



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 10:30 AM JST

PDB ID : 6IJO  
EMDB ID : EMD-9680  
Title : Photosystem I of Chlamydomonas reinhardtii  
Authors : Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.  
Deposited on : 2018-10-10  
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.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

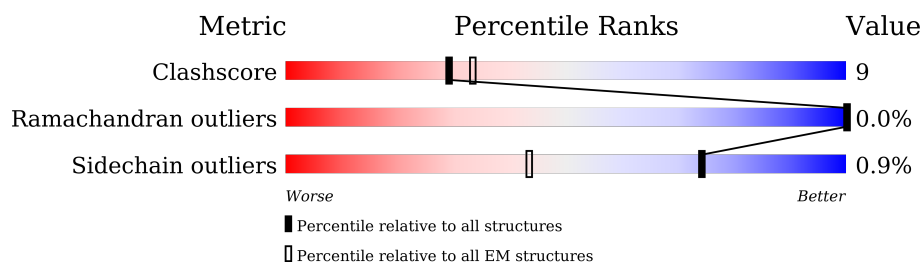
# 1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	751	
2	B	735	
3	C	81	
4	D	247	
5	E	143	
6	F	227	
7	G	159	
8	H	155	

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Mol	Chain	Length	Quality of chain
9	I	106	
10	J	41	
11	K	160	
12	L	258	
13	1	248	
13	a	248	
14	3	298	
15	4	290	
16	5	274	
17	6	318	
18	7	241	
19	8	272	
20	2	227	
21	9	213	
22	X	26	

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
23	CLA	1	601	X	-	-	-
23	CLA	1	602	X	-	-	-
23	CLA	1	603	X	-	-	-
23	CLA	1	604	X	-	-	-
23	CLA	1	606	X	-	-	-
23	CLA	1	607	X	-	-	-
23	CLA	1	608	X	-	-	-
23	CLA	1	609	X	-	-	-
23	CLA	1	610	X	-	-	-
23	CLA	1	611	X	-	-	-
23	CLA	1	612	X	-	-	-
23	CLA	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	1	614	X	-	-	-
23	CLA	1	616	X	-	-	-
23	CLA	2	601	X	-	-	-
23	CLA	2	602	X	-	-	-
23	CLA	2	603	X	-	-	-
23	CLA	2	604	X	-	-	-
23	CLA	2	606	X	-	-	-
23	CLA	2	607	X	-	-	-
23	CLA	2	609	X	-	-	-
23	CLA	2	610	X	-	-	-
23	CLA	2	611	X	-	-	-
23	CLA	2	612	X	-	-	-
23	CLA	2	613	X	-	-	-
23	CLA	2	614	X	-	-	-
23	CLA	2	616	X	-	-	-
23	CLA	3	602	X	-	-	-
23	CLA	3	603	X	-	-	-
23	CLA	3	604	X	-	-	-
23	CLA	3	606	X	-	-	-
23	CLA	3	607	X	-	-	-
23	CLA	3	608	X	-	-	-
23	CLA	3	609	X	-	-	-
23	CLA	3	610	X	-	-	-
23	CLA	3	611	X	-	-	-
23	CLA	3	612	X	-	-	-
23	CLA	3	613	X	-	-	-
23	CLA	3	614	X	-	-	-
23	CLA	3	615	X	-	-	-
23	CLA	3	617	X	-	-	-
23	CLA	4	601	X	-	-	-
23	CLA	4	602	X	-	-	-
23	CLA	4	603	X	-	-	-
23	CLA	4	604	X	-	-	-
23	CLA	4	606	X	-	-	-
23	CLA	4	607	X	-	-	-
23	CLA	4	608	X	-	-	-
23	CLA	4	609	X	-	-	-
23	CLA	4	610	X	-	-	-
23	CLA	4	611	X	-	-	-
23	CLA	4	613	X	-	-	-
23	CLA	4	614	X	-	-	-
23	CLA	4	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	4	618	X	-	-	-
23	CLA	5	601	X	-	-	-
23	CLA	5	602	X	-	-	-
23	CLA	5	603	X	-	-	-
23	CLA	5	604	X	-	-	-
23	CLA	5	606	X	-	-	-
23	CLA	5	607	X	-	-	-
23	CLA	5	608	X	-	-	-
23	CLA	5	609	X	-	-	-
23	CLA	5	610	X	-	-	-
23	CLA	5	611	X	-	-	-
23	CLA	5	612	X	-	-	-
23	CLA	5	613	X	-	-	-
23	CLA	5	614	X	-	-	-
23	CLA	5	616	X	-	-	-
23	CLA	5	617	X	-	-	-
23	CLA	5	618	X	-	-	-
23	CLA	5	619	X	-	-	-
23	CLA	6	601	X	-	-	-
23	CLA	6	602	X	-	-	-
23	CLA	6	603	X	-	-	-
23	CLA	6	604	X	-	-	-
23	CLA	6	606	X	-	-	-
23	CLA	6	607	X	-	-	-
23	CLA	6	608	X	-	-	-
23	CLA	6	609	X	-	-	-
23	CLA	6	610	X	-	-	-
23	CLA	6	611	X	-	-	-
23	CLA	6	612	X	-	-	-
23	CLA	6	613	X	-	-	-
23	CLA	6	614	X	-	-	-
23	CLA	6	616	X	-	-	-
23	CLA	6	617	X	-	-	-
23	CLA	6	618	X	-	-	-
23	CLA	6	620	X	-	-	-
23	CLA	7	601	X	-	-	-
23	CLA	7	602	X	-	-	-
23	CLA	7	603	X	-	-	-
23	CLA	7	604	X	-	-	-
23	CLA	7	606	X	-	-	-
23	CLA	7	607	X	-	-	-
23	CLA	7	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	7	609	X	-	-	-
23	CLA	7	610	X	-	-	-
23	CLA	7	611	X	-	-	-
23	CLA	7	613	X	-	-	-
23	CLA	7	614	X	-	-	-
23	CLA	7	615	X	-	-	-
23	CLA	7	616	X	-	-	-
23	CLA	8	601	X	-	-	-
23	CLA	8	602	X	-	-	-
23	CLA	8	603	X	-	-	-
23	CLA	8	604	X	-	-	-
23	CLA	8	606	X	-	-	-
23	CLA	8	607	X	-	-	-
23	CLA	8	608	X	-	-	-
23	CLA	8	609	X	-	-	-
23	CLA	8	610	X	-	-	-
23	CLA	8	611	X	-	-	-
23	CLA	8	612	X	-	-	-
23	CLA	8	613	X	-	-	-
23	CLA	8	614	X	-	-	-
23	CLA	9	601	X	-	-	-
23	CLA	9	602	X	-	-	-
23	CLA	9	603	X	-	-	-
23	CLA	9	604	X	-	-	-
23	CLA	9	606	X	-	-	-
23	CLA	9	607	X	-	-	-
23	CLA	9	609	X	-	-	-
23	CLA	9	610	X	-	-	-
23	CLA	9	611	X	-	-	-
23	CLA	9	612	X	-	-	-
23	CLA	9	613	X	-	-	-
23	CLA	9	614	X	-	-	-
23	CLA	A	801	X	-	-	-
23	CLA	A	802	X	-	-	-
23	CLA	A	803	X	-	-	-
23	CLA	A	804	X	-	-	-
23	CLA	A	805	X	-	-	-
23	CLA	A	806	X	-	-	-
23	CLA	A	807	X	-	-	-
23	CLA	A	808	X	-	-	-
23	CLA	A	809	X	-	-	-
23	CLA	A	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	811	X	-	-	-
23	CLA	A	812	X	-	-	-
23	CLA	A	813	X	-	-	-
23	CLA	A	814	X	-	-	-
23	CLA	A	815	X	-	-	-
23	CLA	A	816	X	-	-	-
23	CLA	A	817	X	-	-	-
23	CLA	A	818	X	-	-	-
23	CLA	A	819	X	-	-	-
23	CLA	A	820	X	-	-	-
23	CLA	A	821	X	-	-	-
23	CLA	A	822	X	-	-	-
23	CLA	A	823	X	-	-	-
23	CLA	A	824	X	-	-	-
23	CLA	A	825	X	-	-	-
23	CLA	A	826	X	-	-	-
23	CLA	A	827	X	-	-	-
23	CLA	A	828	X	-	-	-
23	CLA	A	829	X	-	-	-
23	CLA	A	830	X	-	-	-
23	CLA	A	831	X	-	-	-
23	CLA	A	832	X	-	-	-
23	CLA	A	833	X	-	-	-
23	CLA	A	834	X	-	-	-
23	CLA	A	835	X	-	-	-
23	CLA	A	836	X	-	-	-
23	CLA	A	837	X	-	-	-
23	CLA	A	838	X	-	-	-
23	CLA	A	839	X	-	-	-
23	CLA	A	840	X	-	-	-
23	CLA	A	841	X	-	-	-
23	CLA	A	842	X	-	-	-
23	CLA	A	843	X	-	-	-
23	CLA	A	845	X	-	-	-
23	CLA	A	854	X	-	-	-
23	CLA	B	802	X	-	-	-
23	CLA	B	803	X	-	-	-
23	CLA	B	804	X	-	-	-
23	CLA	B	805	X	-	-	-
23	CLA	B	806	X	-	-	-
23	CLA	B	807	X	-	-	-
23	CLA	B	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	809	X	-	-	-
23	CLA	B	810	X	-	-	-
23	CLA	B	811	X	-	-	-
23	CLA	B	812	X	-	-	-
23	CLA	B	813	X	-	-	-
23	CLA	B	814	X	-	-	-
23	CLA	B	815	X	-	-	-
23	CLA	B	816	X	-	-	-
23	CLA	B	817	X	-	-	-
23	CLA	B	818	X	-	-	-
23	CLA	B	819	X	-	-	-
23	CLA	B	820	X	-	-	-
23	CLA	B	821	X	-	-	-
23	CLA	B	823	X	-	-	-
23	CLA	B	824	X	-	-	-
23	CLA	B	825	X	-	-	-
23	CLA	B	826	X	-	-	-
23	CLA	B	827	X	-	-	-
23	CLA	B	828	X	-	-	-
23	CLA	B	829	X	-	-	-
23	CLA	B	830	X	-	-	-
23	CLA	B	831	X	-	-	-
23	CLA	B	832	X	-	-	-
23	CLA	B	833	X	-	-	-
23	CLA	B	834	X	-	-	-
23	CLA	B	835	X	-	-	-
23	CLA	B	837	X	-	-	-
23	CLA	B	838	X	-	-	-
23	CLA	B	839	X	-	-	-
23	CLA	B	840	X	-	-	-
23	CLA	B	841	X	-	-	-
23	CLA	F	301	X	-	-	-
23	CLA	F	303	X	-	-	-
23	CLA	F	304	X	-	-	-
23	CLA	G	203	X	-	-	-
23	CLA	G	204	X	-	-	-
23	CLA	J	101	X	-	-	-
23	CLA	K	201	X	-	-	-
23	CLA	K	203	X	-	-	-
23	CLA	K	204	X	-	-	-
23	CLA	K	206	X	-	-	-
23	CLA	L	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	L	303	X	-	-	-
23	CLA	L	304	X	-	-	-
23	CLA	a	601	X	-	-	-
23	CLA	a	602	X	-	-	-
23	CLA	a	603	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	608	X	-	-	-
23	CLA	a	609	X	-	-	-
23	CLA	a	610	X	-	-	-
23	CLA	a	611	X	-	-	-
23	CLA	a	612	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	a	614	X	-	-	-
23	CLA	a	616	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 49685 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5819	3805	993	999	22		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5812	3818	975	1001	18		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1129	722	200	200	7		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			505	322	89	94		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	164	Total	C	N	O	S	0	0
			1254	811	209	231	3		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	70	Total	C	N	O	0	0
			514	334	89	91		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	51	Total	C	N	O	0	0
			357	223	66	68		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			242	166	34	41	1		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	106	Total	C	N	O	S	0	0
			768	507	123	136	2		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1433	932	239	259	3		
13	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 14 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	221	Total	C	N	O	S	0	0
			1683	1099	271	305	8		

- Molecule 15 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 16 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5	226	Total	C	N	O	S	0	0
			1765	1149	295	313	8		

- Molecule 17 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 18 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 19 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	215	Total	C	N	O	S	0	0
			1630	1058	278	290	4		

- Molecule 20 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	173	Total	C	N	O	S	0	0
			1346	874	223	241	8		

- Molecule 21 is a protein called Lhca9.

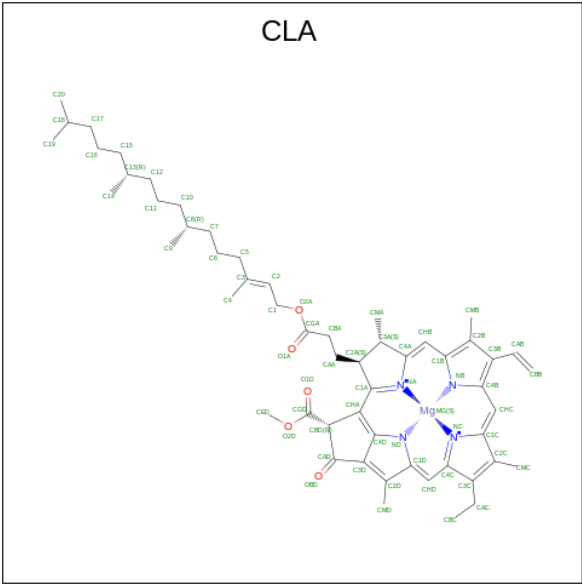


Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	172	Total	C	N	O	S	0	0
			1302	840	220	235	7		

- Molecule 22 is a protein called ChainX.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
23	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
23	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
23	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
23	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	a	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	a	1	Total 44	C 35	Mg 1	N 4	O 4	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	a	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	a	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	a	1	Total 38	C 30	Mg 1	N 4	O 3	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
23	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
23	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
23	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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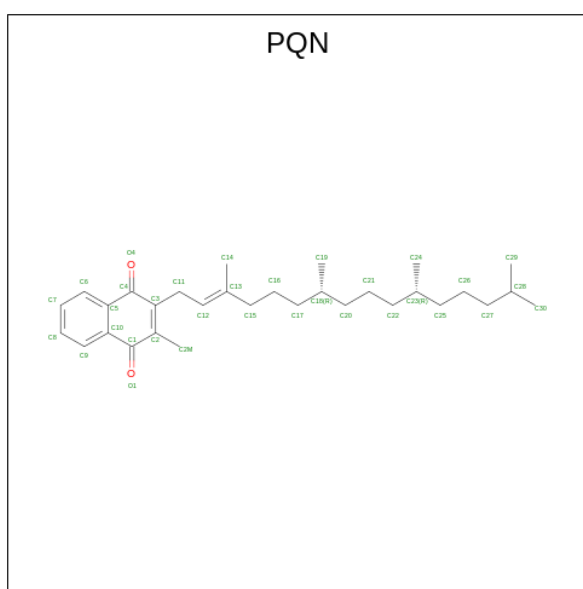
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			26	21	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	

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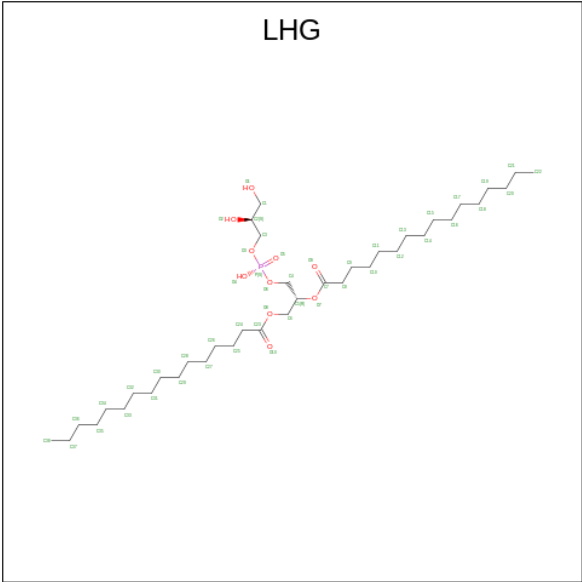
Mol	Chain	Residues	Atoms				AltConf
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	

- Molecule 24 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



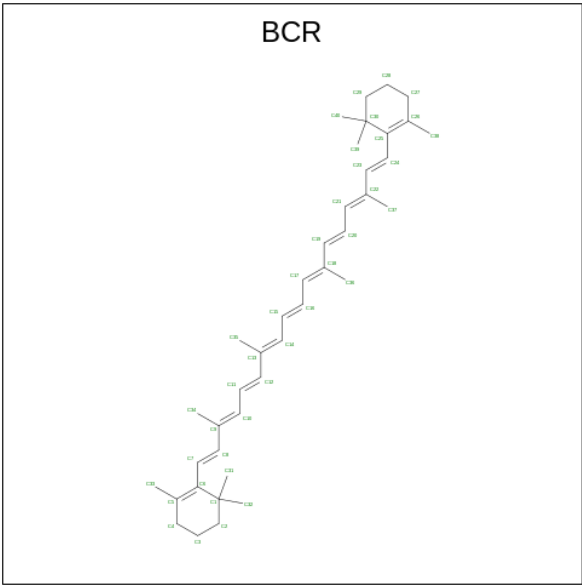
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			30	19	10	1	
25	B	1	Total	C	O	P	0
			38	27	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			45	34	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	6	1	Total	C	O	P	0
			48	37	10	1	
25	7	1	Total	C	O	P	0
			37	26	10	1	
25	8	1	Total	C	O	P	0
			49	38	10	1	
25	8	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
25	2	1	Total	C	O	P	0
			37	26	10	1	
25	9	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	C	0
			40	40	
26	A	1	Total	C	0
			40	40	
26	A	1	Total	C	0
			40	40	
26	A	1	Total	C	0
			40	40	
26	A	1	Total	C	0
			40	40	
26	A	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	1	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	4	1	Total C 40 40	0
26	5	1	Total C 40 40	0
26	6	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	7	1	Total C 40 40	0

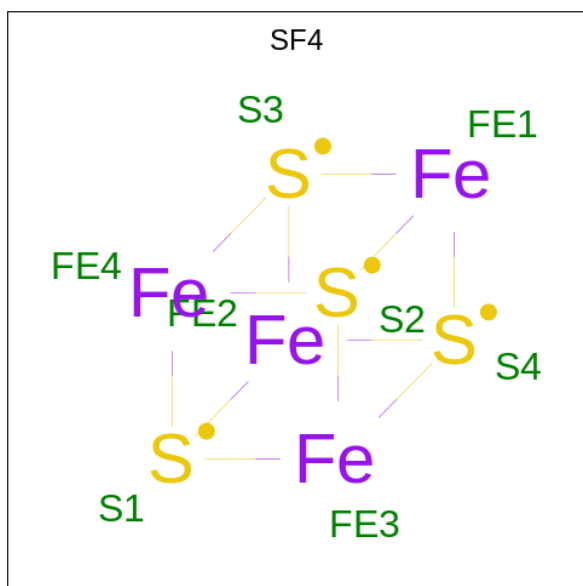
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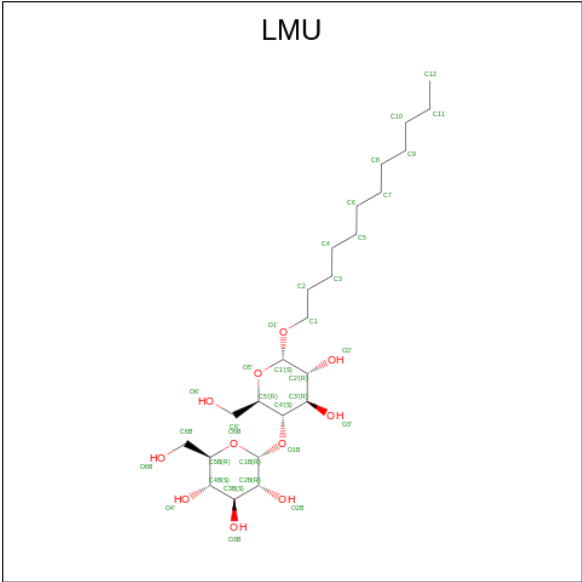
Mol	Chain	Residues	Atoms	AltConf
26	8	1	Total C 40 40	0

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



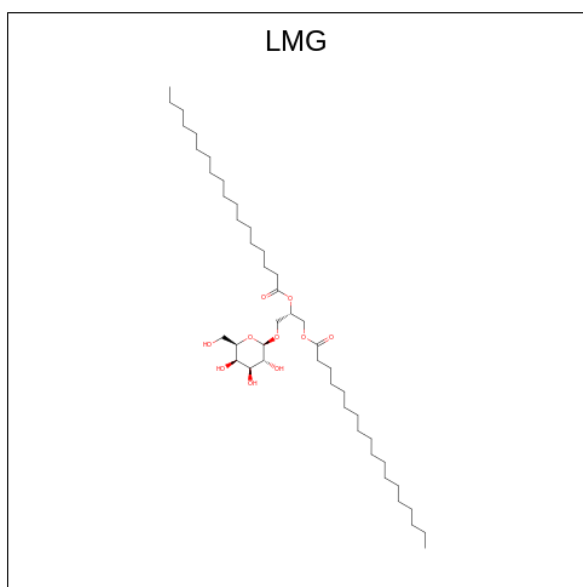
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0

- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).



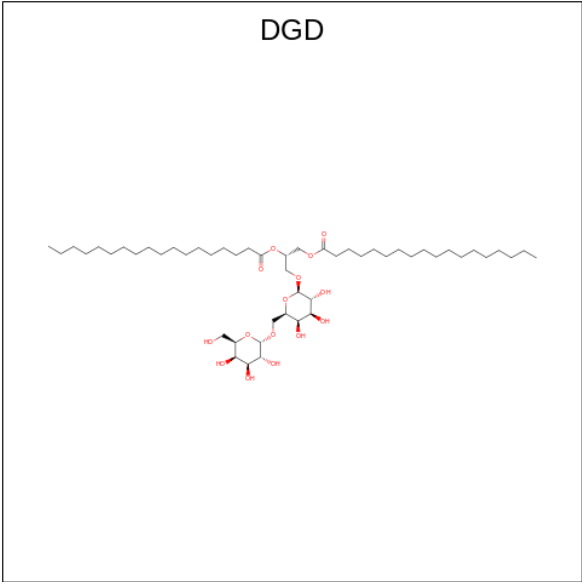
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	A	1	Total	C	O	0
			34	24	10	
28	A	1	Total	C	O	0
			34	24	10	
28	K	1	Total	C	O	0
			35	24	11	
28	5	1	Total	C	O	0
			33	22	11	
28	8	1	Total	C	O	0
			35	24	11	
28	8	1	Total	C	O	0
			35	24	11	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



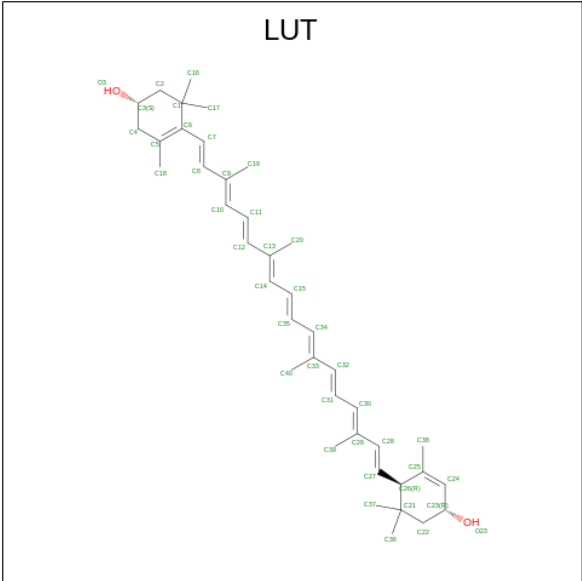
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			40	30	10	
29	J	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	7	1	Total	C	O	0
			44	34	10	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			62	47	15	
30	J	1	Total	C	O	0
			58	43	15	

- Molecule 31 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>).



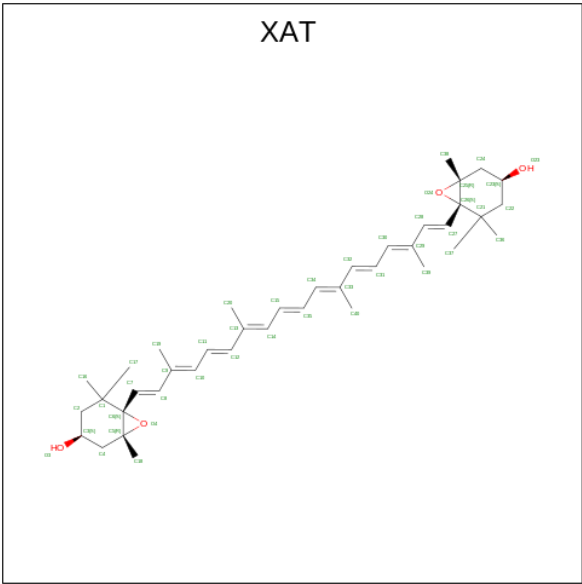
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	

- Molecule 32 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>).



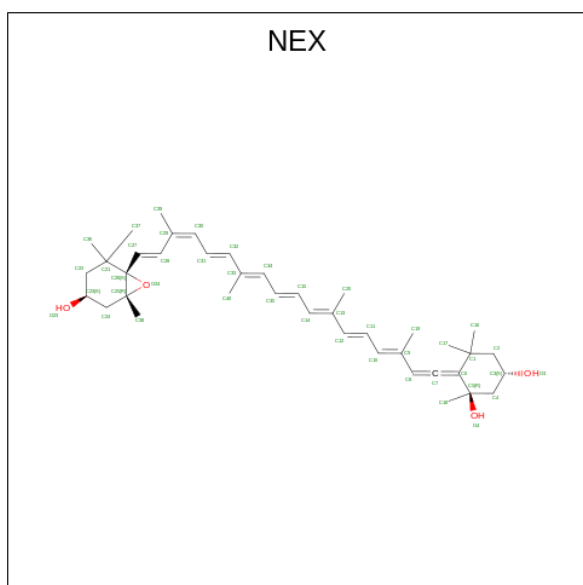
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			44	40	4	
32	a	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
32	3	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	2	1	Total	C	O	0
			44	40	4	
32	9	1	Total	C	O	0
			44	40	4	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-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>).

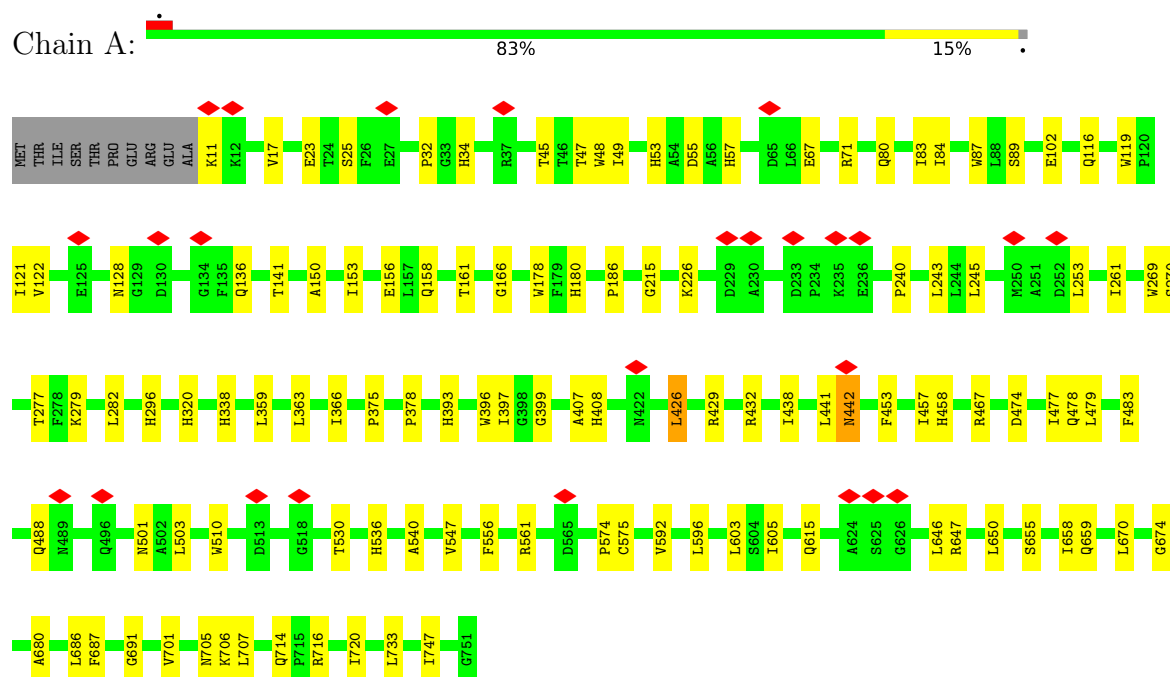


Mol	Chain	Residues	Atoms			AltConf
33	5	1	Total	C	O	0
			44	40	4	
33	6	1	Total	C	O	0
			44	40	4	

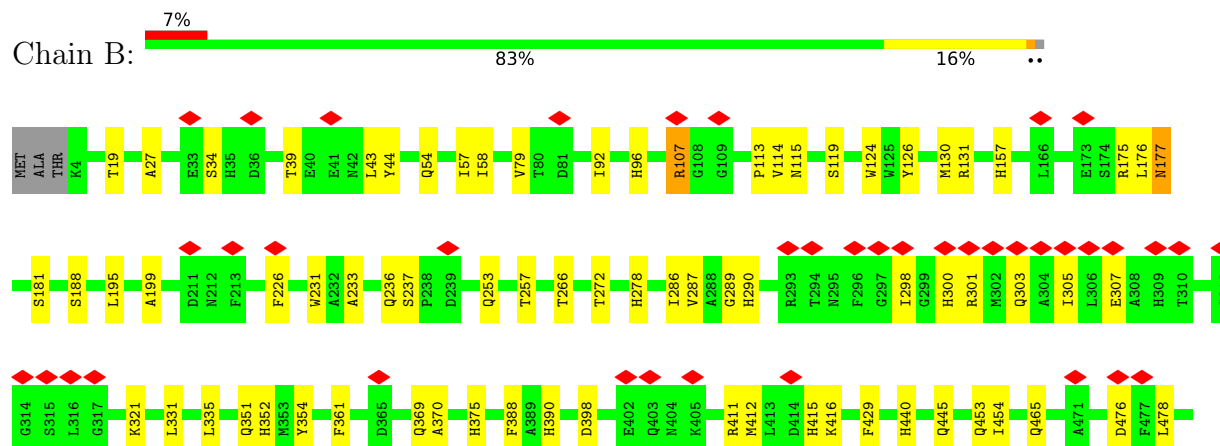
### 3 Residue-property plots [i](#)

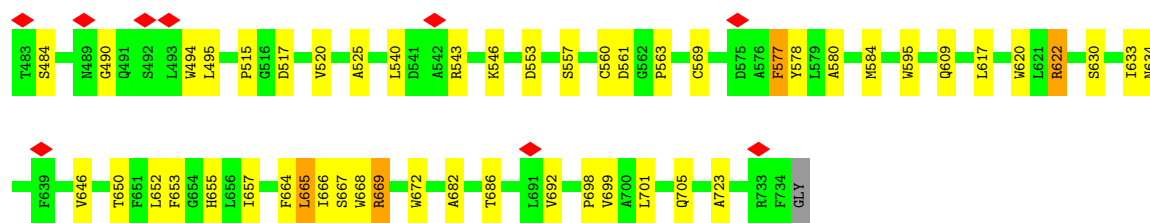
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: PsaA

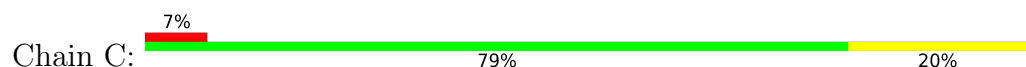


#### • Molecule 2: PsaB

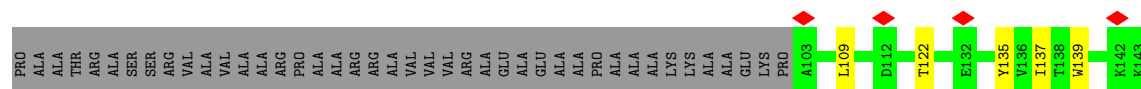
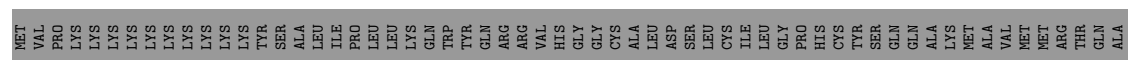




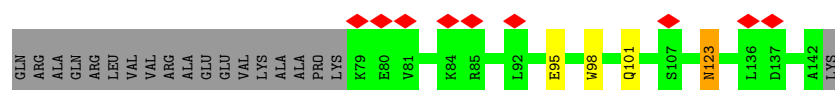
### • Molecule 3: PsuC



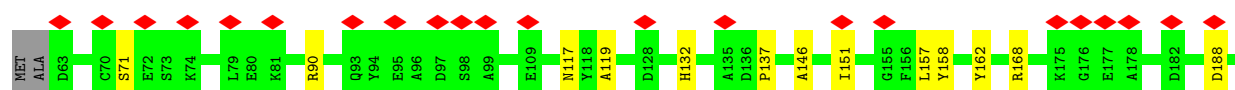
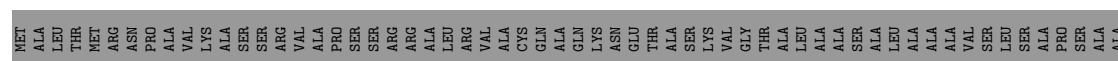
### • Molecule 4: PsuA



### • Molecule 5: PsuE



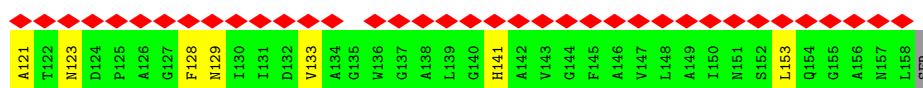
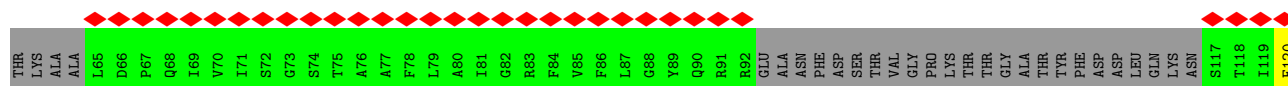
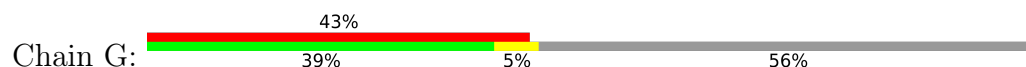
### • Molecule 6: PsuF



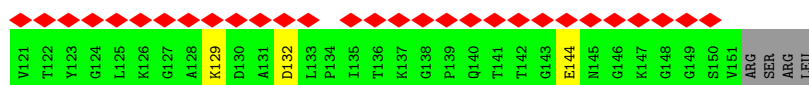
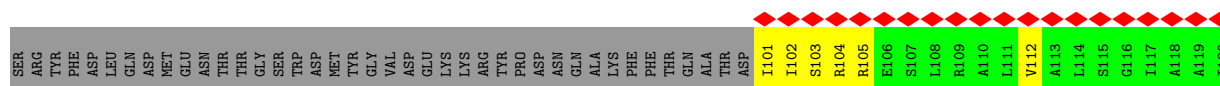




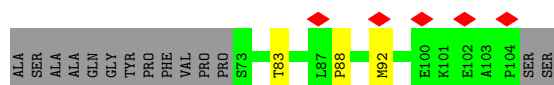
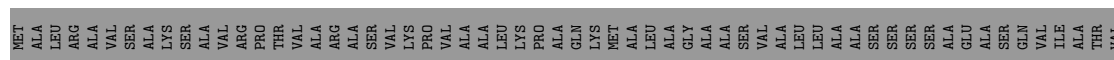
• Molecule 7: Psag



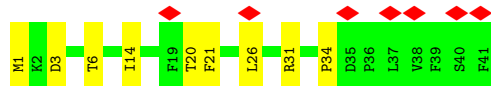
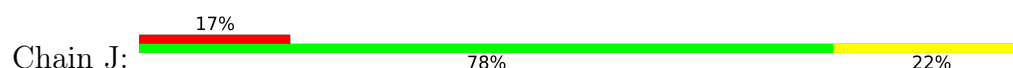
• Molecule 8: PsaH



• Molecule 9: PsaI



• Molecule 10: PsaJ



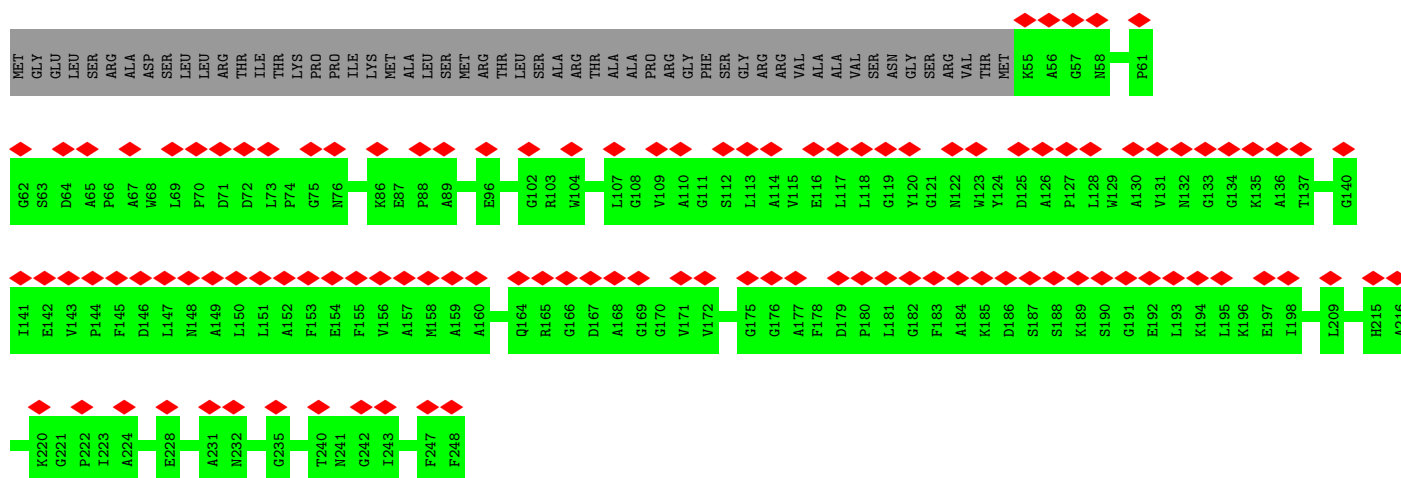
• Molecule 11: PsaK

Chain K:

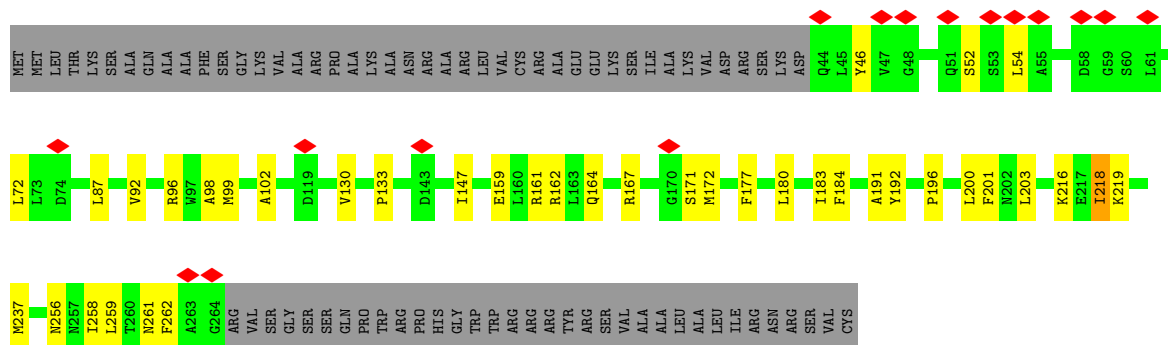
Chain L:

Chain 1:

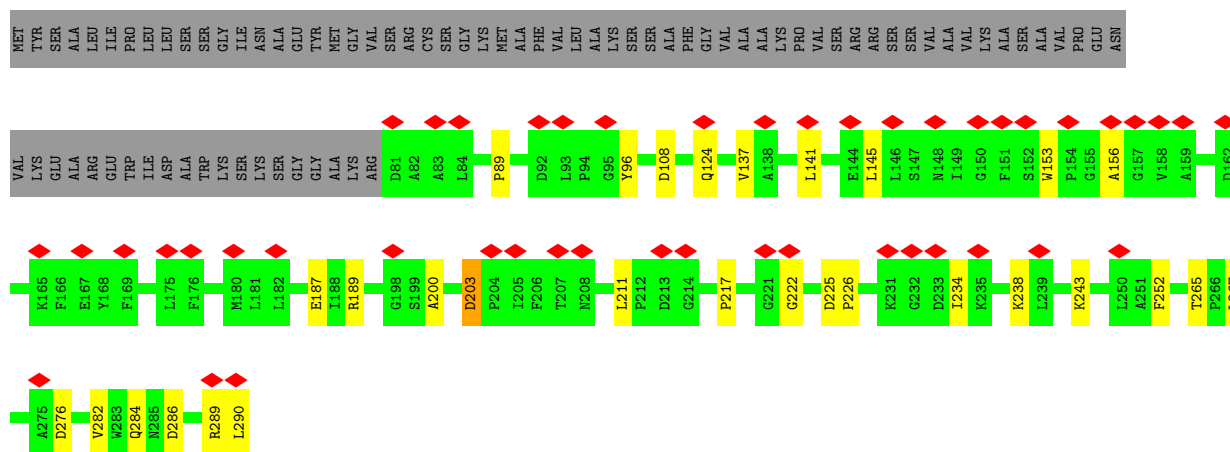
Chain a:



- Molecule 14: Lhca3

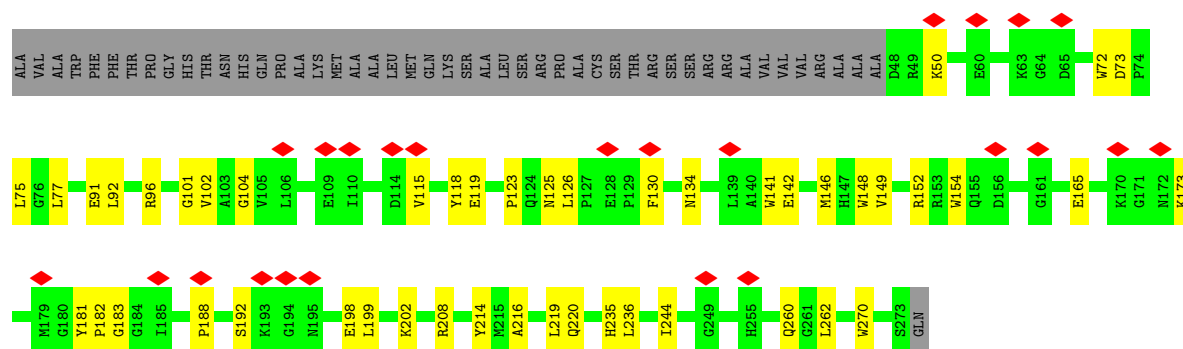


- Molecule 15: Lhca4

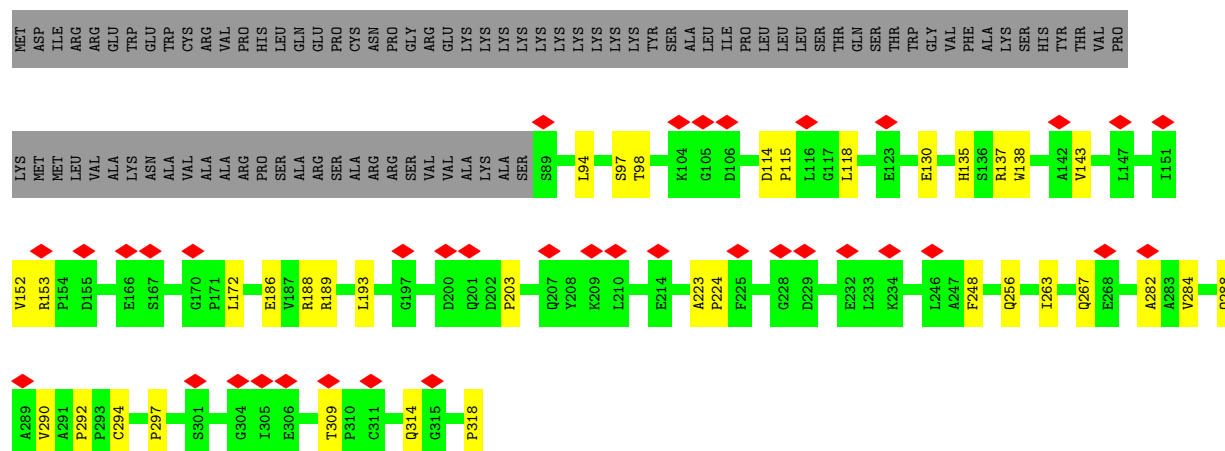


- Molecule 16: Lhca5

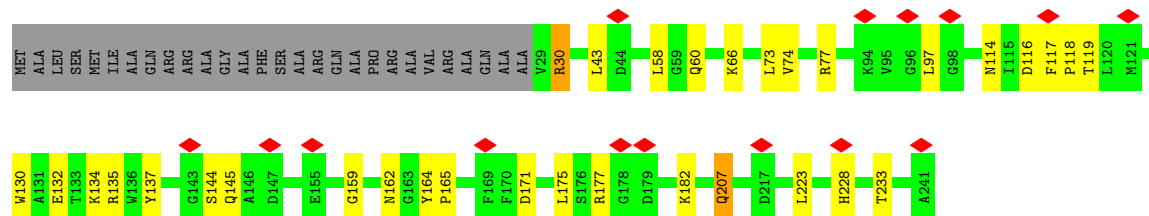
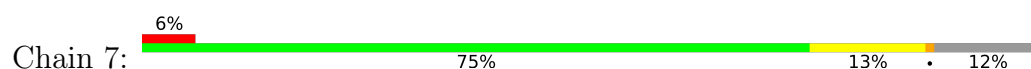




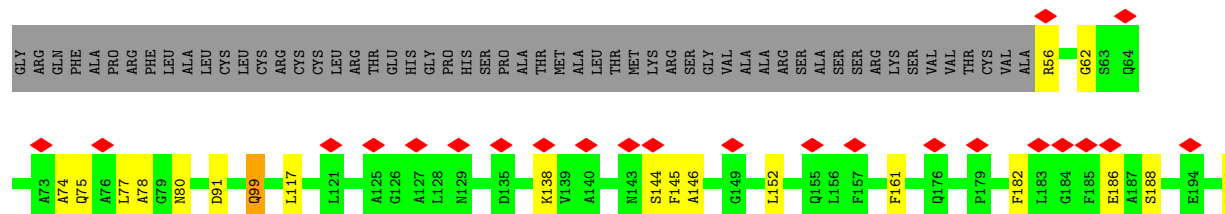
• Molecule 17: Lhca6



• Molecule 18: Lhca7



• Molecule 19: Lhca8





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17420	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 ( $e^-/\text{\AA}^2$ )	60.0	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	0.400	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	A	0.51	0/6015	0.57	1/8201 (0.0%)
2	B	0.49	0/6024	0.59	3/8225 (0.0%)
3	C	0.51	0/610	0.66	0/826
4	D	0.43	0/1157	0.61	0/1563
5	E	0.46	0/515	0.54	0/700
6	F	0.41	0/1280	0.55	0/1733
7	G	0.31	0/524	0.66	1/711 (0.1%)
8	H	0.31	0/359	0.61	0/483
9	I	0.43	0/250	0.63	0/345
10	J	0.43	0/349	0.58	0/478
11	K	0.32	0/583	0.69	1/790 (0.1%)
12	L	0.36	0/787	0.63	0/1074
13	1	0.38	0/1478	0.55	0/2012
13	a	0.39	0/1490	0.55	0/2028
14	3	0.49	0/1731	0.67	3/2349 (0.1%)
15	4	0.37	0/1686	0.53	0/2300
16	5	0.43	0/1820	0.62	0/2480
17	6	0.40	0/1833	0.58	0/2505
18	7	0.48	0/1701	0.61	0/2310
19	8	0.43	0/1680	0.63	1/2288 (0.0%)
20	2	0.29	0/1382	0.56	0/1870
21	9	0.32	0/1337	0.65	1/1814 (0.1%)
22	X	0.24	0/129	0.33	0/179
All	All	0.44	0/34720	0.59	11/47264 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	180	LEU	CA-CB-CG	6.59	130.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	200	LEU	CA-CB-CG	6.43	130.10	115.30
7	G	153	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	426	LEU	CA-CB-CG	6.20	129.56	115.30
11	K	114	LEU	CA-CB-CG	6.05	129.21	115.30
21	9	164	LEU	CA-CB-CG	5.72	128.46	115.30
2	B	665	LEU	CB-CG-CD2	-5.72	101.28	111.00
2	B	176	LEU	CA-CB-CG	5.65	128.29	115.30
2	B	476	ASP	CB-CG-OD1	5.56	123.31	118.30
19	8	117	LEU	CA-CB-CG	5.50	127.95	115.30
14	3	54	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5672	96	0
2	B	5812	0	5569	94	0
3	C	600	0	589	10	0
4	D	1129	0	1144	23	0
5	E	505	0	504	4	0
6	F	1254	0	1288	14	0
7	G	514	0	509	7	0
8	H	357	0	382	6	0
9	I	242	0	252	2	0
10	J	337	0	336	10	0
11	K	578	0	617	7	0
12	L	768	0	776	20	0
13	1	1433	0	1387	29	0
13	a	1444	0	1396	0	0
14	3	1683	0	1641	28	0
15	4	1631	0	1587	26	0
16	5	1765	0	1738	45	0
17	6	1771	0	1770	30	0
18	7	1649	0	1589	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	8	1630	0	1609	26	0
20	2	1346	0	1330	17	0
21	9	1302	0	1275	30	0
22	X	130	0	132	2	0
23	1	674	0	541	19	0
23	2	350	0	39	3	0
23	3	724	0	628	22	0
23	4	782	0	686	24	0
23	5	878	0	758	45	0
23	6	912	0	845	37	0
23	7	760	0	643	26	0
23	8	727	0	635	16	0
23	9	324	0	36	12	0
23	A	2625	0	2614	129	0
23	B	2270	0	2210	101	0
23	F	140	0	113	8	0
23	G	87	0	64	6	0
23	J	42	0	31	2	0
23	K	201	0	171	2	0
23	L	135	0	99	5	0
23	a	709	0	597	0	0
24	A	33	0	46	5	0
24	B	33	0	46	6	0
25	1	49	0	74	6	0
25	2	37	0	44	1	0
25	3	94	0	137	3	0
25	4	49	0	74	6	0
25	5	98	0	148	7	0
25	6	48	0	69	3	0
25	7	37	0	44	2	0
25	8	96	0	141	4	0
25	9	49	0	74	5	0
25	A	79	0	104	4	0
25	B	38	0	46	2	0
25	a	49	0	74	0	0
26	1	40	0	56	2	0
26	3	120	0	168	11	0
26	4	40	0	56	2	0
26	5	40	0	56	4	0
26	6	40	0	56	4	0
26	7	80	0	112	3	0
26	8	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	240	0	336	28	0
26	B	280	0	392	15	0
26	F	40	0	56	4	0
26	G	40	0	56	6	0
26	J	40	0	56	5	0
26	K	80	0	112	6	0
26	L	80	0	112	5	0
26	a	40	0	56	0	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	5	33	0	39	3	0
28	8	70	0	92	3	0
28	A	103	0	134	3	0
28	K	35	0	46	0	0
29	4	80	0	100	1	0
29	5	80	0	100	4	0
29	7	44	0	61	1	0
29	A	40	0	50	2	0
29	J	40	0	50	1	0
30	B	62	0	84	5	0
30	J	58	0	77	1	0
31	1	42	0	56	3	0
31	2	42	0	56	3	0
31	3	42	0	56	1	0
31	4	42	0	56	5	0
31	5	42	0	56	6	0
31	6	42	0	56	4	0
31	7	42	0	56	5	0
31	8	42	0	56	6	0
31	9	42	0	56	1	0
31	a	42	0	56	0	0
32	1	44	0	56	4	0
32	2	44	0	56	3	0
32	3	44	0	56	2	0
32	4	44	0	56	3	0
32	5	44	0	56	10	0
32	6	44	0	56	1	0
32	7	44	0	56	1	0
32	8	44	0	56	1	0
32	9	44	0	56	3	0
32	a	44	0	56	0	0
33	5	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	6	44	0	56	4	0
All	All	49685	0	48724	855	0

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

All (855) 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)
21:9:182:GLN:CB	21:9:183:PRO:HD2	1.85	1.05
1:A:11:LYS:N	14:3:52:SER:HG	1.56	1.04
12:L:223:LEU:HD12	12:L:223:LEU:O	1.78	0.82
23:9:611:CLA:NB	25:9:622:LHG:O4	2.20	0.75
23:A:830:CLA:H2	26:A:849:BCR:HC7	1.68	0.74
11:K:127:ASP:OD1	23:K:201:CLA:NA	2.22	0.73
16:5:216:ALA:O	16:5:220:GLN:HG3	1.87	0.73
23:B:813:CLA:H42	26:B:844:BCR:H21C	1.71	0.72
23:B:841:CLA:HAB	13:1:84:LEU:HD11	1.70	0.72
18:7:207:GLN:NE2	31:7:619:LUT:H42	2.06	0.71
20:2:103:GLU:OE2	23:2:609:CLA:ND	2.23	0.71
26:A:852:BCR:H10C	23:A:854:CLA:H203	1.72	0.70
14:3:161:ARG:HB3	23:3:608:CLA:HMC3	1.73	0.69
1:A:714:GLN:HE22	5:E:123:ASN:HA	1.56	0.69
26:A:856:BCR:H15C	10:J:20:THR:HG22	1.75	0.69
17:6:135:HIS:HE1	23:6:603:CLA:NA	1.89	0.68
1:A:17:VAL:HG11	23:A:811:CLA:HED3	1.74	0.68
2:B:354:TYR:HA	2:B:369:GLN:HE22	1.57	0.68
19:8:213:LYS:HE2	19:8:217:TRP:HE1	1.57	0.68
21:9:182:GLN:O	21:9:183:PRO:C	2.33	0.67
21:9:115:GLU:OE2	23:9:606:CLA:NB	2.27	0.67
23:3:606:CLA:HBA1	26:3:620:BCR:H19C	1.75	0.67
21:9:31:TRP:O	23:9:601:CLA:ND	2.28	0.67
23:A:820:CLA:HAB	23:A:820:CLA:H8	1.77	0.66
1:A:153:ILE:O	1:A:158:GLN:NE2	2.28	0.66
16:5:102:VAL:HG11	31:5:620:LUT:H12	1.77	0.66
23:A:822:CLA:H101	26:A:851:BCR:H10C	1.78	0.65
15:4:226:PRO:HD2	31:4:619:LUT:H23	1.78	0.65
16:5:91:GLU:OE2	16:5:208:ARG:NH2	2.28	0.65
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.79	0.65
23:1:611:CLA:NA	25:1:620:LHG:O4	2.30	0.65
1:A:707:LEU:O	6:F:168:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:HIS:HB3	2:B:305:ILE:HD11	1.78	0.65
2:B:107:ARG:HA	8:H:144:GLU:HA	1.79	0.64
2:B:388:PHE:HZ	23:B:825:CLA:HAB	1.62	0.64
3:C:4:ILE:HB	3:C:68:TYR:HB2	1.79	0.64
18:7:134:LYS:HB3	23:7:608:CLA:HMC3	1.80	0.64
23:A:834:CLA:HBB2	12:L:165:LEU:HD11	1.79	0.64
23:5:609:CLA:HBC3	23:6:616:CLA:H41	1.78	0.64
18:7:132:GLU:OE1	18:7:135:ARG:NH2	2.31	0.63
14:3:159:GLU:OE1	14:3:162:ARG:NH1	2.31	0.63
15:4:284:GLN:HE21	17:6:172:LEU:HB2	1.62	0.63
21:9:160:LYS:HB3	23:9:611:CLA:C2D	2.29	0.63
23:A:811:CLA:HBB2	23:A:814:CLA:HMA3	1.80	0.63
18:7:165:PRO:HB3	23:7:608:CLA:HBC2	1.81	0.62
23:8:607:CLA:HHB	25:8:623:LHG:H191	1.79	0.62
19:8:238:GLN:OE1	23:8:613:CLA:NA	2.33	0.62
1:A:161:THR:HG21	23:A:817:CLA:HAA2	1.82	0.62
23:B:806:CLA:HHB	23:B:829:CLA:HAB	1.81	0.62
8:H:112:VAL:HG11	12:L:192:LEU:HB2	1.82	0.62
13:1:180:PRO:HD2	31:1:617:LUT:H23	1.82	0.62
23:1:601:CLA:O2A	25:1:620:LHG:H142	2.00	0.62
21:9:182:GLN:CB	21:9:183:PRO:CD	2.68	0.62
23:A:829:CLA:H203	26:J:102:BCR:H17C	1.82	0.61
23:A:817:CLA:HMD2	14:3:133:PRO:HG3	1.81	0.61
13:1:158:MET:HG2	23:1:609:CLA:HMC3	1.81	0.61
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.33	0.61
8:H:101:ILE:HG22	8:H:102:ILE:HG23	1.82	0.61
1:A:45:THR:HG22	1:A:47:THR:H	1.66	0.61
17:6:282:ALA:HB2	17:6:292:PRO:HD3	1.82	0.61
18:7:164:TYR:HB3	23:7:610:CLA:HED2	1.82	0.61
26:A:852:BCR:H362	23:A:854:CLA:H42	1.82	0.61
13:1:162:GLU:OE1	13:1:165:ARG:NH2	2.34	0.61
2:B:157:HIS:HE1	23:B:811:CLA:NA	1.98	0.60
1:A:366:ILE:HD13	23:A:827:CLA:HED3	1.82	0.60
16:5:188:PRO:HD2	31:5:620:LUT:H23	1.83	0.60
18:7:77:ARG:NH1	23:7:608:CLA:OBD	2.35	0.60
26:B:801:BCR:H10C	23:B:832:CLA:HMB2	1.83	0.60
12:L:194:LEU:HD23	26:L:305:BCR:H23C	1.82	0.60
23:A:810:CLA:HAB	23:B:833:CLA:HMD2	1.83	0.60
23:B:839:CLA:HAA1	26:L:305:BCR:H362	1.83	0.60
3:C:54:CYS:SG	3:C:55:GLU:N	2.75	0.60
3:C:58:CYS:HB3	3:C:63:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:82:ASN:ND2	23:K:204:CLA:OBD	2.35	0.60
21:9:160:LYS:HD2	23:9:611:CLA:CAD	2.31	0.60
1:A:408:HIS:HE1	23:A:831:CLA:NA	1.98	0.59
23:B:810:CLA:H151	12:L:188:LEU:HD23	1.85	0.59
12:L:133:ASN:HB3	23:L:302:CLA:HAC1	1.83	0.59
23:B:823:CLA:H2A	23:B:823:CLA:HED3	1.85	0.59
17:6:143:VAL:HG11	31:6:619:LUT:H12	1.85	0.59
19:8:182:PHE:HE2	23:8:608:CLA:HBB2	1.67	0.59
25:5:625:LHG:H201	23:6:620:CLA:HAB	1.85	0.59
29:5:627:LMG:HC62	28:5:628:LMU:H6E	1.84	0.59
23:A:843:CLA:H41	23:B:839:CLA:H41	1.85	0.58
17:6:186:GLU:OE1	17:6:189:ARG:NH2	2.35	0.58
17:6:294:CYS:SG	17:6:314:GLN:NE2	2.73	0.58
2:B:398:ASP:OD1	4:D:236:LYS:NZ	2.33	0.58
16:5:123:PRO:HA	16:5:126:LEU:HD13	1.85	0.58
23:5:609:CLA:HBA1	23:5:619:CLA:HMD2	1.85	0.58
20:2:137:LYS:O	20:2:141:ASN:ND2	2.36	0.58
16:5:244:ILE:HB	23:5:613:CLA:H2	1.86	0.58
23:3:617:CLA:HMA2	23:7:601:CLA:H72	1.85	0.58
13:1:77:TYR:OH	13:1:199:LYS:NZ	2.30	0.58
23:5:609:CLA:H43	25:5:625:LHG:H282	1.86	0.58
23:A:843:CLA:H151	26:L:301:BCR:H15C	1.86	0.57
13:1:125:ASP:HA	13:1:128:LEU:HD23	1.85	0.57
24:A:844:PQN:H172	26:B:801:BCR:H382	1.86	0.57
2:B:390:HIS:HE1	23:B:829:CLA:NA	2.02	0.57
4:D:139:TRP:HB3	4:D:187:PRO:HB3	1.86	0.57
23:3:609:CLA:H102	26:3:621:BCR:H10C	1.87	0.57
23:5:602:CLA:H2	32:5:621:XAT:H382	1.86	0.57
1:A:49:ILE:HD11	23:F:301:CLA:HMB3	1.85	0.57
23:A:802:CLA:H171	23:A:842:CLA:H51	1.86	0.57
15:4:276:ASP:OD1	15:4:276:ASP:N	2.36	0.57
23:5:607:CLA:HBB2	23:5:609:CLA:HBC1	1.87	0.57
16:5:220:GLN:OE1	23:5:613:CLA:NA	2.37	0.57
21:9:75:ARG:NH2	21:9:158:GLU:OE2	2.32	0.57
1:A:467:ARG:NH2	23:A:835:CLA:O1D	2.38	0.57
16:5:219:LEU:HD22	16:5:270:TRP:HZ3	1.68	0.57
18:7:66:LYS:O	18:7:162:ASN:ND2	2.34	0.57
12:L:134:LEU:HD12	23:L:303:CLA:HBD	1.84	0.57
2:B:352:HIS:ND1	23:B:817:CLA:OBD	2.37	0.57
19:8:198:PRO:HB3	23:8:608:CLA:HBC2	1.85	0.57
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:613:CLA:H71	25:4:622:LHG:H162	1.86	0.57
2:B:375:HIS:HE1	23:B:827:CLA:ND	2.02	0.56
23:6:616:CLA:HBC3	23:6:620:CLA:HMC3	1.87	0.56
18:7:118:PRO:HB2	19:8:263:ALA:HB1	1.86	0.56
20:2:56:ARG:NH1	20:2:138:GLU:OE2	2.38	0.56
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.70	0.56
1:A:393:HIS:CE1	23:A:829:CLA:ND	2.73	0.56
26:A:848:BCR:H362	26:A:849:BCR:H21C	1.88	0.56
6:F:212:ARG:NH1	19:8:91:ASP:OD2	2.37	0.56
11:K:125:SER:HB2	11:K:132:THR:HG22	1.86	0.56
14:3:96:ARG:HA	14:3:99:MET:HG2	1.86	0.56
14:3:258:ILE:HG23	14:3:259:LEU:HD22	1.87	0.56
19:8:204:PRO:HD2	31:8:619:LUT:H23	1.86	0.56
17:6:314:GLN:HG3	18:7:97:LEU:HD21	1.87	0.56
14:3:192:TYR:HB3	23:3:610:CLA:HED2	1.88	0.56
23:6:604:CLA:H112	26:6:622:BCR:H23C	1.86	0.56
18:7:171:ASP:OD1	31:7:619:LUT:O23	2.23	0.56
23:B:814:CLA:HBC3	26:B:845:BCR:H12C	1.88	0.56
9:I:88:PRO:O	9:I:92:MET:N	2.36	0.56
23:1:601:CLA:CGA	25:1:620:LHG:H161	2.35	0.56
14:3:219:LYS:NZ	25:3:624:LHG:O5	2.37	0.56
21:9:180:ARG:NH1	21:9:204:THR:OG1	2.39	0.56
23:A:804:CLA:H151	26:J:102:BCR:H362	1.86	0.56
23:6:610:CLA:HBB1	23:6:612:CLA:H3A	1.88	0.56
23:A:834:CLA:H192	26:L:305:BCR:H10C	1.88	0.56
4:D:148:GLU:O	4:D:178:GLN:NE2	2.37	0.56
17:6:223:ALA:HB2	23:6:610:CLA:HBD	1.88	0.56
17:6:118:LEU:HD23	18:7:175:LEU:HD21	1.86	0.55
26:B:801:BCR:HC41	23:B:832:CLA:HBB2	1.87	0.55
23:A:813:CLA:H43	14:3:72:LEU:HD21	1.88	0.55
16:5:236:LEU:HD21	23:5:614:CLA:HMC3	1.89	0.55
23:6:601:CLA:H2	25:6:623:LHG:H142	1.87	0.55
14:3:183:ILE:HD13	14:3:196:PRO:HG2	1.88	0.55
2:B:181:SER:HB3	2:B:289:GLY:HA3	1.88	0.55
8:H:129:LYS:HB3	8:H:132:ASP:HB2	1.88	0.55
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.88	0.55
2:B:664:PHE:HA	24:B:842:PQN:H9	1.88	0.55
23:F:303:CLA:HBB2	26:J:102:BCR:H383	1.87	0.55
2:B:175:ARG:HB2	23:B:813:CLA:HBC2	1.89	0.55
2:B:301:ARG:HD3	2:B:303:GLN:HE21	1.72	0.55
23:4:601:CLA:H2	25:4:622:LHG:H132	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:603:CLA:HED2	23:3:609:CLA:H2	1.89	0.55
3:C:13:GLY:O	3:C:38:GLN:NE2	2.40	0.54
18:7:207:GLN:HE22	31:7:619:LUT:H42	1.72	0.54
1:A:441:LEU:HD22	23:A:840:CLA:HBB1	1.88	0.54
2:B:557:SER:O	30:B:850:DGD:O3D	2.25	0.54
15:4:153:TRP:HB2	15:4:156:ALA:HB2	1.89	0.54
23:B:829:CLA:H101	30:B:850:DGD:HAW2	1.89	0.54
12:L:138:ARG:NH1	12:L:149:GLU:OE1	2.41	0.54
17:6:256:GLN:NE2	33:6:624:NEX:O23	2.40	0.54
14:3:171:SER:OG	14:3:172:MET:N	2.41	0.54
15:4:187:GLU:OE2	23:4:609:CLA:ND	2.40	0.54
15:4:203:ASP:N	15:4:203:ASP:OD1	2.39	0.54
23:B:819:CLA:HMB2	23:B:824:CLA:HMA3	1.89	0.54
15:4:286:ASP:OD1	15:4:289:ARG:NH2	2.41	0.54
1:A:670:LEU:HB3	23:A:854:CLA:H62	1.90	0.54
26:3:622:BCR:H333	23:5:601:CLA:H102	1.90	0.54
23:A:820:CLA:HBB2	23:A:820:CLA:H151	1.90	0.54
2:B:630:SER:O	2:B:634:ASN:ND2	2.41	0.54
6:F:162:TYR:OH	6:F:196:ALA:O	2.21	0.54
21:9:160:LYS:HB2	23:9:611:CLA:CAD	2.37	0.54
2:B:177:ASN:ND2	2:B:289:GLY:O	2.41	0.53
3:C:2:ALA:N	3:C:71:SER:O	2.41	0.53
15:4:189:ARG:HE	23:4:608:CLA:HMC3	1.72	0.53
1:A:429:ARG:HG2	1:A:432:ARG:HH21	1.72	0.53
2:B:669:ARG:HB2	24:B:842:PQN:H7	1.89	0.53
23:5:604:CLA:H51	23:5:606:CLA:HBD	1.88	0.53
23:5:608:CLA:H2A	23:5:608:CLA:HED3	1.90	0.53
20:2:181:THR:OG1	22:X:1:ALA:N	2.42	0.53
21:9:164:LEU:HD23	25:9:622:LHG:H262	1.90	0.53
7:G:141:HIS:CE1	26:G:205:BCR:H14C	2.44	0.53
15:4:189:ARG:NH1	15:4:200:ALA:O	2.41	0.53
7:G:123:ASN:ND2	23:G:204:CLA:O2A	2.38	0.53
2:B:195:LEU:HA	2:B:199:ALA:HB3	1.90	0.53
23:B:819:CLA:HBB1	23:B:824:CLA:H61	1.90	0.53
16:5:148:TRP:CD1	26:5:622:BCR:H12C	2.44	0.53
2:B:107:ARG:NH1	2:B:114:VAL:O	2.41	0.52
23:4:601:CLA:HBB1	25:4:622:LHG:H292	1.91	0.52
18:7:165:PRO:HD3	23:7:608:CLA:HMD2	1.90	0.52
2:B:119:SER:HA	23:B:827:CLA:HMA2	1.90	0.52
2:B:126:TYR:O	2:B:131:ARG:NH1	2.42	0.52
25:5:625:LHG:H212	23:7:611:CLA:H122	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:804:CLA:HMB2	25:A:846:LHG:H162	1.90	0.52
2:B:307:GLU:HG3	2:B:321:LYS:HA	1.90	0.52
4:D:109:LEU:HB2	4:D:190:TYR:HE2	1.75	0.52
21:9:184:ILE:O	21:9:184:ILE:HG22	2.08	0.52
12:L:224:PHE:CD1	12:L:224:PHE:N	2.73	0.52
1:A:670:LEU:O	1:A:674:GLY:N	2.41	0.52
23:A:841:CLA:H92	26:B:801:BCR:H17C	1.92	0.52
15:4:243:LYS:NZ	25:4:622:LHG:O5	2.31	0.52
17:6:94:LEU:HD12	23:6:601:CLA:HMA3	1.92	0.52
1:A:89:SER:HB2	1:A:166:GLY:HA3	1.90	0.52
2:B:352:HIS:CE1	23:B:826:CLA:NB	2.78	0.52
16:5:219:LEU:HD11	23:5:616:CLA:HMB3	1.90	0.52
23:A:841:CLA:HMC2	23:A:841:CLA:H111	1.91	0.52
26:A:852:BCR:H24C	23:B:833:CLA:HMC2	1.92	0.52
10:J:1:MET:N	18:7:60:GLN:OE1	2.43	0.52
12:L:138:ARG:O	12:L:146:ARG:NH2	2.42	0.52
23:A:835:CLA:H122	23:L:303:CLA:HAB	1.92	0.52
14:3:92:VAL:HG22	14:3:218:ILE:HD11	1.92	0.52
23:4:602:CLA:H2A	23:4:602:CLA:HED3	1.91	0.52
16:5:72:TRP:HZ3	32:5:621:XAT:H383	1.74	0.52
16:5:188:PRO:HG3	23:5:608:CLA:H43	1.91	0.52
33:5:624:NEX:H172	17:6:290:VAL:HG11	1.92	0.52
1:A:540:ALA:HB2	23:A:839:CLA:HMA1	1.91	0.52
23:A:842:CLA:HMD2	24:A:844:PQN:H192	1.92	0.52
16:5:165:GLU:HG2	16:5:173:LYS:HG2	1.91	0.52
1:A:438:ILE:HG13	1:A:556:PHE:HE2	1.74	0.51
13:1:70:PRO:O	13:1:76:ASN:ND2	2.42	0.51
15:4:141:LEU:O	15:4:145:LEU:N	2.42	0.51
23:8:603:CLA:HED2	23:8:603:CLA:H2A	1.91	0.51
2:B:415:HIS:CE1	23:B:830:CLA:ND	2.79	0.51
18:7:223:LEU:HD21	23:7:614:CLA:HMC3	1.91	0.51
23:5:604:CLA:HMB3	32:5:621:XAT:H162	1.92	0.51
14:3:237:MET:HE2	14:3:261:ASN:HB3	1.93	0.51
2:B:416:LYS:HB2	2:B:540:LEU:HD13	1.92	0.51
23:B:836:CLA:HMB2	23:B:838:CLA:HED3	1.92	0.51
16:5:152:ARG:HB3	23:5:608:CLA:HMC3	1.92	0.51
1:A:128:ASN:O	6:F:90:ARG:NH2	2.44	0.51
12:L:223:LEU:HD12	12:L:223:LEU:C	2.30	0.51
23:5:610:CLA:H2	31:5:620:LUT:H373	1.92	0.51
1:A:407:ALA:HA	1:A:592:VAL:HG11	1.93	0.51
1:A:240:PRO:HA	1:A:243:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:LEU:HD22	2:B:652:LEU:HD21	1.92	0.50
3:C:29:VAL:HG22	4:D:216:ARG:HG3	1.92	0.50
8:H:103:SER:OG	8:H:104:ARG:NH1	2.44	0.50
23:3:613:CLA:H2	23:3:614:CLA:HMD1	1.93	0.50
20:2:68:THR:HB	20:2:73:LEU:HD12	1.92	0.50
29:5:627:LMG:H181	23:7:610:CLA:H92	1.92	0.50
23:B:837:CLA:H162	6:F:157:LEU:HD11	1.93	0.50
13:1:115:VAL:HG13	13:1:120:TYR:HB2	1.92	0.50
23:B:830:CLA:HBC1	26:B:846:BCR:H21C	1.92	0.50
1:A:226:LYS:HD3	1:A:253:LEU:HB3	1.93	0.50
5:E:101:GLN:NE2	5:E:123:ASN:OD1	2.40	0.50
15:4:234:ILE:HG12	15:4:238:LYS:HE3	1.94	0.50
19:8:217:TRP:HB3	23:8:610:CLA:H3A	1.94	0.50
4:D:225:ARG:NE	5:E:95:GLU:OE2	2.33	0.50
2:B:553:ASP:OD2	4:D:229:ASN:ND2	2.45	0.50
23:4:609:CLA:H42	29:4:624:LMG:H191	1.92	0.50
1:A:23:GLU:OE2	29:A:860:LMG:O3	2.28	0.50
23:A:824:CLA:HHB	23:A:845:CLA:HBC3	1.92	0.50
2:B:465:GLN:NE2	23:B:836:CLA:OBD	2.45	0.50
4:D:137:ILE:HD13	4:D:175:LEU:HD23	1.93	0.50
14:3:201:PHE:HD2	31:3:618:LUT:H222	1.77	0.50
29:5:627:LMG:H132	28:5:628:LMU:H61	1.93	0.50
2:B:445:GLN:OE1	2:B:453:GLN:NE2	2.45	0.49
23:1:601:CLA:HAC2	25:1:620:LHG:HC42	1.93	0.49
23:5:606:CLA:HAA1	26:5:622:BCR:H21C	1.93	0.49
23:A:809:CLA:HMC3	23:A:810:CLA:HMD2	1.94	0.49
23:4:606:CLA:HAB	23:4:607:CLA:HMC3	1.93	0.49
23:A:854:CLA:H11	2:B:617:LEU:HD12	1.95	0.49
18:7:58:LEU:HD13	23:7:602:CLA:H42	1.95	0.49
23:A:802:CLA:H18	23:A:842:CLA:H2	1.94	0.49
23:A:829:CLA:H141	23:A:829:CLA:H193	1.93	0.49
23:A:829:CLA:H11	26:A:852:BCR:H323	1.93	0.49
23:7:601:CLA:H112	23:7:616:CLA:HMD2	1.95	0.49
19:8:74:ALA:O	19:8:80:ASN:ND2	2.46	0.49
21:9:175:GLN:OE1	23:9:613:CLA:C4D	2.59	0.49
2:B:580:ALA:O	2:B:584:MET:N	2.46	0.49
23:A:836:CLA:H162	26:A:851:BCR:H372	1.95	0.49
23:B:824:CLA:H71	23:B:826:CLA:H42	1.95	0.49
25:B:851:LHG:H111	13:1:82:LEU:HD22	1.95	0.49
1:A:396:TRP:HB3	23:A:829:CLA:HMC3	1.95	0.49
23:B:831:CLA:HAC1	23:B:838:CLA:HBC3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:607:CLA:H61	23:7:616:CLA:HMC2	1.94	0.49
15:4:96:TYR:OH	15:4:108:ASP:OD2	2.31	0.49
15:4:290:LEU:HB2	23:4:616:CLA:HMA1	1.95	0.49
18:7:144:SER:OG	18:7:145:GLN:N	2.41	0.49
1:A:180:HIS:CE1	23:A:811:CLA:NA	2.81	0.49
1:A:501:ASN:HB2	23:A:837:CLA:HED2	1.95	0.49
23:A:820:CLA:H203	23:A:828:CLA:H3A	1.95	0.49
23:B:807:CLA:O1A	9:I:83:THR:OG1	2.31	0.49
16:5:152:ARG:NH2	23:6:601:CLA:OBD	2.45	0.49
20:2:175:GLY:O	20:2:178:ASN:ND2	2.46	0.49
23:A:801:CLA:HMB1	23:B:802:CLA:HAA1	1.94	0.48
2:B:351:GLN:HE21	23:B:826:CLA:HMD2	1.77	0.48
26:3:620:BCR:HC21	23:7:601:CLA:HMD2	1.95	0.48
1:A:116:GLN:NE2	23:A:810:CLA:OBD	2.44	0.48
1:A:119:TRP:HB3	26:A:856:BCR:H323	1.95	0.48
23:A:841:CLA:H162	23:F:301:CLA:H2	1.93	0.48
23:B:818:CLA:H62	23:B:818:CLA:H41	1.70	0.48
1:A:477:ILE:HG12	28:A:859:LMU:H1B	1.96	0.48
23:B:825:CLA:HMA1	26:B:847:BCR:H14C	1.95	0.48
23:6:613:CLA:HMC2	23:6:613:CLA:H92	1.94	0.48
23:A:811:CLA:HAB	23:A:814:CLA:H111	1.95	0.48
23:A:819:CLA:H72	23:A:836:CLA:H12	1.94	0.48
12:L:193:CYS:SG	26:L:305:BCR:H19C	2.52	0.48
23:3:609:CLA:H2A	23:3:609:CLA:HED2	1.95	0.48
1:A:17:VAL:HA	1:A:186:PRO:HA	1.94	0.48
23:B:821:CLA:HMD2	26:B:843:BCR:H342	1.94	0.48
11:K:89:THR:HA	11:K:143:GLY:HA3	1.95	0.48
16:5:192:SER:HB2	23:5:610:CLA:HAA1	1.96	0.48
29:7:624:LMG:O5	29:7:624:LMG:O9	2.30	0.48
7:G:121:ALA:HB2	21:9:35:LEU:HD23	1.95	0.48
12:L:127:VAL:HG12	12:L:129:THR:H	1.79	0.48
19:8:234:GLY:O	19:8:238:GLN:HG3	2.13	0.48
1:A:83:ILE:HG21	23:A:807:CLA:HMD2	1.96	0.48
26:A:848:BCR:H281	26:3:621:BCR:H281	1.95	0.48
4:D:209:PRO:HA	4:D:216:ARG:HH22	1.77	0.48
23:4:604:CLA:HMB3	32:4:620:XAT:H162	1.96	0.48
16:5:199:LEU:HD23	16:5:202:LYS:HD2	1.95	0.48
17:6:137:ARG:NH2	23:6:608:CLA:OBD	2.47	0.48
5:E:98:TRP:NE1	5:E:123:ASN:O	2.38	0.48
14:3:164:GLN:HE22	14:3:167:ARG:HH11	1.61	0.48
15:4:89:PRO:HG2	23:4:601:CLA:HED2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:154:TRP:NE1	23:5:619:CLA:OBD	2.40	0.48
19:8:78:ALA:HB2	19:8:218:LYS:HB3	1.95	0.48
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.96	0.48
1:A:483:PHE:HB3	23:A:838:CLA:H11	1.95	0.48
1:A:277:THR:HG21	1:A:279:LYS:HE3	1.96	0.47
23:1:601:CLA:HMD2	26:8:621:BCR:H323	1.96	0.47
26:3:622:BCR:H341	26:3:622:BCR:H11C	1.62	0.47
23:6:608:CLA:H41	31:6:619:LUT:H362	1.96	0.47
18:7:130:TRP:HE3	23:8:601:CLA:H11	1.78	0.47
17:6:130:GLU:HG2	17:6:193:LEU:HD12	1.95	0.47
19:8:144:SER:OG	19:8:145:PHE:N	2.46	0.47
19:8:254:LEU:HD21	23:8:614:CLA:HMC3	1.96	0.47
23:6:601:CLA:H61	23:6:614:CLA:H43	1.96	0.47
18:7:130:TRP:CD1	26:7:621:BCR:H12C	2.50	0.47
4:D:146:ILE:HG12	4:D:156:ILE:HG22	1.96	0.47
23:6:620:CLA:H92	33:6:624:NEX:H362	1.97	0.47
18:7:116:ASP:HB3	18:7:119:THR:HG22	1.96	0.47
1:A:686:LEU:HB3	2:B:666:ILE:HG12	1.97	0.47
2:B:525:ALA:HB2	23:B:837:CLA:HMA1	1.95	0.47
23:2:610:CLA:HHC	31:2:619:LUT:H32	1.95	0.47
13:1:73:LEU:HD11	13:1:95:THR:HG21	1.97	0.47
13:1:83:SER:HB2	13:1:86:LYS:HE3	1.96	0.47
16:5:214:TYR:CE2	32:5:621:XAT:H10	2.50	0.47
23:7:613:CLA:H2	23:7:614:CLA:HMD1	1.97	0.47
20:2:29:ASP:OD1	20:2:29:ASP:N	2.47	0.47
20:2:76:PHE:HB2	32:2:620:XAT:H3	1.97	0.47
1:A:320:HIS:HE1	23:A:823:CLA:NA	2.12	0.47
1:A:438:ILE:O	1:A:442:ASN:N	2.44	0.47
28:A:859:LMU:H12	12:L:165:LEU:HD13	1.97	0.47
23:B:805:CLA:H62	23:B:813:CLA:H2	1.96	0.47
23:B:813:CLA:H121	23:B:813:CLA:H8	1.72	0.47
23:B:833:CLA:H61	23:B:833:CLA:H41	1.60	0.47
23:B:839:CLA:H2	23:B:840:CLA:H121	1.96	0.47
4:D:109:LEU:HB2	4:D:190:TYR:CE2	2.50	0.47
4:D:169:LYS:HE3	4:D:201:LEU:HD23	1.96	0.47
6:F:146:ALA:O	6:F:151:ILE:N	2.40	0.47
23:L:304:CLA:H2A	23:L:304:CLA:HED2	1.97	0.47
14:3:184:PHE:CG	23:3:608:CLA:HMC2	2.49	0.47
16:5:104:GLY:HA3	32:5:621:XAT:H182	1.97	0.47
23:5:602:CLA:H112	32:5:621:XAT:H28	1.97	0.47
23:5:610:CLA:H2	31:5:620:LUT:H26	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:7:611:CLA:HBC3	25:7:622:LHG:HC62	1.96	0.47
2:B:188:SER:OG	2:B:278:HIS:O	2.30	0.47
6:F:195:LEU:HD13	6:F:198:GLN:HE21	1.80	0.47
23:3:609:CLA:H3A	23:3:609:CLA:HBA2	1.53	0.47
16:5:183:GLY:N	23:5:610:CLA:OBD	2.47	0.47
1:A:479:LEU:HB2	1:A:530:THR:HG23	1.96	0.47
26:A:856:BCR:HC32	10:J:31:ARG:HH11	1.80	0.47
2:B:494:TRP:CZ2	23:B:835:CLA:H2A	2.49	0.47
23:B:805:CLA:HBA1	23:B:805:CLA:H3A	1.65	0.47
1:A:215:GLY:HA3	23:A:816:CLA:HAB	1.95	0.47
23:A:807:CLA:H161	23:A:830:CLA:HBB2	1.96	0.47
23:B:840:CLA:H11	24:B:842:PQN:H293	1.95	0.47
13:1:60:LEU:HD12	23:1:601:CLA:HMA3	1.97	0.47
14:3:130:VAL:HG21	32:3:619:XAT:H172	1.97	0.47
16:5:216:ALA:HB1	16:5:220:GLN:HE21	1.80	0.47
1:A:596:LEU:HD21	23:A:831:CLA:HBC1	1.97	0.46
23:A:820:CLA:HBA2	23:A:820:CLA:H3A	1.60	0.46
2:B:657:ILE:HG12	23:B:840:CLA:HMB3	1.97	0.46
20:2:144:LEU:HA	20:2:147:LEU:HB2	1.97	0.46
2:B:96:HIS:HE1	23:B:810:CLA:NB	2.14	0.46
23:A:854:CLA:H61	23:A:854:CLA:H41	1.55	0.46
3:C:24:ASP:OD2	4:D:202:HIS:ND1	2.48	0.46
6:F:158:TYR:OH	6:F:200:ALA:O	2.30	0.46
26:F:305:BCR:H20C	26:F:305:BCR:H361	1.63	0.46
10:J:34:PRO:O	30:J:103:DGD:O3D	2.33	0.46
14:3:46:TYR:HE1	25:3:624:LHG:HC12	1.81	0.46
1:A:261:ILE:HG13	14:3:262:PHE:HD1	1.80	0.46
23:L:304:CLA:HBA2	23:L:304:CLA:H3A	1.60	0.46
23:8:610:CLA:H41	23:8:610:CLA:H62	1.55	0.46
1:A:121:ILE:HB	26:A:856:BCR:H322	1.97	0.46
16:5:219:LEU:HD12	23:5:613:CLA:HAC2	1.97	0.46
31:5:620:LUT:H35	31:5:620:LUT:H401	1.80	0.46
23:8:601:CLA:H143	23:8:601:CLA:H161	1.80	0.46
23:A:837:CLA:HBA2	23:A:837:CLA:H3A	1.62	0.46
2:B:429:PHE:CD2	23:B:837:CLA:HAB	2.51	0.46
23:B:824:CLA:HMA2	23:B:824:CLA:H2	1.96	0.46
23:6:602:CLA:H72	23:6:602:CLA:H111	1.83	0.46
21:9:169:PHE:CE1	32:9:620:XAT:H10	2.50	0.46
1:A:102:GLU:OE2	1:A:156:GLU:N	2.48	0.46
2:B:34:SER:HB2	4:D:241:MET:HB3	1.98	0.46
2:B:411:ARG:O	2:B:415:HIS:ND1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:THR:HA	2:B:653:PHE:HB3	1.97	0.46
23:B:831:CLA:H191	23:B:831:CLA:HMD2	1.97	0.46
13:1:222:PRO:O	31:1:617:LUT:O3	2.31	0.46
23:3:607:CLA:H92	23:3:617:CLA:HMB2	1.98	0.46
16:5:216:ALA:O	16:5:220:GLN:CG	2.62	0.46
18:7:228:HIS:HA	18:7:233:THR:HG21	1.98	0.46
22:X:1:ALA:HB1	22:X:4:ALA:HB3	1.97	0.46
1:A:396:TRP:CD1	23:A:829:CLA:HAB	2.51	0.46
2:B:584:MET:HG2	23:B:825:CLA:HBC1	1.98	0.46
3:C:40:ALA:O	4:D:221:GLN:NE2	2.41	0.46
26:J:102:BCR:H15C	26:J:102:BCR:H351	1.79	0.46
25:4:622:LHG:HC92	26:6:622:BCR:HC42	1.98	0.46
17:6:115:PRO:O	18:7:182:LYS:NZ	2.44	0.46
17:6:284:VAL:HB	23:6:616:CLA:C1C	2.45	0.46
23:7:610:CLA:H142	23:7:610:CLA:H112	1.84	0.46
23:A:802:CLA:H102	23:A:842:CLA:HMC2	1.97	0.46
23:A:822:CLA:H192	26:A:850:BCR:H272	1.98	0.46
23:B:806:CLA:HMB2	23:B:829:CLA:HBB2	1.97	0.46
13:1:179:ASP:OD1	31:1:617:LUT:O23	2.31	0.46
15:4:265:THR:HG22	15:4:267:LEU:H	1.81	0.46
23:6:601:CLA:H111	23:6:601:CLA:H152	1.87	0.46
23:7:601:CLA:H51	23:7:601:CLA:H12	1.77	0.46
23:7:610:CLA:H143	31:7:619:LUT:H403	1.97	0.46
1:A:615:GLN:HE21	1:A:747:ILE:HD13	1.80	0.46
23:A:821:CLA:H3A	23:A:821:CLA:HBA2	1.51	0.46
23:A:831:CLA:H93	23:A:842:CLA:HED3	1.98	0.46
2:B:57:ILE:HG21	23:B:806:CLA:HMD2	1.97	0.46
23:1:611:CLA:HAB	26:8:621:BCR:H312	1.97	0.46
1:A:80:GLN:HE21	1:A:84:ILE:HG13	1.81	0.45
23:A:822:CLA:HMD3	23:A:823:CLA:HMC3	1.97	0.45
2:B:233:ALA:HA	2:B:236:GLN:HE21	1.81	0.45
15:4:211:LEU:HD22	15:4:222:GLY:HA3	1.99	0.45
15:4:284:GLN:HG2	17:6:172:LEU:HD12	1.98	0.45
16:5:126:LEU:HD23	16:5:130:PHE:HB3	1.98	0.45
17:6:97:SER:OG	17:6:98:THR:N	2.48	0.45
23:6:604:CLA:H52	23:6:606:CLA:HBD	1.98	0.45
2:B:723:ALA:HB2	23:B:827:CLA:HBB1	1.98	0.45
23:B:814:CLA:H142	23:B:814:CLA:H112	1.83	0.45
26:3:622:BCR:H361	26:3:622:BCR:H20C	1.54	0.45
23:A:841:CLA:HED3	23:A:841:CLA:H2A	1.98	0.45
26:A:852:BCR:H391	23:B:832:CLA:HMA1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ASP:HA	4:D:233:ILE:HD13	1.99	0.45
23:B:817:CLA:H3A	23:B:817:CLA:HBA2	1.52	0.45
12:L:163:ILE:HG13	12:L:176:GLU:HA	1.98	0.45
26:3:620:BCR:H11C	26:3:620:BCR:H341	1.80	0.45
16:5:260:GLN:HB2	33:5:624:NEX:H8	1.98	0.45
17:6:152:VAL:HG23	17:6:153:ARG:HG3	1.99	0.45
32:7:620:XAT:H15	32:7:620:XAT:H201	1.79	0.45
20:2:88:ASN:HA	20:2:91:LEU:HB2	1.98	0.45
1:A:45:THR:HG23	1:A:716:ARG:HG3	1.98	0.45
1:A:55:ASP:OD2	25:A:846:LHG:O2	2.35	0.45
26:A:848:BCR:H20C	26:A:848:BCR:H361	1.81	0.45
16:5:50:LYS:HD3	25:5:623:LHG:HC11	1.98	0.45
18:7:159:GLY:HA2	18:7:165:PRO:HA	1.99	0.45
19:8:182:PHE:HB2	19:8:186:GLU:HB3	1.99	0.45
21:9:140:ASN:OD1	21:9:140:ASN:N	2.49	0.45
1:A:270:SER:HA	23:A:818:CLA:HAA2	1.99	0.45
2:B:646:VAL:HG21	23:B:809:CLA:HMD2	1.97	0.45
10:J:31:ARG:NH2	23:J:101:CLA:O1D	2.50	0.45
13:1:186:ASP:HA	13:1:190:SER:HB3	1.98	0.45
16:5:262:LEU:HD23	17:6:288:GLN:HE21	1.80	0.45
20:2:112:LYS:HG2	20:2:113:THR:HG23	1.98	0.45
20:2:149:PHE:CD2	32:2:620:XAT:H12	2.52	0.45
7:G:133:VAL:HG21	23:G:204:CLA:HMA1	1.99	0.45
23:6:602:CLA:HBC1	25:6:623:LHG:H272	1.99	0.45
19:8:161:PHE:CE2	26:8:621:BCR:H10C	2.52	0.45
1:A:178:TRP:HB2	23:A:812:CLA:HMC3	1.99	0.45
1:A:540:ALA:HB1	23:A:839:CLA:HMB3	1.97	0.45
23:A:802:CLA:CGA	23:A:802:CLA:H3A	2.47	0.45
14:3:216:LYS:HE2	23:3:612:CLA:HAA2	1.98	0.45
15:4:282:VAL:N	23:4:613:CLA:O1A	2.49	0.45
25:9:622:LHG:H262	25:9:622:LHG:H292	1.90	0.45
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.99	0.45
1:A:474:ASP:O	1:A:478:GLN:NE2	2.40	0.45
23:A:809:CLA:H91	23:A:812:CLA:H202	1.98	0.45
23:A:809:CLA:HAA1	23:A:829:CLA:HED2	1.99	0.45
2:B:515:PRO:HG2	6:F:132:HIS:HD2	1.81	0.45
19:8:188:SER:HB3	19:8:201:PRO:HD3	1.99	0.45
21:9:164:LEU:HD13	31:9:619:LUT:H11	1.99	0.45
23:A:806:CLA:H62	23:A:806:CLA:H2	1.73	0.45
23:A:811:CLA:H13	26:A:849:BCR:H372	1.98	0.45
2:B:298:ILE:HB	23:B:821:CLA:HMD1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:ASP:HA	2:B:520:VAL:HG12	1.99	0.45
23:B:822:CLA:HHC	23:B:841:CLA:HED1	1.97	0.45
23:B:830:CLA:HBB2	23:B:838:CLA:HAB	1.98	0.45
3:C:17:CYS:SG	3:C:18:VAL:N	2.90	0.45
4:D:150:PRO:HD3	4:D:175:LEU:HD13	1.99	0.45
8:H:112:VAL:HA	12:L:188:LEU:HD11	1.99	0.45
13:1:104:TRP:NE1	23:1:608:CLA:O1D	2.50	0.45
32:3:619:XAT:H15	32:3:619:XAT:H201	1.81	0.45
16:5:119:GLU:O	16:5:125:ASN:ND2	2.48	0.45
1:A:338:HIS:NE2	23:A:825:CLA:ND	2.65	0.45
23:A:843:CLA:HAB	2:B:692:VAL:HG11	2.00	0.45
13:1:199:LYS:HZ1	25:1:620:LHG:P	2.40	0.45
23:1:612:CLA:HBC1	25:1:620:LHG:H381	1.99	0.45
15:4:137:VAL:HG11	31:4:619:LUT:H10	1.99	0.45
16:5:235:HIS:CG	23:5:613:CLA:HAA2	2.52	0.45
23:5:607:CLA:HBC2	33:5:624:NEX:H15	1.99	0.45
18:7:137:TYR:HB3	19:8:62:GLY:HA3	1.98	0.45
32:8:620:XAT:H35	32:8:620:XAT:H401	1.76	0.45
23:A:841:CLA:H122	23:A:841:CLA:HAB	1.99	0.44
17:6:318:PRO:HD2	23:6:620:CLA:HED2	1.98	0.44
18:7:73:LEU:O	18:7:77:ARG:N	2.40	0.44
1:A:245:LEU:HD23	28:A:857:LMU:H11	1.99	0.44
1:A:279:LYS:HG2	1:A:503:LEU:HD12	1.99	0.44
23:A:802:CLA:H93	23:A:802:CLA:H61	1.80	0.44
26:K:202:BCR:H20C	26:K:202:BCR:H361	1.82	0.44
14:3:147:ILE:HD13	23:3:606:CLA:HMD3	1.99	0.44
23:5:606:CLA:HBB2	23:5:607:CLA:CBB	2.47	0.44
32:5:621:XAT:H35	32:5:621:XAT:H401	1.86	0.44
19:8:152:LEU:HD12	23:8:607:CLA:HBC3	1.99	0.44
21:9:199:ILE:HG23	21:9:200:THR:HG23	1.98	0.44
1:A:34:HIS:NE2	23:A:812:CLA:O1A	2.43	0.44
2:B:560:CYS:SG	2:B:561:ASP:N	2.90	0.44
6:F:188:ASP:HA	29:J:104:LMG:HC61	1.99	0.44
7:G:141:HIS:CE1	23:G:203:CLA:NB	2.85	0.44
23:3:609:CLA:H91	23:3:609:CLA:H112	1.85	0.44
19:8:203:ASP:OD1	31:8:619:LUT:O23	2.27	0.44
1:A:561:ARG:NH1	4:D:122:THR:O	2.51	0.44
23:A:843:CLA:H13	12:L:190:LEU:HD21	1.99	0.44
2:B:577:PHE:CE2	23:B:829:CLA:HMD2	2.52	0.44
11:K:106:LYS:HG2	11:K:116:ASP:HA	2.00	0.44
12:L:224:PHE:N	12:L:224:PHE:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:6:624:NEX:H35	33:6:624:NEX:H401	1.86	0.44
18:7:130:TRP:CE2	26:7:621:BCR:H10C	2.53	0.44
21:9:49:ASN:HD22	21:9:163:ARG:HH11	1.65	0.44
1:A:141:THR:HG22	23:A:809:CLA:HMD1	1.99	0.44
1:A:647:ARG:HA	2:B:633:ILE:HD12	1.99	0.44
1:A:733:LEU:HD22	23:A:842:CLA:HMA1	1.99	0.44
2:B:490:GLY:HA3	2:B:495:LEU:HD13	1.99	0.44
2:B:701:LEU:HD22	2:B:705:GLN:NE2	2.32	0.44
23:B:832:CLA:H62	23:B:832:CLA:H2	1.61	0.44
10:J:3:ASP:O	10:J:6:THR:OG1	2.29	0.44
16:5:146:MET:HG3	23:5:609:CLA:HMC3	1.99	0.44
25:8:623:LHG:H251	28:8:624:LMU:H101	2.00	0.44
21:9:70:GLU:OE2	21:9:163:ARG:NE	2.51	0.44
1:A:453:PHE:CE1	23:A:803:CLA:HBB	2.53	0.44
23:A:829:CLA:H61	23:A:829:CLA:H41	1.80	0.44
2:B:115:ASN:HD21	23:B:809:CLA:HMD1	1.83	0.44
2:B:701:LEU:HD11	24:B:842:PQN:H152	1.99	0.44
14:3:177:PHE:CZ	23:3:608:CLA:HBB2	2.53	0.44
23:6:613:CLA:H93	23:6:613:CLA:H61	1.88	0.44
23:7:613:CLA:H93	25:7:622:LHG:H291	2.00	0.44
1:A:121:ILE:HG12	1:A:122:VAL:HG13	1.99	0.44
2:B:286:ILE:O	2:B:290:HIS:ND1	2.48	0.44
2:B:665:LEU:O	2:B:668:TRP:NE1	2.50	0.44
16:5:73:ASP:HB2	23:5:602:CLA:HBA2	1.99	0.44
23:A:822:CLA:H161	23:A:822:CLA:H141	1.71	0.44
2:B:300:HIS:CE1	23:B:821:CLA:NA	2.85	0.44
23:B:813:CLA:H141	23:B:813:CLA:H162	1.83	0.44
10:J:21:PHE:HA	23:J:101:CLA:HBB2	2.00	0.44
13:1:154:GLU:HG2	23:1:606:CLA:HMA3	2.00	0.44
26:3:620:BCR:H333	23:7:611:CLA:HMC3	2.00	0.44
17:6:297:PRO:O	17:6:309:THR:OG1	2.34	0.44
31:2:619:LUT:H35	31:2:619:LUT:H401	1.83	0.44
21:9:131:LYS:H	21:9:131:LYS:HD2	1.81	0.44
31:2:619:LUT:H11	31:2:619:LUT:H191	1.88	0.44
2:B:682:ALA:O	2:B:686:THR:OG1	2.24	0.43
26:K:202:BCR:H15C	26:K:202:BCR:H351	1.79	0.43
20:2:75:LYS:HG3	20:2:77:TRP:H	1.82	0.43
21:9:38:PRO:HB2	21:9:40:HIS:H	1.83	0.43
21:9:164:LEU:HD23	25:9:622:LHG:H292	2.00	0.43
23:A:831:CLA:H202	23:A:831:CLA:H162	1.87	0.43
2:B:124:TRP:HH2	23:B:828:CLA:H2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:LEU:HD11	23:B:829:CLA:HBB1	1.99	0.43
13:1:214:GLN:HE21	13:1:225:ALA:HB3	1.83	0.43
16:5:214:TYR:CD2	32:5:621:XAT:H12	2.53	0.43
1:A:547:VAL:HG11	23:A:840:CLA:HMB3	2.00	0.43
1:A:650:LEU:HD11	23:A:801:CLA:H72	2.00	0.43
23:A:825:CLA:H202	23:A:840:CLA:HBA2	2.00	0.43
26:A:849:BCR:H20C	26:A:849:BCR:H361	1.87	0.43
2:B:39:THR:O	2:B:43:LEU:N	2.52	0.43
23:B:834:CLA:H2	23:B:834:CLA:H61	1.83	0.43
23:G:203:CLA:HMC1	26:G:205:BCR:H332	2.01	0.43
14:3:203:LEU:HB2	23:3:610:CLA:HBA1	2.00	0.43
16:5:77:LEU:HD13	23:5:602:CLA:H42	2.00	0.43
23:8:601:CLA:H121	23:8:614:CLA:H8	2.00	0.43
23:A:805:CLA:HBA2	23:A:805:CLA:H3A	1.62	0.43
2:B:27:ALA:HA	23:B:829:CLA:H42	2.00	0.43
1:A:458:HIS:CE1	23:A:835:CLA:NA	2.86	0.43
31:7:619:LUT:H15	31:7:619:LUT:H201	1.82	0.43
19:8:77:LEU:HD21	19:8:99:GLN:HG3	2.00	0.43
20:2:106:ARG:HA	20:2:109:ILE:HD12	2.01	0.43
1:A:338:HIS:CD2	23:A:825:CLA:ND	2.87	0.43
23:A:809:CLA:H92	23:A:809:CLA:H62	1.82	0.43
26:A:856:BCR:H15C	26:A:856:BCR:H351	1.89	0.43
4:D:181:ASN:O	4:D:184:LYS:NZ	2.52	0.43
17:6:138:TRP:CD1	23:6:609:CLA:HMD3	2.53	0.43
23:6:613:CLA:H101	25:6:623:LHG:H152	2.00	0.43
26:A:848:BCR:H15C	26:A:848:BCR:H351	1.82	0.43
26:B:844:BCR:H312	26:B:845:BCR:HC41	2.00	0.43
4:D:135:TYR:HE2	4:D:169:LYS:HB2	1.82	0.43
23:4:610:CLA:H93	23:4:610:CLA:H111	1.87	0.43
23:A:829:CLA:H91	23:A:829:CLA:H112	1.84	0.43
26:A:856:BCR:HC22	10:J:31:ARG:HD3	2.01	0.43
2:B:130:MET:HE2	23:B:814:CLA:HMA2	1.99	0.43
2:B:257:THR:H	2:B:272:THR:HB	1.84	0.43
32:4:620:XAT:H35	32:4:620:XAT:H401	1.79	0.43
23:6:602:CLA:H2A	23:6:602:CLA:HED3	2.01	0.43
23:6:604:CLA:H172	23:6:610:CLA:HBC1	2.00	0.43
26:A:848:BCR:H11C	26:A:848:BCR:H341	1.86	0.43
2:B:412:MET:HG2	2:B:540:LEU:HD21	2.01	0.43
23:B:827:CLA:HBA2	23:B:827:CLA:H3A	1.70	0.43
23:B:829:CLA:H141	23:B:829:CLA:H161	1.82	0.43
26:B:847:BCR:H15C	26:B:847:BCR:H351	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:6:609:CLA:H3A	23:6:609:CLA:HBA1	1.73	0.43
1:A:574:PRO:HB3	1:A:720:ILE:HB	2.01	0.43
24:A:844:PQN:H222	24:A:844:PQN:H262	1.78	0.43
6:F:137:PRO:HG2	26:F:305:BCR:H333	2.00	0.43
15:4:124:GLN:NE2	15:4:217:PRO:O	2.50	0.43
16:5:92:LEU:HB3	16:5:96:ARG:NH2	2.33	0.43
23:5:604:CLA:H92	23:5:604:CLA:H61	1.91	0.43
17:6:114:ASP:HB2	23:6:602:CLA:HBA2	2.01	0.43
1:A:680:ALA:O	23:A:802:CLA:HAB	2.19	0.42
23:A:803:CLA:H161	23:A:803:CLA:H141	1.75	0.42
23:B:834:CLA:H61	23:B:834:CLA:H102	1.65	0.42
23:F:301:CLA:H42	10:J:14:ILE:HG22	2.01	0.42
23:1:606:CLA:HBB2	23:1:607:CLA:CBB	2.48	0.42
32:1:618:XAT:H35	32:1:618:XAT:H401	1.85	0.42
14:3:159:GLU:OE2	23:3:609:CLA:NC	2.52	0.42
23:4:601:CLA:H93	23:4:613:CLA:H152	2.01	0.42
31:4:619:LUT:H15	31:4:619:LUT:H201	1.88	0.42
23:6:613:CLA:H12	23:6:614:CLA:HED2	2.01	0.42
21:9:160:LYS:HB3	23:9:611:CLA:C3D	2.49	0.42
23:A:803:CLA:HBD	2:B:655:HIS:HB3	2.01	0.42
23:A:843:CLA:HMC2	23:B:839:CLA:H42	2.00	0.42
23:B:832:CLA:H93	23:B:832:CLA:H111	1.84	0.42
6:F:71:SER:HB3	6:F:119:ALA:HB1	2.02	0.42
23:G:203:CLA:H3A	26:G:205:BCR:H363	2.00	0.42
26:1:619:BCR:H24C	26:1:619:BCR:H371	1.84	0.42
15:4:189:ARG:HB3	23:4:608:CLA:HMC3	2.00	0.42
23:4:614:CLA:H52	23:4:614:CLA:H8	1.90	0.42
23:5:613:CLA:H51	23:5:614:CLA:HMD1	2.02	0.42
28:5:628:LMU:H72	28:5:628:LMU:H41	1.84	0.42
26:6:622:BCR:H11C	26:6:622:BCR:H341	1.84	0.42
1:A:488:GLN:HA	1:A:510:TRP:HE3	1.84	0.42
23:A:803:CLA:H151	23:B:810:CLA:HBC3	1.99	0.42
2:B:287:VAL:HG22	26:B:843:BCR:H14C	2.02	0.42
2:B:478:LEU:O	2:B:484:SER:OG	2.32	0.42
23:B:820:CLA:HBB1	26:G:205:BCR:H342	2.01	0.42
23:B:833:CLA:H152	23:B:833:CLA:H112	1.80	0.42
26:B:844:BCR:H15C	26:B:844:BCR:H351	1.81	0.42
26:G:205:BCR:H15C	26:G:205:BCR:H351	1.87	0.42
23:4:601:CLA:H3A	23:4:601:CLA:HBA2	1.36	0.42
23:7:613:CLA:H142	23:7:613:CLA:H111	1.85	0.42
19:8:138:LYS:NZ	28:8:624:LMU:O6'	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:825:CLA:H3A	23:A:825:CLA:HBA2	1.61	0.42
2:B:440:HIS:CD2	2:B:454:ILE:HG12	2.55	0.42
24:B:842:PQN:H142	24:B:842:PQN:H112	1.81	0.42
14:3:98:ALA:O	14:3:102:ALA:N	2.49	0.42
23:5:613:CLA:H61	23:5:613:CLA:H41	1.89	0.42
32:9:620:XAT:H15	32:9:620:XAT:H201	1.85	0.42
1:A:87:TRP:HA	23:A:808:CLA:HBB2	2.01	0.42
1:A:547:VAL:HG21	23:A:840:CLA:HMA1	2.01	0.42
23:A:832:CLA:HBB2	23:A:840:CLA:HMC2	2.01	0.42
23:4:608:CLA:H11	23:4:608:CLA:H51	1.85	0.42
16:5:101:GLY:HA2	32:5:621:XAT:H181	2.00	0.42
23:5:606:CLA:HMB2	26:5:622:BCR:H373	2.01	0.42
1:A:57:HIS:CE1	23:A:805:CLA:NB	2.86	0.42
15:4:225:ASP:OD1	31:4:619:LUT:O23	2.29	0.42
26:4:621:BCR:H15C	26:4:621:BCR:H351	1.80	0.42
32:5:621:XAT:H373	32:5:621:XAT:H23	1.88	0.42
17:6:118:LEU:HD13	23:6:602:CLA:H42	2.02	0.42
23:A:809:CLA:H203	23:A:809:CLA:H161	1.90	0.42
23:A:841:CLA:H143	23:F:303:CLA:HBC1	2.01	0.42
23:B:824:CLA:H72	23:B:824:CLA:H112	1.77	0.42
23:1:611:CLA:H92	23:1:611:CLA:H62	1.85	0.42
23:3:602:CLA:H72	23:3:602:CLA:H111	1.81	0.42
16:5:115:VAL:HG11	23:5:604:CLA:HED2	2.02	0.42
23:5:604:CLA:H2A	23:5:604:CLA:HED3	2.01	0.42
26:A:852:BCR:H291	26:B:801:BCR:H14C	2.02	0.42
2:B:226:PHE:HA	2:B:231:TRP:HE1	1.83	0.42
2:B:266:THR:HB	2:B:361:PHE:H	1.84	0.42
2:B:546:LYS:HE2	6:F:222:ILE:HD11	2.01	0.42
23:B:803:CLA:H112	26:B:848:BCR:H362	2.02	0.42
23:B:827:CLA:H92	23:B:827:CLA:H62	1.86	0.42
26:K:202:BCR:H11C	26:K:202:BCR:H341	1.87	0.42
23:3:604:CLA:H43	23:5:616:CLA:HED3	2.01	0.42
23:3:610:CLA:H3A	23:3:610:CLA:HBA2	1.72	0.42
23:7:608:CLA:H43	23:7:610:CLA:H201	2.02	0.42
23:8:610:CLA:H92	23:8:612:CLA:HMA1	2.02	0.42
21:9:123:GLU:OE2	23:9:609:CLA:NA	2.53	0.42
23:A:805:CLA:HAA1	23:A:812:CLA:H2	2.02	0.42
23:A:806:CLA:H162	23:A:814:CLA:H51	2.02	0.42
23:A:832:CLA:HBA2	25:A:847:LHG:HC81	2.01	0.42
23:B:830:CLA:H3A	23:B:831:CLA:OBD	2.20	0.42
15:4:203:ASP:OD2	23:4:618:CLA:ND	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ILE:HG23	23:A:803:CLA:H61	2.02	0.42
23:A:801:CLA:C1A	23:B:802:CLA:HAB	2.49	0.42
26:A:856:BCR:H362	26:J:102:BCR:H12C	2.02	0.42
23:B:807:CLA:HHB	23:B:808:CLA:HHB	2.01	0.42
23:B:834:CLA:HBA2	23:B:835:CLA:HMB3	2.01	0.42
13:1:108:GLY:HA2	32:1:618:XAT:H181	2.01	0.42
15:4:252:PHE:CD2	32:4:620:XAT:H12	2.55	0.42
23:5:602:CLA:H112	23:5:602:CLA:H72	1.84	0.42
31:6:619:LUT:H15	31:6:619:LUT:H201	1.91	0.42
19:8:237:ALA:HB1	23:8:616:CLA:HBA2	2.02	0.42
26:8:621:BCR:H15C	26:8:621:BCR:H351	1.83	0.42
23:F:303:CLA:HMB3	10:J:26:LEU:HD21	2.01	0.41
11:K:144:HIS:CE1	26:K:207:BCR:H12C	2.55	0.41
23:1:611:CLA:H152	23:1:611:CLA:H111	1.86	0.41
26:1:619:BCR:H11C	26:1:619:BCR:H341	1.87	0.41
15:4:282:VAL:HB	23:4:613:CLA:H12	2.01	0.41
23:5:606:CLA:HBB2	23:5:607:CLA:CAB	2.50	0.41
25:8:623:LHG:HC81	25:8:623:LHG:H112	1.74	0.41
1:A:296:HIS:CE1	23:A:818:CLA:NA	2.88	0.41
23:A:818:CLA:H61	23:A:818:CLA:H41	1.71	0.41
23:A:836:CLA:H41	23:A:836:CLA:H62	1.74	0.41
25:A:846:LHG:H242	25:A:846:LHG:H272	1.70	0.41
2:B:429:PHE:CE2	23:B:837:CLA:HAB	2.55	0.41
23:B:841:CLA:H3A	25:B:851:LHG:H261	2.02	0.41
13:1:59:TRP:HA	23:1:601:CLA:C4C	2.51	0.41
31:4:619:LUT:H35	31:4:619:LUT:H401	1.78	0.41
16:5:141:TRP:CE2	23:6:614:CLA:H3A	2.55	0.41
16:5:149:VAL:HG21	26:5:622:BCR:H362	2.02	0.41
23:8:609:CLA:HBA1	23:8:609:CLA:H3A	1.89	0.41
1:A:655:SER:HG	1:A:659:GLN:NE2	2.18	0.41
23:A:836:CLA:H62	23:A:836:CLA:H102	1.86	0.41
23:B:805:CLA:H162	23:B:805:CLA:H141	1.77	0.41
17:6:248:PHE:CD2	32:6:621:XAT:H12	2.55	0.41
18:7:74:VAL:HA	18:7:77:ARG:HB2	2.02	0.41
23:7:601:CLA:H61	23:7:613:CLA:H8	2.02	0.41
26:7:621:BCR:H15C	26:7:621:BCR:H351	1.83	0.41
25:8:622:LHG:H141	25:8:622:LHG:H302	2.01	0.41
20:2:149:PHE:CE1	32:2:620:XAT:H10	2.55	0.41
1:A:397:ILE:HD12	23:A:830:CLA:HBB1	2.02	0.41
1:A:536:HIS:CG	23:A:839:CLA:HED3	2.55	0.41
1:A:575:CYS:SG	2:B:563:PRO:HB3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:LYS:HE3	6:F:216:LEU:HD22	2.02	0.41
23:A:819:CLA:H92	23:A:819:CLA:H62	1.89	0.41
4:D:222:ASN:HB3	4:D:224:ARG:HG2	2.01	0.41
26:K:207:BCR:H371	26:K:207:BCR:H24C	1.73	0.41
12:L:156:PHE:HA	12:L:247:ALA:HB2	2.01	0.41
23:1:603:CLA:HBB1	32:1:618:XAT:C35	2.50	0.41
14:3:92:VAL:HG11	14:3:191:ALA:HB1	2.02	0.41
23:5:613:CLA:HMB3	31:5:620:LUT:H162	2.02	0.41
23:6:616:CLA:H192	23:6:620:CLA:HBC1	2.02	0.41
18:7:30:ARG:NH2	18:7:43:LEU:O	2.53	0.41
20:2:19:PRO:HD2	20:2:22:LEU:HD12	2.01	0.41
1:A:269:TRP:O	23:A:818:CLA:H3A	2.20	0.41
23:A:806:CLA:H203	23:A:814:CLA:H62	2.01	0.41
23:B:818:CLA:H93	23:B:818:CLA:H61	1.86	0.41
31:8:619:LUT:H401	31:8:619:LUT:H35	1.79	0.41
21:9:160:LYS:CD	23:9:611:CLA:CAD	2.97	0.41
23:A:804:CLA:H111	23:A:804:CLA:H72	1.83	0.41
23:A:829:CLA:O1D	23:A:830:CLA:HBB	2.21	0.41
2:B:27:ALA:HB2	30:B:850:DGD:HA41	2.02	0.41
2:B:370:ALA:HA	2:B:595:TRP:CZ3	2.56	0.41
2:B:617:LEU:HA	2:B:620:TRP:HD1	1.86	0.41
30:B:850:DGD:O3D	30:B:850:DGD:O6D	2.34	0.41
7:G:120:PHE:HA	7:G:129:ASN:HD22	1.84	0.41
13:1:234:TRP:HB3	19:8:146:ALA:HB2	2.02	0.41
25:3:623:LHG:H312	25:5:625:LHG:H383	2.02	0.41
23:4:609:CLA:HHC	23:4:609:CLA:HBB1	2.02	0.41
23:2:613:CLA:HBB	23:2:614:CLA:HHD	2.02	0.41
21:9:135:THR:HB	21:9:139:ILE:HA	2.03	0.41
21:9:190:HIS:CD2	23:9:614:CLA:NC	2.89	0.41
23:A:801:CLA:HED3	23:A:801:CLA:HBD	1.79	0.41
23:A:802:CLA:H122	26:A:852:BCR:H23C	2.02	0.41
23:A:813:CLA:H12	14:3:72:LEU:HD11	2.03	0.41
23:A:842:CLA:HBA2	23:A:842:CLA:H3A	1.59	0.41
2:B:54:GLN:HE21	2:B:58:ILE:HG13	1.86	0.41
2:B:698:PRO:O	3:C:81:TYR:OH	2.32	0.41
11:K:144:HIS:ND1	26:K:207:BCR:H12C	2.36	0.41
13:1:114:ALA:HA	13:1:117:LEU:HB2	2.03	0.41
23:4:601:CLA:OBD	17:6:188:ARG:NH2	2.54	0.41
25:4:622:LHG:O1	17:6:203:PRO:O	2.36	0.41
17:6:263:ILE:O	17:6:267:GLN:N	2.48	0.41
19:8:75:GLN:HA	19:8:80:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:PHE:CD1	2:B:665:LEU:HB3	2.56	0.41
24:A:844:PQN:H151	23:F:301:CLA:HAB	2.03	0.41
26:3:620:BCR:H15C	26:3:620:BCR:H351	1.98	0.41
19:8:252:ALA:HB1	19:8:260:VAL:HG11	2.02	0.41
23:8:608:CLA:H12	31:8:619:LUT:H383	2.02	0.41
28:8:624:LMU:H22	28:8:624:LMU:H52	1.70	0.41
1:A:53:HIS:HD2	23:A:805:CLA:HAC1	1.85	0.41
1:A:426:LEU:HG	23:A:825:CLA:C1C	2.51	0.41
1:A:691:GLY:N	2:B:569:CYS:O	2.52	0.41
26:A:850:BCR:H11C	26:A:850:BCR:H341	1.92	0.41
2:B:19:THR:HG22	2:B:699:VAL:H	1.85	0.41
2:B:79:VAL:HG13	2:B:126:TYR:HE1	1.85	0.41
2:B:237:SER:O	2:B:253:GLN:N	2.47	0.41
23:B:805:CLA:H93	23:B:805:CLA:H111	1.97	0.41
23:B:809:CLA:H61	23:B:809:CLA:H41	1.85	0.41
23:B:825:CLA:H61	23:B:825:CLA:H2	1.80	0.41
23:B:829:CLA:H93	23:B:829:CLA:H111	1.95	0.41
26:G:205:BCR:H24C	26:G:205:BCR:H371	1.82	0.41
13:1:165:ARG:NH1	23:1:609:CLA:O1D	2.52	0.41
23:5:603:CLA:HMD3	23:6:616:CLA:H72	2.02	0.41
17:6:224:PRO:O	31:6:619:LUT:O23	2.27	0.41
23:6:610:CLA:H141	23:6:610:CLA:H161	1.81	0.41
33:6:624:NEX:H11	33:6:624:NEX:H191	1.85	0.41
31:8:619:LUT:H11	31:8:619:LUT:H191	1.93	0.41
1:A:605:ILE:HD12	23:A:801:CLA:H122	2.02	0.41
24:A:844:PQN:H151	24:A:844:PQN:H18	1.78	0.41
23:B:803:CLA:H142	23:B:803:CLA:H111	1.78	0.41
23:B:830:CLA:CBB	23:B:838:CLA:HAB	2.51	0.41
24:B:842:PQN:H303	30:B:850:DGD:HA81	2.03	0.41
23:F:304:CLA:HED2	23:F:304:CLA:HBD	1.94	0.41
13:1:174:PRO:HD3	23:1:608:CLA:HMD2	2.02	0.41
23:1:611:CLA:H111	23:1:611:CLA:H71	1.83	0.41
23:4:608:CLA:H171	23:4:608:CLA:H13	1.87	0.41
16:5:198:GLU:HG3	16:5:202:LYS:HE2	2.02	0.41
1:A:359:LEU:O	1:A:363:LEU:N	2.47	0.40
1:A:701:VAL:O	1:A:705:ASN:N	2.44	0.40
23:A:826:CLA:HBA1	23:A:830:CLA:H18	2.02	0.40
14:3:87:LEU:HD23	14:3:87:LEU:HA	1.92	0.40
20:2:143:ARG:HB3	25:2:622:LHG:H241	2.03	0.40
1:A:25:SER:OG	29:A:860:LMG:O4	2.29	0.40
26:A:850:BCR:H371	26:A:850:BCR:H24C	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:851:BCR:H20C	26:A:851:BCR:H361	1.87	0.40
23:B:815:CLA:HED2	23:B:815:CLA:H2A	2.03	0.40
26:F:305:BCR:H24C	26:F:305:BCR:H371	1.83	0.40
16:5:142:GLU:HA	23:5:606:CLA:HMA3	2.03	0.40
23:5:609:CLA:H2	23:6:616:CLA:H92	2.03	0.40
23:6:613:CLA:H142	23:6:613:CLA:H112	1.89	0.40
26:6:622:BCR:H20C	26:6:622:BCR:H361	1.95	0.40
2:B:667:SER:HB3	2:B:672:TRP:HE1	1.85	0.40
23:B:803:CLA:H92	23:B:803:CLA:H62	1.86	0.40
7:G:128:PHE:O	23:G:204:CLA:H3A	2.21	0.40
12:L:223:LEU:HD11	12:L:229:TRP:HA	2.03	0.40
13:1:208:PHE:CD2	32:1:618:XAT:H12	2.56	0.40
23:4:613:CLA:HBA2	23:4:613:CLA:H3A	1.74	0.40
25:5:623:LHG:H142	25:5:623:LHG:H172	1.84	0.40
25:5:625:LHG:HC31	29:5:626:LMG:H122	2.03	0.40
23:7:603:CLA:HAC1	23:7:607:CLA:HBB2	2.04	0.40
31:8:619:LUT:H31	31:8:619:LUT:H391	1.94	0.40
21:9:150:ASN:HB3	21:9:154:MET:HB2	2.03	0.40
32:9:620:XAT:H31	32:9:620:XAT:H391	1.91	0.40
25:9:622:LHG:H102	25:9:622:LHG:H131	1.88	0.40
1:A:658:ILE:HB	2:B:622:ARG:HB3	2.02	0.40
23:A:827:CLA:HBA2	23:A:827:CLA:H3A	1.93	0.40
23:A:842:CLA:H101	23:A:842:CLA:H62	1.88	0.40
2:B:44:TYR:HE1	2:B:331:LEU:HD11	1.86	0.40
2:B:543:ARG:NH2	4:D:231:ASN:OD1	2.54	0.40
23:B:837:CLA:HMC2	23:B:837:CLA:H121	2.03	0.40
16:5:182:PRO:HD3	23:5:608:CLA:HMD2	2.02	0.40
18:7:114:ASN:O	19:8:259:HIS:NE2	2.50	0.40
23:7:602:CLA:H71	23:7:603:CLA:HMA1	2.02	0.40
23:B:808:CLA:O1A	23:B:827:CLA:HBD	2.21	0.40
23:B:811:CLA:H61	23:B:811:CLA:H41	1.66	0.40
23:B:832:CLA:H142	26:F:305:BCR:H23C	2.02	0.40
4:D:213:ASN:HB2	4:D:216:ARG:HH11	1.86	0.40
13:1:77:TYR:HH	13:1:199:LYS:HZ3	1.59	0.40
13:1:87:GLU:HA	13:1:88:PRO:HD3	1.94	0.40
13:1:99:VAL:HG22	13:1:198:ILE:HD11	2.04	0.40
23:3:603:CLA:H72	23:3:603:CLA:HED3	2.03	0.40
26:3:622:BCR:H24C	26:3:622:BCR:H371	1.89	0.40
26:4:621:BCR:H341	26:4:621:BCR:H11C	1.79	0.40
16:5:118:TYR:CD1	23:5:607:CLA:HMA2	2.56	0.40
16:5:181:TYR:HB3	23:5:610:CLA:HED2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:6:602:CLA:H192	23:6:602:CLA:H162	1.88	0.40
18:7:117:PHE:HE1	23:7:607:CLA:HHD	1.87	0.40
21:9:160:LYS:CB	23:9:611:CLA:CAD	3.00	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	708 (96%)	31 (4%)	0	100	100
2	B	729/735 (99%)	694 (95%)	35 (5%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	142/247 (58%)	131 (92%)	11 (8%)	0	100	100
5	E	62/143 (43%)	56 (90%)	6 (10%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	G	66/159 (42%)	59 (89%)	7 (11%)	0	100	100
8	H	49/155 (32%)	41 (84%)	8 (16%)	0	100	100
9	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	83/160 (52%)	74 (89%)	9 (11%)	0	100	100
12	L	102/258 (40%)	94 (92%)	8 (8%)	0	100	100
13	1	191/248 (77%)	177 (93%)	14 (7%)	0	100	100
13	a	192/248 (77%)	177 (92%)	15 (8%)	0	100	100
14	3	219/298 (74%)	199 (91%)	20 (9%)	0	100	100
15	4	208/290 (72%)	195 (94%)	13 (6%)	0	100	100
16	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	6	228/318 (72%)	209 (92%)	19 (8%)	0	100	100
18	7	211/241 (88%)	192 (91%)	19 (9%)	0	100	100
19	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
20	2	171/227 (75%)	145 (85%)	26 (15%)	0	100	100
21	9	168/213 (79%)	143 (85%)	23 (14%)	2 (1%)	11	38
22	X	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
All	All	4330/5718 (76%)	3999 (92%)	329 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	9	184	ILE
21	9	183	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	600 (100%)	1 (0%)	92	95
2	B	595/597 (100%)	588 (99%)	7 (1%)	67	80
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/197 (61%)	119 (99%)	1 (1%)	79	87
5	E	55/123 (45%)	54 (98%)	1 (2%)	54	74
6	F	126/169 (75%)	125 (99%)	1 (1%)	79	87
7	G	50/121 (41%)	50 (100%)	0	100	100
8	H	36/126 (29%)	35 (97%)	1 (3%)	38	64
9	I	26/76 (34%)	26 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/123 (48%)	58 (98%)	1 (2%)	56	74
12	L	75/198 (38%)	74 (99%)	1 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1	136/180 (76%)	136 (100%)	0	100	100
13	a	137/180 (76%)	137 (100%)	0	100	100
14	3	167/230 (73%)	165 (99%)	2 (1%)	67	80
15	4	165/226 (73%)	164 (99%)	1 (1%)	84	90
16	5	183/219 (84%)	181 (99%)	2 (1%)	70	82
17	6	184/260 (71%)	184 (100%)	0	100	100
18	7	164/181 (91%)	161 (98%)	3 (2%)	54	74
19	8	161/207 (78%)	159 (99%)	2 (1%)	67	80
20	2	134/183 (73%)	132 (98%)	2 (2%)	60	77
21	9	127/159 (80%)	124 (98%)	3 (2%)	44	68
All	All	3407/4472 (76%)	3378 (99%)	29 (1%)	74	85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	442	ASN
2	B	107	ARG
2	B	177	ASN
2	B	577	PHE
2	B	578	TYR
2	B	609	GLN
2	B	622	ARG
2	B	669	ARG
4	D	213	ASN
5	E	123	ASN
6	F	117	ASN
8	H	105	ARG
11	K	82	ASN
12	L	169	ARG
14	3	218	ILE
14	3	256	ASN
15	4	203	ASP
16	5	75	LEU
16	5	134	ASN
18	7	30	ARG
18	7	177	ARG
18	7	207	GLN
19	8	56	ARG

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Mol	Chain	Res	Type
19	8	99	GLN
20	2	9	ARG
20	2	155	GLN
21	9	131	LYS
21	9	149	MET
21	9	184	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	HIS
1	A	659	GLN
1	A	714	GLN
2	B	15	GLN
2	B	42	ASN
2	B	115	ASN
2	B	177	ASN
2	B	236	GLN
2	B	295	ASN
2	B	303	GLN
2	B	362	GLN
2	B	369	GLN
5	E	101	GLN
5	E	123	ASN
6	F	132	HIS
6	F	198	GLN
10	J	30	ASN
14	3	164	GLN
15	4	284	GLN
16	5	108	GLN
17	6	201	GLN
17	6	288	GLN
19	8	105	HIS
20	2	178	ASN
21	9	49	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

333 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	$\# Z  > 2$
23	CLA	B	818	-	60,68,73	1.49	10 (16%)	70,107,113	1.59	10 (14%)
29	LMG	A	860	-	40,40,55	0.95	3 (7%)	48,48,63	1.32	5 (10%)
23	CLA	5	606	-	39,48,73	1.88	10 (25%)	44,83,113	1.60	7 (15%)
31	LUT	8	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.82	14 (27%)
23	CLA	2	601	20	29,35,73	2.72	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	K	201	11	45,53,73	1.77	7 (15%)	52,89,113	1.79	10 (19%)
23	CLA	a	610	13	59,67,73	1.57	9 (15%)	69,106,113	1.42	7 (10%)
23	CLA	6	601	17	65,73,73	1.42	9 (13%)	76,113,113	1.52	9 (11%)
32	XAT	a	618	-	39,47,47	0.94	2 (5%)	54,74,74	2.57	18 (33%)
23	CLA	6	617	-	45,53,73	1.73	9 (20%)	52,89,113	1.49	7 (13%)
23	CLA	5	614	-	45,52,73	1.86	8 (17%)	48,87,113	1.65	7 (14%)
23	CLA	a	602	13	61,69,73	1.47	8 (13%)	71,108,113	1.51	7 (9%)
23	CLA	5	616	16	41,50,73	1.89	9 (21%)	50,85,113	1.61	9 (18%)
23	CLA	a	616	13	45,53,73	1.76	9 (20%)	52,89,113	1.56	6 (11%)
23	CLA	7	609	18	43,52,73	1.71	7 (16%)	48,87,113	1.87	6 (12%)
23	CLA	7	610	18	65,73,73	1.44	10 (15%)	76,113,113	1.43	8 (10%)
23	CLA	A	809	1	65,73,73	1.43	10 (15%)	76,113,113	1.50	8 (10%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LMU	8	625	-	36,36,36	1.16	2 (5%)	47,47,47	1.41	7 (14%)
26	BCR	F	305	-	41,41,41	0.83	1 (2%)	56,56,56	2.26	23 (41%)
28	LMU	A	857	-	36,36,36	1.20	3 (8%)	47,47,47	1.33	4 (8%)
23	CLA	6	613	-	63,72,73	1.45	10 (15%)	73,112,113	1.43	9 (12%)
26	BCR	A	851	-	41,41,41	0.88	2 (4%)	56,56,56	1.97	16 (28%)
29	LMG	5	626	-	40,40,55	0.94	1 (2%)	48,48,63	1.33	5 (10%)
25	LHG	1	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	7	616	18	43,51,73	1.80	9 (20%)	54,87,113	1.70	10 (18%)
23	CLA	a	613	-	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	8	610	19	60,68,73	1.41	8 (13%)	70,107,113	1.53	8 (11%)
25	LHG	3	623	-	44,44,48	0.66	2 (4%)	47,50,54	1.26	6 (12%)
23	CLA	L	303	-	45,53,73	1.71	8 (17%)	52,89,113	1.67	6 (11%)
23	CLA	a	601	13	53,62,73	1.60	9 (16%)	61,100,113	1.48	7 (11%)
23	CLA	5	610	16	54,62,73	1.59	10 (18%)	62,99,113	1.57	9 (14%)
23	CLA	4	609	15	61,69,73	1.57	7 (11%)	71,108,113	1.49	7 (9%)
26	BCR	B	848	-	41,41,41	0.87	0	56,56,56	1.79	12 (21%)
28	LMU	5	628	-	34,34,36	1.24	3 (8%)	45,45,47	1.50	8 (17%)
23	CLA	B	810	-	64,72,73	1.44	10 (15%)	74,111,113	1.41	8 (10%)
26	BCR	A	849	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	17 (30%)
26	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.10	22 (39%)
31	LUT	a	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	2	614	-	29,35,73	2.64	9 (31%)	28,60,113	1.72	5 (17%)
23	CLA	3	602	14	60,68,73	1.47	10 (16%)	70,107,113	1.48	8 (11%)
23	CLA	4	616	15	43,51,73	1.84	9 (20%)	54,87,113	1.66	9 (16%)
23	CLA	7	614	-	42,50,73	1.71	10 (23%)	48,85,113	1.65	8 (16%)
23	CLA	A	843	-	64,72,73	1.50	11 (17%)	74,111,113	1.46	7 (9%)
23	CLA	8	612	19	40,49,73	1.78	8 (20%)	45,84,113	1.82	8 (17%)
28	LMU	K	208	-	36,36,36	1.19	3 (8%)	47,47,47	1.30	5 (10%)
23	CLA	G	203	-	42,50,73	1.82	6 (14%)	48,85,113	1.74	7 (14%)
23	CLA	8	608	-	51,59,73	1.60	10 (19%)	59,96,113	1.62	7 (11%)
23	CLA	2	616	-	29,35,73	2.65	9 (31%)	28,60,113	1.78	6 (21%)
23	CLA	5	601	16	56,64,73	1.55	8 (14%)	65,102,113	1.42	8 (12%)
26	BCR	B	847	-	41,41,41	0.89	1 (2%)	56,56,56	2.01	19 (33%)
26	BCR	5	622	-	41,41,41	0.71	0	56,56,56	2.17	19 (33%)
30	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.48	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	XAT	4	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	20 (37%)
23	CLA	B	831	-	65,73,73	1.38	7 (10%)	76,113,113	1.61	6 (7%)
23	CLA	9	606	21	29,35,73	2.74	8 (27%)	28,60,113	1.68	4 (14%)
23	CLA	8	603	-	44,52,73	1.87	9 (20%)	55,88,113	1.65	12 (21%)
23	CLA	2	607	-	29,35,73	2.63	9 (31%)	28,60,113	1.72	4 (14%)
23	CLA	B	819	-	55,63,73	1.63	9 (16%)	64,101,113	1.51	6 (9%)
23	CLA	B	813	-	65,73,73	1.43	9 (13%)	76,113,113	1.46	10 (13%)
23	CLA	3	603	-	55,63,73	1.60	12 (21%)	64,101,113	1.71	10 (15%)
23	CLA	4	614	-	56,64,73	1.59	8 (14%)	65,102,113	1.46	9 (13%)
23	CLA	9	610	21	29,35,73	2.63	10 (34%)	28,60,113	1.70	5 (17%)
23	CLA	A	839	-	55,63,73	1.61	9 (16%)	64,101,113	1.50	7 (10%)
23	CLA	A	831	-	65,73,73	1.56	11 (16%)	76,113,113	1.70	12 (15%)
23	CLA	8	604	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
23	CLA	A	822	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	8 (10%)
23	CLA	5	607	-	65,73,73	1.47	10 (15%)	76,113,113	1.58	8 (10%)
23	CLA	8	611	25	42,50,73	1.72	9 (21%)	48,85,113	1.69	9 (18%)
26	BCR	L	305	-	41,41,41	0.80	0	56,56,56	1.88	14 (25%)
23	CLA	5	603	-	54,62,73	1.70	10 (18%)	67,100,113	1.59	10 (14%)
23	CLA	A	825	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	11 (14%)
25	LHG	A	847	23	29,29,48	0.95	1 (3%)	32,35,54	1.37	3 (9%)
23	CLA	B	824	-	65,73,73	1.46	7 (10%)	76,113,113	1.61	11 (14%)
23	CLA	9	609	21	29,35,73	2.62	8 (27%)	28,60,113	1.76	4 (14%)
23	CLA	B	816	-	54,62,73	1.55	7 (12%)	62,99,113	1.65	6 (9%)
26	BCR	B	801	-	41,41,41	0.77	0	56,56,56	2.05	13 (23%)
25	LHG	B	851	23	37,37,48	0.63	0	40,43,54	1.22	4 (10%)
23	CLA	A	837	1	45,53,73	1.76	9 (20%)	52,89,113	1.65	7 (13%)
23	CLA	a	612	13	45,53,73	1.73	8 (17%)	52,89,113	1.69	9 (17%)
23	CLA	B	841	25	43,51,73	1.83	7 (16%)	49,86,113	1.72	7 (14%)
23	CLA	a	608	-	43,52,73	1.77	6 (13%)	49,88,113	1.66	7 (14%)
26	BCR	a	619	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
23	CLA	6	610	17	65,73,73	1.40	7 (10%)	76,113,113	1.45	9 (11%)
26	BCR	B	844	-	41,41,41	0.79	1 (2%)	56,56,56	1.95	15 (26%)
23	CLA	9	611	25	29,35,73	2.73	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	7	606	-	41,49,73	1.81	10 (24%)	47,84,113	1.74	9 (19%)
24	PQN	B	842	-	34,34,34	2.91	11 (32%)	42,45,45	2.04	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	3	609	14	60,68,73	1.53	7 (11%)	70,107,113	1.55	9 (12%)
23	CLA	A	854	-	65,73,73	1.42	9 (13%)	76,113,113	1.56	13 (17%)
23	CLA	B	838	-	47,55,73	1.63	10 (21%)	54,91,113	1.80	8 (14%)
23	CLA	2	610	20	29,35,73	2.61	8 (27%)	28,60,113	1.79	5 (17%)
25	LHG	A	846	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	6 (11%)
24	PQN	A	844	-	34,34,34	2.89	11 (32%)	42,45,45	2.11	5 (11%)
23	CLA	B	834	-	60,68,73	1.51	8 (13%)	70,107,113	1.47	8 (11%)
23	CLA	A	806	-	65,73,73	1.47	13 (20%)	76,113,113	1.69	12 (15%)
26	BCR	J	102	-	41,41,41	0.84	1 (2%)	56,56,56	2.15	16 (28%)
23	CLA	7	603	-	43,52,73	1.79	9 (20%)	49,88,113	1.66	8 (16%)
23	CLA	5	617	-	50,58,73	1.67	10 (20%)	58,95,113	1.58	8 (13%)
23	CLA	8	609	19	45,53,73	1.68	8 (17%)	52,89,113	1.74	8 (15%)
23	CLA	9	614	-	29,35,73	2.65	9 (31%)	28,60,113	1.76	5 (17%)
23	CLA	5	609	16	65,73,73	1.47	10 (15%)	76,113,113	1.38	10 (13%)
23	CLA	A	805	-	52,60,73	1.66	10 (19%)	60,97,113	1.66	7 (11%)
23	CLA	1	601	13	53,62,73	1.60	10 (18%)	61,100,113	1.47	7 (11%)
26	BCR	8	621	-	41,41,41	0.74	0	56,56,56	1.98	18 (32%)
23	CLA	5	608	-	50,58,73	1.66	11 (22%)	58,95,113	1.54	7 (12%)
23	CLA	1	612	13	45,53,73	1.73	8 (17%)	52,89,113	1.69	9 (17%)
26	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.86	16 (28%)
25	LHG	8	622	23	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
23	CLA	3	615	-	39,48,73	1.81	8 (20%)	44,83,113	1.72	7 (15%)
23	CLA	4	607	-	45,53,73	1.77	9 (20%)	52,89,113	1.60	6 (11%)
23	CLA	4	603	15	44,52,73	1.83	9 (20%)	55,88,113	1.69	10 (18%)
23	CLA	K	206	11	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
25	LHG	4	622	23	48,48,48	0.60	0	51,54,54	1.29	6 (11%)
23	CLA	6	604	-	65,73,73	1.42	10 (15%)	76,113,113	1.42	8 (10%)
32	XAT	3	619	-	39,47,47	1.02	2 (5%)	54,74,74	2.60	22 (40%)
23	CLA	B	833	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
26	BCR	A	850	-	41,41,41	0.82	1 (2%)	56,56,56	2.02	18 (32%)
23	CLA	a	604	-	49,57,73	1.67	7 (14%)	55,93,113	1.67	6 (10%)
23	CLA	A	833	-	45,53,73	1.72	9 (20%)	52,89,113	1.73	6 (11%)
23	CLA	6	611	25	42,50,73	1.72	8 (19%)	48,85,113	1.62	7 (14%)
23	CLA	A	803	-	65,73,73	1.52	10 (15%)	76,113,113	1.54	6 (7%)
23	CLA	8	614	-	56,64,73	1.54	9 (16%)	65,102,113	1.53	10 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	A	824	-	41,49,73	1.75	8 (19%)	47,84,113	1.77	9 (19%)
27	SF4	A	853	-	0,12,12	-	-	-		
23	CLA	G	204	7	45,53,73	1.83	5 (11%)	52,89,113	1.78	12 (23%)
23	CLA	B	822	-	42,50,73	1.81	7 (16%)	48,85,113	1.66	7 (14%)
26	BCR	B	845	-	41,41,41	0.84	0	56,56,56	2.06	19 (33%)
23	CLA	7	601	18	60,68,73	1.53	11 (18%)	70,107,113	1.51	9 (12%)
23	CLA	4	610	15	61,69,73	1.47	9 (14%)	71,108,113	1.44	7 (9%)
23	CLA	A	807	1	65,73,73	1.49	10 (15%)	76,113,113	1.42	9 (11%)
23	CLA	6	606	-	39,48,73	1.84	8 (20%)	44,83,113	1.72	7 (15%)
31	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	11 (21%)
23	CLA	B	835	-	45,53,73	1.79	8 (17%)	52,89,113	1.74	11 (21%)
31	LUT	6	619	-	42,43,43	0.81	0	51,60,60	1.69	13 (25%)
23	CLA	1	614	-	37,45,73	2.12	10 (27%)	44,79,113	1.80	8 (18%)
23	CLA	5	604	-	63,71,73	1.54	9 (14%)	78,111,113	1.45	9 (11%)
26	BCR	K	202	-	41,41,41	0.79	0	56,56,56	2.26	20 (35%)
23	CLA	2	613	20	29,35,73	2.70	9 (31%)	28,60,113	1.66	5 (17%)
23	CLA	7	607	-	42,50,73	1.78	8 (19%)	48,85,113	1.86	9 (18%)
23	CLA	B	840	-	65,73,73	1.48	10 (15%)	76,113,113	1.46	7 (9%)
31	LUT	3	618	-	42,43,43	0.88	0	51,60,60	1.73	13 (25%)
25	LHG	7	622	23	36,36,48	0.70	0	39,42,54	1.23	4 (10%)
23	CLA	4	608	-	65,73,73	1.42	7 (10%)	76,113,113	1.56	8 (10%)
26	BCR	G	205	-	41,41,41	0.75	0	56,56,56	2.06	21 (37%)
23	CLA	1	608	-	43,52,73	1.77	5 (11%)	49,88,113	1.67	7 (14%)
23	CLA	2	609	20	29,35,73	2.76	9 (31%)	28,60,113	1.75	6 (21%)
25	LHG	6	623	23	47,47,48	0.64	1 (2%)	50,53,54	1.24	5 (10%)
23	CLA	B	809	2	65,73,73	1.43	11 (16%)	76,113,113	1.55	7 (9%)
23	CLA	6	608	-	51,59,73	1.67	11 (21%)	59,96,113	1.65	9 (15%)
23	CLA	a	614	-	55,62,73	1.72	9 (16%)	60,99,113	1.47	7 (11%)
23	CLA	B	829	-	65,73,73	1.55	10 (15%)	76,113,113	1.69	10 (13%)
23	CLA	A	830	-	65,73,73	1.46	11 (16%)	76,113,113	1.59	11 (14%)
23	CLA	B	806	2	65,73,73	1.47	11 (16%)	76,113,113	1.39	6 (7%)
23	CLA	3	606	-	53,62,73	1.62	9 (16%)	61,100,113	1.45	7 (11%)
28	LMU	A	859	-	35,35,36	1.33	3 (8%)	43,45,47	1.27	6 (13%)
23	CLA	6	603	-	54,62,73	1.67	9 (16%)	67,100,113	1.54	8 (11%)
23	CLA	2	606	20	29,35,73	2.72	8 (27%)	28,60,113	1.61	3 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.80	13 (17%)
23	CLA	4	604	-	54,62,73	1.63	9 (16%)	67,100,113	1.46	7 (10%)
23	CLA	B	805	-	65,73,73	1.42	8 (12%)	76,113,113	1.66	9 (11%)
25	LHG	5	625	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
32	XAT	6	621	-	39,47,47	0.93	2 (5%)	54,74,74	2.61	20 (37%)
23	CLA	4	613	15	65,73,73	1.45	10 (15%)	76,113,113	1.45	7 (9%)
23	CLA	A	811	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	10 (13%)
23	CLA	B	836	-	50,58,73	1.61	8 (16%)	58,95,113	1.73	11 (18%)
23	CLA	5	611	25	42,50,73	1.76	9 (21%)	48,85,113	1.62	8 (16%)
23	CLA	4	611	25	42,50,73	1.76	7 (16%)	48,85,113	1.64	7 (14%)
23	CLA	A	812	-	65,73,73	1.44	10 (15%)	76,113,113	1.52	10 (13%)
23	CLA	A	817	-	45,53,73	1.73	9 (20%)	52,89,113	1.75	9 (17%)
23	CLA	A	804	-	65,73,73	1.40	9 (13%)	76,113,113	1.62	11 (14%)
23	CLA	9	601	21	29,35,73	2.64	9 (31%)	28,60,113	1.68	4 (14%)
26	BCR	A	852	-	41,41,41	0.73	0	56,56,56	1.90	12 (21%)
23	CLA	A	838	-	50,58,73	1.56	8 (16%)	58,95,113	1.77	12 (20%)
23	CLA	A	829	-	65,73,73	1.42	10 (15%)	76,113,113	1.55	9 (11%)
28	LMU	8	624	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
23	CLA	A	823	-	42,50,73	1.77	9 (21%)	48,85,113	1.84	9 (18%)
23	CLA	3	610	14	65,73,73	1.41	9 (13%)	76,113,113	1.57	10 (13%)
23	CLA	6	602	17	65,73,73	1.43	9 (13%)	76,113,113	1.46	6 (7%)
23	CLA	1	610	13	38,47,73	1.90	9 (23%)	44,81,113	1.76	8 (18%)
23	CLA	A	832	-	50,58,73	1.65	11 (22%)	58,95,113	1.66	9 (15%)
23	CLA	B	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.34	7 (9%)
23	CLA	1	604	-	49,57,73	1.68	7 (14%)	55,93,113	1.67	6 (10%)
32	XAT	5	621	-	39,47,47	1.02	2 (5%)	54,74,74	2.89	23 (42%)
31	LUT	2	619	-	42,43,43	0.75	0	51,60,60	1.77	13 (25%)
23	CLA	A	808	-	50,58,73	1.63	10 (20%)	58,95,113	1.65	9 (15%)
23	CLA	A	821	-	53,61,73	1.57	10 (18%)	61,98,113	1.61	7 (11%)
23	CLA	B	823	-	45,53,73	1.73	7 (15%)	52,89,113	1.76	8 (15%)
23	CLA	B	817	-	59,67,73	1.54	10 (16%)	68,105,113	1.57	9 (13%)
23	CLA	A	828	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	8 (10%)
23	CLA	8	602	19	60,68,73	1.52	9 (15%)	70,107,113	1.58	10 (14%)
23	CLA	B	839	-	65,73,73	1.44	10 (15%)	76,113,113	1.51	9 (11%)
30	DGD	B	850	-	63,63,67	1.06	5 (7%)	77,77,81	1.55	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	XAT	7	620	-	39,47,47	1.04	2 (5%)	54,74,74	2.59	18 (33%)
23	CLA	a	606	13	43,52,73	1.78	7 (16%)	48,87,113	1.60	6 (12%)
23	CLA	6	616	17	65,73,73	1.42	7 (10%)	76,113,113	1.68	13 (17%)
23	CLA	F	301	-	57,65,73	1.57	10 (17%)	66,103,113	1.44	5 (7%)
33	NEX	6	624	-	38,46,46	1.01	2 (5%)	50,70,70	2.27	17 (34%)
32	XAT	1	618	-	39,47,47	0.93	2 (5%)	54,74,74	2.58	18 (33%)
23	CLA	A	802	-	65,73,73	1.48	10 (15%)	76,113,113	1.71	10 (13%)
28	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.28	6 (14%)
26	BCR	7	623	-	41,41,41	0.68	0	56,56,56	1.81	13 (23%)
26	BCR	B	846	-	41,41,41	0.88	2 (4%)	56,56,56	2.17	25 (44%)
23	CLA	B	811	-	52,61,73	1.67	9 (17%)	64,99,113	1.56	10 (15%)
29	LMG	4	623	-	40,40,55	0.90	1 (2%)	48,48,63	1.28	5 (10%)
23	CLA	8	601	19	65,73,73	1.44	9 (13%)	76,113,113	1.52	10 (13%)
26	BCR	3	621	-	41,41,41	0.72	0	56,56,56	2.28	19 (33%)
23	CLA	A	826	-	64,72,73	1.43	8 (12%)	74,111,113	1.58	10 (13%)
23	CLA	8	606	-	64,72,73	1.45	9 (14%)	75,112,113	1.48	8 (10%)
23	CLA	2	603	20	29,35,73	2.70	9 (31%)	28,60,113	1.77	6 (21%)
32	XAT	2	620	-	39,47,47	0.89	0	54,74,74	2.65	14 (25%)
23	CLA	F	303	-	42,50,73	1.83	8 (19%)	48,85,113	1.71	10 (20%)
23	CLA	B	828	-	65,73,73	1.48	10 (15%)	76,113,113	1.48	9 (11%)
23	CLA	9	602	21	29,35,73	2.64	9 (31%)	28,60,113	1.76	4 (14%)
23	CLA	B	825	-	62,70,73	1.42	10 (16%)	72,109,113	1.46	11 (15%)
23	CLA	A	845	25	50,58,73	1.63	10 (20%)	58,95,113	1.67	7 (12%)
23	CLA	1	609	13	40,48,73	1.83	7 (17%)	50,83,113	1.84	12 (24%)
26	BCR	1	619	-	41,41,41	0.68	0	56,56,56	2.01	16 (28%)
23	CLA	B	804	-	41,49,73	1.81	10 (24%)	47,84,113	1.85	8 (17%)
31	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	A	816	-	43,52,73	1.76	7 (16%)	48,87,113	1.82	6 (12%)
23	CLA	A	814	-	65,73,73	1.44	10 (15%)	76,113,113	1.56	12 (15%)
23	CLA	2	602	20	29,35,73	2.65	9 (31%)	28,60,113	1.69	3 (10%)
26	BCR	6	622	-	41,41,41	0.69	0	56,56,56	1.94	17 (30%)
23	CLA	1	616	13	43,51,73	1.85	9 (20%)	54,87,113	1.61	8 (14%)
25	LHG	8	623	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
23	CLA	1	606	13	37,47,73	1.90	6 (16%)	41,80,113	1.77	7 (17%)
23	CLA	4	618	15	39,48,73	1.93	9 (23%)	48,83,113	1.67	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	7	602	18	65,73,73	1.48	9 (13%)	76,113,113	1.40	7 (9%)
32	XAT	9	620	-	39,47,47	0.92	0	54,74,74	2.63	16 (29%)
23	CLA	7	613	18	65,73,73	1.46	9 (13%)	76,113,113	1.42	8 (10%)
23	CLA	1	613	-	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	B	821	-	43,51,73	1.86	9 (20%)	48,86,113	1.78	9 (18%)
29	LMG	J	104	-	40,40,55	0.89	2 (5%)	48,48,63	1.26	5 (10%)
33	NEX	5	624	-	38,46,46	0.93	0	50,70,70	2.49	19 (38%)
23	CLA	3	608	-	55,63,73	1.62	10 (18%)	64,101,113	1.62	9 (14%)
23	CLA	F	304	-	41,49,73	1.78	7 (17%)	47,84,113	1.78	7 (14%)
23	CLA	A	841	-	65,73,73	1.42	10 (15%)	76,113,113	1.57	9 (11%)
23	CLA	4	602	15	60,68,73	1.46	7 (11%)	70,107,113	1.62	8 (11%)
23	CLA	A	835	-	61,69,73	1.51	10 (16%)	71,108,113	1.57	8 (11%)
23	CLA	1	602	13	61,69,73	1.46	8 (13%)	71,108,113	1.51	7 (9%)
23	CLA	A	827	-	59,67,73	1.51	8 (13%)	68,105,113	1.59	10 (14%)
23	CLA	B	837	-	65,73,73	1.48	10 (15%)	76,113,113	1.46	7 (9%)
23	CLA	a	611	25	37,46,73	1.88	9 (24%)	46,81,113	1.87	10 (21%)
23	CLA	3	613	14	52,61,73	1.61	9 (17%)	59,98,113	1.55	7 (11%)
23	CLA	6	612	17	40,49,73	1.83	7 (17%)	45,84,113	1.78	9 (20%)
29	LMG	5	627	-	40,40,55	0.91	2 (5%)	48,48,63	1.20	4 (8%)
26	BCR	A	848	-	41,41,41	0.92	1 (2%)	56,56,56	2.07	17 (30%)
23	CLA	3	612	14	43,51,73	1.83	9 (20%)	49,86,113	1.65	8 (16%)
23	CLA	3	614	-	39,48,73	1.85	9 (23%)	44,83,113	1.66	8 (18%)
25	LHG	a	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	5	619	-	43,51,73	1.81	10 (23%)	54,87,113	2.04	12 (22%)
23	CLA	B	814	-	64,72,73	1.43	9 (14%)	74,111,113	1.52	8 (10%)
23	CLA	a	609	13	63,72,73	1.45	7 (11%)	73,112,113	1.39	8 (10%)
23	CLA	L	302	12	45,53,73	1.79	5 (11%)	52,89,113	1.67	8 (15%)
23	CLA	A	819	-	59,67,73	1.57	10 (16%)	68,105,113	1.52	8 (11%)
32	XAT	8	620	-	39,47,47	1.00	2 (5%)	54,74,74	2.70	19 (35%)
23	CLA	9	613	21	29,35,73	2.70	8 (27%)	28,60,113	1.72	4 (14%)
23	CLA	7	615	-	41,50,73	1.90	7 (17%)	50,85,113	1.76	9 (18%)
23	CLA	9	604	-	29,35,73	2.63	9 (31%)	28,60,113	1.73	5 (17%)
23	CLA	A	810	1	50,58,73	1.63	10 (20%)	58,95,113	1.58	7 (12%)
23	CLA	K	204	-	46,54,73	1.72	7 (15%)	53,90,113	1.60	8 (15%)
23	CLA	3	607	14	56,64,73	1.58	9 (16%)	69,102,113	1.54	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	A	820	-	65,73,73	1.52	11 (16%)	76,113,113	1.68	15 (19%)
25	LHG	2	622	23	36,36,48	0.78	1 (2%)	39,42,54	1.29	5 (12%)
23	CLA	B	807	-	52,60,73	1.61	10 (19%)	60,97,113	1.53	7 (11%)
23	CLA	3	604	-	65,73,73	1.47	10 (15%)	76,113,113	1.44	7 (9%)
23	CLA	6	618	17	39,48,73	1.89	9 (23%)	48,83,113	1.75	10 (20%)
25	LHG	3	624	23	48,48,48	0.66	0	51,54,54	1.24	5 (9%)
23	CLA	5	612	16	40,49,73	1.77	8 (20%)	45,84,113	1.81	8 (17%)
23	CLA	B	830	-	43,51,73	1.78	11 (25%)	49,86,113	1.71	6 (12%)
23	CLA	B	827	-	62,70,73	1.48	8 (12%)	72,109,113	1.51	8 (11%)
23	CLA	7	608	-	50,58,73	1.63	10 (20%)	58,95,113	1.53	7 (12%)
23	CLA	2	612	20	29,35,73	2.72	8 (27%)	28,60,113	1.68	3 (10%)
23	CLA	B	826	-	55,63,73	1.58	8 (14%)	64,101,113	1.56	8 (12%)
23	CLA	A	818	-	60,68,73	1.45	8 (13%)	70,107,113	1.60	7 (10%)
23	CLA	a	607	-	45,53,73	1.74	7 (15%)	52,89,113	1.64	7 (13%)
23	CLA	J	101	10	42,50,73	1.80	7 (16%)	48,85,113	1.71	8 (16%)
25	LHG	5	623	23	48,48,48	0.62	1 (2%)	51,54,54	1.21	5 (9%)
23	CLA	A	842	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
23	CLA	K	203	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	7 (9%)
26	BCR	A	856	-	41,41,41	0.70	0	56,56,56	1.99	19 (33%)
31	LUT	7	619	-	42,43,43	0.95	2 (4%)	51,60,60	1.79	16 (31%)
23	CLA	4	601	15	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
23	CLA	1	603	-	52,61,73	1.63	9 (17%)	59,98,113	1.68	9 (15%)
23	CLA	6	609	17	45,53,73	1.78	9 (20%)	52,89,113	1.69	8 (15%)
23	CLA	9	612	21	29,35,73	2.71	9 (31%)	28,60,113	1.67	4 (14%)
23	CLA	A	815	-	50,58,73	1.64	9 (18%)	58,95,113	1.69	11 (18%)
23	CLA	5	602	16	65,73,73	1.44	7 (10%)	76,113,113	1.57	8 (10%)
23	CLA	7	612	18	44,52,73	1.83	9 (20%)	51,88,113	1.63	9 (17%)
29	LMG	7	624	-	44,44,55	0.83	1 (2%)	52,52,63	1.26	6 (11%)
23	CLA	1	611	25	65,73,73	1.40	9 (13%)	76,113,113	1.45	8 (10%)
23	CLA	3	617	14	39,48,73	1.86	9 (23%)	44,83,113	1.78	8 (18%)
23	CLA	9	607	-	29,35,73	2.60	9 (31%)	28,60,113	1.79	6 (21%)
23	CLA	A	840	-	52,60,73	1.62	10 (19%)	60,97,113	1.69	10 (16%)
27	SF4	C	102	-	0,12,12	-	-	-	-	-
23	CLA	9	603	21	29,35,73	2.66	9 (31%)	28,60,113	1.63	4 (14%)
23	CLA	L	304	-	45,53,73	1.76	5 (11%)	52,89,113	1.66	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	LHG	9	622	23	48,48,48	0.62	0	51,54,54	1.23	6 (11%)
23	CLA	5	618	16	39,48,73	1.91	8 (20%)	48,83,113	1.74	9 (18%)
23	CLA	6	607	-	41,49,73	1.84	9 (21%)	51,84,113	1.78	12 (23%)
31	LUT	5	620	-	42,43,43	0.80	0	51,60,60	1.70	13 (25%)
23	CLA	A	834	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	7 (9%)
26	BCR	L	301	-	41,41,41	0.84	0	56,56,56	1.78	16 (28%)
23	CLA	7	604	-	54,62,73	1.56	8 (14%)	63,100,113	1.66	10 (15%)
23	CLA	6	620	-	64,72,73	1.43	10 (15%)	74,111,113	1.49	7 (9%)
23	CLA	4	612	15	40,49,73	1.80	7 (17%)	45,84,113	1.78	8 (17%)
23	CLA	2	611	25	30,33,73	3.40	10 (33%)	24,56,113	1.05	2 (8%)
29	LMG	4	624	-	40,40,55	1.01	4 (10%)	48,48,63	1.29	6 (12%)
23	CLA	A	801	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
23	CLA	8	607	-	41,49,73	1.83	9 (21%)	51,84,113	1.75	9 (17%)
23	CLA	A	836	-	65,73,73	1.44	10 (15%)	76,113,113	1.53	7 (9%)
26	BCR	3	622	-	41,41,41	0.79	0	56,56,56	2.67	21 (37%)
31	LUT	9	619	-	42,43,43	0.76	0	51,60,60	1.67	11 (21%)
23	CLA	8	616	19	43,51,73	1.89	7 (16%)	54,87,113	1.85	12 (22%)
23	CLA	B	832	-	60,68,73	1.48	10 (16%)	70,107,113	1.57	10 (14%)
23	CLA	6	614	-	60,68,73	1.50	7 (11%)	70,107,113	1.47	6 (8%)
23	CLA	B	820	-	50,58,73	1.62	7 (14%)	58,95,113	1.62	7 (12%)
23	CLA	4	606	-	39,48,73	1.84	8 (20%)	44,83,113	1.70	8 (18%)
23	CLA	8	613	19	65,73,73	1.48	9 (13%)	76,113,113	1.64	10 (13%)
23	CLA	B	812	-	43,51,73	1.78	7 (16%)	49,86,113	1.72	7 (14%)
23	CLA	5	613	16	64,72,73	1.56	9 (14%)	74,111,113	1.54	7 (9%)
26	BCR	3	620	-	41,41,41	0.83	0	56,56,56	2.17	20 (35%)
23	CLA	3	611	25	37,46,73	1.94	8 (21%)	46,81,113	1.82	10 (21%)
26	BCR	7	621	-	41,41,41	0.80	0	56,56,56	2.04	18 (32%)
23	CLA	1	607	-	39,48,73	1.85	7 (17%)	44,83,113	1.72	7 (15%)
23	CLA	A	813	-	54,62,73	1.55	9 (16%)	62,99,113	1.64	7 (11%)
23	CLA	a	603	-	42,50,73	1.77	9 (21%)	48,85,113	1.86	9 (18%)
23	CLA	B	808	-	65,73,73	1.46	10 (15%)	76,113,113	1.66	11 (14%)
23	CLA	2	604	-	29,35,73	2.68	8 (27%)	28,60,113	1.80	6 (21%)
26	BCR	B	843	-	41,41,41	0.79	0	56,56,56	1.92	14 (25%)
23	CLA	7	611	25	59,67,73	1.47	9 (15%)	68,105,113	1.56	8 (11%)
23	CLA	B	815	-	43,51,73	1.70	10 (23%)	49,86,113	1.74	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	818	-	1/1/14/20	14/31/109/115	-
29	LMG	A	860	-	-	18/35/55/70	0/1/1/1
23	CLA	5	606	-	1/1/10/20	2/6/84/115	-
31	LUT	8	619	-	-	2/29/67/67	0/2/2/2
23	CLA	2	601	20	1/1/5/20	-	-
23	CLA	K	201	11	1/1/11/20	6/13/91/115	-
23	CLA	a	610	13	1/1/14/20	5/29/107/115	-
23	CLA	6	601	17	1/1/15/20	14/37/115/115	-
32	XAT	a	618	-	-	1/31/93/93	0/4/4/4
23	CLA	6	617	-	1/1/11/20	7/13/91/115	-
23	CLA	5	614	-	1/1/10/20	7/13/87/115	-
23	CLA	a	602	13	1/1/14/20	6/33/111/115	-
23	CLA	5	616	16	1/1/10/20	4/8/84/115	-
23	CLA	a	616	13	1/1/11/20	4/13/91/115	-
23	CLA	7	609	18	1/1/10/20	4/10/88/115	-
23	CLA	7	610	18	1/1/15/20	6/37/115/115	-
23	CLA	A	809	1	1/1/15/20	12/37/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
28	LMU	8	625	-	-	10/21/61/61	0/2/2/2
26	BCR	F	305	-	-	2/29/63/63	0/2/2/2
28	LMU	A	857	-	-	11/21/61/61	0/2/2/2
23	CLA	6	613	-	1/1/15/20	13/35/113/115	-
26	BCR	A	851	-	-	4/29/63/63	0/2/2/2
29	LMG	5	626	-	-	23/35/55/70	0/1/1/1
25	LHG	1	620	23	-	24/53/53/53	-
23	CLA	7	616	18	1/1/11/20	7/11/87/115	-
23	CLA	a	613	-	1/1/15/20	12/37/115/115	-
23	CLA	8	610	19	1/1/14/20	7/31/109/115	-
25	LHG	3	623	-	-	26/49/49/53	-
23	CLA	L	303	-	1/1/11/20	5/13/91/115	-
23	CLA	a	601	13	1/1/13/20	5/23/101/115	-
23	CLA	5	610	16	1/1/12/20	5/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	4	609	15	1/1/14/20	13/33/111/115	-
26	BCR	B	848	-	-	4/29/63/63	0/2/2/2
28	LMU	5	628	-	-	11/19/59/61	0/2/2/2
23	CLA	B	810	-	1/1/14/20	15/35/113/115	-
26	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	BCR	4	621	-	-	1/29/63/63	0/2/2/2
31	LUT	a	617	-	-	2/29/67/67	0/2/2/2
23	CLA	2	614	-	1/1/5/20	-	-
23	CLA	3	602	14	1/1/14/20	8/31/109/115	-
23	CLA	4	616	15	1/1/11/20	6/11/87/115	-
23	CLA	7	614	-	1/1/10/20	3/10/88/115	-
23	CLA	A	843	-	1/1/14/20	16/35/113/115	-
23	CLA	8	612	19	1/1/10/20	2/8/86/115	-
28	LMU	K	208	-	-	10/21/61/61	0/2/2/2
23	CLA	G	203	-	1/1/10/20	3/10/88/115	-
23	CLA	8	608	-	1/1/12/20	4/21/99/115	-
23	CLA	2	616	-	1/1/5/20	-	-
23	CLA	5	601	16	1/1/13/20	6/27/105/115	-
26	BCR	B	847	-	-	1/29/63/63	0/2/2/2
26	BCR	5	622	-	-	3/29/63/63	0/2/2/2
30	DGD	J	103	-	-	25/47/87/95	0/2/2/2
32	XAT	4	620	-	-	1/31/93/93	0/4/4/4
23	CLA	B	831	-	1/1/15/20	12/37/115/115	-
23	CLA	9	606	21	1/1/5/20	-	-
23	CLA	8	603	-	1/1/11/20	8/13/89/115	-
23	CLA	2	607	-	1/1/5/20	-	-
23	CLA	B	819	-	1/1/13/20	11/25/103/115	-
23	CLA	B	813	-	1/1/15/20	20/37/115/115	-
23	CLA	3	603	-	1/1/13/20	11/25/103/115	-
23	CLA	4	614	-	1/1/13/20	7/27/105/115	-
23	CLA	9	610	21	1/1/5/20	-	-
23	CLA	A	839	-	1/1/13/20	5/25/103/115	-
23	CLA	A	831	-	1/1/15/20	14/37/115/115	-
23	CLA	8	604	-	1/1/12/20	5/19/97/115	-
23	CLA	A	822	-	1/1/15/20	13/37/115/115	-
23	CLA	5	607	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	8	611	25	1/1/10/20	4/10/88/115	-
26	BCR	L	305	-	-	10/29/63/63	0/2/2/2
23	CLA	5	603	-	1/1/13/20	10/25/101/115	-
23	CLA	A	825	-	1/1/15/20	18/37/115/115	-
25	LHG	A	847	23	-	11/34/34/53	-
23	CLA	B	824	-	1/1/15/20	9/37/115/115	-
23	CLA	9	609	21	1/1/5/20	-	-
23	CLA	B	816	-	1/1/12/20	10/23/101/115	-
26	BCR	B	801	-	-	4/29/63/63	0/2/2/2
25	LHG	B	851	23	-	22/42/42/53	-
23	CLA	A	837	1	1/1/11/20	7/13/91/115	-
23	CLA	a	612	13	1/1/11/20	6/13/91/115	-
23	CLA	B	841	25	1/1/10/20	1/11/89/115	-
23	CLA	a	608	-	1/1/11/20	4/11/89/115	-
26	BCR	a	619	-	-	4/29/63/63	0/2/2/2
23	CLA	6	610	17	1/1/15/20	10/37/115/115	-
26	BCR	B	844	-	-	9/29/63/63	0/2/2/2
23	CLA	9	611	25	1/1/5/20	-	-
23	CLA	7	606	-	1/1/10/20	2/8/86/115	-
24	PQN	B	842	-	-	7/23/43/43	0/2/2/2
23	CLA	3	609	14	1/1/14/20	16/31/109/115	-
23	CLA	A	854	-	1/1/15/20	13/37/115/115	-
23	CLA	B	838	-	1/1/11/20	5/16/94/115	-
23	CLA	2	610	20	1/1/5/20	-	-
25	LHG	A	846	-	-	25/53/53/53	-
24	PQN	A	844	-	-	8/23/43/43	0/2/2/2
23	CLA	B	834	-	1/1/14/20	13/31/109/115	-
23	CLA	A	806	-	1/1/15/20	15/37/115/115	-
26	BCR	J	102	-	-	5/29/63/63	0/2/2/2
23	CLA	7	603	-	1/1/11/20	2/11/89/115	-
23	CLA	5	617	-	1/1/12/20	6/19/97/115	-
23	CLA	8	609	19	1/1/11/20	4/13/91/115	-
23	CLA	9	614	-	1/1/5/20	-	-
23	CLA	5	609	16	1/1/15/20	13/37/115/115	-
23	CLA	A	805	-	1/1/12/20	5/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1	601	13	1/1/13/20	5/23/101/115	-
26	BCR	8	621	-	-	6/29/63/63	0/2/2/2
23	CLA	5	608	-	1/1/12/20	7/19/97/115	-
23	CLA	1	612	13	1/1/11/20	6/13/91/115	-
26	BCR	K	207	-	-	3/29/63/63	0/2/2/2
25	LHG	8	622	23	-	26/53/53/53	-
23	CLA	3	615	-	1/1/10/20	1/6/84/115	-
23	CLA	4	607	-	1/1/11/20	5/13/91/115	-
23	CLA	4	603	15	1/1/11/20	7/13/89/115	-
23	CLA	K	206	11	1/1/11/20	5/13/91/115	-
25	LHG	4	622	23	-	21/53/53/53	-
23	CLA	6	604	-	1/1/15/20	22/37/115/115	-
32	XAT	3	619	-	-	1/31/93/93	0/4/4/4
23	CLA	B	833	-	1/1/15/20	19/37/115/115	-
26	BCR	A	850	-	-	1/29/63/63	0/2/2/2
23	CLA	a	604	-	1/1/11/20	10/18/96/115	-
23	CLA	A	833	-	1/1/11/20	2/13/91/115	-
23	CLA	6	611	25	1/1/10/20	3/10/88/115	-
23	CLA	A	803	-	1/1/15/20	9/37/115/115	-
23	CLA	8	614	-	1/1/13/20	10/27/105/115	-
23	CLA	A	824	-	1/1/10/20	0/8/86/115	-
27	SF4	A	853	-	-	-	0/6/5/5
23	CLA	G	204	7	1/1/11/20	6/13/91/115	-
23	CLA	B	822	-	-	4/10/88/115	-
26	BCR	B	845	-	-	5/29/63/63	0/2/2/2
23	CLA	7	601	18	1/1/14/20	13/31/109/115	-
23	CLA	4	610	15	1/1/14/20	12/33/111/115	-
23	CLA	A	807	1	1/1/15/20	13/37/115/115	-
23	CLA	6	606	-	1/1/10/20	0/6/84/115	-
31	LUT	4	619	-	-	4/29/67/67	0/2/2/2
23	CLA	B	835	-	1/1/11/20	8/13/91/115	-
31	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	CLA	1	614	-	1/1/9/20	0/4/76/115	-
23	CLA	5	604	-	1/1/15/20	13/35/111/115	-
26	BCR	K	202	-	-	4/29/63/63	0/2/2/2
23	CLA	2	613	20	1/1/5/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	7	607	-	1/1/10/20	6/10/88/115	-
23	CLA	B	840	-	1/1/15/20	9/37/115/115	-
31	LUT	3	618	-	-	2/29/67/67	0/2/2/2
25	LHG	7	622	23	-	24/41/41/53	-
23	CLA	4	608	-	1/1/15/20	11/37/115/115	-
26	BCR	G	205	-	-	0/29/63/63	0/2/2/2
23	CLA	1	608	-	1/1/11/20	4/11/89/115	-
23	CLA	2	609	20	1/1/5/20	-	-
25	LHG	6	623	23	-	23/52/52/53	-
23	CLA	B	809	2	1/1/15/20	15/37/115/115	-
23	CLA	6	608	-	1/1/12/20	8/21/99/115	-
23	CLA	a	614	-	1/1/12/20	10/25/99/115	-
23	CLA	B	829	-	1/1/15/20	7/37/115/115	-
23	CLA	A	830	-	1/1/15/20	14/37/115/115	-
23	CLA	B	806	2	1/1/15/20	13/37/115/115	-
23	CLA	3	606	-	1/1/13/20	10/23/101/115	-
28	LMU	A	859	-	-	13/21/57/61	0/2/2/2
23	CLA	6	603	-	1/1/13/20	4/25/101/115	-
23	CLA	2	606	20	1/1/5/20	-	-
23	CLA	B	803	-	1/1/15/20	15/37/115/115	-
23	CLA	4	604	-	1/1/13/20	6/25/101/115	-
23	CLA	B	805	-	1/1/15/20	16/37/115/115	-
25	LHG	5	625	-	-	23/53/53/53	-
32	XAT	6	621	-	-	2/31/93/93	0/4/4/4
23	CLA	4	613	15	1/1/15/20	12/37/115/115	-
23	CLA	A	811	-	1/1/15/20	16/37/115/115	-
23	CLA	5	611	25	1/1/10/20	3/10/88/115	-
23	CLA	B	836	-	-	6/19/97/115	-
23	CLA	4	611	25	1/1/10/20	4/10/88/115	-
23	CLA	A	812	-	1/1/15/20	11/37/115/115	-
23	CLA	A	817	-	1/1/11/20	5/13/91/115	-
23	CLA	A	804	-	1/1/15/20	11/37/115/115	-
23	CLA	9	601	21	1/1/5/20	-	-
26	BCR	A	852	-	-	11/29/63/63	0/2/2/2
23	CLA	A	838	-	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	829	-	1/1/15/20	11/37/115/115	-
28	LMU	8	624	-	-	6/21/61/61	0/2/2/2
23	CLA	A	823	-	1/1/10/20	5/10/88/115	-
23	CLA	3	610	14	1/1/15/20	16/37/115/115	-
23	CLA	6	602	17	1/1/15/20	8/37/115/115	-
23	CLA	1	610	13	1/1/9/20	1/6/80/115	-
23	CLA	A	832	-	1/1/12/20	7/19/97/115	-
23	CLA	B	802	-	1/1/15/20	19/37/115/115	-
23	CLA	1	604	-	1/1/11/20	10/18/96/115	-
32	XAT	5	621	-	-	2/31/93/93	0/4/4/4
31	LUT	2	619	-	-	2/29/67/67	0/2/2/2
23	CLA	A	808	-	1/1/12/20	0/19/97/115	-
23	CLA	A	821	-	1/1/12/20	12/23/101/115	-
23	CLA	B	823	-	1/1/11/20	4/13/91/115	-
23	CLA	B	817	-	1/1/13/20	10/30/108/115	-
23	CLA	A	828	-	1/1/15/20	9/37/115/115	-
23	CLA	8	602	19	1/1/14/20	8/31/109/115	-
23	CLA	B	839	-	1/1/15/20	12/37/115/115	-
30	DGD	B	850	-	-	22/51/91/95	0/2/2/2
32	XAT	7	620	-	-	1/31/93/93	0/4/4/4
23	CLA	a	606	13	1/1/10/20	3/10/88/115	-
23	CLA	6	616	17	1/1/15/20	18/37/115/115	-
23	CLA	F	301	-	1/1/13/20	9/28/106/115	-
33	NEX	6	624	-	-	4/27/83/83	0/3/3/3
32	XAT	1	618	-	-	1/31/93/93	0/4/4/4
23	CLA	A	802	-	1/1/15/20	9/37/115/115	-
28	LMU	A	858	-	-	6/21/57/61	0/2/2/2
26	BCR	7	623	-	-	0/29/63/63	0/2/2/2
26	BCR	B	846	-	-	5/29/63/63	0/2/2/2
23	CLA	B	811	-	1/1/13/20	8/23/99/115	-
29	LMG	4	623	-	-	11/35/55/70	0/1/1/1
23	CLA	8	601	19	1/1/15/20	20/37/115/115	-
26	BCR	3	621	-	-	6/29/63/63	0/2/2/2
23	CLA	A	826	-	1/1/14/20	12/35/113/115	-
23	CLA	8	606	-	1/1/15/20	14/35/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	2	603	20	1/1/5/20	-	-
32	XAT	2	620	-	-	0/31/93/93	0/4/4/4
23	CLA	F	303	-	1/1/10/20	5/10/88/115	-
23	CLA	B	828	-	1/1/15/20	16/37/115/115	-
23	CLA	9	602	21	1/1/5/20	-	-
23	CLA	B	825	-	1/1/14/20	9/34/112/115	-
23	CLA	A	845	25	1/1/12/20	9/19/97/115	-
23	CLA	1	609	13	1/1/10/20	5/8/84/115	-
26	BCR	1	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	804	-	1/1/10/20	3/8/86/115	-
31	LUT	1	617	-	-	2/29/67/67	0/2/2/2
23	CLA	A	816	-	1/1/10/20	2/10/88/115	-
23	CLA	A	814	-	1/1/15/20	20/37/115/115	-
23	CLA	2	602	20	1/1/5/20	-	-
26	BCR	6	622	-	-	7/29/63/63	0/2/2/2
23	CLA	1	616	13	1/1/11/20	4/11/87/115	-
25	LHG	8	623	-	-	24/51/51/53	-
23	CLA	1	606	13	1/1/8/20	1/5/79/115	-
23	CLA	4	618	15	1/1/10/20	0/8/84/115	-
23	CLA	7	602	18	1/1/15/20	16/37/115/115	-
32	XAT	9	620	-	-	0/31/93/93	0/4/4/4
23	CLA	7	613	18	1/1/15/20	17/37/115/115	-
23	CLA	1	613	-	1/1/15/20	12/37/115/115	-
23	CLA	B	821	-	1/1/11/20	3/11/89/115	-
29	LMG	J	104	-	-	19/35/55/70	0/1/1/1
33	NEX	5	624	-	-	2/27/83/83	0/3/3/3
23	CLA	3	608	-	1/1/13/20	9/25/103/115	-
23	CLA	F	304	-	1/1/10/20	4/8/86/115	-
23	CLA	A	841	-	1/1/15/20	18/37/115/115	-
23	CLA	4	602	15	1/1/14/20	10/31/109/115	-
23	CLA	A	835	-	1/1/14/20	13/33/111/115	-
23	CLA	1	602	13	1/1/14/20	6/33/111/115	-
23	CLA	A	827	-	1/1/13/20	5/30/108/115	-
23	CLA	B	837	-	1/1/15/20	15/37/115/115	-
23	CLA	a	611	25	1/1/10/20	0/4/80/115	-
23	CLA	3	613	14	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	6	612	17	1/1/10/20	2/8/86/115	-
29	LMG	5	627	-	-	13/35/55/70	0/1/1/1
26	BCR	A	848	-	-	4/29/63/63	0/2/2/2
23	CLA	3	612	14	1/1/10/20	3/11/89/115	-
23	CLA	3	614	-	1/1/10/20	0/6/84/115	-
25	LHG	a	620	23	-	24/53/53/53	-
23	CLA	5	619	-	1/1/11/20	7/11/87/115	-
23	CLA	B	814	-	1/1/14/20	12/36/114/115	-
23	CLA	a	609	13	1/1/15/20	19/35/113/115	-
23	CLA	L	302	12	1/1/11/20	3/13/91/115	-
23	CLA	A	819	-	1/1/13/20	8/30/108/115	-
32	XAT	8	620	-	-	2/31/93/93	0/4/4/4
23	CLA	9	613	21	1/1/5/20	-	-
23	CLA	7	615	-	1/1/10/20	4/8/84/115	-
23	CLA	9	604	-	1/1/5/20	-	-
23	CLA	A	810	1	1/1/12/20	5/19/97/115	-
23	CLA	K	204	-	1/1/11/20	7/15/93/115	-
23	CLA	3	607	14	1/1/13/20	9/28/104/115	-
23	CLA	A	820	-	1/1/15/20	15/37/115/115	-
25	LHG	2	622	23	-	19/41/41/53	-
23	CLA	B	807	-	1/1/12/20	4/22/100/115	-
23	CLA	3	604	-	1/1/15/20	11/37/115/115	-
23	CLA	6	618	17	1/1/10/20	2/8/84/115	-
25	LHG	3	624	23	-	26/53/53/53	-
23	CLA	5	612	16	1/1/10/20	3/8/86/115	-
23	CLA	B	830	-	1/1/10/20	2/11/89/115	-
23	CLA	B	827	-	1/1/14/20	14/34/112/115	-
23	CLA	7	608	-	1/1/12/20	4/19/97/115	-
23	CLA	2	612	20	1/1/5/20	-	-
23	CLA	B	826	-	1/1/13/20	8/25/103/115	-
23	CLA	A	818	-	1/1/14/20	12/31/109/115	-
23	CLA	a	607	-	1/1/11/20	6/13/91/115	-
23	CLA	J	101	10	1/1/10/20	5/10/88/115	-
25	LHG	5	623	23	-	23/53/53/53	-
23	CLA	A	842	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	K	203	-	1/1/15/20	10/37/115/115	-
26	BCR	A	856	-	-	8/29/63/63	0/2/2/2
31	LUT	7	619	-	-	5/29/67/67	0/2/2/2
23	CLA	4	601	15	1/1/15/20	16/37/115/115	-
23	CLA	1	603	-	1/1/12/20	11/21/99/115	-
23	CLA	6	609	17	1/1/11/20	4/13/91/115	-
23	CLA	9	612	21	1/1/5/20	-	-
23	CLA	A	815	-	1/1/12/20	7/19/97/115	-
23	CLA	5	602	16	1/1/15/20	11/37/115/115	-
23	CLA	7	612	18	-	6/11/89/115	-
29	LMG	7	624	-	-	19/39/59/70	0/1/1/1
23	CLA	1	611	25	1/1/15/20	11/37/115/115	-
23	CLA	3	617	14	1/1/10/20	0/6/84/115	-
23	CLA	9	607	-	1/1/5/20	-	-
23	CLA	A	840	-	1/1/12/20	5/22/100/115	-
27	SF4	C	102	-	-	-	0/6/5/5
23	CLA	9	603	21	1/1/5/20	-	-
23	CLA	L	304	-	1/1/11/20	6/13/91/115	-
25	LHG	9	622	23	-	23/53/53/53	-
23	CLA	5	618	16	1/1/10/20	2/8/84/115	-
23	CLA	6	607	-	1/1/10/20	6/10/86/115	-
31	LUT	5	620	-	-	2/29/67/67	0/2/2/2
23	CLA	A	834	-	1/1/15/20	17/37/115/115	-
26	BCR	L	301	-	-	6/29/63/63	0/2/2/2
23	CLA	7	604	-	1/1/13/20	8/23/101/115	-
23	CLA	6	620	-	1/1/14/20	14/35/113/115	-
23	CLA	2	611	25	1/1/4/20	-	-
23	CLA	4	612	15	-	2/8/86/115	-
29	LMG	4	624	-	-	15/35/55/70	0/1/1/1
23	CLA	A	801	-	1/1/15/20	10/37/115/115	-
23	CLA	8	607	-	1/1/10/20	3/10/86/115	-
23	CLA	A	836	-	1/1/15/20	11/37/115/115	-
26	BCR	3	622	-	-	8/29/63/63	0/2/2/2
31	LUT	9	619	-	-	3/29/67/67	0/2/2/2
23	CLA	8	616	19	-	7/11/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	832	-	1/1/14/20	7/31/109/115	-
23	CLA	6	614	-	1/1/14/20	7/31/109/115	-
23	CLA	B	820	-	1/1/12/20	7/19/97/115	-
23	CLA	4	606	-	1/1/10/20	3/6/84/115	-
23	CLA	8	613	19	1/1/15/20	16/37/115/115	-
23	CLA	B	812	-	1/1/10/20	6/11/89/115	-
23	CLA	5	613	16	1/1/14/20	19/35/113/115	-
26	BCR	3	620	-	-	4/29/63/63	0/2/2/2
23	CLA	3	611	25	1/1/10/20	2/4/80/115	-
26	BCR	7	621	-	-	6/29/63/63	0/2/2/2
23	CLA	1	607	-	1/1/10/20	3/6/84/115	-
23	CLA	A	813	-	1/1/12/20	5/24/102/115	-
23	CLA	a	603	-	1/1/10/20	3/10/88/115	-
23	CLA	B	808	-	1/1/15/20	14/37/115/115	-
23	CLA	2	604	-	1/1/5/20	-	-
26	BCR	B	843	-	-	8/29/63/63	0/2/2/2
23	CLA	7	611	25	1/1/13/20	10/29/107/115	-
23	CLA	B	815	-	1/1/10/20	2/11/89/115	-

All (2248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	611	CLA	C1A-NA	12.76	1.40	1.29
24	A	844	PQN	C12-C13	8.62	1.53	1.33
24	B	842	PQN	C12-C13	8.55	1.53	1.33
23	4	609	CLA	C4B-NB	8.10	1.42	1.35
23	5	613	CLA	C4B-NB	7.97	1.42	1.35
24	A	844	PQN	O1-C1	7.91	1.40	1.23
23	2	601	CLA	C4B-NB	7.90	1.42	1.35
23	9	611	CLA	C4B-NB	7.79	1.42	1.35
23	G	204	CLA	C4B-NB	7.78	1.42	1.35
23	2	609	CLA	C4B-NB	7.76	1.42	1.35
23	9	613	CLA	C4B-NB	7.69	1.42	1.35
23	B	841	CLA	C4B-NB	7.65	1.42	1.35
23	2	603	CLA	C4B-NB	7.65	1.42	1.35
24	B	842	PQN	O1-C1	7.62	1.39	1.23
23	2	606	CLA	C4B-NB	7.62	1.42	1.35
23	L	302	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	613	CLA	C4B-NB	7.54	1.41	1.35
23	9	606	CLA	C4B-NB	7.53	1.41	1.35
23	B	822	CLA	C4B-NB	7.53	1.41	1.35
23	G	203	CLA	C4B-NB	7.49	1.41	1.35
23	2	616	CLA	C4B-NB	7.48	1.41	1.35
23	7	612	CLA	C4B-NB	7.48	1.41	1.35
23	2	614	CLA	C4B-NB	7.47	1.41	1.35
23	2	612	CLA	C4B-NB	7.46	1.41	1.35
24	A	844	PQN	O4-C4	7.45	1.39	1.23
23	L	304	CLA	C4B-NB	7.43	1.41	1.35
23	3	612	CLA	C4B-NB	7.38	1.41	1.35
24	B	842	PQN	O4-C4	7.37	1.38	1.23
23	6	609	CLA	C4B-NB	7.37	1.41	1.35
23	K	201	CLA	C4B-NB	7.36	1.41	1.35
23	9	612	CLA	C4B-NB	7.36	1.41	1.35
23	9	614	CLA	C4B-NB	7.34	1.41	1.35
23	B	835	CLA	C4B-NB	7.33	1.41	1.35
23	2	604	CLA	C4B-NB	7.32	1.41	1.35
23	9	603	CLA	C4B-NB	7.32	1.41	1.35
23	5	603	CLA	C4B-NB	7.31	1.41	1.35
23	5	618	CLA	C4B-NB	7.31	1.41	1.35
23	8	603	CLA	C4B-NB	7.30	1.41	1.35
23	a	614	CLA	C4B-NB	7.29	1.41	1.35
23	B	824	CLA	C4B-NB	7.27	1.41	1.35
23	2	602	CLA	C4B-NB	7.25	1.41	1.35
23	2	607	CLA	C4B-NB	7.24	1.41	1.35
23	1	606	CLA	C4B-NB	7.24	1.41	1.35
23	2	610	CLA	C4B-NB	7.23	1.41	1.35
23	F	303	CLA	C4B-NB	7.22	1.41	1.35
23	A	805	CLA	C4B-NB	7.21	1.41	1.35
23	a	610	CLA	C4B-NB	7.21	1.41	1.35
23	1	610	CLA	C4B-NB	7.20	1.41	1.35
23	1	614	CLA	C4B-NB	7.20	1.41	1.35
23	J	101	CLA	C4B-NB	7.19	1.41	1.35
23	7	607	CLA	C4B-NB	7.19	1.41	1.35
23	B	819	CLA	C4B-NB	7.19	1.41	1.35
23	4	618	CLA	C4B-NB	7.18	1.41	1.35
23	5	614	CLA	C4B-NB	7.18	1.41	1.35
23	9	610	CLA	C4B-NB	7.18	1.41	1.35
23	2	611	CLA	C4B-NB	7.17	1.41	1.35
23	K	203	CLA	C4B-NB	7.17	1.41	1.35
23	3	611	CLA	C4B-NB	7.16	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	616	CLA	C4B-NB	7.16	1.41	1.35
23	3	609	CLA	C4B-NB	7.15	1.41	1.35
23	B	812	CLA	C4B-NB	7.15	1.41	1.35
23	a	606	CLA	C4B-NB	7.14	1.41	1.35
23	1	612	CLA	C4B-NB	7.14	1.41	1.35
23	1	616	CLA	C4B-NB	7.13	1.41	1.35
23	9	601	CLA	C4B-NB	7.13	1.41	1.35
23	7	615	CLA	C4B-NB	7.13	1.41	1.35
23	4	614	CLA	C4B-NB	7.13	1.41	1.35
23	1	604	CLA	C4B-NB	7.12	1.41	1.35
23	a	616	CLA	C4B-NB	7.12	1.41	1.35
23	3	617	CLA	C4B-NB	7.12	1.41	1.35
23	8	616	CLA	C4B-NB	7.11	1.41	1.35
23	6	603	CLA	C4B-NB	7.10	1.41	1.35
23	a	612	CLA	C4B-NB	7.10	1.41	1.35
23	3	613	CLA	C4B-NB	7.08	1.41	1.35
23	3	604	CLA	C4B-NB	7.08	1.41	1.35
23	1	603	CLA	C4B-NB	7.06	1.41	1.35
23	a	603	CLA	C4B-NB	7.06	1.41	1.35
23	6	612	CLA	C4B-NB	7.05	1.41	1.35
23	a	604	CLA	C4B-NB	7.03	1.41	1.35
23	5	604	CLA	C4B-NB	7.03	1.41	1.35
23	6	606	CLA	C4B-NB	7.03	1.41	1.35
23	6	618	CLA	C4B-NB	7.03	1.41	1.35
23	4	606	CLA	C4B-NB	7.02	1.41	1.35
23	9	607	CLA	C4B-NB	7.02	1.41	1.35
23	B	823	CLA	C4B-NB	7.02	1.41	1.35
23	9	602	CLA	C4B-NB	7.01	1.41	1.35
23	a	613	CLA	C4B-NB	7.00	1.41	1.35
23	4	603	CLA	C4B-NB	7.00	1.41	1.35
23	9	604	CLA	C4B-NB	6.98	1.41	1.35
23	1	613	CLA	C4B-NB	6.98	1.41	1.35
23	B	837	CLA	C4B-NB	6.98	1.41	1.35
23	1	608	CLA	C4B-NB	6.98	1.41	1.35
23	a	607	CLA	C4B-NB	6.97	1.41	1.35
23	1	607	CLA	C4B-NB	6.97	1.41	1.35
23	4	616	CLA	C4B-NB	6.97	1.41	1.35
23	4	607	CLA	C4B-NB	6.96	1.41	1.35
23	5	609	CLA	C4B-NB	6.96	1.41	1.35
23	4	612	CLA	C4B-NB	6.95	1.41	1.35
23	7	602	CLA	C4B-NB	6.95	1.41	1.35
23	F	304	CLA	C4B-NB	6.94	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	816	CLA	C4B-NB	6.94	1.41	1.35
23	a	608	CLA	C4B-NB	6.93	1.41	1.35
23	9	609	CLA	C4B-NB	6.92	1.41	1.35
23	B	804	CLA	C4B-NB	6.91	1.41	1.35
23	B	811	CLA	C4B-NB	6.90	1.41	1.35
23	5	611	CLA	C4B-NB	6.90	1.41	1.35
23	8	612	CLA	C4B-NB	6.89	1.41	1.35
23	4	601	CLA	C4B-NB	6.89	1.41	1.35
23	A	819	CLA	C4B-NB	6.87	1.41	1.35
23	8	604	CLA	C4B-NB	6.86	1.41	1.35
23	8	613	CLA	C4B-NB	6.86	1.41	1.35
23	7	603	CLA	C4B-NB	6.86	1.41	1.35
23	B	820	CLA	C4B-NB	6.85	1.41	1.35
23	A	837	CLA	C4B-NB	6.84	1.41	1.35
23	6	608	CLA	C4B-NB	6.83	1.41	1.35
23	3	606	CLA	C4B-NB	6.82	1.41	1.35
23	5	612	CLA	C4B-NB	6.82	1.41	1.35
23	B	816	CLA	C4B-NB	6.80	1.41	1.35
23	K	206	CLA	C4B-NB	6.80	1.41	1.35
23	5	617	CLA	C4B-NB	6.80	1.41	1.35
23	B	821	CLA	C4B-NB	6.78	1.41	1.35
23	3	614	CLA	C4B-NB	6.78	1.41	1.35
23	B	806	CLA	C4B-NB	6.78	1.41	1.35
23	A	833	CLA	C4B-NB	6.78	1.41	1.35
23	A	823	CLA	C4B-NB	6.77	1.41	1.35
23	8	607	CLA	C4B-NB	6.77	1.41	1.35
23	L	303	CLA	C4B-NB	6.76	1.41	1.35
23	1	609	CLA	C4B-NB	6.76	1.41	1.35
23	4	611	CLA	C4B-NB	6.74	1.41	1.35
23	6	613	CLA	C4B-NB	6.74	1.41	1.35
23	4	608	CLA	C4B-NB	6.73	1.41	1.35
23	A	836	CLA	C4B-NB	6.73	1.41	1.35
23	B	808	CLA	C4B-NB	6.72	1.41	1.35
23	B	834	CLA	C4B-NB	6.72	1.41	1.35
23	F	301	CLA	C4B-NB	6.72	1.41	1.35
23	A	840	CLA	C4B-NB	6.72	1.41	1.35
23	a	601	CLA	C4B-NB	6.71	1.41	1.35
23	5	601	CLA	C4B-NB	6.70	1.41	1.35
23	a	609	CLA	C4B-NB	6.70	1.41	1.35
23	7	609	CLA	C4B-NB	6.70	1.41	1.35
23	8	614	CLA	C4B-NB	6.69	1.41	1.35
23	8	606	CLA	C4B-NB	6.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	617	CLA	C4B-NB	6.68	1.41	1.35
23	1	601	CLA	C4B-NB	6.68	1.41	1.35
23	A	839	CLA	C4B-NB	6.67	1.41	1.35
23	a	602	CLA	C4B-NB	6.67	1.41	1.35
23	B	829	CLA	C4B-NB	6.67	1.41	1.35
23	A	825	CLA	C4B-NB	6.67	1.41	1.35
23	5	608	CLA	C4B-NB	6.66	1.41	1.35
23	5	606	CLA	C4B-NB	6.66	1.41	1.35
23	a	611	CLA	C4B-NB	6.66	1.41	1.35
23	6	614	CLA	C4B-NB	6.65	1.41	1.35
23	8	602	CLA	C4B-NB	6.65	1.41	1.35
23	B	840	CLA	C4B-NB	6.64	1.41	1.35
23	7	616	CLA	C4B-NB	6.64	1.41	1.35
23	5	607	CLA	C4B-NB	6.64	1.41	1.35
23	3	603	CLA	C4B-NB	6.63	1.41	1.35
23	A	834	CLA	C4B-NB	6.63	1.41	1.35
23	A	843	CLA	C4B-NB	6.63	1.41	1.35
23	5	610	CLA	C4B-NB	6.62	1.41	1.35
23	6	607	CLA	C4B-NB	6.62	1.41	1.35
23	4	610	CLA	C4B-NB	6.62	1.41	1.35
23	1	602	CLA	C4B-NB	6.61	1.41	1.35
23	3	615	CLA	C4B-NB	6.61	1.41	1.35
23	A	845	CLA	C4B-NB	6.59	1.41	1.35
23	3	607	CLA	C4B-NB	6.59	1.41	1.35
23	4	613	CLA	C4B-NB	6.58	1.41	1.35
23	B	814	CLA	C4B-NB	6.58	1.41	1.35
23	B	830	CLA	C4B-NB	6.58	1.41	1.35
23	1	611	CLA	C4B-NB	6.58	1.41	1.35
23	B	831	CLA	C4B-NB	6.56	1.41	1.35
23	A	832	CLA	C4B-NB	6.55	1.41	1.35
23	7	610	CLA	C4B-NB	6.54	1.41	1.35
23	7	613	CLA	C4B-NB	6.54	1.41	1.35
23	A	807	CLA	C4B-NB	6.53	1.41	1.35
23	A	835	CLA	C4B-NB	6.53	1.41	1.35
23	4	604	CLA	C4B-NB	6.53	1.41	1.35
23	K	204	CLA	C4B-NB	6.53	1.41	1.35
23	5	602	CLA	C4B-NB	6.53	1.41	1.35
23	A	831	CLA	C4B-NB	6.52	1.41	1.35
23	B	826	CLA	C4B-NB	6.50	1.41	1.35
23	A	808	CLA	C4B-NB	6.50	1.41	1.35
23	A	815	CLA	C4B-NB	6.50	1.41	1.35
23	B	807	CLA	C4B-NB	6.50	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	832	CLA	C4B-NB	6.49	1.41	1.35
23	A	803	CLA	C4B-NB	6.49	1.41	1.35
23	A	809	CLA	C4B-NB	6.49	1.41	1.35
23	8	609	CLA	C4B-NB	6.48	1.41	1.35
23	6	601	CLA	C4B-NB	6.47	1.41	1.35
23	A	841	CLA	C4B-NB	6.47	1.41	1.35
23	6	616	CLA	C4B-NB	6.47	1.41	1.35
23	6	620	CLA	C4B-NB	6.47	1.41	1.35
23	B	828	CLA	C4B-NB	6.46	1.41	1.35
23	5	619	CLA	C4B-NB	6.46	1.41	1.35
23	A	820	CLA	C4B-NB	6.46	1.41	1.35
23	6	602	CLA	C4B-NB	6.45	1.41	1.35
23	7	604	CLA	C4B-NB	6.45	1.41	1.35
23	A	826	CLA	C4B-NB	6.44	1.41	1.35
23	6	611	CLA	C4B-NB	6.44	1.41	1.35
23	A	842	CLA	C4B-NB	6.44	1.40	1.35
23	8	601	CLA	C4B-NB	6.42	1.40	1.35
23	8	608	CLA	C4B-NB	6.42	1.40	1.35
23	7	608	CLA	C4B-NB	6.42	1.40	1.35
23	3	608	CLA	C4B-NB	6.42	1.40	1.35
23	6	610	CLA	C4B-NB	6.41	1.40	1.35
23	B	827	CLA	C4B-NB	6.40	1.40	1.35
23	A	822	CLA	C4B-NB	6.40	1.40	1.35
23	B	838	CLA	C4B-NB	6.38	1.40	1.35
23	7	601	CLA	C4B-NB	6.38	1.40	1.35
23	B	833	CLA	C4B-NB	6.38	1.40	1.35
23	3	610	CLA	C4B-NB	6.38	1.40	1.35
23	A	824	CLA	C4B-NB	6.37	1.40	1.35
23	A	817	CLA	C4B-NB	6.37	1.40	1.35
23	A	821	CLA	C4B-NB	6.36	1.40	1.35
23	4	602	CLA	C4B-NB	6.36	1.40	1.35
23	A	818	CLA	C4B-NB	6.36	1.40	1.35
23	A	802	CLA	C4B-NB	6.35	1.40	1.35
23	A	811	CLA	C4B-NB	6.34	1.40	1.35
23	8	611	CLA	C4B-NB	6.32	1.40	1.35
23	A	812	CLA	C4B-NB	6.32	1.40	1.35
23	A	806	CLA	C4B-NB	6.31	1.40	1.35
23	A	813	CLA	C4B-NB	6.30	1.40	1.35
23	B	809	CLA	C4B-NB	6.28	1.40	1.35
23	7	606	CLA	C4B-NB	6.28	1.40	1.35
23	B	836	CLA	C4B-NB	6.27	1.40	1.35
23	B	810	CLA	C4B-NB	6.27	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	815	CLA	C4B-NB	6.27	1.40	1.35
23	B	813	CLA	C4B-NB	6.26	1.40	1.35
23	B	802	CLA	C4B-NB	6.26	1.40	1.35
23	6	604	CLA	C4B-NB	6.25	1.40	1.35
23	B	839	CLA	C4B-NB	6.23	1.40	1.35
23	B	817	CLA	C4B-NB	6.22	1.40	1.35
23	B	818	CLA	C4B-NB	6.21	1.40	1.35
23	A	801	CLA	C4B-NB	6.20	1.40	1.35
23	B	805	CLA	C4B-NB	6.20	1.40	1.35
23	A	804	CLA	C4B-NB	6.17	1.40	1.35
23	A	810	CLA	C4B-NB	6.15	1.40	1.35
23	7	611	CLA	C4B-NB	6.12	1.40	1.35
23	3	602	CLA	C4B-NB	6.10	1.40	1.35
23	A	830	CLA	C4B-NB	6.09	1.40	1.35
23	A	854	CLA	C4B-NB	6.08	1.40	1.35
23	8	610	CLA	C4B-NB	6.06	1.40	1.35
23	B	803	CLA	C4B-NB	6.06	1.40	1.35
23	A	827	CLA	C4B-NB	6.05	1.40	1.35
23	A	829	CLA	C4B-NB	6.03	1.40	1.35
23	7	614	CLA	C4B-NB	6.00	1.40	1.35
23	A	814	CLA	C4B-NB	5.95	1.40	1.35
23	9	606	CLA	CHB-C4A	5.83	1.39	1.34
23	A	838	CLA	C4B-NB	5.76	1.40	1.35
23	2	609	CLA	C2B-C1B	5.67	1.49	1.39
23	A	828	CLA	C4B-NB	5.64	1.40	1.35
23	2	609	CLA	C3B-C4B	5.64	1.49	1.39
23	9	602	CLA	C2B-C1B	5.61	1.49	1.39
23	9	614	CLA	C2B-C1B	5.58	1.49	1.39
23	9	611	CLA	C2B-C1B	5.58	1.49	1.39
23	9	610	CLA	C3B-C4B	5.57	1.49	1.39
23	9	603	CLA	C2B-C1B	5.55	1.49	1.39
23	9	606	CLA	C2B-C1B	5.55	1.49	1.39
23	9	611	CLA	C3B-C4B	5.53	1.49	1.39
23	2	603	CLA	C2B-C1B	5.52	1.49	1.39
23	2	603	CLA	C3B-C4B	5.52	1.49	1.39
23	2	612	CLA	C3B-C4B	5.52	1.49	1.39
23	2	604	CLA	C2B-C1B	5.51	1.49	1.39
23	9	610	CLA	C2B-C1B	5.51	1.49	1.39
23	9	612	CLA	C2B-C1B	5.50	1.49	1.39
23	2	609	CLA	CHB-C4A	5.48	1.39	1.34
23	2	610	CLA	C3B-C4B	5.48	1.49	1.39
23	2	601	CLA	C2B-C1B	5.46	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	612	CLA	C2B-C1B	5.45	1.49	1.39
23	9	613	CLA	C2B-C1B	5.44	1.49	1.39
23	B	825	CLA	C4B-NB	5.44	1.40	1.35
23	2	602	CLA	C3B-C4B	5.44	1.49	1.39
23	2	602	CLA	C2B-C1B	5.43	1.49	1.39
23	2	611	CLA	C2B-C1B	5.43	1.49	1.39
23	2	613	CLA	C2B-C1B	5.42	1.49	1.39
23	9	603	CLA	C3B-C4B	5.42	1.49	1.39
23	9	609	CLA	C3B-C4B	5.42	1.49	1.39
23	2	614	CLA	C2B-C1B	5.42	1.49	1.39
23	2	606	CLA	C2B-C1B	5.40	1.49	1.39
23	2	607	CLA	C2B-C1B	5.39	1.49	1.39
23	9	607	CLA	C2B-C1B	5.39	1.49	1.39
23	2	611	CLA	C3B-C4B	5.39	1.49	1.39
23	2	606	CLA	C3B-C4B	5.38	1.49	1.39
23	2	616	CLA	C3B-C4B	5.38	1.49	1.39
23	9	614	CLA	C3B-C4B	5.37	1.49	1.39
23	9	609	CLA	C2B-C1B	5.37	1.49	1.39
23	9	602	CLA	C3B-C4B	5.37	1.49	1.39
23	9	612	CLA	C3B-C4B	5.36	1.49	1.39
23	2	601	CLA	C3B-C4B	5.36	1.49	1.39
23	2	607	CLA	C3B-C4B	5.36	1.49	1.39
23	2	614	CLA	C3B-C4B	5.35	1.49	1.39
23	2	604	CLA	C3B-C4B	5.35	1.49	1.39
23	9	601	CLA	CHB-C4A	5.35	1.38	1.34
23	9	613	CLA	C3B-C4B	5.35	1.49	1.39
23	2	612	CLA	CHB-C4A	5.35	1.38	1.34
23	9	606	CLA	C3B-C4B	5.34	1.49	1.39
23	2	610	CLA	C2B-C1B	5.34	1.49	1.39
23	2	613	CLA	C3B-C4B	5.33	1.49	1.39
23	2	606	CLA	CHB-C4A	5.33	1.38	1.34
23	2	604	CLA	CHB-C4A	5.32	1.38	1.34
23	9	604	CLA	C3B-C4B	5.32	1.49	1.39
23	9	604	CLA	C2B-C1B	5.32	1.49	1.39
23	9	612	CLA	CHB-C4A	5.31	1.38	1.34
23	9	607	CLA	C3B-C4B	5.30	1.49	1.39
23	9	601	CLA	C2B-C1B	5.29	1.49	1.39
23	2	616	CLA	C2B-C1B	5.27	1.49	1.39
23	2	601	CLA	CHB-C4A	5.23	1.38	1.34
23	9	613	CLA	CHB-C4A	5.21	1.38	1.34
23	9	611	CLA	CHB-C4A	5.17	1.38	1.34
23	2	613	CLA	CHB-C4A	5.15	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	604	CLA	CHB-C4A	5.14	1.38	1.34
23	9	602	CLA	CHB-C4A	5.14	1.38	1.34
23	9	609	CLA	CHB-C4A	5.14	1.38	1.34
23	9	601	CLA	C3B-C4B	5.13	1.48	1.39
23	2	602	CLA	CHB-C4A	4.98	1.38	1.34
23	9	614	CLA	CHB-C4A	4.97	1.38	1.34
24	B	842	PQN	C2-C1	-4.96	1.37	1.48
23	2	603	CLA	CHB-C4A	4.95	1.38	1.34
23	9	610	CLA	CHB-C4A	4.86	1.38	1.34
23	9	607	CLA	CHB-C4A	4.85	1.38	1.34
23	2	610	CLA	CHB-C4A	4.81	1.38	1.34
23	2	607	CLA	CHB-C4A	4.79	1.38	1.34
23	2	616	CLA	CHB-C4A	4.76	1.38	1.34
23	1	614	CLA	CHB-C4A	4.68	1.38	1.34
23	a	614	CLA	CHB-C4A	4.63	1.38	1.34
23	9	603	CLA	CHB-C4A	4.63	1.38	1.34
23	A	831	CLA	CMB-C2B	-4.50	1.42	1.51
23	2	614	CLA	CHB-C4A	4.37	1.38	1.34
24	A	844	PQN	C2-C1	-4.35	1.38	1.48
23	B	829	CLA	CMB-C2B	-4.14	1.43	1.51
23	7	601	CLA	C4D-ND	-4.09	1.32	1.37
23	B	803	CLA	C4D-ND	-4.07	1.32	1.37
23	G	204	CLA	C1D-ND	4.05	1.42	1.37
23	3	603	CLA	C4D-ND	-4.03	1.32	1.37
23	6	607	CLA	CAB-C3B	-4.01	1.43	1.51
28	A	859	LMU	O5B-C1B	3.99	1.52	1.41
23	8	616	CLA	C1D-ND	3.95	1.42	1.37
23	A	806	CLA	C4D-ND	-3.93	1.32	1.37
23	A	839	CLA	C4D-ND	-3.93	1.32	1.37
23	5	614	CLA	CHB-C4A	3.92	1.37	1.34
23	F	303	CLA	C1D-ND	3.92	1.42	1.37
23	5	613	CLA	C4D-ND	-3.91	1.32	1.37
23	7	611	CLA	C4D-ND	-3.89	1.32	1.37
23	8	613	CLA	C4D-ND	-3.88	1.32	1.37
23	5	619	CLA	CAB-C3B	-3.87	1.43	1.51
23	A	811	CLA	C4D-ND	-3.86	1.32	1.37
23	B	821	CLA	C3C-C4C	3.85	1.46	1.40
23	A	807	CLA	C4D-ND	-3.85	1.32	1.37
23	3	608	CLA	C4D-ND	-3.85	1.32	1.37
23	B	811	CLA	CAB-C3B	-3.83	1.43	1.51
23	K	204	CLA	C1D-ND	3.82	1.42	1.37
23	2	604	CLA	C4B-CHC	-3.82	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	827	CLA	C4D-ND	-3.80	1.32	1.37
23	5	604	CLA	CAB-C3B	-3.80	1.43	1.51
23	K	201	CLA	C1D-ND	3.80	1.42	1.37
23	A	830	CLA	C4D-ND	-3.80	1.32	1.37
28	8	624	LMU	O5B-C1B	3.79	1.51	1.41
23	B	837	CLA	C4D-ND	-3.79	1.32	1.37
23	B	825	CLA	C4D-ND	-3.79	1.32	1.37
23	B	836	CLA	C4D-ND	-3.78	1.32	1.37
23	a	610	CLA	C1D-ND	3.78	1.42	1.37
23	A	812	CLA	C4D-ND	-3.77	1.32	1.37
23	4	604	CLA	CAB-C3B	-3.77	1.43	1.51
23	9	601	CLA	C4B-CHC	-3.77	1.36	1.43
28	5	628	LMU	O5'-C1'	3.77	1.51	1.41
23	8	603	CLA	CAB-C3B	-3.77	1.43	1.51
23	B	805	CLA	C4D-ND	-3.77	1.32	1.37
23	6	603	CLA	CAB-C3B	-3.76	1.43	1.51
23	9	602	CLA	C4B-CHC	-3.76	1.36	1.43
23	9	613	CLA	C4B-CHC	-3.76	1.36	1.43
23	A	820	CLA	CMB-C2B	-3.76	1.43	1.51
23	A	810	CLA	C4D-ND	-3.75	1.32	1.37
23	1	610	CLA	C1D-ND	3.75	1.42	1.37
23	7	603	CLA	C4D-ND	-3.75	1.32	1.37
23	A	820	CLA	C4D-ND	-3.74	1.32	1.37
23	5	603	CLA	CAB-C3B	-3.74	1.43	1.51
23	4	601	CLA	C4D-ND	-3.74	1.32	1.37
23	5	616	CLA	CAB-C3B	-3.73	1.43	1.51
23	2	601	CLA	C4B-CHC	-3.73	1.36	1.43
23	A	831	CLA	C4D-ND	-3.73	1.32	1.37
23	8	607	CLA	CAB-C3B	-3.72	1.43	1.51
23	6	620	CLA	C4D-ND	-3.72	1.32	1.37
23	B	810	CLA	C4D-ND	-3.72	1.32	1.37
23	9	604	CLA	C4B-CHC	-3.72	1.36	1.43
23	6	603	CLA	C4D-ND	-3.71	1.32	1.37
23	3	607	CLA	CAB-C3B	-3.71	1.43	1.51
23	2	613	CLA	C4B-CHC	-3.71	1.36	1.43
23	8	616	CLA	CAB-C3B	-3.71	1.43	1.51
23	L	304	CLA	C1D-ND	3.71	1.42	1.37
23	F	304	CLA	C1D-ND	3.71	1.42	1.37
23	7	616	CLA	CAB-C3B	-3.70	1.44	1.51
23	9	612	CLA	C4B-CHC	-3.69	1.36	1.43
28	K	208	LMU	O5'-C1'	3.69	1.51	1.41
23	B	806	CLA	C4D-ND	-3.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	608	CLA	C4D-ND	-3.69	1.32	1.37
23	B	840	CLA	C4D-ND	-3.69	1.32	1.37
23	A	805	CLA	C4D-ND	-3.68	1.32	1.37
24	B	842	PQN	C3-C4	-3.68	1.37	1.47
28	A	858	LMU	O5B-C1B	3.68	1.51	1.41
23	6	618	CLA	CAB-C3B	-3.68	1.44	1.51
23	4	618	CLA	CAB-C3B	-3.68	1.44	1.51
23	B	833	CLA	C4D-ND	-3.68	1.32	1.37
23	a	609	CLA	C1D-ND	3.68	1.42	1.37
23	9	607	CLA	C4B-CHC	-3.68	1.36	1.43
28	8	625	LMU	O5'-C1'	3.67	1.51	1.41
23	5	603	CLA	C4D-ND	-3.67	1.32	1.37
23	1	609	CLA	C1D-ND	3.67	1.42	1.37
23	4	603	CLA	CAB-C3B	-3.67	1.44	1.51
23	7	602	CLA	C4D-ND	-3.67	1.32	1.37
23	2	616	CLA	C4B-CHC	-3.67	1.36	1.43
23	7	615	CLA	C1D-ND	3.67	1.42	1.37
28	A	859	LMU	O5'-C1'	3.67	1.51	1.42
23	7	615	CLA	CAB-C3B	-3.67	1.44	1.51
23	3	607	CLA	C4D-ND	-3.66	1.32	1.37
23	6	614	CLA	C4D-ND	-3.66	1.32	1.37
23	1	606	CLA	C1D-ND	3.66	1.42	1.37
23	B	809	CLA	C4D-ND	-3.66	1.32	1.37
23	A	803	CLA	C4D-ND	-3.66	1.32	1.37
23	A	822	CLA	C4D-ND	-3.66	1.32	1.37
28	5	628	LMU	O5B-C1B	3.66	1.51	1.41
23	2	614	CLA	C4B-CHC	-3.65	1.36	1.43
23	K	206	CLA	C1D-ND	3.65	1.42	1.37
23	8	602	CLA	C4D-ND	-3.65	1.32	1.37
23	B	807	CLA	C4D-ND	-3.65	1.32	1.37
23	G	203	CLA	C1D-ND	3.65	1.42	1.37
23	5	607	CLA	C4D-ND	-3.64	1.32	1.37
23	A	842	CLA	C4D-ND	-3.64	1.32	1.37
23	B	818	CLA	C1D-ND	3.64	1.42	1.37
23	5	618	CLA	CAB-C3B	-3.63	1.44	1.51
23	4	614	CLA	C1D-ND	3.63	1.42	1.37
23	A	838	CLA	C4D-ND	-3.63	1.32	1.37
23	B	839	CLA	C4D-ND	-3.63	1.32	1.37
23	9	614	CLA	C4B-CHC	-3.63	1.36	1.43
23	1	614	CLA	CAB-C3B	-3.63	1.44	1.51
23	2	606	CLA	C4B-CHC	-3.62	1.36	1.43
23	B	841	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	608	CLA	C4D-ND	-3.62	1.32	1.37
23	2	612	CLA	C4B-CHC	-3.62	1.36	1.43
23	9	609	CLA	C4B-CHC	-3.62	1.36	1.43
23	B	832	CLA	C4D-ND	-3.61	1.32	1.37
23	8	601	CLA	C4D-ND	-3.61	1.32	1.37
23	9	603	CLA	C4B-CHC	-3.61	1.36	1.43
23	L	302	CLA	C1D-ND	3.60	1.42	1.37
23	a	606	CLA	C1D-ND	3.60	1.42	1.37
23	2	602	CLA	C4B-CHC	-3.60	1.36	1.43
23	B	823	CLA	C1D-ND	3.60	1.42	1.37
23	4	616	CLA	CAB-C3B	-3.60	1.44	1.51
23	L	303	CLA	C4D-ND	-3.60	1.32	1.37
23	B	828	CLA	C4D-ND	-3.59	1.32	1.37
23	B	826	CLA	C4D-ND	-3.59	1.32	1.37
23	B	820	CLA	C1D-ND	3.59	1.42	1.37
23	2	611	CLA	C4B-CHC	-3.58	1.36	1.43
23	B	827	CLA	C4D-ND	-3.58	1.32	1.37
23	A	829	CLA	C4D-ND	-3.58	1.32	1.37
23	2	603	CLA	C4B-CHC	-3.58	1.36	1.43
23	K	204	CLA	C4D-ND	-3.58	1.32	1.37
23	1	607	CLA	C1D-ND	3.58	1.42	1.37
23	4	607	CLA	C1D-ND	3.57	1.42	1.37
23	B	817	CLA	C4D-ND	-3.57	1.32	1.37
23	4	616	CLA	C1D-ND	3.57	1.42	1.37
23	3	611	CLA	CAB-C3B	-3.57	1.44	1.51
23	A	833	CLA	C4D-ND	-3.56	1.32	1.37
23	2	607	CLA	C4B-CHC	-3.56	1.36	1.43
23	A	814	CLA	C4D-ND	-3.56	1.32	1.37
23	B	802	CLA	C4D-ND	-3.56	1.32	1.37
23	8	603	CLA	C1D-ND	3.56	1.42	1.37
23	9	606	CLA	C4B-CHC	-3.56	1.36	1.43
23	3	617	CLA	C4D-ND	-3.56	1.32	1.37
23	5	606	CLA	C4D-ND	-3.56	1.32	1.37
23	B	834	CLA	C4D-ND	-3.56	1.32	1.37
23	6	608	CLA	C4D-ND	-3.55	1.32	1.37
23	a	611	CLA	CAB-C3B	-3.55	1.44	1.51
23	1	616	CLA	CAB-C3B	-3.54	1.44	1.51
28	A	857	LMU	O5B-C1B	3.54	1.50	1.41
23	3	612	CLA	C4D-ND	-3.54	1.32	1.37
23	A	808	CLA	C4D-ND	-3.54	1.32	1.37
23	A	845	CLA	C4D-ND	-3.53	1.32	1.37
23	8	614	CLA	C4D-ND	-3.53	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	607	CLA	C1D-ND	3.52	1.42	1.37
23	5	617	CLA	C4D-ND	-3.52	1.32	1.37
23	A	819	CLA	C4D-ND	-3.52	1.32	1.37
23	1	603	CLA	C4D-ND	-3.51	1.32	1.37
23	7	614	CLA	C4D-ND	-3.51	1.32	1.37
23	1	601	CLA	C4D-ND	-3.51	1.32	1.37
23	A	828	CLA	C1D-ND	3.51	1.42	1.37
23	2	609	CLA	C4B-CHC	-3.51	1.36	1.43
23	A	823	CLA	C4D-ND	-3.51	1.32	1.37
23	7	613	CLA	C1D-ND	3.50	1.42	1.37
23	A	809	CLA	C4D-ND	-3.50	1.32	1.37
23	4	603	CLA	C4D-ND	-3.50	1.32	1.37
23	A	815	CLA	C4D-ND	-3.50	1.32	1.37
23	6	601	CLA	C4D-ND	-3.50	1.32	1.37
23	1	608	CLA	C1D-ND	3.50	1.42	1.37
23	A	824	CLA	C4D-ND	-3.49	1.32	1.37
23	B	814	CLA	C4D-ND	-3.49	1.32	1.37
23	a	604	CLA	C1D-ND	3.49	1.42	1.37
23	8	611	CLA	C4D-ND	-3.49	1.32	1.37
23	9	610	CLA	C4B-CHC	-3.49	1.36	1.43
23	1	604	CLA	C1D-ND	3.48	1.42	1.37
23	4	610	CLA	C1D-ND	3.48	1.42	1.37
23	4	612	CLA	C1D-ND	3.48	1.42	1.37
23	A	828	CLA	C4D-ND	-3.48	1.32	1.37
28	A	858	LMU	O5'-C1'	3.48	1.50	1.41
23	6	612	CLA	C1D-ND	3.48	1.42	1.37
23	a	602	CLA	C4D-ND	-3.48	1.32	1.37
23	7	606	CLA	C1D-ND	3.48	1.42	1.37
23	4	602	CLA	C4D-ND	-3.48	1.32	1.37
23	B	819	CLA	C1D-ND	3.47	1.42	1.37
23	B	829	CLA	C4D-ND	-3.47	1.32	1.37
23	1	609	CLA	CAB-C3B	-3.47	1.44	1.51
23	7	608	CLA	C4D-ND	-3.47	1.32	1.37
23	3	604	CLA	C4D-ND	-3.47	1.32	1.37
23	6	610	CLA	C4D-ND	-3.47	1.32	1.37
23	6	618	CLA	C4D-ND	-3.47	1.32	1.37
23	F	301	CLA	C4D-ND	-3.47	1.32	1.37
23	a	601	CLA	C4D-ND	-3.47	1.32	1.37
23	K	203	CLA	C1D-ND	3.47	1.42	1.37
23	5	609	CLA	C4D-ND	-3.46	1.32	1.37
23	7	612	CLA	C4D-ND	-3.46	1.32	1.37
23	B	808	CLA	C4D-ND	-3.45	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	614	CLA	C1D-ND	3.45	1.42	1.37
23	1	602	CLA	C4D-ND	-3.45	1.33	1.37
23	A	802	CLA	C4D-ND	-3.45	1.33	1.37
23	2	612	CLA	C4D-ND	-3.44	1.33	1.37
23	1	614	CLA	C1D-ND	3.44	1.42	1.37
23	a	608	CLA	C1D-ND	3.44	1.42	1.37
23	B	813	CLA	C4D-ND	-3.44	1.33	1.37
23	A	821	CLA	C4D-ND	-3.43	1.33	1.37
23	2	610	CLA	C4B-CHC	-3.43	1.37	1.43
23	B	836	CLA	C1D-ND	3.43	1.42	1.37
23	5	616	CLA	C1D-ND	3.42	1.42	1.37
23	A	837	CLA	C1D-ND	3.42	1.42	1.37
23	B	831	CLA	C4D-ND	-3.42	1.33	1.37
23	A	829	CLA	C1D-ND	3.42	1.42	1.37
23	B	818	CLA	C4D-ND	-3.42	1.33	1.37
23	a	603	CLA	C4D-ND	-3.42	1.33	1.37
23	4	611	CLA	C1D-ND	3.41	1.42	1.37
23	5	602	CLA	C4D-ND	-3.41	1.33	1.37
23	B	835	CLA	C1D-ND	3.41	1.42	1.37
23	B	821	CLA	C1D-ND	3.41	1.42	1.37
23	A	835	CLA	C1D-ND	3.41	1.42	1.37
23	8	606	CLA	C1D-ND	3.41	1.42	1.37
23	1	603	CLA	C1D-ND	3.40	1.42	1.37
23	3	614	CLA	C1D-ND	3.40	1.42	1.37
23	8	616	CLA	C4D-ND	-3.40	1.33	1.37
23	A	834	CLA	C4D-ND	-3.40	1.33	1.37
23	6	606	CLA	C4D-ND	-3.40	1.33	1.37
23	B	812	CLA	C1D-ND	3.40	1.42	1.37
28	8	625	LMU	O5B-C1B	3.40	1.50	1.41
23	9	611	CLA	C4B-CHC	-3.40	1.37	1.43
23	A	818	CLA	C4D-ND	-3.40	1.33	1.37
23	1	612	CLA	C4D-ND	-3.40	1.33	1.37
23	A	854	CLA	C4D-ND	-3.39	1.33	1.37
23	6	617	CLA	C4D-ND	-3.39	1.33	1.37
23	A	813	CLA	C4D-ND	-3.39	1.33	1.37
23	B	830	CLA	C1D-ND	3.39	1.42	1.37
23	B	811	CLA	C4D-ND	-3.39	1.33	1.37
23	A	835	CLA	C4D-ND	-3.39	1.33	1.37
24	A	844	PQN	C3-C4	-3.38	1.38	1.47
23	A	843	CLA	C4D-ND	-3.38	1.33	1.37
23	A	843	CLA	CMB-C2B	-3.38	1.44	1.51
23	6	602	CLA	C1D-ND	3.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	841	CLA	C4D-ND	-3.38	1.33	1.37
23	6	602	CLA	C4D-ND	-3.38	1.33	1.37
23	A	840	CLA	C4D-ND	-3.38	1.33	1.37
23	A	826	CLA	C4D-ND	-3.38	1.33	1.37
28	K	208	LMU	O5B-C1B	3.38	1.50	1.41
23	B	811	CLA	C1D-ND	3.37	1.41	1.37
23	5	614	CLA	C1D-ND	3.37	1.41	1.37
23	A	832	CLA	C4D-ND	-3.37	1.33	1.37
23	B	833	CLA	C1D-ND	3.37	1.41	1.37
23	a	614	CLA	C1D-ND	3.37	1.41	1.37
23	A	804	CLA	C4D-ND	-3.37	1.33	1.37
23	6	604	CLA	C1D-ND	3.37	1.41	1.37
23	B	826	CLA	C1D-ND	3.37	1.41	1.37
23	6	608	CLA	C1D-ND	3.37	1.41	1.37
23	B	822	CLA	C1D-ND	3.37	1.41	1.37
23	6	611	CLA	C1D-ND	3.37	1.41	1.37
23	B	812	CLA	C4D-ND	-3.36	1.33	1.37
23	3	612	CLA	C1D-ND	3.36	1.41	1.37
23	4	604	CLA	C1D-ND	3.36	1.41	1.37
23	8	612	CLA	C4D-ND	-3.36	1.33	1.37
23	A	817	CLA	C1D-ND	3.36	1.41	1.37
23	a	612	CLA	C4D-ND	-3.36	1.33	1.37
23	6	611	CLA	C4D-ND	-3.36	1.33	1.37
23	4	613	CLA	C1D-ND	3.35	1.41	1.37
23	A	817	CLA	C4D-ND	-3.35	1.33	1.37
23	2	609	CLA	C2D-C1D	3.35	1.48	1.42
23	J	101	CLA	C1D-ND	3.35	1.41	1.37
24	B	842	PQN	C10-C1	-3.35	1.41	1.48
23	B	841	CLA	CHC-C1C	3.35	1.43	1.35
23	4	606	CLA	C1D-ND	3.35	1.41	1.37
23	a	613	CLA	C1D-ND	3.34	1.41	1.37
23	A	823	CLA	C1D-ND	3.34	1.41	1.37
23	A	825	CLA	C1D-ND	3.34	1.41	1.37
23	a	601	CLA	C1D-ND	3.34	1.41	1.37
23	5	610	CLA	C4D-ND	-3.34	1.33	1.37
23	2	610	CLA	C2D-C1D	3.34	1.48	1.42
23	6	604	CLA	C4D-ND	-3.34	1.33	1.37
24	A	844	PQN	C3-C2	3.33	1.41	1.35
23	3	608	CLA	CMB-C2B	-3.33	1.44	1.51
23	A	808	CLA	C1D-ND	3.33	1.41	1.37
23	9	612	CLA	C4D-ND	-3.33	1.33	1.37
23	3	614	CLA	C4D-ND	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	601	CLA	C1D-ND	3.33	1.41	1.37
23	B	804	CLA	C4D-ND	-3.32	1.33	1.37
23	4	613	CLA	C4D-ND	-3.32	1.33	1.37
23	2	616	CLA	C2D-C1D	3.32	1.48	1.42
23	a	603	CLA	C1D-ND	3.32	1.41	1.37
23	6	607	CLA	C4D-ND	-3.32	1.33	1.37
23	B	834	CLA	C1D-ND	3.31	1.41	1.37
23	4	604	CLA	C4D-ND	-3.31	1.33	1.37
23	3	615	CLA	C1D-ND	3.31	1.41	1.37
23	A	825	CLA	C4D-ND	-3.31	1.33	1.37
23	9	604	CLA	C2D-C1D	3.31	1.48	1.42
23	9	603	CLA	C4D-ND	-3.30	1.33	1.37
23	K	203	CLA	C4D-ND	-3.30	1.33	1.37
23	7	610	CLA	C4D-ND	-3.30	1.33	1.37
23	9	606	CLA	C2D-C1D	3.30	1.48	1.42
23	A	836	CLA	C4D-ND	-3.30	1.33	1.37
23	B	815	CLA	C4D-ND	-3.30	1.33	1.37
23	A	837	CLA	C4D-ND	-3.30	1.33	1.37
23	2	613	CLA	C2D-C1D	3.30	1.48	1.42
23	7	609	CLA	C4D-ND	-3.30	1.33	1.37
23	8	604	CLA	C1D-ND	3.30	1.41	1.37
23	B	819	CLA	C4D-ND	-3.29	1.33	1.37
23	3	602	CLA	C4D-ND	-3.29	1.33	1.37
23	7	615	CLA	C4D-ND	-3.29	1.33	1.37
23	5	604	CLA	C4D-ND	-3.29	1.33	1.37
23	B	840	CLA	CMB-C2B	-3.28	1.44	1.51
23	6	616	CLA	CHC-C1C	3.28	1.43	1.35
23	B	838	CLA	C4D-ND	-3.28	1.33	1.37
23	3	606	CLA	C1D-ND	3.28	1.41	1.37
23	B	803	CLA	CMC-C2C	-3.28	1.43	1.50
23	1	613	CLA	C1D-ND	3.28	1.41	1.37
33	6	624	NEX	C7-C8	-3.28	1.26	1.32
23	8	604	CLA	C4D-ND	-3.28	1.33	1.37
23	2	606	CLA	C2D-C1D	3.28	1.48	1.42
23	B	835	CLA	C4D-ND	-3.28	1.33	1.37
23	5	612	CLA	C4D-ND	-3.28	1.33	1.37
23	7	604	CLA	C1D-ND	3.28	1.41	1.37
23	4	607	CLA	C4D-ND	-3.27	1.33	1.37
23	5	619	CLA	C1D-ND	3.27	1.41	1.37
23	6	613	CLA	C4D-ND	-3.27	1.33	1.37
23	5	619	CLA	C4D-ND	-3.27	1.33	1.37
23	9	614	CLA	C2D-C1D	3.27	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	607	CLA	C1D-ND	3.26	1.41	1.37
23	1	616	CLA	C4D-ND	-3.26	1.33	1.37
23	3	610	CLA	C4D-ND	-3.26	1.33	1.37
23	9	607	CLA	C2D-C1D	3.26	1.48	1.42
23	F	301	CLA	CMB-C2B	-3.26	1.44	1.51
23	K	206	CLA	C4D-ND	-3.26	1.33	1.37
28	8	624	LMU	O5'-C1'	3.26	1.50	1.41
23	1	612	CLA	C1D-ND	3.25	1.41	1.37
23	A	801	CLA	C4D-ND	-3.25	1.33	1.37
23	2	611	CLA	C4D-ND	-3.25	1.33	1.37
24	B	842	PQN	C11-C12	3.25	1.55	1.50
23	A	845	CLA	C1D-ND	3.25	1.41	1.37
23	4	609	CLA	C1D-ND	3.25	1.41	1.37
23	A	816	CLA	C4D-ND	-3.24	1.33	1.37
23	A	816	CLA	C1D-ND	3.24	1.41	1.37
23	5	614	CLA	C4D-ND	-3.24	1.33	1.37
23	5	618	CLA	C1D-ND	3.24	1.41	1.37
23	3	606	CLA	C4D-ND	-3.24	1.33	1.37
23	5	618	CLA	C4D-ND	-3.24	1.33	1.37
23	9	613	CLA	C2D-C1D	3.23	1.48	1.42
23	8	610	CLA	C1D-ND	3.23	1.41	1.37
23	7	604	CLA	C4D-ND	-3.23	1.33	1.37
23	A	803	CLA	CMB-C2B	-3.23	1.44	1.51
23	B	817	CLA	CMB-C2B	-3.23	1.44	1.51
23	8	603	CLA	C4D-ND	-3.23	1.33	1.37
23	2	604	CLA	C2D-C1D	3.22	1.48	1.42
23	1	608	CLA	C4D-ND	-3.22	1.33	1.37
23	A	801	CLA	C3B-C2B	-3.22	1.35	1.40
23	B	823	CLA	C4D-ND	-3.22	1.33	1.37
23	2	607	CLA	C2D-C1D	3.22	1.48	1.42
23	B	815	CLA	C1D-ND	3.21	1.41	1.37
23	6	616	CLA	C4D-ND	-3.21	1.33	1.37
28	A	857	LMU	O5'-C1'	3.21	1.50	1.41
23	a	608	CLA	C4D-ND	-3.21	1.33	1.37
23	F	303	CLA	C4D-ND	-3.21	1.33	1.37
23	F	304	CLA	C4D-ND	-3.21	1.33	1.37
23	5	601	CLA	C4D-ND	-3.21	1.33	1.37
23	1	607	CLA	C4D-ND	-3.21	1.33	1.37
23	4	608	CLA	C4D-ND	-3.21	1.33	1.37
23	7	613	CLA	C4D-ND	-3.21	1.33	1.37
23	9	603	CLA	C2D-C1D	3.21	1.48	1.42
23	a	611	CLA	C1D-ND	3.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	607	CLA	C4D-ND	-3.20	1.33	1.37
23	B	816	CLA	C1D-ND	3.20	1.41	1.37
23	5	611	CLA	C4D-ND	-3.20	1.33	1.37
23	a	612	CLA	C1D-ND	3.20	1.41	1.37
23	L	304	CLA	CHC-C1C	3.20	1.43	1.35
23	8	610	CLA	C4D-ND	-3.19	1.33	1.37
23	7	612	CLA	C1D-ND	3.19	1.41	1.37
23	4	602	CLA	C1D-ND	3.19	1.41	1.37
23	2	601	CLA	C2D-C1D	3.19	1.48	1.42
23	3	611	CLA	C1D-ND	3.19	1.41	1.37
23	5	610	CLA	C1D-ND	3.19	1.41	1.37
23	7	610	CLA	C1D-ND	3.19	1.41	1.37
23	9	601	CLA	C2D-C1D	3.19	1.48	1.42
23	3	610	CLA	C1D-ND	3.19	1.41	1.37
23	4	616	CLA	C4D-ND	-3.19	1.33	1.37
23	8	606	CLA	C4D-ND	-3.19	1.33	1.37
23	F	303	CLA	CHC-C1C	3.19	1.43	1.35
23	8	607	CLA	C1D-ND	3.19	1.41	1.37
23	7	616	CLA	C4D-ND	-3.18	1.33	1.37
23	8	609	CLA	CHC-C1C	3.18	1.43	1.35
23	A	815	CLA	C1D-ND	3.18	1.41	1.37
23	L	302	CLA	CHC-C1C	3.18	1.43	1.35
23	A	843	CLA	C1D-ND	3.18	1.41	1.37
23	A	854	CLA	CHC-C1C	3.18	1.43	1.35
23	5	609	CLA	C1D-ND	3.18	1.41	1.37
23	8	609	CLA	C1D-ND	3.18	1.41	1.37
23	3	615	CLA	C4D-ND	-3.18	1.33	1.37
23	4	608	CLA	C1D-ND	3.17	1.41	1.37
23	B	828	CLA	C1D-ND	3.17	1.41	1.37
23	1	611	CLA	C1D-ND	3.17	1.41	1.37
23	6	617	CLA	C1D-ND	3.17	1.41	1.37
23	B	810	CLA	C1D-ND	3.17	1.41	1.37
23	a	616	CLA	C4D-ND	-3.17	1.33	1.37
23	5	617	CLA	CMB-C2B	-3.17	1.45	1.51
23	4	618	CLA	CHC-C1C	3.17	1.43	1.35
23	5	611	CLA	C1D-ND	3.16	1.41	1.37
23	B	816	CLA	C4D-ND	-3.16	1.33	1.37
23	7	607	CLA	C1D-ND	3.16	1.41	1.37
23	a	614	CLA	C4D-ND	-3.16	1.33	1.37
23	8	609	CLA	C4D-ND	-3.16	1.33	1.37
23	B	804	CLA	CHC-C1C	3.16	1.43	1.35
23	A	809	CLA	CHC-C1C	3.16	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	614	CLA	C4D-ND	-3.16	1.33	1.37
23	4	603	CLA	C1D-ND	3.16	1.41	1.37
23	6	607	CLA	C1D-ND	3.16	1.41	1.37
23	1	616	CLA	C1D-ND	3.15	1.41	1.37
23	A	814	CLA	C1D-ND	3.15	1.41	1.37
23	B	824	CLA	C1D-ND	3.15	1.41	1.37
23	5	612	CLA	C1D-ND	3.15	1.41	1.37
23	3	604	CLA	C1D-ND	3.15	1.41	1.37
23	B	813	CLA	C1D-ND	3.15	1.41	1.37
23	1	614	CLA	C4D-ND	-3.15	1.33	1.37
23	4	610	CLA	C4D-ND	-3.15	1.33	1.37
23	2	614	CLA	C2D-C1D	3.15	1.48	1.42
23	5	603	CLA	C1D-ND	3.14	1.41	1.37
23	2	603	CLA	C2D-C1D	3.14	1.48	1.42
24	B	842	PQN	C10-C5	-3.14	1.35	1.40
23	B	824	CLA	C4D-ND	-3.14	1.33	1.37
23	9	611	CLA	C2D-C1D	3.14	1.48	1.42
23	A	805	CLA	CHC-C1C	3.14	1.43	1.35
23	a	607	CLA	C4D-ND	-3.14	1.33	1.37
23	B	827	CLA	C1D-ND	3.14	1.41	1.37
23	2	612	CLA	C2D-C1D	3.14	1.48	1.42
23	5	604	CLA	C1D-ND	3.13	1.41	1.37
23	7	611	CLA	C1D-ND	3.13	1.41	1.37
23	B	824	CLA	CHC-C1C	3.13	1.43	1.35
23	8	607	CLA	C4D-ND	-3.13	1.33	1.37
23	A	811	CLA	C1D-ND	3.13	1.41	1.37
23	6	603	CLA	C1D-ND	3.13	1.41	1.37
23	8	601	CLA	C1D-ND	3.13	1.41	1.37
23	B	822	CLA	C4D-ND	-3.13	1.33	1.37
23	4	618	CLA	C1D-ND	3.13	1.41	1.37
23	B	830	CLA	C4D-ND	-3.12	1.33	1.37
23	3	609	CLA	C4D-ND	-3.12	1.33	1.37
23	8	614	CLA	CHC-C1C	3.12	1.43	1.35
23	3	604	CLA	CMB-C2B	-3.12	1.45	1.51
23	9	612	CLA	C2D-C1D	3.12	1.48	1.42
23	a	613	CLA	C4D-ND	-3.12	1.33	1.37
23	A	840	CLA	C1D-ND	3.12	1.41	1.37
23	4	611	CLA	C4D-ND	-3.12	1.33	1.37
23	7	606	CLA	C4D-ND	-3.11	1.33	1.37
23	B	841	CLA	CMC-C2C	-3.11	1.44	1.50
23	6	606	CLA	C1D-ND	3.11	1.41	1.37
23	J	101	CLA	C4D-ND	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	304	CLA	C4D-ND	-3.11	1.33	1.37
23	A	824	CLA	C1D-ND	3.11	1.41	1.37
23	B	807	CLA	C1D-ND	3.11	1.41	1.37
23	5	603	CLA	CMB-C2B	-3.10	1.45	1.51
23	B	812	CLA	CHC-C1C	3.10	1.42	1.35
23	6	616	CLA	C1D-ND	3.10	1.41	1.37
23	7	612	CLA	CHC-C1C	3.10	1.42	1.35
23	5	616	CLA	C4D-ND	-3.10	1.33	1.37
23	2	614	CLA	C4D-ND	-3.10	1.33	1.37
23	B	809	CLA	CMB-C2B	-3.10	1.45	1.51
23	8	613	CLA	C1D-ND	3.10	1.41	1.37
23	1	613	CLA	C4D-ND	-3.10	1.33	1.37
23	3	611	CLA	C4D-ND	-3.10	1.33	1.37
23	A	803	CLA	C1D-ND	3.10	1.41	1.37
23	9	602	CLA	C2D-C1D	3.10	1.48	1.42
23	8	608	CLA	C1D-ND	3.10	1.41	1.37
23	8	602	CLA	CHC-C1C	3.10	1.42	1.35
23	B	820	CLA	C4D-ND	-3.09	1.33	1.37
23	B	817	CLA	C1D-ND	3.09	1.41	1.37
23	7	602	CLA	CHC-C1C	3.09	1.42	1.35
23	B	830	CLA	CMB-C2B	-3.09	1.45	1.51
23	a	616	CLA	C1D-ND	3.09	1.41	1.37
23	8	612	CLA	C1D-ND	3.09	1.41	1.37
24	B	842	PQN	C3-C2	3.09	1.40	1.35
23	1	610	CLA	CHC-C1C	3.09	1.42	1.35
23	B	832	CLA	C1D-ND	3.09	1.41	1.37
23	A	801	CLA	C1D-ND	3.09	1.41	1.37
24	A	844	PQN	C11-C12	3.09	1.55	1.50
23	8	604	CLA	CHC-C1C	3.09	1.42	1.35
23	4	618	CLA	C4D-ND	-3.09	1.33	1.37
23	A	826	CLA	C1D-ND	3.08	1.41	1.37
23	a	602	CLA	C1D-ND	3.08	1.41	1.37
23	a	610	CLA	CHC-C1C	3.08	1.42	1.35
23	2	602	CLA	C2D-C1D	3.08	1.48	1.42
23	5	608	CLA	C1D-ND	3.08	1.41	1.37
23	A	812	CLA	C1D-ND	3.07	1.41	1.37
23	6	609	CLA	CHC-C1C	3.07	1.42	1.35
23	7	615	CLA	CHC-C1C	3.07	1.42	1.35
23	B	841	CLA	C4D-ND	-3.07	1.33	1.37
23	a	610	CLA	C4D-ND	-3.07	1.33	1.37
23	A	819	CLA	C1D-ND	3.07	1.41	1.37
23	3	609	CLA	C1D-ND	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	611	CLA	C1D-ND	3.06	1.41	1.37
23	6	606	CLA	CHC-C1C	3.06	1.42	1.35
23	9	601	CLA	C4D-ND	-3.06	1.33	1.37
23	F	301	CLA	C3B-C2B	-3.06	1.36	1.40
23	2	602	CLA	C4D-ND	-3.06	1.33	1.37
23	B	813	CLA	CHC-C1C	3.06	1.42	1.35
23	a	606	CLA	CHC-C1C	3.05	1.42	1.35
23	A	822	CLA	CHC-C1C	3.05	1.42	1.35
23	G	204	CLA	CHC-C1C	3.05	1.42	1.35
23	B	831	CLA	C1D-ND	3.05	1.41	1.37
23	3	607	CLA	C1D-ND	3.05	1.41	1.37
23	9	610	CLA	C4D-ND	-3.05	1.33	1.37
23	7	603	CLA	C1D-ND	3.05	1.41	1.37
23	3	613	CLA	C4D-ND	-3.05	1.33	1.37
23	2	610	CLA	C4D-ND	-3.05	1.33	1.37
23	4	604	CLA	CHC-C1C	3.05	1.42	1.35
23	A	820	CLA	C3B-C2B	-3.05	1.36	1.40
23	B	805	CLA	C1D-ND	3.05	1.41	1.37
23	1	606	CLA	CHC-C1C	3.04	1.42	1.35
23	5	601	CLA	C1D-ND	3.04	1.41	1.37
23	6	609	CLA	C1D-ND	3.04	1.41	1.37
23	5	613	CLA	CHC-C1C	3.04	1.42	1.35
23	7	604	CLA	CHC-C1C	3.04	1.42	1.35
23	B	837	CLA	C1D-ND	3.04	1.41	1.37
23	A	842	CLA	C1D-ND	3.04	1.41	1.37
23	7	606	CLA	CMB-C2B	-3.03	1.45	1.51
23	a	604	CLA	C4D-ND	-3.03	1.33	1.37
23	6	618	CLA	CHC-C1C	3.03	1.42	1.35
23	3	611	CLA	CHC-C1C	3.03	1.42	1.35
23	A	839	CLA	C3B-C2B	-3.03	1.36	1.40
23	9	611	CLA	C4D-ND	-3.03	1.33	1.37
23	B	802	CLA	C1D-ND	3.03	1.41	1.37
23	5	604	CLA	CHC-C1C	3.03	1.42	1.35
23	B	827	CLA	CHC-C1C	3.03	1.42	1.35
23	3	613	CLA	C1D-ND	3.03	1.41	1.37
23	3	607	CLA	CHC-C1C	3.03	1.42	1.35
23	1	604	CLA	C4D-ND	-3.03	1.33	1.37
23	4	606	CLA	C4D-ND	-3.03	1.33	1.37
23	A	810	CLA	CHC-C1C	3.02	1.42	1.35
23	2	613	CLA	C4D-ND	-3.02	1.33	1.37
23	1	602	CLA	C1D-ND	3.02	1.41	1.37
23	B	823	CLA	CHC-C1C	3.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	303	CLA	CHC-C1C	3.02	1.42	1.35
23	8	614	CLA	C1D-ND	3.02	1.41	1.37
23	B	839	CLA	CHC-C1C	3.02	1.42	1.35
23	A	839	CLA	CMB-C2B	-3.02	1.45	1.51
23	7	601	CLA	CMB-C2B	-3.02	1.45	1.51
23	9	604	CLA	C4D-ND	-3.02	1.33	1.37
23	F	304	CLA	CHC-C1C	3.02	1.42	1.35
23	5	617	CLA	C1D-ND	3.02	1.41	1.37
23	9	602	CLA	C4D-ND	-3.02	1.33	1.37
23	A	836	CLA	CMB-C2B	-3.02	1.45	1.51
23	6	607	CLA	CHC-C1C	3.02	1.42	1.35
23	5	606	CLA	C1D-ND	3.01	1.41	1.37
23	A	801	CLA	CMB-C2B	-3.01	1.45	1.51
23	B	821	CLA	C4D-ND	-3.01	1.33	1.37
23	B	809	CLA	C1D-ND	3.01	1.41	1.37
23	B	838	CLA	C1D-ND	3.01	1.41	1.37
23	6	601	CLA	C1D-ND	3.01	1.41	1.37
23	7	607	CLA	CHC-C1C	3.01	1.42	1.35
23	5	607	CLA	CHC-C1C	3.01	1.42	1.35
23	A	819	CLA	CHC-C1C	3.01	1.42	1.35
23	2	603	CLA	C4D-ND	-3.01	1.33	1.37
23	A	821	CLA	C1D-ND	3.01	1.41	1.37
23	5	612	CLA	CHC-C1C	3.01	1.42	1.35
23	4	607	CLA	CHC-C1C	3.01	1.42	1.35
23	6	620	CLA	CHC-C1C	3.01	1.42	1.35
23	A	830	CLA	C1D-ND	3.01	1.41	1.37
23	A	802	CLA	CHC-C1C	3.01	1.42	1.35
23	B	840	CLA	C3B-C2B	-3.01	1.36	1.40
23	7	610	CLA	CHC-C1C	3.01	1.42	1.35
23	5	608	CLA	CHC-C1C	3.00	1.42	1.35
23	B	829	CLA	CMD-C2D	-3.00	1.44	1.50
23	2	606	CLA	C4D-ND	-3.00	1.33	1.37
23	1	610	CLA	C4D-ND	-3.00	1.33	1.37
23	A	820	CLA	C1D-ND	3.00	1.41	1.37
23	B	816	CLA	CHC-C1C	3.00	1.42	1.35
23	A	842	CLA	CMB-C2B	-3.00	1.45	1.51
30	B	850	DGD	O2G-C2G	-3.00	1.39	1.46
23	B	803	CLA	CHC-C1C	3.00	1.42	1.35
23	B	828	CLA	CHC-C1C	3.00	1.42	1.35
23	4	616	CLA	CHC-C1C	3.00	1.42	1.35
23	4	608	CLA	CHC-C1C	2.99	1.42	1.35
23	2	607	CLA	C4D-ND	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	602	CLA	CMB-C2B	-2.99	1.45	1.51
23	2	611	CLA	C2D-C1D	2.99	1.48	1.42
23	3	617	CLA	CHC-C1C	2.99	1.42	1.35
23	A	829	CLA	CHC-C1C	2.99	1.42	1.35
23	6	612	CLA	C4D-ND	-2.99	1.33	1.37
23	9	609	CLA	C4D-ND	-2.99	1.33	1.37
23	B	821	CLA	CHC-C1C	2.98	1.42	1.35
23	5	610	CLA	CHC-C1C	2.98	1.42	1.35
23	a	613	CLA	CHC-C1C	2.98	1.42	1.35
23	J	101	CLA	CHC-C1C	2.98	1.42	1.35
23	B	819	CLA	CMB-C2B	-2.98	1.45	1.51
23	6	614	CLA	CHC-C1C	2.98	1.42	1.35
23	9	610	CLA	C2D-C1D	2.98	1.48	1.42
23	K	206	CLA	CHC-C1C	2.98	1.42	1.35
23	8	610	CLA	CHC-C1C	2.98	1.42	1.35
23	8	613	CLA	CHC-C1C	2.98	1.42	1.35
23	4	602	CLA	CHC-C1C	2.98	1.42	1.35
23	5	614	CLA	CHC-C1C	2.98	1.42	1.35
23	A	819	CLA	CMB-C2B	-2.98	1.45	1.51
23	2	604	CLA	C4D-ND	-2.97	1.33	1.37
23	B	837	CLA	CHC-C1C	2.97	1.42	1.35
23	6	603	CLA	CHC-C1C	2.97	1.42	1.35
23	5	618	CLA	CHC-C1C	2.97	1.42	1.35
23	3	603	CLA	CMB-C2B	-2.97	1.45	1.51
23	6	618	CLA	C1D-ND	2.97	1.41	1.37
23	6	610	CLA	CHC-C1C	2.97	1.42	1.35
23	G	203	CLA	C4D-ND	-2.97	1.33	1.37
23	5	604	CLA	CMB-C2B	-2.97	1.45	1.51
23	B	820	CLA	CHC-C1C	2.96	1.42	1.35
23	1	613	CLA	CHC-C1C	2.96	1.42	1.35
23	a	611	CLA	C4D-ND	-2.96	1.33	1.37
23	A	833	CLA	CHC-C1C	2.96	1.42	1.35
23	4	609	CLA	CHC-C1C	2.96	1.42	1.35
23	4	611	CLA	CHC-C1C	2.96	1.42	1.35
23	7	606	CLA	CHC-C1C	2.96	1.42	1.35
23	1	611	CLA	C4D-ND	-2.96	1.33	1.37
23	7	616	CLA	C1D-ND	2.96	1.41	1.37
23	4	612	CLA	CHC-C1C	2.96	1.42	1.35
23	G	203	CLA	CHC-C1C	2.96	1.42	1.35
23	B	839	CLA	C1D-ND	2.95	1.41	1.37
23	7	614	CLA	C1D-ND	2.95	1.41	1.37
23	G	204	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	602	CLA	CHC-C1C	2.95	1.42	1.35
23	A	818	CLA	C1D-ND	2.95	1.41	1.37
23	3	608	CLA	C1D-ND	2.95	1.41	1.37
23	K	204	CLA	CHC-C1C	2.95	1.42	1.35
23	5	611	CLA	CHC-C1C	2.95	1.42	1.35
23	6	610	CLA	C1D-ND	2.95	1.41	1.37
23	4	612	CLA	C4D-ND	-2.95	1.33	1.37
23	6	612	CLA	CHC-C1C	2.95	1.42	1.35
23	A	802	CLA	CMD-C2D	-2.95	1.44	1.50
23	A	837	CLA	CHC-C1C	2.95	1.42	1.35
23	A	813	CLA	CHC-C1C	2.95	1.42	1.35
23	7	608	CLA	C1D-ND	2.95	1.41	1.37
23	A	839	CLA	C1D-ND	2.95	1.41	1.37
23	B	817	CLA	C3B-C2B	-2.95	1.36	1.40
23	1	607	CLA	CHC-C1C	2.95	1.42	1.35
23	B	835	CLA	CHC-C1C	2.95	1.42	1.35
23	4	603	CLA	CHC-C1C	2.95	1.42	1.35
23	6	620	CLA	C1D-ND	2.95	1.41	1.37
23	A	817	CLA	CMB-C2B	-2.94	1.45	1.51
23	A	831	CLA	C3B-C2B	-2.94	1.36	1.40
23	A	827	CLA	CHC-C1C	2.94	1.42	1.35
23	1	608	CLA	CHC-C1C	2.94	1.42	1.35
23	3	602	CLA	C1D-ND	2.94	1.41	1.37
23	9	614	CLA	C4D-ND	-2.94	1.33	1.37
23	a	608	CLA	CHC-C1C	2.94	1.42	1.35
23	2	601	CLA	C4D-ND	-2.94	1.33	1.37
25	A	847	LHG	O7-C5	-2.94	1.39	1.46
23	B	806	CLA	C1D-ND	2.94	1.41	1.37
23	A	805	CLA	CMB-C2B	-2.94	1.45	1.51
23	8	602	CLA	C1D-ND	2.93	1.41	1.37
23	A	827	CLA	C1D-ND	2.93	1.41	1.37
25	A	846	LHG	O7-C5	-2.93	1.39	1.46
23	B	828	CLA	CMB-C2B	-2.93	1.45	1.51
23	B	807	CLA	CHC-C1C	2.93	1.42	1.35
23	a	607	CLA	CHC-C1C	2.93	1.42	1.35
23	5	602	CLA	CHC-C1C	2.93	1.42	1.35
23	A	836	CLA	CHC-C1C	2.93	1.42	1.35
23	5	609	CLA	CHC-C1C	2.93	1.42	1.35
23	A	808	CLA	CHC-C1C	2.93	1.42	1.35
23	A	815	CLA	CHC-C1C	2.93	1.42	1.35
23	A	836	CLA	C1D-ND	2.93	1.41	1.37
23	6	601	CLA	CHC-C1C	2.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	613	CLA	CHC-C1C	2.92	1.42	1.35
23	9	607	CLA	C4D-ND	-2.92	1.33	1.37
23	3	613	CLA	CHC-C1C	2.92	1.42	1.35
23	3	609	CLA	CMB-C2B	-2.92	1.45	1.51
23	B	826	CLA	CHC-C1C	2.92	1.42	1.35
23	K	203	CLA	CHC-C1C	2.91	1.42	1.35
23	6	613	CLA	CHC-C1C	2.91	1.42	1.35
23	B	819	CLA	CHC-C1C	2.91	1.42	1.35
23	A	833	CLA	C1D-ND	2.91	1.41	1.37
23	A	810	CLA	CMD-C2D	-2.91	1.44	1.50
23	5	606	CLA	C3B-C2B	-2.91	1.36	1.40
23	1	602	CLA	CHC-C1C	2.90	1.42	1.35
23	5	616	CLA	CHC-C1C	2.90	1.42	1.35
23	a	616	CLA	CHC-C1C	2.90	1.42	1.35
23	1	614	CLA	CHC-C1C	2.90	1.42	1.35
23	A	822	CLA	CMB-C2B	-2.90	1.45	1.51
23	6	608	CLA	CMB-C2B	-2.90	1.45	1.51
23	A	832	CLA	CMB-C2B	-2.90	1.45	1.51
23	a	602	CLA	CHC-C1C	2.90	1.42	1.35
23	a	606	CLA	C4D-ND	-2.90	1.33	1.37
23	a	614	CLA	CHC-C1C	2.90	1.42	1.35
23	A	802	CLA	MG-ND	-2.90	2.00	2.05
23	B	822	CLA	CHC-C1C	2.89	1.42	1.35
23	a	612	CLA	CHC-C1C	2.89	1.42	1.35
23	A	811	CLA	CHC-C1C	2.89	1.42	1.35
23	7	614	CLA	CHC-C1C	2.89	1.42	1.35
23	8	612	CLA	CHC-C1C	2.89	1.42	1.35
23	B	840	CLA	C1D-ND	2.89	1.41	1.37
23	K	201	CLA	C4D-ND	-2.89	1.33	1.37
23	7	616	CLA	CMD-C2D	-2.89	1.44	1.50
23	7	611	CLA	CMB-C2B	-2.89	1.45	1.51
23	A	813	CLA	C1D-ND	2.89	1.41	1.37
23	1	616	CLA	CHC-C1C	2.89	1.42	1.35
23	7	609	CLA	C1D-ND	2.89	1.41	1.37
23	1	604	CLA	CHC-C1C	2.89	1.42	1.35
23	6	604	CLA	CHC-C1C	2.89	1.42	1.35
23	B	825	CLA	CHC-C1C	2.88	1.42	1.35
23	1	606	CLA	C4D-ND	-2.88	1.33	1.37
23	3	604	CLA	CHC-C1C	2.88	1.42	1.35
23	5	601	CLA	CHC-C1C	2.88	1.42	1.35
23	A	834	CLA	C1D-ND	2.88	1.41	1.37
23	A	827	CLA	CMD-C2D	-2.88	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	609	CLA	CHC-C1C	2.88	1.42	1.35
23	8	603	CLA	CHC-C1C	2.88	1.42	1.35
23	A	816	CLA	CHC-C1C	2.88	1.42	1.35
23	4	606	CLA	CMB-C2B	-2.88	1.45	1.51
23	4	614	CLA	CHC-C1C	2.88	1.42	1.35
23	A	822	CLA	C1D-ND	2.88	1.41	1.37
23	A	841	CLA	C1D-ND	2.88	1.41	1.37
23	5	602	CLA	C1D-ND	2.88	1.41	1.37
23	3	608	CLA	CHC-C1C	2.88	1.42	1.35
23	B	831	CLA	CHC-C1C	2.88	1.42	1.35
23	1	609	CLA	CHC-C1C	2.88	1.42	1.35
23	a	601	CLA	CHC-C1C	2.88	1.42	1.35
23	1	612	CLA	CHC-C1C	2.88	1.42	1.35
23	3	617	CLA	C1D-ND	2.88	1.41	1.37
23	B	814	CLA	CHC-C1C	2.87	1.42	1.35
23	A	811	CLA	CMB-C2B	-2.87	1.45	1.51
23	9	606	CLA	C4D-ND	-2.87	1.33	1.37
23	a	604	CLA	CHC-C1C	2.87	1.42	1.35
23	9	612	CLA	CAD-C3D	-2.87	1.45	1.50
23	B	829	CLA	C3B-C2B	-2.87	1.36	1.40
23	A	806	CLA	C1D-ND	2.87	1.41	1.37
23	B	834	CLA	CHC-C1C	2.87	1.42	1.35
23	9	609	CLA	C2D-C1D	2.87	1.47	1.42
23	B	805	CLA	CHC-C1C	2.87	1.42	1.35
23	B	815	CLA	CHC-C1C	2.87	1.42	1.35
23	7	609	CLA	CHC-C1C	2.87	1.42	1.35
23	8	602	CLA	CMB-C2B	-2.87	1.45	1.51
23	8	608	CLA	CHC-C1C	2.87	1.42	1.35
23	3	606	CLA	CHC-C1C	2.87	1.42	1.35
23	4	609	CLA	C4D-ND	-2.87	1.33	1.37
23	B	835	CLA	CMB-C2B	-2.87	1.45	1.51
23	3	614	CLA	CHC-C1C	2.87	1.42	1.35
23	8	601	CLA	CHC-C1C	2.87	1.42	1.35
23	6	611	CLA	CHC-C1C	2.86	1.42	1.35
23	3	615	CLA	CMB-C2B	-2.86	1.45	1.51
23	A	825	CLA	CHC-C1C	2.85	1.42	1.35
23	A	814	CLA	CHC-C1C	2.85	1.42	1.35
23	5	606	CLA	CHC-C1C	2.85	1.42	1.35
23	B	818	CLA	CMB-C2B	-2.85	1.45	1.51
23	5	616	CLA	CMB-C2B	-2.85	1.45	1.51
23	3	612	CLA	C3B-C2B	-2.85	1.36	1.40
23	A	807	CLA	CMB-C2B	-2.85	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	606	CLA	CHC-C1C	2.85	1.42	1.35
23	A	840	CLA	CHC-C1C	2.85	1.42	1.35
23	7	608	CLA	CHC-C1C	2.85	1.42	1.35
23	B	839	CLA	CMB-C2B	-2.85	1.45	1.51
23	2	609	CLA	C4D-ND	-2.85	1.33	1.37
23	A	801	CLA	CMD-C2D	-2.85	1.44	1.50
23	A	835	CLA	CMB-C2B	-2.85	1.45	1.51
23	A	817	CLA	CHC-C1C	2.84	1.42	1.35
23	6	609	CLA	CMB-C2B	-2.84	1.45	1.51
23	1	609	CLA	C4D-ND	-2.84	1.33	1.37
23	5	602	CLA	CMD-C2D	-2.84	1.44	1.50
23	9	613	CLA	C4D-ND	-2.84	1.33	1.37
23	6	603	CLA	CMB-C2B	-2.84	1.45	1.51
23	3	617	CLA	CMB-C2B	-2.84	1.45	1.51
23	B	829	CLA	C1D-ND	2.84	1.41	1.37
23	1	601	CLA	CHC-C1C	2.84	1.42	1.35
23	7	616	CLA	CHC-C1C	2.84	1.42	1.35
23	B	838	CLA	CMB-C2B	-2.84	1.45	1.51
23	A	832	CLA	CMD-C2D	-2.84	1.44	1.50
23	A	826	CLA	CHC-C1C	2.84	1.42	1.35
23	A	830	CLA	CMB-C2B	-2.84	1.45	1.51
23	B	804	CLA	C1D-ND	2.83	1.41	1.37
23	7	601	CLA	C3B-C2B	-2.83	1.36	1.40
23	B	825	CLA	CMD-C2D	-2.83	1.44	1.50
23	7	602	CLA	C1D-ND	2.83	1.41	1.37
23	L	303	CLA	C1D-ND	2.83	1.41	1.37
23	B	811	CLA	CHC-C1C	2.82	1.42	1.35
23	5	601	CLA	CMD-C2D	-2.82	1.44	1.50
23	4	601	CLA	CHC-C1C	2.82	1.42	1.35
23	A	845	CLA	CHC-C1C	2.82	1.42	1.35
23	A	835	CLA	C3B-C2B	-2.82	1.36	1.40
23	4	606	CLA	CHC-C1C	2.82	1.42	1.35
23	4	610	CLA	CHC-C1C	2.82	1.42	1.35
23	A	839	CLA	CHC-C1C	2.82	1.42	1.35
23	6	617	CLA	CHC-C1C	2.82	1.42	1.35
23	6	608	CLA	CHC-C1C	2.82	1.42	1.35
23	a	609	CLA	C4D-ND	-2.82	1.33	1.37
24	A	844	PQN	C10-C5	-2.82	1.36	1.40
23	3	609	CLA	CHC-C1C	2.81	1.42	1.35
23	6	602	CLA	CHC-C1C	2.81	1.42	1.35
23	B	806	CLA	CHC-C1C	2.81	1.42	1.35
23	8	603	CLA	CMB-C2B	-2.81	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	810	CLA	CMB-C2B	-2.81	1.45	1.51
23	5	607	CLA	CMC-C2C	-2.81	1.44	1.50
23	A	813	CLA	CMB-C2B	-2.81	1.45	1.51
23	3	603	CLA	C1D-ND	2.80	1.41	1.37
23	A	818	CLA	CHC-C1C	2.80	1.42	1.35
23	B	833	CLA	CHC-C1C	2.80	1.42	1.35
23	7	603	CLA	CHC-C1C	2.80	1.42	1.35
23	5	619	CLA	CMB-C2B	-2.80	1.45	1.51
23	A	841	CLA	CHC-C1C	2.80	1.42	1.35
23	B	834	CLA	CMB-C2B	-2.80	1.45	1.51
23	5	603	CLA	CHC-C1C	2.80	1.42	1.35
23	A	812	CLA	CMB-C2B	-2.79	1.45	1.51
23	8	611	CLA	CHC-C1C	2.79	1.42	1.35
23	B	808	CLA	CHC-C1C	2.79	1.42	1.35
23	8	616	CLA	CHC-C1C	2.79	1.42	1.35
23	4	613	CLA	CHC-C1C	2.79	1.42	1.35
23	B	813	CLA	CMB-C2B	-2.79	1.45	1.51
23	B	814	CLA	CMB-C2B	-2.79	1.45	1.51
23	5	613	CLA	C1D-ND	2.79	1.41	1.37
23	B	830	CLA	C3B-C2B	-2.79	1.36	1.40
23	B	832	CLA	CHC-C1C	2.79	1.42	1.35
23	B	802	CLA	CHC-C1C	2.78	1.42	1.35
23	2	611	CLA	CAD-C3D	-2.78	1.45	1.50
23	B	811	CLA	CMB-C2B	-2.78	1.45	1.51
23	A	802	CLA	CMB-C2B	-2.78	1.45	1.51
23	A	828	CLA	CMB-C2B	-2.78	1.45	1.51
23	B	817	CLA	CHC-C1C	2.78	1.42	1.35
23	1	611	CLA	CHC-C1C	2.78	1.42	1.35
23	A	843	CLA	C3B-C2B	-2.78	1.36	1.40
23	A	840	CLA	CMB-C2B	-2.77	1.45	1.51
23	3	602	CLA	CMB-C2B	-2.77	1.45	1.51
23	a	611	CLA	CHC-C1C	2.77	1.42	1.35
23	2	616	CLA	C4D-ND	-2.77	1.33	1.37
23	B	807	CLA	CMB-C2B	-2.77	1.45	1.51
23	6	604	CLA	CMB-C2B	-2.77	1.45	1.51
23	B	808	CLA	CMB-C2B	-2.77	1.45	1.51
23	4	604	CLA	CMB-C2B	-2.77	1.45	1.51
23	8	613	CLA	CMB-C2B	-2.77	1.45	1.51
23	6	613	CLA	C1D-ND	2.77	1.41	1.37
23	A	826	CLA	CMB-C2B	-2.77	1.45	1.51
23	B	836	CLA	CHC-C1C	2.77	1.42	1.35
23	A	814	CLA	CMB-C2B	-2.76	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	807	CLA	CHC-C1C	2.76	1.42	1.35
23	A	832	CLA	C1D-ND	2.76	1.41	1.37
23	a	604	CLA	CMB-C2B	-2.76	1.45	1.51
23	K	201	CLA	CHC-C1C	2.75	1.42	1.35
23	1	604	CLA	CMB-C2B	-2.75	1.45	1.51
23	5	606	CLA	CMB-C2B	-2.75	1.45	1.51
23	B	837	CLA	CMB-C2B	-2.75	1.45	1.51
23	4	618	CLA	CMB-C2B	-2.75	1.45	1.51
23	B	808	CLA	CMD-C2D	-2.75	1.45	1.50
23	A	834	CLA	C3B-C2B	-2.75	1.36	1.40
23	3	615	CLA	CHC-C1C	2.75	1.42	1.35
23	9	611	CLA	CAD-C3D	-2.75	1.45	1.50
23	B	810	CLA	CHC-C1C	2.75	1.42	1.35
23	A	837	CLA	CMB-C2B	-2.75	1.45	1.51
23	B	804	CLA	CMB-C2B	-2.75	1.45	1.51
23	A	809	CLA	C1D-ND	2.74	1.41	1.37
23	4	601	CLA	CMB-C2B	-2.74	1.45	1.51
23	8	607	CLA	CHC-C1C	2.74	1.42	1.35
23	3	613	CLA	CMB-C2B	-2.74	1.45	1.51
23	A	823	CLA	CHC-C1C	2.74	1.42	1.35
23	3	606	CLA	CMB-C2B	-2.74	1.45	1.51
23	7	601	CLA	CHC-C1C	2.74	1.42	1.35
23	A	802	CLA	C3B-C2B	-2.74	1.36	1.40
23	A	804	CLA	CHC-C1C	2.74	1.42	1.35
23	7	615	CLA	CMB-C2B	-2.73	1.46	1.51
23	A	831	CLA	C1D-ND	2.73	1.41	1.37
23	3	612	CLA	CHC-C1C	2.73	1.42	1.35
23	A	803	CLA	C3B-C2B	-2.73	1.36	1.40
23	1	610	CLA	CMB-C2B	-2.72	1.46	1.51
23	K	206	CLA	CMB-C2B	-2.72	1.46	1.51
23	8	611	CLA	CMB-C2B	-2.72	1.46	1.51
23	B	829	CLA	MG-ND	-2.72	2.00	2.05
23	3	610	CLA	CHC-C1C	2.72	1.41	1.35
23	2	612	CLA	CAD-C3D	-2.72	1.45	1.50
23	7	603	CLA	CMB-C2B	-2.72	1.46	1.51
23	A	819	CLA	CMD-C2D	-2.72	1.45	1.50
23	A	832	CLA	C3B-C2B	-2.72	1.36	1.40
23	7	604	CLA	CMB-C2B	-2.72	1.46	1.51
23	L	302	CLA	C4D-ND	-2.72	1.34	1.37
23	6	609	CLA	C4D-ND	-2.72	1.34	1.37
23	A	804	CLA	C1D-ND	2.71	1.41	1.37
23	A	816	CLA	CMB-C2B	-2.71	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	842	PQN	C5-C4	-2.71	1.43	1.48
23	A	804	CLA	CMD-C2D	-2.71	1.45	1.50
23	3	602	CLA	CMD-C2D	-2.71	1.45	1.50
23	9	606	CLA	CAD-C3D	-2.71	1.45	1.50
23	3	612	CLA	CMB-C2B	-2.71	1.46	1.51
23	4	613	CLA	CMB-C2B	-2.71	1.46	1.51
23	B	812	CLA	CMB-C2B	-2.71	1.46	1.51
23	A	827	CLA	CMB-C2B	-2.71	1.46	1.51
23	A	833	CLA	CMB-C2B	-2.71	1.46	1.51
23	3	610	CLA	CMB-C2B	-2.70	1.46	1.51
23	B	830	CLA	CHC-C1C	2.70	1.41	1.35
23	A	842	CLA	CHC-C1C	2.70	1.41	1.35
30	B	850	DGD	O3D-C3D	-2.70	1.36	1.43
23	B	838	CLA	CHC-C1C	2.70	1.41	1.35
23	9	607	CLA	CAD-C3D	-2.70	1.45	1.50
23	5	609	CLA	CMB-C2B	-2.70	1.46	1.51
23	7	608	CLA	CMB-C2B	-2.70	1.46	1.51
23	5	606	CLA	C3B-CAB	-2.70	1.42	1.47
23	A	831	CLA	CMD-C2D	-2.70	1.45	1.50
23	B	826	CLA	CMB-C2B	-2.70	1.46	1.51
23	A	808	CLA	CMB-C2B	-2.69	1.46	1.51
24	A	844	PQN	C10-C1	-2.69	1.43	1.48
23	8	616	CLA	CMB-C2B	-2.69	1.46	1.51
23	A	841	CLA	CMB-C2B	-2.69	1.46	1.51
23	a	610	CLA	CMB-C2B	-2.69	1.46	1.51
23	A	809	CLA	CMB-C2B	-2.68	1.46	1.51
31	7	619	LUT	C22-C21	-2.68	1.51	1.54
23	A	807	CLA	MG-ND	-2.68	2.00	2.05
23	A	838	CLA	C1D-ND	2.68	1.41	1.37
23	A	824	CLA	CHC-C1C	2.68	1.41	1.35
23	5	613	CLA	CMB-C2B	-2.68	1.46	1.51
23	a	616	CLA	CMD-C2D	-2.68	1.45	1.50
23	A	824	CLA	CMB-C2B	-2.68	1.46	1.51
23	B	814	CLA	C1D-ND	2.68	1.41	1.37
23	B	824	CLA	CMD-C2D	-2.68	1.45	1.50
23	9	609	CLA	CAD-C3D	-2.68	1.45	1.50
23	9	603	CLA	CAD-C3D	-2.68	1.45	1.50
23	K	204	CLA	CMB-C2B	-2.67	1.46	1.51
23	B	808	CLA	C1D-ND	2.67	1.41	1.37
23	A	825	CLA	CMB-C2B	-2.67	1.46	1.51
23	B	833	CLA	CMB-C2B	-2.67	1.46	1.51
23	1	616	CLA	CMD-C2D	-2.67	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	617	CLA	C3B-C2B	-2.67	1.36	1.40
23	A	801	CLA	CHC-C1C	2.67	1.41	1.35
23	A	803	CLA	CHC-C1C	2.67	1.41	1.35
23	A	812	CLA	CHC-C1C	2.67	1.41	1.35
23	A	834	CLA	CMB-C2B	-2.67	1.46	1.51
23	9	604	CLA	CAD-C3D	-2.67	1.45	1.50
23	A	830	CLA	C3B-C2B	-2.67	1.36	1.40
23	8	606	CLA	CMB-C2B	-2.67	1.46	1.51
23	A	828	CLA	CHC-C1C	2.66	1.41	1.35
23	2	603	CLA	CAD-C3D	-2.66	1.45	1.50
23	A	821	CLA	CMB-C2B	-2.66	1.46	1.51
23	B	809	CLA	CHC-C1C	2.66	1.41	1.35
30	J	103	DGD	C4E-C5E	2.66	1.58	1.53
23	B	802	CLA	C3B-C2B	-2.66	1.36	1.40
23	2	614	CLA	CAD-C3D	-2.66	1.45	1.50
23	A	821	CLA	CMD-C2D	-2.65	1.45	1.50
23	A	823	CLA	CMB-C2B	-2.65	1.46	1.51
23	A	832	CLA	CHC-C1C	2.65	1.41	1.35
23	1	607	CLA	CMB-C2B	-2.65	1.46	1.51
23	A	807	CLA	C1D-ND	2.65	1.41	1.37
23	7	613	CLA	CMB-C2B	-2.65	1.46	1.51
23	2	609	CLA	CAD-C3D	-2.65	1.45	1.50
23	A	802	CLA	C3B-CAB	-2.65	1.42	1.47
23	B	806	CLA	CMB-C2B	-2.65	1.46	1.51
24	A	844	PQN	C11-C3	2.65	1.55	1.51
23	6	617	CLA	CMB-C2B	-2.65	1.46	1.51
23	A	810	CLA	CMB-C2B	-2.64	1.46	1.51
23	F	303	CLA	CMB-C2B	-2.64	1.46	1.51
23	L	303	CLA	CMB-C2B	-2.64	1.46	1.51
23	A	838	CLA	CHC-C1C	2.64	1.41	1.35
23	B	818	CLA	CHC-C1C	2.64	1.41	1.35
23	A	831	CLA	MG-ND	-2.64	2.00	2.05
23	A	820	CLA	CMC-C2C	-2.64	1.45	1.50
23	9	602	CLA	CAD-C3D	-2.64	1.45	1.50
23	B	840	CLA	CHC-C1C	2.64	1.41	1.35
23	3	607	CLA	CMB-C2B	-2.64	1.46	1.51
23	A	806	CLA	CMC-C2C	-2.64	1.45	1.50
23	7	611	CLA	CHC-C1C	2.64	1.41	1.35
23	A	845	CLA	CMB-C2B	-2.64	1.46	1.51
23	9	614	CLA	CAD-C3D	-2.64	1.45	1.50
23	4	610	CLA	CMB-C2B	-2.64	1.46	1.51
23	4	614	CLA	CMB-C2B	-2.64	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	601	CLA	CMD-C2D	-2.64	1.45	1.50
23	B	802	CLA	CMB-C2B	-2.64	1.46	1.51
23	B	815	CLA	CMB-C2B	-2.64	1.46	1.51
23	K	203	CLA	CMB-C2B	-2.63	1.46	1.51
23	2	601	CLA	CAD-C3D	-2.63	1.45	1.50
23	A	806	CLA	CMB-C2B	-2.63	1.46	1.51
23	B	829	CLA	CHC-C1C	2.63	1.41	1.35
23	A	805	CLA	C1D-ND	2.63	1.41	1.37
23	2	607	CLA	CAD-C3D	-2.63	1.45	1.50
23	a	606	CLA	CMB-C2B	-2.63	1.46	1.51
23	1	601	CLA	CMB-C2B	-2.63	1.46	1.51
23	a	613	CLA	CMB-C2B	-2.63	1.46	1.51
23	4	601	CLA	C1D-ND	2.62	1.41	1.37
23	A	834	CLA	CHC-C1C	2.62	1.41	1.35
23	a	607	CLA	CMB-C2B	-2.62	1.46	1.51
23	F	301	CLA	C1D-ND	2.62	1.41	1.37
23	a	609	CLA	CMB-C2B	-2.62	1.46	1.51
23	B	802	CLA	CMC-C2C	-2.62	1.45	1.50
23	1	606	CLA	CMB-C2B	-2.62	1.46	1.51
23	J	101	CLA	CMB-C2B	-2.61	1.46	1.51
23	1	603	CLA	CMB-C2B	-2.61	1.46	1.51
23	3	614	CLA	CMB-C2B	-2.61	1.46	1.51
23	5	610	CLA	CMC-C2C	-2.61	1.45	1.50
32	3	619	XAT	O4-C5	-2.61	1.42	1.46
23	1	609	CLA	CMB-C2B	-2.61	1.46	1.51
23	a	601	CLA	CMB-C2B	-2.61	1.46	1.51
23	A	804	CLA	CMB-C2B	-2.61	1.46	1.51
23	4	603	CLA	CMB-C2B	-2.61	1.46	1.51
23	B	833	CLA	CMC-C2C	-2.61	1.45	1.50
23	B	828	CLA	CMD-C2D	-2.61	1.45	1.50
23	a	603	CLA	CMB-C2B	-2.60	1.46	1.51
23	7	614	CLA	CMB-C2B	-2.60	1.46	1.51
23	5	611	CLA	CMB-C2B	-2.60	1.46	1.51
23	8	607	CLA	CMB-C2B	-2.60	1.46	1.51
23	6	607	CLA	CMB-C2B	-2.60	1.46	1.51
23	1	613	CLA	CMB-C2B	-2.60	1.46	1.51
23	A	806	CLA	CHC-C1C	2.60	1.41	1.35
23	2	606	CLA	CAD-C3D	-2.60	1.45	1.50
23	4	607	CLA	CMB-C2B	-2.60	1.46	1.51
23	1	611	CLA	CMB-C2B	-2.59	1.46	1.51
23	B	802	CLA	CMD-C2D	-2.59	1.45	1.50
23	2	602	CLA	CAD-C3D	-2.59	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	603	CLA	CHC-C1C	2.59	1.41	1.35
23	a	616	CLA	CMB-C2B	-2.59	1.46	1.51
23	5	610	CLA	CMB-C2B	-2.59	1.46	1.51
23	A	842	CLA	C3B-C2B	-2.59	1.36	1.40
23	a	602	CLA	CMB-C2B	-2.59	1.46	1.51
23	1	616	CLA	CMB-C2B	-2.59	1.46	1.51
23	6	613	CLA	CMB-C2B	-2.59	1.46	1.51
23	1	603	CLA	CHC-C1C	2.59	1.41	1.35
29	5	626	LMG	O7-C8	-2.59	1.40	1.46
23	4	609	CLA	C3B-C2B	-2.59	1.36	1.40
23	A	821	CLA	CHC-C1C	2.59	1.41	1.35
23	4	611	CLA	CMB-C2B	-2.58	1.46	1.51
23	2	613	CLA	CAD-C3D	-2.58	1.45	1.50
23	7	608	CLA	C3B-C2B	-2.58	1.36	1.40
23	A	803	CLA	MG-ND	-2.58	2.00	2.05
23	8	604	CLA	CMB-C2B	-2.58	1.46	1.51
23	A	843	CLA	CHC-C1C	2.58	1.41	1.35
23	A	838	CLA	CMB-C2B	-2.58	1.46	1.51
23	9	601	CLA	CAD-C3D	-2.58	1.45	1.50
23	A	818	CLA	CMB-C2B	-2.58	1.46	1.51
23	B	827	CLA	CMB-C2B	-2.58	1.46	1.51
23	2	604	CLA	CAD-C3D	-2.57	1.45	1.50
23	6	601	CLA	CMB-C2B	-2.57	1.46	1.51
23	B	822	CLA	CMB-C2B	-2.57	1.46	1.51
23	B	808	CLA	C3B-C2B	-2.57	1.36	1.40
23	7	601	CLA	C1D-ND	2.57	1.40	1.37
23	7	610	CLA	CMB-C2B	-2.56	1.46	1.51
23	8	612	CLA	CMB-C2B	-2.56	1.46	1.51
23	4	609	CLA	CMB-C2B	-2.56	1.46	1.51
23	A	820	CLA	CHC-C1C	2.56	1.41	1.35
23	1	602	CLA	CMB-C2B	-2.56	1.46	1.51
23	B	836	CLA	CMC-C2C	-2.56	1.45	1.50
23	3	608	CLA	MG-ND	-2.56	2.00	2.05
23	6	612	CLA	CMB-C2B	-2.56	1.46	1.51
23	B	821	CLA	CMB-C2B	-2.56	1.46	1.51
23	5	614	CLA	CMB-C2B	-2.56	1.46	1.51
23	B	825	CLA	CMB-C2B	-2.56	1.46	1.51
23	6	611	CLA	CMB-C2B	-2.56	1.46	1.51
29	4	624	LMG	C4-C5	2.56	1.58	1.53
23	B	825	CLA	MG-ND	-2.55	2.00	2.05
23	B	808	CLA	CMC-C2C	-2.55	1.45	1.50
23	6	602	CLA	CMB-C2B	-2.55	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	616	CLA	CAD-C3D	-2.55	1.45	1.50
23	7	609	CLA	CMB-C2B	-2.55	1.46	1.51
23	A	835	CLA	CHC-C1C	2.55	1.41	1.35
23	B	803	CLA	CMB-C2B	-2.55	1.46	1.51
23	6	616	CLA	CMB-C2B	-2.55	1.46	1.51
23	A	829	CLA	CMB-C2B	-2.55	1.46	1.51
23	3	611	CLA	CMB-C2B	-2.55	1.46	1.51
23	a	611	CLA	CMB-C2B	-2.55	1.46	1.51
23	A	854	CLA	C1D-ND	2.55	1.40	1.37
23	9	613	CLA	CAD-C3D	-2.54	1.45	1.50
23	5	608	CLA	CMB-C2B	-2.54	1.46	1.51
23	6	618	CLA	CMB-C2B	-2.54	1.46	1.51
23	A	815	CLA	C3B-CAB	-2.54	1.42	1.47
23	B	828	CLA	C3B-CAB	-2.54	1.42	1.47
23	B	839	CLA	CMD-C2D	-2.54	1.45	1.50
23	4	616	CLA	CMB-C2B	-2.54	1.46	1.51
23	B	823	CLA	CMB-C2B	-2.54	1.46	1.51
23	B	818	CLA	C3B-C2B	-2.54	1.36	1.40
23	B	817	CLA	CMC-C2C	-2.54	1.45	1.50
23	8	614	CLA	CMB-C2B	-2.53	1.46	1.51
23	A	830	CLA	CHC-C1C	2.53	1.41	1.35
23	7	612	CLA	CMB-C2B	-2.53	1.46	1.51
23	4	612	CLA	CMB-C2B	-2.53	1.46	1.51
23	G	203	CLA	CMB-C2B	-2.53	1.46	1.51
23	G	204	CLA	CMB-C2B	-2.53	1.46	1.51
23	A	854	CLA	CMB-C2B	-2.53	1.46	1.51
23	A	830	CLA	C3B-CAB	-2.53	1.42	1.47
23	5	619	CLA	CHC-C1C	2.52	1.41	1.35
23	5	602	CLA	CMB-C2B	-2.52	1.46	1.51
23	A	824	CLA	CMD-C2D	-2.52	1.45	1.50
23	A	828	CLA	C3B-C2B	-2.52	1.36	1.40
23	B	816	CLA	CMB-C2B	-2.52	1.46	1.51
23	6	614	CLA	CMB-C2B	-2.52	1.46	1.51
23	a	614	CLA	CMB-C2B	-2.52	1.46	1.51
29	4	624	LMG	O1-C7	-2.52	1.39	1.43
23	A	810	CLA	MG-ND	-2.52	2.00	2.05
23	A	831	CLA	CHC-C1C	2.51	1.41	1.35
23	B	813	CLA	C3B-C2B	-2.51	1.36	1.40
23	3	609	CLA	CMD-C2D	-2.51	1.45	1.50
23	6	608	CLA	CMC-C2C	-2.51	1.45	1.50
23	B	803	CLA	CMD-C2D	-2.51	1.45	1.50
23	6	614	CLA	CMD-C2D	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	608	CLA	CMB-C2B	-2.51	1.46	1.51
23	1	614	CLA	CMB-C2B	-2.51	1.46	1.51
23	B	827	CLA	CMD-C2D	-2.51	1.45	1.50
23	7	607	CLA	CMB-C2B	-2.51	1.46	1.51
23	6	604	CLA	C3B-C2B	-2.50	1.36	1.40
23	8	613	CLA	C3B-C2B	-2.50	1.36	1.40
23	A	829	CLA	CMD-C2D	-2.50	1.45	1.50
23	A	838	CLA	CMD-C2D	-2.50	1.45	1.50
23	6	607	CLA	CMC-C2C	-2.50	1.45	1.50
23	B	836	CLA	CMB-C2B	-2.50	1.46	1.51
23	A	830	CLA	CMD-C2D	-2.50	1.45	1.50
23	a	608	CLA	CMB-C2B	-2.50	1.46	1.51
23	B	804	CLA	CMD-C2D	-2.50	1.45	1.50
23	1	608	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	804	CLA	C3B-CAB	-2.49	1.42	1.47
23	A	820	CLA	MG-ND	-2.49	2.00	2.05
23	B	817	CLA	C3B-CAB	-2.49	1.42	1.47
23	B	826	CLA	CMC-C2C	-2.49	1.45	1.50
23	5	601	CLA	MG-ND	-2.49	2.00	2.05
23	B	832	CLA	CMB-C2B	-2.48	1.46	1.51
23	3	603	CLA	MG-ND	-2.48	2.00	2.05
23	A	829	CLA	CMC-C2C	-2.48	1.45	1.50
23	A	814	CLA	CMC-C2C	-2.48	1.45	1.50
23	8	601	CLA	CMB-C2B	-2.48	1.46	1.51
23	5	607	CLA	CMB-C2B	-2.48	1.46	1.51
23	A	832	CLA	MG-ND	-2.48	2.00	2.05
23	B	802	CLA	C3B-CAB	-2.48	1.42	1.47
25	6	623	LHG	O7-C5	-2.48	1.40	1.46
23	A	826	CLA	CMD-C2D	-2.48	1.45	1.50
23	6	620	CLA	CMB-C2B	-2.48	1.46	1.51
23	A	819	CLA	CMC-C2C	-2.48	1.45	1.50
29	A	860	LMG	O7-C8	-2.47	1.40	1.46
23	A	818	CLA	CMD-C2D	-2.47	1.45	1.50
23	B	805	CLA	MG-ND	-2.47	2.00	2.05
23	3	606	CLA	CMD-C2D	-2.47	1.45	1.50
23	1	612	CLA	CMB-C2B	-2.47	1.46	1.51
23	F	301	CLA	CHC-C1C	2.47	1.41	1.35
23	6	610	CLA	CMB-C2B	-2.46	1.46	1.51
23	A	828	CLA	CMD-C2D	-2.46	1.45	1.50
23	A	840	CLA	CMD-C2D	-2.46	1.45	1.50
23	A	854	CLA	MG-ND	-2.46	2.00	2.05
23	6	620	CLA	CMD-C2D	-2.46	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	612	CLA	CMB-C2B	-2.46	1.46	1.51
29	4	623	LMG	O1-C7	-2.46	1.39	1.43
23	3	611	CLA	CMD-C2D	-2.46	1.45	1.50
26	B	844	BCR	C30-C25	-2.45	1.50	1.53
23	7	613	CLA	CMD-C2D	-2.45	1.45	1.50
23	A	810	CLA	C3B-C2B	-2.45	1.37	1.40
23	A	830	CLA	CMC-C2C	-2.45	1.45	1.50
23	5	617	CLA	CMC-C2C	-2.45	1.45	1.50
23	B	841	CLA	CMB-C2B	-2.45	1.46	1.51
23	A	854	CLA	CMD-C2D	-2.45	1.45	1.50
23	B	819	CLA	CMD-C2D	-2.45	1.45	1.50
23	A	807	CLA	CMD-C2D	-2.45	1.45	1.50
23	B	838	CLA	C3B-C2B	-2.45	1.37	1.40
23	7	606	CLA	CMD-C2D	-2.45	1.45	1.50
26	A	848	BCR	C30-C25	-2.45	1.50	1.53
23	B	824	CLA	CMB-C2B	-2.45	1.46	1.51
23	6	609	CLA	CMD-C2D	-2.44	1.45	1.50
23	A	842	CLA	CMD-C2D	-2.44	1.45	1.50
23	B	806	CLA	CMC-C2C	-2.44	1.45	1.50
23	A	817	CLA	CMD-C2D	-2.44	1.45	1.50
23	8	608	CLA	CMB-C2B	-2.44	1.46	1.51
23	7	608	CLA	CMD-C2D	-2.44	1.45	1.50
23	A	815	CLA	CMB-C2B	-2.44	1.46	1.51
23	A	812	CLA	C3B-C2B	-2.44	1.37	1.40
23	9	610	CLA	CAD-C3D	-2.43	1.46	1.50
23	3	608	CLA	CMC-C2C	-2.43	1.45	1.50
23	B	810	CLA	C3B-C2B	-2.43	1.37	1.40
23	5	603	CLA	CMD-C2D	-2.43	1.45	1.50
23	7	613	CLA	CMC-C2C	-2.43	1.45	1.50
23	3	606	CLA	C3B-C2B	-2.43	1.37	1.40
23	B	813	CLA	CMD-C2D	-2.43	1.45	1.50
23	B	837	CLA	C3B-C2B	-2.42	1.37	1.40
23	4	607	CLA	C3B-C2B	-2.42	1.37	1.40
23	A	823	CLA	C3B-C2B	-2.42	1.37	1.40
23	B	814	CLA	CMD-C2D	-2.42	1.45	1.50
23	3	603	CLA	CHC-C1C	2.42	1.41	1.35
26	B	846	BCR	C30-C25	-2.42	1.50	1.53
23	5	618	CLA	CMB-C2B	-2.42	1.46	1.51
23	B	805	CLA	CMB-C2B	-2.42	1.46	1.51
23	B	819	CLA	C3B-C2B	-2.42	1.37	1.40
23	A	842	CLA	CMC-C2C	-2.42	1.45	1.50
23	5	617	CLA	CHC-C1C	2.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	809	CLA	CMD-C2D	-2.42	1.45	1.50
23	3	608	CLA	CMD-C2D	-2.42	1.45	1.50
23	4	602	CLA	CMB-C2B	-2.42	1.46	1.51
23	A	817	CLA	C3B-C2B	-2.42	1.37	1.40
23	B	809	CLA	MG-ND	-2.42	2.01	2.05
23	a	601	CLA	CMD-C2D	-2.41	1.45	1.50
23	A	813	CLA	CMD-C2D	-2.41	1.45	1.50
23	B	827	CLA	CMC-C2C	-2.41	1.45	1.50
23	A	803	CLA	C3B-CAB	-2.41	1.43	1.47
23	7	616	CLA	CMB-C2B	-2.41	1.46	1.51
23	1	601	CLA	CMD-C2D	-2.41	1.45	1.50
23	5	612	CLA	CMB-C2B	-2.41	1.46	1.51
23	5	608	CLA	CMD-C2D	-2.41	1.45	1.50
23	A	831	CLA	CMC-C2C	-2.41	1.45	1.50
23	4	618	CLA	CMD-C2D	-2.41	1.45	1.50
23	B	803	CLA	MG-ND	-2.41	2.01	2.05
23	A	815	CLA	CMC-C2C	-2.41	1.45	1.50
23	A	843	CLA	CMD-C2D	-2.41	1.45	1.50
23	A	839	CLA	CMC-C2C	-2.40	1.45	1.50
23	A	835	CLA	CMC-C2C	-2.40	1.45	1.50
23	B	831	CLA	CMB-C2B	-2.40	1.46	1.51
23	5	601	CLA	CMB-C2B	-2.40	1.46	1.51
23	3	610	CLA	CMC-C2C	-2.40	1.45	1.50
23	3	606	CLA	C3B-CAB	-2.40	1.43	1.47
23	5	618	CLA	CMD-C2D	-2.40	1.45	1.50
23	2	610	CLA	CAD-C3D	-2.40	1.46	1.50
23	8	611	CLA	CMD-C2D	-2.39	1.45	1.50
23	7	607	CLA	CMD-C2D	-2.39	1.45	1.50
23	7	602	CLA	CMD-C2D	-2.39	1.45	1.50
23	7	602	CLA	C3B-C2B	-2.39	1.37	1.40
25	5	623	LHG	O7-C5	-2.39	1.40	1.46
23	A	804	CLA	CMC-C2C	-2.39	1.45	1.50
23	K	201	CLA	CMB-C2B	-2.39	1.46	1.51
23	7	612	CLA	CMC-C2C	-2.39	1.45	1.50
23	A	810	CLA	C1D-ND	2.38	1.40	1.37
23	B	840	CLA	CMD-C2D	-2.38	1.45	1.50
23	A	845	CLA	CMC-C2C	-2.38	1.45	1.50
23	B	815	CLA	CMC-C2C	-2.38	1.45	1.50
23	8	603	CLA	CMD-C2D	-2.38	1.45	1.50
23	A	826	CLA	MG-ND	-2.38	2.01	2.05
23	B	807	CLA	C3B-C2B	-2.38	1.37	1.40
23	A	806	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	611	CLA	CMD-C2D	-2.38	1.45	1.50
23	A	805	CLA	C3B-CAB	-2.38	1.43	1.47
23	A	814	CLA	C3B-C2B	-2.38	1.37	1.40
23	A	822	CLA	CMD-C2D	-2.38	1.45	1.50
23	7	613	CLA	C3B-C2B	-2.38	1.37	1.40
23	7	614	CLA	CMD-C2D	-2.37	1.45	1.50
23	5	610	CLA	CMD-C2D	-2.37	1.45	1.50
23	A	812	CLA	CMC-C2C	-2.37	1.45	1.50
23	4	609	CLA	CMD-C2D	-2.37	1.45	1.50
23	7	606	CLA	C3B-C2B	-2.37	1.37	1.40
32	3	619	XAT	O24-C25	-2.37	1.42	1.46
23	a	601	CLA	MG-ND	-2.37	2.01	2.05
23	3	617	CLA	MG-ND	-2.37	2.01	2.05
23	B	806	CLA	CMD-C2D	-2.37	1.45	1.50
23	A	836	CLA	CMD-C2D	-2.37	1.45	1.50
23	7	601	CLA	CMC-C2C	-2.37	1.45	1.50
23	A	834	CLA	C3B-CAB	-2.37	1.43	1.47
23	A	812	CLA	CMD-C2D	-2.37	1.45	1.50
23	F	304	CLA	CMC-C2C	-2.37	1.45	1.50
23	a	610	CLA	C3B-C2B	-2.37	1.37	1.40
23	B	817	CLA	MG-ND	-2.36	2.01	2.05
23	7	601	CLA	MG-ND	-2.36	2.01	2.05
23	4	613	CLA	C3B-C2B	-2.36	1.37	1.40
23	5	619	CLA	MG-ND	-2.36	2.01	2.05
23	B	815	CLA	CMD-C2D	-2.36	1.45	1.50
23	6	603	CLA	CMD-C2D	-2.36	1.45	1.50
23	A	822	CLA	C3B-C2B	-2.36	1.37	1.40
23	7	609	CLA	CMD-C2D	-2.36	1.45	1.50
23	6	613	CLA	CMD-C2D	-2.36	1.45	1.50
23	3	614	CLA	CMD-C2D	-2.36	1.45	1.50
23	A	842	CLA	C3B-CAB	-2.35	1.43	1.47
23	B	840	CLA	C3B-CAB	-2.35	1.43	1.47
23	8	602	CLA	CMC-C2C	-2.35	1.45	1.50
23	A	808	CLA	C3B-C2B	-2.35	1.37	1.40
23	B	805	CLA	CMD-C2D	-2.35	1.45	1.50
23	B	832	CLA	CMD-C2D	-2.35	1.45	1.50
23	L	302	CLA	CMB-C2B	-2.35	1.46	1.51
23	B	833	CLA	C3B-C2B	-2.35	1.37	1.40
23	5	613	CLA	CMC-C2C	-2.35	1.45	1.50
23	7	604	CLA	CMD-C2D	-2.35	1.45	1.50
23	8	611	CLA	MG-ND	-2.35	2.01	2.05
30	J	103	DGD	O1G-C1G	-2.35	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	803	CLA	CMD-C2D	-2.35	1.45	1.50
23	3	602	CLA	CMC-C2C	-2.35	1.45	1.50
23	8	609	CLA	CMB-C2B	-2.34	1.46	1.51
23	7	610	CLA	C3B-CAB	-2.34	1.43	1.47
23	A	843	CLA	MG-ND	-2.34	2.01	2.05
23	L	304	CLA	CMB-C2B	-2.34	1.46	1.51
23	A	839	CLA	CMD-C2D	-2.34	1.45	1.50
23	6	607	CLA	CMD-C2D	-2.34	1.45	1.50
23	A	803	CLA	CMC-C2C	-2.34	1.45	1.50
23	A	805	CLA	CMC-C2C	-2.34	1.45	1.50
23	A	826	CLA	CMC-C2C	-2.34	1.45	1.50
29	4	624	LMG	C4-C3	2.34	1.58	1.52
30	B	850	DGD	O5D-C6D	-2.34	1.39	1.43
23	5	608	CLA	C3B-C2B	-2.33	1.37	1.40
23	B	818	CLA	CMD-C2D	-2.33	1.45	1.50
23	A	819	CLA	MG-ND	-2.33	2.01	2.05
23	B	804	CLA	CMC-C2C	-2.33	1.45	1.50
23	B	837	CLA	CMC-C2C	-2.33	1.45	1.50
23	A	827	CLA	MG-ND	-2.33	2.01	2.05
23	4	608	CLA	CMC-C2C	-2.33	1.45	1.50
23	7	610	CLA	CMD-C2D	-2.33	1.45	1.50
30	J	103	DGD	C4E-C3E	2.33	1.58	1.52
23	8	609	CLA	CMD-C2D	-2.33	1.45	1.50
23	A	838	CLA	MG-ND	-2.33	2.01	2.05
23	4	603	CLA	CMD-C2D	-2.33	1.45	1.50
23	6	608	CLA	C3B-C2B	-2.32	1.37	1.40
23	A	810	CLA	C3B-CAB	-2.32	1.43	1.47
23	7	606	CLA	MG-ND	-2.32	2.01	2.05
23	B	820	CLA	CMB-C2B	-2.32	1.46	1.51
23	6	606	CLA	CMB-C2B	-2.32	1.46	1.51
23	5	608	CLA	CAC-C3C	-2.32	1.45	1.50
23	B	834	CLA	CMD-C2D	-2.32	1.45	1.50
23	F	301	CLA	CMD-C2D	-2.32	1.45	1.50
23	3	604	CLA	CMD-C2D	-2.32	1.45	1.50
23	8	607	CLA	CMD-C2D	-2.32	1.45	1.50
23	1	610	CLA	C3B-C2B	-2.32	1.37	1.40
23	3	614	CLA	C3B-C2B	-2.32	1.37	1.40
23	8	602	CLA	CMD-C2D	-2.32	1.45	1.50
23	B	807	CLA	C3B-CAB	-2.32	1.43	1.47
23	B	805	CLA	CMC-C2C	-2.32	1.45	1.50
23	5	606	CLA	MG-ND	-2.32	2.01	2.05
23	A	834	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	613	CLA	CMD-C2D	-2.31	1.45	1.50
23	A	821	CLA	C3B-C2B	-2.31	1.37	1.40
25	a	620	LHG	O7-C5	-2.31	1.40	1.46
23	4	614	CLA	CMD-C2D	-2.31	1.45	1.50
23	7	604	CLA	CMC-C2C	-2.31	1.45	1.50
23	A	839	CLA	C3B-CAB	-2.31	1.43	1.47
23	A	840	CLA	MG-ND	-2.31	2.01	2.05
23	7	610	CLA	CMC-C2C	-2.31	1.45	1.50
23	A	807	CLA	CMC-C2C	-2.31	1.45	1.50
23	B	825	CLA	C1D-ND	2.31	1.40	1.37
23	6	602	CLA	C3B-CAB	-2.31	1.43	1.47
23	A	841	CLA	C3B-C2B	-2.31	1.37	1.40
23	B	826	CLA	CMD-C2D	-2.31	1.45	1.50
23	1	601	CLA	MG-ND	-2.31	2.01	2.05
25	1	620	LHG	O7-C5	-2.31	1.40	1.46
23	A	822	CLA	CMC-C2C	-2.31	1.45	1.50
23	3	610	CLA	CMD-C2D	-2.31	1.45	1.50
23	4	616	CLA	CAC-C3C	-2.31	1.45	1.50
23	5	606	CLA	CMD-C2D	-2.31	1.45	1.50
23	A	809	CLA	MG-ND	-2.31	2.01	2.05
23	B	835	CLA	C3B-C2B	-2.30	1.37	1.40
23	B	807	CLA	CMD-C2D	-2.30	1.45	1.50
23	7	608	CLA	CAC-C3C	-2.30	1.45	1.51
23	B	828	CLA	MG-ND	-2.30	2.01	2.05
23	3	606	CLA	CMC-C2C	-2.30	1.45	1.50
23	A	806	CLA	MG-ND	-2.30	2.01	2.05
23	B	821	CLA	CMD-C2D	-2.30	1.45	1.50
23	5	616	CLA	CMC-C2C	-2.30	1.45	1.50
23	6	610	CLA	CMD-C2D	-2.30	1.45	1.50
23	B	829	CLA	CMC-C2C	-2.30	1.45	1.50
23	B	839	CLA	C3B-CAB	-2.30	1.43	1.47
23	F	301	CLA	C3B-CAB	-2.30	1.43	1.47
23	B	838	CLA	CMD-C2D	-2.30	1.45	1.50
23	8	610	CLA	CMB-C2B	-2.30	1.46	1.51
26	A	851	BCR	C30-C25	-2.30	1.50	1.53
23	A	833	CLA	CMD-C2D	-2.30	1.45	1.50
23	A	854	CLA	CMC-C2C	-2.30	1.45	1.50
23	4	616	CLA	CMD-C2D	-2.30	1.45	1.50
23	6	617	CLA	C3B-C2B	-2.30	1.37	1.40
23	3	608	CLA	C3B-C2B	-2.29	1.37	1.40
23	3	613	CLA	CMD-C2D	-2.29	1.45	1.50
23	A	821	CLA	MG-ND	-2.29	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	836	CLA	MG-ND	-2.29	2.01	2.05
23	A	820	CLA	C3B-CAB	-2.29	1.43	1.47
23	A	807	CLA	C3B-C2B	-2.29	1.37	1.40
23	A	837	CLA	C3B-C2B	-2.29	1.37	1.40
23	B	828	CLA	C3B-C2B	-2.29	1.37	1.40
23	6	613	CLA	C3B-C2B	-2.29	1.37	1.40
32	7	620	XAT	O4-C5	-2.29	1.42	1.46
23	A	836	CLA	CMC-C2C	-2.29	1.45	1.50
23	B	825	CLA	CMC-C2C	-2.29	1.45	1.50
23	7	610	CLA	C3B-C2B	-2.29	1.37	1.40
23	3	603	CLA	C3B-C2B	-2.29	1.37	1.40
23	7	612	CLA	C3B-C2B	-2.29	1.37	1.40
23	A	819	CLA	C3B-CAB	-2.29	1.43	1.47
23	A	828	CLA	MG-ND	-2.28	2.01	2.05
25	2	622	LHG	O7-C5	-2.28	1.40	1.46
23	4	612	CLA	CMD-C2D	-2.28	1.46	1.50
23	A	805	CLA	MG-ND	-2.28	2.01	2.05
23	3	608	CLA	CAC-C3C	-2.28	1.45	1.51
23	6	613	CLA	MG-ND	-2.28	2.01	2.05
23	A	843	CLA	CMC-C2C	-2.28	1.46	1.50
23	A	825	CLA	CMC-C2C	-2.28	1.46	1.50
23	7	603	CLA	MG-ND	-2.28	2.01	2.05
23	A	808	CLA	CMC-C2C	-2.28	1.46	1.50
23	7	612	CLA	CMD-C2D	-2.28	1.46	1.50
24	B	842	PQN	C11-C3	2.27	1.55	1.51
23	5	611	CLA	CMD-C2D	-2.27	1.46	1.50
23	B	806	CLA	MG-ND	-2.27	2.01	2.05
23	A	804	CLA	MG-ND	-2.27	2.01	2.05
23	5	608	CLA	MG-ND	-2.27	2.01	2.05
23	7	603	CLA	CMC-C2C	-2.27	1.46	1.50
29	5	627	LMG	C4-C5	2.27	1.57	1.53
23	7	603	CLA	C3B-C2B	-2.27	1.37	1.40
23	A	806	CLA	C3B-C2B	-2.27	1.37	1.40
23	B	814	CLA	CMC-C2C	-2.27	1.46	1.50
23	K	204	CLA	CMD-C2D	-2.27	1.46	1.50
23	B	811	CLA	MG-ND	-2.27	2.01	2.05
23	8	612	CLA	CMD-C2D	-2.27	1.46	1.50
23	A	815	CLA	C3B-C2B	-2.27	1.37	1.40
23	3	615	CLA	C3B-C2B	-2.27	1.37	1.40
23	A	802	CLA	CMC-C2C	-2.27	1.46	1.50
23	1	603	CLA	CMD-C2D	-2.27	1.46	1.50
23	A	831	CLA	C4B-CHC	-2.27	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	601	CLA	CMD-C2D	-2.27	1.46	1.50
23	1	613	CLA	CMD-C2D	-2.27	1.46	1.50
23	B	807	CLA	MG-ND	-2.26	2.01	2.05
23	B	838	CLA	C3B-CAB	-2.26	1.43	1.47
32	7	620	XAT	O24-C25	-2.26	1.43	1.46
23	8	613	CLA	CMC-C2C	-2.26	1.46	1.50
23	8	610	CLA	CMD-C2D	-2.26	1.46	1.50
23	B	819	CLA	CMC-C2C	-2.26	1.46	1.50
23	A	807	CLA	C3B-CAB	-2.26	1.43	1.47
23	B	833	CLA	C3B-CAB	-2.26	1.43	1.47
23	A	812	CLA	MG-ND	-2.26	2.01	2.05
23	A	802	CLA	CAC-C3C	-2.26	1.45	1.51
25	3	623	LHG	O7-C5	-2.26	1.40	1.46
23	6	612	CLA	CMD-C2D	-2.26	1.46	1.50
23	B	811	CLA	CMD-C2D	-2.26	1.46	1.50
23	A	828	CLA	C3B-CAB	-2.26	1.43	1.47
30	B	850	DGD	O1G-C1G	-2.26	1.40	1.45
23	A	815	CLA	CMD-C2D	-2.25	1.46	1.50
23	A	845	CLA	CMD-C2D	-2.25	1.46	1.50
23	7	612	CLA	MG-ND	-2.25	2.01	2.05
23	A	825	CLA	CMD-C2D	-2.25	1.46	1.50
23	5	608	CLA	C3B-CAB	-2.25	1.43	1.47
23	A	805	CLA	CMD-C2D	-2.25	1.46	1.50
23	1	604	CLA	CMD-C2D	-2.25	1.46	1.50
23	7	606	CLA	CMC-C2C	-2.25	1.46	1.50
23	8	610	CLA	CMC-C2C	-2.25	1.46	1.50
23	8	601	CLA	MG-ND	-2.25	2.01	2.05
23	a	604	CLA	CMD-C2D	-2.25	1.46	1.50
23	8	607	CLA	CMC-C2C	-2.25	1.46	1.50
23	F	304	CLA	CMB-C2B	-2.25	1.47	1.51
23	F	304	CLA	CMD-C2D	-2.25	1.46	1.50
23	B	815	CLA	MG-ND	-2.25	2.01	2.05
23	B	825	CLA	C3B-CAB	-2.25	1.43	1.47
23	4	602	CLA	CMC-C2C	-2.25	1.46	1.50
23	7	611	CLA	CMD-C2D	-2.25	1.46	1.50
23	A	833	CLA	MG-ND	-2.25	2.01	2.05
23	A	828	CLA	CMC-C2C	-2.24	1.46	1.50
23	A	811	CLA	C3B-CAB	-2.24	1.43	1.47
23	5	604	CLA	CMD-C2D	-2.24	1.46	1.50
23	5	613	CLA	C3B-C2B	-2.24	1.37	1.40
23	6	602	CLA	CMC-C2C	-2.24	1.46	1.50
23	A	837	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	613	CLA	CMC-C2C	-2.24	1.46	1.50
23	A	836	CLA	C3B-C2B	-2.24	1.37	1.40
23	A	841	CLA	CMC-C2C	-2.24	1.46	1.50
23	6	616	CLA	MG-ND	-2.24	2.01	2.05
23	4	610	CLA	CMC-C2C	-2.24	1.46	1.50
23	B	815	CLA	C3B-C2B	-2.24	1.37	1.40
29	A	860	LMG	O8-C9	-2.24	1.40	1.45
29	4	624	LMG	O7-C8	-2.24	1.41	1.46
23	7	614	CLA	MG-ND	-2.24	2.01	2.05
23	A	819	CLA	C3B-C2B	-2.24	1.37	1.40
23	a	614	CLA	C3B-C2B	-2.24	1.37	1.40
23	6	609	CLA	C3B-C2B	-2.24	1.37	1.40
23	A	816	CLA	CMC-C2C	-2.24	1.46	1.50
23	a	603	CLA	CMD-C2D	-2.24	1.46	1.50
23	B	816	CLA	CMD-C2D	-2.24	1.46	1.50
23	B	832	CLA	CMC-C2C	-2.24	1.46	1.50
23	7	601	CLA	C3B-CAB	-2.24	1.43	1.47
23	4	607	CLA	C3B-CAB	-2.23	1.43	1.47
23	6	618	CLA	MG-ND	-2.23	2.01	2.05
23	B	833	CLA	MG-ND	-2.23	2.01	2.05
23	6	606	CLA	MG-ND	-2.23	2.01	2.05
23	5	613	CLA	CMD-C2D	-2.23	1.46	1.50
23	5	610	CLA	MG-ND	-2.23	2.01	2.05
23	B	823	CLA	CMD-C2D	-2.23	1.46	1.50
31	7	619	LUT	C30-C29	-2.23	1.32	1.35
32	8	620	XAT	O24-C25	-2.23	1.43	1.46
23	A	820	CLA	C4B-CHC	-2.23	1.34	1.41
23	A	817	CLA	CMC-C2C	-2.23	1.46	1.50
23	7	608	CLA	MG-ND	-2.23	2.01	2.05
23	a	613	CLA	C3B-C2B	-2.23	1.37	1.40
23	4	606	CLA	CMD-C2D	-2.23	1.46	1.50
23	A	801	CLA	C3B-CAB	-2.23	1.43	1.47
23	B	814	CLA	MG-ND	-2.23	2.01	2.05
23	5	607	CLA	MG-ND	-2.23	2.01	2.05
23	A	824	CLA	MG-ND	-2.23	2.01	2.05
23	A	834	CLA	MG-ND	-2.23	2.01	2.05
23	8	613	CLA	CMD-C2D	-2.23	1.46	1.50
23	5	602	CLA	MG-ND	-2.23	2.01	2.05
23	7	607	CLA	CMC-C2C	-2.22	1.46	1.50
23	8	606	CLA	MG-ND	-2.22	2.01	2.05
26	B	847	BCR	C30-C25	-2.22	1.50	1.53
23	8	609	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	301	CLA	MG-ND	-2.22	2.01	2.05
23	7	606	CLA	CAC-C3C	-2.22	1.46	1.50
32	a	618	XAT	O24-C25	-2.22	1.43	1.46
23	A	811	CLA	CMC-C2C	-2.22	1.46	1.50
23	5	611	CLA	C3B-C2B	-2.22	1.37	1.40
23	K	201	CLA	CMD-C2D	-2.22	1.46	1.50
28	A	859	LMU	C2'-C3'	-2.22	1.48	1.52
23	A	816	CLA	CMD-C2D	-2.22	1.46	1.50
23	A	835	CLA	CMD-C2D	-2.22	1.46	1.50
23	A	841	CLA	C3B-CAB	-2.22	1.43	1.47
23	5	617	CLA	CMD-C2D	-2.22	1.46	1.50
23	A	840	CLA	C3B-C2B	-2.22	1.37	1.40
23	B	812	CLA	CMD-C2D	-2.22	1.46	1.50
23	4	602	CLA	CMD-C2D	-2.22	1.46	1.50
23	5	609	CLA	CMD-C2D	-2.22	1.46	1.50
23	4	610	CLA	CMD-C2D	-2.22	1.46	1.50
23	A	821	CLA	CMC-C2C	-2.22	1.46	1.50
23	4	603	CLA	CMC-C2C	-2.22	1.46	1.50
23	7	602	CLA	CMC-C2C	-2.22	1.46	1.50
23	7	608	CLA	CMC-C2C	-2.22	1.46	1.50
23	3	613	CLA	MG-ND	-2.21	2.01	2.05
23	A	822	CLA	MG-ND	-2.21	2.01	2.05
23	B	810	CLA	MG-ND	-2.21	2.01	2.05
23	A	814	CLA	C3B-CAB	-2.21	1.43	1.47
23	A	810	CLA	CMC-C2C	-2.21	1.46	1.50
23	8	608	CLA	CMD-C2D	-2.21	1.46	1.50
23	A	822	CLA	C3B-CAB	-2.21	1.43	1.47
23	A	809	CLA	C3B-C2B	-2.21	1.37	1.40
23	8	603	CLA	CMC-C2C	-2.21	1.46	1.50
23	B	816	CLA	CMC-C2C	-2.21	1.46	1.50
23	B	803	CLA	C3B-C2B	-2.21	1.37	1.40
23	B	824	CLA	MG-ND	-2.21	2.01	2.05
23	5	613	CLA	C3B-CAB	-2.21	1.43	1.47
23	3	603	CLA	CMD-C2D	-2.21	1.46	1.50
23	6	601	CLA	MG-ND	-2.21	2.01	2.05
23	A	832	CLA	C3B-CAB	-2.21	1.43	1.47
23	A	830	CLA	MG-ND	-2.21	2.01	2.05
23	3	602	CLA	C3B-CAB	-2.20	1.43	1.47
23	1	609	CLA	CMD-C2D	-2.20	1.46	1.50
23	7	614	CLA	C3B-C2B	-2.20	1.37	1.40
23	B	837	CLA	C3B-CAB	-2.20	1.43	1.47
23	B	821	CLA	C3B-C2B	-2.20	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	614	CLA	CMD-C2D	-2.20	1.46	1.50
23	8	614	CLA	CMD-C2D	-2.20	1.46	1.50
23	A	814	CLA	CMD-C2D	-2.20	1.46	1.50
23	6	608	CLA	CMD-C2D	-2.20	1.46	1.50
23	8	616	CLA	MG-ND	-2.20	2.01	2.05
23	A	854	CLA	C3B-CAB	-2.20	1.43	1.47
23	A	825	CLA	MG-ND	-2.20	2.01	2.05
23	A	812	CLA	C3B-CAB	-2.20	1.43	1.47
23	A	809	CLA	CMD-C2D	-2.20	1.46	1.50
23	3	603	CLA	C4B-CHC	-2.20	1.34	1.41
23	B	837	CLA	CMD-C2D	-2.19	1.46	1.50
23	4	613	CLA	CMC-C2C	-2.19	1.46	1.50
23	B	808	CLA	MG-ND	-2.19	2.01	2.05
23	8	607	CLA	MG-ND	-2.19	2.01	2.05
23	A	808	CLA	CMD-C2D	-2.19	1.46	1.50
23	8	612	CLA	CMC-C2C	-2.19	1.46	1.50
23	A	813	CLA	CMC-C2C	-2.19	1.46	1.50
23	4	612	CLA	CMC-C2C	-2.19	1.46	1.50
23	A	808	CLA	C3B-CAB	-2.19	1.43	1.47
23	A	801	CLA	CMC-C2C	-2.19	1.46	1.50
23	6	617	CLA	CMC-C2C	-2.19	1.46	1.50
23	A	840	CLA	CMC-C2C	-2.19	1.46	1.50
23	3	602	CLA	C3B-C2B	-2.19	1.37	1.40
23	6	606	CLA	CMC-C2C	-2.19	1.46	1.50
23	8	604	CLA	CMD-C2D	-2.19	1.46	1.50
23	B	835	CLA	CMD-C2D	-2.19	1.46	1.50
23	5	617	CLA	MG-ND	-2.19	2.01	2.05
23	4	614	CLA	C3B-C2B	-2.19	1.37	1.40
23	A	806	CLA	CMA-C3A	-2.19	1.48	1.53
23	6	602	CLA	CMD-C2D	-2.19	1.46	1.50
23	4	613	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	860	LMG	O4-C4	-2.18	1.37	1.43
23	5	608	CLA	CMC-C2C	-2.18	1.46	1.50
23	3	613	CLA	C3B-C2B	-2.18	1.37	1.40
23	5	607	CLA	CMD-C2D	-2.18	1.46	1.50
23	B	802	CLA	MG-ND	-2.18	2.01	2.05
23	4	618	CLA	CMC-C2C	-2.18	1.46	1.50
23	B	828	CLA	CMC-C2C	-2.18	1.46	1.50
23	A	809	CLA	C3B-CAB	-2.18	1.43	1.47
23	6	617	CLA	MG-ND	-2.18	2.01	2.05
23	3	613	CLA	CMC-C2C	-2.18	1.46	1.50
23	9	610	CLA	C3C-C2C	2.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	608	CLA	MG-ND	-2.18	2.01	2.05
23	1	613	CLA	C3B-C2B	-2.18	1.37	1.40
23	4	604	CLA	CMD-C2D	-2.18	1.46	1.50
23	4	608	CLA	CMD-C2D	-2.18	1.46	1.50
23	3	604	CLA	MG-ND	-2.18	2.01	2.05
23	5	607	CLA	C3B-CAB	-2.18	1.43	1.47
23	8	614	CLA	MG-ND	-2.18	2.01	2.05
23	B	840	CLA	MG-ND	-2.18	2.01	2.05
23	A	835	CLA	C3B-CAB	-2.18	1.43	1.47
23	A	818	CLA	CMC-C2C	-2.18	1.46	1.50
23	B	804	CLA	MG-ND	-2.18	2.01	2.05
23	6	620	CLA	MG-ND	-2.17	2.01	2.05
23	B	836	CLA	CMD-C2D	-2.17	1.46	1.50
23	A	838	CLA	C3B-CAB	-2.17	1.43	1.47
33	6	624	NEX	O24-C25	-2.17	1.43	1.46
23	3	612	CLA	CMD-C2D	-2.17	1.46	1.50
23	7	616	CLA	MG-ND	-2.17	2.01	2.05
32	1	618	XAT	O24-C25	-2.17	1.43	1.46
23	J	101	CLA	C3B-C2B	-2.17	1.37	1.40
23	5	612	CLA	CMD-C2D	-2.17	1.46	1.50
23	B	823	CLA	CMC-C2C	-2.17	1.46	1.50
23	B	806	CLA	C3B-CAB	-2.17	1.43	1.47
23	1	614	CLA	CMD-C2D	-2.17	1.46	1.50
23	A	845	CLA	MG-ND	-2.17	2.01	2.05
23	B	810	CLA	CMD-C2D	-2.17	1.46	1.50
23	a	609	CLA	CMD-C2D	-2.17	1.46	1.50
23	6	606	CLA	CMD-C2D	-2.17	1.46	1.50
23	1	616	CLA	MG-ND	-2.17	2.01	2.05
23	8	610	CLA	MG-ND	-2.17	2.01	2.05
23	K	203	CLA	CMD-C2D	-2.17	1.46	1.50
23	a	602	CLA	CMC-C2C	-2.17	1.46	1.50
23	6	609	CLA	C3B-CAB	-2.17	1.43	1.47
23	A	811	CLA	CMD-C2D	-2.17	1.46	1.50
23	3	617	CLA	CMD-C2D	-2.17	1.46	1.50
23	6	601	CLA	CMC-C2C	-2.17	1.46	1.50
23	7	610	CLA	MG-ND	-2.16	2.01	2.05
23	B	829	CLA	C3B-CAB	-2.16	1.43	1.47
23	5	612	CLA	CMC-C2C	-2.16	1.46	1.50
23	6	603	CLA	CMC-C2C	-2.16	1.46	1.50
23	a	612	CLA	CMC-C2C	-2.16	1.46	1.50
29	7	624	LMG	O8-C9	-2.16	1.40	1.45
23	6	613	CLA	C3B-CAB	-2.16	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	612	CLA	CMC-C2C	-2.16	1.46	1.50
23	A	827	CLA	CMC-C2C	-2.16	1.46	1.50
23	4	613	CLA	MG-ND	-2.16	2.01	2.05
23	F	303	CLA	CMD-C2D	-2.16	1.46	1.50
23	B	827	CLA	MG-ND	-2.16	2.01	2.05
23	K	204	CLA	CMC-C2C	-2.16	1.46	1.50
23	A	842	CLA	MG-ND	-2.16	2.01	2.05
23	J	101	CLA	CMD-C2D	-2.16	1.46	1.50
23	A	836	CLA	C3B-CAB	-2.16	1.43	1.47
23	A	811	CLA	MG-ND	-2.15	2.01	2.05
23	B	839	CLA	MG-ND	-2.15	2.01	2.05
23	B	808	CLA	C3B-CAB	-2.15	1.43	1.47
23	5	609	CLA	MG-ND	-2.15	2.01	2.05
23	4	616	CLA	CMC-C2C	-2.15	1.46	1.50
23	B	813	CLA	CMC-C2C	-2.15	1.46	1.50
23	1	602	CLA	CMC-C2C	-2.15	1.46	1.50
23	5	603	CLA	CMC-C2C	-2.15	1.46	1.50
23	7	604	CLA	MG-ND	-2.15	2.01	2.05
23	A	806	CLA	C3B-CAB	-2.15	1.43	1.47
23	A	820	CLA	CMD-C2D	-2.15	1.46	1.50
23	L	303	CLA	CMD-C2D	-2.15	1.46	1.50
23	5	603	CLA	CAC-C3C	-2.15	1.45	1.51
23	4	601	CLA	MG-ND	-2.15	2.01	2.05
23	6	620	CLA	CMC-C2C	-2.15	1.46	1.50
23	1	603	CLA	CMC-C2C	-2.14	1.46	1.50
23	5	619	CLA	CMC-C2C	-2.14	1.46	1.50
23	A	817	CLA	MG-ND	-2.14	2.01	2.05
23	5	610	CLA	C3B-CAB	-2.14	1.43	1.47
23	2	607	CLA	C3C-C2C	2.14	1.40	1.35
23	1	612	CLA	CMC-C2C	-2.14	1.46	1.50
23	B	820	CLA	CMD-C2D	-2.14	1.46	1.50
23	6	618	CLA	CMC-C2C	-2.14	1.46	1.50
23	K	203	CLA	CMC-C2C	-2.14	1.46	1.50
23	a	611	CLA	CMD-C2D	-2.14	1.46	1.50
23	3	604	CLA	C3B-C2B	-2.14	1.37	1.40
23	a	603	CLA	CMC-C2C	-2.14	1.46	1.50
23	a	612	CLA	CMD-C2D	-2.14	1.46	1.50
23	3	607	CLA	CMD-C2D	-2.14	1.46	1.50
23	A	841	CLA	MG-ND	-2.14	2.01	2.05
23	6	612	CLA	MG-ND	-2.14	2.01	2.05
23	7	607	CLA	MG-ND	-2.14	2.01	2.05
23	F	301	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	602	CLA	CMD-C2D	-2.14	1.46	1.50
23	A	809	CLA	CMC-C2C	-2.13	1.46	1.50
23	6	610	CLA	CMC-C2C	-2.13	1.46	1.50
23	5	612	CLA	MG-ND	-2.13	2.01	2.05
29	J	104	LMG	O7-C8	-2.13	1.41	1.46
23	B	804	CLA	C3B-C2B	-2.13	1.37	1.40
23	4	607	CLA	CMC-C2C	-2.13	1.46	1.50
23	B	839	CLA	CMC-C2C	-2.13	1.46	1.50
23	6	617	CLA	CMD-C2D	-2.13	1.46	1.50
23	1	613	CLA	CMC-C2C	-2.13	1.46	1.50
23	7	603	CLA	CMD-C2D	-2.13	1.46	1.50
23	8	601	CLA	CMC-C2C	-2.13	1.46	1.50
23	4	606	CLA	CMC-C2C	-2.13	1.46	1.50
23	4	603	CLA	MG-ND	-2.13	2.01	2.05
23	8	606	CLA	CMD-C2D	-2.13	1.46	1.50
23	a	616	CLA	MG-ND	-2.13	2.01	2.05
23	K	203	CLA	MG-ND	-2.13	2.01	2.05
23	B	825	CLA	C3B-C2B	-2.13	1.37	1.40
23	A	841	CLA	CMD-C2D	-2.13	1.46	1.50
23	A	834	CLA	CMC-C2C	-2.12	1.46	1.50
23	B	830	CLA	CMD-C2D	-2.12	1.46	1.50
23	7	613	CLA	C3B-CAB	-2.12	1.43	1.47
23	5	607	CLA	C3B-C2B	-2.12	1.37	1.40
23	1	612	CLA	CMD-C2D	-2.12	1.46	1.50
23	1	601	CLA	C3B-C2B	-2.12	1.37	1.40
32	6	621	XAT	O24-C25	-2.12	1.43	1.46
23	3	604	CLA	CMC-C2C	-2.12	1.46	1.50
23	4	601	CLA	CMD-C2D	-2.12	1.46	1.50
23	4	614	CLA	CMC-C2C	-2.12	1.46	1.50
23	7	614	CLA	CMC-C2C	-2.12	1.46	1.50
23	5	616	CLA	CMD-C2D	-2.12	1.46	1.50
23	A	829	CLA	C3B-C2B	-2.12	1.37	1.40
23	5	610	CLA	C3B-C2B	-2.12	1.37	1.40
23	4	606	CLA	MG-ND	-2.12	2.01	2.05
23	B	807	CLA	CMC-C2C	-2.12	1.46	1.50
23	a	601	CLA	CMC-C2C	-2.12	1.46	1.50
23	a	601	CLA	C3B-C2B	-2.12	1.37	1.40
23	A	829	CLA	C3B-CAB	-2.12	1.43	1.47
23	B	831	CLA	CMD-C2D	-2.12	1.46	1.50
23	6	604	CLA	MG-ND	-2.12	2.01	2.05
23	A	845	CLA	C3B-C2B	-2.12	1.37	1.40
23	5	609	CLA	C3B-CAB	-2.12	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	618	XAT	O4-C5	-2.12	1.43	1.46
23	5	606	CLA	CMC-C2C	-2.12	1.46	1.50
23	A	837	CLA	C3B-CAB	-2.11	1.43	1.47
23	a	612	CLA	MG-ND	-2.11	2.01	2.05
23	B	830	CLA	CMC-C2C	-2.11	1.46	1.50
23	5	603	CLA	MG-ND	-2.11	2.01	2.05
23	B	818	CLA	C3B-CAB	-2.11	1.43	1.47
23	A	833	CLA	CMC-C2C	-2.11	1.46	1.50
23	8	603	CLA	MG-ND	-2.11	2.01	2.05
23	8	612	CLA	MG-ND	-2.11	2.01	2.05
23	6	604	CLA	CMC-C2C	-2.11	1.46	1.50
23	B	826	CLA	MG-ND	-2.11	2.01	2.05
23	4	607	CLA	CMD-C2D	-2.11	1.46	1.50
23	A	805	CLA	C3B-C2B	-2.11	1.37	1.40
23	1	611	CLA	CMD-C2D	-2.11	1.46	1.50
23	3	602	CLA	MG-ND	-2.11	2.01	2.05
23	A	823	CLA	CMD-C2D	-2.11	1.46	1.50
23	9	607	CLA	C3C-C2C	2.11	1.40	1.35
23	3	603	CLA	CAC-C3C	-2.11	1.45	1.51
23	7	616	CLA	CMC-C2C	-2.11	1.46	1.50
23	A	830	CLA	C4B-CHC	-2.11	1.35	1.41
23	6	616	CLA	CMD-C2D	-2.11	1.46	1.50
23	B	830	CLA	MG-ND	-2.10	2.01	2.05
23	9	611	CLA	C3C-C2C	2.10	1.40	1.35
23	1	606	CLA	CMD-C2D	-2.10	1.46	1.50
23	7	611	CLA	CMC-C2C	-2.10	1.46	1.50
23	A	813	CLA	MG-ND	-2.10	2.01	2.05
23	1	602	CLA	CMD-C2D	-2.10	1.46	1.50
23	7	615	CLA	CMD-C2D	-2.10	1.46	1.50
23	8	611	CLA	C3B-C2B	-2.10	1.37	1.40
23	3	615	CLA	CMC-C2C	-2.10	1.46	1.50
23	A	818	CLA	MG-ND	-2.10	2.01	2.05
23	6	611	CLA	CMD-C2D	-2.10	1.46	1.50
32	4	620	XAT	O4-C5	-2.10	1.43	1.46
23	6	620	CLA	C3B-CAB	-2.10	1.43	1.47
23	B	831	CLA	CMC-C2C	-2.10	1.46	1.50
23	6	604	CLA	C3B-CAB	-2.10	1.43	1.47
23	A	825	CLA	C4B-CHC	-2.10	1.35	1.41
23	8	601	CLA	C3B-CAB	-2.10	1.43	1.47
23	B	812	CLA	C3B-C2B	-2.10	1.37	1.40
23	9	610	CLA	C4C-NC	2.10	1.40	1.37
23	B	810	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	844	PQN	C5-C4	-2.10	1.44	1.48
23	A	801	CLA	MG-ND	-2.09	2.01	2.05
23	1	601	CLA	CMC-C2C	-2.09	1.46	1.50
23	B	822	CLA	CMD-C2D	-2.09	1.46	1.50
23	3	610	CLA	C3B-CAB	-2.09	1.43	1.47
32	a	618	XAT	O4-C5	-2.09	1.43	1.46
23	a	609	CLA	C3B-C2B	-2.09	1.37	1.40
23	A	823	CLA	CMC-C2C	-2.09	1.46	1.50
23	a	602	CLA	MG-ND	-2.09	2.01	2.05
23	A	825	CLA	C3B-C2B	-2.09	1.37	1.40
23	1	613	CLA	C3B-CAB	-2.09	1.43	1.47
23	A	832	CLA	CMC-C2C	-2.09	1.46	1.50
23	1	612	CLA	MG-ND	-2.09	2.01	2.05
23	5	614	CLA	CMD-C2D	-2.09	1.46	1.50
23	3	612	CLA	MG-ND	-2.09	2.01	2.05
26	B	846	BCR	C21-C22	-2.09	1.33	1.35
25	8	622	LHG	O7-C5	-2.09	1.41	1.46
23	B	810	CLA	C3B-CAB	-2.09	1.43	1.47
23	3	603	CLA	CMC-C2C	-2.09	1.46	1.50
23	8	604	CLA	CMC-C2C	-2.09	1.46	1.50
23	7	601	CLA	CMA-C3A	-2.09	1.48	1.53
23	A	811	CLA	C3B-C2B	-2.09	1.37	1.40
23	B	803	CLA	C3B-CAB	-2.09	1.43	1.47
23	9	612	CLA	C3C-C2C	2.09	1.40	1.35
23	B	835	CLA	MG-ND	-2.09	2.01	2.05
23	A	837	CLA	CMC-C2C	-2.09	1.46	1.50
23	A	835	CLA	C4B-CHC	-2.09	1.35	1.41
23	A	843	CLA	C4B-CHC	-2.09	1.35	1.41
23	B	839	CLA	C3B-C2B	-2.09	1.37	1.40
23	3	607	CLA	MG-ND	-2.09	2.01	2.05
23	B	817	CLA	CMD-C2D	-2.09	1.46	1.50
29	J	104	LMG	O4-C4	-2.09	1.38	1.43
23	A	806	CLA	C4B-CHC	-2.09	1.35	1.41
23	a	613	CLA	CMC-C2C	-2.08	1.46	1.50
23	A	833	CLA	C3B-CAB	-2.08	1.43	1.47
26	A	850	BCR	C30-C25	-2.08	1.50	1.53
23	6	604	CLA	CMD-C2D	-2.08	1.46	1.50
23	3	610	CLA	MG-ND	-2.08	2.01	2.05
29	5	627	LMG	O7-C8	-2.08	1.41	1.46
23	3	607	CLA	CMC-C2C	-2.08	1.46	1.50
23	5	617	CLA	C4B-CHC	-2.08	1.35	1.41
23	B	841	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	611	CLA	CMC-C2C	-2.08	1.46	1.50
23	A	829	CLA	MG-ND	-2.08	2.01	2.05
23	a	610	CLA	CMD-C2D	-2.08	1.46	1.50
23	6	607	CLA	MG-ND	-2.08	2.01	2.05
23	6	611	CLA	MG-ND	-2.08	2.01	2.05
23	2	614	CLA	C3C-C2C	2.08	1.40	1.35
23	A	831	CLA	C3B-CAB	-2.08	1.43	1.47
23	6	603	CLA	MG-ND	-2.07	2.01	2.05
23	B	830	CLA	C3B-CAB	-2.07	1.43	1.47
28	5	628	LMU	O5'-C5'	2.07	1.49	1.44
23	A	823	CLA	C3B-CAB	-2.07	1.43	1.47
23	8	609	CLA	MG-ND	-2.07	2.01	2.05
23	B	809	CLA	C4B-CHC	-2.07	1.35	1.41
23	L	303	CLA	MG-ND	-2.07	2.01	2.05
23	6	601	CLA	C3B-CAB	-2.07	1.43	1.47
23	5	619	CLA	CMD-C2D	-2.07	1.46	1.50
25	3	623	LHG	P-O6	2.07	1.67	1.59
23	5	604	CLA	MG-ND	-2.07	2.01	2.05
23	A	813	CLA	C3B-C2B	-2.07	1.37	1.40
23	1	611	CLA	C3B-C2B	-2.07	1.37	1.40
23	1	611	CLA	CMC-C2C	-2.07	1.46	1.50
23	a	616	CLA	C3B-C2B	-2.07	1.37	1.40
26	A	849	BCR	C21-C22	-2.07	1.33	1.35
23	2	613	CLA	C3C-C2C	2.07	1.39	1.35
23	1	602	CLA	MG-ND	-2.07	2.01	2.05
23	2	609	CLA	C3C-C2C	2.07	1.39	1.35
23	A	836	CLA	MG-ND	-2.07	2.01	2.05
23	K	201	CLA	MG-ND	-2.07	2.01	2.05
23	7	614	CLA	C3B-CAB	-2.07	1.43	1.47
23	1	610	CLA	CMD-C2D	-2.07	1.46	1.50
23	B	815	CLA	C3B-CAB	-2.07	1.43	1.47
23	A	814	CLA	MG-ND	-2.07	2.01	2.05
23	B	837	CLA	MG-ND	-2.06	2.01	2.05
23	F	303	CLA	CMC-C2C	-2.06	1.46	1.50
23	3	614	CLA	CMC-C2C	-2.06	1.46	1.50
23	4	618	CLA	MG-ND	-2.06	2.01	2.05
23	7	601	CLA	CMD-C2D	-2.06	1.46	1.50
23	7	602	CLA	MG-ND	-2.06	2.01	2.05
23	5	609	CLA	C3B-C2B	-2.06	1.37	1.40
26	J	102	BCR	C10-C9	-2.06	1.33	1.35
23	4	613	CLA	C3B-CAB	-2.06	1.43	1.47
32	8	620	XAT	O4-C5	-2.06	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	602	CLA	C3C-C2C	2.06	1.39	1.35
23	B	818	CLA	MG-ND	-2.06	2.01	2.05
23	5	609	CLA	CMC-C2C	-2.06	1.46	1.50
23	B	806	CLA	C3B-C2B	-2.06	1.37	1.40
23	B	834	CLA	CMC-C2C	-2.06	1.46	1.50
23	5	604	CLA	CMC-C2C	-2.06	1.46	1.50
23	4	610	CLA	C3B-CAB	-2.06	1.43	1.47
32	6	621	XAT	O4-C5	-2.06	1.43	1.46
23	6	608	CLA	C4B-CHC	-2.06	1.35	1.41
23	1	607	CLA	CMD-C2D	-2.05	1.46	1.50
23	8	611	CLA	CMC-C2C	-2.05	1.46	1.50
23	3	611	CLA	MG-ND	-2.05	2.01	2.05
23	a	606	CLA	CMD-C2D	-2.05	1.46	1.50
23	8	602	CLA	C3B-C2B	-2.05	1.37	1.40
31	8	619	LUT	C22-C21	-2.05	1.52	1.54
23	9	601	CLA	C3C-C2C	2.05	1.39	1.35
23	8	608	CLA	C3B-CAB	-2.05	1.43	1.47
23	1	607	CLA	C3B-C2B	-2.05	1.37	1.40
23	G	203	CLA	CMC-C2C	-2.05	1.46	1.50
23	5	616	CLA	MG-ND	-2.05	2.01	2.05
23	6	614	CLA	MG-ND	-2.05	2.01	2.05
23	6	608	CLA	C3B-CAB	-2.05	1.43	1.47
23	K	206	CLA	CMD-C2D	-2.05	1.46	1.50
23	4	604	CLA	CMC-C2C	-2.05	1.46	1.50
23	8	614	CLA	CMC-C2C	-2.05	1.46	1.50
23	a	610	CLA	C3B-CAB	-2.05	1.43	1.47
23	B	834	CLA	C3B-C2B	-2.05	1.37	1.40
23	B	809	CLA	CMC-C2C	-2.05	1.46	1.50
23	6	602	CLA	C3B-C2B	-2.05	1.37	1.40
23	5	614	CLA	CMC-C2C	-2.05	1.46	1.50
23	2	603	CLA	C3C-C2C	2.05	1.39	1.35
23	4	610	CLA	MG-ND	-2.05	2.01	2.05
23	3	617	CLA	CMC-C2C	-2.05	1.46	1.50
23	4	601	CLA	C3B-CAB	-2.05	1.43	1.47
23	6	609	CLA	CMC-C2C	-2.04	1.46	1.50
23	3	603	CLA	C3B-CAB	-2.04	1.43	1.47
23	1	610	CLA	CMC-C2C	-2.04	1.46	1.50
23	a	610	CLA	CMC-C2C	-2.04	1.46	1.50
25	5	625	LHG	P-O6	2.04	1.67	1.59
23	6	620	CLA	C3B-C2B	-2.04	1.37	1.40
23	B	840	CLA	CMC-C2C	-2.04	1.46	1.50
23	a	607	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	611	CLA	MG-ND	-2.04	2.01	2.05
23	8	602	CLA	C3B-CAB	-2.04	1.43	1.47
23	9	614	CLA	C3C-C2C	2.04	1.39	1.35
23	1	614	CLA	MG-ND	-2.04	2.01	2.05
23	2	616	CLA	C3C-C2C	2.04	1.39	1.35
23	6	618	CLA	CMD-C2D	-2.04	1.46	1.50
23	2	611	CLA	C3A-C4A	2.04	1.54	1.50
23	1	611	CLA	MG-ND	-2.04	2.01	2.05
23	B	818	CLA	C4B-CHC	-2.04	1.35	1.41
23	1	601	CLA	C3B-CAB	-2.04	1.43	1.47
23	A	832	CLA	C4B-CHC	-2.04	1.35	1.41
23	8	614	CLA	C3B-C2B	-2.04	1.37	1.40
23	5	619	CLA	C4B-CHC	-2.04	1.35	1.41
23	9	604	CLA	C3C-C2C	2.04	1.39	1.35
23	B	809	CLA	C3B-C2B	-2.04	1.37	1.40
23	8	608	CLA	CMC-C2C	-2.04	1.46	1.50
23	B	809	CLA	C3B-CAB	-2.04	1.43	1.47
32	5	621	XAT	O4-C5	-2.04	1.43	1.46
23	K	206	CLA	C3B-C2B	-2.04	1.37	1.40
23	a	604	CLA	CMC-C2C	-2.03	1.46	1.50
23	4	611	CLA	CMC-C2C	-2.03	1.46	1.50
23	8	613	CLA	C3B-CAB	-2.03	1.43	1.47
23	9	603	CLA	C3C-C2C	2.03	1.39	1.35
23	2	602	CLA	C3C-C2C	2.03	1.39	1.35
23	a	616	CLA	CMC-C2C	-2.03	1.46	1.50
23	6	611	CLA	CMC-C2C	-2.03	1.46	1.50
23	5	611	CLA	MG-ND	-2.03	2.01	2.05
32	5	621	XAT	O24-C25	-2.03	1.43	1.46
23	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
23	A	843	CLA	C3B-CAB	-2.03	1.43	1.47
23	1	616	CLA	CMC-C2C	-2.03	1.46	1.50
23	a	614	CLA	MG-ND	-2.03	2.01	2.05
23	a	603	CLA	CAC-C3C	-2.03	1.45	1.51
23	8	608	CLA	CAC-C3C	-2.03	1.45	1.51
23	4	604	CLA	MG-ND	-2.03	2.01	2.05
23	A	808	CLA	MG-ND	-2.03	2.01	2.05
23	7	609	CLA	CMC-C2C	-2.03	1.46	1.50
23	1	603	CLA	CAC-C3C	-2.03	1.45	1.51
23	3	617	CLA	C3B-C2B	-2.03	1.37	1.40
23	5	618	CLA	CMC-C2C	-2.03	1.46	1.50
23	B	813	CLA	MG-ND	-2.03	2.01	2.05
23	B	832	CLA	C3B-CAB	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	623	LHG	O7-C5	-2.02	1.41	1.46
23	A	824	CLA	C4B-CHC	-2.02	1.35	1.41
23	B	838	CLA	CMC-C2C	-2.02	1.46	1.50
23	1	610	CLA	C3B-CAB	-2.02	1.43	1.47
23	a	608	CLA	CMD-C2D	-2.02	1.46	1.50
23	3	615	CLA	CMD-C2D	-2.02	1.46	1.50
23	A	845	CLA	C3B-CAB	-2.02	1.43	1.47
23	8	606	CLA	C3B-CAB	-2.02	1.43	1.47
23	B	830	CLA	C4B-CHC	-2.02	1.35	1.41
23	a	607	CLA	C3B-C2B	-2.02	1.37	1.40
23	B	806	CLA	CAC-C3C	-2.02	1.45	1.51
23	7	611	CLA	MG-ND	-2.02	2.01	2.05
23	a	613	CLA	C3B-CAB	-2.02	1.43	1.47
23	F	303	CLA	CAC-C3C	-2.02	1.45	1.51
23	5	601	CLA	CMC-C2C	-2.02	1.46	1.50
23	B	821	CLA	C3B-CAB	-2.02	1.43	1.47
23	1	614	CLA	CMC-C2C	-2.02	1.46	1.50
23	B	819	CLA	C3B-CAB	-2.02	1.43	1.47
23	B	820	CLA	CMC-C2C	-2.01	1.46	1.50
28	K	208	LMU	O5'-C5'	2.01	1.49	1.44
23	A	804	CLA	C4B-CHC	-2.01	1.35	1.41
23	1	604	CLA	CMC-C2C	-2.01	1.46	1.50
23	a	603	CLA	MG-ND	-2.01	2.01	2.05
23	B	832	CLA	MG-ND	-2.01	2.01	2.05
23	3	609	CLA	C3B-C2B	-2.01	1.37	1.40
23	B	838	CLA	C4B-CHC	-2.01	1.35	1.41
23	7	611	CLA	C4B-CHC	-2.01	1.35	1.41
23	2	601	CLA	C3C-C2C	2.01	1.39	1.35
23	B	832	CLA	C3B-C2B	-2.01	1.37	1.40
28	A	857	LMU	O1B-C1B	-2.01	1.36	1.41
23	L	303	CLA	CMC-C2C	-2.01	1.46	1.50
23	2	611	CLA	C3C-C2C	2.01	1.39	1.35
30	B	850	DGD	O4E-C4E	-2.01	1.38	1.43
23	A	840	CLA	C3B-CAB	-2.01	1.43	1.47
23	3	604	CLA	C3B-CAB	-2.01	1.43	1.47
23	B	811	CLA	CMC-C2C	-2.00	1.46	1.50
23	8	606	CLA	CMC-C2C	-2.00	1.46	1.50
23	1	603	CLA	MG-ND	-2.00	2.01	2.05
23	8	608	CLA	MG-ND	-2.00	2.01	2.05
23	B	814	CLA	C3B-C2B	-2.00	1.37	1.40
23	5	611	CLA	C3B-CAB	-2.00	1.43	1.47
23	A	806	CLA	CAC-C3C	-2.00	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	821	CLA	C3B-CAB	-2.00	1.43	1.47
23	3	614	CLA	C3B-CAB	-2.00	1.43	1.47
26	A	851	BCR	C10-C9	-2.00	1.33	1.35
26	F	305	BCR	C30-C25	-2.00	1.51	1.53
23	a	606	CLA	C3B-C2B	-2.00	1.37	1.40
23	B	822	CLA	C3B-CAB	-2.00	1.43	1.47

All (3030) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	621	XAT	O24-C25-C24	10.95	121.61	113.38
32	2	620	XAT	O24-C25-C24	10.87	121.55	113.38
32	9	620	XAT	O4-C5-C4	10.55	121.31	113.38
23	B	803	CLA	C4A-NA-C1A	9.04	110.77	106.71
23	8	613	CLA	C4A-NA-C1A	8.99	110.75	106.71
23	B	808	CLA	C4A-NA-C1A	8.68	110.61	106.71
32	2	620	XAT	O4-C5-C4	8.59	119.84	113.38
23	A	841	CLA	C4A-NA-C1A	8.39	110.48	106.71
24	A	844	PQN	C11-C12-C13	-8.27	113.03	126.79
23	A	830	CLA	C4A-NA-C1A	8.23	110.41	106.71
23	1	603	CLA	C4A-NA-C1A	8.21	110.39	106.71
23	A	823	CLA	C4A-NA-C1A	8.20	110.39	106.71
23	5	613	CLA	C4A-NA-C1A	8.20	110.39	106.71
23	a	603	CLA	C4A-NA-C1A	8.19	110.39	106.71
23	B	838	CLA	C4A-NA-C1A	8.12	110.36	106.71
32	8	620	XAT	O24-C25-C24	8.10	119.47	113.38
23	B	831	CLA	C4A-NA-C1A	8.08	110.34	106.71
23	A	804	CLA	C4A-NA-C1A	8.05	110.32	106.71
24	B	842	PQN	C15-C13-C12	-7.96	105.00	121.12
23	G	203	CLA	C4A-NA-C1A	7.91	110.26	106.71
23	B	819	CLA	C4A-NA-C1A	7.88	110.25	106.71
23	A	845	CLA	C4A-NA-C1A	7.86	110.24	106.71
23	B	805	CLA	C4A-NA-C1A	7.85	110.23	106.71
23	A	821	CLA	C4A-NA-C1A	7.84	110.23	106.71
23	5	619	CLA	C4A-NA-C1A	7.83	110.23	106.71
26	B	801	BCR	C24-C23-C22	-7.79	114.47	126.23
23	A	818	CLA	C4A-NA-C1A	7.77	110.20	106.71
23	8	608	CLA	C4A-NA-C1A	7.75	110.19	106.71
23	B	816	CLA	C4A-NA-C1A	7.74	110.18	106.71
23	8	616	CLA	C4A-NA-C1A	7.71	110.17	106.71
23	3	603	CLA	C4A-NA-C1A	7.68	110.16	106.71
23	A	816	CLA	C4A-NA-C1A	7.67	110.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	818	CLA	C4A-NA-C1A	7.60	110.12	106.71
23	A	813	CLA	C4A-NA-C1A	7.59	110.12	106.71
23	4	613	CLA	C4A-NA-C1A	7.58	110.12	106.71
23	A	838	CLA	C4A-NA-C1A	7.57	110.11	106.71
23	B	820	CLA	C4A-NA-C1A	7.57	110.11	106.71
23	7	609	CLA	C4A-NA-C1A	7.57	110.11	106.71
23	F	301	CLA	C4A-NA-C1A	7.55	110.10	106.71
23	J	101	CLA	C4A-NA-C1A	7.53	110.09	106.71
23	7	611	CLA	C4A-NA-C1A	7.53	110.09	106.71
23	4	601	CLA	C4A-NA-C1A	7.49	110.07	106.71
23	K	201	CLA	C4A-NA-C1A	7.48	110.07	106.71
23	B	830	CLA	C4A-NA-C1A	7.47	110.06	106.71
23	5	602	CLA	C4A-NA-C1A	7.45	110.05	106.71
23	A	843	CLA	C4A-NA-C1A	7.43	110.05	106.71
23	B	821	CLA	C4A-NA-C1A	7.43	110.05	106.71
23	1	613	CLA	C4A-NA-C1A	7.43	110.05	106.71
23	1	604	CLA	C4A-NA-C1A	7.43	110.05	106.71
23	5	607	CLA	C4A-NA-C1A	7.40	110.03	106.71
23	A	806	CLA	C4A-NA-C1A	7.39	110.03	106.71
23	A	842	CLA	C4A-NA-C1A	7.39	110.03	106.71
23	a	604	CLA	C4A-NA-C1A	7.38	110.03	106.71
23	a	613	CLA	C4A-NA-C1A	7.35	110.01	106.71
23	7	615	CLA	C4A-NA-C1A	7.35	110.01	106.71
23	3	612	CLA	C4A-NA-C1A	7.34	110.01	106.71
23	A	837	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	7	601	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	A	840	CLA	C4A-NA-C1A	7.32	110.00	106.71
23	G	204	CLA	C4A-NA-C1A	7.31	109.99	106.71
23	3	602	CLA	C4A-NA-C1A	7.31	109.99	106.71
23	5	603	CLA	C4A-NA-C1A	7.29	109.98	106.71
23	A	836	CLA	C4A-NA-C1A	7.29	109.98	106.71
23	4	608	CLA	C4A-NA-C1A	7.29	109.98	106.71
23	B	809	CLA	C4A-NA-C1A	7.28	109.98	106.71
23	L	303	CLA	C4A-NA-C1A	7.26	109.97	106.71
23	A	839	CLA	C4A-NA-C1A	7.25	109.97	106.71
23	3	613	CLA	C4A-NA-C1A	7.23	109.96	106.71
23	1	608	CLA	C4A-NA-C1A	7.22	109.95	106.71
23	B	835	CLA	C4A-NA-C1A	7.19	109.94	106.71
23	B	832	CLA	C4A-NA-C1A	7.18	109.93	106.71
23	1	609	CLA	C4A-NA-C1A	7.17	109.93	106.71
23	A	835	CLA	C4A-NA-C1A	7.16	109.93	106.71
23	3	610	CLA	C4A-NA-C1A	7.16	109.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	831	CLA	CMB-C2B-C1B	-7.15	117.48	128.46
23	A	834	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	3	608	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	4	609	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	a	609	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	3	615	CLA	C4A-NA-C1A	7.12	109.91	106.71
23	A	814	CLA	C4A-NA-C1A	7.11	109.90	106.71
23	a	608	CLA	C4A-NA-C1A	7.11	109.90	106.71
23	B	841	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	6	613	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	A	829	CLA	C4A-NA-C1A	7.08	109.89	106.71
23	6	602	CLA	C4A-NA-C1A	7.07	109.89	106.71
23	B	815	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	7	610	CLA	C4A-NA-C1A	7.04	109.87	106.71
23	F	304	CLA	C4A-NA-C1A	7.02	109.86	106.71
23	A	832	CLA	C4A-NA-C1A	7.02	109.86	106.71
23	B	812	CLA	C4A-NA-C1A	7.01	109.86	106.71
23	6	614	CLA	C4A-NA-C1A	7.01	109.86	106.71
23	B	814	CLA	C4A-NA-C1A	7.00	109.86	106.71
23	A	810	CLA	C4A-NA-C1A	7.00	109.85	106.71
23	B	834	CLA	C4A-NA-C1A	6.98	109.84	106.71
23	A	809	CLA	C4A-NA-C1A	6.98	109.84	106.71
23	B	837	CLA	C4A-NA-C1A	6.96	109.83	106.71
23	3	609	CLA	C4A-NA-C1A	6.96	109.83	106.71
23	5	604	CLA	C4A-NA-C1A	6.91	109.81	106.71
23	2	604	CLA	C4A-NA-C1A	6.91	109.81	106.71
23	A	825	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	B	817	CLA	C4A-NA-C1A	6.88	109.80	106.71
23	6	608	CLA	C4A-NA-C1A	6.86	109.79	106.71
23	B	807	CLA	C4A-NA-C1A	6.86	109.79	106.71
23	K	206	CLA	C4A-NA-C1A	6.85	109.79	106.71
23	4	612	CLA	C4A-NA-C1A	6.85	109.79	106.71
23	7	603	CLA	C4A-NA-C1A	6.85	109.78	106.71
23	6	601	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	A	815	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	6	609	CLA	C4A-NA-C1A	6.80	109.77	106.71
23	4	607	CLA	C4A-NA-C1A	6.78	109.75	106.71
33	5	624	NEX	O24-C25-C24	6.77	118.47	113.38
23	A	828	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	7	616	CLA	C4A-NA-C1A	6.76	109.75	106.71
23	A	824	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	B	839	CLA	C4A-NA-C1A	6.76	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	607	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	A	801	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	K	203	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	6	607	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	8	612	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	B	840	CLA	C4A-NA-C1A	6.73	109.73	106.71
32	1	618	XAT	O24-C25-C24	6.73	118.44	113.38
23	L	302	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	B	811	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	3	604	CLA	C4A-NA-C1A	6.69	109.72	106.71
23	3	611	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	6	618	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	B	828	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	3	606	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	1	607	CLA	C4A-NA-C1A	6.67	109.70	106.71
32	a	618	XAT	O24-C25-C24	6.67	118.39	113.38
23	A	817	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	A	812	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	B	829	CLA	CMB-C2B-C1B	-6.66	118.23	128.46
23	5	610	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	6	620	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	1	602	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	5	616	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	7	607	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	B	842	PQN	C11-C12-C13	-6.62	115.77	126.79
23	8	607	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	B	806	CLA	C4A-NA-C1A	6.60	109.67	106.71
32	5	621	XAT	O4-C5-C4	6.59	118.33	113.38
23	1	616	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	5	611	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	9	602	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	a	602	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	4	604	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	a	611	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	8	610	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	9	609	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	1	614	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	A	803	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	B	810	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	a	614	CLA	C4A-NA-C1A	6.54	109.65	106.71
26	J	102	BCR	C28-C27-C26	-6.54	102.41	114.08
26	3	622	BCR	C11-C10-C9	-6.53	117.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	829	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	9	613	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	3	607	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	4	610	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	8	602	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	7	613	CLA	C4A-NA-C1A	6.51	109.63	106.71
32	7	620	XAT	O24-C25-C24	6.50	118.27	113.38
23	6	603	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	6	610	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	B	833	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	a	616	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	6	612	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	7	614	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	a	612	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	a	606	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	4	616	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	1	612	CLA	C4A-NA-C1A	6.45	109.60	106.71
23	1	606	CLA	C4A-NA-C1A	6.43	109.60	106.71
26	F	305	BCR	C20-C21-C22	-6.43	118.14	127.31
23	1	611	CLA	C4A-NA-C1A	6.42	109.59	106.71
23	A	819	CLA	C4A-NA-C1A	6.42	109.59	106.71
23	L	304	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	5	608	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	2	610	CLA	C4A-NA-C1A	6.40	109.58	106.71
23	7	604	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	8	603	CLA	C4A-NA-C1A	6.39	109.58	106.71
24	A	844	PQN	C15-C13-C12	-6.39	108.19	121.12
23	5	612	CLA	C4A-NA-C1A	6.37	109.57	106.71
32	3	619	XAT	O24-C25-C24	6.36	118.16	113.38
23	7	608	CLA	C4A-NA-C1A	6.36	109.56	106.71
23	2	601	CLA	C4A-NA-C1A	6.36	109.56	106.71
23	A	833	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	8	604	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	a	610	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	8	609	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	A	826	CLA	C4A-NA-C1A	6.32	109.55	106.71
23	A	811	CLA	C4A-NA-C1A	6.31	109.54	106.71
23	9	607	CLA	C4A-NA-C1A	6.31	109.54	106.71
23	B	826	CLA	C4A-NA-C1A	6.29	109.53	106.71
32	4	620	XAT	O24-C25-C24	6.29	118.11	113.38
23	B	813	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	B	827	CLA	C4A-NA-C1A	6.27	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	824	CLA	C4A-NA-C1A	6.27	109.52	106.71
23	1	601	CLA	C4A-NA-C1A	6.27	109.52	106.71
23	A	808	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	4	611	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	4	614	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	a	601	CLA	C4A-NA-C1A	6.25	109.52	106.71
23	1	610	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	5	606	CLA	C4A-NA-C1A	6.22	109.50	106.71
23	6	611	CLA	C4A-NA-C1A	6.22	109.50	106.71
23	9	614	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	5	601	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	9	610	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	2	609	CLA	C4A-NA-C1A	6.21	109.50	106.71
32	6	621	XAT	O24-C25-C24	6.20	118.04	113.38
23	6	616	CLA	CMB-C2B-C1B	-6.19	118.95	128.46
23	A	831	CLA	C4A-NA-C1A	6.18	109.48	106.71
23	B	802	CLA	C4A-NA-C1A	6.16	109.48	106.71
23	5	618	CLA	C4A-NA-C1A	6.16	109.47	106.71
26	3	621	BCR	C11-C10-C9	-6.15	118.53	127.31
26	3	622	BCR	C20-C21-C22	-6.15	118.53	127.31
23	A	827	CLA	C4A-NA-C1A	6.13	109.46	106.71
23	2	612	CLA	C4A-NA-C1A	6.13	109.46	106.71
23	A	822	CLA	C4A-NA-C1A	6.12	109.46	106.71
23	B	823	CLA	C4A-NA-C1A	6.12	109.46	106.71
23	4	603	CLA	C4A-NA-C1A	6.12	109.46	106.71
23	9	606	CLA	C4A-NA-C1A	6.12	109.46	106.71
23	A	820	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	K	204	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	6	604	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	4	606	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	2	603	CLA	C4A-NA-C1A	6.08	109.44	106.71
23	5	617	CLA	C4A-NA-C1A	6.08	109.44	106.71
23	8	611	CLA	C4A-NA-C1A	6.07	109.43	106.71
23	2	607	CLA	C4A-NA-C1A	6.06	109.43	106.71
23	A	802	CLA	C4A-NA-C1A	6.06	109.43	106.71
23	9	612	CLA	C4A-NA-C1A	6.06	109.43	106.71
23	9	604	CLA	C4A-NA-C1A	6.05	109.43	106.71
23	3	617	CLA	C4A-NA-C1A	6.05	109.43	106.71
23	4	602	CLA	C4A-NA-C1A	6.05	109.43	106.71
23	8	601	CLA	C4A-NA-C1A	6.05	109.43	106.71
23	B	822	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	2	616	CLA	C4A-NA-C1A	6.04	109.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	9	611	CLA	C4A-NA-C1A	6.03	109.42	106.71
26	A	852	BCR	C7-C8-C9	-6.03	117.13	126.23
23	4	618	CLA	C4A-NA-C1A	6.02	109.41	106.71
23	9	601	CLA	C4A-NA-C1A	6.01	109.41	106.71
32	4	620	XAT	C26-C27-C28	-6.00	113.32	125.99
24	A	844	PQN	C14-C13-C12	-5.97	108.36	123.68
23	A	820	CLA	CMB-C2B-C1B	-5.97	119.29	128.46
23	A	807	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	7	612	CLA	C4A-NA-C1A	5.94	109.38	106.71
26	3	621	BCR	C35-C13-C14	-5.92	114.63	122.92
32	8	620	XAT	O4-C5-C4	5.92	117.83	113.38
23	A	805	CLA	C4A-NA-C1A	5.91	109.36	106.71
32	6	621	XAT	O4-C5-C4	5.90	117.82	113.38
23	8	614	CLA	C4A-NA-C1A	5.90	109.36	106.71
32	3	619	XAT	C18-C5-C6	-5.88	112.41	122.26
26	3	622	BCR	C36-C18-C17	-5.88	114.69	122.92
23	5	614	CLA	C4A-NA-C1A	5.87	109.35	106.71
32	1	618	XAT	O4-C5-C4	5.87	117.79	113.38
23	6	606	CLA	C4A-NA-C1A	5.85	109.34	106.71
32	a	618	XAT	O4-C5-C4	5.83	117.76	113.38
32	3	619	XAT	C6-C7-C8	-5.83	113.67	125.99
26	A	852	BCR	C20-C21-C22	-5.80	119.03	127.31
26	5	622	BCR	C3-C4-C5	-5.79	103.74	114.08
23	2	606	CLA	C4A-NA-C1A	5.77	109.30	106.71
26	A	851	BCR	C24-C23-C22	-5.76	117.53	126.23
32	a	618	XAT	C26-C27-C28	-5.75	113.83	125.99
32	1	618	XAT	C26-C27-C28	-5.75	113.83	125.99
23	B	825	CLA	C4A-NA-C1A	5.75	109.29	106.71
32	6	621	XAT	C6-C7-C8	-5.74	113.86	125.99
23	2	614	CLA	C4A-NA-C1A	5.73	109.28	106.71
32	6	621	XAT	C26-C27-C28	-5.72	113.90	125.99
32	9	620	XAT	C38-C25-C26	-5.71	112.68	122.26
23	3	614	CLA	C4A-NA-C1A	5.70	109.27	106.71
23	A	826	CLA	CMB-C2B-C1B	-5.68	119.74	128.46
32	6	621	XAT	C38-C25-C26	-5.67	112.75	122.26
26	K	202	BCR	C15-C14-C13	-5.66	119.23	127.31
23	A	802	CLA	CMB-C2B-C1B	-5.66	119.77	128.46
23	5	609	CLA	C4A-NA-C1A	5.63	109.24	106.71
23	2	613	CLA	C4A-NA-C1A	5.61	109.23	106.71
32	4	620	XAT	C6-C7-C8	-5.61	114.13	125.99
23	8	606	CLA	C4A-NA-C1A	5.59	109.22	106.71
32	5	621	XAT	C18-C5-C6	-5.59	112.89	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	620	XAT	C38-C25-C26	-5.57	112.93	122.26
23	F	303	CLA	C4A-NA-C1A	5.56	109.21	106.71
32	3	619	XAT	C38-C25-C26	-5.55	112.95	122.26
32	7	620	XAT	O4-C5-C4	5.55	117.55	113.38
32	7	620	XAT	C38-C25-C26	-5.55	112.96	122.26
33	5	624	NEX	O24-C25-C38	5.53	121.68	115.06
23	B	804	CLA	C4A-NA-C1A	5.52	109.19	106.71
32	6	621	XAT	C18-C5-C6	-5.50	113.04	122.26
26	J	102	BCR	C16-C17-C18	-5.49	119.47	127.31
23	7	602	CLA	C4A-NA-C1A	5.49	109.18	106.71
23	4	602	CLA	CMB-C2B-C1B	-5.48	120.04	128.46
23	2	602	CLA	C4A-NA-C1A	5.46	109.16	106.71
32	1	618	XAT	C38-C25-C26	-5.44	113.14	122.26
23	A	806	CLA	CAA-C2A-C3A	-5.44	97.88	112.78
26	L	305	BCR	C7-C8-C9	-5.44	118.02	126.23
26	K	202	BCR	C28-C27-C26	-5.43	104.37	114.08
23	9	603	CLA	C4A-NA-C1A	5.42	109.14	106.71
23	7	606	CLA	C4A-NA-C1A	5.42	109.14	106.71
23	A	805	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
32	a	618	XAT	C38-C25-C26	-5.40	113.20	122.26
26	A	856	BCR	C20-C21-C22	-5.40	119.61	127.31
32	5	621	XAT	C6-C7-C8	-5.39	114.59	125.99
26	3	622	BCR	C24-C23-C22	-5.39	118.09	126.23
26	K	202	BCR	C3-C4-C5	-5.38	104.47	114.08
32	4	620	XAT	C38-C25-C26	-5.37	113.26	122.26
32	8	620	XAT	O4-C5-C18	5.37	121.49	115.06
26	B	848	BCR	C24-C23-C22	-5.35	118.15	126.23
23	B	823	CLA	CMB-C2B-C1B	-5.34	120.25	128.46
32	8	620	XAT	C26-C27-C28	-5.34	114.70	125.99
32	9	620	XAT	O24-C25-C24	5.33	117.39	113.38
26	B	844	BCR	C30-C25-C26	-5.33	115.11	122.61
26	A	849	BCR	C16-C17-C18	-5.32	119.72	127.31
23	B	831	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
33	6	624	NEX	C38-C25-C26	-5.31	113.36	122.26
23	B	836	CLA	CMB-C2B-C1B	-5.30	120.32	128.46
23	B	805	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
32	4	620	XAT	C18-C5-C6	-5.24	113.48	122.26
23	8	610	CLA	CMB-C2B-C1B	-5.23	120.43	128.46
26	a	619	BCR	C28-C27-C26	-5.21	104.77	114.08
23	5	602	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
32	7	620	XAT	C6-C7-C8	-5.21	114.98	125.99
32	9	620	XAT	O24-C25-C38	5.21	121.30	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	818	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
23	6	616	CLA	CMB-C2B-C3B	5.19	134.39	124.68
23	A	833	CLA	CMB-C2B-C1B	-5.19	120.49	128.46
26	1	619	BCR	C28-C27-C26	-5.19	104.81	114.08
33	6	624	NEX	O24-C25-C24	5.18	117.28	113.38
26	B	801	BCR	C16-C17-C18	-5.17	119.92	127.31
26	3	621	BCR	C12-C13-C14	5.17	126.88	118.94
23	4	608	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
32	2	620	XAT	C18-C5-C6	-5.17	113.60	122.26
23	B	836	CLA	C4A-NA-C1A	5.16	109.03	106.71
26	4	621	BCR	C28-C27-C26	-5.15	104.87	114.08
23	B	804	CLA	CMB-C2B-C1B	-5.15	120.56	128.46
32	a	618	XAT	C6-C7-C8	-5.14	115.12	125.99
32	1	618	XAT	C6-C7-C8	-5.14	115.13	125.99
32	4	620	XAT	O4-C5-C18	5.12	121.19	115.06
26	B	844	BCR	C24-C23-C22	-5.11	118.51	126.23
23	6	617	CLA	C4A-NA-C1A	5.09	108.99	106.71
23	A	803	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
26	5	622	BCR	C16-C17-C18	-5.08	120.05	127.31
26	5	622	BCR	C15-C14-C13	-5.08	120.06	127.31
23	7	607	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
23	B	826	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
26	8	621	BCR	C28-C27-C26	-5.04	105.07	114.08
26	K	202	BCR	C24-C23-C22	-5.03	118.64	126.23
23	5	612	CLA	CMB-C2B-C1B	-5.01	120.77	128.46
23	B	824	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
32	3	619	XAT	O4-C5-C4	4.99	117.13	113.38
26	B	845	BCR	C7-C8-C9	-4.99	118.70	126.23
23	A	827	CLA	CMB-C2B-C1B	-4.98	120.80	128.46
26	A	848	BCR	C20-C21-C22	-4.98	120.20	127.31
26	8	621	BCR	C3-C4-C5	-4.98	105.19	114.08
33	5	624	NEX	C31-C30-C29	-4.98	120.21	127.31
23	7	606	CLA	CMB-C2B-C1B	-4.98	120.82	128.46
26	A	851	BCR	C20-C21-C22	-4.95	120.24	127.31
23	A	802	CLA	CMB-C2B-C3B	4.95	133.93	124.68
32	7	620	XAT	C26-C27-C28	-4.94	115.55	125.99
23	8	612	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
23	A	854	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
23	5	619	CLA	CAB-C3B-C4B	-4.93	120.89	128.46
33	5	624	NEX	C16-C1-C6	4.92	114.88	110.47
26	3	622	BCR	C7-C8-C9	-4.92	118.80	126.23
32	1	618	XAT	C18-C5-C6	-4.90	114.06	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	102	BCR	C15-C14-C13	-4.89	120.33	127.31
23	7	604	CLA	CMB-C2B-C1B	-4.89	120.94	128.46
32	a	618	XAT	C18-C5-C6	-4.89	114.06	122.26
26	3	620	BCR	C28-C27-C26	-4.88	105.37	114.08
23	B	809	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
26	B	846	BCR	C38-C26-C25	-4.87	119.06	124.53
32	2	620	XAT	C38-C25-C26	-4.86	114.12	122.26
23	A	838	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
26	A	856	BCR	C3-C4-C5	-4.85	105.41	114.08
26	B	843	BCR	C28-C27-C26	-4.85	105.41	114.08
33	6	624	NEX	O24-C25-C38	4.85	120.86	115.06
30	J	103	DGD	O3G-C3G-C2G	-4.84	99.23	110.90
32	6	621	XAT	O4-C5-C18	4.83	120.84	115.06
26	F	305	BCR	C16-C17-C18	-4.83	120.42	127.31
26	B	801	BCR	C20-C21-C22	-4.82	120.43	127.31
33	5	624	NEX	C15-C14-C13	-4.82	120.43	127.31
32	8	620	XAT	C18-C5-C6	-4.81	114.20	122.26
23	8	604	CLA	CMB-C2B-C1B	-4.81	121.08	128.46
23	4	602	CLA	CMB-C2B-C3B	4.78	133.63	124.68
26	A	848	BCR	C16-C17-C18	-4.78	120.49	127.31
23	A	854	CLA	C4A-NA-C1A	4.78	108.85	106.71
32	3	619	XAT	O4-C5-C18	4.75	120.75	115.06
23	8	609	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
26	3	620	BCR	C11-C10-C9	-4.75	120.53	127.31
23	6	616	CLA	C4A-NA-C1A	4.72	108.83	106.71
24	B	842	PQN	C14-C13-C12	-4.72	111.57	123.68
31	4	619	LUT	C35-C34-C33	-4.72	120.57	127.31
23	3	609	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
23	7	609	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
23	8	610	CLA	CMB-C2B-C3B	4.71	133.50	124.68
23	A	811	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
26	5	622	BCR	C28-C27-C26	-4.71	105.67	114.08
23	B	803	CLA	CAC-C3C-C4C	4.71	130.91	124.81
26	6	622	BCR	C3-C4-C5	-4.70	105.68	114.08
32	4	620	XAT	O4-C5-C4	4.70	116.91	113.38
23	6	601	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
23	3	608	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
26	3	621	BCR	C7-C8-C9	-4.66	119.19	126.23
23	8	602	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
23	a	612	CLA	CMB-C2B-C1B	-4.66	121.31	128.46
23	8	606	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
23	1	612	CLA	CMB-C2B-C1B	-4.64	121.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	819	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
33	5	624	NEX	C27-C28-C29	-4.62	118.36	125.53
23	6	610	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
32	7	620	XAT	C18-C5-C6	-4.61	114.53	122.26
26	L	301	BCR	C7-C8-C9	-4.61	119.27	126.23
23	B	831	CLA	CMB-C2B-C3B	4.60	133.28	124.68
23	B	814	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
23	B	836	CLA	CMB-C2B-C3B	4.59	133.27	124.68
23	A	813	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
26	B	844	BCR	C7-C8-C9	-4.57	119.33	126.23
23	B	828	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
32	a	618	XAT	O4-C5-C18	4.56	120.52	115.06
23	B	827	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
32	1	618	XAT	O4-C5-C18	4.55	120.51	115.06
26	7	621	BCR	C28-C27-C26	-4.55	105.95	114.08
32	6	621	XAT	O24-C25-C38	4.55	120.51	115.06
23	B	803	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
23	A	826	CLA	CMB-C2B-C3B	4.54	133.18	124.68
26	J	102	BCR	C3-C4-C5	-4.54	105.97	114.08
26	G	205	BCR	C24-C23-C22	-4.54	119.38	126.23
26	3	620	BCR	C7-C8-C9	-4.53	119.39	126.23
32	9	620	XAT	C26-C27-C28	-4.53	116.41	125.99
23	7	611	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
32	5	621	XAT	C38-C25-C26	-4.53	114.67	122.26
26	L	305	BCR	C16-C17-C18	-4.52	120.86	127.31
32	7	620	XAT	O4-C5-C18	4.51	120.46	115.06
26	L	305	BCR	C28-C27-C26	-4.51	106.02	114.08
23	4	606	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
26	B	845	BCR	C24-C23-C22	-4.50	119.43	126.23
23	3	610	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
32	8	620	XAT	O24-C25-C38	4.50	120.45	115.06
31	8	619	LUT	C35-C34-C33	-4.50	120.89	127.31
32	8	620	XAT	C35-C34-C33	-4.49	120.90	127.31
26	A	850	BCR	C24-C23-C22	-4.49	119.45	126.23
32	5	621	XAT	O4-C5-C18	4.48	120.42	115.06
32	7	620	XAT	O24-C25-C38	4.47	120.41	115.06
26	3	622	BCR	C35-C13-C14	-4.47	116.66	122.92
23	A	854	CLA	CMB-C2B-C3B	4.47	133.04	124.68
23	8	601	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
26	3	620	BCR	C20-C21-C22	-4.47	120.94	127.31
23	6	609	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
26	B	848	BCR	C20-C21-C22	-4.46	120.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	805	CLA	CMB-C2B-C3B	4.46	133.01	124.68
32	5	621	XAT	C26-C27-C28	-4.45	116.57	125.99
26	3	622	BCR	C19-C18-C17	4.45	125.78	118.94
26	G	205	BCR	C20-C21-C22	-4.45	120.96	127.31
23	A	822	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
23	4	612	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
23	5	602	CLA	CMB-C2B-C3B	4.44	132.99	124.68
23	3	603	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
23	A	836	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
23	F	304	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
23	7	602	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
26	7	621	BCR	C16-C17-C18	-4.43	120.98	127.31
32	9	620	XAT	C18-C5-C6	-4.42	114.86	122.26
23	6	606	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
31	5	620	LUT	C35-C34-C33	-4.41	121.01	127.31
30	B	850	DGD	O3G-C3G-C2G	-4.40	100.27	110.90
25	4	622	LHG	O4-P-O5	4.40	133.99	112.24
23	A	831	CLA	CMB-C2B-C3B	4.39	132.90	124.68
26	A	851	BCR	C15-C14-C13	-4.39	121.04	127.31
26	K	207	BCR	C24-C23-C22	-4.39	119.60	126.23
26	1	619	BCR	C33-C5-C6	-4.39	119.60	124.53
26	a	619	BCR	C33-C5-C6	-4.39	119.60	124.53
23	B	823	CLA	CMB-C2B-C3B	4.38	132.88	124.68
32	5	621	XAT	C35-C34-C33	-4.38	121.06	127.31
26	6	622	BCR	C16-C17-C18	-4.38	121.06	127.31
23	5	610	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
32	3	619	XAT	C26-C27-C28	-4.37	116.75	125.99
25	8	622	LHG	O4-P-O5	4.37	133.84	112.24
26	7	623	BCR	C7-C8-C9	-4.37	119.63	126.23
23	A	820	CLA	CMB-C2B-C3B	4.37	132.85	124.68
23	A	815	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
23	a	602	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
25	A	847	LHG	O4-P-O5	4.35	133.76	112.24
23	A	809	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
23	3	604	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
26	J	102	BCR	C7-C8-C9	-4.34	119.68	126.23
23	1	602	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
33	5	624	NEX	C38-C25-C26	-4.33	115.00	122.26
23	A	840	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
33	6	624	NEX	C26-C27-C28	-4.33	116.84	125.99
32	7	620	XAT	C15-C14-C13	-4.33	121.13	127.31
23	B	829	CLA	CMB-C2B-C3B	4.33	132.78	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	838	CLA	CMB-C2B-C3B	4.32	132.77	124.68
26	A	848	BCR	C38-C26-C25	-4.31	119.68	124.53
23	7	607	CLA	CMB-C2B-C3B	4.31	132.74	124.68
23	A	818	CLA	CMB-C2B-C3B	4.31	132.74	124.68
26	K	202	BCR	C20-C21-C22	-4.31	121.16	127.31
23	A	805	CLA	CMB-C2B-C3B	4.30	132.73	124.68
25	6	623	LHG	O4-P-O5	4.30	133.49	112.24
26	1	619	BCR	C16-C17-C18	-4.29	121.19	127.31
25	5	623	LHG	O4-P-O5	4.29	133.44	112.24
32	8	620	XAT	C6-C7-C8	-4.29	116.93	125.99
32	3	619	XAT	O24-C25-C38	4.28	120.19	115.06
26	4	621	BCR	C33-C5-C6	-4.28	119.72	124.53
32	a	618	XAT	O24-C25-C38	4.28	120.18	115.06
23	A	829	CLA	CMB-C2B-C1B	-4.27	121.89	128.46
25	A	846	LHG	O4-P-O5	4.27	133.34	112.24
26	4	621	BCR	C15-C14-C13	-4.27	121.22	127.31
32	4	620	XAT	O24-C25-C38	4.27	120.17	115.06
23	B	822	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
26	a	619	BCR	C16-C17-C18	-4.26	121.24	127.31
23	6	608	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
26	B	845	BCR	C15-C14-C13	-4.22	121.29	127.31
23	B	816	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
23	4	608	CLA	CMB-C2B-C3B	4.21	132.56	124.68
26	7	623	BCR	C16-C17-C18	-4.21	121.30	127.31
32	1	618	XAT	O24-C25-C38	4.21	120.10	115.06
26	3	622	BCR	C20-C19-C18	-4.21	114.59	126.42
23	B	824	CLA	CMB-C2B-C3B	4.21	132.55	124.68
26	A	849	BCR	C11-C10-C9	-4.20	121.31	127.31
26	B	848	BCR	C16-C17-C18	-4.20	121.31	127.31
23	8	614	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
26	7	621	BCR	C3-C4-C5	-4.20	106.58	114.08
25	a	620	LHG	O4-P-O5	4.20	133.01	112.24
25	1	620	LHG	O4-P-O5	4.19	132.97	112.24
23	B	804	CLA	CMB-C2B-C3B	4.19	132.52	124.68
23	5	612	CLA	CMB-C2B-C3B	4.19	132.52	124.68
23	A	816	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
26	B	846	BCR	C21-C20-C19	-4.19	110.16	123.22
25	7	622	LHG	O4-P-O5	4.18	132.92	112.24
25	5	625	LHG	O4-P-O5	4.18	132.92	112.24
23	A	833	CLA	CMB-C2B-C3B	4.18	132.50	124.68
31	7	619	LUT	C35-C34-C33	-4.18	121.34	127.31
32	8	620	XAT	C15-C14-C13	-4.18	121.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	850	BCR	C28-C27-C26	-4.18	106.62	114.08
26	B	844	BCR	C3-C4-C5	-4.18	106.62	114.08
31	2	619	LUT	C35-C34-C33	-4.17	121.36	127.31
25	3	623	LHG	O4-P-O5	4.17	132.85	112.24
26	4	621	BCR	C11-C10-C9	-4.17	121.36	127.31
23	5	609	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
23	7	604	CLA	CMB-C2B-C3B	4.16	132.47	124.68
25	8	623	LHG	O4-P-O5	4.16	132.82	112.24
25	2	622	LHG	O4-P-O5	4.16	132.81	112.24
23	8	609	CLA	CMB-C2B-C3B	4.16	132.46	124.68
26	3	622	BCR	C38-C26-C25	-4.16	119.86	124.53
23	A	827	CLA	CMB-C2B-C3B	4.16	132.45	124.68
23	B	839	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
26	F	305	BCR	C24-C23-C22	-4.15	119.97	126.23
23	4	601	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
23	L	304	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
25	9	622	LHG	O4-P-O5	4.15	132.74	112.24
26	A	851	BCR	C16-C17-C18	-4.14	121.39	127.31
23	A	808	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
25	B	851	LHG	O4-P-O5	4.14	132.70	112.24
23	5	618	CLA	CAB-C3B-C4B	-4.13	122.12	128.46
23	F	303	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
26	1	619	BCR	C15-C14-C13	-4.12	121.43	127.31
32	4	620	XAT	C35-C34-C33	-4.12	121.43	127.31
26	B	843	BCR	C7-C8-C9	-4.12	120.01	126.23
26	A	848	BCR	C15-C14-C13	-4.11	121.44	127.31
26	3	621	BCR	C20-C21-C22	-4.11	121.44	127.31
26	B	846	BCR	C7-C8-C9	-4.11	120.03	126.23
32	3	619	XAT	C15-C14-C13	-4.10	121.45	127.31
26	a	619	BCR	C15-C14-C13	-4.10	121.46	127.31
23	6	612	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
23	A	806	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
23	K	203	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
23	7	616	CLA	CAB-C3B-C4B	-4.09	122.18	128.46
23	8	612	CLA	CMB-C2B-C3B	4.09	132.32	124.68
26	B	845	BCR	C16-C17-C18	-4.08	121.48	127.31
25	3	624	LHG	O4-P-O5	4.08	132.39	112.24
23	B	832	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
26	B	847	BCR	C11-C10-C9	-4.05	121.53	127.31
23	5	619	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
26	G	205	BCR	C16-C17-C18	-4.04	121.55	127.31
26	3	620	BCR	C24-C23-C22	-4.04	120.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	817	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
23	1	611	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
31	9	619	LUT	C7-C8-C9	-4.02	120.16	126.23
23	B	827	CLA	CMB-C2B-C3B	4.02	132.19	124.68
23	a	611	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
23	8	604	CLA	CMB-C2B-C3B	4.01	132.19	124.68
26	A	850	BCR	C15-C14-C13	-4.01	121.58	127.31
26	6	622	BCR	C15-C14-C13	-4.01	121.58	127.31
23	6	601	CLA	CMB-C2B-C3B	4.01	132.18	124.68
23	6	620	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
23	1	609	CLA	CAB-C3B-C4B	-4.00	122.31	128.46
24	B	842	PQN	C14-C13-C15	-4.00	108.54	115.27
23	8	601	CLA	CMB-C2B-C3B	4.00	132.16	124.68
23	G	204	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
32	5	621	XAT	C15-C14-C13	-4.00	121.61	127.31
26	A	852	BCR	C16-C17-C18	-3.99	121.62	127.31
33	6	624	NEX	C11-C10-C9	-3.99	121.62	127.31
26	F	305	BCR	C38-C26-C25	-3.99	120.05	124.53
23	a	610	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
23	4	610	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
33	6	624	NEX	C17-C1-C6	-3.98	106.91	110.47
28	A	857	LMU	C1B-O1B-C4'	-3.97	108.13	117.96
23	B	826	CLA	CMB-C2B-C3B	3.97	132.11	124.68
26	B	846	BCR	C11-C10-C9	-3.97	121.65	127.31
23	B	825	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
23	1	606	CLA	CBD-CHA-C1A	3.97	132.26	128.06
23	A	812	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
23	F	304	CLA	CMB-C2B-C3B	3.96	132.10	124.68
23	5	607	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
31	2	619	LUT	C7-C8-C9	-3.96	120.25	126.23
23	A	835	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	A	807	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
26	L	301	BCR	C11-C10-C9	-3.96	121.66	127.31
26	3	620	BCR	C3-C4-C5	-3.95	107.02	114.08
26	B	847	BCR	C7-C8-C9	-3.94	120.28	126.23
32	2	620	XAT	C6-C7-C8	-3.94	117.67	125.99
23	B	806	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
23	L	302	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
23	6	610	CLA	CMB-C2B-C3B	3.93	132.03	124.68
26	B	845	BCR	C34-C9-C10	-3.93	117.42	122.92
23	A	824	CLA	CMA-C3A-C2A	-3.93	106.94	116.10
23	A	803	CLA	CMB-C2B-C3B	3.92	132.02	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	610	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
23	5	608	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
32	2	620	XAT	O4-C5-C18	3.92	119.75	115.06
26	A	856	BCR	C16-C17-C18	-3.92	121.72	127.31
32	5	621	XAT	C10-C11-C12	-3.92	110.99	123.22
23	4	611	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	6	603	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
32	5	621	XAT	C4-C3-C2	-3.91	103.22	110.77
26	1	619	BCR	C11-C10-C9	-3.91	121.73	127.31
26	A	850	BCR	C33-C5-C6	-3.90	120.14	124.53
30	B	850	DGD	O5D-C6D-C5D	-3.90	101.83	109.05
23	K	206	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	A	849	BCR	C24-C23-C22	-3.90	120.34	126.23
23	A	815	CLA	CMB-C2B-C3B	3.90	131.97	124.68
23	A	811	CLA	CMB-C2B-C3B	3.89	131.96	124.68
26	a	619	BCR	C11-C10-C9	-3.89	121.76	127.31
26	B	846	BCR	C38-C26-C27	3.88	121.07	113.62
23	B	838	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
23	B	832	CLA	CMB-C2B-C3B	3.88	131.93	124.68
23	3	617	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
23	a	612	CLA	CMB-C2B-C3B	3.87	131.93	124.68
23	A	813	CLA	CMB-C2B-C3B	3.87	131.92	124.68
23	7	606	CLA	CMB-C2B-C3B	3.87	131.92	124.68
26	B	847	BCR	C15-C14-C13	-3.86	121.79	127.31
31	3	618	LUT	C35-C34-C33	-3.86	121.80	127.31
23	B	828	CLA	CMB-C2B-C3B	3.86	131.89	124.68
23	B	837	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
26	3	621	BCR	C11-C12-C13	-3.85	115.59	126.42
23	B	838	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
26	G	205	BCR	C10-C11-C12	-3.85	111.21	123.22
26	6	622	BCR	C11-C10-C9	-3.85	121.82	127.31
26	7	621	BCR	C15-C14-C13	-3.85	121.82	127.31
23	1	601	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	1	614	CLA	CAB-C3B-C4B	-3.84	122.56	128.46
23	1	612	CLA	CMB-C2B-C3B	3.84	131.86	124.68
32	6	621	XAT	C24-C23-C22	-3.84	103.36	110.77
23	A	829	CLA	CMB-C2B-C3B	3.84	131.86	124.68
23	a	601	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
23	7	609	CLA	CMB-C2B-C3B	3.84	131.86	124.68
23	3	611	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
26	3	620	BCR	C16-C17-C18	-3.83	121.84	127.31
23	6	614	CLA	CMB-C2B-C1B	-3.83	122.58	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	814	CLA	CMB-C2B-C3B	3.83	131.84	124.68
23	4	616	CLA	CAB-C3B-C4B	-3.83	122.58	128.46
23	A	808	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
26	A	849	BCR	C7-C8-C9	-3.82	120.46	126.23
26	7	623	BCR	C33-C5-C6	-3.82	120.24	124.53
26	K	202	BCR	C11-C10-C9	-3.82	121.86	127.31
23	7	612	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
23	5	619	CLA	CAB-C3B-C2B	3.82	132.16	124.69
23	5	614	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
33	6	624	NEX	C31-C30-C29	-3.82	121.86	127.31
26	7	623	BCR	C28-C27-C26	-3.81	107.27	114.08
23	5	618	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
26	K	207	BCR	C7-C8-C9	-3.81	120.47	126.23
31	9	619	LUT	C35-C34-C33	-3.81	121.87	127.31
23	B	833	CLA	CAA-C2A-C3A	-3.81	102.35	112.78
26	7	623	BCR	C24-C23-C22	-3.81	120.48	126.23
31	2	619	LUT	C11-C10-C9	-3.81	121.88	127.31
23	B	813	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
23	B	803	CLA	CMB-C2B-C3B	3.80	131.80	124.68
23	8	602	CLA	CMB-C2B-C3B	3.80	131.79	124.68
26	7	621	BCR	C21-C20-C19	-3.79	111.39	123.22
23	B	829	CLA	C2D-C1D-ND	-3.79	107.31	110.10
26	K	207	BCR	C20-C21-C22	-3.79	121.90	127.31
26	6	622	BCR	C16-C15-C14	-3.79	115.72	123.47
23	8	611	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
23	L	303	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
23	5	619	CLA	C2A-C1A-CHA	3.78	130.46	123.86
23	A	834	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
23	A	817	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	A	837	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
23	A	809	CLA	CMB-C2B-C3B	3.76	131.71	124.68
23	8	606	CLA	CMB-C2B-C3B	3.76	131.71	124.68
26	3	622	BCR	C11-C12-C13	-3.76	115.86	126.42
26	8	621	BCR	C15-C14-C13	-3.75	121.95	127.31
23	7	611	CLA	CMB-C2B-C3B	3.75	131.70	124.68
26	J	102	BCR	C24-C23-C22	-3.75	120.57	126.23
23	A	845	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
23	B	824	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
23	6	602	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
23	1	608	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
26	B	847	BCR	C33-C5-C4	3.74	120.80	113.62
23	7	615	CLA	CMB-C2B-C1B	-3.74	122.72	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	305	BCR	C10-C11-C12	-3.74	111.55	123.22
23	B	835	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
26	F	305	BCR	C16-C15-C14	-3.73	115.83	123.47
26	A	849	BCR	C16-C15-C14	-3.73	115.83	123.47
23	B	804	CLA	CAA-C2A-C3A	-3.73	107.39	116.10
23	7	603	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
23	A	822	CLA	CMB-C2B-C3B	3.73	131.66	124.68
30	J	103	DGD	O6D-C1D-O3G	-3.73	101.14	109.97
23	5	604	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	B	843	BCR	C20-C21-C22	-3.73	121.99	127.31
32	4	620	XAT	C15-C14-C13	-3.72	122.00	127.31
23	a	608	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
23	B	839	CLA	CMB-C2B-C3B	3.72	131.63	124.68
23	6	606	CLA	CMB-C2B-C3B	3.71	131.63	124.68
26	B	843	BCR	C10-C11-C12	-3.71	111.65	123.22
31	7	619	LUT	C15-C14-C13	-3.70	122.03	127.31
32	4	620	XAT	C24-C23-C22	-3.70	103.64	110.77
32	1	618	XAT	C35-C34-C33	-3.70	122.03	127.31
23	B	834	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
23	1	604	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
23	8	613	CLA	CHB-C4A-NA	3.69	129.62	124.51
23	4	603	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	B	801	BCR	C28-C27-C26	-3.69	107.48	114.08
26	4	621	BCR	C16-C17-C18	-3.69	122.04	127.31
23	B	815	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
23	8	616	CLA	C2A-C1A-CHA	3.69	130.31	123.86
26	B	846	BCR	C3-C4-C5	-3.69	107.49	114.08
23	6	620	CLA	CMB-C2B-C3B	3.69	131.58	124.68
23	A	802	CLA	CHB-C4A-NA	3.69	129.61	124.51
23	B	811	CLA	CAB-C3B-C4B	-3.69	122.80	128.46
26	3	621	BCR	C36-C18-C17	-3.68	117.76	122.92
23	A	829	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
23	5	601	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	B	845	BCR	C20-C21-C22	-3.68	122.06	127.31
23	6	616	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
23	a	604	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	4	621	BCR	C7-C8-C9	-3.67	120.69	126.23
23	5	610	CLA	CMB-C2B-C3B	3.67	131.55	124.68
23	3	607	CLA	CAB-C3B-C4B	-3.67	122.83	128.46
23	5	603	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
23	A	804	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
23	5	613	CLA	CMB-C2B-C1B	-3.67	122.83	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	820	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	K	202	BCR	C27-C26-C25	-3.66	117.42	122.73
26	F	305	BCR	C36-C18-C17	-3.66	117.80	122.92
23	3	613	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	A	852	BCR	C20-C19-C18	-3.66	116.15	126.42
32	a	618	XAT	C35-C34-C33	-3.66	122.09	127.31
23	3	615	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
23	a	611	CLA	CAB-C3B-C4B	-3.65	122.85	128.46
26	L	305	BCR	C15-C14-C13	-3.65	122.10	127.31
31	6	619	LUT	C35-C34-C33	-3.65	122.10	127.31
31	8	619	LUT	C7-C8-C9	-3.65	120.72	126.23
23	4	612	CLA	CMB-C2B-C3B	3.65	131.50	124.68
32	3	619	XAT	C24-C23-C22	-3.65	103.73	110.77
33	6	624	NEX	C24-C23-C22	-3.64	103.73	110.77
23	B	840	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
23	K	204	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
26	4	621	BCR	C33-C5-C4	3.64	120.60	113.62
23	6	607	CLA	CAB-C3B-C4B	-3.64	122.88	128.46
26	B	844	BCR	C15-C14-C13	-3.63	122.13	127.31
26	8	621	BCR	C16-C17-C18	-3.63	122.13	127.31
23	B	807	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
23	5	619	CLA	CHB-C4A-NA	3.63	129.53	124.51
26	K	207	BCR	C30-C25-C26	-3.62	117.51	122.61
23	7	615	CLA	CAB-C3B-C4B	-3.62	122.90	128.46
23	A	808	CLA	CMB-C2B-C3B	3.62	131.45	124.68
23	3	614	CLA	CAA-C2A-C3A	-3.62	107.65	116.10
23	3	610	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
26	7	623	BCR	C15-C14-C13	-3.62	122.15	127.31
23	B	812	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
23	B	809	CLA	CMB-C2B-C3B	3.62	131.44	124.68
23	B	816	CLA	CMB-C2B-C3B	3.61	131.44	124.68
23	B	818	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
23	3	610	CLA	CMB-C2B-C3B	3.61	131.43	124.68
33	5	624	NEX	C26-C27-C28	-3.61	118.37	125.99
31	2	619	LUT	C35-C15-C14	-3.61	116.09	123.47
32	7	620	XAT	C4-C3-C2	-3.60	103.81	110.77
23	6	603	CLA	CAB-C3B-C4B	-3.60	122.92	128.46
26	B	847	BCR	C24-C23-C22	-3.60	120.79	126.23
26	B	845	BCR	C11-C10-C9	-3.59	122.18	127.31
32	8	620	XAT	C4-C3-C2	-3.59	103.84	110.77
26	8	621	BCR	C21-C20-C19	-3.59	112.02	123.22
23	A	840	CLA	CMB-C2B-C3B	3.59	131.39	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	825	CLA	CMB-C2B-C3B	3.58	131.38	124.68
26	K	207	BCR	C15-C14-C13	-3.58	122.20	127.31
26	A	850	BCR	C7-C8-C9	-3.58	120.83	126.23
26	B	847	BCR	C3-C4-C5	-3.58	107.69	114.08
23	8	603	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
23	3	611	CLA	CAA-C2A-C3A	-3.58	107.75	116.10
23	a	602	CLA	CMB-C2B-C3B	3.57	131.36	124.68
26	A	848	BCR	C23-C24-C25	-3.57	117.18	127.20
32	7	620	XAT	C24-C23-C22	-3.57	103.89	110.77
23	1	602	CLA	CMB-C2B-C3B	3.56	131.35	124.68
26	A	850	BCR	C16-C17-C18	-3.56	122.22	127.31
23	A	832	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
23	3	617	CLA	CAA-C2A-C3A	-3.56	107.79	116.10
23	1	616	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
33	6	624	NEX	C35-C34-C33	-3.56	122.23	127.31
23	B	808	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
26	7	621	BCR	C11-C10-C9	-3.56	122.23	127.31
23	A	828	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
23	a	606	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
23	6	613	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
23	5	607	CLA	CMB-C2B-C3B	3.55	131.33	124.68
23	8	607	CLA	CAB-C3B-C4B	-3.55	123.00	128.46
31	8	619	LUT	C35-C15-C14	-3.55	116.20	123.47
23	A	836	CLA	CMB-C2B-C3B	3.55	131.32	124.68
26	B	848	BCR	C15-C14-C13	-3.55	122.25	127.31
30	B	850	DGD	O6D-C1D-O3G	-3.54	101.58	109.97
26	A	856	BCR	C28-C27-C26	-3.54	107.75	114.08
23	8	616	CLA	CAB-C3B-C4B	-3.54	123.02	128.46
26	B	847	BCR	C15-C16-C17	-3.54	116.23	123.47
23	a	616	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
23	B	822	CLA	CMB-C2B-C3B	3.54	131.29	124.68
26	B	846	BCR	C24-C23-C22	-3.53	120.89	126.23
26	A	850	BCR	C1-C6-C5	-3.53	117.64	122.61
23	A	819	CLA	CMB-C2B-C3B	3.53	131.29	124.68
23	B	802	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
23	1	607	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
23	1	606	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
23	3	602	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	A	848	BCR	C30-C25-C26	-3.52	117.65	122.61
32	5	621	XAT	C15-C35-C34	-3.52	116.26	123.47
26	B	843	BCR	C29-C30-C25	3.51	115.89	110.48
23	7	604	CLA	O2D-CGD-O1D	-3.51	116.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	202	BCR	C38-C26-C27	3.51	120.36	113.62
23	8	614	CLA	CMB-C2B-C3B	3.51	131.24	124.68
23	6	604	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
23	A	806	CLA	CMB-C2B-C3B	3.51	131.24	124.68
23	4	614	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
23	a	607	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
28	5	628	LMU	C1B-C2B-C3B	3.50	117.30	110.00
23	6	612	CLA	CMB-C2B-C3B	3.50	131.24	124.68
23	A	841	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
32	8	620	XAT	C10-C11-C12	-3.50	112.28	123.22
23	B	841	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
26	B	848	BCR	C10-C11-C12	-3.50	112.29	123.22
26	B	843	BCR	C15-C14-C13	-3.50	122.31	127.31
23	B	808	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
23	F	304	CLA	CAA-C2A-C3A	-3.49	107.95	116.10
23	3	614	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
32	2	620	XAT	C10-C11-C12	-3.48	112.34	123.22
23	3	611	CLA	CAB-C3B-C4B	-3.48	123.11	128.46
23	3	607	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
26	G	205	BCR	C3-C4-C5	-3.48	107.86	114.08
26	F	305	BCR	C20-C19-C18	-3.48	116.64	126.42
32	9	620	XAT	C35-C34-C33	-3.48	122.35	127.31
26	3	621	BCR	C28-C27-C26	-3.48	107.87	114.08
23	A	854	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	A	814	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
23	B	829	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	7	601	CLA	CHB-C4A-NA	3.47	129.31	124.51
23	7	616	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
23	A	822	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
23	A	825	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	A	835	CLA	O2D-CGD-CBD	3.46	117.42	111.27
23	B	816	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
30	B	850	DGD	O3D-C3D-C4D	-3.45	102.36	110.35
24	A	844	PQN	C14-C13-C15	-3.45	109.46	115.27
26	B	845	BCR	C33-C5-C6	-3.45	120.65	124.53
23	6	620	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
23	5	613	CLA	CHB-C4A-NA	3.45	129.28	124.51
28	K	208	LMU	C1'-C2'-C3'	3.45	117.17	110.00
23	7	614	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
23	L	304	CLA	CMB-C2B-C3B	3.44	131.12	124.68
23	3	609	CLA	CMB-C2B-C3B	3.44	131.11	124.68
28	5	628	LMU	O5B-C1B-C2B	3.44	117.62	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	856	BCR	C21-C20-C19	-3.44	112.50	123.22
23	6	609	CLA	CMB-C2B-C3B	3.43	131.10	124.68
26	A	848	BCR	C11-C10-C9	-3.43	122.42	127.31
23	1	611	CLA	CMB-C2B-C3B	3.43	131.09	124.68
31	5	620	LUT	C35-C15-C14	-3.42	116.46	123.47
32	2	620	XAT	C26-C27-C28	-3.42	118.76	125.99
23	7	610	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	A	810	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	8	608	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	B	832	CLA	CHB-C4A-NA	3.41	129.23	124.51
23	6	618	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
23	B	821	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
23	4	616	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
26	A	848	BCR	C24-C23-C22	-3.41	121.08	126.23
26	A	848	BCR	C33-C5-C6	-3.41	120.70	124.53
31	6	619	LUT	C10-C11-C12	-3.40	112.59	123.22
33	6	624	NEX	C15-C14-C13	-3.40	122.46	127.31
23	5	608	CLA	CMB-C2B-C3B	3.40	131.03	124.68
32	4	620	XAT	C4-C3-C2	-3.39	104.22	110.77
26	1	619	BCR	C7-C8-C9	-3.39	121.11	126.23
23	B	806	CLA	CMB-C2B-C3B	3.39	131.02	124.68
26	a	619	BCR	C7-C8-C9	-3.39	121.12	126.23
23	3	603	CLA	CMB-C2B-C3B	3.39	131.01	124.68
23	5	619	CLA	CMB-C2B-C3B	3.39	131.32	124.69
28	A	859	LMU	C1'-O5'-C5'	3.39	118.29	113.03
32	3	619	XAT	C10-C11-C12	-3.39	112.65	123.22
26	7	623	BCR	C11-C10-C9	-3.39	122.48	127.31
26	G	205	BCR	C8-C7-C6	-3.38	117.70	127.20
23	5	609	CLA	CMB-C2B-C3B	3.38	131.01	124.68
26	8	621	BCR	C7-C8-C9	-3.38	121.12	126.23
26	3	622	BCR	C38-C26-C27	3.38	120.11	113.62
23	A	804	CLA	CHB-C4A-NA	3.38	129.19	124.51
26	4	621	BCR	C3-C4-C5	-3.38	108.04	114.08
31	a	617	LUT	C35-C34-C33	-3.38	122.49	127.31
23	4	601	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
26	7	621	BCR	C7-C8-C9	-3.38	121.13	126.23
33	5	624	NEX	C17-C1-C6	-3.38	107.45	110.47
32	6	621	XAT	C4-C3-C2	-3.37	104.26	110.77
23	5	614	CLA	CMB-C2B-C3B	3.37	130.99	124.68
23	G	203	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
23	B	833	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
28	5	628	LMU	C2'-C3'-C4'	3.37	117.37	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	617	LUT	C35-C34-C33	-3.37	122.51	127.31
23	6	608	CLA	CMB-C2B-C3B	3.37	130.97	124.68
23	L	302	CLA	CMB-C2B-C3B	3.36	130.97	124.68
32	3	619	XAT	C4-C3-C2	-3.36	104.28	110.77
32	7	620	XAT	C10-C11-C12	-3.36	112.73	123.22
23	A	820	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
23	B	805	CLA	CHB-C4A-NA	3.36	129.16	124.51
23	4	609	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
32	9	620	XAT	C24-C23-C22	-3.36	104.29	110.77
31	3	618	LUT	C35-C15-C14	-3.35	116.60	123.47
23	4	603	CLA	CAB-C3B-C4B	-3.35	123.32	128.46
23	A	843	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
31	5	620	LUT	C21-C26-C27	-3.35	108.47	112.70
32	7	620	XAT	C35-C34-C33	-3.34	122.54	127.31
26	3	622	BCR	C28-C27-C26	-3.34	108.12	114.08
23	5	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
26	L	305	BCR	C11-C10-C9	-3.34	122.55	127.31
26	B	847	BCR	C4-C5-C6	-3.33	117.89	122.73
23	3	608	CLA	CMB-C2B-C3B	3.33	130.91	124.68
23	6	611	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
23	6	602	CLA	CMB-C2B-C3B	3.33	130.90	124.68
31	6	619	LUT	C35-C15-C14	-3.33	116.66	123.47
23	B	838	CLA	CMB-C2B-C3B	3.32	130.90	124.68
23	B	824	CLA	O2D-CGD-CBD	3.32	117.17	111.27
23	B	840	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
26	3	622	BCR	C3-C4-C5	-3.32	108.15	114.08
23	F	303	CLA	CMB-C2B-C3B	3.32	130.89	124.68
29	5	626	LMG	O1-C1-C2	-3.31	103.13	108.30
23	1	603	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
26	A	850	BCR	C33-C5-C4	3.31	119.98	113.62
23	4	606	CLA	CMB-C2B-C3B	3.31	130.88	124.68
32	a	618	XAT	C15-C14-C13	-3.31	122.59	127.31
23	A	821	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
26	A	848	BCR	C38-C26-C27	3.31	119.97	113.62
23	A	824	CLA	CAA-C2A-C3A	-3.31	108.38	116.10
23	4	610	CLA	CMB-C2B-C3B	3.31	130.87	124.68
26	B	801	BCR	C16-C15-C14	-3.31	116.70	123.47
32	1	618	XAT	C15-C14-C13	-3.31	122.59	127.31
31	5	620	LUT	C10-C11-C12	-3.31	112.90	123.22
26	A	851	BCR	C10-C11-C12	-3.30	112.91	123.22
23	A	841	CLA	CHB-C4A-NA	3.30	129.08	124.51
23	1	614	CLA	C2A-C3A-C4A	-3.30	102.63	106.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	611	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
26	3	620	BCR	C33-C5-C4	3.29	119.94	113.62
23	4	618	CLA	CAB-C3B-C4B	-3.29	123.40	128.46
23	A	825	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
23	A	811	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	4	601	CLA	CMB-C2B-C3B	3.29	130.83	124.68
23	A	803	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
31	6	619	LUT	C15-C14-C13	-3.28	122.63	127.31
23	7	613	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
23	4	607	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
23	A	842	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
32	9	620	XAT	C15-C14-C13	-3.27	122.65	127.31
23	4	604	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
23	8	616	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
23	B	820	CLA	CMB-C2B-C3B	3.27	130.79	124.68
23	7	613	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
26	B	843	BCR	C32-C1-C6	-3.26	105.01	110.30
28	8	625	LMU	C1'-C2'-C3'	3.26	116.78	110.00
23	a	603	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
23	6	614	CLA	CMB-C2B-C3B	3.26	130.77	124.68
23	A	816	CLA	CMB-C2B-C3B	3.26	130.77	124.68
26	J	102	BCR	C11-C10-C9	-3.26	122.66	127.31
31	4	619	LUT	C15-C14-C13	-3.26	122.66	127.31
23	A	807	CLA	CMB-C2B-C3B	3.26	130.77	124.68
23	B	810	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	4	611	CLA	CMB-C2B-C3B	3.25	130.76	124.68
23	8	607	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
26	3	620	BCR	C16-C15-C14	-3.25	116.82	123.47
23	5	603	CLA	CAB-C3B-C4B	-3.25	123.47	128.46
23	a	611	CLA	CMB-C2B-C3B	3.25	131.04	124.69
33	5	624	NEX	C24-C23-C22	-3.24	104.51	110.77
28	5	628	LMU	C1B-O1B-C4'	-3.24	109.94	117.96
23	3	617	CLA	CMA-C3A-C2A	-3.24	108.54	116.10
23	4	618	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
23	B	813	CLA	CMB-C2B-C3B	3.24	130.74	124.68
31	8	619	LUT	C10-C11-C12	-3.23	113.12	123.22
26	B	843	BCR	C7-C6-C5	3.23	129.29	121.46
32	5	621	XAT	O24-C25-C38	3.23	118.93	115.06
26	G	205	BCR	C28-C27-C26	-3.23	108.31	114.08
26	G	205	BCR	C33-C5-C4	3.23	119.82	113.62
31	3	618	LUT	C30-C31-C32	-3.23	113.14	123.22
23	B	815	CLA	CMB-C2B-C3B	3.23	130.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	618	CLA	CAA-C2A-C3A	-3.22	106.21	114.26
23	5	617	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
31	4	619	LUT	C35-C15-C14	-3.22	116.88	123.47
23	K	206	CLA	CMB-C2B-C3B	3.22	130.70	124.68
28	A	858	LMU	O5'-C5'-C4'	3.22	116.54	109.75
23	4	613	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
23	a	601	CLA	CMB-C2B-C3B	3.22	130.70	124.68
26	B	844	BCR	C16-C17-C18	-3.22	122.72	127.31
23	a	613	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
23	1	601	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	B	819	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
23	a	602	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
26	7	621	BCR	C23-C24-C25	-3.21	118.19	127.20
26	B	847	BCR	C21-C20-C19	-3.21	113.21	123.22
23	B	803	CLA	CHB-C4A-NA	3.21	128.94	124.51
23	B	833	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	A	805	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	A	836	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	L	303	CLA	CMB-C2B-C3B	3.20	130.66	124.68
23	B	802	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
30	J	103	DGD	O3G-C1D-C2D	-3.19	103.31	108.30
23	5	604	CLA	CAB-C3B-C4B	-3.19	123.56	128.46
26	K	202	BCR	C16-C17-C18	-3.19	122.76	127.31
23	K	201	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
31	4	619	LUT	C30-C31-C32	-3.19	113.27	123.22
23	1	602	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
23	B	811	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
23	B	818	CLA	CMB-C2B-C3B	3.18	130.63	124.68
23	7	602	CLA	CMB-C2B-C3B	3.18	130.63	124.68
23	K	203	CLA	CMB-C2B-C3B	3.18	130.63	124.68
26	3	620	BCR	C33-C5-C6	-3.18	120.96	124.53
31	1	617	LUT	C7-C8-C9	-3.18	121.44	126.23
23	A	845	CLA	CMB-C2B-C3B	3.17	130.62	124.68
31	1	617	LUT	C10-C11-C12	-3.17	113.32	123.22
23	3	604	CLA	CMB-C2B-C3B	3.17	130.61	124.68
26	K	207	BCR	C16-C17-C18	-3.17	122.79	127.31
23	1	613	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
26	K	207	BCR	C33-C5-C6	-3.17	120.97	124.53
31	a	617	LUT	C10-C11-C12	-3.17	113.34	123.22
23	A	824	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
23	A	814	CLA	CMB-C2B-C3B	3.16	130.60	124.68
23	A	804	CLA	O2D-CGD-O1D	-3.16	117.65	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	204	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	B	823	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	5	616	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
23	B	803	CLA	CBC-CAC-C3C	3.16	121.13	112.43
23	5	607	CLA	CHB-C4A-NA	3.16	128.88	124.51
31	9	619	LUT	C35-C15-C14	-3.15	117.01	123.47
26	A	849	BCR	C38-C26-C27	3.15	119.67	113.62
23	G	204	CLA	CMB-C2B-C3B	3.15	130.58	124.68
23	B	837	CLA	CMB-C2B-C3B	3.15	130.58	124.68
31	a	617	LUT	C7-C8-C9	-3.15	121.48	126.23
26	B	843	BCR	C1-C6-C5	-3.15	118.18	122.61
23	8	613	CLA	CAA-C2A-C3A	-3.14	104.17	112.78
28	A	859	LMU	C1B-O5B-C5B	3.14	119.86	113.69
23	A	831	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	1	610	CLA	CBD-CHA-C1A	3.14	132.20	128.50
23	A	823	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
26	K	202	BCR	C2-C1-C6	3.14	115.32	110.48
23	B	817	CLA	CMB-C2B-C3B	3.14	130.55	124.68
23	a	604	CLA	CHB-C4A-NA	3.14	128.85	124.51
23	a	613	CLA	C1-C2-C3	-3.14	120.62	126.04
23	B	804	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
26	6	622	BCR	C28-C27-C26	-3.13	108.48	114.08
32	3	619	XAT	C31-C30-C29	-3.13	122.84	127.31
23	5	611	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	5	617	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
23	1	604	CLA	CHB-C4A-NA	3.13	128.84	124.51
26	B	843	BCR	C16-C17-C18	-3.13	122.85	127.31
23	8	602	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
26	3	622	BCR	C16-C15-C14	-3.13	117.07	123.47
31	7	619	LUT	C10-C11-C12	-3.12	113.47	123.22
23	6	617	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
26	A	856	BCR	C11-C10-C9	-3.12	122.85	127.31
23	A	812	CLA	CMB-C2B-C3B	3.12	130.52	124.68
32	2	620	XAT	C15-C14-C13	-3.12	122.86	127.31
32	9	620	XAT	O4-C5-C18	3.12	118.79	115.06
23	7	614	CLA	CAA-C2A-C3A	-3.12	106.47	114.26
26	G	205	BCR	C33-C5-C6	-3.12	121.03	124.53
23	3	612	CLA	CHB-C4A-NA	3.11	128.82	124.51
26	L	301	BCR	C16-C17-C18	-3.11	122.86	127.31
23	1	608	CLA	CMB-C2B-C3B	3.11	130.50	124.68
23	a	610	CLA	CMB-C2B-C3B	3.11	130.50	124.68
28	8	625	LMU	C3B-C4B-C5B	3.11	115.79	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	621	BCR	C19-C18-C17	3.11	123.71	118.94
23	3	617	CLA	O2D-CGD-O1D	-3.11	117.03	124.09
23	K	201	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	A	817	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
23	1	610	CLA	CMB-C2B-C3B	3.11	130.49	124.68
23	A	840	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
23	K	201	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
23	2	616	CLA	C3A-C4A-CHB	-3.10	120.11	123.91
23	B	836	CLA	CAC-C3C-C4C	3.10	128.83	124.81
23	5	618	CLA	CAB-C3B-C2B	3.10	130.76	124.69
23	a	608	CLA	CMB-C2B-C3B	3.10	130.48	124.68
23	4	603	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
26	4	621	BCR	C21-C20-C19	-3.10	113.56	123.22
23	1	613	CLA	C1-C2-C3	-3.09	120.69	126.04
23	B	839	CLA	CHB-C4A-NA	3.09	128.79	124.51
26	A	849	BCR	C20-C21-C22	-3.09	122.90	127.31
28	A	859	LMU	O5'-C1'-C2'	3.09	115.53	110.87
23	B	816	CLA	CHB-C4A-NA	3.09	128.78	124.51
33	6	624	NEX	C2-C1-C6	3.09	112.21	109.21
26	K	207	BCR	C10-C11-C12	-3.09	113.58	123.22
23	A	814	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
23	6	601	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
26	3	621	BCR	C29-C30-C25	3.08	115.23	110.48
23	a	603	CLA	CHB-C4A-NA	3.08	128.78	124.51
23	9	609	CLA	C3A-C4A-CHB	-3.08	120.14	123.91
23	7	610	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
26	A	849	BCR	C15-C14-C13	-3.08	122.91	127.31
23	6	618	CLA	CAB-C3B-C4B	-3.08	123.73	128.46
23	7	601	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
23	A	804	CLA	CMB-C2B-C3B	3.08	130.44	124.68
23	A	841	CLA	CMB-C2B-C3B	3.08	130.44	124.68
26	A	848	BCR	C7-C8-C9	-3.08	121.59	126.23
31	5	620	LUT	C30-C31-C32	-3.07	113.62	123.22
23	a	613	CLA	CHB-C4A-NA	3.07	128.76	124.51
26	K	207	BCR	C11-C10-C9	-3.07	122.93	127.31
23	8	606	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	3	607	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	B	808	CLA	CHB-C4A-NA	3.07	128.76	124.51
23	9	604	CLA	C3A-C4A-CHB	-3.07	120.16	123.91
26	A	851	BCR	C38-C26-C27	3.07	119.51	113.62
23	1	616	CLA	CAB-C3B-C4B	-3.07	123.75	128.46
26	B	844	BCR	C34-C9-C10	-3.07	118.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	616	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	1	613	CLA	CHB-C4A-NA	3.07	128.75	124.51
23	a	614	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	9	607	CLA	C3A-C4A-CHB	-3.06	120.16	123.91
23	B	809	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
26	B	847	BCR	C1-C6-C5	-3.06	118.31	122.61
23	6	607	CLA	CHB-C4A-NA	3.05	128.74	124.51
23	B	822	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
23	1	609	CLA	CAB-C3B-C2B	3.05	130.67	124.69
23	8	611	CLA	CMB-C2B-C3B	3.05	130.38	124.68
23	1	603	CLA	CHB-C4A-NA	3.05	128.73	124.51
23	J	101	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
26	A	850	BCR	C20-C21-C22	-3.05	122.96	127.31
31	8	619	LUT	C3-C4-C5	-3.05	105.78	111.85
26	3	621	BCR	C33-C5-C6	-3.05	121.11	124.53
23	7	616	CLA	CAB-C3B-C2B	3.05	130.65	124.69
23	A	811	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
26	B	846	BCR	C28-C27-C26	-3.04	108.64	114.08
23	1	609	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
26	3	622	BCR	C15-C16-C17	-3.04	117.24	123.47
23	1	609	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
23	6	609	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
26	L	305	BCR	C21-C20-C19	-3.04	113.73	123.22
23	B	831	CLA	CHB-C4A-NA	3.04	128.71	124.51
23	a	609	CLA	CHB-C4A-NA	3.04	128.71	124.51
23	5	604	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
26	3	621	BCR	C20-C19-C18	-3.04	117.89	126.42
23	6	616	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
23	1	607	CLA	CAA-C2A-C3A	-3.04	109.01	116.10
23	2	607	CLA	C3A-C4A-CHB	-3.03	120.20	123.91
31	7	619	LUT	C30-C31-C32	-3.03	113.75	123.22
23	A	823	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
26	B	846	BCR	C15-C16-C17	-3.03	117.27	123.47
23	2	603	CLA	C3A-C4A-CHB	-3.03	120.20	123.91
23	6	616	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
23	A	838	CLA	CHB-C4A-NA	3.03	128.70	124.51
32	1	618	XAT	C35-C15-C14	-3.03	117.27	123.47
26	a	619	BCR	C20-C21-C22	-3.03	122.99	127.31
23	A	845	CLA	CHB-C4A-NA	3.02	128.69	124.51
23	B	827	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
32	a	618	XAT	C35-C15-C14	-3.02	117.28	123.47
26	A	852	BCR	C16-C15-C14	-3.02	117.28	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	838	CLA	CHB-C4A-NA	3.02	128.69	124.51
23	7	608	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
23	1	609	CLA	CHB-C4A-NA	3.02	128.69	124.51
26	8	621	BCR	C24-C23-C22	-3.02	121.67	126.23
23	2	614	CLA	C3A-C4A-CHB	-3.02	120.21	123.91
23	A	814	CLA	CHB-C4A-NA	3.02	128.69	124.51
23	A	829	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
32	1	618	XAT	C31-C30-C29	-3.02	123.00	127.31
23	K	201	CLA	CHB-C4A-NA	3.02	128.69	124.51
23	7	604	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	a	609	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
23	8	611	CLA	CAA-C2A-C3A	-3.01	106.73	114.26
23	5	616	CLA	CAB-C3B-C4B	-3.01	123.83	128.46
30	J	103	DGD	C3G-C2G-C1G	-3.01	104.66	111.79
23	A	812	CLA	CAA-CBA-CGA	3.01	122.06	113.25
23	8	603	CLA	CAB-C3B-C4B	-3.01	123.83	128.46
23	9	603	CLA	C3A-C4A-CHB	-3.01	120.22	123.91
23	8	616	CLA	CHB-C4A-NA	3.01	128.68	124.51
23	7	610	CLA	CMB-C2B-C3B	3.01	130.31	124.68
32	8	620	XAT	C24-C23-C22	-3.01	104.96	110.77
23	A	830	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
23	A	813	CLA	CHB-C4A-NA	3.01	128.67	124.51
23	A	816	CLA	CHB-C4A-NA	3.01	128.67	124.51
23	1	604	CLA	CMB-C2B-C3B	3.01	130.30	124.68
23	7	611	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
23	L	304	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
26	5	622	BCR	C33-C5-C4	3.00	119.38	113.62
23	A	828	CLA	CHB-C4A-NA	3.00	128.66	124.51
26	3	622	BCR	C12-C13-C14	3.00	123.54	118.94
23	8	613	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
32	a	618	XAT	C31-C30-C29	-3.00	123.03	127.31
23	5	618	CLA	CMB-C2B-C3B	3.00	130.56	124.69
23	a	604	CLA	CMB-C2B-C3B	3.00	130.28	124.68
26	K	207	BCR	C38-C26-C27	2.99	119.37	113.62
23	B	807	CLA	CMB-C2B-C3B	2.99	130.28	124.68
26	L	305	BCR	C16-C15-C14	-2.99	117.34	123.47
23	6	607	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
26	J	102	BCR	C15-C16-C17	-2.99	117.35	123.47
23	A	823	CLA	CHB-C4A-NA	2.99	128.65	124.51
23	2	602	CLA	C3A-C4A-CHB	-2.99	120.25	123.91
23	7	615	CLA	CMB-C2B-C3B	2.99	130.54	124.69
26	1	619	BCR	C20-C21-C22	-2.99	123.04	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	840	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
23	5	614	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
23	B	812	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
23	B	821	CLA	CHB-C4A-NA	2.98	128.64	124.51
29	4	624	LMG	O1-C7-C8	-2.98	103.70	110.90
23	a	607	CLA	CMB-C2B-C3B	2.98	130.26	124.68
23	3	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	A	830	CLA	CHB-C4A-NA	2.98	128.63	124.51
23	3	606	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
23	a	611	CLA	CAB-C3B-C2B	2.98	130.52	124.69
23	B	834	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	1	607	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	3	610	CLA	CHB-C4A-NA	2.98	128.63	124.51
23	A	809	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
26	1	619	BCR	C24-C23-C22	-2.97	121.74	126.23
23	B	821	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	8	611	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	B	846	BCR	C30-C25-C26	-2.97	118.43	122.61
31	3	618	LUT	C7-C8-C9	-2.97	121.74	126.23
23	a	611	CLA	O2D-CGD-O1D	-2.97	117.34	124.09
28	8	625	LMU	O5'-C1'-C2'	2.97	116.64	110.35
23	B	814	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	L	303	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	A	818	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	6	604	CLA	CMB-C2B-C3B	2.97	130.23	124.68
26	a	619	BCR	C24-C23-C22	-2.97	121.75	126.23
26	A	851	BCR	C38-C26-C25	-2.97	121.19	124.53
26	6	622	BCR	C33-C5-C4	2.97	119.32	113.62
32	8	620	XAT	C35-C15-C14	-2.97	117.39	123.47
23	A	806	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	A	806	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
23	3	613	CLA	CHB-C4A-NA	2.97	128.61	124.51
23	2	610	CLA	C3A-C4A-CHB	-2.97	120.28	123.91
23	a	611	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
28	5	628	LMU	C4B-C3B-C2B	2.96	116.00	110.82
33	6	624	NEX	C27-C28-C29	-2.96	120.93	125.53
31	7	619	LUT	C35-C15-C14	-2.96	117.40	123.47
31	9	619	LUT	C18-C5-C6	-2.96	121.20	124.53
23	B	812	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	B	831	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	A	837	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	4	614	CLA	CMB-C2B-C3B	2.96	130.22	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	A	828	CLA	CMB-C2B-C3B	2.96	130.21	124.68
26	A	849	BCR	C23-C24-C25	-2.96	118.89	127.20
31	8	619	LUT	C38-C25-C24	-2.96	117.23	123.56
26	B	847	BCR	C38-C26-C25	-2.96	121.21	124.53
23	8	609	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
23	8	608	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	7	614	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	A	836	CLA	CHB-C4A-NA	2.95	128.60	124.51
23	A	839	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
23	3	602	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	3	602	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	5	601	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	A	817	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	B	833	CLA	CAA-C2A-C1A	-2.95	102.31	111.97
23	6	603	CLA	CAB-C3B-C2B	2.95	130.46	124.69
23	3	604	CLA	CHB-C4A-NA	2.95	128.59	124.51
23	B	841	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	B	805	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
25	3	624	LHG	O8-C23-C24	2.94	121.15	111.91
23	9	614	CLA	C3A-C4A-CHB	-2.94	120.31	123.91
26	G	205	BCR	C35-C13-C12	2.94	122.71	118.08
23	1	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	8	612	CLA	CHB-C4A-NA	2.94	128.58	124.51
23	6	614	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	3	617	CLA	CMB-C2B-C3B	2.94	130.17	124.68
23	4	607	CLA	CHB-C4A-NA	2.94	128.57	124.51
23	6	602	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	A	835	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
23	8	607	CLA	CAA-C2A-C3A	-2.93	106.93	114.26
23	A	821	CLA	CHB-C4A-NA	2.93	128.57	124.51
23	4	616	CLA	CMB-C2B-C3B	2.93	130.43	124.69
23	8	613	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	1	611	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
23	6	620	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
23	J	101	CLA	CHB-C4A-NA	2.93	128.56	124.51
23	7	615	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
26	A	856	BCR	C33-C5-C6	-2.93	121.24	124.53
23	L	302	CLA	CHB-C4A-NA	2.92	128.56	124.51
26	A	856	BCR	C15-C14-C13	-2.92	123.14	127.31
23	a	604	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
32	9	620	XAT	C10-C11-C12	-2.92	114.10	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	830	CLA	CHB-C4A-NA	2.92	128.55	124.51
23	A	802	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
23	B	825	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
23	3	614	CLA	CMB-C2B-C3B	2.92	130.14	124.68
31	6	619	LUT	C31-C30-C29	-2.92	123.15	127.31
23	F	303	CLA	CAA-C2A-C3A	-2.92	106.97	114.26
23	7	607	CLA	CAA-C2A-C3A	-2.92	106.97	114.26
23	A	813	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	B	808	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
23	B	820	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	8	602	CLA	CHB-C4A-NA	2.91	128.54	124.51
31	3	618	LUT	C11-C10-C9	-2.91	123.15	127.31
23	K	206	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	3	612	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
23	A	826	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	6	611	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	4	613	CLA	CHB-C4A-NA	2.91	128.53	124.51
23	B	833	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	B	841	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	B	805	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	4	609	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	8	619	LUT	C30-C31-C32	-2.91	114.14	123.22
23	a	601	CLA	CHB-C4A-NA	2.91	128.53	124.51
23	B	808	CLA	CMB-C2B-C3B	2.90	130.11	124.68
23	5	613	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
23	B	839	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
26	5	622	BCR	C11-C10-C9	-2.90	123.17	127.31
23	A	826	CLA	C2A-C1A-CHA	2.90	128.93	123.86
23	6	611	CLA	CAA-C2A-C3A	-2.90	107.02	114.26
23	A	809	CLA	CHB-C4A-NA	2.90	128.52	124.51
23	A	830	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
32	a	618	XAT	C4-C3-C2	-2.90	105.18	110.77
26	B	847	BCR	C33-C5-C6	-2.90	121.27	124.53
23	5	618	CLA	CAA-C2A-C3A	-2.90	107.02	114.26
32	1	618	XAT	C4-C3-C2	-2.90	105.18	110.77
32	6	621	XAT	C10-C11-C12	-2.90	114.18	123.22
23	5	606	CLA	CHB-C4A-NA	2.89	128.51	124.51
23	A	841	CLA	C1B-CHB-C4A	-2.89	124.38	130.12
23	1	614	CLA	CAB-C3B-C2B	2.89	130.36	124.69
23	5	614	CLA	CBA-CAA-C2A	-2.89	107.88	113.34
23	1	601	CLA	CHB-C4A-NA	2.89	128.51	124.51
32	1	618	XAT	C24-C23-C22	-2.89	105.19	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	620	CLA	CHB-C4A-NA	2.89	128.51	124.51
23	a	611	CLA	CAA-C2A-C3A	-2.89	109.35	116.10
23	6	608	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
31	a	617	LUT	C30-C31-C32	-2.89	114.20	123.22
23	a	610	CLA	CHB-C4A-NA	2.89	128.51	124.51
28	8	625	LMU	O1B-C4'-C3'	2.89	114.97	107.28
31	3	618	LUT	C10-C11-C12	-2.89	114.20	123.22
23	1	606	CLA	CMB-C2B-C3B	2.89	130.08	124.68
26	5	622	BCR	C8-C7-C6	-2.89	119.09	127.20
26	F	305	BCR	C38-C26-C27	2.89	119.16	113.62
26	J	102	BCR	C10-C11-C12	-2.89	114.21	123.22
23	B	808	CLA	O2D-CGD-CBD	2.89	116.40	111.27
23	F	303	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	a	619	BCR	C33-C5-C4	2.88	119.16	113.62
23	5	607	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
23	5	613	CLA	CMB-C2B-C3B	2.88	130.07	124.68
31	1	617	LUT	C30-C31-C32	-2.88	114.22	123.22
32	a	618	XAT	C24-C23-C22	-2.88	105.20	110.77
26	8	621	BCR	C4-C5-C6	-2.88	118.55	122.73
23	a	606	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	7	603	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	B	815	CLA	CHB-C4A-NA	2.88	128.50	124.51
23	B	810	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	A	825	CLA	CMB-C2B-C3B	2.88	130.06	124.68
26	3	622	BCR	C33-C5-C6	-2.88	121.30	124.53
23	6	606	CLA	CAA-C2A-C3A	-2.88	107.07	114.26
23	7	612	CLA	CHB-C4A-NA	2.88	128.49	124.51
26	1	619	BCR	C33-C5-C4	2.88	119.14	113.62
23	A	819	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	K	201	CLA	CMB-C2B-C3B	2.87	130.06	124.68
23	A	805	CLA	CHB-C4A-NA	2.87	128.49	124.51
23	1	603	CLA	CBA-CAA-C2A	-2.87	109.12	114.28
32	1	618	XAT	C10-C11-C12	-2.87	114.26	123.22
23	A	802	CLA	C3C-C4C-NC	-2.87	107.35	110.57
23	3	611	CLA	CMB-C2B-C3B	2.87	130.31	124.69
23	6	604	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	5	622	BCR	C4-C5-C6	-2.87	118.56	122.73
26	5	622	BCR	C16-C15-C14	-2.87	117.59	123.47
23	L	302	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	B	806	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	8	609	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	A	854	CLA	C1B-CHB-C4A	-2.87	124.44	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	612	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	A	834	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
26	F	305	BCR	C35-C13-C12	2.86	122.59	118.08
26	B	846	BCR	C15-C14-C13	-2.86	123.22	127.31
23	B	828	CLA	C7-C6-C5	-2.86	105.59	113.36
32	4	620	XAT	C10-C11-C12	-2.86	114.29	123.22
23	A	810	CLA	CMB-C2B-C3B	2.86	130.03	124.68
23	B	812	CLA	CHB-C4A-NA	2.86	128.47	124.51
26	L	305	BCR	C29-C30-C25	2.86	114.88	110.48
23	A	801	CLA	C2A-C1A-CHA	2.86	128.85	123.86
26	A	851	BCR	C11-C10-C9	-2.86	123.23	127.31
26	L	301	BCR	C15-C14-C13	-2.86	123.23	127.31
32	a	618	XAT	C10-C11-C12	-2.86	114.31	123.22
23	A	822	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
23	4	601	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	4	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	4	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	K	206	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	1	610	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	K	201	CLA	C2A-C1A-CHA	2.85	128.85	123.86
26	B	846	BCR	C23-C24-C25	-2.85	119.19	127.20
23	a	616	CLA	CMB-C2B-C3B	2.85	130.01	124.68
29	A	860	LMG	C1-C2-C3	-2.85	104.06	110.00
23	6	613	CLA	CMB-C2B-C3B	2.85	130.01	124.68
30	B	850	DGD	CDB-CCB-CBB	-2.85	99.96	114.42
23	3	613	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	8	602	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
23	1	608	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	8	603	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	2	601	CLA	C3A-C4A-CHB	-2.84	120.43	123.91
23	4	609	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	4	607	CLA	CMB-C2B-C3B	2.84	130.00	124.68
25	A	846	LHG	O8-C23-C24	2.84	120.83	111.91
23	8	601	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
23	B	829	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	9	622	LHG	O8-C23-C24	2.84	120.82	111.91
23	5	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	B	836	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	J	101	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
28	8	625	LMU	C4B-C3B-C2B	2.84	115.78	110.82
23	9	613	CLA	C3A-C4A-CHB	-2.84	120.44	123.91
23	8	607	CLA	CAB-C3B-C2B	2.84	130.24	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	202	BCR	C23-C24-C25	-2.84	119.24	127.20
23	4	618	CLA	CHB-C4A-NA	2.84	128.43	124.51
23	B	840	CLA	CHB-C4A-NA	2.83	128.43	124.51
32	6	621	XAT	C31-C30-C29	-2.83	123.27	127.31
31	9	619	LUT	C18-C5-C4	2.83	119.60	114.36
23	5	612	CLA	CHB-C4A-NA	2.83	128.43	124.51
23	7	609	CLA	CHB-C4A-NA	2.83	128.43	124.51
23	A	845	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	7	607	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	A	851	BCR	C30-C25-C26	-2.83	118.63	122.61
23	4	603	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	B	815	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	B	819	CLA	CHB-C4A-NA	2.82	128.42	124.51
23	B	820	CLA	CHB-C4A-NA	2.82	128.42	124.51
23	A	835	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	5	609	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	3	622	BCR	C30-C25-C26	-2.82	118.64	122.61
23	L	303	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	7	612	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	2	612	CLA	C3A-C4A-CHB	-2.82	120.46	123.91
23	3	604	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
33	5	624	NEX	C19-C9-C8	2.82	125.46	118.93
23	7	612	CLA	CMB-C2B-C3B	2.82	129.94	124.68
31	8	619	LUT	C39-C29-C28	2.81	122.51	118.08
23	K	203	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	a	610	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
26	4	621	BCR	C29-C30-C25	2.81	114.81	110.48
23	B	834	CLA	CHB-C4A-NA	2.81	128.40	124.51
26	F	305	BCR	C11-C10-C9	-2.81	123.30	127.31
23	7	607	CLA	CHB-C4A-NA	2.81	128.40	124.51
28	K	208	LMU	C2'-C3'-C4'	2.81	116.09	109.68
23	A	817	CLA	CHB-C4A-NA	2.81	128.39	124.51
23	6	602	CLA	CHB-C4A-NA	2.81	128.39	124.51
28	A	857	LMU	C2'-C3'-C4'	2.81	116.09	109.68
23	8	608	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
23	1	610	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
23	B	818	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	B	824	CLA	CHB-C4A-NA	2.80	128.39	124.51
26	F	305	BCR	C3-C4-C5	-2.80	109.08	114.08
23	3	610	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
23	B	821	CLA	O2D-CGD-O1D	-2.80	117.73	124.09
23	B	835	CLA	CMB-C2B-C3B	2.80	129.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	621	BCR	C29-C30-C25	2.80	114.79	110.48
26	F	305	BCR	C12-C13-C14	-2.80	114.64	118.94
23	2	604	CLA	C3A-C4A-CHB	-2.80	120.48	123.91
23	4	604	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	3	615	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	B	814	CLA	CHB-C4A-NA	2.79	128.38	124.51
23	8	604	CLA	CHB-C4A-NA	2.79	128.38	124.51
23	L	304	CLA	CHB-C4A-NA	2.79	128.38	124.51
23	B	817	CLA	CHB-C4A-NA	2.79	128.38	124.51
23	7	608	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
31	7	619	LUT	C7-C8-C9	-2.79	122.02	126.23
23	a	608	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	B	850	DGD	C3G-C2G-C1G	-2.79	105.19	111.79
23	1	614	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
31	6	619	LUT	C30-C31-C32	-2.79	114.52	123.22
23	B	833	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	6	622	BCR	C21-C20-C19	-2.79	114.52	123.22
23	3	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	6	607	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
26	A	849	BCR	C21-C20-C19	-2.79	114.53	123.22
23	7	610	CLA	CAA-CBA-CGA	-2.78	105.12	113.25
23	B	811	CLA	CAB-C3B-C2B	2.78	130.14	124.69
23	A	837	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	A	831	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
23	a	614	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
26	B	801	BCR	C3-C4-C5	-2.78	109.11	114.08
26	5	622	BCR	C2-C1-C6	2.78	114.76	110.48
23	a	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	A	821	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	B	839	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
31	9	619	LUT	C3-C4-C5	-2.78	106.32	111.85
25	A	847	LHG	O8-C23-C24	2.78	120.62	111.91
23	A	830	CLA	CMB-C2B-C3B	2.78	129.87	124.68
29	4	623	LMG	O6-C1-O1	-2.78	103.40	109.97
23	a	603	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	5	625	LHG	C11-C10-C9	-2.78	100.33	114.42
23	B	834	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	B	829	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	4	603	CLA	CMB-C2B-C3B	2.78	130.12	124.69
26	B	847	BCR	C8-C7-C6	-2.77	119.41	127.20
23	8	607	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	8	613	CLA	CMB-C2B-C3B	2.77	129.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	7	621	BCR	C33-C5-C6	-2.77	121.42	124.53
23	A	827	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
31	4	619	LUT	C10-C11-C12	-2.77	114.57	123.22
23	3	611	CLA	CAB-C3B-C2B	2.77	130.11	124.69
26	3	620	BCR	C1-C6-C7	2.77	123.61	115.78
23	A	809	CLA	O2D-CGD-CBD	2.77	116.19	111.27
23	A	823	CLA	CAA-C2A-C3A	-2.77	107.34	114.26
23	5	608	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	7	606	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
33	5	624	NEX	C15-C35-C34	-2.77	117.80	123.47
26	G	205	BCR	C1-C6-C5	-2.77	118.71	122.61
23	A	812	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
23	1	609	CLA	CAA-C2A-C3A	-2.77	109.64	116.10
23	3	608	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	6	618	CLA	CMB-C2B-C3B	2.76	130.10	124.69
23	8	608	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	5	604	CLA	CMB-C2B-C3B	2.76	130.09	124.69
23	9	606	CLA	C3A-C4A-CHB	-2.76	120.53	123.91
23	4	604	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
31	9	619	LUT	C20-C13-C12	2.76	122.42	118.08
23	3	607	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
23	3	602	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	A	812	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	B	845	BCR	C39-C30-C25	-2.76	105.83	110.30
23	B	813	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	K	203	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	1	610	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	B	844	BCR	C27-C26-C25	-2.75	118.73	122.73
26	A	852	BCR	C10-C11-C12	-2.75	114.62	123.22
23	3	607	CLA	CMB-C2B-C3B	2.75	130.08	124.69
29	A	860	LMG	O6-C1-O1	-2.75	103.46	109.97
23	5	606	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
23	A	807	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	F	301	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	4	603	CLA	CAB-C3B-C2B	2.75	130.07	124.69
23	6	610	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	B	818	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
26	5	622	BCR	C23-C24-C25	-2.75	119.49	127.20
26	A	849	BCR	C38-C26-C25	-2.75	121.44	124.53
23	1	614	CLA	O2D-CGD-O1D	-2.75	117.85	124.09
23	A	840	CLA	CHB-C4A-NA	2.75	128.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	834	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
23	A	840	CLA	CAA-CBA-CGA	-2.75	105.23	113.25
23	a	609	CLA	O2D-CGD-O1D	-2.75	117.86	124.09
23	5	619	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
26	B	846	BCR	C33-C5-C4	2.74	118.89	113.62
32	5	621	XAT	C31-C32-C33	-2.74	118.71	126.42
32	2	620	XAT	C15-C35-C34	-2.74	117.86	123.47
23	A	843	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	G	205	BCR	C15-C16-C17	-2.74	117.86	123.47
23	A	817	CLA	C2D-C1D-ND	-2.74	108.08	110.10
25	5	623	LHG	O8-C23-C24	2.74	120.51	111.91
23	B	817	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
23	7	616	CLA	CMB-C2B-C3B	2.74	130.05	124.69
23	6	603	CLA	CMB-C2B-C3B	2.74	130.05	124.69
23	5	603	CLA	CAB-C3B-C2B	2.74	130.05	124.69
23	8	601	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
23	A	826	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	6	611	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
23	A	825	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	7	610	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	9	602	CLA	C1C-NC-C4C	2.74	107.94	106.71
23	5	608	CLA	CHB-C4A-NA	2.74	128.29	124.51
26	6	622	BCR	C8-C7-C6	-2.74	119.52	127.20
23	4	611	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
23	A	805	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
23	A	804	CLA	O2D-CGD-CBD	2.73	116.13	111.27
26	A	849	BCR	C33-C5-C6	-2.73	121.46	124.53
23	B	809	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
23	6	614	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
23	A	815	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	7	601	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	A	822	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	A	804	CLA	CAA-CBA-CGA	-2.73	105.27	113.25
23	A	824	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	B	801	BCR	C29-C30-C25	2.73	114.68	110.48
23	A	832	CLA	CMB-C2B-C3B	2.73	129.78	124.68
23	3	613	CLA	O2D-CGD-O1D	-2.73	117.89	124.09
23	9	602	CLA	C3A-C4A-CHB	-2.73	120.57	123.91
23	A	807	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	8	616	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	6	611	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
26	A	849	BCR	C3-C4-C5	-2.73	109.21	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	830	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	3	614	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
23	B	811	CLA	O2D-CGD-O1D	-2.73	117.90	124.09
26	A	851	BCR	C15-C16-C17	-2.72	117.89	123.47
28	A	858	LMU	C3B-C4B-C5B	2.72	114.30	110.77
23	B	837	CLA	CHB-C4A-NA	2.72	128.28	124.51
30	J	103	DGD	O6E-C5E-C4E	2.72	114.64	109.69
23	2	610	CLA	C3B-C4B-NB	-2.72	107.72	110.11
23	1	616	CLA	CMB-C2B-C3B	2.72	130.02	124.69
23	6	601	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	5	611	CLA	CMB-C2B-C3B	2.72	129.77	124.68
23	A	842	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	9	611	CLA	C3A-C4A-CHB	-2.72	120.58	123.91
23	A	831	CLA	C2D-C1D-ND	-2.72	108.10	110.10
32	7	620	XAT	C15-C35-C34	-2.72	117.90	123.47
23	B	807	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
26	B	846	BCR	C16-C15-C14	-2.72	117.90	123.47
26	7	623	BCR	C38-C26-C25	-2.72	121.47	124.53
23	A	832	CLA	C2D-C1D-ND	-2.72	108.10	110.10
23	a	613	CLA	CMB-C2B-C3B	2.72	129.76	124.68
23	a	607	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	3	607	CLA	CAB-C3B-C2B	2.72	130.01	124.69
23	a	606	CLA	CHB-C4A-NA	2.72	128.27	124.51
31	2	619	LUT	C18-C5-C4	2.72	119.39	114.36
23	a	607	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
32	9	620	XAT	C6-C7-C8	-2.72	120.25	125.99
23	A	833	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	A	834	CLA	CMB-C2B-C3B	2.71	129.75	124.68
23	1	607	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	A	832	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	6	622	BCR	C4-C5-C6	-2.71	118.80	122.73
23	6	613	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	K	204	CLA	CHB-C4A-NA	2.71	128.25	124.51
23	a	613	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
32	6	621	XAT	C15-C35-C34	-2.70	117.94	123.47
23	6	616	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
26	J	102	BCR	C20-C19-C18	-2.70	118.83	126.42
23	A	808	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	L	301	BCR	C28-C27-C26	-2.70	109.26	114.08
23	B	833	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	9	609	CLA	C3B-C4B-NB	-2.70	107.74	110.11
23	1	613	CLA	O2D-CGD-O1D	-2.70	118.56	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	807	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	A	827	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	3	603	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
23	7	602	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
23	B	835	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	B	807	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	6	617	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	1	618	XAT	C19-C9-C8	2.69	122.32	118.08
31	7	619	LUT	C3-C4-C5	-2.69	106.49	111.85
23	7	609	CLA	CMA-C3A-C2A	-2.69	102.97	113.83
23	9	606	CLA	C3B-C4B-NB	-2.69	107.75	110.11
23	B	827	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
23	7	609	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
23	8	611	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
23	6	607	CLA	CAA-C2A-C3A	-2.69	107.54	114.26
23	1	606	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	F	304	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	B	840	CLA	CMB-C2B-C3B	2.69	129.71	124.68
23	G	203	CLA	CAA-C2A-C3A	-2.69	107.54	114.26
23	4	610	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	7	615	CLA	CAB-C3B-C2B	2.69	129.95	124.69
23	4	616	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
23	5	601	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	4	624	LMG	O6-C1-O1	-2.68	103.62	109.97
23	a	614	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
31	6	619	LUT	C38-C25-C24	-2.68	117.83	123.56
23	G	203	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	B	813	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
26	6	622	BCR	C11-C12-C13	-2.68	118.89	126.42
26	A	849	BCR	C27-C26-C25	-2.68	118.84	122.73
31	5	620	LUT	C16-C1-C6	-2.68	105.96	110.30
23	1	613	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	a	613	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
23	2	616	CLA	C3B-C4B-NB	-2.68	107.76	110.11
32	a	618	XAT	C19-C9-C8	2.68	122.29	118.08
23	7	613	CLA	CMB-C2B-C3B	2.67	129.68	124.68
23	4	616	CLA	CAB-C3B-C2B	2.67	129.93	124.69
23	5	610	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
23	A	815	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	9	601	CLA	C3A-C4A-CHB	-2.67	120.64	123.91
23	F	304	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	1	612	CLA	CHB-C4A-NA	2.67	128.21	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	614	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	8	616	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
26	3	622	BCR	C1-C6-C7	2.67	123.33	115.78
23	B	818	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	6	607	CLA	CAA-C2A-C1A	-2.67	106.23	112.14
23	B	803	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
23	6	617	CLA	CMB-C2B-C3B	2.67	129.67	124.68
26	B	844	BCR	C38-C26-C27	2.67	118.74	113.62
23	1	614	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
31	2	619	LUT	C30-C31-C32	-2.67	114.89	123.22
23	5	616	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	8	616	CLA	CMB-C2B-C3B	2.67	129.91	124.69
23	6	608	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	8	622	LHG	O8-C23-C24	2.66	120.27	111.91
23	A	834	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	5	612	CLA	CAA-C2A-C3A	-2.66	107.61	114.26
23	A	821	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	G	204	CLA	C2A-C1A-CHA	2.66	128.51	123.86
31	3	618	LUT	C16-C1-C6	-2.66	105.98	110.30
23	B	810	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	4	604	CLA	CAB-C3B-C4B	-2.66	124.37	128.46
23	2	614	CLA	C3B-C4B-NB	-2.66	107.77	110.11
33	6	624	NEX	C4-C3-C2	-2.66	105.64	110.77
23	5	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	a	612	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	G	205	BCR	C35-C13-C14	-2.66	119.20	122.92
31	2	619	LUT	C15-C14-C13	-2.66	123.52	127.31
26	F	305	BCR	C30-C25-C26	-2.66	118.87	122.61
23	5	614	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
23	B	825	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	B	817	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	7	613	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	B	828	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	B	838	CLA	O2D-CGD-CBD	2.65	115.97	111.27
31	4	619	LUT	C19-C9-C8	2.65	122.25	118.08
23	4	606	CLA	CAA-C2A-C3A	-2.65	107.65	114.26
23	a	601	CLA	O2D-CGD-O1D	-2.65	118.08	124.09
26	5	622	BCR	C29-C30-C25	2.65	114.55	110.48
23	B	832	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
26	B	844	BCR	C28-C27-C26	-2.65	109.35	114.08
26	A	850	BCR	C39-C30-C25	-2.64	106.01	110.30
26	B	845	BCR	C28-C27-C26	-2.64	109.36	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	613	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
23	B	835	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	A	856	BCR	C31-C1-C6	-2.64	106.02	110.30
23	B	806	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
23	1	603	CLA	CMB-C2B-C3B	2.64	129.62	124.68
23	7	610	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
23	A	832	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
31	1	617	LUT	C11-C10-C9	-2.64	123.55	127.31
26	A	850	BCR	C8-C7-C6	-2.64	119.80	127.20
23	A	827	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
23	1	601	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
23	6	613	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
32	5	621	XAT	C31-C30-C29	-2.63	123.55	127.31
23	6	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	2	613	CLA	C3A-C4A-CHB	-2.63	120.69	123.91
26	A	852	BCR	C33-C5-C6	-2.63	121.57	124.53
23	3	606	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	A	850	BCR	C38-C26-C25	-2.63	121.57	124.53
23	A	810	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
26	G	205	BCR	C34-C9-C8	2.63	122.22	118.08
31	7	619	LUT	C22-C23-C24	-2.63	108.75	111.74
23	B	826	CLA	CHB-C4A-NA	2.63	128.15	124.51
32	8	620	XAT	C19-C9-C8	2.63	122.22	118.08
23	B	837	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
23	5	602	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	2	622	LHG	C11-C10-C9	-2.63	101.09	114.42
31	2	619	LUT	C38-C25-C24	-2.63	117.94	123.56
23	A	830	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	4	623	LMG	O1-C1-C2	-2.63	104.20	108.30
31	a	617	LUT	C11-C10-C9	-2.62	123.56	127.31
23	A	803	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	8	601	CLA	CHB-C4A-NA	2.62	128.14	124.51
28	A	857	LMU	C1'-C2'-C3'	2.62	115.46	110.00
23	A	841	CLA	C1-C2-C3	-2.62	121.51	126.04
32	5	621	XAT	C19-C9-C8	2.62	122.21	118.08
23	8	610	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	8	601	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
23	6	610	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	A	852	BCR	C24-C23-C22	-2.62	122.27	126.23
23	5	603	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	4	614	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
23	8	603	CLA	CMB-C2B-C3B	2.62	129.82	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	603	CLA	O2D-CGD-O1D	-2.62	118.14	124.09
23	4	618	CLA	CMB-C2B-C3B	2.62	129.82	124.69
29	J	104	LMG	O1-C7-C8	-2.62	104.58	110.90
32	6	621	XAT	C35-C34-C33	-2.62	123.57	127.31
23	8	614	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
23	A	840	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
23	A	839	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
23	B	835	CLA	O2D-CGD-CBD	2.61	115.91	111.27
23	5	619	CLA	CAA-C2A-C1A	2.61	120.54	111.97
23	9	607	CLA	C1C-NC-C4C	2.61	107.88	106.71
23	7	615	CLA	CHB-C4A-NA	2.61	128.13	124.51
23	K	204	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
26	3	622	BCR	C15-C14-C13	-2.61	123.58	127.31
32	3	619	XAT	C19-C9-C8	2.61	122.19	118.08
25	7	622	LHG	O8-C23-C24	2.61	120.10	111.91
23	A	841	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	G	203	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	B	804	CLA	CMA-C3A-C2A	-2.61	110.01	116.10
23	a	603	CLA	CMB-C2B-C3B	2.61	129.55	124.68
23	4	613	CLA	CMB-C2B-C3B	2.61	129.55	124.68
23	8	616	CLA	CAB-C3B-C2B	2.61	129.79	124.69
25	1	620	LHG	C11-C10-C9	-2.60	101.20	114.42
23	A	833	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	3	607	CLA	O2D-CGD-CBD	2.60	115.89	111.27
23	6	607	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
26	1	619	BCR	C38-C26-C25	-2.60	121.61	124.53
23	4	613	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
26	a	619	BCR	C38-C26-C25	-2.60	121.61	124.53
23	F	303	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	a	620	LHG	C11-C10-C9	-2.60	101.23	114.42
23	8	614	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	2	606	CLA	C3A-C4A-CHB	-2.60	120.73	123.91
33	5	624	NEX	C11-C10-C9	-2.60	123.60	127.31
26	3	620	BCR	C1-C6-C5	-2.60	118.96	122.61
26	7	621	BCR	C33-C5-C4	2.60	118.60	113.62
26	F	305	BCR	C8-C7-C6	-2.60	119.91	127.20
23	6	604	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
26	K	207	BCR	C27-C26-C25	-2.59	118.97	122.73
26	B	846	BCR	C29-C30-C25	-2.59	106.49	110.48
26	7	621	BCR	C29-C30-C25	2.59	114.47	110.48
23	A	839	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	3	608	CLA	CHB-C4A-NA	2.59	128.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	621	BCR	C16-C15-C14	-2.59	118.17	123.47
26	L	301	BCR	C38-C26-C25	-2.59	121.62	124.53
23	A	843	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
23	6	610	CLA	CHD-C1D-ND	-2.59	122.07	124.45
26	K	207	BCR	C38-C26-C25	-2.59	121.62	124.53
23	a	602	CLA	O1D-CGD-CBD	2.59	129.78	124.48
23	A	835	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
23	2	609	CLA	C3A-C4A-CHB	-2.59	120.74	123.91
23	5	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	a	611	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	A	827	CLA	C2D-C1D-ND	-2.59	108.20	110.10
23	1	602	CLA	O1D-CGD-CBD	2.58	129.77	124.48
26	B	846	BCR	C33-C5-C6	-2.58	121.63	124.53
31	9	619	LUT	C1-C2-C3	2.58	119.48	113.64
23	G	203	CLA	CHB-C4A-NA	2.58	128.09	124.51
23	3	611	CLA	CHB-C4A-NA	2.58	128.09	124.51
23	B	830	CLA	C2D-C1D-ND	-2.58	108.20	110.10
23	6	618	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	B	801	BCR	C23-C22-C21	2.58	122.90	118.94
23	B	830	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
23	8	607	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
23	1	608	CLA	O2D-CGD-O1D	-2.58	118.23	124.09
26	J	102	BCR	C27-C26-C25	-2.58	118.99	122.73
23	B	821	CLA	CHC-C1C-C2C	-2.58	123.64	129.77
23	7	604	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	A	804	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
23	a	608	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
23	B	841	CLA	CHB-C4A-NA	2.58	128.07	124.51
23	G	204	CLA	CHB-C4A-NA	2.58	128.07	124.51
23	3	606	CLA	CMB-C2B-C3B	2.58	129.50	124.68
31	3	618	LUT	C38-C25-C24	-2.57	118.05	123.56
23	5	608	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
26	1	619	BCR	C29-C30-C25	2.57	114.44	110.48
23	A	810	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	7	601	CLA	CMB-C2B-C3B	2.57	129.49	124.68
23	A	822	CLA	O2D-CGD-CBD	2.57	115.84	111.27
23	A	843	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	A	823	CLA	O2D-CGD-CBD	2.57	115.84	111.27
23	4	611	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
23	8	614	CLA	CAA-CBA-CGA	-2.57	105.74	113.25
23	9	604	CLA	C3B-C4B-NB	-2.57	107.85	110.11
23	3	615	CLA	CHB-C4A-NA	2.57	128.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	607	CLA	CMB-C2B-C3B	2.57	129.72	124.69
23	B	841	CLA	CAC-C3C-C4C	2.57	128.14	124.81
32	6	621	XAT	C19-C9-C8	2.57	122.12	118.08
23	A	829	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	7	622	LHG	C11-C10-C9	-2.57	101.39	114.42
26	B	846	BCR	C10-C11-C12	-2.57	115.21	123.22
23	B	819	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	A	852	BCR	C34-C9-C10	-2.57	119.33	122.92
23	6	618	CLA	O2D-CGD-O1D	-2.57	118.26	124.09
23	A	842	CLA	CMB-C2B-C3B	2.56	129.48	124.68
23	A	802	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	A	818	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
23	8	610	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
23	4	607	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	7	611	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	B	838	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
23	A	829	CLA	O2D-CGD-CBD	2.56	115.82	111.27
23	9	611	CLA	C3B-C4B-NB	-2.56	107.86	110.11
23	7	606	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	B	851	LHG	O8-C23-C24	2.56	119.94	111.91
32	2	620	XAT	C31-C30-C29	-2.56	123.66	127.31
32	2	620	XAT	O24-C25-C38	2.56	118.12	115.06
23	A	801	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	8	612	CLA	CAA-C2A-C3A	-2.56	107.87	114.26
23	K	204	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
23	5	610	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	A	814	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
26	a	619	BCR	C29-C30-C25	2.55	114.41	110.48
23	B	810	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	6	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	7	606	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	2	622	LHG	O8-C23-C24	2.55	119.92	111.91
31	2	619	LUT	C16-C1-C6	-2.55	106.16	110.30
26	F	305	BCR	C7-C8-C9	-2.55	122.38	126.23
23	A	820	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
23	B	824	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
23	L	302	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
23	8	607	CLA	CMB-C2B-C3B	2.55	129.68	124.69
23	1	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	B	846	BCR	C37-C22-C23	2.55	122.09	118.08
26	5	622	BCR	C21-C20-C19	-2.55	115.26	123.22
26	L	301	BCR	C21-C20-C19	-2.55	115.26	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	301	BCR	C23-C24-C25	-2.55	120.04	127.20
28	A	858	LMU	O5B-C1B-C2B	2.55	115.87	111.31
23	1	602	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	5	610	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
31	4	619	LUT	C31-C30-C29	-2.55	123.68	127.31
32	5	621	XAT	C8-C9-C10	-2.55	115.03	118.94
23	A	842	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
23	8	601	CLA	C1-C2-C3	-2.54	121.64	126.04
23	A	802	CLA	O1D-CGD-CBD	2.54	129.69	124.48
23	8	614	CLA	CHB-C4A-NA	2.54	128.03	124.51
29	5	626	LMG	O3-C3-C2	-2.54	104.47	110.35
23	8	610	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
23	F	301	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	3	619	XAT	C18-C5-C4	2.54	117.14	114.28
23	4	616	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	8	622	LHG	C20-C19-C18	-2.54	101.53	114.42
28	A	858	LMU	C1'-O5'-C5'	2.54	118.67	113.69
26	B	801	BCR	C20-C19-C18	-2.54	119.28	126.42
26	A	851	BCR	C7-C8-C9	-2.54	122.40	126.23
23	6	620	CLA	O2D-CGD-CBD	2.54	115.78	111.27
23	B	837	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
32	4	620	XAT	C35-C15-C14	-2.54	118.28	123.47
23	2	607	CLA	C3B-C4B-NB	-2.54	107.88	110.11
23	1	608	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
23	2	609	CLA	C3B-C4B-NB	-2.53	107.88	110.11
23	B	826	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	J	101	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
23	8	613	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
23	A	820	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	2	603	CLA	C3B-C4B-NB	-2.53	107.89	110.11
31	1	617	LUT	C35-C15-C14	-2.53	118.29	123.47
32	9	620	XAT	C31-C30-C29	-2.53	123.70	127.31
25	4	622	LHG	C20-C19-C18	-2.53	101.59	114.42
26	4	621	BCR	C27-C26-C25	-2.53	119.06	122.73
23	B	825	CLA	CAA-C2A-C1A	-2.53	103.69	111.97
23	a	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	7	620	XAT	C31-C30-C29	-2.53	123.70	127.31
26	K	202	BCR	C4-C5-C6	-2.52	119.07	122.73
23	3	609	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
31	a	617	LUT	C35-C15-C14	-2.52	118.31	123.47
32	4	620	XAT	C38-C25-C24	2.52	117.12	114.28
23	A	811	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	613	CLA	C3B-C4B-NB	-2.52	107.89	110.11
23	a	601	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
23	B	811	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	a	603	CLA	CAA-C2A-C3A	-2.52	107.96	114.26
23	4	604	CLA	CMB-C2B-C3B	2.52	129.62	124.69
33	5	624	NEX	C19-C9-C10	-2.52	119.39	122.92
26	3	620	BCR	C4-C5-C6	-2.52	119.08	122.73
23	3	604	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
26	A	856	BCR	C23-C24-C25	-2.52	120.13	127.20
26	B	845	BCR	C33-C5-C4	2.52	118.45	113.62
23	6	610	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	B	835	CLA	C2A-C1A-CHA	2.51	128.26	123.86
23	5	611	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	5	603	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
23	7	608	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	a	608	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	B	808	CLA	CBA-CAA-C2A	2.51	121.28	113.86
23	1	603	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
23	8	606	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	4	610	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	F	301	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	1	601	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	3	614	CLA	CMA-C3A-C2A	-2.51	110.25	116.10
23	7	601	CLA	CHD-C1D-ND	-2.51	122.15	124.45
23	5	611	CLA	O2D-CGD-CBD	2.51	115.72	111.27
26	B	845	BCR	C10-C11-C12	-2.51	115.40	123.22
23	7	606	CLA	CAA-C2A-C3A	-2.51	108.00	114.26
23	A	820	CLA	C1-C2-C3	-2.50	121.71	126.04
32	2	620	XAT	C30-C31-C32	-2.50	115.40	123.22
23	4	608	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
23	6	603	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
23	7	606	CLA	C2D-C1D-ND	-2.50	108.26	110.10
31	8	619	LUT	C11-C10-C9	-2.50	123.74	127.31
23	L	303	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
25	4	622	LHG	C11-C10-C9	-2.50	101.72	114.42
26	L	305	BCR	C38-C26-C25	-2.50	121.72	124.53
23	A	833	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
23	B	822	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
23	A	819	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	B	845	BCR	C21-C20-C19	-2.50	115.41	123.22
23	5	604	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
23	3	609	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	847	BCR	C16-C17-C18	-2.50	123.74	127.31
26	A	856	BCR	C16-C15-C14	-2.50	118.35	123.47
26	3	620	BCR	C37-C22-C21	-2.50	119.42	122.92
23	B	819	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	4	610	CLA	C1-C2-C3	-2.50	121.72	126.04
23	6	606	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	8	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	a	614	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	7	603	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	4	609	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
25	8	622	LHG	C11-C10-C9	-2.50	101.75	114.42
23	A	835	CLA	CMB-C2B-C3B	2.50	129.35	124.68
31	5	620	LUT	C7-C8-C9	-2.50	122.46	126.23
23	a	609	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	G	204	CLA	CHD-C1D-ND	-2.50	122.16	124.45
33	5	624	NEX	C35-C34-C33	-2.49	123.75	127.31
23	3	607	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	A	847	LHG	C11-C10-C9	-2.49	101.77	114.42
23	3	606	CLA	O2D-CGD-O1D	-2.49	118.43	124.09
31	2	619	LUT	C20-C13-C14	-2.49	119.43	122.92
23	B	804	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	9	614	CLA	C3B-C4B-NB	-2.49	107.92	110.11
23	3	609	CLA	C2A-C1A-CHA	2.49	128.22	123.86
23	7	601	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
23	7	614	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	B	832	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	3	620	BCR	C38-C26-C25	-2.49	121.73	124.53
23	A	834	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
26	B	844	BCR	C2-C1-C6	2.49	114.31	110.48
23	A	838	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
32	3	619	XAT	C38-C25-C24	2.49	117.08	114.28
23	B	808	CLA	C1-C2-C3	-2.49	121.74	126.04
23	2	612	CLA	C3B-C4B-NB	-2.49	107.92	110.11
23	6	612	CLA	O2D-CGD-O1D	-2.49	118.44	124.09
26	K	207	BCR	C16-C15-C14	-2.49	118.38	123.47
23	8	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	G	205	BCR	C4-C5-C6	-2.49	119.12	122.73
23	A	839	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	6	612	CLA	CAA-C2A-C3A	-2.49	108.05	114.26
23	4	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	2	603	CLA	CHD-C1D-ND	-2.48	122.12	124.52
23	4	614	CLA	CHB-C4A-NA	2.48	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	619	LUT	C30-C31-C32	-2.48	115.47	123.22
26	7	621	BCR	C27-C26-C25	-2.48	119.13	122.73
23	4	601	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
23	A	811	CLA	O1D-CGD-CBD	2.48	129.56	124.48
26	4	621	BCR	C23-C24-C25	-2.48	120.24	127.20
29	A	860	LMG	O1-C7-C8	-2.48	104.92	110.90
23	A	804	CLA	C7-C6-C5	-2.48	106.63	113.36
23	5	619	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	2	616	CLA	C1C-NC-C4C	2.48	107.82	106.71
26	L	301	BCR	C24-C23-C22	-2.48	122.49	126.23
23	A	831	CLA	CHC-C1C-NC	2.48	127.96	124.20
23	B	811	CLA	C4-C3-C5	2.48	119.44	115.27
23	A	825	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
26	7	623	BCR	C20-C21-C22	-2.47	123.78	127.31
23	B	828	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	4	608	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	3	615	CLA	O2D-CGD-O1D	-2.47	118.47	124.09
26	A	850	BCR	C11-C10-C9	-2.47	123.78	127.31
26	4	621	BCR	C38-C26-C27	2.47	118.37	113.62
23	A	823	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	A	824	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	B	813	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	3	613	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	6	616	CLA	CAA-C2A-C1A	-2.47	103.88	111.97
26	B	845	BCR	C15-C16-C17	-2.47	118.41	123.47
25	A	846	LHG	C11-C10-C9	-2.47	101.88	114.42
30	B	850	DGD	CFB-CEB-CDB	-2.47	101.88	114.42
23	3	615	CLA	CAA-C2A-C3A	-2.47	108.09	114.26
26	A	849	BCR	C33-C5-C4	2.47	118.36	113.62
23	B	830	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
23	7	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
30	J	103	DGD	O2D-C2D-C1D	-2.47	104.05	110.05
23	L	304	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
23	2	610	CLA	CHD-C1D-ND	-2.47	122.13	124.52
23	7	601	CLA	O2D-CGD-CBD	2.47	115.65	111.27
26	B	848	BCR	C16-C15-C14	-2.47	118.42	123.47
23	7	607	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
23	4	606	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	6	603	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	B	822	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	A	823	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	6	617	CLA	C1B-CHB-C4A	-2.46	125.24	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	301	BCR	C15-C16-C17	-2.46	118.43	123.47
31	7	619	LUT	C16-C1-C6	-2.46	106.31	110.30
23	8	604	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
26	A	848	BCR	C16-C15-C14	-2.46	118.44	123.47
23	A	808	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	4	611	CLA	CAA-C2A-C3A	-2.46	108.12	114.26
31	9	619	LUT	C10-C11-C12	-2.46	115.55	123.22
23	6	610	CLA	C1-C2-C3	-2.46	121.79	126.04
31	3	618	LUT	C19-C9-C8	2.46	121.95	118.08
31	9	619	LUT	C15-C14-C13	-2.46	123.80	127.31
26	G	205	BCR	C38-C26-C25	-2.46	121.77	124.53
23	5	609	CLA	O2D-CGD-CBD	2.46	115.63	111.27
25	6	623	LHG	C11-C10-C9	-2.46	101.96	114.42
23	7	612	CLA	C2A-C1A-CHA	2.46	128.15	123.86
23	B	824	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
32	6	621	XAT	C39-C29-C28	2.45	121.94	118.08
23	a	604	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
26	G	205	BCR	C16-C15-C14	-2.45	118.45	123.47
23	5	609	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
23	7	611	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	A	848	BCR	C28-C27-C26	-2.45	109.70	114.08
23	A	828	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	B	811	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	a	616	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
26	A	851	BCR	C20-C19-C18	-2.45	119.54	126.42
23	B	804	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	B	813	CLA	C2D-C1D-ND	-2.45	108.30	110.10
23	9	609	CLA	CHB-C4A-NA	2.45	128.09	124.34
23	5	606	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
23	8	604	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
23	A	831	CLA	CMC-C2C-C1C	-2.44	121.32	125.04
23	A	837	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	G	204	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	1	607	CLA	O2D-CGD-O1D	-2.44	118.54	124.09
23	B	831	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	4	620	XAT	C39-C29-C28	2.44	121.93	118.08
26	7	621	BCR	C10-C11-C12	-2.44	115.59	123.22
23	4	612	CLA	O2D-CGD-O1D	-2.44	118.54	124.09
23	1	604	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
26	8	621	BCR	C38-C26-C27	2.44	118.30	113.62
26	A	848	BCR	C30-C25-C24	2.44	122.68	115.78
23	A	803	CLA	CAA-CBA-CGA	-2.44	106.12	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	623	LMG	O3-C3-C2	-2.44	104.71	110.35
23	3	608	CLA	C1-C2-C3	-2.44	121.82	126.04
25	4	622	LHG	O8-C23-C24	2.44	119.56	111.91
26	5	622	BCR	C37-C22-C23	2.44	121.92	118.08
23	A	820	CLA	CMC-C2C-C1C	-2.44	121.33	125.04
23	1	616	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	3	617	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	8	606	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	B	823	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	2	602	CLA	C3B-C4B-NB	-2.44	107.97	110.11
23	4	616	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
26	8	621	BCR	C37-C22-C23	2.44	121.91	118.08
31	6	619	LUT	C19-C9-C8	2.44	121.91	118.08
23	1	606	CLA	C2A-C1A-CHA	2.43	126.49	122.71
32	5	621	XAT	C39-C29-C28	2.43	121.91	118.08
23	a	616	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	9	614	CLA	C1C-NC-C4C	2.43	107.80	106.71
23	7	612	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	B	820	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	B	810	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	4	614	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	A	815	CLA	C1-C2-C3	-2.43	122.82	126.75
23	B	819	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	J	101	CLA	CMB-C2B-C3B	2.43	129.23	124.68
25	8	623	LHG	O8-C23-C24	2.43	119.54	111.91
26	8	621	BCR	C1-C6-C5	-2.43	119.19	122.61
26	B	845	BCR	C29-C28-C27	-2.43	105.95	111.38
26	A	852	BCR	C23-C24-C25	-2.43	120.38	127.20
23	B	805	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	3	606	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	1	616	CLA	CAB-C3B-C2B	2.42	129.44	124.69
23	4	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	7	616	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	8	621	BCR	C27-C26-C25	-2.42	119.21	122.73
30	B	850	DGD	CBB-CAB-C9B	-2.42	102.12	114.42
28	K	208	LMU	C4B-C3B-C2B	2.42	115.05	110.82
23	2	613	CLA	CHD-C1D-ND	-2.42	122.17	124.52
23	5	604	CLA	CAB-C3B-C2B	2.42	129.43	124.69
26	3	620	BCR	C29-C30-C25	2.42	114.21	110.48
25	9	622	LHG	C11-C10-C9	-2.42	102.13	114.42
23	5	602	CLA	C2D-C1D-ND	-2.42	108.32	110.10
25	3	623	LHG	C11-C10-C9	-2.42	102.13	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	619	LUT	C18-C5-C6	-2.42	121.81	124.53
23	B	836	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	B	810	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
23	4	613	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
29	A	860	LMG	O3-C3-C2	-2.42	104.75	110.35
23	B	812	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	7	613	CLA	C2D-C1D-ND	-2.42	108.32	110.10
23	3	602	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	A	838	CLA	C1-C2-C3	-2.42	122.84	126.75
32	3	619	XAT	C15-C35-C34	-2.41	118.53	123.47
23	7	608	CLA	CMB-C2B-C3B	2.41	129.19	124.68
23	4	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	3	614	CLA	O2D-CGD-O1D	-2.41	118.62	124.09
23	4	618	CLA	O2D-CGD-O1D	-2.41	118.62	124.09
23	3	615	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	B	816	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
25	8	623	LHG	C18-C17-C16	-2.41	102.20	114.42
23	6	616	CLA	O2D-CGD-CBD	2.41	115.54	111.27
23	A	815	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	B	825	CLA	O1D-CGD-CBD	2.41	129.41	124.48
25	3	623	LHG	O8-C23-C24	2.41	119.45	111.91
23	A	824	CLA	C2D-C1D-ND	-2.40	108.33	110.10
23	8	606	CLA	C2D-C1D-ND	-2.40	108.33	110.10
26	A	856	BCR	C29-C30-C25	2.40	114.18	110.48
25	a	620	LHG	C20-C19-C18	-2.40	102.23	114.42
23	4	602	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	5	628	LMU	O5'-C5'-C4'	2.40	114.82	109.75
23	a	603	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
26	A	856	BCR	C30-C25-C24	2.40	122.57	115.78
23	A	810	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	1	620	LHG	C20-C19-C18	-2.40	102.24	114.42
26	F	305	BCR	C28-C27-C26	-2.40	109.79	114.08
23	A	814	CLA	CBA-CAA-C2A	-2.40	106.78	113.86
26	5	622	BCR	C38-C26-C27	2.40	118.23	113.62
23	6	616	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	7	619	LUT	C8-C7-C6	-2.40	120.46	127.20
23	5	603	CLA	CMB-C2B-C3B	2.40	129.38	124.69
23	B	824	CLA	C2D-C1D-ND	-2.40	108.34	110.10
23	B	814	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	B	827	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	1	609	CLA	CMB-C2B-C3B	2.40	129.38	124.69
23	8	613	CLA	O2A-CGA-O1A	-2.40	117.54	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	819	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	B	828	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	1	616	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
23	7	612	CLA	O2A-CGA-O1A	-2.40	117.33	123.30
23	A	802	CLA	C1-C2-C3	-2.39	121.90	126.04
23	F	303	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	4	618	CLA	CAA-C2A-C3A	-2.39	108.28	114.26
26	6	622	BCR	C37-C22-C23	2.39	121.85	118.08
23	G	204	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
23	B	803	CLA	CHC-C1C-NC	2.39	127.83	124.20
23	A	807	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	8	602	CLA	C1-C2-C3	-2.39	121.91	126.04
23	B	809	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	A	826	CLA	CHA-C1A-NA	-2.39	120.92	126.40
23	9	610	CLA	C3A-C4A-CHB	-2.39	120.98	123.91
23	5	617	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	4	603	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	G	205	BCR	C20-C19-C18	-2.39	119.70	126.42
23	7	613	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	7	611	CLA	C7-C6-C5	-2.39	109.29	114.49
23	2	604	CLA	CHB-C4A-NA	2.39	128.00	124.34
23	K	206	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
26	A	850	BCR	C16-C15-C14	-2.39	118.58	123.47
23	B	811	CLA	CMB-C2B-C3B	2.39	129.36	124.69
26	8	621	BCR	C33-C5-C4	2.39	118.20	113.62
23	8	616	CLA	CHA-C1A-NA	-2.39	120.94	126.40
26	A	850	BCR	C38-C26-C27	2.38	118.20	113.62
23	A	824	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	1	614	CLA	CMB-C2B-C3B	2.38	129.35	124.69
23	K	203	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
23	1	610	CLA	C2A-C1A-CHA	2.38	126.41	122.71
26	B	847	BCR	C10-C11-C12	-2.38	115.78	123.22
26	6	622	BCR	C33-C5-C6	-2.38	121.85	124.53
23	5	602	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	B	821	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	A	820	CLA	O2D-CGD-CBD	2.38	115.50	111.27
26	A	852	BCR	C15-C14-C13	-2.38	123.91	127.31
23	8	601	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
32	3	619	XAT	C27-C28-C29	-2.38	121.84	125.53
23	3	610	CLA	CAC-C3C-C4C	2.38	127.90	124.81
26	4	621	BCR	C24-C23-C22	-2.38	122.64	126.23
23	a	613	CLA	C1B-CHB-C4A	-2.38	125.41	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	822	CLA	CAA-C2A-C3A	-2.38	108.32	114.26
23	B	802	CLA	O1D-CGD-CBD	2.38	129.35	124.48
29	4	624	LMG	O3-C3-C2	-2.38	104.85	110.35
26	3	621	BCR	C8-C9-C10	2.38	122.59	118.94
23	B	803	CLA	C1C-C2C-C3C	2.38	109.45	106.96
23	A	842	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
23	7	614	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
26	7	621	BCR	C8-C7-C6	-2.38	120.53	127.20
23	4	609	CLA	CMB-C2B-C3B	2.38	129.12	124.68
23	B	808	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
26	A	850	BCR	C1-C6-C7	2.37	122.50	115.78
23	A	812	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	F	304	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	1	603	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	A	851	BCR	C27-C26-C25	-2.37	119.29	122.73
23	5	606	CLA	CMB-C2B-C3B	2.37	129.12	124.68
31	8	619	LUT	C31-C30-C29	-2.37	123.93	127.31
23	5	612	CLA	O2D-CGD-O1D	-2.37	118.71	124.09
26	L	305	BCR	C37-C22-C23	2.37	121.81	118.08
23	6	604	CLA	CAC-C3C-C4C	2.37	127.88	124.81
23	A	836	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	A	806	CLA	C2A-C1A-CHA	2.37	128.00	123.86
26	3	621	BCR	C33-C5-C4	2.37	118.16	113.62
23	A	807	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
23	5	618	CLA	O2D-CGD-O1D	-2.36	118.72	124.09
26	3	621	BCR	C24-C23-C22	-2.36	122.66	126.23
26	A	850	BCR	C3-C4-C5	-2.36	109.86	114.08
23	B	815	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	7	608	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	8	621	BCR	C15-C16-C17	-2.36	118.64	123.47
26	J	102	BCR	C20-C21-C22	-2.36	123.94	127.31
23	a	612	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
31	2	619	LUT	C1-C2-C3	2.36	118.97	113.64
23	A	838	CLA	C2A-C1A-CHA	2.36	127.99	123.86
23	5	616	CLA	CAB-C3B-C2B	2.36	129.31	124.69
29	7	624	LMG	O6-C1-O1	-2.36	104.39	109.97
23	8	612	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	B	821	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
25	3	624	LHG	C18-C17-C16	-2.36	102.46	114.42
26	3	621	BCR	C1-C6-C5	-2.36	119.29	122.61
31	5	620	LUT	C18-C5-C6	-2.36	121.88	124.53
23	a	612	CLA	O2D-CGD-O1D	-2.36	119.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	612	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
26	4	621	BCR	C39-C30-C25	-2.35	106.48	110.30
23	K	203	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
25	3	624	LHG	C20-C19-C18	-2.35	102.48	114.42
23	A	827	CLA	CHB-C4A-NA	2.35	127.77	124.51
23	1	612	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
23	1	612	CLA	C2A-C1A-CHA	2.35	127.97	123.86
26	3	620	BCR	C8-C7-C6	-2.35	120.60	127.20
23	1	613	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	A	832	CLA	CAA-CBA-CGA	-2.35	106.39	113.25
23	B	841	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	A	810	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
23	B	836	CLA	CHA-C1A-NA	-2.35	121.02	126.40
32	7	620	XAT	C19-C9-C8	2.35	121.78	118.08
25	6	623	LHG	C18-C17-C16	-2.35	102.51	114.42
26	B	845	BCR	C16-C15-C14	-2.35	118.67	123.47
23	3	611	CLA	O2D-CGD-O1D	-2.35	118.76	124.09
26	1	619	BCR	C38-C26-C27	2.35	118.12	113.62
25	8	623	LHG	C11-C10-C9	-2.35	102.52	114.42
23	6	601	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
23	5	606	CLA	CAA-C2A-C3A	-2.35	108.40	114.26
24	A	844	PQN	C2M-C2-C3	-2.34	120.58	124.40
33	6	624	NEX	C5-C6-C1	2.34	122.02	119.70
23	a	612	CLA	C2A-C1A-CHA	2.34	127.96	123.86
23	B	818	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
26	K	207	BCR	C23-C24-C25	-2.34	120.62	127.20
26	L	301	BCR	C34-C9-C10	-2.34	119.64	122.92
26	B	801	BCR	C10-C11-C12	-2.34	115.91	123.22
23	9	603	CLA	C3B-C4B-NB	-2.34	108.05	110.11
26	B	845	BCR	C36-C18-C19	2.34	121.77	118.08
23	3	617	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	1	602	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	a	602	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	6	617	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	8	609	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
23	3	603	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
23	5	606	CLA	O2D-CGD-O1D	-2.34	118.78	124.09
31	2	619	LUT	C39-C29-C28	2.34	121.76	118.08
26	a	619	BCR	C1-C6-C5	-2.34	119.32	122.61
23	7	604	CLA	CAA-CBA-CGA	-2.34	106.43	113.25
28	A	858	LMU	C6'-C5'-C4'	-2.33	106.53	113.33
25	a	620	LHG	C18-C17-C16	-2.33	102.58	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	9	620	XAT	C15-C35-C34	-2.33	118.69	123.47
23	4	614	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
29	5	626	LMG	O2-C2-C1	-2.33	104.38	110.05
23	7	603	CLA	O2A-CGA-O1A	-2.33	117.49	123.30
23	5	613	CLA	CBA-CAA-C2A	2.33	118.47	114.28
23	1	616	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	A	848	BCR	C10-C11-C12	-2.33	115.95	123.22
23	A	818	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
23	3	611	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	B	803	CLA	CMD-C2D-C3D	2.33	132.97	127.61
31	4	619	LUT	C21-C26-C27	-2.33	109.76	112.70
23	6	613	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	a	616	CLA	CHB-C4A-NA	2.33	127.73	124.51
31	5	620	LUT	C39-C29-C28	2.33	121.74	118.08
23	5	611	CLA	CAA-C2A-C3A	-2.32	108.46	114.26
23	A	824	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	8	604	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
26	K	202	BCR	C11-C12-C13	-2.32	119.89	126.42
28	A	859	LMU	O5B-C1B-C2B	2.32	115.26	110.35
23	6	602	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	1	620	LHG	C18-C17-C16	-2.32	102.64	114.42
23	F	303	CLA	CHD-C1D-ND	-2.32	122.32	124.45
23	5	603	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	L	305	BCR	C39-C30-C25	-2.32	106.54	110.30
26	B	848	BCR	C20-C19-C18	-2.32	119.90	126.42
25	A	846	LHG	C20-C19-C18	-2.32	102.65	114.42
23	A	806	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	7	623	BCR	C16-C15-C14	-2.32	118.72	123.47
26	B	845	BCR	C8-C9-C10	2.32	122.50	118.94
23	4	604	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
23	2	609	CLA	C1C-NC-C4C	2.32	107.75	106.71
23	A	801	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
28	K	208	LMU	O5'-C1'-C2'	2.32	115.25	110.35
23	6	607	CLA	CAB-C3B-C2B	2.32	129.22	124.69
26	4	621	BCR	C15-C16-C17	-2.31	118.73	123.47
25	a	620	LHG	O8-C23-C24	2.31	119.17	111.91
23	9	612	CLA	C3A-C4A-CHB	-2.31	121.08	123.91
23	A	817	CLA	O2D-CGD-CBD	2.31	115.38	111.27
26	1	619	BCR	C1-C6-C5	-2.31	119.36	122.61
32	8	620	XAT	O4-C5-C6	-2.31	57.05	58.96
25	B	851	LHG	C11-C10-C9	-2.31	102.69	114.42
26	B	801	BCR	C36-C18-C17	-2.31	119.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	620	LHG	O8-C23-C24	2.31	119.15	111.91
23	9	610	CLA	C1C-NC-C4C	2.31	107.74	106.71
23	1	609	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	A	841	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	B	845	BCR	C37-C22-C21	-2.31	119.69	122.92
23	K	201	CLA	O2A-CGA-O1A	-2.31	117.55	123.30
23	A	837	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
26	B	843	BCR	C27-C26-C25	-2.31	119.38	122.73
31	8	619	LUT	C19-C9-C8	2.31	121.71	118.08
23	4	618	CLA	CAB-C3B-C2B	2.31	129.20	124.69
31	3	618	LUT	C15-C14-C13	-2.31	124.02	127.31
32	8	620	XAT	C30-C31-C32	-2.30	116.03	123.22
32	2	620	XAT	C19-C9-C8	2.30	121.70	118.08
23	6	611	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	4	612	CLA	C2A-C1A-CHA	2.30	127.89	123.86
29	J	104	LMG	O7-C10-O9	-2.30	118.14	123.70
23	a	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	A	820	CLA	C2D-C1D-ND	-2.30	108.41	110.10
23	B	818	CLA	C2D-C1D-ND	-2.30	108.41	110.10
26	a	619	BCR	C38-C26-C27	2.30	118.03	113.62
23	L	304	CLA	O2A-CGA-O1A	-2.30	117.57	123.30
23	8	613	CLA	O2D-CGD-CBD	2.30	115.35	111.27
31	4	619	LUT	C39-C29-C28	2.30	121.70	118.08
23	5	619	CLA	CHA-C1A-NA	-2.30	121.13	126.40
25	4	622	LHG	C18-C17-C16	-2.30	102.76	114.42
29	4	624	LMG	O1-C1-C2	-2.30	104.72	108.30
23	3	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
26	G	205	BCR	C38-C26-C27	2.30	118.03	113.62
31	7	619	LUT	C18-C5-C6	-2.30	121.95	124.53
26	B	846	BCR	C23-C22-C21	-2.30	115.42	118.94
23	A	826	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
23	3	612	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
23	A	802	CLA	C2D-C1D-ND	-2.29	108.41	110.10
23	4	618	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
23	7	601	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
23	3	613	CLA	C2D-C1D-ND	-2.29	108.41	110.10
23	4	603	CLA	O2D-CGD-CBD	2.29	115.34	111.27
23	5	610	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
26	K	202	BCR	C30-C25-C26	-2.29	119.39	122.61
23	A	816	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	6	612	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	6	609	CLA	O2D-CGD-CBD	2.29	115.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	607	CLA	O2A-CGA-O1A	-2.29	117.59	123.30
23	8	611	CLA	C2D-C1D-ND	-2.29	108.42	110.10
23	8	613	CLA	C3A-C2A-C1A	2.29	104.77	101.34
23	a	606	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
32	7	620	XAT	O4-C5-C6	-2.29	57.06	58.96
23	2	616	CLA	CHB-C4A-NA	2.29	127.84	124.34
23	2	611	CLA	C3B-C4B-NB	-2.29	108.10	110.11
26	5	622	BCR	C27-C26-C25	-2.29	119.41	122.73
23	8	610	CLA	O2D-CGD-CBD	2.29	115.34	111.27
23	1	609	CLA	C2A-C1A-CHA	2.29	127.85	123.85
23	4	602	CLA	O2D-CGD-CBD	2.29	115.33	111.27
23	a	609	CLA	C2A-C1A-CHA	2.29	127.86	123.86
23	5	601	CLA	C2D-C1D-ND	-2.29	108.42	110.10
23	B	837	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	A	804	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
25	2	622	LHG	O8-C23-O10	-2.29	117.82	123.59
23	4	612	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	9	611	CLA	CHD-C1D-ND	-2.29	122.31	124.52
26	4	621	BCR	C1-C6-C5	-2.29	119.39	122.61
26	K	202	BCR	C16-C15-C14	-2.29	118.79	123.47
32	8	620	XAT	C39-C29-C28	2.29	121.68	118.08
23	5	601	CLA	CHB-C4A-NA	2.29	127.67	124.51
23	9	607	CLA	C3B-C4B-NB	-2.29	108.10	110.11
28	A	859	LMU	O5B-C5B-C4B	2.28	113.84	109.69
23	6	603	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
23	4	606	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
23	A	811	CLA	C2D-C1D-ND	-2.28	108.42	110.10
25	5	623	LHG	C11-C10-C9	-2.28	102.83	114.42
23	A	814	CLA	C11-C10-C8	-2.28	108.54	115.92
23	3	607	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	5	618	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	5	611	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	B	828	CLA	C2D-C1D-ND	-2.28	108.42	110.10
31	a	617	LUT	C15-C35-C34	-2.28	118.80	123.47
23	A	812	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
23	A	840	CLA	C1-C2-C3	-2.28	122.10	126.04
23	5	616	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
26	4	621	BCR	C8-C7-C6	-2.28	120.80	127.20
23	4	601	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	A	848	BCR	C8-C7-C6	-2.28	120.81	127.20
23	A	806	CLA	CAC-C3C-C4C	2.28	127.76	124.81
31	1	617	LUT	C15-C35-C34	-2.28	118.81	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	846	LHG	C18-C17-C16	-2.28	102.87	114.42
23	4	603	CLA	O2A-CGA-O1A	-2.28	117.63	123.30
32	6	621	XAT	C31-C32-C33	-2.28	120.02	126.42
23	3	609	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
29	5	627	LMG	O6-C1-O1	-2.27	104.59	109.97
25	8	622	LHG	C18-C17-C16	-2.27	102.88	114.42
23	5	617	CLA	CHB-C4A-NA	2.27	127.66	124.51
23	A	809	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
25	3	624	LHG	C11-C10-C9	-2.27	102.89	114.42
23	B	836	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	5	607	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
23	4	607	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	7	614	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	A	808	CLA	CHD-C1D-ND	-2.27	122.37	124.45
23	8	607	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	A	848	BCR	C20-C19-C18	-2.27	120.04	126.42
25	5	625	LHG	C20-C19-C18	-2.27	102.91	114.42
23	B	802	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
25	5	625	LHG	C27-C26-C25	-2.27	102.91	114.42
25	7	622	LHG	C27-C26-C25	-2.27	102.91	114.42
23	6	601	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
29	4	624	LMG	O2-C2-C1	-2.27	104.54	110.05
26	J	102	BCR	C23-C24-C25	-2.27	120.84	127.20
23	5	603	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
23	G	204	CLA	C3A-C2A-C1A	2.27	104.73	101.34
23	7	612	CLA	CHA-C1A-NA	-2.26	121.21	126.40
26	8	621	BCR	C10-C11-C12	-2.26	116.15	123.22
26	A	856	BCR	C8-C7-C6	-2.26	120.84	127.20
29	5	626	LMG	O8-C28-O10	-2.26	117.88	123.59
23	2	609	CLA	CHD-C1D-ND	-2.26	122.33	124.52
25	5	625	LHG	O8-C23-C24	2.26	119.01	111.91
23	A	821	CLA	CAC-C3C-C4C	2.26	127.75	124.81
23	B	840	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	A	845	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	8	603	CLA	CAB-C3B-C2B	2.26	129.11	124.69
26	5	622	BCR	C33-C5-C6	-2.26	121.99	124.53
23	6	612	CLA	C2A-C1A-CHA	2.26	127.81	123.86
23	A	830	CLA	CMC-C2C-C1C	-2.26	121.60	125.04
26	B	847	BCR	C23-C24-C25	-2.26	120.86	127.20
23	3	603	CLA	C1-C2-C3	-2.26	122.14	126.04
23	a	606	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	1	603	CLA	CBC-CAC-C3C	-2.26	106.21	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	801	CLA	C11-C12-C13	-2.26	108.62	115.92
31	8	619	LUT	C15-C14-C13	-2.26	124.09	127.31
28	5	628	LMU	C1'-O5'-C5'	2.26	118.12	113.69
23	8	609	CLA	CAC-C3C-C4C	2.26	127.74	124.81
23	B	835	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
23	1	606	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
26	F	305	BCR	C15-C16-C17	-2.25	118.86	123.47
23	6	612	CLA	CAA-C2A-C1A	2.25	117.13	112.14
31	6	619	LUT	C1-C2-C3	2.25	118.73	113.64
23	2	601	CLA	CHD-C1D-ND	-2.25	122.34	124.52
26	B	846	BCR	C4-C5-C6	-2.25	119.46	122.73
23	A	815	CLA	C2A-C1A-CHA	2.25	127.80	123.86
23	G	203	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	9	607	CLA	CHD-C1D-ND	-2.25	122.34	124.52
31	6	619	LUT	C21-C26-C27	-2.25	109.86	112.70
23	B	803	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	a	603	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
23	A	835	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
23	B	827	CLA	O2D-CGD-CBD	2.25	115.26	111.27
23	A	813	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	4	622	LHG	C27-C26-C25	-2.25	103.01	114.42
23	7	615	CLA	O1A-CGA-CBA	2.25	130.30	123.08
23	A	809	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	A	817	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	3	607	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
31	7	619	LUT	C21-C26-C27	-2.25	109.86	112.70
31	1	617	LUT	C39-C29-C28	2.24	121.61	118.08
26	7	621	BCR	C39-C30-C25	-2.24	106.66	110.30
23	8	608	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
23	2	601	CLA	C3B-C4B-NB	-2.24	108.14	110.11
23	8	603	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	6	616	CLA	C16-C15-C13	-2.24	108.68	115.92
23	3	610	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	A	854	CLA	O2D-CGD-CBD	2.24	115.25	111.27
23	K	201	CLA	CHA-C1A-NA	-2.24	121.27	126.40
28	8	624	LMU	C2'-C3'-C4'	2.24	114.79	109.68
23	7	604	CLA	C2D-C1D-ND	-2.24	108.45	110.10
26	A	851	BCR	C30-C25-C24	2.24	122.11	115.78
23	A	828	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
23	7	604	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
23	A	838	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
26	3	621	BCR	C15-C16-C17	-2.24	118.89	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	826	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
32	4	620	XAT	C19-C9-C8	2.23	121.60	118.08
26	B	844	BCR	C21-C20-C19	-2.23	116.25	123.22
23	9	614	CLA	CHB-C4A-NA	2.23	127.76	124.34
23	5	602	CLA	O2A-C1-C2	-2.23	102.77	108.64
23	6	609	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
23	B	802	CLA	CHB-C4A-NA	2.23	127.60	124.51
23	3	603	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	6	622	BCR	C1-C6-C7	2.23	122.09	115.78
23	A	854	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	8	601	CLA	C3A-C2A-C1A	2.23	104.68	101.34
25	6	623	LHG	C5-O7-C7	-2.23	112.30	117.79
23	5	607	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	a	607	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
23	A	839	CLA	CMB-C2B-C3B	2.23	128.85	124.68
28	A	857	LMU	C6B-C5B-C4B	-2.23	107.78	113.00
28	A	859	LMU	C1B-C2B-C3B	2.23	114.64	110.00
23	9	602	CLA	CHB-C4A-NA	2.23	127.75	124.34
26	B	846	BCR	C30-C25-C24	2.23	122.08	115.78
23	8	603	CLA	C2A-C1A-CHA	2.23	127.76	123.86
32	3	619	XAT	O4-C5-C6	-2.23	57.11	58.96
25	5	623	LHG	C20-C19-C18	-2.23	103.11	114.42
23	4	606	CLA	O2D-CGD-O1D	-2.23	119.03	124.09
32	6	621	XAT	C38-C25-C24	2.23	116.78	114.28
23	1	607	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
26	4	621	BCR	C16-C15-C14	-2.23	118.92	123.47
23	2	601	CLA	C1C-NC-C4C	2.22	107.71	106.71
26	F	305	BCR	C34-C9-C8	2.22	121.58	118.08
23	A	845	CLA	C1-C2-C3	-2.22	123.15	126.75
23	F	303	CLA	C3C-C4C-NC	-2.22	108.08	110.57
23	4	608	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
31	a	617	LUT	C39-C29-C28	2.22	121.58	118.08
23	B	826	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	A	840	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
31	4	619	LUT	C8-C7-C6	-2.22	120.97	127.20
23	a	603	CLA	C2A-C1A-CHA	2.22	127.74	123.86
32	3	619	XAT	C30-C31-C32	-2.22	116.29	123.22
23	8	603	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
23	2	614	CLA	C1C-NC-C4C	2.22	107.70	106.71
23	9	611	CLA	C1C-NC-C4C	2.22	107.70	106.71
26	B	843	BCR	C34-C9-C8	2.22	121.57	118.08
25	8	622	LHG	C27-C26-C25	-2.22	103.16	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	628	LMU	C3'-C4'-C5'	2.22	116.01	110.93
23	A	854	CLA	CHA-C1A-NA	-2.22	121.32	126.40
23	A	812	CLA	C1-O2A-CGA	2.22	122.26	116.44
23	3	610	CLA	O2D-CGD-CBD	2.22	115.21	111.27
23	B	829	CLA	C1D-ND-C4D	2.22	107.91	106.33
26	3	621	BCR	C16-C15-C14	-2.22	118.94	123.47
23	3	610	CLA	CMA-C3A-C2A	-2.21	104.90	113.83
23	5	616	CLA	CMB-C2B-C3B	2.21	129.02	124.69
23	3	608	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
23	A	812	CLA	C16-C15-C13	-2.21	108.77	115.92
26	A	851	BCR	C34-C9-C8	2.21	121.56	118.08
30	B	850	DGD	C5B-C4B-C3B	-2.21	103.19	114.42
25	B	851	LHG	C27-C26-C25	-2.21	103.19	114.42
23	A	814	CLA	C11-C12-C13	-2.21	108.77	115.92
33	6	624	NEX	C38-C25-C24	2.21	116.77	114.28
23	A	804	CLA	C2D-C1D-ND	-2.21	108.47	110.10
26	a	619	BCR	C1-C6-C7	2.21	122.03	115.78
23	3	612	CLA	C2A-C1A-CHA	2.21	127.72	123.86
29	5	627	LMG	O3-C3-C2	-2.21	105.24	110.35
23	B	813	CLA	C16-C15-C13	-2.21	108.79	115.92
23	4	614	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	9	607	CLA	CHB-C4A-NA	2.20	127.71	124.34
23	3	609	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
23	A	828	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
23	B	823	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
26	L	301	BCR	C3-C4-C5	-2.20	110.14	114.08
26	K	202	BCR	C20-C19-C18	-2.20	120.23	126.42
23	A	854	CLA	C11-C10-C8	-2.20	108.80	115.92
23	B	812	CLA	CAA-C2A-C1A	2.20	119.19	111.97
32	4	620	XAT	C18-C5-C4	2.20	116.75	114.28
26	K	202	BCR	C10-C11-C12	-2.20	116.35	123.22
26	1	619	BCR	C1-C6-C7	2.20	122.00	115.78
25	5	623	LHG	C27-C26-C25	-2.20	103.26	114.42
26	3	620	BCR	C38-C26-C27	2.20	117.84	113.62
23	B	839	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	6	618	CLA	CAB-C3B-C2B	2.20	128.99	124.69
26	B	848	BCR	C34-C9-C8	2.20	121.54	118.08
25	2	622	LHG	C27-C26-C25	-2.20	103.27	114.42
26	J	102	BCR	C21-C20-C19	-2.20	116.36	123.22
23	6	613	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
23	7	610	CLA	O1D-CGD-CBD	2.20	128.98	124.48
26	B	843	BCR	C16-C15-C14	-2.19	118.98	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	618	XAT	O24-C25-C26	-2.19	57.14	58.96
32	1	618	XAT	O24-C25-C26	-2.19	57.14	58.96
23	6	606	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
31	3	618	LUT	C40-C33-C32	2.19	121.53	118.08
23	9	610	CLA	CHD-C1D-ND	-2.19	122.40	124.52
28	8	625	LMU	C1B-C2B-C3B	2.19	114.56	110.00
23	a	611	CLA	C2A-C1A-CHA	2.19	127.68	123.85
23	A	843	CLA	CMB-C2B-C3B	2.19	128.78	124.68
23	9	604	CLA	CHB-C4A-NA	2.19	127.69	124.34
23	J	101	CLA	CHD-C1D-ND	-2.19	122.44	124.45
33	6	624	NEX	C39-C29-C30	-2.19	119.86	122.92
23	1	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	1	617	LUT	C15-C14-C13	-2.19	124.19	127.31
23	4	612	CLA	CAA-C2A-C3A	-2.19	108.79	114.26
23	A	817	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
26	L	301	BCR	C3-C2-C1	-2.19	106.78	114.60
31	a	617	LUT	C15-C14-C13	-2.19	124.19	127.31
26	3	621	BCR	C34-C9-C10	-2.19	119.86	122.92
23	5	617	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	B	807	CLA	O2D-CGD-CBD	2.19	115.16	111.27
26	L	301	BCR	C10-C11-C12	-2.19	116.39	123.22
23	A	828	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
23	7	616	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
23	B	825	CLA	C2D-C1D-ND	-2.18	108.49	110.10
23	1	603	CLA	C2A-C1A-CHA	2.18	127.68	123.86
23	F	303	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
23	8	606	CLA	O2D-CGD-CBD	2.18	115.15	111.27
23	1	611	CLA	C2A-C1A-CHA	2.18	127.68	123.86
26	7	623	BCR	C33-C5-C4	2.18	117.81	113.62
23	B	815	CLA	C2A-C1A-CHA	2.18	127.67	123.86
26	6	622	BCR	C23-C22-C21	-2.18	115.59	118.94
26	3	620	BCR	C21-C20-C19	-2.18	116.41	123.22
26	B	847	BCR	C20-C21-C22	-2.18	124.20	127.31
23	6	604	CLA	C2D-C1D-ND	-2.18	108.50	110.10
23	5	617	CLA	CMB-C2B-C3B	2.18	128.75	124.68
23	B	832	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
31	7	619	LUT	C39-C29-C28	2.18	121.51	118.08
31	5	620	LUT	C19-C9-C8	2.18	121.51	118.08
23	B	825	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
23	A	808	CLA	O2D-CGD-CBD	2.18	115.14	111.27
23	A	818	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	8	614	CLA	O2A-CGA-O1A	-2.18	118.10	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	621	XAT	C28-C29-C30	-2.18	115.60	118.94
30	B	850	DGD	C7B-C6B-C5B	-2.18	103.38	114.42
23	G	204	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
23	A	807	CLA	C6-C7-C8	-2.17	108.89	115.92
29	5	627	LMG	C1-C2-C3	-2.17	105.47	110.00
23	5	616	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
25	3	623	LHG	C27-C26-C25	-2.17	103.40	114.42
26	B	846	BCR	C35-C13-C12	2.17	121.50	118.08
23	5	610	CLA	C1-C2-C3	-2.17	122.29	126.04
29	J	104	LMG	C3-C4-C5	-2.17	106.37	110.24
29	5	627	LMG	O2-C2-C1	-2.17	104.78	110.05
26	K	207	BCR	C28-C27-C26	-2.17	110.20	114.08
23	A	819	CLA	C2D-C1D-ND	-2.17	108.51	110.10
23	6	613	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	a	612	CLA	CHA-C1A-NA	-2.17	121.44	126.40
23	B	825	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
23	7	607	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	2	603	CLA	C1C-NC-C4C	2.16	107.68	106.71
26	B	801	BCR	C15-C14-C13	-2.16	124.22	127.31
23	A	831	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	B	833	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	B	848	BCR	C39-C30-C25	-2.16	106.79	110.30
23	2	609	CLA	CHB-C4A-NA	2.16	127.65	124.34
23	8	616	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
23	9	604	CLA	CHD-C1D-ND	-2.16	122.43	124.52
23	A	820	CLA	CHC-C1C-NC	2.16	127.48	124.20
25	1	620	LHG	C27-C26-C25	-2.16	103.45	114.42
28	8	625	LMU	O1'-C1'-C2'	2.16	111.68	108.30
26	B	848	BCR	C31-C1-C6	-2.16	106.80	110.30
26	8	621	BCR	C34-C9-C8	2.16	121.48	118.08
31	6	619	LUT	C39-C29-C28	2.16	121.48	118.08
23	8	603	CLA	CHA-C1A-NA	-2.16	121.45	126.40
23	B	811	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	4	609	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	5	612	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	1	612	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
26	4	621	BCR	C11-C12-C13	-2.16	120.36	126.42
23	A	838	CLA	CBA-CAA-C2A	-2.16	107.50	113.86
33	5	624	NEX	O24-C25-C26	-2.16	57.17	58.96
25	3	623	LHG	C20-C19-C18	-2.16	103.48	114.42
23	A	808	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
25	a	620	LHG	C27-C26-C25	-2.15	103.49	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	823	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
23	3	612	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
23	A	811	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	6	618	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
23	K	201	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
26	A	856	BCR	C32-C1-C6	2.15	113.79	110.30
23	A	821	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
25	6	623	LHG	O8-C23-C24	2.15	118.66	111.91
23	A	827	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
25	3	623	LHG	C18-C17-C16	-2.15	103.52	114.42
23	B	833	CLA	C3A-C2A-C1A	2.15	104.56	101.34
23	7	616	CLA	C2D-C1D-ND	-2.15	108.52	110.10
31	5	620	LUT	C38-C25-C24	-2.15	118.97	123.56
23	8	616	CLA	C1D-ND-C4D	-2.15	104.81	106.33
23	7	607	CLA	CBC-CAC-C3C	2.15	118.34	112.43
23	A	820	CLA	C2A-C1A-CHA	2.15	127.61	123.86
23	3	603	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
23	A	819	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
23	A	838	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
23	9	601	CLA	C3B-C4B-NB	-2.14	108.23	110.11
23	A	806	CLA	C3C-C4C-NC	-2.14	108.17	110.57
23	6	616	CLA	C1-C2-C3	-2.14	122.34	126.04
31	a	617	LUT	C16-C1-C6	-2.14	106.82	110.30
32	1	618	XAT	C38-C25-C24	2.14	116.69	114.28
23	B	834	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	A	832	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
29	7	624	LMG	O3-C3-C2	-2.14	105.40	110.35
23	7	615	CLA	C2A-C1A-CHA	2.14	127.60	123.86
23	9	606	CLA	CHB-C4A-NA	2.14	127.61	124.34
26	A	850	BCR	C21-C20-C19	-2.14	116.54	123.22
23	4	614	CLA	C2D-C1D-ND	-2.14	108.53	110.10
32	5	621	XAT	O24-C25-C26	-2.14	57.19	58.96
23	5	607	CLA	CHD-C1D-ND	-2.14	122.49	124.45
29	7	624	LMG	C3-C4-C5	-2.14	106.43	110.24
26	B	801	BCR	C7-C8-C9	-2.14	123.01	126.23
23	5	609	CLA	CHD-C1D-ND	-2.13	122.49	124.45
29	J	104	LMG	O2-C2-C1	-2.13	104.86	110.05
23	1	611	CLA	O2D-CGD-CBD	2.13	115.06	111.27
23	B	835	CLA	CHA-C1A-NA	-2.13	121.51	126.40
23	A	830	CLA	CHC-C1C-NC	2.13	127.44	124.20
23	6	601	CLA	O2D-CGD-CBD	2.13	115.06	111.27
23	a	612	CLA	O2A-CGA-O1A	-2.13	117.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	852	BCR	C40-C30-C25	-2.13	106.84	110.30
23	4	602	CLA	CHD-C1D-ND	-2.13	122.50	124.45
31	5	620	LUT	C28-C29-C30	-2.13	115.67	118.94
23	A	829	CLA	C1-C2-C3	-2.13	122.36	126.04
23	7	604	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	2	603	CLA	CHB-C4A-NA	2.13	127.60	124.34
29	4	623	LMG	O1-C7-C8	-2.13	105.76	110.90
23	A	801	CLA	C1D-ND-C4D	-2.13	104.82	106.33
23	2	604	CLA	CHD-C1D-ND	-2.13	122.46	124.52
23	2	601	CLA	CHB-C4A-NA	2.13	127.60	124.34
23	3	603	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
32	5	621	XAT	C30-C31-C32	-2.13	116.58	123.22
23	A	854	CLA	CHB-C4A-NA	2.13	127.45	124.51
23	8	612	CLA	O2D-CGD-O1D	-2.13	119.26	124.09
23	A	831	CLA	CMC-C2C-C3C	2.13	131.89	126.12
23	G	204	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
23	A	840	CLA	O2D-CGD-CBD	2.13	115.05	111.27
33	5	624	NEX	O23-C23-C24	-2.13	105.58	109.80
31	7	619	LUT	C38-C25-C24	-2.13	119.01	123.56
23	a	610	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
23	A	829	CLA	CAC-C3C-C4C	2.12	127.57	124.81
23	A	807	CLA	C2A-C1A-CHA	2.12	127.57	123.86
25	9	622	LHG	C20-C19-C18	-2.12	103.64	114.42
23	2	607	CLA	CHB-C4A-NA	2.12	127.59	124.34
23	2	616	CLA	CHD-C1D-ND	-2.12	122.46	124.52
23	A	825	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	B	817	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
23	7	613	CLA	CAC-C3C-C4C	2.12	127.56	124.81
26	4	621	BCR	C4-C5-C6	-2.12	119.65	122.73
23	B	820	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
31	1	617	LUT	C31-C30-C29	-2.12	124.28	127.31
31	1	617	LUT	C17-C1-C6	2.12	113.74	110.30
23	9	603	CLA	CHB-C4A-NA	2.12	127.58	124.34
23	A	805	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	A	820	CLA	CMC-C2C-C3C	2.12	131.87	126.12
23	5	612	CLA	C2A-C1A-CHA	2.12	127.56	123.86
23	3	602	CLA	O1D-CGD-CBD	2.12	128.82	124.48
23	B	836	CLA	C2A-C1A-CHA	2.12	127.56	123.86
26	K	202	BCR	C38-C26-C25	-2.12	122.15	124.53
23	A	830	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	G	205	BCR	C11-C10-C9	-2.12	124.29	127.31
25	8	623	LHG	C27-C26-C25	-2.12	103.68	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	305	BCR	C20-C21-C22	-2.12	124.29	127.31
23	7	603	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
26	a	619	BCR	C8-C7-C6	-2.11	121.26	127.20
23	F	301	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
23	A	815	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	5	622	BCR	C39-C30-C25	-2.11	106.87	110.30
23	3	606	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	A	839	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	A	825	CLA	C2D-C1D-ND	-2.11	108.55	110.10
26	A	856	BCR	C11-C12-C13	-2.11	120.48	126.42
26	L	301	BCR	C33-C5-C6	-2.11	122.16	124.53
23	a	614	CLA	O2D-CGD-CBD	2.11	115.02	111.27
23	A	814	CLA	C3A-C2A-C1A	2.11	104.50	101.34
31	8	619	LUT	C28-C29-C30	-2.11	115.70	118.94
23	B	824	CLA	C2A-C1A-CHA	2.11	127.55	123.86
23	A	816	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
26	K	207	BCR	C15-C16-C17	-2.11	119.15	123.47
30	J	103	DGD	O6D-C5D-C6D	-2.11	102.41	106.67
23	6	609	CLA	C2A-C1A-CHA	2.11	127.55	123.86
32	9	620	XAT	C20-C13-C12	2.11	121.40	118.08
24	B	842	PQN	C9-C10-C5	2.11	121.61	119.26
23	8	603	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
23	A	820	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	A	823	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	L	301	BCR	C30-C25-C26	-2.11	119.64	122.61
26	B	848	BCR	C36-C18-C17	-2.11	119.97	122.92
23	8	603	CLA	C2D-C1D-ND	-2.11	108.55	110.10
23	B	805	CLA	C2A-C1A-CHA	2.11	127.54	123.86
23	A	836	CLA	C4-C3-C5	2.11	118.81	115.27
23	3	602	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
23	A	827	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	B	844	BCR	C8-C9-C10	2.11	122.17	118.94
31	a	617	LUT	C17-C1-C6	2.11	113.72	110.30
23	B	814	CLA	C2D-C1D-ND	-2.10	108.55	110.10
26	7	623	BCR	C34-C9-C10	-2.10	119.97	122.92
23	5	601	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	A	830	CLA	C16-C15-C13	-2.10	109.12	115.92
26	1	619	BCR	C8-C7-C6	-2.10	121.29	127.20
26	B	843	BCR	C20-C19-C18	-2.10	120.51	126.42
31	7	619	LUT	C28-C29-C30	-2.10	115.71	118.94
26	G	205	BCR	C15-C14-C13	-2.10	124.31	127.31
23	a	609	CLA	CHA-C1A-NA	-2.10	121.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	832	CLA	O2D-CGD-CBD	2.10	115.00	111.27
23	9	612	CLA	C2A-C1A-CHA	2.10	125.97	122.71
23	B	813	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
26	A	849	BCR	C10-C11-C12	-2.10	116.66	123.22
23	A	815	CLA	CHA-C1A-NA	-2.10	121.58	126.40
31	1	617	LUT	C16-C1-C6	-2.10	106.89	110.30
23	5	617	CLA	O1D-CGD-CBD	2.10	128.78	124.48
32	a	618	XAT	C38-C25-C24	2.10	116.64	114.28
26	F	305	BCR	C23-C24-C25	-2.10	121.30	127.20
23	A	837	CLA	C2A-C1A-CHA	2.10	127.53	123.86
23	4	608	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
29	4	624	LMG	C1-C2-C3	-2.10	105.62	110.00
32	7	620	XAT	C5-C4-C3	-2.10	108.60	112.75
23	a	601	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
31	a	617	LUT	C31-C30-C29	-2.10	124.32	127.31
26	L	305	BCR	C38-C26-C27	2.10	117.64	113.62
23	3	611	CLA	CMA-C3A-C2A	-2.10	111.20	116.10
23	9	611	CLA	CHB-C4A-NA	2.10	127.55	124.34
23	9	613	CLA	CHB-C4A-NA	2.10	127.55	124.34
23	B	838	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	A	846	LHG	C5-O7-C7	-2.09	112.64	117.79
23	a	614	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	2	604	CLA	C1C-NC-C4C	2.09	107.65	106.71
23	A	801	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
23	A	854	CLA	C4D-C3D-CAD	-2.09	105.63	108.10
26	A	856	BCR	C33-C5-C4	2.09	117.64	113.62
31	3	618	LUT	C1-C2-C3	2.09	118.37	113.64
23	7	611	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	6	608	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	8	609	CLA	O1A-CGA-CBA	2.09	129.80	123.08
26	6	622	BCR	C1-C6-C5	-2.09	119.67	122.61
23	1	609	CLA	CHA-C1A-NA	-2.09	121.61	126.40
23	A	841	CLA	C2A-C1A-CHA	2.09	127.51	123.86
23	B	802	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	B	808	CLA	C16-C15-C13	-2.09	109.17	115.92
26	B	847	BCR	C36-C18-C19	2.09	121.37	118.08
23	6	610	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	1	601	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
23	7	603	CLA	CHD-C1D-ND	-2.09	122.54	124.45
23	A	814	CLA	C16-C15-C13	-2.09	109.17	115.92
26	A	849	BCR	C30-C25-C26	-2.09	119.67	122.61
23	B	836	CLA	O2A-CGA-O1A	-2.08	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	102	BCR	C38-C26-C27	2.08	117.62	113.62
23	A	834	CLA	O1D-CGD-CBD	2.08	128.75	124.48
30	J	103	DGD	C5B-C4B-C3B	-2.08	103.85	114.42
33	6	624	NEX	O24-C25-C26	-2.08	57.23	58.96
23	5	610	CLA	O1D-CGD-CBD	2.08	128.75	124.48
23	3	608	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	J	101	CLA	CAA-C2A-C3A	-2.08	109.06	114.26
23	B	805	CLA	O2A-C1-C2	-2.08	103.17	108.64
23	A	832	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
23	B	818	CLA	CGD-CBD-CAD	-2.08	104.00	110.73
23	7	616	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
23	4	613	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	3	614	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	5	614	CLA	C2A-C1A-CHA	2.08	127.31	123.81
23	2	610	CLA	CHB-C4A-NA	2.08	127.52	124.34
23	B	832	CLA	C1-C2-C3	-2.08	122.45	126.04
26	B	846	BCR	C8-C7-C6	-2.08	121.36	127.20
23	4	606	CLA	C2D-C1D-ND	-2.08	108.57	110.10
23	A	831	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	A	815	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	B	809	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	9	613	CLA	CHD-C1D-ND	-2.08	122.51	124.52
23	9	612	CLA	C1C-NC-C4C	2.08	107.64	106.71
23	2	604	CLA	C3B-C4B-NB	-2.08	108.29	110.11
23	B	813	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	5	608	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	B	839	CLA	CMA-C3A-C2A	-2.07	105.46	113.83
26	A	856	BCR	C35-C13-C12	2.07	121.34	118.08
23	A	826	CLA	CAC-C3C-C4C	2.07	127.50	124.81
29	J	104	LMG	C6-C5-C4	-2.07	108.15	113.00
26	7	621	BCR	C23-C22-C21	-2.07	115.76	118.94
23	B	828	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
33	5	624	NEX	C11-C12-C13	-2.07	120.59	126.42
23	4	601	CLA	O2D-CGD-CBD	2.07	114.95	111.27
23	B	824	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
32	9	620	XAT	C38-C25-C24	2.07	116.61	114.28
23	6	606	CLA	O2D-CGD-O1D	-2.07	119.39	124.09
23	1	609	CLA	CMA-C3A-C2A	-2.07	111.27	116.10
26	B	847	BCR	C1-C6-C7	2.07	121.63	115.78
23	A	838	CLA	O1D-CGD-CBD	2.07	128.72	124.48
23	5	609	CLA	CHA-C1A-NA	-2.07	121.66	126.40
23	K	204	CLA	CAA-C2A-C3A	-2.07	107.11	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	621	BCR	C40-C30-C25	2.07	113.65	110.30
31	6	619	LUT	C8-C9-C10	-2.07	115.77	118.94
23	B	834	CLA	C1-C2-C3	-2.07	122.47	126.04
23	B	818	CLA	O2D-CGD-CBD	2.07	114.94	111.27
23	A	830	CLA	O2A-C1-C2	-2.07	103.20	108.64
23	8	611	CLA	O2D-CGD-CBD	2.06	114.94	111.27
23	B	814	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	B	839	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	6	616	CLA	C2D-C1D-ND	-2.06	108.58	110.10
29	4	623	LMG	O2-C2-C1	-2.06	105.03	110.05
23	B	826	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
26	6	622	BCR	C23-C24-C25	-2.06	121.41	127.20
23	8	608	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	7	624	LMG	O1-C7-C8	-2.06	105.92	110.90
23	4	616	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
23	B	817	CLA	CHC-C1C-NC	2.06	127.33	124.20
23	B	803	CLA	C2A-C1A-CHA	2.06	127.46	123.86
23	B	810	CLA	C1-C2-C3	-2.06	122.48	126.04
26	B	848	BCR	C2-C1-C6	2.06	113.65	110.48
23	B	829	CLA	CHA-C4D-ND	2.06	136.80	132.50
23	A	813	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	8	602	CLA	O2D-CGD-CBD	2.06	114.92	111.27
32	6	621	XAT	O4-C5-C6	-2.06	57.26	58.96
23	A	831	CLA	C1D-ND-C4D	2.05	107.79	106.33
23	A	806	CLA	O1D-CGD-CBD	2.05	128.69	124.48
23	A	854	CLA	C4-C3-C5	2.05	118.72	115.27
23	5	618	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
23	B	817	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	6	613	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	5	609	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
26	B	844	BCR	C30-C25-C24	2.05	121.58	115.78
23	A	842	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	9	622	LHG	C18-C17-C16	-2.05	104.02	114.42
23	A	825	CLA	CHC-C1C-NC	2.05	127.31	124.20
26	4	621	BCR	C1-C6-C7	2.05	121.58	115.78
23	B	827	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	B	825	CLA	CMD-C2D-C1D	-2.05	121.10	124.71
23	6	607	CLA	C2D-C1D-ND	-2.05	108.59	110.10
23	4	608	CLA	CHD-C1D-ND	-2.05	122.57	124.45
31	4	619	LUT	C8-C9-C10	-2.05	115.80	118.94
23	B	823	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	A	825	CLA	O1D-CGD-CBD	2.05	128.67	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	617	CLA	C2D-C1D-ND	-2.05	108.59	110.10
23	6	607	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	L	305	BCR	C24-C23-C22	-2.05	123.14	126.23
31	6	619	LUT	C7-C8-C9	-2.05	123.14	126.23
23	A	806	CLA	CHC-C1C-NC	2.05	127.31	124.20
23	9	601	CLA	CHB-C4A-NA	2.05	127.47	124.34
23	B	835	CLA	CED-O2D-CGD	2.04	120.56	115.94
31	8	619	LUT	C18-C5-C6	-2.04	122.23	124.53
26	3	620	BCR	C34-C9-C10	-2.04	120.06	122.92
26	F	305	BCR	C30-C25-C24	2.04	121.56	115.78
23	L	302	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
26	5	622	BCR	C34-C9-C8	2.04	121.30	118.08
32	5	621	XAT	C18-C5-C4	2.04	116.58	114.28
23	5	609	CLA	C2A-C1A-CHA	2.04	127.43	123.86
26	B	844	BCR	C33-C5-C6	-2.04	122.24	124.53
23	5	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	B	832	CLA	CHA-C1A-NA	-2.04	121.73	126.40
28	A	858	LMU	C6B-C5B-C4B	-2.04	110.70	113.54
23	2	611	CLA	C1A-CHA-C4D	-2.04	121.70	125.32
23	B	835	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
23	2	613	CLA	CHB-C4A-NA	2.04	127.46	124.34
26	3	622	BCR	C7-C6-C5	-2.03	116.53	121.46
23	6	608	CLA	CHC-C1C-NC	2.03	127.29	124.20
23	9	610	CLA	CHB-C4A-NA	2.03	127.45	124.34
31	5	620	LUT	C8-C7-C6	-2.03	121.49	127.20
23	1	613	CLA	C1-O2A-CGA	-2.03	111.11	116.44
23	a	608	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
32	4	620	XAT	O24-C25-C26	-2.03	57.28	58.96
29	7	624	LMG	O2-C2-C1	-2.03	105.11	110.05
23	7	608	CLA	C2D-C1D-ND	-2.03	108.61	110.10
26	A	856	BCR	C24-C25-C26	-2.03	116.54	121.46
32	6	621	XAT	C18-C5-C4	2.03	116.56	114.28
23	8	602	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	F	305	BCR	C15-C14-C13	-2.03	124.42	127.31
26	K	202	BCR	C15-C16-C17	-2.03	119.32	123.47
23	8	614	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
23	A	811	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	5	621	XAT	C20-C13-C12	2.03	121.27	118.08
23	5	604	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
25	9	622	LHG	C27-C26-C25	-2.02	104.15	114.42
23	7	606	CLA	C3C-C4C-NC	-2.02	108.36	110.57
23	2	614	CLA	CHB-C4A-NA	2.02	127.44	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	204	CLA	CBA-CAA-C2A	-2.02	107.89	113.86
23	8	612	CLA	C2A-C1A-CHA	2.02	127.40	123.86
23	A	843	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	5	616	CLA	O1A-CGA-CBA	2.02	129.58	123.08
26	a	619	BCR	C11-C12-C13	-2.02	120.74	126.42
26	B	846	BCR	C31-C1-C6	-2.02	107.02	110.30
23	A	814	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
26	J	102	BCR	C16-C15-C14	-2.02	119.33	123.47
23	K	206	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
32	8	620	XAT	C8-C9-C10	-2.02	115.84	118.94
26	F	305	BCR	C40-C30-C25	-2.02	107.02	110.30
23	8	614	CLA	C2D-C1D-ND	-2.02	108.62	110.10
23	B	826	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
26	A	851	BCR	C8-C7-C6	-2.02	121.53	127.20
26	K	202	BCR	C8-C7-C6	-2.02	121.53	127.20
23	B	803	CLA	CMD-C2D-C1D	-2.02	121.16	124.71
23	A	854	CLA	CMD-C2D-C1D	-2.02	121.16	124.71
23	6	618	CLA	C2A-C1A-CHA	2.02	127.38	123.86
23	A	822	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
32	3	619	XAT	C35-C34-C33	-2.02	124.43	127.31
23	3	608	CLA	CHA-C4D-ND	2.01	136.71	132.50
23	a	613	CLA	C1-O2A-CGA	-2.01	111.16	116.44
25	5	625	LHG	C18-C17-C16	-2.01	104.20	114.42
23	A	838	CLA	CHA-C1A-NA	-2.01	121.78	126.40
23	B	829	CLA	O1D-CGD-CBD	2.01	128.60	124.48
23	4	618	CLA	C2D-C1D-ND	-2.01	108.62	110.10
23	A	825	CLA	C2A-C1A-CHA	2.01	127.38	123.86
31	7	619	LUT	C20-C13-C12	2.01	121.25	118.08
23	5	619	CLA	O2D-CGD-CBD	2.01	114.84	111.27
29	7	624	LMG	O7-C10-O9	-2.01	118.84	123.70
23	8	604	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	L	302	CLA	O2D-CGD-CBD	2.01	114.84	111.27
32	4	620	XAT	O4-C5-C6	-2.01	57.29	58.96
26	7	623	BCR	C38-C26-C27	2.01	117.48	113.62
23	7	614	CLA	CHA-C1A-NA	-2.01	121.79	126.40
23	3	609	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	A	820	CLA	C1D-ND-C4D	2.01	107.76	106.33
23	7	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
32	3	619	XAT	O24-C25-C26	-2.01	57.30	58.96
23	B	821	CLA	C2A-C1A-CHA	2.01	127.37	123.86
23	1	608	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
23	2	606	CLA	CHB-C4A-NA	2.01	127.41	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	836	CLA	CHA-C4D-ND	2.01	136.70	132.50
29	A	860	LMG	O2-C2-C1	-2.01	105.17	110.05
23	K	204	CLA	CHA-C1A-NA	-2.01	121.81	126.40
23	6	601	CLA	CHA-C1A-NA	-2.00	121.81	126.40
23	B	806	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
26	8	621	BCR	C16-C15-C14	-2.00	119.37	123.47
23	6	608	CLA	CHD-C1D-ND	-2.00	122.61	124.45
31	3	618	LUT	C8-C7-C6	-2.00	121.58	127.20
33	5	624	NEX	C30-C31-C32	-2.00	116.97	123.22
23	8	602	CLA	CHD-C1D-ND	-2.00	122.61	124.45
29	5	626	LMG	O6-C1-O1	-2.00	105.23	109.97
26	B	846	BCR	C16-C17-C18	-2.00	124.45	127.31
23	3	612	CLA	CMB-C2B-C3B	2.00	128.42	124.68
26	1	619	BCR	C11-C12-C13	-2.00	120.80	126.42
28	K	208	LMU	O5'-C5'-C4'	2.00	113.97	109.75
23	5	601	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (238) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	801	CLA	ND
23	A	802	CLA	ND
23	A	803	CLA	ND
23	A	804	CLA	ND
23	A	805	CLA	ND
23	A	806	CLA	ND
23	A	807	CLA	ND
23	A	808	CLA	ND
23	A	809	CLA	ND
23	A	810	CLA	ND
23	A	811	CLA	ND
23	A	812	CLA	ND
23	A	813	CLA	ND
23	A	814	CLA	ND
23	A	815	CLA	ND
23	A	816	CLA	ND
23	A	817	CLA	ND
23	A	818	CLA	ND
23	A	819	CLA	ND
23	A	820	CLA	ND
23	A	821	CLA	ND
23	A	822	CLA	ND

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Mol	Chain	Res	Type	Atom
23	A	823	CLA	ND
23	A	824	CLA	ND
23	A	825	CLA	ND
23	A	826	CLA	ND
23	A	827	CLA	ND
23	A	828	CLA	ND
23	A	829	CLA	ND
23	A	830	CLA	ND
23	A	831	CLA	ND
23	A	832	CLA	ND
23	A	833	CLA	ND
23	A	834	CLA	ND
23	A	835	CLA	ND
23	A	836	CLA	ND
23	A	837	CLA	ND
23	A	838	CLA	ND
23	A	839	CLA	ND
23	A	840	CLA	ND
23	A	841	CLA	ND
23	A	842	CLA	ND
23	A	843	CLA	ND
23	A	845	CLA	ND
23	A	854	CLA	ND
23	B	802	CLA	ND
23	B	803	CLA	ND
23	B	804	CLA	ND
23	B	805	CLA	ND
23	B	806	CLA	ND
23	B	807	CLA	ND
23	B	808	CLA	ND
23	B	809	CLA	ND
23	B	810	CLA	ND
23	B	811	CLA	ND
23	B	812	CLA	ND
23	B	813	CLA	ND
23	B	814	CLA	ND
23	B	815	CLA	ND
23	B	816	CLA	ND
23	B	817	CLA	ND
23	B	818	CLA	ND
23	B	819	CLA	ND
23	B	820	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	821	CLA	ND
23	B	823	CLA	ND
23	B	824	CLA	ND
23	B	825	CLA	ND
23	B	826	CLA	ND
23	B	827	CLA	ND
23	B	828	CLA	ND
23	B	829	CLA	ND
23	B	830	CLA	ND
23	B	831	CLA	ND
23	B	832	CLA	ND
23	B	833	CLA	ND
23	B	834	CLA	ND
23	B	835	CLA	ND
23	B	837	CLA	ND
23	B	838	CLA	ND
23	B	839	CLA	ND
23	B	840	CLA	ND
23	B	841	CLA	ND
23	F	301	CLA	ND
23	F	303	CLA	ND
23	F	304	CLA	ND
23	G	203	CLA	ND
23	G	204	CLA	ND
23	J	101	CLA	ND
23	K	201	CLA	ND
23	K	203	CLA	ND
23	K	204	CLA	ND
23	K	206	CLA	ND
23	L	302	CLA	ND
23	L	303	CLA	ND
23	L	304	CLA	ND
23	1	601	CLA	ND
23	1	602	CLA	ND
23	1	603	CLA	ND
23	1	604	CLA	ND
23	1	606	CLA	ND
23	1	607	CLA	ND
23	1	608	CLA	ND
23	1	609	CLA	ND
23	1	610	CLA	ND
23	1	611	CLA	ND

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Mol	Chain	Res	Type	Atom
23	1	612	CLA	ND
23	1	613	CLA	ND
23	1	614	CLA	ND
23	1	616	CLA	ND
23	a	601	CLA	ND
23	a	602	CLA	ND
23	a	603	CLA	ND
23	a	604	CLA	ND
23	a	606	CLA	ND
23	a	607	CLA	ND
23	a	608	CLA	ND
23	a	609	CLA	ND
23	a	610	CLA	ND
23	a	611	CLA	ND
23	a	612	CLA	ND
23	a	613	CLA	ND
23	a	614	CLA	ND
23	a	616	CLA	ND
23	3	602	CLA	ND
23	3	603	CLA	ND
23	3	604	CLA	ND
23	3	606	CLA	ND
23	3	607	CLA	ND
23	3	608	CLA	ND
23	3	609	CLA	ND
23	3	610	CLA	ND
23	3	611	CLA	ND
23	3	612	CLA	ND
23	3	613	CLA	ND
23	3	614	CLA	ND
23	3	615	CLA	ND
23	3	617	CLA	ND
23	4	601	CLA	ND
23	4	602	CLA	ND
23	4	603	CLA	ND
23	4	604	CLA	ND
23	4	606	CLA	ND
23	4	607	CLA	ND
23	4	608	CLA	ND
23	4	609	CLA	ND
23	4	610	CLA	ND
23	4	611	CLA	ND

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Mol	Chain	Res	Type	Atom
23	4	613	CLA	ND
23	4	614	CLA	ND
23	4	616	CLA	ND
23	4	618	CLA	ND
23	5	601	CLA	ND
23	5	602	CLA	ND
23	5	603	CLA	ND
23	5	604	CLA	ND
23	5	606	CLA	ND
23	5	607	CLA	ND
23	5	608	CLA	ND
23	5	609	CLA	ND
23	5	610	CLA	ND
23	5	611	CLA	ND
23	5	612	CLA	ND
23	5	613	CLA	ND
23	5	614	CLA	ND
23	5	616	CLA	ND
23	5	617	CLA	ND
23	5	618	CLA	ND
23	5	619	CLA	ND
23	6	601	CLA	ND
23	6	602	CLA	ND
23	6	603	CLA	ND
23	6	604	CLA	ND
23	6	606	CLA	ND
23	6	607	CLA	ND
23	6	608	CLA	ND
23	6	609	CLA	ND
23	6	610	CLA	ND
23	6	611	CLA	ND
23	6	612	CLA	ND
23	6	613	CLA	ND
23	6	614	CLA	ND
23	6	616	CLA	ND
23	6	617	CLA	ND
23	6	618	CLA	ND
23	6	620	CLA	ND
23	7	601	CLA	ND
23	7	602	CLA	ND
23	7	603	CLA	ND
23	7	604	CLA	ND

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Mol	Chain	Res	Type	Atom
23	7	606	CLA	ND
23	7	607	CLA	ND
23	7	608	CLA	ND
23	7	609	CLA	ND
23	7	610	CLA	ND
23	7	611	CLA	ND
23	7	613	CLA	ND
23	7	614	CLA	ND
23	7	615	CLA	ND
23	7	616	CLA	ND
23	8	601	CLA	ND
23	8	602	CLA	ND
23	8	603	CLA	ND
23	8	604	CLA	ND
23	8	606	CLA	ND
23	8	607	CLA	ND
23	8	608	CLA	ND
23	8	609	CLA	ND
23	8	610	CLA	ND
23	8	611	CLA	ND
23	8	612	CLA	ND
23	8	613	CLA	ND
23	8	614	CLA	ND
23	2	601	CLA	ND
23	2	602	CLA	ND
23	2	603	CLA	ND
23	2	604	CLA	ND
23	2	606	CLA	ND
23	2	607	CLA	ND
23	2	609	CLA	ND
23	2	610	CLA	ND
23	2	611	CLA	ND
23	2	612	CLA	ND
23	2	613	CLA	ND
23	2	614	CLA	ND
23	2	616	CLA	ND
23	9	601	CLA	ND
23	9	602	CLA	ND
23	9	603	CLA	ND
23	9	604	CLA	ND
23	9	606	CLA	ND
23	9	607	CLA	ND

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Mol	Chain	Res	Type	Atom
23	9	609	CLA	ND
23	9	610	CLA	ND
23	9	611	CLA	ND
23	9	612	CLA	ND
23	9	613	CLA	ND
23	9	614	CLA	ND

All (2598) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	801	CLA	CBD-CGD-O2D-CED
23	A	804	CLA	C1A-C2A-CAA-CBA
23	A	804	CLA	CHA-CBD-CGD-O1D
23	A	804	CLA	CHA-CBD-CGD-O2D
23	A	805	CLA	C3A-C2A-CAA-CBA
23	A	805	CLA	C3-C5-C6-C7
23	A	806	CLA	C1A-C2A-CAA-CBA
23	A	806	CLA	CHA-CBD-CGD-O1D
23	A	806	CLA	CHA-CBD-CGD-O2D
23	A	806	CLA	CAD-CBD-CGD-O1D
23	A	806	CLA	CAD-CBD-CGD-O2D
23	A	809	CLA	CHA-CBD-CGD-O1D
23	A	809	CLA	CHA-CBD-CGD-O2D
23	A	812	CLA	C4-C3-C5-C6
23	A	814	CLA	CHA-CBD-CGD-O1D
23	A	814	CLA	CHA-CBD-CGD-O2D
23	A	815	CLA	CHA-CBD-CGD-O1D
23	A	815	CLA	CHA-CBD-CGD-O2D
23	A	815	CLA	CAD-CBD-CGD-O1D
23	A	816	CLA	CHA-CBD-CGD-O2D
23	A	817	CLA	CHA-CBD-CGD-O1D
23	A	817	CLA	CHA-CBD-CGD-O2D
23	A	819	CLA	C1A-C2A-CAA-CBA
23	A	819	CLA	C3A-C2A-CAA-CBA
23	A	820	CLA	C1A-C2A-CAA-CBA
23	A	820	CLA	C3A-C2A-CAA-CBA
23	A	821	CLA	C1A-C2A-CAA-CBA
23	A	821	CLA	C3A-C2A-CAA-CBA
23	A	825	CLA	C1A-C2A-CAA-CBA
23	A	825	CLA	C3A-C2A-CAA-CBA
23	A	828	CLA	CHA-CBD-CGD-O1D
23	A	829	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	A	830	CLA	CHA-CBD-CGD-O1D
23	A	830	CLA	CHA-CBD-CGD-O2D
23	A	832	CLA	CHA-CBD-CGD-O1D
23	A	832	CLA	CHA-CBD-CGD-O2D
23	A	834	CLA	CBD-CGD-O2D-CED
23	A	836	CLA	C2-C3-C5-C6
23	A	836	CLA	C4-C3-C5-C6
23	A	837	CLA	C1A-C2A-CAA-CBA
23	A	837	CLA	C3A-C2A-CAA-CBA
23	A	837	CLA	CHA-CBD-CGD-O1D
23	A	837	CLA	CHA-CBD-CGD-O2D
23	A	841	CLA	CHA-CBD-CGD-O1D
23	A	841	CLA	CHA-CBD-CGD-O2D
23	A	842	CLA	C1A-C2A-CAA-CBA
23	A	842	CLA	C3A-C2A-CAA-CBA
23	A	845	CLA	CHA-CBD-CGD-O1D
23	A	845	CLA	CHA-CBD-CGD-O2D
23	B	802	CLA	CHA-CBD-CGD-O1D
23	B	802	CLA	CHA-CBD-CGD-O2D
23	B	802	CLA	CBD-CGD-O2D-CED
23	B	803	CLA	C3A-C2A-CAA-CBA
23	B	803	CLA	CBD-CGD-O2D-CED
23	B	805	CLA	C1A-C2A-CAA-CBA
23	B	805	CLA	C3A-C2A-CAA-CBA
23	B	805	CLA	CHA-CBD-CGD-O1D
23	B	805	CLA	CHA-CBD-CGD-O2D
23	B	805	CLA	CAD-CBD-CGD-O1D
23	B	806	CLA	CBD-CGD-O2D-CED
23	B	809	CLA	C2A-CAA-CBA-CGA
23	B	812	CLA	C1A-C2A-CAA-CBA
23	B	812	CLA	C3A-C2A-CAA-CBA
23	B	813	CLA	CBD-CGD-O2D-CED
23	B	814	CLA	C2A-CAA-CBA-CGA
23	B	818	CLA	C1A-C2A-CAA-CBA
23	B	818	CLA	C3A-C2A-CAA-CBA
23	B	818	CLA	C4-C3-C5-C6
23	B	821	CLA	CBA-CGA-O2A-C1
23	B	821	CLA	O1A-CGA-O2A-C1
23	B	822	CLA	C1A-C2A-CAA-CBA
23	B	822	CLA	C3A-C2A-CAA-CBA
23	B	823	CLA	C1A-C2A-CAA-CBA
23	B	826	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	826	CLA	CHA-CBD-CGD-O2D
23	B	826	CLA	CAD-CBD-CGD-O1D
23	B	827	CLA	C1A-C2A-CAA-CBA
23	B	827	CLA	C3A-C2A-CAA-CBA
23	B	833	CLA	C3A-C2A-CAA-CBA
23	B	833	CLA	C2-C3-C5-C6
23	B	833	CLA	C4-C3-C5-C6
23	B	835	CLA	CBD-CGD-O2D-CED
23	B	837	CLA	CHA-CBD-CGD-O1D
23	B	837	CLA	CHA-CBD-CGD-O2D
23	F	303	CLA	C1A-C2A-CAA-CBA
23	F	303	CLA	CBD-CGD-O2D-CED
23	F	304	CLA	CHA-CBD-CGD-O1D
23	F	304	CLA	CHA-CBD-CGD-O2D
23	F	304	CLA	CBD-CGD-O2D-CED
23	F	304	CLA	O1D-CGD-O2D-CED
23	J	101	CLA	C1A-C2A-CAA-CBA
23	J	101	CLA	CHA-CBD-CGD-O1D
23	J	101	CLA	CHA-CBD-CGD-O2D
23	J	101	CLA	CBD-CGD-O2D-CED
23	J	101	CLA	O1D-CGD-O2D-CED
23	K	204	CLA	CBA-CGA-O2A-C1
23	K	206	CLA	C2A-CAA-CBA-CGA
23	K	206	CLA	CHA-CBD-CGD-O1D
23	K	206	CLA	CHA-CBD-CGD-O2D
23	L	303	CLA	CHA-CBD-CGD-O1D
23	L	303	CLA	CHA-CBD-CGD-O2D
23	L	304	CLA	C1A-C2A-CAA-CBA
23	L	304	CLA	C3A-C2A-CAA-CBA
23	1	603	CLA	CHA-CBD-CGD-O2D
23	1	604	CLA	CHA-CBD-CGD-O1D
23	1	604	CLA	CHA-CBD-CGD-O2D
23	1	604	CLA	CAD-CBD-CGD-O1D
23	1	606	CLA	CBD-CGD-O2D-CED
23	1	609	CLA	CBD-CGD-O2D-CED
23	a	603	CLA	C1A-C2A-CAA-CBA
23	a	604	CLA	CHA-CBD-CGD-O1D
23	a	604	CLA	CHA-CBD-CGD-O2D
23	a	604	CLA	CAD-CBD-CGD-O1D
23	a	606	CLA	C1A-C2A-CAA-CBA
23	a	606	CLA	CBD-CGD-O2D-CED
23	a	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	a	609	CLA	C1A-C2A-CAA-CBA
23	a	609	CLA	C3A-C2A-CAA-CBA
23	a	614	CLA	C1A-C2A-CAA-CBA
23	a	614	CLA	CBD-CGD-O2D-CED
23	3	603	CLA	C3A-C2A-CAA-CBA
23	3	603	CLA	CBD-CGD-O2D-CED
23	3	608	CLA	C2A-CAA-CBA-CGA
23	3	609	CLA	C1A-C2A-CAA-CBA
23	3	609	CLA	C3A-C2A-CAA-CBA
23	3	610	CLA	C1A-C2A-CAA-CBA
23	3	610	CLA	C3A-C2A-CAA-CBA
23	3	610	CLA	C4-C3-C5-C6
23	3	611	CLA	CHA-CBD-CGD-O2D
23	3	612	CLA	CHA-CBD-CGD-O1D
23	3	612	CLA	CHA-CBD-CGD-O2D
23	3	615	CLA	C1A-C2A-CAA-CBA
23	4	601	CLA	C3A-C2A-CAA-CBA
23	4	606	CLA	C1A-C2A-CAA-CBA
23	4	606	CLA	C3A-C2A-CAA-CBA
23	4	608	CLA	CBD-CGD-O2D-CED
23	4	612	CLA	C1A-C2A-CAA-CBA
23	4	612	CLA	C3A-C2A-CAA-CBA
23	4	616	CLA	CHA-CBD-CGD-O1D
23	4	616	CLA	CHA-CBD-CGD-O2D
23	5	601	CLA	C1A-C2A-CAA-CBA
23	5	601	CLA	C3A-C2A-CAA-CBA
23	5	602	CLA	CHA-CBD-CGD-O1D
23	5	602	CLA	CHA-CBD-CGD-O2D
23	5	606	CLA	C1A-C2A-CAA-CBA
23	5	606	CLA	C3A-C2A-CAA-CBA
23	5	607	CLA	CBD-CGD-O2D-CED
23	5	608	CLA	C1A-C2A-CAA-CBA
23	5	608	CLA	C3A-C2A-CAA-CBA
23	5	608	CLA	CBD-CGD-O2D-CED
23	5	609	CLA	C1A-C2A-CAA-CBA
23	5	609	CLA	C3A-C2A-CAA-CBA
23	5	611	CLA	C1A-C2A-CAA-CBA
23	5	612	CLA	C1A-C2A-CAA-CBA
23	5	612	CLA	C3A-C2A-CAA-CBA
23	5	614	CLA	C1A-C2A-CAA-CBA
23	5	614	CLA	C3A-C2A-CAA-CBA
23	5	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	5	614	CLA	O1D-CGD-O2D-CED
23	5	618	CLA	C1A-C2A-CAA-CBA
23	5	619	CLA	C1A-C2A-CAA-CBA
23	6	604	CLA	CHA-CBD-CGD-O1D
23	6	604	CLA	CHA-CBD-CGD-O2D
23	6	607	CLA	C1A-C2A-CAA-CBA
23	6	607	CLA	C3A-C2A-CAA-CBA
23	6	608	CLA	CBD-CGD-O2D-CED
23	6	609	CLA	C1A-C2A-CAA-CBA
23	6	609	CLA	C3A-C2A-CAA-CBA
23	6	610	CLA	CBD-CGD-O2D-CED
23	6	611	CLA	C1A-C2A-CAA-CBA
23	6	612	CLA	C1A-C2A-CAA-CBA
23	6	612	CLA	C3A-C2A-CAA-CBA
23	6	616	CLA	CHA-CBD-CGD-O1D
23	6	616	CLA	CHA-CBD-CGD-O2D
23	6	618	CLA	C1A-C2A-CAA-CBA
23	6	618	CLA	C3A-C2A-CAA-CBA
23	6	620	CLA	C3-C5-C6-C7
23	7	601	CLA	CHA-CBD-CGD-O1D
23	7	601	CLA	CHA-CBD-CGD-O2D
23	7	601	CLA	CAD-CBD-CGD-O1D
23	7	601	CLA	C6-C7-C8-C9
23	7	603	CLA	CHA-CBD-CGD-O2D
23	7	604	CLA	CHA-CBD-CGD-O1D
23	7	604	CLA	CHA-CBD-CGD-O2D
23	7	606	CLA	C1A-C2A-CAA-CBA
23	7	606	CLA	C3A-C2A-CAA-CBA
23	7	607	CLA	C1A-C2A-CAA-CBA
23	7	607	CLA	C3A-C2A-CAA-CBA
23	7	607	CLA	CHA-CBD-CGD-O1D
23	7	609	CLA	C1A-C2A-CAA-CBA
23	7	609	CLA	C3A-C2A-CAA-CBA
23	7	613	CLA	CHA-CBD-CGD-O1D
23	7	613	CLA	CHA-CBD-CGD-O2D
23	7	614	CLA	C1A-C2A-CAA-CBA
23	7	616	CLA	CHA-CBD-CGD-O1D
23	7	616	CLA	CHA-CBD-CGD-O2D
23	7	616	CLA	CBD-CGD-O2D-CED
23	8	601	CLA	CHA-CBD-CGD-O1D
23	8	601	CLA	CHA-CBD-CGD-O2D
23	8	601	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	8	602	CLA	CBD-CGD-O2D-CED
23	8	604	CLA	C1A-C2A-CAA-CBA
23	8	608	CLA	CBD-CGD-O2D-CED
23	8	609	CLA	C1A-C2A-CAA-CBA
23	8	609	CLA	C3A-C2A-CAA-CBA
23	8	611	CLA	C1A-C2A-CAA-CBA
23	8	612	CLA	C1A-C2A-CAA-CBA
23	8	613	CLA	C2-C3-C5-C6
23	8	613	CLA	C4-C3-C5-C6
23	8	614	CLA	CHA-CBD-CGD-O1D
23	8	614	CLA	CHA-CBD-CGD-O2D
23	8	616	CLA	C1A-C2A-CAA-CBA
23	8	616	CLA	CAD-CBD-CGD-O1D
23	8	616	CLA	CAD-CBD-CGD-O2D
24	B	842	PQN	C11-C12-C13-C14
24	B	842	PQN	C19-C18-C20-C21
25	A	846	LHG	C3-O3-P-O4
25	A	846	LHG	O7-C5-C6-O8
25	B	851	LHG	O1-C1-C2-C3
25	B	851	LHG	C4-O6-P-O5
25	1	620	LHG	C3-O3-P-O4
25	a	620	LHG	C3-O3-P-O4
25	3	623	LHG	C3-O3-P-O4
25	3	623	LHG	C3-O3-P-O6
25	3	623	LHG	O9-C7-O7-C5
25	3	624	LHG	O1-C1-C2-O2
25	3	624	LHG	O1-C1-C2-C3
25	3	624	LHG	C4-O6-P-O4
25	3	624	LHG	C8-C7-O7-C5
25	3	624	LHG	O10-C23-O8-C6
25	3	624	LHG	C24-C23-O8-C6
25	4	622	LHG	O1-C1-C2-C3
25	5	623	LHG	C4-O6-P-O5
25	5	623	LHG	O7-C5-C6-O8
25	5	625	LHG	C3-O3-P-O4
25	5	625	LHG	C4-O6-P-O3
25	5	625	LHG	C4-O6-P-O4
25	7	622	LHG	O2-C2-C3-O3
25	7	622	LHG	C3-O3-P-O6
25	7	622	LHG	C4-O6-P-O5
25	8	622	LHG	O1-C1-C2-C3
25	8	622	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	8	622	LHG	C3-O3-P-O4
25	8	623	LHG	O1-C1-C2-C3
25	8	623	LHG	C3-O3-P-O5
25	2	622	LHG	O1-C1-C2-O2
25	2	622	LHG	O1-C1-C2-C3
25	2	622	LHG	C8-C7-O7-C5
25	9	622	LHG	O1-C1-C2-O2
26	A	848	BCR	C21-C22-C23-C24
26	A	848	BCR	C37-C22-C23-C24
26	A	849	BCR	C21-C22-C23-C24
26	A	849	BCR	C37-C22-C23-C24
26	A	851	BCR	C21-C22-C23-C24
26	A	851	BCR	C37-C22-C23-C24
26	A	852	BCR	C17-C18-C19-C20
26	A	852	BCR	C36-C18-C19-C20
26	A	852	BCR	C21-C22-C23-C24
26	A	852	BCR	C37-C22-C23-C24
26	A	856	BCR	C21-C22-C23-C24
26	A	856	BCR	C37-C22-C23-C24
26	B	801	BCR	C7-C8-C9-C34
26	B	843	BCR	C1-C6-C7-C8
26	B	843	BCR	C5-C6-C7-C8
26	B	843	BCR	C7-C8-C9-C10
26	B	843	BCR	C7-C8-C9-C34
26	B	843	BCR	C36-C18-C19-C20
26	B	843	BCR	C21-C22-C23-C24
26	B	843	BCR	C37-C22-C23-C24
26	B	844	BCR	C21-C22-C23-C24
26	B	844	BCR	C37-C22-C23-C24
26	B	846	BCR	C21-C22-C23-C24
26	B	846	BCR	C37-C22-C23-C24
26	B	848	BCR	C21-C22-C23-C24
26	B	848	BCR	C37-C22-C23-C24
26	J	102	BCR	C17-C18-C19-C20
26	J	102	BCR	C36-C18-C19-C20
26	K	202	BCR	C37-C22-C23-C24
26	L	301	BCR	C11-C12-C13-C14
26	L	301	BCR	C11-C12-C13-C35
26	L	305	BCR	C1-C6-C7-C8
26	1	619	BCR	C11-C12-C13-C14
26	1	619	BCR	C11-C12-C13-C35
26	a	619	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	a	619	BCR	C11-C12-C13-C35
26	3	621	BCR	C23-C24-C25-C30
26	3	622	BCR	C1-C6-C7-C8
26	3	622	BCR	C5-C6-C7-C8
26	3	622	BCR	C21-C22-C23-C24
26	3	622	BCR	C37-C22-C23-C24
26	6	622	BCR	C7-C8-C9-C10
26	6	622	BCR	C7-C8-C9-C34
26	6	622	BCR	C11-C12-C13-C14
26	6	622	BCR	C11-C12-C13-C35
26	8	621	BCR	C7-C8-C9-C10
26	8	621	BCR	C7-C8-C9-C34
28	A	857	LMU	O5'-C1'-O1'-C1
28	A	859	LMU	C2'-C1'-O1'-C1
28	A	859	LMU	O5'-C1'-O1'-C1
28	5	628	LMU	O5'-C1'-O1'-C1
28	8	624	LMU	C2-C1-O1'-C1'
29	J	104	LMG	C11-C10-O7-C8
29	7	624	LMG	C11-C10-O7-C8
30	B	850	DGD	C2B-C1B-O2G-C2G
30	B	850	DGD	O1B-C1B-O2G-C2G
30	J	103	DGD	O6E-C1E-O5D-C6D
31	4	619	LUT	C1-C6-C7-C8
31	6	619	LUT	C1-C6-C7-C8
31	2	619	LUT	C31-C32-C33-C34
31	2	619	LUT	C31-C32-C33-C40
32	5	621	XAT	C27-C28-C29-C30
32	5	621	XAT	C27-C28-C29-C39
32	8	620	XAT	C27-C28-C29-C39
33	6	624	NEX	C27-C28-C29-C30
33	6	624	NEX	C27-C28-C29-C39
23	A	801	CLA	O1D-CGD-O2D-CED
23	F	303	CLA	O1D-CGD-O2D-CED
23	1	609	CLA	O1D-CGD-O2D-CED
23	a	607	CLA	O1D-CGD-O2D-CED
23	7	604	CLA	O1D-CGD-O2D-CED
23	7	616	CLA	O1D-CGD-O2D-CED
23	8	611	CLA	O1D-CGD-O2D-CED
23	A	811	CLA	O1D-CGD-O2D-CED
23	A	817	CLA	O1D-CGD-O2D-CED
23	B	803	CLA	O1D-CGD-O2D-CED
23	B	835	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	5	607	CLA	O1D-CGD-O2D-CED
23	8	608	CLA	O1D-CGD-O2D-CED
23	A	811	CLA	CBD-CGD-O2D-CED
23	A	817	CLA	CBD-CGD-O2D-CED
23	A	825	CLA	CBD-CGD-O2D-CED
23	A	836	CLA	CBD-CGD-O2D-CED
23	A	854	CLA	CBD-CGD-O2D-CED
23	B	810	CLA	CBD-CGD-O2D-CED
23	B	812	CLA	CBD-CGD-O2D-CED
23	B	814	CLA	CBD-CGD-O2D-CED
23	B	815	CLA	CBD-CGD-O2D-CED
23	B	816	CLA	CBD-CGD-O2D-CED
23	B	819	CLA	CBD-CGD-O2D-CED
23	B	822	CLA	CBD-CGD-O2D-CED
23	B	823	CLA	CBD-CGD-O2D-CED
23	B	834	CLA	CBD-CGD-O2D-CED
23	G	204	CLA	CBD-CGD-O2D-CED
23	K	204	CLA	CBD-CGD-O2D-CED
23	1	602	CLA	CBD-CGD-O2D-CED
23	1	604	CLA	CBD-CGD-O2D-CED
23	1	612	CLA	CBD-CGD-O2D-CED
23	a	602	CLA	CBD-CGD-O2D-CED
23	a	604	CLA	CBD-CGD-O2D-CED
23	a	612	CLA	CBD-CGD-O2D-CED
23	4	607	CLA	CBD-CGD-O2D-CED
23	4	611	CLA	CBD-CGD-O2D-CED
23	4	613	CLA	CBD-CGD-O2D-CED
23	6	604	CLA	CBD-CGD-O2D-CED
23	6	607	CLA	CBD-CGD-O2D-CED
23	7	602	CLA	CBD-CGD-O2D-CED
23	7	604	CLA	CBD-CGD-O2D-CED
23	7	607	CLA	CBD-CGD-O2D-CED
23	7	608	CLA	CBD-CGD-O2D-CED
23	7	612	CLA	CBD-CGD-O2D-CED
23	8	603	CLA	CBD-CGD-O2D-CED
23	8	611	CLA	CBD-CGD-O2D-CED
23	8	616	CLA	CBD-CGD-O2D-CED
25	B	851	LHG	O10-C23-O8-C6
25	9	622	LHG	O10-C23-O8-C6
29	4	624	LMG	O10-C28-O8-C9
23	K	204	CLA	O1A-CGA-O2A-C1
23	A	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	G	204	CLA	O1D-CGD-O2D-CED
23	6	607	CLA	O1D-CGD-O2D-CED
23	7	608	CLA	O1D-CGD-O2D-CED
23	8	616	CLA	O1D-CGD-O2D-CED
28	K	208	LMU	O5B-C1B-O1B-C4'
28	8	624	LMU	O5B-C1B-O1B-C4'
23	A	834	CLA	O1D-CGD-O2D-CED
23	B	802	CLA	O1D-CGD-O2D-CED
23	B	813	CLA	O1D-CGD-O2D-CED
23	7	607	CLA	O1D-CGD-O2D-CED
23	8	602	CLA	O1D-CGD-O2D-CED
23	5	603	CLA	CBA-CGA-O2A-C1
25	9	622	LHG	C24-C23-O8-C6
29	J	104	LMG	C29-C28-O8-C9
23	A	814	CLA	CBD-CGD-O2D-CED
23	A	815	CLA	CBD-CGD-O2D-CED
23	A	822	CLA	CBD-CGD-O2D-CED
23	A	835	CLA	CBD-CGD-O2D-CED
23	A	840	CLA	CBD-CGD-O2D-CED
23	B	804	CLA	CBD-CGD-O2D-CED
23	B	809	CLA	CBD-CGD-O2D-CED
23	B	829	CLA	CBD-CGD-O2D-CED
23	B	831	CLA	CBD-CGD-O2D-CED
23	B	833	CLA	CBD-CGD-O2D-CED
23	B	840	CLA	CBD-CGD-O2D-CED
23	F	301	CLA	CBD-CGD-O2D-CED
23	G	203	CLA	CBD-CGD-O2D-CED
23	1	611	CLA	CBD-CGD-O2D-CED
23	3	602	CLA	CBD-CGD-O2D-CED
23	3	609	CLA	CBD-CGD-O2D-CED
23	4	601	CLA	CBD-CGD-O2D-CED
23	4	602	CLA	CBD-CGD-O2D-CED
23	4	603	CLA	CBD-CGD-O2D-CED
23	5	604	CLA	CBD-CGD-O2D-CED
23	5	613	CLA	CBD-CGD-O2D-CED
23	5	617	CLA	CBD-CGD-O2D-CED
23	6	602	CLA	CBD-CGD-O2D-CED
23	6	614	CLA	CBD-CGD-O2D-CED
23	7	613	CLA	CBD-CGD-O2D-CED
23	7	614	CLA	CBD-CGD-O2D-CED
23	a	614	CLA	O1A-CGA-O2A-C1
23	4	609	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	5	603	CLA	O1A-CGA-O2A-C1
23	5	607	CLA	O1A-CGA-O2A-C1
23	6	614	CLA	O1A-CGA-O2A-C1
23	7	604	CLA	O1A-CGA-O2A-C1
23	8	604	CLA	O1A-CGA-O2A-C1
23	8	613	CLA	O1A-CGA-O2A-C1
29	J	104	LMG	O10-C28-O8-C9
23	5	608	CLA	O1D-CGD-O2D-CED
23	B	806	CLA	O1D-CGD-O2D-CED
23	B	816	CLA	O1D-CGD-O2D-CED
23	a	614	CLA	O1D-CGD-O2D-CED
23	4	608	CLA	O1D-CGD-O2D-CED
23	6	610	CLA	O1D-CGD-O2D-CED
23	B	824	CLA	CBD-CGD-O2D-CED
23	B	832	CLA	CBD-CGD-O2D-CED
23	L	304	CLA	CBD-CGD-O2D-CED
23	3	603	CLA	O1D-CGD-O2D-CED
23	4	611	CLA	O1D-CGD-O2D-CED
23	6	608	CLA	O1D-CGD-O2D-CED
25	5	625	LHG	O9-C7-O7-C5
25	2	622	LHG	O9-C7-O7-C5
29	J	104	LMG	O9-C10-O7-C8
29	7	624	LMG	O9-C10-O7-C8
23	A	802	CLA	C3-C5-C6-C7
23	A	807	CLA	C3-C5-C6-C7
23	A	834	CLA	C3-C5-C6-C7
23	A	836	CLA	C3-C5-C6-C7
23	B	827	CLA	C3-C5-C6-C7
23	B	832	CLA	C3-C5-C6-C7
23	1	611	CLA	C3-C5-C6-C7
23	3	607	CLA	C3-C5-C6-C7
23	3	608	CLA	C3-C5-C6-C7
23	4	604	CLA	C3-C5-C6-C7
23	5	603	CLA	C3-C5-C6-C7
23	5	607	CLA	C3-C5-C6-C7
23	7	601	CLA	C3-C5-C6-C7
23	7	602	CLA	C3-C5-C6-C7
23	7	610	CLA	C3-C5-C6-C7
23	7	613	CLA	C3-C5-C6-C7
24	A	844	PQN	C13-C15-C16-C17
23	4	609	CLA	CBA-CGA-O2A-C1
23	7	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	8	604	CLA	CBA-CGA-O2A-C1
23	8	613	CLA	CBA-CGA-O2A-C1
25	2	622	LHG	C24-C23-O8-C6
29	4	624	LMG	C29-C28-O8-C9
25	5	625	LHG	C8-C7-O7-C5
23	4	607	CLA	O1D-CGD-O2D-CED
23	A	827	CLA	CBD-CGD-O2D-CED
23	3	604	CLA	CBD-CGD-O2D-CED
23	8	613	CLA	CBD-CGD-O2D-CED
23	A	834	CLA	O1A-CGA-O2A-C1
23	A	839	CLA	O1A-CGA-O2A-C1
29	7	624	LMG	O6-C5-C6-O5
28	K	208	LMU	O5'-C5'-C6'-O6'
23	A	818	CLA	C4-C3-C5-C6
23	A	830	CLA	C4-C3-C5-C6
23	A	812	CLA	C2-C3-C5-C6
23	B	818	CLA	C2-C3-C5-C6
23	3	610	CLA	C2-C3-C5-C6
23	B	827	CLA	CBD-CGD-O2D-CED
23	3	608	CLA	CBD-CGD-O2D-CED
23	A	814	CLA	C2A-CAA-CBA-CGA
23	A	825	CLA	C2A-CAA-CBA-CGA
23	A	837	CLA	C2A-CAA-CBA-CGA
23	A	854	CLA	C2A-CAA-CBA-CGA
23	B	819	CLA	C2A-CAA-CBA-CGA
23	B	829	CLA	C2A-CAA-CBA-CGA
23	B	831	CLA	C2A-CAA-CBA-CGA
23	B	839	CLA	C2A-CAA-CBA-CGA
23	4	601	CLA	C2A-CAA-CBA-CGA
23	4	607	CLA	C2A-CAA-CBA-CGA
23	5	604	CLA	C2A-CAA-CBA-CGA
23	6	620	CLA	C2A-CAA-CBA-CGA
23	8	603	CLA	C2A-CAA-CBA-CGA
23	3	610	CLA	O1A-CGA-O2A-C1
23	1	602	CLA	O1D-CGD-O2D-CED
23	a	602	CLA	O1D-CGD-O2D-CED
23	6	604	CLA	O1D-CGD-O2D-CED
23	A	825	CLA	C3-C5-C6-C7
23	B	819	CLA	C3-C5-C6-C7
23	B	834	CLA	C3-C5-C6-C7
23	1	603	CLA	C3-C5-C6-C7
23	a	609	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	3	603	CLA	C3-C5-C6-C7
23	3	606	CLA	C3-C5-C6-C7
23	4	601	CLA	C3-C5-C6-C7
23	A	814	CLA	CBA-CGA-O2A-C1
23	A	820	CLA	CBA-CGA-O2A-C1
23	B	820	CLA	CBA-CGA-O2A-C1
23	a	614	CLA	CBA-CGA-O2A-C1
23	3	603	CLA	CBA-CGA-O2A-C1
23	5	607	CLA	CBA-CGA-O2A-C1
23	6	614	CLA	CBA-CGA-O2A-C1
25	B	851	LHG	C24-C23-O8-C6
25	7	622	LHG	C24-C23-O8-C6
28	A	859	LMU	O5B-C5B-C6B-O6B
28	5	628	LMU	O5B-C5B-C6B-O6B
28	8	625	LMU	C3'-C4'-O1B-C1B
23	B	834	CLA	O1D-CGD-O2D-CED
23	K	204	CLA	O1D-CGD-O2D-CED
23	a	612	CLA	O1D-CGD-O2D-CED
24	A	844	PQN	C11-C12-C13-C14
23	K	206	CLA	CBD-CGD-O2D-CED
23	B	815	CLA	O1D-CGD-O2D-CED
23	1	612	CLA	O1D-CGD-O2D-CED
23	A	820	CLA	O1A-CGA-O2A-C1
23	A	822	CLA	O1A-CGA-O2A-C1
23	B	820	CLA	O1A-CGA-O2A-C1
23	1	604	CLA	O1A-CGA-O2A-C1
23	a	604	CLA	O1A-CGA-O2A-C1
25	7	622	LHG	O10-C23-O8-C6
29	5	626	LMG	O10-C28-O8-C9
23	A	854	CLA	O1D-CGD-O2D-CED
23	B	823	CLA	O1D-CGD-O2D-CED
23	B	803	CLA	C2C-C3C-CAC-CBC
23	A	823	CLA	CBD-CGD-O2D-CED
23	A	832	CLA	CBD-CGD-O2D-CED
23	A	841	CLA	CBD-CGD-O2D-CED
23	B	818	CLA	CBD-CGD-O2D-CED
23	B	836	CLA	CBD-CGD-O2D-CED
23	B	837	CLA	CBD-CGD-O2D-CED
23	5	603	CLA	CBD-CGD-O2D-CED
23	6	601	CLA	CBD-CGD-O2D-CED
23	6	616	CLA	CBD-CGD-O2D-CED
23	6	617	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	8	606	CLA	CBD-CGD-O2D-CED
23	B	810	CLA	O1D-CGD-O2D-CED
23	4	613	CLA	O1D-CGD-O2D-CED
30	J	103	DGD	O6D-C5D-C6D-O5D
25	A	846	LHG	O2-C2-C3-O3
25	B	851	LHG	O2-C2-C3-O3
23	A	818	CLA	C3-C5-C6-C7
23	A	854	CLA	C3-C5-C6-C7
23	B	806	CLA	C3-C5-C6-C7
23	8	601	CLA	C3-C5-C6-C7
23	8	606	CLA	C3-C5-C6-C7
23	A	801	CLA	CBA-CGA-O2A-C1
23	A	818	CLA	CBA-CGA-O2A-C1
23	A	822	CLA	CBA-CGA-O2A-C1
23	A	834	CLA	CBA-CGA-O2A-C1
23	A	839	CLA	CBA-CGA-O2A-C1
23	3	610	CLA	CBA-CGA-O2A-C1
23	4	604	CLA	CBA-CGA-O2A-C1
23	4	614	CLA	CBA-CGA-O2A-C1
25	B	851	LHG	C28-C29-C30-C31
23	B	818	CLA	O1A-CGA-O2A-C1
23	B	831	CLA	O1A-CGA-O2A-C1
25	2	622	LHG	O10-C23-O8-C6
23	B	814	CLA	O1D-CGD-O2D-CED
23	B	819	CLA	O1D-CGD-O2D-CED
29	5	626	LMG	C11-C10-O7-C8
23	B	822	CLA	O1D-CGD-O2D-CED
23	A	837	CLA	CBD-CGD-O2D-CED
23	A	845	CLA	CBD-CGD-O2D-CED
23	4	609	CLA	CBD-CGD-O2D-CED
28	A	857	LMU	O5B-C5B-C6B-O6B
29	5	627	LMG	O6-C5-C6-O5
28	5	628	LMU	C4B-C5B-C6B-O6B
28	8	625	LMU	O5'-C5'-C6'-O6'
23	B	812	CLA	O1D-CGD-O2D-CED
23	8	603	CLA	O1D-CGD-O2D-CED
23	8	607	CLA	CBD-CGD-O2D-CED
23	B	805	CLA	C3-C5-C6-C7
23	B	818	CLA	CBA-CGA-O2A-C1
23	B	831	CLA	CBA-CGA-O2A-C1
23	1	604	CLA	CBA-CGA-O2A-C1
23	a	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	836	CLA	O1D-CGD-O2D-CED
23	7	612	CLA	O1D-CGD-O2D-CED
28	A	859	LMU	O5'-C5'-C6'-O6'
29	A	860	LMG	O6-C5-C6-O5
28	A	858	LMU	C5'-C4'-O1B-C1B
28	A	859	LMU	C3'-C4'-O1B-C1B
25	3	623	LHG	C2-C3-O3-P
23	A	801	CLA	O1A-CGA-O2A-C1
23	A	814	CLA	O1A-CGA-O2A-C1
23	A	818	CLA	O1A-CGA-O2A-C1
23	4	604	CLA	O1A-CGA-O2A-C1
23	A	854	CLA	C4-C3-C5-C6
23	B	811	CLA	C4-C3-C5-C6
23	8	610	CLA	C4-C3-C5-C6
29	7	624	LMG	C4-C5-C6-O5
23	A	830	CLA	C2-C3-C5-C6
23	A	854	CLA	C2-C3-C5-C6
23	B	811	CLA	C2-C3-C5-C6
23	8	610	CLA	C2-C3-C5-C6
23	A	819	CLA	C2A-CAA-CBA-CGA
23	A	821	CLA	C2A-CAA-CBA-CGA
23	A	843	CLA	C2A-CAA-CBA-CGA
23	3	609	CLA	C2A-CAA-CBA-CGA
23	a	604	CLA	O1D-CGD-O2D-CED
23	3	603	CLA	O1A-CGA-O2A-C1
28	K	208	LMU	O5'-C1'-O1'-C1
29	J	104	LMG	O6-C1-O1-C7
23	1	604	CLA	O1D-CGD-O2D-CED
23	A	830	CLA	CBA-CGA-O2A-C1
23	B	819	CLA	CBA-CGA-O2A-C1
23	4	601	CLA	CBA-CGA-O2A-C1
28	A	859	LMU	C4B-C5B-C6B-O6B
28	K	208	LMU	C4'-C5'-C6'-O6'
23	A	825	CLA	O1D-CGD-O2D-CED
23	3	602	CLA	O1D-CGD-O2D-CED
23	4	601	CLA	O1D-CGD-O2D-CED
23	7	602	CLA	O1D-CGD-O2D-CED
23	4	614	CLA	O1A-CGA-O2A-C1
29	5	627	LMG	C4-C5-C6-O5
23	A	822	CLA	O1D-CGD-O2D-CED
23	F	301	CLA	O1D-CGD-O2D-CED
23	1	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	7	613	CLA	O1D-CGD-O2D-CED
23	A	835	CLA	O1D-CGD-O2D-CED
23	B	809	CLA	O1D-CGD-O2D-CED
25	3	624	LHG	O9-C7-O7-C5
28	A	857	LMU	C4'-C5'-C6'-O6'
28	8	625	LMU	C4'-C5'-C6'-O6'
23	B	802	CLA	O1A-CGA-O2A-C1
23	A	821	CLA	C3-C5-C6-C7
23	B	808	CLA	C3-C5-C6-C7
23	5	613	CLA	O1D-CGD-O2D-CED
23	A	821	CLA	CBA-CGA-O2A-C1
23	A	835	CLA	CBA-CGA-O2A-C1
23	A	843	CLA	CBA-CGA-O2A-C1
23	B	802	CLA	CBA-CGA-O2A-C1
23	B	811	CLA	CBA-CGA-O2A-C1
23	B	813	CLA	CBA-CGA-O2A-C1
23	B	837	CLA	CBA-CGA-O2A-C1
23	1	613	CLA	CBA-CGA-O2A-C1
23	a	613	CLA	CBA-CGA-O2A-C1
23	3	607	CLA	CBA-CGA-O2A-C1
23	6	604	CLA	CBA-CGA-O2A-C1
23	6	608	CLA	CBA-CGA-O2A-C1
23	7	613	CLA	CBA-CGA-O2A-C1
29	5	626	LMG	C29-C28-O8-C9
29	5	627	LMG	C29-C28-O8-C9
23	A	831	CLA	CBD-CGD-O2D-CED
23	B	839	CLA	CBD-CGD-O2D-CED
29	A	860	LMG	C4-C5-C6-O5
30	J	103	DGD	C4D-C5D-C6D-O5D
23	4	603	CLA	O1D-CGD-O2D-CED
23	A	812	CLA	C5-C6-C7-C8
23	B	813	CLA	C5-C6-C7-C8
23	B	824	CLA	C13-C15-C16-C17
23	B	816	CLA	C2A-CAA-CBA-CGA
29	4	624	LMG	O6-C5-C6-O5
28	A	857	LMU	C4B-C5B-C6B-O6B
23	A	806	CLA	C15-C16-C17-C18
23	A	842	CLA	C15-C16-C17-C18
23	B	808	CLA	C5-C6-C7-C8
23	B	816	CLA	C5-C6-C7-C8
25	5	623	LHG	O2-C2-C3-O3
29	J	104	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	7	624	LMG	C2-C1-O1-C7
25	8	622	LHG	O7-C5-C6-O8
29	J	104	LMG	O1-C7-C8-O7
23	1	613	CLA	O1A-CGA-O2A-C1
23	a	613	CLA	O1A-CGA-O2A-C1
28	A	859	LMU	C4'-C5'-C6'-O6'
28	8	625	LMU	C4B-C5B-C6B-O6B
23	A	807	CLA	C11-C10-C8-C9
23	A	828	CLA	C6-C7-C8-C9
23	B	810	CLA	C11-C12-C13-C14
23	B	828	CLA	C14-C13-C15-C16
23	B	829	CLA	C14-C13-C15-C16
23	a	610	CLA	C6-C7-C8-C9
23	5	604	CLA	C6-C7-C8-C9
23	6	604	CLA	C14-C13-C15-C16
23	7	601	CLA	C11-C10-C8-C9
23	7	611	CLA	C11-C10-C8-C9
23	7	613	CLA	C11-C10-C8-C9
23	8	601	CLA	C6-C7-C8-C9
23	6	614	CLA	O1D-CGD-O2D-CED
23	A	812	CLA	C13-C15-C16-C17
23	A	843	CLA	C13-C15-C16-C17
23	B	808	CLA	C15-C16-C17-C18
23	1	616	CLA	C2A-CAA-CBA-CGA
23	a	616	CLA	C2A-CAA-CBA-CGA
26	A	852	BCR	C7-C8-C9-C34
26	B	801	BCR	C37-C22-C23-C24
26	J	102	BCR	C11-C12-C13-C35
26	K	202	BCR	C7-C8-C9-C34
26	L	305	BCR	C7-C8-C9-C34
26	L	305	BCR	C37-C22-C23-C24
26	3	620	BCR	C37-C22-C23-C24
31	4	619	LUT	C31-C32-C33-C40
31	7	619	LUT	C27-C28-C29-C39
26	K	202	BCR	C21-C22-C23-C24
26	L	305	BCR	C7-C8-C9-C10
26	L	305	BCR	C21-C22-C23-C24
26	3	620	BCR	C21-C22-C23-C24
29	A	860	LMG	C11-C10-O7-C8
30	J	103	DGD	C4E-C5E-C6E-O5E
25	A	847	LHG	C23-C24-C25-C26
29	J	104	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
23	A	821	CLA	O1A-CGA-O2A-C1
29	5	627	LMG	O10-C28-O8-C9
23	A	834	CLA	C15-C16-C17-C18
23	B	806	CLA	C5-C6-C7-C8
23	B	809	CLA	C5-C6-C7-C8
23	4	604	CLA	C5-C6-C7-C8
23	5	602	CLA	C10-C11-C12-C13
23	5	607	CLA	C15-C16-C17-C18
23	6	613	CLA	C5-C6-C7-C8
24	A	844	PQN	C18-C20-C21-C22
23	B	833	CLA	O1D-CGD-O2D-CED
23	A	832	CLA	CBA-CGA-O2A-C1
23	4	613	CLA	CBA-CGA-O2A-C1
25	8	623	LHG	C24-C23-O8-C6
23	A	825	CLA	C15-C16-C17-C18
23	A	829	CLA	C5-C6-C7-C8
23	A	831	CLA	C5-C6-C7-C8
23	B	809	CLA	C13-C15-C16-C17
23	B	810	CLA	C8-C10-C11-C12
23	B	824	CLA	C5-C6-C7-C8
23	B	840	CLA	C13-C15-C16-C17
23	1	611	CLA	C15-C16-C17-C18
23	a	609	CLA	C8-C10-C11-C12
23	a	610	CLA	C5-C6-C7-C8
23	3	609	CLA	C5-C6-C7-C8
23	3	609	CLA	C8-C10-C11-C12
23	5	602	CLA	C8-C10-C11-C12
23	5	613	CLA	C13-C15-C16-C17
23	6	601	CLA	C5-C6-C7-C8
23	A	815	CLA	O1D-CGD-O2D-CED
23	B	840	CLA	O1D-CGD-O2D-CED
23	5	604	CLA	O1D-CGD-O2D-CED
23	A	843	CLA	O1A-CGA-O2A-C1
23	A	803	CLA	C15-C16-C17-C18
23	B	818	CLA	C8-C10-C11-C12
23	B	833	CLA	C5-C6-C7-C8
23	B	837	CLA	C15-C16-C17-C18
23	K	203	CLA	C15-C16-C17-C18
23	1	601	CLA	C5-C6-C7-C8
23	a	601	CLA	C5-C6-C7-C8
23	4	613	CLA	C15-C16-C17-C18
23	5	609	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	6	604	CLA	C5-C6-C7-C8
23	6	613	CLA	C15-C16-C17-C18
23	8	606	CLA	C10-C11-C12-C13
23	A	814	CLA	O1D-CGD-O2D-CED
23	B	804	CLA	O1D-CGD-O2D-CED
23	B	831	CLA	O1D-CGD-O2D-CED
23	G	203	CLA	O1D-CGD-O2D-CED
23	3	609	CLA	O1D-CGD-O2D-CED
25	7	622	LHG	C23-C24-C25-C26
25	2	622	LHG	C23-C24-C25-C26
29	A	860	LMG	C10-C11-C12-C13
29	7	624	LMG	C10-C11-C12-C13
28	A	857	LMU	O5'-C5'-C6'-O6'
23	B	829	CLA	O1D-CGD-O2D-CED
23	A	806	CLA	C5-C6-C7-C8
23	A	834	CLA	C5-C6-C7-C8
23	B	802	CLA	C15-C16-C17-C18
23	B	805	CLA	C13-C15-C16-C17
23	B	814	CLA	C5-C6-C7-C8
23	B	818	CLA	C5-C6-C7-C8
23	3	604	CLA	C10-C11-C12-C13
23	3	604	CLA	C13-C15-C16-C17
23	4	601	CLA	C13-C15-C16-C17
23	7	614	CLA	O1D-CGD-O2D-CED
23	A	802	CLA	C15-C16-C17-C18
23	B	827	CLA	C10-C11-C12-C13
23	1	611	CLA	C8-C10-C11-C12
23	3	607	CLA	C5-C6-C7-C8
23	A	838	CLA	CBD-CGD-O2D-CED
23	B	827	CLA	C13-C15-C16-C17
23	3	607	CLA	C8-C10-C11-C12
23	A	840	CLA	C3-C5-C6-C7
23	A	842	CLA	C13-C15-C16-C17
23	B	833	CLA	C15-C16-C17-C18
23	5	604	CLA	C13-C15-C16-C17
23	6	620	CLA	C8-C10-C11-C12
23	A	825	CLA	C6-C7-C8-C10
23	A	826	CLA	C11-C10-C8-C7
23	B	802	CLA	C12-C13-C15-C16
23	B	805	CLA	C11-C12-C13-C15
23	4	609	CLA	C6-C7-C8-C10
23	6	616	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	8	613	CLA	C11-C10-C8-C7
23	B	811	CLA	C3-C5-C6-C7
23	F	301	CLA	C3-C5-C6-C7
23	B	811	CLA	O1A-CGA-O2A-C1
23	3	607	CLA	O1A-CGA-O2A-C1
23	6	616	CLA	CBA-CGA-O2A-C1
23	A	833	CLA	C2A-CAA-CBA-CGA
23	A	834	CLA	C2A-CAA-CBA-CGA
23	B	821	CLA	C2A-CAA-CBA-CGA
23	1	601	CLA	C2A-CAA-CBA-CGA
23	a	601	CLA	C2A-CAA-CBA-CGA
23	3	607	CLA	C2A-CAA-CBA-CGA
23	A	840	CLA	O1D-CGD-O2D-CED
23	B	832	CLA	O1D-CGD-O2D-CED
23	L	304	CLA	O1D-CGD-O2D-CED
23	5	617	CLA	O1D-CGD-O2D-CED
23	6	602	CLA	O1D-CGD-O2D-CED
23	A	804	CLA	C8-C10-C11-C12
23	A	841	CLA	C5-C6-C7-C8
23	B	802	CLA	C10-C11-C12-C13
23	B	814	CLA	C10-C11-C12-C13
23	B	828	CLA	C10-C11-C12-C13
23	1	603	CLA	C5-C6-C7-C8
23	4	610	CLA	C8-C10-C11-C12
23	7	613	CLA	C15-C16-C17-C18
23	8	601	CLA	C15-C16-C17-C18
24	B	842	PQN	C25-C26-C27-C28
23	1	603	CLA	CAA-CBA-CGA-O2A
23	A	835	CLA	O1A-CGA-O2A-C1
23	B	813	CLA	O1A-CGA-O2A-C1
23	B	837	CLA	O1A-CGA-O2A-C1
23	6	604	CLA	O1A-CGA-O2A-C1
23	6	608	CLA	O1A-CGA-O2A-C1
23	7	613	CLA	O1A-CGA-O2A-C1
23	7	611	CLA	C5-C6-C7-C8
29	5	626	LMG	O9-C10-O7-C8
30	J	103	DGD	O1B-C1B-O2G-C2G
23	A	828	CLA	C15-C16-C17-C18
23	B	809	CLA	C10-C11-C12-C13
23	B	825	CLA	C8-C10-C11-C12
23	K	203	CLA	C5-C6-C7-C8
23	3	608	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	4	601	CLA	C15-C16-C17-C18
23	3	606	CLA	CBA-CGA-O2A-C1
23	8	601	CLA	CBA-CGA-O2A-C1
29	4	623	LMG	C29-C28-O8-C9
23	A	830	CLA	O1A-CGA-O2A-C1
23	B	819	CLA	O1A-CGA-O2A-C1
23	4	601	CLA	O1A-CGA-O2A-C1
23	8	613	CLA	O1D-CGD-O2D-CED
23	B	803	CLA	C8-C10-C11-C12
23	B	803	CLA	C10-C11-C12-C13
23	B	824	CLA	C10-C11-C12-C13
23	B	829	CLA	C13-C15-C16-C17
23	6	604	CLA	C13-C15-C16-C17
23	6	610	CLA	C13-C15-C16-C17
23	8	614	CLA	C5-C6-C7-C8
23	3	613	CLA	CAA-CBA-CGA-O2A
23	A	827	CLA	O1D-CGD-O2D-CED
23	3	604	CLA	O1D-CGD-O2D-CED
23	4	602	CLA	O1D-CGD-O2D-CED
23	A	832	CLA	O1A-CGA-O2A-C1
23	4	613	CLA	O1A-CGA-O2A-C1
23	6	616	CLA	O1A-CGA-O2A-C1
23	A	804	CLA	C13-C15-C16-C17
23	A	822	CLA	C13-C15-C16-C17
23	A	827	CLA	C8-C10-C11-C12
23	3	603	CLA	C5-C6-C7-C8
23	5	613	CLA	C10-C11-C12-C13
23	6	601	CLA	C13-C15-C16-C17
23	6	616	CLA	C5-C6-C7-C8
23	7	601	CLA	C8-C10-C11-C12
23	7	613	CLA	C10-C11-C12-C13
23	8	601	CLA	C10-C11-C12-C13
24	B	842	PQN	C15-C16-C17-C18
25	A	847	LHG	C3-O3-P-O6
25	1	620	LHG	C3-O3-P-O6
25	a	620	LHG	C3-O3-P-O6
25	3	624	LHG	C4-O6-P-O3
25	7	622	LHG	C4-O6-P-O3
25	8	622	LHG	C3-O3-P-O6
23	8	610	CLA	C3-C5-C6-C7
23	A	811	CLA	CBA-CGA-O2A-C1
23	B	824	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	828	CLA	CBA-CGA-O2A-C1
23	1	601	CLA	CBA-CGA-O2A-C1
23	1	611	CLA	CBA-CGA-O2A-C1
23	a	601	CLA	CBA-CGA-O2A-C1
23	B	827	CLA	O1D-CGD-O2D-CED
23	1	613	CLA	C10-C11-C12-C13
23	a	613	CLA	C10-C11-C12-C13
23	B	824	CLA	O1D-CGD-O2D-CED
25	A	846	LHG	C1-C2-C3-O3
25	3	624	LHG	C1-C2-C3-O3
25	7	622	LHG	C1-C2-C3-O3
25	8	622	LHG	C1-C2-C3-O3
25	A	846	LHG	O9-C7-O7-C5
23	A	818	CLA	C2-C3-C5-C6
23	A	830	CLA	C8-C10-C11-C12
23	K	206	CLA	O1D-CGD-O2D-CED
23	A	818	CLA	C2A-CAA-CBA-CGA
23	B	827	CLA	C2A-CAA-CBA-CGA
23	L	304	CLA	C2A-CAA-CBA-CGA
23	3	606	CLA	C6-C7-C8-C9
23	6	604	CLA	C16-C17-C18-C20
23	7	604	CLA	C3-C5-C6-C7
23	5	602	CLA	CBA-CGA-O2A-C1
23	3	602	CLA	C10-C11-C12-C13
23	3	608	CLA	O1D-CGD-O2D-CED
26	A	856	BCR	C19-C20-C21-C22
25	6	623	LHG	C23-C24-C25-C26
25	8	623	LHG	C23-C24-C25-C26
25	5	623	LHG	C30-C31-C32-C33
25	5	625	LHG	C29-C30-C31-C32
25	3	623	LHG	C8-C7-O7-C5
25	6	623	LHG	C8-C7-O7-C5
30	J	103	DGD	C2B-C1B-O2G-C2G
23	B	810	CLA	C15-C16-C17-C18
23	5	609	CLA	C13-C15-C16-C17
23	5	613	CLA	C2A-CAA-CBA-CGA
30	B	850	DGD	C3B-C4B-C5B-C6B
23	B	809	CLA	C16-C17-C18-C20
23	K	203	CLA	C16-C17-C18-C20
23	a	609	CLA	C16-C17-C18-C20
23	3	609	CLA	C11-C12-C13-C15
23	5	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	5	604	CLA	C16-C17-C18-C20
23	B	840	CLA	CBA-CGA-O2A-C1
23	A	843	CLA	C8-C10-C11-C12
25	3	624	LHG	C11-C10-C9-C8
25	7	622	LHG	C29-C30-C31-C32
25	8	623	LHG	C24-C25-C26-C27
29	4	624	LMG	C32-C33-C34-C35
29	5	626	LMG	C14-C15-C16-C17
29	5	626	LMG	C30-C31-C32-C33
23	6	601	CLA	O1D-CGD-O2D-CED
23	6	616	CLA	O1D-CGD-O2D-CED
25	B	851	LHG	O9-C7-O7-C5
29	4	623	LMG	O9-C10-O7-C8
23	7	611	CLA	C8-C10-C11-C12
25	8	623	LHG	C12-C13-C14-C15
25	2	622	LHG	C27-C28-C29-C30
29	5	626	LMG	C15-C16-C17-C18
25	3	623	LHG	C11-C12-C13-C14
25	3	624	LHG	C29-C30-C31-C32
25	5	625	LHG	C11-C12-C13-C14
25	8	622	LHG	C31-C32-C33-C34
25	8	622	LHG	C33-C34-C35-C36
28	A	857	LMU	C7-C8-C9-C10
29	7	624	LMG	C16-C17-C18-C19
23	B	836	CLA	O1D-CGD-O2D-CED
23	8	606	CLA	C13-C15-C16-C17
25	a	620	LHG	C27-C28-C29-C30
25	5	623	LHG	C16-C17-C18-C19
25	7	622	LHG	C9-C10-C11-C12
23	B	833	CLA	C3-C5-C6-C7
25	3	624	LHG	C7-C8-C9-C10
25	5	623	LHG	C7-C8-C9-C10
23	6	617	CLA	O1D-CGD-O2D-CED
23	A	838	CLA	CBA-CGA-O2A-C1
25	1	620	LHG	C27-C28-C29-C30
25	3	623	LHG	C28-C29-C30-C31
25	5	623	LHG	C32-C33-C34-C35
25	8	623	LHG	C10-C11-C12-C13
25	8	623	LHG	C28-C29-C30-C31
29	4	623	LMG	C32-C33-C34-C35
30	B	850	DGD	C4B-C5B-C6B-C7B
23	A	831	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	6	601	CLA	C8-C10-C11-C12
23	1	601	CLA	O1A-CGA-O2A-C1
23	a	601	CLA	O1A-CGA-O2A-C1
23	A	803	CLA	C16-C17-C18-C19
23	B	832	CLA	C11-C12-C13-C15
23	B	837	CLA	C16-C17-C18-C19
23	5	603	CLA	C6-C7-C8-C10
23	7	601	CLA	C11-C12-C13-C14
23	5	603	CLA	O1D-CGD-O2D-CED
23	B	825	CLA	C4-C3-C5-C6
23	3	613	CLA	C4-C3-C5-C6
25	A	846	LHG	C27-C28-C29-C30
25	3	623	LHG	C24-C25-C26-C27
25	3	623	LHG	C30-C31-C32-C33
25	8	623	LHG	C29-C30-C31-C32
23	A	825	CLA	C6-C7-C8-C9
23	A	826	CLA	C11-C10-C8-C9
23	1	613	CLA	C11-C12-C13-C14
23	a	609	CLA	C11-C10-C8-C9
23	a	613	CLA	C11-C12-C13-C14
23	B	837	CLA	O1D-CGD-O2D-CED
25	3	624	LHG	C23-C24-C25-C26
30	J	103	DGD	C3A-C4A-C5A-C6A
23	A	803	CLA	C2A-CAA-CBA-CGA
23	B	813	CLA	C2A-CAA-CBA-CGA
23	5	609	CLA	C2A-CAA-CBA-CGA
23	6	616	CLA	C2A-CAA-CBA-CGA
23	8	616	CLA	C2A-CAA-CBA-CGA
23	A	832	CLA	O1D-CGD-O2D-CED
23	8	601	CLA	O1A-CGA-O2A-C1
25	5	623	LHG	C12-C13-C14-C15
29	7	624	LMG	C29-C30-C31-C32
25	1	620	LHG	O1-C1-C2-C3
25	a	620	LHG	O1-C1-C2-C3
25	6	623	LHG	O1-C1-C2-C3
25	9	622	LHG	O1-C1-C2-C3
26	B	801	BCR	C21-C22-C23-C24
26	B	843	BCR	C17-C18-C19-C20
23	A	828	CLA	C3-C5-C6-C7
23	4	613	CLA	C3-C5-C6-C7
23	6	613	CLA	C3-C5-C6-C7
23	6	616	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	A	834	CLA	C13-C15-C16-C17
23	8	613	CLA	C10-C11-C12-C13
23	B	814	CLA	C15-C16-C17-C18
25	9	622	LHG	C17-C18-C19-C20
25	4	622	LHG	C23-C24-C25-C26
29	A	860	LMG	C28-C29-C30-C31
25	1	620	LHG	C26-C27-C28-C29
25	a	620	LHG	C26-C27-C28-C29
25	3	624	LHG	C11-C12-C13-C14
25	4	622	LHG	C27-C28-C29-C30
25	5	623	LHG	C11-C12-C13-C14
29	J	104	LMG	C12-C13-C14-C15
29	5	626	LMG	C16-C17-C18-C19
29	5	626	LMG	C32-C33-C34-C35
30	B	850	DGD	CAB-CBB-CCB-CDB
30	J	103	DGD	C4B-C5B-C6B-C7B
23	1	603	CLA	C6-C7-C8-C10
23	a	609	CLA	C16-C17-C18-C19
23	3	606	CLA	C6-C7-C8-C10
23	5	613	CLA	C16-C17-C18-C19
23	6	601	CLA	C16-C17-C18-C20
23	8	601	CLA	C16-C17-C18-C19
23	8	601	CLA	C16-C17-C18-C20
23	A	836	CLA	C8-C10-C11-C12
23	3	610	CLA	C5-C6-C7-C8
23	7	601	CLA	C5-C6-C7-C8
25	B	851	LHG	C26-C27-C28-C29
25	B	851	LHG	C27-C28-C29-C30
25	8	622	LHG	C32-C33-C34-C35
28	A	858	LMU	C6-C7-C8-C9
29	4	623	LMG	C16-C17-C18-C19
29	5	627	LMG	C31-C32-C33-C34
29	7	624	LMG	C12-C13-C14-C15
30	J	103	DGD	C6A-C7A-C8A-C9A
23	K	201	CLA	CBD-CGD-O2D-CED
23	A	841	CLA	O1D-CGD-O2D-CED
23	8	606	CLA	O1D-CGD-O2D-CED
25	1	620	LHG	C15-C16-C17-C18
25	a	620	LHG	C15-C16-C17-C18
30	J	103	DGD	C5B-C6B-C7B-C8B
23	6	613	CLA	C8-C10-C11-C12
23	B	824	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	1	611	CLA	O1A-CGA-O2A-C1
25	A	846	LHG	C12-C13-C14-C15
23	B	818	CLA	O1D-CGD-O2D-CED
25	A	846	LHG	C24-C23-O8-C6
25	9	622	LHG	C15-C16-C17-C18
28	K	208	LMU	C3-C4-C5-C6
23	A	801	CLA	C3A-C2A-CAA-CBA
23	A	803	CLA	C3A-C2A-CAA-CBA
23	A	804	CLA	C3A-C2A-CAA-CBA
23	A	814	CLA	C3A-C2A-CAA-CBA
23	B	810	CLA	C3A-C2A-CAA-CBA
23	B	813	CLA	C3A-C2A-CAA-CBA
23	B	823	CLA	C3A-C2A-CAA-CBA
23	F	301	CLA	C3A-C2A-CAA-CBA
23	G	204	CLA	C3A-C2A-CAA-CBA
23	K	201	CLA	C3A-C2A-CAA-CBA
23	a	606	CLA	C3A-C2A-CAA-CBA
23	5	619	CLA	C3A-C2A-CAA-CBA
23	6	616	CLA	C3A-C2A-CAA-CBA
23	6	620	CLA	C3A-C2A-CAA-CBA
23	8	616	CLA	C3A-C2A-CAA-CBA
23	7	602	CLA	C5-C6-C7-C8
25	5	623	LHG	C27-C28-C29-C30
30	B	850	DGD	C3A-C4A-C5A-C6A
30	B	850	DGD	C1B-C2B-C3B-C4B
23	B	828	CLA	O1A-CGA-O2A-C1
23	3	606	CLA	O1A-CGA-O2A-C1
23	A	803	CLA	C16-C17-C18-C20
23	3	609	CLA	C11-C12-C13-C14
23	5	604	CLA	C16-C17-C18-C19
23	5	613	CLA	C16-C17-C18-C20
23	6	604	CLA	C16-C17-C18-C19
25	3	624	LHG	C9-C10-C11-C12
25	3	624	LHG	C27-C28-C29-C30
29	5	626	LMG	O1-C7-C8-C9
25	A	847	LHG	C7-C8-C9-C10
25	5	625	LHG	C23-C24-C25-C26
28	A	857	LMU	C1-C2-C3-C4
25	7	622	LHG	C27-C28-C29-C30
28	A	857	LMU	C4-C5-C6-C7
23	A	811	CLA	O1A-CGA-O2A-C1
23	B	834	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	3	604	CLA	CBA-CGA-O2A-C1
23	8	610	CLA	CBA-CGA-O2A-C1
23	B	825	CLA	C2-C3-C5-C6
23	B	834	CLA	C2-C3-C5-C6
23	3	613	CLA	C2-C3-C5-C6
23	B	803	CLA	C4C-C3C-CAC-CBC
25	1	620	LHG	C32-C33-C34-C35
25	a	620	LHG	C32-C33-C34-C35
25	5	623	LHG	C10-C11-C12-C13
23	B	828	CLA	C2A-CAA-CBA-CGA
25	B	851	LHG	O1-C1-C2-O2
25	4	622	LHG	O1-C1-C2-O2
25	8	622	LHG	O1-C1-C2-O2
25	8	623	LHG	O1-C1-C2-O2
23	B	814	CLA	C13-C15-C16-C17
25	A	846	LHG	C11-C10-C9-C8
25	2	622	LHG	C29-C30-C31-C32
29	A	860	LMG	C11-C12-C13-C14
23	B	812	CLA	C2A-CAA-CBA-CGA
23	A	801	CLA	C16-C17-C18-C19
25	3	624	LHG	O2-C2-C3-O3
23	A	802	CLA	C10-C11-C12-C13
25	A	846	LHG	C28-C29-C30-C31
25	2	622	LHG	C11-C10-C9-C8
25	B	851	LHG	C11-C10-C9-C8
23	B	840	CLA	O1A-CGA-O2A-C1
23	5	602	CLA	O1A-CGA-O2A-C1
25	3	623	LHG	C7-C8-C9-C10
28	5	628	LMU	O5B-C1B-O1B-C4'
25	B	851	LHG	C1-C2-C3-O3
25	A	846	LHG	C13-C14-C15-C16
25	A	846	LHG	C30-C31-C32-C33
25	5	625	LHG	C13-C14-C15-C16
25	6	623	LHG	C11-C10-C9-C8
25	8	623	LHG	C11-C12-C13-C14
29	J	104	LMG	C17-C18-C19-C20
29	A	860	LMG	O9-C10-O7-C8
25	8	622	LHG	C27-C28-C29-C30
23	6	616	CLA	C13-C15-C16-C17
23	8	610	CLA	O1A-CGA-O2A-C1
25	6	623	LHG	C27-C28-C29-C30
25	8	622	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	A	851	BCR	C23-C24-C25-C26
26	A	851	BCR	C23-C24-C25-C30
26	A	856	BCR	C1-C6-C7-C8
26	A	856	BCR	C5-C6-C7-C8
26	A	856	BCR	C23-C24-C25-C26
26	A	856	BCR	C23-C24-C25-C30
26	B	844	BCR	C1-C6-C7-C8
26	B	844	BCR	C5-C6-C7-C8
26	B	848	BCR	C1-C6-C7-C8
26	B	848	BCR	C5-C6-C7-C8
26	L	305	BCR	C5-C6-C7-C8
26	L	305	BCR	C23-C24-C25-C26
26	L	305	BCR	C23-C24-C25-C30
26	3	620	BCR	C23-C24-C25-C26
26	3	620	BCR	C23-C24-C25-C30
26	3	621	BCR	C23-C24-C25-C26
26	6	622	BCR	C23-C24-C25-C26
26	6	622	BCR	C23-C24-C25-C30
26	8	621	BCR	C1-C6-C7-C8
26	8	621	BCR	C5-C6-C7-C8
31	4	619	LUT	C5-C6-C7-C8
31	5	620	LUT	C1-C6-C7-C8
31	5	620	LUT	C5-C6-C7-C8
31	6	619	LUT	C5-C6-C7-C8
31	7	619	LUT	C1-C6-C7-C8
31	8	619	LUT	C1-C6-C7-C8
31	8	619	LUT	C5-C6-C7-C8
25	B	851	LHG	C30-C31-C32-C33
25	4	622	LHG	C13-C14-C15-C16
25	5	625	LHG	C27-C28-C29-C30
23	B	803	CLA	CBA-CGA-O2A-C1
25	3	623	LHG	C24-C23-O8-C6
23	4	601	CLA	C5-C6-C7-C8
23	4	608	CLA	C5-C6-C7-C8
23	5	604	CLA	C5-C6-C7-C8
28	A	859	LMU	C1-C2-C3-C4
25	5	625	LHG	C16-C17-C18-C19
29	4	624	LMG	C15-C16-C17-C18
25	3	623	LHG	C23-C24-C25-C26
29	5	626	LMG	C13-C14-C15-C16
29	5	627	LMG	C12-C13-C14-C15
23	A	807	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	4	608	CLA	C10-C11-C12-C13
25	3	623	LHG	C11-C10-C9-C8
30	J	103	DGD	C4A-C5A-C6A-C7A
23	A	820	CLA	C4-C3-C5-C6
23	4	610	CLA	C4-C3-C5-C6
23	A	837	CLA	O1D-CGD-O2D-CED
23	A	804	CLA	C12-C13-C15-C16
23	A	809	CLA	C12-C13-C15-C16
23	A	814	CLA	C11-C10-C8-C7
23	A	820	CLA	C2-C3-C5-C6
23	A	822	CLA	C11-C12-C13-C15
23	A	843	CLA	C11-C12-C13-C15
23	B	803	CLA	C11-C10-C8-C7
23	B	806	CLA	C12-C13-C15-C16
23	B	810	CLA	C11-C12-C13-C15
23	B	834	CLA	C6-C7-C8-C10
23	1	613	CLA	C11-C12-C13-C15
23	a	613	CLA	C11-C12-C13-C15
23	5	607	CLA	C12-C13-C15-C16
23	6	604	CLA	C11-C10-C8-C7
23	7	611	CLA	C6-C7-C8-C10
23	8	602	CLA	C2-C3-C5-C6
23	A	838	CLA	O1A-CGA-O2A-C1
23	3	604	CLA	O1A-CGA-O2A-C1
23	8	601	CLA	C13-C15-C16-C17
23	B	809	CLA	C16-C17-C18-C19
23	B	819	CLA	C6-C7-C8-C10
23	B	832	CLA	C11-C12-C13-C14
23	K	203	CLA	C16-C17-C18-C19
23	A	845	CLA	O1D-CGD-O2D-CED
25	6	623	LHG	O9-C7-O7-C5
25	2	622	LHG	C7-C8-C9-C10
29	5	626	LMG	C28-C29-C30-C31
23	A	831	CLA	CBA-CGA-O2A-C1
23	B	805	CLA	CBA-CGA-O2A-C1
29	7	624	LMG	C29-C28-O8-C9
25	1	620	LHG	C25-C26-C27-C28
28	8	625	LMU	C11-C10-C9-C8
23	B	835	CLA	C2A-CAA-CBA-CGA
23	5	601	CLA	C2A-CAA-CBA-CGA
23	5	602	CLA	C2A-CAA-CBA-CGA
23	8	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	A	842	CLA	C10-C11-C12-C13
23	5	610	CLA	C5-C6-C7-C8
25	a	620	LHG	C25-C26-C27-C28
25	5	623	LHG	C9-C10-C11-C12
29	5	627	LMG	C17-C18-C19-C20
23	8	607	CLA	O1D-CGD-O2D-CED
25	5	625	LHG	C32-C33-C34-C35
25	8	622	LHG	C34-C35-C36-C37
28	K	208	LMU	O1'-C1-C2-C3
23	4	609	CLA	C12-C13-C15-C16
23	B	837	CLA	C5-C6-C7-C8
23	3	610	CLA	C8-C10-C11-C12
25	6	623	LHG	C33-C34-C35-C36
29	4	623	LMG	C17-C18-C19-C20
23	A	806	CLA	C3-C5-C6-C7
23	4	609	CLA	O1D-CGD-O2D-CED
25	5	625	LHG	C34-C35-C36-C37
30	B	850	DGD	CEB-CFB-CGB-CHB
23	A	814	CLA	C10-C11-C12-C13
23	A	823	CLA	O1D-CGD-O2D-CED
25	A	846	LHG	C32-C33-C34-C35
29	4	623	LMG	C11-C10-O7-C8
25	3	624	LHG	C28-C29-C30-C31
28	A	859	LMU	C2-C3-C4-C5
28	K	208	LMU	C5-C6-C7-C8
23	A	854	CLA	C8-C10-C11-C12
23	A	807	CLA	CBD-CGD-O2D-CED
23	B	828	CLA	CBD-CGD-O2D-CED
23	7	611	CLA	C2-C3-C5-C6
30	B	850	DGD	C5A-C6A-C7A-C8A
29	4	624	LMG	O9-C10-O7-C8
23	6	604	CLA	C3-C5-C6-C7
28	5	628	LMU	C2'-C1'-O1'-C1
30	J	103	DGD	C2E-C1E-O5D-C6D
25	9	622	LHG	O7-C5-C6-O8
25	3	623	LHG	C15-C16-C17-C18
23	6	601	CLA	C16-C17-C18-C19
23	7	601	CLA	C11-C12-C13-C15
25	B	851	LHG	C10-C11-C12-C13
30	J	103	DGD	O6E-C5E-C6E-O5E
23	A	826	CLA	C5-C6-C7-C8
23	7	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	8	602	CLA	C4-C3-C5-C6
23	A	804	CLA	C14-C13-C15-C16
23	A	814	CLA	C11-C10-C8-C9
23	A	843	CLA	C11-C12-C13-C14
23	B	802	CLA	C11-C10-C8-C9
23	B	805	CLA	C11-C12-C13-C14
23	B	806	CLA	C14-C13-C15-C16
23	B	818	CLA	C11-C10-C8-C9
23	5	607	CLA	C14-C13-C15-C16
23	7	611	CLA	C6-C7-C8-C9
30	B	850	DGD	C4A-C5A-C6A-C7A
23	A	809	CLA	C2A-CAA-CBA-CGA
23	L	302	CLA	C2A-CAA-CBA-CGA
23	4	602	CLA	C2A-CAA-CBA-CGA
23	5	619	CLA	C2A-CAA-CBA-CGA
23	6	602	CLA	C2A-CAA-CBA-CGA
23	6	610	CLA	C2A-CAA-CBA-CGA
29	5	627	LMG	C14-C15-C16-C17
30	B	850	DGD	C7B-C8B-C9B-CAB
26	L	305	BCR	C36-C18-C19-C20
23	A	831	CLA	C15-C16-C17-C18
23	8	606	CLA	C5-C6-C7-C8
25	A	846	LHG	C31-C32-C33-C34
25	6	623	LHG	C28-C29-C30-C31
23	B	803	CLA	O1A-CGA-O2A-C1
23	A	805	CLA	C1A-C2A-CAA-CBA
23	A	810	CLA	C1A-C2A-CAA-CBA
23	A	811	CLA	C1A-C2A-CAA-CBA
23	A	812	CLA	C1A-C2A-CAA-CBA
23	A	814	CLA	C1A-C2A-CAA-CBA
23	A	831	CLA	C1A-C2A-CAA-CBA
23	A	838	CLA	C1A-C2A-CAA-CBA
23	B	803	CLA	C1A-C2A-CAA-CBA
23	B	810	CLA	C1A-C2A-CAA-CBA
23	B	811	CLA	C1A-C2A-CAA-CBA
23	B	813	CLA	C1A-C2A-CAA-CBA
23	B	814	CLA	C1A-C2A-CAA-CBA
23	B	816	CLA	C1A-C2A-CAA-CBA
23	B	820	CLA	C1A-C2A-CAA-CBA
23	B	833	CLA	C1A-C2A-CAA-CBA
23	B	834	CLA	C1A-C2A-CAA-CBA
23	B	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	F	301	CLA	C1A-C2A-CAA-CBA
23	G	204	CLA	C1A-C2A-CAA-CBA
23	K	201	CLA	C1A-C2A-CAA-CBA
23	K	203	CLA	C1A-C2A-CAA-CBA
23	1	602	CLA	C1A-C2A-CAA-CBA
23	a	602	CLA	C1A-C2A-CAA-CBA
23	a	610	CLA	C1A-C2A-CAA-CBA
23	3	603	CLA	C1A-C2A-CAA-CBA
23	3	607	CLA	C1A-C2A-CAA-CBA
23	4	601	CLA	C1A-C2A-CAA-CBA
23	4	610	CLA	C1A-C2A-CAA-CBA
23	4	614	CLA	C1A-C2A-CAA-CBA
23	4	616	CLA	C1A-C2A-CAA-CBA
23	5	607	CLA	C1A-C2A-CAA-CBA
23	5	610	CLA	C1A-C2A-CAA-CBA
23	6	604	CLA	C1A-C2A-CAA-CBA
23	6	610	CLA	C1A-C2A-CAA-CBA
23	6	616	CLA	C1A-C2A-CAA-CBA
23	6	620	CLA	C1A-C2A-CAA-CBA
23	7	610	CLA	C1A-C2A-CAA-CBA
23	8	608	CLA	C1A-C2A-CAA-CBA
23	8	610	CLA	C1A-C2A-CAA-CBA
23	8	614	CLA	C1A-C2A-CAA-CBA
23	B	837	CLA	C16-C17-C18-C20
23	1	603	CLA	C6-C7-C8-C9
23	3	603	CLA	C6-C7-C8-C9
23	3	603	CLA	C6-C7-C8-C10
23	3	604	CLA	C16-C17-C18-C19
23	4	601	CLA	C16-C17-C18-C19
25	A	846	LHG	C8-C7-O7-C5
25	9	622	LHG	C4-O6-P-O3
28	8	625	LMU	O5B-C5B-C6B-O6B
23	A	801	CLA	C3-C5-C6-C7
23	B	839	CLA	O1D-CGD-O2D-CED
28	A	858	LMU	C7-C8-C9-C10
28	A	858	LMU	C1-C2-C3-C4
23	a	609	CLA	C13-C15-C16-C17
25	1	620	LHG	C24-C23-O8-C6
25	a	620	LHG	C24-C23-O8-C6
25	4	622	LHG	C24-C23-O8-C6
29	5	627	LMG	C13-C14-C15-C16
23	A	831	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	5	623	LHG	C29-C30-C31-C32
25	8	622	LHG	C28-C29-C30-C31
28	8	624	LMU	C4-C5-C6-C7
29	J	104	LMG	C8-C9-O8-C28
23	A	807	CLA	C16-C17-C18-C19
23	A	812	CLA	C16-C17-C18-C19
29	5	626	LMG	C31-C32-C33-C34
29	5	627	LMG	C32-C33-C34-C35
25	9	622	LHG	C11-C10-C9-C8
29	5	626	LMG	C17-C18-C19-C20
23	A	804	CLA	C15-C16-C17-C18
25	9	622	LHG	C32-C33-C34-C35
23	A	807	CLA	CBA-CGA-O2A-C1
25	4	622	LHG	C1-C2-C3-O3
23	B	808	CLA	C4-C3-C5-C6
23	F	303	CLA	C3A-C2A-CAA-CBA
23	a	603	CLA	C3A-C2A-CAA-CBA
23	5	611	CLA	C3A-C2A-CAA-CBA
23	5	618	CLA	C3A-C2A-CAA-CBA
23	6	611	CLA	C3A-C2A-CAA-CBA
23	8	611	CLA	C3A-C2A-CAA-CBA
23	8	612	CLA	C3A-C2A-CAA-CBA
25	6	623	LHG	C10-C11-C12-C13
23	6	601	CLA	C15-C16-C17-C18
23	6	610	CLA	C8-C10-C11-C12
28	A	859	LMU	C11-C10-C9-C8
29	J	104	LMG	C16-C17-C18-C19
23	7	611	CLA	C2A-CAA-CBA-CGA
23	3	604	CLA	C16-C17-C18-C20
29	J	104	LMG	O6-C5-C6-O5
25	1	620	LHG	C4-C5-C6-O8
25	a	620	LHG	C4-C5-C6-O8
25	3	624	LHG	C12-C13-C14-C15
25	5	623	LHG	C4-C5-C6-O8
25	5	625	LHG	C33-C34-C35-C36
25	8	623	LHG	C4-C5-C6-O8
30	J	103	DGD	O1G-C1G-C2G-C3G
30	J	103	DGD	C1G-C2G-C3G-O3G
24	A	844	PQN	C20-C21-C22-C23
25	4	622	LHG	C32-C33-C34-C35
29	4	623	LMG	C8-C7-O1-C1
25	4	622	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	7	622	LHG	C30-C31-C32-C33
29	A	860	LMG	C30-C31-C32-C33
29	A	860	LMG	C31-C32-C33-C34
29	4	624	LMG	C18-C19-C20-C21
23	5	602	CLA	CBD-CGD-O2D-CED
23	4	609	CLA	C14-C13-C15-C16
23	K	201	CLA	O1D-CGD-O2D-CED
28	5	628	LMU	O5'-C5'-C6'-O6'
23	A	804	CLA	O1A-CGA-O2A-C1
25	B	851	LHG	C31-C32-C33-C34
29	7	624	LMG	O6-C1-O1-C7
25	6	623	LHG	C32-C33-C34-C35
23	4	610	CLA	CBD-CGD-O2D-CED
25	6	623	LHG	O1-C1-C2-O2
28	A	859	LMU	C5-C6-C7-C8
23	A	831	CLA	O1A-CGA-O2A-C1
23	B	805	CLA	O1A-CGA-O2A-C1
23	6	620	CLA	CBD-CGD-O2D-CED
25	8	622	LHG	C13-C14-C15-C16
29	4	623	LMG	C14-C15-C16-C17
29	4	623	LMG	C18-C19-C20-C21
23	3	613	CLA	C2A-CAA-CBA-CGA
29	5	626	LMG	O6-C5-C6-O5
23	B	802	CLA	C4-C3-C5-C6
23	B	827	CLA	C4-C3-C5-C6
29	4	624	LMG	C16-C17-C18-C19
30	J	103	DGD	C2A-C3A-C4A-C5A
25	7	622	LHG	C7-C8-C9-C10
23	A	807	CLA	C16-C17-C18-C20
23	B	819	CLA	C6-C7-C8-C9
23	a	609	CLA	CBA-CGA-O2A-C1
30	J	103	DGD	CEA-CFA-CGA-CHA
23	A	807	CLA	C15-C16-C17-C18
23	B	809	CLA	C15-C16-C17-C18
23	B	810	CLA	C13-C15-C16-C17
23	4	613	CLA	C8-C10-C11-C12
23	5	613	CLA	C8-C10-C11-C12
23	A	842	CLA	CAA-CBA-CGA-O2A
25	8	622	LHG	C24-C25-C26-C27
28	A	857	LMU	C9-C10-C11-C12
23	B	803	CLA	C15-C16-C17-C18
23	6	601	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
30	B	850	DGD	O6E-C5E-C6E-O5E
28	5	628	LMU	C3'-C4'-O1B-C1B
24	B	842	PQN	C23-C25-C26-C27
23	A	804	CLA	CBA-CGA-O2A-C1
23	1	613	CLA	C5-C6-C7-C8
23	a	613	CLA	C5-C6-C7-C8
23	A	826	CLA	CAA-CBA-CGA-O2A
23	B	827	CLA	C8-C10-C11-C12
23	7	613	CLA	C8-C10-C11-C12
30	J	103	DGD	CFA-CGA-CHA-CIA
25	A	847	LHG	O7-C5-C6-O8
29	7	624	LMG	O7-C8-C9-O8
23	5	610	CLA	C6-C7-C8-C9
23	B	828	CLA	C13-C15-C16-C17
23	A	807	CLA	O1A-CGA-O2A-C1
23	a	609	CLA	O1A-CGA-O2A-C1
23	B	816	CLA	C2-C1-O2A-CGA
23	A	807	CLA	C4-C3-C5-C6
23	B	816	CLA	C4-C3-C5-C6
23	A	807	CLA	C2-C3-C5-C6
23	A	807	CLA	C11-C10-C8-C7
23	A	811	CLA	C11-C10-C8-C7
23	A	825	CLA	C11-C12-C13-C15
23	B	802	CLA	C11-C10-C8-C7
23	B	808	CLA	C2-C3-C5-C6
23	B	810	CLA	C6-C7-C8-C10
23	B	813	CLA	C11-C12-C13-C15
23	B	817	CLA	C11-C10-C8-C7
23	B	818	CLA	C11-C10-C8-C7
23	B	827	CLA	C2-C3-C5-C6
23	B	828	CLA	C11-C10-C8-C7
23	B	829	CLA	C6-C7-C8-C10
23	B	834	CLA	C11-C10-C8-C7
23	a	609	CLA	C11-C10-C8-C7
23	4	608	CLA	C11-C10-C8-C7
23	4	610	CLA	C6-C7-C8-C10
23	5	609	CLA	C11-C10-C8-C7
23	5	609	CLA	C12-C13-C15-C16
23	6	601	CLA	C12-C13-C15-C16
23	6	604	CLA	C12-C13-C15-C16
23	6	610	CLA	C6-C7-C8-C10
23	7	601	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	7	613	CLA	C11-C10-C8-C7
23	8	601	CLA	C11-C10-C8-C7
23	8	606	CLA	C11-C12-C13-C15
23	8	614	CLA	C6-C7-C8-C10
24	B	842	PQN	C17-C18-C20-C21
28	8	625	LMU	C1-C2-C3-C4
23	B	809	CLA	C3-C5-C6-C7
23	A	809	CLA	C14-C13-C15-C16
23	A	811	CLA	C11-C10-C8-C9
23	A	820	CLA	C11-C10-C8-C9
23	A	825	CLA	C11-C12-C13-C14
23	A	825	CLA	C14-C13-C15-C16
23	A	826	CLA	C11-C12-C13-C14
23	A	831	CLA	C14-C13-C15-C16
23	A	836	CLA	C11-C10-C8-C9
23	A	841	CLA	C11-C12-C13-C14
23	B	802	CLA	C6-C7-C8-C9
23	B	806	CLA	C11-C12-C13-C14
23	B	809	CLA	C6-C7-C8-C9
23	B	810	CLA	C6-C7-C8-C9
23	B	817	CLA	C6-C7-C8-C9
23	B	828	CLA	C11-C10-C8-C9
23	B	834	CLA	C11-C10-C8-C9
23	1	613	CLA	C6-C7-C8-C9
23	a	613	CLA	C6-C7-C8-C9
23	3	610	CLA	C11-C10-C8-C9
23	5	609	CLA	C6-C7-C8-C9
23	5	609	CLA	C11-C10-C8-C9
23	5	609	CLA	C14-C13-C15-C16
23	6	616	CLA	C6-C7-C8-C9
23	8	601	CLA	C11-C10-C8-C9
23	8	602	CLA	C11-C10-C8-C9
23	8	606	CLA	C11-C12-C13-C14
23	8	613	CLA	C11-C12-C13-C14
23	8	614	CLA	C6-C7-C8-C9
25	9	622	LHG	C27-C28-C29-C30
23	A	838	CLA	O1D-CGD-O2D-CED
26	L	301	BCR	C36-C18-C19-C20
26	7	621	BCR	C7-C8-C9-C34
26	7	621	BCR	C36-C18-C19-C20
23	4	601	CLA	C16-C17-C18-C20
29	5	626	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	B	801	BCR	C7-C8-C9-C10
23	4	608	CLA	C3-C5-C6-C7
23	6	620	CLA	C10-C11-C12-C13
23	7	610	CLA	C8-C10-C11-C12
29	4	624	LMG	C11-C10-O7-C8
23	A	810	CLA	CBA-CGA-O2A-C1
23	B	808	CLA	CBA-CGA-O2A-C1
23	B	825	CLA	CBA-CGA-O2A-C1
23	7	602	CLA	CBA-CGA-O2A-C1
25	8	622	LHG	C24-C23-O8-C6
29	4	624	LMG	C33-C34-C35-C36
25	9	622	LHG	C7-C8-C9-C10
23	5	607	CLA	C8-C10-C11-C12
29	4	624	LMG	C31-C32-C33-C34
23	A	843	CLA	C5-C6-C7-C8
23	4	609	CLA	C8-C10-C11-C12
23	8	606	CLA	C15-C16-C17-C18
25	3	623	LHG	O6-C4-C5-C6
25	2	622	LHG	O6-C4-C5-C6
23	B	813	CLA	C3-C5-C6-C7
23	B	839	CLA	CBA-CGA-O2A-C1
23	5	601	CLA	CBA-CGA-O2A-C1
25	9	622	LHG	C26-C27-C28-C29
23	A	826	CLA	C4-C3-C5-C6
23	A	826	CLA	C2-C3-C5-C6
23	B	802	CLA	C2-C3-C5-C6
23	B	816	CLA	C2-C3-C5-C6
25	A	847	LHG	C9-C10-C11-C12
29	A	860	LMG	O10-C28-O8-C9
25	1	620	LHG	C31-C32-C33-C34
25	a	620	LHG	C31-C32-C33-C34
25	6	623	LHG	C35-C36-C37-C38
23	A	806	CLA	C13-C15-C16-C17
23	A	819	CLA	CBA-CGA-O2A-C1
25	5	625	LHG	C30-C31-C32-C33
23	A	838	CLA	C3A-C2A-CAA-CBA
23	7	615	CLA	CBD-CGD-O2D-CED
23	8	604	CLA	C3A-C2A-CAA-CBA
23	A	814	CLA	C13-C15-C16-C17
25	3	623	LHG	C25-C26-C27-C28
30	B	850	DGD	CBB-CCB-CDB-CEB
28	A	858	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
25	6	623	LHG	C12-C13-C14-C15
25	A	847	LHG	C11-C10-C9-C8
29	5	626	LMG	C12-C13-C14-C15
23	A	801	CLA	C16-C17-C18-C20
29	A	860	LMG	C29-C28-O8-C9
29	A	860	LMG	C16-C17-C18-C19
23	A	834	CLA	C8-C10-C11-C12
23	B	833	CLA	C13-C15-C16-C17
23	5	609	CLA	C8-C10-C11-C12
23	6	602	CLA	C8-C10-C11-C12
23	B	810	CLA	C2A-CAA-CBA-CGA
25	A	847	LHG	C4-C5-C6-O8
25	8	622	LHG	C4-C5-C6-O8
29	7	624	LMG	C7-C8-C9-O8
30	B	850	DGD	O1G-C1G-C2G-C3G
30	B	850	DGD	C1G-C2G-C3G-O3G
29	A	860	LMG	C14-C15-C16-C17
23	B	802	CLA	C5-C6-C7-C8
25	2	622	LHG	C9-C10-C11-C12
23	B	824	CLA	C8-C10-C11-C12
23	6	604	CLA	C10-C11-C12-C13
23	A	845	CLA	CBA-CGA-O2A-C1
23	F	301	CLA	CBA-CGA-O2A-C1
28	A	859	LMU	C5'-C4'-O1B-C1B
25	B	851	LHG	C23-C24-C25-C26
25	1	620	LHG	O1-C1-C2-O2
25	a	620	LHG	O1-C1-C2-O2
25	5	623	LHG	O1-C1-C2-O2
23	A	842	CLA	C5-C6-C7-C8
25	3	623	LHG	C12-C13-C14-C15
25	3	623	LHG	O6-C4-C5-O7
23	A	841	CLA	CBA-CGA-O2A-C1
23	A	807	CLA	O1D-CGD-O2D-CED
25	8	623	LHG	O10-C23-O8-C6
23	A	826	CLA	C10-C11-C12-C13
23	A	803	CLA	C13-C15-C16-C17
23	A	810	CLA	O1A-CGA-O2A-C1
25	7	622	LHG	C11-C10-C9-C8
23	6	602	CLA	C3-C5-C6-C7
29	J	104	LMG	C11-C12-C13-C14
25	8	623	LHG	O7-C5-C6-O8
29	5	626	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
29	5	626	LMG	O7-C8-C9-O8
30	B	850	DGD	O2G-C2G-C3G-O3G
25	7	622	LHG	C25-C26-C27-C28
25	B	851	LHG	C8-C7-O7-C5
23	A	829	CLA	C8-C10-C11-C12
23	B	833	CLA	C8-C10-C11-C12
30	B	850	DGD	CFB-CGB-CHB-CIB
23	A	835	CLA	C2-C1-O2A-CGA
23	A	841	CLA	C2-C1-O2A-CGA
23	B	836	CLA	C2-C1-O2A-CGA
23	B	839	CLA	C2-C1-O2A-CGA
23	B	840	CLA	C2-C1-O2A-CGA
23	a	614	CLA	C2-C1-O2A-CGA
23	A	809	CLA	C11-C12-C13-C14
23	A	820	CLA	C6-C7-C8-C9
23	A	854	CLA	C14-C13-C15-C16
23	B	813	CLA	C11-C12-C13-C14
23	B	817	CLA	C11-C10-C8-C9
23	B	833	CLA	C14-C13-C15-C16
23	B	837	CLA	C14-C13-C15-C16
23	4	610	CLA	C6-C7-C8-C9
23	6	604	CLA	C6-C7-C8-C9
23	6	604	CLA	C11-C10-C8-C9
23	6	620	CLA	C11-C12-C13-C14
25	3	623	LHG	C9-C10-C11-C12
23	B	839	CLA	C13-C15-C16-C17
25	4	622	LHG	C34-C35-C36-C37
23	A	830	CLA	C2A-CAA-CBA-CGA
26	1	619	BCR	C23-C24-C25-C26
26	a	619	BCR	C23-C24-C25-C26
26	7	621	BCR	C23-C24-C25-C30
26	8	621	BCR	C23-C24-C25-C26
31	1	617	LUT	C5-C6-C7-C8
31	a	617	LUT	C5-C6-C7-C8
31	3	618	LUT	C1-C6-C7-C8
31	3	618	LUT	C5-C6-C7-C8
31	7	619	LUT	C5-C6-C7-C8
26	A	849	BCR	C7-C8-C9-C34
26	A	852	BCR	C7-C8-C9-C10
31	4	619	LUT	C31-C32-C33-C34
31	7	619	LUT	C27-C28-C29-C30
32	8	620	XAT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	5	626	LMG	C18-C19-C20-C21
23	B	817	CLA	C5-C6-C7-C8
23	A	812	CLA	C16-C17-C18-C20
23	4	614	CLA	C11-C10-C8-C9
23	B	825	CLA	O1A-CGA-O2A-C1
28	8	625	LMU	C9-C10-C11-C12
25	3	624	LHG	C32-C33-C34-C35
29	4	624	LMG	C29-C30-C31-C32
23	A	809	CLA	C11-C12-C13-C15
23	A	811	CLA	C6-C7-C8-C10
23	A	820	CLA	C6-C7-C8-C10
23	A	820	CLA	C11-C10-C8-C7
23	A	825	CLA	C12-C13-C15-C16
23	A	830	CLA	C6-C7-C8-C10
23	A	831	CLA	C12-C13-C15-C16
23	A	834	CLA	C11-C12-C13-C15
23	A	836	CLA	C11-C10-C8-C7
23	A	841	CLA	C11-C10-C8-C7
23	A	843	CLA	C12-C13-C15-C16
23	A	854	CLA	C12-C13-C15-C16
23	B	802	CLA	C6-C7-C8-C10
23	B	806	CLA	C11-C12-C13-C15
23	B	809	CLA	C6-C7-C8-C10
23	B	813	CLA	C11-C10-C8-C7
23	B	814	CLA	C12-C13-C15-C16
23	B	817	CLA	C6-C7-C8-C10
23	B	831	CLA	C12-C13-C15-C16
23	B	833	CLA	C11-C10-C8-C7
23	B	833	CLA	C12-C13-C15-C16
23	B	837	CLA	C12-C13-C15-C16
23	B	839	CLA	C6-C7-C8-C10
23	1	613	CLA	C6-C7-C8-C10
23	a	609	CLA	C12-C13-C15-C16
23	a	613	CLA	C6-C7-C8-C10
23	3	610	CLA	C11-C10-C8-C7
23	4	602	CLA	C11-C10-C8-C7
23	4	610	CLA	C11-C12-C13-C15
23	5	604	CLA	C11-C10-C8-C7
23	6	604	CLA	C6-C7-C8-C10
23	6	604	CLA	C11-C12-C13-C15
23	6	620	CLA	C11-C12-C13-C15
23	7	601	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	7	602	CLA	C11-C10-C8-C7
23	7	602	CLA	C12-C13-C15-C16
23	7	611	CLA	C11-C10-C8-C7
23	8	601	CLA	C6-C7-C8-C10
23	8	601	CLA	C11-C12-C13-C15
23	8	602	CLA	C11-C10-C8-C7
23	8	613	CLA	C11-C12-C13-C15
24	A	844	PQN	C21-C22-C23-C25
23	A	841	CLA	C3-C5-C6-C7
25	5	623	LHG	C15-C16-C17-C18
26	6	622	BCR	C13-C14-C15-C16
31	9	619	LUT	C29-C30-C31-C32
32	4	620	XAT	C29-C30-C31-C32
23	3	610	CLA	CBD-CGD-O2D-CED
23	3	602	CLA	CBA-CGA-O2A-C1
23	5	613	CLA	C5-C6-C7-C8
29	4	623	LMG	O10-C28-O8-C9
23	1	604	CLA	C2A-CAA-CBA-CGA
23	a	604	CLA	C2A-CAA-CBA-CGA
25	a	620	LHG	C8-C7-O7-C5
23	B	832	CLA	C8-C10-C11-C12
23	1	603	CLA	C2A-CAA-CBA-CGA
25	A	846	LHG	C23-C24-C25-C26
23	3	609	CLA	C3-C5-C6-C7
23	6	602	CLA	CBA-CGA-O2A-C1
23	4	614	CLA	C11-C10-C8-C7
23	A	841	CLA	C15-C16-C17-C18
23	A	843	CLA	C15-C16-C17-C18
23	A	805	CLA	CAD-CBD-CGD-O2D
23	A	813	CLA	CAD-CBD-CGD-O2D
23	A	821	CLA	CAD-CBD-CGD-O2D
23	A	831	CLA	CAD-CBD-CGD-O2D
23	A	842	CLA	CAD-CBD-CGD-O2D
23	A	854	CLA	CAD-CBD-CGD-O2D
23	B	804	CLA	CAD-CBD-CGD-O2D
23	B	812	CLA	CAD-CBD-CGD-O2D
23	B	824	CLA	CAD-CBD-CGD-O2D
23	B	833	CLA	CAD-CBD-CGD-O2D
23	K	201	CLA	CAD-CBD-CGD-O2D
23	1	602	CLA	CAD-CBD-CGD-O2D
23	1	612	CLA	CAD-CBD-CGD-O2D
23	a	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	a	612	CLA	CAD-CBD-CGD-O2D
23	3	603	CLA	CAD-CBD-CGD-O2D
23	3	610	CLA	CAD-CBD-CGD-O2D
23	4	601	CLA	CAD-CBD-CGD-O2D
23	4	609	CLA	CAD-CBD-CGD-O2D
23	4	610	CLA	CAD-CBD-CGD-O2D
23	4	611	CLA	CAD-CBD-CGD-O2D
23	5	611	CLA	CAD-CBD-CGD-O2D
23	5	614	CLA	CAD-CBD-CGD-O2D
23	6	617	CLA	CAD-CBD-CGD-O2D
23	7	601	CLA	CAD-CBD-CGD-O2D
23	7	610	CLA	CAD-CBD-CGD-O2D
23	8	607	CLA	CAD-CBD-CGD-O2D
23	8	608	CLA	CAD-CBD-CGD-O2D
30	J	103	DGD	C3G-C2G-O2G-C1B
25	7	622	LHG	C11-C12-C13-C14
23	A	814	CLA	C8-C10-C11-C12
23	7	602	CLA	O1A-CGA-O2A-C1
23	6	601	CLA	CBA-CGA-O2A-C1
23	A	829	CLA	C10-C11-C12-C13
25	A	846	LHG	C4-C5-C6-O8
25	5	625	LHG	C2-C3-O3-P
29	J	104	LMG	O1-C7-C8-C9
29	5	626	LMG	C7-C8-C9-O8
29	5	627	LMG	O1-C7-C8-C9
23	5	601	CLA	O1A-CGA-O2A-C1
25	1	620	LHG	C8-C7-O7-C5
25	8	623	LHG	C16-C17-C18-C19
25	8	623	LHG	O6-C4-C5-O7
25	2	622	LHG	O6-C4-C5-O7
23	B	834	CLA	C8-C10-C11-C12
25	5	623	LHG	C28-C29-C30-C31
23	1	602	CLA	C2A-CAA-CBA-CGA
23	a	602	CLA	C2A-CAA-CBA-CGA
23	4	613	CLA	C2A-CAA-CBA-CGA
23	8	604	CLA	C2A-CAA-CBA-CGA
23	F	301	CLA	O1A-CGA-O2A-C1
30	J	103	DGD	O1A-C1A-O1G-C1G
23	5	613	CLA	CBA-CGA-O2A-C1
23	A	802	CLA	CHA-CBD-CGD-O1D
23	A	802	CLA	CHA-CBD-CGD-O2D
23	A	811	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	A	811	CLA	CHA-CBD-CGD-O2D
23	A	820	CLA	CHA-CBD-CGD-O1D
23	A	820	CLA	CHA-CBD-CGD-O2D
23	A	822	CLA	CHA-CBD-CGD-O1D
23	A	822	CLA	CHA-CBD-CGD-O2D
23	A	823	CLA	CHA-CBD-CGD-O1D
23	A	823	CLA	CHA-CBD-CGD-O2D
23	A	825	CLA	CHA-CBD-CGD-O1D
23	A	825	CLA	CHA-CBD-CGD-O2D
23	A	828	CLA	CHA-CBD-CGD-O2D
23	A	835	CLA	CHA-CBD-CGD-O1D
23	A	835	CLA	CHA-CBD-CGD-O2D
23	A	840	CLA	CHA-CBD-CGD-O1D
23	A	840	CLA	CHA-CBD-CGD-O2D
23	B	806	CLA	CHA-CBD-CGD-O1D
23	B	808	CLA	CHA-CBD-CGD-O1D
23	B	808	CLA	CHA-CBD-CGD-O2D
23	B	828	CLA	CHA-CBD-CGD-O1D
23	B	836	CLA	CHA-CBD-CGD-O1D
23	B	836	CLA	CHA-CBD-CGD-O2D
23	K	204	CLA	CHA-CBD-CGD-O1D
23	K	204	CLA	CHA-CBD-CGD-O2D
23	1	611	CLA	CHA-CBD-CGD-O1D
23	4	603	CLA	CHA-CBD-CGD-O1D
23	4	603	CLA	CHA-CBD-CGD-O2D
23	5	603	CLA	CHA-CBD-CGD-O1D
23	7	607	CLA	CHA-CBD-CGD-O2D
23	8	613	CLA	CHA-CBD-CGD-O1D
23	8	613	CLA	CHA-CBD-CGD-O2D
23	A	831	CLA	C3-C5-C6-C7
23	B	818	CLA	C3-C5-C6-C7
24	A	844	PQN	C15-C16-C17-C18
30	B	850	DGD	O1G-C1G-C2G-O2G
30	J	103	DGD	O1G-C1G-C2G-O2G
23	4	610	CLA	O1D-CGD-O2D-CED
23	A	819	CLA	O1A-CGA-O2A-C1
23	A	841	CLA	O1A-CGA-O2A-C1
23	B	839	CLA	O1A-CGA-O2A-C1
25	1	620	LHG	C12-C13-C14-C15
25	a	620	LHG	C12-C13-C14-C15
23	B	828	CLA	O1D-CGD-O2D-CED
23	A	828	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	A	845	CLA	O1A-CGA-O2A-C1
28	5	628	LMU	C5'-C4'-O1B-C1B
23	A	811	CLA	C6-C7-C8-C9
23	A	811	CLA	C11-C12-C13-C14
23	A	830	CLA	C6-C7-C8-C9
23	A	830	CLA	C14-C13-C15-C16
23	A	843	CLA	C14-C13-C15-C16
23	4	610	CLA	C11-C12-C13-C14
23	6	604	CLA	C11-C12-C13-C14
23	7	602	CLA	C14-C13-C15-C16
23	8	606	CLA	C11-C10-C8-C9
29	J	104	LMG	C30-C31-C32-C33
25	1	620	LHG	C23-C24-C25-C26
23	8	613	CLA	C8-C10-C11-C12
23	K	201	CLA	C2A-CAA-CBA-CGA
23	8	613	CLA	C2A-CAA-CBA-CGA
23	B	830	CLA	CBD-CGD-O2D-CED
23	7	611	CLA	CBA-CGA-O2A-C1
25	a	620	LHG	C23-C24-C25-C26
25	9	622	LHG	C23-C24-C25-C26
26	K	202	BCR	C7-C8-C9-C10
23	B	810	CLA	C3-C5-C6-C7
29	J	104	LMG	C33-C34-C35-C36
23	A	801	CLA	C1A-C2A-CAA-CBA
23	A	803	CLA	C1A-C2A-CAA-CBA
23	A	809	CLA	C1A-C2A-CAA-CBA
23	B	838	CLA	C1A-C2A-CAA-CBA
23	B	839	CLA	C1A-C2A-CAA-CBA
23	1	611	CLA	C1A-C2A-CAA-CBA
23	5	612	CLA	CHA-CBD-CGD-O2D
23	5	617	CLA	C1A-C2A-CAA-CBA
23	6	614	CLA	C1A-C2A-CAA-CBA
23	3	606	CLA	C5-C6-C7-C8
23	8	601	CLA	C5-C6-C7-C8
23	A	806	CLA	CBA-CGA-O2A-C1
23	K	203	CLA	CBA-CGA-O2A-C1
25	5	625	LHG	C15-C16-C17-C18
29	A	860	LMG	C17-C18-C19-C20
23	A	854	CLA	C5-C6-C7-C8
23	B	813	CLA	C8-C10-C11-C12
25	2	622	LHG	C4-O6-P-O3
25	8	622	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	A	858	LMU	C3'-C4'-O1B-C1B
23	4	610	CLA	C2-C3-C5-C6
25	1	620	LHG	C13-C14-C15-C16
25	a	620	LHG	C13-C14-C15-C16
23	B	808	CLA	O1A-CGA-O2A-C1
25	A	847	LHG	C3-O3-P-O5
25	7	622	LHG	C3-O3-P-O5
25	7	622	LHG	C4-O6-P-O4
25	9	622	LHG	C3-O3-P-O4
25	9	622	LHG	C4-O6-P-O5
28	8	625	LMU	O5'-C1'-O1'-C1
29	5	626	LMG	O6-C1-O1-C7
23	A	834	CLA	C10-C11-C12-C13
23	A	836	CLA	C13-C15-C16-C17
23	5	617	CLA	CBA-CGA-O2A-C1
25	6	623	LHG	O6-C4-C5-C6
25	8	622	LHG	O6-C4-C5-C6
25	8	623	LHG	O6-C4-C5-C6
23	7	611	CLA	O1A-CGA-O2A-C1
23	A	829	CLA	C15-C16-C17-C18
23	A	814	CLA	C3-C5-C6-C7
25	4	622	LHG	C12-C13-C14-C15
23	A	811	CLA	CAD-CBD-CGD-O1D
23	A	814	CLA	CAD-CBD-CGD-O1D
23	A	825	CLA	CAD-CBD-CGD-O1D
23	A	828	CLA	CAD-CBD-CGD-O1D
23	A	832	CLA	CAD-CBD-CGD-O1D
23	A	834	CLA	CAD-CBD-CGD-O1D
23	A	845	CLA	CAD-CBD-CGD-O1D
23	B	838	CLA	CAD-CBD-CGD-O1D
23	K	204	CLA	CAD-CBD-CGD-O1D
23	4	616	CLA	CAD-CBD-CGD-O1D
23	6	620	CLA	CAD-CBD-CGD-O1D
23	7	616	CLA	CAD-CBD-CGD-O1D
23	5	603	CLA	C5-C6-C7-C8
28	8	625	LMU	C5'-C4'-O1B-C1B
23	1	603	CLA	C2-C1-O2A-CGA
23	A	829	CLA	C4-C3-C5-C6
23	A	802	CLA	C12-C13-C15-C16
23	A	811	CLA	C11-C12-C13-C15
23	A	812	CLA	C12-C13-C15-C16
23	A	814	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	A	818	CLA	C6-C7-C8-C10
23	A	828	CLA	C6-C7-C8-C10
23	A	830	CLA	C12-C13-C15-C16
23	B	825	CLA	C11-C10-C8-C7
23	1	607	CLA	CAD-CBD-CGD-O2D
23	1	608	CLA	CAD-CBD-CGD-O2D
23	a	608	CLA	CAD-CBD-CGD-O2D
23	a	609	CLA	CAD-CBD-CGD-O2D
23	4	608	CLA	C11-C12-C13-C15
23	4	611	CLA	C3A-C2A-CAA-CBA
23	4	614	CLA	C6-C7-C8-C10
23	5	613	CLA	C11-C12-C13-C15
23	8	606	CLA	C11-C10-C8-C7
25	6	623	LHG	O6-C4-C5-O7
25	8	622	LHG	O6-C4-C5-O7
25	9	622	LHG	O6-C4-C5-O7
23	6	601	CLA	O1A-CGA-O2A-C1
25	1	620	LHG	C24-C25-C26-C27
29	5	627	LMG	C18-C19-C20-C21
29	4	624	LMG	C4-C5-C6-O5
25	a	620	LHG	C24-C25-C26-C27
28	8	624	LMU	C1-C2-C3-C4
23	A	806	CLA	O1A-CGA-O2A-C1
23	6	602	CLA	O1A-CGA-O2A-C1
25	4	622	LHG	O2-C2-C3-O3
25	A	846	LHG	C19-C20-C21-C22
29	4	623	LMG	C15-C16-C17-C18
23	a	614	CLA	C5-C6-C7-C8
23	B	808	CLA	C16-C17-C18-C20
23	8	613	CLA	C3-C5-C6-C7
23	B	832	CLA	CAA-CBA-CGA-O2A
23	8	601	CLA	CAA-CBA-CGA-O2A
23	K	203	CLA	O1A-CGA-O2A-C1
25	1	620	LHG	O7-C5-C6-O8
25	a	620	LHG	O7-C5-C6-O8
29	5	627	LMG	O1-C7-C8-O7
30	J	103	DGD	O2G-C2G-C3G-O3G
25	a	620	LHG	C30-C31-C32-C33
23	6	620	CLA	O1D-CGD-O2D-CED
25	1	620	LHG	C30-C31-C32-C33
25	5	625	LHG	C12-C13-C14-C15
29	4	624	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
23	6	616	CLA	C10-C11-C12-C13
23	7	610	CLA	C15-C16-C17-C18
25	2	622	LHG	C5-C4-O6-P
23	5	617	CLA	O1A-CGA-O2A-C1
24	B	842	PQN	C14-C13-C15-C16
23	A	819	CLA	C11-C10-C8-C9
23	A	829	CLA	C14-C13-C15-C16
23	A	834	CLA	C11-C12-C13-C14
23	A	841	CLA	C11-C10-C8-C9
23	B	802	CLA	C14-C13-C15-C16
23	B	814	CLA	C14-C13-C15-C16
23	B	829	CLA	C6-C7-C8-C9
23	B	831	CLA	C14-C13-C15-C16
23	B	833	CLA	C11-C10-C8-C9
23	B	839	CLA	C6-C7-C8-C9
23	a	609	CLA	C14-C13-C15-C16
23	3	609	CLA	C11-C10-C8-C9
23	4	602	CLA	C11-C10-C8-C9
23	5	604	CLA	C11-C10-C8-C9
23	6	601	CLA	C14-C13-C15-C16
23	6	613	CLA	C6-C7-C8-C9
23	7	602	CLA	C11-C10-C8-C9
23	8	613	CLA	C11-C10-C8-C9
29	A	860	LMG	C33-C34-C35-C36
25	6	623	LHG	C17-C18-C19-C20
25	6	623	LHG	C34-C35-C36-C37
23	B	816	CLA	CBA-CGA-O2A-C1
23	3	613	CLA	CBA-CGA-O2A-C1
25	3	623	LHG	O8-C23-C24-C25
25	A	846	LHG	O1-C1-C2-O2
23	B	839	CLA	C5-C6-C7-C8
25	5	625	LHG	C31-C32-C33-C34
25	1	620	LHG	C28-C29-C30-C31
25	5	623	LHG	C19-C20-C21-C22
25	a	620	LHG	C28-C29-C30-C31
25	3	624	LHG	C13-C14-C15-C16
23	1	604	CLA	C1-C2-C3-C4
23	a	604	CLA	C1-C2-C3-C4
23	8	614	CLA	O1A-CGA-O2A-C1
23	A	802	CLA	C2A-CAA-CBA-CGA
23	A	829	CLA	C2A-CAA-CBA-CGA
23	A	841	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	3	602	CLA	C2A-CAA-CBA-CGA
23	7	602	CLA	C2A-CAA-CBA-CGA
23	A	829	CLA	C13-C15-C16-C17
23	B	831	CLA	C2-C1-O2A-CGA
25	6	623	LHG	C7-C8-C9-C10
25	7	622	LHG	C10-C11-C12-C13
25	2	622	LHG	C24-C25-C26-C27
23	A	835	CLA	C8-C10-C11-C12
29	7	624	LMG	C18-C19-C20-C21
23	7	613	CLA	C4-C3-C5-C6
25	3	624	LHG	C30-C31-C32-C33
25	8	622	LHG	C12-C13-C14-C15
23	3	610	CLA	O1D-CGD-O2D-CED
26	B	844	BCR	C23-C24-C25-C26
26	7	621	BCR	C23-C24-C25-C26
26	8	621	BCR	C23-C24-C25-C30
23	A	828	CLA	C2-C3-C5-C6
25	a	620	LHG	C34-C35-C36-C37
23	1	613	CLA	C16-C17-C18-C19
23	a	613	CLA	C16-C17-C18-C19
23	8	606	CLA	C16-C17-C18-C20
25	1	620	LHG	C34-C35-C36-C37
23	A	820	CLA	C5-C6-C7-C8
23	B	817	CLA	C8-C10-C11-C12
23	4	604	CLA	C2A-CAA-CBA-CGA
23	5	616	CLA	C2A-CAA-CBA-CGA
28	A	857	LMU	C2'-C1'-O1'-C1
25	4	622	LHG	C16-C17-C18-C19
25	4	622	LHG	C3-O3-P-O6
25	5	623	LHG	C3-O3-P-O6
25	6	623	LHG	C3-O3-P-O6
25	8	623	LHG	C3-O3-P-O6
25	8	623	LHG	C4-O6-P-O3
25	9	622	LHG	C3-O3-P-O6
23	B	830	CLA	O1D-CGD-O2D-CED
25	8	622	LHG	C9-C10-C11-C12
25	5	625	LHG	C26-C27-C28-C29
25	9	622	LHG	C4-C5-C6-O8
23	A	803	CLA	C4-C3-C5-C6
25	3	623	LHG	C27-C28-C29-C30
23	4	613	CLA	C13-C15-C16-C17
23	A	831	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	5	607	CLA	C6-C7-C8-C10
23	A	802	CLA	C14-C13-C15-C16
23	A	812	CLA	C14-C13-C15-C16
23	B	813	CLA	C11-C10-C8-C9
23	4	608	CLA	C11-C10-C8-C9
23	4	608	CLA	C11-C12-C13-C14
23	4	609	CLA	C6-C7-C8-C9
23	4	614	CLA	C6-C7-C8-C9
23	6	610	CLA	C6-C7-C8-C9
23	8	601	CLA	C11-C12-C13-C14
24	A	844	PQN	C21-C22-C23-C24
26	A	852	BCR	C19-C20-C21-C22
26	K	207	BCR	C9-C10-C11-C12
23	B	808	CLA	C16-C17-C18-C19
23	5	602	CLA	O1D-CGD-O2D-CED
23	A	819	CLA	CAA-CBA-CGA-O2A
23	3	608	CLA	CBA-CGA-O2A-C1
25	4	622	LHG	C2-C3-O3-P
25	9	622	LHG	C2-C3-O3-P
26	L	305	BCR	C17-C18-C19-C20
23	A	835	CLA	C12-C13-C15-C16
23	A	820	CLA	C15-C16-C17-C18
23	B	806	CLA	C10-C11-C12-C13
23	B	814	CLA	CBA-CGA-O2A-C1
23	8	614	CLA	CBA-CGA-O2A-C1
25	4	622	LHG	C10-C11-C12-C13
25	7	622	LHG	C24-C25-C26-C27
23	5	613	CLA	C15-C16-C17-C18
23	3	602	CLA	O1A-CGA-O2A-C1
25	1	620	LHG	C11-C12-C13-C14
25	a	620	LHG	C11-C12-C13-C14
23	7	610	CLA	C2A-CAA-CBA-CGA
23	1	613	CLA	C16-C17-C18-C20
23	a	613	CLA	C16-C17-C18-C20
23	4	613	CLA	C10-C11-C12-C13
26	5	622	BCR	C13-C14-C15-C16
31	7	619	LUT	C29-C30-C31-C32
25	A	846	LHG	C33-C34-C35-C36
25	5	623	LHG	C11-C10-C9-C8
25	5	625	LHG	C24-C25-C26-C27
23	6	617	CLA	CAA-CBA-CGA-O1A
23	A	821	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	B	811	CLA	C2-C1-O2A-CGA
23	a	610	CLA	C2-C1-O2A-CGA
23	4	609	CLA	C2-C1-O2A-CGA
23	8	610	CLA	C2-C1-O2A-CGA
23	3	608	CLA	O1A-CGA-O2A-C1
23	8	606	CLA	C16-C17-C18-C19
25	4	622	LHG	C30-C31-C32-C33
23	A	813	CLA	C2A-CAA-CBA-CGA
23	A	820	CLA	C2A-CAA-CBA-CGA
23	a	609	CLA	C2A-CAA-CBA-CGA
23	7	613	CLA	C2A-CAA-CBA-CGA
30	J	103	DGD	C1B-C2B-C3B-C4B
25	3	624	LHG	C2-C3-O3-P
25	5	625	LHG	C10-C11-C12-C13
23	A	806	CLA	C3A-C2A-CAA-CBA
23	B	809	CLA	C3A-C2A-CAA-CBA
23	B	826	CLA	C3A-C2A-CAA-CBA
23	B	828	CLA	C3A-C2A-CAA-CBA
23	5	609	CLA	C16-C17-C18-C20
32	1	618	XAT	C29-C30-C31-C32
32	a	618	XAT	C29-C30-C31-C32
23	B	835	CLA	CAA-CBA-CGA-O2A
23	6	614	CLA	C3-C5-C6-C7
25	1	620	LHG	C16-C17-C18-C19
25	a	620	LHG	C16-C17-C18-C19
28	K	208	LMU	C4B-C5B-C6B-O6B
23	A	818	CLA	C6-C7-C8-C9
23	B	805	CLA	C14-C13-C15-C16
23	B	808	CLA	C6-C7-C8-C9
23	5	613	CLA	C11-C10-C8-C9
25	A	846	LHG	C15-C16-C17-C18
23	B	814	CLA	O1A-CGA-O2A-C1
26	A	852	BCR	C11-C10-C9-C34
26	A	852	BCR	C16-C17-C18-C36
26	B	844	BCR	C11-C10-C9-C34
26	B	845	BCR	C11-C10-C9-C34
26	B	845	BCR	C20-C21-C22-C37
26	F	305	BCR	C16-C17-C18-C36
26	L	301	BCR	C11-C10-C9-C34
26	3	621	BCR	C35-C13-C14-C15
26	3	621	BCR	C16-C17-C18-C36
26	3	622	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	3	622	BCR	C16-C17-C18-C36
33	5	624	NEX	C39-C29-C30-C31
33	6	624	NEX	C39-C29-C30-C31
23	B	835	CLA	CAA-CBA-CGA-O1A
23	3	612	CLA	C2A-CAA-CBA-CGA
23	A	815	CLA	C2A-CAA-CBA-CGA
23	B	817	CLA	C2A-CAA-CBA-CGA
23	a	614	CLA	C2A-CAA-CBA-CGA
23	A	842	CLA	CAA-CBA-CGA-O1A
23	5	609	CLA	C16-C17-C18-C19
23	B	803	CLA	O2A-C1-C2-C3
30	B	850	DGD	O6E-C1E-O5D-C6D
23	K	203	CLA	C13-C15-C16-C17
26	B	846	BCR	C7-C8-C9-C34
23	6	620	CLA	C5-C6-C7-C8
25	4	622	LHG	C24-C25-C26-C27
30	B	850	DGD	C1G-C2G-O2G-C1B
23	B	831	CLA	C4-C3-C5-C6
23	A	822	CLA	C1A-C2A-CAA-CBA
23	A	836	CLA	C1A-C2A-CAA-CBA
23	B	809	CLA	C1A-C2A-CAA-CBA
23	B	826	CLA	C1A-C2A-CAA-CBA
23	B	828	CLA	C1A-C2A-CAA-CBA
23	1	603	CLA	C1A-C2A-CAA-CBA
23	1	616	CLA	C1A-C2A-CAA-CBA
23	a	616	CLA	C1A-C2A-CAA-CBA
23	6	608	CLA	C1A-C2A-CAA-CBA
23	7	608	CLA	C1A-C2A-CAA-CBA
23	A	806	CLA	CAA-CBA-CGA-O2A
23	B	806	CLA	C11-C10-C8-C7
23	B	808	CLA	C6-C7-C8-C10
23	B	813	CLA	C6-C7-C8-C10
23	B	828	CLA	C12-C13-C15-C16
23	5	602	CLA	C11-C10-C8-C7
23	5	604	CLA	C6-C7-C8-C10
23	6	613	CLA	C11-C10-C8-C7
23	7	612	CLA	CAA-CBA-CGA-O1A
28	A	857	LMU	C11-C10-C9-C8
25	3	623	LHG	C4-O6-P-O3
25	5	623	LHG	C4-O6-P-O3
23	5	619	CLA	CAA-CBA-CGA-O2A
25	B	851	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	7	624	LMG	C14-C15-C16-C17
23	A	839	CLA	C2A-CAA-CBA-CGA
23	A	842	CLA	C2A-CAA-CBA-CGA
23	B	807	CLA	C2A-CAA-CBA-CGA
23	a	609	CLA	C15-C16-C17-C18
25	3	624	LHG	O6-C4-C5-O7
25	7	622	LHG	O6-C4-C5-C6
25	4	622	LHG	C19-C20-C21-C22
23	B	805	CLA	CBD-CGD-O2D-CED
23	A	835	CLA	C5-C6-C7-C8
30	B	850	DGD	O1A-C1A-O1G-C1G
23	4	603	CLA	CAA-CBA-CGA-O1A
23	5	619	CLA	CAA-CBA-CGA-O1A
25	A	846	LHG	O10-C23-O8-C6
29	7	624	LMG	O10-C28-O8-C9
23	A	821	CLA	CBD-CGD-O2D-CED
23	5	613	CLA	CAA-CBA-CGA-O2A
26	A	852	BCR	C11-C10-C9-C8
26	A	852	BCR	C16-C17-C18-C19
26	B	844	BCR	C11-C10-C9-C8
26	B	845	BCR	C11-C10-C9-C8
26	B	845	BCR	C20-C21-C22-C23
26	F	305	BCR	C16-C17-C18-C19
26	L	301	BCR	C11-C10-C9-C8
26	3	621	BCR	C12-C13-C14-C15
26	3	621	BCR	C16-C17-C18-C19
26	3	622	BCR	C12-C13-C14-C15
26	3	622	BCR	C16-C17-C18-C19
33	5	624	NEX	C28-C29-C30-C31
33	6	624	NEX	C28-C29-C30-C31
28	8	624	LMU	C9-C10-C11-C12
26	B	846	BCR	C9-C10-C11-C12
32	7	620	XAT	C29-C30-C31-C32
25	5	623	LHG	C1-C2-C3-O3
23	B	805	CLA	C10-C11-C12-C13
23	5	608	CLA	C2-C1-O2A-CGA
23	7	604	CLA	C2-C1-O2A-CGA
23	B	837	CLA	C8-C10-C11-C12
23	B	827	CLA	CAA-CBA-CGA-O2A
23	A	814	CLA	C14-C13-C15-C16
23	B	817	CLA	C11-C12-C13-C14
23	B	825	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	B	839	CLA	C3-C5-C6-C7
23	7	612	CLA	CAA-CBA-CGA-O2A
29	7	624	LMG	C17-C18-C19-C20
23	6	604	CLA	C15-C16-C17-C18
23	4	610	CLA	C2A-CAA-CBA-CGA
23	6	613	CLA	C2A-CAA-CBA-CGA
23	B	826	CLA	C6-C7-C8-C9
23	6	617	CLA	CAA-CBA-CGA-O2A
26	A	848	BCR	C1-C6-C7-C8
26	B	844	BCR	C23-C24-C25-C30
26	K	207	BCR	C1-C6-C7-C8
26	1	619	BCR	C23-C24-C25-C30
26	a	619	BCR	C23-C24-C25-C30
26	4	621	BCR	C23-C24-C25-C30
26	5	622	BCR	C23-C24-C25-C26
26	5	622	BCR	C23-C24-C25-C30
31	1	617	LUT	C1-C6-C7-C8
31	a	617	LUT	C1-C6-C7-C8
31	9	619	LUT	C1-C6-C7-C8
23	A	821	CLA	O1D-CGD-O2D-CED
23	A	825	CLA	C13-C15-C16-C17
25	A	846	LHG	O1-C1-C2-C3
25	5	623	LHG	O1-C1-C2-C3
26	B	844	BCR	C9-C10-C11-C12
25	3	623	LHG	C29-C30-C31-C32
23	3	607	CLA	C4-C3-C5-C6
23	6	613	CLA	C4-C3-C5-C6
23	A	823	CLA	C1A-C2A-CAA-CBA
26	A	856	BCR	C11-C12-C13-C14
23	A	803	CLA	C2-C3-C5-C6
23	7	613	CLA	C2-C3-C5-C6
23	3	604	CLA	C3-C5-C6-C7
29	7	624	LMG	C8-C7-O1-C1
23	A	819	CLA	C11-C12-C13-C14
23	1	612	CLA	CAA-CBA-CGA-O2A
23	a	612	CLA	CAA-CBA-CGA-O2A
23	4	603	CLA	CAA-CBA-CGA-O2A
23	6	609	CLA	CAA-CBA-CGA-O2A
23	A	826	CLA	C13-C15-C16-C17
23	B	803	CLA	C5-C6-C7-C8
25	A	846	LHG	O6-C4-C5-O7
23	A	835	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	A	860	LMG	C18-C19-C20-C21
23	K	203	CLA	C4-C3-C5-C6
28	K	208	LMU	C2-C3-C4-C5
23	B	833	CLA	C11-C12-C13-C15
23	L	302	CLA	CAA-CBA-CGA-O2A
30	J	103	DGD	C8A-C9A-CAA-CBA
23	A	827	CLA	C3-C5-C6-C7
25	8	622	LHG	C19-C20-C21-C22
26	A	849	BCR	C9-C10-C11-C12
23	A	839	CLA	C6-C7-C8-C10
23	a	612	CLA	CAA-CBA-CGA-O1A
23	6	616	CLA	C8-C10-C11-C12
23	1	612	CLA	CAA-CBA-CGA-O1A
23	B	813	CLA	CAA-CBA-CGA-O2A
23	7	616	CLA	C2A-CAA-CBA-CGA
23	4	616	CLA	CAA-CBA-CGA-O2A
23	A	809	CLA	CBA-CGA-O2A-C1
23	A	818	CLA	CAA-CBA-CGA-O2A
28	5	628	LMU	C2B-C1B-O1B-C4'
23	A	834	CLA	C4-C3-C5-C6
23	B	805	CLA	C4-C3-C5-C6
23	B	809	CLA	C4-C3-C5-C6
23	3	604	CLA	C4-C3-C5-C6
23	3	608	CLA	C4-C3-C5-C6
23	5	610	CLA	C4-C3-C5-C6
23	5	613	CLA	C4-C3-C5-C6
23	A	854	CLA	C10-C11-C12-C13
23	B	828	CLA	C8-C10-C11-C12
28	K	208	LMU	C7-C8-C9-C10
23	L	303	CLA	CAA-CBA-CGA-O2A
23	1	616	CLA	CAA-CBA-CGA-O2A
23	a	616	CLA	CAA-CBA-CGA-O2A
25	4	622	LHG	C4-O6-P-O3
23	A	829	CLA	C2-C3-C5-C6
23	A	812	CLA	C6-C7-C8-C9
23	A	826	CLA	C14-C13-C15-C16
23	A	831	CLA	C11-C10-C8-C9
23	B	818	CLA	C6-C7-C8-C9
23	B	825	CLA	C11-C10-C8-C9
23	5	613	CLA	C11-C12-C13-C14
23	7	602	CLA	C6-C7-C8-C9
23	B	805	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	3	623	LHG	C18-C19-C20-C21
23	7	615	CLA	CAA-CBA-CGA-O1A
23	8	603	CLA	CAA-CBA-CGA-O2A
23	A	841	CLA	C3A-C2A-CAA-CBA
23	B	835	CLA	C3A-C2A-CAA-CBA
23	1	603	CLA	C3A-C2A-CAA-CBA
23	4	609	CLA	C3A-C2A-CAA-CBA
23	5	616	CLA	CBD-CGD-O2D-CED
23	6	617	CLA	C3A-C2A-CAA-CBA
23	A	809	CLA	O1A-CGA-O2A-C1
23	A	843	CLA	CAA-CBA-CGA-O2A
25	8	622	LHG	O8-C23-C24-C25
23	4	607	CLA	CAA-CBA-CGA-O2A
23	A	818	CLA	CAD-CBD-CGD-O2D
23	A	826	CLA	CAD-CBD-CGD-O2D
23	A	838	CLA	CAD-CBD-CGD-O2D
23	B	825	CLA	CAD-CBD-CGD-O2D
23	B	826	CLA	CAD-CBD-CGD-O2D
23	B	835	CLA	CAD-CBD-CGD-O2D
23	B	840	CLA	CAD-CBD-CGD-O2D
23	B	841	CLA	CAD-CBD-CGD-O2D
23	F	301	CLA	CAD-CBD-CGD-O2D
23	F	303	CLA	CAD-CBD-CGD-O2D
23	G	203	CLA	CAD-CBD-CGD-O2D
23	1	604	CLA	CAD-CBD-CGD-O2D
23	1	610	CLA	CAD-CBD-CGD-O2D
23	1	613	CLA	CAD-CBD-CGD-O2D
23	a	604	CLA	CAD-CBD-CGD-O2D
23	a	610	CLA	CAD-CBD-CGD-O2D
23	a	613	CLA	CAD-CBD-CGD-O2D
23	5	601	CLA	CAD-CBD-CGD-O2D
23	5	610	CLA	CAD-CBD-CGD-O2D
23	5	617	CLA	CAD-CBD-CGD-O2D
23	6	610	CLA	CAD-CBD-CGD-O2D
23	6	611	CLA	CAD-CBD-CGD-O2D
23	7	602	CLA	CAD-CBD-CGD-O2D
23	7	612	CLA	CAD-CBD-CGD-O2D
23	8	601	CLA	CAD-CBD-CGD-O2D
23	A	809	CLA	C16-C17-C18-C19
23	B	826	CLA	C6-C7-C8-C10
23	1	611	CLA	C10-C11-C12-C13
23	3	610	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	A	850	BCR	C13-C14-C15-C16
32	6	621	XAT	C29-C30-C31-C32
28	5	628	LMU	C7-C8-C9-C10
30	J	103	DGD	C9A-CAA-CBA-CCA
23	6	608	CLA	C2-C1-O2A-CGA
23	8	609	CLA	CAA-CBA-CGA-O2A
23	A	841	CLA	CAA-CBA-CGA-O2A
23	6	608	CLA	CAA-CBA-CGA-O2A
23	A	843	CLA	C11-C10-C8-C7
23	A	814	CLA	C4-C3-C5-C6
23	F	301	CLA	C4-C3-C5-C6
23	5	616	CLA	CAA-CBA-CGA-O2A
23	3	608	CLA	C2-C3-C5-C6
23	A	835	CLA	CAA-CBA-CGA-O2A
23	8	614	CLA	CAA-CBA-CGA-O2A
25	8	623	LHG	O7-C7-C8-C9
26	A	849	BCR	C7-C8-C9-C10
26	J	102	BCR	C11-C12-C13-C14
26	L	301	BCR	C17-C18-C19-C20
26	7	621	BCR	C7-C8-C9-C10
29	J	104	LMG	C7-C8-C9-O8
32	3	619	XAT	O24-C26-C27-C28
32	6	621	XAT	O4-C6-C7-C8
23	6	609	CLA	CAA-CBA-CGA-O1A
25	7	622	LHG	O6-C4-C5-O7
23	A	821	CLA	CAA-CBA-CGA-O2A
23	A	834	CLA	CAA-CBA-CGA-O2A
23	G	204	CLA	CAA-CBA-CGA-O2A
23	A	826	CLA	O2A-C1-C2-C3
23	B	817	CLA	O2A-C1-C2-C3
29	J	104	LMG	C14-C15-C16-C17
23	A	805	CLA	C2A-CAA-CBA-CGA
23	6	603	CLA	CAA-CBA-CGA-O2A
23	6	613	CLA	CAA-CBA-CGA-O2A
23	G	204	CLA	CAA-CBA-CGA-O1A
23	4	607	CLA	CAA-CBA-CGA-O1A
25	1	620	LHG	C9-C10-C11-C12
23	B	806	CLA	CHA-CBD-CGD-O2D
23	B	807	CLA	CHA-CBD-CGD-O2D
23	B	810	CLA	CHA-CBD-CGD-O2D
23	B	813	CLA	CHA-CBD-CGD-O1D
23	B	819	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	819	CLA	CHA-CBD-CGD-O2D
23	B	820	CLA	CHA-CBD-CGD-O1D
23	B	820	CLA	CHA-CBD-CGD-O2D
23	B	827	CLA	CHA-CBD-CGD-O1D
23	B	827	CLA	CHA-CBD-CGD-O2D
23	B	828	CLA	CHA-CBD-CGD-O2D
23	1	609	CLA	CHA-CBD-CGD-O1D
23	1	609	CLA	CHA-CBD-CGD-O2D
23	1	611	CLA	CHA-CBD-CGD-O2D
23	a	603	CLA	CHA-CBD-CGD-O1D
23	a	607	CLA	CHA-CBD-CGD-O1D
23	a	607	CLA	CHA-CBD-CGD-O2D
23	3	602	CLA	CHA-CBD-CGD-O2D
23	3	609	CLA	CHA-CBD-CGD-O1D
23	3	609	CLA	CHA-CBD-CGD-O2D
23	4	602	CLA	CHA-CBD-CGD-O2D
23	4	604	CLA	CHA-CBD-CGD-O2D
23	5	603	CLA	CHA-CBD-CGD-O2D
23	5	604	CLA	CHA-CBD-CGD-O1D
23	5	604	CLA	CHA-CBD-CGD-O2D
23	5	607	CLA	CHA-CBD-CGD-O1D
23	5	607	CLA	CHA-CBD-CGD-O2D
23	5	613	CLA	CHA-CBD-CGD-O1D
23	5	613	CLA	CHA-CBD-CGD-O2D
23	5	619	CLA	CHA-CBD-CGD-O1D
23	5	619	CLA	CHA-CBD-CGD-O2D
23	6	603	CLA	CHA-CBD-CGD-O1D
23	6	603	CLA	CHA-CBD-CGD-O2D
23	6	607	CLA	CHA-CBD-CGD-O1D
23	6	607	CLA	CHA-CBD-CGD-O2D
23	8	603	CLA	CHA-CBD-CGD-O1D
23	8	603	CLA	CHA-CBD-CGD-O2D
23	3	604	CLA	C15-C16-C17-C18
23	L	302	CLA	CAA-CBA-CGA-O1A
23	5	616	CLA	CAA-CBA-CGA-O1A
23	6	613	CLA	C2-C3-C5-C6
25	a	620	LHG	C9-C10-C11-C12
29	7	624	LMG	C15-C16-C17-C18
25	9	622	LHG	O6-C4-C5-C6
23	4	616	CLA	CAA-CBA-CGA-O1A
23	7	615	CLA	CAA-CBA-CGA-O2A
23	A	830	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	B	834	CLA	CAA-CBA-CGA-O2A
23	6	616	CLA	CAA-CBA-CGA-O2A
23	6	620	CLA	CAA-CBA-CGA-O2A
29	A	860	LMG	O8-C28-C29-C30
23	L	303	CLA	CAA-CBA-CGA-O1A
23	A	806	CLA	C8-C10-C11-C12
23	A	810	CLA	CAA-CBA-CGA-O2A
23	3	606	CLA	CAA-CBA-CGA-O2A
25	B	851	LHG	O8-C23-C24-C25
23	B	820	CLA	C2A-CAA-CBA-CGA
23	1	616	CLA	CAA-CBA-CGA-O1A
23	8	603	CLA	CAA-CBA-CGA-O1A
25	A	847	LHG	C11-C12-C13-C14
23	5	613	CLA	C2-C1-O2A-CGA
23	B	831	CLA	C11-C10-C8-C7
23	7	602	CLA	C6-C7-C8-C10
25	A	847	LHG	O9-C7-O7-C5
23	A	845	CLA	CAA-CBA-CGA-O2A
23	a	616	CLA	CAA-CBA-CGA-O1A
23	B	803	CLA	C11-C10-C8-C9
23	B	831	CLA	C11-C10-C8-C9
23	4	608	CLA	C14-C13-C15-C16
23	4	613	CLA	C14-C13-C15-C16
23	5	607	CLA	C6-C7-C8-C9
23	6	613	CLA	C11-C10-C8-C9
26	B	845	BCR	C9-C10-C11-C12
23	B	813	CLA	C10-C11-C12-C13
23	A	815	CLA	CBA-CGA-O2A-C1
23	A	813	CLA	C3-C5-C6-C7
23	B	837	CLA	C2A-CAA-CBA-CGA
28	5	628	LMU	C2-C3-C4-C5
25	B	851	LHG	O7-C7-C8-C9
23	8	609	CLA	CAA-CBA-CGA-O1A
23	A	841	CLA	CAA-CBA-CGA-O1A
23	A	843	CLA	C4-C3-C5-C6
23	B	837	CLA	C4-C3-C5-C6
23	K	203	CLA	C2-C3-C5-C6
24	A	844	PQN	C12-C13-C15-C16
23	B	807	CLA	CAA-CBA-CGA-O2A
25	8	623	LHG	O9-C7-C8-C9
25	8	623	LHG	C30-C31-C32-C33
23	A	813	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	843	CLA	C6-C7-C8-C10
23	A	816	CLA	CAD-CBD-CGD-O2D
23	A	833	CLA	C1A-C2A-CAA-CBA
23	A	841	CLA	C1A-C2A-CAA-CBA
23	B	811	CLA	CHA-CBD-CGD-O2D
23	L	303	CLA	C1A-C2A-CAA-CBA
23	1	607	CLA	CHA-CBD-CGD-O2D
23	1	612	CLA	C1A-C2A-CAA-CBA
23	a	609	CLA	CHA-CBD-CGD-O2D
23	a	612	CLA	C1A-C2A-CAA-CBA
23	3	606	CLA	CHA-CBD-CGD-O2D
23	4	609	CLA	C1A-C2A-CAA-CBA
23	4	613	CLA	C1A-C2A-CAA-CBA
23	6	617	CLA	C1A-C2A-CAA-CBA
23	7	609	CLA	CAD-CBD-CGD-O2D
23	7	615	CLA	CAD-CBD-CGD-O2D
23	7	616	CLA	C1A-C2A-CAA-CBA
23	8	603	CLA	C1A-C2A-CAA-CBA
23	8	606	CLA	C1A-C2A-CAA-CBA
23	A	839	CLA	C6-C7-C8-C9
23	A	845	CLA	CAA-CBA-CGA-O1A
23	6	603	CLA	CAA-CBA-CGA-O1A
25	6	623	LHG	O10-C23-C24-C25
23	A	827	CLA	C2-C1-O2A-CGA
23	A	854	CLA	C2-C1-O2A-CGA
25	9	622	LHG	C33-C34-C35-C36
23	B	838	CLA	CBA-CGA-O2A-C1
23	A	835	CLA	CAA-CBA-CGA-O1A
23	B	813	CLA	CAA-CBA-CGA-O1A
23	B	834	CLA	CAA-CBA-CGA-O1A
23	4	602	CLA	CAA-CBA-CGA-O2A
23	A	822	CLA	C2A-CAA-CBA-CGA
23	4	603	CLA	C2A-CAA-CBA-CGA
23	A	818	CLA	C11-C12-C13-C15
23	A	818	CLA	CAA-CBA-CGA-O1A
23	A	821	CLA	CAA-CBA-CGA-O1A
23	A	843	CLA	CAA-CBA-CGA-O1A
23	6	608	CLA	CAA-CBA-CGA-O1A
25	6	623	LHG	O9-C7-C8-C9
23	a	609	CLA	C5-C6-C7-C8
23	5	614	CLA	CAA-CBA-CGA-O2A
23	B	808	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	810	CLA	C10-C11-C12-C13
23	A	834	CLA	CAA-CBA-CGA-O1A
23	8	614	CLA	CAA-CBA-CGA-O1A
29	A	860	LMG	O10-C28-C29-C30
23	a	607	CLA	CAA-CBA-CGA-O2A
30	B	850	DGD	C2E-C1E-O5D-C6D
23	A	806	CLA	C10-C11-C12-C13
25	B	851	LHG	C3-O3-P-O5
25	3	623	LHG	C4-O6-P-O4
25	3	623	LHG	C4-O6-P-O5
25	4	622	LHG	C3-O3-P-O5
25	6	623	LHG	C4-O6-P-O5
25	8	623	LHG	C4-O6-P-O5
25	2	622	LHG	C4-O6-P-O4
23	A	809	CLA	C16-C17-C18-C20
23	A	810	CLA	CAA-CBA-CGA-O1A
23	3	606	CLA	CAA-CBA-CGA-O1A
23	B	802	CLA	CAA-CBA-CGA-O2A
23	7	602	CLA	CAA-CBA-CGA-O2A
23	7	608	CLA	CAA-CBA-CGA-O2A
25	6	623	LHG	O7-C7-C8-C9
26	A	848	BCR	C5-C6-C7-C8
26	B	847	BCR	C23-C24-C25-C30
26	K	207	BCR	C5-C6-C7-C8
31	9	619	LUT	C5-C6-C7-C8
23	A	813	CLA	C6-C7-C8-C9
23	5	602	CLA	C13-C15-C16-C17
25	B	851	LHG	O9-C7-C8-C9
25	8	622	LHG	O10-C23-C24-C25
25	8	623	LHG	C15-C16-C17-C18
23	1	613	CLA	C2A-CAA-CBA-CGA
23	a	613	CLA	C2A-CAA-CBA-CGA
23	6	620	CLA	CAA-CBA-CGA-O1A
23	B	833	CLA	CAA-CBA-CGA-O2A
25	9	622	LHG	C16-C17-C18-C19
23	6	613	CLA	CAA-CBA-CGA-O1A
28	8	624	LMU	C2-C3-C4-C5
23	A	811	CLA	C8-C10-C11-C12
23	A	817	CLA	CAD-CBD-CGD-O1D
23	B	813	CLA	CAD-CBD-CGD-O1D
23	B	816	CLA	CAD-CBD-CGD-O1D
23	B	819	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	820	CLA	CAD-CBD-CGD-O1D
23	1	609	CLA	CAD-CBD-CGD-O1D
23	4	602	CLA	CAD-CBD-CGD-O1D
23	5	608	CLA	C2-C3-C5-C6
23	6	602	CLA	CAD-CBD-CGD-O1D
23	7	602	CLA	CAD-CBD-CGD-O1D
23	A	830	CLA	CAA-CBA-CGA-O1A
23	4	602	CLA	C10-C11-C12-C13
23	A	802	CLA	C11-C10-C8-C9
23	A	822	CLA	C11-C12-C13-C14
23	B	802	CLA	C11-C12-C13-C14
23	B	834	CLA	C6-C7-C8-C9
23	B	840	CLA	C6-C7-C8-C9
23	4	601	CLA	C11-C12-C13-C14
23	6	614	CLA	C11-C10-C8-C9
28	A	859	LMU	O1'-C1-C2-C3
23	A	822	CLA	CAA-CBA-CGA-O2A
23	a	602	CLA	CAA-CBA-CGA-O2A
25	3	624	LHG	O8-C23-C24-C25
23	a	607	CLA	CAA-CBA-CGA-O1A
23	B	838	CLA	CAA-CBA-CGA-O2A
23	6	601	CLA	CAA-CBA-CGA-O2A
23	6	610	CLA	CAA-CBA-CGA-O2A
25	A	846	LHG	O7-C7-C8-C9
23	6	616	CLA	CAA-CBA-CGA-O1A
23	A	825	CLA	C8-C10-C11-C12
23	A	812	CLA	C6-C7-C8-C10
23	B	831	CLA	C2-C3-C5-C6
23	B	840	CLA	C6-C7-C8-C10
23	1	601	CLA	CAD-CBD-CGD-O2D
23	1	603	CLA	CHA-CBD-CGD-O1D
23	1	607	CLA	CHA-CBD-CGD-O1D
23	1	608	CLA	CHA-CBD-CGD-O1D
23	a	601	CLA	CAD-CBD-CGD-O2D
23	a	608	CLA	CHA-CBD-CGD-O1D
23	a	609	CLA	CHA-CBD-CGD-O1D
23	3	602	CLA	C11-C10-C8-C7
23	3	606	CLA	CHA-CBD-CGD-O1D
23	3	607	CLA	C2-C3-C5-C6
23	3	610	CLA	C11-C12-C13-C15
23	3	611	CLA	CHA-CBD-CGD-O1D
23	4	601	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	4	606	CLA	CAD-CBD-CGD-O2D
23	4	608	CLA	C12-C13-C15-C16
23	5	607	CLA	C11-C10-C8-C7
23	6	613	CLA	C6-C7-C8-C10
23	7	603	CLA	CHA-CBD-CGD-O1D
23	7	613	CLA	C6-C7-C8-C10
23	B	807	CLA	CAA-CBA-CGA-O1A
23	L	304	CLA	CAA-CBA-CGA-O2A
23	5	614	CLA	CAA-CBA-CGA-O1A
23	A	836	CLA	CAA-CBA-CGA-O2A
23	a	614	CLA	CAA-CBA-CGA-O2A
23	3	609	CLA	CAA-CBA-CGA-O2A
25	7	622	LHG	O8-C23-C24-C25
29	5	626	LMG	O8-C28-C29-C30
26	B	846	BCR	C7-C8-C9-C10
26	7	621	BCR	C17-C18-C19-C20
23	3	609	CLA	CAA-CBA-CGA-O1A
25	5	625	LHG	O9-C7-C8-C9
23	1	608	CLA	CAA-CBA-CGA-O2A
23	a	608	CLA	CAA-CBA-CGA-O2A
26	J	102	BCR	C15-C16-C17-C18
23	B	817	CLA	CAA-CBA-CGA-O2A
23	1	602	CLA	CAA-CBA-CGA-O2A
23	8	602	CLA	CAA-CBA-CGA-O2A
25	A	847	LHG	O8-C23-C24-C25
25	2	622	LHG	O7-C7-C8-C9
29	4	624	LMG	O7-C10-C11-C12
23	A	801	CLA	C15-C16-C17-C18
23	B	838	CLA	O1A-CGA-O2A-C1
23	3	609	CLA	O1A-CGA-O2A-C1
25	3	624	LHG	O10-C23-C24-C25
23	B	836	CLA	CBA-CGA-O2A-C1
23	3	610	CLA	C13-C15-C16-C17
23	B	806	CLA	CAA-CBA-CGA-O2A
23	5	608	CLA	C2A-CAA-CBA-CGA
23	7	609	CLA	C2A-CAA-CBA-CGA
23	7	612	CLA	C2A-CAA-CBA-CGA
23	A	811	CLA	C5-C6-C7-C8
23	A	822	CLA	CAA-CBA-CGA-O1A
23	B	833	CLA	CAA-CBA-CGA-O1A
23	a	614	CLA	CAA-CBA-CGA-O1A
23	4	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	7	622	LHG	O10-C23-C24-C25
23	A	814	CLA	CAA-CBA-CGA-O2A
23	1	608	CLA	CAA-CBA-CGA-O1A
23	a	608	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

257 monomers are involved in 596 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	818	CLA	2	0
29	A	860	LMG	2	0
23	5	606	CLA	6	0
31	8	619	LUT	6	0
23	K	201	CLA	1	0
23	6	601	CLA	5	0
23	5	614	CLA	2	0
23	5	616	CLA	2	0
23	7	610	CLA	5	0
23	A	809	CLA	6	0
26	F	305	BCR	4	0
28	A	857	LMU	1	0
23	6	613	CLA	5	0
26	A	851	BCR	3	0
29	5	626	LMG	1	0
25	1	620	LHG	6	0
23	7	616	CLA	2	0
23	8	610	CLA	3	0
25	3	623	LHG	1	0
23	L	303	CLA	2	0
23	5	610	CLA	5	0
23	4	609	CLA	3	0
26	B	848	BCR	1	0
28	5	628	LMU	3	0
23	B	810	CLA	3	0
26	A	849	BCR	4	0
26	4	621	BCR	2	0
23	2	614	CLA	1	0
23	3	602	CLA	1	0
23	4	616	CLA	1	0
23	7	614	CLA	2	0
23	A	843	CLA	5	0
23	8	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	203	CLA	3	0
23	8	608	CLA	3	0
23	5	601	CLA	1	0
26	B	847	BCR	2	0
26	5	622	BCR	4	0
30	J	103	DGD	1	0
32	4	620	XAT	3	0
23	B	831	CLA	3	0
23	9	606	CLA	1	0
23	8	603	CLA	1	0
23	B	819	CLA	2	0
23	B	813	CLA	5	0
23	3	603	CLA	2	0
23	4	614	CLA	1	0
23	A	839	CLA	3	0
23	A	831	CLA	4	0
23	A	822	CLA	4	0
23	5	607	CLA	5	0
26	L	305	BCR	4	0
23	5	603	CLA	1	0
23	A	825	CLA	5	0
25	A	847	LHG	1	0
23	B	824	CLA	5	0
23	9	609	CLA	1	0
26	B	801	BCR	5	0
25	B	851	LHG	2	0
23	A	837	CLA	2	0
23	B	841	CLA	3	0
23	6	610	CLA	4	0
26	B	844	BCR	3	0
23	9	611	CLA	7	0
24	B	842	PQN	6	0
23	3	609	CLA	6	0
23	A	854	CLA	5	0
23	B	838	CLA	4	0
23	2	610	CLA	1	0
25	A	846	LHG	3	0
24	A	844	PQN	5	0
23	B	834	CLA	3	0
23	A	806	CLA	3	0
26	J	102	BCR	5	0
23	7	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	8	609	CLA	1	0
23	9	614	CLA	1	0
23	5	609	CLA	6	0
23	A	805	CLA	4	0
23	1	601	CLA	6	0
26	8	621	BCR	4	0
23	5	608	CLA	4	0
23	1	612	CLA	1	0
26	K	207	BCR	3	0
25	8	622	LHG	1	0
23	4	607	CLA	1	0
25	4	622	LHG	6	0
23	6	604	CLA	3	0
32	3	619	XAT	2	0
23	B	833	CLA	4	0
26	A	850	BCR	3	0
23	A	803	CLA	5	0
23	8	614	CLA	2	0
23	A	824	CLA	1	0
23	G	204	CLA	3	0
23	B	822	CLA	1	0
26	B	845	BCR	2	0
23	7	601	CLA	5	0
23	4	610	CLA	1	0
23	A	807	CLA	2	0
23	6	606	CLA	1	0
31	4	619	LUT	5	0
23	B	835	CLA	2	0
31	6	619	LUT	4	0
23	5	604	CLA	5	0
26	K	202	BCR	3	0
23	2	613	CLA	1	0
23	7	607	CLA	2	0
23	B	840	CLA	3	0
31	3	618	LUT	1	0
25	7	622	LHG	2	0
23	4	608	CLA	4	0
26	G	205	BCR	6	0
23	1	608	CLA	2	0
23	2	609	CLA	1	0
25	6	623	LHG	3	0
23	B	809	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	608	CLA	2	0
23	B	829	CLA	9	0
23	A	830	CLA	5	0
23	B	806	CLA	3	0
23	3	606	CLA	2	0
28	A	859	LMU	2	0
23	6	603	CLA	1	0
23	B	803	CLA	3	0
23	4	604	CLA	1	0
23	B	805	CLA	4	0
25	5	625	LHG	5	0
32	6	621	XAT	1	0
23	4	613	CLA	5	0
23	A	811	CLA	5	0
23	B	836	CLA	2	0
23	A	812	CLA	4	0
23	A	817	CLA	2	0
23	A	804	CLA	3	0
23	9	601	CLA	1	0
26	A	852	BCR	7	0
23	A	838	CLA	1	0
23	A	829	CLA	10	0
28	8	624	LMU	3	0
23	A	823	CLA	2	0
23	3	610	CLA	3	0
23	6	602	CLA	6	0
23	A	832	CLA	2	0
23	B	802	CLA	2	0
32	5	621	XAT	10	0
31	2	619	LUT	3	0
23	A	808	CLA	1	0
23	A	821	CLA	1	0
23	B	823	CLA	1	0
23	B	817	CLA	2	0
23	A	828	CLA	1	0
23	B	839	CLA	4	0
30	B	850	DGD	5	0
32	7	620	XAT	1	0
23	6	616	CLA	6	0
23	F	301	CLA	4	0
33	6	624	NEX	4	0
32	1	618	XAT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	802	CLA	7	0
26	B	846	BCR	1	0
23	B	811	CLA	2	0
23	8	601	CLA	3	0
26	3	621	BCR	2	0
23	A	826	CLA	1	0
32	2	620	XAT	3	0
23	F	303	CLA	3	0
23	B	828	CLA	1	0
23	B	825	CLA	4	0
23	A	845	CLA	1	0
23	1	609	CLA	2	0
26	1	619	BCR	2	0
31	1	617	LUT	3	0
23	A	816	CLA	1	0
23	A	814	CLA	4	0
26	6	622	BCR	4	0
25	8	623	LHG	3	0
23	1	606	CLA	2	0
23	4	618	CLA	1	0
23	7	602	CLA	2	0
32	9	620	XAT	3	0
23	7	613	CLA	4	0
23	B	821	CLA	3	0
29	J	104	LMG	1	0
33	5	624	NEX	3	0
23	3	608	CLA	3	0
23	F	304	CLA	1	0
23	A	841	CLA	6	0
23	4	602	CLA	1	0
23	A	835	CLA	3	0
23	A	827	CLA	2	0
23	B	837	CLA	5	0
23	3	613	CLA	1	0
23	6	612	CLA	1	0
29	5	627	LMG	3	0
26	A	848	BCR	5	0
23	3	612	CLA	1	0
23	3	614	CLA	1	0
23	5	619	CLA	2	0
23	B	814	CLA	3	0
23	L	302	CLA	1	0

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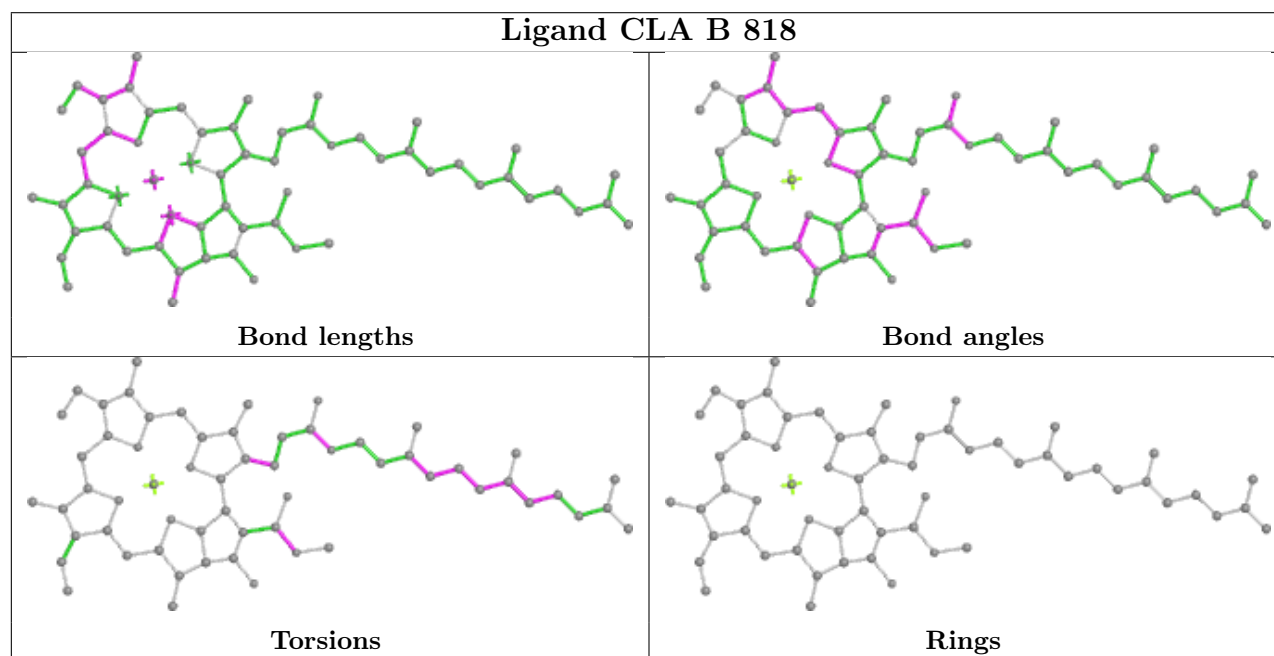
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	819	CLA	2	0
32	8	620	XAT	1	0
23	9	613	CLA	1	0
23	A	810	CLA	3	0
23	K	204	CLA	1	0
23	3	607	CLA	2	0
23	A	820	CLA	4	0
25	2	622	LHG	1	0
23	B	807	CLA	2	0
23	3	604	CLA	1	0
25	3	624	LHG	2	0
23	B	830	CLA	5	0
23	B	827	CLA	6	0
23	7	608	CLA	5	0
23	B	826	CLA	3	0
23	A	818	CLA	4	0
23	J	101	CLA	2	0
25	5	623	LHG	2	0
23	A	842	CLA	8	0
26	A	856	BCR	7	0
31	7	619	LUT	5	0
23	4	601	CLA	6	0
23	1	603	CLA	1	0
23	6	609	CLA	2	0
23	5	602	CLA	5	0
29	7	624	LMG	1	0
23	1	611	CLA	5	0
23	3	617	CLA	2	0
23	A	840	CLA	5	0
23	L	304	CLA	2	0
25	9	622	LHG	5	0
31	5	620	LUT	6	0
23	A	834	CLA	2	0
26	L	301	BCR	1	0
23	6	620	CLA	5	0
29	4	624	LMG	1	0
23	A	801	CLA	5	0
23	8	607	CLA	2	0
23	A	836	CLA	4	0
26	3	622	BCR	4	0
31	9	619	LUT	1	0
23	8	616	CLA	1	0

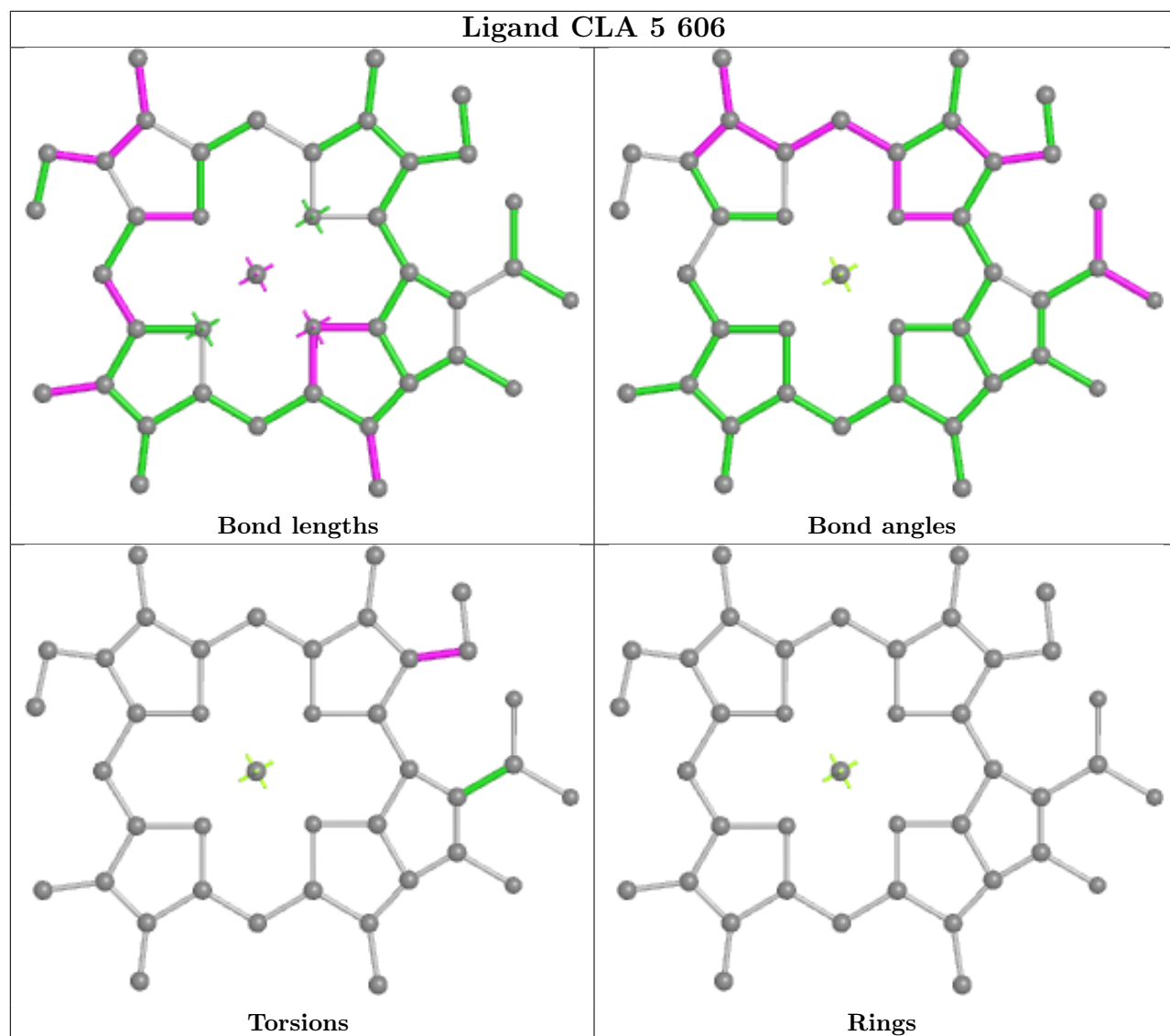
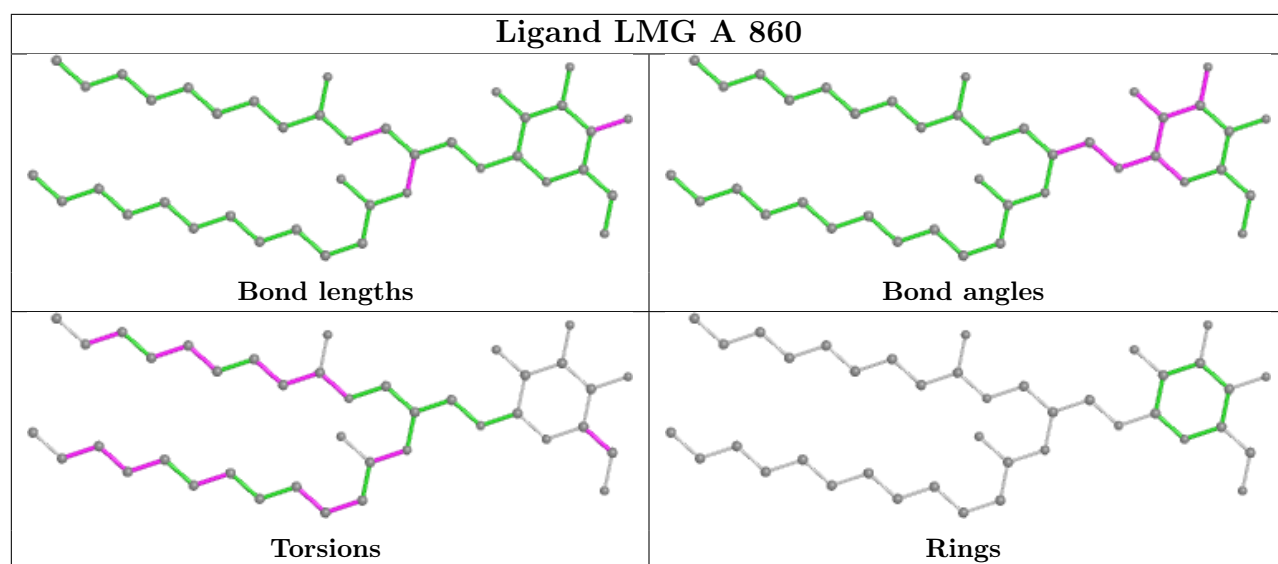
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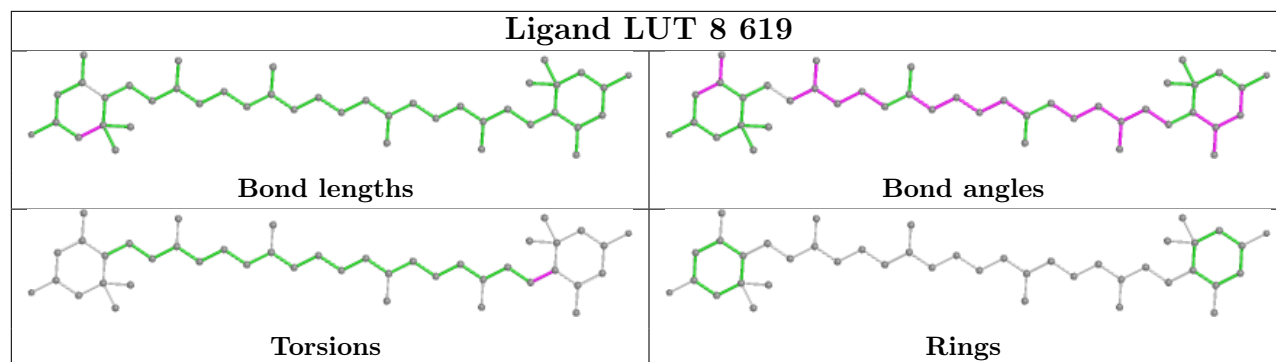
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	832	CLA	6	0
23	6	614	CLA	3	0
23	B	820	CLA	1	0
23	4	606	CLA	1	0
23	8	613	CLA	1	0
23	5	613	CLA	7	0
26	3	620	BCR	5	0
26	7	621	BCR	3	0
23	1	607	CLA	1	0
23	A	813	CLA	2	0
23	B	808	CLA	2	0
26	B	843	BCR	2	0
23	7	611	CLA	3	0
23	B	815	CLA	1	0

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

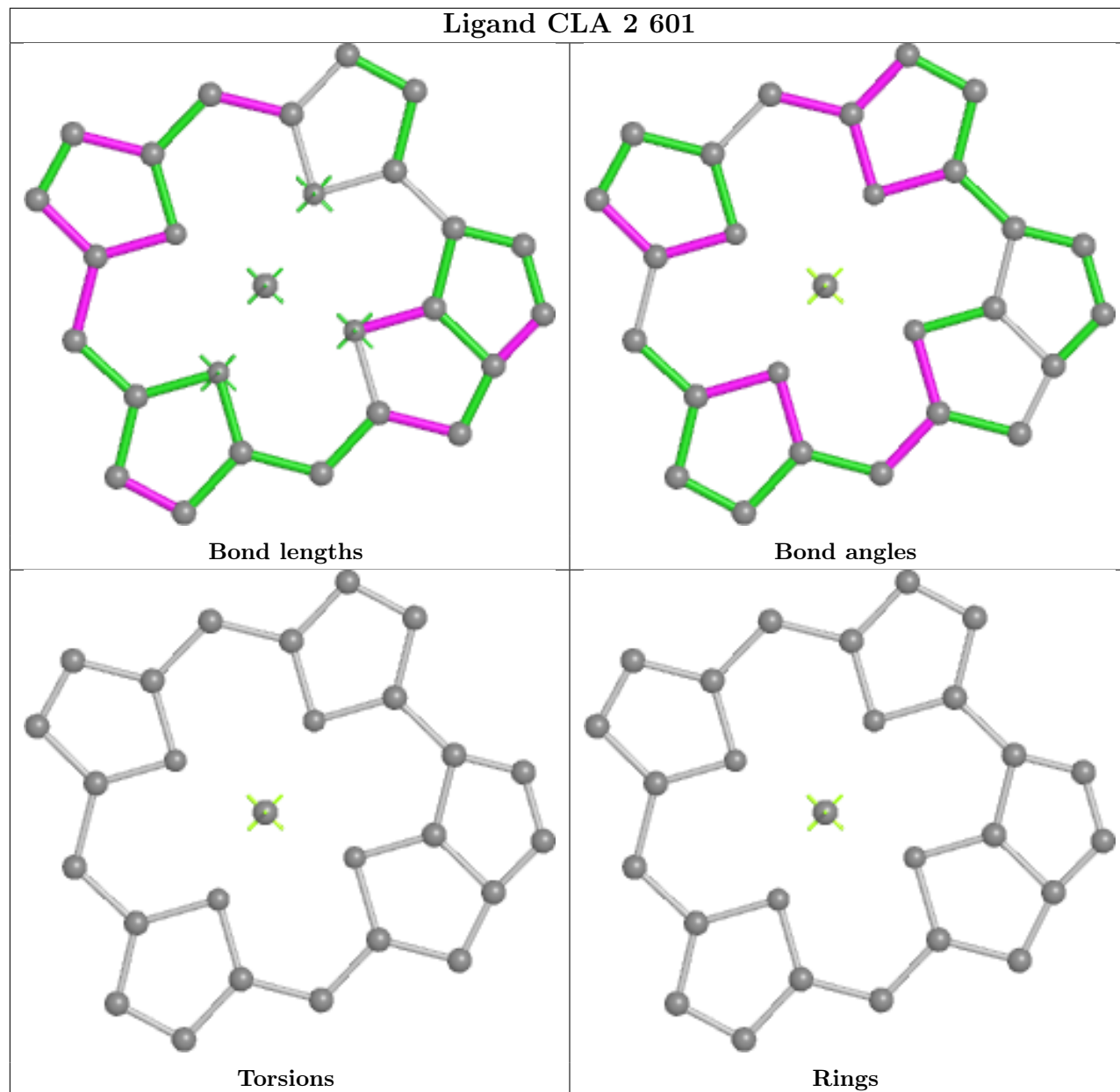


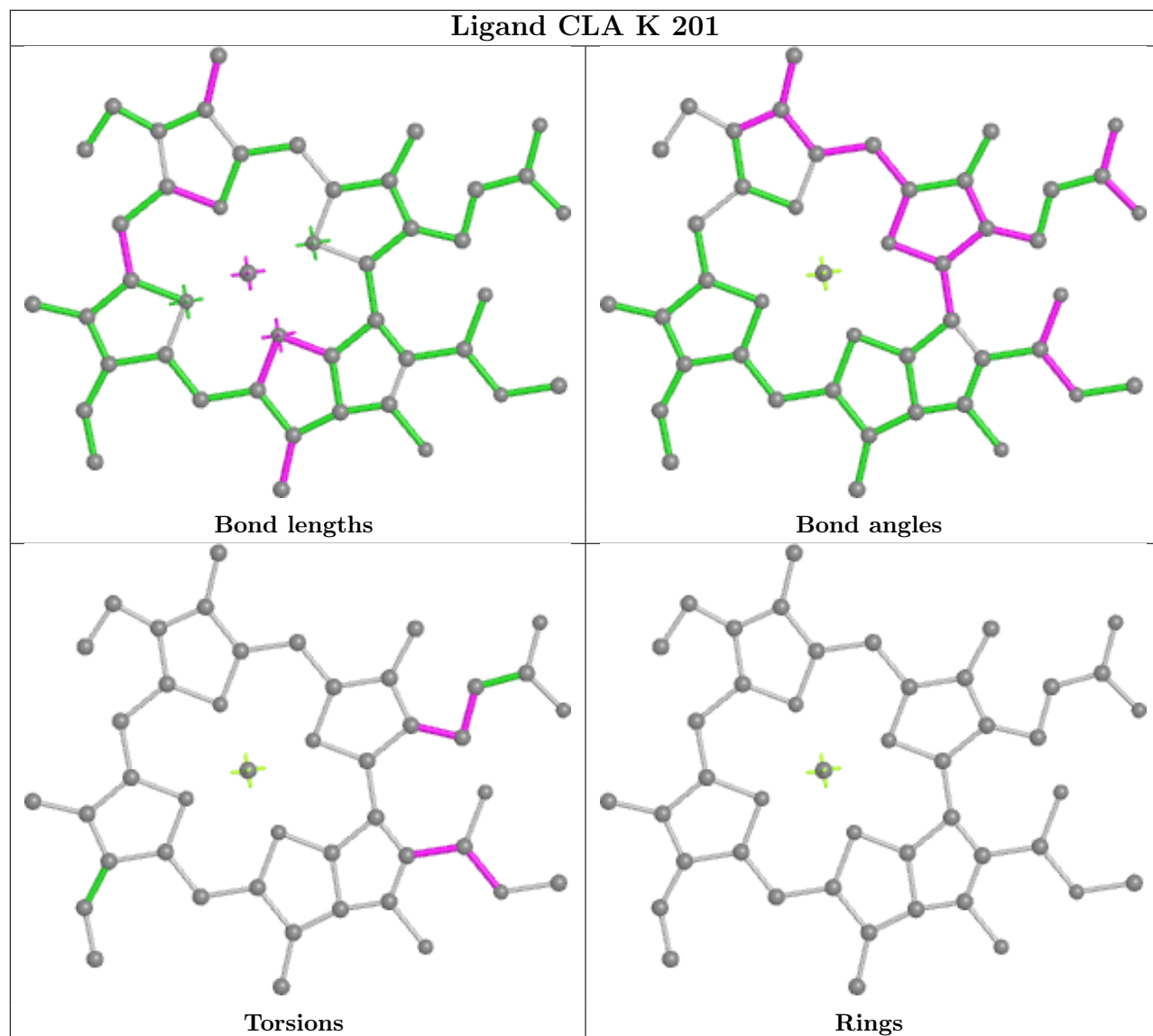


## Ligand LUT 8 619

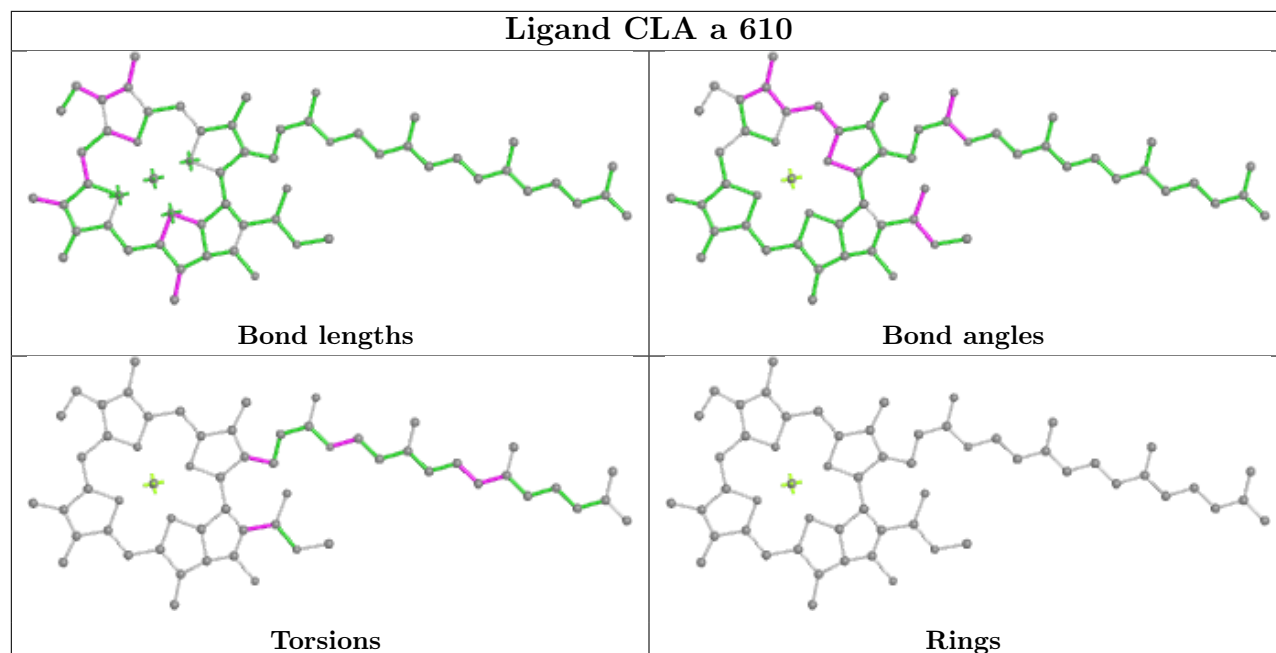


## Ligand CLA 2 601

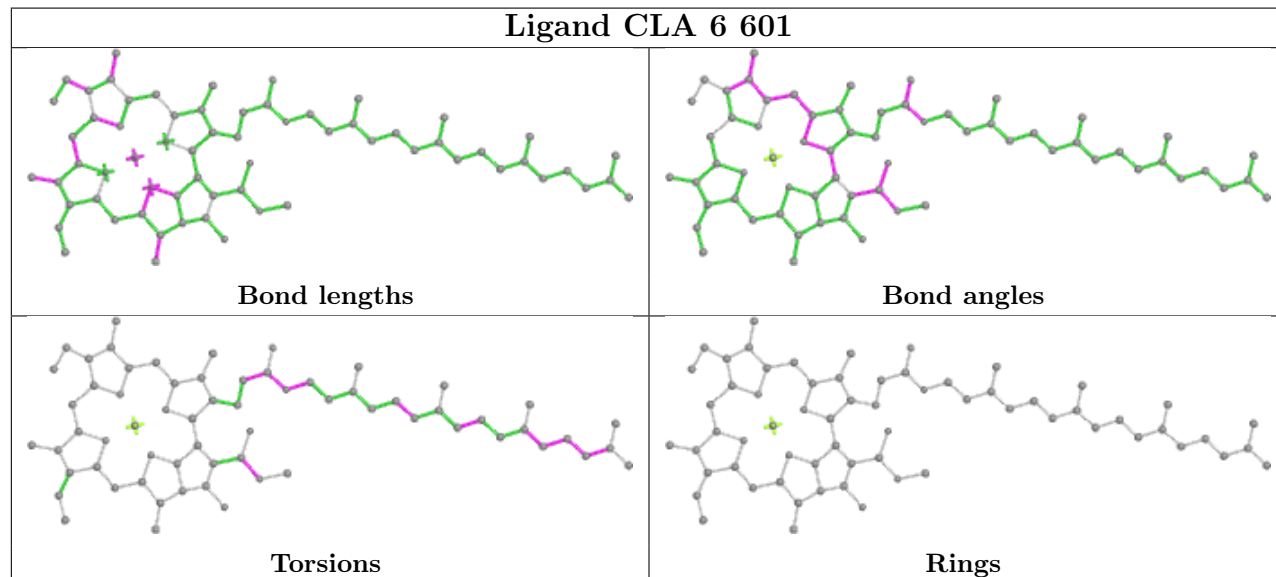




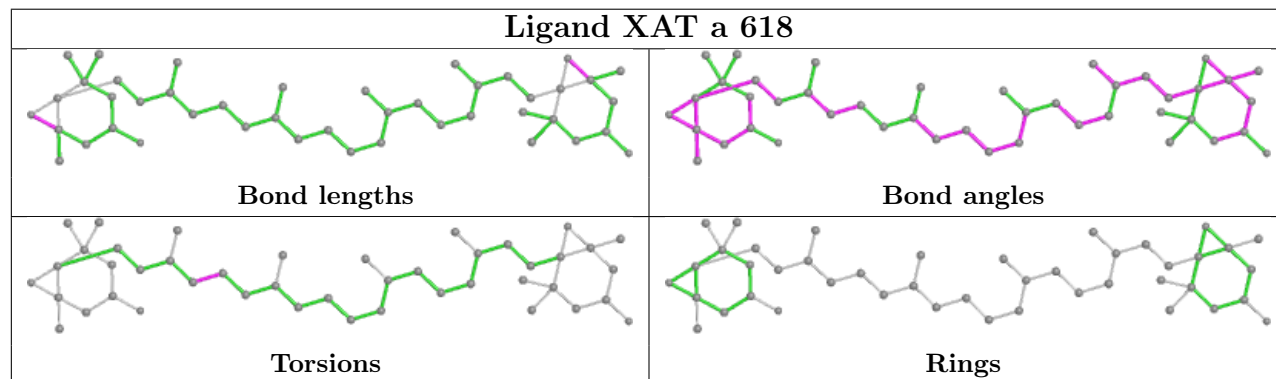
## Ligand CLA a 610



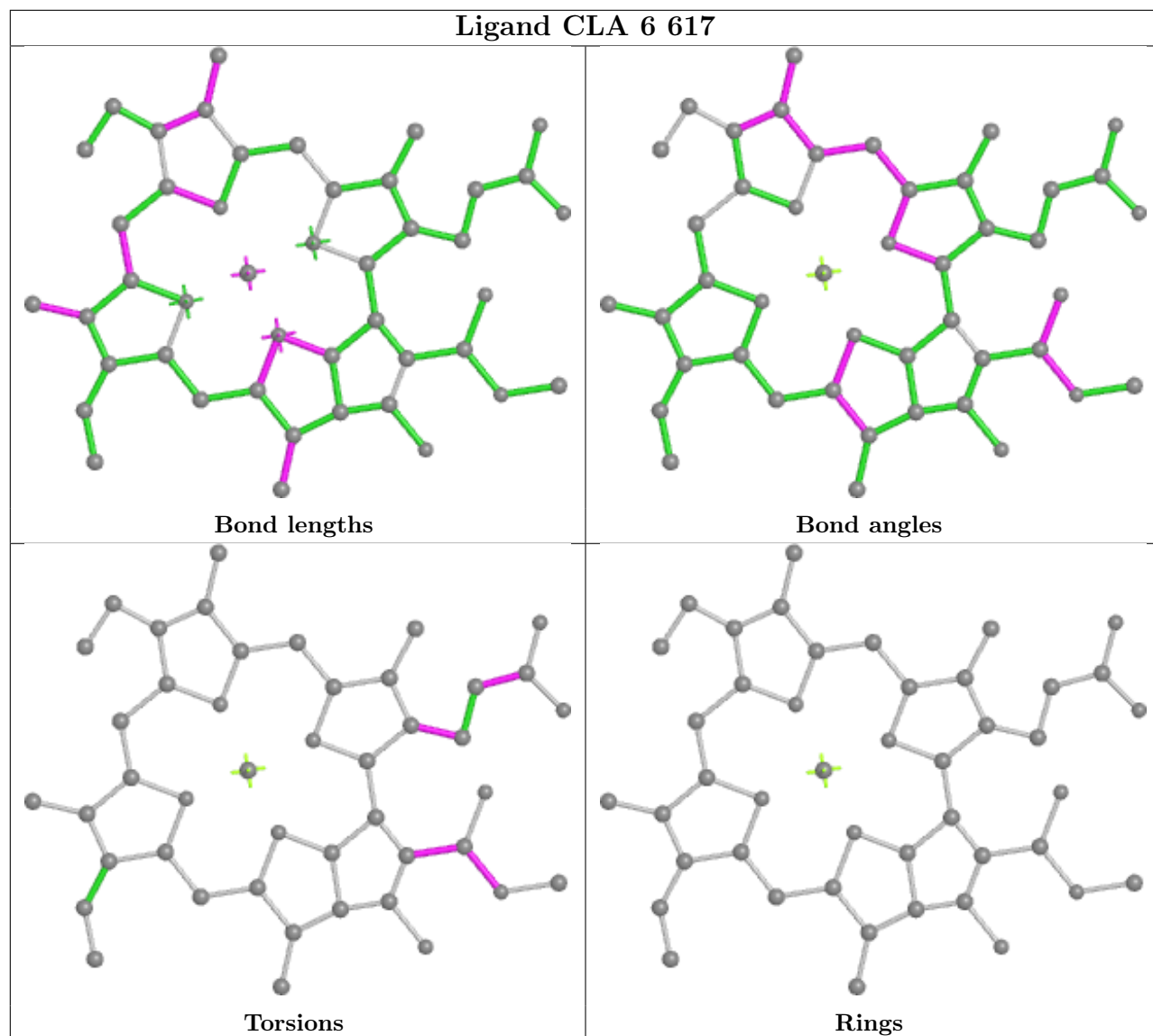
## Ligand CLA 6 601



## Ligand XAT a 618

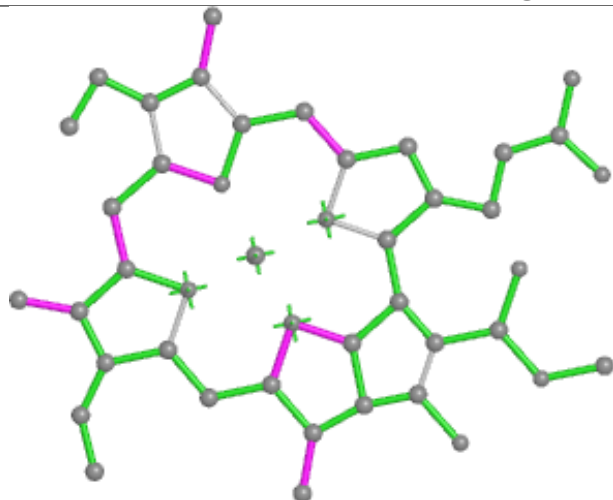


## Ligand CLA 6 617

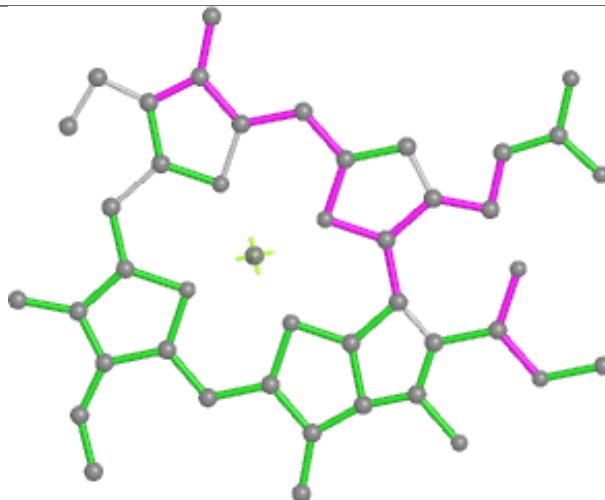




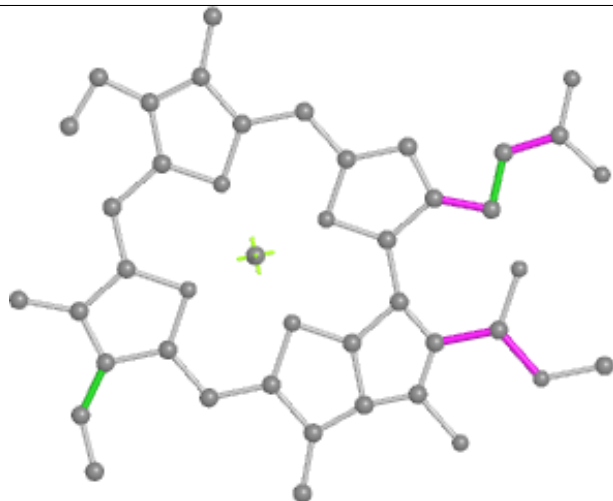
## Ligand CLA 5 614



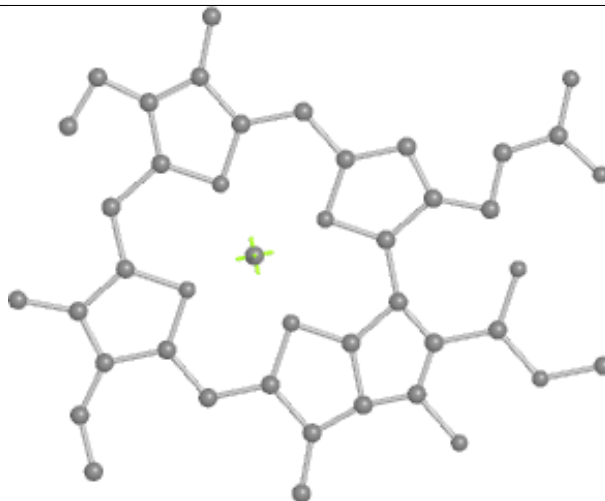
Bond lengths



Bond angles

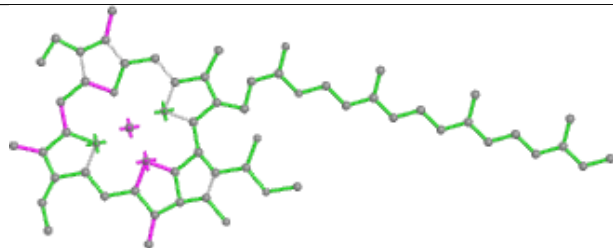


Torsions

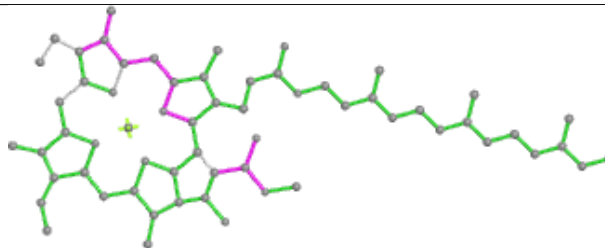


Rings

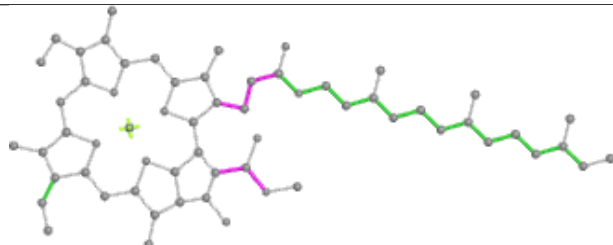
## Ligand CLA a 602



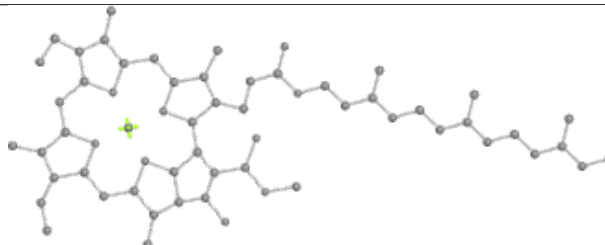
Bond lengths



Bond angles

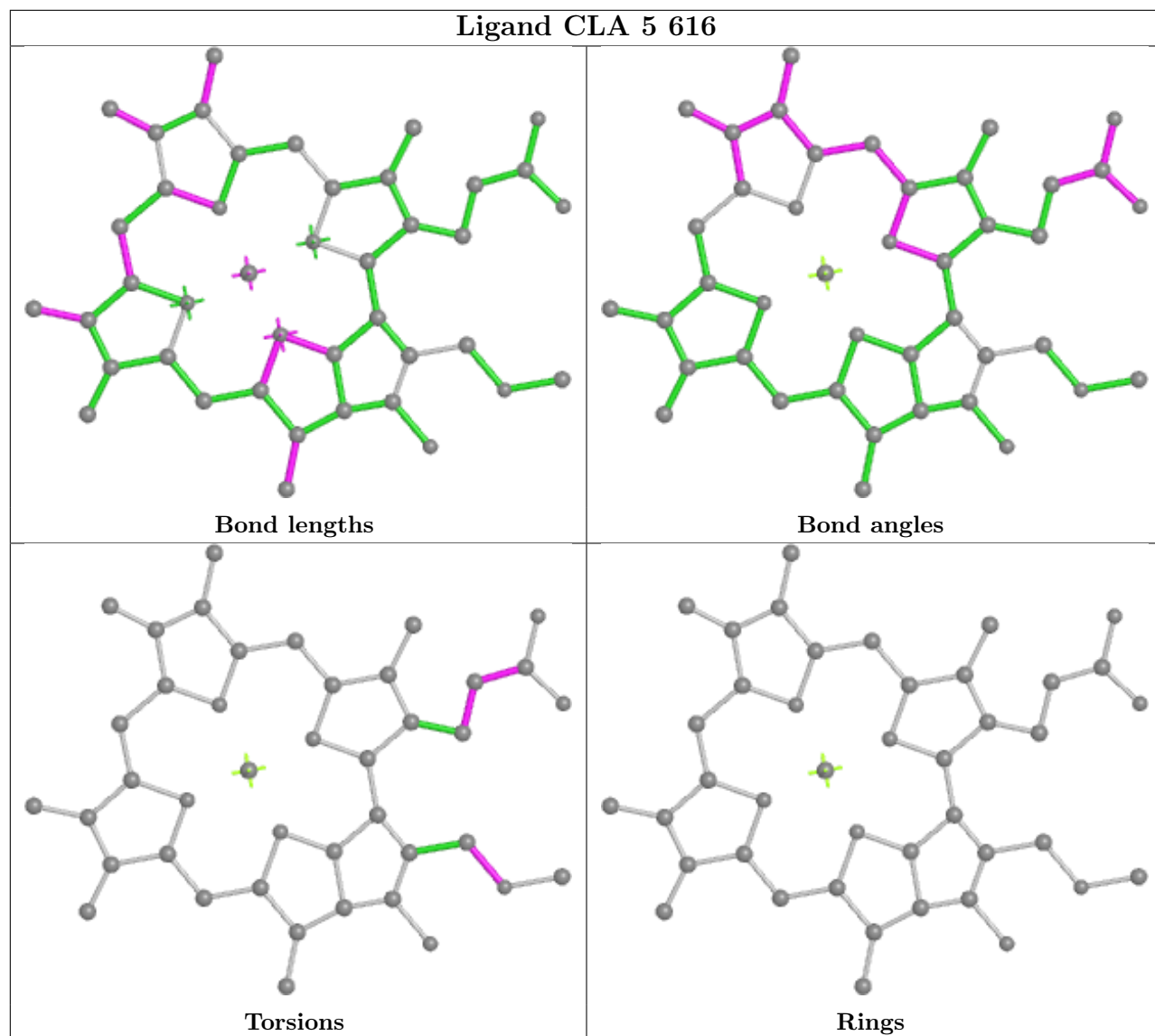


Torsions

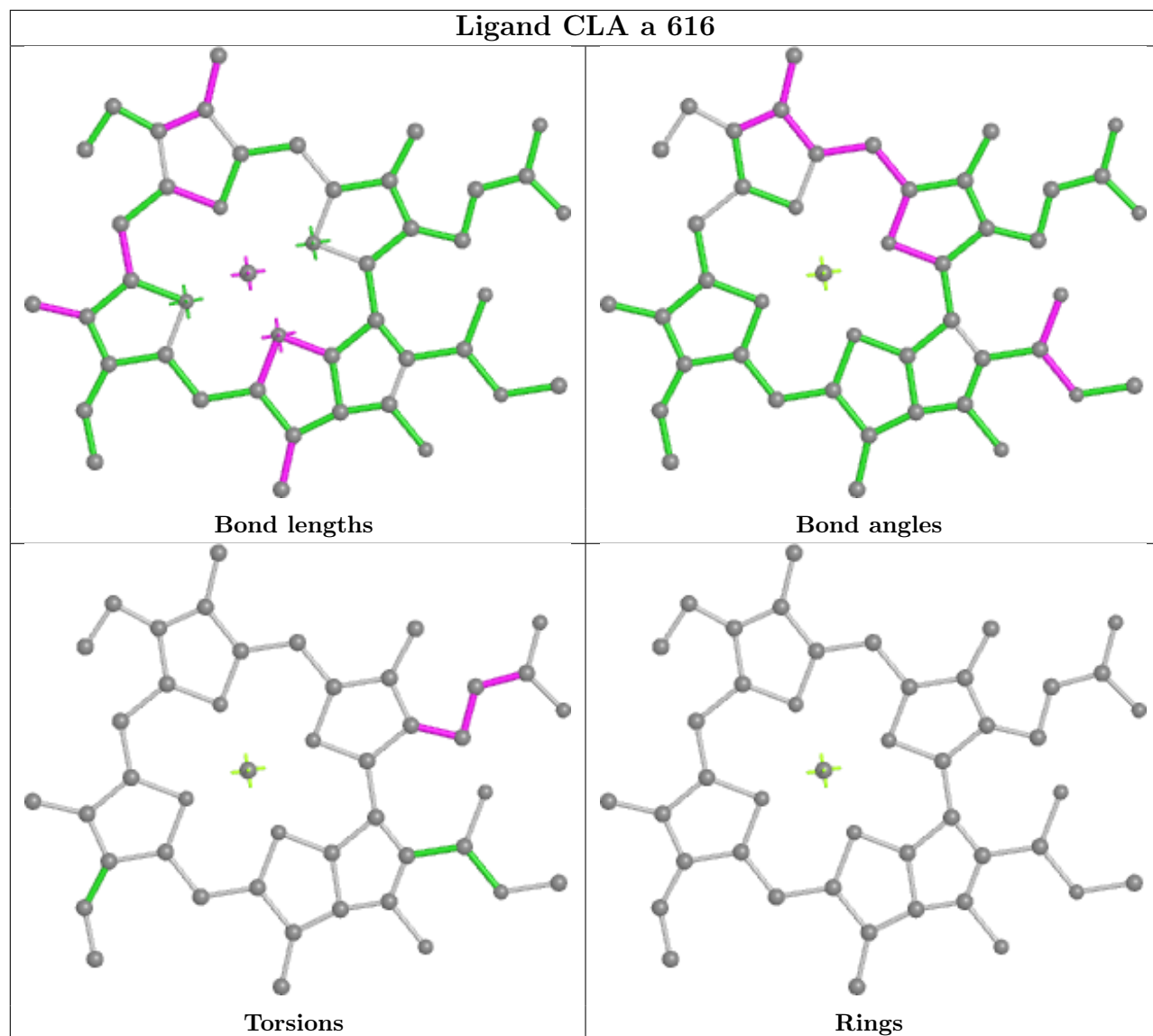


Rings

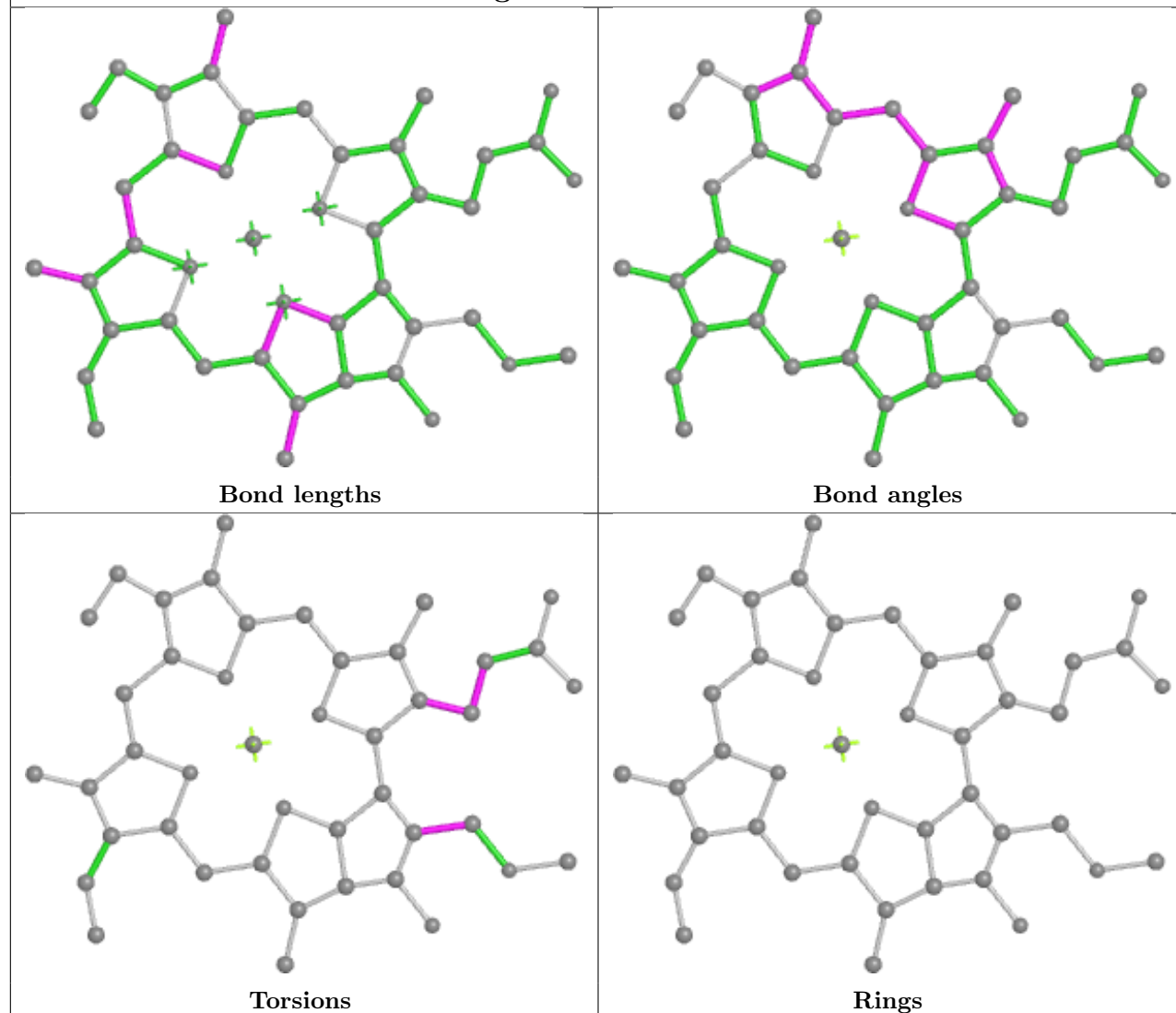
## Ligand CLA 5 616



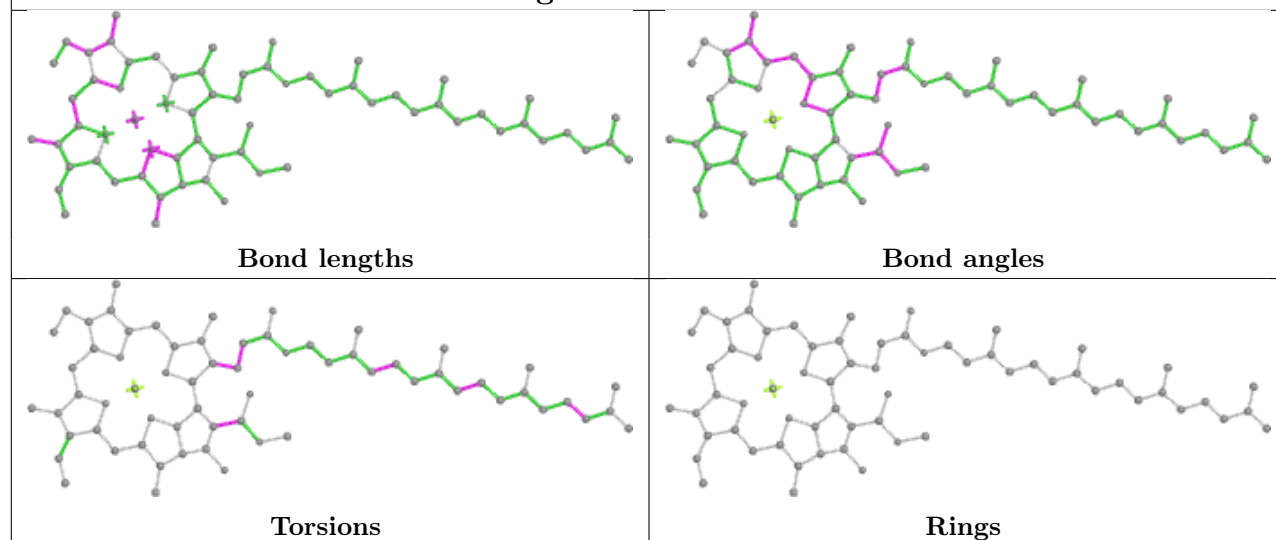
## Ligand CLA a 616



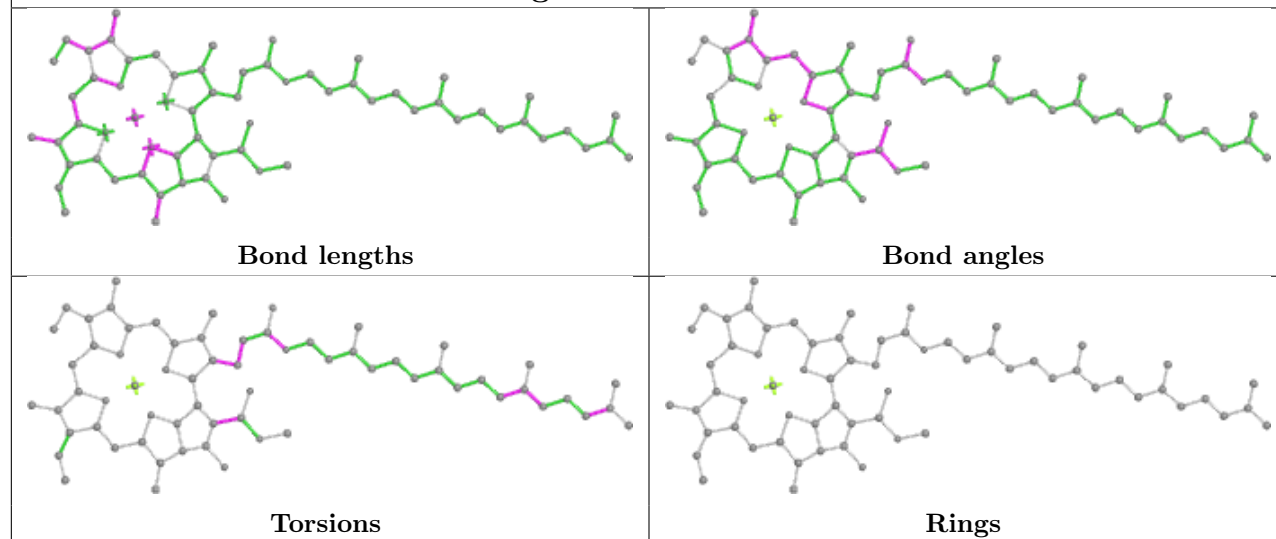
## Ligand CLA 7 609



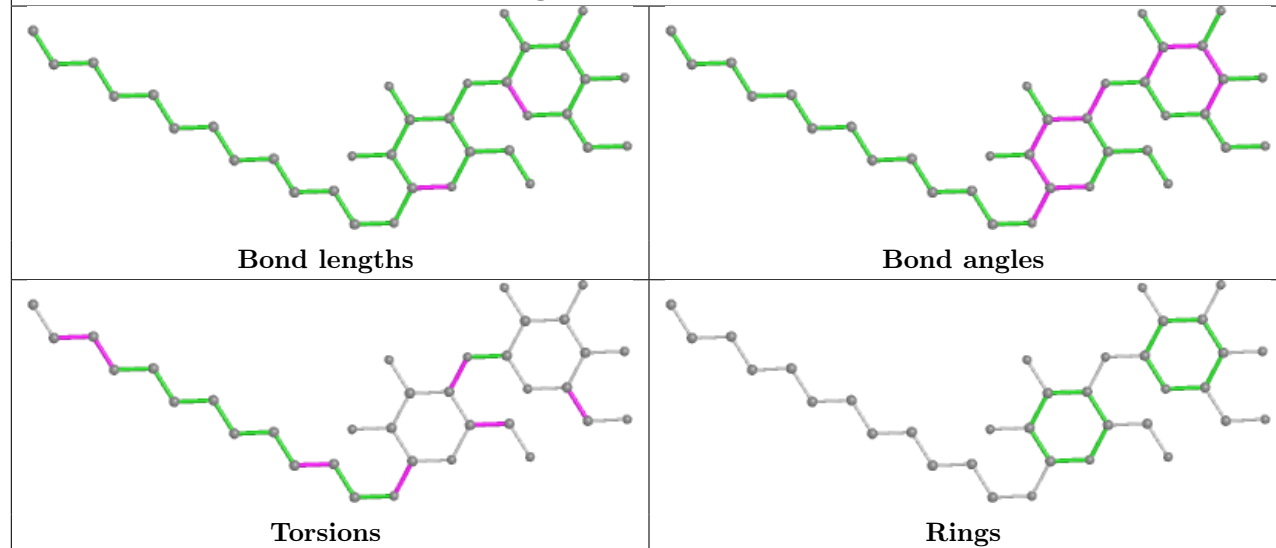
## Ligand CLA 7 610



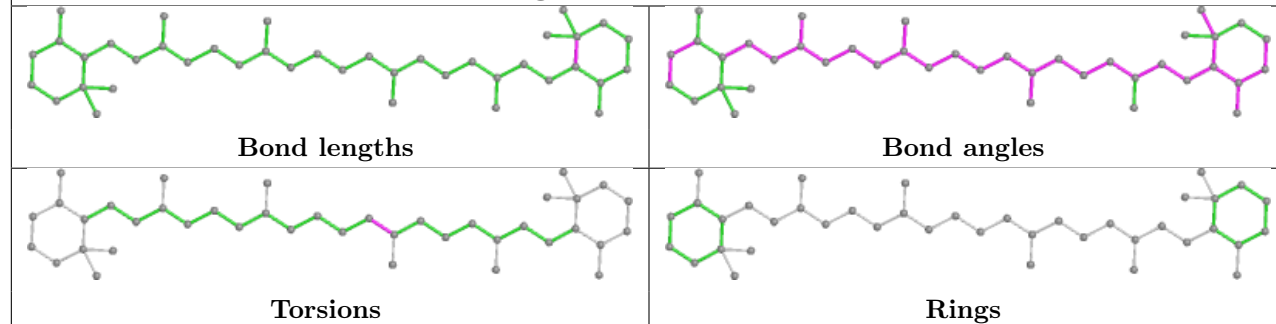
## Ligand CLA A 809

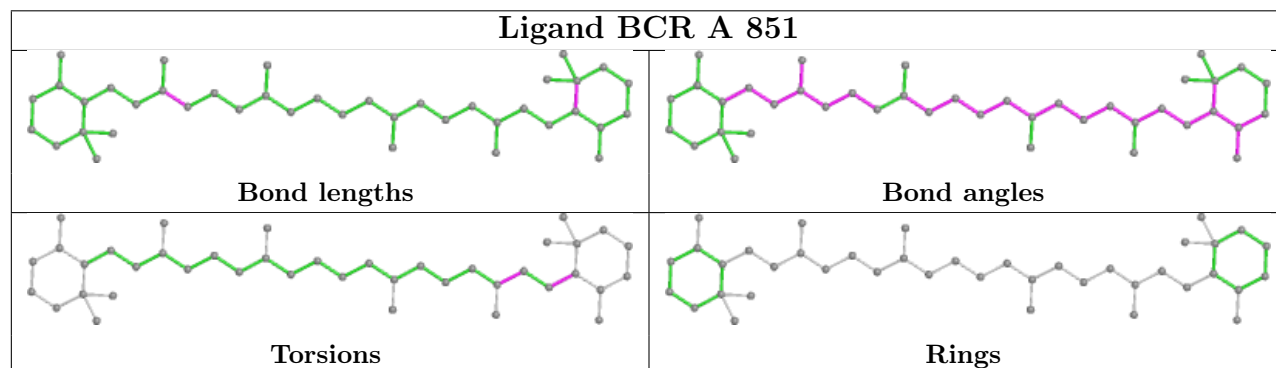
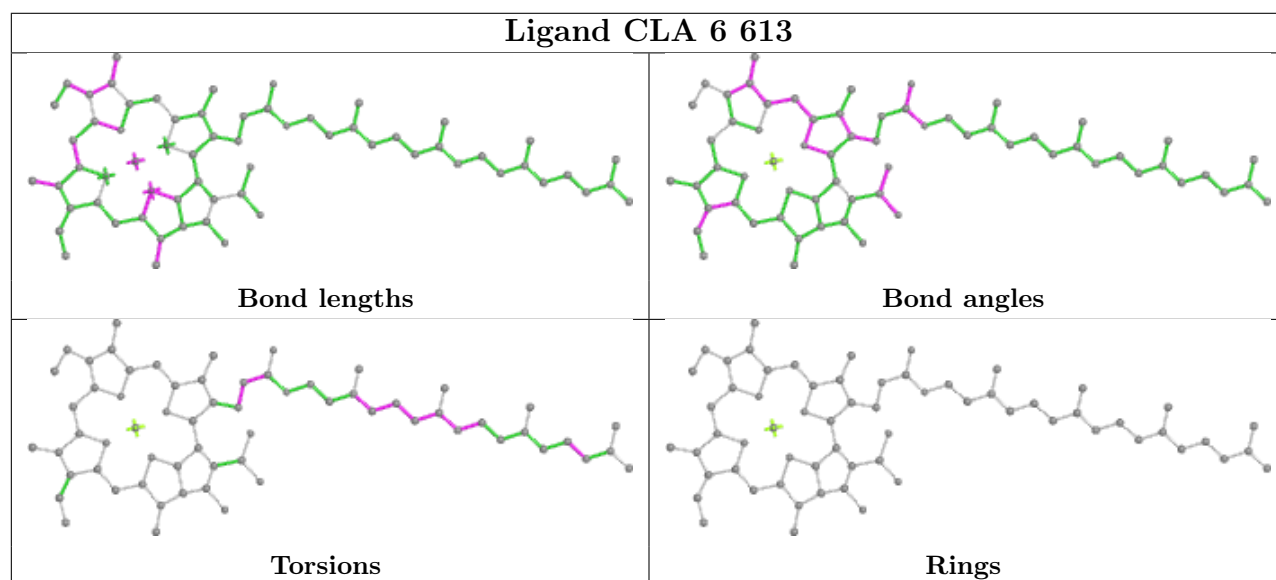
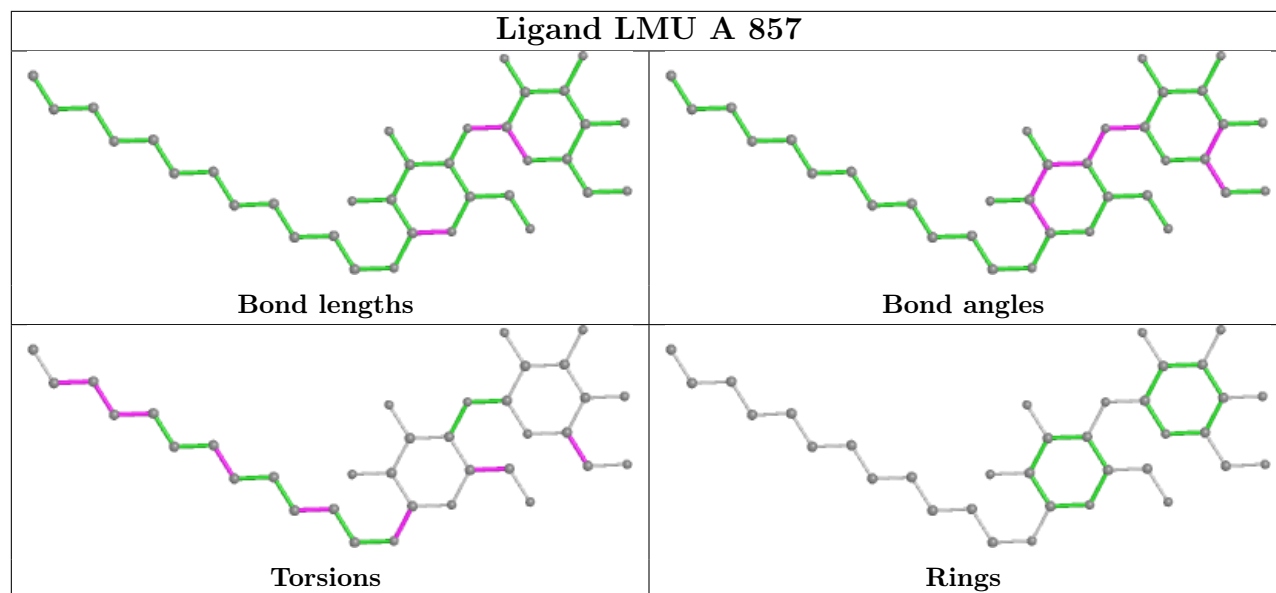


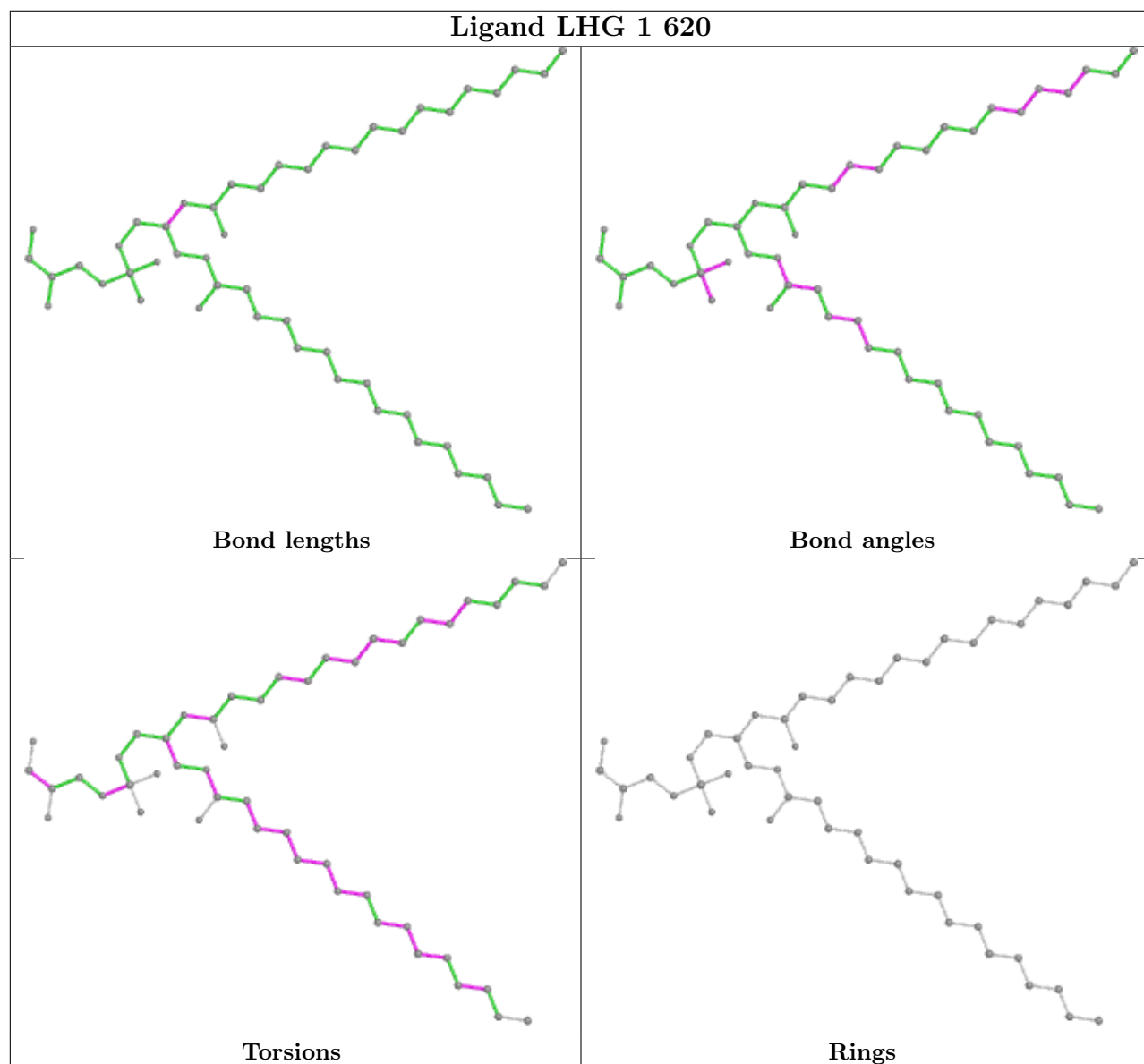
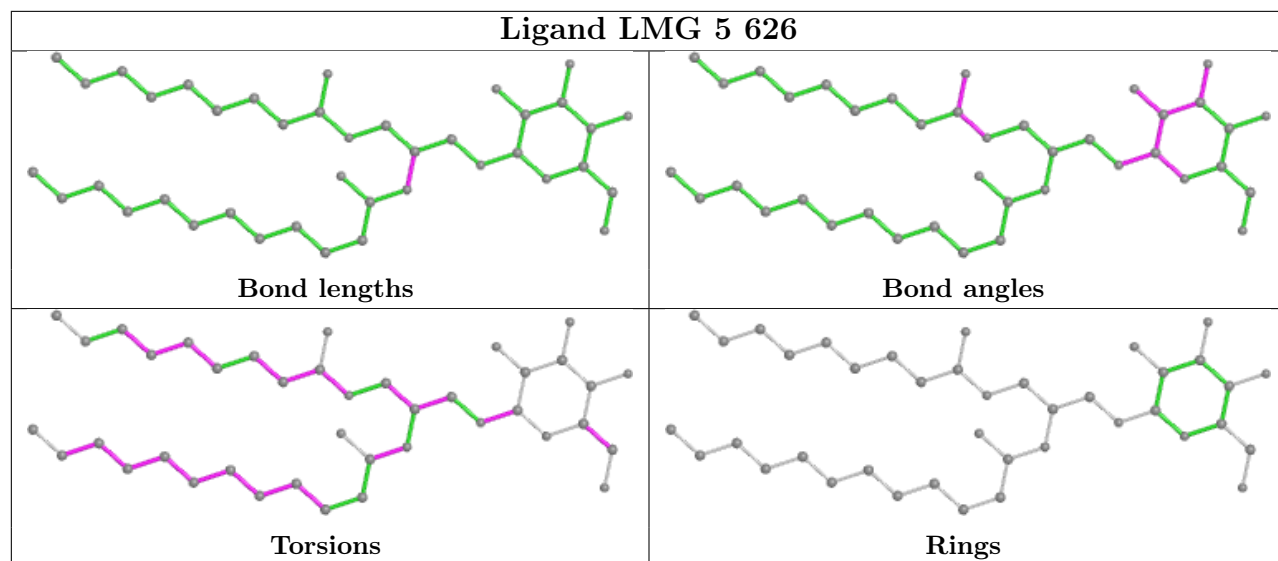
## Ligand LMU 8 625



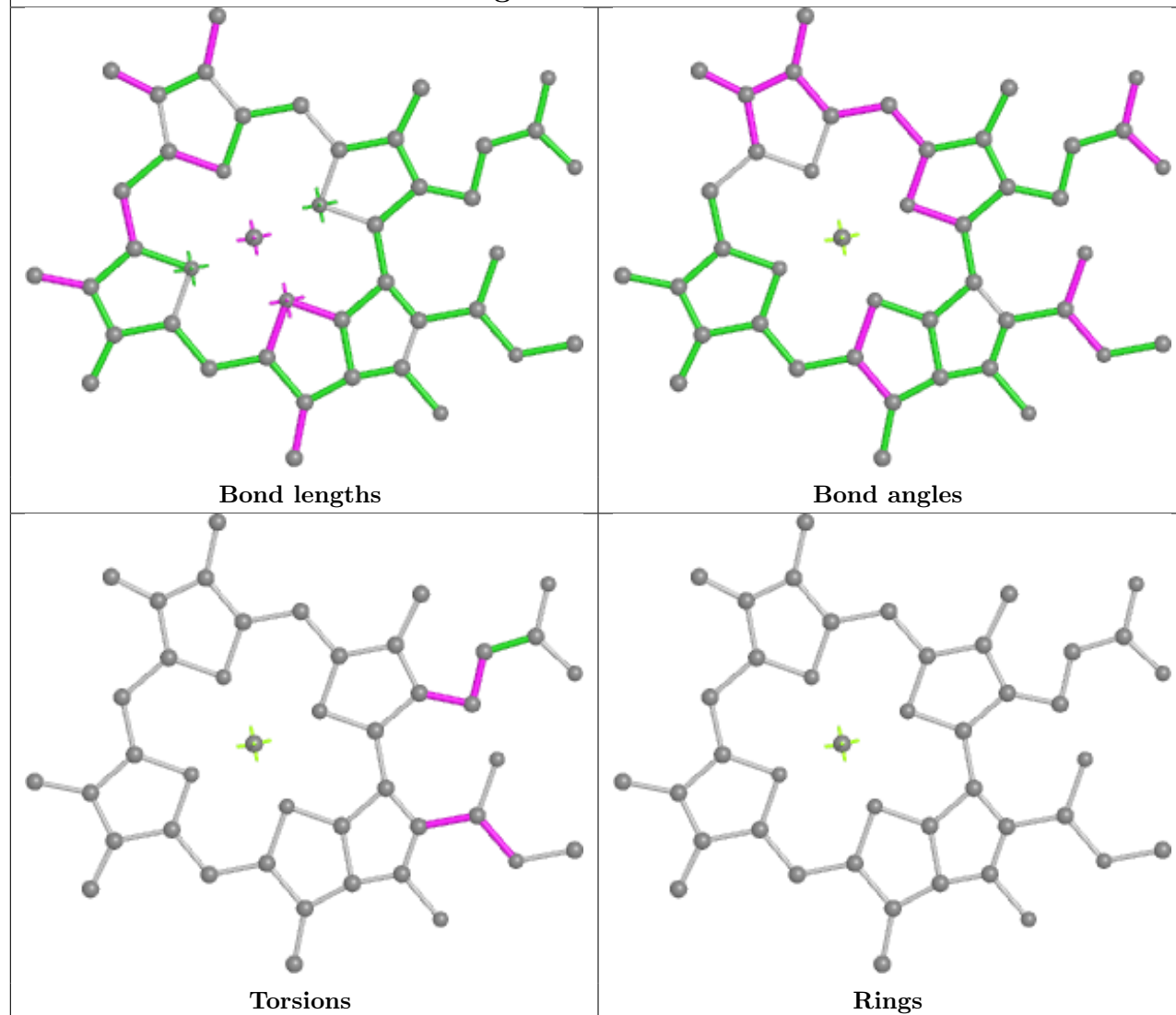
## Ligand BCR F 305



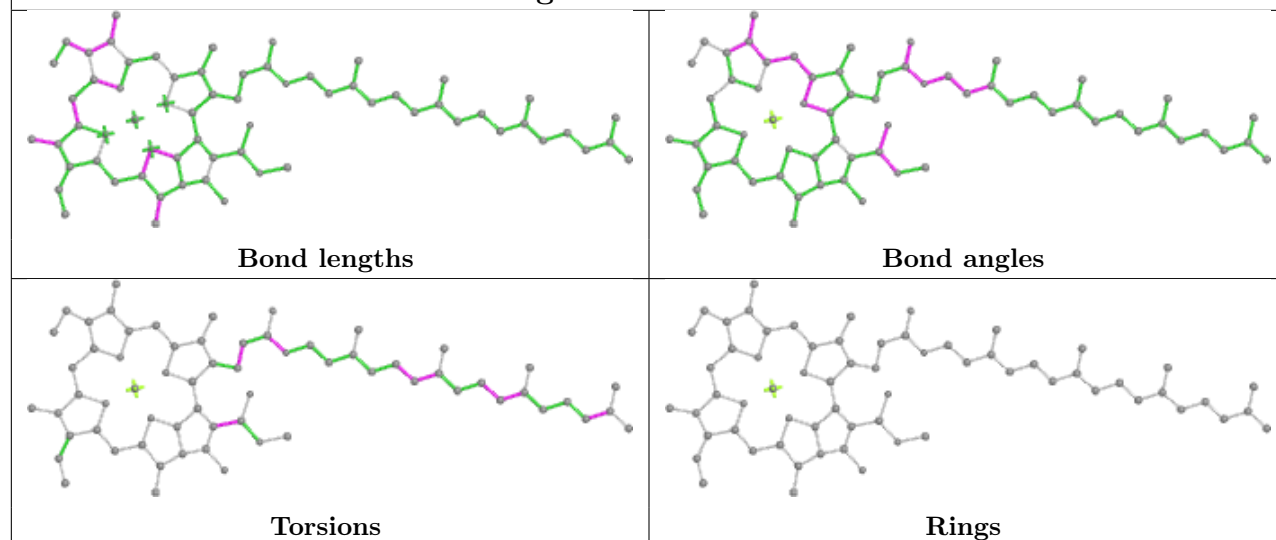




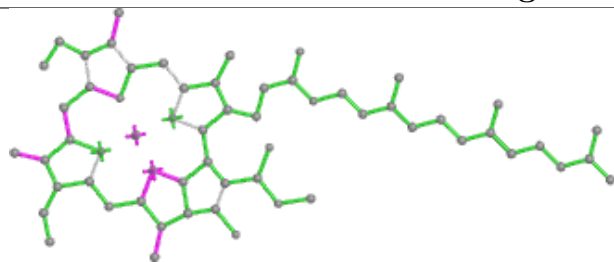
## Ligand CLA 7 616



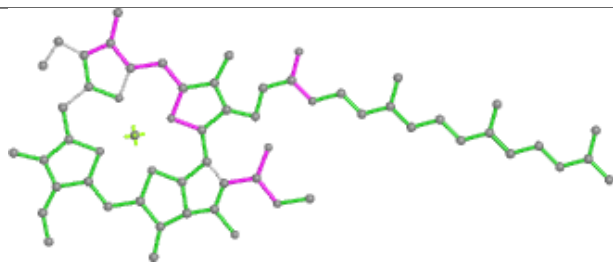
## Ligand CLA a 613



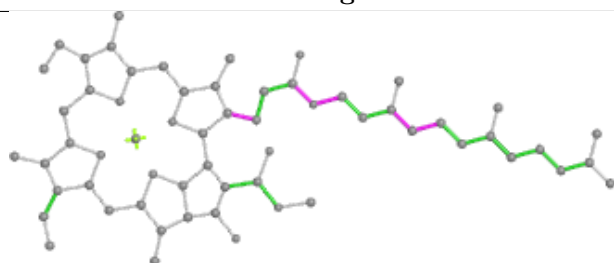


**Ligand CLA 8 610**

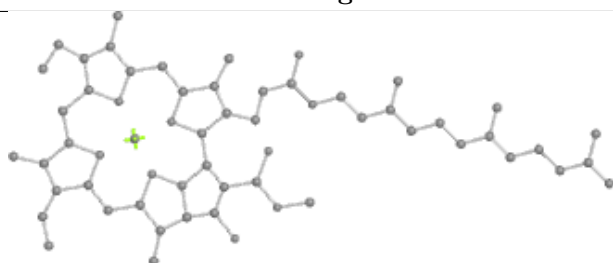
Bond lengths



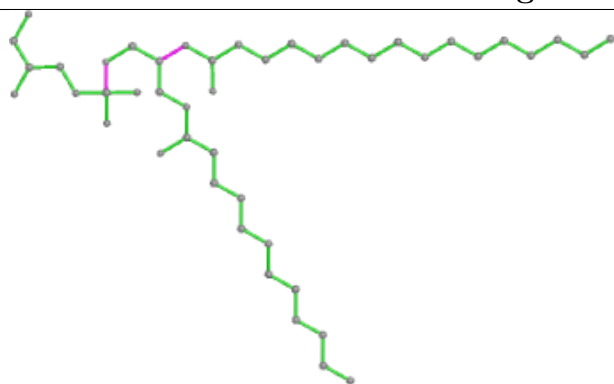
Bond angles



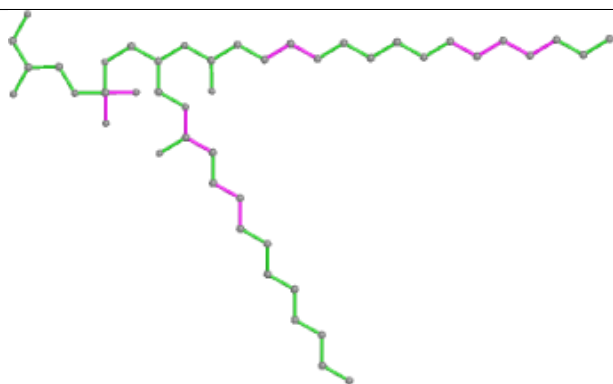
Torsions



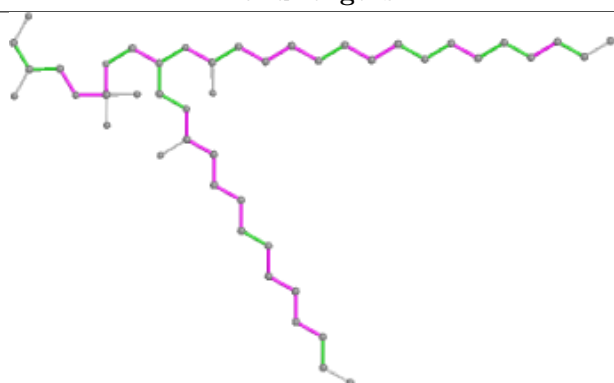
Rings

**Ligand LHG 3 623**

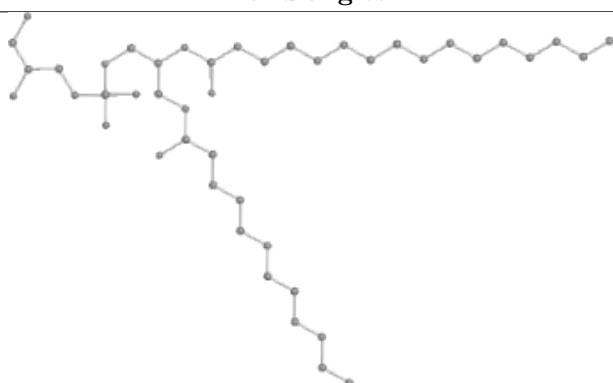
Bond lengths



Bond angles

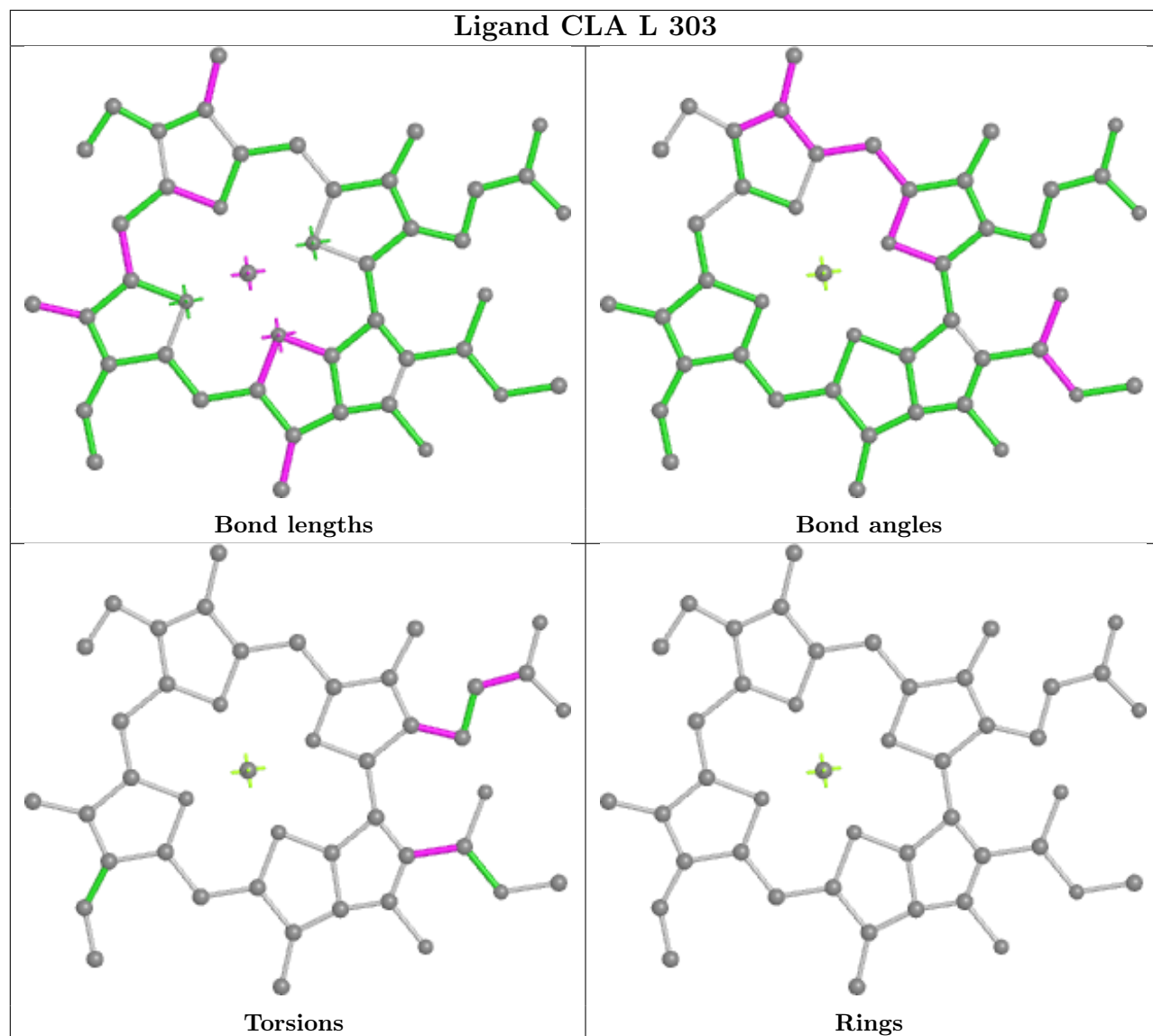


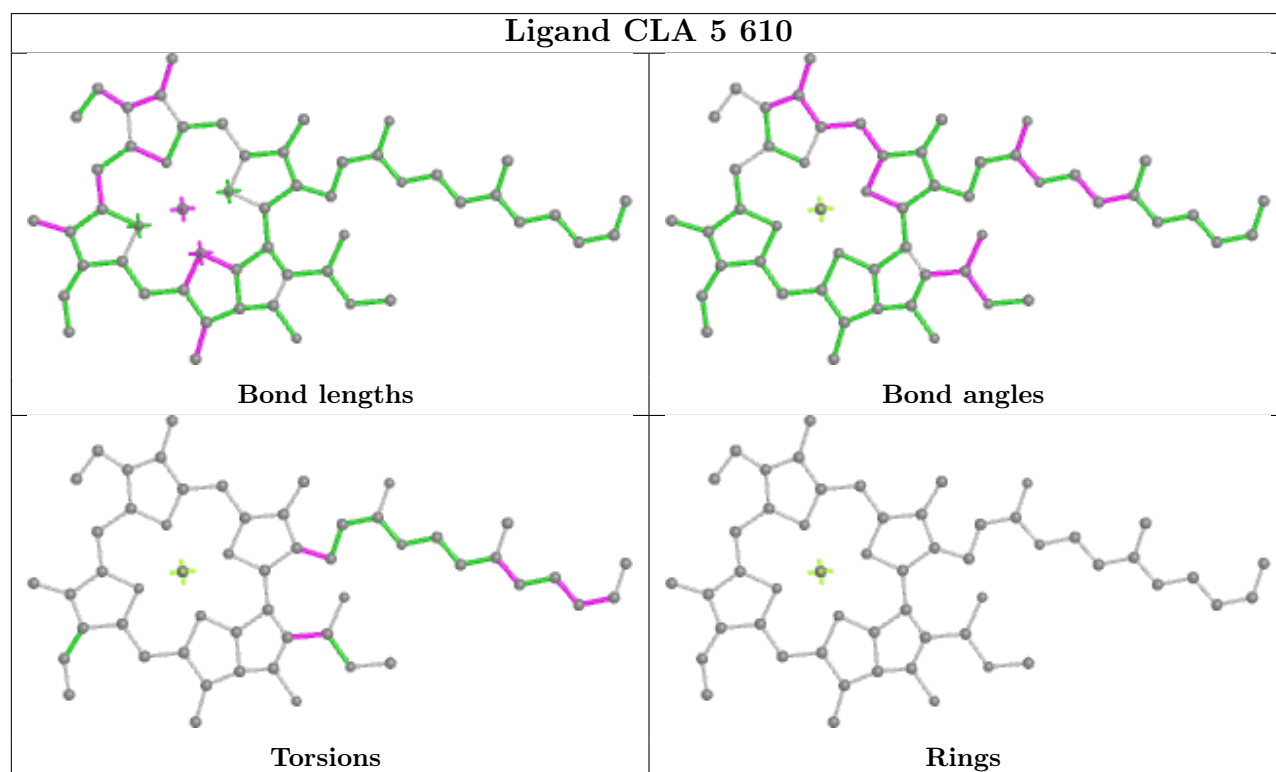
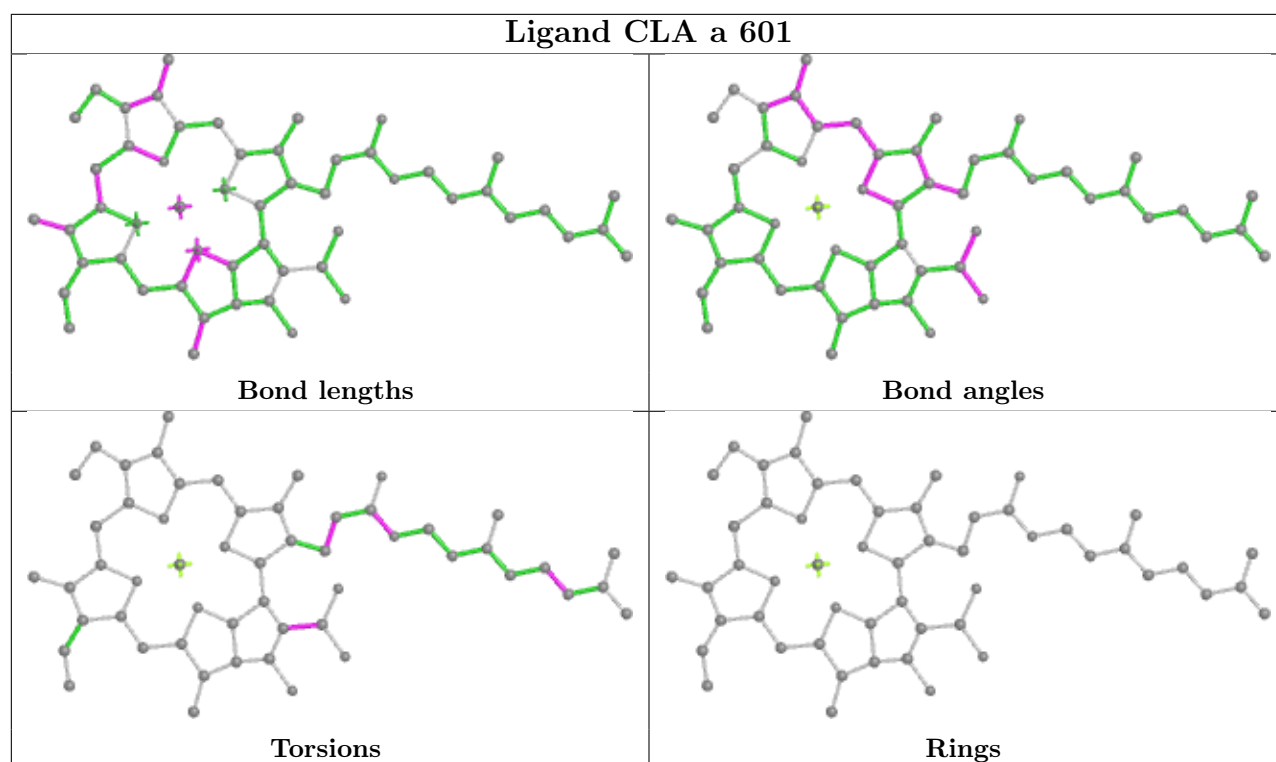
Torsions

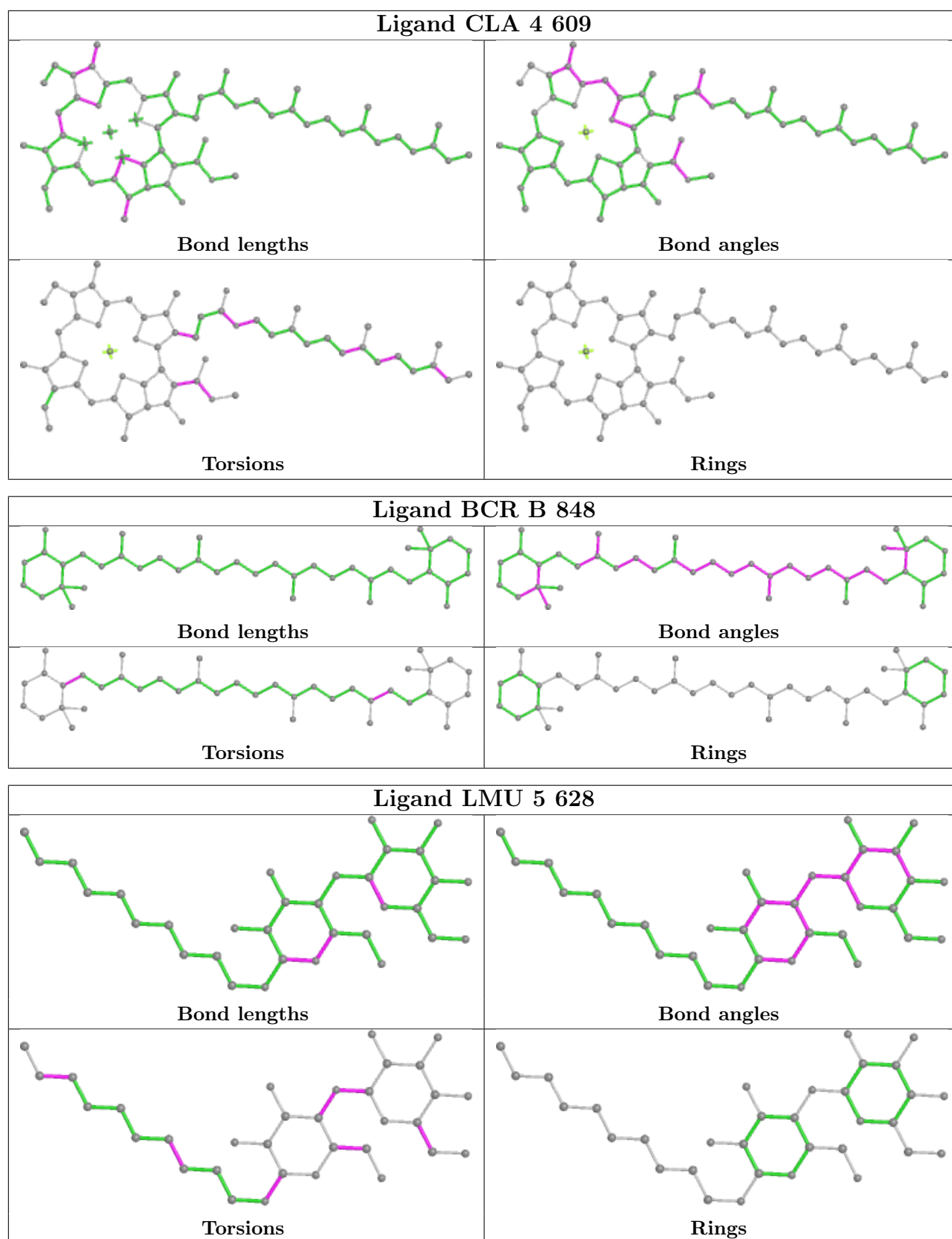


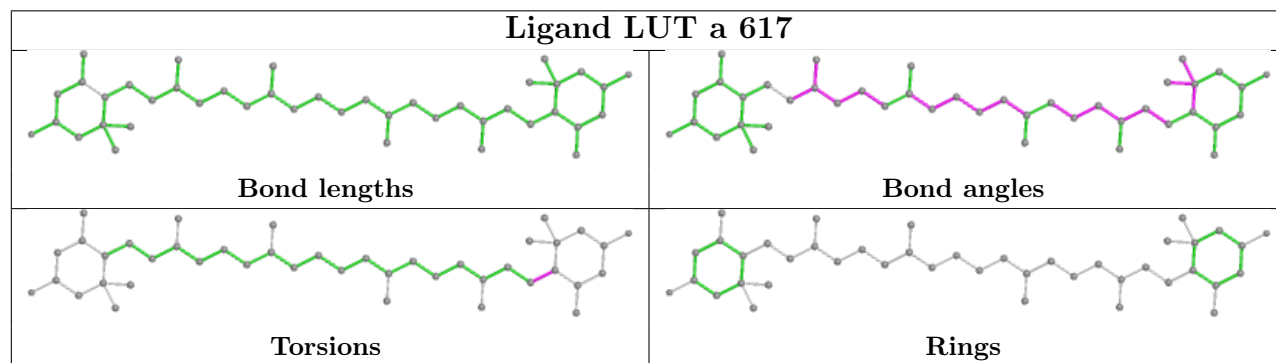
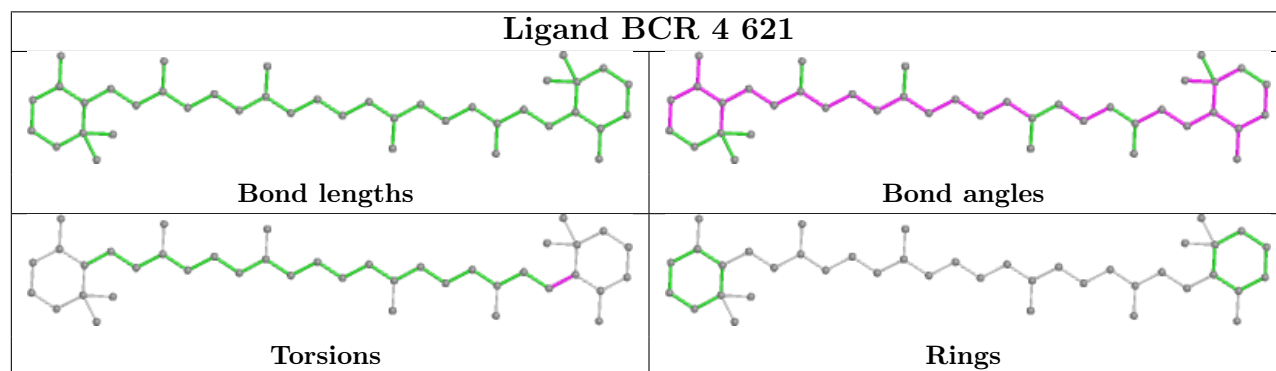
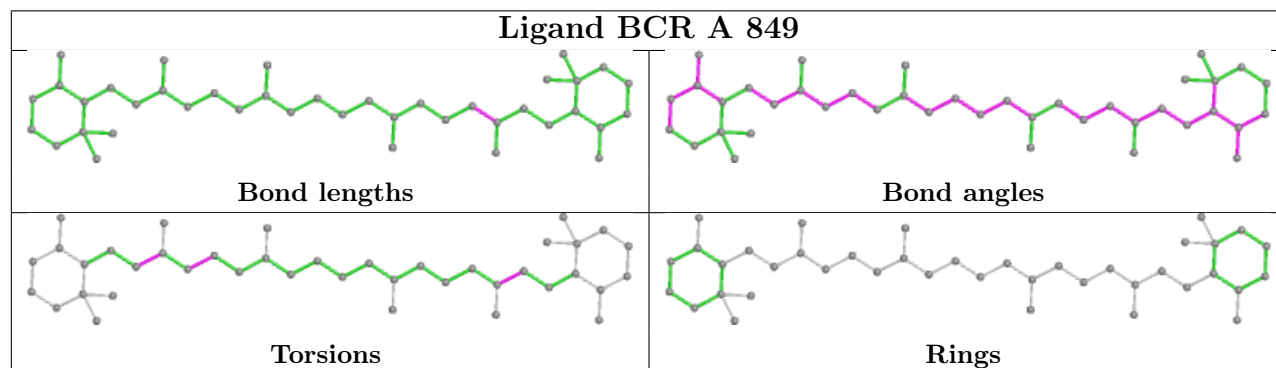
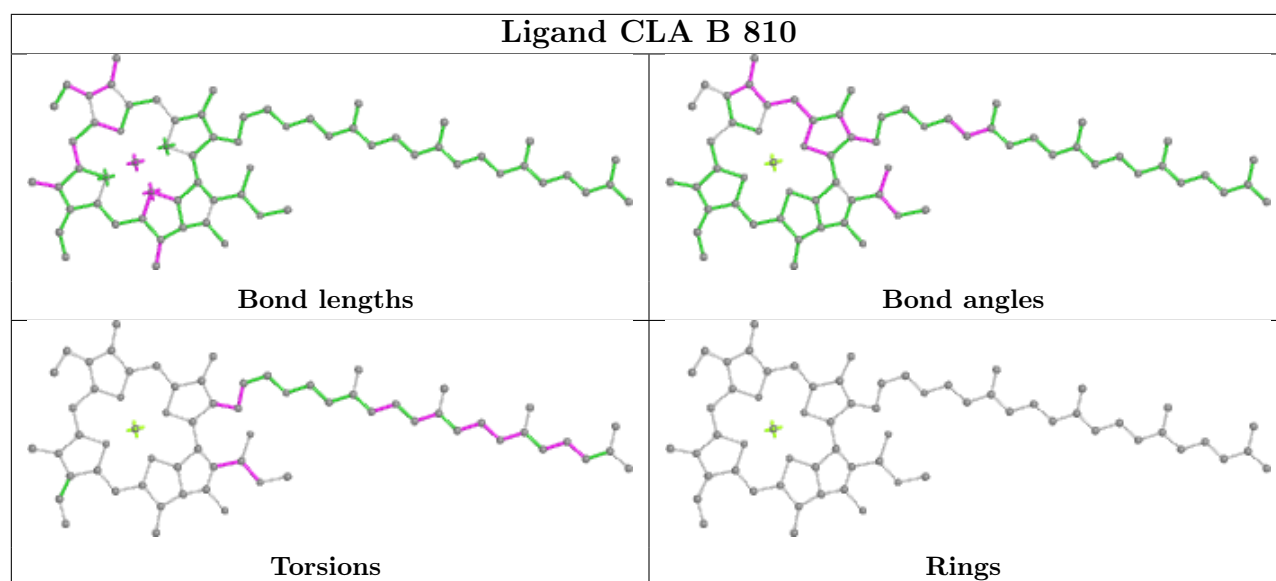
Rings

## Ligand CLA L 303

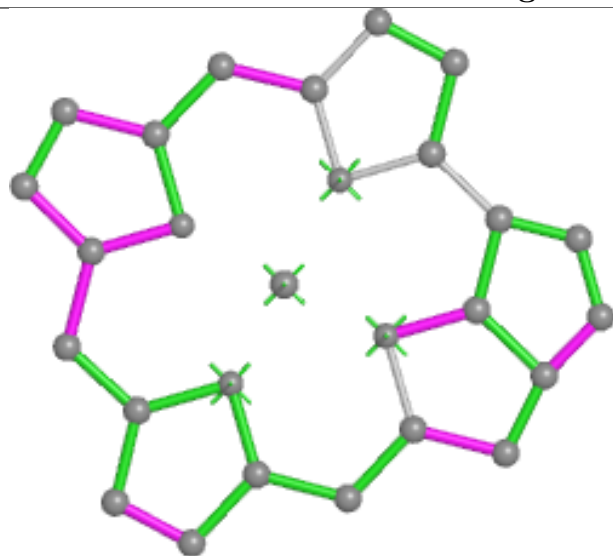




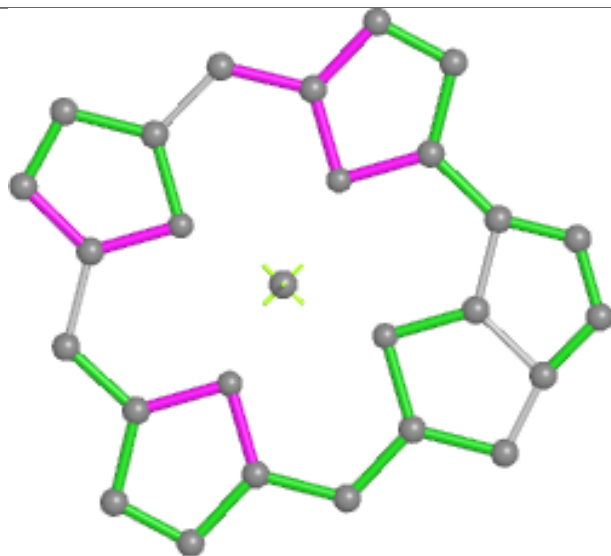




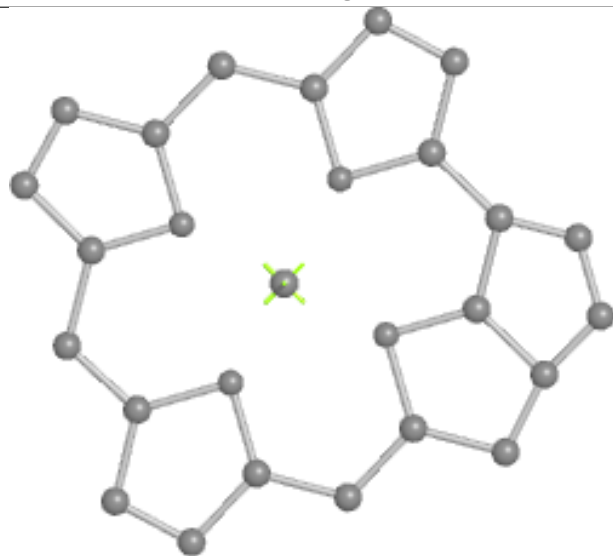
## Ligand CLA 2 614



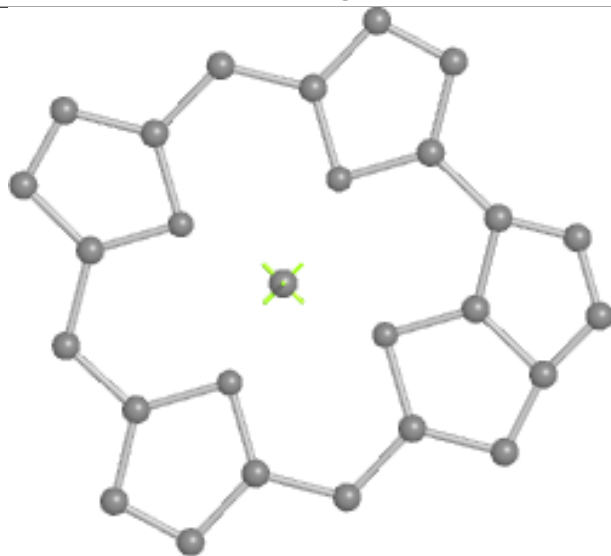
Bond lengths



Bond angles

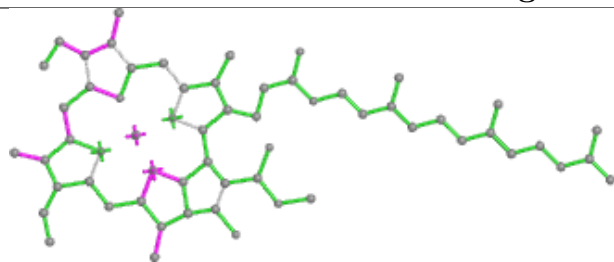


Torsions

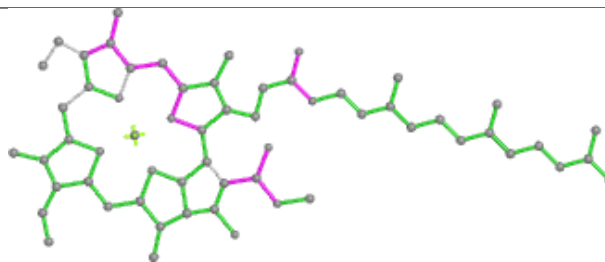


Rings

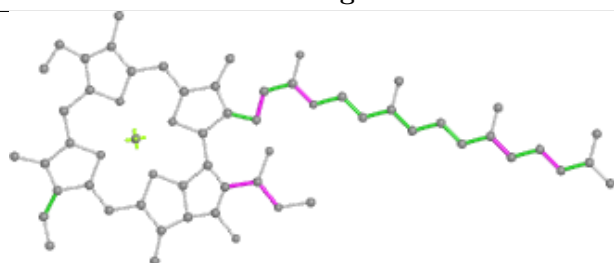
## Ligand CLA 3 602



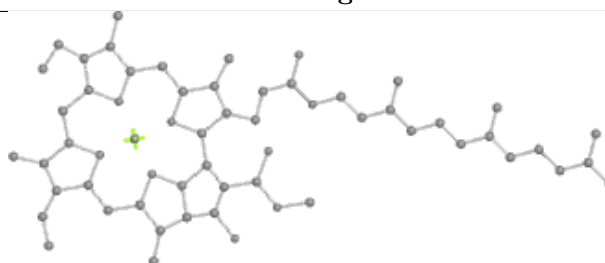
Bond lengths



Bond angles

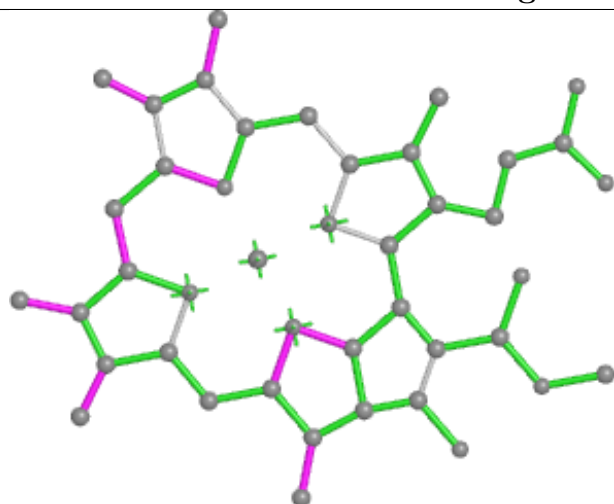


Torsions

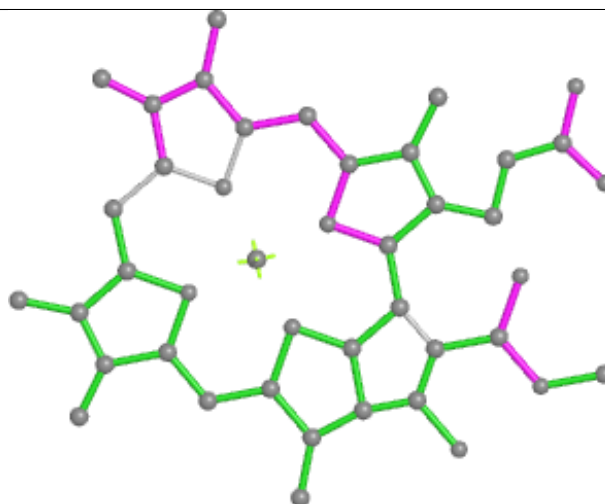


Rings

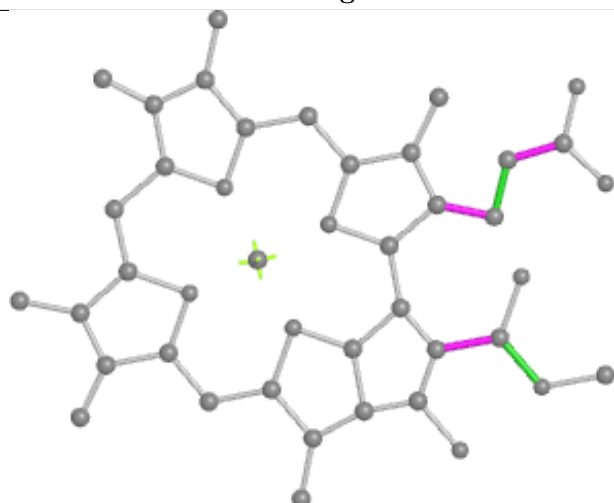
## Ligand CLA 4 616



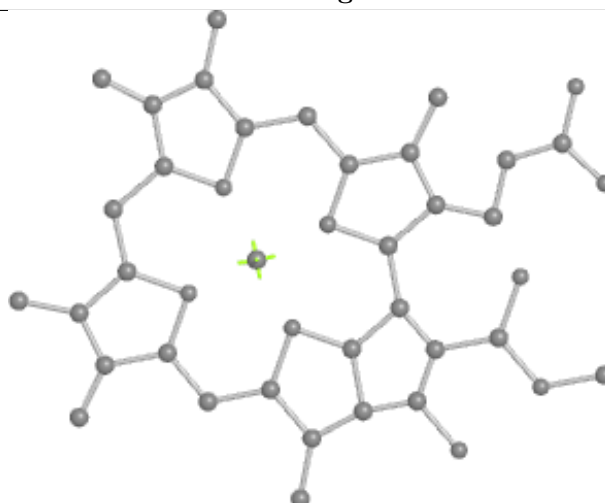
Bond lengths



Bond angles

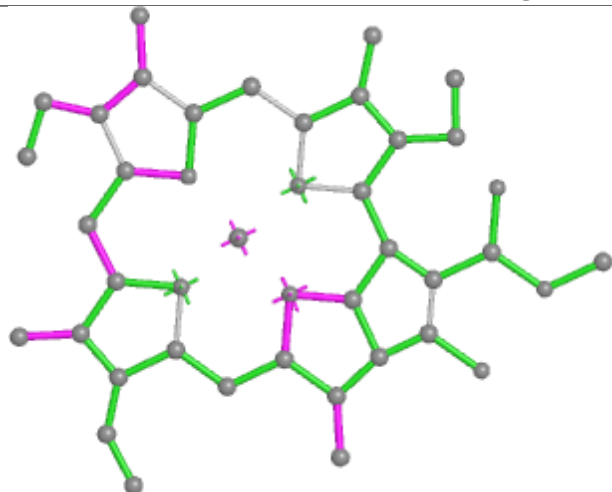


Torsions

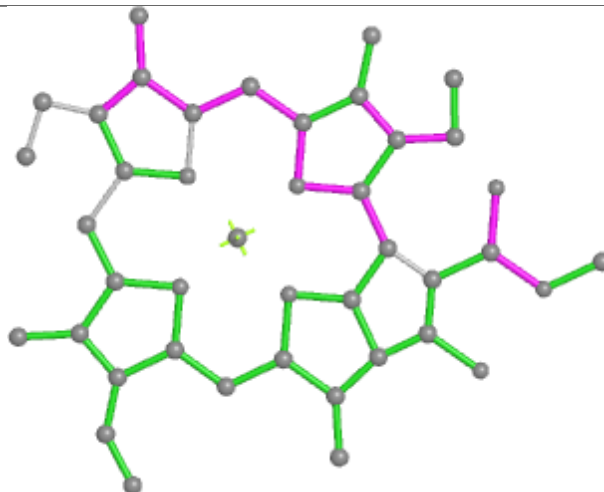


Rings

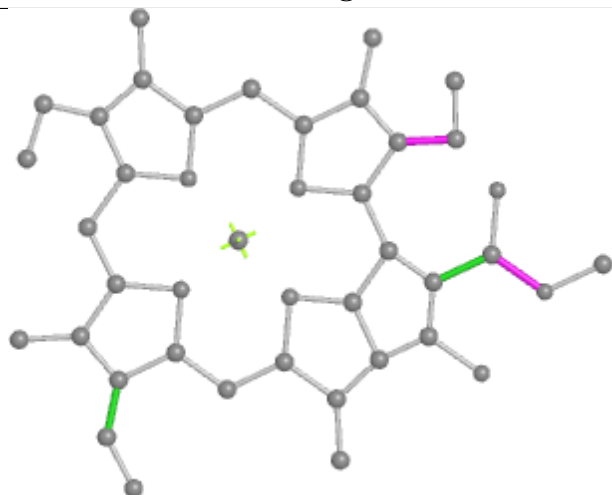
## Ligand CLA 7 614



Bond lengths



Bond angles

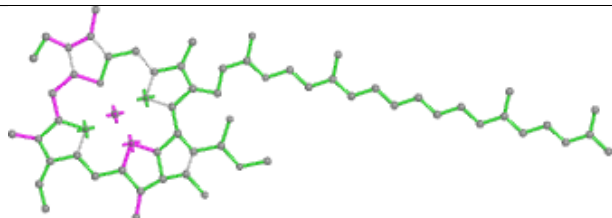


Torsions

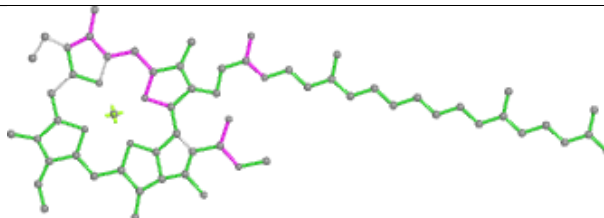


Rings

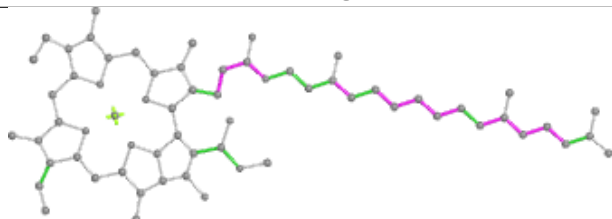
## Ligand CLA A 843



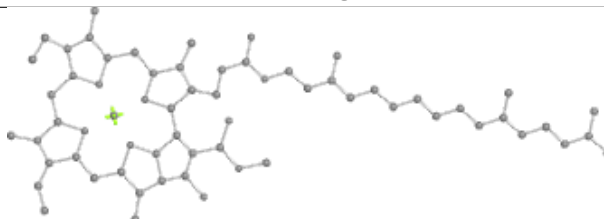
Bond lengths



Bond angles



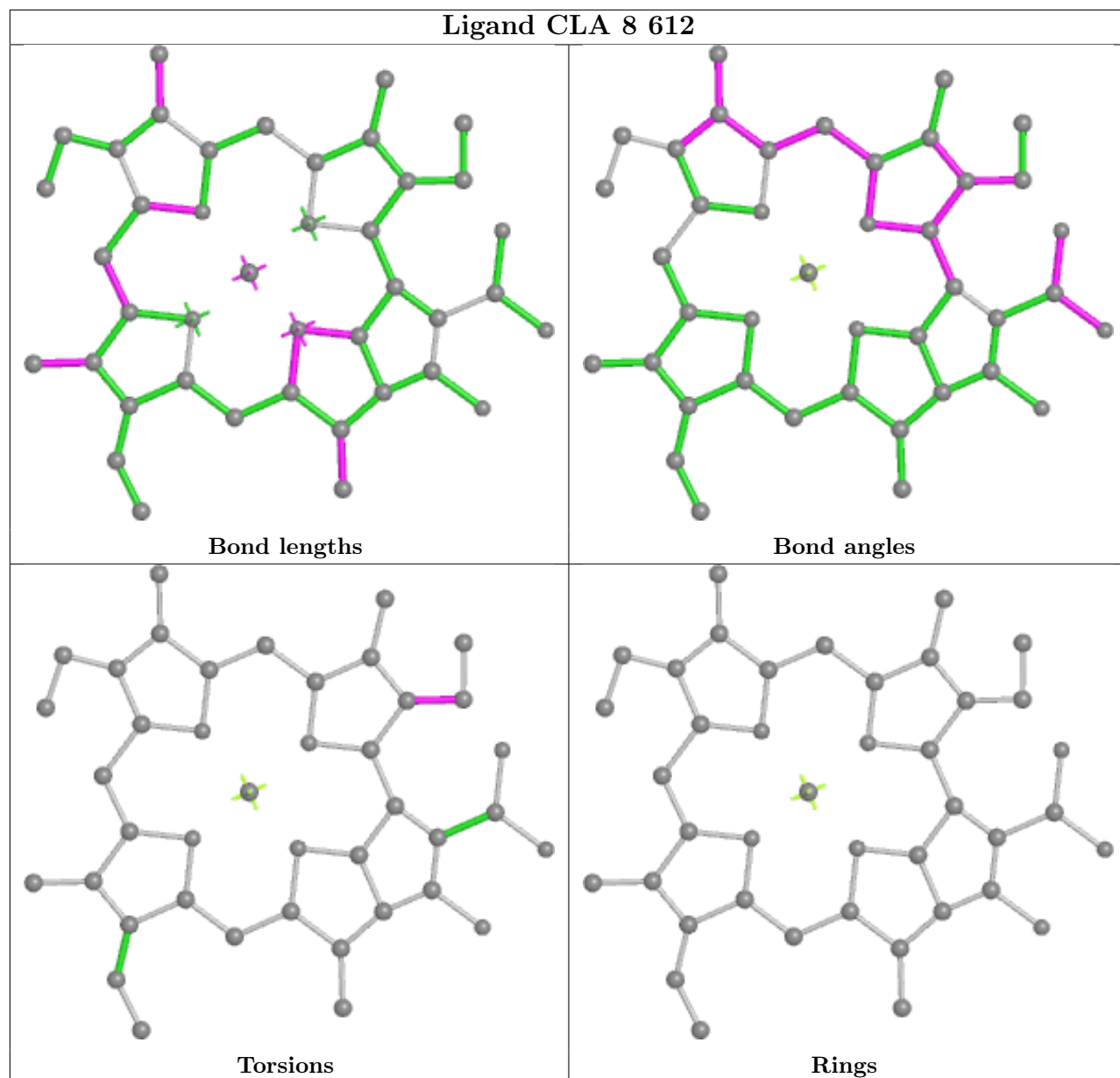
Torsions

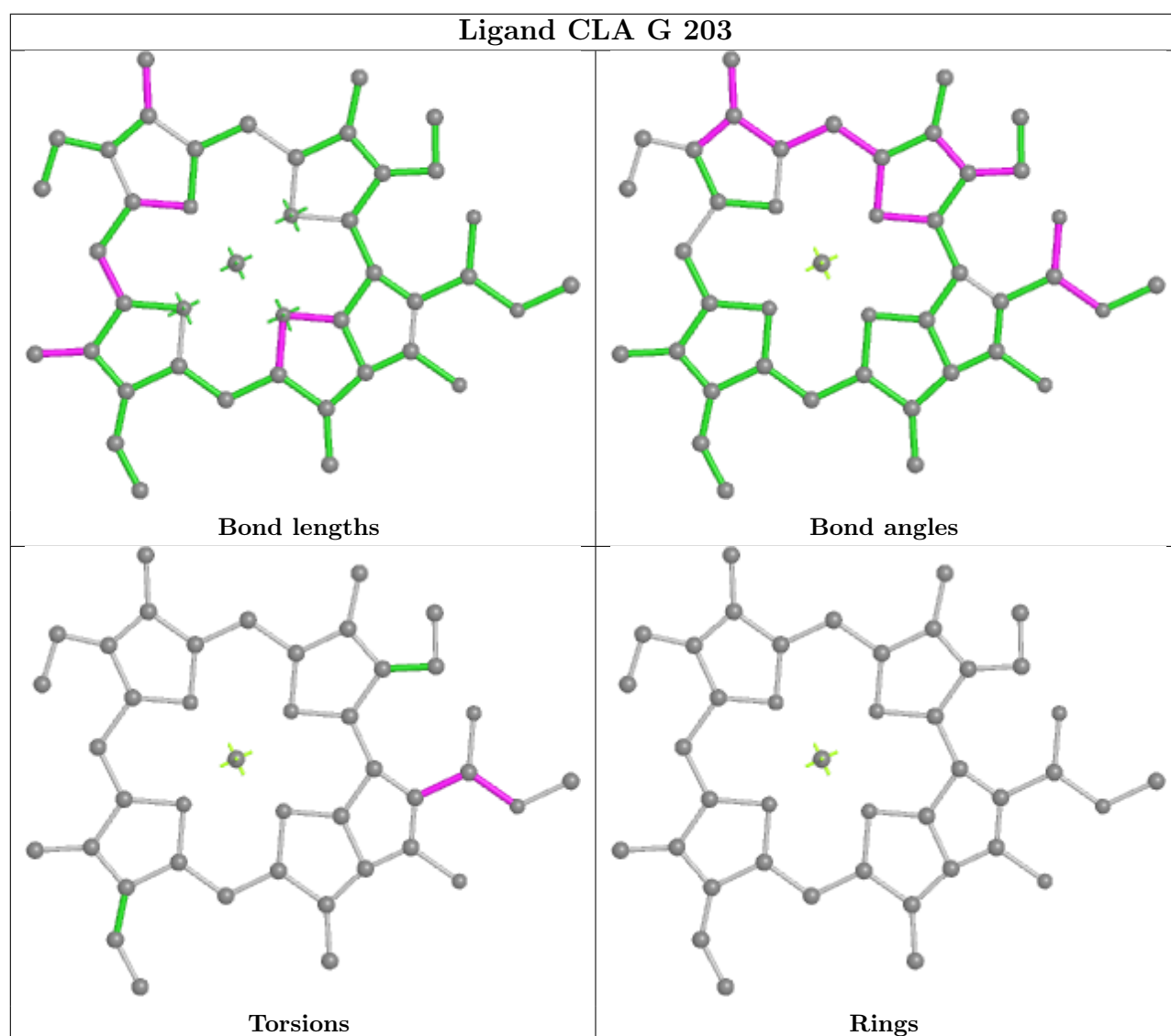
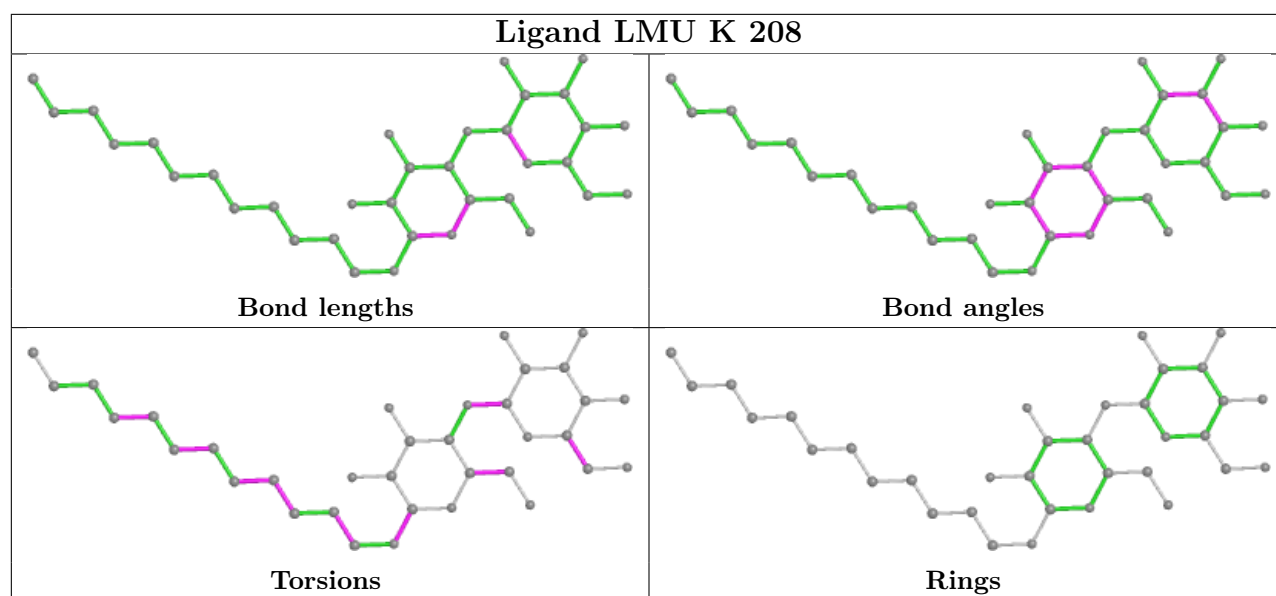


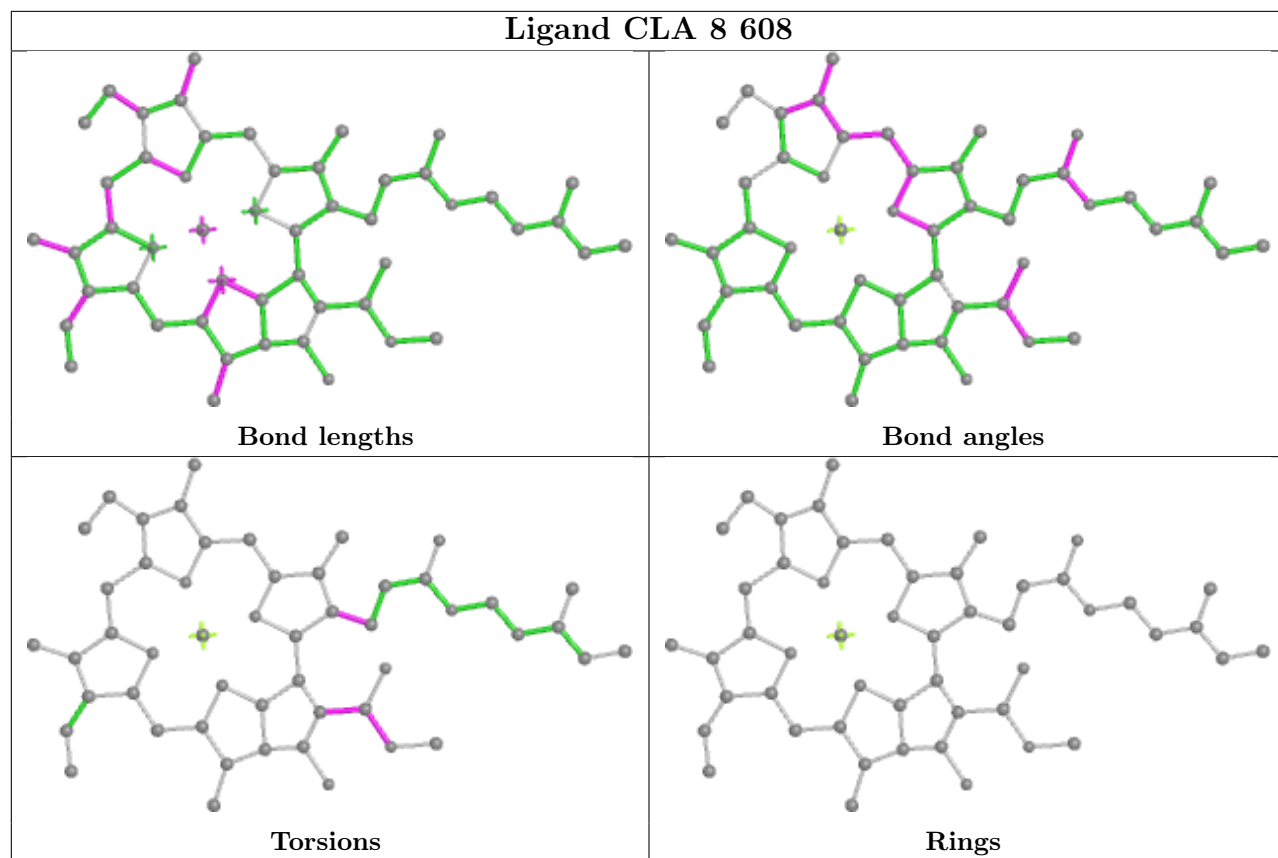
Rings



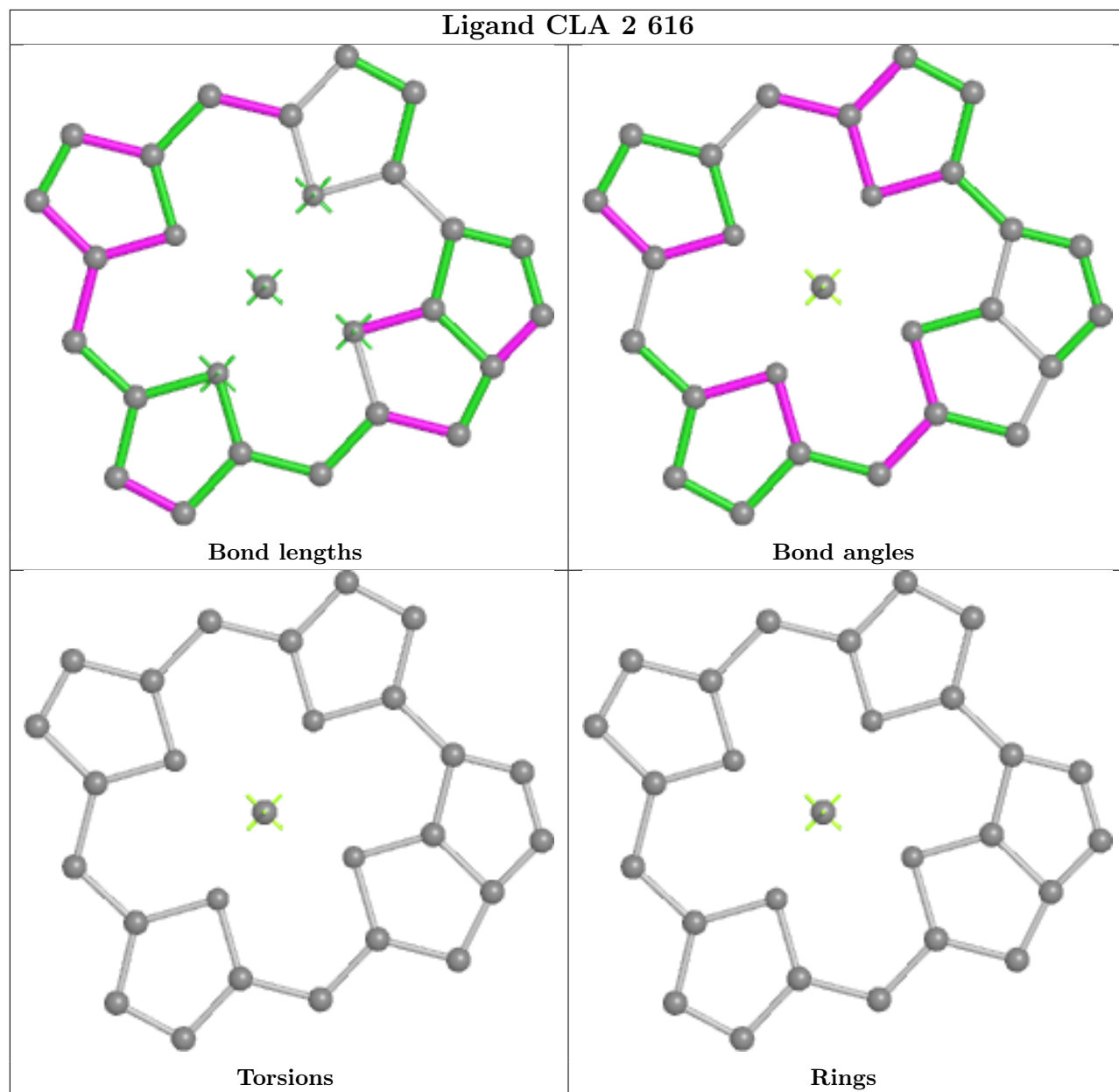
## Ligand CLA 8 612

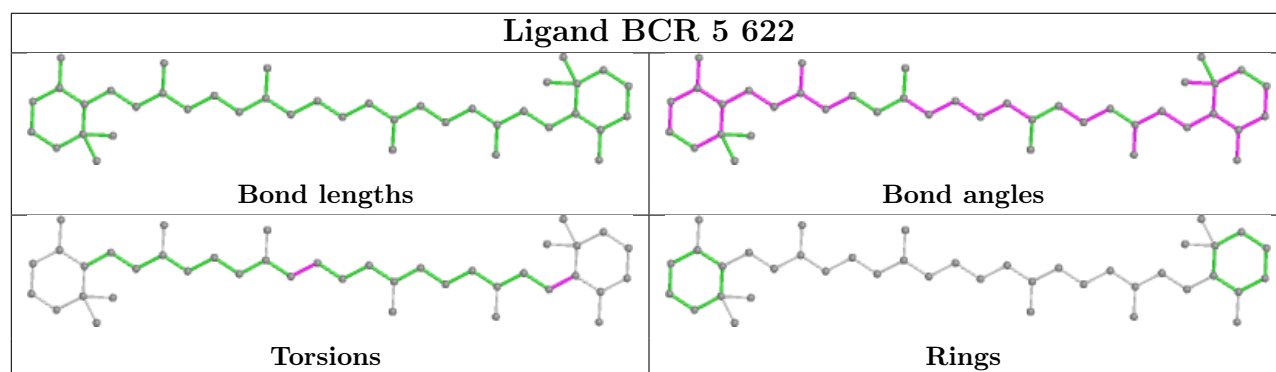
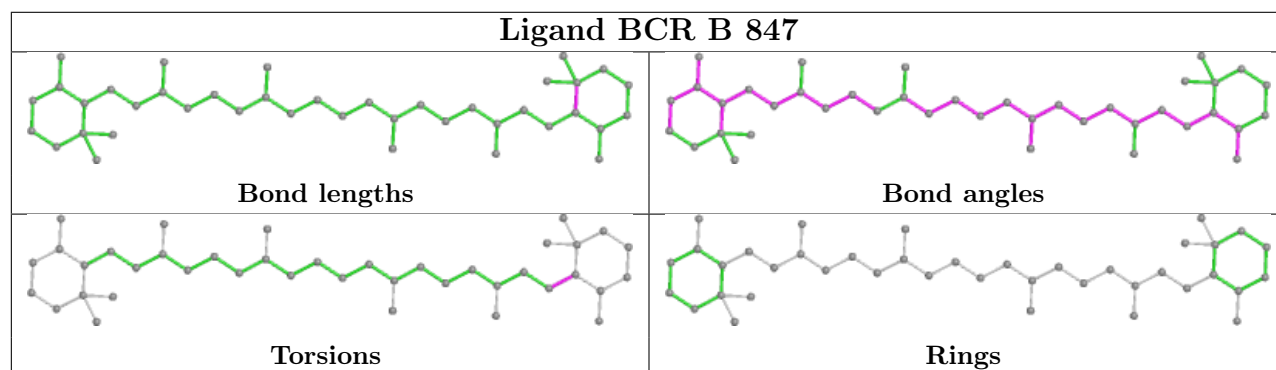
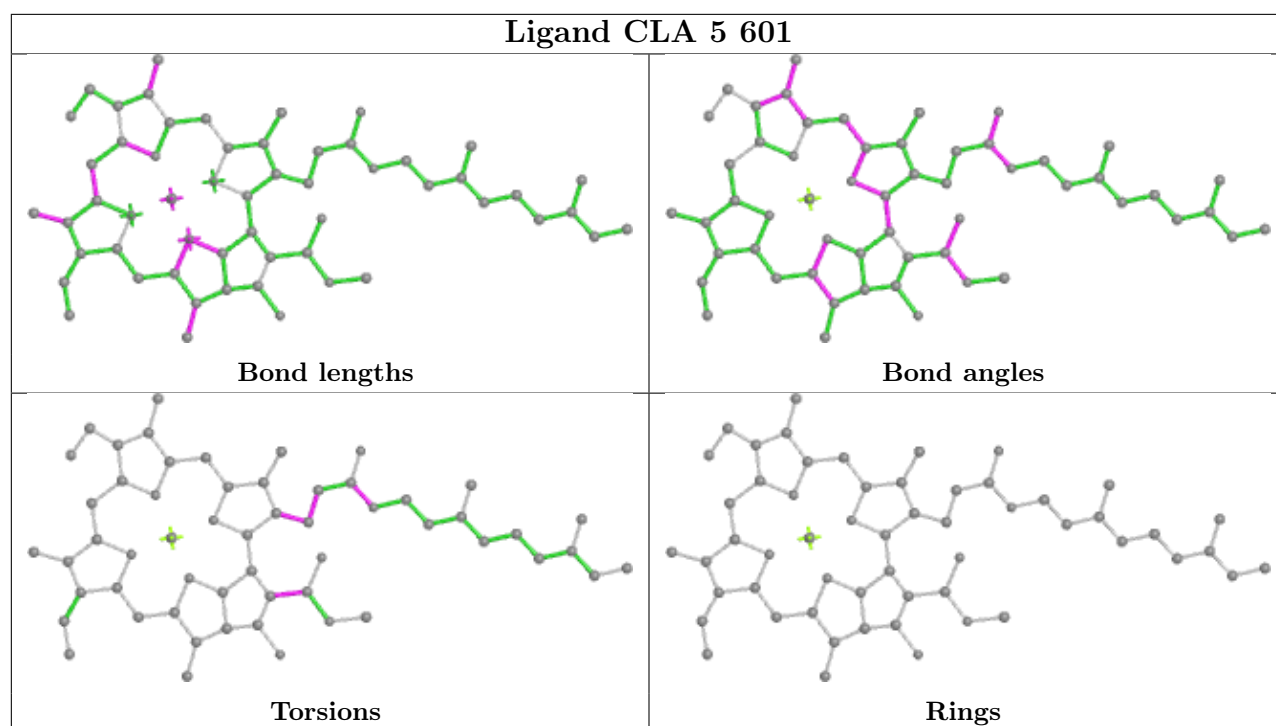


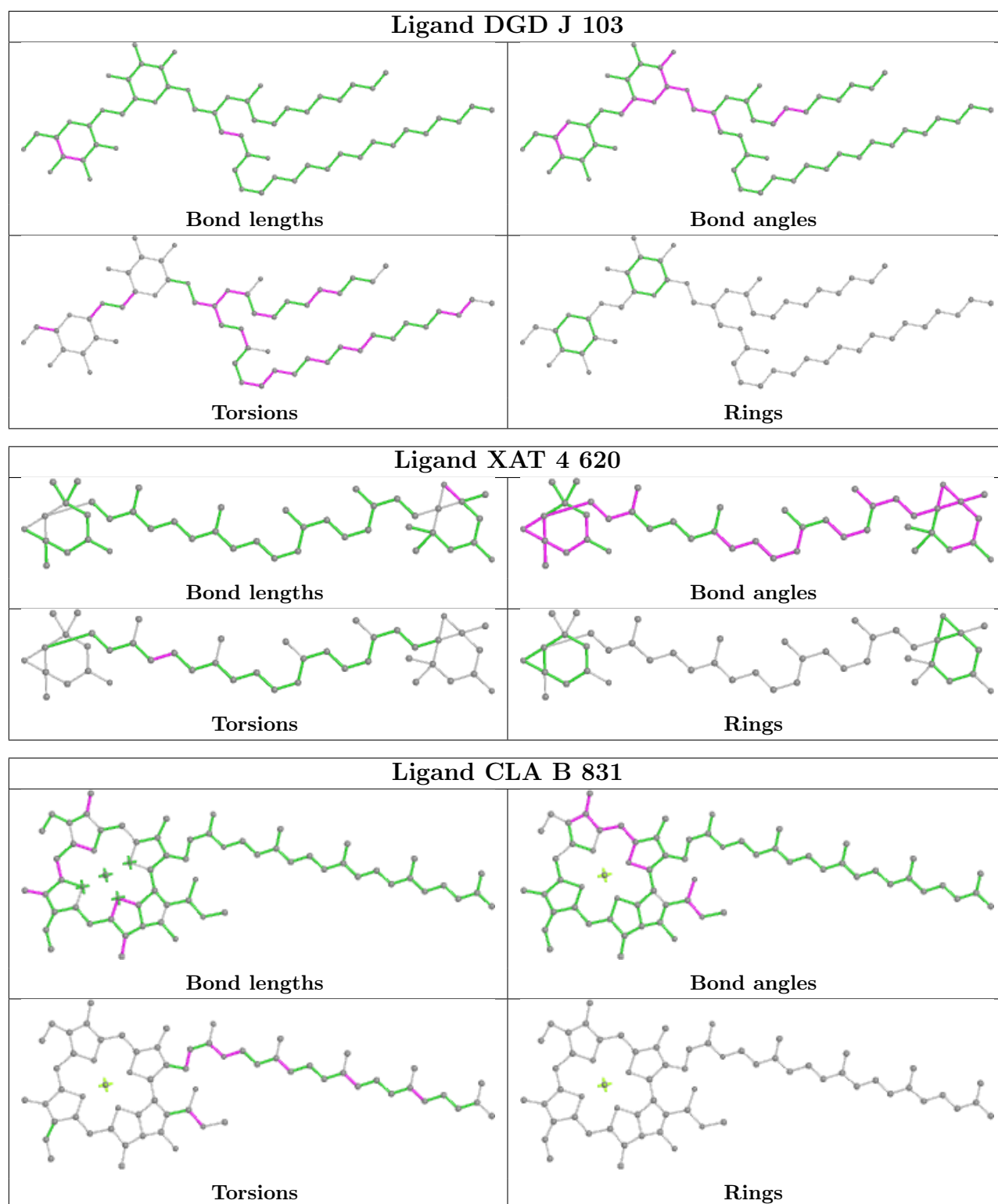




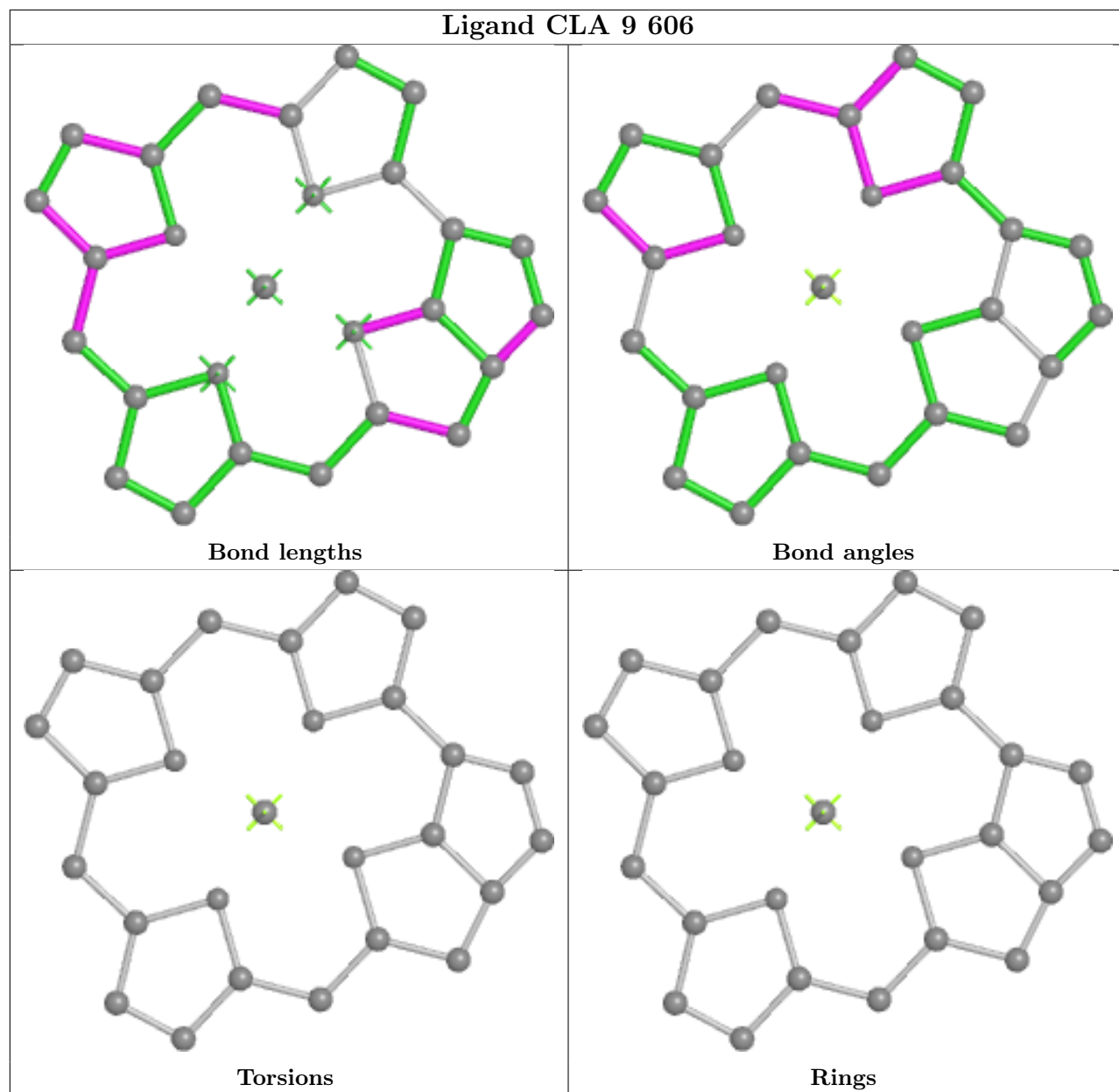
## Ligand CLA 2 616



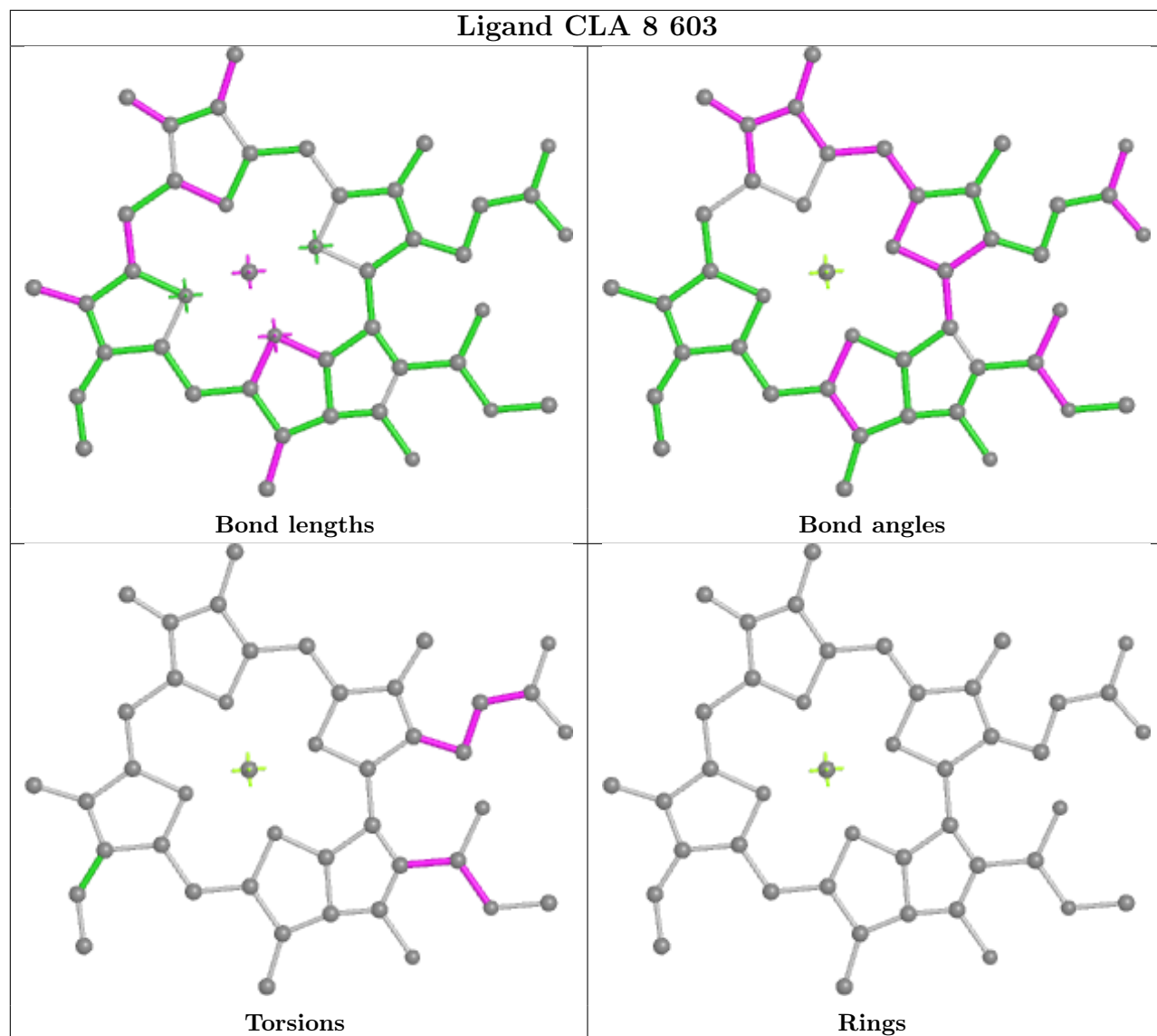




## Ligand CLA 9 606

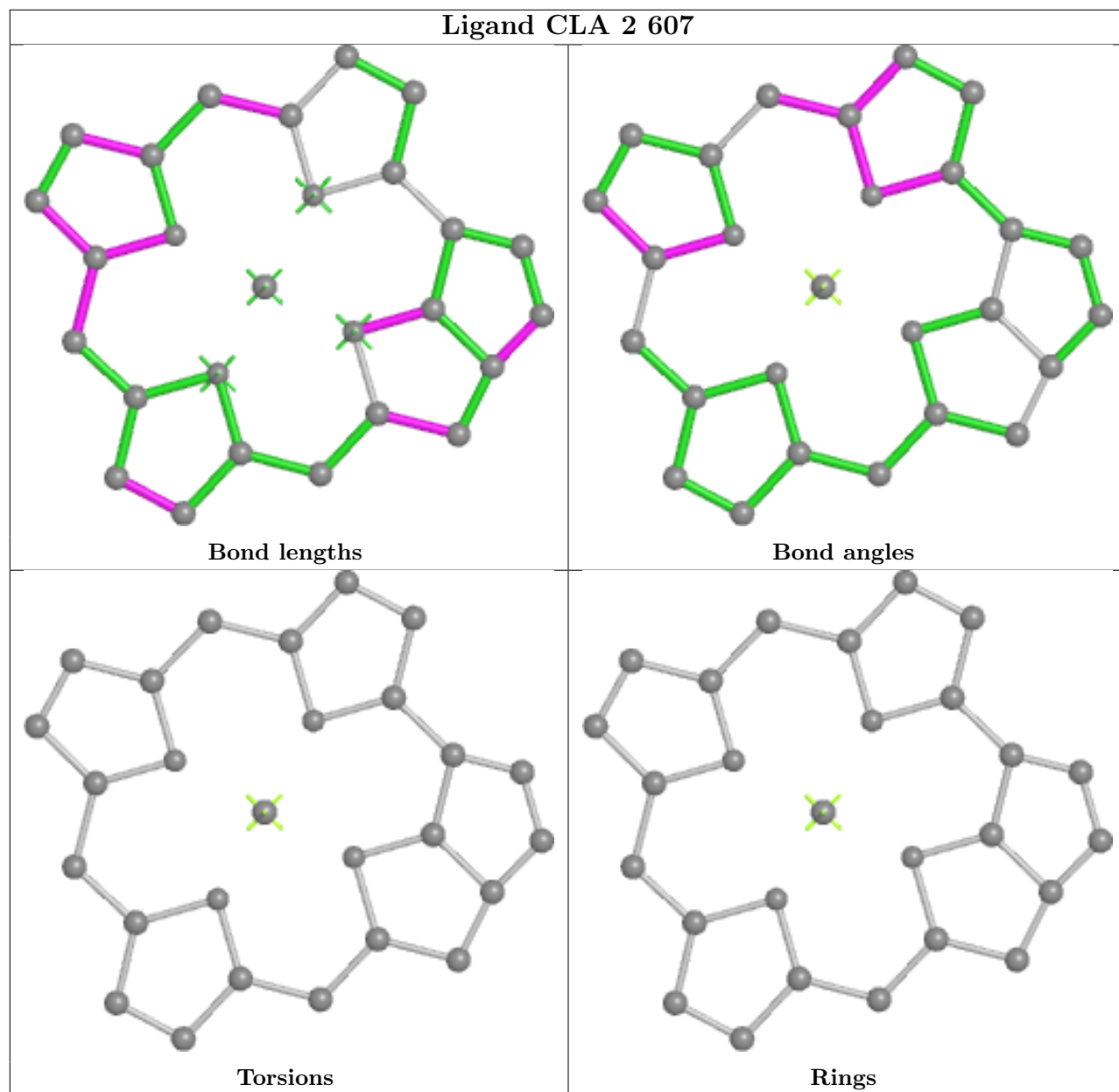


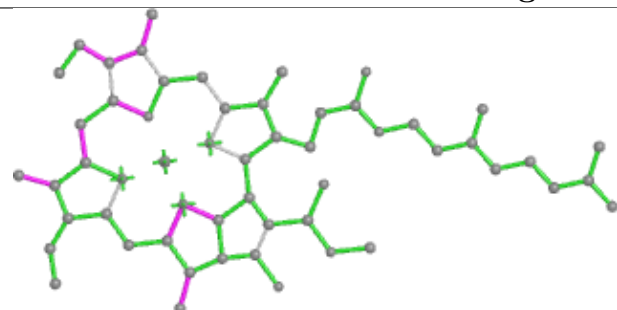
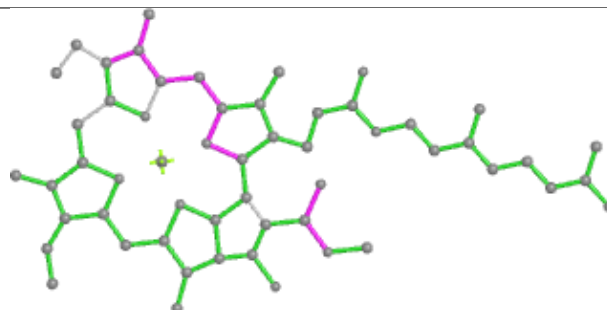
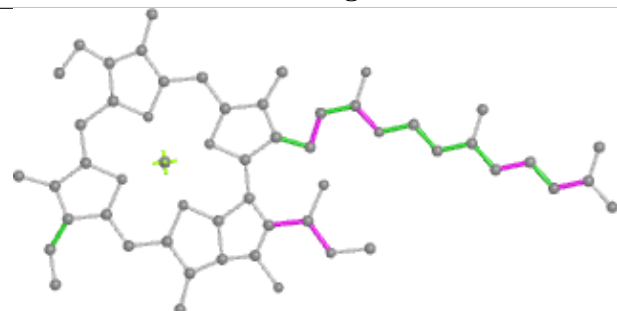
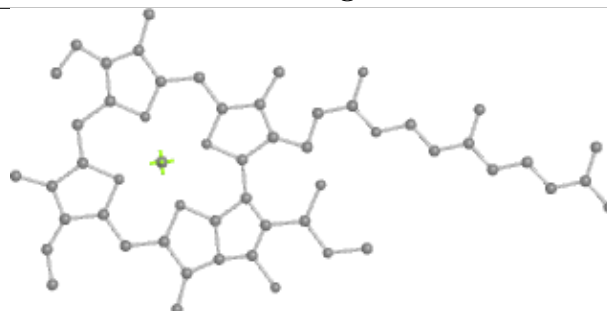
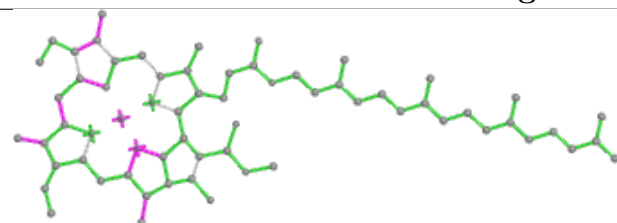
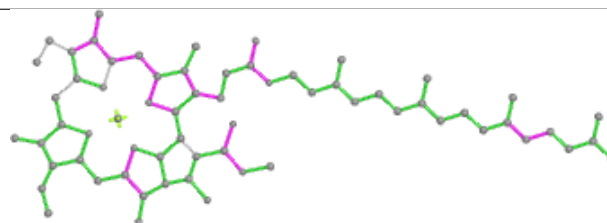
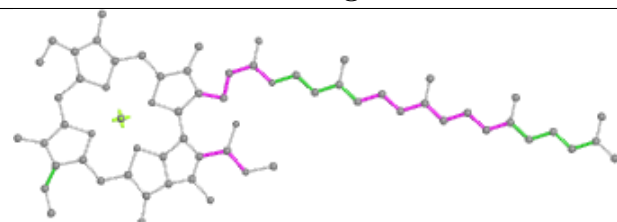
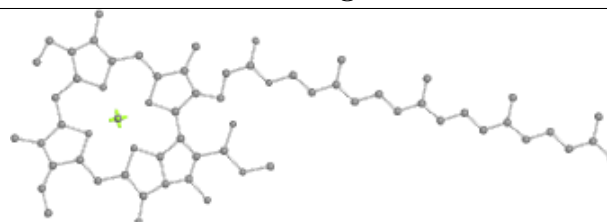
## Ligand CLA 8 603



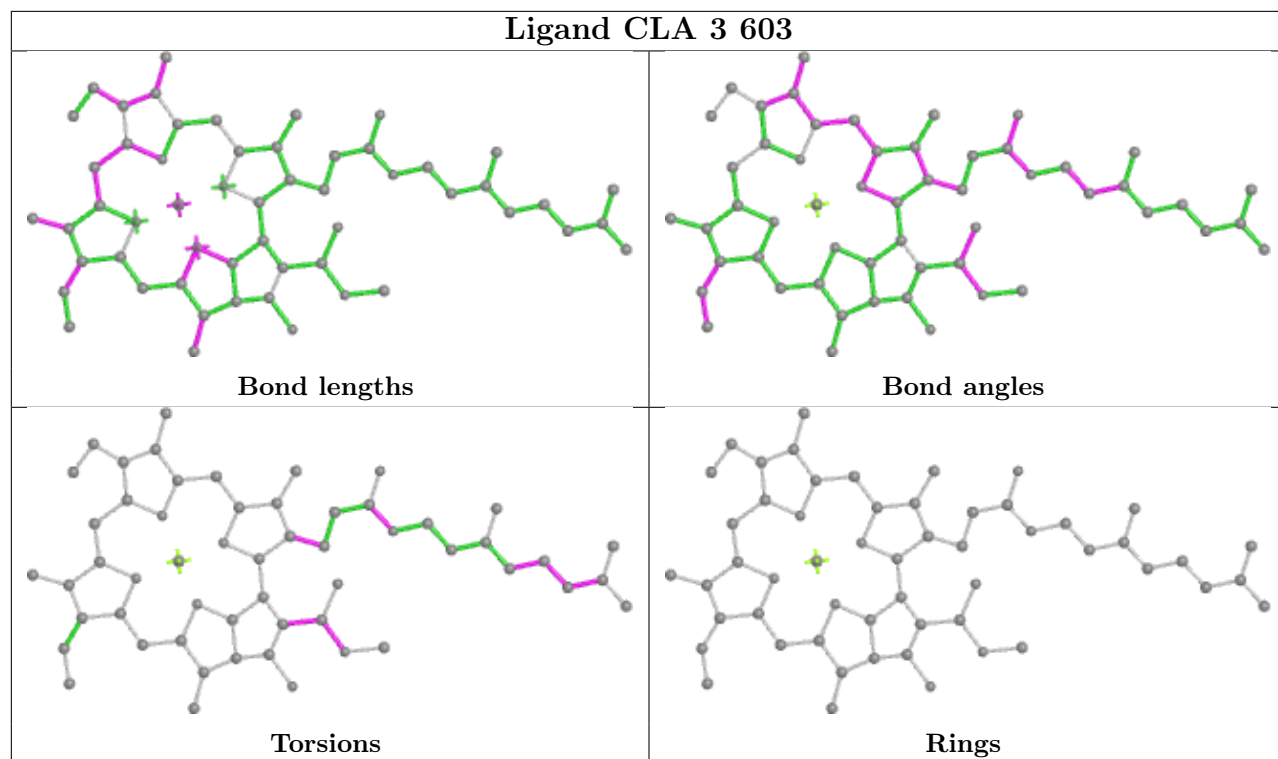


## Ligand CLA 2 607

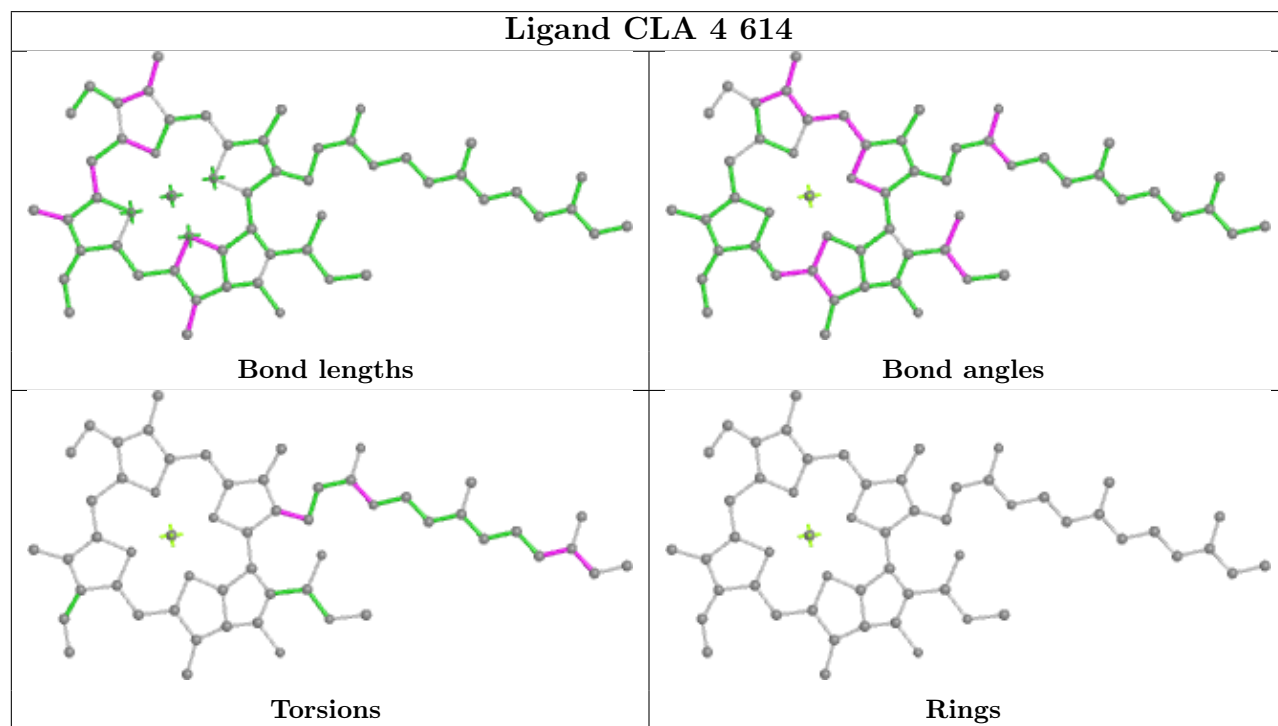


**Ligand CLA B 819****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 813****Bond lengths****Bond angles****Torsions****Rings**

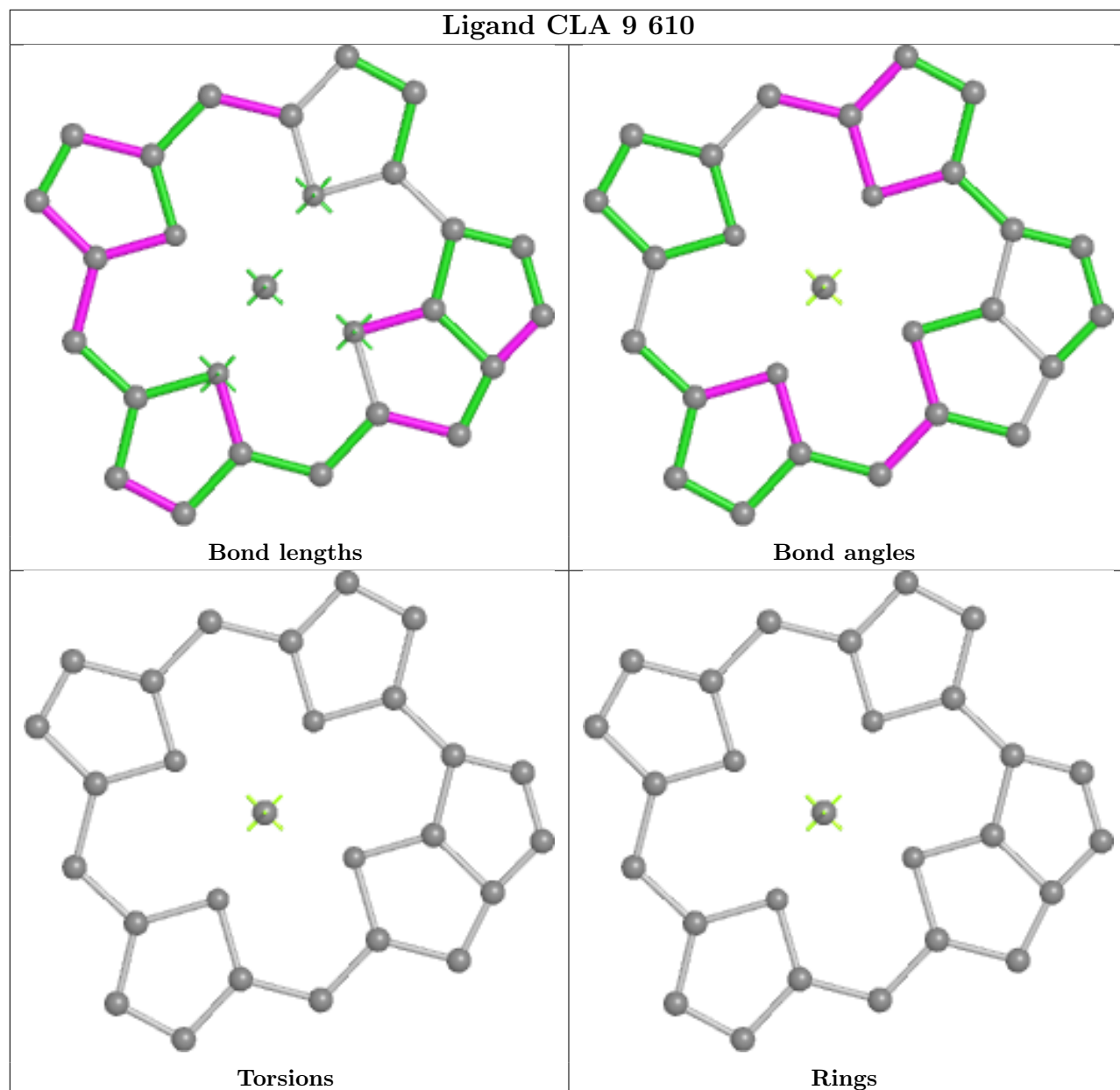
## Ligand CLA 3 603



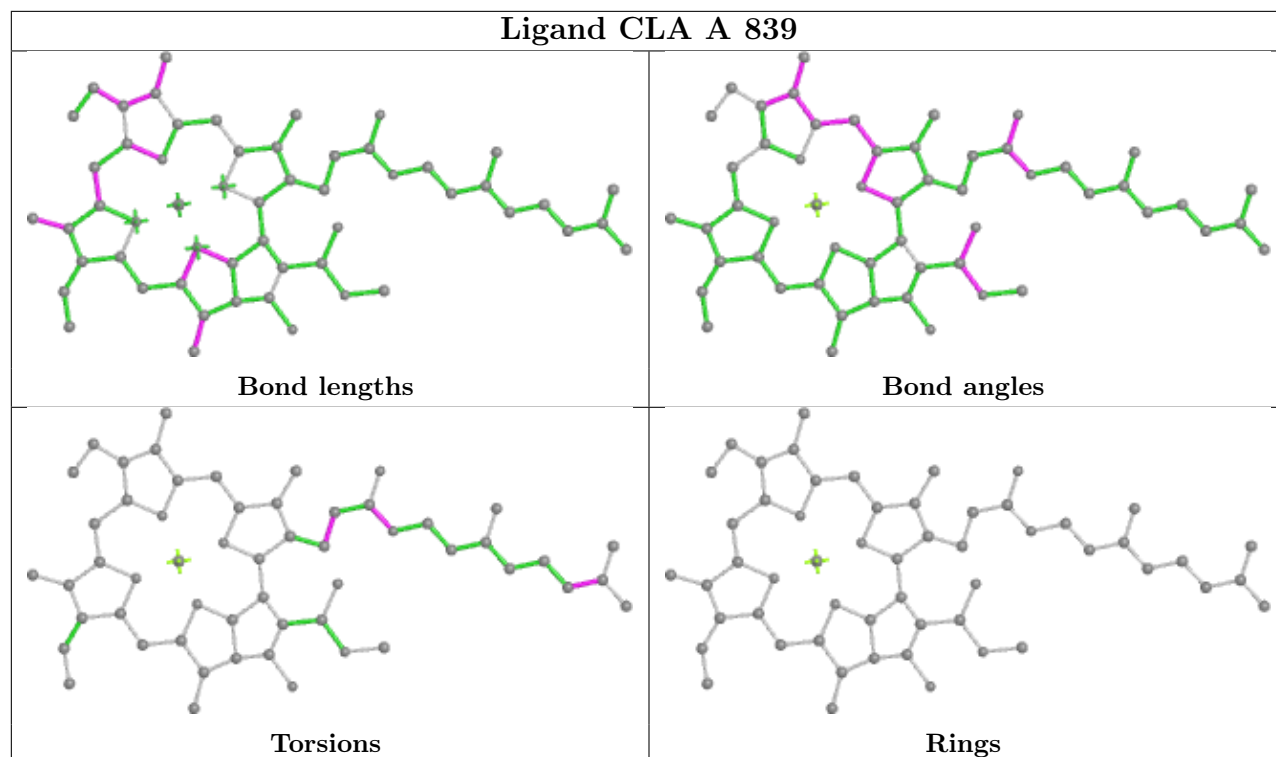
## Ligand CLA 4 614



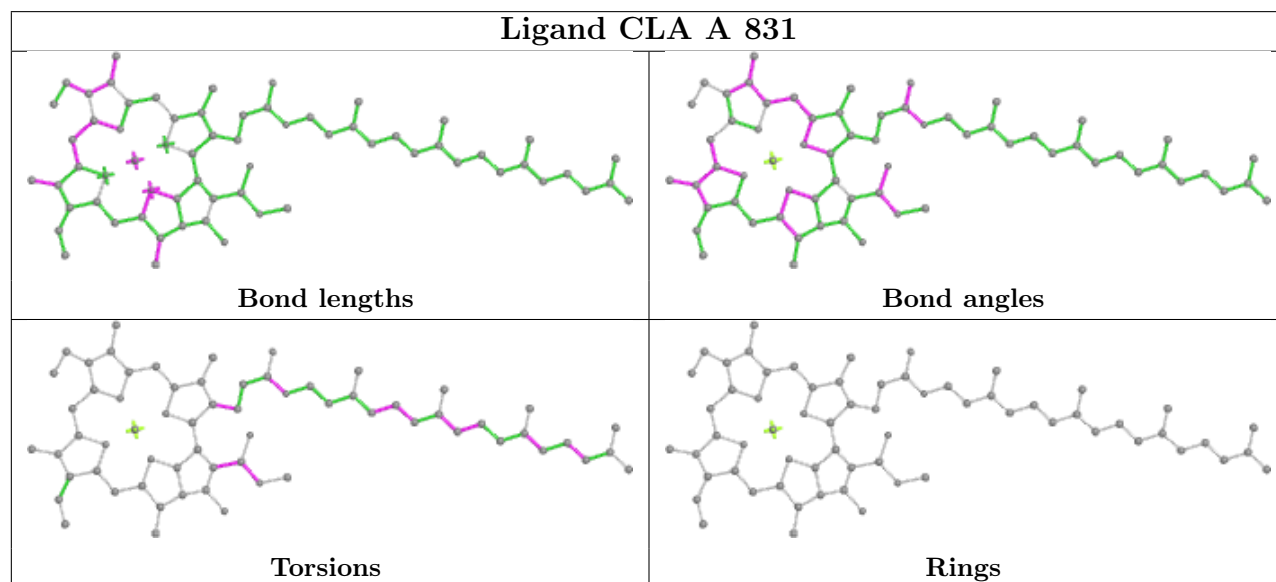
## Ligand CLA 9 610



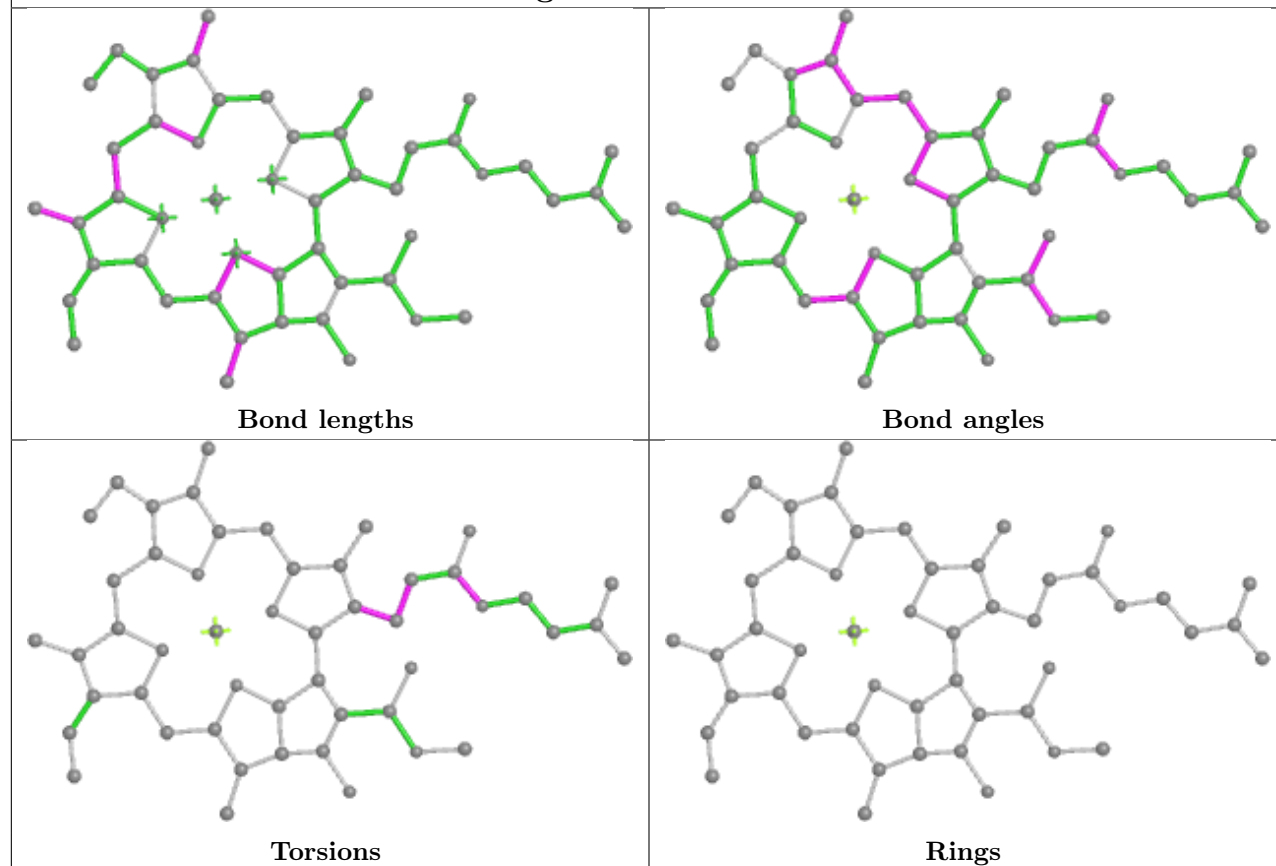
## Ligand CLA A 839



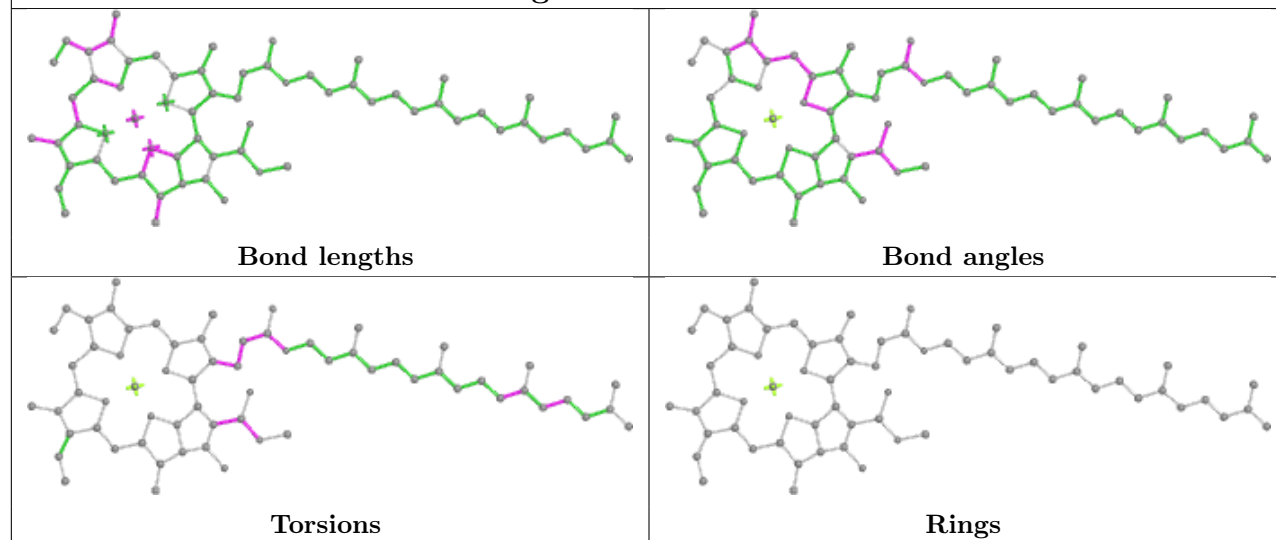
## Ligand CLA A 831



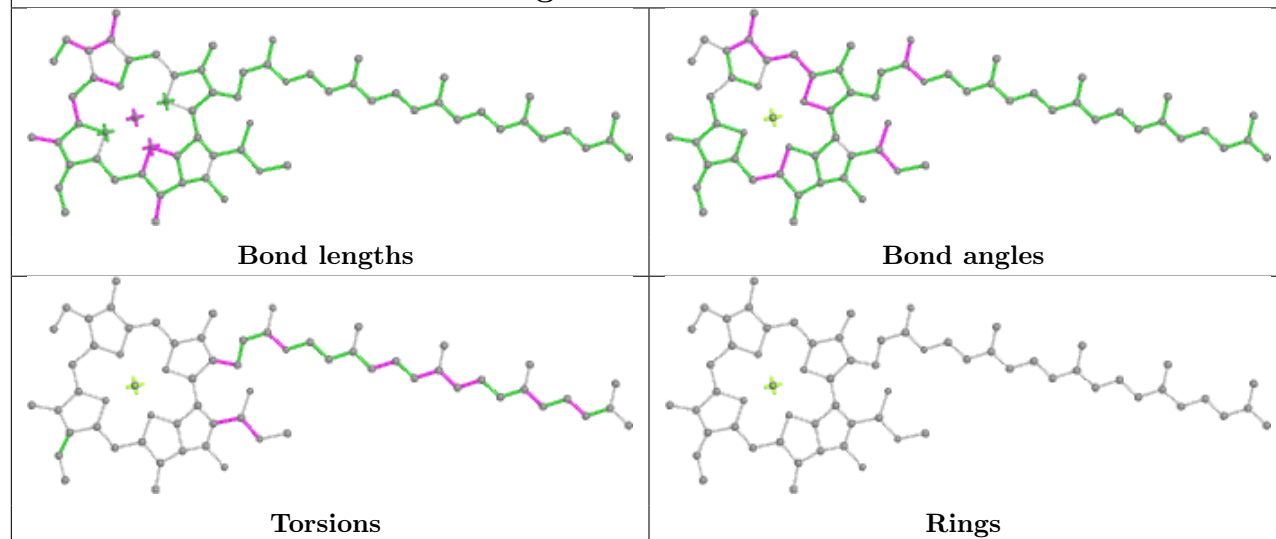
## Ligand CLA 8 604



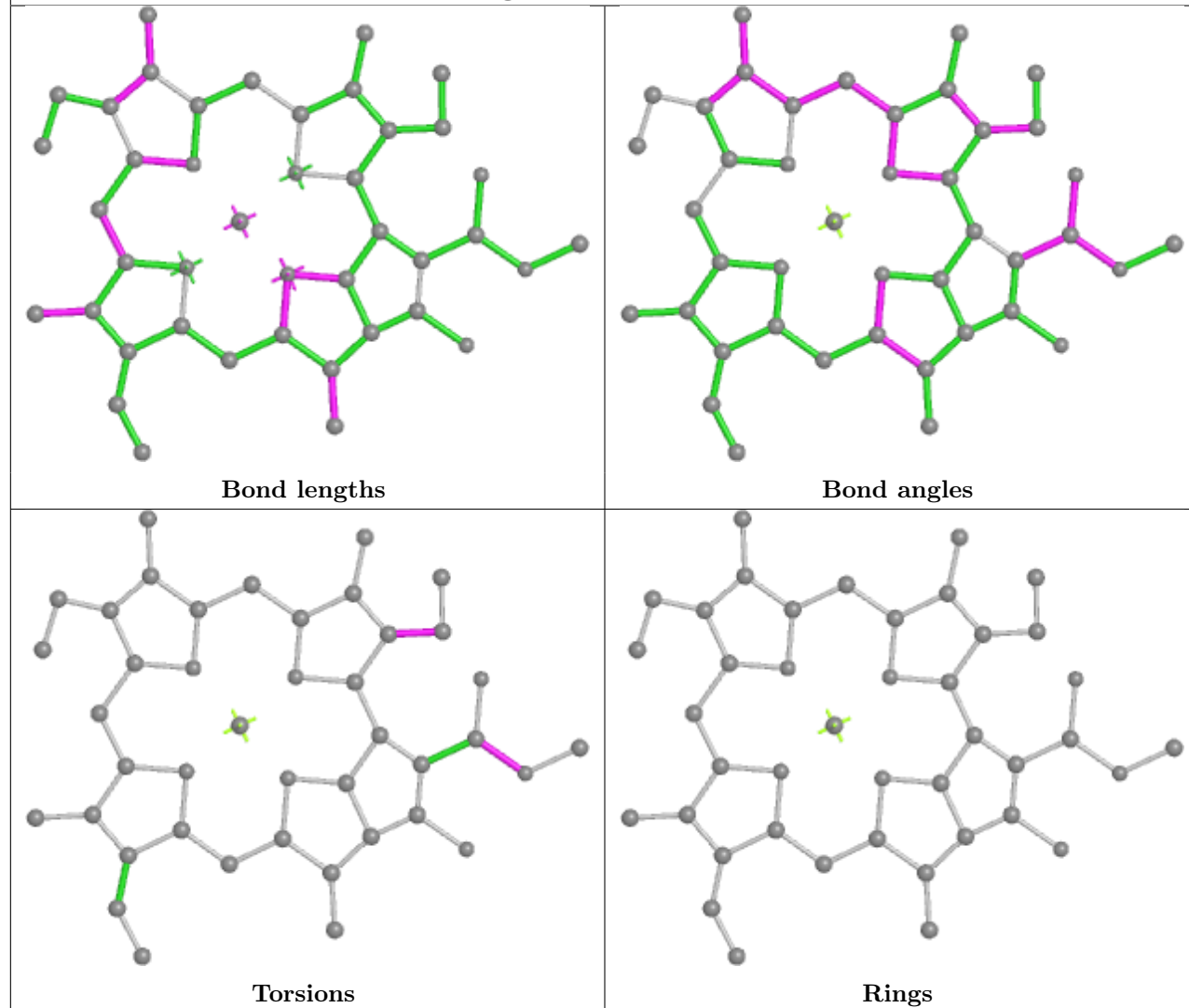
## Ligand CLA A 822

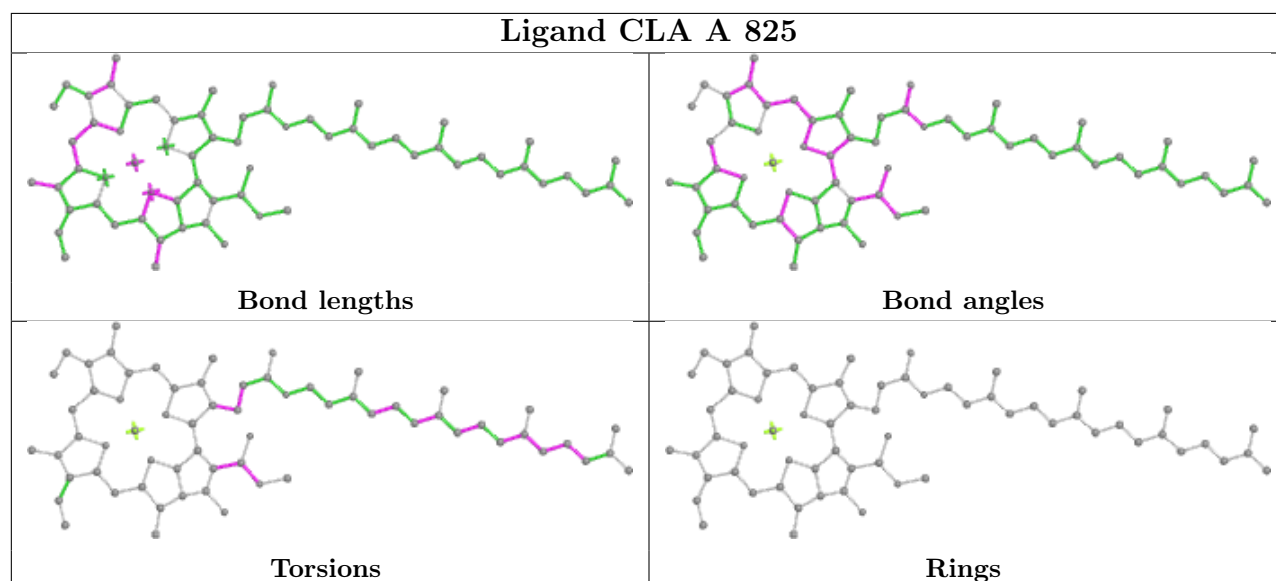
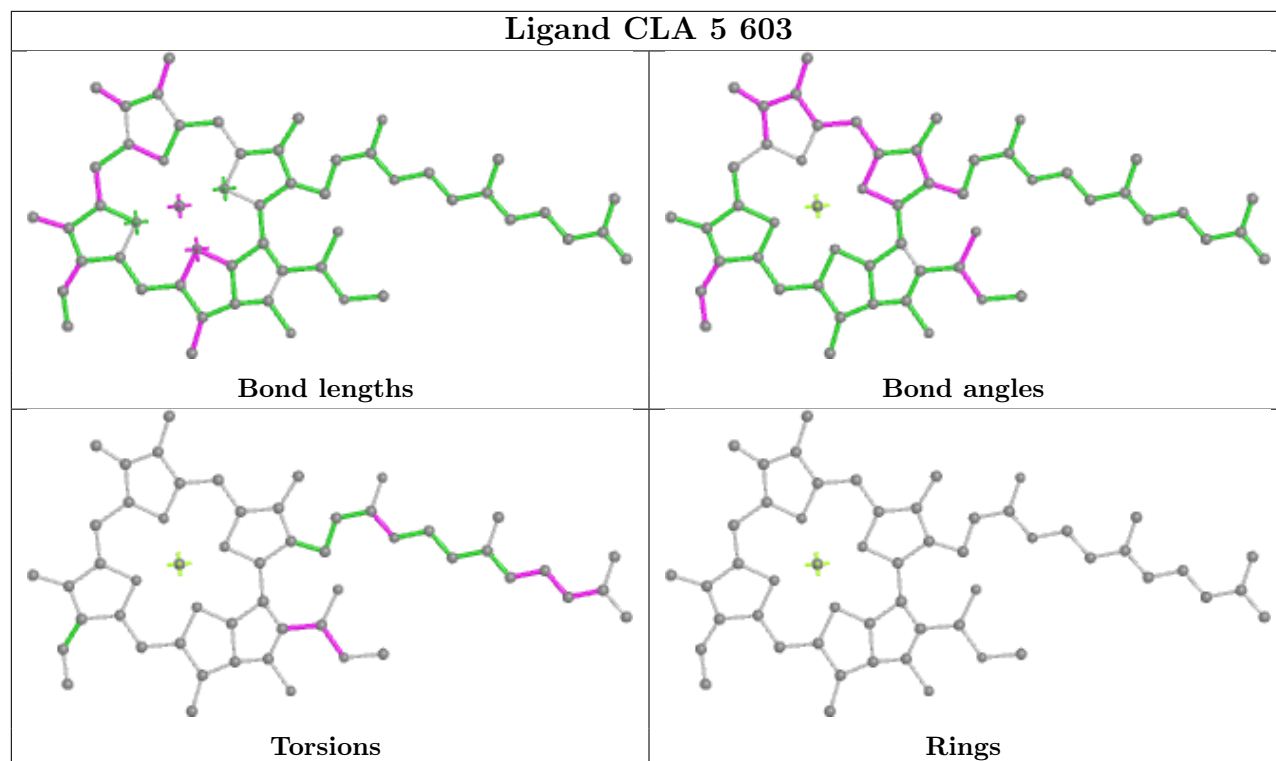
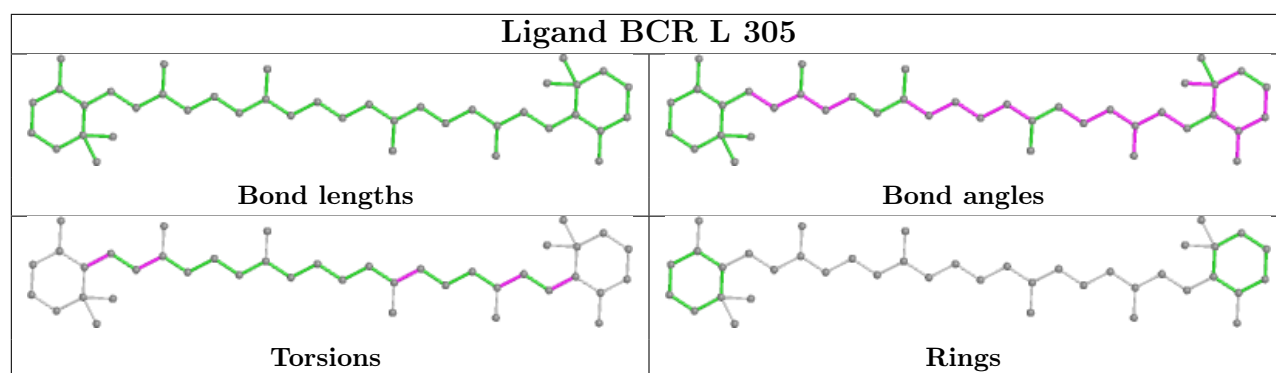


## Ligand CLA 5 607

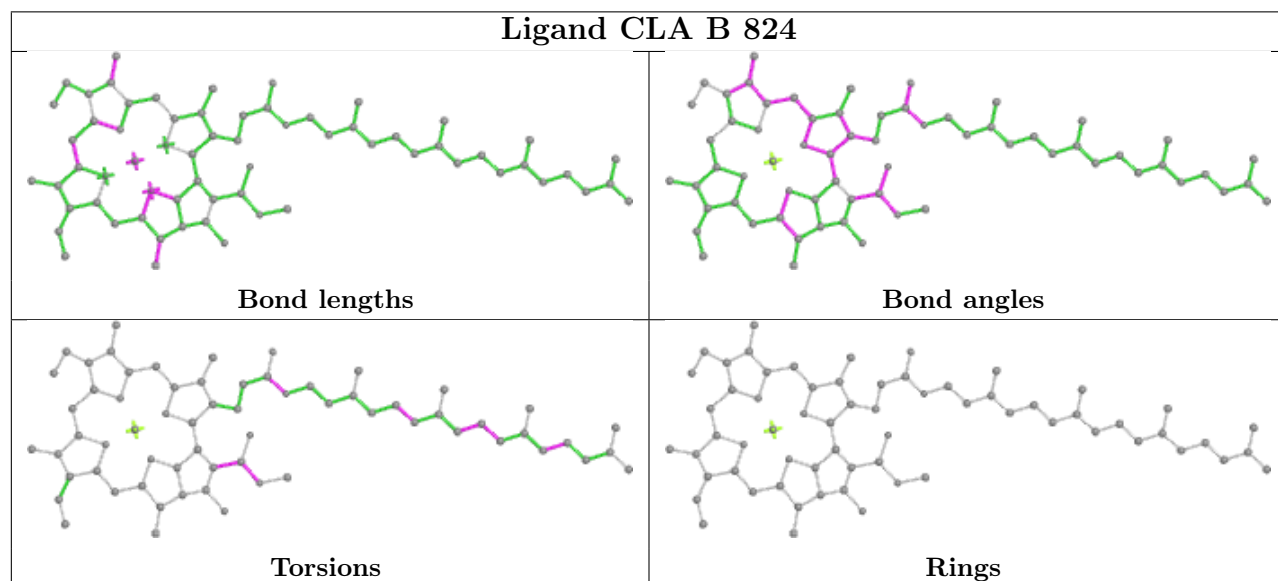
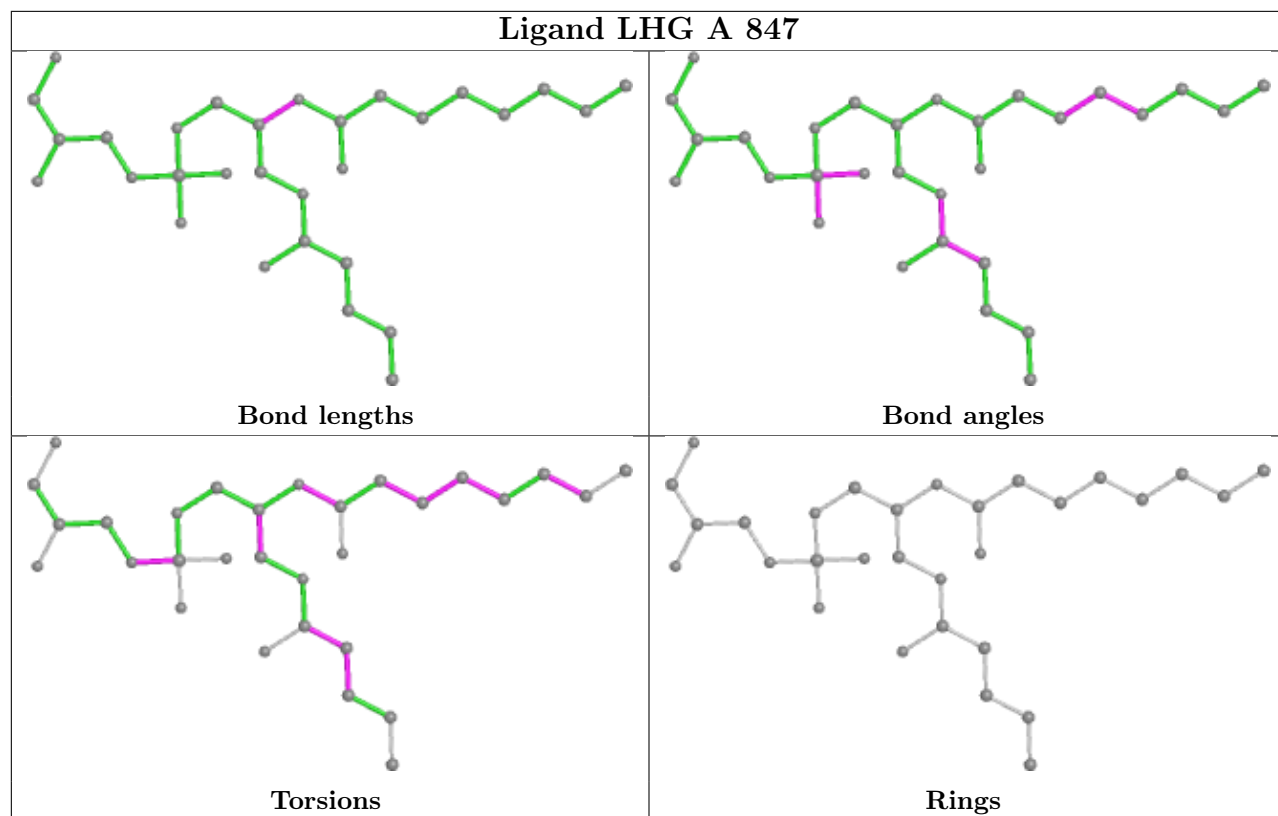


## Ligand CLA 8 611

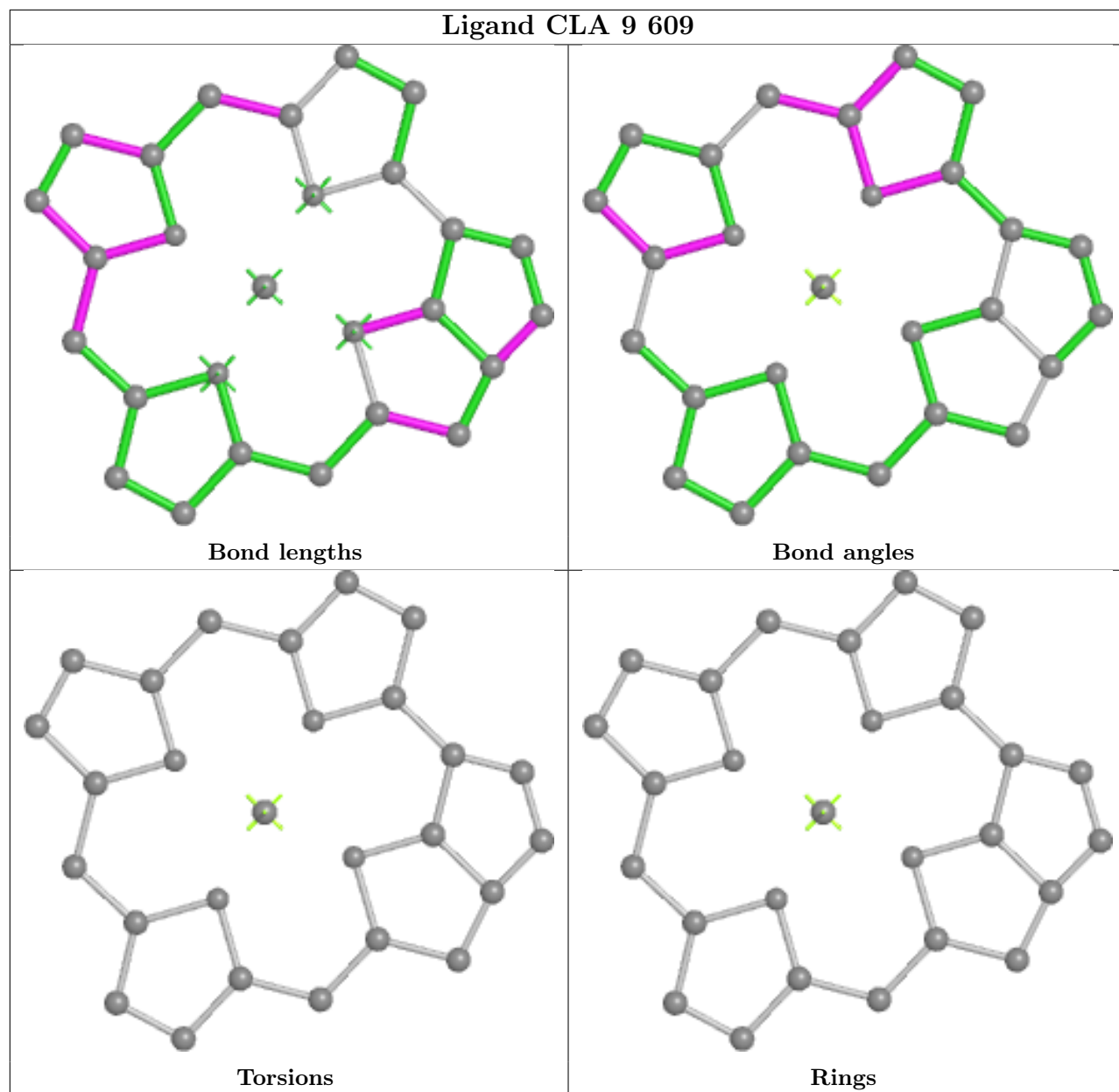


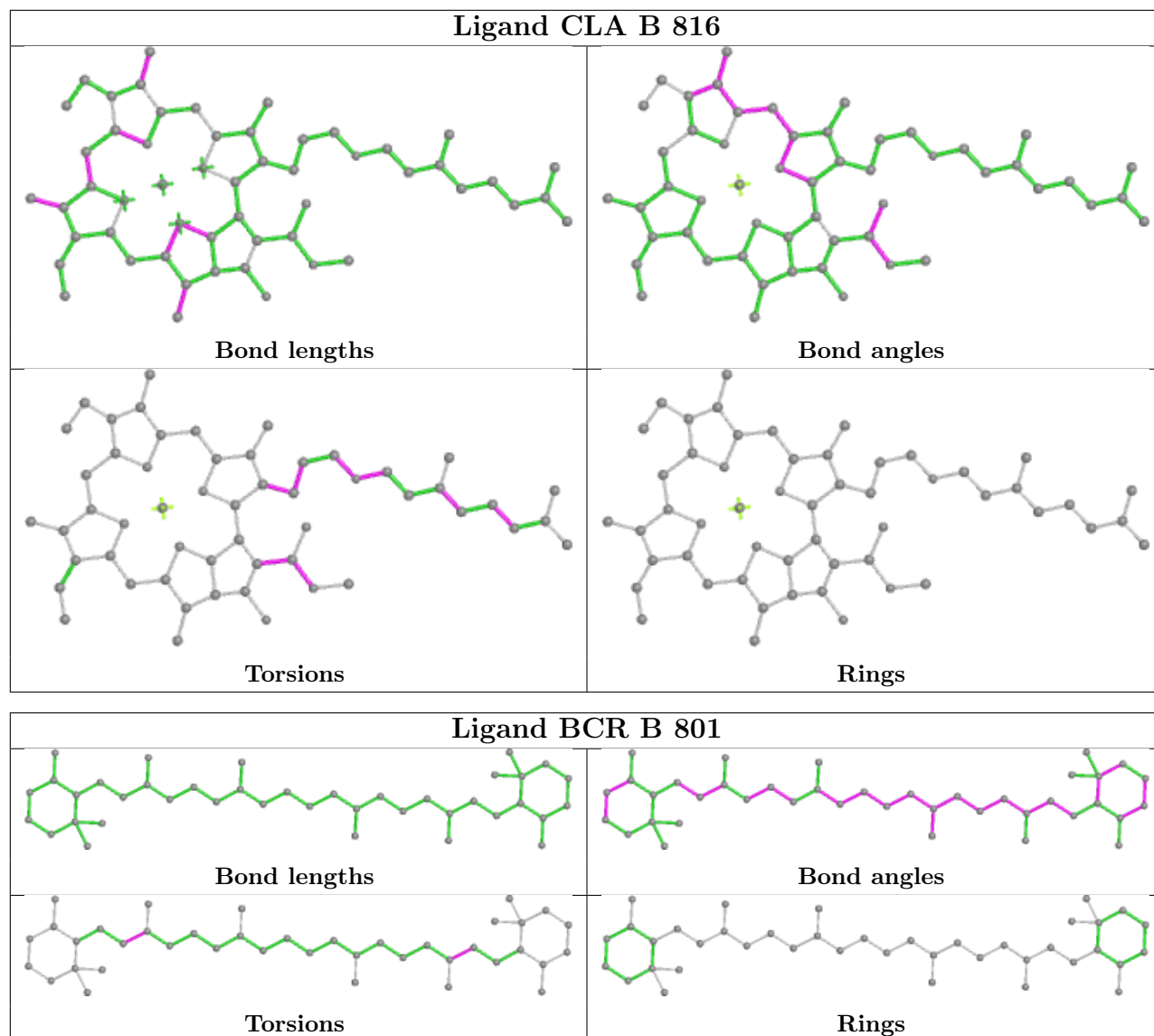


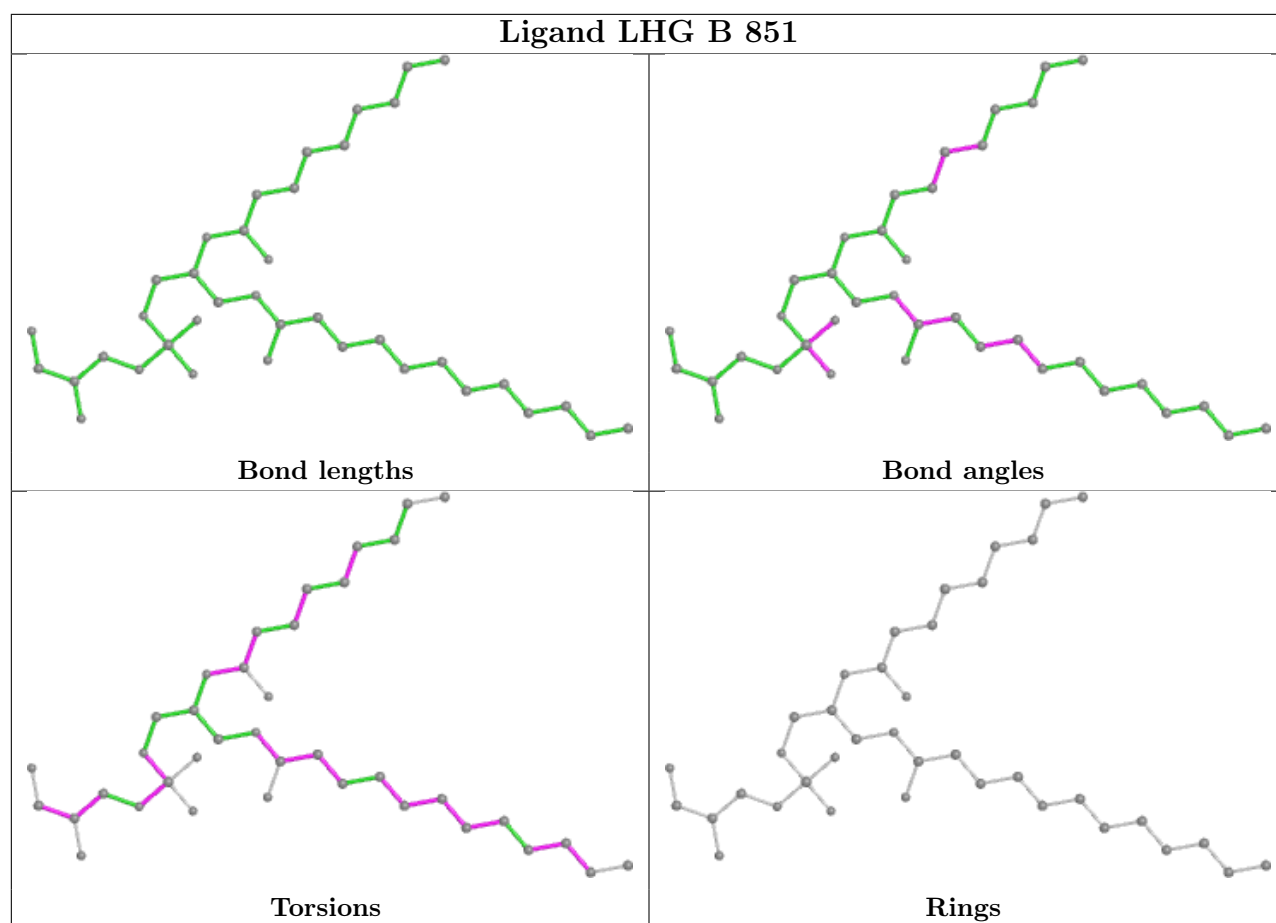




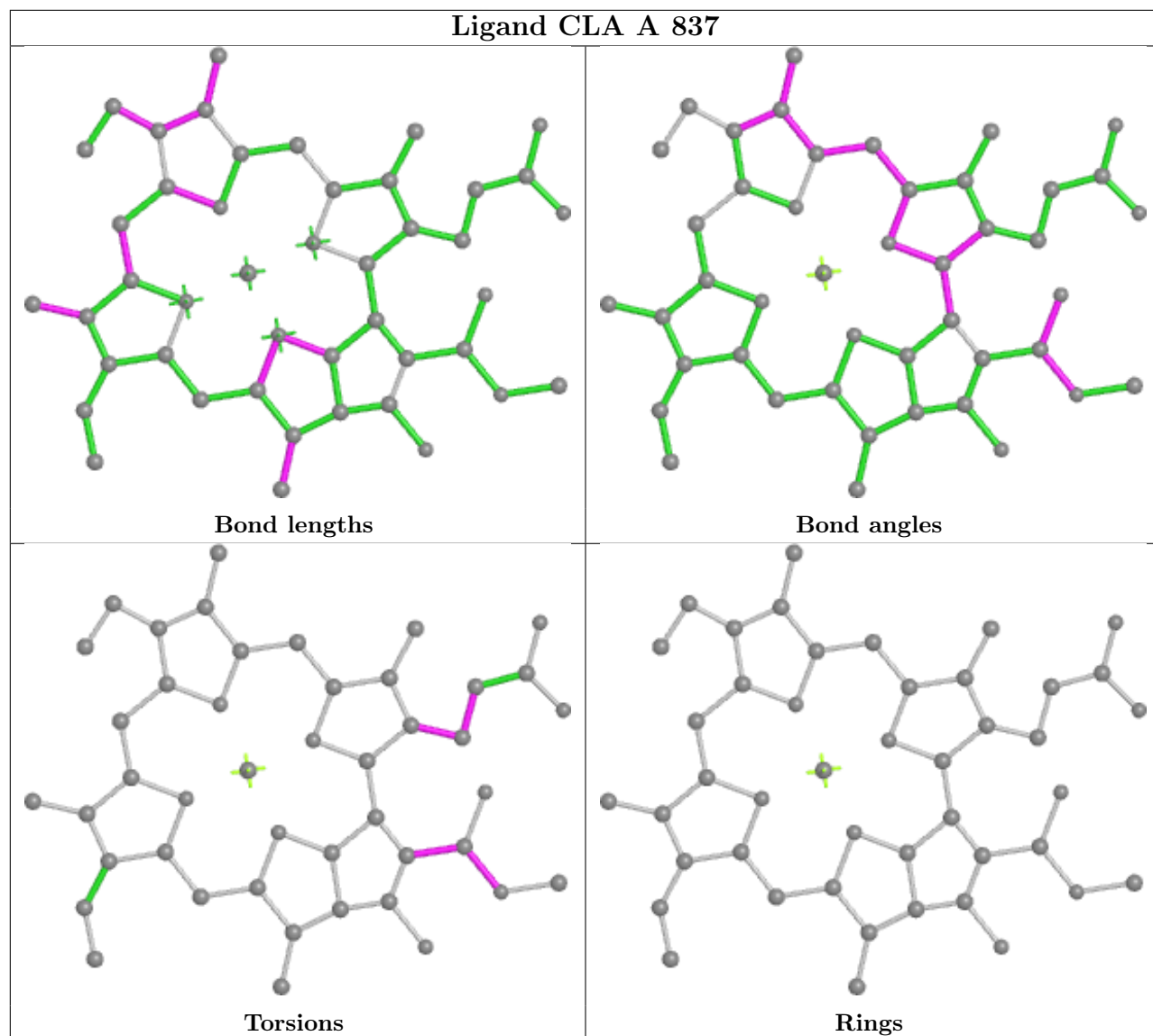
## Ligand CLA 9 609



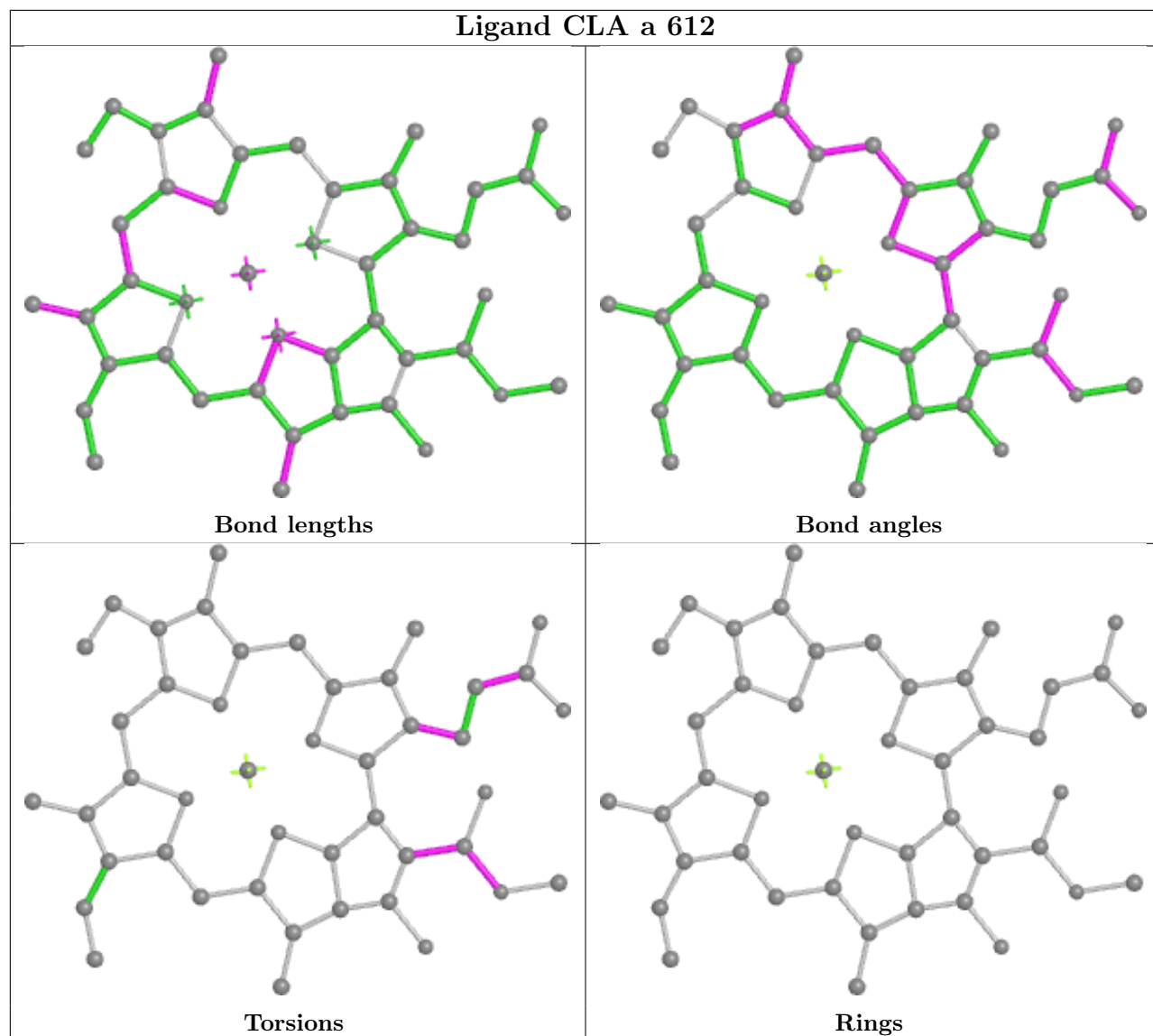




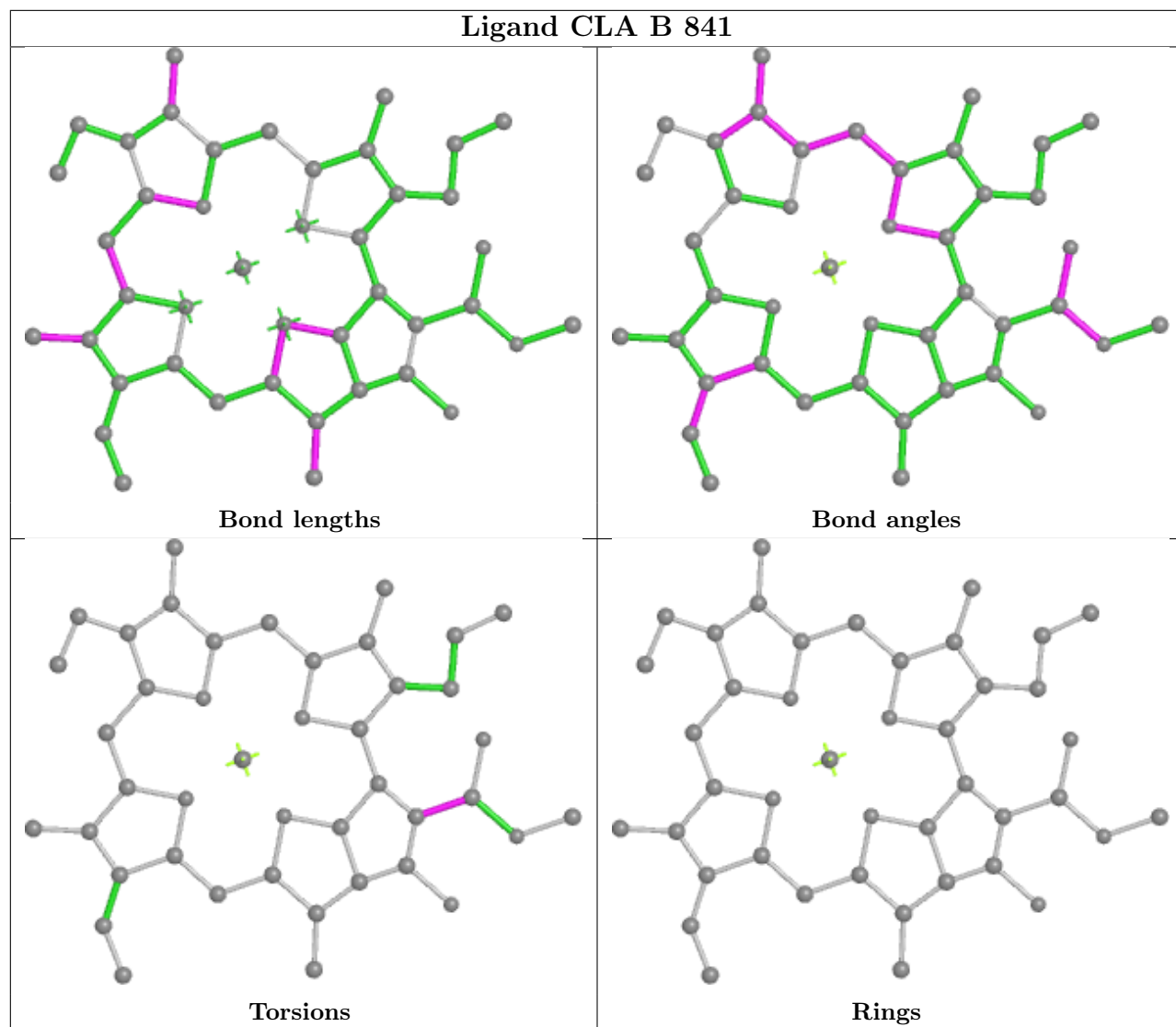
## Ligand CLA A 837



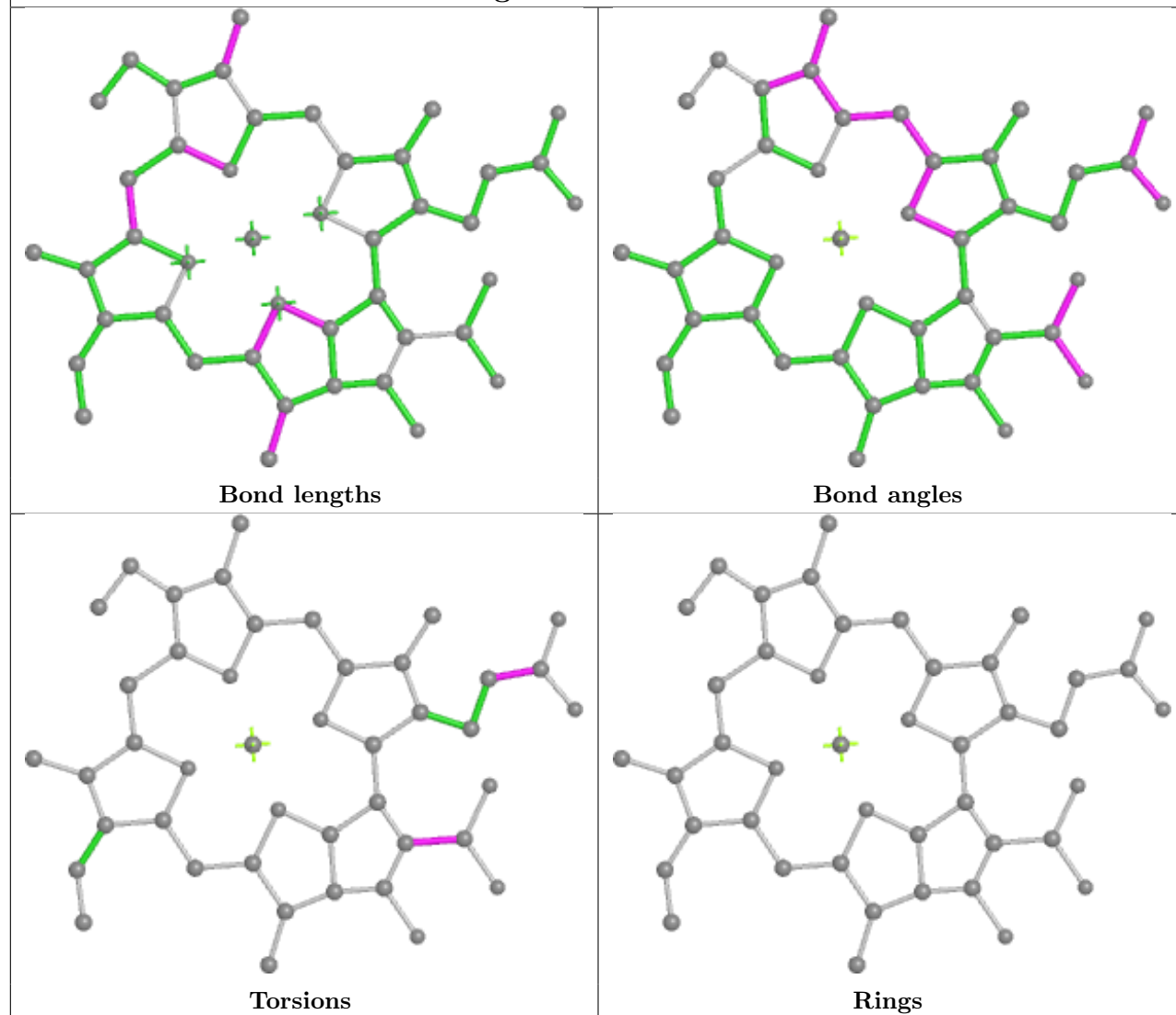
## Ligand CLA a 612



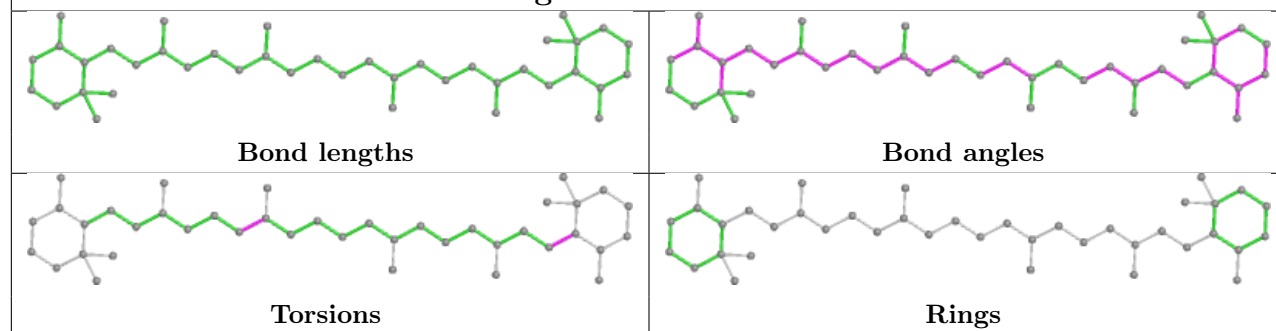
## Ligand CLA B 841



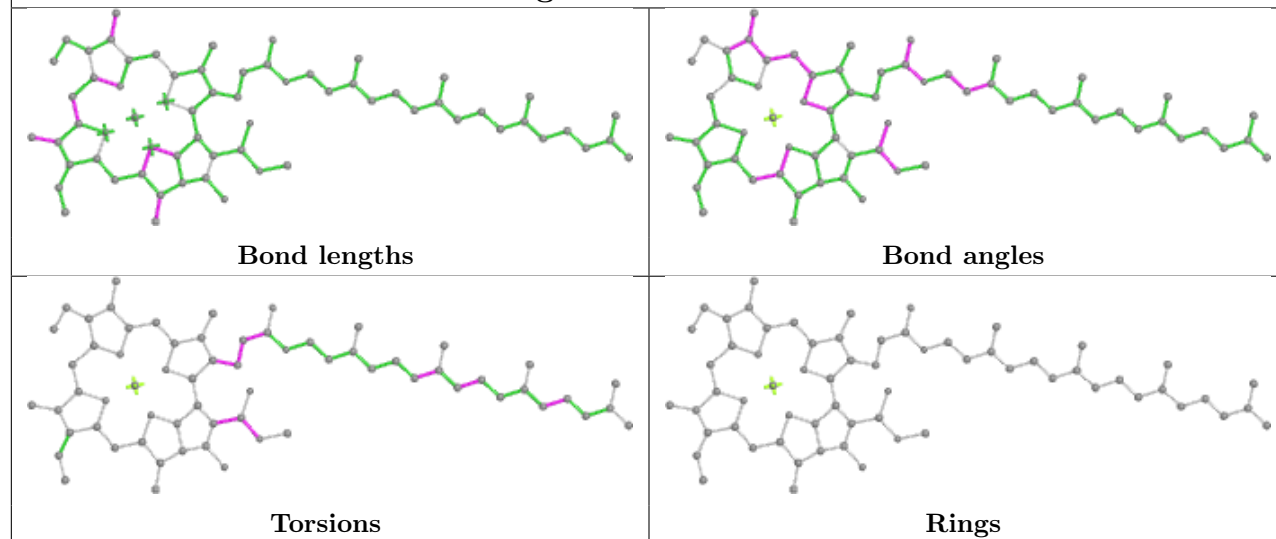
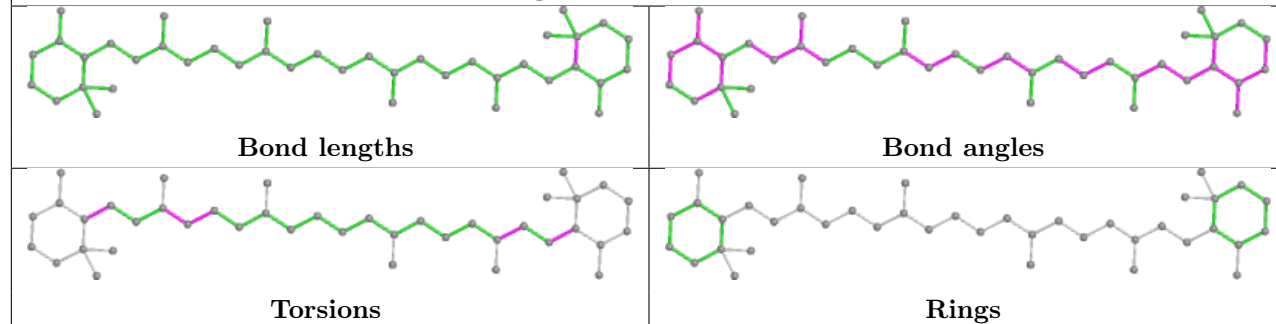
## Ligand CLA a 608



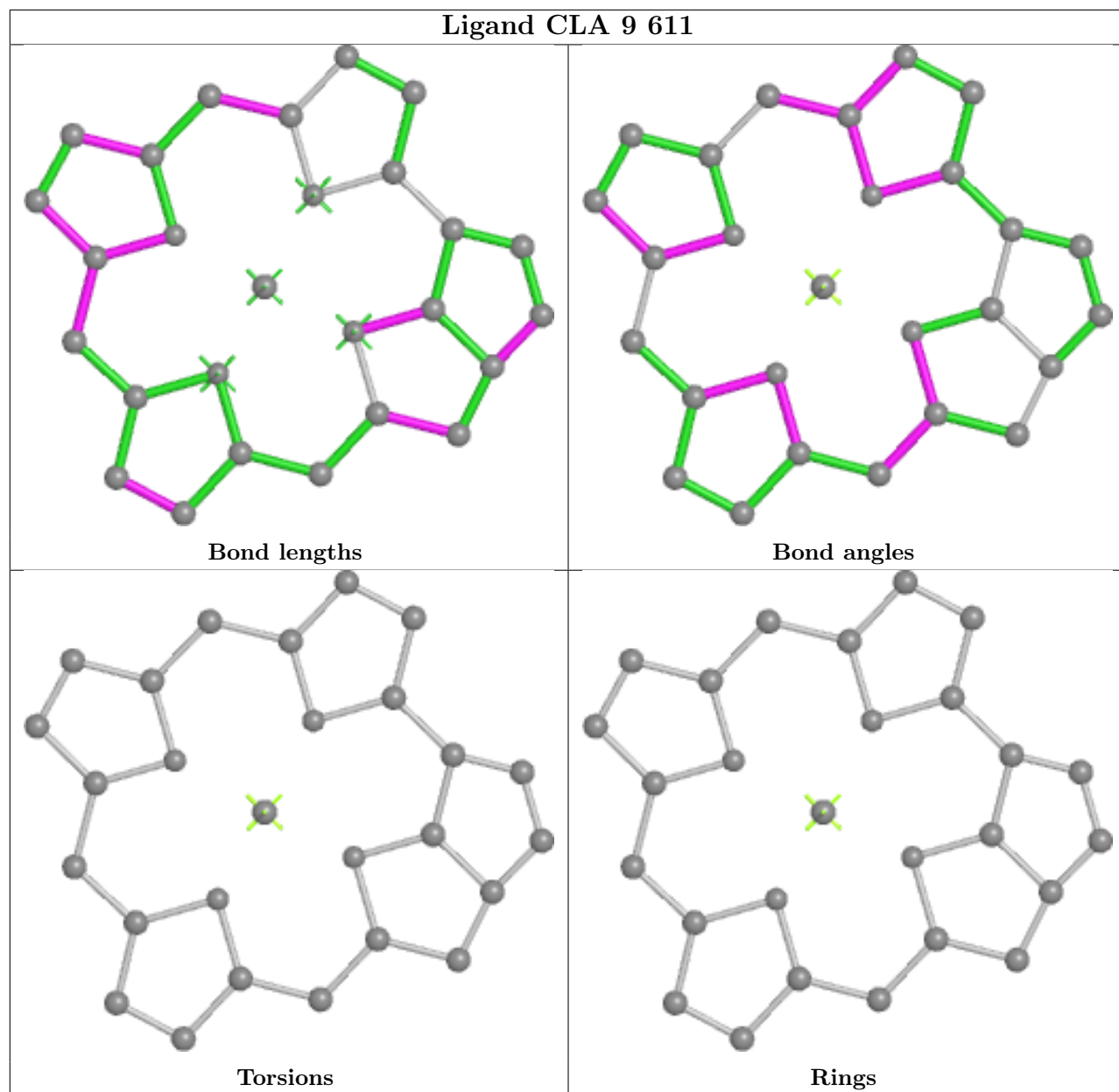
## Ligand BCR a 619



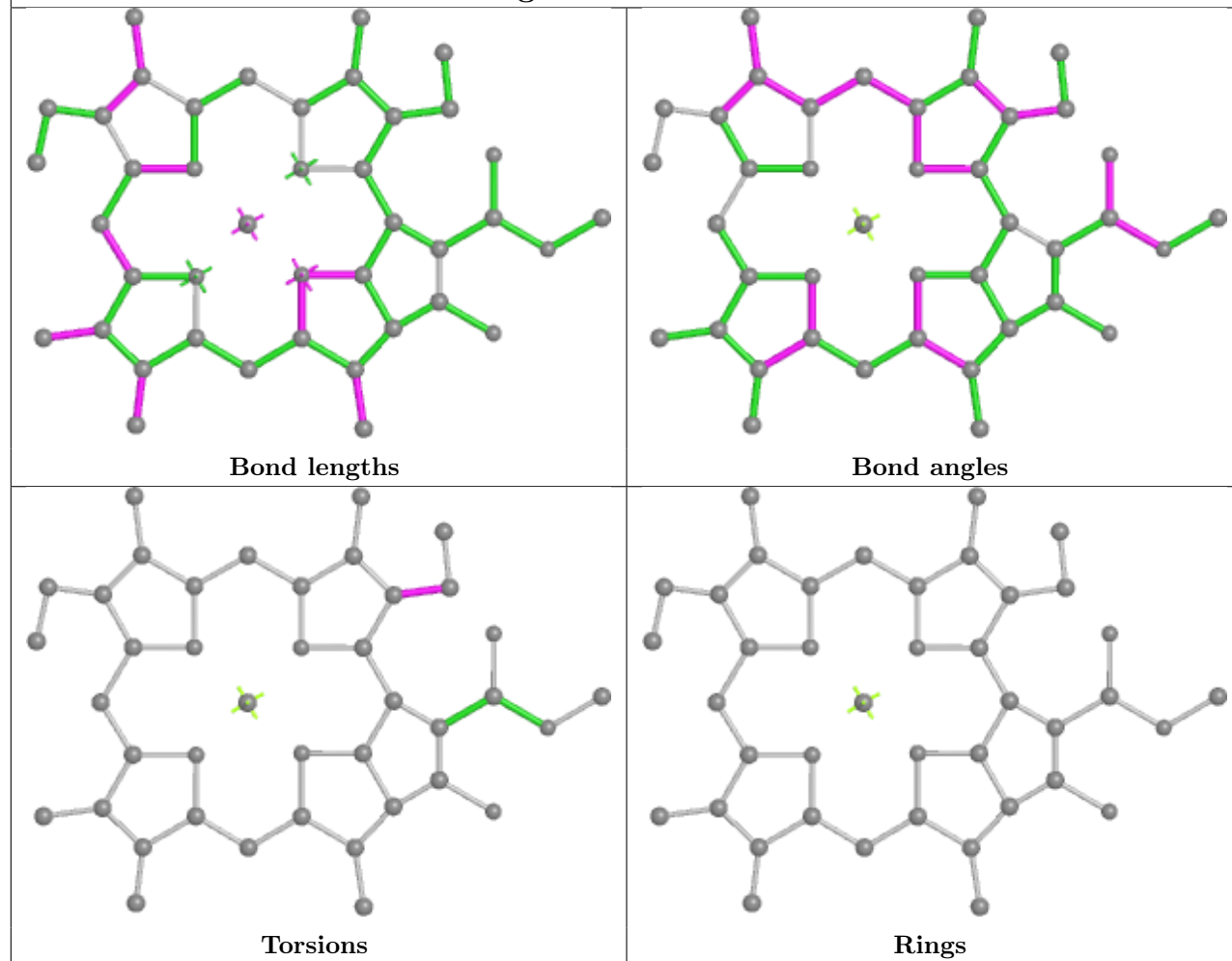


**Ligand CLA 6 610****Ligand BCR B 844**

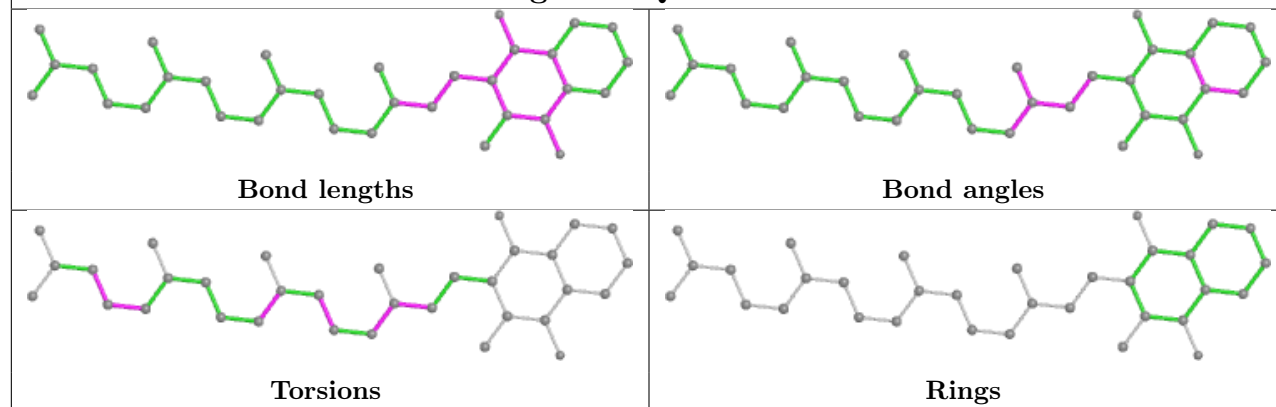
## Ligand CLA 9 611

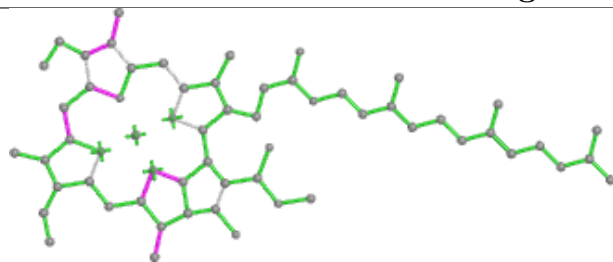


## Ligand CLA 7 606

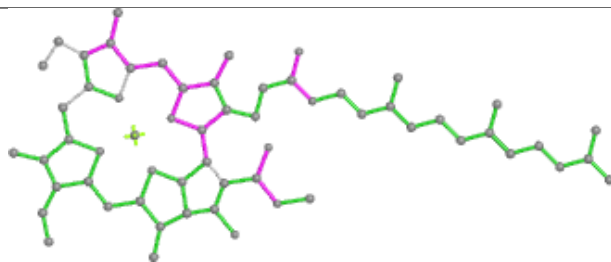


## Ligand PQN B 842

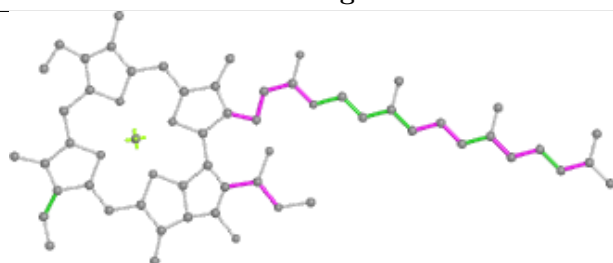


**Ligand CLA 3 609**

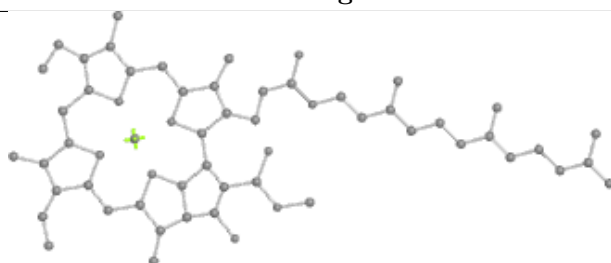
Bond lengths



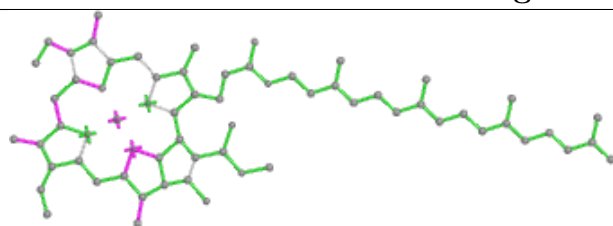
Bond angles



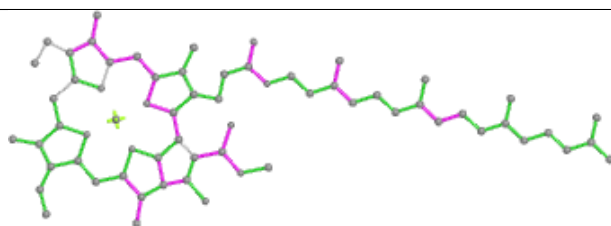
Torsions



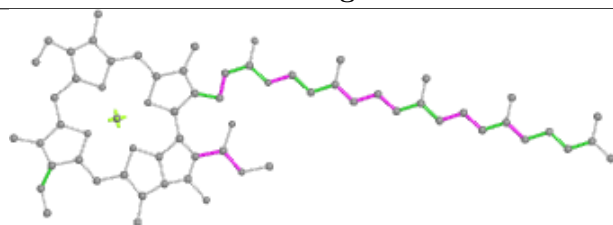
Rings

**Ligand CLA A 854**

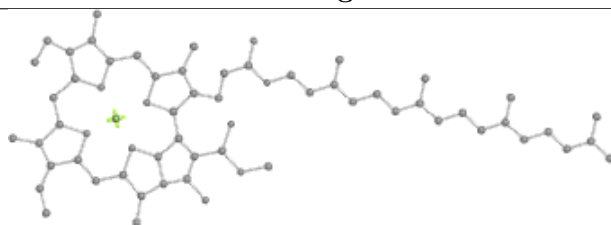
Bond lengths



Bond angles

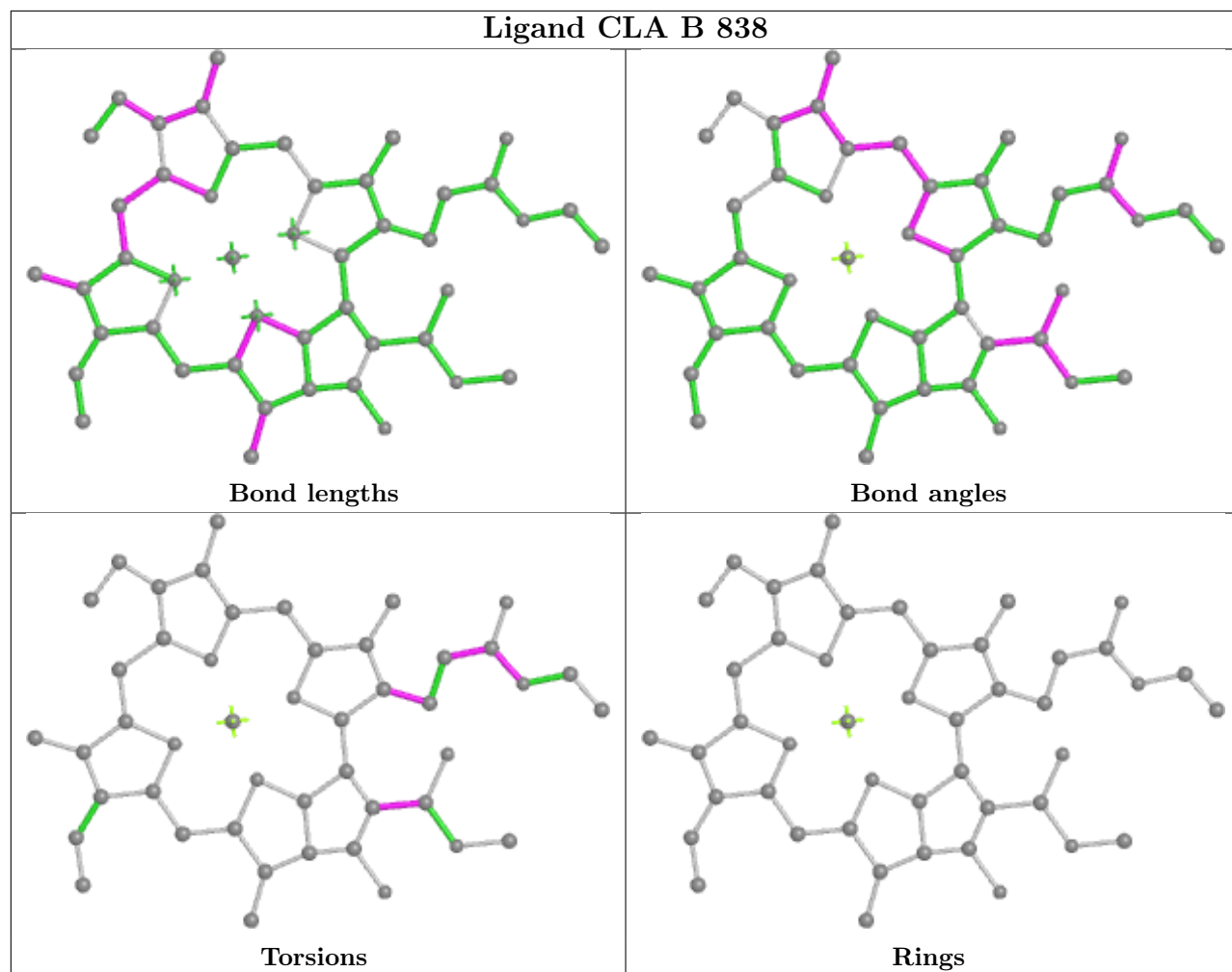


Torsions

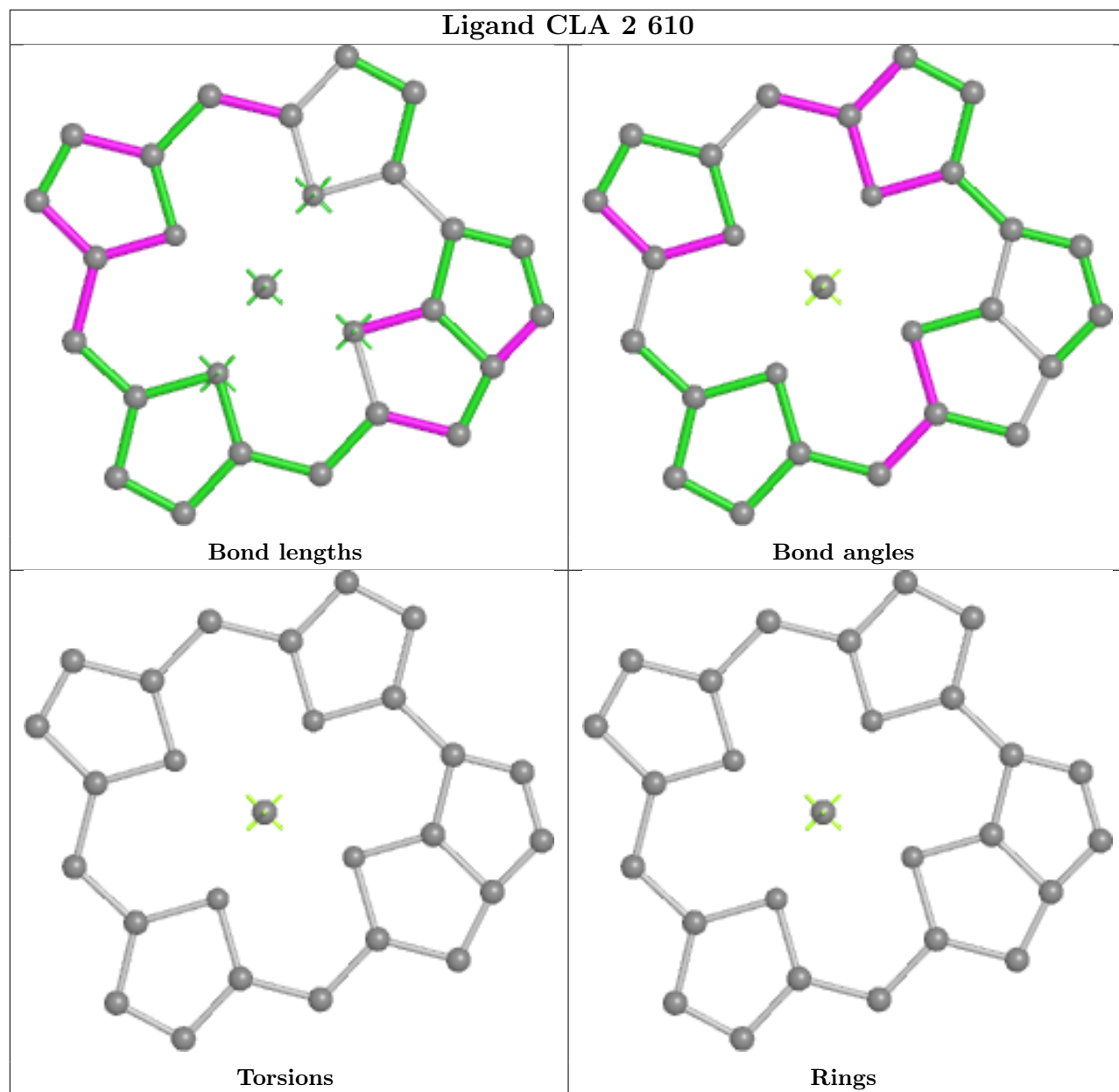


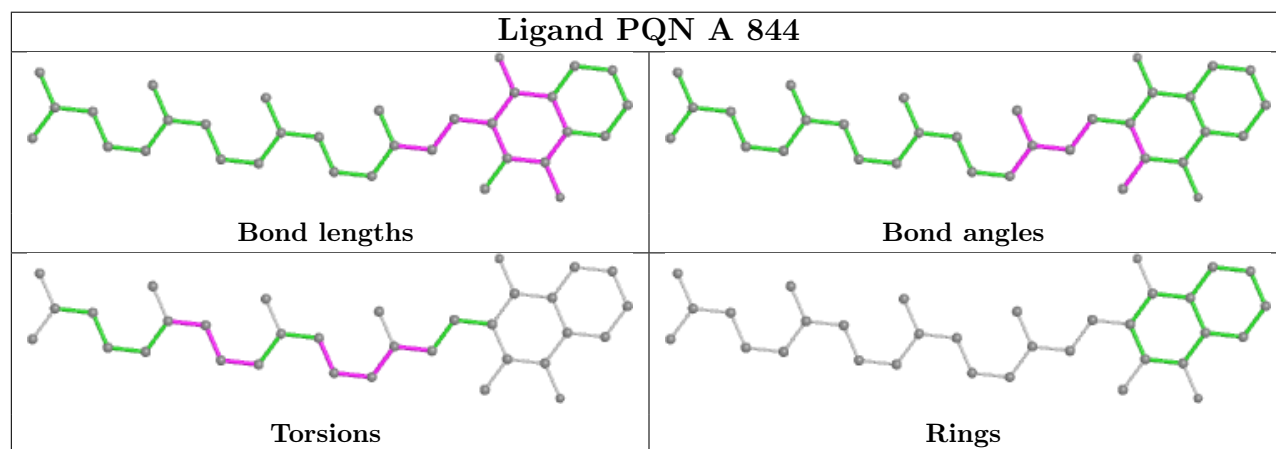
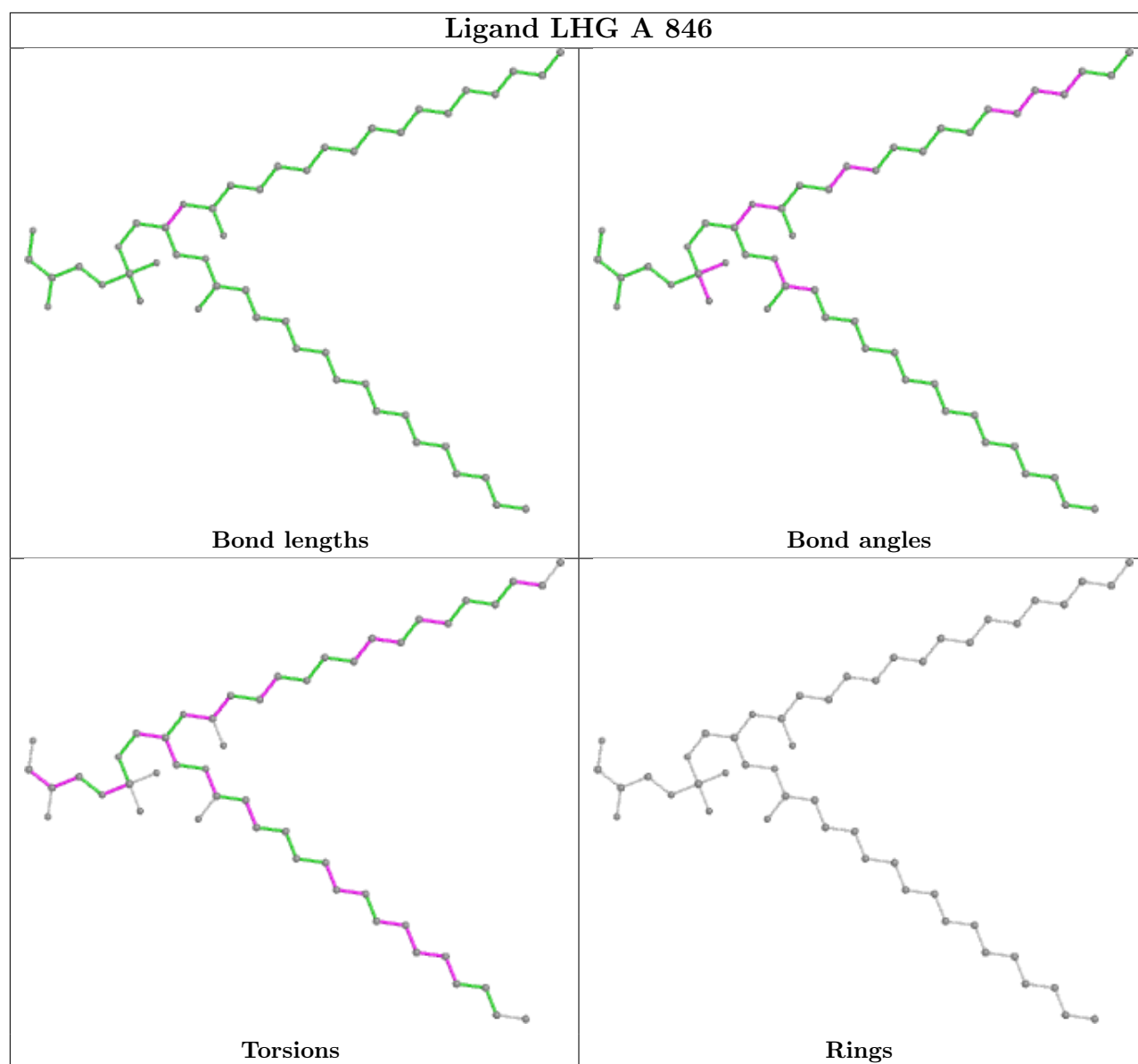
Rings

## Ligand CLA B 838

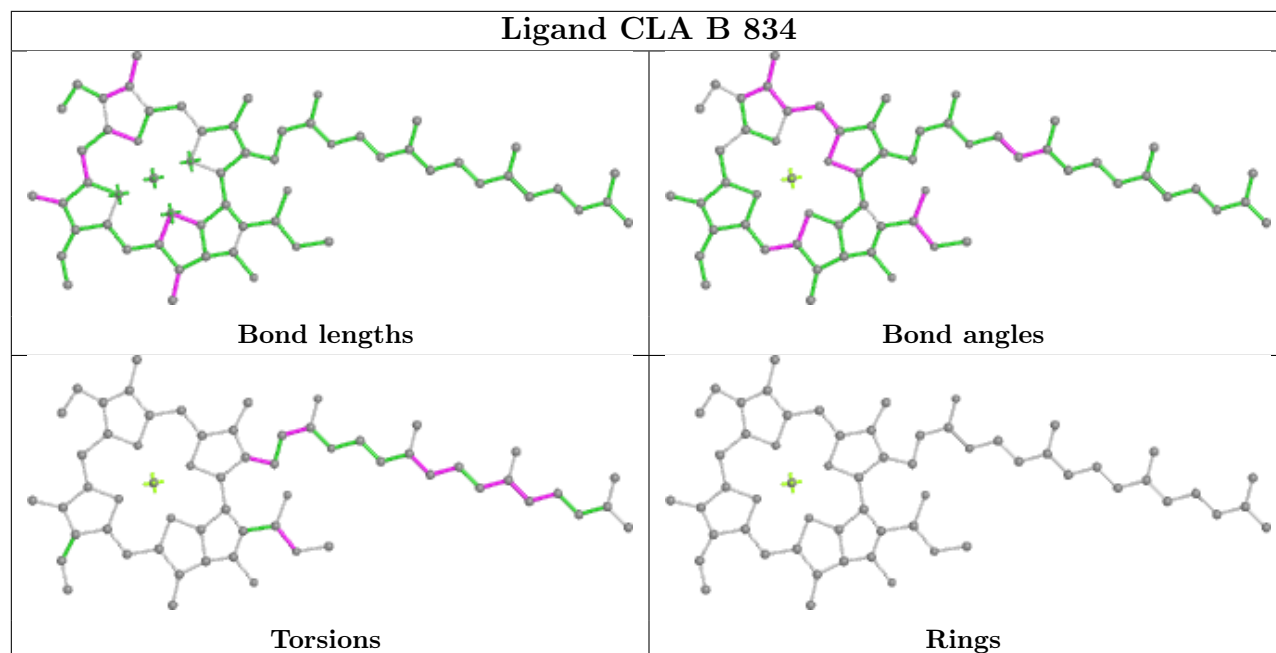


## Ligand CLA 2 610

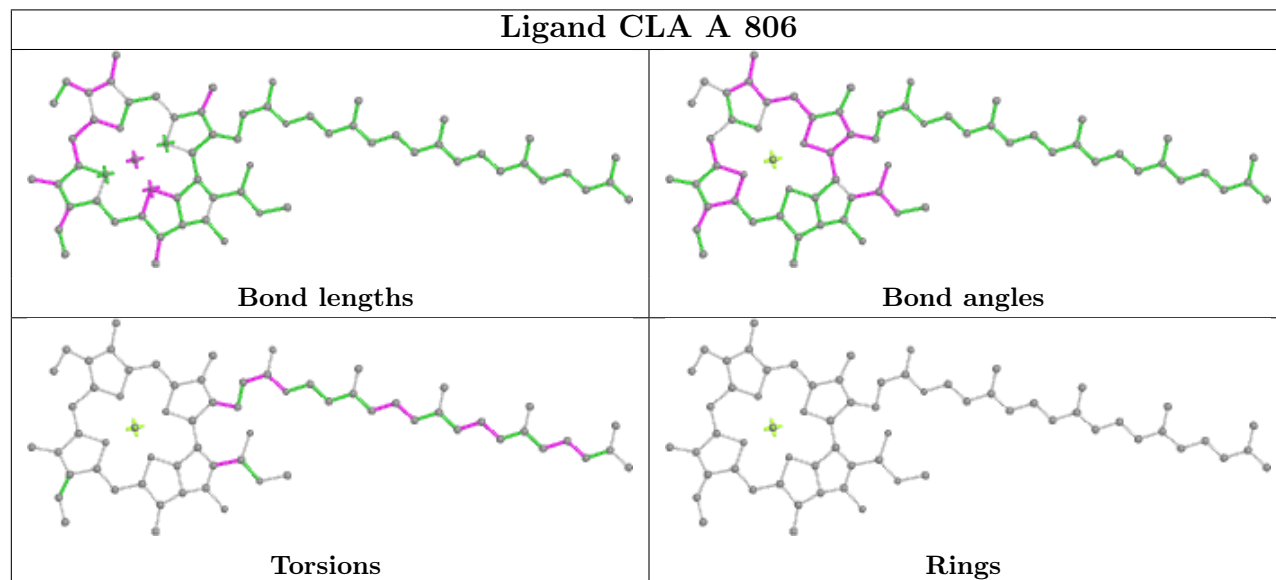




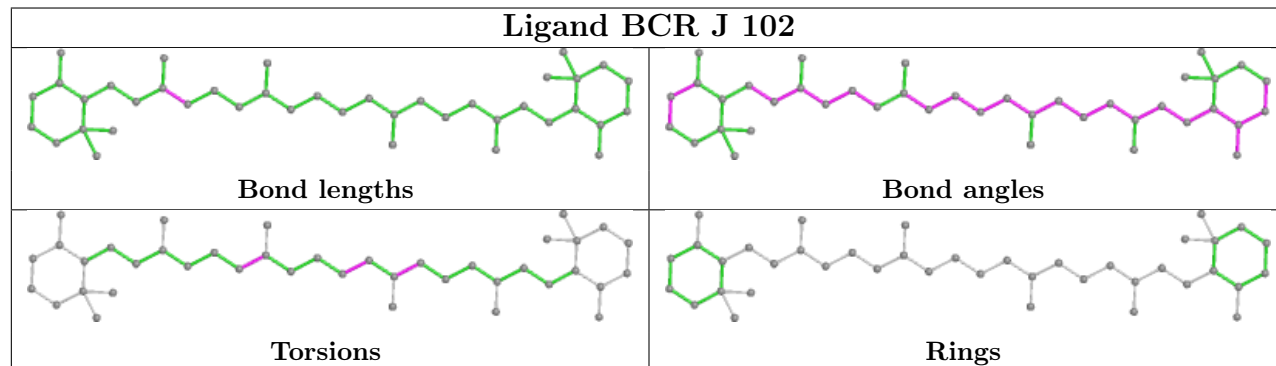
## Ligand CLA B 834



## Ligand CLA A 806

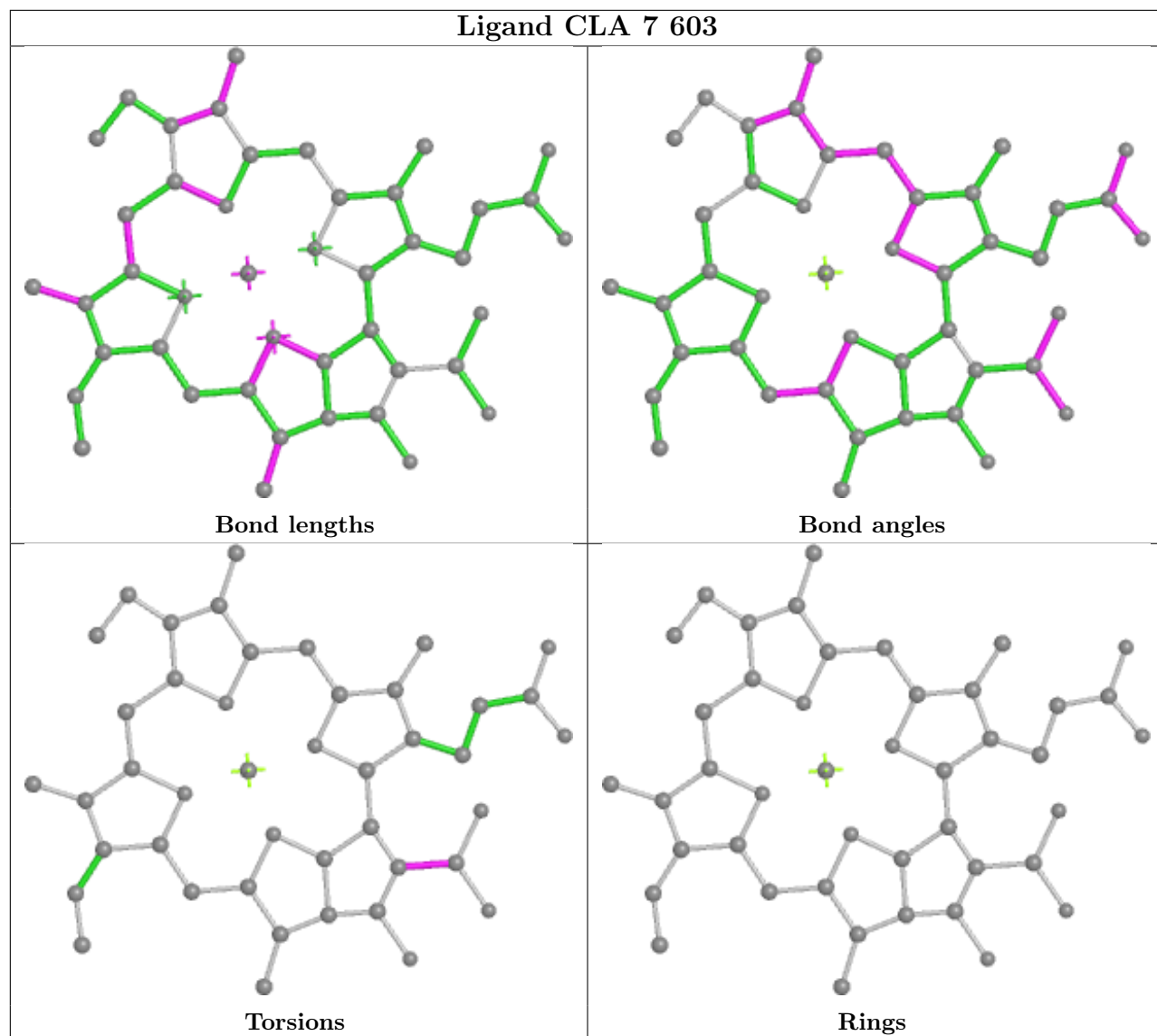


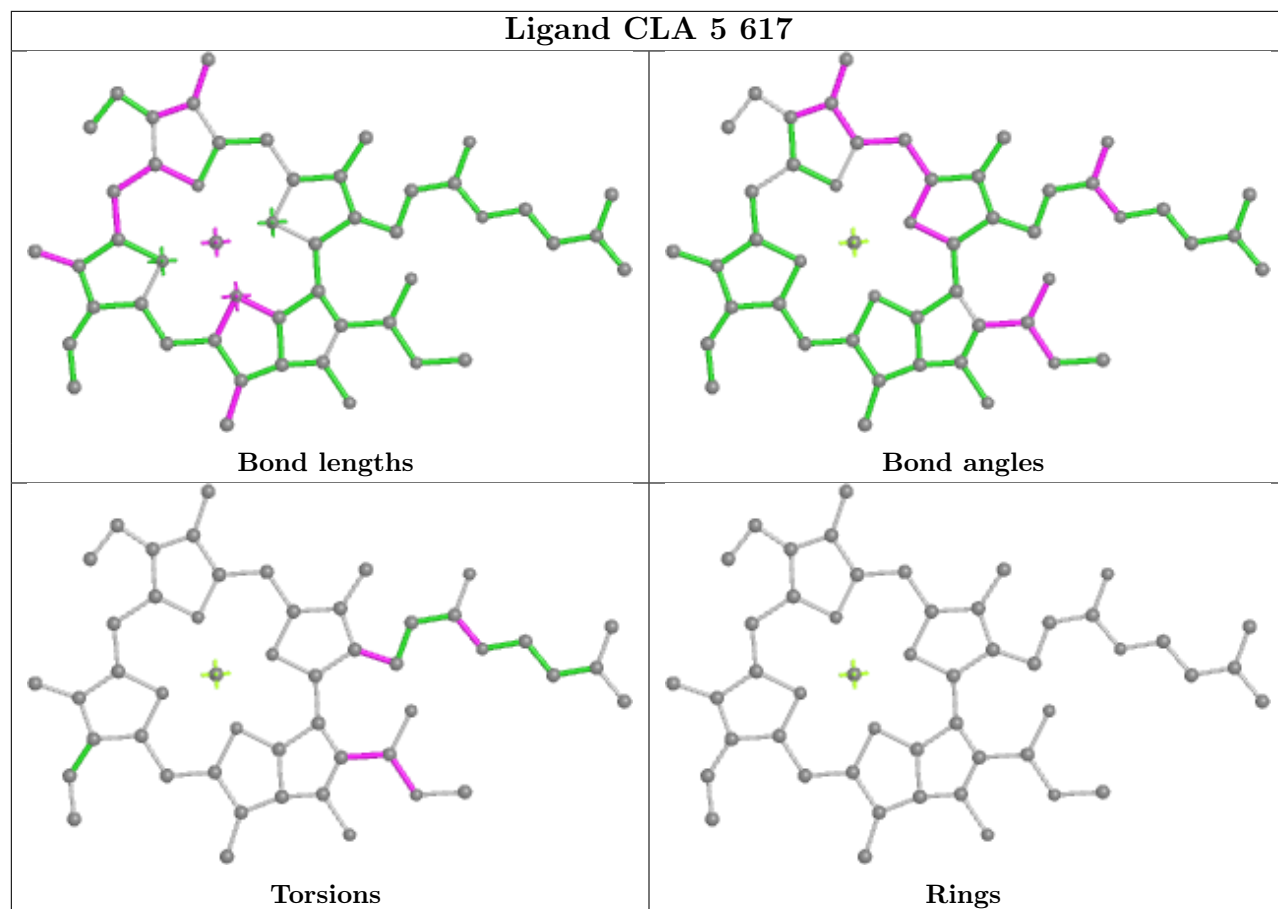
## Ligand BCR J 102



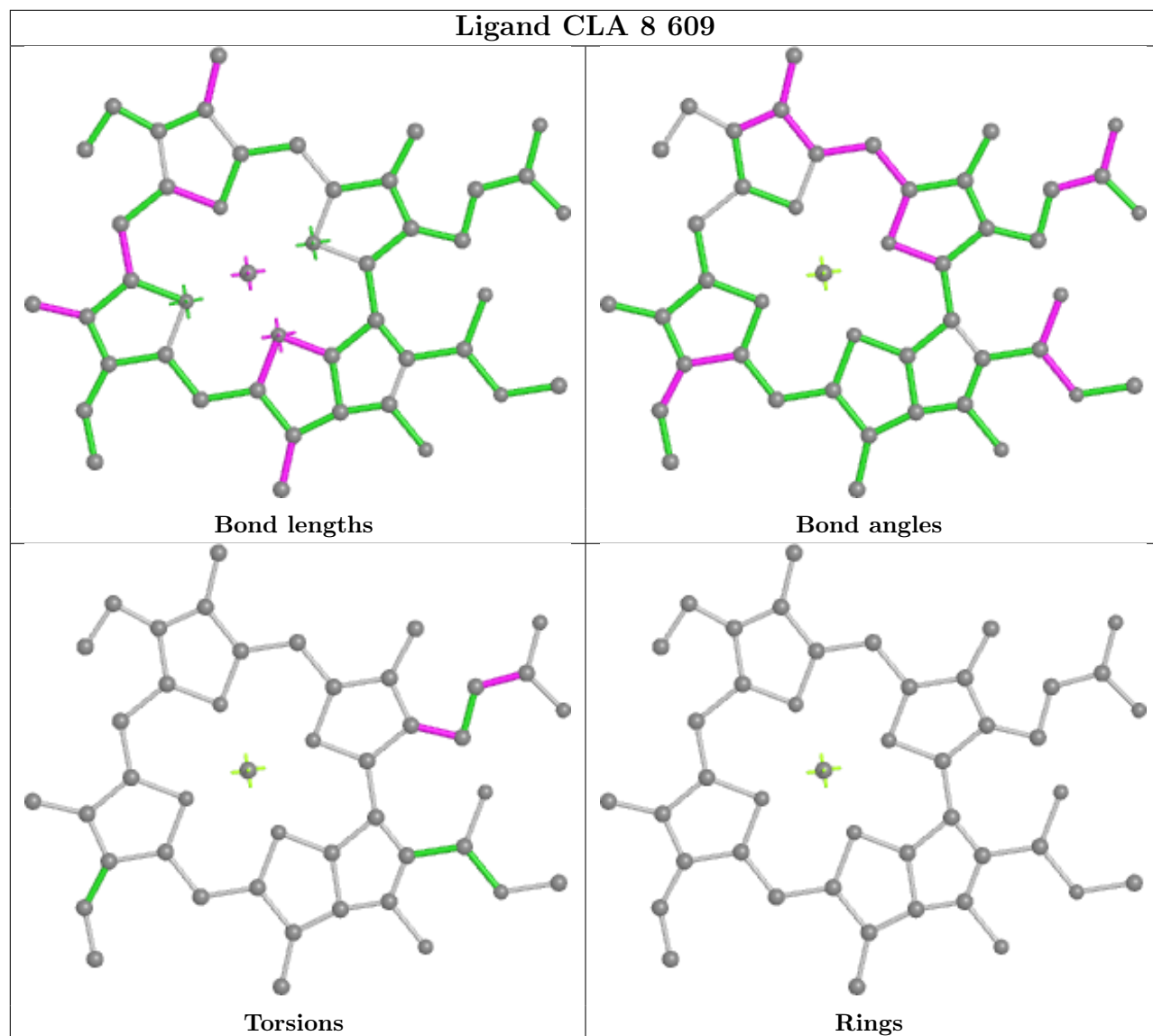


## Ligand CLA 7 603

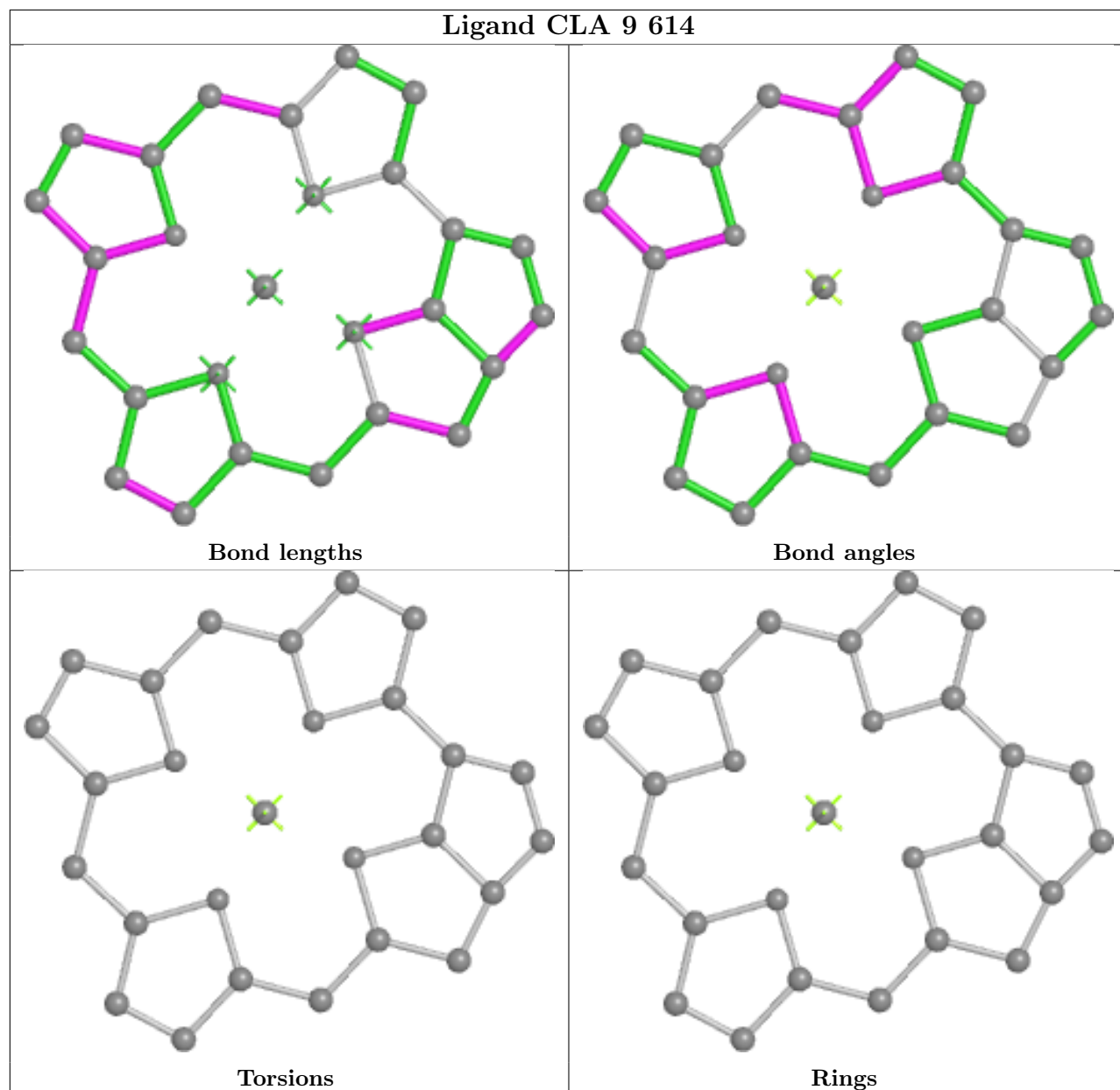




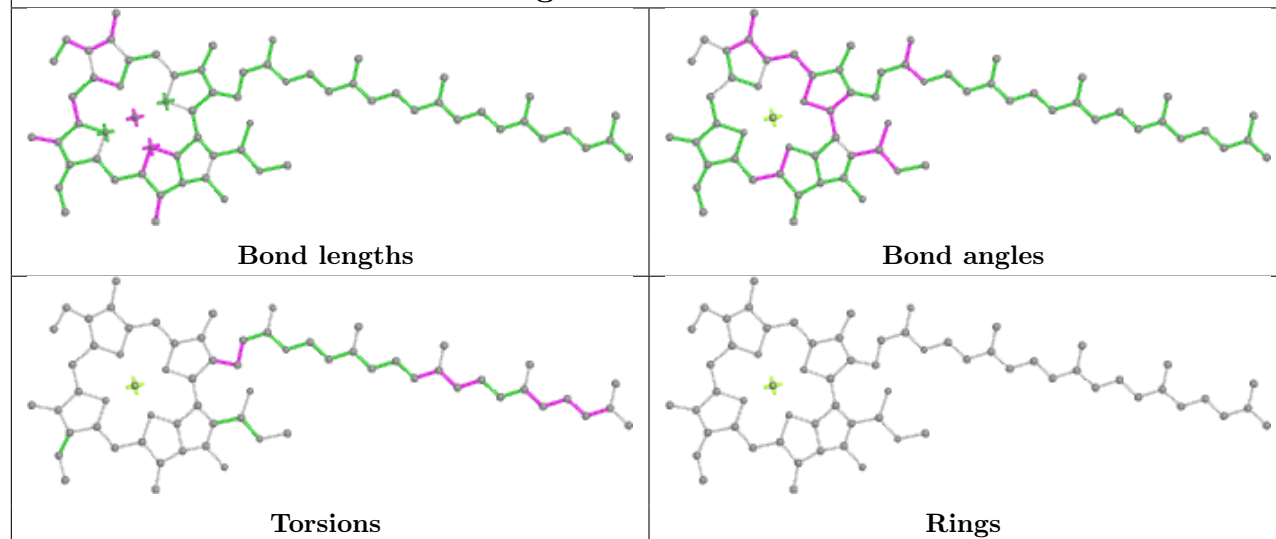
## Ligand CLA 8 609



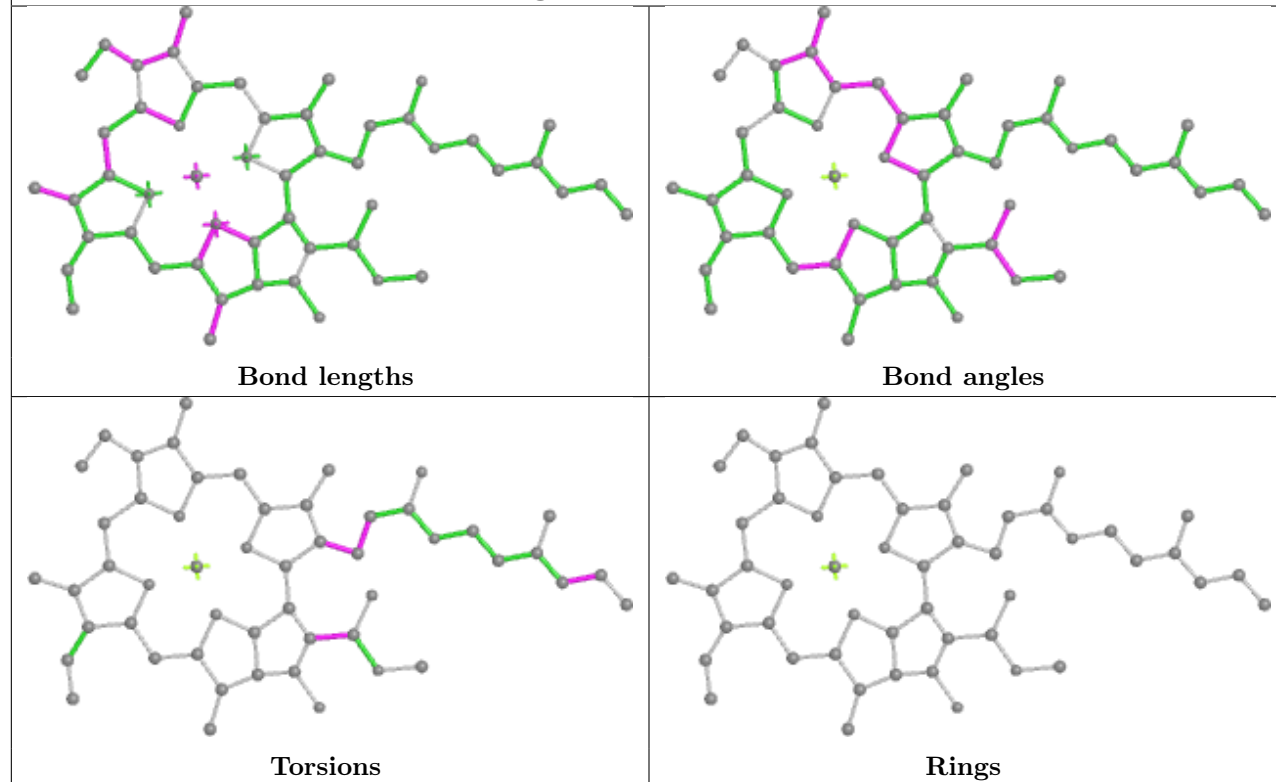
## Ligand CLA 9 614

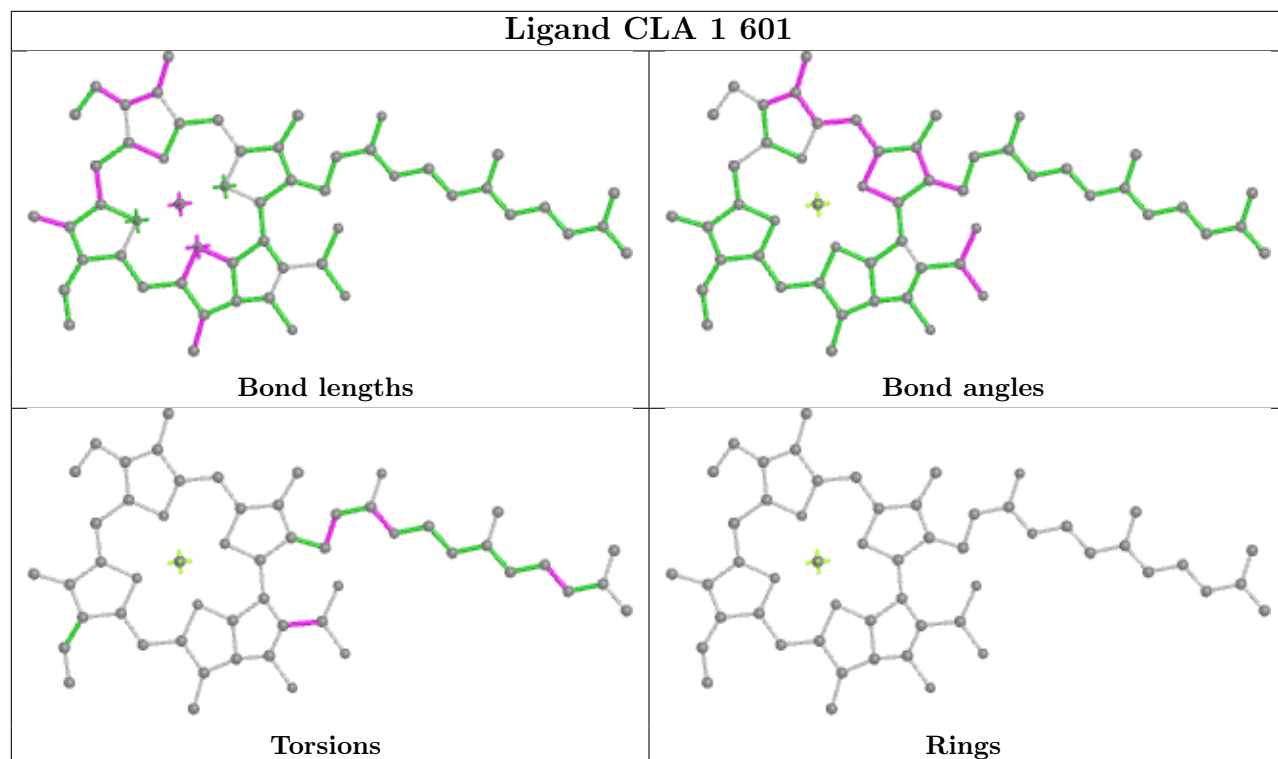
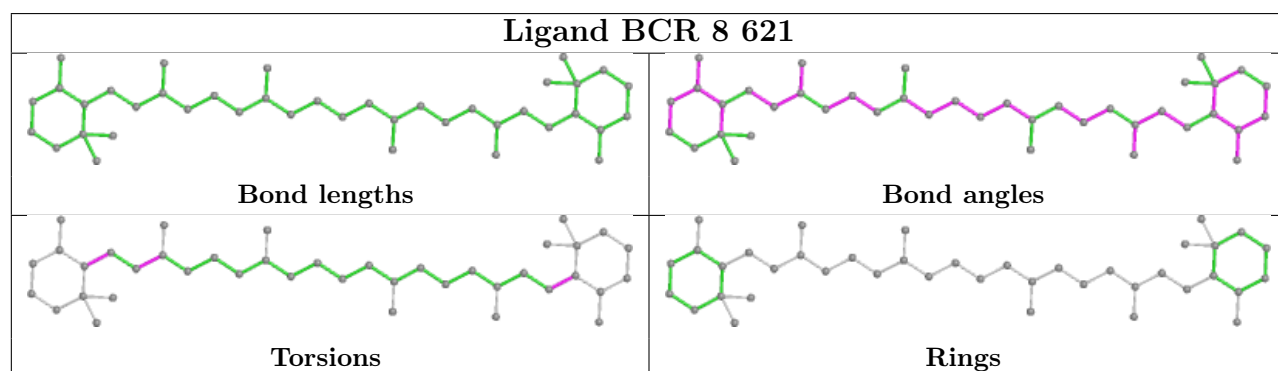


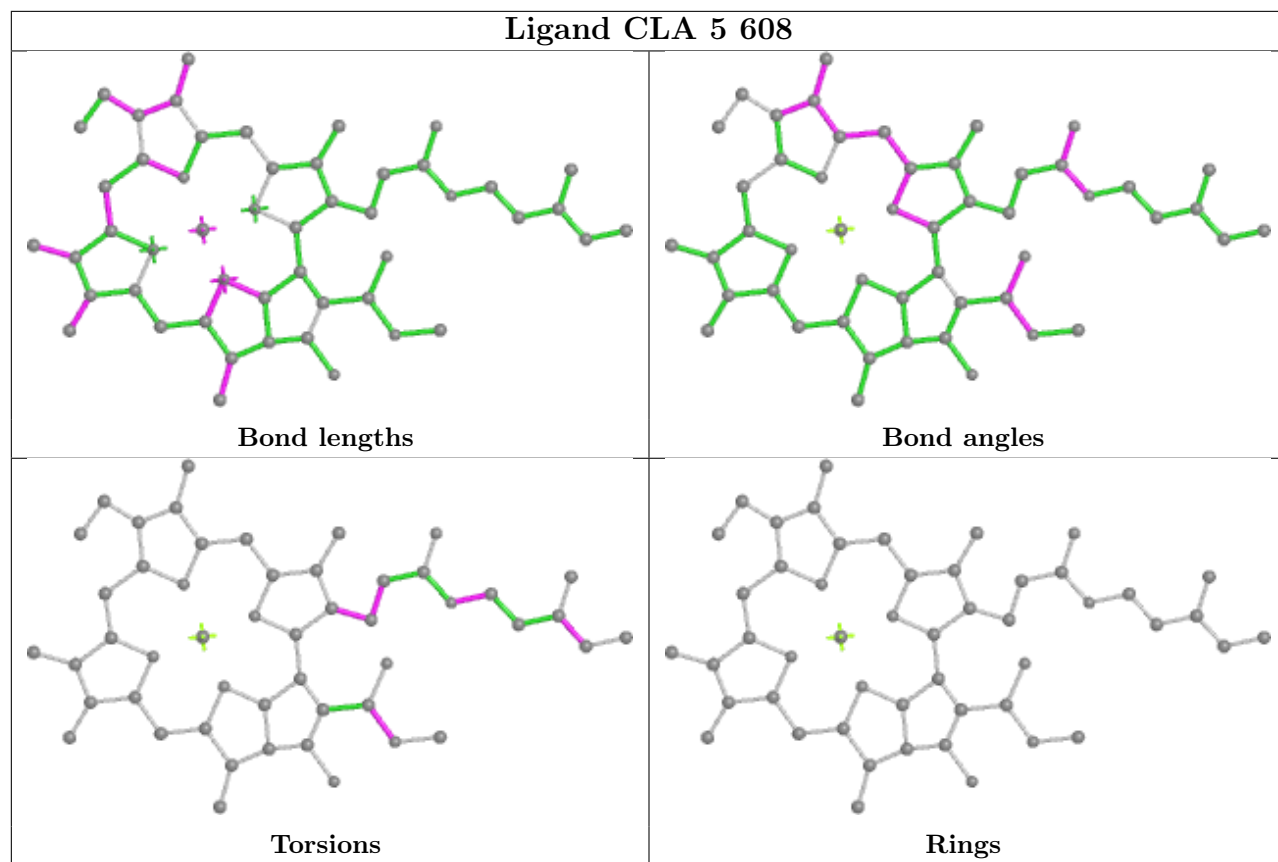
## Ligand CLA 5 609



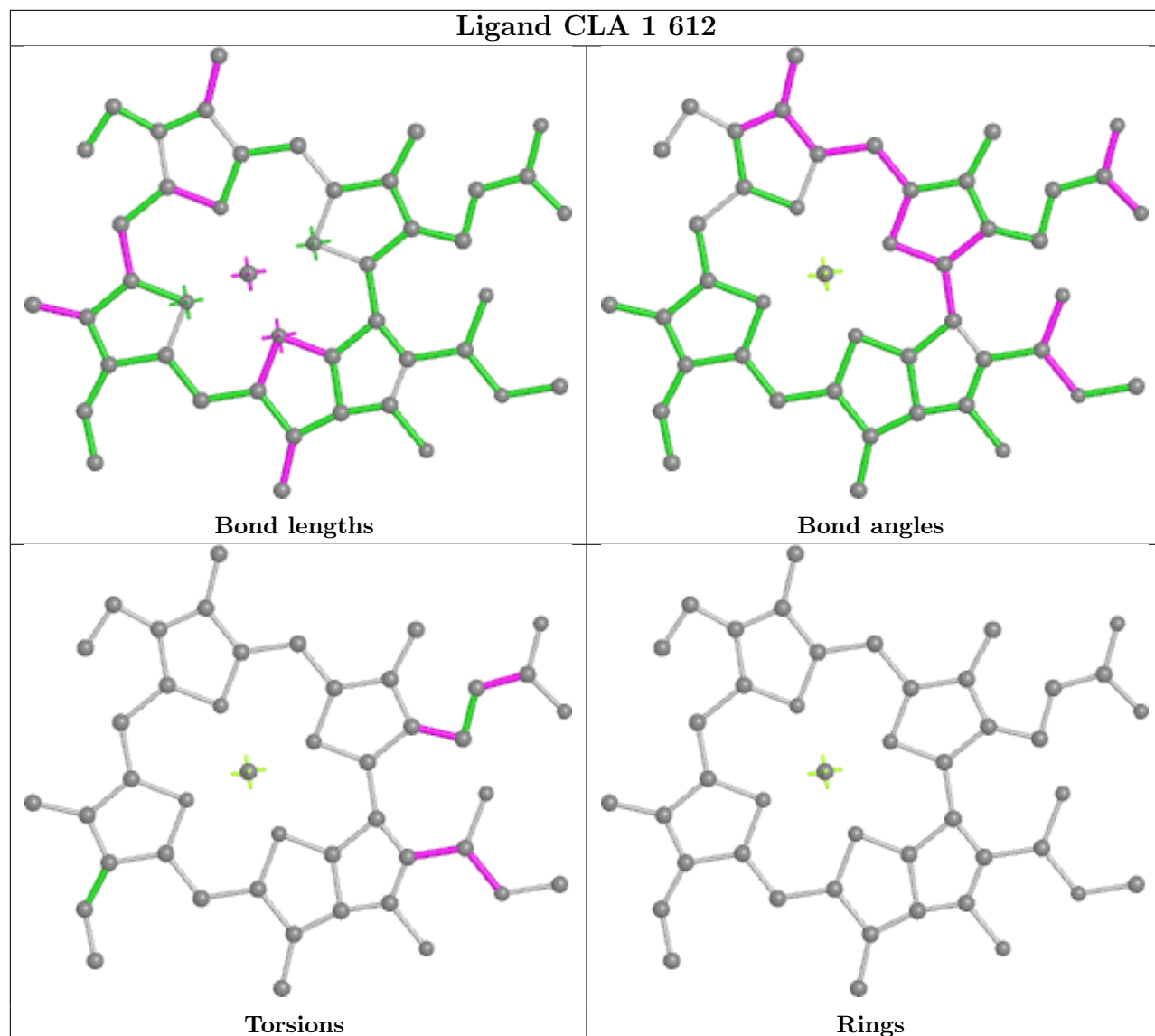
## Ligand CLA A 805



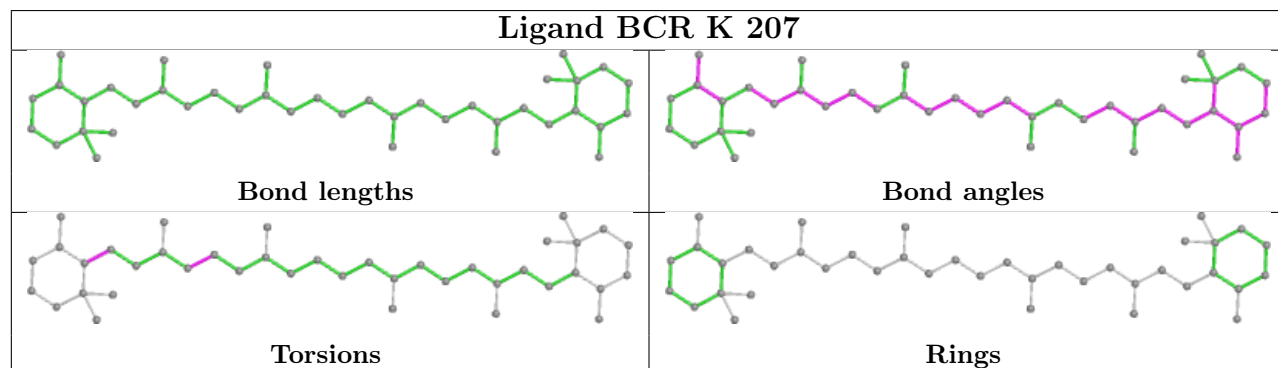
**Ligand CLA 1 601****Ligand BCR 8 621**



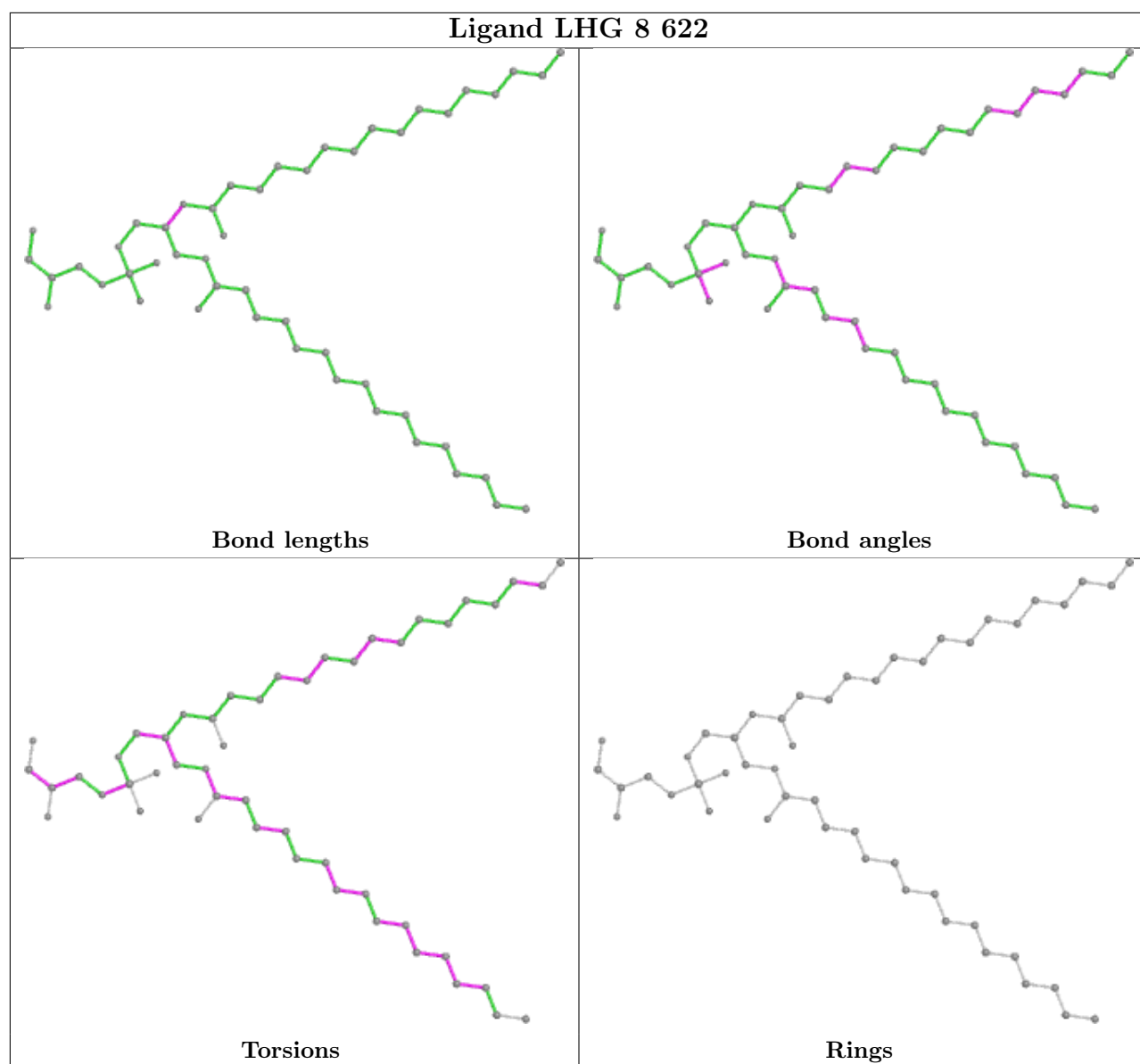
## Ligand CLA 1 612



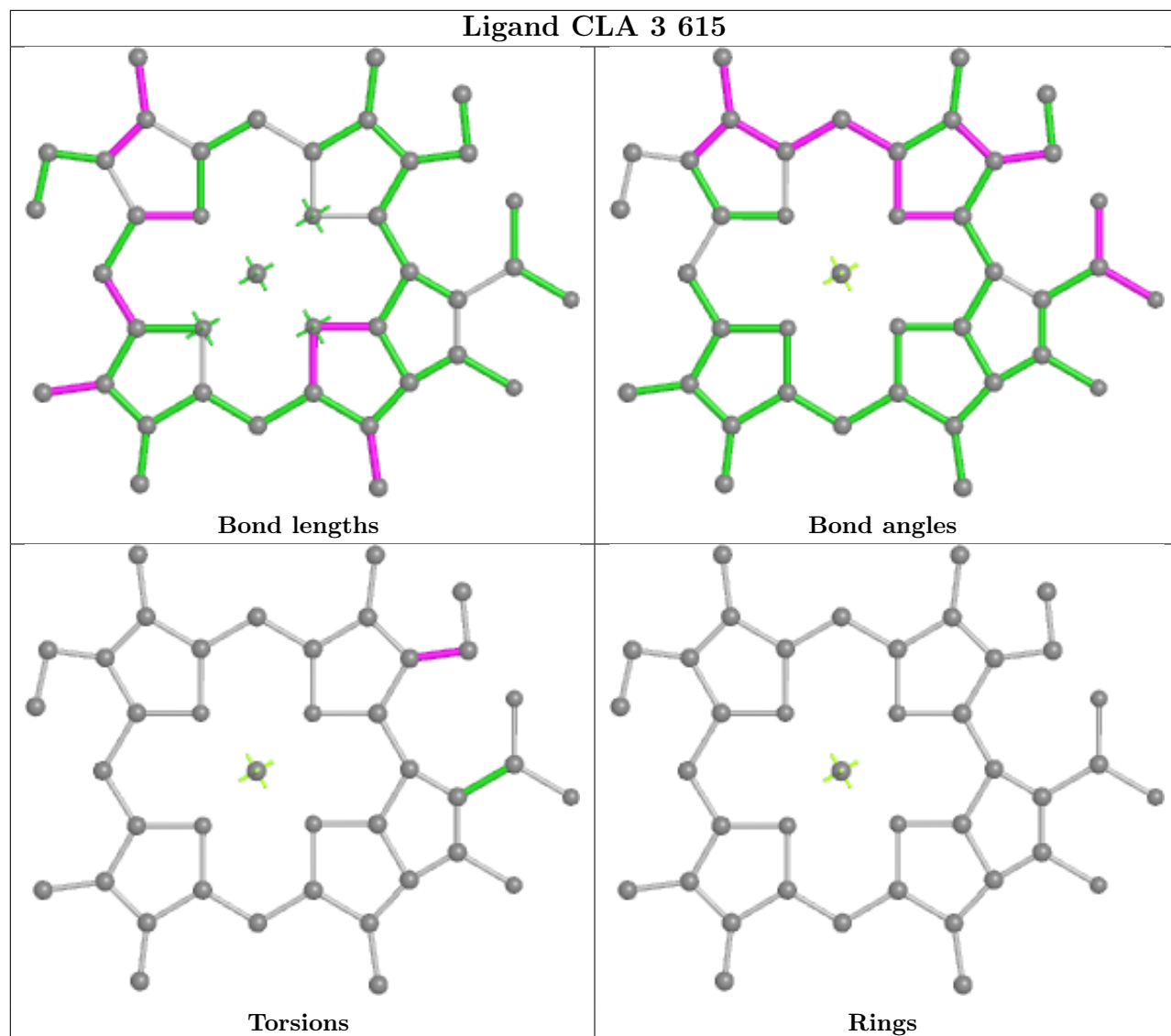
## Ligand BCR K 207



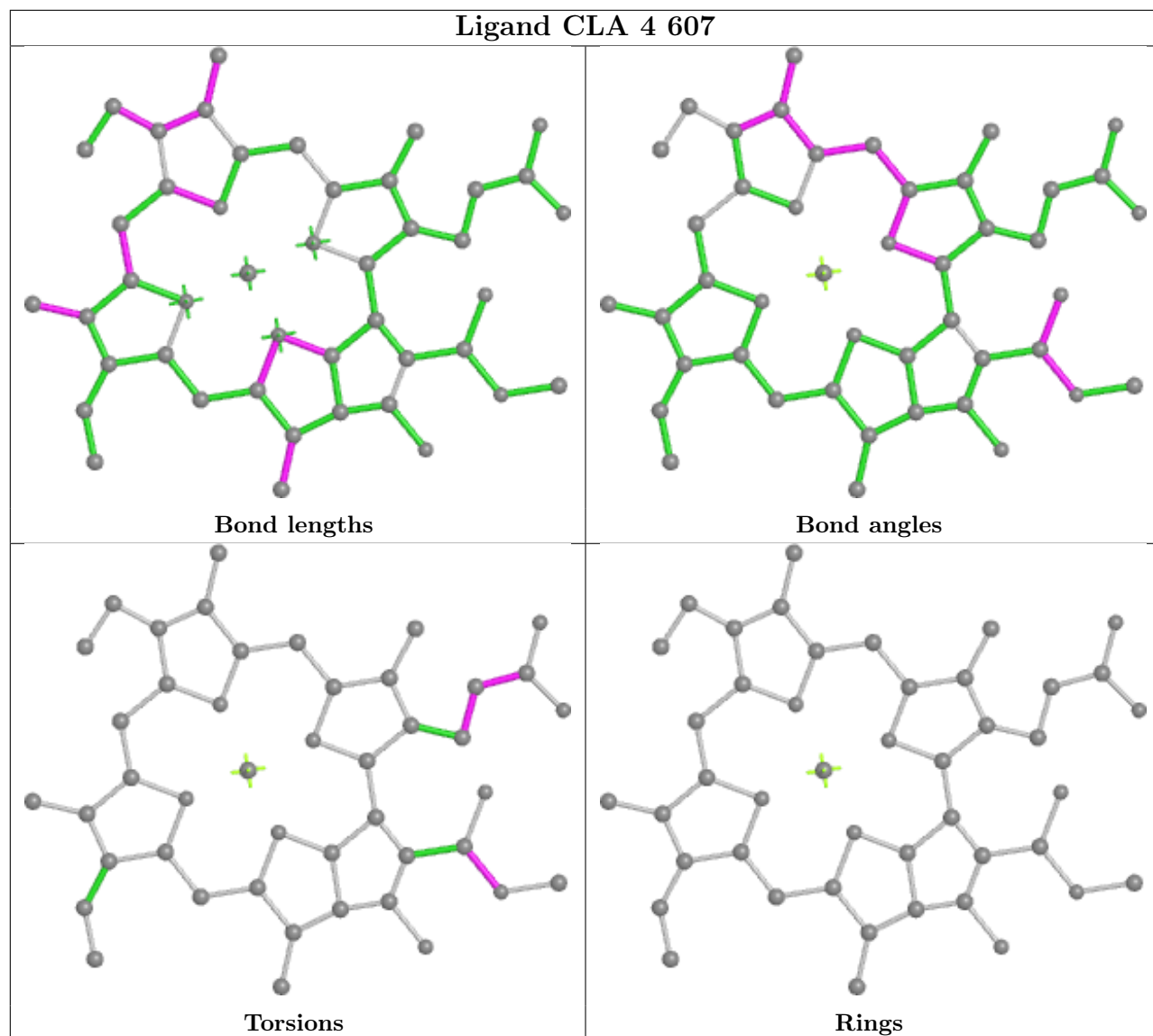




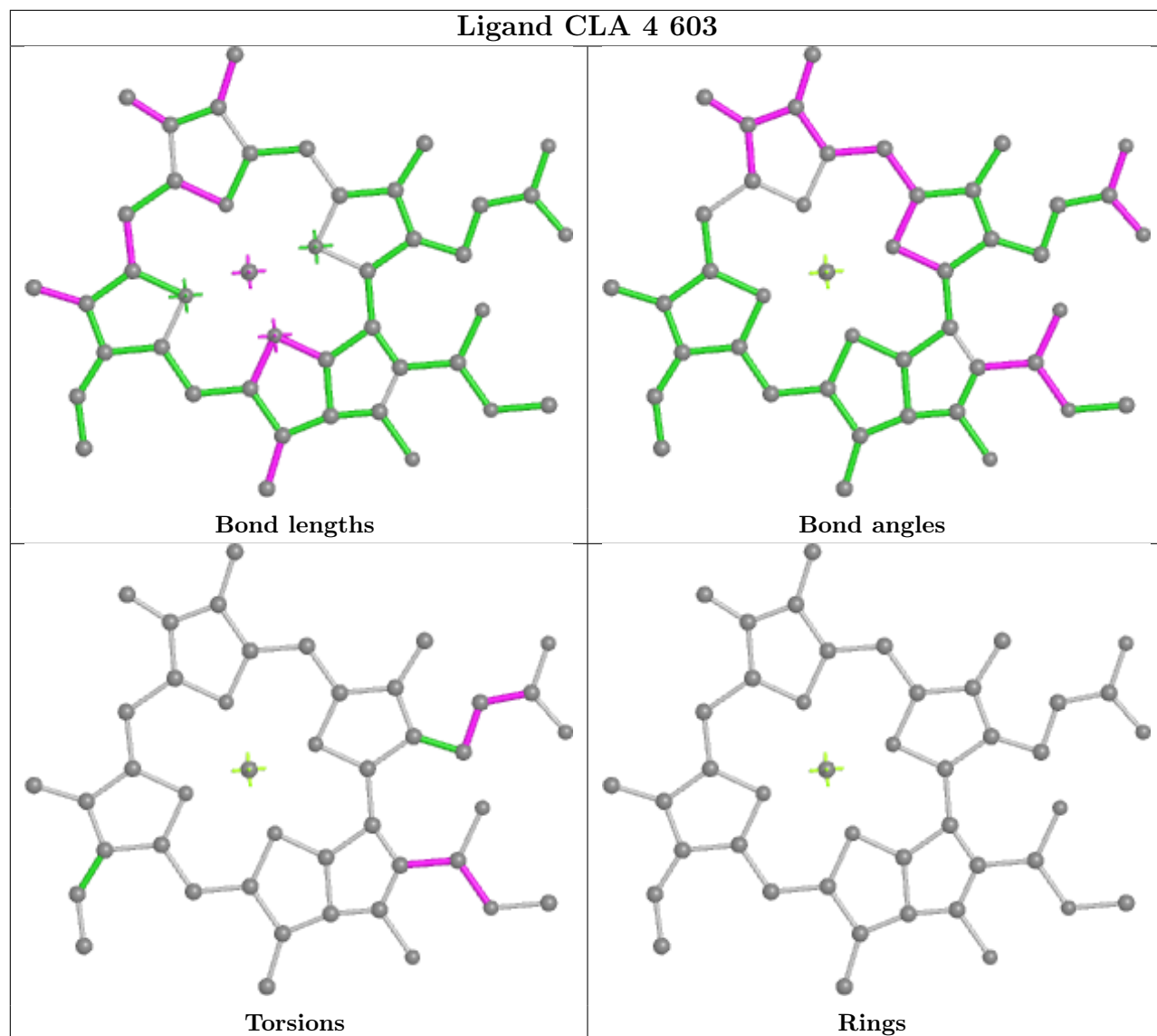
## Ligand CLA 3 615



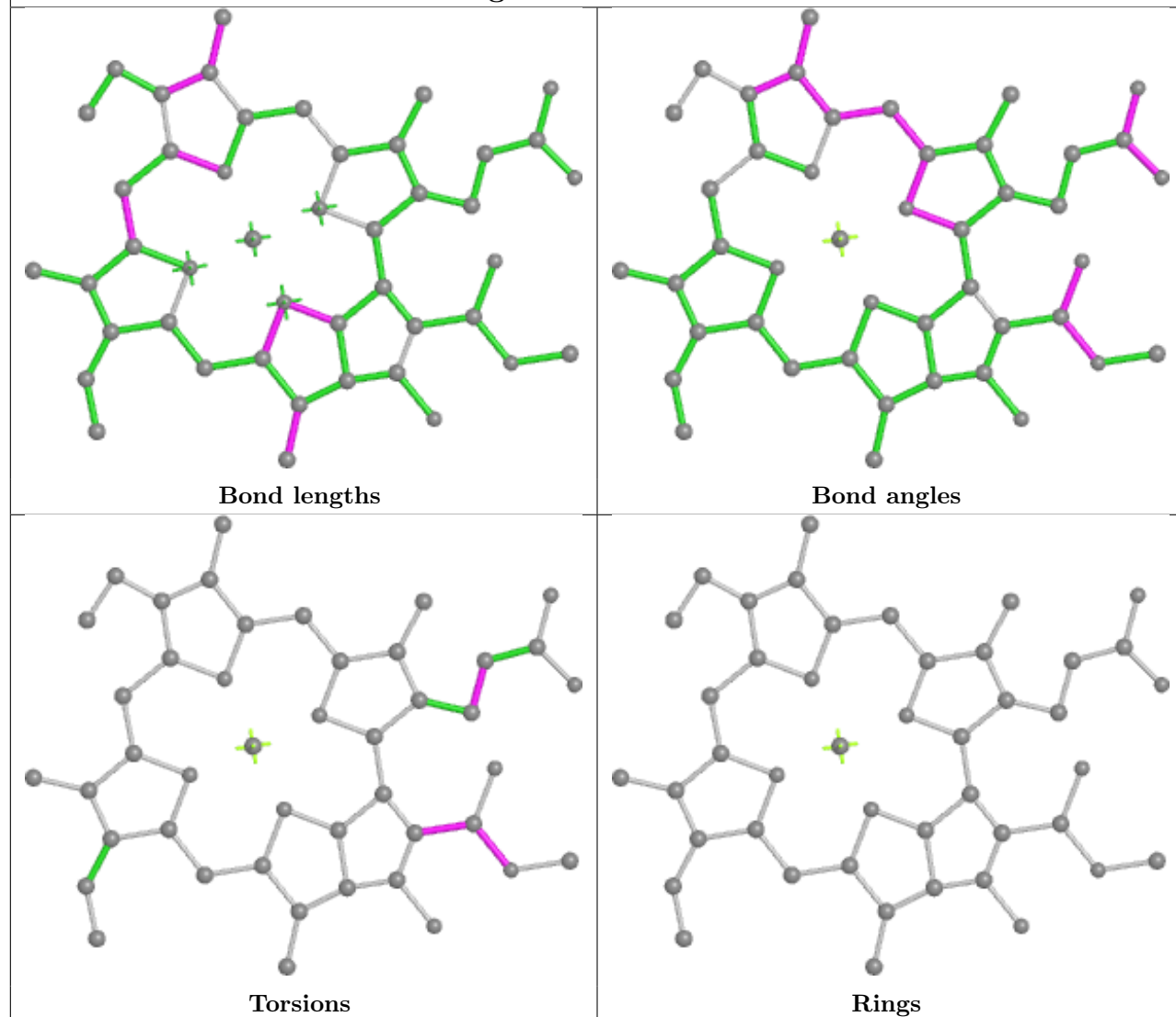
## Ligand CLA 4 607

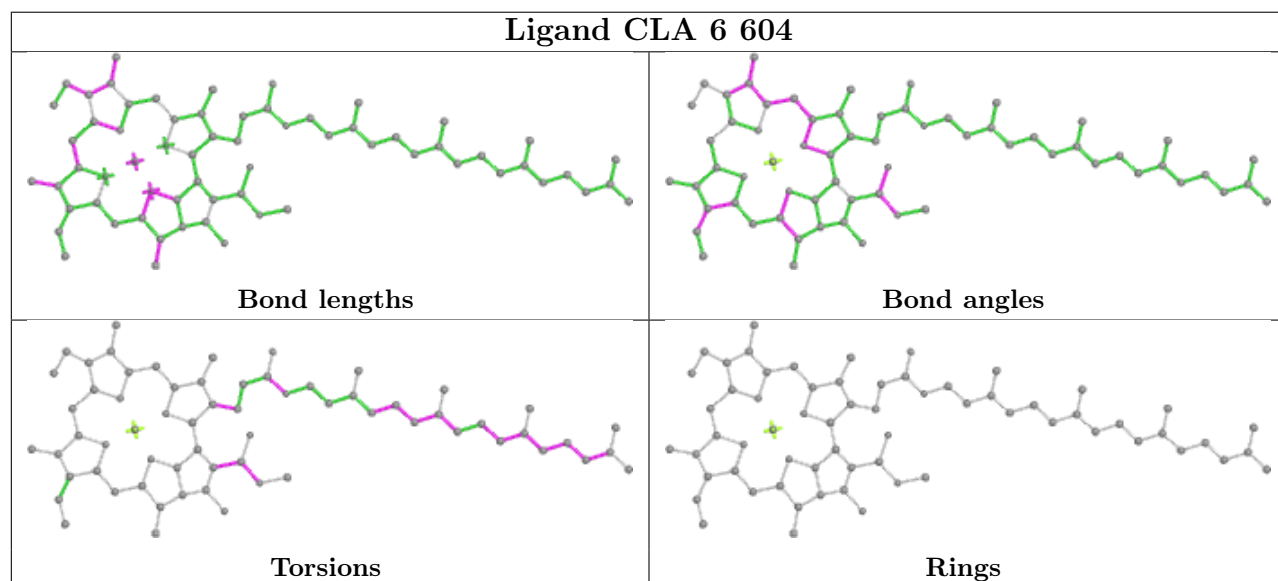
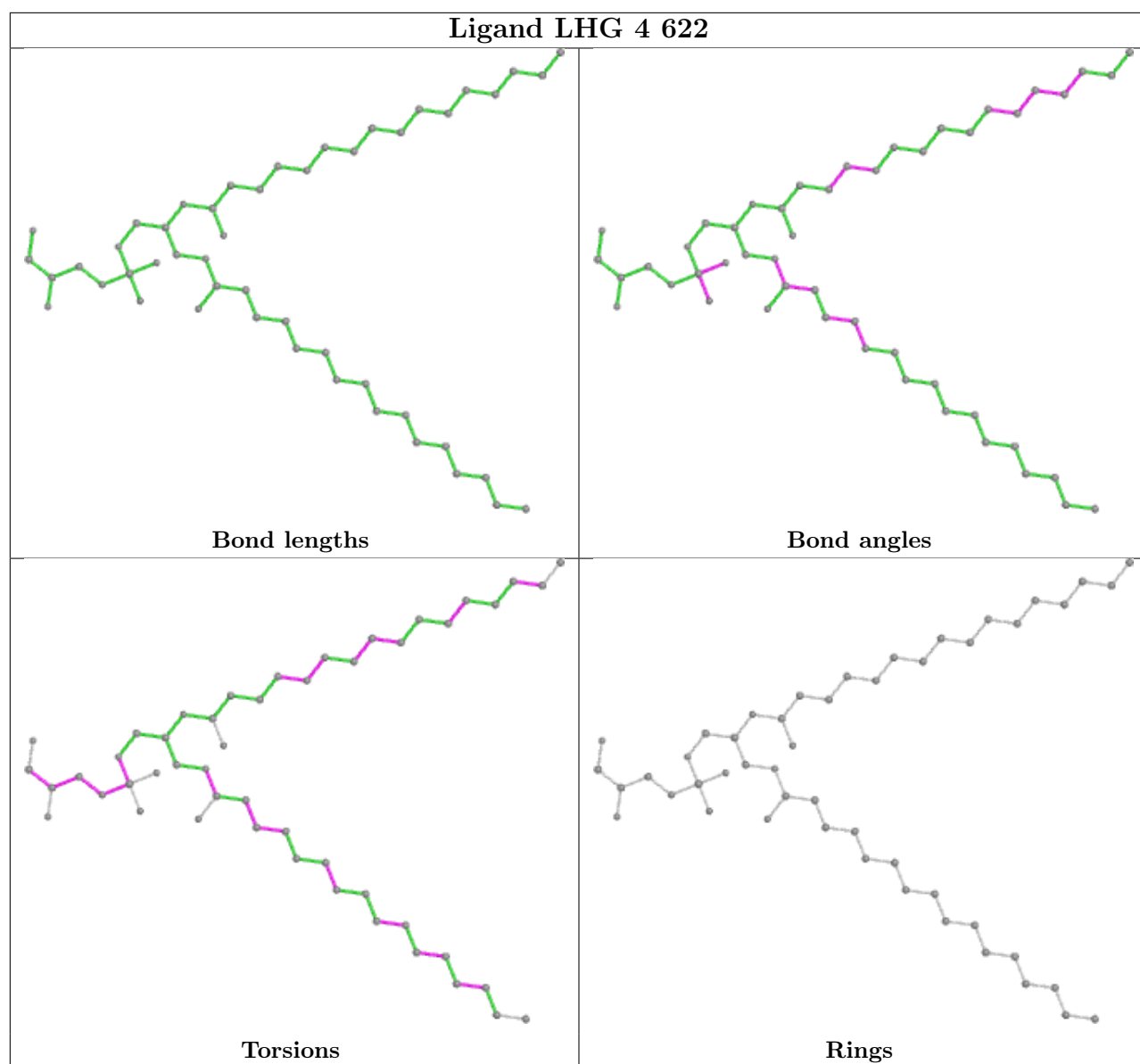


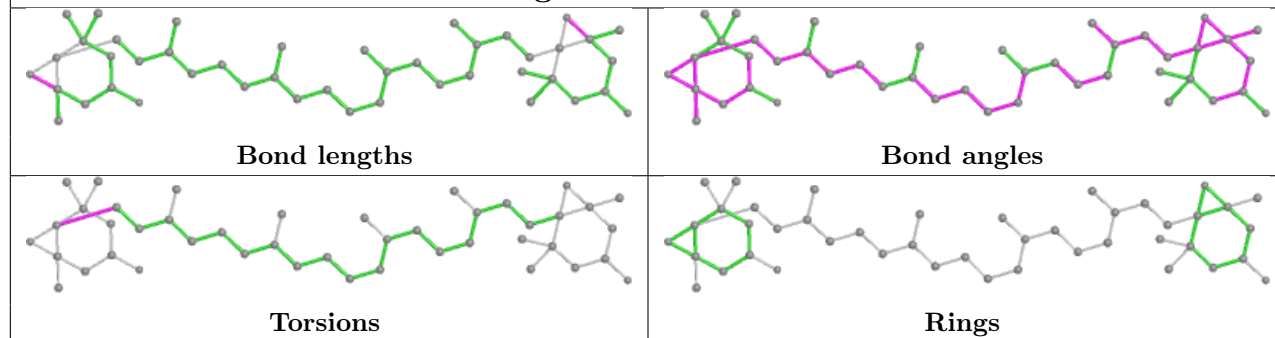
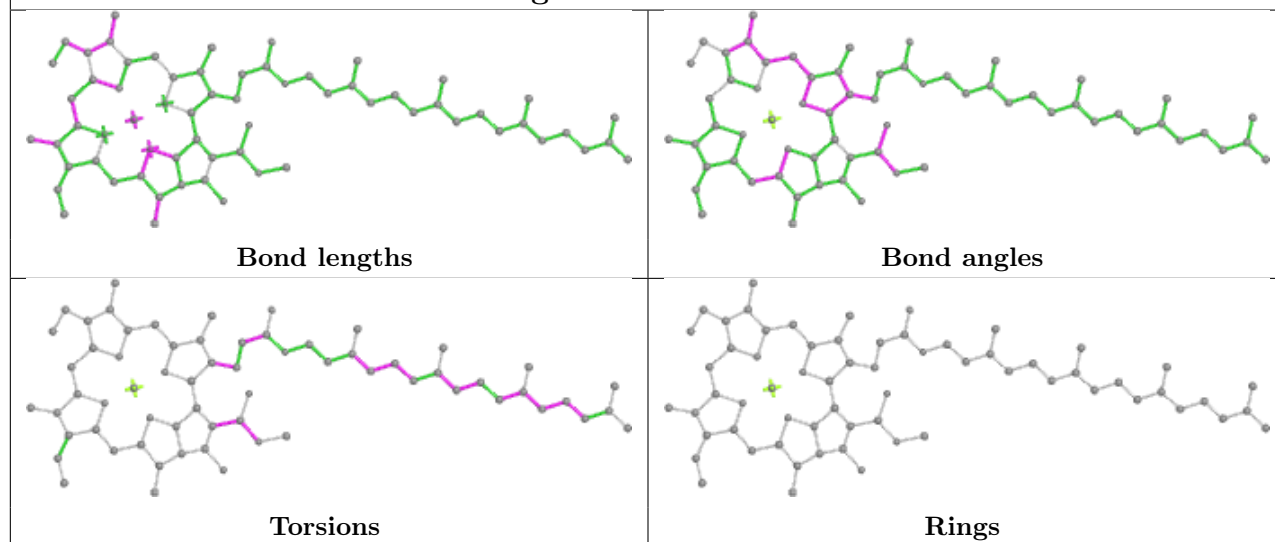
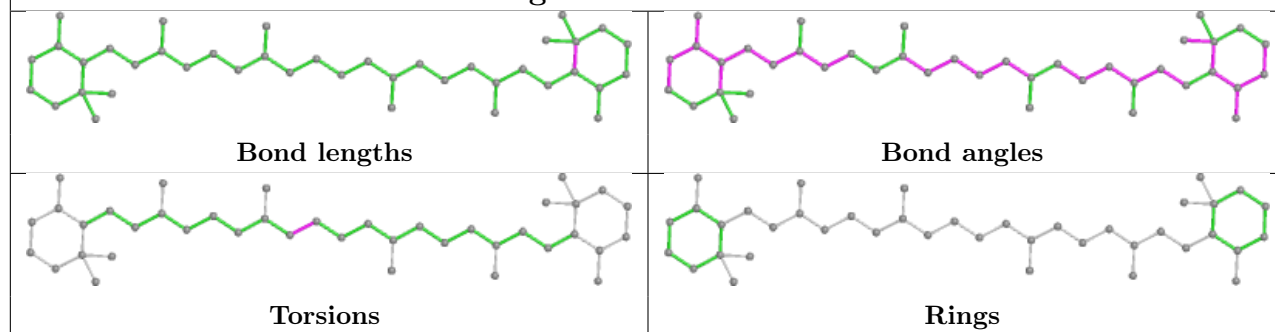
## Ligand CLA 4 603

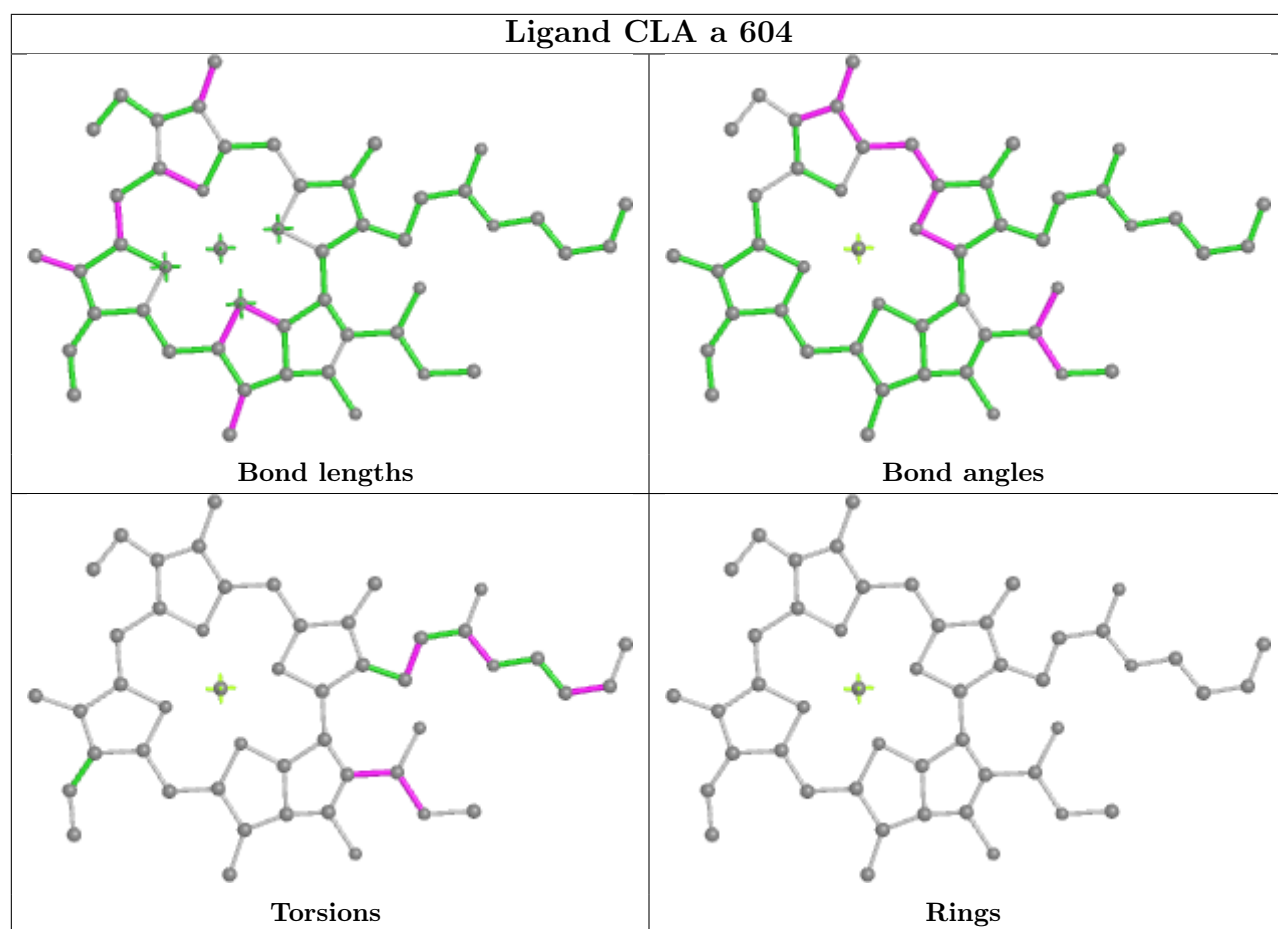


## Ligand CLA K 206



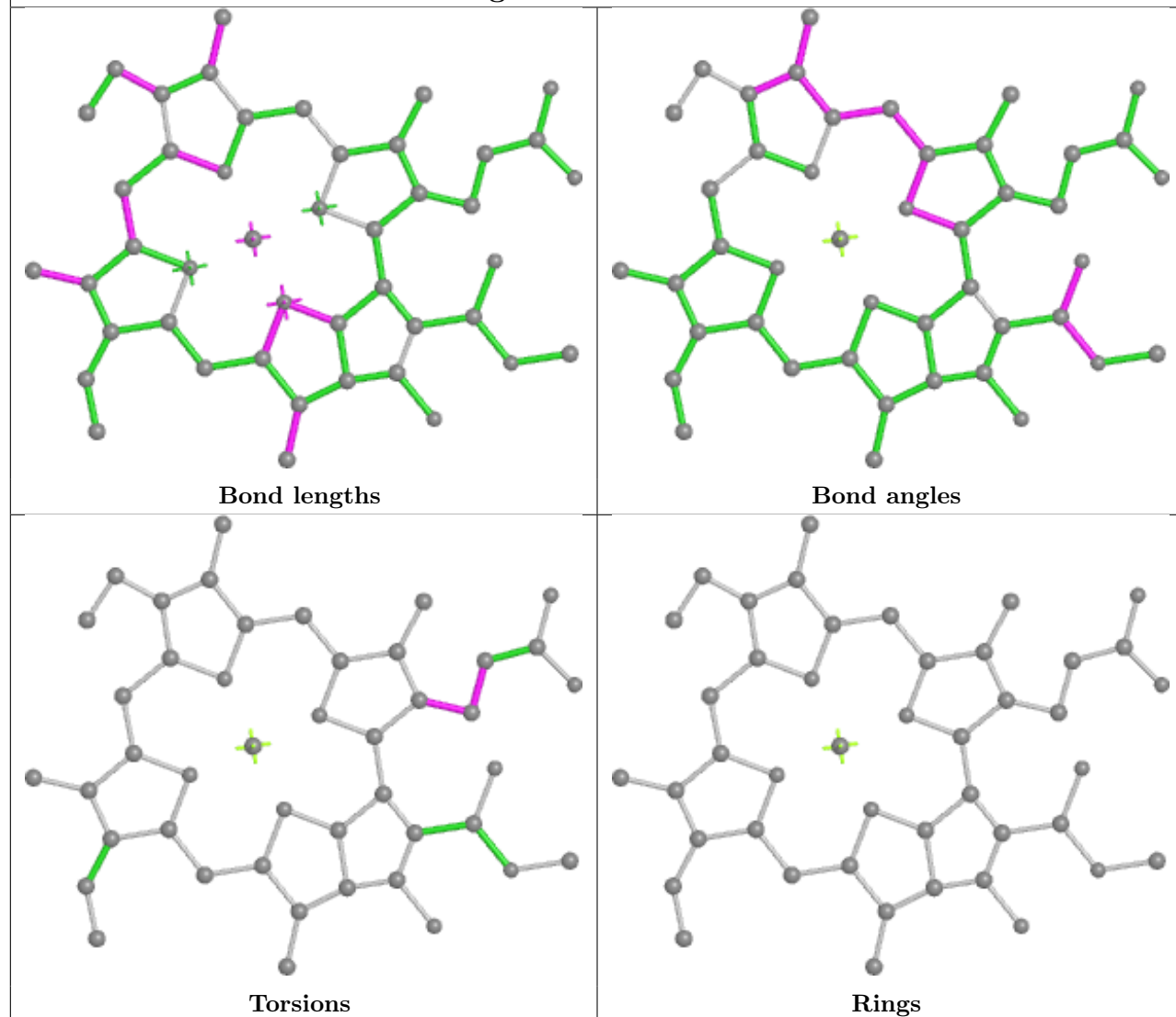


**Ligand XAT 3 619****Ligand CLA B 833****Ligand BCR A 850**

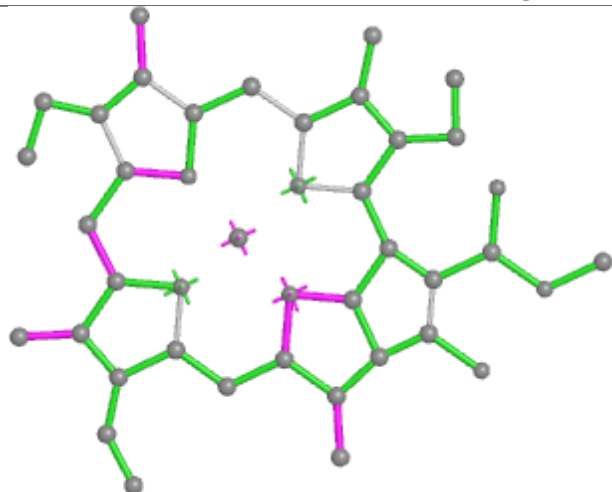




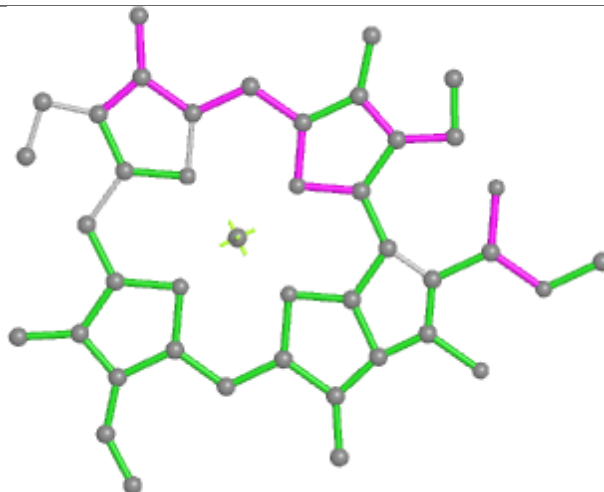
## Ligand CLA A 833



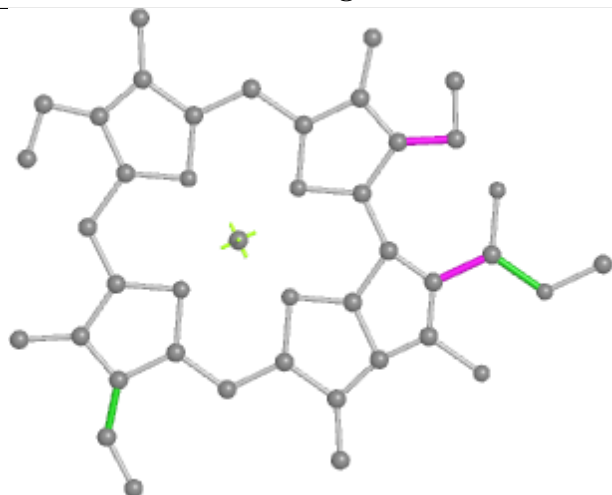
## Ligand CLA 6 611



Bond lengths



Bond angles

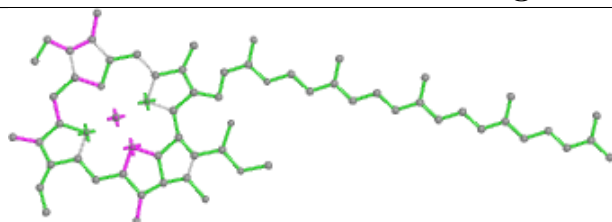


Torsions

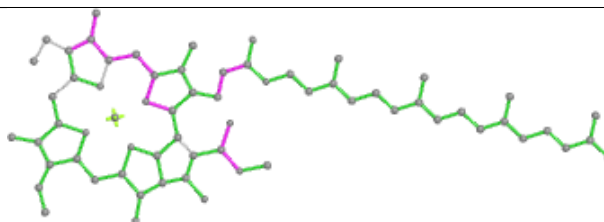


Rings

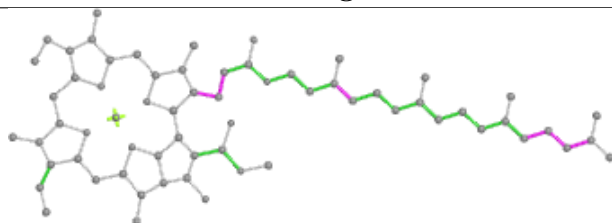
## Ligand CLA A 803



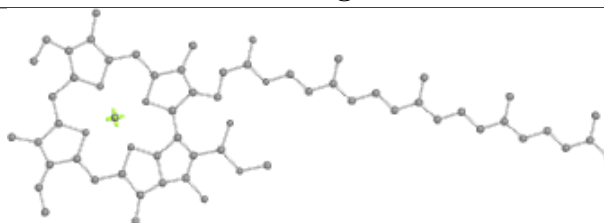
Bond lengths



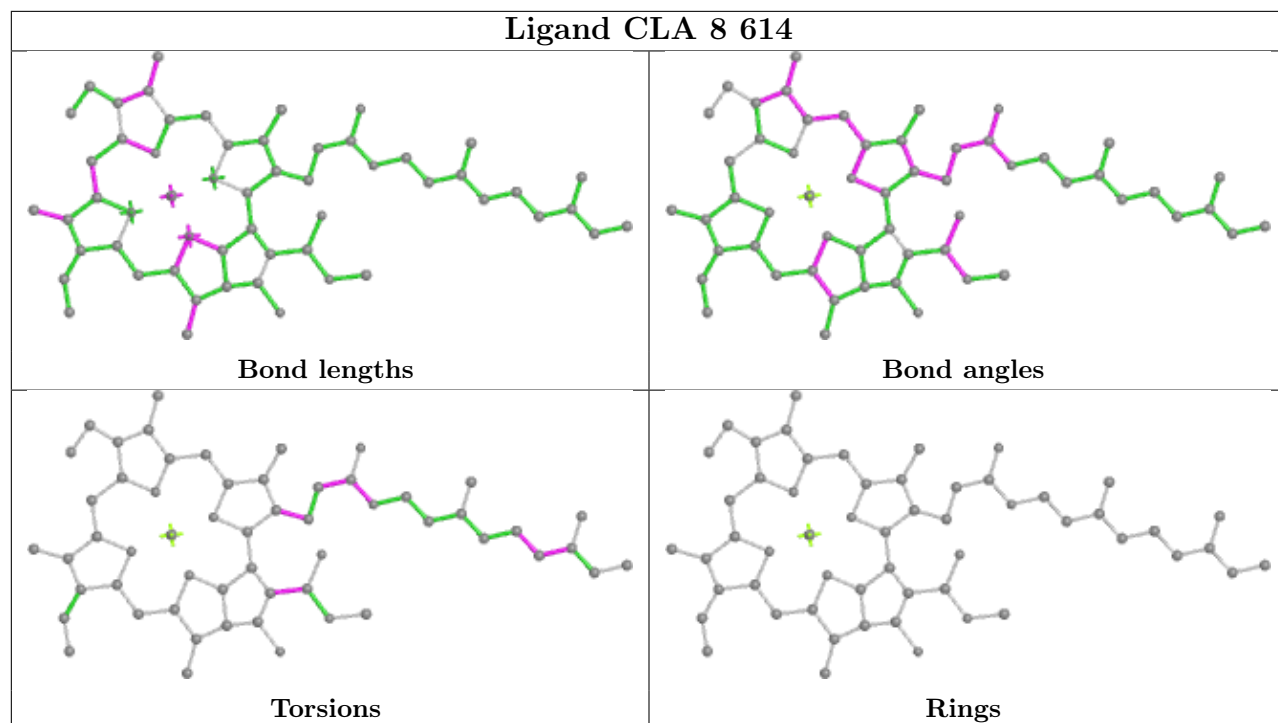
Bond angles

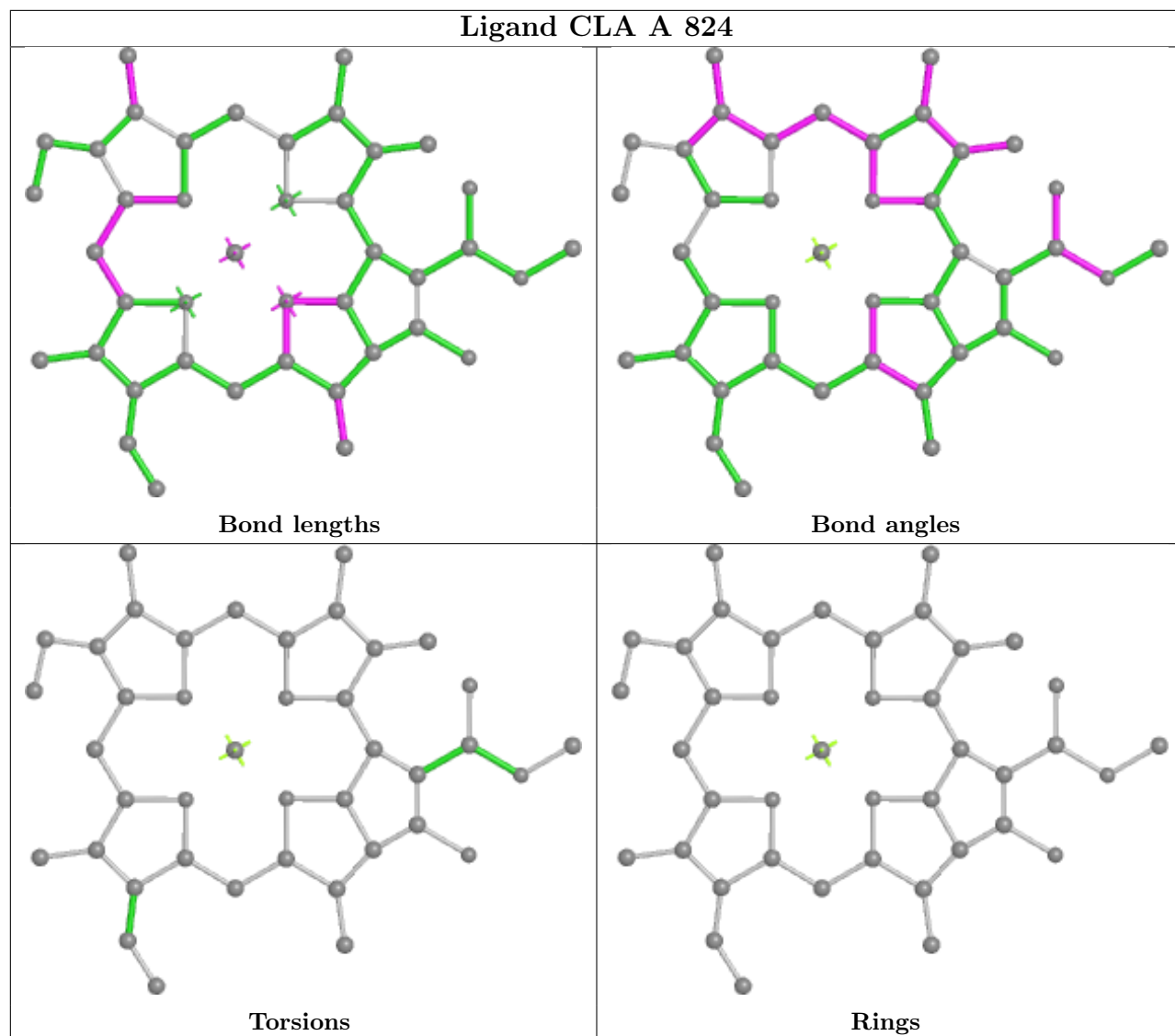


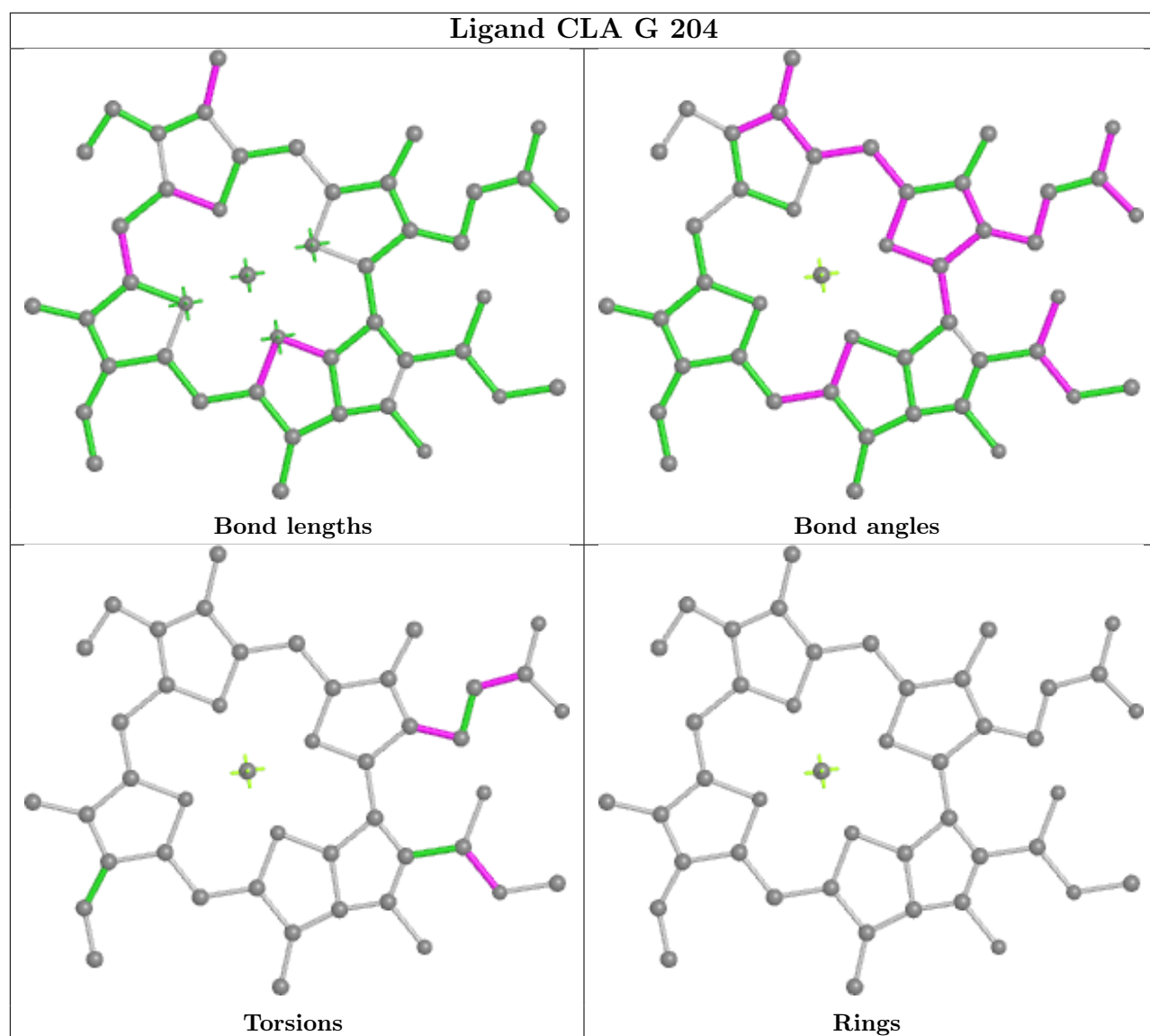
Torsions



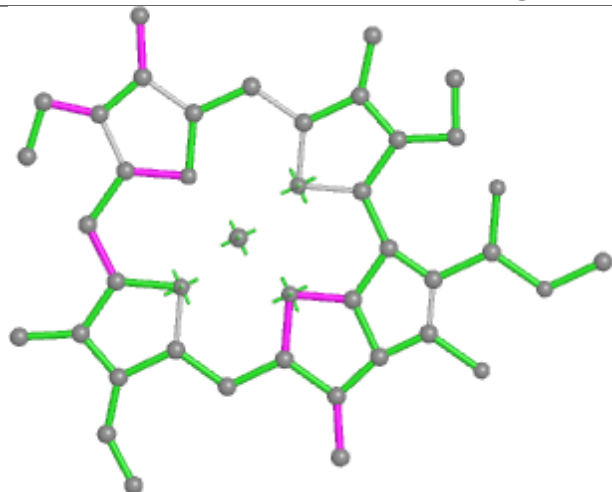
Rings



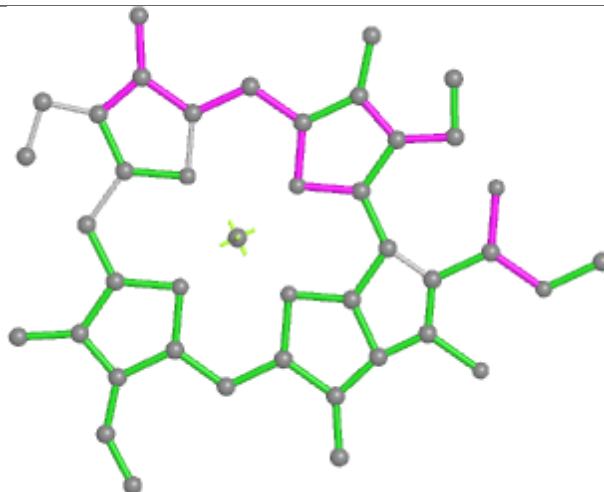




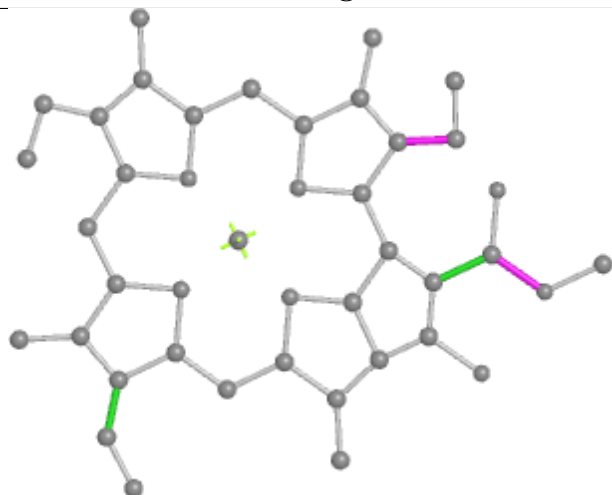
## Ligand CLA B 822



Bond lengths



Bond angles

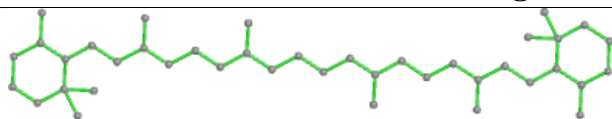


Torsions

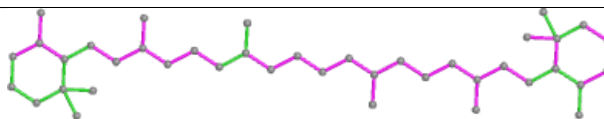


Rings

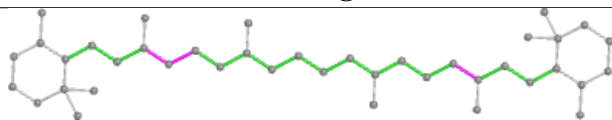
## Ligand BCR B 845



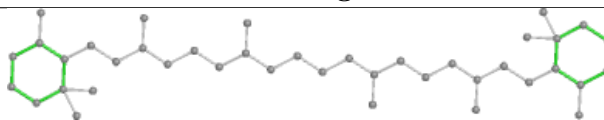
Bond lengths



Bond angles

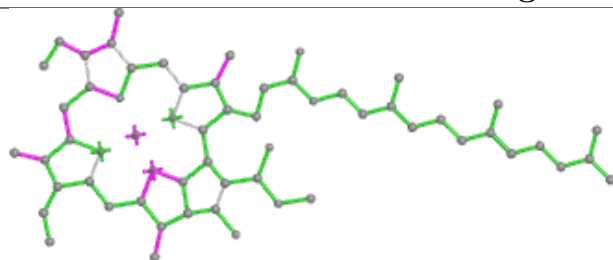


Torsions

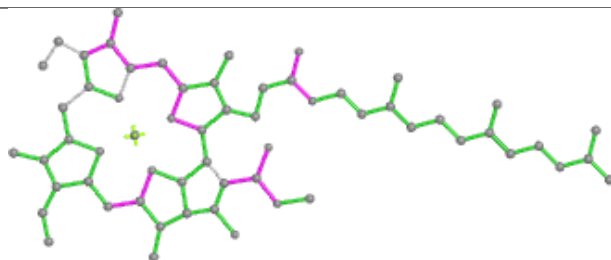


Rings

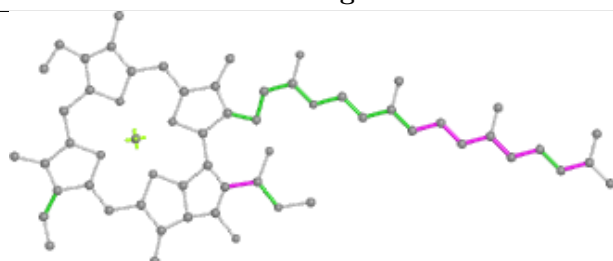
## Ligand CLA 7 601



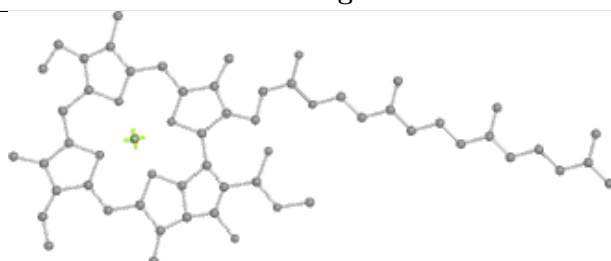
Bond lengths



Bond angles

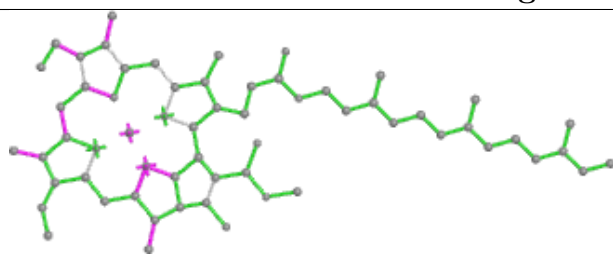


Torsions

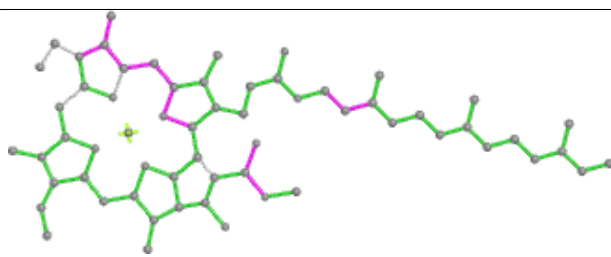


Rings

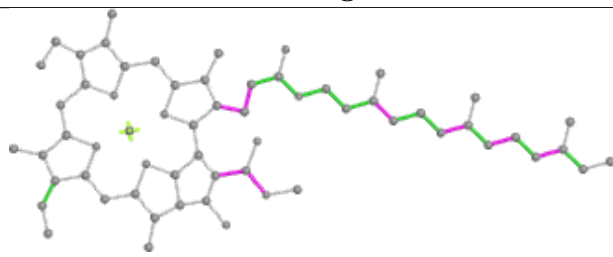
## Ligand CLA 4 610



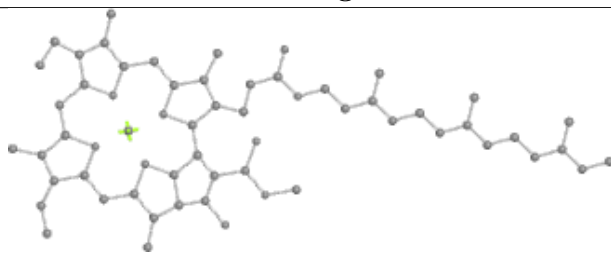
Bond lengths



Bond angles

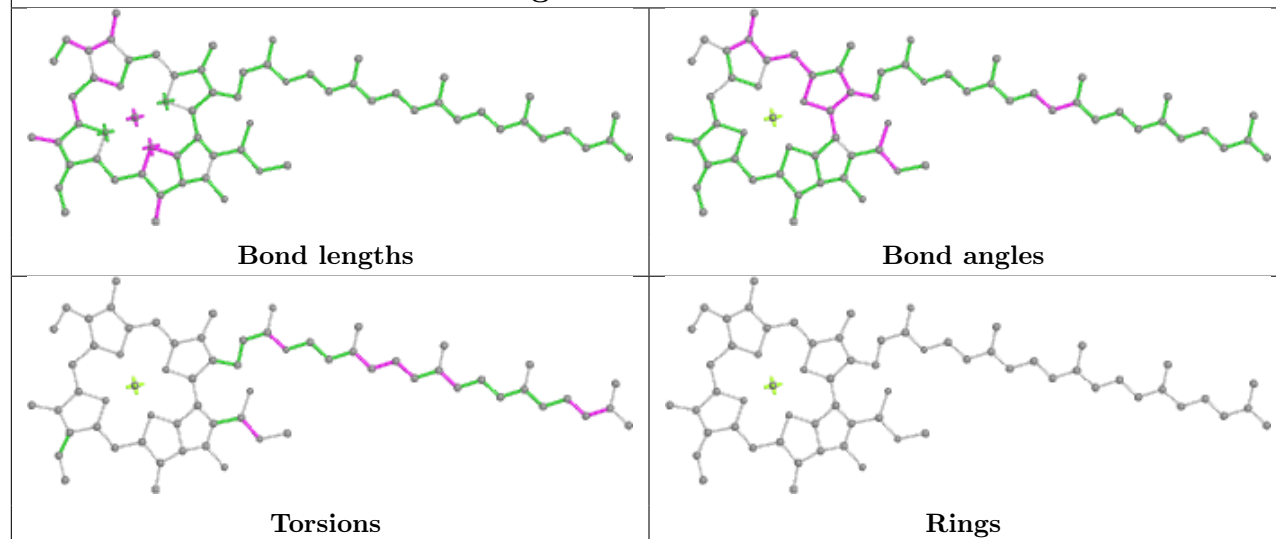


Torsions

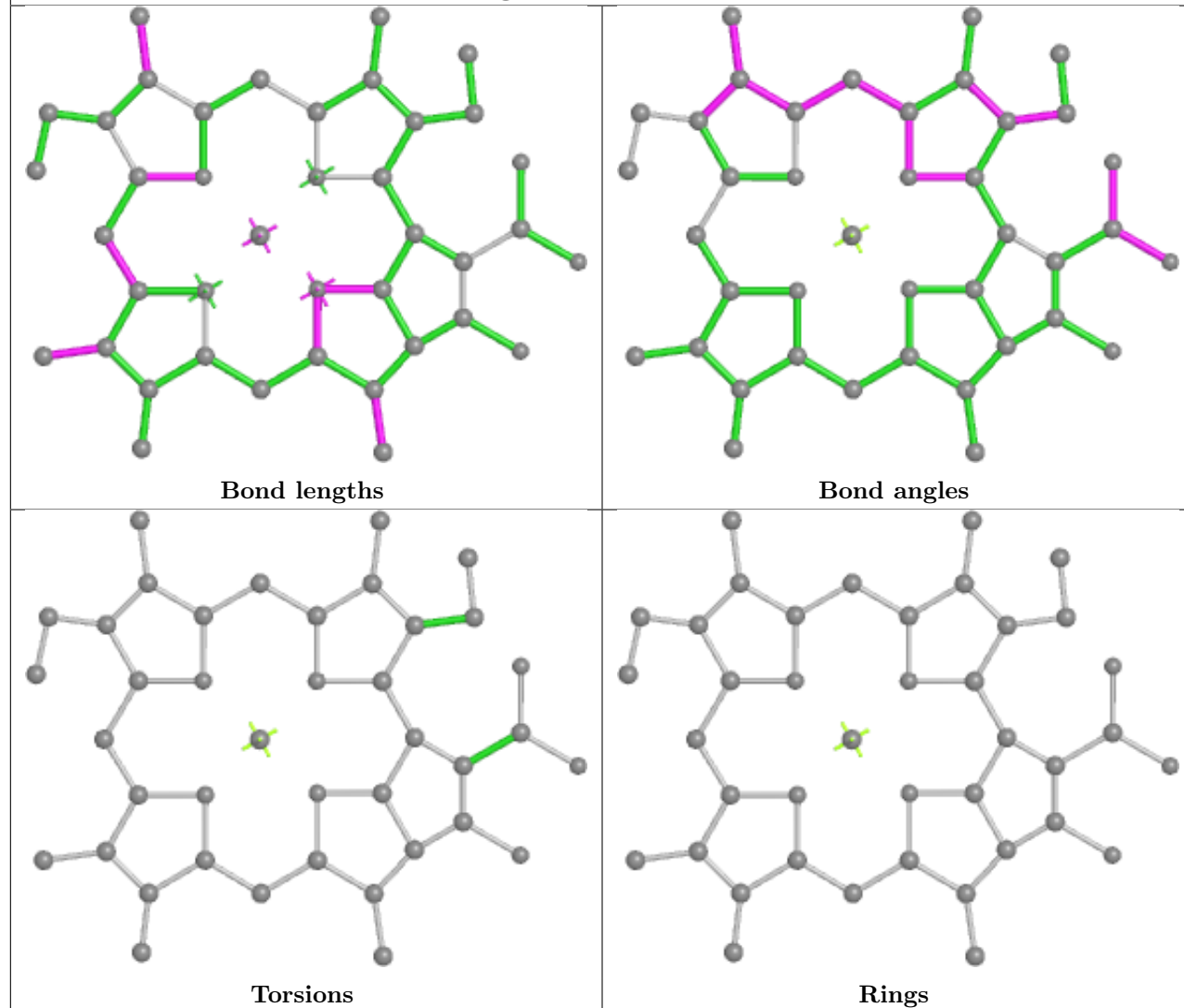


Rings

## Ligand CLA A 807

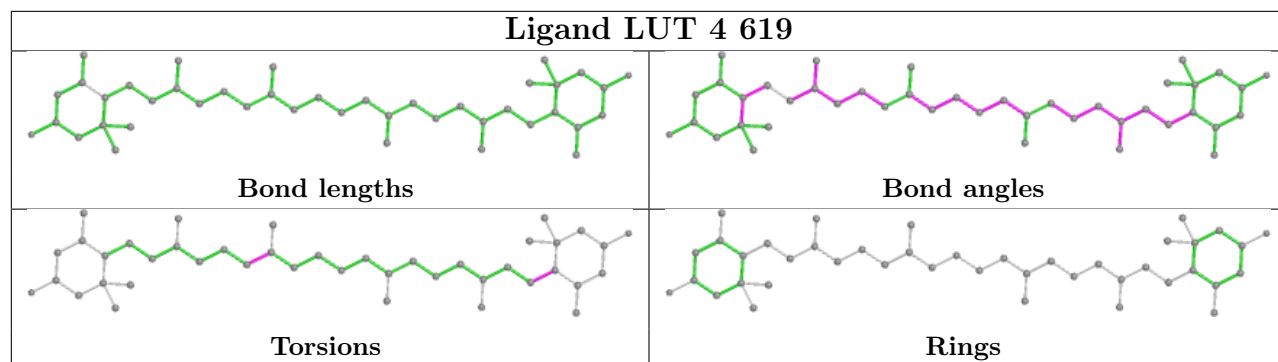


## Ligand CLA 6 606

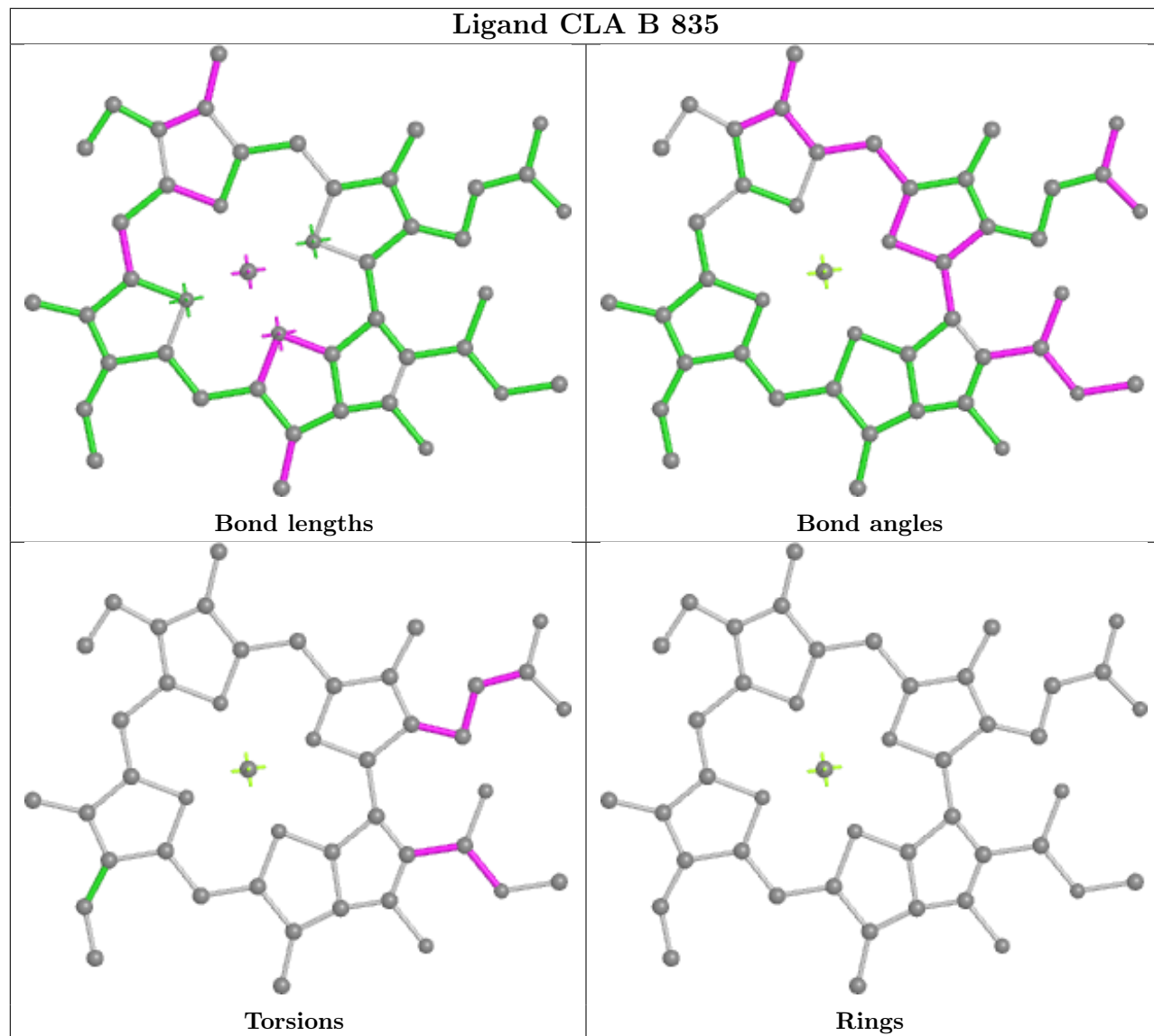




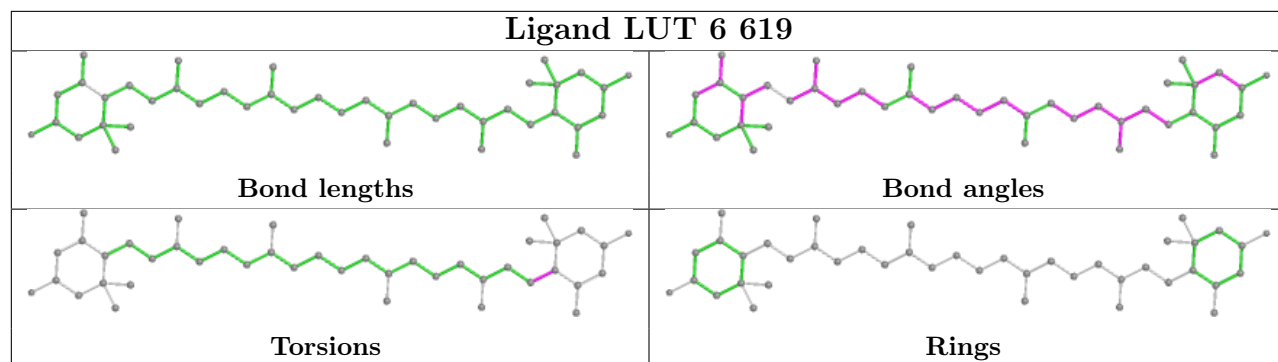
## Ligand LUT 4 619



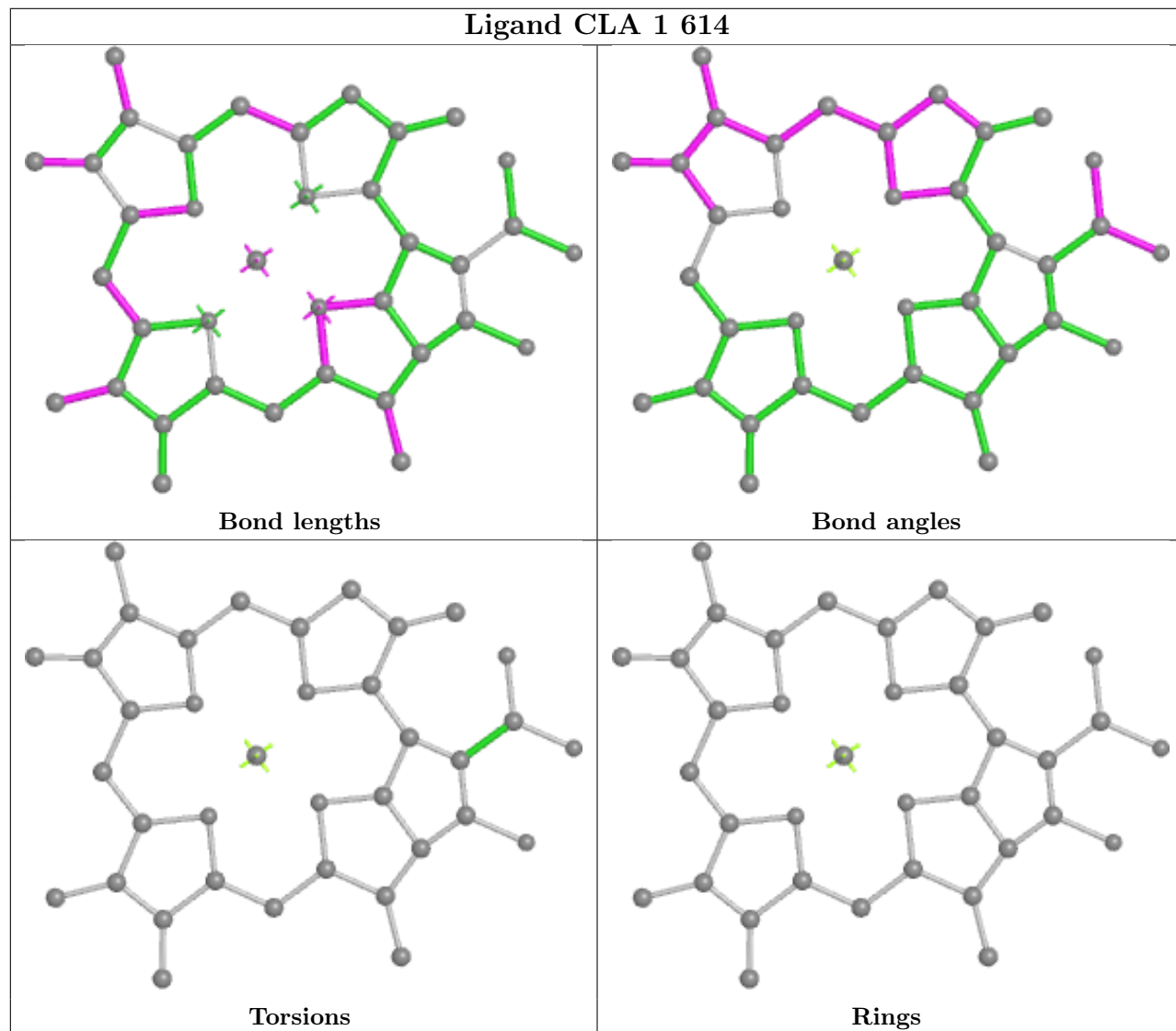
## Ligand CLA B 835



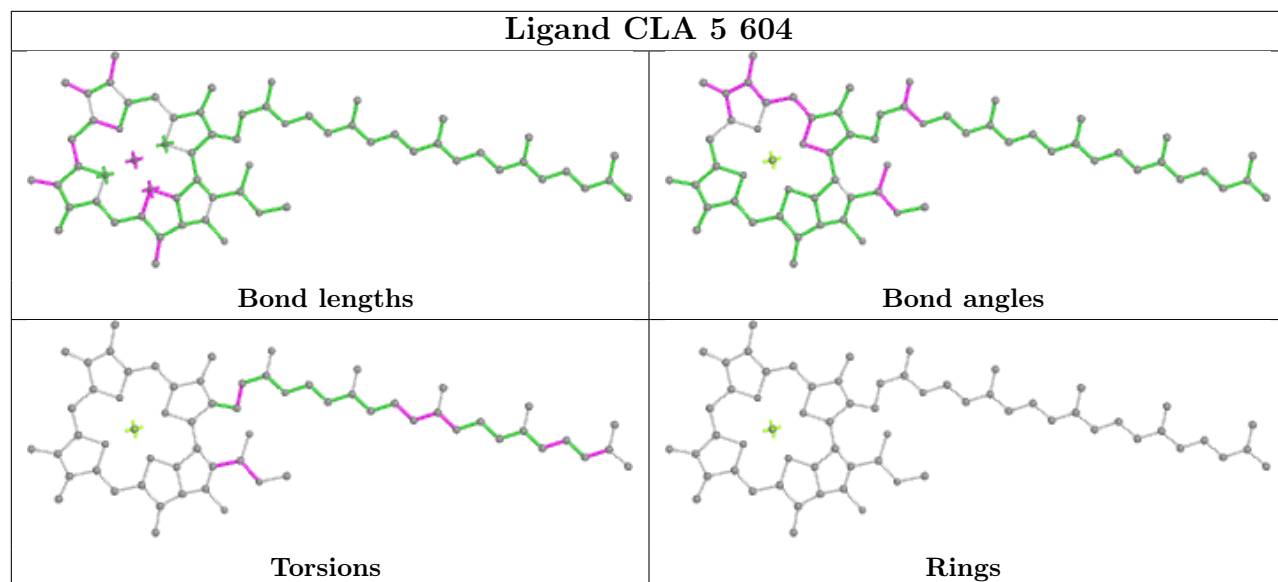
## Ligand LUT 6 619



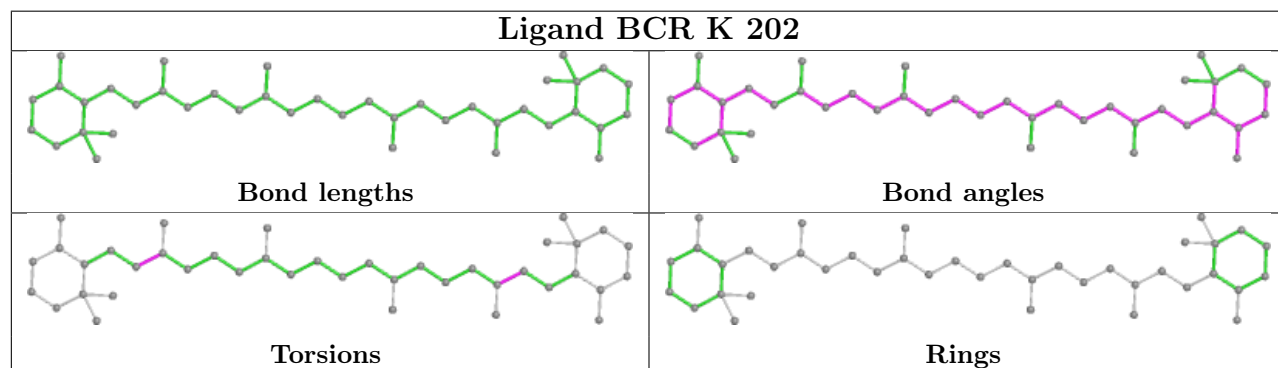
## Ligand CLA 1 614



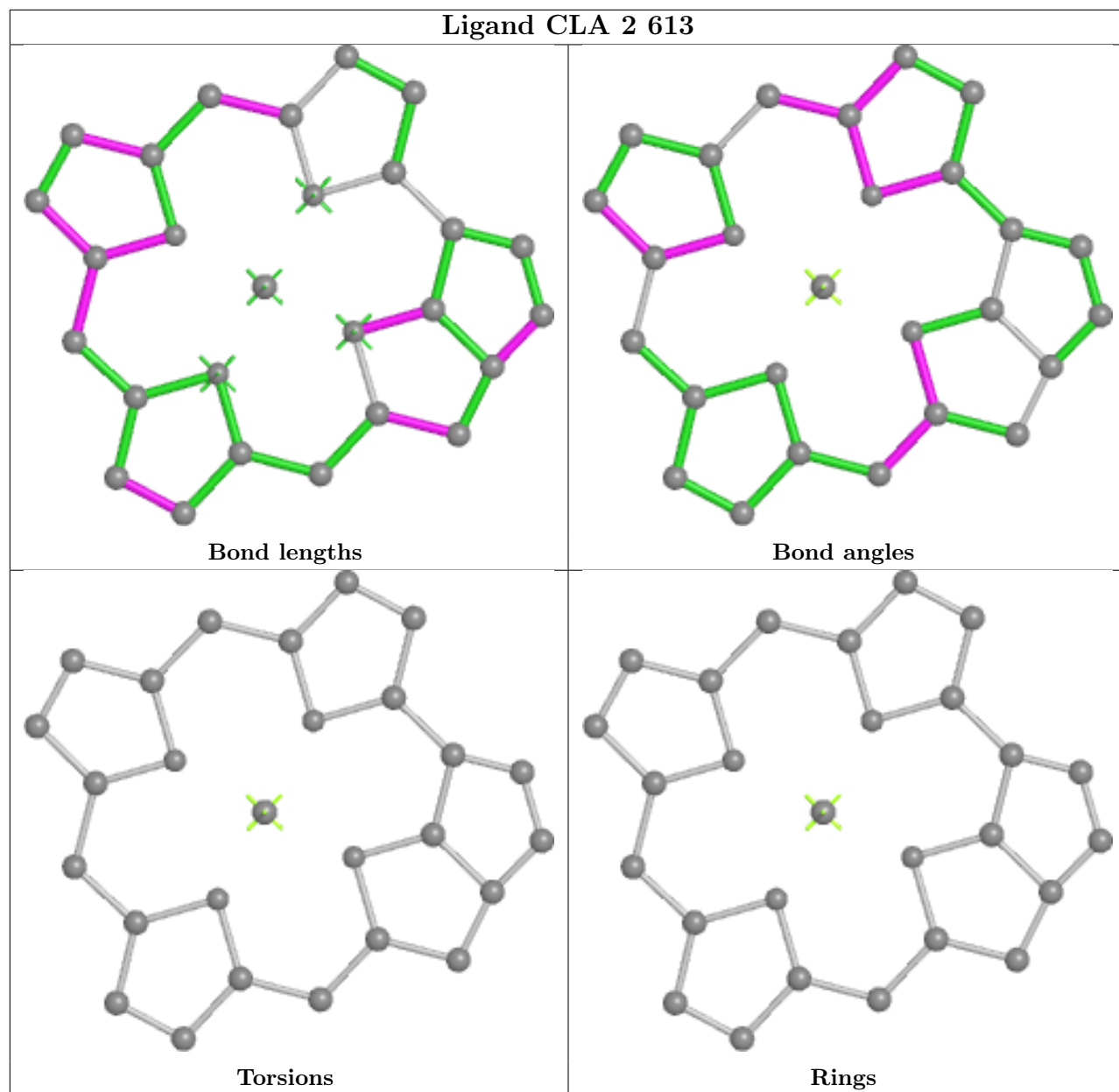
## Ligand CLA 5 604



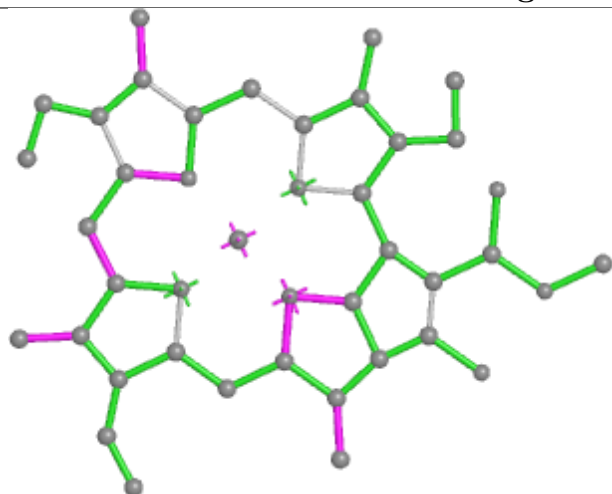
## Ligand BCR K 202



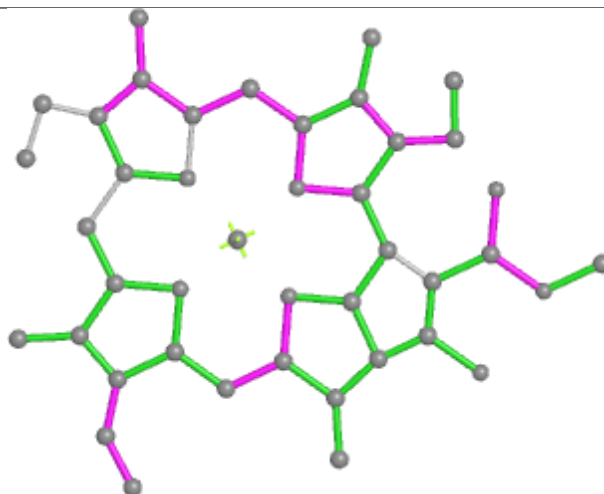
## Ligand CLA 2 613



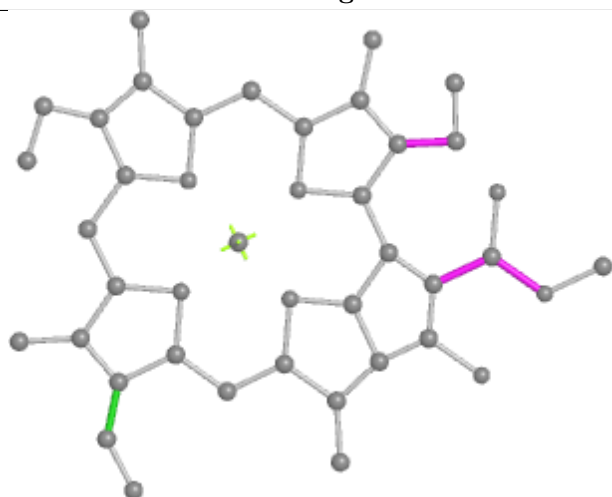
## Ligand CLA 7 607



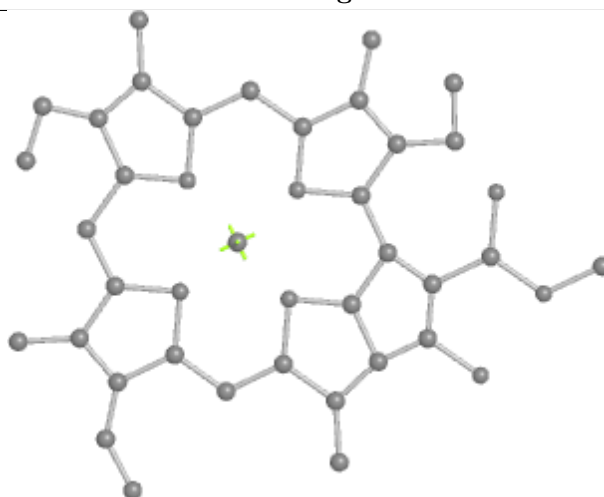
Bond lengths



Bond angles

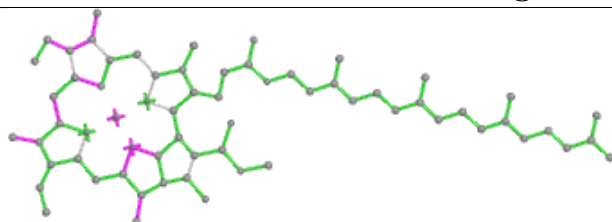


Torsions

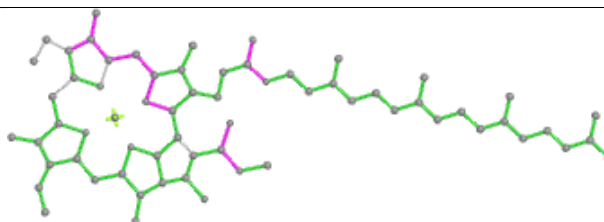


Rings

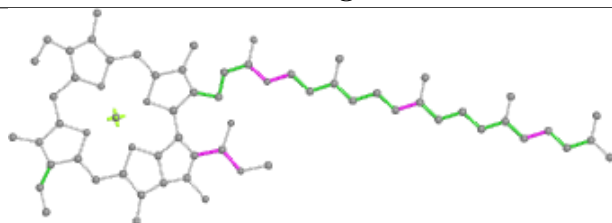
## Ligand CLA B 840



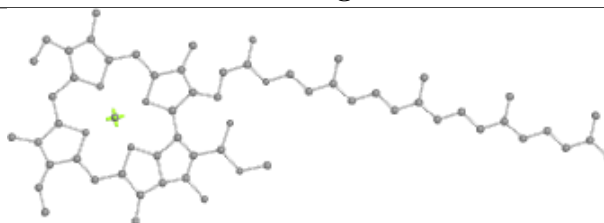
Bond lengths



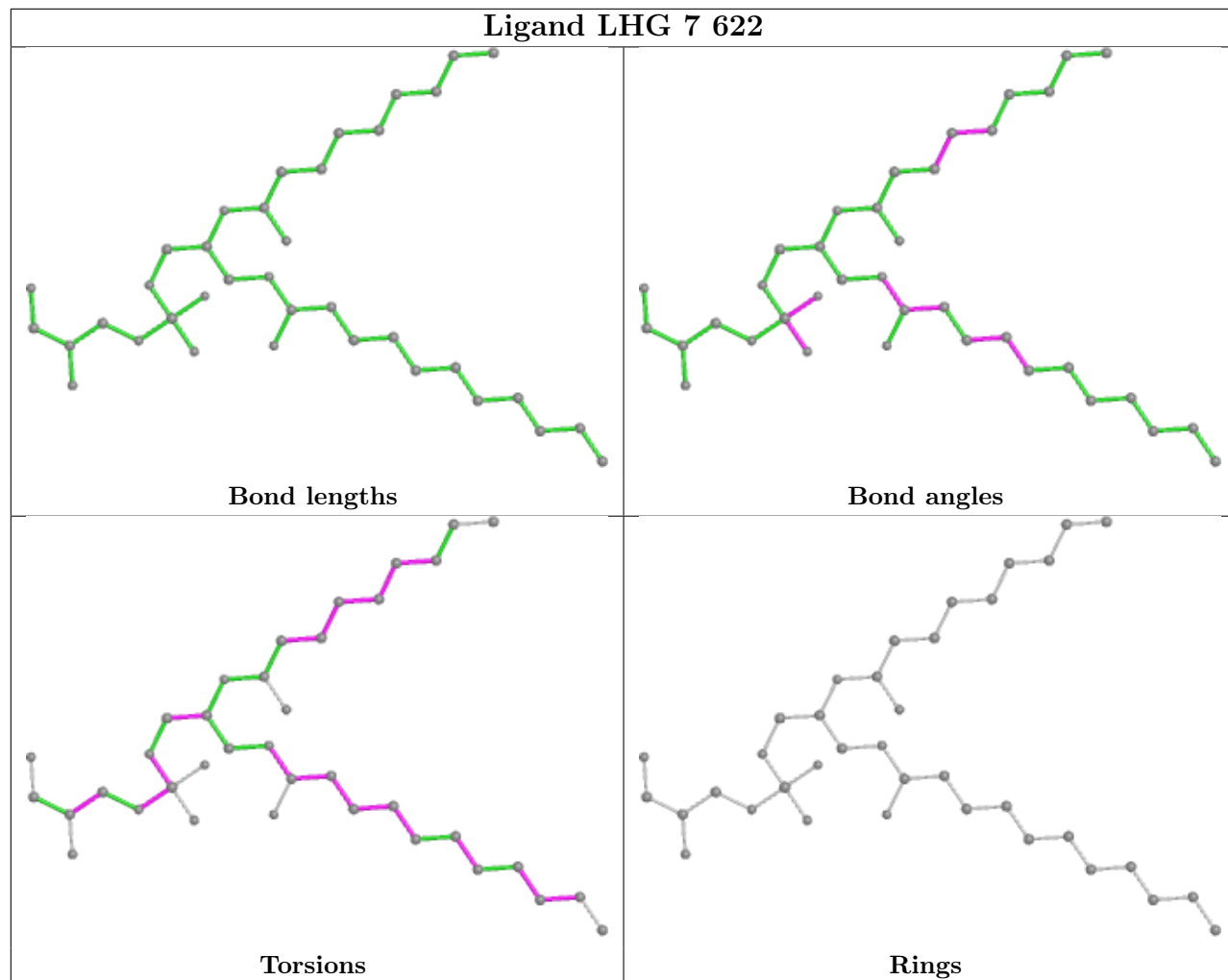
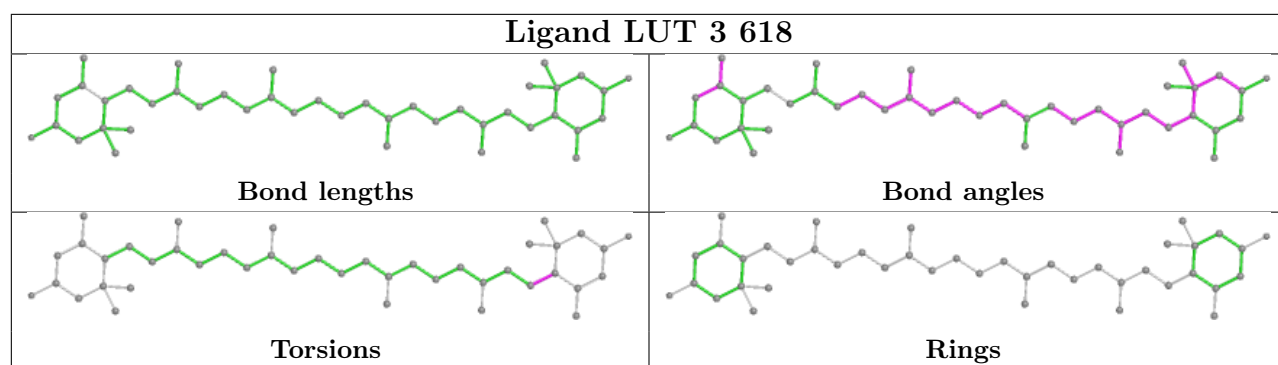
Bond angles

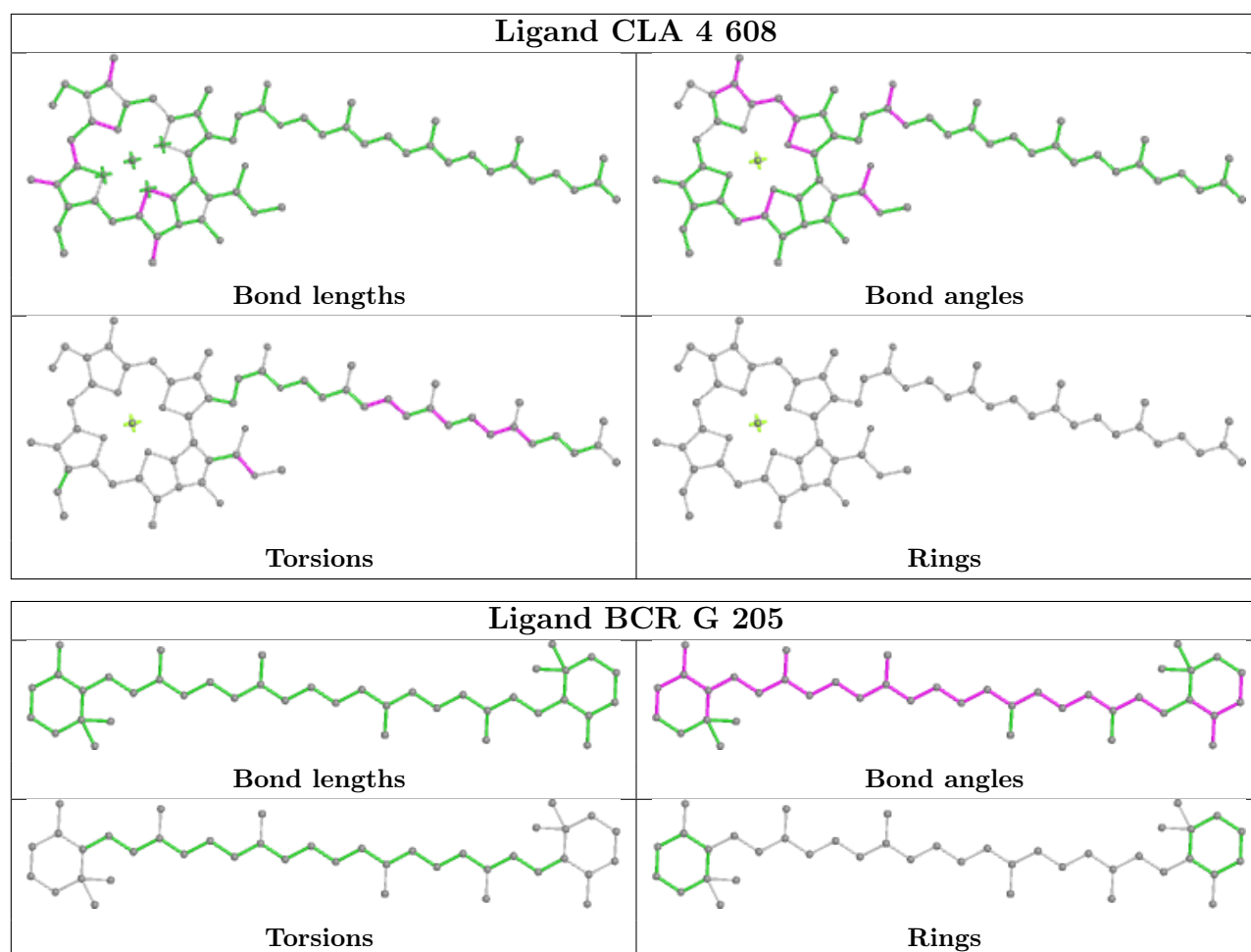


Torsions

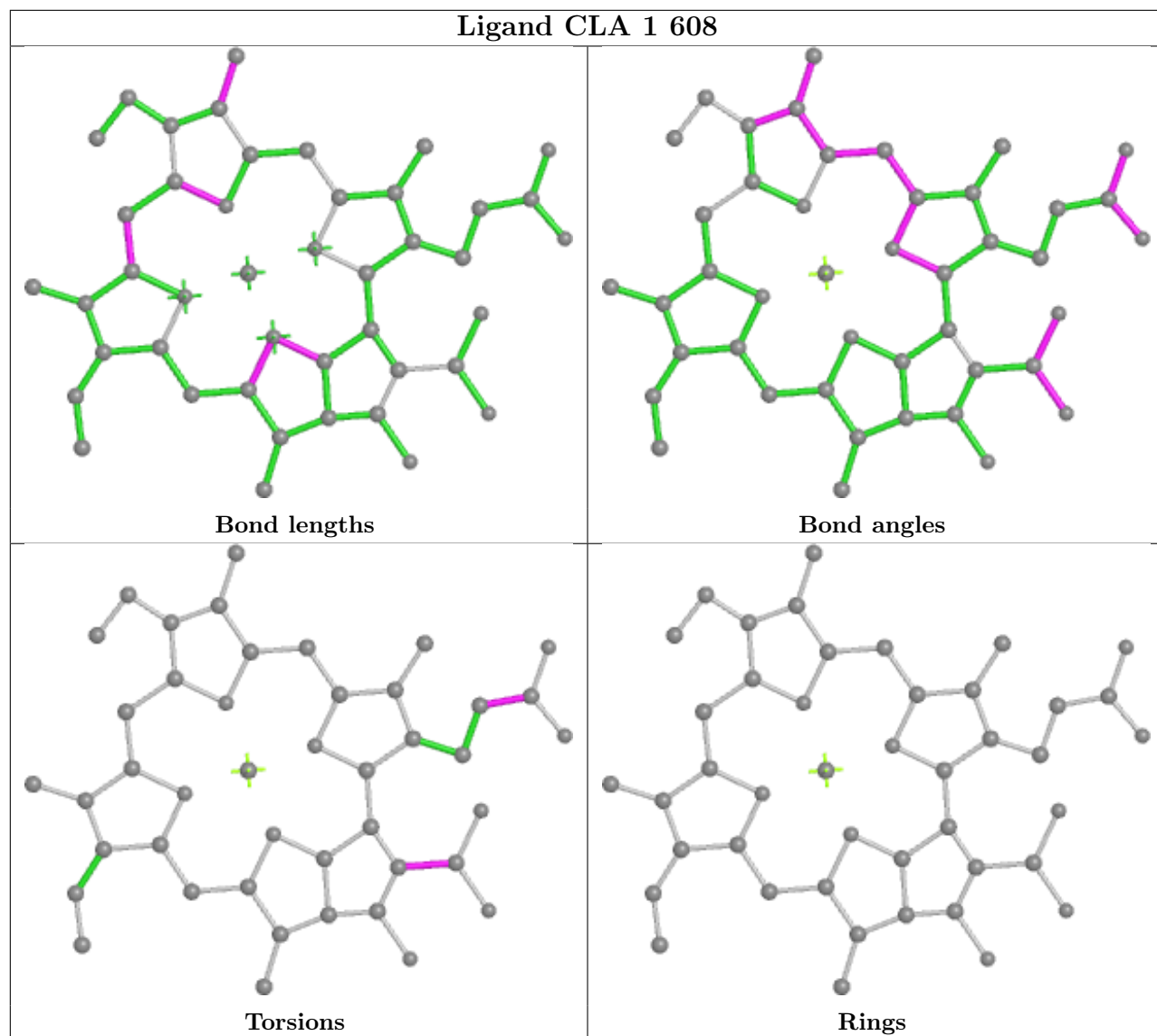


Rings



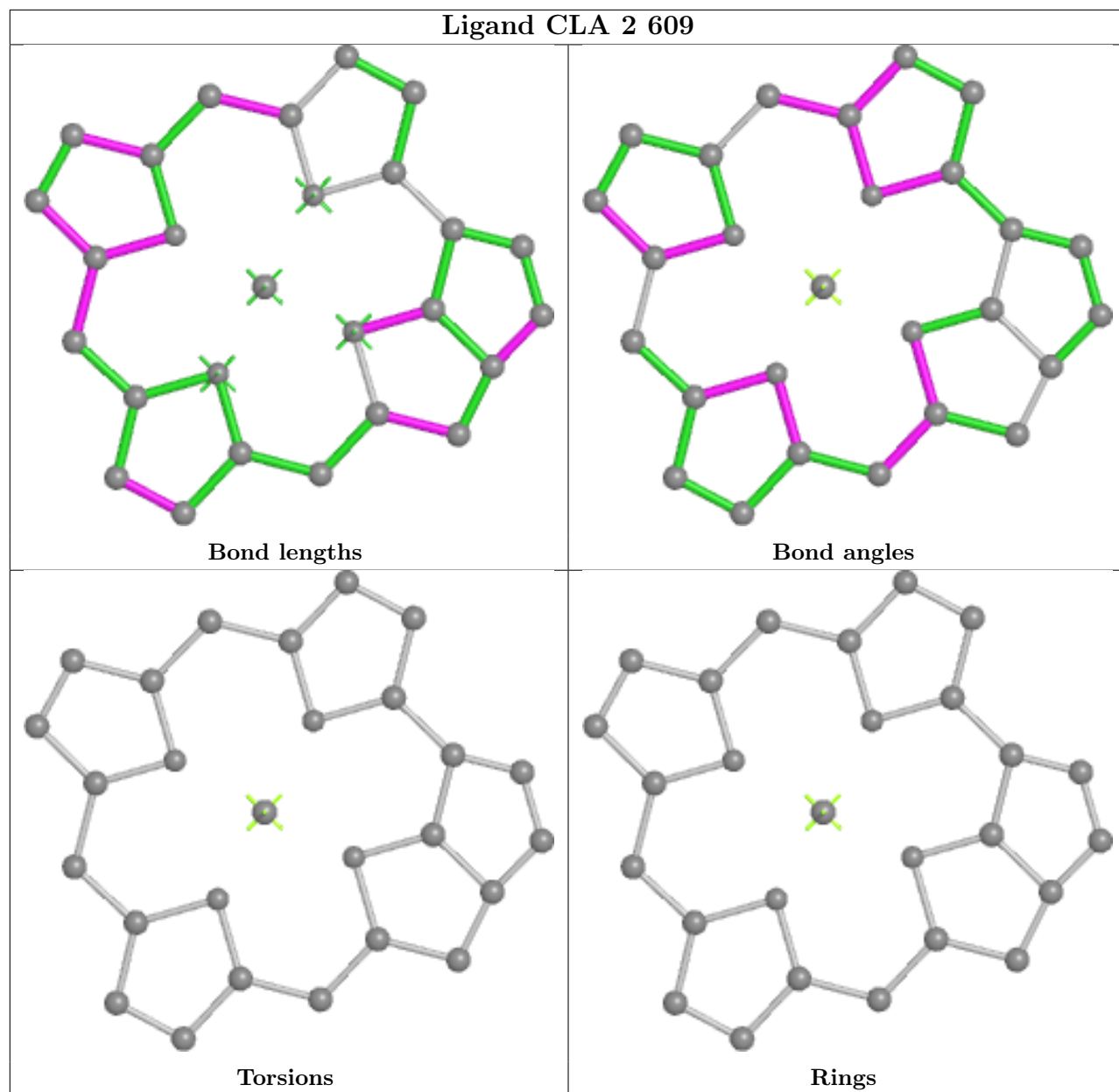


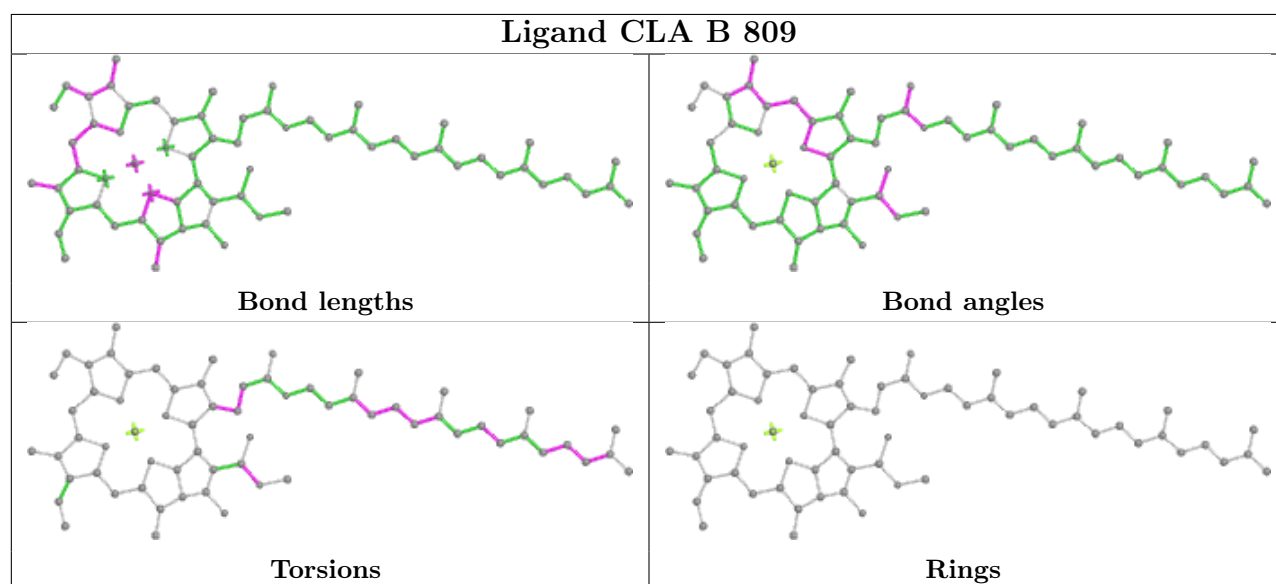
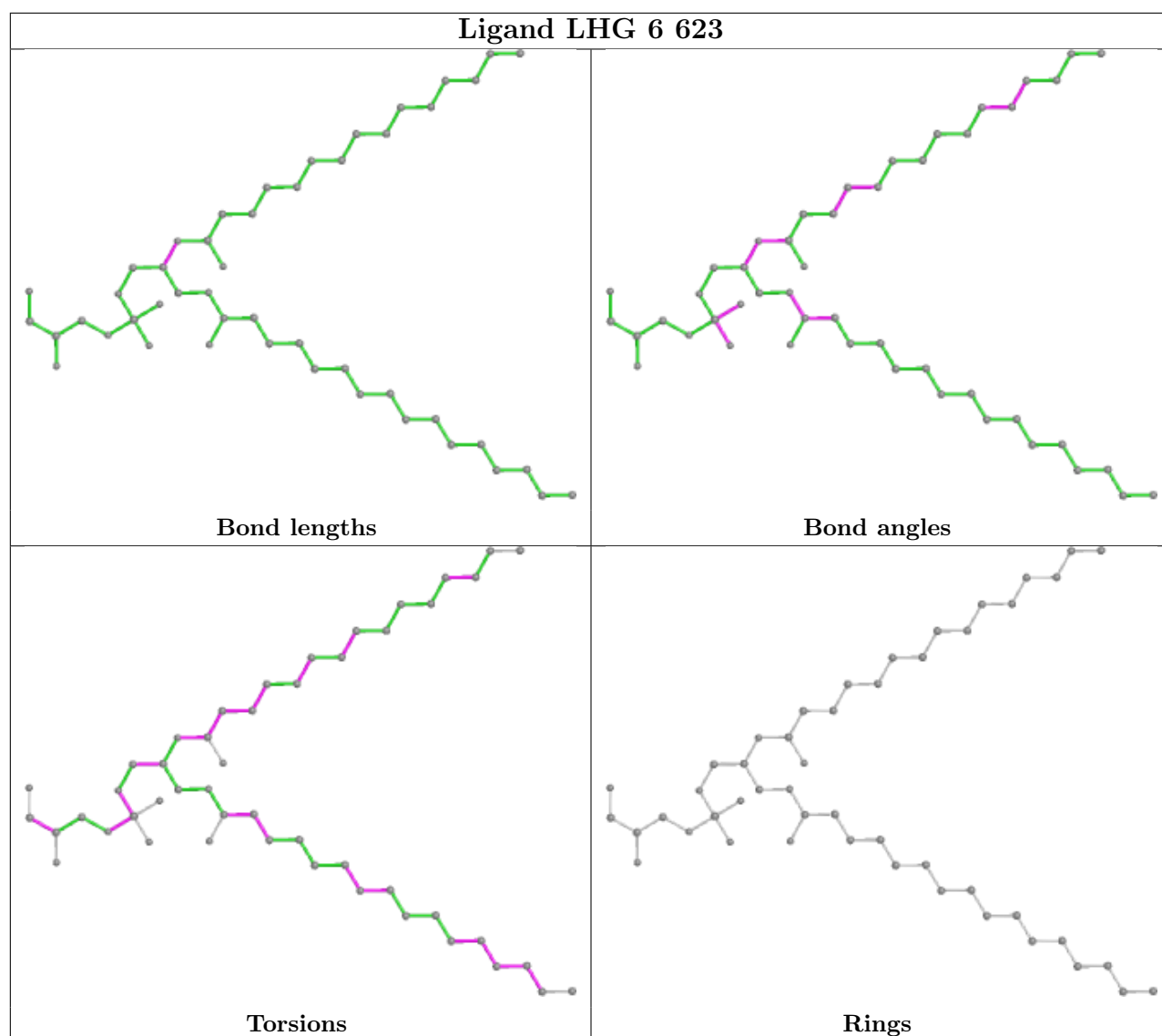
## Ligand CLA 1 608



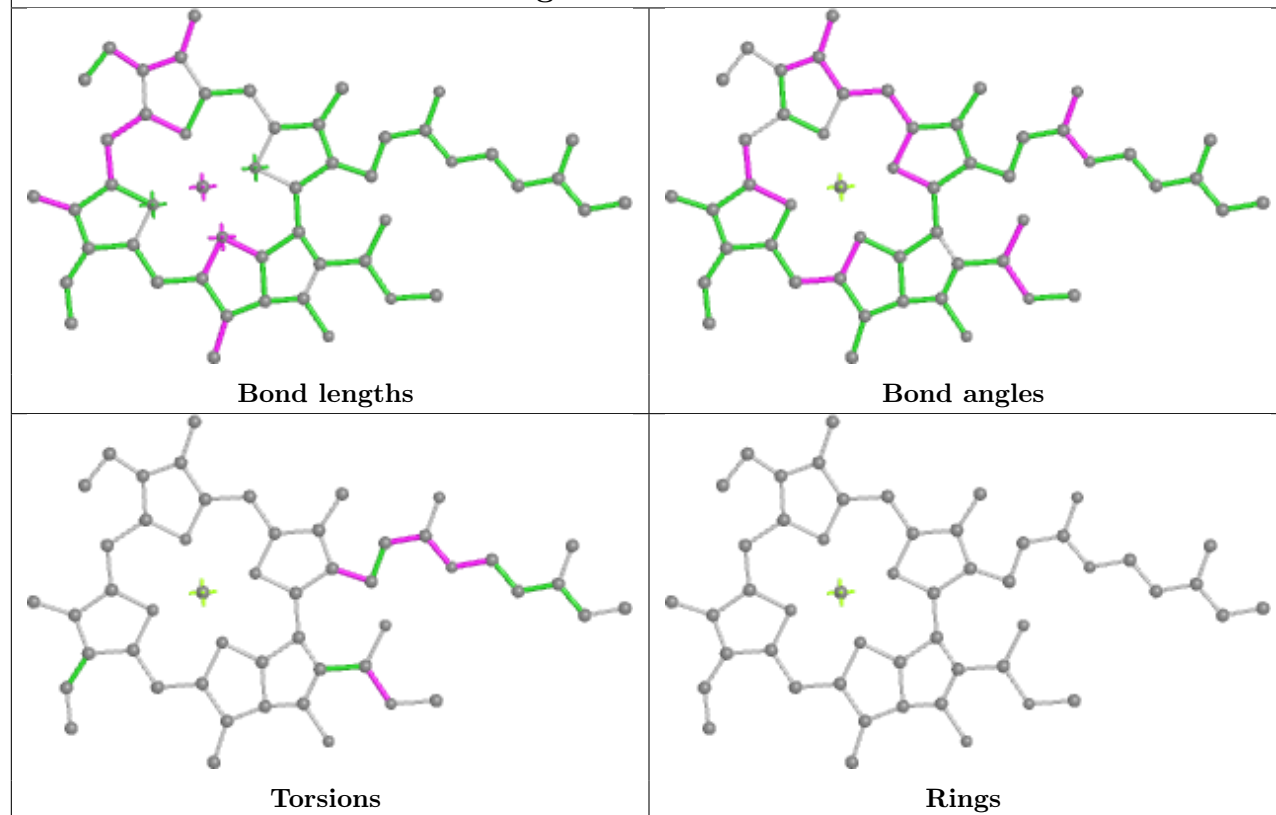


## Ligand CLA 2 609

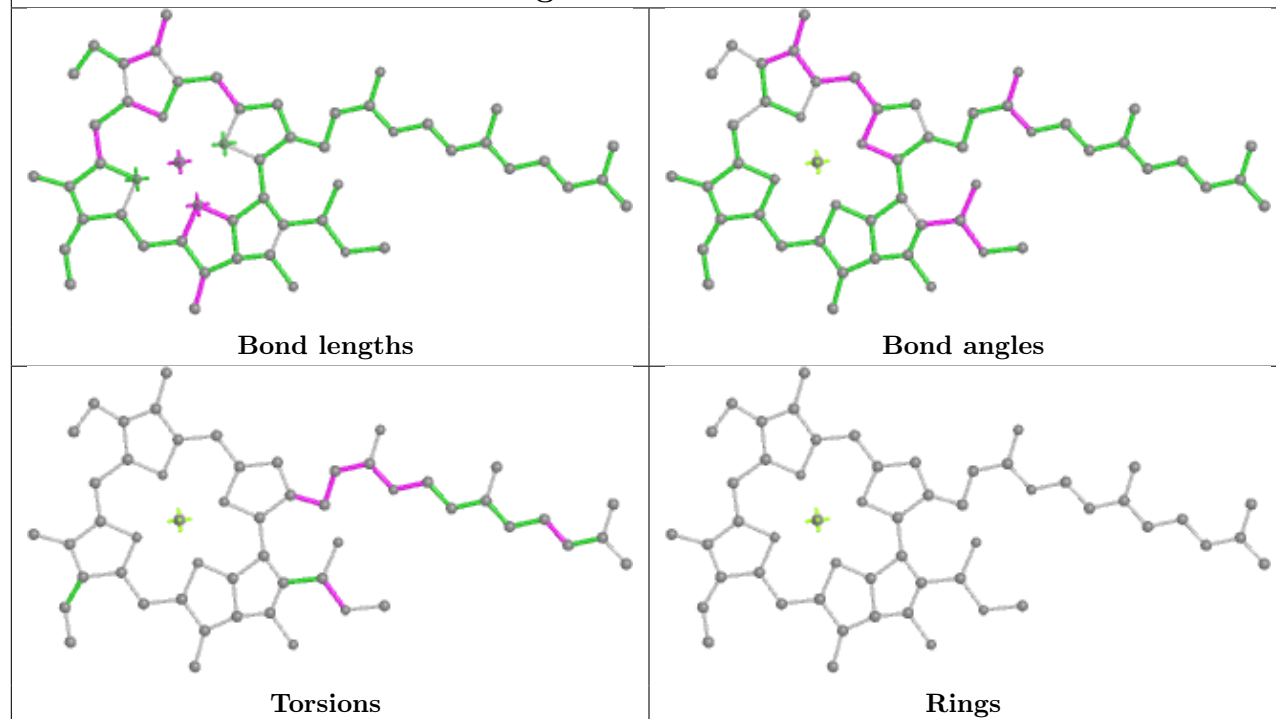




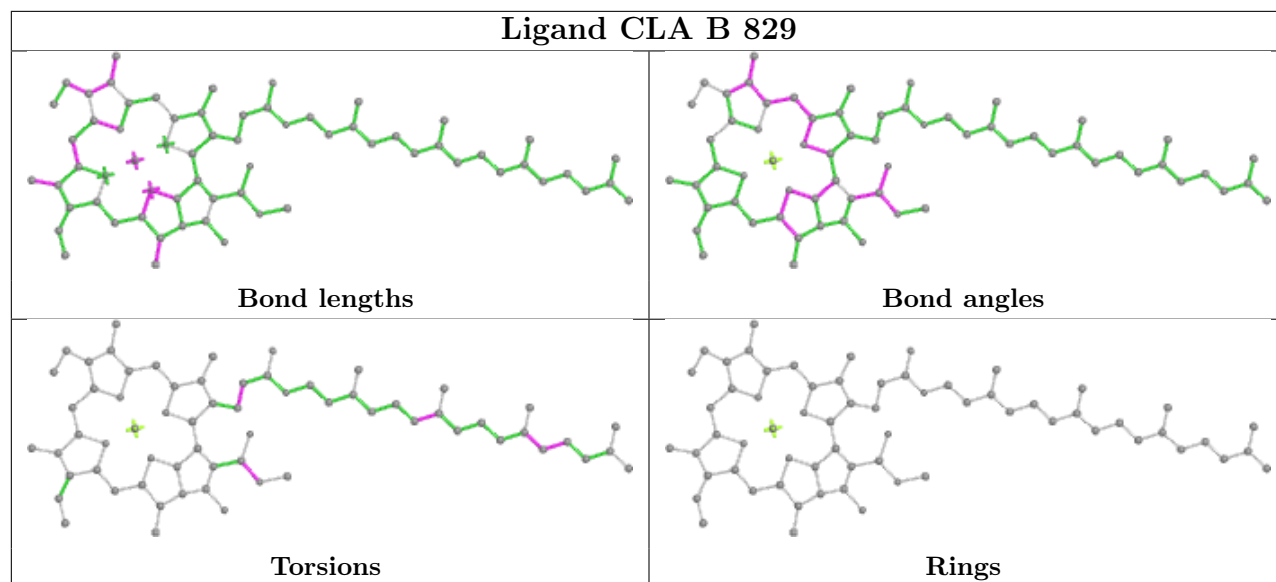
## Ligand CLA 6 608



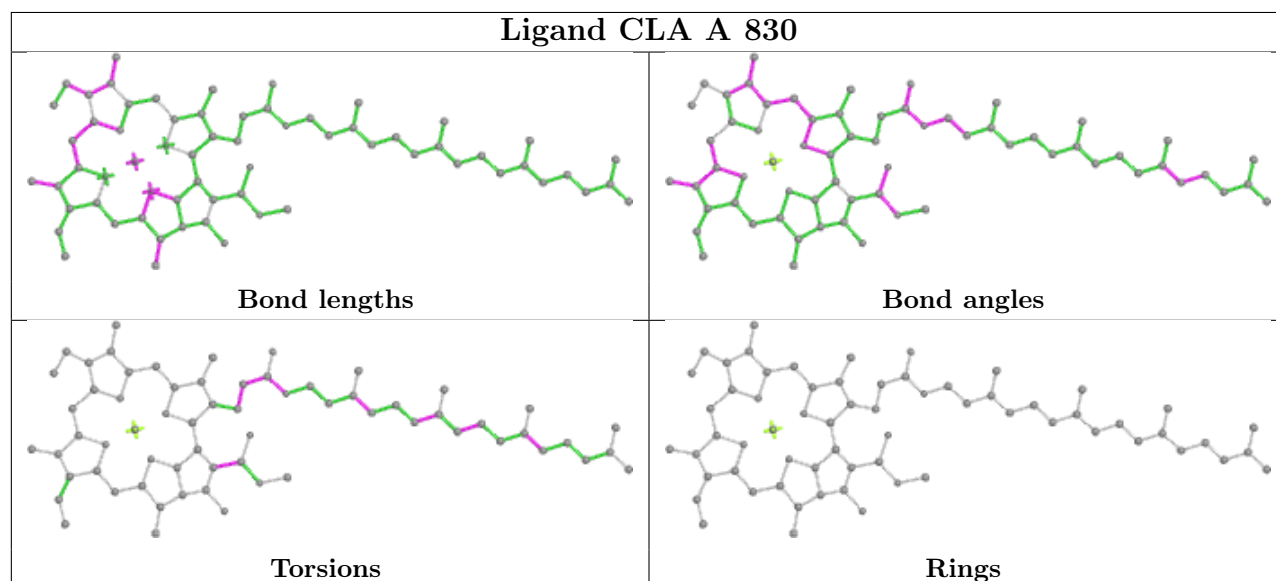
## Ligand CLA a 614



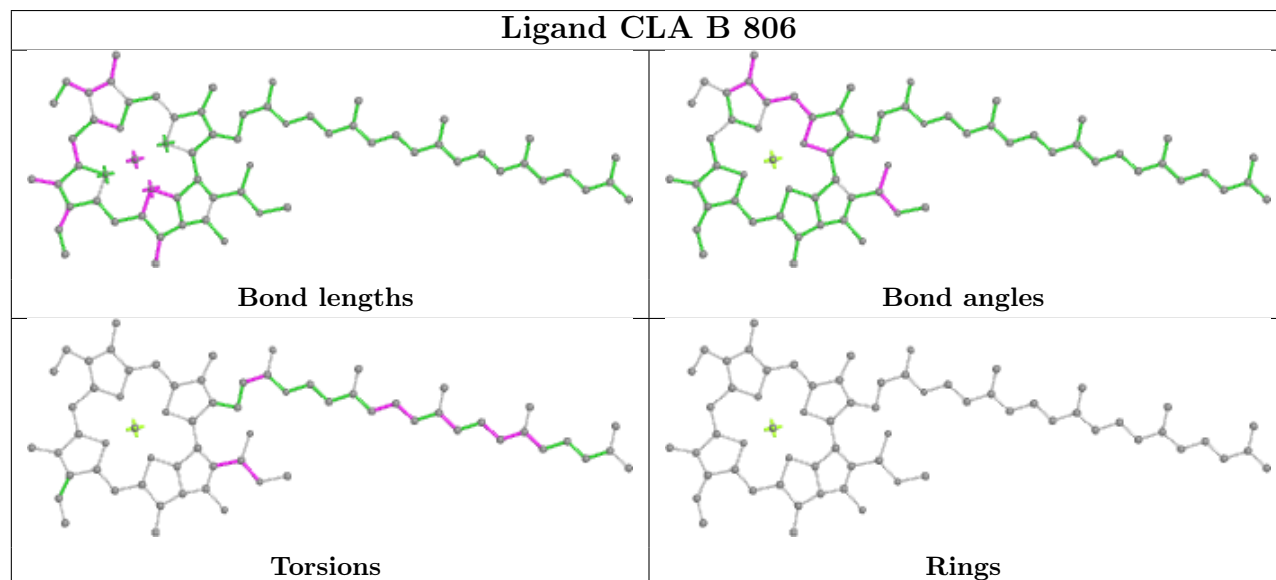
## Ligand CLA B 829

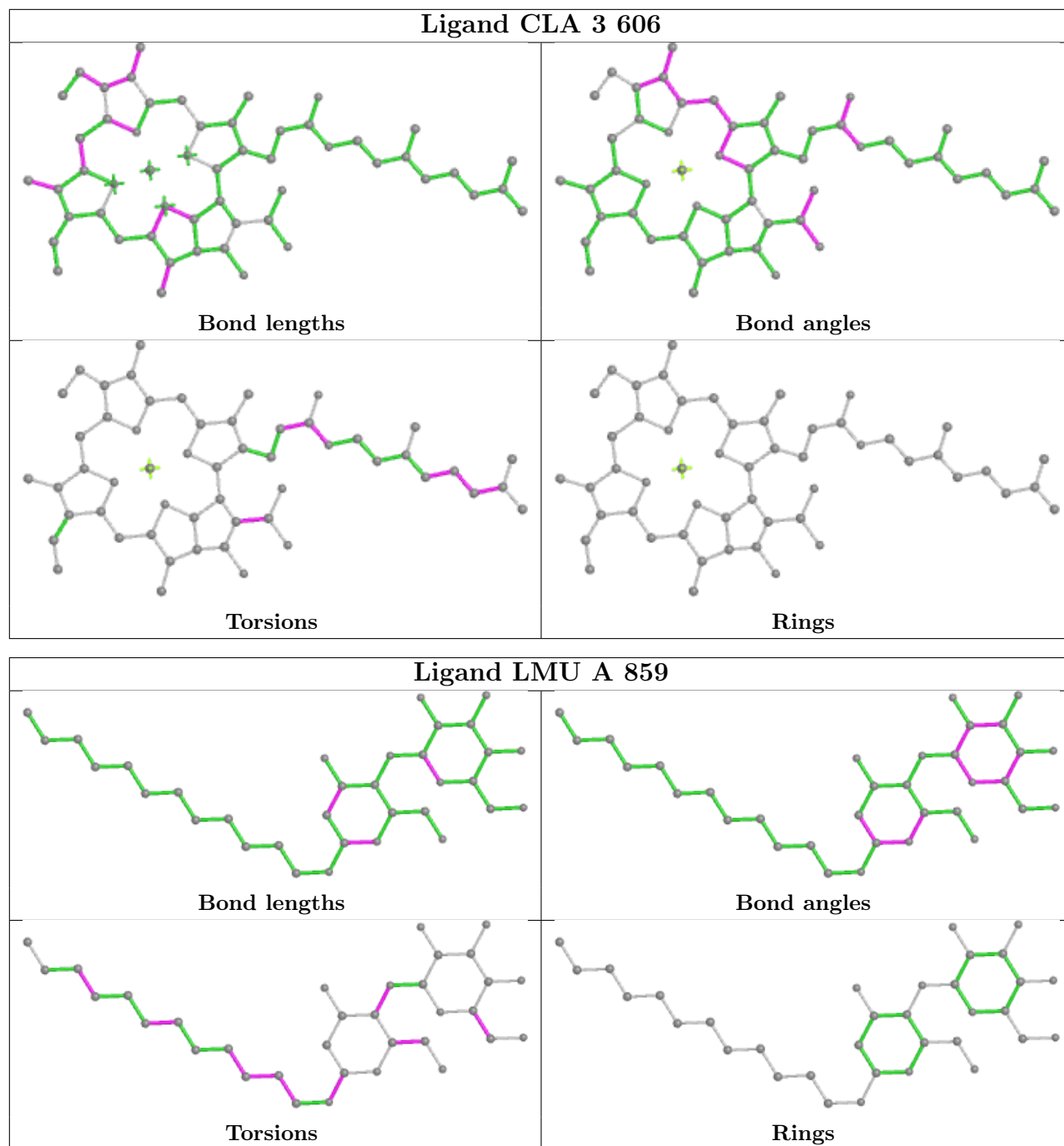


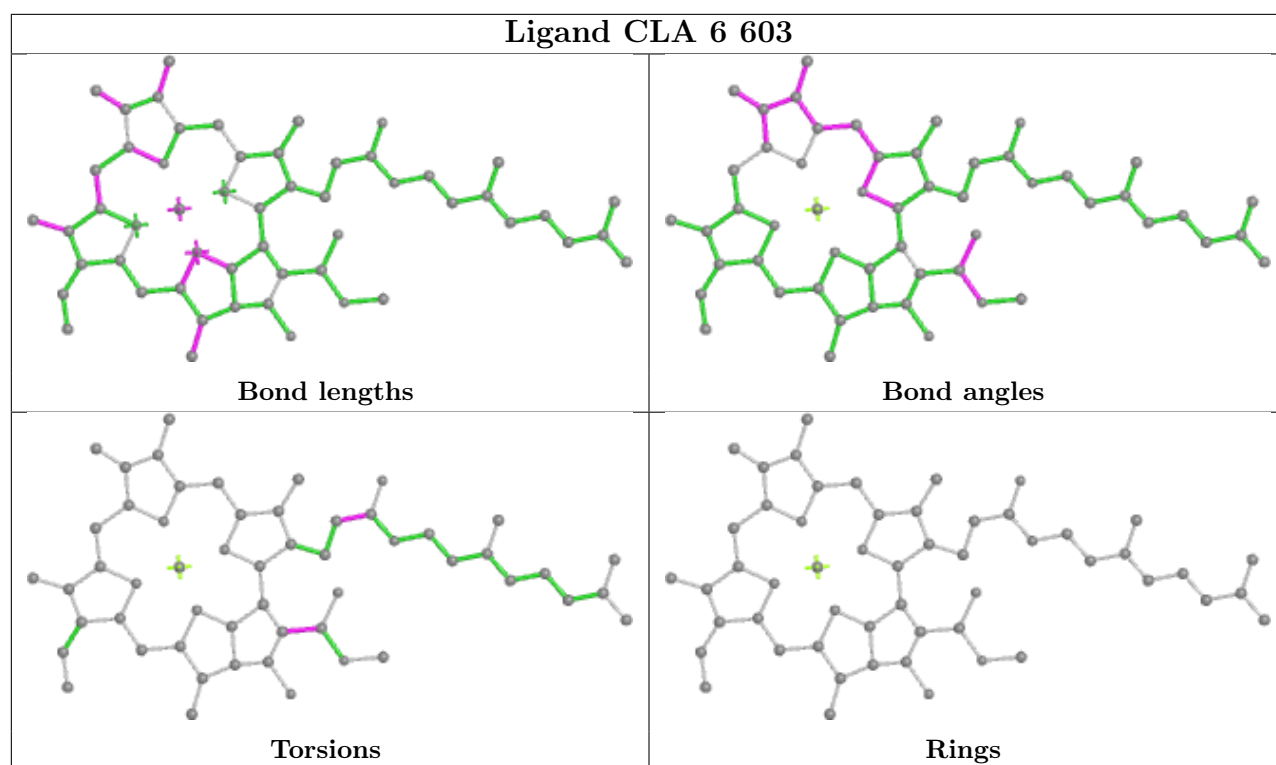
## Ligand CLA A 830



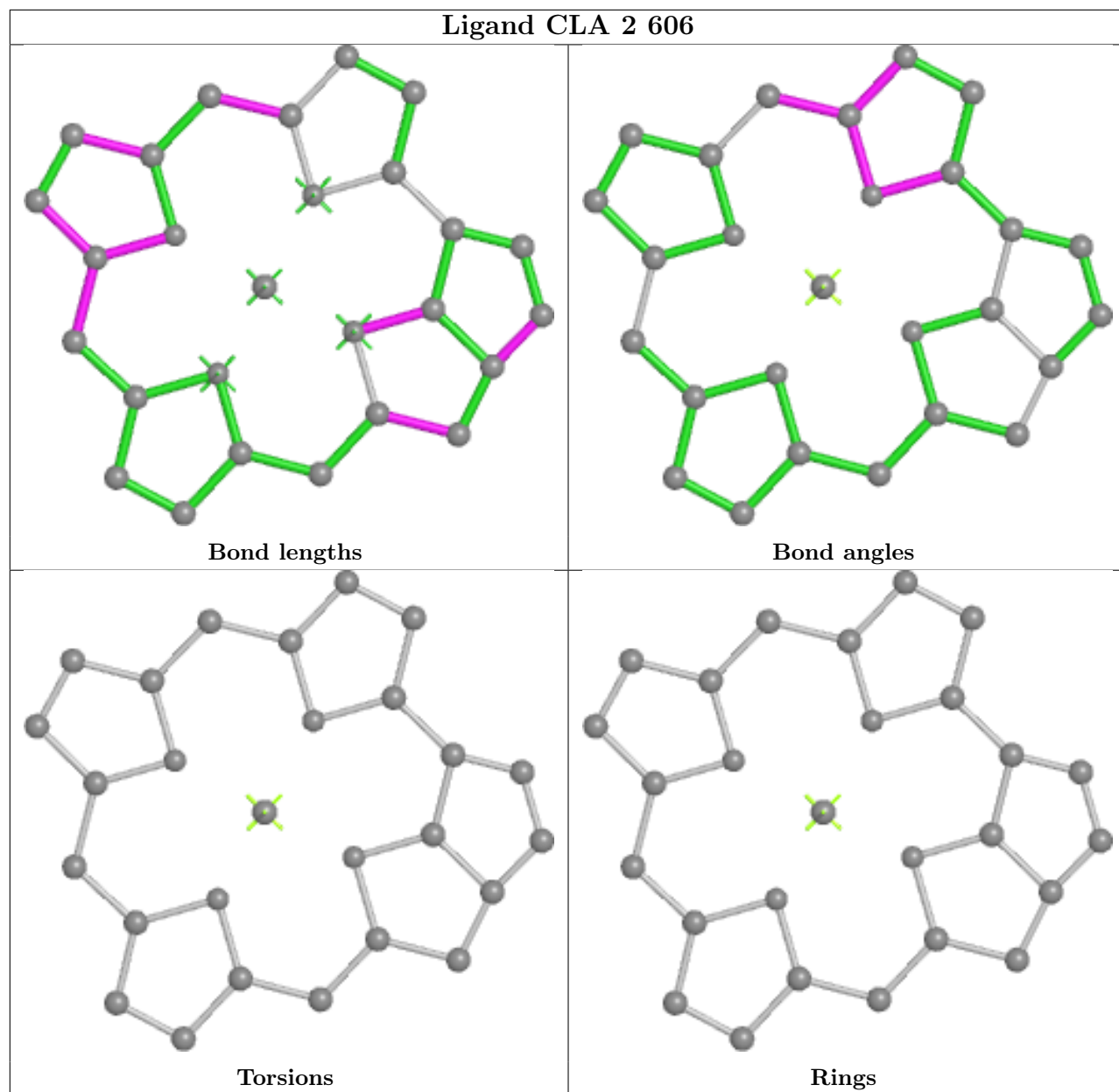
## Ligand CLA B 806



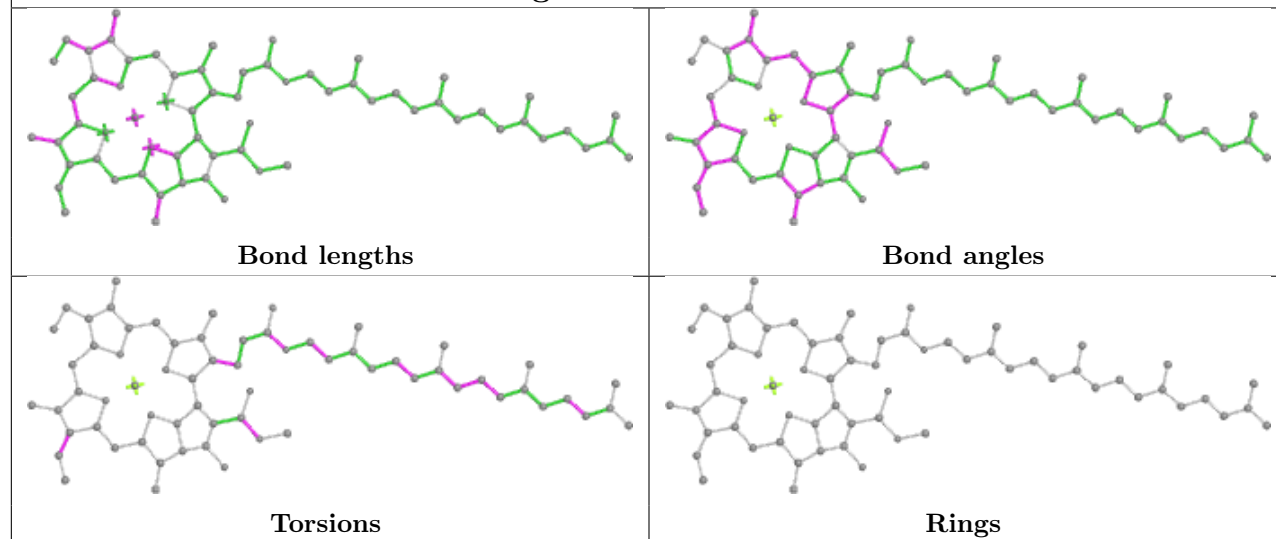




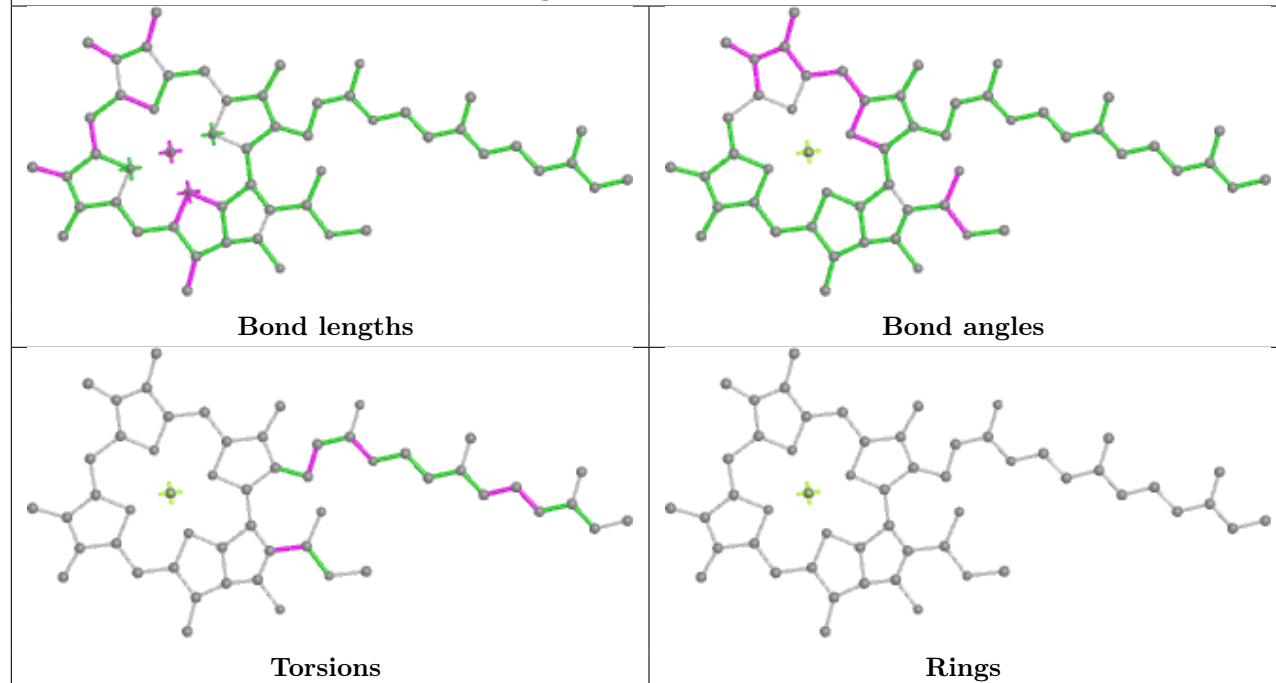
## Ligand CLA 2 606



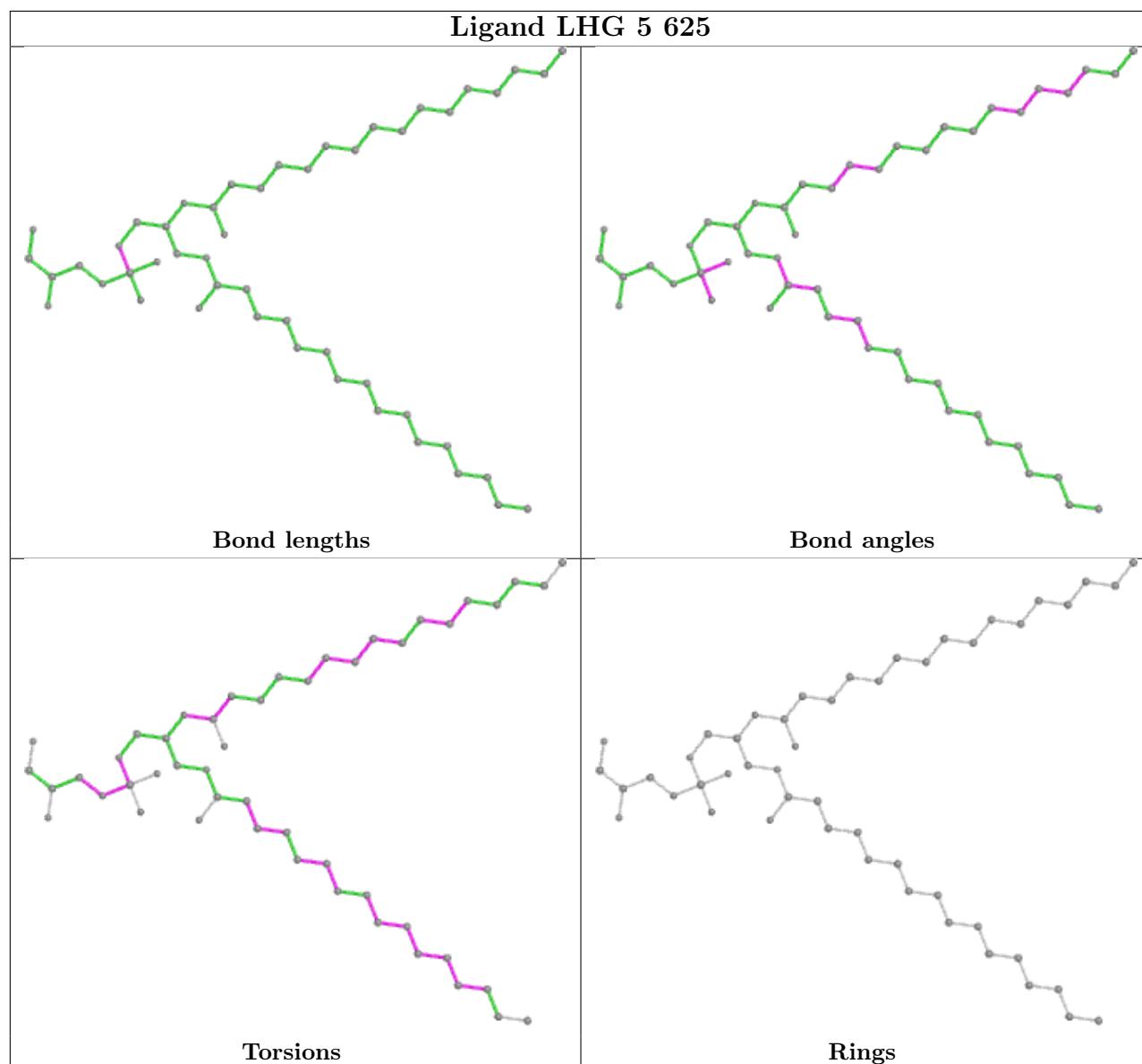
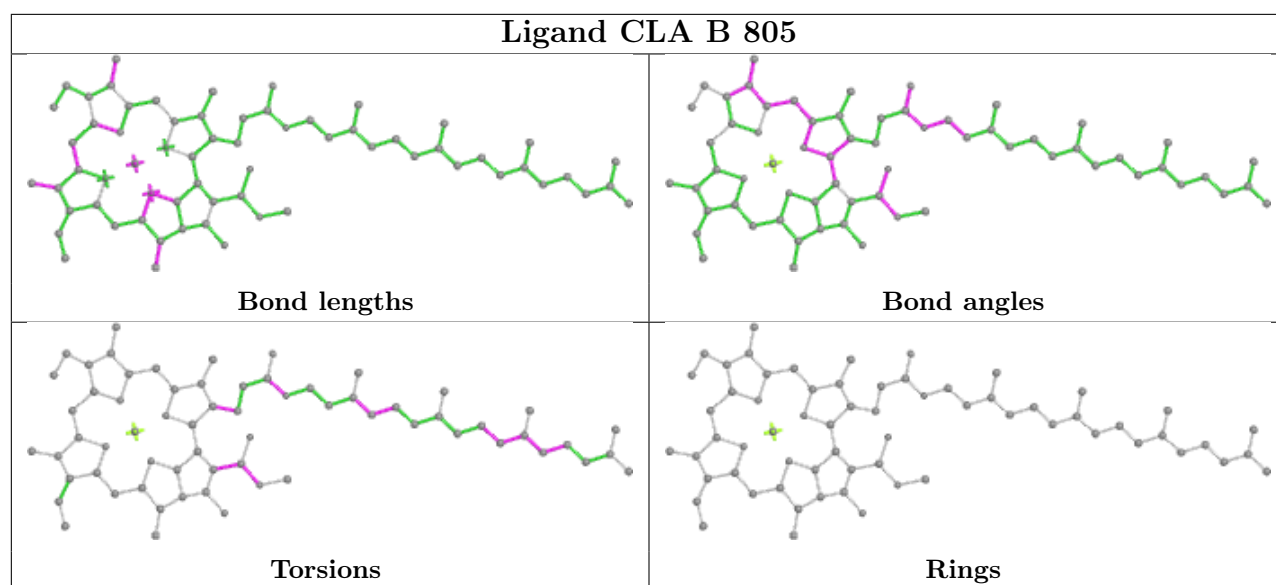
## Ligand CLA B 803

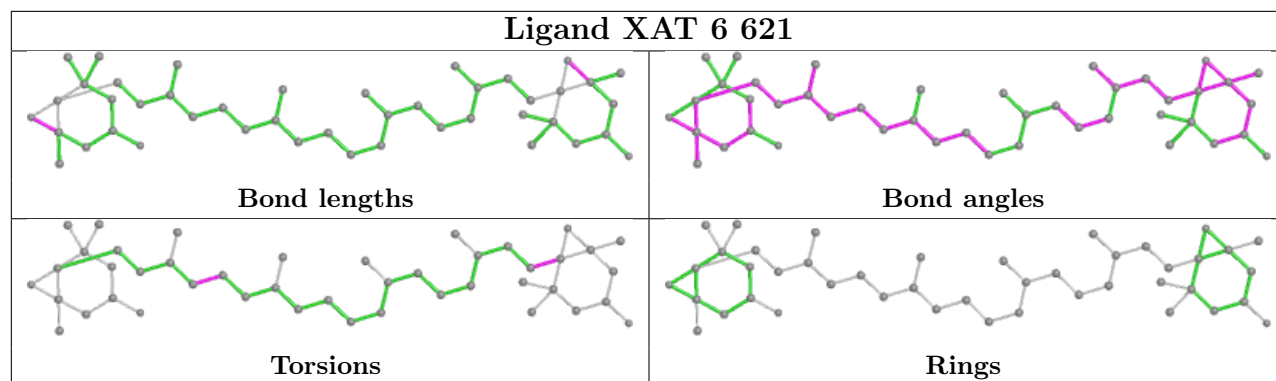
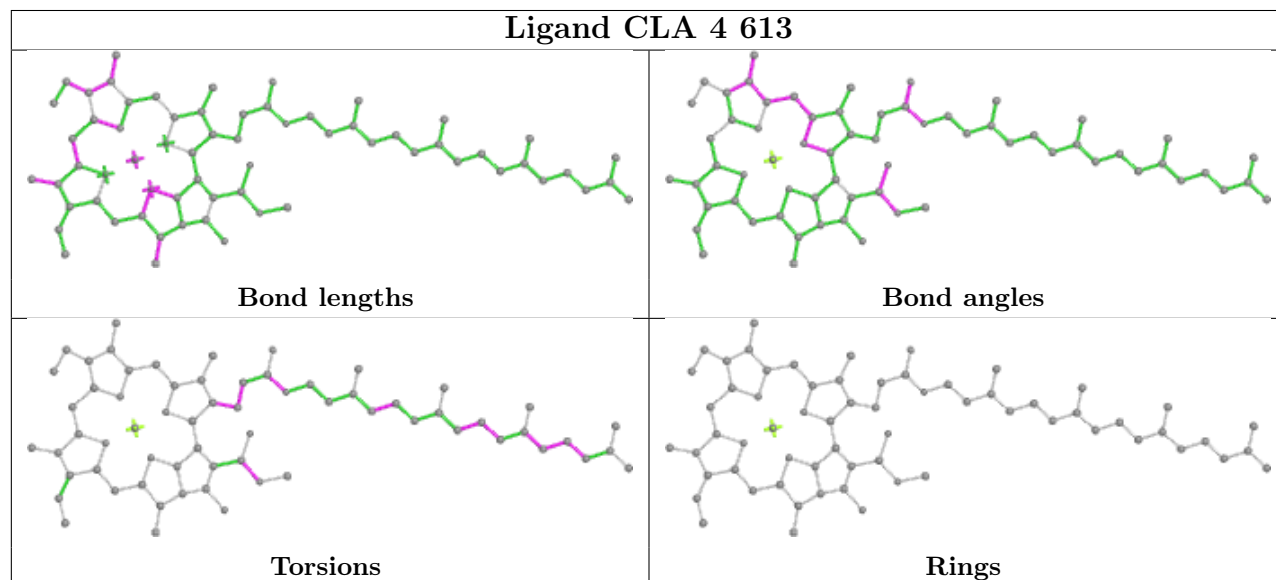
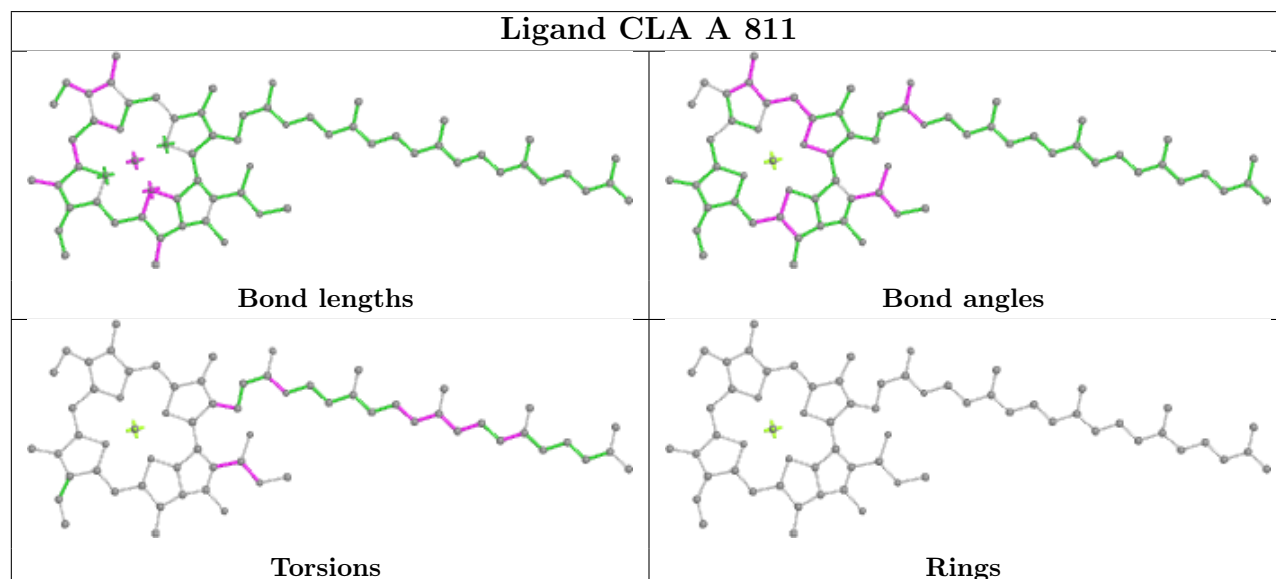


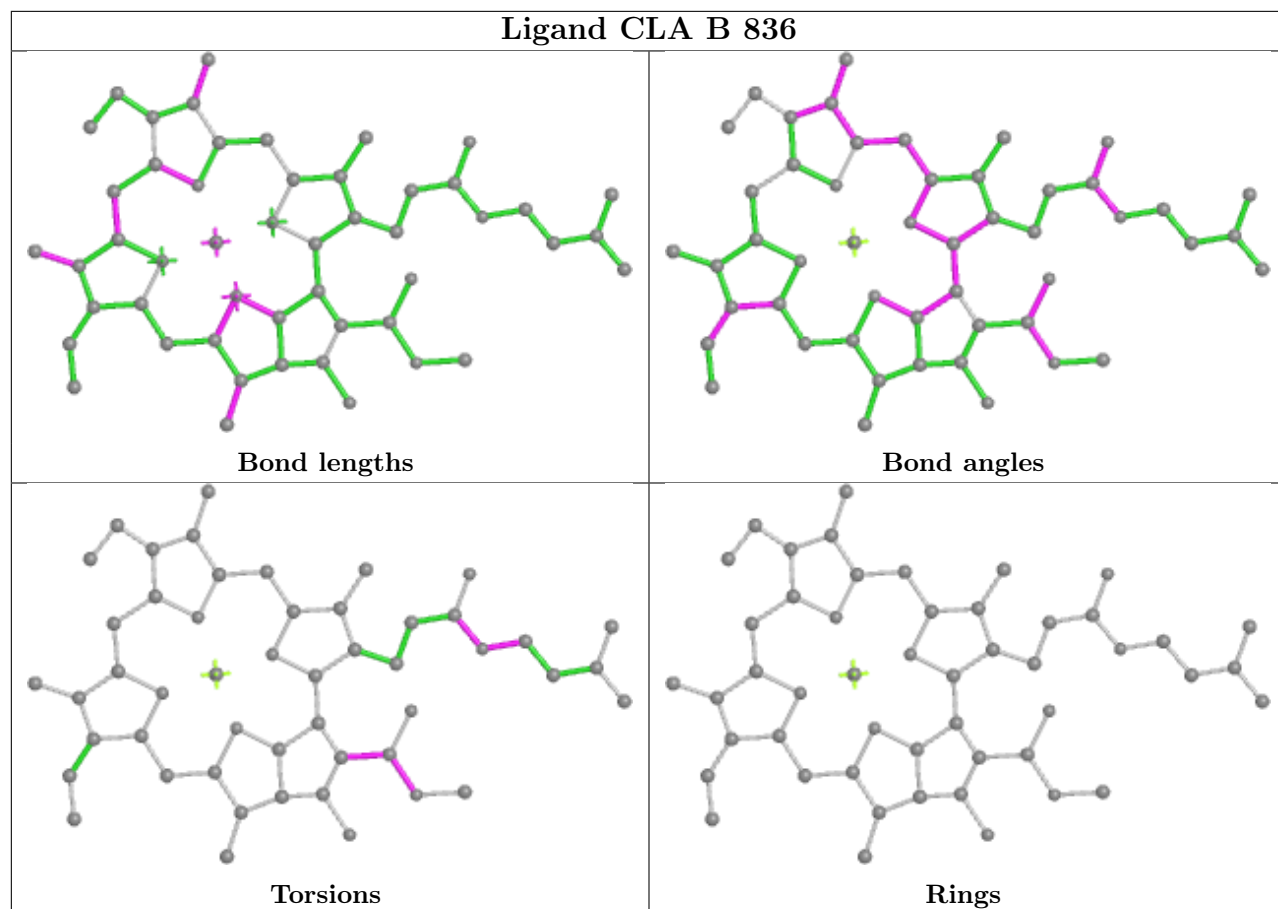
## Ligand CLA 4 604



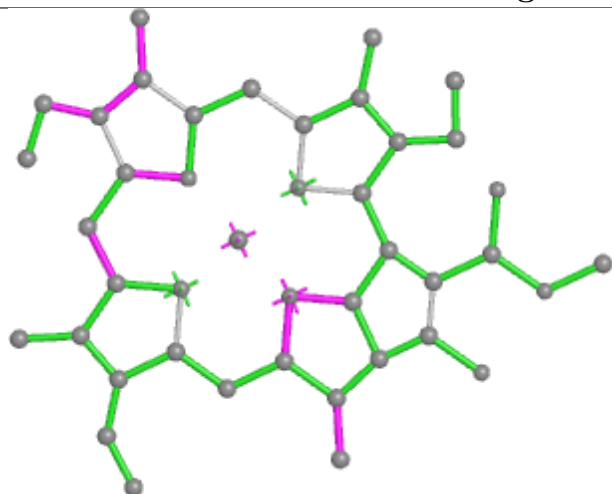




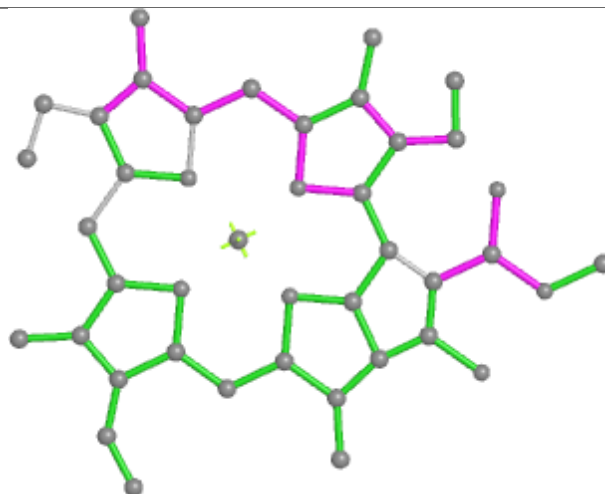
**Ligand XAT 6 621****Ligand CLA 4 613****Ligand CLA A 811**



## Ligand CLA 5 611



Bond lengths



Bond angles

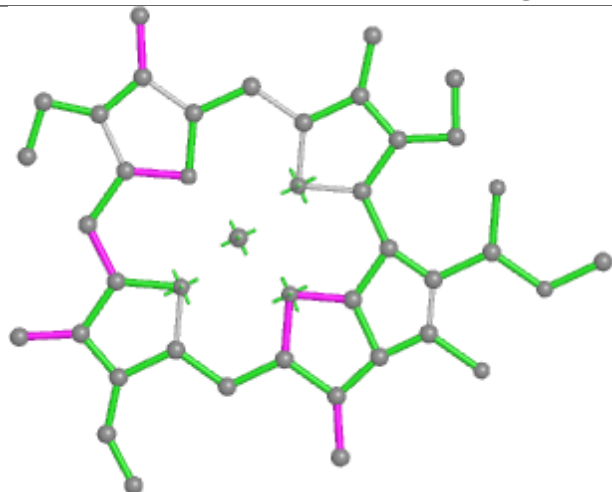


Torsions

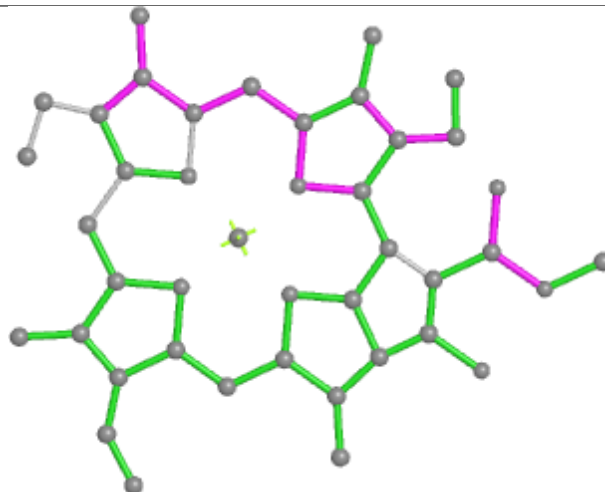


Rings

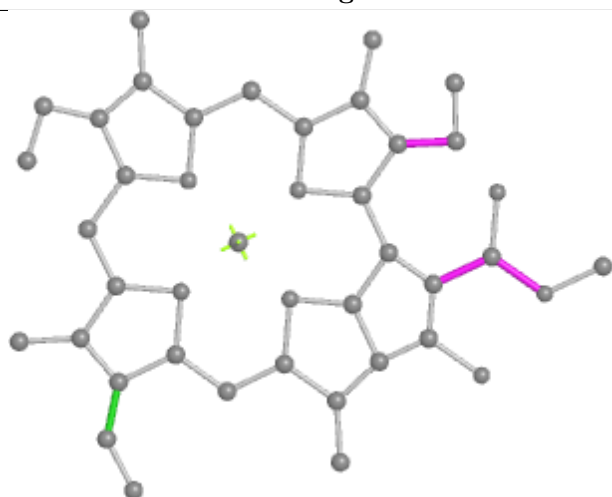
## Ligand CLA 4 611



Bond lengths



Bond angles

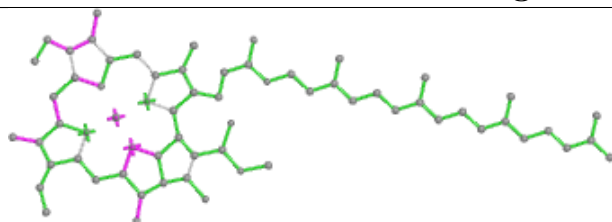


Torsions

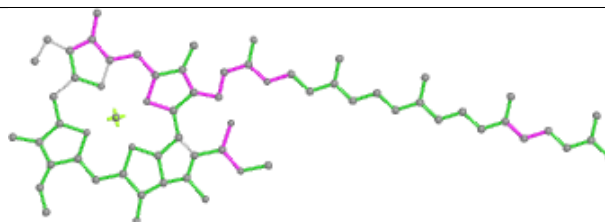


Rings

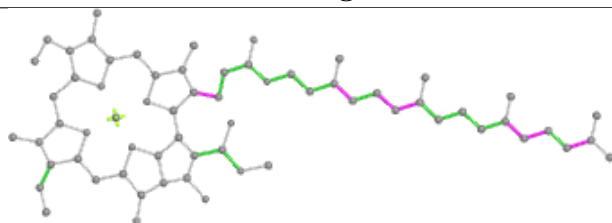
## Ligand CLA A 812



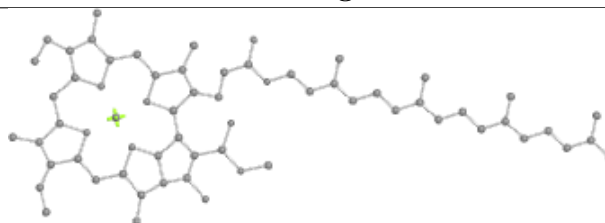
Bond lengths



Bond angles

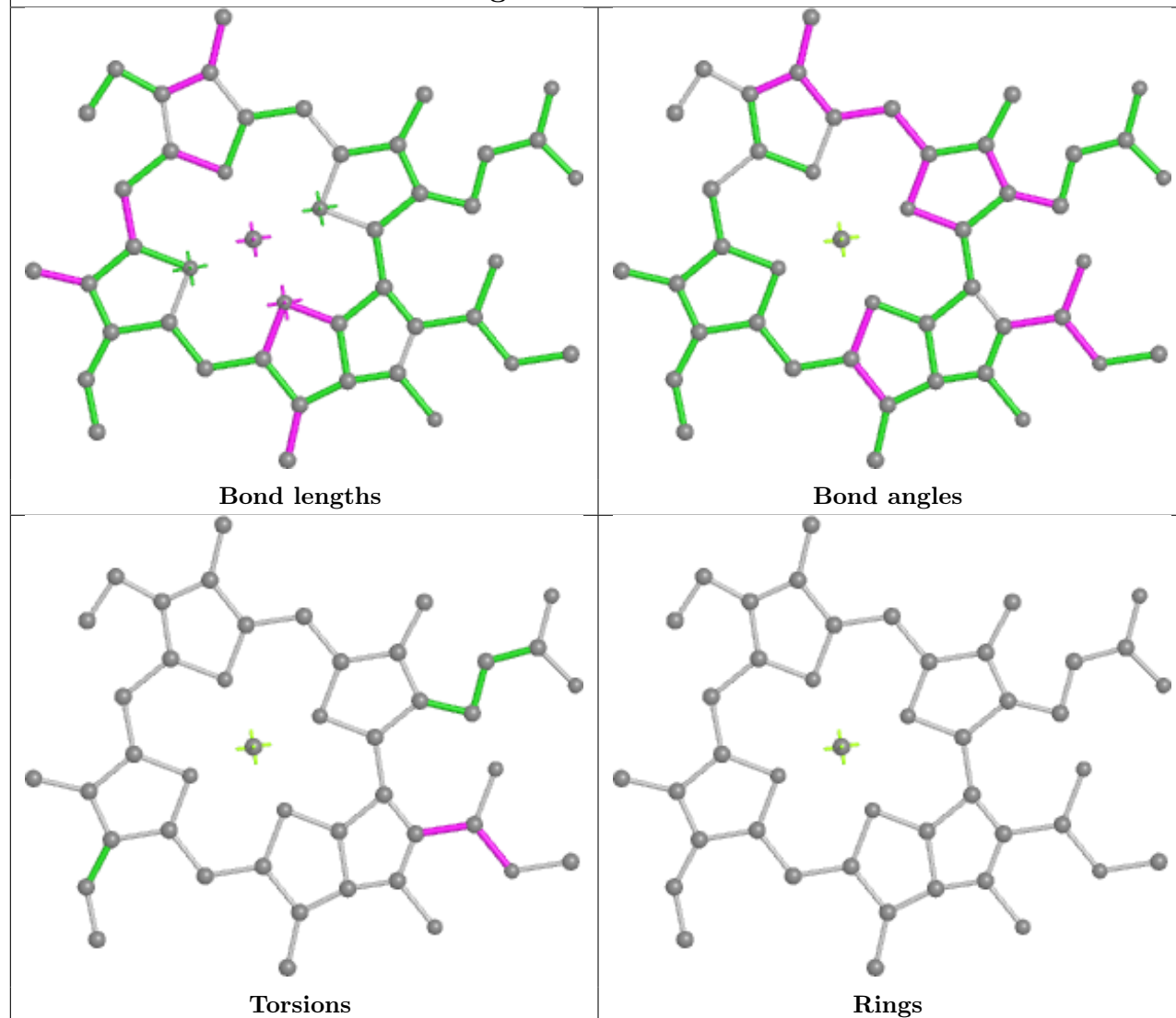


Torsions

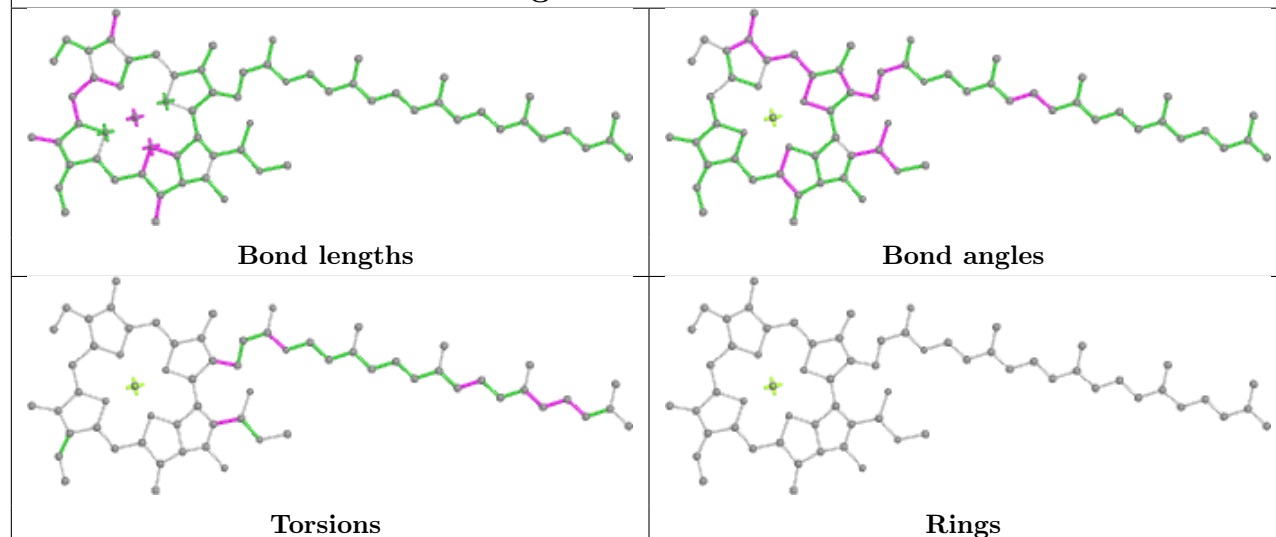


Rings

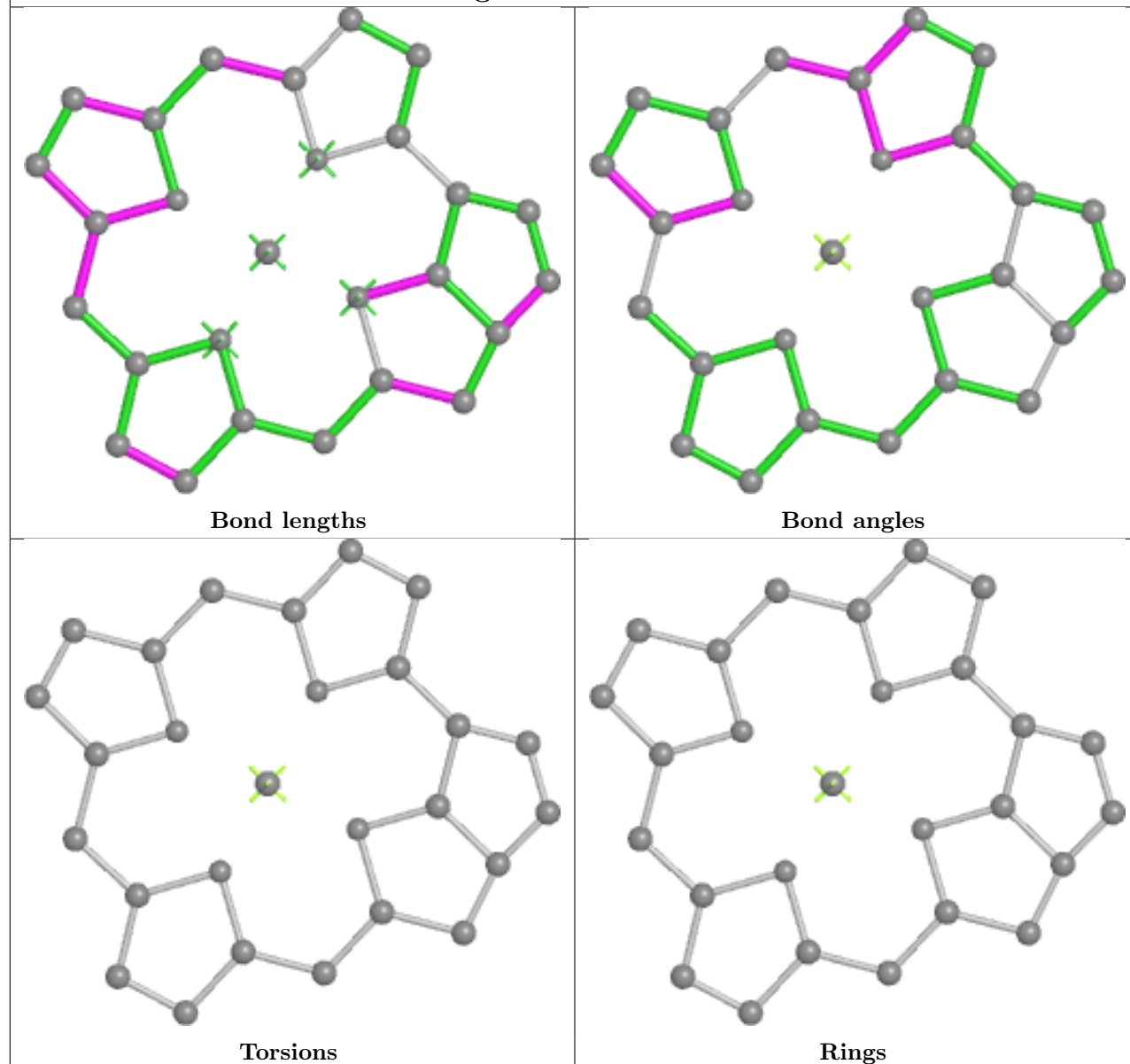
## Ligand CLA A 817



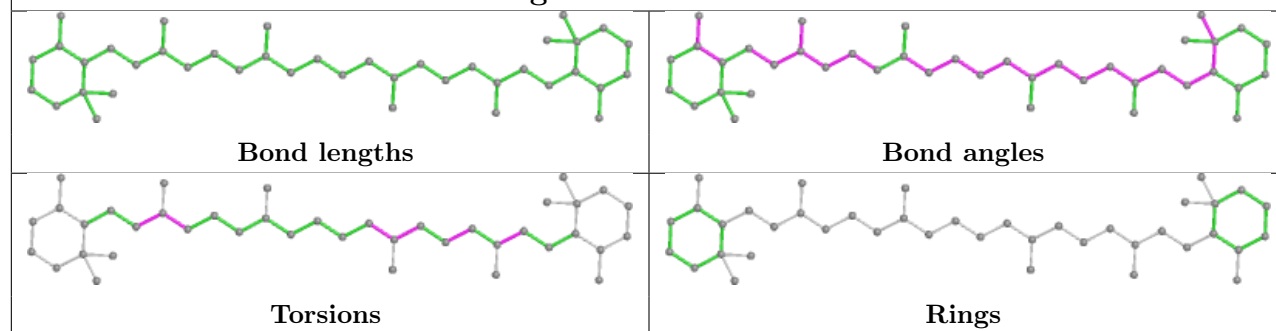
## Ligand CLA A 804



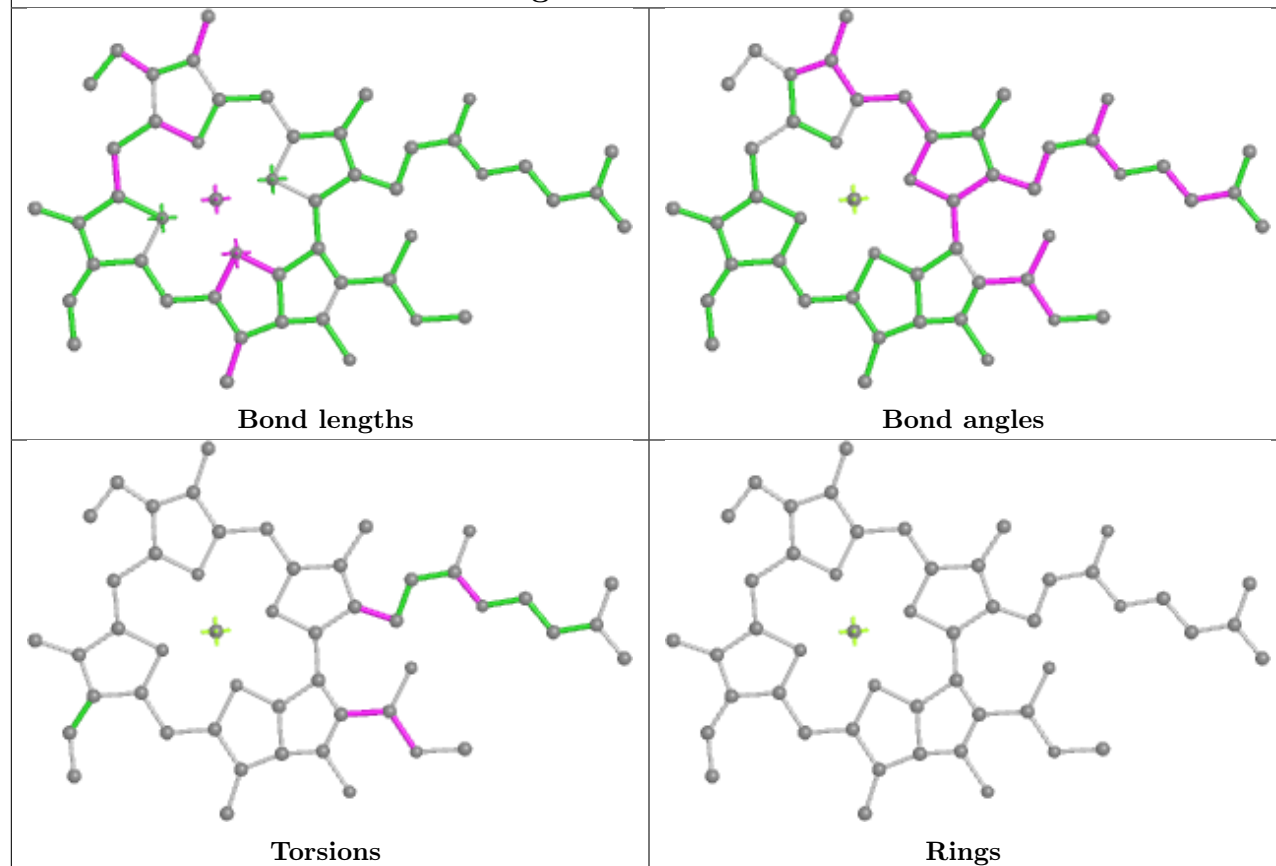
## Ligand CLA 9 601



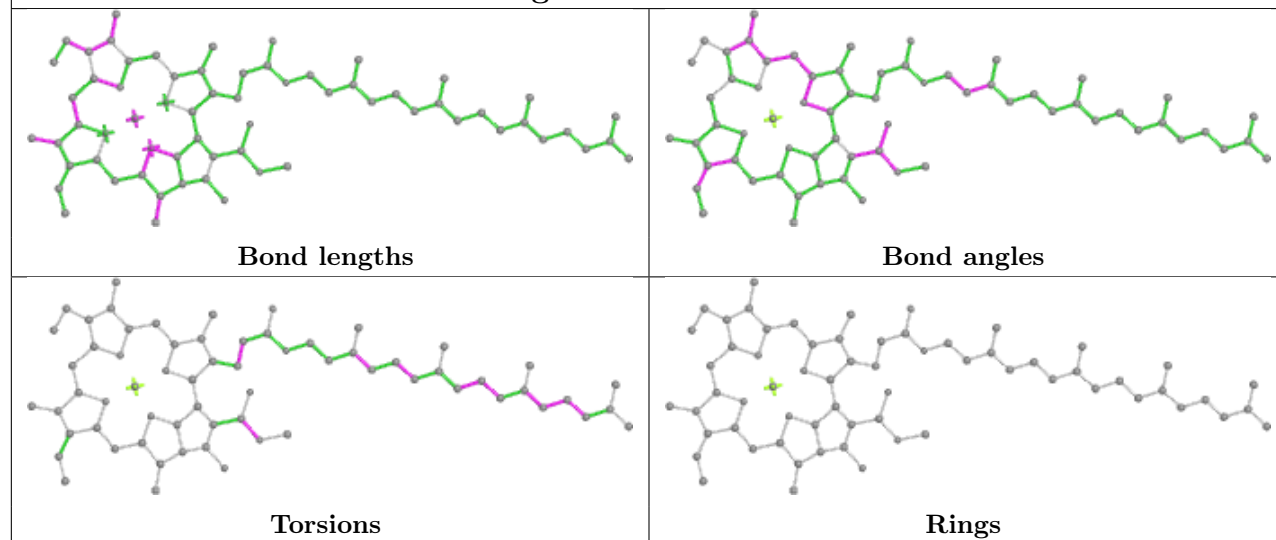
## Ligand BCR A 852



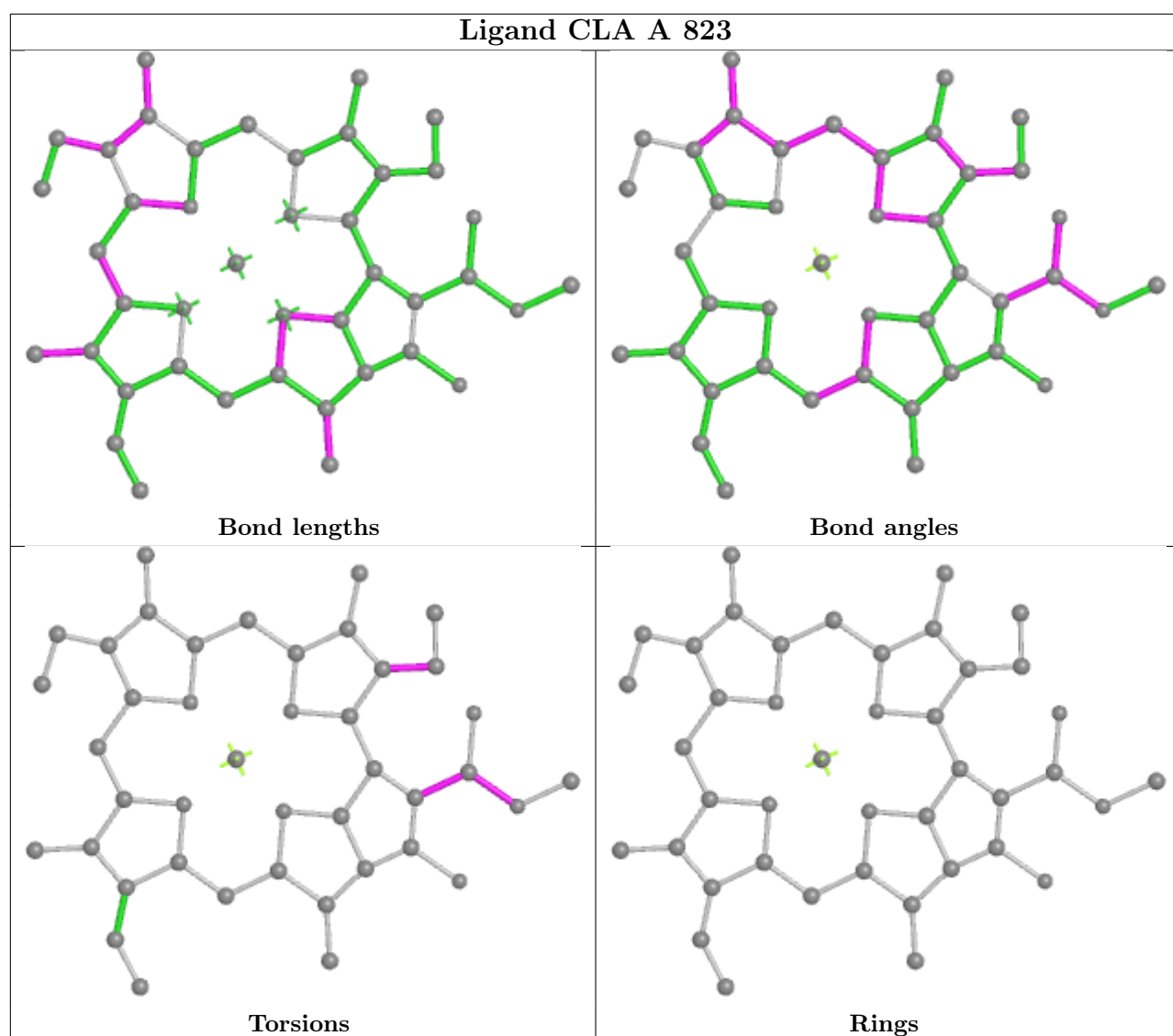
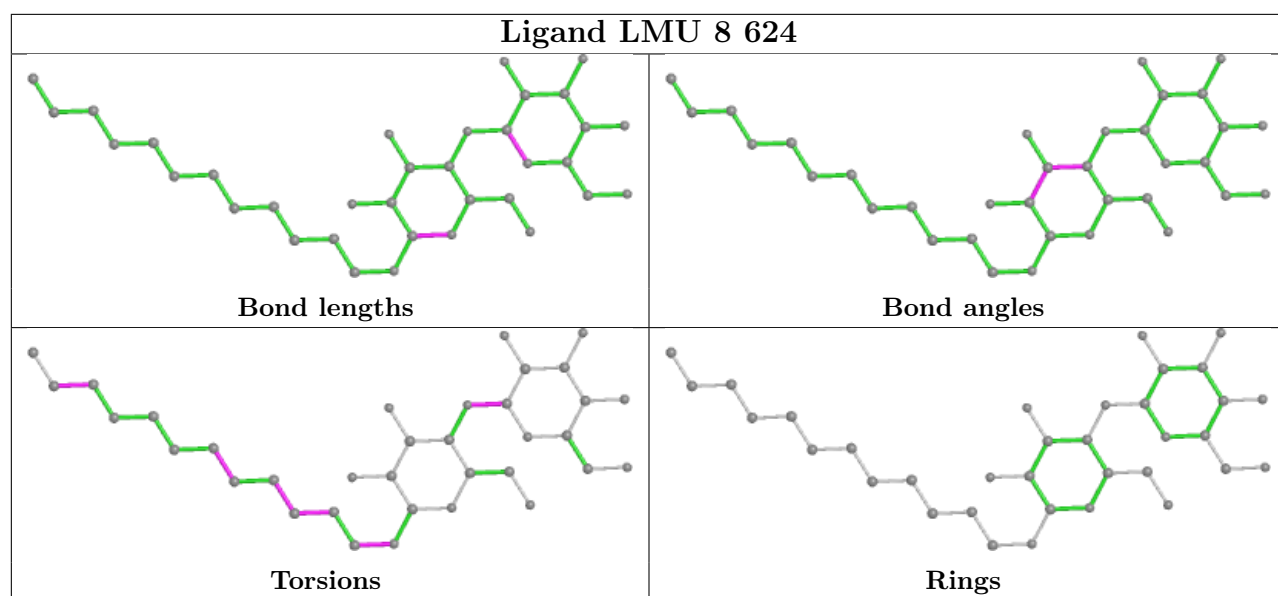
## Ligand CLA A 838



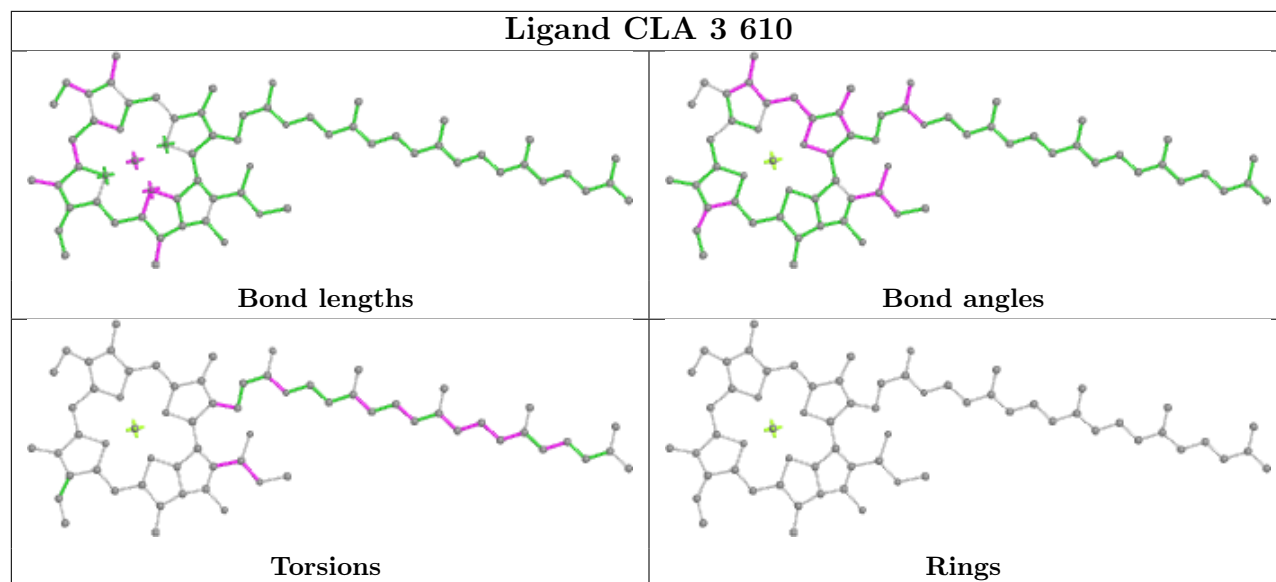
## Ligand CLA A 829



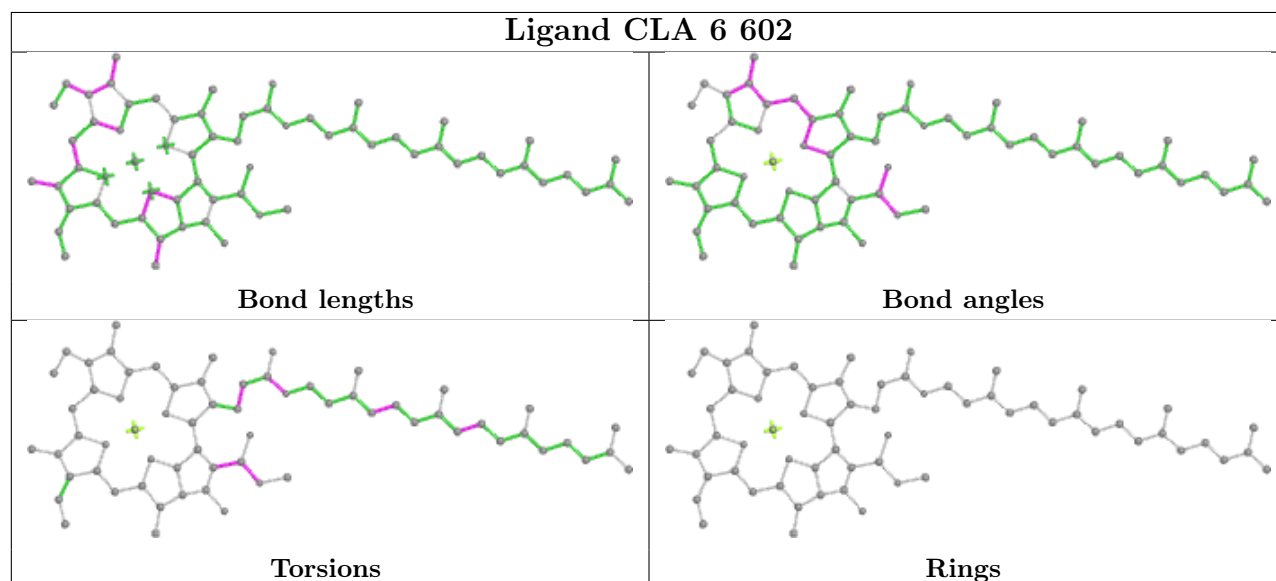




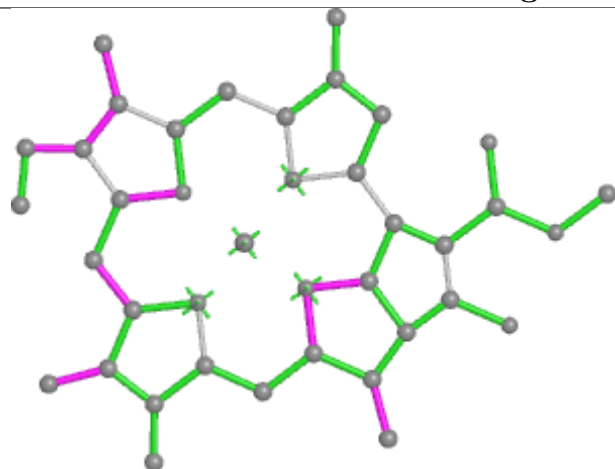
## Ligand CLA 3 610



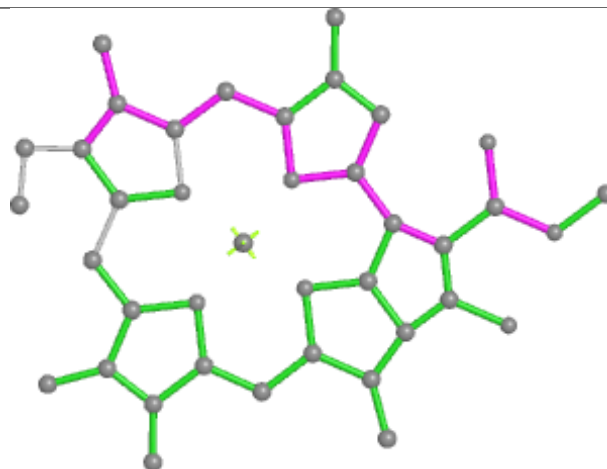
## Ligand CLA 6 602



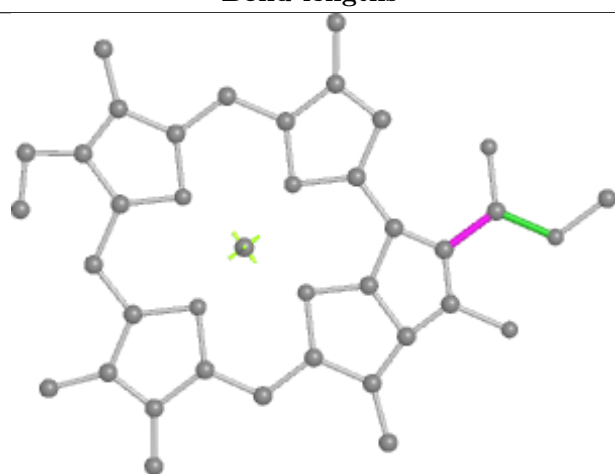
## Ligand CLA 1 610



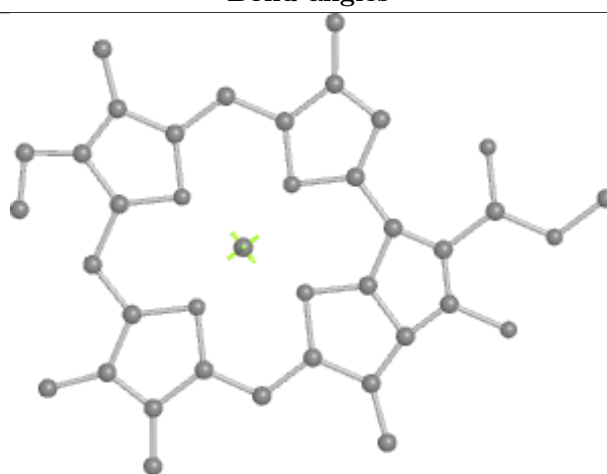
Bond lengths



Bond angles

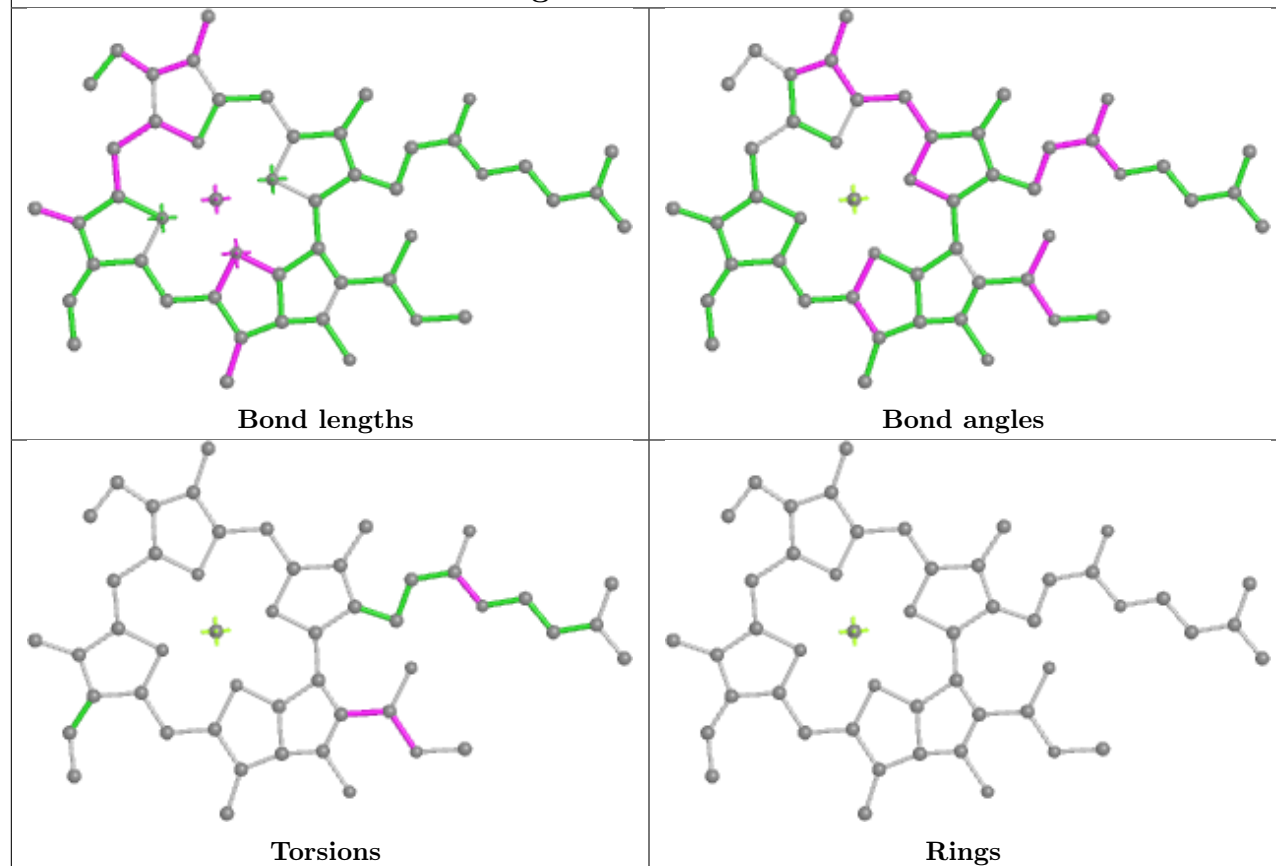


Torsions

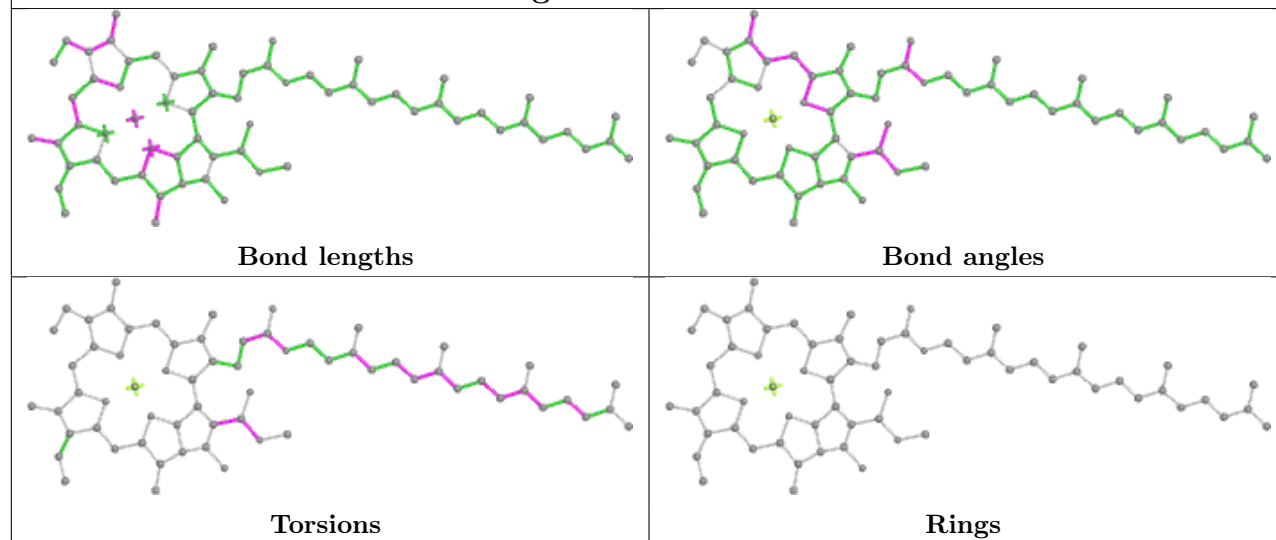


Rings

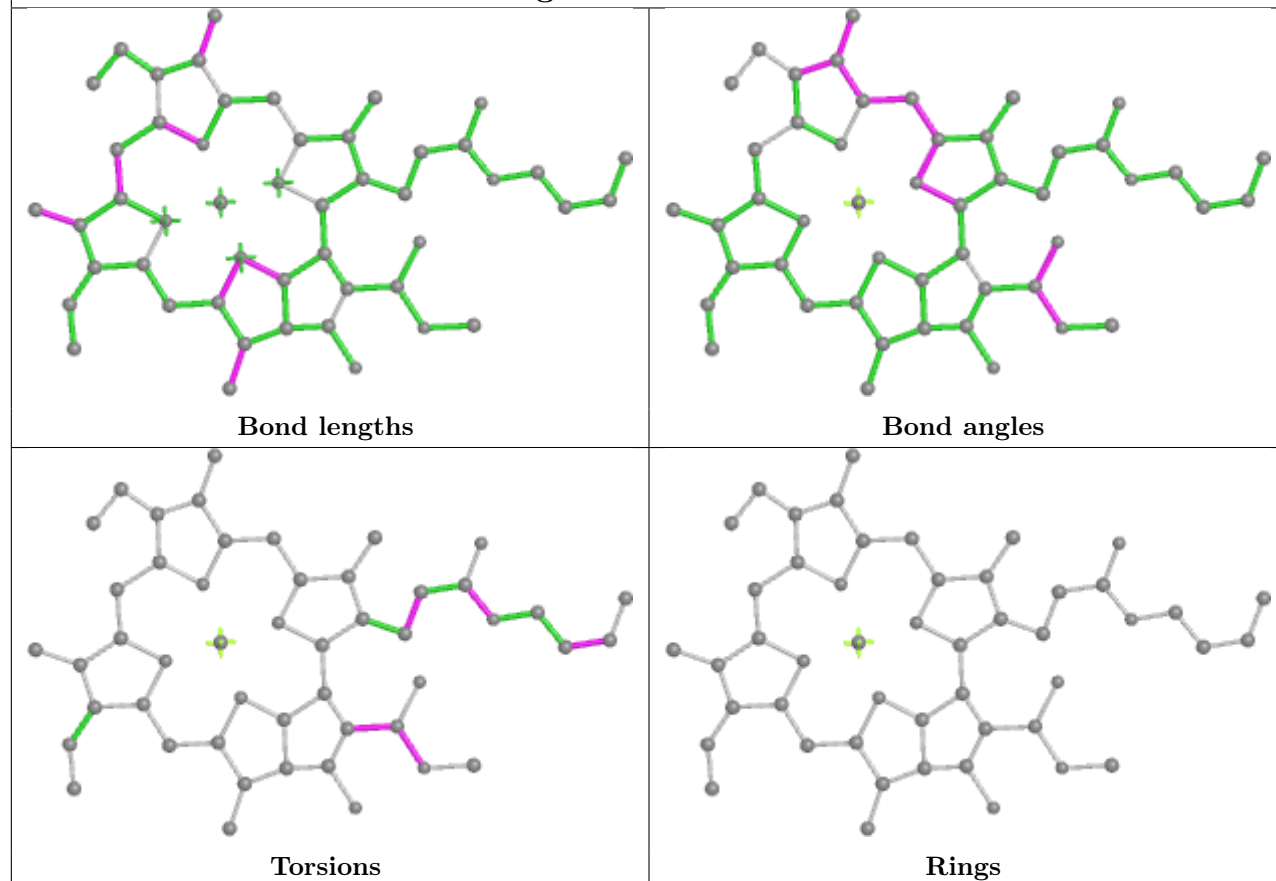
## Ligand CLA A 832



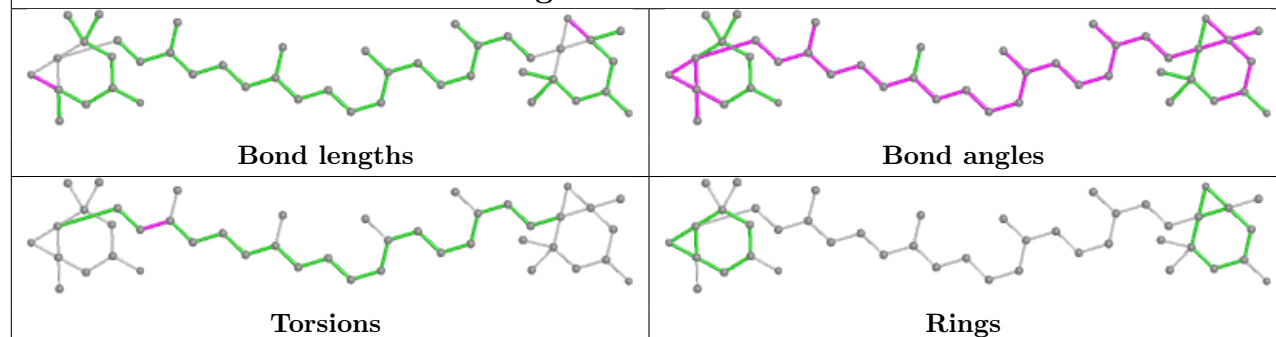
## Ligand CLA B 802



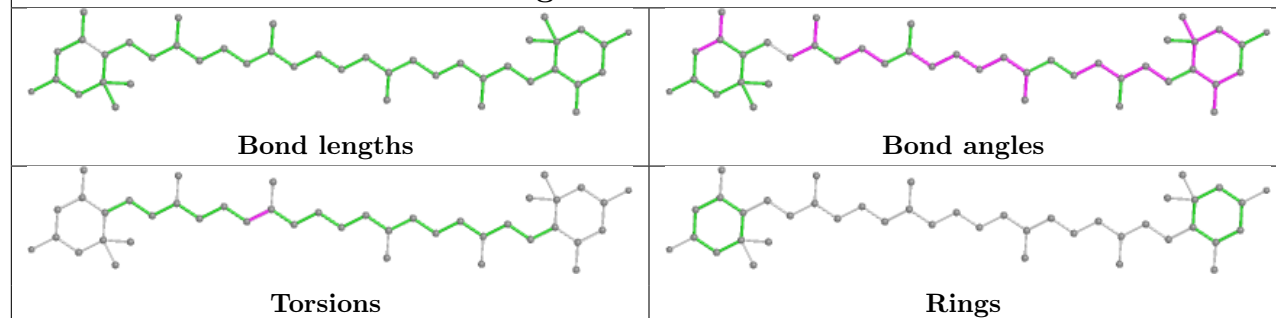
## Ligand CLA 1 604



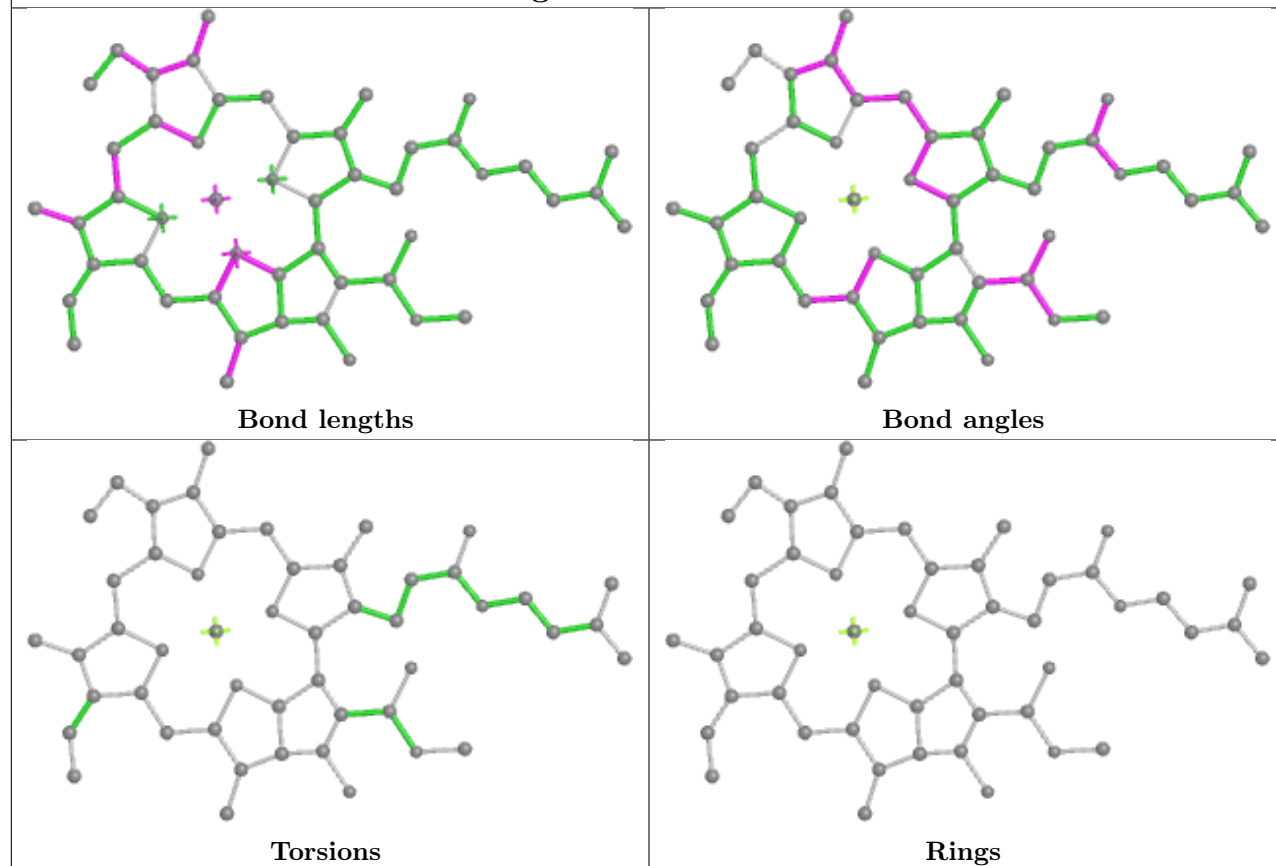
## Ligand XAT 5 621



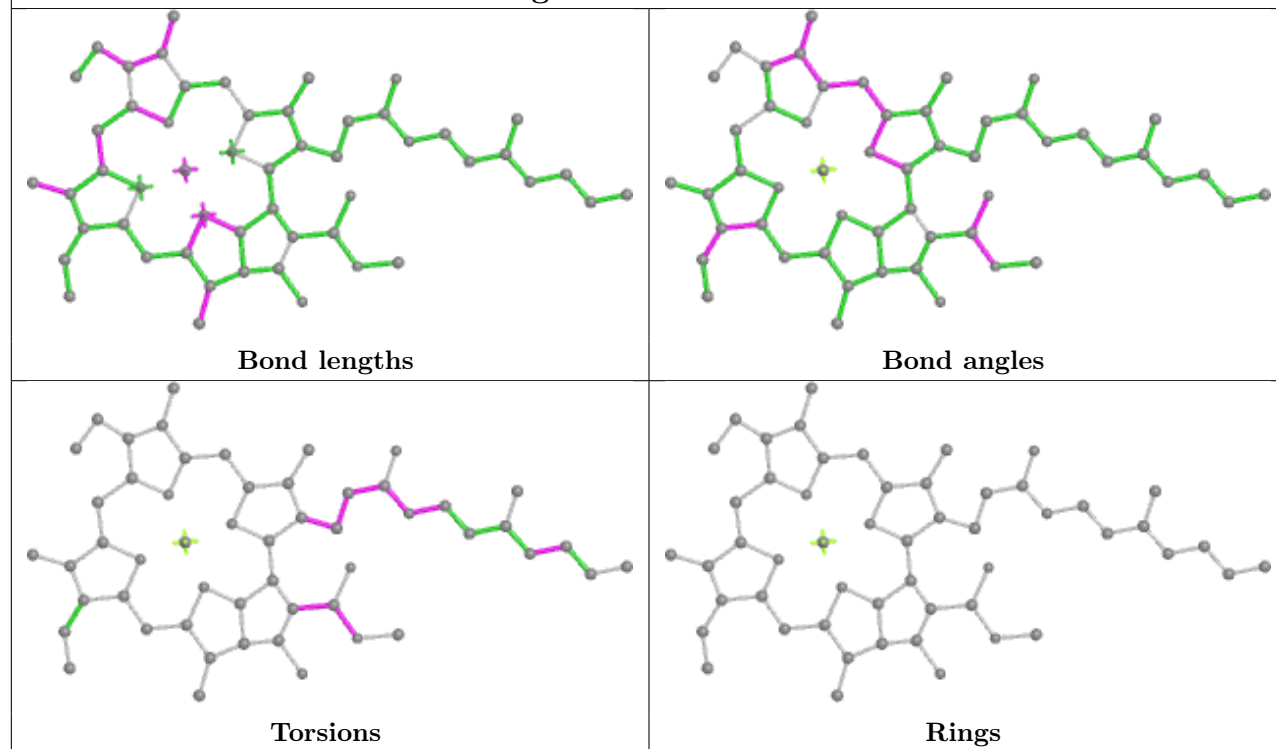
## Ligand LUT 2 619



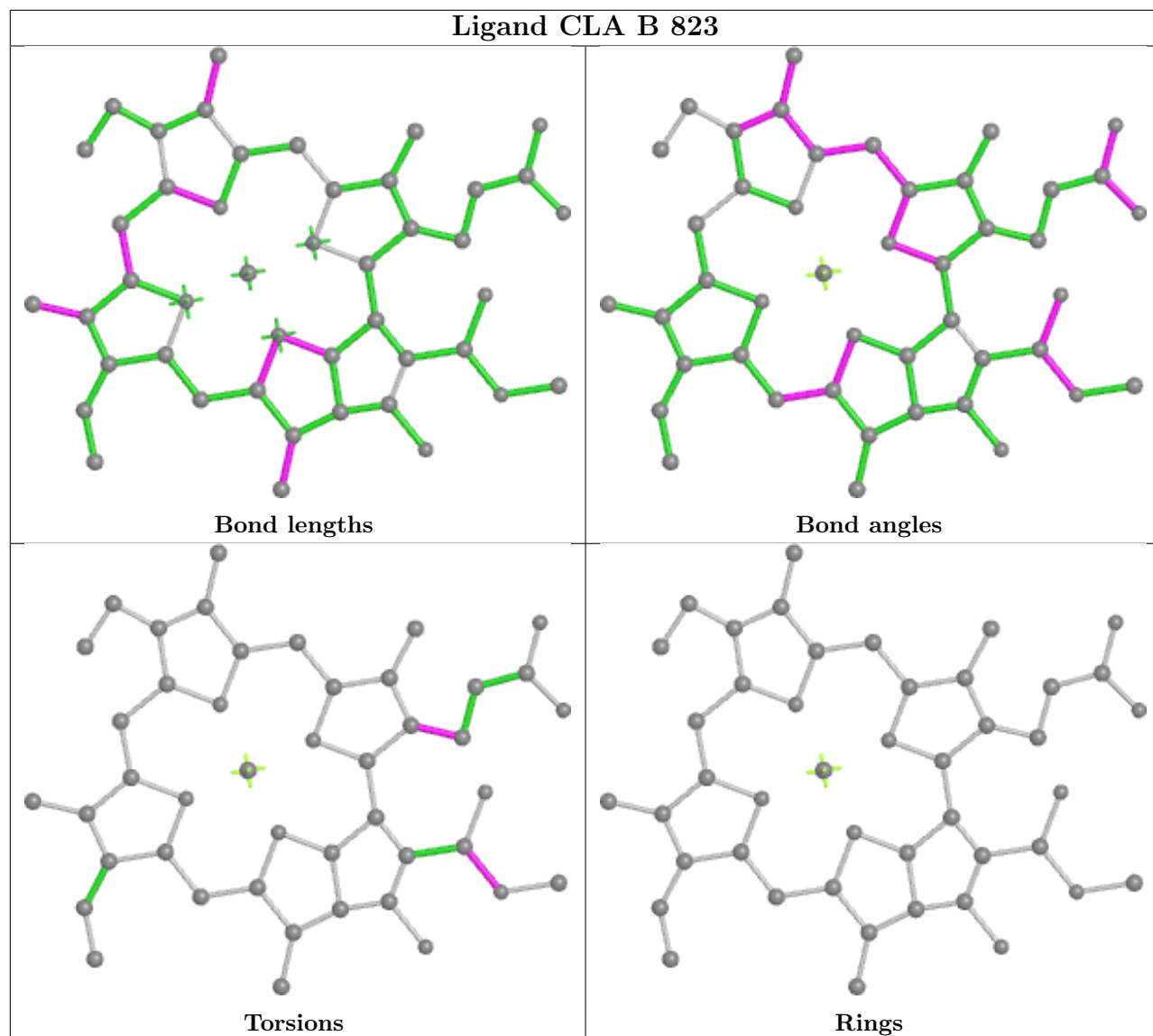
## Ligand CLA A 808



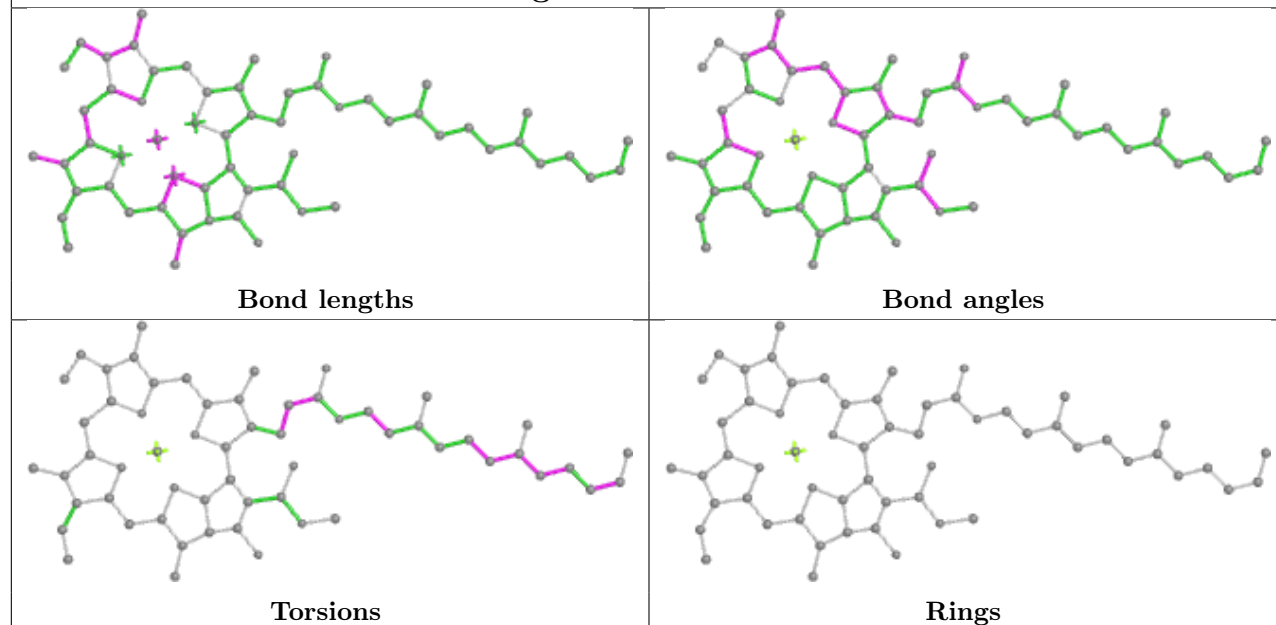
## Ligand CLA A 821



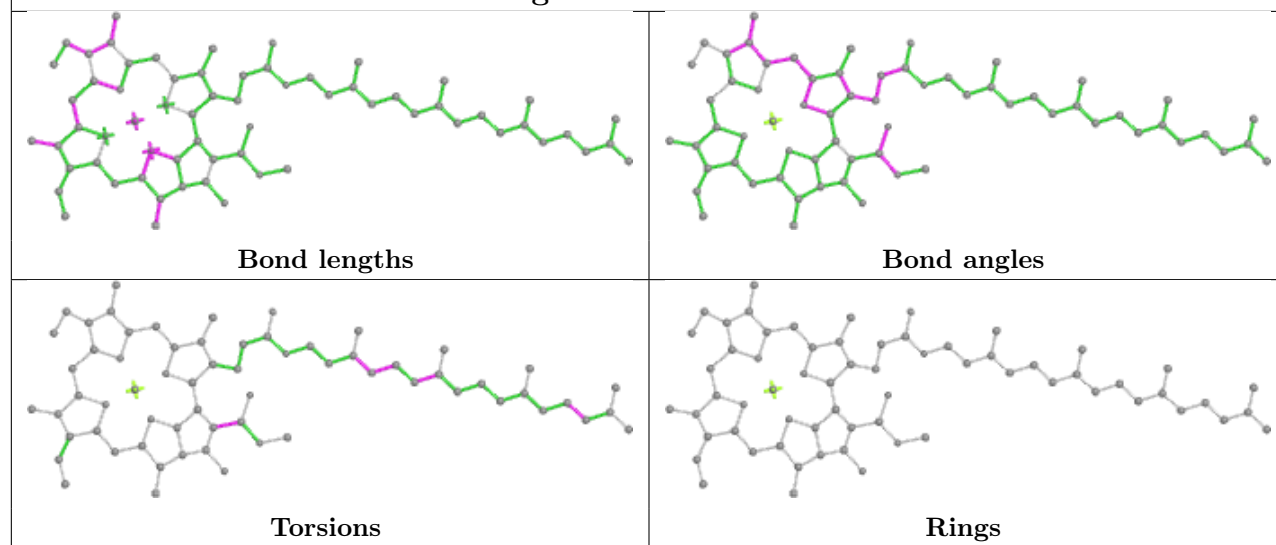
## Ligand CLA B 823



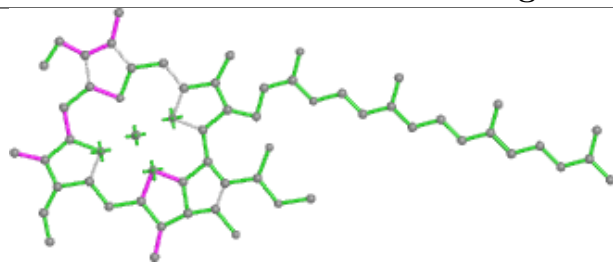
## Ligand CLA B 817



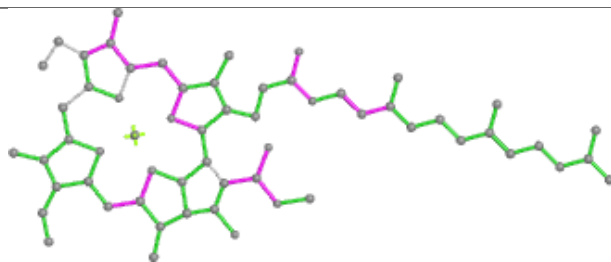
## Ligand CLA A 828



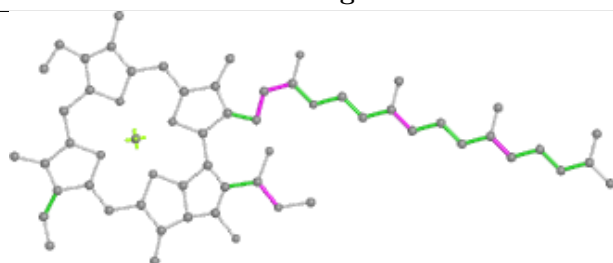


**Ligand CLA 8 602**

Bond lengths



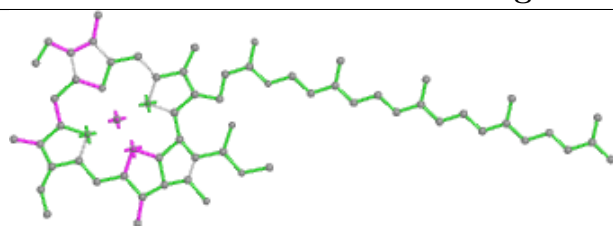
Bond angles



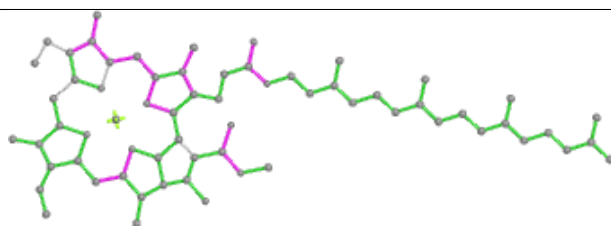
Torsions



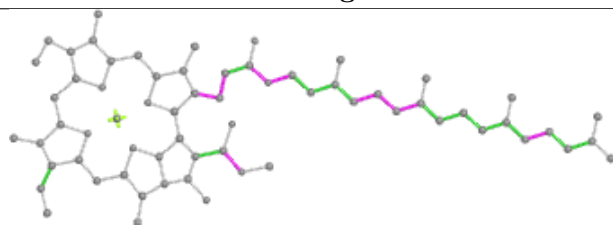
Rings

**Ligand CLA B 839**

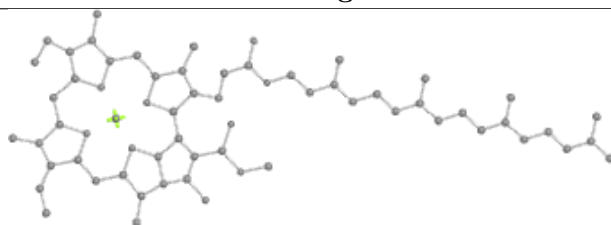
Bond lengths



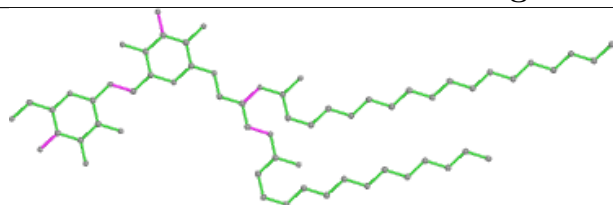
Bond angles



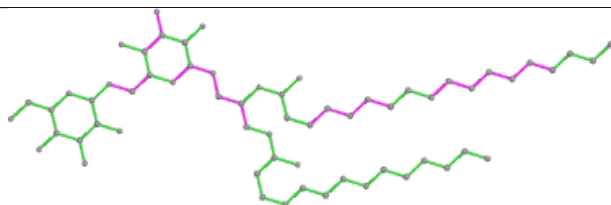
Torsions



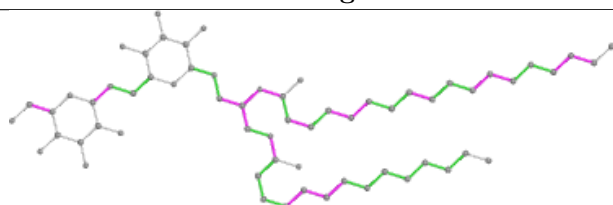
Rings

**Ligand DGD B 850**

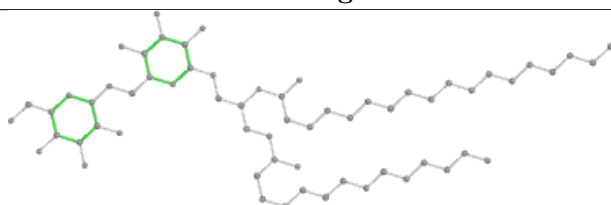
Bond lengths



Bond angles

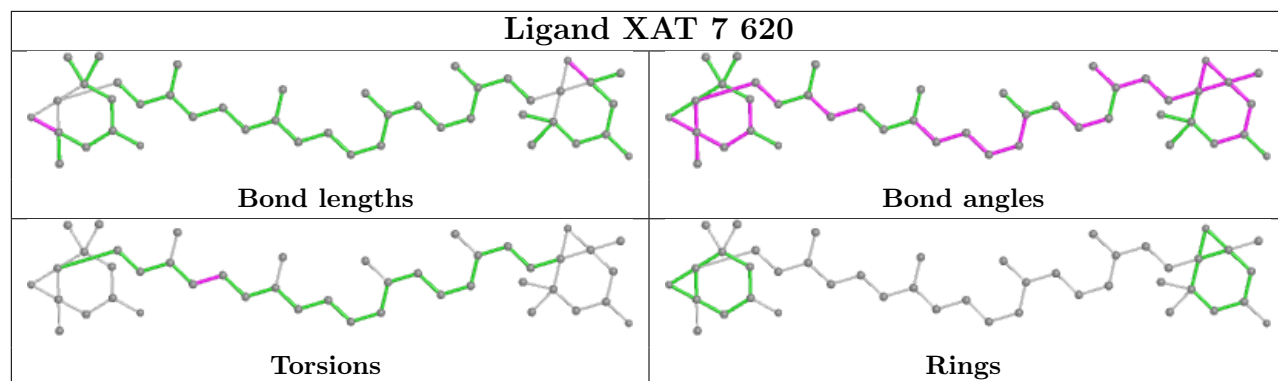


Torsions

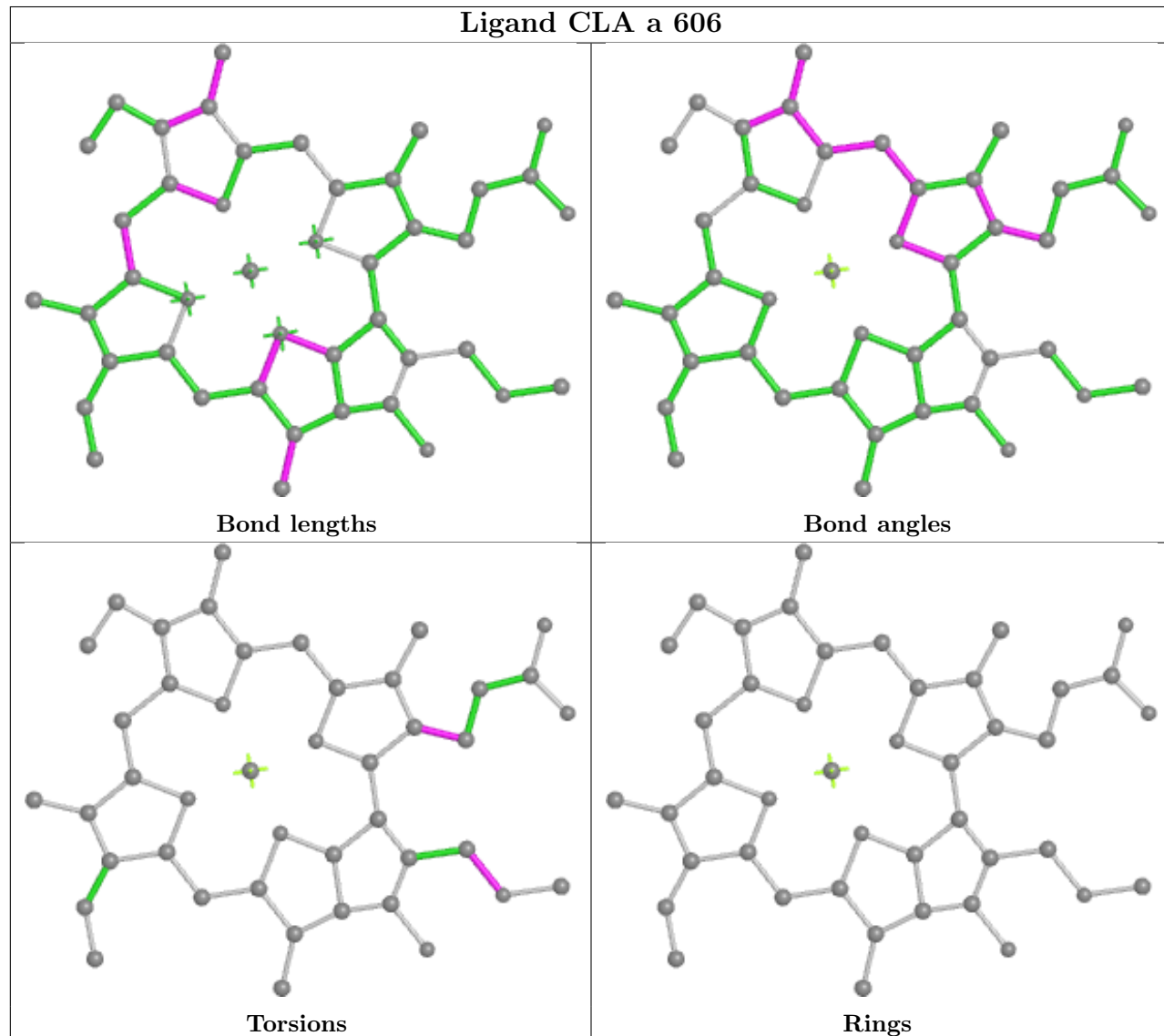


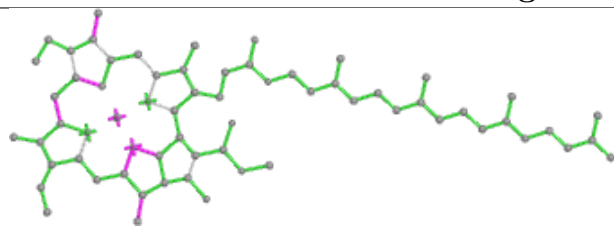
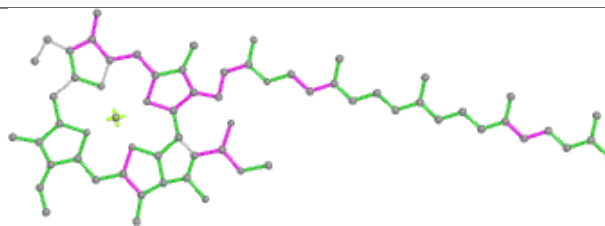
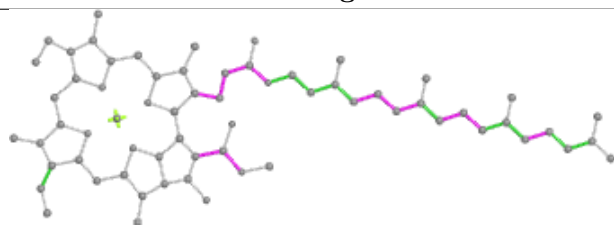
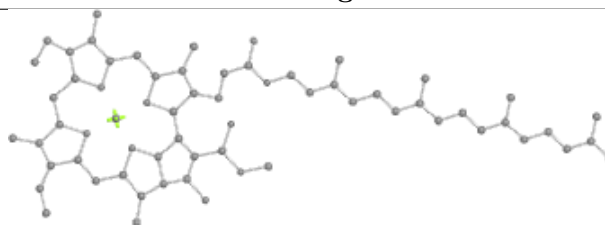
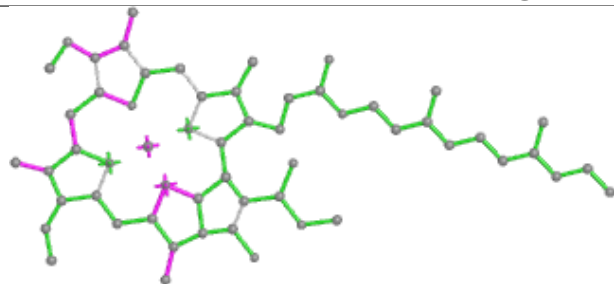
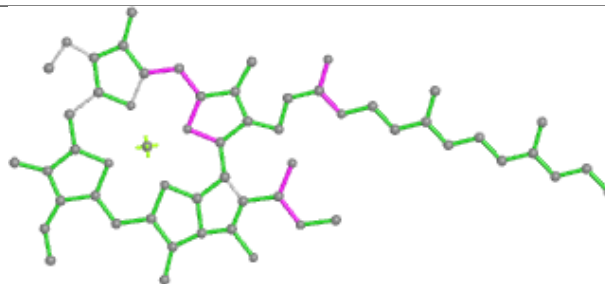
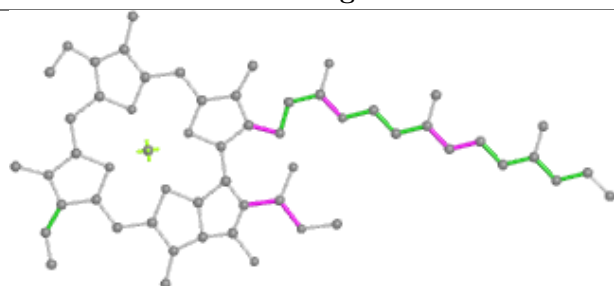
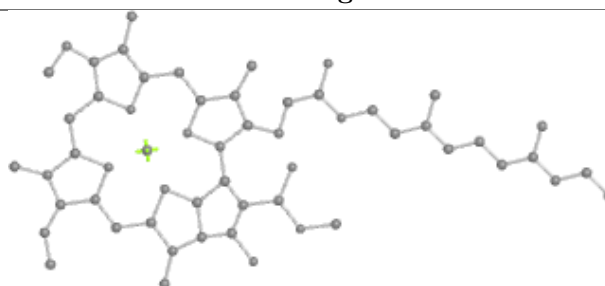
Rings

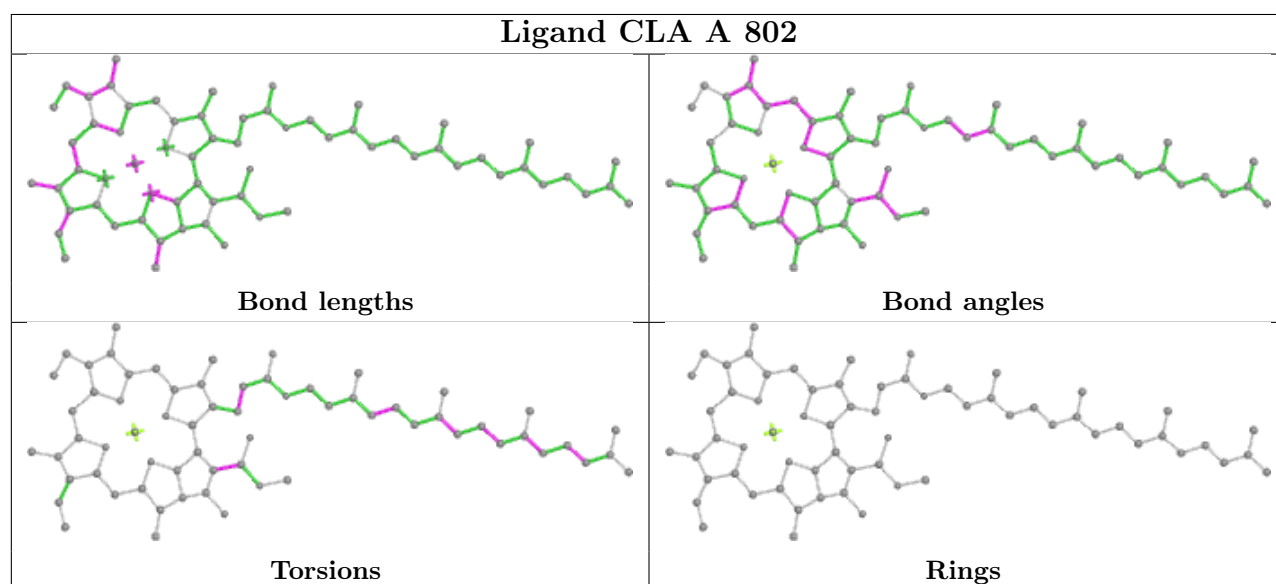
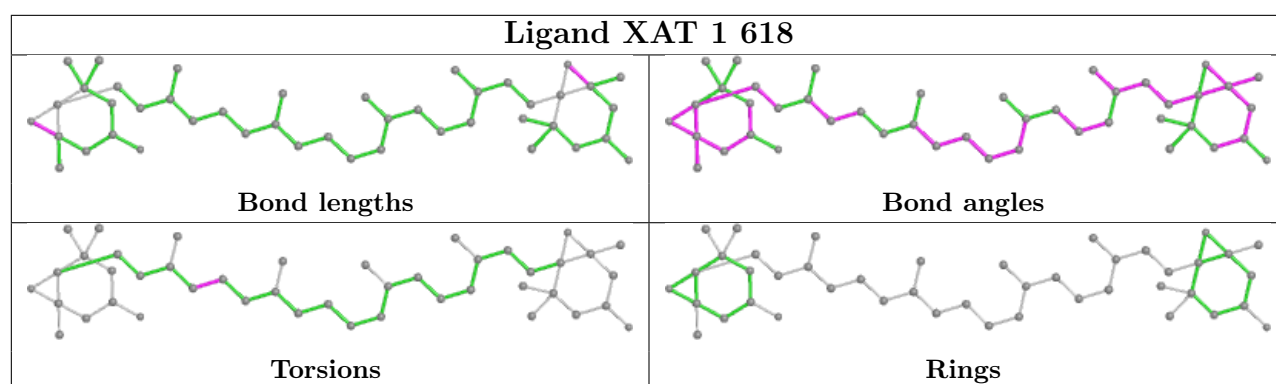
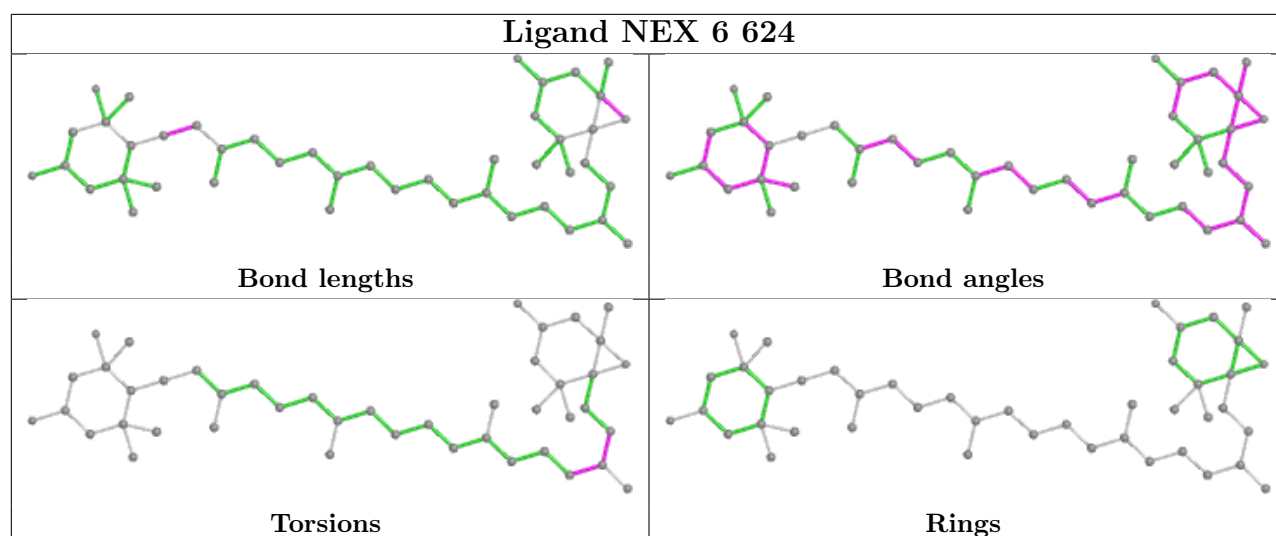
## Ligand XAT 7 620

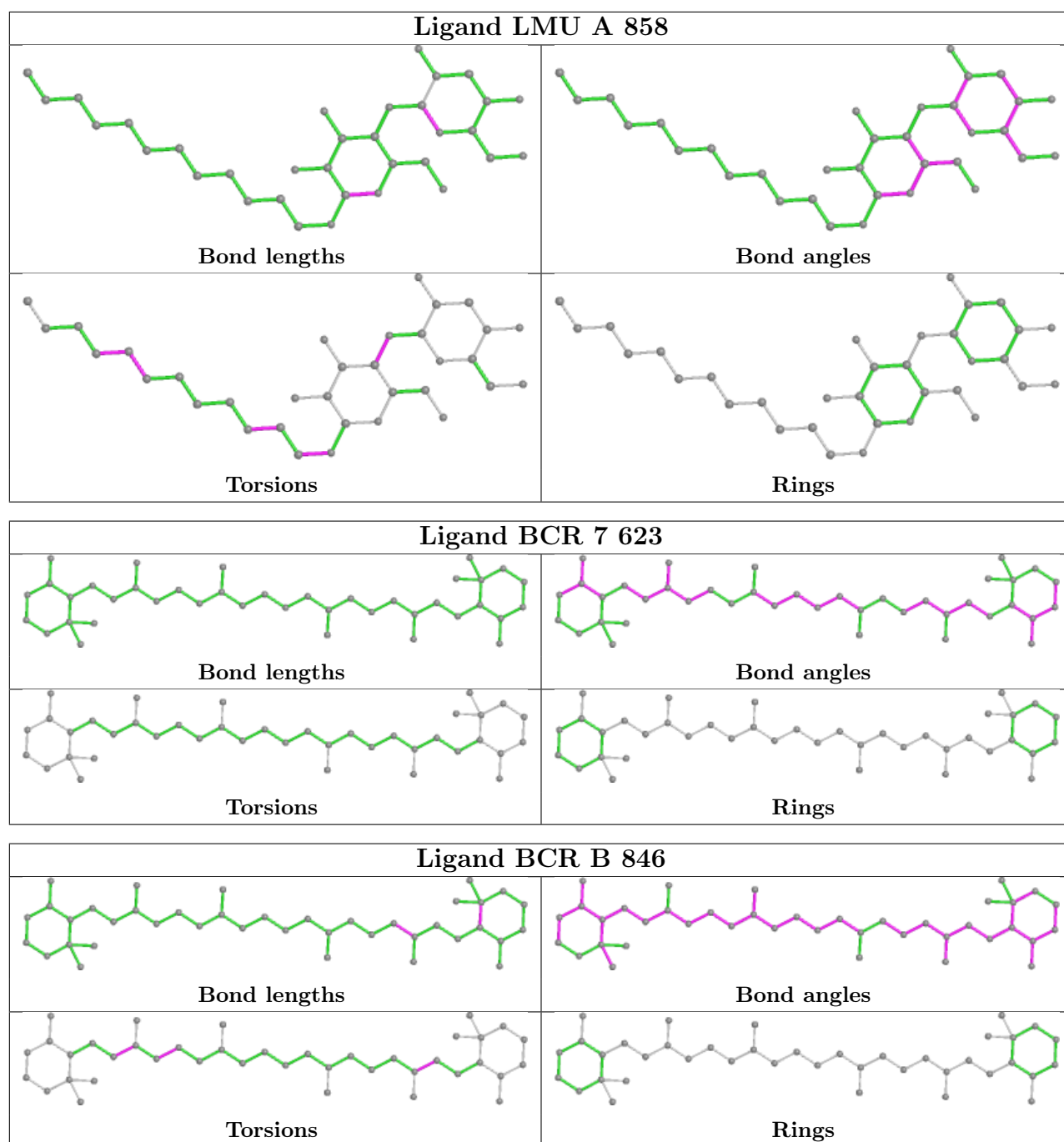


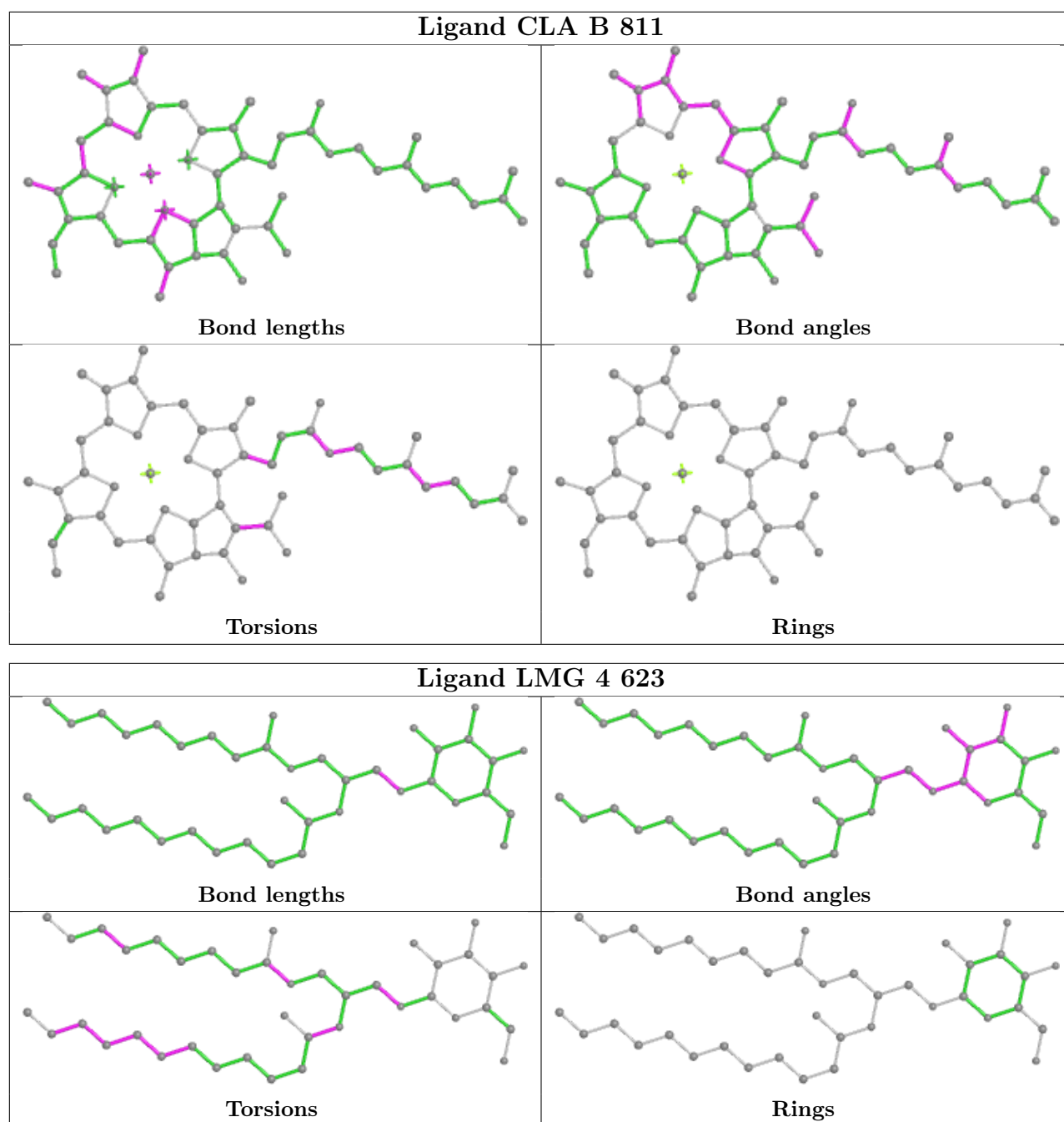
## Ligand CLA a 606

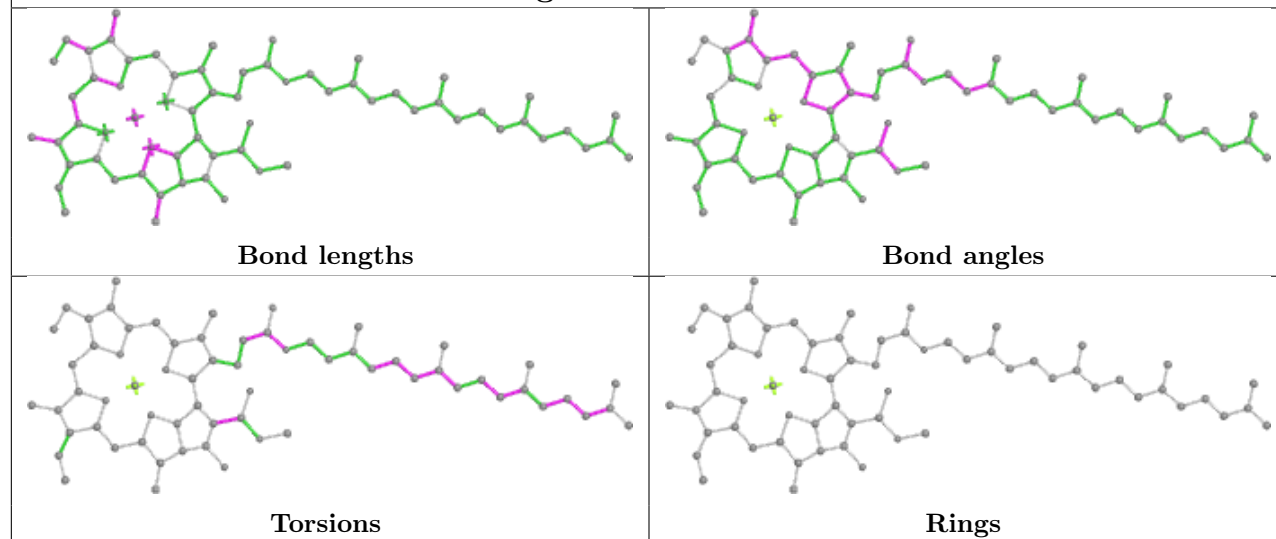
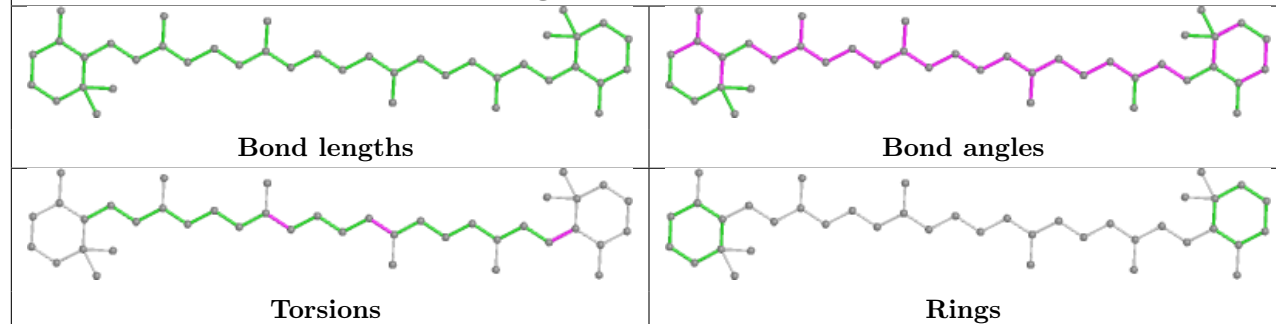
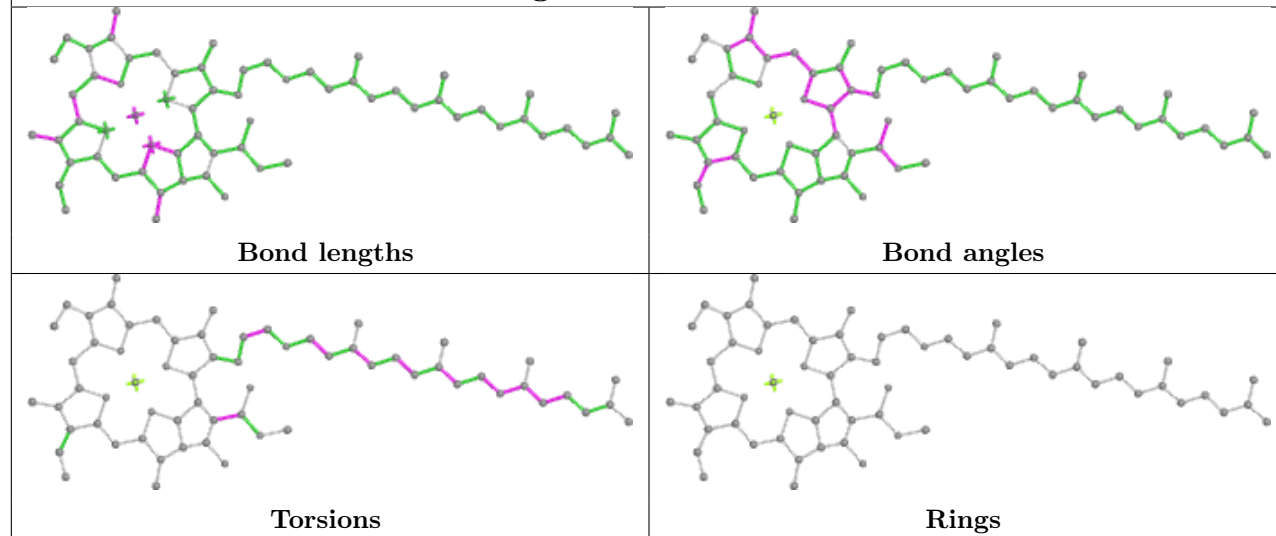


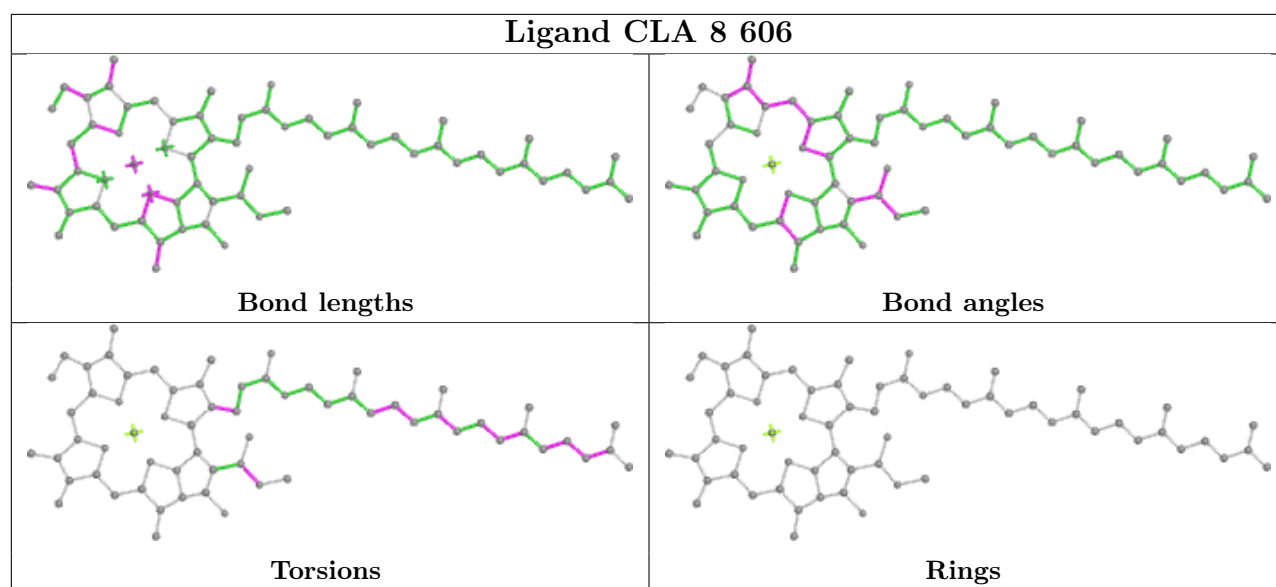
**Ligand CLA 6 616****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA F 301****Bond lengths****Bond angles****Torsions****Rings**





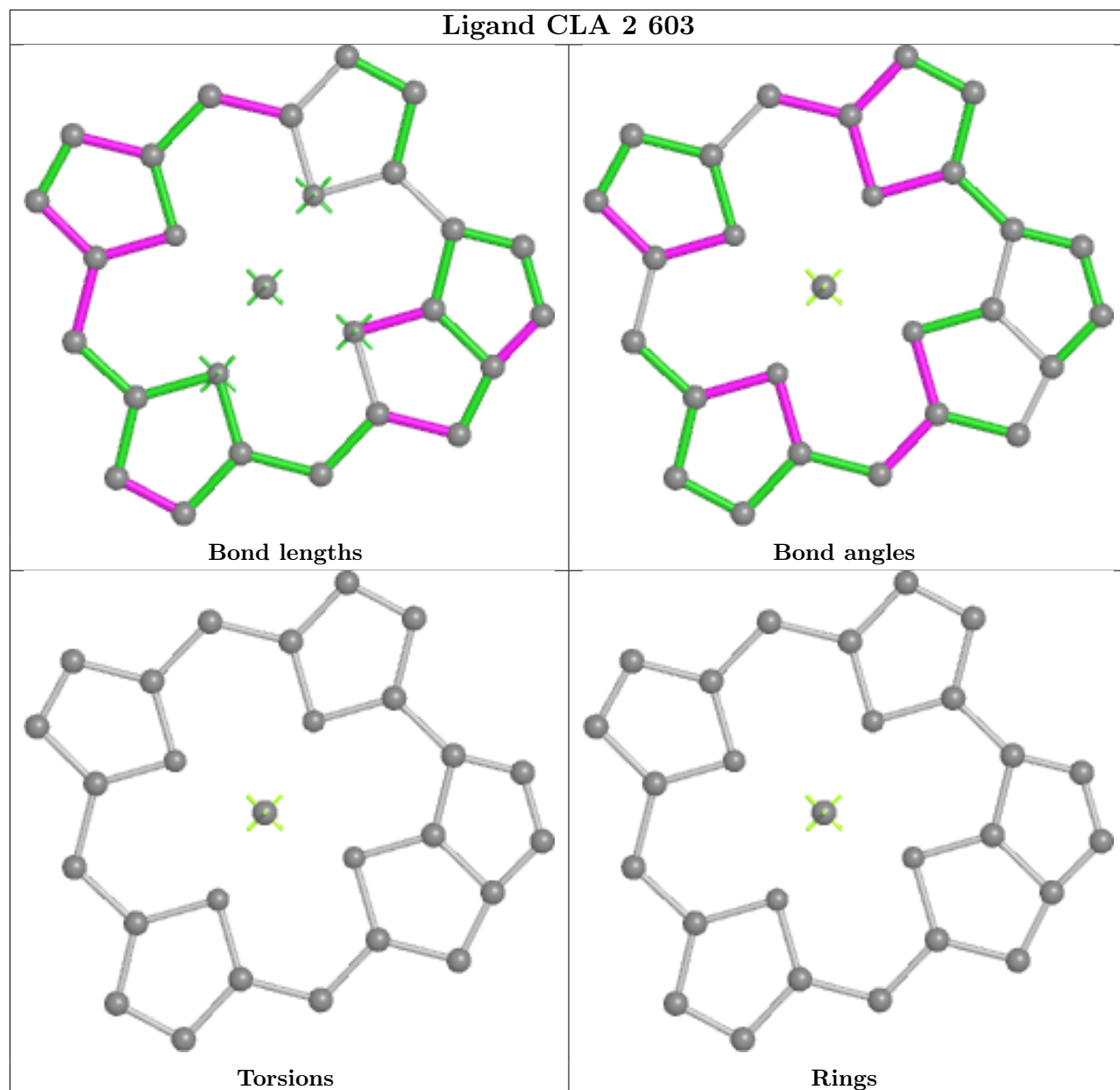


**Ligand CLA 8 601****Ligand BCR 3 621****Ligand CLA A 826**

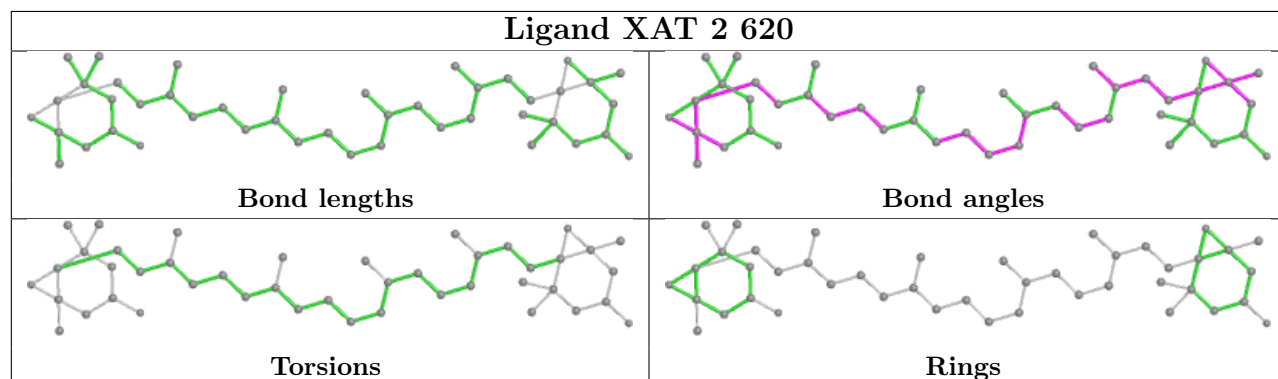




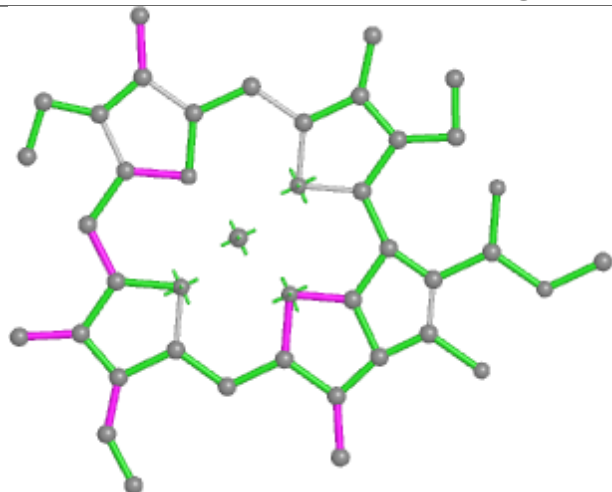
## Ligand CLA 2 603



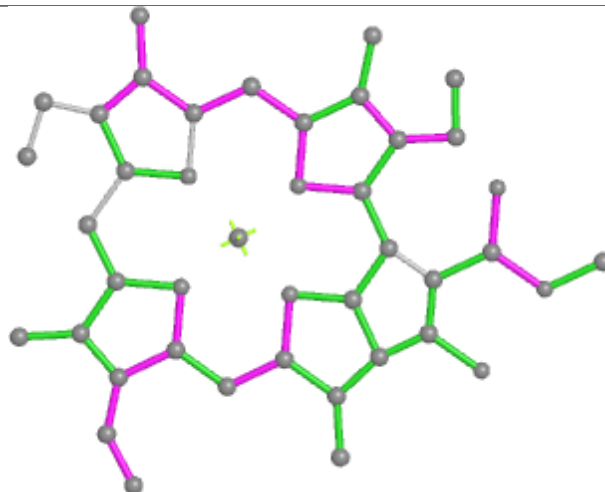
## Ligand XAT 2 620



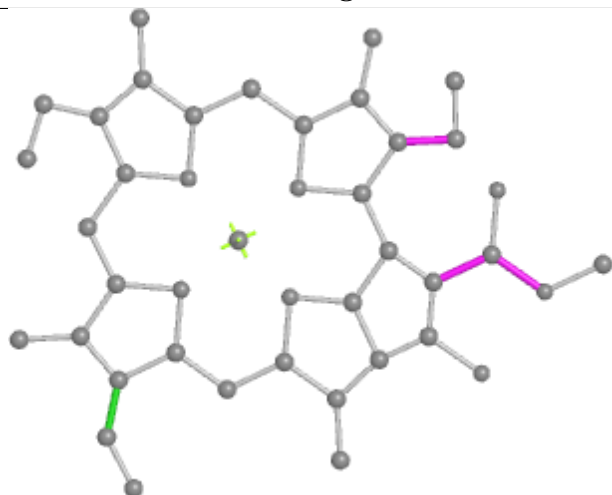
## Ligand CLA F 303



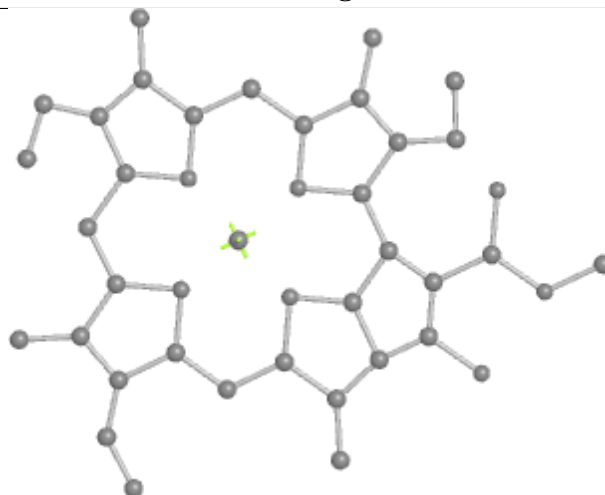
Bond lengths



Bond angles

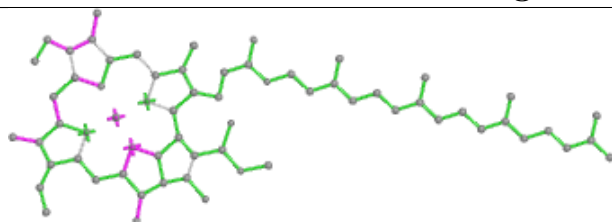


Torsions

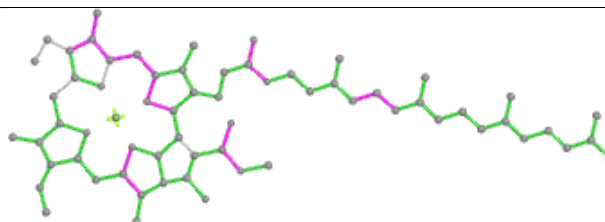


Rings

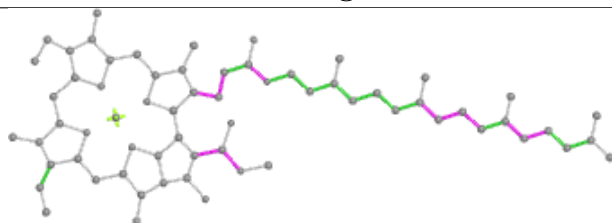
## Ligand CLA B 828



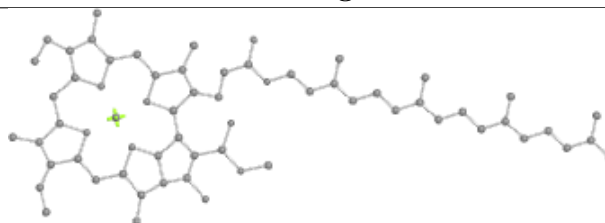
Bond lengths



Bond angles

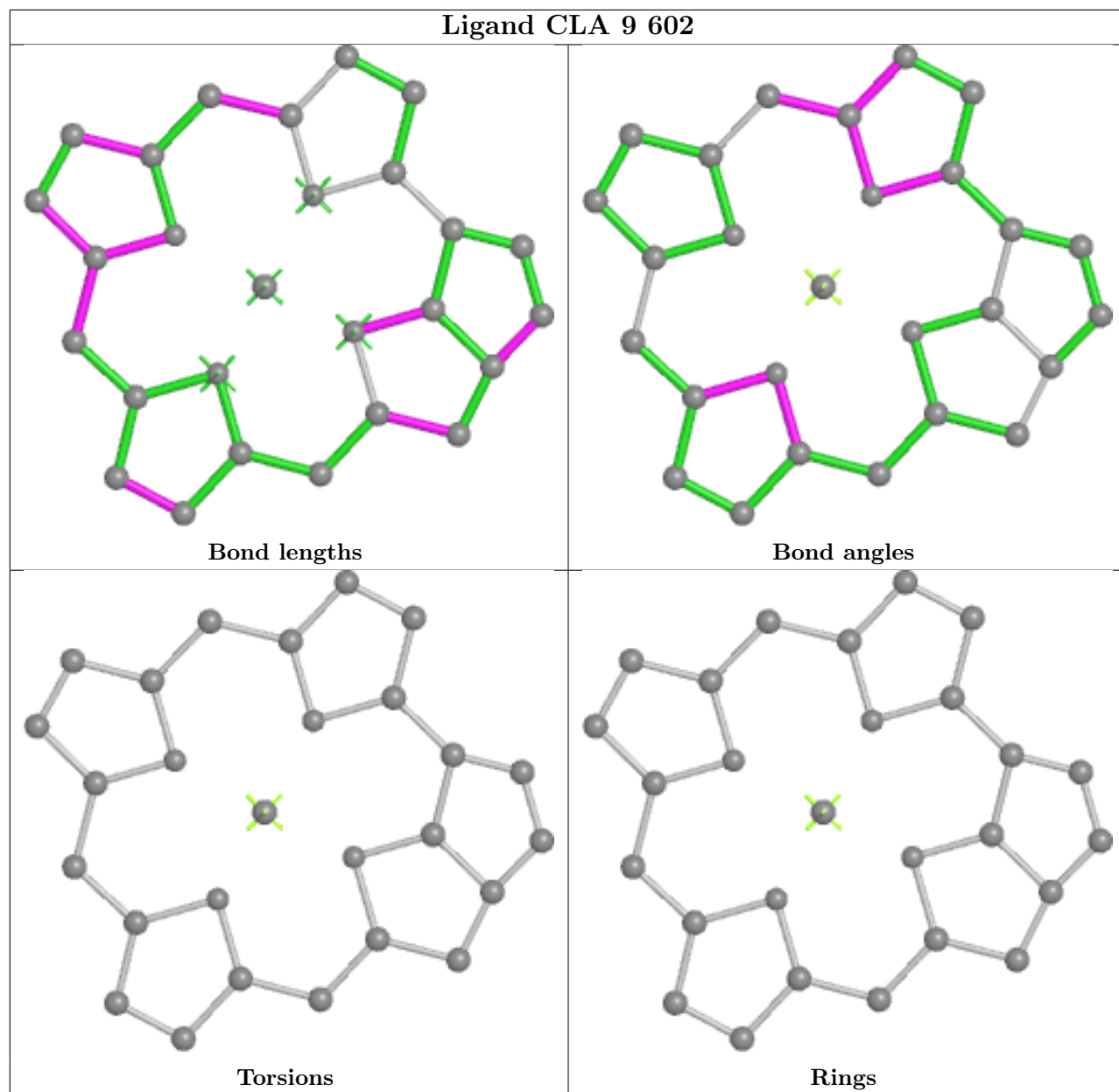


Torsions

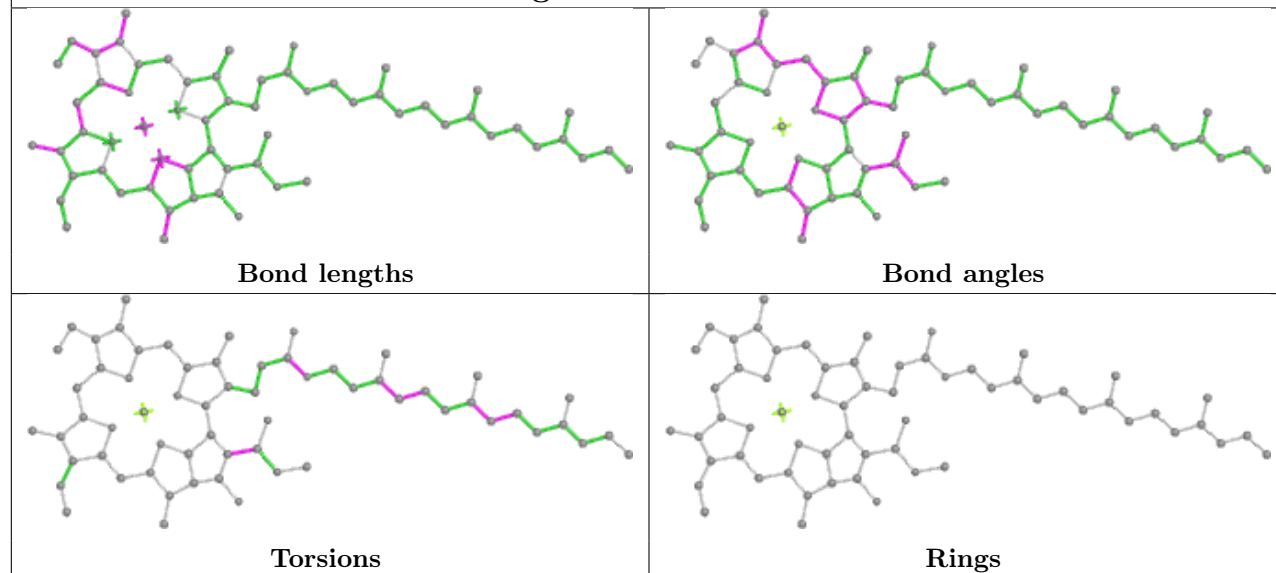


Rings

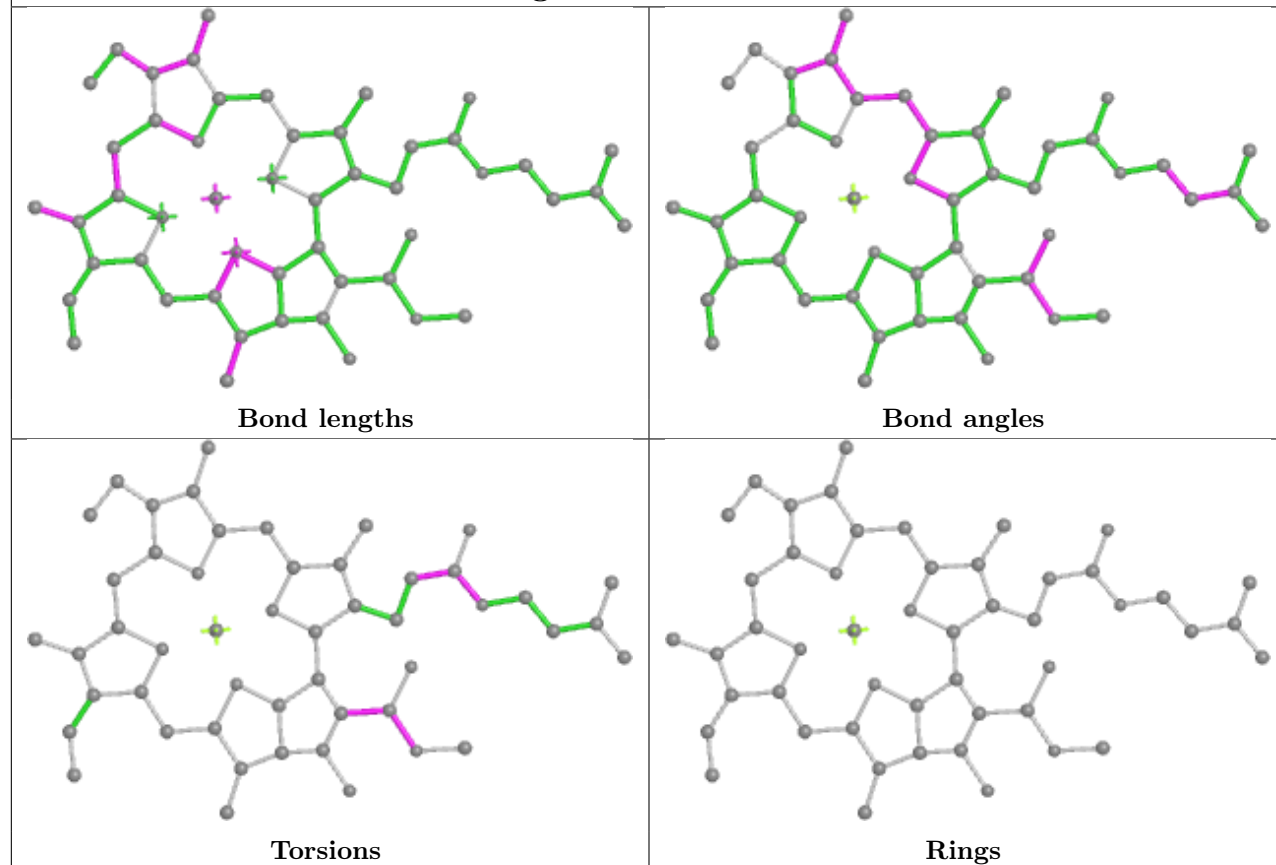
## Ligand CLA 9 602



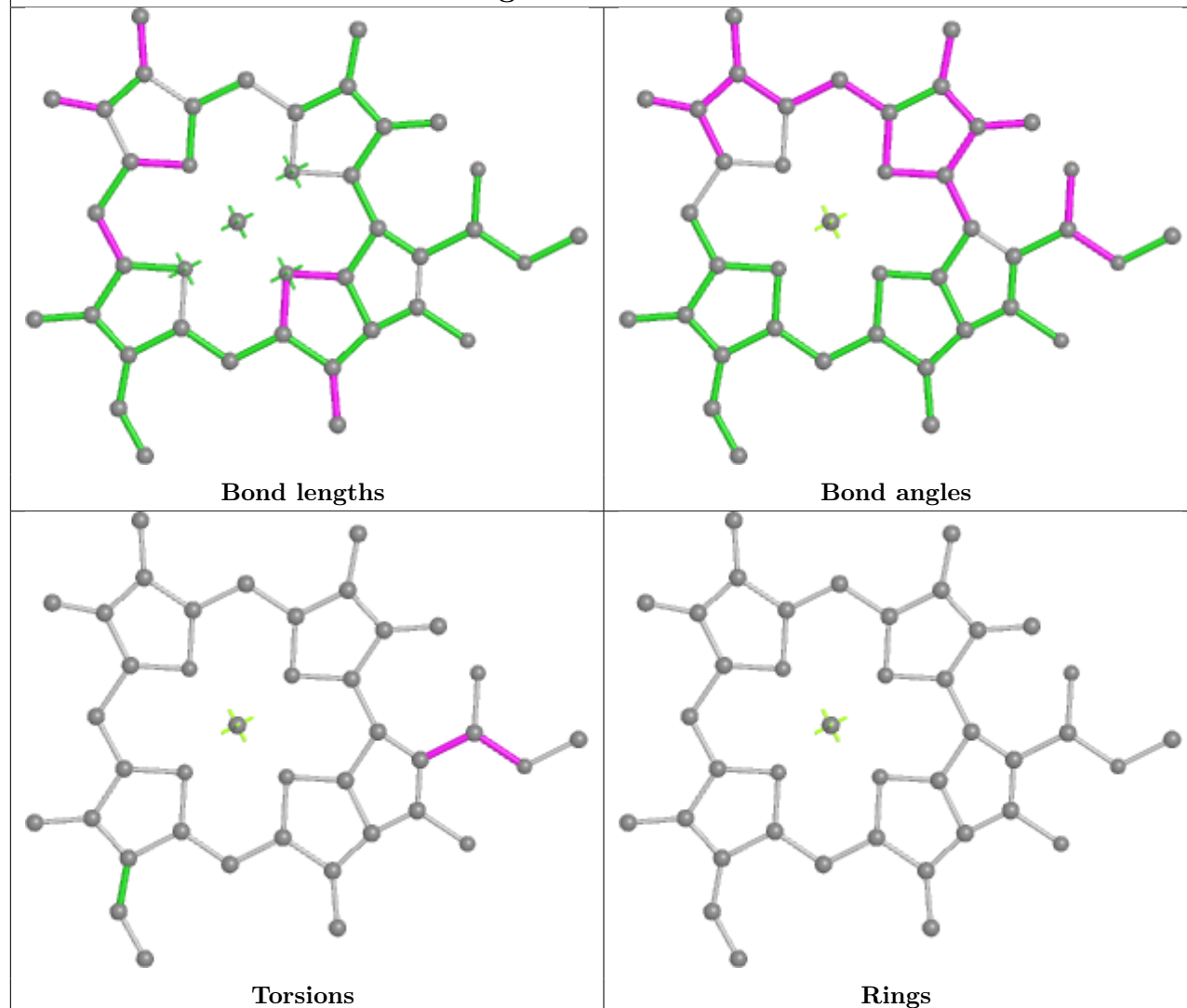
## Ligand CLA B 825



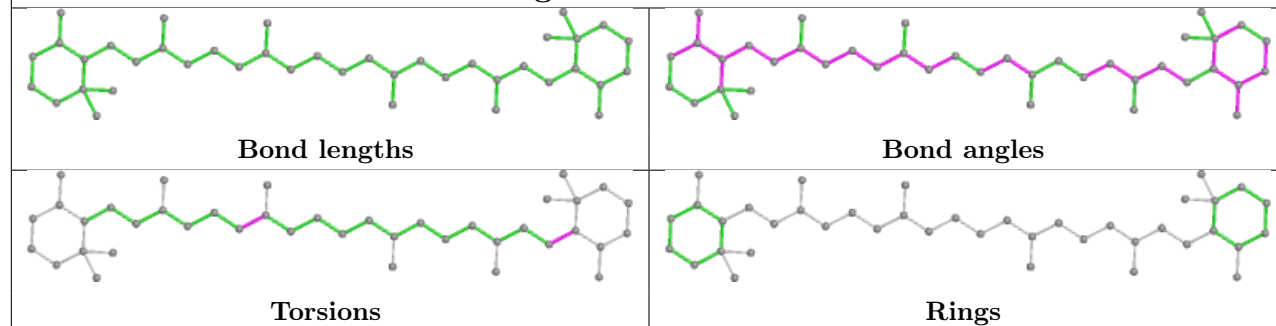
## Ligand CLA A 845



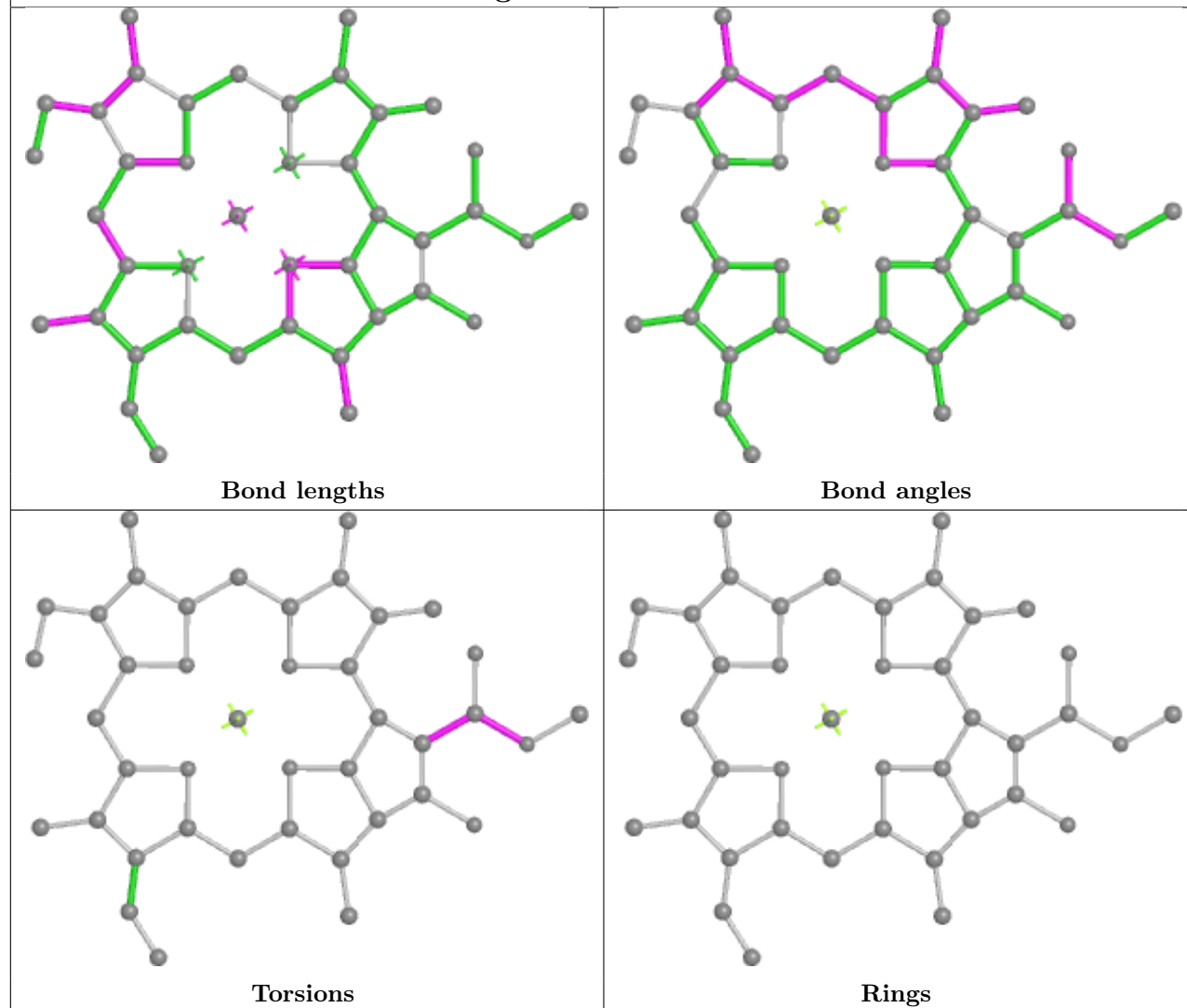
## Ligand CLA 1 609



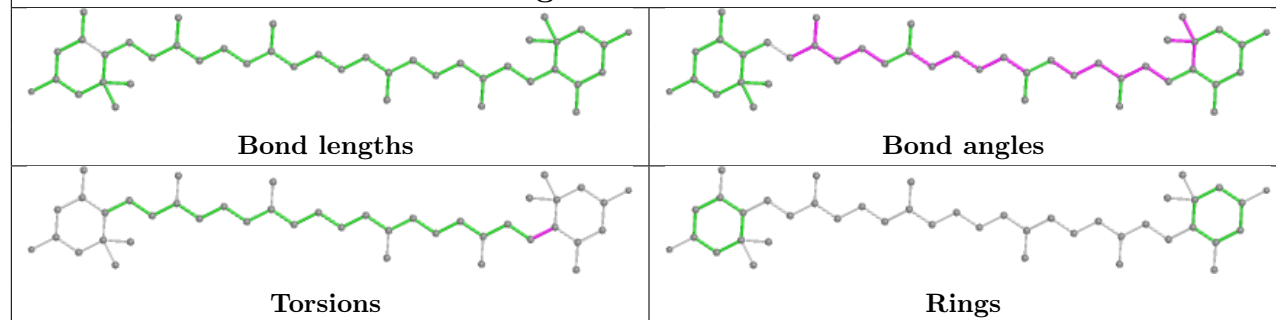
## Ligand BCR 1 619



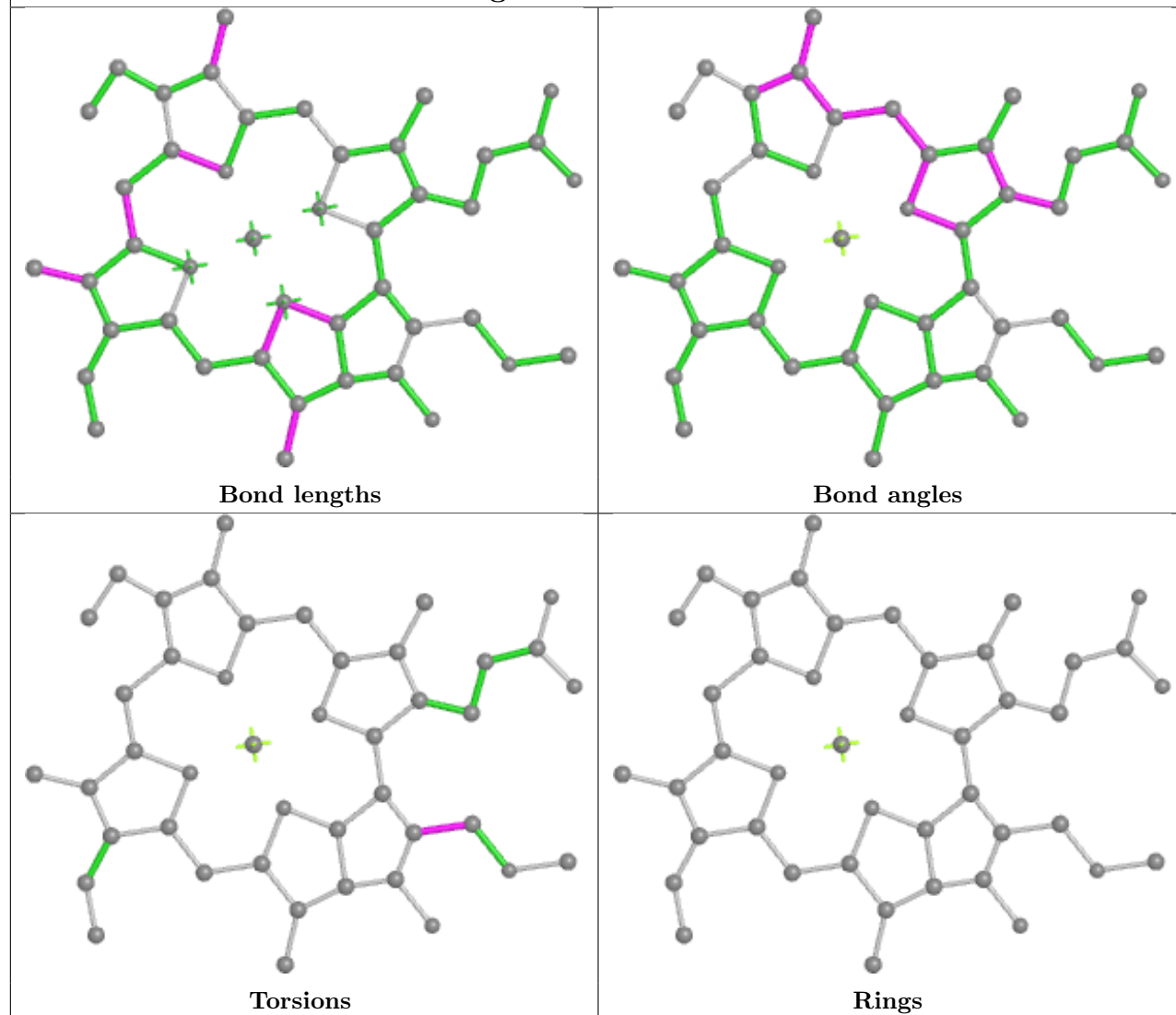
## Ligand CLA B 804



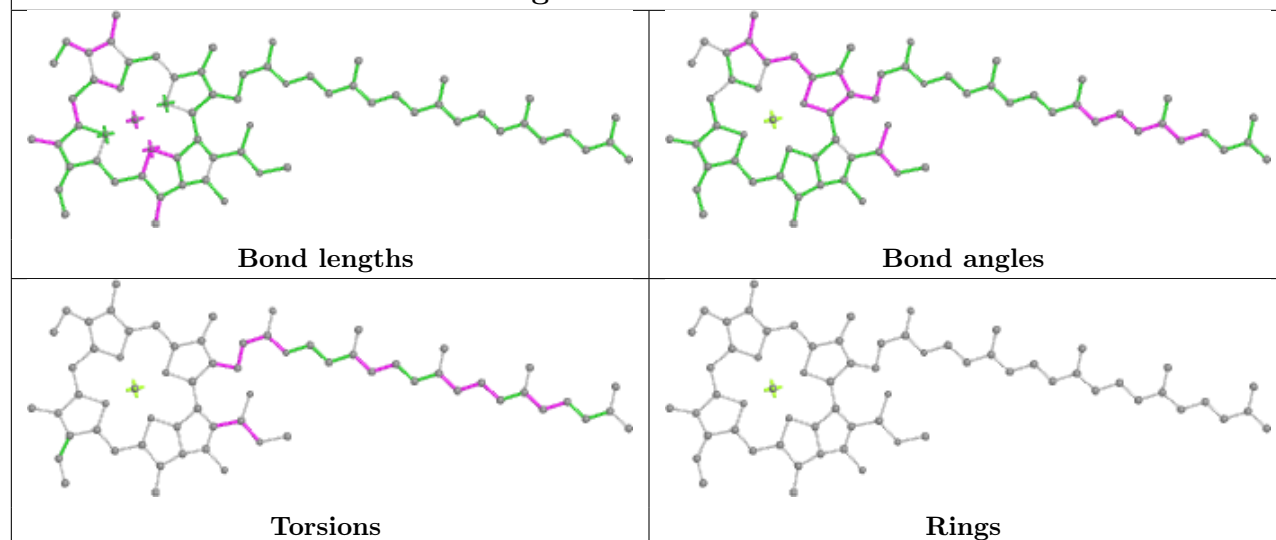
## Ligand LUT 1 617

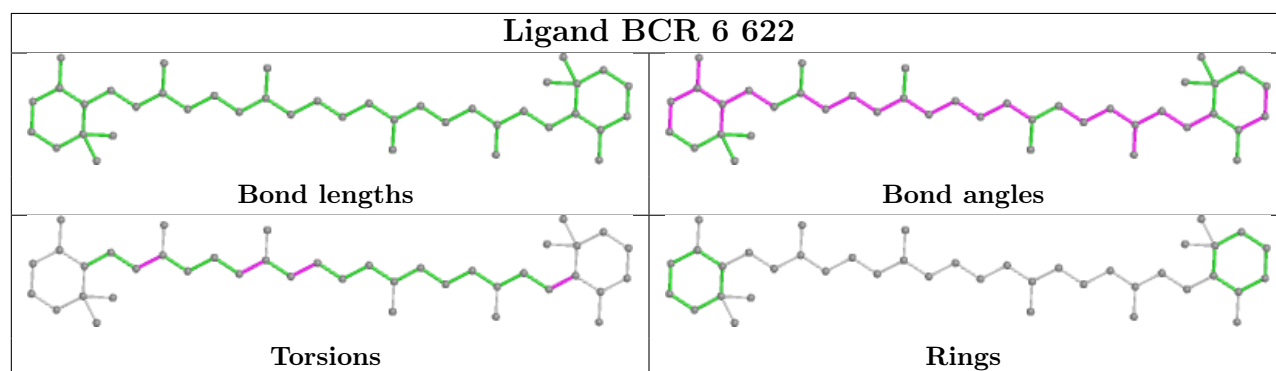
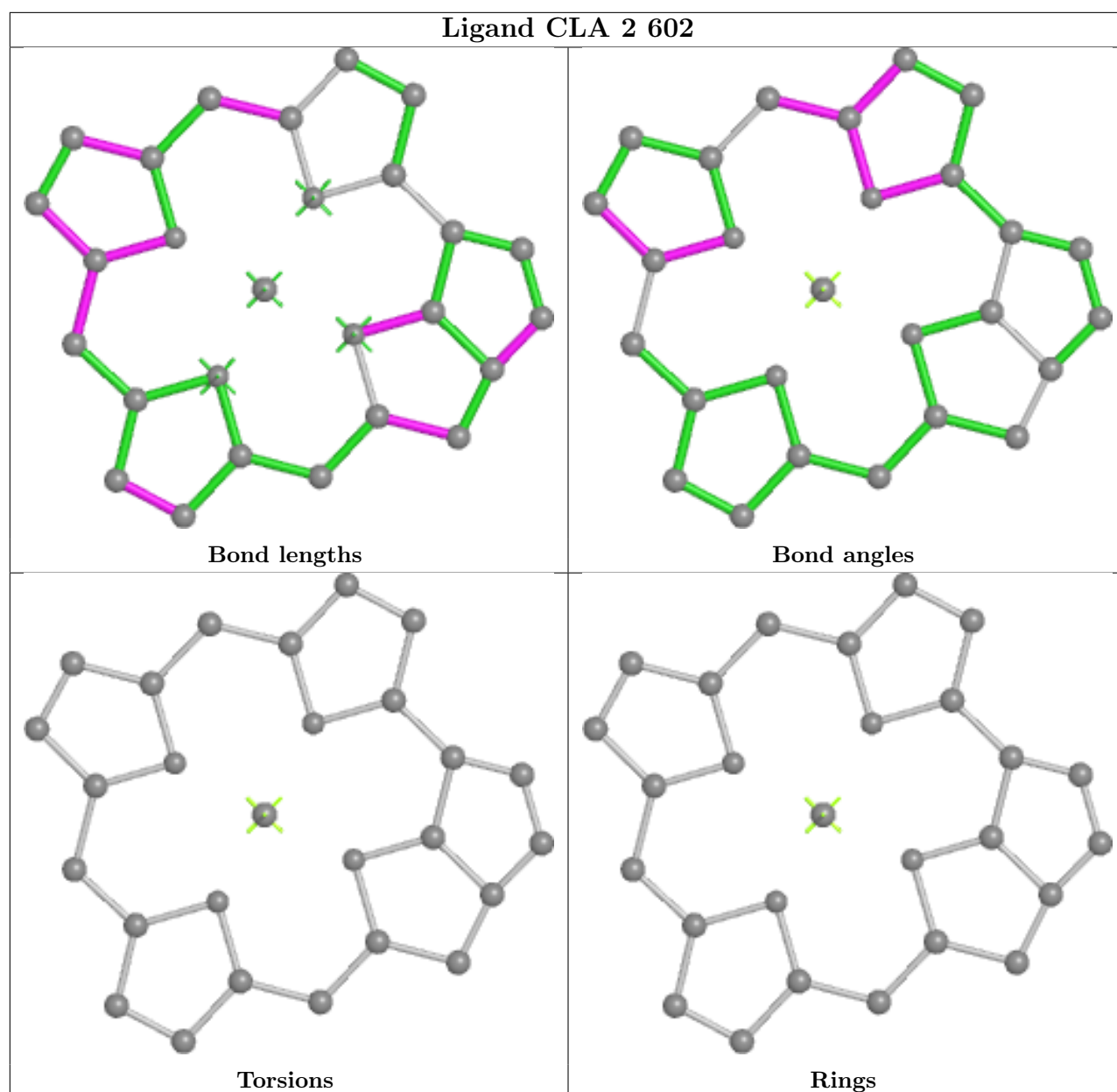


## Ligand CLA A 816



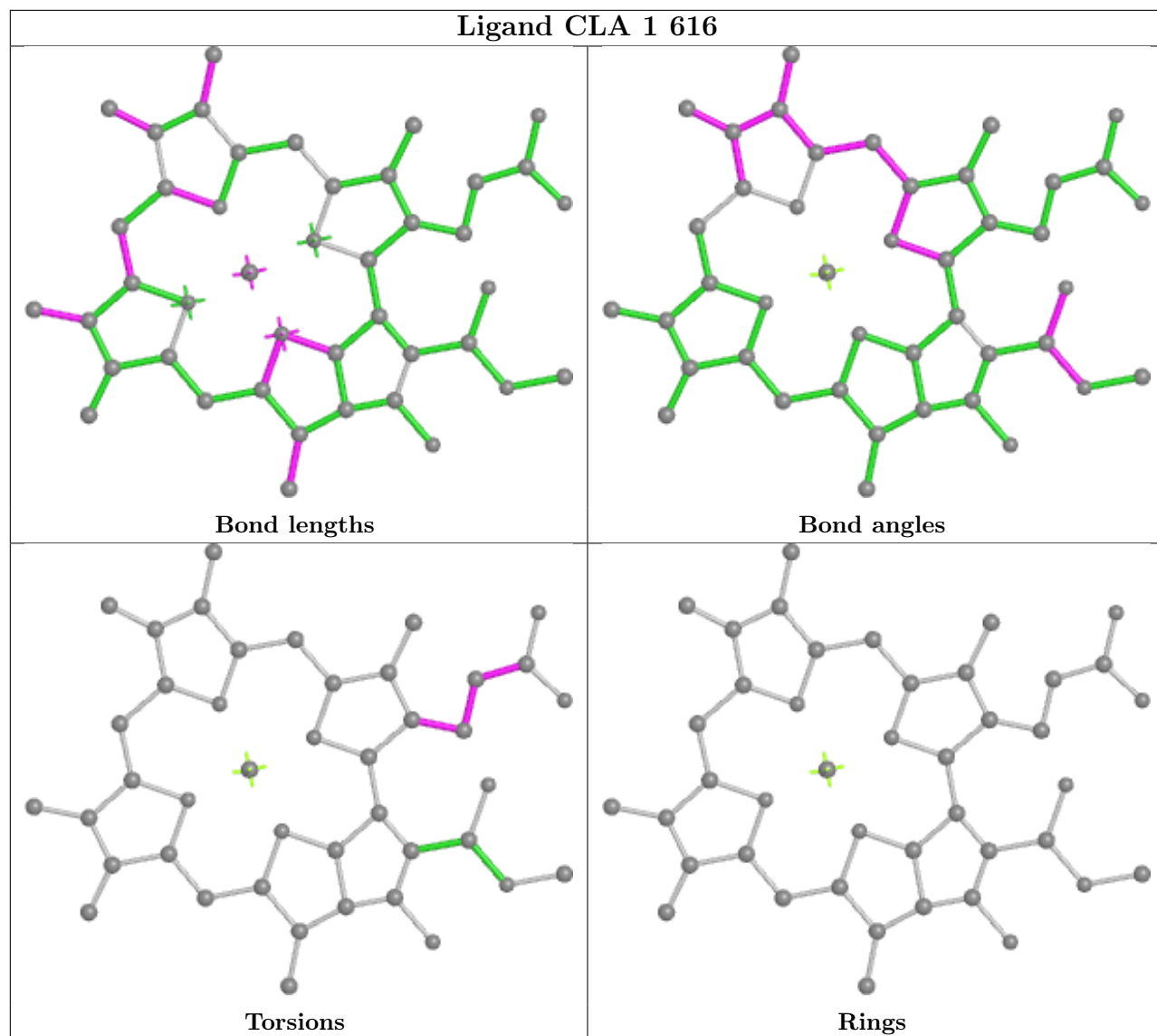
## Ligand CLA A 814

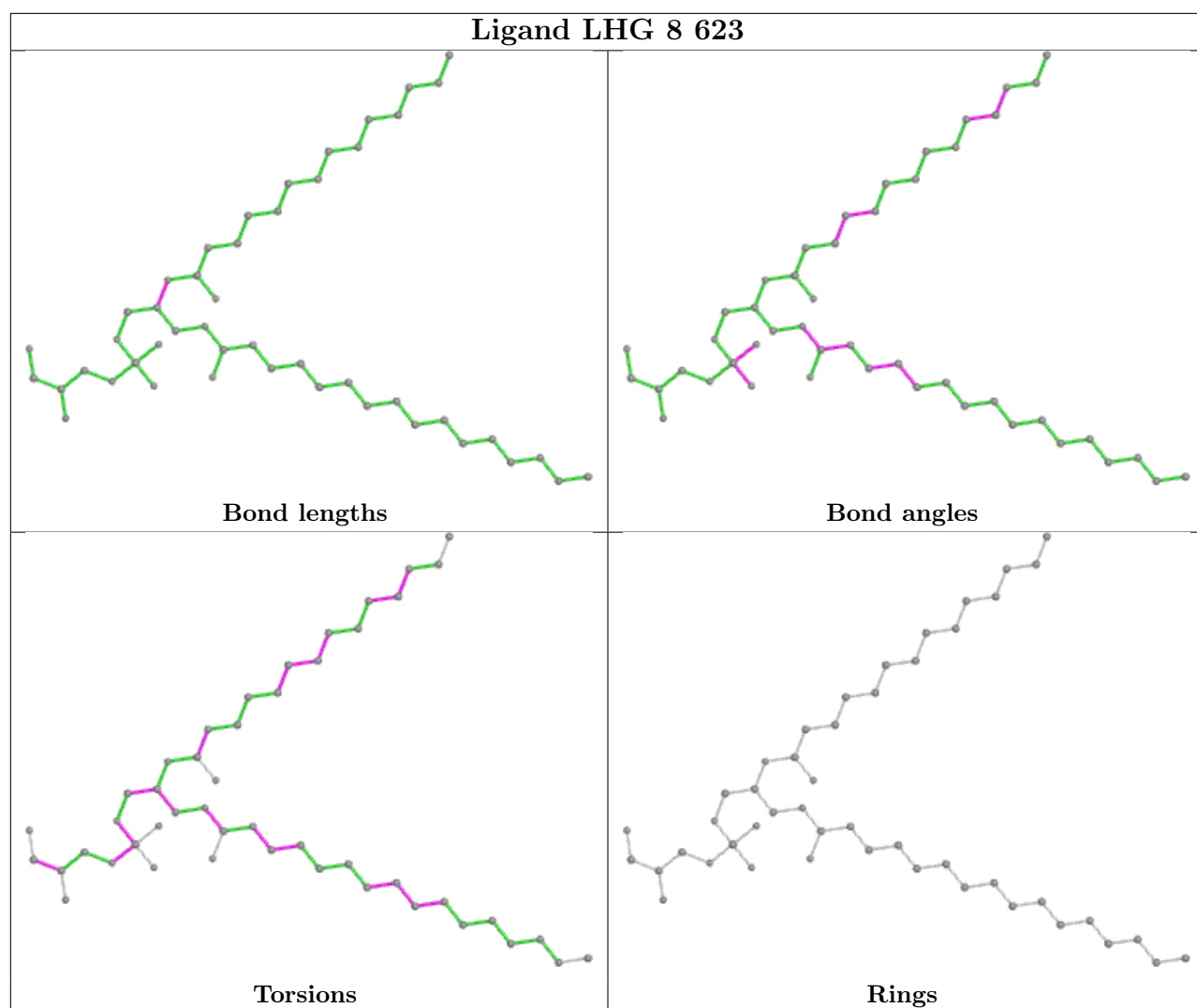




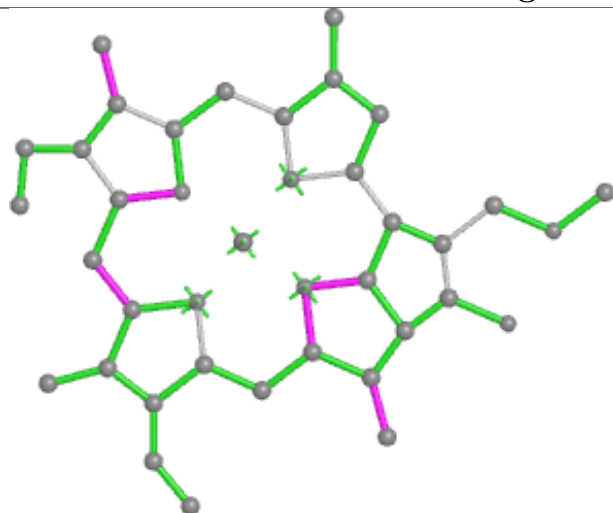


## Ligand CLA 1 616

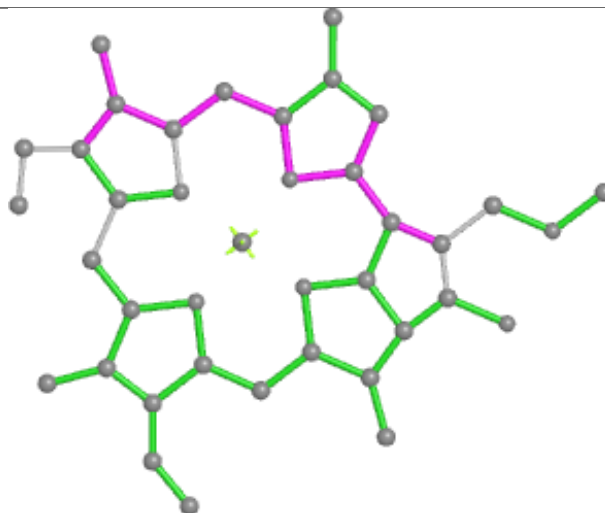




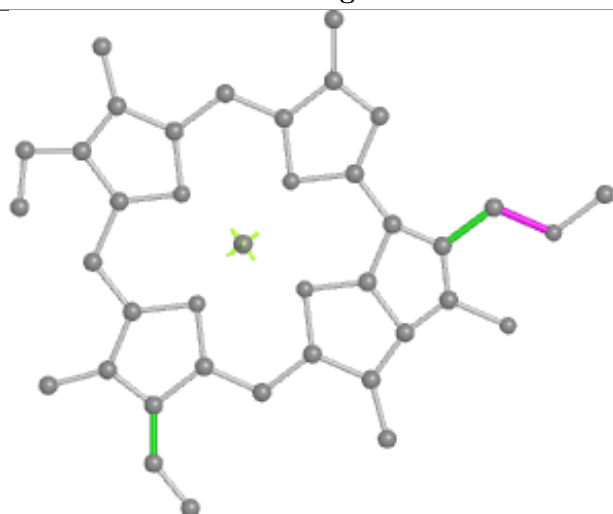
## Ligand CLA 1 606



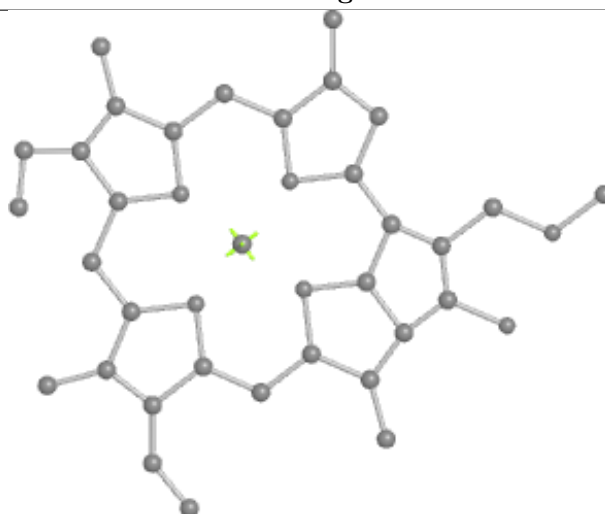
Bond lengths



Bond angles

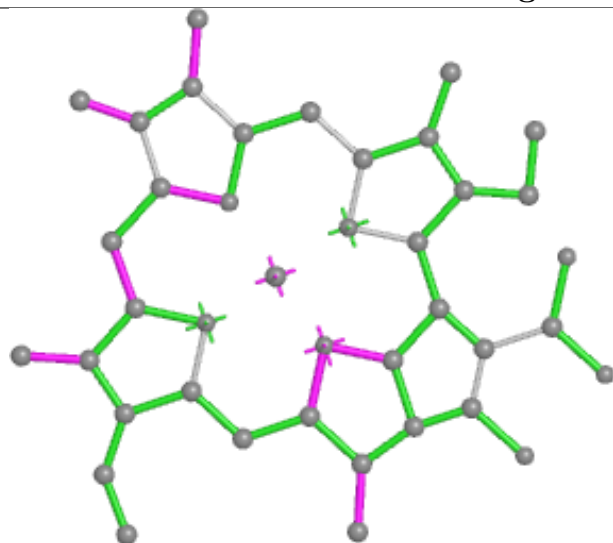


Torsions

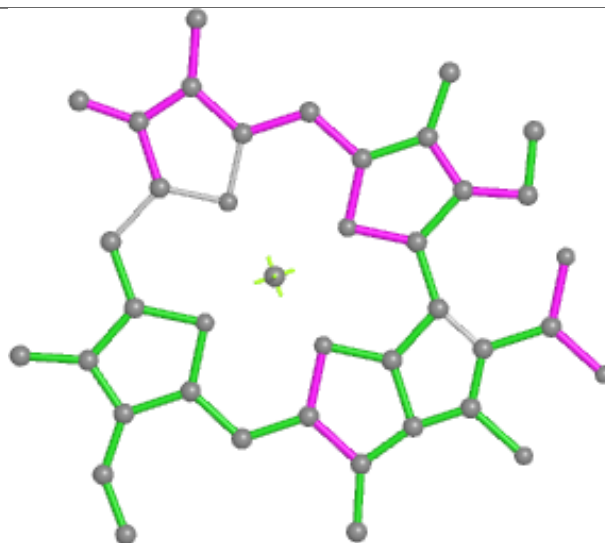


Rings

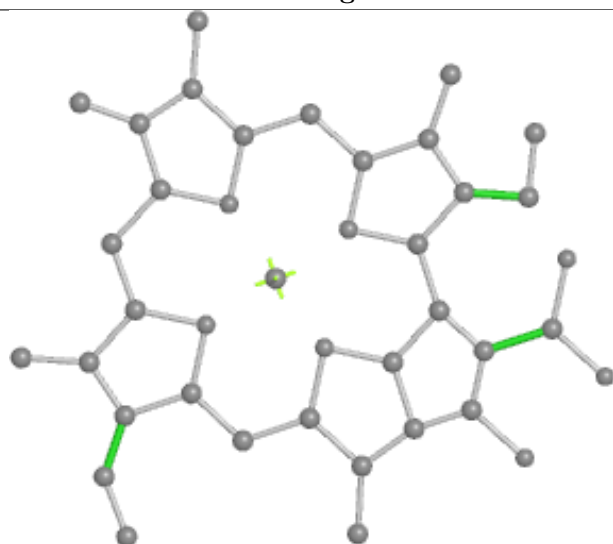
## Ligand CLA 4 618



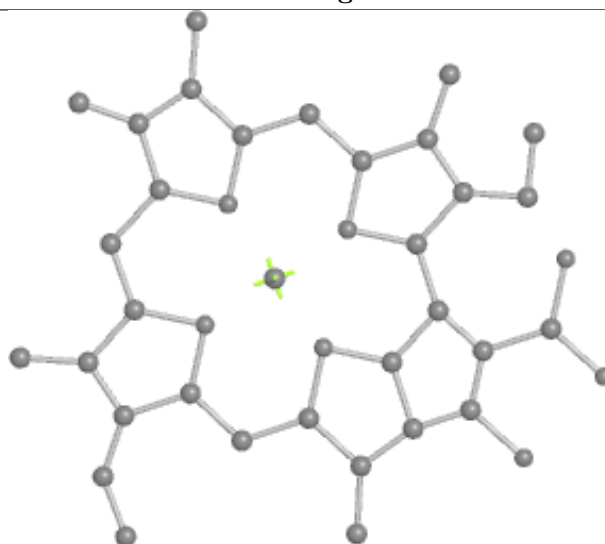
Bond lengths



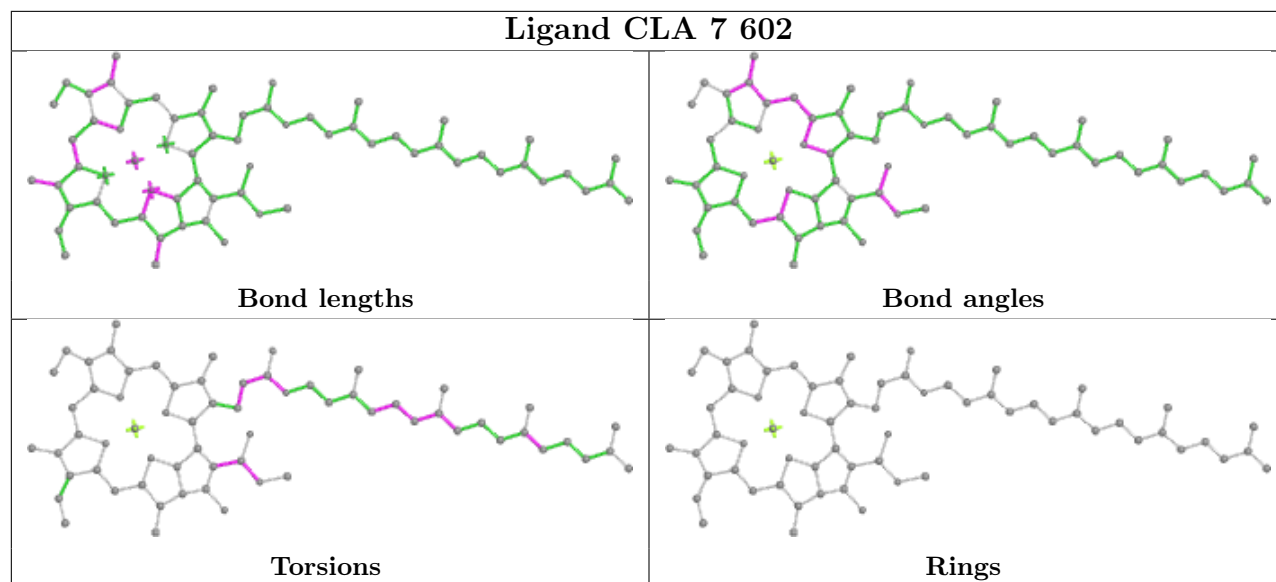
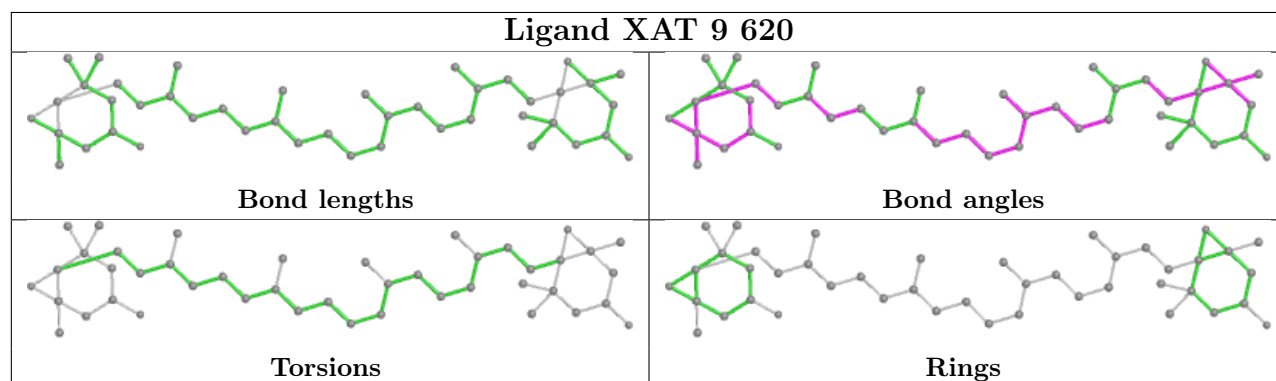
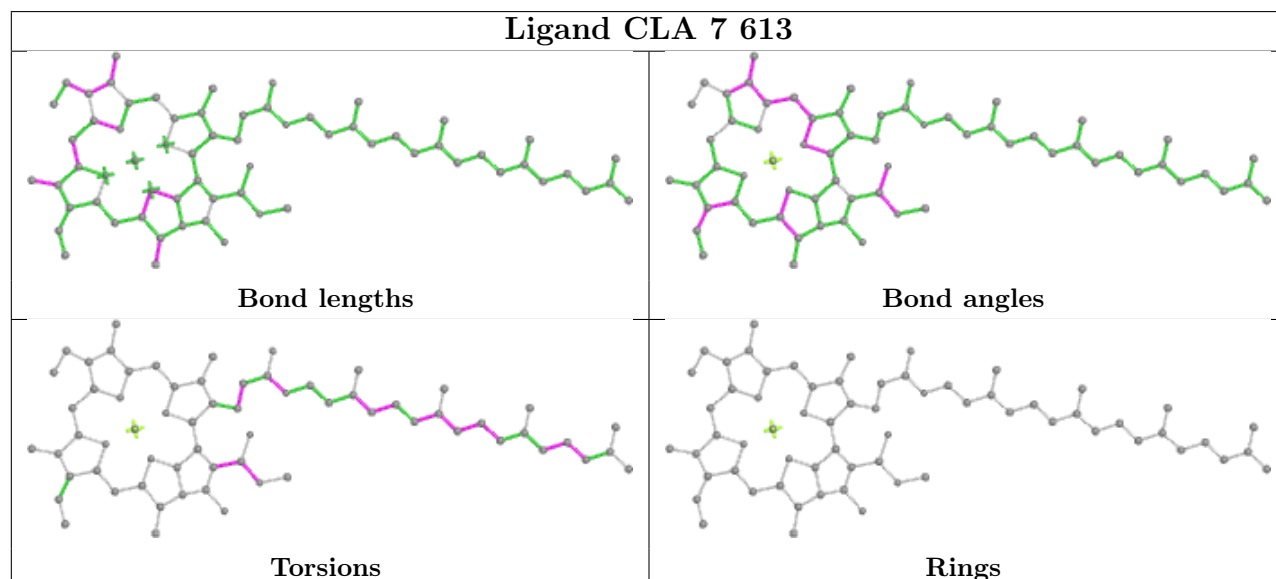
Bond angles



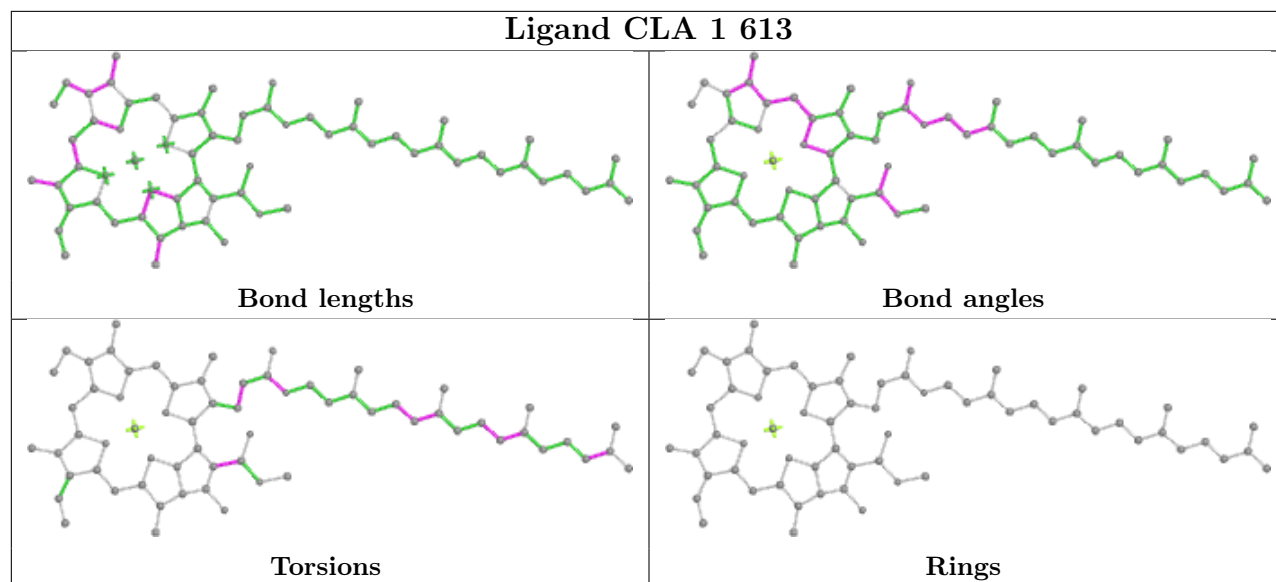
Torsions



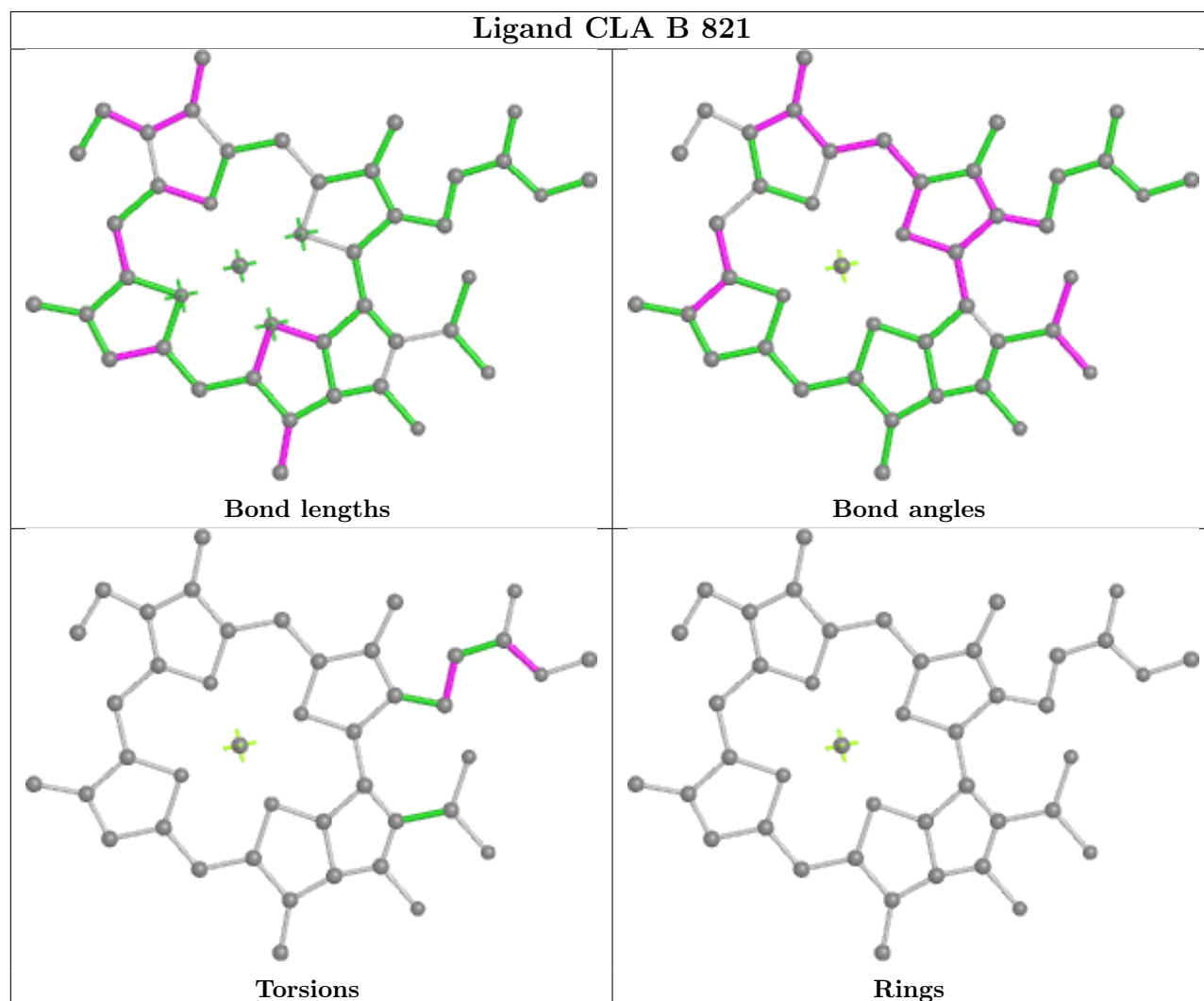
Rings

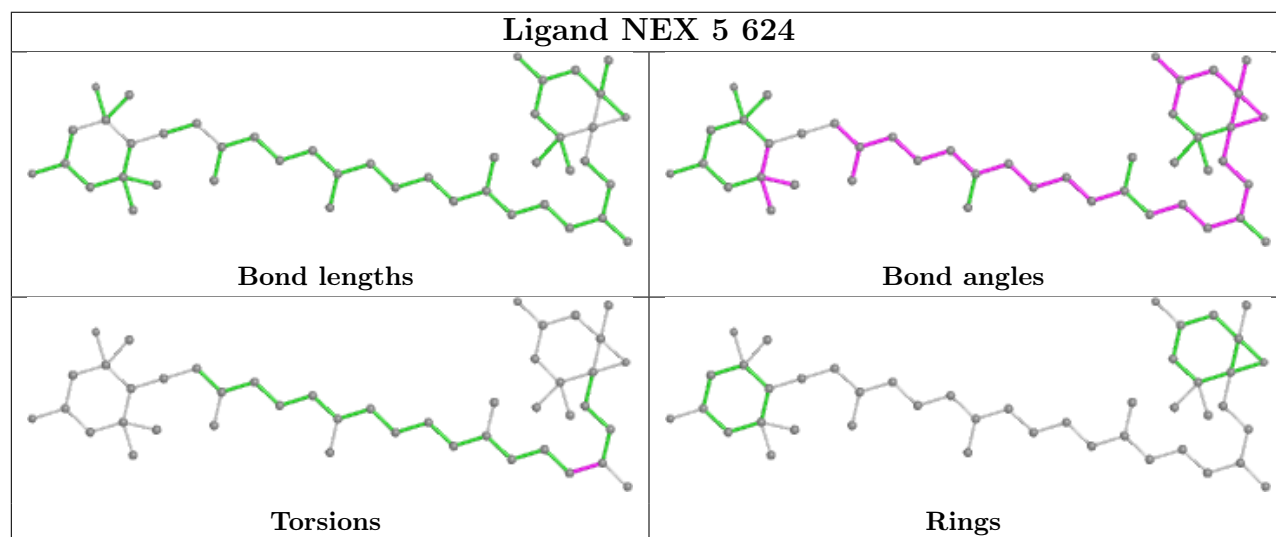
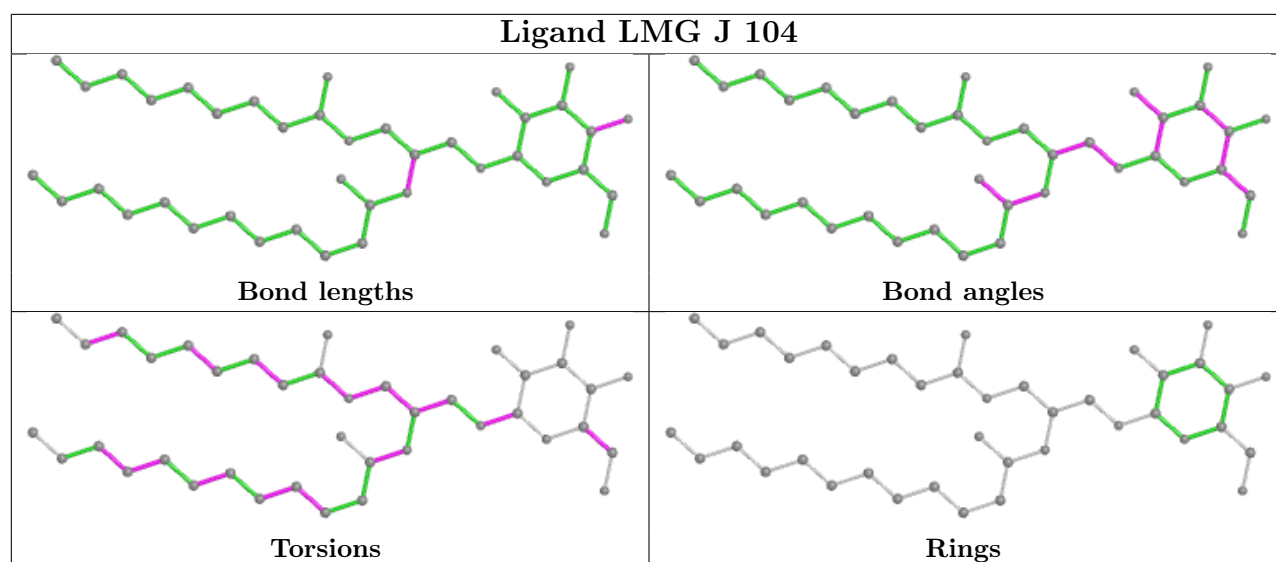
**Ligand CLA 7 602****Ligand XAT 9 620****Ligand CLA 7 613**

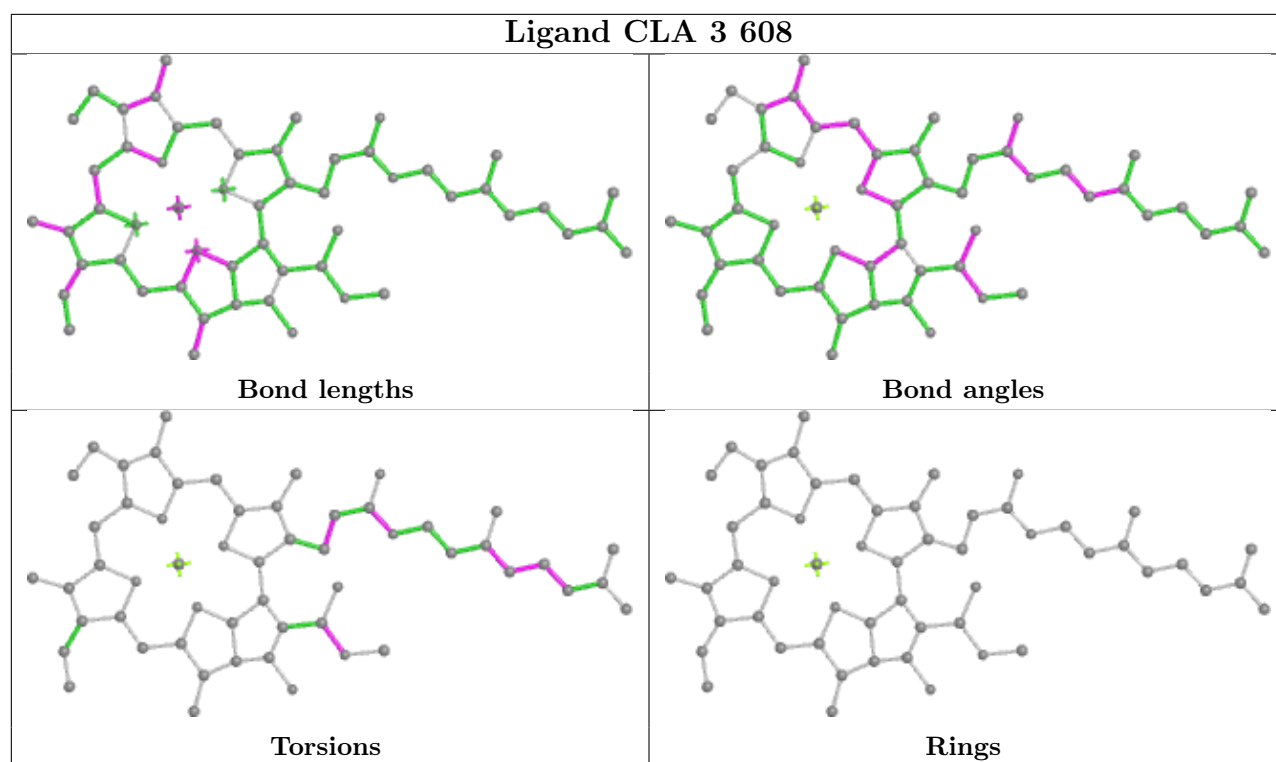
## Ligand CLA 1 613



## Ligand CLA B 821

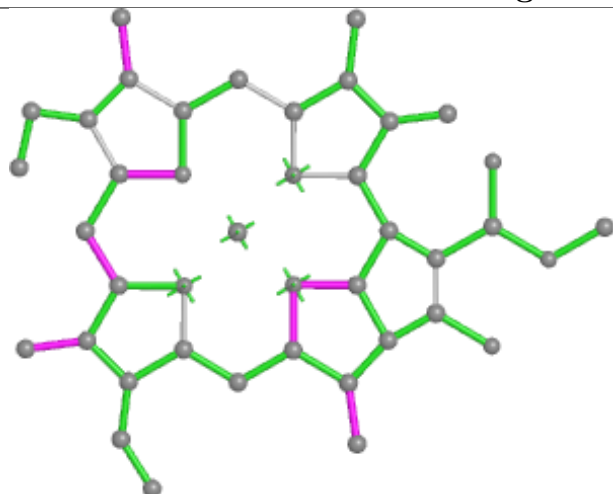




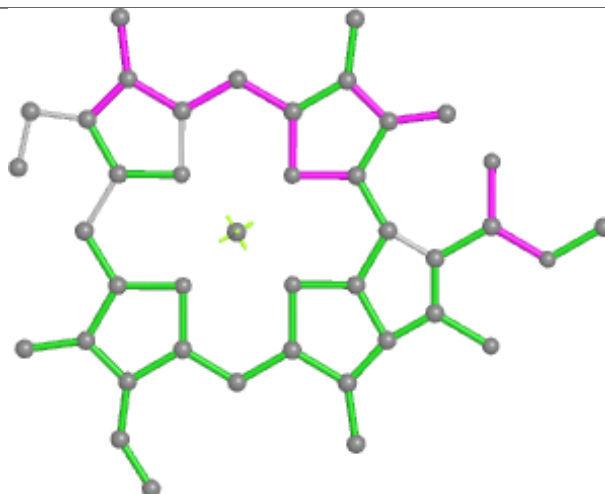




## Ligand CLA F 304



Bond lengths



Bond angles

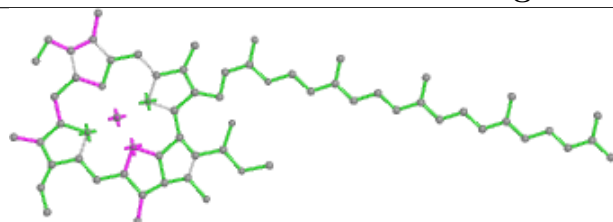


Torsions

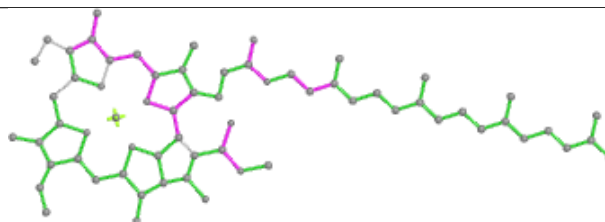


Rings

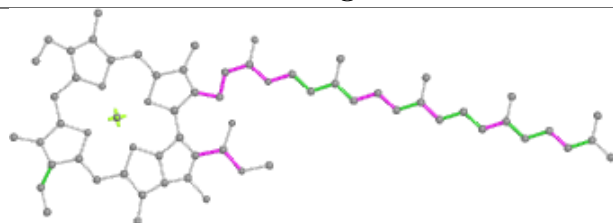
## Ligand CLA A 841



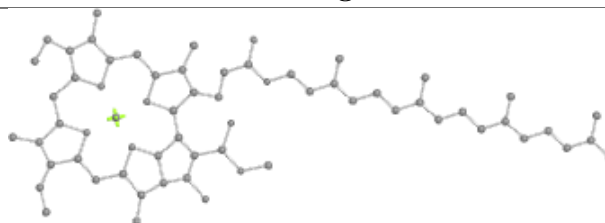
Bond lengths



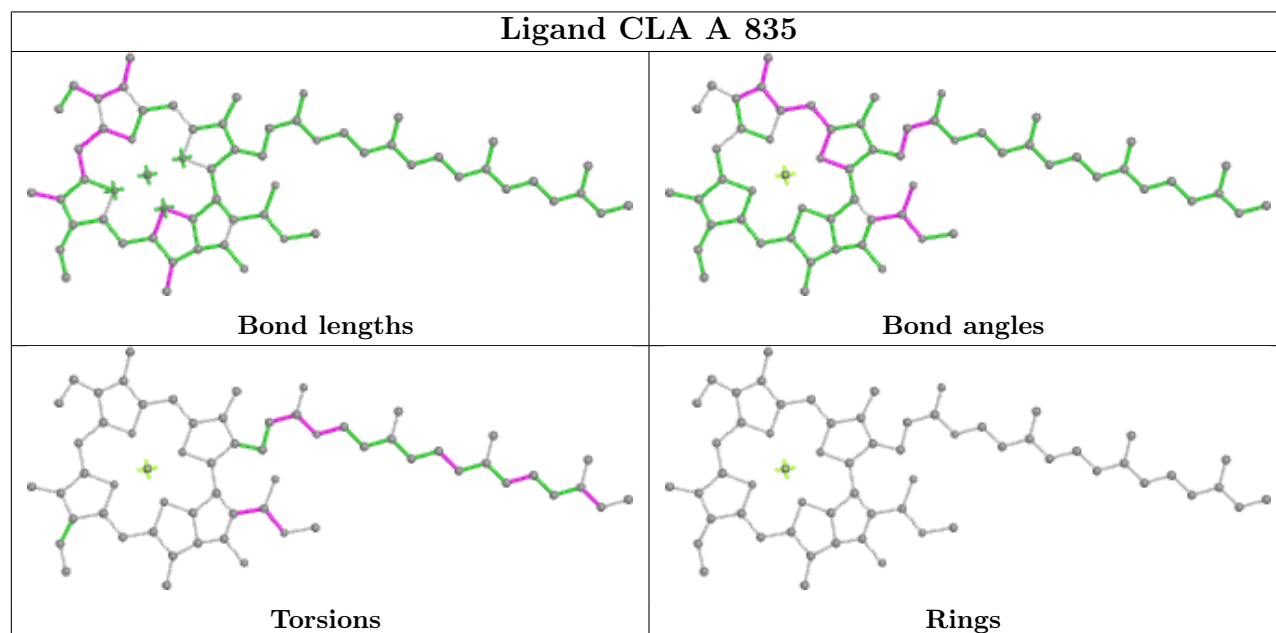
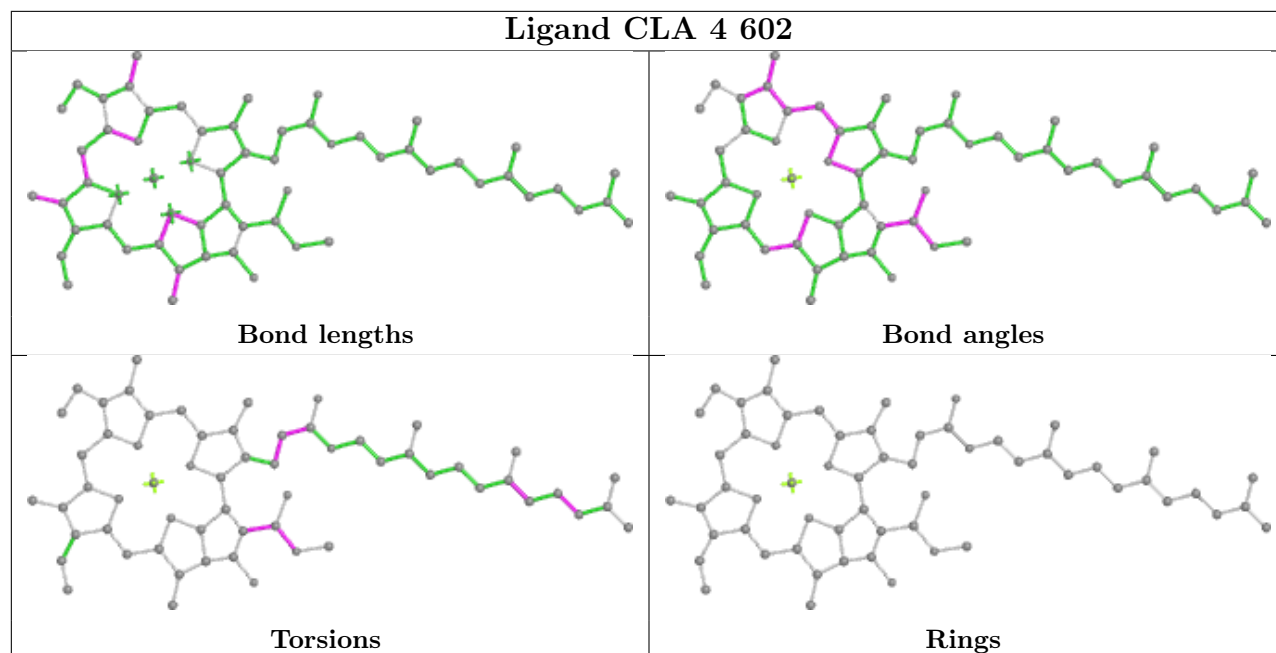
Bond angles



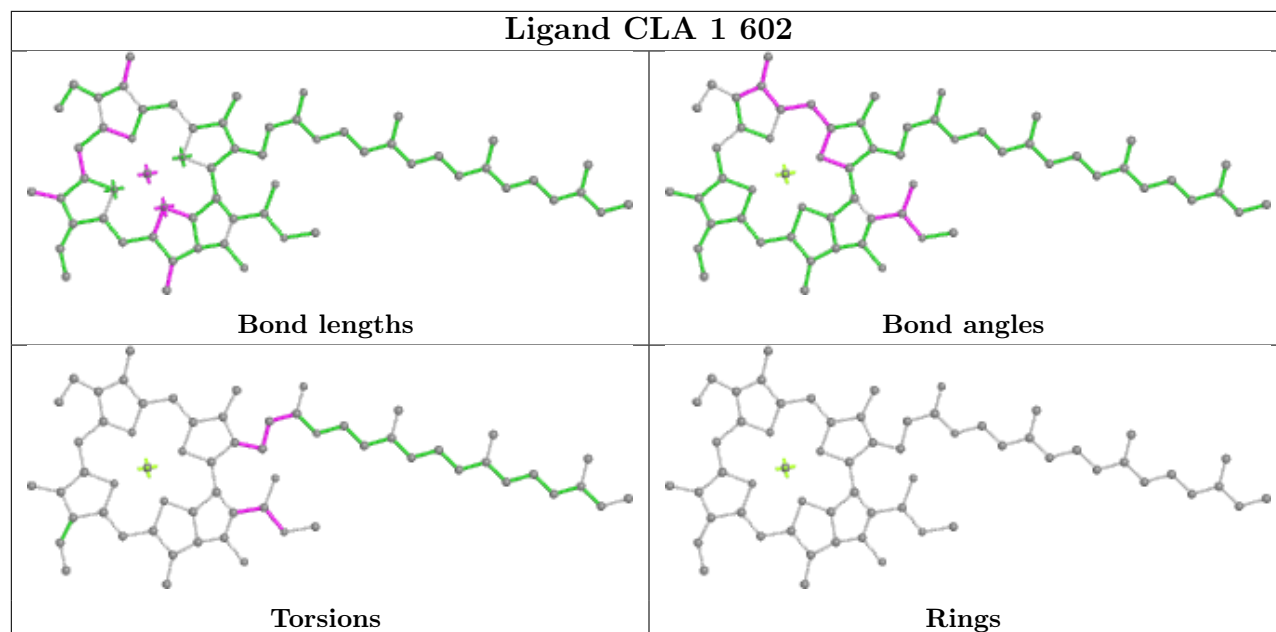
Torsions



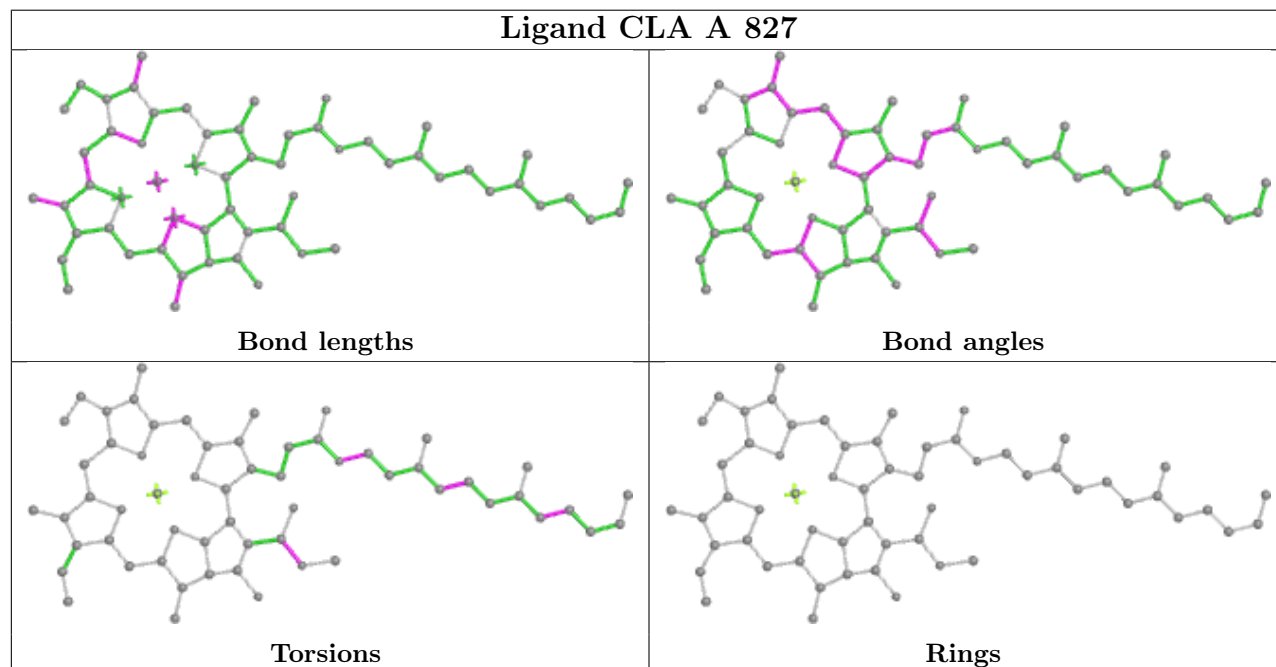
Rings



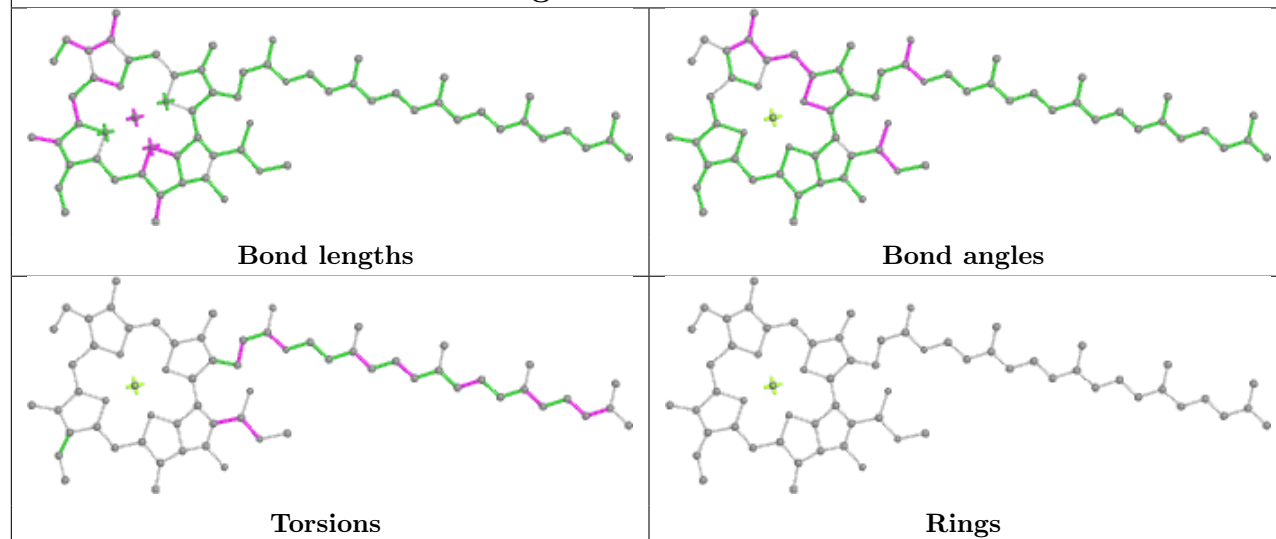
## Ligand CLA 1 602



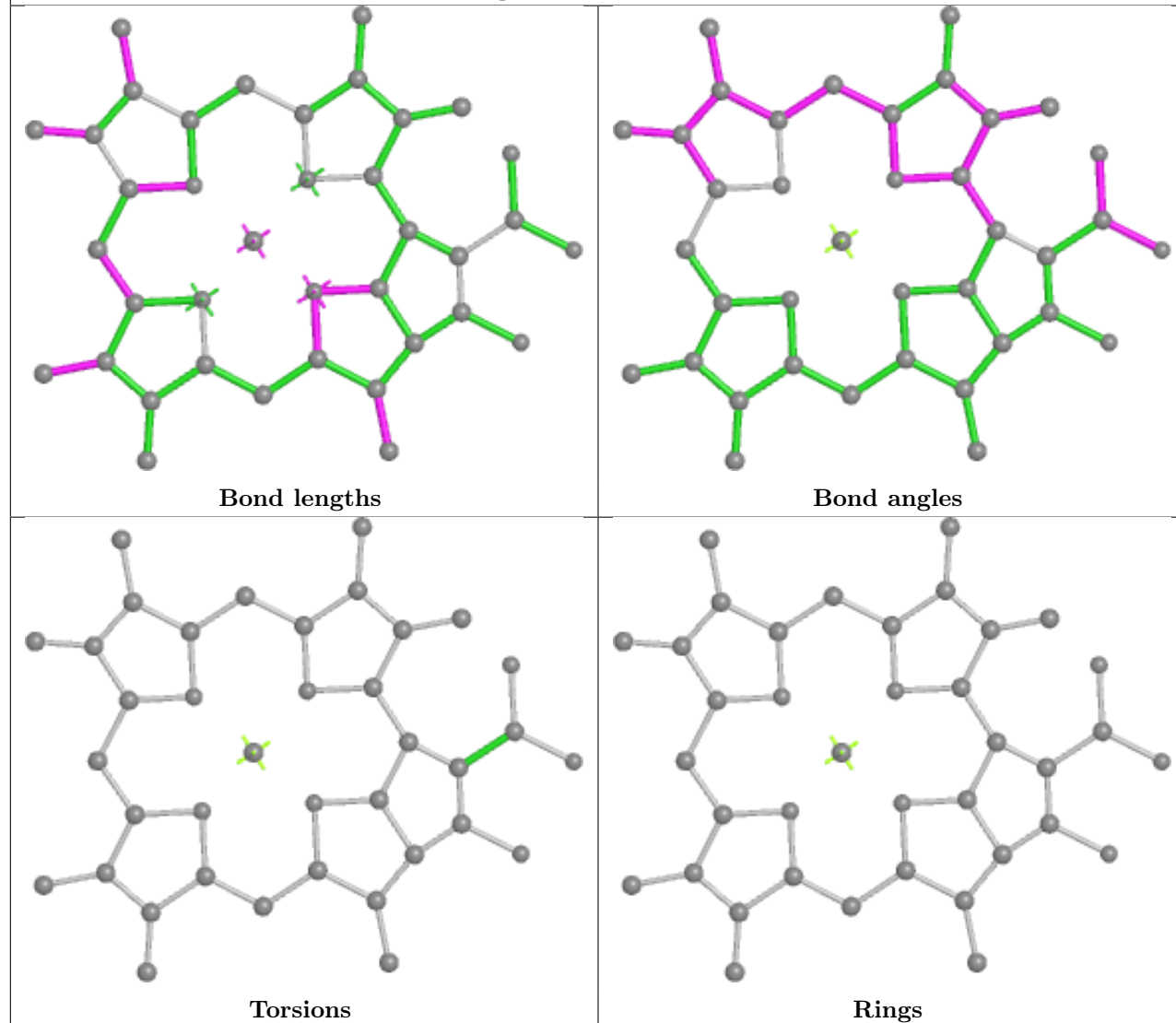
## Ligand CLA A 827

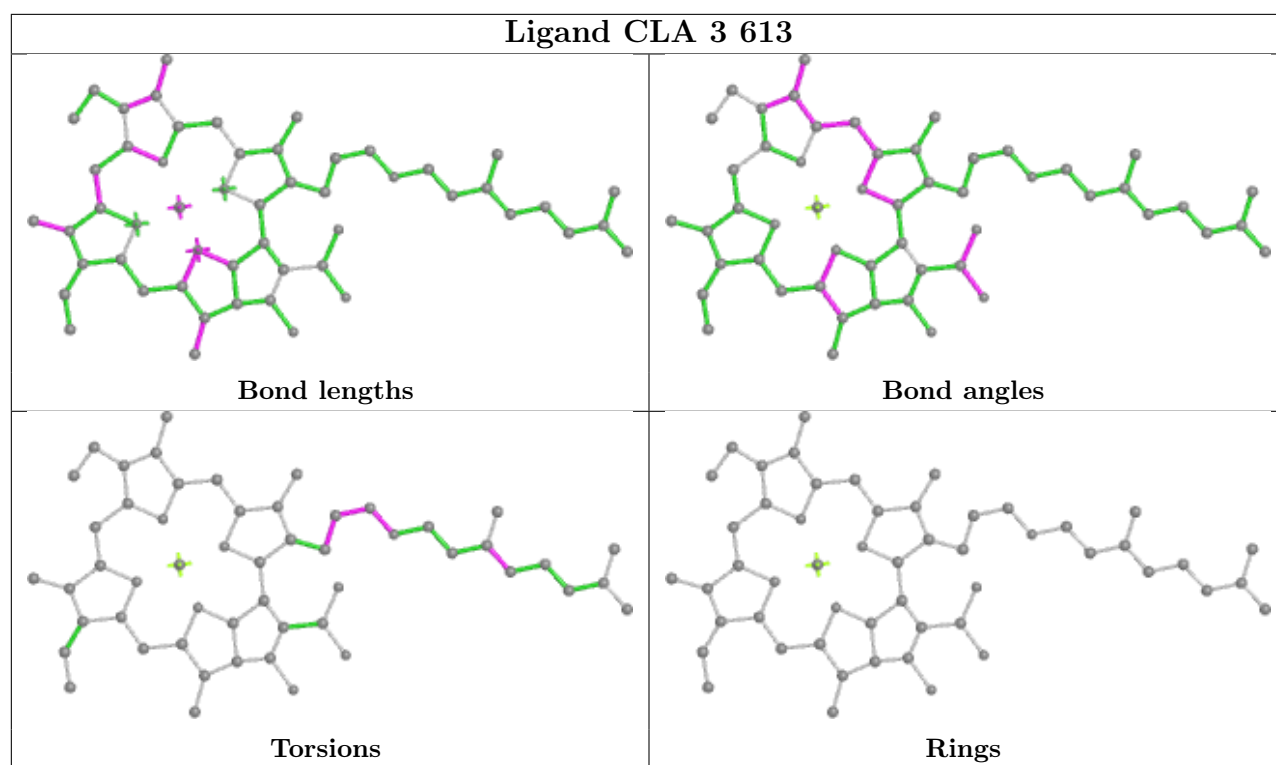


## Ligand CLA B 837

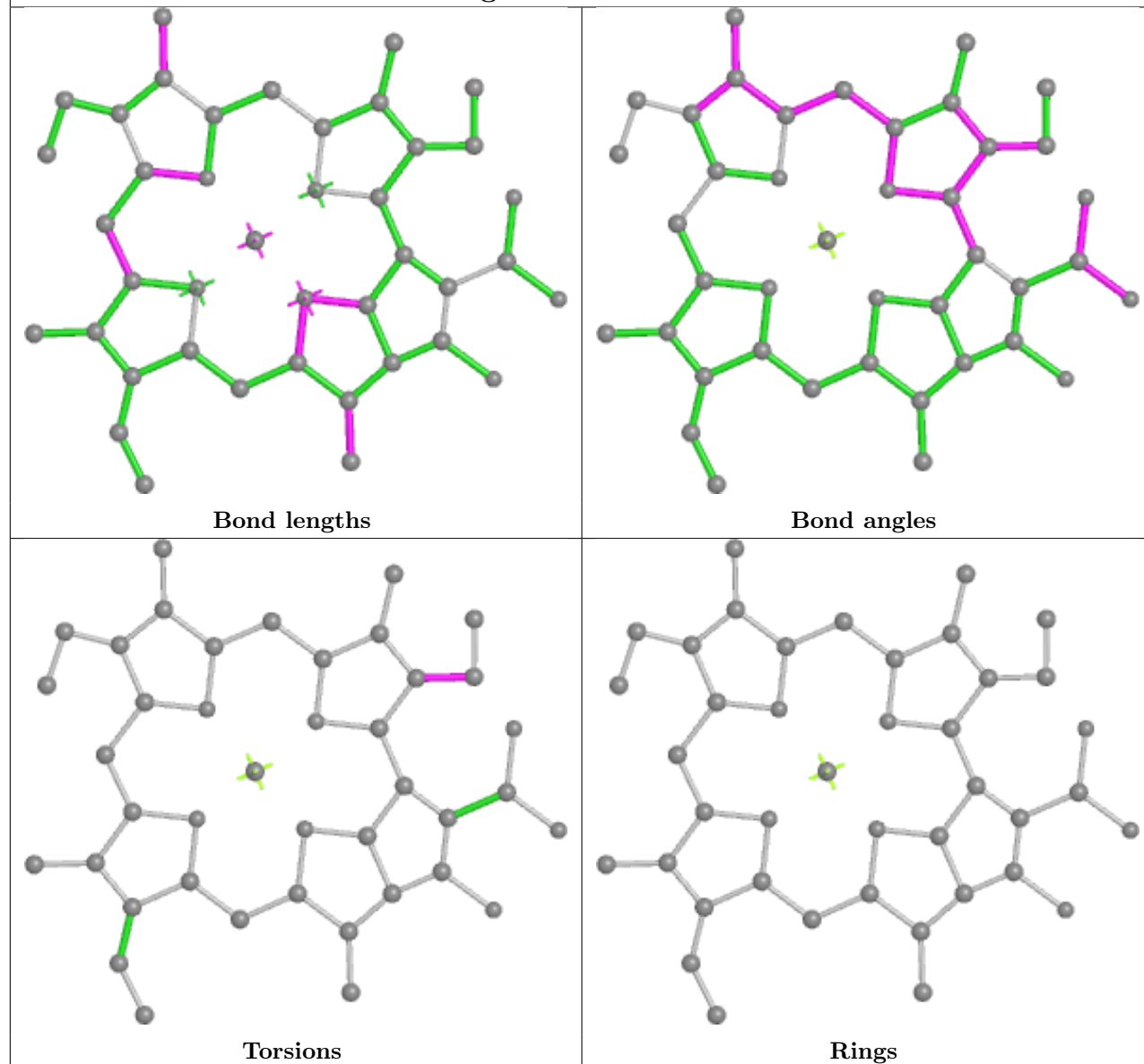


## Ligand CLA a 611

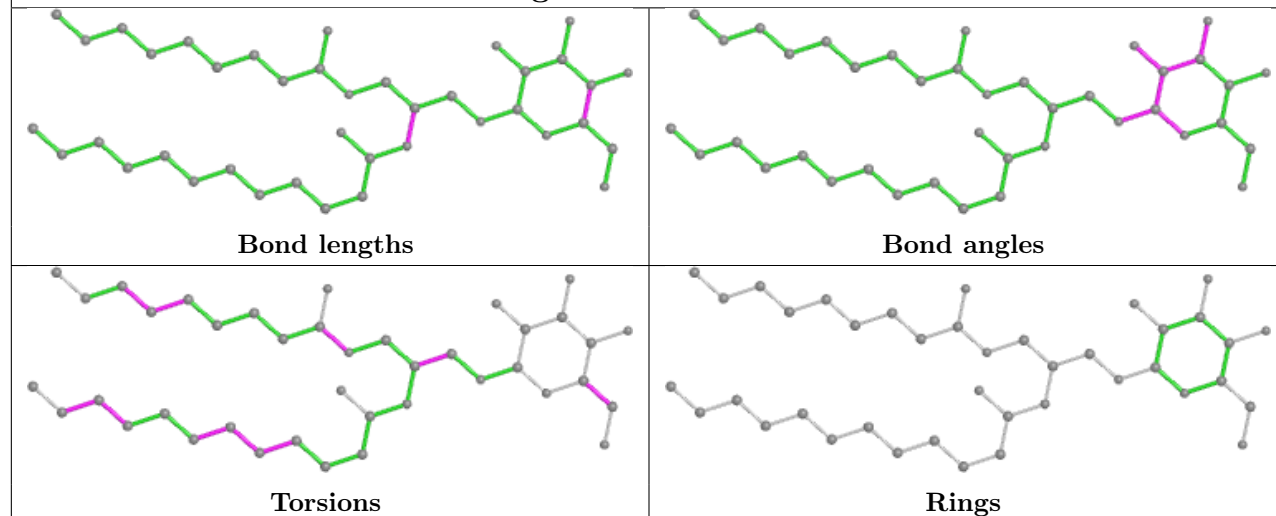


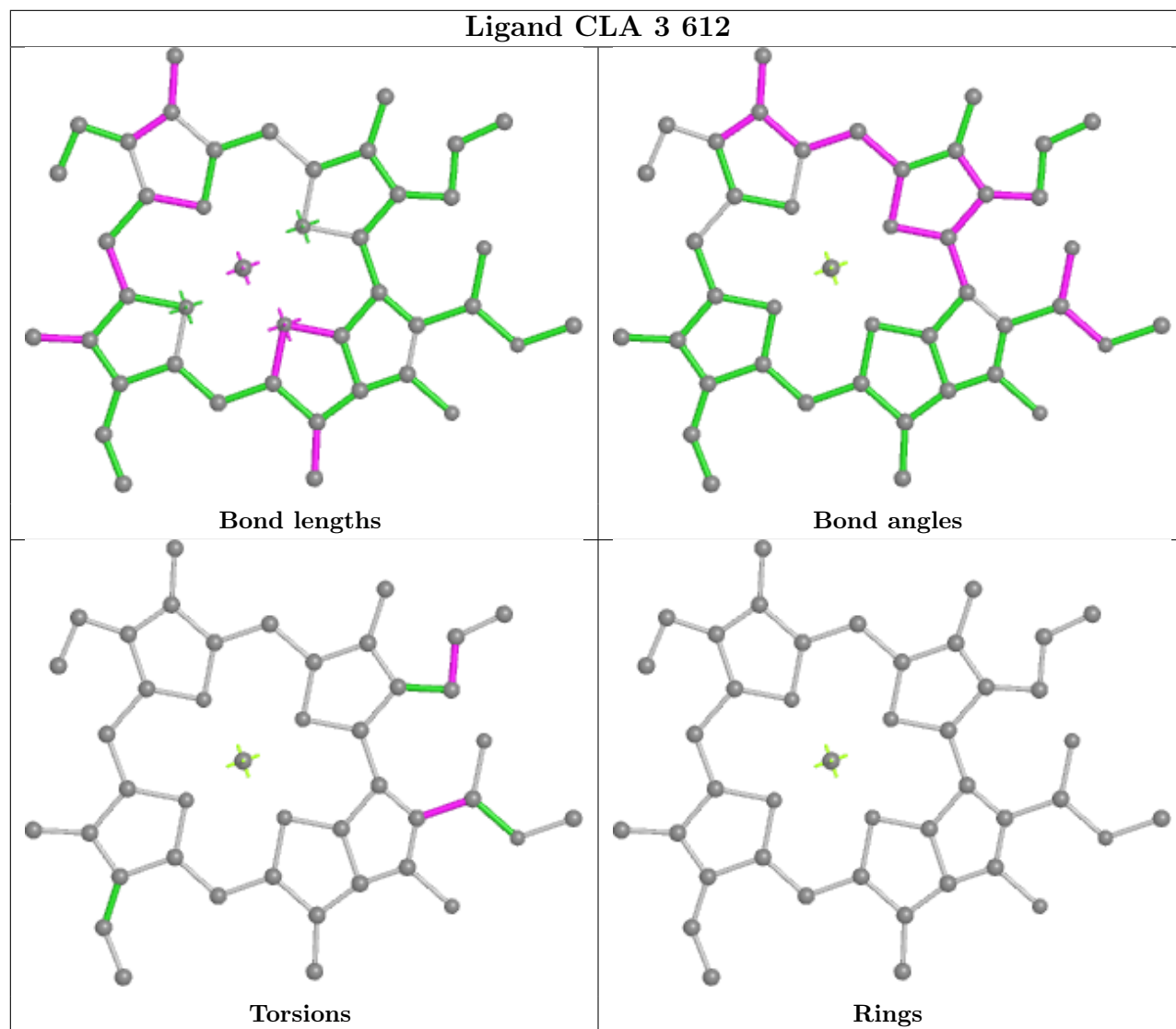
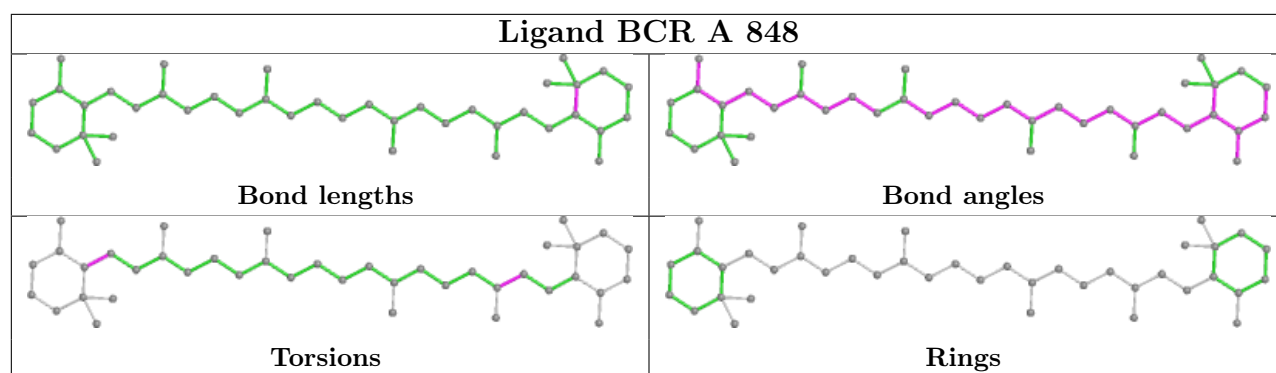


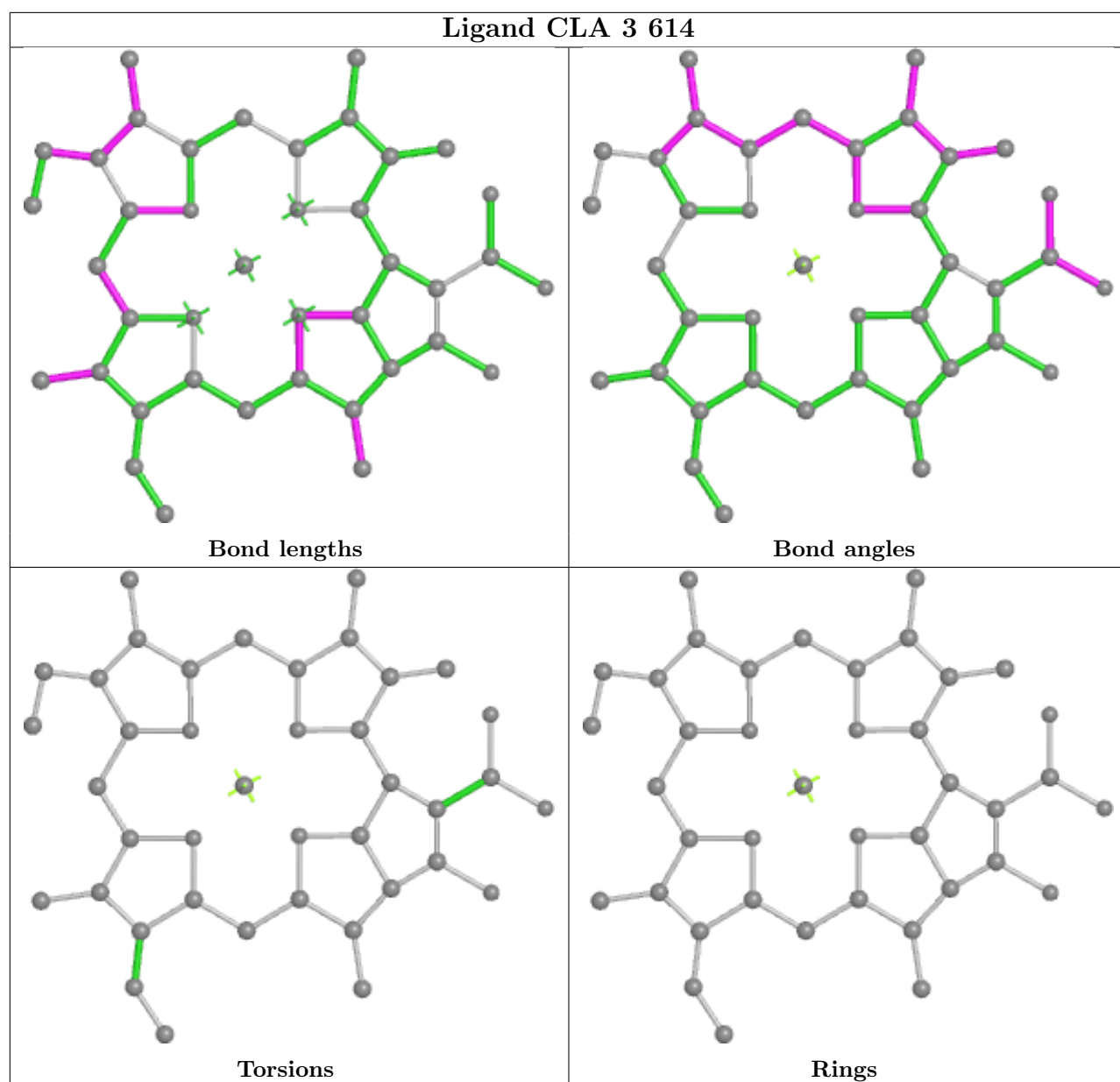
## Ligand CLA 6 612



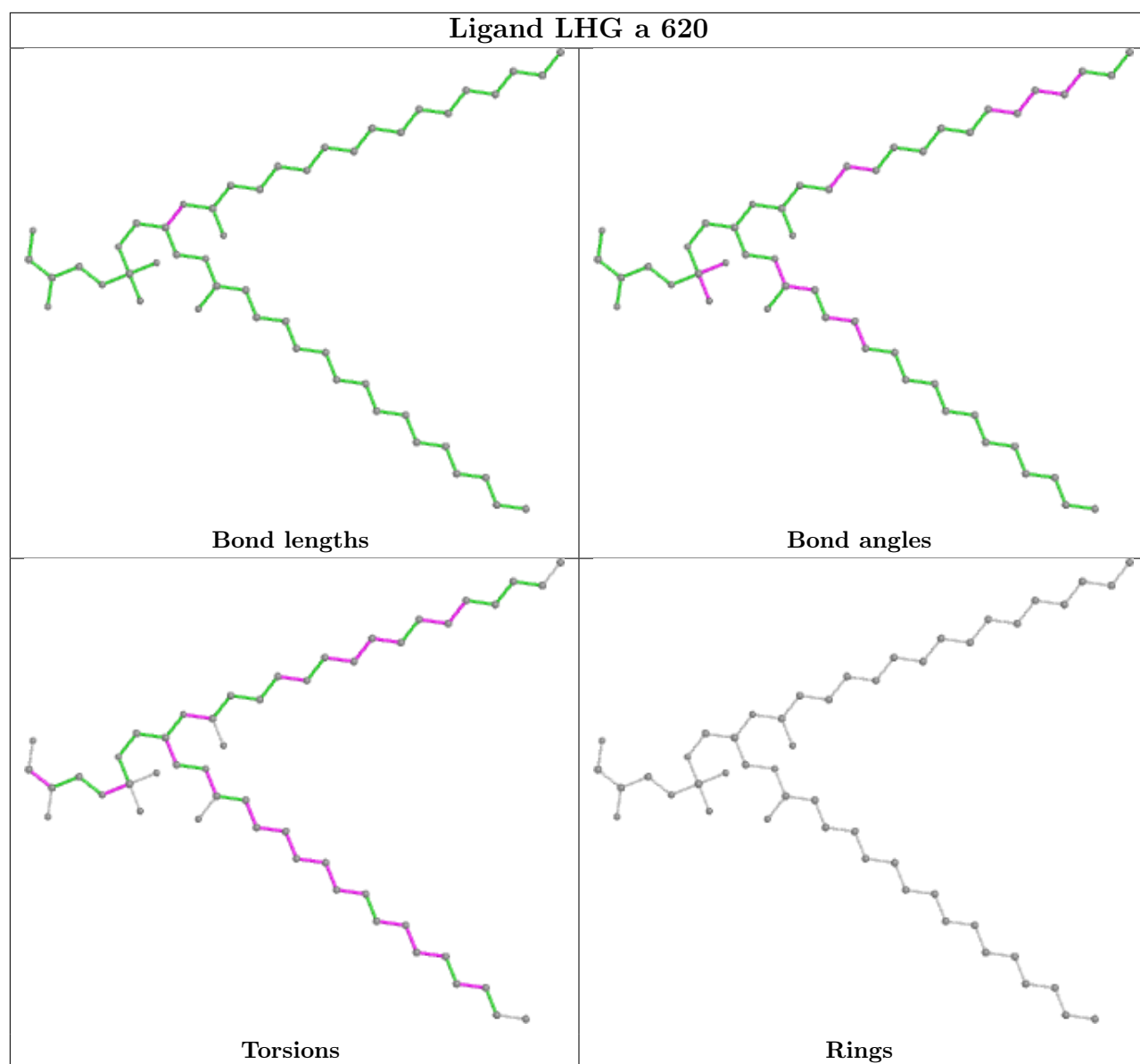
## Ligand LMG 5 627



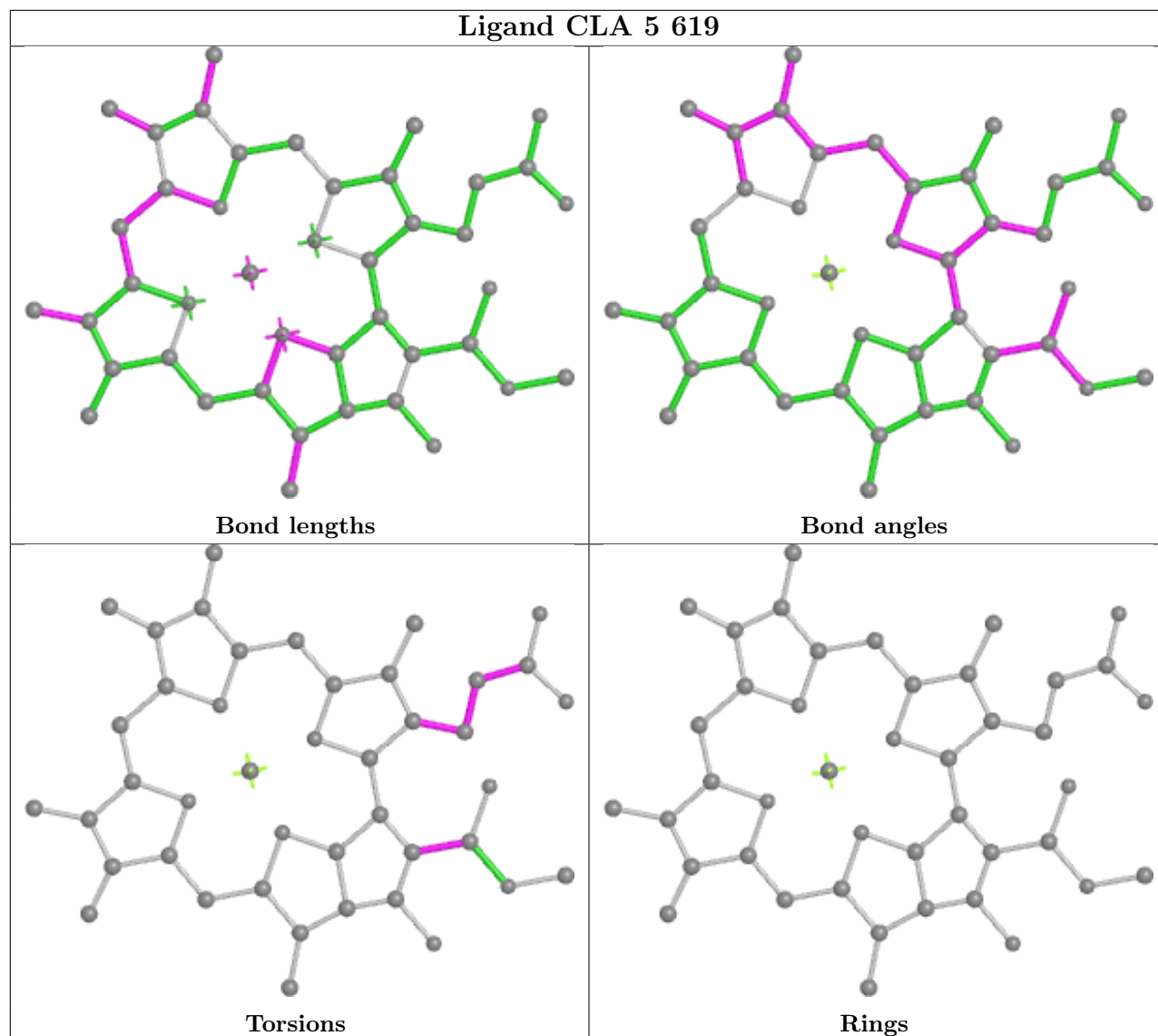




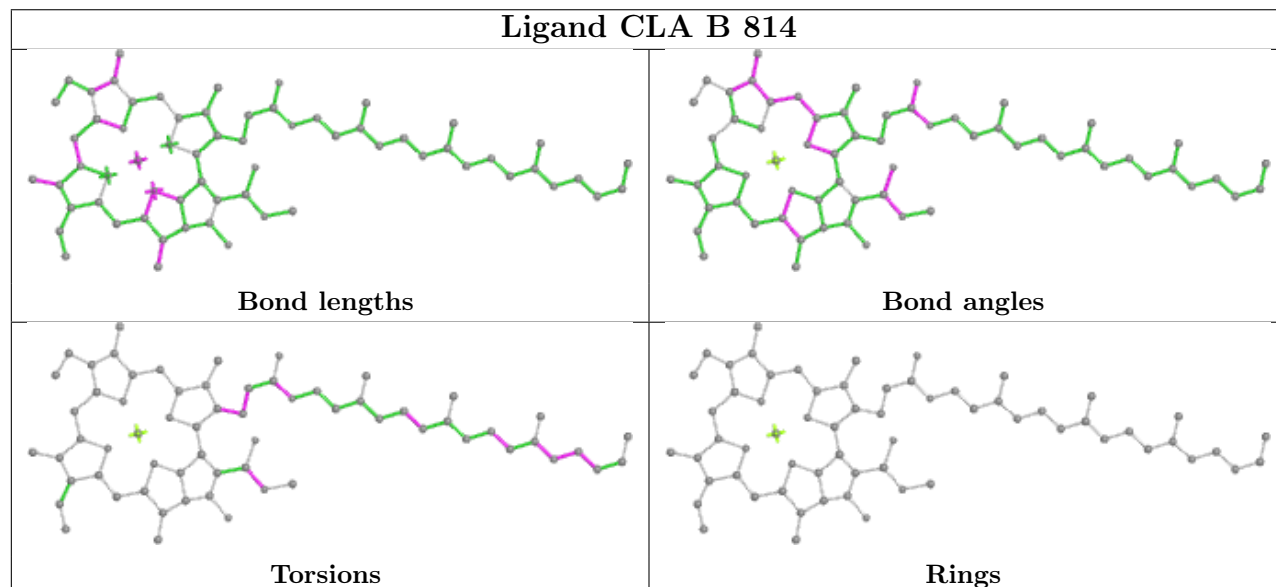


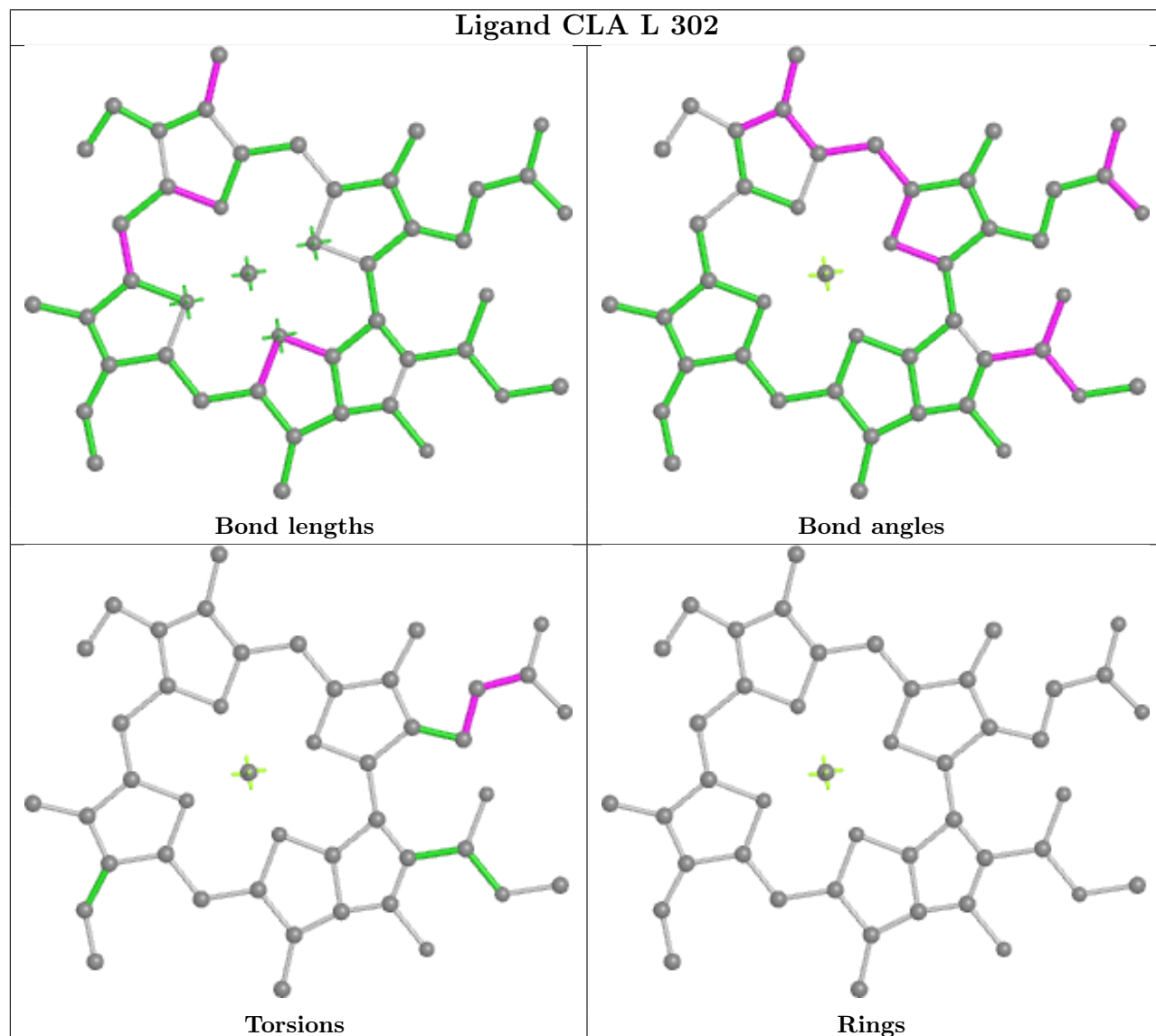
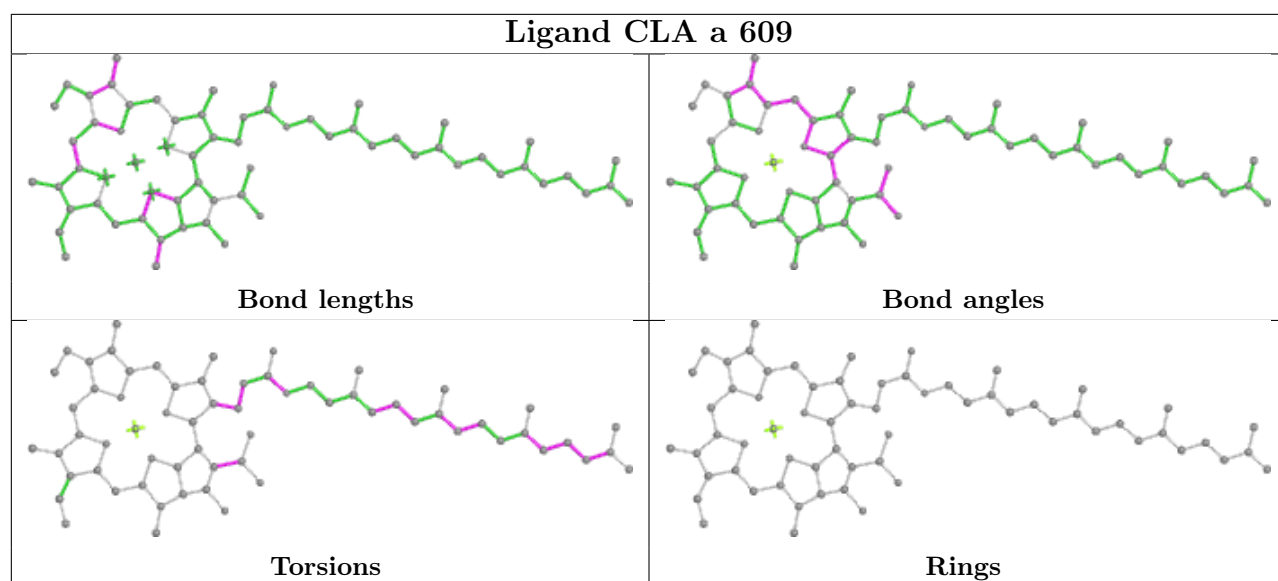


## Ligand CLA 5 619

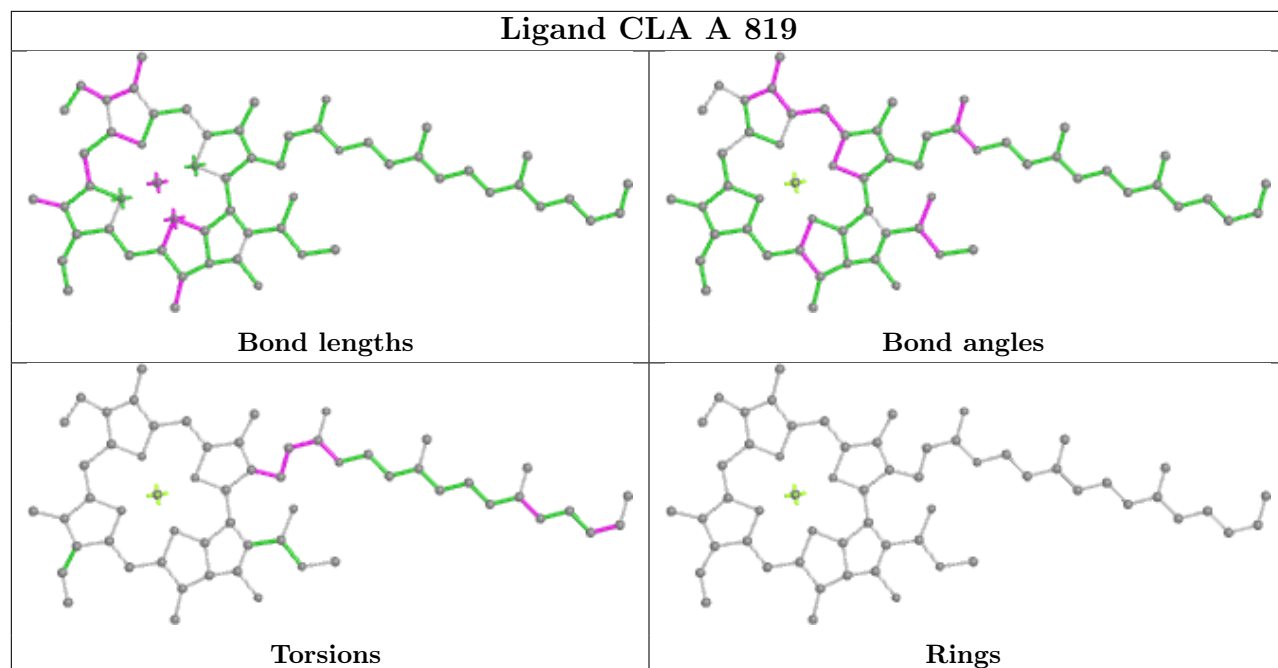


## Ligand CLA B 814

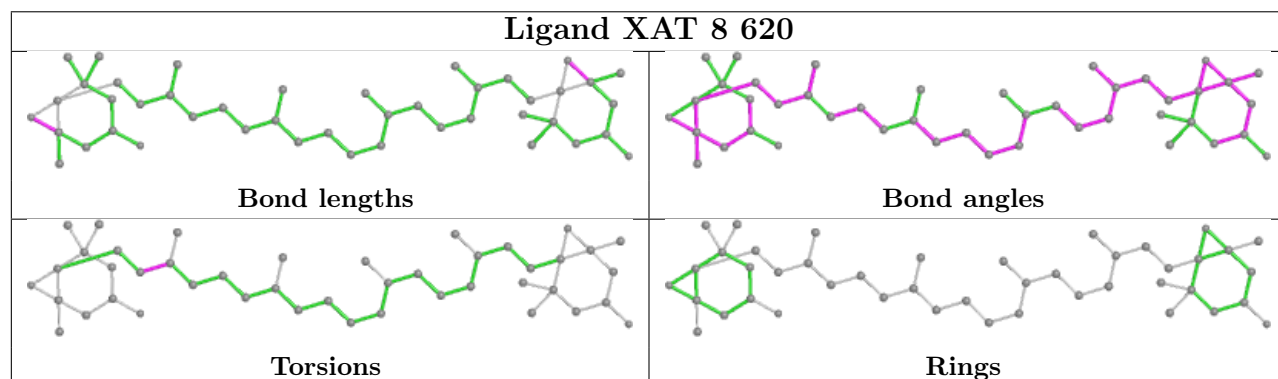




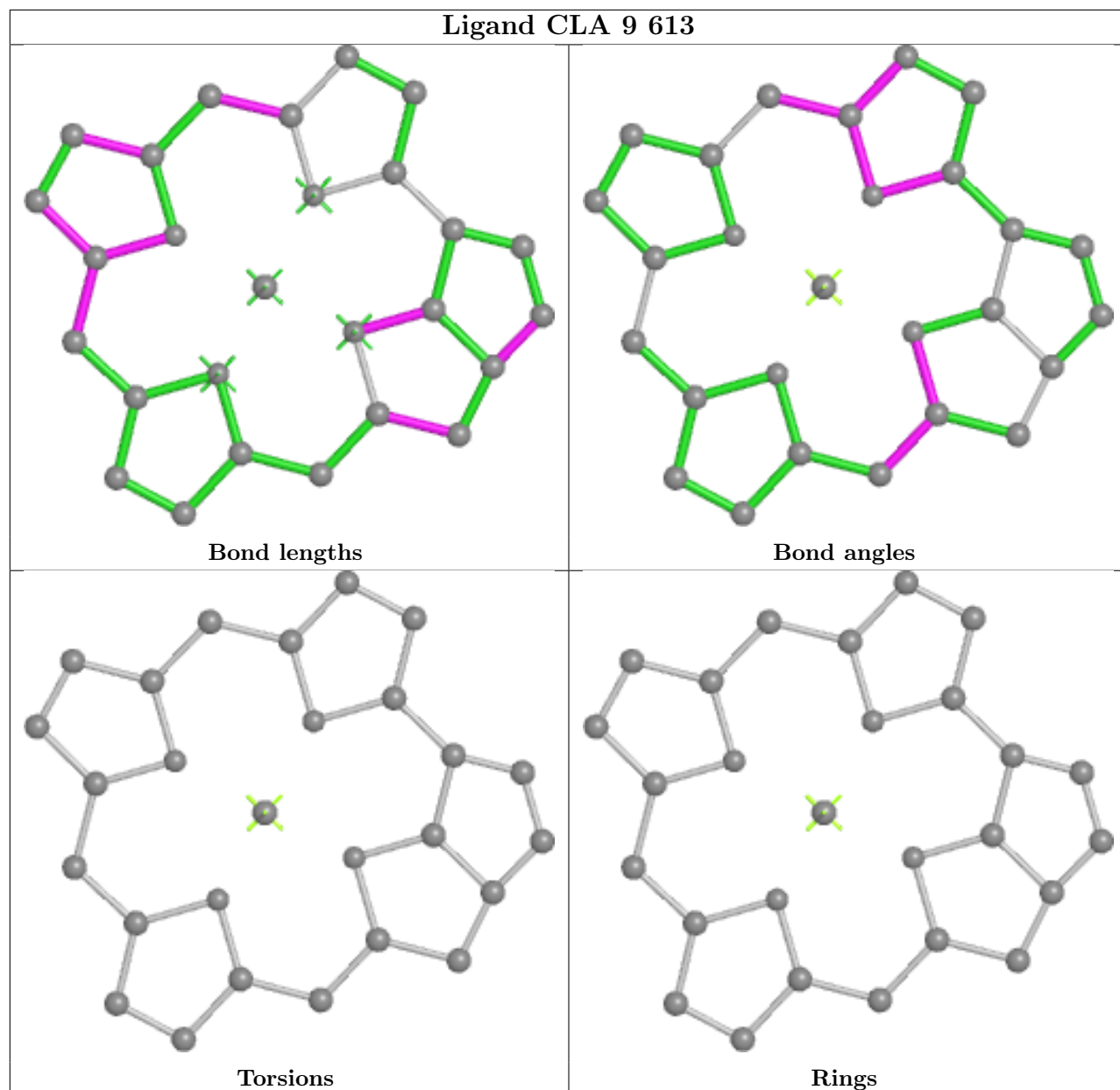
## Ligand CLA A 819



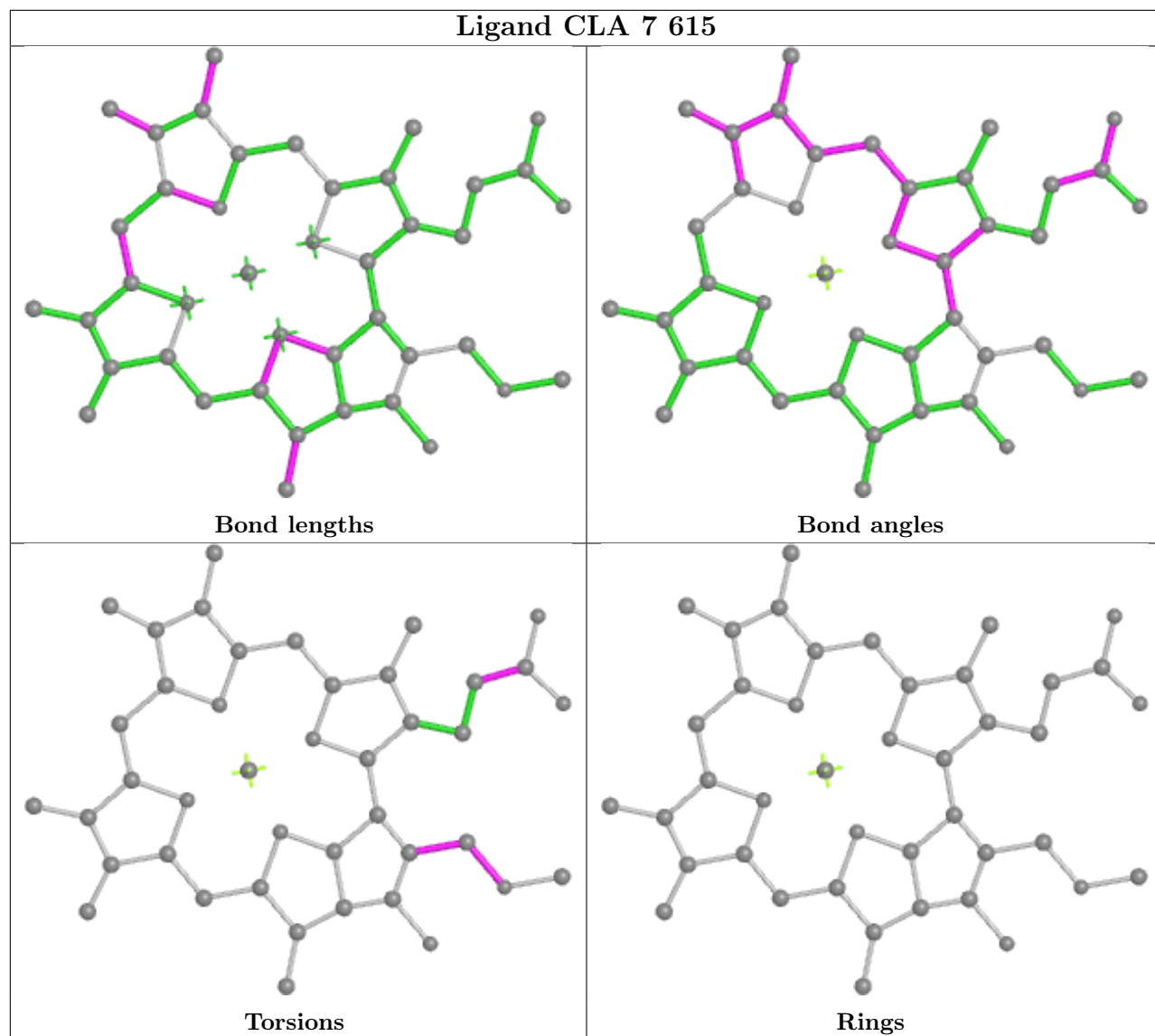
## Ligand XAT 8 620



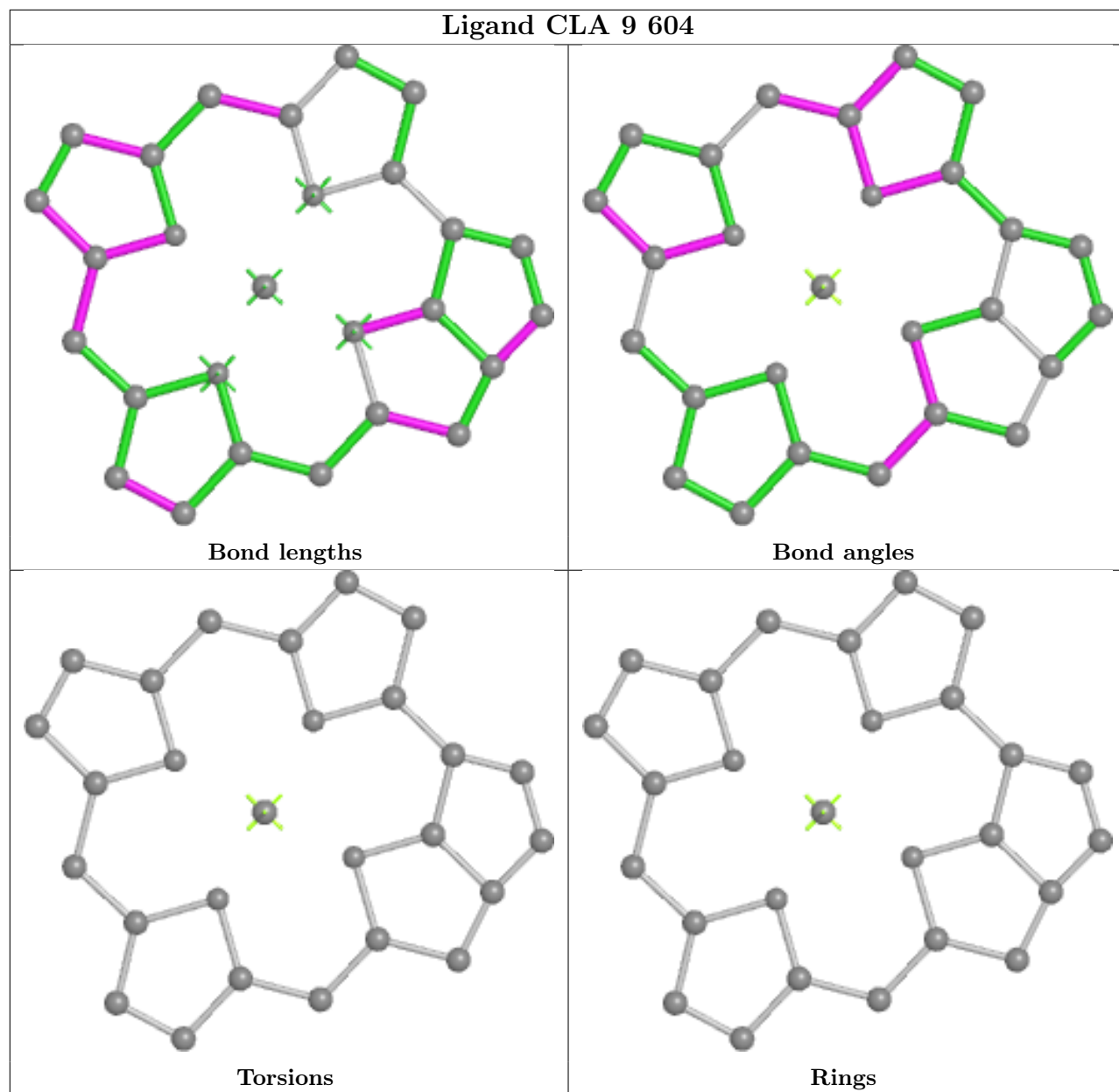
## Ligand CLA 9 613

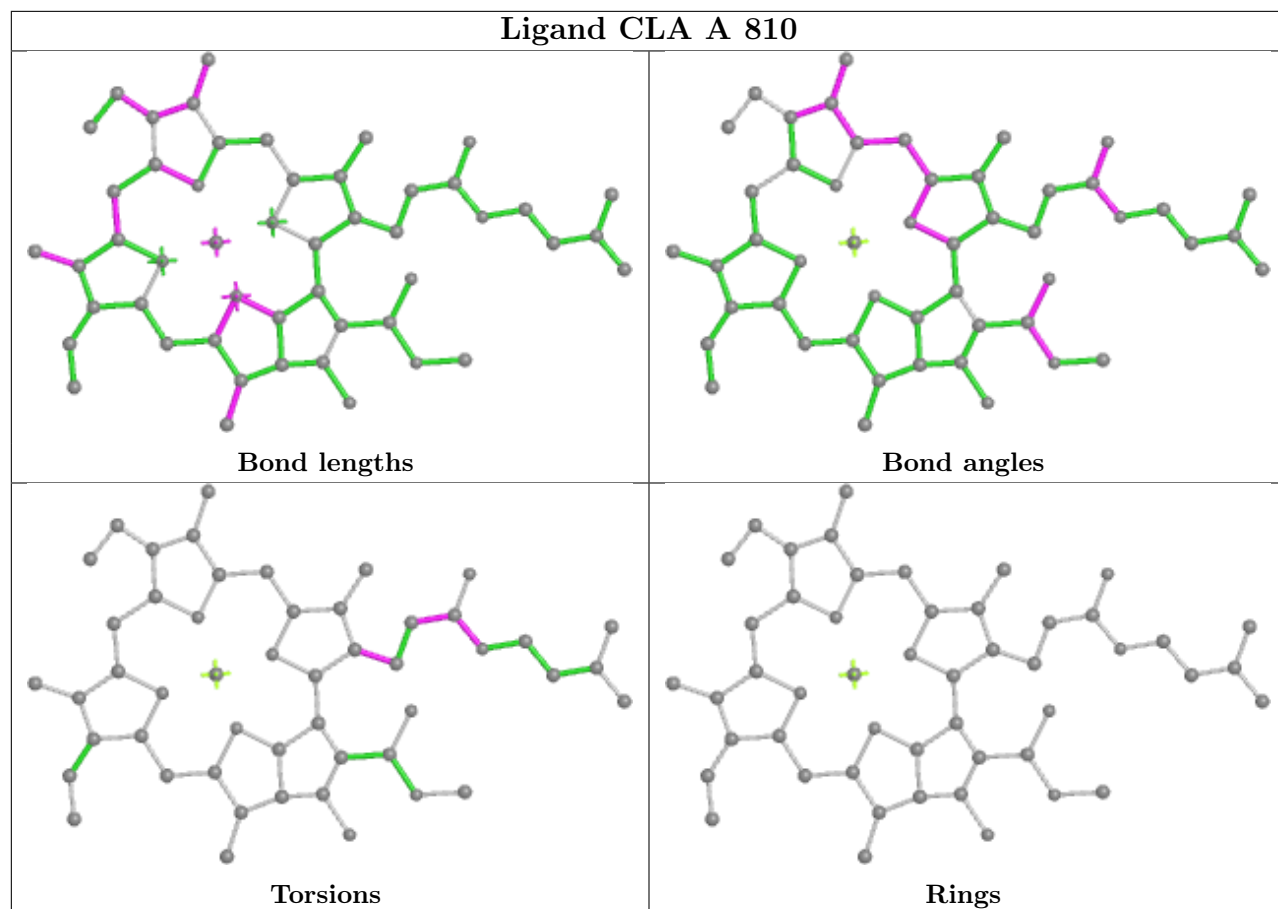


## Ligand CLA 7 615



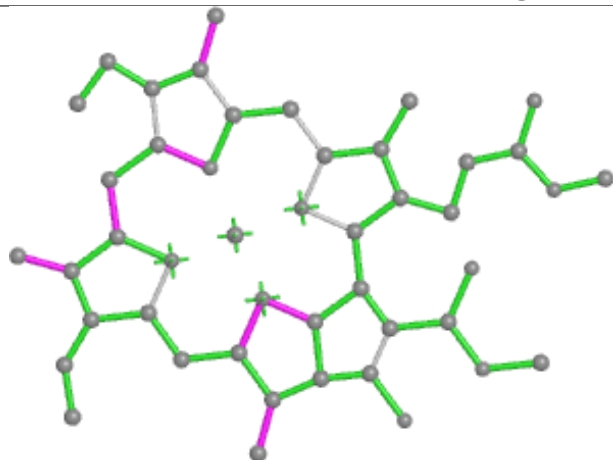
## Ligand CLA 9 604



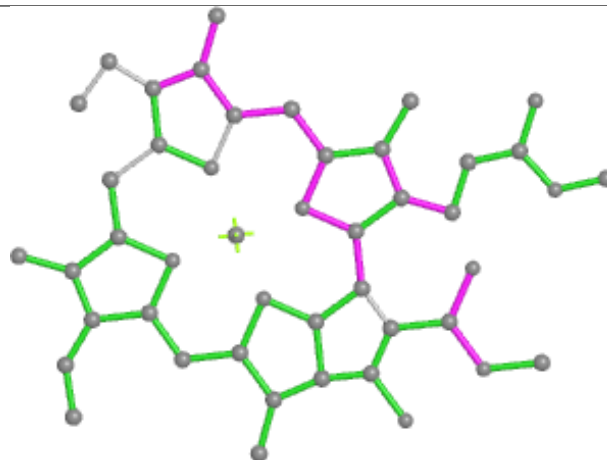




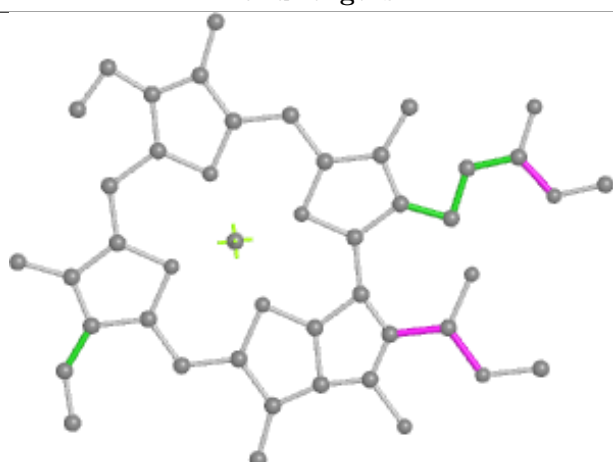
## Ligand CLA K 204



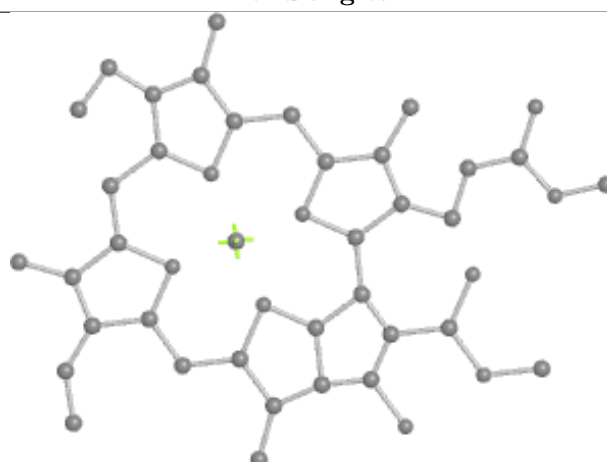
Bond lengths



Bond angles

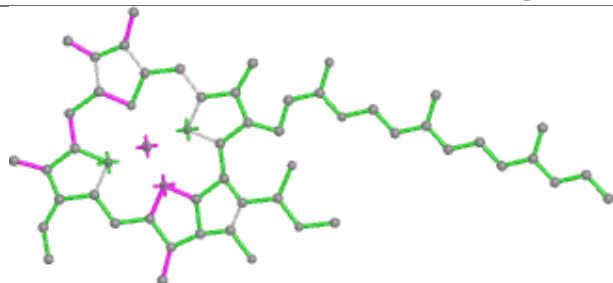


Torsions

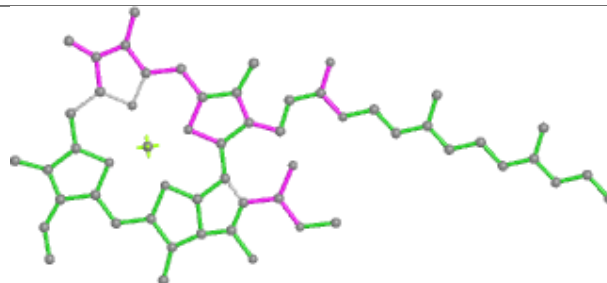


Rings

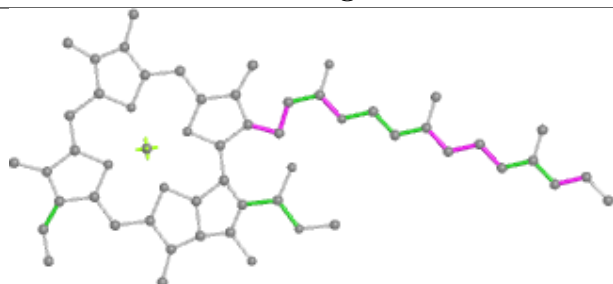
## Ligand CLA 3 607



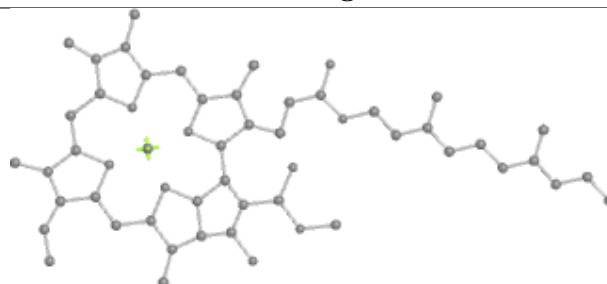
Bond lengths



Bond angles

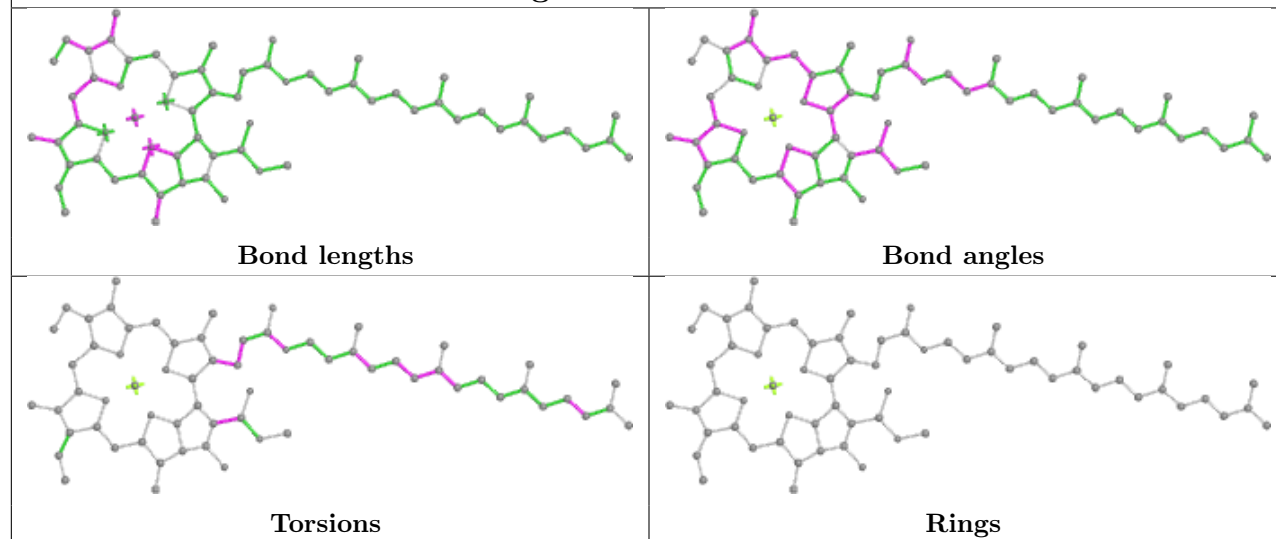


Torsions

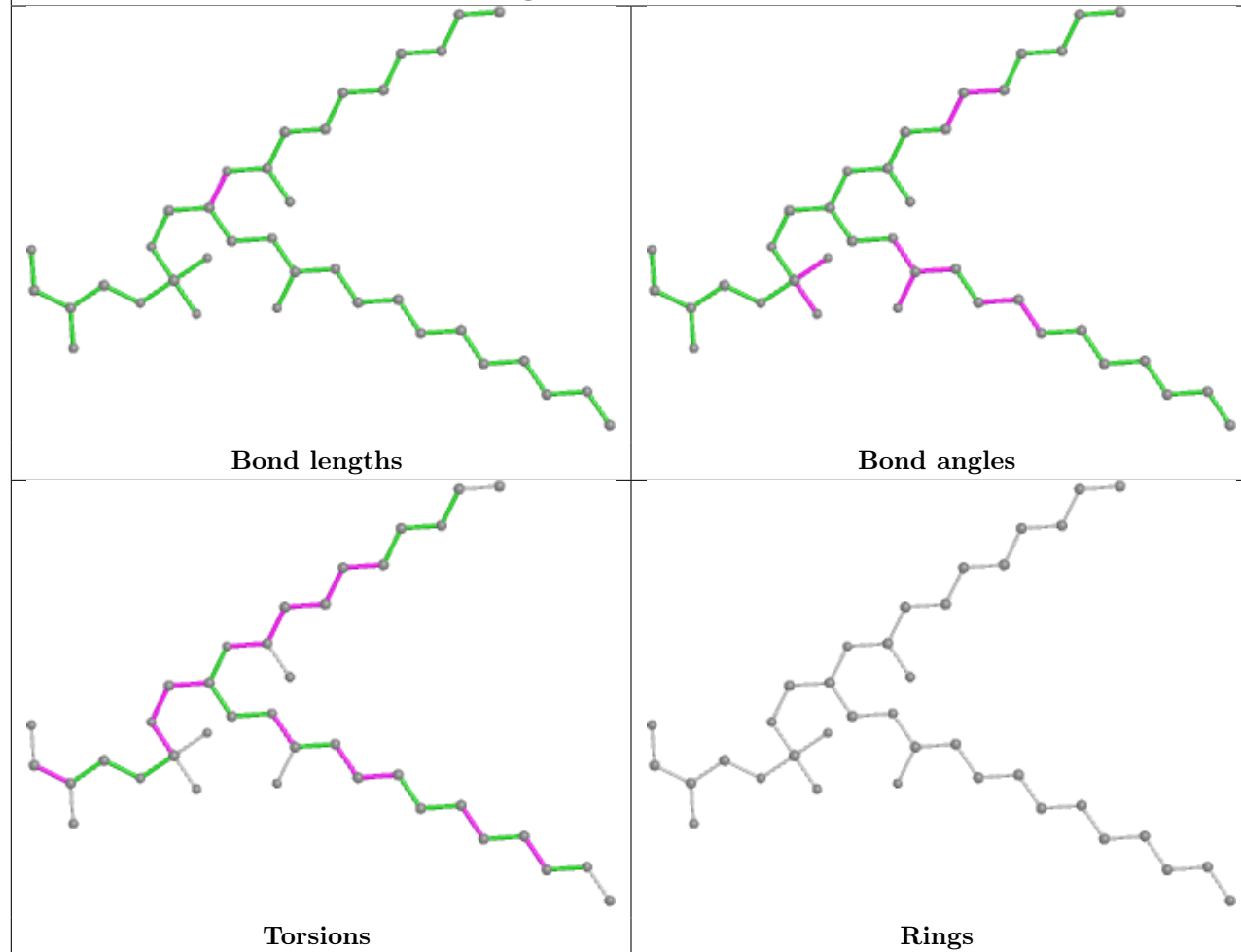


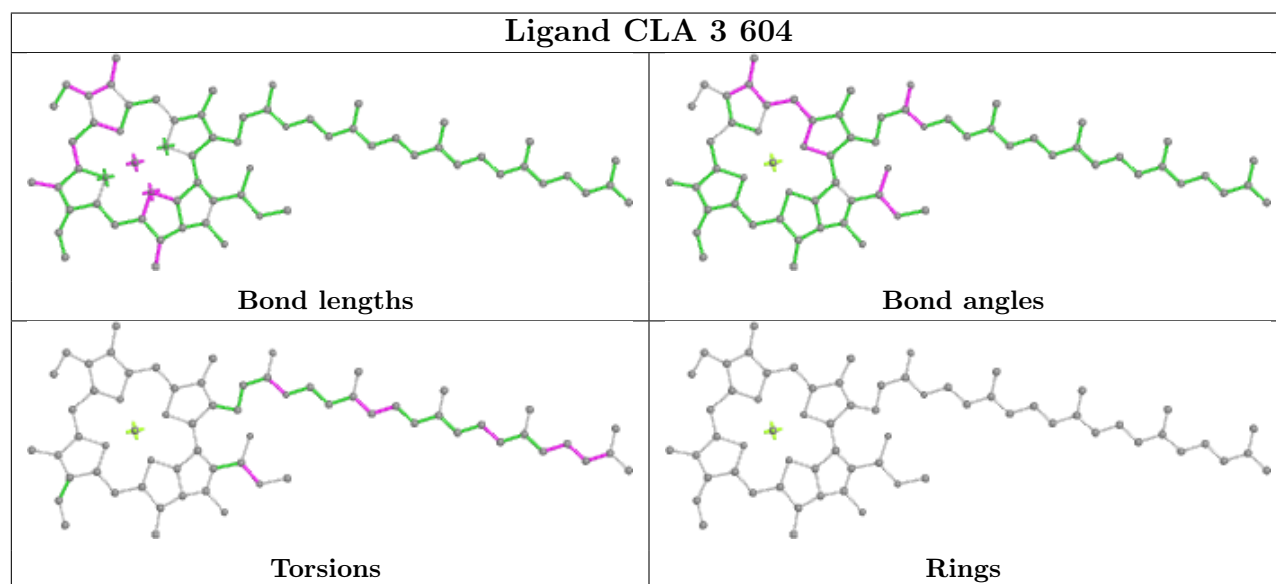
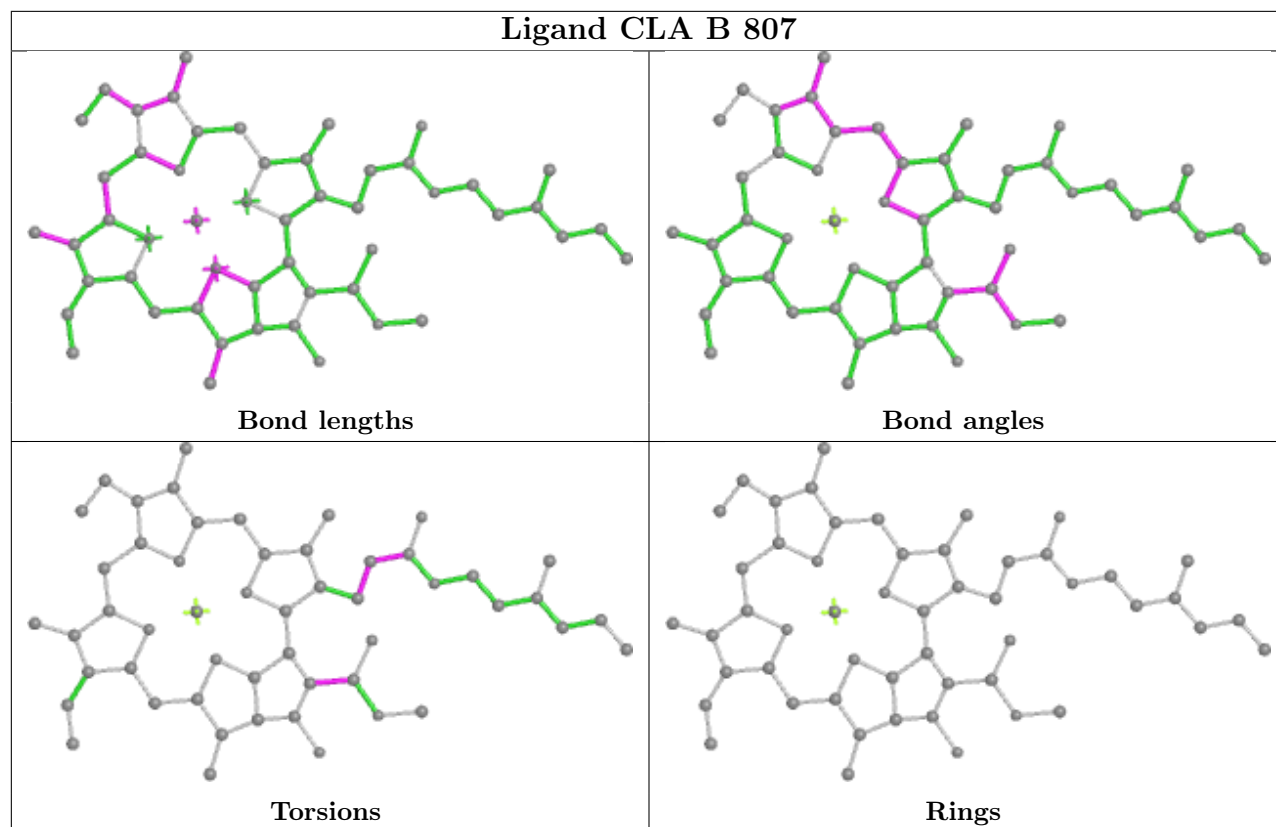
Rings

## Ligand CLA A 820

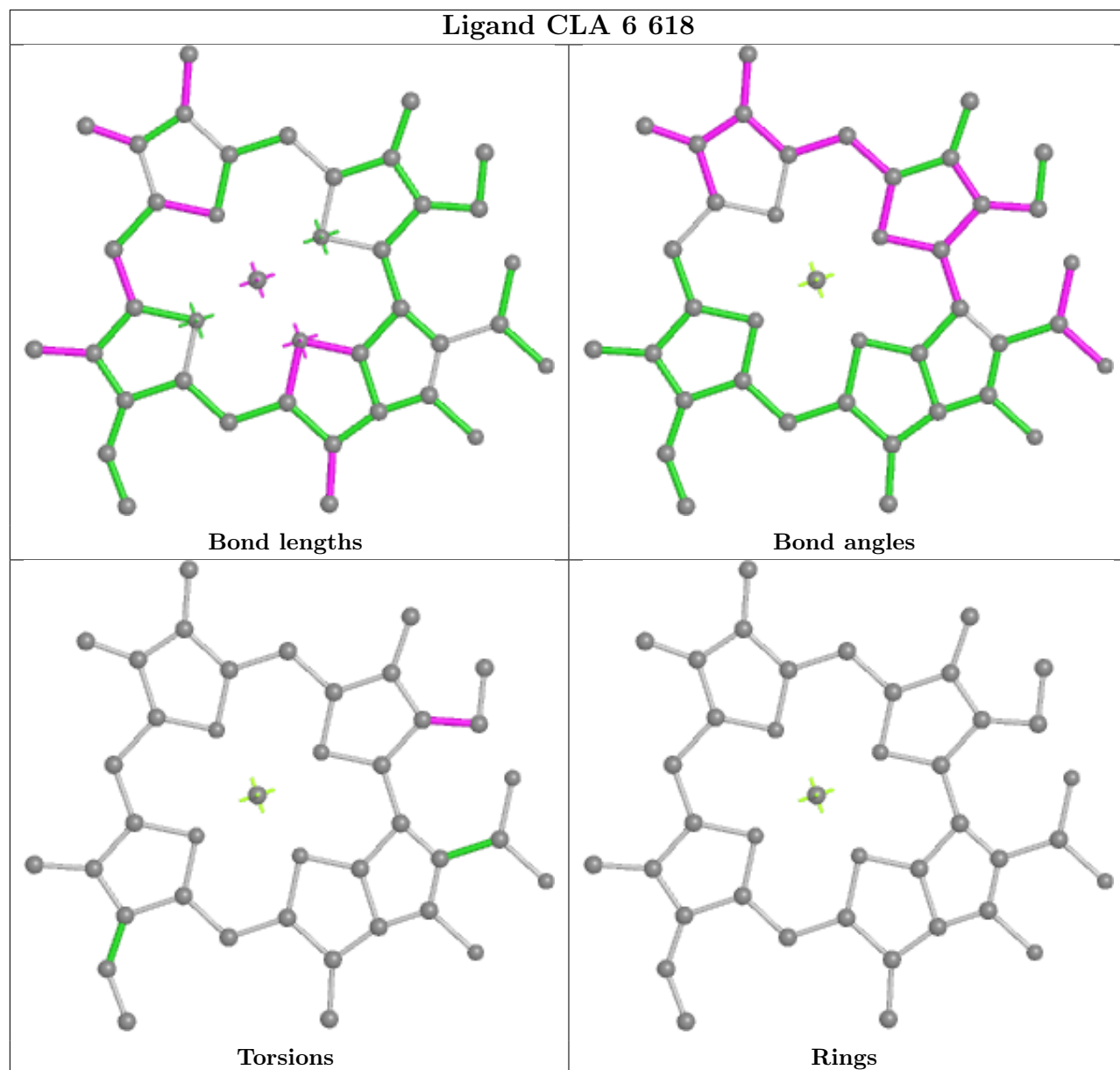


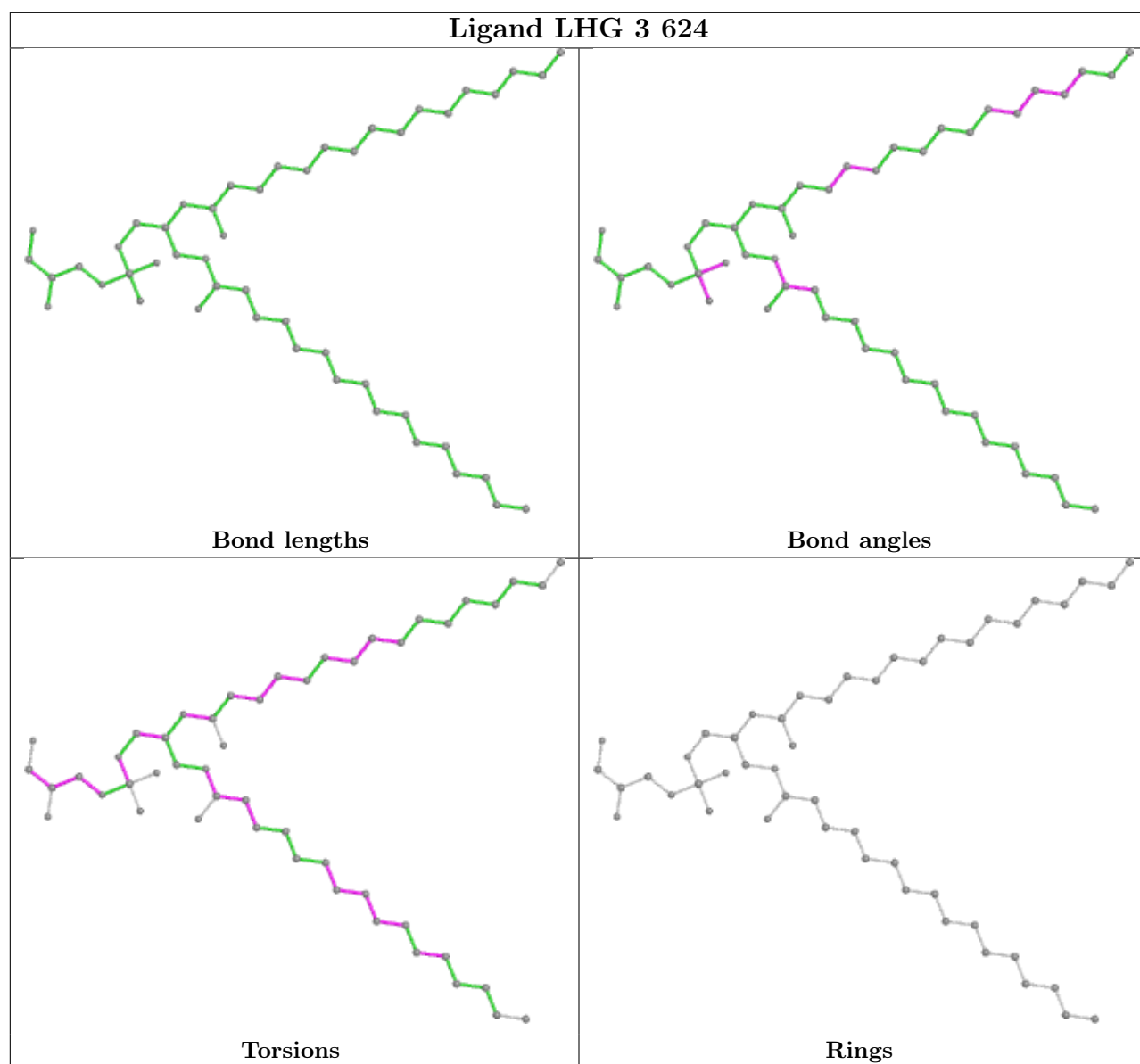
## Ligand LHG 2 622



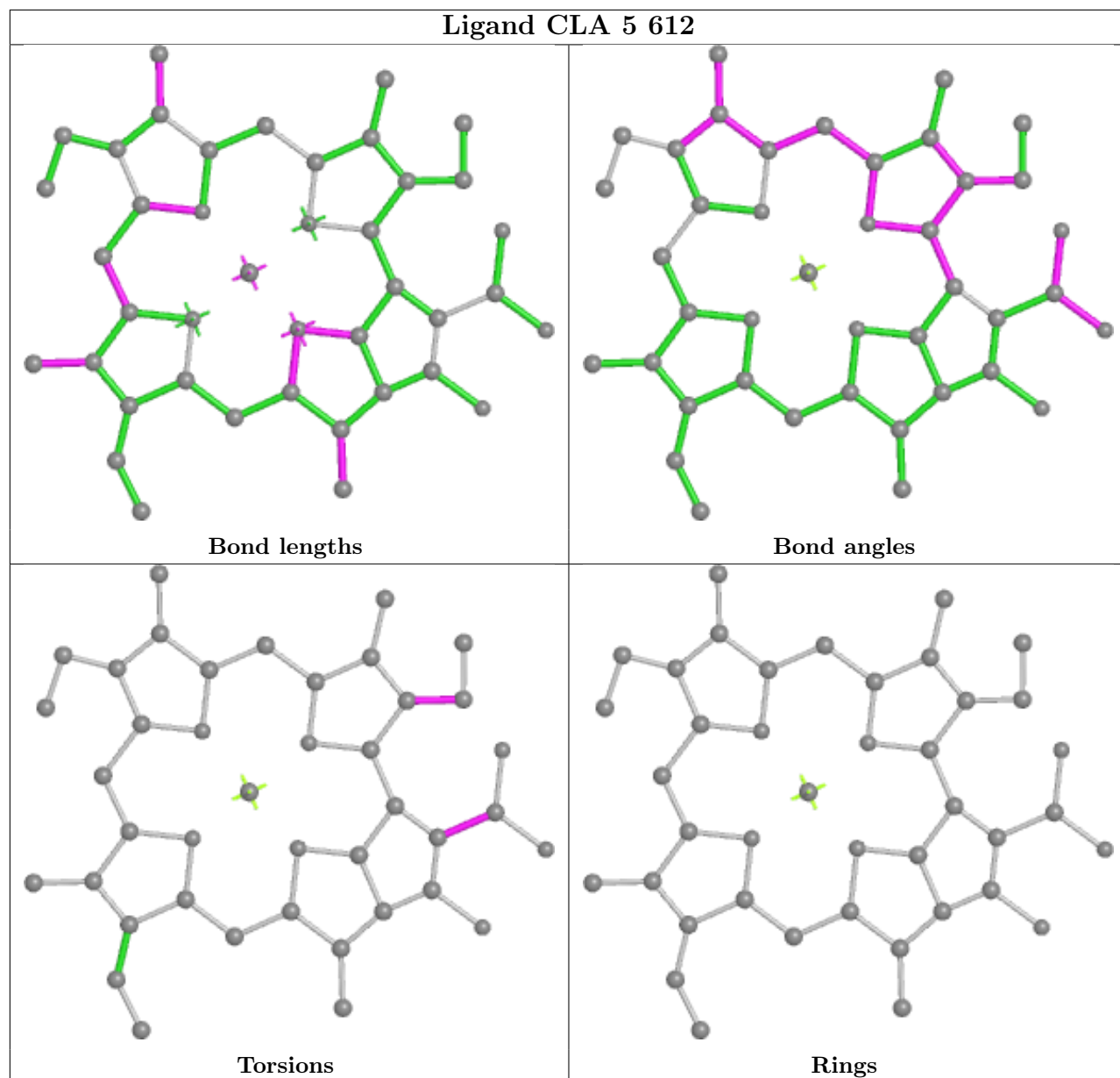


## Ligand CLA 6 618

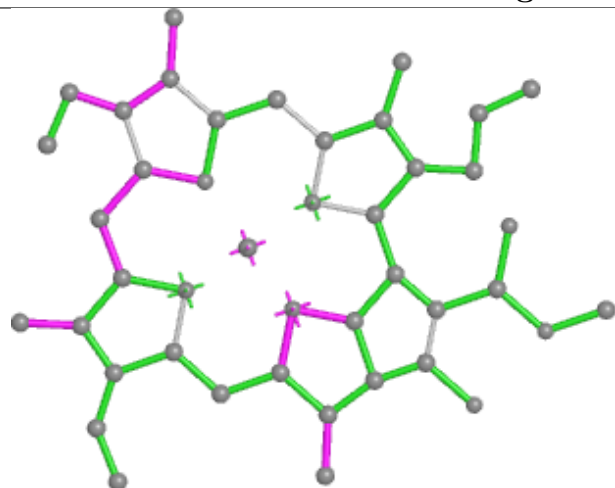




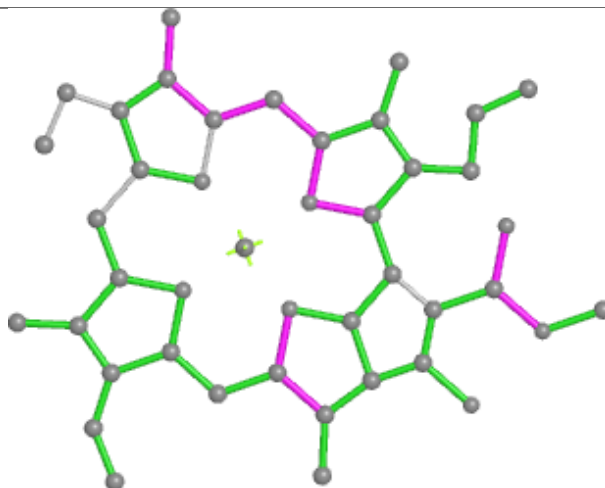
## Ligand CLA 5 612



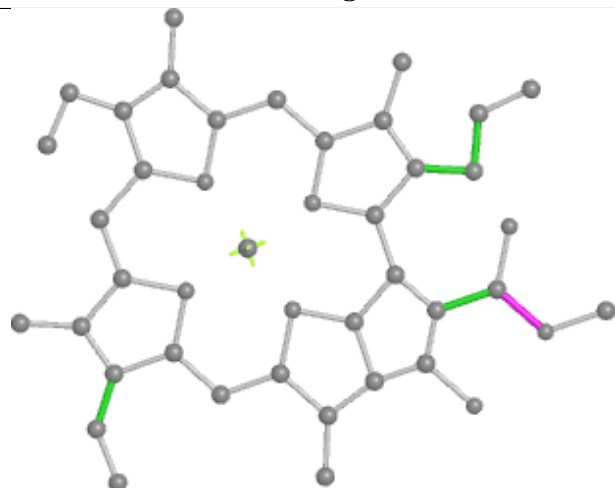
## Ligand CLA B 830



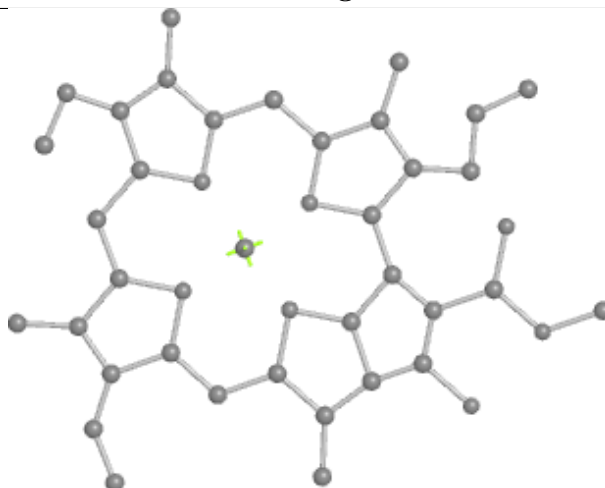
Bond lengths



Bond angles

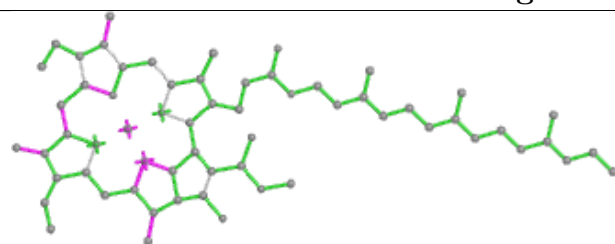


Torsions

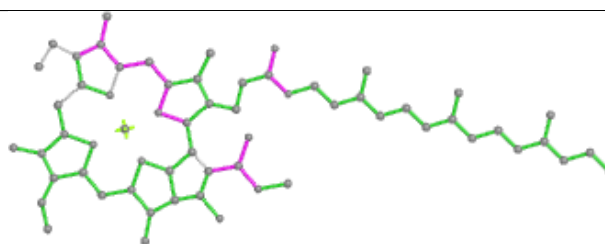


Rings

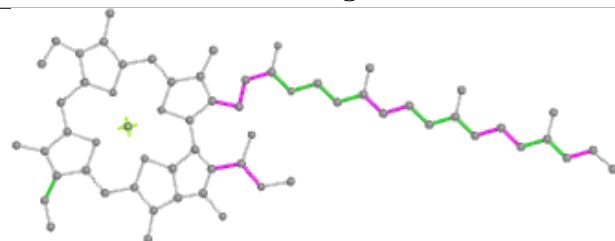
## Ligand CLA B 827



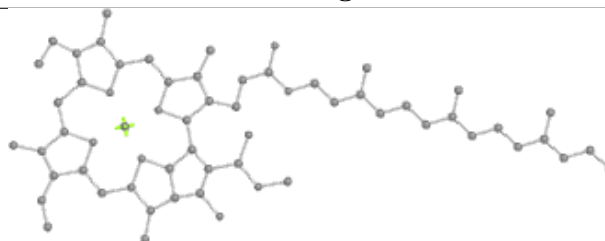
Bond lengths



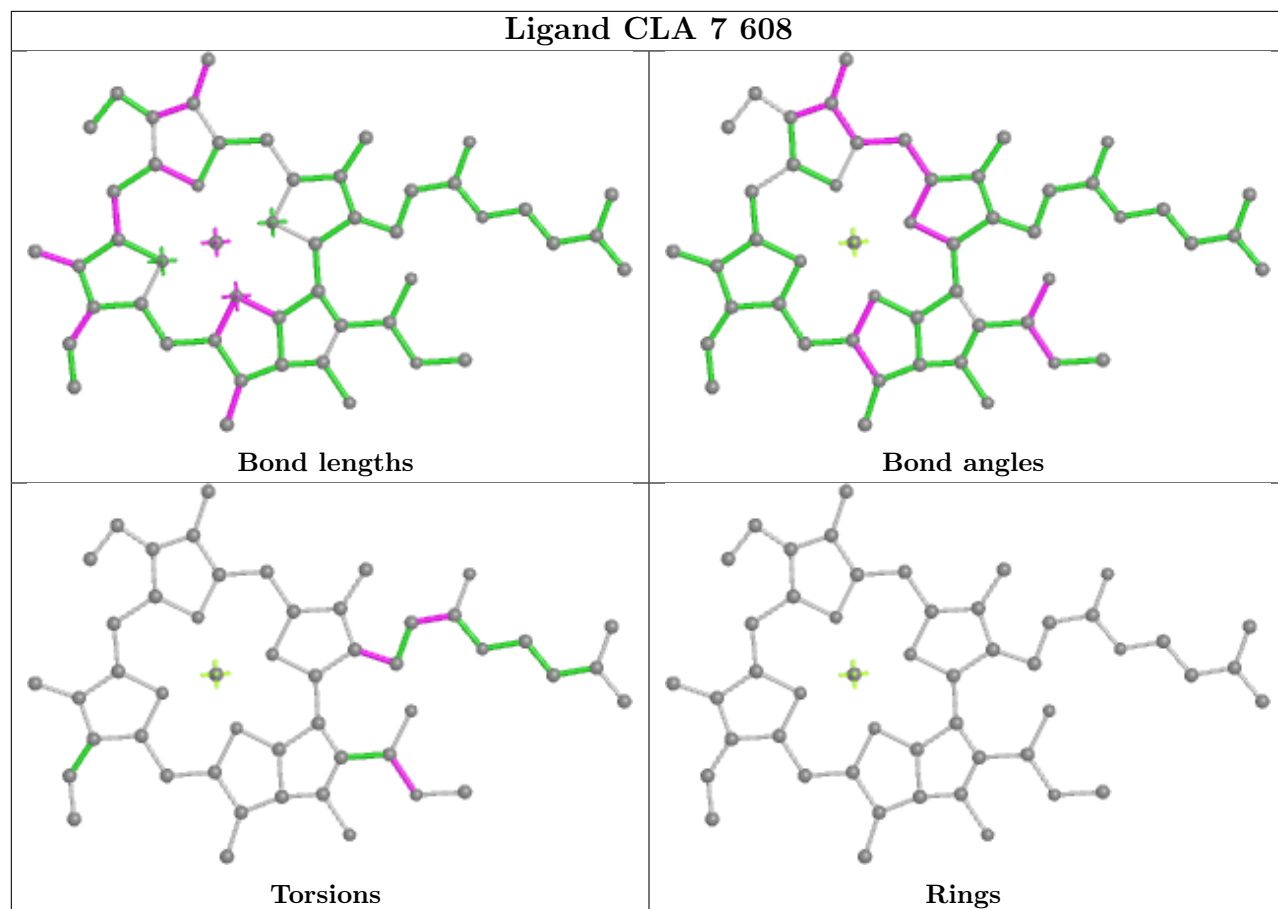
Bond angles



Torsions

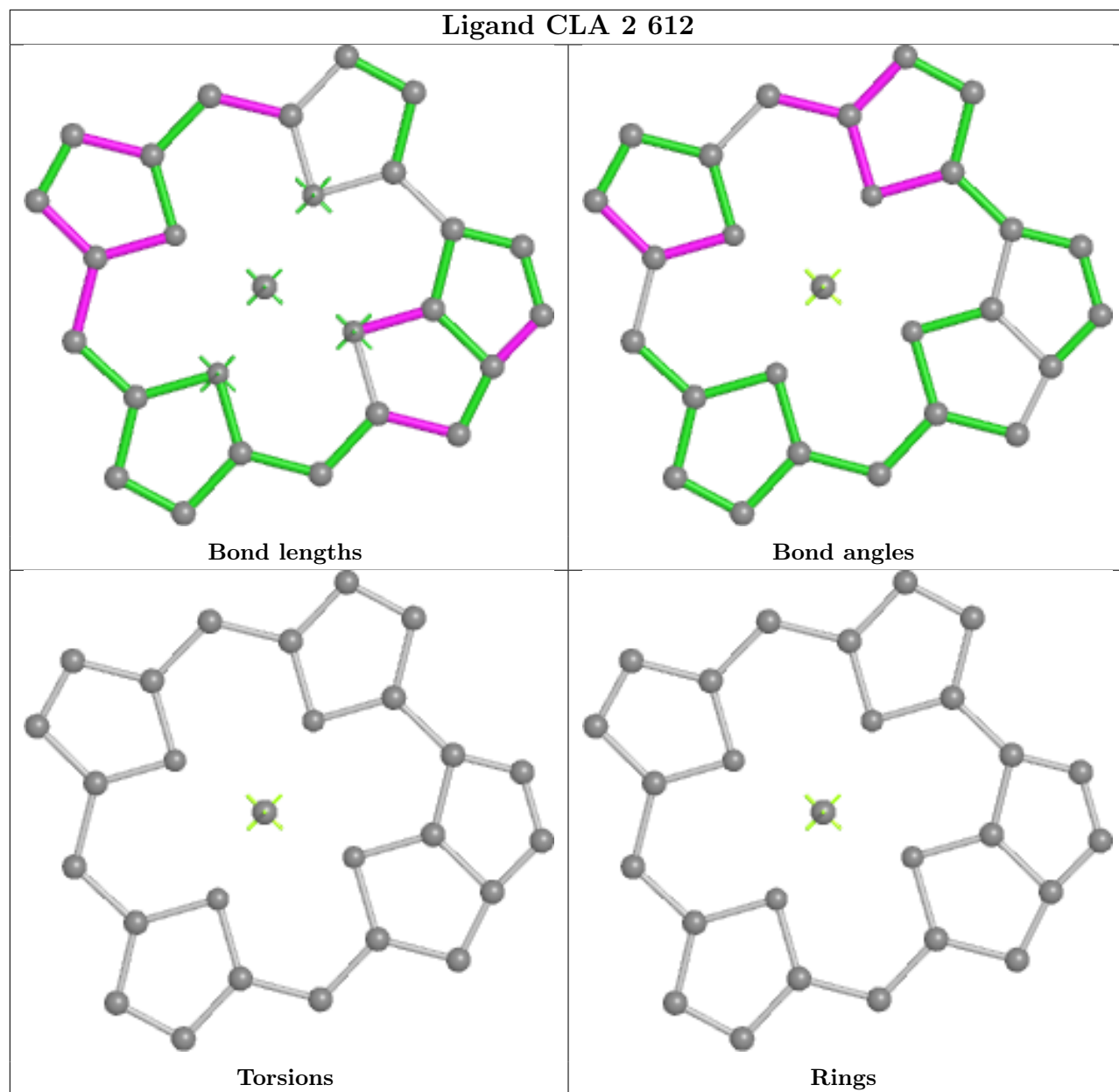


Rings

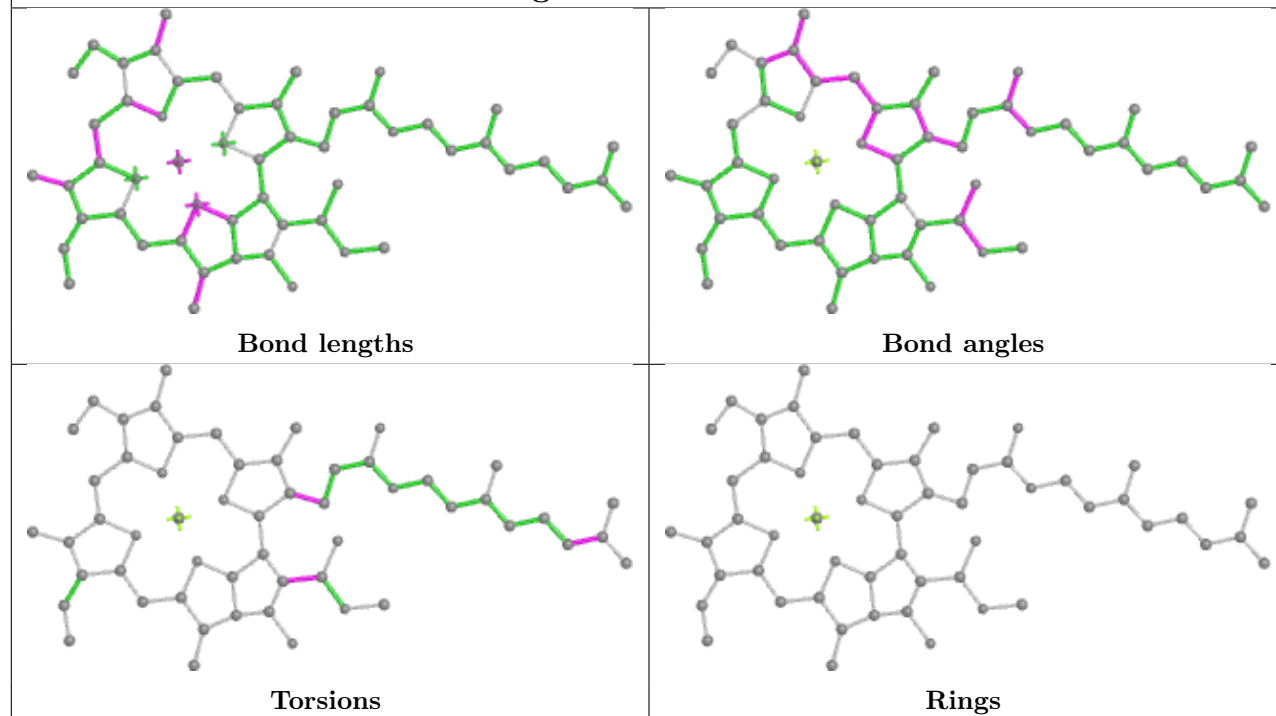




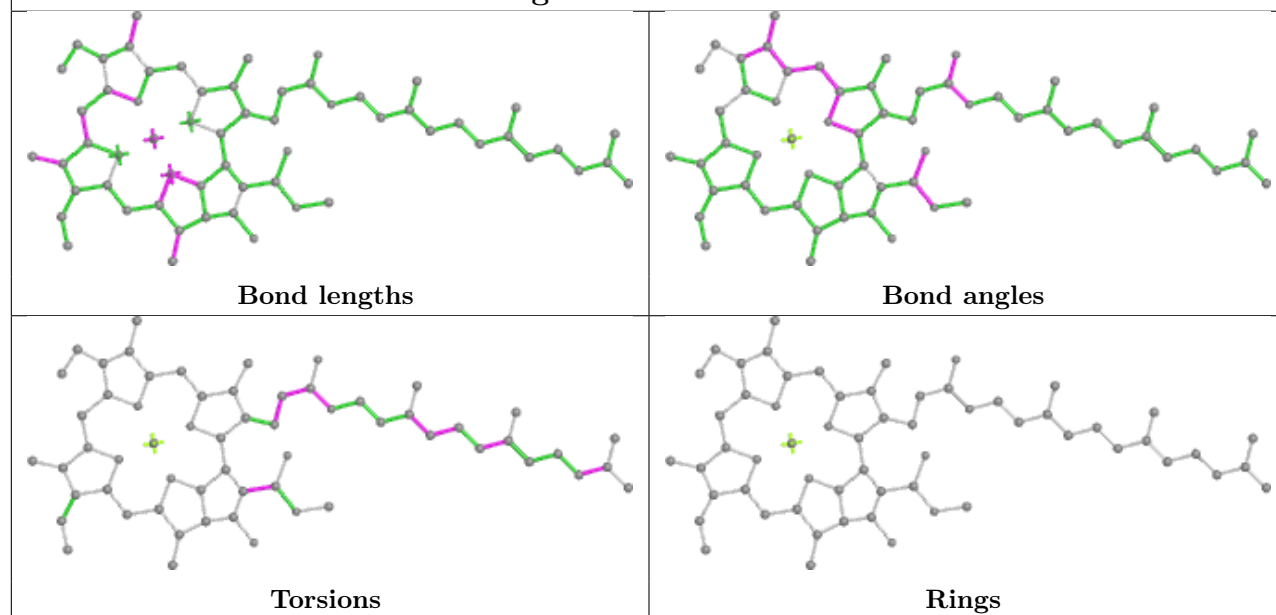
## Ligand CLA 2 612



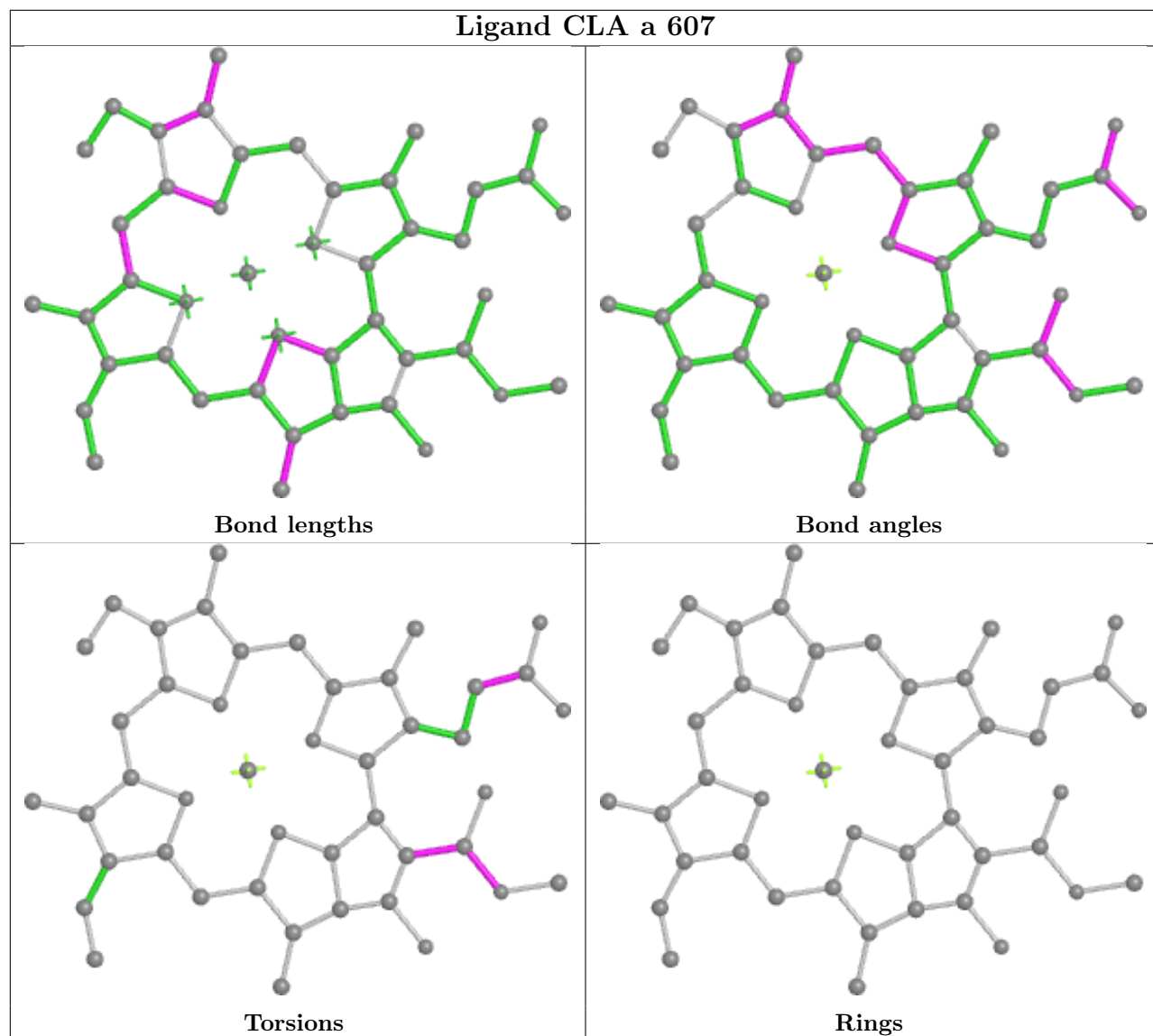
## Ligand CLA B 826



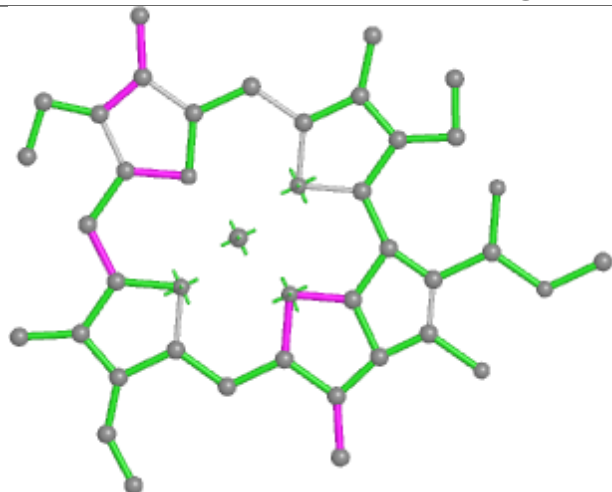
## Ligand CLA A 818



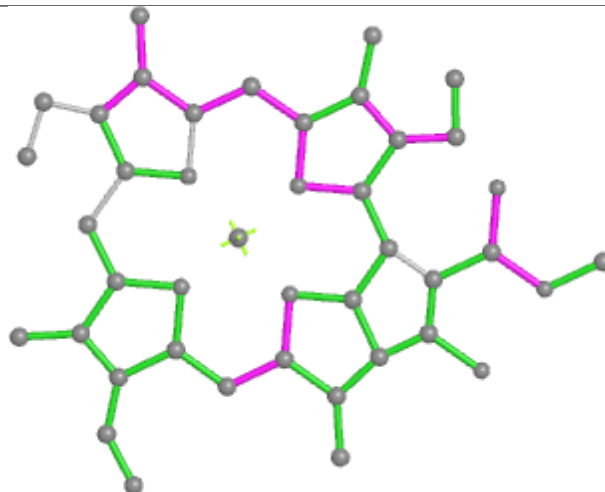
## Ligand CLA a 607



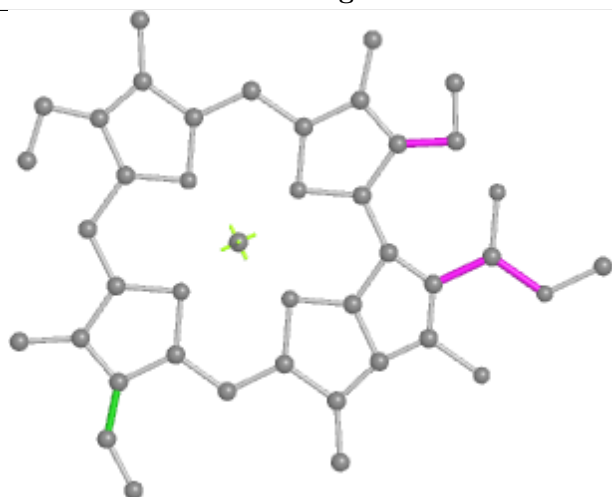
## Ligand CLA J 101



Bond lengths



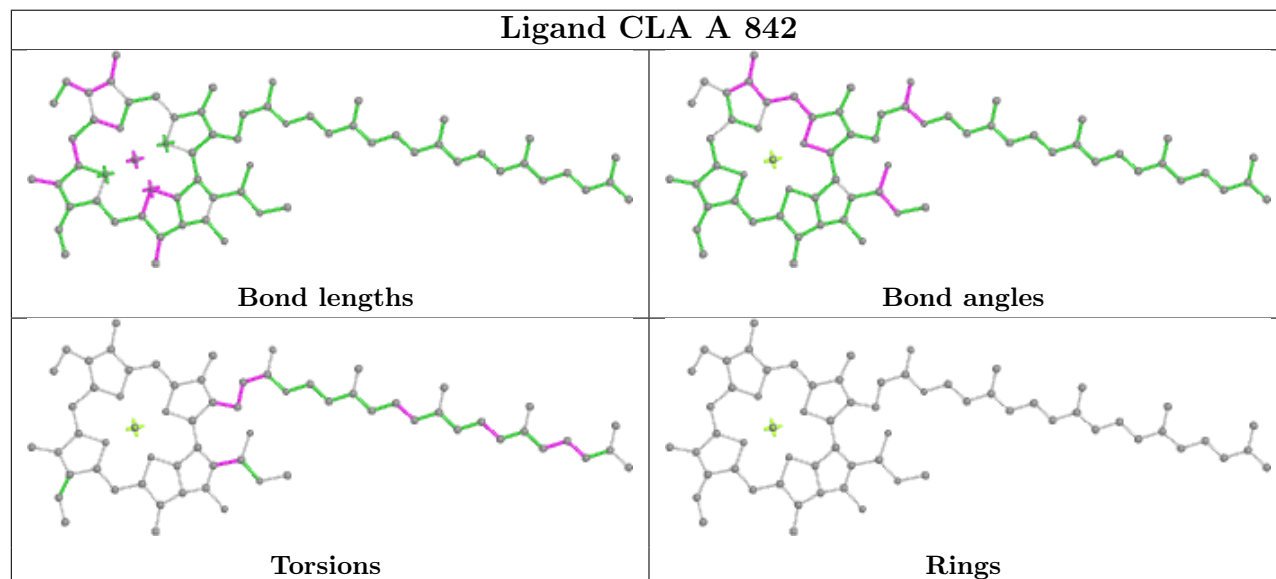
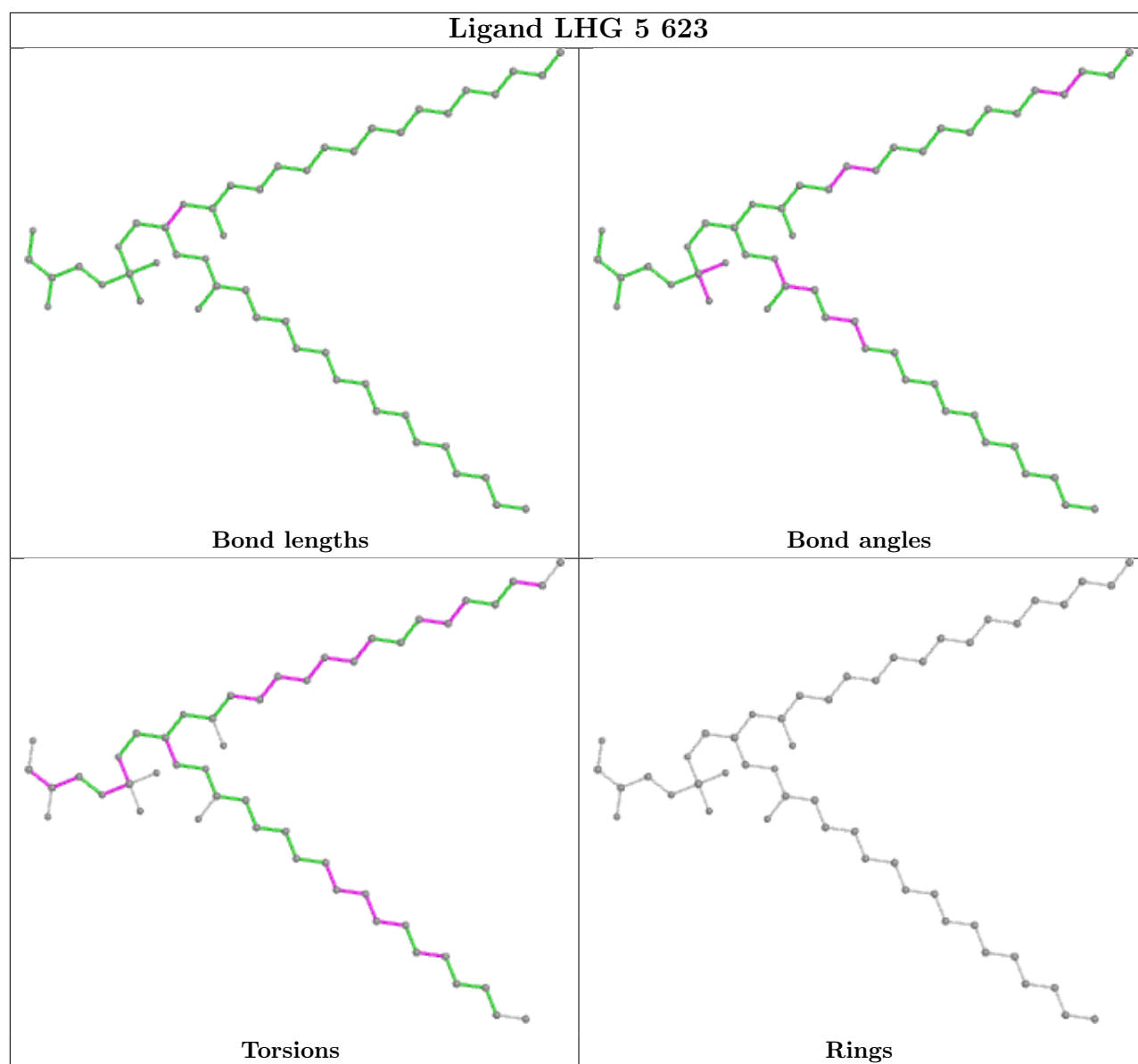
Bond angles

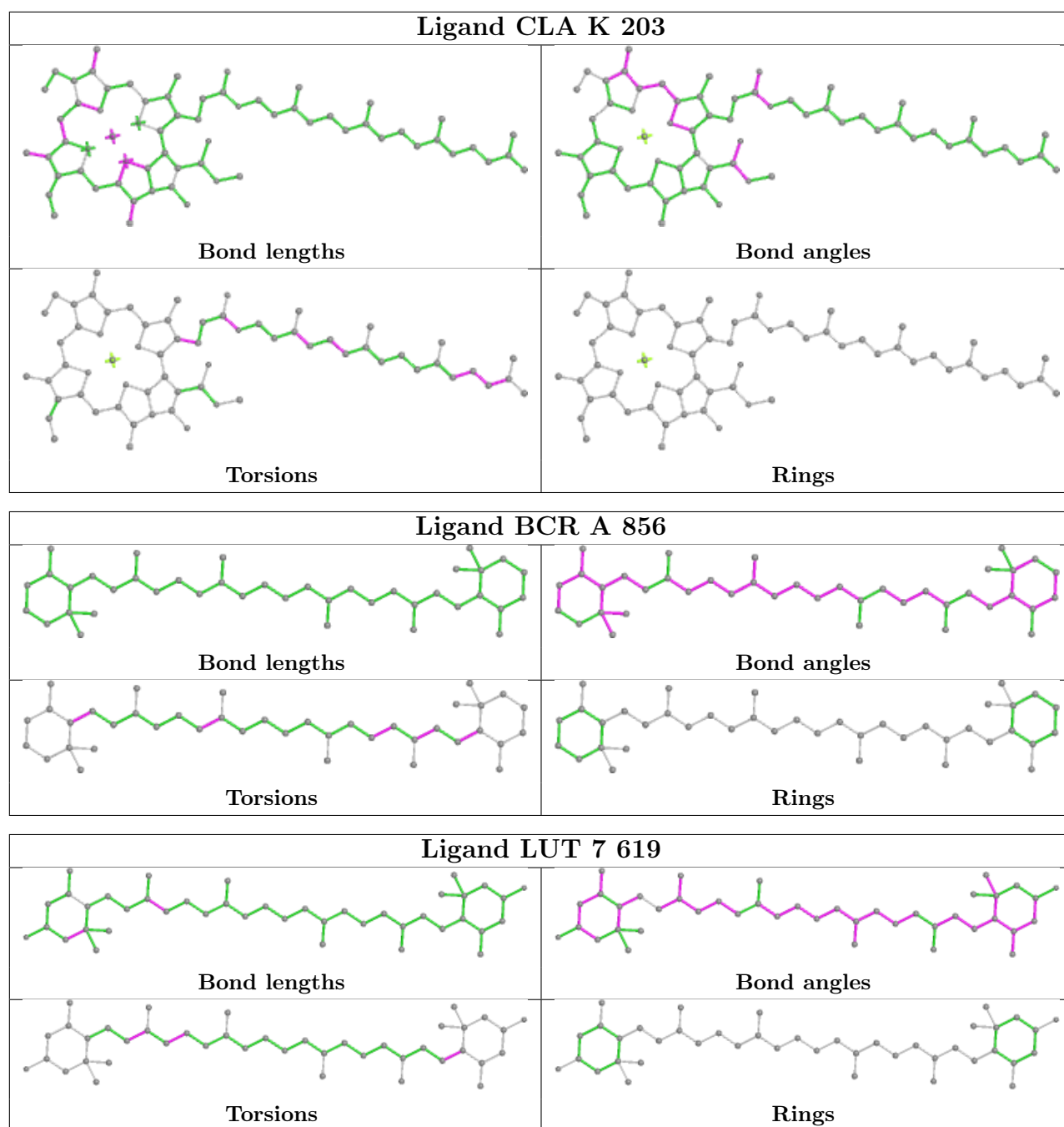


Torsions

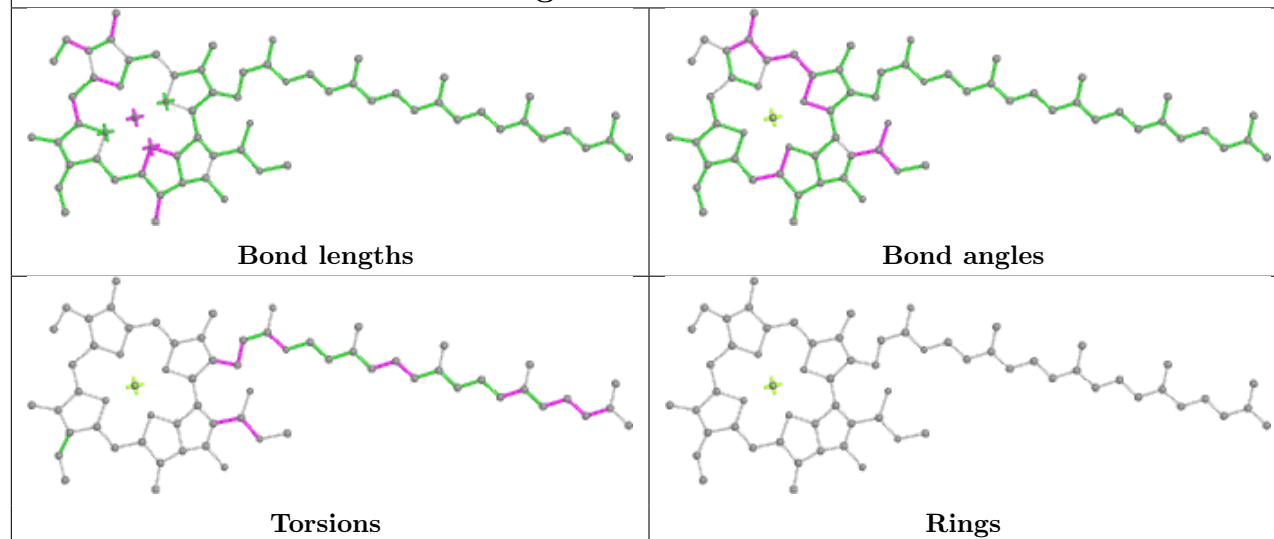


Rings

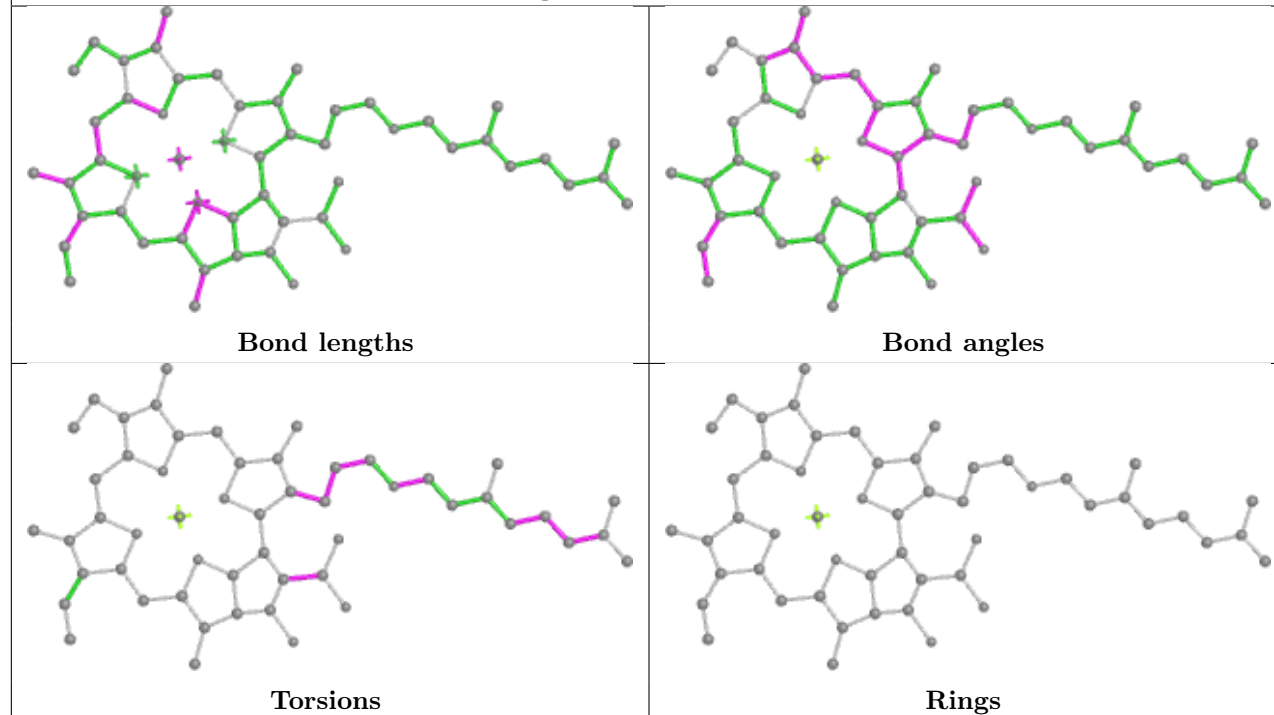




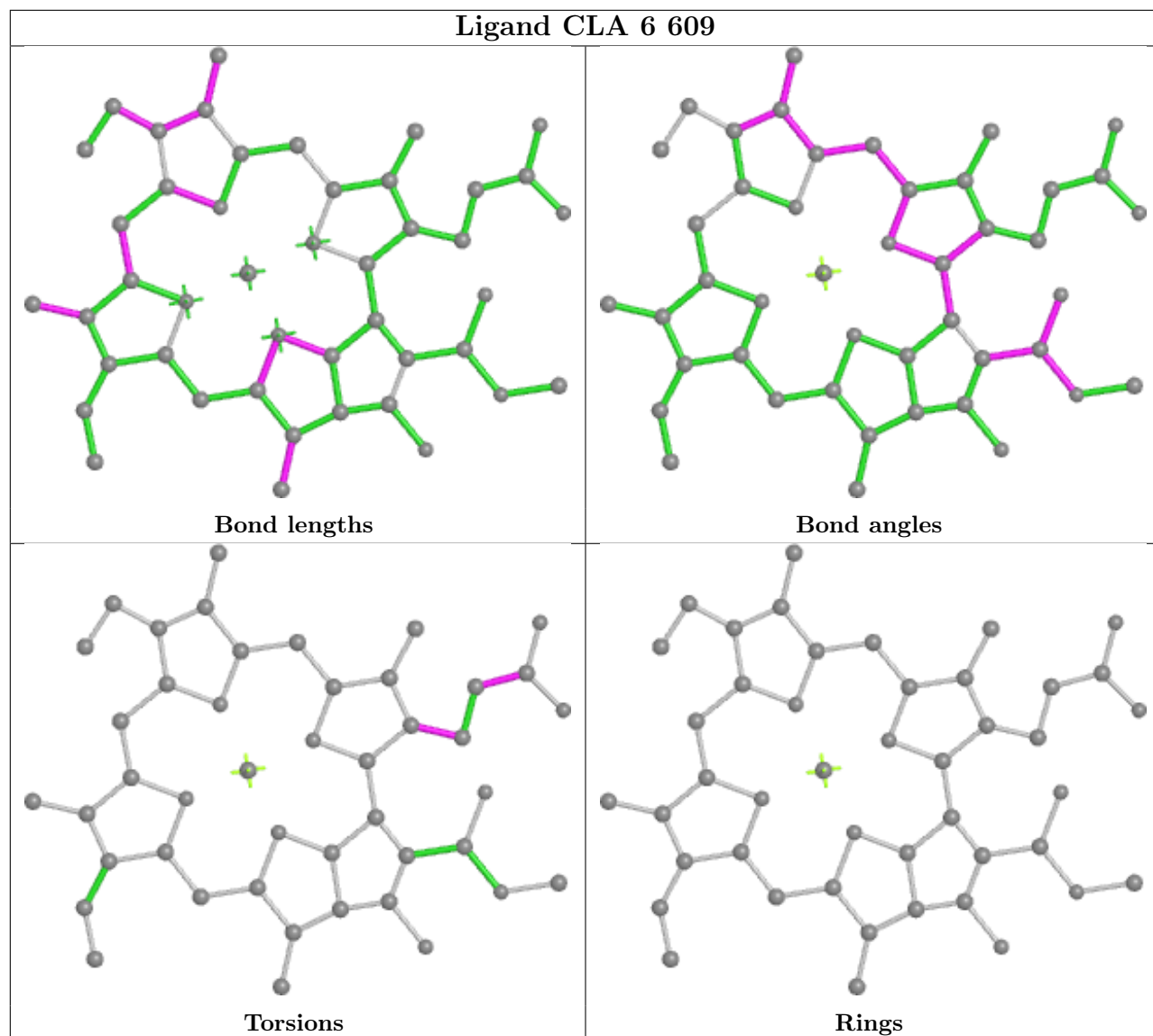
## Ligand CLA 4 601



## Ligand CLA 1 603

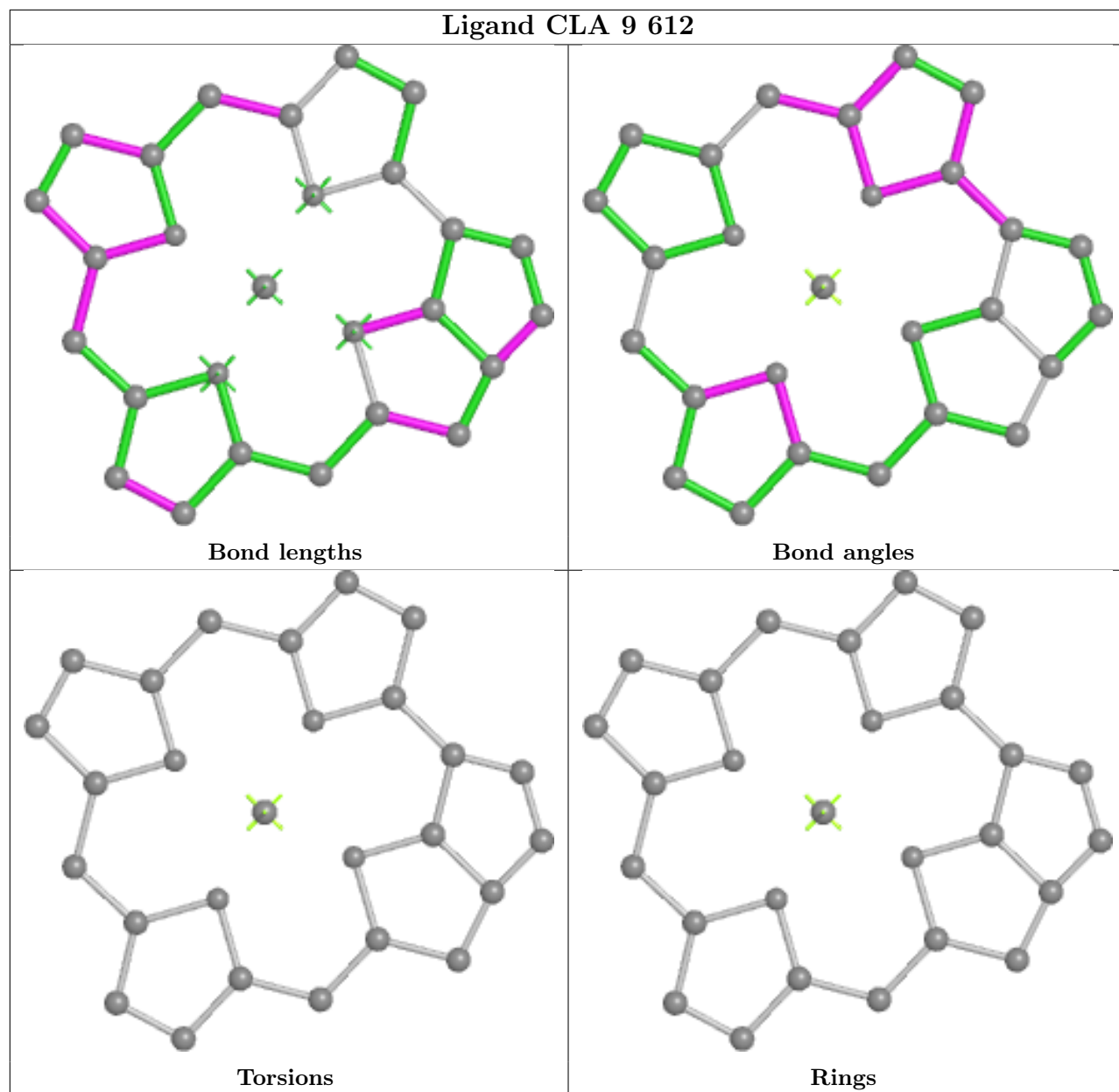


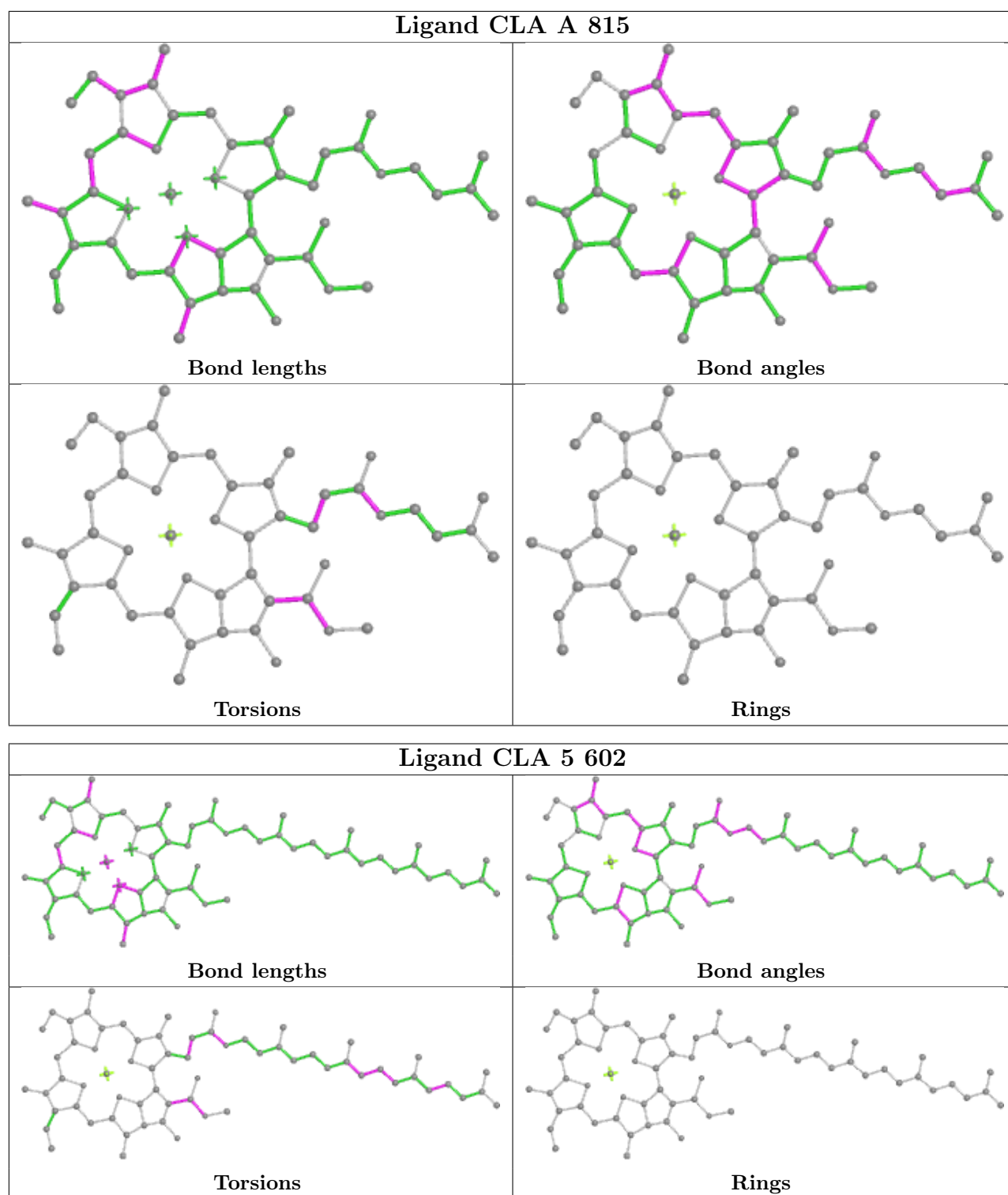
## Ligand CLA 6 609



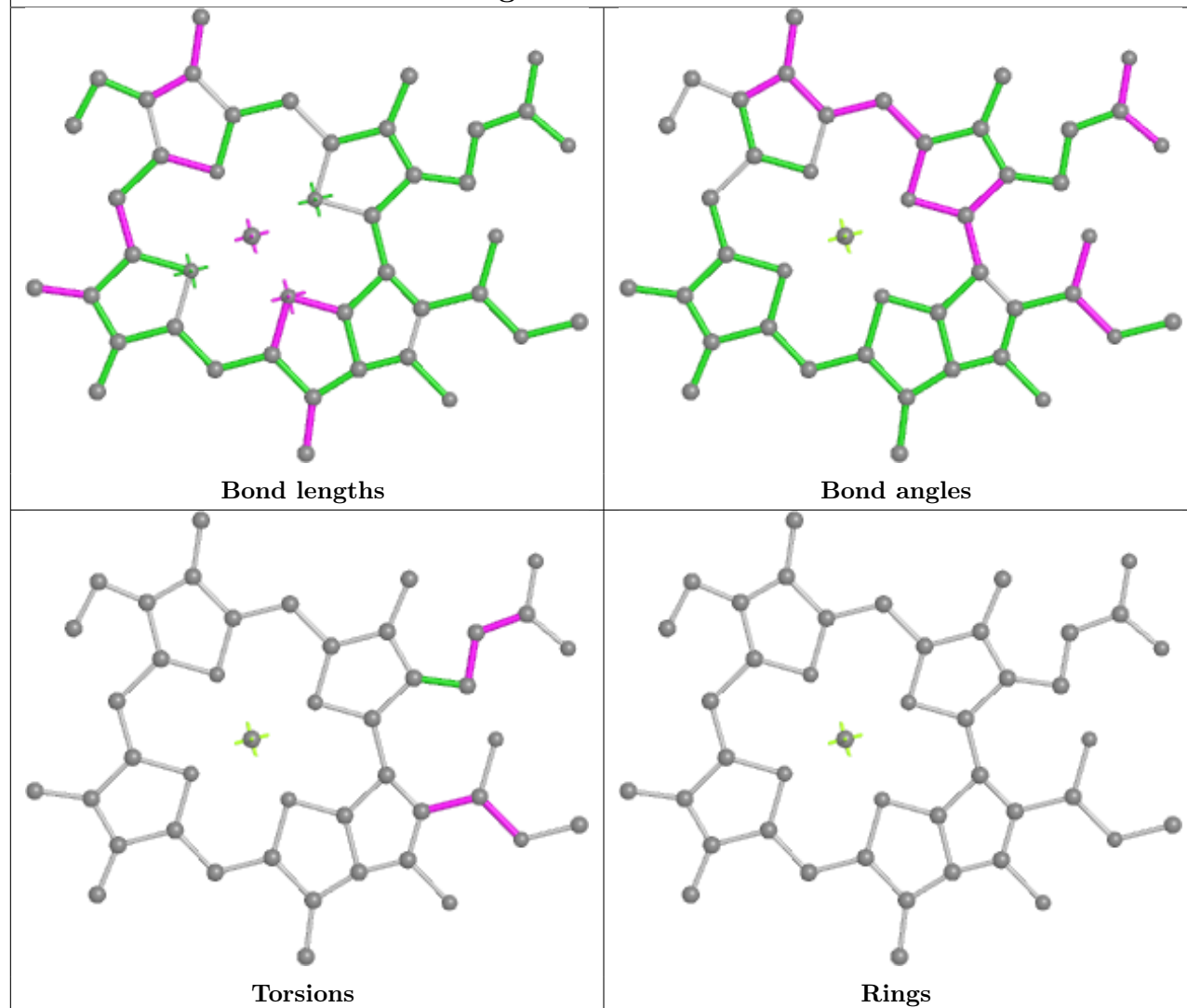


## Ligand CLA 9 612

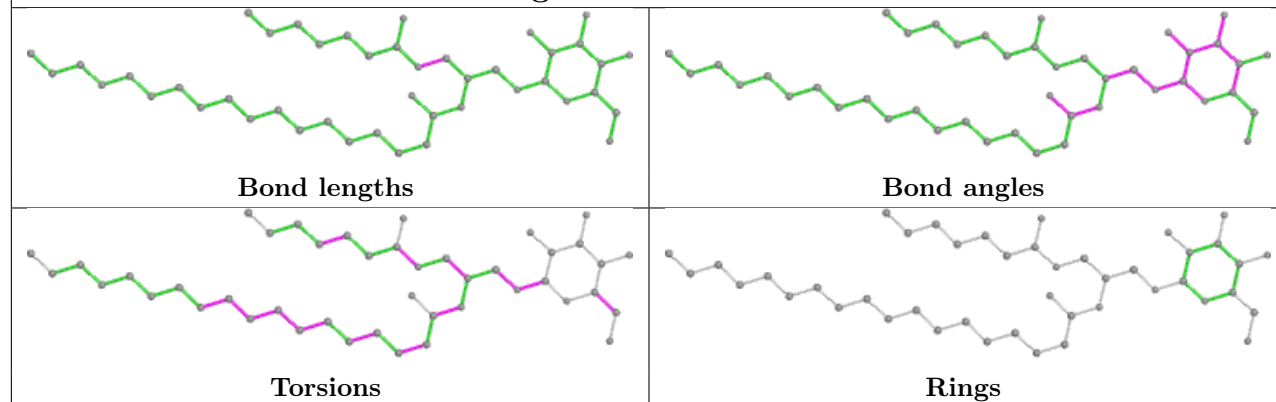


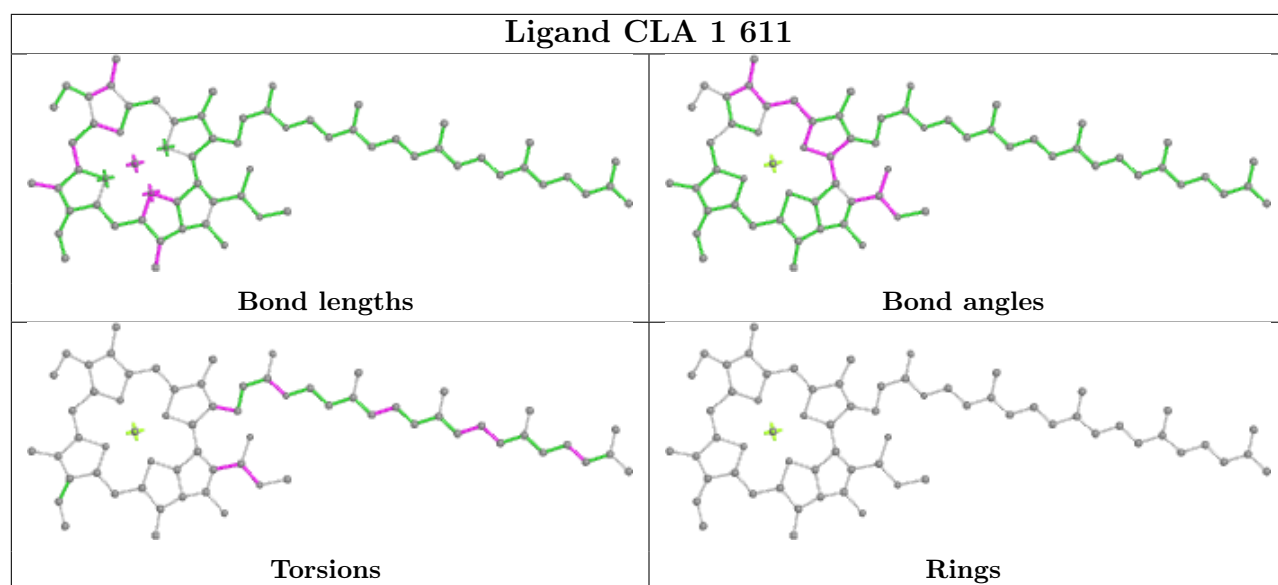


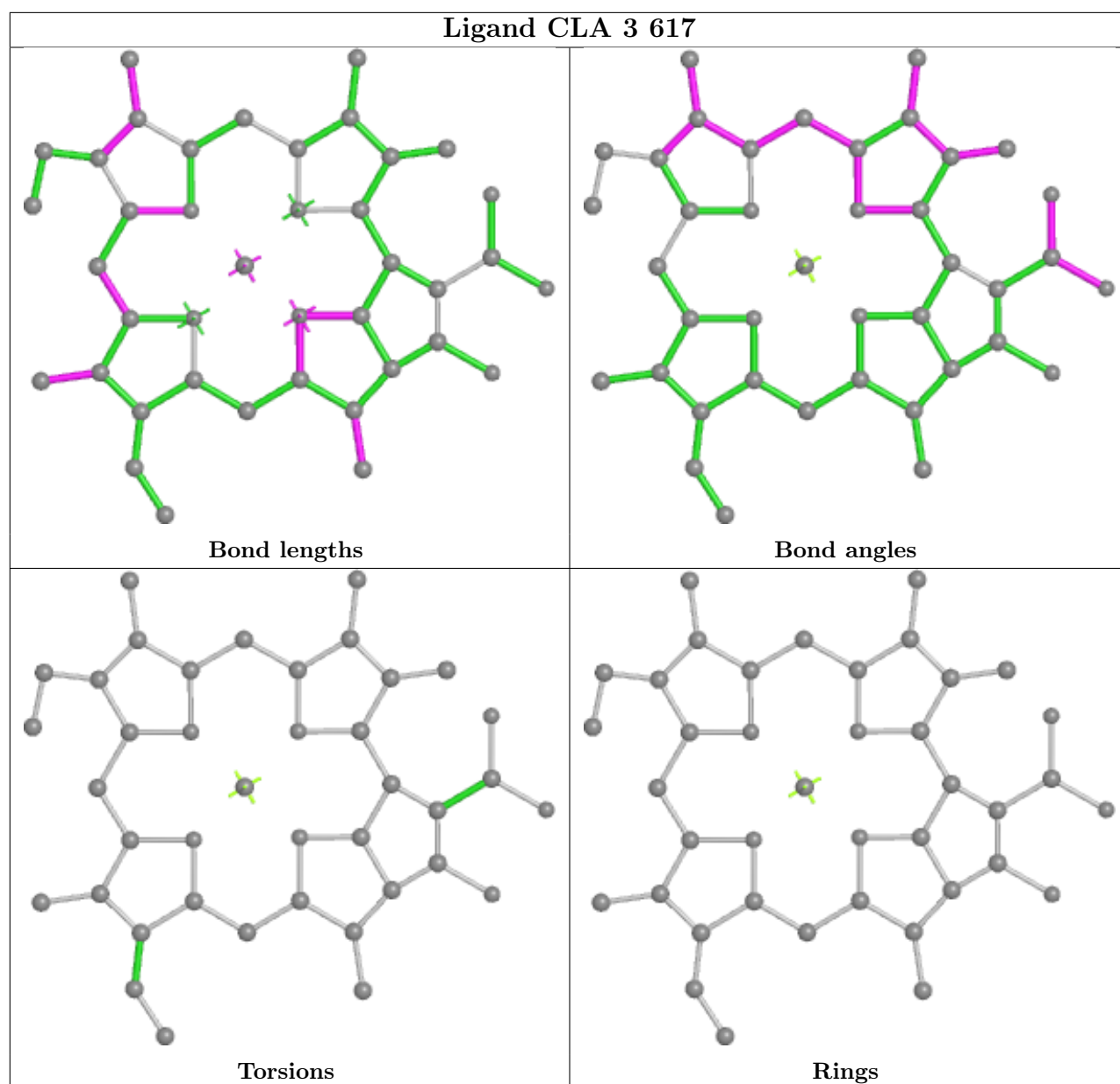
## Ligand CLA 7 612



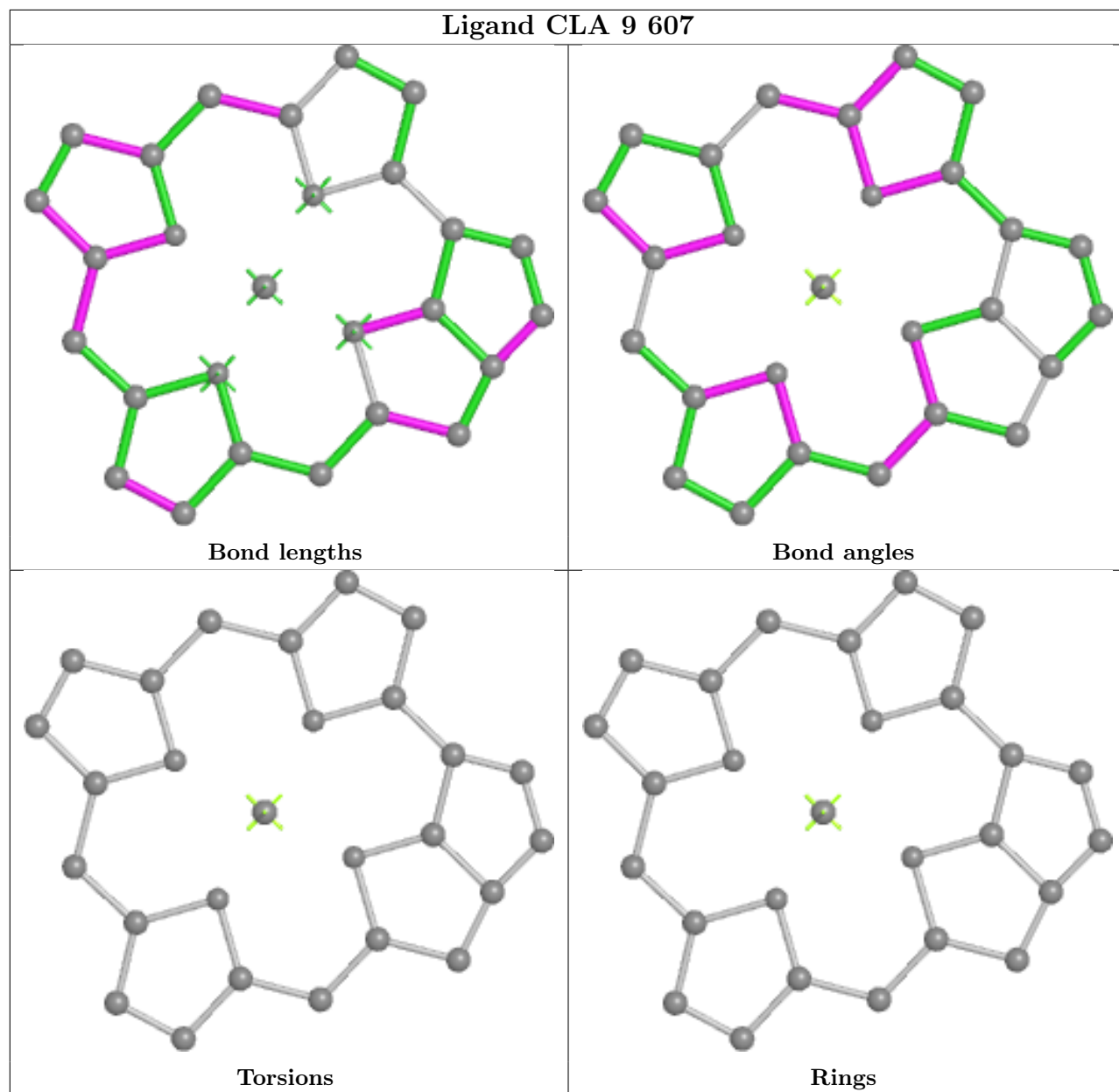
## Ligand LMG 7 624

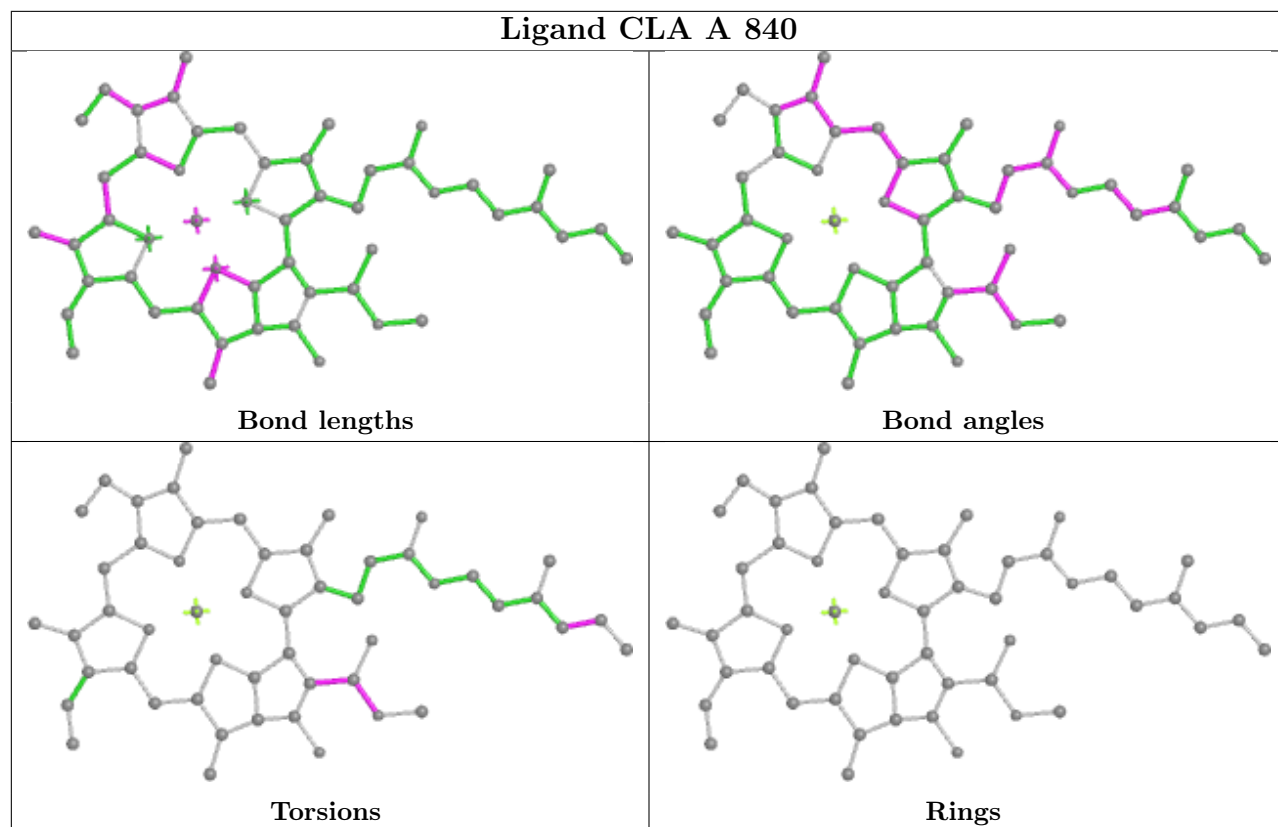




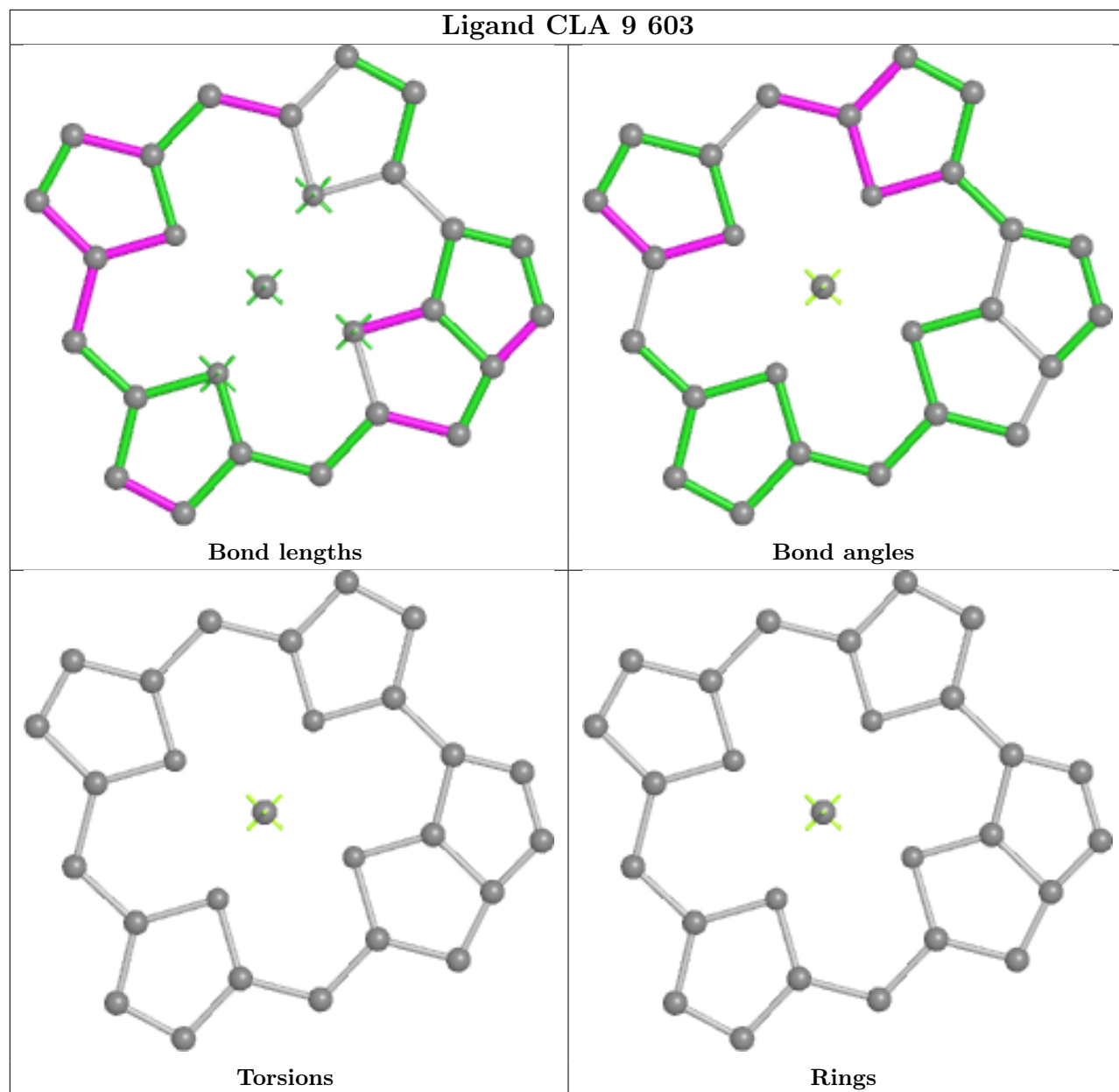


## Ligand CLA 9 607



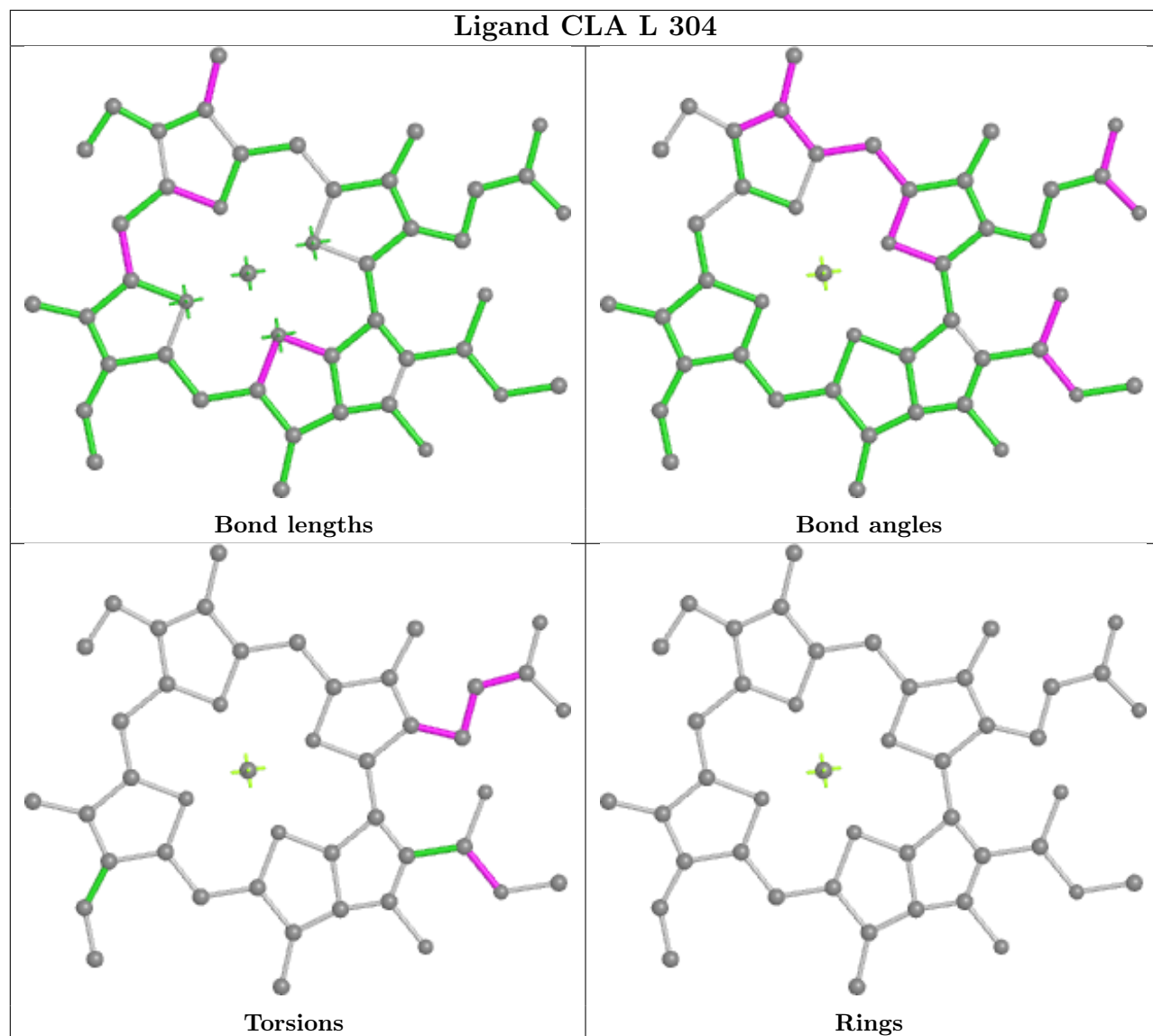


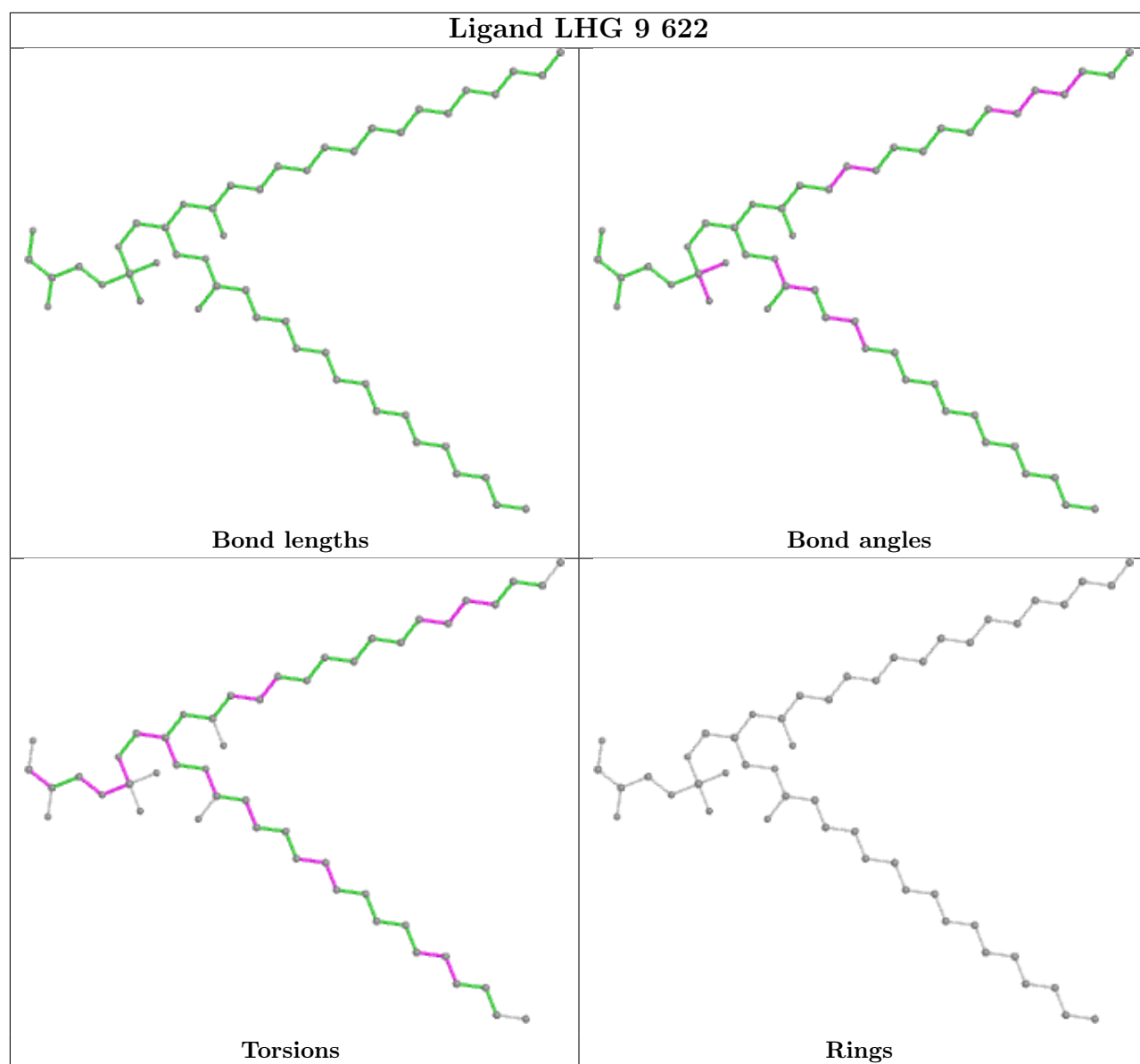
## Ligand CLA 9 603



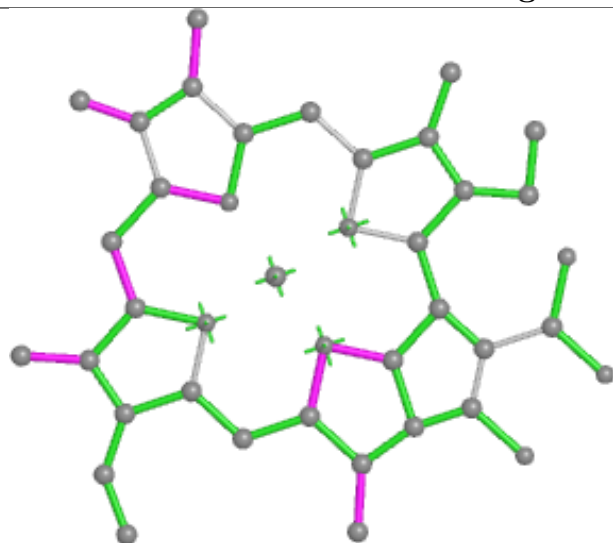


## Ligand CLA L 304

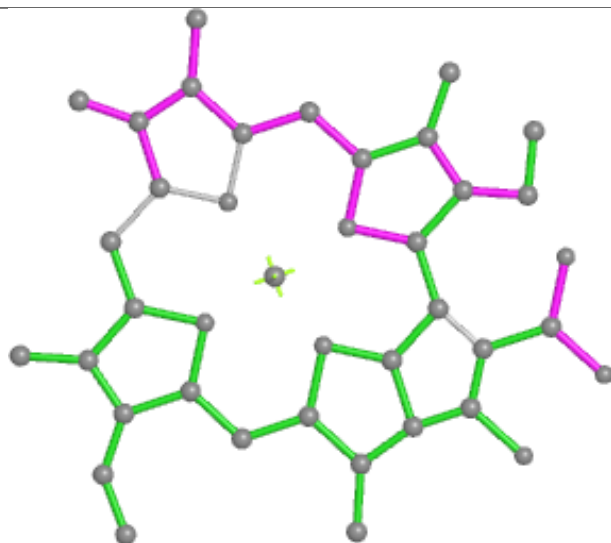




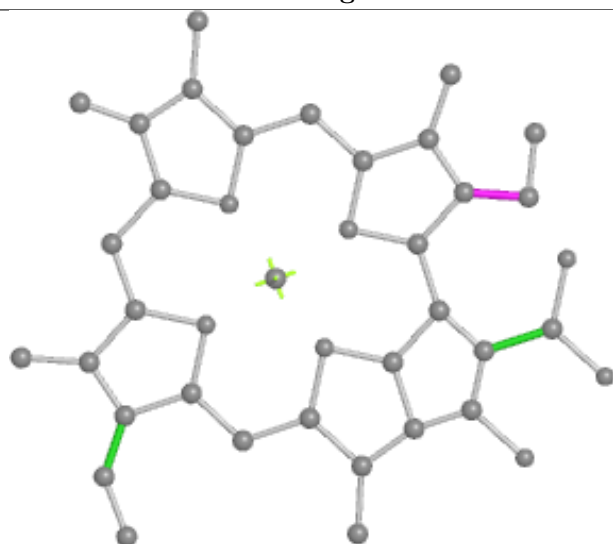
## Ligand CLA 5 618



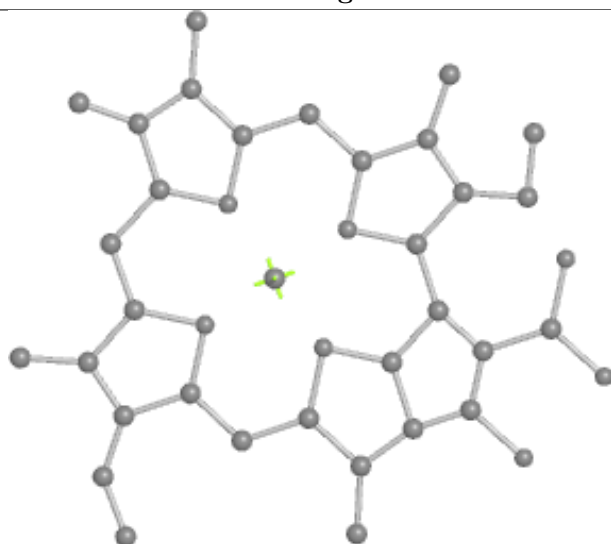
Bond lengths



Bond angles

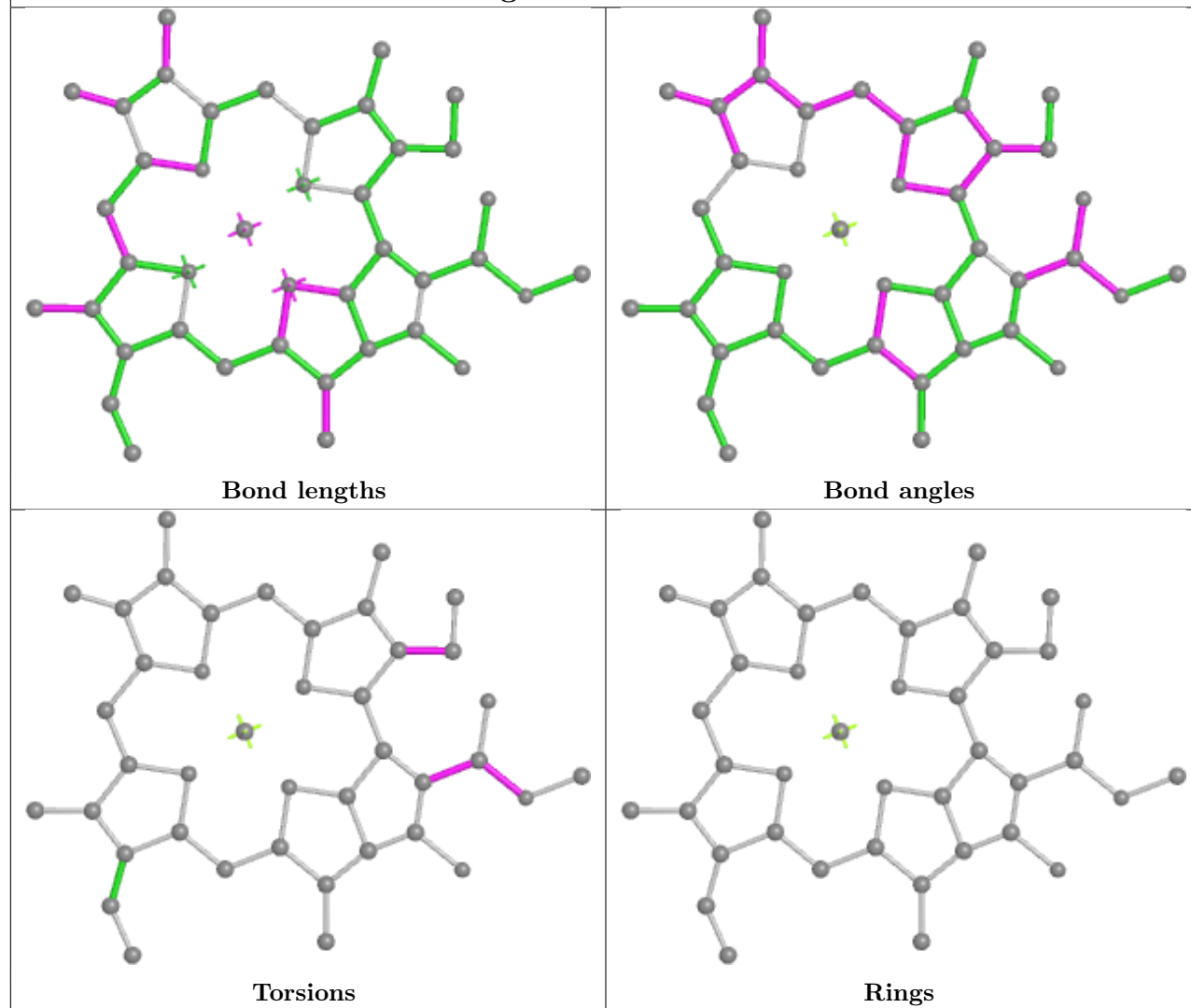


Torsions

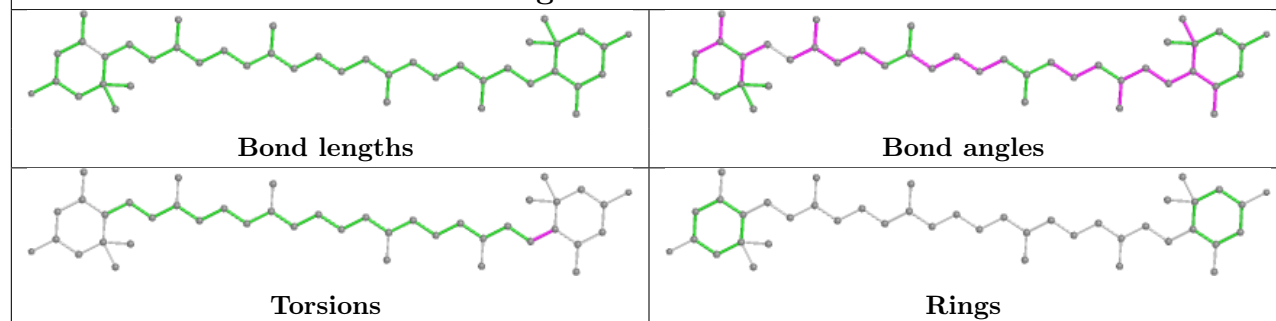


Rings

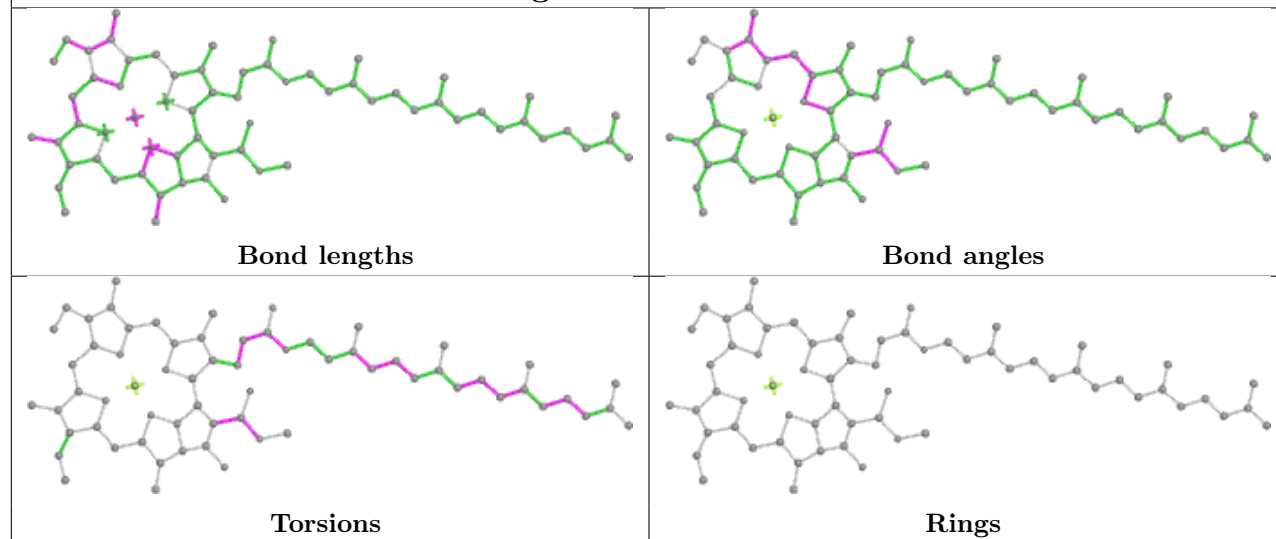
## Ligand CLA 6 607



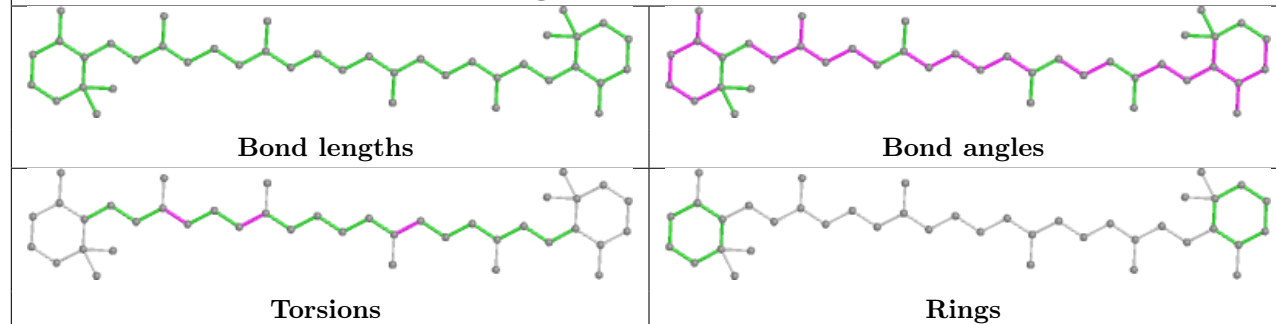
## Ligand LUT 5 620



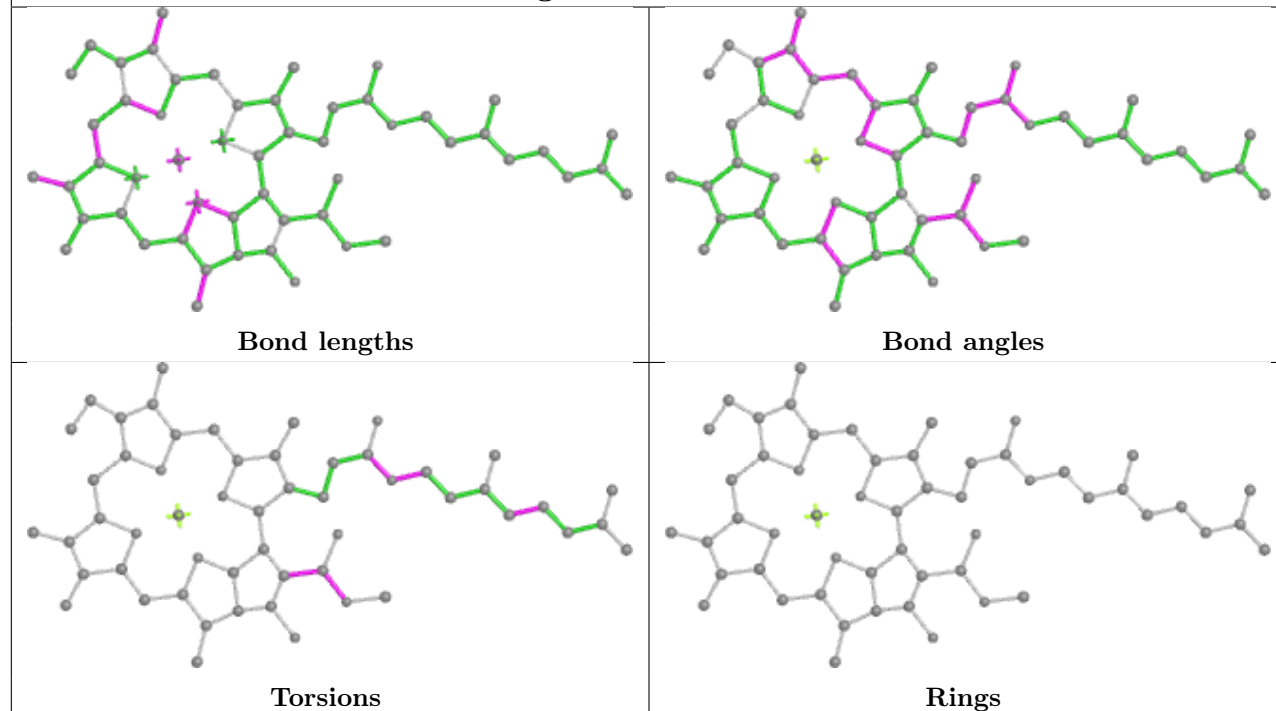
## Ligand CLA A 834

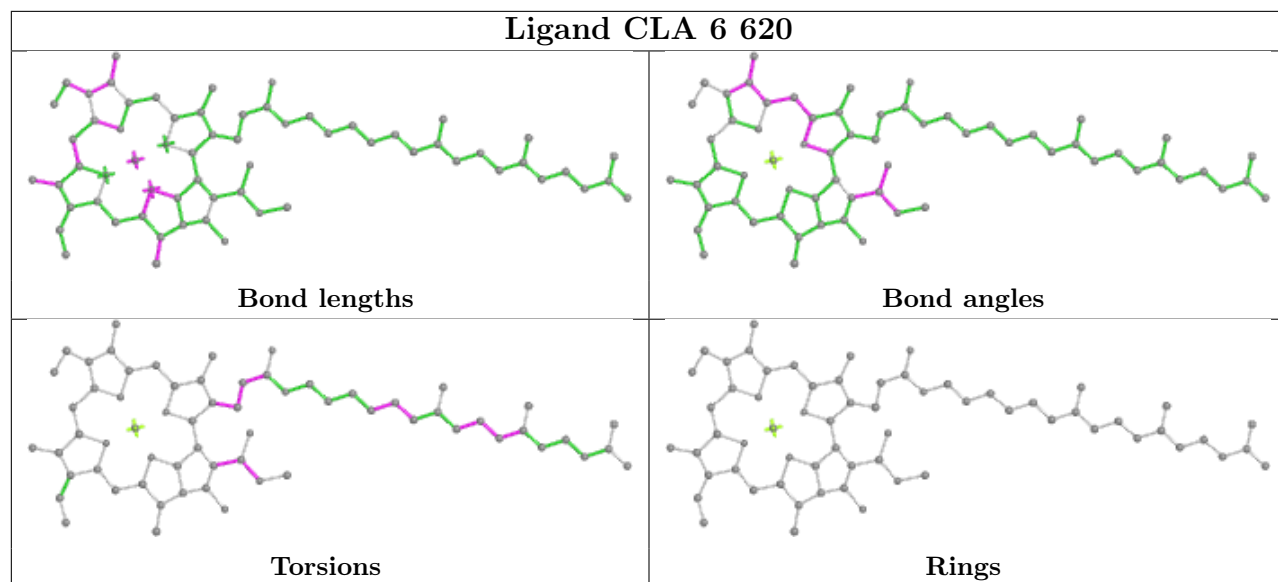


## Ligand BCR L 301

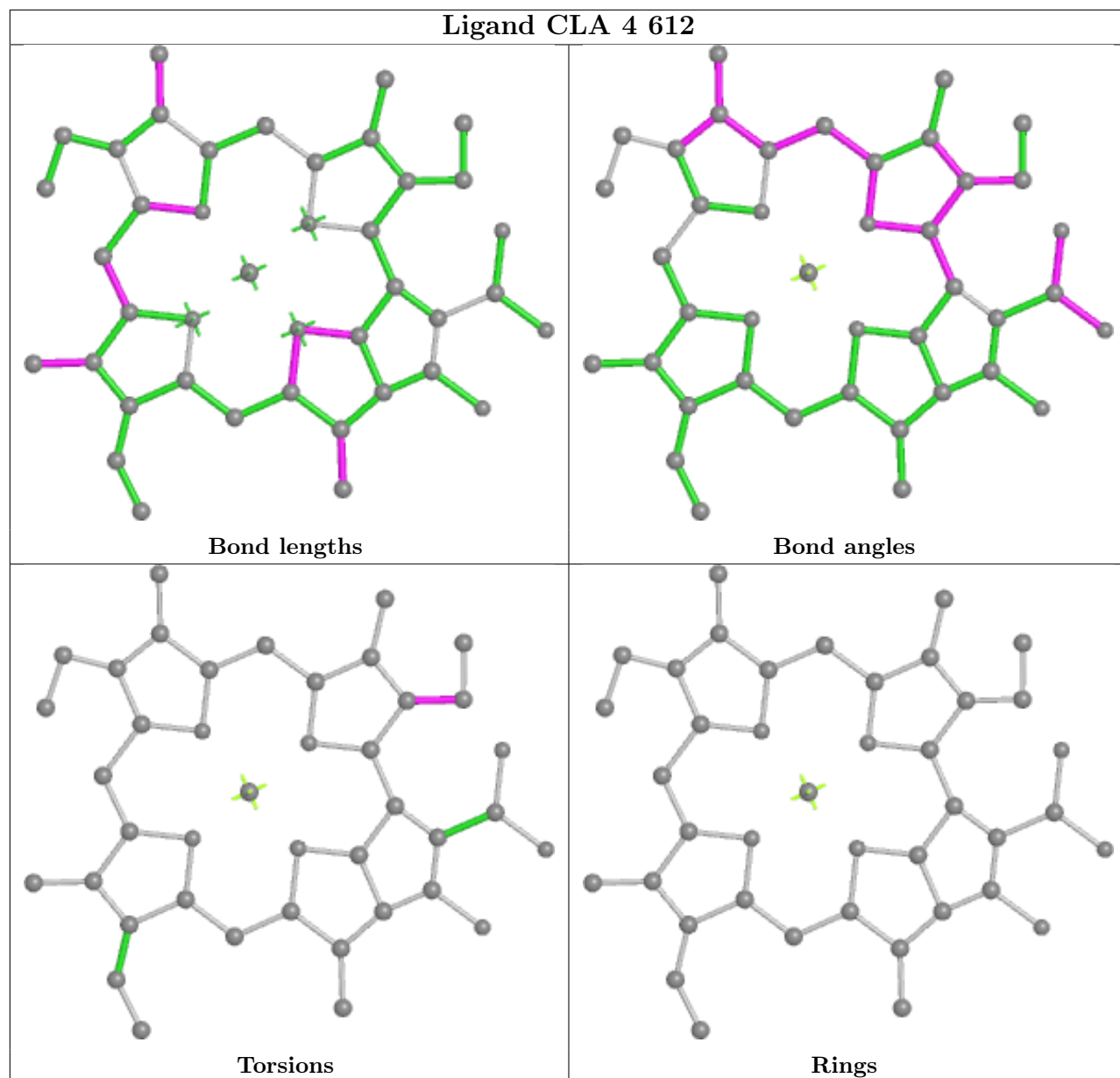


## Ligand CLA 7 604

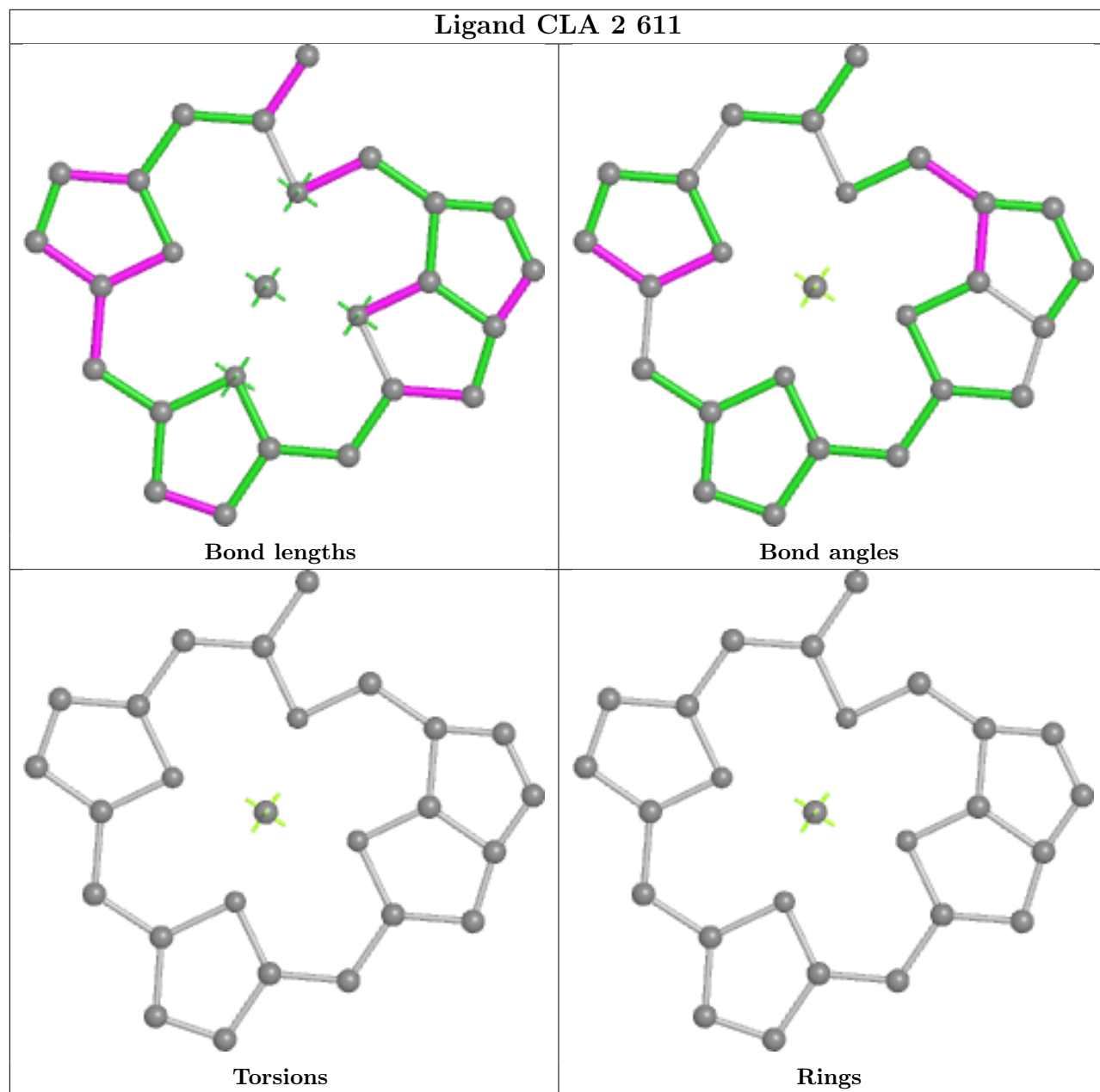




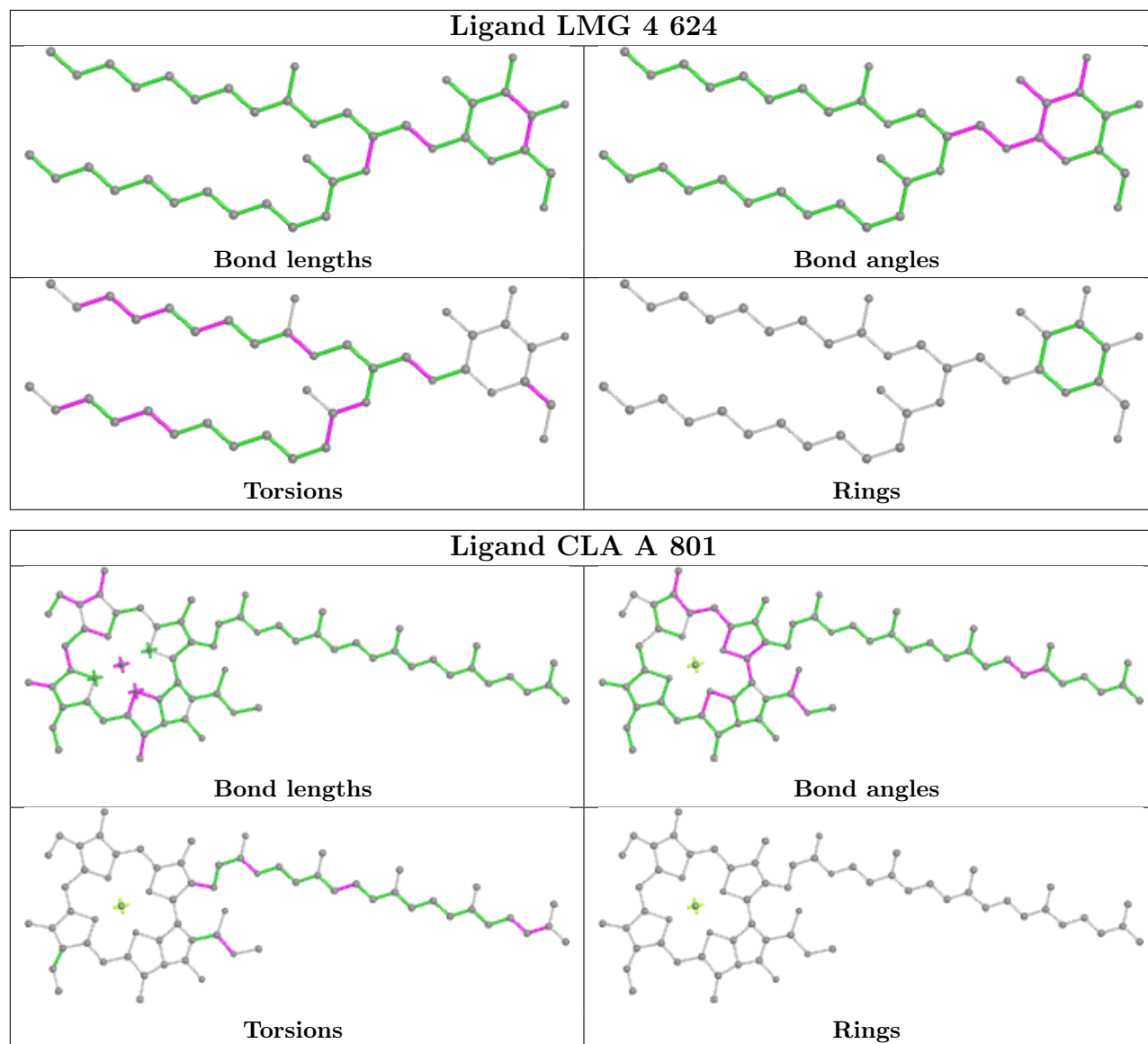
## Ligand CLA 4 612



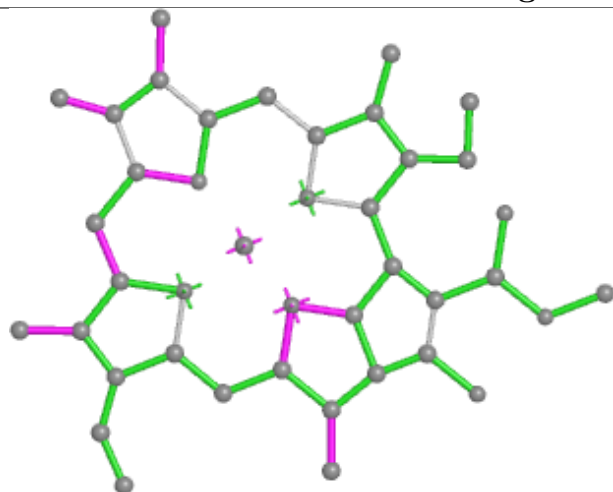
## Ligand CLA 2 611



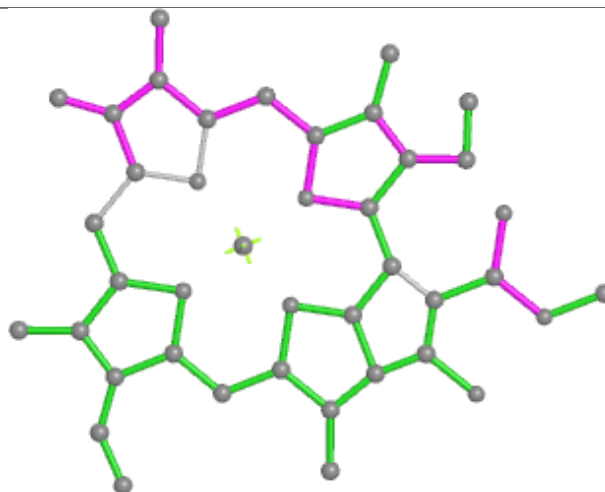




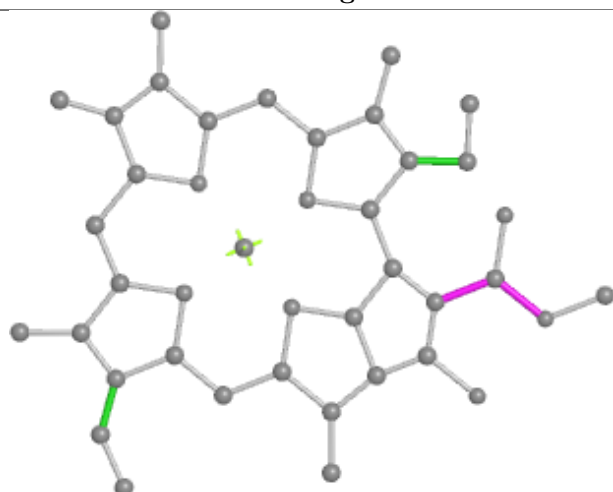
## Ligand CLA 8 607



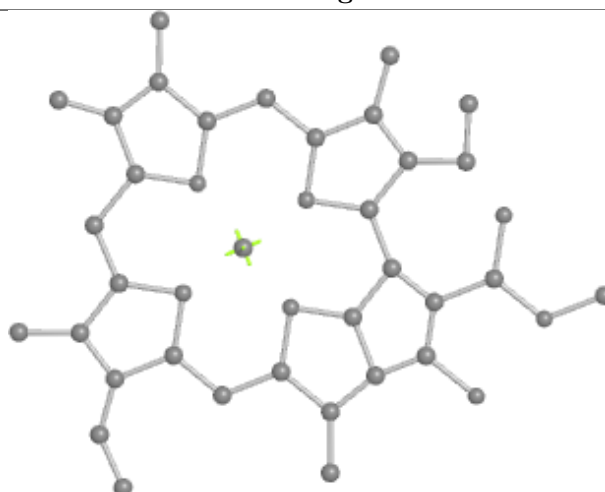
Bond lengths



Bond angles

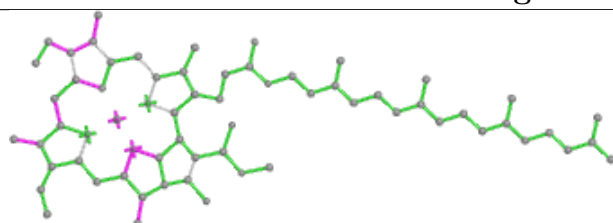


Torsions

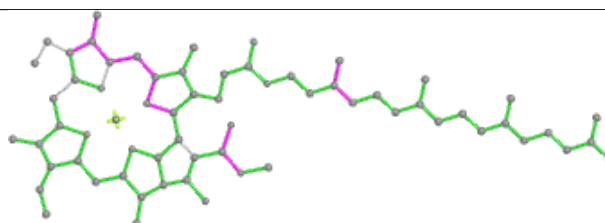


Rings

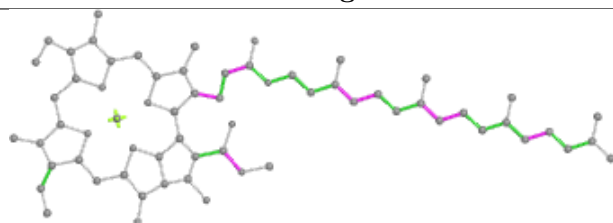
## Ligand CLA A 836



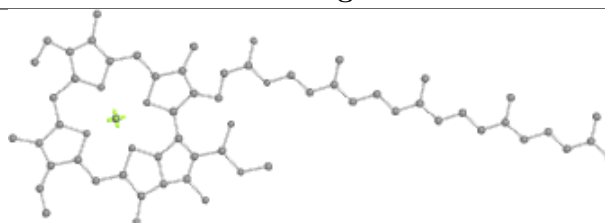
Bond lengths



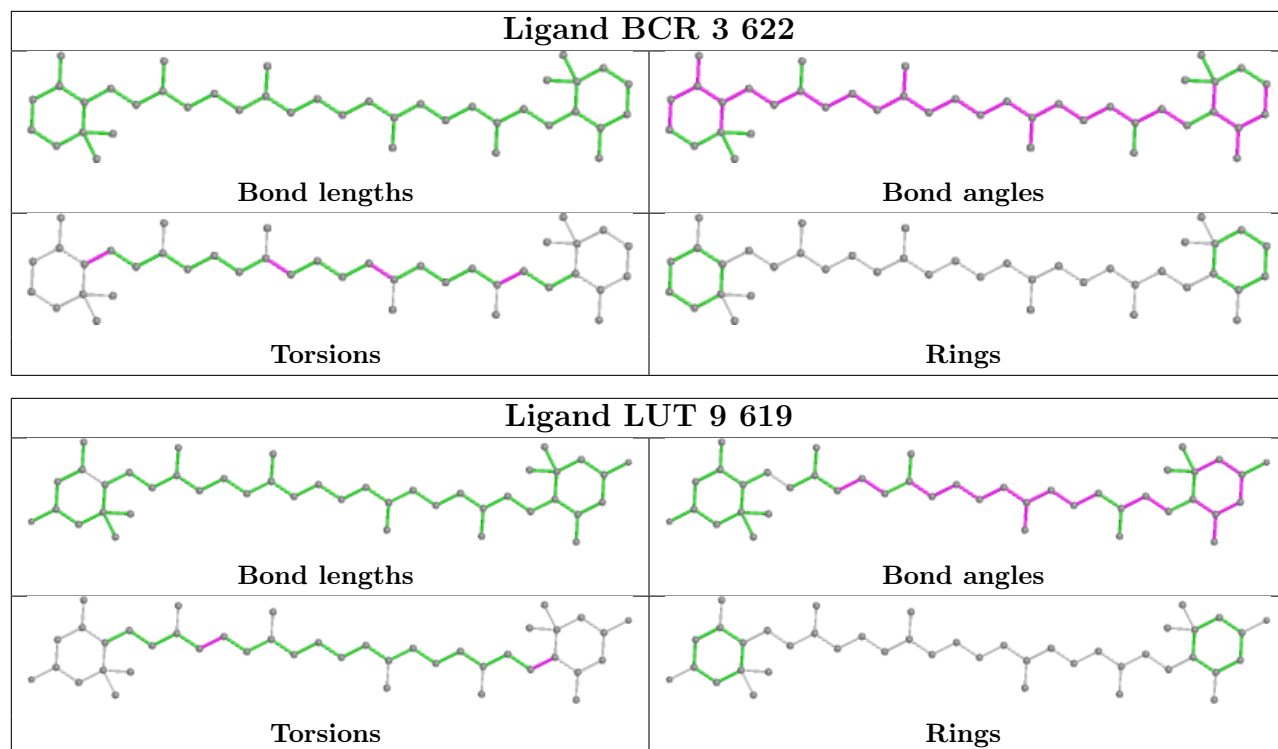
Bond angles



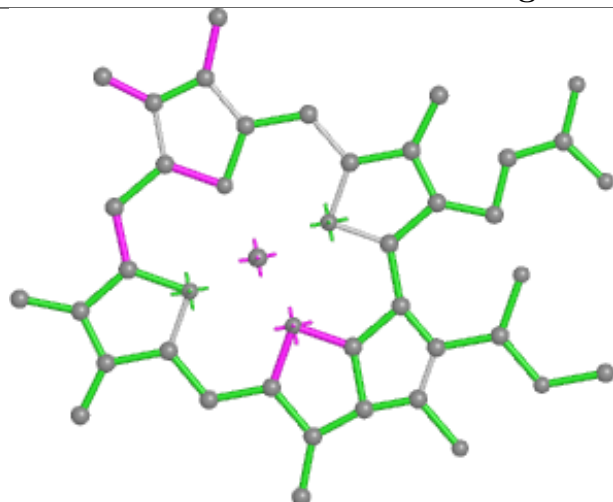
Torsions



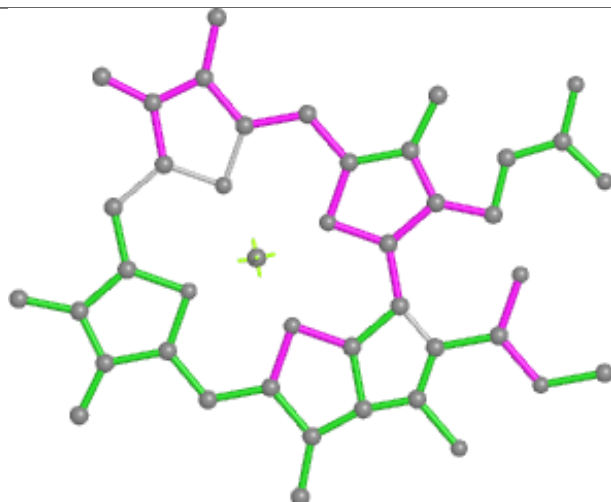
Rings



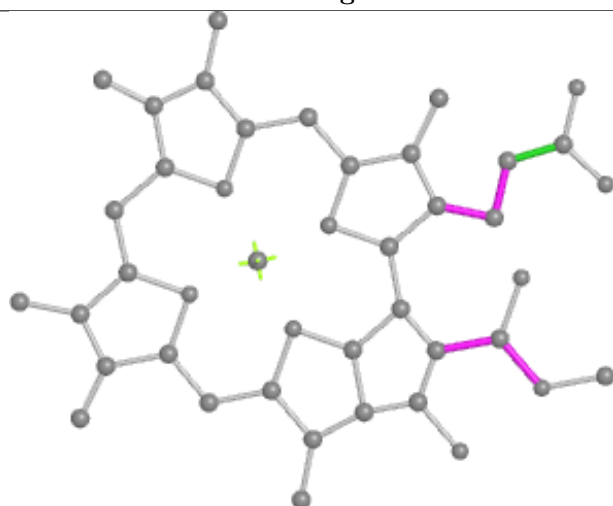
## Ligand CLA 8 616



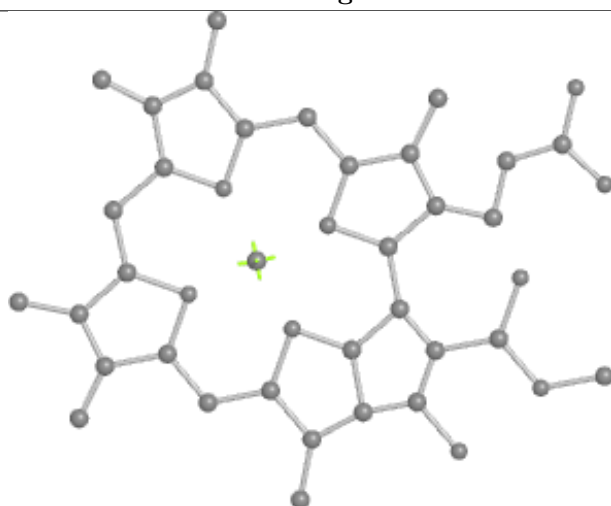
Bond lengths



Bond angles

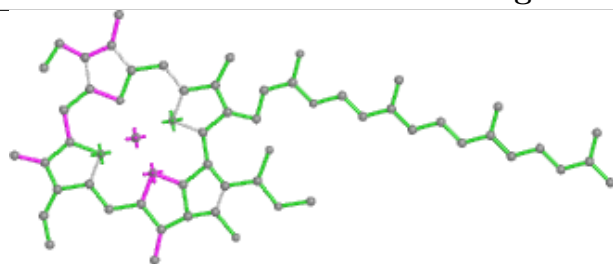


Torsions

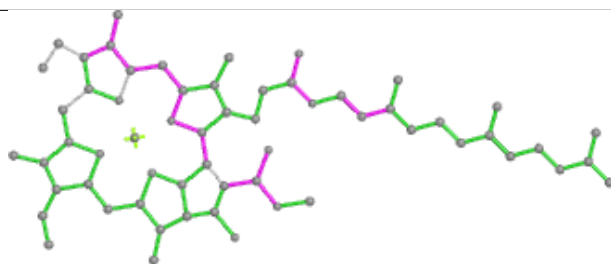


Rings

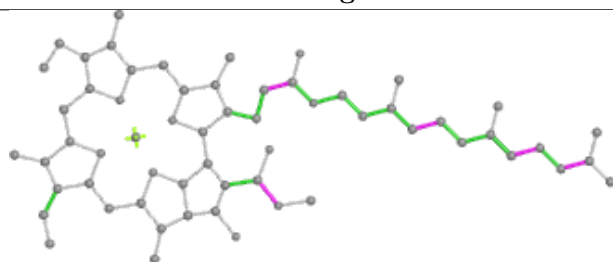
## Ligand CLA B 832



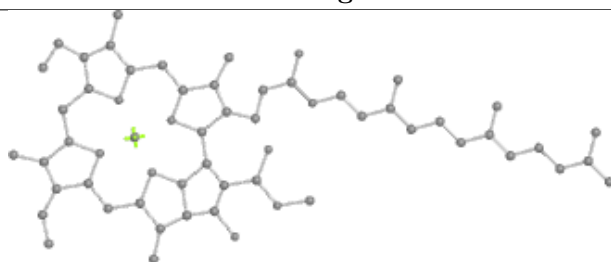
Bond lengths



Bond angles

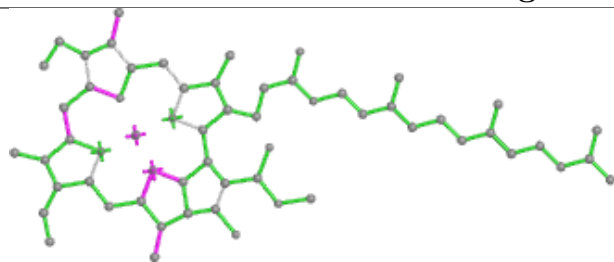


Torsions

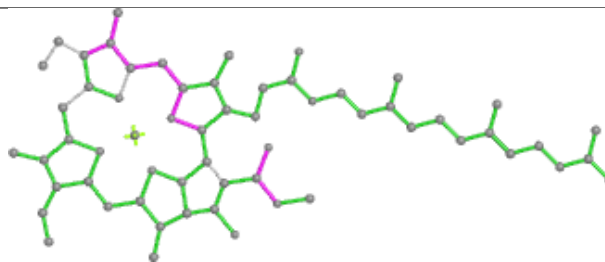


Rings

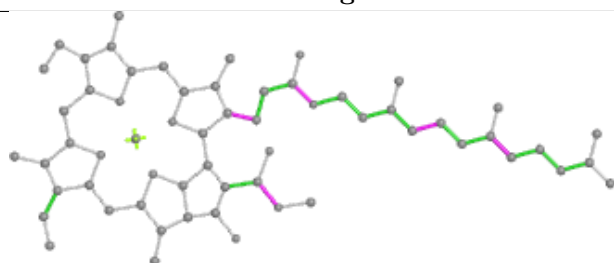
## Ligand CLA 6 614



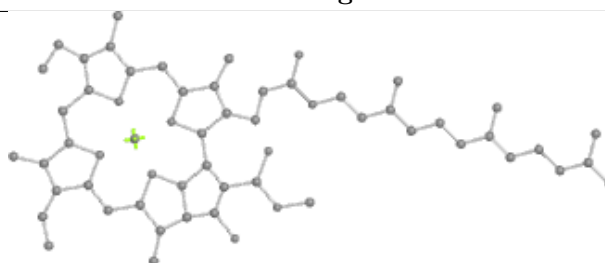
Bond lengths



Bond angles

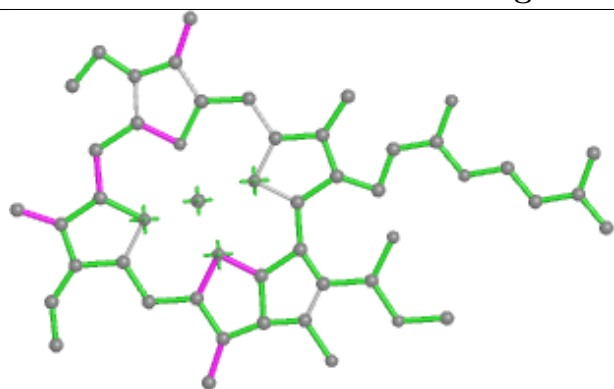


Torsions

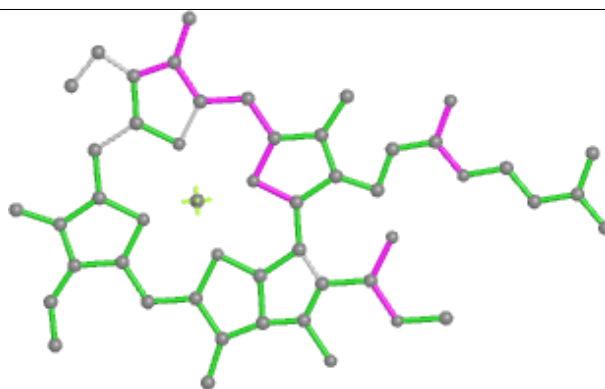


Rings

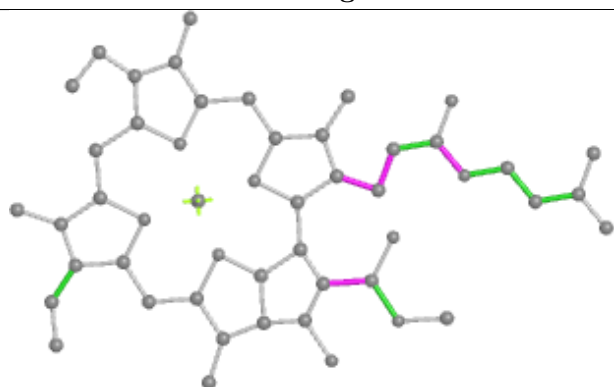
## Ligand CLA B 820



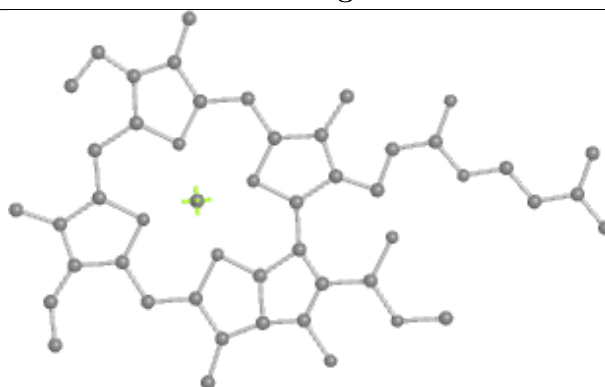
Bond lengths



Bond angles

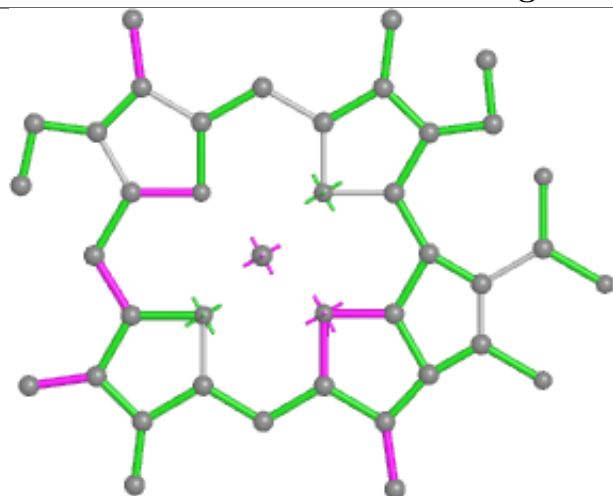


Torsions

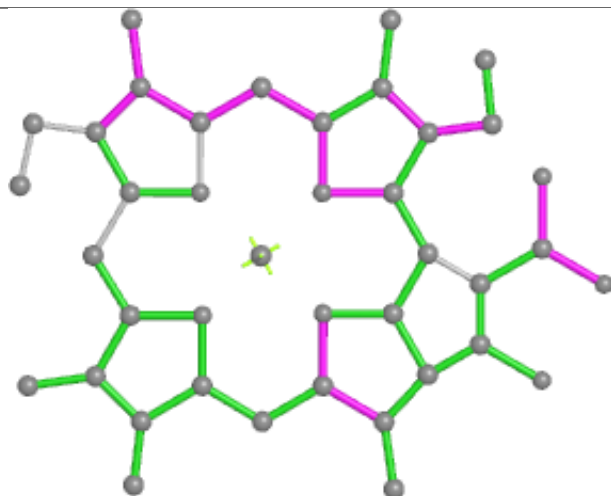


Rings

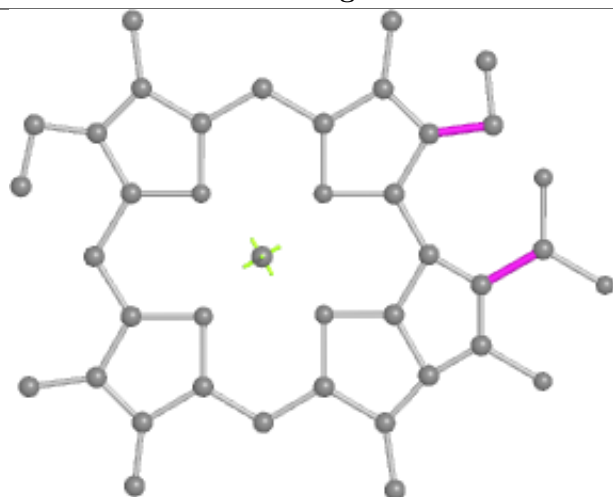
## Ligand CLA 4 606



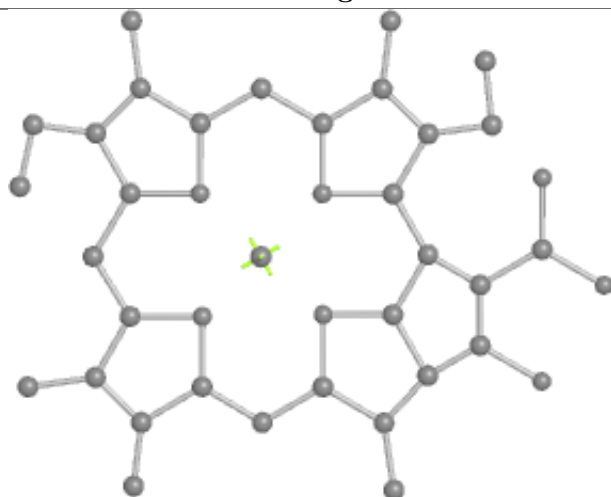
Bond lengths



Bond angles

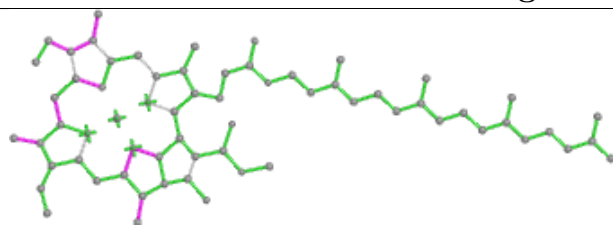


Torsions

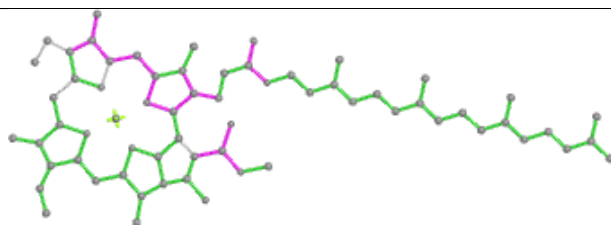


Rings

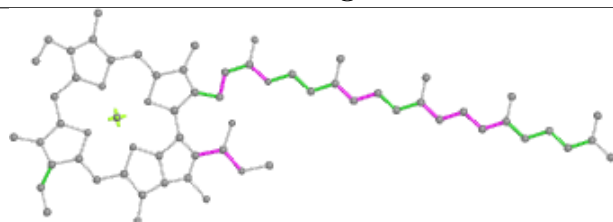
## Ligand CLA 8 613



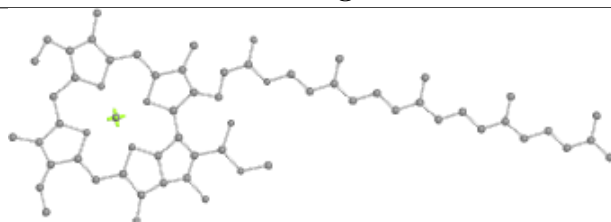
Bond lengths



Bond angles

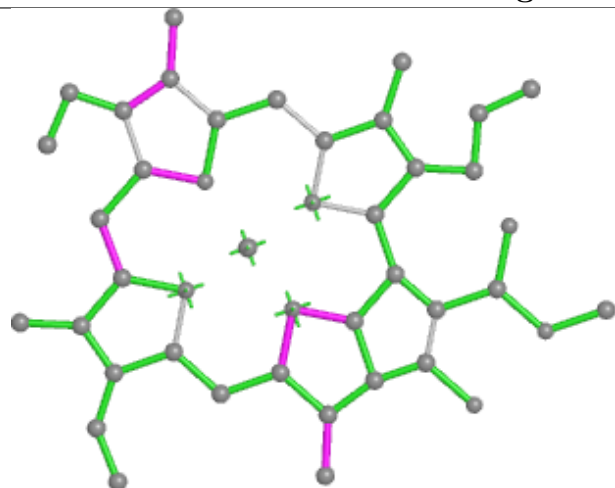


Torsions

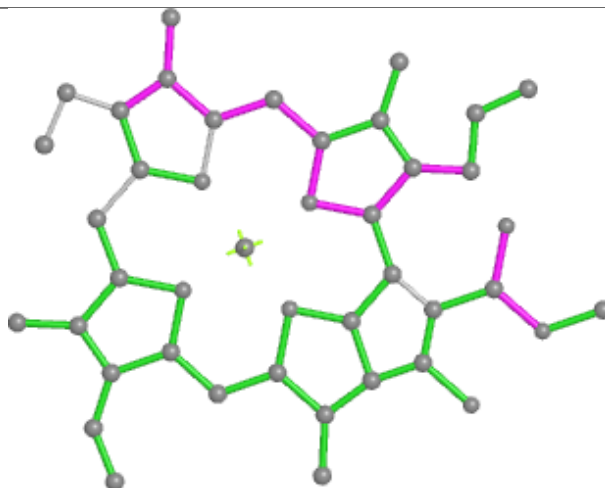


Rings

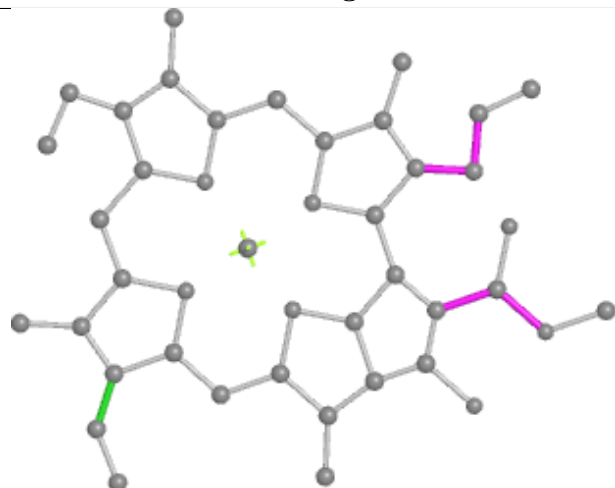
## Ligand CLA B 812



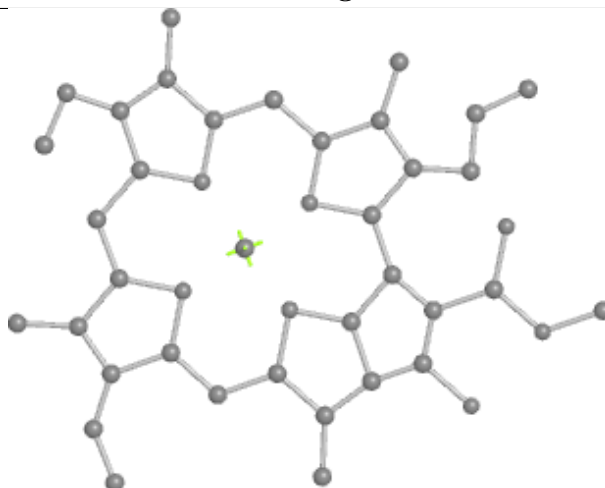
Bond lengths



Bond angles

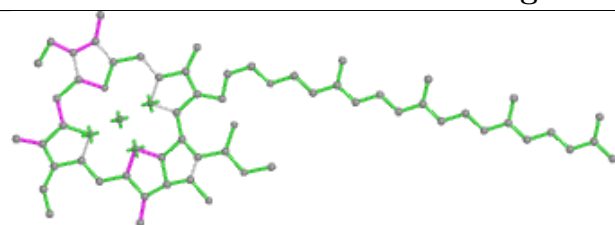


Torsions

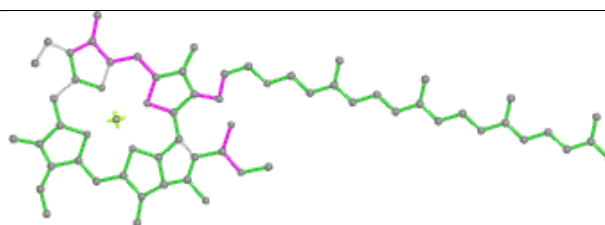


Rings

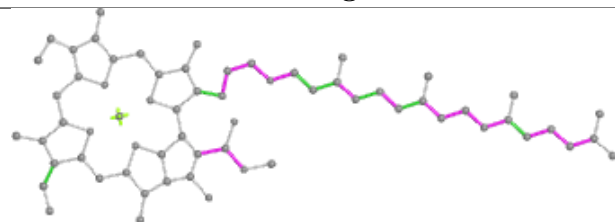
## Ligand CLA 5 613



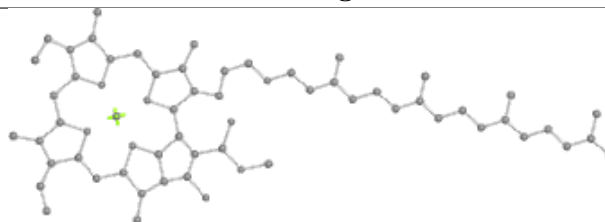
Bond lengths



Bond angles

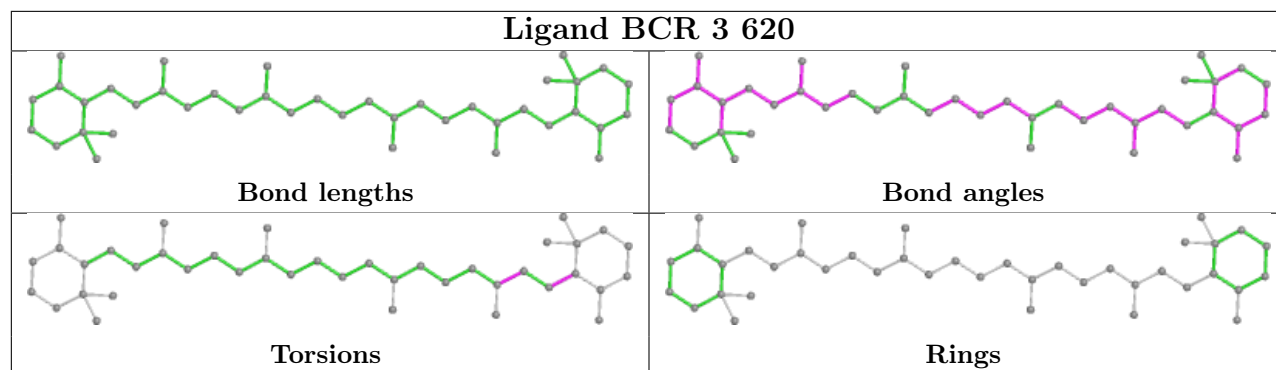


Torsions

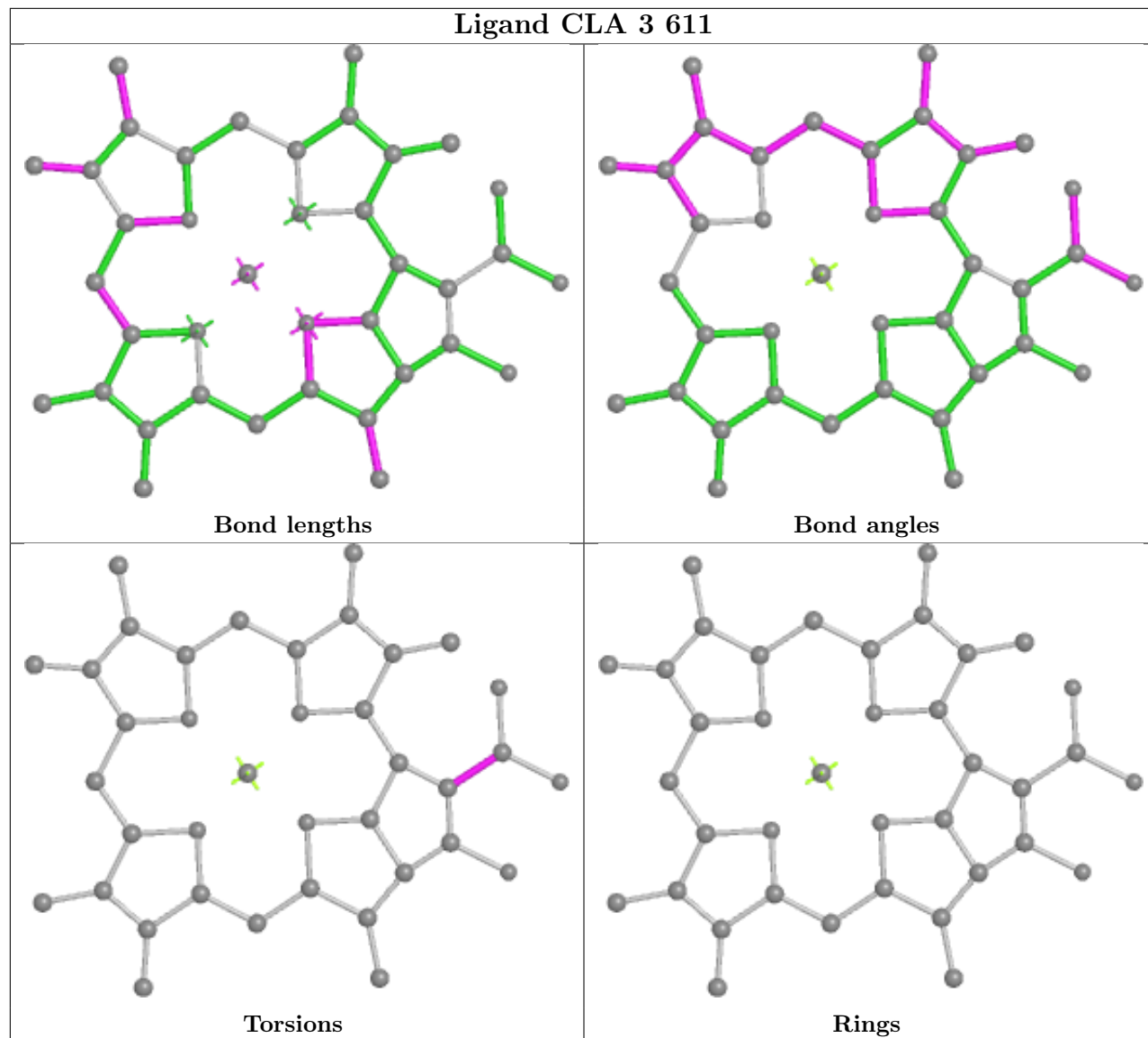


Rings

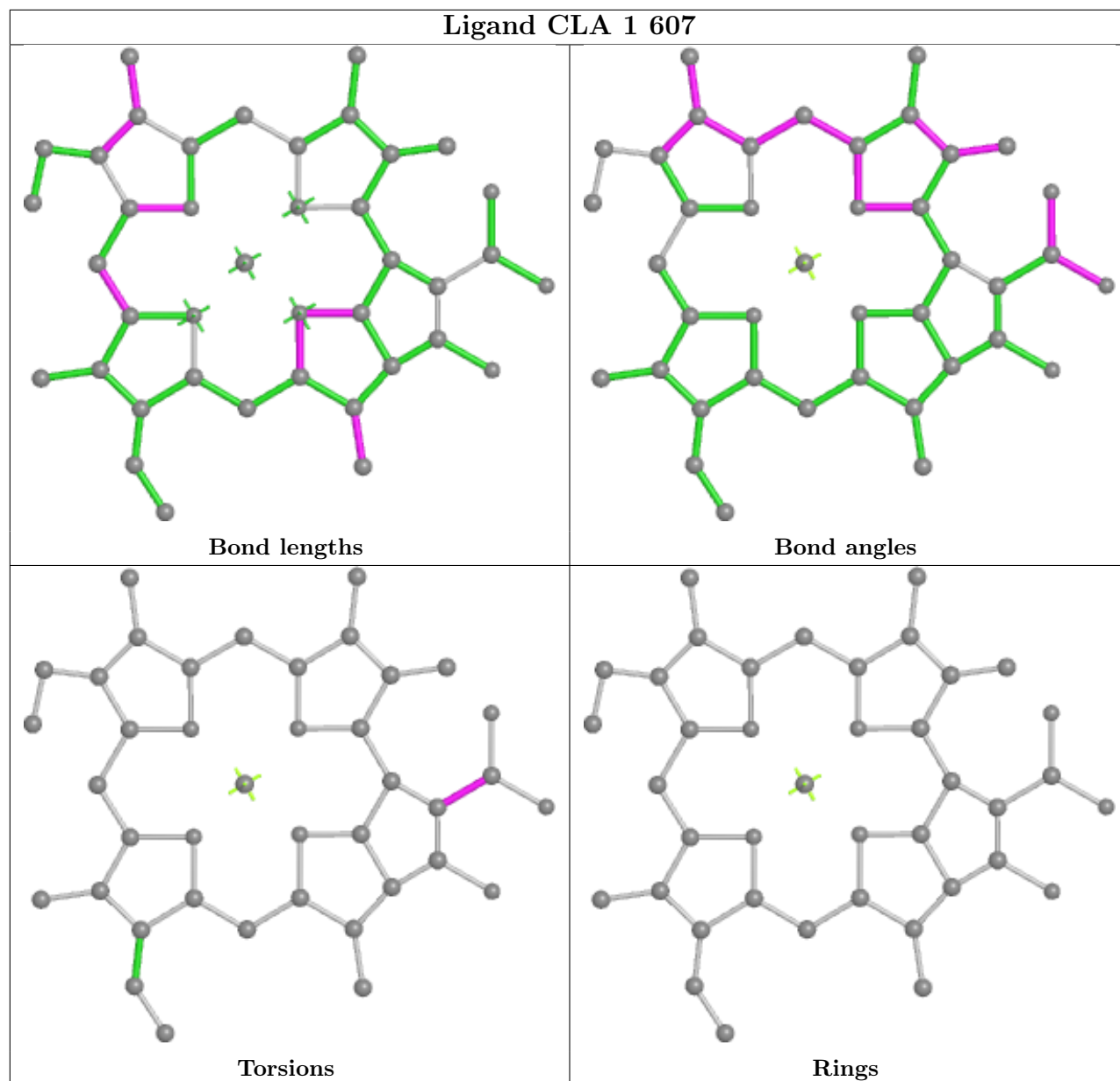
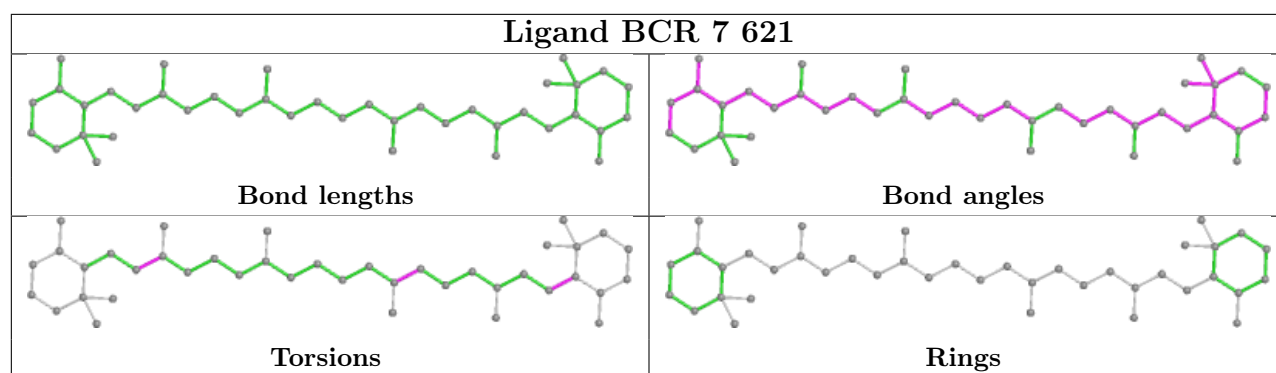
## Ligand BCR 3 620

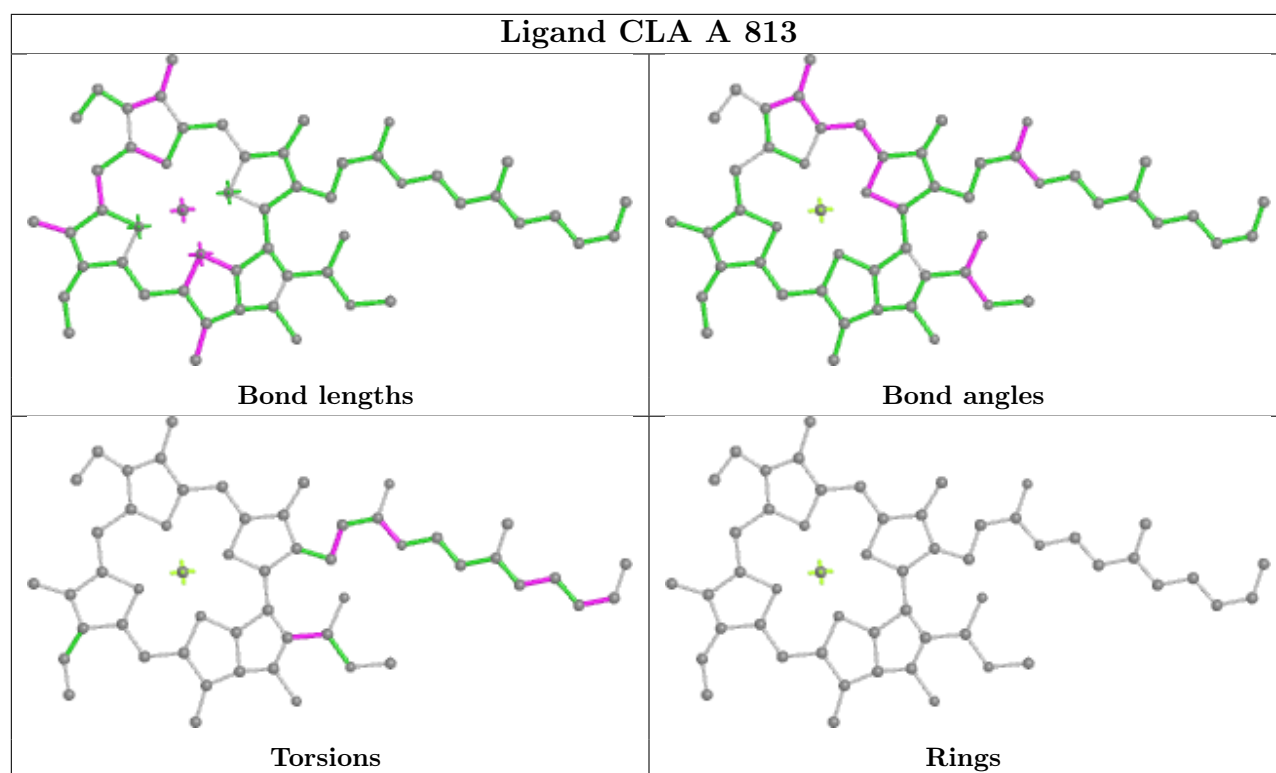


## Ligand CLA 3 611

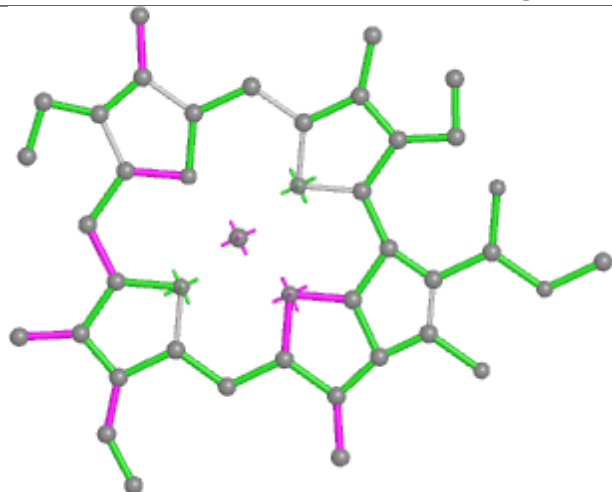




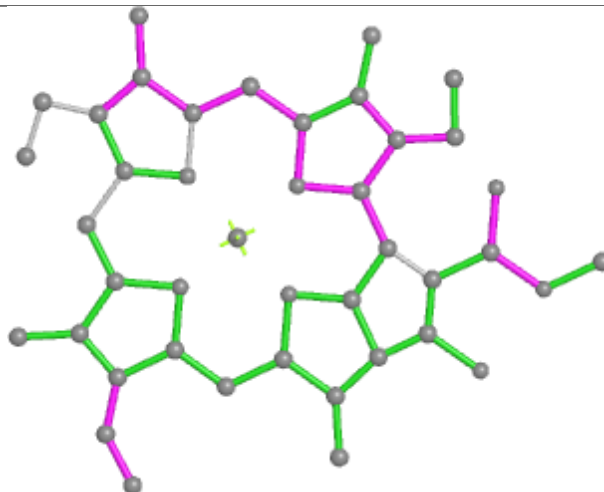




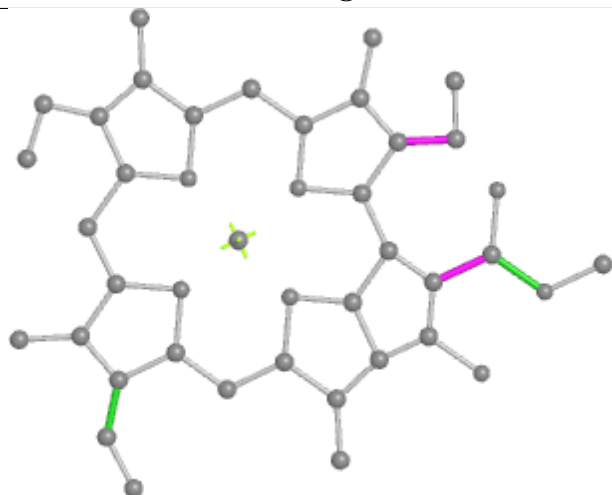
## Ligand CLA a 603



Bond lengths



Bond angles

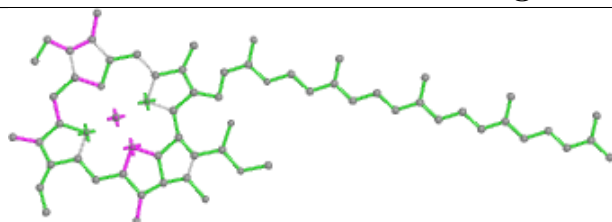


Torsions

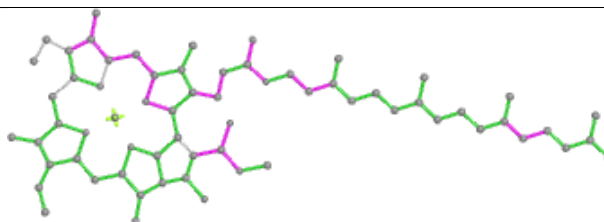


Rings

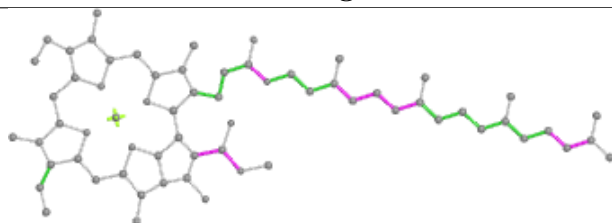
## Ligand CLA B 808



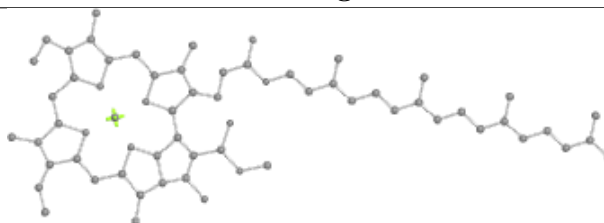
Bond lengths



Bond angles

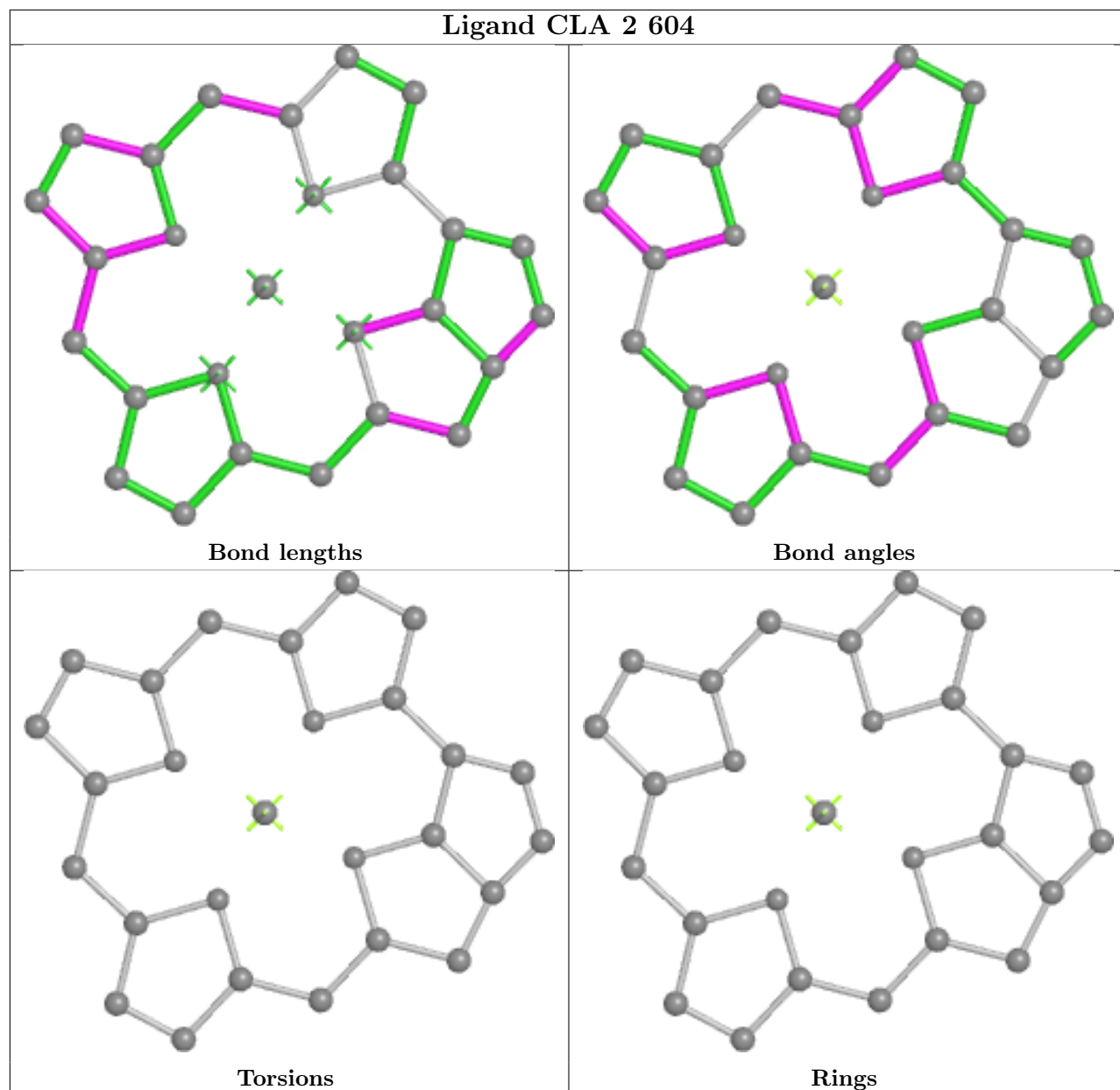


Torsions

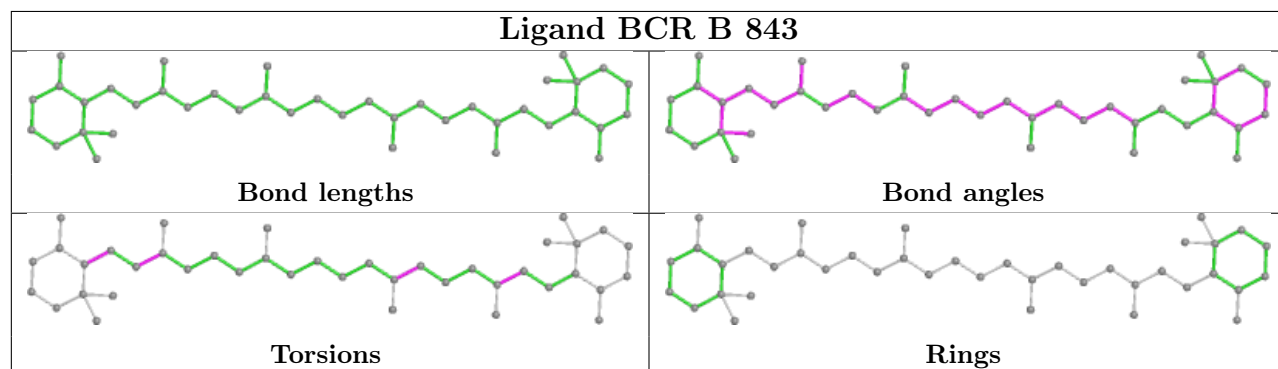


Rings

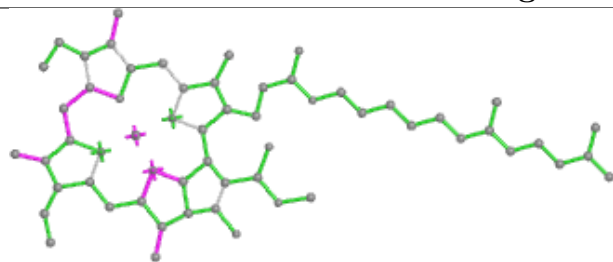
## Ligand CLA 2 604



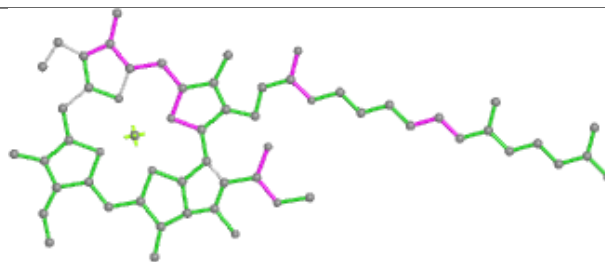
## Ligand BCR B 843



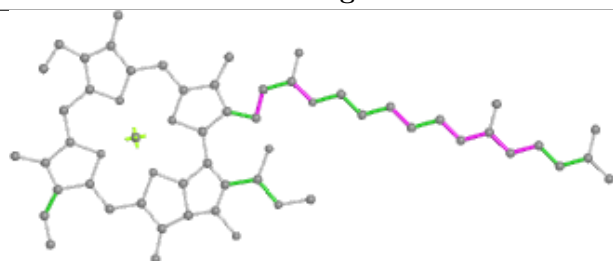
## Ligand CLA 7 611



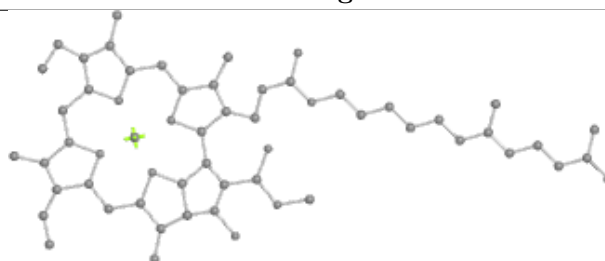
Bond lengths



Bond angles

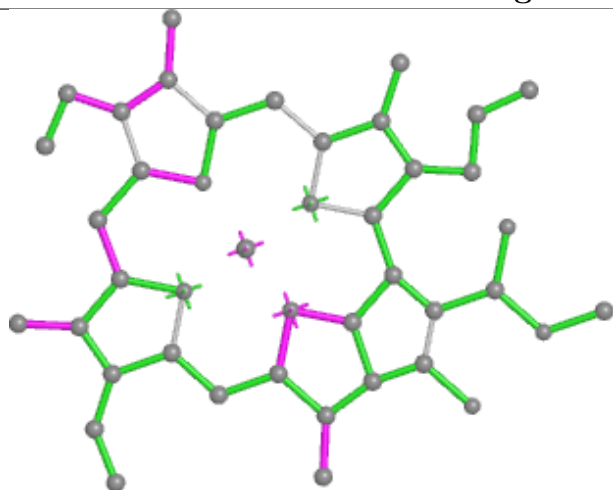


Torsions

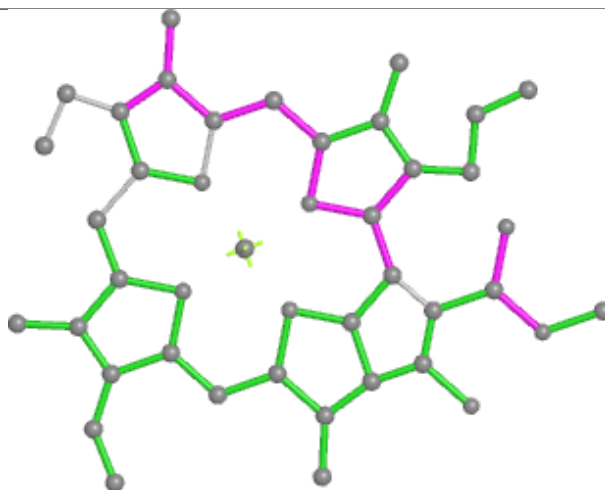


Rings

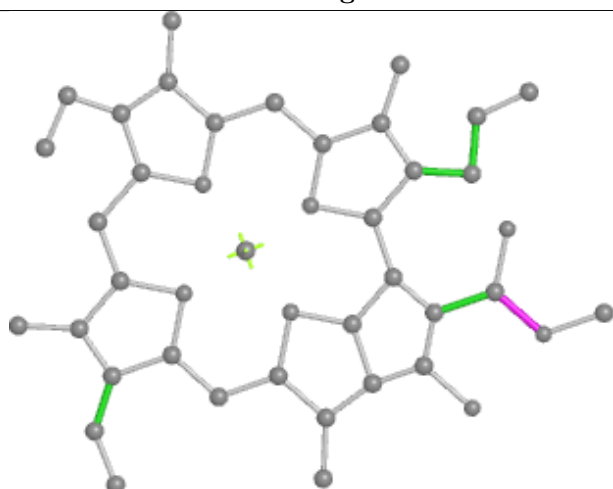
## Ligand CLA B 815



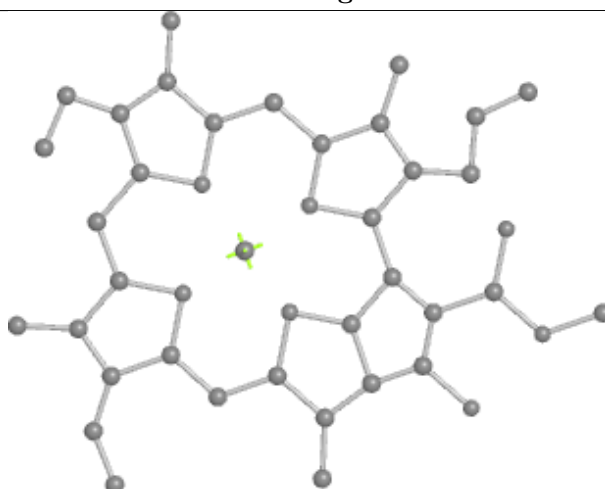
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

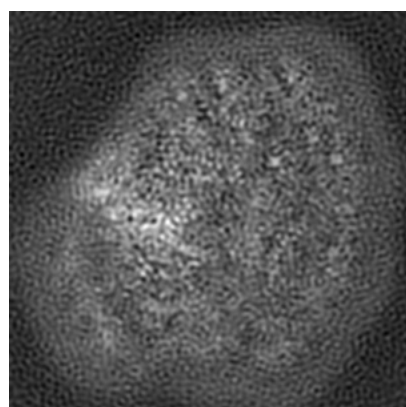
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9680. These allow visual inspection of the internal detail of the map and identification of artifacts.

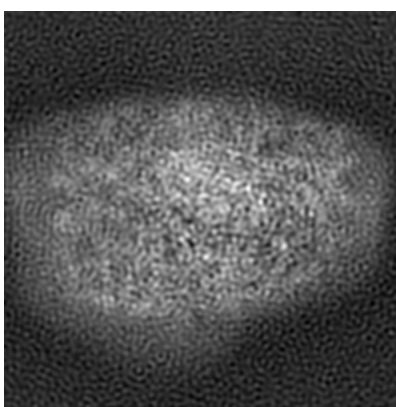
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

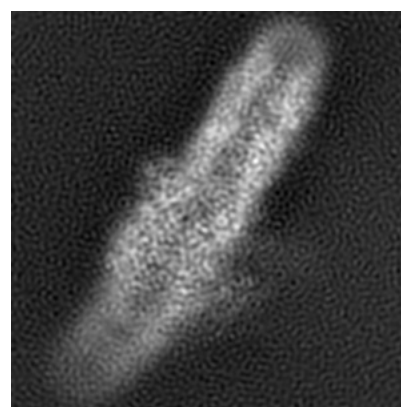
#### 6.1.1 Primary map



X



Y

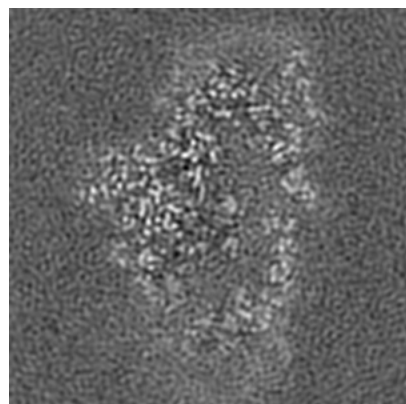


Z

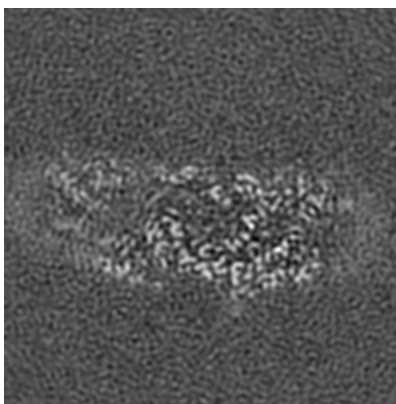
The images above show the map projected in three orthogonal directions.

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

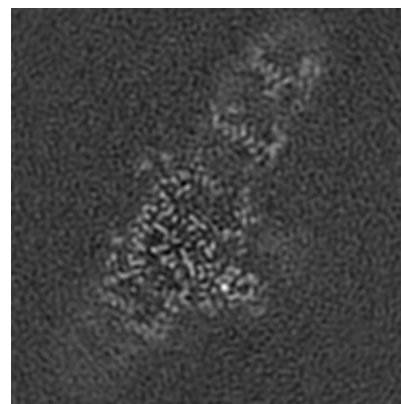
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

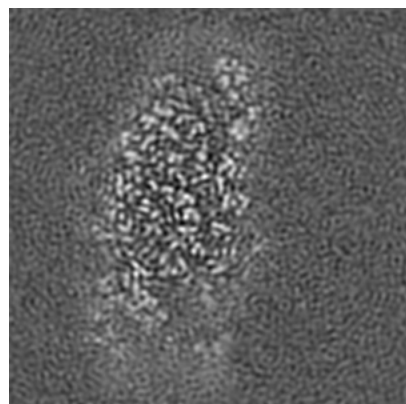


Z Index: 100

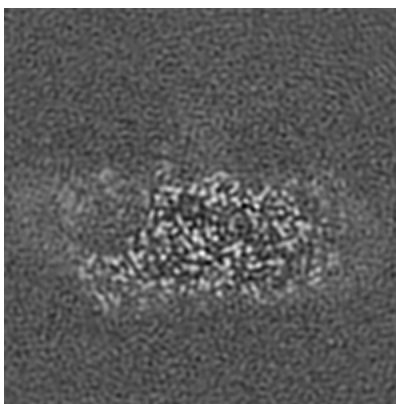
The images above show central slices of the map in three orthogonal directions.

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

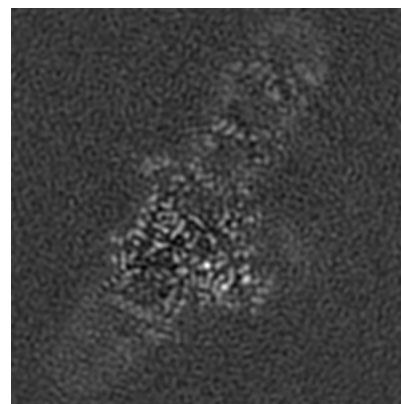
### 6.3.1 Primary map



X Index: 84



Y Index: 88

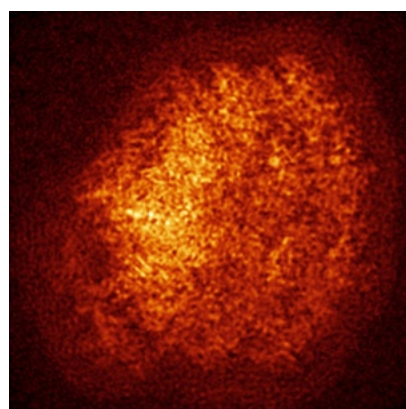


Z Index: 98

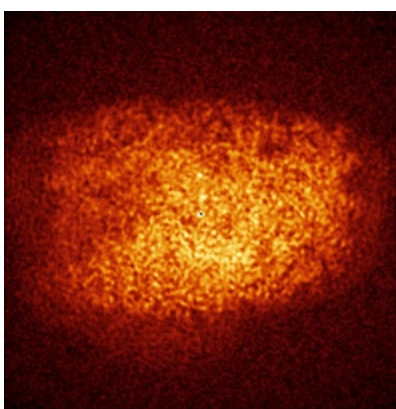
The images above show the largest variance slices of the map in three orthogonal directions.

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

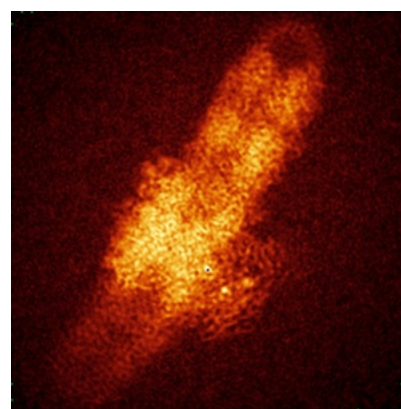
### 6.4.1 Primary map



X



Y



Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

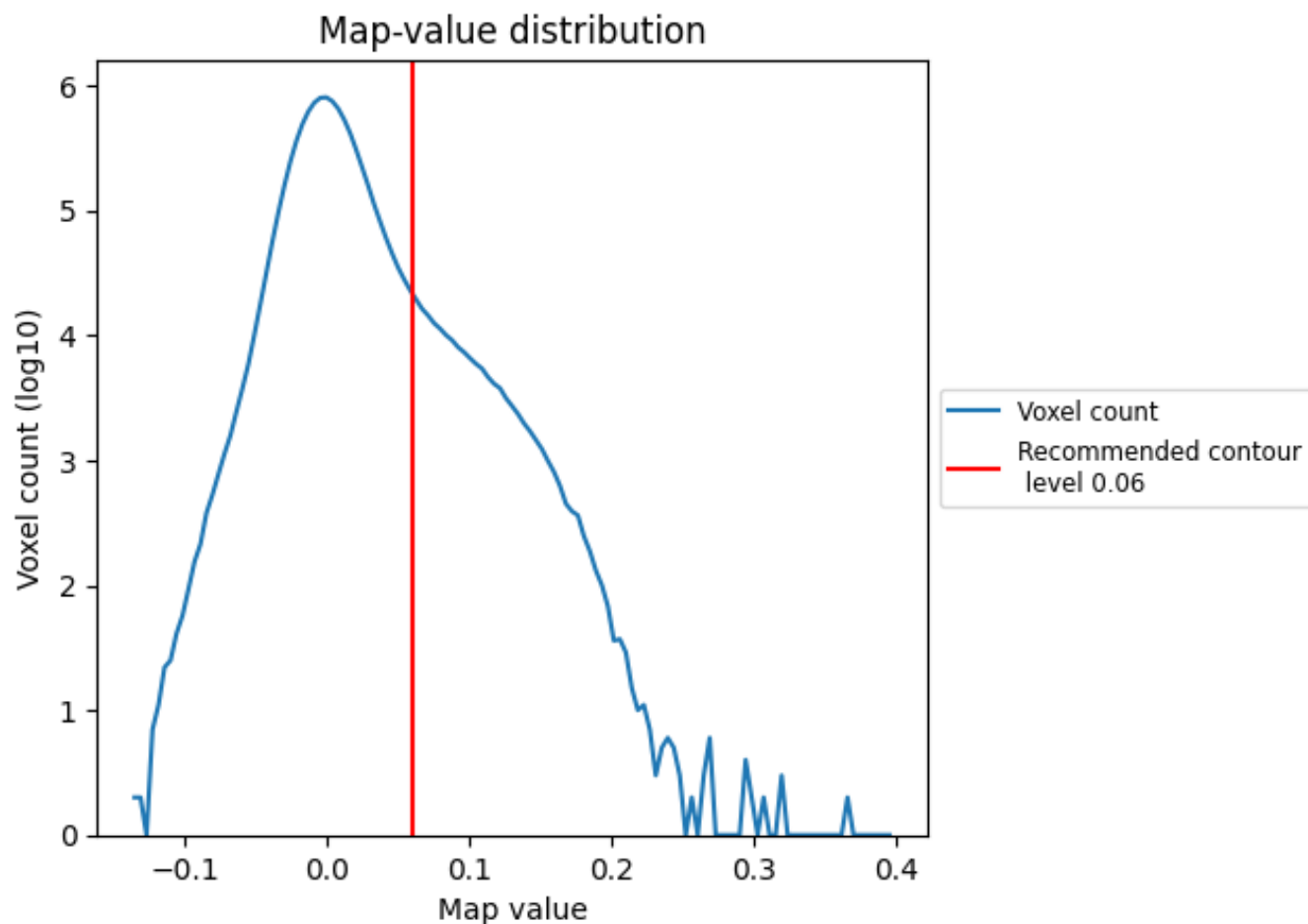
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

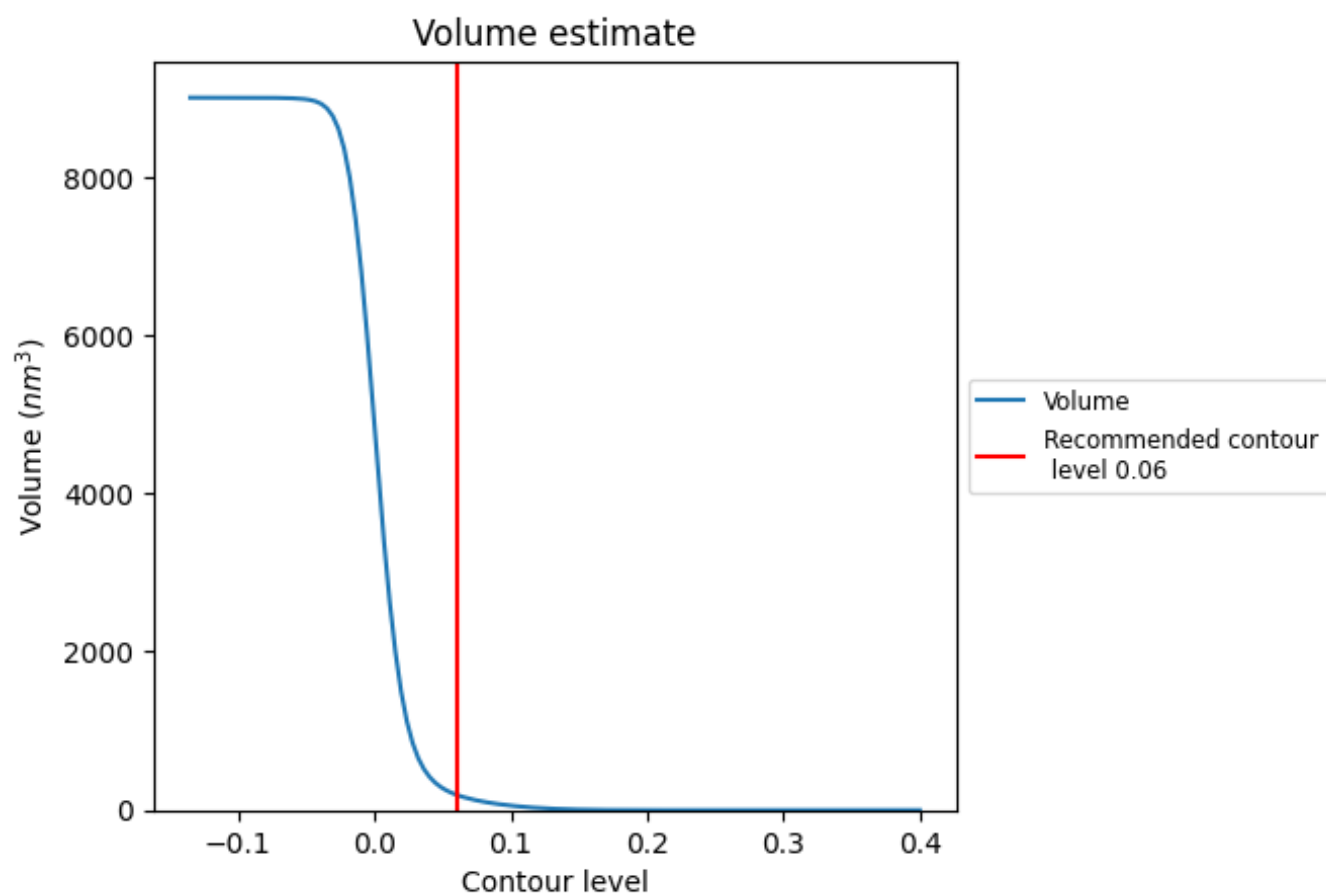
This section contains the results of statistical analysis of the map.

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



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

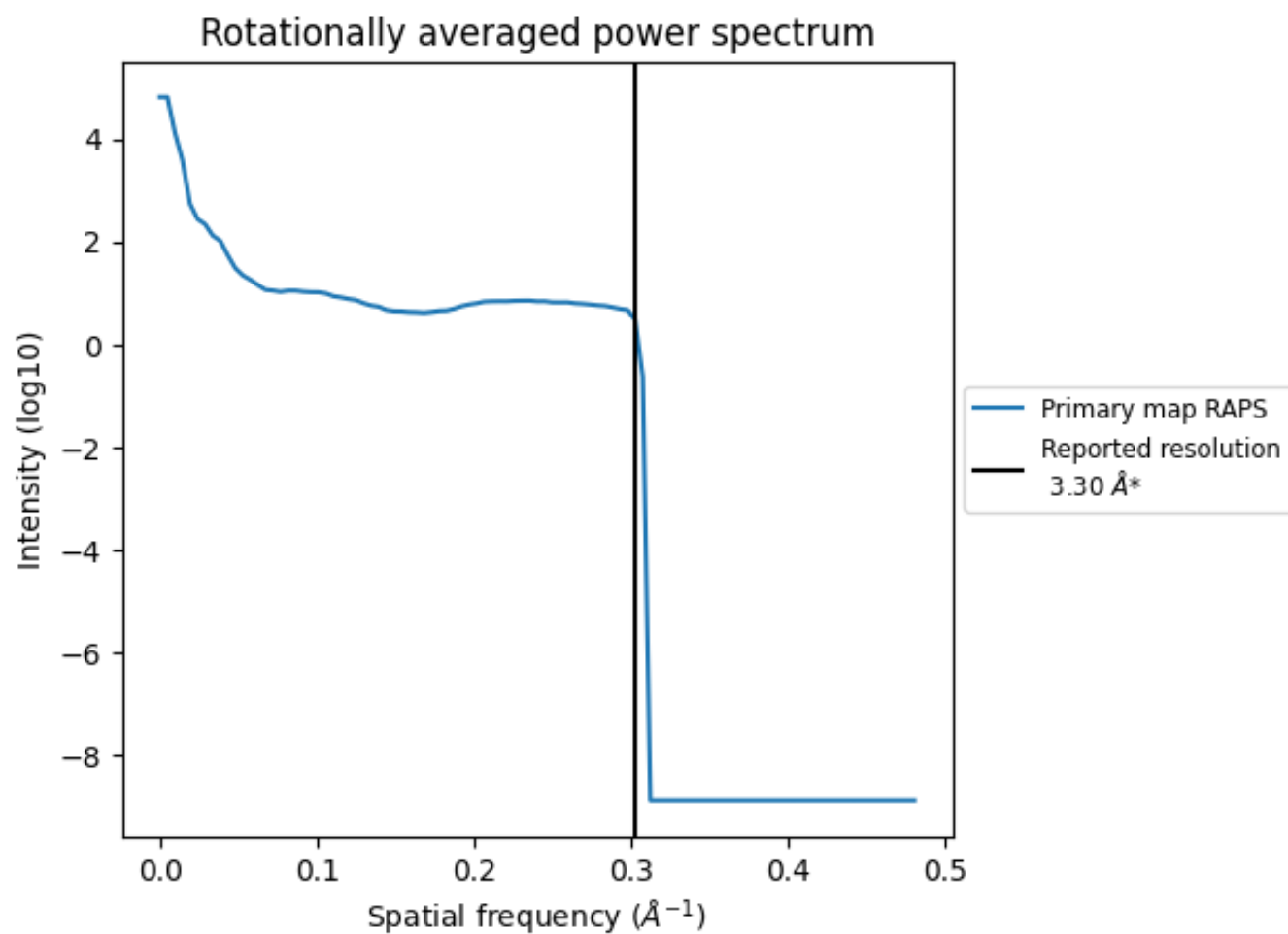
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm<sup>3</sup>; this corresponds to an approximate mass of 177 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

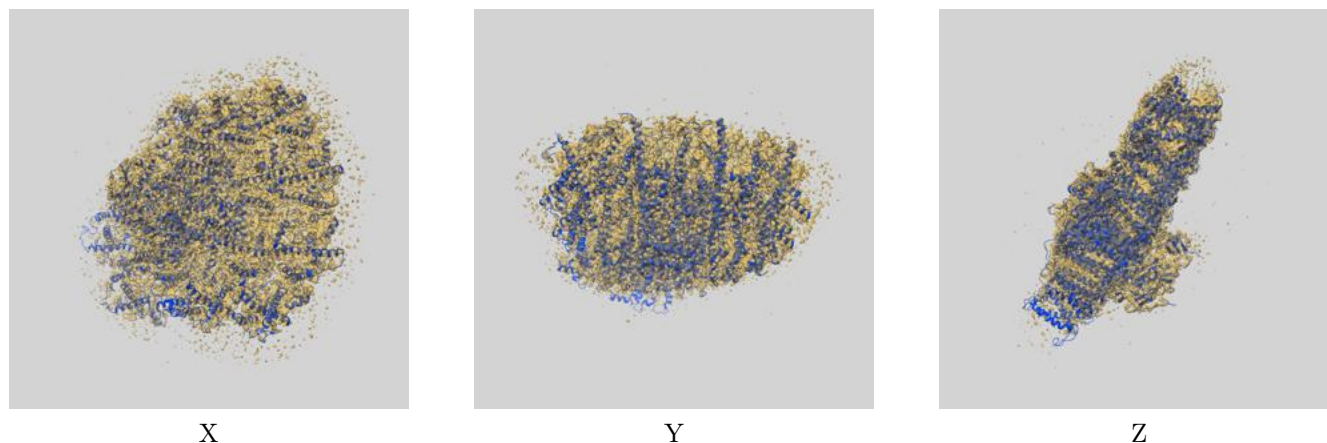
## 8 Fourier-Shell correlation

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

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

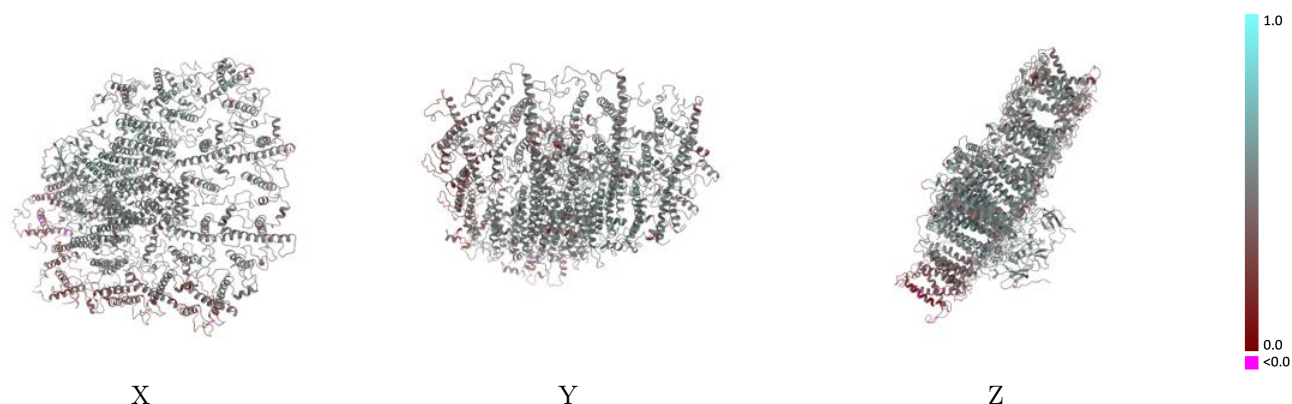
This section contains information regarding the fit between EMDB map EMD-9680 and PDB model 6IJO. Per-residue inclusion information can be found in section 3 on page 35.

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



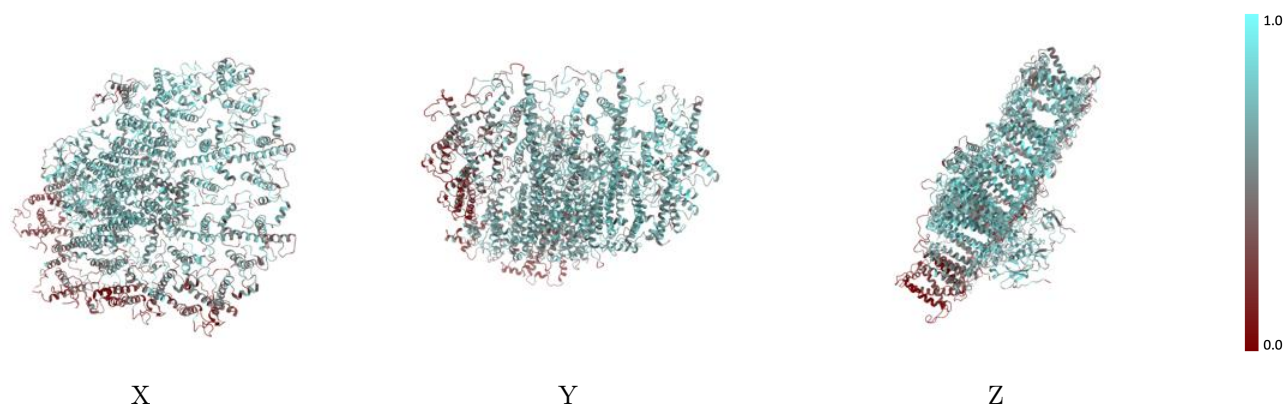
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



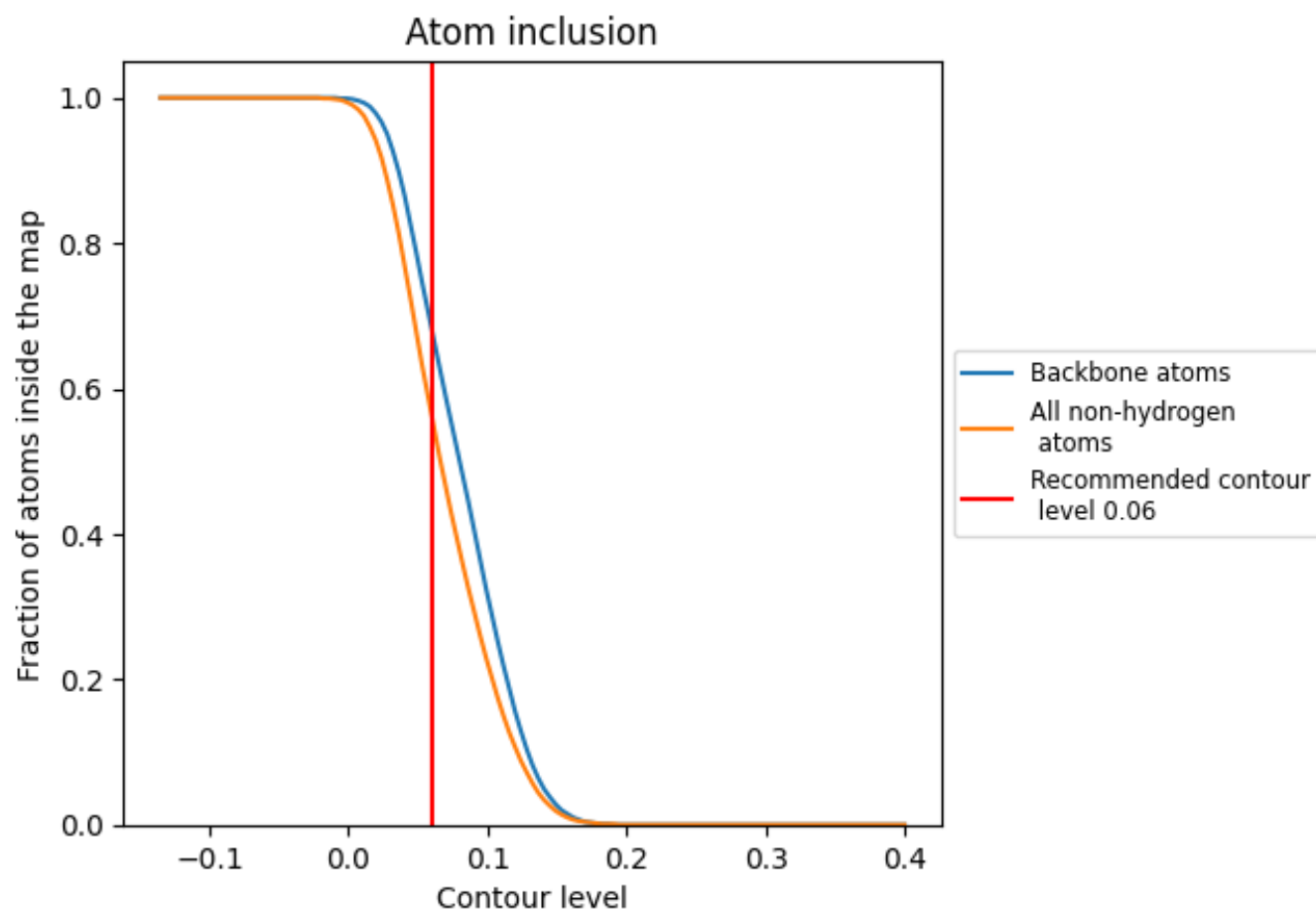
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



















































At the recommended contour level, 68% of all backbone atoms, 56% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5620	 0.4690
1	 0.4300	 0.3900
2	 0.0930	 0.2380
3	 0.6630	 0.5120
4	 0.5190	 0.4540
5	 0.5820	 0.4790
6	 0.5810	 0.4770
7	 0.6370	 0.4970
8	 0.5960	 0.4870
9	 0.2720	 0.2900
A	 0.7080	 0.5400
B	 0.6440	 0.5150
C	 0.7140	 0.4870
D	 0.6490	 0.4900
E	 0.6160	 0.4570
F	 0.5690	 0.4590
G	 0.0740	 0.3300
H	 0.0910	 0.3340
I	 0.5670	 0.4660
J	 0.4220	 0.4370
K	 0.4790	 0.4470
L	 0.4380	 0.4150
X	 0.2620	 0.2840
a	 0.4000	 0.4140

