



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 12:48 PM JST

PDB ID : 8J6Z  
EMDB ID : EMD-36021  
Title : Cryo-EM structure of the Arabidopsis thaliana photosystem I(PSI-LHCII-ST2)  
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.  
Deposited on : 2023-04-26  
Resolution : 2.79 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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

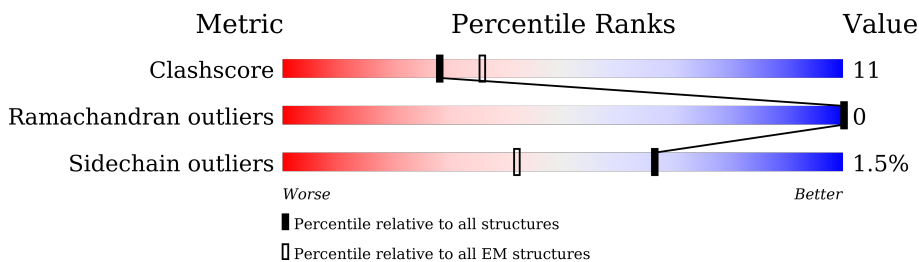
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 Å.

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















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

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

Mol	Chain	Length	Quality of chain
1	1	241	64% 15% 20%
2	2	257	65% 12% 22%
3	3	273	69% 11% 20%
4	4	251	71% 7% 22%
5	A	750	89% 9%
6	B	734	90% 10%
7	C	81	90% 7%
8	D	204	66% 30%

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Mol	Chain	Length	Quality of chain
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	
17	O	140	
18	x	267	
18	y	267	
19	z	265	

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
20	CHL	1	601	X	-	-	-
20	CHL	1	606	X	-	-	-
20	CHL	2	601	X	-	-	-
20	CHL	2	605	X	-	-	-
20	CHL	2	606	X	-	-	-
20	CHL	2	607	X	-	-	-
20	CHL	2	615	X	-	-	-
20	CHL	3	606	X	-	-	-
20	CHL	4	605	X	-	-	-
20	CHL	4	606	X	-	-	-
20	CHL	4	607	X	-	-	-
20	CHL	4	615	X	-	-	-
20	CHL	x	601	X	-	-	-
20	CHL	x	605	X	-	-	-
20	CHL	x	606	X	-	-	-
20	CHL	x	607	X	-	-	-
20	CHL	x	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CHL	x	609	X	-	-	-
20	CHL	y	601	X	-	-	-
20	CHL	y	605	X	-	-	-
20	CHL	y	606	X	-	-	-
20	CHL	y	607	X	-	-	-
20	CHL	y	608	X	-	-	-
20	CHL	y	609	X	-	-	-
20	CHL	z	601	X	-	-	-
20	CHL	z	605	X	-	-	-
20	CHL	z	606	X	-	-	-
20	CHL	z	607	X	-	-	-
20	CHL	z	608	X	-	-	-
20	CHL	z	609	X	-	-	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	605	X	-	-	-
21	CLA	1	607	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	609	X	-	-	-
21	CLA	1	610	X	-	-	-
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	613	X	-	-	-
21	CLA	2	602	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	-	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	601	X	-	-	-
21	CLA	3	602	X	-	-	-
21	CLA	3	603	X	-	-	-
21	CLA	3	604	X	-	-	-
21	CLA	3	605	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	608	X	-	-	-
21	CLA	3	609	X	-	-	-
21	CLA	3	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	3	611	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	609	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	4	614	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	844	X	-	-	-
21	CLA	A	845	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-
21	CLA	F	301	X	-	-	-
21	CLA	F	302	X	-	-	-
21	CLA	F	303	X	-	-	-
21	CLA	G	201	X	-	-	-
21	CLA	G	202	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	H	201	X	-	-	-
21	CLA	J	101	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	K	206	X	-	-	-
21	CLA	L	302	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	O	201	X	-	-	-
21	CLA	O	202	X	-	-	-
21	CLA	O	203	X	-	-	-
21	CLA	x	602	X	-	-	-
21	CLA	x	603	X	-	-	-
21	CLA	x	604	X	-	-	-
21	CLA	x	610	X	-	-	-
21	CLA	x	611	X	-	-	-
21	CLA	x	612	X	-	-	-
21	CLA	x	613	X	-	-	-
21	CLA	x	614	X	-	-	-
21	CLA	y	602	X	-	-	-
21	CLA	y	603	X	-	-	-
21	CLA	y	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	y	610	X	-	-	-
21	CLA	y	611	X	-	-	-
21	CLA	y	612	X	-	-	-
21	CLA	y	613	X	-	-	-
21	CLA	y	614	X	-	-	-
21	CLA	z	602	X	-	-	-
21	CLA	z	603	X	-	-	-
21	CLA	z	604	X	-	-	-
21	CLA	z	610	X	-	-	-
21	CLA	z	611	X	-	-	-
21	CLA	z	612	X	-	-	-
21	CLA	z	613	X	-	-	-
21	CLA	z	614	X	-	-	-
27	CL0	A	801	X	-	-	-
28	SF4	A	854	-	-	X	-
28	SF4	C	101	-	-	X	-
28	SF4	C	102	-	-	X	-



## 2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 43924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	193	1496	975	248	268	5	0	0

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	201	1566	1024	256	282	4	0	0

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	218	1666	1088	270	303	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	196	1551	1013	253	282	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	737	5807	3807	986	996	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	732	5854	3842	997	1001	14	0	0

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	80	616	381	107	117	11	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	143	1128	723	195	206	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	64	517	331	92	94	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	152	1208	789	207	209	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	91	708	458	118	132	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	H	90	693	451	112	130	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	31	239	162	39	37	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			327	221	50	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			593	373	104	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1207	799	191	215	2		

- Molecule 17 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	86	Total	C	N	O	S	0	0
			686	456	114	115	1		

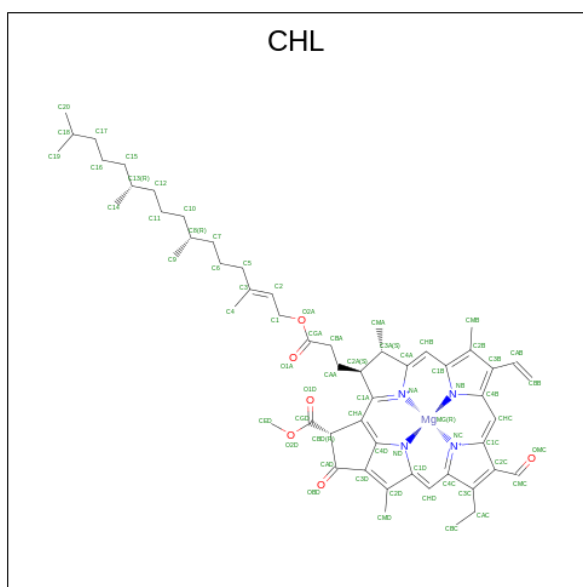
- Molecule 18 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	x	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
18	y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 2.1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	z	227	Total	C	N	O	P	S	0	0
			1759	1140	286	327	1	5		

- Molecule 20 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



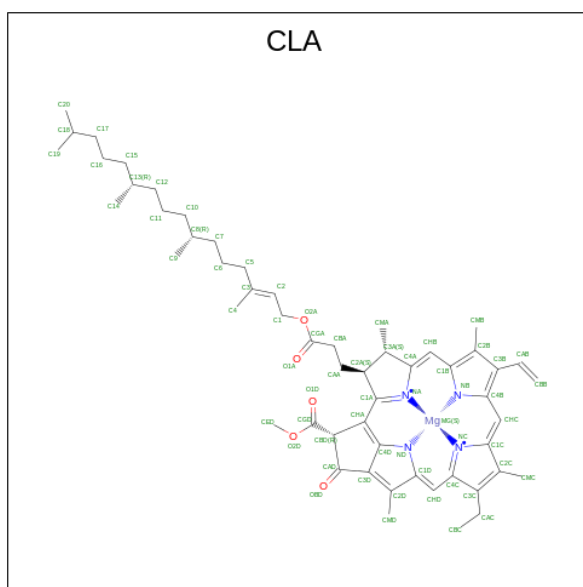
Mol	Chain	Residues	Atoms				AltConf	
20	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms				AltConf	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	z	1	Total	C	Mg	N	O	0
			52	41	1	4	6	

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
21	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	2	1	38	30	1	4	3	0
21	2	1	65	55	1	4	5	0
21	2	1	44	34	1	4	5	0
21	2	1	45	35	1	4	5	0
21	2	1	47	37	1	4	5	0
21	2	1	43	35	1	4	3	0
21	3	1	60	50	1	4	5	0
21	3	1	36	30	1	4	1	0
21	3	1	41	33	1	4	3	0
21	3	1	45	35	1	4	5	0
21	3	1	40	32	1	4	3	0
21	3	1	45	35	1	4	5	0
21	3	1	41	33	1	4	3	0
21	3	1	40	32	1	4	3	0
21	3	1	55	45	1	4	5	0
21	3	1	54	44	1	4	5	0
21	3	1	41	33	1	4	3	0
21	4	1	45	35	1	4	5	0
21	4	1	54	44	1	4	5	0
21	4	1	45	35	1	4	5	0
21	4	1	44	34	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	41	33	1	4	3	0
21	4	1	57	47	1	4	5	0
21	4	1	46	36	1	4	5	0
21	4	1	60	50	1	4	5	0
21	4	1	42	34	1	4	3	0
21	4	1	50	40	1	4	5	0
21	4	1	43	33	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	54	44	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	60	50	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	42	34	1	4	3	0
21	A	1	41	33	1	4	3	0
21	A	1	59	49	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	55	45	1	4	5	0
21	A	1	52	42	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	42	34	1	4	3	0
21	A	1	65	55	1	4	5	0
21	A	1	59	49	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	51	41	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	56	46	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	52	42	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	55	45	1	4	5	0
21	B	1	55	45	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	50	40	1	4	5	0
21	B	1	41	33	1	4	3	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	59	49	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	56	46	1	4	5	0
21	B	1	43	35	1	4	3	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	43	35	1	4	3	0
21	B	1	54	44	1	4	5	0
21	B	1	45	35	1	4	5	0
21	B	1	62	52	1	4	5	0
21	B	1	50	40	1	4	5	0
21	B	1	47	37	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	52	42	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	42	34	1	4	3	0
21	B	1	47	37	1	4	5	0
21	B	1	62	52	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	45	35	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	55	45	1	4	5	0
21	B	1	60	50	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
21	B	1	43	35	1	4	3	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	60	50	1	4	5	0
21	B	1	43	35	1	4	3	0
21	B	1	65	55	1	4	5	0
21	F	1	51	41	1	4	5	0
21	F	1	41	33	1	4	3	0
21	F	1	57	47	1	4	5	0
21	G	1	45	35	1	4	5	0
21	G	1	42	34	1	4	3	0
21	G	1	45	35	1	4	5	0
21	H	1	60	50	1	4	5	0
21	J	1	51	41	1	4	5	0
21	K	1	37	31	1	4	1	0
21	K	1	46	36	1	4	5	0
21	K	1	39	31	1	4	3	0
21	K	1	45	35	1	4	5	0
21	L	1	45	35	1	4	5	0
21	L	1	65	55	1	4	5	0

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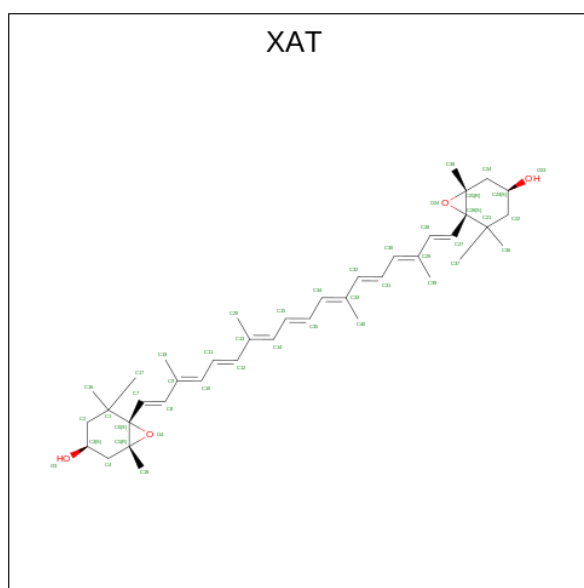
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	L	1	45	35	1	4	5	0
21	O	1	38	30	1	4	3	0
21	O	1	38	30	1	4	3	0
21	O	1	65	55	1	4	5	0
21	x	1	65	55	1	4	5	0
21	x	1	52	42	1	4	5	0
21	x	1	45	35	1	4	5	0
21	x	1	65	55	1	4	5	0
21	x	1	45	35	1	4	5	0
21	x	1	59	49	1	4	5	0
21	x	1	45	35	1	4	5	0
21	x	1	60	50	1	4	5	0
21	y	1	53	43	1	4	5	0
21	y	1	58	48	1	4	5	0
21	y	1	45	35	1	4	5	0
21	y	1	45	35	1	4	5	0
21	y	1	65	55	1	4	5	0
21	y	1	51	41	1	4	5	0
21	y	1	65	55	1	4	5	0
21	y	1	45	35	1	4	5	0
21	z	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	z	1	65	55	1	4	5	0
21	z	1	45	35	1	4	5	0
21	z	1	65	55	1	4	5	0
21	z	1	51	41	1	4	5	0
21	z	1	45	35	1	4	5	0
21	z	1	45	35	1	4	5	0
21	z	1	57	47	1	4	5	0

- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



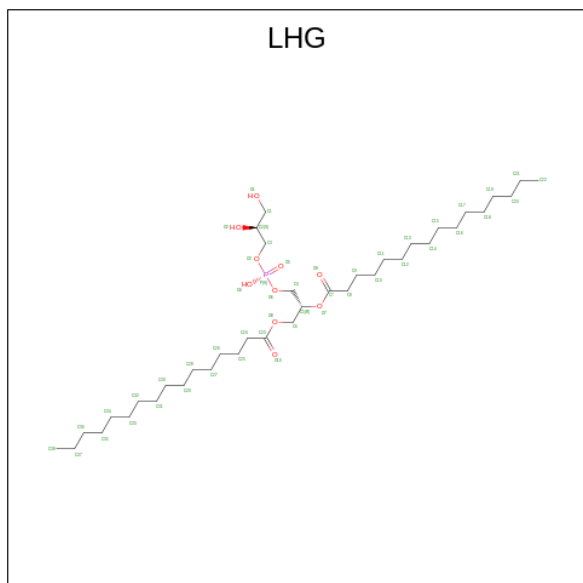
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	1	1	44	40	4	0
22	2	1	44	40	4	0
22	4	1	44	40	4	0
22	x	1	44	40	4	0

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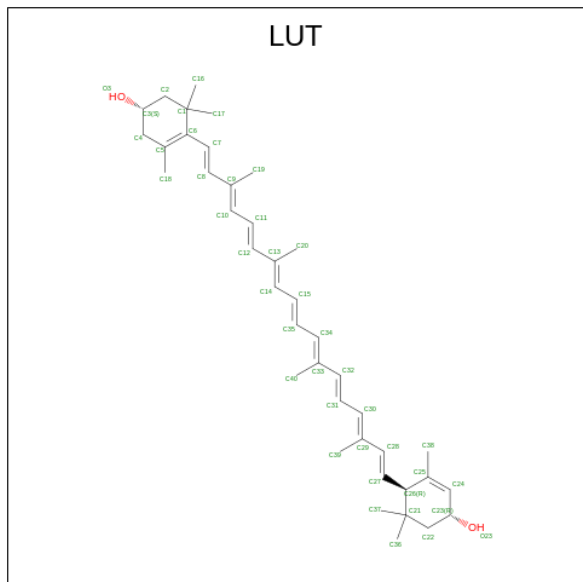
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	y	1	44	40	4	0
22	z	1	44	40	4	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{76}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	1	1	49	38	10	1	0
23	2	1	37	26	10	1	0
23	A	1	30	19	10	1	0
23	A	1	49	38	10	1	0
23	B	1	38	27	10	1	0
23	B	1	49	38	10	1	0
23	x	1	49	38	10	1	0
23	y	1	49	38	10	1	0
23	z	1	49	38	10	1	0

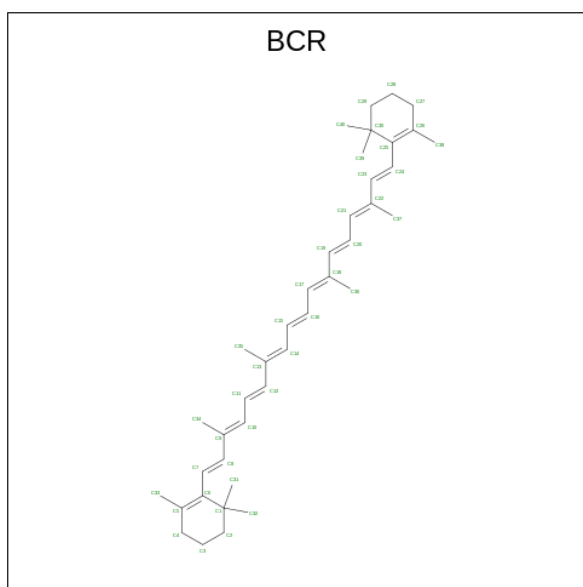
- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula:  $C_{40}H_{56}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	4	1	Total	C	O	0
			42	40	2	
24	x	1	Total	C	O	0
			42	40	2	
24	x	1	Total	C	O	0
			42	40	2	
24	y	1	Total	C	O	0
			42	40	2	
24	y	1	Total	C	O	0
			42	40	2	
24	z	1	Total	C	O	0
			42	40	2	
24	z	1	Total	C	O	0
			42	40	2	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





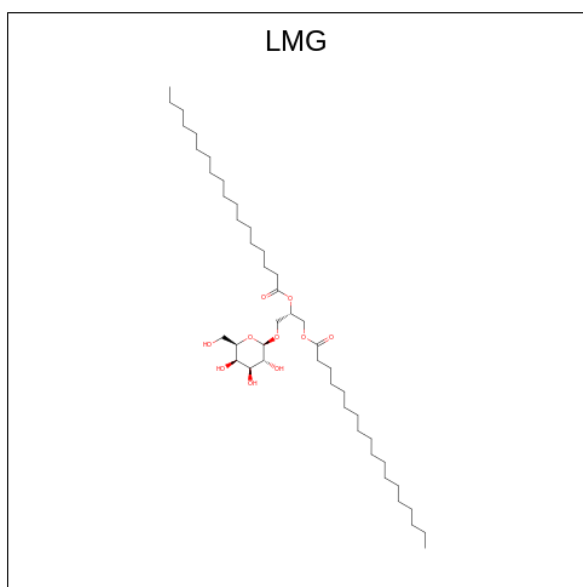
Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C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

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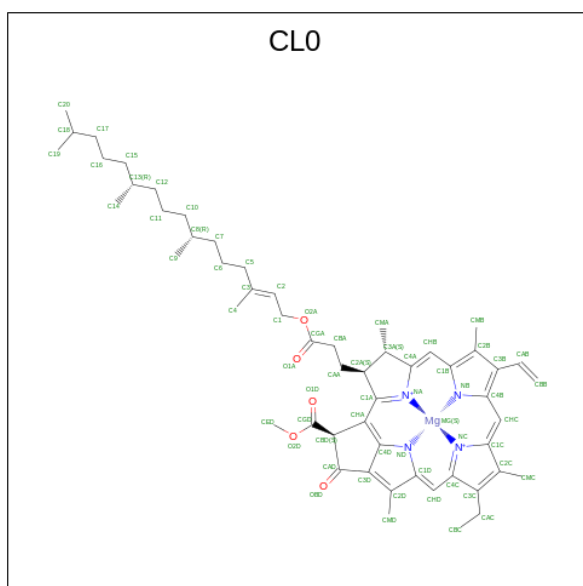
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



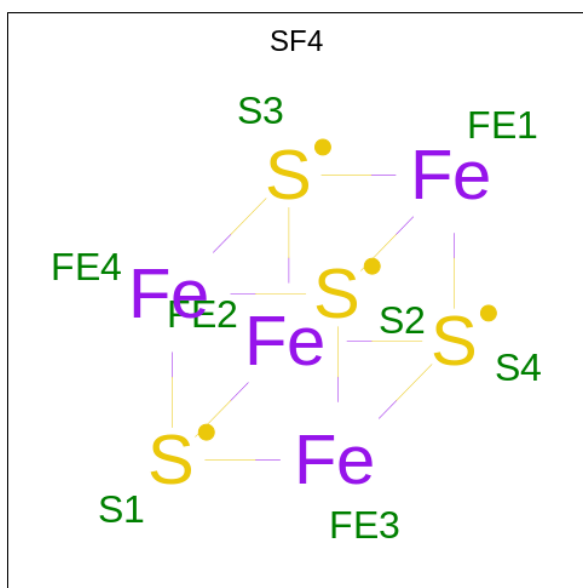
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			39	29	10	
26	4	1	Total	C	O	0
			33	23	10	

- Molecule 27 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



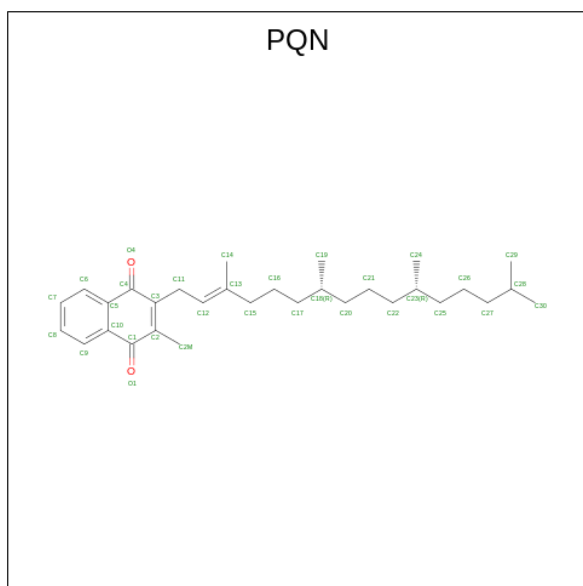
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			61	53	1	4	3	

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



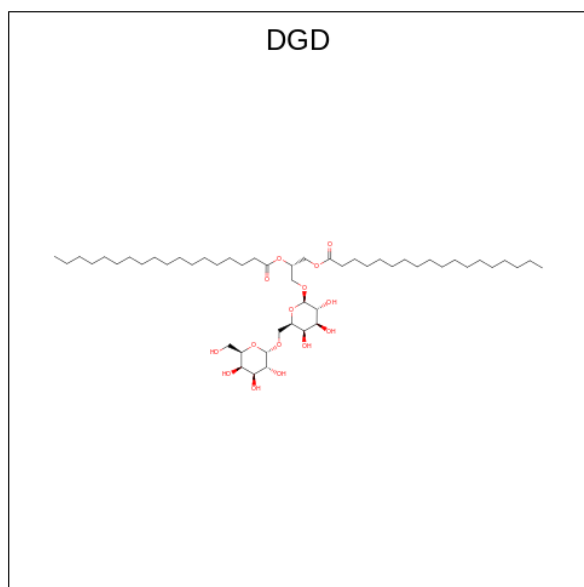
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Fe S	0
			8	4 4	
28	C	1	Total	Fe S	0
			8	4 4	
28	C	1	Total	Fe S	0
			8	4 4	

- Molecule 29 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



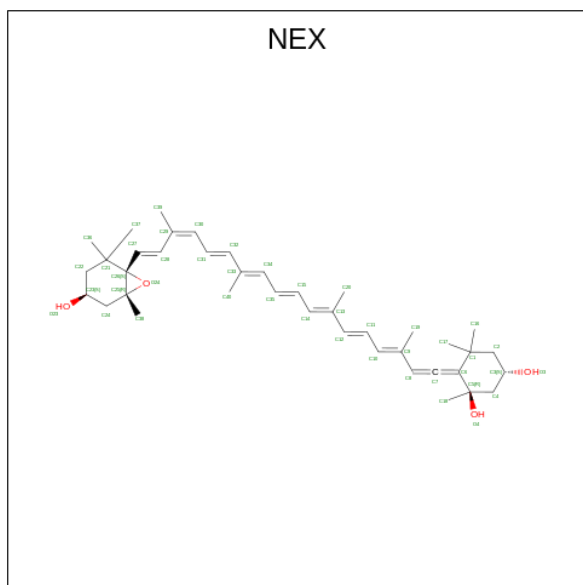
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

- 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
			66	51	15	

- Molecule 31 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula:  $C_{40}H_{56}O_4$ ).

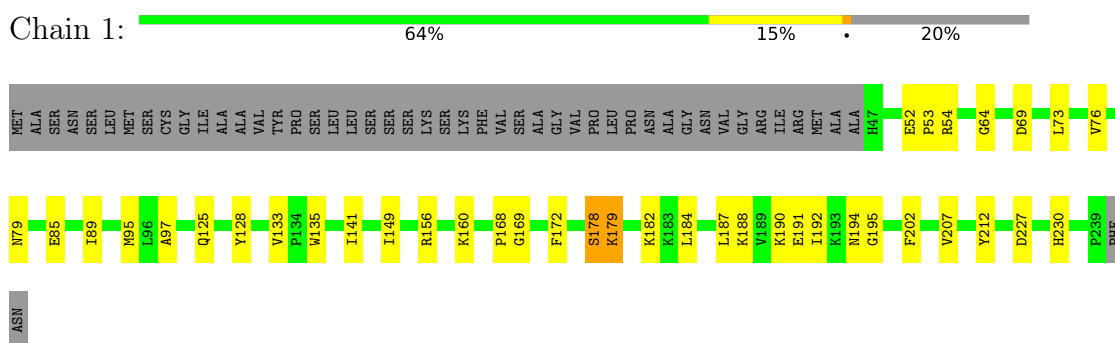


Mol	Chain	Residues	Atoms			AltConf
31	x	1	Total	C	O	0
			44	40	4	
31	y	1	Total	C	O	0
			44	40	4	
31	z	1	Total	C	O	0
			44	40	4	

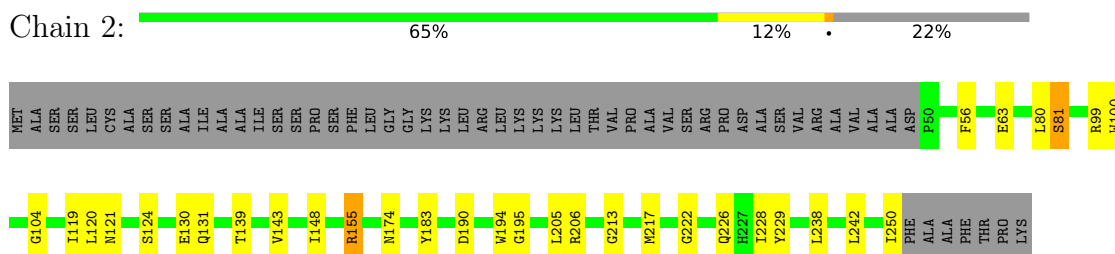
### 3 Residue-property plots [i](#)

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

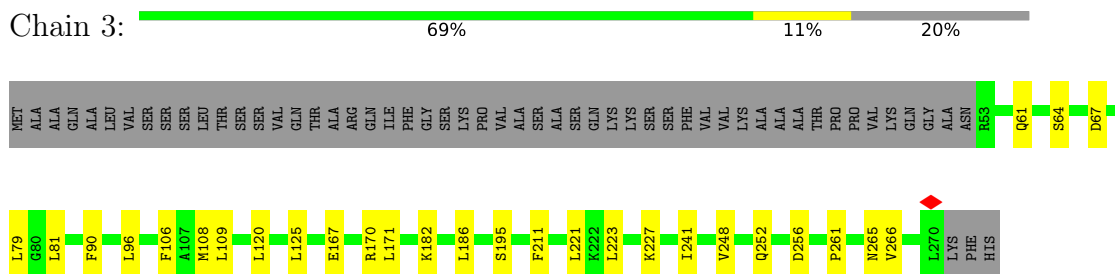
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

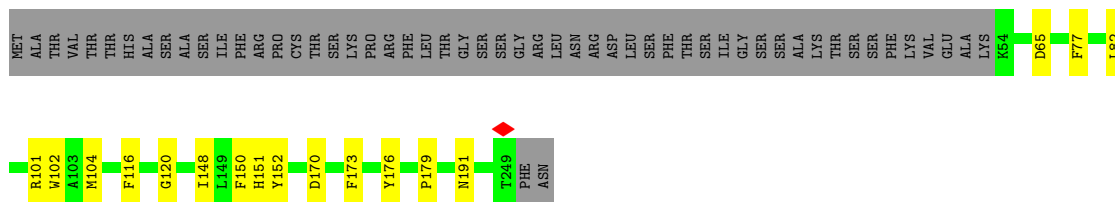


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

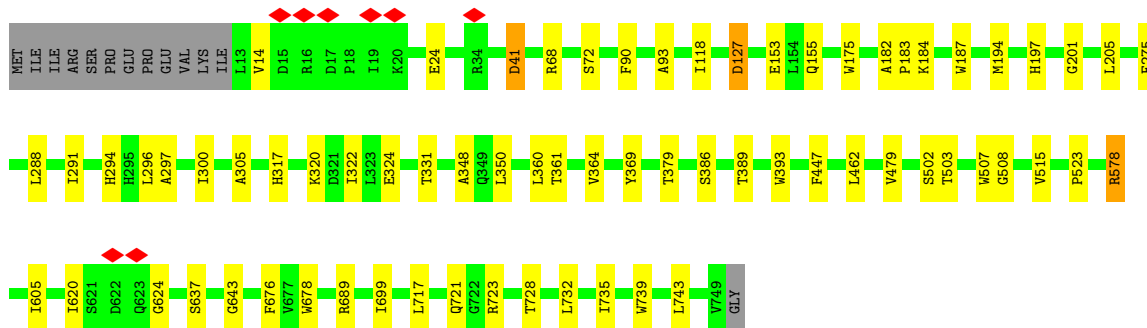
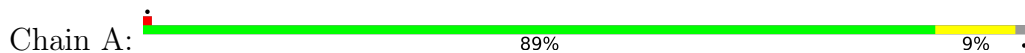


- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic

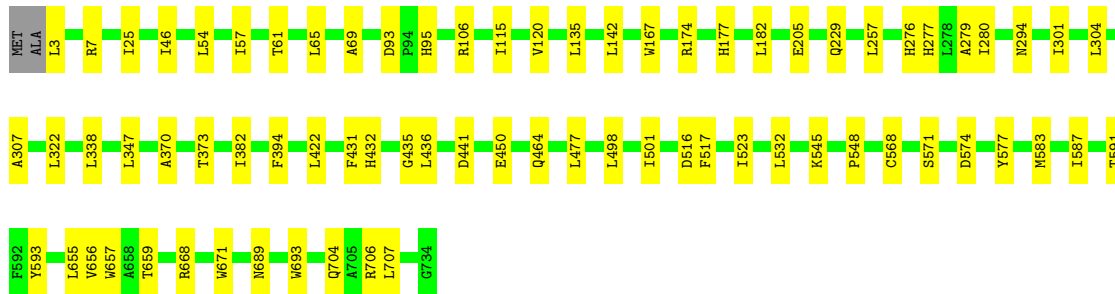
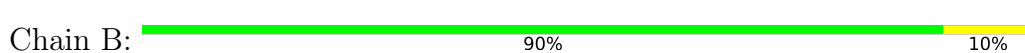




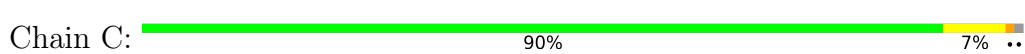
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 7: Photosystem I iron-sulfur center



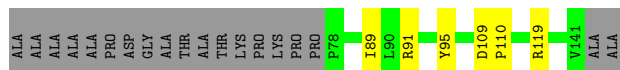
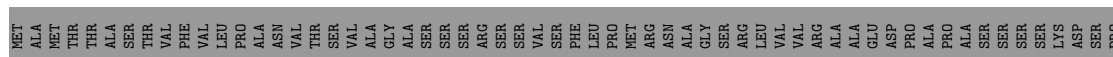
• Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic







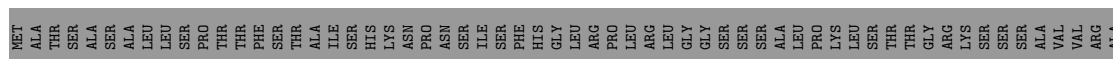
• Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic



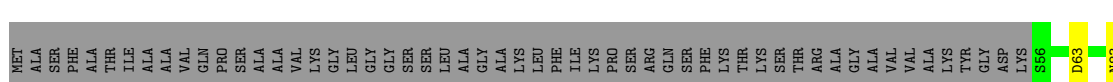
• Molecule 10: Photosystem I reaction center subunit III, chloroplastic



• Molecule 11: Photosystem I reaction center subunit V, chloroplastic



• Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic



• Molecule 13: Photosystem I reaction center subunit VIII



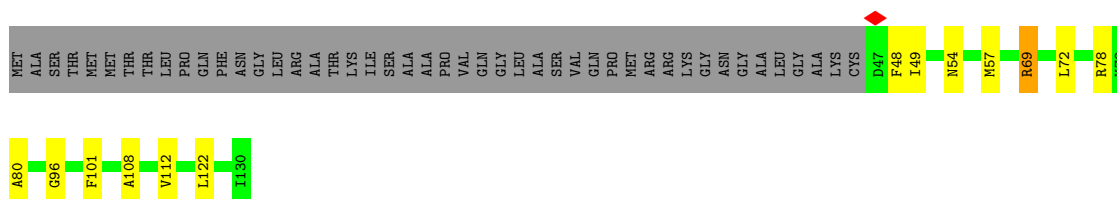
- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  68% 25% 7%



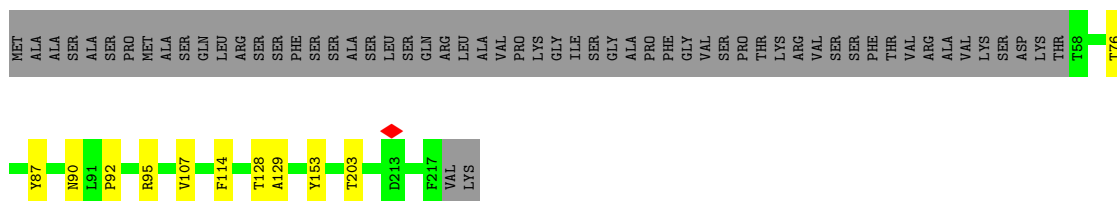
- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  55% 9% 35%



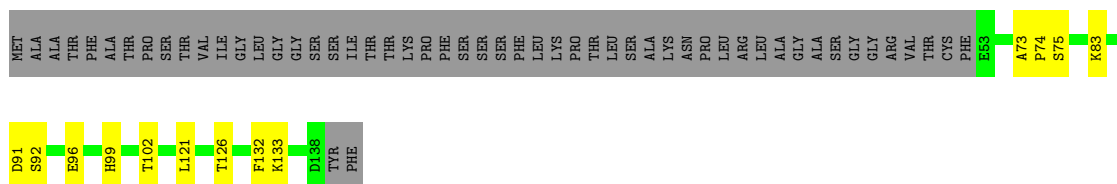
- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L:  68% 5% 27%




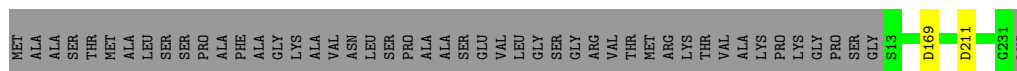
- Molecule 17: Photosystem I subunit O

Chain O:  52% 9% 39%




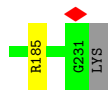
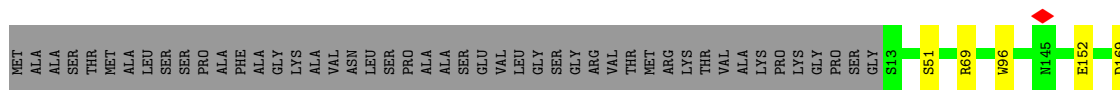
- Molecule 18: Chlorophyll a-b binding protein 2, chloroplastic

Chain x:  81% 18%

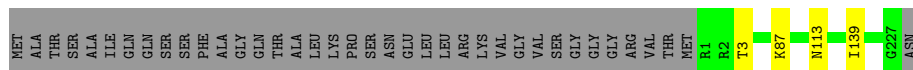
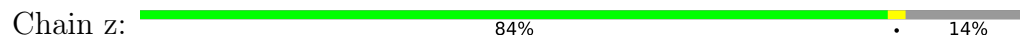


- Molecule 18: Chlorophyll a-b binding protein 2, chloroplastic

Chain y:  80% 18%



- Molecule 19: Chlorophyll a-b binding protein 2.1, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	38.962	Depositor
Minimum map value	-20.964	Depositor
Average map value	0.022	Depositor
Map value standard deviation	1.157	Depositor
Recommended contour level	3.59	Depositor
Map size (Å)	365.232, 365.232, 365.232	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.29	0/1546	0.44	0/2110
2	2	0.43	0/1622	0.66	3/2219 (0.1%)
3	3	0.31	0/1717	0.49	0/2336
4	4	0.28	0/1599	0.42	0/2178
5	A	0.32	0/6005	0.52	5/8194 (0.1%)
6	B	0.32	0/6065	0.53	2/8279 (0.0%)
7	C	0.47	0/629	1.04	5/852 (0.6%)
8	D	0.49	0/1157	0.77	3/1563 (0.2%)
9	E	0.30	0/528	0.50	0/715
10	F	0.27	0/1238	0.47	0/1670
11	G	0.29	0/724	0.45	0/981
12	H	0.42	0/713	0.56	0/968
13	I	0.27	0/245	0.43	0/333
14	J	0.25	0/336	0.46	0/458
15	K	0.48	0/599	0.82	2/809 (0.2%)
16	L	0.31	0/1244	0.48	0/1700
17	O	0.29	0/710	0.49	0/969
18	x	0.37	0/1716	0.59	1/2336 (0.0%)
18	y	0.47	0/1716	0.73	2/2336 (0.1%)
19	z	0.34	0/1802	0.52	0/2450
All	All	0.35	0/31911	0.56	23/43456 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	1
7	C	0	1
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	44	ARG	NE-CZ-NH2	10.05	125.33	120.30
7	C	81	TYR	CB-CG-CD2	-9.85	115.09	121.00
15	K	78	ARG	NE-CZ-NH2	8.36	124.48	120.30
5	A	127	ASP	CB-CG-OD1	8.14	125.63	118.30
8	D	150	ARG	NE-CZ-NH2	8.04	124.32	120.30
15	K	69	ARG	NE-CZ-NH2	7.61	124.10	120.30
8	D	139	ARG	NE-CZ-NH2	7.33	123.96	120.30
6	B	706	ARG	NE-CZ-NH2	7.25	123.92	120.30
5	A	578	ARG	NE-CZ-NH2	7.12	123.86	120.30
5	A	723	ARG	NE-CZ-NH2	7.06	123.83	120.30
2	2	155	ARG	NE-CZ-NH2	6.25	123.43	120.30
18	y	69	ARG	NE-CZ-NH2	6.02	123.31	120.30
6	B	668	ARG	NE-CZ-NH2	6.02	123.31	120.30
18	y	185	ARG	NE-CZ-NH2	5.96	123.28	120.30
7	C	81	TYR	CB-CG-CD1	5.86	124.52	121.00
8	D	127	ARG	NE-CZ-NH2	5.85	123.23	120.30
18	x	169	ASP	CB-CG-OD1	5.66	123.39	118.30
5	A	127	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	2	99	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	2	206	ARG	NE-CZ-NH2	5.46	123.03	120.30
7	C	81	TYR	CA-CB-CG	5.20	123.28	113.40
5	A	689	ARG	NE-CZ-NH2	5.17	122.89	120.30
7	C	19	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	578	ARG	Sidechain
7	C	44	ARG	Sidechain

## 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	1	1496	0	1471	38	0
2	2	1566	0	1519	32	0
3	3	1666	0	1627	29	0
4	4	1551	0	1508	18	0
5	A	5807	0	5657	54	0
6	B	5854	0	5645	68	0
7	C	616	0	595	7	0
8	D	1128	0	1134	2	0
9	E	517	0	526	3	0
10	F	1208	0	1243	12	0
11	G	708	0	700	2	0
12	H	693	0	690	4	0
13	I	239	0	258	4	0
14	J	327	0	342	11	0
15	K	593	0	614	19	0
16	L	1207	0	1209	9	0
17	O	686	0	677	6	0
18	x	1666	0	1593	0	0
18	y	1666	0	1593	0	0
19	z	1759	0	1693	0	0
20	1	93	0	62	7	0
20	2	226	0	150	12	0
20	3	45	0	30	2	0
20	4	169	0	100	5	0
20	x	293	0	212	0	0
20	y	296	0	215	0	0
20	z	295	0	213	0	0
21	1	496	0	354	31	0
21	2	434	0	352	43	0
21	3	498	0	377	35	0
21	4	527	0	412	21	0
21	A	2533	0	2495	134	0
21	B	2284	0	2242	123	0
21	F	149	0	123	9	0
21	G	132	0	97	3	0
21	H	60	0	59	4	0
21	J	51	0	41	1	0
21	K	167	0	116	16	0
21	L	155	0	138	7	0
21	O	141	0	110	3	0
21	x	436	0	403	0	0
21	y	427	0	384	0	0
21	z	438	0	409	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	1	44	0	56	13	0
22	2	44	0	56	5	0
22	4	44	0	54	6	0
22	x	44	0	56	0	0
22	y	44	0	56	0	0
22	z	44	0	56	0	0
23	1	49	0	74	12	0
23	2	37	0	44	2	0
23	A	79	0	104	8	0
23	B	87	0	120	6	0
23	x	49	0	74	0	0
23	y	49	0	74	0	0
23	z	49	0	74	0	0
24	1	42	0	56	3	0
24	2	84	0	112	11	0
24	3	42	0	56	8	0
24	4	42	0	56	2	0
24	x	84	0	112	0	0
24	y	84	0	112	0	0
24	z	84	0	112	0	0
25	3	40	0	56	6	0
25	4	40	0	56	6	0
25	A	240	0	336	27	0
25	B	320	0	448	46	0
25	F	40	0	56	2	0
25	G	40	0	56	4	0
25	I	40	0	56	2	0
25	J	40	0	56	5	0
25	K	80	0	112	10	0
25	L	120	0	168	14	0
25	O	80	0	112	3	0
26	4	72	0	84	0	0
27	A	61	0	68	15	0
28	A	8	0	0	2	0
28	C	16	0	0	5	0
29	A	33	0	46	3	0
29	B	33	0	46	3	0
30	B	66	0	96	5	0
31	x	44	0	56	0	0
31	y	44	0	56	0	0
31	z	44	0	56	0	0
All	All	43924	0	42922	712	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 11.

All (712) 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)
4:4:77:PHE:HE2	22:4:617:XAT:H383	1.22	1.05
4:4:77:PHE:CE2	22:4:617:XAT:H383	1.91	1.05
21:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.52	0.90
21:B:814:CLA:H3A	25:B:845:BCR:H393	1.53	0.90
2:2:143:VAL:HG22	21:4:613:CLA:HBA2	1.58	0.85
21:2:604:CLA:HBB2	20:2:605:CHL:C1C	2.07	0.85
27:A:801:CL0:H7	21:B:802:CLA:HAB	1.59	0.83
20:1:601:CHL:HAA1	23:1:615:LHG:H142	1.62	0.82
21:1:602:CLA:H51	22:1:614:XAT:H373	1.60	0.81
25:B:801:BCR:H12C	25:B:801:BCR:H341	1.62	0.79
28:A:854:SF4:S4	6:B:568:CYS:SG	2.78	0.79
1:1:172:PHE:HB2	21:1:609:CLA:HMD2	1.65	0.78
25:L:306:BCR:H321	25:L:306:BCR:HC8	1.67	0.77
21:3:607:CLA:HHC	21:3:607:CLA:HBB1	1.67	0.76
22:2:617:XAT:H401	22:2:617:XAT:H15	1.66	0.76
7:C:14:CYS:SG	28:C:102:SF4:S4	2.83	0.76
7:C:21:CYS:SG	28:C:101:SF4:FE4	1.77	0.76
25:B:848:BCR:H403	25:B:848:BCR:H23C	1.66	0.76
25:A:853:BCR:H12C	25:A:853:BCR:H341	1.67	0.76
21:F:301:CLA:HHC	21:F:301:CLA:HBB1	1.68	0.75
28:A:854:SF4:FE2	6:B:568:CYS:SG	1.77	0.75
15:K:101:PHE:CE2	21:K:201:CLA:HMC2	2.21	0.75
21:3:607:CLA:HBA1	21:3:612:CLA:HAB	1.70	0.74
21:A:804:CLA:HBD	21:A:804:CLA:HBA2	1.70	0.73
2:2:194:TRP:HB2	21:2:609:CLA:O2A	1.86	0.73
21:A:803:CLA:HMA3	27:A:801:CL0:H43	1.70	0.73
6:B:517:PHE:HA	21:B:837:CLA:HED1	1.71	0.73
21:B:822:CLA:H52	23:B:852:LHG:H121	1.70	0.73
21:B:816:CLA:O1A	11:G:152:ASN:ND2	2.21	0.72
25:A:848:BCR:H403	25:A:848:BCR:H23C	1.71	0.72
20:3:606:CHL:HHC	20:3:606:CHL:HBB1	1.70	0.72
21:A:826:CLA:HMA3	21:A:822:CLA:HMB2	1.71	0.72
21:A:840:CLA:HHC	21:A:840:CLA:HBB1	1.72	0.72
5:A:175:TRP:HB2	21:A:812:CLA:HMC3	1.72	0.71
7:C:14:CYS:SG	28:C:102:SF4:FE3	1.81	0.71
24:2:619:LUT:H8	24:2:619:LUT:H181	1.72	0.71
25:A:850:BCR:H16C	25:A:850:BCR:H351	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:2:619:LUT:H172	21:4:610:CLA:HHC	1.73	0.70
2:2:119:ILE:HG22	2:2:120:LEU:HD12	1.73	0.70
6:B:432:HIS:HB2	25:B:849:BCR:H402	1.72	0.70
27:A:801:CL0:H7	21:B:802:CLA:CAB	2.21	0.70
27:A:801:CL0:H38	27:A:801:CL0:H67	1.72	0.70
3:3:266:VAL:HG22	21:3:609:CLA:HBD	1.73	0.69
5:A:393:TRP:CD1	21:A:829:CLA:HAB	2.28	0.69
21:1:602:CLA:CBB	22:1:614:XAT:H32	2.23	0.69
3:3:252:GLN:NE2	3:3:256:ASP:OD1	2.26	0.69
25:3:614:BCR:H403	25:3:614:BCR:H23C	1.73	0.69
17:O:99:HIS:O	17:O:102:THR:OG1	2.10	0.69
23:1:615:LHG:H101	25:4:618:BCR:H393	1.74	0.68
5:A:14:VAL:HG11	21:A:811:CLA:HED3	1.75	0.68
5:A:386:SER:HB3	21:A:829:CLA:HMA1	1.75	0.68
15:K:101:PHE:HE2	21:K:201:CLA:HMC2	1.58	0.68
21:A:821:CLA:HHC	21:A:821:CLA:HBB1	1.74	0.68
20:1:601:CHL:HHC	20:1:601:CHL:HBB1	1.74	0.68
21:4:613:CLA:HBD	21:4:613:CLA:HBA1	1.75	0.68
21:A:810:CLA:HMD2	21:A:809:CLA:HMC3	1.74	0.68
25:A:851:BCR:H16C	25:A:851:BCR:H351	1.76	0.68
25:A:849:BCR:H383	25:A:849:BCR:H23C	1.76	0.68
27:A:801:CL0:H14	21:B:802:CLA:C4A	2.24	0.67
21:A:829:CLA:H202	25:J:102:BCR:H19C	1.76	0.67
3:3:79:LEU:HD13	21:A:813:CLA:H2	1.77	0.67
25:B:846:BCR:H332	23:B:852:LHG:H382	1.77	0.66
21:B:822:CLA:HBB1	25:B:846:BCR:H321	1.77	0.66
3:3:81:LEU:HD13	21:3:601:CLA:H42	1.76	0.66
21:A:842:CLA:HBC2	29:A:855:PQN:H192	1.77	0.66
3:3:170:ARG:NH1	21:3:607:CLA:O1D	2.29	0.66
4:4:82:LEU:HD22	21:4:602:CLA:H42	1.77	0.66
29:A:855:PQN:H172	25:B:801:BCR:H382	1.77	0.66
25:A:853:BCR:HC8	25:A:853:BCR:H311	1.79	0.65
27:A:801:CL0:H9	21:B:802:CLA:HMB1	1.79	0.65
6:B:656:VAL:HG22	21:B:840:CLA:HMB3	1.77	0.65
21:B:805:CLA:H52	21:B:813:CLA:H61	1.78	0.65
10:F:118:ARG:NH2	10:F:121:ASP:OD2	2.29	0.65
21:1:602:CLA:HBB2	22:1:614:XAT:H32	1.78	0.65
4:4:104:MET:HE1	21:4:609:CLA:HHC	1.78	0.65
25:J:102:BCR:HC8	25:J:102:BCR:H311	1.77	0.65
24:4:616:LUT:H8	24:4:616:LUT:H171	1.78	0.64
21:H:201:CLA:HMA1	21:L:302:CLA:HAA1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:803:CLA:OBD	21:B:802:CLA:HMB3	1.97	0.64
21:A:831:CLA:H13	23:A:846:LHG:H202	1.79	0.64
14:J:32:LEU:HD11	21:J:101:CLA:HBA2	1.79	0.64
25:B:845:BCR:H16C	25:B:845:BCR:H20C	1.78	0.64
2:2:205:LEU:HB3	21:2:609:CLA:HMA1	1.79	0.64
5:A:699:ILE:HA	21:A:841:CLA:HED1	1.80	0.64
25:L:301:BCR:H21C	25:L:301:BCR:H361	1.79	0.63
24:3:613:LUT:H401	24:3:613:LUT:H15	1.79	0.63
21:A:809:CLA:H201	23:A:846:LHG:H211	1.80	0.63
25:4:618:BCR:H383	25:4:618:BCR:H23C	1.80	0.63
25:L:305:BCR:H321	25:L:305:BCR:HC8	1.79	0.63
20:4:605:CHL:HHC	20:4:605:CHL:HBB1	1.80	0.63
25:B:847:BCR:HC8	25:B:847:BCR:H311	1.81	0.62
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.81	0.62
6:B:450:GLU:OE2	10:F:119:ARG:NH2	2.32	0.62
1:1:135:TRP:HE1	21:1:605:CLA:HBA2	1.63	0.62
6:B:659:THR:HA	21:B:803:CLA:HAB	1.80	0.62
1:1:168:PRO:HG2	21:1:609:CLA:HMD3	1.81	0.62
25:K:205:BCR:H321	25:K:205:BCR:HC8	1.81	0.62
21:4:601:CLA:HHC	21:4:601:CLA:HBB1	1.81	0.62
21:F:302:CLA:HBA1	14:J:26:LEU:HD21	1.83	0.61
16:L:90:ASN:HB3	21:L:302:CLA:HAC1	1.81	0.60
4:4:176:TYR:HE2	20:4:615:CHL:HAA2	1.66	0.60
21:A:842:CLA:HBD	21:A:842:CLA:HBA1	1.83	0.60
21:A:809:CLA:H143	21:A:804:CLA:H18	1.83	0.60
5:A:732:LEU:HA	23:A:846:LHG:H383	1.82	0.60
25:A:851:BCR:H23C	25:A:851:BCR:H403	1.83	0.60
24:1:616:LUT:H391	24:1:616:LUT:H32	1.83	0.60
1:1:73:LEU:HD12	22:1:614:XAT:H221	1.84	0.60
1:1:169:GLY:H	21:1:609:CLA:HMD1	1.67	0.60
25:B:846:BCR:HC8	25:B:846:BCR:H311	1.83	0.60
6:B:65:LEU:HD11	25:B:845:BCR:H282	1.84	0.60
1:1:95:MET:HE2	21:1:609:CLA:HAB	1.84	0.59
10:F:70:SER:OG	10:F:70:SER:O	2.20	0.59
25:K:205:BCR:H403	25:K:205:BCR:H23C	1.83	0.59
21:2:604:CLA:HBB2	20:2:605:CHL:C2C	2.32	0.59
1:1:156:ARG:NH1	21:1:608:CLA:O1D	2.29	0.59
21:4:602:CLA:HMB1	21:4:602:CLA:HBB1	1.84	0.59
21:2:604:CLA:HED2	21:2:604:CLA:H2A	1.85	0.59
25:G:204:BCR:HC8	25:G:204:BCR:H311	1.85	0.58
3:3:186:LEU:HD11	25:3:614:BCR:H343	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:613:LUT:H161	24:3:613:LUT:H8	1.85	0.58
21:B:824:CLA:H93	21:B:819:CLA:HBB1	1.85	0.58
21:1:602:CLA:H43	21:1:602:CLA:HMB2	1.85	0.58
24:3:613:LUT:H12	24:3:613:LUT:H191	1.85	0.58
5:A:41:ASP:OD1	5:A:41:ASP:N	2.36	0.58
1:1:97:ALA:CB	22:1:614:XAT:H10	2.32	0.58
21:A:834:CLA:HMC2	21:L:304:CLA:HBB2	1.84	0.58
21:B:824:CLA:HMB1	21:B:824:CLA:HBB1	1.86	0.58
21:B:818:CLA:HBB1	21:B:818:CLA:HMB1	1.86	0.58
1:1:95:MET:CE	21:1:609:CLA:HAB	2.33	0.58
25:A:853:BCR:H23C	25:A:853:BCR:H393	1.84	0.58
25:4:618:BCR:HC8	25:4:618:BCR:H321	1.86	0.58
6:B:3:LEU:HD13	6:B:7:ARG:HH11	1.67	0.58
6:B:657:TRP:CE3	21:B:802:CLA:HMA1	2.39	0.57
15:K:72:LEU:HD22	21:K:206:CLA:H3A	1.85	0.57
25:B:844:BCR:H361	25:B:844:BCR:H21C	1.85	0.57
21:A:831:CLA:H172	23:A:846:LHG:H182	1.87	0.57
2:2:104:GLY:HA2	22:2:617:XAT:H181	1.87	0.57
3:3:211:PHE:HD2	24:3:613:LUT:H41	1.70	0.57
25:A:852:BCR:H403	25:A:852:BCR:H23C	1.86	0.57
24:2:616:LUT:H203	21:2:609:CLA:HAB	1.86	0.57
21:A:820:CLA:HMB1	21:A:820:CLA:HBB1	1.87	0.57
21:A:802:CLA:H202	21:A:842:CLA:H2	1.86	0.57
17:O:83:LYS:NZ	17:O:91:ASP:OD2	2.39	0.56
1:1:95:MET:SD	1:1:195:GLY:HA2	2.45	0.56
21:1:602:CLA:ND	22:1:614:XAT:H382	2.20	0.56
2:2:183:TYR:HD1	21:2:609:CLA:O1D	1.88	0.56
21:2:611:CLA:HBB1	21:2:611:CLA:HMB1	1.87	0.56
3:3:61:GLN:O	3:3:64:SER:OG	2.22	0.56
25:A:850:BCR:H311	25:A:850:BCR:HC8	1.86	0.56
21:B:832:CLA:HHC	21:B:832:CLA:HBB1	1.88	0.56
21:1:604:CLA:C1B	22:1:614:XAT:H42	2.36	0.56
21:1:609:CLA:CBB	21:1:609:CLA:HHC	2.35	0.56
21:A:841:CLA:H143	21:F:302:CLA:HBC1	1.86	0.56
6:B:671:TRP:HZ3	21:B:803:CLA:O1D	1.89	0.56
21:A:812:CLA:H141	21:A:812:CLA:H203	1.88	0.56
27:A:801:CL0:H14	21:B:802:CLA:NA	2.21	0.56
5:A:728:THR:HG23	23:A:846:LHG:H341	1.88	0.55
21:A:830:CLA:HBD	21:A:830:CLA:HBA1	1.88	0.55
21:A:831:CLA:H152	21:A:842:CLA:HAA2	1.87	0.55
2:2:213:GLY:O	2:2:217:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:612:CLA:C2B	24:2:616:LUT:H373	2.36	0.55
21:2:604:CLA:HBB2	20:2:605:CHL:NC	2.21	0.55
5:A:361:THR:HA	21:A:830:CLA:HBC2	1.88	0.55
13:I:27:LEU:HD22	25:L:305:BCR:H323	1.88	0.55
15:K:48:PHE:HZ	21:K:204:CLA:HBC3	1.72	0.55
3:3:221:LEU:HB3	21:3:608:CLA:HMA1	1.89	0.55
21:4:612:CLA:HBB1	21:4:612:CLA:HMB1	1.88	0.55
21:G:203:CLA:HMB1	21:G:203:CLA:HBB1	1.89	0.54
1:1:149:ILE:HG21	21:1:608:CLA:HMC3	1.87	0.54
21:4:608:CLA:C1D	21:4:603:CLA:HMD2	2.37	0.54
5:A:739:TRP:HH2	21:A:809:CLA:HBC2	1.72	0.54
21:B:826:CLA:OBD	21:B:825:CLA:HAA2	2.06	0.54
24:2:616:LUT:H401	24:2:616:LUT:H15	1.89	0.54
21:2:613:CLA:H2A	21:2:613:CLA:HED2	1.88	0.54
6:B:707:LEU:HD23	30:B:850:DGD:HA21	1.90	0.54
21:3:608:CLA:HMB1	21:3:608:CLA:HBB1	1.89	0.54
5:A:93:ALA:HA	5:A:153:GLU:HG2	1.89	0.54
5:A:288:LEU:HD23	5:A:291:ILE:HD12	1.89	0.54
6:B:57:ILE:HA	21:B:806:CLA:HBC3	1.89	0.54
21:B:830:CLA:HBC2	21:B:823:CLA:HBB1	1.88	0.54
14:J:24:GLY:O	14:J:28:GLU:HG2	2.07	0.54
21:B:806:CLA:H2	21:B:806:CLA:HED3	1.90	0.54
21:B:814:CLA:HMB1	21:B:814:CLA:HBB1	1.88	0.54
21:A:841:CLA:HMB1	21:A:841:CLA:HBB1	1.90	0.54
21:A:842:CLA:HBA2	23:A:846:LHG:H162	1.89	0.54
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.73	0.54
5:A:348:ALA:HB1	25:A:850:BCR:H393	1.88	0.54
21:A:803:CLA:H2	6:B:655:LEU:HD22	1.89	0.54
21:B:825:CLA:H42	21:B:834:CLA:HBB2	1.89	0.54
21:A:802:CLA:H161	21:A:804:CLA:H71	1.90	0.54
5:A:735:ILE:HD12	23:A:846:LHG:H382	1.89	0.53
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.90	0.53
15:K:108:ALA:O	15:K:112:VAL:HG23	2.08	0.53
1:1:128:TYR:HD1	21:1:604:CLA:HBA1	1.73	0.53
1:1:178:SER:O	1:1:178:SER:OG	2.25	0.53
23:1:615:LHG:H342	23:1:615:LHG:H181	1.90	0.53
4:4:82:LEU:HD21	10:F:202:ILE:HD12	1.91	0.53
6:B:7:ARG:HE	6:B:7:ARG:HA	1.73	0.53
7:C:21:CYS:HG	28:C:101:SF4:FE4	1.26	0.53
16:L:107:VAL:HA	21:L:303:CLA:HED1	1.91	0.53
21:A:824:CLA:HBC2	21:A:825:CLA:HAA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:801:BCR:HC8	25:B:801:BCR:H331	1.91	0.53
1:1:207:VAL:HG11	21:1:612:CLA:HMD2	1.91	0.53
20:2:601:CHL:HMD2	25:3:614:BCR:H323	1.90	0.53
6:B:279:ALA:HA	21:B:816:CLA:HMC3	1.91	0.53
21:2:604:CLA:HBB2	20:2:605:CHL:C4C	2.39	0.53
21:B:828:CLA:H171	25:B:845:BCR:H362	1.89	0.53
25:B:849:BCR:H10C	14:J:38:THR:O	2.09	0.53
3:3:109:LEU:HD22	21:3:603:CLA:HBC1	1.90	0.53
21:A:842:CLA:HMB1	21:A:842:CLA:HBB1	1.89	0.53
1:1:227:ASP:OD2	1:1:230:HIS:HB2	2.09	0.52
21:1:609:CLA:HHC	21:1:609:CLA:HBB1	1.91	0.52
21:2:603:CLA:HMD2	21:2:608:CLA:C1D	2.39	0.52
6:B:477:LEU:HD13	21:B:834:CLA:HMD3	1.90	0.52
21:B:824:CLA:HMA3	21:B:819:CLA:HMB2	1.90	0.52
21:B:824:CLA:H141	21:B:824:CLA:H193	1.91	0.52
1:1:125:GLN:NE2	1:1:133:VAL:O	2.40	0.52
22:4:617:XAT:H162	22:4:617:XAT:H42	1.92	0.52
25:F:304:BCR:H14C	25:F:304:BCR:H10C	1.90	0.52
25:K:202:BCR:H23C	25:K:202:BCR:H392	1.91	0.52
13:I:34:ASN:OD1	13:I:35:LYS:N	2.42	0.52
5:A:620:ILE:HD11	5:A:624:GLY:HA2	1.90	0.52
21:A:831:CLA:HMB1	21:A:831:CLA:HBB1	1.92	0.52
21:B:828:CLA:H192	25:B:844:BCR:H352	1.92	0.52
1:1:191:GLU:HB2	21:1:609:CLA:HMA1	1.92	0.52
21:2:604:CLA:H2A	21:2:604:CLA:CED	2.39	0.52
21:A:811:CLA:HMB1	21:A:811:CLA:HBB1	1.91	0.52
23:B:851:LHG:H261	23:B:851:LHG:H302	1.91	0.52
20:1:601:CHL:O1A	4:4:151:HIS:ND1	2.41	0.52
3:3:120:LEU:HD22	3:3:125:LEU:HD13	1.92	0.52
4:4:104:MET:HE1	21:4:609:CLA:HAB	1.91	0.52
21:A:802:CLA:H42	21:A:802:CLA:HMA1	1.91	0.52
6:B:422:LEU:HD13	6:B:532:LEU:HA	1.90	0.52
6:B:707:LEU:HD11	30:B:850:DGD:HB81	1.92	0.52
2:2:148:ILE:HG21	21:2:608:CLA:HMC3	1.92	0.52
21:B:822:CLA:HBA1	21:B:822:CLA:HBD	1.92	0.52
10:F:160:ILE:HG21	21:F:302:CLA:HMA3	1.92	0.52
6:B:301:ILE:HG21	21:B:824:CLA:HAC1	1.92	0.51
3:3:108:MET:HE1	21:3:608:CLA:HHC	1.92	0.51
21:B:824:CLA:HBA1	21:B:805:CLA:H101	1.92	0.51
21:4:609:CLA:CGA	21:4:609:CLA:H3A	2.39	0.51
5:A:320:LYS:NZ	5:A:324:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:830:CLA:HBA1	21:A:830:CLA:CHA	2.40	0.51
21:3:601:CLA:HBB1	21:3:601:CLA:HMB1	1.92	0.51
5:A:296:LEU:O	5:A:300:ILE:HG12	2.11	0.51
6:B:523:ILE:HG21	21:B:836:CLA:HAB	1.92	0.51
6:B:517:PHE:HE2	25:B:849:BCR:H271	1.76	0.51
29:B:842:PQN:H272	21:B:840:CLA:H11	1.92	0.51
15:K:72:LEU:HB3	21:K:206:CLA:C4A	2.41	0.51
5:A:294:HIS:HB2	21:A:819:CLA:C1B	2.41	0.51
6:B:304:LEU:HA	21:B:822:CLA:HED1	1.92	0.51
24:2:619:LUT:H181	24:2:619:LUT:C8	2.41	0.51
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.92	0.51
21:A:803:CLA:C2B	27:A:801:CL0:H64	2.41	0.51
1:1:141:ILE:HD12	21:1:605:CLA:H3A	1.93	0.51
21:2:602:CLA:CGA	21:2:602:CLA:H3A	2.41	0.51
6:B:93:ASP:H	12:H:129:ILE:HD13	1.76	0.51
6:B:167:TRP:CZ2	21:B:811:CLA:HMA1	2.46	0.51
1:1:212:TYR:HE1	21:1:612:CLA:HMC2	1.76	0.50
23:1:615:LHG:H312	23:1:615:LHG:H161	1.94	0.50
5:A:297:ALA:HB1	21:A:818:CLA:HBC2	1.93	0.50
5:A:393:TRP:HD1	21:A:829:CLA:HAB	1.76	0.50
29:B:842:PQN:H172	21:B:840:CLA:HMD2	1.92	0.50
21:A:809:CLA:HBB1	21:A:809:CLA:HMB1	1.93	0.50
22:4:617:XAT:C32	21:4:603:CLA:HMB2	2.41	0.50
21:A:819:CLA:CGA	21:A:819:CLA:H3A	2.37	0.50
6:B:46:ILE:HG21	21:B:805:CLA:H202	1.94	0.50
2:2:56:PHE:CE1	20:2:601:CHL:HED1	2.46	0.50
5:A:502:SER:OG	5:A:507:TRP:HD1	1.95	0.50
21:A:844:CLA:H3A	21:A:844:CLA:O1A	2.11	0.50
6:B:435:GLY:HA3	21:B:833:CLA:HAB	1.94	0.50
25:B:843:BCR:H16C	25:B:843:BCR:H351	1.92	0.50
20:1:601:CHL:H11	4:4:152:TYR:HB2	1.94	0.50
1:1:190:LYS:HD3	21:1:611:CLA:HAA2	1.93	0.49
21:A:820:CLA:H91	21:A:820:CLA:H151	1.94	0.49
21:B:806:CLA:HAB	21:B:828:CLA:HBB1	1.94	0.49
21:B:808:CLA:O1A	21:B:827:CLA:HBD	2.12	0.49
21:A:803:CLA:ND	27:A:801:CL0:H39	2.27	0.49
21:A:818:CLA:H51	15:K:122:LEU:HD13	1.94	0.49
21:A:833:CLA:HMB1	21:A:833:CLA:HBB1	1.94	0.49
1:1:169:GLY:N	21:1:609:CLA:HMD1	2.27	0.49
21:A:820:CLA:H91	21:A:820:CLA:H172	1.94	0.49
25:A:853:BCR:H343	14:J:27:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:72:LEU:HD22	21:K:206:CLA:C3A	2.42	0.49
5:A:72:SER:HB2	21:A:812:CLA:HMD3	1.95	0.49
21:A:802:CLA:H51	6:B:431:PHE:HE1	1.77	0.49
25:B:801:BCR:H312	21:B:832:CLA:CBB	2.43	0.49
15:K:69:ARG:HG2	21:K:201:CLA:HAC1	1.95	0.49
6:B:370:ALA:HB1	21:B:827:CLA:HMA1	1.95	0.49
21:B:805:CLA:H61	21:B:805:CLA:H93	1.61	0.49
21:B:803:CLA:H3A	21:B:803:CLA:O2A	2.12	0.49
24:3:613:LUT:H373	21:3:609:CLA:C2B	2.42	0.49
21:B:813:CLA:HMB1	21:B:813:CLA:HBB1	1.95	0.49
21:2:604:CLA:CBB	21:2:604:CLA:HHC	2.43	0.49
25:A:853:BCR:H332	14:J:31:ARG:HD3	1.95	0.49
6:B:464:GLN:NE2	21:B:836:CLA:OBD	2.40	0.49
21:B:829:CLA:HBB1	21:B:829:CLA:HMB1	1.94	0.49
21:A:806:CLA:HBA1	21:A:806:CLA:H3A	1.50	0.49
1:1:187:LEU:HD13	21:1:609:CLA:HAA2	1.93	0.49
2:2:205:LEU:HB3	21:2:609:CLA:CMA	2.43	0.49
21:B:809:CLA:H41	21:B:809:CLA:H61	1.52	0.49
5:A:678:TRP:CE2	27:A:801:CL0:H4	2.48	0.48
21:A:824:CLA:CAB	21:A:845:CLA:HBB1	2.43	0.48
6:B:174:ARG:HB2	21:B:813:CLA:HBC2	1.94	0.48
6:B:656:VAL:CG2	21:B:840:CLA:HMB3	2.43	0.48
1:1:64:GLY:HA3	1:1:192:ILE:HG21	1.95	0.48
2:2:121:ASN:OD1	2:2:121:ASN:N	2.45	0.48
20:2:615:CHL:HHC	20:2:615:CHL:HBB1	1.94	0.48
5:A:735:ILE:HG21	21:A:829:CLA:HMC2	1.94	0.48
21:F:301:CLA:H62	21:F:301:CLA:H41	1.63	0.48
15:K:101:PHE:CE2	21:K:201:CLA:CMC	2.94	0.48
6:B:307:ALA:HB3	21:B:822:CLA:HED3	1.95	0.48
5:A:479:VAL:HG21	21:O:201:CLA:H43	1.96	0.48
21:B:838:CLA:HHC	21:B:838:CLA:HBB1	1.95	0.48
21:B:809:CLA:HBB1	21:B:809:CLA:HMB1	1.94	0.48
21:A:835:CLA:H93	21:A:835:CLA:H111	1.73	0.48
25:L:301:BCR:H361	25:L:301:BCR:C21	2.42	0.48
3:3:261:PRO:HG2	21:3:610:CLA:HMB3	1.95	0.48
8:D:90:VAL:HG12	8:D:91:GLU:HG3	1.95	0.48
5:A:305:ALA:HB2	21:A:822:CLA:HBC2	1.95	0.48
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.96	0.48
21:F:302:CLA:HAA2	14:J:22:LEU:HD11	1.95	0.48
15:K:101:PHE:CD2	21:K:201:CLA:HMC2	2.48	0.48
25:L:305:BCR:H402	25:L:305:BCR:H23C	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:617:XAT:H373	22:4:617:XAT:H23	1.50	0.48
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.96	0.48
21:A:823:CLA:HAA2	15:K:80:ALA:CB	2.44	0.48
21:B:818:CLA:H62	21:B:818:CLA:H41	1.72	0.48
21:K:204:CLA:H3A	21:K:204:CLA:HBA2	1.66	0.48
21:A:812:CLA:H172	21:A:812:CLA:H13	1.49	0.47
25:B:801:BCR:HC21	21:F:302:CLA:H51	1.96	0.47
21:L:302:CLA:HHC	21:L:302:CLA:HBB1	1.96	0.47
21:3:609:CLA:H3A	21:3:609:CLA:HBA2	1.43	0.47
5:A:502:SER:HG	5:A:507:TRP:HD1	1.62	0.47
21:A:827:CLA:HAA2	21:A:828:CLA:OBD	2.15	0.47
16:L:128:THR:HG22	16:L:129:ALA:H	1.80	0.47
21:1:603:CLA:HMD2	21:1:608:CLA:C1D	2.45	0.47
15:K:72:LEU:HD13	21:K:206:CLA:H3A	1.96	0.47
1:1:135:TRP:NE1	21:1:605:CLA:HBA2	2.29	0.47
4:4:170:ASP:OD1	4:4:173:PHE:N	2.39	0.47
21:B:805:CLA:H61	21:B:805:CLA:H2	1.60	0.47
21:3:612:CLA:O2D	21:3:612:CLA:H2A	2.15	0.47
4:4:151:HIS:HA	21:4:608:CLA:HAB	1.96	0.47
21:A:802:CLA:H202	21:A:802:CLA:H162	1.65	0.47
21:A:823:CLA:HAA2	15:K:80:ALA:HB3	1.96	0.47
6:B:25:ILE:HD11	25:L:305:BCR:H312	1.97	0.47
25:A:851:BCR:H351	25:A:851:BCR:C16	2.39	0.47
6:B:205:GLU:OE1	6:B:205:GLU:HA	2.15	0.47
16:L:87:TYR:OH	21:L:303:CLA:O1A	2.31	0.47
21:1:604:CLA:HMB3	22:1:614:XAT:H162	1.97	0.47
23:1:615:LHG:H301	23:1:615:LHG:H152	1.95	0.47
21:2:602:CLA:H101	21:2:603:CLA:HMA1	1.95	0.47
3:3:96:LEU:HD13	21:3:601:CLA:H12	1.97	0.47
21:4:614:CLA:CED	21:4:614:CLA:H2A	2.44	0.47
21:A:845:CLA:H2A	21:A:845:CLA:O2D	2.14	0.47
21:B:841:CLA:H121	21:B:841:CLA:H161	1.47	0.47
2:2:228:ILE:HG22	2:2:229:TYR:HD1	1.80	0.47
2:2:194:TRP:CE3	21:2:609:CLA:H11	2.50	0.46
21:A:832:CLA:HMA2	16:L:76:THR:HG21	1.96	0.46
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.22	0.46
15:K:101:PHE:HE2	21:K:201:CLA:CMC	2.27	0.46
2:2:195:GLY:HA3	21:2:609:CLA:HED3	1.96	0.46
21:A:804:CLA:HBA2	21:A:804:CLA:CBD	2.43	0.46
27:A:801:CL0:H72	21:B:802:CLA:HMB1	1.97	0.46
6:B:373:THR:HG23	6:B:591:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:199:ARG:HE	10:F:199:ARG:HB2	1.54	0.46
21:3:607:CLA:C1D	21:3:602:CLA:HMD2	2.45	0.46
21:B:834:CLA:H3A	21:B:834:CLA:HBA1	1.57	0.46
6:B:517:PHE:CE2	25:B:849:BCR:H271	2.50	0.46
21:B:824:CLA:H62	21:B:824:CLA:H41	1.50	0.46
25:B:843:BCR:H383	25:B:843:BCR:H23C	1.97	0.46
4:4:116:PHE:O	4:4:120:GLY:N	2.29	0.46
21:A:812:CLA:H91	21:A:812:CLA:H111	1.67	0.46
3:3:167:GLU:OE1	3:3:170:ARG:NH2	2.49	0.46
5:A:739:TRP:CH2	21:A:809:CLA:HBC2	2.50	0.46
25:K:202:BCR:H24C	25:K:202:BCR:H371	1.69	0.46
21:A:810:CLA:HBB1	21:A:829:CLA:H203	1.97	0.46
21:B:827:CLA:H111	21:B:827:CLA:H152	1.39	0.46
5:A:447:PHE:O	21:A:835:CLA:HBB2	2.16	0.46
5:A:678:TRP:CZ3	27:A:801:CL0:H13	2.50	0.46
6:B:704:GLN:HG3	30:B:850:DGD:HA22	1.98	0.46
21:B:802:CLA:H161	21:B:802:CLA:H121	1.73	0.46
1:1:202:PHE:CD2	22:1:614:XAT:H14	2.51	0.46
4:4:101:ARG:NH2	20:4:607:CHL:OBD	2.47	0.46
23:1:615:LHG:C10	25:4:618:BCR:H281	2.46	0.46
2:2:217:MET:HE1	21:2:602:CLA:HAB	1.98	0.46
5:A:331:THR:OG1	23:A:847:LHG:HC12	2.16	0.46
21:A:820:CLA:H3A	21:A:820:CLA:HBA2	1.32	0.46
6:B:61:THR:HB	6:B:142:LEU:HD13	1.98	0.46
21:B:826:CLA:HBB1	21:B:826:CLA:HMB1	1.97	0.46
21:3:607:CLA:HBC2	21:3:604:CLA:HMB1	1.98	0.45
20:3:606:CHL:HBA1	21:3:608:CLA:HBC1	1.98	0.45
21:A:803:CLA:H171	21:B:810:CLA:HMC2	1.98	0.45
21:B:808:CLA:H141	21:B:808:CLA:H162	1.63	0.45
21:B:822:CLA:HMB3	21:B:841:CLA:C1D	2.45	0.45
21:B:840:CLA:H111	21:B:840:CLA:H151	1.78	0.45
22:1:614:XAT:H242	22:1:614:XAT:H362	1.97	0.45
2:2:81:SER:O	2:2:81:SER:OG	2.26	0.45
2:2:104:GLY:HA3	22:2:617:XAT:H192	1.97	0.45
3:3:182:LYS:HE2	3:3:182:LYS:HB2	1.68	0.45
21:A:833:CLA:H41	21:A:833:CLA:H61	1.46	0.45
25:B:801:BCR:H383	25:B:801:BCR:H23C	1.97	0.45
23:B:851:LHG:HC41	23:B:851:LHG:HC31	1.98	0.45
1:1:73:LEU:O	23:B:851:LHG:O1	2.25	0.45
3:3:90:PHE:HB2	21:3:602:CLA:H43	1.97	0.45
2:2:174:ASN:HD22	20:2:615:CHL:CHA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:602:CLA:H111	21:2:602:CLA:H152	1.78	0.45
27:A:801:CL0:H47	27:A:801:CL0:H51	1.69	0.45
21:B:817:CLA:CGA	21:B:817:CLA:H3A	2.45	0.45
21:A:818:CLA:H92	21:A:818:CLA:H61	1.79	0.45
21:A:835:CLA:H202	21:A:835:CLA:H161	1.71	0.45
15:K:57:MET:HG3	21:K:204:CLA:HAC2	1.99	0.45
21:A:807:CLA:H161	21:A:807:CLA:H121	1.74	0.45
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.52	0.45
21:B:828:CLA:H202	25:B:845:BCR:H362	1.98	0.45
2:2:190:ASP:OD1	21:2:609:CLA:C2	2.65	0.45
3:3:223:LEU:O	3:3:227:LYS:HG3	2.17	0.45
21:A:818:CLA:H142	21:A:818:CLA:H112	1.78	0.45
21:A:820:CLA:H62	21:A:820:CLA:H92	1.63	0.45
21:B:828:CLA:H122	25:B:845:BCR:H372	1.99	0.45
12:H:83:ASN:ND2	21:H:201:CLA:HAC2	2.32	0.45
23:2:618:LHG:HC91	25:3:614:BCR:HC41	1.98	0.45
21:4:609:CLA:H3A	21:4:609:CLA:O1A	2.17	0.45
21:A:829:CLA:H112	21:A:829:CLA:H142	1.73	0.45
21:A:802:CLA:HBA1	21:A:802:CLA:H3A	1.30	0.45
21:B:820:CLA:H3A	21:B:820:CLA:HBA2	1.34	0.45
21:B:828:CLA:H3A	21:B:828:CLA:HBA2	1.30	0.45
21:B:805:CLA:HBA1	21:B:805:CLA:H3A	1.42	0.45
25:K:202:BCR:H20C	25:K:202:BCR:H361	1.79	0.45
25:L:301:BCR:H15C	25:L:301:BCR:H351	1.68	0.45
1:1:97:ALA:HB2	22:1:614:XAT:H10	1.98	0.45
1:1:184:LEU:O	1:1:188:LYS:HG3	2.17	0.45
3:3:106:PHE:CE1	21:3:607:CLA:HBC3	2.52	0.45
24:3:613:LUT:H191	24:3:613:LUT:C12	2.46	0.45
6:B:177:HIS:CG	21:B:813:CLA:HMC2	2.51	0.45
21:B:824:CLA:H91	21:B:824:CLA:H112	1.78	0.45
25:K:205:BCR:H24C	25:K:205:BCR:H371	1.77	0.45
21:A:803:CLA:HBA1	21:A:803:CLA:H3A	1.54	0.45
6:B:671:TRP:CZ3	21:B:803:CLA:O1D	2.70	0.45
29:B:842:PQN:H161	29:B:842:PQN:H141	1.78	0.45
25:B:843:BCR:H331	25:B:843:BCR:HC7	1.72	0.45
15:K:96:GLY:O	21:K:201:CLA:H3A	2.16	0.45
3:3:241:ILE:HG21	21:3:609:CLA:HMD3	1.98	0.44
25:B:846:BCR:H11C	25:B:846:BCR:H341	1.80	0.44
12:H:116:THR:HG21	13:I:14:LEU:HD13	1.98	0.44
17:O:92:SER:O	17:O:96:GLU:HG2	2.17	0.44
4:4:176:TYR:CE2	20:4:615:CHL:HBD	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:805:CLA:H3A	21:A:805:CLA:HBA2	1.57	0.44
21:A:841:CLA:H62	21:A:841:CLA:H41	1.68	0.44
25:B:843:BCR:H372	25:G:204:BCR:HC21	1.99	0.44
21:2:603:CLA:HMC2	22:2:617:XAT:H12	1.98	0.44
24:2:616:LUT:H31	24:2:616:LUT:H391	1.77	0.44
21:3:602:CLA:H92	21:A:811:CLA:HMD2	2.00	0.44
4:4:148:ILE:HD13	4:4:148:ILE:HA	1.87	0.44
5:A:187:TRP:CZ2	21:A:811:CLA:HMA1	2.52	0.44
21:A:826:CLA:H202	21:A:826:CLA:H161	1.78	0.44
7:C:14:CYS:HG	28:C:102:SF4:FE3	1.32	0.44
3:3:108:MET:HE2	21:3:608:CLA:HMC3	1.99	0.44
21:4:612:CLA:H91	21:4:612:CLA:H111	1.73	0.44
21:A:812:CLA:H92	21:A:812:CLA:H62	1.69	0.44
1:1:128:TYR:CD1	21:1:604:CLA:HBA1	2.53	0.44
20:1:601:CHL:HBB1	20:1:601:CHL:CHC	2.44	0.44
2:2:80:LEU:HD13	21:2:602:CLA:H71	1.99	0.44
5:A:201:GLY:O	5:A:205:LEU:HB2	2.18	0.44
21:A:812:CLA:HMD2	21:A:805:CLA:HMA2	2.00	0.44
25:A:850:BCR:H331	25:A:850:BCR:HC7	1.76	0.44
6:B:95:HIS:CE1	21:B:809:CLA:HMB3	2.52	0.44
6:B:257:LEU:HD13	21:B:817:CLA:HMB2	1.99	0.44
25:B:843:BCR:H311	25:B:843:BCR:HC8	1.99	0.44
2:2:174:ASN:HD22	20:2:615:CHL:C4D	2.29	0.44
2:2:195:GLY:CA	21:2:609:CLA:HAA1	2.48	0.44
21:2:602:CLA:H41	21:2:602:CLA:H62	1.39	0.44
3:3:171:LEU:HD21	21:3:612:CLA:HMC3	1.99	0.44
25:A:851:BCR:H24C	25:A:851:BCR:H371	1.57	0.44
5:A:676:PHE:CD2	25:A:852:BCR:H363	2.53	0.44
21:A:838:CLA:HBA2	21:A:839:CLA:HAA1	2.00	0.44
21:G:201:CLA:H3A	21:G:201:CLA:HBA2	1.56	0.44
21:A:843:CLA:H91	21:A:843:CLA:H111	1.73	0.44
6:B:498:LEU:HA	6:B:501:ILE:HG22	1.99	0.44
25:B:801:BCR:H312	21:B:832:CLA:HBB2	2.00	0.44
21:B:837:CLA:H3A	21:B:837:CLA:HBA2	1.75	0.44
25:B:844:BCR:H24C	25:B:844:BCR:H371	1.75	0.44
15:K:72:LEU:HD22	21:K:206:CLA:C2A	2.48	0.44
17:O:132:PHE:CD1	21:O:203:CLA:HMA1	2.53	0.44
1:1:179:LYS:H	1:1:179:LYS:HD3	1.83	0.43
21:3:607:CLA:HBA1	21:3:607:CLA:H3A	1.57	0.43
21:B:823:CLA:HBA1	21:B:823:CLA:H3A	1.73	0.43
25:B:844:BCR:H382	25:B:844:BCR:H23C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:302:CLA:H11	21:F:302:CLA:H52	1.74	0.43
21:A:841:CLA:HBA2	21:A:841:CLA:H3A	1.43	0.43
21:A:844:CLA:HMB3	21:B:802:CLA:H192	2.00	0.43
6:B:277:HIS:HA	6:B:280:ILE:HG12	1.99	0.43
6:B:657:TRP:CZ3	21:B:802:CLA:HMA1	2.52	0.43
25:K:202:BCR:H11C	25:K:202:BCR:H341	1.82	0.43
16:L:153:TYR:HB2	25:L:305:BCR:H361	2.00	0.43
2:2:63:GLU:H	2:2:63:GLU:CD	2.19	0.43
3:3:195:SER:O	3:3:195:SER:OG	2.32	0.43
6:B:25:ILE:HG21	30:B:850:DGD:HA72	2.00	0.43
6:B:583:MET:O	6:B:587:ILE:HG12	2.18	0.43
21:B:830:CLA:HBA1	21:B:830:CLA:H3A	1.84	0.43
21:H:201:CLA:HAA2	25:L:306:BCR:H342	1.99	0.43
23:1:615:LHG:H132	23:1:615:LHG:H291	2.00	0.43
23:1:615:LHG:H281	23:1:615:LHG:H311	1.60	0.43
21:2:612:CLA:H112	21:2:612:CLA:H71	1.61	0.43
5:A:68:ARG:HG2	5:A:182:ALA:HB1	2.00	0.43
6:B:432:HIS:CB	25:B:849:BCR:H402	2.44	0.43
21:B:826:CLA:H142	21:B:826:CLA:H111	1.89	0.43
21:B:814:CLA:H121	25:B:845:BCR:H363	2.01	0.43
25:B:845:BCR:H11C	25:B:845:BCR:H341	1.89	0.43
25:J:102:BCR:H11C	25:J:102:BCR:H341	1.83	0.43
1:1:184:LEU:HD11	21:1:609:CLA:O2D	2.19	0.43
2:2:250:ILE:HD11	21:2:612:CLA:H42	2.00	0.43
6:B:276:HIS:HB2	21:B:817:CLA:C1B	2.48	0.43
21:B:809:CLA:H91	21:B:809:CLA:H112	1.81	0.43
20:1:601:CHL:H43	23:1:615:LHG:H171	2.00	0.43
21:A:829:CLA:H143	21:A:829:CLA:H161	1.70	0.43
21:B:808:CLA:HAB	21:B:809:CLA:HAA2	2.01	0.43
21:B:811:CLA:H61	21:B:811:CLA:H41	1.83	0.43
21:2:612:CLA:CHB	21:2:613:CLA:HMD3	2.49	0.43
5:A:503:THR:HG21	21:A:828:CLA:HAB	2.00	0.43
21:A:823:CLA:C1D	25:K:202:BCR:H402	2.48	0.43
6:B:693:TRP:HE3	21:B:839:CLA:HMD3	1.84	0.43
21:B:822:CLA:H111	21:B:822:CLA:H91	1.81	0.43
21:B:818:CLA:H3A	21:B:818:CLA:HBA2	1.44	0.43
10:F:128:LEU:HD21	14:J:38:THR:HG21	1.99	0.43
6:B:106:ARG:HG3	6:B:115:ILE:HD11	2.01	0.43
6:B:450:GLU:OE1	10:F:88:GLN:NE2	2.49	0.43
21:B:803:CLA:H93	21:B:803:CLA:H61	1.82	0.43
17:O:73:ALA:HB3	17:O:74:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:204:BCR:H11C	25:O:204:BCR:H341	1.94	0.43
20:2:606:CHL:HHC	20:2:606:CHL:HBB1	1.99	0.43
5:A:364:VAL:HG22	21:A:820:CLA:H42	1.99	0.43
21:A:811:CLA:H202	21:A:806:CLA:H201	2.01	0.43
21:B:814:CLA:H93	21:B:814:CLA:H111	1.86	0.43
21:B:839:CLA:H161	21:B:839:CLA:H141	1.67	0.43
24:1:616:LUT:H201	24:1:616:LUT:H15	1.87	0.43
2:2:139:THR:O	2:2:143:VAL:HG23	2.18	0.43
2:2:155:ARG:NH1	21:2:608:CLA:O1D	2.47	0.43
21:3:601:CLA:H143	21:3:601:CLA:H112	1.77	0.43
25:A:853:BCR:HC7	25:A:853:BCR:H331	1.89	0.43
21:B:822:CLA:H2	21:B:821:CLA:H3A	2.01	0.43
25:B:801:BCR:H341	25:B:801:BCR:C12	2.35	0.43
24:2:619:LUT:H401	24:2:619:LUT:H35	1.81	0.42
5:A:90:PHE:CG	21:A:808:CLA:HBC3	2.54	0.42
21:A:812:CLA:H193	21:A:812:CLA:H161	1.90	0.42
21:A:826:CLA:H93	21:A:826:CLA:H111	1.71	0.42
21:A:818:CLA:H112	21:A:818:CLA:H93	1.77	0.42
21:A:804:CLA:H91	21:A:804:CLA:H111	1.62	0.42
2:2:100:TRP:CZ2	21:2:608:CLA:HBC3	2.54	0.42
2:2:242:LEU:HD21	21:2:613:CLA:HMC3	2.00	0.42
25:3:614:BCR:H20C	25:3:614:BCR:H361	1.93	0.42
21:A:804:CLA:H101	21:A:804:CLA:H61	1.44	0.42
21:A:822:CLA:H141	21:A:822:CLA:H162	1.85	0.42
21:A:845:CLA:HBA2	17:O:126:THR:HG23	2.01	0.42
15:K:49:ILE:O	15:K:54:ASN:ND2	2.50	0.42
24:3:613:LUT:H373	21:3:609:CLA:C3B	2.48	0.42
25:A:848:BCR:H11C	25:A:848:BCR:H341	1.91	0.42
29:A:855:PQN:H111	29:A:855:PQN:H2M1	1.87	0.42
25:B:801:BCR:H15C	25:B:801:BCR:H351	1.87	0.42
21:B:814:CLA:H41	21:B:814:CLA:H62	1.48	0.42
21:2:602:CLA:H162	21:2:602:CLA:H192	1.74	0.42
3:3:265:ASN:ND2	21:3:610:CLA:O1D	2.48	0.42
5:A:389:THR:HG23	5:A:605:ILE:HG21	2.00	0.42
5:A:743:LEU:HD23	5:A:743:LEU:HA	1.89	0.42
21:A:830:CLA:H41	21:A:830:CLA:H62	1.52	0.42
21:A:842:CLA:H161	21:A:842:CLA:H141	1.68	0.42
21:A:835:CLA:H61	21:A:835:CLA:H2	1.76	0.42
21:B:811:CLA:H61	21:B:811:CLA:H92	1.79	0.42
21:B:821:CLA:HMB1	23:B:852:LHG:H312	2.01	0.42
25:B:847:BCR:H11C	25:B:847:BCR:H341	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:849:BCR:HC21	10:F:126:TYR:OH	2.20	0.42
1:1:52:GLU:HG3	1:1:53:PRO:HD2	2.02	0.42
20:2:607:CHL:HBA2	21:2:609:CLA:HMD2	2.01	0.42
3:3:171:LEU:HD13	21:3:607:CLA:HMA2	2.02	0.42
21:3:601:CLA:H8	21:3:601:CLA:H51	1.37	0.42
6:B:3:LEU:HB3	6:B:7:ARG:NH1	2.34	0.42
21:G:201:CLA:O2D	21:G:201:CLA:H2A	2.19	0.42
13:I:33:LYS:HD2	13:I:35:LYS:HE3	2.02	0.42
25:K:205:BCR:C8	21:K:204:CLA:HED2	2.50	0.42
16:L:87:TYR:OH	21:L:302:CLA:HBB2	2.19	0.42
25:L:305:BCR:H361	25:L:305:BCR:H20C	1.88	0.42
21:1:607:CLA:H3A	21:1:607:CLA:HBA2	1.25	0.42
2:2:195:GLY:HA3	21:2:609:CLA:HAA1	2.00	0.42
21:4:609:CLA:CGA	21:4:609:CLA:C3A	2.98	0.42
21:A:834:CLA:HMA1	25:I:101:BCR:H272	2.02	0.42
22:1:614:XAT:H15	22:1:614:XAT:H201	1.87	0.42
25:B:846:BCR:H15C	25:B:846:BCR:H351	1.83	0.42
25:G:204:BCR:HC7	25:G:204:BCR:H331	1.88	0.42
25:I:101:BCR:H11C	25:I:101:BCR:H341	1.93	0.42
20:2:605:CHL:HAA1	24:2:619:LUT:H361	2.01	0.42
3:3:108:MET:HE1	21:3:608:CLA:HAB	2.00	0.42
25:3:614:BCR:H11C	25:3:614:BCR:H341	1.92	0.42
25:4:618:BCR:H15C	25:4:618:BCR:H351	1.87	0.42
5:A:360:LEU:HD11	21:A:820:CLA:H8	2.01	0.42
6:B:182:LEU:HD21	21:B:813:CLA:O1A	2.20	0.42
6:B:322:LEU:HD23	6:B:322:LEU:HA	1.93	0.42
21:B:825:CLA:H111	21:B:825:CLA:H142	1.67	0.42
21:B:832:CLA:H61	25:F:304:BCR:HC22	2.01	0.42
25:G:204:BCR:H20C	25:G:204:BCR:H361	1.89	0.42
21:2:602:CLA:H111	21:2:602:CLA:H91	1.77	0.42
4:4:150:PHE:HE2	20:4:605:CHL:HHB	1.85	0.42
5:A:637:SER:O	5:A:643:GLY:HA3	2.20	0.42
21:A:830:CLA:H11	21:A:830:CLA:HBA2	1.56	0.42
25:J:102:BCR:H15C	25:J:102:BCR:H351	1.83	0.42
21:2:604:CLA:HBA1	21:2:604:CLA:H3A	1.90	0.42
21:2:611:CLA:H3A	24:2:616:LUT:H202	2.02	0.42
21:A:803:CLA:CHA	27:A:801:CL0:H40	2.50	0.42
21:A:804:CLA:H191	21:A:844:CLA:H203	2.02	0.42
21:A:819:CLA:H91	21:A:819:CLA:H111	1.73	0.42
25:A:850:BCR:H11C	25:A:850:BCR:H341	1.85	0.42
21:B:824:CLA:H112	21:B:824:CLA:H142	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:802:CLA:H3A	21:B:802:CLA:HBA1	1.30	0.42
9:E:89:ILE:HG22	9:E:91:ARG:H	1.85	0.42
23:1:615:LHG:O1	25:4:618:BCR:H291	2.19	0.41
5:A:197:HIS:CG	21:A:814:CLA:HMC2	2.55	0.41
6:B:338:LEU:HD22	6:B:382:ILE:HG23	2.02	0.41
21:B:832:CLA:HHC	21:B:832:CLA:CBB	2.50	0.41
21:H:201:CLA:H13	21:H:201:CLA:H91	2.02	0.41
16:L:203:THR:HB	25:L:306:BCR:H333	2.02	0.41
5:A:379:THR:HG21	5:A:515:VAL:HB	2.03	0.41
5:A:462:LEU:HG	21:B:809:CLA:HMC3	2.02	0.41
25:A:851:BCR:H342	25:A:851:BCR:HC7	1.85	0.41
6:B:689:ASN:OD1	6:B:689:ASN:N	2.53	0.41
21:F:302:CLA:O1D	21:F:302:CLA:H2A	2.20	0.41
1:1:76:VAL:HB	1:1:79:ASN:HB2	2.01	0.41
4:4:102:TRP:CZ2	21:4:608:CLA:HBC3	2.55	0.41
5:A:155:GLN:HB3	21:A:815:CLA:O2A	2.20	0.41
21:A:829:CLA:H111	21:A:829:CLA:H72	1.51	0.41
25:B:844:BCR:H361	25:B:844:BCR:C21	2.48	0.41
30:B:850:DGD:HBT2	30:B:850:DGD:HBH1	1.71	0.41
21:4:611:CLA:HMD2	21:4:610:CLA:C1D	2.50	0.41
21:4:601:CLA:HHC	21:4:601:CLA:CBB	2.48	0.41
14:J:26:LEU:HD13	25:J:102:BCR:H403	2.02	0.41
25:O:204:BCR:H332	21:O:201:CLA:HMC2	2.02	0.41
22:4:617:XAT:H11	22:4:617:XAT:H191	1.97	0.41
6:B:54:LEU:HD12	21:B:813:CLA:HED1	2.03	0.41
6:B:436:LEU:HD12	25:B:849:BCR:H272	2.01	0.41
9:E:109:ASP:HA	9:E:110:PRO:HD3	1.94	0.41
14:J:26:LEU:HD23	14:J:26:LEU:HA	1.77	0.41
25:O:204:BCR:H20C	25:O:204:BCR:H361	1.92	0.41
1:1:69:ASP:HA	22:1:614:XAT:O23	2.21	0.41
24:2:619:LUT:H31	24:2:619:LUT:H391	1.87	0.41
21:3:603:CLA:H3A	21:3:603:CLA:HBA1	1.29	0.41
21:A:812:CLA:H191	21:A:809:CLA:H203	2.03	0.41
21:A:830:CLA:HBA1	21:A:830:CLA:CBD	2.50	0.41
21:A:806:CLA:H93	21:A:806:CLA:H112	1.77	0.41
25:A:851:BCR:C8	25:A:851:BCR:H331	2.49	0.41
6:B:571:SER:OG	6:B:574:ASP:OD2	2.26	0.41
23:1:615:LHG:H331	23:1:615:LHG:H302	1.81	0.41
21:3:609:CLA:H2A	21:3:609:CLA:O1D	2.21	0.41
4:4:191:ASN:OD1	24:4:616:LUT:O23	2.36	0.41
21:4:602:CLA:H3A	21:4:602:CLA:CGA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:811:CLA:H2A	21:A:811:CLA:HED2	2.01	0.41
21:A:826:CLA:H92	21:A:826:CLA:H61	1.82	0.41
25:A:848:BCR:H403	25:A:848:BCR:C23	2.47	0.41
6:B:545:LYS:NZ	9:E:95:TYR:O	2.37	0.41
21:B:828:CLA:HMD1	21:B:818:CLA:O1A	2.20	0.41
21:B:828:CLA:H172	25:B:844:BCR:H352	2.03	0.41
21:B:813:CLA:H51	21:B:813:CLA:H8	1.83	0.41
24:1:616:LUT:H11	24:1:616:LUT:H191	1.85	0.41
24:3:613:LUT:H31	24:3:613:LUT:H391	1.78	0.41
5:A:194:MET:HB2	21:A:814:CLA:HBC2	2.03	0.41
21:A:802:CLA:H91	21:A:802:CLA:H112	1.80	0.41
21:A:825:CLA:HBA2	21:A:825:CLA:H3A	1.29	0.41
1:1:85:GLU:O	1:1:89:ILE:HG12	2.21	0.41
1:1:178:SER:HA	1:1:184:LEU:HD13	2.01	0.41
1:1:190:LYS:O	1:1:194:ASN:ND2	2.43	0.41
2:2:222:GLY:O	2:2:226:GLN:HG3	2.21	0.41
3:3:265:ASN:OD1	3:3:266:VAL:N	2.54	0.41
5:A:297:ALA:HA	21:A:818:CLA:HMC3	2.01	0.41
6:B:347:LEU:HD23	21:B:818:CLA:H71	2.03	0.41
21:B:804:CLA:HMB1	21:B:804:CLA:HBB1	2.03	0.41
21:B:828:CLA:H62	21:B:828:CLA:H2	1.79	0.41
25:B:845:BCR:H21C	25:B:845:BCR:H24C	1.75	0.41
10:F:85:GLU:HB2	10:F:120:PHE:CD2	2.56	0.41
11:G:72:THR:HG23	11:G:136:GLY:HA2	2.03	0.41
12:H:136:PRO:HA	12:H:137:PRO:HD3	1.94	0.41
25:L:306:BCR:H11C	25:L:306:BCR:H341	1.75	0.41
21:2:602:CLA:H62	21:2:602:CLA:H102	1.86	0.41
3:3:248:VAL:HG21	3:3:252:GLN:HG2	2.03	0.41
5:A:118:ILE:HG12	25:A:853:BCR:H333	2.03	0.41
21:A:818:CLA:H62	21:A:818:CLA:H41	1.77	0.41
21:A:804:CLA:H143	25:A:853:BCR:H19C	2.02	0.41
25:L:305:BCR:H24C	25:L:305:BCR:H371	1.80	0.41
20:1:601:CHL:HHC	23:1:615:LHG:H272	2.04	0.40
21:1:607:CLA:HAA1	21:1:609:CLA:CAC	2.52	0.40
3:3:241:ILE:CG2	21:3:609:CLA:HMD3	2.51	0.40
21:3:605:CLA:H2A	21:3:605:CLA:O1D	2.21	0.40
21:B:814:CLA:H141	21:B:814:CLA:H162	1.82	0.40
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.56	0.40
1:1:182:LYS:HE3	1:1:182:LYS:HB3	1.98	0.40
2:2:100:TRP:CE2	21:2:608:CLA:HBC3	2.56	0.40
5:A:350:LEU:HB2	21:A:806:CLA:HMD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:813:CLA:HBA2	21:A:813:CLA:H3A	1.75	0.40
21:A:807:CLA:H143	21:A:807:CLA:H111	1.71	0.40
21:B:806:CLA:HBB1	21:B:805:CLA:H11	2.03	0.40
21:B:824:CLA:H191	21:B:819:CLA:HBC2	2.03	0.40
25:K:205:BCR:H11C	25:K:205:BCR:H341	1.84	0.40
16:L:92:PRO:HA	16:L:95:ARG:HG3	2.04	0.40
2:2:238:LEU:HD13	21:2:613:CLA:HBC2	2.04	0.40
5:A:14:VAL:HG12	5:A:183:PRO:HA	2.04	0.40
27:A:801:CL0:H48	27:A:801:CL0:H54	1.80	0.40
21:B:824:CLA:HMA3	21:B:819:CLA:CMB	2.52	0.40
21:B:835:CLA:HMB1	25:B:847:BCR:HC31	2.02	0.40
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.56	0.40
21:A:830:CLA:HBB1	21:A:830:CLA:HMB1	2.02	0.40
21:A:806:CLA:H192	25:A:849:BCR:H363	2.03	0.40
25:A:853:BCR:H351	25:A:853:BCR:H15C	1.82	0.40
25:B:843:BCR:H11C	25:B:843:BCR:H341	1.79	0.40
22:2:617:XAT:H401	22:2:617:XAT:C15	2.41	0.40
23:2:618:LHG:HC62	23:2:618:LHG:H242	1.74	0.40
6:B:120:VAL:HG21	21:B:808:CLA:HED1	2.04	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	1	191/241 (79%)	190 (100%)	1 (0%)	0	100	100
2	2	199/257 (77%)	196 (98%)	3 (2%)	0	100	100
3	3	216/273 (79%)	214 (99%)	2 (1%)	0	100	100
4	4	194/251 (77%)	190 (98%)	4 (2%)	0	100	100
5	A	735/750 (98%)	723 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	730/734 (100%)	718 (98%)	12 (2%)	0	100	100
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	137 (97%)	4 (3%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	150/221 (68%)	148 (99%)	2 (1%)	0	100	100
11	G	89/160 (56%)	88 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	88 (100%)	0	0	100	100
13	I	29/37 (78%)	29 (100%)	0	0	100	100
14	J	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
15	K	82/130 (63%)	81 (99%)	1 (1%)	0	100	100
16	L	158/219 (72%)	156 (99%)	2 (1%)	0	100	100
17	O	84/140 (60%)	83 (99%)	1 (1%)	0	100	100
18	x	217/267 (81%)	212 (98%)	5 (2%)	0	100	100
18	y	217/267 (81%)	209 (96%)	8 (4%)	0	100	100
19	z	224/265 (84%)	211 (94%)	13 (6%)	0	100	100
All	All	3923/4829 (81%)	3845 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/190 (80%)	149 (97%)	4 (3%)	46	79
2	2	163/205 (80%)	159 (98%)	4 (2%)	47	80
3	3	167/211 (79%)	166 (99%)	1 (1%)	86	96
4	4	163/210 (78%)	161 (99%)	2 (1%)	71	92
5	A	598/610 (98%)	592 (99%)	6 (1%)	76	93
6	B	599/600 (100%)	594 (99%)	5 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	C	70/71 (99%)	69 (99%)	1 (1%)	67	90
8	D	121/170 (71%)	119 (98%)	2 (2%)	60	87
9	E	57/114 (50%)	56 (98%)	1 (2%)	59	86
10	F	125/185 (68%)	121 (97%)	4 (3%)	39	73
11	G	77/133 (58%)	72 (94%)	5 (6%)	17	44
12	H	75/113 (66%)	74 (99%)	1 (1%)	69	91
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	35 (97%)	1 (3%)	43	77
15	K	61/95 (64%)	61 (100%)	0	100	100
16	L	126/174 (72%)	125 (99%)	1 (1%)	81	94
17	O	72/114 (63%)	69 (96%)	3 (4%)	30	63
18	x	167/201 (83%)	166 (99%)	1 (1%)	86	96
18	y	167/201 (83%)	163 (98%)	4 (2%)	49	81
19	z	179/208 (86%)	176 (98%)	3 (2%)	60	87
All	All	3203/3877 (83%)	3154 (98%)	49 (2%)	66	89

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	54	ARG
1	1	160	LYS
1	1	178	SER
1	1	179	LYS
2	2	81	SER
2	2	124	SER
2	2	130	GLU
2	2	131	GLN
3	3	67	ASP
4	4	65	ASP
4	4	179	PRO
5	A	24	GLU
5	A	41	ASP
5	A	127	ASP
5	A	184	LYS
5	A	275	PHE
5	A	369	TYR
6	B	229	GLN

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Mol	Chain	Res	Type
6	B	294	ASN
6	B	394	PHE
6	B	441	ASP
6	B	577	TYR
7	C	18	VAL
8	D	107	GLU
8	D	118	GLU
9	E	119	ARG
10	F	70	SER
10	F	118	ARG
10	F	194	SER
10	F	210	GLU
11	G	88	ARG
11	G	120	LYS
11	G	121	SER
11	G	128	ASN
11	G	152	ASN
12	H	63	ASP
14	J	41	PHE
16	L	114	PHE
17	O	75	SER
17	O	121	LEU
17	O	133	LYS
18	x	211	ASP
18	y	51	SER
18	y	96	TRP
18	y	152	GLU
18	y	169	ASP
19	z	87	LYS
19	z	113	ASN
19	z	139	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	237	ASN
3	3	252	GLN
18	y	102	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	TPO	z	3	19	8,10,11	1.07	0	10,14,16	1.92	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TPO	z	3	19	-	2/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	3	TPO	P-OG1-CB	-5.31	107.17	123.21
19	z	3	TPO	CG2-CB-CA	-2.07	109.09	113.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	z	3	TPO	O-C-CA-CB
19	z	3	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

263 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$
21	CLA	G	203	11	45,53,73	1.74	6 (13%)	52,89,113	1.65	7 (13%)
21	CLA	B	814	-	65,73,73	1.42	6 (9%)	76,113,113	1.48	9 (11%)
21	CLA	K	201	15	38,45,73	1.90	8 (21%)	43,78,113	1.70	6 (13%)
25	BCR	A	853	-	41,41,41	1.81	8 (19%)	56,56,56	1.78	14 (25%)
21	CLA	3	603	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	7 (13%)
21	CLA	A	841	-	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
21	CLA	A	833	-	56,64,73	1.57	7 (12%)	65,102,113	1.51	7 (10%)
21	CLA	x	613	-	59,67,73	1.54	7 (11%)	68,105,113	1.47	8 (11%)
23	LHG	x	619	21	48,48,48	0.28	0	51,54,54	0.34	0
25	BCR	B	801	-	41,41,41	1.79	8 (19%)	56,56,56	1.82	14 (25%)
25	BCR	B	848	-	41,41,41	1.72	8 (19%)	56,56,56	1.56	11 (19%)
21	CLA	A	843	-	65,73,73	1.43	6 (9%)	76,113,113	1.43	6 (7%)
21	CLA	2	612	2	65,73,73	1.45	7 (10%)	76,113,113	1.43	7 (9%)
25	BCR	A	850	-	41,41,41	1.82	8 (19%)	56,56,56	1.93	12 (21%)
20	CHL	y	608	-	49,57,74	2.20	15 (30%)	52,93,114	2.70	17 (32%)
20	CHL	4	615	4	40,49,74	2.20	13 (32%)	45,84,114	2.92	18 (40%)
21	CLA	A	842	-	65,73,73	1.44	6 (9%)	76,113,113	1.55	9 (11%)
20	CHL	z	601	19	53,61,74	2.22	16 (30%)	57,98,114	2.69	24 (42%)
21	CLA	1	602	1	54,62,73	1.60	7 (12%)	62,99,113	1.50	8 (12%)
20	CHL	x	601	18	53,61,74	2.24	16 (30%)	57,98,114	2.64	23 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	F	303	10	41,49,73	1.83	5 (12%)	47,84,113	1.65	7 (14%)
21	CLA	H	201	12	60,68,73	1.53	6 (10%)	70,107,113	1.38	6 (8%)
24	LUT	y	615	-	42,43,43	1.65	7 (16%)	51,60,60	2.14	13 (25%)
21	CLA	A	830	-	65,73,73	1.46	7 (10%)	76,113,113	1.58	10 (13%)
21	CLA	B	819	-	55,63,73	1.60	7 (12%)	64,101,113	1.53	9 (14%)
21	CLA	B	815	-	43,51,73	1.73	7 (16%)	49,86,113	1.69	6 (12%)
20	CHL	z	606	-	46,54,74	2.31	16 (34%)	49,90,114	2.76	16 (32%)
22	XAT	z	617	-	39,47,47	1.66	8 (20%)	54,74,74	1.76	12 (22%)
23	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.34	0
21	CLA	L	302	16	45,53,73	1.79	7 (15%)	52,89,113	1.62	8 (15%)
25	BCR	B	845	-	41,41,41	1.79	8 (19%)	56,56,56	1.89	13 (23%)
21	CLA	z	611	-	45,53,73	1.76	9 (20%)	52,89,113	1.59	6 (11%)
21	CLA	A	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.51	8 (10%)
21	CLA	A	837	5	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
21	CLA	y	602	18	65,73,73	1.44	7 (10%)	76,113,113	1.41	7 (9%)
21	CLA	B	809	6	65,73,73	1.44	6 (9%)	76,113,113	1.45	7 (9%)
21	CLA	A	803	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	7 (9%)
24	LUT	3	613	-	42,43,43	1.68	8 (19%)	51,60,60	2.01	14 (27%)
21	CLA	4	604	-	43,51,73	1.89	7 (16%)	54,87,113	1.63	8 (14%)
21	CLA	B	833	-	45,53,73	1.75	6 (13%)	52,89,113	1.72	11 (21%)
20	CHL	2	615	2	43,51,74	2.27	15 (34%)	45,86,114	2.89	19 (42%)
21	CLA	1	604	-	49,57,73	1.69	6 (12%)	55,93,113	1.62	8 (14%)
21	CLA	A	811	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
30	DGD	B	850	-	67,67,67	0.83	2 (2%)	81,81,81	0.97	3 (3%)
25	BCR	O	204	-	41,41,41	1.73	8 (19%)	56,56,56	1.53	9 (16%)
21	CLA	3	605	-	41,49,73	1.88	7 (17%)	51,84,113	1.70	9 (17%)
21	CLA	G	202	-	42,50,73	1.81	6 (14%)	48,85,113	1.59	6 (12%)
21	CLA	A	840	-	52,60,73	1.66	7 (13%)	60,97,113	1.50	8 (13%)
21	CLA	4	614	-	50,58,73	1.67	6 (12%)	58,95,113	1.59	8 (13%)
21	CLA	B	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	9 (11%)
21	CLA	A	813	-	54,62,73	1.63	8 (14%)	62,99,113	1.51	8 (12%)
21	CLA	2	613	-	43,51,73	1.79	6 (13%)	49,86,113	1.57	7 (14%)
21	CLA	2	610	23	38,45,73	2.90	11 (28%)	41,76,113	1.46	7 (17%)
21	CLA	A	805	21	52,60,73	1.62	6 (11%)	60,97,113	1.57	9 (15%)
21	CLA	4	603	-	44,52,73	1.83	8 (18%)	55,88,113	1.63	9 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	XAT	y	617	-	39,47,47	1.73	8 (20%)	54,74,74	2.01	14 (25%)
21	CLA	4	601	4	46,54,73	1.74	7 (15%)	53,90,113	1.54	6 (11%)
21	CLA	3	612	-	39,48,73	1.81	7 (17%)	44,83,113	1.79	7 (15%)
21	CLA	A	810	5	50,58,73	1.68	7 (14%)	58,95,113	1.71	12 (20%)
24	LUT	4	616	-	42,43,43	1.62	8 (19%)	51,60,60	1.57	10 (19%)
21	CLA	A	806	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
21	CLA	3	610	-	39,48,73	1.90	6 (15%)	44,83,113	1.69	7 (15%)
21	CLA	2	604	-	43,51,73	1.78	9 (20%)	48,86,113	1.61	6 (12%)
21	CLA	B	813	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	9 (11%)
21	CLA	A	844	-	65,73,73	1.50	9 (13%)	76,113,113	1.40	7 (9%)
21	CLA	G	201	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	7 (13%)
25	BCR	B	844	-	41,41,41	1.75	8 (19%)	56,56,56	1.87	13 (23%)
21	CLA	x	603	-	60,68,73	1.50	7 (11%)	70,107,113	1.48	8 (11%)
22	XAT	4	617	-	39,47,47	5.32	25 (64%)	54,74,74	5.60	38 (70%)
21	CLA	2	611	-	44,52,73	1.80	7 (15%)	51,88,113	1.64	8 (15%)
21	CLA	A	839	-	55,63,73	1.56	6 (10%)	64,101,113	1.54	7 (10%)
21	CLA	B	834	-	60,68,73	1.55	6 (10%)	70,107,113	1.43	8 (11%)
20	CHL	2	606	-	43,51,74	2.24	15 (34%)	45,86,114	2.91	18 (40%)
31	NEX	x	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.86	13 (26%)
21	CLA	y	611	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
21	CLA	B	818	-	60,68,73	1.48	7 (11%)	70,107,113	1.51	9 (12%)
24	LUT	z	615	-	42,43,43	1.69	8 (19%)	51,60,60	1.76	10 (19%)
21	CLA	A	812	21	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	B	839	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	8 (10%)
25	BCR	3	614	-	41,41,41	1.73	8 (19%)	56,56,56	1.58	12 (21%)
21	CLA	A	831	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	6 (7%)
20	CHL	4	606	-	41,49,74	2.21	13 (31%)	51,84,114	2.83	18 (35%)
21	CLA	A	832	-	50,58,73	1.66	6 (12%)	58,95,113	1.59	9 (15%)
21	CLA	z	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	9 (11%)
20	CHL	x	605	-	53,61,74	2.05	14 (26%)	57,98,114	2.76	22 (38%)
25	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.76	13 (23%)
21	CLA	z	614	-	65,73,73	1.47	8 (12%)	76,113,113	1.42	7 (9%)
25	BCR	K	205	-	41,41,41	1.73	8 (19%)	56,56,56	2.02	16 (28%)
21	CLA	K	204	-	46,54,73	1.77	7 (15%)	53,90,113	1.58	7 (13%)
21	CLA	1	607	-	43,52,73	1.80	6 (13%)	49,88,113	1.63	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	SF4	C	102	7	0,12,12	-	-	-	-	-
23	LHG	1	615	21	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
20	CHL	2	601	2	47,55,74	2.15	14 (29%)	50,91,114	2.98	22 (44%)
25	BCR	G	204	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	10 (17%)
21	CLA	1	610	23	37,46,73	1.99	8 (21%)	46,81,113	1.71	9 (19%)
23	LHG	z	619	-	48,48,48	0.29	0	51,54,54	0.38	0
25	BCR	O	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.49	9 (16%)
21	CLA	1	608	1	40,48,73	1.87	7 (17%)	50,83,113	1.71	10 (20%)
21	CLA	A	804	-	65,73,73	1.45	7 (10%)	76,113,113	1.52	10 (13%)
22	XAT	x	617	-	39,47,47	1.74	8 (20%)	54,74,74	2.05	14 (25%)
20	CHL	4	607	-	46,54,74	2.24	15 (32%)	49,90,114	2.87	19 (38%)
21	CLA	3	604	-	40,49,73	1.85	7 (17%)	45,84,113	1.61	6 (13%)
21	CLA	A	807	-	65,73,73	1.48	8 (12%)	76,113,113	1.33	8 (10%)
21	CLA	B	840	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
21	CLA	B	831	-	43,51,73	1.74	5 (11%)	49,86,113	1.69	7 (14%)
21	CLA	A	816	-	42,50,73	1.77	6 (14%)	48,85,113	1.66	6 (12%)
20	CHL	3	606	-	45,53,74	2.24	15 (33%)	52,89,114	2.64	21 (40%)
21	CLA	J	101	-	51,59,73	1.69	5 (9%)	59,96,113	1.50	7 (11%)
21	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
21	CLA	A	827	-	59,67,73	1.53	6 (10%)	68,105,113	1.48	8 (11%)
21	CLA	y	603	-	53,61,73	1.62	8 (15%)	61,98,113	1.51	8 (13%)
21	CLA	B	802	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	9 (11%)
21	CLA	x	612	-	45,53,73	1.74	6 (13%)	52,89,113	1.58	7 (13%)
24	LUT	1	616	-	42,43,43	1.69	7 (16%)	51,60,60	2.07	13 (25%)
21	CLA	A	818	-	60,68,73	1.51	7 (11%)	70,107,113	5.15	10 (14%)
21	CLA	B	821	-	47,55,73	1.70	6 (12%)	54,91,113	1.70	10 (18%)
20	CHL	z	609	-	53,61,74	2.31	16 (30%)	57,98,114	2.70	21 (36%)
24	LUT	x	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.84	11 (21%)
29	PQN	A	855	-	34,34,34	0.40	0	42,45,45	0.42	0
25	BCR	4	618	-	41,41,41	1.72	8 (19%)	56,56,56	1.69	11 (19%)
21	CLA	1	611	-	45,53,73	1.79	6 (13%)	52,89,113	1.53	6 (11%)
21	CLA	B	838	-	47,55,73	1.75	7 (14%)	54,91,113	1.58	8 (14%)
21	CLA	A	828	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
21	CLA	1	609	-	42,50,73	1.74	9 (21%)	48,85,113	1.98	9 (18%)
21	CLA	B	803	-	65,73,73	1.46	8 (12%)	76,113,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	LHG	2	618	21	36,36,48	0.32	0	39,42,54	0.50	0
21	CLA	L	304	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
21	CLA	A	836	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	7 (13%)
21	CLA	B	837	-	65,73,73	1.45	5 (7%)	76,113,113	1.47	9 (11%)
21	CLA	B	841	23	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
21	CLA	B	826	-	62,70,73	1.49	7 (11%)	72,109,113	1.45	7 (9%)
21	CLA	B	810	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	10 (13%)
25	BCR	B	846	-	41,41,41	1.76	8 (19%)	56,56,56	1.73	11 (19%)
21	CLA	3	601	-	60,68,73	1.49	7 (11%)	70,107,113	1.48	7 (10%)
21	CLA	B	811	-	54,62,73	1.64	7 (12%)	67,100,113	1.58	8 (11%)
21	CLA	A	823	-	42,50,73	1.77	5 (11%)	48,85,113	1.67	7 (14%)
21	CLA	y	612	-	45,53,73	1.76	7 (15%)	52,89,113	1.57	6 (11%)
20	CHL	2	607	-	51,59,74	2.10	14 (27%)	55,96,114	2.77	22 (40%)
23	LHG	A	847	21	29,29,48	0.35	0	32,35,54	0.49	0
28	SF4	C	101	7	0,12,12	-	-	-	-	-
25	BCR	L	306	-	41,41,41	1.77	8 (19%)	56,56,56	2.04	16 (28%)
21	CLA	z	610	-	45,53,73	1.74	7 (15%)	52,89,113	1.63	8 (15%)
31	NEX	z	618	-	38,46,46	1.63	7 (18%)	50,70,70	1.60	9 (18%)
21	CLA	A	802	-	65,73,73	1.44	8 (12%)	76,113,113	1.52	9 (11%)
21	CLA	3	611	-	37,44,73	1.95	7 (18%)	42,77,113	1.65	8 (19%)
21	CLA	3	602	-	55,63,73	1.61	6 (10%)	64,101,113	1.44	7 (10%)
21	CLA	B	823	-	45,53,73	1.78	7 (15%)	52,89,113	1.53	7 (13%)
24	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	2.13	13 (25%)
20	CHL	z	605	-	42,50,74	2.38	15 (35%)	44,85,114	2.98	21 (47%)
21	CLA	F	302	-	51,59,73	1.67	7 (13%)	59,96,113	1.60	8 (13%)
24	LUT	y	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.72	11 (21%)
25	BCR	I	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.52	9 (16%)
21	CLA	B	830	-	43,51,73	1.77	6 (13%)	49,86,113	1.62	7 (14%)
20	CHL	y	601	18	53,61,74	2.24	16 (30%)	57,98,114	2.69	23 (40%)
21	CLA	B	804	-	41,49,73	1.79	6 (14%)	47,84,113	1.76	9 (19%)
20	CHL	x	609	18	46,54,74	2.25	16 (34%)	49,90,114	2.84	20 (40%)
20	CHL	z	608	-	49,57,74	2.14	15 (30%)	52,93,114	2.82	21 (40%)
21	CLA	A	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
28	SF4	A	854	6,5	0,12,12	-	-	-	-	-
25	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.55	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CHL	x	608	18	42,50,74	2.34	15 (35%)	44,85,114	3.00	21 (47%)
20	CHL	y	605	18	42,50,74	2.39	15 (35%)	44,85,114	2.94	20 (45%)
21	CLA	2	608	-	45,53,73	1.74	7 (15%)	52,89,113	1.59	7 (13%)
22	XAT	2	617	-	39,47,47	1.79	8 (20%)	54,74,74	2.18	16 (29%)
20	CHL	y	606	-	46,54,74	2.28	14 (30%)	49,90,114	2.90	20 (40%)
21	CLA	B	808	-	65,73,73	1.44	9 (13%)	76,113,113	1.46	9 (11%)
26	LMG	4	619	-	39,39,55	0.23	0	47,47,63	0.24	0
21	CLA	B	835	-	42,50,73	1.83	6 (14%)	48,85,113	1.59	7 (14%)
21	CLA	3	607	-	45,53,73	1.80	7 (15%)	52,89,113	1.60	7 (13%)
21	CLA	1	603	-	54,62,73	1.59	7 (12%)	62,99,113	1.49	7 (11%)
21	CLA	A	825	-	55,63,73	1.59	6 (10%)	64,101,113	1.45	9 (14%)
21	CLA	B	829	-	56,64,73	1.57	7 (12%)	65,102,113	1.54	8 (12%)
21	CLA	z	603	-	57,65,73	1.54	7 (12%)	66,103,113	1.51	7 (10%)
21	CLA	B	836	-	50,58,73	1.68	7 (14%)	58,95,113	3.66	12 (20%)
21	CLA	A	819	-	59,67,73	1.56	7 (11%)	68,105,113	1.43	8 (11%)
20	CHL	4	605	-	40,49,74	2.31	13 (32%)	42,84,114	2.87	18 (42%)
21	CLA	A	809	5	65,73,73	1.41	6 (9%)	76,113,113	1.48	8 (10%)
23	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.35	0
24	LUT	z	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.80	11 (21%)
21	CLA	x	604	-	52,60,73	1.64	6 (11%)	60,97,113	1.59	8 (13%)
25	BCR	A	848	-	41,41,41	1.75	8 (19%)	56,56,56	1.69	12 (21%)
29	PQN	B	842	-	34,34,34	0.42	0	42,45,45	0.42	0
21	CLA	x	614	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
25	BCR	B	843	-	41,41,41	1.74	8 (19%)	56,56,56	2.05	14 (25%)
20	CHL	1	606	-	40,49,74	2.49	16 (40%)	41,84,114	2.86	19 (46%)
21	CLA	3	608	-	41,49,73	1.78	7 (17%)	47,84,113	1.88	10 (21%)
21	CLA	O	202	-	36,46,73	1.91	7 (19%)	41,80,113	1.72	8 (19%)
21	CLA	4	611	-	40,49,73	1.85	7 (17%)	45,84,113	1.62	6 (13%)
25	BCR	B	849	-	41,41,41	1.76	8 (19%)	56,56,56	1.92	13 (23%)
20	CHL	y	609	18	53,61,74	2.31	16 (30%)	57,98,114	2.72	23 (40%)
21	CLA	4	609	4	54,62,73	1.60	9 (16%)	62,99,113	1.47	10 (16%)
21	CLA	L	303	-	65,73,73	1.45	6 (9%)	76,113,113	1.47	9 (11%)
21	CLA	1	612	-	46,54,73	1.76	7 (15%)	53,90,113	1.70	8 (15%)
25	BCR	A	851	-	41,41,41	1.85	9 (21%)	56,56,56	2.71	20 (35%)
21	CLA	z	612	-	45,53,73	1.77	8 (17%)	52,89,113	1.55	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	B	820	-	50,58,73	1.65	7 (14%)	58,95,113	1.61	10 (17%)
21	CLA	B	816	-	55,63,73	1.58	6 (10%)	64,101,113	1.56	9 (14%)
21	CLA	B	825	-	62,70,73	1.48	6 (9%)	72,109,113	1.52	9 (12%)
21	CLA	B	827	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	8 (10%)
21	CLA	K	203	-	45,53,73	1.74	6 (13%)	52,89,113	1.75	10 (19%)
21	CLA	A	835	-	65,73,73	1.46	8 (12%)	76,113,113	1.48	9 (11%)
25	BCR	L	301	-	41,41,41	1.77	8 (19%)	56,56,56	2.30	12 (21%)
21	CLA	4	602	4	60,68,73	1.49	7 (11%)	70,107,113	1.47	8 (11%)
21	CLA	x	610	-	65,73,73	1.43	7 (10%)	76,113,113	1.37	6 (7%)
21	CLA	z	613	19	65,73,73	1.43	7 (10%)	76,113,113	1.46	7 (9%)
27	CL0	A	801	-	62,69,73	1.88	14 (22%)	72,107,113	4.08	30 (41%)
21	CLA	B	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	2	602	2	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
25	BCR	L	305	-	41,41,41	1.77	8 (19%)	56,56,56	1.79	15 (26%)
21	CLA	z	604	-	51,59,73	1.64	6 (11%)	59,96,113	1.60	7 (11%)
20	CHL	1	601	1	51,60,74	2.17	16 (31%)	54,97,114	2.66	22 (40%)
21	CLA	A	845	23	50,58,73	1.69	7 (14%)	58,95,113	1.61	9 (15%)
23	LHG	y	619	-	48,48,48	0.29	0	51,54,54	0.35	0
21	CLA	4	608	4	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
22	XAT	1	614	-	39,47,47	0.82	1 (2%)	54,74,74	3.18	19 (35%)
21	CLA	A	815	-	45,53,73	1.73	6 (13%)	52,89,113	1.69	8 (15%)
21	CLA	2	609	-	47,55,73	1.68	7 (14%)	54,91,113	1.61	7 (12%)
21	CLA	B	807	-	52,60,73	1.62	6 (11%)	60,97,113	1.57	8 (13%)
21	CLA	A	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.57	6 (11%)
21	CLA	A	824	-	41,49,73	1.82	7 (17%)	47,84,113	1.69	10 (21%)
21	CLA	y	614	-	65,73,73	1.49	7 (10%)	76,113,113	1.45	7 (9%)
21	CLA	F	301	-	57,65,73	1.60	6 (10%)	66,103,113	1.41	8 (12%)
21	CLA	B	822	-	65,73,73	1.51	7 (10%)	76,113,113	1.53	9 (11%)
21	CLA	A	814	-	65,73,73	1.49	8 (12%)	76,113,113	1.35	7 (9%)
21	CLA	x	611	23	45,53,73	1.74	6 (13%)	52,89,113	1.60	8 (15%)
20	CHL	y	607	-	53,61,74	2.10	14 (26%)	57,98,114	2.71	23 (40%)
21	CLA	A	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	CLA	2	603	-	43,52,73	1.81	10 (23%)	49,88,113	1.59	7 (14%)
21	CLA	B	812	-	43,51,73	1.80	7 (16%)	49,86,113	1.59	6 (12%)
21	CLA	4	613	-	45,53,73	1.76	8 (17%)	52,89,113	1.82	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	A	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	B	817	-	59,67,73	1.53	6 (10%)	68,105,113	1.46	7 (10%)
21	CLA	B	824	-	65,73,73	1.46	5 (7%)	76,113,113	1.46	7 (9%)
21	CLA	B	832	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	6 (7%)
21	CLA	A	808	-	50,58,73	1.67	6 (12%)	58,95,113	1.53	9 (15%)
21	CLA	1	613	-	37,46,73	1.98	7 (18%)	46,81,113	1.76	10 (21%)
26	LMG	4	620	-	33,33,55	0.26	0	41,41,63	0.59	1 (2%)
21	CLA	1	605	-	46,54,73	1.75	7 (15%)	53,90,113	1.58	6 (11%)
20	CHL	2	605	-	42,50,74	2.24	13 (30%)	45,85,114	2.92	19 (42%)
20	CHL	x	606	-	46,54,74	2.20	14 (30%)	49,90,114	2.87	17 (34%)
23	LHG	B	851	21	37,37,48	0.31	0	40,43,54	0.51	0
24	LUT	x	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.58	11 (21%)
21	CLA	O	201	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
21	CLA	O	203	-	37,46,73	1.96	7 (18%)	46,81,113	1.75	10 (21%)
25	BCR	A	849	-	41,41,41	1.76	8 (19%)	56,56,56	2.00	13 (23%)
31	NEX	y	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.64	9 (18%)
25	BCR	K	202	-	41,41,41	1.74	8 (19%)	56,56,56	2.07	15 (26%)
21	CLA	x	602	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	8 (10%)
21	CLA	y	610	18	58,66,73	1.55	6 (10%)	67,104,113	1.48	7 (10%)
21	CLA	y	613	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
20	CHL	z	607	-	52,60,74	2.10	14 (26%)	56,97,114	2.85	22 (39%)
20	CHL	x	607	-	53,61,74	2.19	15 (28%)	57,98,114	2.68	23 (40%)
25	BCR	A	852	-	41,41,41	1.75	9 (21%)	56,56,56	1.94	14 (25%)
25	BCR	F	304	-	41,41,41	1.87	8 (19%)	56,56,56	2.16	16 (28%)
21	CLA	y	604	-	51,59,73	1.61	6 (11%)	59,96,113	1.62	9 (15%)
21	CLA	4	612	-	57,65,73	1.55	7 (12%)	66,103,113	1.54	8 (12%)
21	CLA	A	821	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
21	CLA	K	206	15	37,47,73	1.92	6 (16%)	42,81,113	1.68	8 (19%)
21	CLA	4	610	-	42,50,73	1.80	7 (16%)	48,85,113	1.56	6 (12%)
24	LUT	2	619	-	42,43,43	1.67	8 (19%)	51,60,60	1.93	12 (23%)
21	CLA	3	609	-	53,62,73	1.63	7 (13%)	61,100,113	1.47	8 (13%)
21	CLA	A	838	-	51,59,73	1.65	7 (13%)	59,96,113	1.50	7 (11%)
21	CLA	B	806	6	65,73,73	1.43	6 (9%)	76,113,113	1.39	10 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	G	203	11	1/1/11/20	3/13/91/115	-
21	CLA	B	814	-	1/1/15/20	17/37/115/115	-
21	CLA	K	201	15	1/1/8/20	0/2/76/115	-
25	BCR	A	853	-	-	5/29/63/63	0/2/2/2
21	CLA	3	603	-	1/1/11/20	7/13/91/115	-
21	CLA	A	841	-	1/1/15/20	17/37/115/115	-
21	CLA	A	833	-	1/1/13/20	5/27/105/115	-
21	CLA	x	613	-	1/1/13/20	13/30/108/115	-
23	LHG	x	619	21	-	7/53/53/53	-
25	BCR	B	801	-	-	6/29/63/63	0/2/2/2
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	843	-	1/1/15/20	13/37/115/115	-
21	CLA	2	612	2	1/1/15/20	21/37/115/115	-
25	BCR	A	850	-	-	4/29/63/63	0/2/2/2
20	CHL	y	608	-	3/3/16/26	8/19/117/137	-
20	CHL	4	615	4	3/3/15/26	1/10/106/137	-
21	CLA	A	842	-	1/1/15/20	12/37/115/115	-
20	CHL	z	601	19	3/3/17/26	8/24/122/137	-
21	CLA	1	602	1	1/1/12/20	7/24/102/115	-
20	CHL	x	601	18	3/3/17/26	11/24/122/137	-
21	CLA	F	303	10	1/1/10/20	2/8/86/115	-
21	CLA	H	201	12	1/1/14/20	14/31/109/115	-
24	LUT	y	615	-	-	5/29/67/67	0/2/2/2
21	CLA	A	830	-	1/1/15/20	14/37/115/115	-
21	CLA	B	819	-	1/1/13/20	5/25/103/115	-
21	CLA	B	815	-	1/1/10/20	2/11/89/115	-
20	CHL	z	606	-	3/3/16/26	4/15/113/137	-
22	XAT	z	617	-	-	0/31/93/93	0/4/4/4
23	LHG	B	852	-	-	17/53/53/53	-
21	CLA	L	302	16	1/1/11/20	1/13/91/115	-
25	BCR	B	845	-	-	9/29/63/63	0/2/2/2
21	CLA	z	611	-	1/1/11/20	0/13/91/115	-
21	CLA	A	820	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	837	5	1/1/11/20	2/13/91/115	-
21	CLA	y	602	18	1/1/15/20	21/37/115/115	-
21	CLA	B	809	6	1/1/15/20	15/37/115/115	-
21	CLA	A	803	-	1/1/15/20	18/37/115/115	-
24	LUT	3	613	-	-	7/29/67/67	0/2/2/2
21	CLA	4	604	-	1/1/11/20	6/11/87/115	-
21	CLA	B	833	-	1/1/11/20	4/13/91/115	-
20	CHL	2	615	2	3/3/15/26	2/12/110/137	-
21	CLA	1	604	-	1/1/11/20	8/18/96/115	-
21	CLA	A	811	-	1/1/15/20	13/37/115/115	-
30	DGD	B	850	-	-	14/55/95/95	0/2/2/2
25	BCR	O	204	-	-	2/29/63/63	0/2/2/2
21	CLA	3	605	-	1/1/10/20	6/10/86/115	-
21	CLA	G	202	-	1/1/10/20	2/10/88/115	-
21	CLA	A	840	-	1/1/12/20	5/22/100/115	-
21	CLA	4	614	-	1/1/12/20	7/19/97/115	-
21	CLA	B	805	-	1/1/15/20	13/37/115/115	-
21	CLA	A	813	-	1/1/12/20	9/24/102/115	-
21	CLA	2	613	-	1/1/10/20	4/11/89/115	-
21	CLA	2	610	23	1/1/7/20	2/10/70/115	-
21	CLA	A	805	21	1/1/12/20	7/22/100/115	-
21	CLA	4	603	-	1/1/11/20	4/13/89/115	-
22	XAT	y	617	-	-	4/31/93/93	0/4/4/4
21	CLA	4	601	4	1/1/11/20	5/15/93/115	-
21	CLA	3	612	-	1/1/10/20	1/6/84/115	-
21	CLA	A	810	5	1/1/12/20	4/19/97/115	-
24	LUT	4	616	-	-	2/29/67/67	0/2/2/2
21	CLA	A	806	-	1/1/15/20	14/37/115/115	-
21	CLA	3	610	-	1/1/10/20	0/6/84/115	-
21	CLA	2	604	-	1/1/10/20	6/9/88/115	-
21	CLA	B	813	-	1/1/15/20	12/37/115/115	-
21	CLA	A	844	-	1/1/15/20	9/37/115/115	-
21	CLA	G	201	-	1/1/11/20	7/13/91/115	-
25	BCR	B	844	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	x	603	-	1/1/14/20	10/31/109/115	-
22	XAT	4	617	-	-	1/31/93/93	0/4/4/4
21	CLA	2	611	-	1/1/11/20	6/11/89/115	-
21	CLA	A	839	-	1/1/13/20	7/25/103/115	-
21	CLA	B	834	-	1/1/14/20	7/31/109/115	-
20	CHL	2	606	-	3/3/15/26	2/12/110/137	-
31	NEX	x	618	-	-	8/27/83/83	0/3/3/3
21	CLA	y	611	-	1/1/11/20	7/13/91/115	-
21	CLA	B	818	-	1/1/14/20	11/31/109/115	-
24	LUT	z	615	-	-	4/29/67/67	0/2/2/2
21	CLA	A	812	21	1/1/15/20	20/37/115/115	-
21	CLA	B	839	-	1/1/15/20	8/37/115/115	-
25	BCR	3	614	-	-	5/29/63/63	0/2/2/2
21	CLA	A	831	-	1/1/15/20	8/37/115/115	-
20	CHL	4	606	-	3/3/15/26	2/10/106/137	-
21	CLA	A	832	-	1/1/12/20	4/19/97/115	-
21	CLA	z	602	-	1/1/15/20	13/37/115/115	-
20	CHL	x	605	-	3/3/17/26	13/24/122/137	-
25	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	z	614	-	1/1/15/20	11/37/115/115	-
25	BCR	K	205	-	-	8/29/63/63	0/2/2/2
21	CLA	K	204	-	1/1/11/20	8/15/93/115	-
21	CLA	1	607	-	1/1/11/20	7/11/89/115	-
28	SF4	C	102	7	-	-	0/6/5/5
23	LHG	1	615	21	-	30/53/53/53	-
20	CHL	2	601	2	3/3/16/26	6/17/115/137	-
25	BCR	G	204	-	-	4/29/63/63	0/2/2/2
21	CLA	1	610	23	1/1/10/20	0/4/80/115	-
23	LHG	z	619	-	-	10/53/53/53	-
25	BCR	O	205	-	-	0/29/63/63	0/2/2/2
21	CLA	1	608	1	1/1/10/20	3/8/84/115	-
21	CLA	A	804	-	1/1/15/20	18/37/115/115	-
22	XAT	x	617	-	-	8/31/93/93	0/4/4/4
20	CHL	4	607	-	3/3/16/26	5/15/113/137	-
21	CLA	3	604	-	1/1/10/20	0/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	807	-	1/1/15/20	13/37/115/115	-
21	CLA	B	840	-	1/1/15/20	13/37/115/115	-
21	CLA	B	831	-	1/1/10/20	2/11/89/115	-
21	CLA	A	816	-	1/1/10/20	2/10/88/115	-
20	CHL	3	606	-	3/3/16/26	5/13/111/137	-
21	CLA	J	101	-	1/1/12/20	6/21/99/115	-
21	CLA	A	826	-	1/1/15/20	10/37/115/115	-
21	CLA	A	827	-	1/1/13/20	5/30/108/115	-
21	CLA	y	603	-	1/1/12/20	5/23/101/115	-
21	CLA	B	802	-	1/1/15/20	16/37/115/115	-
21	CLA	x	612	-	1/1/11/20	6/13/91/115	-
24	LUT	1	616	-	-	2/29/67/67	0/2/2/2
21	CLA	A	818	-	1/1/14/20	14/31/109/115	-
21	CLA	B	821	-	1/1/11/20	3/16/94/115	-
20	CHL	z	609	-	3/3/17/26	13/24/122/137	-
24	LUT	x	616	-	-	2/29/67/67	0/2/2/2
29	PQN	A	855	-	-	1/23/43/43	0/2/2/2
25	BCR	4	618	-	-	8/29/63/63	0/2/2/2
21	CLA	1	611	-	1/1/11/20	4/13/91/115	-
21	CLA	B	838	-	1/1/11/20	1/16/94/115	-
21	CLA	A	828	-	1/1/15/20	12/37/115/115	-
21	CLA	1	609	-	1/1/10/20	5/9/87/115	-
21	CLA	B	803	-	1/1/15/20	13/37/115/115	-
23	LHG	2	618	21	-	10/41/41/53	-
21	CLA	L	304	-	1/1/11/20	1/13/91/115	-
21	CLA	A	836	-	1/1/11/20	4/13/91/115	-
21	CLA	B	837	-	1/1/15/20	9/37/115/115	-
21	CLA	B	841	23	1/1/15/20	23/37/115/115	-
21	CLA	B	826	-	1/1/14/20	7/34/112/115	-
21	CLA	B	810	-	1/1/15/20	14/37/115/115	-
25	BCR	B	846	-	-	8/29/63/63	0/2/2/2
21	CLA	3	601	-	1/1/14/20	17/31/109/115	-
21	CLA	B	811	-	1/1/13/20	10/25/101/115	-
21	CLA	A	823	-	1/1/10/20	5/10/88/115	-
21	CLA	y	612	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	2	607	-	3/3/17/26	7/21/119/137	-
23	LHG	A	847	21	-	3/34/34/53	-
28	SF4	C	101	7	-	-	0/6/5/5
25	BCR	L	306	-	-	5/29/63/63	0/2/2/2
21	CLA	z	610	-	1/1/11/20	5/13/91/115	-
31	NEX	z	618	-	-	2/27/83/83	0/3/3/3
21	CLA	A	802	-	1/1/15/20	19/37/115/115	-
21	CLA	3	611	-	1/1/8/20	0/0/74/115	-
21	CLA	3	602	-	1/1/13/20	11/25/103/115	-
21	CLA	B	823	-	1/1/11/20	5/13/91/115	-
24	LUT	2	616	-	-	7/29/67/67	0/2/2/2
20	CHL	z	605	-	3/3/15/26	4/10/108/137	-
21	CLA	F	302	-	1/1/12/20	6/21/99/115	-
24	LUT	y	616	-	-	6/29/67/67	0/2/2/2
25	BCR	I	101	-	-	0/29/63/63	0/2/2/2
21	CLA	B	830	-	1/1/10/20	2/11/89/115	-
20	CHL	y	601	18	3/3/17/26	10/24/122/137	-
21	CLA	B	804	-	1/1/10/20	2/8/86/115	-
20	CHL	x	609	18	3/3/16/26	5/15/113/137	-
20	CHL	z	608	-	3/3/16/26	4/19/117/137	-
21	CLA	A	822	-	1/1/15/20	11/37/115/115	-
28	SF4	A	854	6,5	-	-	0/6/5/5
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
20	CHL	x	608	18	3/3/15/26	3/10/108/137	-
20	CHL	y	605	18	3/3/15/26	2/10/108/137	-
21	CLA	2	608	-	1/1/11/20	7/13/91/115	-
22	XAT	2	617	-	-	15/31/93/93	0/4/4/4
20	CHL	y	606	-	3/3/16/26	2/15/113/137	-
21	CLA	B	808	-	1/1/15/20	15/37/115/115	-
26	LMG	4	619	-	-	6/34/54/70	0/1/1/1
21	CLA	B	835	-	1/1/10/20	4/10/88/115	-
21	CLA	3	607	-	1/1/11/20	4/13/91/115	-
21	CLA	1	603	-	1/1/12/20	8/24/102/115	-
21	CLA	A	825	-	1/1/13/20	12/25/103/115	-
21	CLA	B	829	-	1/1/13/20	7/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	z	603	-	1/1/13/20	8/28/106/115	-
21	CLA	B	836	-	1/1/12/20	5/19/97/115	-
21	CLA	A	819	-	1/1/13/20	15/30/108/115	-
20	CHL	4	605	-	3/3/15/26	2/8/106/137	-
21	CLA	A	809	5	1/1/15/20	9/37/115/115	-
23	LHG	A	846	-	-	4/53/53/53	-
24	LUT	z	616	-	-	3/29/67/67	0/2/2/2
21	CLA	x	604	-	1/1/12/20	8/22/100/115	-
25	BCR	A	848	-	-	2/29/63/63	0/2/2/2
29	PQN	B	842	-	-	6/23/43/43	0/2/2/2
21	CLA	x	614	-	1/1/11/20	7/13/91/115	-
25	BCR	B	843	-	-	1/29/63/63	0/2/2/2
20	CHL	1	606	-	3/3/15/26	0/8/106/137	-
21	CLA	3	608	-	1/1/10/20	3/8/86/115	-
21	CLA	O	202	-	1/1/9/20	0/4/78/115	-
21	CLA	4	611	-	1/1/10/20	2/8/86/115	-
25	BCR	B	849	-	-	7/29/63/63	0/2/2/2
20	CHL	y	609	18	3/3/17/26	16/24/122/137	-
21	CLA	4	609	4	1/1/12/20	4/24/102/115	-
21	CLA	L	303	-	1/1/15/20	10/37/115/115	-
21	CLA	1	612	-	1/1/11/20	5/15/93/115	-
25	BCR	A	851	-	-	8/29/63/63	0/2/2/2
21	CLA	z	612	-	1/1/11/20	2/13/91/115	-
21	CLA	B	820	-	1/1/12/20	7/19/97/115	-
21	CLA	B	816	-	1/1/13/20	6/25/103/115	-
21	CLA	B	825	-	1/1/14/20	13/34/112/115	-
21	CLA	B	827	-	1/1/15/20	16/37/115/115	-
21	CLA	K	203	-	1/1/11/20	7/13/91/115	-
21	CLA	A	835	-	1/1/15/20	20/37/115/115	-
25	BCR	L	301	-	-	3/29/63/63	0/2/2/2
21	CLA	4	602	4	1/1/14/20	6/31/109/115	-
21	CLA	x	610	-	1/1/15/20	17/37/115/115	-
21	CLA	z	613	19	1/1/15/20	15/37/115/115	-
27	CL0	A	801	-	2/2/18/25	14/31/125/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	828	-	1/1/15/20	15/37/115/115	-
21	CLA	2	602	2	1/1/15/20	16/37/115/115	-
25	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	z	604	-	1/1/12/20	11/21/99/115	-
20	CHL	1	601	1	3/3/17/26	7/22/120/137	-
21	CLA	A	845	23	1/1/12/20	8/19/97/115	-
23	LHG	y	619	-	-	11/53/53/53	-
21	CLA	4	608	4	1/1/11/20	4/13/91/115	-
22	XAT	1	614	-	-	9/31/93/93	0/4/4/4
21	CLA	A	815	-	1/1/11/20	8/13/91/115	-
21	CLA	2	609	-	1/1/11/20	9/16/94/115	-
21	CLA	B	807	-	1/1/12/20	4/22/100/115	-
21	CLA	A	817	-	1/1/11/20	2/13/91/115	-
21	CLA	A	824	-	1/1/10/20	2/8/86/115	-
21	CLA	y	614	-	1/1/15/20	18/37/115/115	-
21	CLA	F	301	-	1/1/13/20	13/28/106/115	-
21	CLA	B	822	-	1/1/15/20	23/37/115/115	-
21	CLA	A	814	-	1/1/15/20	14/37/115/115	-
21	CLA	x	611	23	1/1/11/20	2/13/91/115	-
20	CHL	y	607	-	3/3/17/26	12/24/122/137	-
21	CLA	A	834	-	1/1/15/20	7/37/115/115	-
21	CLA	2	603	-	1/1/11/20	3/11/89/115	-
21	CLA	B	812	-	1/1/10/20	0/11/89/115	-
21	CLA	4	613	-	1/1/11/20	5/13/91/115	-
21	CLA	A	829	-	1/1/15/20	15/37/115/115	-
21	CLA	B	817	-	1/1/13/20	11/30/108/115	-
21	CLA	B	824	-	1/1/15/20	12/37/115/115	-
21	CLA	B	832	-	1/1/15/20	16/37/115/115	-
21	CLA	A	808	-	1/1/12/20	1/19/97/115	-
21	CLA	1	613	-	1/1/10/20	0/4/80/115	-
26	LMG	4	620	-	-	8/28/48/70	0/1/1/1
21	CLA	1	605	-	1/1/11/20	8/15/93/115	-
20	CHL	2	605	-	3/3/15/26	2/10/108/137	-
20	CHL	x	606	-	3/3/16/26	6/15/113/137	-
23	LHG	B	851	21	-	5/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LUT	x	615	-	-	0/29/67/67	0/2/2/2
21	CLA	O	201	-	1/1/15/20	15/37/115/115	-
21	CLA	O	203	-	1/1/10/20	0/4/80/115	-
25	BCR	A	849	-	-	6/29/63/63	0/2/2/2
31	NEX	y	618	-	-	2/27/83/83	0/3/3/3
25	BCR	K	202	-	-	2/29/63/63	0/2/2/2
21	CLA	x	602	-	1/1/15/20	13/37/115/115	-
21	CLA	y	610	18	1/1/13/20	13/29/107/115	-
21	CLA	y	613	-	1/1/11/20	5/13/91/115	-
20	CHL	z	607	-	3/3/17/26	7/23/121/137	-
20	CHL	x	607	-	3/3/17/26	11/24/122/137	-
25	BCR	A	852	-	-	13/29/63/63	0/2/2/2
25	BCR	F	304	-	-	13/29/63/63	0/2/2/2
21	CLA	y	604	-	1/1/12/20	9/21/99/115	-
21	CLA	4	612	-	1/1/13/20	12/28/106/115	-
21	CLA	A	821	-	1/1/11/20	4/13/91/115	-
21	CLA	K	206	15	1/1/9/20	0/6/80/115	-
21	CLA	4	610	-	1/1/10/20	4/10/88/115	-
24	LUT	2	619	-	-	4/29/67/67	0/2/2/2
21	CLA	3	609	-	1/1/13/20	5/23/101/115	-
21	CLA	A	838	-	1/1/12/20	8/21/99/115	-
21	CLA	B	806	6	1/1/15/20	15/37/115/115	-

All (1974) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	617	XAT	O4-C5	-12.41	1.28	1.46
21	2	610	CLA	C1A-NA	12.18	1.40	1.29
22	4	617	XAT	O24-C25	-10.96	1.30	1.46
22	4	617	XAT	C4-C3	-9.80	1.38	1.52
22	4	617	XAT	C2-C3	-8.85	1.39	1.52
27	A	801	CL0	C1D-ND	8.30	1.48	1.37
22	4	617	XAT	C19-C9	-7.82	1.34	1.50
21	G	201	CLA	C4B-NB	7.67	1.42	1.35
21	B	838	CLA	C4B-NB	7.66	1.42	1.35
21	F	301	CLA	C4B-NB	7.62	1.42	1.35
21	A	821	CLA	C4B-NB	7.61	1.42	1.35
21	3	607	CLA	C4B-NB	7.60	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	817	CLA	C4B-NB	7.56	1.41	1.35
21	A	813	CLA	C4B-NB	7.54	1.41	1.35
21	B	805	CLA	C4B-NB	7.54	1.41	1.35
21	B	812	CLA	C4B-NB	7.53	1.41	1.35
21	L	302	CLA	C4B-NB	7.53	1.41	1.35
21	A	840	CLA	C4B-NB	7.53	1.41	1.35
21	B	835	CLA	C4B-NB	7.51	1.41	1.35
21	3	610	CLA	C4B-NB	7.51	1.41	1.35
21	3	611	CLA	C4B-NB	7.48	1.41	1.35
21	A	845	CLA	C4B-NB	7.48	1.41	1.35
21	1	611	CLA	C4B-NB	7.48	1.41	1.35
21	A	819	CLA	C4B-NB	7.47	1.41	1.35
21	B	832	CLA	C4B-NB	7.46	1.41	1.35
21	J	101	CLA	C4B-NB	7.45	1.41	1.35
21	4	604	CLA	C4B-NB	7.44	1.41	1.35
21	A	812	CLA	C4B-NB	7.44	1.41	1.35
21	1	610	CLA	C4B-NB	7.43	1.41	1.35
21	K	204	CLA	C4B-NB	7.42	1.41	1.35
21	B	822	CLA	C4B-NB	7.42	1.41	1.35
21	1	613	CLA	C4B-NB	7.41	1.41	1.35
21	A	814	CLA	C4B-NB	7.41	1.41	1.35
21	G	202	CLA	C4B-NB	7.40	1.41	1.35
21	1	612	CLA	C4B-NB	7.40	1.41	1.35
21	A	807	CLA	C4B-NB	7.39	1.41	1.35
21	F	302	CLA	C4B-NB	7.39	1.41	1.35
21	A	836	CLA	C4B-NB	7.38	1.41	1.35
21	K	201	CLA	C4B-NB	7.38	1.41	1.35
21	y	613	CLA	C4B-NB	7.37	1.41	1.35
21	4	601	CLA	C4B-NB	7.37	1.41	1.35
21	x	613	CLA	C4B-NB	7.36	1.41	1.35
21	1	607	CLA	C4B-NB	7.33	1.41	1.35
21	B	823	CLA	C4B-NB	7.33	1.41	1.35
21	1	605	CLA	C4B-NB	7.33	1.41	1.35
21	L	304	CLA	C4B-NB	7.33	1.41	1.35
21	4	611	CLA	C4B-NB	7.33	1.41	1.35
21	H	201	CLA	C4B-NB	7.32	1.41	1.35
21	3	605	CLA	C4B-NB	7.32	1.41	1.35
21	F	303	CLA	C4B-NB	7.32	1.41	1.35
21	K	206	CLA	C4B-NB	7.31	1.41	1.35
21	2	611	CLA	C4B-NB	7.30	1.41	1.35
21	4	614	CLA	C4B-NB	7.30	1.41	1.35
21	3	604	CLA	C4B-NB	7.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	834	CLA	C4B-NB	7.29	1.41	1.35
21	A	844	CLA	C4B-NB	7.29	1.41	1.35
21	3	603	CLA	C4B-NB	7.28	1.41	1.35
21	3	602	CLA	C4B-NB	7.28	1.41	1.35
21	A	810	CLA	C4B-NB	7.28	1.41	1.35
21	B	819	CLA	C4B-NB	7.27	1.41	1.35
21	O	201	CLA	C4B-NB	7.27	1.41	1.35
22	4	617	XAT	C22-C23	-7.26	1.41	1.52
21	A	837	CLA	C4B-NB	7.26	1.41	1.35
21	1	604	CLA	C4B-NB	7.26	1.41	1.35
21	A	830	CLA	C4B-NB	7.26	1.41	1.35
21	B	804	CLA	C4B-NB	7.26	1.41	1.35
21	2	613	CLA	C4B-NB	7.25	1.41	1.35
21	A	824	CLA	C4B-NB	7.25	1.41	1.35
21	A	806	CLA	C4B-NB	7.25	1.41	1.35
21	y	614	CLA	C4B-NB	7.25	1.41	1.35
21	B	820	CLA	C4B-NB	7.24	1.41	1.35
21	B	802	CLA	C4B-NB	7.24	1.41	1.35
21	B	810	CLA	C4B-NB	7.24	1.41	1.35
21	A	833	CLA	C4B-NB	7.24	1.41	1.35
21	B	840	CLA	C4B-NB	7.24	1.41	1.35
21	B	828	CLA	C4B-NB	7.23	1.41	1.35
21	B	841	CLA	C4B-NB	7.23	1.41	1.35
21	z	612	CLA	C4B-NB	7.23	1.41	1.35
21	4	610	CLA	C4B-NB	7.23	1.41	1.35
21	x	614	CLA	C4B-NB	7.23	1.41	1.35
21	B	824	CLA	C4B-NB	7.22	1.41	1.35
21	B	811	CLA	C4B-NB	7.22	1.41	1.35
21	2	610	CLA	C4B-NB	7.21	1.41	1.35
21	A	811	CLA	C4B-NB	7.21	1.41	1.35
21	A	818	CLA	C4B-NB	7.20	1.41	1.35
21	y	612	CLA	C4B-NB	7.20	1.41	1.35
21	z	611	CLA	C4B-NB	7.20	1.41	1.35
21	4	603	CLA	C4B-NB	7.19	1.41	1.35
21	A	834	CLA	C4B-NB	7.18	1.41	1.35
21	A	827	CLA	C4B-NB	7.18	1.41	1.35
21	A	808	CLA	C4B-NB	7.18	1.41	1.35
21	B	807	CLA	C4B-NB	7.18	1.41	1.35
21	A	826	CLA	C4B-NB	7.18	1.41	1.35
21	y	610	CLA	C4B-NB	7.18	1.41	1.35
21	B	836	CLA	C4B-NB	7.17	1.41	1.35
21	4	608	CLA	C4B-NB	7.17	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	803	CLA	C4B-NB	7.17	1.41	1.35
21	A	820	CLA	C4B-NB	7.16	1.41	1.35
21	L	303	CLA	C4B-NB	7.16	1.41	1.35
21	A	832	CLA	C4B-NB	7.16	1.41	1.35
21	3	609	CLA	C4B-NB	7.15	1.41	1.35
21	B	816	CLA	C4B-NB	7.15	1.41	1.35
21	y	603	CLA	C4B-NB	7.15	1.41	1.35
21	B	839	CLA	C4B-NB	7.15	1.41	1.35
21	y	611	CLA	C4B-NB	7.14	1.41	1.35
21	z	614	CLA	C4B-NB	7.14	1.41	1.35
21	A	805	CLA	C4B-NB	7.14	1.41	1.35
21	A	825	CLA	C4B-NB	7.14	1.41	1.35
21	x	604	CLA	C4B-NB	7.14	1.41	1.35
21	A	829	CLA	C4B-NB	7.14	1.41	1.35
21	B	825	CLA	C4B-NB	7.14	1.41	1.35
21	A	831	CLA	C4B-NB	7.14	1.41	1.35
21	B	831	CLA	C4B-NB	7.14	1.41	1.35
21	B	833	CLA	C4B-NB	7.13	1.41	1.35
21	B	813	CLA	C4B-NB	7.13	1.41	1.35
21	B	837	CLA	C4B-NB	7.13	1.41	1.35
21	B	826	CLA	C4B-NB	7.13	1.41	1.35
21	O	202	CLA	C4B-NB	7.12	1.41	1.35
21	G	203	CLA	C4B-NB	7.12	1.41	1.35
21	4	613	CLA	C4B-NB	7.11	1.41	1.35
21	A	816	CLA	C4B-NB	7.10	1.41	1.35
21	2	612	CLA	C4B-NB	7.09	1.41	1.35
21	z	604	CLA	C4B-NB	7.09	1.41	1.35
21	B	829	CLA	C4B-NB	7.08	1.41	1.35
21	B	817	CLA	C4B-NB	7.07	1.41	1.35
21	A	828	CLA	C4B-NB	7.07	1.41	1.35
21	B	827	CLA	C4B-NB	7.07	1.41	1.35
21	A	838	CLA	C4B-NB	7.06	1.41	1.35
21	4	612	CLA	C4B-NB	7.06	1.41	1.35
21	B	830	CLA	C4B-NB	7.05	1.41	1.35
21	A	823	CLA	C4B-NB	7.05	1.41	1.35
21	A	815	CLA	C4B-NB	7.05	1.41	1.35
21	x	611	CLA	C4B-NB	7.04	1.41	1.35
22	4	617	XAT	C22-C21	-7.04	1.43	1.54
21	A	842	CLA	C4B-NB	7.03	1.41	1.35
21	A	822	CLA	C4B-NB	7.03	1.41	1.35
21	B	821	CLA	C4B-NB	7.03	1.41	1.35
21	1	608	CLA	C4B-NB	7.03	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	602	CLA	C4B-NB	7.03	1.41	1.35
22	4	617	XAT	C4-C5	-7.02	1.42	1.52
21	z	603	CLA	C4B-NB	7.02	1.41	1.35
21	1	603	CLA	C4B-NB	7.01	1.41	1.35
21	A	804	CLA	C4B-NB	7.00	1.41	1.35
21	x	612	CLA	C4B-NB	7.00	1.41	1.35
21	K	203	CLA	C4B-NB	6.99	1.41	1.35
21	A	841	CLA	C4B-NB	6.99	1.41	1.35
21	2	608	CLA	C4B-NB	6.99	1.41	1.35
21	y	604	CLA	C4B-NB	6.99	1.41	1.35
21	1	602	CLA	C4B-NB	6.98	1.41	1.35
21	B	809	CLA	C4B-NB	6.98	1.41	1.35
21	z	610	CLA	C4B-NB	6.96	1.41	1.35
21	O	203	CLA	C4B-NB	6.96	1.41	1.35
22	4	617	XAT	C38-C25	-6.95	1.40	1.51
21	A	843	CLA	C4B-NB	6.95	1.41	1.35
21	4	609	CLA	C4B-NB	6.95	1.41	1.35
21	A	839	CLA	C4B-NB	6.93	1.41	1.35
21	3	608	CLA	C4B-NB	6.92	1.41	1.35
21	A	835	CLA	C4B-NB	6.92	1.41	1.35
21	3	612	CLA	C4B-NB	6.91	1.41	1.35
21	A	803	CLA	C4B-NB	6.90	1.41	1.35
21	B	815	CLA	C4B-NB	6.90	1.41	1.35
21	4	602	CLA	C4B-NB	6.88	1.41	1.35
21	z	613	CLA	C4B-NB	6.88	1.41	1.35
21	3	601	CLA	C4B-NB	6.88	1.41	1.35
21	B	808	CLA	C4B-NB	6.87	1.41	1.35
21	B	814	CLA	C4B-NB	6.86	1.41	1.35
21	y	602	CLA	C4B-NB	6.86	1.41	1.35
21	x	603	CLA	C4B-NB	6.84	1.41	1.35
21	2	609	CLA	C4B-NB	6.83	1.41	1.35
21	B	806	CLA	C4B-NB	6.83	1.41	1.35
21	A	802	CLA	C4B-NB	6.82	1.41	1.35
21	2	603	CLA	C4B-NB	6.80	1.41	1.35
21	B	818	CLA	C4B-NB	6.79	1.41	1.35
21	A	809	CLA	C4B-NB	6.77	1.41	1.35
21	x	602	CLA	C4B-NB	6.68	1.41	1.35
21	x	610	CLA	C4B-NB	6.65	1.41	1.35
21	1	609	CLA	C4B-NB	6.61	1.41	1.35
21	z	602	CLA	C4B-NB	6.52	1.41	1.35
21	2	604	CLA	C4B-NB	6.35	1.40	1.35
22	4	617	XAT	C24-C23	-6.34	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	617	XAT	C10-C9	-6.26	1.27	1.35
22	4	617	XAT	C2-C1	-5.95	1.45	1.54
22	4	617	XAT	C40-C33	-5.90	1.38	1.50
22	4	617	XAT	C20-C13	-5.73	1.39	1.50
22	4	617	XAT	C16-C1	-5.42	1.43	1.53
20	z	609	CHL	C3B-C2B	5.34	1.47	1.40
20	y	609	CHL	C3B-C2B	5.32	1.47	1.40
21	2	610	CLA	CHB-C4A	5.28	1.38	1.34
20	z	609	CHL	CHC-C1C	5.26	1.48	1.35
20	y	609	CHL	CHC-C1C	5.26	1.48	1.35
22	4	617	XAT	C37-C21	-5.20	1.43	1.53
20	y	605	CHL	O2D-CGD	5.18	1.45	1.33
20	4	606	CHL	O2D-CGD	5.17	1.45	1.33
20	z	609	CHL	O2D-CGD	5.16	1.45	1.33
20	y	601	CHL	C3B-C2B	5.15	1.47	1.40
20	y	609	CHL	O2D-CGD	5.13	1.45	1.33
20	x	601	CHL	O2D-CGD	5.13	1.45	1.33
25	F	304	BCR	C17-C18	5.11	1.42	1.35
20	z	601	CHL	O2D-CGD	5.11	1.45	1.33
20	y	601	CHL	O2D-CGD	5.11	1.45	1.33
20	x	607	CHL	O2D-CGD	5.11	1.45	1.33
25	F	304	BCR	C21-C22	5.10	1.42	1.35
20	1	606	CHL	CHC-C1C	5.10	1.48	1.35
20	2	606	CHL	O2D-CGD	5.09	1.45	1.33
20	2	615	CHL	O2D-CGD	5.09	1.45	1.33
20	z	605	CHL	O2D-CGD	5.09	1.45	1.33
20	z	606	CHL	O2D-CGD	5.09	1.45	1.33
20	x	601	CHL	C3B-C2B	5.08	1.47	1.40
20	x	606	CHL	O2D-CGD	5.07	1.45	1.33
20	2	605	CHL	O2D-CGD	5.07	1.45	1.33
25	A	853	BCR	C10-C9	5.07	1.42	1.35
20	z	606	CHL	CHC-C1C	5.06	1.47	1.35
20	x	608	CHL	O2D-CGD	5.06	1.45	1.33
20	y	608	CHL	CHC-C1C	5.04	1.47	1.35
20	y	606	CHL	CHC-C1C	5.02	1.47	1.35
20	y	606	CHL	O2D-CGD	5.01	1.45	1.33
20	1	606	CHL	C3B-C2B	5.01	1.47	1.40
20	y	601	CHL	CHC-C1C	5.00	1.47	1.35
20	y	607	CHL	O2D-CGD	5.00	1.45	1.33
20	y	609	CHL	C2C-C3C	4.99	1.47	1.36
22	x	617	XAT	C10-C9	4.99	1.42	1.35
20	z	609	CHL	C2C-C3C	4.97	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	z	608	CHL	O2D-CGD	4.97	1.45	1.33
20	z	607	CHL	O2D-CGD	4.97	1.45	1.33
20	1	601	CHL	CHC-C1C	4.96	1.47	1.35
20	4	607	CHL	O2D-CGD	4.96	1.45	1.33
20	x	601	CHL	CHC-C1C	4.96	1.47	1.35
20	z	601	CHL	CHC-C1C	4.96	1.47	1.35
25	B	845	BCR	C21-C22	4.96	1.42	1.35
20	2	615	CHL	CHC-C1C	4.95	1.47	1.35
20	z	609	CHL	CHD-C1D	4.95	1.48	1.38
20	2	607	CHL	O2D-CGD	4.94	1.45	1.33
20	x	605	CHL	O2D-CGD	4.94	1.45	1.33
22	4	617	XAT	C39-C29	-4.93	1.40	1.50
20	y	609	CHL	CHD-C1D	4.92	1.48	1.38
20	x	607	CHL	C3B-C2B	4.91	1.47	1.40
20	x	609	CHL	CHC-C1C	4.91	1.47	1.35
20	z	601	CHL	C3B-C2B	4.90	1.47	1.40
20	x	606	CHL	CHC-C1C	4.90	1.47	1.35
20	y	605	CHL	C3B-C2B	4.90	1.47	1.40
20	x	608	CHL	CHC-C1C	4.89	1.47	1.35
20	2	607	CHL	C3D-C4D	-4.87	1.33	1.44
20	y	605	CHL	CHC-C1C	4.87	1.47	1.35
20	3	606	CHL	O2D-CGD	4.87	1.45	1.33
20	2	605	CHL	CHC-C1C	4.86	1.47	1.35
20	2	607	CHL	CHC-C1C	4.86	1.47	1.35
20	2	606	CHL	CHC-C1C	4.85	1.47	1.35
22	2	617	XAT	C34-C33	4.84	1.42	1.35
20	4	615	CHL	CHC-C1C	4.83	1.47	1.35
20	z	605	CHL	CHC-C1C	4.83	1.47	1.35
20	y	607	CHL	CHC-C1C	4.83	1.47	1.35
22	y	617	XAT	C30-C29	4.83	1.42	1.35
20	4	606	CHL	CHC-C1C	4.83	1.47	1.35
20	1	601	CHL	C3D-C4D	-4.83	1.33	1.44
20	4	607	CHL	CHC-C1C	4.81	1.47	1.35
20	2	601	CHL	C3D-C4D	-4.81	1.33	1.44
20	x	601	CHL	C2C-C3C	4.81	1.47	1.36
20	x	609	CHL	C3D-C4D	-4.80	1.33	1.44
20	y	608	CHL	O2D-CGD	4.79	1.44	1.33
20	4	607	CHL	C3D-C4D	-4.79	1.33	1.44
20	3	606	CHL	C3D-C4D	-4.79	1.33	1.44
20	4	605	CHL	CHC-C1C	4.79	1.47	1.35
25	A	850	BCR	C14-C13	4.79	1.42	1.35
20	y	607	CHL	C3D-C4D	-4.78	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	850	BCR	C17-C18	4.78	1.42	1.35
20	y	601	CHL	C2C-C3C	4.78	1.47	1.36
20	z	605	CHL	C3D-C4D	-4.78	1.33	1.44
20	x	605	CHL	CHC-C1C	4.77	1.47	1.35
20	y	608	CHL	C3D-C4D	-4.77	1.33	1.44
20	x	605	CHL	C3D-C4D	-4.77	1.33	1.44
20	z	609	CHL	C3D-C4D	-4.77	1.33	1.44
20	1	606	CHL	C2C-C3C	4.77	1.47	1.36
20	z	607	CHL	CHC-C1C	4.77	1.47	1.35
20	z	608	CHL	C3D-C4D	-4.76	1.33	1.44
24	3	613	LUT	C10-C9	4.76	1.42	1.35
20	2	605	CHL	C3D-C4D	-4.76	1.33	1.44
20	y	606	CHL	C3D-C4D	-4.75	1.33	1.44
20	4	605	CHL	C3D-C4D	-4.75	1.33	1.44
20	x	607	CHL	CHC-C1C	4.73	1.47	1.35
20	z	608	CHL	CHC-C1C	4.73	1.47	1.35
20	z	607	CHL	C3D-C4D	-4.73	1.33	1.44
20	2	615	CHL	C3D-C4D	-4.72	1.33	1.44
20	y	609	CHL	C3D-C4D	-4.72	1.33	1.44
20	x	607	CHL	C2C-C3C	4.71	1.46	1.36
20	z	606	CHL	C3D-C4D	-4.71	1.33	1.44
20	1	606	CHL	CHD-C1D	4.70	1.47	1.38
20	z	605	CHL	C3B-C2B	4.70	1.46	1.40
20	z	601	CHL	C3D-C4D	-4.70	1.33	1.44
20	z	601	CHL	C2C-C3C	4.70	1.46	1.36
20	2	601	CHL	CHC-C1C	4.69	1.47	1.35
20	4	607	CHL	C3B-C2B	4.69	1.46	1.40
20	x	601	CHL	CHD-C1D	4.68	1.47	1.38
20	2	606	CHL	C3D-C4D	-4.68	1.33	1.44
20	x	607	CHL	C3D-C4D	-4.68	1.33	1.44
20	3	606	CHL	CHC-C1C	4.67	1.47	1.35
22	4	617	XAT	C36-C21	-4.67	1.44	1.53
20	4	605	CHL	O2D-CGD	4.67	1.45	1.30
20	z	601	CHL	CHD-C1D	4.67	1.47	1.38
20	x	608	CHL	C3D-C4D	-4.67	1.33	1.44
20	y	601	CHL	C3D-C4D	-4.66	1.33	1.44
20	2	601	CHL	O2D-CGD	4.66	1.44	1.33
20	x	609	CHL	O2D-CGD	4.66	1.44	1.33
20	1	606	CHL	C3D-C4D	-4.65	1.33	1.44
24	y	615	LUT	C14-C13	4.65	1.41	1.35
20	4	605	CHL	C2C-C3C	4.64	1.46	1.37
20	1	606	CHL	O2D-CGD	4.63	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	x	601	CHL	C3D-C4D	-4.63	1.33	1.44
20	y	605	CHL	C3D-C4D	-4.63	1.33	1.44
20	y	606	CHL	C2C-C3C	4.63	1.46	1.36
20	x	606	CHL	C3D-C4D	-4.62	1.33	1.44
20	4	606	CHL	C3D-C4D	-4.62	1.33	1.44
20	y	601	CHL	CHD-C1D	4.62	1.47	1.38
24	1	616	LUT	C30-C29	4.61	1.41	1.35
20	4	615	CHL	C3D-C4D	-4.61	1.33	1.44
20	y	605	CHL	C2C-C3C	4.60	1.46	1.36
25	A	851	BCR	C21-C22	4.60	1.41	1.35
25	B	801	BCR	C10-C9	4.57	1.41	1.35
20	1	601	CHL	O2D-CGD	4.56	1.45	1.30
20	2	615	CHL	C3B-C2B	4.56	1.46	1.40
20	x	607	CHL	CHD-C1D	4.56	1.47	1.38
20	4	615	CHL	C2C-C3C	4.55	1.46	1.36
25	A	851	BCR	C14-C13	4.54	1.41	1.35
20	4	615	CHL	O2D-CGD	4.54	1.45	1.30
20	4	606	CHL	C3C-C2C	4.54	1.46	1.36
22	4	617	XAT	C30-C29	-4.53	1.29	1.35
20	y	608	CHL	C3B-C2B	4.53	1.46	1.40
20	z	605	CHL	C2C-C3C	4.53	1.46	1.36
20	3	606	CHL	O2A-CGA	4.52	1.46	1.30
20	z	606	CHL	C3B-C2B	4.52	1.46	1.40
25	A	849	BCR	C21-C22	4.51	1.41	1.35
20	2	615	CHL	C2C-C3C	4.51	1.46	1.36
20	1	601	CHL	CHD-C1D	4.51	1.47	1.38
27	A	801	CL0	C3D-C4D	-4.49	1.34	1.44
20	z	606	CHL	C2C-C3C	4.48	1.46	1.36
20	z	606	CHL	CHD-C1D	4.47	1.47	1.38
20	y	606	CHL	O2A-CGA	4.47	1.45	1.30
20	1	601	CHL	C3B-C2B	4.46	1.46	1.40
25	F	304	BCR	C10-C9	4.45	1.41	1.35
25	A	851	BCR	C17-C18	4.44	1.41	1.35
20	4	607	CHL	O2A-CGA	4.43	1.45	1.30
20	z	606	CHL	O2A-CGA	4.43	1.45	1.30
20	x	606	CHL	O2A-CGA	4.43	1.45	1.30
22	2	617	XAT	C14-C13	4.43	1.41	1.35
20	x	609	CHL	O2A-CGA	4.42	1.45	1.30
20	x	608	CHL	C3B-C2B	4.41	1.46	1.40
20	1	601	CHL	C2C-C3C	4.41	1.46	1.36
20	y	605	CHL	CHD-C1D	4.40	1.46	1.38
20	x	609	CHL	C3B-C2B	4.40	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	x	608	CHL	C2C-C3C	4.39	1.46	1.36
20	y	607	CHL	C3B-C2B	4.39	1.46	1.40
20	y	607	CHL	C2C-C3C	4.38	1.46	1.36
20	z	607	CHL	C2C-C3C	4.38	1.46	1.36
20	2	615	CHL	CHD-C1D	4.37	1.46	1.38
25	L	306	BCR	C10-C9	4.36	1.41	1.35
20	y	608	CHL	C2C-C3C	4.35	1.46	1.36
20	z	609	CHL	CHD-C4C	4.35	1.49	1.39
20	x	607	CHL	O2A-CGA	4.35	1.46	1.33
25	F	304	BCR	C14-C13	4.35	1.41	1.35
20	z	605	CHL	CHD-C1D	4.34	1.46	1.38
20	3	606	CHL	C3C-C2C	4.34	1.45	1.36
24	z	615	LUT	C34-C33	4.33	1.41	1.35
20	z	607	CHL	C3B-C2B	4.33	1.46	1.40
20	y	607	CHL	O2A-CGA	4.33	1.46	1.33
20	2	606	CHL	C3B-C2B	4.32	1.46	1.40
20	2	605	CHL	C2C-C3C	4.32	1.46	1.37
20	2	606	CHL	CHD-C1D	4.32	1.46	1.38
25	A	851	BCR	C10-C9	4.31	1.41	1.35
20	2	606	CHL	C2C-C3C	4.31	1.46	1.36
20	y	609	CHL	CHD-C4C	4.30	1.49	1.39
20	4	607	CHL	C2C-C3C	4.30	1.46	1.36
20	y	601	CHL	O2A-CGA	4.30	1.45	1.33
20	y	606	CHL	C3B-C2B	4.30	1.46	1.40
20	x	605	CHL	C2C-C3C	4.30	1.46	1.36
20	x	601	CHL	O2A-CGA	4.29	1.45	1.33
20	z	601	CHL	O2A-CGA	4.29	1.45	1.33
20	z	609	CHL	O2A-CGA	4.29	1.45	1.33
20	4	605	CHL	CHD-C1D	4.29	1.46	1.38
20	y	606	CHL	CHD-C1D	4.28	1.46	1.38
25	L	306	BCR	C17-C18	4.27	1.41	1.35
22	4	617	XAT	C18-C5	-4.27	1.45	1.51
20	2	607	CHL	C2C-C3C	4.27	1.45	1.36
25	B	846	BCR	C10-C9	4.27	1.41	1.35
20	y	607	CHL	CHD-C1D	4.27	1.46	1.38
20	z	608	CHL	O2A-CGA	4.27	1.45	1.33
20	4	605	CHL	C3B-C2B	4.26	1.46	1.40
23	1	615	LHG	O8-C23	4.26	1.45	1.33
24	z	615	LUT	C14-C13	4.26	1.41	1.35
20	2	601	CHL	C3B-C2B	4.26	1.46	1.40
20	z	607	CHL	O2A-CGA	4.25	1.45	1.33
25	A	849	BCR	C17-C18	4.25	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	849	BCR	C14-C13	4.25	1.41	1.35
20	x	609	CHL	C2C-C3C	4.25	1.45	1.36
24	2	616	LUT	C34-C33	4.25	1.41	1.35
20	y	608	CHL	O2A-CGA	4.24	1.45	1.33
20	x	608	CHL	CHD-C1D	4.24	1.46	1.38
20	2	607	CHL	O2A-CGA	4.23	1.45	1.33
20	y	608	CHL	CHD-C1D	4.23	1.46	1.38
25	A	853	BCR	C21-C22	4.23	1.41	1.35
20	x	605	CHL	O2A-CGA	4.22	1.45	1.33
25	A	848	BCR	C14-C13	4.22	1.41	1.35
20	1	606	CHL	CHD-C4C	4.22	1.48	1.39
20	x	601	CHL	CHD-C4C	4.22	1.48	1.39
25	A	848	BCR	C21-C22	4.22	1.41	1.35
20	4	615	CHL	CHD-C1D	4.21	1.46	1.38
25	L	301	BCR	C17-C18	4.21	1.41	1.35
20	z	605	CHL	C3A-C2A	-4.21	1.50	1.54
25	B	843	BCR	C21-C22	4.20	1.41	1.35
20	x	609	CHL	CHD-C1D	4.20	1.46	1.38
22	y	617	XAT	C10-C9	4.20	1.41	1.35
20	z	608	CHL	C2C-C3C	4.20	1.45	1.36
20	4	606	CHL	CHD-C1D	4.20	1.46	1.38
25	K	205	BCR	C21-C22	4.20	1.41	1.35
22	2	617	XAT	C10-C9	4.20	1.41	1.35
25	K	202	BCR	C21-C22	4.19	1.41	1.35
20	2	605	CHL	CHD-C1D	4.19	1.46	1.38
30	B	850	DGD	O1G-C1A	4.18	1.45	1.33
27	A	801	CL0	C3C-C2C	4.18	1.45	1.36
24	1	616	LUT	C10-C9	4.18	1.41	1.35
20	x	606	CHL	C3B-C2B	4.18	1.46	1.40
24	1	616	LUT	C14-C13	4.18	1.41	1.35
25	B	801	BCR	C17-C18	4.18	1.41	1.35
25	B	846	BCR	C17-C18	4.18	1.41	1.35
25	A	852	BCR	C17-C18	4.18	1.41	1.35
24	y	616	LUT	C34-C33	4.17	1.41	1.35
20	1	601	CHL	O2A-CGA	4.17	1.45	1.33
25	J	102	BCR	C10-C9	4.17	1.41	1.35
25	K	202	BCR	C10-C9	4.17	1.41	1.35
20	x	606	CHL	C2C-C3C	4.17	1.45	1.36
25	A	853	BCR	C17-C18	4.16	1.41	1.35
25	B	844	BCR	C10-C9	4.16	1.41	1.35
25	L	305	BCR	C21-C22	4.16	1.41	1.35
20	2	601	CHL	C2C-C3C	4.16	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	102	BCR	C21-C22	4.16	1.41	1.35
25	B	849	BCR	C10-C9	4.16	1.41	1.35
20	y	609	CHL	O2A-CGA	4.15	1.45	1.33
20	z	607	CHL	CHD-C1D	4.15	1.46	1.38
27	A	801	CL0	O2A-CGA	4.15	1.45	1.33
24	x	616	LUT	C10-C9	4.15	1.41	1.35
25	B	845	BCR	C10-C9	4.14	1.41	1.35
20	x	608	CHL	C3A-C2A	-4.14	1.50	1.54
20	3	606	CHL	C3B-C2B	4.14	1.46	1.40
24	2	619	LUT	C30-C29	4.14	1.41	1.35
24	2	616	LUT	C10-C9	4.14	1.41	1.35
25	J	102	BCR	C17-C18	4.14	1.41	1.35
25	A	852	BCR	C21-C22	4.13	1.41	1.35
25	L	301	BCR	C10-C9	4.13	1.41	1.35
25	L	301	BCR	C14-C13	4.12	1.41	1.35
25	B	843	BCR	C14-C13	4.12	1.41	1.35
25	B	843	BCR	C17-C18	4.12	1.41	1.35
22	x	617	XAT	C30-C29	4.11	1.41	1.35
25	L	306	BCR	C21-C22	4.11	1.41	1.35
25	B	844	BCR	C14-C13	4.11	1.41	1.35
25	L	305	BCR	C14-C13	4.11	1.41	1.35
20	2	607	CHL	C3B-C2B	4.11	1.46	1.40
24	y	616	LUT	C30-C29	4.11	1.41	1.35
24	3	613	LUT	C34-C33	4.10	1.41	1.35
20	x	605	CHL	C3B-C2B	4.10	1.46	1.40
25	B	844	BCR	C21-C22	4.09	1.41	1.35
24	z	616	LUT	C30-C29	4.09	1.41	1.35
24	2	619	LUT	C14-C13	4.09	1.41	1.35
25	A	848	BCR	C17-C18	4.09	1.41	1.35
25	B	845	BCR	C17-C18	4.09	1.41	1.35
30	B	850	DGD	O2G-C1B	4.09	1.45	1.34
20	z	601	CHL	CHD-C4C	4.08	1.48	1.39
20	2	607	CHL	CHD-C1D	4.08	1.46	1.38
25	B	846	BCR	C14-C13	4.08	1.41	1.35
25	L	301	BCR	C21-C22	4.08	1.41	1.35
31	y	618	NEX	C14-C13	4.08	1.41	1.35
23	1	615	LHG	O7-C7	4.08	1.45	1.34
24	2	619	LUT	C10-C9	4.08	1.41	1.35
20	4	607	CHL	CHD-C1D	4.08	1.46	1.38
25	B	849	BCR	C17-C18	4.08	1.41	1.35
25	L	306	BCR	C14-C13	4.07	1.41	1.35
25	J	102	BCR	C14-C13	4.07	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	z	615	LUT	C10-C9	4.07	1.41	1.35
20	z	608	CHL	CHD-C1D	4.07	1.46	1.38
25	B	801	BCR	C14-C13	4.06	1.41	1.35
20	z	606	CHL	CHD-C4C	4.06	1.48	1.39
24	4	616	LUT	C34-C33	4.06	1.41	1.35
25	A	853	BCR	C14-C13	4.06	1.41	1.35
25	I	101	BCR	C14-C13	4.06	1.41	1.35
22	2	617	XAT	C30-C29	4.05	1.41	1.35
20	3	606	CHL	CHD-C1D	4.05	1.46	1.38
25	A	849	BCR	C14-C13	4.05	1.41	1.35
25	L	305	BCR	C10-C9	4.05	1.41	1.35
20	2	601	CHL	CHD-C1D	4.05	1.46	1.38
25	G	204	BCR	C17-C18	4.04	1.41	1.35
20	1	601	CHL	CHD-C4C	4.04	1.48	1.39
22	x	617	XAT	C14-C13	4.04	1.41	1.35
20	z	608	CHL	C3B-C2B	4.04	1.46	1.40
24	y	615	LUT	C10-C9	4.04	1.41	1.35
20	y	601	CHL	CHD-C4C	4.04	1.48	1.39
25	O	204	BCR	C10-C9	4.03	1.41	1.35
25	B	848	BCR	C14-C13	4.03	1.41	1.35
22	4	617	XAT	C17-C1	-4.03	1.45	1.53
22	y	617	XAT	C14-C13	4.02	1.41	1.35
25	A	848	BCR	C10-C9	4.02	1.41	1.35
24	2	619	LUT	C34-C33	4.01	1.41	1.35
24	x	615	LUT	C14-C13	4.01	1.41	1.35
20	2	605	CHL	C3B-C2B	4.01	1.45	1.40
31	z	618	NEX	C30-C29	4.01	1.41	1.35
20	y	605	CHL	C3A-C2A	-4.01	1.50	1.54
24	x	616	LUT	C14-C13	4.00	1.41	1.35
20	x	607	CHL	CHD-C4C	4.00	1.48	1.39
22	x	617	XAT	C34-C33	4.00	1.41	1.35
25	B	847	BCR	C10-C9	4.00	1.41	1.35
25	B	846	BCR	C21-C22	4.00	1.41	1.35
25	A	850	BCR	C21-C22	4.00	1.41	1.35
25	B	801	BCR	C21-C22	4.00	1.41	1.35
20	4	605	CHL	CHD-C4C	3.99	1.48	1.39
25	G	204	BCR	C21-C22	3.99	1.41	1.35
24	z	616	LUT	C14-C13	3.99	1.41	1.35
25	A	852	BCR	C14-C13	3.99	1.41	1.35
25	K	202	BCR	C14-C13	3.98	1.41	1.35
20	x	605	CHL	CHD-C1D	3.98	1.46	1.38
31	x	618	NEX	C30-C29	3.97	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	601	CHL	O2A-CGA	3.97	1.45	1.33
25	I	101	BCR	C17-C18	3.97	1.41	1.35
25	K	205	BCR	C14-C13	3.97	1.41	1.35
20	4	606	CHL	CHD-C4C	3.96	1.48	1.39
22	y	617	XAT	C34-C33	3.96	1.41	1.35
25	A	852	BCR	C10-C9	3.96	1.41	1.35
25	L	305	BCR	C17-C18	3.96	1.41	1.35
25	G	204	BCR	C14-C13	3.96	1.41	1.35
31	z	618	NEX	C14-C13	3.96	1.41	1.35
24	y	615	LUT	C30-C29	3.96	1.41	1.35
25	4	618	BCR	C17-C18	3.96	1.41	1.35
25	O	204	BCR	C17-C18	3.96	1.41	1.35
25	4	618	BCR	C14-C13	3.94	1.41	1.35
20	y	605	CHL	CHD-C4C	3.94	1.48	1.39
21	2	611	CLA	C1D-ND	3.94	1.42	1.37
21	F	303	CLA	C1D-ND	3.94	1.42	1.37
25	3	614	BCR	C21-C22	3.93	1.41	1.35
25	A	849	BCR	C10-C9	3.93	1.41	1.35
24	y	616	LUT	C14-C13	3.92	1.41	1.35
20	y	606	CHL	CHD-C4C	3.92	1.48	1.39
22	z	617	XAT	C14-C13	3.91	1.41	1.35
25	B	849	BCR	C21-C22	3.91	1.41	1.35
25	3	614	BCR	C17-C18	3.91	1.41	1.35
20	4	615	CHL	CHD-C4C	3.90	1.48	1.39
22	4	617	XAT	O23-C23	-3.90	1.31	1.43
25	3	614	BCR	C14-C13	3.90	1.41	1.35
20	x	606	CHL	CHD-C1D	3.90	1.46	1.38
25	4	618	BCR	C10-C9	3.90	1.41	1.35
25	K	205	BCR	C10-C9	3.90	1.40	1.35
20	y	607	CHL	CHD-C4C	3.89	1.48	1.39
20	z	605	CHL	CHD-C4C	3.89	1.48	1.39
25	B	844	BCR	C17-C18	3.89	1.40	1.35
25	3	614	BCR	C10-C9	3.88	1.40	1.35
25	O	205	BCR	C14-C13	3.88	1.40	1.35
25	B	847	BCR	C21-C22	3.88	1.40	1.35
25	4	618	BCR	C21-C22	3.88	1.40	1.35
25	K	202	BCR	C17-C18	3.88	1.40	1.35
25	B	843	BCR	C10-C9	3.88	1.40	1.35
20	y	608	CHL	CHD-C4C	3.87	1.48	1.39
24	1	616	LUT	C34-C33	3.87	1.40	1.35
21	A	817	CLA	C1D-ND	3.87	1.42	1.37
25	O	204	BCR	C14-C13	3.87	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	801	CL0	C3B-C2B	3.87	1.45	1.40
24	z	616	LUT	C10-C9	3.87	1.40	1.35
25	O	204	BCR	C21-C22	3.87	1.40	1.35
21	A	845	CLA	C1D-ND	3.86	1.42	1.37
20	x	609	CHL	CHD-C4C	3.86	1.48	1.39
24	x	616	LUT	C30-C29	3.86	1.40	1.35
21	G	201	CLA	C1D-ND	3.86	1.42	1.37
25	B	847	BCR	C14-C13	3.86	1.40	1.35
20	2	605	CHL	CHD-C4C	3.85	1.48	1.39
24	z	615	LUT	C30-C29	3.85	1.40	1.35
20	x	608	CHL	CHD-C4C	3.85	1.48	1.39
20	2	615	CHL	CHD-C4C	3.85	1.48	1.39
24	3	613	LUT	C30-C29	3.85	1.40	1.35
31	x	618	NEX	C14-C13	3.85	1.40	1.35
20	2	606	CHL	CHD-C4C	3.85	1.48	1.39
24	z	616	LUT	C34-C33	3.84	1.40	1.35
25	B	845	BCR	C14-C13	3.84	1.40	1.35
24	4	616	LUT	C30-C29	3.84	1.40	1.35
24	x	615	LUT	C34-C33	3.84	1.40	1.35
25	B	848	BCR	C17-C18	3.84	1.40	1.35
21	1	604	CLA	C1D-ND	3.84	1.42	1.37
21	L	304	CLA	C1D-ND	3.84	1.42	1.37
25	I	101	BCR	C10-C9	3.84	1.40	1.35
24	4	616	LUT	C14-C13	3.83	1.40	1.35
21	3	610	CLA	C1D-ND	3.83	1.42	1.37
21	1	605	CLA	C1D-ND	3.83	1.42	1.37
21	O	201	CLA	C1D-ND	3.83	1.42	1.37
24	x	616	LUT	C34-C33	3.82	1.40	1.35
25	O	205	BCR	C17-C18	3.82	1.40	1.35
21	J	101	CLA	C1D-ND	3.82	1.42	1.37
20	z	607	CHL	CHD-C4C	3.82	1.47	1.39
25	A	850	BCR	C10-C9	3.81	1.40	1.35
25	O	205	BCR	C21-C22	3.81	1.40	1.35
25	I	101	BCR	C21-C22	3.81	1.40	1.35
25	B	848	BCR	C10-C9	3.80	1.40	1.35
21	3	603	CLA	C1D-ND	3.80	1.42	1.37
20	4	607	CHL	CHD-C4C	3.79	1.47	1.39
21	A	828	CLA	C1D-ND	3.79	1.42	1.37
21	B	834	CLA	C1D-ND	3.79	1.42	1.37
21	2	604	CLA	C1D-ND	3.79	1.42	1.37
25	K	205	BCR	C17-C18	3.79	1.40	1.35
21	K	201	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	204	BCR	C10-C9	3.78	1.40	1.35
24	x	615	LUT	C10-C9	3.78	1.40	1.35
31	z	618	NEX	C34-C33	3.78	1.40	1.35
20	3	606	CHL	CHD-C4C	3.77	1.47	1.39
21	1	612	CLA	C1D-ND	3.77	1.42	1.37
21	B	822	CLA	C1D-ND	3.77	1.42	1.37
21	F	302	CLA	C1D-ND	3.76	1.42	1.37
21	1	610	CLA	C1D-ND	3.76	1.42	1.37
21	A	840	CLA	C1D-ND	3.76	1.42	1.37
24	x	615	LUT	C30-C29	3.75	1.40	1.35
22	z	617	XAT	C34-C33	3.75	1.40	1.35
31	y	618	NEX	C34-C33	3.75	1.40	1.35
25	B	847	BCR	C17-C18	3.75	1.40	1.35
20	4	605	CHL	OBD-CAD	3.75	1.28	1.22
21	A	811	CLA	C1D-ND	3.74	1.42	1.37
21	A	833	CLA	C1D-ND	3.74	1.42	1.37
21	A	823	CLA	C1D-ND	3.74	1.42	1.37
31	x	618	NEX	C34-C33	3.74	1.40	1.35
21	3	611	CLA	C1D-ND	3.73	1.42	1.37
20	z	605	CHL	OBD-CAD	3.73	1.28	1.22
21	A	839	CLA	C1D-ND	3.73	1.42	1.37
22	z	617	XAT	C10-C9	3.73	1.40	1.35
21	B	837	CLA	C1D-ND	3.72	1.42	1.37
21	G	203	CLA	C1D-ND	3.72	1.42	1.37
21	y	614	CLA	C1D-ND	3.71	1.42	1.37
20	x	605	CHL	CHD-C4C	3.71	1.47	1.39
21	B	824	CLA	C1D-ND	3.71	1.42	1.37
24	y	616	LUT	C10-C9	3.71	1.40	1.35
20	2	607	CHL	CHD-C4C	3.71	1.47	1.39
21	A	831	CLA	C1D-ND	3.71	1.42	1.37
21	4	601	CLA	C1D-ND	3.70	1.42	1.37
24	2	616	LUT	C14-C13	3.70	1.40	1.35
21	B	841	CLA	C1D-ND	3.70	1.42	1.37
20	2	601	CHL	CHD-C4C	3.70	1.47	1.39
21	A	820	CLA	C1D-ND	3.70	1.42	1.37
20	2	606	CHL	OBD-CAD	3.70	1.28	1.22
21	4	604	CLA	C1D-ND	3.70	1.42	1.37
21	F	301	CLA	C1D-ND	3.70	1.42	1.37
21	B	835	CLA	C1D-ND	3.69	1.42	1.37
20	z	601	CHL	OBD-CAD	3.69	1.28	1.22
21	A	807	CLA	C1D-ND	3.69	1.42	1.37
24	2	616	LUT	C30-C29	3.69	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	608	CLA	C1D-ND	3.69	1.42	1.37
20	z	608	CHL	CHD-C4C	3.69	1.47	1.39
20	4	606	CHL	OBD-CAD	3.69	1.28	1.22
21	B	830	CLA	C1D-ND	3.69	1.42	1.37
21	K	204	CLA	C1D-ND	3.69	1.42	1.37
20	x	608	CHL	OBD-CAD	3.69	1.28	1.22
21	x	602	CLA	C1D-ND	3.68	1.42	1.37
21	A	808	CLA	C1D-ND	3.68	1.42	1.37
21	A	838	CLA	C1D-ND	3.68	1.42	1.37
27	A	801	CL0	CHC-C1C	3.68	1.44	1.35
21	x	614	CLA	C1D-ND	3.68	1.42	1.37
21	A	819	CLA	C1D-ND	3.67	1.42	1.37
21	3	609	CLA	C1D-ND	3.67	1.42	1.37
21	B	827	CLA	C1D-ND	3.67	1.42	1.37
21	O	203	CLA	CAB-C3B	-3.67	1.44	1.51
21	A	813	CLA	C1D-ND	3.67	1.42	1.37
25	B	848	BCR	C21-C22	3.67	1.40	1.35
20	x	606	CHL	CHD-C4C	3.67	1.47	1.39
21	A	821	CLA	C1D-ND	3.67	1.42	1.37
21	A	837	CLA	C1D-ND	3.66	1.42	1.37
21	B	836	CLA	C1D-ND	3.66	1.42	1.37
21	A	832	CLA	C1D-ND	3.66	1.42	1.37
21	A	826	CLA	C1D-ND	3.65	1.42	1.37
24	4	616	LUT	C10-C9	3.65	1.40	1.35
21	1	607	CLA	C1D-ND	3.65	1.42	1.37
20	z	608	CHL	OBD-CAD	3.65	1.28	1.22
21	z	604	CLA	C1D-ND	3.65	1.42	1.37
21	A	825	CLA	C1D-ND	3.65	1.42	1.37
21	A	805	CLA	C1D-ND	3.65	1.42	1.37
21	A	816	CLA	C1D-ND	3.65	1.42	1.37
21	B	804	CLA	C1D-ND	3.65	1.42	1.37
21	1	602	CLA	C1D-ND	3.65	1.42	1.37
20	y	605	CHL	OBD-CAD	3.64	1.28	1.22
21	4	610	CLA	C1D-ND	3.64	1.42	1.37
21	y	611	CLA	C1D-ND	3.64	1.42	1.37
21	A	829	CLA	C1D-ND	3.64	1.42	1.37
21	1	608	CLA	CAB-C3B	-3.64	1.44	1.51
21	B	812	CLA	C1D-ND	3.64	1.42	1.37
22	z	617	XAT	C30-C29	3.64	1.40	1.35
21	1	609	CLA	C4D-ND	-3.64	1.32	1.37
20	x	601	CHL	OBD-CAD	3.64	1.28	1.22
21	A	822	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	820	CLA	C1D-ND	3.63	1.42	1.37
21	G	202	CLA	C1D-ND	3.63	1.42	1.37
24	y	615	LUT	C34-C33	3.63	1.40	1.35
21	4	612	CLA	C1D-ND	3.63	1.42	1.37
21	4	604	CLA	CAB-C3B	-3.63	1.44	1.51
21	B	821	CLA	C1D-ND	3.62	1.42	1.37
21	B	833	CLA	C1D-ND	3.62	1.42	1.37
21	A	812	CLA	C1D-ND	3.62	1.42	1.37
21	A	815	CLA	C1D-ND	3.62	1.42	1.37
21	B	817	CLA	C1D-ND	3.62	1.42	1.37
20	z	609	CHL	OBD-CAD	3.62	1.28	1.22
21	y	612	CLA	C1D-ND	3.62	1.42	1.37
21	B	813	CLA	C1D-ND	3.62	1.42	1.37
21	4	608	CLA	C1D-ND	3.62	1.42	1.37
21	1	611	CLA	C1D-ND	3.62	1.42	1.37
21	A	827	CLA	C1D-ND	3.61	1.42	1.37
21	B	839	CLA	C1D-ND	3.61	1.42	1.37
31	y	618	NEX	C30-C29	3.61	1.40	1.35
21	K	203	CLA	C1D-ND	3.61	1.42	1.37
21	B	819	CLA	C1D-ND	3.61	1.42	1.37
21	K	206	CLA	C1D-ND	3.61	1.42	1.37
20	x	607	CHL	OBD-CAD	3.61	1.28	1.22
21	1	613	CLA	CAB-C3B	-3.61	1.44	1.51
21	2	610	CLA	CAB-C3B	-3.61	1.44	1.51
21	L	302	CLA	C1D-ND	3.61	1.42	1.37
21	B	815	CLA	C1D-ND	3.60	1.42	1.37
20	1	606	CHL	OBD-CAD	3.60	1.28	1.22
21	B	806	CLA	C1D-ND	3.60	1.42	1.37
21	1	613	CLA	C1D-ND	3.60	1.42	1.37
21	H	201	CLA	C1D-ND	3.60	1.42	1.37
24	3	613	LUT	C14-C13	3.60	1.40	1.35
21	x	613	CLA	C1D-ND	3.60	1.42	1.37
20	y	608	CHL	OBD-CAD	3.59	1.28	1.22
21	3	605	CLA	C1D-ND	3.59	1.42	1.37
21	A	824	CLA	C1D-ND	3.59	1.42	1.37
21	B	807	CLA	C1D-ND	3.59	1.42	1.37
21	B	805	CLA	C1D-ND	3.59	1.42	1.37
21	B	826	CLA	C1D-ND	3.59	1.42	1.37
21	4	603	CLA	C1D-ND	3.59	1.42	1.37
21	4	611	CLA	C1D-ND	3.59	1.42	1.37
21	B	823	CLA	C1D-ND	3.59	1.42	1.37
21	B	814	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	613	CLA	C1D-ND	3.59	1.42	1.37
21	B	810	CLA	C1D-ND	3.59	1.42	1.37
21	y	604	CLA	C1D-ND	3.59	1.42	1.37
25	O	205	BCR	C10-C9	3.59	1.40	1.35
21	2	613	CLA	C1D-ND	3.59	1.42	1.37
21	B	818	CLA	C1D-ND	3.59	1.42	1.37
21	y	610	CLA	C1D-ND	3.59	1.42	1.37
21	4	603	CLA	CAB-C3B	-3.58	1.44	1.51
21	B	831	CLA	C1D-ND	3.58	1.42	1.37
21	A	834	CLA	C1D-ND	3.58	1.42	1.37
21	4	614	CLA	C1D-ND	3.58	1.42	1.37
21	1	610	CLA	CAB-C3B	-3.58	1.44	1.51
21	y	613	CLA	C1D-ND	3.58	1.42	1.37
21	A	802	CLA	C1D-ND	3.57	1.42	1.37
21	A	806	CLA	C1D-ND	3.57	1.42	1.37
20	2	601	CHL	OBD-CAD	3.57	1.28	1.22
21	B	803	CLA	C1D-ND	3.57	1.42	1.37
21	z	603	CLA	C1D-ND	3.57	1.42	1.37
21	A	814	CLA	C1D-ND	3.57	1.42	1.37
21	B	829	CLA	C1D-ND	3.57	1.42	1.37
20	4	615	CHL	OBD-CAD	3.57	1.28	1.22
21	A	804	CLA	C1D-ND	3.57	1.42	1.37
20	y	606	CHL	OBD-CAD	3.57	1.28	1.22
21	3	602	CLA	C1D-ND	3.57	1.42	1.37
21	B	825	CLA	C1D-ND	3.57	1.42	1.37
20	y	609	CHL	OBD-CAD	3.57	1.28	1.22
20	1	601	CHL	OBD-CAD	3.57	1.28	1.22
20	2	605	CHL	OBD-CAD	3.57	1.28	1.22
21	x	603	CLA	C1D-ND	3.56	1.42	1.37
21	3	601	CLA	C1D-ND	3.56	1.42	1.37
21	z	613	CLA	C1D-ND	3.56	1.42	1.37
21	3	605	CLA	CAB-C3B	-3.56	1.44	1.51
21	O	203	CLA	C1D-ND	3.56	1.42	1.37
21	A	836	CLA	C1D-ND	3.55	1.42	1.37
21	y	603	CLA	C1D-ND	3.55	1.42	1.37
21	B	811	CLA	CAB-C3B	-3.55	1.44	1.51
20	x	605	CHL	OBD-CAD	3.55	1.28	1.22
21	A	844	CLA	C1D-ND	3.55	1.42	1.37
21	O	202	CLA	C1D-ND	3.54	1.42	1.37
21	2	610	CLA	C1D-ND	3.54	1.42	1.37
21	x	604	CLA	C1D-ND	3.54	1.42	1.37
21	3	607	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	615	CHL	OBD-CAD	3.54	1.28	1.22
21	B	840	CLA	C1D-ND	3.54	1.42	1.37
21	A	830	CLA	C1D-ND	3.53	1.42	1.37
21	4	602	CLA	C1D-ND	3.53	1.42	1.37
21	B	838	CLA	C1D-ND	3.53	1.42	1.37
21	A	835	CLA	C1D-ND	3.53	1.42	1.37
21	A	843	CLA	C1D-ND	3.52	1.42	1.37
20	z	607	CHL	OBD-CAD	3.52	1.28	1.22
21	1	603	CLA	C1D-ND	3.52	1.42	1.37
21	B	816	CLA	C1D-ND	3.51	1.42	1.37
21	L	303	CLA	C1D-ND	3.51	1.42	1.37
20	y	607	CHL	OBD-CAD	3.51	1.28	1.22
21	x	610	CLA	C1D-ND	3.51	1.42	1.37
20	3	606	CHL	OBD-CAD	3.51	1.28	1.22
20	x	609	CHL	OBD-CAD	3.50	1.28	1.22
21	y	602	CLA	C1D-ND	3.50	1.42	1.37
20	z	606	CHL	OBD-CAD	3.50	1.28	1.22
21	3	604	CLA	C1D-ND	3.49	1.42	1.37
21	B	832	CLA	C1D-ND	3.49	1.42	1.37
21	x	612	CLA	C1D-ND	3.49	1.42	1.37
21	2	602	CLA	C1D-ND	3.49	1.42	1.37
21	A	810	CLA	C1D-ND	3.49	1.42	1.37
21	z	614	CLA	C1D-ND	3.48	1.42	1.37
20	y	601	CHL	OBD-CAD	3.48	1.28	1.22
21	B	809	CLA	C1D-ND	3.48	1.42	1.37
21	z	612	CLA	C1D-ND	3.47	1.42	1.37
21	A	818	CLA	C1D-ND	3.47	1.42	1.37
20	2	607	CHL	OBD-CAD	3.46	1.28	1.22
21	A	803	CLA	C1D-ND	3.46	1.42	1.37
21	4	609	CLA	C1D-ND	3.45	1.42	1.37
21	A	809	CLA	C1D-ND	3.45	1.42	1.37
20	x	606	CHL	OBD-CAD	3.44	1.28	1.22
21	2	608	CLA	C1D-ND	3.44	1.42	1.37
21	B	811	CLA	C1D-ND	3.44	1.42	1.37
20	4	607	CHL	OBD-CAD	3.44	1.28	1.22
21	A	841	CLA	C1D-ND	3.44	1.42	1.37
21	B	808	CLA	C1D-ND	3.43	1.42	1.37
21	A	842	CLA	C1D-ND	3.43	1.42	1.37
21	3	612	CLA	C1D-ND	3.43	1.42	1.37
21	z	602	CLA	C1D-ND	3.43	1.42	1.37
21	2	603	CLA	C1D-ND	3.42	1.42	1.37
21	z	610	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	612	CLA	C1D-ND	3.40	1.42	1.37
21	2	609	CLA	C1D-ND	3.40	1.42	1.37
20	1	606	CHL	C3A-C2A	-3.40	1.51	1.54
21	x	611	CLA	C1D-ND	3.38	1.41	1.37
21	3	608	CLA	C4D-ND	-3.36	1.33	1.37
21	z	602	CLA	C4D-ND	-3.35	1.33	1.37
31	y	618	NEX	C10-C9	3.33	1.40	1.35
31	z	618	NEX	C10-C9	3.32	1.40	1.35
20	y	609	CHL	C3D-C2D	3.29	1.48	1.39
22	4	617	XAT	O3-C3	-3.29	1.33	1.43
21	x	610	CLA	C4D-ND	-3.28	1.33	1.37
21	z	611	CLA	C1D-ND	3.28	1.41	1.37
21	3	608	CLA	CHC-C1C	3.27	1.43	1.35
21	3	608	CLA	C1D-ND	3.26	1.41	1.37
21	2	604	CLA	C4D-ND	-3.26	1.33	1.37
21	B	828	CLA	C1D-ND	3.26	1.41	1.37
20	y	609	CHL	C1D-C2D	3.26	1.51	1.45
21	B	802	CLA	C1D-ND	3.25	1.41	1.37
21	K	204	CLA	C4D-ND	-3.25	1.33	1.37
21	B	826	CLA	C4D-ND	-3.24	1.33	1.37
21	B	829	CLA	C4D-ND	-3.23	1.33	1.37
20	z	609	CHL	C1D-C2D	3.23	1.51	1.45
21	x	603	CLA	C4D-ND	-3.21	1.33	1.37
21	B	838	CLA	C4D-ND	-3.21	1.33	1.37
21	4	609	CLA	CHC-C1C	3.20	1.43	1.35
20	1	606	CHL	C3D-C2D	3.20	1.47	1.39
21	1	605	CLA	CHC-C1C	3.19	1.43	1.35
21	A	803	CLA	C4D-ND	-3.19	1.33	1.37
21	B	816	CLA	CHC-C1C	3.19	1.43	1.35
21	B	836	CLA	C4D-ND	-3.19	1.33	1.37
21	B	822	CLA	CHC-C1C	3.18	1.43	1.35
20	1	606	CHL	C1D-C2D	3.18	1.51	1.45
21	A	814	CLA	CHC-C1C	3.18	1.43	1.35
21	3	605	CLA	C4D-ND	-3.17	1.33	1.37
21	4	609	CLA	C4D-ND	-3.17	1.33	1.37
21	A	812	CLA	CHC-C1C	3.17	1.43	1.35
21	A	828	CLA	CHC-C1C	3.17	1.43	1.35
20	y	601	CHL	C3D-C2D	3.17	1.47	1.39
21	y	603	CLA	C4D-ND	-3.17	1.33	1.37
21	B	806	CLA	C4D-ND	-3.17	1.33	1.37
21	A	824	CLA	C4D-ND	-3.17	1.33	1.37
21	A	844	CLA	CHC-C1C	3.16	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	610	CLA	C4D-ND	-3.16	1.33	1.37
21	1	604	CLA	CHC-C1C	3.16	1.43	1.35
21	B	823	CLA	CHC-C1C	3.16	1.43	1.35
21	A	808	CLA	CHC-C1C	3.16	1.43	1.35
20	z	609	CHL	C3D-C2D	3.16	1.47	1.39
21	A	842	CLA	C4D-ND	-3.16	1.33	1.37
21	B	817	CLA	C4D-ND	-3.15	1.33	1.37
21	z	613	CLA	C4D-ND	-3.15	1.33	1.37
21	B	836	CLA	CHC-C1C	3.15	1.43	1.35
21	A	819	CLA	CHC-C1C	3.15	1.43	1.35
21	G	203	CLA	CHC-C1C	3.15	1.43	1.35
21	B	835	CLA	CHC-C1C	3.15	1.43	1.35
21	A	810	CLA	C4D-ND	-3.14	1.33	1.37
21	2	602	CLA	CHC-C1C	3.14	1.43	1.35
21	2	602	CLA	C4D-ND	-3.14	1.33	1.37
21	A	844	CLA	C4D-ND	-3.14	1.33	1.37
21	B	826	CLA	CHC-C1C	3.14	1.43	1.35
21	2	613	CLA	C4D-ND	-3.14	1.33	1.37
21	A	805	CLA	CHC-C1C	3.14	1.43	1.35
21	y	602	CLA	C4D-ND	-3.14	1.33	1.37
21	O	202	CLA	C4D-ND	-3.13	1.33	1.37
21	K	203	CLA	C4D-ND	-3.13	1.33	1.37
21	z	612	CLA	C4D-ND	-3.13	1.33	1.37
21	z	610	CLA	C4D-ND	-3.13	1.33	1.37
21	B	821	CLA	CHC-C1C	3.13	1.43	1.35
21	2	611	CLA	CHC-C1C	3.13	1.43	1.35
21	L	302	CLA	CHC-C1C	3.13	1.43	1.35
21	2	603	CLA	C4D-ND	-3.13	1.33	1.37
21	A	806	CLA	CHC-C1C	3.13	1.43	1.35
21	B	830	CLA	CHC-C1C	3.13	1.43	1.35
20	x	601	CHL	C3D-C2D	3.13	1.47	1.39
21	A	822	CLA	CHC-C1C	3.13	1.43	1.35
21	A	820	CLA	CHC-C1C	3.12	1.43	1.35
21	x	612	CLA	C4D-ND	-3.12	1.33	1.37
21	3	603	CLA	C4D-ND	-3.12	1.33	1.37
21	2	613	CLA	CHC-C1C	3.12	1.43	1.35
21	A	833	CLA	CHC-C1C	3.12	1.43	1.35
21	J	101	CLA	CHC-C1C	3.12	1.43	1.35
21	y	610	CLA	C4D-ND	-3.12	1.33	1.37
21	y	611	CLA	CHC-C1C	3.12	1.43	1.35
21	L	304	CLA	CHC-C1C	3.12	1.43	1.35
21	1	612	CLA	C4D-ND	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	y	610	CLA	CHC-C1C	3.12	1.43	1.35
21	B	805	CLA	CHC-C1C	3.12	1.43	1.35
21	y	612	CLA	CHC-C1C	3.12	1.43	1.35
21	z	611	CLA	C4D-ND	-3.12	1.33	1.37
21	B	804	CLA	CHC-C1C	3.12	1.43	1.35
21	B	824	CLA	C4D-ND	-3.12	1.33	1.37
21	A	843	CLA	C4D-ND	-3.11	1.33	1.37
21	4	610	CLA	CHC-C1C	3.11	1.42	1.35
21	F	301	CLA	CHC-C1C	3.11	1.42	1.35
21	A	815	CLA	CHC-C1C	3.11	1.42	1.35
21	B	829	CLA	CHC-C1C	3.11	1.42	1.35
21	G	201	CLA	CHC-C1C	3.11	1.42	1.35
21	3	605	CLA	CHC-C1C	3.11	1.42	1.35
21	O	203	CLA	C4D-ND	-3.11	1.33	1.37
21	A	845	CLA	CHC-C1C	3.11	1.42	1.35
21	y	613	CLA	CHC-C1C	3.11	1.42	1.35
21	4	602	CLA	CHC-C1C	3.10	1.42	1.35
21	A	831	CLA	CHC-C1C	3.10	1.42	1.35
21	A	834	CLA	C4D-ND	-3.10	1.33	1.37
21	L	303	CLA	CHC-C1C	3.10	1.42	1.35
21	B	811	CLA	CHC-C1C	3.10	1.42	1.35
21	1	611	CLA	CHC-C1C	3.10	1.42	1.35
21	A	838	CLA	CHC-C1C	3.10	1.42	1.35
21	B	815	CLA	CHC-C1C	3.10	1.42	1.35
21	1	610	CLA	CHC-C1C	3.10	1.42	1.35
21	2	612	CLA	C4D-ND	-3.10	1.33	1.37
21	B	825	CLA	CHC-C1C	3.10	1.42	1.35
21	B	833	CLA	CHC-C1C	3.09	1.42	1.35
20	z	601	CHL	C3D-C2D	3.09	1.47	1.39
21	3	607	CLA	C4D-ND	-3.09	1.33	1.37
21	A	811	CLA	CHC-C1C	3.09	1.42	1.35
21	2	608	CLA	C4D-ND	-3.09	1.33	1.37
21	3	611	CLA	CHC-C1C	3.09	1.42	1.35
21	B	813	CLA	CHC-C1C	3.09	1.42	1.35
21	2	609	CLA	C4D-ND	-3.09	1.33	1.37
21	A	823	CLA	CHC-C1C	3.09	1.42	1.35
21	B	834	CLA	CHC-C1C	3.09	1.42	1.35
21	B	816	CLA	C4D-ND	-3.09	1.33	1.37
21	y	602	CLA	CHC-C1C	3.09	1.42	1.35
21	A	824	CLA	CHC-C1C	3.09	1.42	1.35
21	z	604	CLA	CHC-C1C	3.09	1.42	1.35
21	A	837	CLA	CHC-C1C	3.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	828	CLA	CHC-C1C	3.08	1.42	1.35
21	B	838	CLA	CHC-C1C	3.08	1.42	1.35
21	O	202	CLA	CHC-C1C	3.08	1.42	1.35
21	K	201	CLA	CHC-C1C	3.08	1.42	1.35
21	4	602	CLA	C4D-ND	-3.08	1.33	1.37
21	A	828	CLA	C4D-ND	-3.08	1.33	1.37
21	A	827	CLA	CHC-C1C	3.08	1.42	1.35
21	B	837	CLA	CHC-C1C	3.08	1.42	1.35
21	B	821	CLA	C4D-ND	-3.08	1.33	1.37
21	A	809	CLA	CHC-C1C	3.08	1.42	1.35
21	A	829	CLA	CHC-C1C	3.08	1.42	1.35
21	4	604	CLA	C4D-ND	-3.08	1.33	1.37
21	B	839	CLA	C4D-ND	-3.08	1.33	1.37
21	x	614	CLA	CHC-C1C	3.08	1.42	1.35
21	x	602	CLA	C4D-ND	-3.08	1.33	1.37
21	K	206	CLA	CHC-C1C	3.07	1.42	1.35
21	z	602	CLA	CHC-C1C	3.07	1.42	1.35
21	A	816	CLA	CHC-C1C	3.07	1.42	1.35
21	A	834	CLA	CHC-C1C	3.07	1.42	1.35
21	K	201	CLA	C4D-ND	-3.07	1.33	1.37
21	y	611	CLA	C4D-ND	-3.07	1.33	1.37
21	A	830	CLA	CHC-C1C	3.07	1.42	1.35
21	A	813	CLA	CHC-C1C	3.07	1.42	1.35
20	x	607	CHL	C3D-C2D	3.07	1.47	1.39
21	B	830	CLA	C4D-ND	-3.07	1.33	1.37
25	B	845	BCR	C23-C22	-3.07	1.39	1.45
21	2	609	CLA	CHC-C1C	3.06	1.42	1.35
21	A	825	CLA	CHC-C1C	3.06	1.42	1.35
21	4	603	CLA	C4D-ND	-3.06	1.33	1.37
21	B	808	CLA	C4D-ND	-3.06	1.33	1.37
21	B	807	CLA	CHC-C1C	3.06	1.42	1.35
21	B	817	CLA	CHC-C1C	3.06	1.42	1.35
21	z	614	CLA	CHC-C1C	3.06	1.42	1.35
21	B	814	CLA	C4D-ND	-3.06	1.33	1.37
21	x	611	CLA	C4D-ND	-3.06	1.33	1.37
21	B	831	CLA	C4D-ND	-3.06	1.33	1.37
21	A	807	CLA	CHC-C1C	3.06	1.42	1.35
21	B	841	CLA	C4D-ND	-3.06	1.33	1.37
21	2	612	CLA	CHC-C1C	3.06	1.42	1.35
21	A	827	CLA	C4D-ND	-3.06	1.33	1.37
21	3	607	CLA	CHC-C1C	3.06	1.42	1.35
21	4	613	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	812	CLA	CHC-C1C	3.06	1.42	1.35
21	B	818	CLA	C4D-ND	-3.06	1.33	1.37
31	x	618	NEX	C10-C9	3.06	1.39	1.35
21	3	609	CLA	CHC-C1C	3.06	1.42	1.35
21	F	303	CLA	C4D-ND	-3.06	1.33	1.37
21	4	611	CLA	CHC-C1C	3.06	1.42	1.35
21	3	610	CLA	CHC-C1C	3.06	1.42	1.35
21	A	822	CLA	C4D-ND	-3.06	1.33	1.37
21	A	839	CLA	C4D-ND	-3.06	1.33	1.37
21	B	810	CLA	CHC-C1C	3.06	1.42	1.35
21	A	832	CLA	CHC-C1C	3.06	1.42	1.35
21	B	831	CLA	CHC-C1C	3.05	1.42	1.35
21	A	817	CLA	CHC-C1C	3.05	1.42	1.35
21	1	613	CLA	CHC-C1C	3.05	1.42	1.35
21	O	203	CLA	CHC-C1C	3.05	1.42	1.35
21	B	841	CLA	CHC-C1C	3.05	1.42	1.35
21	B	812	CLA	C4D-ND	-3.05	1.33	1.37
21	y	614	CLA	C4D-ND	-3.05	1.33	1.37
21	3	604	CLA	CHC-C1C	3.05	1.42	1.35
21	4	614	CLA	CHC-C1C	3.05	1.42	1.35
21	A	831	CLA	C4D-ND	-3.05	1.33	1.37
21	A	838	CLA	C4D-ND	-3.05	1.33	1.37
21	F	302	CLA	CHC-C1C	3.05	1.42	1.35
21	K	206	CLA	C4D-ND	-3.05	1.33	1.37
21	B	809	CLA	CHC-C1C	3.05	1.42	1.35
21	B	832	CLA	C4D-ND	-3.05	1.33	1.37
21	A	804	CLA	CHC-C1C	3.05	1.42	1.35
21	G	202	CLA	CHC-C1C	3.05	1.42	1.35
21	3	604	CLA	C4D-ND	-3.05	1.33	1.37
21	A	830	CLA	C4D-ND	-3.05	1.33	1.37
21	A	812	CLA	C4D-ND	-3.05	1.33	1.37
20	y	609	CHL	MG-NA	-3.05	1.99	2.06
21	4	604	CLA	CHC-C1C	3.04	1.42	1.35
21	K	204	CLA	CHC-C1C	3.04	1.42	1.35
21	1	602	CLA	C4D-ND	-3.04	1.33	1.37
21	3	601	CLA	C4D-ND	-3.04	1.33	1.37
21	A	821	CLA	CHC-C1C	3.04	1.42	1.35
21	A	829	CLA	C4D-ND	-3.04	1.33	1.37
21	O	201	CLA	CHC-C1C	3.04	1.42	1.35
21	x	604	CLA	CHC-C1C	3.04	1.42	1.35
21	A	806	CLA	C4D-ND	-3.04	1.33	1.37
21	x	612	CLA	CHC-C1C	3.04	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	603	CLA	CHC-C1C	3.04	1.42	1.35
21	B	824	CLA	CHC-C1C	3.04	1.42	1.35
21	B	810	CLA	C4D-ND	-3.04	1.33	1.37
21	B	802	CLA	CHC-C1C	3.04	1.42	1.35
21	1	608	CLA	C4D-ND	-3.04	1.33	1.37
21	B	809	CLA	C4D-ND	-3.04	1.33	1.37
21	A	804	CLA	C4D-ND	-3.04	1.33	1.37
21	x	613	CLA	C4D-ND	-3.04	1.33	1.37
21	B	820	CLA	CHC-C1C	3.03	1.42	1.35
21	A	818	CLA	C4D-ND	-3.03	1.33	1.37
21	z	604	CLA	C4D-ND	-3.03	1.33	1.37
21	y	603	CLA	CHC-C1C	3.03	1.42	1.35
21	z	610	CLA	CHC-C1C	3.03	1.42	1.35
21	A	835	CLA	C4D-ND	-3.03	1.33	1.37
21	4	612	CLA	CHC-C1C	3.03	1.42	1.35
21	B	803	CLA	C4D-ND	-3.03	1.33	1.37
21	2	608	CLA	CHC-C1C	3.03	1.42	1.35
20	x	601	CHL	C1D-C2D	3.03	1.51	1.45
21	1	607	CLA	CHC-C1C	3.03	1.42	1.35
21	L	303	CLA	C4D-ND	-3.03	1.33	1.37
21	A	803	CLA	CHC-C1C	3.03	1.42	1.35
21	A	810	CLA	CHC-C1C	3.03	1.42	1.35
21	B	827	CLA	CHC-C1C	3.03	1.42	1.35
21	x	613	CLA	CHC-C1C	3.03	1.42	1.35
21	A	841	CLA	C4D-ND	-3.03	1.33	1.37
20	y	606	CHL	C1D-C2D	3.03	1.51	1.45
21	A	823	CLA	C4D-ND	-3.03	1.33	1.37
21	4	601	CLA	CHC-C1C	3.03	1.42	1.35
21	4	601	CLA	C4D-ND	-3.03	1.33	1.37
21	y	604	CLA	C4D-ND	-3.03	1.33	1.37
21	4	608	CLA	C4D-ND	-3.03	1.33	1.37
21	A	807	CLA	C4D-ND	-3.03	1.33	1.37
21	B	807	CLA	C4D-ND	-3.03	1.33	1.37
21	K	203	CLA	CHC-C1C	3.02	1.42	1.35
21	1	608	CLA	CHC-C1C	3.02	1.42	1.35
20	z	601	CHL	C1D-C2D	3.02	1.51	1.45
20	z	609	CHL	MG-NA	-3.02	1.99	2.06
21	1	602	CLA	CHC-C1C	3.02	1.42	1.35
21	A	839	CLA	CHC-C1C	3.02	1.42	1.35
21	B	819	CLA	CHC-C1C	3.02	1.42	1.35
21	4	603	CLA	CHC-C1C	3.02	1.42	1.35
21	A	835	CLA	CHC-C1C	3.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	839	CLA	CHC-C1C	3.02	1.42	1.35
21	B	823	CLA	C4D-ND	-3.02	1.33	1.37
21	4	612	CLA	C4D-ND	-3.02	1.33	1.37
21	4	610	CLA	C4D-ND	-3.01	1.33	1.37
21	y	604	CLA	CHC-C1C	3.01	1.42	1.35
21	1	613	CLA	C4D-ND	-3.01	1.33	1.37
21	B	813	CLA	C4D-ND	-3.01	1.33	1.37
21	4	608	CLA	CHC-C1C	3.01	1.42	1.35
21	A	826	CLA	CHC-C1C	3.01	1.42	1.35
21	3	609	CLA	C4D-ND	-3.01	1.33	1.37
20	y	605	CHL	C1D-C2D	3.01	1.51	1.45
21	B	833	CLA	C4D-ND	-3.01	1.33	1.37
21	B	832	CLA	CHC-C1C	3.01	1.42	1.35
21	B	802	CLA	C4D-ND	-3.01	1.33	1.37
21	z	614	CLA	C4D-ND	-3.01	1.33	1.37
21	4	613	CLA	C4D-ND	-3.01	1.33	1.37
21	A	819	CLA	C4D-ND	-3.01	1.33	1.37
21	3	602	CLA	C4D-ND	-3.01	1.33	1.37
21	B	834	CLA	C4D-ND	-3.01	1.33	1.37
21	A	816	CLA	C4D-ND	-3.01	1.33	1.37
21	B	840	CLA	C4D-ND	-3.00	1.33	1.37
21	F	303	CLA	CHC-C1C	3.00	1.42	1.35
21	2	610	CLA	CHC-C1C	3.00	1.42	1.35
21	F	301	CLA	C4D-ND	-3.00	1.33	1.37
21	x	611	CLA	CHC-C1C	3.00	1.42	1.35
21	z	611	CLA	CHC-C1C	3.00	1.42	1.35
21	G	203	CLA	C4D-ND	-3.00	1.33	1.37
21	z	612	CLA	CHC-C1C	3.00	1.42	1.35
21	A	826	CLA	C4D-ND	-3.00	1.33	1.37
21	3	611	CLA	C4D-ND	-3.00	1.33	1.37
21	4	614	CLA	C4D-ND	-3.00	1.33	1.37
21	A	802	CLA	CHC-C1C	3.00	1.42	1.35
21	x	602	CLA	CHC-C1C	3.00	1.42	1.35
21	A	818	CLA	CHC-C1C	3.00	1.42	1.35
21	B	814	CLA	CHC-C1C	2.99	1.42	1.35
21	A	836	CLA	CHC-C1C	2.99	1.42	1.35
21	B	815	CLA	C4D-ND	-2.99	1.33	1.37
21	A	841	CLA	CHC-C1C	2.99	1.42	1.35
21	L	302	CLA	C4D-ND	-2.99	1.33	1.37
21	x	604	CLA	C4D-ND	-2.99	1.33	1.37
21	B	808	CLA	CHC-C1C	2.99	1.42	1.35
21	B	840	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	833	CLA	C4D-ND	-2.99	1.33	1.37
21	H	201	CLA	C4D-ND	-2.99	1.33	1.37
21	A	820	CLA	C4D-ND	-2.99	1.33	1.37
21	1	603	CLA	C4D-ND	-2.99	1.33	1.37
21	x	610	CLA	CHC-C1C	2.99	1.42	1.35
25	B	847	BCR	C23-C22	-2.98	1.39	1.45
21	A	814	CLA	C4D-ND	-2.98	1.33	1.37
21	1	612	CLA	CHC-C1C	2.98	1.42	1.35
21	B	828	CLA	C4D-ND	-2.98	1.33	1.37
21	B	825	CLA	C4D-ND	-2.98	1.33	1.37
21	A	840	CLA	CHC-C1C	2.98	1.42	1.35
21	3	612	CLA	C4D-ND	-2.98	1.33	1.37
21	3	603	CLA	CHC-C1C	2.98	1.42	1.35
20	x	607	CHL	C1D-C2D	2.98	1.51	1.45
21	y	614	CLA	CHC-C1C	2.98	1.42	1.35
21	3	602	CLA	CHC-C1C	2.98	1.42	1.35
21	B	818	CLA	CHC-C1C	2.97	1.42	1.35
21	J	101	CLA	C4D-ND	-2.97	1.33	1.37
21	B	806	CLA	CHC-C1C	2.97	1.42	1.35
21	B	805	CLA	C4D-ND	-2.97	1.33	1.37
21	x	614	CLA	C4D-ND	-2.97	1.33	1.37
21	z	603	CLA	C4D-ND	-2.97	1.33	1.37
25	B	848	BCR	C23-C22	-2.97	1.39	1.45
21	A	837	CLA	C4D-ND	-2.97	1.33	1.37
20	1	601	CHL	C3D-C2D	2.96	1.47	1.39
21	A	805	CLA	C4D-ND	-2.96	1.33	1.37
25	B	849	BCR	C23-C22	-2.96	1.39	1.45
21	H	201	CLA	CHC-C1C	2.96	1.42	1.35
21	1	611	CLA	C4D-ND	-2.96	1.33	1.37
21	B	822	CLA	C4D-ND	-2.96	1.33	1.37
21	z	603	CLA	CHC-C1C	2.96	1.42	1.35
25	4	618	BCR	C23-C22	-2.96	1.39	1.45
21	A	808	CLA	C4D-ND	-2.96	1.33	1.37
21	3	601	CLA	CHC-C1C	2.96	1.42	1.35
20	4	615	CHL	C3D-C2D	2.95	1.47	1.39
21	B	803	CLA	CHC-C1C	2.95	1.42	1.35
21	3	610	CLA	C4D-ND	-2.95	1.33	1.37
21	A	825	CLA	C4D-ND	-2.95	1.33	1.37
21	z	613	CLA	CHC-C1C	2.95	1.42	1.35
21	2	603	CLA	CHC-C1C	2.95	1.42	1.35
20	2	606	CHL	C3D-C2D	2.94	1.47	1.39
21	A	843	CLA	CHC-C1C	2.94	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	827	CLA	C4D-ND	-2.94	1.33	1.37
21	B	837	CLA	C4D-ND	-2.94	1.33	1.37
21	B	811	CLA	C4D-ND	-2.94	1.33	1.37
21	A	842	CLA	CHC-C1C	2.94	1.42	1.35
21	A	821	CLA	C4D-ND	-2.93	1.33	1.37
20	4	606	CHL	C3D-C2D	2.93	1.47	1.39
20	2	615	CHL	C3D-C2D	2.93	1.47	1.39
21	4	611	CLA	C4D-ND	-2.93	1.33	1.37
21	1	610	CLA	C4D-ND	-2.93	1.33	1.37
21	A	817	CLA	C4D-ND	-2.93	1.33	1.37
21	x	603	CLA	CHC-C1C	2.93	1.42	1.35
21	A	836	CLA	C4D-ND	-2.92	1.33	1.37
20	y	605	CHL	C3D-C2D	2.92	1.47	1.39
21	B	820	CLA	C4D-ND	-2.91	1.33	1.37
25	A	852	BCR	C23-C22	-2.91	1.39	1.45
21	B	819	CLA	C4D-ND	-2.91	1.33	1.37
21	A	802	CLA	C4D-ND	-2.91	1.33	1.37
25	I	101	BCR	C23-C22	-2.91	1.39	1.45
21	y	612	CLA	C4D-ND	-2.91	1.33	1.37
21	A	811	CLA	C4D-ND	-2.91	1.33	1.37
20	4	605	CHL	C1D-C2D	2.90	1.51	1.45
21	A	832	CLA	C4D-ND	-2.90	1.33	1.37
20	z	605	CHL	C3D-C2D	2.90	1.47	1.39
21	L	304	CLA	C4D-ND	-2.90	1.33	1.37
25	B	801	BCR	C8-C9	-2.89	1.39	1.45
21	1	604	CLA	C4D-ND	-2.89	1.33	1.37
20	y	601	CHL	MG-NA	-2.89	1.99	2.06
20	3	606	CHL	C3D-C2D	2.89	1.47	1.39
20	x	608	CHL	C3D-C2D	2.89	1.47	1.39
25	3	614	BCR	C23-C22	-2.89	1.39	1.45
27	A	801	CL0	OBD-CAD	2.89	1.28	1.23
25	L	305	BCR	C8-C9	-2.89	1.39	1.45
21	G	202	CLA	C4D-ND	-2.88	1.33	1.37
25	B	847	BCR	C8-C9	-2.88	1.39	1.45
21	A	845	CLA	C4D-ND	-2.88	1.33	1.37
20	z	606	CHL	C3D-C2D	2.87	1.47	1.39
21	B	835	CLA	C4D-ND	-2.87	1.33	1.37
21	A	809	CLA	C4D-ND	-2.87	1.33	1.37
20	x	608	CHL	C1D-C2D	2.87	1.51	1.45
25	B	846	BCR	C23-C22	-2.87	1.39	1.45
21	A	840	CLA	C4D-ND	-2.87	1.33	1.37
24	x	615	LUT	C8-C9	-2.86	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	y	608	CHL	C3D-C2D	2.86	1.46	1.39
21	3	612	CLA	CHC-C1C	2.86	1.42	1.35
20	z	605	CHL	C1D-C2D	2.86	1.51	1.45
21	2	611	CLA	C4D-ND	-2.86	1.33	1.37
21	A	815	CLA	C4D-ND	-2.86	1.33	1.37
21	A	813	CLA	C4D-ND	-2.86	1.33	1.37
25	O	205	BCR	C8-C9	-2.86	1.39	1.45
21	1	605	CLA	C4D-ND	-2.85	1.33	1.37
21	y	613	CLA	C4D-ND	-2.85	1.33	1.37
20	x	609	CHL	C3D-C2D	2.85	1.46	1.39
25	A	850	BCR	C8-C9	-2.85	1.39	1.45
25	4	618	BCR	C8-C9	-2.85	1.39	1.45
20	4	615	CHL	C1D-C2D	2.85	1.50	1.45
27	A	801	CL0	CHD-C1D	2.84	1.43	1.38
21	1	607	CLA	C4D-ND	-2.84	1.33	1.37
20	y	601	CHL	C1D-C2D	2.84	1.50	1.45
25	A	849	BCR	C8-C9	-2.84	1.39	1.45
20	1	601	CHL	C1D-C2D	2.84	1.50	1.45
20	2	606	CHL	C1D-C2D	2.84	1.50	1.45
20	4	605	CHL	C3D-C2D	2.83	1.46	1.39
20	2	605	CHL	C3D-C2D	2.83	1.46	1.39
25	A	850	BCR	C23-C22	-2.82	1.39	1.45
21	F	302	CLA	C4D-ND	-2.82	1.33	1.37
25	B	848	BCR	C8-C9	-2.82	1.39	1.45
20	z	606	CHL	C1D-C2D	2.81	1.50	1.45
25	O	205	BCR	C23-C22	-2.81	1.39	1.45
21	B	804	CLA	C4D-ND	-2.81	1.33	1.37
25	O	204	BCR	C8-C9	-2.81	1.39	1.45
25	A	852	BCR	C8-C9	-2.81	1.39	1.45
21	O	201	CLA	C4D-ND	-2.80	1.33	1.37
25	A	848	BCR	C8-C9	-2.80	1.39	1.45
25	G	204	BCR	C8-C9	-2.80	1.39	1.45
25	L	306	BCR	C23-C22	-2.80	1.39	1.45
20	4	606	CHL	C1D-C2D	2.80	1.50	1.45
20	x	601	CHL	MG-NA	-2.79	1.99	2.06
24	y	616	LUT	C8-C9	-2.79	1.39	1.45
25	A	849	BCR	C23-C22	-2.79	1.40	1.45
25	3	614	BCR	C8-C9	-2.79	1.40	1.45
20	y	607	CHL	C3D-C2D	2.78	1.46	1.39
24	3	613	LUT	C8-C9	-2.78	1.40	1.45
25	K	205	BCR	C8-C9	-2.78	1.40	1.45
24	z	616	LUT	C8-C9	-2.78	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	605	CHL	C1D-C2D	2.78	1.50	1.45
24	y	615	LUT	C8-C9	-2.78	1.40	1.45
20	2	615	CHL	C1D-C2D	2.77	1.50	1.45
21	2	604	CLA	C3B-CAB	-2.77	1.42	1.47
21	A	842	CLA	CMB-C2B	-2.76	1.45	1.51
25	L	306	BCR	C8-C9	-2.76	1.40	1.45
27	A	801	CL0	CHD-C4C	2.76	1.45	1.39
25	G	204	BCR	C23-C22	-2.76	1.40	1.45
25	I	101	BCR	C8-C9	-2.76	1.40	1.45
20	4	607	CHL	C3D-C2D	2.75	1.46	1.39
25	L	301	BCR	C23-C22	-2.75	1.40	1.45
25	B	844	BCR	C8-C9	-2.74	1.40	1.45
25	B	844	BCR	C23-C22	-2.74	1.40	1.45
25	O	204	BCR	C23-C22	-2.74	1.40	1.45
20	2	607	CHL	C3D-C2D	2.74	1.46	1.39
24	1	616	LUT	C8-C9	-2.74	1.40	1.45
20	x	605	CHL	C3D-C2D	2.74	1.46	1.39
20	z	607	CHL	C3D-C2D	2.73	1.46	1.39
21	2	604	CLA	CHC-C1C	2.73	1.42	1.35
20	z	607	CHL	C1D-C2D	2.73	1.50	1.45
24	z	615	LUT	C8-C9	-2.72	1.40	1.45
24	4	616	LUT	C8-C9	-2.72	1.40	1.45
21	G	201	CLA	C4D-ND	-2.71	1.34	1.37
20	z	608	CHL	C3D-C2D	2.71	1.46	1.39
25	K	202	BCR	C8-C9	-2.71	1.40	1.45
20	x	606	CHL	C3D-C2D	2.71	1.46	1.39
25	A	853	BCR	C23-C22	-2.70	1.40	1.45
25	L	305	BCR	C23-C22	-2.70	1.40	1.45
21	B	819	CLA	CMB-C2B	-2.70	1.46	1.51
24	2	616	LUT	C8-C9	-2.69	1.40	1.45
21	3	607	CLA	CMB-C2B	-2.69	1.46	1.51
21	A	836	CLA	CMB-C2B	-2.69	1.46	1.51
21	1	609	CLA	CMD-C2D	-2.68	1.45	1.50
25	J	102	BCR	C23-C22	-2.68	1.40	1.45
20	1	606	CHL	MG-NA	-2.68	1.99	2.06
24	x	616	LUT	C8-C9	-2.68	1.40	1.45
25	A	853	BCR	C8-C9	-2.68	1.40	1.45
21	1	609	CLA	C1D-ND	2.67	1.41	1.37
25	K	205	BCR	C23-C22	-2.67	1.40	1.45
25	B	843	BCR	C23-C22	-2.67	1.40	1.45
25	J	102	BCR	C8-C9	-2.67	1.40	1.45
25	B	846	BCR	C8-C9	-2.66	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	822	CLA	CMB-C2B	-2.66	1.46	1.51
21	4	608	CLA	CMB-C2B	-2.66	1.46	1.51
21	L	302	CLA	CMB-C2B	-2.66	1.46	1.51
25	L	301	BCR	C8-C9	-2.66	1.40	1.45
21	3	602	CLA	CMB-C2B	-2.66	1.46	1.51
21	2	604	CLA	CMB-C2B	-2.66	1.46	1.51
21	A	822	CLA	CMB-C2B	-2.66	1.46	1.51
24	2	619	LUT	C8-C9	-2.65	1.40	1.45
20	2	601	CHL	C3D-C2D	2.65	1.46	1.39
25	B	849	BCR	C8-C9	-2.65	1.40	1.45
25	B	801	BCR	C23-C22	-2.65	1.40	1.45
25	A	848	BCR	C23-C22	-2.64	1.40	1.45
25	B	845	BCR	C8-C9	-2.64	1.40	1.45
20	y	607	CHL	C1D-C2D	2.64	1.50	1.45
25	B	843	BCR	C8-C9	-2.64	1.40	1.45
21	x	604	CLA	CMB-C2B	-2.64	1.46	1.51
21	z	611	CLA	CMB-C2B	-2.64	1.46	1.51
21	4	604	CLA	CMB-C2B	-2.64	1.46	1.51
21	4	613	CLA	CMB-C2B	-2.63	1.46	1.51
21	2	604	CLA	C3B-C2B	-2.63	1.36	1.40
21	B	829	CLA	CMB-C2B	-2.63	1.46	1.51
20	4	607	CHL	C1D-C2D	2.63	1.50	1.45
21	x	603	CLA	CMB-C2B	-2.63	1.46	1.51
21	B	802	CLA	CMB-C2B	-2.62	1.46	1.51
21	z	612	CLA	CMB-C2B	-2.62	1.46	1.51
21	1	612	CLA	CMB-C2B	-2.61	1.46	1.51
20	x	609	CHL	C1D-C2D	2.61	1.50	1.45
20	z	608	CHL	C1D-C2D	2.61	1.50	1.45
20	x	605	CHL	C1D-C2D	2.61	1.50	1.45
25	F	304	BCR	C8-C9	-2.61	1.40	1.45
20	y	608	CHL	MG-NA	-2.60	2.00	2.06
21	1	611	CLA	CMB-C2B	-2.60	1.46	1.51
20	x	606	CHL	C1D-C2D	2.59	1.50	1.45
21	3	604	CLA	CMB-C2B	-2.59	1.46	1.51
20	y	608	CHL	C1D-C2D	2.59	1.50	1.45
21	B	828	CLA	CMB-C2B	-2.59	1.46	1.51
21	A	831	CLA	CMB-C2B	-2.59	1.46	1.51
21	B	809	CLA	CMB-C2B	-2.58	1.46	1.51
20	y	606	CHL	C3D-C2D	2.58	1.46	1.39
21	3	605	CLA	CMB-C2B	-2.58	1.46	1.51
21	B	834	CLA	CMB-C2B	-2.58	1.46	1.51
21	A	806	CLA	CMB-C2B	-2.58	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	z	601	CHL	MG-NA	-2.58	2.00	2.06
21	2	612	CLA	CMB-C2B	-2.58	1.46	1.51
20	2	601	CHL	C1D-C2D	2.57	1.50	1.45
20	3	606	CHL	C1D-C2D	2.57	1.50	1.45
21	4	603	CLA	CMB-C2B	-2.57	1.46	1.51
21	A	810	CLA	CMB-C2B	-2.57	1.46	1.51
21	1	609	CLA	CMB-C2B	-2.57	1.46	1.51
20	1	601	CHL	MG-NA	-2.57	2.00	2.06
20	2	607	CHL	C1D-C2D	2.57	1.50	1.45
21	A	844	CLA	CMB-C2B	-2.57	1.46	1.51
21	2	610	CLA	CMB-C2B	-2.56	1.46	1.51
21	x	612	CLA	CMB-C2B	-2.56	1.46	1.51
21	A	845	CLA	CMB-C2B	-2.56	1.46	1.51
21	A	832	CLA	CMB-C2B	-2.56	1.46	1.51
21	2	613	CLA	CMB-C2B	-2.56	1.46	1.51
21	z	603	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	835	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	839	CLA	CMB-C2B	-2.56	1.46	1.51
21	4	611	CLA	CMB-C2B	-2.56	1.46	1.51
21	y	614	CLA	CMB-C2B	-2.56	1.46	1.51
21	3	611	CLA	CMB-C2B	-2.55	1.46	1.51
21	B	840	CLA	CMB-C2B	-2.55	1.46	1.51
21	x	611	CLA	CMB-C2B	-2.55	1.46	1.51
20	x	607	CHL	C4C-C3C	2.55	1.49	1.45
21	z	604	CLA	CMB-C2B	-2.55	1.46	1.51
21	B	836	CLA	CMB-C2B	-2.55	1.46	1.51
21	B	811	CLA	CMB-C2B	-2.55	1.46	1.51
21	2	603	CLA	C3B-CAB	-2.55	1.42	1.47
21	1	613	CLA	CMB-C2B	-2.54	1.46	1.51
25	A	851	BCR	C8-C9	-2.54	1.40	1.45
21	1	602	CLA	CMB-C2B	-2.54	1.46	1.51
21	L	304	CLA	CMB-C2B	-2.54	1.46	1.51
21	K	204	CLA	CMB-C2B	-2.54	1.46	1.51
21	x	613	CLA	CMB-C2B	-2.54	1.46	1.51
21	y	603	CLA	CMB-C2B	-2.54	1.46	1.51
21	3	609	CLA	CMB-C2B	-2.54	1.46	1.51
21	2	602	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	826	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	803	CLA	CMB-C2B	-2.54	1.46	1.51
21	4	609	CLA	CMB-C2B	-2.54	1.46	1.51
25	K	202	BCR	C23-C22	-2.54	1.40	1.45
21	A	813	CLA	CMB-C2B	-2.53	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	y	613	CLA	CMB-C2B	-2.53	1.46	1.51
21	A	824	CLA	CMB-C2B	-2.53	1.46	1.51
21	B	827	CLA	CMB-C2B	-2.53	1.46	1.51
20	z	609	CHL	C4C-C3C	2.53	1.49	1.45
21	B	838	CLA	CMB-C2B	-2.53	1.46	1.51
21	z	614	CLA	CMB-C2B	-2.53	1.46	1.51
25	A	851	BCR	C23-C22	-2.53	1.40	1.45
21	B	821	CLA	CMB-C2B	-2.53	1.46	1.51
21	O	202	CLA	CMB-C2B	-2.52	1.46	1.51
21	O	203	CLA	CMB-C2B	-2.52	1.46	1.51
21	B	813	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	804	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	802	CLA	CMB-C2B	-2.52	1.46	1.51
21	4	614	CLA	CMB-C2B	-2.52	1.46	1.51
21	y	604	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	827	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	814	CLA	CMB-C2B	-2.52	1.46	1.51
21	1	604	CLA	CMB-C2B	-2.52	1.46	1.51
21	1	603	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	808	CLA	CMB-C2B	-2.52	1.46	1.51
20	z	609	CHL	C4B-CHC	2.52	1.48	1.41
21	1	608	CLA	CMB-C2B	-2.51	1.46	1.51
21	B	803	CLA	CMB-C2B	-2.51	1.46	1.51
21	1	607	CLA	CMB-C2B	-2.51	1.46	1.51
21	B	808	CLA	CMB-C2B	-2.51	1.46	1.51
21	G	202	CLA	CMB-C2B	-2.51	1.46	1.51
21	B	805	CLA	CMB-C2B	-2.51	1.46	1.51
20	y	609	CHL	C4B-CHC	2.51	1.48	1.41
21	1	610	CLA	CMB-C2B	-2.50	1.46	1.51
21	4	601	CLA	CMB-C2B	-2.50	1.46	1.51
21	x	602	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	823	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	820	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	812	CLA	CMB-C2B	-2.50	1.46	1.51
21	y	612	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	837	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	818	CLA	CMB-C2B	-2.50	1.46	1.51
21	2	603	CLA	C3B-C2B	-2.50	1.36	1.40
21	A	838	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	819	CLA	CMB-C2B	-2.50	1.46	1.51
31	y	618	NEX	C12-C13	-2.50	1.40	1.45
21	B	817	CLA	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	605	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	825	CLA	CMB-C2B	-2.50	1.46	1.51
21	K	206	CLA	CMB-C2B	-2.50	1.46	1.51
21	z	613	CLA	CMB-C2B	-2.49	1.46	1.51
21	3	603	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	810	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	830	CLA	CMB-C2B	-2.49	1.46	1.51
31	x	618	NEX	C12-C13	-2.49	1.40	1.45
21	K	203	CLA	CMB-C2B	-2.49	1.46	1.51
21	2	608	CLA	CMB-C2B	-2.49	1.46	1.51
21	z	610	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	840	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	821	CLA	CMB-C2B	-2.49	1.46	1.51
21	F	301	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	826	CLA	CMB-C2B	-2.48	1.46	1.51
21	2	603	CLA	CMB-C2B	-2.48	1.46	1.51
21	A	829	CLA	CMB-C2B	-2.48	1.46	1.51
21	A	817	CLA	CMB-C2B	-2.48	1.46	1.51
21	3	610	CLA	CMB-C2B	-2.48	1.46	1.51
21	4	612	CLA	CMB-C2B	-2.48	1.46	1.51
21	B	825	CLA	CMB-C2B	-2.48	1.46	1.51
21	4	610	CLA	CMB-C2B	-2.48	1.46	1.51
21	y	602	CLA	CMB-C2B	-2.48	1.46	1.51
21	A	843	CLA	CMB-C2B	-2.48	1.46	1.51
20	y	609	CHL	C4C-C3C	2.47	1.49	1.45
21	A	835	CLA	CMB-C2B	-2.47	1.46	1.51
24	x	615	LUT	C12-C13	-2.47	1.40	1.45
21	A	807	CLA	CMB-C2B	-2.47	1.46	1.51
21	A	830	CLA	CMB-C2B	-2.47	1.46	1.51
20	z	601	CHL	C4C-C3C	2.47	1.49	1.45
21	2	609	CLA	CMB-C2B	-2.47	1.46	1.51
21	F	303	CLA	CMB-C2B	-2.47	1.46	1.51
21	A	812	CLA	CMB-C2B	-2.47	1.46	1.51
25	L	305	BCR	C12-C13	-2.47	1.40	1.45
21	y	611	CLA	CMB-C2B	-2.46	1.46	1.51
24	2	616	LUT	C12-C13	-2.46	1.40	1.45
21	A	834	CLA	CMB-C2B	-2.46	1.46	1.51
21	B	818	CLA	CMB-C2B	-2.46	1.46	1.51
24	x	616	LUT	C28-C29	-2.46	1.40	1.45
21	y	610	CLA	CMB-C2B	-2.46	1.46	1.51
21	L	303	CLA	CMB-C2B	-2.45	1.46	1.51
31	y	618	NEX	C28-C29	-2.45	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	608	CLA	CMB-C2B	-2.45	1.46	1.51
21	z	602	CLA	CMB-C2B	-2.45	1.46	1.51
21	4	602	CLA	CMB-C2B	-2.45	1.46	1.51
21	B	832	CLA	CMB-C2B	-2.45	1.46	1.51
21	O	201	CLA	CMB-C2B	-2.45	1.46	1.51
24	x	615	LUT	C32-C33	-2.45	1.40	1.45
21	A	816	CLA	CMB-C2B	-2.44	1.46	1.51
21	G	201	CLA	CMB-C2B	-2.44	1.46	1.51
21	H	201	CLA	CMB-C2B	-2.44	1.46	1.51
21	B	806	CLA	CMB-C2B	-2.44	1.46	1.51
21	3	601	CLA	CMB-C2B	-2.44	1.46	1.51
24	z	616	LUT	C32-C33	-2.44	1.40	1.45
21	B	807	CLA	CMB-C2B	-2.44	1.46	1.51
20	y	609	CHL	C1B-CHB	2.44	1.47	1.41
22	z	617	XAT	C12-C13	-2.43	1.40	1.45
25	I	101	BCR	C12-C13	-2.43	1.40	1.45
25	B	845	BCR	C12-C13	-2.43	1.40	1.45
21	B	815	CLA	CMB-C2B	-2.43	1.46	1.51
20	x	601	CHL	C4C-C3C	2.43	1.49	1.45
21	B	816	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	848	BCR	C12-C13	-2.43	1.40	1.45
20	z	606	CHL	C4B-CHC	2.43	1.47	1.41
21	A	823	CLA	CMB-C2B	-2.43	1.46	1.51
20	x	607	CHL	MG-NA	-2.43	2.00	2.06
25	4	618	BCR	C19-C18	-2.43	1.40	1.45
21	x	610	CLA	CMB-C2B	-2.43	1.46	1.51
27	A	801	CL0	C3D-C2D	2.43	1.45	1.39
21	x	614	CLA	CMB-C2B	-2.43	1.46	1.51
21	B	841	CLA	CMB-C2B	-2.42	1.46	1.51
21	A	805	CLA	CMB-C2B	-2.42	1.46	1.51
20	x	609	CHL	C1D-ND	-2.42	1.34	1.37
21	A	841	CLA	CMB-C2B	-2.42	1.46	1.51
21	2	611	CLA	CMB-C2B	-2.42	1.46	1.51
20	1	606	CHL	C4C-C3C	2.42	1.49	1.45
21	B	820	CLA	CMB-C2B	-2.41	1.46	1.51
25	3	614	BCR	C19-C18	-2.41	1.40	1.45
21	B	804	CLA	CMB-C2B	-2.41	1.46	1.51
21	3	612	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	848	BCR	C19-C18	-2.41	1.40	1.45
24	z	616	LUT	C12-C13	-2.41	1.40	1.45
24	4	616	LUT	C32-C33	-2.41	1.40	1.45
21	A	839	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	609	CLA	CHC-C1C	2.40	1.41	1.35
21	A	828	CLA	CMB-C2B	-2.40	1.46	1.51
24	z	616	LUT	C28-C29	-2.40	1.40	1.45
22	z	617	XAT	C8-C9	-2.40	1.40	1.45
22	4	617	XAT	C24-C25	-2.40	1.48	1.52
21	B	824	CLA	CMB-C2B	-2.40	1.46	1.51
21	B	802	CLA	C3B-C2B	-2.40	1.37	1.40
21	A	809	CLA	CMB-C2B	-2.40	1.46	1.51
21	B	833	CLA	CMB-C2B	-2.39	1.46	1.51
21	J	101	CLA	CMB-C2B	-2.39	1.46	1.51
21	K	201	CLA	CMB-C2B	-2.39	1.46	1.51
25	O	205	BCR	C12-C13	-2.39	1.40	1.45
22	2	617	XAT	C28-C29	-2.39	1.40	1.45
21	A	833	CLA	CMB-C2B	-2.39	1.46	1.51
31	x	618	NEX	C32-C33	-2.39	1.40	1.45
25	B	847	BCR	C12-C13	-2.39	1.40	1.45
24	z	615	LUT	C28-C29	-2.39	1.40	1.45
20	z	609	CHL	C1B-CHB	2.38	1.47	1.41
21	2	609	CLA	CMD-C2D	-2.38	1.45	1.50
21	B	814	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	849	BCR	C19-C18	-2.38	1.40	1.45
20	y	606	CHL	C4B-CHC	2.38	1.47	1.41
24	z	615	LUT	C32-C33	-2.38	1.40	1.45
20	4	606	CHL	C4C-C3C	2.37	1.49	1.45
21	G	203	CLA	CMB-C2B	-2.37	1.46	1.51
20	1	606	CHL	C4B-CHC	2.37	1.47	1.41
20	y	601	CHL	C4B-CHC	2.37	1.47	1.41
25	L	301	BCR	C12-C13	-2.37	1.40	1.45
25	3	614	BCR	C12-C13	-2.37	1.40	1.45
21	A	815	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	847	BCR	C19-C18	-2.36	1.40	1.45
20	1	601	CHL	C4B-CHC	2.36	1.47	1.41
20	2	615	CHL	C4B-CHC	2.36	1.47	1.41
21	B	831	CLA	CMB-C2B	-2.36	1.46	1.51
25	O	205	BCR	C19-C18	-2.36	1.40	1.45
24	4	616	LUT	C12-C13	-2.36	1.40	1.45
22	z	617	XAT	C32-C33	-2.36	1.40	1.45
27	A	801	CL0	C1D-C2D	2.35	1.50	1.45
25	A	850	BCR	C19-C18	-2.35	1.40	1.45
21	B	828	CLA	CMD-C2D	-2.35	1.45	1.50
31	z	618	NEX	C32-C33	-2.35	1.40	1.45
24	3	613	LUT	C12-C13	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	204	BCR	C19-C18	-2.34	1.40	1.45
24	4	616	LUT	C28-C29	-2.34	1.40	1.45
21	F	302	CLA	CMB-C2B	-2.33	1.46	1.51
25	B	801	BCR	C12-C13	-2.33	1.40	1.45
31	y	618	NEX	C32-C33	-2.33	1.40	1.45
25	F	304	BCR	C23-C22	-2.33	1.40	1.45
20	x	609	CHL	MG-NA	-2.33	2.00	2.06
22	z	617	XAT	C28-C29	-2.33	1.40	1.45
20	y	608	CHL	C4B-CHC	2.33	1.47	1.41
20	1	606	CHL	C1B-CHB	2.33	1.47	1.41
21	B	837	CLA	CMB-C2B	-2.33	1.46	1.51
20	z	606	CHL	MG-NA	-2.33	2.00	2.06
21	A	811	CLA	CMB-C2B	-2.32	1.46	1.51
20	2	606	CHL	C4C-C3C	2.32	1.49	1.45
20	2	615	CHL	MG-NA	-2.32	2.00	2.06
24	3	613	LUT	C32-C33	-2.32	1.41	1.45
31	x	618	NEX	C28-C29	-2.32	1.41	1.45
20	y	601	CHL	C4C-C3C	2.32	1.49	1.45
31	z	618	NEX	C28-C29	-2.31	1.41	1.45
25	I	101	BCR	C19-C18	-2.31	1.41	1.45
20	x	606	CHL	C4B-CHC	2.31	1.47	1.41
21	B	802	CLA	CMD-C2D	-2.31	1.45	1.50
24	2	616	LUT	C32-C33	-2.31	1.41	1.45
25	B	801	BCR	C19-C18	-2.30	1.41	1.45
25	B	846	BCR	C19-C18	-2.30	1.41	1.45
24	y	616	LUT	C12-C13	-2.30	1.41	1.45
24	y	616	LUT	C28-C29	-2.30	1.41	1.45
20	2	605	CHL	C4B-CHC	2.30	1.47	1.41
25	O	204	BCR	C12-C13	-2.30	1.41	1.45
21	z	610	CLA	CMD-C2D	-2.30	1.45	1.50
24	1	616	LUT	C12-C13	-2.30	1.41	1.45
24	2	616	LUT	C28-C29	-2.30	1.41	1.45
20	2	607	CHL	C4B-CHC	2.30	1.47	1.41
24	x	616	LUT	C32-C33	-2.29	1.41	1.45
21	2	603	CLA	CMD-C2D	-2.29	1.45	1.50
20	z	605	CHL	C4B-CHC	2.29	1.47	1.41
25	G	204	BCR	C12-C13	-2.29	1.41	1.45
20	1	601	CHL	C1D-ND	-2.28	1.35	1.37
20	z	607	CHL	C4C-C3C	2.28	1.49	1.45
20	y	605	CHL	C4B-CHC	2.28	1.47	1.41
21	z	602	CLA	CMC-C2C	-2.28	1.46	1.50
25	B	849	BCR	C12-C13	-2.28	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	x	608	CHL	C4B-CHC	2.28	1.47	1.41
20	x	601	CHL	C4B-CHC	2.28	1.47	1.41
20	1	601	CHL	C4C-C3C	2.28	1.49	1.45
24	2	619	LUT	C12-C13	-2.28	1.41	1.45
20	x	609	CHL	C4B-CHC	2.28	1.47	1.41
20	z	605	CHL	C4C-C3C	2.28	1.49	1.45
20	y	607	CHL	C4C-C3C	2.28	1.49	1.45
20	x	608	CHL	C4C-C3C	2.27	1.49	1.45
25	B	845	BCR	C19-C18	-2.27	1.41	1.45
25	O	204	BCR	C19-C18	-2.27	1.41	1.45
24	3	613	LUT	C28-C29	-2.27	1.41	1.45
20	x	601	CHL	C1B-CHB	2.27	1.47	1.41
25	4	618	BCR	C12-C13	-2.26	1.41	1.45
25	A	850	BCR	C12-C13	-2.26	1.41	1.45
22	y	617	XAT	C8-C9	-2.26	1.41	1.45
24	2	619	LUT	C32-C33	-2.26	1.41	1.45
20	4	605	CHL	MG-NA	-2.26	2.00	2.06
20	2	606	CHL	C4B-CHC	2.26	1.47	1.41
25	L	305	BCR	C19-C18	-2.26	1.41	1.45
21	4	603	CLA	CMD-C2D	-2.26	1.46	1.50
21	A	803	CLA	C3B-CAB	-2.25	1.43	1.47
21	2	604	CLA	CMD-C2D	-2.25	1.46	1.50
20	3	606	CHL	MG-NA	-2.25	2.00	2.06
20	z	601	CHL	C4B-CHC	2.24	1.47	1.41
25	K	205	BCR	C19-C18	-2.24	1.41	1.45
25	B	844	BCR	C12-C13	-2.24	1.41	1.45
20	z	606	CHL	C4C-C3C	2.24	1.48	1.45
20	y	608	CHL	C1D-ND	-2.24	1.35	1.37
25	J	102	BCR	C12-C13	-2.23	1.41	1.45
20	4	605	CHL	C4B-CHC	2.23	1.47	1.41
21	B	817	CLA	CMC-C2C	-2.23	1.46	1.50
20	2	605	CHL	MG-NA	-2.23	2.01	2.06
21	3	609	CLA	CMD-C2D	-2.22	1.46	1.50
21	1	603	CLA	CMD-C2D	-2.22	1.46	1.50
21	1	608	CLA	CMD-C2D	-2.22	1.46	1.50
20	4	605	CHL	C4C-C3C	2.22	1.48	1.44
25	A	849	BCR	C19-C18	-2.22	1.41	1.45
24	x	616	LUT	C12-C13	-2.22	1.41	1.45
21	z	603	CLA	CMD-C2D	-2.22	1.46	1.50
20	4	615	CHL	MG-NA	-2.22	2.01	2.06
21	O	203	CLA	CMD-C2D	-2.22	1.46	1.50
25	A	848	BCR	C12-C13	-2.22	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	x	607	CHL	C4B-CHC	2.22	1.47	1.41
21	y	603	CLA	CMD-C2D	-2.22	1.46	1.50
21	2	613	CLA	CMD-C2D	-2.22	1.46	1.50
20	z	605	CHL	MG-NA	-2.21	2.01	2.06
20	y	601	CHL	C1D-ND	-2.21	1.35	1.37
21	x	603	CLA	CMD-C2D	-2.21	1.46	1.50
20	z	607	CHL	C4B-CHC	2.21	1.47	1.41
25	A	852	BCR	C19-C18	-2.21	1.41	1.45
25	A	849	BCR	C12-C13	-2.21	1.41	1.45
31	z	618	NEX	C12-C13	-2.21	1.41	1.45
20	y	601	CHL	C1B-CHB	2.20	1.47	1.41
21	3	612	CLA	CMD-C2D	-2.20	1.46	1.50
20	x	607	CHL	C1B-CHB	2.20	1.47	1.41
21	2	602	CLA	CMD-C2D	-2.20	1.46	1.50
21	B	803	CLA	CMC-C2C	-2.20	1.46	1.50
20	x	608	CHL	MG-NA	-2.20	2.01	2.06
22	x	617	XAT	C32-C33	-2.20	1.41	1.45
21	A	830	CLA	CMD-C2D	-2.20	1.46	1.50
21	1	605	CLA	CMD-C2D	-2.20	1.46	1.50
20	y	605	CHL	MG-NA	-2.19	2.01	2.06
24	x	615	LUT	C28-C29	-2.19	1.41	1.45
21	A	810	CLA	CMD-C2D	-2.19	1.46	1.50
25	B	843	BCR	C12-C13	-2.19	1.41	1.45
20	z	608	CHL	C4B-CHC	2.19	1.47	1.41
21	2	611	CLA	CMD-C2D	-2.19	1.46	1.50
25	K	202	BCR	C19-C18	-2.19	1.41	1.45
20	y	607	CHL	C4B-CHC	2.19	1.47	1.41
22	2	617	XAT	C32-C33	-2.19	1.41	1.45
21	z	614	CLA	CMD-C2D	-2.19	1.46	1.50
24	y	615	LUT	C32-C33	-2.18	1.41	1.45
20	4	615	CHL	C4B-CHC	2.18	1.47	1.41
20	4	615	CHL	C4C-C3C	2.18	1.48	1.45
21	z	611	CLA	CMD-C2D	-2.18	1.46	1.50
21	x	602	CLA	CMD-C2D	-2.18	1.46	1.50
25	A	853	BCR	C19-C18	-2.18	1.41	1.45
20	x	605	CHL	C4B-CHC	2.17	1.47	1.41
21	4	613	CLA	CMD-C2D	-2.17	1.46	1.50
21	1	609	CLA	MG-ND	-2.17	2.01	2.05
21	A	835	CLA	C3B-CAB	-2.17	1.43	1.47
20	4	607	CHL	C4B-CHC	2.17	1.47	1.41
20	z	609	CHL	C1D-ND	-2.17	1.35	1.37
21	A	844	CLA	C3B-CAB	-2.17	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	z	602	CLA	CMD-C2D	-2.17	1.46	1.50
21	3	608	CLA	CMD-C2D	-2.17	1.46	1.50
20	z	608	CHL	C1D-ND	-2.17	1.35	1.37
20	x	601	CHL	C1D-ND	-2.17	1.35	1.37
21	3	602	CLA	CMD-C2D	-2.17	1.46	1.50
21	z	612	CLA	CMD-C2D	-2.16	1.46	1.50
21	2	609	CLA	CMC-C2C	-2.16	1.46	1.50
21	B	813	CLA	CMC-C2C	-2.16	1.46	1.50
20	2	606	CHL	MG-NA	-2.16	2.01	2.06
21	B	808	CLA	CMD-C2D	-2.16	1.46	1.50
21	2	612	CLA	CMD-C2D	-2.16	1.46	1.50
21	z	613	CLA	CMD-C2D	-2.16	1.46	1.50
21	1	607	CLA	CMD-C2D	-2.16	1.46	1.50
21	3	607	CLA	CMD-C2D	-2.16	1.46	1.50
21	B	829	CLA	CMD-C2D	-2.16	1.46	1.50
24	y	616	LUT	C32-C33	-2.16	1.41	1.45
21	x	611	CLA	CMD-C2D	-2.16	1.46	1.50
20	y	609	CHL	C1D-ND	-2.16	1.35	1.37
21	A	814	CLA	CMD-C2D	-2.16	1.46	1.50
20	2	601	CHL	C4B-CHC	2.16	1.47	1.41
21	O	202	CLA	CMD-C2D	-2.16	1.46	1.50
22	2	617	XAT	C12-C13	-2.16	1.41	1.45
21	z	614	CLA	C3B-C2B	-2.15	1.37	1.40
21	B	834	CLA	CMD-C2D	-2.15	1.46	1.50
25	L	301	BCR	C20-C19	2.15	1.40	1.34
20	y	606	CHL	MG-NA	-2.15	2.01	2.06
21	4	601	CLA	CMD-C2D	-2.15	1.46	1.50
21	B	833	CLA	CMD-C2D	-2.15	1.46	1.50
24	2	619	LUT	C28-C29	-2.15	1.41	1.45
20	4	606	CHL	MG-NA	-2.15	2.01	2.06
21	3	601	CLA	CMD-C2D	-2.15	1.46	1.50
20	z	601	CHL	C1B-CHB	2.15	1.47	1.41
21	y	603	CLA	CMC-C2C	-2.14	1.46	1.50
21	x	613	CLA	CMD-C2D	-2.14	1.46	1.50
21	4	611	CLA	CMD-C2D	-2.14	1.46	1.50
20	x	605	CHL	MG-NA	-2.14	2.01	2.06
21	4	602	CLA	CMD-C2D	-2.14	1.46	1.50
21	A	803	CLA	CMD-C2D	-2.14	1.46	1.50
22	x	617	XAT	C28-C29	-2.14	1.41	1.45
21	A	842	CLA	CMD-C2D	-2.14	1.46	1.50
21	y	604	CLA	CMD-C2D	-2.14	1.46	1.50
21	y	610	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	202	BCR	C12-C13	-2.14	1.41	1.45
21	A	835	CLA	C3B-C2B	-2.14	1.37	1.40
20	y	606	CHL	C4C-C3C	2.14	1.48	1.45
22	y	617	XAT	C28-C29	-2.14	1.41	1.45
21	B	832	CLA	C3B-C2B	-2.14	1.37	1.40
21	B	814	CLA	CMD-C2D	-2.14	1.46	1.50
24	y	615	LUT	C12-C13	-2.14	1.41	1.45
21	2	610	CLA	CMD-C2D	-2.13	1.46	1.50
21	A	839	CLA	CMD-C2D	-2.13	1.46	1.50
21	x	610	CLA	CMC-C2C	-2.13	1.46	1.50
25	A	848	BCR	C19-C18	-2.13	1.41	1.45
21	A	835	CLA	CMD-C2D	-2.13	1.46	1.50
20	4	607	CHL	C1D-ND	-2.13	1.35	1.37
27	A	801	CL0	MG-NC	2.13	2.11	2.06
21	3	601	CLA	CMC-C2C	-2.13	1.46	1.50
20	3	606	CHL	C1D-ND	-2.13	1.35	1.37
22	x	617	XAT	C8-C9	-2.13	1.41	1.45
21	2	608	CLA	CMD-C2D	-2.13	1.46	1.50
21	B	823	CLA	CMD-C2D	-2.13	1.46	1.50
21	z	610	CLA	CMC-C2C	-2.13	1.46	1.50
20	x	609	CHL	C4C-C3C	2.13	1.48	1.45
21	A	812	CLA	CMD-C2D	-2.13	1.46	1.50
25	B	844	BCR	C20-C19	2.13	1.40	1.34
21	x	610	CLA	CMD-C2D	-2.13	1.46	1.50
21	B	822	CLA	C3B-C2B	-2.13	1.37	1.40
21	y	602	CLA	CMD-C2D	-2.12	1.46	1.50
21	4	610	CLA	CMD-C2D	-2.12	1.46	1.50
20	2	605	CHL	C4C-C3C	2.12	1.48	1.44
20	y	605	CHL	C4C-C3C	2.12	1.48	1.45
21	A	809	CLA	CMD-C2D	-2.12	1.46	1.50
21	G	202	CLA	CMD-C2D	-2.12	1.46	1.50
21	y	612	CLA	CMD-C2D	-2.12	1.46	1.50
22	4	617	XAT	C35-C15	-2.12	1.30	1.36
21	y	614	CLA	CMD-C2D	-2.12	1.46	1.50
20	z	601	CHL	C1D-ND	-2.12	1.35	1.37
21	A	806	CLA	CMD-C2D	-2.12	1.46	1.50
21	A	814	CLA	CMC-C2C	-2.12	1.46	1.50
21	A	806	CLA	CMC-C2C	-2.12	1.46	1.50
21	1	610	CLA	CMD-C2D	-2.12	1.46	1.50
21	B	840	CLA	C3B-C2B	-2.12	1.37	1.40
21	B	810	CLA	CMD-C2D	-2.12	1.46	1.50
21	z	604	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	808	CLA	CMC-C2C	-2.12	1.46	1.50
25	A	852	BCR	C11-C12	2.11	1.40	1.34
21	4	608	CLA	CMD-C2D	-2.11	1.46	1.50
25	B	843	BCR	C19-C18	-2.11	1.41	1.45
21	B	803	CLA	C3B-CAB	-2.11	1.43	1.47
21	K	201	CLA	CBD-CAD	2.11	1.56	1.51
21	A	819	CLA	CMC-C2C	-2.11	1.46	1.50
20	3	606	CHL	C4B-CHC	2.11	1.46	1.41
21	A	814	CLA	C3B-C2B	-2.11	1.37	1.40
20	z	606	CHL	C1D-ND	-2.11	1.35	1.37
21	A	836	CLA	CMD-C2D	-2.11	1.46	1.50
21	x	604	CLA	CMD-C2D	-2.11	1.46	1.50
20	x	609	CHL	C1B-CHB	2.11	1.46	1.41
24	z	615	LUT	C12-C13	-2.11	1.41	1.45
21	4	612	CLA	CMD-C2D	-2.11	1.46	1.50
22	y	617	XAT	C12-C13	-2.11	1.41	1.45
20	4	606	CHL	C4B-CHC	2.11	1.46	1.41
22	x	617	XAT	C12-C13	-2.11	1.41	1.45
21	A	843	CLA	CMD-C2D	-2.11	1.46	1.50
21	1	609	CLA	C4B-CHC	-2.10	1.35	1.41
21	x	603	CLA	CMC-C2C	-2.10	1.46	1.50
25	A	853	BCR	C12-C13	-2.10	1.41	1.45
21	A	818	CLA	CMC-C2C	-2.10	1.46	1.50
21	B	840	CLA	CMD-C2D	-2.10	1.46	1.50
25	B	846	BCR	C12-C13	-2.10	1.41	1.45
20	1	601	CHL	C1B-CHB	2.10	1.46	1.41
21	B	815	CLA	CMD-C2D	-2.10	1.46	1.50
20	z	608	CHL	C4C-C3C	2.10	1.48	1.45
20	4	607	CHL	MG-NA	-2.10	2.01	2.06
21	1	602	CLA	CMD-C2D	-2.10	1.46	1.50
21	A	824	CLA	CMD-C2D	-2.10	1.46	1.50
21	B	820	CLA	CMD-C2D	-2.10	1.46	1.50
21	L	302	CLA	C3B-C2B	-2.10	1.37	1.40
21	A	821	CLA	CMD-C2D	-2.10	1.46	1.50
21	H	201	CLA	CMD-C2D	-2.09	1.46	1.50
21	1	613	CLA	CMD-C2D	-2.09	1.46	1.50
21	4	609	CLA	C3B-C2B	-2.09	1.37	1.40
22	y	617	XAT	C32-C33	-2.09	1.41	1.45
21	A	802	CLA	CMD-C2D	-2.09	1.46	1.50
21	z	611	CLA	CMC-C2C	-2.09	1.46	1.50
21	4	609	CLA	CMC-C2C	-2.09	1.46	1.50
21	A	837	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	841	CLA	CMD-C2D	-2.09	1.46	1.50
21	z	602	CLA	C3B-CAB	-2.09	1.43	1.47
21	B	805	CLA	CMD-C2D	-2.09	1.46	1.50
21	B	809	CLA	CMD-C2D	-2.09	1.46	1.50
20	2	606	CHL	C1D-ND	-2.09	1.35	1.37
21	A	819	CLA	CMD-C2D	-2.09	1.46	1.50
25	L	306	BCR	C12-C13	-2.09	1.41	1.45
21	F	302	CLA	CMD-C2D	-2.09	1.46	1.50
20	y	605	CHL	C1B-CHB	2.09	1.46	1.41
21	A	826	CLA	CMD-C2D	-2.09	1.46	1.50
21	B	822	CLA	CMD-C2D	-2.09	1.46	1.50
25	L	306	BCR	C19-C18	-2.09	1.41	1.45
21	B	821	CLA	CMD-C2D	-2.08	1.46	1.50
21	x	612	CLA	CMD-C2D	-2.08	1.46	1.50
21	1	612	CLA	CMD-C2D	-2.08	1.46	1.50
21	3	604	CLA	CMD-C2D	-2.08	1.46	1.50
21	3	612	CLA	CMC-C2C	-2.08	1.46	1.50
21	z	612	CLA	C3B-C2B	-2.08	1.37	1.40
21	B	811	CLA	CMD-C2D	-2.08	1.46	1.50
21	3	607	CLA	C3B-C2B	-2.08	1.37	1.40
21	A	822	CLA	CMD-C2D	-2.08	1.46	1.50
21	1	603	CLA	CMC-C2C	-2.08	1.46	1.50
21	A	817	CLA	CMD-C2D	-2.08	1.46	1.50
25	J	102	BCR	C19-C18	-2.08	1.41	1.45
21	3	604	CLA	CMC-C2C	-2.08	1.46	1.50
21	O	201	CLA	CMD-C2D	-2.08	1.46	1.50
27	A	801	CL0	C4C-C3C	2.08	1.48	1.45
21	A	804	CLA	CMD-C2D	-2.08	1.46	1.50
20	y	607	CHL	MG-NA	-2.08	2.01	2.06
21	2	612	CLA	CMC-C2C	-2.08	1.46	1.50
21	A	815	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	818	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	820	CLA	CMD-C2D	-2.08	1.46	1.50
21	3	608	CLA	CMC-C2C	-2.08	1.46	1.50
21	1	611	CLA	CMD-C2D	-2.08	1.46	1.50
25	K	205	BCR	C11-C12	2.08	1.39	1.34
21	A	834	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	845	CLA	CMD-C2D	-2.08	1.46	1.50
21	x	614	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	819	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	824	CLA	C3B-C2B	-2.07	1.37	1.40
21	B	836	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	605	CLA	CMD-C2D	-2.07	1.46	1.50
25	F	304	BCR	C19-C18	-2.07	1.41	1.45
21	B	813	CLA	CMD-C2D	-2.07	1.46	1.50
25	F	304	BCR	C11-C12	2.07	1.39	1.34
21	y	602	CLA	CMC-C2C	-2.07	1.46	1.50
21	B	819	CLA	C3B-C2B	-2.07	1.37	1.40
21	A	831	CLA	CMD-C2D	-2.07	1.46	1.50
25	A	852	BCR	C12-C13	-2.07	1.41	1.45
25	A	851	BCR	C12-C13	-2.07	1.41	1.45
20	4	607	CHL	C4C-C3C	2.07	1.48	1.45
21	A	844	CLA	C3B-C2B	-2.07	1.37	1.40
21	B	806	CLA	CMD-C2D	-2.07	1.46	1.50
21	K	204	CLA	CMC-C2C	-2.07	1.46	1.50
20	2	601	CHL	MG-NA	-2.07	2.01	2.06
21	F	301	CLA	CMD-C2D	-2.07	1.46	1.50
20	4	615	CHL	C1B-CHB	2.07	1.46	1.41
21	B	808	CLA	C3B-C2B	-2.07	1.37	1.40
21	4	612	CLA	CMC-C2C	-2.07	1.46	1.50
20	4	606	CHL	C1B-CHB	2.07	1.46	1.41
21	4	614	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	815	CLA	CMC-C2C	-2.07	1.46	1.50
21	K	201	CLA	CMC-C2C	-2.07	1.46	1.50
20	z	607	CHL	MG-NA	-2.07	2.01	2.06
21	4	609	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	808	CLA	C3B-CAB	-2.06	1.43	1.47
21	A	845	CLA	CMC-C2C	-2.06	1.46	1.50
21	A	807	CLA	C3B-C2B	-2.06	1.37	1.40
21	A	832	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	839	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	813	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	836	CLA	CMC-C2C	-2.06	1.46	1.50
20	y	608	CHL	C4C-C3C	2.06	1.48	1.45
20	2	606	CHL	C1B-CHB	2.06	1.46	1.41
21	3	609	CLA	CMC-C2C	-2.06	1.46	1.50
21	B	826	CLA	CMD-C2D	-2.06	1.46	1.50
21	K	201	CLA	CMD-C2D	-2.06	1.46	1.50
21	z	611	CLA	C3B-C2B	-2.06	1.37	1.40
22	1	614	XAT	O24-C25	-2.06	1.43	1.46
21	A	827	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	825	CLA	CMD-C2D	-2.06	1.46	1.50
21	2	604	CLA	CMC-C2C	-2.06	1.46	1.50
21	G	203	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	206	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	844	CLA	CMD-C2D	-2.06	1.46	1.50
25	A	851	BCR	C19-C18	-2.06	1.41	1.45
21	A	838	CLA	CMD-C2D	-2.05	1.46	1.50
21	2	602	CLA	CMC-C2C	-2.05	1.46	1.50
21	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	805	CLA	CMC-C2C	-2.05	1.46	1.50
20	2	601	CHL	C1D-ND	-2.05	1.35	1.37
21	y	611	CLA	CMD-C2D	-2.05	1.46	1.50
21	z	612	CLA	CMC-C2C	-2.05	1.46	1.50
21	4	604	CLA	CMD-C2D	-2.05	1.46	1.50
21	2	603	CLA	MG-ND	-2.05	2.01	2.05
21	B	823	CLA	CMC-C2C	-2.05	1.46	1.50
20	z	605	CHL	C1B-CHB	2.05	1.46	1.41
21	A	802	CLA	C3B-CAB	-2.05	1.43	1.47
21	A	813	CLA	C3B-C2B	-2.05	1.37	1.40
21	2	603	CLA	CMC-C2C	-2.05	1.46	1.50
21	B	816	CLA	CMD-C2D	-2.05	1.46	1.50
21	L	303	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	840	CLA	C3B-C2B	-2.05	1.37	1.40
20	x	605	CHL	C1D-ND	-2.05	1.35	1.37
21	B	838	CLA	CMD-C2D	-2.05	1.46	1.50
21	1	602	CLA	CMC-C2C	-2.04	1.46	1.50
21	A	808	CLA	CMD-C2D	-2.04	1.46	1.50
21	4	602	CLA	CMC-C2C	-2.04	1.46	1.50
21	L	302	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	803	CLA	C3B-C2B	-2.04	1.37	1.40
21	A	805	CLA	CMD-C2D	-2.04	1.46	1.50
20	x	606	CHL	MG-NA	-2.04	2.01	2.06
21	4	611	CLA	CMC-C2C	-2.04	1.46	1.50
21	L	304	CLA	CMD-C2D	-2.04	1.46	1.50
21	y	614	CLA	CMC-C2C	-2.04	1.46	1.50
21	A	844	CLA	CMC-C2C	-2.04	1.46	1.50
21	B	829	CLA	CMC-C2C	-2.04	1.46	1.50
21	A	807	CLA	CMC-C2C	-2.04	1.46	1.50
21	B	803	CLA	C3B-C2B	-2.04	1.37	1.40
21	1	605	CLA	CMC-C2C	-2.04	1.46	1.50
20	2	615	CHL	C4C-C3C	2.04	1.48	1.45
21	4	609	CLA	C3B-CAB	-2.04	1.43	1.47
20	1	606	CHL	C1D-ND	-2.04	1.35	1.37
21	1	604	CLA	CMD-C2D	-2.04	1.46	1.50
24	1	616	LUT	C32-C33	-2.04	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	830	CLA	CMD-C2D	-2.04	1.46	1.50
21	y	613	CLA	CMD-C2D	-2.04	1.46	1.50
21	1	612	CLA	CMC-C2C	-2.03	1.46	1.50
21	B	832	CLA	CMC-C2C	-2.03	1.46	1.50
21	B	812	CLA	CMD-C2D	-2.03	1.46	1.50
21	O	202	CLA	CMC-C2C	-2.03	1.46	1.50
20	x	606	CHL	C1D-ND	-2.03	1.35	1.37
22	2	617	XAT	C8-C9	-2.03	1.41	1.45
21	A	807	CLA	CMD-C2D	-2.03	1.46	1.50
21	A	811	CLA	CMD-C2D	-2.03	1.46	1.50
20	2	615	CHL	C1B-CHB	2.03	1.46	1.41
21	B	832	CLA	CMD-C2D	-2.03	1.46	1.50
20	2	607	CHL	C4C-C3C	2.03	1.48	1.45
21	A	816	CLA	CMD-C2D	-2.03	1.46	1.50
21	x	613	CLA	CMC-C2C	-2.03	1.46	1.50
21	4	613	CLA	CMC-C2C	-2.03	1.46	1.50
21	B	835	CLA	CMD-C2D	-2.03	1.46	1.50
20	2	615	CHL	C1D-ND	-2.02	1.35	1.37
21	B	827	CLA	CMD-C2D	-2.02	1.46	1.50
21	2	611	CLA	CMC-C2C	-2.02	1.46	1.50
21	y	612	CLA	CMC-C2C	-2.02	1.46	1.50
20	z	606	CHL	C1B-CHB	2.02	1.46	1.41
21	3	611	CLA	C3B-C2B	-2.02	1.37	1.40
21	A	813	CLA	CMC-C2C	-2.02	1.46	1.50
21	A	802	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	818	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	805	CLA	C3B-C2B	-2.02	1.37	1.40
21	A	830	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	804	CLA	CMD-C2D	-2.02	1.46	1.50
21	K	204	CLA	CMD-C2D	-2.02	1.46	1.50
21	1	609	CLA	CAC-C3C	-2.02	1.46	1.50
21	4	601	CLA	CMC-C2C	-2.02	1.46	1.50
20	x	608	CHL	C1B-CHB	2.02	1.46	1.41
27	A	801	CL0	C1C-C2C	2.02	1.48	1.44
21	3	610	CLA	CMD-C2D	-2.02	1.46	1.50
21	B	841	CLA	CMD-C2D	-2.02	1.46	1.50
21	4	613	CLA	C3B-C2B	-2.02	1.37	1.40
21	A	810	CLA	C3B-C2B	-2.02	1.37	1.40
21	z	613	CLA	CMC-C2C	-2.02	1.46	1.50
21	A	804	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	826	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	807	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	602	CLA	CMC-C2C	-2.02	1.46	1.50
20	z	608	CHL	MG-NA	-2.01	2.01	2.06
20	3	606	CHL	C1B-CHB	2.01	1.46	1.41
21	A	820	CLA	CMC-C2C	-2.01	1.46	1.50
21	B	812	CLA	CMC-C2C	-2.01	1.46	1.50
21	4	603	CLA	CMC-C2C	-2.01	1.46	1.50
21	y	603	CLA	C3B-C2B	-2.01	1.37	1.40
21	1	610	CLA	CMC-C2C	-2.01	1.46	1.50
21	A	833	CLA	CMC-C2C	-2.01	1.46	1.50
21	K	203	CLA	CMD-C2D	-2.01	1.46	1.50
21	z	603	CLA	CMC-C2C	-2.01	1.46	1.50
20	2	607	CHL	MG-NA	-2.01	2.01	2.06
21	B	838	CLA	CMC-C2C	-2.01	1.46	1.50
21	4	610	CLA	CMC-C2C	-2.01	1.46	1.50
21	B	825	CLA	CMD-C2D	-2.01	1.46	1.50
21	z	611	CLA	C3B-CAB	-2.01	1.43	1.47
21	2	610	CLA	CMC-C2C	-2.01	1.46	1.50
21	3	611	CLA	CMD-C2D	-2.01	1.46	1.50
21	A	840	CLA	CMD-C2D	-2.01	1.46	1.50
21	B	818	CLA	CMD-C2D	-2.01	1.46	1.50
21	A	838	CLA	CMC-C2C	-2.01	1.46	1.50
21	A	833	CLA	CMD-C2D	-2.00	1.46	1.50
25	A	851	BCR	C20-C19	2.00	1.39	1.34
21	A	828	CLA	CMD-C2D	-2.00	1.46	1.50
21	2	610	CLA	C1A-CHA	-2.00	1.36	1.40
21	F	302	CLA	CMC-C2C	-2.00	1.46	1.50
21	2	608	CLA	CMC-C2C	-2.00	1.46	1.50
21	z	614	CLA	CMC-C2C	-2.00	1.46	1.50
21	B	827	CLA	C3B-CAB	-2.00	1.43	1.47
21	B	820	CLA	CMC-C2C	-2.00	1.46	1.50

All (2575) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	818	CLA	O2D-CGD-CBD	25.89	157.28	111.27
21	A	818	CLA	O2D-CGD-O1D	-25.26	74.45	123.84
22	4	617	XAT	O24-C25-C24	23.78	131.25	113.38
21	A	818	CLA	O1D-CGD-CBD	-20.36	82.83	124.48
27	A	801	CL0	C1D-ND-C4D	-17.19	94.13	106.33
21	B	836	CLA	C5-C3-C4	-16.61	77.91	114.60
21	B	836	CLA	C4-C3-C2	-13.91	82.45	122.65
21	B	836	CLA	C5-C3-C2	13.05	160.36	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	801	CL0	C2C-C1C-NC	10.58	119.89	109.97
22	4	617	XAT	C5-C4-C3	-10.21	92.54	112.75
22	4	617	XAT	C4-C3-C2	-10.03	91.40	110.77
27	A	801	CL0	C4A-NA-C1A	-9.73	102.33	106.71
22	4	617	XAT	O4-C5-C4	9.14	120.25	113.38
27	A	801	CL0	C1B-CHB-C4A	-9.14	112.03	130.12
20	y	606	CHL	CMD-C2D-C1D	9.05	140.66	124.71
22	1	614	XAT	C38-C25-C26	-8.94	107.27	122.26
27	A	801	CL0	C2D-C1D-ND	8.87	116.64	110.10
25	B	843	BCR	C16-C15-C14	8.61	141.12	123.47
22	1	614	XAT	C18-C5-C6	-8.48	108.05	122.26
22	x	617	XAT	C35-C15-C14	8.43	140.74	123.47
20	x	606	CHL	CMD-C2D-C1D	8.41	139.53	124.71
20	2	605	CHL	CMD-C2D-C1D	8.39	139.50	124.71
20	4	605	CHL	CMD-C2D-C1D	8.38	139.48	124.71
20	z	606	CHL	CMD-C2D-C1D	8.36	139.45	124.71
20	y	605	CHL	CMD-C2D-C1D	8.35	139.43	124.71
20	z	607	CHL	CMD-C2D-C1D	8.35	139.43	124.71
20	x	605	CHL	CMD-C2D-C1D	8.33	139.40	124.71
20	2	601	CHL	CMD-C2D-C1D	8.33	139.39	124.71
20	4	607	CHL	CMD-C2D-C1D	8.33	139.38	124.71
20	2	607	CHL	CMD-C2D-C1D	8.28	139.30	124.71
25	L	301	BCR	C16-C15-C14	8.27	140.41	123.47
20	z	609	CHL	CMD-C2D-C1D	8.24	139.23	124.71
20	x	608	CHL	CMD-C2D-C1D	8.21	139.19	124.71
20	z	605	CHL	CMD-C2D-C1D	8.20	139.16	124.71
22	4	617	XAT	O4-C5-C6	-8.19	52.18	58.96
20	y	607	CHL	CMD-C2D-C1D	8.17	139.11	124.71
20	z	608	CHL	CMD-C2D-C1D	8.16	139.09	124.71
20	z	601	CHL	CMD-C2D-C1D	8.14	139.07	124.71
20	1	601	CHL	CMD-C2D-C1D	8.14	139.05	124.71
22	1	614	XAT	O24-C25-C24	8.13	119.49	113.38
20	2	615	CHL	CMD-C2D-C1D	8.11	139.01	124.71
20	y	608	CHL	CMD-C2D-C1D	8.11	139.00	124.71
20	x	609	CHL	CMD-C2D-C1D	8.10	138.99	124.71
20	x	601	CHL	CMD-C2D-C1D	8.08	138.95	124.71
20	4	606	CHL	CMD-C2D-C1D	8.04	138.88	124.71
20	y	609	CHL	CMD-C2D-C1D	8.03	138.87	124.71
20	2	606	CHL	CMD-C2D-C1D	8.03	138.86	124.71
25	L	301	BCR	C15-C16-C17	8.03	139.92	123.47
20	3	606	CHL	CMD-C2D-C1D	8.02	138.85	124.71
20	4	615	CHL	CMD-C2D-C1D	8.02	138.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	617	XAT	C18-C5-C6	-7.98	108.88	122.26
20	1	606	CHL	CMD-C2D-C1D	7.90	138.64	124.71
20	z	607	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
20	y	609	CHL	CHD-C1D-ND	-7.87	117.22	124.45
20	x	607	CHL	CMD-C2D-C1D	7.87	138.58	124.71
27	A	801	CL0	CMD-C2D-C1D	7.84	138.52	124.71
20	x	607	CHL	C2C-C3C-C4C	-7.83	100.91	106.49
20	x	606	CHL	C2C-C3C-C4C	-7.81	100.92	106.49
27	A	801	CL0	C3C-C4C-NC	7.80	119.31	110.57
20	2	607	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
20	y	601	CHL	CMD-C2D-C1D	7.70	138.29	124.71
20	z	608	CHL	C2C-C3C-C4C	-7.69	101.00	106.49
20	x	608	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
21	F	302	CLA	C4A-NA-C1A	7.62	110.13	106.71
27	A	801	CL0	C3D-C4D-ND	7.62	122.56	110.24
20	y	607	CHL	C2C-C3C-C4C	-7.61	101.06	106.49
20	y	608	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
20	2	615	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
20	4	607	CHL	C2C-C3C-C4C	-7.60	101.08	106.49
22	4	617	XAT	O23-C23-C24	-7.57	94.76	109.80
20	y	606	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
22	4	617	XAT	C18-C5-C4	7.56	122.78	114.28
20	x	605	CHL	C2C-C3C-C4C	-7.54	101.12	106.49
20	y	601	CHL	C2C-C3C-C4C	-7.52	101.12	106.49
22	1	614	XAT	O4-C5-C4	7.49	119.01	113.38
20	z	609	CHL	CHD-C1D-ND	-7.48	117.58	124.45
24	3	613	LUT	C15-C35-C34	7.42	138.67	123.47
20	z	606	CHL	C2C-C3C-C4C	-7.42	101.20	106.49
20	2	601	CHL	C2C-C3C-C4C	-7.41	101.21	106.49
22	4	617	XAT	C24-C23-C22	-7.40	96.48	110.77
20	1	606	CHL	CHD-C1D-ND	-7.40	117.66	124.45
20	2	606	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
21	y	614	CLA	C4A-NA-C1A	7.39	110.03	106.71
25	A	849	BCR	C15-C16-C17	7.39	138.61	123.47
22	4	617	XAT	C7-C8-C9	7.34	136.92	125.53
21	B	811	CLA	C4A-NA-C1A	7.34	110.00	106.71
20	z	601	CHL	C2C-C3C-C4C	-7.33	101.26	106.49
25	A	851	BCR	C8-C9-C10	7.28	130.12	118.94
21	z	613	CLA	C4A-NA-C1A	7.27	109.97	106.71
20	2	605	CHL	C2C-C3C-C4C	-7.27	101.09	106.49
20	z	605	CHL	C2C-C3C-C4C	-7.24	101.33	106.49
21	3	612	CLA	C4A-NA-C1A	7.23	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	601	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
21	B	814	CLA	C4A-NA-C1A	7.22	109.95	106.71
20	2	601	CHL	O2D-CGD-CBD	7.22	124.10	111.27
20	4	615	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	1	609	CLA	C4A-NA-C1A	7.19	109.94	106.71
20	1	601	CHL	C2C-C3C-C4C	-7.19	101.37	106.49
20	z	601	CHL	CHD-C1D-ND	-7.18	117.86	124.45
22	4	617	XAT	C40-C33-C32	-7.14	106.82	118.08
20	x	609	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
22	4	617	XAT	C36-C21-C22	-7.13	96.59	108.98
20	y	605	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
21	4	613	CLA	C4A-NA-C1A	7.11	109.90	106.71
21	1	607	CLA	C4A-NA-C1A	7.11	109.90	106.71
20	y	609	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
20	z	609	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
21	B	805	CLA	C4A-NA-C1A	7.10	109.90	106.71
20	1	606	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
21	B	817	CLA	C4A-NA-C1A	7.07	109.89	106.71
21	A	826	CLA	C4A-NA-C1A	7.07	109.88	106.71
21	4	614	CLA	C4A-NA-C1A	7.06	109.88	106.71
21	B	824	CLA	C4A-NA-C1A	7.03	109.87	106.71
20	4	606	CHL	C1B-C2B-C3B	-7.02	100.39	106.92
21	A	818	CLA	C4A-NA-C1A	7.02	109.86	106.71
21	B	803	CLA	C4A-NA-C1A	7.01	109.86	106.71
21	A	813	CLA	C4A-NA-C1A	6.99	109.85	106.71
21	1	604	CLA	C4A-NA-C1A	6.98	109.84	106.71
21	A	830	CLA	C4A-NA-C1A	6.98	109.84	106.71
21	A	845	CLA	C4A-NA-C1A	6.98	109.84	106.71
21	3	605	CLA	C4A-NA-C1A	6.97	109.84	106.71
22	1	614	XAT	O4-C5-C18	6.97	123.40	115.06
21	x	613	CLA	C4A-NA-C1A	6.94	109.83	106.71
21	B	831	CLA	C4A-NA-C1A	6.93	109.82	106.71
21	z	603	CLA	C4A-NA-C1A	6.93	109.82	106.71
21	B	820	CLA	C4A-NA-C1A	6.93	109.82	106.71
21	B	804	CLA	C4A-NA-C1A	6.92	109.82	106.71
20	x	601	CHL	CHD-C1D-ND	-6.92	118.09	124.45
21	z	614	CLA	C4A-NA-C1A	6.92	109.82	106.71
21	3	610	CLA	C4A-NA-C1A	6.92	109.81	106.71
27	A	801	CL0	CHD-C1D-ND	-6.91	118.10	124.45
21	K	201	CLA	C4A-NA-C1A	6.91	109.81	106.71
21	K	204	CLA	C4A-NA-C1A	6.91	109.81	106.71
21	A	836	CLA	C4A-NA-C1A	6.90	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	838	CLA	C4A-NA-C1A	6.90	109.81	106.71
21	A	816	CLA	C4A-NA-C1A	6.90	109.81	106.71
25	A	851	BCR	C16-C15-C14	6.90	137.60	123.47
21	B	829	CLA	C4A-NA-C1A	6.89	109.80	106.71
21	3	609	CLA	C4A-NA-C1A	6.86	109.79	106.71
21	B	815	CLA	C4A-NA-C1A	6.85	109.79	106.71
21	B	808	CLA	C4A-NA-C1A	6.85	109.78	106.71
21	G	201	CLA	C4A-NA-C1A	6.84	109.78	106.71
21	4	612	CLA	C4A-NA-C1A	6.84	109.78	106.71
21	A	827	CLA	C4A-NA-C1A	6.84	109.78	106.71
21	2	609	CLA	C4A-NA-C1A	6.83	109.78	106.71
21	A	843	CLA	C4A-NA-C1A	6.82	109.77	106.71
21	B	807	CLA	C4A-NA-C1A	6.82	109.77	106.71
21	A	820	CLA	C4A-NA-C1A	6.81	109.77	106.71
21	B	840	CLA	C4A-NA-C1A	6.81	109.77	106.71
20	4	615	CHL	C1B-C2B-C3B	-6.79	100.60	106.92
21	z	611	CLA	C4A-NA-C1A	6.79	109.76	106.71
21	A	831	CLA	C4A-NA-C1A	6.79	109.76	106.71
21	G	203	CLA	C4A-NA-C1A	6.79	109.76	106.71
21	A	823	CLA	C4A-NA-C1A	6.78	109.75	106.71
24	2	616	LUT	C15-C35-C34	6.77	137.35	123.47
20	y	601	CHL	CHD-C1D-ND	-6.77	118.23	124.45
21	H	201	CLA	C4A-NA-C1A	6.77	109.75	106.71
21	A	832	CLA	C4A-NA-C1A	6.77	109.75	106.71
21	1	605	CLA	C4A-NA-C1A	6.76	109.75	106.71
21	A	819	CLA	C4A-NA-C1A	6.76	109.75	106.71
21	B	837	CLA	C4A-NA-C1A	6.76	109.75	106.71
21	A	835	CLA	C4A-NA-C1A	6.76	109.74	106.71
21	B	839	CLA	C4A-NA-C1A	6.75	109.74	106.71
20	4	605	CHL	C2C-C3C-C4C	-6.74	101.48	106.49
21	A	842	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	2	611	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	A	839	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	B	826	CLA	C4A-NA-C1A	6.74	109.73	106.71
21	y	604	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	A	841	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	A	837	CLA	C4A-NA-C1A	6.73	109.73	106.71
20	1	601	CHL	CHD-C1D-ND	-6.72	118.27	124.45
21	1	612	CLA	C4A-NA-C1A	6.72	109.73	106.71
21	B	809	CLA	C4A-NA-C1A	6.72	109.73	106.71
21	L	303	CLA	C4A-NA-C1A	6.72	109.73	106.71
21	4	603	CLA	C4A-NA-C1A	6.71	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	604	CLA	C4A-NA-C1A	6.71	109.72	106.71
21	A	833	CLA	C4A-NA-C1A	6.70	109.72	106.71
21	B	825	CLA	C4A-NA-C1A	6.70	109.72	106.71
21	B	813	CLA	C4A-NA-C1A	6.69	109.72	106.71
21	B	827	CLA	C4A-NA-C1A	6.69	109.71	106.71
21	A	817	CLA	C4A-NA-C1A	6.69	109.71	106.71
21	A	804	CLA	C4A-NA-C1A	6.68	109.71	106.71
21	A	809	CLA	C4A-NA-C1A	6.65	109.70	106.71
21	3	601	CLA	C4A-NA-C1A	6.64	109.69	106.71
21	A	815	CLA	C4A-NA-C1A	6.64	109.69	106.71
21	G	202	CLA	C4A-NA-C1A	6.63	109.69	106.71
21	J	101	CLA	C4A-NA-C1A	6.63	109.69	106.71
21	z	612	CLA	C4A-NA-C1A	6.62	109.68	106.71
21	A	828	CLA	C4A-NA-C1A	6.62	109.68	106.71
21	B	812	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	A	850	BCR	C15-C16-C17	6.61	137.02	123.47
21	A	822	CLA	C4A-NA-C1A	6.61	109.68	106.71
21	A	834	CLA	C4A-NA-C1A	6.60	109.67	106.71
21	x	602	CLA	C4A-NA-C1A	6.59	109.67	106.71
21	y	611	CLA	C4A-NA-C1A	6.59	109.67	106.71
20	z	606	CHL	CHD-C1D-ND	-6.59	118.40	124.45
21	A	806	CLA	C4A-NA-C1A	6.59	109.67	106.71
21	L	302	CLA	C4A-NA-C1A	6.58	109.67	106.71
20	x	607	CHL	CHD-C1D-ND	-6.58	118.41	124.45
21	A	808	CLA	C4A-NA-C1A	6.58	109.66	106.71
22	2	617	XAT	C35-C15-C14	6.57	136.94	123.47
21	4	611	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	A	811	CLA	C4A-NA-C1A	6.57	109.66	106.71
20	x	609	CHL	CHD-C1D-ND	-6.55	118.44	124.45
21	A	812	CLA	C4A-NA-C1A	6.55	109.65	106.71
21	1	611	CLA	C4A-NA-C1A	6.54	109.65	106.71
21	B	833	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	y	613	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	3	604	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	A	821	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	3	602	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	x	612	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	A	829	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	A	802	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	3	611	CLA	C4A-NA-C1A	6.51	109.63	106.71
21	B	830	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	y	615	LUT	C35-C15-C14	6.50	136.78	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	824	CLA	C4A-NA-C1A	6.49	109.63	106.71
21	B	816	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	A	840	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	4	602	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	B	832	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	y	603	CLA	C4A-NA-C1A	6.48	109.62	106.71
20	4	605	CHL	CHD-C1D-ND	-6.48	118.50	124.45
21	x	603	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	z	602	CLA	C4A-NA-C1A	6.48	109.62	106.71
25	B	849	BCR	C30-C25-C26	-6.48	113.49	122.61
21	4	601	CLA	C4A-NA-C1A	6.47	109.62	106.71
21	A	810	CLA	C4A-NA-C1A	6.47	109.62	106.71
21	B	802	CLA	C4A-NA-C1A	6.47	109.62	106.71
21	y	610	CLA	C4A-NA-C1A	6.47	109.62	106.71
21	z	610	CLA	C4A-NA-C1A	6.47	109.61	106.71
21	x	614	CLA	C4A-NA-C1A	6.47	109.61	106.71
21	x	610	CLA	C4A-NA-C1A	6.46	109.61	106.71
21	x	604	CLA	C4A-NA-C1A	6.46	109.61	106.71
21	B	819	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	2	612	CLA	C4A-NA-C1A	6.45	109.61	106.71
20	2	606	CHL	CHD-C1D-ND	-6.45	118.53	124.45
21	y	602	CLA	C4A-NA-C1A	6.44	109.60	106.71
21	B	806	CLA	C4A-NA-C1A	6.44	109.60	106.71
21	F	301	CLA	C4A-NA-C1A	6.44	109.60	106.71
21	3	608	CLA	C4A-NA-C1A	6.43	109.60	106.71
21	B	841	CLA	C4A-NA-C1A	6.43	109.60	106.71
20	4	615	CHL	CHD-C1D-ND	-6.43	118.54	124.45
21	L	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
21	1	613	CLA	C4A-NA-C1A	6.43	109.59	106.71
21	1	602	CLA	C4A-NA-C1A	6.42	109.59	106.71
21	A	807	CLA	C4A-NA-C1A	6.42	109.59	106.71
20	2	615	CHL	CHD-C1D-ND	-6.42	118.56	124.45
21	B	835	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	B	834	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	2	603	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	A	825	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	K	206	CLA	C4A-NA-C1A	6.39	109.58	106.71
20	y	606	CHL	CHD-C1D-ND	-6.39	118.59	124.45
21	F	303	CLA	C4A-NA-C1A	6.38	109.58	106.71
21	A	805	CLA	C4A-NA-C1A	6.37	109.57	106.71
20	z	605	CHL	CHD-C1D-ND	-6.37	118.60	124.45
21	B	810	CLA	C4A-NA-C1A	6.37	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	828	CLA	C4A-NA-C1A	6.36	109.56	106.71
21	B	818	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	x	608	CHL	CHD-C1D-ND	-6.34	118.63	124.45
21	z	604	CLA	C4A-NA-C1A	6.34	109.56	106.71
21	1	608	CLA	C4A-NA-C1A	6.34	109.56	106.71
21	2	613	CLA	C4A-NA-C1A	6.34	109.56	106.71
21	2	602	CLA	C4A-NA-C1A	6.33	109.55	106.71
21	A	838	CLA	C4A-NA-C1A	6.33	109.55	106.71
21	y	612	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	2	617	XAT	C15-C35-C34	6.32	136.41	123.47
21	B	822	CLA	C4A-NA-C1A	6.31	109.54	106.71
21	x	611	CLA	C4A-NA-C1A	6.30	109.54	106.71
25	A	851	BCR	C23-C22-C21	6.29	128.60	118.94
22	1	614	XAT	O24-C25-C38	6.29	122.59	115.06
20	x	609	CHL	O2D-CGD-CBD	6.27	122.41	111.27
21	1	610	CLA	C4A-NA-C1A	6.26	109.52	106.71
20	y	605	CHL	CHD-C1D-ND	-6.26	118.70	124.45
21	B	823	CLA	C4A-NA-C1A	6.25	109.52	106.71
21	2	608	CLA	C4A-NA-C1A	6.25	109.52	106.71
20	2	605	CHL	CHD-C1D-ND	-6.25	118.71	124.45
21	4	610	CLA	C4A-NA-C1A	6.25	109.52	106.71
25	A	850	BCR	C16-C15-C14	6.24	136.26	123.47
21	4	608	CLA	C4A-NA-C1A	6.23	109.51	106.71
20	3	606	CHL	CHD-C1D-ND	-6.22	118.73	124.45
21	1	603	CLA	C4A-NA-C1A	6.22	109.50	106.71
21	K	203	CLA	C4A-NA-C1A	6.22	109.50	106.71
20	y	608	CHL	CHD-C1D-ND	-6.20	118.75	124.45
20	4	607	CHL	CHD-C1D-ND	-6.19	118.77	124.45
21	B	821	CLA	C4A-NA-C1A	6.18	109.49	106.71
21	O	201	CLA	C4A-NA-C1A	6.17	109.48	106.71
21	A	814	CLA	C4A-NA-C1A	6.17	109.48	106.71
20	z	607	CHL	CHD-C1D-ND	-6.16	118.79	124.45
27	A	801	CL0	C3B-C4B-NB	6.13	117.13	109.21
21	O	203	CLA	C4A-NA-C1A	6.11	109.45	106.71
20	x	606	CHL	CHD-C1D-ND	-6.11	118.84	124.45
20	4	606	CHL	CHD-C1D-ND	-6.10	118.85	124.45
21	O	202	CLA	C4A-NA-C1A	6.07	109.43	106.71
21	3	607	CLA	C4A-NA-C1A	6.06	109.43	106.71
21	2	604	CLA	C4A-NA-C1A	6.03	109.42	106.71
20	x	605	CHL	CHD-C1D-ND	-6.01	118.93	124.45
20	y	607	CHL	CHD-C1D-ND	-6.01	118.93	124.45
21	4	609	CLA	C4A-NA-C1A	5.97	109.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	836	CLA	C4A-NA-C1A	5.96	109.38	106.71
20	2	607	CHL	CHD-C1D-ND	-5.95	118.98	124.45
20	z	608	CHL	CHD-C1D-ND	-5.94	118.99	124.45
22	4	617	XAT	C26-C27-C28	-5.89	113.53	125.99
20	2	601	CHL	CHD-C1D-ND	-5.89	119.04	124.45
25	F	304	BCR	C15-C16-C17	5.89	135.54	123.47
21	1	609	CLA	CMB-C2B-C1B	-5.88	119.42	128.46
25	K	202	BCR	C16-C15-C14	5.70	135.16	123.47
25	F	304	BCR	C24-C23-C22	5.68	134.81	126.23
21	A	844	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	A	851	BCR	C7-C8-C9	-5.65	117.70	126.23
24	2	616	LUT	C7-C8-C9	5.63	134.75	126.23
25	K	205	BCR	C15-C16-C17	5.63	135.00	123.47
21	3	603	CLA	C4A-NA-C1A	5.60	109.22	106.71
21	A	803	CLA	C4A-NA-C1A	5.58	109.22	106.71
22	4	617	XAT	O3-C3-C2	-5.58	98.72	109.80
24	2	619	LUT	C15-C35-C34	5.56	134.86	123.47
20	z	609	CHL	C1B-CHB-C4A	-5.55	119.12	130.12
25	A	851	BCR	C34-C9-C10	-5.55	115.15	122.92
22	1	614	XAT	C35-C34-C33	-5.48	119.48	127.31
24	y	615	LUT	C8-C9-C10	5.45	127.31	118.94
27	A	801	CL0	CHD-C4C-C3C	-5.44	116.84	124.84
20	2	607	CHL	C3C-C4C-NC	5.39	116.61	110.57
20	x	606	CHL	C3C-C4C-NC	5.38	116.60	110.57
22	4	617	XAT	C15-C14-C13	5.36	134.96	127.31
20	y	601	CHL	C1B-CHB-C4A	-5.33	119.55	130.12
22	4	617	XAT	C32-C33-C34	5.33	127.12	118.94
20	z	608	CHL	C3C-C4C-NC	5.32	116.53	110.57
20	z	607	CHL	C3C-C4C-NC	5.27	116.49	110.57
20	2	601	CHL	C3C-C4C-NC	5.27	116.48	110.57
20	2	605	CHL	C3C-C4C-NC	5.26	116.32	110.57
22	4	617	XAT	O24-C25-C26	-5.24	54.62	58.96
20	x	605	CHL	C3C-C4C-NC	5.21	116.41	110.57
20	z	607	CHL	O2D-CGD-CBD	5.21	120.53	111.27
25	B	845	BCR	C19-C18-C17	5.20	126.92	118.94
20	y	606	CHL	C3C-C4C-NC	5.19	116.40	110.57
20	4	607	CHL	C3C-C4C-NC	5.19	116.40	110.57
20	x	601	CHL	C1B-CHB-C4A	-5.15	119.92	130.12
24	x	616	LUT	C28-C29-C30	5.12	126.79	118.94
25	A	851	BCR	C37-C22-C21	-5.10	115.77	122.92
20	y	607	CHL	C3C-C4C-NC	5.08	116.27	110.57
25	A	851	BCR	C11-C10-C9	5.07	134.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	615	CHL	O2D-CGD-CBD	5.06	120.26	111.27
20	x	608	CHL	C3C-C4C-NC	5.06	116.24	110.57
20	4	606	CHL	C3C-C4C-NC	5.03	116.21	110.57
24	z	616	LUT	C15-C35-C34	5.02	133.76	123.47
31	x	618	NEX	C15-C35-C34	5.02	133.76	123.47
20	y	609	CHL	O2D-CGD-CBD	5.02	120.18	111.27
27	A	801	CL0	C3D-C2D-C1D	-5.00	99.00	105.83
20	z	605	CHL	C3C-C4C-NC	5.00	116.18	110.57
20	z	601	CHL	O2D-CGD-CBD	5.00	120.15	111.27
27	A	801	CL0	C1C-C2C-C3C	-4.98	101.73	106.96
20	2	606	CHL	C3C-C4C-NC	4.96	116.14	110.57
20	y	609	CHL	C1B-CHB-C4A	-4.96	120.30	130.12
25	B	846	BCR	C16-C15-C14	4.95	133.61	123.47
20	2	615	CHL	C3C-C4C-NC	4.94	116.12	110.57
24	1	616	LUT	C30-C31-C32	4.93	138.61	123.22
20	2	605	CHL	O2D-CGD-CBD	4.93	120.03	111.27
27	A	801	CL0	C1D-CHD-C4C	-4.92	115.44	126.06
20	3	606	CHL	C3C-C4C-NC	4.92	116.09	110.57
24	z	615	LUT	C35-C15-C14	4.92	133.55	123.47
25	L	306	BCR	C8-C9-C10	4.92	126.49	118.94
20	x	607	CHL	O2D-CGD-CBD	4.92	120.00	111.27
20	4	606	CHL	O2D-CGD-CBD	4.91	120.00	111.27
20	z	605	CHL	O2D-CGD-CBD	4.90	119.98	111.27
20	4	605	CHL	C3C-C4C-NC	4.90	115.92	110.57
20	x	608	CHL	O2D-CGD-CBD	4.88	119.95	111.27
20	4	615	CHL	C3C-C4C-NC	4.88	116.05	110.57
24	2	616	LUT	C39-C29-C30	-4.88	116.08	122.92
20	z	609	CHL	O2D-CGD-CBD	4.86	119.90	111.27
20	y	605	CHL	C3C-C4C-NC	4.85	116.01	110.57
20	3	606	CHL	C2C-C1C-NC	4.84	114.51	109.97
25	B	849	BCR	C16-C15-C14	4.84	133.38	123.47
24	y	615	LUT	C39-C29-C30	-4.84	116.15	122.92
25	J	102	BCR	C16-C15-C14	4.83	133.38	123.47
25	A	853	BCR	C16-C15-C14	4.80	133.31	123.47
20	x	606	CHL	C3D-C2D-C1D	-4.80	99.29	105.83
20	z	608	CHL	O2D-CGD-CBD	4.79	119.78	111.27
21	A	842	CLA	CMB-C2B-C1B	-4.78	121.11	128.46
20	2	606	CHL	O2D-CGD-CBD	4.78	119.76	111.27
24	2	616	LUT	C28-C29-C30	4.77	126.27	118.94
20	2	601	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
21	4	613	CLA	CAA-C2A-C3A	-4.76	99.74	112.78
25	B	843	BCR	C34-C9-C10	-4.76	116.26	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	605	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
20	z	606	CHL	C3C-C4C-NC	4.74	115.88	110.57
24	2	619	LUT	C19-C9-C10	-4.74	116.29	122.92
20	y	608	CHL	C3C-C4C-NC	4.72	115.86	110.57
20	x	609	CHL	C3C-C4C-NC	4.71	115.85	110.57
21	B	822	CLA	CAA-C2A-C3A	-4.71	99.89	112.78
20	4	607	CHL	O2D-CGD-CBD	4.70	119.63	111.27
21	A	820	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
20	3	606	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
20	4	606	CHL	C2C-C1C-NC	4.69	114.37	109.97
24	y	615	LUT	C19-C9-C10	-4.69	116.35	122.92
20	2	607	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
22	y	617	XAT	C8-C9-C10	4.68	126.11	118.94
22	y	617	XAT	C19-C9-C10	-4.67	116.38	122.92
20	4	607	CHL	C3D-C2D-C1D	-4.67	99.45	105.83
20	x	606	CHL	CHD-C4C-C3C	-4.66	117.99	124.84
25	K	205	BCR	C19-C18-C17	4.66	126.09	118.94
24	2	619	LUT	C8-C9-C10	4.65	126.08	118.94
31	y	618	NEX	C35-C15-C14	4.65	133.00	123.47
20	y	601	CHL	O2D-CGD-CBD	4.65	119.53	111.27
20	y	607	CHL	O2D-CGD-CBD	4.64	119.51	111.27
20	2	605	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
25	B	843	BCR	C8-C9-C10	4.63	126.05	118.94
21	B	818	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
24	x	616	LUT	C15-C35-C34	4.62	132.95	123.47
20	y	605	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
20	z	608	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
25	L	306	BCR	C34-C9-C10	-4.61	116.46	122.92
25	B	847	BCR	C16-C15-C14	4.61	132.92	123.47
25	B	845	BCR	C36-C18-C17	-4.61	116.47	122.92
24	x	616	LUT	C39-C29-C30	-4.60	116.48	122.92
24	3	613	LUT	C39-C29-C30	-4.59	116.49	122.92
20	y	608	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
22	z	617	XAT	C35-C15-C14	4.58	132.85	123.47
20	2	607	CHL	CHD-C4C-C3C	-4.58	118.11	124.84
20	x	606	CHL	O2D-CGD-CBD	4.58	119.40	111.27
20	x	607	CHL	C3C-C4C-NC	4.57	115.69	110.57
20	x	605	CHL	CHD-C4C-C3C	-4.57	118.13	124.84
20	4	606	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
20	y	601	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
20	z	605	CHL	C3D-C2D-C1D	-4.53	99.64	105.83
25	A	851	BCR	C12-C13-C14	4.53	125.89	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	z	607	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
20	x	608	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
20	z	606	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
25	L	306	BCR	C16-C15-C14	4.51	132.71	123.47
25	K	202	BCR	C37-C22-C21	-4.51	116.61	122.92
20	4	615	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
25	L	301	BCR	C12-C13-C14	4.49	125.83	118.94
20	x	609	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
24	z	616	LUT	C30-C31-C32	4.49	137.22	123.22
25	K	202	BCR	C15-C16-C17	4.48	132.66	123.47
21	z	604	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
20	2	606	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
25	G	204	BCR	C15-C16-C17	4.47	132.63	123.47
22	1	614	XAT	C15-C14-C13	-4.47	120.93	127.31
25	A	848	BCR	C15-C16-C17	4.46	132.61	123.47
20	2	607	CHL	O2D-CGD-CBD	4.45	119.17	111.27
22	4	617	XAT	C28-C29-C30	4.45	125.76	118.94
24	3	613	LUT	C28-C29-C30	4.44	125.76	118.94
20	y	606	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
24	z	615	LUT	C19-C9-C10	-4.44	116.70	122.92
20	y	607	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
20	1	601	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
20	2	601	CHL	CHD-C4C-C3C	-4.43	118.32	124.84
25	K	205	BCR	C37-C22-C21	-4.43	116.72	122.92
20	4	607	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
21	B	813	CLA	O2D-CGD-O1D	-4.43	115.19	123.84
25	B	844	BCR	C37-C22-C21	-4.42	116.73	122.92
25	L	306	BCR	C37-C22-C21	-4.42	116.73	122.92
20	x	606	CHL	C2D-C1D-ND	4.42	113.36	110.10
20	z	608	CHL	CHD-C4C-C3C	-4.41	118.36	124.84
20	1	606	CHL	C3D-C2D-C1D	-4.40	99.82	105.83
25	B	846	BCR	C34-C9-C10	-4.40	116.76	122.92
21	3	608	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
20	y	606	CHL	CHD-C4C-C3C	-4.39	118.39	124.84
21	B	813	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
21	4	612	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
20	y	606	CHL	O2D-CGD-CBD	4.39	119.07	111.27
20	z	601	CHL	C3D-C2D-C1D	-4.39	99.84	105.83
22	z	617	XAT	C39-C29-C30	-4.38	116.78	122.92
25	F	304	BCR	C16-C15-C14	4.38	132.45	123.47
22	y	617	XAT	C35-C15-C14	4.38	132.45	123.47
21	3	601	CLA	CMB-C2B-C1B	-4.38	121.73	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	615	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
20	z	607	CHL	CHD-C4C-C3C	-4.38	118.41	124.84
21	4	602	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
20	x	601	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
20	x	605	CHL	O2D-CGD-CBD	4.37	119.03	111.27
20	z	601	CHL	C3C-C4C-NC	4.36	115.47	110.57
25	B	844	BCR	C21-C20-C19	4.35	136.79	123.22
25	L	305	BCR	C16-C15-C14	4.34	132.37	123.47
20	y	601	CHL	C3C-C4C-NC	4.34	115.43	110.57
20	1	601	CHL	C3C-C4C-NC	4.34	115.43	110.57
25	K	205	BCR	C34-C9-C10	-4.33	116.85	122.92
21	A	831	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
24	y	616	LUT	C15-C35-C34	4.32	132.33	123.47
25	B	844	BCR	C16-C15-C14	4.32	132.33	123.47
25	K	205	BCR	C36-C18-C17	-4.32	116.87	122.92
25	L	305	BCR	C37-C22-C21	-4.31	116.88	122.92
25	J	102	BCR	C34-C9-C10	-4.31	116.88	122.92
21	A	830	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
22	2	617	XAT	C39-C29-C30	-4.30	116.90	122.92
25	B	844	BCR	C34-C9-C10	-4.30	116.90	122.92
25	F	304	BCR	C34-C9-C10	-4.30	116.90	122.92
30	B	850	DGD	O2G-C1B-C2B	4.30	120.77	111.50
25	K	202	BCR	C12-C13-C14	4.30	125.54	118.94
21	z	613	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
31	z	618	NEX	C39-C29-C30	-4.29	116.92	122.92
25	L	301	BCR	C37-C22-C21	-4.28	116.92	122.92
24	1	616	LUT	C15-C35-C34	4.27	132.22	123.47
25	K	202	BCR	C35-C13-C14	-4.27	116.94	122.92
25	A	849	BCR	C21-C20-C19	4.27	136.54	123.22
25	A	850	BCR	C34-C9-C10	-4.27	116.94	122.92
20	x	605	CHL	C2D-C1D-ND	4.26	113.25	110.10
22	2	617	XAT	C28-C29-C30	4.26	125.48	118.94
20	4	605	CHL	C3D-C2D-C1D	-4.26	100.02	105.83
21	B	829	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
20	1	606	CHL	C3C-C4C-NC	4.26	115.35	110.57
21	B	825	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
24	1	616	LUT	C19-C9-C10	-4.25	116.97	122.92
21	A	841	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
22	z	617	XAT	C19-C9-C10	-4.25	116.97	122.92
20	z	606	CHL	O2D-CGD-CBD	4.24	118.81	111.27
27	A	801	CL0	CAD-CBD-CHA	-4.24	100.36	105.14
20	2	605	CHL	CHD-C4C-C3C	-4.24	118.36	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	821	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
20	y	605	CHL	O2D-CGD-CBD	4.24	118.80	111.27
21	A	833	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
20	x	607	CHL	C3D-C2D-C1D	-4.23	100.06	105.83
21	B	809	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
20	3	606	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
20	y	609	CHL	C3D-C2D-C1D	-4.23	100.06	105.83
25	K	202	BCR	C34-C9-C10	-4.22	117.01	122.92
21	A	809	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
25	A	852	BCR	C37-C22-C21	-4.22	117.02	122.92
20	y	609	CHL	C4A-NA-C1A	4.22	108.60	106.71
21	G	203	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
22	4	617	XAT	C39-C29-C28	-4.21	111.44	118.08
21	3	603	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
25	A	849	BCR	C30-C25-C26	-4.21	116.69	122.61
25	G	204	BCR	C37-C22-C21	-4.21	117.03	122.92
21	B	814	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
22	4	617	XAT	C16-C1-C6	-4.20	98.70	110.05
21	y	604	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
25	A	852	BCR	C16-C15-C14	4.20	132.07	123.47
25	B	801	BCR	C16-C15-C14	4.19	132.06	123.47
22	2	617	XAT	C19-C9-C10	-4.19	117.05	122.92
20	2	601	CHL	C2D-C1D-ND	4.19	113.19	110.10
21	B	831	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
20	y	605	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
24	2	619	LUT	C39-C29-C30	-4.18	117.06	122.92
20	x	601	CHL	O2D-CGD-CBD	4.18	118.70	111.27
24	z	616	LUT	C19-C9-C10	-4.18	117.07	122.92
20	x	608	CHL	CHD-C4C-C3C	-4.17	118.70	124.84
22	4	617	XAT	C38-C25-C26	-4.17	115.27	122.26
21	B	824	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
24	1	616	LUT	C35-C15-C14	4.16	132.00	123.47
20	4	606	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
24	1	616	LUT	C31-C30-C29	4.16	133.25	127.31
20	3	606	CHL	C2D-C1D-ND	4.16	113.17	110.10
20	3	606	CHL	O2D-CGD-CBD	4.16	118.66	111.27
25	L	301	BCR	C35-C13-C14	-4.16	117.10	122.92
25	O	204	BCR	C37-C22-C21	-4.16	117.10	122.92
20	4	606	CHL	C4C-C3C-C2C	-4.15	100.84	106.90
21	2	612	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
20	z	608	CHL	C2D-C1D-ND	4.15	113.16	110.10
25	L	306	BCR	C23-C22-C21	4.15	125.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	y	601	CHL	C4A-NA-C1A	4.14	108.57	106.71
25	B	801	BCR	C8-C9-C10	4.13	125.28	118.94
24	y	616	LUT	C39-C29-C30	-4.13	117.14	122.92
25	B	845	BCR	C34-C9-C10	-4.12	117.16	122.92
20	4	615	CHL	CHD-C4C-C3C	-4.12	118.79	124.84
25	A	852	BCR	C10-C11-C12	4.11	136.05	123.22
25	3	614	BCR	C34-C9-C10	-4.11	117.17	122.92
25	4	618	BCR	C16-C15-C14	4.11	131.89	123.47
24	y	616	LUT	C19-C9-C10	-4.11	117.17	122.92
25	L	301	BCR	C36-C18-C17	-4.10	117.17	122.92
21	B	826	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
21	x	603	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
20	z	609	CHL	C3D-C2D-C1D	-4.09	100.25	105.83
24	1	616	LUT	C40-C33-C34	-4.09	117.20	122.92
24	x	615	LUT	C19-C9-C10	-4.09	117.20	122.92
24	1	616	LUT	C32-C33-C34	4.08	125.20	118.94
25	B	801	BCR	C37-C22-C21	-4.08	117.21	122.92
21	x	610	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
25	I	101	BCR	C15-C16-C17	4.07	131.82	123.47
21	1	609	CLA	CMB-C2B-C3B	4.07	132.30	124.68
25	O	205	BCR	C34-C9-C10	-4.07	117.22	122.92
25	4	618	BCR	C34-C9-C10	-4.07	117.22	122.92
22	x	617	XAT	C39-C29-C30	-4.07	117.22	122.92
21	A	828	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
25	A	853	BCR	C37-C22-C21	-4.06	117.23	122.92
31	x	618	NEX	C32-C33-C34	4.06	125.18	118.94
21	A	806	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
25	A	848	BCR	C37-C22-C21	-4.06	117.24	122.92
21	A	802	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
21	A	811	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
20	x	601	CHL	C3C-C4C-NC	4.05	115.11	110.57
25	J	102	BCR	C37-C22-C21	-4.05	117.25	122.92
20	y	607	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
21	A	839	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
20	4	607	CHL	C2D-C1D-ND	4.04	113.08	110.10
20	1	601	CHL	C6-C5-C3	-4.04	108.02	114.62
25	L	301	BCR	C21-C20-C19	4.03	135.81	123.22
25	K	202	BCR	C23-C22-C21	4.03	125.13	118.94
21	x	604	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
21	y	610	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
25	4	618	BCR	C30-C25-C26	-4.03	116.94	122.61
25	L	301	BCR	C34-C9-C10	-4.03	117.28	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	847	BCR	C34-C9-C10	-4.03	117.28	122.92
31	y	618	NEX	C39-C29-C30	-4.03	117.28	122.92
24	1	616	LUT	C39-C29-C28	4.03	124.42	118.08
25	O	204	BCR	C15-C16-C17	4.02	131.71	123.47
25	F	304	BCR	C12-C13-C14	4.02	125.10	118.94
21	A	805	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
25	I	101	BCR	C37-C22-C21	-4.01	117.30	122.92
25	A	848	BCR	C34-C9-C10	-4.01	117.31	122.92
20	z	605	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
25	G	204	BCR	C34-C9-C10	-4.01	117.31	122.92
25	B	845	BCR	C20-C21-C22	4.00	133.03	127.31
24	2	616	LUT	C19-C9-C10	-4.00	117.32	122.92
21	B	815	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
21	B	820	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
21	2	611	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
21	2	602	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
24	y	615	LUT	C40-C33-C34	-3.98	117.34	122.92
24	y	615	LUT	C32-C33-C34	3.98	125.05	118.94
25	B	849	BCR	C37-C22-C21	-3.98	117.35	122.92
20	z	607	CHL	C2D-C1D-ND	3.98	113.03	110.10
20	2	601	CHL	O2D-CGD-O1D	-3.97	116.08	123.84
25	L	305	BCR	C34-C9-C10	-3.97	117.36	122.92
25	O	205	BCR	C37-C22-C21	-3.96	117.37	122.92
20	4	606	CHL	C2D-C1D-ND	3.96	113.02	110.10
25	I	101	BCR	C34-C9-C10	-3.96	117.38	122.92
20	2	606	CHL	CAC-C3C-C4C	3.96	129.94	124.81
24	z	615	LUT	C8-C9-C10	3.95	125.01	118.94
21	A	804	CLA	CAA-C2A-C3A	-3.95	101.95	112.78
25	B	844	BCR	C15-C16-C17	3.95	131.57	123.47
24	x	616	LUT	C19-C9-C10	-3.95	117.38	122.92
21	B	804	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
24	z	616	LUT	C32-C33-C34	3.95	125.00	118.94
31	x	618	NEX	C40-C33-C34	-3.95	117.39	122.92
25	F	304	BCR	C20-C21-C22	3.95	132.94	127.31
25	A	852	BCR	C23-C22-C21	3.95	125.00	118.94
21	y	611	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
21	x	602	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
25	B	847	BCR	C37-C22-C21	-3.93	117.42	122.92
24	4	616	LUT	C19-C9-C10	-3.93	117.42	122.92
20	1	601	CHL	CAC-C3C-C4C	3.93	129.91	124.81
25	B	848	BCR	C34-C9-C10	-3.92	117.42	122.92
25	B	848	BCR	C37-C22-C21	-3.92	117.43	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	837	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
21	y	602	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
24	4	616	LUT	C39-C29-C30	-3.92	117.43	122.92
24	z	615	LUT	C39-C29-C30	-3.92	117.43	122.92
21	3	612	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	A	850	BCR	C37-C22-C21	-3.92	117.44	122.92
20	y	608	CHL	O2D-CGD-CBD	3.92	118.23	111.27
20	2	606	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
20	2	607	CHL	C2D-C1D-ND	3.91	112.99	110.10
25	O	204	BCR	C34-C9-C10	-3.91	117.45	122.92
20	z	608	CHL	CAC-C3C-C4C	3.91	129.88	124.81
25	A	852	BCR	C19-C18-C17	3.91	124.93	118.94
21	A	815	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
21	B	818	CLA	CMB-C2B-C3B	3.90	131.98	124.68
20	2	615	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
25	A	851	BCR	C15-C16-C17	3.89	131.45	123.47
22	1	614	XAT	C6-C7-C8	-3.89	117.77	125.99
20	x	609	CHL	CAC-C3C-C4C	3.88	129.85	124.81
21	B	833	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
21	O	202	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
22	y	617	XAT	C30-C31-C32	3.88	135.32	123.22
25	A	851	BCR	C24-C23-C22	-3.88	120.37	126.23
25	A	849	BCR	C34-C9-C10	-3.88	117.49	122.92
25	K	202	BCR	C19-C18-C17	3.88	124.89	118.94
20	4	615	CHL	C2D-C1D-ND	3.88	112.96	110.10
20	y	608	CHL	C1B-CHB-C4A	-3.88	122.44	130.12
25	B	843	BCR	C37-C22-C21	-3.87	117.50	122.92
25	F	304	BCR	C35-C13-C14	-3.87	117.50	122.92
20	2	605	CHL	C2D-C1D-ND	3.87	112.96	110.10
21	O	203	CLA	CAB-C3B-C4B	-3.87	122.51	128.46
20	z	607	CHL	C1D-ND-C4D	-3.87	103.59	106.33
21	L	303	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
24	2	619	LUT	C40-C33-C34	-3.86	117.51	122.92
21	x	614	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
21	x	613	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
21	A	820	CLA	CMB-C2B-C3B	3.85	131.89	124.68
25	F	304	BCR	C21-C20-C19	3.85	135.25	123.22
21	B	816	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
22	y	617	XAT	C20-C13-C14	-3.85	117.52	122.92
25	L	306	BCR	C15-C16-C17	3.85	131.37	123.47
20	z	608	CHL	C1D-ND-C4D	-3.85	103.60	106.33
23	1	615	LHG	O7-C7-C8	3.85	119.79	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	y	607	CHL	CAC-C3C-C4C	3.84	129.80	124.81
24	4	616	LUT	C15-C35-C34	3.84	131.35	123.47
21	K	203	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
21	1	605	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
20	z	607	CHL	C1-C2-C3	-3.84	119.41	126.04
21	z	602	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
21	A	804	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
21	3	607	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
21	1	612	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
21	B	807	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
20	4	605	CHL	C1D-ND-C4D	-3.83	103.62	106.33
25	L	306	BCR	C35-C13-C14	-3.83	117.56	122.92
20	x	608	CHL	C2D-C1D-ND	3.83	112.92	110.10
25	3	614	BCR	C37-C22-C21	-3.82	117.57	122.92
21	A	823	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
21	1	612	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
24	x	615	LUT	C39-C29-C30	-3.82	117.57	122.92
21	L	303	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
20	4	605	CHL	CHD-C4C-C3C	-3.82	119.02	124.98
25	L	306	BCR	C12-C13-C14	3.81	124.79	118.94
20	y	605	CHL	C2D-C1D-ND	3.81	112.91	110.10
21	3	608	CLA	CMB-C2B-C3B	3.81	131.81	124.68
24	2	619	LUT	C32-C33-C34	3.81	124.78	118.94
25	B	844	BCR	C36-C18-C17	-3.81	117.59	122.92
20	x	605	CHL	C1D-ND-C4D	-3.81	103.63	106.33
22	y	617	XAT	C12-C13-C14	3.81	124.78	118.94
21	2	609	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
20	y	608	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
20	2	601	CHL	C3B-C4B-NB	3.80	114.12	109.21
20	z	606	CHL	CAC-C3C-C4C	3.80	129.74	124.81
21	z	604	CLA	CMB-C2B-C3B	3.80	131.79	124.68
24	y	615	LUT	C15-C35-C34	3.80	131.26	123.47
25	A	852	BCR	C34-C9-C10	-3.80	117.60	122.92
31	z	618	NEX	C15-C35-C34	3.80	131.25	123.47
25	4	618	BCR	C37-C22-C21	-3.79	117.61	122.92
20	2	606	CHL	C2D-C1D-ND	3.79	112.90	110.10
21	K	203	CLA	CAA-C2A-C3A	-3.79	102.40	112.78
20	4	607	CHL	C3B-C4B-NB	3.79	114.11	109.21
21	z	603	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	B	845	BCR	C1-C6-C5	-3.78	117.28	122.61
24	x	616	LUT	C32-C33-C34	3.78	124.75	118.94
24	z	616	LUT	C40-C33-C34	-3.78	117.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	822	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
21	A	842	CLA	CMB-C2B-C3B	3.78	131.74	124.68
25	A	852	BCR	C36-C18-C17	-3.78	117.63	122.92
20	y	609	CHL	C3C-C4C-NC	3.77	114.80	110.57
21	A	816	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	L	306	BCR	C7-C8-C9	3.77	131.93	126.23
25	B	801	BCR	C10-C11-C12	3.77	134.98	123.22
25	B	846	BCR	C37-C22-C21	-3.76	117.65	122.92
20	y	607	CHL	C2D-C1D-ND	3.76	112.88	110.10
21	2	610	CLA	CAB-C3B-C4B	-3.76	122.68	128.46
25	A	853	BCR	C35-C13-C14	-3.76	117.66	122.92
25	B	844	BCR	C23-C22-C21	3.75	124.70	118.94
24	x	616	LUT	C40-C33-C34	-3.75	117.67	122.92
20	z	605	CHL	C2D-C1D-ND	3.75	112.87	110.10
25	A	852	BCR	C35-C13-C14	-3.75	117.67	122.92
20	1	601	CHL	C1-C2-C3	-3.75	119.56	126.04
27	A	801	CL0	CHC-C1C-C2C	-3.74	116.36	126.72
21	z	610	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
20	x	606	CHL	C1D-ND-C4D	-3.74	103.68	106.33
25	K	205	BCR	C23-C22-C21	3.74	124.68	118.94
25	B	846	BCR	C35-C13-C14	-3.74	117.69	122.92
20	z	607	CHL	C4-C3-C5	3.73	120.25	115.98
25	K	202	BCR	C36-C18-C17	-3.73	117.70	122.92
24	2	616	LUT	C20-C13-C14	-3.73	117.70	122.92
25	B	846	BCR	C8-C9-C10	3.73	124.66	118.94
31	x	618	NEX	C39-C29-C30	-3.72	117.71	122.92
27	A	801	CL0	C1-C2-C3	-3.72	119.60	126.04
25	L	305	BCR	C36-C18-C17	-3.72	117.71	122.92
20	4	605	CHL	C3B-C4B-NB	3.72	114.02	109.21
21	A	843	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
20	y	606	CHL	C1D-ND-C4D	-3.72	103.69	106.33
20	y	609	CHL	C1-C2-C3	-3.71	119.62	126.04
20	3	606	CHL	C4C-C3C-C2C	-3.71	101.48	106.90
20	z	607	CHL	C3B-C4B-NB	3.71	114.00	109.21
20	z	606	CHL	CHD-C4C-C3C	-3.70	119.40	124.84
21	1	603	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
20	z	607	CHL	CAC-C3C-C4C	3.70	129.61	124.81
20	4	605	CHL	C3D-C4D-ND	3.70	116.23	110.24
25	A	853	BCR	C11-C10-C9	3.70	132.59	127.31
25	A	853	BCR	C10-C11-C12	3.70	134.76	123.22
25	B	849	BCR	C34-C9-C10	-3.70	117.74	122.92
20	4	606	CHL	C1D-ND-C4D	-3.70	103.71	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	z	609	CHL	C3C-C4C-NC	3.69	114.71	110.57
21	A	844	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
25	A	851	BCR	C20-C21-C22	3.69	132.57	127.31
24	2	619	LUT	C7-C8-C9	-3.67	120.69	126.23
21	4	602	CLA	CMB-C2B-C3B	3.67	131.54	124.68
20	2	607	CHL	C1-C2-C3	-3.66	120.82	126.75
24	2	616	LUT	C12-C13-C14	3.66	124.56	118.94
21	1	602	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
25	B	849	BCR	C35-C13-C14	-3.66	117.79	122.92
20	2	601	CHL	C1D-ND-C4D	-3.66	103.73	106.33
24	z	615	LUT	C20-C13-C14	-3.66	117.80	122.92
21	B	819	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
21	B	841	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
22	1	614	XAT	C26-C27-C28	-3.65	118.27	125.99
25	J	102	BCR	C35-C13-C14	-3.65	117.81	122.92
20	y	608	CHL	C2D-C1D-ND	3.65	112.80	110.10
25	J	102	BCR	C12-C13-C14	3.65	124.55	118.94
25	3	614	BCR	C16-C15-C14	3.65	130.95	123.47
24	y	615	LUT	C7-C8-C9	-3.65	120.72	126.23
21	4	612	CLA	CMB-C2B-C3B	3.65	131.50	124.68
22	4	617	XAT	C12-C13-C14	3.65	124.54	118.94
25	B	801	BCR	C7-C8-C9	-3.65	120.72	126.23
21	A	832	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
25	O	205	BCR	C16-C15-C14	3.64	130.94	123.47
21	x	612	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
25	B	849	BCR	C12-C13-C14	3.64	124.53	118.94
21	A	809	CLA	CMB-C2B-C3B	3.64	131.49	124.68
21	B	825	CLA	CMB-C2B-C3B	3.64	131.48	124.68
25	K	205	BCR	C10-C11-C12	3.63	134.55	123.22
21	1	613	CLA	CAB-C3B-C4B	-3.63	122.88	128.46
20	y	607	CHL	C1D-ND-C4D	-3.63	103.76	106.33
25	B	846	BCR	C12-C13-C14	3.63	124.51	118.94
20	z	606	CHL	C1B-CHB-C4A	-3.63	122.94	130.12
20	x	609	CHL	CHD-C4C-C3C	-3.63	119.51	124.84
24	x	615	LUT	C15-C35-C34	3.62	130.90	123.47
20	y	607	CHL	C3B-C4B-NB	3.62	113.89	109.21
25	B	848	BCR	C15-C16-C17	3.62	130.89	123.47
20	4	607	CHL	CAC-C3C-C4C	3.61	129.50	124.81
21	A	810	CLA	CAA-C2A-C3A	-3.61	102.89	112.78
20	x	607	CHL	C3B-C4B-NB	3.61	113.88	109.21
31	y	618	NEX	C12-C13-C14	3.61	124.48	118.94
21	B	821	CLA	CAA-C2A-C3A	-3.61	102.91	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	605	CHL	C3B-C4B-NB	3.60	113.87	109.21
21	A	845	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
21	A	813	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
21	B	819	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
21	B	813	CLA	O2D-CGD-CBD	3.60	117.66	111.27
20	2	607	CHL	CAC-C3C-C4C	3.60	129.47	124.81
20	x	608	CHL	C1D-ND-C4D	-3.59	103.78	106.33
21	z	613	CLA	CMB-C2B-C3B	3.59	131.40	124.68
20	y	605	CHL	C3B-C4B-NB	3.59	113.85	109.21
21	3	601	CLA	CMB-C2B-C3B	3.59	131.40	124.68
24	x	615	LUT	C35-C15-C14	3.59	130.83	123.47
20	z	605	CHL	C3B-C4B-NB	3.59	113.85	109.21
20	4	606	CHL	CAC-C3C-C4C	3.59	129.47	124.81
20	x	607	CHL	CAC-C3C-C4C	3.59	129.47	124.81
21	A	830	CLA	CAA-C2A-C3A	-3.59	102.95	112.78
20	z	608	CHL	C3B-C4B-NB	3.59	113.85	109.21
21	1	612	CLA	O2D-CGD-CBD	3.59	117.64	111.27
21	B	813	CLA	CMB-C2B-C3B	3.59	131.39	124.68
21	4	603	CLA	CAB-C3B-C4B	-3.58	122.95	128.46
25	A	853	BCR	C12-C13-C14	3.58	124.44	118.94
20	2	606	CHL	C3B-C4B-NB	3.58	113.84	109.21
20	4	607	CHL	C1D-ND-C4D	-3.58	103.79	106.33
22	4	617	XAT	C19-C9-C8	-3.58	112.44	118.08
21	A	841	CLA	CMB-C2B-C3B	3.58	131.37	124.68
31	y	618	NEX	C20-C13-C14	-3.57	117.92	122.92
20	3	606	CHL	C1D-ND-C4D	-3.57	103.80	106.33
21	A	802	CLA	CMB-C2B-C3B	3.57	131.35	124.68
21	K	201	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	4	617	XAT	C17-C1-C16	3.56	112.63	107.37
20	z	609	CHL	C4A-NA-C1A	3.56	108.31	106.71
21	y	613	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
20	3	606	CHL	C3B-C4B-NB	3.56	113.81	109.21
20	4	615	CHL	C1D-ND-C4D	-3.56	103.81	106.33
24	1	616	LUT	C1-C6-C5	-3.56	117.60	122.61
25	B	847	BCR	C35-C13-C14	-3.56	117.94	122.92
21	B	835	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
25	A	848	BCR	C36-C18-C17	-3.55	117.95	122.92
20	x	606	CHL	CAC-C3C-C4C	3.55	129.41	124.81
20	2	605	CHL	C1D-ND-C4D	-3.55	103.81	106.33
25	L	306	BCR	C36-C18-C17	-3.55	117.96	122.92
21	A	830	CLA	CMB-C2B-C3B	3.55	131.31	124.68
21	A	827	CLA	CMB-C2B-C1B	-3.54	123.02	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	608	CHL	C3B-C4B-NB	3.54	113.79	109.21
21	A	818	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
20	4	605	CHL	C2D-C1D-ND	3.54	112.71	110.10
20	x	608	CHL	CAC-C3C-C4C	3.54	129.40	124.81
24	z	615	LUT	C12-C13-C14	3.54	124.37	118.94
27	A	801	CL0	C4C-C3C-C2C	-3.54	101.74	106.90
25	A	850	BCR	C16-C17-C18	3.54	132.36	127.31
20	y	608	CHL	CAC-C3C-C4C	3.54	129.40	124.81
21	2	612	CLA	CMB-C2B-C3B	3.54	131.29	124.68
22	y	617	XAT	C15-C35-C34	3.54	130.72	123.47
25	A	849	BCR	C20-C21-C22	3.53	132.35	127.31
25	L	305	BCR	C19-C18-C17	3.53	124.36	118.94
20	2	607	CHL	C1D-ND-C4D	-3.53	103.83	106.33
20	z	601	CHL	CAC-C3C-C4C	3.53	129.39	124.81
20	x	607	CHL	C3D-C4D-ND	3.53	115.94	110.24
21	A	833	CLA	CMB-C2B-C3B	3.52	131.27	124.68
20	z	605	CHL	C1D-ND-C4D	-3.52	103.83	106.33
25	L	305	BCR	C15-C16-C17	3.52	130.69	123.47
25	B	845	BCR	C12-C13-C14	3.52	124.35	118.94
25	K	205	BCR	C35-C13-C14	-3.52	117.99	122.92
25	A	851	BCR	C35-C13-C14	-3.52	117.99	122.92
20	y	606	CHL	C3B-C4B-NB	3.52	113.76	109.21
25	F	304	BCR	C10-C11-C12	3.51	134.19	123.22
20	2	606	CHL	C1D-ND-C4D	-3.51	103.84	106.33
21	K	206	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
21	B	821	CLA	CMB-C2B-C3B	3.51	131.25	124.68
25	3	614	BCR	C15-C16-C17	3.51	130.66	123.47
21	2	608	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
24	y	616	LUT	C40-C33-C34	-3.51	118.01	122.92
21	B	837	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
21	B	814	CLA	CMB-C2B-C3B	3.50	131.23	124.68
21	1	610	CLA	CAB-C3B-C4B	-3.50	123.08	128.46
25	A	852	BCR	C15-C16-C17	3.50	130.65	123.47
21	B	830	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
20	2	615	CHL	C1B-CHB-C4A	-3.50	123.19	130.12
20	y	606	CHL	CMD-C2D-C3D	-3.50	119.57	127.61
25	J	102	BCR	C8-C9-C10	3.50	124.31	118.94
25	B	801	BCR	C35-C13-C14	-3.49	118.03	122.92
21	G	203	CLA	CMB-C2B-C3B	3.49	131.21	124.68
20	2	606	CHL	C3D-C4D-ND	3.49	115.88	110.24
21	A	820	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
21	B	818	CLA	O2D-CGD-O1D	-3.49	117.02	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	617	XAT	C20-C13-C12	-3.48	112.59	118.08
21	B	805	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
20	x	609	CHL	C2D-C1D-ND	3.48	112.67	110.10
21	A	845	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
20	y	606	CHL	C2D-C1D-ND	3.48	112.67	110.10
21	A	839	CLA	CMB-C2B-C3B	3.48	131.19	124.68
21	3	608	CLA	CAA-C2A-C3A	-3.48	107.98	116.10
25	G	204	BCR	C36-C18-C17	-3.48	118.05	122.92
21	A	837	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
22	y	617	XAT	C40-C33-C34	-3.48	118.06	122.92
21	x	611	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
21	A	810	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	y	604	CLA	CMB-C2B-C3B	3.47	131.17	124.68
25	L	306	BCR	C19-C18-C17	3.47	124.27	118.94
25	L	305	BCR	C35-C13-C14	-3.47	118.06	122.92
21	x	610	CLA	CMB-C2B-C3B	3.46	131.15	124.68
21	B	812	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
21	B	829	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
21	B	811	CLA	CAB-C3B-C4B	-3.45	123.16	128.46
25	B	844	BCR	C8-C9-C10	3.45	124.24	118.94
21	A	840	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
21	4	609	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
21	B	809	CLA	CMB-C2B-C3B	3.45	131.13	124.68
21	A	826	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
21	A	805	CLA	CMB-C2B-C3B	3.45	131.12	124.68
21	L	302	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
20	2	601	CHL	CAC-C3C-C4C	3.44	129.28	124.81
21	A	831	CLA	CMB-C2B-C3B	3.44	131.12	124.68
21	B	807	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
20	y	606	CHL	C3D-C4D-ND	3.44	115.81	110.24
22	2	617	XAT	C32-C33-C34	3.44	124.22	118.94
22	y	617	XAT	C31-C30-C29	3.44	132.22	127.31
20	z	607	CHL	C3D-C4D-ND	3.44	115.80	110.24
25	B	845	BCR	C35-C13-C14	-3.44	118.11	122.92
21	3	604	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
20	4	606	CHL	C3D-C4D-ND	3.44	115.80	110.24
21	A	812	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
21	B	824	CLA	CMB-C2B-C3B	3.44	131.11	124.68
20	4	615	CHL	C3D-C4D-ND	3.44	115.80	110.24
21	B	826	CLA	CMB-C2B-C3B	3.43	131.10	124.68
21	1	608	CLA	CAB-C3B-C4B	-3.43	123.19	128.46
25	B	844	BCR	C35-C13-C14	-3.43	118.11	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	608	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
21	F	303	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
21	B	829	CLA	CMB-C2B-C3B	3.43	131.10	124.68
22	z	617	XAT	C20-C13-C14	-3.43	118.12	122.92
21	F	302	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
21	4	614	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
20	y	605	CHL	C1D-ND-C4D	-3.43	103.90	106.33
21	F	301	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
21	K	203	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
21	y	612	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
20	1	606	CHL	CAC-C3C-C4C	3.43	129.25	124.81
21	B	831	CLA	CMB-C2B-C3B	3.42	131.09	124.68
21	4	601	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
21	z	614	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
21	A	815	CLA	CMB-C2B-C3B	3.42	131.08	124.68
20	y	607	CHL	C3D-C4D-ND	3.42	115.77	110.24
21	4	611	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
24	1	616	LUT	C39-C29-C30	-3.42	118.13	122.92
21	A	828	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
20	x	608	CHL	C3D-C4D-ND	3.42	115.77	110.24
21	B	825	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
21	2	613	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	L	301	BCR	C19-C18-C17	3.41	124.18	118.94
21	J	101	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	L	305	BCR	C12-C13-C14	3.41	124.18	118.94
31	x	618	NEX	C19-C9-C10	-3.41	118.14	122.92
21	3	602	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
20	z	608	CHL	C3D-C4D-ND	3.41	115.75	110.24
24	1	616	LUT	C20-C13-C14	-3.41	118.15	122.92
21	A	835	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
21	A	821	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
20	z	605	CHL	C3D-C4D-ND	3.41	115.75	110.24
21	B	815	CLA	CMB-C2B-C3B	3.41	131.05	124.68
25	B	845	BCR	C16-C17-C18	3.41	132.17	127.31
25	B	843	BCR	C7-C8-C9	-3.41	121.09	126.23
21	B	808	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
20	1	601	CHL	C1B-CHB-C4A	-3.40	123.38	130.12
21	1	613	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
21	B	810	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
21	3	603	CLA	CMB-C2B-C3B	3.40	131.04	124.68
24	z	616	LUT	C31-C30-C29	3.40	132.16	127.31
21	A	810	CLA	O2D-CGD-O1D	-3.40	117.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	608	CLA	CMA-C3A-C2A	-3.40	108.17	116.10
25	A	851	BCR	C36-C18-C17	-3.40	118.17	122.92
31	x	618	NEX	C5-C4-C3	3.39	115.76	111.75
21	A	828	CLA	CMB-C2B-C3B	3.39	131.02	124.68
21	B	806	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
31	z	618	NEX	C40-C33-C34	-3.39	118.18	122.92
21	B	828	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
20	1	606	CHL	C1B-CHB-C4A	-3.39	123.41	130.12
21	B	838	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
24	1	616	LUT	C12-C13-C14	3.38	124.13	118.94
25	B	801	BCR	C12-C13-C14	3.38	124.13	118.94
22	x	617	XAT	C11-C10-C9	3.38	132.13	127.31
31	z	618	NEX	C35-C15-C14	3.38	130.40	123.47
21	B	837	CLA	CMB-C2B-C3B	3.38	131.00	124.68
21	4	613	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
21	A	824	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
20	x	601	CHL	CAC-C3C-C4C	3.37	129.19	124.81
21	A	811	CLA	CMB-C2B-C3B	3.37	130.99	124.68
21	3	609	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
21	A	817	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
20	2	605	CHL	C3D-C4D-ND	3.37	115.69	110.24
21	1	608	CLA	CAA-C2A-C3A	-3.37	108.24	116.10
20	y	601	CHL	CAC-C3C-C4C	3.37	129.18	124.81
24	y	615	LUT	C39-C29-C28	3.37	123.38	118.08
22	x	617	XAT	C10-C11-C12	3.37	133.72	123.22
21	y	603	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
20	z	601	CHL	C1B-CHB-C4A	-3.36	123.46	130.12
21	4	614	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
20	1	606	CHL	C3D-C4D-ND	3.36	115.67	110.24
25	F	304	BCR	C8-C9-C10	3.36	124.09	118.94
21	4	610	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
25	4	618	BCR	C35-C13-C14	-3.36	118.22	122.92
21	2	611	CLA	CMB-C2B-C3B	3.35	130.95	124.68
21	A	806	CLA	CMB-C2B-C3B	3.35	130.94	124.68
21	y	610	CLA	CMB-C2B-C3B	3.35	130.94	124.68
25	A	848	BCR	C19-C18-C17	3.35	124.08	118.94
21	B	816	CLA	CMB-C2B-C3B	3.35	130.94	124.68
21	z	602	CLA	CMB-C2B-C3B	3.35	130.94	124.68
24	y	616	LUT	C32-C33-C34	3.35	124.08	118.94
21	A	804	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
21	x	603	CLA	CMB-C2B-C3B	3.35	130.94	124.68
20	2	605	CHL	C3B-C4B-NB	3.35	113.54	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	603	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
24	2	616	LUT	C19-C9-C8	3.35	123.35	118.08
22	1	614	XAT	C27-C28-C29	-3.34	120.34	125.53
27	A	801	CL0	CAC-C3C-C4C	3.34	129.15	124.81
31	y	618	NEX	C40-C33-C34	-3.34	118.24	122.92
21	B	836	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
21	y	603	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	K	202	BCR	C8-C9-C10	3.34	124.06	118.94
21	B	815	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
21	A	802	CLA	CHB-C4A-NA	3.34	129.13	124.51
20	2	607	CHL	C3B-C4B-NB	3.34	113.52	109.21
21	A	803	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
20	4	607	CHL	CMB-C2B-C3B	3.33	130.91	124.68
20	y	605	CHL	C3D-C4D-ND	3.33	115.62	110.24
21	x	602	CLA	CMB-C2B-C3B	3.32	130.90	124.68
20	z	606	CHL	C2D-C1D-ND	3.32	112.55	110.10
21	B	827	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
21	2	602	CLA	CMB-C2B-C3B	3.32	130.88	124.68
21	B	820	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
21	G	201	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
21	B	804	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
25	B	801	BCR	C34-C9-C10	-3.31	118.28	122.92
25	A	850	BCR	C15-C14-C13	3.31	132.04	127.31
21	A	813	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
21	3	605	CLA	CAB-C3B-C4B	-3.31	123.38	128.46
21	3	612	CLA	CMB-C2B-C3B	3.31	130.87	124.68
25	O	204	BCR	C36-C18-C17	-3.31	118.29	122.92
21	A	836	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
21	B	820	CLA	CMB-C2B-C3B	3.30	130.86	124.68
20	x	607	CHL	CHD-C4C-C3C	-3.30	119.99	124.84
21	A	805	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
25	L	301	BCR	C23-C22-C21	3.30	124.01	118.94
21	B	804	CLA	CMB-C2B-C3B	3.30	130.85	124.68
21	4	604	CLA	CAB-C3B-C4B	-3.30	123.39	128.46
21	B	832	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
20	2	615	CHL	C2D-C1D-ND	3.30	112.53	110.10
21	L	302	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
21	1	607	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
22	1	614	XAT	C11-C10-C9	-3.29	122.61	127.31
25	B	847	BCR	C12-C13-C14	3.29	123.99	118.94
20	y	609	CHL	C4-C3-C5	3.29	120.81	115.27
21	A	827	CLA	O2D-CGD-O1D	-3.29	117.40	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	609	CLA	CMB-C2B-C3B	3.29	130.83	124.68
20	2	615	CHL	C3B-C4B-NB	3.29	113.46	109.21
21	B	826	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
20	2	615	CHL	CAC-C3C-C4C	3.29	129.08	124.81
20	x	605	CHL	CAC-C3C-C4C	3.29	129.07	124.81
20	x	605	CHL	C3D-C4D-ND	3.29	115.55	110.24
21	A	825	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
25	F	304	BCR	C37-C22-C21	-3.29	118.32	122.92
21	B	840	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
21	y	602	CLA	CMB-C2B-C3B	3.28	130.82	124.68
20	y	608	CHL	C3B-C4B-NB	3.28	113.45	109.21
20	z	605	CHL	CAC-C3C-C4C	3.28	129.06	124.81
25	3	614	BCR	C35-C13-C14	-3.28	118.33	122.92
21	1	604	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
25	A	852	BCR	C1-C6-C5	-3.28	118.00	122.61
25	3	614	BCR	C36-C18-C17	-3.28	118.33	122.92
20	3	606	CHL	C3D-C4D-ND	3.28	115.54	110.24
20	4	607	CHL	C3D-C4D-ND	3.27	115.53	110.24
21	y	604	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
21	z	612	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
21	B	808	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
21	L	303	CLA	CMB-C2B-C3B	3.27	130.79	124.68
21	K	204	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	O	205	BCR	C15-C16-C17	3.27	130.17	123.47
20	x	609	CHL	C3B-C4B-NB	3.27	113.43	109.21
21	3	605	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
21	O	203	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
21	A	842	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
21	B	841	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
21	A	808	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
21	O	202	CLA	CMB-C2B-C3B	3.26	130.77	124.68
21	A	838	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
31	z	618	NEX	C20-C13-C14	-3.25	118.37	122.92
21	4	604	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
21	z	611	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
21	1	611	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
21	x	614	CLA	CMB-C2B-C3B	3.25	130.75	124.68
25	I	101	BCR	C36-C18-C17	-3.25	118.38	122.92
21	A	835	CLA	CMB-C2B-C1B	-3.25	123.48	128.46
25	G	204	BCR	C19-C18-C17	3.24	123.92	118.94
20	1	606	CHL	C3B-C4B-NB	3.24	113.40	109.21
25	B	801	BCR	C15-C16-C17	3.24	130.11	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	z	601	CHL	C3B-C4B-NB	3.24	113.40	109.21
21	A	819	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
21	A	841	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
20	2	607	CHL	C3D-C4D-ND	3.23	115.47	110.24
21	B	822	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
21	y	611	CLA	CMB-C2B-C3B	3.23	130.72	124.68
21	B	833	CLA	CMB-C2B-C3B	3.23	130.72	124.68
31	z	618	NEX	C28-C29-C30	3.23	123.90	118.94
21	K	203	CLA	CMB-C2B-C3B	3.23	130.72	124.68
24	1	616	LUT	C8-C9-C10	3.23	123.90	118.94
24	y	616	LUT	C20-C13-C14	-3.23	118.40	122.92
22	x	617	XAT	C6-C7-C8	3.23	132.81	125.99
21	H	201	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	B	849	BCR	C36-C18-C17	-3.22	118.41	122.92
24	2	616	LUT	C35-C15-C14	3.22	130.07	123.47
21	2	610	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
24	z	615	LUT	C15-C35-C34	3.22	130.06	123.47
21	3	610	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
21	B	838	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
21	A	815	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
21	A	834	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	B	849	BCR	C30-C25-C24	3.21	124.87	115.78
31	x	618	NEX	C20-C13-C14	-3.21	118.42	122.92
20	x	601	CHL	C3B-C4B-NB	3.21	113.36	109.21
27	A	801	CL0	C2A-C1A-CHA	-3.21	118.24	123.86
21	G	202	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
24	z	616	LUT	C39-C29-C30	-3.21	118.43	122.92
21	x	603	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
24	x	616	LUT	C30-C31-C32	3.21	133.23	123.22
21	x	604	CLA	CMB-C2B-C3B	3.21	130.68	124.68
21	L	304	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
20	1	601	CHL	CHD-C4C-C3C	-3.21	120.13	124.84
21	B	811	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
21	A	823	CLA	CMB-C2B-C3B	3.20	130.67	124.68
21	A	829	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
25	G	204	BCR	C35-C13-C14	-3.20	118.44	122.92
21	A	831	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
20	z	609	CHL	C3D-C4D-ND	3.20	115.41	110.24
21	z	611	CLA	CMB-C2B-C1B	-3.19	123.55	128.46
21	G	201	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
21	B	823	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
20	2	615	CHL	C3D-C4D-ND	3.19	115.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	z	617	XAT	C12-C13-C14	3.19	123.83	118.94
25	A	850	BCR	C8-C9-C10	3.19	123.83	118.94
21	B	834	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
22	y	617	XAT	C32-C33-C34	3.19	123.83	118.94
21	1	610	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
20	x	609	CHL	O2D-CGD-O1D	-3.18	117.61	123.84
21	B	832	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
20	4	615	CHL	CAC-C3C-C4C	3.18	128.94	124.81
20	y	601	CHL	C1-C2-C3	-3.18	120.55	126.04
20	z	609	CHL	CAC-C3C-C4C	3.18	128.93	124.81
20	y	608	CHL	OMC-CMC-C2C	-3.18	118.51	125.69
21	A	816	CLA	CMB-C2B-C3B	3.17	130.62	124.68
25	L	305	BCR	C23-C22-C21	3.17	123.81	118.94
24	x	615	LUT	C20-C13-C14	-3.17	118.48	122.92
21	1	612	CLA	CMB-C2B-C3B	3.17	130.61	124.68
22	y	617	XAT	C39-C29-C30	-3.17	118.48	122.92
25	4	618	BCR	C15-C16-C17	3.17	129.96	123.47
25	A	851	BCR	C19-C18-C17	3.17	123.80	118.94
21	A	826	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
21	z	610	CLA	CMB-C2B-C3B	3.16	130.60	124.68
21	A	839	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
25	O	204	BCR	C35-C13-C14	-3.16	118.49	122.92
25	B	801	BCR	C36-C18-C17	-3.16	118.49	122.92
25	A	853	BCR	C36-C18-C17	-3.16	118.50	122.92
25	L	306	BCR	C10-C11-C12	3.16	133.08	123.22
25	A	848	BCR	C35-C13-C14	-3.16	118.50	122.92
21	B	839	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
25	O	204	BCR	C16-C15-C14	3.16	129.94	123.47
20	x	609	CHL	C3D-C4D-ND	3.16	115.34	110.24
20	x	606	CHL	C3B-C4B-NB	3.16	113.29	109.21
24	4	616	LUT	C35-C15-C14	3.16	129.94	123.47
20	z	601	CHL	C1-C2-C3	-3.16	120.59	126.04
21	B	816	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
21	3	605	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
21	4	601	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
20	y	609	CHL	C3D-C4D-ND	3.15	115.33	110.24
20	2	601	CHL	CHB-C4A-NA	3.15	128.86	124.51
25	A	849	BCR	C1-C6-C5	-3.15	118.18	122.61
25	J	102	BCR	C36-C18-C17	-3.14	118.52	122.92
20	x	606	CHL	C3D-C4D-ND	3.14	115.32	110.24
22	1	614	XAT	C31-C30-C29	-3.14	122.83	127.31
20	x	605	CHL	C6-C5-C3	-3.14	109.48	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	843	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	B	833	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	B	843	BCR	C15-C14-C13	3.14	131.79	127.31
21	z	614	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
24	z	616	LUT	C20-C13-C14	-3.13	118.53	122.92
21	B	817	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
21	A	844	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	B	803	CLA	CHB-C4A-NA	3.13	128.84	124.51
21	3	601	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
21	B	805	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
25	4	618	BCR	C36-C18-C17	-3.13	118.54	122.92
21	B	807	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	x	602	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
21	y	614	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
20	1	601	CHL	C3D-C4D-ND	3.12	115.28	110.24
22	x	617	XAT	C19-C9-C10	-3.12	118.56	122.92
24	3	613	LUT	C8-C9-C10	3.12	123.72	118.94
21	A	838	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	B	849	BCR	C15-C16-C17	3.11	129.85	123.47
21	B	810	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
21	A	840	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
22	2	617	XAT	C20-C13-C14	-3.11	118.57	122.92
21	1	602	CLA	CMB-C2B-C3B	3.11	130.50	124.68
21	1	603	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	4	617	XAT	C8-C9-C10	3.11	123.71	118.94
24	3	613	LUT	C19-C9-C10	-3.11	118.57	122.92
21	B	831	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
20	2	601	CHL	C3D-C4D-ND	3.11	115.26	110.24
22	z	617	XAT	C40-C33-C34	-3.10	118.57	122.92
24	x	616	LUT	C20-C13-C14	-3.10	118.57	122.92
24	x	615	LUT	C40-C33-C34	-3.10	118.58	122.92
20	y	609	CHL	CAC-C3C-C4C	3.10	128.84	124.81
21	1	603	CLA	CMB-C2B-C3B	3.10	130.48	124.68
21	B	811	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
21	3	611	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
21	A	809	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	4	617	XAT	C36-C21-C26	3.09	118.40	110.05
25	O	205	BCR	C35-C13-C14	-3.09	118.59	122.92
21	y	613	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
25	A	849	BCR	C37-C22-C21	-3.09	118.59	122.92
21	x	613	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	4	605	CHL	CMD-C2D-C3D	-3.09	120.50	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	101	BCR	C35-C13-C14	-3.09	118.59	122.92
21	O	201	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
22	4	617	XAT	C25-C24-C23	-3.08	106.65	112.75
20	z	609	CHL	CMD-C2D-C3D	-3.08	120.52	127.61
20	1	606	CHL	CHD-C4C-C3C	-3.08	120.31	124.84
21	z	603	CLA	CMB-C2B-C3B	3.08	130.44	124.68
21	1	608	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
21	B	814	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	K	205	BCR	C21-C20-C19	3.08	132.82	123.22
24	y	615	LUT	C15-C14-C13	3.08	131.70	127.31
21	1	605	CLA	CMB-C2B-C3B	3.08	130.44	124.68
21	B	803	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
21	B	822	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	2	616	LUT	C35-C34-C33	3.07	131.70	127.31
22	2	617	XAT	C12-C13-C14	3.07	123.66	118.94
24	y	616	LUT	C35-C15-C14	3.07	129.77	123.47
25	B	844	BCR	C12-C13-C14	3.07	123.65	118.94
21	B	827	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
20	z	609	CHL	C6-C5-C3	-3.07	109.60	114.62
24	3	613	LUT	C20-C13-C14	-3.07	118.63	122.92
24	z	615	LUT	C40-C33-C34	-3.07	118.63	122.92
21	A	824	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
20	z	601	CHL	C3D-C4D-ND	3.07	115.20	110.24
24	4	616	LUT	C40-C33-C34	-3.07	118.63	122.92
25	B	848	BCR	C36-C18-C17	-3.07	118.63	122.92
21	4	613	CLA	CHB-C4A-NA	3.07	128.75	124.51
20	y	608	CHL	C3D-C4D-ND	3.06	115.19	110.24
31	z	618	NEX	C32-C33-C34	3.06	123.64	118.94
21	A	822	CLA	CMB-C2B-C3B	3.06	130.41	124.68
31	y	618	NEX	C32-C33-C34	3.05	123.63	118.94
31	x	618	NEX	C30-C31-C32	3.05	132.74	123.22
20	4	605	CHL	C2A-C1A-CHA	-3.05	118.52	123.86
21	B	809	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	y	617	XAT	C10-C11-C12	3.05	132.74	123.22
20	z	609	CHL	C1-C2-C3	-3.05	120.77	126.04
21	B	841	CLA	CMB-C2B-C3B	3.05	130.39	124.68
21	B	833	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
21	A	822	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
20	4	605	CHL	CHB-C4A-NA	3.05	128.73	124.51
21	A	806	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
25	O	205	BCR	C36-C18-C17	-3.05	118.66	122.92
21	A	832	CLA	CMB-C2B-C3B	3.04	130.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	602	CLA	C1-C2-C3	-3.04	120.78	126.04
21	4	613	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
21	A	814	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
21	B	812	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
20	x	601	CHL	C3D-C4D-ND	3.03	115.14	110.24
21	B	808	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
20	z	605	CHL	O2D-CGD-O1D	-3.03	117.91	123.84
20	2	605	CHL	CAC-C3C-C4C	3.03	129.66	125.04
21	1	605	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	A	819	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	B	824	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	3	613	LUT	C35-C34-C33	3.03	131.63	127.31
20	z	606	CHL	C3D-C4D-ND	3.02	115.13	110.24
22	x	617	XAT	C40-C33-C34	-3.02	118.69	122.92
21	x	611	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	B	849	BCR	C19-C18-C17	3.02	123.58	118.94
25	A	849	BCR	C35-C13-C14	-3.02	118.69	122.92
20	z	608	CHL	O2A-CGA-CBA	3.02	121.38	111.91
25	4	618	BCR	C12-C13-C14	3.02	123.57	118.94
20	y	605	CHL	CAC-C3C-C4C	3.01	128.72	124.81
21	z	602	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
24	4	616	LUT	C20-C13-C14	-3.01	118.70	122.92
20	1	601	CHL	C2D-C1D-ND	3.01	112.32	110.10
21	1	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	y	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	B	839	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
21	A	807	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
21	2	608	CLA	CMB-C2B-C3B	3.00	130.30	124.68
21	2	602	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
21	A	837	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
21	A	834	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
20	x	605	CHL	O2A-CGA-CBA	3.00	121.31	111.91
21	A	832	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
21	O	203	CLA	CAA-C2A-C3A	-2.99	109.11	116.10
21	F	302	CLA	CHB-C4A-NA	2.99	128.65	124.51
21	K	206	CLA	CMB-C2B-C3B	2.99	130.28	124.68
21	A	816	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	B	834	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	x	617	XAT	C15-C14-C13	2.99	131.58	127.31
21	B	802	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	1	604	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	2	604	CLA	CHB-C4A-NA	2.99	128.64	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	617	XAT	O23-C23-C22	-2.99	103.87	109.80
20	y	601	CHL	C4-C3-C5	2.99	120.29	115.27
25	O	204	BCR	C19-C18-C17	2.98	123.52	118.94
21	B	836	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
20	z	601	CHL	C4A-NA-C1A	2.98	108.05	106.71
21	2	604	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
21	A	821	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	O	201	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
21	A	830	CLA	CHB-C4A-NA	2.97	128.62	124.51
25	A	849	BCR	C19-C18-C17	2.97	123.50	118.94
31	y	618	NEX	C19-C9-C10	-2.97	118.76	122.92
25	3	614	BCR	C19-C18-C17	2.97	123.50	118.94
21	F	302	CLA	CMB-C2B-C3B	2.97	130.23	124.68
21	B	817	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	A	830	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
21	B	830	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
20	y	607	CHL	C6-C5-C3	-2.97	109.77	114.62
21	4	610	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
25	F	304	BCR	C1-C6-C5	-2.96	118.44	122.61
25	K	202	BCR	C21-C20-C19	2.96	132.47	123.22
24	y	616	LUT	C28-C29-C30	2.96	123.49	118.94
21	A	818	CLA	CMB-C2B-C3B	2.96	130.22	124.68
20	1	601	CHL	C3B-C4B-NB	2.96	113.04	109.21
20	1	606	CHL	C2D-C1D-ND	2.96	112.29	110.10
20	z	601	CHL	CHD-C4C-C3C	-2.96	120.49	124.84
21	A	814	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
31	x	618	NEX	C36-C21-C22	-2.96	103.84	108.98
21	B	830	CLA	CMB-C2B-C3B	2.96	130.21	124.68
21	F	303	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
20	x	607	CHL	C2D-C1D-ND	2.96	112.28	110.10
21	A	823	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
21	A	833	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
31	x	618	NEX	C12-C13-C14	2.95	123.47	118.94
25	A	848	BCR	C16-C15-C14	2.95	129.52	123.47
21	A	803	CLA	CMB-C2B-C3B	2.95	130.20	124.68
21	4	609	CLA	CMB-C2B-C3B	2.95	130.19	124.68
20	z	606	CHL	C3B-C4B-NB	2.95	113.02	109.21
25	B	848	BCR	C16-C15-C14	2.95	129.51	123.47
25	B	848	BCR	C35-C13-C14	-2.95	118.79	122.92
20	x	607	CHL	C4-C3-C5	2.95	120.23	115.27
21	A	824	CLA	CAA-C2A-C3A	-2.95	109.22	116.10
21	A	827	CLA	CMB-C2B-C3B	2.94	130.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	853	BCR	C34-C9-C10	-2.94	118.80	122.92
25	B	843	BCR	C36-C18-C17	-2.94	118.80	122.92
21	y	612	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	2	617	XAT	C40-C33-C34	-2.94	118.81	122.92
21	x	612	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	B	845	BCR	C21-C20-C19	2.94	132.38	123.22
21	1	610	CLA	CAA-C2A-C3A	-2.94	109.25	116.10
20	y	607	CHL	CHB-C4A-NA	2.93	128.57	124.51
21	2	604	CLA	CMB-C2B-C3B	2.93	130.17	124.68
21	K	201	CLA	CMB-C2B-C3B	2.93	130.17	124.68
21	B	840	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	y	608	CHL	O2A-CGA-CBA	2.93	121.11	111.91
20	z	606	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
21	x	604	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	z	601	CHL	C6-C5-C3	-2.93	109.83	114.62
21	A	825	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	y	613	CLA	CMB-C2B-C3B	2.92	130.15	124.68
21	1	609	CLA	CHB-C4A-NA	2.92	128.56	124.51
31	x	618	NEX	C35-C15-C14	2.92	129.46	123.47
20	z	607	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
21	B	828	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	2	607	CHL	CHB-C4A-NA	2.92	128.55	124.51
25	B	846	BCR	C36-C18-C17	-2.92	118.84	122.92
21	1	613	CLA	CAA-C2A-C3A	-2.92	109.30	116.10
21	G	203	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
21	B	803	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
20	z	607	CHL	CHB-C4A-NA	2.91	128.54	124.51
25	F	304	BCR	C16-C17-C18	2.91	131.47	127.31
21	J	101	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	B	801	BCR	C11-C10-C9	2.91	131.47	127.31
21	B	823	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	x	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	4	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	A	852	BCR	C21-C20-C19	2.91	132.30	123.22
21	G	202	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	A	802	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
21	A	808	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
21	y	614	CLA	CHB-C4A-NA	2.90	128.53	124.51
25	A	849	BCR	C36-C18-C17	-2.90	118.86	122.92
20	x	607	CHL	C1-C2-C3	-2.90	121.02	126.04
25	G	204	BCR	C16-C15-C14	2.90	129.42	123.47
25	A	852	BCR	C12-C13-C14	2.90	123.39	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	611	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	x	615	LUT	C39-C29-C28	2.90	122.64	118.08
25	I	101	BCR	C19-C18-C17	2.90	123.39	118.94
21	2	610	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
21	B	835	CLA	CMB-C2B-C3B	2.89	130.09	124.68
20	1	601	CHL	O2A-CGA-CBA	2.89	120.99	111.91
20	4	607	CHL	CHB-C4A-NA	2.89	128.51	124.51
21	2	610	CLA	C1A-CHA-C4D	-2.89	121.67	125.72
24	x	616	LUT	C35-C15-C14	2.89	129.40	123.47
20	y	608	CHL	C1D-ND-C4D	-2.89	104.28	106.33
21	2	604	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
31	z	618	NEX	C12-C13-C14	2.89	123.37	118.94
20	x	609	CHL	C1B-CHB-C4A	-2.89	124.40	130.12
25	I	101	BCR	C16-C15-C14	2.89	129.39	123.47
21	z	603	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	3	614	BCR	C12-C13-C14	2.89	123.37	118.94
20	z	608	CHL	CHB-C4A-NA	2.89	128.50	124.51
22	2	617	XAT	C30-C31-C32	2.89	132.22	123.22
25	B	844	BCR	C19-C18-C17	2.89	123.37	118.94
25	G	204	BCR	C30-C25-C26	-2.88	118.55	122.61
20	y	601	CHL	CHD-C4C-C3C	-2.88	120.60	124.84
21	1	609	CLA	C1C-C2C-C3C	-2.88	104.43	107.07
20	y	601	CHL	C3B-C4B-NB	2.88	112.94	109.21
21	3	607	CLA	CMB-C2B-C3B	2.88	130.07	124.68
21	B	806	CLA	CMB-C2B-C3B	2.88	130.07	124.68
21	A	843	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	2	605	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
21	A	835	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	B	847	BCR	C36-C18-C17	-2.88	118.89	122.92
20	2	607	CHL	O2A-CGA-CBA	2.88	120.94	111.91
21	B	811	CLA	CHB-C4A-NA	2.88	128.49	124.51
21	B	822	CLA	CHB-C4A-NA	2.87	128.49	124.51
21	y	614	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	4	605	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
20	z	607	CHL	O2A-CGA-CBA	2.87	120.90	111.91
21	A	804	CLA	CMB-C2B-C3B	2.87	130.04	124.68
21	1	611	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
21	A	817	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
21	A	804	CLA	CHB-C4A-NA	2.86	128.47	124.51
21	z	604	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
21	B	827	CLA	CHB-C4A-NA	2.86	128.47	124.51
21	3	607	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	304	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	2	615	CHL	C1D-ND-C4D	-2.86	104.31	106.33
21	A	803	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
21	A	810	CLA	C1-C2-C3	-2.86	122.13	126.75
27	A	801	CL0	O2A-CGA-CBA	2.86	120.87	111.91
20	y	605	CHL	CMD-C2D-C3D	-2.86	121.05	127.61
22	4	617	XAT	C15-C35-C34	2.85	129.32	123.47
21	B	810	CLA	CMB-C2B-C3B	2.85	130.00	124.68
21	A	826	CLA	CMB-C2B-C3B	2.85	130.00	124.68
24	x	615	LUT	C12-C13-C14	2.84	123.31	118.94
24	2	616	LUT	C30-C31-C32	2.84	132.09	123.22
31	z	618	NEX	C19-C9-C10	-2.84	118.94	122.92
20	y	609	CHL	CMD-C2D-C3D	-2.84	121.07	127.61
21	B	808	CLA	CMB-C2B-C3B	2.84	130.00	124.68
21	4	612	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	A	853	BCR	C15-C16-C17	2.84	129.29	123.47
21	A	844	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	2	617	XAT	C35-C34-C33	2.84	131.36	127.31
20	z	601	CHL	CMD-C2D-C3D	-2.84	121.09	127.61
21	4	608	CLA	CMB-C2B-C3B	2.84	129.98	124.68
21	z	602	CLA	C1-C2-C3	2.83	130.94	126.04
21	A	811	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	A	815	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	A	814	CLA	CHB-C4A-NA	2.83	128.43	124.51
30	B	850	DGD	C2G-O2G-C1B	-2.83	110.83	117.79
25	A	849	BCR	C16-C17-C18	2.83	131.34	127.31
24	z	615	LUT	C32-C33-C34	2.83	123.28	118.94
21	z	614	CLA	CHB-C4A-NA	2.83	128.42	124.51
21	2	612	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
21	A	807	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	B	843	BCR	C35-C13-C14	-2.82	118.97	122.92
20	y	607	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
20	x	607	CHL	C1D-ND-C4D	-2.82	104.33	106.33
21	A	812	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
21	2	613	CLA	CMB-C2B-C3B	2.82	129.95	124.68
21	3	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	2	615	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
20	x	608	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
21	J	101	CLA	CMB-C2B-C3B	2.81	129.94	124.68
21	4	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
21	B	827	CLA	CMB-C2B-C3B	2.81	129.94	124.68
21	2	603	CLA	CMB-C2B-C1B	-2.81	124.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	601	CHL	C4A-NA-C1A	2.81	107.97	106.71
20	x	607	CHL	C1B-CHB-C4A	-2.81	124.55	130.12
20	x	607	CHL	C6-C5-C3	-2.81	110.03	114.62
21	3	612	CLA	O2D-CGD-O1D	-2.81	117.71	124.09
21	B	806	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	4	614	CLA	CMB-C2B-C3B	2.81	129.93	124.68
20	4	607	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
21	4	613	CLA	CMB-C2B-C3B	2.80	129.93	124.68
20	1	601	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
21	A	836	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	y	612	CLA	CMB-C2B-C3B	2.80	129.92	124.68
20	x	605	CHL	C1-C2-C3	-2.80	121.20	126.04
21	A	845	CLA	CHB-C4A-NA	2.80	128.39	124.51
20	x	609	CHL	C1D-ND-C4D	-2.80	104.34	106.33
21	A	829	CLA	CMB-C2B-C3B	2.80	129.92	124.68
21	B	804	CLA	CAA-C2A-C3A	-2.80	109.57	116.10
20	x	601	CHL	CMD-C2D-C3D	-2.80	121.18	127.61
21	4	608	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
21	y	611	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
24	y	615	LUT	C10-C11-C12	2.79	131.94	123.22
20	y	606	CHL	CAC-C3C-C4C	2.79	128.44	124.81
20	x	606	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
21	B	819	CLA	CMB-C2B-C3B	2.79	129.91	124.68
21	x	614	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
20	x	601	CHL	C6-C5-C3	-2.79	110.05	114.62
21	B	825	CLA	CHB-C4A-NA	2.79	128.37	124.51
20	x	601	CHL	CHD-C4C-C3C	-2.79	120.74	124.84
20	2	606	CHL	CHB-C4A-NA	2.79	128.37	124.51
21	A	837	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	z	605	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
21	3	607	CLA	CHB-C4A-NA	2.79	128.37	124.51
20	x	605	CHL	C4-C3-C5	2.79	119.96	115.27
21	4	610	CLA	CMB-C2B-C3B	2.79	129.89	124.68
21	O	203	CLA	CAB-C3B-C2B	2.78	130.14	124.69
20	z	607	CHL	C2A-C1A-CHA	-2.78	118.99	123.86
20	z	609	CHL	C3B-C4B-NB	2.78	112.81	109.21
21	4	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
21	1	607	CLA	CHB-C4A-NA	2.78	128.36	124.51
24	y	615	LUT	C12-C13-C14	2.78	123.20	118.94
31	y	618	NEX	C15-C35-C34	2.78	129.16	123.47
21	3	612	CLA	CHB-C4A-NA	2.78	128.35	124.51
21	2	610	CLA	CAB-C3B-C2B	2.77	130.12	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	832	CLA	CHB-C4A-NA	2.77	128.34	124.51
21	z	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
21	B	836	CLA	CMB-C2B-C3B	2.77	129.86	124.68
21	B	834	CLA	CHB-C4A-NA	2.77	128.34	124.51
21	3	604	CLA	O2D-CGD-O1D	-2.77	117.81	124.09
20	z	609	CHL	CMB-C2B-C3B	2.77	129.85	124.68
21	A	810	CLA	CMB-C2B-C3B	2.77	129.85	124.68
21	2	611	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	x	617	XAT	C20-C13-C14	-2.77	119.05	122.92
21	O	202	CLA	O2D-CGD-O1D	-2.77	117.81	124.09
20	x	605	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
24	3	613	LUT	C10-C11-C12	2.76	131.84	123.22
21	2	613	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
21	y	610	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
25	B	801	BCR	C19-C18-C17	2.76	123.18	118.94
21	A	812	CLA	CMB-C2B-C3B	2.76	129.85	124.68
21	3	604	CLA	CMB-C2B-C3B	2.76	129.84	124.68
20	2	607	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
21	A	809	CLA	CHB-C4A-NA	2.76	128.33	124.51
21	1	608	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
20	2	601	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
24	y	616	LUT	C12-C13-C14	2.75	123.16	118.94
20	z	609	CHL	O2A-CGA-CBA	2.75	120.54	111.91
20	z	609	CHL	C4-C3-C5	2.75	119.90	115.27
20	3	606	CHL	CAC-C3C-C4C	2.75	128.38	124.81
21	F	303	CLA	CMB-C2B-C3B	2.75	129.82	124.68
24	y	615	LUT	C20-C13-C14	-2.75	119.07	122.92
20	x	609	CHL	CMD-C2D-C3D	-2.74	121.30	127.61
20	x	601	CHL	OMC-CMC-C2C	-2.74	119.49	125.69
20	y	605	CHL	CAA-C2A-C3A	-2.74	109.70	116.10
20	2	606	CHL	C2A-C1A-CHA	-2.74	119.07	123.86
22	2	617	XAT	C15-C14-C13	2.74	131.22	127.31
20	y	609	CHL	C6-C5-C3	-2.74	110.14	114.62
21	B	812	CLA	CMB-C2B-C3B	2.74	129.80	124.68
21	B	837	CLA	CHB-C4A-NA	2.74	128.30	124.51
21	B	817	CLA	CHB-C4A-NA	2.74	128.29	124.51
20	x	605	CHL	CHB-C4A-NA	2.73	128.29	124.51
21	F	303	CLA	CAA-C2A-C3A	-2.73	109.72	116.10
21	A	845	CLA	CMB-C2B-C3B	2.73	129.79	124.68
20	y	607	CHL	C2A-C1A-CHA	-2.73	119.08	123.86
21	2	603	CLA	CMB-C2B-C3B	2.73	129.79	124.68
21	B	809	CLA	CHB-C4A-NA	2.73	128.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	205	BCR	C8-C9-C10	2.73	123.13	118.94
20	x	601	CHL	C2D-C1D-ND	2.73	112.12	110.10
20	y	601	CHL	CMB-C2B-C3B	2.73	129.79	124.68
25	J	102	BCR	C15-C16-C17	2.73	129.07	123.47
20	y	609	CHL	CMB-C2B-C3B	2.73	129.79	124.68
21	x	613	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	B	844	BCR	C30-C25-C26	-2.73	118.77	122.61
21	B	802	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
21	A	825	CLA	CMB-C2B-C3B	2.73	129.78	124.68
21	B	835	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	A	842	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
21	4	611	CLA	CMB-C2B-C3B	2.73	129.78	124.68
25	K	205	BCR	C16-C15-C14	2.73	129.06	123.47
24	z	616	LUT	C35-C15-C14	2.73	129.06	123.47
21	1	604	CLA	CHB-C4A-NA	2.72	128.28	124.51
24	2	619	LUT	C28-C29-C30	2.72	123.12	118.94
25	A	848	BCR	C12-C13-C14	2.72	123.12	118.94
25	L	301	BCR	C10-C11-C12	2.72	131.71	123.22
21	A	829	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	A	848	BCR	C29-C30-C25	2.72	114.67	110.48
20	y	607	CHL	C4-C3-C5	2.72	119.85	115.27
20	4	606	CHL	CHB-C4A-NA	2.72	128.27	124.51
21	1	609	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
20	x	607	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
20	z	609	CHL	OMC-CMC-C2C	-2.72	119.54	125.69
21	B	830	CLA	CHB-C4A-NA	2.72	128.27	124.51
21	2	608	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
21	4	603	CLA	CAB-C3B-C2B	2.71	130.00	124.69
21	B	836	CLA	C1-C2-C3	-2.71	122.36	126.75
20	y	601	CHL	OMC-CMC-C2C	-2.71	119.55	125.69
20	x	608	CHL	CAA-C2A-C3A	-2.71	109.77	116.10
21	1	604	CLA	CMB-C2B-C3B	2.71	129.75	124.68
21	B	816	CLA	CHB-C4A-NA	2.71	128.26	124.51
21	z	610	CLA	CHB-C4A-NA	2.71	128.26	124.51
20	z	608	CHL	CMD-C2D-C3D	-2.71	121.37	127.61
20	x	608	CHL	CMB-C2B-C3B	2.71	129.75	124.68
21	1	613	CLA	CAB-C3B-C2B	2.71	130.00	124.69
20	z	605	CHL	CHB-C4A-NA	2.71	128.26	124.51
21	A	835	CLA	CHB-C4A-NA	2.71	128.25	124.51
21	K	201	CLA	CHB-C4A-NA	2.71	128.25	124.51
21	L	303	CLA	O2D-CGD-CBD	2.70	116.07	111.27
20	x	609	CHL	CMB-C2B-C3B	2.70	129.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	834	CLA	CMB-C2B-C3B	2.70	129.73	124.68
25	4	618	BCR	C19-C18-C17	2.70	123.08	118.94
21	B	805	CLA	CHB-C4A-NA	2.70	128.24	124.51
21	B	811	CLA	CAB-C3B-C2B	2.70	129.97	124.69
21	2	603	CLA	CHB-C4A-NA	2.70	128.24	124.51
21	B	821	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	A	853	BCR	C19-C18-C17	2.70	123.08	118.94
24	3	613	LUT	C40-C33-C34	-2.70	119.14	122.92
21	2	609	CLA	CHB-C4A-NA	2.70	128.24	124.51
20	y	601	CHL	O2A-CGA-CBA	2.69	120.36	111.91
25	A	851	BCR	C10-C11-C12	-2.69	114.81	123.22
20	y	608	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
20	2	606	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
21	A	804	CLA	O2D-CGD-CBD	2.69	116.05	111.27
20	x	601	CHL	O2A-CGA-CBA	2.69	120.35	111.91
20	y	605	CHL	CMB-C2B-C3B	2.69	129.71	124.68
21	A	842	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	B	814	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	x	610	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	3	605	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	K	202	BCR	C10-C11-C12	2.69	131.60	123.22
21	2	608	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	A	819	CLA	CHB-C4A-NA	2.69	128.23	124.51
20	z	601	CHL	C2D-C1D-ND	2.69	112.08	110.10
22	z	617	XAT	C15-C35-C34	2.68	128.97	123.47
21	x	604	CLA	CHB-C4A-NA	2.68	128.22	124.51
21	3	609	CLA	CHB-C4A-NA	2.68	128.22	124.51
20	y	601	CHL	C2D-C1D-ND	2.68	112.08	110.10
20	y	609	CHL	CHD-C1D-C2D	2.68	131.10	125.48
22	z	617	XAT	C28-C29-C30	2.68	123.06	118.94
21	A	836	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	x	617	XAT	C37-C21-C22	-2.68	104.33	108.98
21	4	614	CLA	CHB-C4A-NA	2.68	128.22	124.51
21	F	301	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
21	A	808	CLA	CMB-C2B-C3B	2.68	129.69	124.68
20	4	615	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
21	A	805	CLA	CHB-C4A-NA	2.68	128.21	124.51
21	1	607	CLA	CMB-C2B-C3B	2.68	129.68	124.68
21	1	610	CLA	O2D-CGD-O1D	-2.67	118.02	124.09
21	B	802	CLA	CHB-C4A-NA	2.67	128.21	124.51
21	4	601	CLA	CMB-C2B-C3B	2.67	129.68	124.68
21	A	844	CLA	O2A-CGA-O1A	-2.67	116.84	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	z	616	LUT	C12-C13-C14	2.67	123.04	118.94
20	z	601	CHL	O2A-CGA-CBA	2.67	120.30	111.91
20	y	609	CHL	C3B-C4B-NB	2.67	112.67	109.21
21	K	204	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
21	3	601	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	G	204	BCR	C23-C22-C21	2.67	123.04	118.94
25	O	204	BCR	C12-C13-C14	2.67	123.04	118.94
24	3	613	LUT	C11-C10-C9	2.67	131.12	127.31
20	4	606	CHL	C2A-C1A-CHA	-2.67	119.19	123.86
25	B	846	BCR	C15-C16-C17	2.67	128.94	123.47
21	y	613	CLA	CHB-C4A-NA	2.67	128.20	124.51
21	z	602	CLA	CHB-C4A-NA	2.67	128.20	124.51
21	A	838	CLA	CMB-C2B-C3B	2.66	129.66	124.68
21	3	611	CLA	CAA-C2A-C3A	-2.66	109.88	116.10
21	A	841	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	2	619	LUT	C20-C13-C14	-2.66	119.20	122.92
20	y	607	CHL	CMB-C2B-C3B	2.66	129.65	124.68
21	y	603	CLA	CMB-C2B-C3B	2.66	129.65	124.68
24	2	619	LUT	C11-C10-C9	2.66	131.10	127.31
21	B	804	CLA	CHB-C4A-NA	2.66	128.19	124.51
21	B	834	CLA	CMB-C2B-C3B	2.66	129.65	124.68
21	O	203	CLA	CMB-C2B-C3B	2.66	129.89	124.69
24	x	616	LUT	C12-C13-C14	2.66	123.02	118.94
20	y	601	CHL	C3D-C4D-ND	2.66	114.53	110.24
21	L	302	CLA	CMB-C2B-C3B	2.65	129.65	124.68
21	3	608	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	G	202	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	y	604	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	K	202	BCR	C24-C23-C22	-2.65	122.23	126.23
20	4	606	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
21	A	813	CLA	CHB-C4A-NA	2.65	128.18	124.51
20	x	607	CHL	OMC-CMC-C2C	-2.65	119.69	125.69
21	4	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	4	617	XAT	C6-C7-C8	-2.65	120.39	125.99
21	B	816	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
21	2	603	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
20	z	605	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
21	B	817	CLA	CMB-C2B-C3B	2.65	129.63	124.68
20	z	606	CHL	C1D-ND-C4D	-2.65	104.45	106.33
21	z	613	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
25	I	101	BCR	C12-C13-C14	2.64	123.00	118.94
21	B	815	CLA	CHB-C4A-NA	2.64	128.17	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	606	CHL	CMD-C2D-C3D	-2.64	121.54	127.61
21	4	601	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	A	834	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	3	610	CLA	CAA-C2A-C3A	-2.64	109.94	116.10
21	A	843	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	B	839	CLA	CMB-C2B-C3B	2.64	129.62	124.68
21	3	608	CLA	CMC-C2C-C1C	2.64	129.06	125.04
21	B	807	CLA	CHB-C4A-NA	2.64	128.16	124.51
20	y	606	CHL	C2A-C1A-CHA	-2.64	119.25	123.86
21	A	822	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	A	819	CLA	CMB-C2B-C3B	2.64	129.61	124.68
20	1	601	CHL	C4-C3-C5	2.64	119.71	115.27
21	B	828	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	B	810	CLA	CHB-C4A-NA	2.63	128.16	124.51
21	3	610	CLA	CMB-C2B-C3B	2.63	129.61	124.68
23	1	615	LHG	O8-C23-C24	2.63	120.17	111.91
21	A	823	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	A	821	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	x	617	XAT	O4-C5-C4	-2.63	111.41	113.38
21	4	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	A	821	CLA	CMB-C2B-C3B	2.63	129.60	124.68
21	J	101	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	B	828	CLA	CMB-C2B-C3B	2.63	129.60	124.68
24	x	615	LUT	C32-C33-C34	2.63	122.97	118.94
31	x	618	NEX	C28-C29-C30	2.63	122.97	118.94
21	3	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	G	201	CLA	CHB-C4A-NA	2.63	128.15	124.51
20	x	607	CHL	O2A-CGA-CBA	2.63	120.15	111.91
20	y	605	CHL	C1B-CHB-C4A	-2.63	124.92	130.12
20	y	608	CHL	CMB-C2B-C3B	2.63	129.59	124.68
21	1	613	CLA	CMB-C2B-C3B	2.62	129.83	124.69
21	B	806	CLA	CHB-C4A-NA	2.62	128.14	124.51
21	B	841	CLA	O2D-CGD-CBD	2.62	115.93	111.27
20	y	609	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
24	3	613	LUT	C32-C33-C34	2.62	122.96	118.94
21	A	816	CLA	CHB-C4A-NA	2.62	128.14	124.51
21	B	819	CLA	CHB-C4A-NA	2.62	128.14	124.51
21	1	608	CLA	CHB-C4A-NA	2.62	128.13	124.51
21	B	838	CLA	CHB-C4A-NA	2.62	128.13	124.51
21	L	304	CLA	CMB-C2B-C3B	2.62	129.57	124.68
20	z	605	CHL	CMB-C2B-C3B	2.62	129.57	124.68
21	4	611	CLA	CHB-C4A-NA	2.62	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	803	CLA	CMB-C2B-C3B	2.61	129.57	124.68
21	1	602	CLA	CHB-C4A-NA	2.61	128.13	124.51
21	x	614	CLA	CHB-C4A-NA	2.61	128.13	124.51
20	2	607	CHL	C5-C3-C4	2.61	120.37	114.60
21	3	604	CLA	CHB-C4A-NA	2.61	128.12	124.51
21	1	613	CLA	O2D-CGD-O1D	-2.61	118.17	124.09
21	y	614	CLA	CMB-C2B-C3B	2.61	129.56	124.68
24	x	615	LUT	C8-C9-C10	2.61	122.94	118.94
21	4	608	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	O	205	BCR	C12-C13-C14	2.61	122.94	118.94
21	F	301	CLA	CMB-C2B-C3B	2.61	129.55	124.68
21	B	822	CLA	CMB-C2B-C3B	2.61	129.55	124.68
20	z	606	CHL	CMB-C2B-C3B	2.60	129.55	124.68
25	L	306	BCR	C21-C20-C19	2.60	131.34	123.22
25	F	304	BCR	C37-C22-C23	2.60	122.18	118.08
21	B	819	CLA	O2D-CGD-CBD	2.60	115.89	111.27
27	A	801	CL0	C4-C3-C5	2.60	119.65	115.27
25	G	204	BCR	C12-C13-C14	2.60	122.93	118.94
21	H	201	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	4	612	CLA	CHB-C4A-NA	2.60	128.10	124.51
21	A	828	CLA	CHB-C4A-NA	2.60	128.10	124.51
21	3	602	CLA	CHB-C4A-NA	2.59	128.10	124.51
21	A	818	CLA	CHB-C4A-NA	2.59	128.10	124.51
21	B	835	CLA	CHB-C4A-NA	2.59	128.10	124.51
21	x	602	CLA	CHB-C4A-NA	2.59	128.10	124.51
21	B	816	CLA	C1-C2-C3	-2.59	121.56	126.04
20	y	605	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
20	z	608	CHL	C2A-C1A-CHA	-2.59	119.33	123.86
21	z	614	CLA	CMB-C2B-C3B	2.59	129.52	124.68
21	A	827	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	B	818	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	x	607	CHL	CMB-C2B-C3B	2.59	129.52	124.68
21	A	833	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	A	839	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	4	615	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
21	3	610	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
21	A	817	CLA	CMB-C2B-C3B	2.59	129.51	124.68
21	z	611	CLA	CMB-C2B-C3B	2.59	129.51	124.68
21	A	836	CLA	CMB-C2B-C3B	2.58	129.51	124.68
25	A	851	BCR	C11-C12-C13	2.58	133.67	126.42
21	L	303	CLA	CHB-C4A-NA	2.58	128.08	124.51
20	z	601	CHL	CMB-C2B-C3B	2.58	129.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	102	BCR	C19-C18-C17	2.58	122.90	118.94
21	2	602	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	A	837	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	y	610	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	x	613	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	A	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	K	204	CLA	CMB-C2B-C3B	2.58	129.50	124.68
25	B	845	BCR	C24-C23-C22	-2.58	122.34	126.23
20	z	601	CHL	OMC-CMC-C2C	-2.57	119.87	125.69
21	4	603	CLA	CMB-C2B-C3B	2.57	129.73	124.69
21	3	605	CLA	CMB-C2B-C3B	2.57	129.73	124.69
25	K	202	BCR	C30-C25-C24	2.57	123.06	115.78
21	K	201	CLA	CAA-C2A-C3A	-2.57	110.09	116.10
25	B	846	BCR	C10-C11-C12	2.57	131.24	123.22
21	B	840	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	z	617	XAT	C32-C33-C34	2.57	122.89	118.94
21	3	602	CLA	CMB-C2B-C3B	2.57	129.49	124.68
21	O	201	CLA	CMB-C2B-C3B	2.57	129.49	124.68
20	z	601	CHL	C4-C3-C5	2.57	119.59	115.27
21	B	826	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	1	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	4	610	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	A	811	CLA	CHB-C4A-NA	2.56	128.06	124.51
21	x	603	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	z	617	XAT	C17-C1-C2	-2.56	104.53	108.98
21	B	808	CLA	CHB-C4A-NA	2.56	128.06	124.51
20	z	609	CHL	CHD-C1D-C2D	2.56	130.86	125.48
21	1	610	CLA	CHB-C4A-NA	2.56	128.06	124.51
21	K	203	CLA	CHB-C4A-NA	2.56	128.06	124.51
25	F	304	BCR	C36-C18-C17	-2.56	119.33	122.92
21	1	608	CLA	CAB-C3B-C2B	2.56	129.70	124.69
21	3	609	CLA	CMB-C2B-C3B	2.56	129.47	124.68
21	A	826	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	B	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	y	612	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	3	606	CHL	CMD-C2D-C3D	-2.56	121.72	127.61
25	B	848	BCR	C19-C18-C17	2.56	122.87	118.94
21	1	610	CLA	CAB-C3B-C2B	2.56	129.70	124.69
21	1	609	CLA	C2D-C1D-ND	-2.56	108.22	110.10
21	A	831	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	z	612	CLA	CMB-C2B-C3B	2.56	129.46	124.68
21	4	603	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	202	CLA	CMB-C2B-C3B	2.56	129.46	124.68
24	4	616	LUT	C19-C9-C8	2.56	122.10	118.08
21	4	611	CLA	O2D-CGD-O1D	-2.56	118.29	124.09
21	A	824	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	F	303	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	y	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	B	841	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	B	813	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	A	844	CLA	CHB-C4A-NA	2.55	128.03	124.51
21	3	611	CLA	CHB-C4A-NA	2.55	128.03	124.51
21	4	609	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
21	z	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	y	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	G	201	CLA	CMB-C2B-C3B	2.54	129.43	124.68
21	B	823	CLA	CMB-C2B-C3B	2.54	129.43	124.68
21	2	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	B	812	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	3	603	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	4	616	LUT	C32-C33-C34	2.54	122.83	118.94
21	B	820	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	A	813	CLA	CMB-C2B-C3B	2.54	129.42	124.68
21	z	604	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	B	831	CLA	CHB-C4A-NA	2.53	128.02	124.51
21	z	612	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	B	829	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	z	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	z	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	A	838	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	L	304	CLA	CHB-C4A-NA	2.53	128.00	124.51
20	4	607	CHL	C2A-C1A-CHA	-2.52	119.44	123.86
21	4	604	CLA	CAB-C3B-C2B	2.52	129.63	124.69
21	B	832	CLA	CMB-C2B-C3B	2.52	129.40	124.68
21	B	836	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
20	2	601	CHL	C2A-C1A-CHA	-2.52	119.45	123.86
25	B	843	BCR	C12-C13-C14	2.52	122.81	118.94
21	1	611	CLA	CMB-C2B-C3B	2.52	129.39	124.68
21	A	841	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
21	A	808	CLA	CHB-C4A-NA	2.52	127.99	124.51
21	O	203	CLA	CHB-C4A-NA	2.52	127.99	124.51
21	2	613	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	3	612	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
21	L	302	CLA	CHB-C4A-NA	2.51	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	611	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	z	610	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	1	614	XAT	C38-C25-C24	2.51	117.11	114.28
25	B	843	BCR	C16-C17-C18	2.51	130.90	127.31
22	2	617	XAT	C8-C9-C10	2.51	122.79	118.94
21	A	825	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	y	606	CHL	CMB-C2B-C3B	2.51	129.37	124.68
21	1	612	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	4	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	y	607	CHL	O2A-CGA-CBA	2.51	119.78	111.91
25	O	205	BCR	C19-C18-C17	2.51	122.79	118.94
21	B	840	CLA	CMB-C2B-C3B	2.51	129.37	124.68
20	x	601	CHL	C1-C2-C3	-2.50	121.71	126.04
21	B	839	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	2	601	CHL	CMB-C2B-C3B	2.50	129.36	124.68
21	A	814	CLA	CMB-C2B-C3B	2.50	129.36	124.68
21	A	812	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	y	606	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
20	4	615	CHL	C1B-CHB-C4A	-2.50	125.16	130.12
21	B	833	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	B	849	BCR	C7-C8-C9	2.50	130.01	126.23
21	G	203	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	1	605	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	x	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	x	604	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
21	O	201	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	1	603	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	4	613	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
21	A	806	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	y	603	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	A	824	CLA	CMB-C2B-C3B	2.49	129.34	124.68
21	2	603	CLA	O2D-CGD-O1D	-2.49	118.43	124.09
21	1	610	CLA	CMB-C2B-C3B	2.49	129.56	124.69
24	2	616	LUT	C40-C33-C34	-2.49	119.44	122.92
21	O	202	CLA	CBD-CHA-C1A	2.49	131.43	128.50
20	4	615	CHL	CMB-C2B-C3B	2.49	129.56	124.69
21	A	840	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	H	201	CLA	CMB-C2B-C3B	2.48	129.33	124.68
22	4	617	XAT	C35-C34-C33	2.48	130.86	127.31
21	3	611	CLA	CMB-C2B-C3B	2.48	129.33	124.68
21	H	201	CLA	CHB-C4A-NA	2.48	127.95	124.51
20	2	605	CHL	OMC-CMC-C2C	-2.48	120.07	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	609	CLA	O2D-CGD-O1D	-2.48	118.45	124.09
20	2	615	CHL	CMB-C2B-C3B	2.48	129.32	124.68
21	B	832	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	z	616	LUT	C8-C9-C10	2.48	122.75	118.94
25	J	102	BCR	C23-C22-C21	2.48	122.75	118.94
25	B	845	BCR	C37-C22-C21	-2.48	119.45	122.92
20	1	606	CHL	CMB-C2B-C3B	2.48	129.32	124.68
20	z	607	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
21	A	803	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	y	606	CHL	CHB-C4A-NA	2.48	127.94	124.51
21	K	204	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	2	601	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
21	B	805	CLA	CMB-C2B-C3B	2.48	129.31	124.68
24	y	616	LUT	C8-C9-C10	2.48	122.74	118.94
21	A	810	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	G	201	CLA	O2D-CGD-CBD	2.47	115.67	111.27
21	2	610	CLA	CMB-C2B-C3B	2.47	129.53	124.69
21	3	603	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	y	617	XAT	C7-C8-C9	2.47	129.37	125.53
20	4	606	CHL	CMB-C2B-C3B	2.47	129.53	124.69
21	z	602	CLA	O2A-C1-C2	2.47	115.13	108.64
21	A	822	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
20	x	606	CHL	CMB-C2B-C3B	2.47	129.30	124.68
20	1	606	CHL	C1D-ND-C4D	-2.47	104.58	106.33
25	F	304	BCR	C19-C18-C17	2.47	122.72	118.94
20	y	601	CHL	C6-C5-C3	-2.47	110.59	114.62
20	2	601	CHL	C4D-CHA-C1A	-2.46	118.25	121.25
20	4	605	CHL	CAC-C3C-C4C	2.46	128.79	125.04
21	A	802	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
21	A	817	CLA	CHB-C4A-NA	2.46	127.91	124.51
21	A	829	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
27	A	801	CL0	CMC-C2C-C1C	2.46	128.78	125.04
25	B	843	BCR	C1-C6-C7	2.46	122.73	115.78
20	z	609	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
20	y	607	CHL	C1-C2-C3	-2.46	121.80	126.04
20	z	609	CHL	CHD-C4C-C3C	-2.45	121.23	124.84
21	B	803	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
20	y	609	CHL	CHD-C4C-C3C	-2.45	121.24	124.84
21	B	816	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	3	605	CLA	CAB-C3B-C2B	2.45	129.48	124.69
21	B	811	CLA	CMB-C2B-C3B	2.45	129.48	124.69
21	1	608	CLA	CMB-C2B-C3B	2.45	129.48	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	801	BCR	C23-C22-C21	2.44	122.69	118.94
21	A	835	CLA	O2D-CGD-CBD	2.44	115.61	111.27
21	2	609	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
20	x	605	CHL	CMB-C2B-C3B	2.44	129.25	124.68
21	A	813	CLA	O2D-CGD-CBD	2.44	115.61	111.27
24	z	615	LUT	C10-C11-C12	2.44	130.84	123.22
20	x	605	CHL	OMC-CMC-C2C	-2.44	120.18	125.69
21	B	821	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	3	613	LUT	C30-C31-C32	2.43	130.81	123.22
21	A	807	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	K	204	CLA	CHD-C1D-ND	-2.43	122.22	124.45
21	K	206	CLA	CBD-CHA-C1A	2.43	131.36	128.50
21	K	201	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
21	z	603	CLA	C1-C2-C3	-2.43	121.85	126.04
25	L	306	BCR	C1-C6-C5	-2.42	119.20	122.61
20	2	605	CHL	C1B-CHB-C4A	-2.42	125.32	130.12
21	4	609	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
25	K	205	BCR	C12-C13-C14	2.42	122.66	118.94
21	1	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	z	602	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
25	B	849	BCR	C34-C9-C8	2.42	121.89	118.08
21	B	836	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	4	617	XAT	C37-C21-C22	-2.42	104.78	108.98
26	4	620	LMG	O1-C7-C8	-2.42	105.07	110.90
21	A	810	CLA	CAA-CBA-CGA	-2.42	106.19	113.25
20	x	601	CHL	CMB-C2B-C3B	2.42	129.20	124.68
20	2	615	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
21	B	821	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
21	A	810	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
22	1	614	XAT	O24-C25-C26	-2.41	56.96	58.96
25	K	202	BCR	C30-C25-C26	-2.41	119.22	122.61
21	B	834	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
20	y	601	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
21	B	822	CLA	CAA-CBA-CGA	-2.40	106.23	113.25
21	A	827	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
21	F	301	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	z	605	CHL	C2A-C1A-CHA	-2.40	119.66	123.85
21	B	814	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
21	y	603	CLA	O2D-CGD-CBD	2.39	115.52	111.27
21	B	825	CLA	O2D-CGD-CBD	2.39	115.52	111.27
21	y	610	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	L	306	BCR	C24-C23-C22	2.39	129.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	102	BCR	C1-C6-C5	-2.39	119.25	122.61
20	1	606	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
20	z	608	CHL	CMB-C2B-C3B	2.38	129.13	124.68
25	B	846	BCR	C19-C18-C17	2.38	122.59	118.94
21	1	607	CLA	O2D-CGD-O1D	-2.38	118.69	124.09
21	K	206	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	A	848	BCR	C23-C22-C21	2.38	122.59	118.94
20	1	606	CHL	C4A-NA-C1A	2.38	107.78	106.71
21	3	609	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
21	3	607	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
20	1	601	CHL	C1D-ND-C4D	-2.37	104.65	106.33
20	z	605	CHL	C4D-CHA-C1A	-2.37	118.36	121.25
22	2	617	XAT	C27-C28-C29	-2.37	121.85	125.53
21	A	832	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
21	B	819	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
21	B	805	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
21	x	610	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
21	x	603	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
20	x	609	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
20	z	607	CHL	CMB-C2B-C3B	2.37	129.11	124.68
21	B	810	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
20	2	607	CHL	C2A-C1A-CHA	-2.37	119.72	123.86
21	4	604	CLA	CMB-C2B-C3B	2.37	129.32	124.69
20	x	608	CHL	C1B-CHB-C4A	-2.37	125.43	130.12
21	A	802	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	A	809	CLA	C1-C2-C3	-2.36	121.96	126.04
21	B	825	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	B	821	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	J	102	BCR	C10-C11-C12	2.36	130.58	123.22
21	B	822	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
30	B	850	DGD	O1G-C1A-C2A	2.36	119.31	111.91
21	A	839	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
20	1	601	CHL	CMB-C2B-C3B	2.36	129.09	124.68
22	4	617	XAT	C37-C21-C36	-2.36	103.89	107.37
21	x	604	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	B	833	CLA	CAA-C2A-C1A	-2.35	104.26	111.97
21	B	818	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
21	2	613	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
21	A	835	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
21	A	845	CLA	O2D-CGD-CBD	2.35	115.45	111.27
25	O	204	BCR	C23-C22-C21	2.35	122.55	118.94
24	2	619	LUT	C15-C14-C13	2.35	130.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	807	CLA	CMB-C2B-C3B	2.35	129.08	124.68
25	A	850	BCR	C35-C13-C14	-2.35	119.63	122.92
22	x	617	XAT	C35-C34-C33	2.35	130.67	127.31
21	B	827	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	2	607	CHL	CMB-C2B-C3B	2.35	129.07	124.68
21	J	101	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
20	4	615	CHL	C2A-C1A-CHA	-2.35	119.76	123.86
25	A	848	BCR	C30-C25-C26	-2.35	119.31	122.61
24	4	616	LUT	C12-C13-C14	2.35	122.54	118.94
21	A	814	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	4	617	XAT	C31-C30-C29	2.34	130.66	127.31
20	x	601	CHL	C4-C3-C5	2.34	119.21	115.27
21	3	603	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	B	830	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	A	814	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
20	x	608	CHL	C2A-C1A-CHA	-2.34	119.76	123.85
21	4	614	CLA	O2D-CGD-CBD	2.34	115.43	111.27
21	2	602	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	2	604	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	A	851	BCR	C30-C25-C26	-2.34	119.32	122.61
21	B	838	CLA	CMB-C2B-C3B	2.34	129.05	124.68
21	3	608	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	A	849	BCR	C12-C13-C14	2.34	122.53	118.94
25	B	849	BCR	C23-C22-C21	2.34	122.53	118.94
21	A	804	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	B	823	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	2	605	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
20	x	606	CHL	CHB-C4A-NA	2.33	127.73	124.51
21	K	203	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
20	1	601	CHL	O2D-CGD-O1D	-2.33	118.81	124.09
21	B	825	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
21	A	823	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
21	F	302	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
21	A	820	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
21	B	810	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	A	842	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
27	A	801	CL0	CMB-C2B-C3B	2.32	129.02	124.68
21	A	844	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	3	606	CHL	CMB-C2B-C3B	2.32	129.02	124.68
21	A	835	CLA	C1-C2-C3	-2.32	122.03	126.04
21	4	609	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
21	B	828	CLA	C1B-CHB-C4A	-2.32	125.53	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	614	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	1	615	LHG	C5-O7-C7	-2.32	112.09	117.79
21	2	608	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
21	B	829	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
21	A	836	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
21	4	611	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
22	4	617	XAT	C11-C12-C13	2.31	132.92	126.42
20	2	606	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
21	K	204	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
20	x	605	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
21	A	808	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	3	605	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	A	841	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	K	206	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	y	602	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	1	604	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	K	206	CLA	CHD-C1D-ND	-2.31	122.33	124.45
21	4	602	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
20	y	607	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
25	A	848	BCR	C30-C25-C24	2.31	122.30	115.78
21	1	602	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	B	843	BCR	C19-C18-C17	2.30	122.48	118.94
21	A	803	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
21	A	809	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	L	302	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
25	A	851	BCR	C30-C25-C24	2.30	122.29	115.78
25	B	843	BCR	C10-C11-C12	2.30	130.40	123.22
25	L	305	BCR	C8-C9-C10	2.30	122.47	118.94
21	B	833	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	z	610	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	A	815	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
25	B	848	BCR	C34-C9-C8	2.30	121.70	118.08
20	y	609	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
21	A	834	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
21	B	840	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
25	O	205	BCR	C37-C22-C23	2.30	121.70	118.08
21	L	302	CLA	O2D-CGD-CBD	2.30	115.35	111.27
25	K	205	BCR	C1-C6-C5	-2.30	119.38	122.61
21	y	612	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
21	A	810	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	A	839	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
21	O	202	CLA	CHB-C4A-NA	2.29	127.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	606	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
21	O	203	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
20	4	605	CHL	CMB-C2B-C3B	2.29	128.96	124.68
21	A	825	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	3	602	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
22	2	617	XAT	C16-C1-C2	-2.29	105.01	108.98
20	x	607	CHL	C2A-C1A-CHA	-2.29	119.86	123.86
21	1	613	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	A	843	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	x	603	CLA	O2D-CGD-CBD	2.28	115.33	111.27
20	x	609	CHL	OMC-CMC-C2C	-2.28	120.52	125.69
21	B	837	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
20	y	609	CHL	O2A-CGA-CBA	2.28	119.08	111.91
21	B	836	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
25	B	848	BCR	C12-C13-C14	2.28	122.44	118.94
21	A	838	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
25	A	851	BCR	C15-C14-C13	2.28	130.57	127.31
21	A	829	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
21	B	812	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
25	J	102	BCR	C1-C6-C7	2.28	122.23	115.78
21	B	821	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
22	1	614	XAT	O4-C5-C6	-2.28	57.07	58.96
21	4	604	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	y	611	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
20	x	605	CHL	C1C-C2C-C3C	-2.28	105.31	107.11
21	z	614	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
20	2	601	CHL	O1D-CGD-CBD	-2.28	119.83	124.48
21	3	601	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	4	608	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	A	805	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	x	602	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
25	K	205	BCR	C1-C6-C7	2.27	122.21	115.78
21	A	812	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
21	B	839	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
21	B	816	CLA	CHD-C1D-ND	-2.27	122.37	124.45
21	A	815	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	A	824	CLA	O2D-CGD-CBD	2.27	115.30	111.27
21	K	206	CLA	O2D-CGD-O1D	-2.27	118.93	124.09
25	B	847	BCR	C15-C16-C17	2.27	128.13	123.47
21	3	610	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	B	817	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	B	809	CLA	C1B-CHB-C4A	-2.27	125.62	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	840	CLA	CMB-C2B-C3B	2.27	128.92	124.68
21	x	612	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	A	831	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
21	z	613	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
21	B	833	CLA	O2D-CGD-CBD	2.27	115.30	111.27
20	3	606	CHL	C1B-CHB-C4A	-2.27	125.63	130.12
21	B	808	CLA	C1-C2-C3	-2.27	122.12	126.04
25	K	205	BCR	C30-C25-C24	2.26	122.18	115.78
21	1	602	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
20	y	605	CHL	C2A-C1A-CHA	-2.26	119.90	123.85
21	3	604	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	A	840	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	A	833	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	4	618	BCR	C37-C22-C23	2.26	121.64	118.08
21	B	815	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	z	604	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	1	612	CLA	CHD-C1D-ND	-2.26	122.38	124.45
20	2	606	CHL	CMB-C2B-C3B	2.26	128.90	124.68
20	z	608	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
21	B	807	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
21	K	203	CLA	CAA-CBA-CGA	-2.26	106.52	112.51
21	z	603	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
21	3	602	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
20	4	606	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
25	L	305	BCR	C30-C25-C24	2.25	122.15	115.78
21	B	835	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
21	O	202	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
21	B	837	CLA	CHD-C1D-ND	-2.25	122.38	124.45
22	x	617	XAT	C32-C33-C34	2.25	122.40	118.94
21	B	808	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	1	607	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
20	y	607	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
21	1	605	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	x	611	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	y	603	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
20	x	608	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
21	B	839	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
21	1	610	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
21	F	301	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
20	z	601	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
21	A	818	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
21	y	614	CLA	C1-C2-C3	-2.24	122.16	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	607	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
21	B	813	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
20	2	605	CHL	CMB-C2B-C3B	2.24	128.87	124.68
21	B	804	CLA	O2D-CGD-CBD	2.24	115.25	111.27
21	4	610	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
24	3	613	LUT	C12-C13-C14	2.24	122.38	118.94
21	2	609	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
21	y	613	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
21	A	816	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
20	z	608	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
22	z	617	XAT	C8-C9-C10	2.24	122.38	118.94
21	x	613	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
21	3	611	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
21	B	831	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
25	A	850	BCR	C36-C18-C17	-2.24	119.79	122.92
27	A	801	CL0	CMD-C2D-C3D	-2.24	122.47	127.61
25	B	845	BCR	C30-C25-C26	-2.23	119.47	122.61
21	G	202	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	B	822	CLA	C1-C2-C3	-2.23	122.19	126.04
21	A	824	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	A	830	CLA	CAC-C3C-C4C	2.23	127.70	124.81
21	B	838	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	B	802	CLA	CGD-CBD-CAD	2.23	117.95	110.73
21	L	304	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	1	614	XAT	C35-C15-C14	-2.23	118.91	123.47
21	B	803	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	B	827	CLA	O2D-CGD-CBD	2.23	115.22	111.27
21	z	614	CLA	O2D-CGD-CBD	2.23	115.22	111.27
21	F	303	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
31	y	618	NEX	C10-C11-C12	2.22	130.16	123.22
21	A	807	CLA	CHD-C1D-ND	-2.22	122.41	124.45
21	A	827	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
21	A	819	CLA	CHD-C1D-ND	-2.22	122.41	124.45
21	2	612	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
21	4	614	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
21	B	832	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
25	A	850	BCR	C1-C6-C7	2.22	122.06	115.78
20	x	608	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
20	z	608	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
25	L	301	BCR	C8-C9-C10	2.22	122.34	118.94
25	L	306	BCR	C1-C6-C7	2.22	122.05	115.78
21	A	821	CLA	C1B-CHB-C4A	-2.22	125.73	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	808	CLA	O1D-CGD-CBD	2.21	129.01	124.48
21	1	604	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
21	A	830	CLA	O2A-C1-C2	2.21	114.45	108.64
21	4	602	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
27	A	801	CL0	C4D-C3D-CAD	2.21	110.65	107.70
21	1	612	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	B	837	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	B	823	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	4	616	LUT	C39-C29-C28	2.21	121.56	118.08
21	A	819	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	A	828	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	4	612	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
21	A	806	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
25	A	850	BCR	C12-C13-C14	2.21	122.33	118.94
21	B	841	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
25	3	614	BCR	C37-C22-C23	2.20	121.55	118.08
21	A	825	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
20	x	609	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
20	x	601	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
24	2	616	LUT	C32-C33-C34	2.20	122.32	118.94
21	A	825	CLA	C1-C2-C3	-2.20	122.24	126.04
21	B	802	CLA	C1-C2-C3	-2.20	122.24	126.04
25	B	843	BCR	C1-C6-C5	-2.20	119.52	122.61
21	z	612	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
21	G	203	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
20	x	608	CHL	CHB-C4A-NA	2.20	127.55	124.51
20	1	606	CHL	O2D-CGD-O1D	-2.20	119.10	124.09
21	4	614	CLA	C1-C2-C3	-2.20	123.20	126.75
21	y	614	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
21	B	805	CLA	CHD-C1D-ND	-2.19	122.44	124.45
21	2	611	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
21	A	835	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	B	848	BCR	C30-C25-C24	2.19	121.98	115.78
21	A	820	CLA	O2D-CGD-CBD	2.19	115.17	111.27
25	L	305	BCR	C21-C20-C19	2.19	130.06	123.22
21	A	811	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
21	A	817	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
21	B	838	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
20	z	601	CHL	O2D-CGD-O1D	-2.19	119.55	123.84
21	z	602	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
21	L	303	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
21	B	828	CLA	O2A-CGA-O1A	-2.19	118.06	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	z	610	CLA	CHD-C1D-ND	-2.19	122.44	124.45
21	2	603	CLA	C2D-C1D-ND	-2.19	108.49	110.10
21	B	817	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
21	4	609	CLA	CHD-C1D-ND	-2.19	122.44	124.45
21	A	837	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
21	B	802	CLA	CMB-C2B-C3B	2.19	128.77	124.68
21	3	609	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
20	2	607	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
21	B	807	CLA	O2D-CGD-CBD	2.19	115.15	111.27
20	x	606	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
27	A	801	CL0	C3D-C4D-CHA	-2.19	107.72	112.72
21	4	603	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
21	B	820	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
21	B	804	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
25	L	305	BCR	C1-C6-C7	2.18	121.95	115.78
21	4	612	CLA	C1-C2-C3	-2.18	122.27	126.04
21	A	826	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
21	3	608	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
21	B	829	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
21	A	810	CLA	O2D-CGD-CBD	2.18	115.14	111.27
21	B	834	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	A	808	CLA	C1-C2-C3	-2.18	123.23	126.75
20	1	606	CHL	CHD-C1D-C2D	2.18	130.05	125.48
21	H	201	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
21	A	825	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	z	601	CHL	CHD-C1D-C2D	2.18	130.04	125.48
21	B	820	CLA	C1-C2-C3	-2.18	123.23	126.75
31	x	618	NEX	C27-C28-C29	-2.17	122.16	125.53
21	A	812	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	B	848	BCR	C37-C22-C23	2.17	121.50	118.08
21	G	201	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
25	K	205	BCR	C30-C25-C26	-2.17	119.56	122.61
21	F	302	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
21	1	608	CLA	CMA-C3A-C2A	-2.17	111.05	116.10
21	B	824	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
25	A	853	BCR	C23-C22-C21	2.16	122.26	118.94
21	y	602	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
22	4	617	XAT	C40-C33-C34	2.16	125.95	122.92
20	z	607	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
25	A	850	BCR	C1-C6-C5	-2.16	119.57	122.61
21	B	806	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	2	617	XAT	C36-C21-C22	-2.16	105.23	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	834	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
21	3	612	CLA	CAA-C2A-C3A	-2.16	111.06	116.10
21	B	837	CLA	O2D-CGD-CBD	2.16	115.11	111.27
25	A	853	BCR	C30-C25-C24	2.16	121.89	115.78
20	2	615	CHL	OMC-CMC-C2C	-2.16	120.80	125.69
21	x	603	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
21	1	613	CLA	CMA-C3A-C2A	-2.16	111.06	116.10
21	B	818	CLA	O2D-CGD-CBD	2.16	115.10	111.27
21	1	603	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
27	A	801	CL0	C6-C5-C3	-2.16	107.80	113.45
20	x	608	CHL	C1C-C2C-C3C	-2.15	105.40	107.11
22	4	617	XAT	C16-C1-C2	2.15	112.72	108.98
21	A	804	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
21	B	819	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
21	A	813	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
21	B	823	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	A	845	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
27	A	801	CL0	CMB-C2B-C1B	2.15	131.77	128.46
21	2	611	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
21	B	814	CLA	O2D-CGD-CBD	2.15	115.09	111.27
21	B	826	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
21	B	839	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	4	601	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
21	A	828	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
21	A	827	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	A	832	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	A	842	CLA	CBA-CAA-C2A	2.15	120.20	113.86
22	x	617	XAT	C12-C13-C14	2.15	122.23	118.94
21	A	815	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	3	614	BCR	C30-C25-C24	2.14	121.84	115.78
21	A	822	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
25	B	845	BCR	C8-C9-C10	2.14	122.23	118.94
21	1	611	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
21	A	807	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
21	3	605	CLA	CAA-C2A-C3A	-2.14	108.91	114.26
21	K	203	CLA	O2D-CGD-CBD	2.14	115.08	111.27
21	4	609	CLA	C1-C2-C3	-2.14	122.34	126.04
21	B	807	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	B	820	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	A	809	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	B	834	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	2	615	CHL	C1C-C2C-C3C	-2.14	105.42	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	609	CLA	CMC-C2C-C3C	2.14	131.18	126.75
20	y	601	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
21	B	830	CLA	CHD-C1D-ND	-2.13	122.49	124.45
21	B	806	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
21	A	833	CLA	CHD-C1D-ND	-2.13	122.49	124.45
20	z	606	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
20	4	607	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
21	A	811	CLA	CHD-C1D-ND	-2.13	122.50	124.45
21	A	829	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
20	x	601	CHL	CED-O2D-CGD	2.13	120.76	115.94
22	1	614	XAT	C18-C5-C4	2.13	116.68	114.28
25	B	847	BCR	C37-C22-C23	2.13	121.43	118.08
21	A	832	CLA	C1-C2-C3	-2.13	123.31	126.75
21	y	604	CLA	CHD-C1D-ND	-2.13	122.50	124.45
20	z	605	CHL	CAA-C2A-C3A	-2.13	111.13	116.10
21	z	611	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
21	B	804	CLA	CMA-C3A-C2A	-2.13	111.14	116.10
21	K	203	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
21	1	603	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
25	A	851	BCR	C34-C9-C8	-2.12	114.73	118.08
25	3	614	BCR	C8-C9-C10	2.12	122.20	118.94
20	y	609	CHL	C2D-C1D-ND	2.12	111.67	110.10
21	B	810	CLA	CHD-C1D-ND	-2.12	122.50	124.45
20	y	601	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
21	A	842	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	B	805	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
21	2	602	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	A	830	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
25	A	849	BCR	C15-C14-C13	2.12	130.33	127.31
21	B	813	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
21	2	610	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
21	x	602	CLA	O2D-CGD-CBD	2.12	115.03	111.27
21	A	808	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
21	y	613	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	A	838	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
21	A	824	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	B	806	CLA	CHD-C1D-ND	-2.11	122.51	124.45
21	L	303	CLA	CHD-C1D-ND	-2.11	122.51	124.45
20	4	615	CHL	C4B-C3B-C2B	-2.11	104.95	106.92
20	2	605	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
21	L	302	CLA	CHD-C1D-ND	-2.11	122.51	124.45
21	A	806	CLA	O2A-CGA-O1A	-2.11	118.26	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	803	CLA	C1-C2-C3	-2.11	122.39	126.04
21	B	826	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
20	x	607	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
21	F	301	CLA	CHD-C1D-ND	-2.11	122.52	124.45
21	B	818	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
20	4	605	CHL	O2D-CGD-O1D	-2.11	119.31	124.09
21	z	613	CLA	CHD-C1D-ND	-2.10	122.52	124.45
22	z	617	XAT	C25-C24-C23	2.10	116.91	112.75
21	y	603	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
21	A	845	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
21	B	841	CLA	CHD-C1D-ND	-2.10	122.52	124.45
21	L	303	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
21	J	101	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	x	615	LUT	C31-C30-C29	2.10	130.31	127.31
21	1	609	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
21	y	604	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
21	A	820	CLA	CHD-C1D-ND	-2.10	122.53	124.45
20	4	607	CHL	O2D-CGD-O1D	-2.09	119.74	123.84
21	B	809	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
21	B	838	CLA	O2D-CGD-CBD	2.09	114.98	111.27
20	2	615	CHL	CAA-C2A-C3A	-2.09	109.03	114.26
20	4	615	CHL	CHB-C4A-NA	2.09	127.40	124.51
20	4	607	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
20	3	606	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
25	A	853	BCR	C29-C30-C25	2.09	113.70	110.48
21	x	604	CLA	CHD-C1D-ND	-2.09	122.53	124.45
21	z	612	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
21	A	802	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
20	1	606	CHL	CMA-C3A-C2A	-2.09	111.23	116.10
21	3	608	CLA	CHD-C1D-ND	-2.09	122.54	124.45
21	B	821	CLA	CHD-C1D-ND	-2.09	122.54	124.45
20	3	606	CHL	C2A-C1A-CHA	-2.08	120.21	123.86
20	1	601	CHL	OMC-CMC-C2C	-2.08	120.98	125.69
21	B	811	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
21	B	831	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	A	845	CLA	C1-C2-C3	-2.08	123.38	126.75
21	2	609	CLA	CHD-C1D-ND	-2.08	122.54	124.45
24	x	616	LUT	C8-C9-C10	2.08	122.13	118.94
20	2	607	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
20	3	606	CHL	CHB-C4A-NA	2.08	127.39	124.51
25	4	618	BCR	C8-C9-C10	2.08	122.13	118.94
21	B	810	CLA	C1-C2-C3	-2.08	122.45	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	z	604	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	1	604	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
21	A	840	CLA	CHD-C1D-ND	-2.08	122.55	124.45
21	O	202	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	B	847	BCR	C19-C18-C17	2.08	122.13	118.94
25	3	614	BCR	C30-C25-C26	-2.07	119.69	122.61
21	x	610	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
25	L	305	BCR	C30-C25-C26	-2.07	119.69	122.61
25	I	101	BCR	C34-C9-C8	2.07	121.34	118.08
21	A	806	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	B	829	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	3	611	CLA	CMA-C3A-C2A	-2.07	111.26	116.10
25	A	853	BCR	C30-C25-C26	-2.07	119.69	122.61
21	L	304	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	z	607	CHL	OMC-CMC-C2C	-2.07	121.00	125.69
21	B	824	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
21	y	604	CLA	O2D-CGD-CBD	2.07	114.95	111.27
20	1	601	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
21	B	814	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	A	852	BCR	C24-C23-C22	2.07	129.36	126.23
25	B	846	BCR	C1-C6-C7	2.07	121.63	115.78
20	2	605	CHL	CHB-C4A-NA	2.07	127.37	124.51
20	2	601	CHL	OMC-CMC-C2C	-2.07	121.02	125.69
21	A	818	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
21	x	613	CLA	C1-C2-C3	-2.07	122.47	126.04
21	F	301	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
25	L	305	BCR	C1-C6-C5	-2.06	119.71	122.61
25	A	852	BCR	C30-C25-C24	2.06	121.62	115.78
21	B	827	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
27	A	801	CL0	O2A-CGA-O1A	-2.06	118.39	123.59
21	3	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	2	613	CLA	O1D-CGD-CBD	2.06	128.70	124.48
20	x	606	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
20	3	606	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
21	B	802	CLA	CMA-C3A-C2A	-2.06	105.52	113.83
21	B	814	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	B	819	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	O	201	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	B	847	BCR	C8-C9-C10	2.06	122.10	118.94
21	B	825	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	A	830	CLA	C2A-C1A-CHA	2.06	127.46	123.86
21	1	608	CLA	C1B-CHB-C4A	-2.06	126.04	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	607	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	A	823	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	A	824	CLA	CMA-C3A-C2A	-2.06	111.30	116.10
20	x	601	CHL	CHD-C1D-C2D	2.05	129.79	125.48
21	y	604	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
20	2	601	CHL	O2A-CGA-CBA	2.05	120.34	112.23
20	4	605	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
22	y	617	XAT	C28-C29-C30	2.05	122.09	118.94
21	B	813	CLA	C1-C2-C3	-2.05	122.49	126.04
21	4	612	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
21	3	609	CLA	C1-C2-C3	-2.05	122.50	126.04
20	y	609	CHL	C1C-C2C-C3C	-2.05	105.49	107.11
21	A	841	CLA	O1D-CGD-CBD	2.05	128.67	124.48
21	4	609	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
20	z	601	CHL	O1D-CGD-CBD	-2.05	120.30	124.48
21	F	302	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
21	A	828	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	B	818	CLA	C1-C2-C3	-2.05	122.50	126.04
21	A	804	CLA	C1-C2-C3	-2.05	122.50	126.04
21	A	811	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
21	2	611	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	B	802	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	A	836	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
21	A	810	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	x	611	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
21	B	806	CLA	O1D-CGD-CBD	2.04	128.66	124.48
21	O	203	CLA	O2D-CGD-O1D	-2.04	119.45	124.09
21	O	201	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
20	x	609	CHL	O2A-CGA-CBA	2.04	120.58	114.03
21	B	820	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	B	835	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	1	601	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
21	A	832	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
21	B	833	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
20	y	605	CHL	CED-O2D-CGD	2.04	120.55	115.94
21	A	805	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
21	A	802	CLA	C7-C6-C5	-2.04	107.82	113.36
21	A	808	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	4	613	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
21	x	613	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
21	2	608	CLA	O1D-CGD-CBD	2.04	128.65	124.48
21	x	614	CLA	CHD-C1D-ND	-2.04	122.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	613	LUT	C7-C8-C9	-2.04	123.16	126.23
21	A	813	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
20	y	606	CHL	C4D-C3D-CAD	2.04	110.50	108.10
20	y	606	CHL	C4D-CHA-C1A	-2.03	118.77	121.25
21	F	302	CLA	C2A-C1A-CHA	2.03	127.42	123.86
21	B	810	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
21	G	203	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
21	2	612	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	2	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
20	y	605	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
20	y	607	CHL	OMC-CMC-C2C	-2.03	121.10	125.69
25	B	844	BCR	C20-C19-C18	2.03	132.11	126.42
21	A	840	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
21	A	818	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	A	837	CLA	O2D-CGD-CBD	2.02	114.87	111.27
21	B	840	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
21	4	602	CLA	CHD-C1D-ND	-2.02	122.59	124.45
24	y	616	LUT	C30-C31-C32	2.02	129.53	123.22
21	A	807	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	B	801	BCR	C1-C6-C5	-2.02	119.77	122.61
21	O	203	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	y	606	CHL	C1B-CHB-C4A	-2.02	126.11	130.12
21	B	806	CLA	C1-C2-C3	-2.02	122.55	126.04
21	A	834	CLA	CHD-C1D-ND	-2.02	122.60	124.45
21	4	603	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
21	A	819	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
20	3	606	CHL	O2A-CGA-CBA	2.02	120.51	114.03
21	B	805	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	1	614	XAT	C20-C13-C14	-2.01	120.10	122.92
21	A	805	CLA	C1-C2-C3	-2.01	122.56	126.04
21	2	611	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
21	x	611	CLA	CHD-C1D-ND	-2.01	122.60	124.45
21	z	610	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
21	B	836	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	1	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	A	805	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	z	605	CHL	CMA-C3A-C2A	-2.01	111.41	116.10
20	z	608	CHL	O2A-CGA-O1A	-2.01	118.53	123.59
21	3	601	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	3	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	y	601	CHL	CHD-C1D-C2D	2.00	129.69	125.48
21	A	803	CLA	C2D-C1D-ND	-2.00	108.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	612	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
24	2	619	LUT	C30-C31-C32	2.00	129.47	123.22
21	B	833	CLA	CHD-C1D-ND	-2.00	122.61	124.45
21	y	610	CLA	CHD-C1D-ND	-2.00	122.61	124.45
21	B	820	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (260) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	601	CHL	ND
20	1	601	CHL	NA
20	1	601	CHL	NC
20	1	606	CHL	ND
20	1	606	CHL	NA
20	1	606	CHL	NC
20	2	605	CHL	ND
20	2	605	CHL	NA
20	2	605	CHL	NC
20	2	606	CHL	ND
20	2	606	CHL	NA
20	2	606	CHL	NC
20	2	601	CHL	ND
20	2	601	CHL	NA
20	2	601	CHL	NC
20	2	607	CHL	ND
20	2	607	CHL	NA
20	2	607	CHL	NC
20	2	615	CHL	ND
20	2	615	CHL	NA
20	2	615	CHL	NC
20	3	606	CHL	ND
20	3	606	CHL	NA
20	3	606	CHL	NC
20	4	605	CHL	ND
20	4	605	CHL	NA
20	4	605	CHL	NC
20	4	606	CHL	ND
20	4	606	CHL	NA
20	4	606	CHL	NC
20	4	615	CHL	ND
20	4	615	CHL	NA
20	4	615	CHL	NC

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	4	607	CHL	ND
20	4	607	CHL	NA
20	4	607	CHL	NC
20	x	608	CHL	ND
20	x	608	CHL	NA
20	x	608	CHL	NC
20	x	606	CHL	ND
20	x	606	CHL	NA
20	x	606	CHL	NC
20	x	607	CHL	ND
20	x	607	CHL	NA
20	x	607	CHL	NC
20	x	609	CHL	ND
20	x	609	CHL	NA
20	x	609	CHL	NC
20	x	601	CHL	ND
20	x	601	CHL	NA
20	x	601	CHL	NC
20	x	605	CHL	ND
20	x	605	CHL	NA
20	x	605	CHL	NC
20	y	607	CHL	ND
20	y	607	CHL	NA
20	y	607	CHL	NC
20	y	606	CHL	ND
20	y	606	CHL	NA
20	y	606	CHL	NC
20	y	601	CHL	ND
20	y	601	CHL	NA
20	y	601	CHL	NC
20	y	605	CHL	ND
20	y	605	CHL	NA
20	y	605	CHL	NC
20	y	608	CHL	ND
20	y	608	CHL	NA
20	y	608	CHL	NC
20	y	609	CHL	ND
20	y	609	CHL	NA
20	y	609	CHL	NC
20	z	606	CHL	ND
20	z	606	CHL	NA
20	z	606	CHL	NC

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
21	3	612	CLA	ND
21	3	602	CLA	ND
21	3	609	CLA	ND
21	3	608	CLA	ND
21	4	613	CLA	ND
21	4	609	CLA	ND
21	4	608	CLA	ND
21	4	603	CLA	ND
21	4	611	CLA	ND
21	4	612	CLA	ND
21	4	601	CLA	ND
21	4	602	CLA	ND
21	4	610	CLA	ND
21	4	614	CLA	ND
21	4	604	CLA	ND
21	A	803	CLA	ND
21	A	811	CLA	ND
21	A	810	CLA	ND
21	A	812	CLA	ND
21	A	813	CLA	ND
21	A	826	CLA	ND
21	A	829	CLA	ND
21	A	830	CLA	ND
21	A	831	CLA	ND
21	A	818	CLA	ND
21	A	808	CLA	ND
21	A	809	CLA	ND
21	A	807	CLA	ND
21	A	820	CLA	ND
21	A	802	CLA	ND
21	A	804	CLA	ND
21	A	823	CLA	ND
21	A	824	CLA	ND
21	A	827	CLA	ND
21	A	828	CLA	ND
21	A	825	CLA	ND
21	A	805	CLA	ND
21	A	815	CLA	ND
21	A	816	CLA	ND
21	A	814	CLA	ND
21	A	819	CLA	ND
21	A	806	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
21	A	817	CLA	ND
21	A	821	CLA	ND
21	A	822	CLA	ND
21	A	841	CLA	ND
21	A	832	CLA	ND
21	A	838	CLA	ND
21	A	834	CLA	ND
21	A	833	CLA	ND
21	A	842	CLA	ND
21	A	844	CLA	ND
21	A	835	CLA	ND
21	A	837	CLA	ND
21	A	845	CLA	ND
21	A	836	CLA	ND
21	A	840	CLA	ND
21	A	843	CLA	ND
21	A	839	CLA	ND
21	B	816	CLA	ND
21	B	806	CLA	ND
21	B	820	CLA	ND
21	B	804	CLA	ND
21	B	808	CLA	ND
21	B	822	CLA	ND
21	B	817	CLA	ND
21	B	828	CLA	ND
21	B	829	CLA	ND
21	B	830	CLA	ND
21	B	824	CLA	ND
21	B	837	CLA	ND
21	B	815	CLA	ND
21	B	811	CLA	ND
21	B	823	CLA	ND
21	B	826	CLA	ND
21	B	836	CLA	ND
21	B	838	CLA	ND
21	B	840	CLA	ND
21	B	807	CLA	ND
21	B	841	CLA	ND
21	B	835	CLA	ND
21	B	821	CLA	ND
21	B	825	CLA	ND
21	B	814	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
21	B	832	CLA	ND
21	B	833	CLA	ND
21	B	809	CLA	ND
21	B	819	CLA	ND
21	B	818	CLA	ND
21	B	827	CLA	ND
21	B	802	CLA	ND
21	B	805	CLA	ND
21	B	810	CLA	ND
21	B	831	CLA	ND
21	B	839	CLA	ND
21	B	813	CLA	ND
21	B	834	CLA	ND
21	B	812	CLA	ND
21	B	803	CLA	ND
21	F	302	CLA	ND
21	F	303	CLA	ND
21	F	301	CLA	ND
21	G	203	CLA	ND
21	G	202	CLA	ND
21	G	201	CLA	ND
21	H	201	CLA	ND
21	J	101	CLA	ND
21	K	201	CLA	ND
21	K	204	CLA	ND
21	K	206	CLA	ND
21	K	203	CLA	ND
21	L	302	CLA	ND
21	L	303	CLA	ND
21	L	304	CLA	ND
21	O	203	CLA	ND
21	O	202	CLA	ND
21	O	201	CLA	ND
21	x	610	CLA	ND
21	x	604	CLA	ND
21	x	612	CLA	ND
21	x	602	CLA	ND
21	x	611	CLA	ND
21	x	613	CLA	ND
21	x	614	CLA	ND
21	x	603	CLA	ND
21	y	603	CLA	ND

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Mol	Chain	Res	Type	Atom
21	y	610	CLA	ND
21	y	613	CLA	ND
21	y	612	CLA	ND
21	y	602	CLA	ND
21	y	604	CLA	ND
21	y	614	CLA	ND
21	y	611	CLA	ND
21	z	602	CLA	ND
21	z	614	CLA	ND
21	z	612	CLA	ND
21	z	613	CLA	ND
21	z	604	CLA	ND
21	z	611	CLA	ND
21	z	610	CLA	ND
21	z	603	CLA	ND
27	A	801	CL0	NA
27	A	801	CL0	NC

All (1936) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	2	605	CHL	C3C-C2C-CMC-OMC
20	2	607	CHL	C1A-C2A-CAA-CBA
20	2	607	CHL	CBD-CGD-O2D-CED
20	3	606	CHL	C2A-CAA-CBA-CGA
20	3	606	CHL	CHA-CBD-CGD-O1D
20	3	606	CHL	CHA-CBD-CGD-O2D
20	4	605	CHL	C1A-C2A-CAA-CBA
20	x	606	CHL	C1A-C2A-CAA-CBA
20	x	606	CHL	C1C-C2C-CMC-OMC
20	x	606	CHL	C3C-C2C-CMC-OMC
20	x	607	CHL	C1C-C2C-CMC-OMC
20	x	607	CHL	C3C-C2C-CMC-OMC
20	x	607	CHL	C3-C5-C6-C7
20	x	609	CHL	C1A-C2A-CAA-CBA
20	x	601	CHL	C1A-C2A-CAA-CBA
20	x	601	CHL	C3A-C2A-CAA-CBA
20	x	601	CHL	C1C-C2C-CMC-OMC
20	x	601	CHL	C3C-C2C-CMC-OMC
20	x	601	CHL	CHA-CBD-CGD-O1D
20	x	601	CHL	CHA-CBD-CGD-O2D
20	x	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	x	605	CHL	C3A-C2A-CAA-CBA
20	x	605	CHL	C3C-C2C-CMC-OMC
20	x	605	CHL	CBD-CGD-O2D-CED
20	y	607	CHL	C3A-C2A-CAA-CBA
20	y	601	CHL	C1C-C2C-CMC-OMC
20	y	601	CHL	C3C-C2C-CMC-OMC
20	y	601	CHL	CBD-CGD-O2D-CED
20	y	605	CHL	CBD-CGD-O2D-CED
20	y	608	CHL	C1A-C2A-CAA-CBA
20	y	608	CHL	C3A-C2A-CAA-CBA
20	y	608	CHL	C1C-C2C-CMC-OMC
20	y	608	CHL	C3C-C2C-CMC-OMC
20	y	608	CHL	CBD-CGD-O2D-CED
20	y	609	CHL	C1A-C2A-CAA-CBA
20	y	609	CHL	C3A-C2A-CAA-CBA
20	y	609	CHL	CBA-CGA-O2A-C1
20	y	609	CHL	O1A-CGA-O2A-C1
20	y	609	CHL	C1C-C2C-CMC-OMC
20	y	609	CHL	C3C-C2C-CMC-OMC
20	y	609	CHL	CHA-CBD-CGD-O1D
20	y	609	CHL	CHA-CBD-CGD-O2D
20	y	609	CHL	C2-C3-C5-C6
20	y	609	CHL	C4-C3-C5-C6
20	z	606	CHL	C3C-C2C-CMC-OMC
20	z	609	CHL	C1A-C2A-CAA-CBA
20	z	609	CHL	C3A-C2A-CAA-CBA
20	z	609	CHL	C1C-C2C-CMC-OMC
20	z	609	CHL	C3C-C2C-CMC-OMC
20	z	609	CHL	C3-C5-C6-C7
20	z	601	CHL	C1C-C2C-CMC-OMC
20	z	601	CHL	C3C-C2C-CMC-OMC
20	z	601	CHL	CHA-CBD-CGD-O1D
20	z	601	CHL	CHA-CBD-CGD-O2D
20	z	605	CHL	CAD-CBD-CGD-O1D
20	z	605	CHL	CAD-CBD-CGD-O2D
21	1	603	CLA	C4-C3-C5-C6
21	1	604	CLA	C1A-C2A-CAA-CBA
21	1	605	CLA	C1A-C2A-CAA-CBA
21	1	605	CLA	C3A-C2A-CAA-CBA
21	1	605	CLA	C2A-CAA-CBA-CGA
21	1	605	CLA	CBA-CGA-O2A-C1
21	1	607	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	1	607	CLA	C3A-C2A-CAA-CBA
21	1	608	CLA	CBD-CGD-O2D-CED
21	1	609	CLA	CBD-CGD-O2D-CED
21	2	602	CLA	C2-C3-C5-C6
21	2	602	CLA	C4-C3-C5-C6
21	2	604	CLA	C1A-C2A-CAA-CBA
21	2	604	CLA	C3A-C2A-CAA-CBA
21	2	610	CLA	CMA-C3A-C4A-CHB
21	2	612	CLA	CBD-CGD-O2D-CED
21	2	608	CLA	C3A-C2A-CAA-CBA
21	3	605	CLA	C1A-C2A-CAA-CBA
21	3	605	CLA	CAD-CBD-CGD-O1D
21	3	605	CLA	CAD-CBD-CGD-O2D
21	3	603	CLA	C1A-C2A-CAA-CBA
21	3	603	CLA	C3A-C2A-CAA-CBA
21	3	609	CLA	C1A-C2A-CAA-CBA
21	3	609	CLA	C3A-C2A-CAA-CBA
21	3	608	CLA	CBD-CGD-O2D-CED
21	4	613	CLA	C1A-C2A-CAA-CBA
21	4	609	CLA	CBD-CGD-O2D-CED
21	4	611	CLA	CHA-CBD-CGD-O2D
21	4	612	CLA	CHA-CBD-CGD-O1D
21	4	612	CLA	CHA-CBD-CGD-O2D
21	4	610	CLA	C3A-C2A-CAA-CBA
21	4	610	CLA	CHA-CBD-CGD-O1D
21	4	610	CLA	CHA-CBD-CGD-O2D
21	4	604	CLA	CBD-CGD-O2D-CED
21	4	604	CLA	O1D-CGD-O2D-CED
21	A	829	CLA	CHA-CBD-CGD-O1D
21	A	829	CLA	CHA-CBD-CGD-O2D
21	A	829	CLA	CBD-CGD-O2D-CED
21	A	830	CLA	C1A-C2A-CAA-CBA
21	A	830	CLA	CBA-CGA-O2A-C1
21	A	830	CLA	O1A-CGA-O2A-C1
21	A	830	CLA	O2A-C1-C2-C3
21	A	830	CLA	C2-C3-C5-C6
21	A	830	CLA	C4-C3-C5-C6
21	A	818	CLA	CBD-CGD-O2D-CED
21	A	820	CLA	C1A-C2A-CAA-CBA
21	A	820	CLA	C3A-C2A-CAA-CBA
21	A	802	CLA	C1A-C2A-CAA-CBA
21	A	802	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	802	CLA	CBD-CGD-O2D-CED
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	804	CLA	CHA-CBD-CGD-O1D
21	A	804	CLA	CHA-CBD-CGD-O2D
21	A	804	CLA	CAD-CBD-CGD-O1D
21	A	804	CLA	CAD-CBD-CGD-O2D
21	A	823	CLA	C1A-C2A-CAA-CBA
21	A	823	CLA	C3A-C2A-CAA-CBA
21	A	824	CLA	CHA-CBD-CGD-O1D
21	A	824	CLA	CHA-CBD-CGD-O2D
21	A	827	CLA	C3A-C2A-CAA-CBA
21	A	825	CLA	C1A-C2A-CAA-CBA
21	A	825	CLA	C3A-C2A-CAA-CBA
21	A	825	CLA	C2-C3-C5-C6
21	A	825	CLA	C4-C3-C5-C6
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	814	CLA	C1A-C2A-CAA-CBA
21	A	814	CLA	C3A-C2A-CAA-CBA
21	A	819	CLA	C1A-C2A-CAA-CBA
21	A	819	CLA	C3A-C2A-CAA-CBA
21	A	819	CLA	C2-C3-C5-C6
21	A	819	CLA	C4-C3-C5-C6
21	A	819	CLA	C6-C7-C8-C9
21	A	806	CLA	C1A-C2A-CAA-CBA
21	A	806	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D
21	A	822	CLA	CHA-CBD-CGD-O1D
21	A	822	CLA	CHA-CBD-CGD-O2D
21	A	841	CLA	C1A-C2A-CAA-CBA
21	A	841	CLA	C3A-C2A-CAA-CBA
21	A	841	CLA	CHA-CBD-CGD-O1D
21	A	841	CLA	CHA-CBD-CGD-O2D
21	A	841	CLA	CAD-CBD-CGD-O1D
21	A	841	CLA	CBD-CGD-O2D-CED
21	A	838	CLA	C2A-CAA-CBA-CGA
21	A	842	CLA	C1A-C2A-CAA-CBA
21	A	844	CLA	C2-C3-C5-C6
21	A	844	CLA	C4-C3-C5-C6
21	A	835	CLA	CHA-CBD-CGD-O1D
21	A	835	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	CHA-CBD-CGD-O1D
21	A	837	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	A	845	CLA	C1A-C2A-CAA-CBA
21	A	845	CLA	C3A-C2A-CAA-CBA
21	A	836	CLA	C1A-C2A-CAA-CBA
21	A	840	CLA	CHA-CBD-CGD-O1D
21	A	840	CLA	CHA-CBD-CGD-O2D
21	A	840	CLA	C2-C3-C5-C6
21	A	840	CLA	C4-C3-C5-C6
21	A	843	CLA	C2-C1-O2A-CGA
21	A	839	CLA	C4-C3-C5-C6
21	B	820	CLA	C3A-C2A-CAA-CBA
21	B	822	CLA	C1A-C2A-CAA-CBA
21	B	822	CLA	CBD-CGD-O2D-CED
21	B	828	CLA	C1A-C2A-CAA-CBA
21	B	828	CLA	C3A-C2A-CAA-CBA
21	B	824	CLA	C3A-C2A-CAA-CBA
21	B	824	CLA	C2-C3-C5-C6
21	B	824	CLA	C4-C3-C5-C6
21	B	811	CLA	C1A-C2A-CAA-CBA
21	B	823	CLA	C1A-C2A-CAA-CBA
21	B	823	CLA	C3A-C2A-CAA-CBA
21	B	826	CLA	C1A-C2A-CAA-CBA
21	B	835	CLA	C3A-C2A-CAA-CBA
21	B	821	CLA	C1A-C2A-CAA-CBA
21	B	825	CLA	C3A-C2A-CAA-CBA
21	B	825	CLA	CHA-CBD-CGD-O2D
21	B	814	CLA	C4-C3-C5-C6
21	B	833	CLA	CHA-CBD-CGD-O1D
21	B	833	CLA	CHA-CBD-CGD-O2D
21	B	809	CLA	C1A-C2A-CAA-CBA
21	B	809	CLA	C2-C3-C5-C6
21	B	809	CLA	C4-C3-C5-C6
21	B	819	CLA	C1A-C2A-CAA-CBA
21	B	819	CLA	C3A-C2A-CAA-CBA
21	B	818	CLA	C1A-C2A-CAA-CBA
21	B	818	CLA	C3A-C2A-CAA-CBA
21	B	827	CLA	C1A-C2A-CAA-CBA
21	B	827	CLA	C3A-C2A-CAA-CBA
21	B	802	CLA	C3A-C2A-CAA-CBA
21	B	802	CLA	C11-C12-C13-C14
21	B	805	CLA	C1A-C2A-CAA-CBA
21	B	805	CLA	C3A-C2A-CAA-CBA
21	B	810	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	803	CLA	CHA-CBD-CGD-O1D
21	B	803	CLA	CHA-CBD-CGD-O2D
21	B	803	CLA	CBD-CGD-O2D-CED
21	B	803	CLA	O1D-CGD-O2D-CED
21	F	302	CLA	CBD-CGD-O2D-CED
21	F	301	CLA	CBD-CGD-O2D-CED
21	F	301	CLA	C2-C3-C5-C6
21	F	301	CLA	C4-C3-C5-C6
21	G	202	CLA	C1A-C2A-CAA-CBA
21	G	202	CLA	C3A-C2A-CAA-CBA
21	G	201	CLA	C1A-C2A-CAA-CBA
21	G	201	CLA	C3A-C2A-CAA-CBA
21	G	201	CLA	CBD-CGD-O2D-CED
21	K	204	CLA	CBD-CGD-O2D-CED
21	K	203	CLA	C1A-C2A-CAA-CBA
21	x	610	CLA	C3A-C2A-CAA-CBA
21	x	604	CLA	CBA-CGA-O2A-C1
21	x	612	CLA	CBD-CGD-O2D-CED
21	x	602	CLA	C3A-C2A-CAA-CBA
21	x	613	CLA	CHA-CBD-CGD-O1D
21	x	613	CLA	CHA-CBD-CGD-O2D
21	x	613	CLA	CBD-CGD-O2D-CED
21	x	603	CLA	C6-C7-C8-C9
21	y	610	CLA	C1A-C2A-CAA-CBA
21	y	610	CLA	C3A-C2A-CAA-CBA
21	y	610	CLA	CBD-CGD-O2D-CED
21	y	612	CLA	CBD-CGD-O2D-CED
21	y	602	CLA	C3A-C2A-CAA-CBA
21	y	602	CLA	C2-C3-C5-C6
21	y	602	CLA	C4-C3-C5-C6
21	y	604	CLA	C1A-C2A-CAA-CBA
21	y	604	CLA	CHA-CBD-CGD-O1D
21	y	604	CLA	CHA-CBD-CGD-O2D
21	y	614	CLA	C1A-C2A-CAA-CBA
21	y	614	CLA	O1A-CGA-O2A-C1
21	y	614	CLA	CBD-CGD-O2D-CED
21	y	614	CLA	C6-C7-C8-C10
21	y	611	CLA	C1A-C2A-CAA-CBA
21	y	611	CLA	C3A-C2A-CAA-CBA
21	z	602	CLA	O2A-C1-C2-C3
21	z	614	CLA	C1A-C2A-CAA-CBA
21	z	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	z	614	CLA	CHA-CBD-CGD-O2D
22	1	614	XAT	O24-C26-C27-C28
22	2	617	XAT	O4-C6-C7-C8
22	2	617	XAT	C11-C10-C9-C19
22	2	617	XAT	C10-C11-C12-C13
22	2	617	XAT	C13-C14-C15-C35
22	2	617	XAT	O24-C26-C27-C28
22	2	617	XAT	C28-C29-C30-C31
22	2	617	XAT	C39-C29-C30-C31
22	2	617	XAT	C31-C32-C33-C34
22	2	617	XAT	C31-C32-C33-C40
22	4	617	XAT	O4-C6-C7-C8
22	x	617	XAT	C1-C6-C7-C8
22	x	617	XAT	C5-C6-C7-C8
22	x	617	XAT	C6-C7-C8-C9
22	x	617	XAT	O24-C26-C27-C28
22	y	617	XAT	C7-C8-C9-C10
22	y	617	XAT	C7-C8-C9-C19
22	y	617	XAT	O24-C26-C27-C28
23	1	615	LHG	C2-C3-O3-P
23	1	615	LHG	C3-O3-P-O4
23	1	615	LHG	O7-C5-C6-O8
23	2	618	LHG	C3-O3-P-O5
23	2	618	LHG	C3-O3-P-O6
23	2	618	LHG	O9-C7-O7-C5
23	2	618	LHG	C8-C7-O7-C5
23	2	618	LHG	O10-C23-O8-C6
23	2	618	LHG	C24-C23-O8-C6
23	A	846	LHG	O10-C23-O8-C6
23	A	846	LHG	C24-C23-O8-C6
23	B	851	LHG	C8-C7-O7-C5
23	B	852	LHG	C2-C3-O3-P
23	z	619	LHG	C3-O3-P-O5
23	z	619	LHG	O10-C23-O8-C6
23	z	619	LHG	C24-C23-O8-C6
24	2	619	LUT	C21-C26-C27-C28
24	2	619	LUT	C25-C26-C27-C28
24	2	616	LUT	C6-C7-C8-C9
24	2	616	LUT	C31-C32-C33-C34
24	2	616	LUT	C31-C32-C33-C40
24	3	613	LUT	C21-C26-C27-C28
24	3	613	LUT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
24	4	616	LUT	C1-C6-C7-C8
24	4	616	LUT	C5-C6-C7-C8
24	x	616	LUT	C27-C28-C29-C30
24	x	616	LUT	C27-C28-C29-C39
24	y	616	LUT	C1-C6-C7-C8
24	y	616	LUT	C5-C6-C7-C8
24	y	616	LUT	C21-C26-C27-C28
24	y	616	LUT	C25-C26-C27-C28
24	y	616	LUT	C27-C28-C29-C30
24	y	616	LUT	C27-C28-C29-C39
24	y	615	LUT	C26-C27-C28-C29
24	y	615	LUT	C31-C32-C33-C34
24	y	615	LUT	C31-C32-C33-C40
24	z	615	LUT	C7-C8-C9-C10
24	z	615	LUT	C7-C8-C9-C19
24	z	616	LUT	C21-C26-C27-C28
24	z	616	LUT	C25-C26-C27-C28
25	3	614	BCR	C21-C22-C23-C24
25	3	614	BCR	C37-C22-C23-C24
25	4	618	BCR	C7-C8-C9-C10
25	4	618	BCR	C7-C8-C9-C34
25	4	618	BCR	C23-C24-C25-C26
25	A	852	BCR	C14-C15-C16-C17
25	A	852	BCR	C16-C17-C18-C19
25	A	852	BCR	C16-C17-C18-C36
25	A	852	BCR	C21-C22-C23-C24
25	A	852	BCR	C37-C22-C23-C24
25	A	850	BCR	C7-C8-C9-C10
25	A	850	BCR	C7-C8-C9-C34
25	A	851	BCR	C11-C12-C13-C14
25	A	851	BCR	C11-C12-C13-C35
25	A	849	BCR	C23-C24-C25-C26
25	A	849	BCR	C23-C24-C25-C30
25	B	801	BCR	C1-C6-C7-C8
25	B	801	BCR	C5-C6-C7-C8
25	B	844	BCR	C12-C13-C14-C15
25	B	844	BCR	C35-C13-C14-C15
25	B	844	BCR	C14-C15-C16-C17
25	B	844	BCR	C16-C17-C18-C36
25	B	845	BCR	C21-C22-C23-C24
25	B	846	BCR	C23-C24-C25-C26
25	B	846	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	B	849	BCR	C11-C10-C9-C34
25	B	849	BCR	C22-C23-C24-C25
25	F	304	BCR	C11-C12-C13-C14
25	F	304	BCR	C11-C12-C13-C35
25	F	304	BCR	C15-C16-C17-C18
25	K	205	BCR	C7-C8-C9-C10
25	K	205	BCR	C7-C8-C9-C34
25	K	205	BCR	C17-C18-C19-C20
25	K	205	BCR	C36-C18-C19-C20
25	K	205	BCR	C18-C19-C20-C21
29	B	842	PQN	C14-C13-C15-C16
30	B	850	DGD	O2G-C2G-C3G-O3G
31	x	618	NEX	C21-C26-C27-C28
31	x	618	NEX	C25-C26-C27-C28
31	x	618	NEX	O24-C26-C27-C28
31	x	618	NEX	C28-C29-C30-C31
31	x	618	NEX	C39-C29-C30-C31
21	1	608	CLA	O1D-CGD-O2D-CED
21	2	609	CLA	O1D-CGD-O2D-CED
21	A	802	CLA	O1D-CGD-O2D-CED
21	B	822	CLA	O1D-CGD-O2D-CED
21	B	830	CLA	O1D-CGD-O2D-CED
21	H	201	CLA	O1D-CGD-O2D-CED
21	x	610	CLA	O1D-CGD-O2D-CED
20	3	606	CHL	O1D-CGD-O2D-CED
21	4	609	CLA	O1D-CGD-O2D-CED
21	A	818	CLA	O1D-CGD-O2D-CED
21	B	802	CLA	O1D-CGD-O2D-CED
21	K	204	CLA	O1D-CGD-O2D-CED
20	3	606	CHL	CBD-CGD-O2D-CED
20	4	607	CHL	CBD-CGD-O2D-CED
20	z	606	CHL	CBD-CGD-O2D-CED
21	2	609	CLA	CBD-CGD-O2D-CED
21	2	613	CLA	CBD-CGD-O2D-CED
21	3	605	CLA	CBD-CGD-O2D-CED
21	3	607	CLA	CBD-CGD-O2D-CED
21	4	614	CLA	CBD-CGD-O2D-CED
21	A	811	CLA	CBD-CGD-O2D-CED
21	A	812	CLA	CBD-CGD-O2D-CED
21	B	830	CLA	CBD-CGD-O2D-CED
21	B	802	CLA	CBD-CGD-O2D-CED
21	H	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	x	610	CLA	CBD-CGD-O2D-CED
21	y	613	CLA	CBD-CGD-O2D-CED
21	z	610	CLA	CBD-CGD-O2D-CED
20	x	607	CHL	O1A-CGA-O2A-C1
21	A	803	CLA	O1A-CGA-O2A-C1
21	x	604	CLA	O1A-CGA-O2A-C1
21	y	610	CLA	O1A-CGA-O2A-C1
21	2	613	CLA	O1D-CGD-O2D-CED
21	A	811	CLA	O1D-CGD-O2D-CED
21	F	302	CLA	O1D-CGD-O2D-CED
21	y	613	CLA	O1D-CGD-O2D-CED
21	z	610	CLA	O1D-CGD-O2D-CED
20	x	605	CHL	O1D-CGD-O2D-CED
20	y	605	CHL	O1D-CGD-O2D-CED
21	1	609	CLA	O1D-CGD-O2D-CED
21	3	605	CLA	O1D-CGD-O2D-CED
21	3	608	CLA	O1D-CGD-O2D-CED
21	A	829	CLA	O1D-CGD-O2D-CED
21	x	613	CLA	O1D-CGD-O2D-CED
21	y	610	CLA	O1D-CGD-O2D-CED
21	y	612	CLA	O1D-CGD-O2D-CED
20	x	607	CHL	CBA-CGA-O2A-C1
21	A	803	CLA	CBA-CGA-O2A-C1
20	y	606	CHL	CBD-CGD-O2D-CED
20	z	608	CHL	CBD-CGD-O2D-CED
20	z	601	CHL	CBD-CGD-O2D-CED
21	1	604	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	CBD-CGD-O2D-CED
21	A	803	CLA	CBD-CGD-O2D-CED
21	A	813	CLA	CBD-CGD-O2D-CED
21	A	816	CLA	CBD-CGD-O2D-CED
21	B	823	CLA	CBD-CGD-O2D-CED
21	x	614	CLA	CBD-CGD-O2D-CED
21	z	613	CLA	CBD-CGD-O2D-CED
20	x	601	CHL	O1A-CGA-O2A-C1
20	z	609	CHL	O1A-CGA-O2A-C1
21	3	602	CLA	O1A-CGA-O2A-C1
21	A	835	CLA	O1A-CGA-O2A-C1
21	A	839	CLA	O1A-CGA-O2A-C1
21	B	836	CLA	O1A-CGA-O2A-C1
21	B	802	CLA	O1A-CGA-O2A-C1
21	y	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	1	605	CLA	O1A-CGA-O2A-C1
20	y	601	CHL	O1D-CGD-O2D-CED
21	2	612	CLA	O1D-CGD-O2D-CED
21	F	301	CLA	O1D-CGD-O2D-CED
21	G	201	CLA	O1D-CGD-O2D-CED
20	2	607	CHL	O1D-CGD-O2D-CED
20	y	608	CHL	O1D-CGD-O2D-CED
21	A	841	CLA	O1D-CGD-O2D-CED
21	x	612	CLA	O1D-CGD-O2D-CED
21	y	614	CLA	O1D-CGD-O2D-CED
21	2	608	CLA	CBD-CGD-O2D-CED
21	3	603	CLA	CBD-CGD-O2D-CED
21	A	822	CLA	CBD-CGD-O2D-CED
21	y	602	CLA	CBD-CGD-O2D-CED
21	y	604	CLA	CBD-CGD-O2D-CED
21	A	812	CLA	C13-C15-C16-C17
23	B	851	LHG	O9-C7-O7-C5
30	B	850	DGD	O1B-C1B-O2G-C2G
21	A	820	CLA	O1A-CGA-O2A-C1
21	3	602	CLA	C3-C5-C6-C7
21	4	602	CLA	C3-C5-C6-C7
21	A	803	CLA	C3-C5-C6-C7
21	A	829	CLA	C3-C5-C6-C7
21	A	814	CLA	C3-C5-C6-C7
21	A	819	CLA	C3-C5-C6-C7
21	A	833	CLA	C3-C5-C6-C7
21	A	843	CLA	C3-C5-C6-C7
21	B	829	CLA	C3-C5-C6-C7
21	B	840	CLA	C3-C5-C6-C7
21	B	841	CLA	C3-C5-C6-C7
21	B	814	CLA	C3-C5-C6-C7
21	B	827	CLA	C3-C5-C6-C7
21	B	805	CLA	C3-C5-C6-C7
21	L	303	CLA	C3-C5-C6-C7
21	x	613	CLA	C3-C5-C6-C7
27	A	801	CL0	C3-C5-C6-C7
20	z	609	CHL	CBA-CGA-O2A-C1
21	3	602	CLA	CBA-CGA-O2A-C1
21	A	835	CLA	CBA-CGA-O2A-C1
21	B	836	CLA	CBA-CGA-O2A-C1
21	y	610	CLA	CBA-CGA-O2A-C1
21	y	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	y	614	CLA	CBA-CGA-O2A-C1
30	B	850	DGD	C2B-C1B-O2G-C2G
20	y	607	CHL	CBD-CGD-O2D-CED
21	A	814	CLA	CBD-CGD-O2D-CED
21	A	838	CLA	CBD-CGD-O2D-CED
21	O	201	CLA	CBD-CGD-O2D-CED
21	x	603	CLA	CBD-CGD-O2D-CED
20	1	601	CHL	C3-C5-C6-C7
20	z	609	CHL	C4-C3-C5-C6
21	A	818	CLA	C4-C3-C5-C6
21	A	805	CLA	C4-C3-C5-C6
21	A	841	CLA	C4-C3-C5-C6
21	x	610	CLA	C4-C3-C5-C6
21	A	818	CLA	C2-C3-C5-C6
21	A	839	CLA	C2-C3-C5-C6
21	B	814	CLA	C2-C3-C5-C6
21	x	610	CLA	C2-C3-C5-C6
20	x	607	CHL	CBD-CGD-O2D-CED
21	1	602	CLA	CBD-CGD-O2D-CED
21	A	823	CLA	CBD-CGD-O2D-CED
21	B	840	CLA	CBD-CGD-O2D-CED
21	B	834	CLA	CBD-CGD-O2D-CED
20	2	601	CHL	C2A-CAA-CBA-CGA
20	2	607	CHL	C2A-CAA-CBA-CGA
20	x	601	CHL	C2A-CAA-CBA-CGA
20	y	601	CHL	C2A-CAA-CBA-CGA
20	z	609	CHL	C2A-CAA-CBA-CGA
20	z	607	CHL	C2A-CAA-CBA-CGA
21	2	608	CLA	C2A-CAA-CBA-CGA
21	A	809	CLA	C2A-CAA-CBA-CGA
21	A	843	CLA	C2A-CAA-CBA-CGA
21	B	802	CLA	C2A-CAA-CBA-CGA
21	B	839	CLA	C2A-CAA-CBA-CGA
21	B	813	CLA	C2A-CAA-CBA-CGA
21	G	201	CLA	C2A-CAA-CBA-CGA
21	H	201	CLA	C2A-CAA-CBA-CGA
21	x	602	CLA	C2A-CAA-CBA-CGA
21	y	613	CLA	C2A-CAA-CBA-CGA
21	z	602	CLA	C2A-CAA-CBA-CGA
21	A	818	CLA	C3-C5-C6-C7
21	A	828	CLA	C3-C5-C6-C7
21	B	806	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	B	808	CLA	C3-C5-C6-C7
20	x	601	CHL	CBA-CGA-O2A-C1
20	y	601	CHL	CBA-CGA-O2A-C1
21	A	802	CLA	CBA-CGA-O2A-C1
21	A	839	CLA	CBA-CGA-O2A-C1
21	B	811	CLA	CBA-CGA-O2A-C1
21	B	802	CLA	CBA-CGA-O2A-C1
21	x	602	CLA	CBA-CGA-O2A-C1
20	z	606	CHL	O1D-CGD-O2D-CED
21	A	820	CLA	CBD-CGD-O2D-CED
21	B	835	CLA	CBD-CGD-O2D-CED
21	x	604	CLA	CBD-CGD-O2D-CED
21	3	607	CLA	O1D-CGD-O2D-CED
21	4	614	CLA	O1D-CGD-O2D-CED
21	1	603	CLA	O1A-CGA-O2A-C1
21	2	609	CLA	O1A-CGA-O2A-C1
21	A	818	CLA	O1A-CGA-O2A-C1
21	A	802	CLA	O1A-CGA-O2A-C1
21	B	811	CLA	O1A-CGA-O2A-C1
21	B	827	CLA	O1A-CGA-O2A-C1
21	L	303	CLA	O1A-CGA-O2A-C1
22	2	617	XAT	C33-C34-C35-C15
22	x	617	XAT	C9-C10-C11-C12
22	y	617	XAT	C29-C30-C31-C32
24	1	616	LUT	C29-C30-C31-C32
24	2	616	LUT	C33-C34-C35-C15
24	3	613	LUT	C9-C10-C11-C12
24	3	613	LUT	C33-C34-C35-C15
24	y	615	LUT	C13-C14-C15-C35
24	z	616	LUT	C29-C30-C31-C32
25	A	853	BCR	C9-C10-C11-C12
25	A	850	BCR	C13-C14-C15-C16
25	A	850	BCR	C15-C16-C17-C18
25	A	851	BCR	C13-C14-C15-C16
25	A	849	BCR	C15-C16-C17-C18
25	A	849	BCR	C19-C20-C21-C22
25	B	801	BCR	C9-C10-C11-C12
25	B	843	BCR	C13-C14-C15-C16
25	B	845	BCR	C19-C20-C21-C22
25	F	304	BCR	C19-C20-C21-C22
31	x	618	NEX	C29-C30-C31-C32
20	4	606	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	817	CLA	CBD-CGD-O2D-CED
21	A	836	CLA	CBD-CGD-O2D-CED
21	B	813	CLA	CBD-CGD-O2D-CED
21	J	101	CLA	CBD-CGD-O2D-CED
23	1	615	LHG	O2-C2-C3-O3
21	2	612	CLA	C3-C5-C6-C7
21	3	601	CLA	C3-C5-C6-C7
21	A	807	CLA	C3-C5-C6-C7
21	A	844	CLA	C3-C5-C6-C7
21	A	811	CLA	CBA-CGA-O2A-C1
21	A	818	CLA	CBA-CGA-O2A-C1
21	A	820	CLA	CBA-CGA-O2A-C1
21	L	303	CLA	CBA-CGA-O2A-C1
23	y	619	LHG	C24-C23-O8-C6
23	1	615	LHG	C28-C29-C30-C31
21	A	811	CLA	O1A-CGA-O2A-C1
21	K	204	CLA	CBA-CGA-O2A-C1
20	z	605	CHL	CBD-CGD-O2D-CED
21	4	613	CLA	CBD-CGD-O2D-CED
21	4	612	CLA	CBD-CGD-O2D-CED
21	K	203	CLA	CBD-CGD-O2D-CED
21	3	601	CLA	C5-C6-C7-C8
21	A	812	CLA	O1D-CGD-O2D-CED
23	1	615	LHG	C11-C10-C9-C8
23	1	615	LHG	C34-C35-C36-C37
21	A	841	CLA	C3-C5-C6-C7
21	B	803	CLA	C3-C5-C6-C7
21	H	201	CLA	C3-C5-C6-C7
21	1	603	CLA	CBA-CGA-O2A-C1
21	2	609	CLA	CBA-CGA-O2A-C1
21	B	827	CLA	CBA-CGA-O2A-C1
20	4	607	CHL	O1D-CGD-O2D-CED
20	y	601	CHL	O1A-CGA-O2A-C1
21	x	602	CLA	O1A-CGA-O2A-C1
20	x	605	CHL	C3-C5-C6-C7
20	y	608	CHL	O2A-C1-C2-C3
20	y	601	CHL	C4-C3-C5-C6
21	A	833	CLA	C4-C3-C5-C6
20	y	601	CHL	C2-C3-C5-C6
21	1	603	CLA	C2-C3-C5-C6
21	A	833	CLA	C2-C3-C5-C6
29	B	842	PQN	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	830	CLA	C2A-CAA-CBA-CGA
30	B	850	DGD	O6D-C1D-O3G-C3G
21	A	842	CLA	CBA-CGA-O2A-C1
21	F	301	CLA	CBA-CGA-O2A-C1
21	x	610	CLA	CBA-CGA-O2A-C1
26	4	620	LMG	C29-C28-O8-C9
23	y	619	LHG	O10-C23-O8-C6
21	A	813	CLA	O1D-CGD-O2D-CED
21	A	816	CLA	O1D-CGD-O2D-CED
21	y	611	CLA	CBD-CGD-O2D-CED
21	x	610	CLA	O1A-CGA-O2A-C1
26	4	620	LMG	O10-C28-O8-C9
20	1	601	CHL	CBA-CGA-O2A-C1
20	y	607	CHL	CBA-CGA-O2A-C1
21	A	805	CLA	CBA-CGA-O2A-C1
21	A	843	CLA	CBA-CGA-O2A-C1
21	B	840	CLA	CBA-CGA-O2A-C1
21	B	814	CLA	CBA-CGA-O2A-C1
21	J	101	CLA	CBA-CGA-O2A-C1
21	z	602	CLA	CBA-CGA-O2A-C1
21	z	604	CLA	CBA-CGA-O2A-C1
21	z	603	CLA	CBA-CGA-O2A-C1
27	A	801	CL0	CBA-CGA-O2A-C1
20	x	606	CHL	CBD-CGD-O2D-CED
21	2	604	CLA	O1D-CGD-O2D-CED
22	x	617	XAT	C13-C14-C15-C35
21	A	835	CLA	C2C-C3C-CAC-CBC
20	y	607	CHL	O1A-CGA-O2A-C1
21	A	835	CLA	C8-C10-C11-C12
21	z	613	CLA	C15-C16-C17-C18
20	y	607	CHL	C3-C5-C6-C7
20	z	601	CHL	O1D-CGD-O2D-CED
20	z	609	CHL	C2-C3-C5-C6
21	A	841	CLA	C2-C3-C5-C6
21	2	612	CLA	C11-C12-C13-C14
21	3	601	CLA	C11-C10-C8-C9
21	4	612	CLA	C6-C7-C8-C9
21	A	803	CLA	C6-C7-C8-C9
21	A	811	CLA	C14-C13-C15-C16
21	A	812	CLA	C6-C7-C8-C9
21	A	826	CLA	C11-C10-C8-C9
21	A	826	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	A	831	CLA	C6-C7-C8-C9
21	A	818	CLA	C11-C10-C8-C9
21	A	807	CLA	C11-C10-C8-C9
21	A	820	CLA	C11-C10-C8-C9
21	A	802	CLA	C11-C12-C13-C14
21	A	804	CLA	C11-C10-C8-C9
21	A	828	CLA	C11-C10-C8-C9
21	A	841	CLA	C14-C13-C15-C16
21	A	835	CLA	C11-C10-C8-C9
21	B	808	CLA	C6-C7-C8-C9
21	B	808	CLA	C14-C13-C15-C16
21	B	828	CLA	C14-C13-C15-C16
21	B	840	CLA	C6-C7-C8-C9
21	B	840	CLA	C14-C13-C15-C16
21	B	825	CLA	C11-C12-C13-C14
21	B	825	CLA	C14-C13-C15-C16
21	B	814	CLA	C11-C10-C8-C9
21	B	809	CLA	C6-C7-C8-C9
21	B	805	CLA	C11-C10-C8-C9
21	B	839	CLA	C14-C13-C15-C16
21	B	803	CLA	C6-C7-C8-C9
21	B	803	CLA	C11-C10-C8-C9
21	F	301	CLA	C6-C7-C8-C9
21	H	201	CLA	C6-C7-C8-C9
21	L	303	CLA	C11-C12-C13-C14
21	O	201	CLA	C11-C10-C8-C9
21	x	610	CLA	C6-C7-C8-C9
21	x	610	CLA	C11-C12-C13-C14
21	y	602	CLA	C14-C13-C15-C16
21	y	614	CLA	C11-C12-C13-C14
27	A	801	CL0	C11-C10-C8-C9
21	1	604	CLA	O1D-CGD-O2D-CED
21	A	825	CLA	CBD-CGD-O2D-CED
21	4	602	CLA	C5-C6-C7-C8
21	B	813	CLA	C13-C15-C16-C17
21	L	303	CLA	C8-C10-C11-C12
21	O	201	CLA	C15-C16-C17-C18
21	y	610	CLA	C5-C6-C7-C8
21	G	203	CLA	C2A-CAA-CBA-CGA
22	1	614	XAT	C7-C8-C9-C19
22	x	617	XAT	C7-C8-C9-C19
25	A	853	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
25	B	801	BCR	C7-C8-C9-C34
25	B	845	BCR	C36-C18-C19-C20
25	B	845	BCR	C37-C22-C23-C24
25	B	846	BCR	C7-C8-C9-C34
25	B	846	BCR	C37-C22-C23-C24
25	J	102	BCR	C7-C8-C9-C34
25	L	306	BCR	C7-C8-C9-C34
25	L	306	BCR	C37-C22-C23-C24
22	1	614	XAT	C7-C8-C9-C10
22	x	617	XAT	C7-C8-C9-C10
25	A	853	BCR	C11-C12-C13-C14
25	B	845	BCR	C17-C18-C19-C20
25	B	846	BCR	C7-C8-C9-C10
25	J	102	BCR	C7-C8-C9-C10
25	L	306	BCR	C7-C8-C9-C10
25	L	306	BCR	C21-C22-C23-C24
21	B	840	CLA	O1A-CGA-O2A-C1
21	B	814	CLA	O1A-CGA-O2A-C1
21	z	604	CLA	O1A-CGA-O2A-C1
21	A	812	CLA	C5-C6-C7-C8
21	A	828	CLA	C8-C10-C11-C12
21	B	808	CLA	C13-C15-C16-C17
21	z	613	CLA	O1D-CGD-O2D-CED
21	A	845	CLA	CBA-CGA-O2A-C1
21	y	602	CLA	CBA-CGA-O2A-C1
21	B	814	CLA	C8-C10-C11-C12
21	O	201	CLA	C13-C15-C16-C17
20	z	609	CHL	C2C-C3C-CAC-CBC
21	2	602	CLA	C5-C6-C7-C8
21	2	602	CLA	C13-C15-C16-C17
21	A	831	CLA	C13-C15-C16-C17
21	A	820	CLA	C5-C6-C7-C8
21	A	828	CLA	C5-C6-C7-C8
21	A	842	CLA	C8-C10-C11-C12
21	B	837	CLA	C10-C11-C12-C13
21	B	805	CLA	C10-C11-C12-C13
21	H	201	CLA	C5-C6-C7-C8
21	x	602	CLA	C5-C6-C7-C8
21	x	602	CLA	C10-C11-C12-C13
21	z	613	CLA	C10-C11-C12-C13
27	A	801	CL0	C8-C10-C11-C12
27	A	801	CL0	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	A	843	CLA	O1A-CGA-O2A-C1
23	B	851	LHG	C23-C24-C25-C26
20	z	608	CHL	O1D-CGD-O2D-CED
21	2	602	CLA	C15-C16-C17-C18
21	A	812	CLA	C10-C11-C12-C13
21	A	826	CLA	C8-C10-C11-C12
21	A	806	CLA	C10-C11-C12-C13
21	B	822	CLA	C5-C6-C7-C8
21	B	809	CLA	C5-C6-C7-C8
21	y	602	CLA	C5-C6-C7-C8
21	A	838	CLA	CBA-CGA-O2A-C1
21	A	828	CLA	C13-C15-C16-C17
21	A	841	CLA	C5-C6-C7-C8
21	A	844	CLA	C5-C6-C7-C8
23	y	619	LHG	C2-C3-O3-P
21	x	614	CLA	O1D-CGD-O2D-CED
21	1	605	CLA	CBD-CGD-O2D-CED
21	A	839	CLA	CBD-CGD-O2D-CED
21	B	841	CLA	CBD-CGD-O2D-CED
21	3	601	CLA	C11-C10-C8-C7
21	A	803	CLA	C11-C12-C13-C15
21	A	804	CLA	C6-C7-C8-C10
21	A	804	CLA	C12-C13-C15-C16
21	B	806	CLA	C11-C10-C8-C7
21	B	827	CLA	C11-C12-C13-C15
21	B	810	CLA	C6-C7-C8-C10
21	B	803	CLA	C11-C10-C8-C7
21	z	613	CLA	C6-C7-C8-C10
21	z	614	CLA	C3-C5-C6-C7
21	z	613	CLA	C3-C5-C6-C7
21	A	805	CLA	O1A-CGA-O2A-C1
21	z	603	CLA	O1A-CGA-O2A-C1
21	1	607	CLA	C2A-CAA-CBA-CGA
21	3	609	CLA	C2A-CAA-CBA-CGA
21	B	828	CLA	C2A-CAA-CBA-CGA
20	y	606	CHL	O1D-CGD-O2D-CED
21	A	803	CLA	O1D-CGD-O2D-CED
21	A	822	CLA	O1D-CGD-O2D-CED
21	B	823	CLA	O1D-CGD-O2D-CED
21	y	602	CLA	O1D-CGD-O2D-CED
21	B	837	CLA	C5-C6-C7-C8
21	H	201	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	L	303	CLA	C13-C15-C16-C17
20	1	601	CHL	O1A-CGA-O2A-C1
21	J	101	CLA	O1A-CGA-O2A-C1
21	z	602	CLA	O1A-CGA-O2A-C1
27	A	801	CL0	O1A-CGA-O2A-C1
20	y	609	CHL	CBD-CGD-O2D-CED
21	A	804	CLA	C8-C10-C11-C12
21	A	828	CLA	C15-C16-C17-C18
21	B	832	CLA	C15-C16-C17-C18
21	2	608	CLA	O1D-CGD-O2D-CED
22	2	617	XAT	C30-C31-C32-C33
24	2	616	LUT	C10-C11-C12-C13
25	B	849	BCR	C10-C11-C12-C13
21	B	802	CLA	C3-C5-C6-C7
21	2	612	CLA	C10-C11-C12-C13
21	A	819	CLA	C5-C6-C7-C8
21	A	806	CLA	C8-C10-C11-C12
21	A	843	CLA	C8-C10-C11-C12
21	B	806	CLA	C5-C6-C7-C8
21	B	822	CLA	C10-C11-C12-C13
21	B	841	CLA	C8-C10-C11-C12
21	B	810	CLA	C5-C6-C7-C8
21	y	604	CLA	O1D-CGD-O2D-CED
21	A	842	CLA	O1A-CGA-O2A-C1
21	F	301	CLA	O1A-CGA-O2A-C1
21	y	602	CLA	O1A-CGA-O2A-C1
21	A	812	CLA	C8-C10-C11-C12
21	A	842	CLA	C13-C15-C16-C17
21	B	817	CLA	C5-C6-C7-C8
21	L	303	CLA	C10-C11-C12-C13
21	O	201	CLA	C5-C6-C7-C8
21	x	603	CLA	C5-C6-C7-C8
21	y	602	CLA	C13-C15-C16-C17
21	y	614	CLA	C10-C11-C12-C13
21	K	204	CLA	O1A-CGA-O2A-C1
20	y	607	CHL	O1D-CGD-O2D-CED
21	O	201	CLA	O1D-CGD-O2D-CED
21	x	603	CLA	O1D-CGD-O2D-CED
21	3	603	CLA	O1D-CGD-O2D-CED
21	B	822	CLA	C8-C10-C11-C12
21	B	811	CLA	C5-C6-C7-C8
21	B	825	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	814	CLA	C5-C6-C7-C8
21	B	818	CLA	C8-C10-C11-C12
21	z	602	CLA	C5-C6-C7-C8
23	1	615	LHG	C3-O3-P-O6
23	B	852	LHG	C3-O3-P-O6
21	B	820	CLA	CBA-CGA-O2A-C1
21	B	813	CLA	CBA-CGA-O2A-C1
20	x	607	CHL	O1D-CGD-O2D-CED
21	A	814	CLA	O1D-CGD-O2D-CED
21	A	845	CLA	CBD-CGD-O2D-CED
21	A	835	CLA	C10-C11-C12-C13
20	z	608	CHL	O2A-C1-C2-C3
21	A	838	CLA	O1D-CGD-O2D-CED
21	B	813	CLA	C4-C3-C5-C6
21	A	834	CLA	C13-C15-C16-C17
21	2	611	CLA	C2A-CAA-CBA-CGA
21	2	609	CLA	C2A-CAA-CBA-CGA
21	3	601	CLA	C2A-CAA-CBA-CGA
21	B	817	CLA	C2A-CAA-CBA-CGA
21	B	816	CLA	C6-C7-C8-C10
21	B	817	CLA	CBA-CGA-O2A-C1
21	B	841	CLA	CBA-CGA-O2A-C1
21	A	807	CLA	C5-C6-C7-C8
21	A	814	CLA	C13-C15-C16-C17
30	B	850	DGD	C3B-C4B-C5B-C6B
21	4	608	CLA	CBD-CGD-O2D-CED
22	2	617	XAT	C20-C13-C14-C15
24	3	613	LUT	C11-C10-C9-C19
25	A	852	BCR	C35-C13-C14-C15
25	F	304	BCR	C11-C10-C9-C34
25	K	205	BCR	C20-C21-C22-C37
23	1	615	LHG	C11-C12-C13-C14
30	B	850	DGD	C5B-C6B-C7B-C8B
21	1	602	CLA	O1D-CGD-O2D-CED
21	A	823	CLA	O1D-CGD-O2D-CED
21	2	612	CLA	C16-C17-C18-C20
21	A	812	CLA	C16-C17-C18-C20
21	B	808	CLA	C16-C17-C18-C20
21	B	822	CLA	C16-C17-C18-C19
21	B	818	CLA	C11-C12-C13-C14
21	O	201	CLA	C16-C17-C18-C19
23	B	852	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
21	A	820	CLA	O1D-CGD-O2D-CED
21	B	840	CLA	O1D-CGD-O2D-CED
21	B	835	CLA	O1D-CGD-O2D-CED
21	B	834	CLA	O1D-CGD-O2D-CED
21	B	811	CLA	CBD-CGD-O2D-CED
23	1	615	LHG	C29-C30-C31-C32
21	x	604	CLA	O1D-CGD-O2D-CED
21	x	610	CLA	C3-C5-C6-C7
22	2	617	XAT	C11-C10-C9-C8
25	A	852	BCR	C12-C13-C14-C15
25	B	844	BCR	C16-C17-C18-C19
25	B	849	BCR	C11-C10-C9-C8
25	F	304	BCR	C11-C10-C9-C8
25	K	205	BCR	C20-C21-C22-C23
21	A	813	CLA	CBA-CGA-O2A-C1
21	A	834	CLA	CBA-CGA-O2A-C1
21	2	612	CLA	C5-C6-C7-C8
21	A	838	CLA	O1A-CGA-O2A-C1
21	A	845	CLA	O1A-CGA-O2A-C1
21	B	822	CLA	C16-C17-C18-C20
21	B	841	CLA	C16-C17-C18-C20
21	z	613	CLA	C4-C3-C5-C6
23	1	615	LHG	C26-C27-C28-C29
21	B	813	CLA	C2-C3-C5-C6
21	A	818	CLA	C6-C7-C8-C9
21	A	834	CLA	C11-C10-C8-C9
21	B	806	CLA	C14-C13-C15-C16
21	B	841	CLA	C6-C7-C8-C9
21	B	839	CLA	C6-C7-C8-C9
21	z	602	CLA	C14-C13-C15-C16
21	J	101	CLA	O1D-CGD-O2D-CED
23	1	615	LHG	C13-C14-C15-C16
21	A	820	CLA	C13-C15-C16-C17
21	A	806	CLA	C13-C15-C16-C17
21	B	837	CLA	C8-C10-C11-C12
21	B	839	CLA	C13-C15-C16-C17
20	y	609	CHL	C2A-CAA-CBA-CGA
21	1	604	CLA	C2A-CAA-CBA-CGA
21	2	603	CLA	C2A-CAA-CBA-CGA
21	4	614	CLA	C2A-CAA-CBA-CGA
21	A	822	CLA	C2A-CAA-CBA-CGA
21	A	832	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	B	809	CLA	C2A-CAA-CBA-CGA
22	1	614	XAT	C11-C12-C13-C20
21	A	835	CLA	C4C-C3C-CAC-CBC
23	1	615	LHG	C33-C34-C35-C36
23	1	615	LHG	O1-C1-C2-C3
22	1	614	XAT	C11-C12-C13-C14
21	2	602	CLA	C3-C5-C6-C7
21	A	814	CLA	C10-C11-C12-C13
30	B	850	DGD	CCA-CDA-CEA-CFA
23	y	619	LHG	C9-C10-C11-C12
21	2	612	CLA	C16-C17-C18-C19
21	B	824	CLA	C16-C17-C18-C19
21	B	818	CLA	C11-C12-C13-C15
21	O	201	CLA	C16-C17-C18-C20
21	B	802	CLA	C8-C10-C11-C12
21	z	613	CLA	C2C-C3C-CAC-CBC
21	A	835	CLA	CBD-CGD-O2D-CED
20	4	606	CHL	O1D-CGD-O2D-CED
21	A	817	CLA	O1D-CGD-O2D-CED
21	F	301	CLA	C8-C10-C11-C12
20	x	605	CHL	CBA-CGA-O2A-C1
21	2	612	CLA	CBA-CGA-O2A-C1
23	1	615	LHG	C24-C23-O8-C6
21	A	836	CLA	O1D-CGD-O2D-CED
20	x	606	CHL	C3A-C2A-CAA-CBA
21	1	612	CLA	C3A-C2A-CAA-CBA
21	2	611	CLA	C3A-C2A-CAA-CBA
21	A	810	CLA	C3A-C2A-CAA-CBA
21	A	830	CLA	C3A-C2A-CAA-CBA
21	A	815	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	C3A-C2A-CAA-CBA
21	A	842	CLA	C3A-C2A-CAA-CBA
21	B	815	CLA	C3A-C2A-CAA-CBA
21	B	811	CLA	C3A-C2A-CAA-CBA
21	B	826	CLA	C3A-C2A-CAA-CBA
21	B	821	CLA	C3A-C2A-CAA-CBA
21	B	833	CLA	C3A-C2A-CAA-CBA
21	B	809	CLA	C3A-C2A-CAA-CBA
21	B	810	CLA	C3A-C2A-CAA-CBA
21	x	614	CLA	C3A-C2A-CAA-CBA
21	y	604	CLA	C3A-C2A-CAA-CBA
21	y	614	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	z	614	CLA	C3A-C2A-CAA-CBA
22	1	614	XAT	C9-C10-C11-C12
21	B	820	CLA	O1A-CGA-O2A-C1
21	B	813	CLA	O1A-CGA-O2A-C1
21	B	824	CLA	C16-C17-C18-C20
21	B	813	CLA	O1D-CGD-O2D-CED
26	4	620	LMG	C7-C8-C9-O8
21	B	841	CLA	O1A-CGA-O2A-C1
21	B	828	CLA	C4-C3-C5-C6
21	A	835	CLA	C2-C3-C5-C6
21	B	828	CLA	C2-C3-C5-C6
21	y	603	CLA	C2-C3-C5-C6
21	B	820	CLA	C2A-CAA-CBA-CGA
30	B	850	DGD	C9A-CAA-CBA-CCA
21	B	808	CLA	C16-C17-C18-C19
21	A	835	CLA	C15-C16-C17-C18
21	B	824	CLA	C3-C5-C6-C7
21	A	825	CLA	CBA-CGA-O2A-C1
21	B	817	CLA	O1A-CGA-O2A-C1
21	x	610	CLA	C5-C6-C7-C8
21	A	812	CLA	C2-C1-O2A-CGA
27	A	801	CL0	C2-C1-O2A-CGA
21	A	812	CLA	C15-C16-C17-C18
21	A	813	CLA	O1A-CGA-O2A-C1
21	y	614	CLA	C16-C17-C18-C20
21	x	602	CLA	C3-C5-C6-C7
25	4	618	BCR	C23-C24-C25-C30
25	A	852	BCR	C5-C6-C7-C8
25	B	844	BCR	C23-C24-C25-C26
25	B	845	BCR	C5-C6-C7-C8
25	B	847	BCR	C1-C6-C7-C8
25	B	847	BCR	C5-C6-C7-C8
25	B	849	BCR	C23-C24-C25-C26
25	F	304	BCR	C5-C6-C7-C8
25	G	204	BCR	C23-C24-C25-C26
21	A	829	CLA	C8-C10-C11-C12
21	A	807	CLA	C10-C11-C12-C13
21	A	802	CLA	C15-C16-C17-C18
23	x	619	LHG	C12-C13-C14-C15
21	2	612	CLA	O1A-CGA-O2A-C1
21	A	834	CLA	O1A-CGA-O2A-C1
21	B	829	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	A	855	PQN	C25-C26-C27-C28
21	B	818	CLA	C4-C3-C5-C6
21	x	613	CLA	C4-C3-C5-C6
21	z	603	CLA	C4-C3-C5-C6
21	4	613	CLA	O1D-CGD-O2D-CED
20	x	601	CHL	C2-C3-C5-C6
21	A	826	CLA	C11-C12-C13-C15
21	A	818	CLA	C11-C10-C8-C7
21	A	807	CLA	C11-C10-C8-C7
21	A	828	CLA	C11-C10-C8-C7
21	A	805	CLA	C2-C3-C5-C6
21	A	835	CLA	C11-C10-C8-C7
21	B	806	CLA	C12-C13-C15-C16
21	B	841	CLA	C6-C7-C8-C10
21	B	841	CLA	C12-C13-C15-C16
21	B	839	CLA	C6-C7-C8-C10
21	B	803	CLA	C6-C7-C8-C10
21	y	602	CLA	C11-C12-C13-C15
21	y	602	CLA	C12-C13-C15-C16
21	z	613	CLA	C2-C3-C5-C6
27	A	801	CL0	C11-C10-C8-C7
20	x	605	CHL	O1A-CGA-O2A-C1
23	1	615	LHG	O10-C23-O8-C6
21	B	828	CLA	C13-C15-C16-C17
23	z	619	LHG	C23-C24-C25-C26
21	2	602	CLA	CBA-CGA-O2A-C1
21	B	832	CLA	CBA-CGA-O2A-C1
21	4	612	CLA	C2A-CAA-CBA-CGA
21	A	829	CLA	C2A-CAA-CBA-CGA
21	A	825	CLA	C2A-CAA-CBA-CGA
21	y	602	CLA	C2A-CAA-CBA-CGA
21	z	614	CLA	C13-C15-C16-C17
20	z	605	CHL	O1D-CGD-O2D-CED
21	4	612	CLA	O1D-CGD-O2D-CED
21	K	203	CLA	O1D-CGD-O2D-CED
21	A	811	CLA	C8-C10-C11-C12
21	A	829	CLA	C13-C15-C16-C17
21	A	834	CLA	C3-C5-C6-C7
21	y	602	CLA	C3-C5-C6-C7
21	A	835	CLA	C16-C17-C18-C19
23	1	615	LHG	C23-C24-C25-C26
25	K	205	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	z	604	CLA	CBD-CGD-O2D-CED
26	4	620	LMG	C2-C1-O1-C7
21	A	829	CLA	C15-C16-C17-C18
30	B	850	DGD	C6B-C7B-C8B-C9B
21	A	825	CLA	O1A-CGA-O2A-C1
21	A	812	CLA	C16-C17-C18-C19
21	B	841	CLA	C16-C17-C18-C19
20	x	601	CHL	C4-C3-C5-C6
21	A	835	CLA	C4-C3-C5-C6
21	x	613	CLA	C2-C3-C5-C6
21	z	603	CLA	C2-C3-C5-C6
26	4	619	LMG	C30-C31-C32-C33
21	A	803	CLA	C11-C12-C13-C14
21	A	804	CLA	C14-C13-C15-C16
21	B	806	CLA	C11-C10-C8-C9
21	B	829	CLA	C6-C7-C8-C9
21	B	805	CLA	C6-C7-C8-C9
21	B	809	CLA	C3-C5-C6-C7
20	y	607	CHL	C2A-CAA-CBA-CGA
21	3	603	CLA	C2A-CAA-CBA-CGA
21	3	602	CLA	C2A-CAA-CBA-CGA
21	4	604	CLA	C2A-CAA-CBA-CGA
21	A	818	CLA	C2A-CAA-CBA-CGA
21	A	806	CLA	C2A-CAA-CBA-CGA
21	B	822	CLA	C2A-CAA-CBA-CGA
21	B	832	CLA	C2A-CAA-CBA-CGA
20	x	606	CHL	O1D-CGD-O2D-CED
21	B	805	CLA	C5-C6-C7-C8
20	y	607	CHL	C1A-C2A-CAA-CBA
21	1	612	CLA	C1A-C2A-CAA-CBA
21	2	611	CLA	C1A-C2A-CAA-CBA
21	2	608	CLA	C1A-C2A-CAA-CBA
21	2	609	CLA	C1A-C2A-CAA-CBA
21	4	604	CLA	C1A-C2A-CAA-CBA
21	A	810	CLA	C1A-C2A-CAA-CBA
21	A	812	CLA	C1A-C2A-CAA-CBA
21	A	827	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C1A-C2A-CAA-CBA
21	A	815	CLA	C1A-C2A-CAA-CBA
21	A	833	CLA	C1A-C2A-CAA-CBA
21	B	820	CLA	C1A-C2A-CAA-CBA
21	B	824	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	815	CLA	C1A-C2A-CAA-CBA
21	B	825	CLA	C1A-C2A-CAA-CBA
21	B	833	CLA	C1A-C2A-CAA-CBA
21	B	802	CLA	C1A-C2A-CAA-CBA
21	B	834	CLA	C1A-C2A-CAA-CBA
21	F	302	CLA	C1A-C2A-CAA-CBA
21	x	610	CLA	C1A-C2A-CAA-CBA
21	x	602	CLA	C1A-C2A-CAA-CBA
21	x	614	CLA	C1A-C2A-CAA-CBA
21	y	613	CLA	C1A-C2A-CAA-CBA
21	y	602	CLA	C1A-C2A-CAA-CBA
21	B	816	CLA	C6-C7-C8-C9
21	B	828	CLA	C16-C17-C18-C19
21	B	828	CLA	C16-C17-C18-C20
21	y	614	CLA	C16-C17-C18-C19
30	B	850	DGD	CEB-CFB-CGB-CHB
21	B	841	CLA	C13-C15-C16-C17
23	1	615	LHG	C5-C4-O6-P
23	z	619	LHG	C2-C3-O3-P
21	A	804	CLA	C15-C16-C17-C18
21	B	806	CLA	C10-C11-C12-C13
21	B	827	CLA	C10-C11-C12-C13
21	B	822	CLA	CBA-CGA-O2A-C1
21	y	611	CLA	O1D-CGD-O2D-CED
23	x	619	LHG	C25-C26-C27-C28
26	4	619	LMG	O6-C5-C6-O5
21	B	841	CLA	C15-C16-C17-C18
21	B	813	CLA	C15-C16-C17-C18
21	A	809	CLA	C16-C17-C18-C20
20	z	609	CHL	C4C-C3C-CAC-CBC
23	1	615	LHG	C1-C2-C3-O3
21	y	603	CLA	C4-C3-C5-C6
21	3	601	CLA	C2-C3-C5-C6
21	3	605	CLA	C3A-C2A-CAA-CBA
21	A	829	CLA	C10-C11-C12-C13
21	z	602	CLA	C13-C15-C16-C17
21	2	602	CLA	O1A-CGA-O2A-C1
21	B	832	CLA	O1A-CGA-O2A-C1
21	4	603	CLA	C2A-CAA-CBA-CGA
23	1	615	LHG	C4-C5-C6-O8
26	4	620	LMG	O1-C7-C8-C9
30	B	850	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
21	1	609	CLA	C2A-CAA-CBA-CGA
21	A	814	CLA	C15-C16-C17-C18
21	A	806	CLA	C15-C16-C17-C18
21	B	822	CLA	C13-C15-C16-C17
23	1	615	LHG	C14-C15-C16-C17
23	1	615	LHG	O8-C23-C24-C25
23	1	615	LHG	C7-C8-C9-C10
21	B	834	CLA	C3-C5-C6-C7
21	3	601	CLA	C10-C11-C12-C13
23	A	847	LHG	C5-C6-O8-C23
26	4	620	LMG	C8-C9-O8-C28
21	A	820	CLA	C8-C10-C11-C12
21	4	612	CLA	C5-C6-C7-C8
25	A	849	BCR	C20-C21-C22-C37
25	F	304	BCR	C35-C13-C14-C15
21	3	601	CLA	C4-C3-C5-C6
21	A	828	CLA	C16-C17-C18-C20
21	B	828	CLA	CBA-CGA-O2A-C1
21	A	804	CLA	C5-C6-C7-C8
21	B	840	CLA	C5-C6-C7-C8
21	y	610	CLA	C8-C10-C11-C12
30	B	850	DGD	CCB-CDB-CEB-CFB
23	2	618	LHG	C6-C5-O7-C7
21	J	101	CLA	C2A-CAA-CBA-CGA
21	4	602	CLA	C10-C11-C12-C13
21	B	826	CLA	C8-C10-C11-C12
21	B	827	CLA	C2-C1-O2A-CGA
21	A	825	CLA	O1D-CGD-O2D-CED
21	y	603	CLA	C5-C6-C7-C8
21	1	605	CLA	O1D-CGD-O2D-CED
21	1	603	CLA	C6-C7-C8-C9
21	A	828	CLA	C16-C17-C18-C19
21	B	819	CLA	C6-C7-C8-C9
21	y	610	CLA	C10-C11-C12-C13
21	z	613	CLA	C4C-C3C-CAC-CBC
21	A	807	CLA	C8-C10-C11-C12
21	B	805	CLA	C8-C10-C11-C12
21	O	201	CLA	C8-C10-C11-C12
23	B	852	LHG	C12-C13-C14-C15
22	2	617	XAT	C12-C13-C14-C15
26	4	619	LMG	C2-C1-O1-C7
21	A	803	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	811	CLA	C10-C11-C12-C13
21	2	602	CLA	C6-C7-C8-C10
21	A	803	CLA	C6-C7-C8-C10
21	A	811	CLA	C11-C10-C8-C7
21	A	811	CLA	C11-C12-C13-C15
21	A	812	CLA	C12-C13-C15-C16
21	A	826	CLA	C11-C10-C8-C7
21	A	829	CLA	C11-C10-C8-C7
21	A	831	CLA	C11-C12-C13-C15
21	A	802	CLA	C11-C12-C13-C15
21	A	802	CLA	C12-C13-C15-C16
21	A	828	CLA	C11-C12-C13-C15
21	A	842	CLA	C11-C10-C8-C7
21	A	844	CLA	C12-C13-C15-C16
21	A	843	CLA	C6-C7-C8-C10
21	B	806	CLA	C6-C7-C8-C10
21	B	806	CLA	C11-C12-C13-C15
21	B	808	CLA	C11-C12-C13-C15
21	B	828	CLA	C6-C7-C8-C10
21	B	828	CLA	C12-C13-C15-C16
21	B	829	CLA	C6-C7-C8-C10
21	B	825	CLA	C12-C13-C15-C16
21	B	814	CLA	C11-C10-C8-C7
21	B	809	CLA	C12-C13-C15-C16
21	L	303	CLA	C11-C12-C13-C15
21	O	201	CLA	C11-C10-C8-C7
21	x	610	CLA	C11-C12-C13-C15
21	y	602	CLA	C11-C10-C8-C7
21	z	602	CLA	C11-C12-C13-C15
27	A	801	CL0	C12-C13-C15-C16
29	B	842	PQN	C22-C23-C25-C26
21	A	811	CLA	C11-C12-C13-C14
21	A	812	CLA	C14-C13-C15-C16
21	A	802	CLA	C6-C7-C8-C9
21	A	802	CLA	C14-C13-C15-C16
21	A	814	CLA	C14-C13-C15-C16
21	A	842	CLA	C11-C10-C8-C9
21	A	844	CLA	C14-C13-C15-C16
21	A	835	CLA	C11-C12-C13-C14
21	A	843	CLA	C6-C7-C8-C9
21	B	806	CLA	C6-C7-C8-C9
21	B	806	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	808	CLA	C11-C12-C13-C14
21	B	817	CLA	C6-C7-C8-C9
21	B	824	CLA	C14-C13-C15-C16
21	B	841	CLA	C11-C10-C8-C9
21	B	809	CLA	C14-C13-C15-C16
21	B	827	CLA	C14-C13-C15-C16
21	B	813	CLA	C11-C12-C13-C14
21	H	201	CLA	C11-C10-C8-C9
21	x	610	CLA	C11-C10-C8-C9
21	y	602	CLA	C11-C12-C13-C14
21	y	614	CLA	C14-C13-C15-C16
21	z	602	CLA	C11-C12-C13-C14
27	A	801	CL0	C14-C13-C15-C16
21	A	830	CLA	C2C-C3C-CAC-CBC
21	A	812	CLA	CBA-CGA-O2A-C1
21	A	809	CLA	C16-C17-C18-C19
27	A	801	CL0	C16-C17-C18-C19
21	4	608	CLA	O1D-CGD-O2D-CED
25	F	304	BCR	C22-C23-C24-C25
21	3	602	CLA	C6-C7-C8-C10
21	3	601	CLA	C8-C10-C11-C12
21	B	802	CLA	C5-C6-C7-C8
21	A	810	CLA	CBD-CGD-O2D-CED
21	A	818	CLA	C5-C6-C7-C8
20	y	609	CHL	O1D-CGD-O2D-CED
21	B	817	CLA	C11-C12-C13-C14
21	3	602	CLA	C4-C3-C5-C6
21	A	839	CLA	O1D-CGD-O2D-CED
21	B	802	CLA	C15-C16-C17-C18
21	B	822	CLA	O1A-CGA-O2A-C1
21	B	828	CLA	O1A-CGA-O2A-C1
21	B	841	CLA	O1D-CGD-O2D-CED
21	z	602	CLA	C10-C11-C12-C13
21	A	835	CLA	O1D-CGD-O2D-CED
20	x	609	CHL	C3A-C2A-CAA-CBA
20	z	601	CHL	C3A-C2A-CAA-CBA
21	A	803	CLA	C3A-C2A-CAA-CBA
21	A	833	CLA	C3A-C2A-CAA-CBA
21	A	836	CLA	C3A-C2A-CAA-CBA
21	B	834	CLA	C3A-C2A-CAA-CBA
21	K	204	CLA	C3A-C2A-CAA-CBA
21	K	203	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	A	801	CL0	C3A-C2A-CAA-CBA
23	B	852	LHG	C4-C5-C6-O8
21	B	811	CLA	O1D-CGD-O2D-CED
21	A	841	CLA	CAA-CBA-CGA-O2A
21	A	803	CLA	C4-C3-C5-C6
20	2	601	CHL	C3C-C2C-CMC-OMC
20	4	615	CHL	C3C-C2C-CMC-OMC
21	A	812	CLA	C2A-CAA-CBA-CGA
21	A	845	CLA	O1D-CGD-O2D-CED
23	B	852	LHG	O6-C4-C5-O7
21	3	602	CLA	C6-C7-C8-C9
21	B	806	CLA	C16-C17-C18-C19
27	A	801	CL0	C16-C17-C18-C20
21	A	812	CLA	O1A-CGA-O2A-C1
21	A	835	CLA	C16-C17-C18-C20
23	x	619	LHG	C9-C10-C11-C12
20	z	609	CHL	C2-C1-O2A-CGA
21	3	602	CLA	C2-C1-O2A-CGA
21	A	822	CLA	C2-C1-O2A-CGA
21	B	841	CLA	C2-C1-O2A-CGA
21	A	806	CLA	C14-C13-C15-C16
21	B	841	CLA	C11-C12-C13-C14
21	B	825	CLA	C11-C10-C8-C9
21	B	814	CLA	C11-C12-C13-C14
21	x	602	CLA	C14-C13-C15-C16
21	y	610	CLA	C11-C10-C8-C9
21	z	614	CLA	C11-C10-C8-C9
21	B	829	CLA	CBA-CGA-O2A-C1
21	B	818	CLA	CBD-CGD-O2D-CED
21	A	826	CLA	C15-C16-C17-C18
21	A	822	CLA	C15-C16-C17-C18
23	2	618	LHG	C2-C3-O3-P
21	A	802	CLA	C2A-CAA-CBA-CGA
21	z	613	CLA	C2A-CAA-CBA-CGA
21	B	819	CLA	C6-C7-C8-C10
25	4	618	BCR	C5-C6-C7-C8
25	A	853	BCR	C1-C6-C7-C8
25	A	853	BCR	C5-C6-C7-C8
25	A	848	BCR	C5-C6-C7-C8
25	B	844	BCR	C23-C24-C25-C30
25	B	845	BCR	C1-C6-C7-C8
25	F	304	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	z	607	CHL	CBA-CGA-O2A-C1
20	2	606	CHL	C1A-C2A-CAA-CBA
21	A	818	CLA	C8-C10-C11-C12
23	A	846	LHG	C27-C28-C29-C30
21	A	819	CLA	CBD-CGD-O2D-CED
21	B	832	CLA	C2C-C3C-CAC-CBC
23	1	615	LHG	O6-C4-C5-C6
21	z	604	CLA	O1D-CGD-O2D-CED
21	2	602	CLA	C12-C13-C15-C16
21	2	612	CLA	C11-C12-C13-C15
21	2	612	CLA	C12-C13-C15-C16
21	3	601	CLA	C6-C7-C8-C10
21	A	803	CLA	C2-C3-C5-C6
21	A	809	CLA	C11-C10-C8-C7
21	A	820	CLA	C11-C10-C8-C7
21	A	802	CLA	C6-C7-C8-C10
21	A	814	CLA	C12-C13-C15-C16
21	A	819	CLA	C6-C7-C8-C10
21	A	806	CLA	C12-C13-C15-C16
21	A	841	CLA	C12-C13-C15-C16
21	A	834	CLA	C11-C10-C8-C7
21	A	835	CLA	C11-C12-C13-C15
21	B	808	CLA	C6-C7-C8-C10
21	B	822	CLA	C12-C13-C15-C16
21	B	824	CLA	C12-C13-C15-C16
21	B	840	CLA	C12-C13-C15-C16
21	B	841	CLA	C11-C10-C8-C7
21	B	814	CLA	C11-C12-C13-C15
21	B	818	CLA	C11-C10-C8-C7
21	B	827	CLA	C12-C13-C15-C16
21	B	802	CLA	C11-C12-C13-C15
21	B	805	CLA	C6-C7-C8-C10
21	B	805	CLA	C11-C10-C8-C7
21	B	813	CLA	C11-C12-C13-C15
21	H	201	CLA	C6-C7-C8-C10
21	H	201	CLA	C11-C10-C8-C7
21	x	610	CLA	C11-C10-C8-C7
21	x	603	CLA	C6-C7-C8-C10
21	y	610	CLA	C11-C10-C8-C7
21	y	614	CLA	C11-C12-C13-C15
21	y	614	CLA	C12-C13-C15-C16
21	z	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	z	603	CLA	C6-C7-C8-C10
21	B	827	CLA	C8-C10-C11-C12
21	B	809	CLA	C15-C16-C17-C18
21	B	826	CLA	C2A-CAA-CBA-CGA
21	4	608	CLA	C2C-C3C-CAC-CBC
24	2	616	LUT	C11-C10-C9-C19
25	3	614	BCR	C20-C21-C22-C37
25	B	849	BCR	C20-C21-C22-C37
21	A	830	CLA	C3-C5-C6-C7
21	A	832	CLA	CBA-CGA-O2A-C1
20	y	609	CHL	C3-C5-C6-C7
21	x	604	CLA	C3-C5-C6-C7
21	B	829	CLA	C11-C10-C8-C7
21	1	608	CLA	CAD-CBD-CGD-O2D
21	1	609	CLA	CAD-CBD-CGD-O2D
21	1	612	CLA	CAD-CBD-CGD-O2D
21	2	611	CLA	CAD-CBD-CGD-O2D
21	2	613	CLA	CAD-CBD-CGD-O2D
21	3	602	CLA	CAD-CBD-CGD-O2D
21	3	608	CLA	CAD-CBD-CGD-O2D
21	4	603	CLA	CAD-CBD-CGD-O2D
21	A	807	CLA	CAD-CBD-CGD-O2D
21	A	802	CLA	CAD-CBD-CGD-O2D
21	A	823	CLA	CAD-CBD-CGD-O2D
21	A	805	CLA	CAD-CBD-CGD-O2D
21	A	834	CLA	CAD-CBD-CGD-O2D
21	B	802	CLA	CAD-CBD-CGD-O2D
21	B	805	CLA	CAD-CBD-CGD-O2D
21	B	810	CLA	CAD-CBD-CGD-O2D
21	B	839	CLA	CAD-CBD-CGD-O2D
21	B	813	CLA	CAD-CBD-CGD-O2D
21	K	203	CLA	CAD-CBD-CGD-O2D
21	L	304	CLA	CAD-CBD-CGD-O2D
21	x	610	CLA	CAD-CBD-CGD-O2D
21	z	610	CLA	CAD-CBD-CGD-O2D
21	z	603	CLA	CAD-CBD-CGD-O2D
23	B	851	LHG	C4-C5-O7-C7
21	B	803	CLA	C13-C15-C16-C17
24	y	615	LUT	C6-C7-C8-C9
25	B	801	BCR	C6-C7-C8-C9
25	B	849	BCR	C6-C7-C8-C9
21	B	814	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	z	613	CLA	C8-C10-C11-C12
23	B	852	LHG	C5-C4-O6-P
23	1	615	LHG	O6-C4-C5-O7
25	F	304	BCR	C14-C15-C16-C17
21	B	829	CLA	O1A-CGA-O2A-C1
21	3	601	CLA	C11-C12-C13-C14
21	B	809	CLA	C16-C17-C18-C20
21	1	604	CLA	CHA-CBD-CGD-O1D
21	1	604	CLA	CHA-CBD-CGD-O2D
21	2	604	CLA	CHA-CBD-CGD-O1D
21	2	604	CLA	CHA-CBD-CGD-O2D
21	2	612	CLA	CHA-CBD-CGD-O1D
21	2	612	CLA	CHA-CBD-CGD-O2D
21	4	601	CLA	CHA-CBD-CGD-O1D
21	4	601	CLA	CHA-CBD-CGD-O2D
21	4	614	CLA	CHA-CBD-CGD-O1D
21	4	614	CLA	CHA-CBD-CGD-O2D
21	A	813	CLA	CHA-CBD-CGD-O1D
21	A	813	CLA	CHA-CBD-CGD-O2D
21	A	809	CLA	CHA-CBD-CGD-O1D
21	A	809	CLA	CHA-CBD-CGD-O2D
21	A	815	CLA	CHA-CBD-CGD-O1D
21	B	822	CLA	CHA-CBD-CGD-O1D
21	B	822	CLA	CHA-CBD-CGD-O2D
21	B	841	CLA	CHA-CBD-CGD-O1D
21	B	825	CLA	CHA-CBD-CGD-O1D
21	G	201	CLA	CHA-CBD-CGD-O1D
21	x	612	CLA	CHA-CBD-CGD-O1D
21	x	612	CLA	CHA-CBD-CGD-O2D
21	x	602	CLA	CHA-CBD-CGD-O1D
21	x	602	CLA	CHA-CBD-CGD-O2D
21	y	603	CLA	CHA-CBD-CGD-O1D
21	y	603	CLA	CHA-CBD-CGD-O2D
21	y	612	CLA	CHA-CBD-CGD-O1D
21	y	612	CLA	CHA-CBD-CGD-O2D
21	z	602	CLA	CHA-CBD-CGD-O1D
21	z	602	CLA	CHA-CBD-CGD-O2D
21	z	604	CLA	CHA-CBD-CGD-O1D
25	F	304	BCR	C12-C13-C14-C15
26	4	620	LMG	O1-C7-C8-O7
20	z	607	CHL	O1A-CGA-O2A-C1
21	A	819	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	y	619	LHG	C26-C27-C28-C29
21	A	829	CLA	C16-C17-C18-C20
21	x	603	CLA	C11-C12-C13-C14
21	A	812	CLA	C3-C5-C6-C7
21	B	827	CLA	C4-C3-C5-C6
21	B	818	CLA	C2-C3-C5-C6
21	2	612	CLA	C14-C13-C15-C16
21	A	809	CLA	C11-C10-C8-C9
21	B	818	CLA	C11-C10-C8-C9
21	y	614	CLA	C6-C7-C8-C9
21	A	832	CLA	O1A-CGA-O2A-C1
21	A	814	CLA	C2A-CAA-CBA-CGA
21	O	201	CLA	C2A-CAA-CBA-CGA
21	A	814	CLA	CAA-CBA-CGA-O2A
25	A	849	BCR	C37-C22-C23-C24
21	B	827	CLA	C15-C16-C17-C18
21	4	601	CLA	CBD-CGD-O2D-CED
25	B	846	BCR	C21-C22-C23-C24
21	1	603	CLA	C5-C6-C7-C8
20	4	607	CHL	C1A-C2A-CAA-CBA
20	z	607	CHL	C1A-C2A-CAA-CBA
21	B	806	CLA	C16-C17-C18-C20
21	B	808	CLA	CBD-CGD-O2D-CED
25	B	844	BCR	C15-C16-C17-C18
23	A	847	LHG	C4-O6-P-O3
21	B	831	CLA	CBD-CGD-O2D-CED
21	A	807	CLA	C4-C3-C5-C6
21	B	828	CLA	C15-C16-C17-C18
23	2	618	LHG	C5-C4-O6-P
23	B	852	LHG	C3-O3-P-O5
21	4	612	CLA	CBA-CGA-O2A-C1
21	A	827	CLA	CBD-CGD-O2D-CED
21	2	613	CLA	C2A-CAA-CBA-CGA
21	4	613	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	838	CLA	C2-C3-C5-C6
21	B	822	CLA	CAD-CBD-CGD-O1D
21	F	302	CLA	CAD-CBD-CGD-O1D
21	y	604	CLA	CAD-CBD-CGD-O1D
21	z	604	CLA	C2-C3-C5-C6
20	z	607	CHL	C3A-C2A-CAA-CBA
21	3	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	4	612	CLA	C6-C7-C8-C10
21	A	829	CLA	C6-C7-C8-C10
21	A	804	CLA	C11-C12-C13-C15
21	B	808	CLA	C12-C13-C15-C16
21	B	817	CLA	C6-C7-C8-C10
21	B	840	CLA	C6-C7-C8-C10
21	B	814	CLA	C6-C7-C8-C10
21	B	809	CLA	C6-C7-C8-C10
29	B	842	PQN	C16-C17-C18-C20
21	4	612	CLA	O1A-CGA-O2A-C1
20	y	608	CHL	C2A-CAA-CBA-CGA
21	A	839	CLA	C2A-CAA-CBA-CGA
21	x	613	CLA	C2A-CAA-CBA-CGA
21	A	844	CLA	C16-C17-C18-C20
20	1	601	CHL	CAD-CBD-CGD-O1D
20	2	605	CHL	C1C-C2C-CMC-OMC
20	2	601	CHL	C1C-C2C-CMC-OMC
20	x	605	CHL	C1C-C2C-CMC-OMC
20	z	606	CHL	C1C-C2C-CMC-OMC
21	3	609	CLA	CAD-CBD-CGD-O1D
23	B	852	LHG	O7-C5-C6-O8
26	4	620	LMG	O7-C8-C9-O8
21	A	829	CLA	C16-C17-C18-C19
21	y	614	CLA	C3-C5-C6-C7
21	B	816	CLA	C5-C6-C7-C8
21	2	602	CLA	C14-C13-C15-C16
21	3	601	CLA	C6-C7-C8-C9
21	A	804	CLA	C6-C7-C8-C9
21	B	822	CLA	C14-C13-C15-C16
21	B	827	CLA	C11-C12-C13-C14
21	B	805	CLA	C14-C13-C15-C16
21	B	810	CLA	C11-C12-C13-C14
21	z	603	CLA	C6-C7-C8-C9
21	4	601	CLA	O1D-CGD-O2D-CED
25	A	851	BCR	C6-C7-C8-C9
20	1	601	CHL	C2A-CAA-CBA-CGA
23	1	615	LHG	O1-C1-C2-O2
25	A	852	BCR	C10-C11-C12-C13
25	B	844	BCR	C18-C19-C20-C21
25	F	304	BCR	C10-C11-C12-C13
25	L	301	BCR	C18-C19-C20-C21
21	A	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	810	CLA	O1D-CGD-O2D-CED
21	A	842	CLA	C2C-C3C-CAC-CBC
21	3	601	CLA	C11-C12-C13-C15
21	A	807	CLA	C2-C3-C5-C6
21	A	814	CLA	C16-C17-C18-C20
21	1	604	CLA	C1-C2-C3-C4
21	B	831	CLA	O1D-CGD-O2D-CED
21	A	803	CLA	C2A-CAA-CBA-CGA
21	A	813	CLA	C2A-CAA-CBA-CGA
21	A	819	CLA	C2A-CAA-CBA-CGA
21	B	807	CLA	C2A-CAA-CBA-CGA
20	z	607	CHL	C2-C1-O2A-CGA
21	1	602	CLA	C2-C1-O2A-CGA
21	1	603	CLA	C2-C1-O2A-CGA
21	B	817	CLA	C2-C1-O2A-CGA
21	B	825	CLA	C2-C1-O2A-CGA
21	B	810	CLA	C2-C1-O2A-CGA
21	4	608	CLA	C4C-C3C-CAC-CBC
24	3	613	LUT	C26-C27-C28-C29
23	1	615	LHG	C15-C16-C17-C18
25	A	852	BCR	C1-C6-C7-C8
25	A	848	BCR	C1-C6-C7-C8
25	G	204	BCR	C5-C6-C7-C8
21	B	827	CLA	C2-C3-C5-C6
21	z	604	CLA	C2C-C3C-CAC-CBC
20	2	615	CHL	O1D-CGD-O2D-CED
21	A	819	CLA	C8-C10-C11-C12
21	x	603	CLA	C11-C12-C13-C15
23	x	619	LHG	C29-C30-C31-C32
21	z	614	CLA	C2A-CAA-CBA-CGA
25	L	301	BCR	C11-C10-C9-C8
21	B	816	CLA	C2C-C3C-CAC-CBC
26	4	619	LMG	C29-C28-O8-C9
23	2	618	LHG	C4-O6-P-O3
23	A	846	LHG	C3-O3-P-O6
23	B	852	LHG	C4-O6-P-O3
23	x	619	LHG	C3-O3-P-O6
23	y	619	LHG	C3-O3-P-O6
23	z	619	LHG	C3-O3-P-O6
21	A	819	CLA	C11-C12-C13-C14
23	y	619	LHG	C27-C28-C29-C30
21	A	830	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	A	843	CLA	C11-C12-C13-C15
21	B	827	CLA	C11-C10-C8-C7
21	F	301	CLA	C6-C7-C8-C10
21	A	811	CLA	C11-C10-C8-C9
21	A	831	CLA	C11-C12-C13-C14
21	B	828	CLA	C6-C7-C8-C9
21	B	841	CLA	C14-C13-C15-C16
21	B	810	CLA	C6-C7-C8-C9
21	y	602	CLA	C11-C10-C8-C9
21	z	613	CLA	C6-C7-C8-C9
29	B	842	PQN	C24-C23-C25-C26
25	B	844	BCR	C13-C14-C15-C16
21	B	818	CLA	O1D-CGD-O2D-CED
21	2	612	CLA	C2A-CAA-CBA-CGA
21	A	802	CLA	C4-C3-C5-C6
21	3	602	CLA	C2-C3-C5-C6
21	A	844	CLA	C16-C17-C18-C19
21	B	807	CLA	CBA-CGA-O2A-C1
20	2	615	CHL	CBD-CGD-O2D-CED
20	x	605	CHL	C2A-CAA-CBA-CGA
21	2	602	CLA	C2A-CAA-CBA-CGA
21	B	816	CLA	C2A-CAA-CBA-CGA
21	x	613	CLA	C11-C12-C13-C14
21	A	842	CLA	C4C-C3C-CAC-CBC
21	x	612	CLA	CAA-CBA-CGA-O2A
21	B	826	CLA	C5-C6-C7-C8
21	A	822	CLA	C2-C3-C5-C6
21	B	807	CLA	O1A-CGA-O2A-C1
21	B	802	CLA	C10-C11-C12-C13
23	x	619	LHG	C16-C17-C18-C19
21	1	607	CLA	CAA-CBA-CGA-O1A
21	2	602	CLA	C2-C1-O2A-CGA
21	A	830	CLA	C2-C1-O2A-CGA
21	A	820	CLA	C2-C1-O2A-CGA
21	x	603	CLA	C2-C1-O2A-CGA
20	2	606	CHL	O1D-CGD-O2D-CED
21	K	203	CLA	CAA-CBA-CGA-O1A
21	1	602	CLA	C2A-CAA-CBA-CGA
21	1	603	CLA	C2A-CAA-CBA-CGA
21	z	603	CLA	C2A-CAA-CBA-CGA
21	B	837	CLA	C15-C16-C17-C18
30	B	850	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
20	2	601	CHL	C3A-C2A-CAA-CBA
21	3	607	CLA	C3A-C2A-CAA-CBA
21	A	822	CLA	C3A-C2A-CAA-CBA
21	A	843	CLA	C3A-C2A-CAA-CBA
21	B	832	CLA	C3A-C2A-CAA-CBA
21	4	601	CLA	CAA-CBA-CGA-O2A
21	A	804	CLA	CAA-CBA-CGA-O2A
23	1	615	LHG	O10-C23-C24-C25
22	1	614	XAT	C13-C14-C15-C35
21	A	822	CLA	C4-C3-C5-C6
21	A	829	CLA	C6-C7-C8-C9
21	A	802	CLA	C11-C10-C8-C9
21	z	602	CLA	C11-C10-C8-C9
21	z	614	CLA	C14-C13-C15-C16
21	3	603	CLA	CAA-CBA-CGA-O1A
21	z	604	CLA	C4C-C3C-CAC-CBC
20	x	608	CHL	O1D-CGD-O2D-CED
21	A	827	CLA	O1D-CGD-O2D-CED
25	4	618	BCR	C20-C21-C22-C37
25	A	852	BCR	C11-C10-C9-C34
25	K	202	BCR	C16-C17-C18-C36
25	L	301	BCR	C11-C10-C9-C34
25	L	305	BCR	C16-C17-C18-C36
31	y	618	NEX	C39-C29-C30-C31
21	B	837	CLA	C3-C5-C6-C7
21	A	845	CLA	C2A-CAA-CBA-CGA
21	B	808	CLA	O1D-CGD-O2D-CED
23	z	619	LHG	C26-C27-C28-C29
25	B	801	BCR	C7-C8-C9-C10
20	2	601	CHL	C1A-C2A-CAA-CBA
20	z	601	CHL	C1A-C2A-CAA-CBA
21	A	803	CLA	C1A-C2A-CAA-CBA
21	A	843	CLA	C1A-C2A-CAA-CBA
21	B	832	CLA	C1A-C2A-CAA-CBA
21	K	204	CLA	C1A-C2A-CAA-CBA
27	A	801	CL0	C1A-C2A-CAA-CBA
21	A	811	CLA	C12-C13-C15-C16
21	A	812	CLA	C6-C7-C8-C10
21	A	803	CLA	C10-C11-C12-C13
22	2	617	XAT	C29-C30-C31-C32
20	x	608	CHL	C3C-C2C-CMC-OMC
20	y	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
21	1	607	CLA	CAA-CBA-CGA-O2A
21	2	611	CLA	CAA-CBA-CGA-O1A
21	A	835	CLA	C3-C5-C6-C7
21	1	612	CLA	C2A-CAA-CBA-CGA
21	A	815	CLA	C2A-CAA-CBA-CGA
21	B	819	CLA	C2A-CAA-CBA-CGA
21	L	303	CLA	C15-C16-C17-C18
21	x	613	CLA	C8-C10-C11-C12
21	B	837	CLA	C16-C17-C18-C20
21	K	203	CLA	CAA-CBA-CGA-O2A
21	B	841	CLA	C4-C3-C5-C6
21	B	810	CLA	C4-C3-C5-C6
21	x	613	CLA	CBA-CGA-O2A-C1
21	2	608	CLA	CAA-CBA-CGA-O1A
21	3	603	CLA	CAA-CBA-CGA-O2A
21	x	613	CLA	O1A-CGA-O2A-C1
24	2	616	LUT	C11-C10-C9-C8
24	3	613	LUT	C11-C10-C9-C8
25	A	852	BCR	C11-C10-C9-C8
25	K	202	BCR	C16-C17-C18-C19
25	L	305	BCR	C16-C17-C18-C19
31	y	618	NEX	C28-C29-C30-C31
21	4	604	CLA	CAA-CBA-CGA-O1A
21	B	837	CLA	CBA-CGA-O2A-C1
23	B	851	LHG	C26-C27-C28-C29
21	2	611	CLA	CAA-CBA-CGA-O2A
21	A	803	CLA	C2-C1-O2A-CGA
21	B	802	CLA	C2-C1-O2A-CGA
21	A	843	CLA	C5-C6-C7-C8
21	4	603	CLA	CAA-CBA-CGA-O1A
21	x	612	CLA	CAA-CBA-CGA-O1A
21	A	820	CLA	C6-C7-C8-C9
21	B	810	CLA	C14-C13-C15-C16
21	2	608	CLA	CAA-CBA-CGA-O2A
21	A	838	CLA	C4-C3-C5-C6
21	z	604	CLA	C4-C3-C5-C6
21	4	602	CLA	C2A-CAA-CBA-CGA
21	x	603	CLA	C2A-CAA-CBA-CGA
21	y	611	CLA	C2A-CAA-CBA-CGA
21	B	837	CLA	O1A-CGA-O2A-C1
24	1	616	LUT	C1-C6-C7-C8
24	z	615	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	z	615	LUT	C5-C6-C7-C8
25	3	614	BCR	C23-C24-C25-C26
25	4	618	BCR	C1-C6-C7-C8
25	L	306	BCR	C5-C6-C7-C8
25	O	204	BCR	C23-C24-C25-C30
23	B	852	LHG	C10-C11-C12-C13
21	4	603	CLA	CAA-CBA-CGA-O2A
21	4	604	CLA	CAA-CBA-CGA-O2A
21	B	810	CLA	C15-C16-C17-C18
21	B	825	CLA	O1A-CGA-O2A-C1
22	1	614	XAT	C33-C34-C35-C15
25	A	852	BCR	C13-C14-C15-C16
20	y	607	CHL	C4-C3-C5-C6
21	B	811	CLA	C4-C3-C5-C6
21	4	610	CLA	C1A-C2A-CAA-CBA
21	B	821	CLA	CAA-CBA-CGA-O2A
21	A	807	CLA	O1A-CGA-O2A-C1
20	1	601	CHL	CAA-CBA-CGA-O2A
21	B	840	CLA	C16-C17-C18-C20
23	B	852	LHG	C11-C10-C9-C8
21	x	614	CLA	CAA-CBA-CGA-O2A
21	1	611	CLA	CAA-CBA-CGA-O2A
21	1	602	CLA	C4-C3-C5-C6
21	A	831	CLA	C12-C13-C15-C16
21	A	804	CLA	C11-C10-C8-C7
21	B	825	CLA	C11-C10-C8-C7
21	x	610	CLA	C6-C7-C8-C10
21	A	806	CLA	CBA-CGA-O2A-C1
21	A	830	CLA	C16-C17-C18-C20
21	y	612	CLA	CAA-CBA-CGA-O2A
21	A	807	CLA	CBA-CGA-O2A-C1
21	4	612	CLA	C8-C10-C11-C12
21	x	614	CLA	CAA-CBA-CGA-O1A
21	3	601	CLA	CAA-CBA-CGA-O2A
21	B	817	CLA	CAA-CBA-CGA-O2A
23	y	619	LHG	O8-C23-C24-C25
21	A	806	CLA	O1A-CGA-O2A-C1
21	A	831	CLA	C10-C11-C12-C13
21	B	837	CLA	C16-C17-C18-C19
20	x	609	CHL	CAA-CBA-CGA-O2A
24	2	619	LUT	C11-C10-C9-C19
25	4	618	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
25	A	851	BCR	C11-C10-C9-C34
25	A	851	BCR	C20-C21-C22-C37
25	B	844	BCR	C11-C10-C9-C34
25	B	845	BCR	C16-C17-C18-C36
31	x	618	NEX	C11-C10-C9-C19
31	z	618	NEX	C39-C29-C30-C31
21	A	820	CLA	C4-C3-C5-C6
21	A	821	CLA	CAA-CBA-CGA-O2A
21	A	802	CLA	C2-C3-C5-C6
21	4	612	CLA	C11-C10-C8-C9
21	4	602	CLA	C6-C7-C8-C9
21	B	814	CLA	C6-C7-C8-C9
29	B	842	PQN	C16-C17-C18-C19
21	B	826	CLA	C10-C11-C12-C13
23	B	852	LHG	C11-C12-C13-C14
20	x	607	CHL	C3A-C2A-CAA-CBA
21	1	604	CLA	C3A-C2A-CAA-CBA
21	A	813	CLA	C3A-C2A-CAA-CBA
21	B	822	CLA	C3A-C2A-CAA-CBA
21	B	817	CLA	C3A-C2A-CAA-CBA
21	F	302	CLA	C3A-C2A-CAA-CBA
21	A	809	CLA	C2C-C3C-CAC-CBC
21	x	602	CLA	C13-C15-C16-C17
21	B	809	CLA	CAA-CBA-CGA-O2A
21	B	803	CLA	CAA-CBA-CGA-O2A
21	1	611	CLA	CAA-CBA-CGA-O1A
20	x	609	CHL	CAD-CBD-CGD-O2D
21	1	602	CLA	CAD-CBD-CGD-O2D
21	2	610	CLA	CAD-CBD-CGD-O2D
21	2	609	CLA	CAD-CBD-CGD-O2D
21	4	609	CLA	CAD-CBD-CGD-O2D
21	A	811	CLA	CAD-CBD-CGD-O2D
21	A	812	CLA	CAD-CBD-CGD-O2D
21	A	808	CLA	CAD-CBD-CGD-O2D
21	A	827	CLA	CAD-CBD-CGD-O2D
21	A	814	CLA	CAD-CBD-CGD-O2D
21	A	821	CLA	CAD-CBD-CGD-O2D
21	A	841	CLA	CAD-CBD-CGD-O2D
21	A	838	CLA	CAD-CBD-CGD-O2D
21	A	845	CLA	CAD-CBD-CGD-O2D
21	B	808	CLA	CAD-CBD-CGD-O2D
21	B	824	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	838	CLA	CAD-CBD-CGD-O2D
21	B	841	CLA	CAD-CBD-CGD-O2D
21	B	835	CLA	CAD-CBD-CGD-O2D
21	B	814	CLA	CAD-CBD-CGD-O2D
21	B	832	CLA	CAD-CBD-CGD-O2D
21	F	301	CLA	CAD-CBD-CGD-O2D
21	L	302	CLA	CAD-CBD-CGD-O2D
21	L	303	CLA	CAD-CBD-CGD-O2D
21	O	201	CLA	CAD-CBD-CGD-O2D
21	x	604	CLA	CAD-CBD-CGD-O2D
21	x	614	CLA	CAD-CBD-CGD-O2D
21	x	603	CLA	CAD-CBD-CGD-O2D
21	y	610	CLA	CAD-CBD-CGD-O2D
21	y	613	CLA	CAD-CBD-CGD-O2D
21	B	832	CLA	C16-C17-C18-C20
21	A	841	CLA	C2A-CAA-CBA-CGA
21	B	806	CLA	CAA-CBA-CGA-O2A
21	A	841	CLA	CAA-CBA-CGA-O1A
21	y	602	CLA	C8-C10-C11-C12
21	B	825	CLA	CBA-CGA-O2A-C1
21	4	602	CLA	C4-C3-C5-C6
21	B	822	CLA	C4-C3-C5-C6
21	y	611	CLA	CAA-CBA-CGA-O2A
21	B	841	CLA	C2-C3-C5-C6
21	B	810	CLA	C2-C3-C5-C6
20	y	601	CHL	CAA-CBA-CGA-O2A
21	A	807	CLA	CAA-CBA-CGA-O2A
21	B	811	CLA	CAA-CBA-CGA-O2A
26	4	619	LMG	O10-C28-O8-C9
22	1	614	XAT	O4-C6-C7-C8
21	y	602	CLA	CAA-CBA-CGA-O2A
21	x	611	CLA	CAA-CBA-CGA-O1A
21	x	611	CLA	CAA-CBA-CGA-O2A
21	y	612	CLA	CAA-CBA-CGA-O1A
21	4	614	CLA	O2A-C1-C2-C3
21	A	826	CLA	O2A-C1-C2-C3
21	B	841	CLA	O2A-C1-C2-C3
21	B	832	CLA	O2A-C1-C2-C3
21	F	301	CLA	O2A-C1-C2-C3
21	H	201	CLA	O2A-C1-C2-C3
21	J	101	CLA	O2A-C1-C2-C3
21	O	201	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	x	604	CLA	O2A-C1-C2-C3
21	z	614	CLA	O2A-C1-C2-C3
21	B	814	CLA	C10-C11-C12-C13
20	4	607	CHL	CAA-CBA-CGA-O2A
21	G	203	CLA	CAA-CBA-CGA-O2A
21	B	803	CLA	C16-C17-C18-C20
20	2	601	CHL	CHA-CBD-CGD-O2D
20	x	607	CHL	CHA-CBD-CGD-O1D
20	x	607	CHL	CHA-CBD-CGD-O2D
21	1	611	CLA	CHA-CBD-CGD-O1D
21	1	611	CLA	CHA-CBD-CGD-O2D
21	2	602	CLA	CHA-CBD-CGD-O2D
21	3	601	CLA	CHA-CBD-CGD-O1D
21	3	601	CLA	CHA-CBD-CGD-O2D
21	A	818	CLA	CHA-CBD-CGD-O2D
21	A	828	CLA	CHA-CBD-CGD-O1D
21	A	828	CLA	CHA-CBD-CGD-O2D
21	A	825	CLA	CHA-CBD-CGD-O1D
21	A	825	CLA	CHA-CBD-CGD-O2D
21	A	815	CLA	CHA-CBD-CGD-O2D
21	A	821	CLA	CHA-CBD-CGD-O1D
21	A	832	CLA	CHA-CBD-CGD-O2D
21	B	804	CLA	CHA-CBD-CGD-O1D
21	B	804	CLA	CHA-CBD-CGD-O2D
21	B	823	CLA	CHA-CBD-CGD-O2D
21	B	826	CLA	CHA-CBD-CGD-O2D
21	B	836	CLA	CHA-CBD-CGD-O1D
21	B	836	CLA	CHA-CBD-CGD-O2D
21	B	807	CLA	CHA-CBD-CGD-O2D
21	F	303	CLA	CHA-CBD-CGD-O1D
21	F	303	CLA	CHA-CBD-CGD-O2D
21	G	201	CLA	CHA-CBD-CGD-O2D
21	H	201	CLA	CHA-CBD-CGD-O1D
21	H	201	CLA	CHA-CBD-CGD-O2D
21	K	204	CLA	CHA-CBD-CGD-O1D
21	K	204	CLA	CHA-CBD-CGD-O2D
21	z	612	CLA	CHA-CBD-CGD-O1D
21	z	612	CLA	CHA-CBD-CGD-O2D
21	z	604	CLA	CHA-CBD-CGD-O2D
20	2	607	CHL	CAA-CBA-CGA-O2A
21	2	612	CLA	CAA-CBA-CGA-O2A
21	B	832	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	822	CLA	C2-C3-C5-C6
24	2	619	LUT	C11-C10-C9-C8
25	A	851	BCR	C11-C10-C9-C8
25	A	851	BCR	C20-C21-C22-C23
25	B	844	BCR	C11-C10-C9-C8
25	B	845	BCR	C16-C17-C18-C19
31	x	618	NEX	C11-C10-C9-C8
31	z	618	NEX	C28-C29-C30-C31
20	4	607	CHL	CAA-CBA-CGA-O1A
21	A	842	CLA	CAA-CBA-CGA-O2A
21	F	301	CLA	CAA-CBA-CGA-O2A
21	y	614	CLA	CAA-CBA-CGA-O2A
23	z	619	LHG	C24-C25-C26-C27
20	z	607	CHL	O1D-CGD-O2D-CED
21	G	203	CLA	CAA-CBA-CGA-O1A
21	A	809	CLA	C4C-C3C-CAC-CBC
20	x	605	CHL	CAA-CBA-CGA-O2A
20	y	609	CHL	CAA-CBA-CGA-O2A
21	B	822	CLA	C3-C5-C6-C7
21	2	609	CLA	CAA-CBA-CGA-O2A
21	B	805	CLA	CAA-CBA-CGA-O2A
21	B	808	CLA	C4-C3-C5-C6
21	B	832	CLA	C2-C3-C5-C6
21	B	834	CLA	C6-C7-C8-C10
21	B	822	CLA	CAA-CBA-CGA-O2A
21	A	831	CLA	C14-C13-C15-C16
21	A	804	CLA	C11-C12-C13-C14
21	A	843	CLA	C11-C12-C13-C14
21	B	834	CLA	C6-C7-C8-C9
23	y	619	LHG	C30-C31-C32-C33
21	A	826	CLA	CAA-CBA-CGA-O2A
21	B	840	CLA	C15-C16-C17-C18
20	x	609	CHL	CAA-CBA-CGA-O1A
21	A	821	CLA	CAA-CBA-CGA-O1A
20	x	608	CHL	CBD-CGD-O2D-CED
21	y	602	CLA	CAA-CBA-CGA-O1A
21	O	201	CLA	CAA-CBA-CGA-O2A
23	y	619	LHG	O10-C23-C24-C25
21	B	840	CLA	C16-C17-C18-C19
21	2	612	CLA	C4-C3-C5-C6
21	y	611	CLA	CAA-CBA-CGA-O1A
21	B	839	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	4	605	CHL	CHA-CBD-CGD-O2D
20	x	607	CHL	C1A-C2A-CAA-CBA
21	1	607	CLA	CHA-CBD-CGD-O2D
21	1	609	CLA	C1A-C2A-CAA-CBA
21	3	607	CLA	C1A-C2A-CAA-CBA
21	A	813	CLA	C1A-C2A-CAA-CBA
21	A	822	CLA	C1A-C2A-CAA-CBA
21	B	817	CLA	C1A-C2A-CAA-CBA
21	B	803	CLA	C1A-C2A-CAA-CBA
21	B	832	CLA	C16-C17-C18-C19
21	3	601	CLA	CAA-CBA-CGA-O1A
21	A	807	CLA	CAA-CBA-CGA-O1A
21	4	609	CLA	C5-C6-C7-C8
20	x	605	CHL	C2-C1-O2A-CGA
21	B	836	CLA	C2-C1-O2A-CGA
21	2	612	CLA	C15-C16-C17-C18
21	H	201	CLA	C10-C11-C12-C13
23	A	847	LHG	C24-C23-O8-C6
20	2	607	CHL	CAA-CBA-CGA-O1A
21	B	811	CLA	CAA-CBA-CGA-O1A
21	B	809	CLA	CAA-CBA-CGA-O1A
21	A	820	CLA	C2A-CAA-CBA-CGA
21	A	844	CLA	C2A-CAA-CBA-CGA
21	2	602	CLA	C16-C17-C18-C19
21	B	832	CLA	C3-C5-C6-C7
21	B	806	CLA	CAA-CBA-CGA-O1A
21	A	815	CLA	CAA-CBA-CGA-O2A
23	y	619	LHG	C3-O3-P-O5
21	A	803	CLA	C16-C17-C18-C20
20	y	609	CHL	CAA-CBA-CGA-O1A
21	A	842	CLA	CAA-CBA-CGA-O1A
21	B	832	CLA	CAA-CBA-CGA-O1A
23	B	852	LHG	O6-C4-C5-C6
25	3	614	BCR	C23-C24-C25-C30
25	B	846	BCR	C1-C6-C7-C8
25	B	846	BCR	C5-C6-C7-C8
25	B	848	BCR	C23-C24-C25-C26
25	B	848	BCR	C23-C24-C25-C30
25	G	204	BCR	C1-C6-C7-C8
25	G	204	BCR	C23-C24-C25-C30
25	O	204	BCR	C23-C24-C25-C26
26	4	619	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
21	B	822	CLA	CAA-CBA-CGA-O1A
21	O	201	CLA	CAA-CBA-CGA-O1A
21	z	610	CLA	CAA-CBA-CGA-O2A
21	y	610	CLA	C3-C5-C6-C7
21	A	826	CLA	C5-C6-C7-C8
21	B	824	CLA	CAA-CBA-CGA-O2A
21	F	301	CLA	CAA-CBA-CGA-O1A
21	y	614	CLA	CAA-CBA-CGA-O1A
21	x	604	CLA	C4-C3-C5-C6
23	1	615	LHG	C30-C31-C32-C33
21	1	605	CLA	CAD-CBD-CGD-O1D
21	1	612	CLA	CAD-CBD-CGD-O1D
21	A	825	CLA	CAD-CBD-CGD-O1D
21	A	815	CLA	CAD-CBD-CGD-O1D
21	F	302	CLA	C2-C3-C5-C6
21	z	604	CLA	CAD-CBD-CGD-O1D
23	z	619	LHG	C6-C5-O7-C7
23	z	619	LHG	C35-C36-C37-C38
21	A	840	CLA	CAA-CBA-CGA-O2A
21	B	808	CLA	C5-C6-C7-C8
21	x	602	CLA	C6-C7-C8-C9
23	B	852	LHG	C25-C26-C27-C28
21	2	603	CLA	CAA-CBA-CGA-O2A
20	x	605	CHL	CAA-CBA-CGA-O1A
21	2	612	CLA	CAA-CBA-CGA-O1A
23	B	852	LHG	O7-C7-C8-C9
21	B	839	CLA	O1A-CGA-O2A-C1
21	z	610	CLA	C2A-CAA-CBA-CGA
21	B	820	CLA	CAA-CBA-CGA-O2A
21	x	613	CLA	CAA-CBA-CGA-O2A
21	z	613	CLA	CAA-CBA-CGA-O2A
21	A	820	CLA	C15-C16-C17-C18
30	B	850	DGD	C1B-C2B-C3B-C4B
21	B	814	CLA	C16-C17-C18-C19
20	1	601	CHL	CAD-CBD-CGD-O2D
20	2	607	CHL	C3A-C2A-CAA-CBA
21	1	607	CLA	CHA-CBD-CGD-O1D
21	3	612	CLA	CHA-CBD-CGD-O1D
21	4	613	CLA	C3A-C2A-CAA-CBA
21	4	611	CLA	CHA-CBD-CGD-O1D
21	A	831	CLA	C6-C7-C8-C10
21	A	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	810	CLA	C11-C12-C13-C15
21	B	810	CLA	C12-C13-C15-C16
23	B	852	LHG	O9-C7-C8-C9
20	y	607	CHL	CAA-CBA-CGA-O2A
21	3	602	CLA	CAA-CBA-CGA-O2A
23	1	615	LHG	O7-C7-C8-C9
23	x	619	LHG	C11-C12-C13-C14
21	2	602	CLA	C8-C10-C11-C12
21	2	609	CLA	CAA-CBA-CGA-O1A
21	1	602	CLA	CAA-CBA-CGA-O2A
21	4	614	CLA	CAA-CBA-CGA-O2A
21	2	612	CLA	C8-C10-C11-C12
21	A	830	CLA	C8-C10-C11-C12
20	y	607	CHL	CAA-CBA-CGA-O1A
21	A	826	CLA	CAA-CBA-CGA-O1A
21	A	819	CLA	CAA-CBA-CGA-O1A
21	B	820	CLA	CAA-CBA-CGA-O1A
21	A	802	CLA	CAA-CBA-CGA-O2A
21	B	824	CLA	C13-C15-C16-C17
21	z	613	CLA	CAA-CBA-CGA-O1A
20	z	608	CHL	C2A-CAA-CBA-CGA
21	2	603	CLA	CAA-CBA-CGA-O1A
21	B	832	CLA	C4-C3-C5-C6
21	B	816	CLA	CAA-CBA-CGA-O2A
21	A	815	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

184 monomers are involved in 611 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	203	CLA	1	0
21	B	814	CLA	6	0
21	K	201	CLA	7	0
25	A	853	BCR	9	0
21	3	603	CLA	2	0
21	A	841	CLA	5	0
21	A	833	CLA	2	0
25	B	801	BCR	9	0
25	B	848	BCR	1	0
21	A	843	CLA	1	0
21	2	612	CLA	4	0
25	A	850	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	615	CHL	2	0
21	A	842	CLA	7	0
21	1	602	CLA	5	0
21	H	201	CLA	4	0
21	A	830	CLA	7	0
21	B	819	CLA	4	0
23	B	852	LHG	3	0
21	L	302	CLA	4	0
25	B	845	BCR	9	0
21	A	820	CLA	7	0
21	B	809	CLA	6	0
21	A	803	CLA	9	0
24	3	613	LUT	8	0
21	B	833	CLA	1	0
20	2	615	CHL	3	0
21	1	604	CLA	4	0
21	A	811	CLA	6	0
30	B	850	DGD	5	0
25	O	204	BCR	3	0
21	3	605	CLA	1	0
21	A	840	CLA	1	0
21	4	614	CLA	1	0
21	B	805	CLA	7	0
21	A	813	CLA	2	0
21	2	613	CLA	4	0
21	A	805	CLA	2	0
21	4	603	CLA	2	0
21	4	601	CLA	2	0
21	3	612	CLA	3	0
21	A	810	CLA	2	0
24	4	616	LUT	2	0
21	A	806	CLA	5	0
21	3	610	CLA	2	0
21	2	604	CLA	8	0
21	B	813	CLA	7	0
21	A	844	CLA	3	0
21	G	201	CLA	2	0
25	B	844	BCR	6	0
22	4	617	XAT	6	0
21	2	611	CLA	2	0
21	A	839	CLA	1	0
21	B	834	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	606	CHL	1	0
21	B	818	CLA	5	0
21	A	812	CLA	9	0
21	B	839	CLA	2	0
25	3	614	BCR	6	0
21	A	831	CLA	4	0
21	A	832	CLA	1	0
25	J	102	BCR	5	0
25	K	205	BCR	5	0
21	K	204	CLA	4	0
21	1	607	CLA	2	0
28	C	102	SF4	3	0
23	1	615	LHG	12	0
20	2	601	CHL	2	0
25	G	204	BCR	4	0
21	1	608	CLA	3	0
21	A	804	CLA	8	0
20	4	607	CHL	1	0
21	3	604	CLA	1	0
21	A	807	CLA	2	0
21	B	840	CLA	5	0
20	3	606	CHL	2	0
21	J	101	CLA	1	0
21	A	826	CLA	4	0
21	A	827	CLA	1	0
21	B	802	CLA	12	0
24	1	616	LUT	3	0
21	A	818	CLA	7	0
21	B	821	CLA	2	0
29	A	855	PQN	3	0
25	4	618	BCR	6	0
21	1	611	CLA	1	0
21	B	838	CLA	1	0
21	A	828	CLA	2	0
21	1	609	CLA	12	0
21	B	803	CLA	5	0
23	2	618	LHG	2	0
21	L	304	CLA	1	0
21	B	837	CLA	2	0
21	B	841	CLA	2	0
21	B	826	CLA	3	0
21	B	810	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	846	BCR	5	0
21	3	601	CLA	5	0
21	B	811	CLA	3	0
21	A	823	CLA	3	0
20	2	607	CHL	1	0
23	A	847	LHG	1	0
28	C	101	SF4	2	0
25	L	306	BCR	4	0
21	A	802	CLA	7	0
21	3	602	CLA	3	0
21	B	823	CLA	2	0
24	2	616	LUT	5	0
21	F	302	CLA	7	0
25	I	101	BCR	2	0
21	B	830	CLA	2	0
21	B	804	CLA	1	0
21	A	822	CLA	3	0
28	A	854	SF4	2	0
25	B	847	BCR	3	0
21	2	608	CLA	5	0
22	2	617	XAT	5	0
21	B	808	CLA	4	0
21	B	835	CLA	1	0
21	3	607	CLA	8	0
21	1	603	CLA	1	0
21	A	825	CLA	2	0
21	B	829	CLA	1	0
21	B	836	CLA	2	0
21	A	819	CLA	3	0
20	4	605	CHL	2	0
21	A	809	CLA	7	0
23	A	846	LHG	7	0
25	A	848	BCR	3	0
29	B	842	PQN	3	0
25	B	843	BCR	6	0
21	3	608	CLA	6	0
21	4	611	CLA	1	0
25	B	849	BCR	7	0
21	4	609	CLA	5	0
21	L	303	CLA	2	0
21	1	612	CLA	2	0
25	A	851	BCR	6	0

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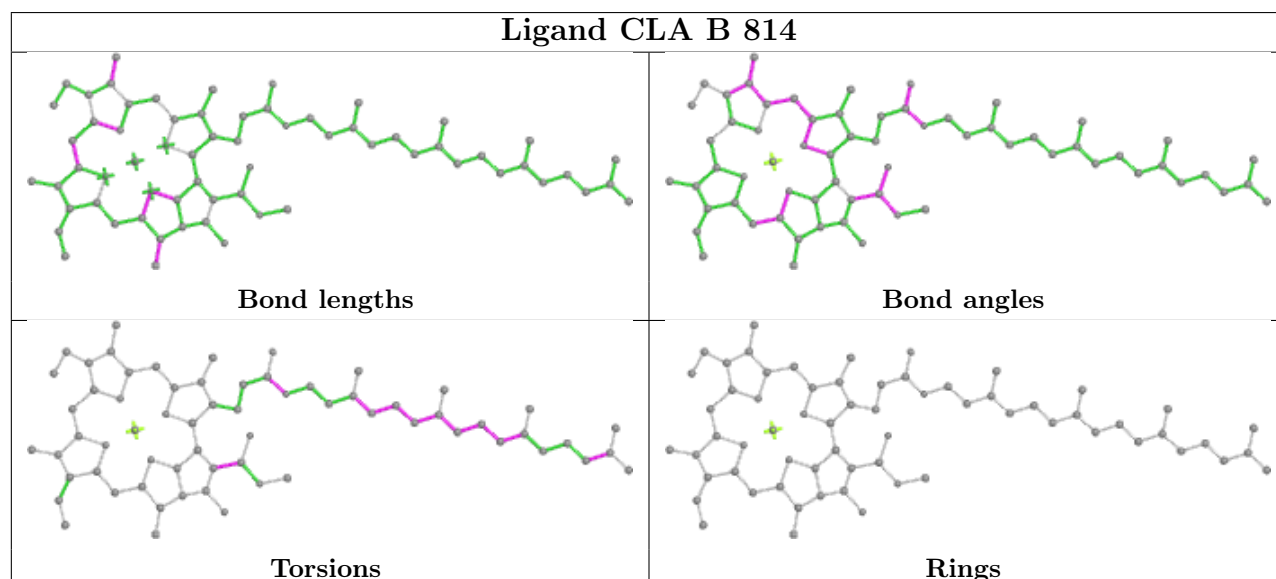
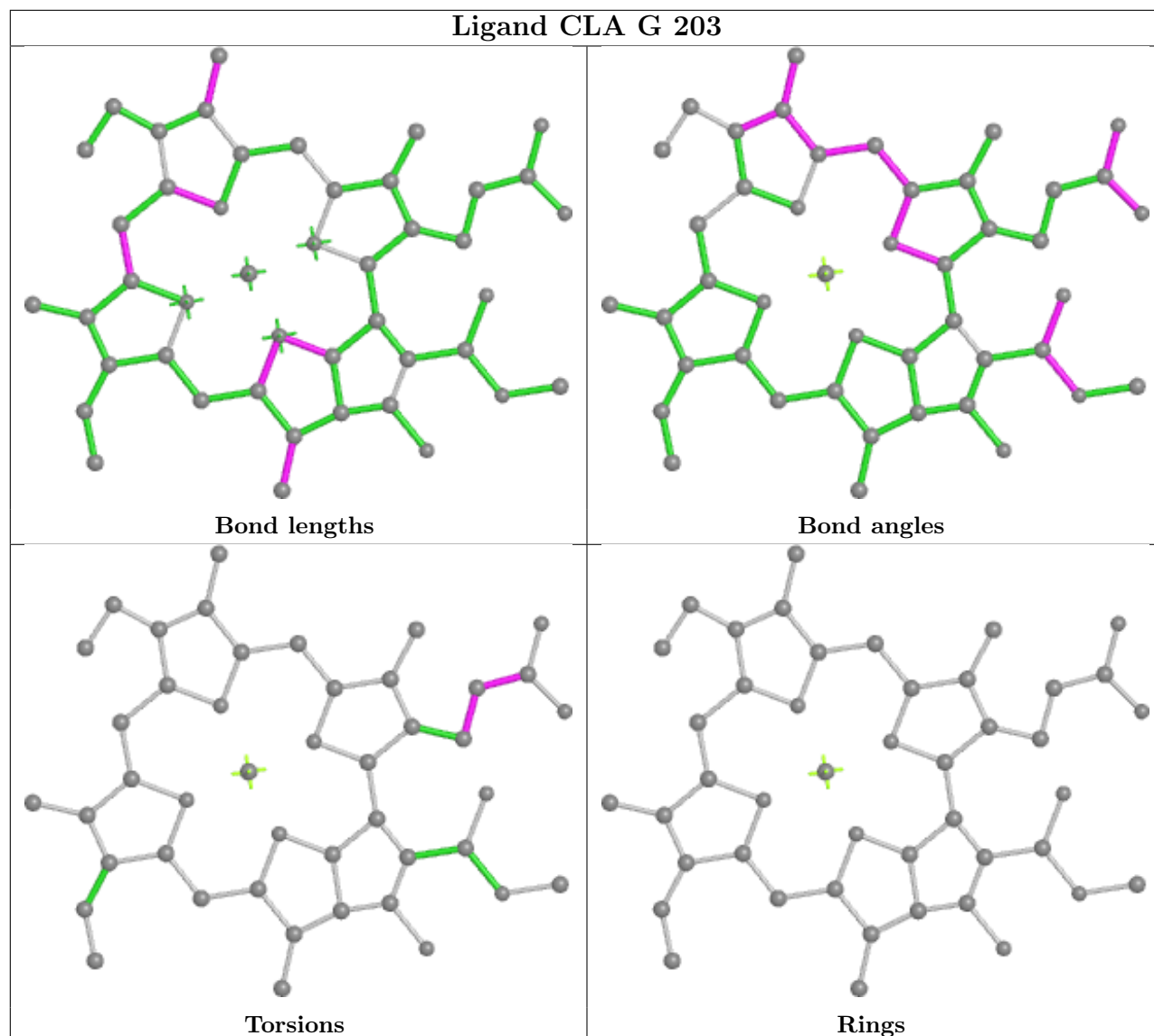
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	B	816	CLA	2	0
21	B	825	CLA	3	0
21	B	827	CLA	3	0
21	A	835	CLA	4	0
25	L	301	BCR	3	0
21	4	602	CLA	3	0
27	A	801	CL0	15	0
21	B	828	CLA	9	0
21	2	602	CLA	9	0
25	L	305	BCR	7	0
20	1	601	CHL	7	0
21	A	845	CLA	3	0
21	4	608	CLA	3	0
22	1	614	XAT	13	0
21	A	815	CLA	1	0
21	2	609	CLA	11	0
21	A	824	CLA	2	0
21	F	301	CLA	2	0
21	B	822	CLA	8	0
21	A	814	CLA	2	0
21	A	834	CLA	2	0
21	2	603	CLA	3	0
21	4	613	CLA	2	0
21	A	829	CLA	9	0
21	B	817	CLA	3	0
21	B	824	CLA	11	0
21	B	832	CLA	5	0
21	A	808	CLA	1	0
21	1	605	CLA	3	0
20	2	605	CHL	5	0
23	B	851	LHG	3	0
21	O	201	CLA	2	0
21	O	203	CLA	1	0
25	A	849	BCR	2	0
25	K	202	BCR	5	0
25	A	852	BCR	2	0
25	F	304	BCR	2	0
21	4	612	CLA	2	0
21	A	821	CLA	1	0
21	K	206	CLA	5	0
21	4	610	CLA	2	0

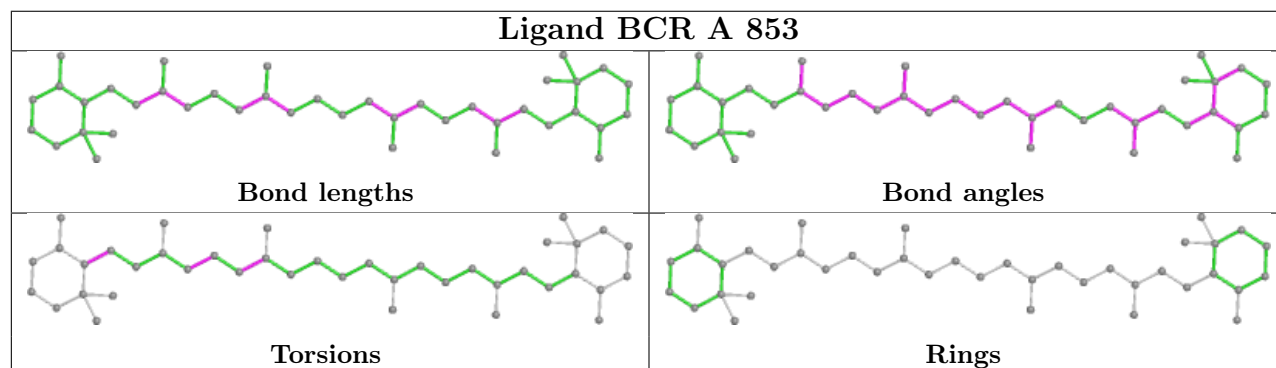
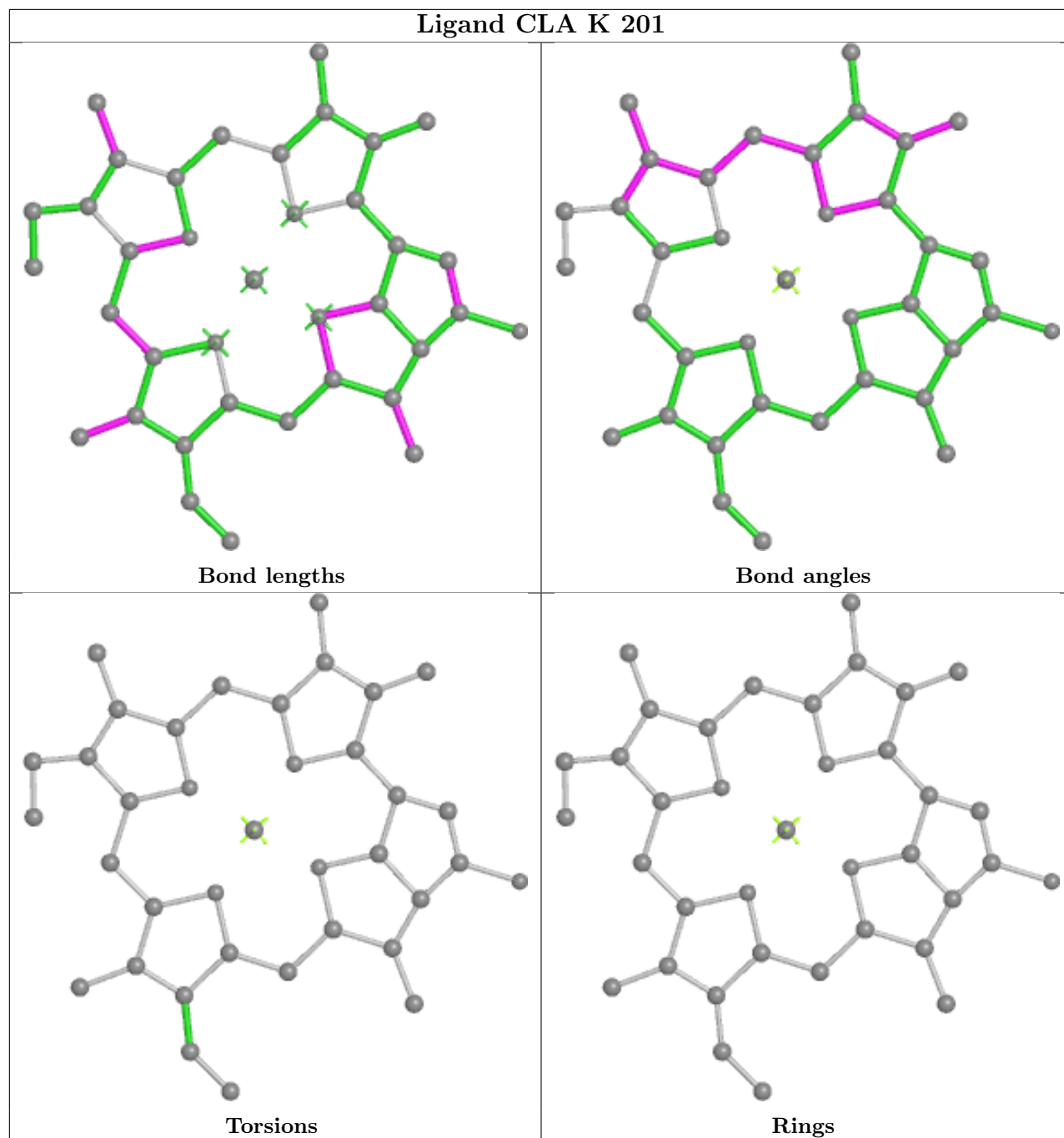
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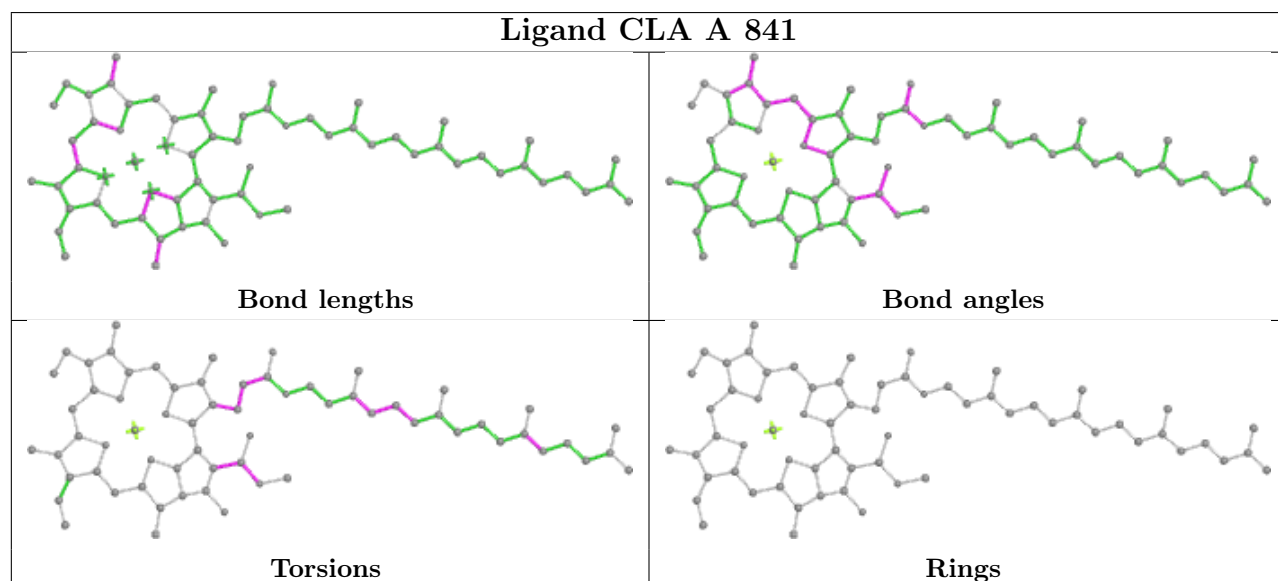
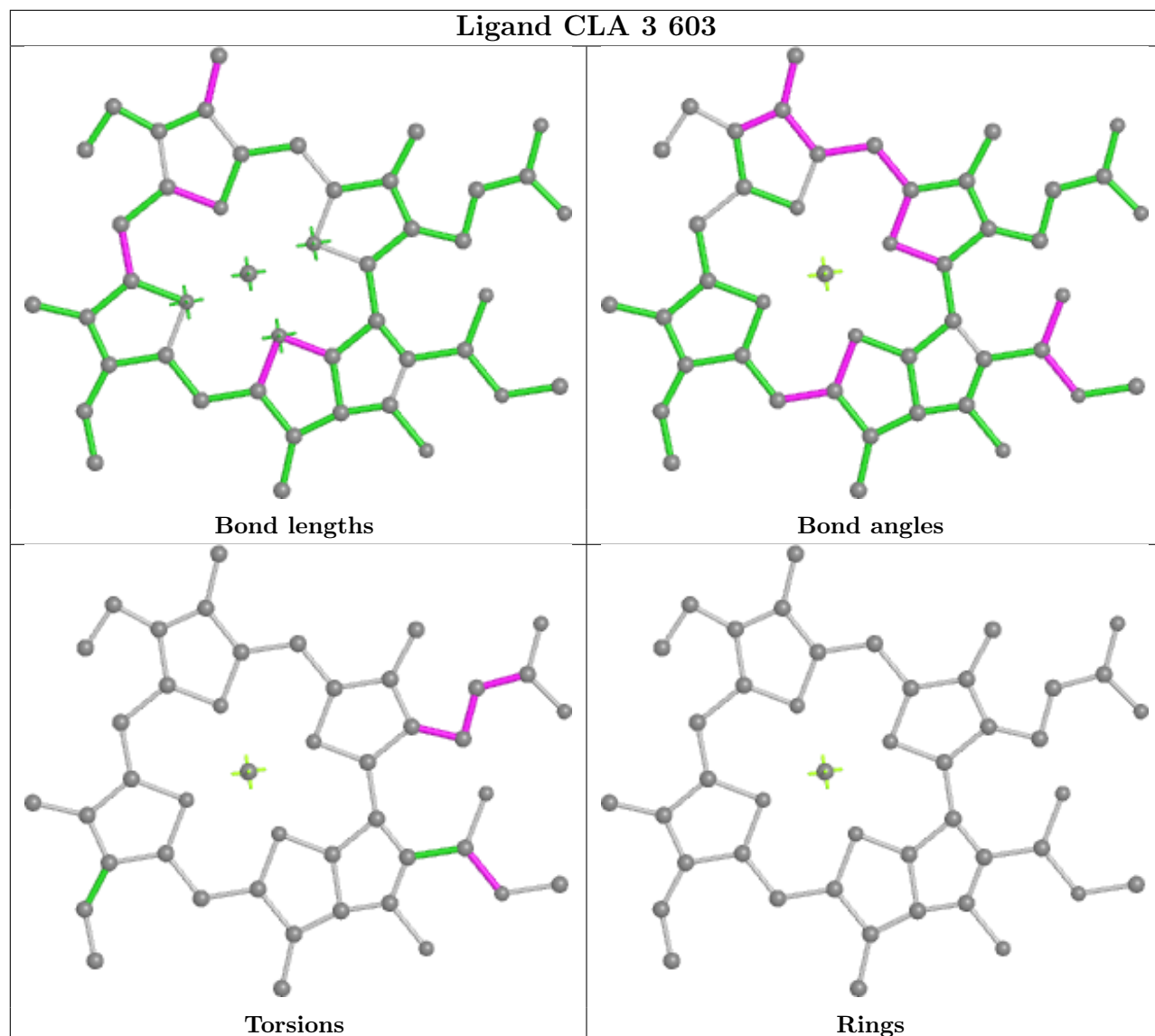
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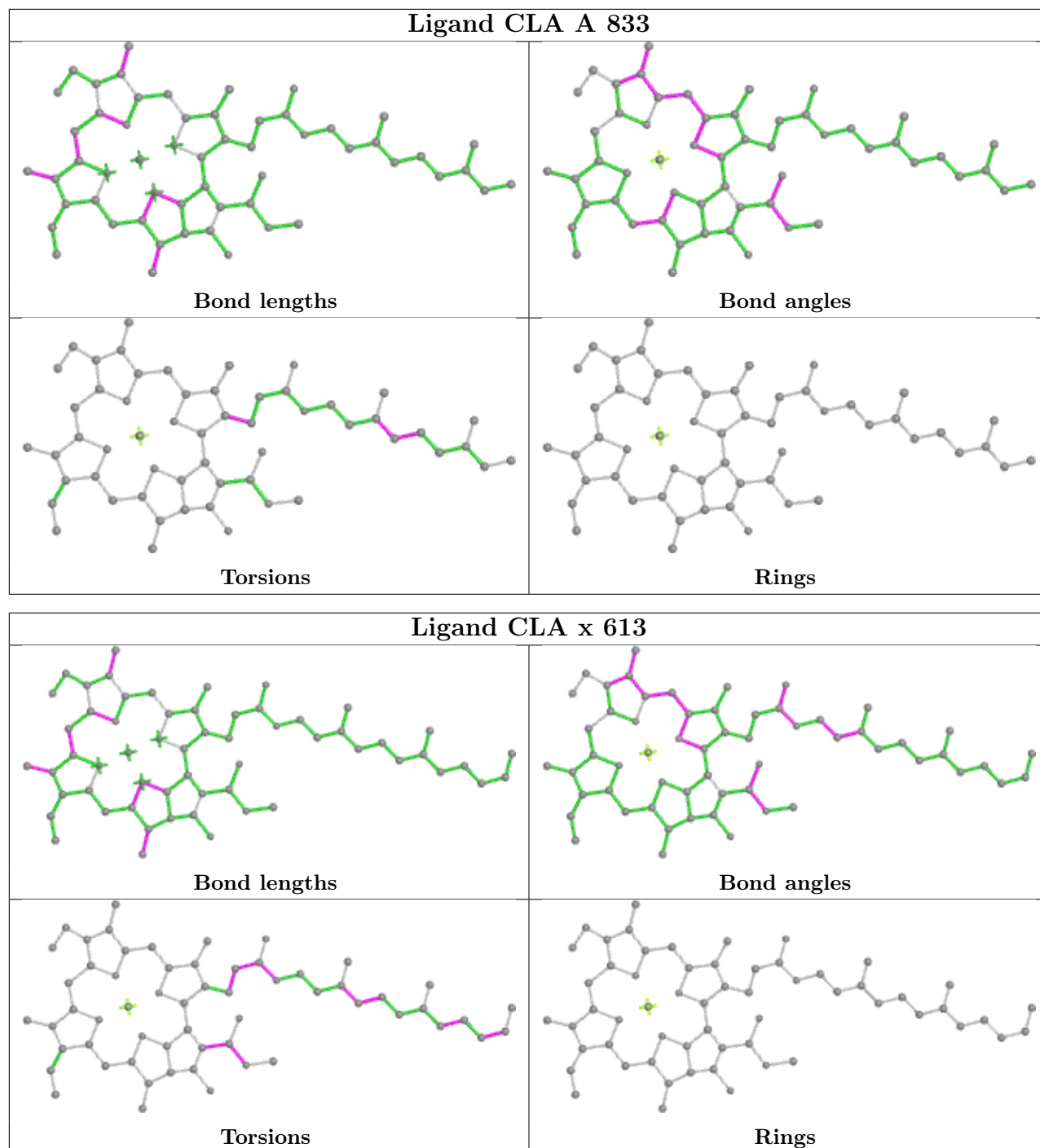
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	2	619	LUT	6	0
21	3	609	CLA	7	0
21	A	838	CLA	1	0
21	B	806	CLA	4	0

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

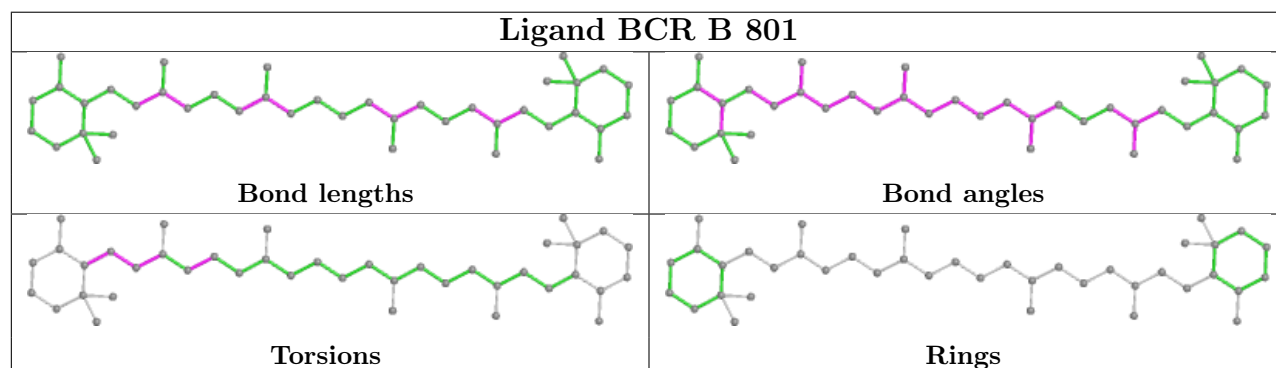
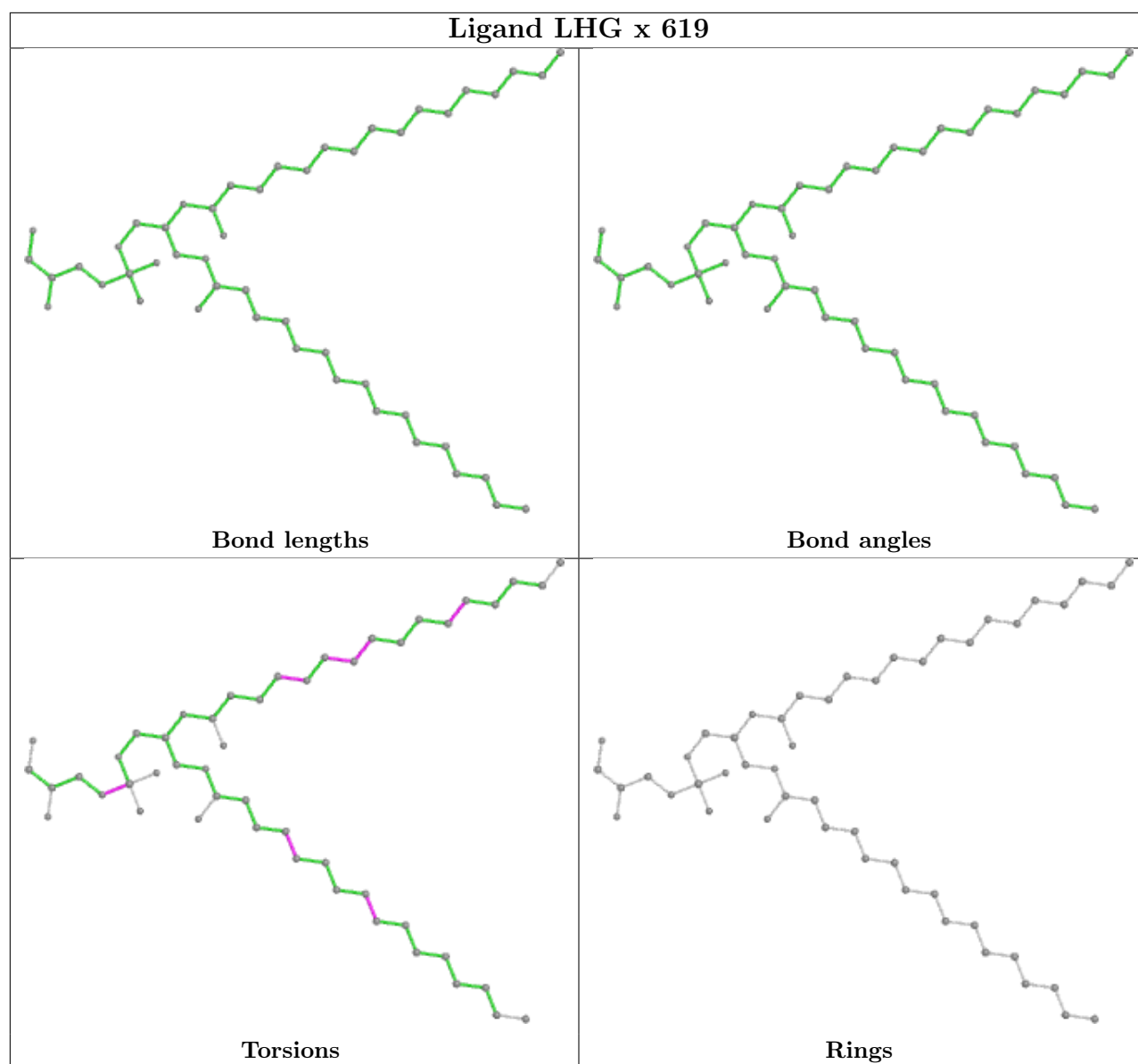


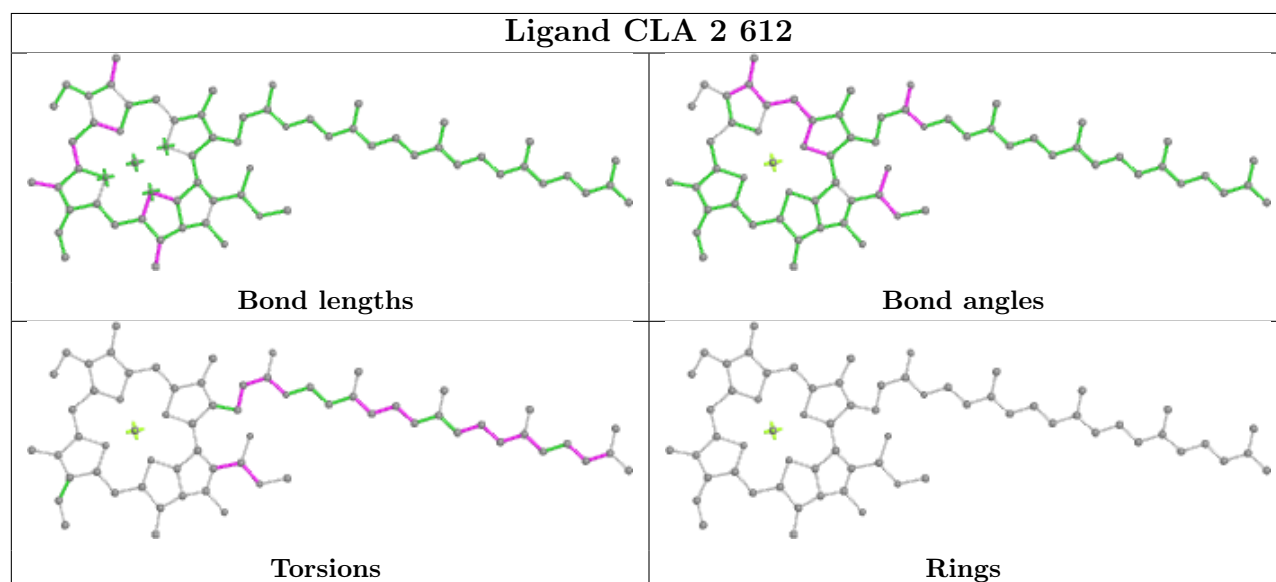
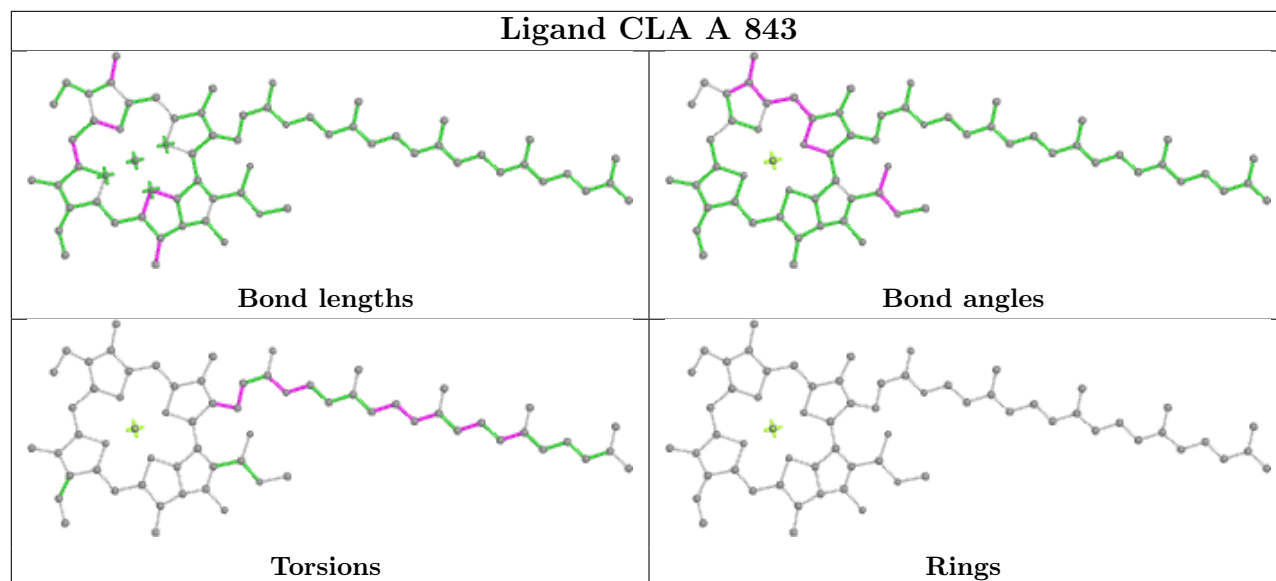
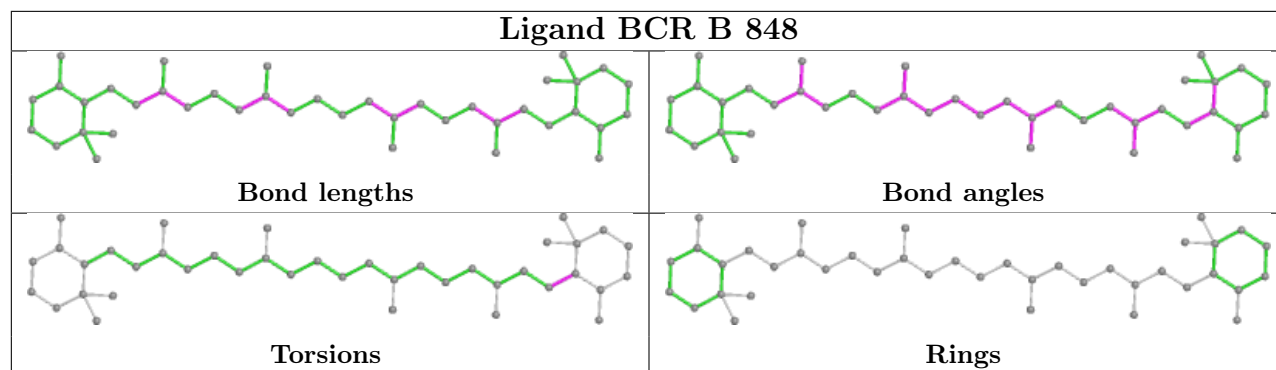


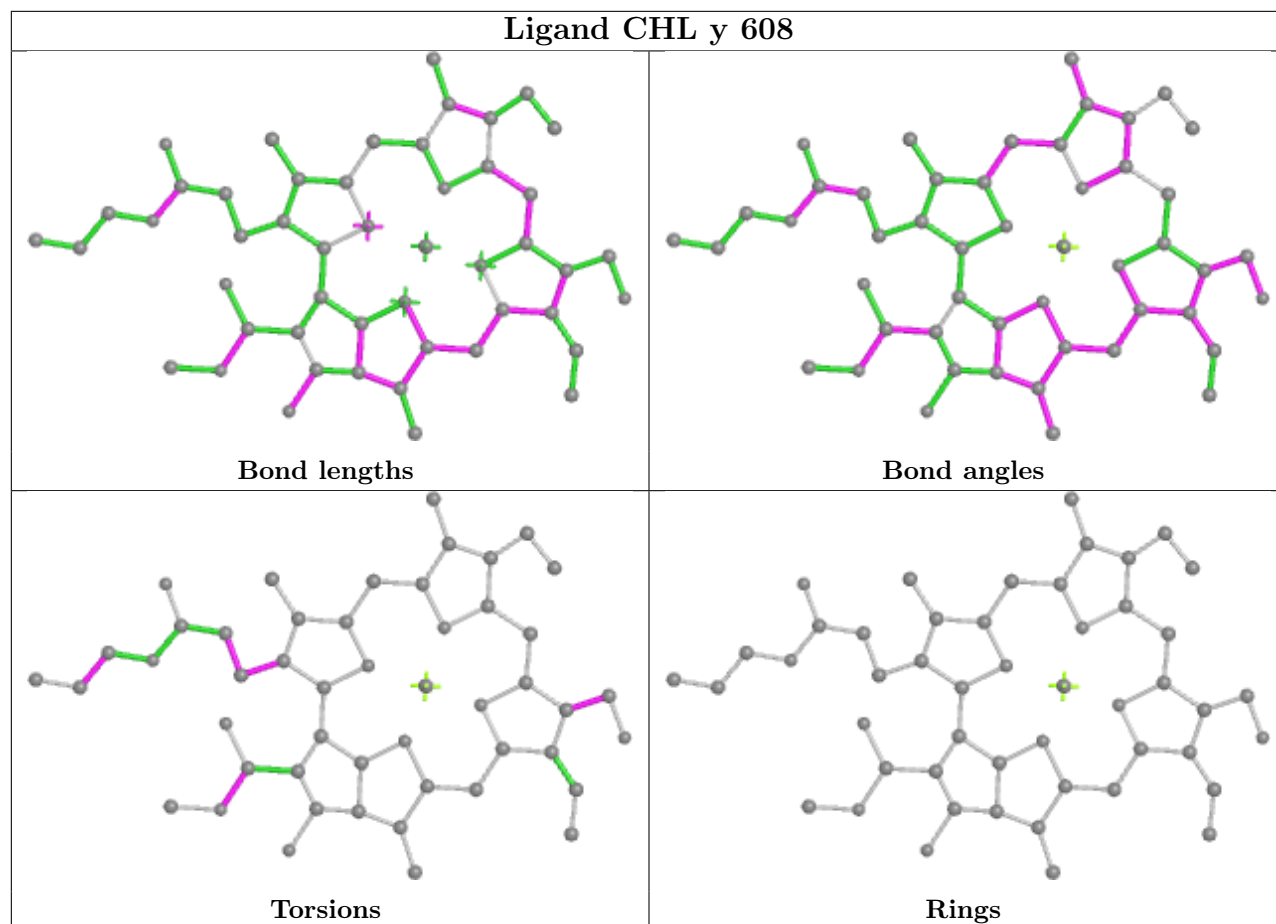
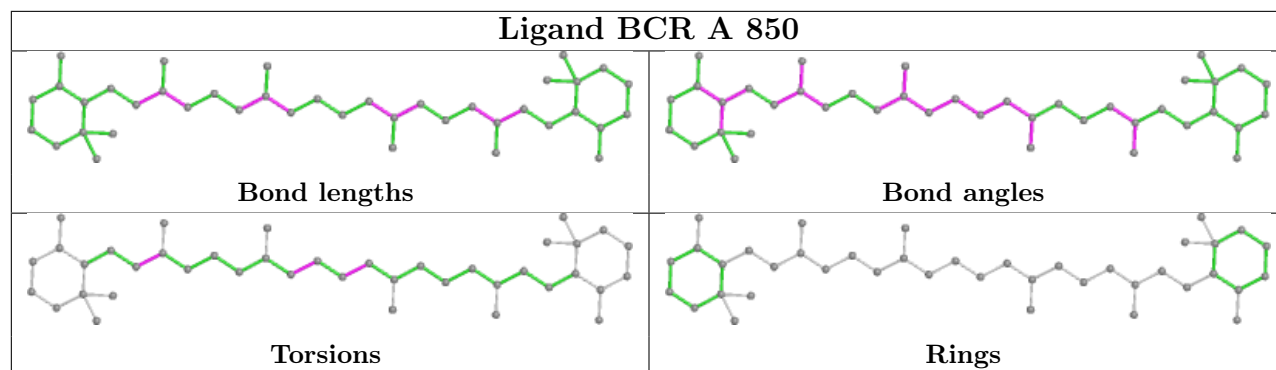


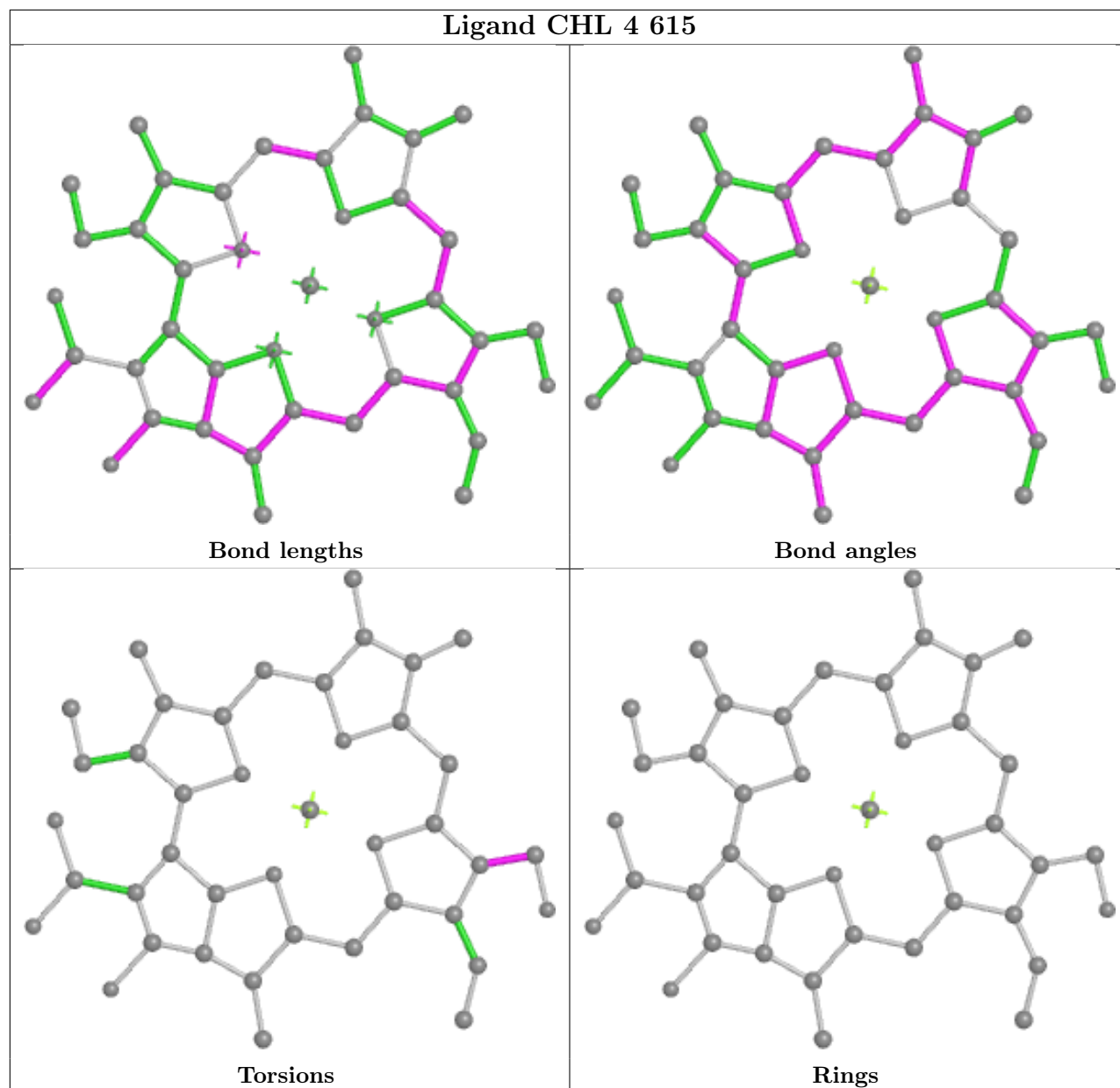


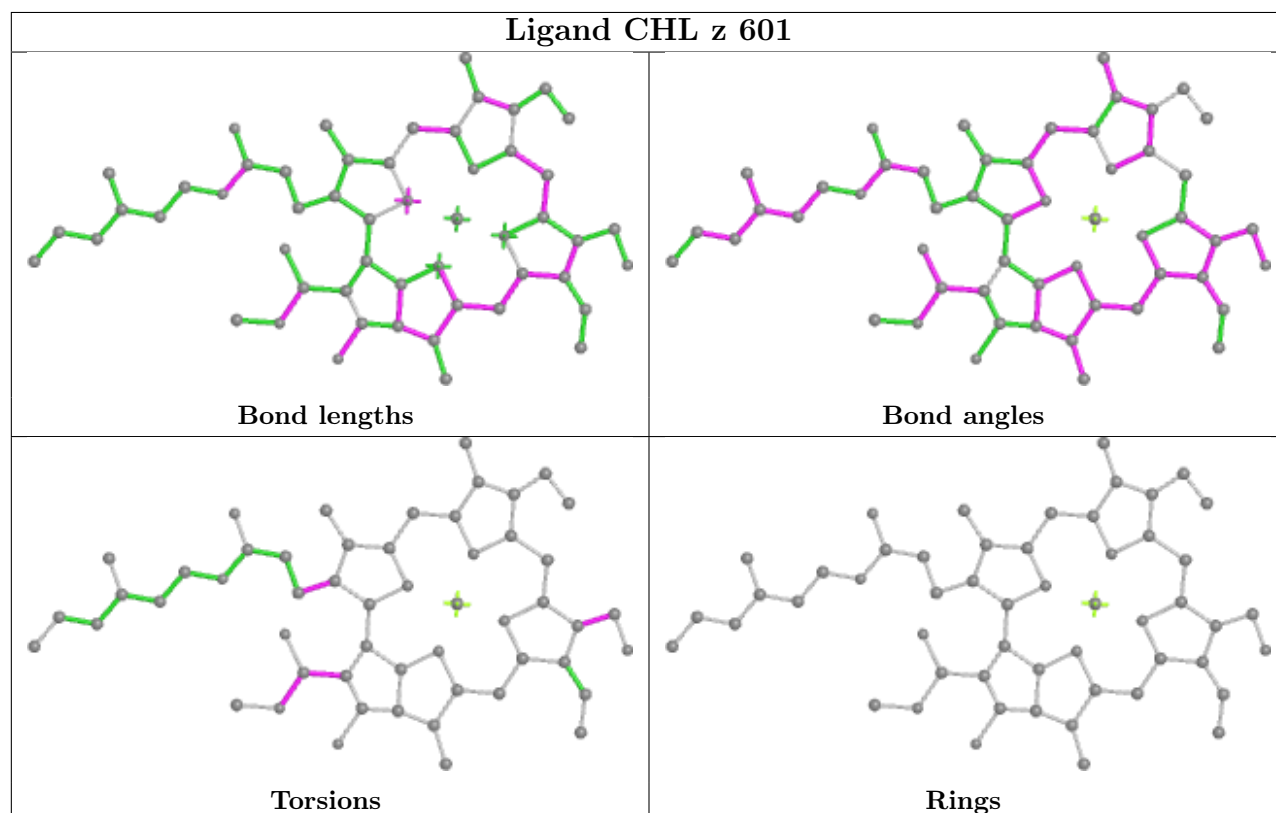
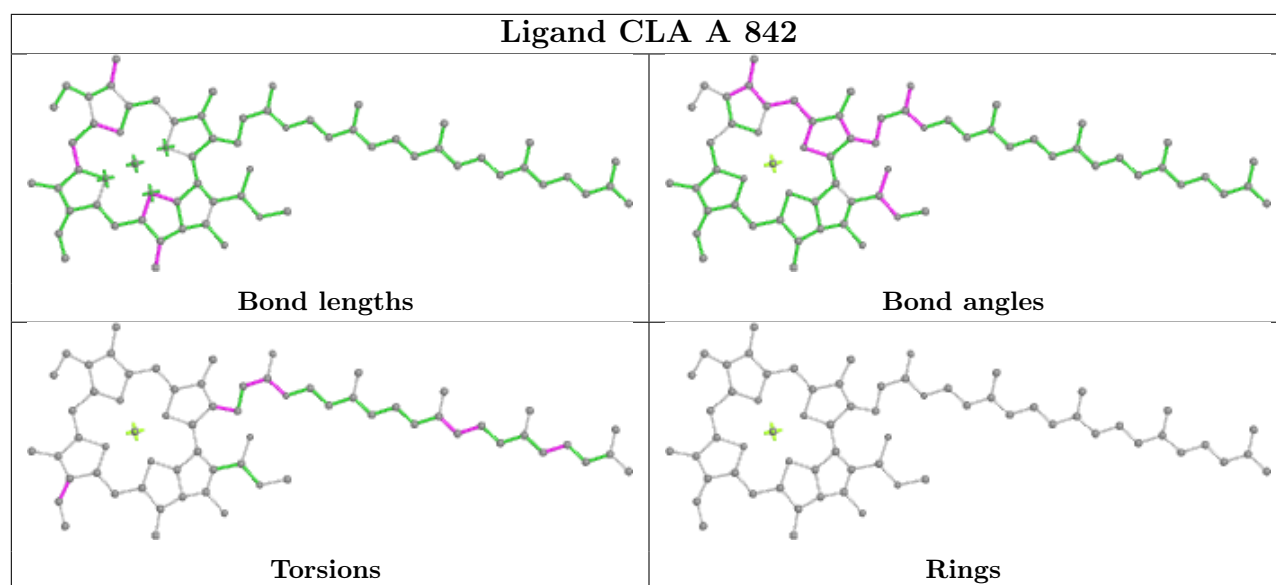


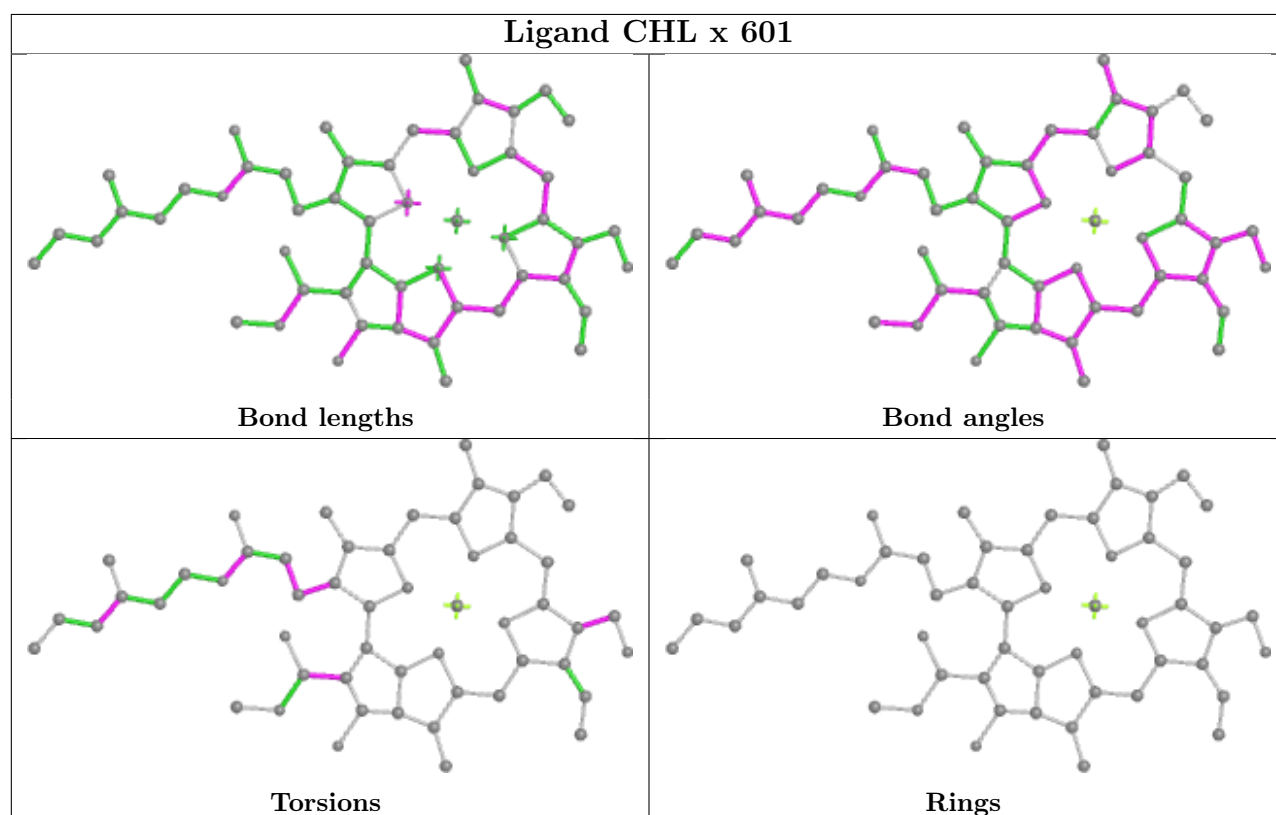
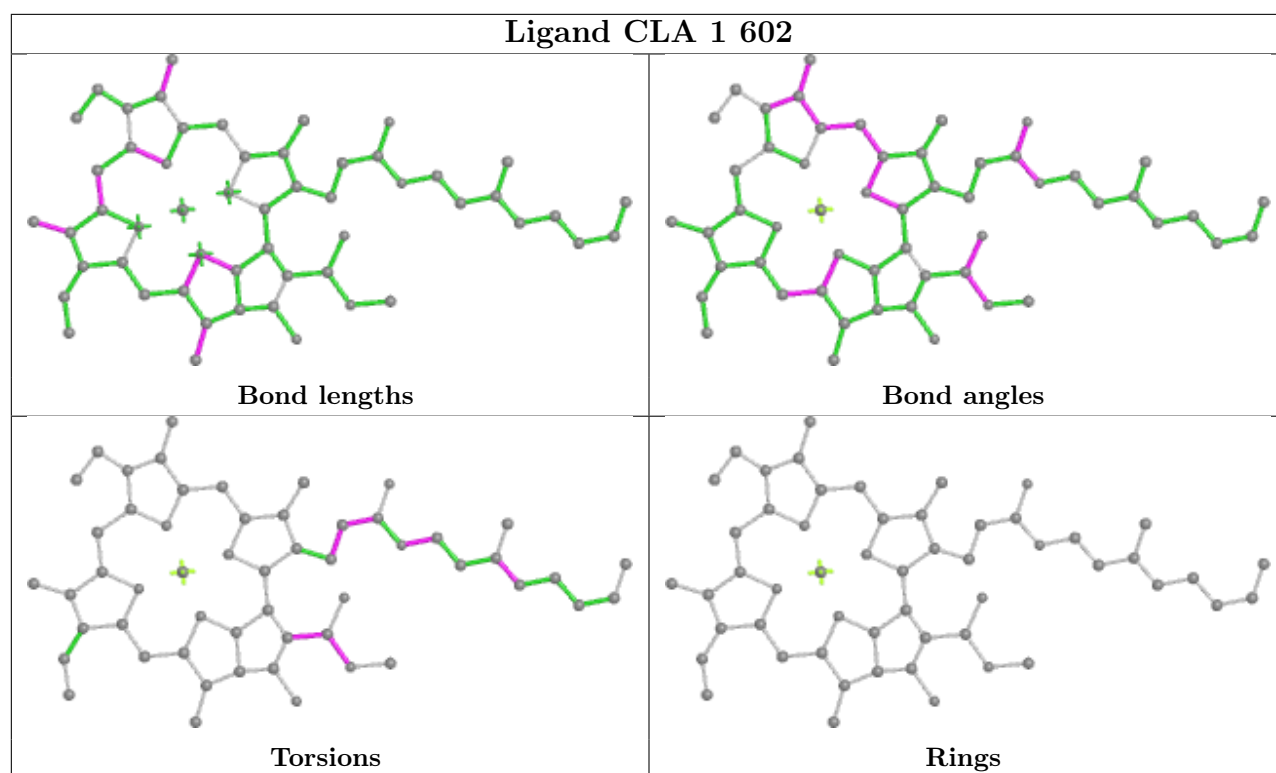


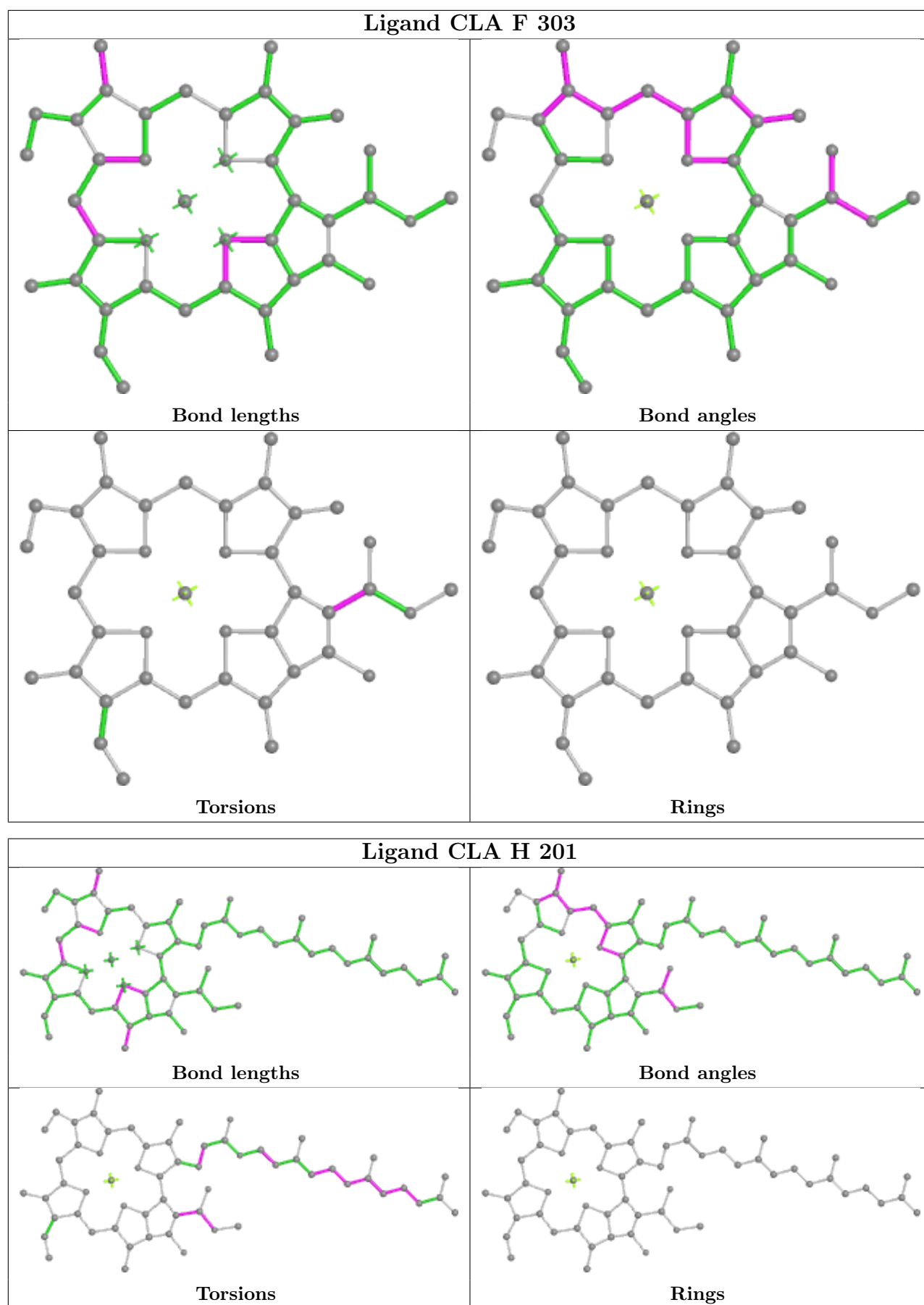


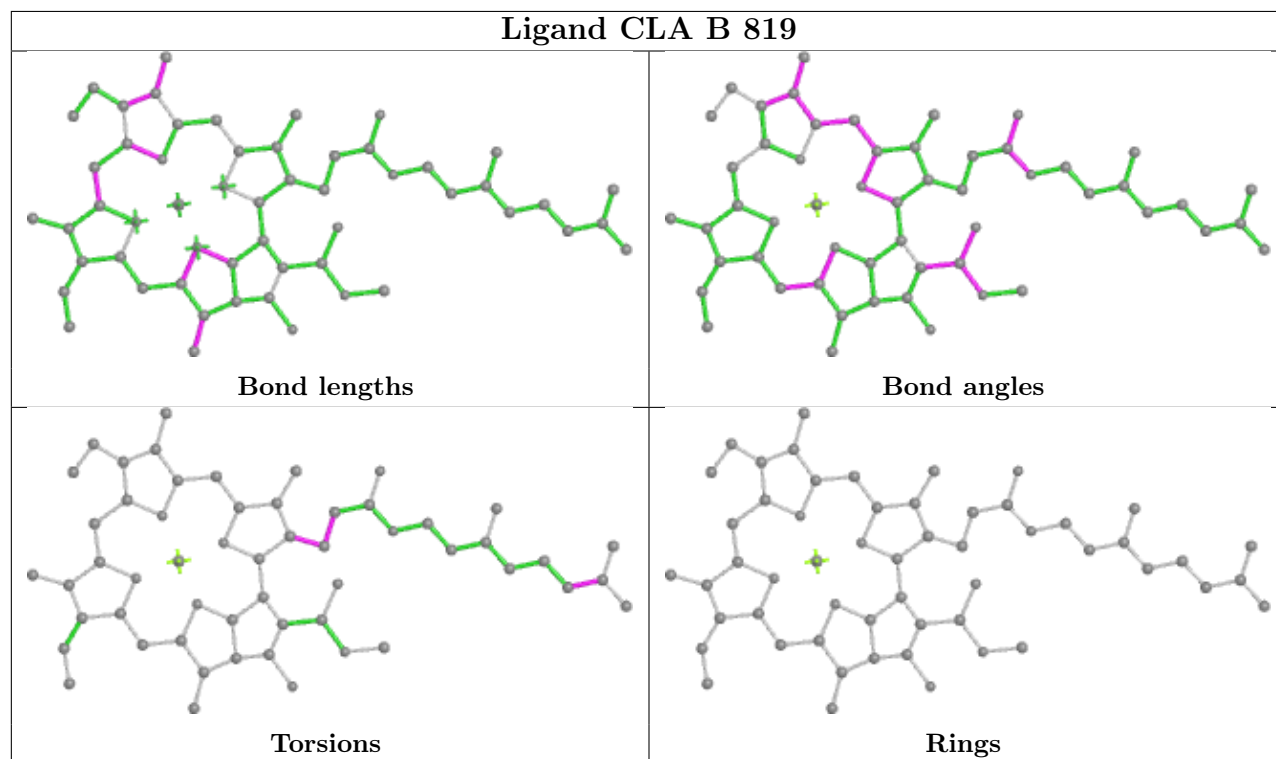
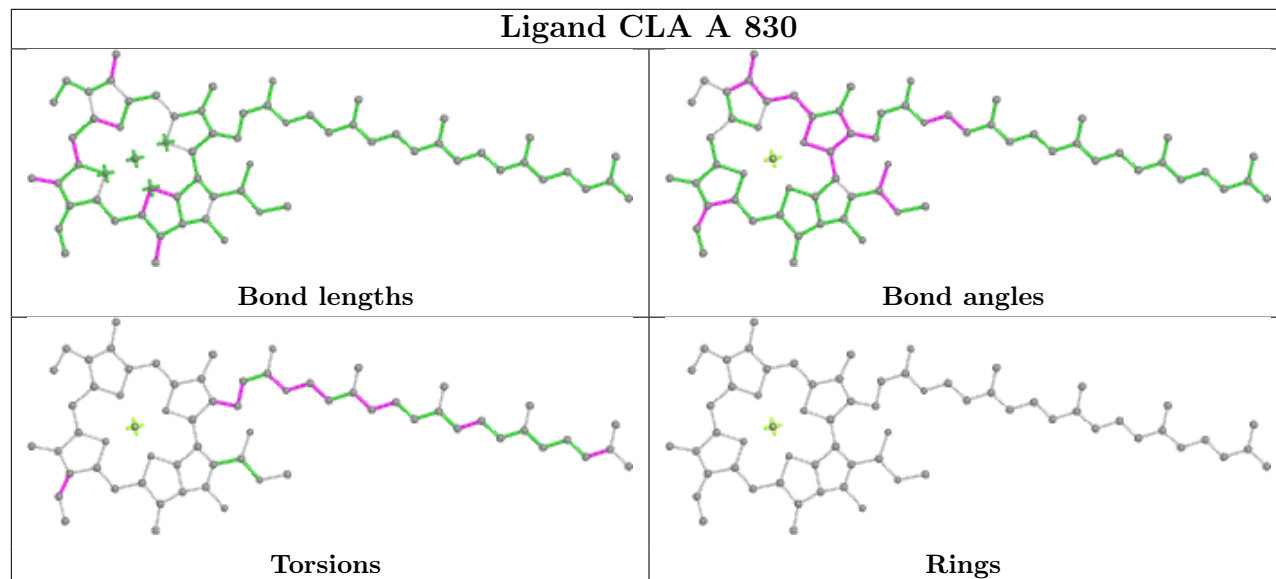
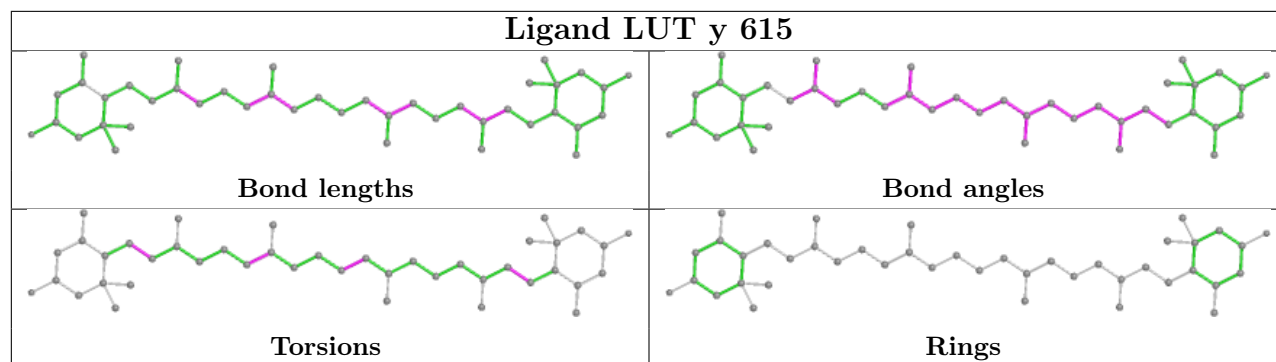




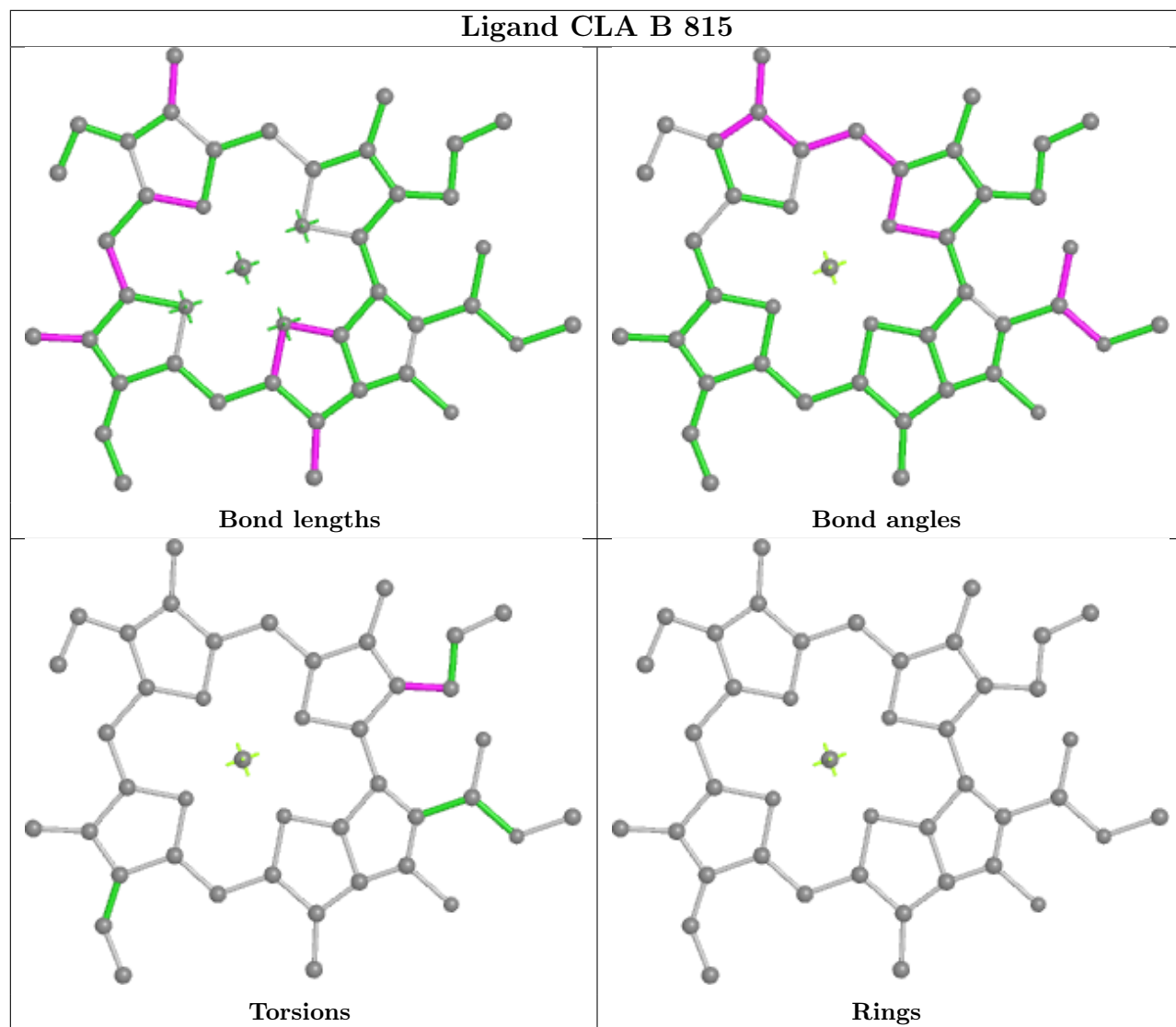


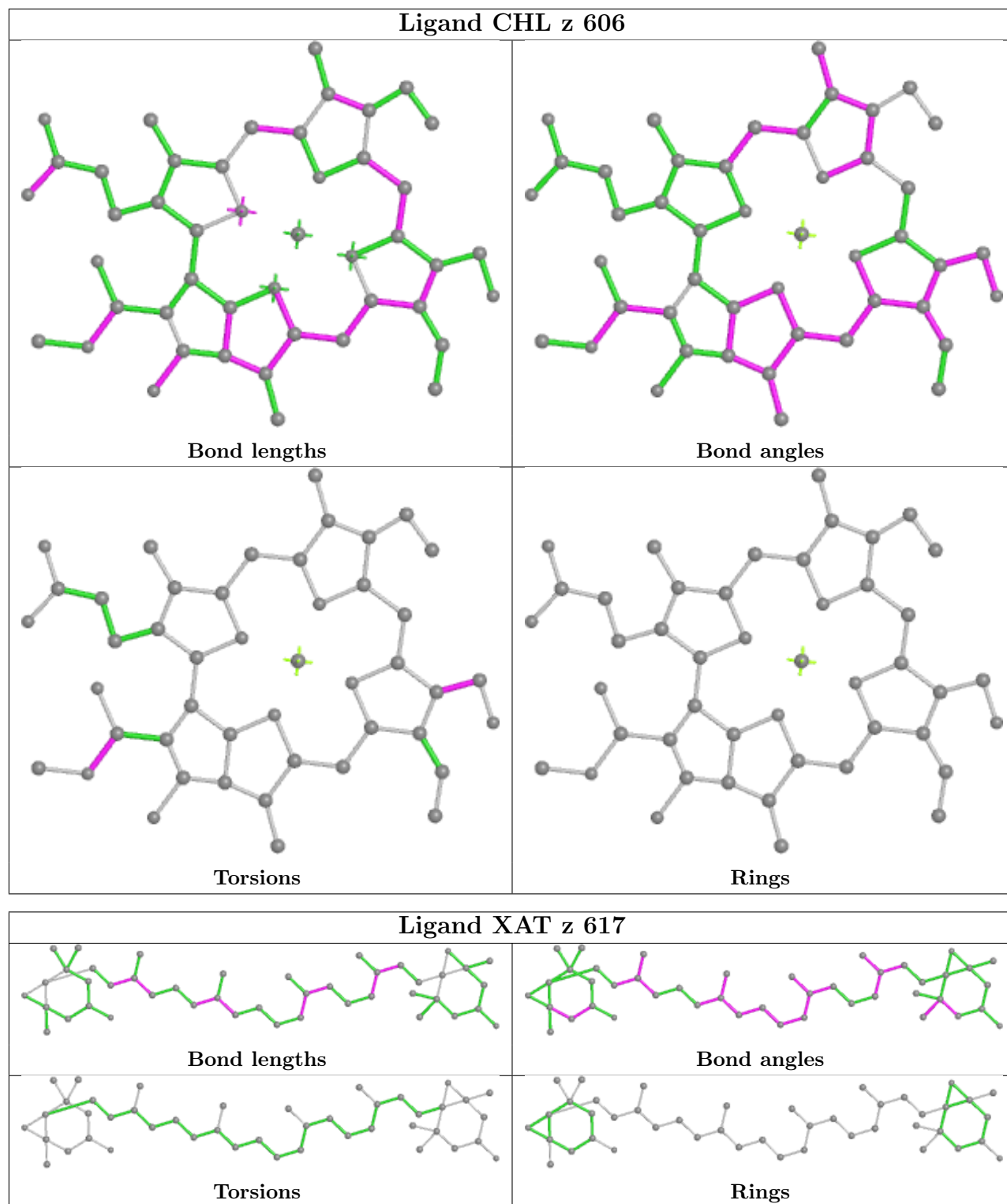


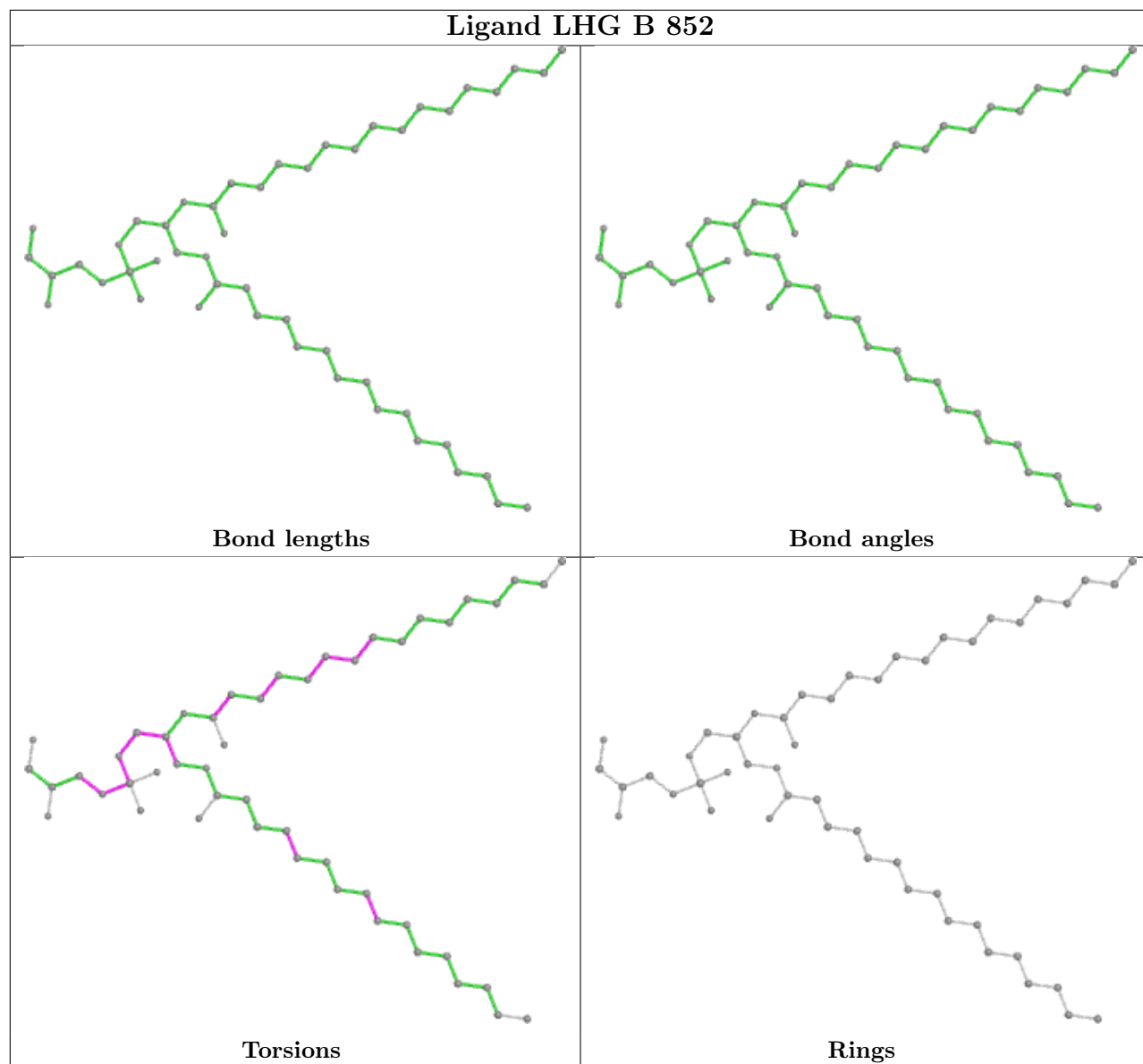


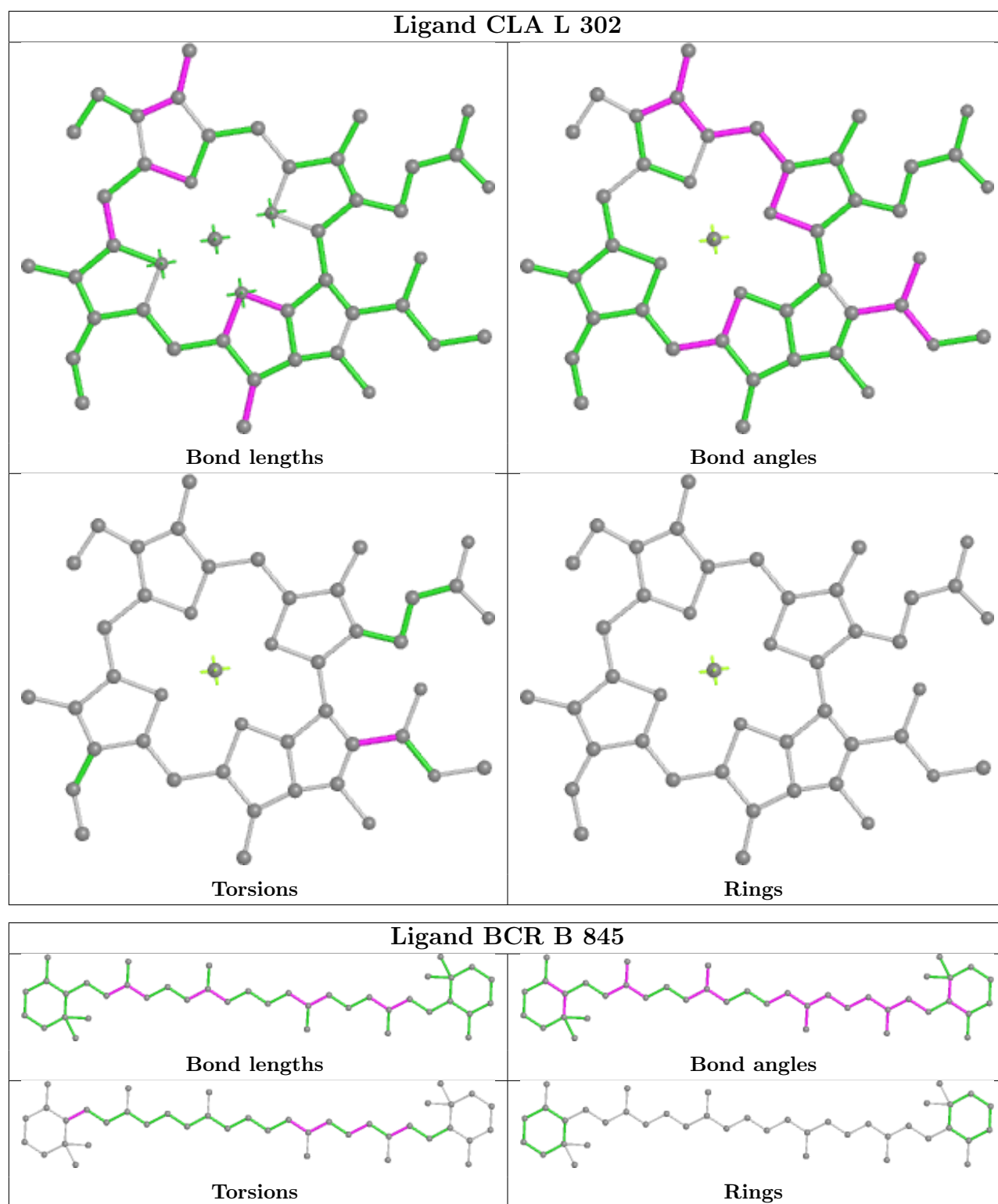


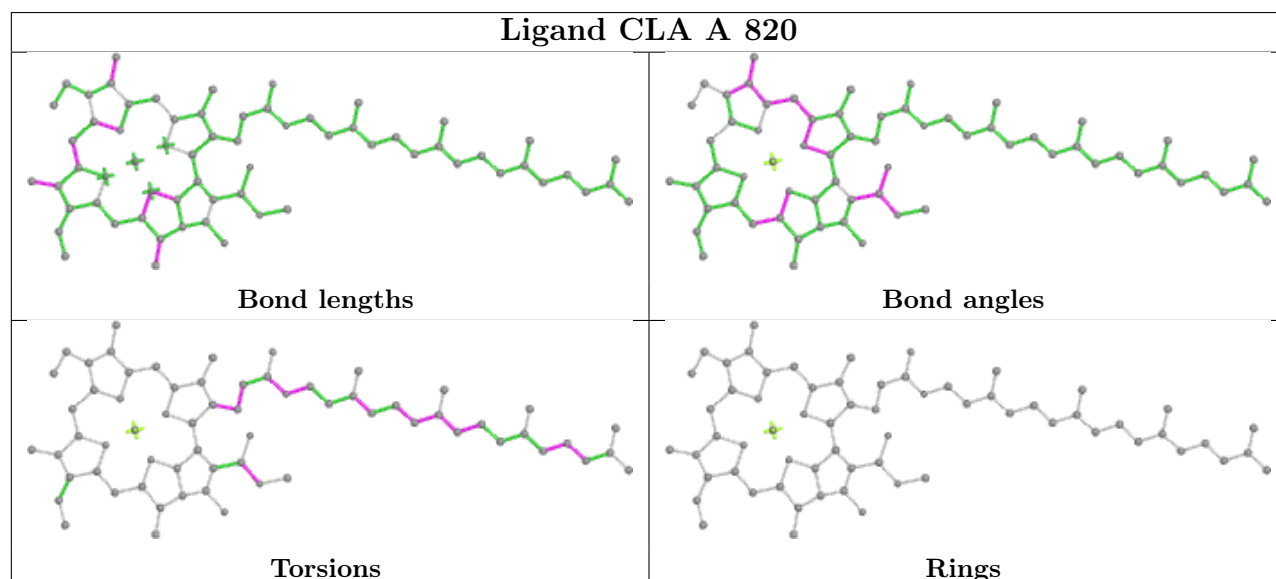
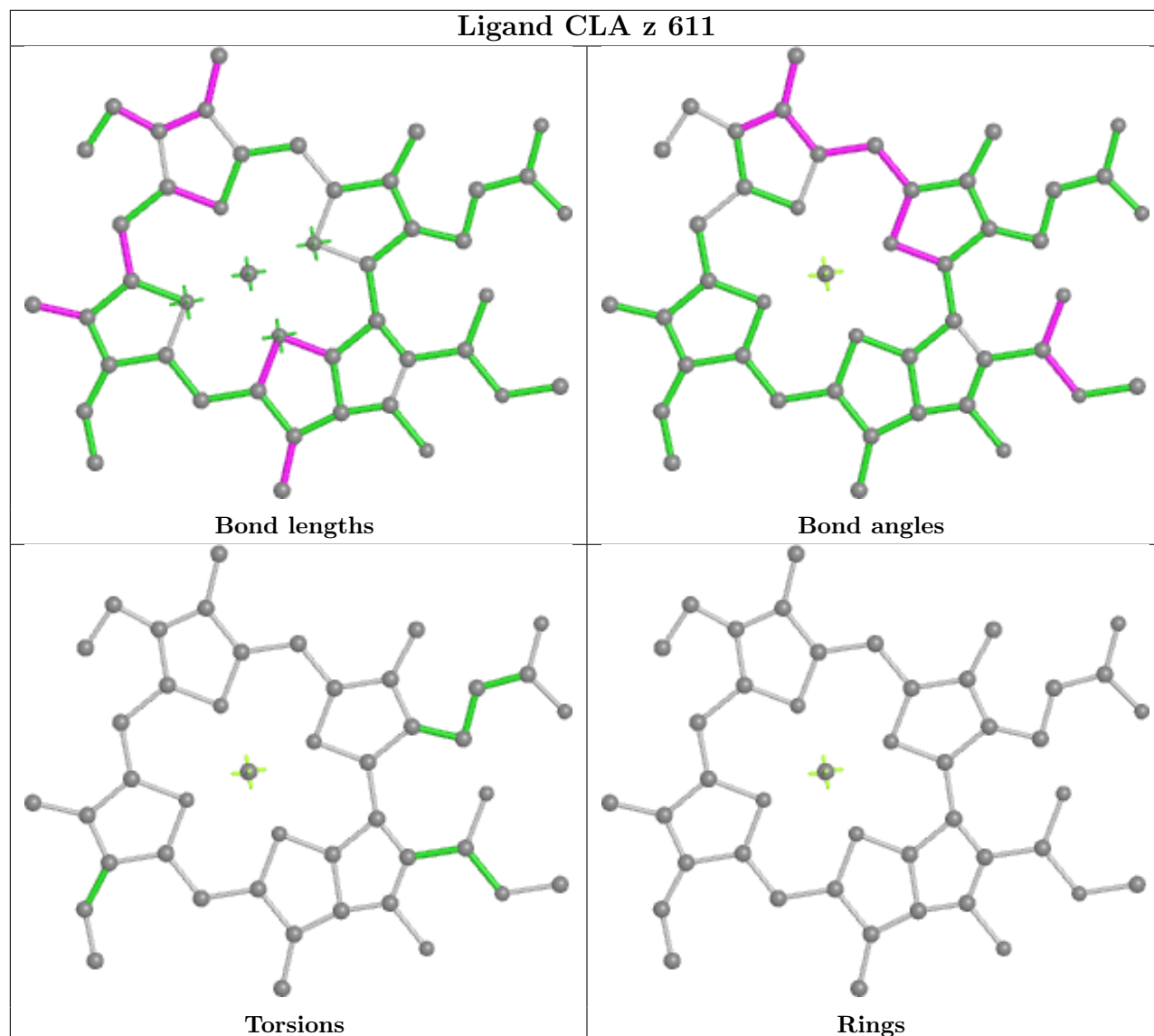


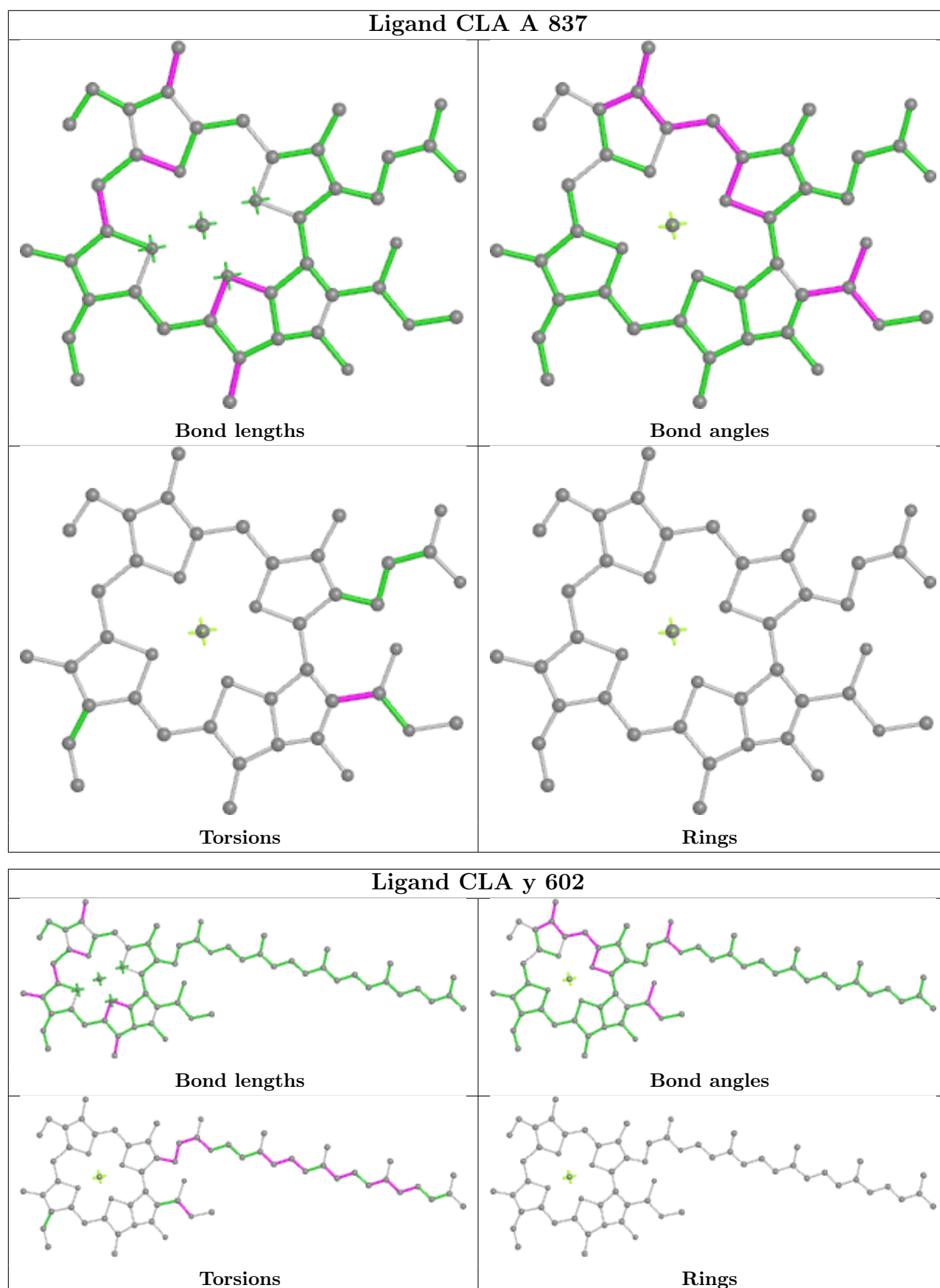


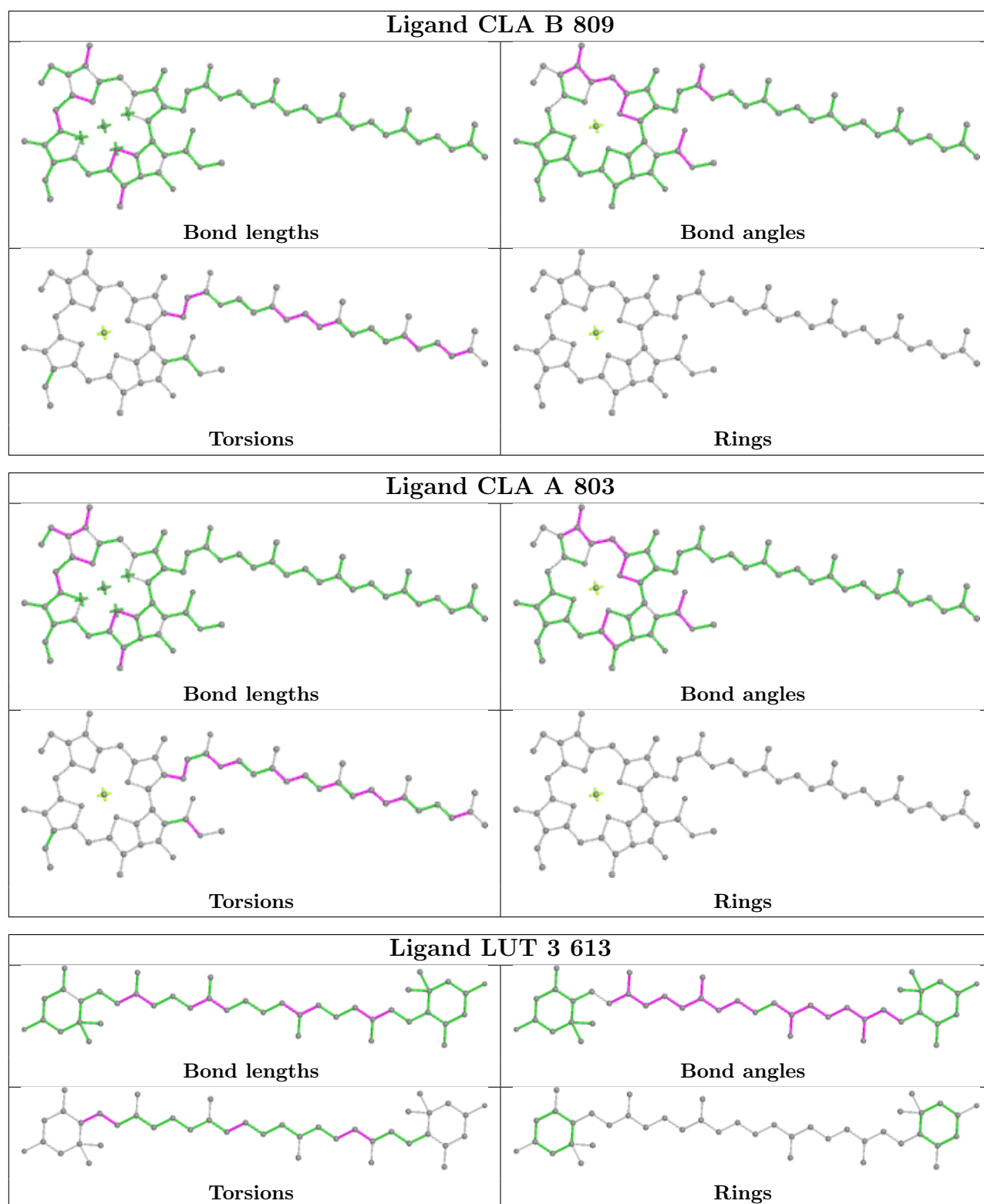


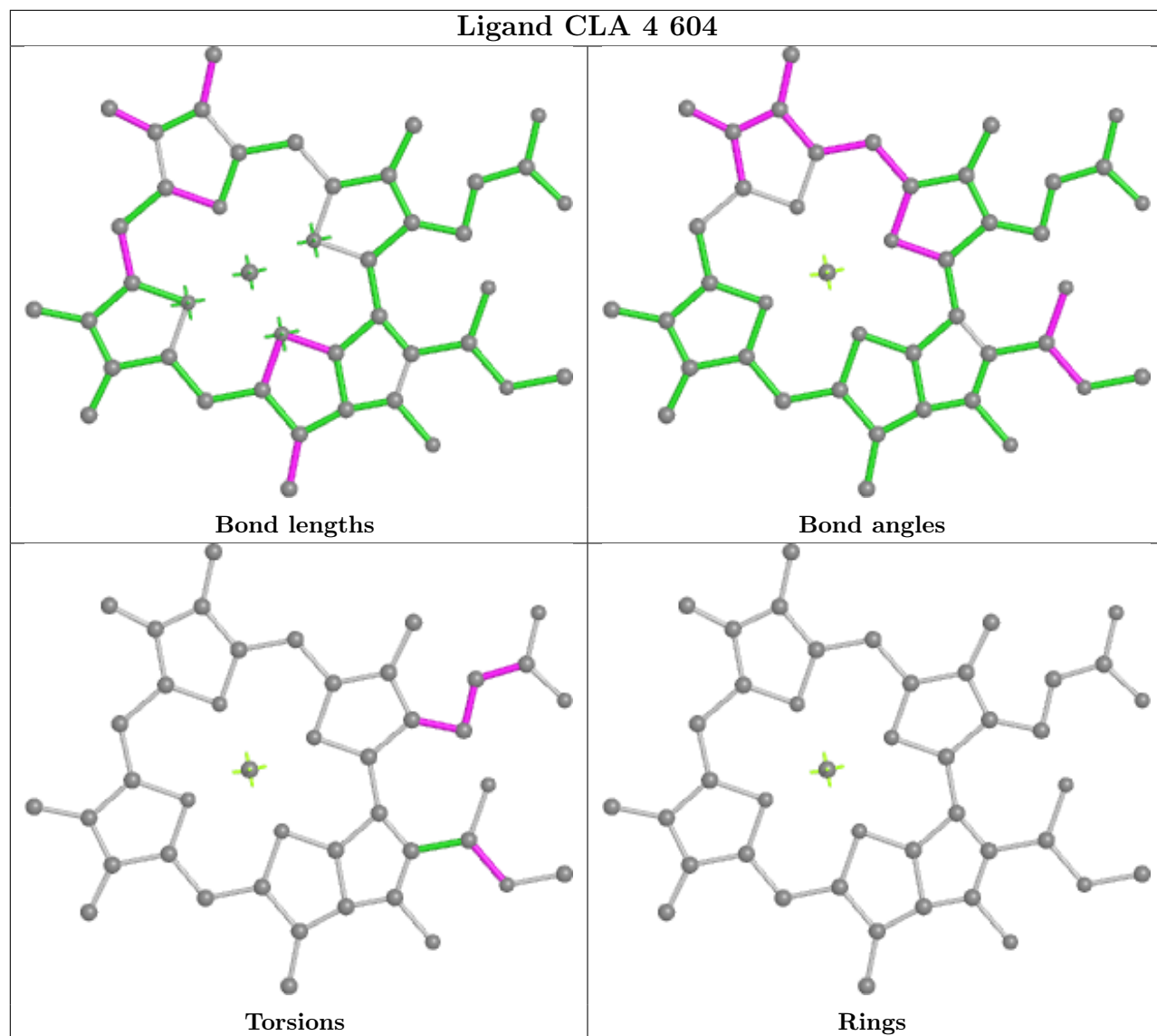




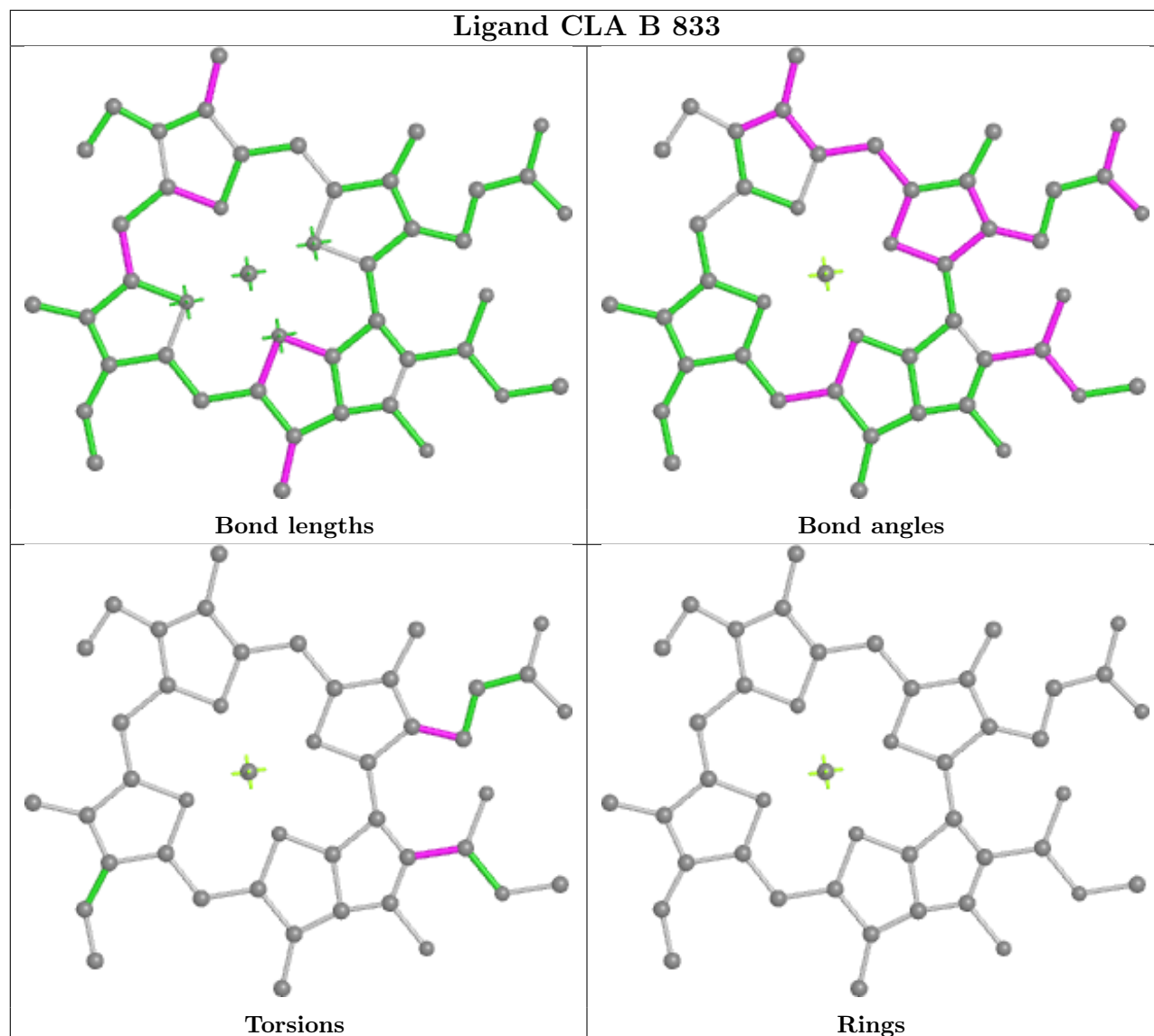


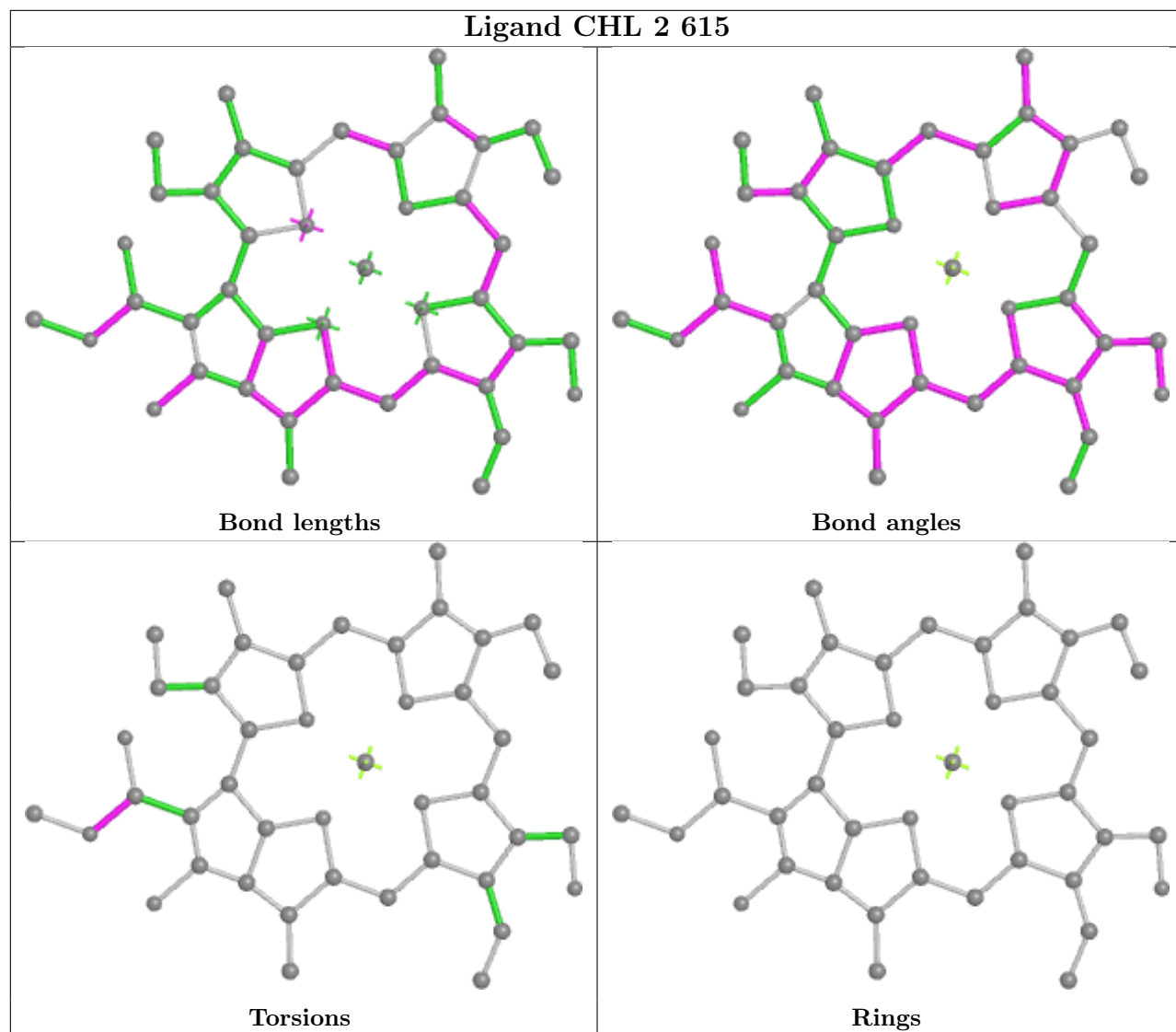


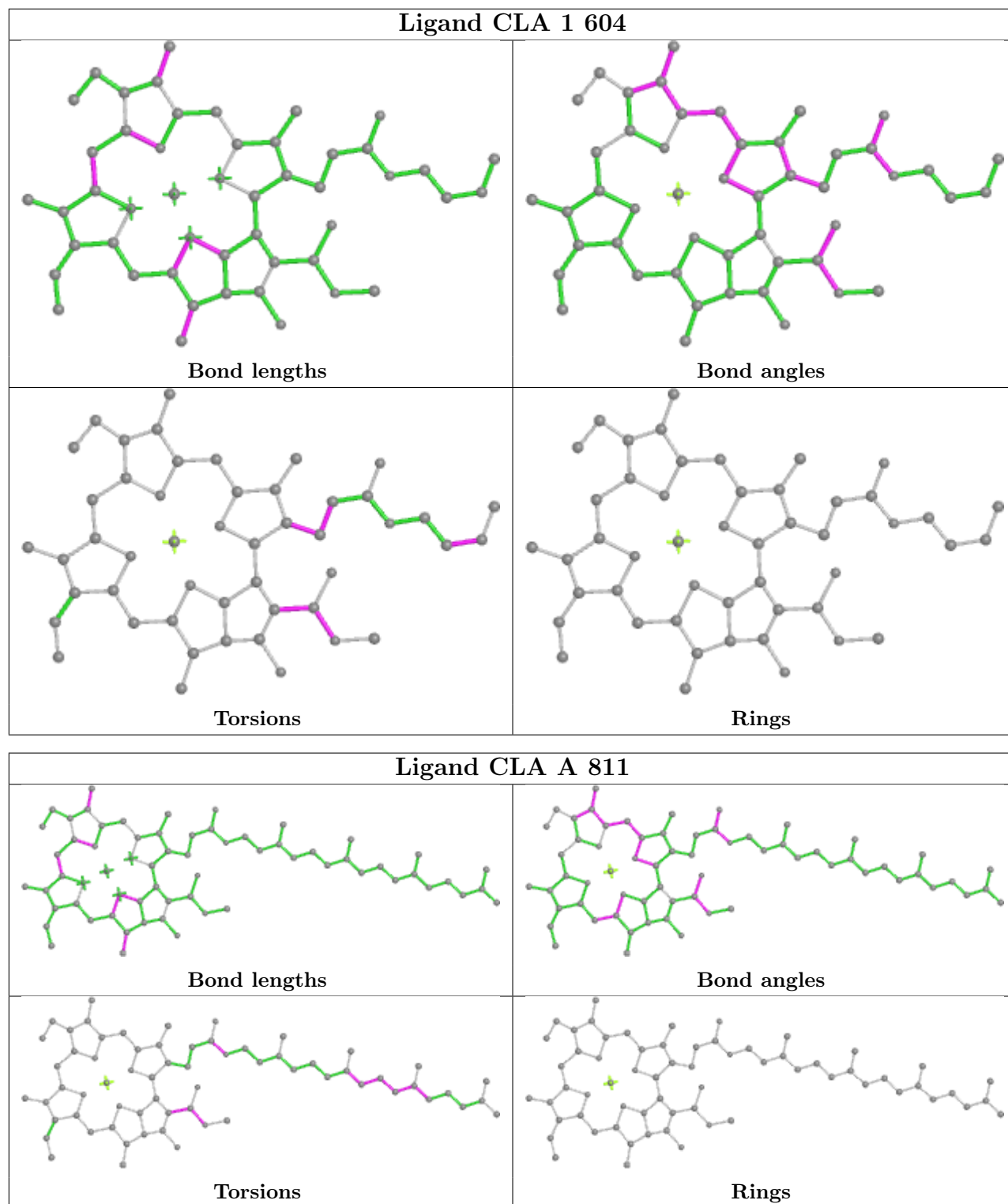


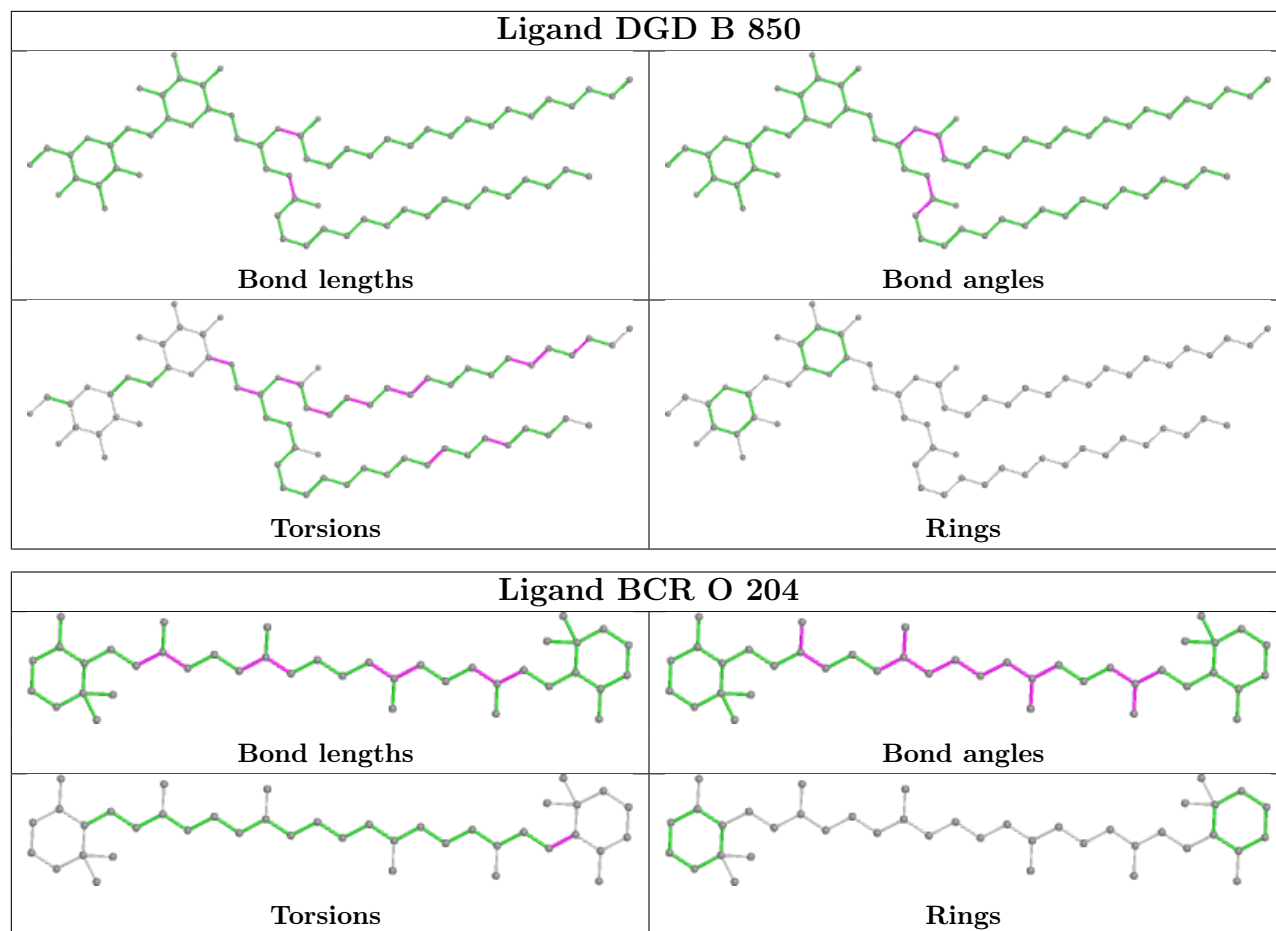


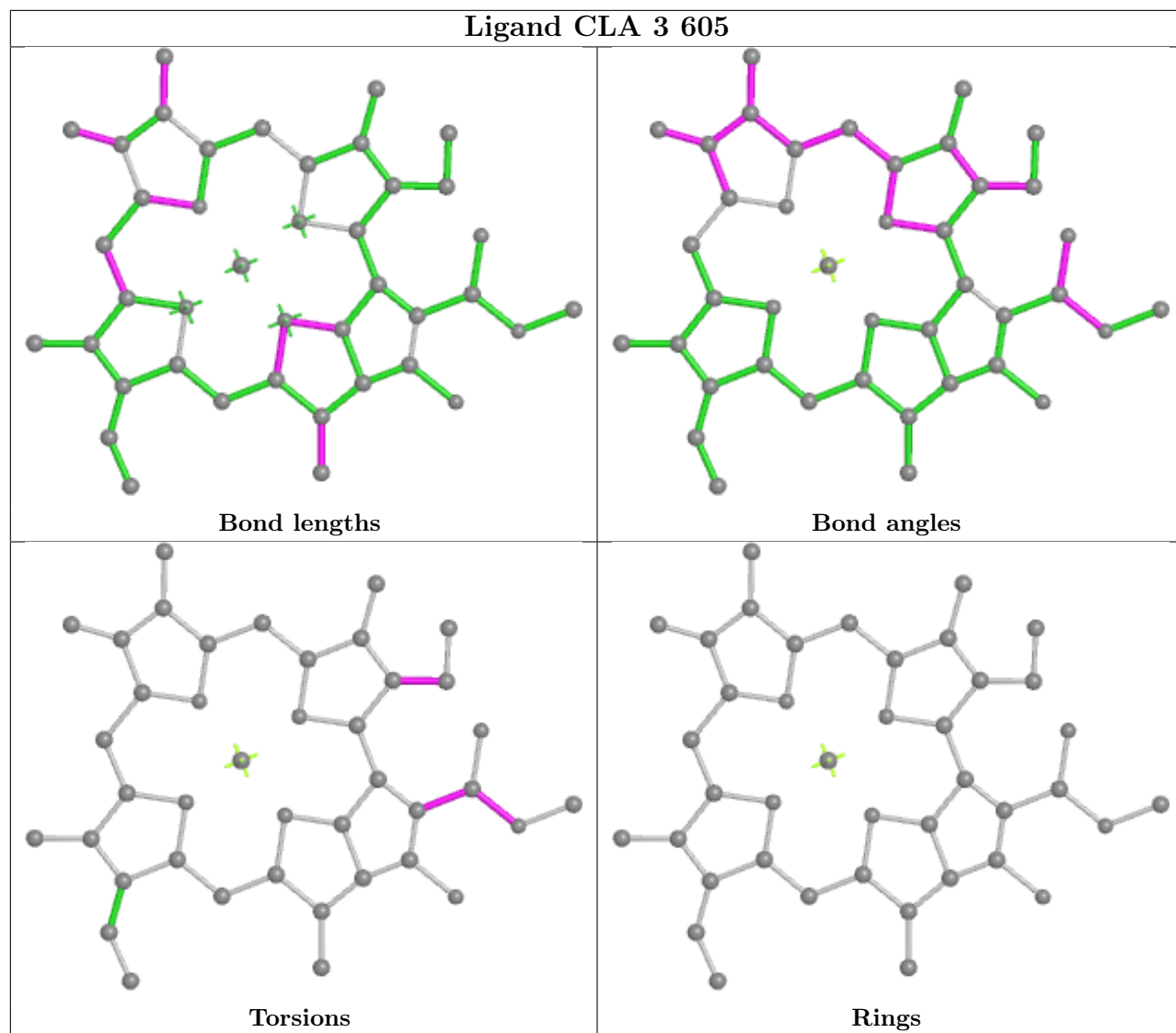


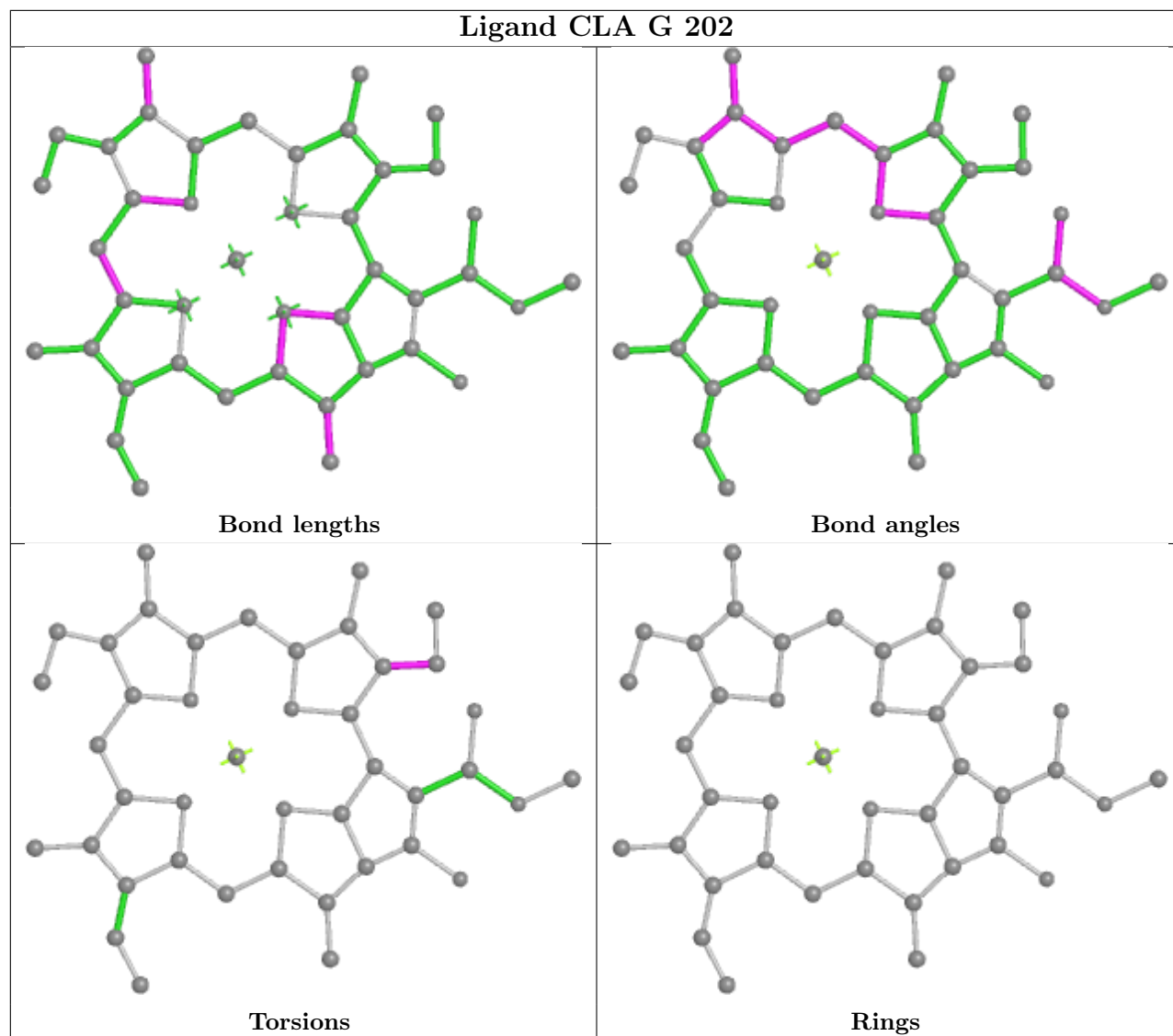


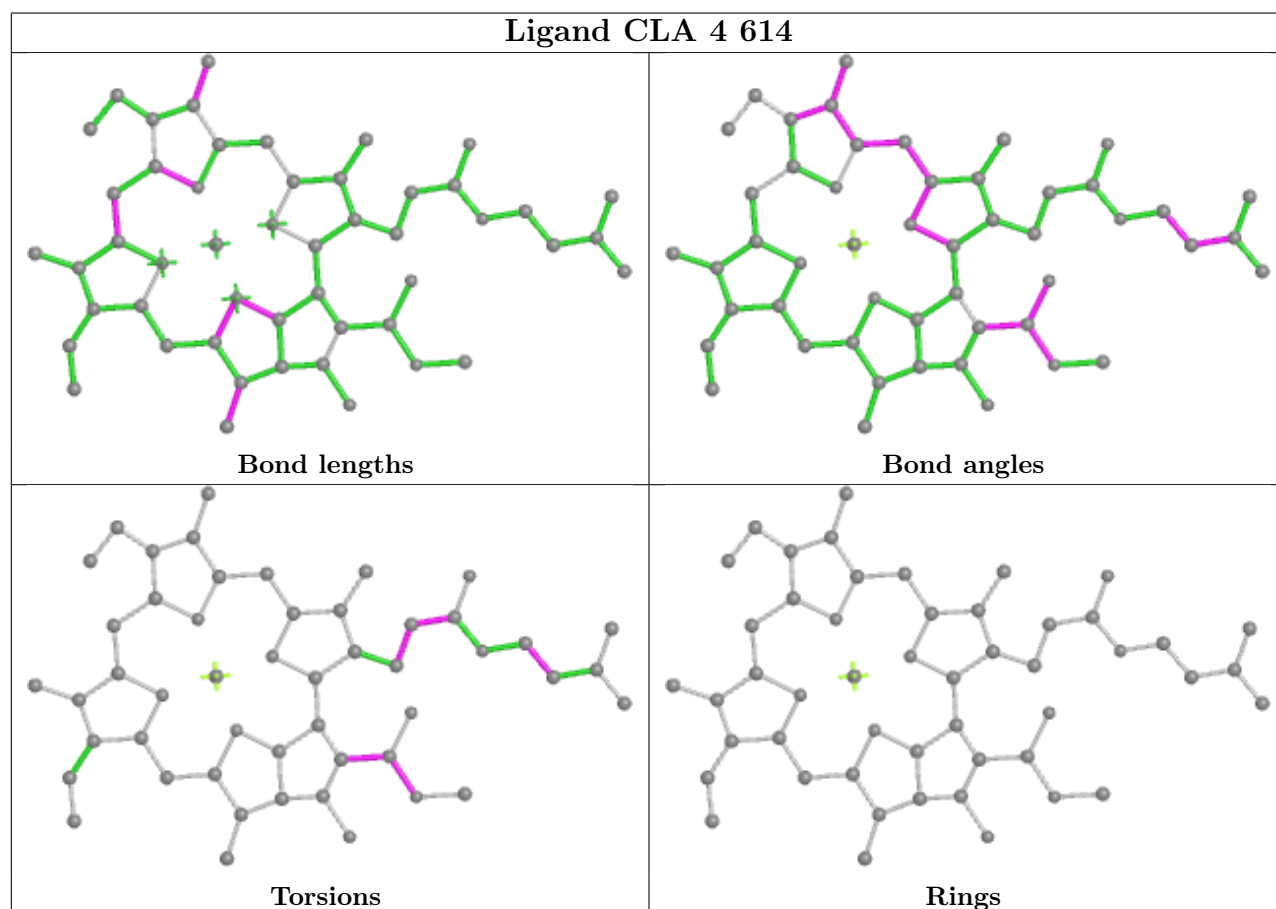
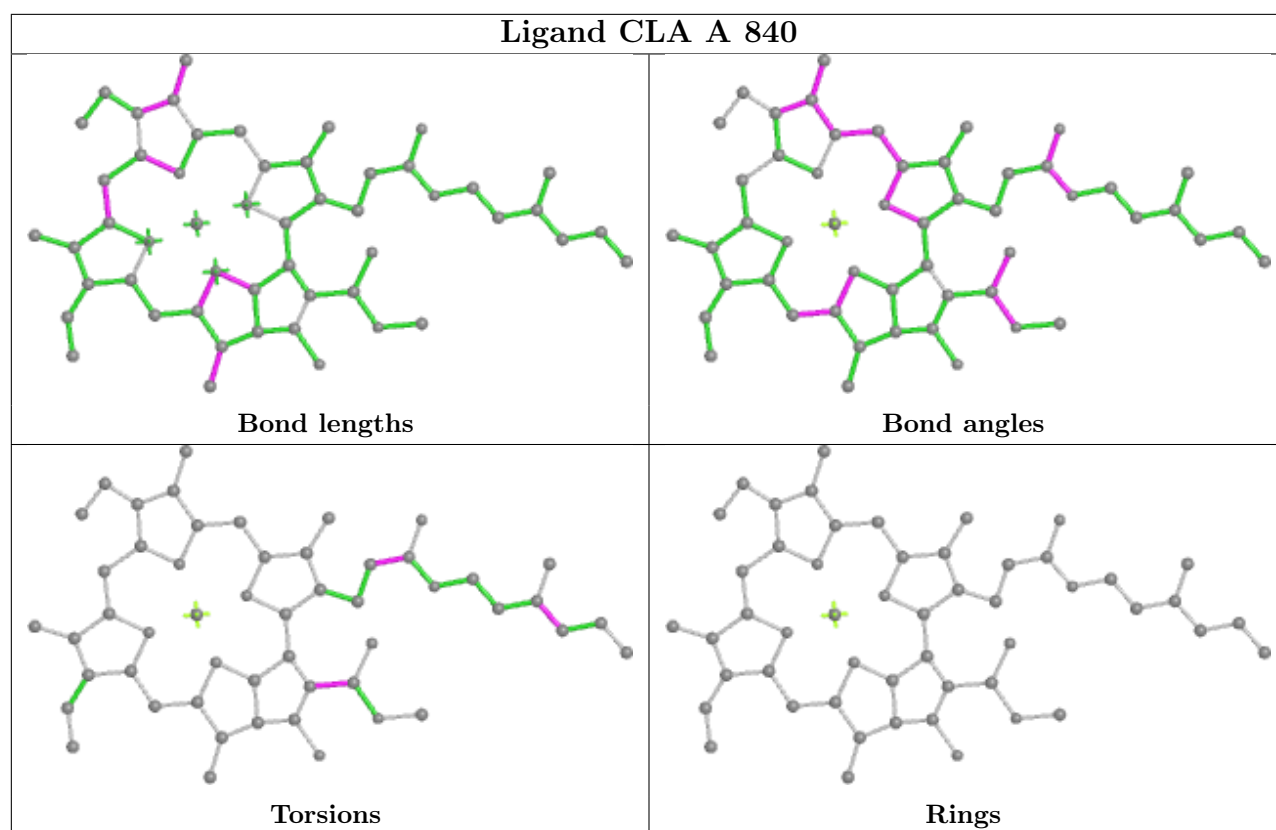


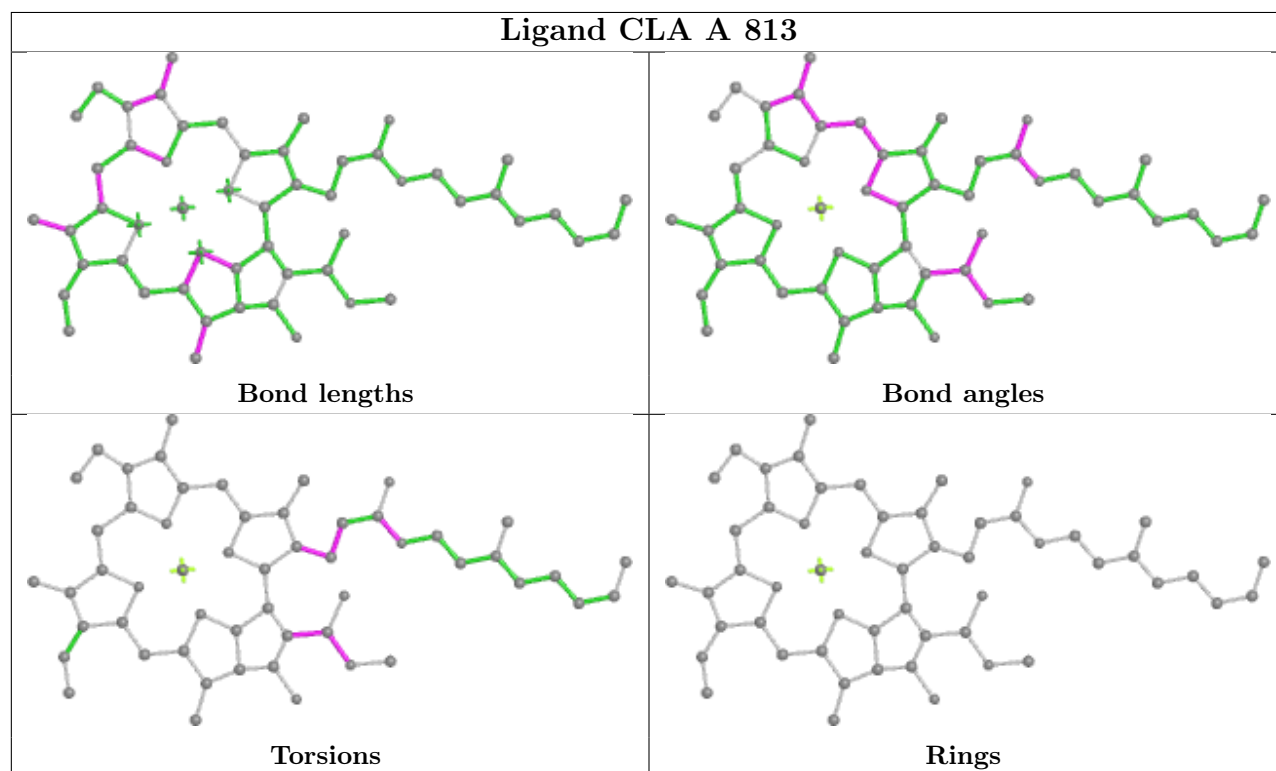
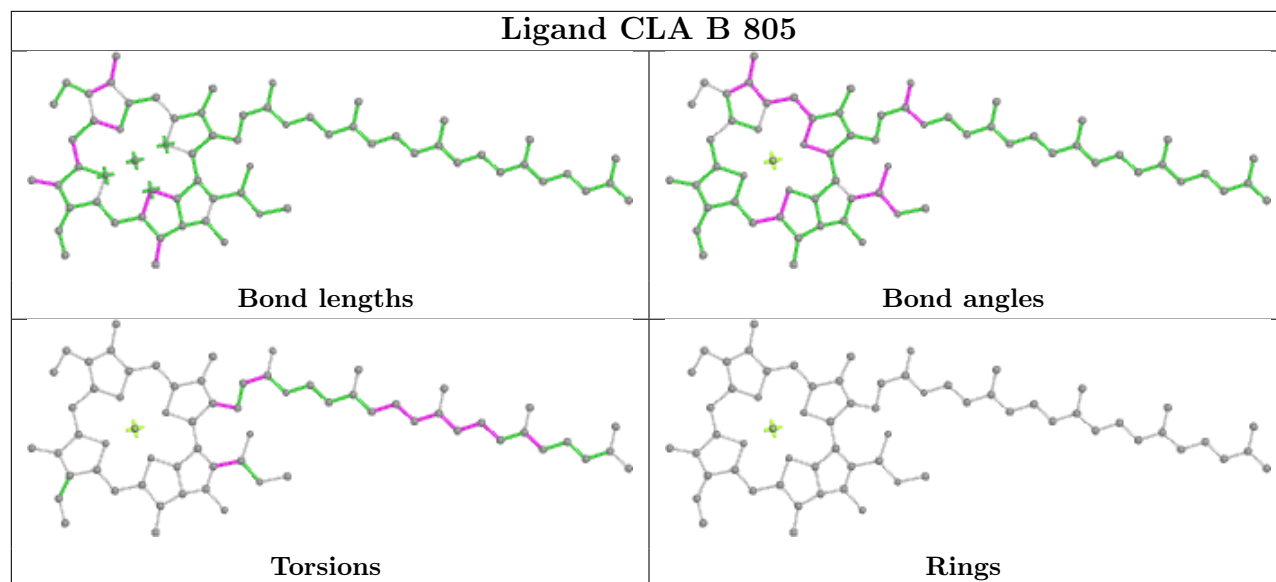




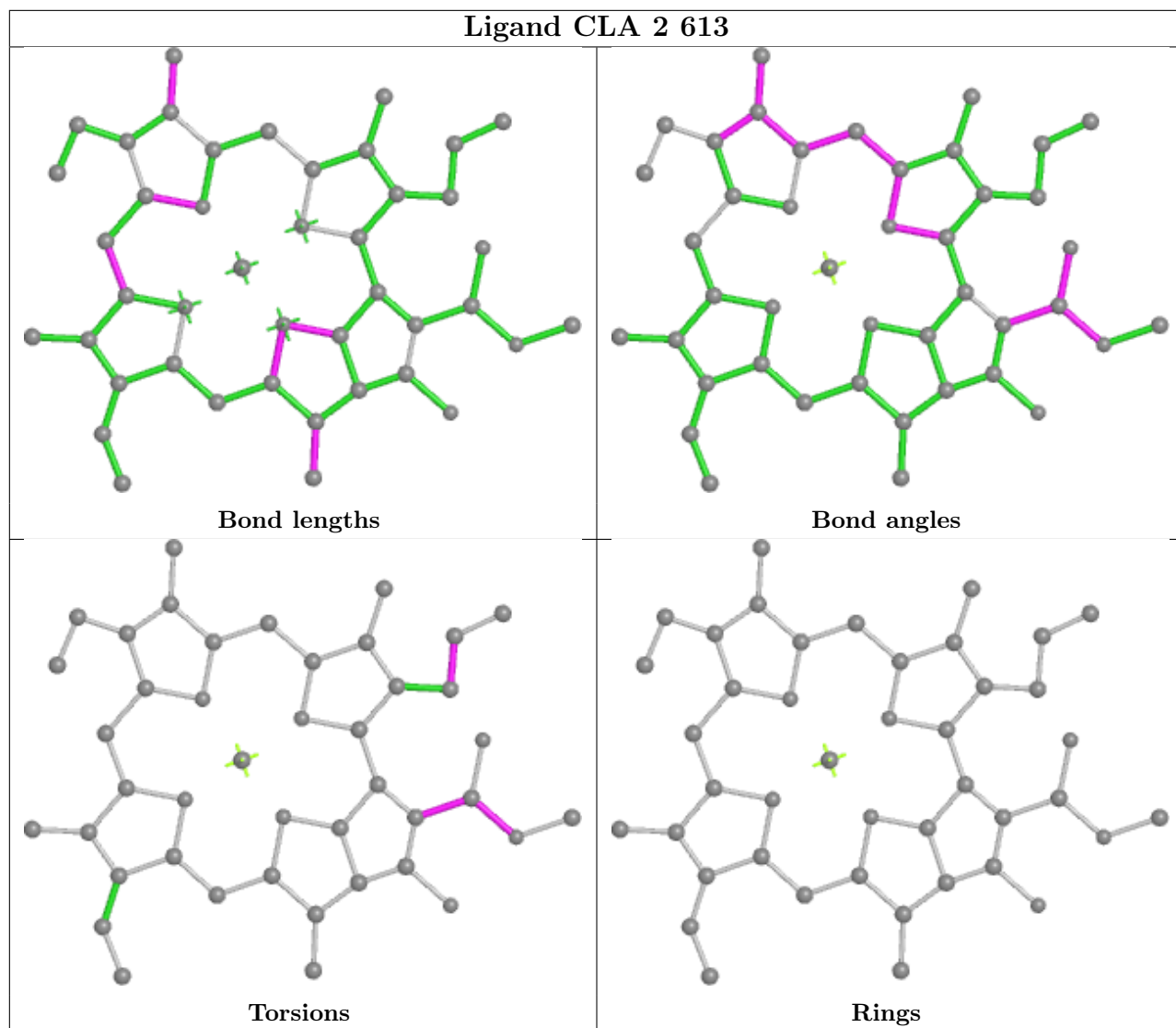


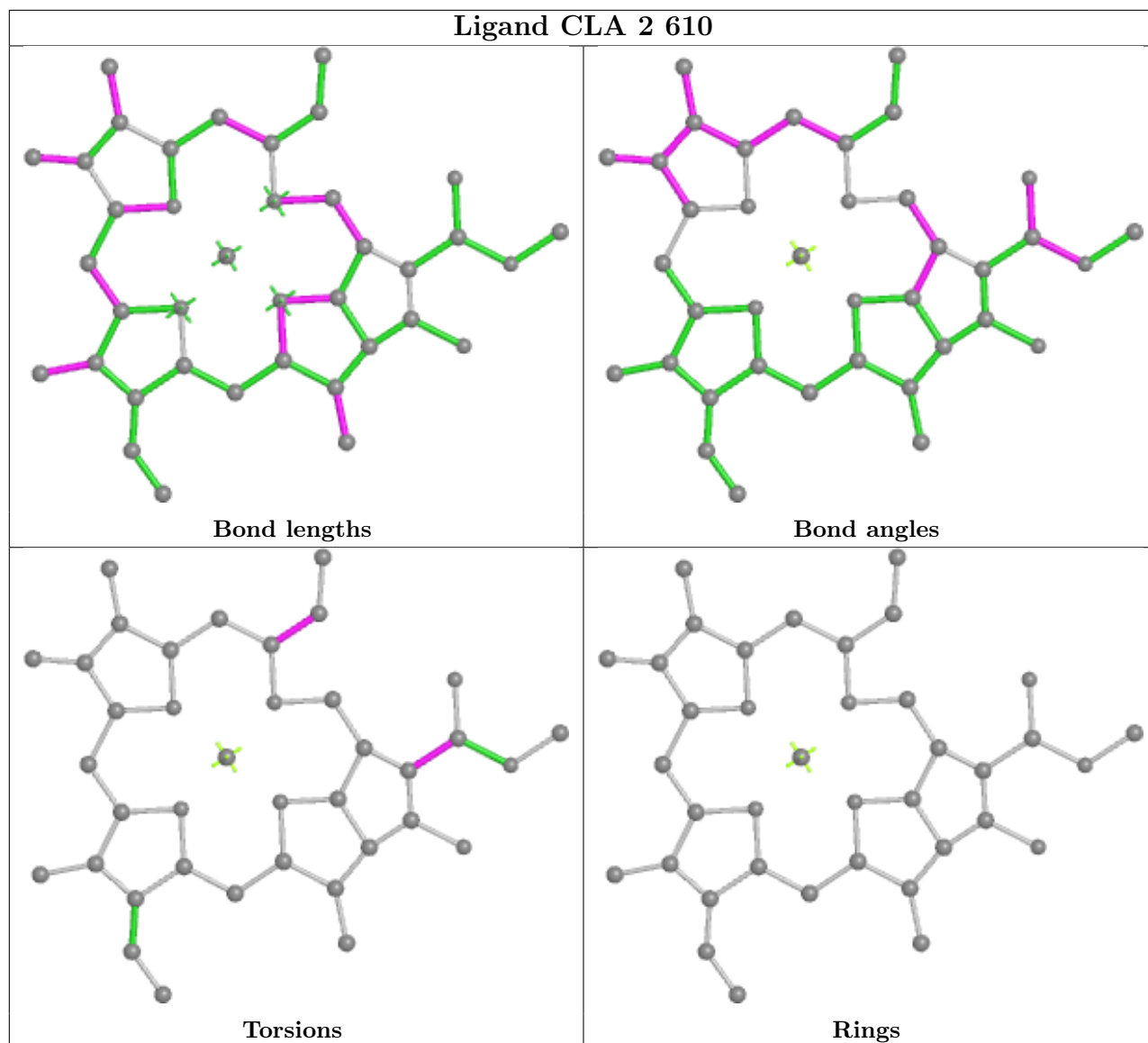


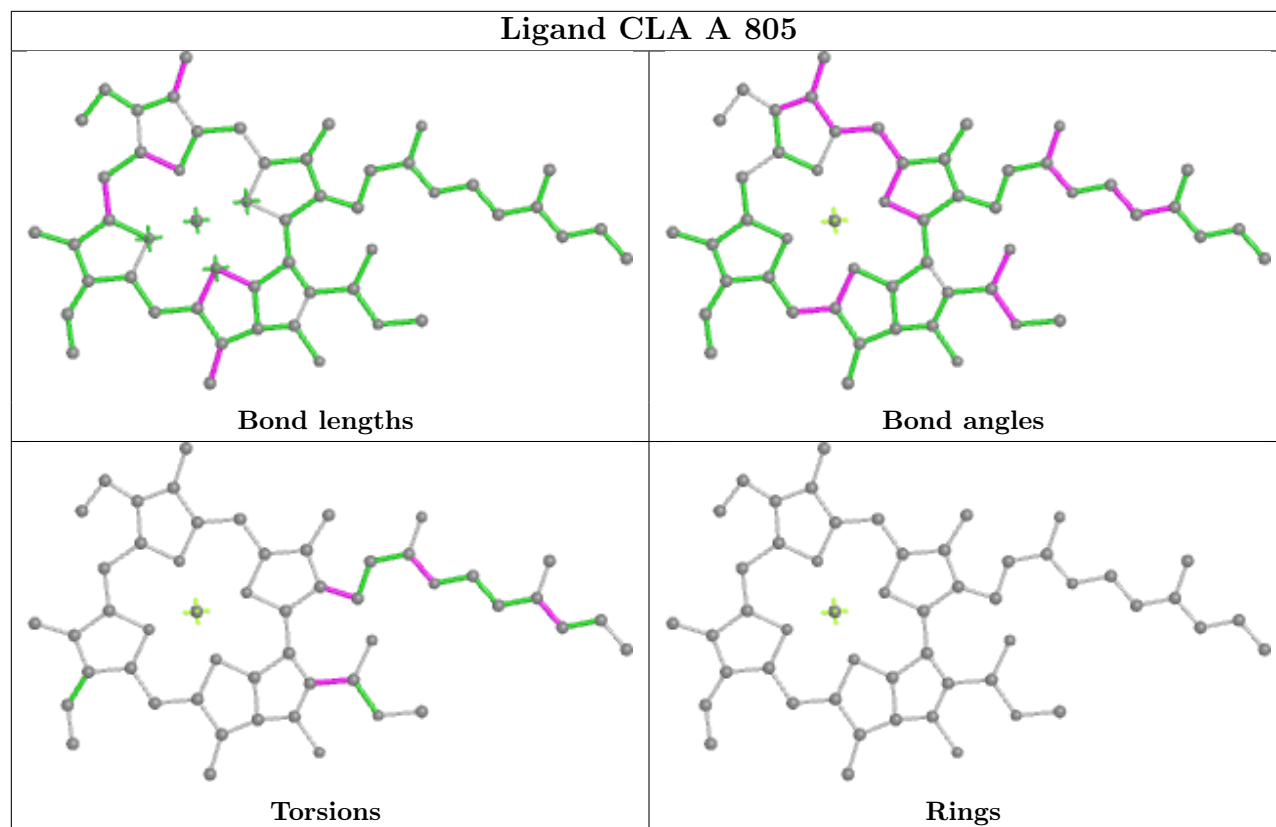


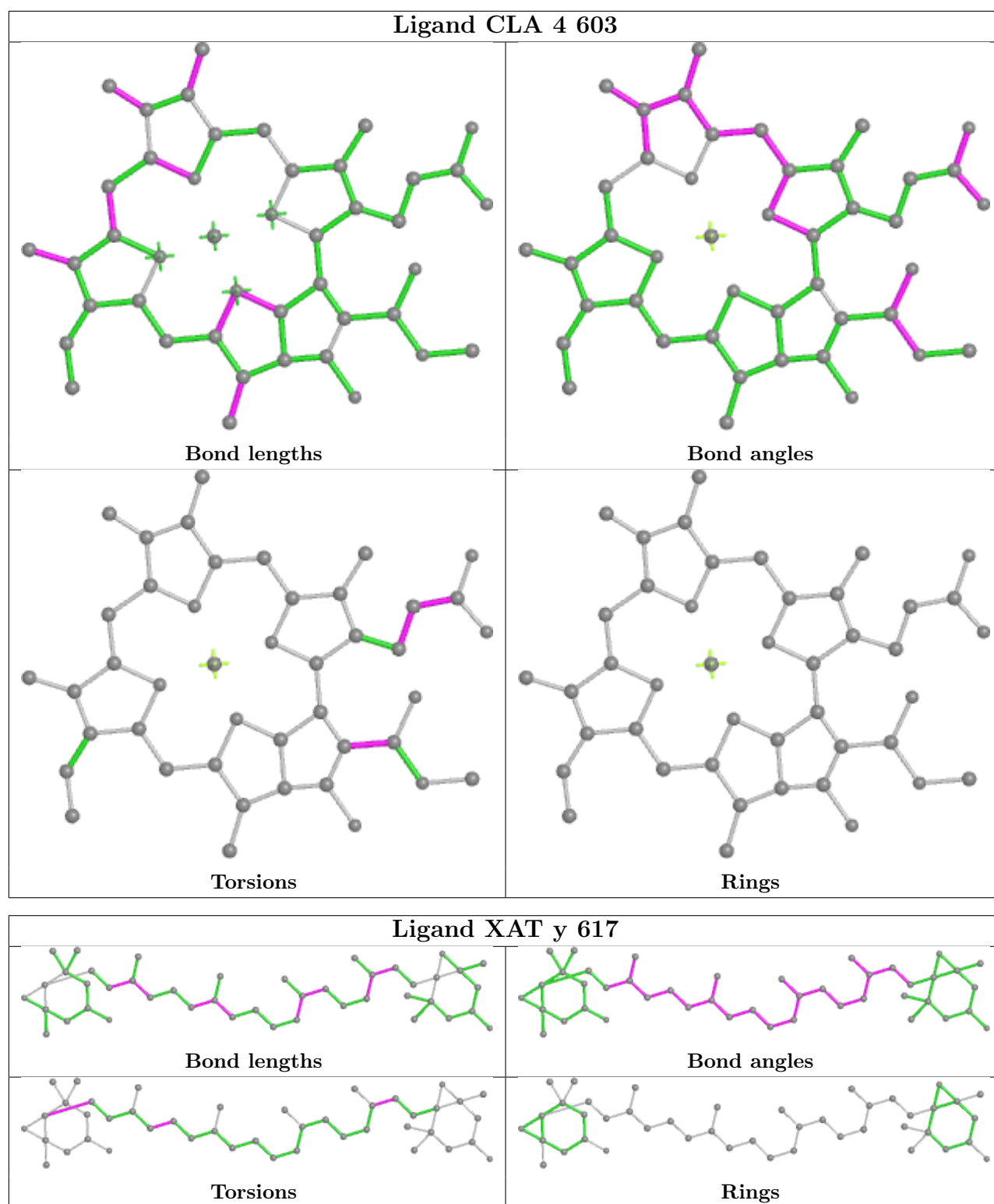


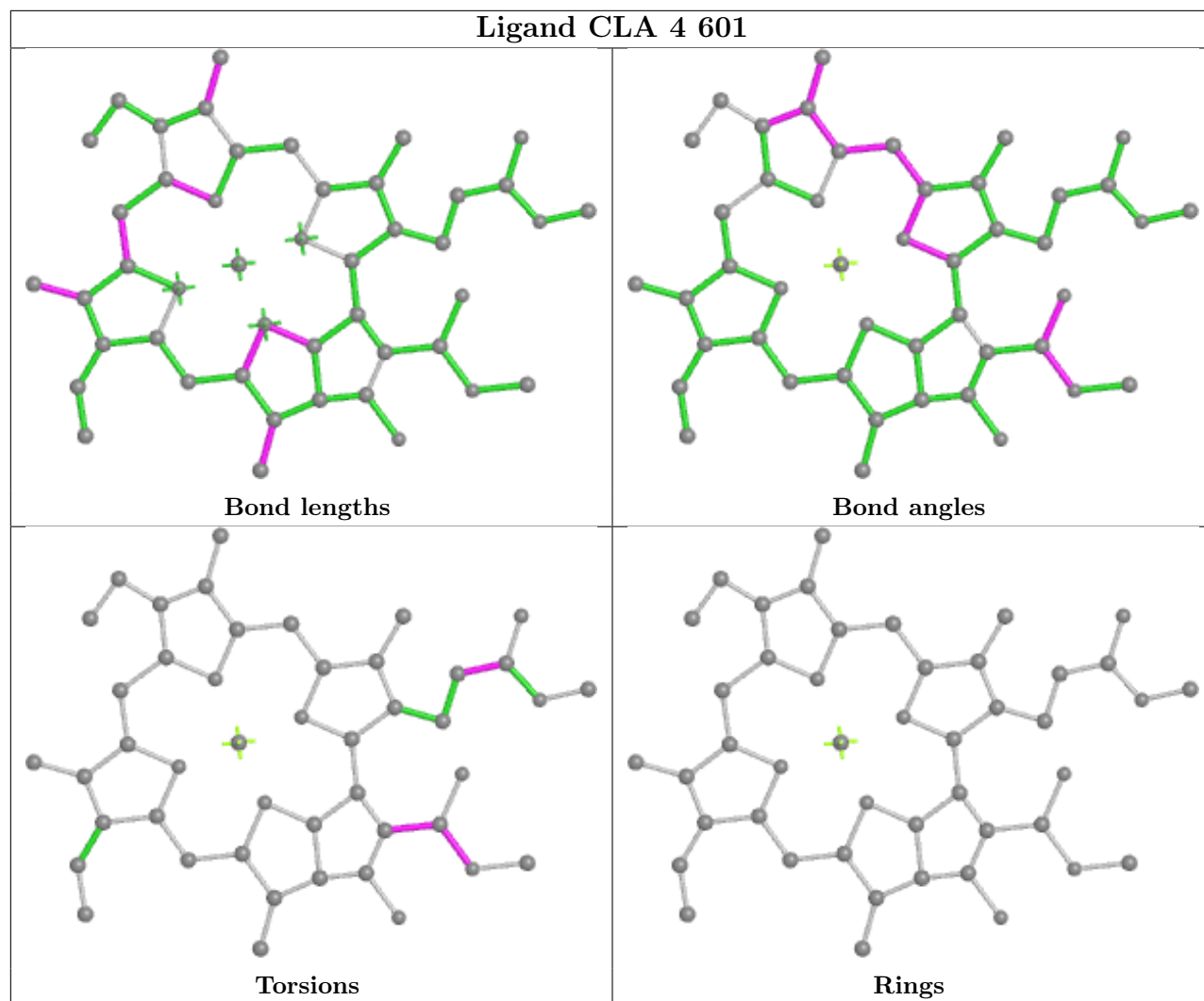


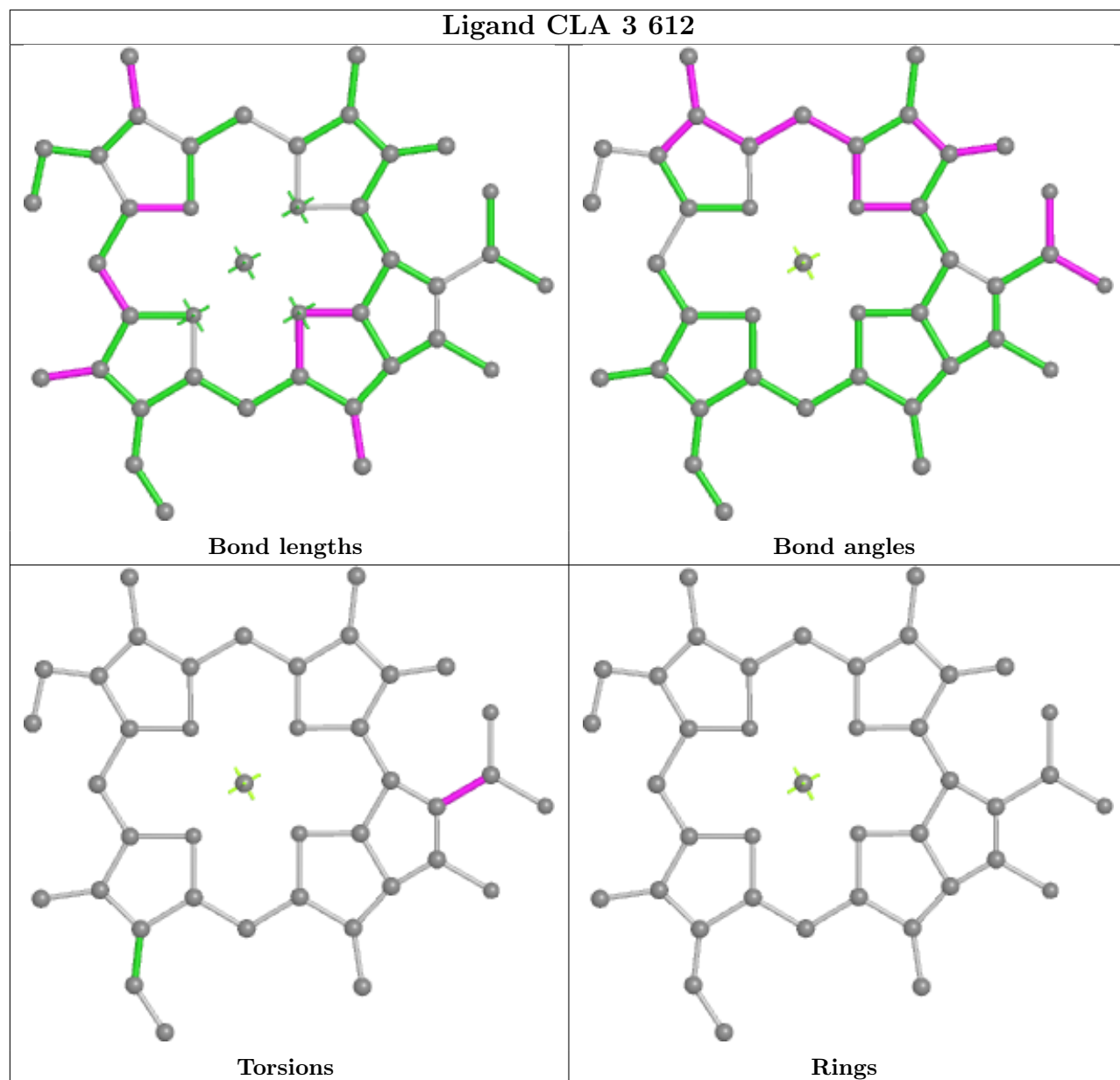


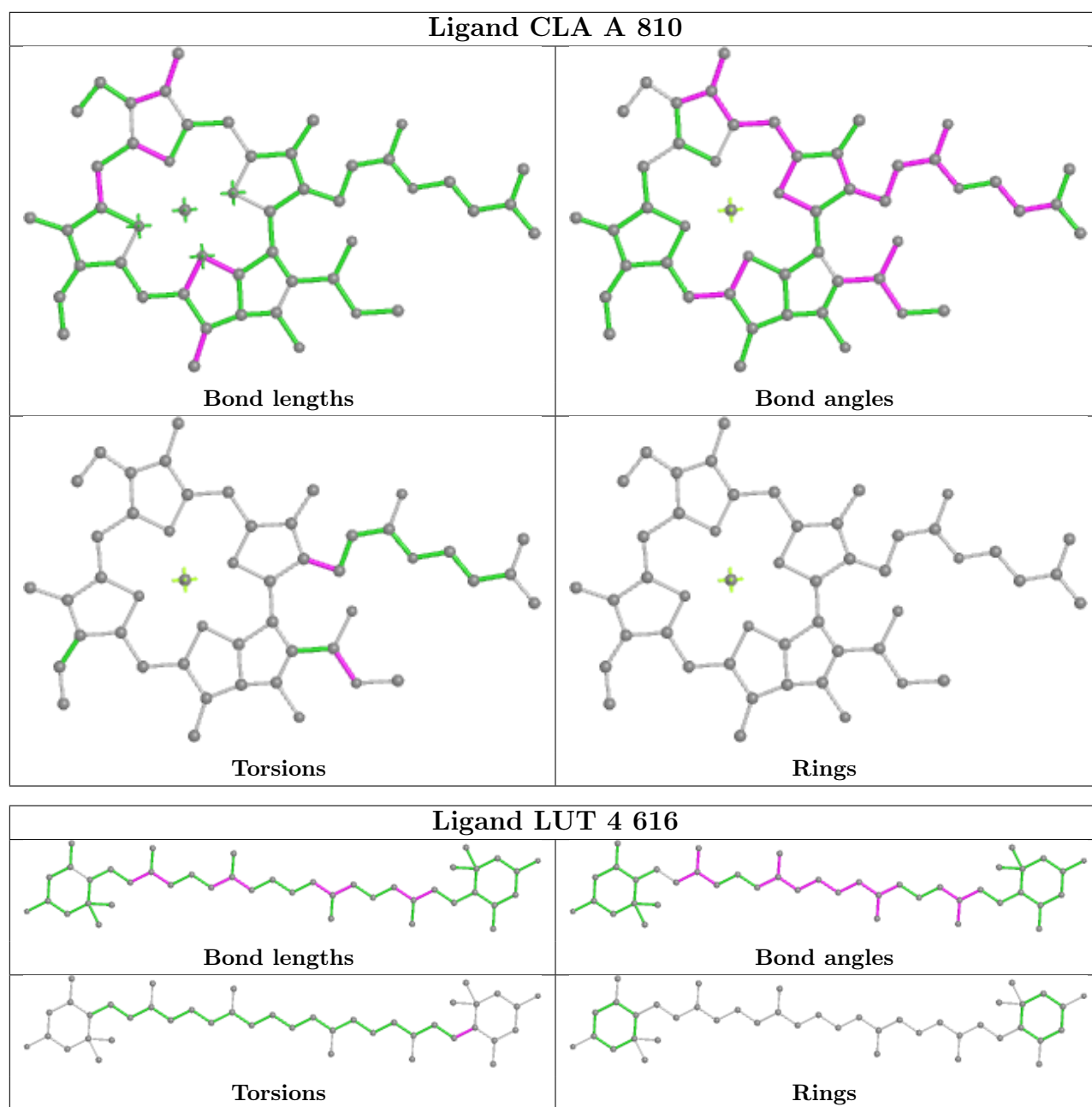


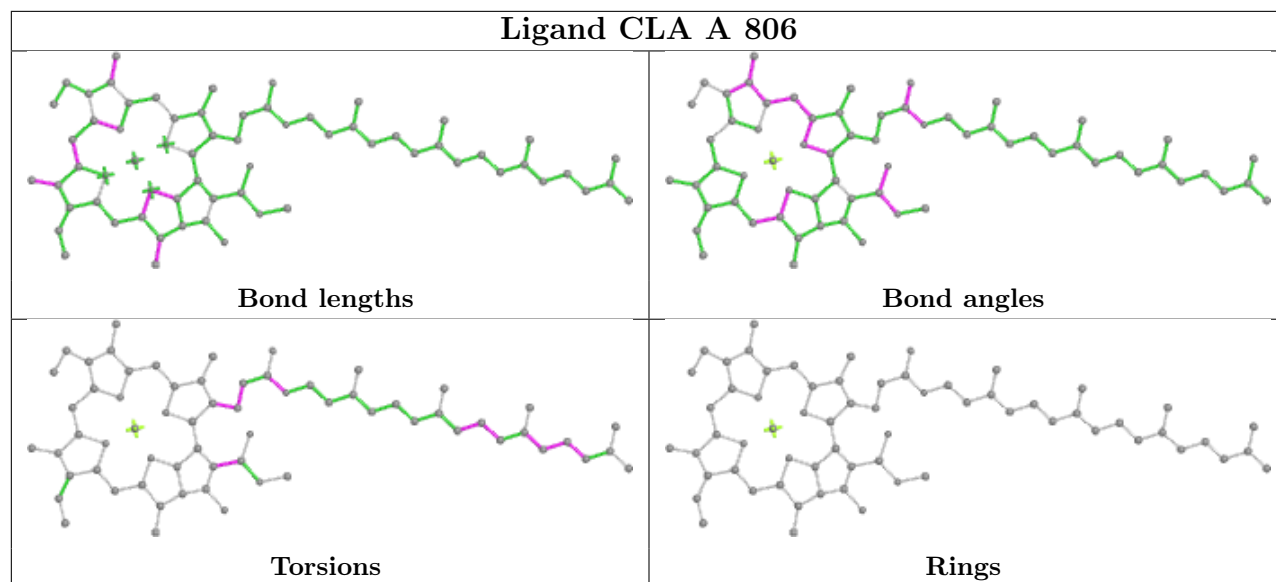




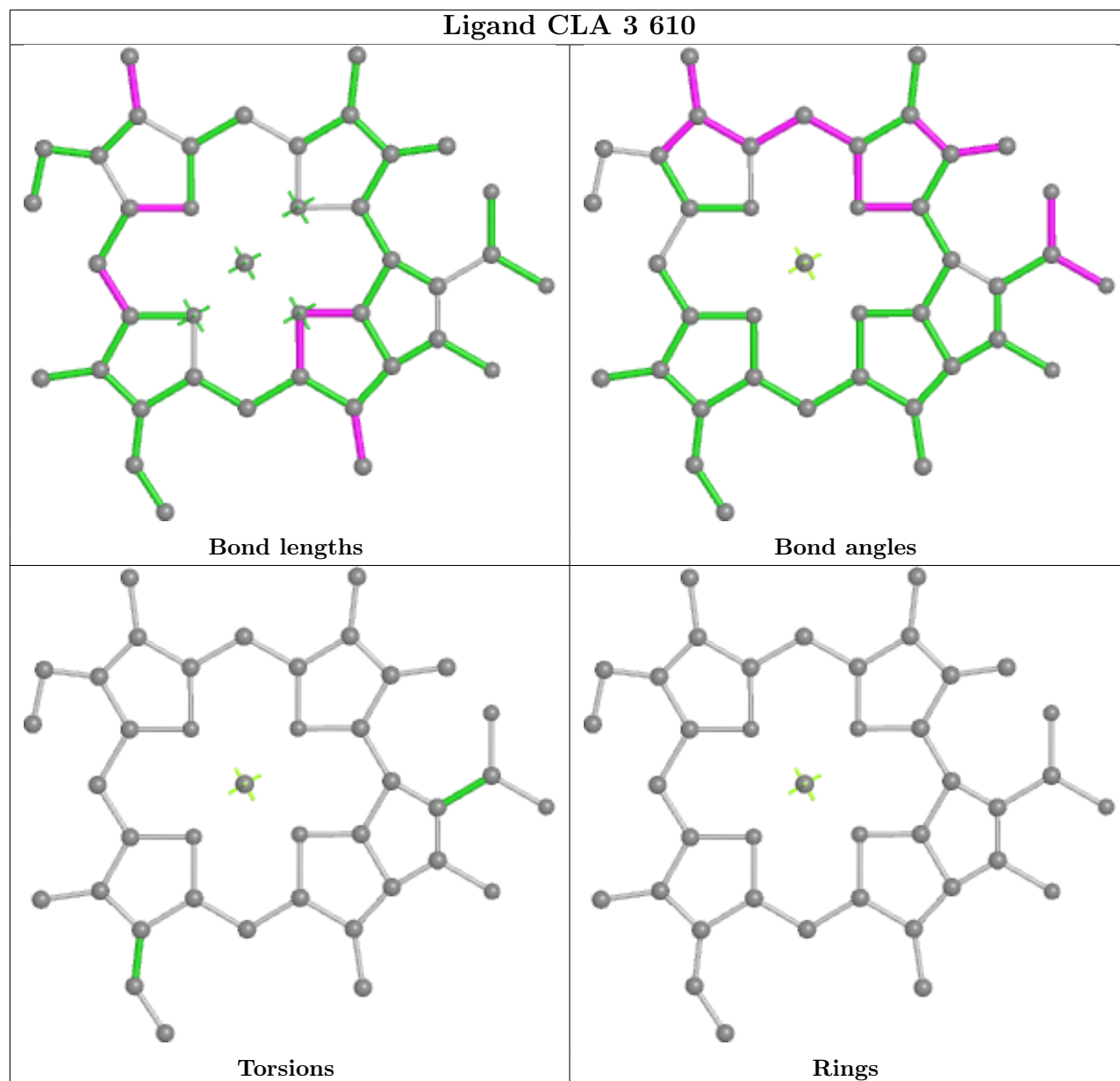


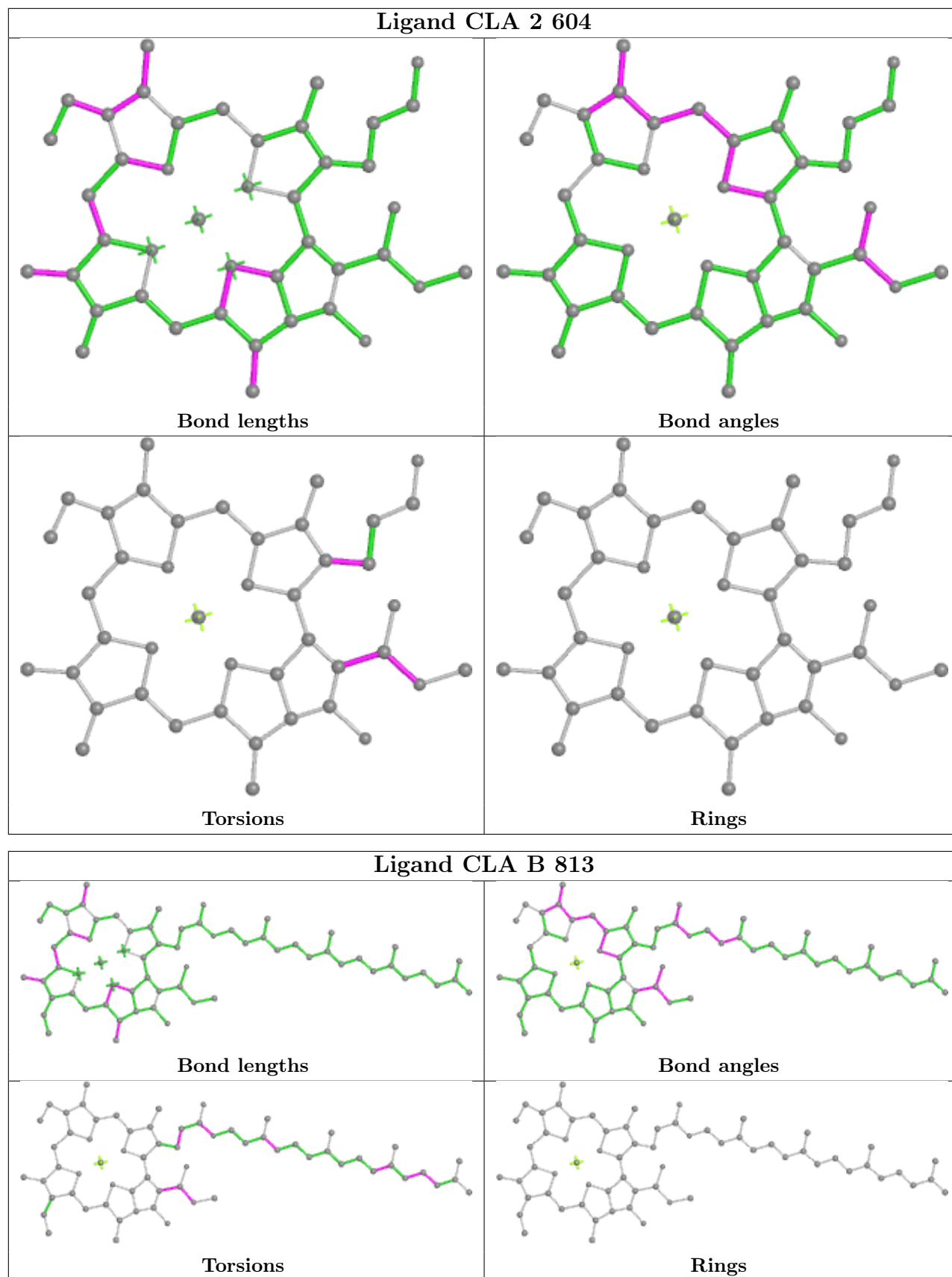


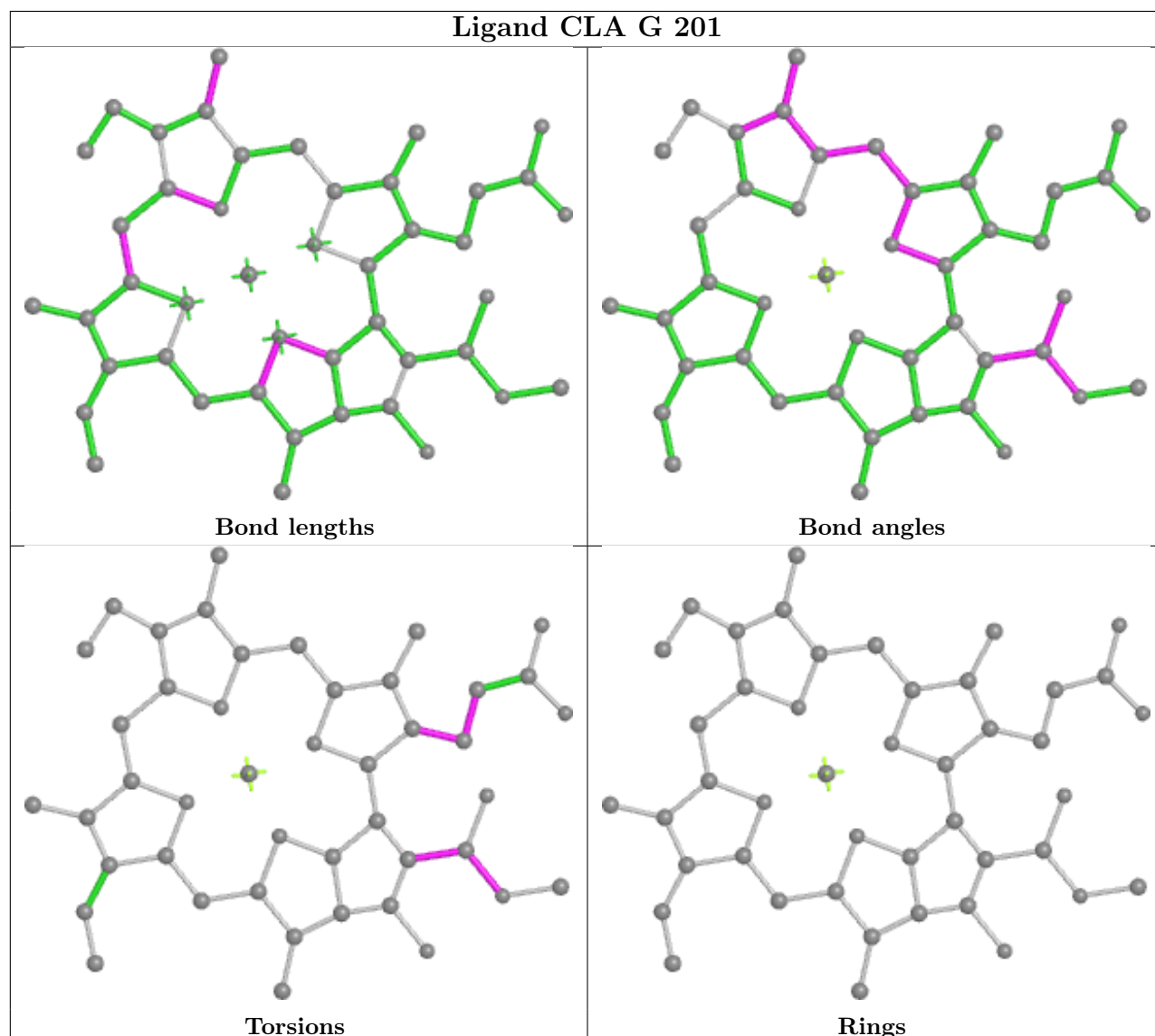
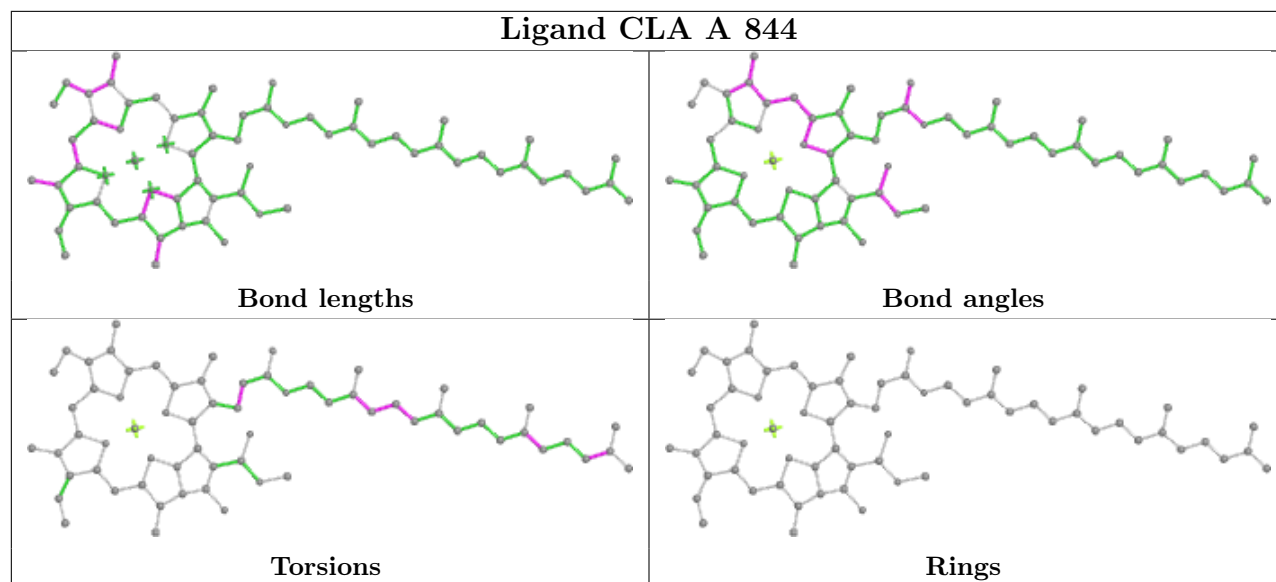


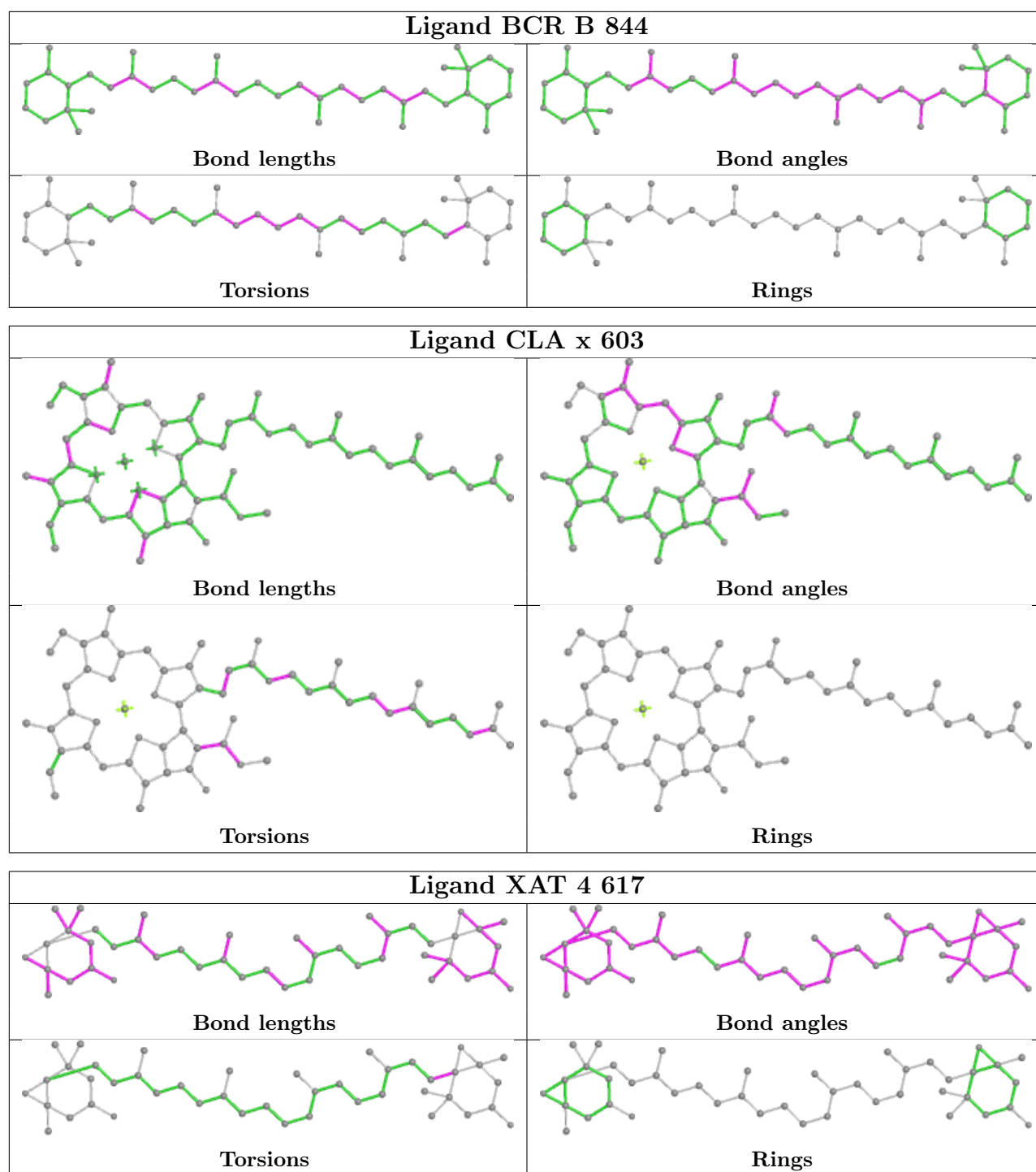


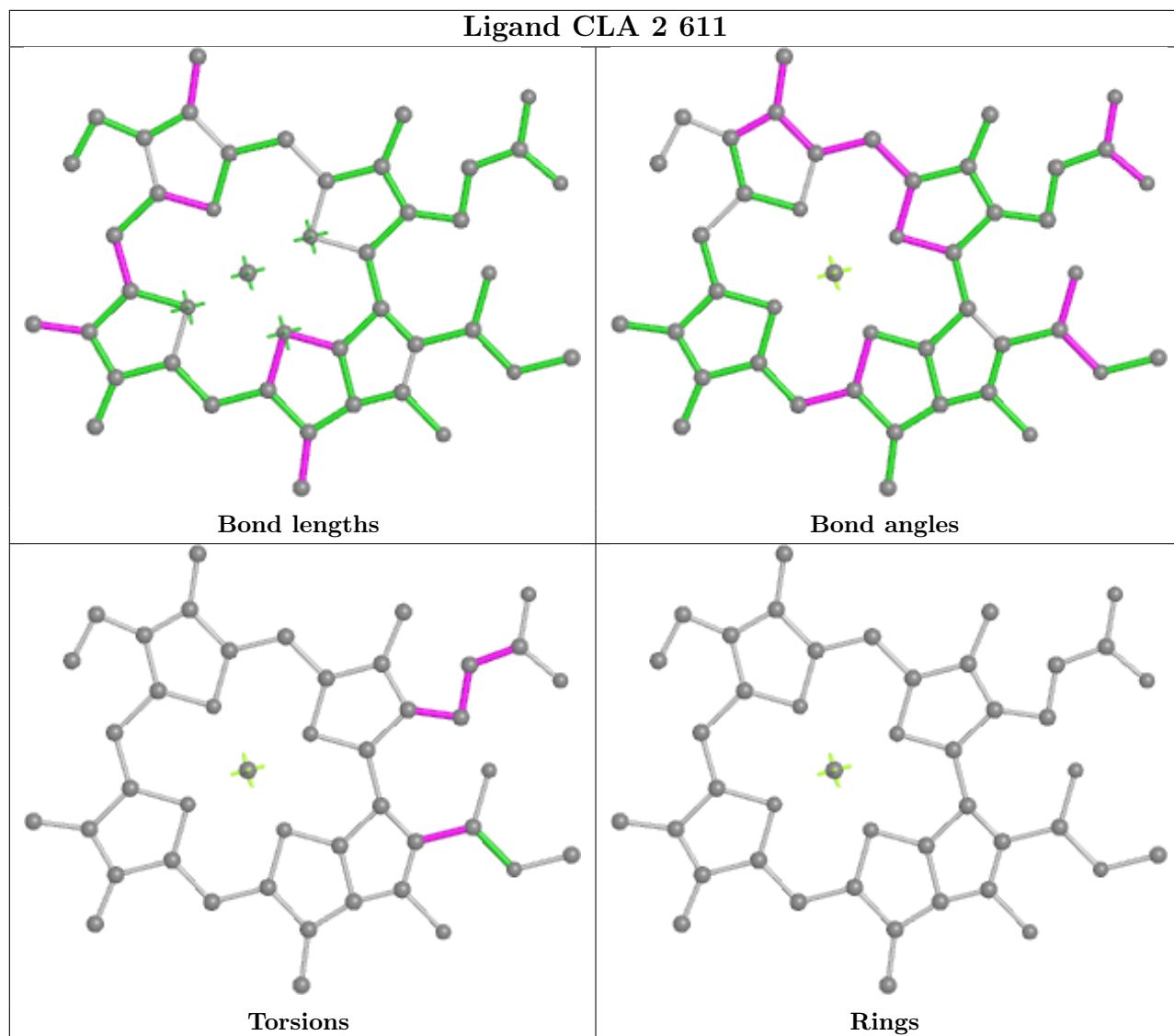


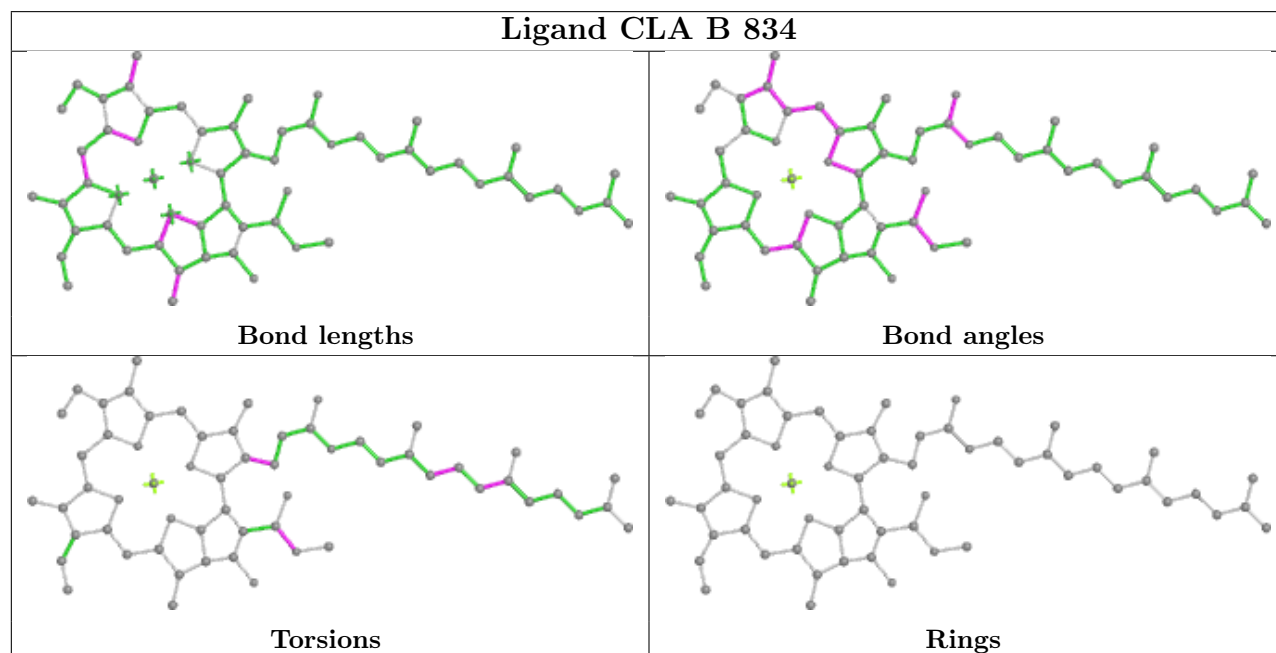
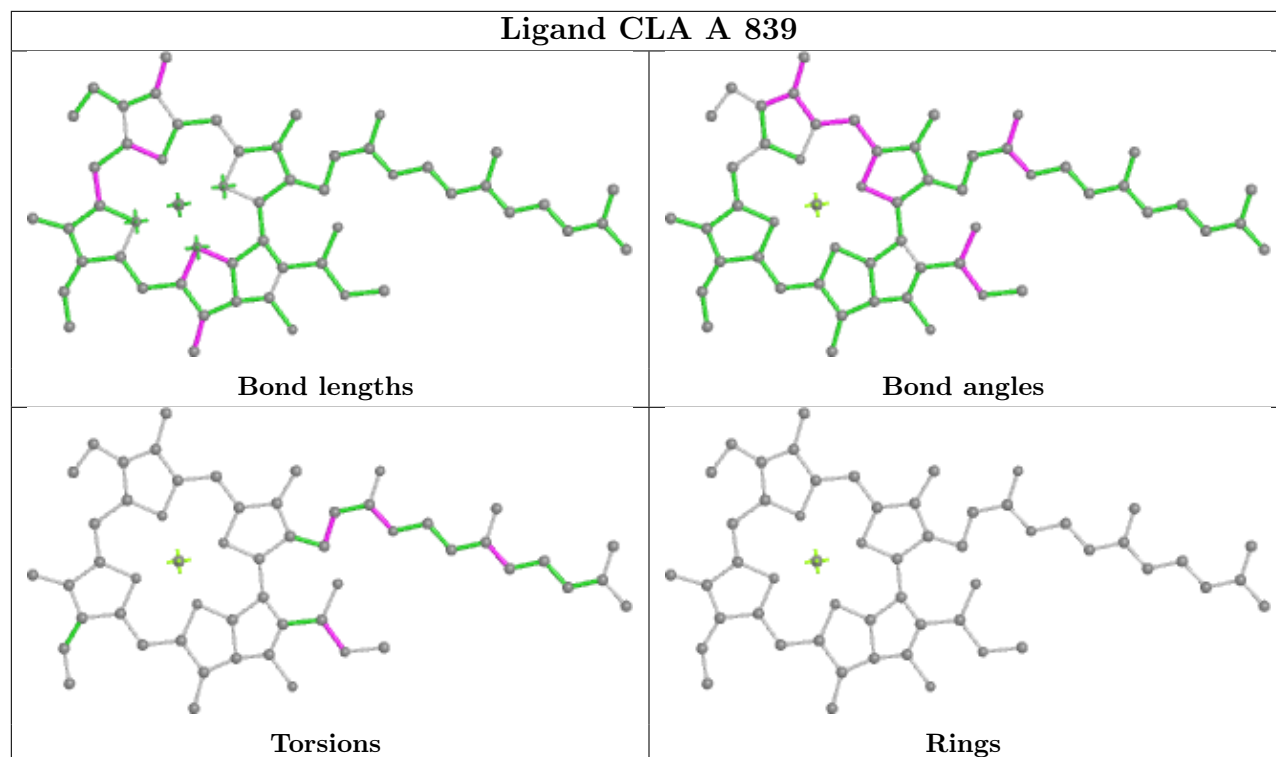


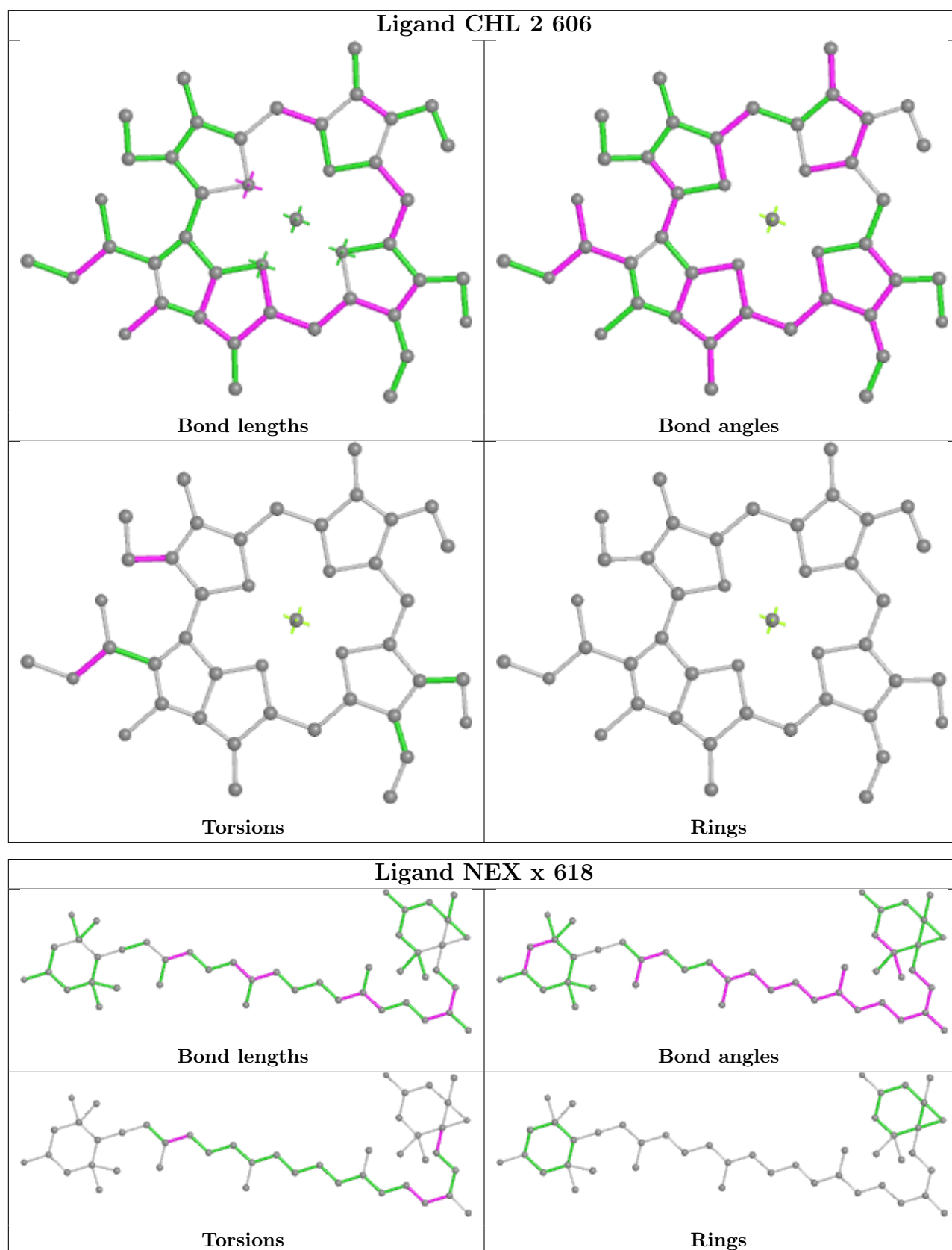


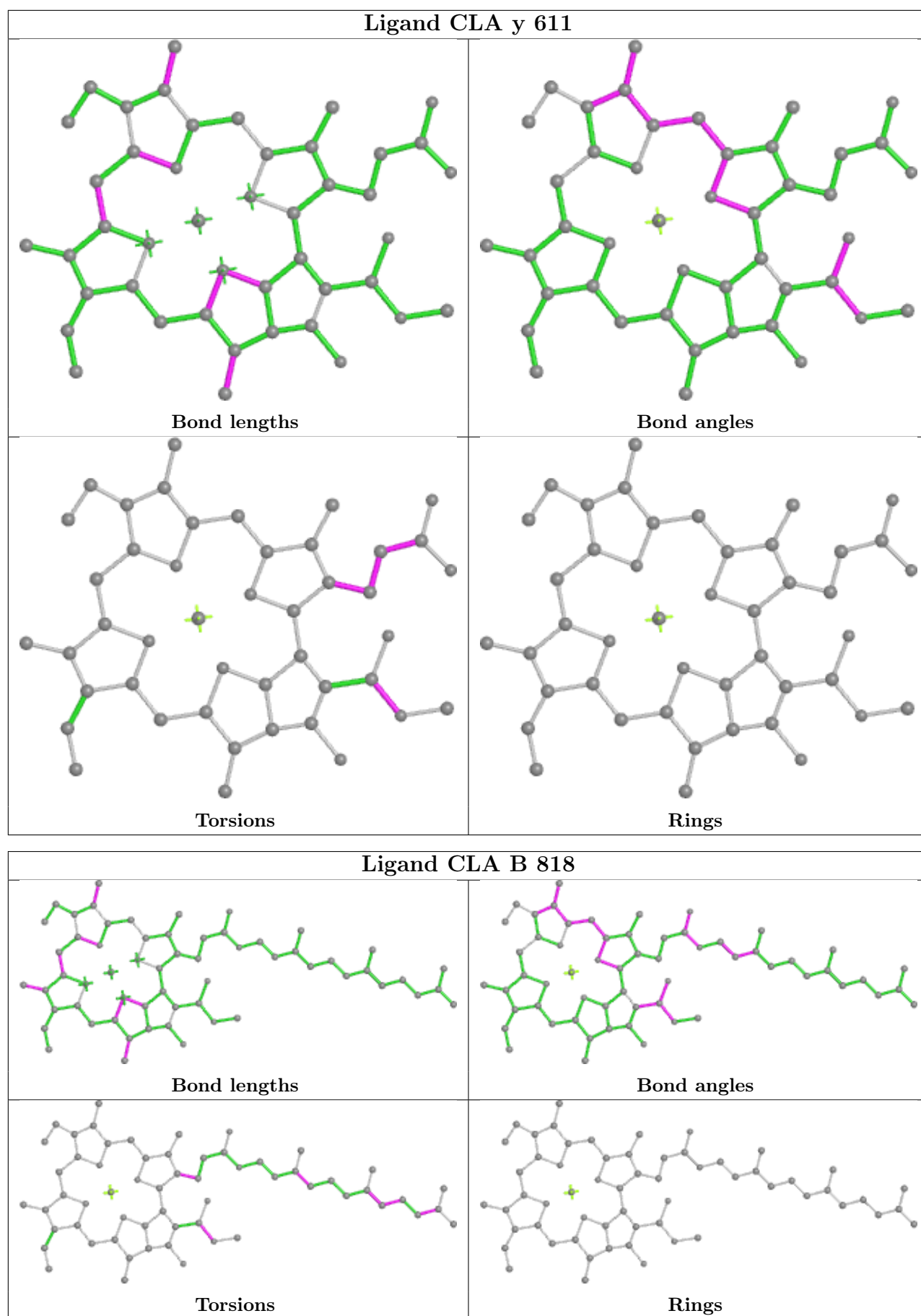




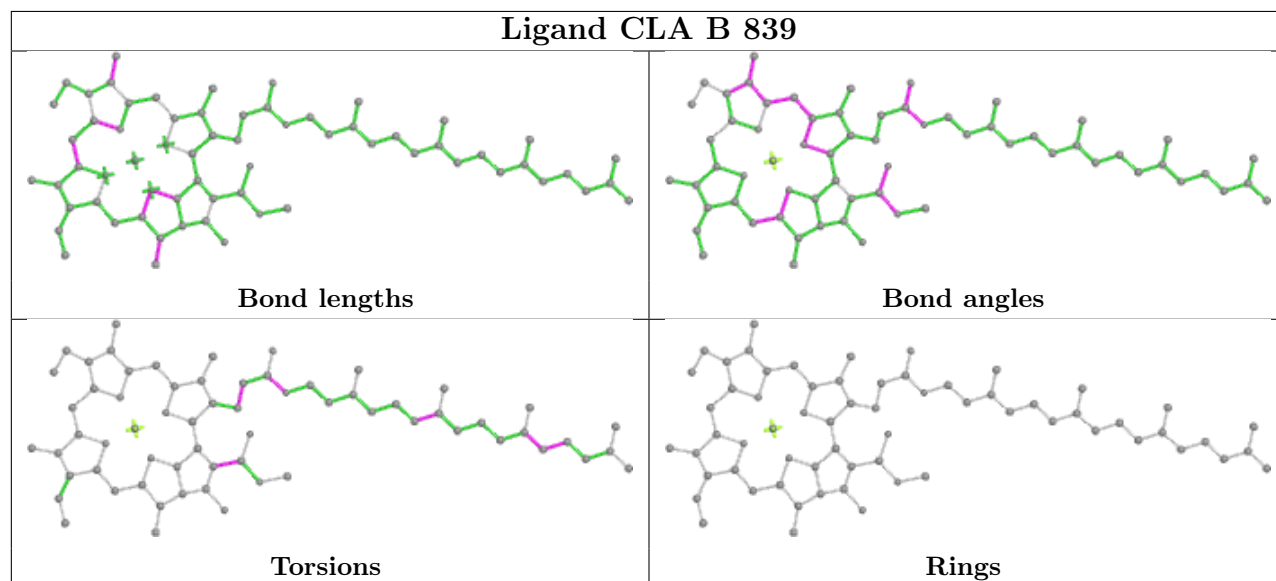
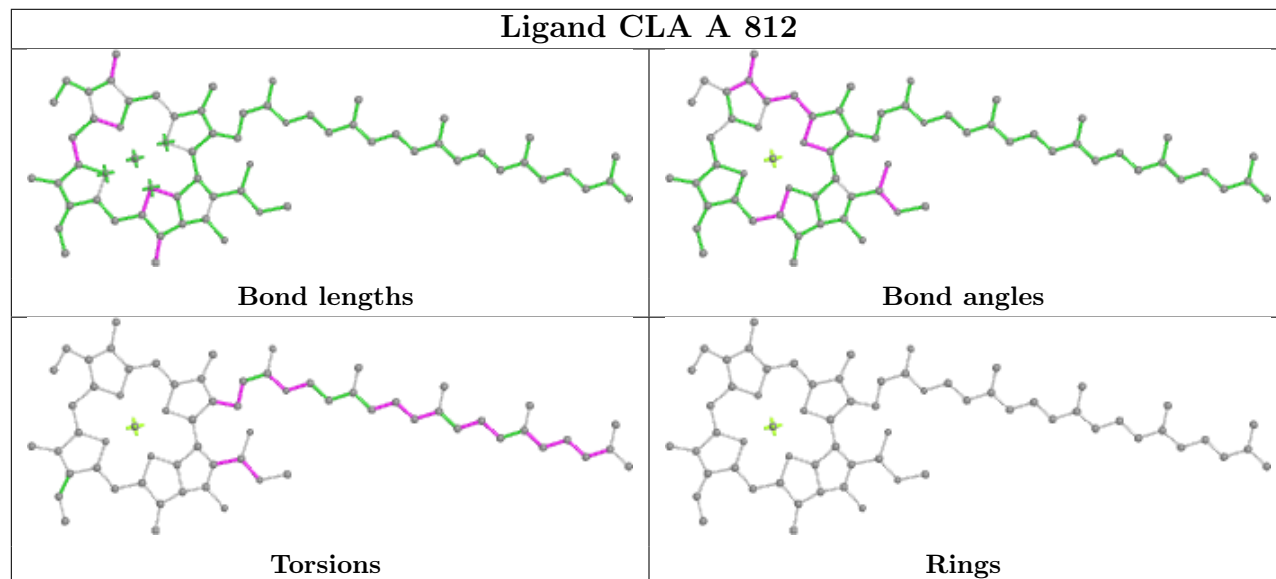
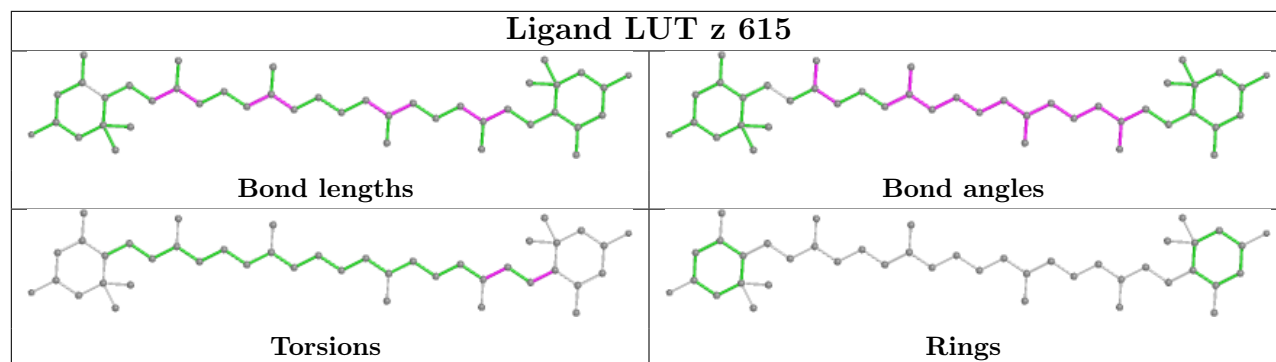


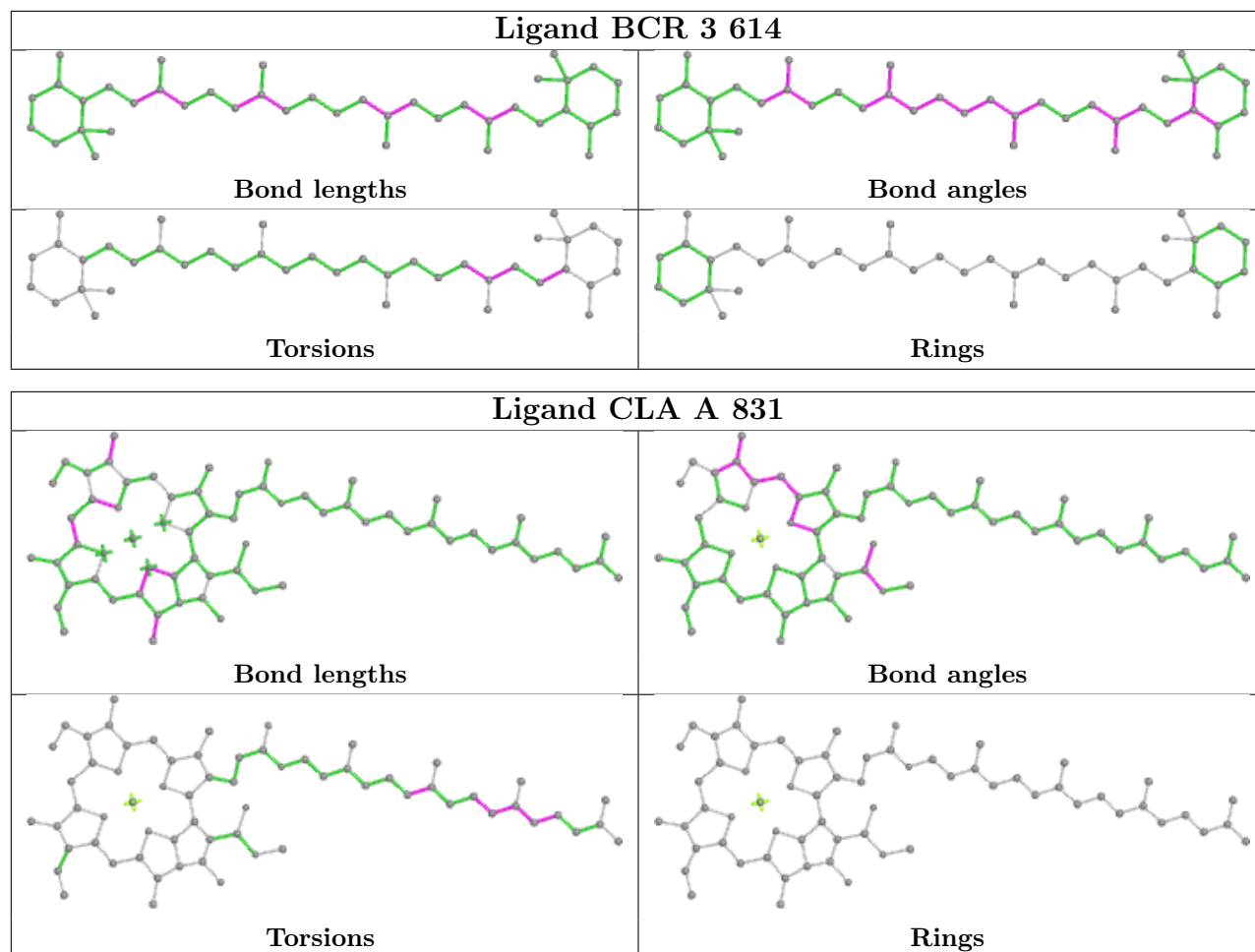


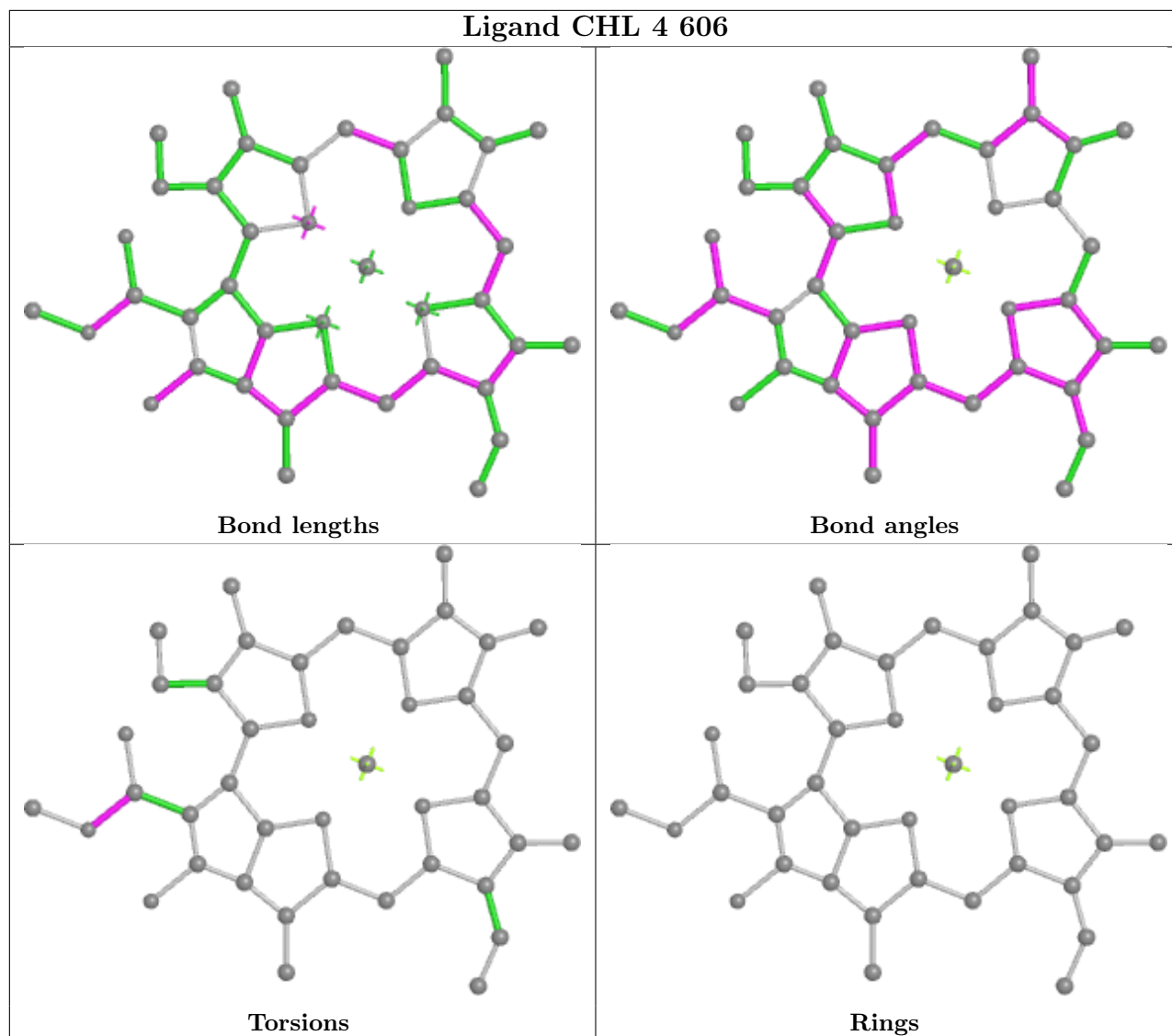


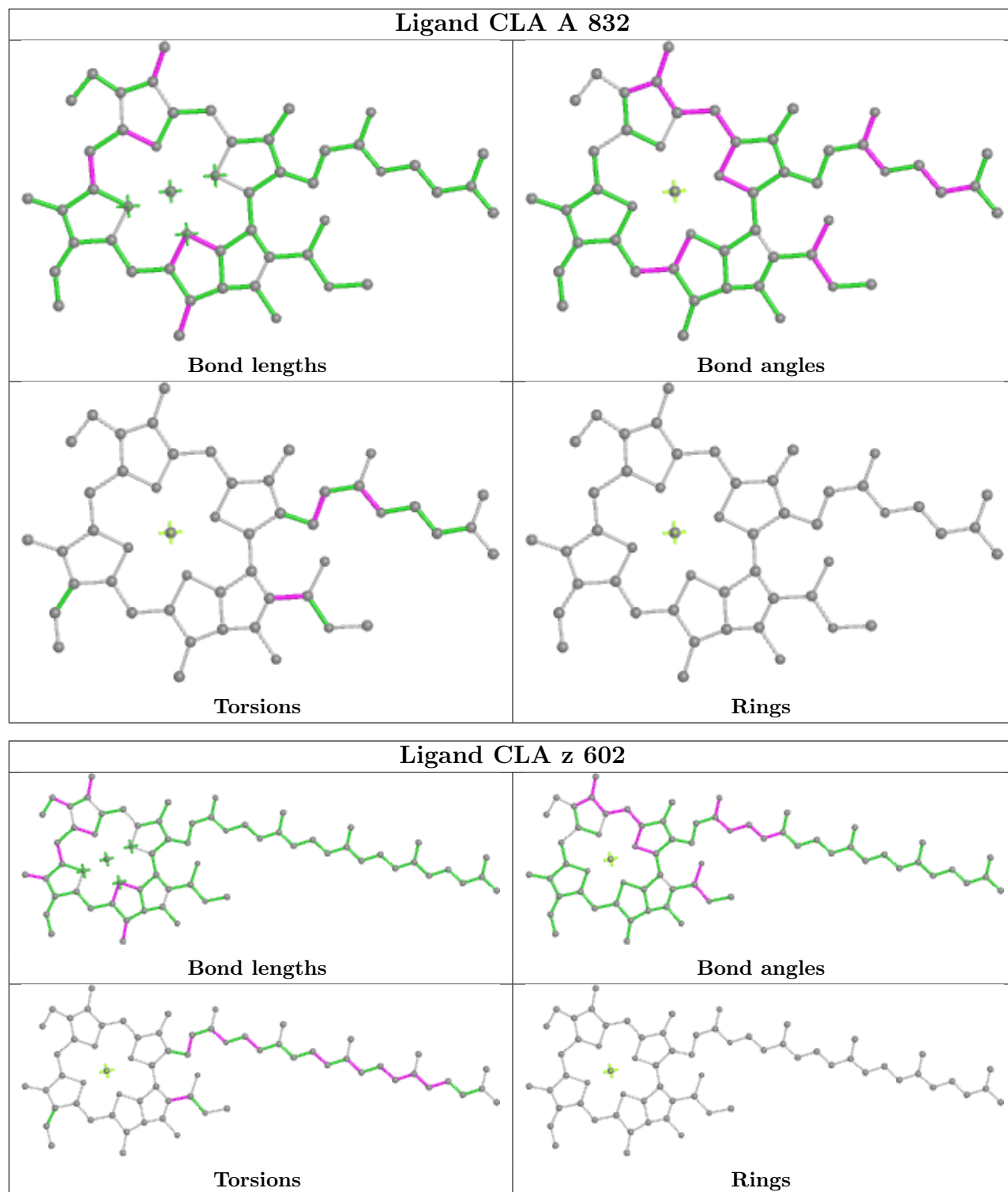


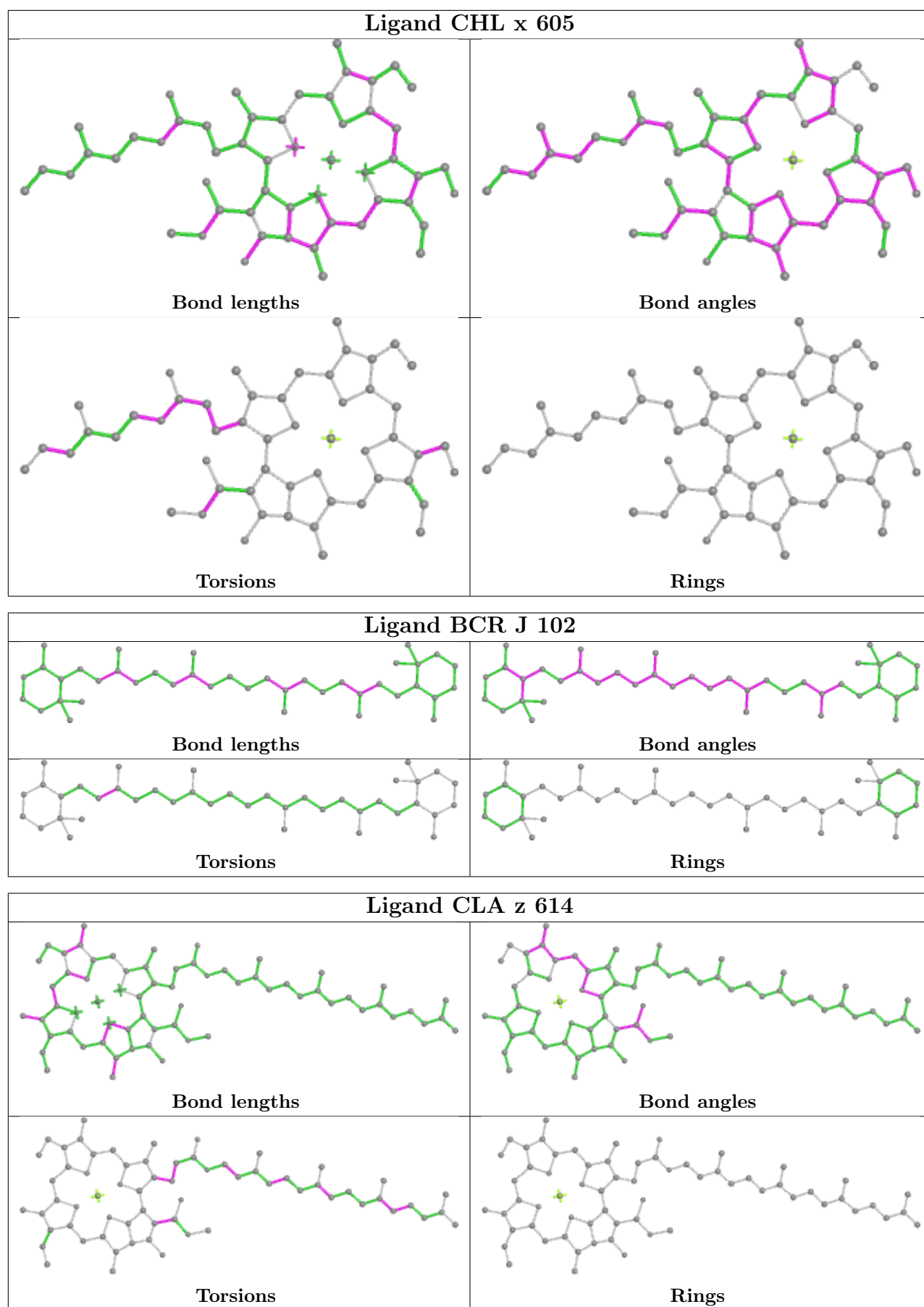


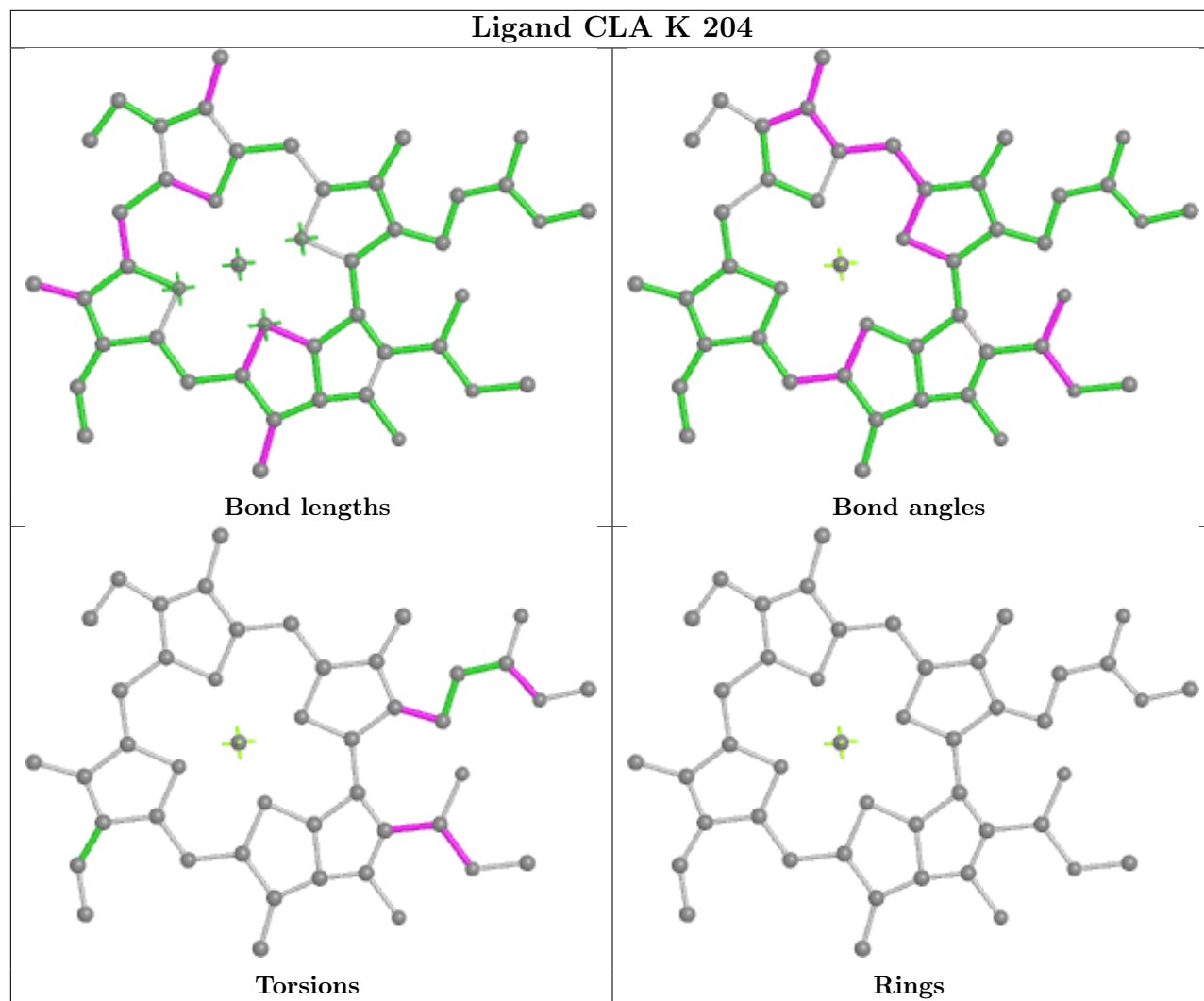
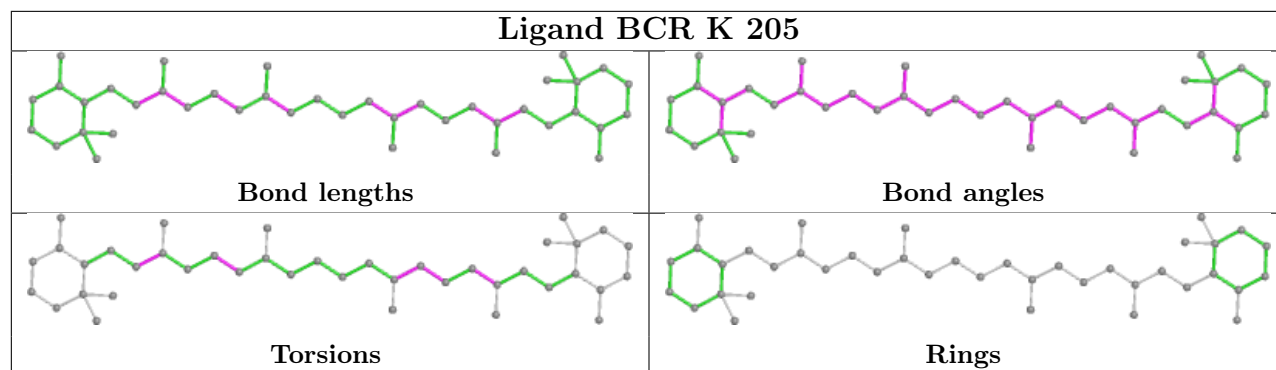


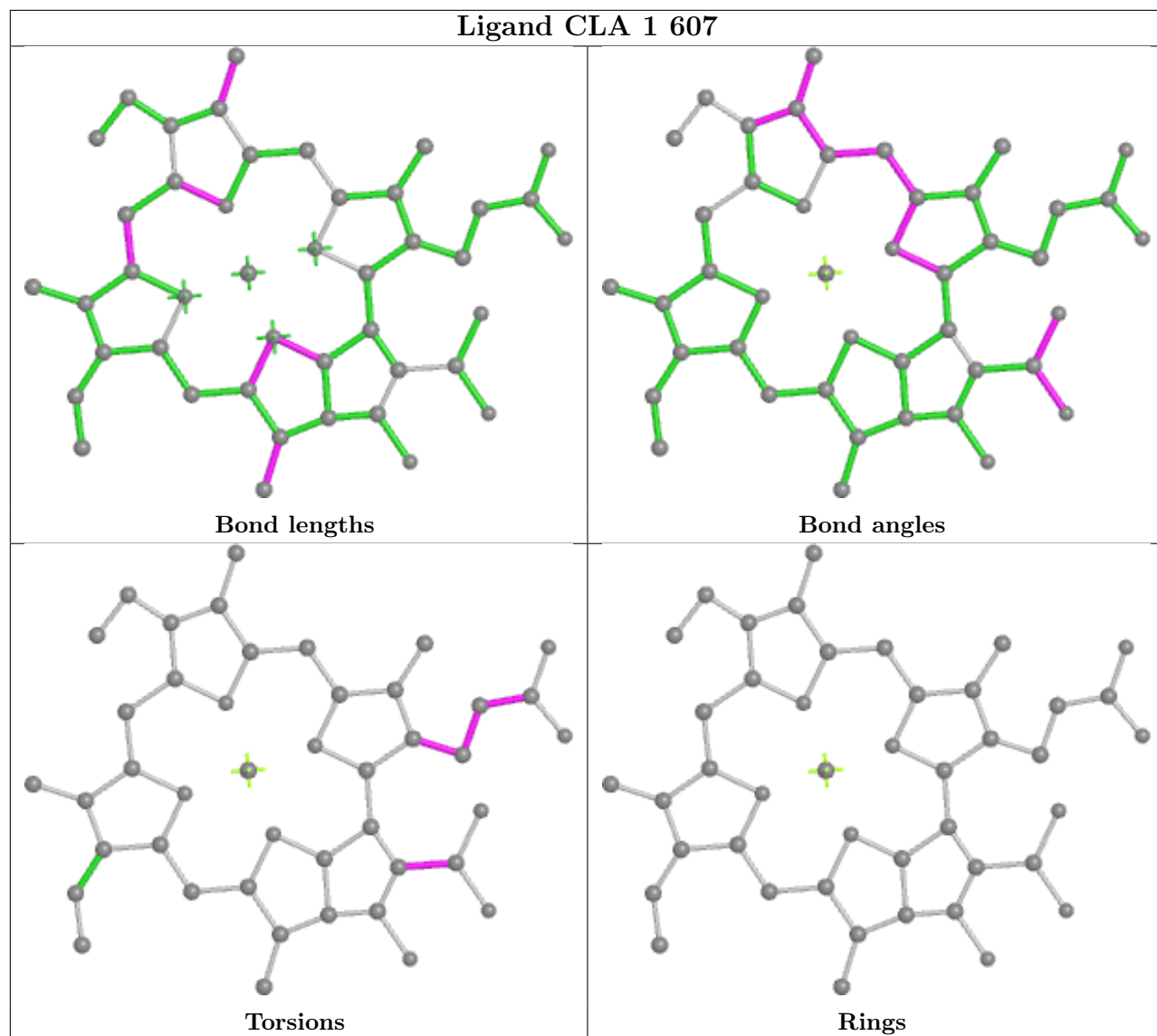


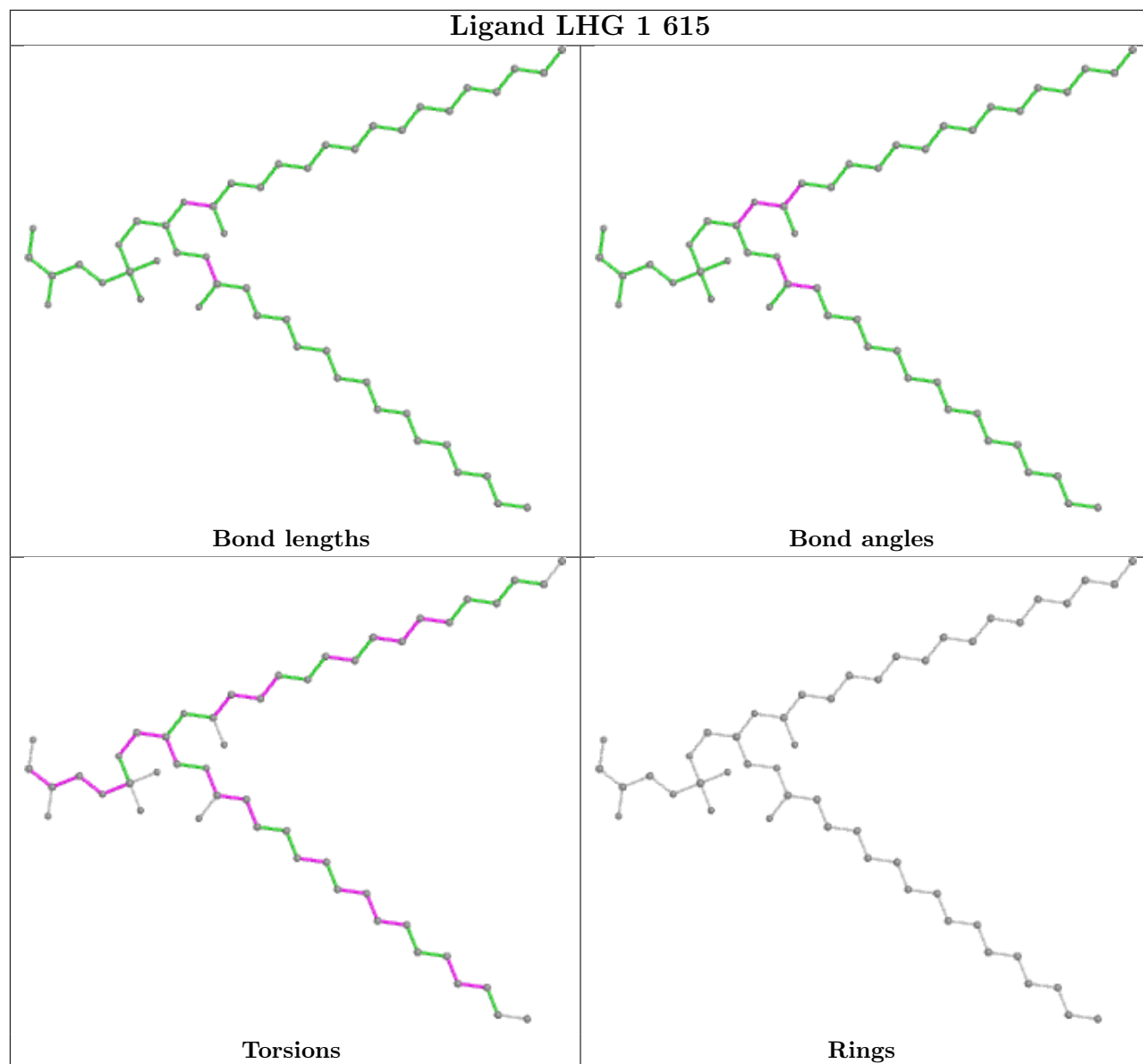




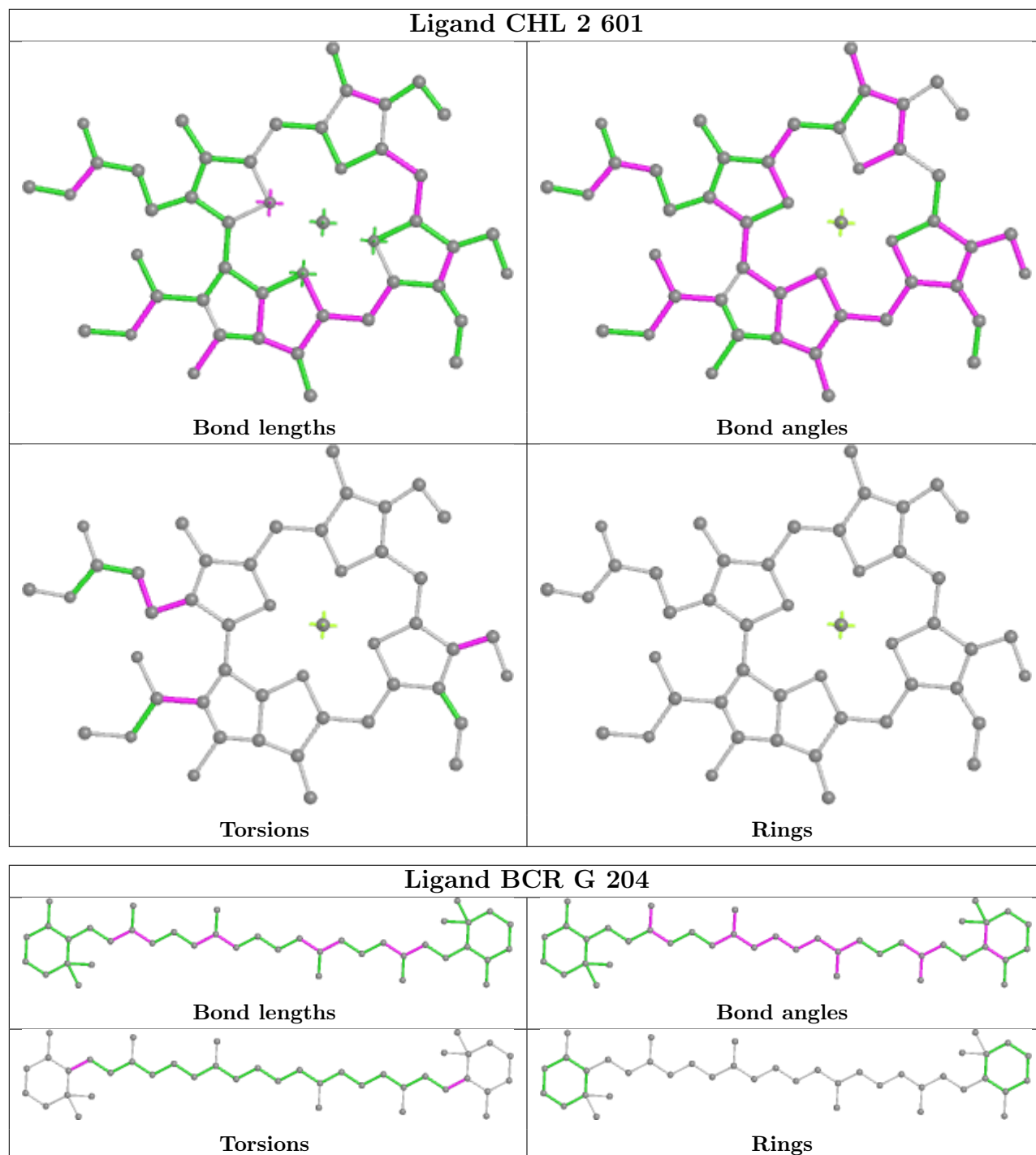


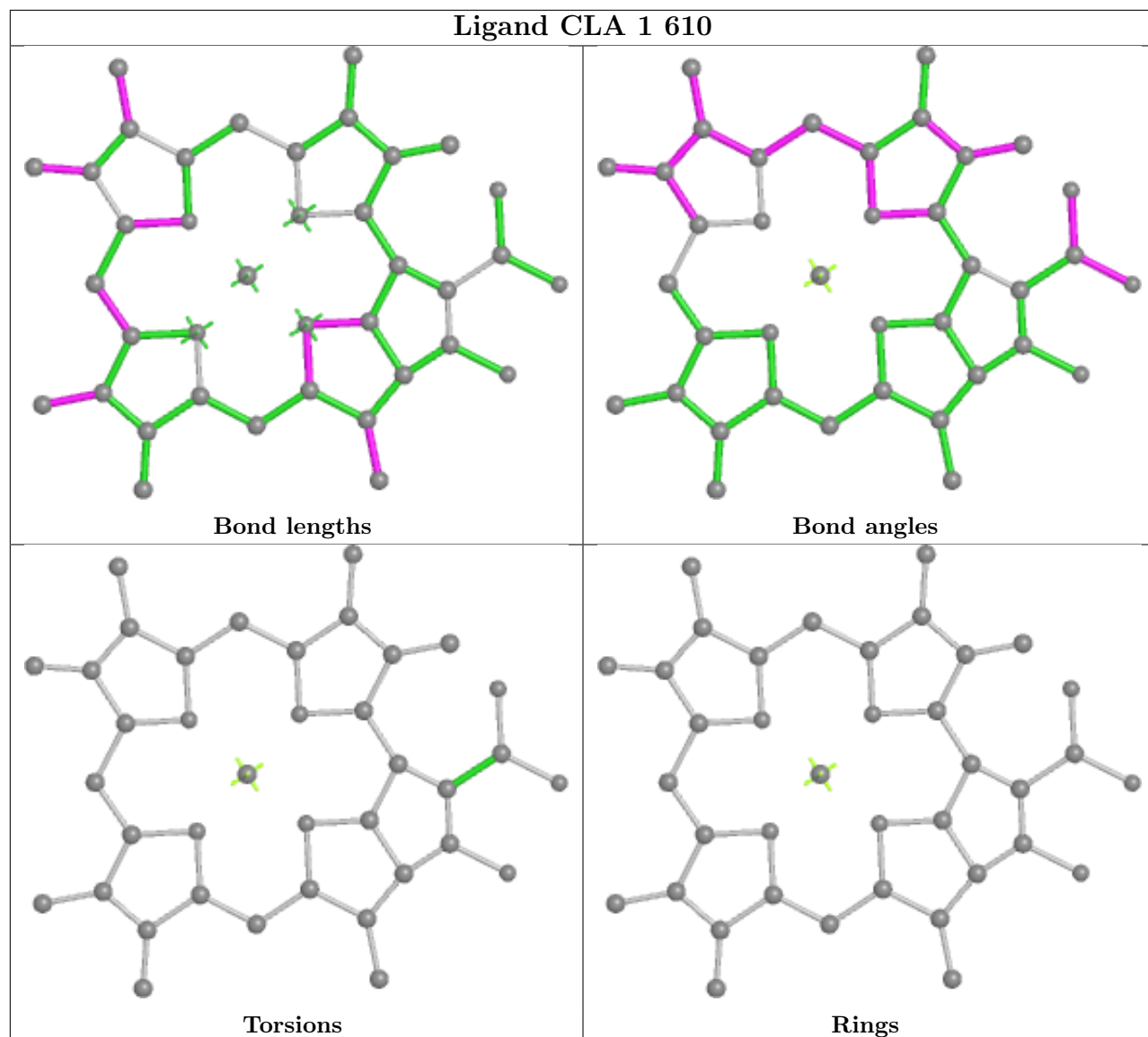


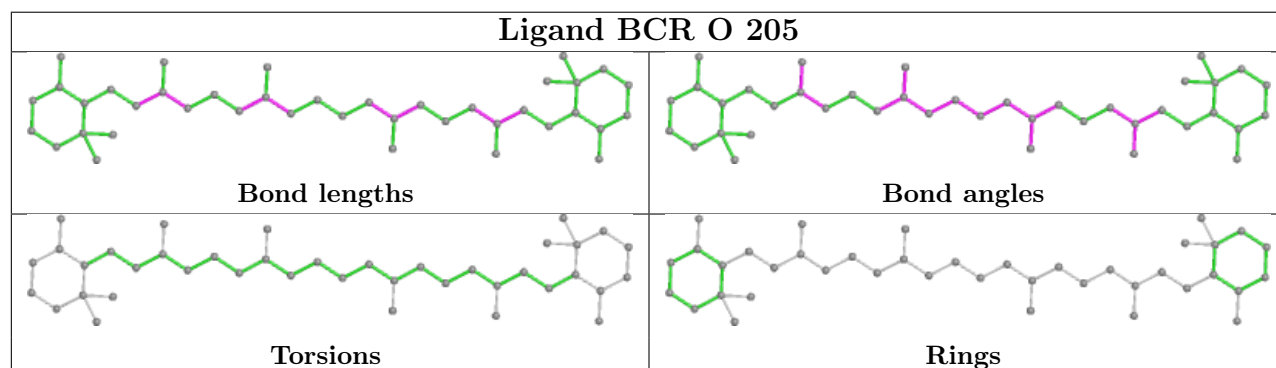
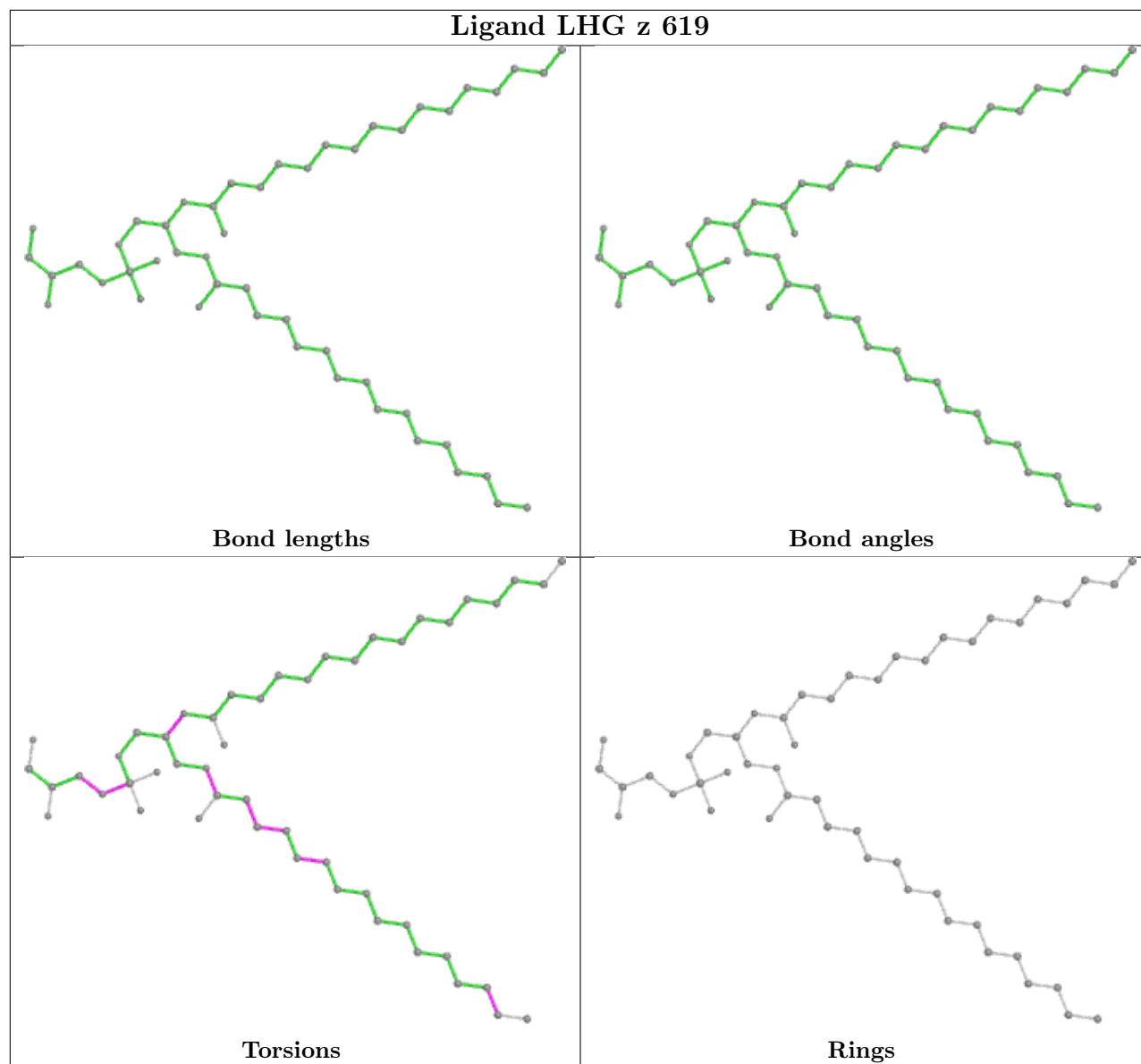


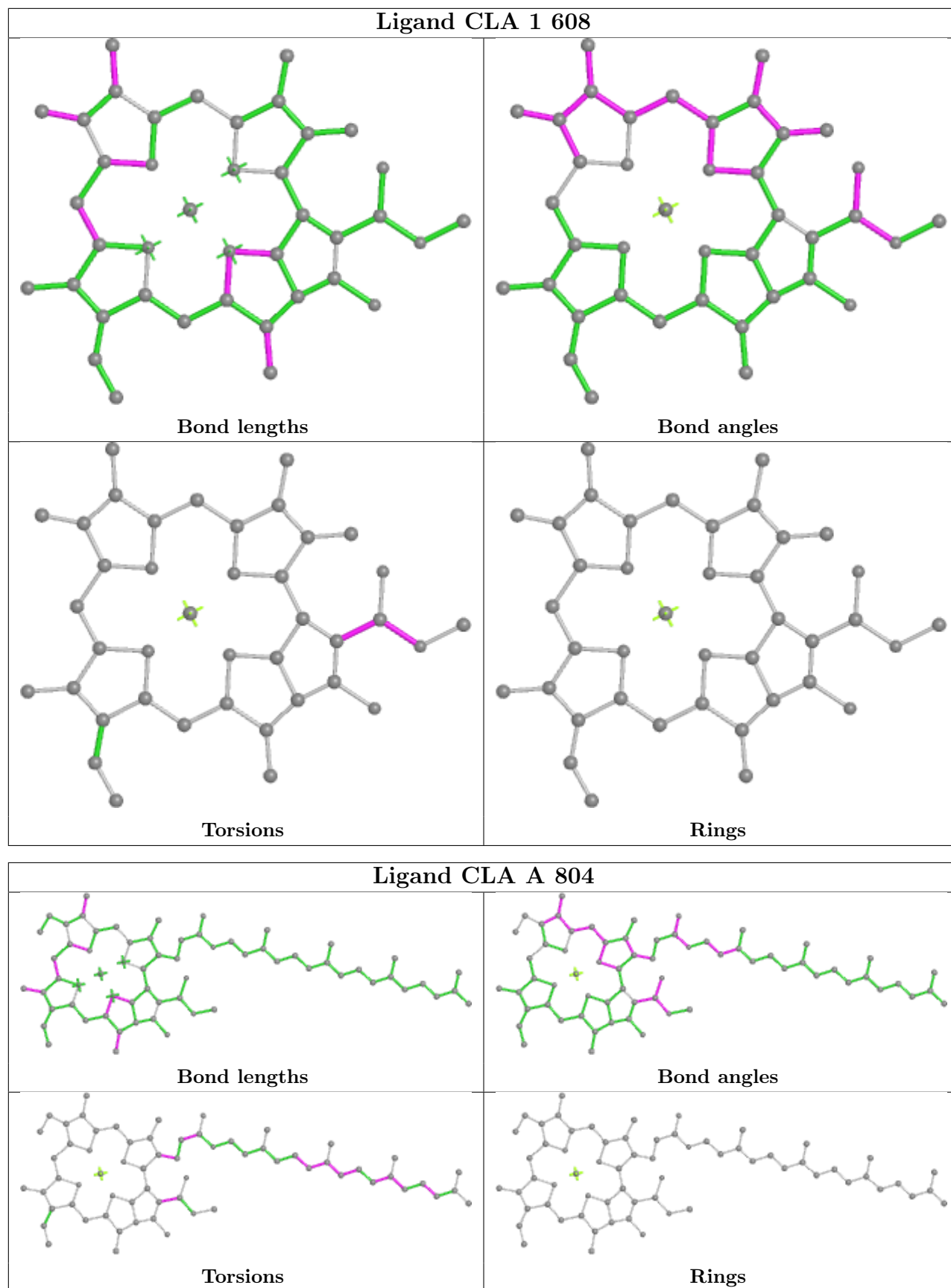


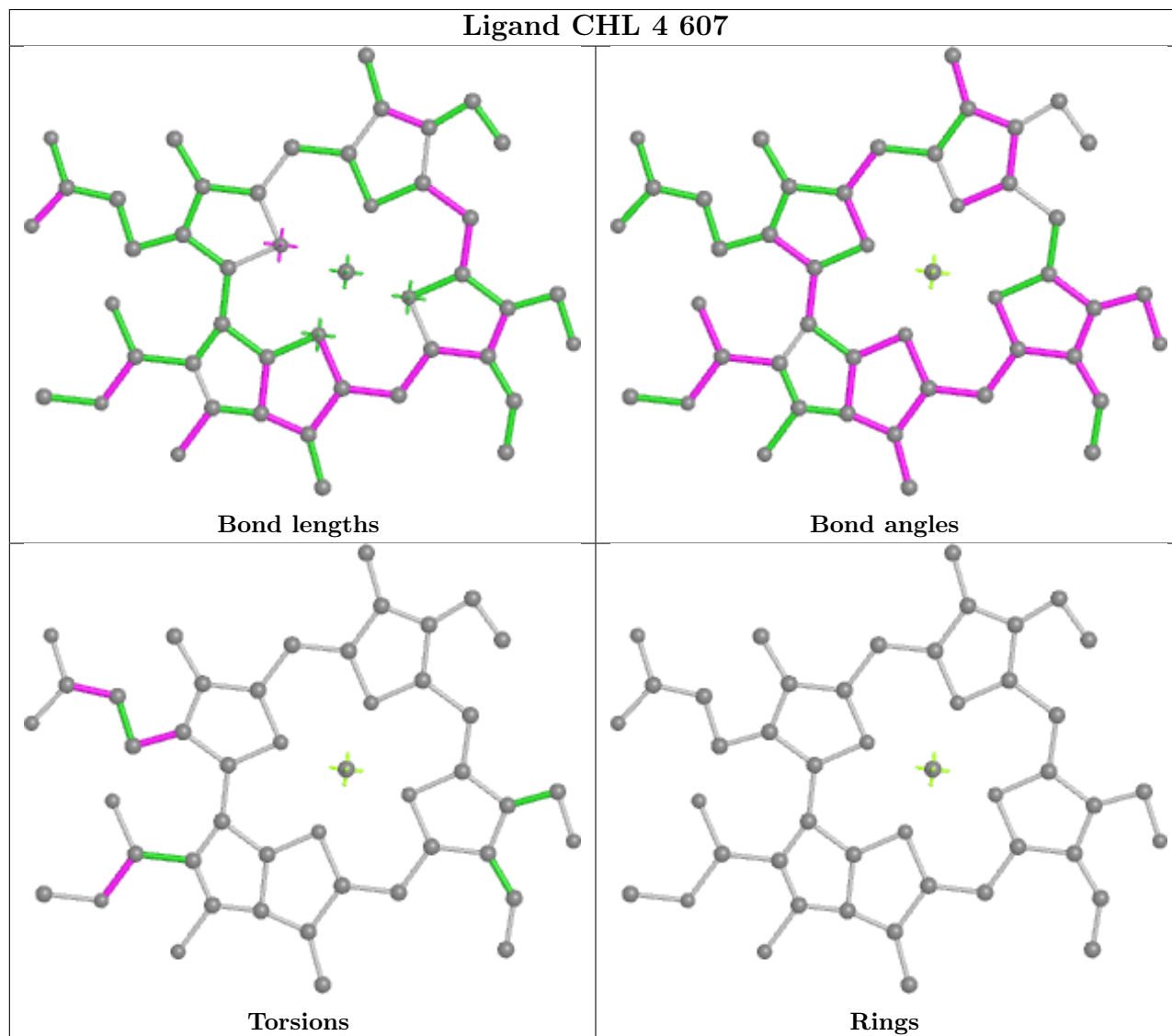
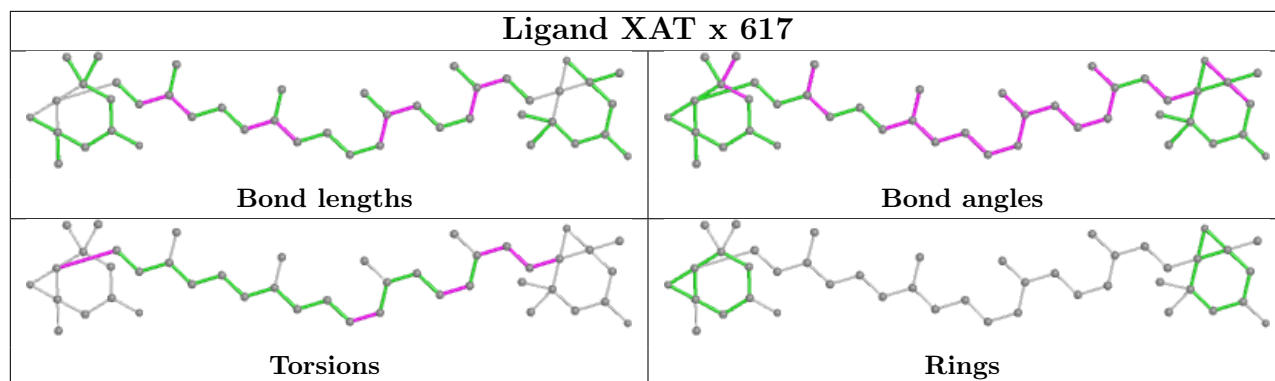


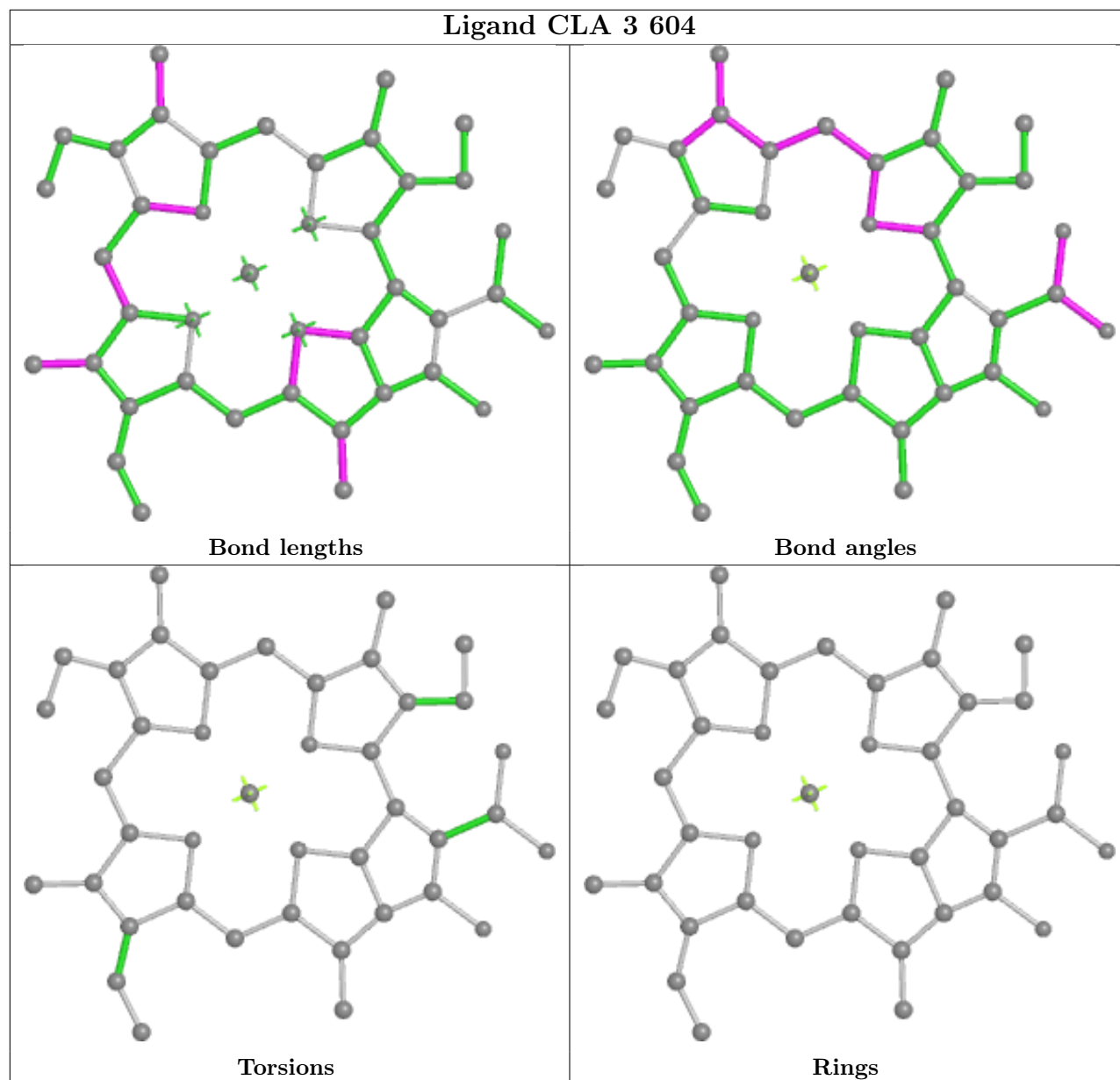


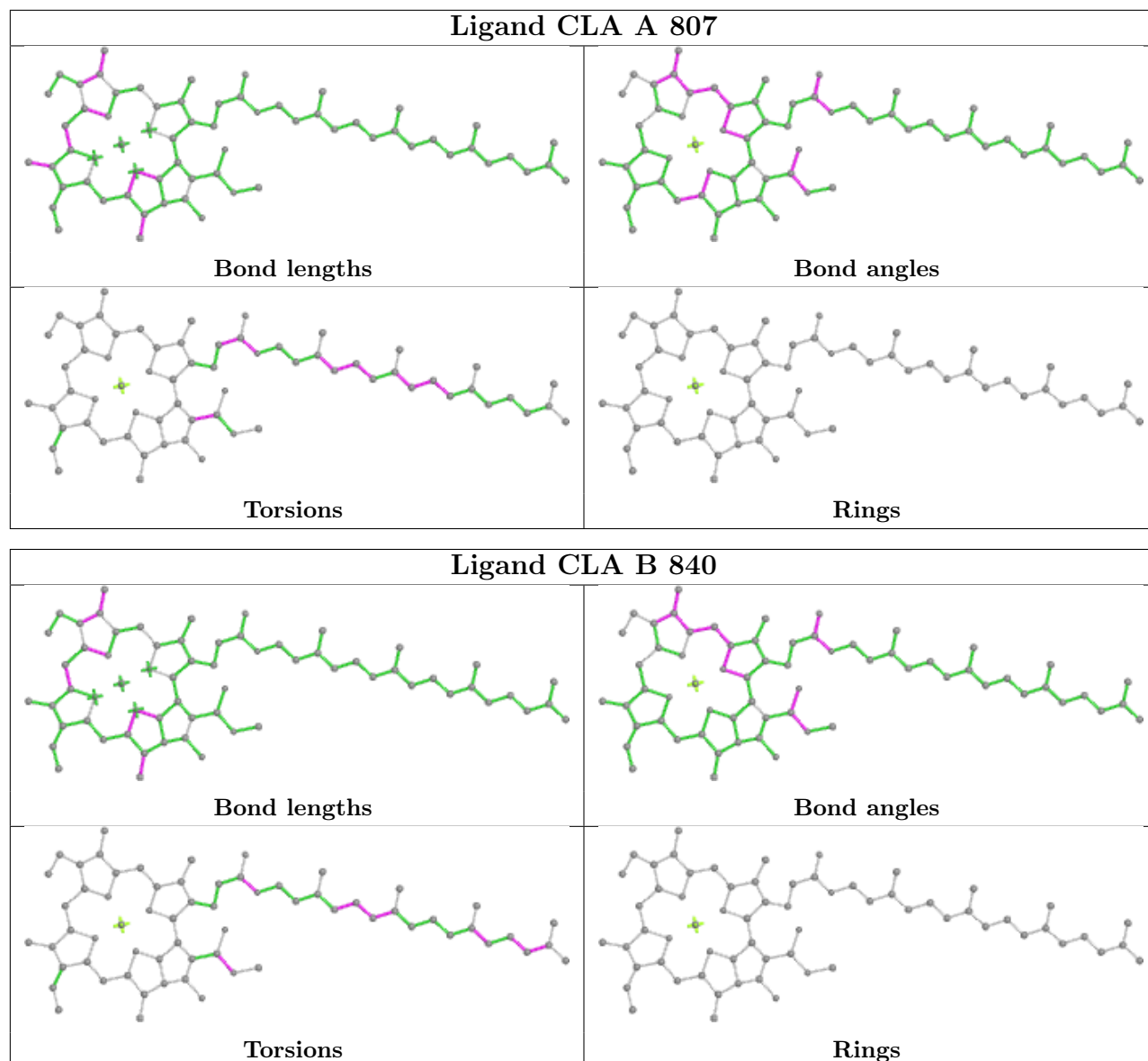


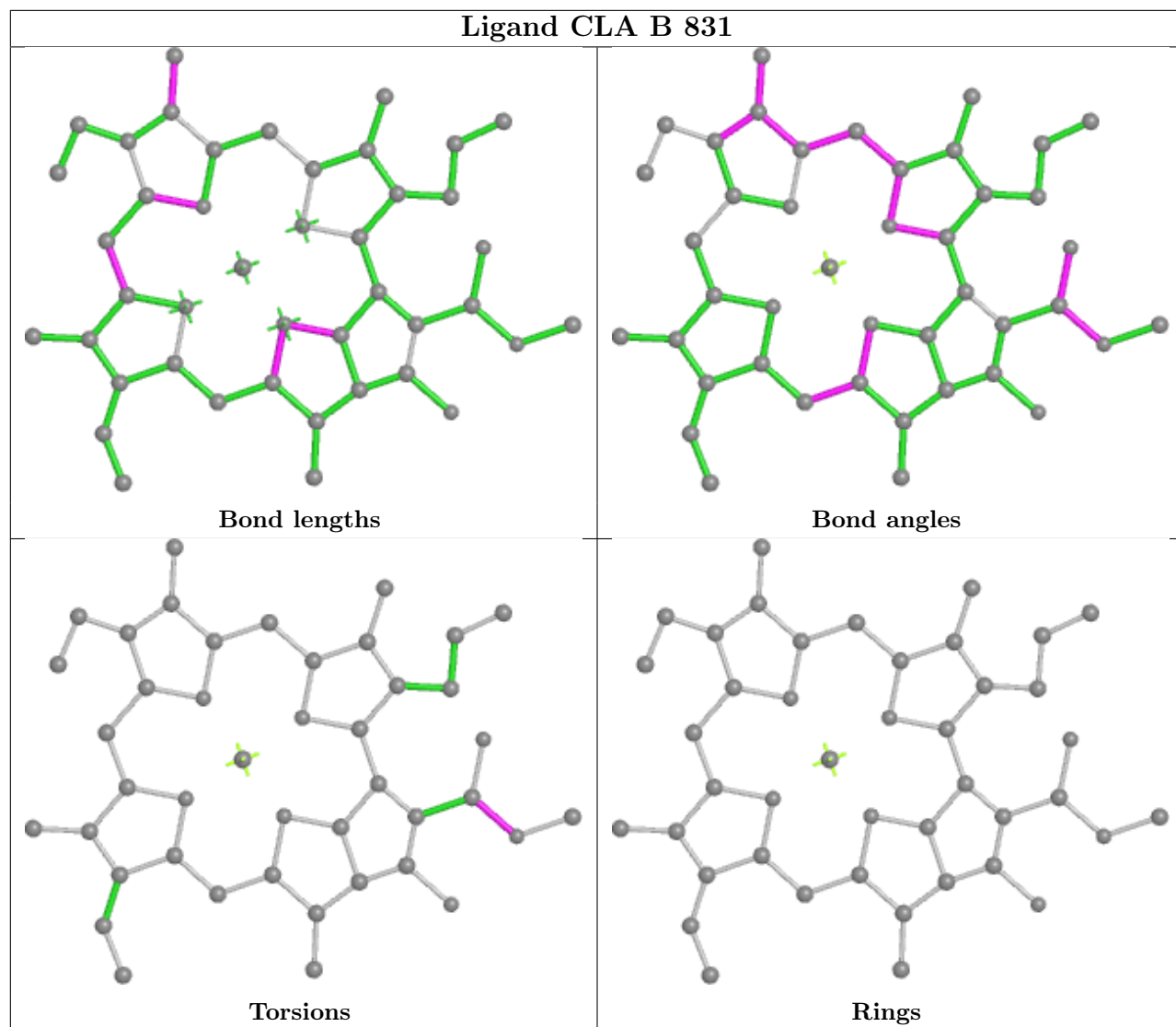




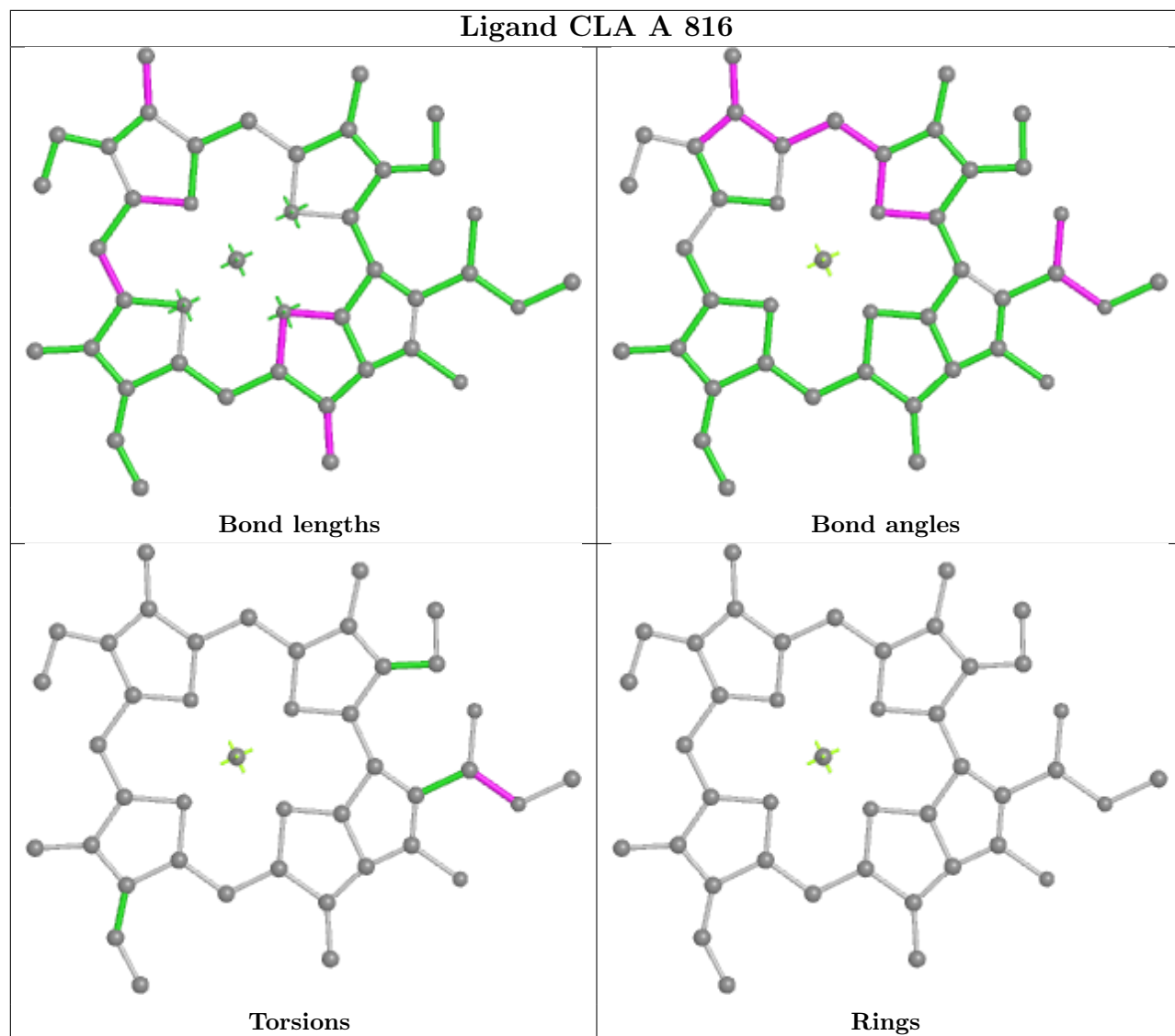


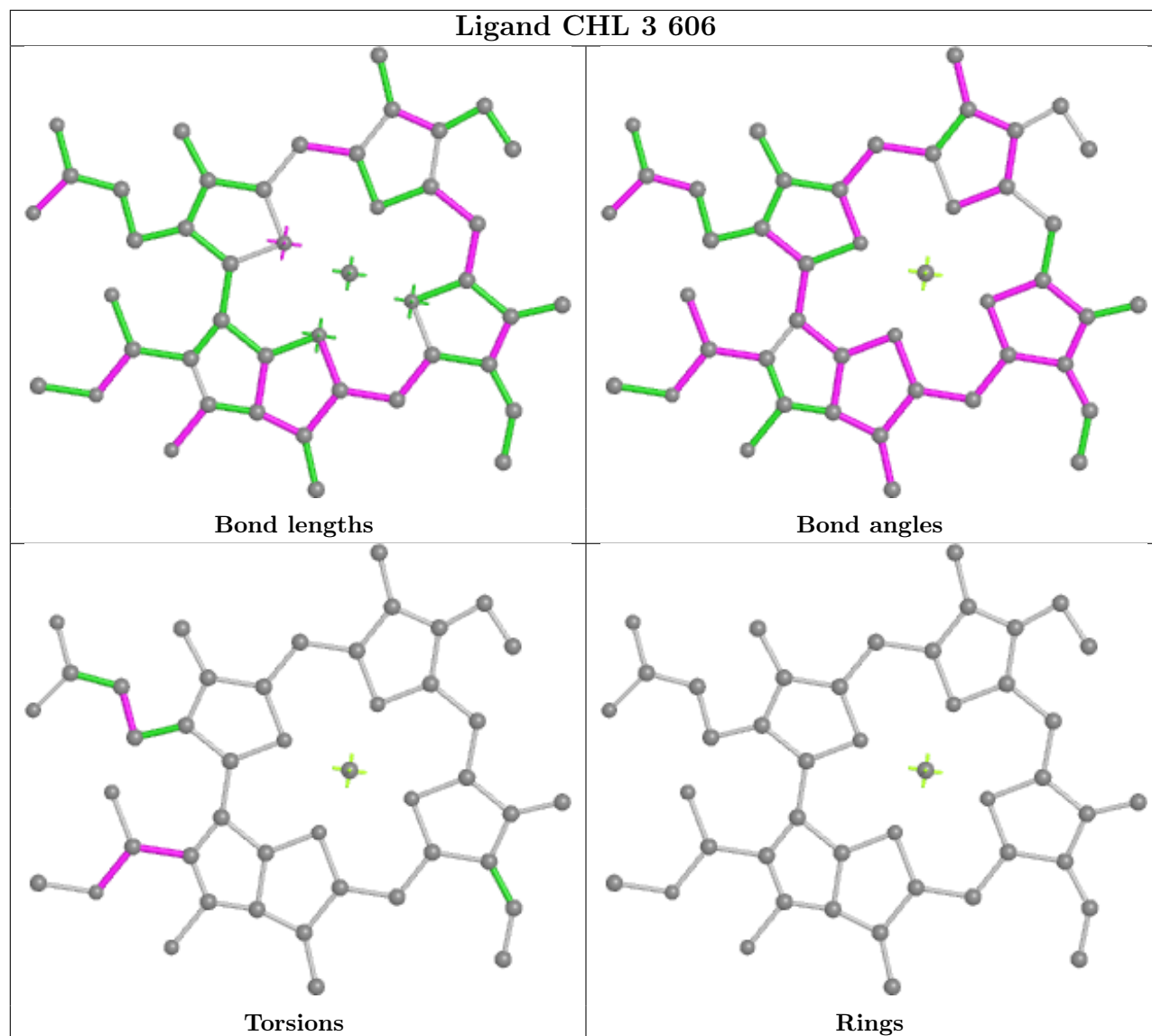


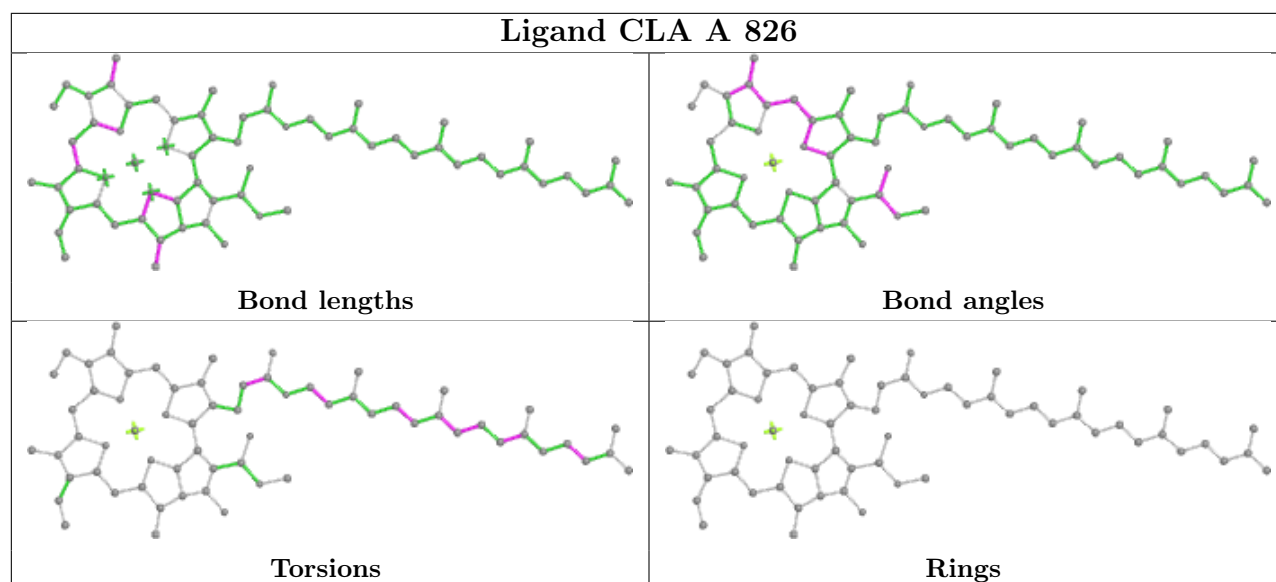
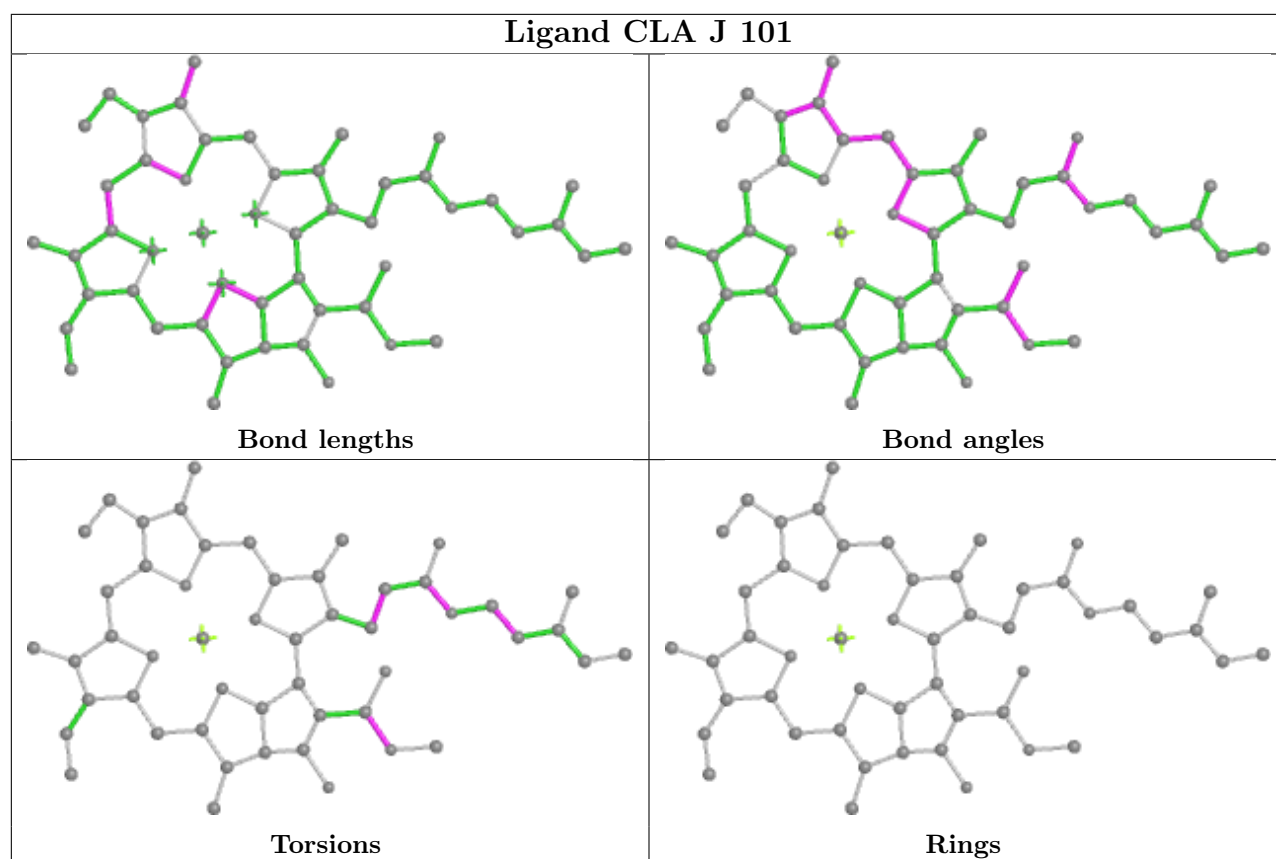


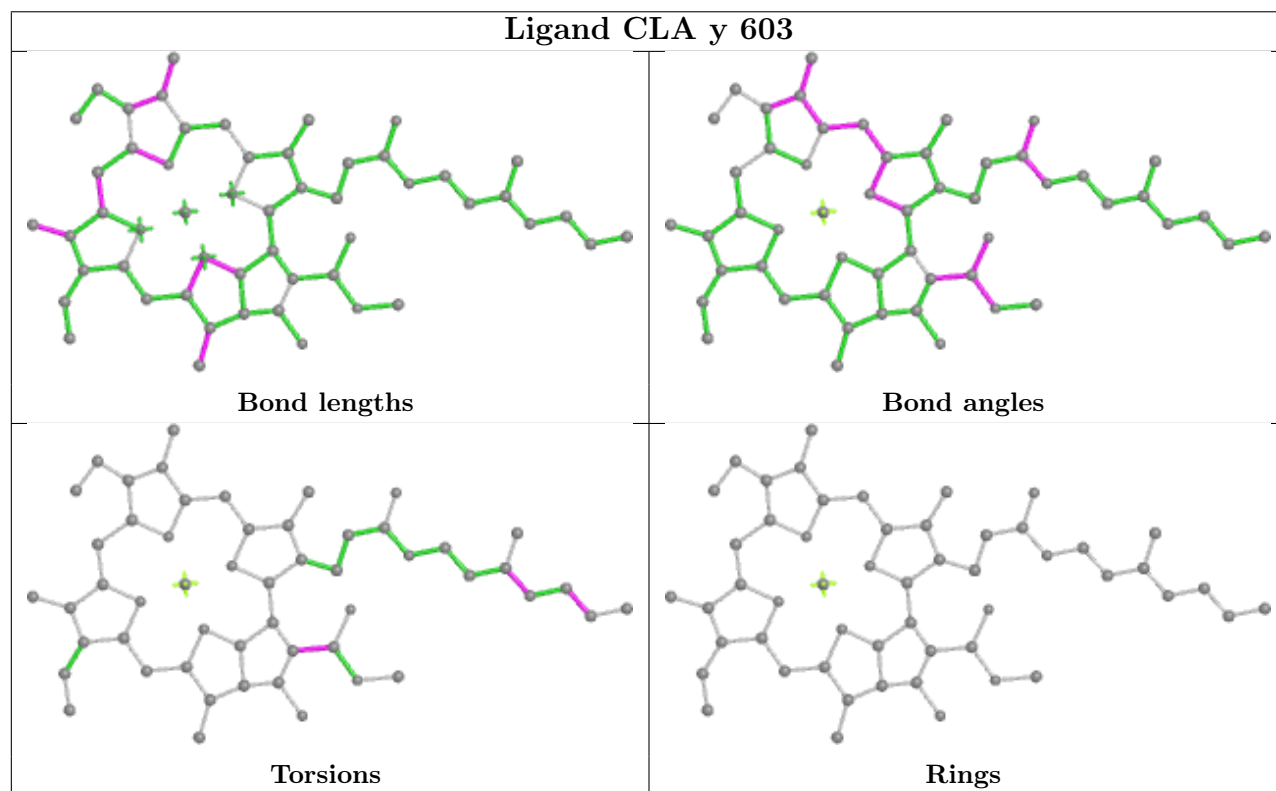
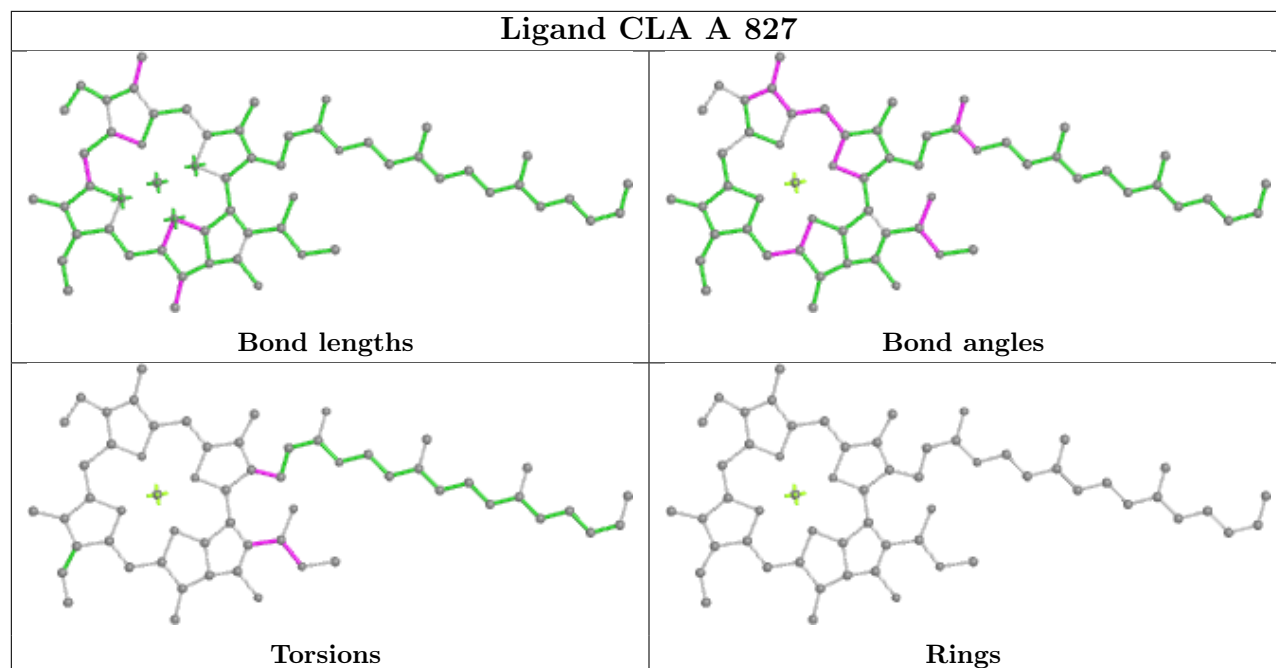


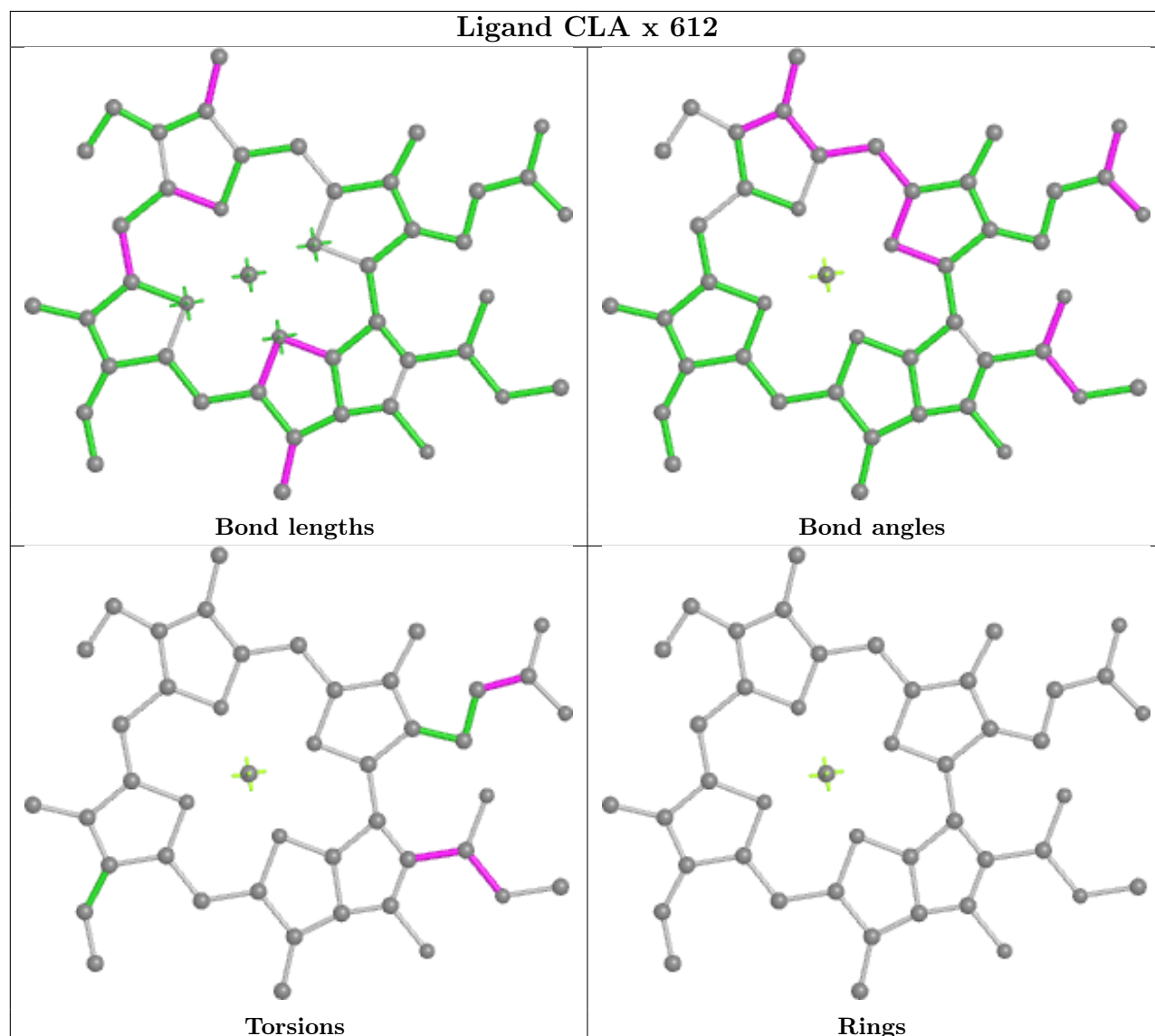
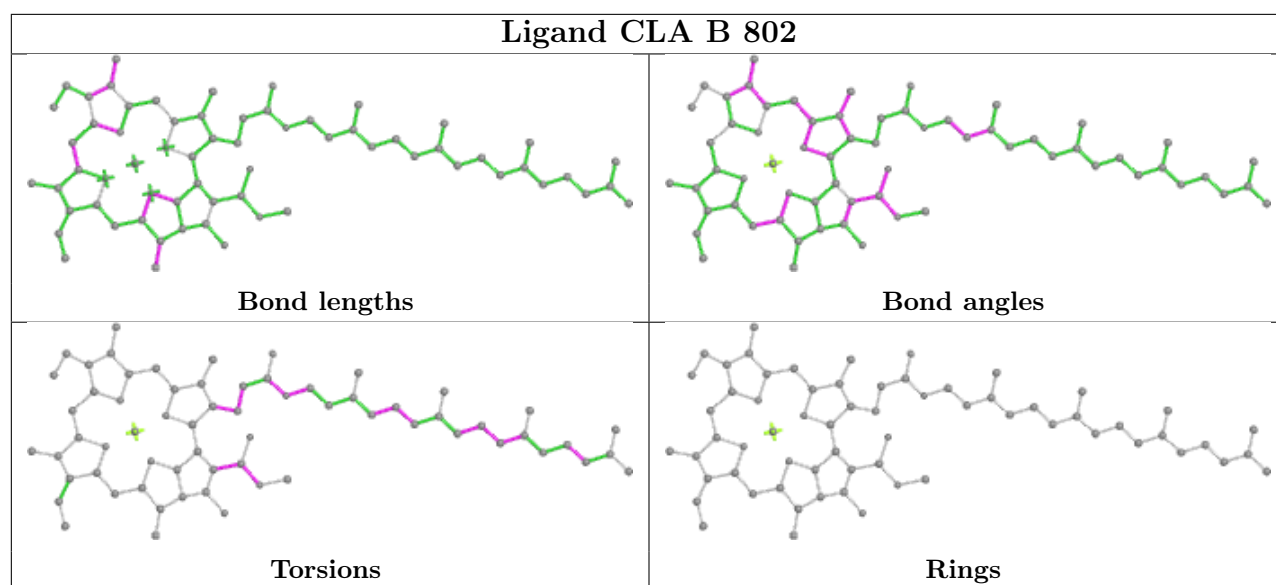


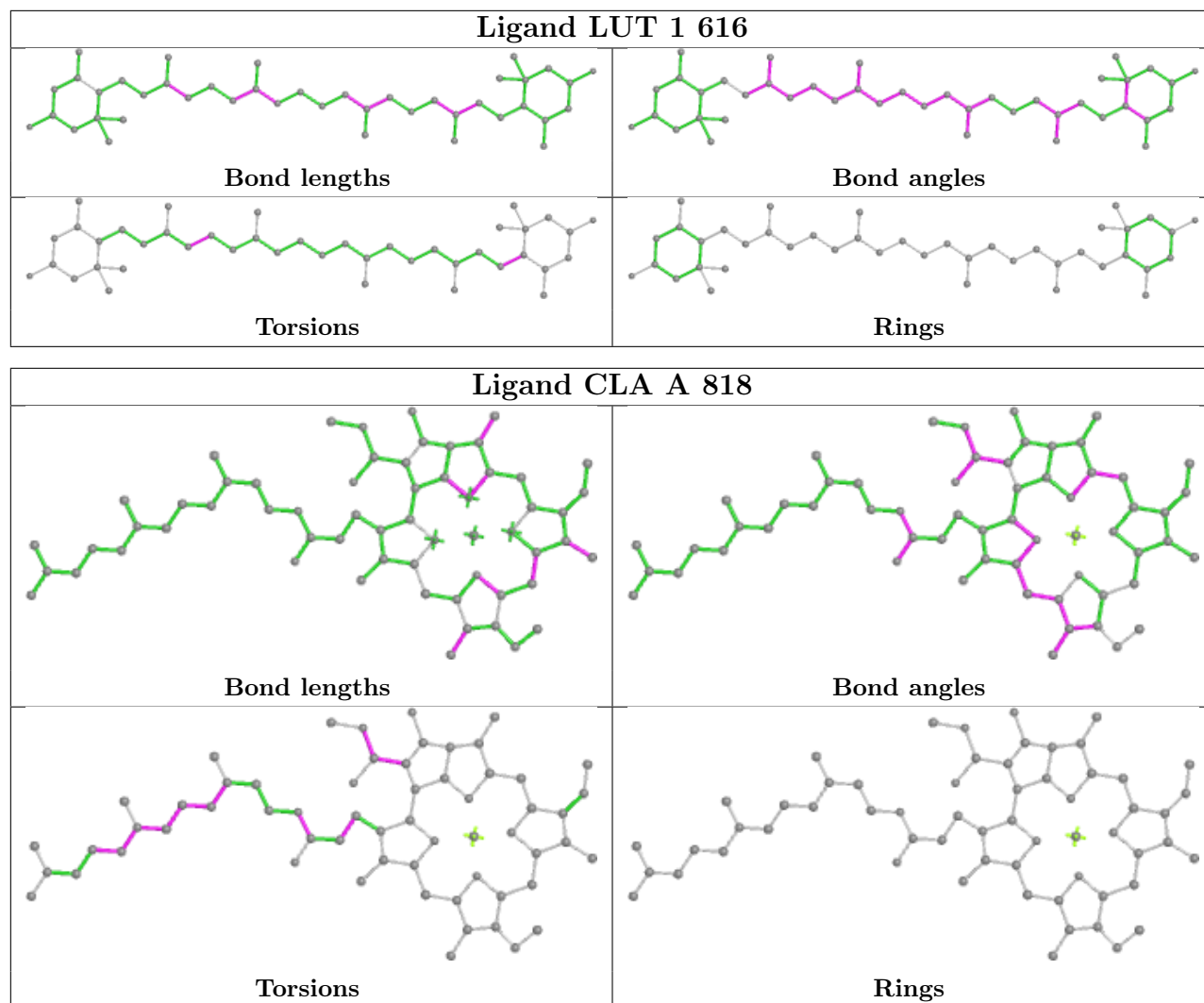


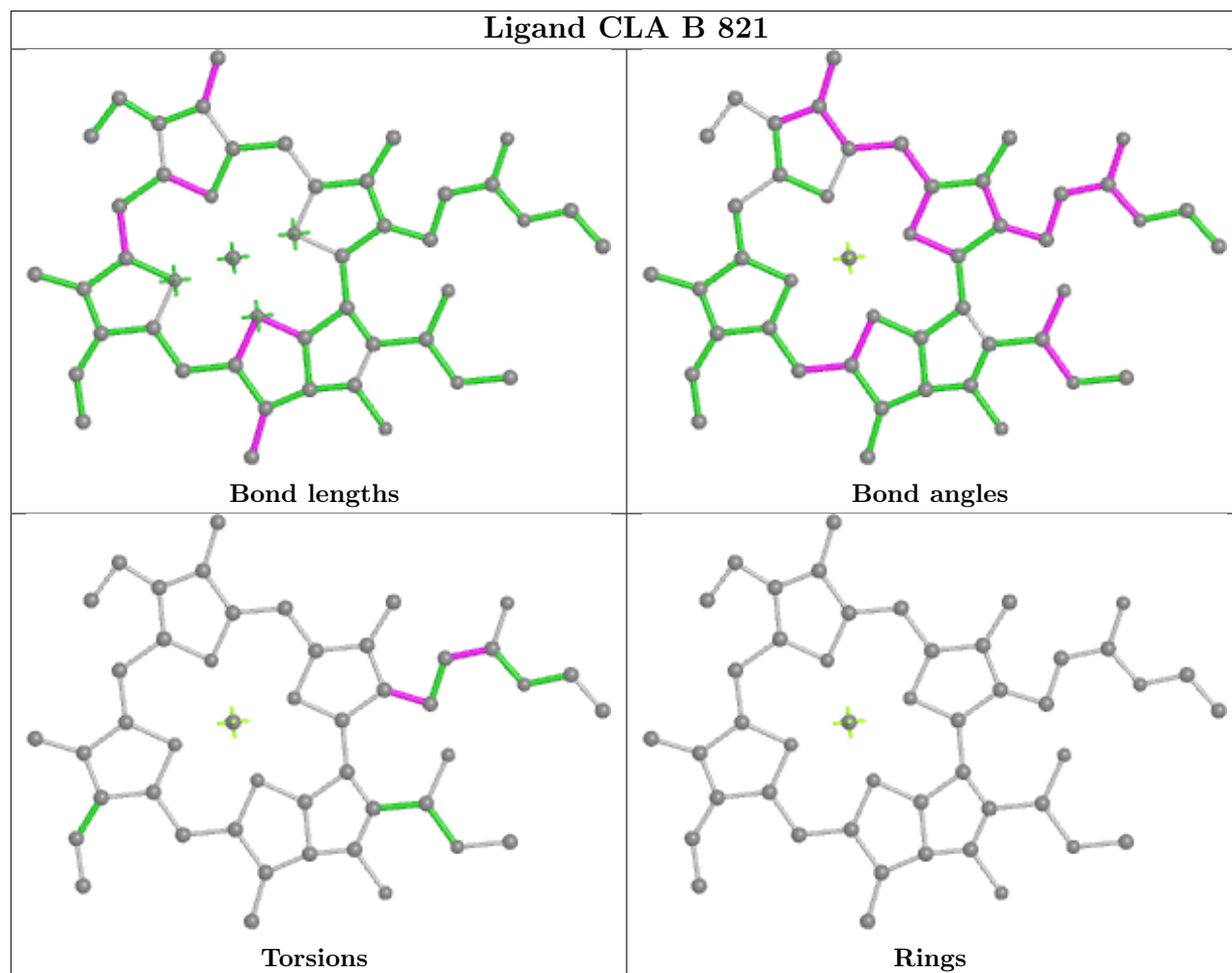


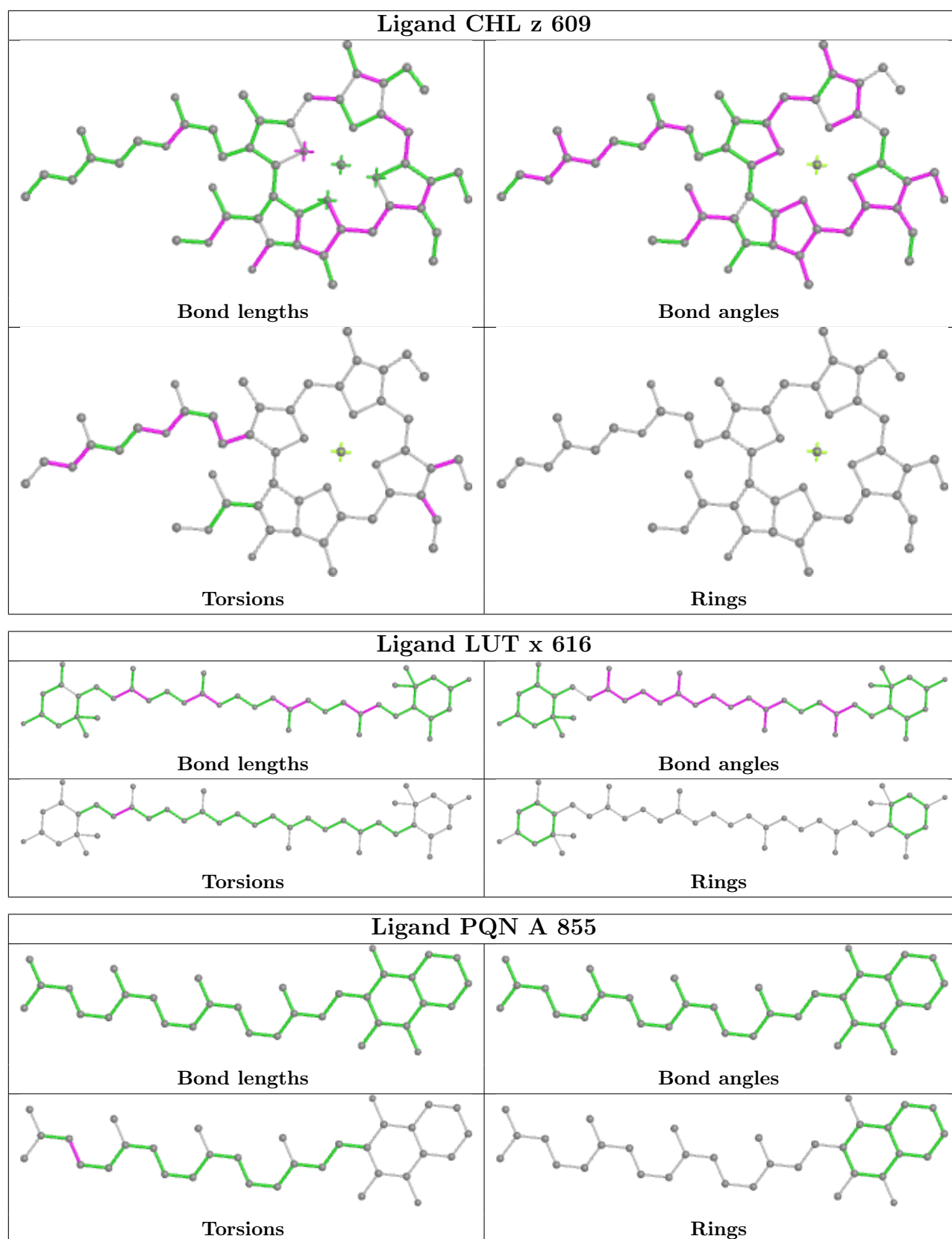




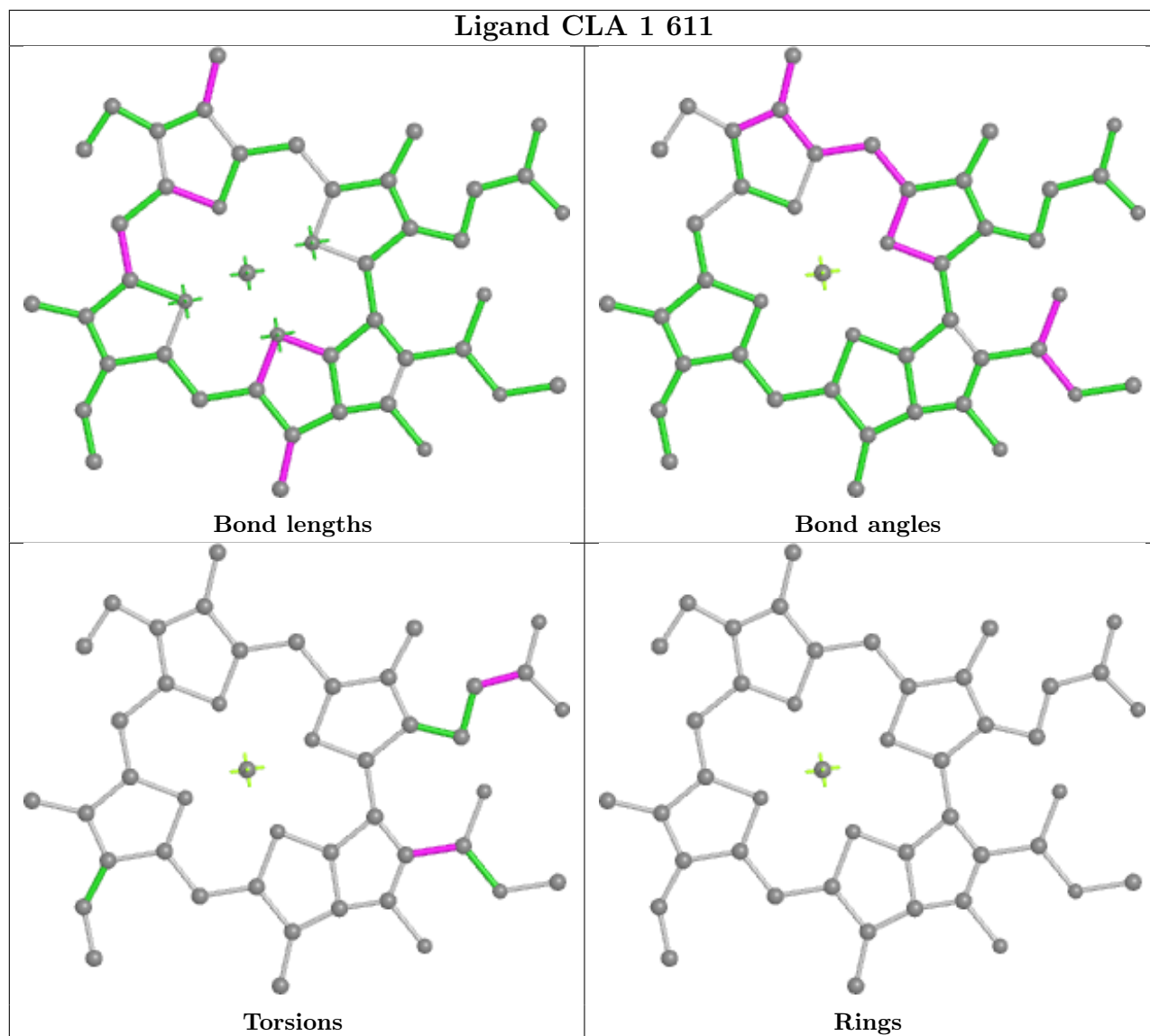
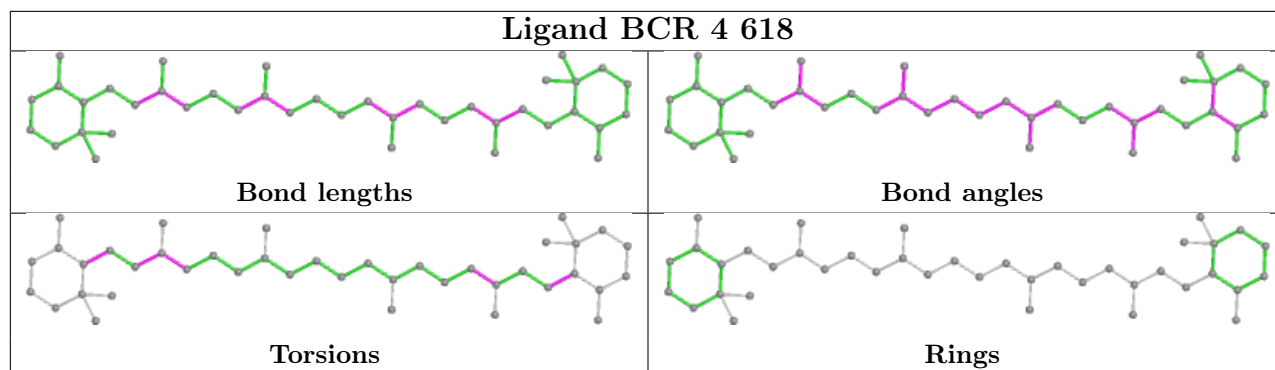


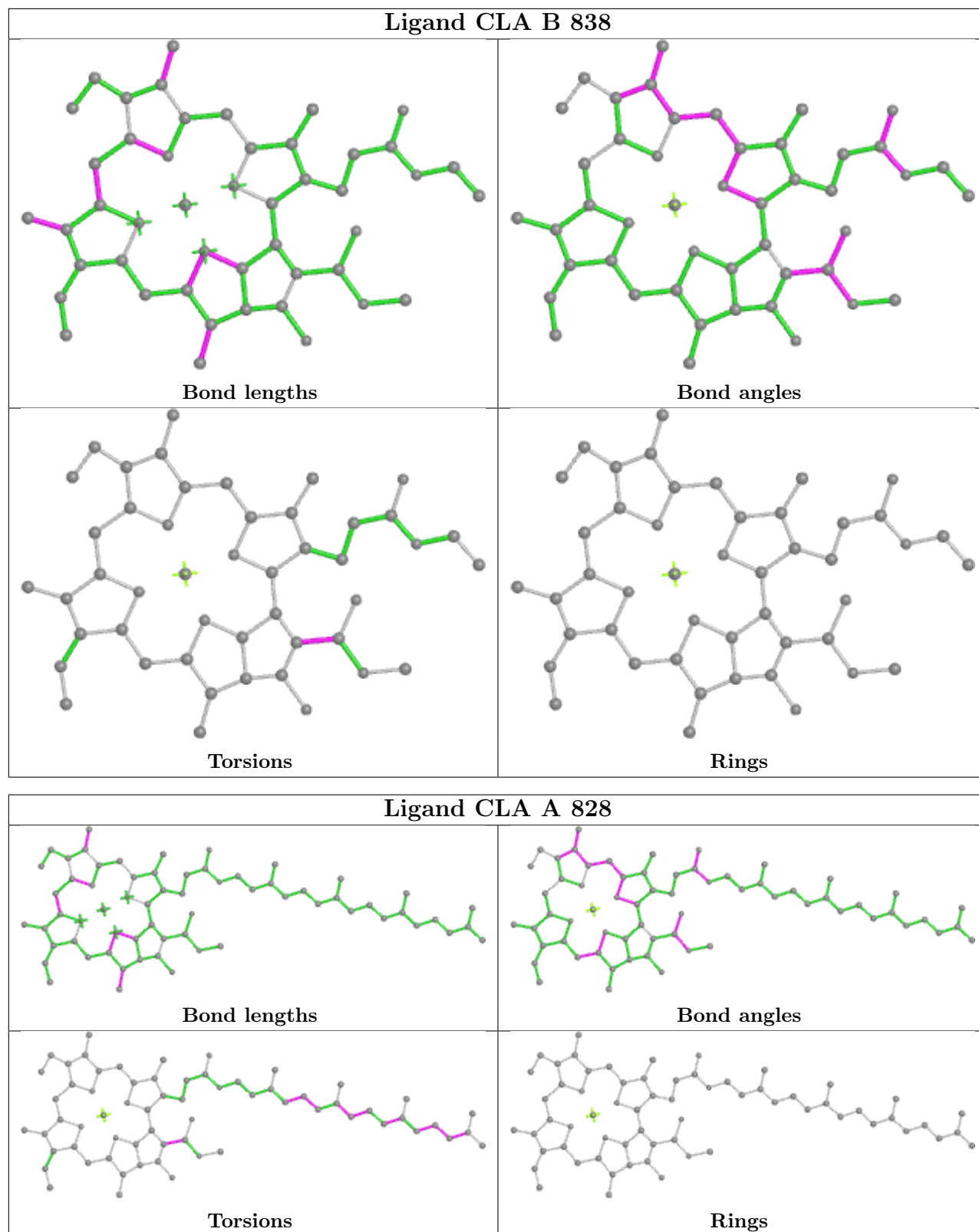




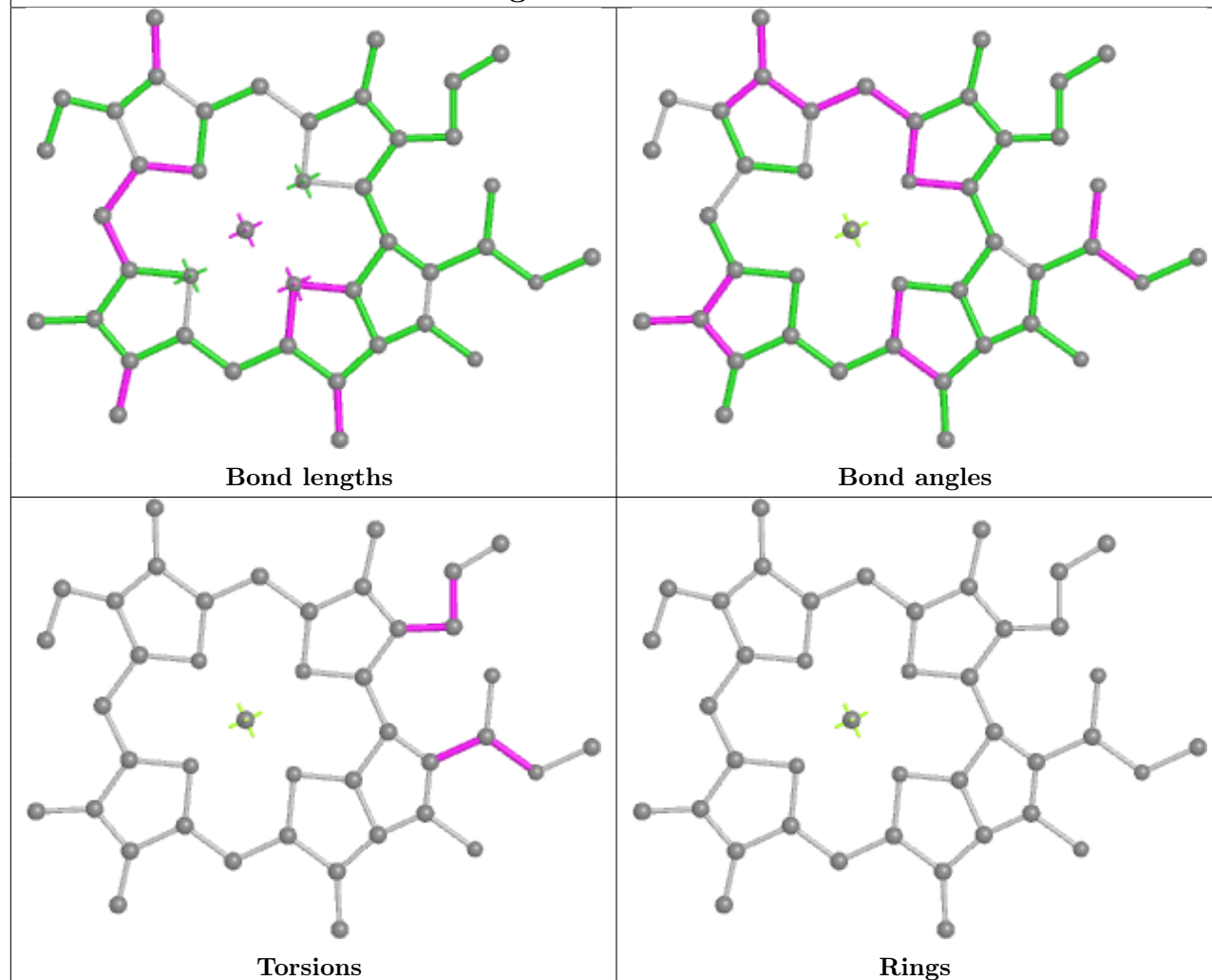




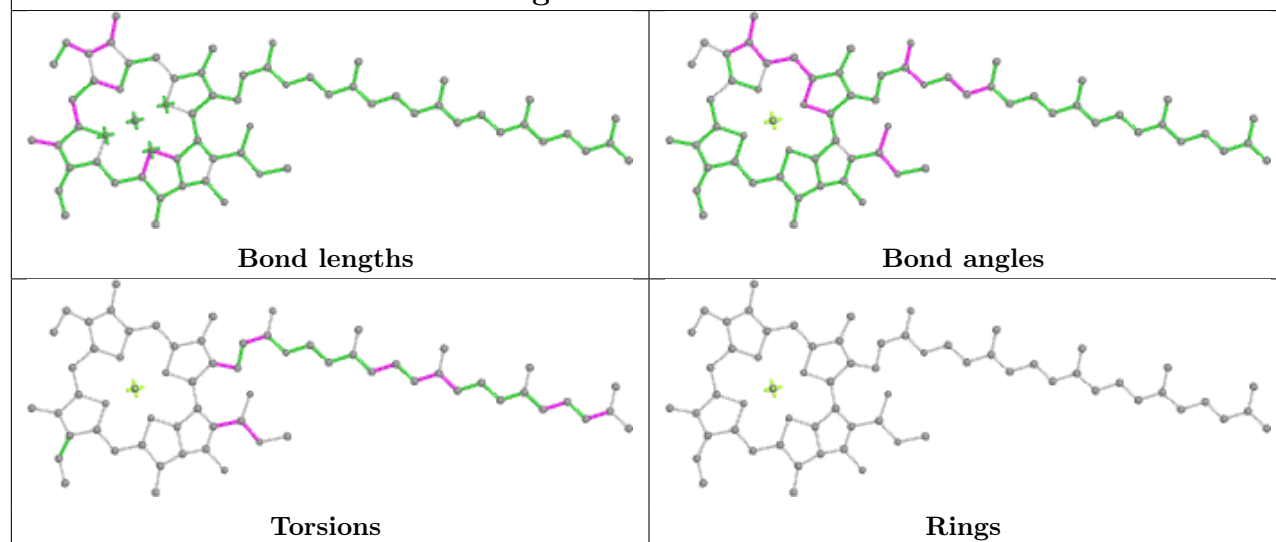


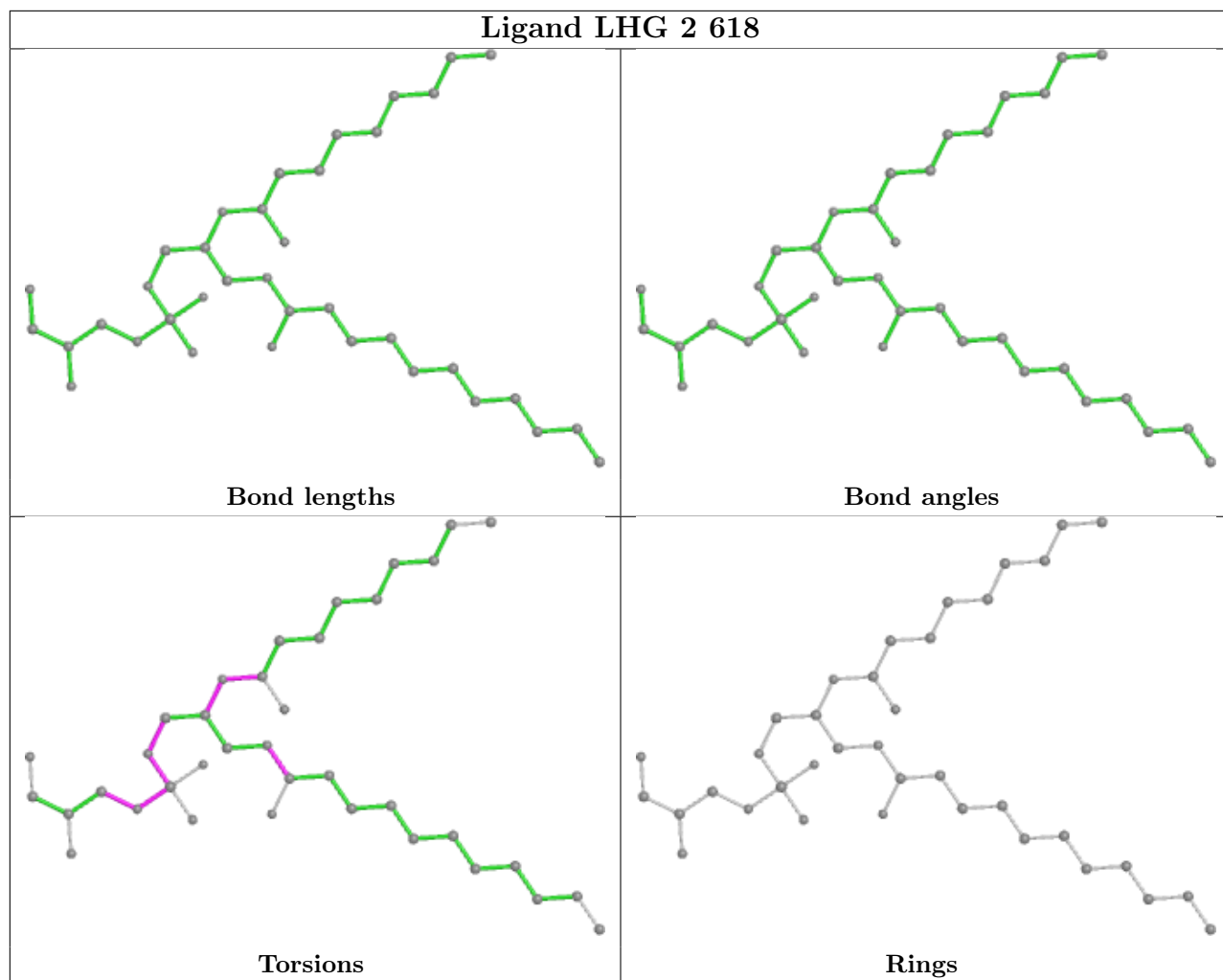


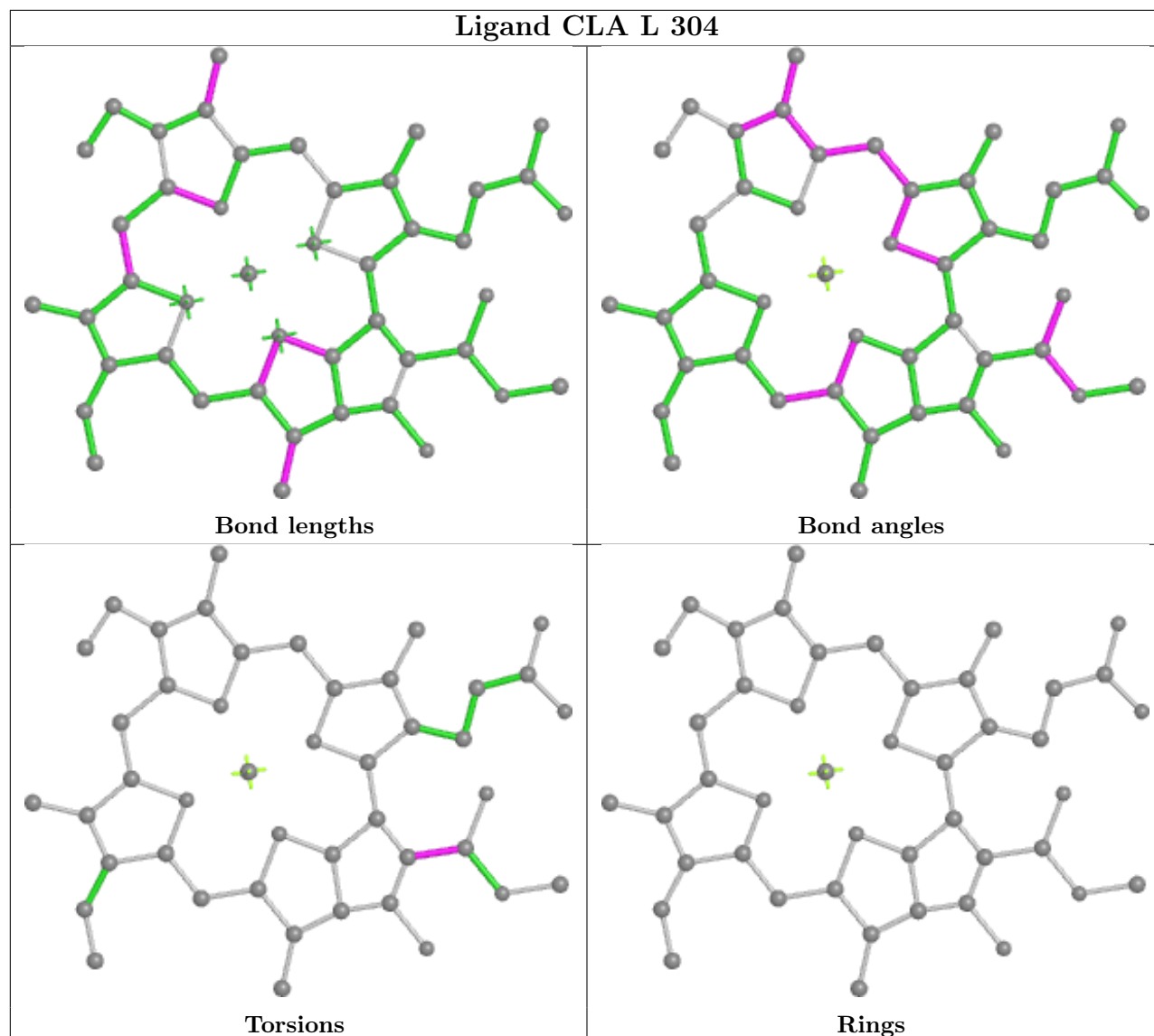
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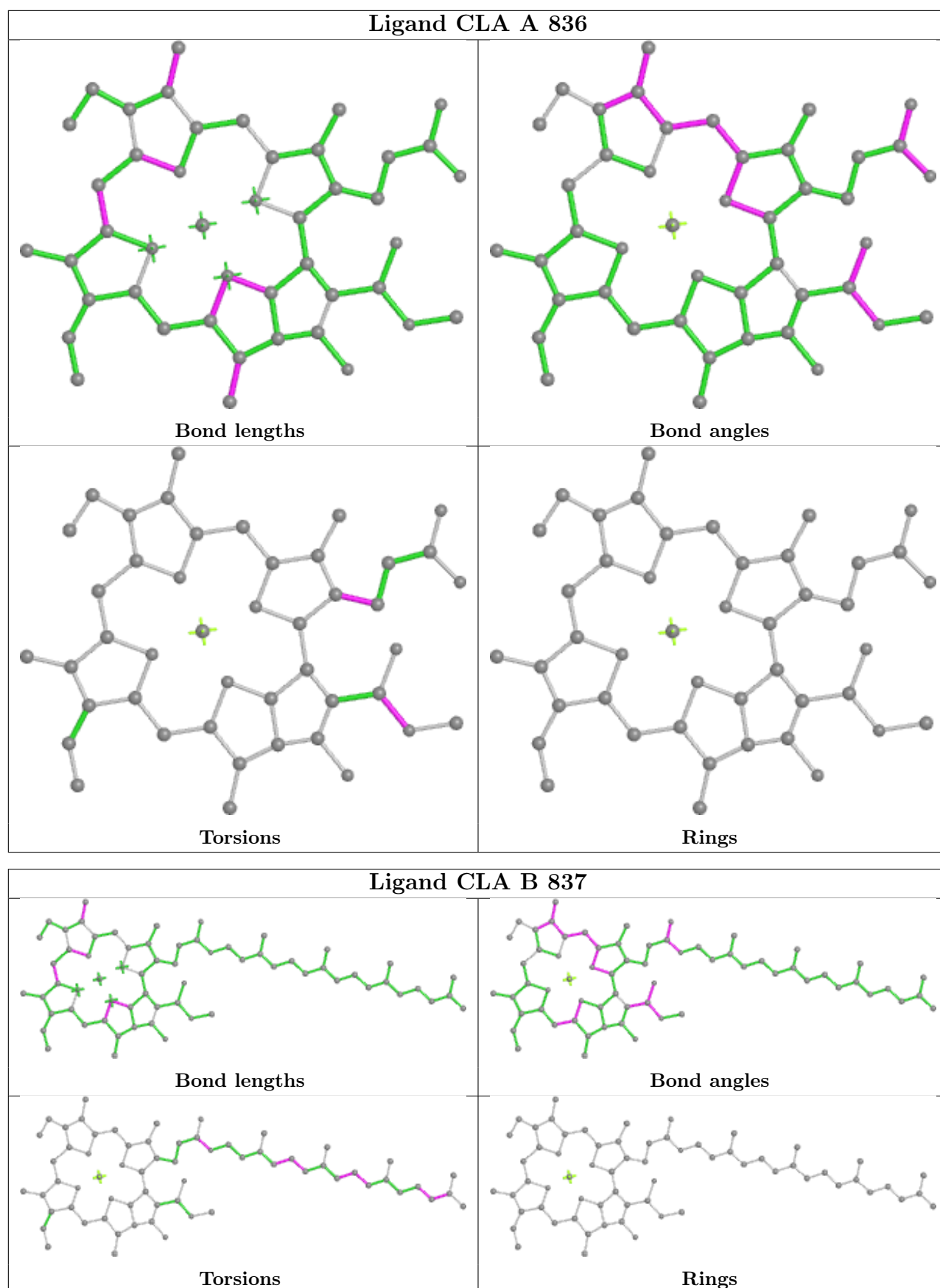


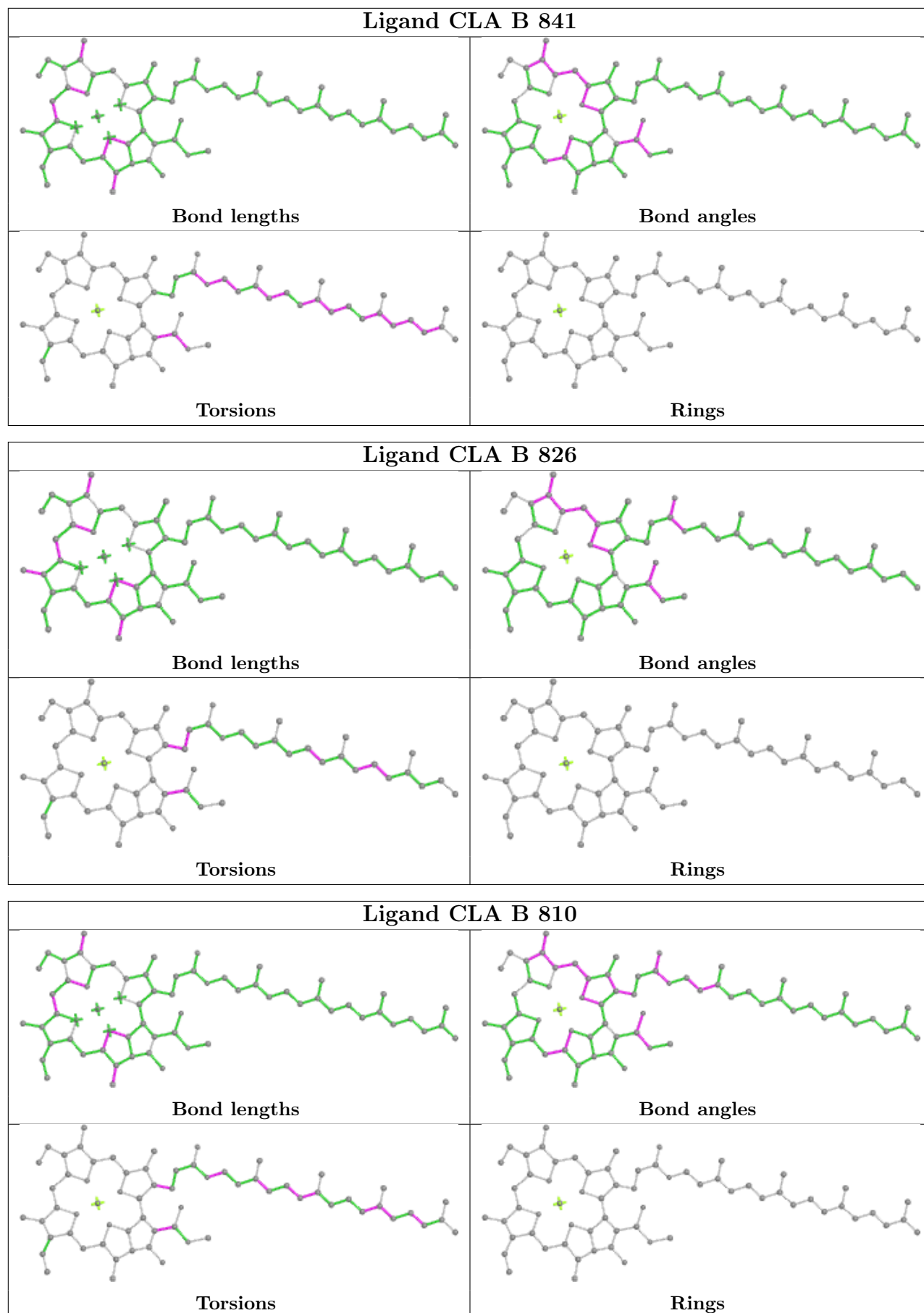
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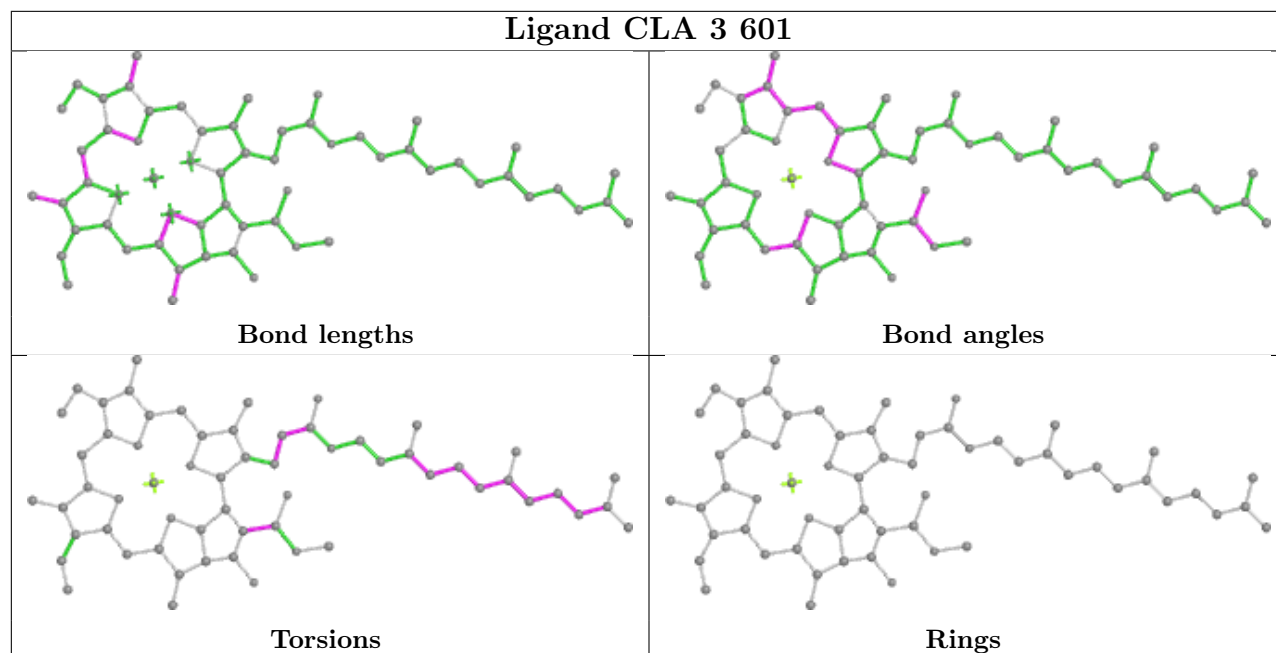
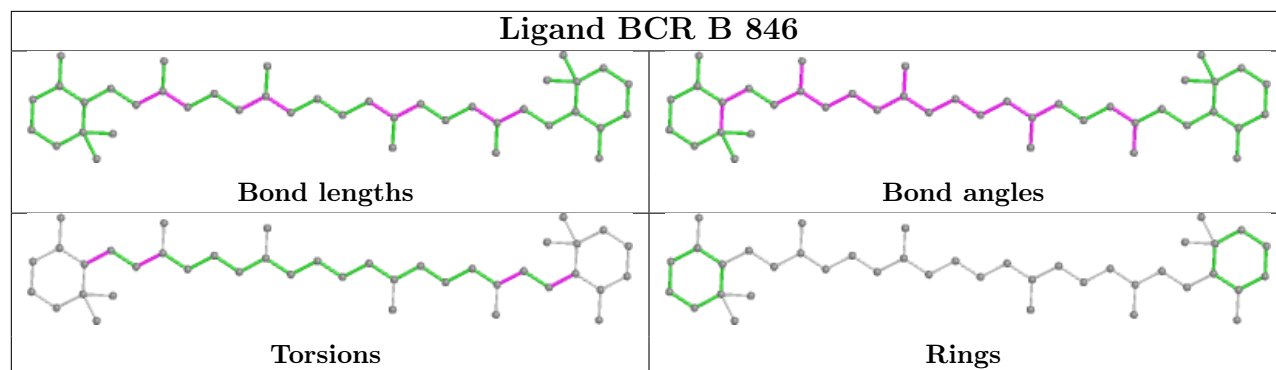




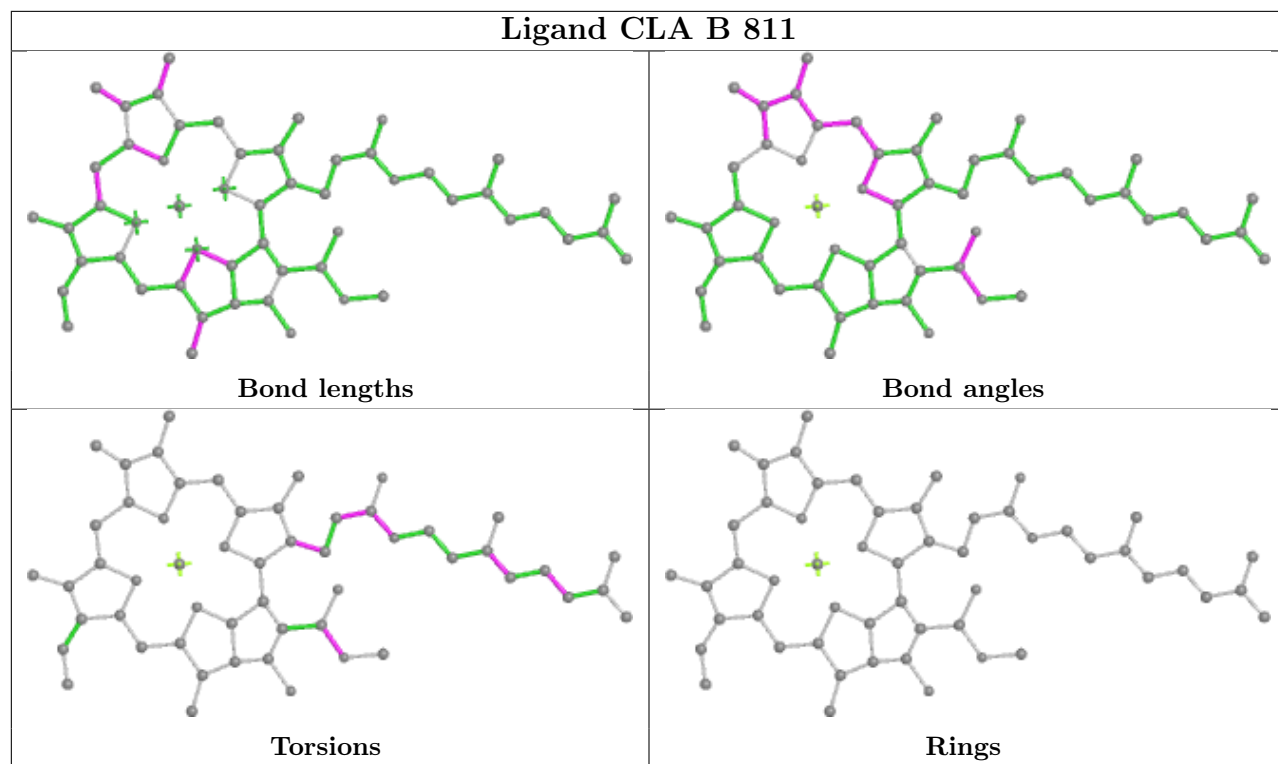


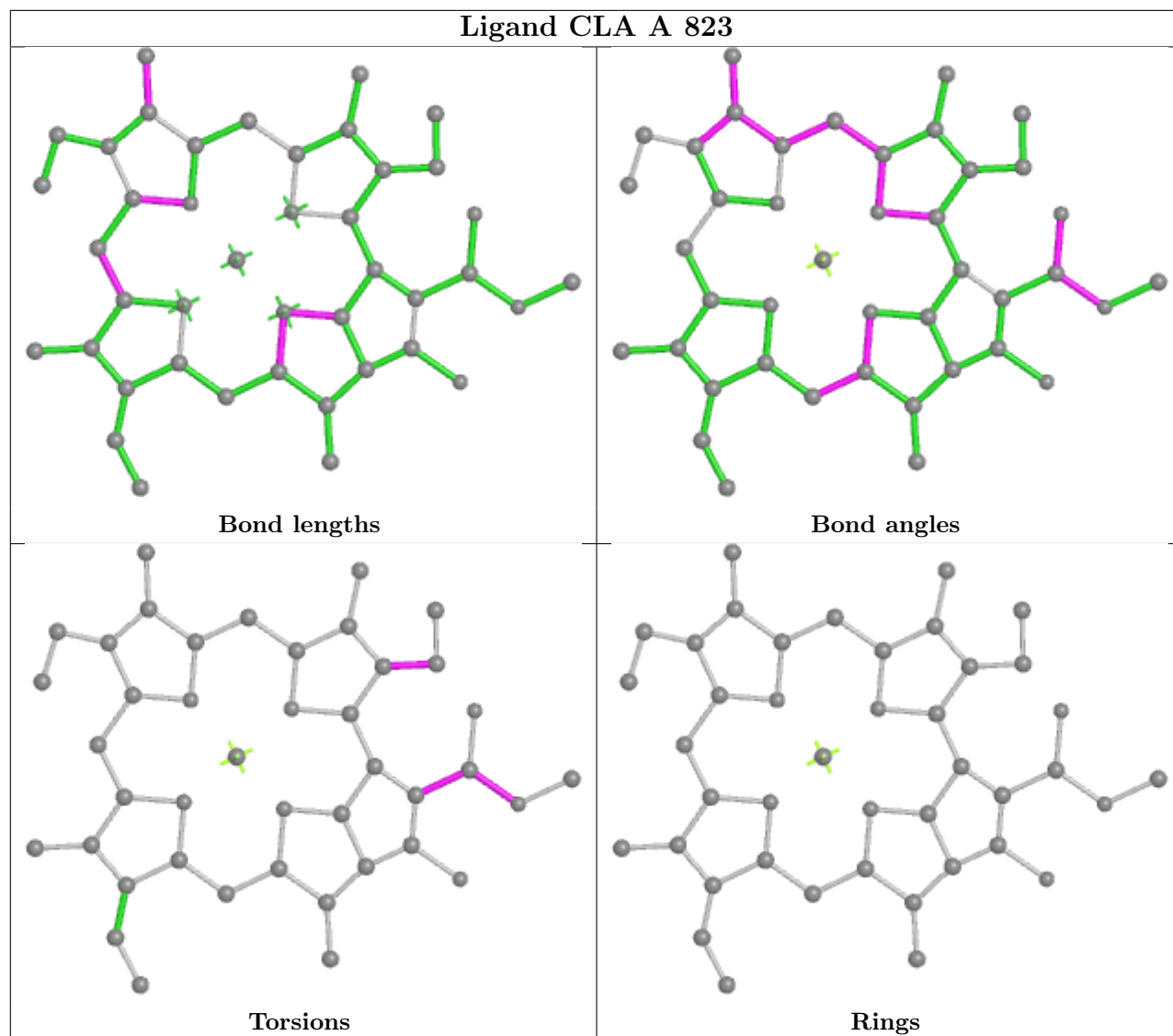


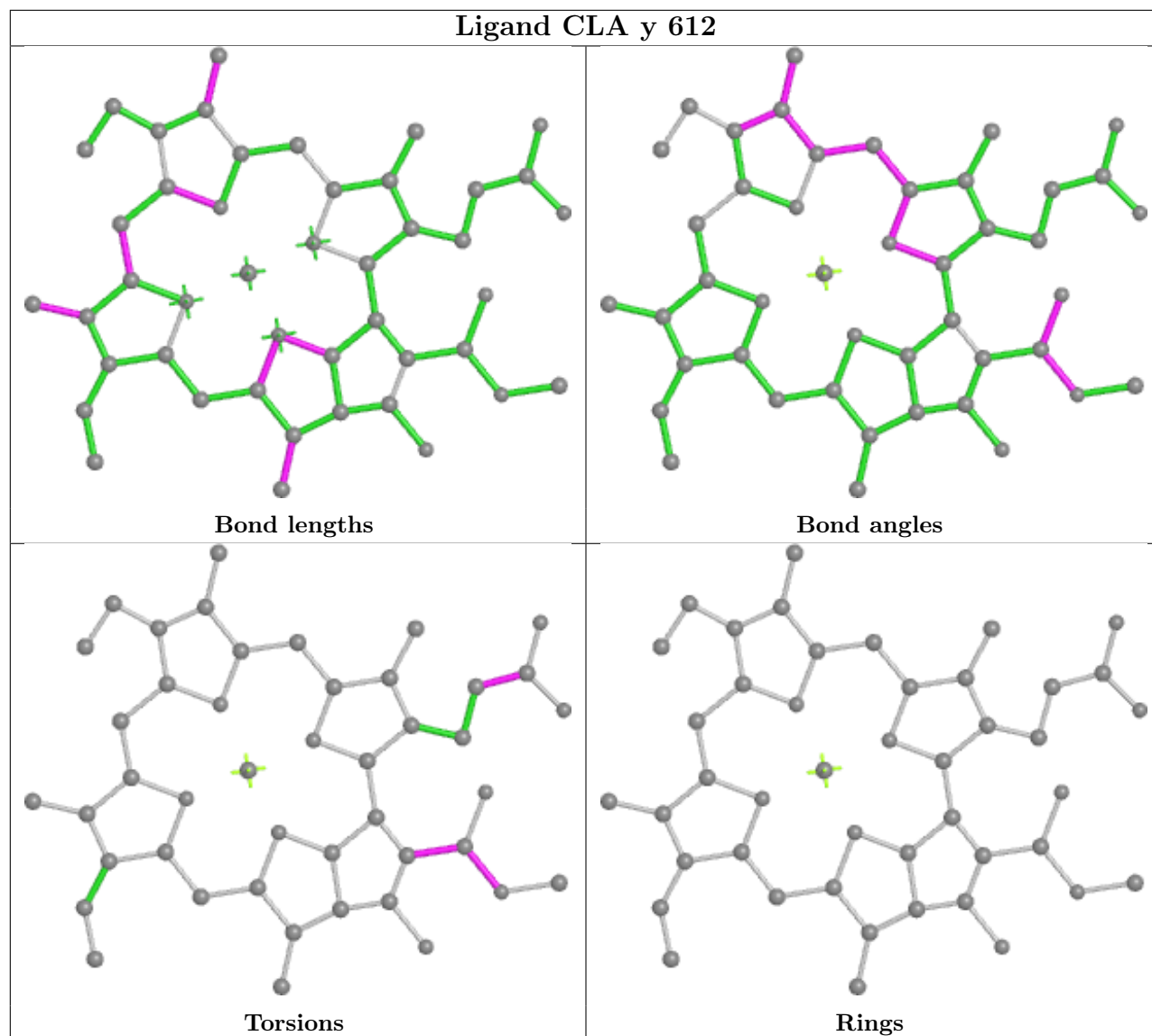


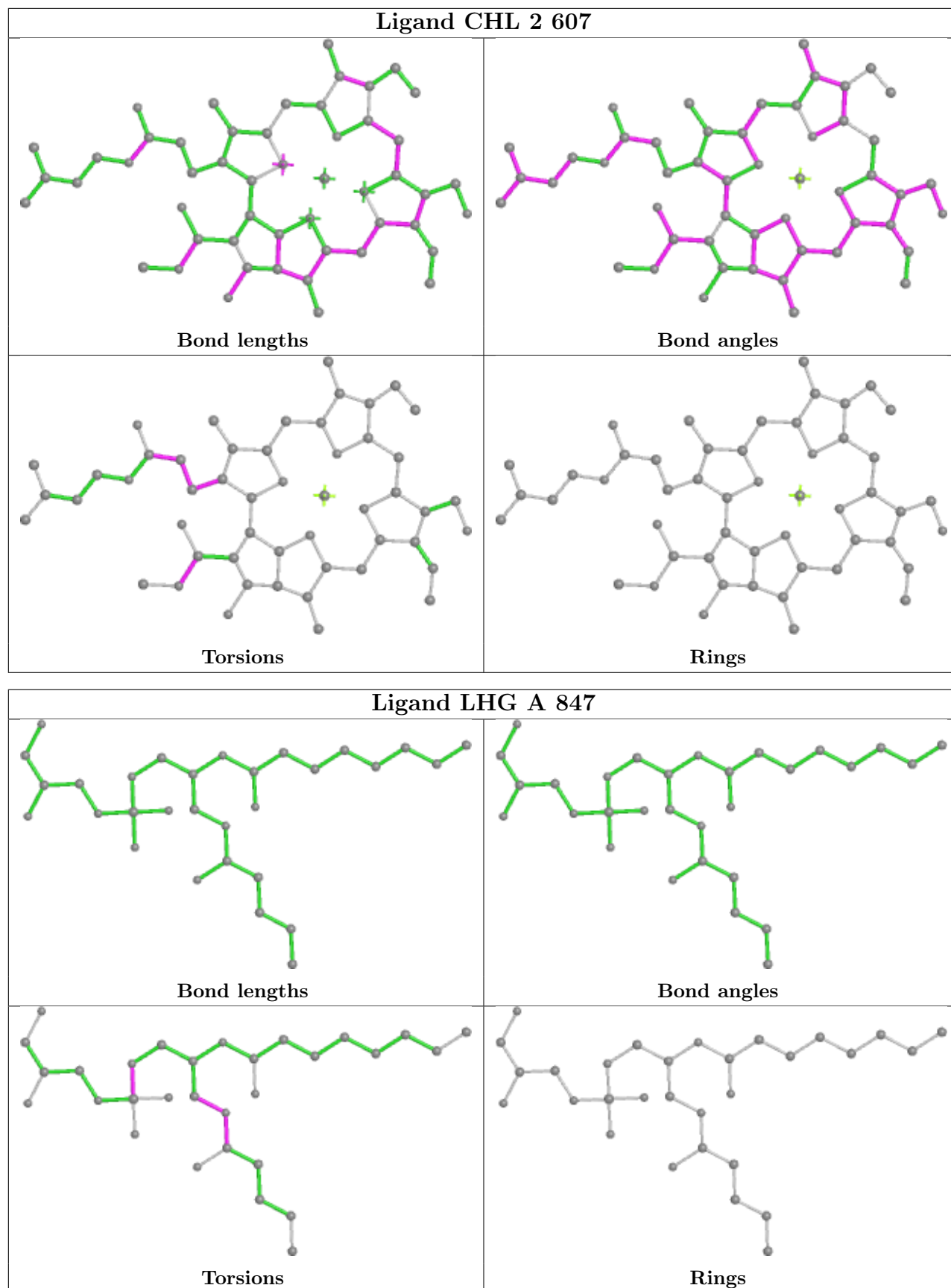


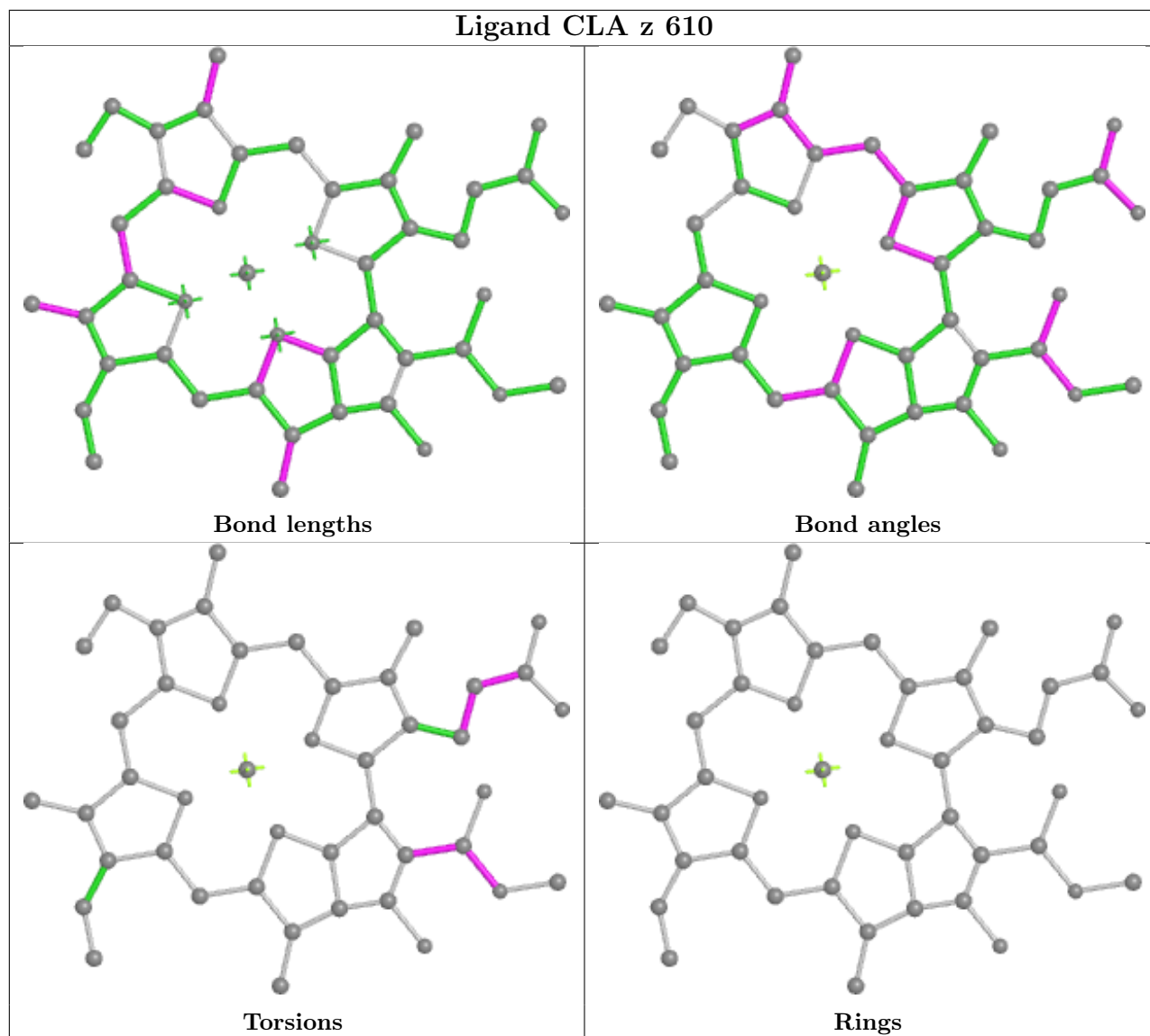
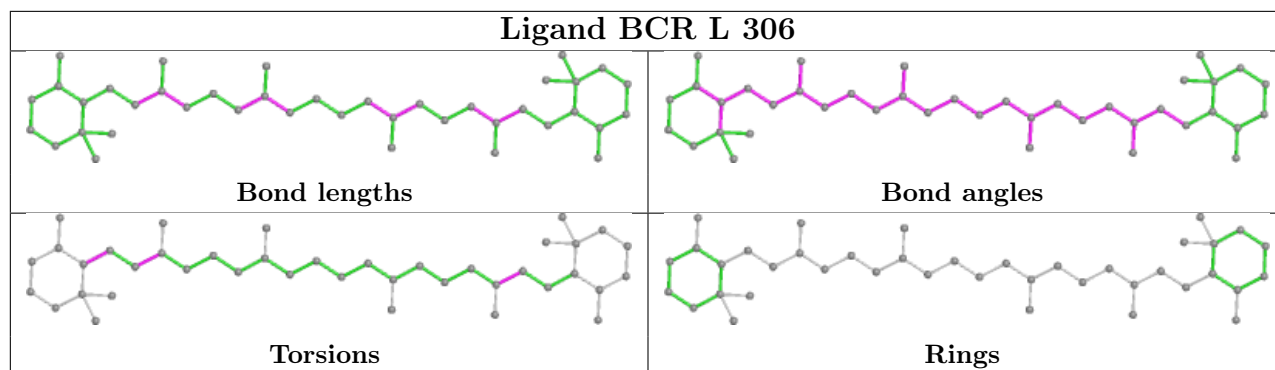


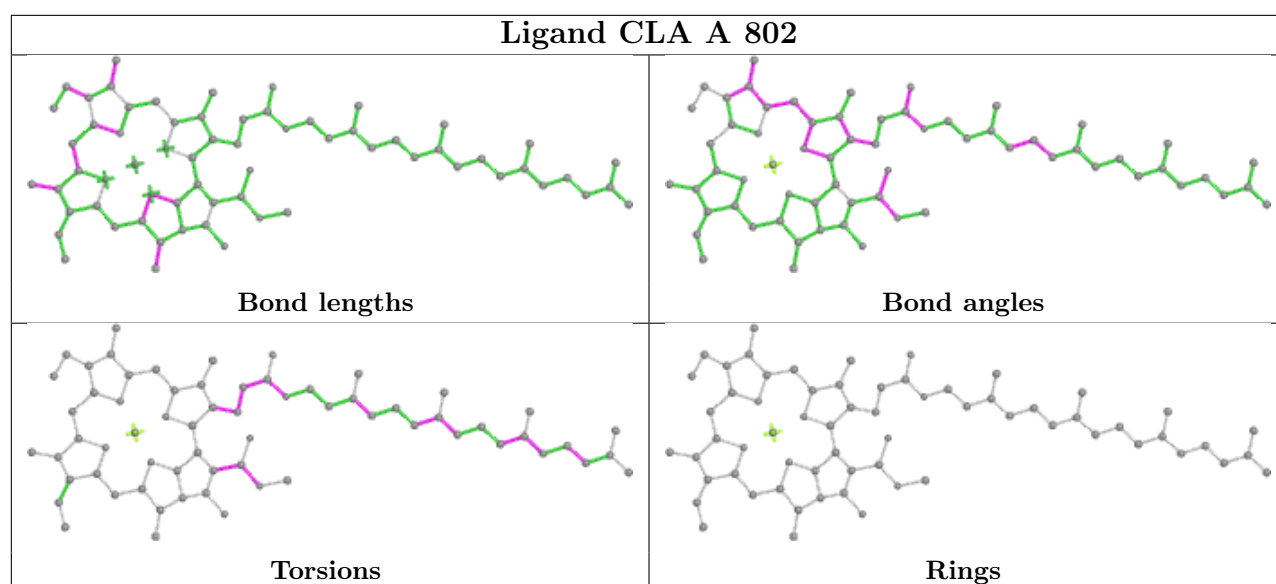
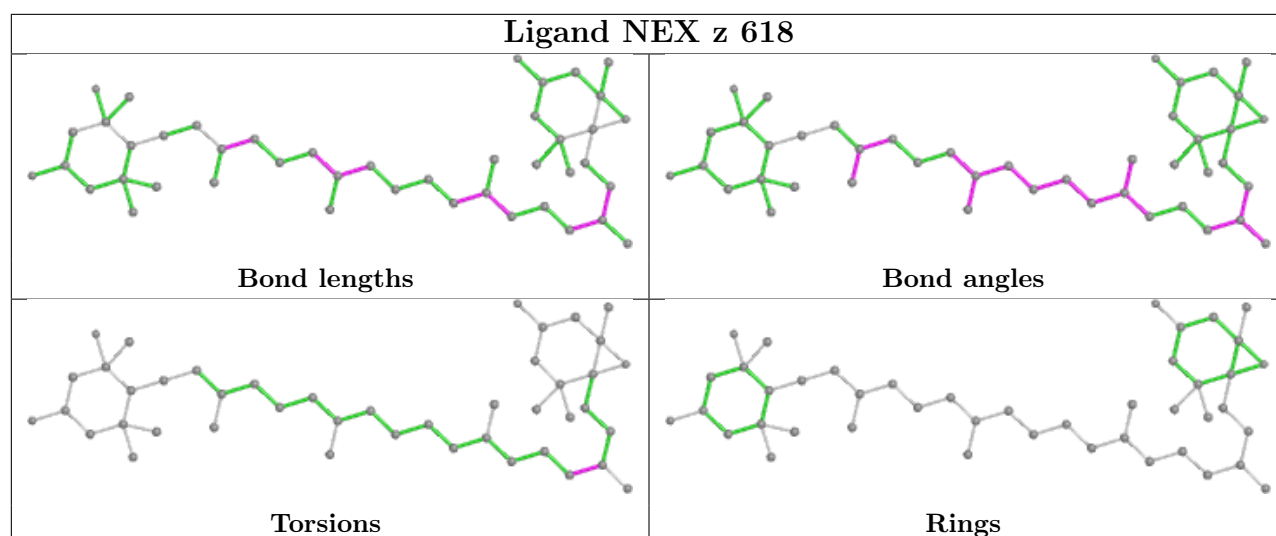


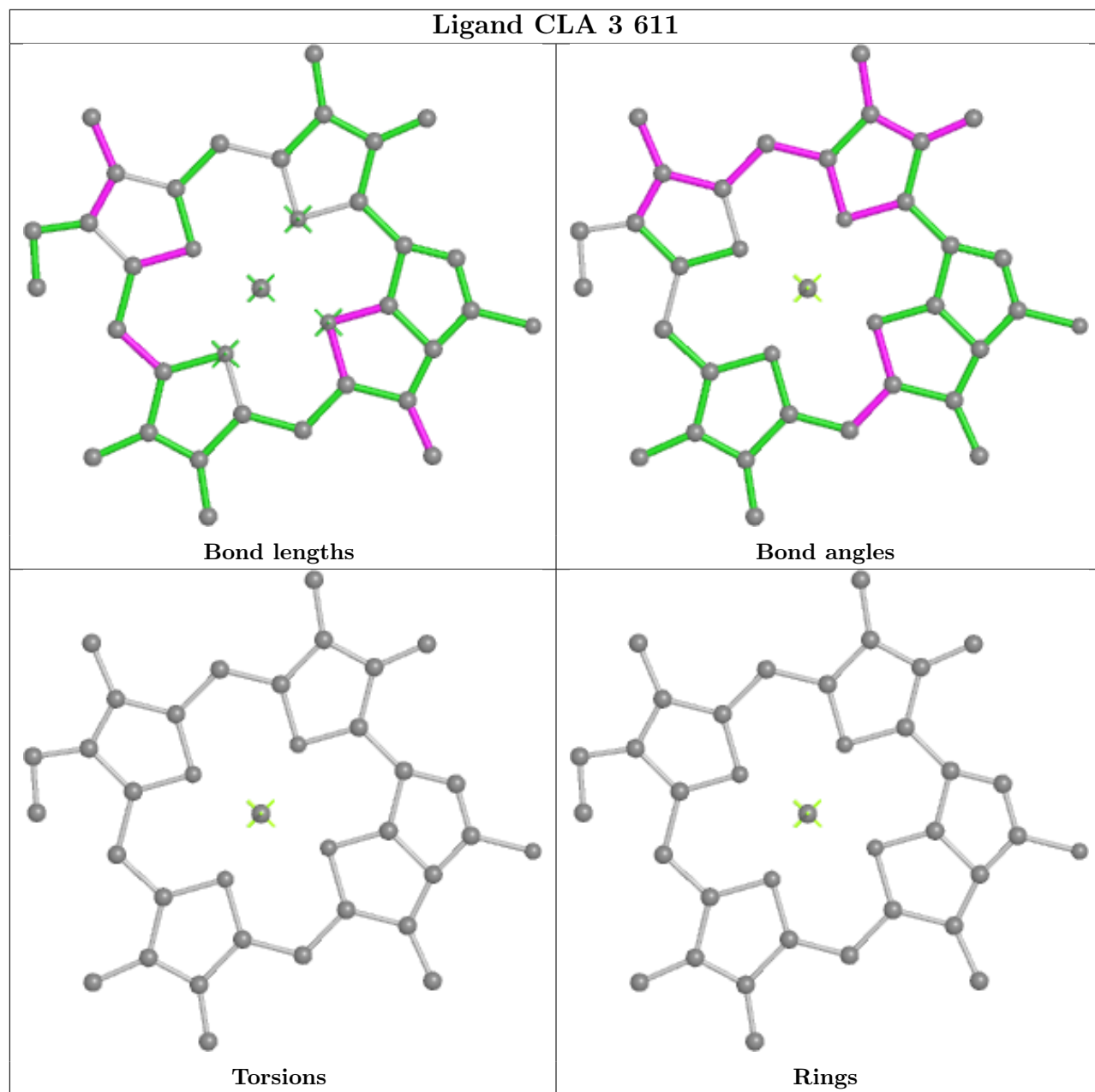


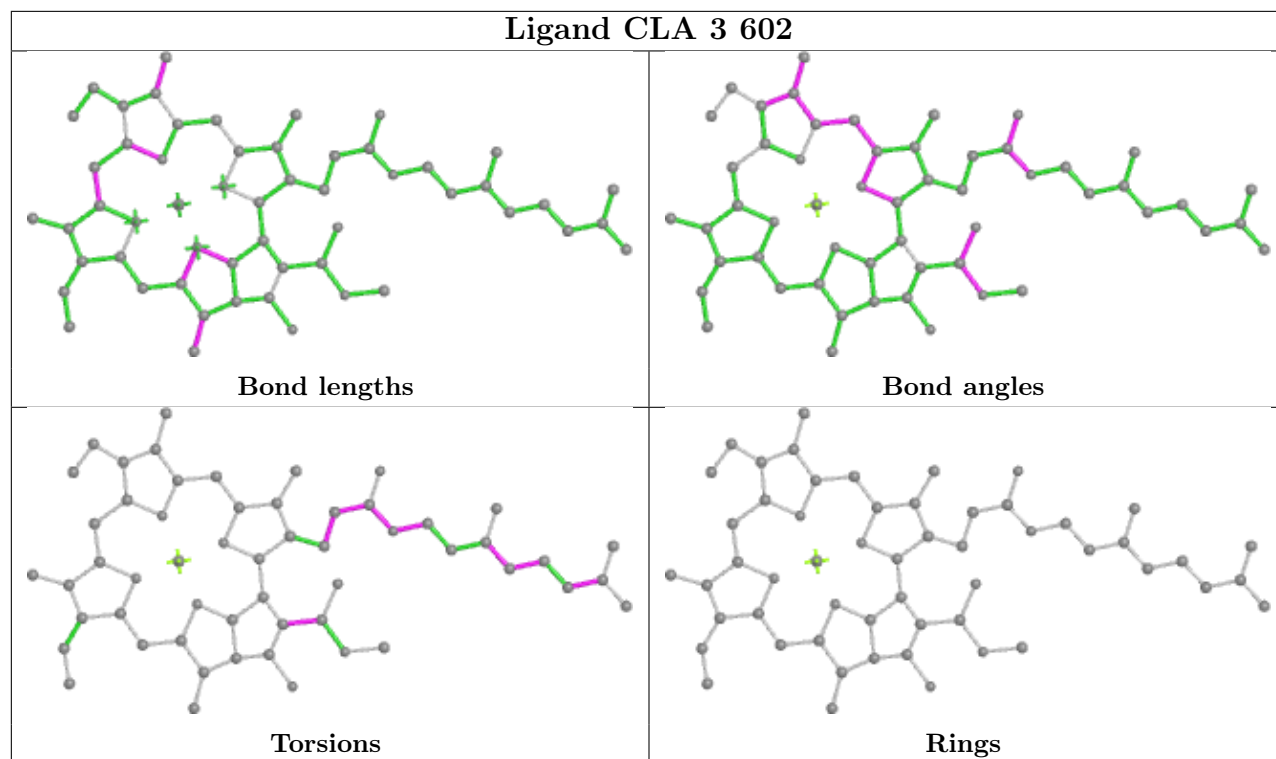




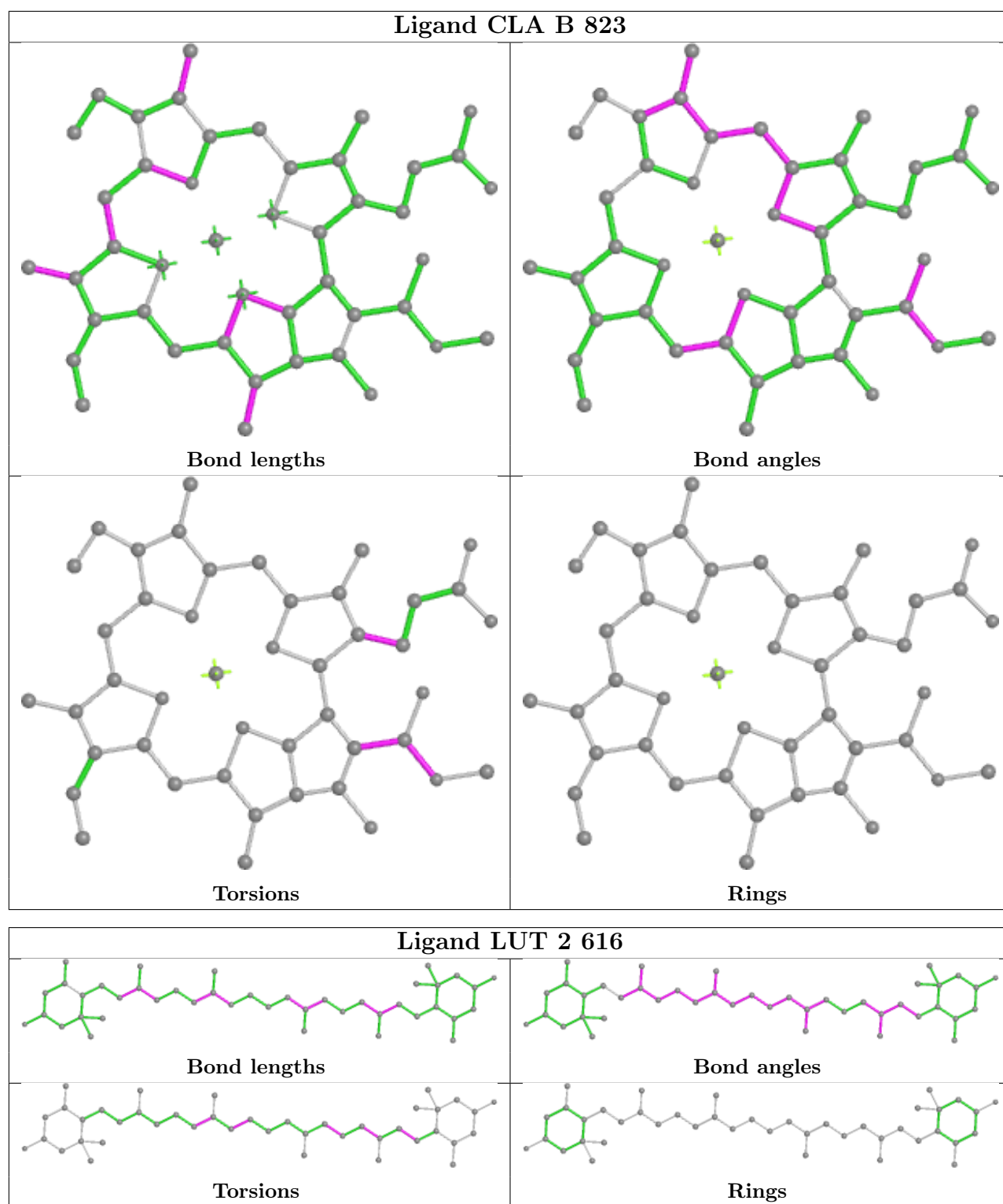


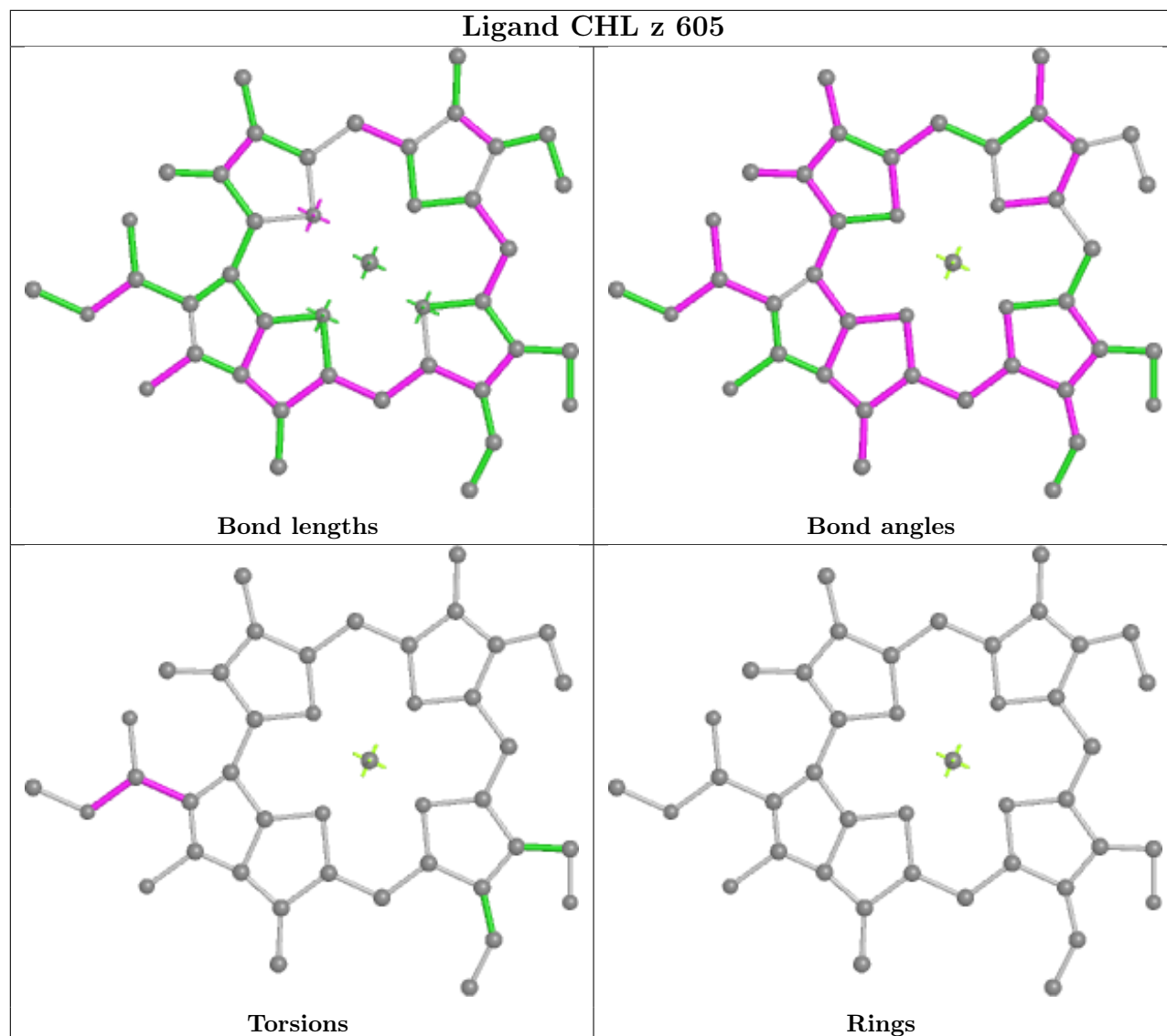


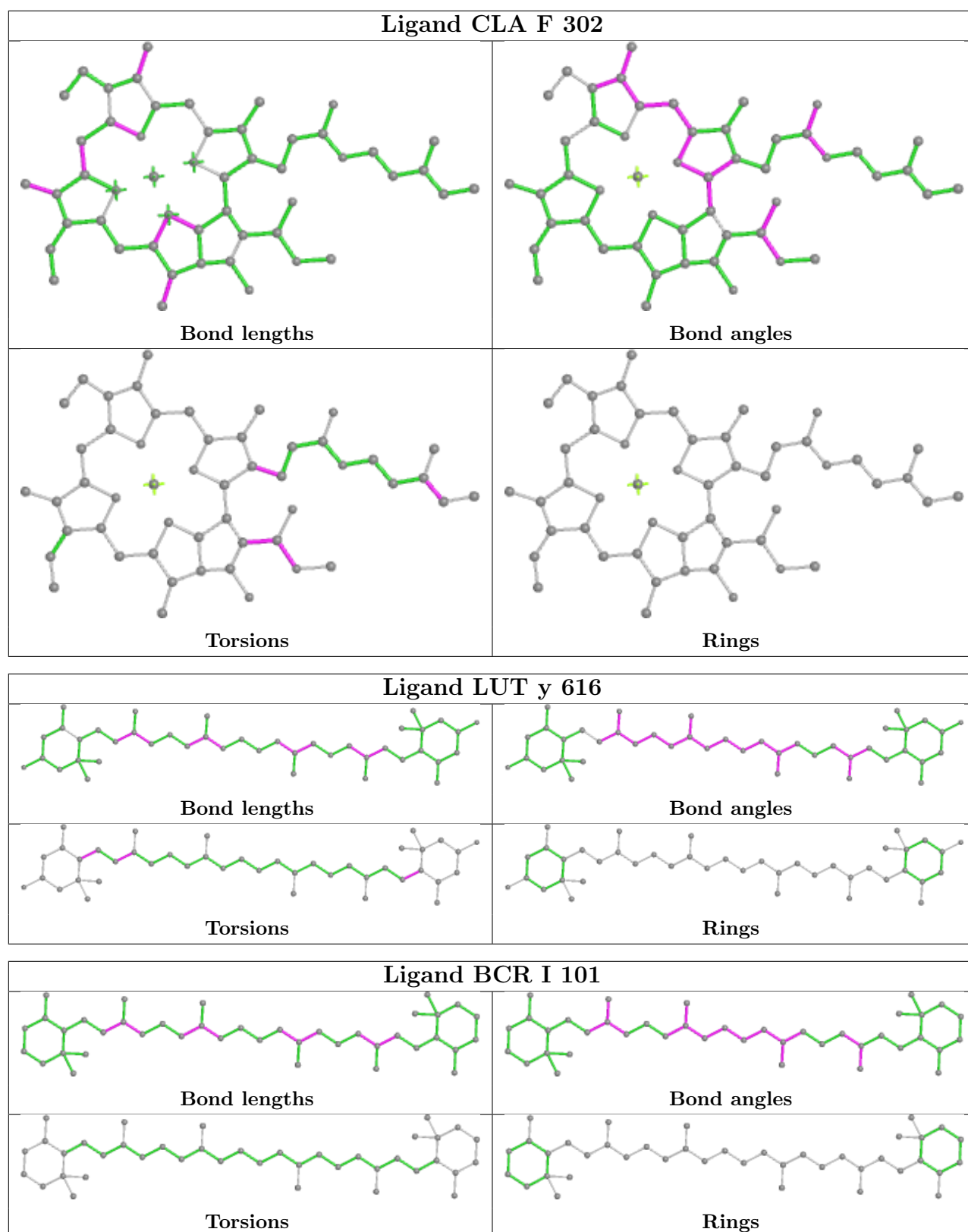


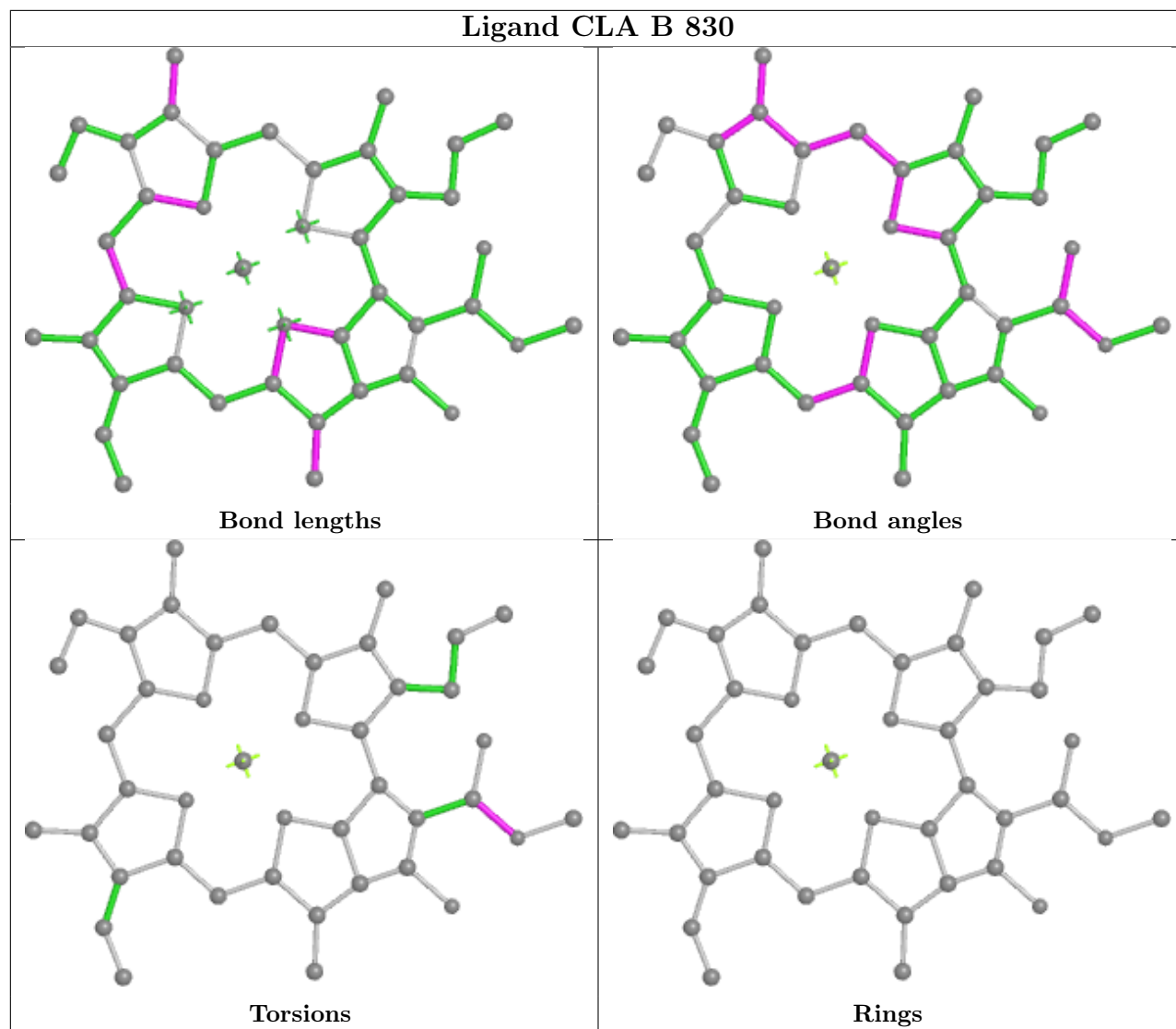


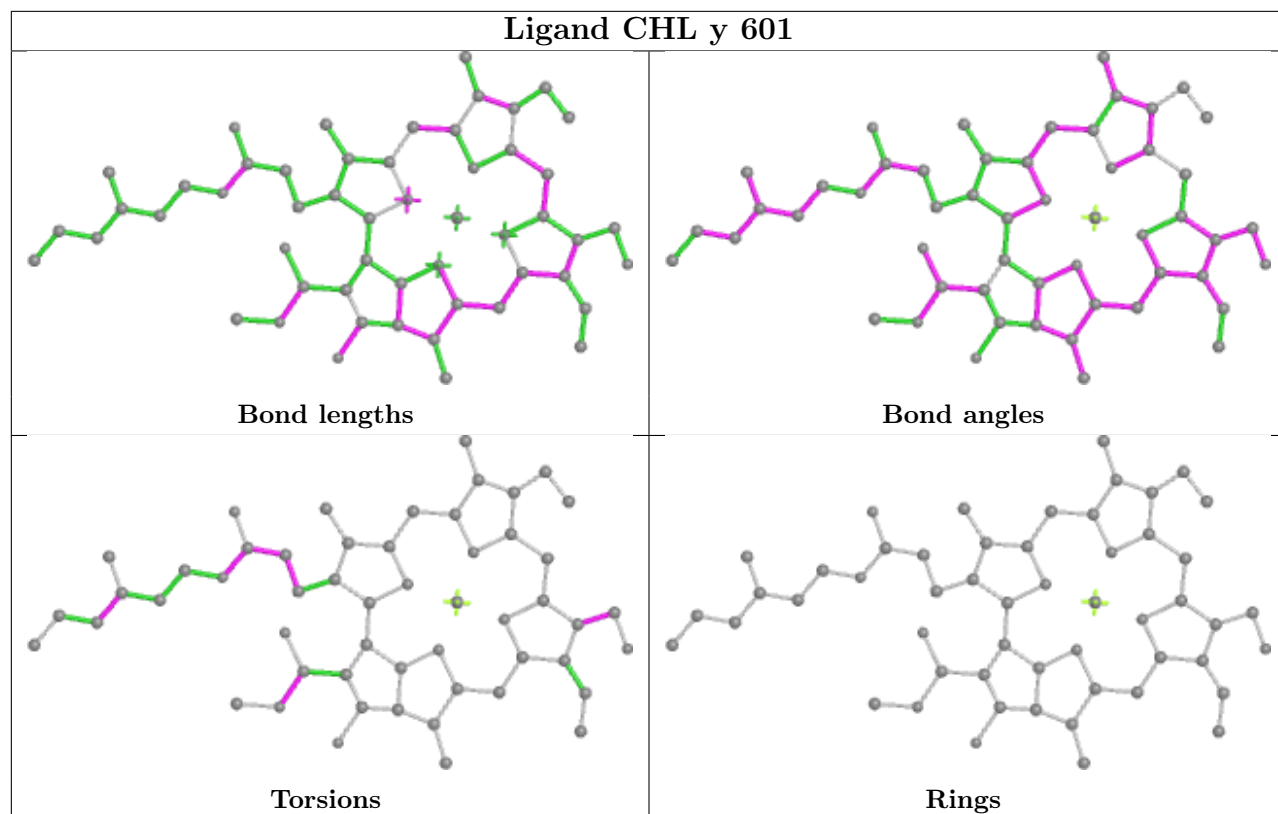


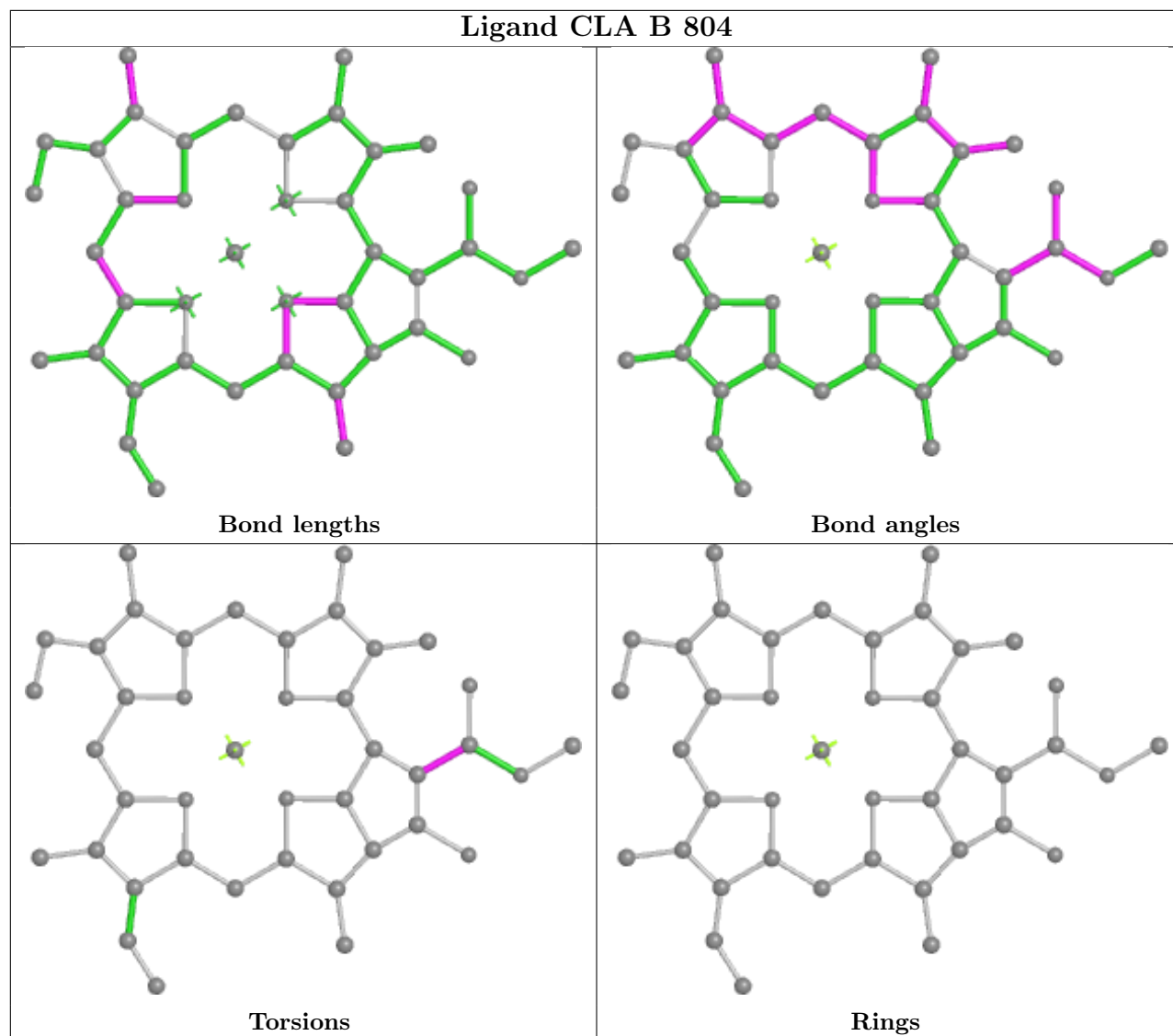


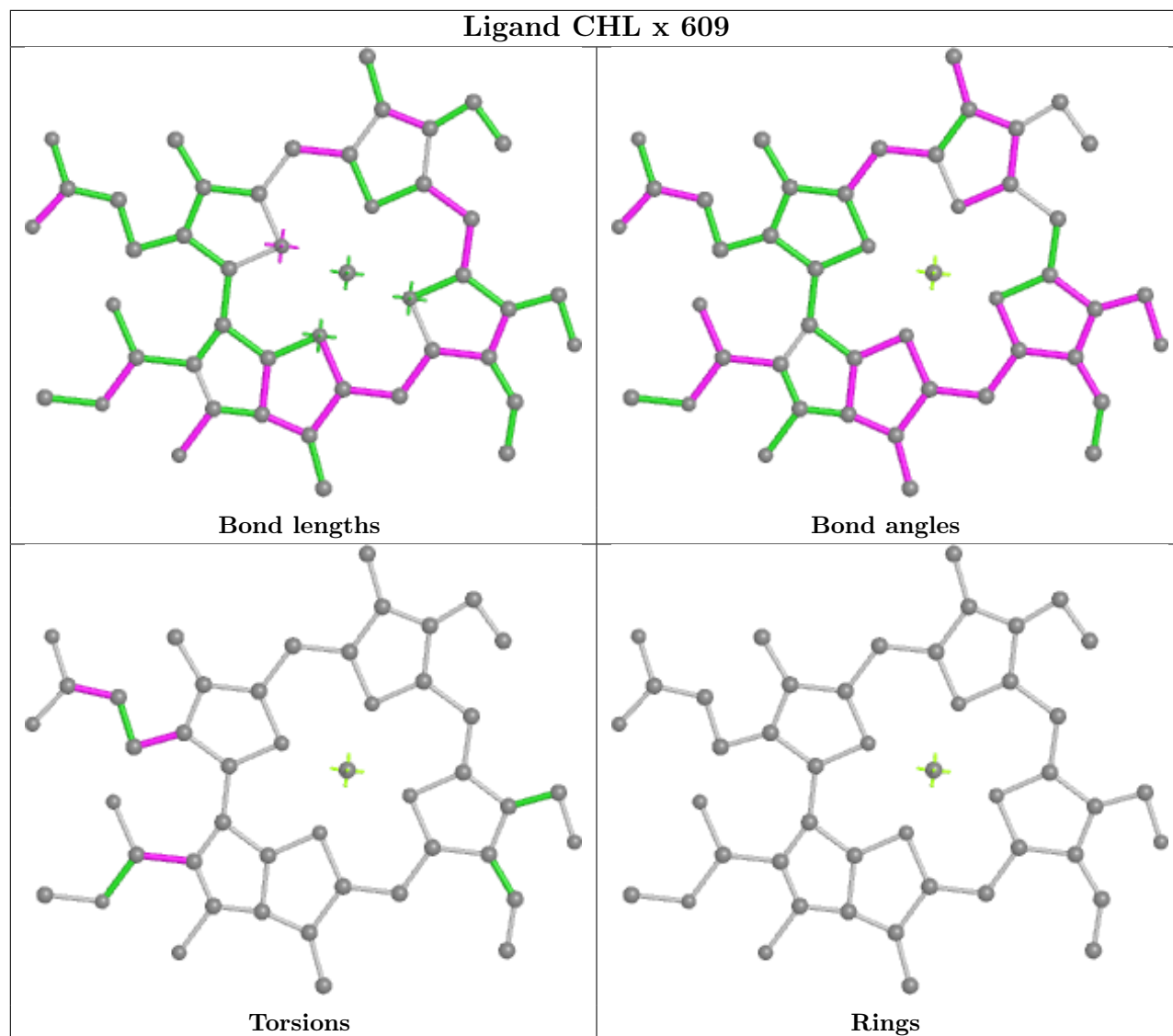


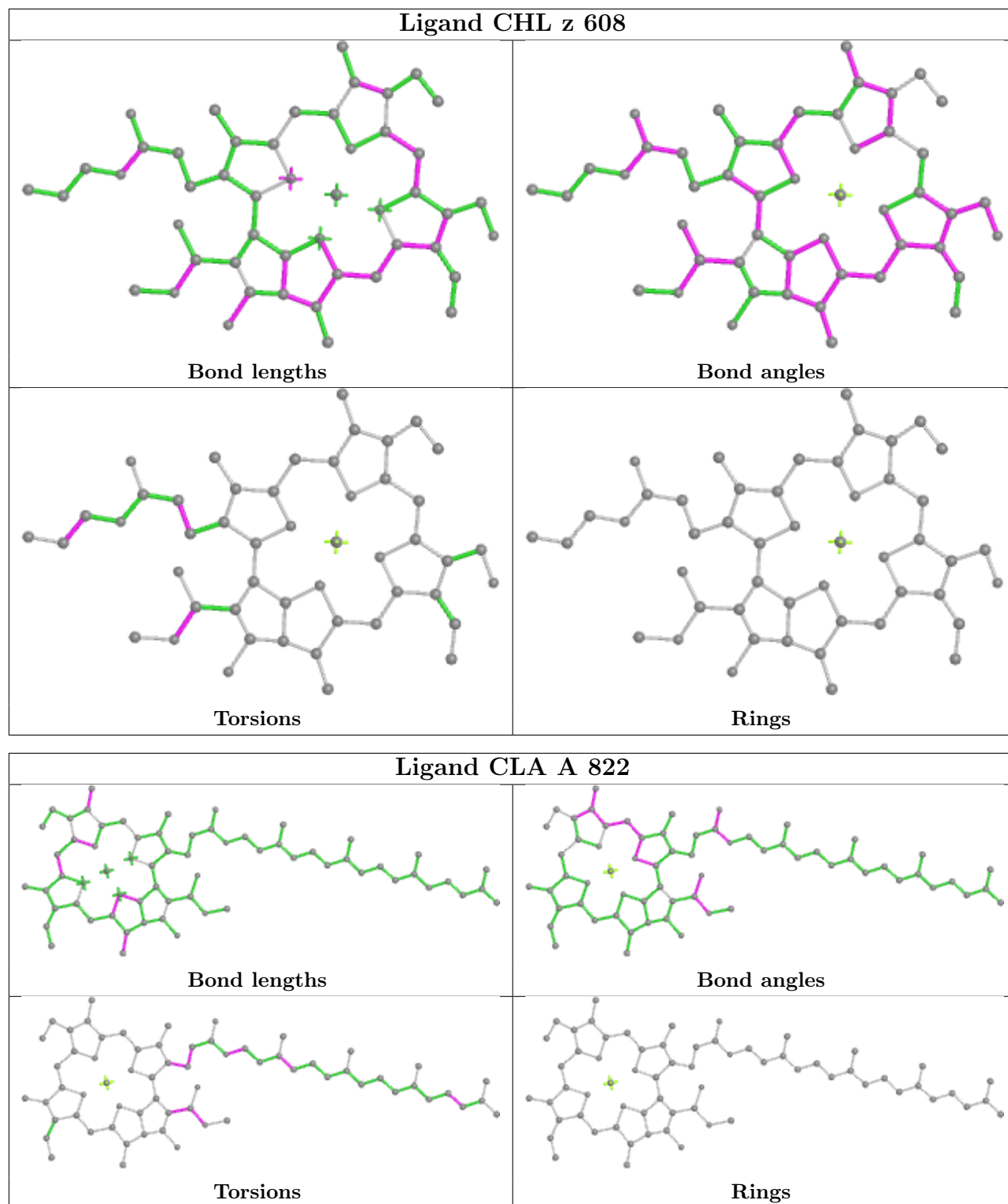




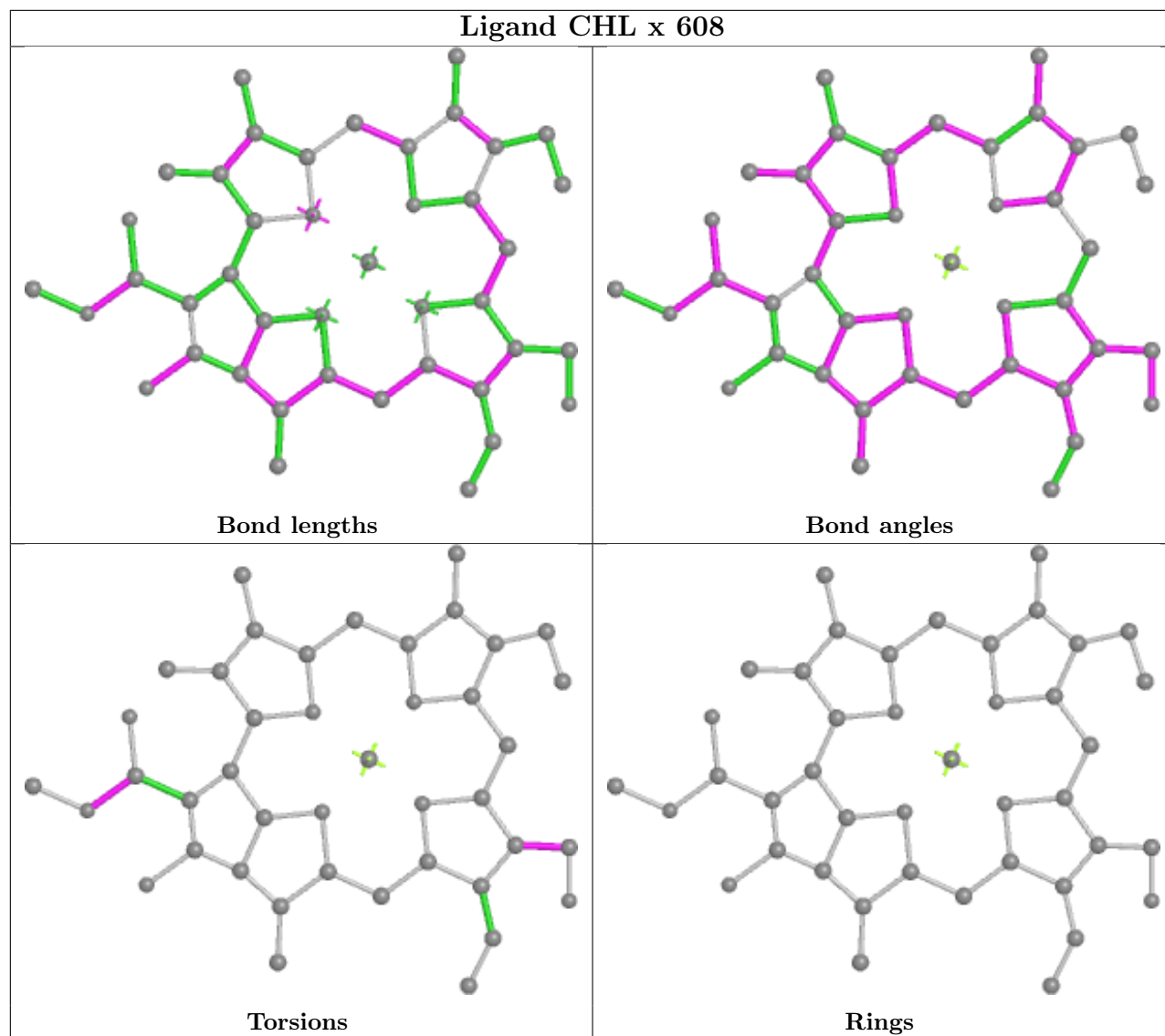
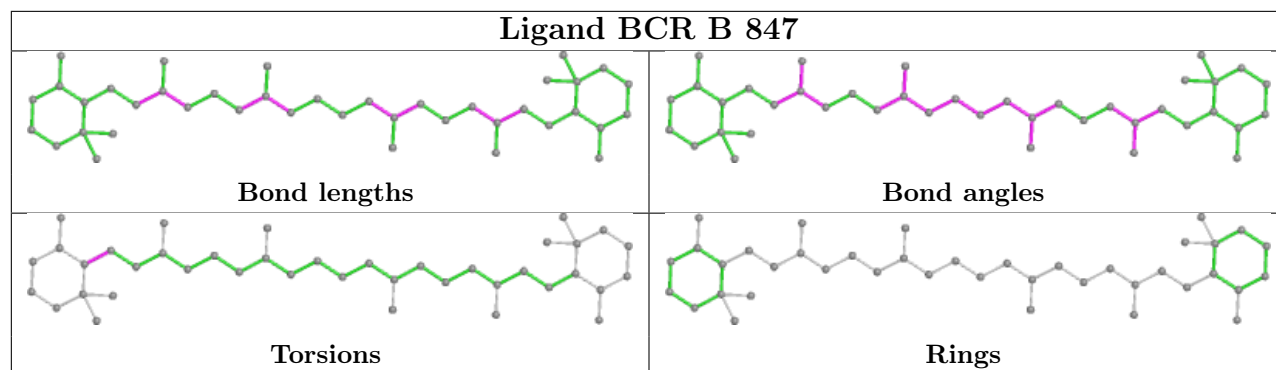


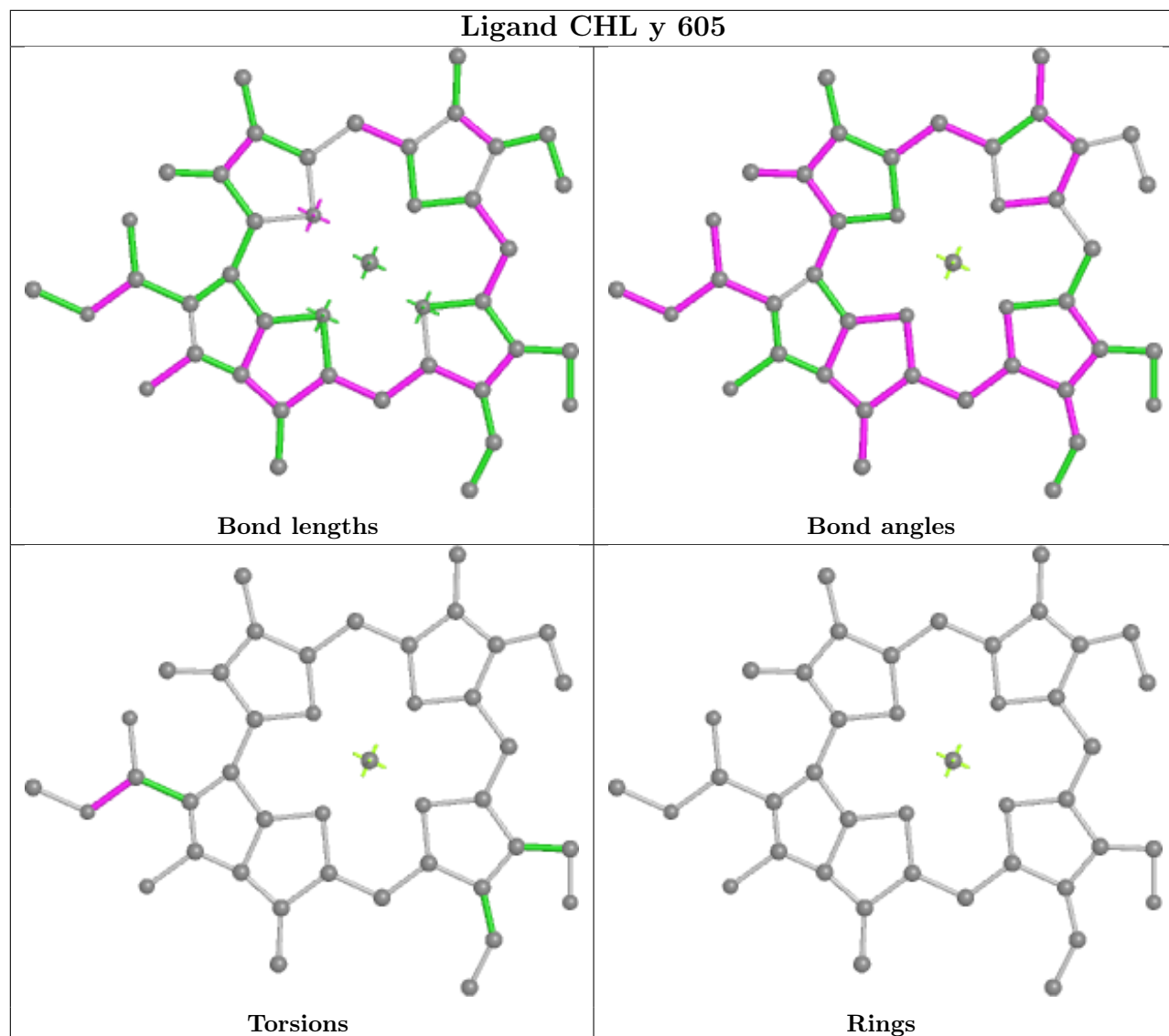


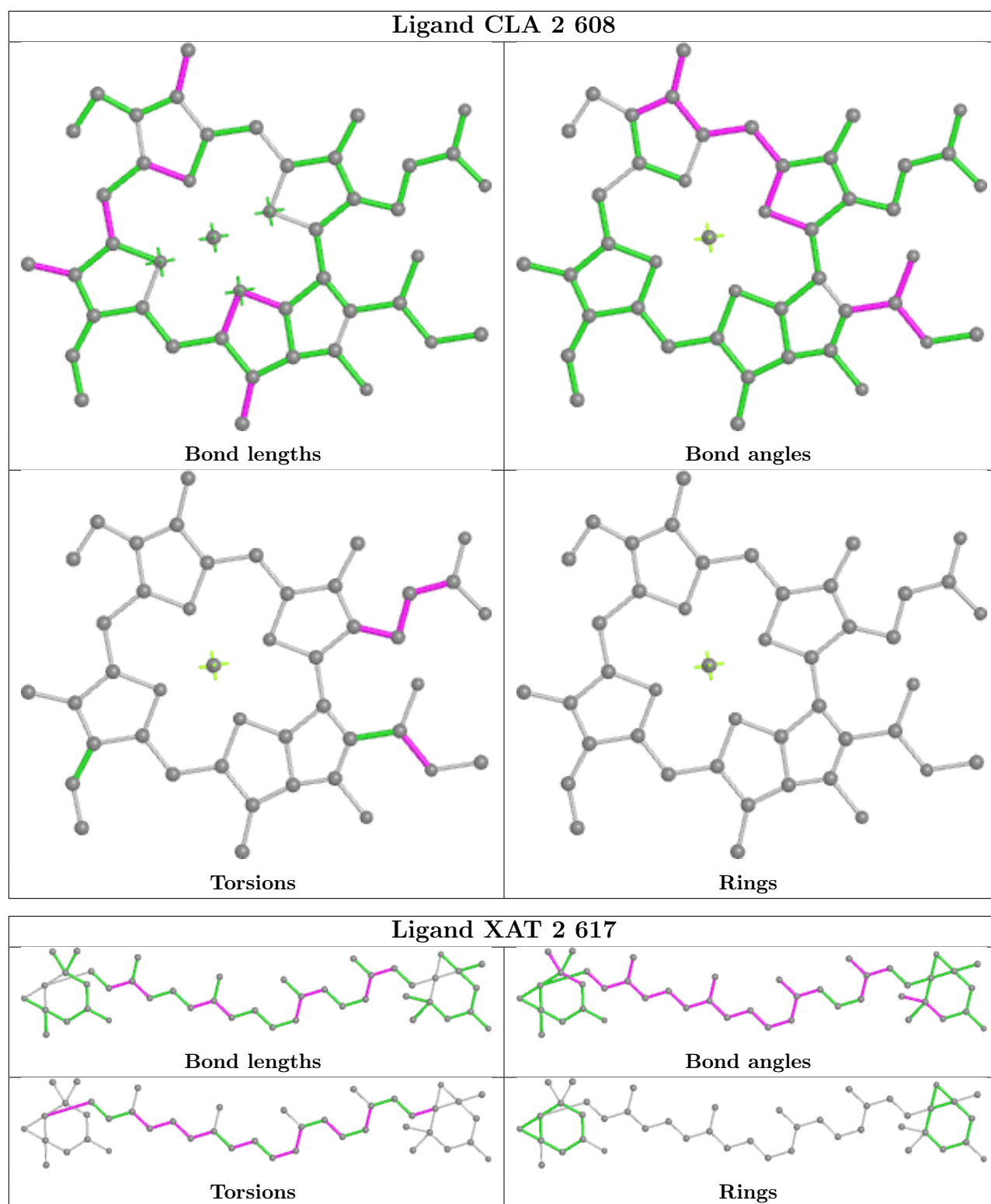


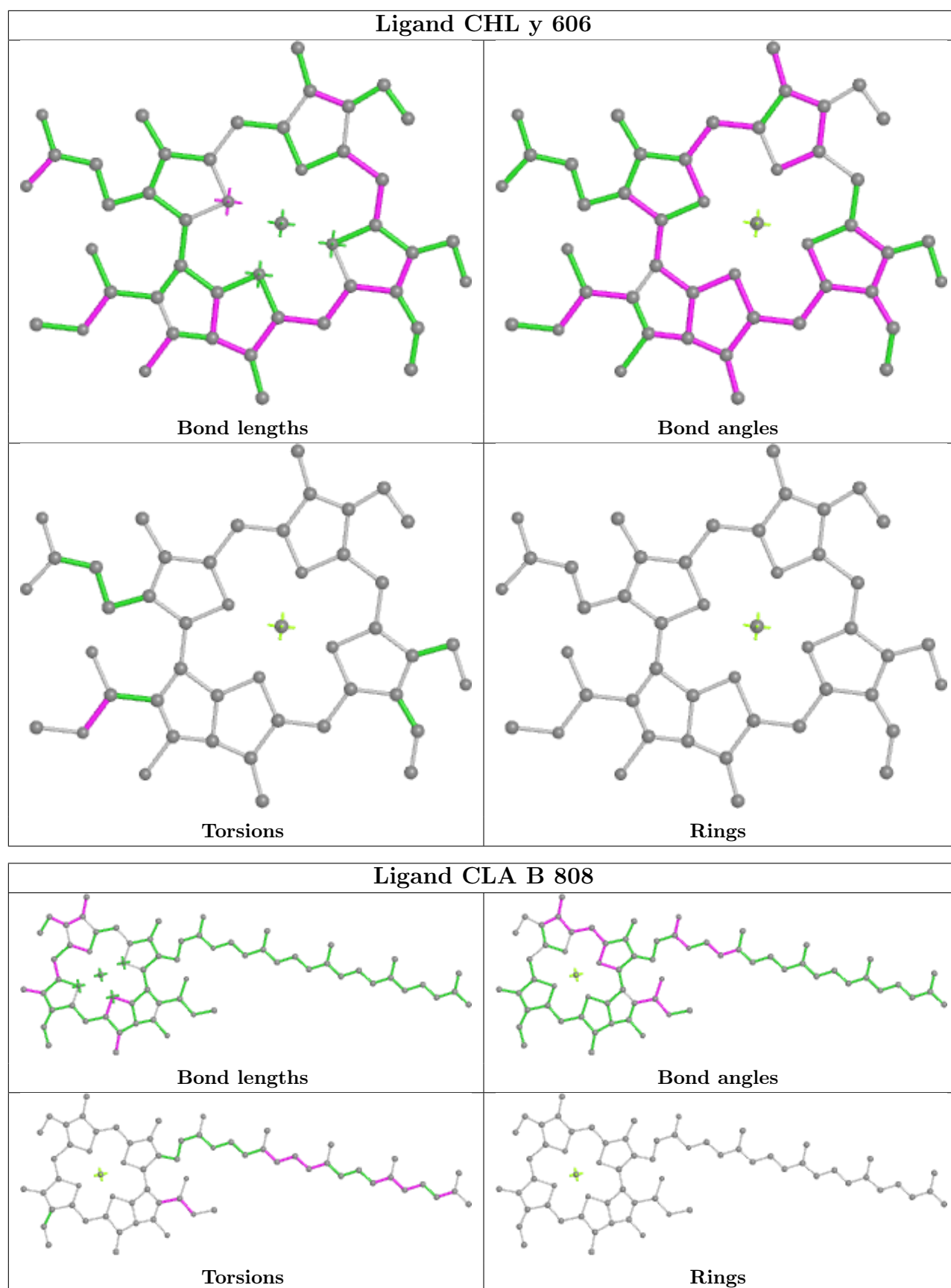


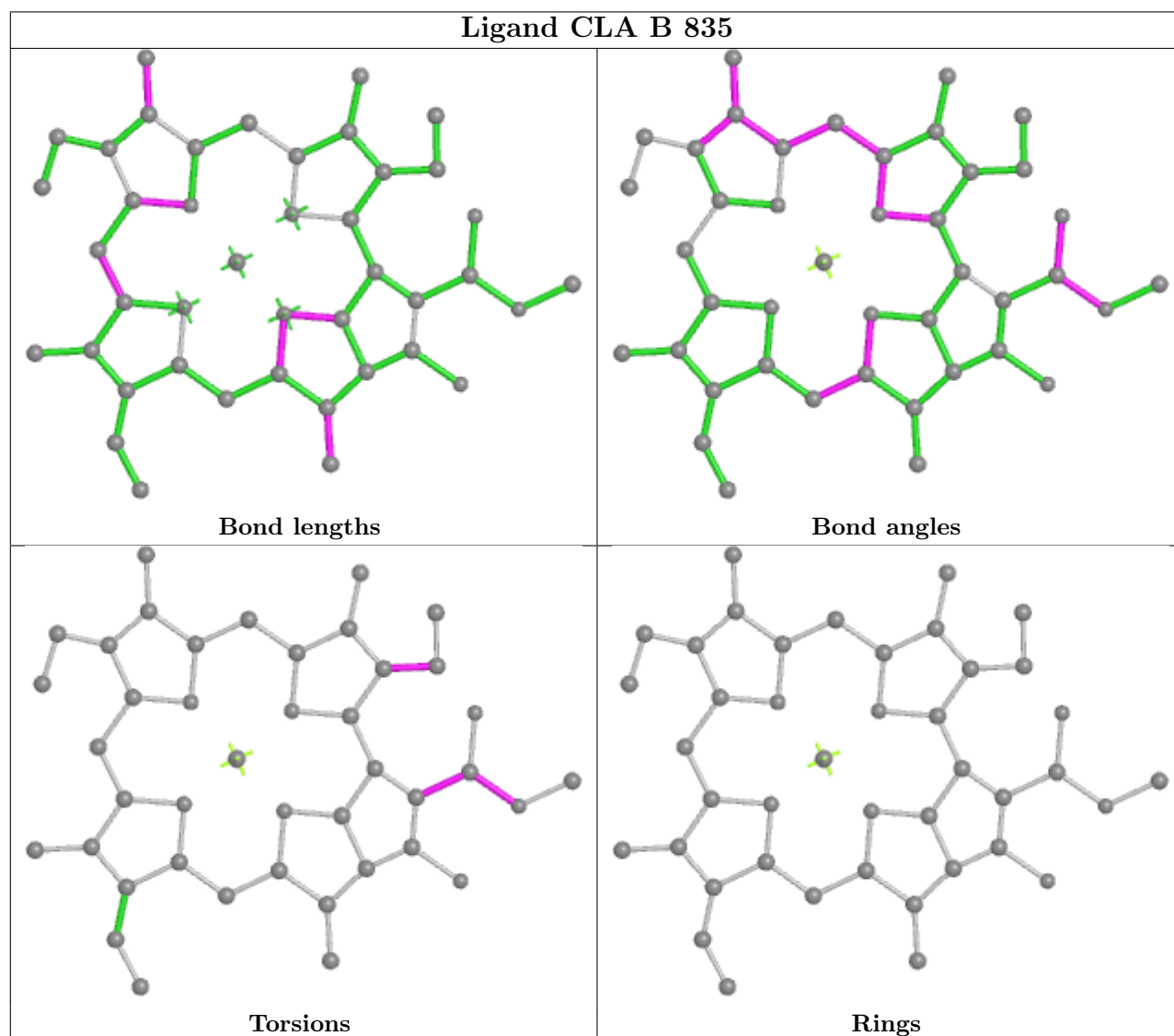
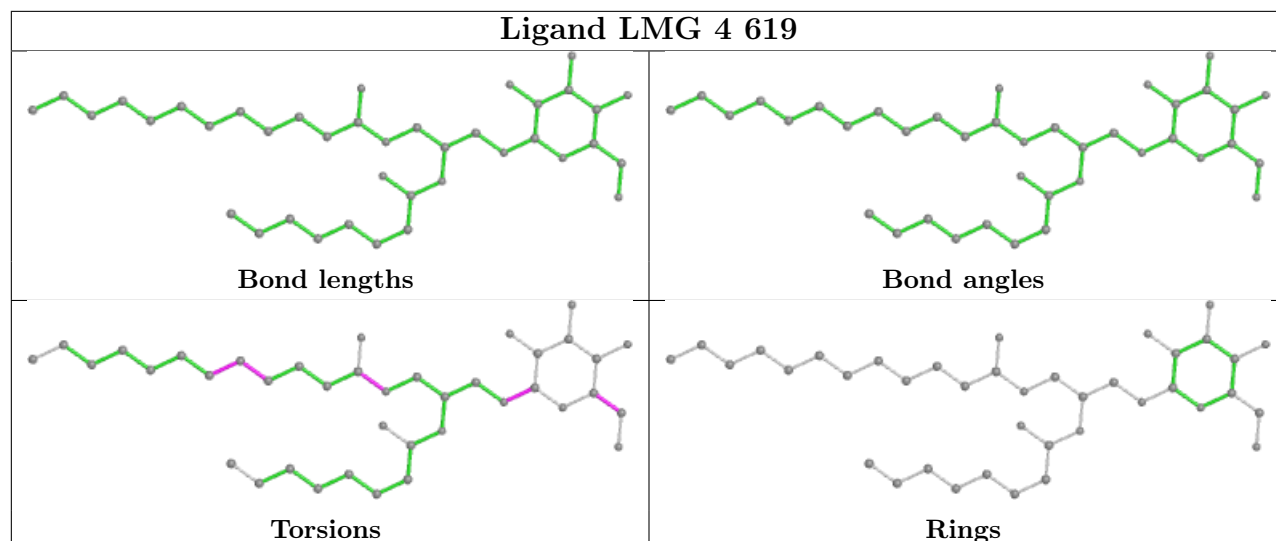


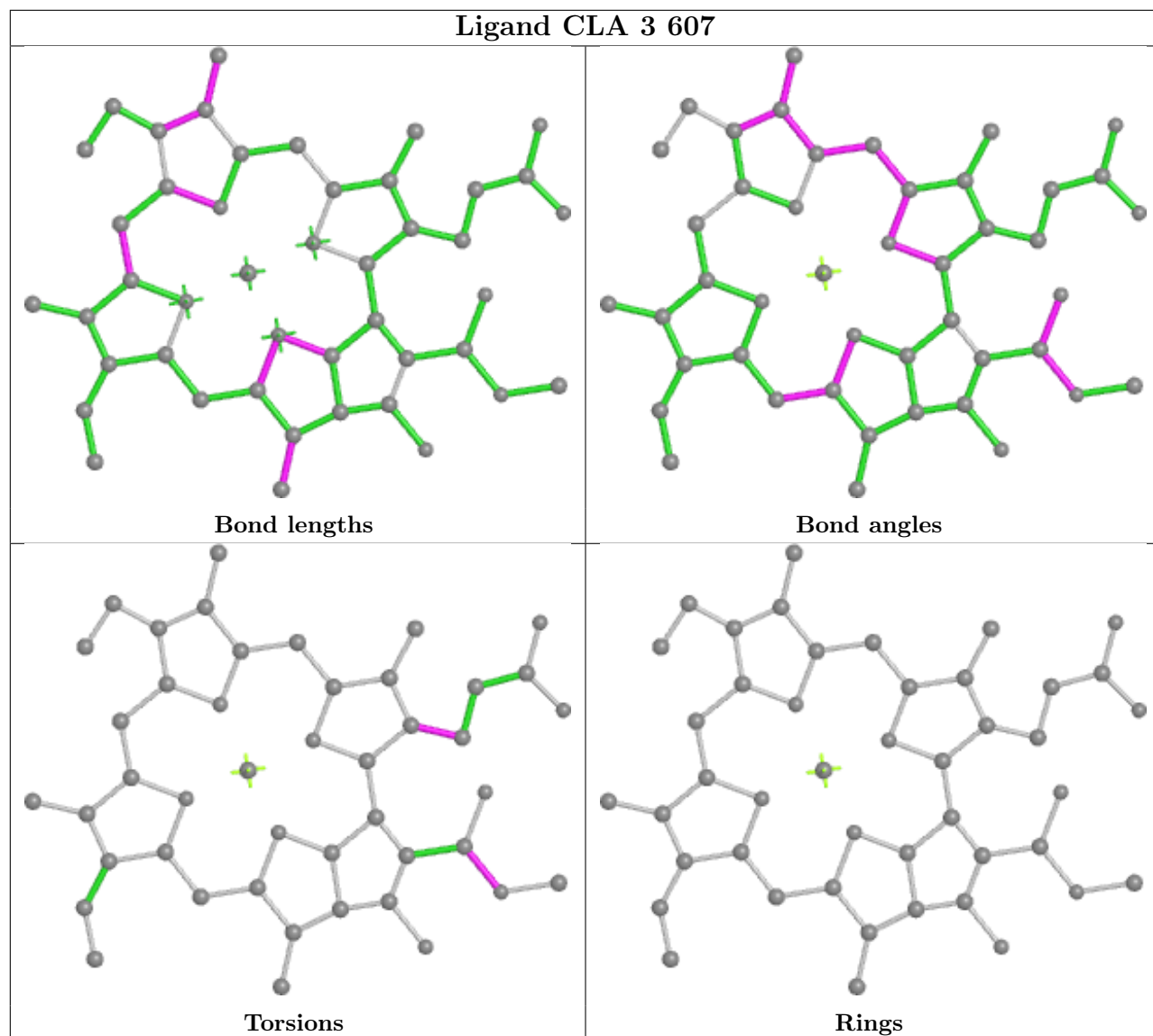


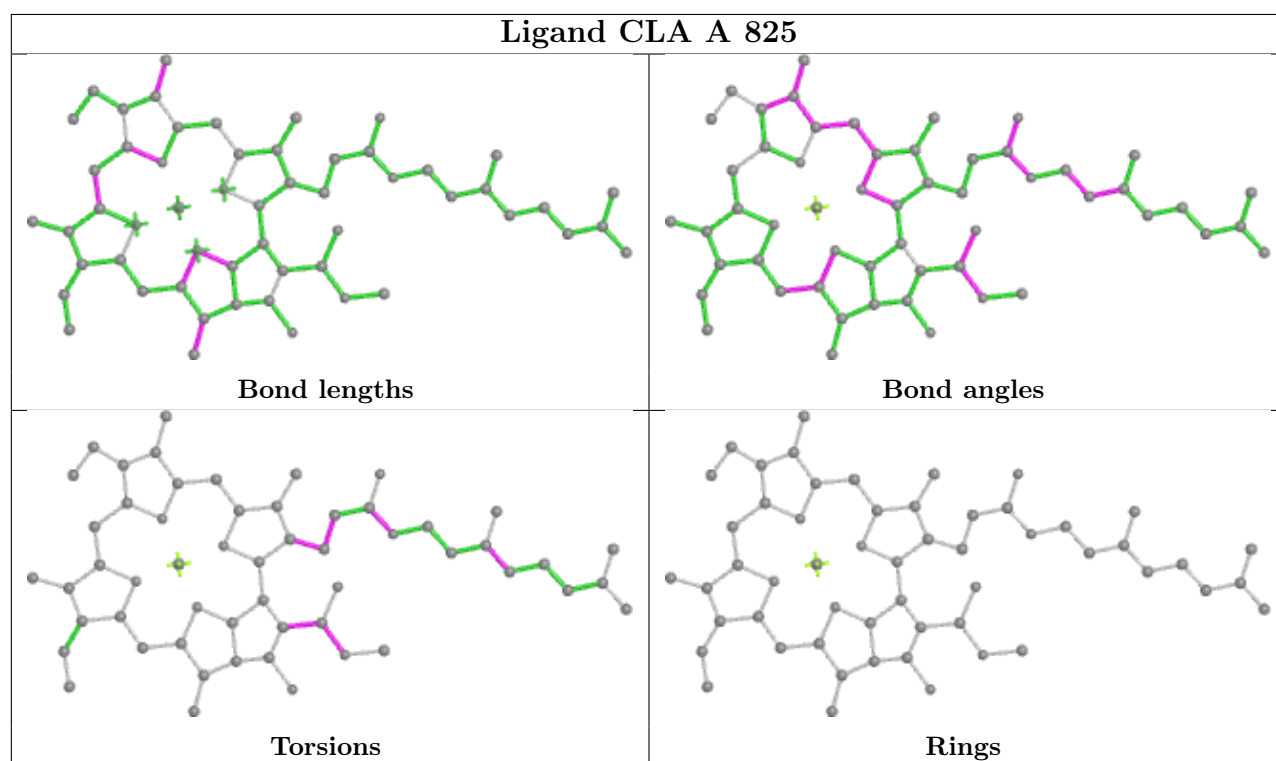
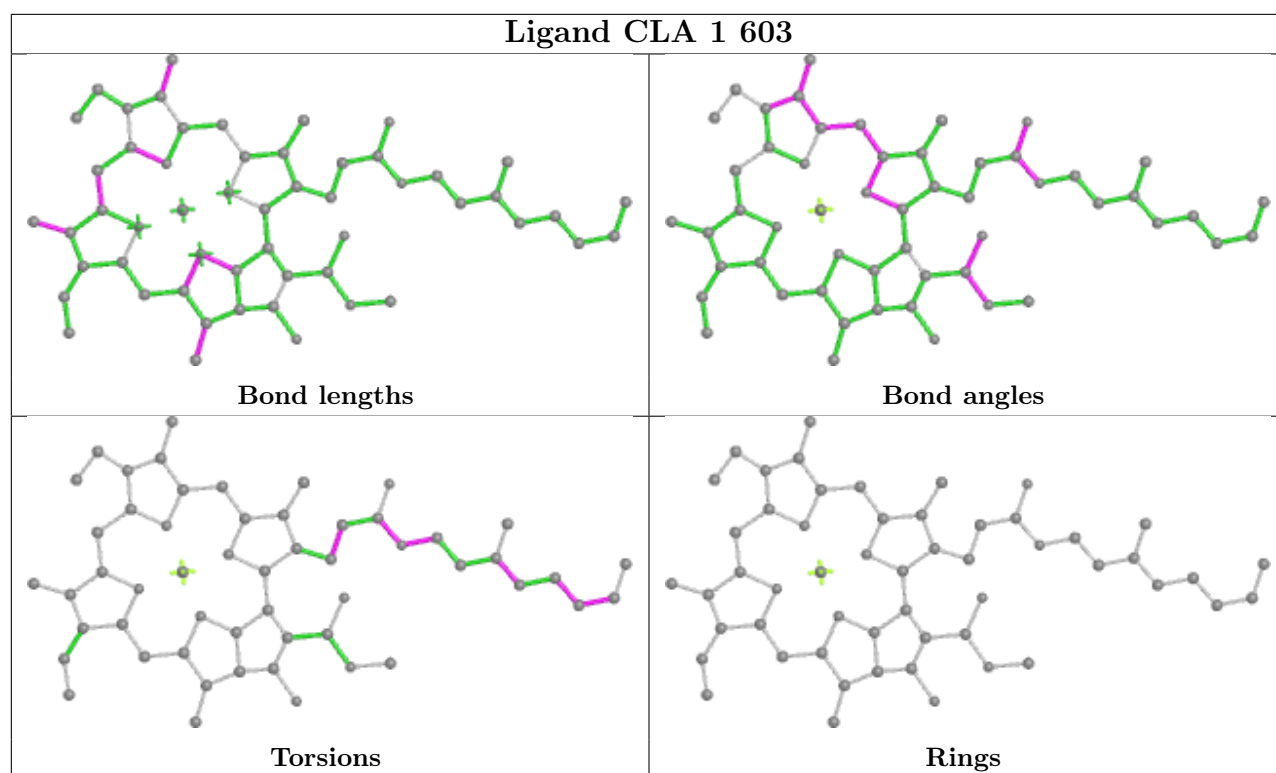


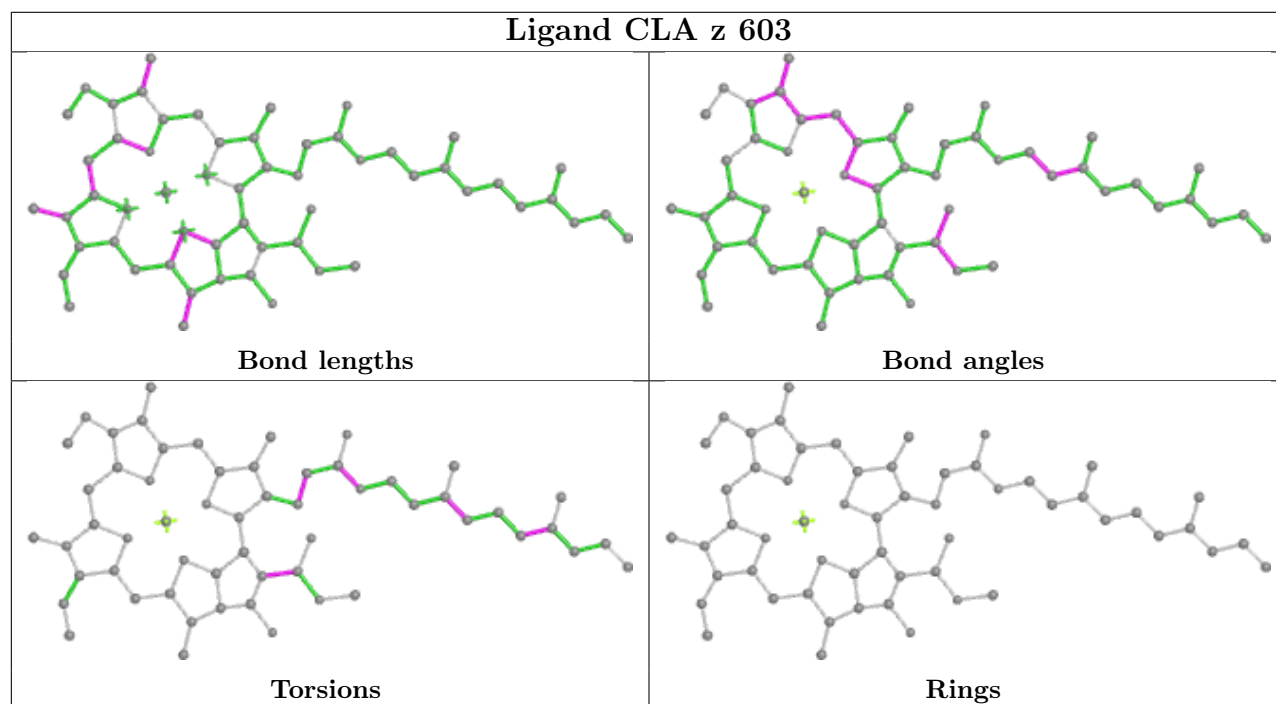
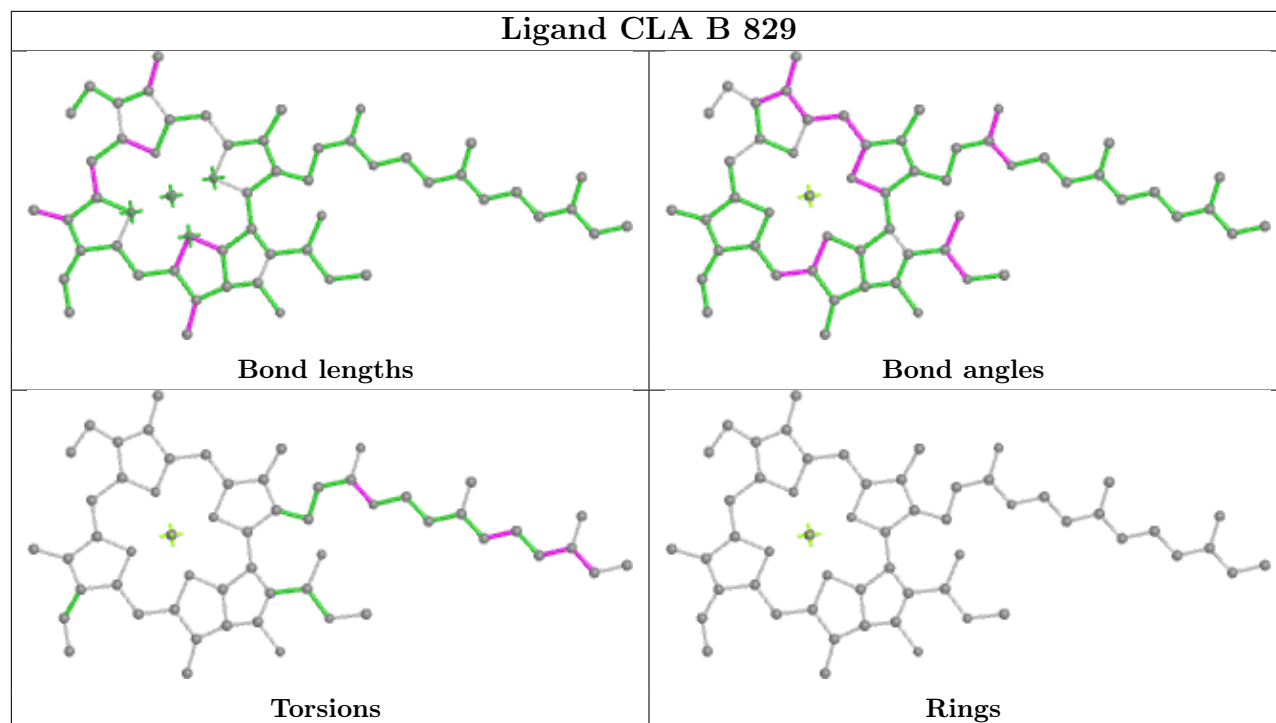




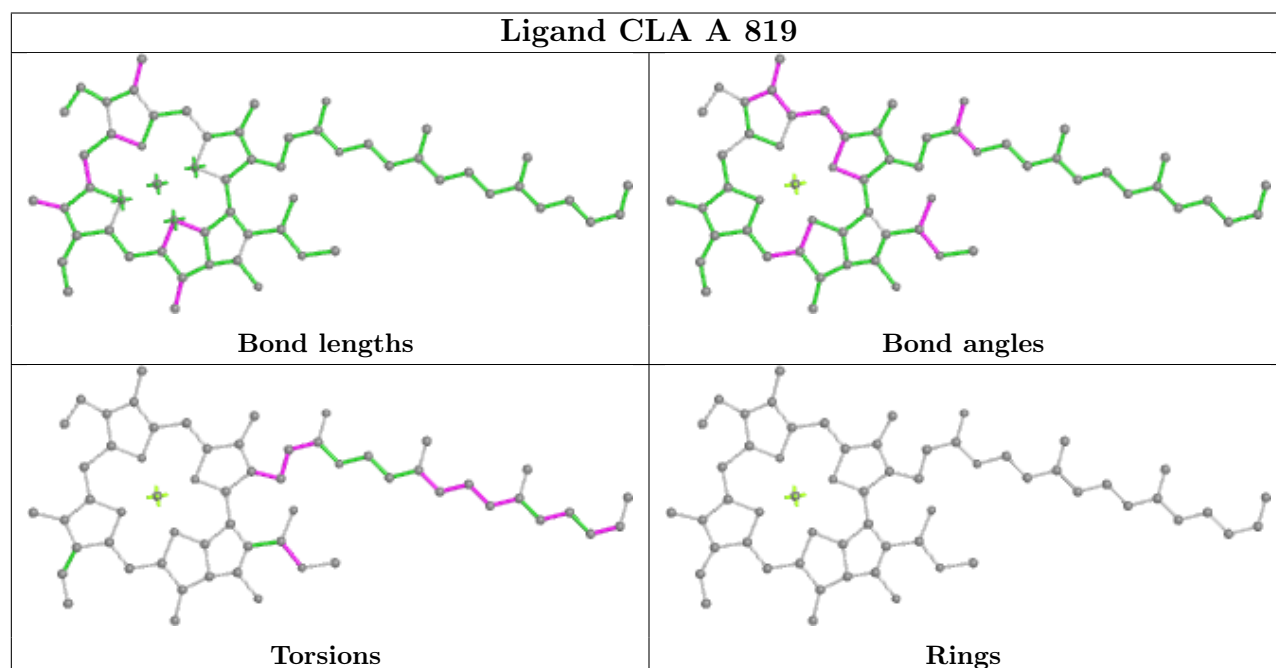
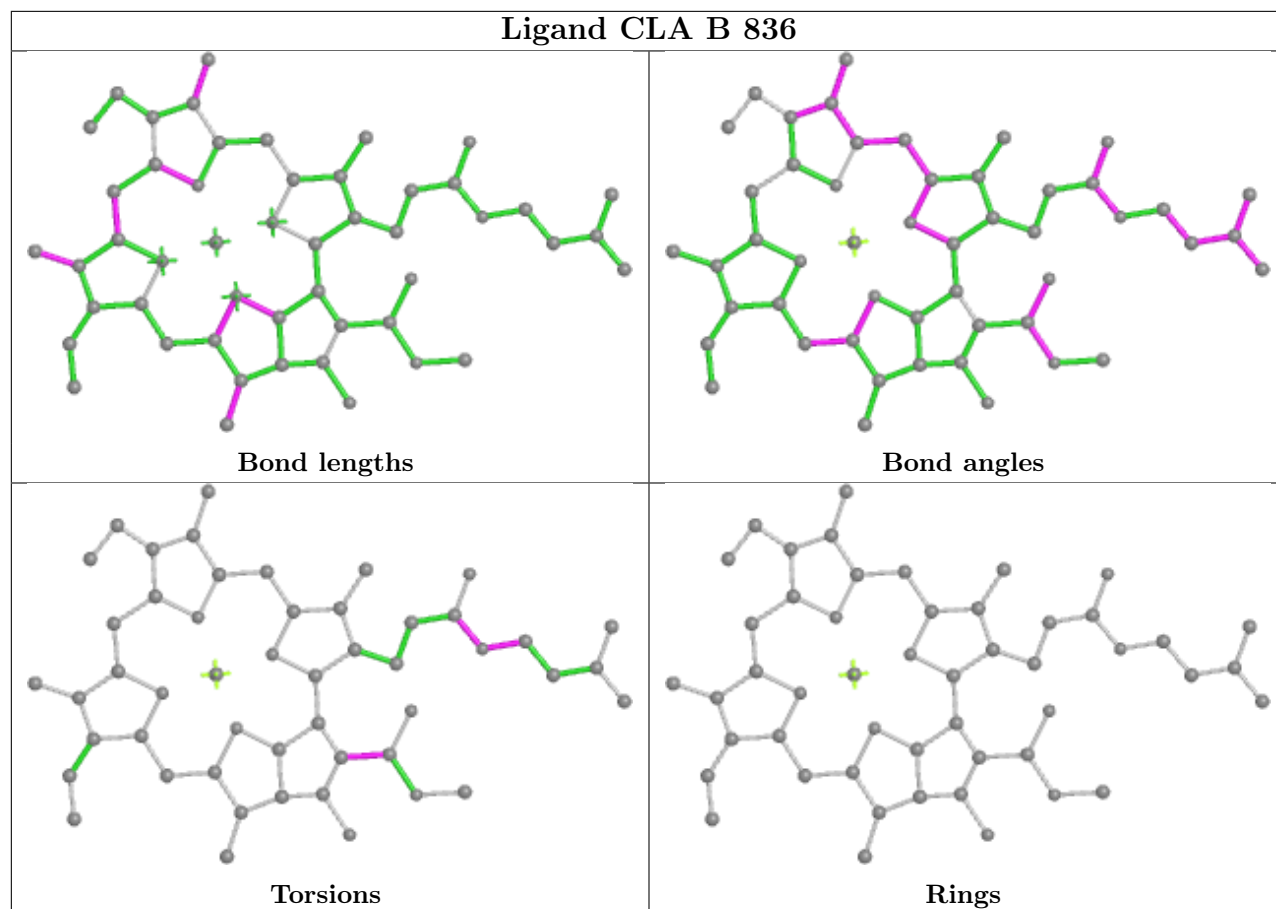


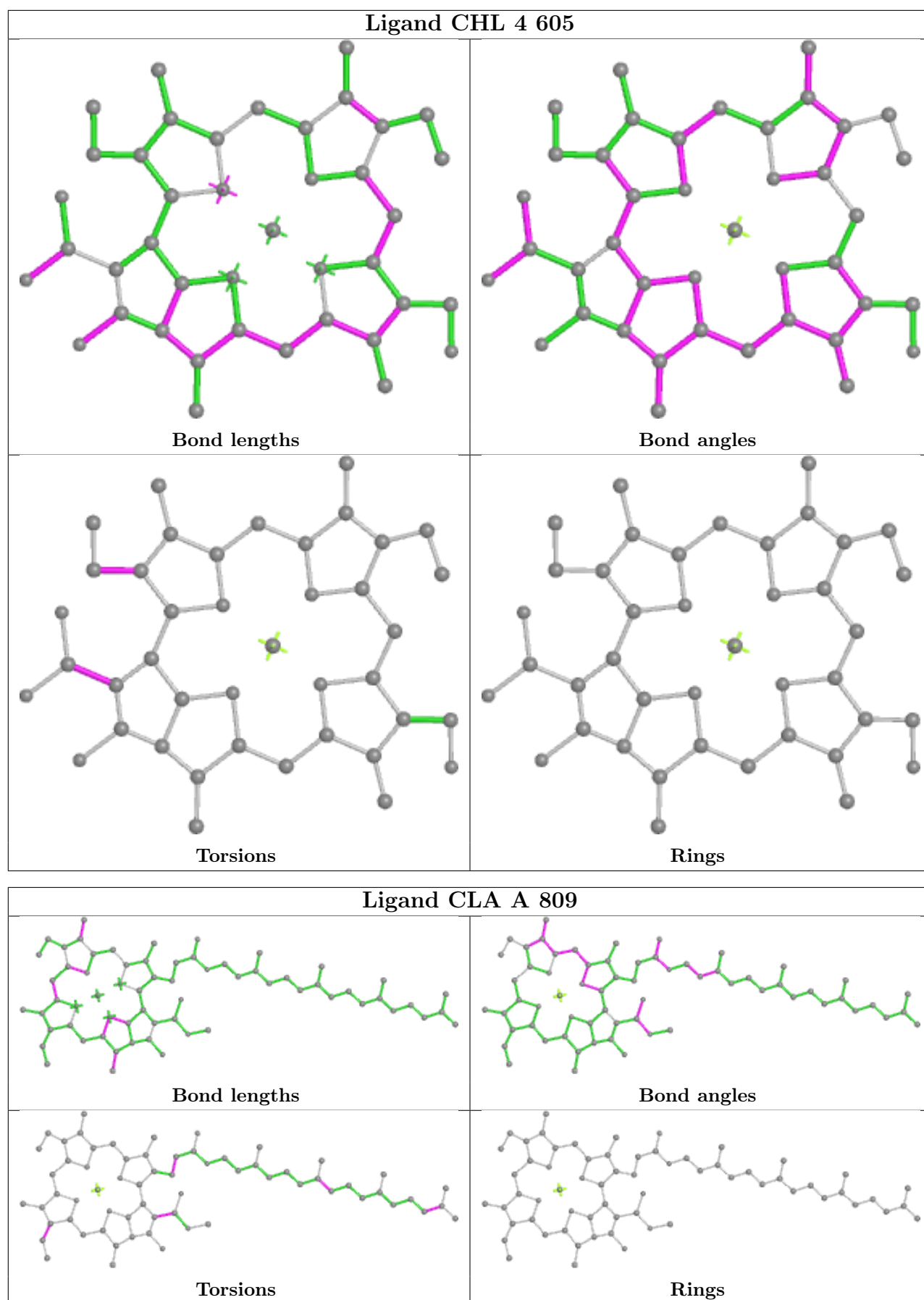


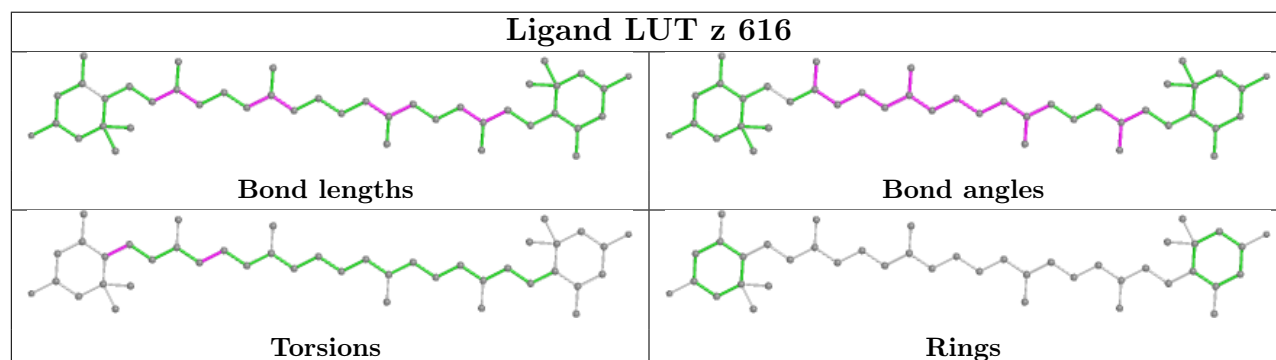
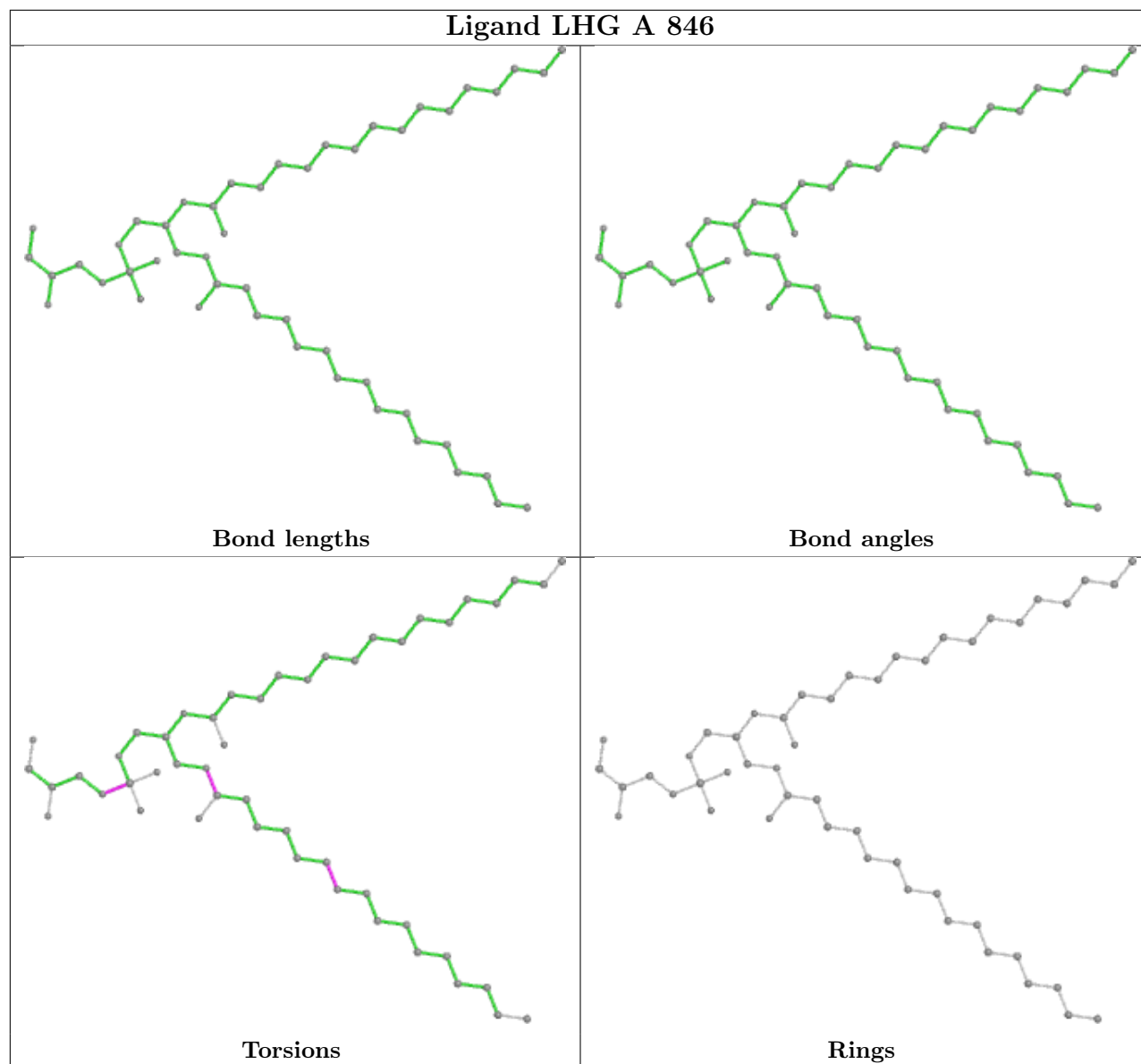


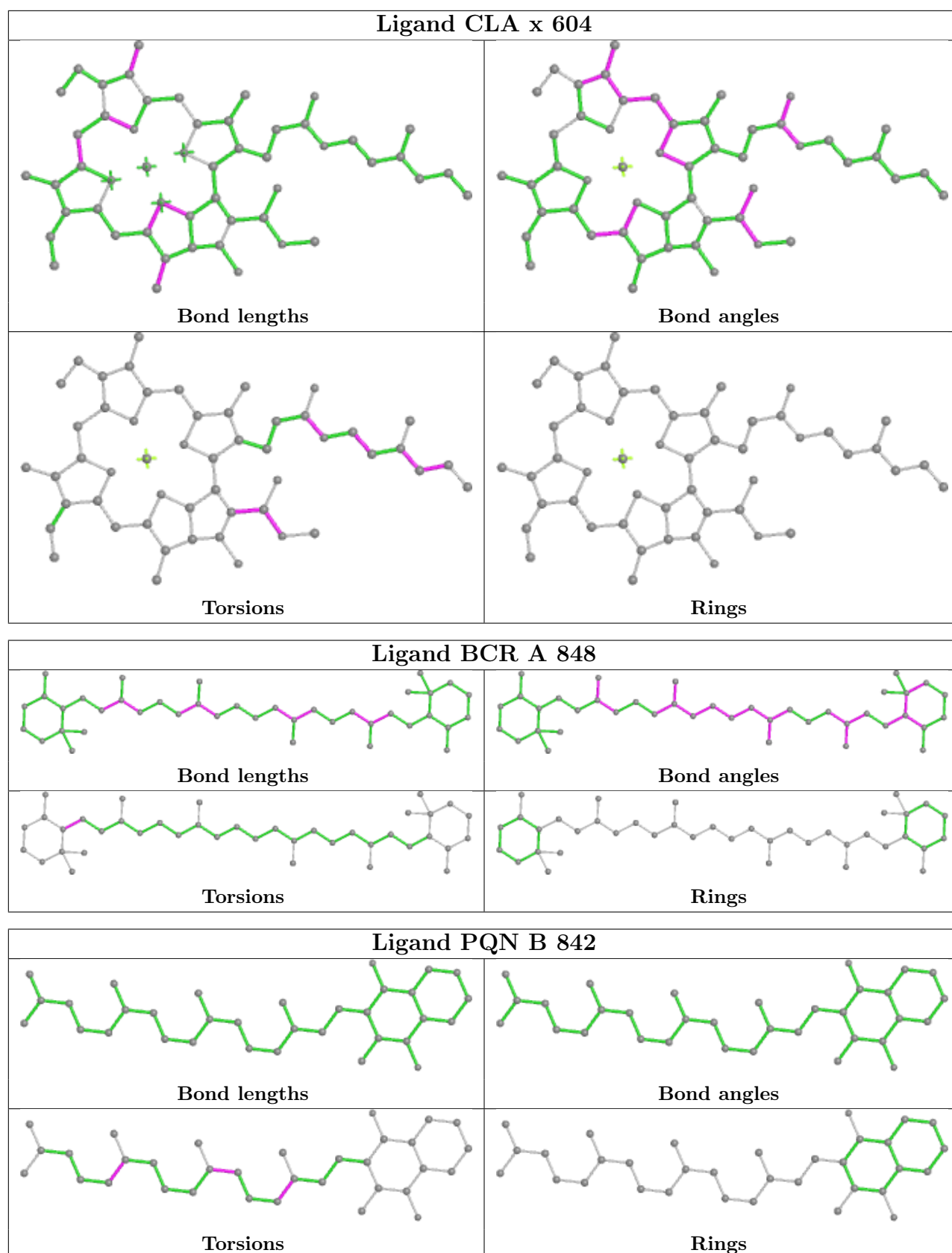


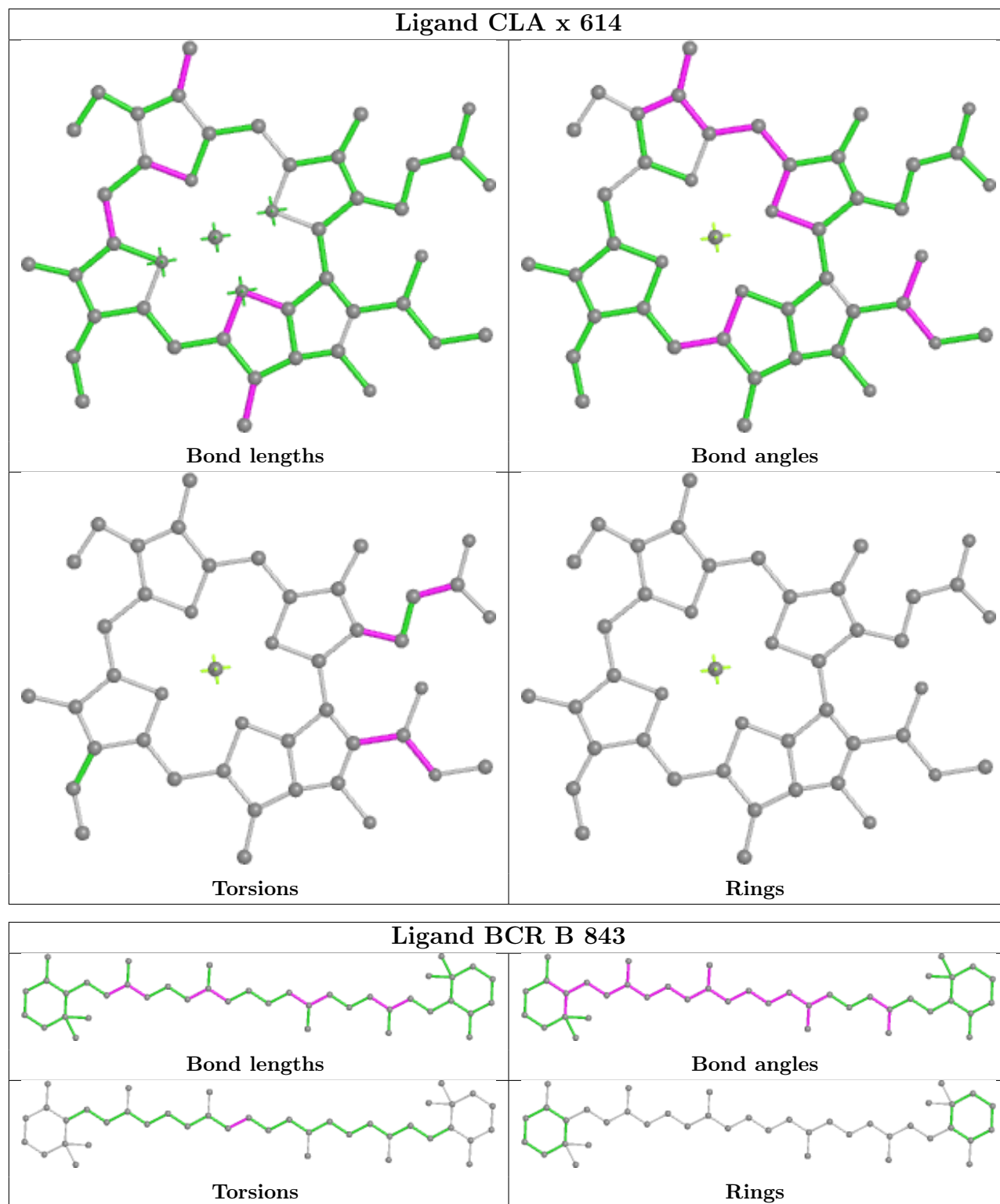


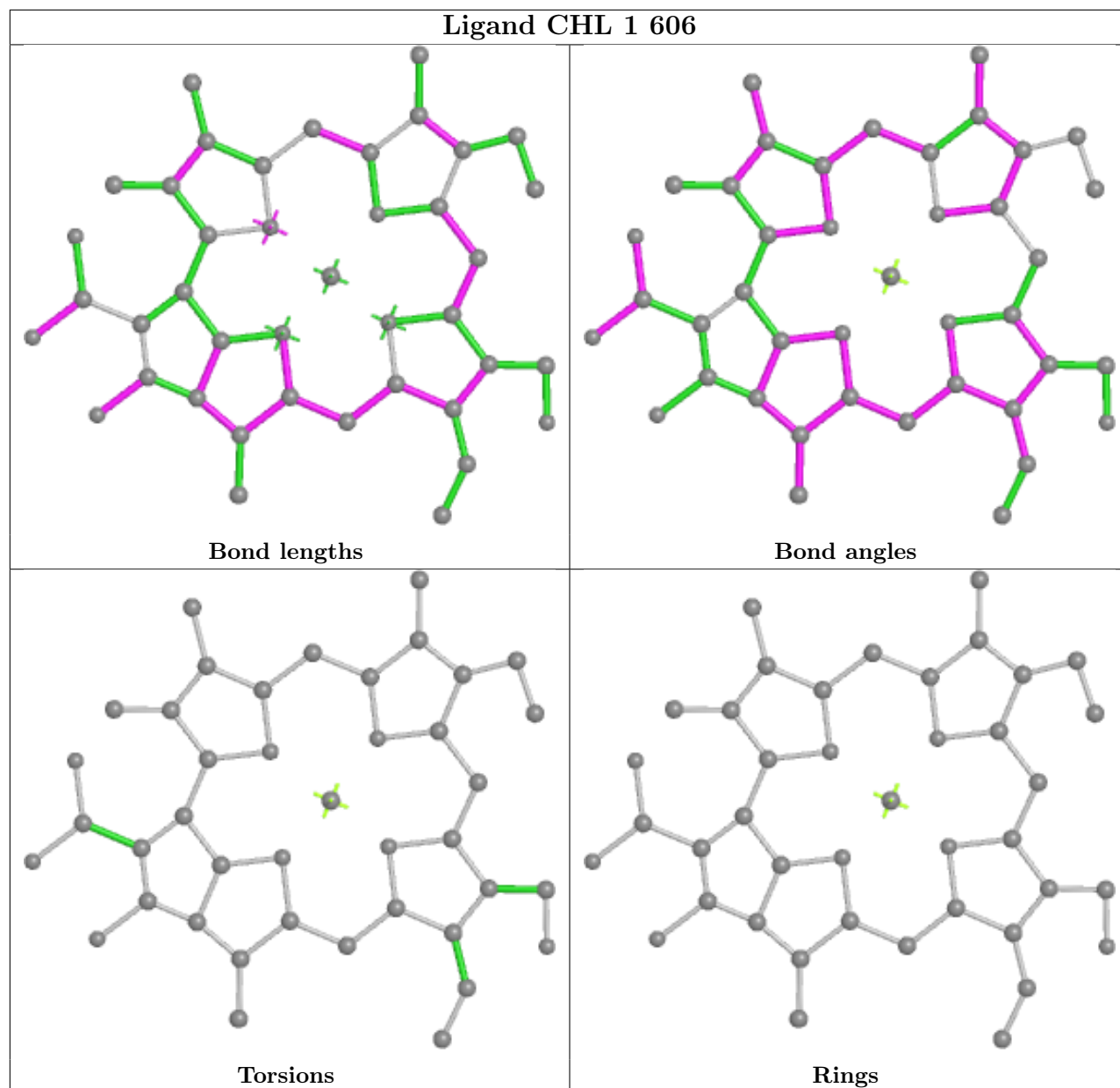


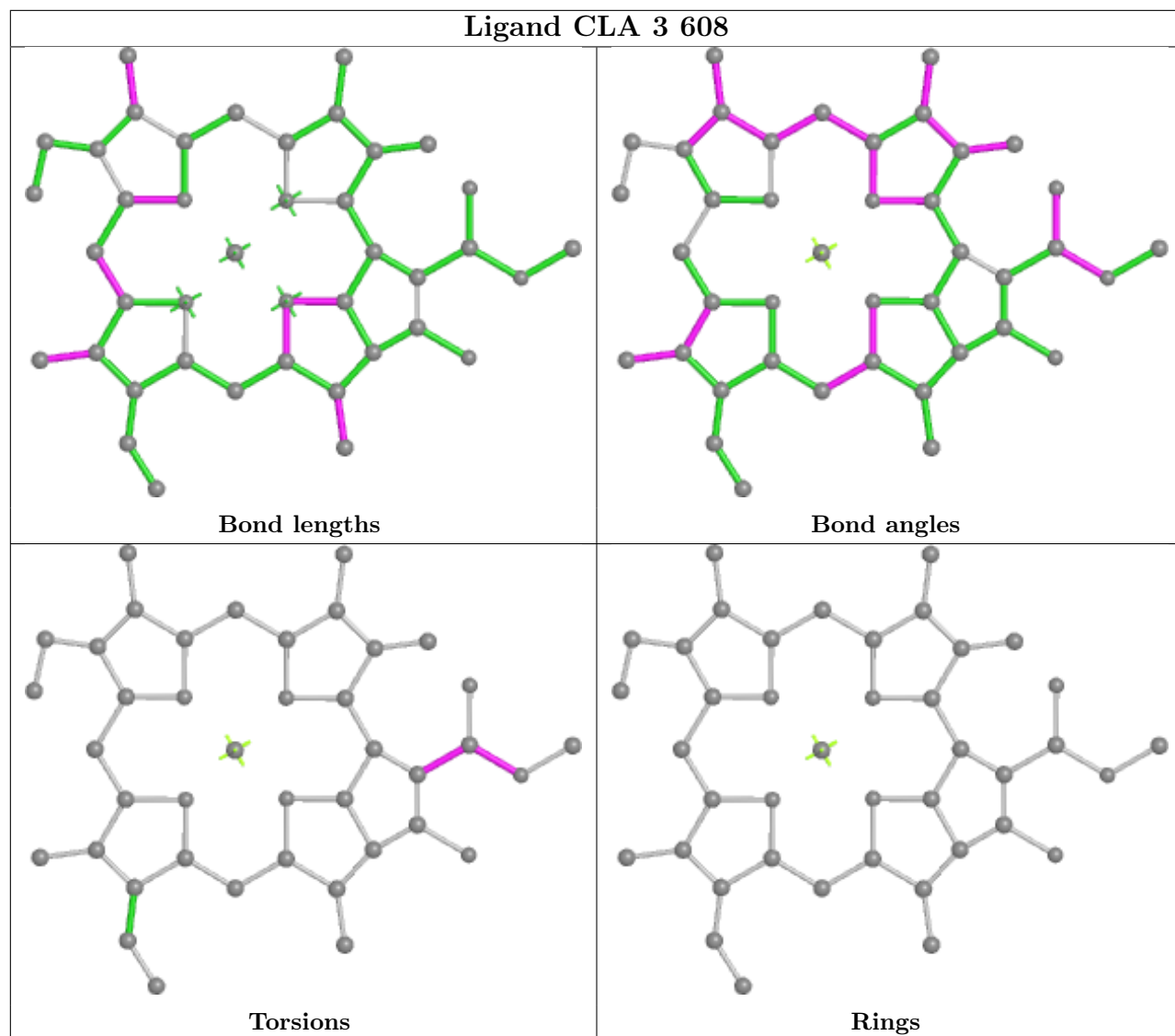


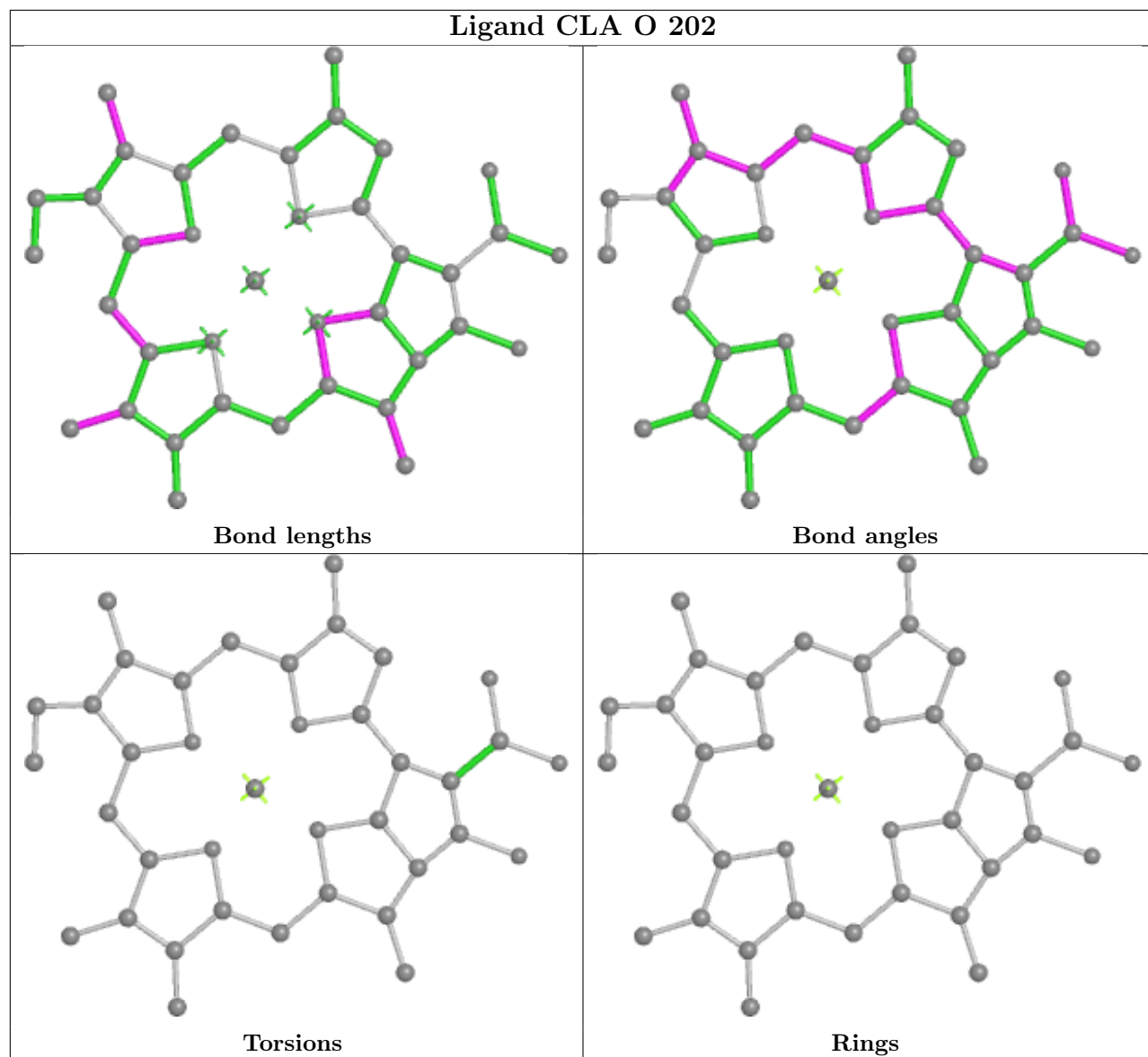




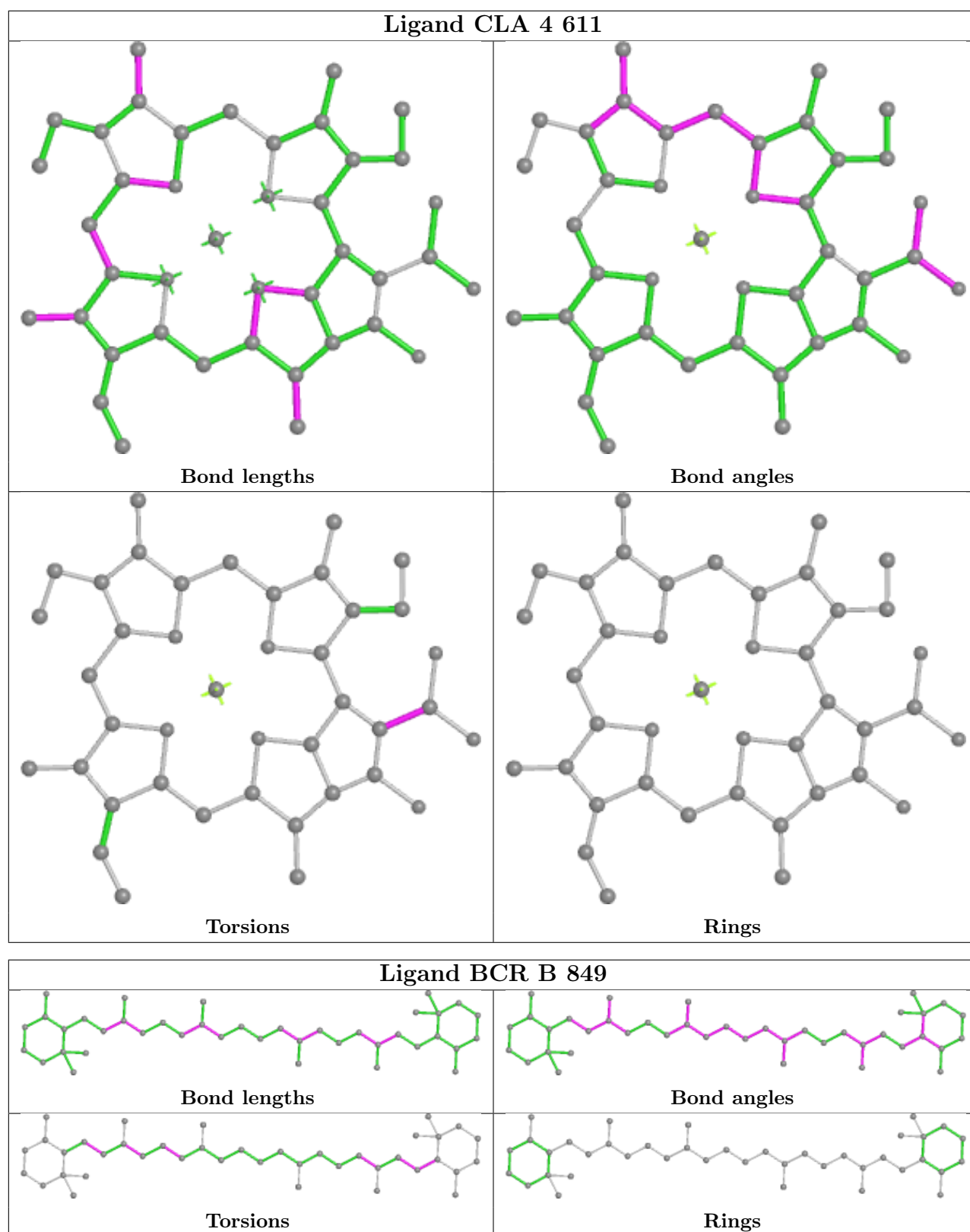


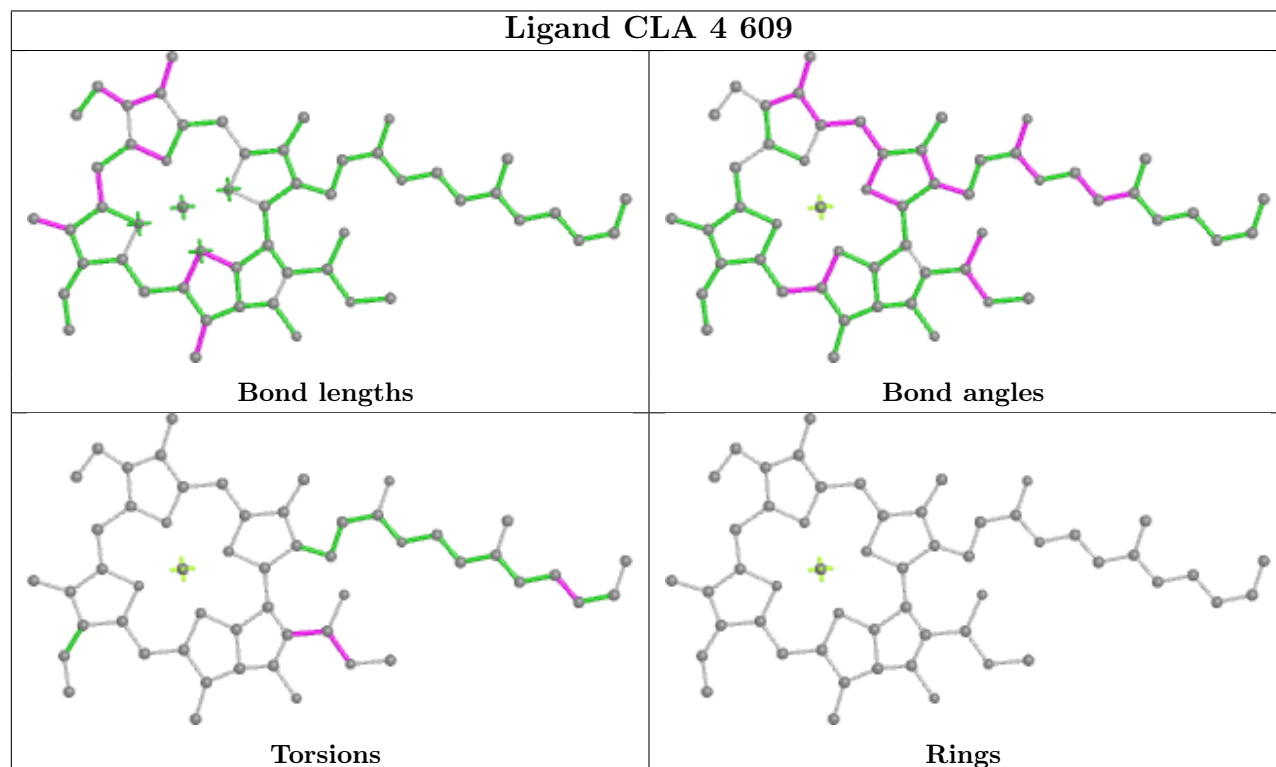
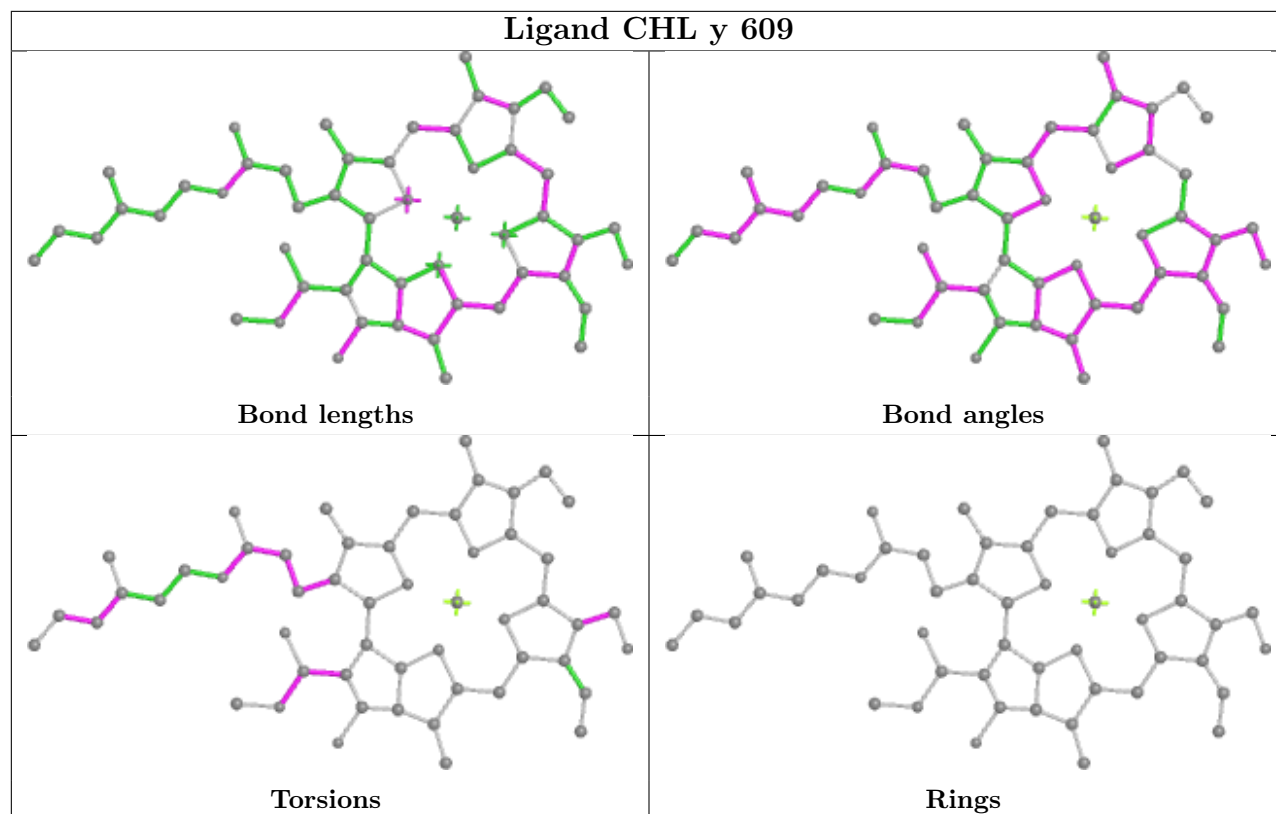


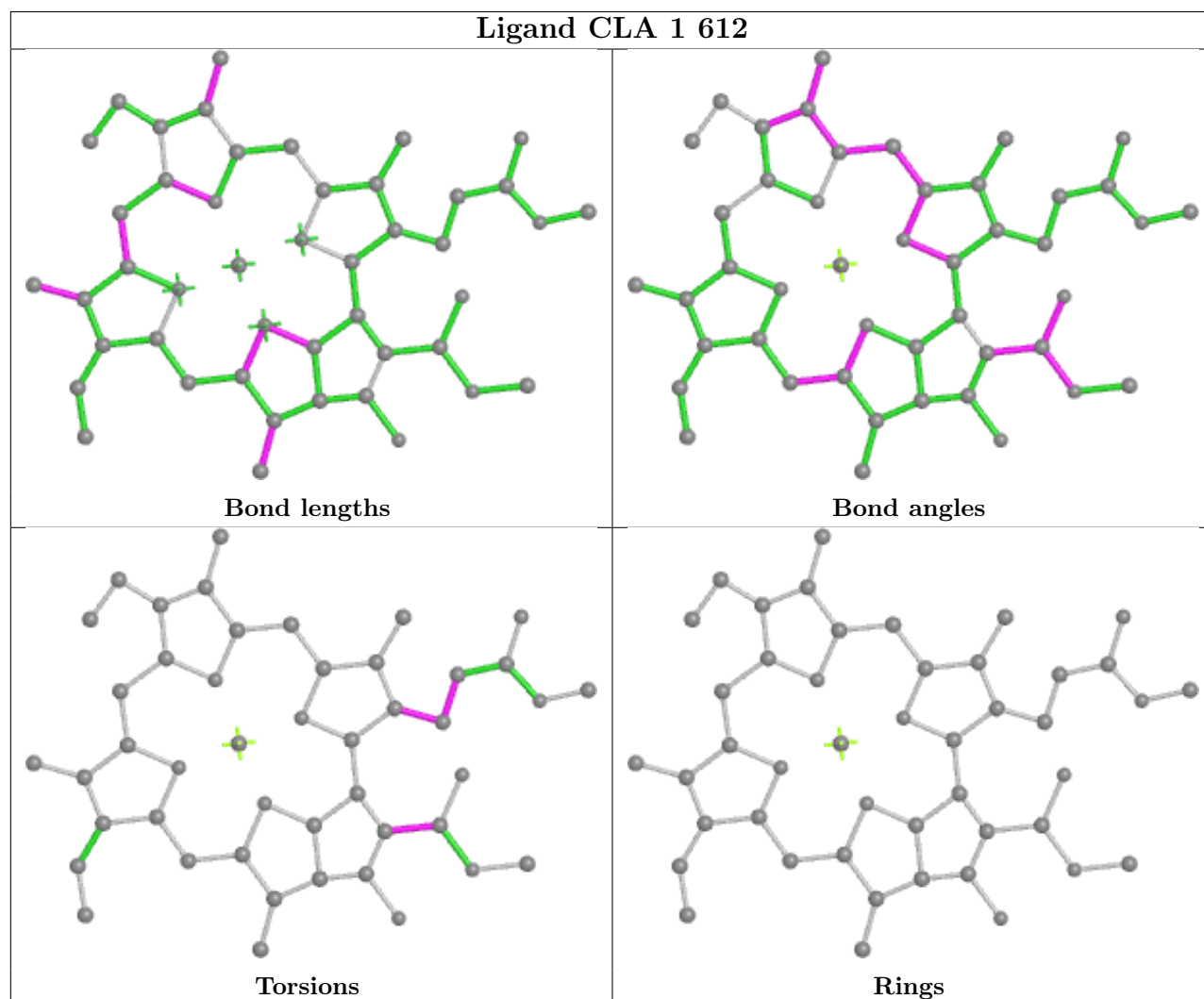
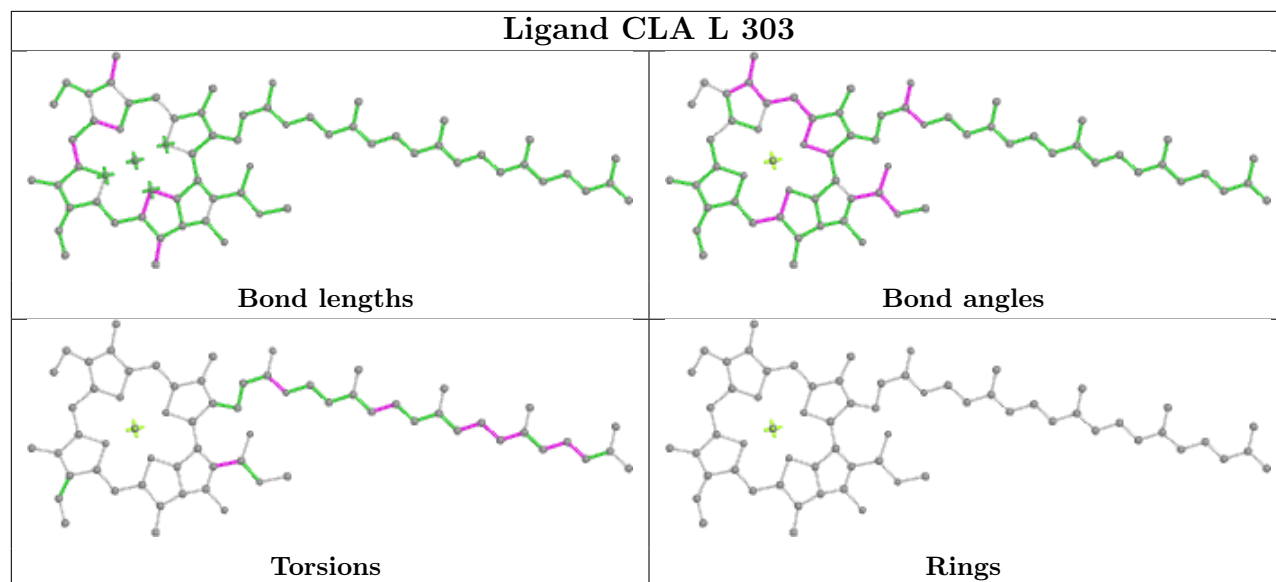


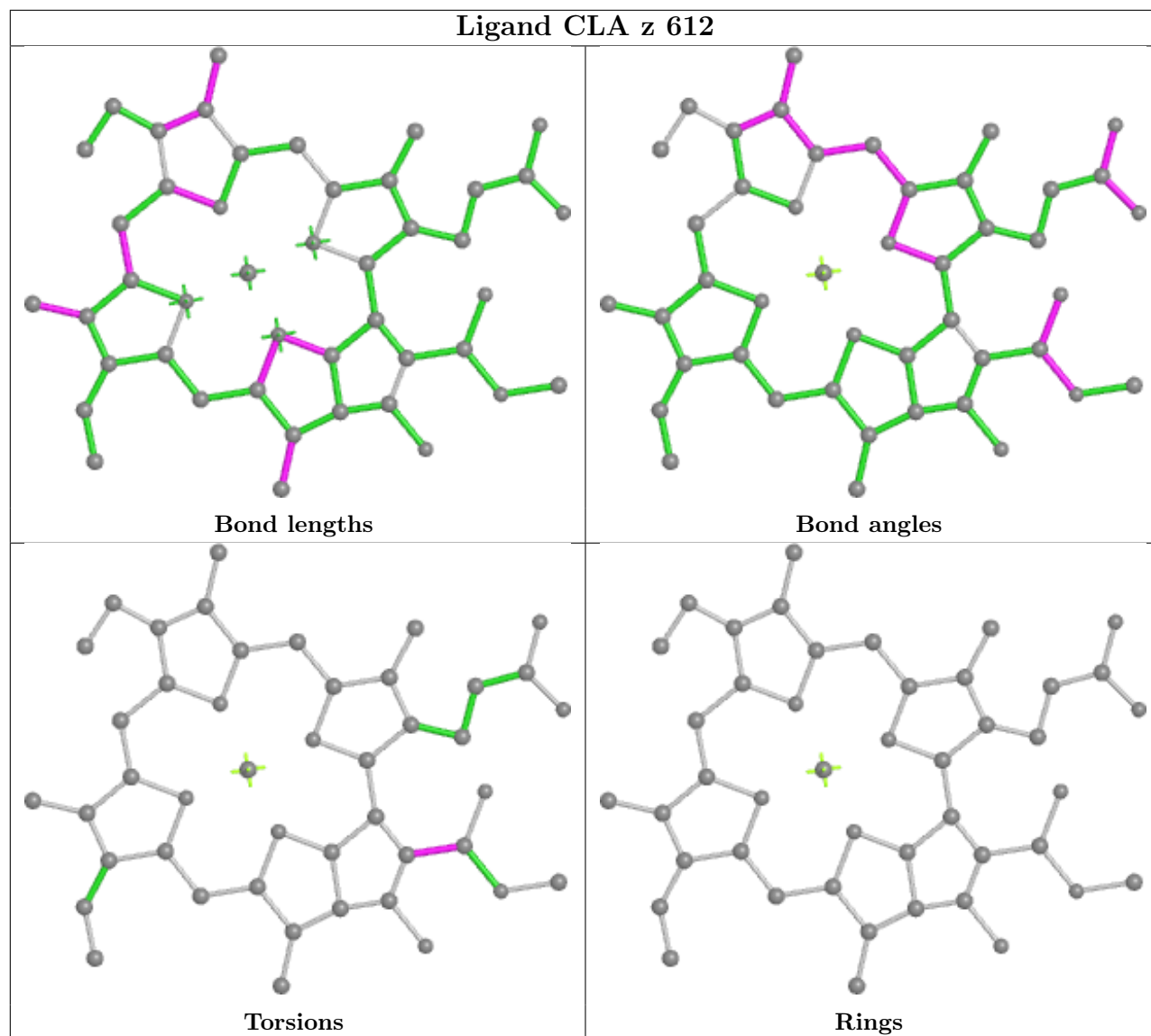
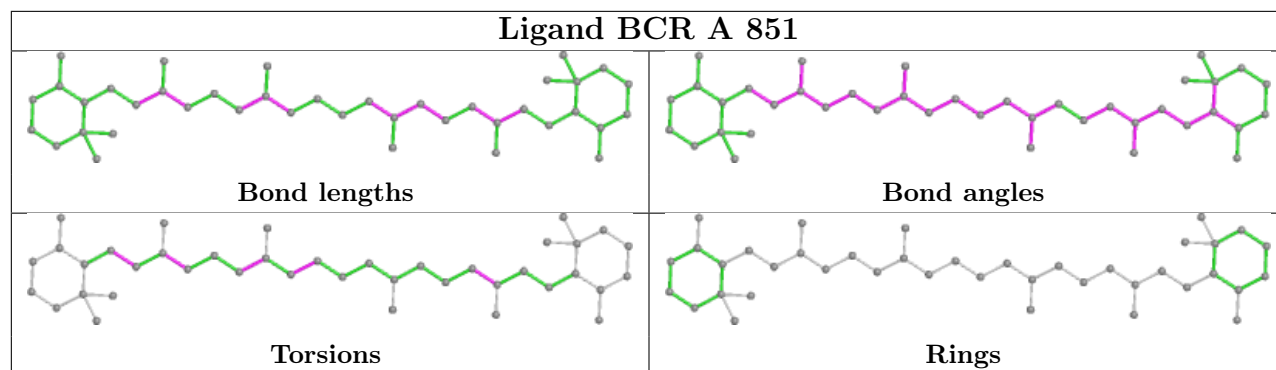


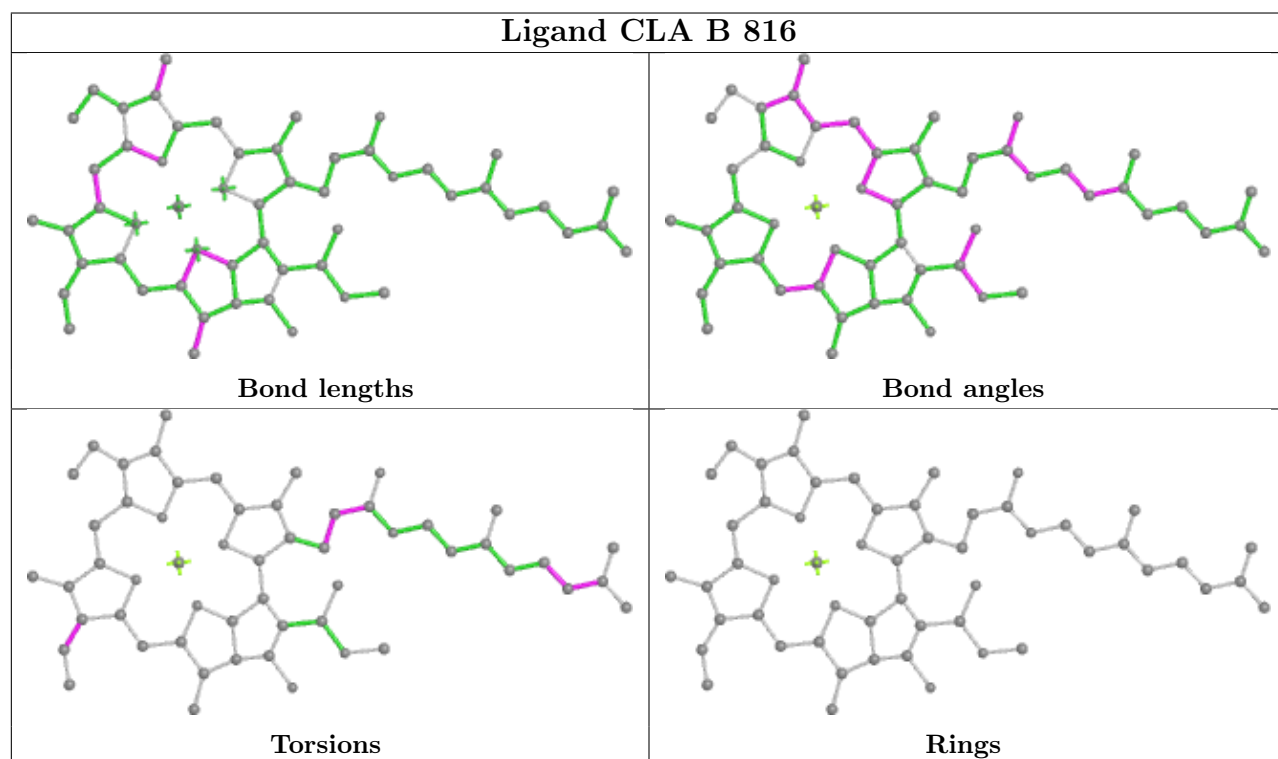
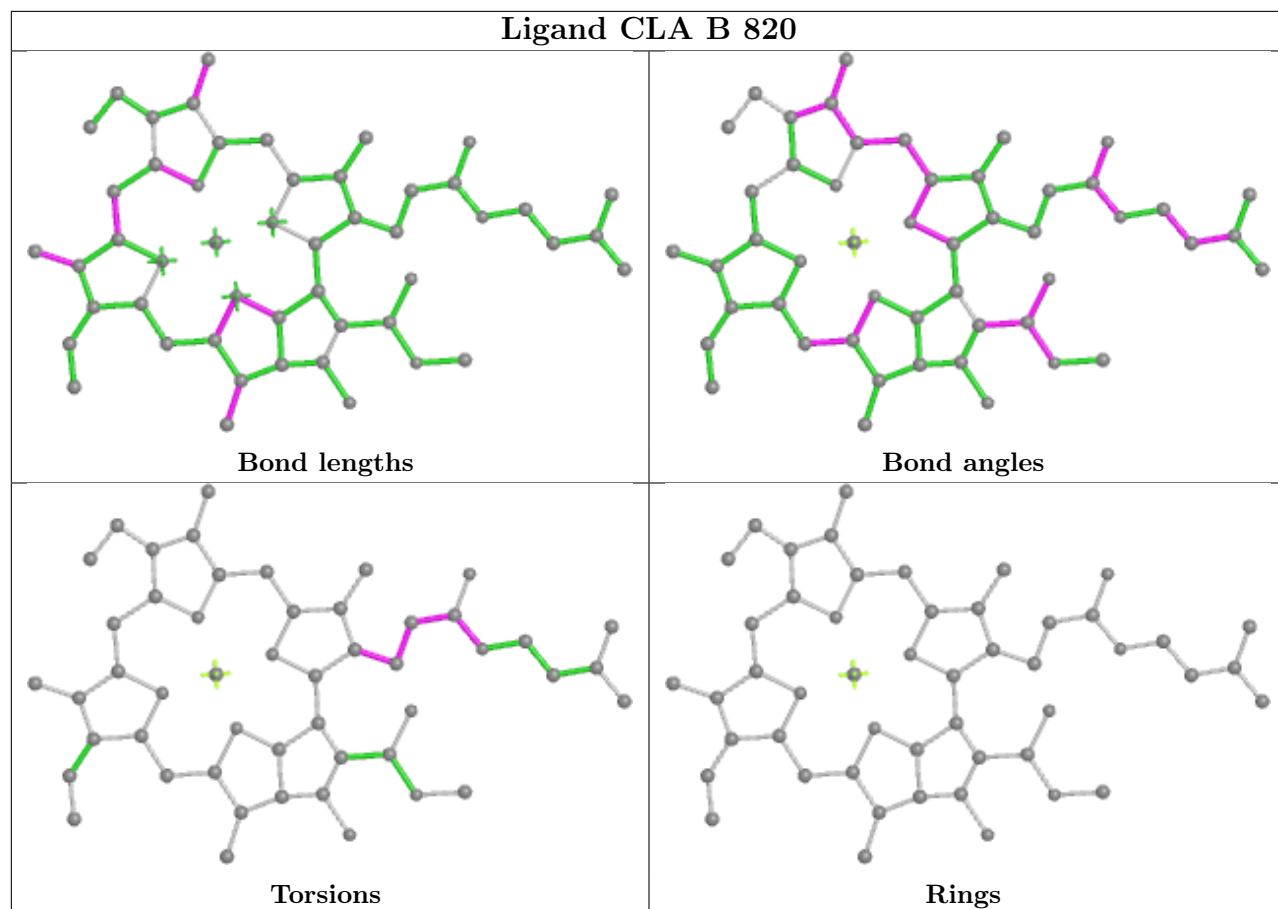


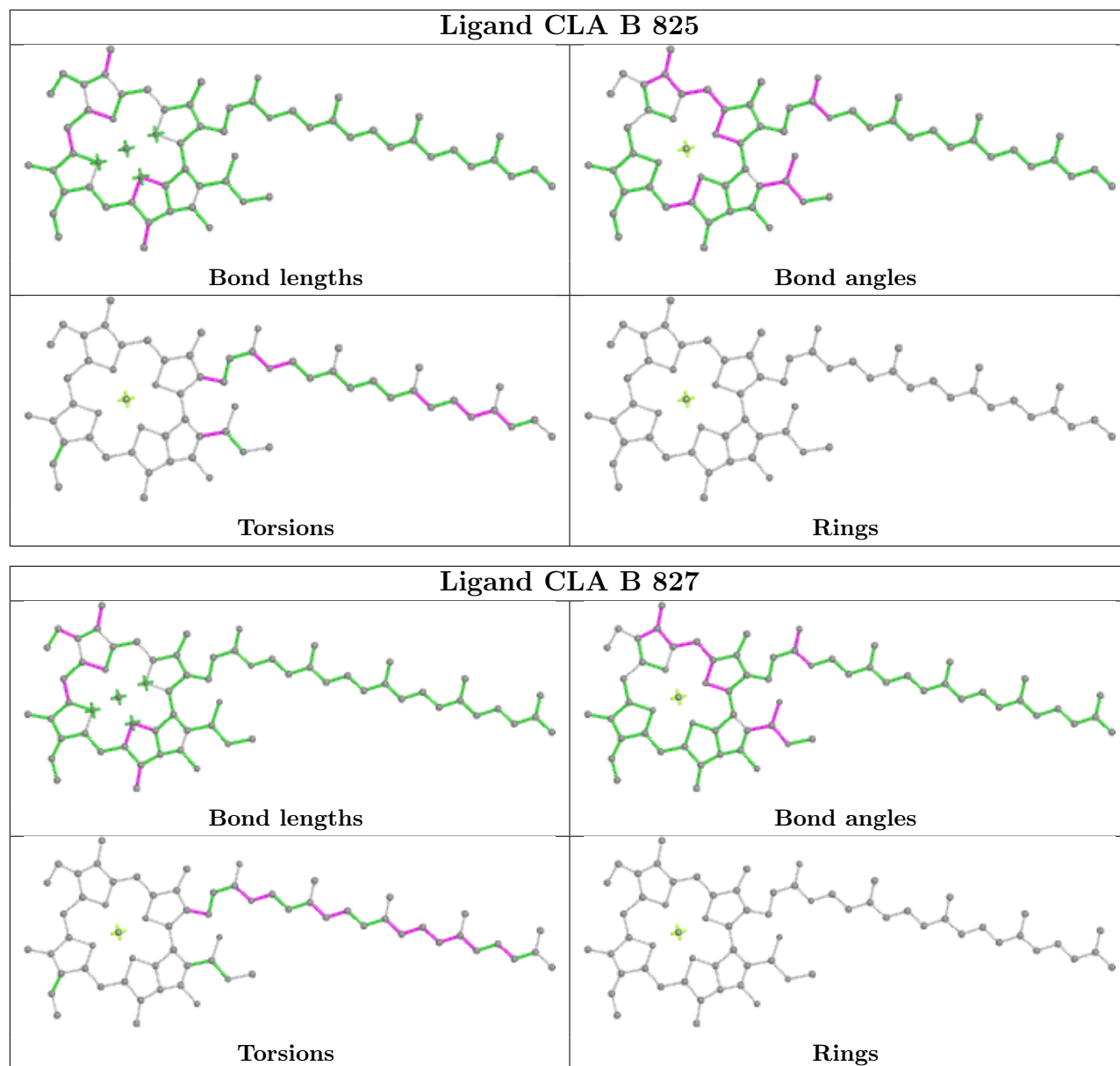


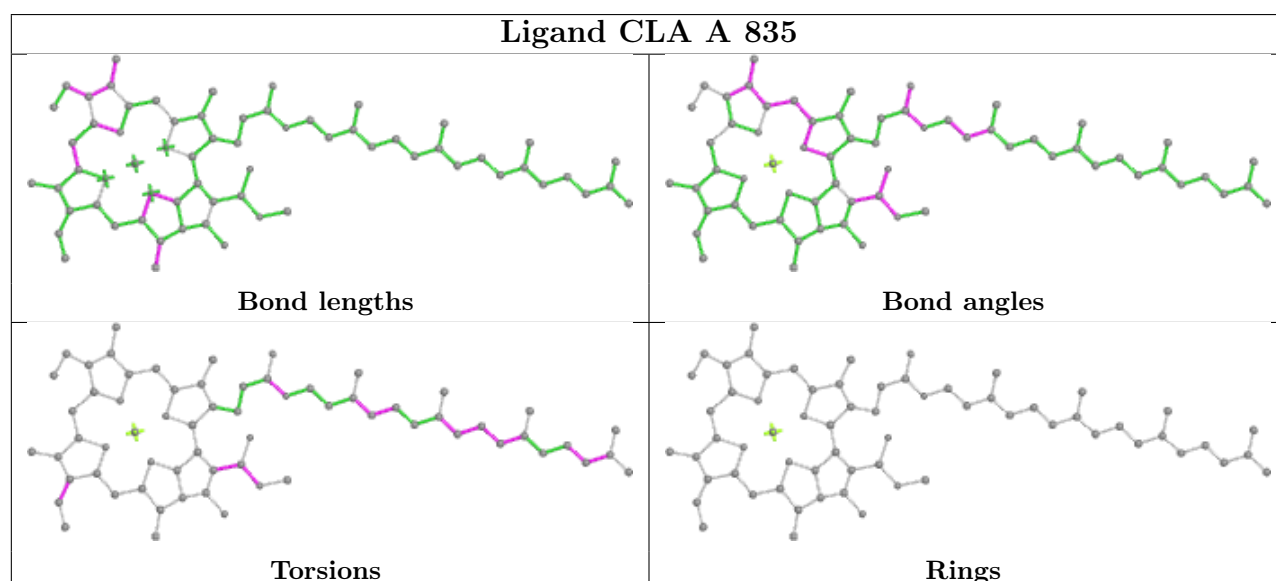
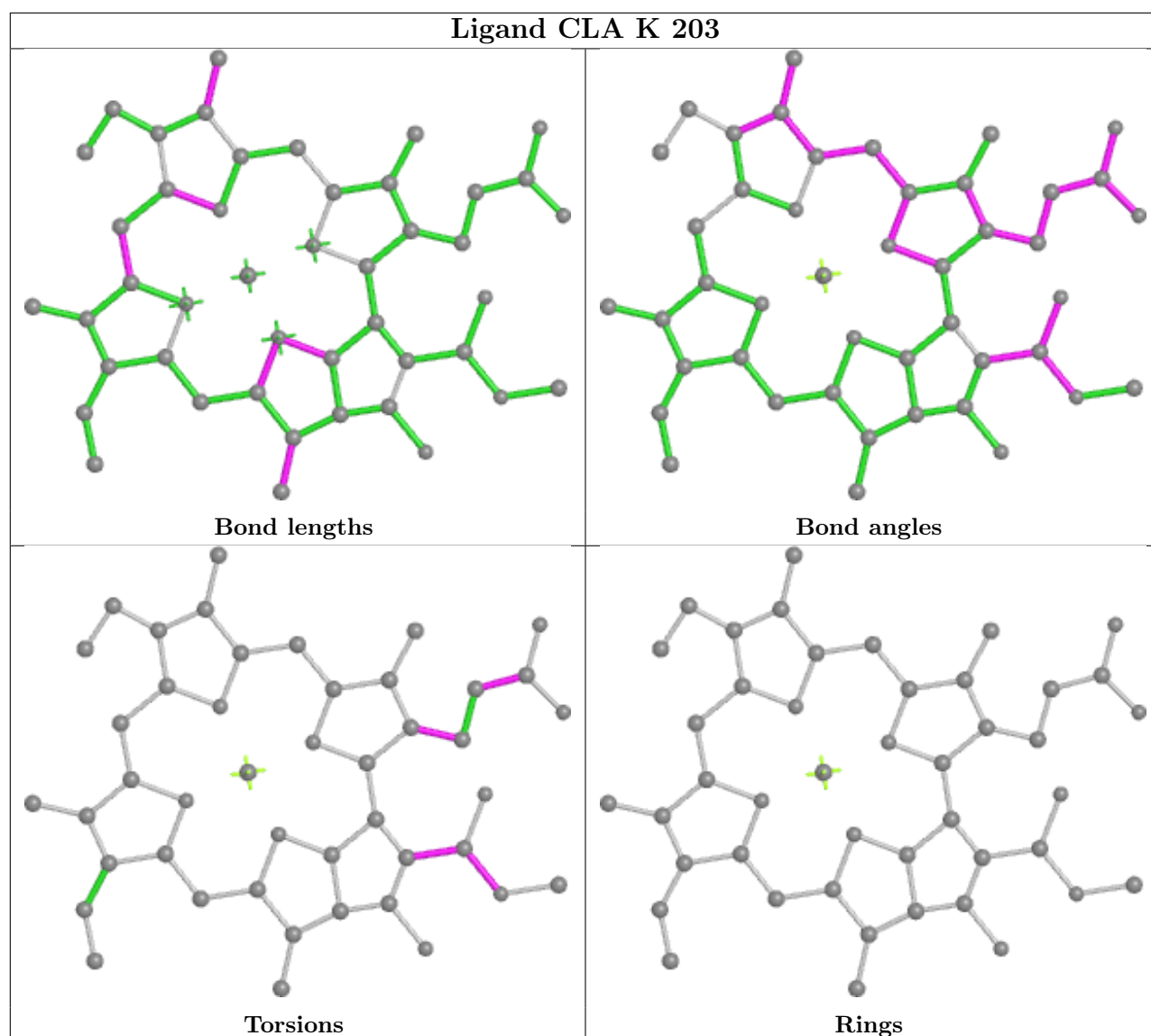


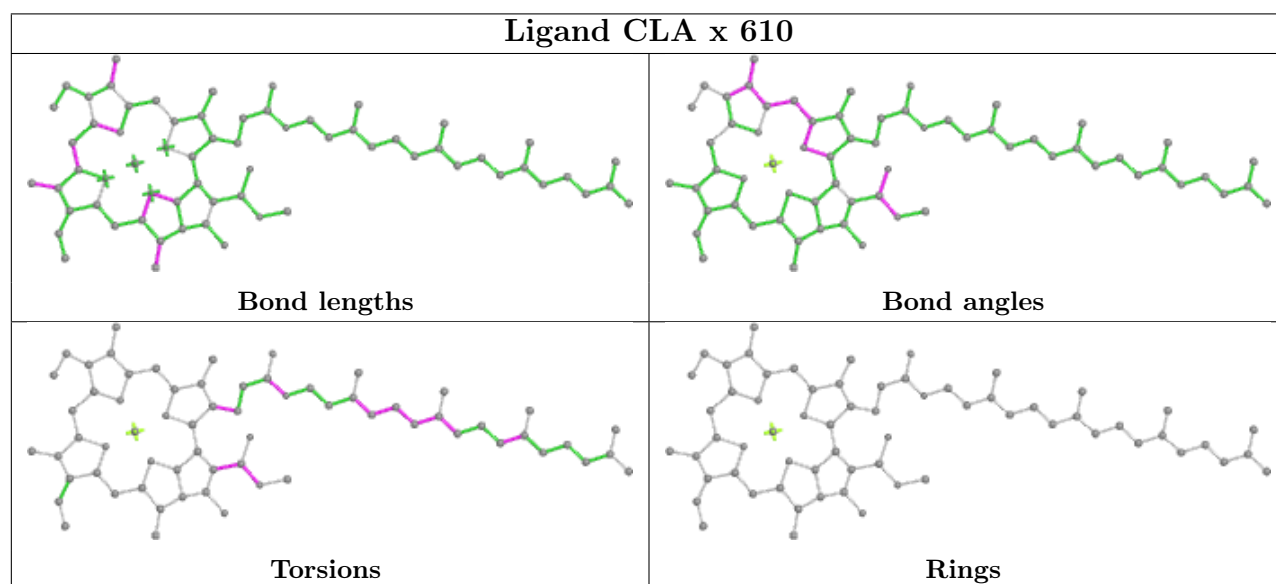
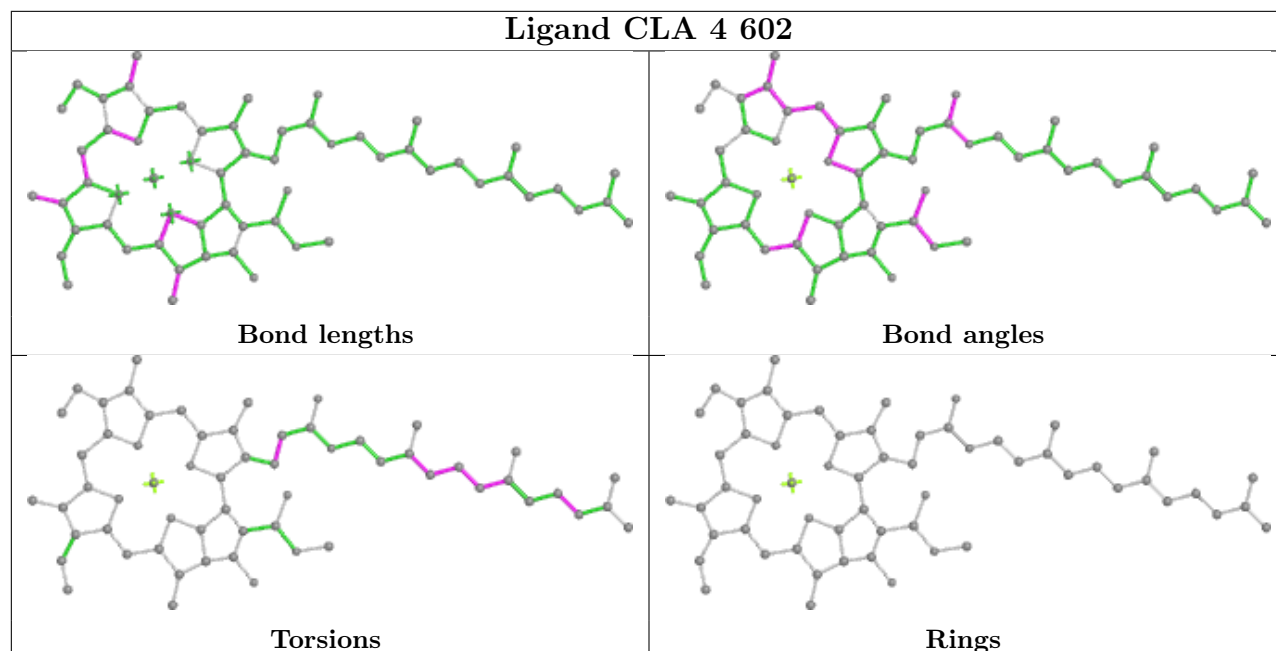
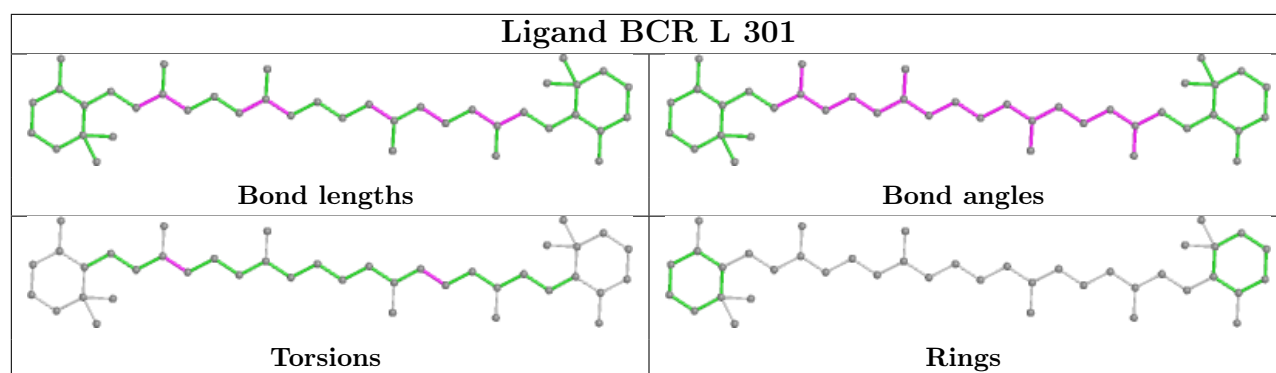




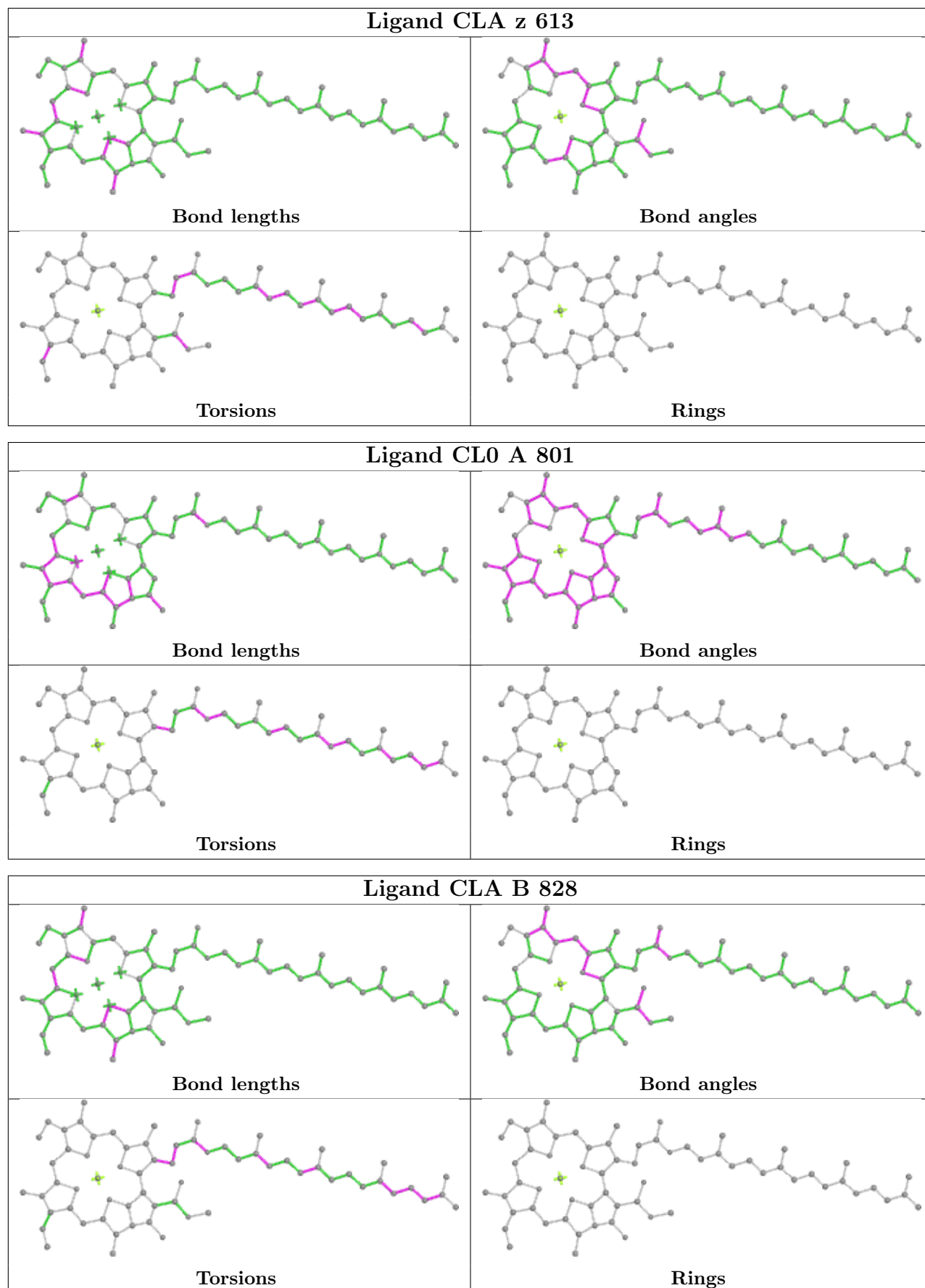


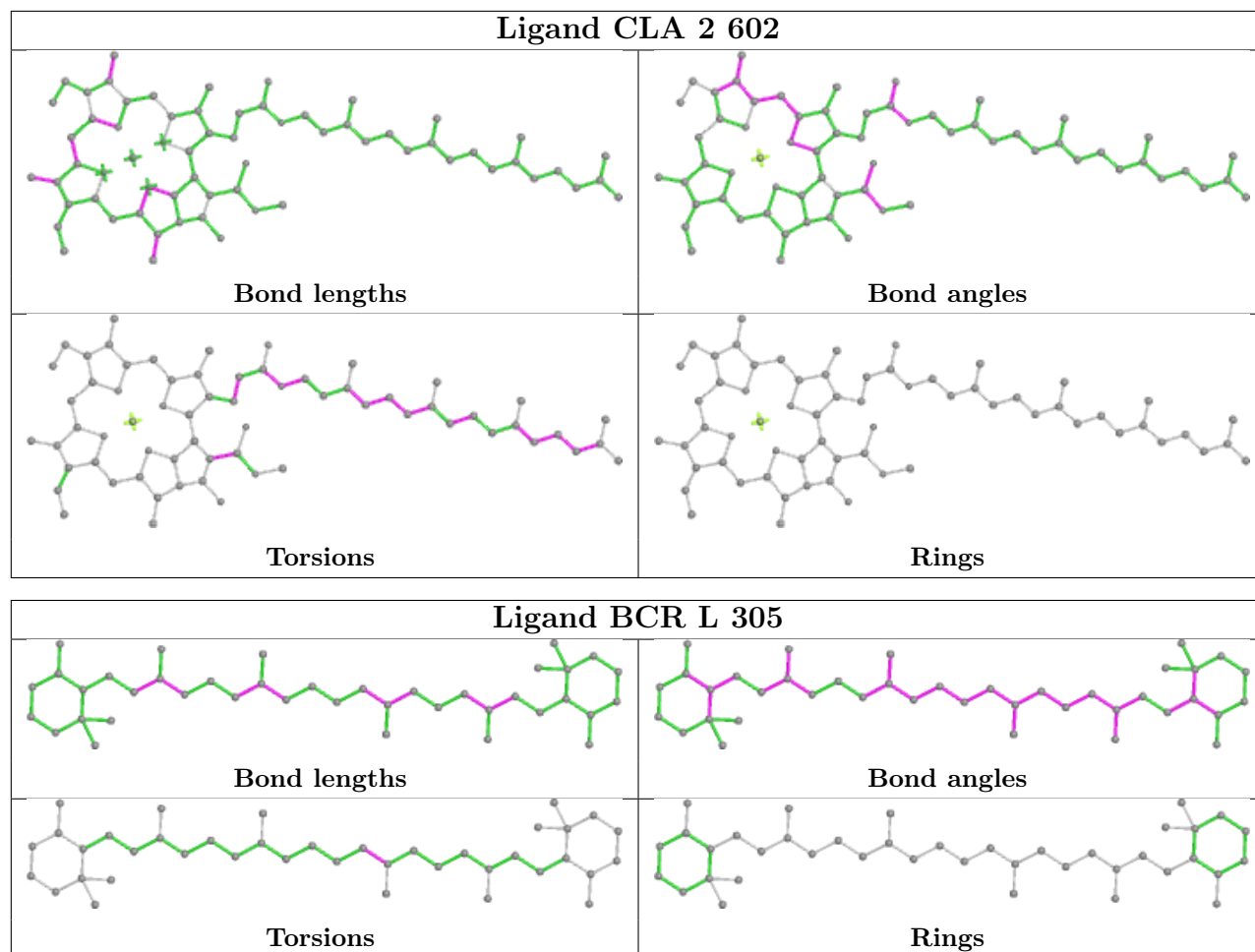


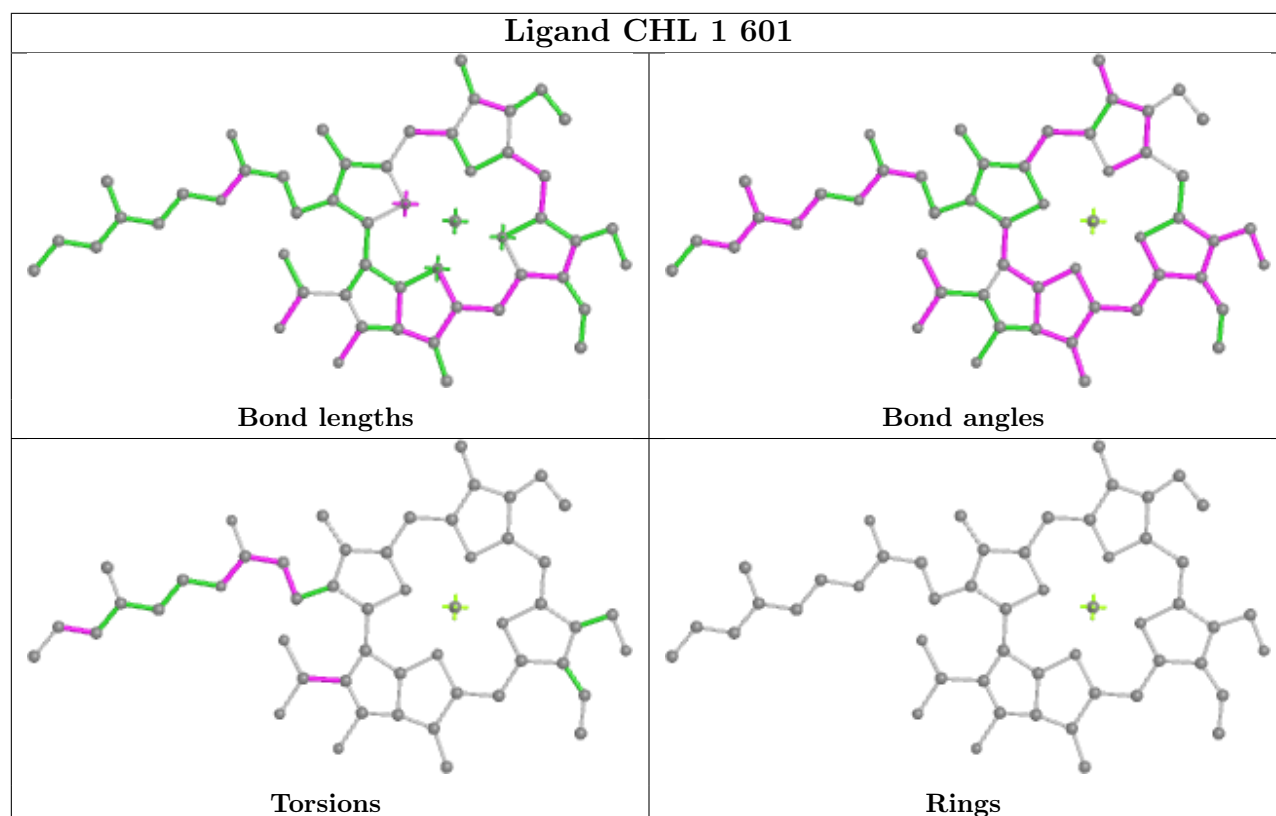
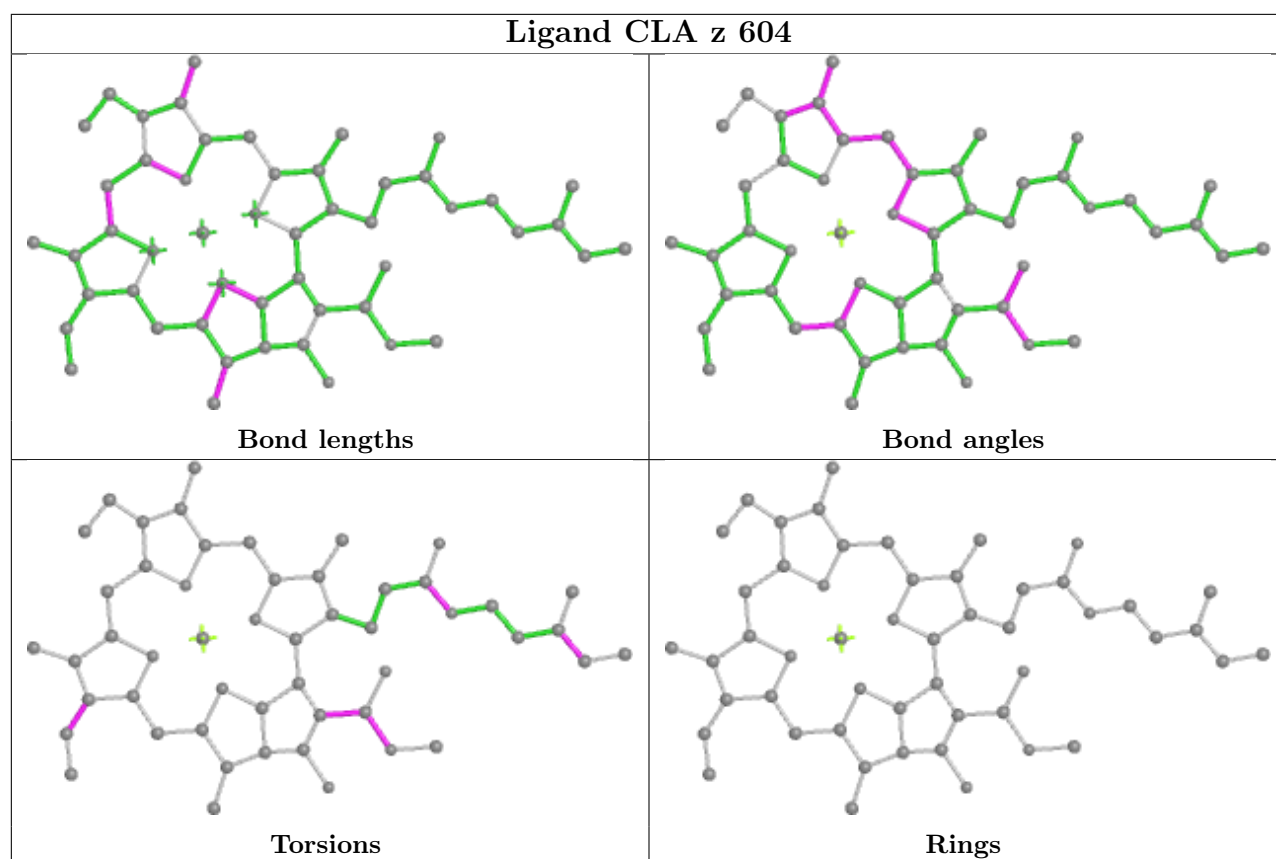


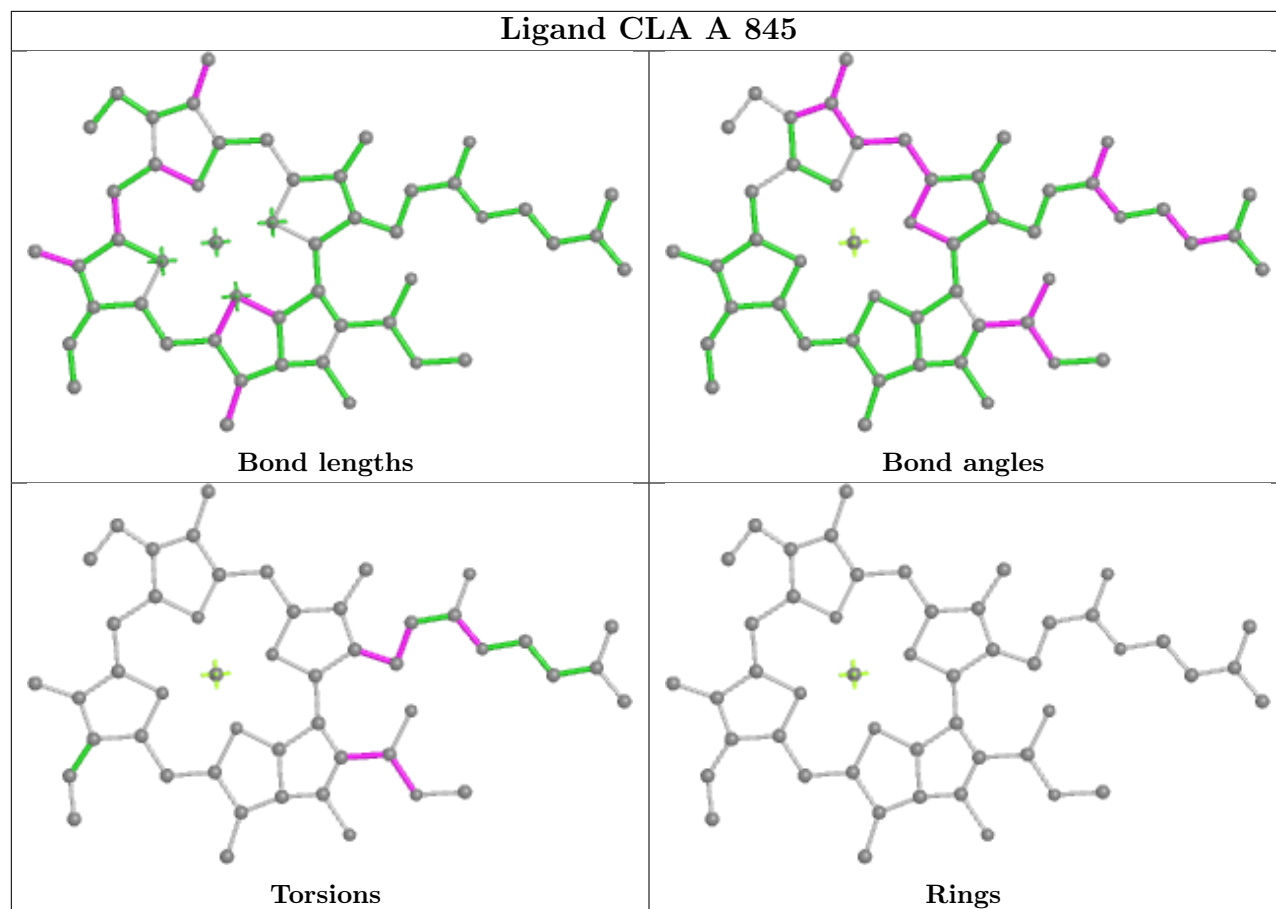


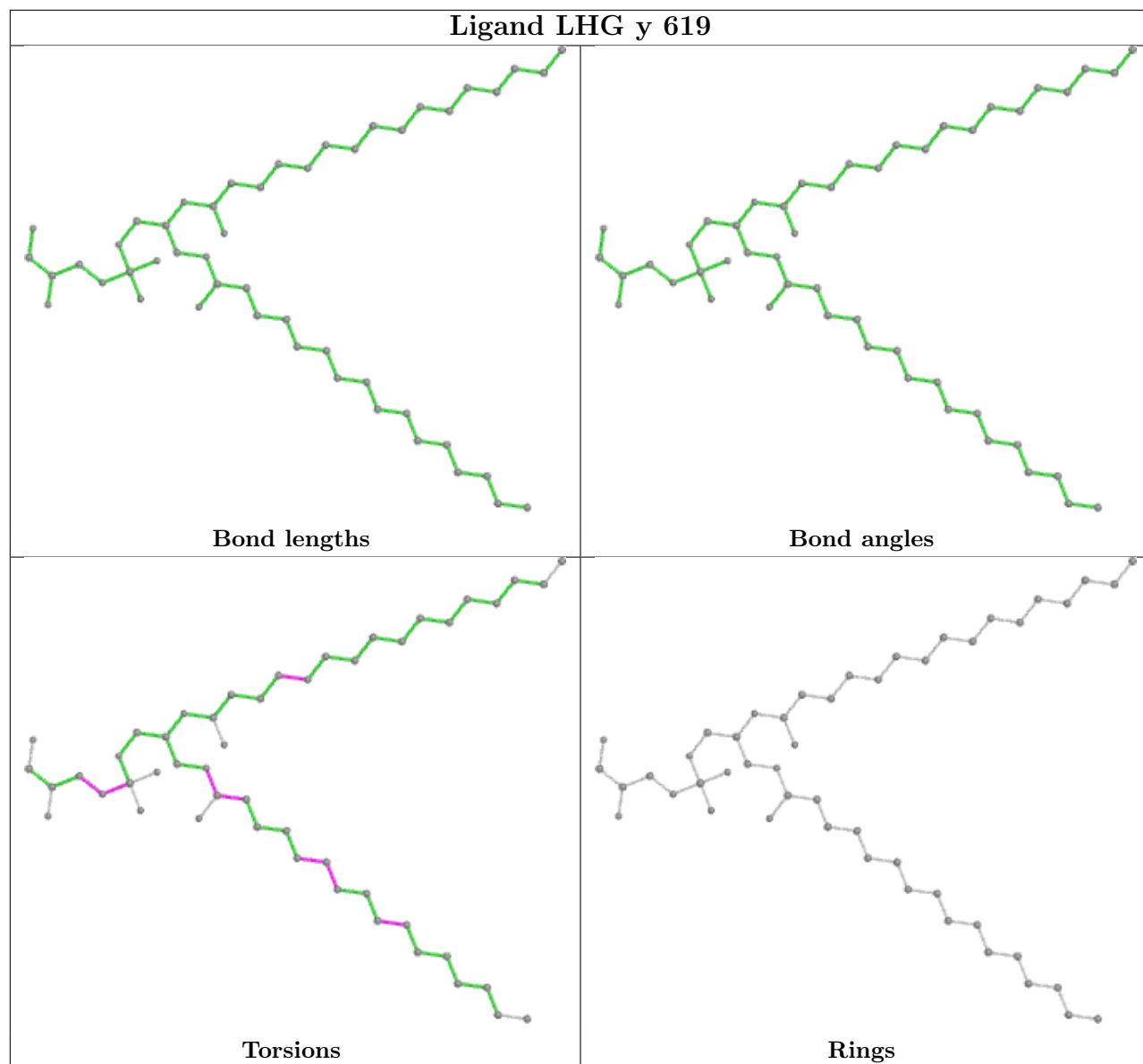


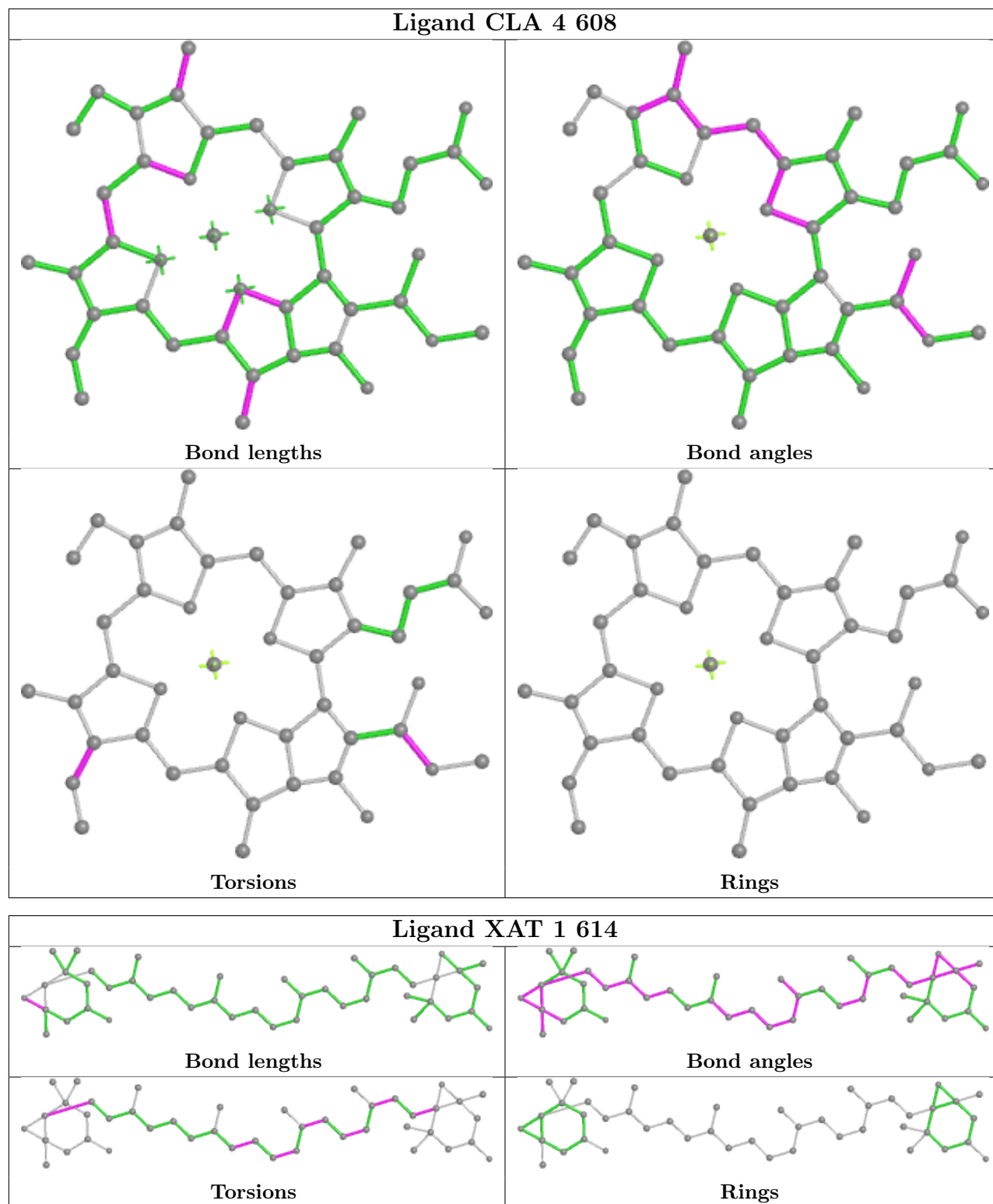


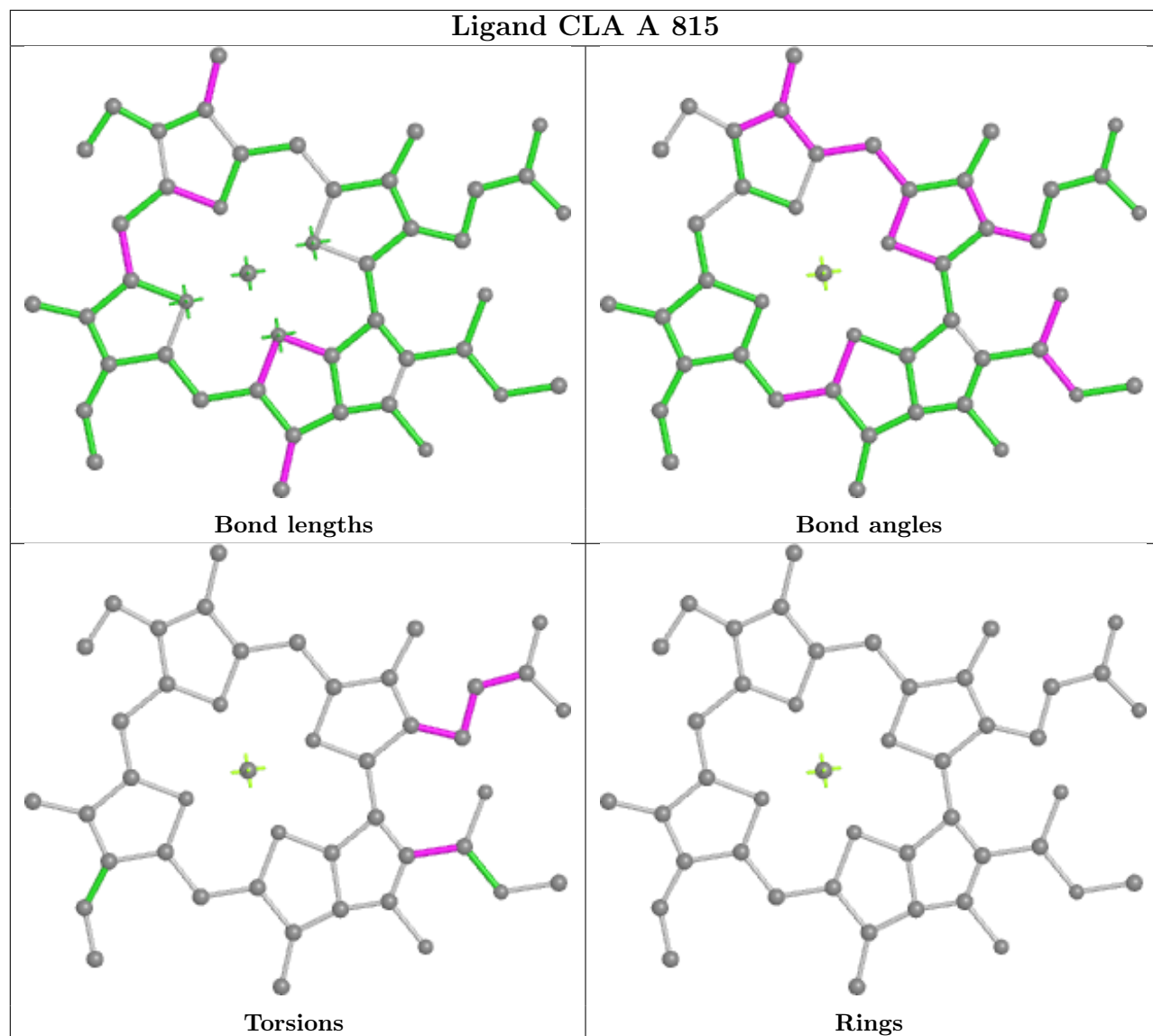


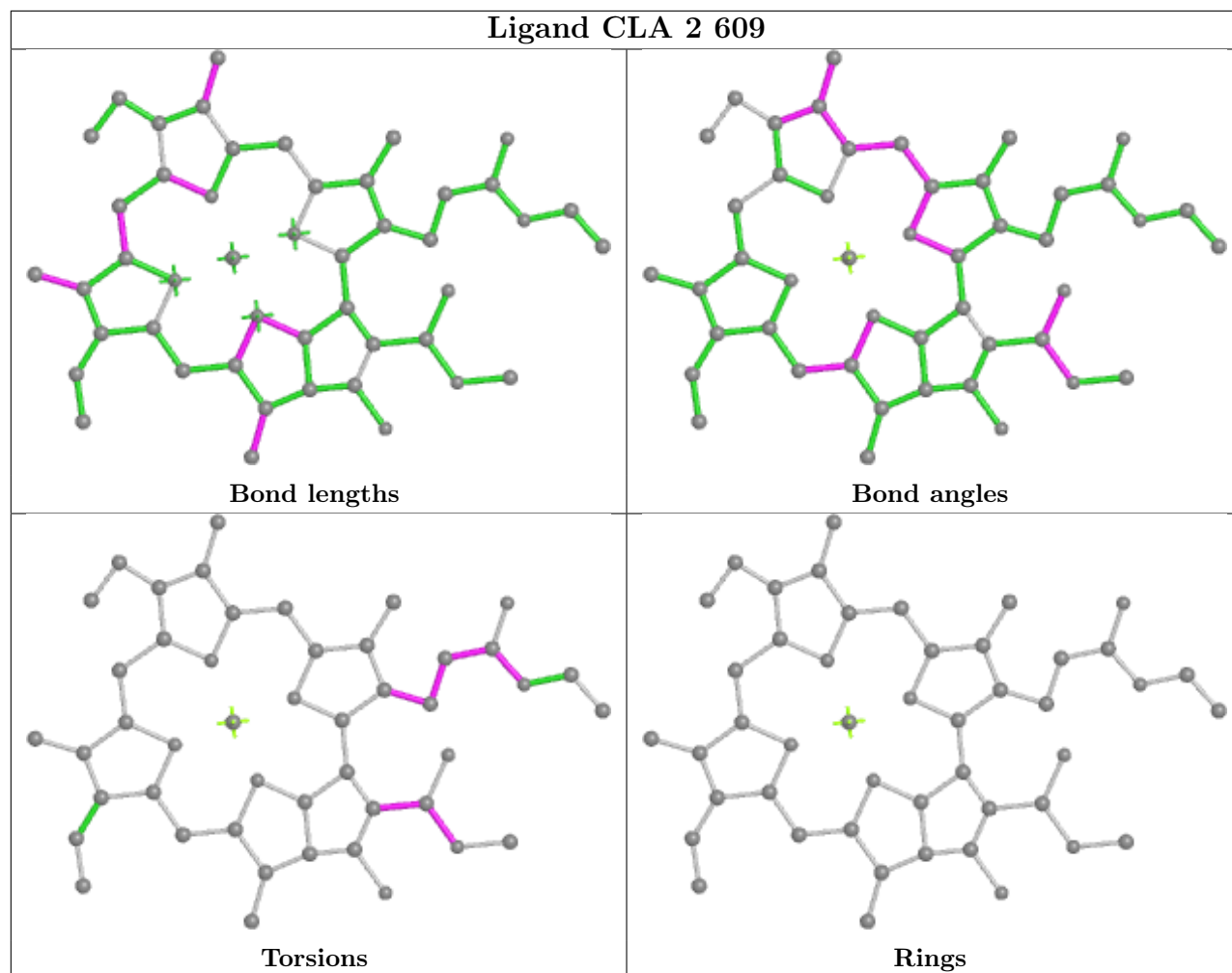




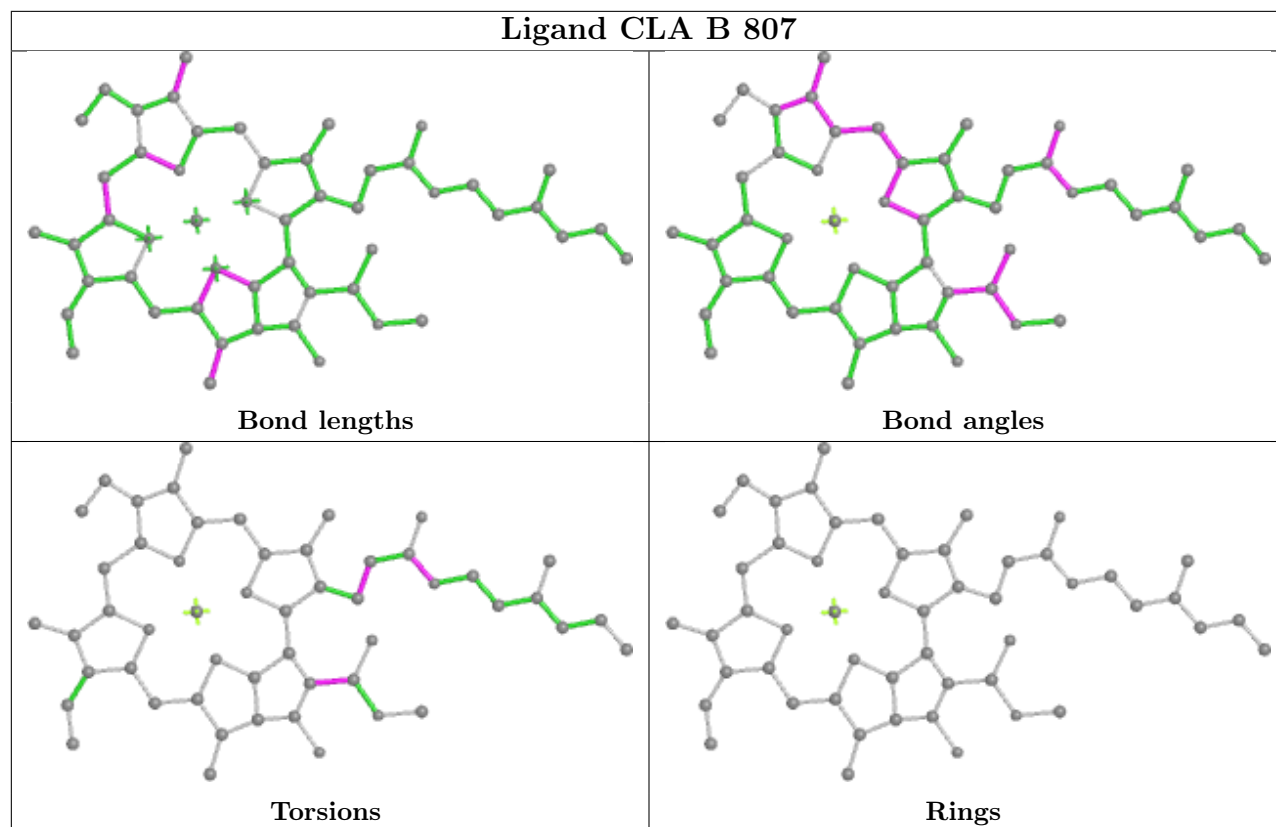


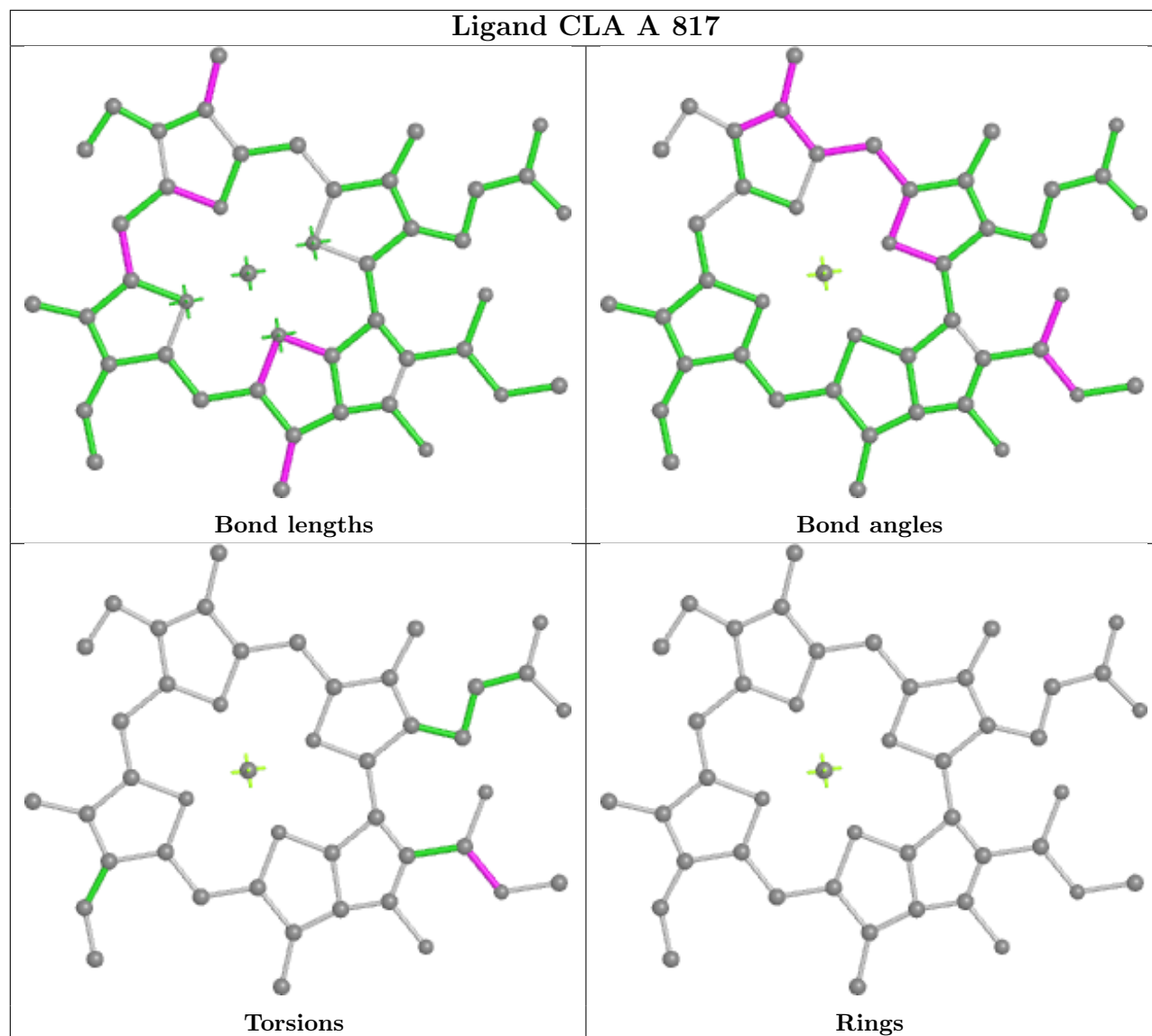


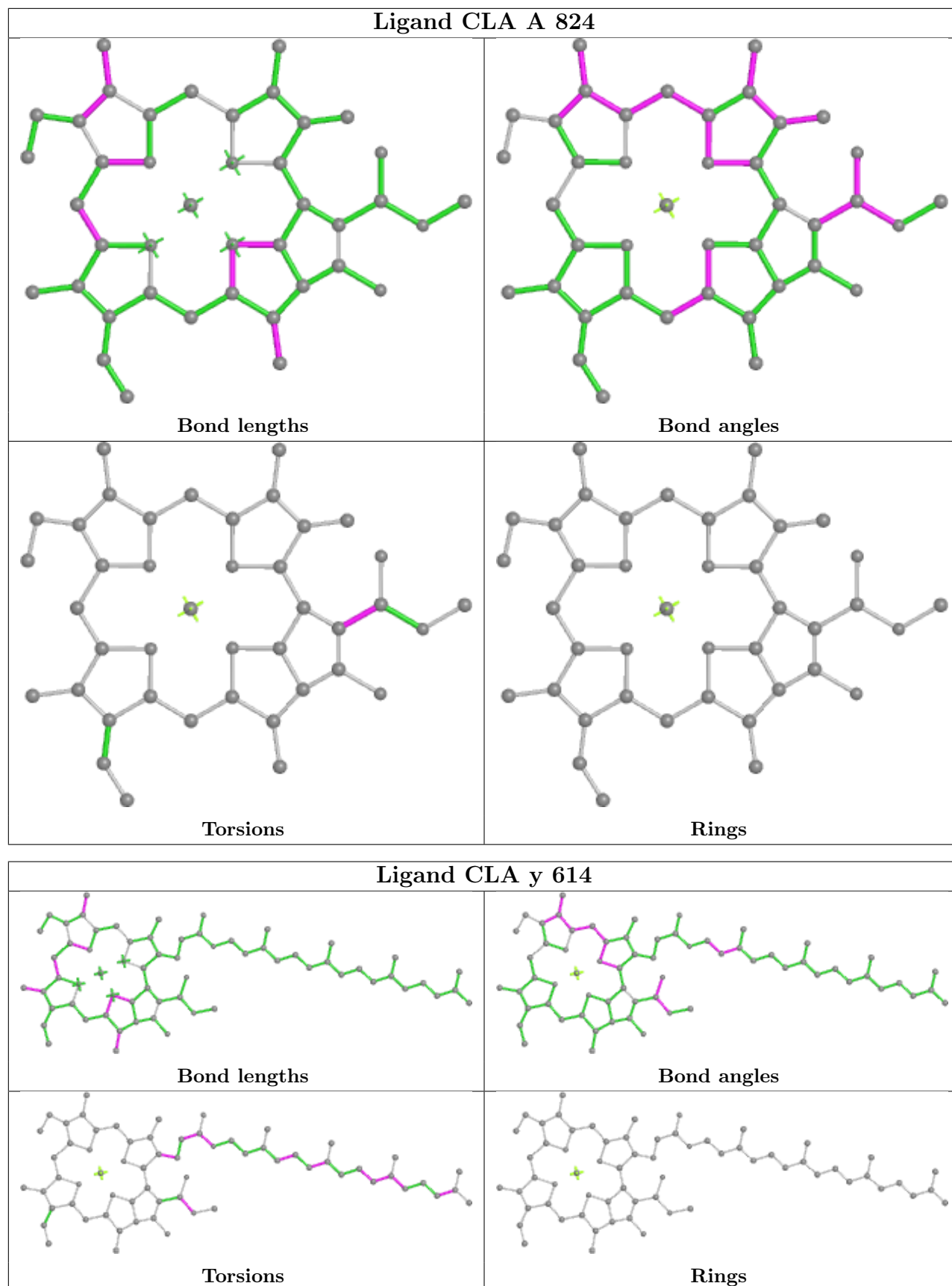


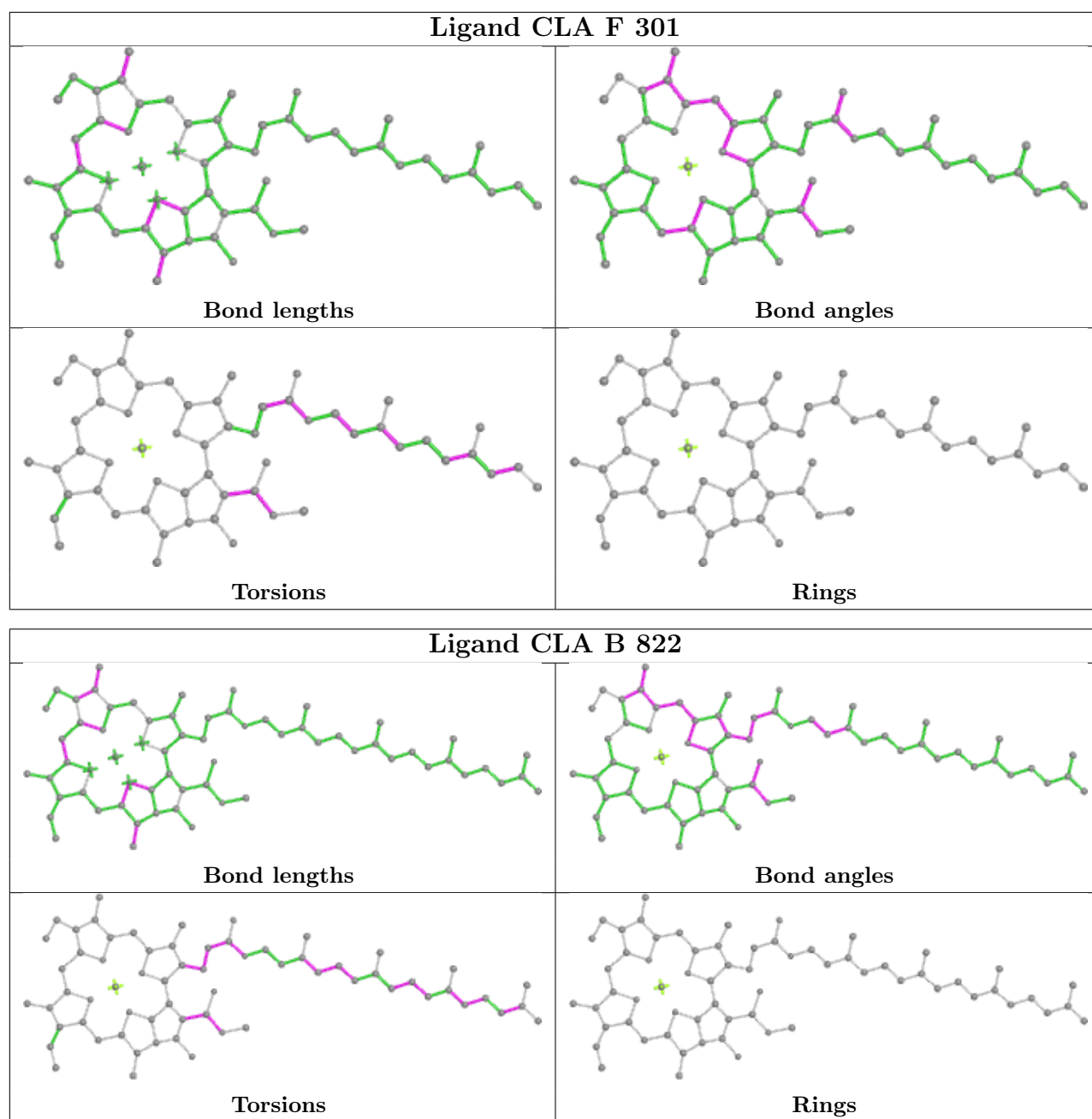


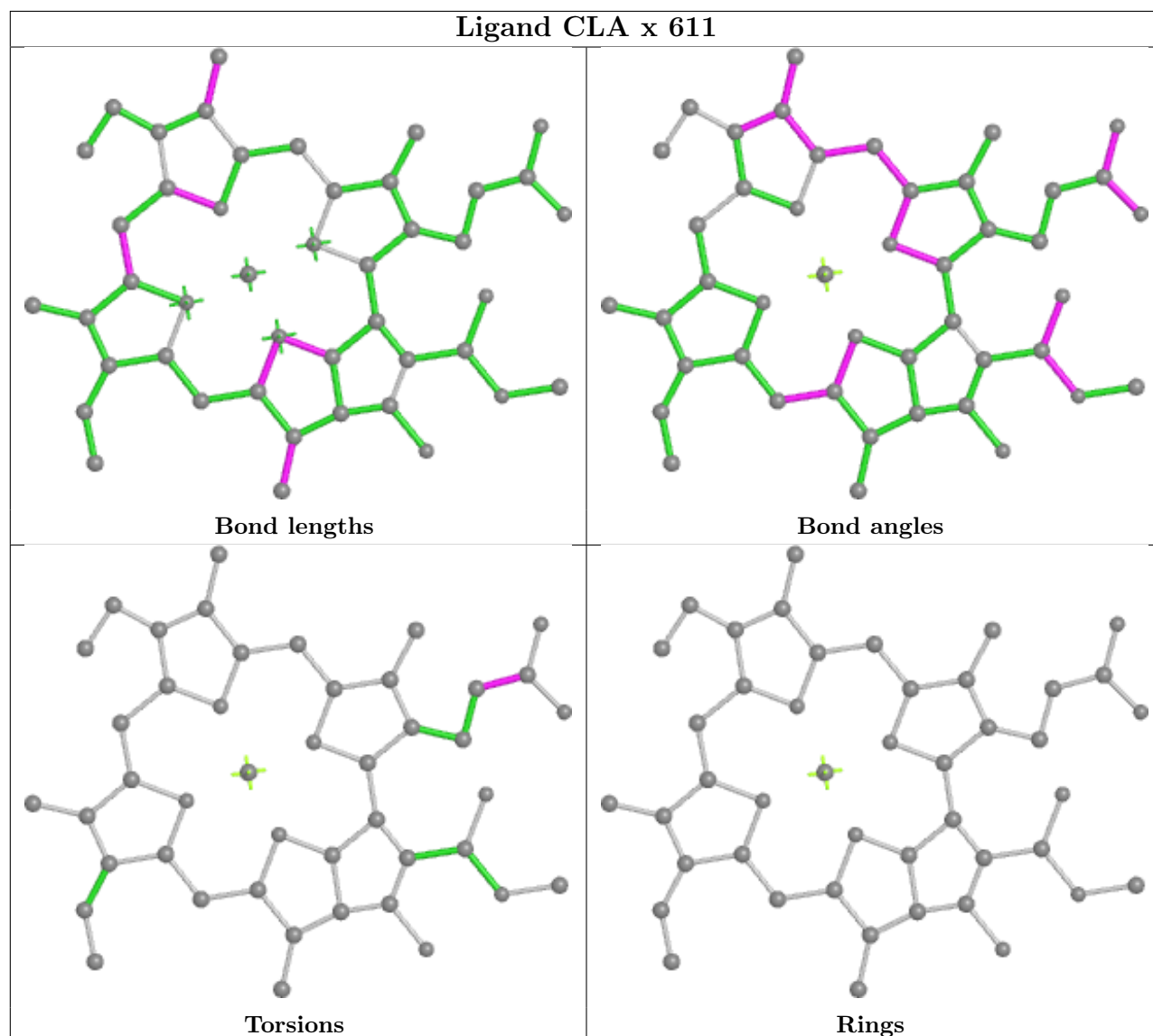
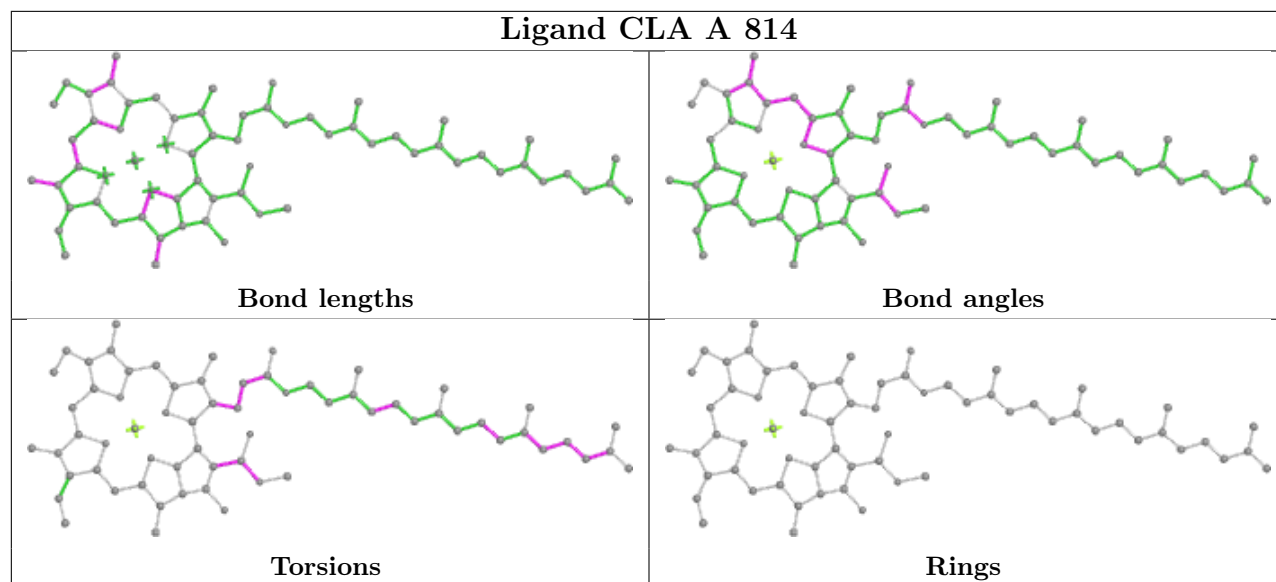


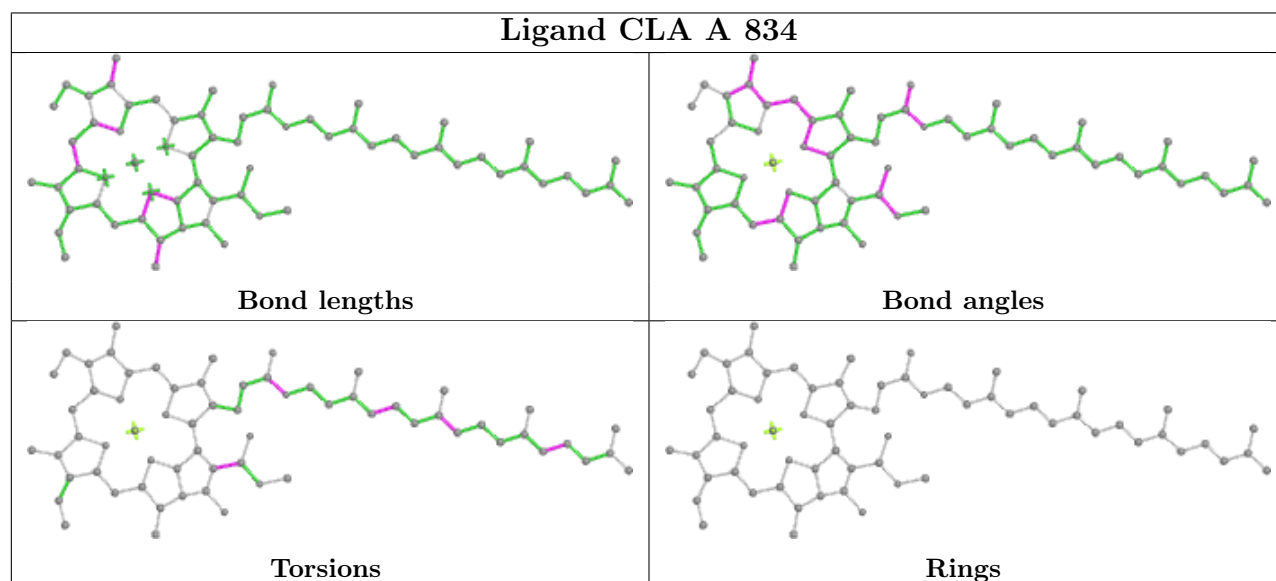
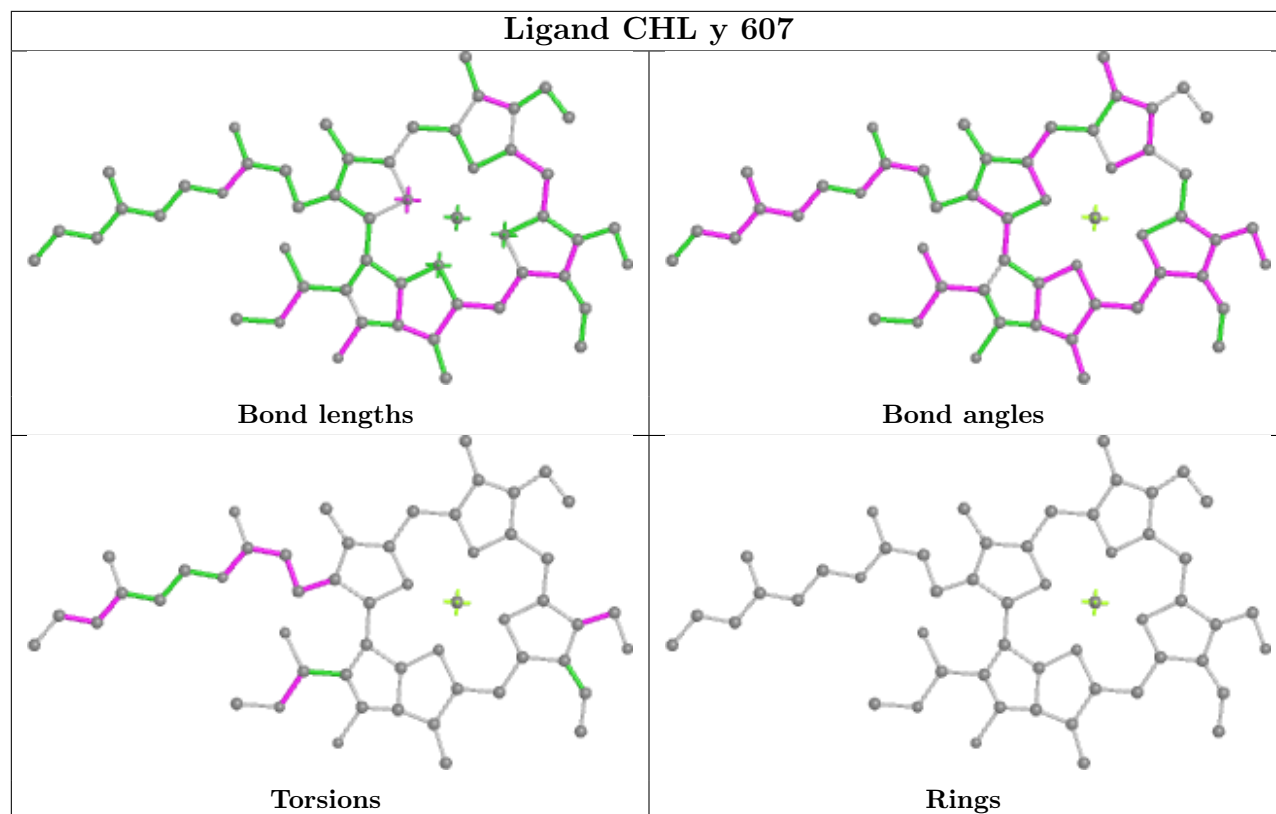


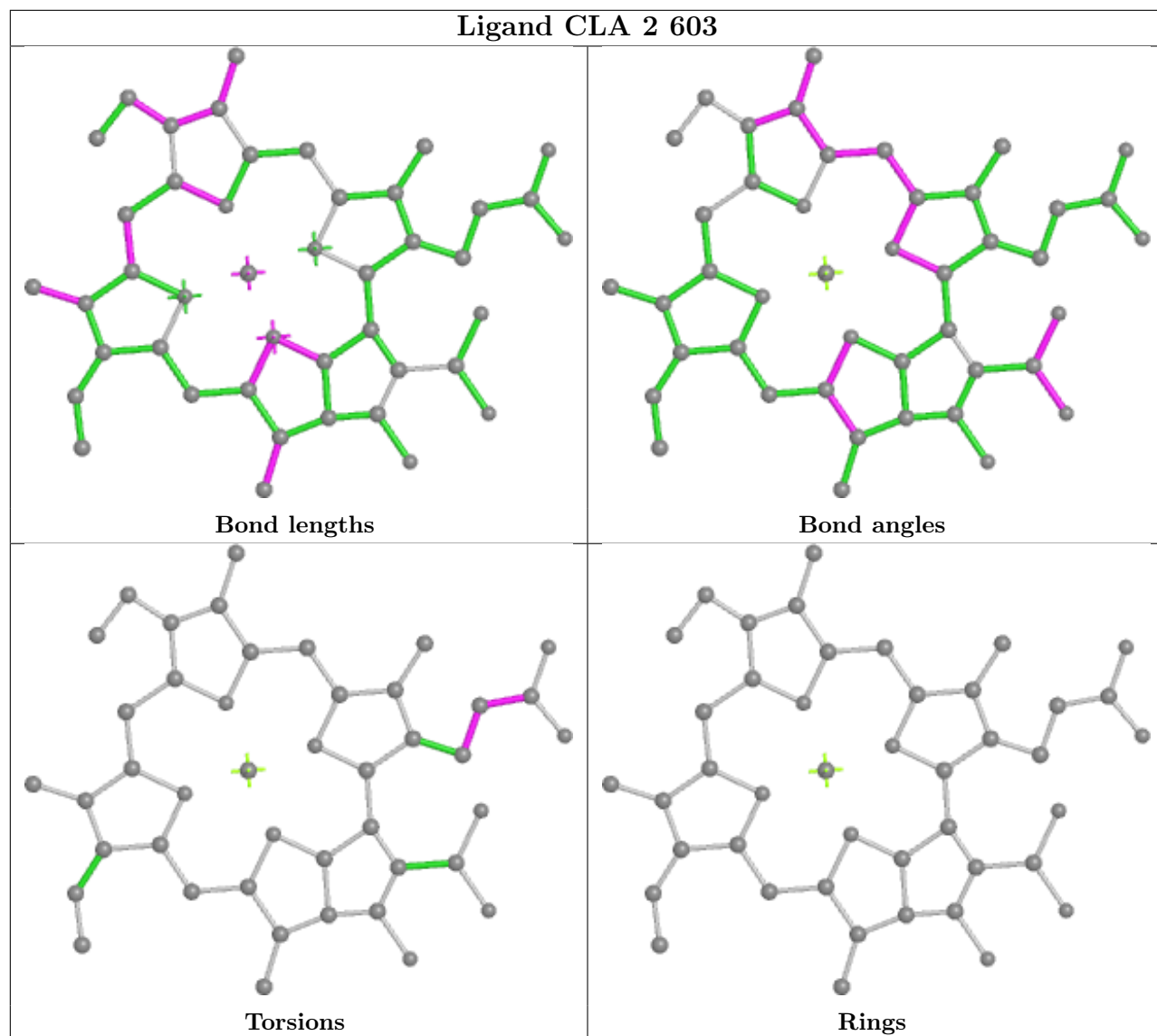


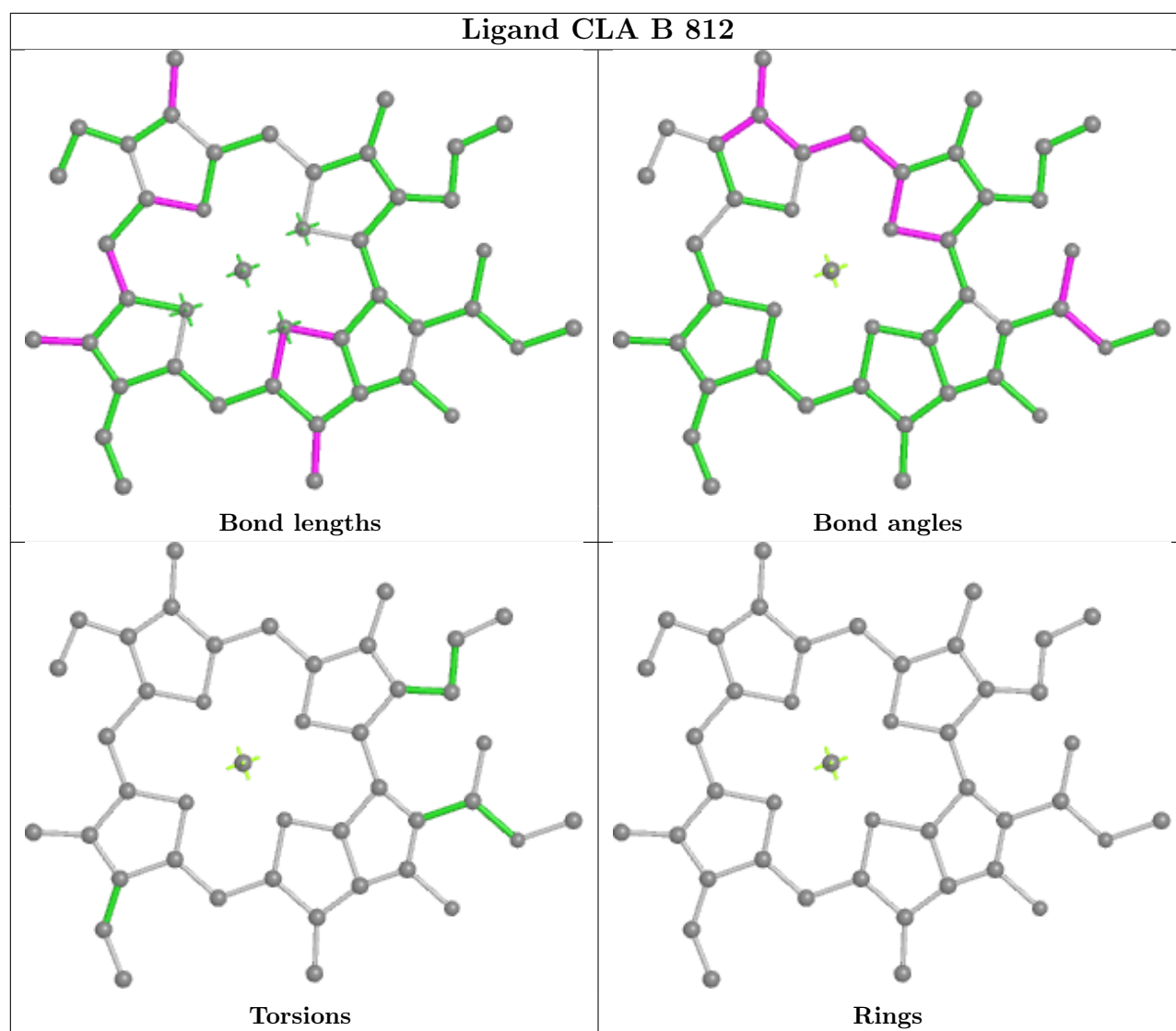




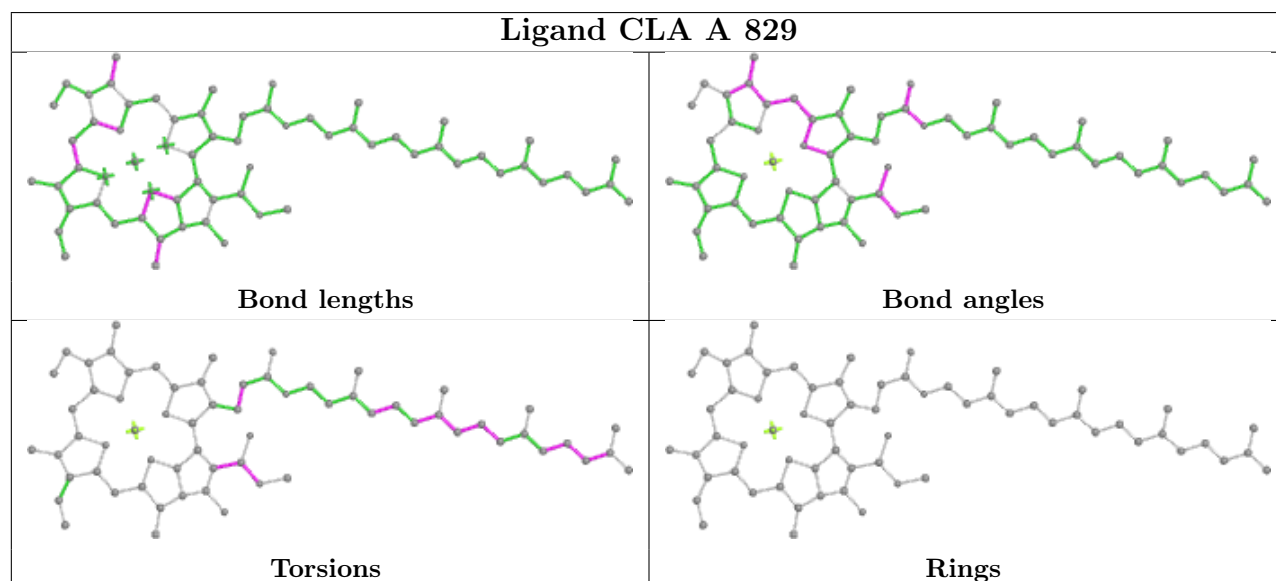
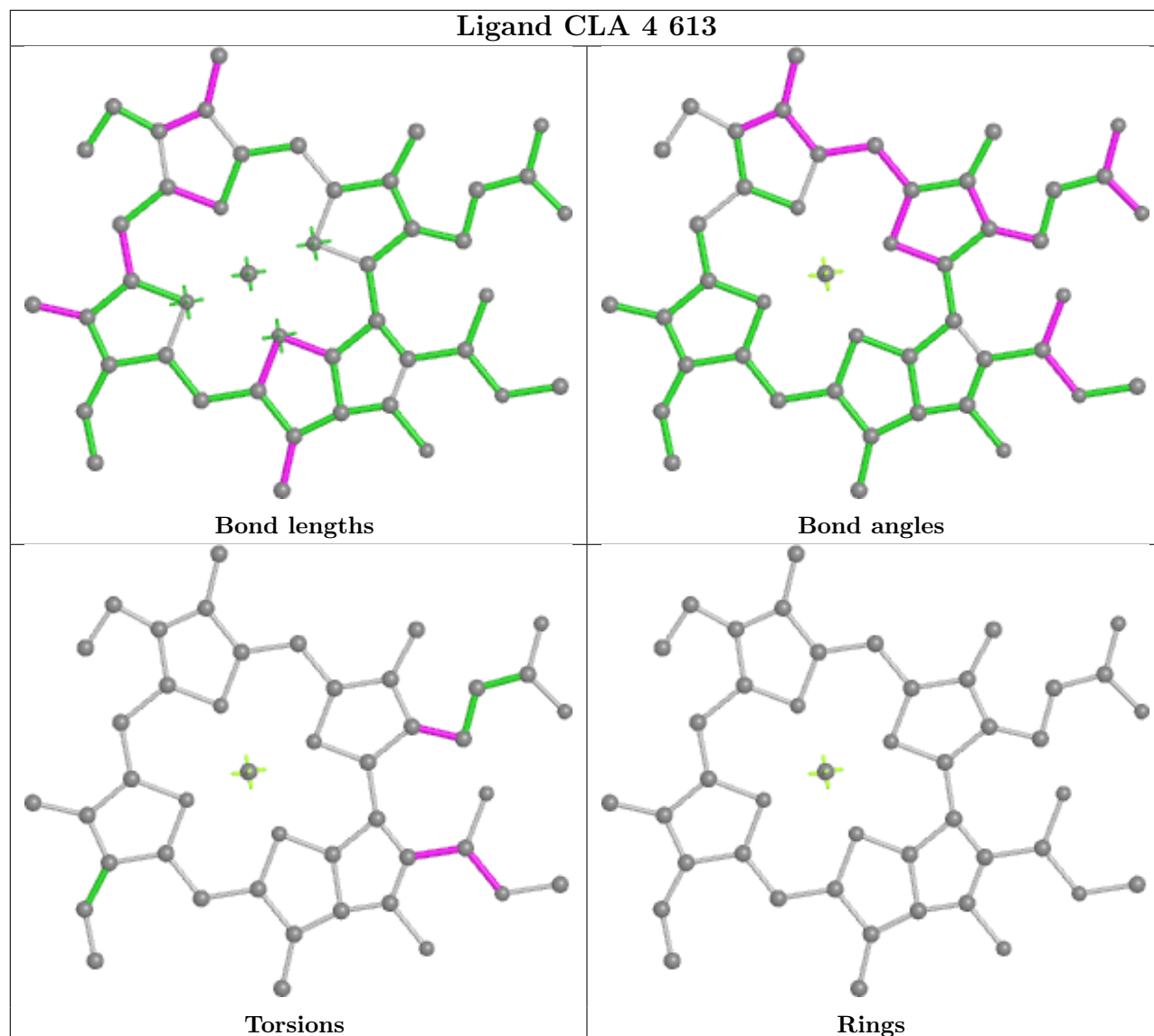


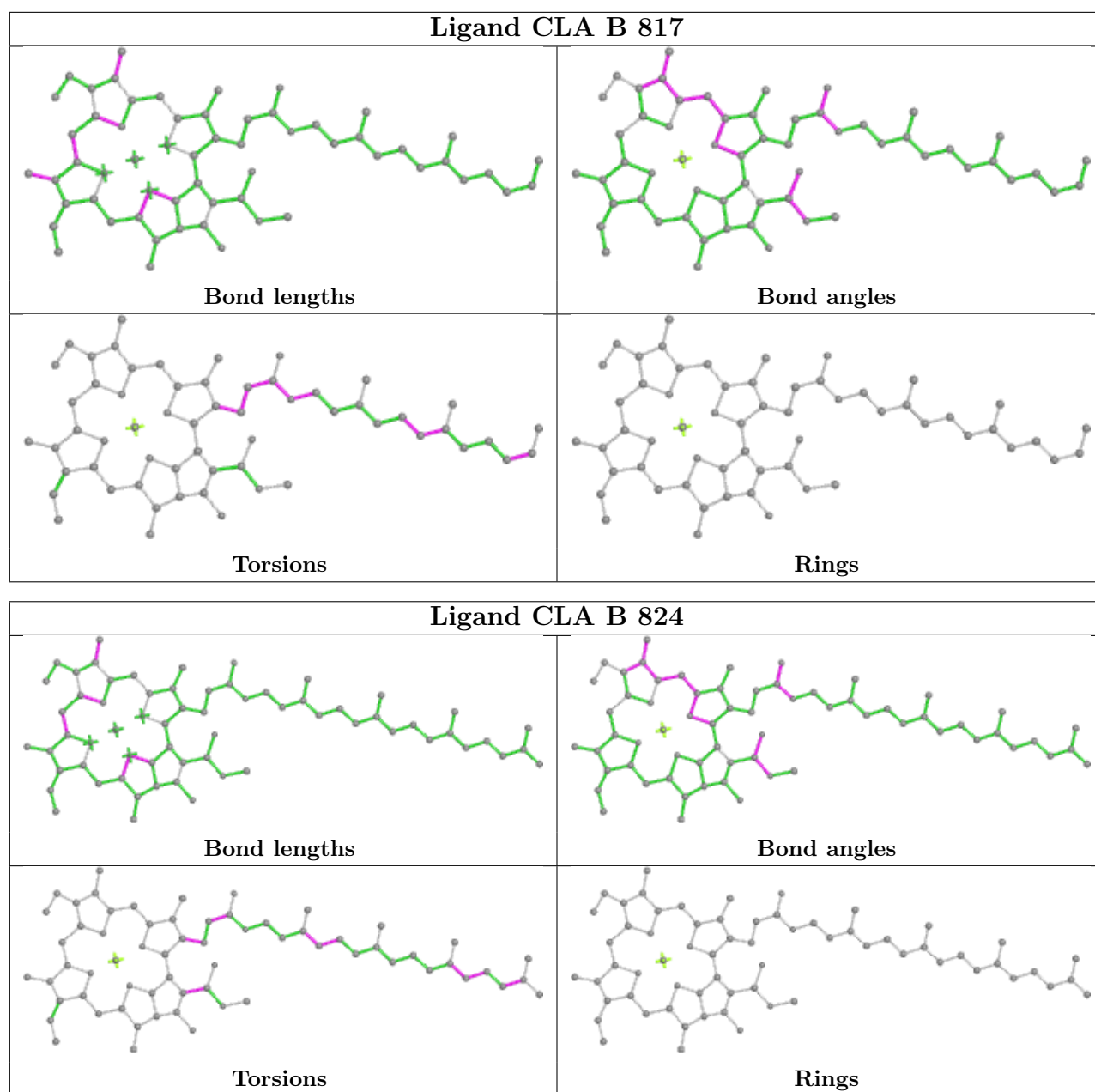


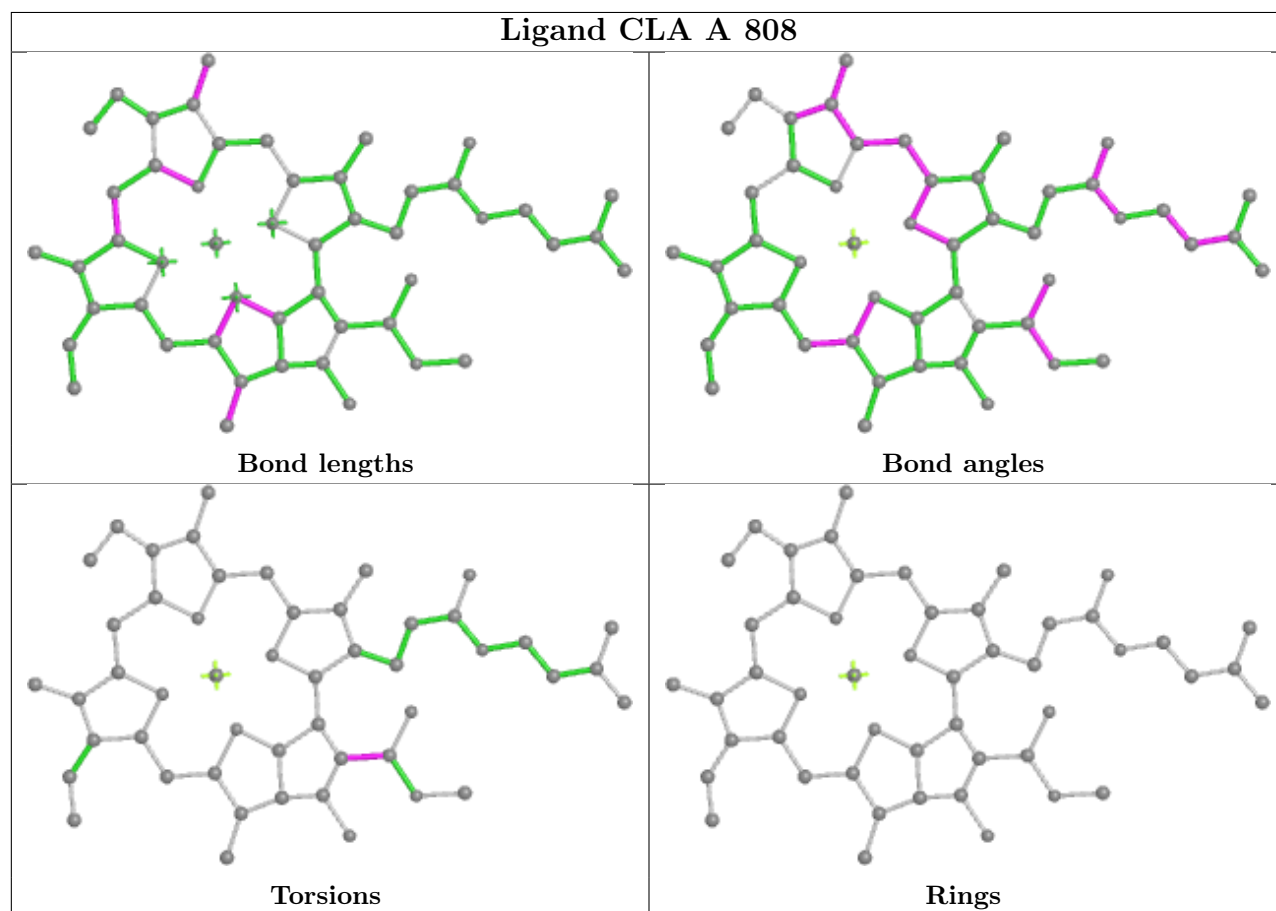
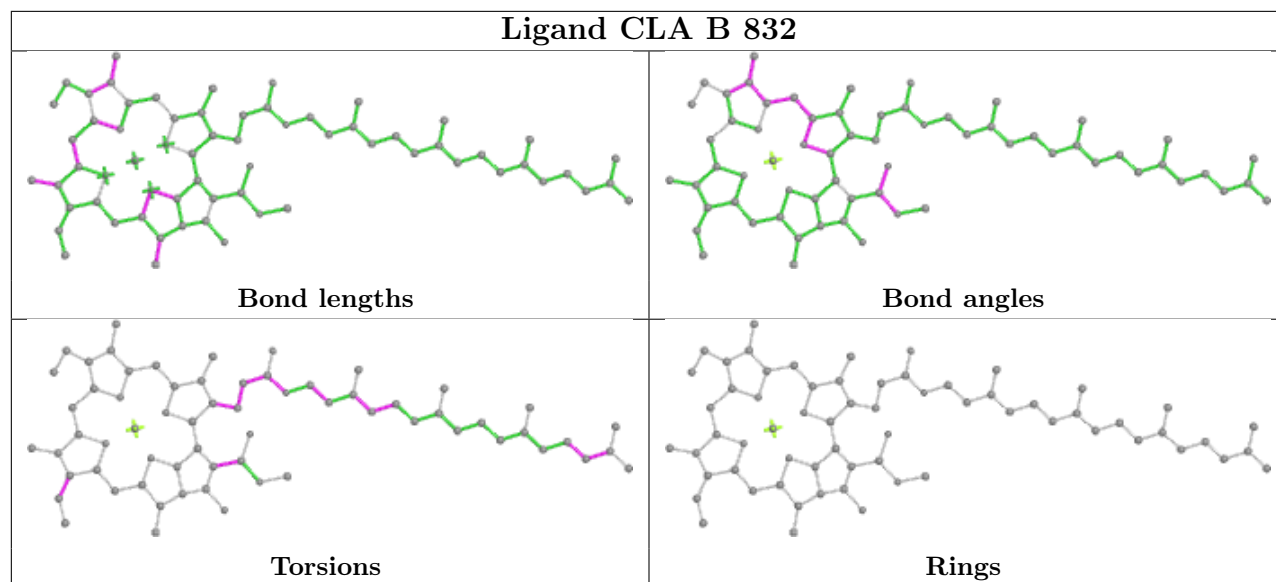


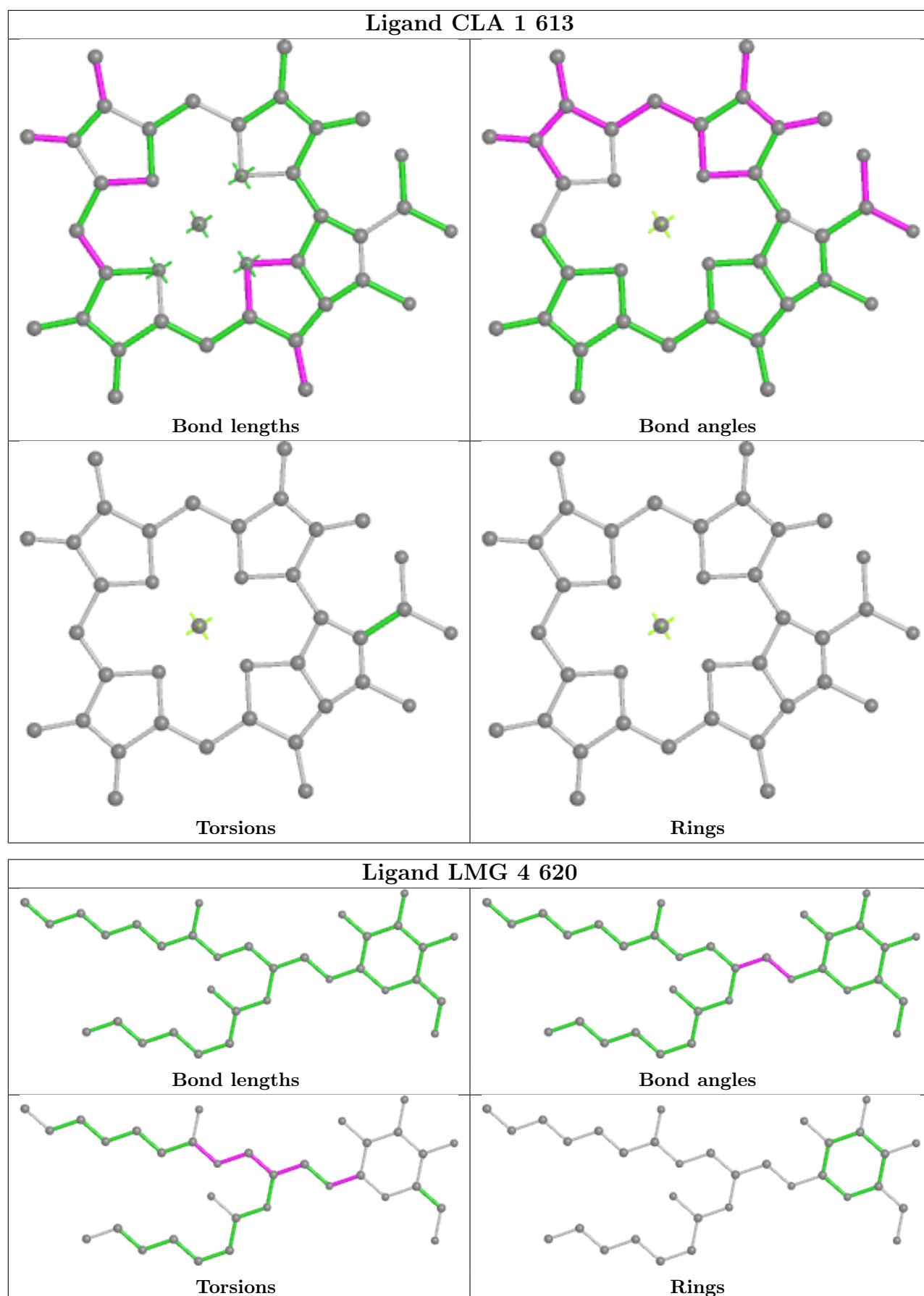


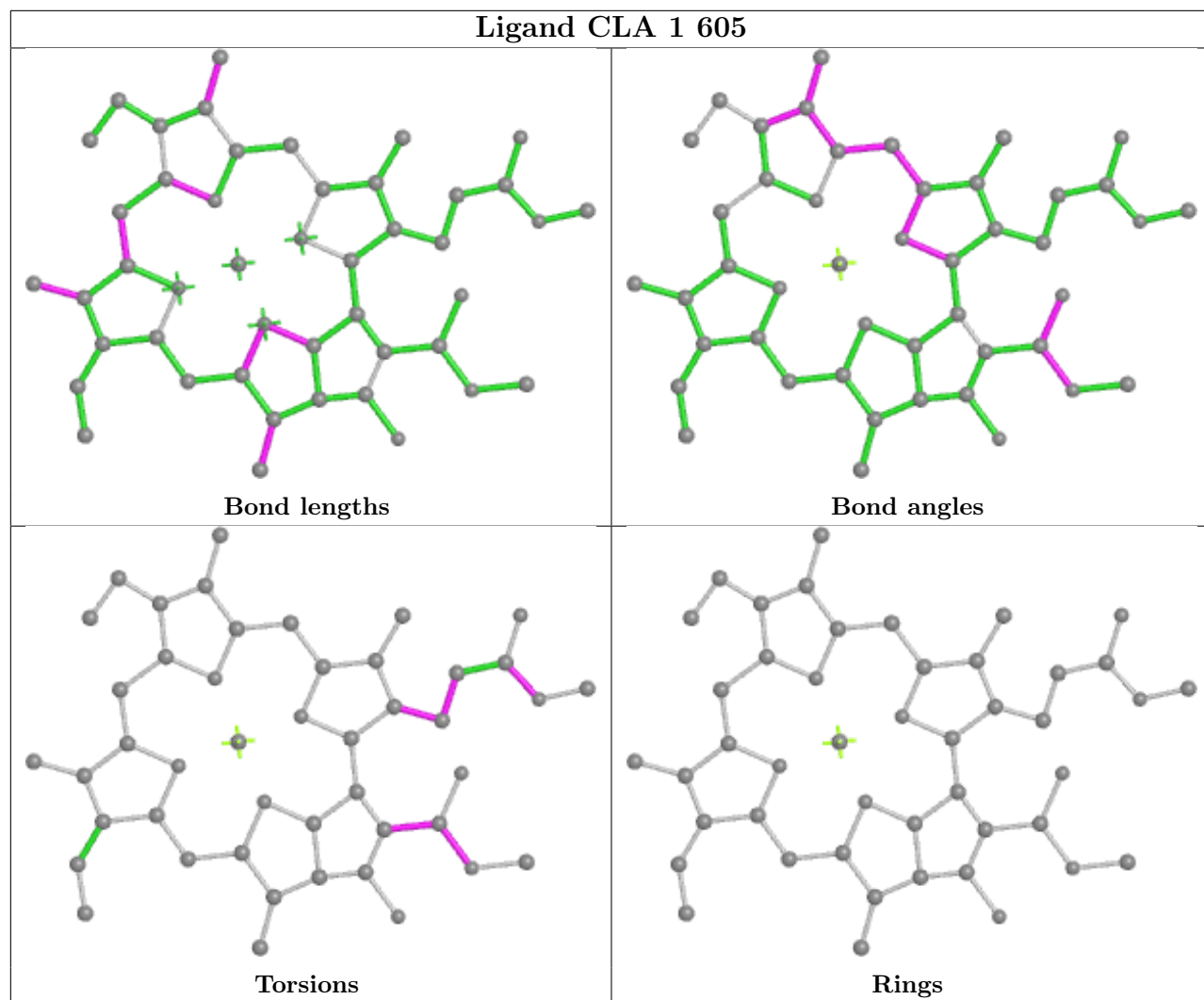


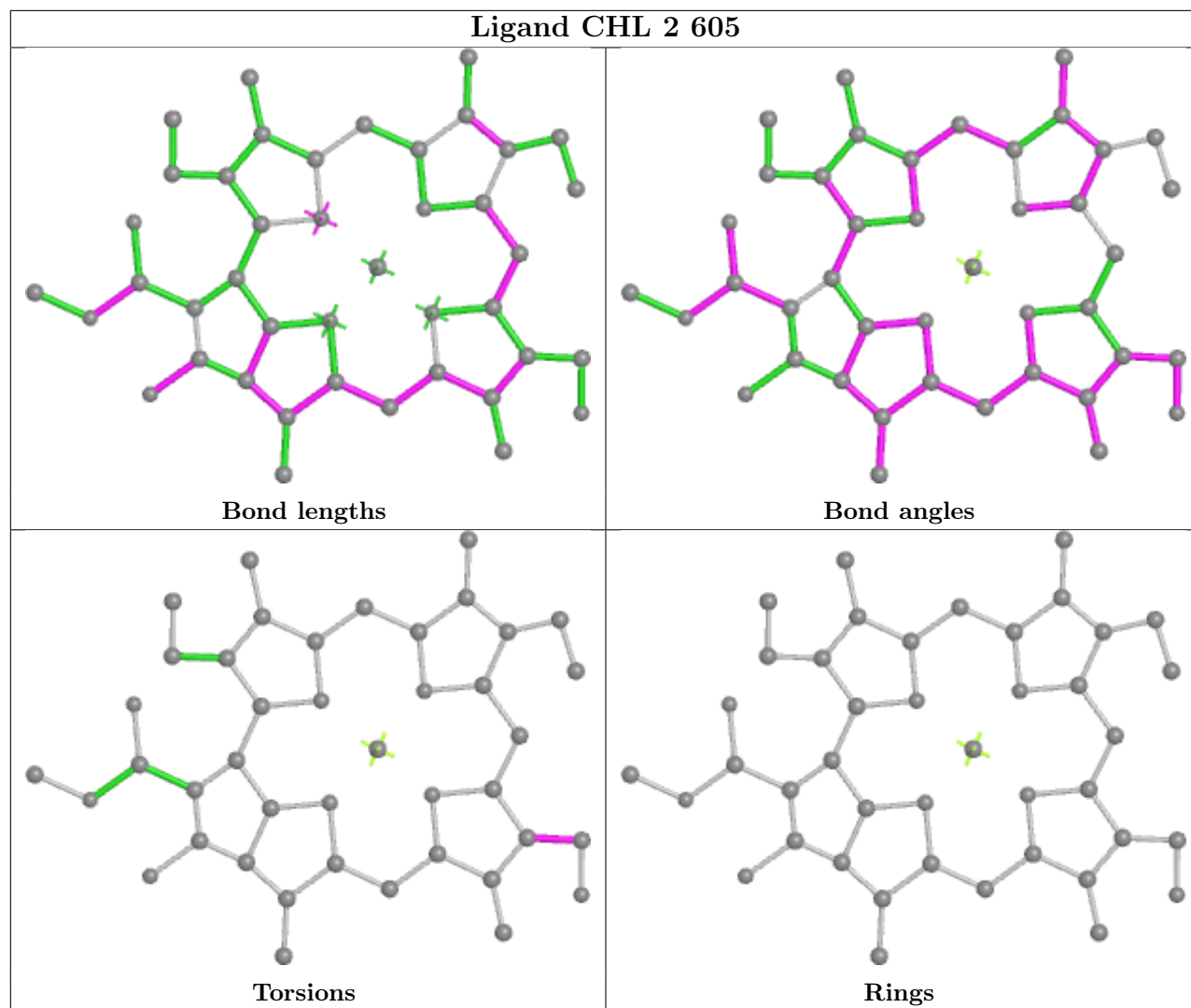


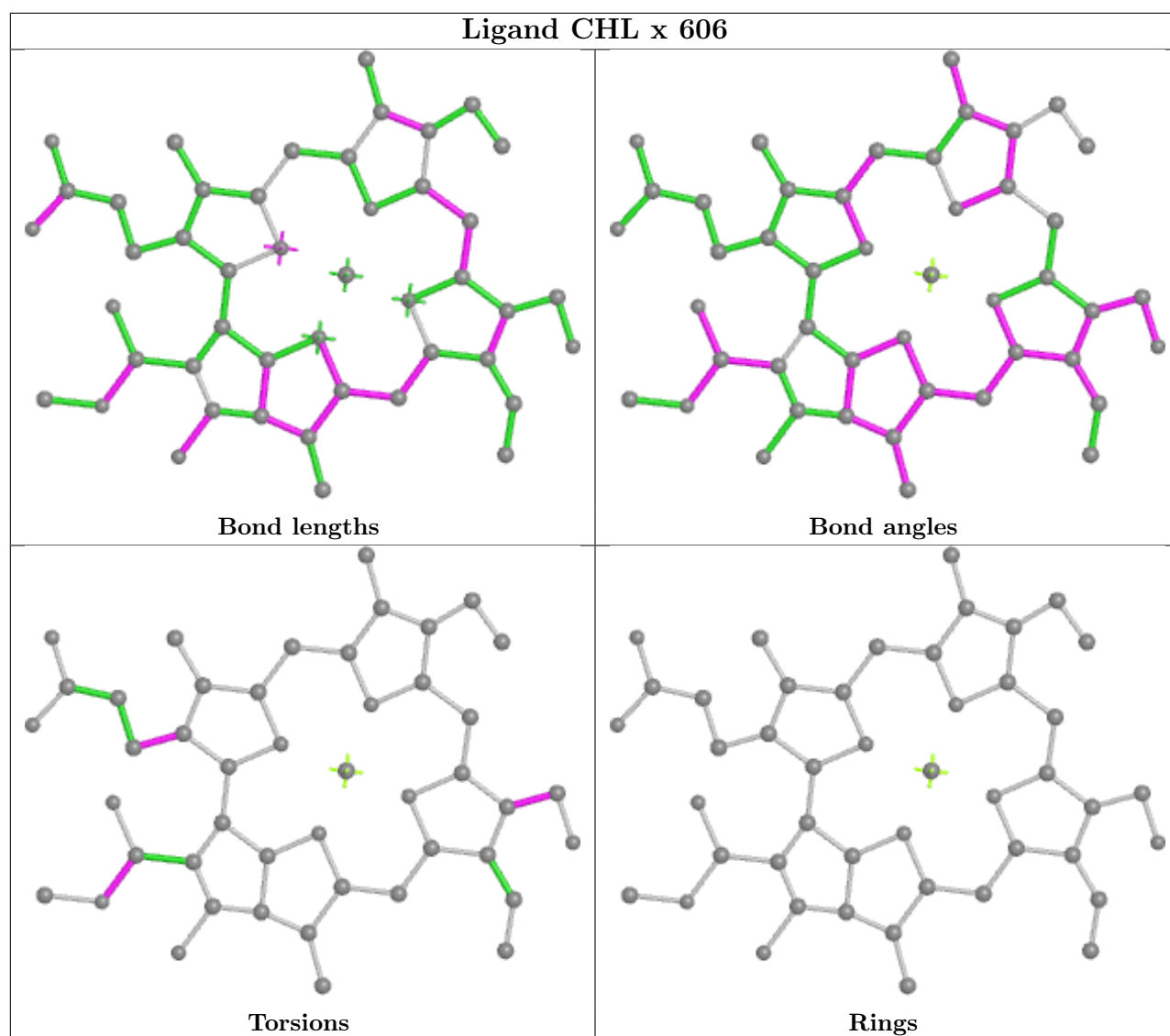


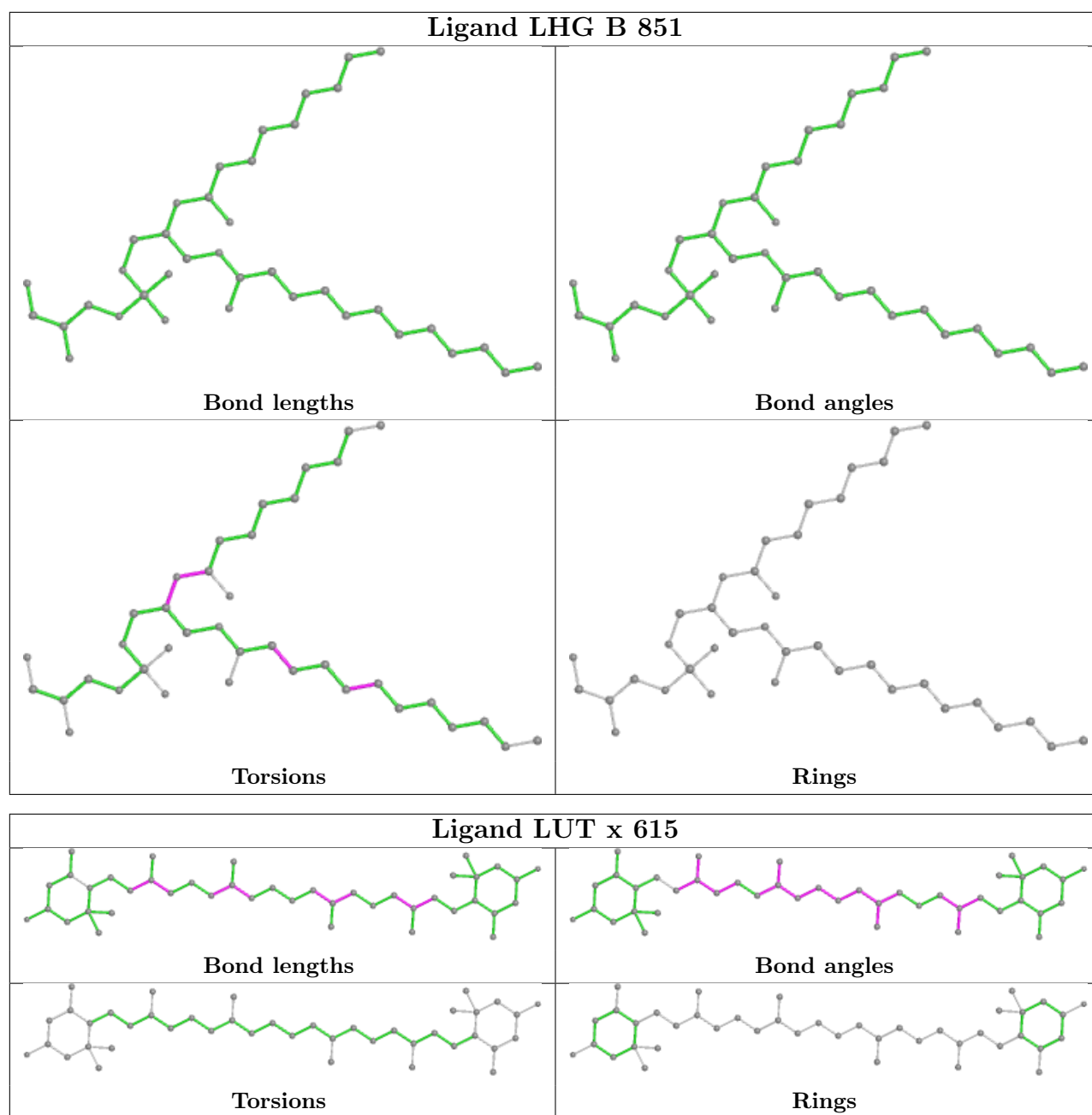




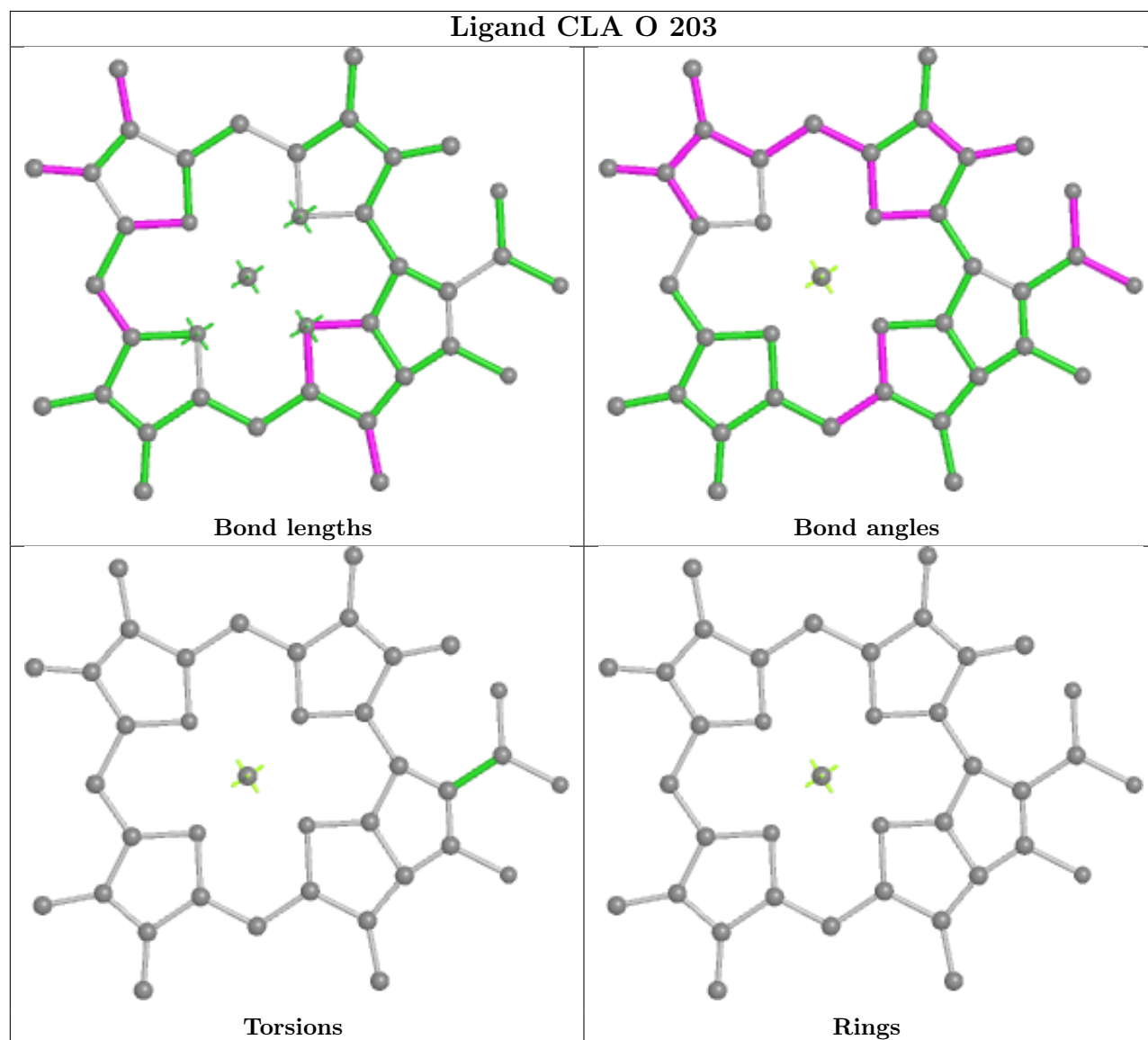
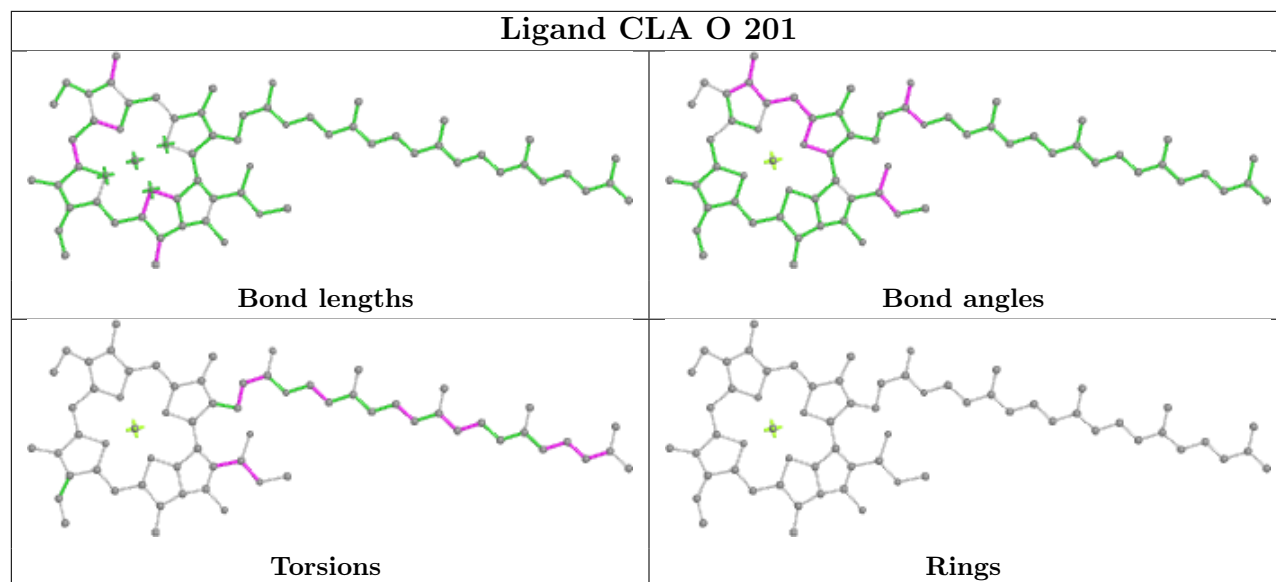


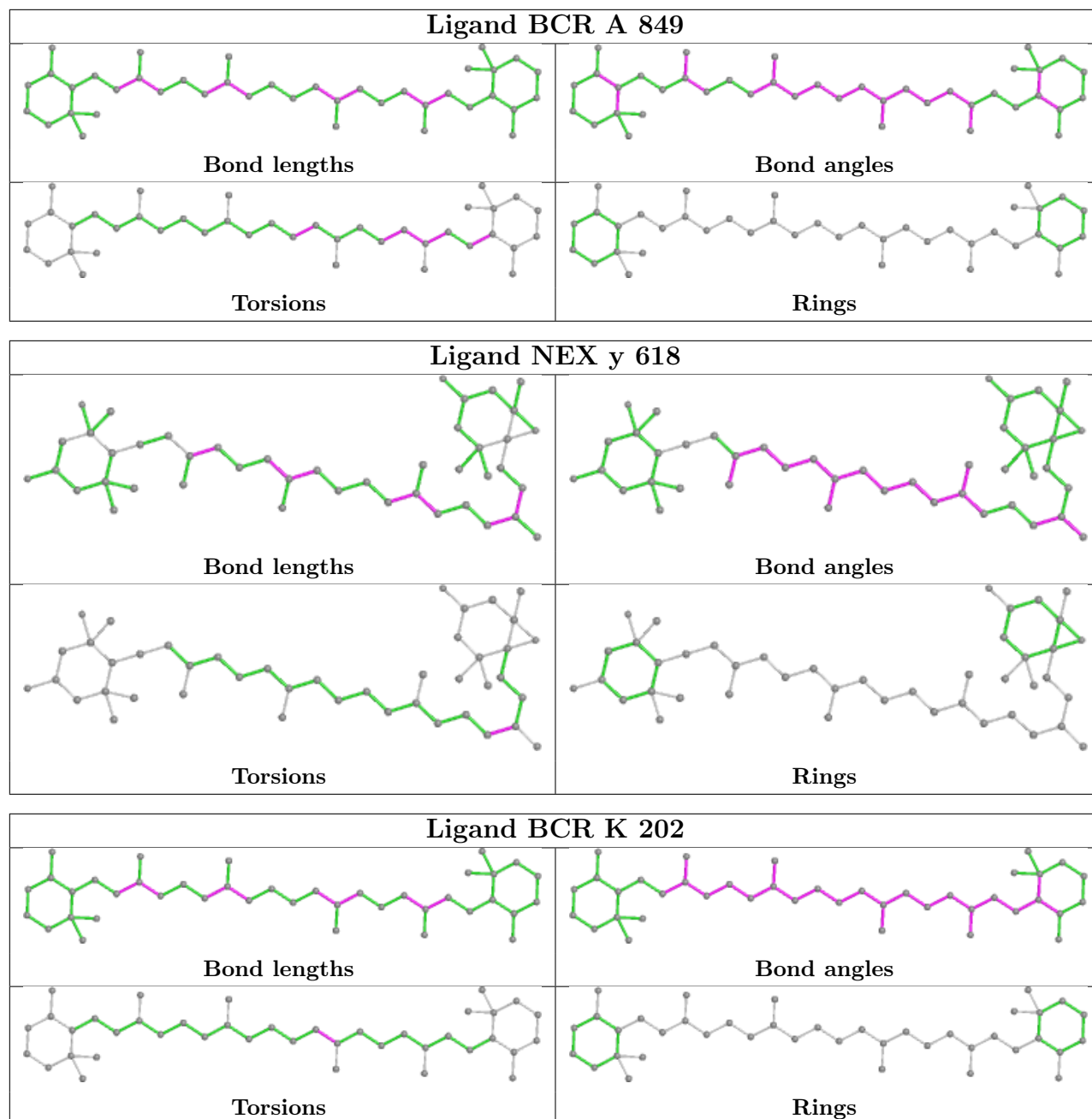


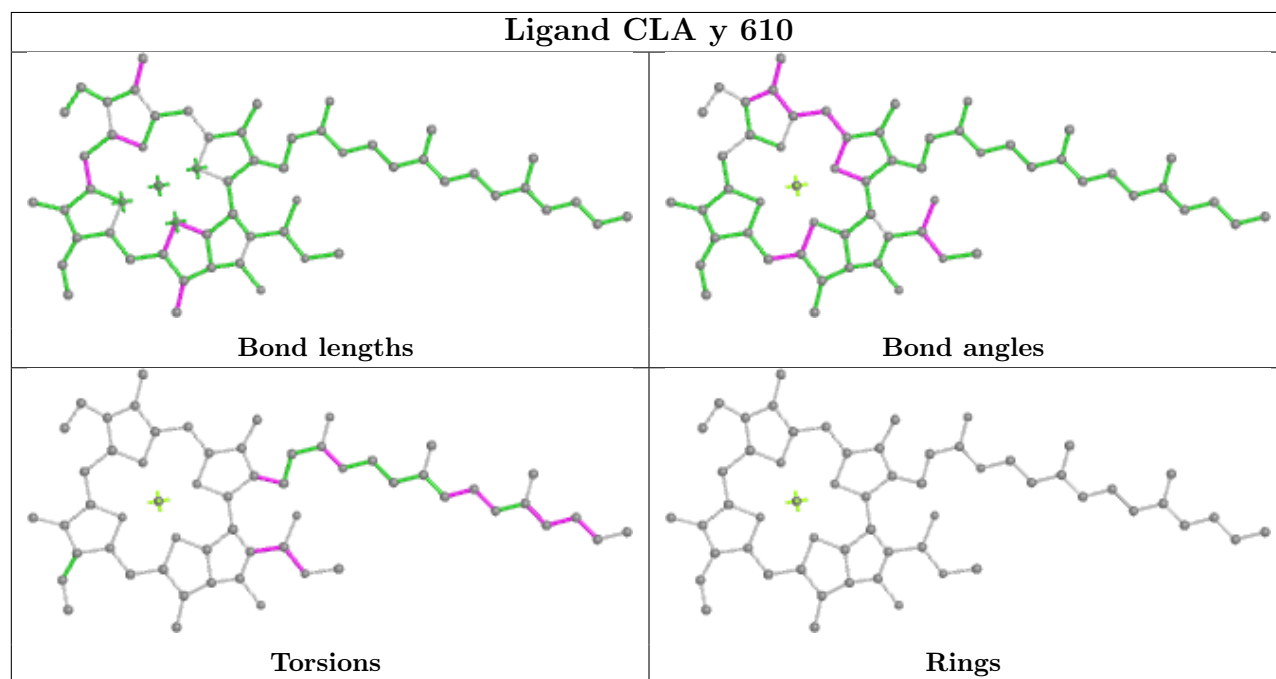
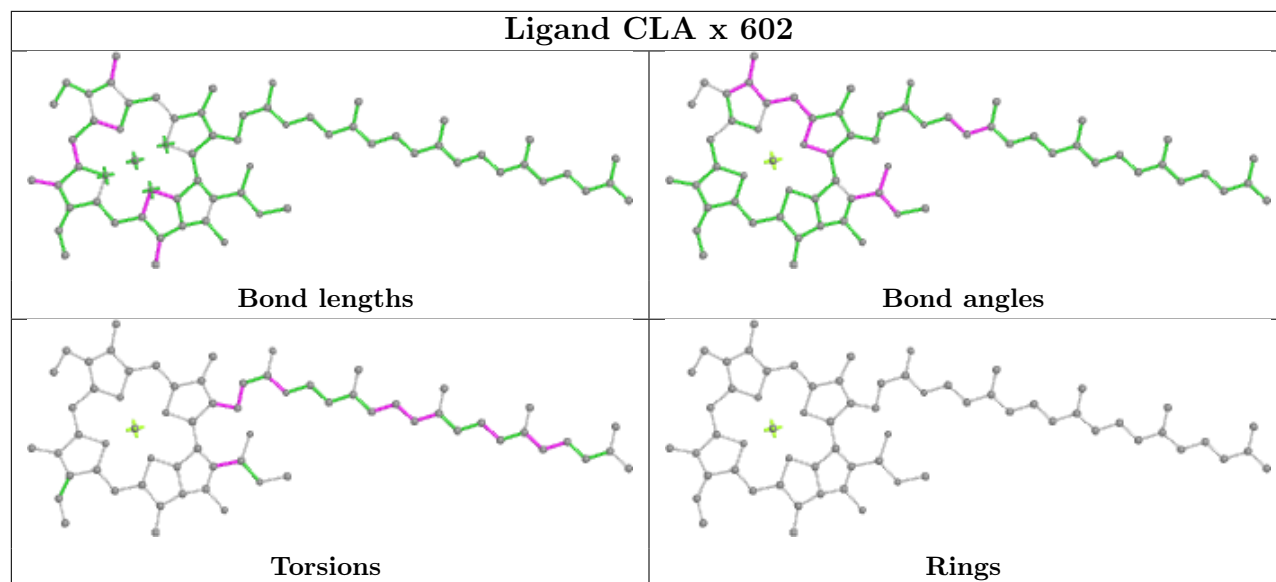


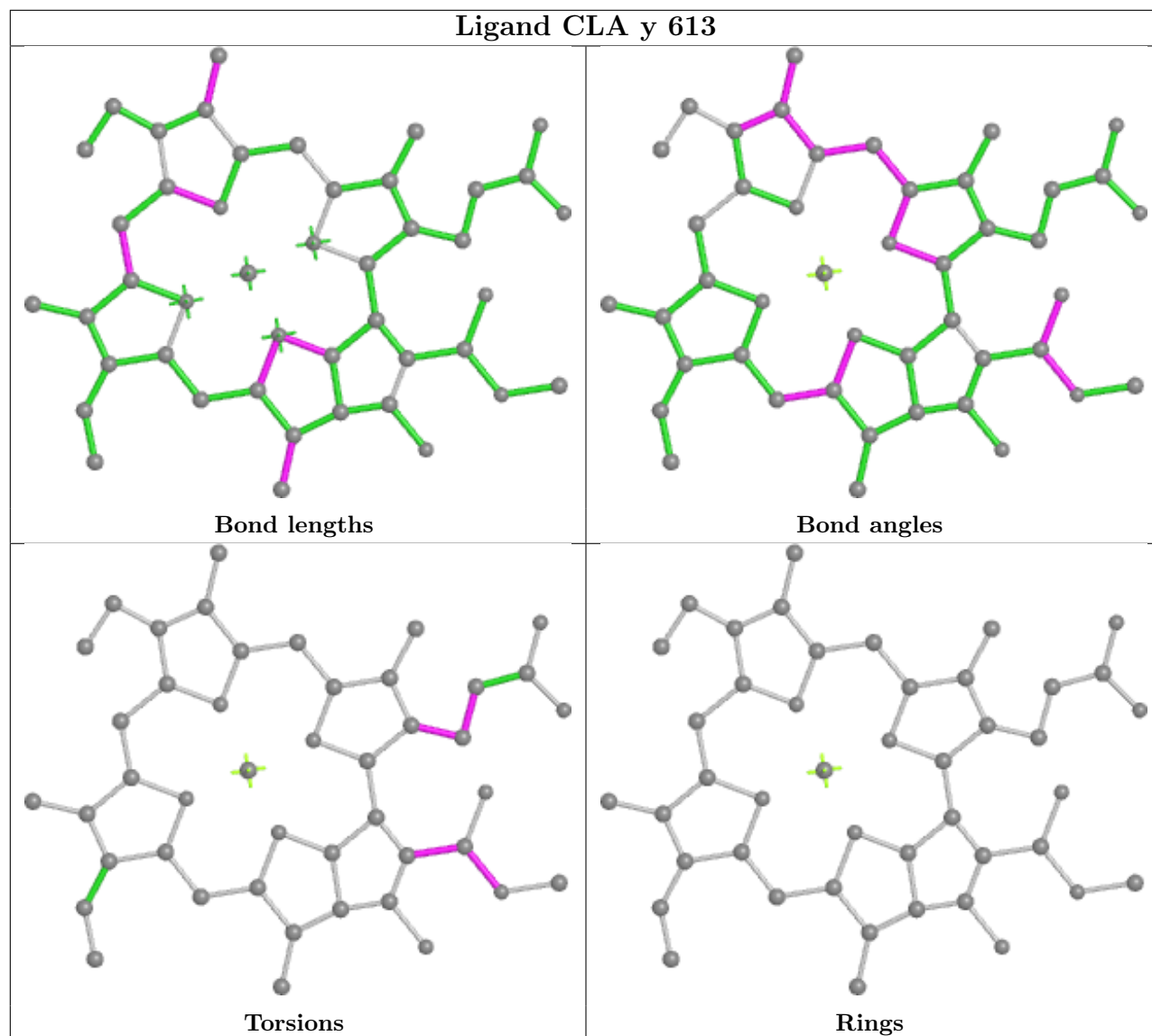


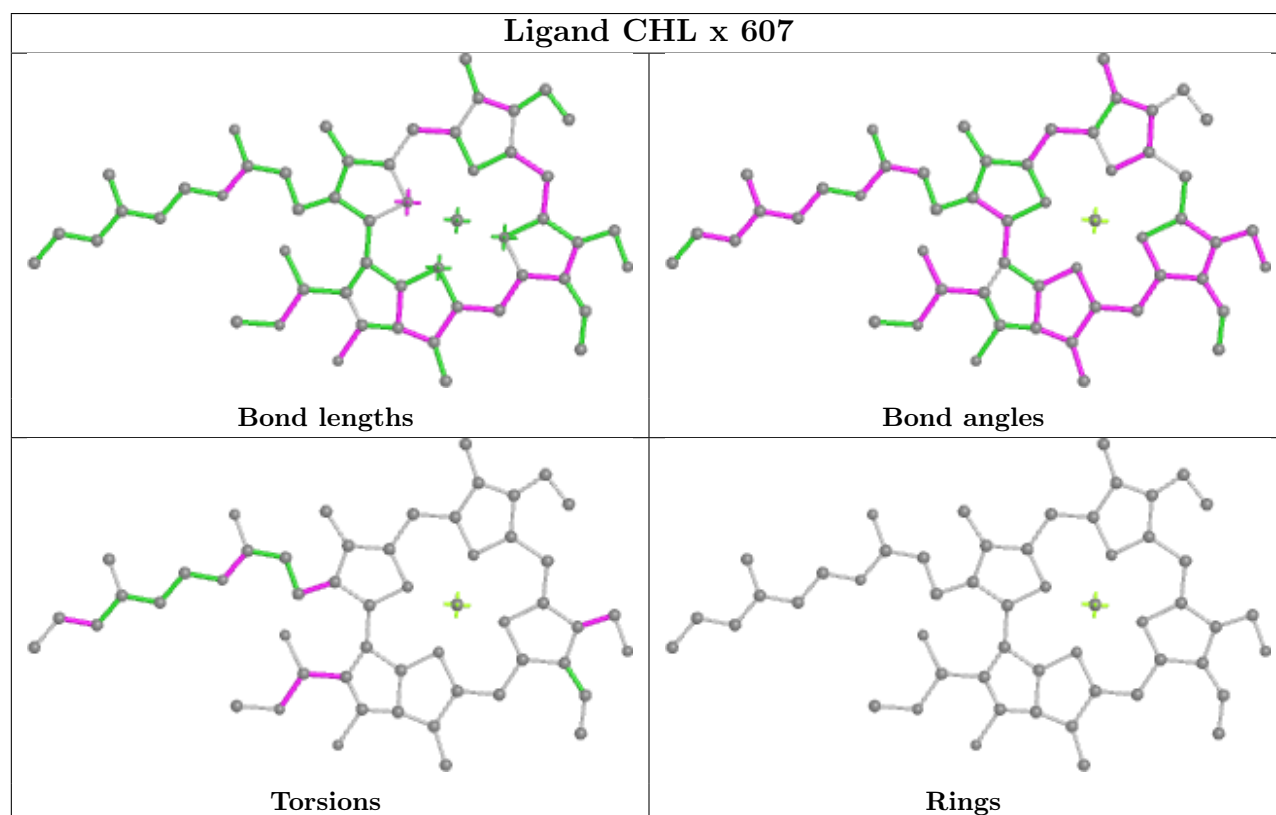
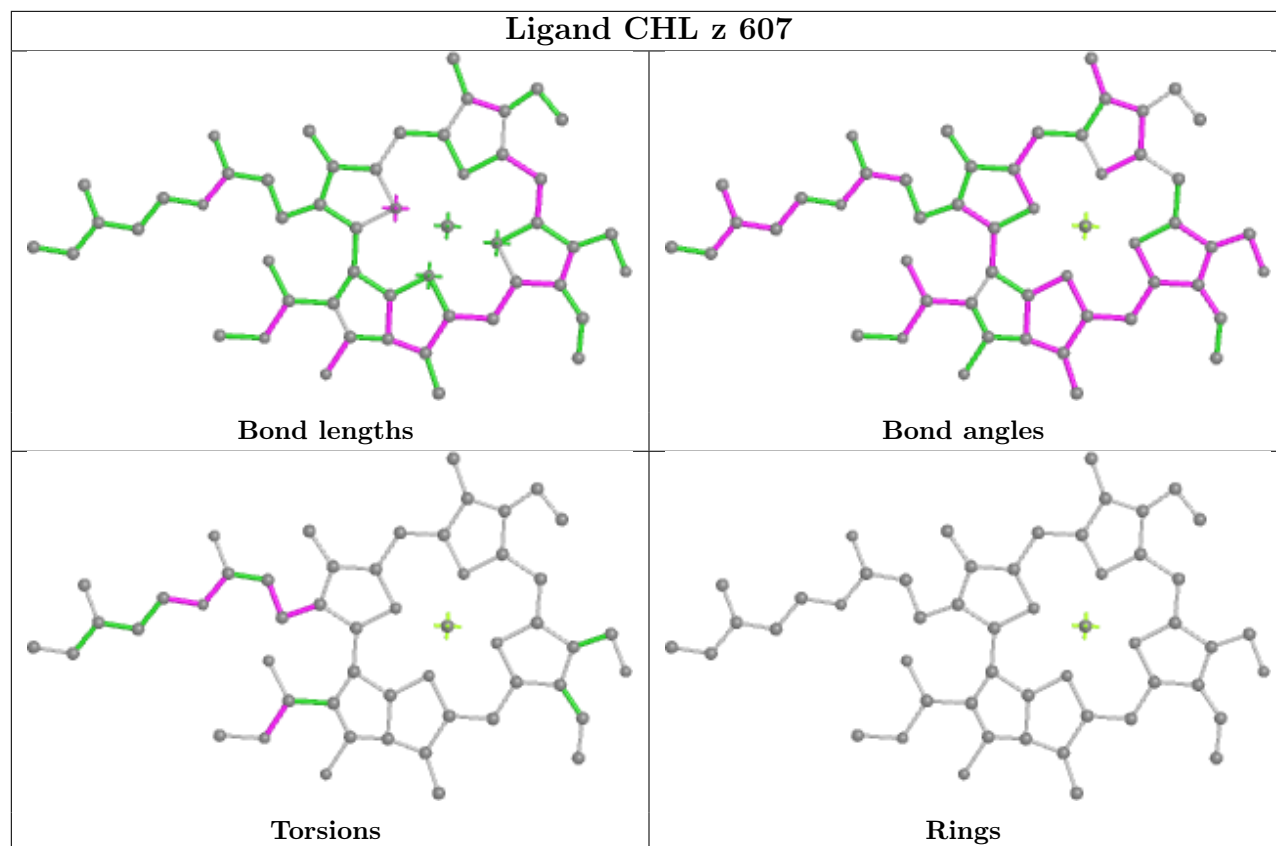


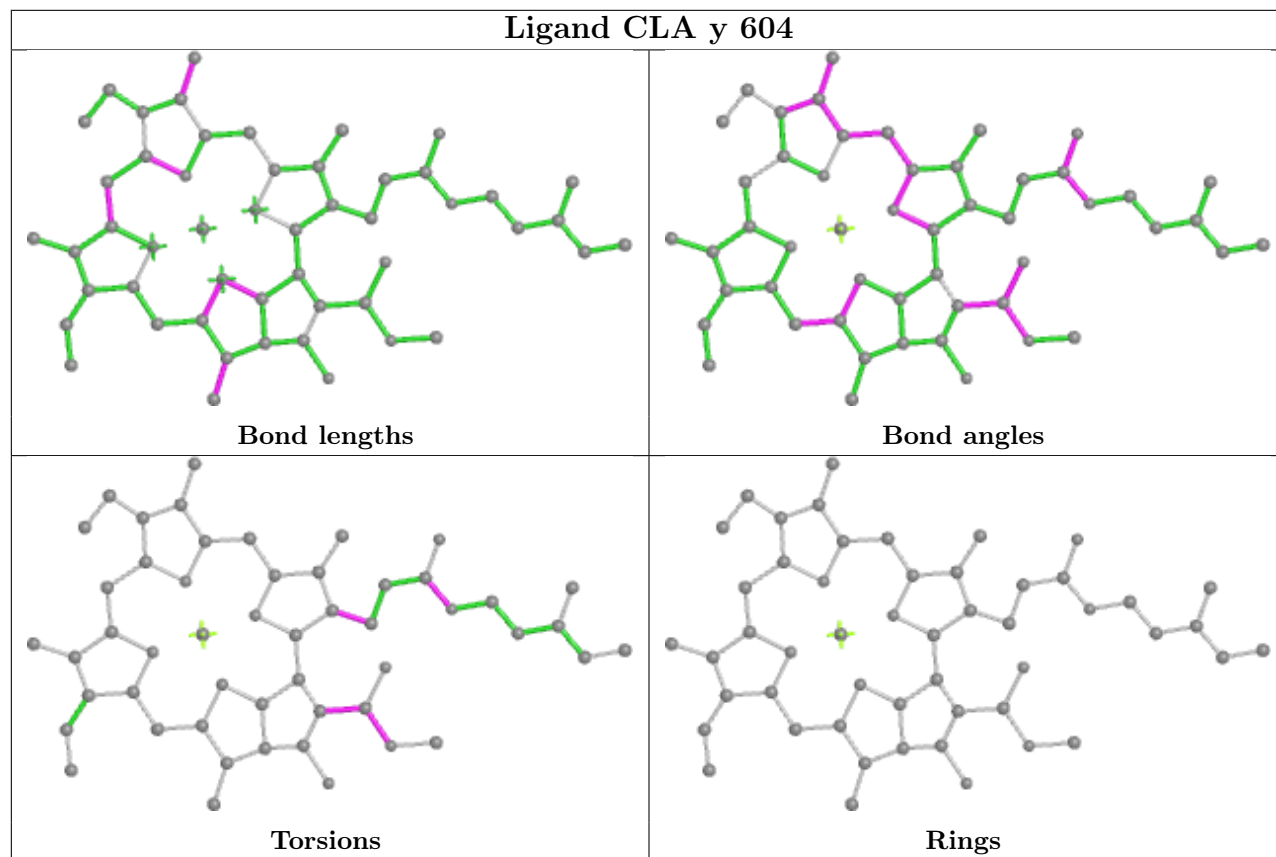
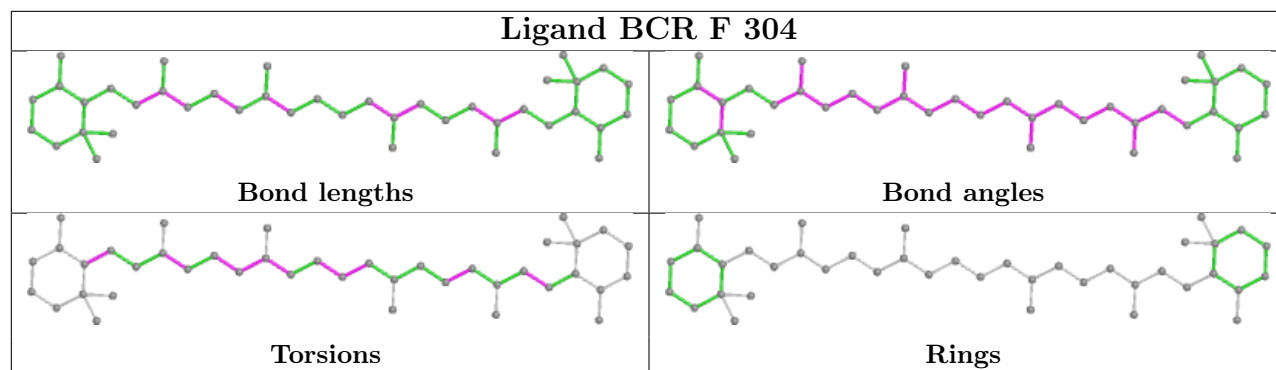
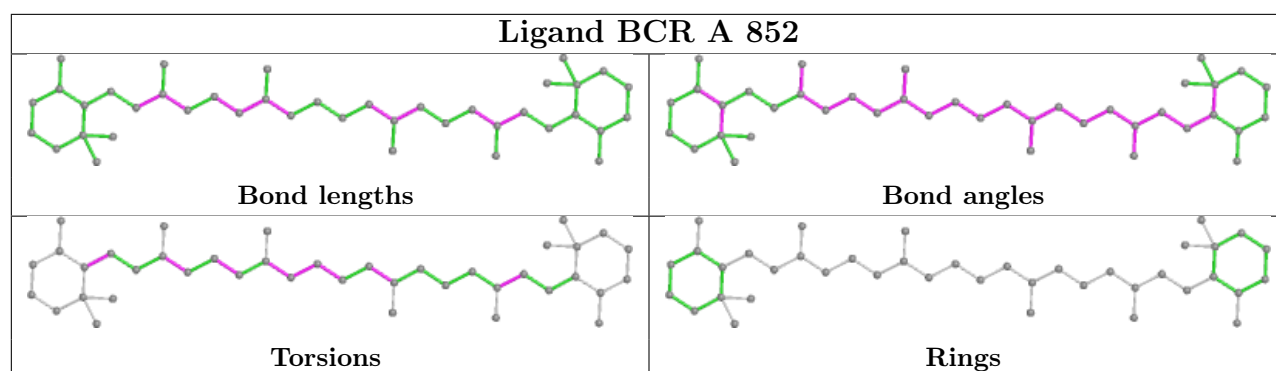


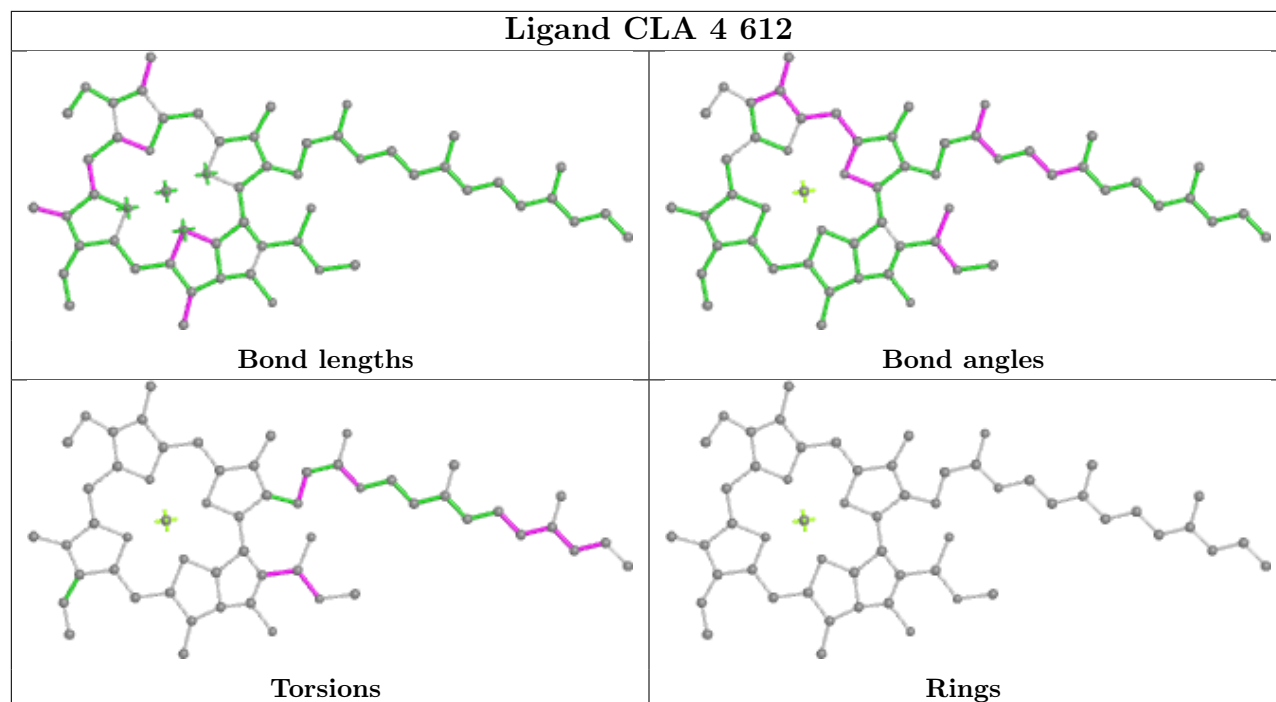


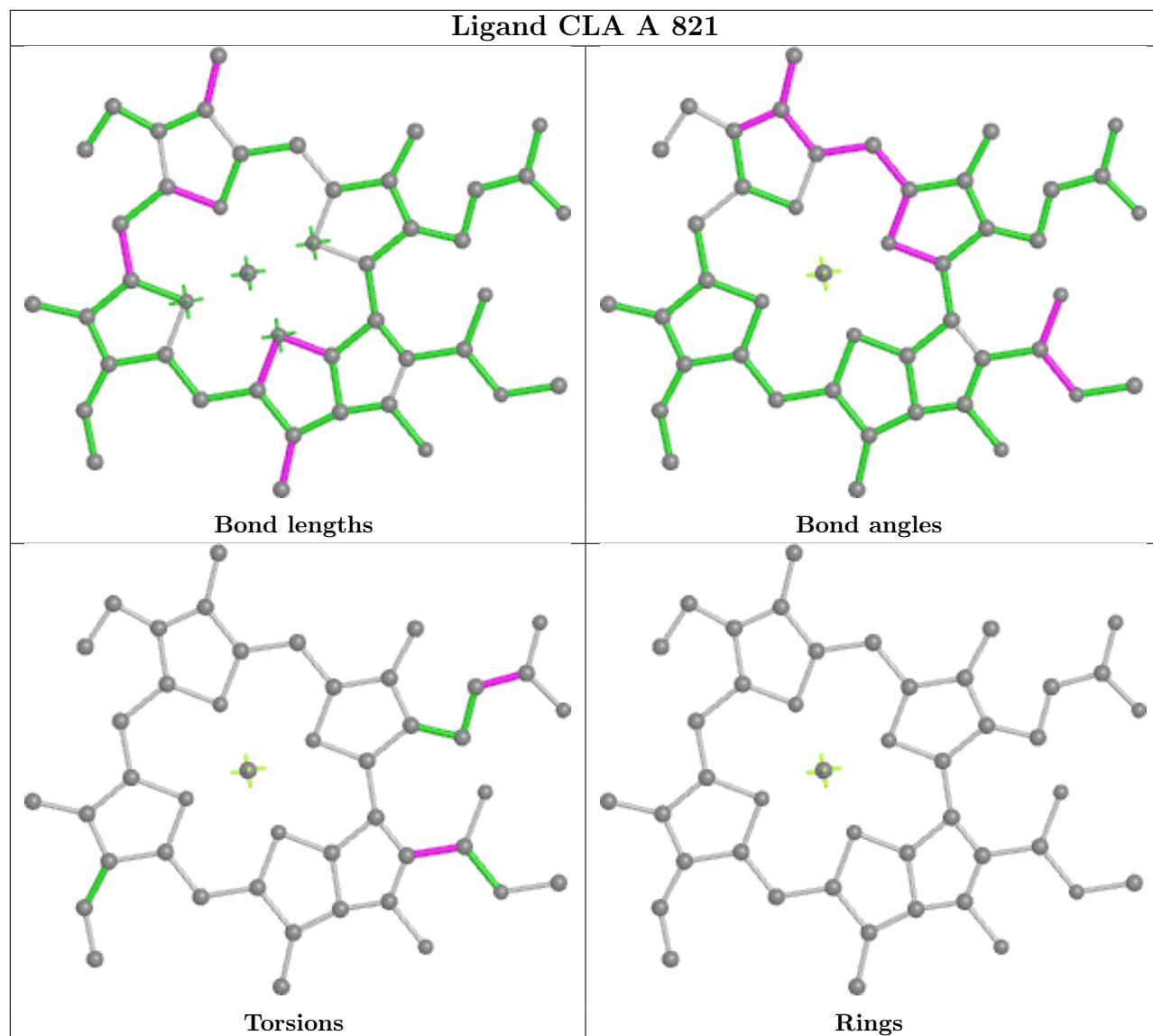




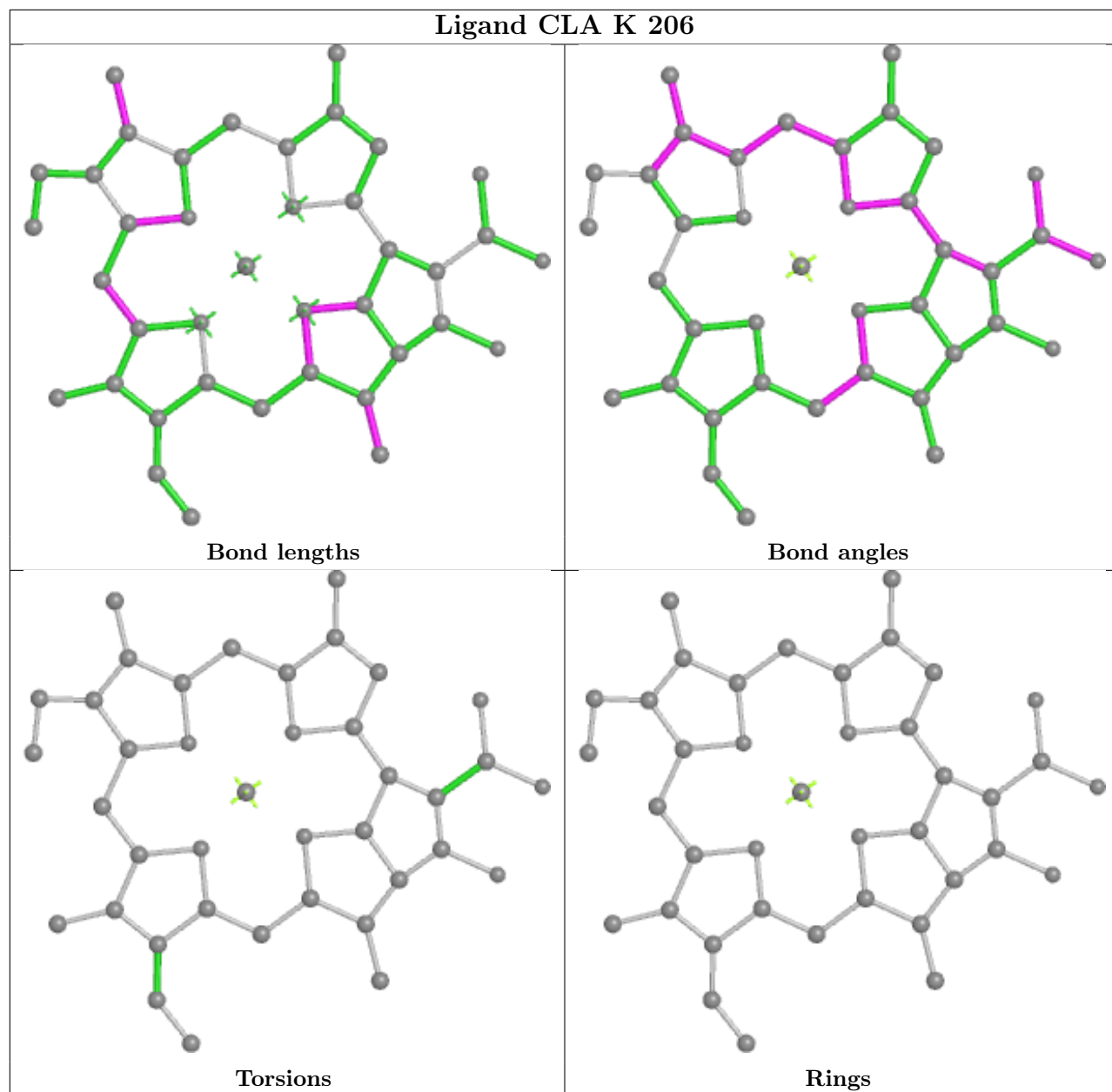


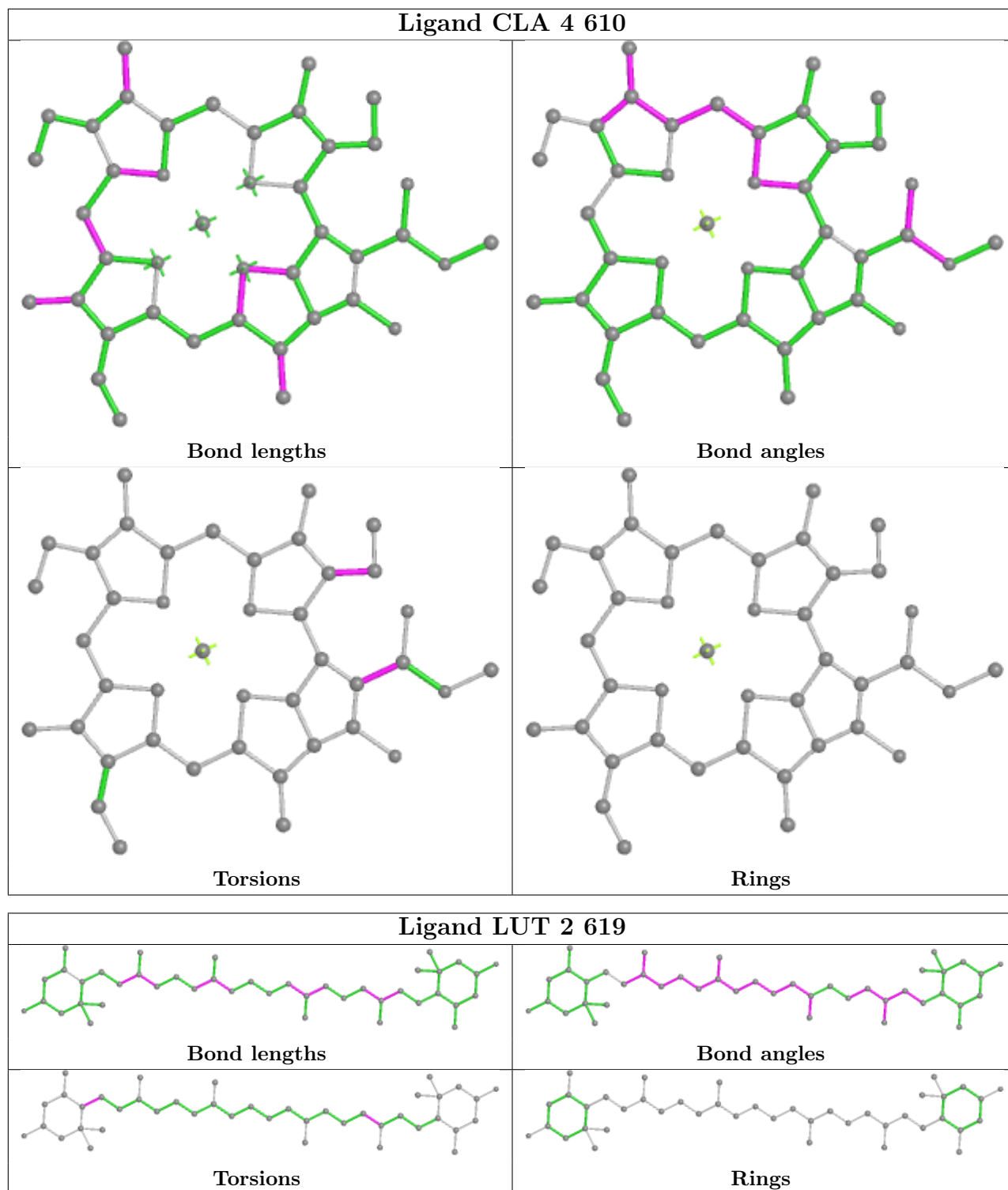


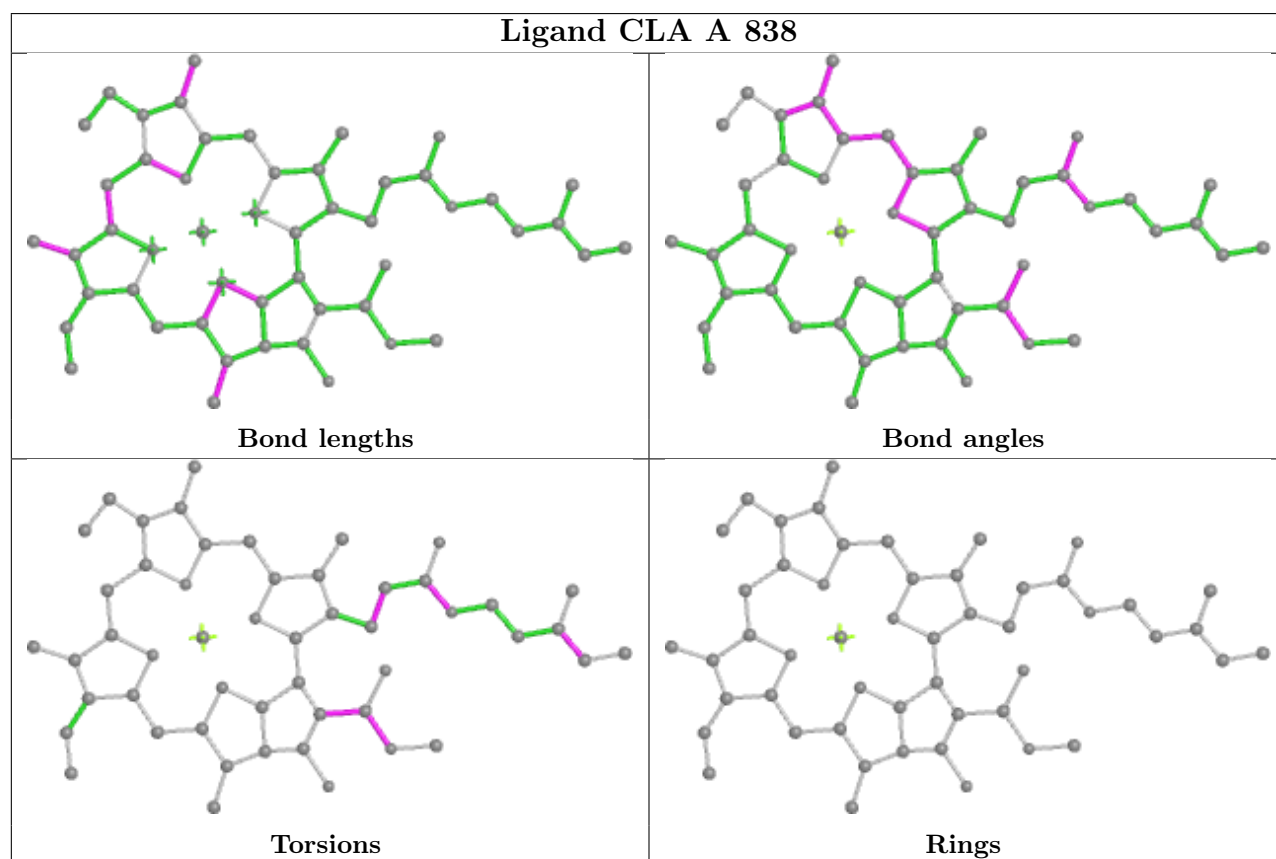
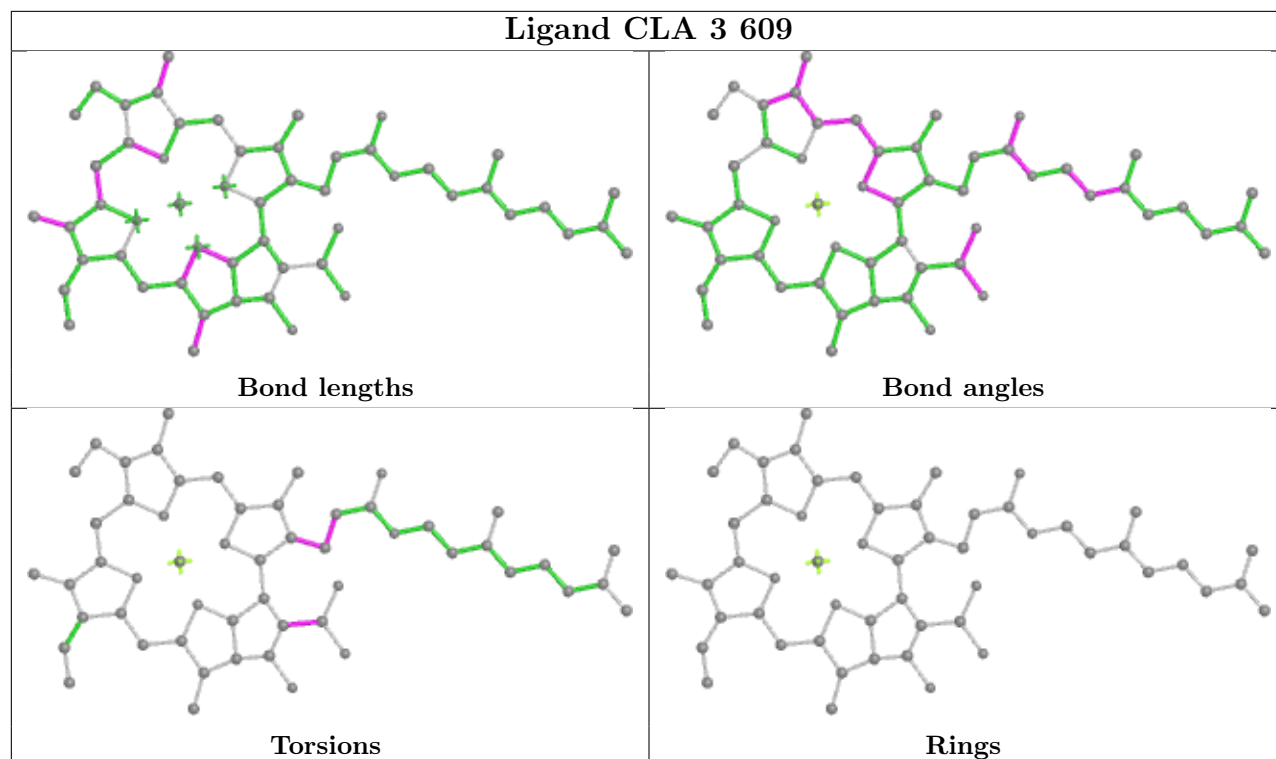


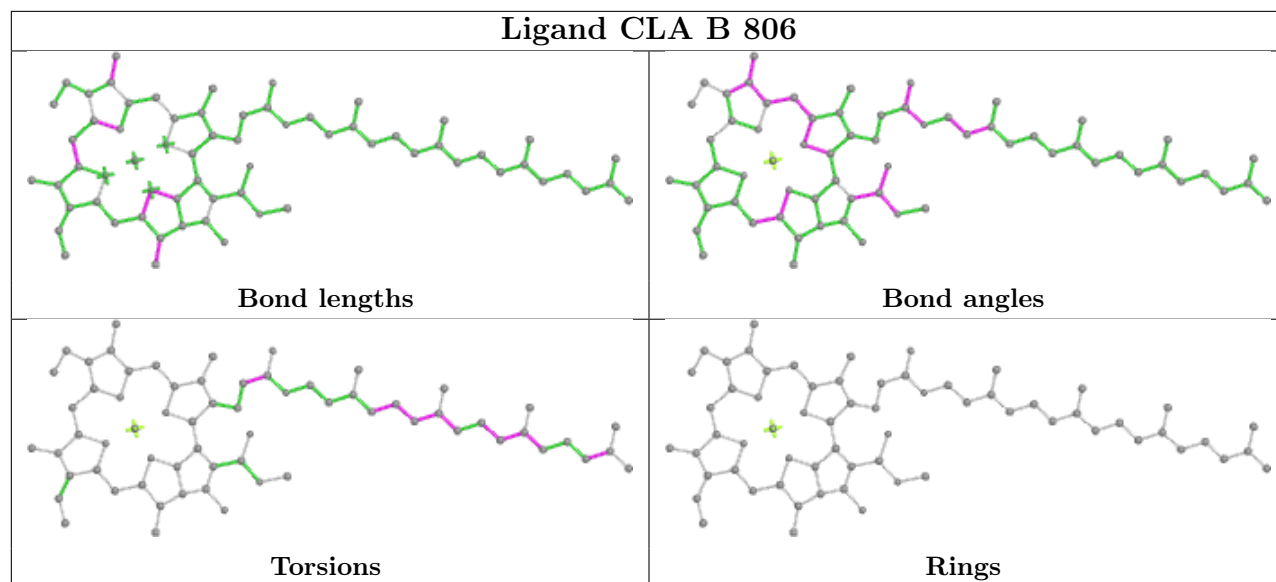












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

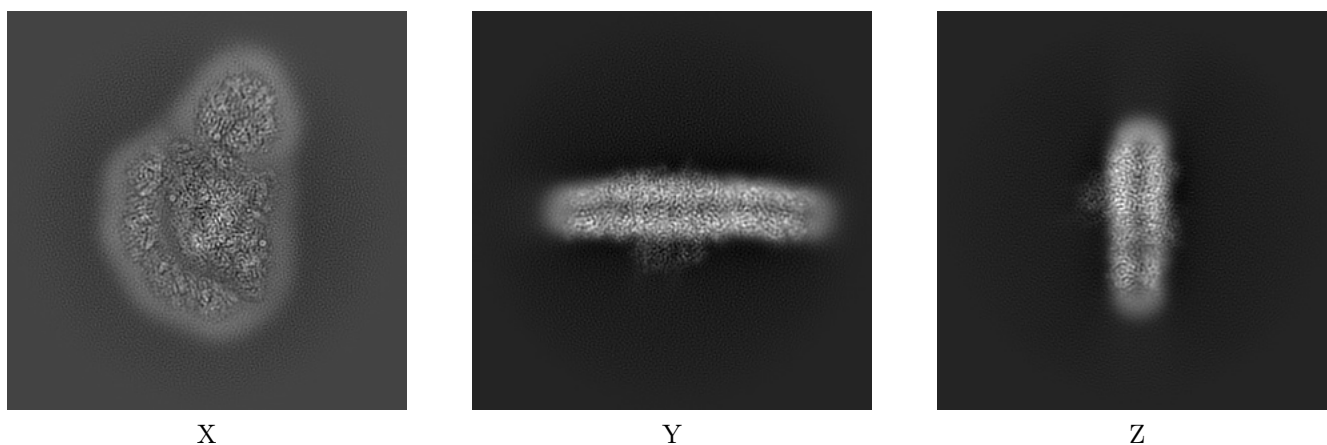
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36021. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

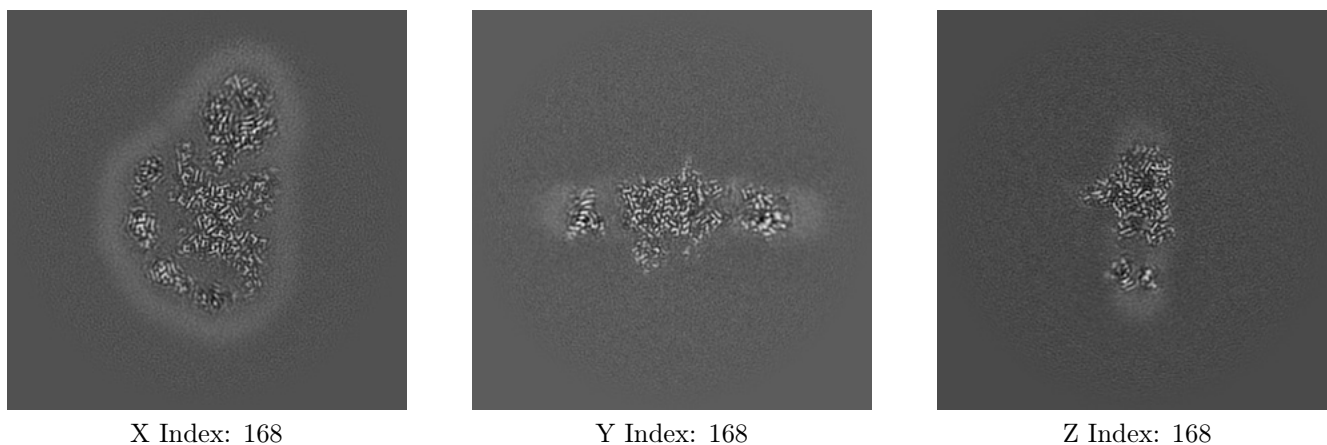
#### 6.1.1 Primary map



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

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

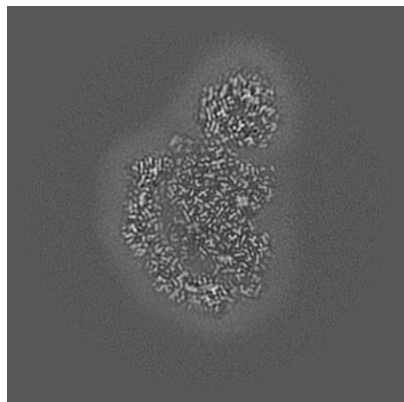
#### 6.2.1 Primary map



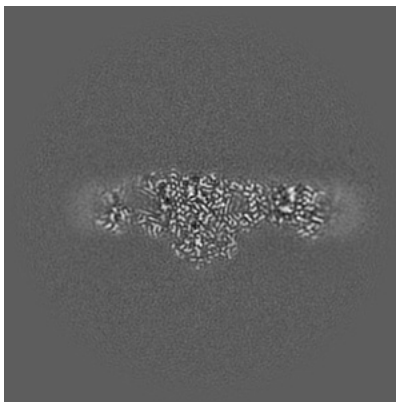
The images above show central slices of the map in three orthogonal directions.

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

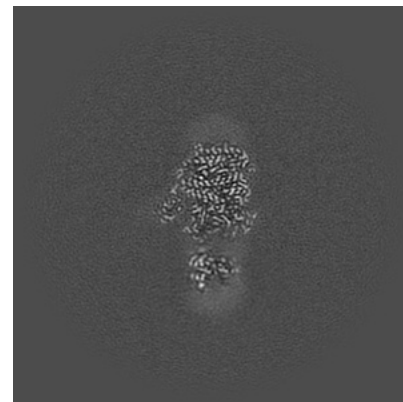
### 6.3.1 Primary map



X Index: 157



Y Index: 180

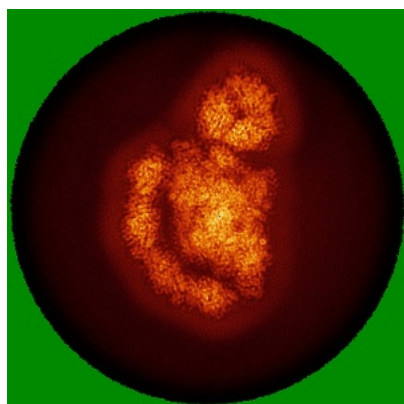


Z Index: 142

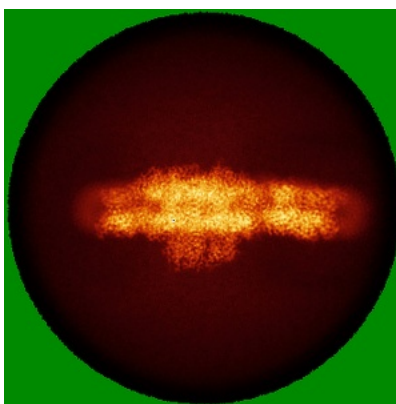
The images above show the largest variance slices of the map in three orthogonal directions.

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

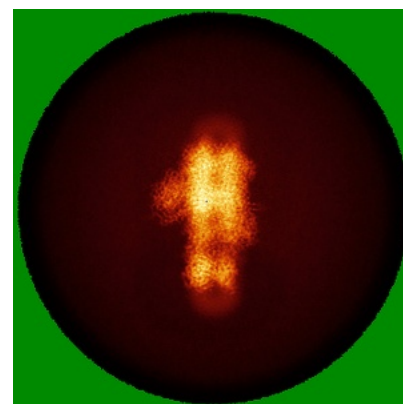
### 6.4.1 Primary map



X



Y

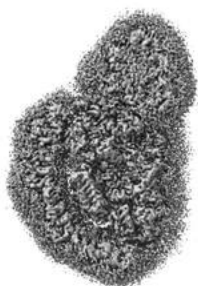


Z

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](#)

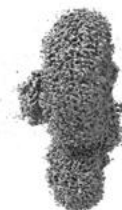
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.59. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

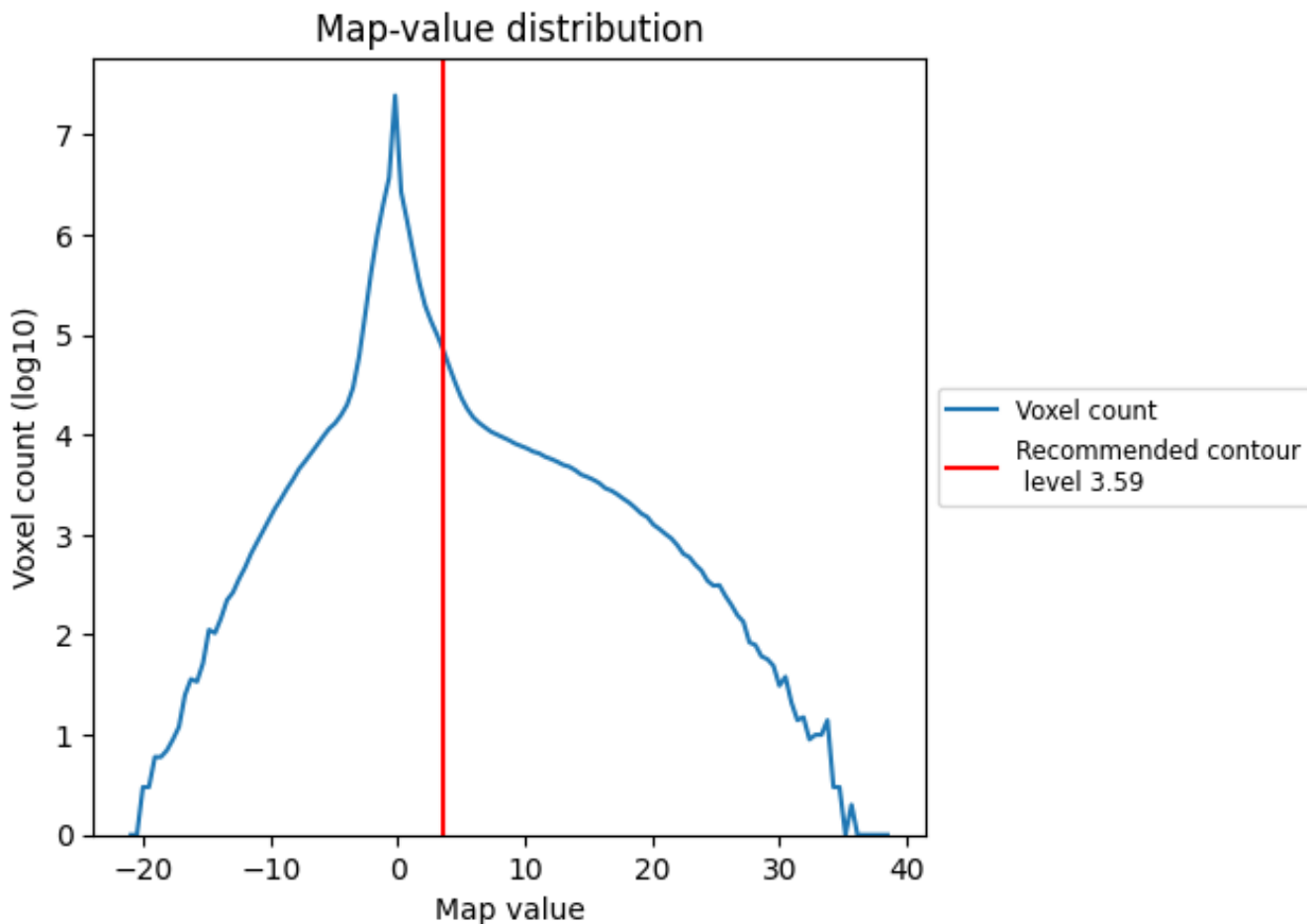
## 6.6 Mask visualisation [i](#)

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.

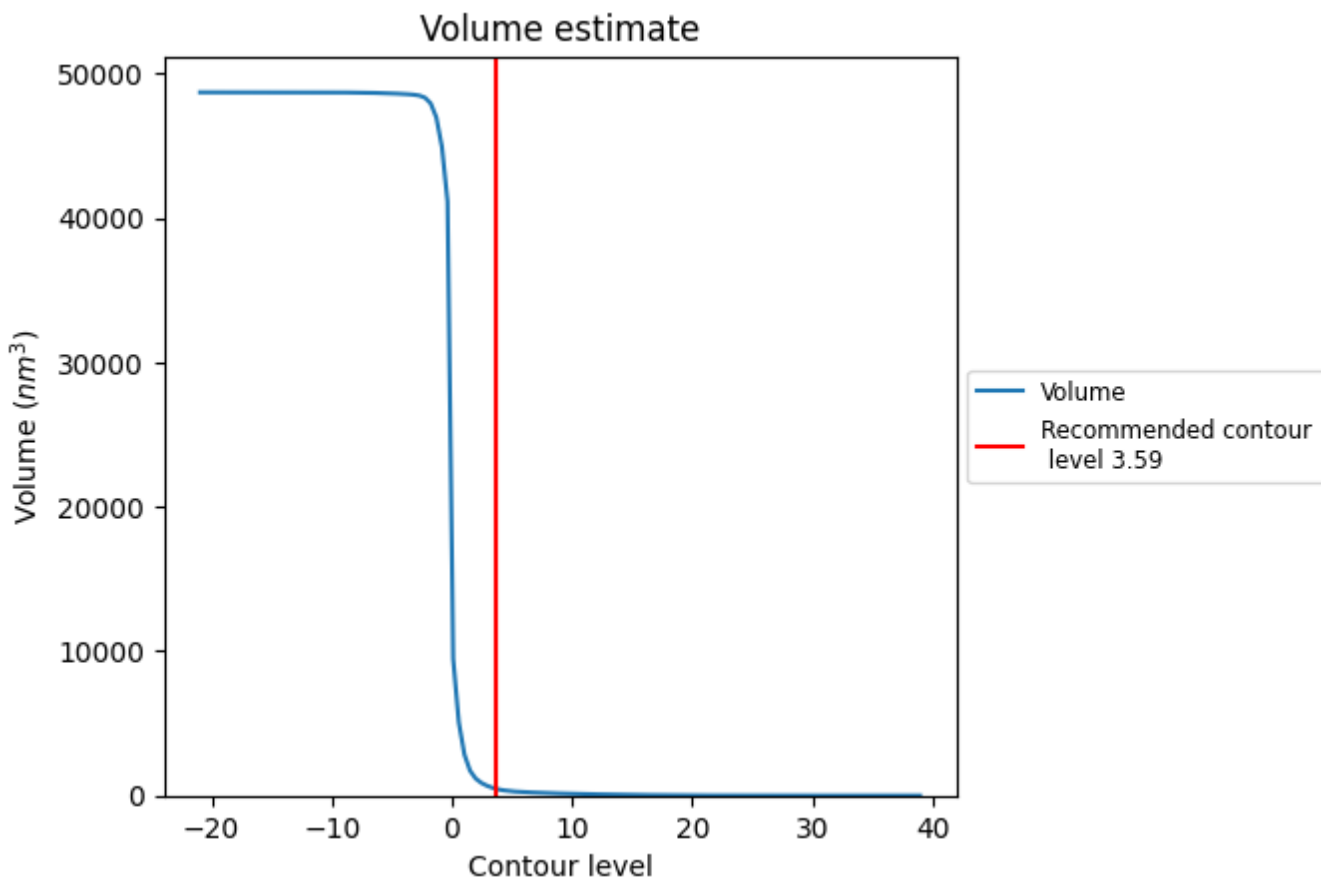
### 7.1 Map-value distribution [i](#)



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.



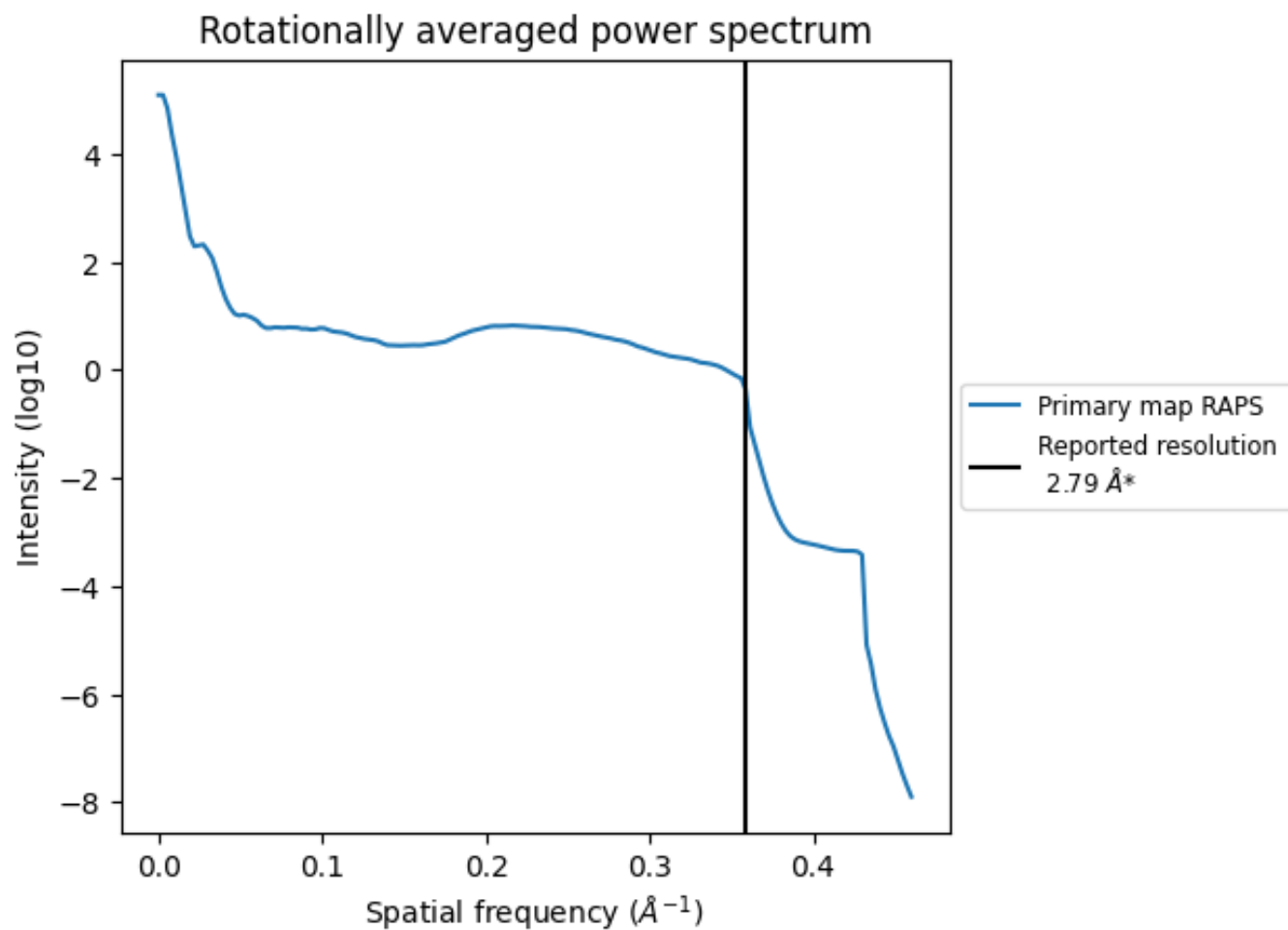
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm<sup>3</sup>; this corresponds to an approximate mass of 444 kDa.

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

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.358 Å<sup>-1</sup>

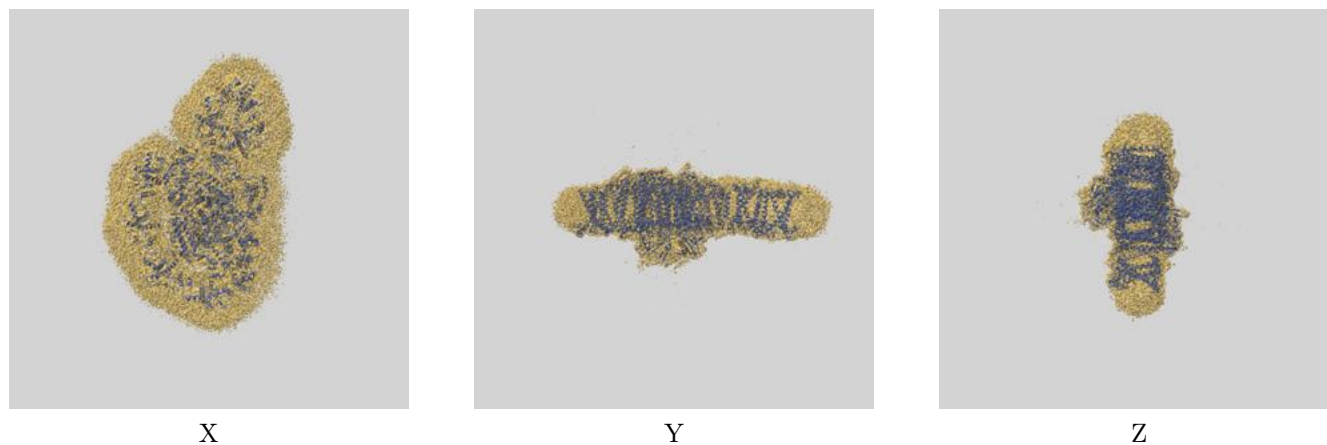
## 8 Fourier-Shell correlation

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

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

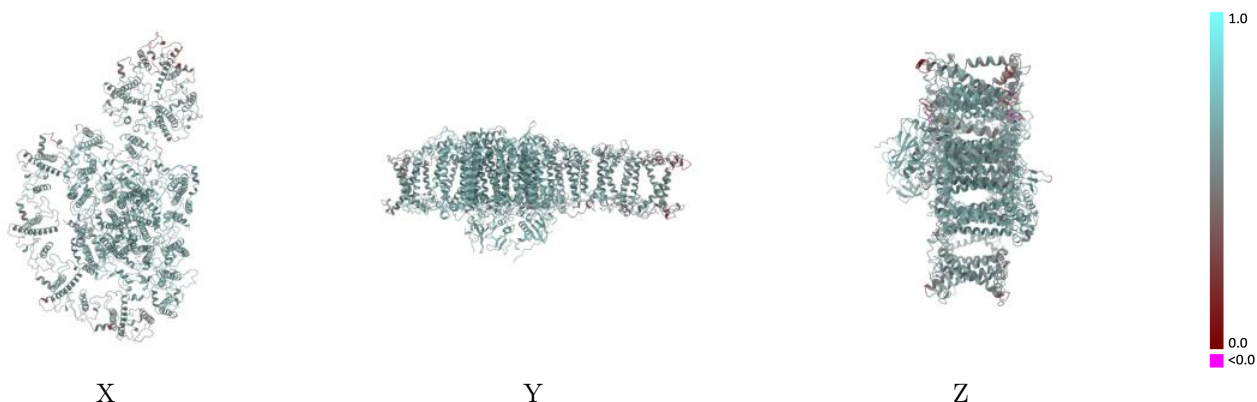
This section contains information regarding the fit between EMDB map EMD-36021 and PDB model 8J6Z. Per-residue inclusion information can be found in section 3 on page 31.

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



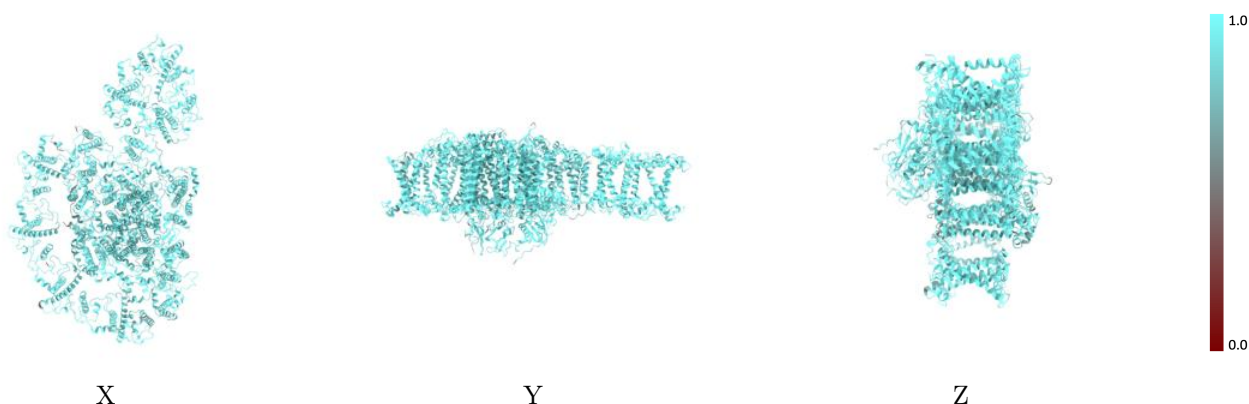
The images above show the 3D surface view of the map at the recommended contour level 3.59 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



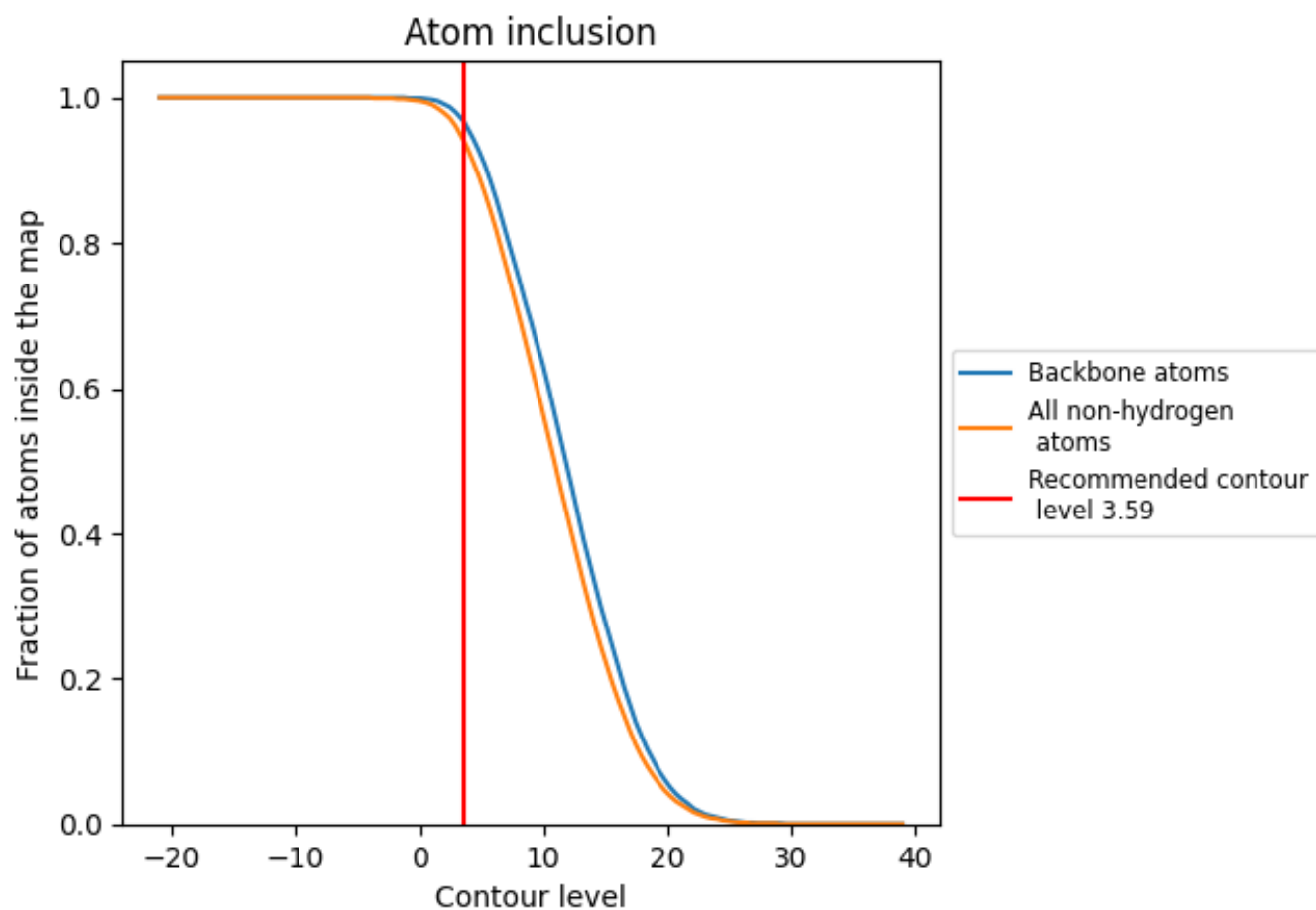
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.59).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (3.59) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.5870
1	 0.9140	 0.5120
2	 0.9470	 0.5510
3	 0.9300	 0.5400
4	 0.9350	 0.5600
A	 0.9480	 0.6270
B	 0.9600	 0.6330
C	 0.9790	 0.6360
D	 0.9550	 0.6250
E	 0.9480	 0.6200
F	 0.8810	 0.5920
G	 0.9060	 0.5880
H	 0.9160	 0.5880
I	 0.9680	 0.6200
J	 0.7920	 0.5530
K	 0.8900	 0.5620
L	 0.9590	 0.6250
O	 0.9570	 0.5820
x	 0.9460	 0.5470
y	 0.9200	 0.4890
z	 0.9480	 0.5580

