



Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 02:23 PM JST

PDB ID : 8J7B
EMDB ID : EMD-36037
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 2 (PSI-ST2)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-27
Resolution : 3.22 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

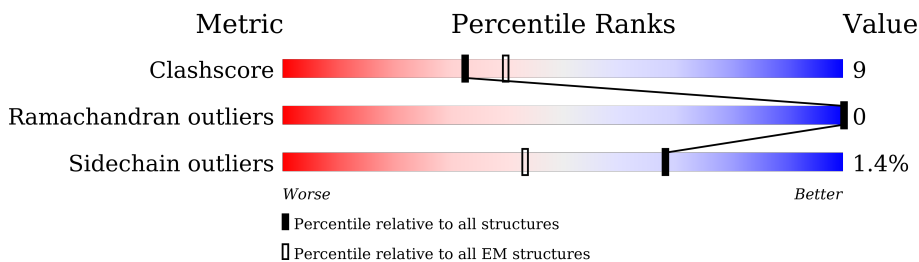
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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 ≥ 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	
2	2	257	
3	3	273	
4	4	251	
5	A	750	
6	B	734	
7	C	81	
8	D	204	

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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	

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
17	CHL	1	601	X	-	-	-
17	CHL	1	606	X	-	-	-
17	CHL	2	601	X	-	-	-
17	CHL	2	605	X	-	-	-
17	CHL	2	606	X	-	-	-
17	CHL	2	607	X	-	-	-
17	CHL	2	615	X	-	-	-
17	CHL	3	606	X	-	-	-
17	CHL	4	605	X	-	-	-
17	CHL	4	606	X	-	-	-
17	CHL	4	607	X	-	-	-
17	CHL	4	615	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	608	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	3	601	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	605	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	608	X	-	-	-
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	844	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	202	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	H	201	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
24	CL0	A	801	X	-	-	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 35077 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
			Total	C	N	O	S		
14	J	41	327	221	50	55	1	0	0

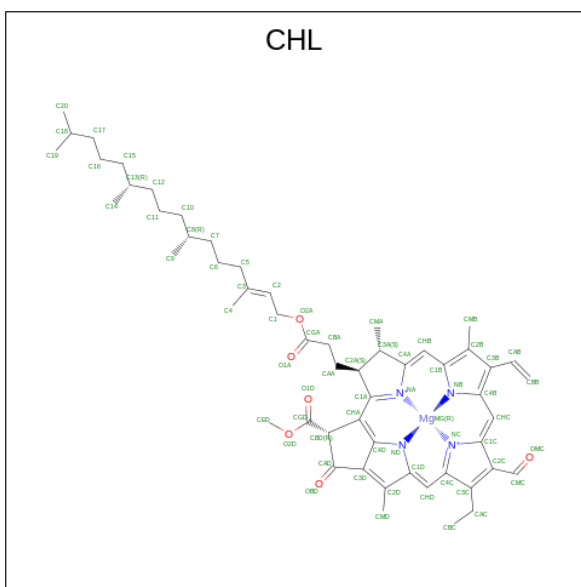
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

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

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

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

- Molecule 17 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



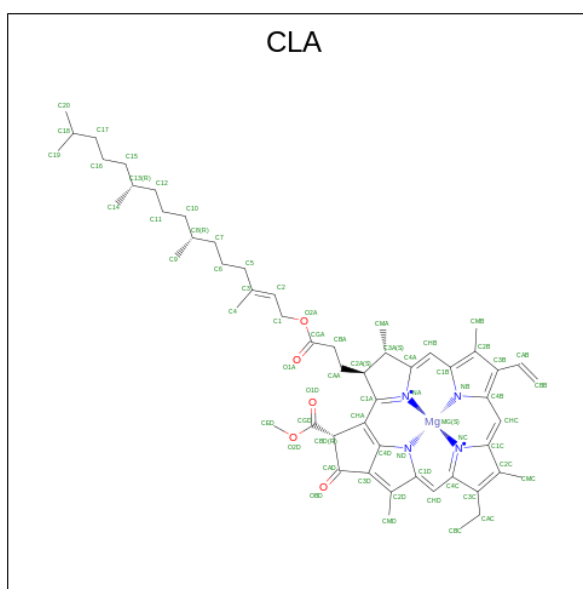
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	1	1	52	41	1	4	6	0
17	1	1	41	32	1	4	4	0
17	2	1	42	33	1	4	4	0
17	2	1	43	34	1	4	4	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 18 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
			Total	C	Mg	N	O	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	1	1	46	36	1	4	5	0
18	1	1	44	34	1	4	5	0
18	1	1	40	32	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	38	30	1	4	3	0
18	1	1	45	35	1	4	5	0
18	1	1	46	36	1	4	5	0
18	1	1	38	30	1	4	3	0
18	2	1	44	34	1	4	5	0
18	2	1	65	55	1	4	5	0
18	2	1	47	37	1	4	5	0
18	2	1	65	55	1	4	5	0
18	2	1	43	34	1	4	4	0
18	2	1	43	35	1	4	3	0
18	2	1	38	30	1	4	3	0
18	2	1	45	35	1	4	5	0
18	2	1	44	34	1	4	5	0
18	3	1	41	33	1	4	3	0
18	3	1	36	30	1	4	1	0
18	3	1	41	33	1	4	3	0
18	3	1	54	44	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	3	1	41	33	1	4	3	0
18	3	1	45	35	1	4	5	0
18	3	1	60	50	1	4	5	0
18	3	1	40	32	1	4	3	0
18	3	1	40	32	1	4	3	0
18	3	1	45	35	1	4	5	0
18	3	1	55	45	1	4	5	0
18	4	1	60	50	1	4	5	0
18	4	1	46	36	1	4	5	0
18	4	1	45	35	1	4	5	0
18	4	1	54	44	1	4	5	0
18	4	1	45	35	1	4	5	0
18	4	1	57	47	1	4	5	0
18	4	1	41	33	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	43	33	1	4	5	0
18	4	1	50	40	1	4	5	0
18	4	1	44	34	1	4	5	0
18	A	1	59	49	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	60	50	1	4	5	0
18	A	1	55	45	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	54	44	1	4	5	0
18	A	1	50	40	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	50	40	1	4	5	0
18	A	1	42	34	1	4	3	0
18	A	1	41	33	1	4	3	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	52	42	1	4	5	0
18	A	1	50	40	1	4	5	0
18	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	55	45	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	42	34	1	4	3	0
18	A	1	65	55	1	4	5	0
18	A	1	59	49	1	4	5	0
18	A	1	56	46	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	51	41	1	4	5	0
18	A	1	50	40	1	4	5	0
18	A	1	45	35	1	4	5	0
18	B	1	60	50	1	4	5	0

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

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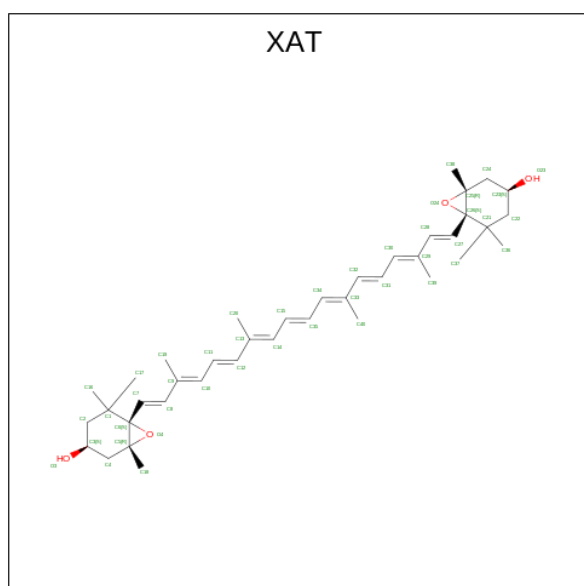
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	43	35	1	4	3	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	62	52	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	52	42	1	4	5	0
18	B	1	50	40	1	4	5	0
18	B	1	43	35	1	4	3	0
18	B	1	65	55	1	4	5	0
18	B	1	56	46	1	4	5	0
18	B	1	41	33	1	4	3	0
18	B	1	59	49	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	50	40	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	47	37	1	4	5	0
18	F	1	41	33	1	4	3	0
18	F	1	57	47	1	4	5	0
18	F	1	51	41	1	4	5	0

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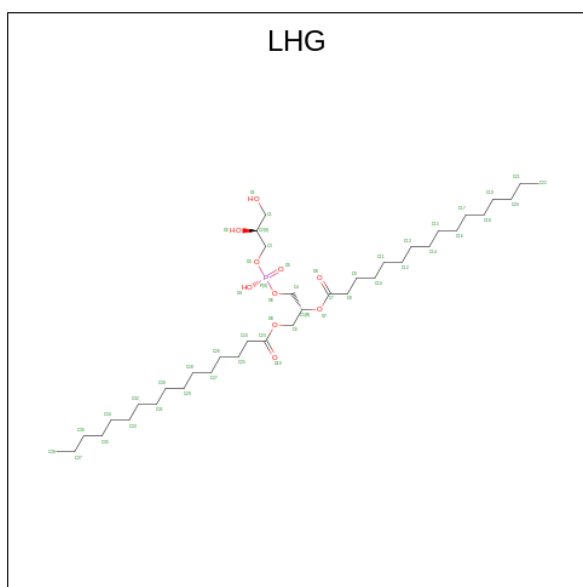
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	J	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	K	1	Total 39	C 31	Mg 1	N 4	O 3	0
18	K	1	Total 37	C 31	Mg 1	N 4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

- Molecule 19 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: C₄₀H₅₆O₄).



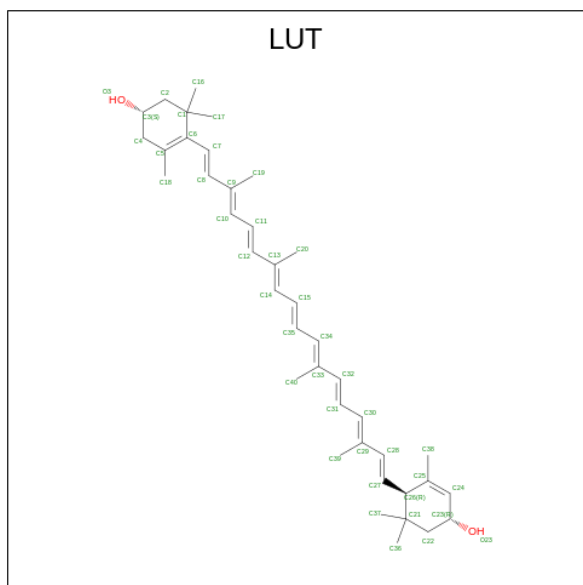
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	2	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



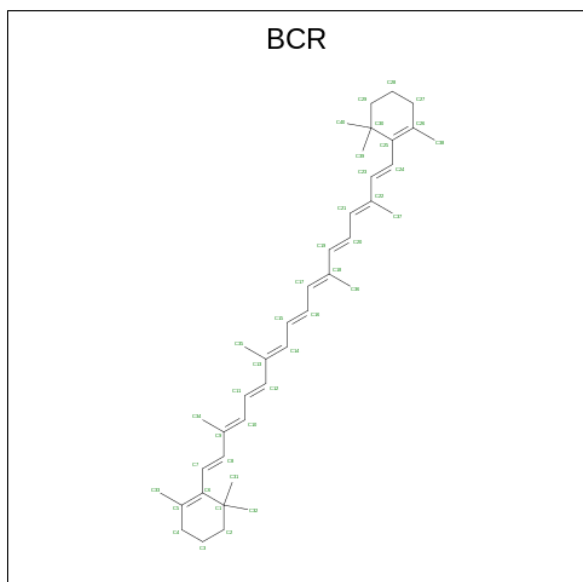
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			37	26	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			38	27	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 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
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



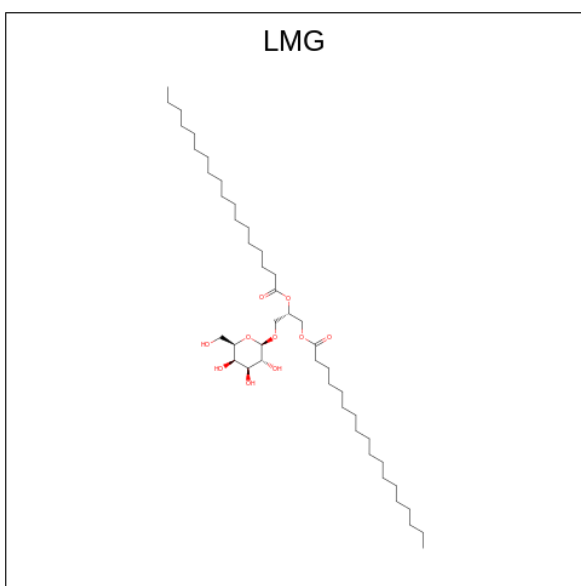
Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0

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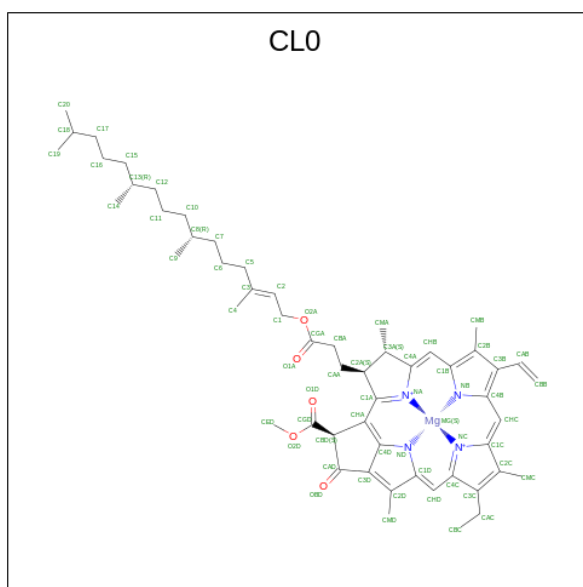
Mol	Chain	Residues	Atoms	AltConf
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



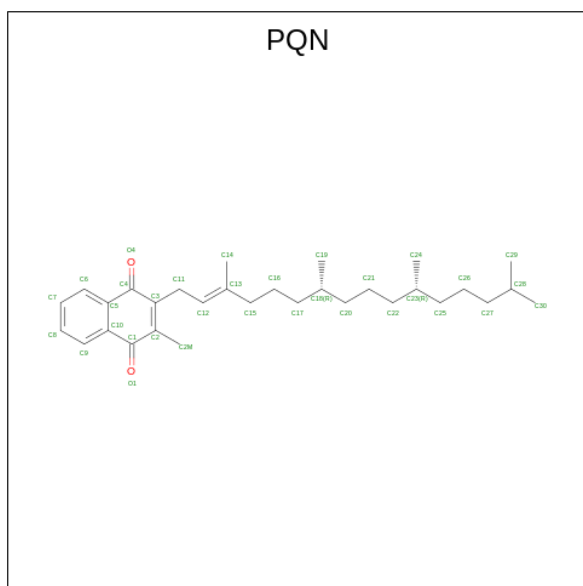
Mol	Chain	Residues	Atoms	AltConf
23	4	1	Total C O 39 29 10	0
23	4	1	Total C O 33 23 10	0

- Molecule 24 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	
			Total	C	Mg	N		O
24	A	1	60	52	1	4	3	0

- Molecule 25 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



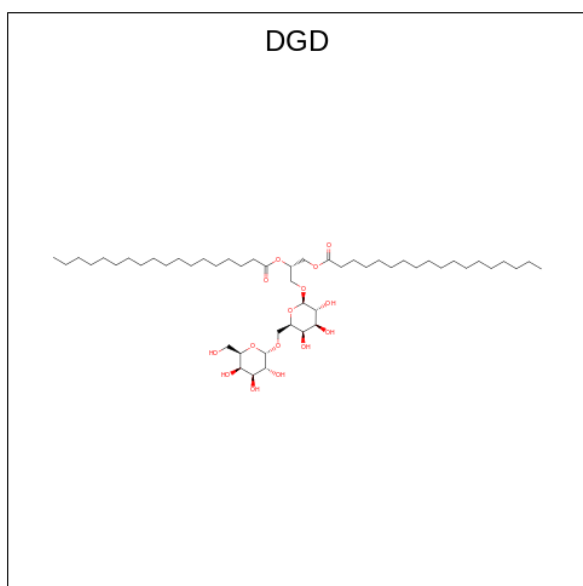
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	A	1	33	31	2	0
25	B	1	33	31	2	0

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

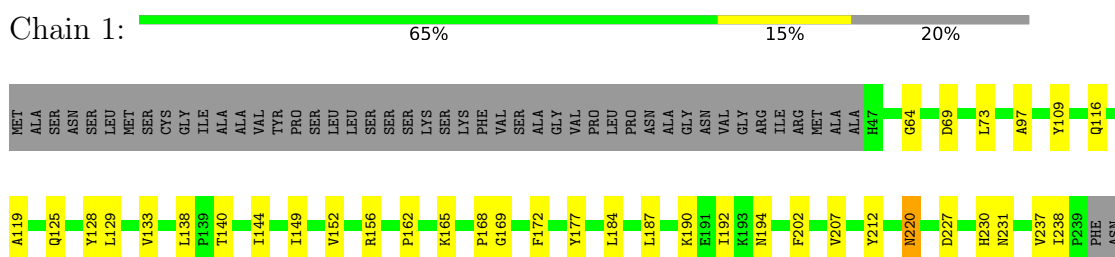


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	66	51	15	0

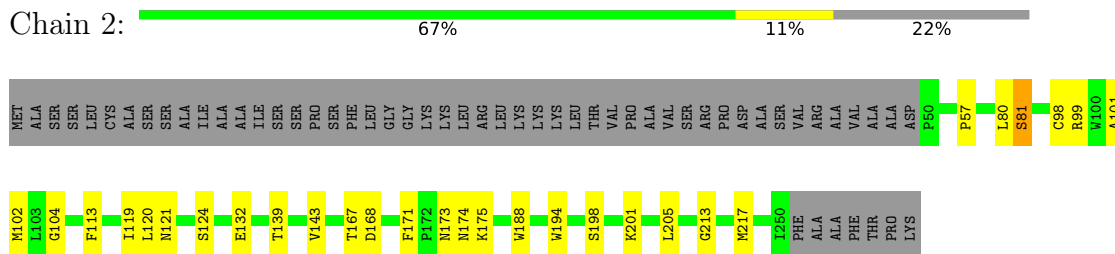
3 Residue-property plots [i](#)

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.

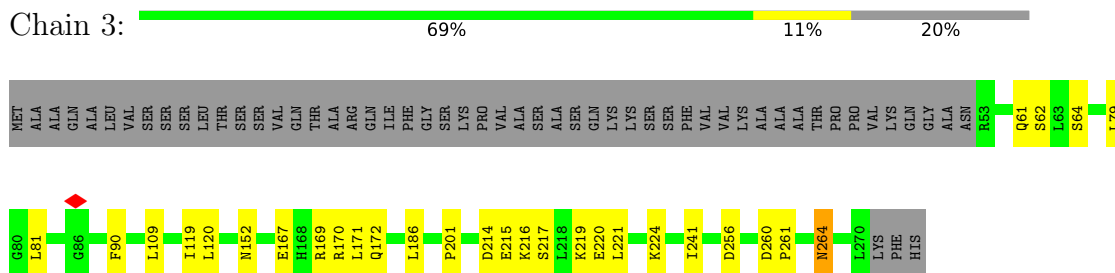
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



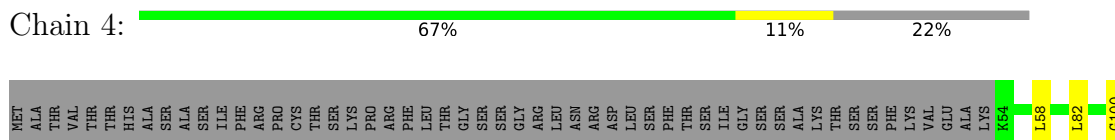
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

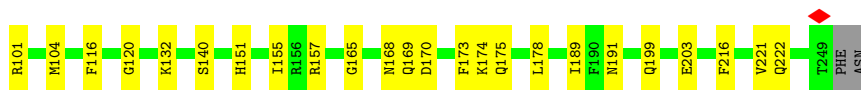


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

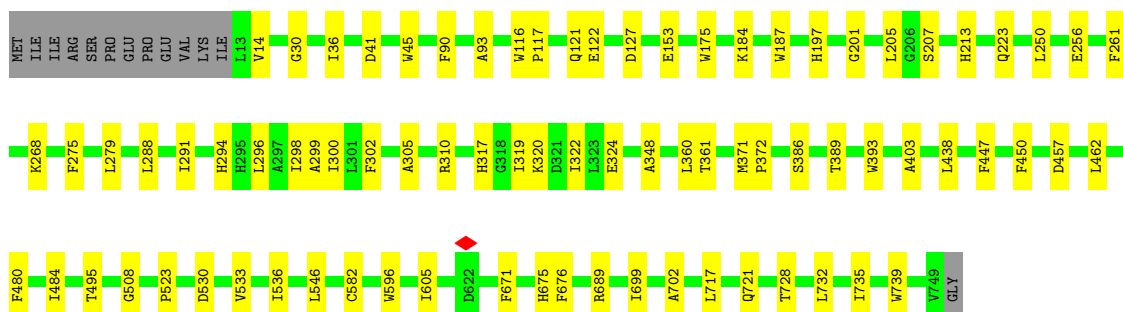
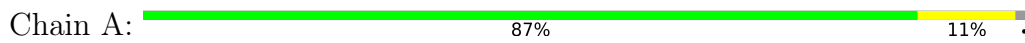


- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic

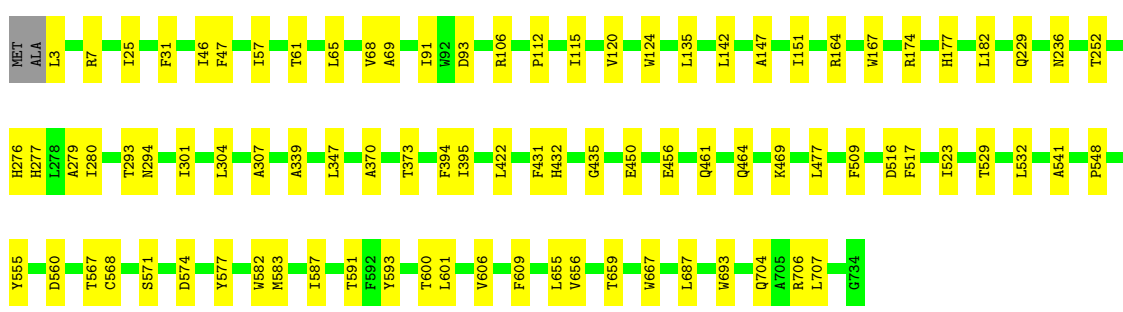
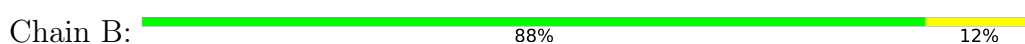




• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



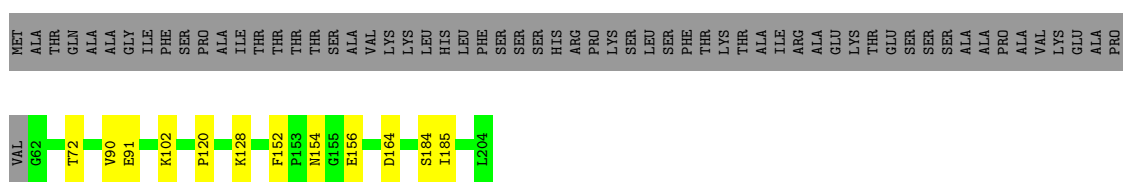
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



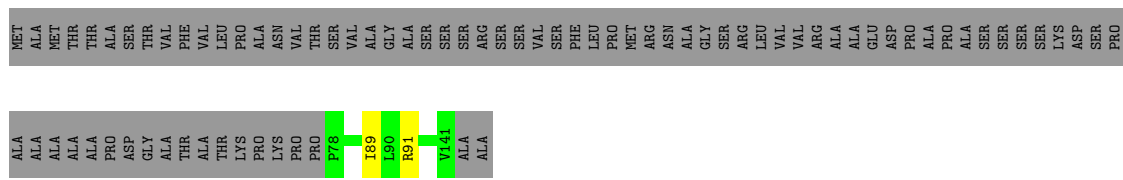
• Molecule 7: Photosystem I iron-sulfur center



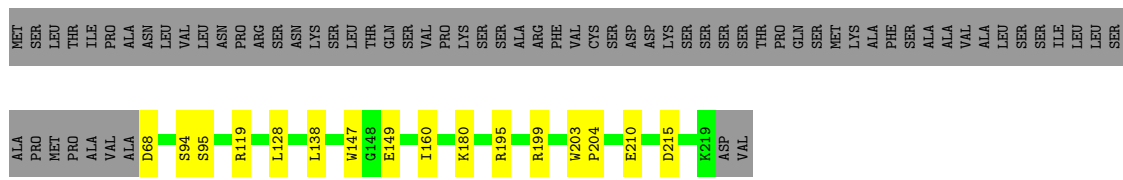
• Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic



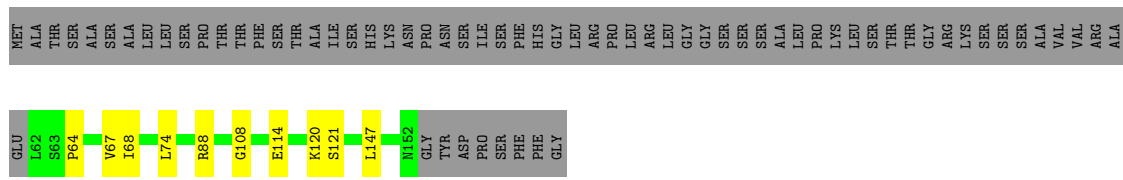
• Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic



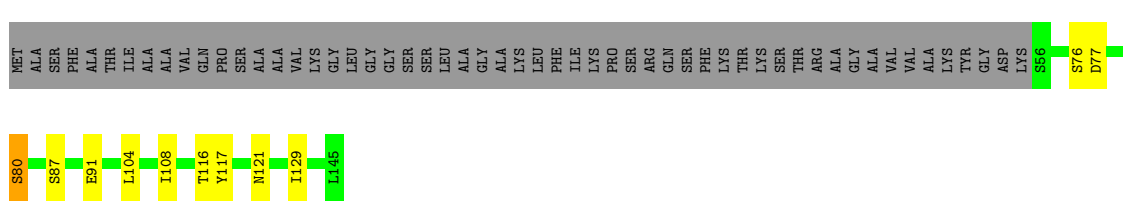
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic



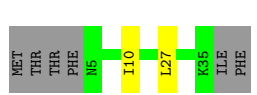
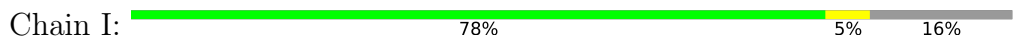
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic



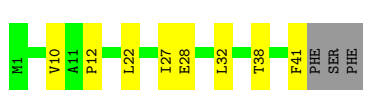
- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII

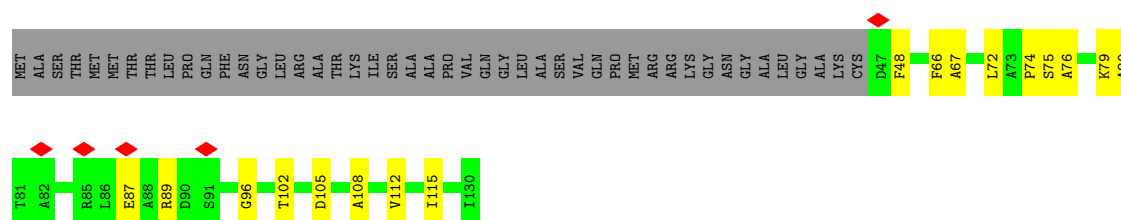


- Molecule 14: Photosystem I reaction center subunit IX



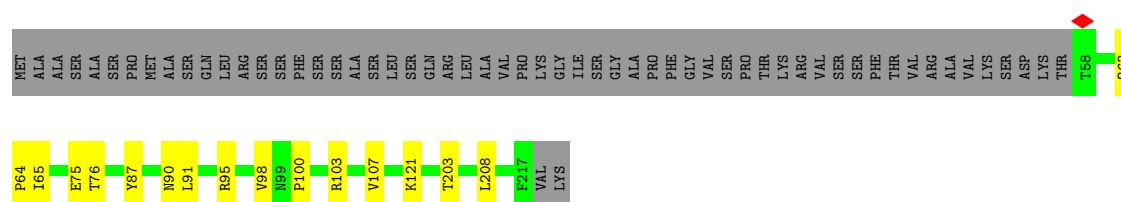
- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  52% 13% 35%



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

Chain L:  66% 7% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	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	35.714	Depositor
Minimum map value	-22.642	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	3.21	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.25	0/1546	0.46	0/2110
2	2	0.25	0/1622	0.45	0/2219
3	3	0.26	0/1717	0.47	0/2336
4	4	0.25	0/1599	0.42	0/2178
5	A	0.24	0/6005	0.42	0/8194
6	B	0.24	0/6065	0.43	0/8279
7	C	0.24	0/629	0.50	0/852
8	D	0.25	0/1157	0.50	0/1563
9	E	0.25	0/528	0.48	0/715
10	F	0.25	0/1238	0.45	0/1670
11	G	0.24	0/724	0.42	0/981
12	H	0.25	0/713	0.46	0/968
13	I	0.25	0/245	0.40	0/333
14	J	0.24	0/336	0.46	0/458
15	K	0.27	0/599	0.63	2/809 (0.2%)
16	L	0.26	0/1244	0.43	0/1700
All	All	0.25	0/25967	0.45	2/35365 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	74	PRO	CA-N-CD	-7.33	101.24	111.50
15	K	74	PRO	N-CD-CG	-5.20	95.41	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1496	0	1471	34	0
2	2	1566	0	1519	21	0
3	3	1666	0	1627	23	0
4	4	1551	0	1508	22	0
5	A	5807	0	5659	61	0
6	B	5854	0	5646	67	0
7	C	616	0	600	4	0
8	D	1128	0	1134	8	0
9	E	517	0	526	1	0
10	F	1208	0	1243	10	0
11	G	708	0	700	6	0
12	H	693	0	690	6	0
13	I	239	0	258	2	0
14	J	327	0	342	7	0
15	K	593	0	614	12	0
16	L	1207	0	1209	14	0
17	1	93	0	62	10	0
17	2	226	0	150	13	0
17	3	45	0	30	2	0
17	4	169	0	100	3	0
18	1	496	0	354	30	0
18	2	434	0	352	29	0
18	3	498	0	377	16	0
18	4	527	0	412	21	0
18	A	2533	0	2495	115	0
18	B	2284	0	2242	106	0
18	F	149	0	123	8	0
18	G	132	0	97	1	0
18	H	60	0	59	3	0
18	J	51	0	41	2	0
18	K	167	0	116	2	0
18	L	155	0	138	8	0
19	1	44	0	56	18	0
19	2	44	0	56	9	0
19	4	44	0	56	5	0
20	1	49	0	74	13	0
20	2	37	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	79	0	104	6	0
20	B	87	0	120	5	0
21	1	42	0	56	3	0
21	2	84	0	112	11	0
21	3	42	0	56	5	0
21	4	42	0	56	4	0
22	3	40	0	56	4	0
22	4	40	0	56	4	0
22	A	240	0	336	27	0
22	B	320	0	448	43	0
22	F	40	0	56	3	0
22	G	40	0	56	2	0
22	I	40	0	56	0	0
22	J	40	0	56	6	0
22	K	80	0	112	7	0
22	L	120	0	168	16	0
23	4	72	0	84	1	0
24	A	60	0	68	4	0
25	A	33	0	46	4	0
25	B	33	0	46	3	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	5	0
All	All	35077	0	34424	647	0

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

All (647) 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)
18:B:814:CLA:H3A	22:B:845:BCR:H393	1.51	0.91
1:1:172:PHE:HB2	18:1:609:CLA:HMD2	1.60	0.84
17:1:601:CHL:HBB1	20:1:615:LHG:H252	1.57	0.84
21:2:619:LUT:H8	21:2:619:LUT:H181	1.60	0.82
22:B:801:BCR:H12C	22:B:801:BCR:H341	1.63	0.81
3:3:79:LEU:HD13	18:A:813:CLA:H2	1.63	0.81
2:2:143:VAL:HG22	18:4:613:CLA:HBA2	1.61	0.80
22:A:853:BCR:H12C	22:A:853:BCR:H341	1.68	0.76
1:1:202:PHE:CE1	19:1:614:XAT:H10	2.20	0.76
22:B:845:BCR:H16C	22:B:845:BCR:H20C	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:306:BCR:H321	22:L:306:BCR:HC8	1.68	0.75
18:3:612:CLA:HAB	18:3:607:CLA:HBA1	1.66	0.75
18:1:602:CLA:H51	19:1:614:XAT:H373	1.69	0.75
3:3:170:ARG:NH2	18:3:607:CLA:O1D	2.21	0.74
22:A:850:BCR:H16C	22:A:850:BCR:H351	1.69	0.74
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.69	0.72
17:1:601:CHL:HBB1	17:1:601:CHL:HHC	1.72	0.72
18:B:812:CLA:HHC	18:B:812:CLA:HBB1	1.68	0.72
21:3:613:LUT:H401	21:3:613:LUT:H15	1.72	0.72
8:D:154:ASN:ND2	8:D:156:GLU:OE2	2.19	0.71
18:1:602:CLA:CBB	19:1:614:XAT:H32	2.21	0.71
17:4:605:CHL:HHC	17:4:605:CHL:HBB1	1.73	0.71
5:A:386:SER:HB3	18:A:829:CLA:HMA1	1.73	0.71
6:B:304:LEU:HA	18:B:822:CLA:HED1	1.72	0.70
21:4:616:LUT:H8	21:4:616:LUT:H171	1.73	0.70
5:A:175:TRP:HB2	18:A:812:CLA:HMC3	1.73	0.70
18:1:602:CLA:HBB2	19:1:614:XAT:H32	1.73	0.69
17:1:601:CHL:HHC	20:1:615:LHG:H252	1.75	0.69
18:A:809:CLA:HMC3	18:A:810:CLA:HMD2	1.75	0.69
22:3:614:BCR:H403	22:3:614:BCR:H23C	1.74	0.69
3:3:256:ASP:O	3:3:264:ASN:ND2	2.26	0.69
18:A:805:CLA:H43	18:A:812:CLA:HBB1	1.73	0.68
3:3:215:GLU:N	3:3:215:GLU:OE2	2.23	0.68
1:1:97:ALA:HA	19:1:614:XAT:H181	1.76	0.68
3:3:81:LEU:HD13	18:3:601:CLA:H42	1.76	0.68
18:A:804:CLA:H191	18:A:844:CLA:H203	1.75	0.68
2:2:98:CYS:O	2:2:102:MET:HG3	1.93	0.67
22:A:853:BCR:HC8	22:A:853:BCR:H311	1.75	0.67
16:L:107:VAL:HA	18:L:303:CLA:HED1	1.74	0.67
12:H:87:SER:O	12:H:91:GLU:HG3	1.95	0.67
18:A:829:CLA:H202	22:J:102:BCR:H19C	1.76	0.66
22:L:301:BCR:H21C	22:L:301:BCR:H361	1.77	0.66
1:1:187:LEU:HD13	18:1:609:CLA:HAA2	1.78	0.66
6:B:65:LEU:HD11	22:B:845:BCR:H282	1.75	0.66
18:B:805:CLA:H52	18:B:813:CLA:H61	1.78	0.66
18:A:804:CLA:HBD	18:A:804:CLA:HBA2	1.78	0.65
2:2:217:MET:HE3	18:2:602:CLA:HMC3	1.79	0.65
5:A:393:TRP:CD1	18:A:829:CLA:HAB	2.31	0.65
18:2:609:CLA:HMD2	17:2:607:CHL:HBA2	1.78	0.65
18:2:613:CLA:H2A	18:2:613:CLA:HED2	1.78	0.65
6:B:164:ARG:NH2	11:G:108:GLY:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:517:PHE:HA	18:B:837:CLA:HED1	1.79	0.65
18:3:602:CLA:H92	18:A:811:CLA:HMD2	1.79	0.65
18:B:828:CLA:H171	22:B:845:BCR:H362	1.79	0.65
22:J:102:BCR:HC8	22:J:102:BCR:H311	1.79	0.65
5:A:320:LYS:NZ	5:A:324:GLU:OE2	2.31	0.64
18:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.79	0.64
25:A:855:PQN:H172	22:B:801:BCR:H382	1.78	0.64
18:A:802:CLA:H202	18:A:842:CLA:H2	1.80	0.64
16:L:65:ILE:HA	16:L:75:GLU:HG3	1.81	0.64
22:B:848:BCR:H403	22:B:848:BCR:H23C	1.80	0.63
22:B:847:BCR:HC8	22:B:847:BCR:H311	1.80	0.63
18:A:822:CLA:HMB2	18:A:826:CLA:HMA3	1.81	0.63
22:A:851:BCR:H16C	22:A:851:BCR:H351	1.80	0.63
22:K:205:BCR:H403	22:K:205:BCR:H23C	1.80	0.63
1:1:116:GLN:HG2	18:1:605:CLA:HBB2	1.80	0.63
22:B:801:BCR:HC8	22:B:801:BCR:H331	1.80	0.63
18:A:842:CLA:HBC2	25:A:855:PQN:H192	1.81	0.62
4:4:165:GLY:HA2	4:4:168:ASN:HD22	1.63	0.62
22:A:849:BCR:H383	22:A:849:BCR:H23C	1.80	0.62
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.31	0.62
6:B:307:ALA:HB3	18:B:822:CLA:HED3	1.80	0.62
18:B:841:CLA:HED1	18:B:822:CLA:HAB	1.80	0.62
2:2:119:ILE:HG22	2:2:120:LEU:HD12	1.81	0.61
18:3:607:CLA:HHC	18:3:607:CLA:HBB1	1.82	0.61
6:B:57:ILE:HA	18:B:806:CLA:HBC3	1.83	0.61
22:B:846:BCR:H343	18:B:822:CLA:HBB2	1.83	0.61
15:K:75:SER:OG	15:K:76:ALA:N	2.33	0.61
15:K:75:SER:O	15:K:89:ARG:NH2	2.34	0.61
1:1:73:LEU:HD12	19:1:614:XAT:H221	1.81	0.60
5:A:302:PHE:HE1	18:A:822:CLA:HAB	1.66	0.60
16:L:100:PRO:HA	16:L:103:ARG:HD3	1.83	0.60
22:A:851:BCR:H23C	22:A:851:BCR:H403	1.82	0.60
22:L:305:BCR:H321	22:L:305:BCR:HC8	1.82	0.60
22:G:204:BCR:HC8	22:G:204:BCR:H311	1.82	0.60
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.81	0.60
24:A:801:CL0:H15	24:A:801:CL0:H2	1.84	0.60
21:1:616:LUT:H391	21:1:616:LUT:H32	1.81	0.60
18:2:602:CLA:HMC2	19:2:617:XAT:H31	1.83	0.60
6:B:469:LYS:NZ	6:B:509:PHE:O	2.33	0.60
22:B:846:BCR:HC8	22:B:846:BCR:H311	1.84	0.60
4:4:100:GLY:O	4:4:104:MET:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:216:PHE:CD2	19:4:617:XAT:H14	2.37	0.60
18:1:609:CLA:HHC	18:1:609:CLA:HBB1	1.84	0.59
20:1:615:LHG:H151	18:4:614:CLA:HED3	1.83	0.59
22:K:205:BCR:H321	22:K:205:BCR:HC8	1.82	0.59
6:B:293:THR:HG22	6:B:294:ASN:H	1.67	0.59
5:A:732:LEU:HA	20:A:846:LHG:H383	1.83	0.59
18:A:821:CLA:HHC	18:A:821:CLA:HBB1	1.85	0.59
6:B:432:HIS:HB2	22:B:849:BCR:H402	1.84	0.59
1:1:169:GLY:H	18:1:609:CLA:HMD1	1.68	0.59
12:H:117:TYR:O	12:H:121:ASN:ND2	2.30	0.59
18:4:613:CLA:HBD	18:4:613:CLA:HBA1	1.85	0.59
22:A:852:BCR:H403	22:A:852:BCR:H23C	1.85	0.59
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.68	0.59
17:1:601:CHL:O1A	4:4:151:HIS:ND1	2.35	0.58
18:A:822:CLA:H2	18:A:826:CLA:HBB1	1.85	0.58
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.85	0.58
21:2:619:LUT:H172	18:4:610:CLA:HHC	1.84	0.58
6:B:600:THR:HG21	6:B:609:PHE:HB2	1.85	0.58
22:4:618:BCR:HC8	22:4:618:BCR:H321	1.85	0.58
18:A:831:CLA:H172	20:A:846:LHG:H182	1.85	0.58
1:1:125:GLN:NE2	1:1:133:VAL:O	2.31	0.58
5:A:348:ALA:HB1	22:A:850:BCR:H393	1.86	0.58
17:1:601:CHL:HAA1	20:1:615:LHG:H141	1.85	0.58
2:2:205:LEU:HB3	18:2:609:CLA:HMA1	1.85	0.58
5:A:288:LEU:HD23	5:A:291:ILE:HD12	1.86	0.58
6:B:147:ALA:O	6:B:151:ILE:HG13	2.04	0.58
18:4:602:CLA:HMB1	18:4:602:CLA:HBB1	1.85	0.57
4:4:178:LEU:HD21	4:4:189:ILE:HG22	1.86	0.57
18:A:820:CLA:H91	18:A:820:CLA:H151	1.86	0.57
5:A:36:ILE:O	5:A:45:TRP:NE1	2.29	0.57
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.86	0.57
18:A:809:CLA:HAB	18:A:829:CLA:H122	1.86	0.57
18:A:834:CLA:HMC2	18:L:304:CLA:HBB2	1.86	0.57
18:A:809:CLA:H201	20:A:846:LHG:H211	1.86	0.57
1:1:187:LEU:HB3	18:1:609:CLA:HMA2	1.86	0.57
2:2:104:GLY:HA2	19:2:617:XAT:H181	1.87	0.57
4:4:169:GLN:NE2	4:4:174:LYS:O	2.38	0.57
22:A:850:BCR:H311	22:A:850:BCR:HC8	1.86	0.57
3:3:186:LEU:HD11	22:3:614:BCR:H343	1.87	0.56
6:B:571:SER:OG	6:B:574:ASP:OD2	2.21	0.56
5:A:117:PRO:HB3	5:A:122:GLU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.21	0.56
22:B:843:BCR:H16C	22:B:843:BCR:H351	1.87	0.56
5:A:739:TRP:HH2	18:A:809:CLA:HBC2	1.70	0.56
5:A:495:THR:OG1	18:A:836:CLA:OBD	2.21	0.56
4:4:82:LEU:HD13	18:4:602:CLA:H42	1.86	0.56
3:3:217:SER:O	3:3:221:LEU:HD12	2.06	0.56
1:1:149:ILE:HD13	18:1:608:CLA:HMC3	1.87	0.56
5:A:294:HIS:HB2	18:A:819:CLA:C1B	2.36	0.56
6:B:707:LEU:HD11	27:B:850:DGD:HB81	1.87	0.55
6:B:395:ILE:HG13	6:B:541:ALA:HB1	1.89	0.55
18:A:825:CLA:H41	22:A:851:BCR:H15C	1.87	0.55
6:B:523:ILE:HG21	18:B:836:CLA:HAB	1.89	0.55
16:L:90:ASN:O	16:L:95:ARG:NH1	2.38	0.55
4:4:104:MET:HE1	18:4:609:CLA:HHC	1.89	0.55
5:A:735:ILE:HD12	20:A:846:LHG:H382	1.87	0.55
18:H:201:CLA:HAA2	22:L:306:BCR:H342	1.89	0.55
5:A:279:LEU:HD21	5:A:372:PRO:HD2	1.89	0.55
18:A:808:CLA:H2	18:A:810:CLA:H42	1.87	0.55
17:2:615:CHL:HHC	17:2:615:CHL:HBB1	1.88	0.55
18:A:805:CLA:HMA2	18:A:812:CLA:HMD2	1.89	0.55
25:B:842:PQN:H272	18:B:840:CLA:H42	1.89	0.55
18:H:201:CLA:HMA1	18:L:302:CLA:HAA1	1.89	0.55
18:B:824:CLA:H141	18:B:824:CLA:H193	1.87	0.55
20:1:615:LHG:H171	20:1:615:LHG:H342	1.89	0.55
18:B:818:CLA:HBB1	18:B:818:CLA:HMB1	1.89	0.55
5:A:296:LEU:O	5:A:300:ILE:HG12	2.07	0.55
5:A:728:THR:HG23	20:A:846:LHG:H341	1.88	0.55
8:D:72:THR:HG23	8:D:120:PRO:HB2	1.88	0.55
6:B:704:GLN:HG3	27:B:850:DGD:HA22	1.89	0.54
25:B:842:PQN:H172	18:B:840:CLA:HMD2	1.87	0.54
6:B:373:THR:HG23	6:B:591:THR:HG21	1.90	0.54
13:I:27:LEU:HD22	22:L:305:BCR:H323	1.89	0.54
18:1:602:CLA:H2	19:1:614:XAT:H221	1.89	0.54
5:A:360:LEU:HD11	18:A:820:CLA:H8	1.90	0.54
22:A:853:BCR:H23C	22:A:853:BCR:H393	1.89	0.54
6:B:276:HIS:HB2	18:B:817:CLA:C1B	2.38	0.54
6:B:370:ALA:HB1	18:B:827:CLA:HMA1	1.90	0.54
6:B:477:LEU:HD13	18:B:834:CLA:HMD3	1.88	0.54
22:F:304:BCR:H14C	22:F:304:BCR:H10C	1.90	0.54
18:A:842:CLA:HBD	18:A:842:CLA:HBA1	1.90	0.53
21:3:613:LUT:H161	21:3:613:LUT:H8	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:808:CLA:O1A	18:B:827:CLA:HBD	2.09	0.53
16:L:63:GLN:HG2	16:L:64:PRO:HD2	1.90	0.53
4:4:116:PHE:O	4:4:120:GLY:N	2.30	0.53
22:4:618:BCR:H383	22:4:618:BCR:H23C	1.91	0.53
18:B:805:CLA:H101	18:B:824:CLA:HBA1	1.89	0.53
1:1:237:VAL:HG13	1:1:238:ILE:HG23	1.90	0.53
18:A:830:CLA:CHA	18:A:830:CLA:HBA1	2.38	0.53
20:B:851:LHG:H261	20:B:851:LHG:H302	1.90	0.53
20:B:852:LHG:H121	18:B:822:CLA:H52	1.90	0.53
6:B:659:THR:HA	18:B:803:CLA:HAB	1.89	0.53
18:B:819:CLA:HMB2	18:B:824:CLA:HMA3	1.90	0.53
6:B:707:LEU:HD23	27:B:850:DGD:HA21	1.91	0.53
5:A:689:ARG:H	6:B:568:CYS:HB2	1.74	0.53
4:4:191:ASN:OD1	21:4:616:LUT:O23	2.27	0.53
18:A:828:CLA:HBB1	18:A:828:CLA:HMB1	1.91	0.53
1:1:64:GLY:HA3	1:1:192:ILE:HG21	1.90	0.52
6:B:25:ILE:HG21	27:B:850:DGD:HA72	1.91	0.52
18:B:828:CLA:H122	22:B:845:BCR:H372	1.91	0.52
22:B:849:BCR:H10C	14:J:38:THR:O	2.09	0.52
1:1:69:ASP:HA	19:1:614:XAT:O23	2.10	0.52
18:A:841:CLA:H143	18:F:302:CLA:HBC1	1.92	0.52
3:3:61:GLN:O	3:3:64:SER:OG	2.26	0.52
18:A:812:CLA:H141	18:A:812:CLA:H203	1.91	0.52
17:2:605:CHL:HHB	21:2:619:LUT:H392	1.91	0.52
18:1:602:CLA:H43	18:1:602:CLA:HMB2	1.91	0.52
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.92	0.52
5:A:536:ILE:HG23	24:A:801:CL0:H70	1.92	0.52
4:4:170:ASP:OD1	4:4:173:PHE:N	2.42	0.52
5:A:403:ALA:HB2	22:A:851:BCR:H323	1.92	0.52
18:B:840:CLA:H122	22:L:305:BCR:H351	1.92	0.52
5:A:14:VAL:HG11	18:A:811:CLA:HED3	1.91	0.52
18:A:803:CLA:H2	6:B:655:LEU:HD22	1.92	0.52
25:B:842:PQN:H272	18:B:840:CLA:H11	1.91	0.52
16:L:90:ASN:HB3	18:L:302:CLA:HAC1	1.92	0.52
22:B:843:BCR:H311	22:B:843:BCR:HC8	1.92	0.51
5:A:699:ILE:HA	18:A:841:CLA:HED1	1.92	0.51
18:A:841:CLA:H72	18:B:832:CLA:H42	1.92	0.51
15:K:102:THR:OG1	15:K:105:ASP:OD2	2.23	0.51
2:2:80:LEU:HD13	18:2:602:CLA:H71	1.92	0.51
3:3:214:ASP:OD1	3:3:216:LYS:N	2.44	0.51
5:A:256:GLU:OE2	5:A:268:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:806:CLA:H51	18:A:814:CLA:H12	1.93	0.51
7:C:47:ASP:OD2	8:D:128:LYS:NZ	2.41	0.51
6:B:236:ASN:HB3	6:B:252:THR:HG22	1.93	0.51
22:B:844:BCR:H382	22:B:844:BCR:H23C	1.93	0.51
2:2:167:THR:HG22	2:2:175:LYS:HD3	1.93	0.51
1:1:156:ARG:NH2	18:1:608:CLA:O1D	2.38	0.51
17:2:605:CHL:C2C	18:2:604:CLA:HBB2	2.41	0.51
18:B:832:CLA:HHC	18:B:832:CLA:HBB1	1.93	0.51
19:1:614:XAT:H242	19:1:614:XAT:H362	1.93	0.51
14:J:28:GLU:HG3	18:J:101:CLA:CHA	2.40	0.50
18:A:809:CLA:H202	18:A:809:CLA:H91	1.93	0.50
11:G:68:ILE:HG21	11:G:147:LEU:HG	1.93	0.50
15:K:108:ALA:O	15:K:112:VAL:HG23	2.10	0.50
5:A:371:MET:HE2	18:A:819:CLA:HAA2	1.93	0.50
12:H:80:SER:HB2	16:L:98:VAL:HG13	1.93	0.50
18:B:838:CLA:HHC	18:B:838:CLA:HBB1	1.93	0.50
18:A:820:CLA:HMB1	18:A:820:CLA:HBB1	1.93	0.50
18:1:602:CLA:ND	19:1:614:XAT:H382	2.27	0.50
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.92	0.50
17:2:601:CHL:HHC	17:2:601:CHL:HBB1	1.94	0.49
18:A:811:CLA:H2A	18:A:811:CLA:HED2	1.93	0.49
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.44	0.49
6:B:120:VAL:HG21	18:B:808:CLA:HED1	1.94	0.49
18:4:614:CLA:CED	18:4:614:CLA:H2A	2.42	0.49
6:B:422:LEU:HD13	6:B:532:LEU:HA	1.94	0.49
2:2:104:GLY:HA3	19:2:617:XAT:H192	1.93	0.49
4:4:175:GLN:OE1	4:4:175:GLN:N	2.28	0.49
22:B:844:BCR:H352	18:B:828:CLA:H192	1.94	0.49
8:D:90:VAL:HG12	8:D:91:GLU:HG3	1.94	0.49
10:F:210:GLU:HG3	10:F:215:ASP:HB3	1.95	0.49
18:4:609:CLA:CGA	18:4:609:CLA:H3A	2.42	0.49
3:3:171:LEU:HD21	18:3:612:CLA:HMC3	1.94	0.49
1:1:149:ILE:HA	1:1:152:VAL:HG22	1.94	0.49
5:A:371:MET:SD	18:A:828:CLA:HMC2	2.53	0.49
5:A:447:PHE:O	18:A:835:CLA:HBB2	2.13	0.49
2:2:99:ARG:NH1	17:2:607:CHL:OBD	2.34	0.49
2:2:213:GLY:O	2:2:217:MET:HG3	2.12	0.49
18:A:844:CLA:H3A	18:A:844:CLA:O1A	2.13	0.49
18:B:819:CLA:HBB1	18:B:824:CLA:H93	1.95	0.49
5:A:261:PHE:HE1	18:A:818:CLA:HBB1	1.77	0.48
18:A:803:CLA:OBD	18:B:802:CLA:HMB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:843:CLA:H152	22:L:301:BCR:H16C	1.95	0.48
6:B:395:ILE:HD13	6:B:555:TYR:HA	1.94	0.48
8:D:152:PHE:HB2	8:D:156:GLU:HG2	1.94	0.48
1:1:238:ILE:HD12	23:4:620:LMG:H132	1.94	0.48
21:2:616:LUT:H401	21:2:616:LUT:H15	1.95	0.48
15:K:79:LYS:O	15:K:87:GLU:N	2.45	0.48
17:2:605:CHL:C4C	18:2:604:CLA:HAB	2.44	0.48
5:A:197:HIS:CG	18:A:814:CLA:HMC2	2.48	0.48
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.96	0.48
5:A:361:THR:HA	18:A:830:CLA:HBC2	1.96	0.48
5:A:739:TRP:CH2	18:A:809:CLA:HBC2	2.47	0.48
18:A:802:CLA:H202	18:A:802:CLA:H162	1.70	0.48
16:L:203:THR:HB	22:L:306:BCR:H333	1.94	0.48
17:1:601:CHL:NB	20:1:615:LHG:H131	2.29	0.48
6:B:177:HIS:CG	18:B:813:CLA:HMC2	2.49	0.48
10:F:199:ARG:HE	10:F:199:ARG:HB2	1.53	0.48
2:2:201:LYS:HE3	2:2:205:LEU:HD11	1.95	0.48
4:4:199:GLN:O	4:4:203:GLU:HG3	2.14	0.48
18:B:818:CLA:O1A	18:B:828:CLA:HMD1	2.13	0.48
16:L:87:TYR:OH	18:L:303:CLA:O1A	2.30	0.48
1:1:177:TYR:HB2	18:1:609:CLA:HBA2	1.96	0.48
5:A:41:ASP:OD1	5:A:41:ASP:N	2.46	0.48
18:A:809:CLA:H151	18:A:804:CLA:H161	1.95	0.48
18:A:812:CLA:H92	18:A:812:CLA:H62	1.71	0.48
1:1:190:LYS:HD3	18:1:611:CLA:HAA2	1.95	0.48
17:1:601:CHL:H12	20:1:615:LHG:H181	1.96	0.48
19:2:617:XAT:H401	19:2:617:XAT:H15	1.95	0.48
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.95	0.48
18:A:806:CLA:H192	22:A:849:BCR:H363	1.96	0.48
25:A:855:PQN:H271	18:A:841:CLA:H91	1.96	0.48
3:3:220:GLU:O	3:3:224:LYS:HG3	2.14	0.47
4:4:151:HIS:HA	18:4:608:CLA:HAB	1.96	0.47
18:4:612:CLA:H91	18:4:612:CLA:H111	1.70	0.47
18:B:821:CLA:HBA1	18:B:821:CLA:HBD	1.95	0.47
4:4:157:ARG:NH2	18:4:608:CLA:O1D	2.33	0.47
18:B:830:CLA:HBC2	18:B:823:CLA:HBB1	1.96	0.47
15:K:48:PHE:HZ	18:K:204:CLA:HBC3	1.80	0.47
3:3:261:PRO:HG2	18:3:610:CLA:HMB3	1.97	0.47
18:A:802:CLA:HBA1	18:A:802:CLA:H3A	1.43	0.47
18:B:814:CLA:H121	22:B:845:BCR:H363	1.97	0.47
6:B:106:ARG:HG3	6:B:115:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:805:CLA:H2	18:B:805:CLA:H61	1.58	0.47
11:G:64:PRO:HG2	11:G:67:VAL:HB	1.97	0.47
6:B:277:HIS:HA	6:B:280:ILE:HG12	1.95	0.47
18:B:818:CLA:H3A	18:B:818:CLA:HBA2	1.42	0.47
5:A:702:ALA:HB3	18:A:841:CLA:HED3	1.96	0.47
6:B:279:ALA:HA	18:B:816:CLA:HMC3	1.97	0.47
12:H:104:LEU:O	12:H:108:ILE:HG12	2.15	0.47
22:L:301:BCR:H361	22:L:301:BCR:C21	2.41	0.47
18:2:602:CLA:H192	18:2:602:CLA:H162	1.74	0.47
18:B:834:CLA:HBA1	18:B:834:CLA:H3A	1.57	0.47
18:F:302:CLA:H11	18:F:302:CLA:H52	1.72	0.47
18:1:602:CLA:CBB	19:1:614:XAT:H30	2.45	0.47
18:F:301:CLA:H62	18:F:301:CLA:H41	1.56	0.47
5:A:393:TRP:HD1	18:A:829:CLA:HAB	1.78	0.47
22:A:848:BCR:H403	22:A:848:BCR:H23C	1.96	0.47
17:2:606:CHL:HHC	17:2:606:CHL:HBB1	1.97	0.46
3:3:90:PHE:HB2	18:3:602:CLA:H43	1.97	0.46
5:A:207:SER:HB3	5:A:299:ALA:HB2	1.97	0.46
6:B:31:PHE:HE1	18:B:804:CLA:HED1	1.80	0.46
10:F:128:LEU:HD21	14:J:38:THR:HG21	1.96	0.46
6:B:456:GLU:OE1	6:B:461:GLN:NE2	2.48	0.46
18:A:833:CLA:H61	18:A:833:CLA:H41	1.44	0.46
18:1:612:CLA:O2D	18:1:612:CLA:H2A	2.15	0.46
5:A:450:PHE:CE1	18:A:803:CLA:HMA1	2.50	0.46
6:B:182:LEU:HD21	18:B:813:CLA:O1A	2.16	0.46
18:B:825:CLA:HMB1	18:B:825:CLA:HBB1	1.97	0.46
12:H:116:THR:HG23	13:I:10:ILE:HG23	1.97	0.46
21:1:616:LUT:H35	21:1:616:LUT:H401	1.79	0.46
17:2:606:CHL:HMB3	19:2:617:XAT:H171	1.98	0.46
18:A:805:CLA:H3A	18:A:805:CLA:HBA2	1.38	0.46
18:B:832:CLA:HBB2	22:B:801:BCR:H312	1.98	0.46
1:1:109:TYR:HE1	1:1:129:LEU:HA	1.80	0.46
21:2:616:LUT:H22	18:2:609:CLA:H12	1.98	0.46
6:B:46:ILE:HG21	18:B:805:CLA:H202	1.96	0.46
18:A:835:CLA:H161	18:A:835:CLA:H202	1.69	0.46
16:L:87:TYR:OH	18:L:302:CLA:HBB2	2.16	0.46
6:B:435:GLY:HA3	18:B:833:CLA:HAB	1.98	0.46
18:B:840:CLA:HBA1	18:B:840:CLA:H3A	1.66	0.46
18:1:603:CLA:H41	18:1:603:CLA:H62	1.67	0.46
22:K:202:BCR:H23C	22:K:202:BCR:H392	1.97	0.46
18:A:845:CLA:H3A	18:A:845:CLA:HBA1	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.51	0.46
10:F:138:LEU:HD22	10:F:149:GLU:HG2	1.98	0.46
1:1:238:ILE:O	1:1:238:ILE:HG13	2.15	0.45
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.72	0.45
1:1:169:GLY:N	18:1:609:CLA:HMD1	2.31	0.45
18:A:828:CLA:OBD	18:A:827:CLA:HAA2	2.16	0.45
18:A:833:CLA:HBA1	18:A:833:CLA:H3A	1.86	0.45
3:3:260:ASP:OD2	3:3:264:ASN:ND2	2.49	0.45
24:A:801:CL0:H51	24:A:801:CL0:H59	1.67	0.45
18:A:804:CLA:H143	22:A:853:BCR:H19C	1.98	0.45
18:H:201:CLA:H93	18:H:201:CLA:H62	1.78	0.45
1:1:212:TYR:HD1	1:1:220:ASN:HD21	1.62	0.45
20:1:615:LHG:H341	20:1:615:LHG:H371	1.50	0.45
2:2:194:TRP:HB2	18:2:609:CLA:O2A	2.16	0.45
3:3:119:ILE:HG13	3:3:120:LEU:HD23	1.98	0.45
22:A:853:BCR:H343	14:J:27:ILE:HG21	1.99	0.45
22:A:851:BCR:H351	22:A:851:BCR:C16	2.42	0.45
6:B:61:THR:HB	6:B:142:LEU:HD13	1.97	0.45
1:1:119:ALA:HB1	1:1:138:LEU:HD12	1.98	0.45
3:3:260:ASP:HA	3:3:261:PRO:HD3	1.86	0.45
21:3:613:LUT:H12	21:3:613:LUT:H191	1.98	0.45
18:4:612:CLA:HBB1	18:4:612:CLA:HMB1	1.98	0.45
6:B:301:ILE:HG21	18:B:824:CLA:HAC1	1.98	0.45
18:B:806:CLA:H72	18:B:806:CLA:H111	1.52	0.45
18:B:808:CLA:H141	18:B:808:CLA:H162	1.62	0.45
10:F:180:LYS:HB3	10:F:180:LYS:HE3	1.78	0.45
18:A:844:CLA:HMB3	18:B:802:CLA:H192	1.99	0.45
18:A:832:CLA:HMA2	16:L:76:THR:HG21	1.99	0.45
18:B:805:CLA:H61	18:B:805:CLA:H93	1.66	0.45
18:B:841:CLA:C1D	18:B:822:CLA:HMB3	2.46	0.45
18:B:827:CLA:H152	18:B:827:CLA:H111	1.39	0.45
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.82	0.45
21:2:619:LUT:H31	21:2:619:LUT:H391	1.82	0.45
6:B:656:VAL:HG22	18:B:840:CLA:HMB3	1.97	0.45
6:B:339:ALA:HB2	22:B:847:BCR:H372	1.99	0.45
22:B:846:BCR:H332	20:B:852:LHG:H351	1.98	0.45
22:B:801:BCR:H383	22:B:801:BCR:H23C	1.99	0.45
1:1:190:LYS:O	1:1:194:ASN:ND2	2.42	0.45
5:A:201:GLY:O	5:A:205:LEU:HB2	2.16	0.45
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.45	0.45
18:A:843:CLA:HMC2	18:B:839:CLA:H11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:841:CLA:HBA2	18:A:841:CLA:H3A	1.41	0.44
18:B:805:CLA:HBA1	18:B:805:CLA:H3A	1.44	0.44
22:A:853:BCR:HC7	22:A:853:BCR:H331	1.82	0.44
6:B:687:LEU:HD11	16:L:91:LEU:HD13	1.99	0.44
18:B:809:CLA:HBB1	18:B:809:CLA:HMB1	1.98	0.44
2:2:81:SER:O	2:2:81:SER:OG	2.30	0.44
18:2:609:CLA:HMB1	18:2:609:CLA:HBB1	1.98	0.44
4:4:58:LEU:HD13	18:4:601:CLA:HMA3	2.00	0.44
18:4:608:CLA:C1D	18:4:603:CLA:HMD2	2.47	0.44
5:A:735:ILE:HG21	18:A:829:CLA:HMC2	2.00	0.44
18:A:820:CLA:H62	18:A:820:CLA:H92	1.67	0.44
6:B:693:TRP:HE3	18:B:839:CLA:HMD3	1.81	0.44
7:C:58:CYS:HB3	7:C:63:LEU:HD23	2.00	0.44
15:K:96:GLY:O	18:K:201:CLA:H3A	2.18	0.44
1:1:97:ALA:HA	19:1:614:XAT:C18	2.46	0.44
20:1:615:LHG:H342	20:1:615:LHG:H192	1.99	0.44
18:2:602:CLA:H41	18:2:602:CLA:H62	1.51	0.44
4:4:101:ARG:NH1	17:4:607:CHL:OBD	2.43	0.44
18:A:803:CLA:HBA1	18:A:803:CLA:H3A	1.63	0.44
18:A:842:CLA:H102	18:A:842:CLA:H62	1.78	0.44
10:F:160:ILE:HG21	18:F:302:CLA:HMA3	1.98	0.44
18:2:612:CLA:H112	18:2:612:CLA:H71	1.68	0.44
18:2:602:CLA:H62	18:2:602:CLA:H102	1.83	0.44
18:2:608:CLA:C1D	18:2:603:CLA:HMD2	2.47	0.44
18:4:602:CLA:H92	18:4:603:CLA:HMB	1.99	0.44
5:A:90:PHE:CG	18:A:808:CLA:HBC3	2.53	0.44
20:1:615:LHG:H261	20:1:615:LHG:H292	1.32	0.44
9:E:89:ILE:HG22	9:E:91:ARG:H	1.82	0.44
11:G:120:LYS:HB3	11:G:120:LYS:HE3	1.71	0.44
18:G:201:CLA:CGA	18:G:201:CLA:H3A	2.48	0.44
22:K:202:BCR:H24C	22:K:202:BCR:H371	1.77	0.44
1:1:140:THR:O	1:1:144:ILE:HG13	2.17	0.44
18:1:609:CLA:HHC	18:1:609:CLA:CBB	2.47	0.44
6:B:167:TRP:CZ2	18:B:811:CLA:HMA1	2.53	0.44
22:B:847:BCR:H11C	22:B:847:BCR:H341	1.89	0.44
18:B:826:CLA:H102	18:B:826:CLA:H61	1.74	0.44
18:A:822:CLA:H141	18:A:822:CLA:H162	1.71	0.44
21:2:619:LUT:H35	21:2:619:LUT:H401	1.82	0.44
5:A:582:CYS:HB2	6:B:667:TRP:HB3	2.00	0.44
18:A:842:CLA:HMB1	18:A:842:CLA:HBB1	1.99	0.44
25:A:855:PQN:H111	25:A:855:PQN:H2M1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:156:GLU:OE2	8:D:156:GLU:N	2.51	0.44
19:1:614:XAT:H35	19:1:614:XAT:H401	1.87	0.43
18:2:602:CLA:CGA	18:2:602:CLA:H3A	2.48	0.43
4:4:165:GLY:HA2	4:4:168:ASN:ND2	2.31	0.43
18:A:819:CLA:H3A	18:A:819:CLA:HBA2	1.63	0.43
22:A:853:BCR:H15C	22:A:853:BCR:H351	1.85	0.43
6:B:517:PHE:HE1	22:B:849:BCR:H271	1.83	0.43
22:B:846:BCR:H11C	22:B:846:BCR:H341	1.81	0.43
22:B:847:BCR:HC7	22:B:847:BCR:H331	1.85	0.43
18:B:825:CLA:H3A	18:B:825:CLA:HBA1	1.43	0.43
1:1:238:ILE:HD11	4:4:140:SER:HB3	1.99	0.43
2:2:57:PRO:O	3:3:172:GLN:HG2	2.19	0.43
18:3:601:CLA:H8	18:3:601:CLA:H51	1.74	0.43
6:B:395:ILE:HD12	6:B:555:TYR:HD1	1.82	0.43
18:F:303:CLA:HMB2	22:F:304:BCR:H393	1.99	0.43
18:3:603:CLA:HBA1	18:3:603:CLA:H3A	1.30	0.43
21:3:613:LUT:H181	21:3:613:LUT:H7	1.72	0.43
4:4:222:GLN:HE22	21:4:616:LUT:H41	1.83	0.43
15:K:67:ALA:HA	15:K:72:LEU:HD12	2.00	0.43
1:1:184:LEU:HD11	18:1:609:CLA:O2D	2.18	0.43
18:1:604:CLA:C1B	19:1:614:XAT:H42	2.48	0.43
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.99	0.43
5:A:676:PHE:CD2	22:A:852:BCR:H363	2.52	0.43
6:B:93:ASP:H	12:H:129:ILE:HD13	1.84	0.43
6:B:174:ARG:HB2	18:B:813:CLA:HBC2	2.00	0.43
18:B:822:CLA:H91	18:B:822:CLA:H111	1.82	0.43
5:A:480:PHE:O	5:A:484:ILE:HG12	2.18	0.43
18:A:825:CLA:H3A	18:A:825:CLA:HBA2	1.40	0.43
22:B:847:BCR:H14C	18:B:825:CLA:HMA1	2.01	0.43
18:B:809:CLA:H92	18:B:809:CLA:H62	1.72	0.43
5:A:294:HIS:CE1	5:A:298:ILE:HG13	2.54	0.43
18:B:827:CLA:H193	27:B:850:DGD:HAN2	2.01	0.43
18:B:803:CLA:H61	18:B:803:CLA:H93	1.78	0.43
15:K:115:ILE:HG12	22:K:205:BCR:H313	2.01	0.43
20:2:618:LHG:O4	20:2:618:LHG:O2	2.33	0.43
5:A:93:ALA:HA	5:A:153:GLU:HG2	1.99	0.43
1:1:128:TYR:HD1	18:1:604:CLA:HBA1	1.82	0.43
18:1:602:CLA:H72	19:1:614:XAT:C37	2.49	0.43
19:2:617:XAT:H12	18:2:603:CLA:HMC2	2.00	0.43
2:2:171:PHE:HE2	17:2:615:CHL:HHB	1.84	0.43
19:4:617:XAT:H31	19:4:617:XAT:H391	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:530:ASP:HA	5:A:533:VAL:HG12	2.01	0.43
3:3:201:PRO:HD3	17:3:606:CHL:HMD2	2.00	0.43
3:3:219:LYS:HA	3:3:219:LYS:HD2	1.83	0.43
5:A:223:GLN:HG2	5:A:250:LEU:HD21	2.01	0.43
22:B:846:BCR:H15C	22:B:846:BCR:H351	1.81	0.43
18:B:809:CLA:H41	18:B:809:CLA:H61	1.64	0.43
18:B:841:CLA:H121	18:B:841:CLA:H161	1.75	0.43
17:1:601:CHL:C2C	20:1:615:LHG:HC81	2.49	0.42
18:2:612:CLA:H142	18:2:612:CLA:H111	1.74	0.42
21:2:619:LUT:H181	21:2:619:LUT:C8	2.37	0.42
18:A:807:CLA:H93	18:A:807:CLA:H112	1.88	0.42
22:J:102:BCR:H11C	22:J:102:BCR:H341	1.83	0.42
18:L:303:CLA:H142	18:L:303:CLA:H111	1.72	0.42
2:2:168:ASP:HB3	2:2:171:PHE:O	2.19	0.42
20:2:618:LHG:HC81	20:2:618:LHG:HC41	2.01	0.42
17:4:615:CHL:HMC	17:4:607:CHL:OMC	2.18	0.42
18:A:835:CLA:H3A	18:A:835:CLA:HBA1	1.77	0.42
18:A:835:CLA:HBB	18:A:834:CLA:HAB	2.01	0.42
22:A:848:BCR:H11C	22:A:848:BCR:H341	1.90	0.42
6:B:583:MET:O	6:B:587:ILE:HG12	2.19	0.42
20:B:852:LHG:H121	18:B:822:CLA:H41	2.01	0.42
22:B:801:BCR:HC21	18:F:302:CLA:H51	2.00	0.42
22:B:845:BCR:H21C	22:B:845:BCR:H24C	1.78	0.42
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.54	0.42
18:F:302:CLA:HAA2	14:J:22:LEU:HD11	2.02	0.42
18:1:604:CLA:C3B	19:1:614:XAT:H183	2.49	0.42
2:2:101:ALA:CB	2:2:217:MET:HG2	2.49	0.42
2:2:139:THR:O	2:2:143:VAL:HG23	2.19	0.42
21:3:613:LUT:H191	21:3:613:LUT:C12	2.48	0.42
4:4:221:VAL:HG11	18:4:612:CLA:HAC2	2.00	0.42
18:A:807:CLA:H193	18:A:807:CLA:H161	1.87	0.42
18:A:809:CLA:H71	22:J:102:BCR:H343	2.00	0.42
18:A:817:CLA:HBA1	18:A:817:CLA:H3A	1.65	0.42
22:A:851:BCR:H371	22:A:851:BCR:H24C	1.69	0.42
6:B:529:THR:HG21	6:B:582:TRP:CZ2	2.54	0.42
22:L:305:BCR:H24C	22:L:305:BCR:H371	1.81	0.42
18:3:604:CLA:HMB1	18:3:607:CLA:HBC2	2.02	0.42
18:A:807:CLA:HBA1	18:A:807:CLA:H3A	1.79	0.42
6:B:347:LEU:HD23	18:B:818:CLA:H72	2.02	0.42
19:1:614:XAT:H42	19:1:614:XAT:H162	2.01	0.42
21:2:616:LUT:H373	18:2:612:CLA:C2B	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:241:ILE:CG2	18:3:609:CLA:HMD3	2.49	0.42
24:A:801:CL0:H51	24:A:801:CL0:H42	1.79	0.42
18:A:823:CLA:HAA2	15:K:80:ALA:HB3	2.02	0.42
18:B:808:CLA:C1A	18:B:808:CLA:CGA	2.97	0.42
18:B:828:CLA:H3A	18:B:828:CLA:HBA2	1.30	0.42
22:B:801:BCR:H15C	22:B:801:BCR:H351	1.87	0.42
1:1:73:LEU:O	20:B:851:LHG:O1	2.28	0.42
18:A:804:CLA:O1D	18:A:804:CLA:H2A	2.19	0.42
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.54	0.42
5:A:30:GLY:HA3	5:A:36:ILE:HG22	2.01	0.42
22:B:848:BCR:H403	22:B:848:BCR:C23	2.49	0.42
22:K:202:BCR:H351	22:K:202:BCR:H15C	1.80	0.42
18:3:605:CLA:O1D	18:3:605:CLA:H2A	2.20	0.42
22:B:846:BCR:H373	18:B:826:CLA:H121	2.01	0.42
22:B:801:BCR:H341	22:B:801:BCR:C12	2.37	0.42
22:L:305:BCR:H393	22:L:305:BCR:H23C	2.01	0.42
18:2:602:CLA:H122	19:2:617:XAT:H371	2.00	0.42
18:2:604:CLA:HBA1	18:2:604:CLA:H3A	1.92	0.42
6:B:294:ASN:HB2	11:G:114:GLU:HA	2.02	0.42
22:L:305:BCR:H20C	22:L:305:BCR:H361	1.88	0.42
1:1:168:PRO:HG2	18:1:609:CLA:HMD3	2.02	0.42
18:B:840:CLA:H93	18:B:840:CLA:H61	1.91	0.42
1:1:227:ASP:OD2	1:1:230:HIS:HB2	2.20	0.41
18:A:844:CLA:H12	18:A:844:CLA:H52	1.84	0.41
18:A:839:CLA:H61	18:A:839:CLA:H41	1.77	0.41
22:A:851:BCR:H331	22:A:851:BCR:C8	2.49	0.41
18:B:825:CLA:H93	18:B:825:CLA:H111	1.85	0.41
22:B:801:BCR:H24C	22:B:801:BCR:H371	1.87	0.41
8:D:102:LYS:HB2	8:D:102:LYS:HE2	1.91	0.41
1:1:207:VAL:HG11	18:1:612:CLA:HMD2	2.02	0.41
17:1:601:CHL:C3B	20:1:615:LHG:H282	2.50	0.41
18:2:612:CLA:HBB1	18:2:612:CLA:HMB1	2.02	0.41
19:4:617:XAT:H32	18:4:602:CLA:HAB	2.00	0.41
5:A:310:ARG:HH22	15:K:79:LYS:HD3	1.85	0.41
18:A:804:CLA:HBA2	18:A:804:CLA:CBP	2.46	0.41
18:A:842:CLA:HBA2	20:A:846:LHG:H162	2.01	0.41
18:A:812:CLA:H111	18:A:812:CLA:H91	1.69	0.41
18:B:817:CLA:CGA	18:B:817:CLA:H3A	2.50	0.41
22:L:305:BCR:H23C	22:L:305:BCR:H402	2.02	0.41
21:1:616:LUT:H391	21:1:616:LUT:C32	2.49	0.41
19:2:617:XAT:H201	19:2:617:XAT:H35	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:608:CLA:H3A	18:2:608:CLA:HBA2	1.22	0.41
5:A:187:TRP:CZ2	18:A:811:CLA:HMA1	2.55	0.41
5:A:213:HIS:HB2	18:A:815:CLA:CHC	2.50	0.41
18:A:813:CLA:HBA2	18:A:813:CLA:H3A	1.75	0.41
18:A:830:CLA:H41	18:A:830:CLA:H62	1.68	0.41
18:B:824:CLA:H62	18:B:824:CLA:H41	1.55	0.41
18:A:821:CLA:HHC	18:A:821:CLA:CBB	2.50	0.41
18:A:809:CLA:H92	18:A:809:CLA:H62	1.77	0.41
18:A:830:CLA:H11	18:A:830:CLA:HBA2	1.55	0.41
22:B:848:BCR:H11C	22:B:848:BCR:H341	1.95	0.41
18:B:840:CLA:H111	18:B:840:CLA:H151	1.83	0.41
3:3:169:ARG:HB3	17:3:606:CHL:CMC	2.51	0.41
18:3:601:CLA:H2	18:3:601:CLA:H62	1.76	0.41
18:4:602:CLA:CGA	18:4:602:CLA:H3A	2.51	0.41
22:4:618:BCR:H11C	22:4:618:BCR:H341	1.92	0.41
22:A:851:BCR:H321	22:A:851:BCR:HC7	1.86	0.41
22:B:848:BCR:H20C	22:B:848:BCR:H361	1.92	0.41
18:B:818:CLA:H62	18:B:818:CLA:H41	1.77	0.41
18:B:823:CLA:HBA1	18:B:823:CLA:H3A	1.72	0.41
18:B:832:CLA:H143	18:B:832:CLA:H161	1.80	0.41
21:2:616:LUT:H11	21:2:616:LUT:H191	1.87	0.41
18:2:604:CLA:C2C	19:2:617:XAT:H183	2.50	0.41
19:4:617:XAT:H35	19:4:617:XAT:H401	1.89	0.41
21:4:616:LUT:H15	21:4:616:LUT:H201	1.96	0.41
5:A:462:LEU:HG	18:B:809:CLA:HMC3	2.01	0.41
18:A:825:CLA:HBB1	18:A:832:CLA:HBC2	2.02	0.41
18:B:809:CLA:H142	18:B:809:CLA:H111	1.91	0.41
18:B:802:CLA:HHC	18:B:802:CLA:HBB1	2.02	0.41
20:1:615:LHG:HC12	22:4:618:BCR:H291	2.03	0.41
18:A:805:CLA:HBA1	18:A:812:CLA:C1D	2.50	0.41
18:A:835:CLA:H93	18:A:835:CLA:H111	1.71	0.41
22:A:848:BCR:H23C	22:A:848:BCR:H392	2.02	0.41
22:A:850:BCR:H331	22:A:850:BCR:HC7	1.77	0.41
18:B:828:CLA:HBB1	18:B:806:CLA:HAB	2.03	0.41
18:B:828:CLA:H142	18:B:828:CLA:H112	1.90	0.41
22:B:845:BCR:H15C	22:B:845:BCR:H351	1.94	0.41
14:J:32:LEU:HD21	18:J:101:CLA:HBA2	2.03	0.41
2:2:171:PHE:CE2	17:2:615:CHL:HHB	2.55	0.41
21:2:619:LUT:H172	18:4:610:CLA:HMC3	2.03	0.41
5:A:596:TRP:HE1	18:B:803:CLA:C1D	2.33	0.41
18:A:813:CLA:H2A	18:A:813:CLA:O2D	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:829:CLA:H72	18:A:829:CLA:H111	1.35	0.41
18:B:802:CLA:HBA1	18:B:802:CLA:H3A	1.29	0.41
18:B:820:CLA:C4B	22:B:843:BCR:H15C	2.50	0.41
22:G:204:BCR:HC7	22:G:204:BCR:H331	1.84	0.41
22:J:102:BCR:H15C	22:J:102:BCR:H351	1.82	0.41
22:L:301:BCR:H15C	22:L:301:BCR:H351	1.72	0.41
18:1:607:CLA:HBA2	18:1:607:CLA:H3A	1.23	0.41
18:2:602:CLA:H101	18:2:603:CLA:HMA1	2.02	0.41
5:A:116:TRP:O	5:A:121:GLN:NE2	2.38	0.41
5:A:305:ALA:HB2	18:A:822:CLA:HBC2	2.02	0.41
18:A:813:CLA:H2A	18:A:813:CLA:CED	2.51	0.41
18:A:834:CLA:H162	18:A:834:CLA:H141	1.82	0.41
22:A:850:BCR:H11C	22:A:850:BCR:H341	1.84	0.41
18:A:812:CLA:H172	18:A:812:CLA:H13	1.73	0.41
6:B:464:GLN:NE2	18:B:836:CLA:OBD	2.44	0.41
6:B:601:LEU:HA	6:B:606:VAL:HG12	2.03	0.41
18:B:832:CLA:H62	18:B:832:CLA:H2	1.70	0.41
18:B:803:CLA:H202	18:B:803:CLA:H162	1.76	0.41
18:F:302:CLA:O1D	18:F:302:CLA:H2A	2.20	0.41
22:J:102:BCR:HC7	22:J:102:BCR:H331	1.90	0.41
16:L:121:LYS:HB3	16:L:121:LYS:HE3	1.84	0.41
16:L:208:LEU:HD23	16:L:208:LEU:HA	1.92	0.41
22:L:306:BCR:H15C	22:L:306:BCR:H351	1.84	0.41
2:2:174:ASN:HD22	17:2:615:CHL:C4D	2.33	0.41
4:4:155:ILE:HD13	4:4:155:ILE:HA	1.92	0.41
19:4:617:XAT:H11	19:4:617:XAT:H191	1.84	0.41
18:B:820:CLA:HBA2	18:B:820:CLA:H3A	1.32	0.41
22:L:305:BCR:H11C	22:L:305:BCR:H341	1.88	0.41
17:1:601:CHL:H61	17:1:601:CHL:H41	1.70	0.40
18:1:602:CLA:CGA	18:1:602:CLA:H3A	2.51	0.40
17:2:615:CHL:HBB1	17:2:615:CHL:CHC	2.50	0.40
18:2:612:CLA:H3A	18:2:612:CLA:HBA2	1.81	0.40
18:2:604:CLA:HED2	18:2:604:CLA:H2A	2.03	0.40
18:B:808:CLA:HAB	18:B:809:CLA:HAA2	2.03	0.40
18:B:814:CLA:H162	18:B:814:CLA:H141	1.81	0.40
18:B:824:CLA:H91	18:B:824:CLA:H112	1.87	0.40
15:K:75:SER:OG	15:K:105:ASP:OD1	2.27	0.40
22:3:614:BCR:H11C	22:3:614:BCR:H341	1.90	0.40
18:4:602:CLA:H91	18:4:602:CLA:H112	1.81	0.40
6:B:560:ASP:H	6:B:567:THR:HG1	1.69	0.40
18:B:822:CLA:O1D	18:B:822:CLA:HBA1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:601:CLA:H91	18:3:601:CLA:H112	1.87	0.40
5:A:319:ILE:HG21	18:A:826:CLA:HAC1	2.03	0.40
6:B:3:LEU:HD13	6:B:7:ARG:HH21	1.85	0.40
18:B:826:CLA:H111	18:B:826:CLA:H142	1.83	0.40
18:B:827:CLA:HBA2	18:B:827:CLA:H3A	1.39	0.40
22:B:843:BCR:H331	22:B:843:BCR:HC7	1.78	0.40
18:L:303:CLA:H112	18:L:303:CLA:H71	1.72	0.40
1:1:162:PRO:HA	1:1:165:LYS:HG3	2.03	0.40
19:1:614:XAT:H183	19:1:614:XAT:H7	1.85	0.40
18:2:602:CLA:H91	18:2:602:CLA:H111	1.82	0.40
20:2:618:LHG:HC91	22:3:614:BCR:HC41	2.04	0.40
5:A:671:PHE:O	5:A:675:HIS:ND1	2.54	0.40
18:A:809:CLA:H101	18:A:809:CLA:H13	1.92	0.40
18:B:813:CLA:O2D	18:B:813:CLA:H2A	2.22	0.40
18:B:832:CLA:CBB	22:B:801:BCR:H312	2.51	0.40
3:3:109:LEU:HD22	18:3:603:CLA:HBC1	2.04	0.40
3:3:167:GLU:OE1	3:3:170:ARG:NH1	2.54	0.40
6:B:432:HIS:CB	22:B:849:BCR:H402	2.49	0.40
10:F:195:ARG:HD2	10:F:195:ARG:HA	1.96	0.40
22:F:304:BCR:H361	22:F:304:BCR:H20C	1.80	0.40
11:G:74:LEU:HD12	11:G:74:LEU:HA	1.97	0.40
22:K:205:BCR:H24C	22:K:205:BCR:H371	1.90	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%)	198 (100%)	1 (0%)	0	100	100
3	3	216/273 (79%)	213 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	194/251 (77%)	191 (98%)	3 (2%)	0	100	100
5	A	735/750 (98%)	725 (99%)	10 (1%)	0	100	100
6	B	730/734 (100%)	716 (98%)	14 (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%)	149 (99%)	1 (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%)	28 (97%)	1 (3%)	0	100	100
14	J	39/44 (89%)	38 (97%)	1 (3%)	0	100	100
15	K	82/130 (63%)	82 (100%)	0	0	100	100
16	L	158/219 (72%)	155 (98%)	3 (2%)	0	100	100
All	All	3181/3890 (82%)	3133 (98%)	48 (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%)	151 (99%)	2 (1%)	69	86
2	2	163/205 (80%)	155 (95%)	8 (5%)	25	60
3	3	167/211 (79%)	164 (98%)	3 (2%)	59	81
4	4	163/210 (78%)	162 (99%)	1 (1%)	86	93
5	A	598/610 (98%)	594 (99%)	4 (1%)	84	93
6	B	599/600 (100%)	594 (99%)	5 (1%)	81	92
7	C	70/71 (99%)	69 (99%)	1 (1%)	67	85
8	D	121/170 (71%)	119 (98%)	2 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	125/185 (68%)	121 (97%)	4 (3%)	39	70
11	G	77/133 (58%)	75 (97%)	2 (3%)	46	75
12	H	75/113 (66%)	72 (96%)	3 (4%)	31	65
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	35 (97%)	1 (3%)	43	73
15	K	61/95 (64%)	60 (98%)	1 (2%)	62	83
16	L	126/174 (72%)	126 (100%)	0	100	100
All	All	2618/3153 (83%)	2581 (99%)	37 (1%)	68	85

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	220	ASN
1	1	231	ASN
2	2	81	SER
2	2	113	PHE
2	2	121	ASN
2	2	124	SER
2	2	132	GLU
2	2	173	ASN
2	2	188	TRP
2	2	198	SER
3	3	62	SER
3	3	152	ASN
3	3	264	ASN
4	4	132	LYS
5	A	127	ASP
5	A	184	LYS
5	A	275	PHE
5	A	457	ASP
6	B	47	PHE
6	B	229	GLN
6	B	394	PHE
6	B	431	PHE
6	B	577	TYR
7	C	35	LYS
8	D	164	ASP
8	D	184	SER

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Mol	Chain	Res	Type
10	F	68	ASP
10	F	94	SER
10	F	95	SER
10	F	147	TRP
11	G	88	ARG
11	G	121	SER
12	H	76	SER
12	H	77	ASP
12	H	80	SER
14	J	41	PHE
15	K	66	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	222	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

201 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
18	CLA	A	831	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
18	CLA	3	609	-	53,62,73	1.66	6 (11%)	61,100,113	1.45	8 (13%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	4	610	-	42,50,73	1.83	5 (11%)	48,85,113	1.58	6 (12%)
18	CLA	A	829	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	7 (9%)
18	CLA	2	608	-	45,53,73	1.76	5 (11%)	52,89,113	1.61	6 (11%)
22	BCR	B	844	-	41,41,41	1.74	8 (19%)	56,56,56	1.79	12 (21%)
18	CLA	B	832	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	7 (9%)
18	CLA	B	836	-	50,58,73	1.71	6 (12%)	58,95,113	3.64	12 (20%)
18	CLA	B	841	20	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
17	CHL	2	605	-	42,50,74	2.37	14 (33%)	45,85,114	2.85	18 (40%)
18	CLA	A	815	-	45,53,73	1.75	5 (11%)	52,89,113	1.61	6 (11%)
18	CLA	1	609	-	42,50,73	1.81	6 (14%)	48,85,113	1.66	6 (12%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.33	0
18	CLA	A	814	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
22	BCR	B	849	-	41,41,41	1.75	8 (19%)	56,56,56	1.80	13 (23%)
19	XAT	2	617	-	39,47,47	1.78	7 (17%)	54,74,74	2.05	14 (25%)
17	CHL	2	607	-	51,59,74	2.22	16 (31%)	55,96,114	2.68	21 (38%)
18	CLA	3	607	-	45,53,73	1.81	6 (13%)	52,89,113	1.58	7 (13%)
22	BCR	B	845	-	41,41,41	1.80	8 (19%)	56,56,56	1.80	14 (25%)
18	CLA	B	830	-	43,51,73	1.80	5 (11%)	49,86,113	1.61	7 (14%)
18	CLA	4	611	-	40,49,73	1.89	6 (15%)	45,84,113	1.60	6 (13%)
18	CLA	A	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	9 (15%)
18	CLA	3	602	-	55,63,73	1.63	5 (9%)	64,101,113	1.42	7 (10%)
18	CLA	B	815	-	43,51,73	1.79	6 (13%)	49,86,113	1.61	6 (12%)
18	CLA	B	840	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
18	CLA	J	101	-	51,59,73	1.70	5 (9%)	59,96,113	1.49	8 (13%)
18	CLA	A	820	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	7 (9%)
17	CHL	1	606	-	40,49,74	2.55	16 (40%)	41,84,114	2.90	18 (43%)
17	CHL	1	601	1	51,60,74	2.22	15 (29%)	54,97,114	2.68	21 (38%)
18	CLA	K	204	-	46,54,73	1.78	6 (13%)	53,90,113	1.57	7 (13%)
18	CLA	K	203	-	45,53,73	1.78	5 (11%)	52,89,113	1.63	8 (15%)
22	BCR	L	306	-	41,41,41	1.75	8 (19%)	56,56,56	1.91	16 (28%)
18	CLA	2	612	2	65,73,73	1.47	6 (9%)	76,113,113	1.42	6 (7%)
18	CLA	A	826	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	G	202	-	42,50,73	1.83	6 (14%)	48,85,113	1.59	6 (12%)
21	LUT	3	613	-	42,43,43	1.71	8 (19%)	51,60,60	1.92	14 (27%)
18	CLA	A	843	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	6 (7%)
18	CLA	B	823	-	45,53,73	1.80	6 (13%)	52,89,113	1.55	7 (13%)
18	CLA	B	819	-	55,63,73	1.63	5 (9%)	64,101,113	1.47	8 (12%)
18	CLA	A	833	-	56,64,73	1.59	5 (8%)	65,102,113	1.48	6 (9%)
22	BCR	K	205	-	41,41,41	1.75	8 (19%)	56,56,56	1.97	16 (28%)
18	CLA	B	838	-	47,55,73	1.76	6 (12%)	54,91,113	1.54	8 (14%)
22	BCR	B	801	-	41,41,41	1.81	8 (19%)	56,56,56	1.77	13 (23%)
18	CLA	A	837	5	45,53,73	1.81	5 (11%)	52,89,113	1.57	7 (13%)
25	PQN	B	842	-	34,34,34	0.42	0	42,45,45	0.40	0
27	DGD	B	850	-	67,67,67	0.84	2 (2%)	81,81,81	0.94	4 (4%)
18	CLA	2	611	-	44,52,73	1.81	6 (13%)	51,88,113	1.67	6 (11%)
18	CLA	B	805	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	8 (10%)
22	BCR	L	305	-	41,41,41	1.76	8 (19%)	56,56,56	1.75	14 (25%)
18	CLA	A	827	-	59,67,73	1.56	5 (8%)	68,105,113	1.48	8 (11%)
19	XAT	1	614	-	39,47,47	0.83	1 (2%)	54,74,74	3.20	18 (33%)
18	CLA	A	804	-	65,73,73	1.48	5 (7%)	76,113,113	1.47	9 (11%)
18	CLA	A	842	-	65,73,73	1.48	6 (9%)	76,113,113	1.50	8 (10%)
18	CLA	A	819	-	59,67,73	1.58	6 (10%)	68,105,113	1.45	7 (10%)
18	CLA	A	838	-	51,59,73	1.70	5 (9%)	59,96,113	1.50	9 (15%)
18	CLA	4	603	-	44,52,73	1.86	7 (15%)	55,88,113	1.62	8 (14%)
18	CLA	F	303	10	41,49,73	1.86	5 (12%)	47,84,113	1.67	7 (14%)
18	CLA	K	206	15	37,47,73	1.95	5 (13%)	42,81,113	1.68	8 (19%)
18	CLA	B	803	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	A	805	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	6 (10%)
18	CLA	B	806	6	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
18	CLA	4	612	-	57,65,73	1.57	5 (8%)	66,103,113	1.49	7 (10%)
18	CLA	A	824	-	41,49,73	1.85	6 (14%)	47,84,113	1.64	8 (17%)
18	CLA	B	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (11%)
18	CLA	A	806	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
18	CLA	A	836	-	45,53,73	1.82	5 (11%)	52,89,113	1.58	7 (13%)
18	CLA	1	605	-	46,54,73	1.77	5 (10%)	53,90,113	1.57	6 (11%)
17	CHL	2	601	2	47,55,74	2.32	15 (31%)	50,91,114	2.77	19 (38%)
22	BCR	B	848	-	41,41,41	1.72	8 (19%)	56,56,56	1.58	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SF4	C	101	-	0,12,12	-	-	-	-	-
18	CLA	1	613	-	37,46,73	2.00	7 (18%)	46,81,113	1.75	10 (21%)
18	CLA	A	844	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
18	CLA	B	835	-	42,50,73	1.84	6 (14%)	48,85,113	1.60	7 (14%)
18	CLA	3	610	-	39,48,73	1.91	5 (12%)	44,83,113	1.65	7 (15%)
18	CLA	1	607	-	43,52,73	1.84	5 (11%)	49,88,113	1.57	7 (14%)
21	LUT	1	616	-	42,43,43	1.69	7 (16%)	51,60,60	2.00	12 (23%)
18	CLA	F	302	-	51,59,73	1.69	5 (9%)	59,96,113	1.55	7 (11%)
18	CLA	A	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	9 (11%)
18	CLA	B	824	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
22	BCR	A	849	-	41,41,41	1.79	8 (19%)	56,56,56	1.95	13 (23%)
17	CHL	2	615	2	43,51,74	2.36	14 (32%)	45,86,114	2.90	20 (44%)
25	PQN	A	855	-	34,34,34	0.41	0	42,45,45	0.42	0
18	CLA	B	834	-	60,68,73	1.56	6 (10%)	70,107,113	1.43	9 (12%)
17	CHL	2	606	-	43,51,74	2.36	14 (32%)	45,86,114	2.86	18 (40%)
18	CLA	A	830	-	65,73,73	1.47	6 (9%)	76,113,113	1.52	11 (14%)
18	CLA	A	813	-	54,62,73	1.63	6 (11%)	62,99,113	1.51	8 (12%)
18	CLA	4	604	-	43,51,73	1.88	6 (13%)	54,87,113	1.62	8 (14%)
18	CLA	B	812	-	43,51,73	1.84	5 (11%)	49,86,113	1.55	6 (12%)
18	CLA	A	834	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
18	CLA	4	608	4	45,53,73	1.78	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	A	840	-	52,60,73	1.68	5 (9%)	60,97,113	1.51	7 (11%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.53	1 (2%)
18	CLA	1	608	1	40,48,73	1.91	7 (17%)	50,83,113	1.71	9 (18%)
20	LHG	A	847	18	29,29,48	0.33	0	32,35,54	0.43	0
22	BCR	B	846	-	41,41,41	1.74	8 (19%)	56,56,56	1.70	10 (17%)
18	CLA	B	822	-	65,73,73	1.49	5 (7%)	76,113,113	1.49	9 (11%)
22	BCR	A	853	-	41,41,41	1.81	8 (19%)	56,56,56	1.75	14 (25%)
18	CLA	B	818	-	60,68,73	1.54	5 (8%)	70,107,113	1.47	7 (10%)
22	BCR	3	614	-	41,41,41	1.73	8 (19%)	56,56,56	1.57	12 (21%)
18	CLA	B	813	-	65,73,73	1.48	6 (9%)	76,113,113	1.46	9 (11%)
18	CLA	B	828	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	7 (9%)
18	CLA	A	802	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	8 (10%)
18	CLA	A	818	-	60,68,73	1.52	5 (8%)	70,107,113	5.15	9 (12%)
18	CLA	B	816	-	55,63,73	1.60	5 (9%)	64,101,113	1.49	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SF4	A	854	-	0,12,12	-	-	-	-	-
18	CLA	G	203	11	45,53,73	1.77	5 (11%)	52,89,113	1.62	6 (11%)
18	CLA	B	802	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	6 (7%)
18	CLA	3	612	-	39,48,73	1.87	6 (15%)	44,83,113	1.69	7 (15%)
18	CLA	B	829	-	56,64,73	1.60	6 (10%)	65,102,113	1.47	8 (12%)
18	CLA	K	201	15	38,45,73	1.92	6 (15%)	43,78,113	1.64	6 (13%)
22	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.57	10 (17%)
22	BCR	A	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.61	11 (19%)
18	CLA	B	817	-	59,67,73	1.57	5 (8%)	68,105,113	1.42	8 (11%)
20	LHG	A	846	-	48,48,48	0.27	0	51,54,54	0.33	0
18	CLA	A	822	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
18	CLA	2	610	20	38,45,73	2.98	8 (21%)	41,76,113	1.50	8 (19%)
18	CLA	H	201	-	60,68,73	1.54	5 (8%)	70,107,113	1.40	6 (8%)
18	CLA	1	610	20	37,46,73	2.01	6 (16%)	46,81,113	1.74	9 (19%)
22	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.77	14 (25%)
22	BCR	4	618	-	41,41,41	1.73	8 (19%)	56,56,56	1.69	10 (17%)
22	BCR	A	850	-	41,41,41	1.82	8 (19%)	56,56,56	1.90	13 (23%)
22	BCR	F	304	-	41,41,41	1.84	7 (17%)	56,56,56	2.14	16 (28%)
20	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.33	0
18	CLA	3	604	-	40,49,73	1.88	6 (15%)	45,84,113	1.58	7 (15%)
18	CLA	4	602	4	60,68,73	1.53	5 (8%)	70,107,113	1.46	7 (10%)
22	BCR	K	202	-	41,41,41	1.74	8 (19%)	56,56,56	1.93	14 (25%)
23	LMG	4	619	-	39,39,55	0.22	0	47,47,63	0.24	0
18	CLA	A	812	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
18	CLA	A	807	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	8 (10%)
18	CLA	4	609	-	54,62,73	1.62	6 (11%)	62,99,113	1.49	9 (14%)
18	CLA	A	835	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
18	CLA	1	604	-	49,57,73	1.72	5 (10%)	55,93,113	1.60	8 (14%)
18	CLA	3	605	-	41,49,73	1.90	7 (17%)	51,84,113	1.69	8 (15%)
18	CLA	B	809	6	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
18	CLA	2	603	-	43,52,73	1.82	5 (11%)	49,88,113	1.59	6 (12%)
18	CLA	A	828	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	6 (7%)
18	CLA	B	831	-	43,51,73	1.79	5 (11%)	49,86,113	1.64	7 (14%)
18	CLA	3	611	-	37,44,73	1.97	6 (16%)	42,77,113	1.65	6 (14%)
18	CLA	1	612	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	XAT	4	617	-	39,47,47	1.72	8 (20%)	54,74,74	1.72	12 (22%)
22	BCR	B	843	-	41,41,41	1.78	8 (19%)	56,56,56	1.92	14 (25%)
18	CLA	A	821	-	45,53,73	1.81	5 (11%)	52,89,113	1.58	6 (11%)
17	CHL	3	606	-	45,53,74	2.33	15 (33%)	52,89,114	2.65	18 (34%)
18	CLA	A	845	20	50,58,73	1.71	5 (10%)	58,95,113	1.52	8 (13%)
18	CLA	A	810	5	50,58,73	1.70	6 (12%)	58,95,113	1.64	12 (20%)
18	CLA	A	811	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	B	814	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
22	BCR	A	851	-	41,41,41	1.88	8 (19%)	56,56,56	2.48	19 (33%)
21	LUT	4	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.55	11 (21%)
22	BCR	G	204	-	41,41,41	1.73	8 (19%)	56,56,56	1.64	11 (19%)
18	CLA	4	614	-	50,58,73	1.70	5 (10%)	58,95,113	1.57	8 (13%)
18	CLA	F	301	-	57,65,73	1.61	5 (8%)	66,103,113	1.40	7 (10%)
22	BCR	L	301	-	41,41,41	1.76	8 (19%)	56,56,56	2.17	12 (21%)
18	CLA	B	807	-	52,60,73	1.66	6 (11%)	60,97,113	1.52	7 (11%)
17	CHL	4	605	-	40,49,74	2.38	14 (35%)	42,84,114	2.83	18 (42%)
18	CLA	A	839	-	55,63,73	1.60	5 (9%)	64,101,113	1.48	7 (10%)
18	CLA	4	601	4	46,54,73	1.76	5 (10%)	53,90,113	1.56	6 (11%)
18	CLA	4	613	-	45,53,73	1.78	6 (13%)	52,89,113	1.74	8 (15%)
18	CLA	L	304	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	7 (13%)
17	CHL	4	615	4	40,49,74	2.24	13 (32%)	45,84,114	2.97	18 (40%)
17	CHL	4	607	-	46,54,74	2.29	15 (32%)	49,90,114	2.81	20 (40%)
18	CLA	2	602	2	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
18	CLA	B	839	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
18	CLA	1	602	1	54,62,73	1.62	5 (9%)	62,99,113	1.48	7 (11%)
18	CLA	B	821	-	47,55,73	1.72	5 (10%)	54,91,113	1.72	9 (16%)
18	CLA	B	810	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	7 (9%)
21	LUT	2	619	-	42,43,43	1.66	8 (19%)	51,60,60	1.88	12 (23%)
22	BCR	I	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.50	10 (17%)
26	SF4	C	102	-	0,12,12	-	-	-	-	-
18	CLA	3	601	-	60,68,73	1.54	6 (10%)	70,107,113	1.44	8 (11%)
18	CLA	L	303	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (11%)
18	CLA	2	609	-	47,55,73	1.70	6 (12%)	54,91,113	1.62	7 (12%)
18	CLA	A	809	-	65,73,73	1.46	5 (7%)	76,113,113	1.41	7 (9%)
18	CLA	A	803	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	613	-	43,51,73	1.82	5 (11%)	49,86,113	1.57	7 (14%)
18	CLA	A	817	-	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
22	BCR	A	852	-	41,41,41	1.74	8 (19%)	56,56,56	1.90	14 (25%)
18	CLA	B	820	-	50,58,73	1.68	6 (12%)	58,95,113	1.57	8 (13%)
18	CLA	A	816	-	42,50,73	1.83	6 (14%)	48,85,113	1.61	7 (14%)
18	CLA	A	823	-	42,50,73	1.80	5 (11%)	48,85,113	1.65	6 (12%)
24	CL0	A	801	-	60,67,73	2.09	15 (25%)	68,102,113	3.89	29 (42%)
18	CLA	B	826	-	62,70,73	1.51	6 (9%)	72,109,113	1.44	7 (9%)
18	CLA	B	811	-	54,62,73	1.68	6 (11%)	67,100,113	1.54	9 (13%)
18	CLA	3	603	-	45,53,73	1.78	5 (11%)	52,89,113	1.61	7 (13%)
18	CLA	B	825	-	62,70,73	1.50	5 (8%)	72,109,113	1.48	10 (13%)
18	CLA	2	604	-	43,51,73	1.81	6 (13%)	48,86,113	1.61	6 (12%)
18	CLA	B	833	-	45,53,73	1.77	5 (11%)	52,89,113	1.66	9 (17%)
18	CLA	3	608	-	41,49,73	1.80	5 (12%)	47,84,113	1.75	9 (19%)
17	CHL	4	606	-	41,49,74	2.25	13 (31%)	51,84,114	2.77	17 (33%)
21	LUT	2	616	-	42,43,43	1.66	8 (19%)	51,60,60	2.02	12 (23%)
18	CLA	1	603	-	54,62,73	1.63	6 (11%)	62,99,113	1.51	8 (12%)
18	CLA	B	808	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	B	827	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	7 (9%)
18	CLA	B	804	-	41,49,73	1.82	5 (12%)	47,84,113	1.72	7 (14%)
18	CLA	G	201	-	45,53,73	1.79	5 (11%)	52,89,113	1.56	6 (11%)
20	LHG	B	851	18	37,37,48	0.30	0	40,43,54	0.49	0
18	CLA	A	825	-	55,63,73	1.63	5 (9%)	64,101,113	1.43	8 (12%)
18	CLA	A	808	-	50,58,73	1.70	5 (10%)	58,95,113	1.54	9 (15%)
18	CLA	1	611	-	45,53,73	1.80	5 (11%)	52,89,113	1.57	6 (11%)
18	CLA	L	302	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	7 (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
18	CLA	A	831	-	1/1/15/20	11/37/115/115	-
18	CLA	3	609	-	1/1/13/20	7/23/101/115	-
20	LHG	1	615	18	-	34/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	610	-	1/1/10/20	2/10/88/115	-
18	CLA	A	829	-	1/1/15/20	15/37/115/115	-
18	CLA	2	608	-	1/1/11/20	7/13/91/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
18	CLA	B	832	-	1/1/15/20	15/37/115/115	-
18	CLA	B	836	-	1/1/12/20	5/19/97/115	-
18	CLA	B	841	20	1/1/15/20	22/37/115/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-
18	CLA	A	815	-	1/1/11/20	6/13/91/115	-
18	CLA	1	609	-	1/1/10/20	4/9/87/115	-
23	LMG	4	620	-	-	7/28/48/70	0/1/1/1
18	CLA	A	814	-	1/1/15/20	10/37/115/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
19	XAT	2	617	-	-	16/31/93/93	0/4/4/4
17	CHL	2	607	-	3/3/17/26	5/21/119/137	-
18	CLA	3	607	-	1/1/11/20	4/13/91/115	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	B	830	-	1/1/10/20	2/11/89/115	-
18	CLA	4	611	-	1/1/10/20	4/8/86/115	-
18	CLA	A	832	-	1/1/12/20	5/19/97/115	-
18	CLA	3	602	-	1/1/13/20	9/25/103/115	-
18	CLA	B	815	-	1/1/10/20	2/11/89/115	-
18	CLA	B	840	-	1/1/15/20	17/37/115/115	-
18	CLA	J	101	-	1/1/12/20	7/21/99/115	-
18	CLA	A	820	-	1/1/15/20	14/37/115/115	-
17	CHL	1	606	-	3/3/15/26	0/8/106/137	-
17	CHL	1	601	1	3/3/17/26	10/22/120/137	-
18	CLA	K	204	-	1/1/11/20	10/15/93/115	-
18	CLA	K	203	-	1/1/11/20	6/13/91/115	-
22	BCR	L	306	-	-	5/29/63/63	0/2/2/2
18	CLA	2	612	2	1/1/15/20	17/37/115/115	-
18	CLA	A	826	-	1/1/15/20	9/37/115/115	-
18	CLA	G	202	-	1/1/10/20	3/10/88/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	843	-	1/1/15/20	11/37/115/115	-
18	CLA	B	823	-	1/1/11/20	6/13/91/115	-
18	CLA	B	819	-	1/1/13/20	9/25/103/115	-
18	CLA	A	833	-	1/1/13/20	7/27/105/115	-
22	BCR	K	205	-	-	9/29/63/63	0/2/2/2
18	CLA	B	838	-	1/1/11/20	1/16/94/115	-
22	BCR	B	801	-	-	3/29/63/63	0/2/2/2
18	CLA	A	837	5	1/1/11/20	3/13/91/115	-
25	PQN	B	842	-	-	6/23/43/43	0/2/2/2
27	DGD	B	850	-	-	11/55/95/95	0/2/2/2
18	CLA	2	611	-	1/1/11/20	5/11/89/115	-
18	CLA	B	805	-	1/1/15/20	16/37/115/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	A	827	-	1/1/13/20	3/30/108/115	-
19	XAT	1	614	-	-	8/31/93/93	0/4/4/4
18	CLA	A	804	-	1/1/15/20	19/37/115/115	-
18	CLA	A	842	-	1/1/15/20	17/37/115/115	-
18	CLA	A	819	-	1/1/13/20	14/30/108/115	-
18	CLA	A	838	-	1/1/12/20	4/21/99/115	-
18	CLA	4	603	-	1/1/11/20	6/13/89/115	-
18	CLA	F	303	10	1/1/10/20	0/8/86/115	-
18	CLA	K	206	15	1/1/9/20	0/6/80/115	-
18	CLA	B	803	-	1/1/15/20	10/37/115/115	-
18	CLA	A	805	-	1/1/12/20	5/22/100/115	-
18	CLA	B	806	6	1/1/15/20	12/37/115/115	-
18	CLA	4	612	-	1/1/13/20	13/28/106/115	-
18	CLA	A	824	-	1/1/10/20	2/8/86/115	-
18	CLA	B	837	-	1/1/15/20	13/37/115/115	-
18	CLA	A	806	-	1/1/15/20	20/37/115/115	-
18	CLA	A	836	-	1/1/11/20	6/13/91/115	-
18	CLA	1	605	-	1/1/11/20	8/15/93/115	-
17	CHL	2	601	2	3/3/16/26	7/17/115/137	-
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
26	SF4	C	101	-	-	-	0/6/5/5
18	CLA	1	613	-	1/1/10/20	0/4/80/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	844	-	1/1/15/20	10/37/115/115	-
18	CLA	B	835	-	1/1/10/20	4/10/88/115	-
18	CLA	3	610	-	1/1/10/20	1/6/84/115	-
18	CLA	1	607	-	1/1/11/20	6/11/89/115	-
21	LUT	1	616	-	-	1/29/67/67	0/2/2/2
18	CLA	F	302	-	1/1/12/20	5/21/99/115	-
18	CLA	A	841	-	1/1/15/20	14/37/115/115	-
18	CLA	B	824	-	1/1/15/20	14/37/115/115	-
22	BCR	A	849	-	-	6/29/63/63	0/2/2/2
17	CHL	2	615	2	3/3/15/26	2/12/110/137	-
25	PQN	A	855	-	-	1/23/43/43	0/2/2/2
18	CLA	B	834	-	1/1/14/20	7/31/109/115	-
17	CHL	2	606	-	3/3/15/26	2/12/110/137	-
18	CLA	A	830	-	1/1/15/20	13/37/115/115	-
18	CLA	A	813	-	1/1/12/20	9/24/102/115	-
18	CLA	4	604	-	1/1/11/20	6/11/87/115	-
18	CLA	B	812	-	1/1/10/20	1/11/89/115	-
18	CLA	A	834	-	1/1/15/20	7/37/115/115	-
18	CLA	4	608	4	1/1/11/20	4/13/91/115	-
18	CLA	A	840	-	1/1/12/20	6/22/100/115	-
20	LHG	2	618	18	-	11/41/41/53	-
18	CLA	1	608	1	1/1/10/20	2/8/84/115	-
20	LHG	A	847	18	-	2/34/34/53	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	B	822	-	1/1/15/20	16/37/115/115	-
22	BCR	A	853	-	-	3/29/63/63	0/2/2/2
18	CLA	B	818	-	1/1/14/20	7/31/109/115	-
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	B	813	-	1/1/15/20	15/37/115/115	-
18	CLA	B	828	-	1/1/15/20	19/37/115/115	-
18	CLA	A	802	-	1/1/15/20	17/37/115/115	-
18	CLA	A	818	-	1/1/14/20	13/31/109/115	-
18	CLA	B	816	-	1/1/13/20	6/25/103/115	-
26	SF4	A	854	-	-	-	0/6/5/5
18	CLA	G	203	11	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	802	-	1/1/15/20	15/37/115/115	-
18	CLA	3	612	-	1/1/10/20	0/6/84/115	-
18	CLA	B	829	-	1/1/13/20	4/27/105/115	-
18	CLA	K	201	15	1/1/8/20	0/2/76/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	BCR	A	848	-	-	0/29/63/63	0/2/2/2
18	CLA	B	817	-	1/1/13/20	9/30/108/115	-
20	LHG	A	846	-	-	5/53/53/53	-
18	CLA	A	822	-	1/1/15/20	13/37/115/115	-
18	CLA	2	610	20	1/1/7/20	5/10/70/115	-
18	CLA	H	201	-	1/1/14/20	15/31/109/115	-
18	CLA	1	610	20	1/1/10/20	1/4/80/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	BCR	4	618	-	-	6/29/63/63	0/2/2/2
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
20	LHG	B	852	-	-	14/53/53/53	-
18	CLA	3	604	-	1/1/10/20	0/8/86/115	-
18	CLA	4	602	4	1/1/14/20	6/31/109/115	-
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
23	LMG	4	619	-	-	5/34/54/70	0/1/1/1
18	CLA	A	812	-	1/1/15/20	17/37/115/115	-
18	CLA	A	807	-	1/1/15/20	13/37/115/115	-
18	CLA	4	609	-	1/1/12/20	6/24/102/115	-
18	CLA	A	835	-	1/1/15/20	16/37/115/115	-
18	CLA	1	604	-	1/1/11/20	7/18/96/115	-
18	CLA	3	605	-	1/1/10/20	6/10/86/115	-
18	CLA	B	809	6	1/1/15/20	18/37/115/115	-
18	CLA	2	603	-	1/1/11/20	3/11/89/115	-
18	CLA	A	828	-	1/1/15/20	8/37/115/115	-
18	CLA	B	831	-	1/1/10/20	0/11/89/115	-
18	CLA	3	611	-	1/1/8/20	0/0/74/115	-
18	CLA	1	612	-	1/1/11/20	4/15/93/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	A	821	-	1/1/11/20	1/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CHL	3	606	-	3/3/16/26	5/13/111/137	-
18	CLA	A	845	20	1/1/12/20	6/19/97/115	-
18	CLA	A	810	5	1/1/12/20	3/19/97/115	-
18	CLA	A	811	-	1/1/15/20	10/37/115/115	-
18	CLA	B	814	-	1/1/15/20	15/37/115/115	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
22	BCR	G	204	-	-	2/29/63/63	0/2/2/2
18	CLA	4	614	-	1/1/12/20	8/19/97/115	-
18	CLA	F	301	-	1/1/13/20	14/28/106/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
18	CLA	B	807	-	1/1/12/20	5/22/100/115	-
17	CHL	4	605	-	3/3/15/26	2/8/106/137	-
18	CLA	A	839	-	1/1/13/20	11/25/103/115	-
18	CLA	4	601	4	1/1/11/20	5/15/93/115	-
18	CLA	4	613	-	1/1/11/20	4/13/91/115	-
18	CLA	L	304	-	1/1/11/20	1/13/91/115	-
17	CHL	4	615	4	3/3/15/26	0/10/106/137	-
17	CHL	4	607	-	3/3/16/26	4/15/113/137	-
18	CLA	2	602	2	1/1/15/20	16/37/115/115	-
18	CLA	B	839	-	1/1/15/20	8/37/115/115	-
18	CLA	1	602	1	1/1/12/20	6/24/102/115	-
18	CLA	B	821	-	1/1/11/20	3/16/94/115	-
18	CLA	B	810	-	1/1/15/20	11/37/115/115	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
26	SF4	C	102	-	-	-	0/6/5/5
18	CLA	3	601	-	1/1/14/20	13/31/109/115	-
18	CLA	L	303	-	1/1/15/20	11/37/115/115	-
18	CLA	2	609	-	1/1/11/20	9/16/94/115	-
18	CLA	A	809	-	1/1/15/20	14/37/115/115	-
18	CLA	A	803	-	1/1/15/20	19/37/115/115	-
18	CLA	2	613	-	1/1/10/20	4/11/89/115	-
18	CLA	A	817	-	1/1/11/20	3/13/91/115	-
22	BCR	A	852	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	820	-	1/1/12/20	5/19/97/115	-
18	CLA	A	816	-	1/1/10/20	2/10/88/115	-
18	CLA	A	823	-	1/1/10/20	4/10/88/115	-
24	CL0	A	801	-	2/2/16/25	8/33/115/135	-
18	CLA	B	826	-	1/1/14/20	6/34/112/115	-
18	CLA	B	811	-	1/1/13/20	11/25/101/115	-
18	CLA	3	603	-	1/1/11/20	8/13/91/115	-
18	CLA	B	825	-	1/1/14/20	10/34/112/115	-
18	CLA	2	604	-	1/1/10/20	6/9/88/115	-
18	CLA	B	833	-	1/1/11/20	4/13/91/115	-
18	CLA	3	608	-	1/1/10/20	3/8/86/115	-
17	CHL	4	606	-	3/3/15/26	2/10/106/137	-
21	LUT	2	616	-	-	4/29/67/67	0/2/2/2
18	CLA	1	603	-	1/1/12/20	8/24/102/115	-
18	CLA	B	808	-	1/1/15/20	16/37/115/115	-
18	CLA	B	827	-	1/1/15/20	20/37/115/115	-
18	CLA	B	804	-	1/1/10/20	2/8/86/115	-
18	CLA	G	201	-	1/1/11/20	7/13/91/115	-
20	LHG	B	851	18	-	5/42/42/53	-
18	CLA	A	825	-	1/1/13/20	7/25/103/115	-
18	CLA	A	808	-	1/1/12/20	2/19/97/115	-
18	CLA	1	611	-	1/1/11/20	4/13/91/115	-
18	CLA	L	302	-	1/1/11/20	1/13/91/115	-

All (1220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	610	CLA	C1A-NA	12.67	1.40	1.29
24	A	801	CL0	C1D-ND	8.48	1.48	1.37
18	B	812	CLA	C4B-NB	7.96	1.42	1.35
18	B	805	CLA	C4B-NB	7.83	1.42	1.35
18	B	838	CLA	C4B-NB	7.78	1.42	1.35
18	A	821	CLA	C4B-NB	7.77	1.42	1.35
18	A	814	CLA	C4B-NB	7.70	1.42	1.35
18	3	607	CLA	C4B-NB	7.70	1.42	1.35
18	3	611	CLA	C4B-NB	7.68	1.42	1.35
18	A	836	CLA	C4B-NB	7.68	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	828	CLA	C4B-NB	7.66	1.42	1.35
18	J	101	CLA	C4B-NB	7.66	1.42	1.35
18	B	802	CLA	C4B-NB	7.63	1.42	1.35
18	A	807	CLA	C4B-NB	7.63	1.42	1.35
18	B	832	CLA	C4B-NB	7.62	1.42	1.35
18	F	301	CLA	C4B-NB	7.62	1.42	1.35
18	A	817	CLA	C4B-NB	7.62	1.42	1.35
18	A	837	CLA	C4B-NB	7.61	1.42	1.35
18	4	611	CLA	C4B-NB	7.60	1.42	1.35
18	B	835	CLA	C4B-NB	7.60	1.42	1.35
18	A	819	CLA	C4B-NB	7.60	1.42	1.35
18	A	845	CLA	C4B-NB	7.60	1.42	1.35
18	1	607	CLA	C4B-NB	7.59	1.42	1.35
18	1	605	CLA	C4B-NB	7.57	1.42	1.35
18	L	302	CLA	C4B-NB	7.57	1.42	1.35
18	B	836	CLA	C4B-NB	7.57	1.42	1.35
18	F	303	CLA	C4B-NB	7.57	1.42	1.35
18	1	604	CLA	C4B-NB	7.56	1.42	1.35
18	3	610	CLA	C4B-NB	7.56	1.42	1.35
18	A	838	CLA	C4B-NB	7.56	1.42	1.35
18	3	605	CLA	C4B-NB	7.55	1.41	1.35
18	B	823	CLA	C4B-NB	7.54	1.41	1.35
18	K	201	CLA	C4B-NB	7.54	1.41	1.35
18	A	812	CLA	C4B-NB	7.54	1.41	1.35
18	4	610	CLA	C4B-NB	7.53	1.41	1.35
18	F	302	CLA	C4B-NB	7.53	1.41	1.35
18	G	201	CLA	C4B-NB	7.53	1.41	1.35
18	B	819	CLA	C4B-NB	7.53	1.41	1.35
18	3	602	CLA	C4B-NB	7.52	1.41	1.35
18	B	810	CLA	C4B-NB	7.52	1.41	1.35
18	3	604	CLA	C4B-NB	7.52	1.41	1.35
18	A	828	CLA	C4B-NB	7.52	1.41	1.35
18	2	613	CLA	C4B-NB	7.51	1.41	1.35
18	K	204	CLA	C4B-NB	7.51	1.41	1.35
18	4	601	CLA	C4B-NB	7.51	1.41	1.35
18	1	611	CLA	C4B-NB	7.51	1.41	1.35
18	A	841	CLA	C4B-NB	7.51	1.41	1.35
18	A	840	CLA	C4B-NB	7.50	1.41	1.35
18	3	609	CLA	C4B-NB	7.50	1.41	1.35
18	4	614	CLA	C4B-NB	7.50	1.41	1.35
18	A	834	CLA	C4B-NB	7.49	1.41	1.35
18	B	840	CLA	C4B-NB	7.49	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	808	CLA	C4B-NB	7.49	1.41	1.35
18	G	202	CLA	C4B-NB	7.49	1.41	1.35
18	B	834	CLA	C4B-NB	7.49	1.41	1.35
18	B	829	CLA	C4B-NB	7.48	1.41	1.35
18	2	611	CLA	C4B-NB	7.48	1.41	1.35
18	4	603	CLA	C4B-NB	7.48	1.41	1.35
18	B	811	CLA	C4B-NB	7.48	1.41	1.35
18	1	603	CLA	C4B-NB	7.47	1.41	1.35
18	B	826	CLA	C4B-NB	7.47	1.41	1.35
18	A	827	CLA	C4B-NB	7.47	1.41	1.35
18	B	827	CLA	C4B-NB	7.47	1.41	1.35
18	1	610	CLA	C4B-NB	7.46	1.41	1.35
18	K	206	CLA	C4B-NB	7.46	1.41	1.35
18	2	610	CLA	C4B-NB	7.46	1.41	1.35
18	B	815	CLA	C4B-NB	7.45	1.41	1.35
18	A	822	CLA	C4B-NB	7.45	1.41	1.35
18	1	612	CLA	C4B-NB	7.44	1.41	1.35
18	B	839	CLA	C4B-NB	7.44	1.41	1.35
18	A	816	CLA	C4B-NB	7.44	1.41	1.35
18	B	818	CLA	C4B-NB	7.44	1.41	1.35
18	B	817	CLA	C4B-NB	7.44	1.41	1.35
18	4	604	CLA	C4B-NB	7.43	1.41	1.35
18	A	825	CLA	C4B-NB	7.43	1.41	1.35
18	3	603	CLA	C4B-NB	7.43	1.41	1.35
18	A	813	CLA	C4B-NB	7.43	1.41	1.35
18	A	824	CLA	C4B-NB	7.43	1.41	1.35
18	A	820	CLA	C4B-NB	7.42	1.41	1.35
18	1	608	CLA	C4B-NB	7.42	1.41	1.35
18	1	613	CLA	C4B-NB	7.42	1.41	1.35
18	B	813	CLA	C4B-NB	7.41	1.41	1.35
18	L	303	CLA	C4B-NB	7.41	1.41	1.35
18	1	609	CLA	C4B-NB	7.41	1.41	1.35
18	A	810	CLA	C4B-NB	7.41	1.41	1.35
18	A	803	CLA	C4B-NB	7.41	1.41	1.35
18	B	830	CLA	C4B-NB	7.40	1.41	1.35
18	B	807	CLA	C4B-NB	7.40	1.41	1.35
18	A	843	CLA	C4B-NB	7.40	1.41	1.35
18	A	844	CLA	C4B-NB	7.40	1.41	1.35
18	L	304	CLA	C4B-NB	7.39	1.41	1.35
18	G	203	CLA	C4B-NB	7.39	1.41	1.35
18	K	203	CLA	C4B-NB	7.39	1.41	1.35
18	4	602	CLA	C4B-NB	7.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	831	CLA	C4B-NB	7.38	1.41	1.35
18	B	837	CLA	C4B-NB	7.38	1.41	1.35
18	4	608	CLA	C4B-NB	7.38	1.41	1.35
18	A	802	CLA	C4B-NB	7.38	1.41	1.35
18	A	805	CLA	C4B-NB	7.38	1.41	1.35
18	B	803	CLA	C4B-NB	7.37	1.41	1.35
18	1	602	CLA	C4B-NB	7.36	1.41	1.35
18	B	831	CLA	C4B-NB	7.36	1.41	1.35
18	B	825	CLA	C4B-NB	7.36	1.41	1.35
18	B	804	CLA	C4B-NB	7.36	1.41	1.35
18	B	820	CLA	C4B-NB	7.36	1.41	1.35
18	B	841	CLA	C4B-NB	7.36	1.41	1.35
18	2	603	CLA	C4B-NB	7.35	1.41	1.35
18	4	613	CLA	C4B-NB	7.35	1.41	1.35
18	A	826	CLA	C4B-NB	7.34	1.41	1.35
18	B	814	CLA	C4B-NB	7.34	1.41	1.35
18	B	822	CLA	C4B-NB	7.34	1.41	1.35
18	A	842	CLA	C4B-NB	7.34	1.41	1.35
18	H	201	CLA	C4B-NB	7.34	1.41	1.35
18	A	823	CLA	C4B-NB	7.34	1.41	1.35
18	3	601	CLA	C4B-NB	7.33	1.41	1.35
18	A	804	CLA	C4B-NB	7.32	1.41	1.35
18	A	833	CLA	C4B-NB	7.32	1.41	1.35
18	2	602	CLA	C4B-NB	7.32	1.41	1.35
18	A	832	CLA	C4B-NB	7.31	1.41	1.35
18	A	806	CLA	C4B-NB	7.31	1.41	1.35
18	A	830	CLA	C4B-NB	7.30	1.41	1.35
18	B	824	CLA	C4B-NB	7.30	1.41	1.35
18	B	806	CLA	C4B-NB	7.30	1.41	1.35
18	B	821	CLA	C4B-NB	7.30	1.41	1.35
18	B	808	CLA	C4B-NB	7.29	1.41	1.35
18	B	816	CLA	C4B-NB	7.29	1.41	1.35
18	A	839	CLA	C4B-NB	7.28	1.41	1.35
18	A	818	CLA	C4B-NB	7.27	1.41	1.35
18	4	612	CLA	C4B-NB	7.27	1.41	1.35
18	A	835	CLA	C4B-NB	7.27	1.41	1.35
18	B	833	CLA	C4B-NB	7.27	1.41	1.35
18	B	809	CLA	C4B-NB	7.26	1.41	1.35
18	2	604	CLA	C4B-NB	7.24	1.41	1.35
18	3	612	CLA	C4B-NB	7.23	1.41	1.35
18	2	608	CLA	C4B-NB	7.23	1.41	1.35
18	4	609	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	829	CLA	C4B-NB	7.22	1.41	1.35
18	2	612	CLA	C4B-NB	7.21	1.41	1.35
18	A	809	CLA	C4B-NB	7.20	1.41	1.35
18	A	815	CLA	C4B-NB	7.20	1.41	1.35
18	3	608	CLA	C4B-NB	7.17	1.41	1.35
18	A	811	CLA	C4B-NB	7.16	1.41	1.35
18	2	609	CLA	C4B-NB	7.13	1.41	1.35
24	A	801	CL0	C3D-C4D	-6.44	1.34	1.46
18	2	610	CLA	CHB-C4A	5.36	1.38	1.34
17	1	606	CHL	C3B-C2B	5.32	1.47	1.40
17	1	606	CHL	CHC-C1C	5.28	1.48	1.35
17	2	606	CHL	O2D-CGD	5.18	1.45	1.33
17	4	606	CHL	O2D-CGD	5.17	1.45	1.33
17	2	605	CHL	O2D-CGD	5.15	1.45	1.33
17	4	607	CHL	O2D-CGD	5.15	1.45	1.33
17	2	615	CHL	O2D-CGD	5.14	1.45	1.33
17	2	607	CHL	O2D-CGD	5.11	1.45	1.33
17	2	605	CHL	CHC-C1C	5.11	1.48	1.35
17	2	615	CHL	CHC-C1C	5.11	1.48	1.35
17	1	601	CHL	CHC-C1C	5.10	1.48	1.35
17	2	607	CHL	CHC-C1C	5.10	1.48	1.35
22	A	853	BCR	C10-C9	5.10	1.42	1.35
17	2	601	CHL	O2D-CGD	5.08	1.45	1.33
17	2	601	CHL	CHC-C1C	5.07	1.48	1.35
17	2	606	CHL	CHC-C1C	5.07	1.48	1.35
17	3	606	CHL	O2D-CGD	5.06	1.45	1.33
22	B	801	BCR	C10-C9	5.05	1.42	1.35
22	F	304	BCR	C21-C22	5.02	1.42	1.35
17	4	605	CHL	CHC-C1C	5.01	1.47	1.35
22	F	304	BCR	C17-C18	5.00	1.42	1.35
17	2	615	CHL	C3B-C2B	5.00	1.47	1.40
22	B	845	BCR	C21-C22	4.99	1.42	1.35
17	4	606	CHL	CHC-C1C	4.98	1.47	1.35
17	2	606	CHL	C3B-C2B	4.97	1.47	1.40
17	4	607	CHL	CHC-C1C	4.96	1.47	1.35
17	2	601	CHL	C3B-C2B	4.96	1.47	1.40
17	4	615	CHL	CHC-C1C	4.95	1.47	1.35
17	2	605	CHL	C3B-C2B	4.93	1.47	1.40
17	1	606	CHL	CHD-C1D	4.92	1.47	1.38
17	1	606	CHL	C2C-C3C	4.91	1.47	1.36
17	1	601	CHL	C3B-C2B	4.91	1.47	1.40
22	A	850	BCR	C14-C13	4.89	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	613	LUT	C10-C9	4.87	1.42	1.35
17	3	606	CHL	CHC-C1C	4.84	1.47	1.35
22	A	851	BCR	C14-C13	4.84	1.42	1.35
17	3	606	CHL	C3B-C2B	4.81	1.47	1.40
17	4	605	CHL	C3B-C2B	4.81	1.47	1.40
22	A	851	BCR	C21-C22	4.81	1.42	1.35
21	1	616	LUT	C30-C29	4.79	1.42	1.35
22	A	849	BCR	C21-C22	4.73	1.42	1.35
17	1	601	CHL	C2C-C3C	4.73	1.46	1.36
17	2	615	CHL	C2C-C3C	4.73	1.46	1.36
17	2	606	CHL	C2C-C3C	4.72	1.46	1.36
19	2	617	XAT	C34-C33	4.71	1.42	1.35
22	A	850	BCR	C17-C18	4.71	1.42	1.35
17	1	606	CHL	C3D-C4D	-4.70	1.33	1.44
17	2	601	CHL	C2C-C3C	4.70	1.46	1.36
17	2	605	CHL	C2C-C3C	4.70	1.46	1.37
17	4	605	CHL	C3D-C4D	-4.69	1.33	1.44
19	2	617	XAT	C14-C13	4.69	1.42	1.35
22	A	851	BCR	C17-C18	4.68	1.42	1.35
17	2	601	CHL	C3D-C4D	-4.67	1.33	1.44
17	2	607	CHL	C3D-C4D	-4.67	1.33	1.44
17	1	601	CHL	C3D-C4D	-4.66	1.33	1.44
17	4	607	CHL	C3D-C4D	-4.66	1.33	1.44
17	4	605	CHL	C2C-C3C	4.66	1.46	1.37
17	4	615	CHL	O2D-CGD	4.66	1.45	1.30
17	4	606	CHL	C3C-C2C	4.66	1.46	1.36
17	1	606	CHL	O2D-CGD	4.65	1.45	1.30
17	4	605	CHL	O2D-CGD	4.65	1.45	1.30
17	2	615	CHL	CHD-C1D	4.65	1.47	1.38
17	3	606	CHL	C3D-C4D	-4.64	1.33	1.44
17	2	606	CHL	CHD-C1D	4.64	1.47	1.38
17	1	601	CHL	CHD-C1D	4.64	1.47	1.38
17	2	606	CHL	C3D-C4D	-4.63	1.33	1.44
17	1	601	CHL	O2D-CGD	4.62	1.45	1.30
17	4	615	CHL	C2C-C3C	4.62	1.46	1.36
17	2	605	CHL	C3D-C4D	-4.62	1.33	1.44
17	2	607	CHL	C3B-C2B	4.61	1.46	1.40
17	4	615	CHL	C3D-C4D	-4.61	1.33	1.44
17	2	607	CHL	C2C-C3C	4.60	1.46	1.36
22	A	849	BCR	C17-C18	4.60	1.41	1.35
17	2	615	CHL	C3D-C4D	-4.59	1.33	1.44
17	4	607	CHL	C3B-C2B	4.58	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	843	BCR	C14-C13	4.56	1.41	1.35
17	2	601	CHL	CHD-C1D	4.55	1.47	1.38
17	4	606	CHL	C3D-C4D	-4.54	1.33	1.44
21	3	613	LUT	C34-C33	4.53	1.41	1.35
17	3	606	CHL	O2A-CGA	4.53	1.46	1.30
17	4	605	CHL	CHD-C1D	4.52	1.47	1.38
21	2	616	LUT	C34-C33	4.49	1.41	1.35
17	2	607	CHL	CHD-C1D	4.49	1.47	1.38
17	2	605	CHL	CHD-C1D	4.49	1.47	1.38
17	4	607	CHL	C2C-C3C	4.48	1.46	1.36
17	4	607	CHL	O2A-CGA	4.48	1.45	1.30
17	4	615	CHL	CHD-C1D	4.44	1.47	1.38
22	A	851	BCR	C10-C9	4.44	1.41	1.35
17	3	606	CHL	C3C-C2C	4.44	1.46	1.36
17	4	606	CHL	CHD-C1D	4.43	1.47	1.38
17	3	606	CHL	CHD-C1D	4.41	1.47	1.38
17	1	606	CHL	CHD-C4C	4.38	1.49	1.39
22	B	845	BCR	C17-C18	4.36	1.41	1.35
17	4	607	CHL	CHD-C1D	4.33	1.46	1.38
22	B	844	BCR	C21-C22	4.32	1.41	1.35
17	2	607	CHL	O2A-CGA	4.32	1.46	1.33
22	F	304	BCR	C14-C13	4.29	1.41	1.35
22	B	843	BCR	C17-C18	4.27	1.41	1.35
22	F	304	BCR	C10-C9	4.26	1.41	1.35
22	K	205	BCR	C21-C22	4.26	1.41	1.35
22	L	301	BCR	C17-C18	4.26	1.41	1.35
17	1	601	CHL	O2A-CGA	4.24	1.45	1.33
22	L	301	BCR	C21-C22	4.24	1.41	1.35
19	4	617	XAT	C34-C33	4.23	1.41	1.35
22	L	306	BCR	C17-C18	4.23	1.41	1.35
22	B	849	BCR	C14-C13	4.22	1.41	1.35
20	1	615	LHG	O8-C23	4.22	1.45	1.33
22	B	843	BCR	C21-C22	4.22	1.41	1.35
22	J	102	BCR	C10-C9	4.22	1.41	1.35
22	A	849	BCR	C14-C13	4.21	1.41	1.35
21	1	616	LUT	C34-C33	4.21	1.41	1.35
24	A	801	CL0	C3D-C2D	4.21	1.45	1.37
22	L	306	BCR	C10-C9	4.21	1.41	1.35
27	B	850	DGD	O1G-C1A	4.20	1.45	1.33
22	L	306	BCR	C21-C22	4.20	1.41	1.35
19	4	617	XAT	C10-C9	4.20	1.41	1.35
22	K	202	BCR	C10-C9	4.20	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	843	BCR	C10-C9	4.19	1.41	1.35
21	2	616	LUT	C14-C13	4.19	1.41	1.35
19	2	617	XAT	C30-C29	4.19	1.41	1.35
22	L	301	BCR	C14-C13	4.19	1.41	1.35
24	A	801	CL0	O2A-CGA	4.19	1.45	1.33
21	1	616	LUT	C14-C13	4.18	1.41	1.35
19	2	617	XAT	C10-C9	4.18	1.41	1.35
19	4	617	XAT	C30-C29	4.18	1.41	1.35
22	K	205	BCR	C10-C9	4.18	1.41	1.35
22	J	102	BCR	C14-C13	4.18	1.41	1.35
17	2	606	CHL	CHD-C4C	4.18	1.48	1.39
22	B	801	BCR	C14-C13	4.17	1.41	1.35
22	B	846	BCR	C21-C22	4.17	1.41	1.35
22	A	850	BCR	C10-C9	4.16	1.41	1.35
17	2	615	CHL	CHD-C4C	4.16	1.48	1.39
19	4	617	XAT	C14-C13	4.16	1.41	1.35
22	J	102	BCR	C17-C18	4.15	1.41	1.35
22	B	849	BCR	C17-C18	4.15	1.41	1.35
22	B	801	BCR	C17-C18	4.15	1.41	1.35
22	L	306	BCR	C14-C13	4.15	1.41	1.35
22	B	844	BCR	C10-C9	4.15	1.41	1.35
22	J	102	BCR	C21-C22	4.15	1.41	1.35
22	L	305	BCR	C14-C13	4.15	1.41	1.35
22	L	305	BCR	C17-C18	4.14	1.41	1.35
22	A	853	BCR	C21-C22	4.13	1.41	1.35
20	1	615	LHG	O7-C7	4.13	1.46	1.34
22	G	204	BCR	C21-C22	4.13	1.41	1.35
17	4	605	CHL	CHD-C4C	4.13	1.48	1.39
17	2	601	CHL	CHD-C4C	4.13	1.48	1.39
22	L	301	BCR	C10-C9	4.12	1.41	1.35
22	A	853	BCR	C14-C13	4.12	1.41	1.35
17	2	605	CHL	CHD-C4C	4.12	1.48	1.39
22	4	618	BCR	C17-C18	4.12	1.41	1.35
22	B	846	BCR	C14-C13	4.12	1.41	1.35
22	L	305	BCR	C21-C22	4.12	1.41	1.35
22	B	846	BCR	C10-C9	4.11	1.41	1.35
22	L	305	BCR	C10-C9	4.11	1.41	1.35
21	1	616	LUT	C10-C9	4.11	1.41	1.35
24	A	801	CL0	C3C-C2C	4.11	1.45	1.36
22	B	801	BCR	C21-C22	4.10	1.41	1.35
22	A	849	BCR	C10-C9	4.10	1.41	1.35
22	B	847	BCR	C14-C13	4.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	202	BCR	C14-C13	4.10	1.41	1.35
22	A	853	BCR	C17-C18	4.10	1.41	1.35
22	A	852	BCR	C21-C22	4.10	1.41	1.35
27	B	850	DGD	O2G-C1B	4.09	1.45	1.34
22	B	849	BCR	C10-C9	4.09	1.41	1.35
17	1	601	CHL	CHD-C4C	4.09	1.48	1.39
22	A	852	BCR	C10-C9	4.09	1.41	1.35
22	A	852	BCR	C14-C13	4.09	1.41	1.35
22	4	618	BCR	C14-C13	4.09	1.41	1.35
22	B	846	BCR	C17-C18	4.09	1.41	1.35
17	2	607	CHL	CHD-C4C	4.08	1.48	1.39
22	K	202	BCR	C17-C18	4.08	1.41	1.35
22	K	205	BCR	C14-C13	4.08	1.41	1.35
22	A	852	BCR	C17-C18	4.08	1.41	1.35
22	K	202	BCR	C21-C22	4.08	1.41	1.35
22	A	848	BCR	C21-C22	4.07	1.41	1.35
22	B	844	BCR	C14-C13	4.07	1.41	1.35
21	2	619	LUT	C30-C29	4.07	1.41	1.35
22	3	614	BCR	C17-C18	4.07	1.41	1.35
21	2	619	LUT	C34-C33	4.06	1.41	1.35
22	4	618	BCR	C21-C22	4.06	1.41	1.35
17	3	606	CHL	CHD-C4C	4.06	1.48	1.39
22	3	614	BCR	C10-C9	4.05	1.41	1.35
21	2	619	LUT	C14-C13	4.05	1.41	1.35
22	B	847	BCR	C10-C9	4.05	1.41	1.35
22	B	845	BCR	C10-C9	4.05	1.41	1.35
22	G	204	BCR	C17-C18	4.04	1.41	1.35
21	2	619	LUT	C10-C9	4.04	1.41	1.35
22	B	849	BCR	C21-C22	4.04	1.41	1.35
22	B	844	BCR	C17-C18	4.04	1.41	1.35
22	4	618	BCR	C10-C9	4.04	1.41	1.35
22	K	205	BCR	C17-C18	4.03	1.41	1.35
22	B	847	BCR	C17-C18	4.03	1.41	1.35
22	3	614	BCR	C14-C13	4.03	1.41	1.35
17	4	615	CHL	CHD-C4C	4.02	1.48	1.39
21	4	616	LUT	C34-C33	4.01	1.41	1.35
17	2	601	CHL	O2A-CGA	4.01	1.45	1.33
22	A	848	BCR	C10-C9	4.01	1.41	1.35
18	L	304	CLA	C1D-ND	4.01	1.42	1.37
17	4	606	CHL	CHD-C4C	4.00	1.48	1.39
22	I	101	BCR	C17-C18	4.00	1.41	1.35
22	I	101	BCR	C10-C9	4.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	616	LUT	C30-C29	3.99	1.41	1.35
22	G	204	BCR	C10-C9	3.99	1.41	1.35
22	B	848	BCR	C10-C9	3.98	1.41	1.35
22	A	848	BCR	C17-C18	3.98	1.41	1.35
22	B	848	BCR	C17-C18	3.98	1.41	1.35
22	A	848	BCR	C14-C13	3.97	1.41	1.35
22	B	848	BCR	C14-C13	3.97	1.41	1.35
17	4	607	CHL	CHD-C4C	3.97	1.48	1.39
22	I	101	BCR	C14-C13	3.97	1.41	1.35
21	2	616	LUT	C10-C9	3.97	1.41	1.35
18	A	826	CLA	C1D-ND	3.95	1.42	1.37
22	G	204	BCR	C14-C13	3.95	1.41	1.35
21	4	616	LUT	C14-C13	3.95	1.41	1.35
21	3	613	LUT	C14-C13	3.95	1.41	1.35
18	F	303	CLA	C1D-ND	3.95	1.42	1.37
18	2	611	CLA	C1D-ND	3.94	1.42	1.37
18	3	609	CLA	C1D-ND	3.94	1.42	1.37
21	4	616	LUT	C10-C9	3.94	1.41	1.35
22	B	847	BCR	C21-C22	3.93	1.41	1.35
18	4	614	CLA	C1D-ND	3.93	1.42	1.37
18	A	836	CLA	C1D-ND	3.93	1.42	1.37
18	B	837	CLA	C1D-ND	3.93	1.42	1.37
18	B	834	CLA	C1D-ND	3.92	1.42	1.37
18	B	820	CLA	C1D-ND	3.91	1.42	1.37
18	A	816	CLA	C1D-ND	3.91	1.42	1.37
18	G	201	CLA	C1D-ND	3.91	1.42	1.37
18	A	820	CLA	C1D-ND	3.91	1.42	1.37
18	K	206	CLA	C1D-ND	3.91	1.42	1.37
18	1	611	CLA	C1D-ND	3.91	1.42	1.37
22	B	845	BCR	C14-C13	3.91	1.41	1.35
18	4	613	CLA	C1D-ND	3.91	1.42	1.37
18	4	611	CLA	C1D-ND	3.90	1.42	1.37
18	A	840	CLA	C1D-ND	3.90	1.42	1.37
18	A	817	CLA	C1D-ND	3.90	1.42	1.37
22	3	614	BCR	C21-C22	3.90	1.41	1.35
18	1	610	CLA	C1D-ND	3.90	1.42	1.37
18	1	613	CLA	C1D-ND	3.90	1.42	1.37
18	B	840	CLA	C1D-ND	3.90	1.42	1.37
18	K	201	CLA	C1D-ND	3.90	1.42	1.37
18	A	845	CLA	C1D-ND	3.90	1.42	1.37
18	3	611	CLA	C1D-ND	3.90	1.42	1.37
18	H	201	CLA	C1D-ND	3.90	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	604	CLA	C1D-ND	3.90	1.42	1.37
18	A	825	CLA	C1D-ND	3.90	1.42	1.37
18	A	813	CLA	C1D-ND	3.90	1.42	1.37
18	B	833	CLA	C1D-ND	3.90	1.42	1.37
18	A	804	CLA	C1D-ND	3.90	1.42	1.37
18	A	824	CLA	C1D-ND	3.90	1.42	1.37
18	3	603	CLA	C1D-ND	3.89	1.42	1.37
18	A	835	CLA	C1D-ND	3.89	1.42	1.37
18	1	607	CLA	C1D-ND	3.89	1.42	1.37
18	3	610	CLA	C1D-ND	3.89	1.42	1.37
18	2	602	CLA	C1D-ND	3.89	1.42	1.37
18	B	827	CLA	C1D-ND	3.89	1.42	1.37
18	G	202	CLA	C1D-ND	3.89	1.42	1.37
18	2	604	CLA	C1D-ND	3.88	1.42	1.37
18	3	601	CLA	C1D-ND	3.88	1.42	1.37
22	B	848	BCR	C21-C22	3.88	1.40	1.35
18	F	302	CLA	C1D-ND	3.88	1.42	1.37
18	A	832	CLA	C1D-ND	3.88	1.42	1.37
18	4	612	CLA	C1D-ND	3.88	1.42	1.37
18	2	612	CLA	C1D-ND	3.88	1.42	1.37
18	3	607	CLA	C1D-ND	3.88	1.42	1.37
24	A	801	CL0	C3B-C2B	3.88	1.45	1.40
18	2	613	CLA	C1D-ND	3.88	1.42	1.37
18	A	809	CLA	C1D-ND	3.88	1.42	1.37
18	2	603	CLA	C1D-ND	3.88	1.42	1.37
18	B	831	CLA	C1D-ND	3.87	1.42	1.37
18	A	821	CLA	C1D-ND	3.87	1.42	1.37
18	B	841	CLA	C1D-ND	3.87	1.42	1.37
18	A	806	CLA	C1D-ND	3.87	1.42	1.37
18	J	101	CLA	C1D-ND	3.87	1.42	1.37
22	A	850	BCR	C21-C22	3.87	1.40	1.35
18	A	823	CLA	C1D-ND	3.86	1.42	1.37
18	B	818	CLA	C1D-ND	3.86	1.42	1.37
18	1	612	CLA	C1D-ND	3.86	1.42	1.37
18	B	804	CLA	C1D-ND	3.86	1.42	1.37
18	3	602	CLA	C1D-ND	3.86	1.42	1.37
18	B	835	CLA	C1D-ND	3.86	1.42	1.37
18	A	808	CLA	C1D-ND	3.86	1.42	1.37
18	A	833	CLA	C1D-ND	3.86	1.42	1.37
18	B	830	CLA	C1D-ND	3.86	1.42	1.37
18	1	605	CLA	C1D-ND	3.86	1.42	1.37
18	A	837	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	101	BCR	C21-C22	3.86	1.40	1.35
18	B	824	CLA	C1D-ND	3.86	1.42	1.37
18	B	810	CLA	C1D-ND	3.85	1.42	1.37
18	A	839	CLA	C1D-ND	3.85	1.42	1.37
18	B	812	CLA	C1D-ND	3.85	1.42	1.37
18	1	604	CLA	C1D-ND	3.85	1.42	1.37
18	A	841	CLA	C1D-ND	3.85	1.42	1.37
18	B	819	CLA	C1D-ND	3.85	1.42	1.37
18	G	203	CLA	C1D-ND	3.85	1.42	1.37
18	4	604	CLA	C1D-ND	3.85	1.42	1.37
18	A	838	CLA	C1D-ND	3.84	1.42	1.37
21	3	613	LUT	C30-C29	3.84	1.40	1.35
18	F	301	CLA	C1D-ND	3.84	1.42	1.37
18	A	807	CLA	C1D-ND	3.84	1.42	1.37
18	A	828	CLA	C1D-ND	3.84	1.42	1.37
18	B	822	CLA	C1D-ND	3.84	1.42	1.37
18	K	203	CLA	C1D-ND	3.84	1.42	1.37
18	B	839	CLA	C1D-ND	3.84	1.42	1.37
18	A	834	CLA	C1D-ND	3.83	1.42	1.37
18	3	605	CLA	C1D-ND	3.83	1.42	1.37
18	A	810	CLA	C1D-ND	3.83	1.42	1.37
18	B	815	CLA	C1D-ND	3.83	1.42	1.37
18	A	819	CLA	C1D-ND	3.83	1.42	1.37
18	3	612	CLA	C1D-ND	3.82	1.42	1.37
18	B	817	CLA	C1D-ND	3.82	1.42	1.37
18	A	822	CLA	C1D-ND	3.82	1.42	1.37
18	A	811	CLA	C1D-ND	3.82	1.42	1.37
18	2	608	CLA	C1D-ND	3.82	1.42	1.37
18	L	303	CLA	C1D-ND	3.82	1.42	1.37
18	A	818	CLA	C1D-ND	3.82	1.42	1.37
18	A	843	CLA	C1D-ND	3.82	1.42	1.37
18	B	813	CLA	C1D-ND	3.82	1.42	1.37
18	A	812	CLA	C1D-ND	3.81	1.42	1.37
18	A	805	CLA	C1D-ND	3.81	1.42	1.37
18	B	809	CLA	C1D-ND	3.81	1.42	1.37
18	B	821	CLA	C1D-ND	3.81	1.42	1.37
18	B	811	CLA	C1D-ND	3.81	1.42	1.37
18	B	807	CLA	C1D-ND	3.81	1.42	1.37
18	B	805	CLA	C1D-ND	3.81	1.42	1.37
18	B	814	CLA	C1D-ND	3.81	1.42	1.37
18	A	827	CLA	C1D-ND	3.81	1.42	1.37
18	4	603	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	814	CLA	C1D-ND	3.80	1.42	1.37
18	A	844	CLA	C1D-ND	3.80	1.42	1.37
18	B	829	CLA	C1D-ND	3.80	1.42	1.37
18	2	610	CLA	C1D-ND	3.80	1.42	1.37
18	4	608	CLA	C1D-ND	3.80	1.42	1.37
18	4	610	CLA	C1D-ND	3.80	1.42	1.37
18	A	802	CLA	C1D-ND	3.79	1.42	1.37
21	2	616	LUT	C30-C29	3.79	1.40	1.35
18	A	831	CLA	C1D-ND	3.79	1.42	1.37
18	B	823	CLA	C1D-ND	3.79	1.42	1.37
18	A	815	CLA	C1D-ND	3.79	1.42	1.37
18	B	836	CLA	C1D-ND	3.78	1.42	1.37
18	B	816	CLA	C1D-ND	3.78	1.42	1.37
18	A	829	CLA	C1D-ND	3.78	1.42	1.37
18	B	838	CLA	C1D-ND	3.77	1.42	1.37
18	K	204	CLA	C1D-ND	3.77	1.42	1.37
18	1	602	CLA	C1D-ND	3.77	1.42	1.37
18	B	825	CLA	C1D-ND	3.77	1.42	1.37
18	4	602	CLA	C1D-ND	3.77	1.42	1.37
18	L	302	CLA	C1D-ND	3.77	1.42	1.37
18	1	603	CLA	C1D-ND	3.76	1.42	1.37
18	B	826	CLA	C1D-ND	3.76	1.42	1.37
18	B	802	CLA	C1D-ND	3.76	1.42	1.37
18	3	608	CLA	C1D-ND	3.76	1.42	1.37
18	A	842	CLA	C1D-ND	3.76	1.42	1.37
18	2	609	CLA	C1D-ND	3.76	1.42	1.37
18	B	806	CLA	C1D-ND	3.76	1.42	1.37
18	4	601	CLA	C1D-ND	3.75	1.42	1.37
18	4	609	CLA	C1D-ND	3.75	1.42	1.37
18	1	608	CLA	C1D-ND	3.75	1.42	1.37
18	A	830	CLA	C1D-ND	3.75	1.42	1.37
18	B	803	CLA	C1D-ND	3.75	1.42	1.37
18	A	803	CLA	C1D-ND	3.74	1.42	1.37
17	4	605	CHL	OBD-CAD	3.74	1.28	1.22
17	2	606	CHL	OBD-CAD	3.74	1.28	1.22
17	4	606	CHL	OBD-CAD	3.73	1.28	1.22
17	2	615	CHL	OBD-CAD	3.72	1.28	1.22
17	2	601	CHL	OBD-CAD	3.72	1.28	1.22
17	3	606	CHL	OBD-CAD	3.72	1.28	1.22
18	B	832	CLA	C1D-ND	3.71	1.42	1.37
17	4	615	CHL	OBD-CAD	3.70	1.28	1.22
17	1	606	CHL	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	601	CHL	OBD-CAD	3.69	1.28	1.22
17	2	605	CHL	OBD-CAD	3.69	1.28	1.22
24	A	801	CL0	CHC-C1C	3.68	1.44	1.35
17	4	607	CHL	OBD-CAD	3.66	1.28	1.22
18	B	828	CLA	C1D-ND	3.65	1.42	1.37
18	B	808	CLA	C1D-ND	3.64	1.42	1.37
17	2	607	CHL	OBD-CAD	3.64	1.28	1.22
18	1	610	CLA	CAB-C3B	-3.57	1.44	1.51
18	2	610	CLA	CAB-C3B	-3.56	1.44	1.51
18	1	608	CLA	CAB-C3B	-3.56	1.44	1.51
18	4	604	CLA	CAB-C3B	-3.53	1.44	1.51
18	4	603	CLA	CAB-C3B	-3.53	1.44	1.51
18	1	613	CLA	CAB-C3B	-3.52	1.44	1.51
18	1	609	CLA	C1D-ND	3.52	1.42	1.37
18	B	811	CLA	CAB-C3B	-3.51	1.44	1.51
18	3	605	CLA	CAB-C3B	-3.51	1.44	1.51
18	A	828	CLA	CHC-C1C	3.30	1.43	1.35
18	4	609	CLA	CHC-C1C	3.27	1.43	1.35
17	1	606	CHL	C3D-C2D	3.24	1.48	1.39
18	F	301	CLA	CHC-C1C	3.24	1.43	1.35
18	A	844	CLA	CHC-C1C	3.24	1.43	1.35
18	B	825	CLA	CHC-C1C	3.24	1.43	1.35
18	A	814	CLA	CHC-C1C	3.23	1.43	1.35
18	A	819	CLA	CHC-C1C	3.22	1.43	1.35
18	A	835	CLA	CHC-C1C	3.22	1.43	1.35
18	A	837	CLA	CHC-C1C	3.22	1.43	1.35
18	B	836	CLA	CHC-C1C	3.22	1.43	1.35
18	A	805	CLA	CHC-C1C	3.22	1.43	1.35
18	A	810	CLA	CHC-C1C	3.22	1.43	1.35
17	1	606	CHL	C1D-C2D	3.21	1.51	1.45
18	A	824	CLA	CHC-C1C	3.20	1.43	1.35
18	K	206	CLA	CHC-C1C	3.20	1.43	1.35
18	B	804	CLA	CHC-C1C	3.20	1.43	1.35
18	A	803	CLA	CHC-C1C	3.20	1.43	1.35
18	2	602	CLA	CHC-C1C	3.20	1.43	1.35
18	B	828	CLA	CHC-C1C	3.20	1.43	1.35
18	1	608	CLA	CHC-C1C	3.20	1.43	1.35
18	B	822	CLA	CHC-C1C	3.19	1.43	1.35
18	3	607	CLA	CHC-C1C	3.19	1.43	1.35
18	B	837	CLA	CHC-C1C	3.19	1.43	1.35
18	A	827	CLA	CHC-C1C	3.19	1.43	1.35
18	1	605	CLA	CHC-C1C	3.19	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	815	CLA	CHC-C1C	3.19	1.43	1.35
18	B	813	CLA	CHC-C1C	3.19	1.43	1.35
18	J	101	CLA	CHC-C1C	3.19	1.43	1.35
18	B	829	CLA	CHC-C1C	3.18	1.43	1.35
18	A	811	CLA	CHC-C1C	3.18	1.43	1.35
18	B	811	CLA	CHC-C1C	3.18	1.43	1.35
18	1	604	CLA	CHC-C1C	3.18	1.43	1.35
18	4	610	CLA	CHC-C1C	3.18	1.43	1.35
18	B	824	CLA	CHC-C1C	3.18	1.43	1.35
18	2	609	CLA	CHC-C1C	3.18	1.43	1.35
18	B	805	CLA	CHC-C1C	3.18	1.43	1.35
18	A	808	CLA	CHC-C1C	3.18	1.43	1.35
18	A	833	CLA	CHC-C1C	3.18	1.43	1.35
18	A	836	CLA	CHC-C1C	3.18	1.43	1.35
18	B	833	CLA	CHC-C1C	3.18	1.43	1.35
18	4	602	CLA	CHC-C1C	3.17	1.43	1.35
18	4	611	CLA	CHC-C1C	3.17	1.43	1.35
18	A	809	CLA	CHC-C1C	3.17	1.43	1.35
18	2	612	CLA	CHC-C1C	3.17	1.43	1.35
18	B	818	CLA	CHC-C1C	3.17	1.43	1.35
18	3	608	CLA	CHC-C1C	3.17	1.43	1.35
18	A	841	CLA	CHC-C1C	3.17	1.43	1.35
18	1	613	CLA	CHC-C1C	3.17	1.43	1.35
18	2	608	CLA	CHC-C1C	3.17	1.43	1.35
18	B	814	CLA	CHC-C1C	3.17	1.43	1.35
18	A	802	CLA	CHC-C1C	3.16	1.43	1.35
18	B	816	CLA	CHC-C1C	3.16	1.43	1.35
18	B	810	CLA	CHC-C1C	3.16	1.43	1.35
18	B	809	CLA	CHC-C1C	3.16	1.43	1.35
18	K	203	CLA	CHC-C1C	3.16	1.43	1.35
18	3	601	CLA	CHC-C1C	3.16	1.43	1.35
18	B	831	CLA	CHC-C1C	3.16	1.43	1.35
18	4	613	CLA	CHC-C1C	3.16	1.43	1.35
18	A	812	CLA	CHC-C1C	3.16	1.43	1.35
18	A	816	CLA	CHC-C1C	3.16	1.43	1.35
18	A	838	CLA	CHC-C1C	3.16	1.43	1.35
18	B	815	CLA	CHC-C1C	3.16	1.43	1.35
18	3	611	CLA	CHC-C1C	3.16	1.43	1.35
18	A	823	CLA	CHC-C1C	3.16	1.43	1.35
18	B	835	CLA	CHC-C1C	3.16	1.43	1.35
18	B	821	CLA	CHC-C1C	3.16	1.43	1.35
18	3	610	CLA	CHC-C1C	3.16	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	302	CLA	CHC-C1C	3.15	1.43	1.35
18	A	822	CLA	CHC-C1C	3.15	1.43	1.35
18	B	803	CLA	CHC-C1C	3.15	1.43	1.35
18	A	845	CLA	CHC-C1C	3.15	1.43	1.35
18	A	831	CLA	CHC-C1C	3.15	1.43	1.35
18	B	807	CLA	CHC-C1C	3.15	1.43	1.35
18	1	610	CLA	CHC-C1C	3.15	1.43	1.35
18	B	827	CLA	CHC-C1C	3.15	1.43	1.35
18	G	203	CLA	CHC-C1C	3.15	1.43	1.35
18	1	603	CLA	CHC-C1C	3.15	1.43	1.35
18	L	304	CLA	CHC-C1C	3.15	1.43	1.35
18	A	832	CLA	CHC-C1C	3.15	1.43	1.35
18	B	812	CLA	CHC-C1C	3.15	1.43	1.35
18	A	807	CLA	CHC-C1C	3.15	1.43	1.35
18	A	840	CLA	CHC-C1C	3.15	1.43	1.35
18	2	613	CLA	CHC-C1C	3.15	1.43	1.35
18	4	601	CLA	CHC-C1C	3.15	1.43	1.35
18	G	201	CLA	CHC-C1C	3.15	1.43	1.35
18	A	839	CLA	CHC-C1C	3.15	1.43	1.35
18	3	605	CLA	CHC-C1C	3.14	1.43	1.35
18	4	604	CLA	CHC-C1C	3.14	1.43	1.35
18	B	834	CLA	CHC-C1C	3.14	1.43	1.35
18	L	303	CLA	CHC-C1C	3.14	1.43	1.35
18	3	609	CLA	CHC-C1C	3.14	1.43	1.35
18	A	806	CLA	CHC-C1C	3.14	1.43	1.35
18	B	841	CLA	CHC-C1C	3.14	1.43	1.35
18	1	611	CLA	CHC-C1C	3.14	1.43	1.35
18	1	602	CLA	CHC-C1C	3.14	1.43	1.35
18	B	840	CLA	CHC-C1C	3.14	1.43	1.35
18	A	825	CLA	CHC-C1C	3.14	1.43	1.35
17	2	606	CHL	C1D-C2D	3.14	1.51	1.45
18	A	813	CLA	CHC-C1C	3.14	1.43	1.35
18	K	201	CLA	CHC-C1C	3.13	1.43	1.35
18	4	603	CLA	CHC-C1C	3.13	1.43	1.35
18	3	602	CLA	CHC-C1C	3.13	1.43	1.35
18	B	817	CLA	CHC-C1C	3.13	1.43	1.35
18	F	303	CLA	CHC-C1C	3.13	1.43	1.35
18	A	829	CLA	CHC-C1C	3.13	1.43	1.35
18	A	817	CLA	CHC-C1C	3.13	1.43	1.35
18	4	614	CLA	CHC-C1C	3.13	1.43	1.35
18	A	804	CLA	CHC-C1C	3.13	1.43	1.35
18	B	832	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	830	CLA	CHC-C1C	3.13	1.43	1.35
18	A	830	CLA	CHC-C1C	3.13	1.43	1.35
18	A	820	CLA	CHC-C1C	3.13	1.43	1.35
18	B	823	CLA	CHC-C1C	3.13	1.43	1.35
18	L	302	CLA	CHC-C1C	3.13	1.43	1.35
18	4	608	CLA	CHC-C1C	3.12	1.43	1.35
18	A	826	CLA	CHC-C1C	3.12	1.43	1.35
18	2	603	CLA	CHC-C1C	3.12	1.43	1.35
18	2	610	CLA	CHC-C1C	3.12	1.43	1.35
18	1	607	CLA	CHC-C1C	3.12	1.43	1.35
18	3	604	CLA	CHC-C1C	3.12	1.43	1.35
18	B	826	CLA	CHC-C1C	3.12	1.43	1.35
18	B	808	CLA	CHC-C1C	3.12	1.43	1.35
18	4	612	CLA	CHC-C1C	3.12	1.43	1.35
18	G	202	CLA	CHC-C1C	3.11	1.42	1.35
18	K	204	CLA	CHC-C1C	3.11	1.42	1.35
18	B	838	CLA	CHC-C1C	3.11	1.42	1.35
18	B	819	CLA	CHC-C1C	3.11	1.42	1.35
18	A	821	CLA	CHC-C1C	3.11	1.42	1.35
18	2	611	CLA	CHC-C1C	3.10	1.42	1.35
18	A	834	CLA	CHC-C1C	3.10	1.42	1.35
17	2	606	CHL	C3D-C2D	3.10	1.47	1.39
18	B	820	CLA	CHC-C1C	3.10	1.42	1.35
18	A	843	CLA	CHC-C1C	3.10	1.42	1.35
18	3	603	CLA	CHC-C1C	3.10	1.42	1.35
18	B	839	CLA	CHC-C1C	3.09	1.42	1.35
18	B	802	CLA	CHC-C1C	3.09	1.42	1.35
18	K	204	CLA	C4D-ND	-3.09	1.33	1.37
18	2	604	CLA	CHC-C1C	3.09	1.42	1.35
18	B	806	CLA	CHC-C1C	3.09	1.42	1.35
18	H	201	CLA	CHC-C1C	3.09	1.42	1.35
17	1	601	CHL	C1D-C2D	3.08	1.51	1.45
18	A	818	CLA	CHC-C1C	3.07	1.42	1.35
17	3	606	CHL	C1D-C2D	3.06	1.51	1.45
18	3	612	CLA	CHC-C1C	3.05	1.42	1.35
18	A	842	CLA	CHC-C1C	3.05	1.42	1.35
17	2	601	CHL	C3D-C2D	3.04	1.47	1.39
17	2	605	CHL	C3D-C2D	3.04	1.47	1.39
17	4	605	CHL	C1D-C2D	3.04	1.51	1.45
17	2	615	CHL	C1D-C2D	3.04	1.51	1.45
17	2	615	CHL	C3D-C2D	3.04	1.47	1.39
17	4	615	CHL	C1D-C2D	3.03	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	607	CHL	C3D-C2D	3.03	1.47	1.39
18	1	609	CLA	CHC-C1C	3.02	1.42	1.35
17	2	601	CHL	C1D-C2D	3.02	1.51	1.45
17	4	606	CHL	C3D-C2D	3.02	1.47	1.39
18	1	612	CLA	CHC-C1C	3.02	1.42	1.35
18	A	828	CLA	C4D-ND	-3.00	1.33	1.37
17	1	601	CHL	C3D-C2D	3.00	1.47	1.39
18	B	841	CLA	C4D-ND	-3.00	1.33	1.37
18	B	826	CLA	C4D-ND	-2.98	1.33	1.37
18	A	829	CLA	C4D-ND	-2.97	1.33	1.37
18	B	829	CLA	C4D-ND	-2.97	1.33	1.37
18	1	609	CLA	C4D-ND	-2.97	1.33	1.37
22	B	845	BCR	C23-C22	-2.97	1.39	1.45
18	1	605	CLA	C4D-ND	-2.96	1.33	1.37
18	A	839	CLA	C4D-ND	-2.96	1.33	1.37
18	K	206	CLA	C4D-ND	-2.96	1.33	1.37
18	2	609	CLA	C4D-ND	-2.96	1.33	1.37
17	2	607	CHL	C1D-C2D	2.96	1.51	1.45
18	F	301	CLA	C4D-ND	-2.96	1.33	1.37
17	4	606	CHL	C1D-C2D	2.96	1.51	1.45
18	A	810	CLA	C4D-ND	-2.96	1.33	1.37
17	2	605	CHL	C1D-C2D	2.96	1.51	1.45
18	A	803	CLA	C4D-ND	-2.95	1.33	1.37
18	B	817	CLA	C4D-ND	-2.95	1.33	1.37
18	B	821	CLA	C4D-ND	-2.95	1.33	1.37
17	3	606	CHL	C3D-C2D	2.95	1.47	1.39
18	3	608	CLA	C4D-ND	-2.94	1.33	1.37
18	3	602	CLA	C4D-ND	-2.94	1.33	1.37
18	B	816	CLA	C4D-ND	-2.94	1.33	1.37
18	B	808	CLA	C4D-ND	-2.94	1.33	1.37
18	B	840	CLA	C4D-ND	-2.94	1.33	1.37
18	A	826	CLA	C4D-ND	-2.94	1.33	1.37
18	2	604	CLA	C4D-ND	-2.93	1.33	1.37
18	B	810	CLA	C4D-ND	-2.93	1.33	1.37
17	4	615	CHL	C3D-C2D	2.93	1.47	1.39
18	3	609	CLA	C4D-ND	-2.93	1.33	1.37
17	4	607	CHL	C3D-C2D	2.93	1.47	1.39
18	2	602	CLA	C4D-ND	-2.93	1.33	1.37
18	4	613	CLA	C4D-ND	-2.93	1.33	1.37
18	K	203	CLA	C4D-ND	-2.93	1.33	1.37
18	B	824	CLA	C4D-ND	-2.93	1.33	1.37
18	A	830	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	834	CLA	C4D-ND	-2.92	1.33	1.37
17	4	605	CHL	C3D-C2D	2.92	1.47	1.39
18	A	812	CLA	C4D-ND	-2.92	1.33	1.37
18	2	610	CLA	C4D-ND	-2.92	1.33	1.37
18	4	609	CLA	C4D-ND	-2.92	1.33	1.37
18	B	833	CLA	C4D-ND	-2.92	1.33	1.37
18	B	837	CLA	C4D-ND	-2.92	1.33	1.37
18	A	831	CLA	C4D-ND	-2.92	1.33	1.37
17	4	607	CHL	C1D-C2D	2.92	1.51	1.45
18	3	601	CLA	C4D-ND	-2.92	1.33	1.37
18	A	804	CLA	C4D-ND	-2.92	1.33	1.37
18	4	603	CLA	C4D-ND	-2.92	1.33	1.37
18	2	608	CLA	C4D-ND	-2.92	1.33	1.37
18	A	835	CLA	C4D-ND	-2.91	1.33	1.37
18	B	836	CLA	C4D-ND	-2.91	1.33	1.37
18	3	604	CLA	C4D-ND	-2.91	1.33	1.37
18	K	201	CLA	C4D-ND	-2.91	1.33	1.37
18	A	820	CLA	C4D-ND	-2.91	1.33	1.37
18	A	838	CLA	C4D-ND	-2.91	1.33	1.37
18	1	603	CLA	C4D-ND	-2.91	1.33	1.37
18	A	816	CLA	C4D-ND	-2.91	1.33	1.37
18	A	817	CLA	C4D-ND	-2.91	1.33	1.37
18	A	825	CLA	C4D-ND	-2.91	1.33	1.37
18	A	818	CLA	C4D-ND	-2.90	1.33	1.37
18	A	819	CLA	C4D-ND	-2.90	1.33	1.37
17	1	606	CHL	MG-NA	-2.90	1.99	2.06
18	4	612	CLA	C4D-ND	-2.90	1.33	1.37
18	B	832	CLA	C4D-ND	-2.90	1.33	1.37
22	A	850	BCR	C23-C22	-2.90	1.39	1.45
18	3	603	CLA	C4D-ND	-2.90	1.33	1.37
18	B	823	CLA	C4D-ND	-2.90	1.33	1.37
18	L	302	CLA	C4D-ND	-2.90	1.33	1.37
22	B	801	BCR	C8-C9	-2.90	1.39	1.45
18	A	842	CLA	C4D-ND	-2.90	1.33	1.37
18	A	811	CLA	C4D-ND	-2.89	1.33	1.37
18	B	811	CLA	C4D-ND	-2.89	1.33	1.37
18	B	828	CLA	C4D-ND	-2.89	1.33	1.37
18	A	843	CLA	C4D-ND	-2.89	1.33	1.37
18	2	603	CLA	C4D-ND	-2.89	1.33	1.37
18	4	602	CLA	C4D-ND	-2.89	1.33	1.37
18	A	841	CLA	C4D-ND	-2.89	1.33	1.37
18	4	610	CLA	C4D-ND	-2.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	830	CLA	C4D-ND	-2.89	1.33	1.37
18	2	613	CLA	C4D-ND	-2.88	1.33	1.37
22	I	101	BCR	C23-C22	-2.88	1.39	1.45
18	B	819	CLA	C4D-ND	-2.88	1.33	1.37
18	A	833	CLA	C4D-ND	-2.88	1.33	1.37
18	B	814	CLA	C4D-ND	-2.88	1.33	1.37
18	L	304	CLA	C4D-ND	-2.88	1.33	1.37
18	2	612	CLA	C4D-ND	-2.87	1.33	1.37
18	A	844	CLA	C4D-ND	-2.87	1.33	1.37
18	4	604	CLA	C4D-ND	-2.87	1.33	1.37
18	2	611	CLA	C4D-ND	-2.87	1.33	1.37
18	B	804	CLA	C4D-ND	-2.87	1.33	1.37
18	B	805	CLA	C4D-ND	-2.87	1.33	1.37
18	3	607	CLA	C4D-ND	-2.86	1.33	1.37
18	A	821	CLA	C4D-ND	-2.86	1.33	1.37
18	A	815	CLA	C4D-ND	-2.86	1.33	1.37
18	B	806	CLA	C4D-ND	-2.86	1.33	1.37
18	A	822	CLA	C4D-ND	-2.86	1.33	1.37
18	3	610	CLA	C4D-ND	-2.86	1.33	1.37
18	1	610	CLA	C4D-ND	-2.86	1.33	1.37
18	A	806	CLA	C4D-ND	-2.86	1.33	1.37
18	B	802	CLA	C4D-ND	-2.86	1.33	1.37
18	B	838	CLA	C4D-ND	-2.86	1.33	1.37
24	A	801	CL0	OBD-CAD	2.86	1.28	1.22
22	B	849	BCR	C23-C22	-2.86	1.39	1.45
18	A	807	CLA	C4D-ND	-2.86	1.33	1.37
18	A	840	CLA	C4D-ND	-2.86	1.33	1.37
18	B	822	CLA	C4D-ND	-2.86	1.33	1.37
18	A	805	CLA	C4D-ND	-2.85	1.33	1.37
18	H	201	CLA	C4D-ND	-2.85	1.33	1.37
18	B	815	CLA	C4D-ND	-2.85	1.33	1.37
22	B	847	BCR	C23-C22	-2.85	1.39	1.45
18	B	807	CLA	C4D-ND	-2.85	1.33	1.37
22	B	848	BCR	C23-C22	-2.85	1.39	1.45
18	B	827	CLA	C4D-ND	-2.85	1.33	1.37
18	A	814	CLA	C4D-ND	-2.84	1.33	1.37
18	4	611	CLA	C4D-ND	-2.84	1.33	1.37
18	B	809	CLA	C4D-ND	-2.84	1.33	1.37
18	3	611	CLA	C4D-ND	-2.84	1.33	1.37
18	A	827	CLA	C4D-ND	-2.84	1.33	1.37
18	A	832	CLA	C4D-ND	-2.84	1.33	1.37
18	B	834	CLA	C4D-ND	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	839	CLA	C4D-ND	-2.84	1.33	1.37
18	B	803	CLA	C4D-ND	-2.84	1.33	1.37
18	4	601	CLA	C4D-ND	-2.84	1.33	1.37
18	4	614	CLA	C4D-ND	-2.83	1.33	1.37
18	L	303	CLA	C4D-ND	-2.83	1.33	1.37
18	G	203	CLA	C4D-ND	-2.83	1.33	1.37
18	A	845	CLA	C4D-ND	-2.83	1.33	1.37
18	B	831	CLA	C4D-ND	-2.83	1.33	1.37
18	B	820	CLA	C4D-ND	-2.83	1.33	1.37
18	1	608	CLA	C4D-ND	-2.83	1.33	1.37
18	G	202	CLA	C4D-ND	-2.83	1.33	1.37
18	1	613	CLA	C4D-ND	-2.82	1.33	1.37
18	B	818	CLA	C4D-ND	-2.82	1.33	1.37
18	A	824	CLA	C4D-ND	-2.82	1.33	1.37
18	1	604	CLA	C4D-ND	-2.82	1.33	1.37
18	1	602	CLA	C4D-ND	-2.81	1.33	1.37
22	3	614	BCR	C23-C22	-2.81	1.39	1.45
18	A	823	CLA	C4D-ND	-2.81	1.33	1.37
18	A	808	CLA	C4D-ND	-2.81	1.33	1.37
18	A	836	CLA	C4D-ND	-2.81	1.33	1.37
18	B	812	CLA	C4D-ND	-2.81	1.33	1.37
18	B	825	CLA	C4D-ND	-2.81	1.33	1.37
18	4	608	CLA	C4D-ND	-2.81	1.33	1.37
18	A	837	CLA	C4D-ND	-2.80	1.33	1.37
18	B	835	CLA	C4D-ND	-2.80	1.33	1.37
18	A	813	CLA	C4D-ND	-2.80	1.33	1.37
18	J	101	CLA	C4D-ND	-2.80	1.33	1.37
18	1	611	CLA	C4D-ND	-2.80	1.33	1.37
18	A	809	CLA	C4D-ND	-2.80	1.33	1.37
22	A	852	BCR	C8-C9	-2.80	1.39	1.45
18	F	302	CLA	C4D-ND	-2.79	1.33	1.37
18	3	605	CLA	C4D-ND	-2.79	1.33	1.37
18	3	612	CLA	C4D-ND	-2.79	1.33	1.37
22	B	846	BCR	C8-C9	-2.79	1.40	1.45
18	1	607	CLA	C4D-ND	-2.79	1.33	1.37
22	I	101	BCR	C8-C9	-2.78	1.40	1.45
22	A	852	BCR	C23-C22	-2.78	1.40	1.45
22	B	849	BCR	C8-C9	-2.78	1.40	1.45
22	G	204	BCR	C8-C9	-2.78	1.40	1.45
22	4	618	BCR	C8-C9	-2.78	1.40	1.45
22	B	845	BCR	C8-C9	-2.78	1.40	1.45
21	4	616	LUT	C8-C9	-2.77	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	813	CLA	C4D-ND	-2.77	1.33	1.37
18	F	303	CLA	C4D-ND	-2.77	1.33	1.37
22	A	849	BCR	C23-C22	-2.76	1.40	1.45
21	3	613	LUT	C8-C9	-2.76	1.40	1.45
18	G	201	CLA	C4D-ND	-2.76	1.33	1.37
22	A	848	BCR	C23-C22	-2.76	1.40	1.45
22	3	614	BCR	C8-C9	-2.75	1.40	1.45
22	G	204	BCR	C23-C22	-2.75	1.40	1.45
22	L	305	BCR	C8-C9	-2.74	1.40	1.45
18	1	612	CLA	C4D-ND	-2.73	1.33	1.37
22	B	847	BCR	C8-C9	-2.73	1.40	1.45
22	L	305	BCR	C23-C22	-2.72	1.40	1.45
18	A	802	CLA	C4D-ND	-2.72	1.33	1.37
22	A	853	BCR	C23-C22	-2.71	1.40	1.45
22	B	848	BCR	C8-C9	-2.71	1.40	1.45
17	1	606	CHL	C3A-C2A	-2.71	1.52	1.54
22	4	618	BCR	C23-C22	-2.71	1.40	1.45
22	L	301	BCR	C8-C9	-2.71	1.40	1.45
22	B	844	BCR	C23-C22	-2.70	1.40	1.45
22	K	205	BCR	C8-C9	-2.70	1.40	1.45
22	A	853	BCR	C8-C9	-2.70	1.40	1.45
21	2	619	LUT	C8-C9	-2.69	1.40	1.45
22	A	848	BCR	C8-C9	-2.69	1.40	1.45
22	J	102	BCR	C23-C22	-2.68	1.40	1.45
24	A	801	CL0	CHD-C1D	2.68	1.43	1.38
22	L	306	BCR	C23-C22	-2.68	1.40	1.45
22	K	205	BCR	C23-C22	-2.68	1.40	1.45
22	B	801	BCR	C23-C22	-2.67	1.40	1.45
21	1	616	LUT	C8-C9	-2.67	1.40	1.45
22	A	850	BCR	C8-C9	-2.67	1.40	1.45
22	J	102	BCR	C8-C9	-2.67	1.40	1.45
22	F	304	BCR	C8-C9	-2.66	1.40	1.45
22	B	844	BCR	C8-C9	-2.66	1.40	1.45
22	K	202	BCR	C23-C22	-2.66	1.40	1.45
22	B	846	BCR	C23-C22	-2.65	1.40	1.45
22	A	849	BCR	C8-C9	-2.64	1.40	1.45
22	K	202	BCR	C8-C9	-2.63	1.40	1.45
18	A	842	CLA	CMB-C2B	-2.63	1.46	1.51
22	L	301	BCR	C23-C22	-2.61	1.40	1.45
22	L	306	BCR	C8-C9	-2.61	1.40	1.45
22	B	843	BCR	C8-C9	-2.59	1.40	1.45
17	1	606	CHL	C4B-CHC	2.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	843	BCR	C23-C22	-2.56	1.40	1.45
18	L	302	CLA	CMB-C2B	-2.54	1.46	1.51
17	2	615	CHL	MG-NA	-2.54	2.00	2.06
24	A	801	CL0	CHD-C4C	2.54	1.45	1.39
18	B	817	CLA	CMB-C2B	-2.52	1.46	1.51
22	A	851	BCR	C8-C9	-2.51	1.40	1.45
18	4	604	CLA	CMB-C2B	-2.50	1.46	1.51
18	B	819	CLA	CMB-C2B	-2.49	1.46	1.51
18	B	829	CLA	CMB-C2B	-2.49	1.46	1.51
17	2	605	CHL	C4B-CHC	2.48	1.47	1.41
18	B	822	CLA	CMB-C2B	-2.47	1.46	1.51
18	3	609	CLA	CMB-C2B	-2.47	1.46	1.51
18	B	838	CLA	CMB-C2B	-2.47	1.46	1.51
18	A	810	CLA	CMB-C2B	-2.47	1.46	1.51
18	4	603	CLA	CMB-C2B	-2.47	1.46	1.51
18	A	840	CLA	CMB-C2B	-2.47	1.46	1.51
18	A	844	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	830	CLA	CMB-C2B	-2.46	1.46	1.51
17	2	605	CHL	MG-NA	-2.45	2.00	2.06
18	1	612	CLA	CMB-C2B	-2.45	1.46	1.51
18	2	613	CLA	CMB-C2B	-2.45	1.46	1.51
18	A	812	CLA	CMB-C2B	-2.45	1.46	1.51
18	K	204	CLA	CMB-C2B	-2.45	1.46	1.51
18	A	822	CLA	CMB-C2B	-2.45	1.46	1.51
18	F	303	CLA	CMB-C2B	-2.44	1.46	1.51
17	1	601	CHL	C4B-CHC	2.44	1.47	1.41
18	A	838	CLA	CMB-C2B	-2.44	1.46	1.51
18	3	603	CLA	CMB-C2B	-2.44	1.46	1.51
18	A	832	CLA	CMB-C2B	-2.44	1.46	1.51
18	J	101	CLA	CMB-C2B	-2.44	1.46	1.51
18	B	835	CLA	CMB-C2B	-2.44	1.46	1.51
17	1	606	CHL	C4C-C3C	2.44	1.49	1.45
18	B	839	CLA	CMB-C2B	-2.43	1.46	1.51
18	4	609	CLA	CMB-C2B	-2.43	1.46	1.51
18	B	827	CLA	CMB-C2B	-2.43	1.46	1.51
18	B	828	CLA	CMB-C2B	-2.43	1.46	1.51
17	1	601	CHL	MG-NA	-2.43	2.00	2.06
17	2	601	CHL	MG-NA	-2.43	2.00	2.06
18	1	603	CLA	CMB-C2B	-2.43	1.46	1.51
18	A	808	CLA	CMB-C2B	-2.43	1.46	1.51
18	3	611	CLA	CMB-C2B	-2.43	1.46	1.51
18	4	608	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	851	BCR	C23-C22	-2.42	1.40	1.45
18	1	613	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	834	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	834	CLA	CMB-C2B	-2.42	1.46	1.51
18	2	604	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	821	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	805	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	845	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	831	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	809	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	807	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	812	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	802	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	836	CLA	CMB-C2B	-2.42	1.46	1.51
18	1	607	CLA	CMB-C2B	-2.42	1.46	1.51
21	2	616	LUT	C8-C9	-2.42	1.40	1.45
18	3	604	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	813	CLA	CMB-C2B	-2.42	1.46	1.51
18	A	814	CLA	CMB-C2B	-2.42	1.46	1.51
18	H	201	CLA	CMB-C2B	-2.42	1.46	1.51
18	3	605	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	815	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	808	CLA	CMB-C2B	-2.42	1.46	1.51
17	2	615	CHL	C4B-CHC	2.42	1.47	1.41
18	A	819	CLA	CMB-C2B	-2.41	1.46	1.51
18	A	802	CLA	CMB-C2B	-2.41	1.46	1.51
17	2	606	CHL	C4C-C3C	2.41	1.49	1.45
18	1	605	CLA	CMB-C2B	-2.41	1.46	1.51
18	4	601	CLA	CMB-C2B	-2.41	1.46	1.51
18	L	304	CLA	CMB-C2B	-2.41	1.46	1.51
18	A	817	CLA	CMB-C2B	-2.41	1.46	1.51
18	3	602	CLA	CMB-C2B	-2.41	1.46	1.51
18	B	811	CLA	CMB-C2B	-2.41	1.46	1.51
18	F	301	CLA	CMB-C2B	-2.41	1.46	1.51
17	2	606	CHL	MG-NA	-2.41	2.00	2.06
17	2	607	CHL	C4B-CHC	2.41	1.47	1.41
18	B	820	CLA	CMB-C2B	-2.40	1.46	1.51
18	1	604	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	836	CLA	CMB-C2B	-2.40	1.46	1.51
18	1	611	CLA	CMB-C2B	-2.40	1.46	1.51
17	4	606	CHL	C4C-C3C	2.40	1.49	1.45
18	B	823	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	201	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	816	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	824	CLA	CMB-C2B	-2.40	1.46	1.51
18	4	614	CLA	CMB-C2B	-2.40	1.46	1.51
18	1	610	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	825	CLA	CMB-C2B	-2.40	1.46	1.51
17	1	606	CHL	C1B-CHB	2.40	1.47	1.41
17	2	606	CHL	C4B-CHC	2.40	1.47	1.41
18	B	806	CLA	CMB-C2B	-2.40	1.46	1.51
18	3	607	CLA	CMB-C2B	-2.40	1.46	1.51
18	1	609	CLA	CMB-C2B	-2.40	1.46	1.51
18	2	602	CLA	CMB-C2B	-2.40	1.46	1.51
18	2	610	CLA	CMB-C2B	-2.40	1.46	1.51
18	1	608	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	804	CLA	CMB-C2B	-2.40	1.46	1.51
18	4	611	CLA	CMB-C2B	-2.39	1.46	1.51
18	B	840	CLA	CMB-C2B	-2.39	1.46	1.51
18	3	610	CLA	CMB-C2B	-2.39	1.46	1.51
18	2	603	CLA	CMB-C2B	-2.39	1.46	1.51
18	K	201	CLA	CMB-C2B	-2.39	1.46	1.51
18	1	602	CLA	CMB-C2B	-2.39	1.46	1.51
18	B	841	CLA	CMB-C2B	-2.39	1.46	1.51
17	4	605	CHL	MG-NA	-2.39	2.00	2.06
18	4	613	CLA	CMB-C2B	-2.39	1.46	1.51
18	A	803	CLA	CMB-C2B	-2.39	1.46	1.51
24	A	801	CL0	C1D-C2D	2.39	1.50	1.45
18	4	610	CLA	CMB-C2B	-2.39	1.46	1.51
18	B	807	CLA	CMB-C2B	-2.39	1.46	1.51
18	3	601	CLA	CMB-C2B	-2.38	1.46	1.51
18	B	826	CLA	CMB-C2B	-2.38	1.46	1.51
18	B	832	CLA	CMB-C2B	-2.38	1.46	1.51
17	4	605	CHL	C4C-C3C	2.38	1.49	1.44
18	A	839	CLA	CMB-C2B	-2.38	1.46	1.51
18	2	609	CLA	CMB-C2B	-2.38	1.46	1.51
17	2	601	CHL	C4B-CHC	2.38	1.47	1.41
18	2	608	CLA	CMB-C2B	-2.38	1.46	1.51
18	G	202	CLA	CMB-C2B	-2.38	1.46	1.51
18	3	612	CLA	CMB-C2B	-2.38	1.46	1.51
18	A	841	CLA	CMB-C2B	-2.38	1.46	1.51
18	A	837	CLA	CMB-C2B	-2.38	1.46	1.51
18	A	826	CLA	CMB-C2B	-2.38	1.46	1.51
18	B	833	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	811	CLA	CMB-C2B	-2.37	1.46	1.51
18	F	302	CLA	CMB-C2B	-2.37	1.46	1.51
17	2	601	CHL	C4C-C3C	2.37	1.49	1.45
18	B	810	CLA	CMB-C2B	-2.37	1.46	1.51
18	A	833	CLA	CMB-C2B	-2.37	1.46	1.51
18	K	203	CLA	CMB-C2B	-2.37	1.46	1.51
18	A	843	CLA	CMB-C2B	-2.37	1.46	1.51
18	B	813	CLA	CMB-C2B	-2.36	1.46	1.51
18	B	803	CLA	CMB-C2B	-2.36	1.46	1.51
18	A	827	CLA	CMB-C2B	-2.36	1.46	1.51
18	B	814	CLA	CMB-C2B	-2.36	1.46	1.51
18	A	835	CLA	CMB-C2B	-2.36	1.46	1.51
18	A	823	CLA	CMB-C2B	-2.36	1.46	1.51
18	A	820	CLA	CMB-C2B	-2.36	1.46	1.51
18	B	804	CLA	CMB-C2B	-2.36	1.46	1.51
18	B	831	CLA	CMB-C2B	-2.36	1.46	1.51
18	K	206	CLA	CMB-C2B	-2.35	1.46	1.51
18	L	303	CLA	CMB-C2B	-2.35	1.46	1.51
18	A	830	CLA	CMB-C2B	-2.35	1.46	1.51
17	2	605	CHL	C4C-C3C	2.35	1.49	1.44
18	2	611	CLA	CMB-C2B	-2.35	1.46	1.51
18	A	806	CLA	CMB-C2B	-2.35	1.46	1.51
18	B	837	CLA	CMB-C2B	-2.35	1.46	1.51
18	B	821	CLA	CMB-C2B	-2.35	1.46	1.51
21	2	616	LUT	C28-C29	-2.35	1.40	1.45
18	B	816	CLA	CMB-C2B	-2.34	1.46	1.51
18	B	824	CLA	CMB-C2B	-2.34	1.46	1.51
18	2	612	CLA	CMB-C2B	-2.34	1.46	1.51
18	3	608	CLA	CMB-C2B	-2.34	1.46	1.51
17	4	605	CHL	C4B-CHC	2.34	1.47	1.41
18	1	609	CLA	CMD-C2D	-2.34	1.45	1.50
18	A	805	CLA	CMB-C2B	-2.34	1.46	1.51
22	I	101	BCR	C12-C13	-2.34	1.40	1.45
22	B	848	BCR	C19-C18	-2.34	1.40	1.45
18	A	828	CLA	CMB-C2B	-2.34	1.46	1.51
18	B	818	CLA	CMB-C2B	-2.34	1.46	1.51
18	4	612	CLA	CMB-C2B	-2.33	1.46	1.51
18	A	829	CLA	CMB-C2B	-2.33	1.46	1.51
21	2	616	LUT	C32-C33	-2.33	1.40	1.45
17	4	615	CHL	C4C-C3C	2.33	1.49	1.45
21	3	613	LUT	C28-C29	-2.33	1.40	1.45
22	B	845	BCR	C12-C13	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	613	LUT	C32-C33	-2.33	1.40	1.45
22	A	850	BCR	C19-C18	-2.32	1.41	1.45
17	4	606	CHL	C4B-CHC	2.32	1.47	1.41
17	4	607	CHL	C4B-CHC	2.32	1.47	1.41
17	1	601	CHL	C4C-C3C	2.32	1.49	1.45
18	G	203	CLA	CMB-C2B	-2.32	1.46	1.51
21	3	613	LUT	C12-C13	-2.32	1.41	1.45
22	3	614	BCR	C19-C18	-2.32	1.41	1.45
18	A	815	CLA	CMB-C2B	-2.32	1.46	1.51
18	4	602	CLA	CMB-C2B	-2.31	1.46	1.51
18	A	818	CLA	CMB-C2B	-2.31	1.46	1.51
18	B	825	CLA	CMB-C2B	-2.31	1.46	1.51
21	4	616	LUT	C32-C33	-2.31	1.41	1.45
17	2	607	CHL	MG-NA	-2.31	2.00	2.06
24	A	801	CL0	CHA-C1A	2.31	1.45	1.39
22	L	301	BCR	C12-C13	-2.30	1.41	1.45
17	2	615	CHL	C4C-C3C	2.30	1.49	1.45
22	F	304	BCR	C23-C22	-2.30	1.41	1.45
18	A	809	CLA	CMB-C2B	-2.30	1.46	1.51
17	3	606	CHL	MG-NA	-2.29	2.00	2.06
17	4	606	CHL	MG-NA	-2.29	2.00	2.06
17	2	607	CHL	C4C-C3C	2.29	1.49	1.45
21	4	616	LUT	C12-C13	-2.29	1.41	1.45
22	I	101	BCR	C19-C18	-2.29	1.41	1.45
22	B	848	BCR	C12-C13	-2.29	1.41	1.45
22	G	204	BCR	C12-C13	-2.28	1.41	1.45
21	2	619	LUT	C32-C33	-2.28	1.41	1.45
22	A	848	BCR	C19-C18	-2.28	1.41	1.45
22	L	305	BCR	C12-C13	-2.28	1.41	1.45
21	2	619	LUT	C12-C13	-2.27	1.41	1.45
19	2	617	XAT	C28-C29	-2.27	1.41	1.45
24	A	801	CL0	MG-NC	2.27	2.11	2.06
17	3	606	CHL	C4B-CHC	2.27	1.47	1.41
17	4	615	CHL	C4B-CHC	2.26	1.47	1.41
22	B	847	BCR	C19-C18	-2.26	1.41	1.45
22	G	204	BCR	C19-C18	-2.25	1.41	1.45
17	4	607	CHL	C4C-C3C	2.25	1.48	1.45
22	3	614	BCR	C12-C13	-2.25	1.41	1.45
17	2	601	CHL	C1B-CHB	2.25	1.47	1.41
17	1	601	CHL	C1B-CHB	2.25	1.47	1.41
22	4	618	BCR	C12-C13	-2.25	1.41	1.45
22	B	847	BCR	C12-C13	-2.25	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	301	BCR	C20-C19	2.23	1.40	1.34
17	2	606	CHL	C1B-CHB	2.23	1.47	1.41
22	A	848	BCR	C12-C13	-2.23	1.41	1.45
22	B	849	BCR	C12-C13	-2.23	1.41	1.45
21	4	616	LUT	C28-C29	-2.23	1.41	1.45
22	B	801	BCR	C12-C13	-2.23	1.41	1.45
17	2	605	CHL	C1B-CHB	2.22	1.47	1.41
17	3	606	CHL	C4C-C3C	2.22	1.48	1.45
17	4	605	CHL	C1B-CHB	2.22	1.47	1.41
22	B	849	BCR	C19-C18	-2.21	1.41	1.45
22	A	853	BCR	C19-C18	-2.21	1.41	1.45
22	B	844	BCR	C12-C13	-2.21	1.41	1.45
22	A	849	BCR	C19-C18	-2.20	1.41	1.45
22	B	846	BCR	C19-C18	-2.20	1.41	1.45
22	A	852	BCR	C19-C18	-2.20	1.41	1.45
21	2	619	LUT	C28-C29	-2.20	1.41	1.45
22	B	801	BCR	C19-C18	-2.20	1.41	1.45
22	K	205	BCR	C19-C18	-2.19	1.41	1.45
22	J	102	BCR	C19-C18	-2.19	1.41	1.45
22	4	618	BCR	C19-C18	-2.19	1.41	1.45
22	A	853	BCR	C12-C13	-2.18	1.41	1.45
21	2	616	LUT	C12-C13	-2.18	1.41	1.45
17	2	615	CHL	C1B-CHB	2.18	1.47	1.41
17	2	607	CHL	C1B-CHB	2.18	1.47	1.41
22	L	305	BCR	C19-C18	-2.17	1.41	1.45
17	3	606	CHL	C1B-CHB	2.17	1.47	1.41
24	A	801	CL0	C1C-C2C	2.17	1.48	1.44
24	A	801	CL0	CHA-C4D	2.17	1.42	1.38
22	B	846	BCR	C12-C13	-2.16	1.41	1.45
19	4	617	XAT	C32-C33	-2.16	1.41	1.45
17	4	606	CHL	C1B-CHB	2.16	1.47	1.41
22	K	202	BCR	C19-C18	-2.16	1.41	1.45
22	A	850	BCR	C12-C13	-2.16	1.41	1.45
19	4	617	XAT	C8-C9	-2.15	1.41	1.45
19	4	617	XAT	C28-C29	-2.15	1.41	1.45
22	A	849	BCR	C12-C13	-2.15	1.41	1.45
21	1	616	LUT	C12-C13	-2.14	1.41	1.45
18	B	808	CLA	CMD-C2D	-2.14	1.46	1.50
17	4	607	CHL	MG-NA	-2.14	2.01	2.06
18	A	842	CLA	CMD-C2D	-2.14	1.46	1.50
22	J	102	BCR	C12-C13	-2.14	1.41	1.45
18	B	802	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	202	BCR	C12-C13	-2.12	1.41	1.45
17	4	615	CHL	MG-NA	-2.11	2.01	2.06
18	K	201	CLA	CBD-CAD	2.11	1.56	1.51
22	B	843	BCR	C19-C18	-2.11	1.41	1.45
22	B	845	BCR	C19-C18	-2.11	1.41	1.45
17	4	615	CHL	C1B-CHB	2.11	1.46	1.41
17	4	607	CHL	C1B-CHB	2.10	1.46	1.41
22	K	205	BCR	C11-C12	2.10	1.40	1.34
19	2	617	XAT	C32-C33	-2.10	1.41	1.45
19	4	617	XAT	C12-C13	-2.10	1.41	1.45
22	L	306	BCR	C19-C18	-2.09	1.41	1.45
22	A	852	BCR	C11-C12	2.09	1.40	1.34
22	B	843	BCR	C12-C13	-2.09	1.41	1.45
18	B	823	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	828	CLA	CMD-C2D	-2.09	1.46	1.50
21	1	616	LUT	C32-C33	-2.08	1.41	1.45
19	1	614	XAT	O24-C25	-2.08	1.43	1.46
22	B	844	BCR	C20-C19	2.08	1.39	1.34
17	1	606	CHL	C1D-ND	-2.08	1.35	1.37
18	B	839	CLA	CMD-C2D	-2.07	1.46	1.50
19	2	617	XAT	C12-C13	-2.07	1.41	1.45
18	B	829	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	609	CLA	CMD-C2D	-2.07	1.46	1.50
18	3	612	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	613	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	851	BCR	C20-C19	2.06	1.39	1.34
22	F	304	BCR	C19-C18	-2.06	1.41	1.45
18	4	611	CLA	CMD-C2D	-2.06	1.46	1.50
18	3	611	CLA	CBD-CAD	2.06	1.56	1.51
18	4	603	CLA	CMD-C2D	-2.06	1.46	1.50
18	K	204	CLA	CMC-C2C	-2.06	1.46	1.50
18	A	810	CLA	CMD-C2D	-2.05	1.46	1.50
22	L	306	BCR	C12-C13	-2.05	1.41	1.45
18	3	609	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	807	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	811	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	613	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	608	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	819	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	803	CLA	CMC-C2C	-2.04	1.46	1.50
18	2	612	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	836	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	608	CLA	CMD-C2D	-2.03	1.46	1.50
17	2	607	CHL	C1D-ND	-2.03	1.35	1.37
18	B	826	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	607	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	813	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	828	CLA	CMC-C2C	-2.02	1.46	1.50
18	1	603	CLA	CMD-C2D	-2.02	1.46	1.50
18	3	601	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.02	1.46	1.50
18	3	604	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	834	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	802	CLA	CMD-C2D	-2.02	1.46	1.50
18	G	202	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	840	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	824	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	820	CLA	CMD-C2D	-2.01	1.46	1.50
18	4	609	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	830	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	817	CLA	CMD-C2D	-2.01	1.46	1.50
18	2	611	CLA	CMD-C2D	-2.01	1.46	1.50
18	3	605	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	807	CLA	CMD-C2D	-2.01	1.46	1.50
18	1	612	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	805	CLA	CMD-C2D	-2.01	1.46	1.50
18	2	602	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.00	1.46	1.50
18	2	604	CLA	CMD-C2D	-2.00	1.46	1.50
18	B	838	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	851	BCR	C12-C13	-2.00	1.41	1.45
18	B	835	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	806	CLA	CMC-C2C	-2.00	1.46	1.50
18	A	832	CLA	CMD-C2D	-2.00	1.46	1.50

All (1744) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	O2D-CGD-CBD	26.04	157.54	111.27
18	A	818	CLA	O2D-CGD-O1D	-25.22	74.53	123.84
18	A	818	CLA	O1D-CGD-CBD	-20.27	83.01	124.48
18	B	836	CLA	C5-C3-C4	-16.66	77.79	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	836	CLA	C4-C3-C2	-13.89	82.51	122.65
18	B	836	CLA	C5-C3-C2	13.03	160.30	122.65
24	A	801	CL0	C4A-NA-C1A	-11.97	101.33	106.71
19	1	614	XAT	O4-C5-C4	11.64	122.12	113.38
24	A	801	CL0	C2C-C1C-NC	10.78	120.08	109.97
24	A	801	CL0	CHA-C4D-C3D	-9.77	108.54	125.26
19	1	614	XAT	C38-C25-C26	-9.20	106.84	122.26
19	1	614	XAT	O24-C25-C24	9.17	120.27	113.38
24	A	801	CL0	C3D-C2D-C1D	-8.74	98.73	107.08
17	4	605	CHL	CMD-C2D-C1D	8.42	139.54	124.71
24	A	801	CL0	CMD-C2D-C1D	8.41	139.53	124.71
17	3	606	CHL	CMD-C2D-C1D	8.33	139.40	124.71
17	4	615	CHL	CMD-C2D-C1D	8.30	139.34	124.71
17	2	615	CHL	CMD-C2D-C1D	8.26	139.28	124.71
17	4	607	CHL	CMD-C2D-C1D	8.25	139.25	124.71
17	2	606	CHL	CMD-C2D-C1D	8.22	139.19	124.71
17	1	601	CHL	CMD-C2D-C1D	8.21	139.19	124.71
17	2	601	CHL	CMD-C2D-C1D	8.21	139.18	124.71
24	A	801	CL0	C3C-C4C-NC	8.17	119.73	110.57
17	2	605	CHL	CMD-C2D-C1D	8.16	139.09	124.71
17	2	607	CHL	CMD-C2D-C1D	8.15	139.07	124.71
17	1	606	CHL	CMD-C2D-C1D	8.10	138.99	124.71
17	4	606	CHL	CMD-C2D-C1D	8.03	138.87	124.71
22	B	843	BCR	C16-C15-C14	7.85	139.55	123.47
19	1	614	XAT	C18-C5-C6	-7.71	109.34	122.26
17	4	615	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
17	1	606	CHL	CHD-C1D-ND	-7.49	117.58	124.45
22	L	301	BCR	C16-C15-C14	7.45	138.73	123.47
17	4	607	CHL	C2C-C3C-C4C	-7.44	101.18	106.49
22	L	301	BCR	C15-C16-C17	7.41	138.65	123.47
17	2	615	CHL	C2C-C3C-C4C	-7.38	101.22	106.49
17	1	601	CHL	C2C-C3C-C4C	-7.27	101.30	106.49
17	2	605	CHL	C2C-C3C-C4C	-7.24	101.11	106.49
24	A	801	CL0	C2D-C1D-ND	7.21	115.42	110.10
18	1	609	CLA	C4A-NA-C1A	7.20	109.94	106.71
17	2	601	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
17	2	607	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
24	A	801	CL0	CHA-C4D-ND	7.11	130.99	124.45
17	2	606	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
18	2	611	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	A	849	BCR	C15-C16-C17	7.08	137.98	123.47
21	2	616	LUT	C15-C35-C34	7.07	137.95	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	612	CLA	C4A-NA-C1A	7.04	109.87	106.71
17	2	606	CHL	CHD-C1D-ND	-7.00	118.02	124.45
17	4	605	CHL	C2C-C3C-C4C	-7.00	101.30	106.49
17	4	615	CHL	C1B-C2B-C3B	-6.96	100.44	106.92
18	4	614	CLA	C4A-NA-C1A	6.95	109.83	106.71
18	A	818	CLA	C4A-NA-C1A	6.95	109.83	106.71
17	4	606	CHL	C1B-C2B-C3B	-6.94	100.46	106.92
18	A	830	CLA	C4A-NA-C1A	6.94	109.83	106.71
18	A	828	CLA	C4A-NA-C1A	6.94	109.82	106.71
18	A	819	CLA	C4A-NA-C1A	6.91	109.81	106.71
17	1	601	CHL	CHD-C1D-ND	-6.90	118.12	124.45
18	F	302	CLA	C4A-NA-C1A	6.90	109.81	106.71
17	1	606	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
17	2	615	CHL	CHD-C1D-ND	-6.89	118.12	124.45
18	A	813	CLA	C4A-NA-C1A	6.85	109.78	106.71
18	A	827	CLA	C4A-NA-C1A	6.84	109.78	106.71
18	B	841	CLA	C4A-NA-C1A	6.83	109.78	106.71
17	4	605	CHL	CHD-C1D-ND	-6.83	118.18	124.45
18	1	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	2	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
21	3	613	LUT	C15-C35-C34	6.81	137.43	123.47
18	A	843	CLA	C4A-NA-C1A	6.81	109.77	106.71
18	B	807	CLA	C4A-NA-C1A	6.81	109.77	106.71
18	B	804	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	B	811	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	B	840	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	K	204	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	B	826	CLA	C4A-NA-C1A	6.76	109.75	106.71
18	B	809	CLA	C4A-NA-C1A	6.76	109.74	106.71
17	2	601	CHL	CHD-C1D-ND	-6.76	118.25	124.45
18	3	605	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	H	201	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	A	831	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	A	808	CLA	C4A-NA-C1A	6.74	109.74	106.71
18	B	808	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	B	819	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	G	202	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	2	613	CLA	C4A-NA-C1A	6.73	109.73	106.71
18	A	812	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	B	814	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	817	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	1	605	CLA	C4A-NA-C1A	6.72	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	602	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	4	601	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	A	839	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	L	302	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	2	608	CLA	C4A-NA-C1A	6.69	109.71	106.71
18	3	612	CLA	C4A-NA-C1A	6.69	109.71	106.71
17	2	607	CHL	CHD-C1D-ND	-6.69	118.31	124.45
18	4	613	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	A	806	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	818	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	837	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	815	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	1	603	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	A	826	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	A	829	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	4	612	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	L	304	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	3	601	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	B	825	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	1	611	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	L	303	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	G	203	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	4	608	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	B	813	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	4	610	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	827	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	A	851	BCR	C8-C9-C10	6.63	129.11	118.94
18	A	840	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	3	609	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	831	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	J	101	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	816	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	1	607	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	A	804	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	A	842	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	B	806	CLA	C4A-NA-C1A	6.60	109.67	106.71
17	2	605	CHL	CHD-C1D-ND	-6.60	118.39	124.45
18	A	805	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	A	825	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	4	603	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	A	816	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	A	841	CLA	C4A-NA-C1A	6.58	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	A	838	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	1	614	XAT	O24-C25-C38	6.57	122.93	115.06
18	A	833	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	820	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	A	845	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	830	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	829	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	A	802	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	A	851	BCR	C16-C15-C14	6.56	136.91	123.47
18	A	832	CLA	C4A-NA-C1A	6.56	109.65	106.71
18	1	610	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	B	824	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	K	201	CLA	C4A-NA-C1A	6.54	109.64	106.71
18	A	836	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	3	608	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	4	607	CHL	CHD-C1D-ND	-6.53	118.45	124.45
18	B	839	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	2	609	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	A	820	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	B	823	CLA	C4A-NA-C1A	6.51	109.64	106.71
18	2	612	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	A	850	BCR	C15-C16-C17	6.51	136.81	123.47
18	B	803	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	809	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	B	817	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	F	303	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	B	821	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	G	201	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	B	838	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	3	611	CLA	C4A-NA-C1A	6.49	109.63	106.71
18	2	603	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	B	805	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	4	604	CLA	C4A-NA-C1A	6.47	109.62	106.71
18	A	811	CLA	C4A-NA-C1A	6.47	109.62	106.71
18	3	610	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	B	835	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	B	812	CLA	C4A-NA-C1A	6.46	109.61	106.71
17	3	606	CHL	CHD-C1D-ND	-6.45	118.52	124.45
18	1	602	CLA	C4A-NA-C1A	6.45	109.61	106.71
18	3	607	CLA	C4A-NA-C1A	6.45	109.61	106.71
18	A	834	CLA	C4A-NA-C1A	6.45	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	611	CLA	C4A-NA-C1A	6.45	109.60	106.71
18	A	823	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	B	802	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	A	824	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	1	613	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	A	801	CL0	C3B-C4B-NB	6.42	117.50	109.21
18	A	821	CLA	C4A-NA-C1A	6.41	109.59	106.71
18	A	815	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	A	835	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	A	837	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	B	833	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	A	822	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	B	810	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	B	832	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	3	602	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	3	604	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	F	301	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	A	801	CL0	CHD-C4C-C3C	-6.35	115.51	124.84
17	4	606	CHL	CHD-C1D-ND	-6.34	118.62	124.45
18	B	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	4	615	CHL	CHD-C1D-ND	-6.33	118.64	124.45
18	1	608	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	3	603	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	K	203	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	2	602	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	A	850	BCR	C16-C15-C14	6.32	136.41	123.47
18	K	206	CLA	C4A-NA-C1A	6.31	109.54	106.71
18	A	810	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	B	822	CLA	C4A-NA-C1A	6.23	109.51	106.71
18	A	807	CLA	C4A-NA-C1A	6.19	109.49	106.71
18	B	836	CLA	C4A-NA-C1A	6.16	109.47	106.71
18	A	814	CLA	C4A-NA-C1A	6.08	109.44	106.71
18	4	609	CLA	C4A-NA-C1A	6.07	109.44	106.71
19	2	617	XAT	C15-C35-C34	6.06	135.88	123.47
21	2	619	LUT	C15-C35-C34	5.84	135.44	123.47
19	2	617	XAT	C35-C15-C14	5.84	135.43	123.47
22	K	205	BCR	C15-C16-C17	5.78	135.32	123.47
18	A	803	CLA	C4A-NA-C1A	5.71	109.27	106.71
18	A	844	CLA	C4A-NA-C1A	5.61	109.23	106.71
17	2	601	CHL	O2D-CGD-CBD	5.57	121.17	111.27
22	F	304	BCR	C15-C16-C17	5.54	134.82	123.47
22	A	851	BCR	C23-C22-C21	5.50	127.38	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	304	BCR	C24-C23-C22	5.44	134.45	126.23
17	1	606	CHL	C1B-CHB-C4A	-5.36	119.50	130.12
24	A	801	CL0	CHD-C1D-ND	-5.33	119.55	124.45
22	B	846	BCR	C16-C15-C14	5.27	134.27	123.47
22	A	851	BCR	C34-C9-C10	-5.22	115.61	122.92
22	B	849	BCR	C30-C25-C26	-5.22	115.27	122.61
24	A	801	CL0	C1C-C2C-C3C	-5.13	101.57	106.96
22	K	202	BCR	C16-C15-C14	5.09	133.90	123.47
24	A	801	CL0	C4D-CHA-C1A	-5.08	114.37	126.62
21	1	616	LUT	C15-C35-C34	5.02	133.76	123.47
17	4	615	CHL	C3C-C4C-NC	4.97	116.14	110.57
24	A	801	CL0	C1D-CHD-C4C	-4.96	115.36	126.06
22	A	851	BCR	C7-C8-C9	-4.95	118.76	126.23
17	4	607	CHL	C3C-C4C-NC	4.94	116.11	110.57
17	2	615	CHL	O2D-CGD-CBD	4.94	120.05	111.27
17	2	606	CHL	O2D-CGD-CBD	4.92	120.01	111.27
22	J	102	BCR	C16-C15-C14	4.90	133.50	123.47
22	B	845	BCR	C19-C18-C17	4.87	126.42	118.94
19	1	614	XAT	O4-C5-C18	4.87	120.89	115.06
17	4	606	CHL	C3C-C4C-NC	4.85	116.02	110.57
22	A	851	BCR	C37-C22-C21	-4.84	116.14	122.92
21	1	616	LUT	C30-C31-C32	4.82	138.26	123.22
17	2	605	CHL	O2D-CGD-CBD	4.78	119.76	111.27
22	B	847	BCR	C16-C15-C14	4.77	133.25	123.47
19	1	614	XAT	C35-C34-C33	-4.74	120.54	127.31
17	4	605	CHL	C3C-C4C-NC	4.70	115.70	110.57
17	2	605	CHL	C3C-C4C-NC	4.70	115.70	110.57
17	2	607	CHL	O2D-CGD-CBD	4.68	119.59	111.27
21	2	616	LUT	C7-C8-C9	4.68	133.30	126.23
17	2	607	CHL	C3C-C4C-NC	4.67	115.81	110.57
17	4	607	CHL	O2D-CGD-CBD	4.66	119.55	111.27
17	4	606	CHL	O2D-CGD-CBD	4.65	119.52	111.27
17	3	606	CHL	O2D-CGD-CBD	4.63	119.49	111.27
21	2	616	LUT	C19-C9-C10	-4.62	116.44	122.92
17	4	615	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
17	4	607	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
21	2	616	LUT	C39-C29-C30	-4.60	116.48	122.92
22	L	306	BCR	C34-C9-C10	-4.59	116.49	122.92
17	3	606	CHL	C2C-C1C-NC	4.57	114.26	109.97
18	A	842	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
17	2	601	CHL	C3C-C4C-NC	4.55	115.68	110.57
17	3	606	CHL	C3D-C2D-C1D	-4.55	99.62	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	304	BCR	C16-C15-C14	4.55	132.79	123.47
17	1	601	CHL	C3C-C4C-NC	4.54	115.67	110.57
17	2	605	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
17	2	607	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
17	3	606	CHL	C3C-C4C-NC	4.50	115.62	110.57
17	4	606	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
21	3	613	LUT	C39-C29-C30	-4.50	116.62	122.92
22	B	843	BCR	C34-C9-C10	-4.49	116.64	122.92
17	1	601	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
21	2	619	LUT	C19-C9-C10	-4.48	116.64	122.92
17	2	615	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
17	2	615	CHL	C3C-C4C-NC	4.46	115.58	110.57
22	A	853	BCR	C16-C15-C14	4.46	132.61	123.47
22	L	306	BCR	C16-C15-C14	4.45	132.58	123.47
22	K	202	BCR	C15-C16-C17	4.44	132.56	123.47
17	2	606	CHL	C3C-C4C-NC	4.43	115.54	110.57
17	2	606	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
22	A	851	BCR	C11-C10-C9	4.42	133.62	127.31
17	2	615	CHL	C1B-CHB-C4A	-4.42	121.36	130.12
17	2	601	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
22	B	845	BCR	C36-C18-C17	-4.41	116.75	122.92
22	G	204	BCR	C15-C16-C17	4.41	132.50	123.47
22	K	205	BCR	C19-C18-C17	4.40	125.70	118.94
22	L	306	BCR	C37-C22-C21	-4.40	116.76	122.92
22	A	848	BCR	C15-C16-C17	4.39	132.46	123.47
17	4	606	CHL	C2C-C1C-NC	4.38	114.08	109.97
22	K	202	BCR	C34-C9-C10	-4.37	116.80	122.92
22	K	202	BCR	C37-C22-C21	-4.37	116.80	122.92
22	B	844	BCR	C37-C22-C21	-4.37	116.80	122.92
22	K	205	BCR	C37-C22-C21	-4.35	116.83	122.92
18	A	820	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
22	A	852	BCR	C37-C22-C21	-4.32	116.87	122.92
17	2	605	CHL	C1B-CHB-C4A	-4.32	121.57	130.12
19	2	617	XAT	C39-C29-C30	-4.31	116.88	122.92
17	4	605	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
19	4	617	XAT	C19-C9-C10	-4.31	116.89	122.92
22	J	102	BCR	C34-C9-C10	-4.30	116.89	122.92
22	B	846	BCR	C34-C9-C10	-4.30	116.90	122.92
22	B	801	BCR	C16-C15-C14	4.30	132.27	123.47
17	1	606	CHL	C3D-C2D-C1D	-4.29	99.98	105.83
22	A	850	BCR	C34-C9-C10	-4.29	116.92	122.92
18	A	828	CLA	CMB-C2B-C1B	-4.28	121.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	301	BCR	C12-C13-C14	4.27	125.49	118.94
22	F	304	BCR	C34-C9-C10	-4.26	116.95	122.92
21	2	619	LUT	C39-C29-C30	-4.24	116.98	122.92
22	L	305	BCR	C37-C22-C21	-4.24	116.98	122.92
19	2	617	XAT	C19-C9-C10	-4.24	116.98	122.92
21	1	616	LUT	C19-C9-C10	-4.24	116.98	122.92
22	A	852	BCR	C16-C15-C14	4.24	132.16	123.47
22	L	301	BCR	C37-C22-C21	-4.24	116.98	122.92
18	4	602	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
22	F	304	BCR	C21-C20-C19	4.23	136.42	123.22
18	B	818	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
22	B	848	BCR	C15-C16-C17	4.23	132.13	123.47
22	B	849	BCR	C16-C15-C14	4.23	132.13	123.47
24	A	801	CL0	C1B-CHB-C4A	-4.21	121.78	130.12
22	L	306	BCR	C8-C9-C10	4.21	125.41	118.94
22	K	205	BCR	C34-C9-C10	-4.21	117.03	122.92
22	K	205	BCR	C36-C18-C17	-4.21	117.03	122.92
18	B	825	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
22	4	618	BCR	C30-C25-C26	-4.19	116.71	122.61
22	B	844	BCR	C34-C9-C10	-4.17	117.09	122.92
18	2	612	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
22	B	844	BCR	C16-C15-C14	4.16	132.00	123.47
22	G	204	BCR	C37-C22-C21	-4.16	117.09	122.92
21	1	616	LUT	C31-C30-C29	4.16	133.25	127.31
21	1	616	LUT	C39-C29-C28	4.16	124.62	118.08
22	A	851	BCR	C15-C16-C17	4.13	131.94	123.47
18	2	609	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	L	301	BCR	C36-C18-C17	-4.13	117.14	122.92
22	B	849	BCR	C37-C22-C21	-4.12	117.15	122.92
22	B	801	BCR	C37-C22-C21	-4.12	117.15	122.92
22	A	851	BCR	C12-C13-C14	4.12	125.26	118.94
22	A	848	BCR	C37-C22-C21	-4.11	117.16	122.92
18	2	611	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
22	3	614	BCR	C34-C9-C10	-4.11	117.17	122.92
21	1	616	LUT	C32-C33-C34	4.10	125.24	118.94
18	B	809	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
18	B	822	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
17	4	607	CHL	CHD-C4C-C3C	-4.09	118.82	124.84
27	B	850	DGD	O2G-C1B-C2B	4.09	120.32	111.50
22	B	845	BCR	C34-C9-C10	-4.09	117.19	122.92
22	J	102	BCR	C37-C22-C21	-4.07	117.22	122.92
22	A	853	BCR	C37-C22-C21	-4.07	117.22	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	826	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
18	4	612	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
22	L	305	BCR	C34-C9-C10	-4.06	117.24	122.92
18	A	831	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
21	2	619	LUT	C8-C9-C10	4.05	125.16	118.94
17	4	615	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
22	L	301	BCR	C34-C9-C10	-4.05	117.25	122.92
22	F	304	BCR	C12-C13-C14	4.05	125.16	118.94
22	L	301	BCR	C35-C13-C14	-4.05	117.25	122.92
17	4	606	CHL	C4C-C3C-C2C	-4.05	101.00	106.90
21	2	616	LUT	C28-C29-C30	4.04	125.14	118.94
19	4	617	XAT	C39-C29-C30	-4.03	117.28	122.92
22	B	847	BCR	C34-C9-C10	-4.03	117.28	122.92
22	A	848	BCR	C34-C9-C10	-4.01	117.30	122.92
22	K	202	BCR	C12-C13-C14	4.01	125.10	118.94
21	1	616	LUT	C40-C33-C34	-4.01	117.30	122.92
18	4	613	CLA	CAA-C2A-C3A	-4.01	101.81	112.78
18	B	813	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
18	A	823	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
17	1	606	CHL	C4A-NA-C1A	3.99	108.50	106.71
18	G	203	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
18	3	603	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
22	4	618	BCR	C34-C9-C10	-3.98	117.34	122.92
22	A	849	BCR	C34-C9-C10	-3.98	117.34	122.92
22	B	848	BCR	C37-C22-C21	-3.98	117.34	122.92
22	4	618	BCR	C37-C22-C21	-3.98	117.34	122.92
22	B	846	BCR	C37-C22-C21	-3.98	117.35	122.92
22	K	202	BCR	C35-C13-C14	-3.98	117.35	122.92
22	A	852	BCR	C34-C9-C10	-3.98	117.35	122.92
22	L	305	BCR	C16-C15-C14	3.98	131.62	123.47
22	I	101	BCR	C15-C16-C17	3.97	131.61	123.47
22	3	614	BCR	C16-C15-C14	3.96	131.59	123.47
18	A	830	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
18	B	831	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
18	B	829	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
22	B	843	BCR	C8-C9-C10	3.94	124.99	118.94
18	A	815	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
22	B	848	BCR	C34-C9-C10	-3.93	117.42	122.92
22	4	618	BCR	C16-C15-C14	3.92	131.51	123.47
22	B	847	BCR	C37-C22-C21	-3.92	117.43	122.92
22	A	849	BCR	C30-C25-C26	-3.92	117.09	122.61
22	3	614	BCR	C37-C22-C21	-3.92	117.44	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	304	BCR	C35-C13-C14	-3.91	117.44	122.92
22	I	101	BCR	C37-C22-C21	-3.91	117.44	122.92
22	B	844	BCR	C21-C20-C19	3.91	135.41	123.22
18	A	802	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
18	B	821	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
18	B	821	CLA	CAA-C2A-C3A	-3.90	102.11	112.78
18	3	608	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
18	A	811	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
18	A	833	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
17	4	606	CHL	CHD-C4C-C3C	-3.89	119.12	124.84
18	A	818	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
21	3	613	LUT	C28-C29-C30	3.89	124.91	118.94
18	2	610	CLA	CAB-C3B-C4B	-3.89	122.49	128.46
18	A	805	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
22	B	843	BCR	C37-C22-C21	-3.88	117.49	122.92
22	G	204	BCR	C34-C9-C10	-3.88	117.49	122.92
22	A	850	BCR	C37-C22-C21	-3.88	117.49	122.92
20	1	615	LHG	O7-C7-C8	3.87	119.85	111.50
22	I	101	BCR	C34-C9-C10	-3.87	117.50	122.92
22	B	849	BCR	C34-C9-C10	-3.86	117.52	122.92
21	2	619	LUT	C40-C33-C34	-3.84	117.54	122.92
22	B	845	BCR	C1-C6-C5	-3.84	117.21	122.61
19	4	617	XAT	C15-C35-C34	3.84	131.33	123.47
22	A	852	BCR	C10-C11-C12	3.83	135.18	123.22
17	4	615	CHL	C2D-C1D-ND	3.83	112.93	110.10
22	F	304	BCR	C20-C21-C22	3.82	132.76	127.31
18	A	806	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
21	4	616	LUT	C19-C9-C10	-3.82	117.57	122.92
19	2	617	XAT	C28-C29-C30	3.82	124.80	118.94
17	1	606	CHL	C3C-C4C-NC	3.81	114.85	110.57
22	B	844	BCR	C15-C16-C17	3.81	131.28	123.47
21	2	619	LUT	C32-C33-C34	3.80	124.78	118.94
18	B	804	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
21	4	616	LUT	C39-C29-C30	-3.80	117.61	122.92
18	A	809	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
18	B	814	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	L	306	BCR	C35-C13-C14	-3.77	117.64	122.92
18	1	605	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
17	3	606	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
18	A	841	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
17	4	607	CHL	C2D-C1D-ND	3.77	112.88	110.10
22	A	849	BCR	C21-C20-C19	3.75	134.94	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	801	BCR	C8-C9-C10	3.75	124.69	118.94
22	L	306	BCR	C23-C22-C21	3.75	124.69	118.94
22	L	305	BCR	C15-C16-C17	3.74	131.14	123.47
22	B	846	BCR	C35-C13-C14	-3.74	117.68	122.92
22	L	306	BCR	C12-C13-C14	3.74	124.68	118.94
22	L	301	BCR	C21-C20-C19	3.74	134.87	123.22
22	A	852	BCR	C35-C13-C14	-3.73	117.69	122.92
18	A	839	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	A	852	BCR	C19-C18-C17	3.73	124.67	118.94
18	3	601	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
18	A	827	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
22	B	845	BCR	C20-C21-C22	3.72	132.62	127.31
17	4	606	CHL	C2D-C1D-ND	3.70	112.83	110.10
18	A	826	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
22	J	102	BCR	C35-C13-C14	-3.70	117.74	122.92
18	F	302	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
18	1	610	CLA	CAB-C3B-C4B	-3.69	122.79	128.46
18	L	303	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
17	1	601	CHL	C6-C5-C3	-3.68	108.60	114.62
22	B	846	BCR	C12-C13-C14	3.68	124.59	118.94
17	3	606	CHL	C3B-C4B-NB	3.67	113.95	109.21
17	2	607	CHL	CHD-C4C-C3C	-3.67	119.45	124.84
18	B	830	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
18	A	822	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
18	K	203	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
18	1	613	CLA	CAB-C3B-C4B	-3.66	122.83	128.46
22	B	801	BCR	C10-C11-C12	3.66	134.64	123.22
22	A	852	BCR	C23-C22-C21	3.66	124.56	118.94
22	A	852	BCR	C36-C18-C17	-3.66	117.80	122.92
18	B	824	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
22	J	102	BCR	C8-C9-C10	3.65	124.54	118.94
18	K	206	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
18	B	833	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
18	A	828	CLA	CMB-C2B-C3B	3.64	131.49	124.68
17	3	606	CHL	C4C-C3C-C2C	-3.64	101.60	106.90
18	4	602	CLA	CMB-C2B-C3B	3.64	131.48	124.68
18	4	603	CLA	CAB-C3B-C4B	-3.63	122.88	128.46
22	B	844	BCR	C36-C18-C17	-3.63	117.83	122.92
18	B	811	CLA	CAB-C3B-C4B	-3.63	122.88	128.46
18	4	613	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
18	1	602	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	1	608	CLA	CAB-C3B-C4B	-3.62	122.90	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	606	CHL	CAC-C3C-C4C	3.62	129.50	124.81
18	A	843	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
18	1	603	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
18	B	825	CLA	CMB-C2B-C3B	3.61	131.44	124.68
18	A	820	CLA	CMB-C2B-C3B	3.61	131.43	124.68
18	B	815	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
18	B	816	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
22	J	102	BCR	C12-C13-C14	3.61	124.48	118.94
18	A	842	CLA	CMB-C2B-C3B	3.61	131.43	124.68
18	2	608	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
22	K	205	BCR	C10-C11-C12	3.60	134.46	123.22
18	B	818	CLA	CMB-C2B-C3B	3.59	131.40	124.68
18	3	605	CLA	CAB-C3B-C4B	-3.59	122.95	128.46
22	A	853	BCR	C10-C11-C12	3.59	134.41	123.22
17	3	606	CHL	C2D-C1D-ND	3.59	112.75	110.10
18	2	609	CLA	CMB-C2B-C3B	3.59	131.39	124.68
18	B	837	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
24	A	801	CL0	C4C-C3C-C2C	-3.58	101.67	106.90
17	2	601	CHL	C1B-CHB-C4A	-3.58	123.02	130.12
17	4	607	CHL	CAC-C3C-C4C	3.58	129.45	124.81
18	B	820	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
22	A	853	BCR	C35-C13-C14	-3.57	117.92	122.92
22	K	202	BCR	C8-C9-C10	3.57	124.41	118.94
21	4	616	LUT	C15-C35-C34	3.57	130.78	123.47
18	B	813	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
17	4	615	CHL	C1D-ND-C4D	-3.56	103.81	106.33
17	1	601	CHL	CHD-C4C-C3C	-3.56	119.61	124.84
22	B	844	BCR	C23-C22-C21	3.55	124.39	118.94
18	B	827	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
18	A	832	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
24	A	801	CL0	C1-C2-C3	-3.54	119.92	126.04
18	A	844	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
18	2	602	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	K	202	BCR	C36-C18-C17	-3.53	117.97	122.92
22	L	306	BCR	C15-C16-C17	3.53	130.71	123.47
22	G	204	BCR	C36-C18-C17	-3.53	117.98	122.92
18	B	803	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
18	A	804	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
22	B	844	BCR	C35-C13-C14	-3.52	117.99	122.92
17	2	607	CHL	CAC-C3C-C4C	3.52	129.38	124.81
18	2	612	CLA	CMB-C2B-C3B	3.52	131.26	124.68
18	A	816	CLA	CMB-C2B-C1B	-3.52	123.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	606	CHL	CAC-C3C-C4C	3.52	129.37	124.81
18	B	806	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	L	305	BCR	C36-C18-C17	-3.51	118.01	122.92
22	L	306	BCR	C36-C18-C17	-3.50	118.02	122.92
22	B	847	BCR	C35-C13-C14	-3.50	118.02	122.92
18	4	609	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
18	B	812	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
18	A	804	CLA	O2D-CGD-O1D	-3.49	117.00	123.84
22	A	848	BCR	C36-C18-C17	-3.49	118.03	122.92
17	2	601	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
18	2	603	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
18	B	841	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
18	B	835	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
22	A	853	BCR	C11-C10-C9	3.48	132.28	127.31
18	A	821	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
18	B	832	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
18	1	612	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
18	A	810	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	L	305	BCR	C35-C13-C14	-3.47	118.06	122.92
18	A	804	CLA	CAA-C2A-C3A	-3.47	103.28	112.78
18	B	805	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
18	B	828	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	B	801	BCR	C35-C13-C14	-3.47	118.07	122.92
18	3	609	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
17	4	605	CHL	C3D-C4D-ND	3.46	115.84	110.24
18	A	835	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
18	4	604	CLA	CAB-C3B-C4B	-3.46	123.14	128.46
17	4	615	CHL	CAC-C3C-C4C	3.46	129.30	124.81
18	B	807	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
21	1	616	LUT	C20-C13-C14	-3.45	118.09	122.92
19	4	617	XAT	C35-C15-C14	3.45	130.54	123.47
22	K	205	BCR	C35-C13-C14	-3.45	118.09	122.92
18	3	607	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
18	B	809	CLA	CMB-C2B-C3B	3.45	131.12	124.68
22	K	202	BCR	C19-C18-C17	3.44	124.22	118.94
18	A	813	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
18	A	830	CLA	CMB-C2B-C3B	3.44	131.11	124.68
22	B	849	BCR	C35-C13-C14	-3.44	118.11	122.92
22	K	205	BCR	C23-C22-C21	3.44	124.21	118.94
18	4	612	CLA	CMB-C2B-C3B	3.43	131.10	124.68
18	F	303	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	K	201	CLA	CMB-C2B-C1B	-3.43	123.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	838	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
18	2	611	CLA	CMB-C2B-C3B	3.42	131.09	124.68
17	4	605	CHL	C3B-C4B-NB	3.42	113.63	109.21
17	2	605	CHL	CHD-C4C-C3C	-3.41	119.65	124.98
21	1	616	LUT	C39-C29-C30	-3.41	118.15	122.92
17	1	601	CHL	C1B-CHB-C4A	-3.41	123.37	130.12
17	4	605	CHL	CHD-C4C-C3C	-3.41	119.66	124.98
17	2	615	CHL	CAC-C3C-C4C	3.41	129.23	124.81
18	A	837	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
17	2	606	CHL	CAC-C3C-C4C	3.40	129.23	124.81
22	A	853	BCR	C12-C13-C14	3.40	124.16	118.94
18	A	823	CLA	CMB-C2B-C3B	3.40	131.04	124.68
18	A	807	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
17	4	607	CHL	C1D-ND-C4D	-3.39	103.92	106.33
17	2	607	CHL	C2D-C1D-ND	3.39	112.60	110.10
18	1	609	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
18	3	604	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
17	1	606	CHL	CAC-C3C-C4C	3.38	129.20	124.81
18	F	301	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	B	826	CLA	CMB-C2B-C3B	3.38	131.00	124.68
18	J	101	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	B	845	BCR	C21-C20-C19	3.38	133.76	123.22
18	A	808	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	L	302	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
17	2	615	CHL	CHD-C4C-C3C	-3.37	119.88	124.84
17	4	615	CHL	C3D-C4D-ND	3.37	115.69	110.24
17	1	601	CHL	CAC-C3C-C4C	3.37	129.18	124.81
22	A	852	BCR	C15-C16-C17	3.37	130.38	123.47
17	3	606	CHL	C3D-C4D-ND	3.37	115.69	110.24
18	A	819	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
22	4	618	BCR	C15-C16-C17	3.37	130.37	123.47
18	G	203	CLA	CMB-C2B-C3B	3.36	130.97	124.68
18	B	834	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
18	A	836	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	4	618	BCR	C35-C13-C14	-3.36	118.22	122.92
18	A	815	CLA	CMB-C2B-C3B	3.36	130.96	124.68
18	3	611	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
19	4	617	XAT	C20-C13-C14	-3.35	118.23	122.92
18	A	802	CLA	CMB-C2B-C3B	3.35	130.95	124.68
18	G	201	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
18	1	604	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
18	A	831	CLA	CMB-C2B-C3B	3.35	130.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	607	CHL	C3D-C4D-ND	3.35	115.65	110.24
18	4	614	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
22	K	202	BCR	C23-C22-C21	3.34	124.07	118.94
24	A	801	CL0	CHC-C1C-C2C	-3.34	117.48	126.72
18	B	821	CLA	CMB-C2B-C3B	3.34	130.93	124.68
18	A	811	CLA	CMB-C2B-C3B	3.34	130.92	124.68
18	4	611	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
18	B	822	CLA	CMB-C2B-C3B	3.34	130.92	124.68
18	B	840	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
22	A	851	BCR	C35-C13-C14	-3.34	118.25	122.92
17	2	606	CHL	C1B-CHB-C4A	-3.33	123.52	130.12
22	B	845	BCR	C35-C13-C14	-3.33	118.26	122.92
17	4	606	CHL	C3D-C4D-ND	3.33	115.62	110.24
18	B	831	CLA	CMB-C2B-C3B	3.33	130.91	124.68
18	3	608	CLA	CMB-C2B-C3B	3.33	130.91	124.68
18	1	608	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
17	1	601	CHL	C3D-C4D-ND	3.33	115.62	110.24
17	4	606	CHL	C1D-ND-C4D	-3.32	103.97	106.33
22	B	848	BCR	C36-C18-C17	-3.32	118.27	122.92
18	3	603	CLA	CMB-C2B-C3B	3.32	130.90	124.68
18	A	805	CLA	CMB-C2B-C3B	3.32	130.90	124.68
18	B	813	CLA	CMB-C2B-C3B	3.32	130.90	124.68
22	B	849	BCR	C15-C16-C17	3.32	130.28	123.47
18	3	605	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
22	3	614	BCR	C35-C13-C14	-3.32	118.27	122.92
17	2	606	CHL	CHD-C4C-C3C	-3.32	119.96	124.84
17	2	606	CHL	C3D-C4D-ND	3.32	115.61	110.24
18	A	818	CLA	CMB-C2B-C3B	3.32	130.88	124.68
17	3	606	CHL	C1D-ND-C4D	-3.32	103.98	106.33
18	A	833	CLA	CMB-C2B-C3B	3.31	130.88	124.68
18	B	810	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
18	B	817	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
22	A	851	BCR	C36-C18-C17	-3.31	118.28	122.92
18	3	612	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
18	3	610	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
18	A	814	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	B	849	BCR	C12-C13-C14	3.31	124.02	118.94
17	2	601	CHL	C3D-C4D-ND	3.31	115.59	110.24
18	B	839	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
18	L	304	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
18	1	611	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
18	2	610	CLA	CMB-C2B-C1B	-3.30	123.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	824	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
17	1	601	CHL	C2D-C1D-ND	3.30	112.54	110.10
17	4	607	CHL	C3B-C4B-NB	3.30	113.48	109.21
18	K	204	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
22	A	849	BCR	C1-C6-C5	-3.30	117.97	122.61
17	2	606	CHL	C3B-C4B-NB	3.30	113.47	109.21
18	A	834	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
18	1	613	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
18	A	812	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
18	A	840	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	4	617	XAT	C40-C33-C34	-3.29	118.32	122.92
22	B	847	BCR	C12-C13-C14	3.29	123.98	118.94
18	A	813	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
18	1	612	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
24	A	801	CL0	CMB-C2B-C3B	3.28	130.82	124.68
18	G	202	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
18	A	845	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	B	844	BCR	C12-C13-C14	3.28	123.97	118.94
22	F	304	BCR	C37-C22-C21	-3.28	118.33	122.92
22	A	849	BCR	C20-C21-C22	3.28	131.99	127.31
17	2	605	CHL	C2D-C1D-ND	3.28	112.52	110.10
21	1	616	LUT	C12-C13-C14	3.28	123.97	118.94
17	1	601	CHL	C1-C2-C3	-3.28	120.38	126.04
19	2	617	XAT	C32-C33-C34	3.27	123.97	118.94
17	2	601	CHL	CAC-C3C-C4C	3.27	129.06	124.81
22	B	849	BCR	C36-C18-C17	-3.27	118.34	122.92
22	F	304	BCR	C1-C6-C5	-3.27	118.00	122.61
17	2	607	CHL	C3D-C4D-ND	3.27	115.52	110.24
18	A	809	CLA	CMB-C2B-C3B	3.27	130.79	124.68
18	B	811	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	G	204	BCR	C19-C18-C17	3.26	123.95	118.94
22	L	306	BCR	C19-C18-C17	3.26	123.95	118.94
22	L	305	BCR	C19-C18-C17	3.26	123.94	118.94
17	2	615	CHL	C3B-C4B-NB	3.26	113.42	109.21
22	B	801	BCR	C36-C18-C17	-3.26	118.36	122.92
22	L	301	BCR	C19-C18-C17	3.25	123.93	118.94
22	L	305	BCR	C12-C13-C14	3.25	123.93	118.94
21	1	616	LUT	C35-C15-C14	3.25	130.13	123.47
22	A	848	BCR	C19-C18-C17	3.25	123.92	118.94
18	B	814	CLA	CMB-C2B-C3B	3.25	130.75	124.68
18	1	607	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
18	3	602	CLA	CMB-C2B-C1B	-3.24	123.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	829	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
22	I	101	BCR	C36-C18-C17	-3.24	118.38	122.92
18	4	608	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
18	B	836	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
18	A	803	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
18	B	829	CLA	CMB-C2B-C3B	3.24	130.74	124.68
17	2	607	CHL	C1-C2-C3	-3.23	121.52	126.75
17	2	601	CHL	C3B-C4B-NB	3.23	113.38	109.21
18	A	817	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
18	A	838	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
18	B	804	CLA	CMB-C2B-C3B	3.22	130.71	124.68
21	2	616	LUT	C35-C34-C33	3.22	131.91	127.31
17	4	605	CHL	C2D-C1D-ND	3.22	112.48	110.10
18	4	614	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
18	H	201	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
18	L	303	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
18	A	835	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
18	3	605	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
22	F	304	BCR	C10-C11-C12	3.21	133.23	123.22
22	B	846	BCR	C8-C9-C10	3.21	123.86	118.94
17	2	601	CHL	C2D-C1D-ND	3.20	112.46	110.10
18	4	601	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
22	B	801	BCR	C12-C13-C14	3.20	123.85	118.94
18	A	839	CLA	CMB-C2B-C3B	3.20	130.67	124.68
18	1	610	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
18	3	601	CLA	CMB-C2B-C3B	3.20	130.66	124.68
17	2	615	CHL	C2D-C1D-ND	3.20	112.46	110.10
18	A	806	CLA	CMB-C2B-C3B	3.19	130.65	124.68
18	2	604	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
22	B	843	BCR	C15-C14-C13	3.19	131.86	127.31
18	B	823	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
18	A	841	CLA	CMB-C2B-C3B	3.18	130.63	124.68
18	2	613	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
18	A	810	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
21	3	613	LUT	C19-C9-C10	-3.18	118.47	122.92
18	F	302	CLA	CMB-C2B-C3B	3.18	130.62	124.68
22	3	614	BCR	C15-C16-C17	3.18	129.98	123.47
22	3	614	BCR	C36-C18-C17	-3.17	118.48	122.92
22	J	102	BCR	C36-C18-C17	-3.17	118.49	122.92
22	4	618	BCR	C36-C18-C17	-3.17	118.49	122.92
18	4	610	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
22	G	204	BCR	C35-C13-C14	-3.16	118.49	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	605	CHL	C1D-ND-C4D	-3.16	104.09	106.33
18	B	819	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
18	B	825	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
18	B	822	CLA	CAA-C2A-C3A	-3.16	104.13	112.78
18	4	604	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
17	2	606	CHL	C2D-C1D-ND	3.16	112.43	110.10
22	A	850	BCR	C16-C17-C18	3.15	131.81	127.31
22	A	853	BCR	C36-C18-C17	-3.15	118.51	122.92
18	4	603	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
18	1	605	CLA	CMB-C2B-C3B	3.15	130.57	124.68
18	B	827	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
17	1	601	CHL	C3B-C4B-NB	3.14	113.27	109.21
22	A	848	BCR	C35-C13-C14	-3.14	118.52	122.92
18	B	802	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
18	L	303	CLA	CMB-C2B-C3B	3.14	130.55	124.68
18	B	824	CLA	CMB-C2B-C3B	3.13	130.54	124.68
18	A	826	CLA	CMB-C2B-C3B	3.13	130.54	124.68
21	4	616	LUT	C40-C33-C34	-3.13	118.54	122.92
18	B	808	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
17	2	607	CHL	C3B-C4B-NB	3.12	113.25	109.21
18	B	814	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	B	837	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
21	2	616	LUT	C20-C13-C14	-3.12	118.56	122.92
18	1	602	CLA	CMB-C2B-C3B	3.12	130.51	124.68
18	4	613	CLA	CMB-C2B-C3B	3.11	130.50	124.68
18	B	822	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
18	A	827	CLA	CMB-C2B-C3B	3.11	130.49	124.68
17	2	615	CHL	C3D-C4D-ND	3.11	115.26	110.24
18	A	825	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
17	2	607	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
17	1	606	CHL	C3D-C4D-ND	3.10	115.26	110.24
18	K	203	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	F	304	BCR	C8-C9-C10	3.10	123.70	118.94
22	B	801	BCR	C7-C8-C9	-3.10	121.55	126.23
22	A	849	BCR	C35-C13-C14	-3.10	118.58	122.92
18	2	608	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	B	803	CLA	CMB-C2B-C3B	3.10	130.47	124.68
17	4	605	CHL	CMD-C2D-C3D	-3.09	120.50	127.61
22	K	205	BCR	C21-C20-C19	3.09	132.85	123.22
18	B	804	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
22	B	801	BCR	C11-C10-C9	3.09	131.71	127.31
18	B	837	CLA	CMB-C2B-C3B	3.08	130.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	850	BCR	C15-C14-C13	3.08	131.71	127.31
24	A	801	CL0	O2A-CGA-CBA	3.08	121.57	111.91
18	B	833	CLA	CMB-C2B-C3B	3.08	130.43	124.68
18	B	816	CLA	CMB-C2B-C3B	3.07	130.42	124.68
18	A	802	CLA	CHB-C4A-NA	3.07	128.76	124.51
18	4	601	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	B	801	BCR	C15-C16-C17	3.07	129.75	123.47
22	B	845	BCR	C12-C13-C14	3.06	123.64	118.94
22	A	849	BCR	C37-C22-C21	-3.06	118.64	122.92
18	B	819	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	A	850	BCR	C8-C9-C10	3.06	123.63	118.94
17	2	605	CHL	C3D-C4D-ND	3.06	115.18	110.24
17	4	606	CHL	C1B-CHB-C4A	-3.06	124.07	130.12
24	A	801	CL0	CAC-C3C-C4C	3.06	128.77	124.81
22	B	801	BCR	C34-C9-C10	-3.05	118.64	122.92
22	A	851	BCR	C20-C21-C22	3.05	131.67	127.31
18	2	602	CLA	CMB-C2B-C3B	3.05	130.38	124.68
19	2	617	XAT	C40-C33-C34	-3.05	118.66	122.92
19	4	617	XAT	C8-C9-C10	3.05	123.62	118.94
18	B	830	CLA	CMB-C2B-C3B	3.05	130.38	124.68
18	B	805	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	A	844	CLA	CMB-C2B-C3B	3.04	130.37	124.68
18	A	809	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	B	826	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	2	605	CHL	C3B-C4B-NB	3.04	113.14	109.21
18	A	822	CLA	CMB-C2B-C3B	3.04	130.36	124.68
18	B	803	CLA	CHB-C4A-NA	3.03	128.70	124.51
18	B	815	CLA	CMB-C2B-C3B	3.03	130.35	124.68
22	4	618	BCR	C12-C13-C14	3.03	123.59	118.94
18	A	840	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
18	K	206	CLA	CMB-C2B-C3B	3.03	130.34	124.68
18	A	843	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	B	849	BCR	C19-C18-C17	3.03	123.58	118.94
18	B	841	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
18	4	609	CLA	CMB-C2B-C3B	3.02	130.33	124.68
18	A	804	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	I	101	BCR	C35-C13-C14	-3.02	118.69	122.92
18	A	810	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
18	B	818	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	A	849	BCR	C16-C17-C18	3.02	131.62	127.31
18	B	833	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
18	A	832	CLA	CMB-C2B-C3B	3.02	130.32	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	603	CLA	CMB-C2B-C3B	3.02	130.32	124.68
21	4	616	LUT	C35-C15-C14	3.02	129.65	123.47
22	B	846	BCR	C36-C18-C17	-3.01	118.70	122.92
18	A	830	CLA	CHB-C4A-NA	3.01	128.68	124.51
18	B	820	CLA	CMB-C2B-C3B	3.01	130.31	124.68
17	3	606	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
22	A	853	BCR	C15-C16-C17	3.01	129.63	123.47
18	3	608	CLA	CAA-C2A-C3A	-3.01	109.09	116.10
19	2	617	XAT	C20-C13-C14	-3.00	118.72	122.92
18	B	827	CLA	CMB-C2B-C3B	3.00	130.29	124.68
18	1	608	CLA	CAA-C2A-C3A	-3.00	109.11	116.10
22	B	848	BCR	C35-C13-C14	-3.00	118.73	122.92
22	B	843	BCR	C36-C18-C17	-2.99	118.73	122.92
18	G	201	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
18	B	806	CLA	CMB-C2B-C3B	2.99	130.27	124.68
18	A	835	CLA	CMB-C2B-C3B	2.99	130.27	124.68
24	A	801	CL0	CMC-C2C-C1C	2.99	129.59	125.04
21	3	613	LUT	C8-C9-C10	2.98	123.52	118.94
18	1	609	CLA	CHB-C4A-NA	2.98	128.64	124.51
18	H	201	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	B	807	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	F	304	BCR	C19-C18-C17	2.97	123.50	118.94
18	2	603	CLA	CMB-C2B-C3B	2.97	130.24	124.68
18	A	810	CLA	C1-C2-C3	-2.97	121.94	126.75
18	K	204	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	2	619	LUT	C28-C29-C30	2.97	123.50	118.94
18	B	832	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	B	848	BCR	C19-C18-C17	2.97	123.50	118.94
21	4	616	LUT	C20-C13-C14	-2.97	118.76	122.92
18	2	610	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	B	838	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	1	614	XAT	C27-C28-C29	-2.97	120.92	125.53
19	1	614	XAT	C15-C14-C13	-2.97	123.08	127.31
18	A	826	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	F	303	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	B	815	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	A	853	BCR	C34-C9-C10	-2.96	118.77	122.92
22	B	847	BCR	C36-C18-C17	-2.96	118.77	122.92
18	K	203	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	4	617	XAT	C12-C13-C14	2.96	123.48	118.94
22	L	305	BCR	C23-C22-C21	2.96	123.48	118.94
21	2	616	LUT	C30-C31-C32	2.96	132.45	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	834	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	B	820	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	A	815	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	B	841	CLA	CMB-C2B-C3B	2.95	130.20	124.68
18	B	823	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	A	844	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	B	811	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	4	613	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	A	852	BCR	C1-C6-C5	-2.95	118.46	122.61
18	2	612	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	2	617	XAT	C30-C31-C32	2.95	132.42	123.22
19	2	617	XAT	C12-C13-C14	2.95	123.46	118.94
18	4	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
18	A	816	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	L	306	BCR	C10-C11-C12	2.94	132.40	123.22
18	B	807	CLA	CMB-C2B-C3B	2.94	130.17	124.68
17	1	601	CHL	C1D-ND-C4D	-2.93	104.25	106.33
18	A	832	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	A	821	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	A	838	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	3	613	LUT	C20-C13-C14	-2.93	118.82	122.92
18	A	833	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	B	836	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
22	3	614	BCR	C12-C13-C14	2.93	123.43	118.94
18	2	604	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
18	A	820	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	L	302	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
17	4	605	CHL	C1B-CHB-C4A	-2.91	124.35	130.12
18	2	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	A	823	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
18	1	603	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
18	1	611	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
18	A	845	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
18	3	601	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	4	602	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	4	617	XAT	C32-C33-C34	2.90	123.39	118.94
18	2	610	CLA	CAB-C3B-C2B	2.90	130.36	124.69
18	A	842	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
21	1	616	LUT	C8-C9-C10	2.90	123.39	118.94
18	1	604	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	A	851	BCR	C19-C18-C17	2.89	123.38	118.94
18	B	840	CLA	O2D-CGD-O1D	-2.89	118.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	817	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	A	827	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	4	613	CLA	CHB-C4A-NA	2.89	128.50	124.51
17	3	606	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
18	B	830	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	B	824	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	A	801	CL0	C2A-C1A-CHA	-2.88	117.24	123.39
18	B	816	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
18	A	810	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	1	601	CHL	O2A-CGA-CBA	2.87	120.93	111.91
24	A	801	CL0	C4-C3-C5	2.87	120.11	115.27
18	A	819	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	A	837	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	3	608	CLA	CMA-C3A-C2A	-2.87	109.39	116.10
17	2	615	CHL	CMD-C2D-C3D	-2.87	121.00	127.61
18	A	836	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	L	306	BCR	C7-C8-C9	2.87	130.57	126.23
17	2	601	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
17	2	606	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
21	2	616	LUT	C12-C13-C14	2.87	123.34	118.94
18	A	805	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	A	848	BCR	C16-C15-C14	2.86	129.33	123.47
17	1	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
18	1	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	607	CHL	O2A-CGA-CBA	2.86	120.88	111.91
18	A	828	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	607	CHL	C1D-ND-C4D	-2.86	104.30	106.33
18	B	810	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	A	816	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	A	829	CLA	CMB-C2B-C3B	2.86	130.02	124.68
18	A	806	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
18	3	607	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	F	304	BCR	C36-C18-C17	-2.85	118.93	122.92
18	B	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	A	801	CL0	C4D-C3D-C2D	2.85	109.09	106.75
18	B	802	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	K	201	CLA	CMB-C2B-C3B	2.85	130.01	124.68
18	A	839	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	J	101	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	4	605	CHL	CAC-C3C-C4C	2.85	129.37	125.04
18	A	807	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	A	811	CLA	O2D-CGD-O1D	-2.85	118.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	822	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	A	831	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	B	831	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	3	603	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	B	813	CLA	O2D-CGD-CBD	2.84	116.32	111.27
22	A	851	BCR	C24-C23-C22	-2.84	121.94	126.23
18	B	834	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
18	3	612	CLA	CMB-C2B-C3B	2.84	129.99	124.68
18	B	804	CLA	CAA-C2A-C3A	-2.84	109.48	116.10
21	3	613	LUT	C35-C34-C33	2.84	131.36	127.31
18	A	819	CLA	CMB-C2B-C3B	2.84	129.98	124.68
18	1	604	CLA	CMB-C2B-C3B	2.83	129.98	124.68
17	2	605	CHL	CAC-C3C-C4C	2.83	129.35	125.04
18	B	808	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	1	601	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
18	3	609	CLA	CMB-C2B-C3B	2.83	129.97	124.68
27	B	850	DGD	C2G-O2G-C1B	-2.83	110.83	117.79
18	B	812	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	4	608	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	4	615	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
18	B	835	CLA	CMB-C2B-C3B	2.82	129.96	124.68
18	2	613	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	4	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	G	203	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	1	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	G	204	BCR	C16-C15-C14	2.82	129.24	123.47
18	G	202	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	A	814	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
22	I	101	BCR	C19-C18-C17	2.81	123.26	118.94
18	B	803	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	B	828	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	4	610	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	I	101	BCR	C16-C15-C14	2.81	129.23	123.47
19	1	614	XAT	C26-C27-C28	-2.81	120.05	125.99
18	A	824	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	B	835	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	B	801	BCR	C19-C18-C17	2.81	123.25	118.94
18	A	804	CLA	CHB-C4A-NA	2.80	128.39	124.51
18	A	837	CLA	CMB-C2B-C3B	2.80	129.92	124.68
18	4	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	A	841	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	B	839	CLA	O2D-CGD-O1D	-2.80	118.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	601	CHL	C1D-ND-C4D	-2.80	104.35	106.33
18	A	817	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	L	301	BCR	C23-C22-C21	2.80	123.23	118.94
18	J	101	CLA	CMB-C2B-C3B	2.80	129.91	124.68
18	A	803	CLA	CMB-C2B-C3B	2.80	129.91	124.68
18	1	610	CLA	CAA-C2A-C3A	-2.80	109.58	116.10
18	A	814	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	A	802	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	A	819	CLA	CHB-C4A-NA	2.79	128.37	124.51
21	2	619	LUT	C20-C13-C14	-2.79	119.02	122.92
18	B	832	CLA	CMB-C2B-C3B	2.79	129.90	124.68
17	4	607	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
18	A	825	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
18	F	302	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	F	301	CLA	CMB-C2B-C3B	2.79	129.89	124.68
22	F	304	BCR	C37-C22-C23	2.79	122.47	118.08
18	3	602	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	F	301	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	B	834	CLA	CMB-C2B-C3B	2.78	129.88	124.68
18	2	610	CLA	C1A-CHA-C4D	-2.78	121.83	125.72
18	A	808	CLA	CMB-C2B-C3B	2.78	129.87	124.68
18	F	303	CLA	CAA-C2A-C3A	-2.78	109.62	116.10
18	B	811	CLA	CHB-C4A-NA	2.77	128.35	124.51
17	2	605	CHL	CMD-C2D-C3D	-2.77	121.23	127.61
18	1	604	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	A	843	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	4	614	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	B	825	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	2	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
18	3	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
18	1	605	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
18	3	610	CLA	CMB-C2B-C3B	2.77	129.86	124.68
18	B	817	CLA	CMB-C2B-C3B	2.77	129.86	124.68
21	3	613	LUT	C35-C15-C14	2.77	129.14	123.47
22	J	102	BCR	C15-C16-C17	2.77	129.14	123.47
17	2	607	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
22	B	844	BCR	C30-C25-C26	-2.76	118.72	122.61
21	2	616	LUT	C19-C9-C8	2.76	122.43	118.08
17	2	606	CHL	C1D-ND-C4D	-2.76	104.38	106.33
18	2	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	A	824	CLA	CMB-C2B-C3B	2.76	129.84	124.68
18	B	839	CLA	CMB-C2B-C3B	2.76	129.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	830	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
18	G	201	CLA	CMB-C2B-C3B	2.76	129.84	124.68
18	B	829	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
18	B	834	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	1	612	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	A	836	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	A	842	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	A	829	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	A	828	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	1	609	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	3	611	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	A	812	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	2	609	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	A	824	CLA	CAA-C2A-C3A	-2.75	109.69	116.10
18	4	611	CLA	CMB-C2B-C3B	2.75	129.81	124.68
18	A	834	CLA	CMB-C2B-C3B	2.75	129.81	124.68
18	4	608	CLA	CMB-C2B-C3B	2.74	129.81	124.68
18	4	609	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	A	845	CLA	CMB-C2B-C3B	2.74	129.81	124.68
18	2	608	CLA	CHB-C4A-NA	2.74	128.30	124.51
18	B	822	CLA	C1-C2-C3	-2.74	121.30	126.04
18	F	303	CLA	CMB-C2B-C3B	2.74	129.80	124.68
18	A	830	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	3	607	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	L	303	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	4	601	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	L	304	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	B	828	CLA	CMB-C2B-C3B	2.73	129.78	124.68
18	1	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	A	803	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
18	B	806	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
18	B	822	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	A	807	CLA	CMB-C2B-C3B	2.72	129.78	124.68
18	L	304	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	B	808	CLA	CMB-C2B-C3B	2.72	129.77	124.68
18	A	802	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
18	A	838	CLA	CMB-C2B-C3B	2.72	129.77	124.68
18	B	840	CLA	CMB-C2B-C3B	2.72	129.77	124.68
18	B	821	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	A	805	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	B	809	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	2	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	4	601	CLA	CMB-C2B-C3B	2.72	129.77	124.68
18	L	304	CLA	CMB-C2B-C3B	2.72	129.77	124.68
22	K	202	BCR	C10-C11-C12	2.72	131.70	123.22
18	3	612	CLA	CAA-C2A-C3A	-2.72	109.75	116.10
18	B	809	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	3	612	CLA	O2D-CGD-O1D	-2.72	117.92	124.09
18	L	302	CLA	CMB-C2B-C3B	2.72	129.76	124.68
18	4	614	CLA	CMB-C2B-C3B	2.71	129.76	124.68
18	2	609	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
18	A	835	CLA	CHB-C4A-NA	2.71	128.26	124.51
21	2	619	LUT	C7-C8-C9	-2.71	122.14	126.23
22	B	844	BCR	C8-C9-C10	2.71	123.09	118.94
18	4	603	CLA	CAB-C3B-C2B	2.70	129.98	124.69
18	B	805	CLA	CMB-C2B-C3B	2.70	129.74	124.68
18	K	204	CLA	CMB-C2B-C3B	2.70	129.74	124.68
18	4	609	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	B	848	BCR	C16-C15-C14	2.70	129.01	123.47
18	A	813	CLA	CMB-C2B-C3B	2.70	129.74	124.68
18	2	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
18	1	613	CLA	CAB-C3B-C2B	2.70	129.98	124.69
18	B	841	CLA	CHB-C4A-NA	2.70	128.24	124.51
17	2	601	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
18	B	810	CLA	CMB-C2B-C3B	2.70	129.72	124.68
18	A	812	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
18	A	808	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
18	A	809	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	B	833	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
18	A	843	CLA	CHB-C4A-NA	2.69	128.24	124.51
18	3	607	CLA	CMB-C2B-C3B	2.69	129.72	124.68
22	4	618	BCR	C19-C18-C17	2.69	123.07	118.94
17	1	606	CHL	C3B-C4B-NB	2.69	112.69	109.21
18	A	813	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	A	853	BCR	C19-C18-C17	2.69	123.07	118.94
18	1	610	CLA	CAB-C3B-C2B	2.69	129.95	124.69
22	B	844	BCR	C19-C18-C17	2.69	123.06	118.94
18	K	206	CLA	CBD-CHA-C1A	2.69	131.67	128.50
18	A	840	CLA	CMB-C2B-C3B	2.69	129.70	124.68
18	1	613	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
18	3	611	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
18	3	612	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	1	611	CLA	CMB-C2B-C3B	2.68	129.70	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	852	BCR	C12-C13-C14	2.68	123.06	118.94
24	A	801	CL0	CMD-C2D-C3D	-2.68	121.73	128.30
18	1	608	CLA	CAB-C3B-C2B	2.68	129.94	124.69
17	4	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
18	4	608	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	813	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	806	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	804	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	836	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	821	CLA	CMB-C2B-C3B	2.68	129.69	124.68
18	1	607	CLA	CMB-C2B-C3B	2.68	129.69	124.68
18	G	202	CLA	CMB-C2B-C3B	2.68	129.69	124.68
18	A	832	CLA	CHB-C4A-NA	2.68	128.21	124.51
18	A	829	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	B	839	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	2	602	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	J	102	BCR	C19-C18-C17	2.67	123.04	118.94
18	A	808	CLA	CHB-C4A-NA	2.67	128.21	124.51
17	2	605	CHL	CMB-C2B-C3B	2.67	129.67	124.68
22	A	849	BCR	C36-C18-C17	-2.67	119.18	122.92
18	B	838	CLA	CMB-C2B-C3B	2.67	129.67	124.68
18	3	608	CLA	CHB-C4A-NA	2.67	128.20	124.51
18	B	811	CLA	CAB-C3B-C2B	2.67	129.91	124.69
18	3	610	CLA	CAA-C2A-C3A	-2.67	109.88	116.10
18	A	833	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	B	845	BCR	C16-C17-C18	2.67	131.11	127.31
18	A	844	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	B	808	CLA	CHB-C4A-NA	2.66	128.20	124.51
17	2	601	CHL	CMB-C2B-C3B	2.66	129.66	124.68
18	A	818	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	A	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	836	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	B	845	BCR	C37-C22-C21	-2.66	119.19	122.92
18	1	612	CLA	O2D-CGD-CBD	2.66	116.00	111.27
18	1	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	827	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	840	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	2	613	CLA	CMB-C2B-C3B	2.66	129.65	124.68
18	A	834	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	A	812	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	4	610	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	A	849	BCR	C19-C18-C17	2.66	123.02	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	814	CLA	CMB-C2B-C3B	2.66	129.65	124.68
22	B	843	BCR	C35-C13-C14	-2.66	119.20	122.92
18	B	818	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	K	201	CLA	CAA-C2A-C3A	-2.66	109.90	116.10
18	3	602	CLA	CMB-C2B-C3B	2.65	129.65	124.68
21	3	613	LUT	C30-C31-C32	2.65	131.50	123.22
21	3	613	LUT	C32-C33-C34	2.65	123.01	118.94
18	B	810	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	3	605	CLA	CAB-C3B-C2B	2.65	129.88	124.69
18	1	608	CLA	CMB-C2B-C3B	2.65	129.88	124.69
22	A	852	BCR	C21-C20-C19	2.65	131.49	123.22
18	B	819	CLA	CHB-C4A-NA	2.65	128.17	124.51
17	1	606	CHL	CMB-C2B-C3B	2.64	129.63	124.68
18	B	812	CLA	CMB-C2B-C3B	2.64	129.63	124.68
18	A	831	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	B	820	CLA	C1-C2-C3	-2.64	122.47	126.75
18	1	609	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
18	3	601	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	G	202	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	H	201	CLA	CMB-C2B-C3B	2.64	129.62	124.68
18	3	610	CLA	O2D-CGD-O1D	-2.64	118.09	124.09
18	B	830	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	4	610	CLA	CMB-C2B-C3B	2.64	129.62	124.68
18	4	602	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	817	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	837	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	3	603	CLA	CHB-C4A-NA	2.63	128.16	124.51
22	A	849	BCR	C16-C15-C14	2.63	128.86	123.47
18	B	824	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	B	831	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	1	602	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	A	848	BCR	C12-C13-C14	2.63	122.97	118.94
18	1	607	CLA	CHB-C4A-NA	2.63	128.14	124.51
18	A	813	CLA	O2D-CGD-CBD	2.62	115.93	111.27
22	3	614	BCR	C19-C18-C17	2.62	122.97	118.94
18	A	827	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	B	828	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	821	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	4	604	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	825	CLA	CMB-C2B-C3B	2.62	129.58	124.68
18	1	613	CLA	CMB-C2B-C3B	2.62	129.82	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	605	CLA	CHB-C4A-NA	2.62	128.13	124.51
17	4	615	CHL	C1B-CHB-C4A	-2.62	124.93	130.12
18	B	820	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	B	811	CLA	CMB-C2B-C3B	2.61	129.81	124.69
18	A	825	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	A	841	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	4	611	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	G	203	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	2	615	CHL	CMB-C2B-C3B	2.61	129.56	124.68
17	2	605	CHL	C1D-ND-C4D	-2.61	104.48	106.33
18	2	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	B	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	B	812	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	B	815	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	G	201	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	B	807	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	A	817	CLA	CMB-C2B-C3B	2.60	129.55	124.68
18	B	823	CLA	CMB-C2B-C3B	2.60	129.54	124.68
18	1	610	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	B	838	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	K	203	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	1	613	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	A	816	CLA	CHB-C4A-NA	2.60	128.10	124.51
17	3	606	CHL	CMB-C2B-C3B	2.59	129.53	124.68
18	1	608	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	B	826	CLA	CHB-C4A-NA	2.59	128.10	124.51
17	2	615	CHL	C1D-ND-C4D	-2.59	104.49	106.33
18	4	612	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	A	845	CLA	CHB-C4A-NA	2.58	128.09	124.51
18	B	816	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	A	838	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	4	616	LUT	C32-C33-C34	2.58	122.90	118.94
18	2	610	CLA	CMB-C2B-C3B	2.58	129.74	124.69
18	A	826	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	A	806	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	K	201	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	B	849	BCR	C23-C22-C21	2.57	122.89	118.94
18	B	832	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	B	836	CLA	C1-C2-C3	-2.57	122.59	126.75
18	A	839	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	B	833	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	3	613	LUT	C40-C33-C34	-2.57	119.32	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	604	CLA	CAB-C3B-C2B	2.57	129.72	124.69
18	J	101	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	1	610	CLA	CMB-C2B-C3B	2.57	129.72	124.69
18	2	612	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	A	822	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	F	303	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	L	302	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	B	819	CLA	CMB-C2B-C3B	2.57	129.48	124.68
18	K	206	CLA	O2D-CGD-O1D	-2.56	118.27	124.09
19	1	614	XAT	C6-C7-C8	-2.56	120.57	125.99
18	A	815	CLA	CHB-C4A-NA	2.56	128.06	124.51
18	A	803	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	A	837	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	1	613	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
18	A	810	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	H	201	CLA	CHB-C4A-NA	2.56	128.05	124.51
17	4	615	CHL	CMB-C2B-C3B	2.56	129.70	124.69
22	F	304	BCR	C16-C17-C18	2.56	130.96	127.31
22	A	850	BCR	C35-C13-C14	-2.56	119.34	122.92
18	A	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	1	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	808	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
21	2	616	LUT	C35-C15-C14	2.55	128.70	123.47
18	A	823	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	B	829	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	G	204	BCR	C12-C13-C14	2.55	122.85	118.94
18	A	832	CLA	C1-C2-C3	-2.55	122.63	126.75
21	3	613	LUT	C11-C10-C9	2.54	130.94	127.31
18	B	835	CLA	CHB-C4A-NA	2.54	128.03	124.51
18	2	611	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	4	606	CHL	CMB-C2B-C3B	2.54	129.66	124.69
18	2	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	B	805	CLA	CHB-C4A-NA	2.54	128.02	124.51
17	2	607	CHL	CMB-C2B-C3B	2.54	129.42	124.68
18	3	605	CLA	CMB-C2B-C3B	2.54	129.65	124.69
17	1	606	CHL	CHD-C4C-C3C	-2.53	121.11	124.84
18	A	820	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	2	606	CHL	CMB-C2B-C3B	2.53	129.42	124.68
18	B	802	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	A	849	BCR	C12-C13-C14	2.53	122.83	118.94
18	3	610	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	2	603	CLA	O2D-CGD-O1D	-2.53	118.35	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	807	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	B	802	CLA	CMB-C2B-C3B	2.52	129.40	124.68
18	1	605	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	3	609	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	3	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	B	846	BCR	C15-C16-C17	2.51	128.62	123.47
18	3	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	L	301	BCR	C10-C11-C12	2.51	131.05	123.22
18	3	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	1	607	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
18	3	609	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
18	4	611	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
18	A	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	2	617	XAT	C35-C34-C33	2.50	130.88	127.31
18	3	604	CLA	O2D-CGD-O1D	-2.50	118.42	124.09
17	4	607	CHL	CMB-C2B-C3B	2.50	129.35	124.68
18	K	203	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	A	850	BCR	C12-C13-C14	2.50	122.77	118.94
18	1	610	CLA	O2D-CGD-O1D	-2.49	118.43	124.09
21	4	616	LUT	C19-C9-C8	2.49	122.00	118.08
18	4	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	801	BCR	C23-C22-C21	2.49	122.76	118.94
18	K	204	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	F	301	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	B	836	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	1	601	CHL	CMB-C2B-C3B	2.48	129.32	124.68
27	B	850	DGD	O1G-C1A-C2A	2.48	119.69	111.91
21	4	616	LUT	C39-C29-C28	2.47	121.97	118.08
18	4	603	CLA	CMB-C2B-C3B	2.46	129.51	124.69
18	B	823	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	G	204	BCR	C23-C22-C21	2.45	122.70	118.94
17	4	607	CHL	C1B-CHB-C4A	-2.45	125.26	130.12
18	4	604	CLA	CMB-C2B-C3B	2.44	129.47	124.69
21	3	613	LUT	C10-C11-C12	2.44	130.82	123.22
18	A	803	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
17	1	601	CHL	C4-C3-C5	2.44	119.37	115.27
17	1	606	CHL	CHD-C1D-C2D	2.44	130.59	125.48
18	2	609	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	2	617	XAT	C8-C9-C10	2.43	122.67	118.94
22	B	849	BCR	C30-C25-C24	2.43	122.66	115.78
18	B	816	CLA	C1-C2-C3	-2.43	121.84	126.04
18	A	844	CLA	C1B-CHB-C4A	-2.43	125.31	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	202	BCR	C30-C25-C24	2.43	122.64	115.78
22	B	846	BCR	C10-C11-C12	2.42	130.76	123.22
22	K	205	BCR	C8-C9-C10	2.42	122.65	118.94
17	2	605	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
18	4	609	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
22	B	847	BCR	C15-C16-C17	2.41	128.42	123.47
22	G	204	BCR	C30-C25-C26	-2.41	119.22	122.61
18	B	818	CLA	C1-C2-C3	-2.41	121.88	126.04
22	A	851	BCR	C15-C14-C13	2.41	130.75	127.31
19	2	617	XAT	C15-C14-C13	2.40	130.74	127.31
18	F	302	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	B	843	BCR	C1-C6-C7	2.40	122.56	115.78
17	2	607	CHL	C5-C3-C4	2.40	119.90	114.60
22	I	101	BCR	C12-C13-C14	2.39	122.61	118.94
18	B	825	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	K	202	BCR	C30-C25-C26	-2.39	119.25	122.61
18	2	604	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	A	851	BCR	C30-C25-C26	-2.38	119.26	122.61
22	J	102	BCR	C1-C6-C5	-2.38	119.26	122.61
18	4	614	CLA	O2D-CGD-CBD	2.38	115.50	111.27
18	A	810	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	B	821	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
18	A	802	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
18	B	839	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
17	2	606	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
22	L	306	BCR	C1-C6-C5	-2.37	119.28	122.61
18	B	833	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
18	B	822	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
22	B	846	BCR	C19-C18-C17	2.36	122.57	118.94
18	B	821	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
18	A	814	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	J	102	BCR	C10-C11-C12	2.36	130.58	123.22
17	2	606	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
22	K	205	BCR	C16-C15-C14	2.36	128.31	123.47
18	2	602	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
22	K	205	BCR	C1-C6-C5	-2.35	119.30	122.61
24	A	801	CL0	C2A-C3A-C4A	-2.35	98.07	101.87
18	3	607	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
18	A	835	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
17	1	606	CHL	C2D-C1D-ND	2.35	111.83	110.10
22	B	843	BCR	C1-C6-C5	-2.34	119.31	122.61
18	B	808	CLA	C1B-CHB-C4A	-2.34	125.48	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	814	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
18	L	304	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
22	B	848	BCR	C12-C13-C14	2.33	122.52	118.94
18	1	609	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	3	613	LUT	C12-C13-C14	2.33	122.52	118.94
22	A	850	BCR	C36-C18-C17	-2.33	119.66	122.92
22	B	843	BCR	C12-C13-C14	2.33	122.52	118.94
18	A	808	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
18	A	809	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	2	616	LUT	C40-C33-C34	-2.33	119.66	122.92
22	K	205	BCR	C30-C25-C26	-2.33	119.33	122.61
17	4	605	CHL	CMB-C2B-C3B	2.33	129.03	124.68
18	F	301	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	B	816	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	K	201	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	A	844	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
18	3	603	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	L	303	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	3	612	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	4	613	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
17	1	601	CHL	O2D-CGD-O1D	-2.32	118.82	124.09
18	4	612	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	L	302	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	4	616	LUT	C12-C13-C14	2.32	122.50	118.94
18	3	608	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	B	834	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
18	K	206	CLA	CHB-C4A-NA	2.31	127.71	124.51
18	A	834	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
18	4	609	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
22	B	849	BCR	C34-C9-C8	2.31	121.72	118.08
17	2	615	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
18	2	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
18	A	818	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
17	2	601	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
22	B	847	BCR	C19-C18-C17	2.31	122.48	118.94
19	2	617	XAT	C27-C28-C29	-2.31	121.95	125.53
18	A	822	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	4	608	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
18	A	808	CLA	C1-C2-C3	-2.30	123.02	126.75
18	A	839	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
18	A	819	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	A	836	CLA	C1B-CHB-C4A	-2.30	125.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	817	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	2	608	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	B	830	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	A	851	BCR	C30-C25-C24	2.30	122.29	115.78
18	B	835	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	A	830	CLA	C1-C2-C3	2.30	130.02	126.04
18	1	604	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	A	811	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	J	102	BCR	C23-C22-C21	2.30	122.47	118.94
22	A	851	BCR	C11-C12-C13	2.30	132.87	126.42
18	B	824	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	4	614	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	B	829	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	B	804	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	A	829	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
18	A	842	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
18	3	601	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
18	A	827	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	4	604	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	A	805	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	B	834	CLA	CHD-C1D-ND	-2.29	122.35	124.45
18	1	613	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	A	823	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	A	831	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	B	837	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	1	610	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
18	4	611	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
18	1	605	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	B	831	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	B	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	I	101	BCR	C34-C9-C8	2.28	121.67	118.08
18	B	836	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	B	840	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	A	812	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	A	837	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	B	827	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	2	619	LUT	C30-C31-C32	2.28	130.32	123.22
18	A	833	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
18	A	804	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
18	B	828	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
18	3	609	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	A	810	CLA	O2A-CGA-O1A	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	841	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	K	203	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
17	4	615	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
18	1	602	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	A	821	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	F	302	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	B	832	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	K	206	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
17	2	607	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
18	A	820	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	A	824	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	2	613	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
17	4	605	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
18	A	841	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	B	819	CLA	C1-C2-C3	-2.26	122.13	126.04
18	A	838	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	4	610	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	B	843	BCR	C19-C18-C17	2.26	122.41	118.94
18	A	816	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	B	809	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	1	615	LHG	O8-C23-C24	2.26	119.00	111.91
22	A	853	BCR	C30-C25-C24	2.26	122.17	115.78
18	A	845	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	A	853	BCR	C30-C25-C26	-2.26	119.43	122.61
18	F	303	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	A	840	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	B	819	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	B	848	BCR	C30-C25-C24	2.26	122.16	115.78
18	A	826	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
18	A	830	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	2	605	CHL	O2D-CGD-O1D	-2.26	119.43	123.84
18	H	201	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
22	L	305	BCR	C30-C25-C24	2.25	122.16	115.78
18	A	845	CLA	C1-C2-C3	-2.25	123.11	126.75
18	K	204	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	A	848	BCR	C23-C22-C21	2.25	122.39	118.94
22	L	305	BCR	C1-C6-C7	2.25	122.14	115.78
18	B	841	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
18	2	603	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
18	3	605	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
18	4	614	CLA	C1-C2-C3	-2.25	123.11	126.75
18	2	611	CLA	C1B-CHB-C4A	-2.25	125.66	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	601	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
22	L	306	BCR	C21-C20-C19	2.25	130.23	123.22
18	A	843	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
18	1	603	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	B	811	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	3	602	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	A	804	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
18	3	611	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	A	832	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	J	101	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	A	825	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	B	806	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
18	4	601	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
18	B	820	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	J	102	BCR	C1-C6-C7	2.24	122.11	115.78
21	2	619	LUT	C15-C14-C13	2.24	130.50	127.31
18	A	806	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
18	B	832	CLA	CHD-C1D-ND	-2.23	122.40	124.45
18	4	609	CLA	C1-C2-C3	-2.23	122.18	126.04
18	A	803	CLA	CHD-C1D-ND	-2.23	122.40	124.45
18	1	612	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	1	611	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	1	607	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
17	3	606	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
18	B	812	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	3	610	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
22	L	301	BCR	C8-C9-C10	2.23	122.36	118.94
18	A	815	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
18	B	810	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
18	G	203	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
18	A	813	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
18	1	608	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
18	4	602	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
18	B	821	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
18	B	815	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
18	B	841	CLA	O2D-CGD-CBD	2.22	115.21	111.27
18	2	609	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	A	848	BCR	C30-C25-C24	2.22	122.06	115.78
22	K	205	BCR	C30-C25-C24	2.22	122.06	115.78
18	A	835	CLA	O2D-CGD-CBD	2.22	115.21	111.27
17	2	607	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
18	A	828	CLA	C1B-CHB-C4A	-2.21	125.73	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	205	BCR	C1-C6-C7	2.21	122.04	115.78
17	4	615	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
18	B	838	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
17	4	605	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
18	G	202	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
18	A	814	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
18	A	810	CLA	CHD-C1D-ND	-2.21	122.43	124.45
22	B	849	BCR	C7-C8-C9	2.21	129.57	126.23
18	A	807	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
18	G	201	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
17	4	606	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
21	2	619	LUT	C11-C10-C9	2.20	130.46	127.31
22	B	845	BCR	C8-C9-C10	2.20	122.32	118.94
20	1	615	LHG	C5-O7-C7	-2.20	112.37	117.79
22	B	843	BCR	C16-C17-C18	2.20	130.45	127.31
22	L	305	BCR	C1-C6-C5	-2.20	119.52	122.61
24	A	801	CL0	CHB-C4A-NA	2.20	127.55	124.51
18	B	807	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
22	J	102	BCR	C7-C8-C9	2.19	129.55	126.23
17	1	606	CHL	O2D-CGD-O1D	-2.19	119.11	124.09
18	4	603	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	4	607	CHL	C2A-C1A-CHA	-2.19	120.03	123.86
18	B	805	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	B	823	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
18	A	844	CLA	CHD-C1D-ND	-2.19	122.44	124.45
18	A	819	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	4	607	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
18	A	827	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
18	A	817	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
22	A	852	BCR	C24-C23-C22	2.18	129.53	126.23
18	B	813	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
18	3	602	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
18	B	818	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
18	B	839	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
22	K	205	BCR	C12-C13-C14	2.18	122.28	118.94
18	B	816	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	B	805	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
18	3	604	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	G	204	BCR	C34-C9-C8	2.17	121.50	118.08
18	B	816	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	B	836	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	A	850	BCR	C19-C18-C17	2.17	122.26	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	808	CLA	C1-C2-C3	-2.16	122.30	126.04
22	L	305	BCR	C8-C9-C10	2.16	122.26	118.94
17	2	615	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
22	K	202	BCR	C21-C20-C19	2.16	129.94	123.22
22	B	848	BCR	C34-C9-C8	2.15	121.47	118.08
17	4	615	CHL	O2D-CGD-O1D	-2.15	119.20	124.09
18	2	610	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
17	4	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
22	A	850	BCR	C1-C6-C7	2.15	121.86	115.78
22	A	848	BCR	C30-C25-C26	-2.15	119.59	122.61
18	K	204	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	B	847	BCR	C8-C9-C10	2.15	122.23	118.94
18	4	609	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	B	814	CLA	CHD-C1D-ND	-2.14	122.48	124.45
18	A	804	CLA	O2D-CGD-CBD	2.14	115.07	111.27
22	L	305	BCR	C30-C25-C26	-2.14	119.60	122.61
18	B	813	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	B	838	CLA	CHD-C1D-ND	-2.13	122.49	124.45
17	1	601	CHL	C4A-NA-C1A	2.13	107.66	106.71
17	1	606	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
18	A	809	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	L	306	BCR	C1-C6-C7	2.13	121.80	115.78
18	B	837	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	I	101	BCR	C37-C22-C23	2.13	121.43	118.08
18	1	613	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	A	808	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	A	801	CL0	O2A-CGA-O1A	-2.13	118.22	123.59
18	A	807	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	A	853	BCR	C1-C6-C5	-2.12	119.62	122.61
18	A	838	CLA	C1-C2-C3	-2.12	122.37	126.04
18	A	841	CLA	C1-C2-C3	-2.12	122.37	126.04
18	B	820	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	4	616	LUT	C7-C8-C9	2.12	129.44	126.23
19	1	614	XAT	O24-C25-C26	-2.12	57.20	58.96
18	B	834	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	A	841	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	1	614	XAT	C35-C15-C14	-2.12	119.14	123.47
18	B	833	CLA	CHD-C1D-ND	-2.11	122.51	124.45
18	B	826	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	B	826	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
18	B	825	CLA	C1-C2-C3	-2.11	122.39	126.04
18	A	829	CLA	O2A-CGA-O1A	-2.11	118.26	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	614	BCR	C30-C25-C24	2.11	121.75	115.78
22	A	853	BCR	C23-C22-C21	2.11	122.18	118.94
19	1	614	XAT	C31-C30-C29	-2.11	124.30	127.31
18	B	814	CLA	O2D-CGD-CBD	2.11	115.01	111.27
18	B	827	CLA	O2D-CGD-CBD	2.11	115.01	111.27
18	A	836	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	2	602	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
18	B	825	CLA	O2D-CGD-CBD	2.10	115.01	111.27
27	B	850	DGD	O2G-C1B-O1B	-2.10	118.62	123.70
18	L	303	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	L	303	CLA	O2D-CGD-CBD	2.10	115.00	111.27
18	3	601	CLA	C1-C2-C3	-2.10	122.41	126.04
18	L	302	CLA	CHD-C1D-ND	-2.10	122.53	124.45
18	A	825	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	L	304	CLA	CHD-C1D-ND	-2.10	122.53	124.45
17	4	607	CHL	CHB-C4A-NA	2.10	127.41	124.51
18	B	819	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	B	829	CLA	CHD-C1D-ND	-2.10	122.53	124.45
17	4	605	CHL	O2D-CGD-O1D	-2.09	119.33	124.09
22	B	843	BCR	C10-C11-C12	2.09	129.75	123.22
18	B	805	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	B	824	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	3	614	BCR	C8-C9-C10	2.09	122.15	118.94
18	A	834	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	A	839	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	B	803	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	B	810	CLA	C1-C2-C3	-2.09	122.43	126.04
22	B	845	BCR	C24-C23-C22	-2.09	123.08	126.23
18	1	604	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
17	4	615	CHL	CHB-C4A-NA	2.08	127.39	124.51
22	3	614	BCR	C37-C22-C23	2.08	121.36	118.08
17	2	606	CHL	C4A-NA-C1A	2.08	107.64	106.71
18	3	608	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	A	812	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	A	825	CLA	C1-C2-C3	-2.08	122.44	126.04
18	B	833	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
22	B	845	BCR	C16-C15-C14	2.08	127.73	123.47
18	A	838	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	A	802	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	831	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	829	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	B	836	CLA	CHD-C1D-ND	-2.07	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	607	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	A	820	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	B	822	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	J	101	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
17	2	615	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
18	3	604	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	A	810	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
20	2	618	LHG	O7-C7-C8	2.07	115.95	111.50
17	2	601	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
19	1	614	XAT	O4-C5-C6	-2.06	57.25	58.96
17	4	605	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
17	2	615	CHL	C4A-NA-C1A	2.06	107.63	106.71
18	1	602	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
18	B	817	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	1	614	XAT	C7-C8-C9	-2.06	122.34	125.53
18	2	610	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	4	617	XAT	C28-C29-C30	2.06	122.10	118.94
18	B	828	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	1	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	3	609	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	818	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	843	BCR	C7-C8-C9	-2.05	123.14	126.23
22	4	618	BCR	C8-C9-C10	2.05	122.09	118.94
19	4	617	XAT	C16-C1-C2	-2.05	105.42	108.98
18	3	601	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	4	607	CHL	OMC-CMC-C2C	-2.05	121.06	125.69
18	B	807	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
18	A	837	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	B	806	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	F	301	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	B	814	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	2	605	CHL	CAA-C2A-C3A	-2.04	109.16	114.26
18	A	834	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	B	830	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	K	206	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	B	825	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	B	835	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	K	203	CLA	CHD-C1D-ND	-2.04	122.58	124.45
17	2	615	CHL	CAA-C2A-C3A	-2.04	109.17	114.26
18	A	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	840	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	B	838	CLA	O2A-CGA-O1A	-2.04	118.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	808	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	824	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	817	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	B	817	CLA	CHD-C1D-ND	-2.03	122.58	124.45
18	B	806	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	B	802	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	F	302	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	1	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	4	613	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
18	A	813	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	A	842	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
18	A	832	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	L	306	BCR	C24-C23-C22	2.03	129.30	126.23
18	2	602	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	2	601	CHL	O2A-CGA-CBA	2.03	120.24	112.23
18	B	837	CLA	O2D-CGD-CBD	2.03	114.87	111.27
18	A	830	CLA	C2A-C1A-CHA	2.03	127.40	123.86
18	J	101	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	848	BCR	C37-C22-C23	2.03	121.27	118.08
18	B	811	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	A	850	BCR	C1-C6-C5	-2.02	119.76	122.61
18	B	809	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
19	1	614	XAT	C10-C11-C12	-2.02	116.90	123.22
22	A	852	BCR	C30-C25-C24	2.02	121.50	115.78
18	B	840	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	1	614	XAT	C40-C33-C34	-2.02	120.10	122.92
22	3	614	BCR	C30-C25-C26	-2.02	119.77	122.61
18	4	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
17	1	606	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
18	3	609	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	A	831	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
18	A	807	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	L	303	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	B	847	BCR	C37-C22-C23	2.01	121.25	118.08
18	3	603	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
18	2	613	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	B	837	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	822	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	B	825	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	B	813	CLA	C1-C2-C3	-2.01	122.57	126.04
22	A	851	BCR	C10-C11-C12	-2.01	116.95	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	832	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	2	607	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
18	4	612	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	1	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	822	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
22	B	845	BCR	C30-C25-C26	-2.00	119.79	122.61
18	B	834	CLA	C1-C2-C3	-2.00	122.58	126.04
18	A	842	CLA	C2D-C1D-ND	-2.00	108.63	110.10
18	A	830	CLA	O2A-C1-C2	2.00	113.90	108.64
18	A	845	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	A	810	CLA	O2D-CGD-CBD	2.00	114.82	111.27
18	A	816	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	B	823	CLA	CHD-C1D-ND	-2.00	122.61	124.45
17	3	606	CHL	CMC-C2C-C1C	2.00	128.09	125.04
18	A	811	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	4	617	XAT	C10-C11-C12	2.00	129.46	123.22
18	3	607	CLA	CHD-C1D-ND	-2.00	122.62	124.45
18	A	830	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (179) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	601	CHL	NC
17	1	601	CHL	ND
17	1	601	CHL	NA
17	1	606	CHL	NC
17	1	606	CHL	ND
17	1	606	CHL	NA
17	2	605	CHL	NC
17	2	605	CHL	ND
17	2	605	CHL	NA
17	2	615	CHL	NC
17	2	615	CHL	ND
17	2	615	CHL	NA
17	2	601	CHL	NC
17	2	601	CHL	ND
17	2	601	CHL	NA
17	2	606	CHL	NC
17	2	606	CHL	ND
17	2	606	CHL	NA
17	2	607	CHL	NC
17	2	607	CHL	ND

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Mol	Chain	Res	Type	Atom
17	2	607	CHL	NA
17	3	606	CHL	NC
17	3	606	CHL	ND
17	3	606	CHL	NA
17	4	606	CHL	NC
17	4	606	CHL	ND
17	4	606	CHL	NA
17	4	615	CHL	NC
17	4	615	CHL	ND
17	4	615	CHL	NA
17	4	605	CHL	NC
17	4	605	CHL	ND
17	4	605	CHL	NA
17	4	607	CHL	NC
17	4	607	CHL	ND
17	4	607	CHL	NA
18	1	602	CLA	ND
18	1	603	CLA	ND
18	1	604	CLA	ND
18	1	605	CLA	ND
18	1	607	CLA	ND
18	1	608	CLA	ND
18	1	609	CLA	ND
18	1	610	CLA	ND
18	1	611	CLA	ND
18	1	612	CLA	ND
18	1	613	CLA	ND
18	2	611	CLA	ND
18	2	612	CLA	ND
18	2	609	CLA	ND
18	2	602	CLA	ND
18	2	604	CLA	ND
18	2	613	CLA	ND
18	2	610	CLA	ND
18	2	608	CLA	ND
18	2	603	CLA	ND
18	3	605	CLA	ND
18	3	611	CLA	ND
18	3	608	CLA	ND
18	3	609	CLA	ND
18	3	604	CLA	ND
18	3	603	CLA	ND

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Mol	Chain	Res	Type	Atom
18	3	601	CLA	ND
18	3	612	CLA	ND
18	3	610	CLA	ND
18	3	607	CLA	ND
18	3	602	CLA	ND
18	4	602	CLA	ND
18	4	601	CLA	ND
18	4	608	CLA	ND
18	4	609	CLA	ND
18	4	613	CLA	ND
18	4	612	CLA	ND
18	4	611	CLA	ND
18	4	610	CLA	ND
18	4	604	CLA	ND
18	4	614	CLA	ND
18	4	603	CLA	ND
18	A	819	CLA	ND
18	A	807	CLA	ND
18	A	805	CLA	ND
18	A	822	CLA	ND
18	A	821	CLA	ND
18	A	818	CLA	ND
18	A	825	CLA	ND
18	A	820	CLA	ND
18	A	806	CLA	ND
18	A	809	CLA	ND
18	A	804	CLA	ND
18	A	813	CLA	ND
18	A	808	CLA	ND
18	A	811	CLA	ND
18	A	810	CLA	ND
18	A	823	CLA	ND
18	A	824	CLA	ND
18	A	826	CLA	ND
18	A	803	CLA	ND
18	A	802	CLA	ND
18	A	830	CLA	ND
18	A	840	CLA	ND
18	A	845	CLA	ND
18	A	831	CLA	ND
18	A	835	CLA	ND
18	A	842	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	834	CLA	ND
18	A	843	CLA	ND
18	A	844	CLA	ND
18	A	841	CLA	ND
18	A	839	CLA	ND
18	A	817	CLA	ND
18	A	815	CLA	ND
18	A	814	CLA	ND
18	A	816	CLA	ND
18	A	828	CLA	ND
18	A	827	CLA	ND
18	A	833	CLA	ND
18	A	812	CLA	ND
18	A	829	CLA	ND
18	A	836	CLA	ND
18	A	838	CLA	ND
18	A	832	CLA	ND
18	A	837	CLA	ND
18	B	818	CLA	ND
18	B	830	CLA	ND
18	B	837	CLA	ND
18	B	821	CLA	ND
18	B	805	CLA	ND
18	B	826	CLA	ND
18	B	835	CLA	ND
18	B	834	CLA	ND
18	B	823	CLA	ND
18	B	833	CLA	ND
18	B	808	CLA	ND
18	B	819	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	816	CLA	ND
18	B	841	CLA	ND
18	B	831	CLA	ND
18	B	814	CLA	ND
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	813	CLA	ND
18	B	812	CLA	ND
18	B	806	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	832	CLA	ND
18	B	839	CLA	ND
18	B	802	CLA	ND
18	B	807	CLA	ND
18	B	820	CLA	ND
18	B	815	CLA	ND
18	B	803	CLA	ND
18	B	829	CLA	ND
18	B	804	CLA	ND
18	B	817	CLA	ND
18	B	822	CLA	ND
18	B	836	CLA	ND
18	B	840	CLA	ND
18	B	838	CLA	ND
18	F	303	CLA	ND
18	F	301	CLA	ND
18	F	302	CLA	ND
18	G	201	CLA	ND
18	G	202	CLA	ND
18	G	203	CLA	ND
18	H	201	CLA	ND
18	J	101	CLA	ND
18	K	206	CLA	ND
18	K	201	CLA	ND
18	K	204	CLA	ND
18	K	203	CLA	ND
18	L	304	CLA	ND
18	L	303	CLA	ND
18	L	302	CLA	ND
24	A	801	CL0	NC
24	A	801	CL0	NA

All (1437) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	2	605	CHL	C3C-C2C-CMC-OMC
17	2	601	CHL	C1A-C2A-CAA-CBA
17	2	601	CHL	C3A-C2A-CAA-CBA
17	2	601	CHL	CHA-CBD-CGD-O1D
17	2	601	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	3	606	CHL	CHA-CBD-CGD-O1D
17	3	606	CHL	CHA-CBD-CGD-O2D
17	3	606	CHL	CBD-CGD-O2D-CED
17	4	605	CHL	C1A-C2A-CAA-CBA
18	1	604	CLA	C1A-C2A-CAA-CBA
18	1	604	CLA	CHA-CBD-CGD-O1D
18	1	604	CLA	CHA-CBD-CGD-O2D
18	1	605	CLA	C1A-C2A-CAA-CBA
18	1	605	CLA	C3A-C2A-CAA-CBA
18	1	605	CLA	CBA-CGA-O2A-C1
18	1	607	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C3A-C2A-CAA-CBA
18	1	608	CLA	CBD-CGD-O2D-CED
18	1	609	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	2	612	CLA	C11-C12-C13-C14
18	2	602	CLA	C2-C3-C5-C6
18	2	602	CLA	C4-C3-C5-C6
18	2	613	CLA	CBD-CGD-O2D-CED
18	2	610	CLA	CMA-C3A-C4A-CHB
18	2	608	CLA	C3A-C2A-CAA-CBA
18	3	605	CLA	C1A-C2A-CAA-CBA
18	3	605	CLA	C3A-C2A-CAA-CBA
18	3	605	CLA	CAD-CBD-CGD-O1D
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	C1A-C2A-CAA-CBA
18	4	612	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	C6-C7-C8-C9
18	4	604	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	804	CLA	C11-C10-C8-C9
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	823	CLA	C1A-C2A-CAA-CBA
18	A	823	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	C11-C12-C13-C14
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	O2A-C1-C2-C3
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	845	CLA	C3A-C2A-CAA-CBA
18	A	845	CLA	CHA-CBD-CGD-O1D
18	A	845	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	817	CLA	C3A-C2A-CAA-CBA
18	A	814	CLA	C1A-C2A-CAA-CBA
18	A	814	CLA	C3A-C2A-CAA-CBA
18	A	827	CLA	C3A-C2A-CAA-CBA
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C6-C7-C8-C9
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C3A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C3A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	814	CLA	C2-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
18	B	814	CLA	C11-C10-C8-C9
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C11-C12-C13-C15
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	C2-C3-C5-C6
18	B	824	CLA	C4-C3-C5-C6
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	CHA-CBD-CGD-O1D
18	B	825	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	C11-C12-C13-C14
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	C6-C7-C8-C9
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C2-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	F	302	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CHA-CBD-CGD-O1D
18	G	201	CLA	CHA-CBD-CGD-O2D
18	G	202	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	C1A-C2A-CAA-CBA
18	K	204	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	C1A-C2A-CAA-CBA
19	1	614	XAT	C5-C6-C7-C8
19	1	614	XAT	O4-C6-C7-C8
19	1	614	XAT	C7-C8-C9-C10
19	1	614	XAT	C7-C8-C9-C19
19	1	614	XAT	C11-C12-C13-C14
19	1	614	XAT	C11-C12-C13-C20
19	1	614	XAT	O24-C26-C27-C28
19	2	617	XAT	O4-C6-C7-C8
19	2	617	XAT	C11-C10-C9-C19
19	2	617	XAT	C10-C11-C12-C13
19	2	617	XAT	C13-C14-C15-C35
19	2	617	XAT	O24-C26-C27-C28
19	2	617	XAT	C28-C29-C30-C31
19	2	617	XAT	C39-C29-C30-C31
19	2	617	XAT	C33-C34-C35-C15
19	4	617	XAT	C7-C8-C9-C10
19	4	617	XAT	C7-C8-C9-C19
20	1	615	LHG	C1-C2-C3-O3
20	1	615	LHG	C2-C3-O3-P
20	1	615	LHG	C3-O3-P-O4
20	1	615	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	O7-C5-C6-O8
20	2	618	LHG	C3-O3-P-O5
20	2	618	LHG	O9-C7-O7-C5
20	2	618	LHG	C8-C7-O7-C5
20	2	618	LHG	O10-C23-O8-C6
20	2	618	LHG	C24-C23-O8-C6
20	A	846	LHG	O10-C23-O8-C6
20	A	846	LHG	C24-C23-O8-C6
20	B	851	LHG	C8-C7-O7-C5
20	B	852	LHG	C2-C3-O3-P
20	B	852	LHG	C3-O3-P-O5
20	B	852	LHG	C4-O6-P-O3
21	2	619	LUT	C5-C6-C7-C8
21	3	613	LUT	C9-C10-C11-C12
21	3	613	LUT	C21-C26-C27-C28
21	3	613	LUT	C25-C26-C27-C28
22	3	614	BCR	C21-C22-C23-C24
22	3	614	BCR	C37-C22-C23-C24
22	4	618	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C30
22	A	852	BCR	C35-C13-C14-C15
22	A	852	BCR	C14-C15-C16-C17
22	A	852	BCR	C16-C17-C18-C19
22	A	852	BCR	C16-C17-C18-C36
22	A	852	BCR	C21-C22-C23-C24
22	A	852	BCR	C37-C22-C23-C24
22	A	850	BCR	C7-C8-C9-C10
22	A	850	BCR	C7-C8-C9-C34
22	A	851	BCR	C11-C12-C13-C14
22	A	851	BCR	C11-C12-C13-C35
22	B	846	BCR	C7-C8-C9-C10
22	B	846	BCR	C7-C8-C9-C34
22	B	846	BCR	C23-C24-C25-C26
22	B	846	BCR	C23-C24-C25-C30
22	B	844	BCR	C12-C13-C14-C15
22	B	844	BCR	C35-C13-C14-C15
22	B	844	BCR	C18-C19-C20-C21
22	B	801	BCR	C1-C6-C7-C8
22	B	801	BCR	C5-C6-C7-C8
22	B	845	BCR	C17-C18-C19-C20
22	B	845	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	B	845	BCR	C21-C22-C23-C24
22	B	845	BCR	C37-C22-C23-C24
22	B	849	BCR	C22-C23-C24-C25
22	F	304	BCR	C11-C12-C13-C14
22	F	304	BCR	C11-C12-C13-C35
22	F	304	BCR	C15-C16-C17-C18
22	J	102	BCR	C7-C8-C9-C10
22	J	102	BCR	C7-C8-C9-C34
27	B	850	DGD	O2G-C2G-C3G-O3G
18	2	609	CLA	O1D-CGD-O2D-CED
18	4	604	CLA	O1D-CGD-O2D-CED
18	B	802	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED
18	1	608	CLA	O1D-CGD-O2D-CED
18	3	608	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1D-CGD-O2D-CED
18	K	204	CLA	O1D-CGD-O2D-CED
18	1	605	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CBD-CGD-O2D-CED
18	2	609	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	CBD-CGD-O2D-CED
18	3	605	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	803	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	O1A-CGA-O2A-C1
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	835	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1D-CGD-O2D-CED
18	F	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	1	609	CLA	O1D-CGD-O2D-CED
18	2	613	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	G	201	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	CBA-CGA-O2A-C1
17	2	607	CHL	CBD-CGD-O2D-CED
17	4	607	CHL	CBD-CGD-O2D-CED
18	2	604	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	O1A-CGA-O2A-C1
18	2	609	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1A-CGA-O2A-C1
18	1	605	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	O1D-CGD-O2D-CED
18	A	841	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
17	2	601	CHL	CBD-CGD-O2D-CED
18	3	603	CLA	CBD-CGD-O2D-CED
18	B	840	CLA	CBD-CGD-O2D-CED
17	3	606	CHL	O1D-CGD-O2D-CED
20	B	851	LHG	O9-C7-O7-C5
18	B	827	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C3-C5-C6-C7
18	A	819	CLA	C3-C5-C6-C7
18	A	807	CLA	C3-C5-C6-C7
18	A	818	CLA	C3-C5-C6-C7
18	A	803	CLA	C3-C5-C6-C7
18	A	834	CLA	C3-C5-C6-C7
18	A	843	CLA	C3-C5-C6-C7
18	A	844	CLA	C3-C5-C6-C7
18	A	841	CLA	C3-C5-C6-C7
18	A	814	CLA	C3-C5-C6-C7
18	A	828	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	B	805	CLA	C3-C5-C6-C7
18	B	841	CLA	C3-C5-C6-C7
18	B	814	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	B	840	CLA	C3-C5-C6-C7
18	H	201	CLA	C3-C5-C6-C7
18	B	802	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
17	4	606	CHL	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	CBD-CGD-O2D-CED
18	A	820	CLA	C4-C3-C5-C6
18	A	839	CLA	C4-C3-C5-C6
18	B	809	CLA	C4-C3-C5-C6
18	A	820	CLA	C2-C3-C5-C6
18	A	839	CLA	C2-C3-C5-C6
18	1	602	CLA	CBD-CGD-O2D-CED
18	4	603	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	CBD-CGD-O2D-CED
18	J	101	CLA	CBD-CGD-O2D-CED
17	2	601	CHL	C2A-CAA-CBA-CGA
17	2	607	CHL	C2A-CAA-CBA-CGA
17	3	606	CHL	C2A-CAA-CBA-CGA
18	1	605	CLA	C2A-CAA-CBA-CGA
18	2	611	CLA	C2A-CAA-CBA-CGA
18	2	608	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	A	832	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	C3-C5-C6-C7
18	B	829	CLA	C3-C5-C6-C7
18	1	603	CLA	CBA-CGA-O2A-C1
18	2	609	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
17	2	606	CHL	CBD-CGD-O2D-CED
18	4	614	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	820	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	811	CLA	O1A-CGA-O2A-C1
18	A	839	CLA	O1A-CGA-O2A-C1
18	L	303	CLA	O1A-CGA-O2A-C1
21	1	616	LUT	C29-C30-C31-C32
21	2	616	LUT	C33-C34-C35-C15
21	3	613	LUT	C33-C34-C35-C15
22	A	849	BCR	C15-C16-C17-C18
22	A	849	BCR	C19-C20-C21-C22
22	A	853	BCR	C9-C10-C11-C12
22	A	850	BCR	C13-C14-C15-C16
22	A	850	BCR	C15-C16-C17-C18
22	A	851	BCR	C13-C14-C15-C16
22	B	801	BCR	C9-C10-C11-C12
22	B	843	BCR	C13-C14-C15-C16
22	B	845	BCR	C19-C20-C21-C22
22	F	304	BCR	C19-C20-C21-C22
18	1	612	CLA	CBD-CGD-O2D-CED
18	2	610	CLA	CBD-CGD-O2D-CED
18	3	601	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	O2-C2-C3-O3
18	B	827	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
24	A	801	CL0	C3-C5-C6-C7
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	CBA-CGA-O2A-C1
18	L	303	CLA	CBA-CGA-O2A-C1
18	1	605	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	O1D-CGD-O2D-CED
18	K	203	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	O1D-CGD-O2D-CED
18	4	602	CLA	C3-C5-C6-C7
18	B	803	CLA	C3-C5-C6-C7
18	B	822	CLA	C3-C5-C6-C7
18	A	820	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C26-C27-C28-C29
18	A	833	CLA	C4-C3-C5-C6
25	B	842	PQN	C14-C13-C15-C16
18	A	833	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	842	PQN	C12-C13-C15-C16
18	A	822	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	O1D-CGD-O2D-CED
18	A	842	CLA	CBA-CGA-O2A-C1
18	A	838	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBD-CGD-O2D-CED
18	3	605	CLA	O1D-CGD-O2D-CED
18	3	607	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
17	2	607	CHL	O1D-CGD-O2D-CED
17	4	607	CHL	O1D-CGD-O2D-CED
17	2	615	CHL	CBD-CGD-O2D-CED
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	842	CLA	O1A-CGA-O2A-C1
18	A	838	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	CBA-CGA-O2A-C1
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	CBA-CGA-O2A-C1
18	A	845	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBD-CGD-O2D-CED
18	B	808	CLA	CBD-CGD-O2D-CED
18	A	812	CLA	C5-C6-C7-C8
18	4	602	CLA	C5-C6-C7-C8
18	A	828	CLA	C15-C16-C17-C18
18	B	822	CLA	O1A-CGA-O2A-C1
18	B	809	CLA	C2-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C9
18	4	612	CLA	C11-C10-C8-C9
18	A	819	CLA	C6-C7-C8-C9
18	A	807	CLA	C11-C10-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	806	CLA	C11-C10-C8-C9
18	A	811	CLA	C14-C13-C15-C16
18	A	826	CLA	C11-C10-C8-C9
18	A	802	CLA	C11-C12-C13-C14
18	A	835	CLA	C11-C10-C8-C9
18	A	841	CLA	C14-C13-C15-C16
18	A	812	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	B	808	CLA	C6-C7-C8-C9
18	B	808	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C10-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	B	825	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C14
18	B	803	CLA	C11-C10-C8-C9
18	B	840	CLA	C14-C13-C15-C16
18	F	301	CLA	C6-C7-C8-C9
18	H	201	CLA	C6-C7-C8-C9
18	2	604	CLA	O1D-CGD-O2D-CED
18	B	809	CLA	O1D-CGD-O2D-CED
18	A	816	CLA	CBD-CGD-O2D-CED
19	2	617	XAT	C31-C32-C33-C40
21	2	616	LUT	C31-C32-C33-C40
22	4	618	BCR	C7-C8-C9-C34
22	A	853	BCR	C11-C12-C13-C35
22	B	846	BCR	C37-C22-C23-C24
22	K	205	BCR	C7-C8-C9-C34
22	K	205	BCR	C36-C18-C19-C20
22	L	306	BCR	C7-C8-C9-C34
22	L	306	BCR	C37-C22-C23-C24
21	2	616	LUT	C31-C32-C33-C34
22	A	853	BCR	C11-C12-C13-C14
22	L	306	BCR	C7-C8-C9-C10
22	L	306	BCR	C21-C22-C23-C24
18	A	806	CLA	C13-C15-C16-C17
18	A	832	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	C15-C16-C17-C18
18	A	806	CLA	C10-C11-C12-C13
18	A	835	CLA	C15-C16-C17-C18
18	A	842	CLA	C13-C15-C16-C17
18	A	812	CLA	C10-C11-C12-C13
18	B	814	CLA	C5-C6-C7-C8
18	B	835	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C34-C35-C36-C37
18	2	602	CLA	C5-C6-C7-C8
18	A	819	CLA	C5-C6-C7-C8
18	A	820	CLA	C5-C6-C7-C8
18	A	804	CLA	C8-C10-C11-C12
18	A	831	CLA	C13-C15-C16-C17
18	A	828	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	A	812	CLA	C8-C10-C11-C12
18	B	805	CLA	C10-C11-C12-C13
18	B	826	CLA	C8-C10-C11-C12
18	B	808	CLA	C13-C15-C16-C17
18	B	806	CLA	C10-C11-C12-C13
18	B	822	CLA	C13-C15-C16-C17
20	1	615	LHG	C7-C8-C9-C10
18	A	835	CLA	C8-C10-C11-C12
18	B	837	CLA	C5-C6-C7-C8
18	B	819	CLA	O1D-CGD-O2D-CED
18	A	843	CLA	C2-C1-O2A-CGA
18	2	602	CLA	C15-C16-C17-C18
18	A	844	CLA	C5-C6-C7-C8
20	1	615	LHG	C5-C4-O6-P
18	H	201	CLA	C8-C10-C11-C12
18	A	804	CLA	C6-C7-C8-C10
18	A	803	CLA	C11-C12-C13-C15
18	A	835	CLA	C11-C10-C8-C7
18	A	829	CLA	C11-C10-C8-C7
18	B	805	CLA	C6-C7-C8-C10
18	B	834	CLA	C6-C7-C8-C10
18	B	810	CLA	C6-C7-C8-C10
18	B	841	CLA	C11-C10-C8-C7
18	B	841	CLA	C12-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C15
18	2	612	CLA	C3-C5-C6-C7
18	B	802	CLA	C3-C5-C6-C7
17	1	601	CHL	O1A-CGA-O2A-C1
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	845	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	C2A-CAA-CBA-CGA
18	1	607	CLA	C2A-CAA-CBA-CGA
18	2	609	CLA	C2A-CAA-CBA-CGA
18	2	603	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	832	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	O1D-CGD-O2D-CED
18	A	828	CLA	C5-C6-C7-C8
18	H	201	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	F	301	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	C5-C6-C7-C8
19	2	617	XAT	C30-C31-C32-C33
22	B	849	BCR	C10-C11-C12-C13
22	K	205	BCR	C10-C11-C12-C13
22	K	205	BCR	C18-C19-C20-C21
18	A	828	CLA	C13-C15-C16-C17
18	A	829	CLA	C8-C10-C11-C12
18	B	813	CLA	C13-C15-C16-C17
18	B	841	CLA	CBA-CGA-O2A-C1
18	3	602	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	O1A-CGA-O2A-C1
18	3	601	CLA	C8-C10-C11-C12
18	A	806	CLA	C8-C10-C11-C12
18	A	829	CLA	C15-C16-C17-C18
18	B	814	CLA	C8-C10-C11-C12
18	B	817	CLA	C5-C6-C7-C8
18	B	840	CLA	C5-C6-C7-C8
18	3	603	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1A-CGA-O2A-C1
17	2	601	CHL	O1D-CGD-O2D-CED
18	A	839	CLA	O1D-CGD-O2D-CED
18	A	807	CLA	C5-C6-C7-C8
18	A	842	CLA	C8-C10-C11-C12
18	B	806	CLA	C5-C6-C7-C8
20	1	615	LHG	C3-O3-P-O6
18	B	808	CLA	C3-C5-C6-C7
18	A	813	CLA	CBA-CGA-O2A-C1
18	J	101	CLA	CBA-CGA-O2A-C1
17	4	606	CHL	O1D-CGD-O2D-CED
18	A	840	CLA	C4-C3-C5-C6
18	B	832	CLA	C15-C16-C17-C18
24	A	801	CL0	C10-C11-C12-C13
18	1	602	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	C2A-CAA-CBA-CGA
18	4	604	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C2A-CAA-CBA-CGA
18	G	201	CLA	C2A-CAA-CBA-CGA
18	A	839	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	A	830	CLA	C3-C5-C6-C7
18	A	843	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
18	4	602	CLA	C10-C11-C12-C13
18	A	811	CLA	C8-C10-C11-C12
18	B	839	CLA	C13-C15-C16-C17
18	J	101	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C13-C14-C15-C16
17	2	606	CHL	O1D-CGD-O2D-CED
18	4	603	CLA	O1D-CGD-O2D-CED
19	2	617	XAT	C20-C13-C14-C15
21	3	613	LUT	C11-C10-C9-C19
22	A	849	BCR	C20-C21-C22-C37
22	B	844	BCR	C16-C17-C18-C36
22	B	849	BCR	C11-C10-C9-C34
22	F	304	BCR	C35-C13-C14-C15
22	K	205	BCR	C20-C21-C22-C37
18	1	603	CLA	C5-C6-C7-C8
18	B	828	CLA	C16-C17-C18-C20
18	B	824	CLA	C16-C17-C18-C19
18	B	813	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
18	3	601	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C15-C16-C17-C18
18	B	813	CLA	O1D-CGD-O2D-CED
19	2	617	XAT	C11-C10-C9-C8
22	A	852	BCR	C12-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C19
22	B	849	BCR	C11-C10-C9-C8
22	K	205	BCR	C20-C21-C22-C23
18	A	819	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C25-C26-C27-C28
18	2	612	CLA	C10-C11-C12-C13
18	A	813	CLA	O1A-CGA-O2A-C1
18	A	843	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C6-C7-C8-C10
18	B	824	CLA	C16-C17-C18-C20
18	B	822	CLA	C16-C17-C18-C19
18	A	822	CLA	C4-C3-C5-C6
18	A	835	CLA	C4-C3-C5-C6
18	B	805	CLA	C11-C12-C13-C14
18	B	810	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	B	839	CLA	C6-C7-C8-C9
18	B	802	CLA	C11-C10-C8-C9
20	1	615	LHG	C23-C24-C25-C26
20	1	615	LHG	C27-C28-C29-C30
18	B	805	CLA	C5-C6-C7-C8
18	A	829	CLA	C2A-CAA-CBA-CGA
18	B	826	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C3-C5-C6-C7
18	B	809	CLA	C8-C10-C11-C12
20	1	615	LHG	C11-C10-C9-C8
27	B	850	DGD	C9A-CAA-CBA-CCA
18	2	612	CLA	C16-C17-C18-C20
18	A	839	CLA	C6-C7-C8-C9
18	2	610	CLA	O1D-CGD-O2D-CED
18	B	811	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	C8-C10-C11-C12
23	4	620	LMG	C29-C28-O8-C9
20	1	615	LHG	C12-C13-C14-C15
18	B	834	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C3A-C2A-CAA-CBA
18	B	815	CLA	C3A-C2A-CAA-CBA
18	G	201	CLA	C3A-C2A-CAA-CBA
18	K	203	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C8-C10-C11-C12
18	4	601	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	O1D-CGD-O2D-CED
18	J	101	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	C10-C11-C12-C13
18	B	811	CLA	CBD-CGD-O2D-CED
20	1	615	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	844	BCR	C14-C15-C16-C17
18	2	602	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	3	609	CLA	C4-C3-C5-C6
18	B	828	CLA	C4-C3-C5-C6
18	A	834	CLA	CBA-CGA-O2A-C1
18	3	609	CLA	C2-C3-C5-C6
18	B	817	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C6-C7-C8-C9
18	L	303	CLA	C8-C10-C11-C12
25	A	855	PQN	C25-C26-C27-C28
18	A	802	CLA	C3-C5-C6-C7
20	1	615	LHG	C18-C19-C20-C21
18	2	602	CLA	C13-C15-C16-C17
18	B	841	CLA	C13-C15-C16-C17
18	B	813	CLA	O1A-CGA-O2A-C1
20	B	851	LHG	C23-C24-C25-C26
21	2	619	LUT	C1-C6-C7-C8
21	4	616	LUT	C1-C6-C7-C8
21	4	616	LUT	C5-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C30
22	B	844	BCR	C23-C24-C25-C26
22	B	844	BCR	C23-C24-C25-C30
22	B	845	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C26
22	F	304	BCR	C1-C6-C7-C8
22	F	304	BCR	C5-C6-C7-C8
18	2	613	CLA	C2A-CAA-CBA-CGA
18	B	840	CLA	CBA-CGA-O2A-C1
18	A	834	CLA	C13-C15-C16-C17
18	A	819	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	C6-C7-C8-C10
18	3	601	CLA	C2-C3-C5-C6
18	A	819	CLA	C6-C7-C8-C10
18	A	807	CLA	C2-C3-C5-C6
18	A	807	CLA	C11-C10-C8-C7
18	A	822	CLA	C2-C3-C5-C6
18	A	806	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C10-C8-C7
18	A	835	CLA	C2-C3-C5-C6
18	B	808	CLA	C6-C7-C8-C10
18	B	810	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	B	828	CLA	C2-C3-C5-C6
18	B	806	CLA	C12-C13-C15-C16
18	B	839	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	840	CLA	C12-C13-C15-C16
18	A	834	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C20
18	3	609	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C2A-CAA-CBA-CGA
27	B	850	DGD	CCB-CDB-CEB-CFB
18	4	609	CLA	C5-C6-C7-C8
21	2	616	LUT	C6-C7-C8-C9
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	C16-C17-C18-C20
18	B	805	CLA	C8-C10-C11-C12
18	K	203	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	C2B-C1B-O2G-C2G
22	F	304	BCR	C10-C11-C12-C13
18	B	823	CLA	CBD-CGD-O2D-CED
27	B	850	DGD	O1B-C1B-O2G-C2G
23	4	619	LMG	C2-C1-O1-C7
20	1	615	LHG	C17-C18-C19-C20
18	B	828	CLA	C16-C17-C18-C19
18	3	601	CLA	C4-C3-C5-C6
18	A	830	CLA	C4-C3-C5-C6
18	A	840	CLA	C2-C3-C5-C6
18	A	818	CLA	C6-C7-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	831	CLA	C11-C10-C8-C9
18	A	828	CLA	C11-C10-C8-C9
18	A	829	CLA	C11-C10-C8-C9
18	B	834	CLA	C6-C7-C8-C9
18	B	841	CLA	C11-C10-C8-C9
18	B	806	CLA	C14-C13-C15-C16
17	2	615	CHL	O1D-CGD-O2D-CED
18	A	809	CLA	O1D-CGD-O2D-CED
18	B	818	CLA	C3-C5-C6-C7
18	A	806	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2A-CAA-CBA-CGA
23	4	619	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
18	B	840	CLA	O1A-CGA-O2A-C1
23	4	620	LMG	O10-C28-O8-C9
18	1	609	CLA	C1A-C2A-CAA-CBA
18	1	612	CLA	C1A-C2A-CAA-CBA
18	2	611	CLA	C1A-C2A-CAA-CBA
18	2	604	CLA	C1A-C2A-CAA-CBA
18	2	608	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	845	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	827	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA
18	B	815	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	G	201	CLA	C1A-C2A-CAA-CBA
18	2	612	CLA	C16-C17-C18-C19
18	2	612	CLA	C5-C6-C7-C8
20	2	618	LHG	C3-O3-P-O6
18	A	805	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C10-C11-C12-C13
18	B	808	CLA	C5-C6-C7-C8
18	B	802	CLA	C8-C10-C11-C12
18	B	808	CLA	O1D-CGD-O2D-CED
18	A	807	CLA	C4-C3-C5-C6
18	4	611	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C5-C6-C7-C8
18	B	840	CLA	C16-C17-C18-C20
18	B	841	CLA	O1D-CGD-O2D-CED
18	B	832	CLA	C3-C5-C6-C7
20	1	615	LHG	C4-C5-C6-O8
27	B	850	DGD	C1G-C2G-C3G-O3G
18	B	817	CLA	C11-C12-C13-C14
18	A	819	CLA	O1D-CGD-O2D-CED
18	A	816	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
18	B	828	CLA	C13-C15-C16-C17
21	2	619	LUT	C11-C10-C9-C19
22	F	304	BCR	C11-C10-C9-C34
18	A	803	CLA	C4-C3-C5-C6
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
18	B	829	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C10-C11-C12-C13
18	L	303	CLA	C10-C11-C12-C13
20	2	618	LHG	C6-C5-O7-C7
18	3	603	CLA	C2A-CAA-CBA-CGA
18	A	820	CLA	C13-C15-C16-C17
18	A	812	CLA	C2-C1-O2A-CGA
23	4	619	LMG	C30-C31-C32-C33
18	B	807	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	C8-C10-C11-C12
18	A	805	CLA	O1A-CGA-O2A-C1
18	A	822	CLA	CBD-CGD-O2D-CED
19	2	617	XAT	C12-C13-C14-C15
22	F	304	BCR	C12-C13-C14-C15
23	4	620	LMG	C2-C1-O1-C7
18	B	810	CLA	C5-C6-C7-C8
18	1	603	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	827	CLA	C4-C3-C5-C6
18	B	813	CLA	C4-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C7
18	A	809	CLA	C11-C10-C8-C7
18	A	804	CLA	C11-C12-C13-C15
18	A	804	CLA	C12-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C15
18	A	811	CLA	C12-C13-C15-C16
18	A	802	CLA	C6-C7-C8-C10
18	A	802	CLA	C11-C12-C13-C15
18	A	802	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C7
18	A	831	CLA	C12-C13-C15-C16
18	A	842	CLA	C11-C10-C8-C7
18	A	844	CLA	C6-C7-C8-C10
18	A	844	CLA	C12-C13-C15-C16
18	A	828	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	808	CLA	C11-C12-C13-C15
18	B	809	CLA	C11-C10-C8-C7
18	B	809	CLA	C12-C13-C15-C16
18	B	827	CLA	C12-C13-C15-C16
18	B	828	CLA	C12-C13-C15-C16
18	B	813	CLA	C11-C12-C13-C15
18	B	806	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C12-C13-C15
18	B	825	CLA	C12-C13-C15-C16
18	H	201	CLA	C6-C7-C8-C10
18	H	201	CLA	C11-C10-C8-C7
18	B	837	CLA	C3-C5-C6-C7
20	1	615	LHG	C19-C20-C21-C22
18	A	806	CLA	C14-C13-C15-C16
18	A	809	CLA	C11-C10-C8-C9
18	A	804	CLA	C6-C7-C8-C9
18	A	804	CLA	C14-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C14
18	A	803	CLA	C6-C7-C8-C9
18	A	802	CLA	C6-C7-C8-C9
18	A	802	CLA	C14-C13-C15-C16
18	A	843	CLA	C6-C7-C8-C9
18	A	844	CLA	C14-C13-C15-C16
18	A	812	CLA	C14-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C9
18	B	808	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	841	CLA	C6-C7-C8-C9
18	B	806	CLA	C11-C12-C13-C14
18	B	824	CLA	C14-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C9
18	H	201	CLA	C11-C10-C8-C9
18	B	822	CLA	C2A-CAA-CBA-CGA
18	B	825	CLA	C10-C11-C12-C13
18	B	840	CLA	C16-C17-C18-C19
22	K	205	BCR	C7-C8-C9-C10
20	B	852	LHG	C8-C7-O7-C5
18	A	819	CLA	C11-C12-C13-C14
18	A	807	CLA	C15-C16-C17-C18
18	A	812	CLA	C13-C15-C16-C17
18	A	812	CLA	C15-C16-C17-C18
18	1	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	846	LHG	C27-C28-C29-C30
18	A	807	CLA	C8-C10-C11-C12
20	1	615	LHG	O6-C4-C5-C6
18	1	603	CLA	C3-C5-C6-C7
18	B	813	CLA	C15-C16-C17-C18
18	A	836	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	C2-C3-C5-C6
18	B	810	CLA	C2-C3-C5-C6
18	B	827	CLA	C2-C3-C5-C6
18	B	813	CLA	C2-C3-C5-C6
18	4	612	CLA	C5-C6-C7-C8
20	A	847	LHG	C5-C6-O8-C23
18	3	601	CLA	C3-C5-C6-C7
18	B	824	CLA	C3-C5-C6-C7
18	A	834	CLA	C5-C6-C7-C8
18	B	819	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	CAA-CBA-CGA-O2A
18	B	829	CLA	O1A-CGA-O2A-C1
18	2	604	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	836	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA
18	K	204	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	C15-C16-C17-C18
20	1	615	LHG	C14-C15-C16-C17
18	B	841	CLA	C16-C17-C18-C20
17	1	601	CHL	C3-C5-C6-C7
18	A	841	CLA	C5-C6-C7-C8
20	B	852	LHG	C4-C5-C6-O8
23	4	620	LMG	C7-C8-C9-O8
18	B	828	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C19
18	B	811	CLA	C5-C6-C7-C8
18	B	811	CLA	O1D-CGD-O2D-CED
18	B	841	CLA	C2A-CAA-CBA-CGA
18	B	820	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	O6-C4-C5-O7
18	B	827	CLA	C15-C16-C17-C18
18	B	807	CLA	O1A-CGA-O2A-C1
18	A	831	CLA	C3-C5-C6-C7
18	A	822	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	A	809	CLA	C2-C1-O2A-CGA
18	A	830	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	A	835	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C10-C8-C9
18	A	814	CLA	C14-C13-C15-C16
18	B	809	CLA	C6-C7-C8-C9
18	B	814	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	B	806	CLA	C6-C7-C8-C9
18	B	837	CLA	C15-C16-C17-C18
20	2	618	LHG	C2-C3-O3-P
20	B	852	LHG	C5-C4-O6-P
18	B	828	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C3-C5-C6-C7
22	B	845	BCR	C1-C6-C7-C8
18	4	611	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
19	2	617	XAT	C31-C32-C33-C34
22	4	618	BCR	C7-C8-C9-C10
22	K	205	BCR	C17-C18-C19-C20
18	B	841	CLA	C15-C16-C17-C18
18	B	827	CLA	C8-C10-C11-C12
22	F	304	BCR	C14-C15-C16-C17
18	B	832	CLA	C16-C17-C18-C19
18	A	806	CLA	C15-C16-C17-C18
18	2	612	CLA	C12-C13-C15-C16
18	A	806	CLA	C12-C13-C15-C16
18	A	804	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C12-C13-C15
18	A	831	CLA	C11-C12-C13-C15
18	A	835	CLA	C11-C12-C13-C15
18	A	842	CLA	C11-C12-C13-C15
18	A	843	CLA	C6-C7-C8-C10
18	A	841	CLA	C12-C13-C15-C16
18	A	814	CLA	C12-C13-C15-C16
18	A	812	CLA	C12-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C10
18	B	818	CLA	C11-C10-C8-C7
18	B	841	CLA	C6-C7-C8-C10
18	B	814	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	B	814	CLA	C11-C12-C13-C15
18	B	806	CLA	C6-C7-C8-C10
18	B	824	CLA	C12-C13-C15-C16
18	B	803	CLA	C11-C10-C8-C7
18	B	817	CLA	C6-C7-C8-C10
18	B	840	CLA	C6-C7-C8-C10
18	F	301	CLA	C6-C7-C8-C10
18	A	831	CLA	C10-C11-C12-C13
18	A	833	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	C15-C16-C17-C18
18	A	829	CLA	C13-C15-C16-C17
18	B	840	CLA	C15-C16-C17-C18
18	A	841	CLA	C2A-CAA-CBA-CGA
19	2	617	XAT	C40-C33-C34-C35
18	1	609	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	C16-C17-C18-C19
18	A	820	CLA	C8-C10-C11-C12
18	2	602	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	A	826	CLA	C8-C10-C11-C12
18	1	602	CLA	CAD-CBD-CGD-O2D
18	1	605	CLA	CAD-CBD-CGD-O2D
18	2	610	CLA	CAD-CBD-CGD-O2D
18	3	608	CLA	CAD-CBD-CGD-O2D
18	3	607	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	810	CLA	CAD-CBD-CGD-O2D
18	A	842	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	832	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	B	802	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	L	303	CLA	CAD-CBD-CGD-O2D
22	B	849	BCR	C6-C7-C8-C9
22	K	205	BCR	C22-C23-C24-C25
18	A	809	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
18	A	818	CLA	C5-C6-C7-C8
18	B	837	CLA	C10-C11-C12-C13
18	L	303	CLA	C15-C16-C17-C18
18	4	603	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C8-C10-C11-C12
18	A	824	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	C16-C17-C18-C20
18	1	611	CLA	CHA-CBD-CGD-O1D
18	1	611	CLA	CHA-CBD-CGD-O2D
18	2	602	CLA	CHA-CBD-CGD-O1D
18	2	602	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O2D
18	4	601	CLA	CHA-CBD-CGD-O1D
18	4	601	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	CHA-CBD-CGD-O1D
18	4	612	CLA	CHA-CBD-CGD-O2D
18	4	614	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O1D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	CHA-CBD-CGD-O1D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	CHA-CBD-CGD-O1D
18	H	201	CLA	CHA-CBD-CGD-O1D
21	3	613	LUT	C11-C10-C9-C8
22	A	849	BCR	C20-C21-C22-C23
22	F	304	BCR	C11-C10-C9-C8
20	1	615	LHG	O1-C1-C2-O2
18	B	823	CLA	O1D-CGD-O2D-CED
18	B	834	CLA	C3-C5-C6-C7
18	4	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	2	602	CLA	C14-C13-C15-C16
18	B	827	CLA	C11-C12-C13-C14
17	1	601	CHL	C2A-CAA-CBA-CGA
18	F	301	CLA	C3-C5-C6-C7
17	4	605	CHL	CHA-CBD-CGD-O2D
18	4	611	CLA	CHA-CBD-CGD-O2D
18	A	844	CLA	C16-C17-C18-C20
18	B	819	CLA	C6-C7-C8-C10
18	B	826	CLA	C5-C6-C7-C8
20	2	618	LHG	C4-O6-P-O3
20	B	852	LHG	C3-O3-P-O6
18	A	822	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	C4-C3-C5-C6
20	2	618	LHG	C5-C4-O6-P
18	A	842	CLA	C2C-C3C-CAC-CBC
18	2	602	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	O1A-CGA-O2A-C1
18	A	809	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C3-O3-P-O5
20	B	852	LHG	C4-O6-P-O4
18	A	812	CLA	CBA-CGA-O2A-C1
18	B	839	CLA	CBA-CGA-O2A-C1
18	A	841	CLA	CAD-CBD-CGD-O1D
18	B	813	CLA	CAD-CBD-CGD-O1D
18	B	822	CLA	CAD-CBD-CGD-O1D
18	F	302	CLA	CAD-CBD-CGD-O1D
18	B	837	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	C5-C6-C7-C8
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C16-C17-C18-C20
18	2	602	CLA	C12-C13-C15-C16
18	A	830	CLA	C2-C3-C5-C6
18	A	812	CLA	C6-C7-C8-C10
18	B	805	CLA	C11-C10-C8-C7
18	B	808	CLA	C12-C13-C15-C16
18	B	814	CLA	C6-C7-C8-C10
18	F	301	CLA	C11-C10-C8-C7
25	B	842	PQN	C16-C17-C18-C20
25	B	842	PQN	C22-C23-C25-C26
20	1	615	LHG	C8-C7-O7-C5
18	4	614	CLA	C2A-CAA-CBA-CGA
24	A	801	CL0	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	4	601	CLA	CAA-CBA-CGA-O2A
17	1	601	CHL	CAD-CBD-CGD-O1D
17	2	605	CHL	C1C-C2C-CMC-OMC
18	3	609	CLA	CAD-CBD-CGD-O1D
23	4	620	LMG	O7-C8-C9-O8
27	B	850	DGD	CBB-CCB-CDB-CEB
18	A	812	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	O1A-CGA-O2A-C1
18	4	609	CLA	C4-C3-C5-C6
18	1	602	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	C13-C15-C16-C17
18	2	612	CLA	C14-C13-C15-C16
18	A	820	CLA	C6-C7-C8-C9
18	A	802	CLA	C11-C10-C8-C9
18	A	831	CLA	C11-C12-C13-C14
18	A	831	CLA	C14-C13-C15-C16
18	A	842	CLA	C11-C12-C13-C14
18	B	818	CLA	C11-C10-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	808	CLA	C11-C10-C8-C9
18	B	810	CLA	C6-C7-C8-C9
18	1	602	CLA	O1A-CGA-O2A-C1
18	A	841	CLA	CAA-CBA-CGA-O2A
22	A	852	BCR	C10-C11-C12-C13
22	L	301	BCR	C18-C19-C20-C21
18	B	808	CLA	C16-C17-C18-C20
22	B	846	BCR	C21-C22-C23-C24
20	1	615	LHG	O9-C7-O7-C5
20	B	851	LHG	C26-C27-C28-C29
27	B	850	DGD	C6B-C7B-C8B-C9B
18	2	612	CLA	C15-C16-C17-C18
18	1	604	CLA	C1-C2-C3-C4
18	3	601	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	808	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	C2-C1-O2A-CGA
18	A	842	CLA	C2-C1-O2A-CGA
18	B	827	CLA	C2-C1-O2A-CGA
18	A	844	CLA	C16-C17-C18-C19
18	A	824	CLA	O1D-CGD-O2D-CED
18	L	303	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	B	832	CLA	C13-C15-C16-C17
18	2	610	CLA	CMA-C3A-C4A-NA
18	4	614	CLA	O1A-CGA-O2A-C1
18	A	818	CLA	C4-C3-C5-C6
18	1	603	CLA	C2-C3-C5-C6
20	B	852	LHG	O9-C7-O7-C5
18	B	826	CLA	C10-C11-C12-C13
18	A	822	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CAA-CBA-CGA-O2A
23	4	620	LMG	O7-C10-C11-C12
24	A	801	CL0	CAA-CBA-CGA-O2A
18	K	204	CLA	CBA-CGA-O2A-C1
21	2	619	LUT	C11-C10-C9-C8
22	L	301	BCR	C11-C10-C9-C8
20	B	852	LHG	O7-C5-C6-O8
20	A	847	LHG	C4-O6-P-O3
20	A	846	LHG	C3-O3-P-O6
18	A	842	CLA	C4C-C3C-CAC-CBC
17	2	605	CHL	O1D-CGD-O2D-CED
18	A	828	CLA	C11-C10-C8-C7
18	A	804	CLA	C11-C12-C13-C14
18	A	844	CLA	C6-C7-C8-C9
18	B	841	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C12-C13-C14
18	A	814	CLA	C10-C11-C12-C13
19	1	614	XAT	C33-C34-C35-C15
18	4	614	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	C2A-CAA-CBA-CGA
18	A	822	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C31-C32-C33-C34
20	1	615	LHG	C32-C33-C34-C35
18	A	829	CLA	C16-C17-C18-C20
18	B	819	CLA	C6-C7-C8-C9
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C2-C1-O2A-CGA
18	B	836	CLA	C2-C1-O2A-CGA
18	A	835	CLA	O1D-CGD-O2D-CED
18	B	808	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	1	607	CLA	CAA-CBA-CGA-O2A
18	1	602	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	C2A-CAA-CBA-CGA
18	4	613	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	813	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C6-C7-C8-C9
18	B	825	CLA	C11-C10-C8-C9
18	L	303	CLA	C11-C12-C13-C14
25	B	842	PQN	C24-C23-C25-C26
18	1	607	CLA	CAA-CBA-CGA-O1A
22	A	852	BCR	C11-C10-C9-C34
22	A	851	BCR	C11-C10-C9-C34
22	A	851	BCR	C20-C21-C22-C37
22	B	845	BCR	C16-C17-C18-C36
22	K	202	BCR	C16-C17-C18-C36
22	L	305	BCR	C16-C17-C18-C36
22	L	301	BCR	C11-C10-C9-C34
18	1	611	CLA	CAA-CBA-CGA-O1A
18	2	611	CLA	CAA-CBA-CGA-O1A
18	2	608	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	C5-C6-C7-C8
18	B	805	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	CBD-CGD-O2D-CED
20	B	851	LHG	C4-C5-O7-C7
18	A	818	CLA	C8-C10-C11-C12
18	B	841	CLA	C4-C3-C5-C6
18	2	609	CLA	C1A-C2A-CAA-CBA
18	4	604	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	C1A-C2A-CAA-CBA
18	4	612	CLA	C11-C10-C8-C7
18	B	828	CLA	C6-C7-C8-C10
18	B	813	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	B	840	CLA	C11-C10-C8-C7
24	A	801	CL0	C11-C12-C13-C15
18	B	816	CLA	C5-C6-C7-C8
18	3	603	CLA	CAA-CBA-CGA-O2A
24	A	801	CL0	CBA-CGA-O2A-C1
24	A	801	CL0	O1A-CGA-O2A-C1
18	3	603	CLA	CAA-CBA-CGA-O1A
18	G	203	CLA	CAA-CBA-CGA-O1A
18	1	604	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C11-C12-C13-C14
18	B	839	CLA	C15-C16-C17-C18
17	2	605	CHL	CBD-CGD-O2D-CED
19	2	617	XAT	C32-C33-C34-C35
22	A	852	BCR	C11-C10-C9-C8
22	A	851	BCR	C11-C10-C9-C8
22	A	851	BCR	C20-C21-C22-C23
22	B	845	BCR	C16-C17-C18-C19
22	K	202	BCR	C16-C17-C18-C19
22	L	305	BCR	C16-C17-C18-C19
18	4	603	CLA	CAA-CBA-CGA-O1A
18	A	809	CLA	C16-C17-C18-C20
18	2	611	CLA	CAA-CBA-CGA-O2A
18	B	818	CLA	C4-C3-C5-C6
18	A	803	CLA	C2-C1-O2A-CGA
18	A	832	CLA	C2-C1-O2A-CGA
18	B	841	CLA	C2-C1-O2A-CGA
18	B	817	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	C11-C10-C8-C9
18	2	608	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	CAA-CBA-CGA-O2A
18	2	612	CLA	C2A-CAA-CBA-CGA
18	K	204	CLA	C2A-CAA-CBA-CGA
18	L	303	CLA	C16-C17-C18-C20
22	A	852	BCR	C1-C6-C7-C8
22	A	852	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C30
18	A	819	CLA	C4-C3-C5-C6
18	A	829	CLA	C16-C17-C18-C19
18	A	835	CLA	CBD-CGD-O2D-CED
18	2	603	CLA	CAA-CBA-CGA-O2A
18	4	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	G	203	CLA	CAA-CBA-CGA-O2A
18	3	601	CLA	C11-C12-C13-C14
18	A	802	CLA	C5-C6-C7-C8
27	B	850	DGD	C1B-C2B-C3B-C4B
18	A	815	CLA	CAA-CBA-CGA-O2A
18	K	203	CLA	CAA-CBA-CGA-O2A
18	B	828	CLA	C3-C5-C6-C7
18	B	821	CLA	CAA-CBA-CGA-O2A
17	1	601	CHL	C2-C3-C5-C6
18	A	820	CLA	C11-C10-C8-C7
18	A	803	CLA	C6-C7-C8-C10
18	A	803	CLA	C11-C10-C8-C7
18	B	808	CLA	C11-C10-C8-C7
18	B	841	CLA	C2-C3-C5-C6
18	A	843	CLA	C5-C6-C7-C8
18	K	203	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	CAA-CBA-CGA-O2A
18	B	827	CLA	C16-C17-C18-C20
22	3	614	BCR	C20-C21-C22-C37
22	B	844	BCR	C11-C10-C9-C34
24	A	801	CL0	C4-C3-C5-C6
17	4	607	CHL	CAA-CBA-CGA-O2A
18	B	809	CLA	CAA-CBA-CGA-O2A
18	A	818	CLA	C11-C10-C8-C9
18	B	814	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	B	813	CLA	C11-C10-C8-C9
18	B	832	CLA	C11-C10-C8-C9
25	B	842	PQN	C16-C17-C18-C19
18	3	607	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	CAA-CBA-CGA-O2A
18	2	613	CLA	CAD-CBD-CGD-O2D
18	3	605	CLA	CAD-CBD-CGD-O2D
18	4	602	CLA	CAD-CBD-CGD-O2D
18	4	609	CLA	CAD-CBD-CGD-O2D
18	A	807	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	803	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	815	CLA	CAD-CBD-CGD-O2D
18	A	832	CLA	CAD-CBD-CGD-O2D
18	B	808	CLA	CAD-CBD-CGD-O2D
18	B	810	CLA	CAD-CBD-CGD-O2D
18	B	841	CLA	CAD-CBD-CGD-O2D
18	B	812	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	G	202	CLA	CAD-CBD-CGD-O2D
18	J	101	CLA	CAD-CBD-CGD-O2D
18	L	302	CLA	CAD-CBD-CGD-O2D
18	2	612	CLA	C8-C10-C11-C12
22	B	844	BCR	C15-C16-C17-C18
18	A	821	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	CBA-CGA-O2A-C1
18	2	603	CLA	CAA-CBA-CGA-O1A
18	A	815	CLA	CAA-CBA-CGA-O1A
17	1	601	CHL	CAA-CBA-CGA-O2A
17	2	607	CHL	CAA-CBA-CGA-O2A
18	3	609	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CAA-CBA-CGA-O2A
19	4	617	XAT	O4-C6-C7-C8
18	A	814	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	C30-C31-C32-C33
18	B	828	CLA	C15-C16-C17-C18
18	B	832	CLA	CAA-CBA-CGA-O2A
18	4	604	CLA	CAA-CBA-CGA-O2A
18	A	826	CLA	O2A-C1-C2-C3
18	B	832	CLA	O2A-C1-C2-C3
18	F	301	CLA	O2A-C1-C2-C3
18	H	201	CLA	O2A-C1-C2-C3
18	J	101	CLA	O2A-C1-C2-C3
18	A	825	CLA	C2A-CAA-CBA-CGA
18	J	101	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	CAA-CBA-CGA-O2A
18	4	604	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	C16-C17-C18-C20
18	3	603	CLA	CHA-CBD-CGD-O1D
18	3	601	CLA	CHA-CBD-CGD-O1D
18	3	601	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	4	610	CLA	CHA-CBD-CGD-O1D
18	4	610	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	839	CLA	CHA-CBD-CGD-O1D
18	A	839	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	838	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	CHA-CBD-CGD-O1D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	CHA-CBD-CGD-O2D
18	H	201	CLA	CHA-CBD-CGD-O2D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	4	608	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O2A
22	B	844	BCR	C11-C10-C9-C8
17	4	607	CHL	CAA-CBA-CGA-O1A
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	840	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CBA-CGA-O2A-C1
23	4	619	LMG	C8-C9-O8-C28
18	2	609	CLA	C2-C1-O2A-CGA
18	4	609	CLA	C2-C3-C5-C6
18	4	612	CLA	C6-C7-C8-C10
18	A	804	CLA	C2-C3-C5-C6
18	B	837	CLA	C16-C17-C18-C20
18	A	803	CLA	C11-C10-C8-C9
18	A	843	CLA	C8-C10-C11-C12
18	A	809	CLA	C16-C17-C18-C19
18	A	842	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
18	B	827	CLA	C16-C17-C18-C19
18	L	303	CLA	C16-C17-C18-C19
18	A	807	CLA	O1A-CGA-O2A-C1
18	B	818	CLA	C2A-CAA-CBA-CGA
17	2	607	CHL	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O1A
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	818	CLA	C2-C3-C5-C6
18	A	805	CLA	C3-C5-C6-C7
23	4	619	LMG	C29-C28-O8-C9
18	K	204	CLA	O1A-CGA-O2A-C1
18	1	610	CLA	CHA-CBD-CGD-O2D
18	A	803	CLA	C1A-C2A-CAA-CBA
18	B	837	CLA	C1A-C2A-CAA-CBA
18	3	602	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	O7-C7-C8-C9
18	B	811	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	C11-C12-C13-C14
18	2	602	CLA	C2A-CAA-CBA-CGA
18	4	602	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C2A-CAA-CBA-CGA
18	2	602	CLA	C16-C17-C18-C19
18	B	809	CLA	CAA-CBA-CGA-O1A
20	1	615	LHG	C4-O6-P-O4
20	A	846	LHG	C3-O3-P-O5
18	A	840	CLA	CAA-CBA-CGA-O1A
22	4	618	BCR	C1-C6-C7-C8
22	4	618	BCR	C5-C6-C7-C8
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C5-C6-C7-C8
22	B	847	BCR	C1-C6-C7-C8
22	B	847	BCR	C5-C6-C7-C8
22	G	204	BCR	C1-C6-C7-C8
22	G	204	BCR	C5-C6-C7-C8
22	L	306	BCR	C5-C6-C7-C8
20	B	852	LHG	O9-C7-C8-C9
18	4	602	CLA	CAA-CBA-CGA-O2A
18	4	614	CLA	CAA-CBA-CGA-O2A
18	4	608	CLA	CAA-CBA-CGA-O1A
18	A	804	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	3	601	CLA	CAA-CBA-CGA-O2A
20	2	618	LHG	O7-C7-C8-C9
27	B	850	DGD	CFB-CGB-CHB-CIB
18	A	809	CLA	C4C-C3C-CAC-CBC
18	4	613	CLA	CAD-CBD-CGD-O1D
18	A	844	CLA	CAD-CBD-CGD-O1D
18	B	837	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	O1A-CGA-O2A-C1
18	B	832	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O2A
18	B	828	CLA	C5-C6-C7-C8
18	2	602	CLA	C6-C7-C8-C9
18	A	820	CLA	C11-C12-C13-C14
18	B	810	CLA	C11-C12-C13-C14
18	B	840	CLA	C11-C10-C8-C9
23	4	620	LMG	C8-C9-O8-C28
18	K	204	CLA	CAA-CBA-CGA-O2A
18	B	822	CLA	C8-C10-C11-C12
18	2	612	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	C8-C10-C11-C12
18	A	842	CLA	CAA-CBA-CGA-O1A
18	A	804	CLA	C4-C3-C5-C6
17	1	601	CHL	CAD-CBD-CGD-O2D
18	1	607	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	C11-C12-C13-C15
18	3	609	CLA	CAD-CBD-CGD-O2D
18	3	610	CLA	CAD-CBD-CGD-O2D
18	4	611	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	C6-C7-C8-C10
18	B	825	CLA	C11-C12-C13-C15
21	2	619	LUT	C25-C26-C27-C28
18	2	609	CLA	CAA-CBA-CGA-O2A
18	A	837	CLA	CAA-CBA-CGA-O2A
22	A	852	BCR	C13-C14-C15-C16
18	B	824	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O2A
18	2	609	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O1A
18	B	802	CLA	C5-C6-C7-C8
18	1	604	CLA	O1D-CGD-O2D-CED
18	B	814	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	4	613	CLA	C2A-CAA-CBA-CGA
18	A	844	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2C-C3C-CAC-CBC
18	F	301	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

170 monomers are involved in 505 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	831	CLA	1	0
18	3	609	CLA	1	0
20	1	615	LHG	13	0
18	4	610	CLA	2	0
18	A	829	CLA	7	0
18	2	608	CLA	2	0
22	B	844	BCR	2	0
18	B	832	CLA	6	0
18	B	836	CLA	2	0
18	B	841	CLA	3	0
17	2	605	CHL	3	0
18	A	815	CLA	1	0
18	1	609	CLA	10	0
23	4	620	LMG	1	0
18	A	814	CLA	3	0
22	B	849	BCR	4	0
19	2	617	XAT	9	0
17	2	607	CHL	2	0
18	3	607	CLA	4	0
22	B	845	BCR	8	0
18	B	830	CLA	1	0
18	A	832	CLA	2	0
18	3	602	CLA	2	0
18	B	840	CLA	8	0
18	J	101	CLA	2	0
18	A	820	CLA	4	0
17	1	601	CHL	10	0
18	K	204	CLA	1	0
22	L	306	BCR	4	0
18	2	612	CLA	5	0
18	A	826	CLA	3	0
21	3	613	LUT	5	0
18	A	843	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	823	CLA	2	0
18	B	819	CLA	2	0
18	A	833	CLA	2	0
22	K	205	BCR	4	0
18	B	838	CLA	1	0
22	B	801	BCR	10	0
25	B	842	PQN	3	0
27	B	850	DGD	5	0
18	B	805	CLA	6	0
22	L	305	BCR	8	0
18	A	827	CLA	1	0
19	1	614	XAT	18	0
18	A	804	CLA	6	0
18	A	842	CLA	6	0
18	A	819	CLA	3	0
18	4	603	CLA	2	0
18	F	303	CLA	1	0
18	B	803	CLA	4	0
18	A	805	CLA	4	0
18	B	806	CLA	3	0
18	4	612	CLA	3	0
18	B	837	CLA	2	0
18	A	806	CLA	3	0
18	A	836	CLA	1	0
18	1	605	CLA	1	0
17	2	601	CHL	1	0
22	B	848	BCR	4	0
18	A	844	CLA	4	0
18	3	610	CLA	1	0
18	1	607	CLA	1	0
21	1	616	LUT	3	0
18	F	302	CLA	6	0
18	A	841	CLA	6	0
18	B	824	CLA	7	0
22	A	849	BCR	2	0
17	2	615	CHL	5	0
25	A	855	PQN	4	0
18	B	834	CLA	2	0
17	2	606	CHL	2	0
18	A	830	CLA	4	0
18	A	813	CLA	4	0
18	B	812	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	834	CLA	3	0
18	4	608	CLA	3	0
20	2	618	LHG	3	0
18	1	608	CLA	2	0
22	B	846	BCR	6	0
18	B	822	CLA	9	0
22	A	853	BCR	7	0
18	B	818	CLA	5	0
22	3	614	BCR	4	0
18	B	813	CLA	5	0
18	B	828	CLA	7	0
18	A	802	CLA	3	0
18	A	818	CLA	1	0
18	B	816	CLA	1	0
18	B	802	CLA	4	0
18	3	612	CLA	2	0
18	K	201	CLA	1	0
22	B	847	BCR	5	0
22	A	848	BCR	3	0
18	B	817	CLA	2	0
20	A	846	LHG	6	0
18	A	822	CLA	5	0
18	H	201	CLA	3	0
22	J	102	BCR	6	0
22	4	618	BCR	4	0
22	A	850	BCR	5	0
22	F	304	BCR	3	0
20	B	852	LHG	3	0
18	3	604	CLA	1	0
18	4	602	CLA	6	0
22	K	202	BCR	3	0
18	A	812	CLA	8	0
18	A	807	CLA	3	0
18	4	609	CLA	2	0
18	A	835	CLA	5	0
18	1	604	CLA	3	0
18	3	605	CLA	1	0
18	B	809	CLA	6	0
18	2	603	CLA	3	0
18	A	828	CLA	3	0
18	1	612	CLA	2	0
19	4	617	XAT	5	0

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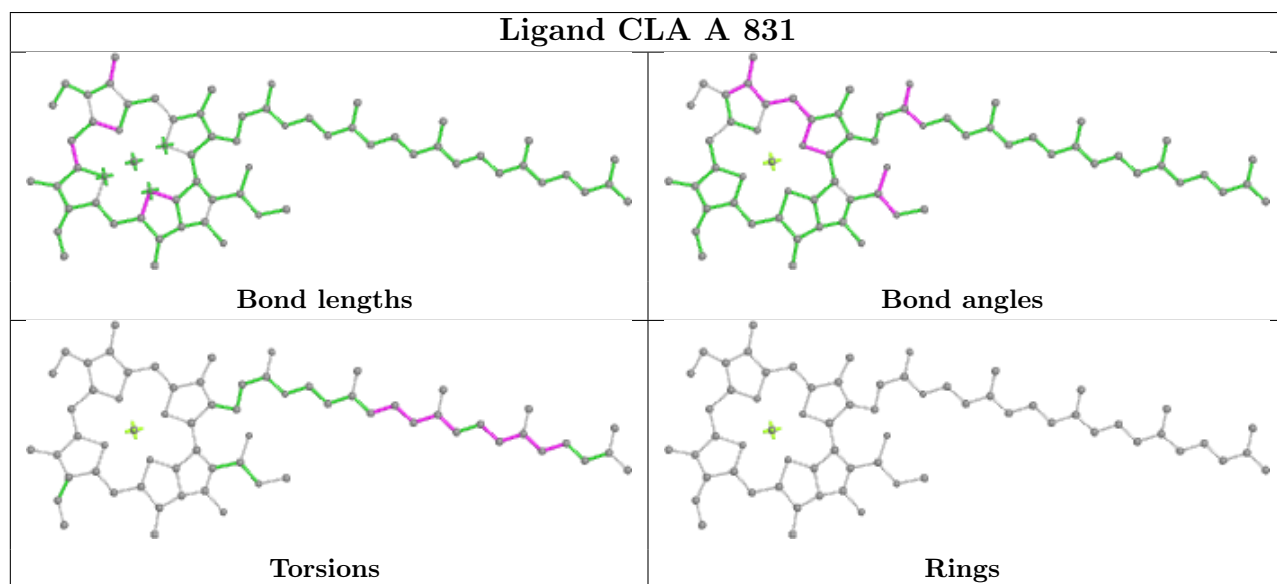
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	843	BCR	4	0
18	A	821	CLA	2	0
17	3	606	CHL	2	0
18	A	845	CLA	1	0
18	A	810	CLA	2	0
18	A	811	CLA	4	0
18	B	814	CLA	3	0
22	A	851	BCR	8	0
21	4	616	LUT	4	0
22	G	204	BCR	2	0
18	4	614	CLA	2	0
18	F	301	CLA	1	0
22	L	301	BCR	4	0
17	4	605	CHL	1	0
18	A	839	CLA	1	0
18	4	601	CLA	1	0
18	4	613	CLA	2	0
18	L	304	CLA	1	0
17	4	615	CHL	1	0
17	4	607	CHL	2	0
18	2	602	CLA	10	0
18	B	839	CLA	2	0
18	1	602	CLA	9	0
18	B	821	CLA	1	0
21	2	619	LUT	7	0
18	3	601	CLA	4	0
18	L	303	CLA	4	0
18	2	609	CLA	5	0
18	A	809	CLA	10	0
18	A	803	CLA	5	0
18	2	613	CLA	1	0
18	A	817	CLA	1	0
22	A	852	BCR	2	0
18	B	820	CLA	2	0
18	A	823	CLA	1	0
24	A	801	CL0	4	0
18	B	826	CLA	3	0
18	B	811	CLA	1	0
18	3	603	CLA	2	0
18	B	825	CLA	4	0
18	2	604	CLA	5	0
18	B	833	CLA	1	0

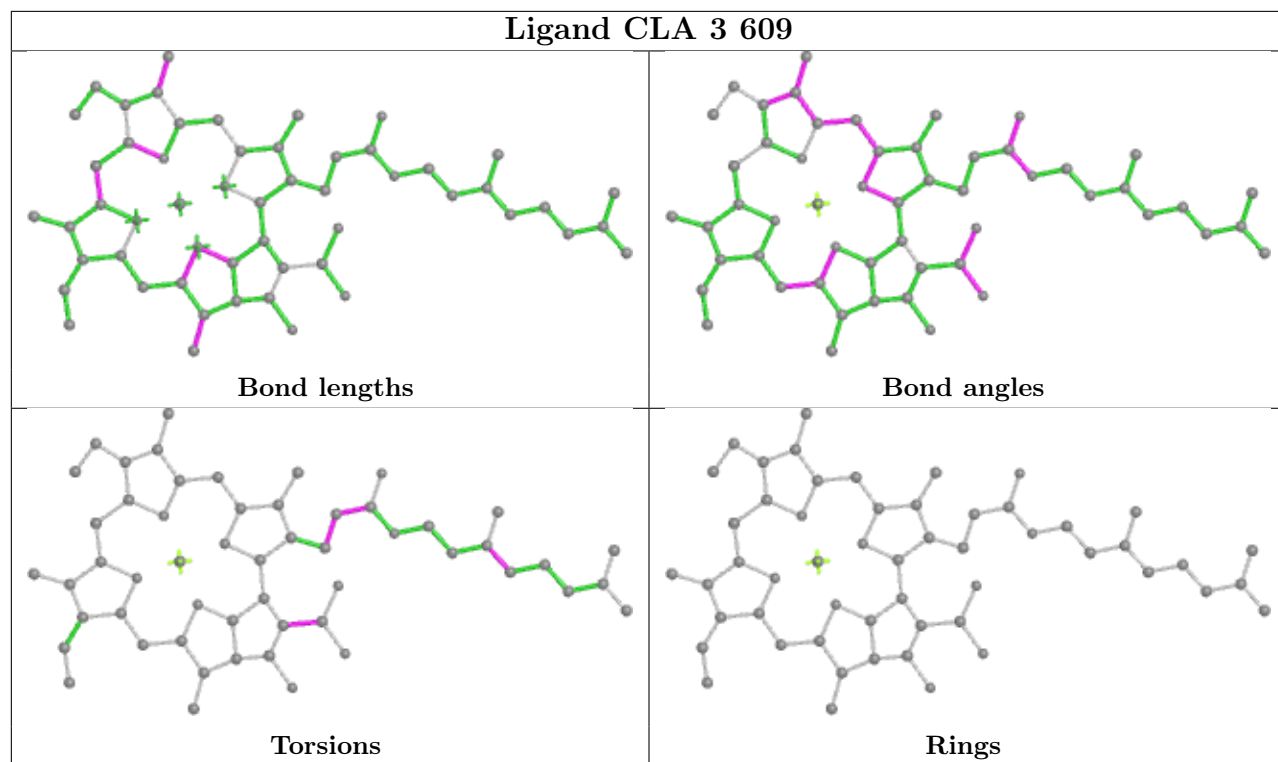
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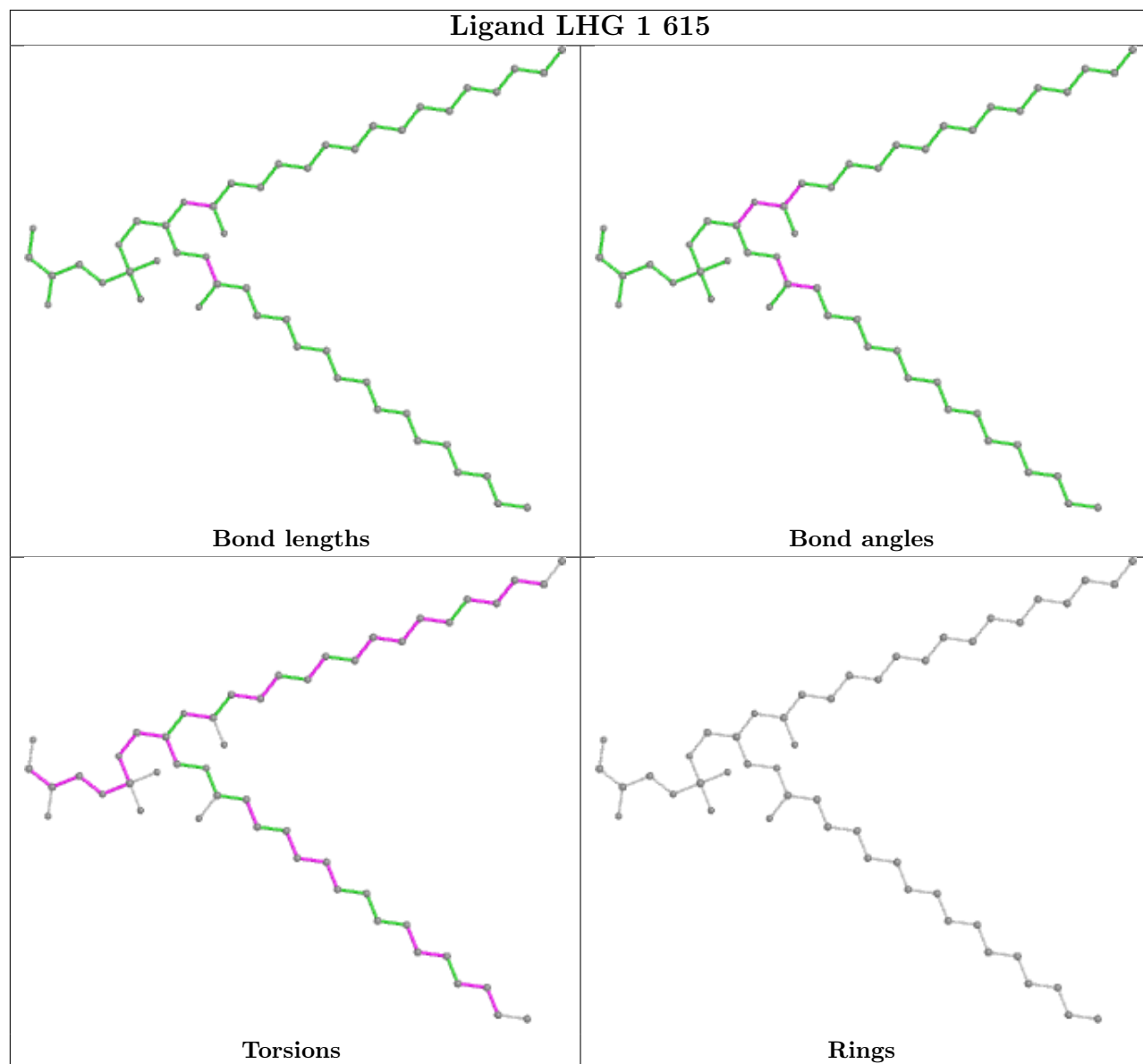
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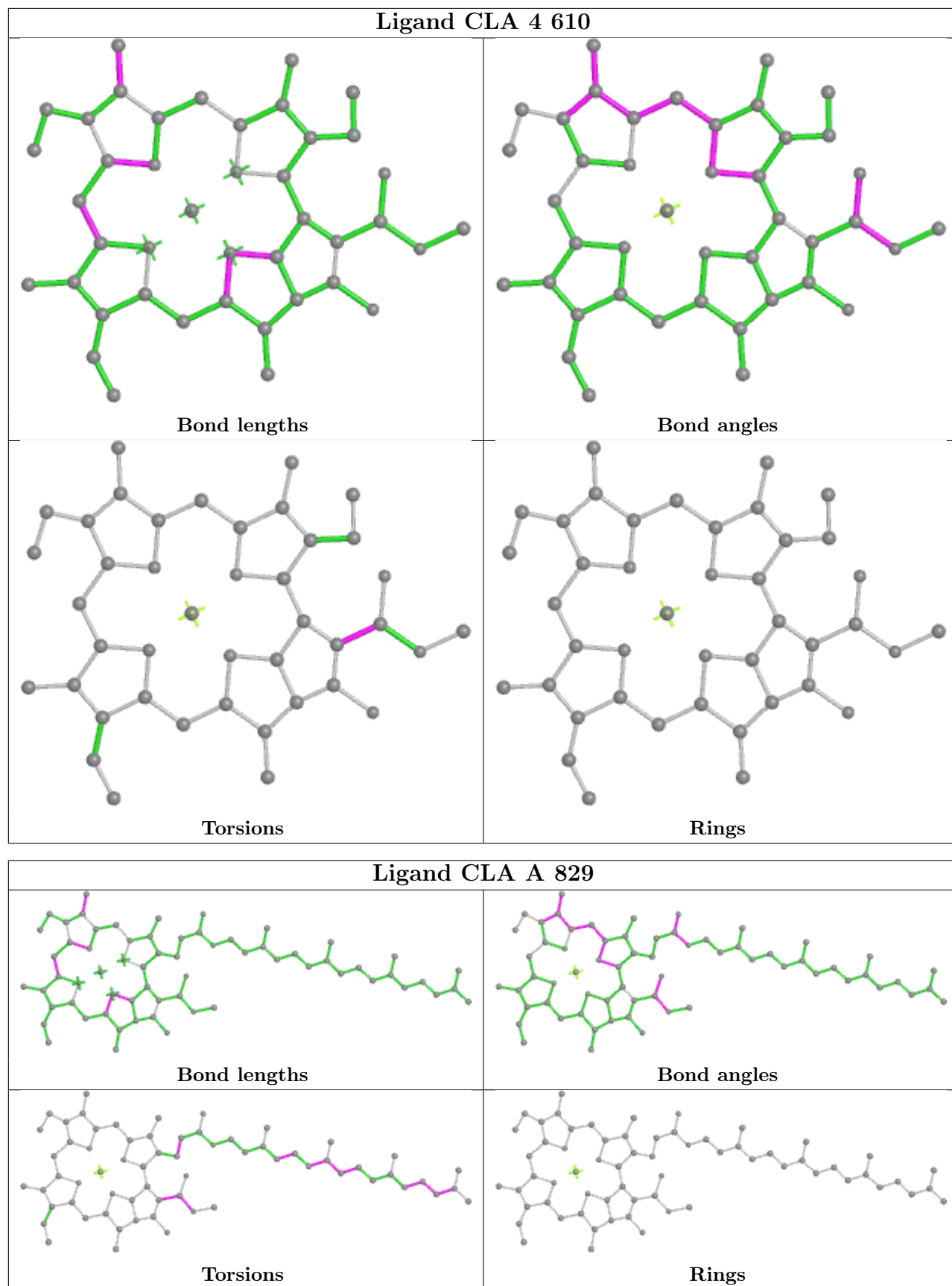
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	616	LUT	4	0
18	1	603	CLA	1	0
18	B	808	CLA	5	0
18	B	827	CLA	5	0
18	B	804	CLA	1	0
18	G	201	CLA	1	0
20	B	851	LHG	2	0
18	A	825	CLA	3	0
18	A	808	CLA	2	0
18	1	611	CLA	1	0
18	L	302	CLA	3	0

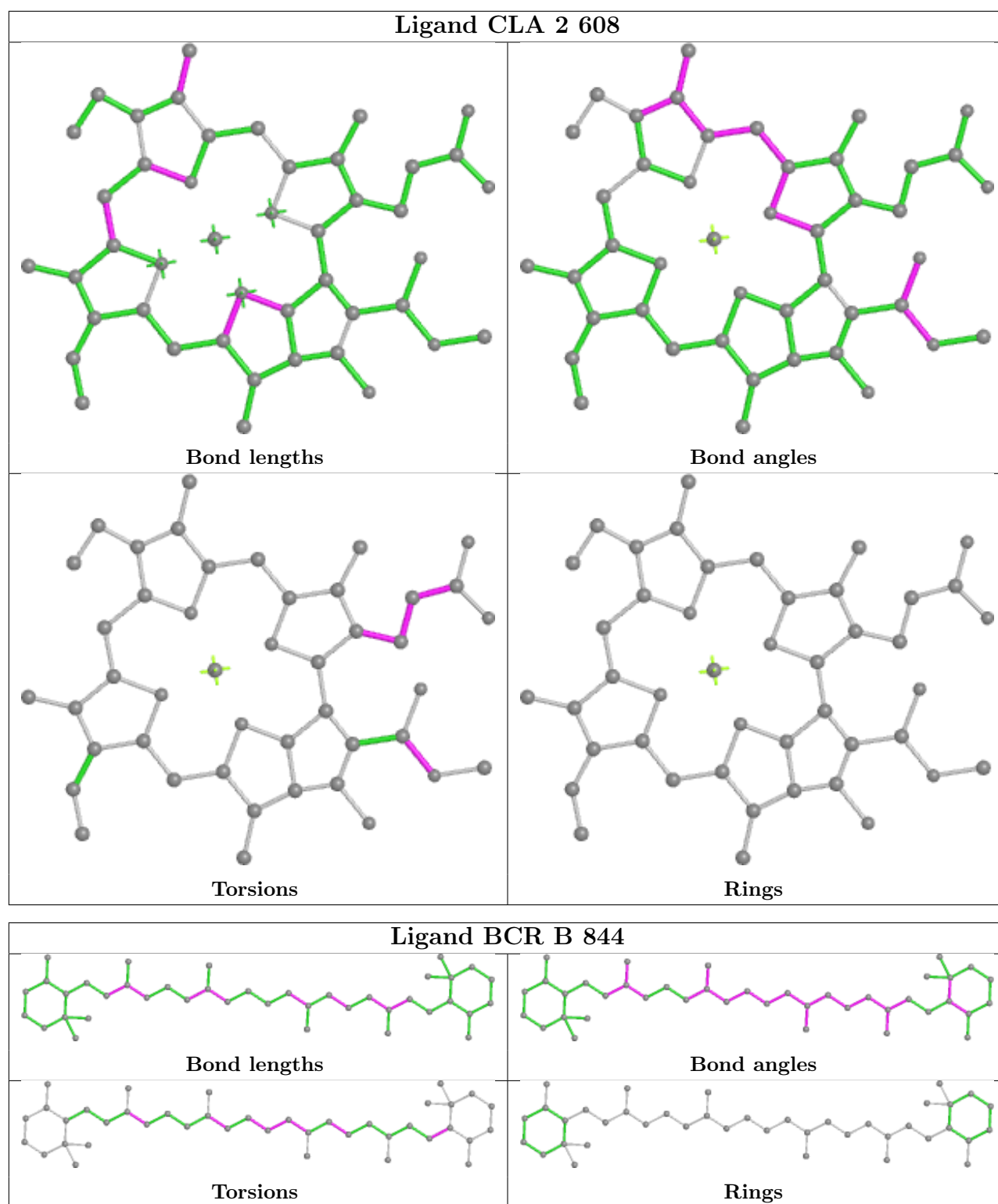
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

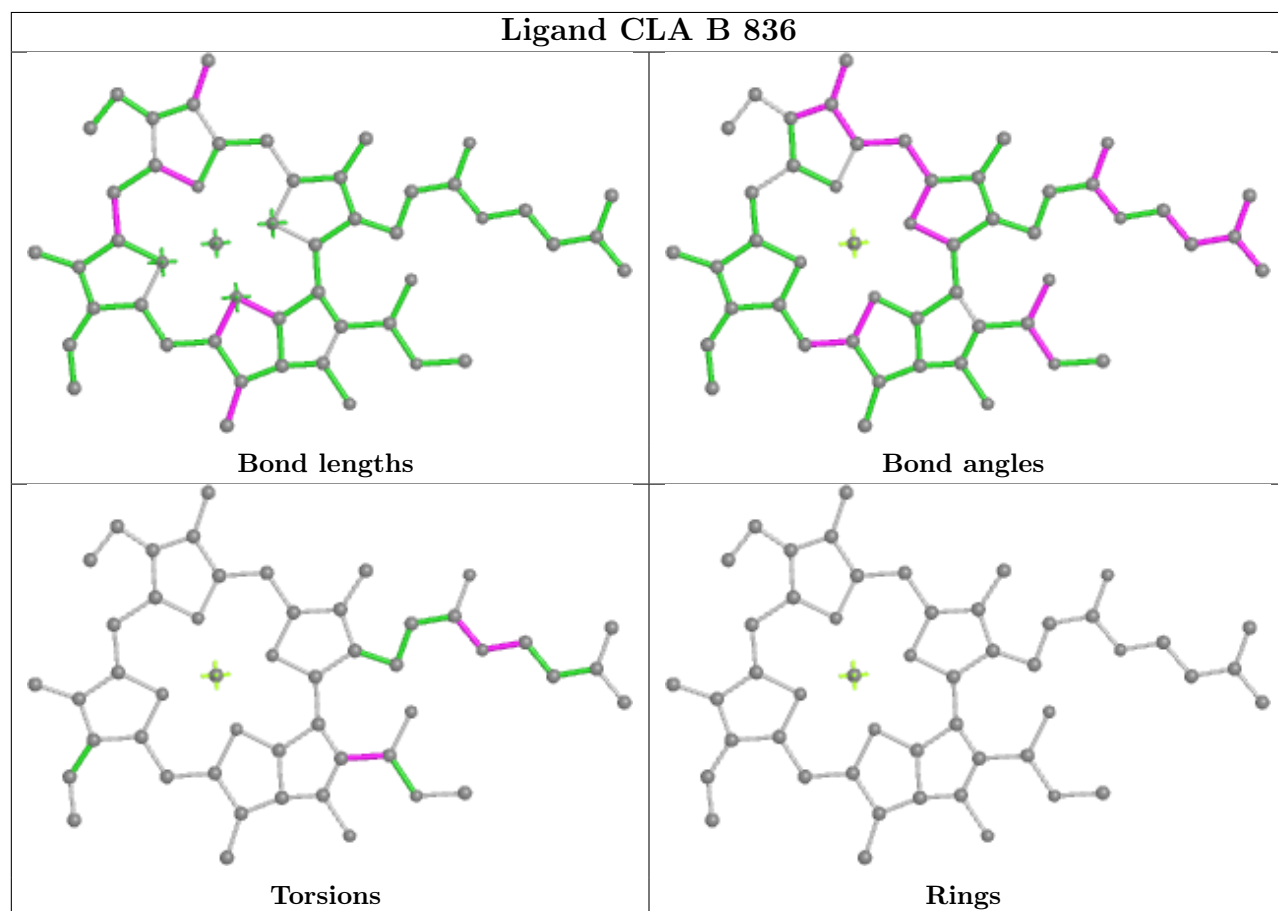
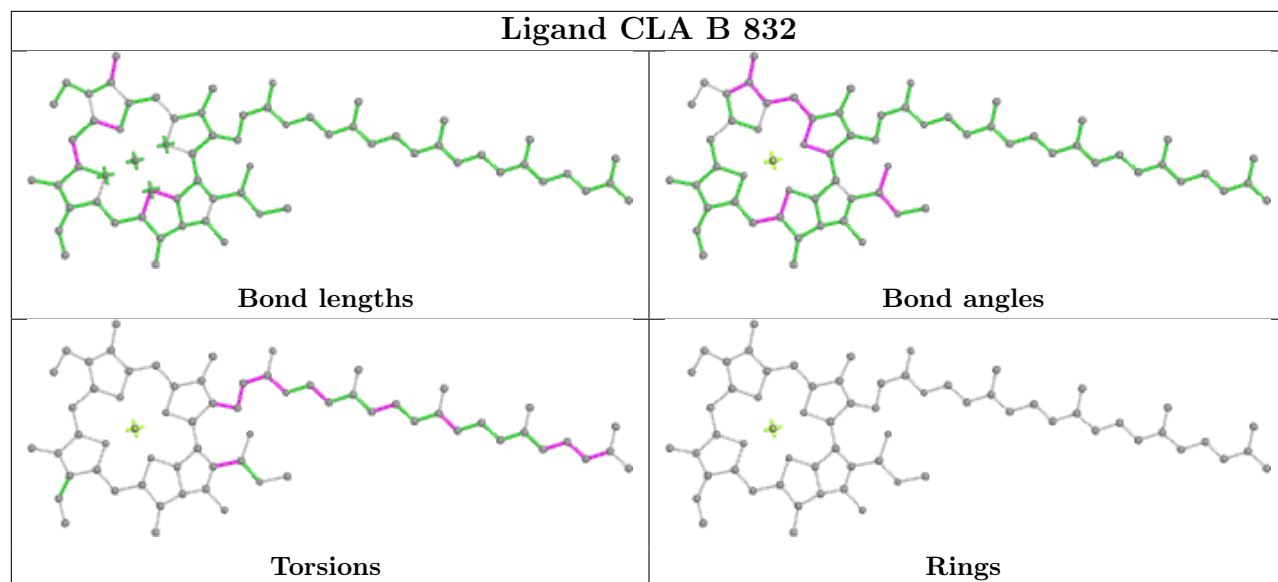


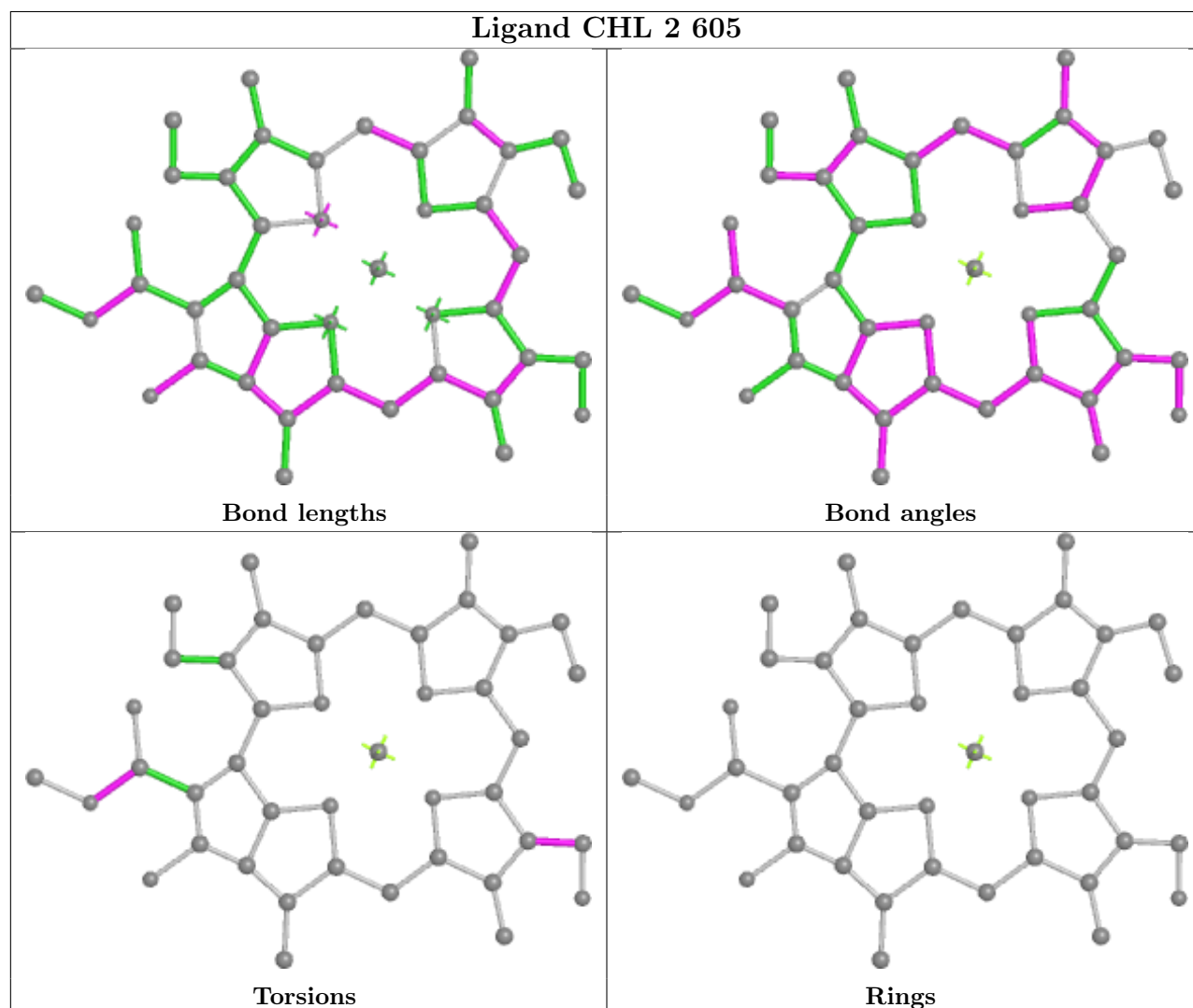
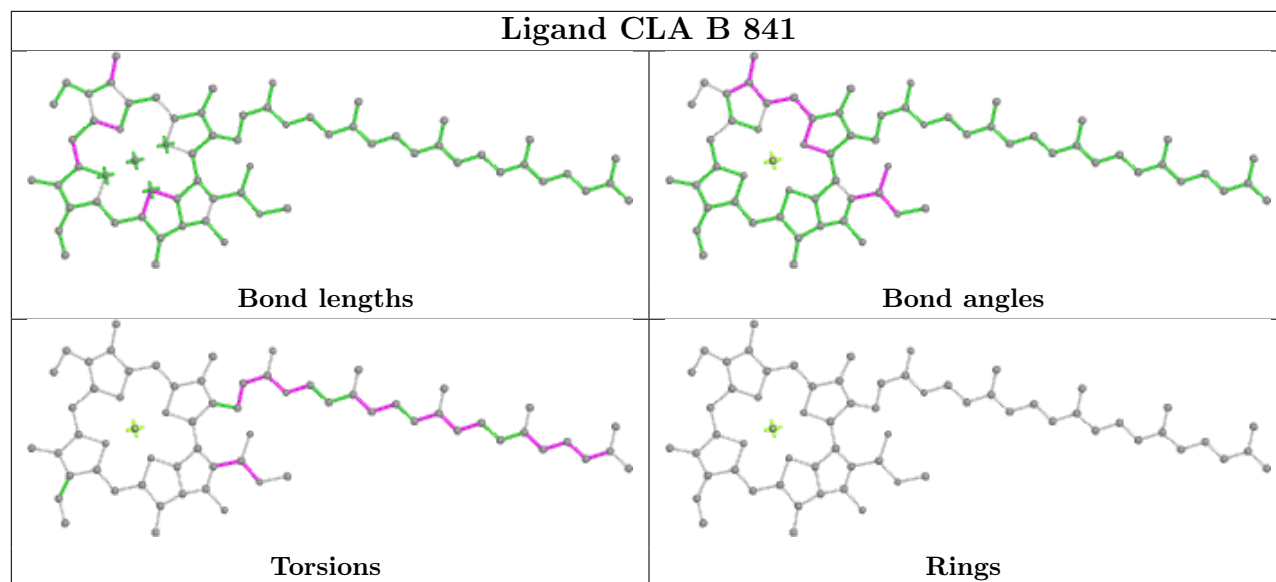


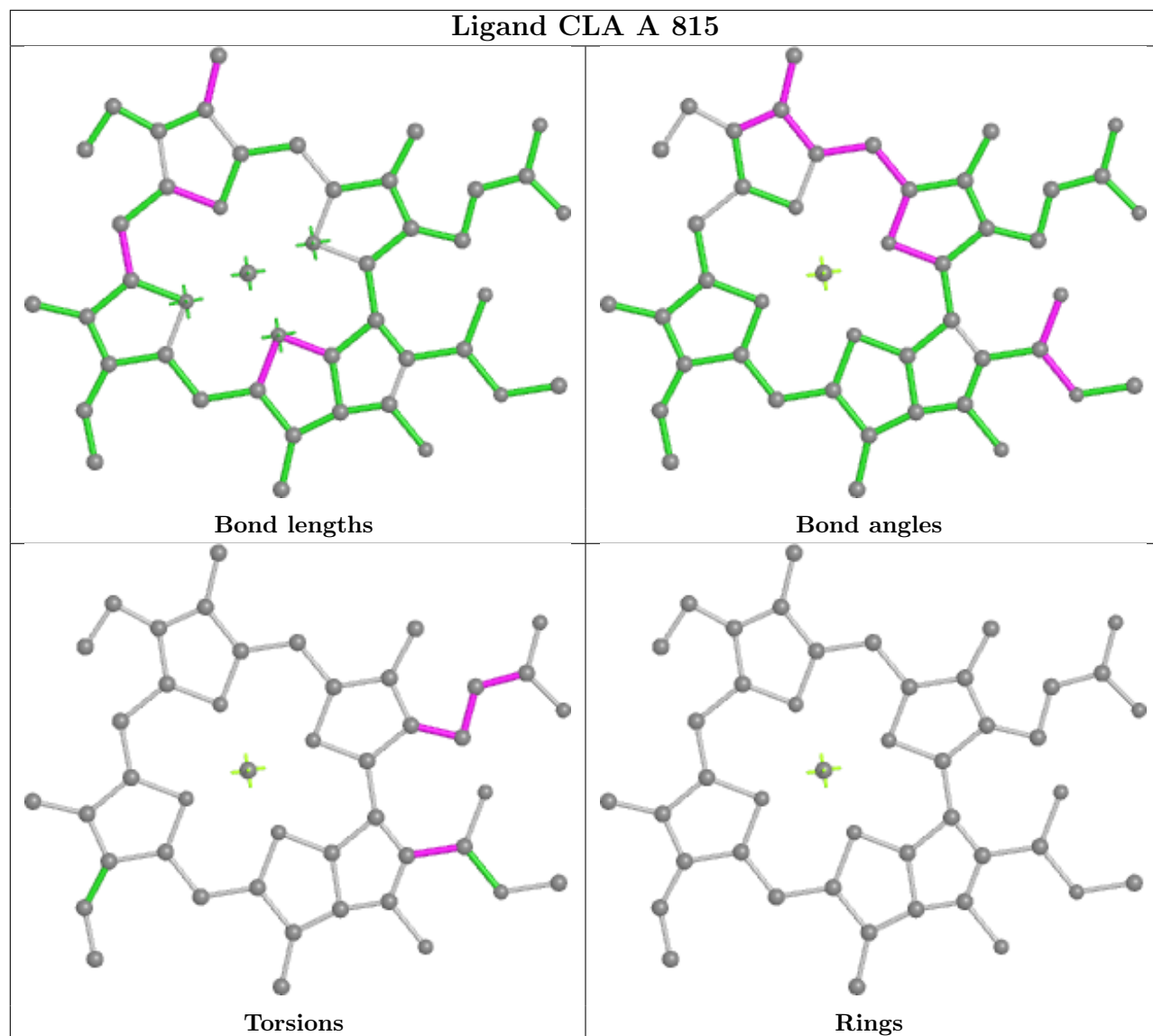


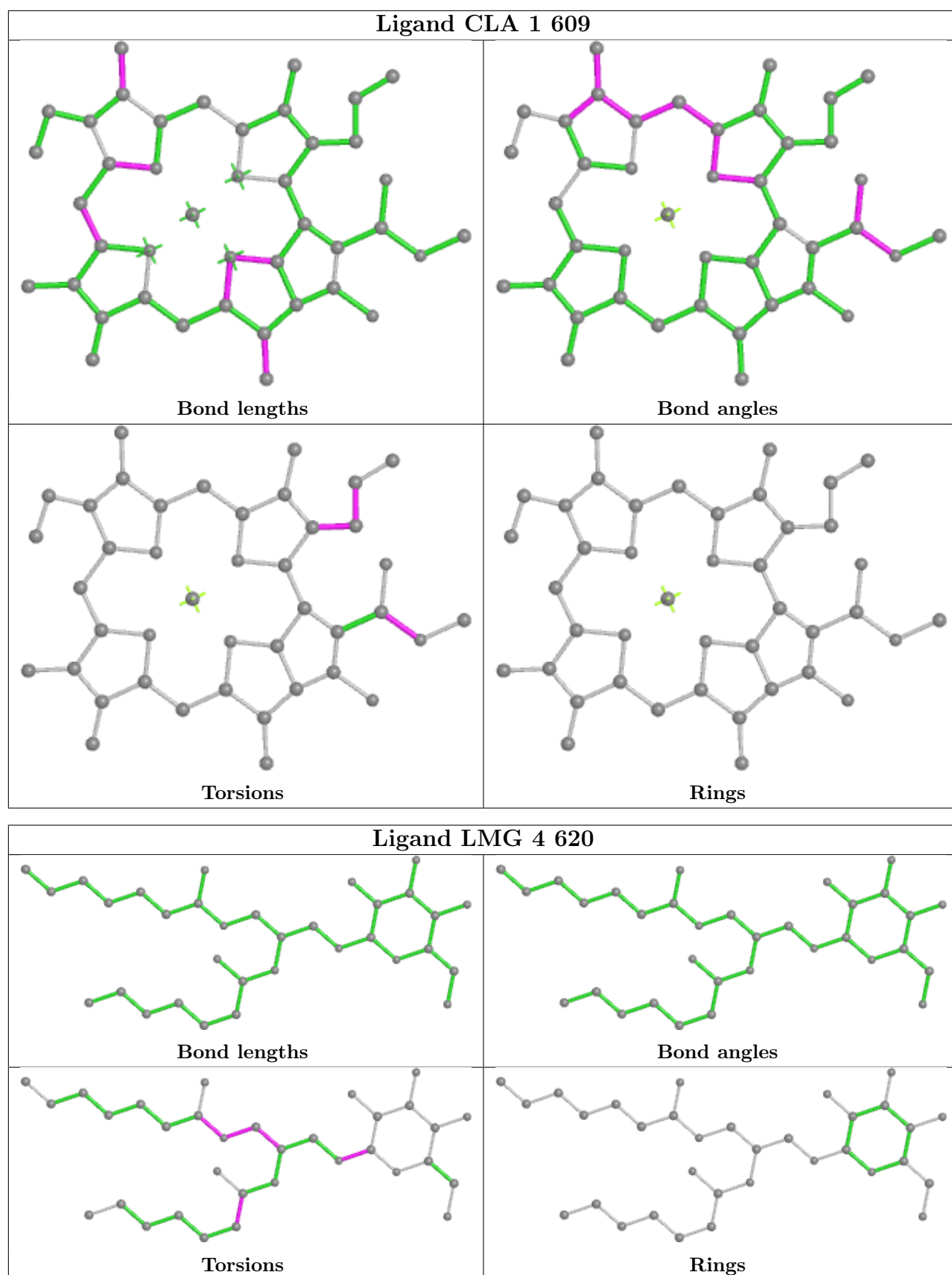


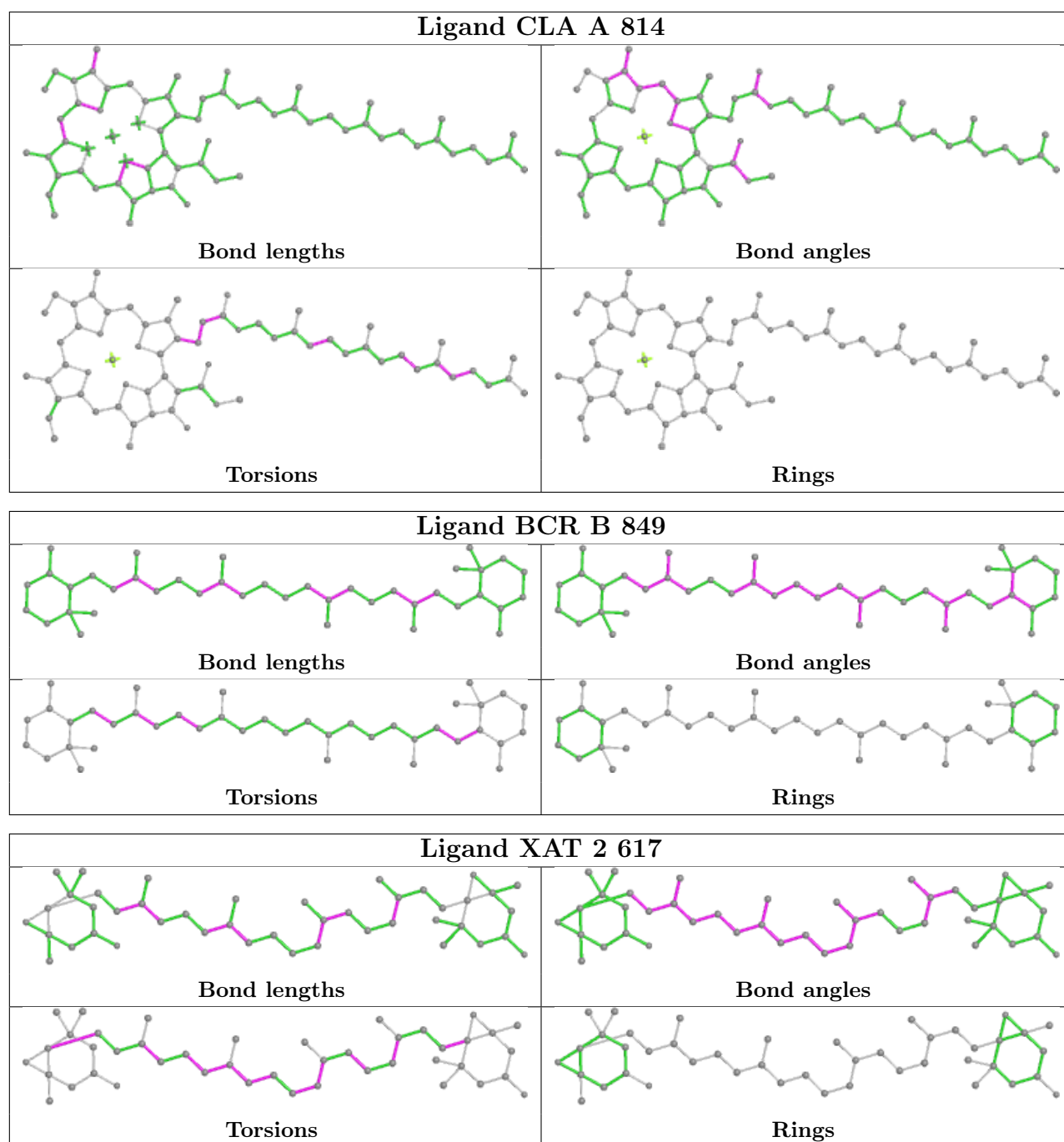


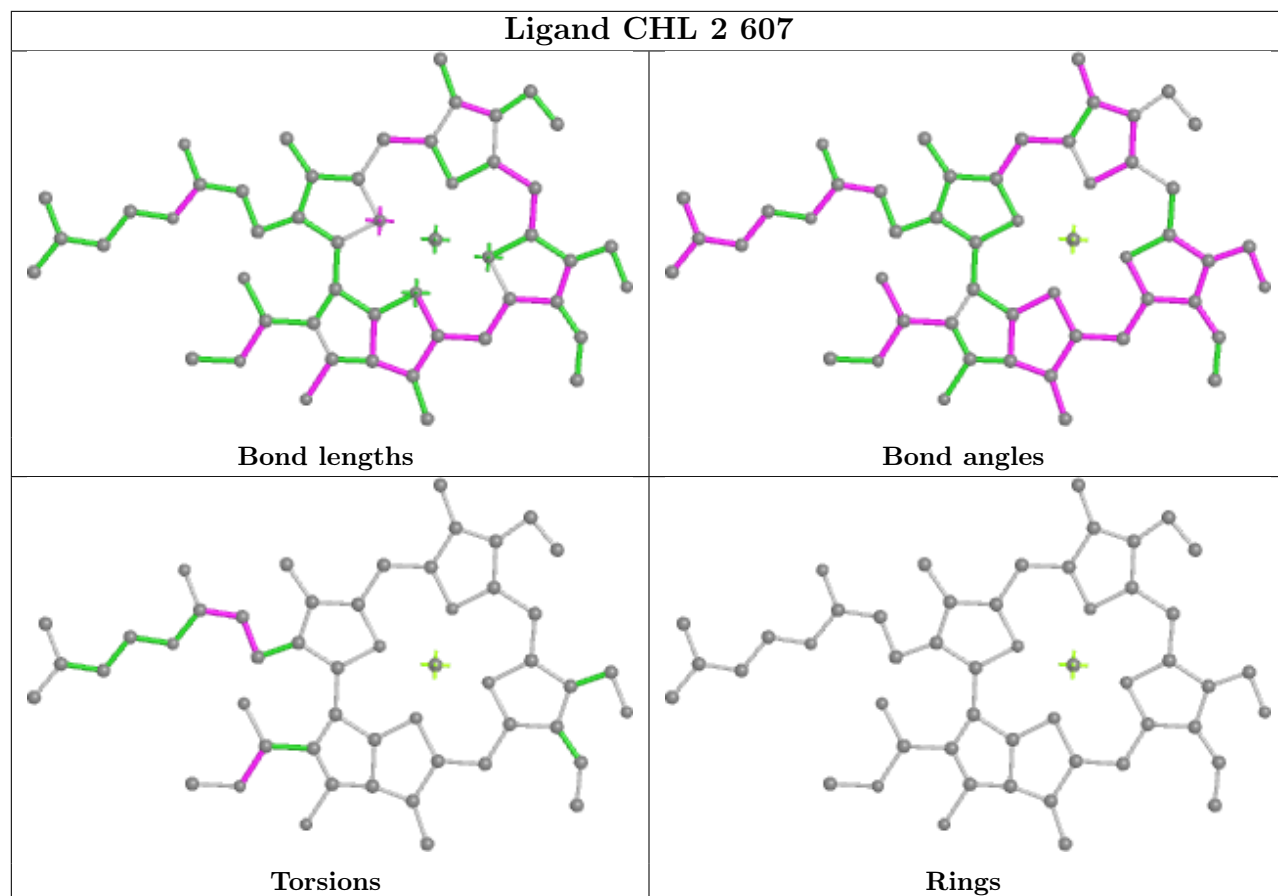


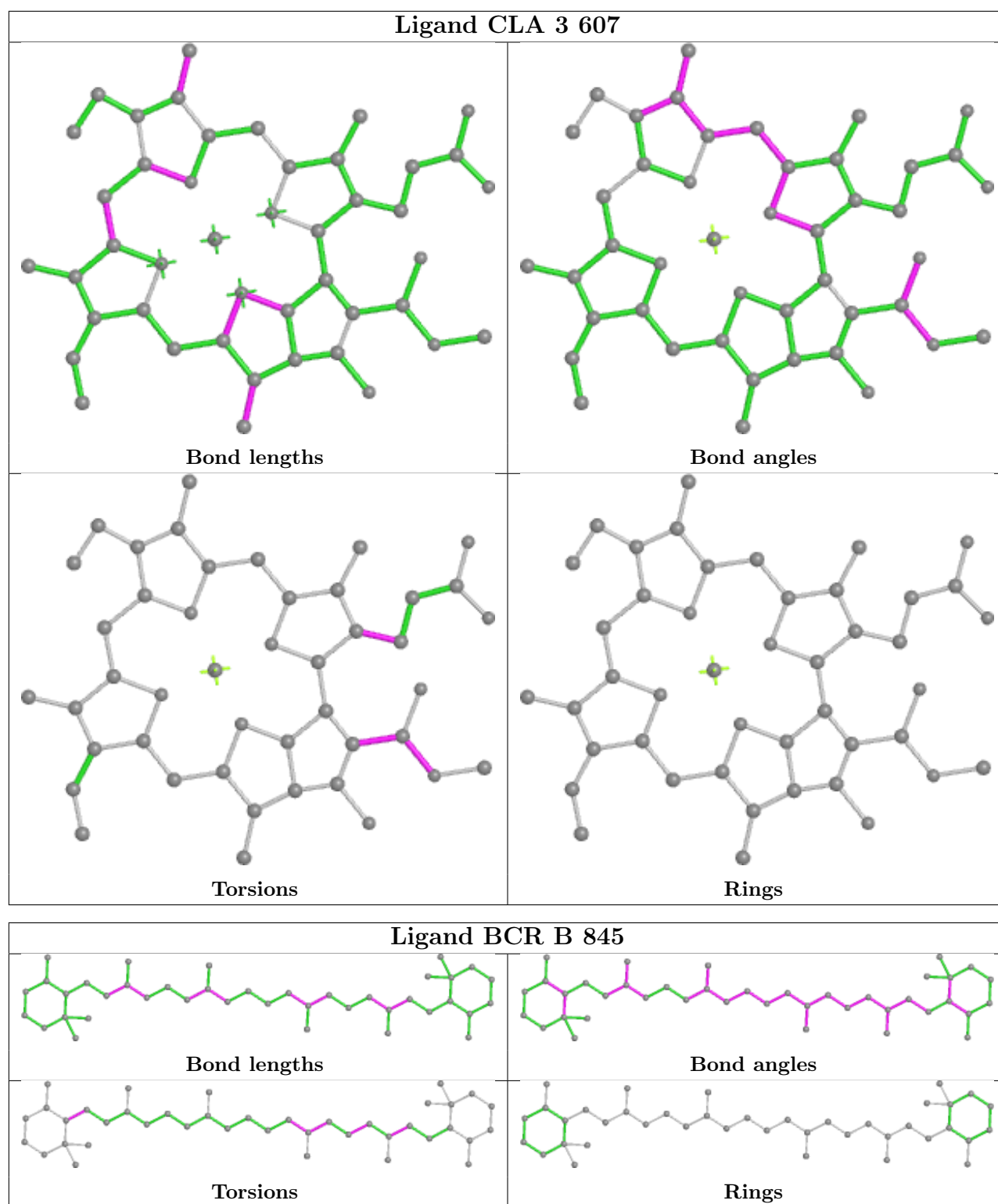


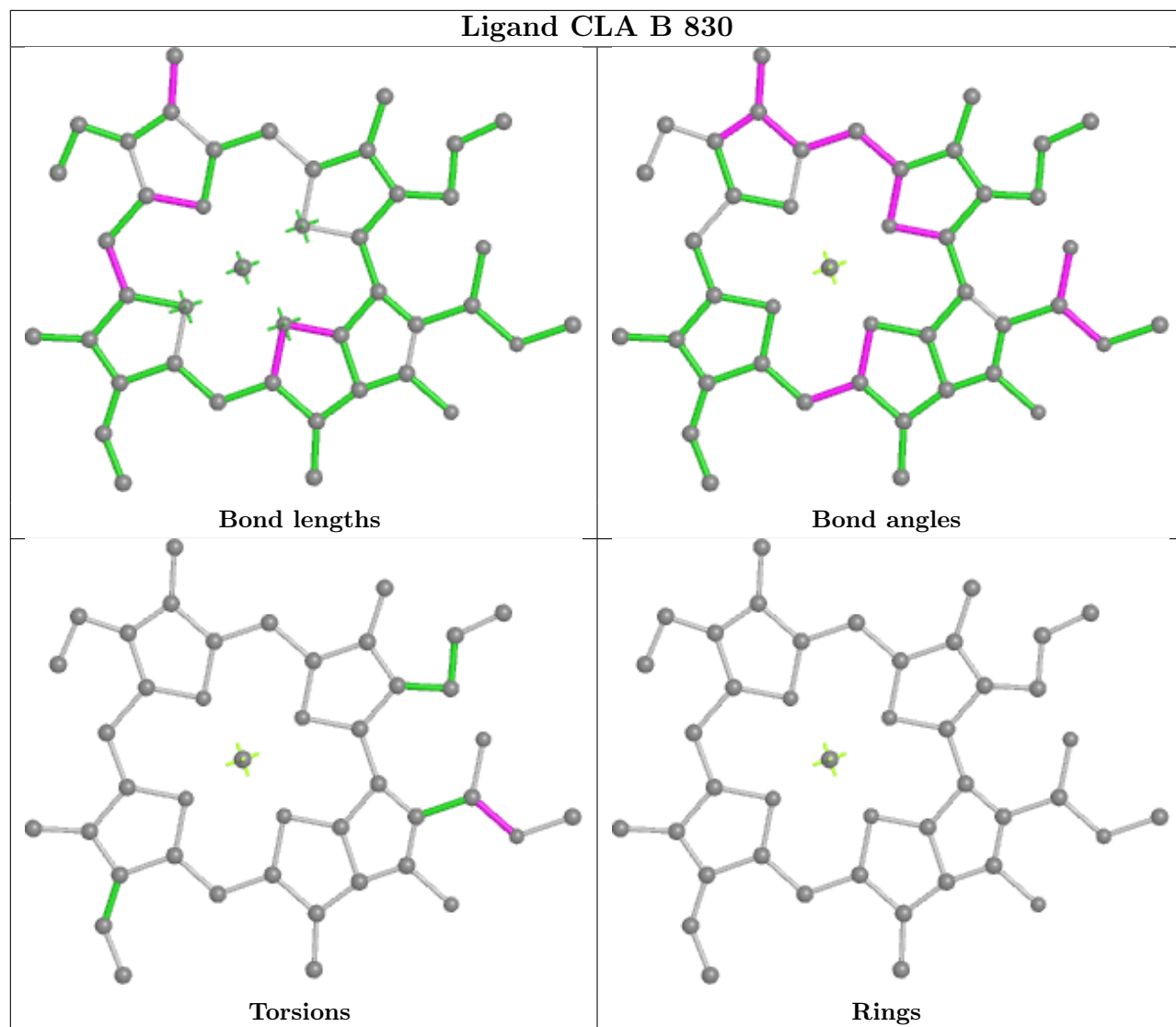


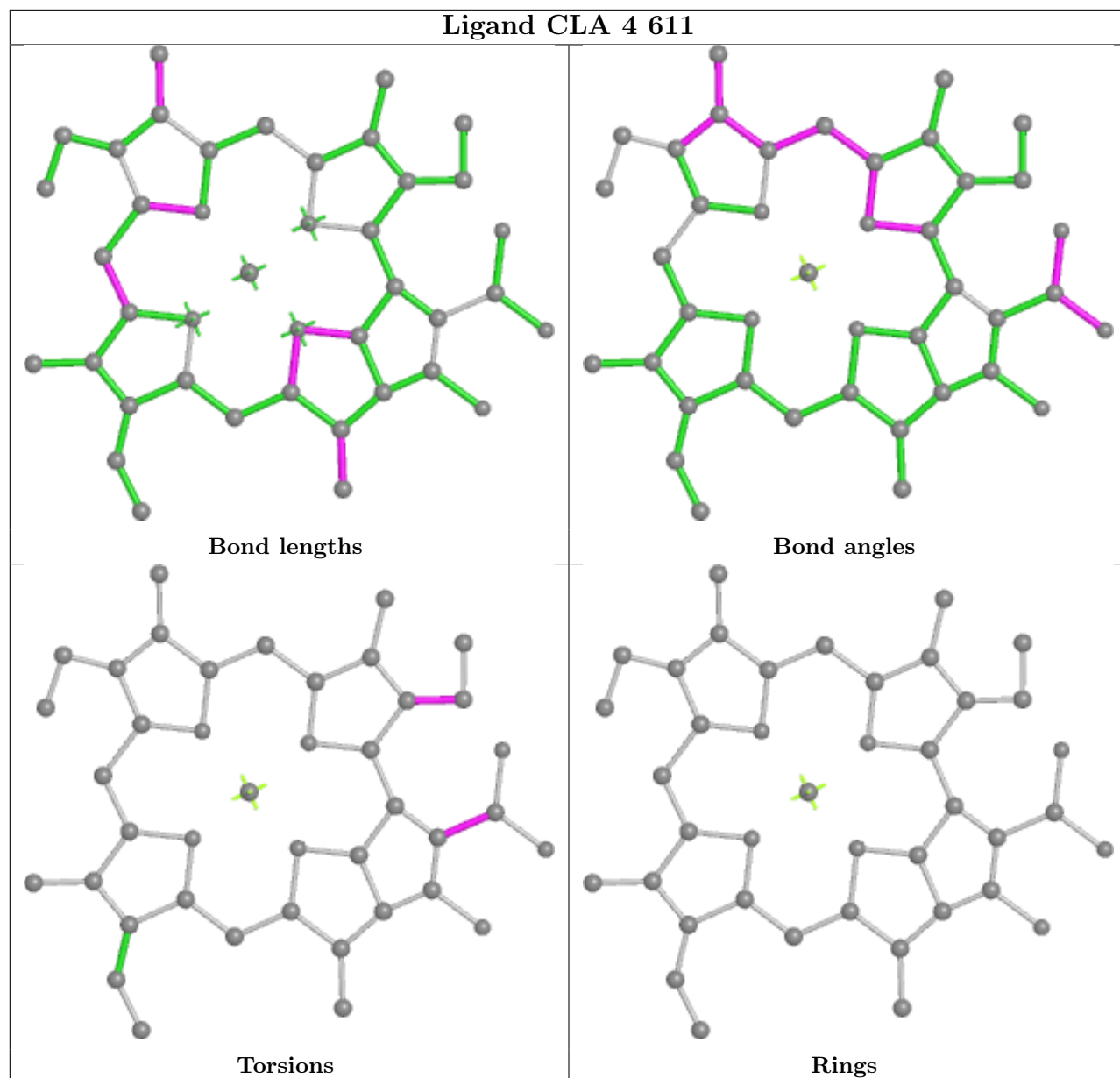


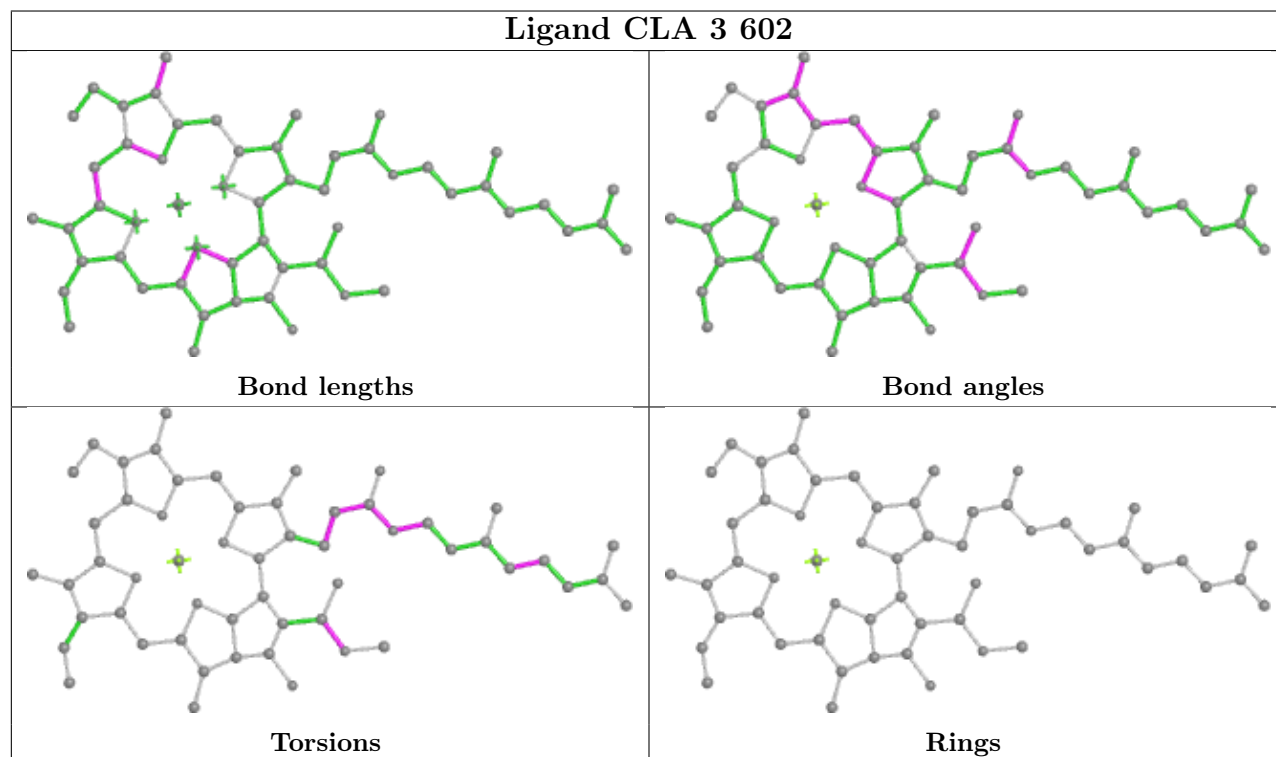
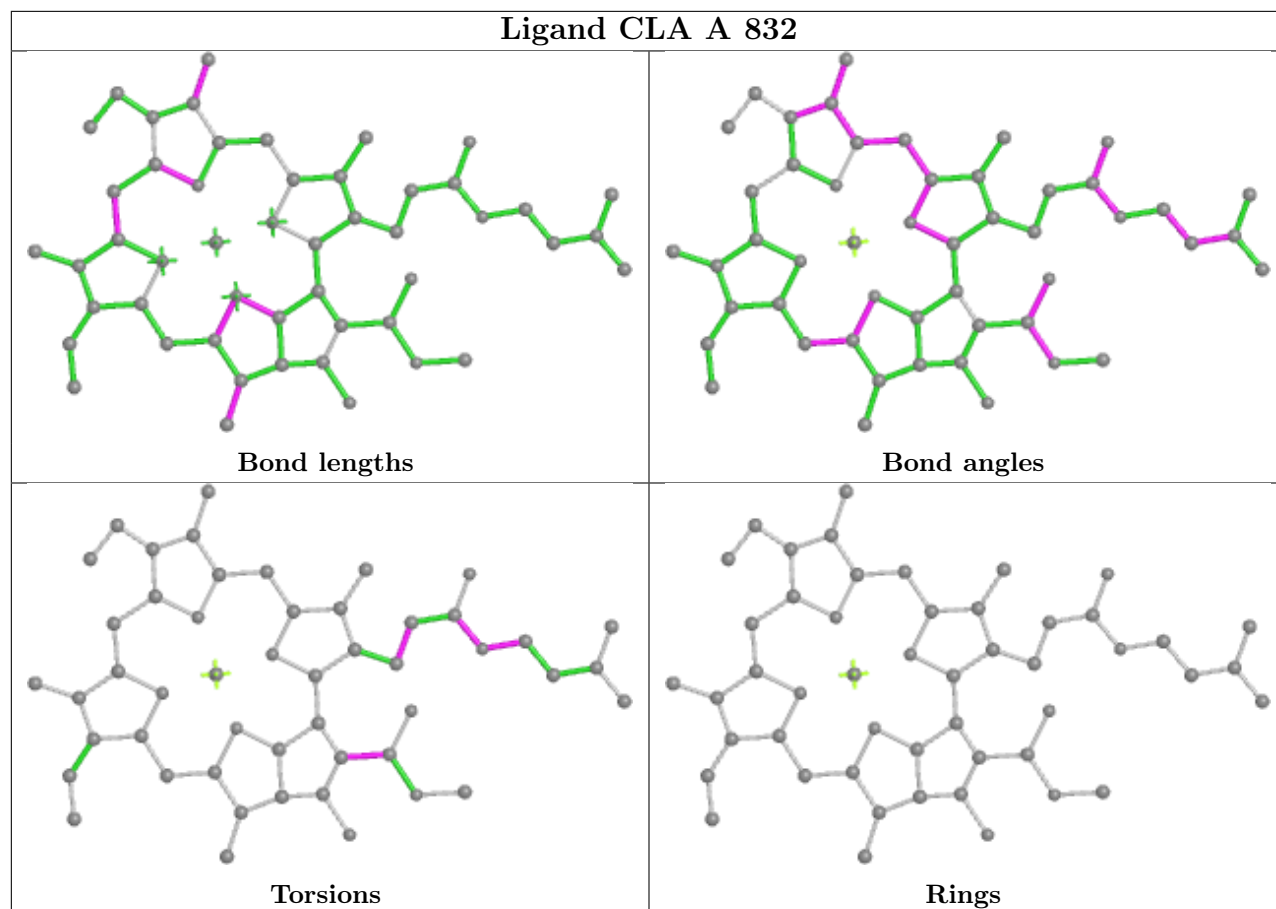


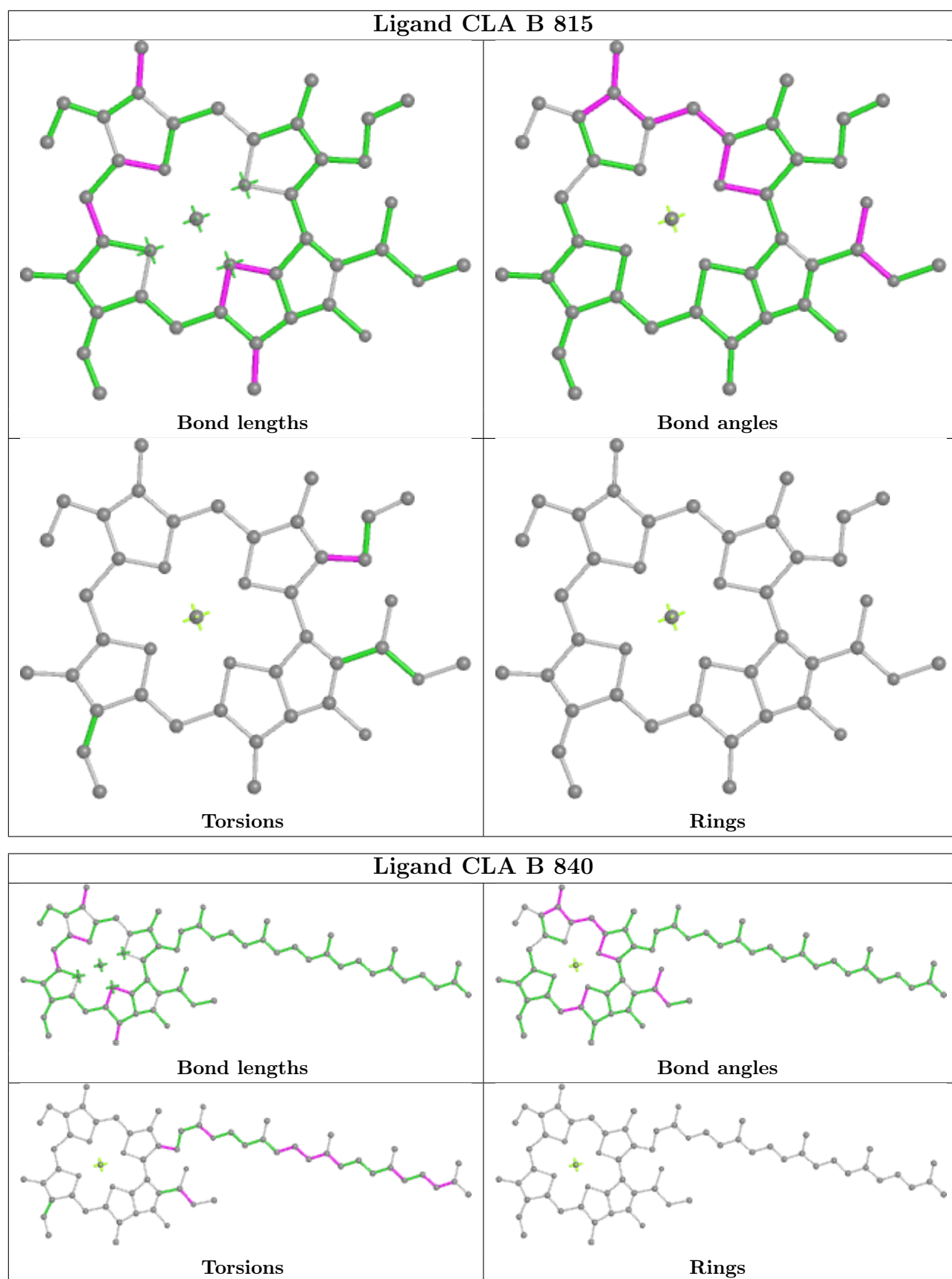


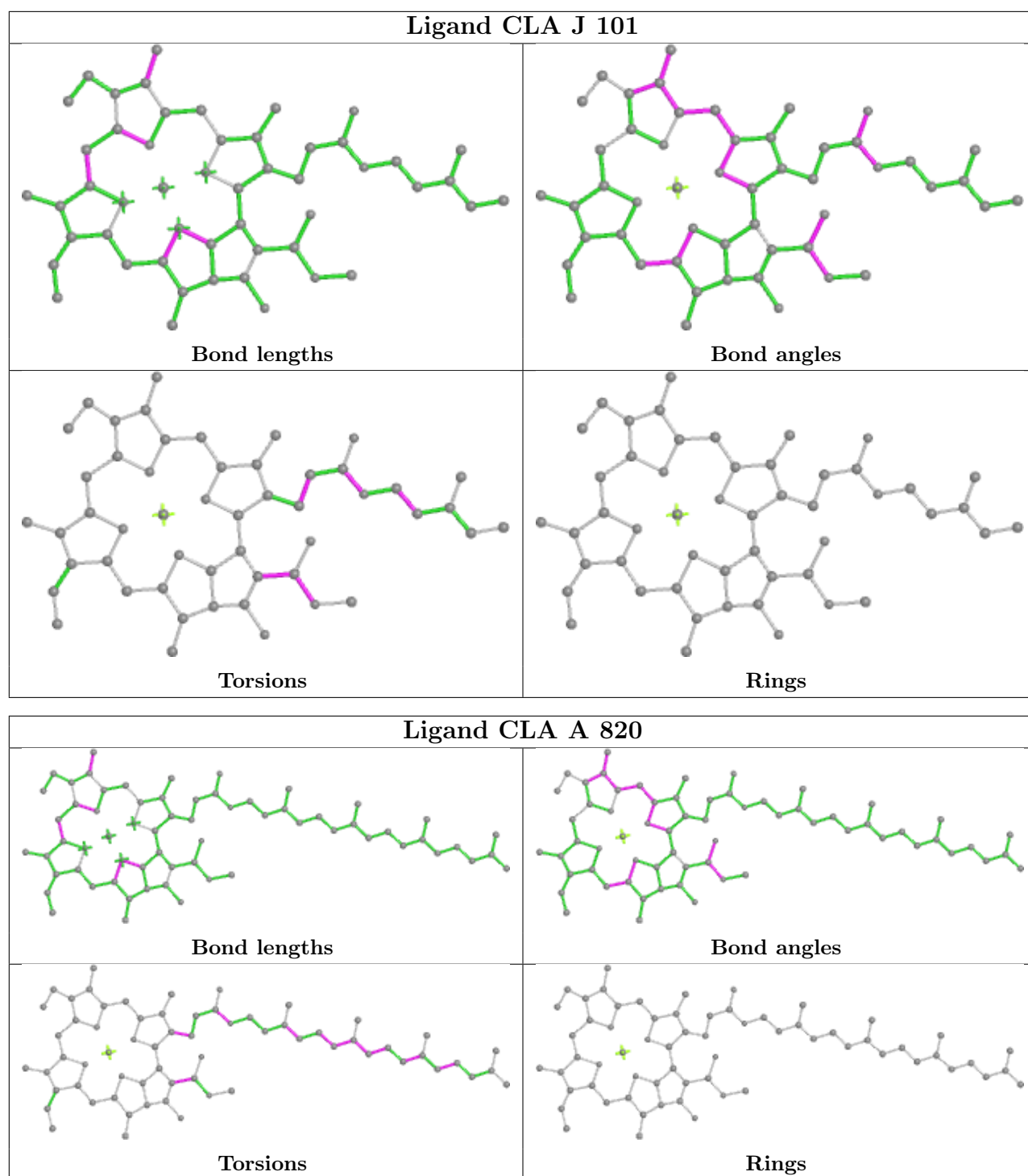


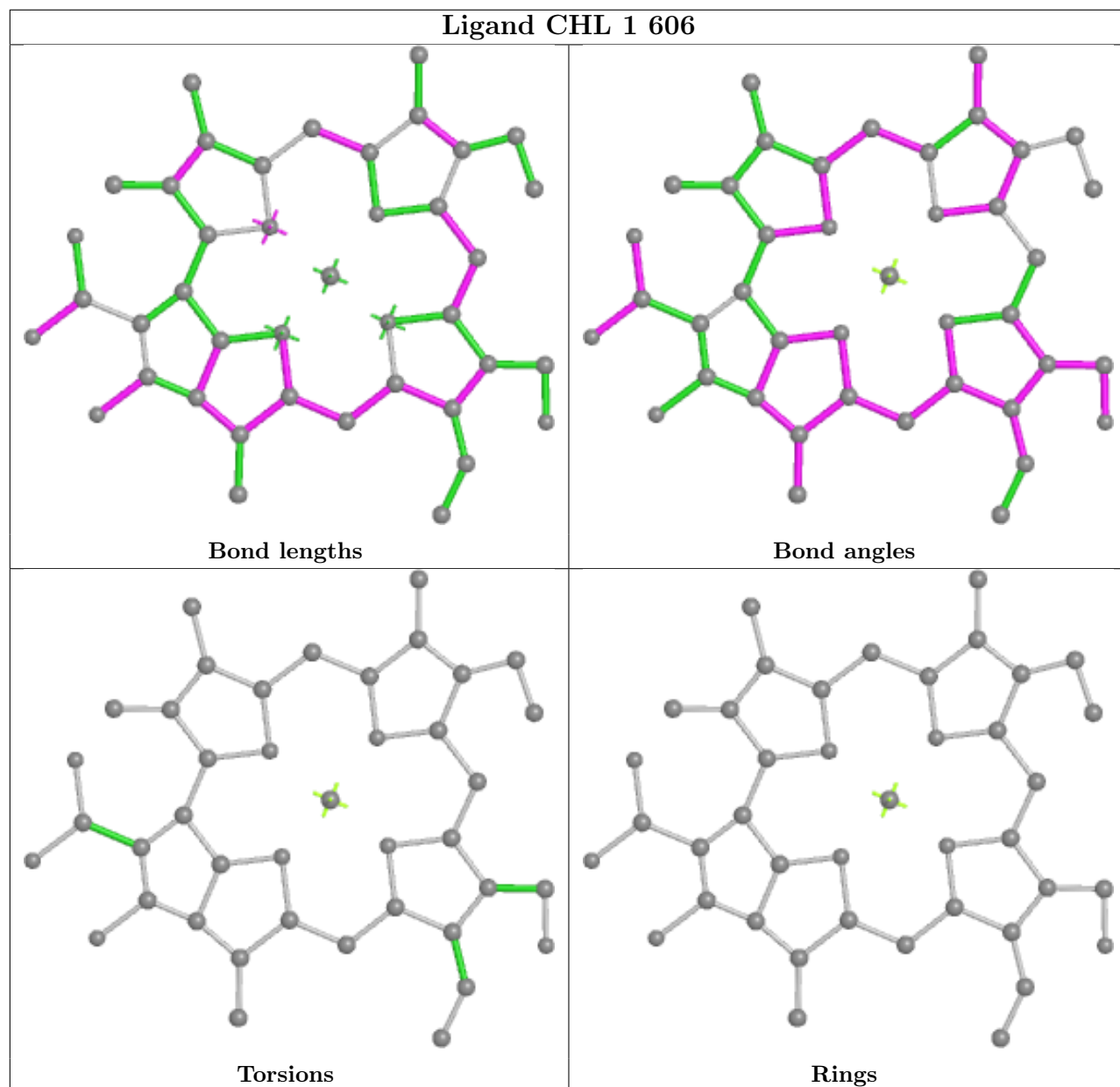


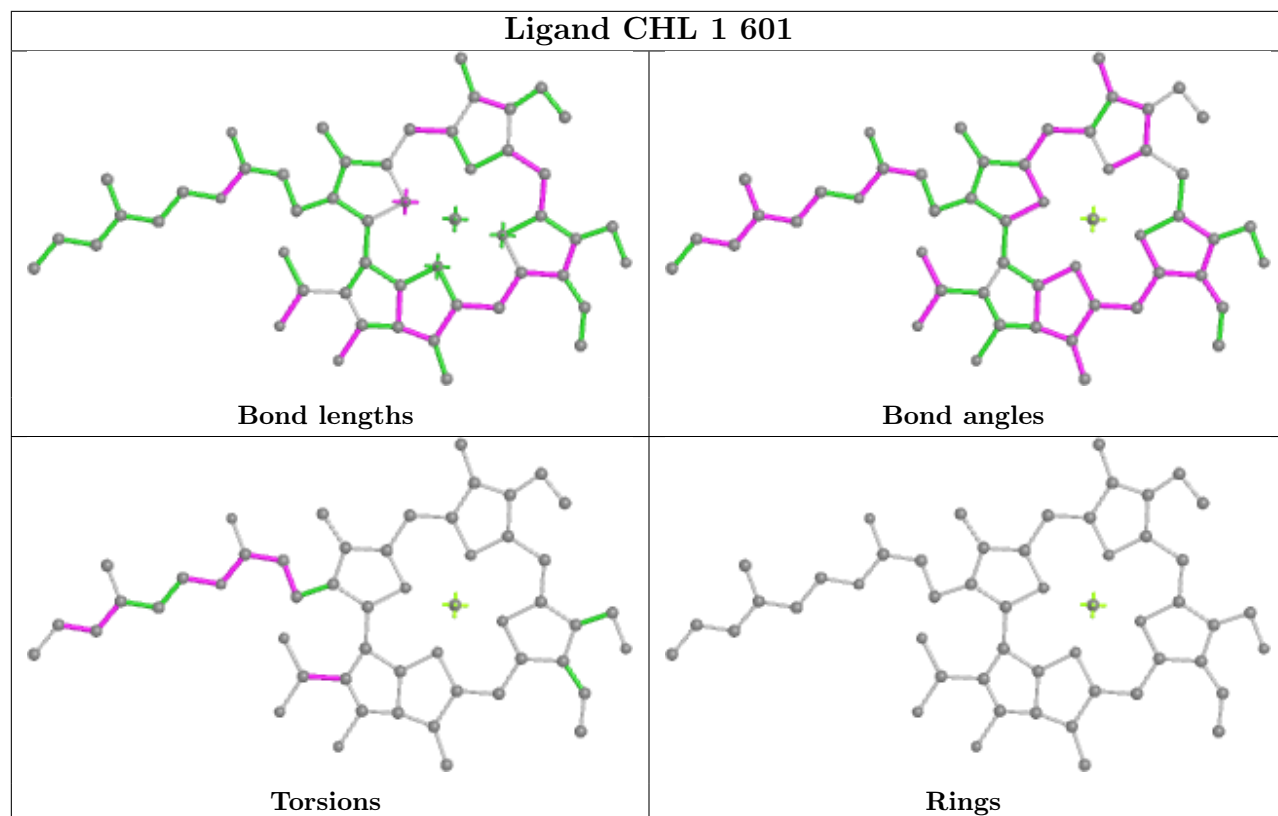


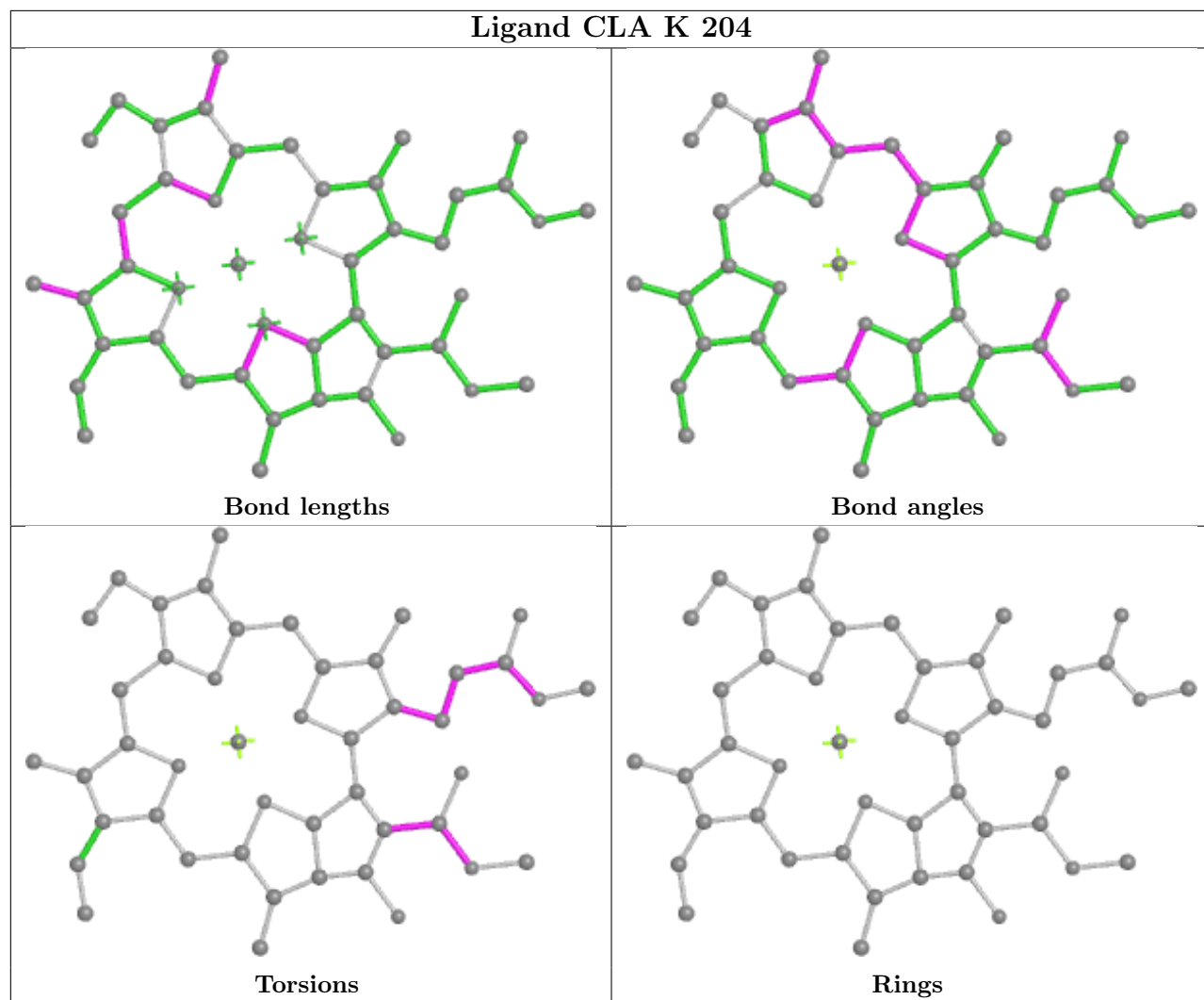


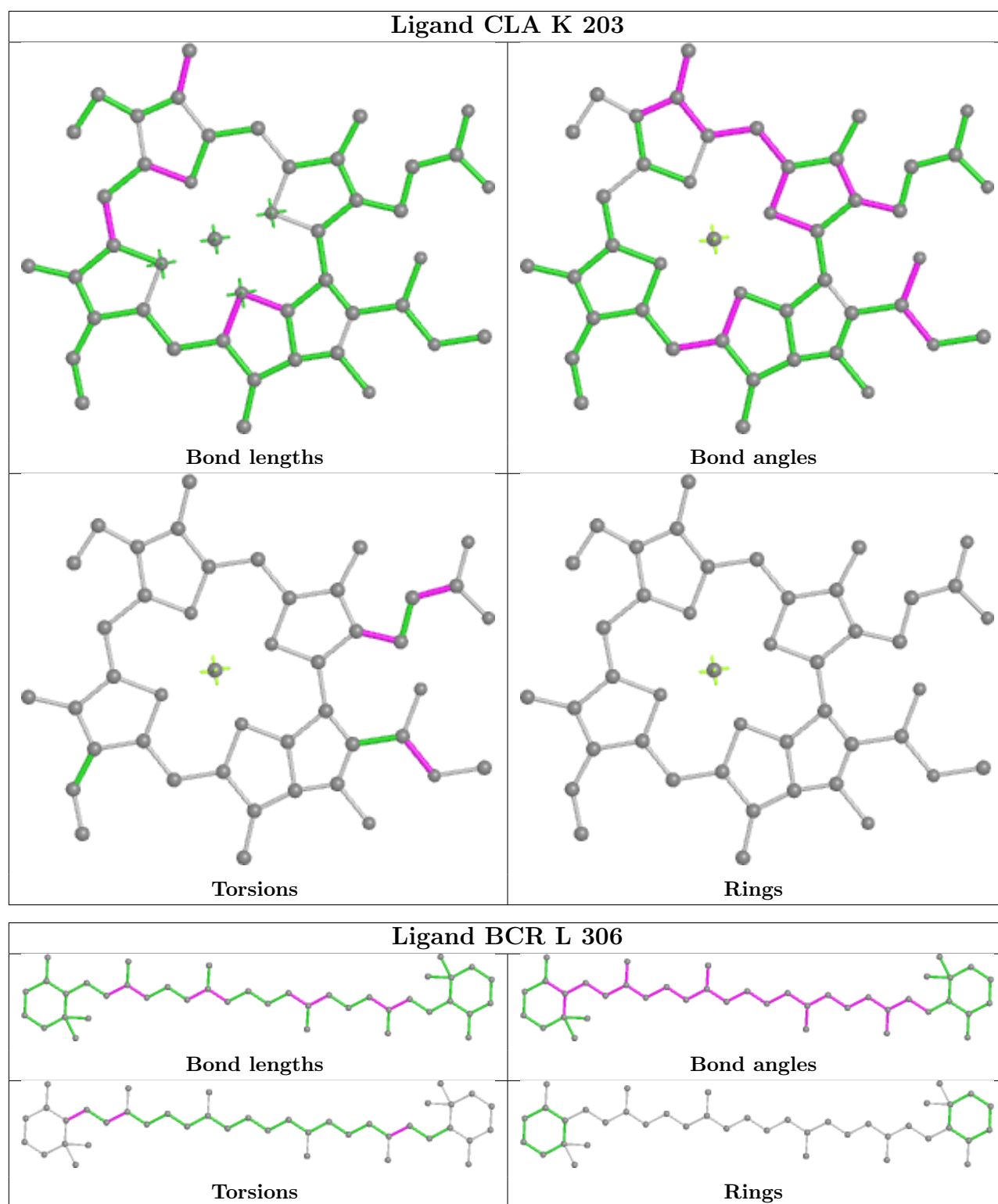


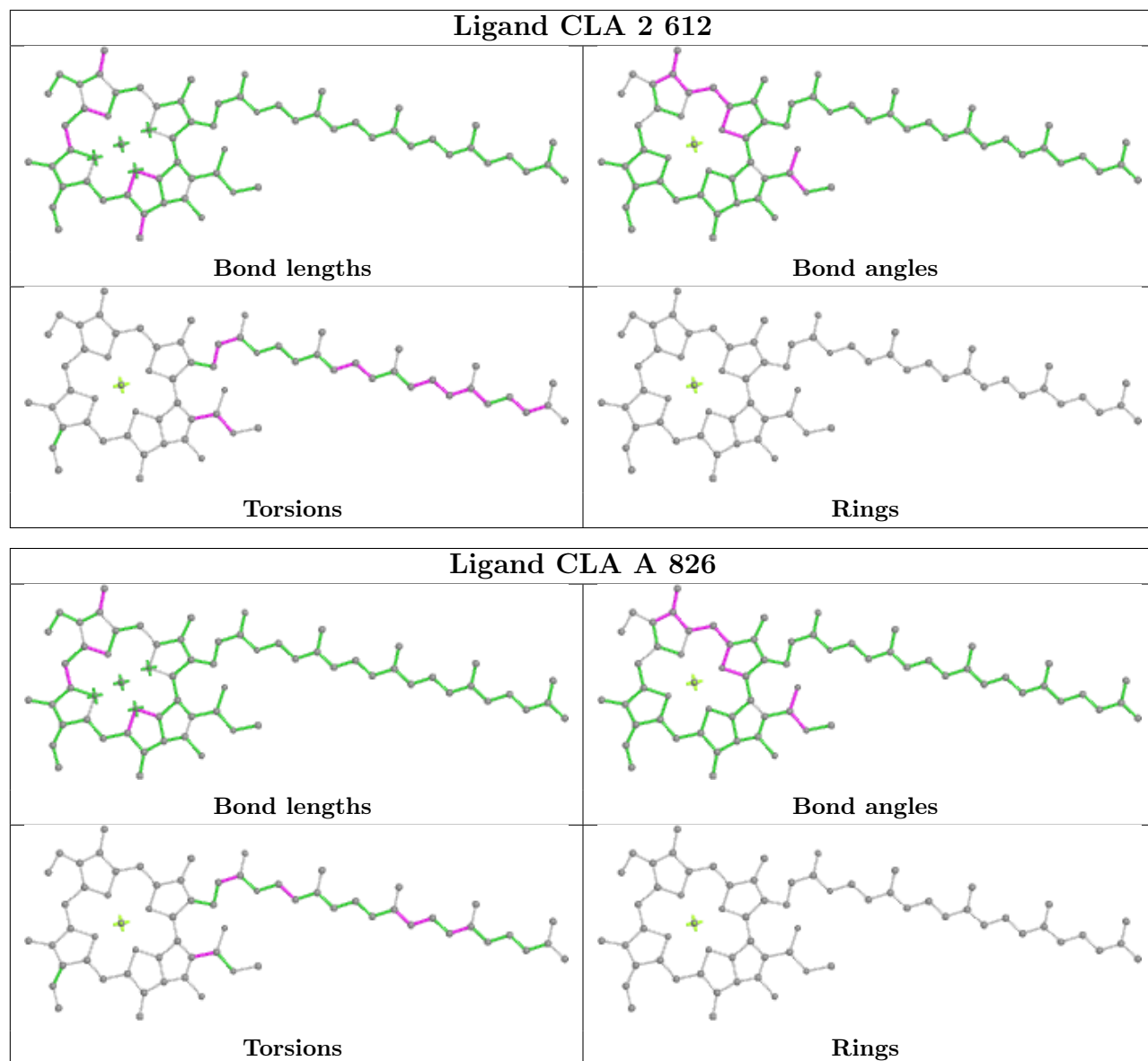


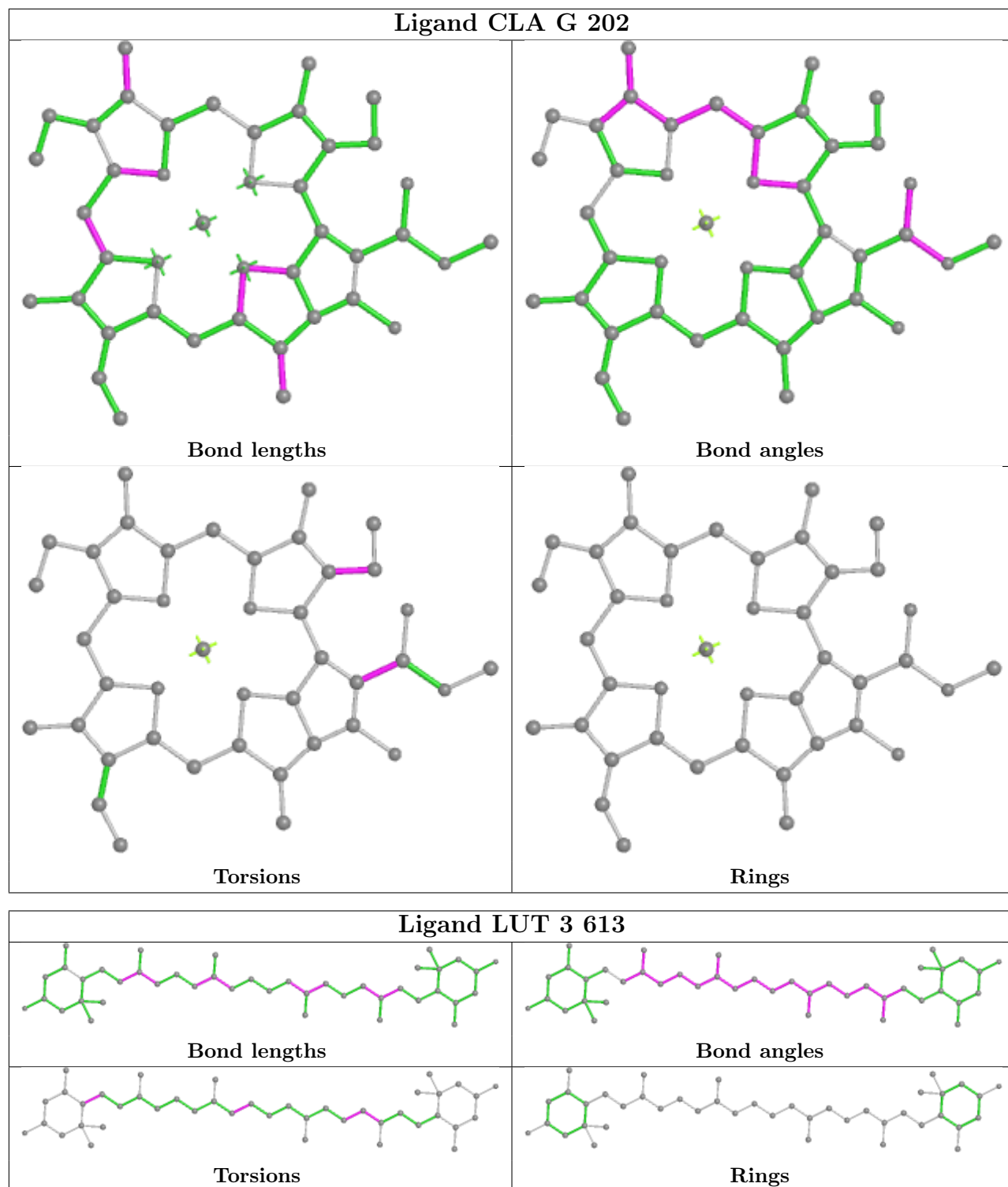


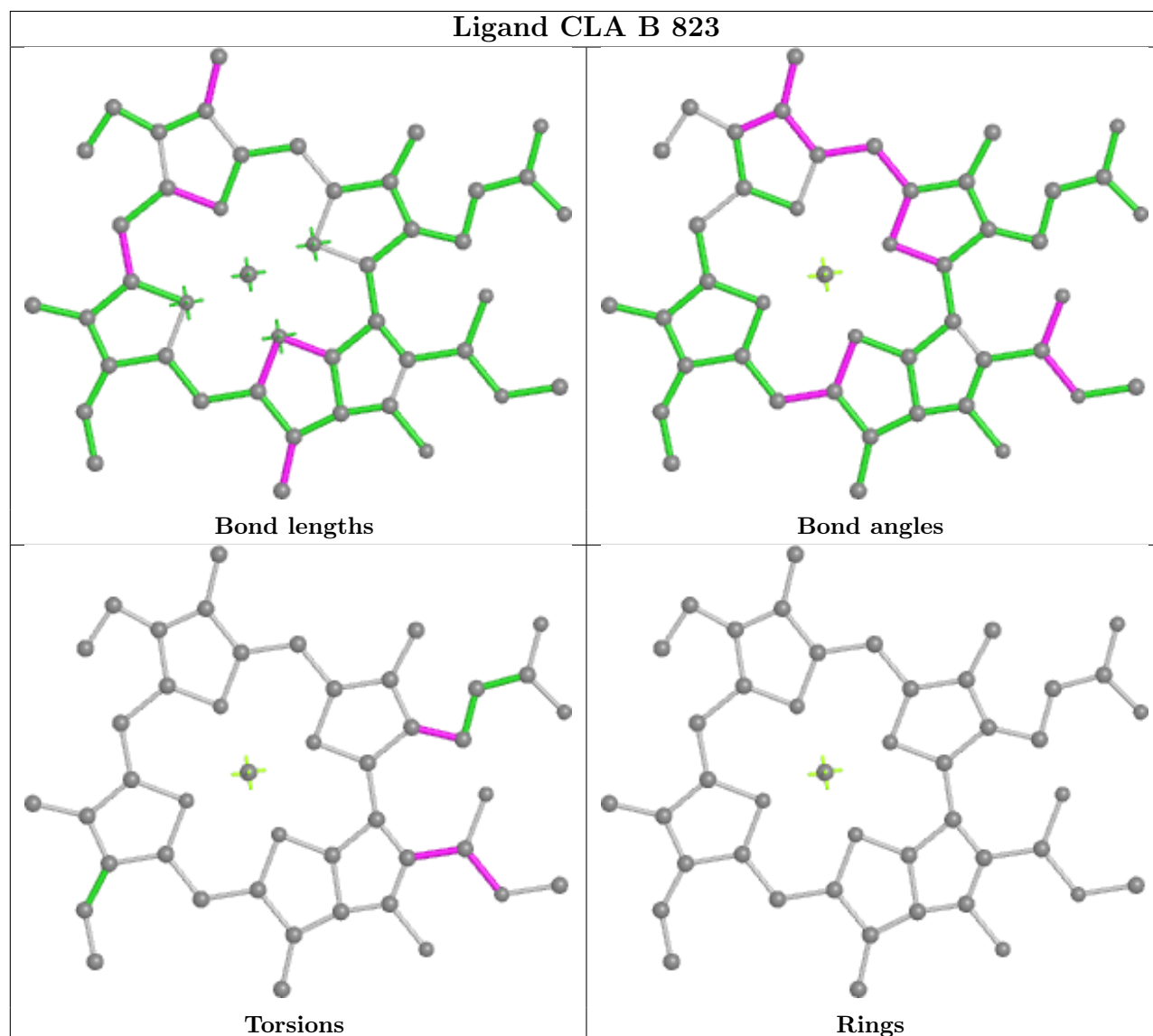
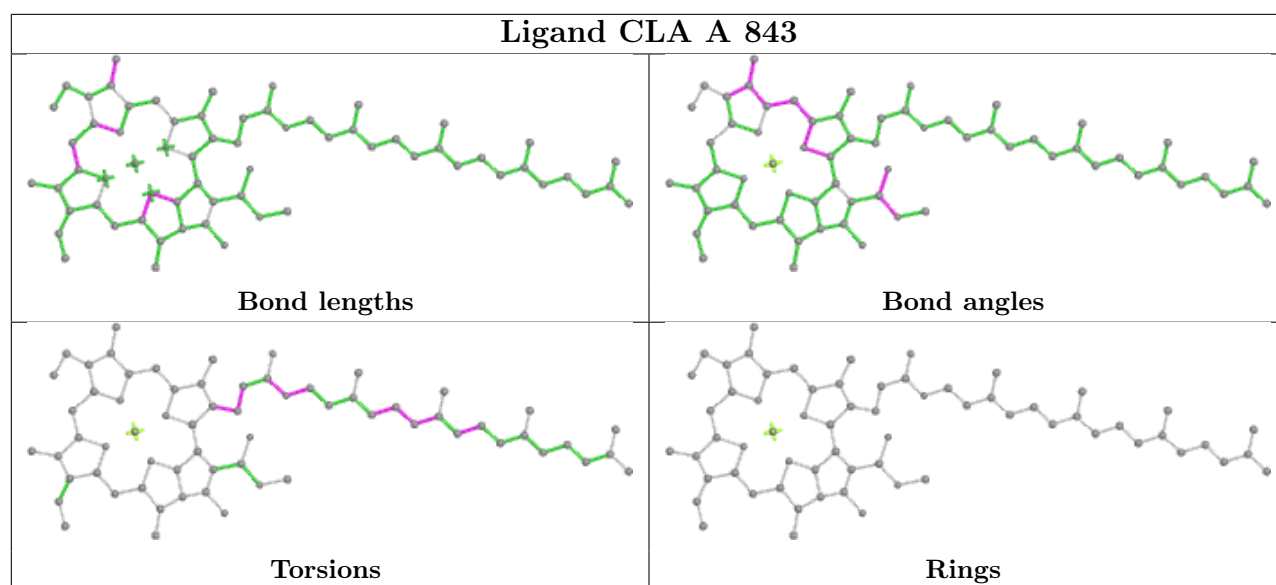


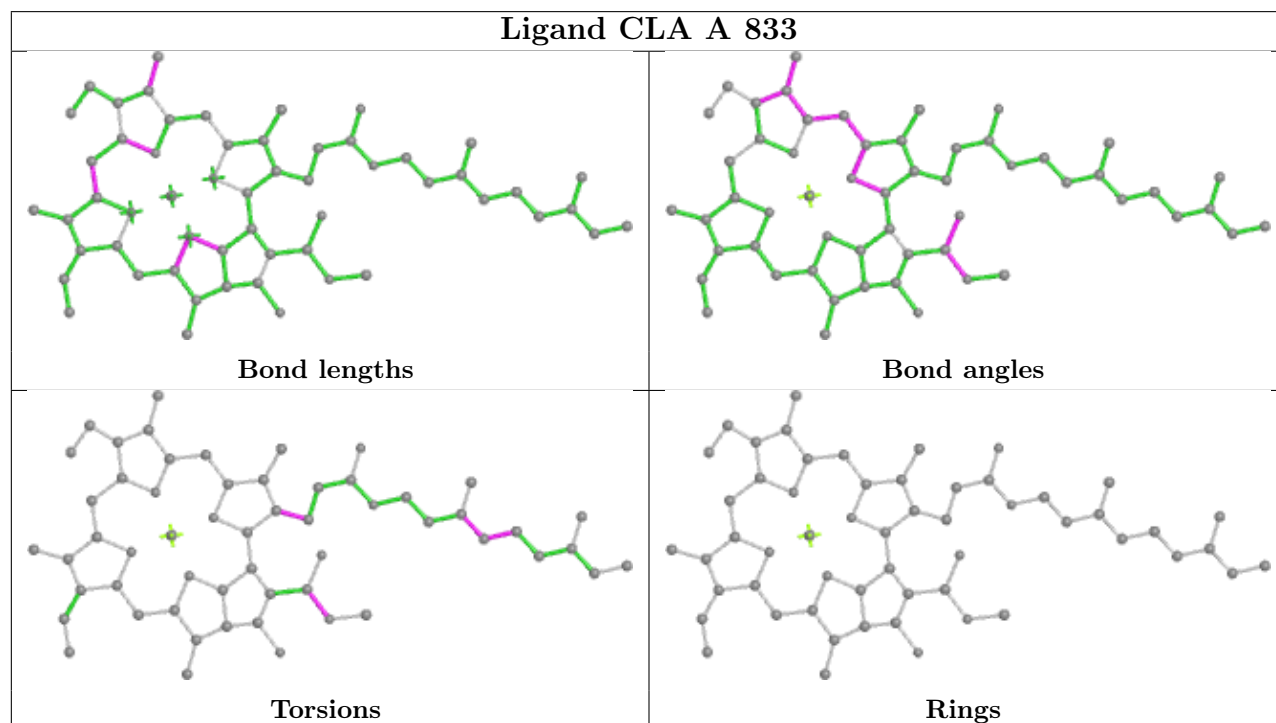
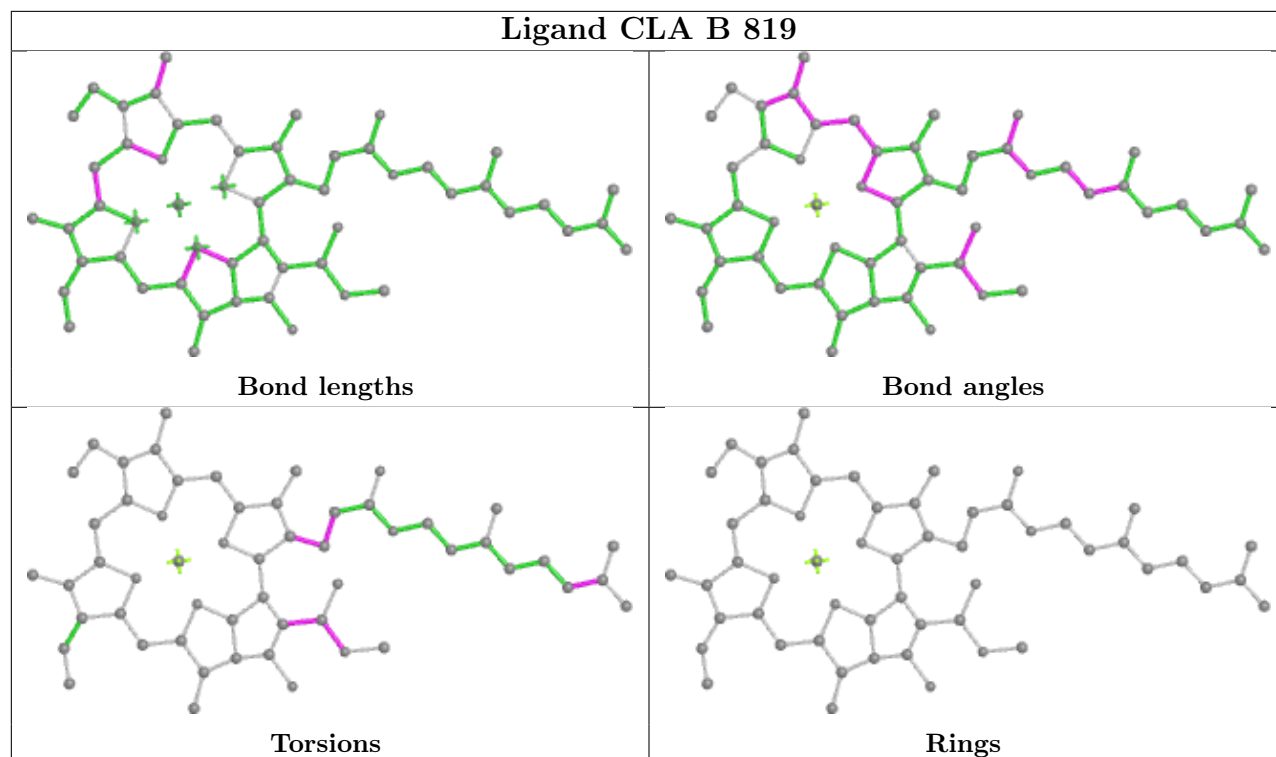


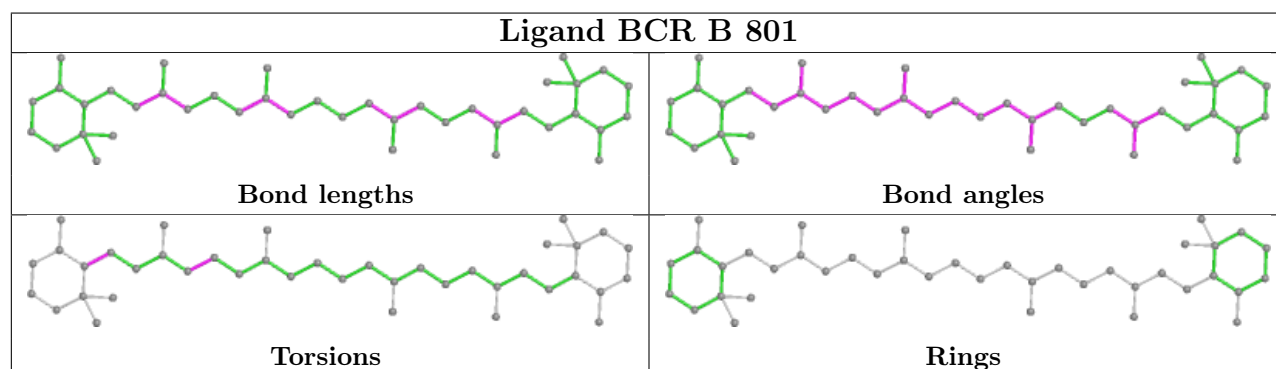
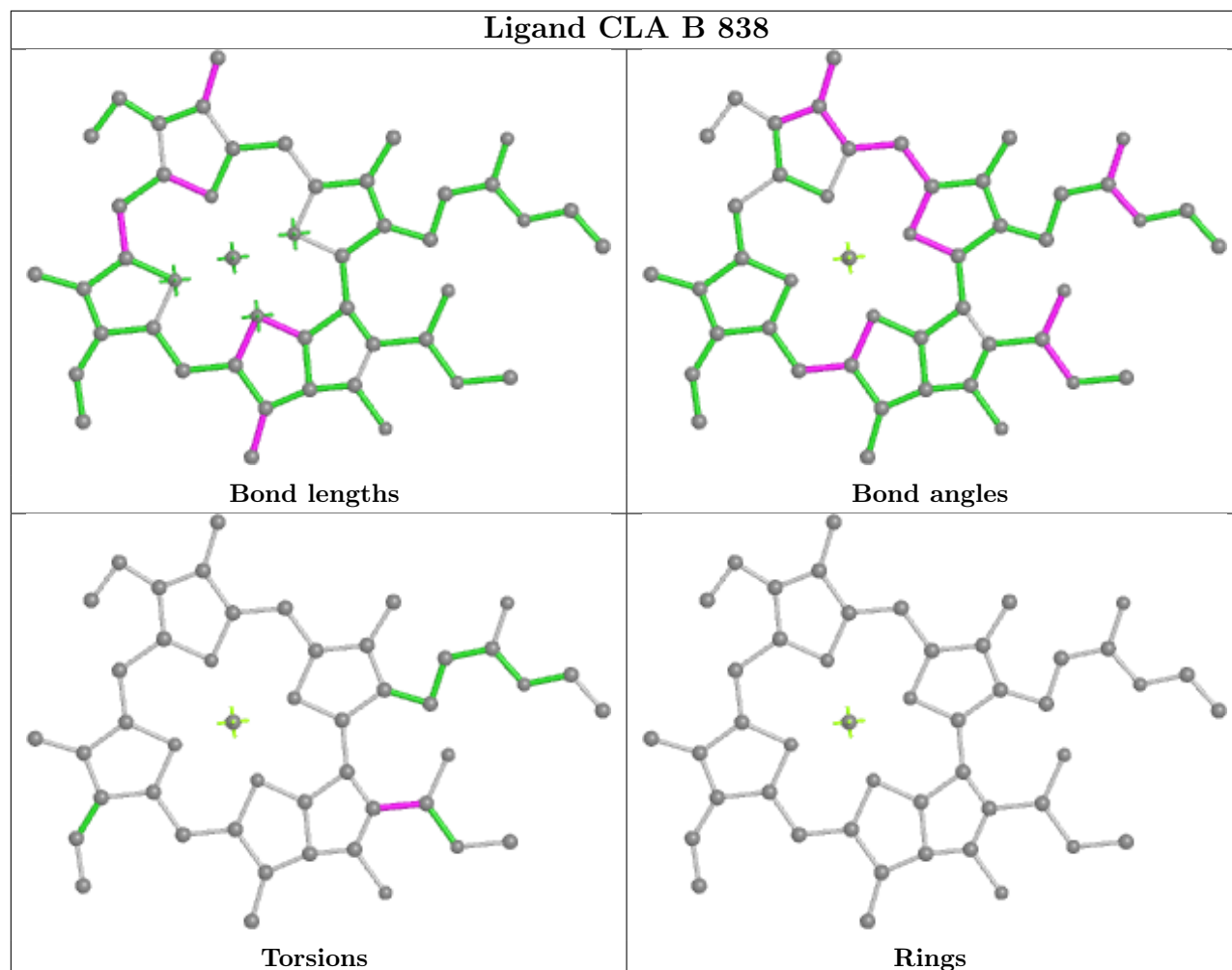
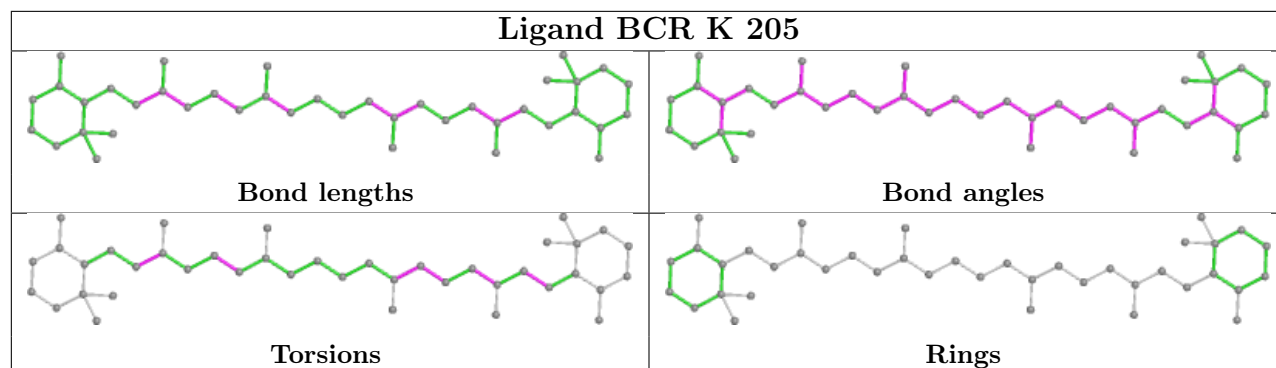


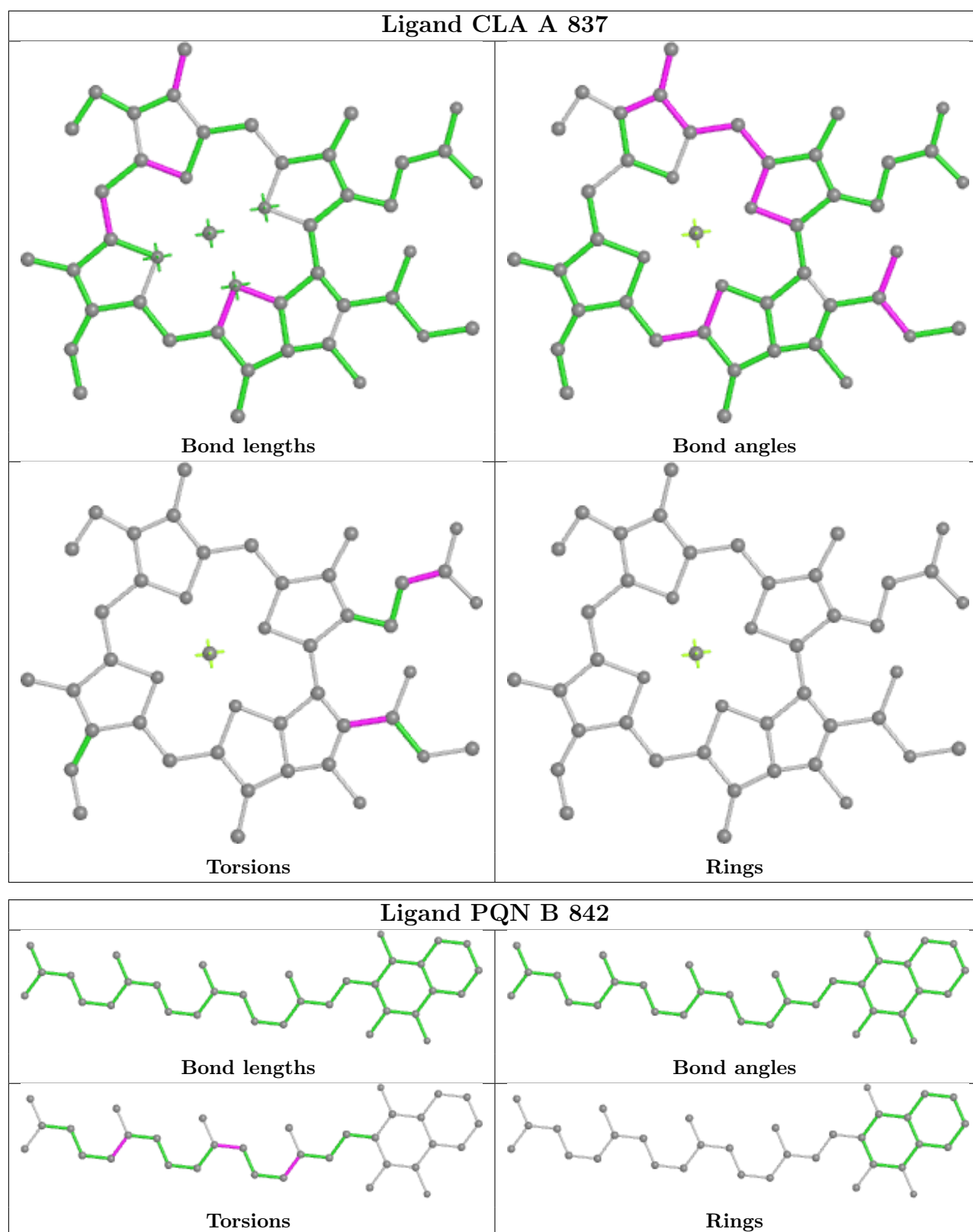


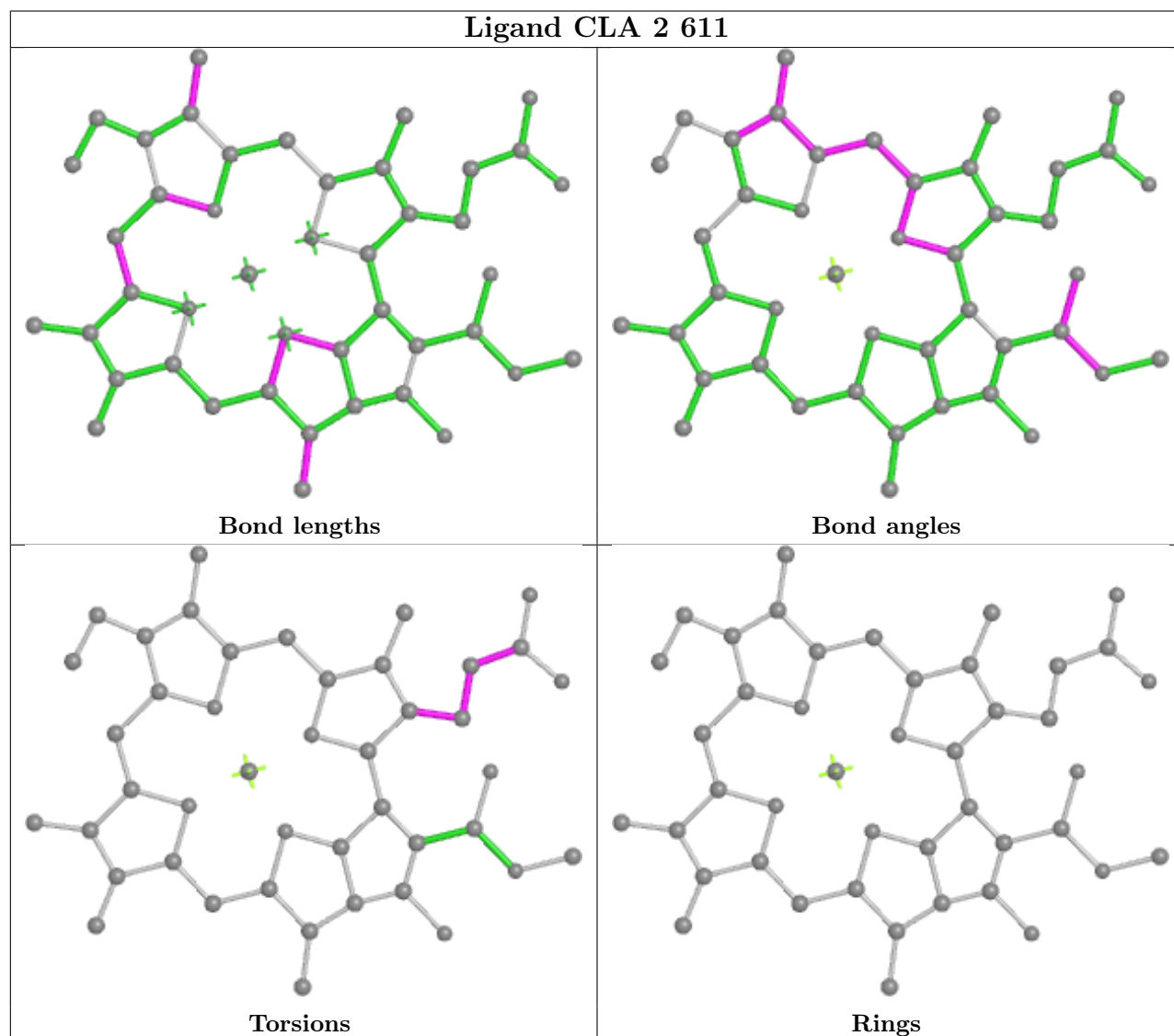
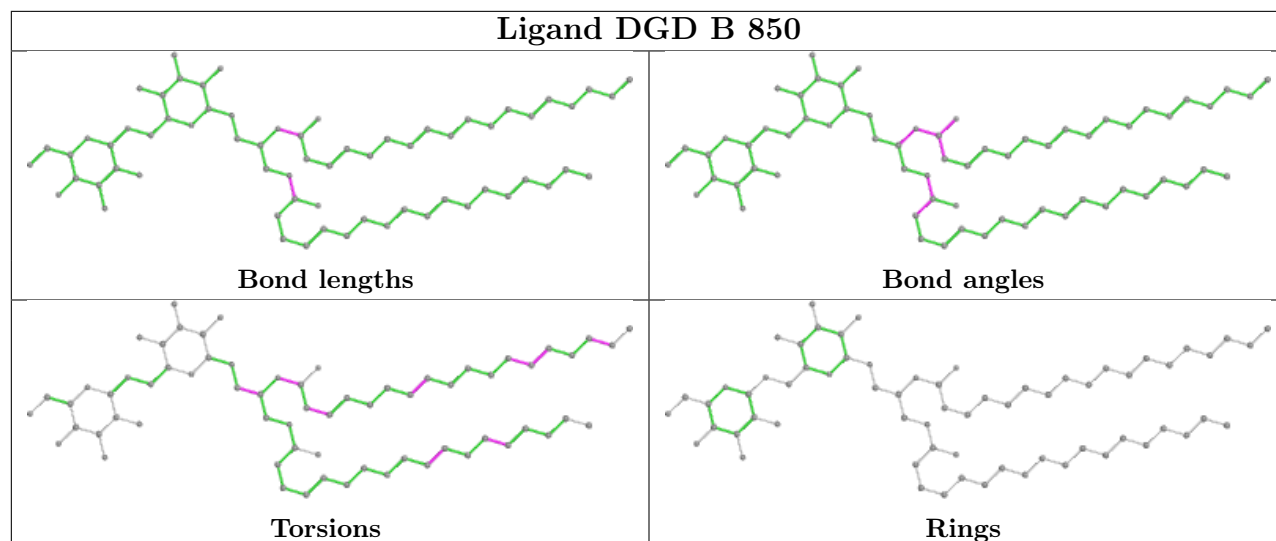


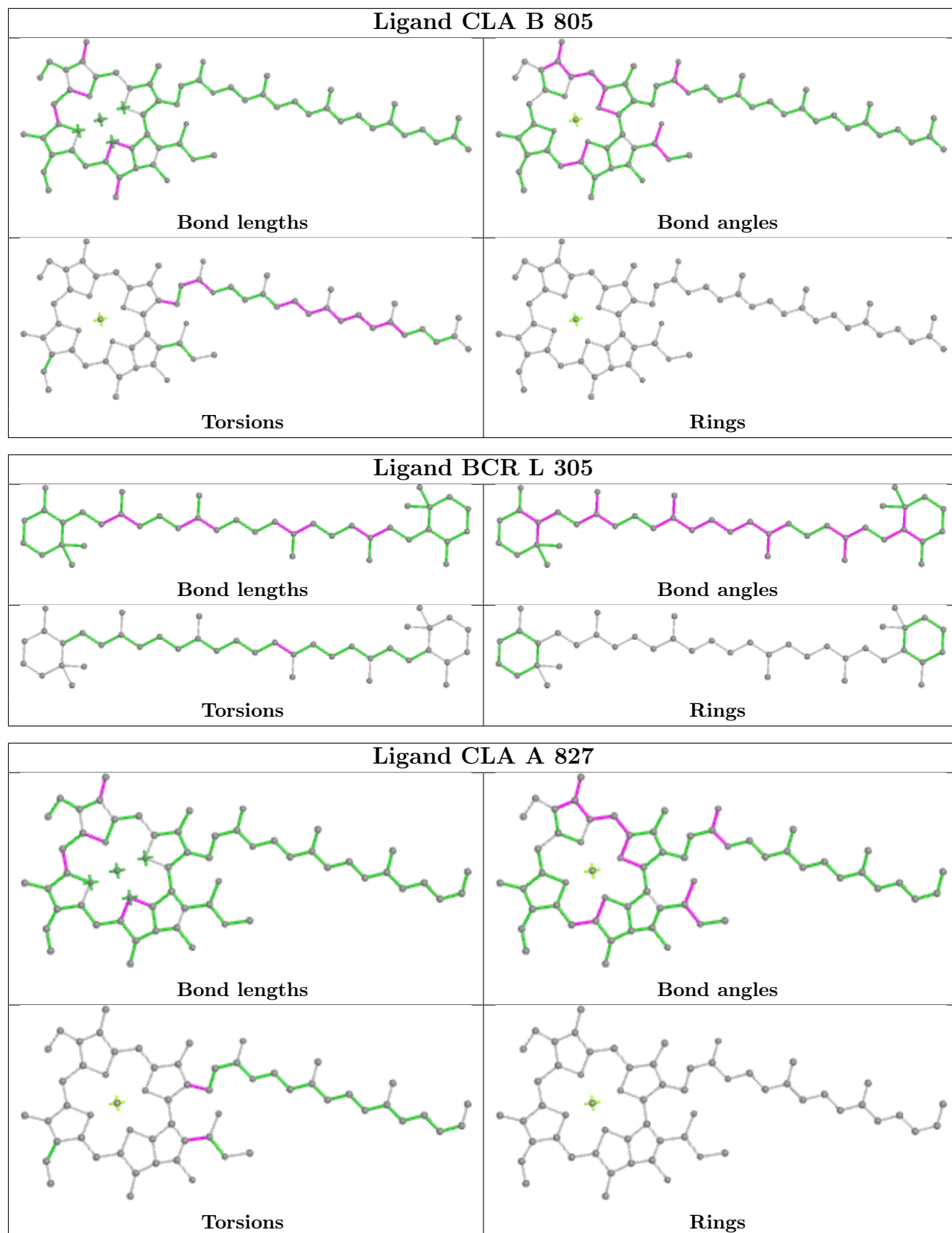


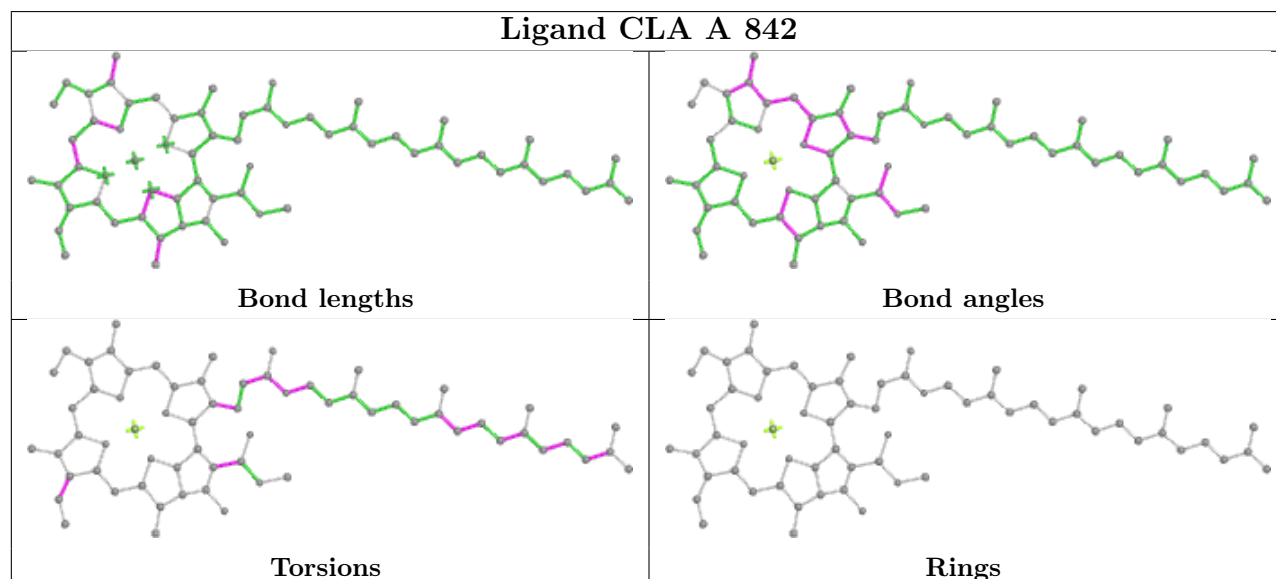
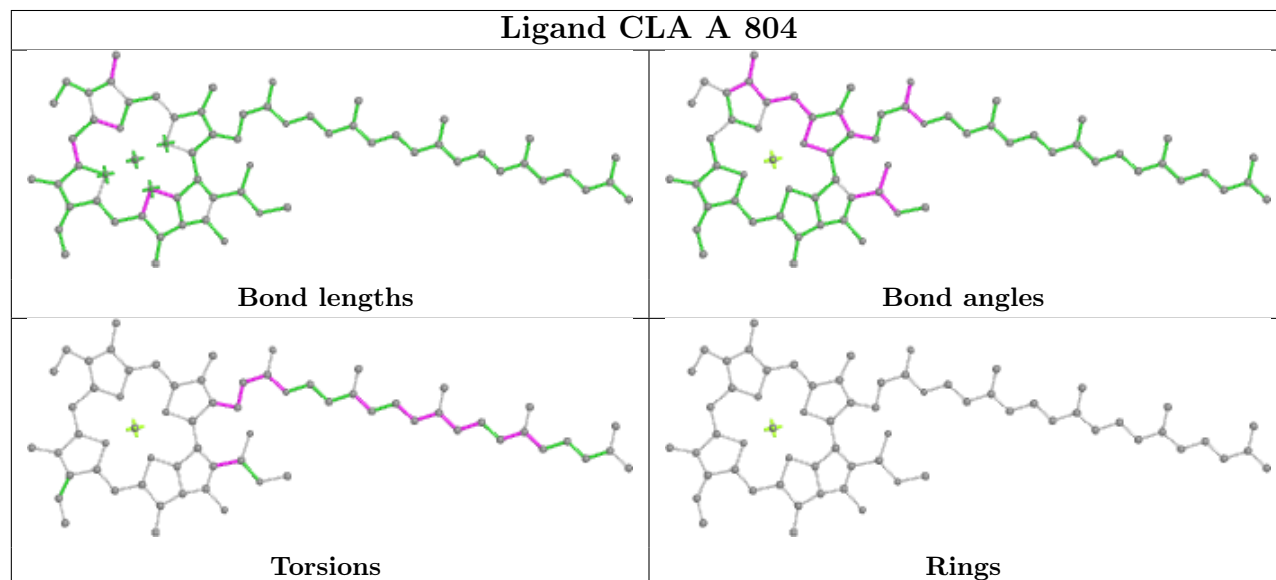
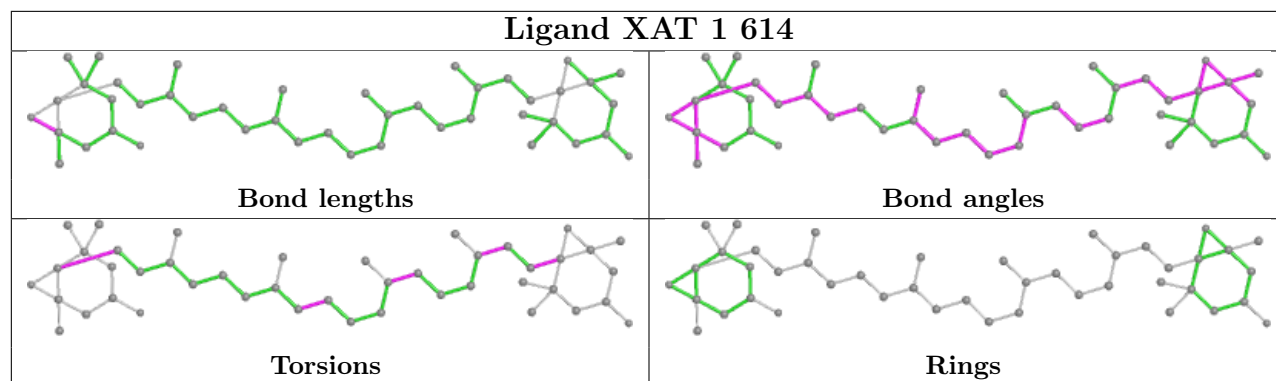


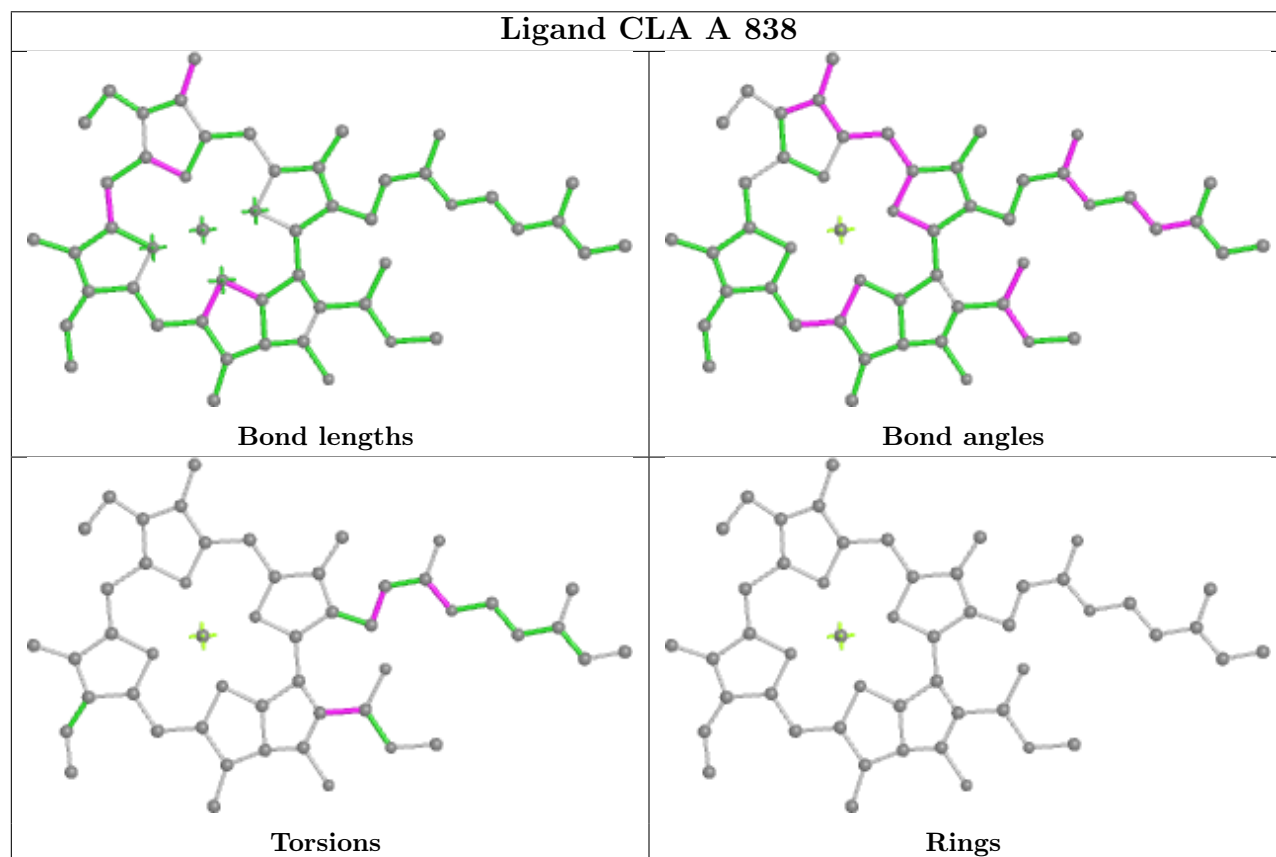
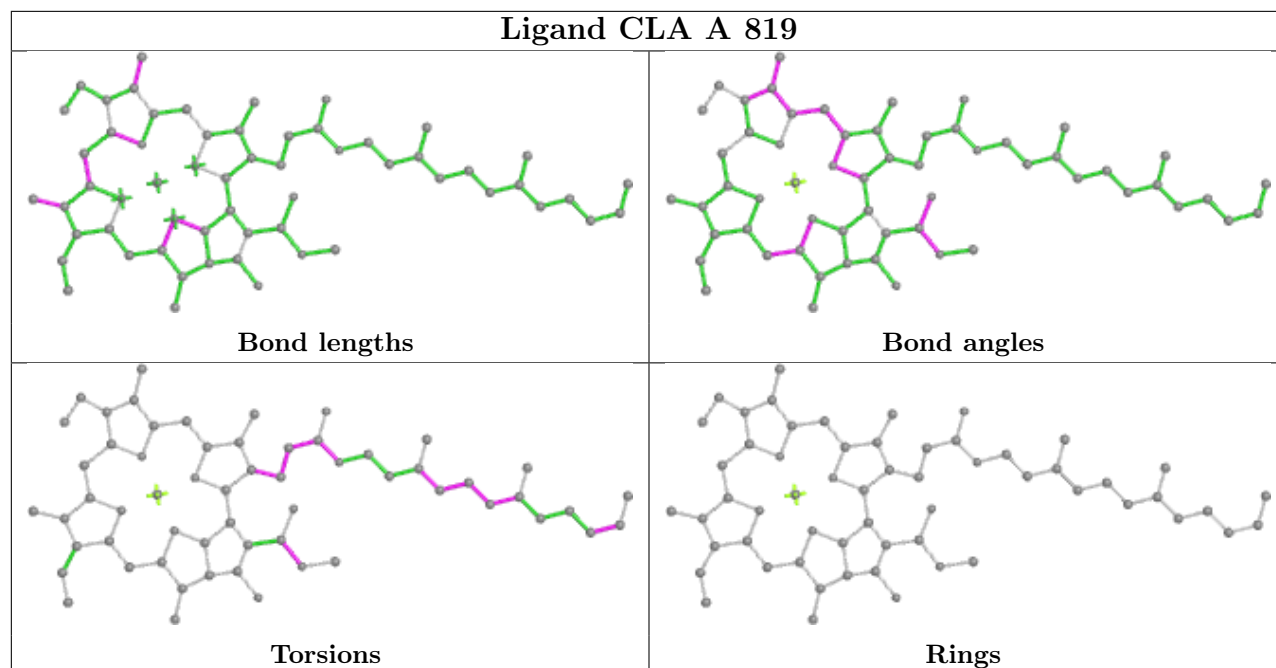


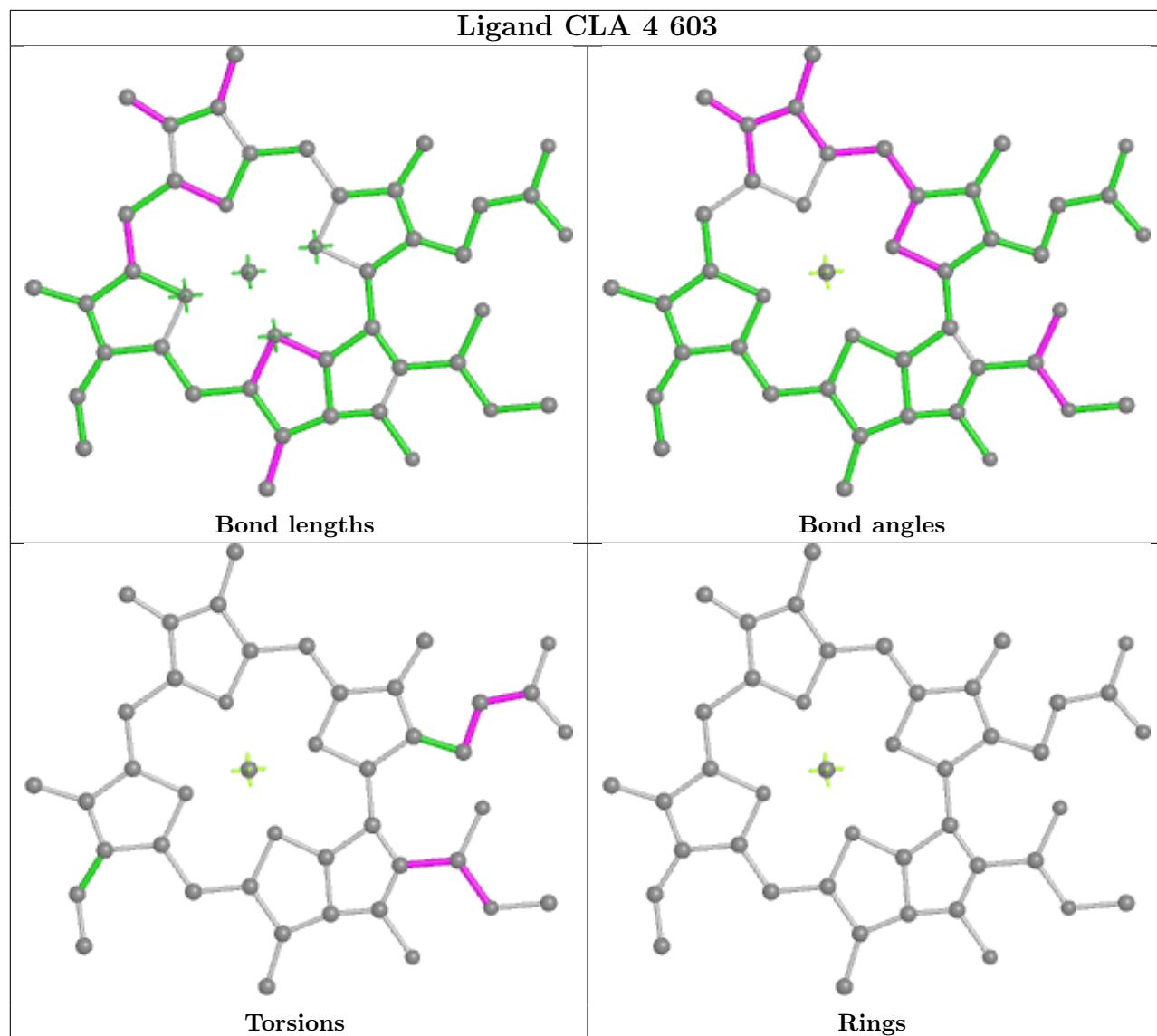


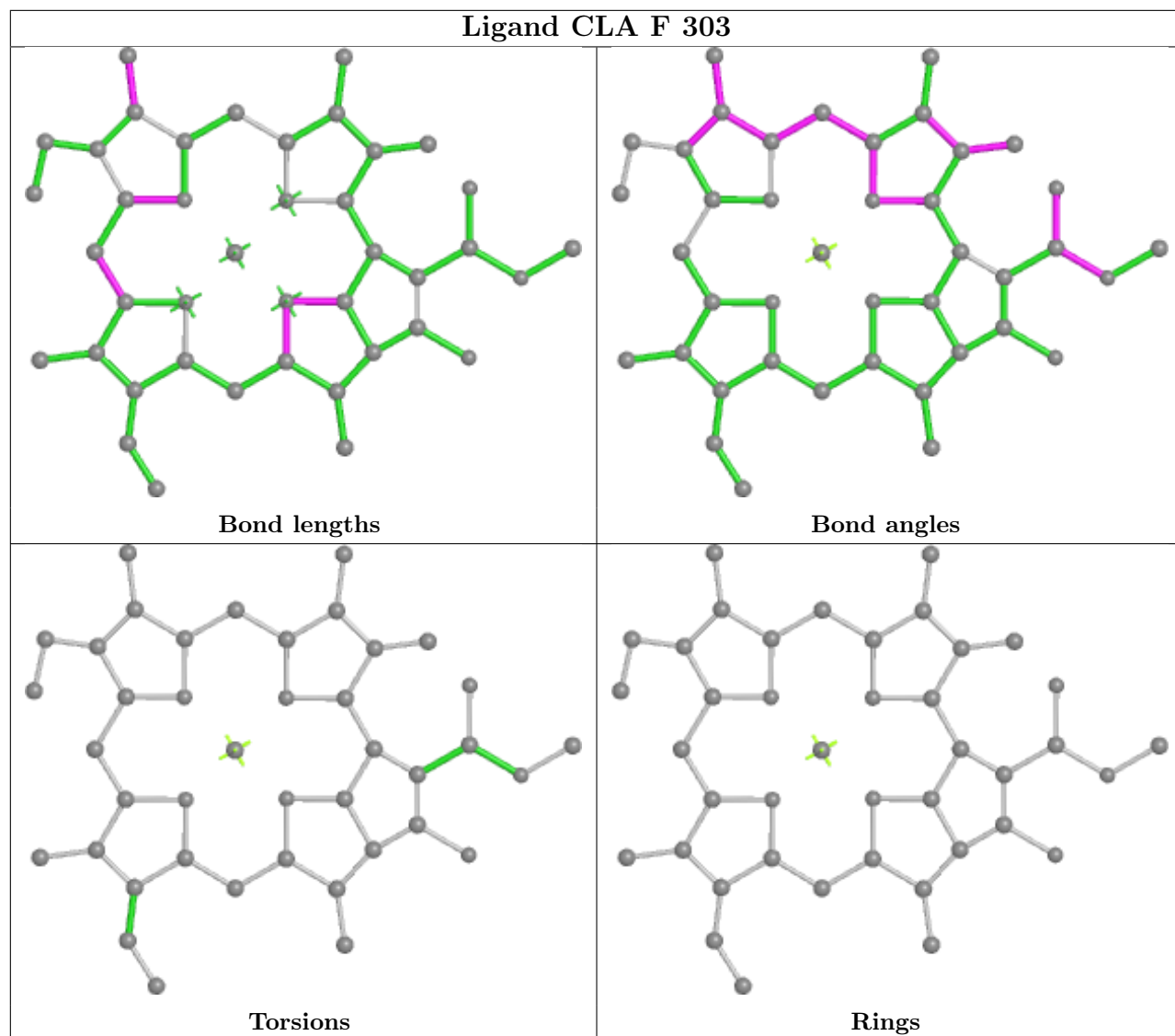


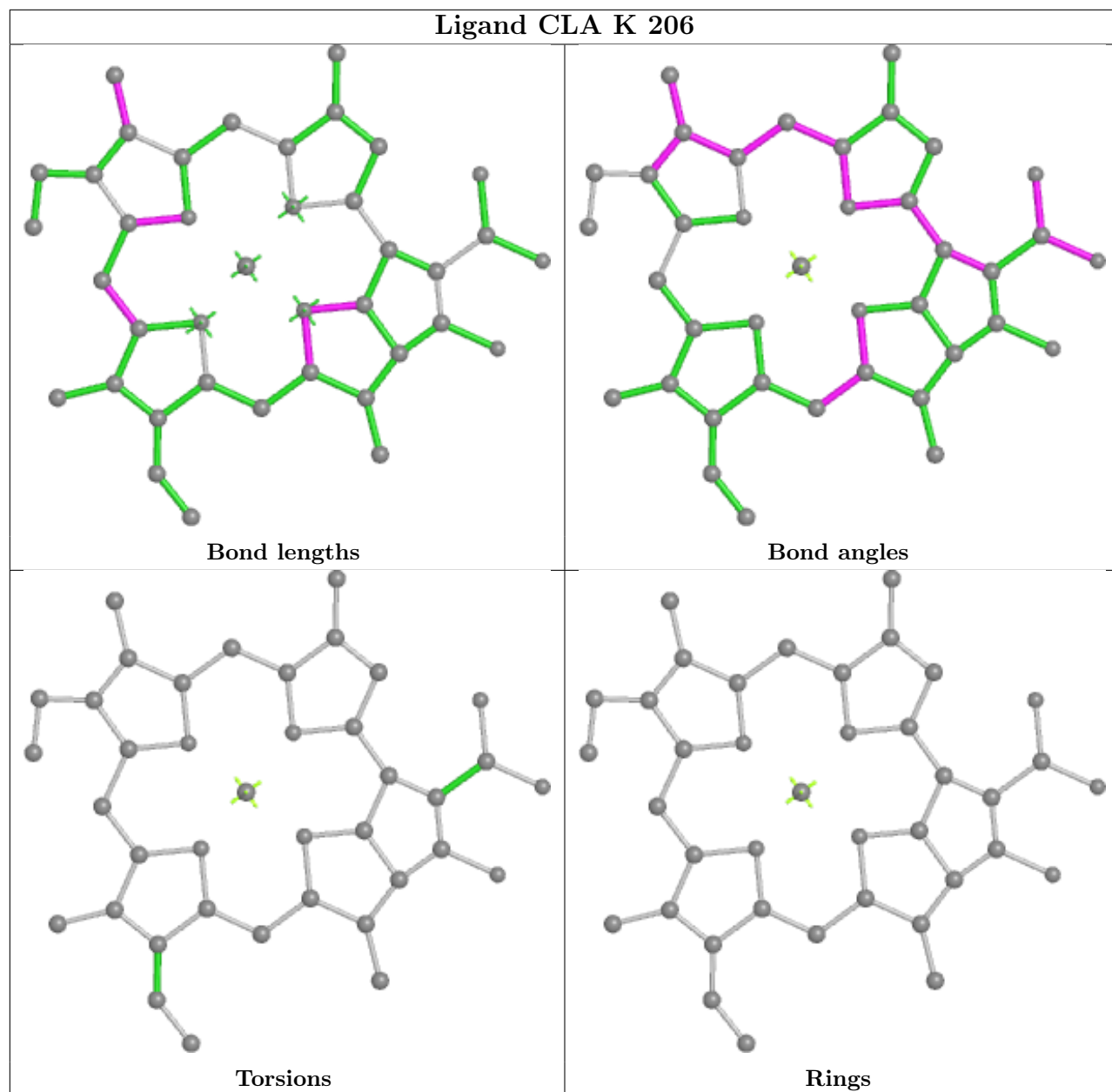


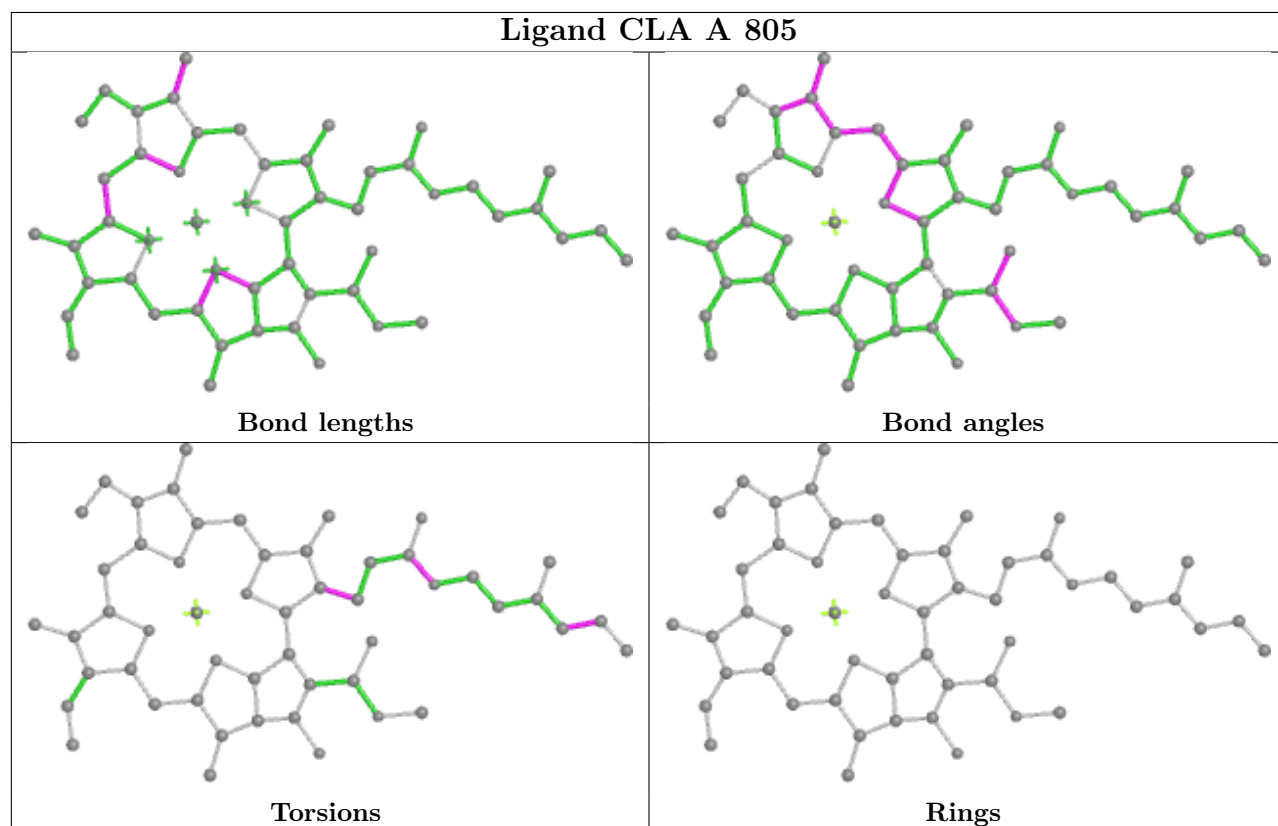
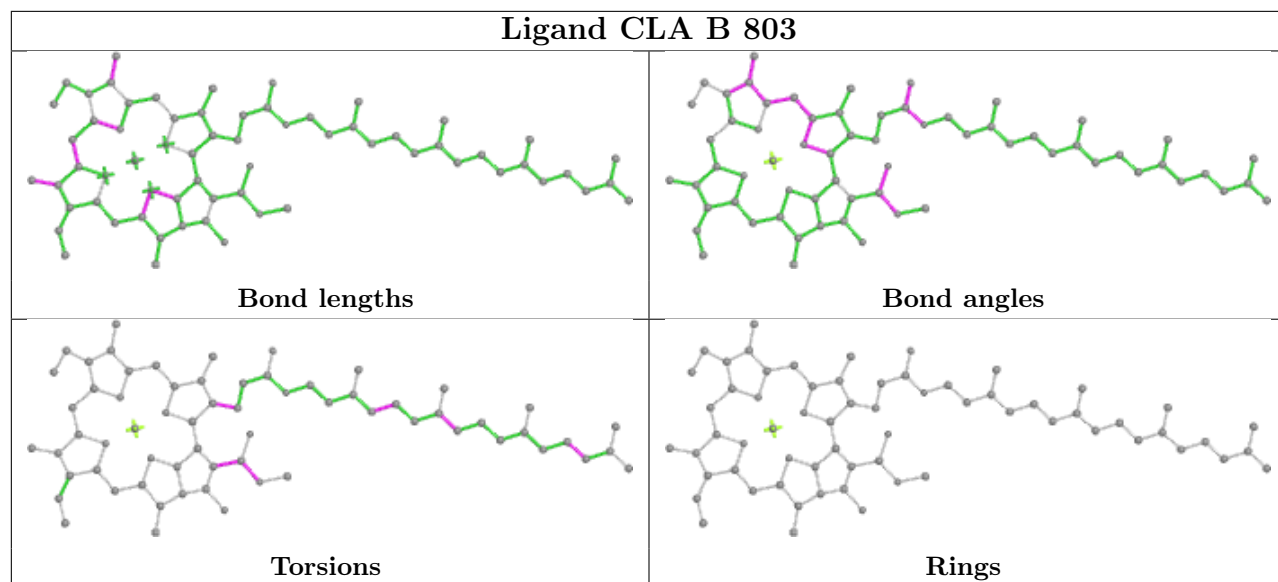


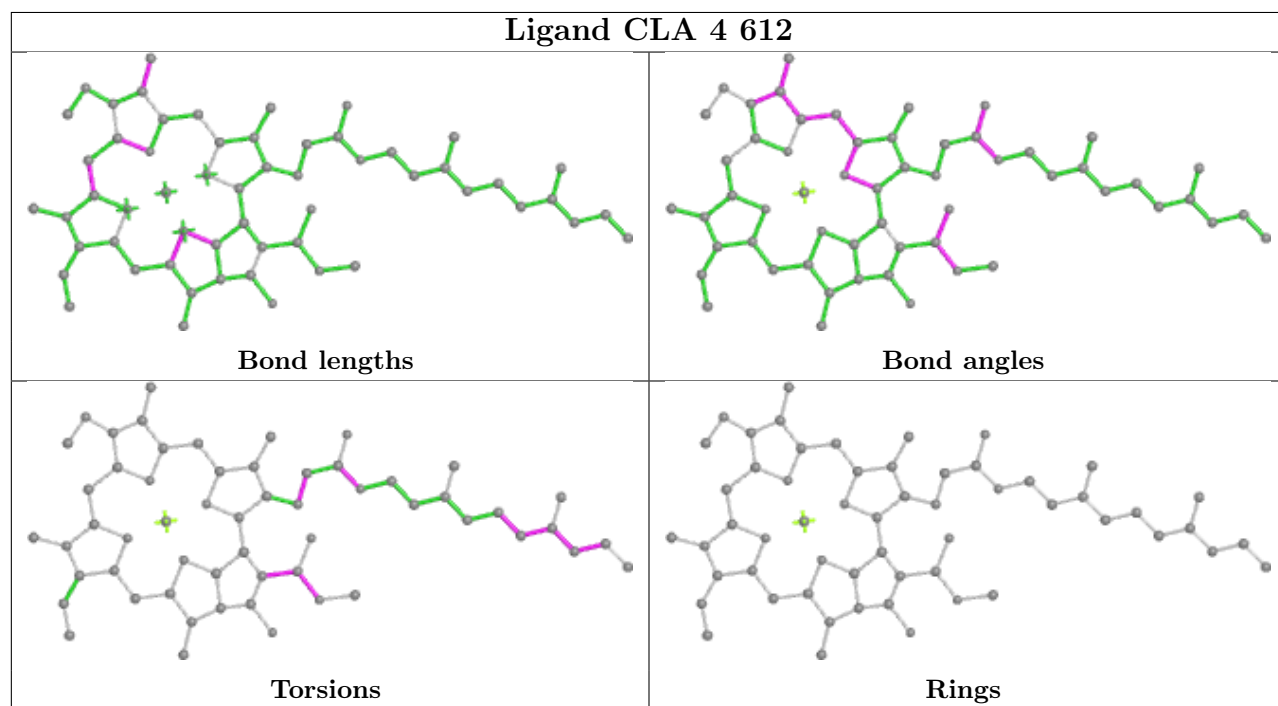
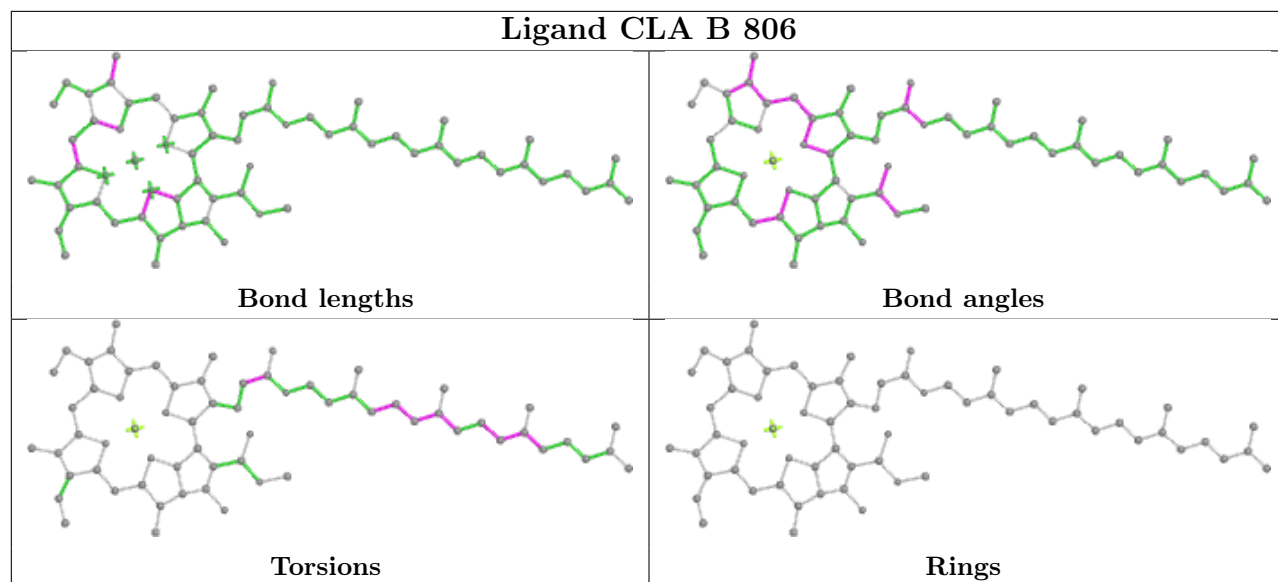


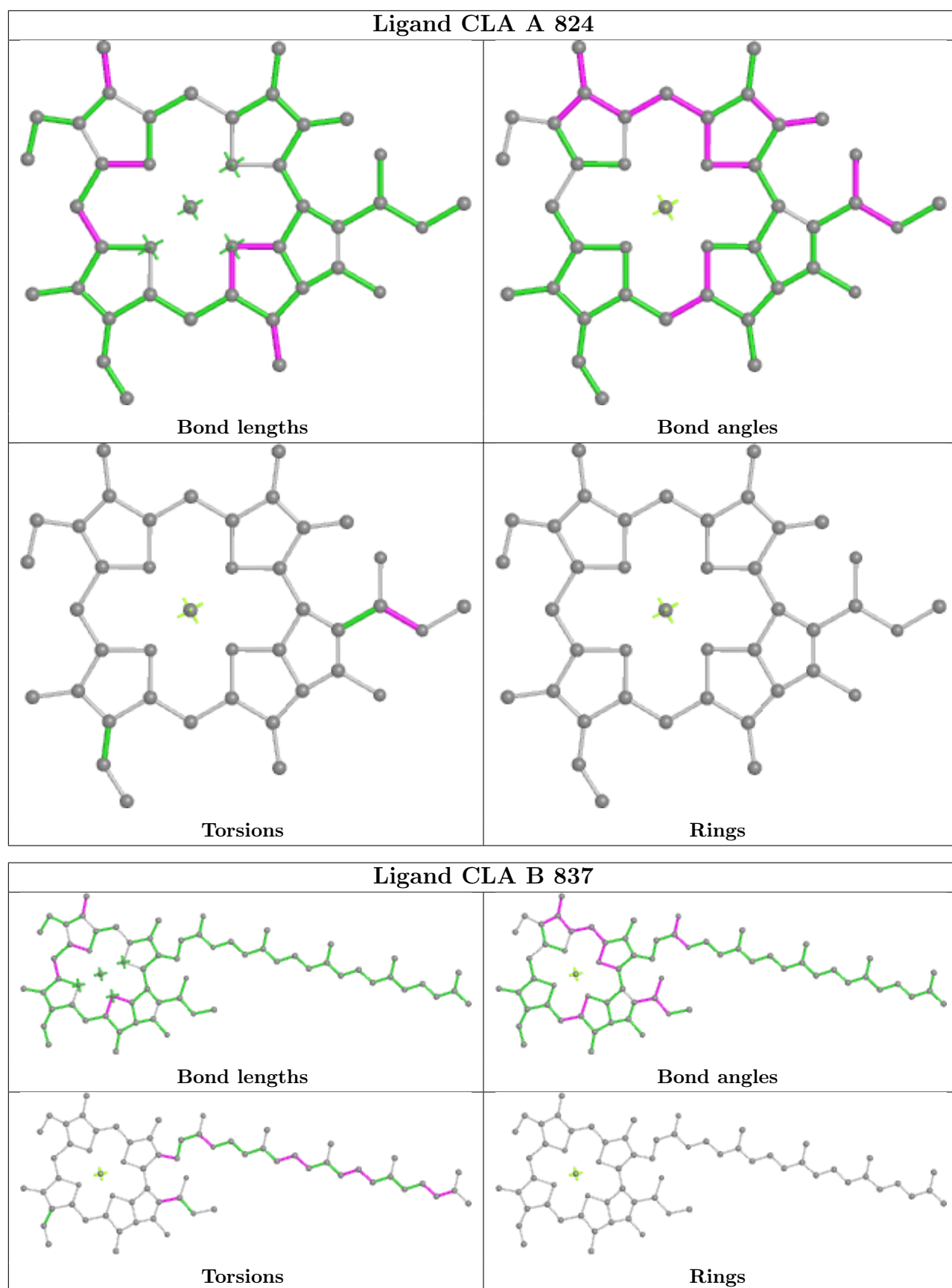


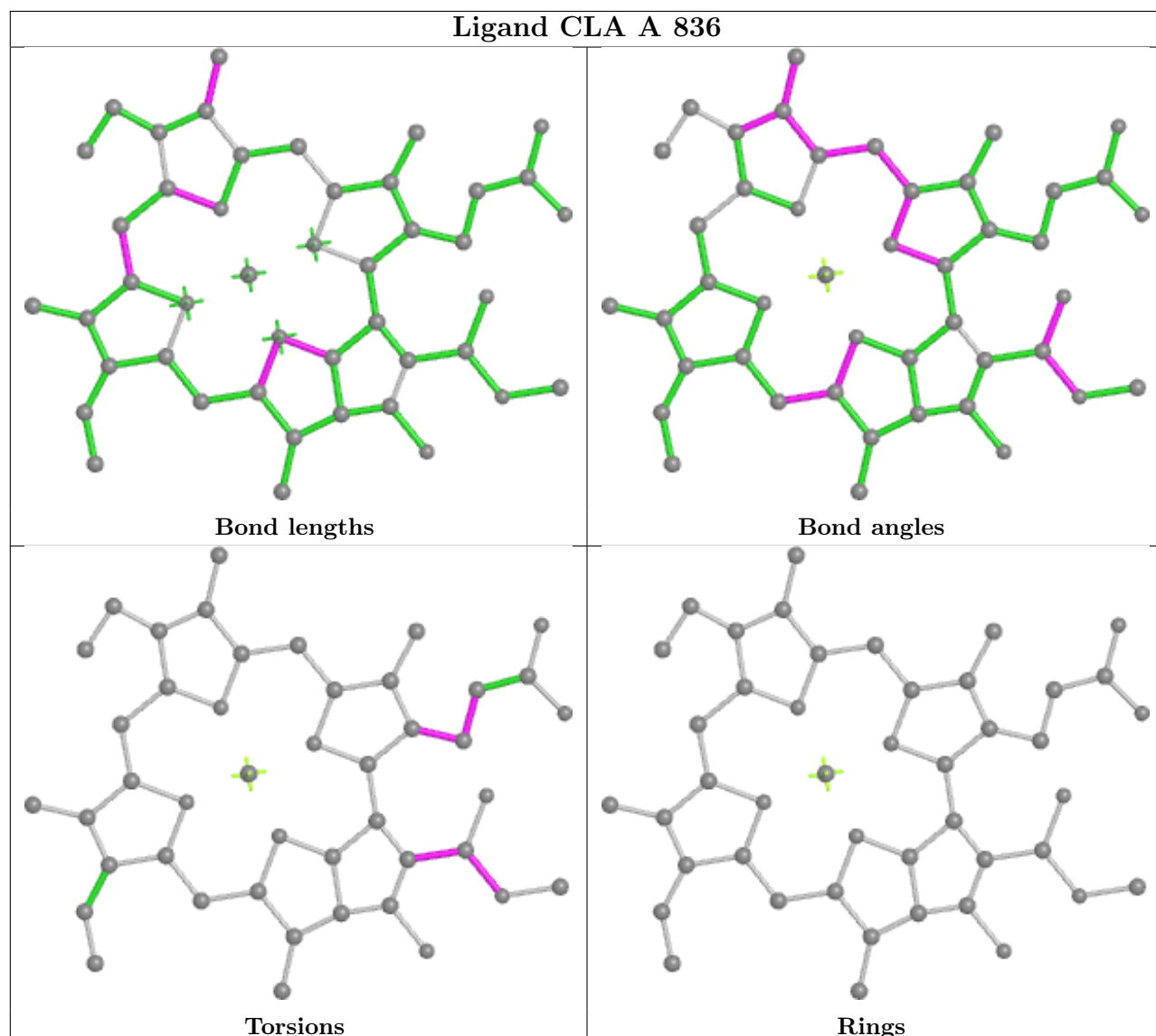
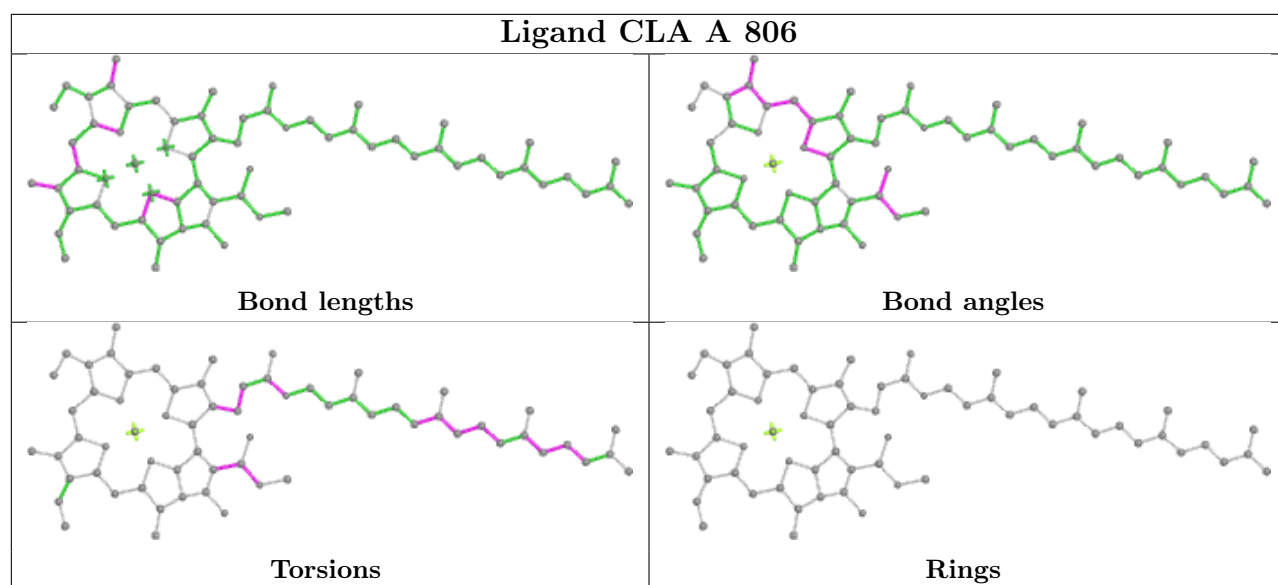


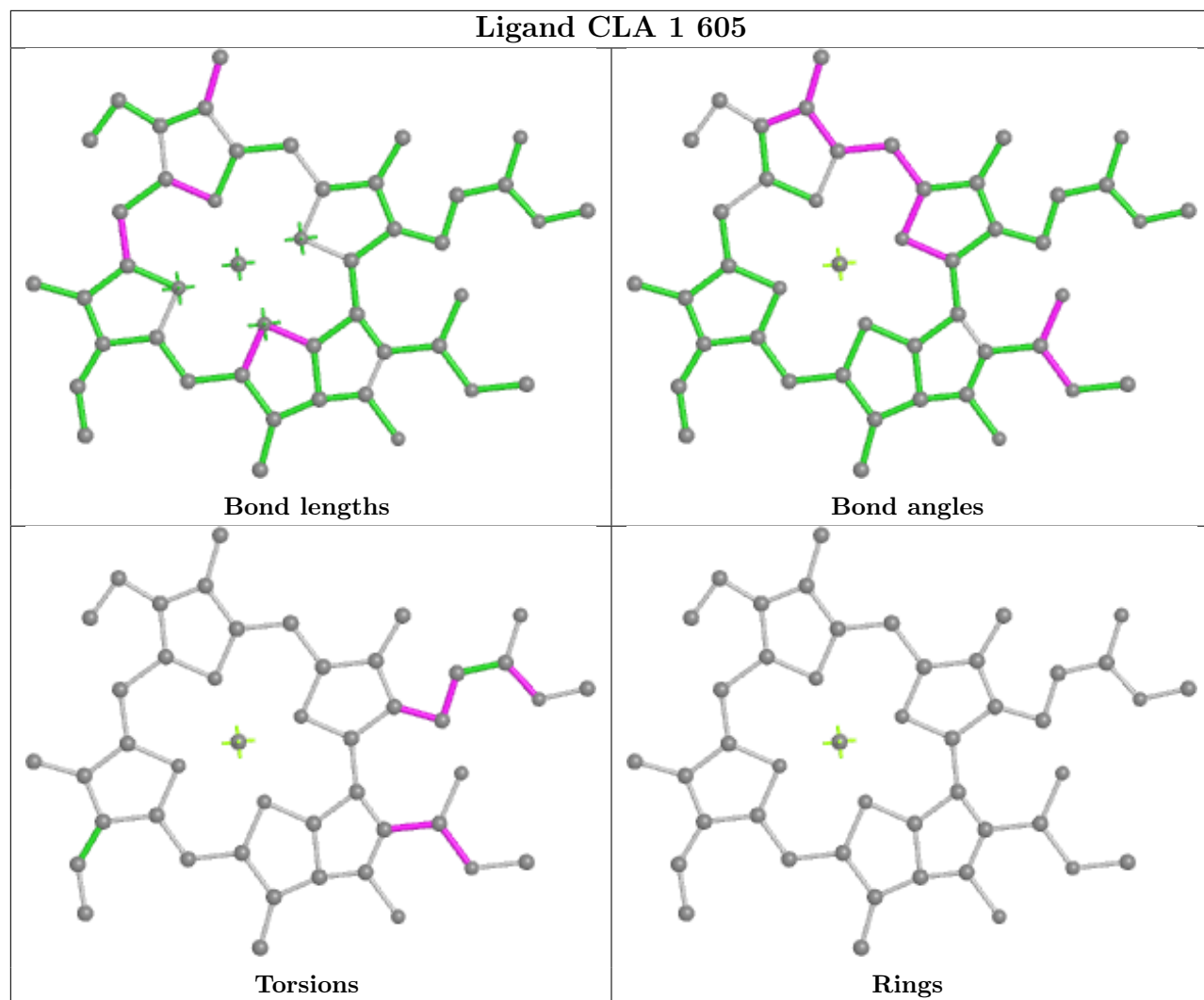


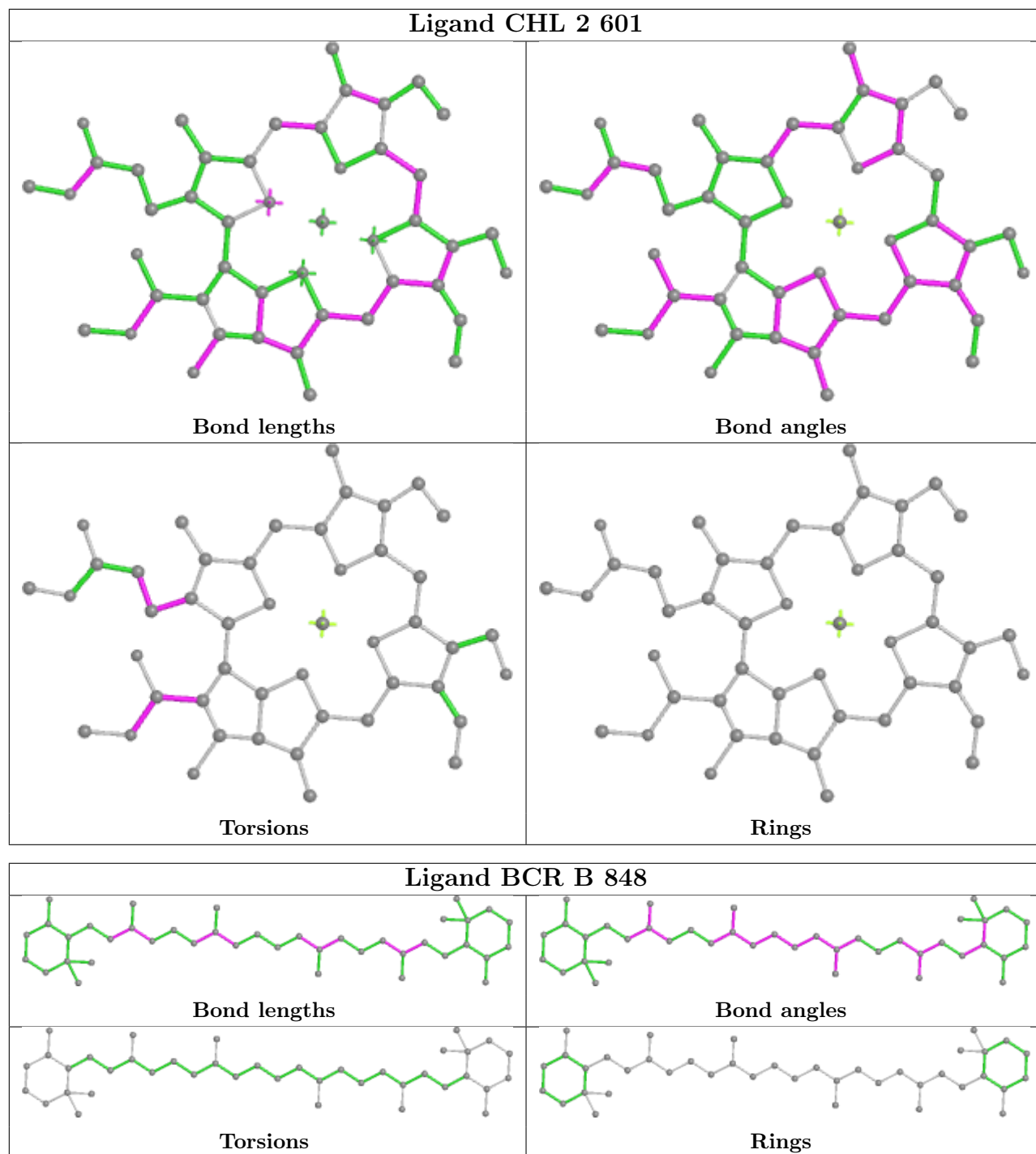


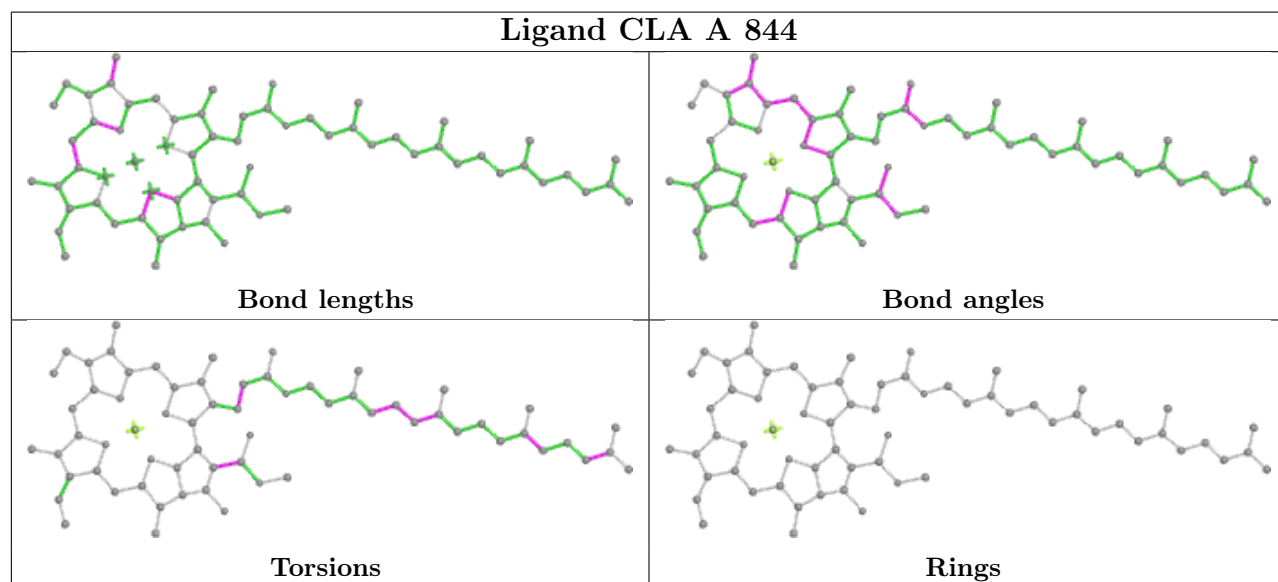
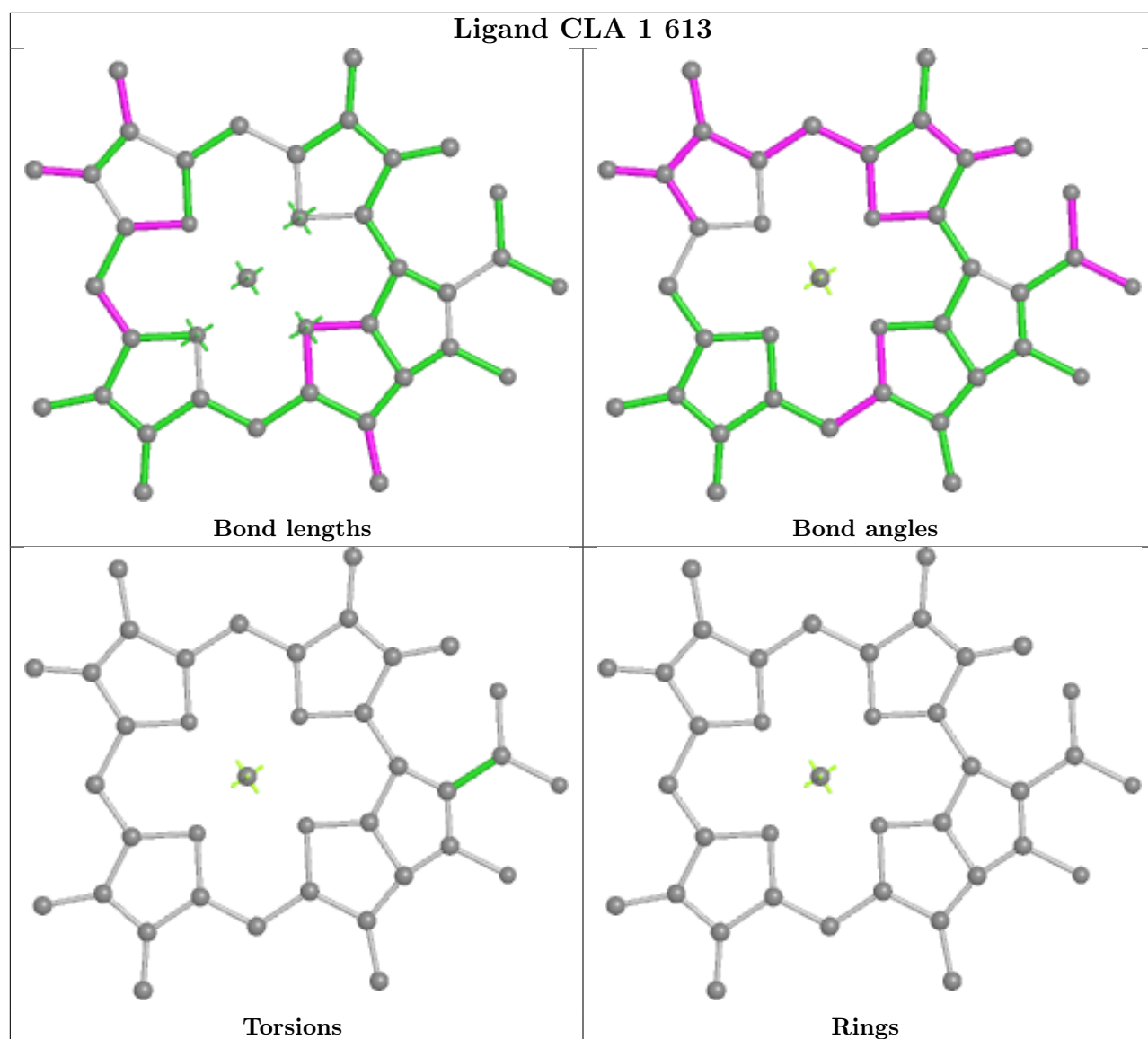


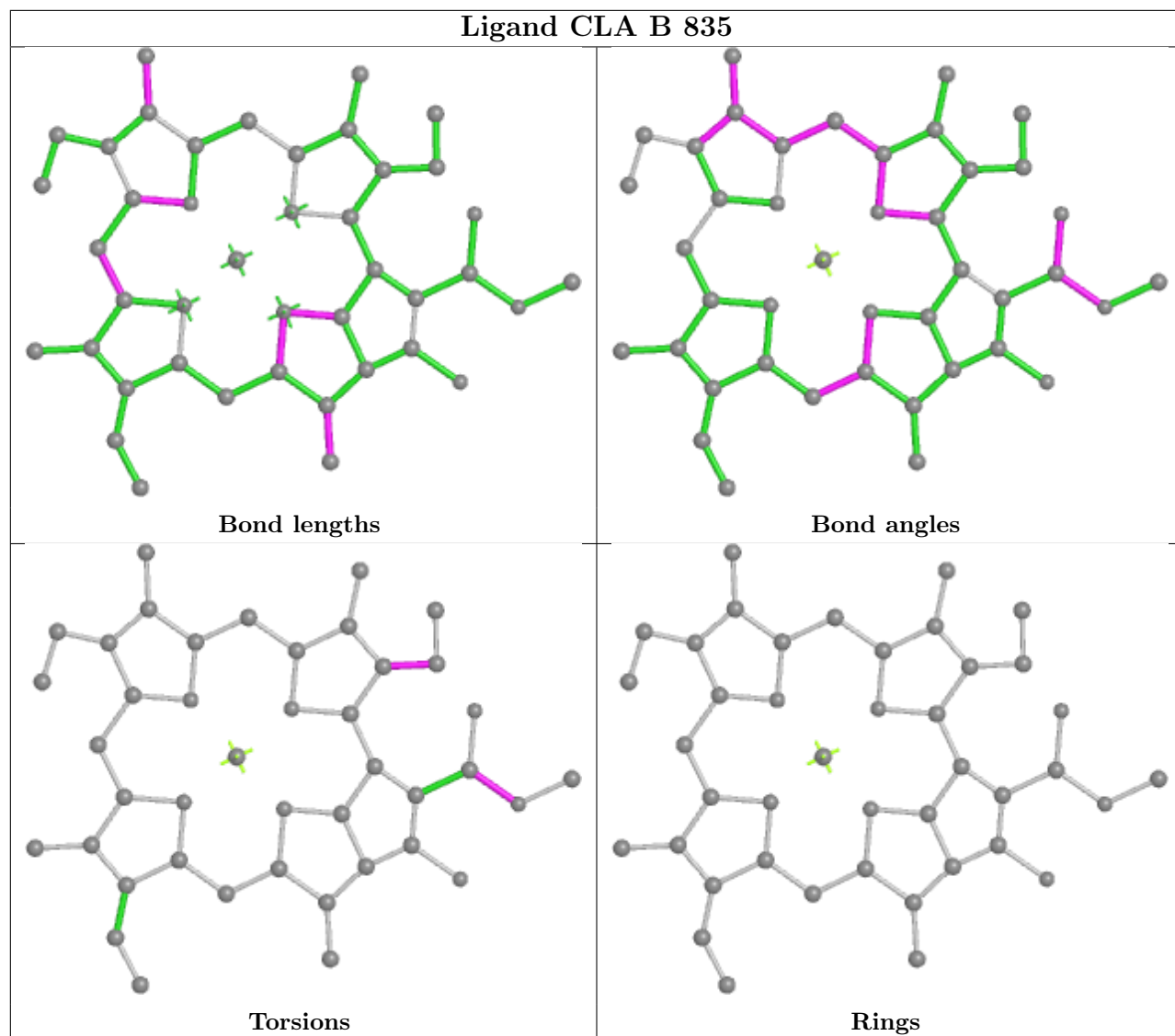


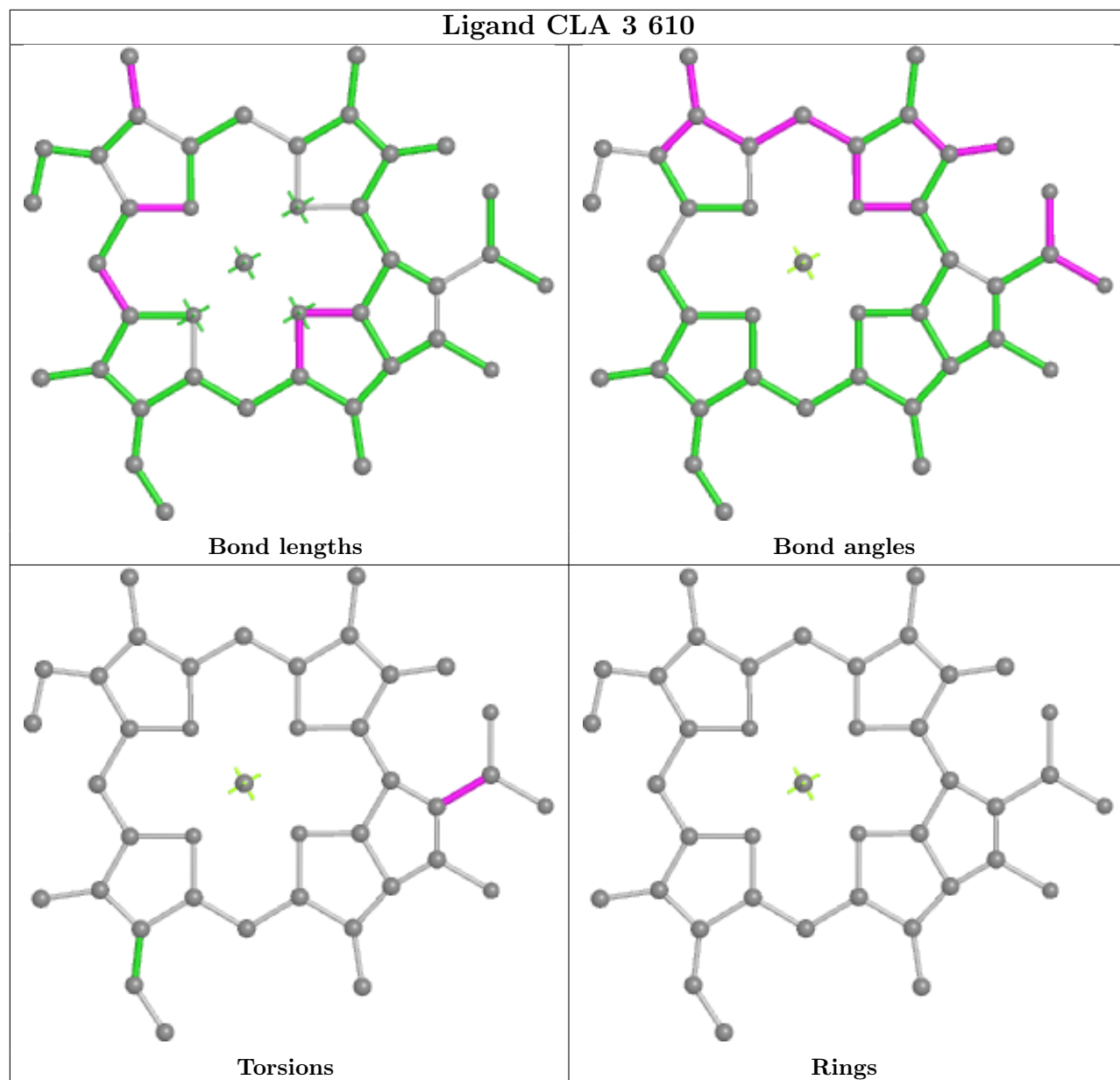


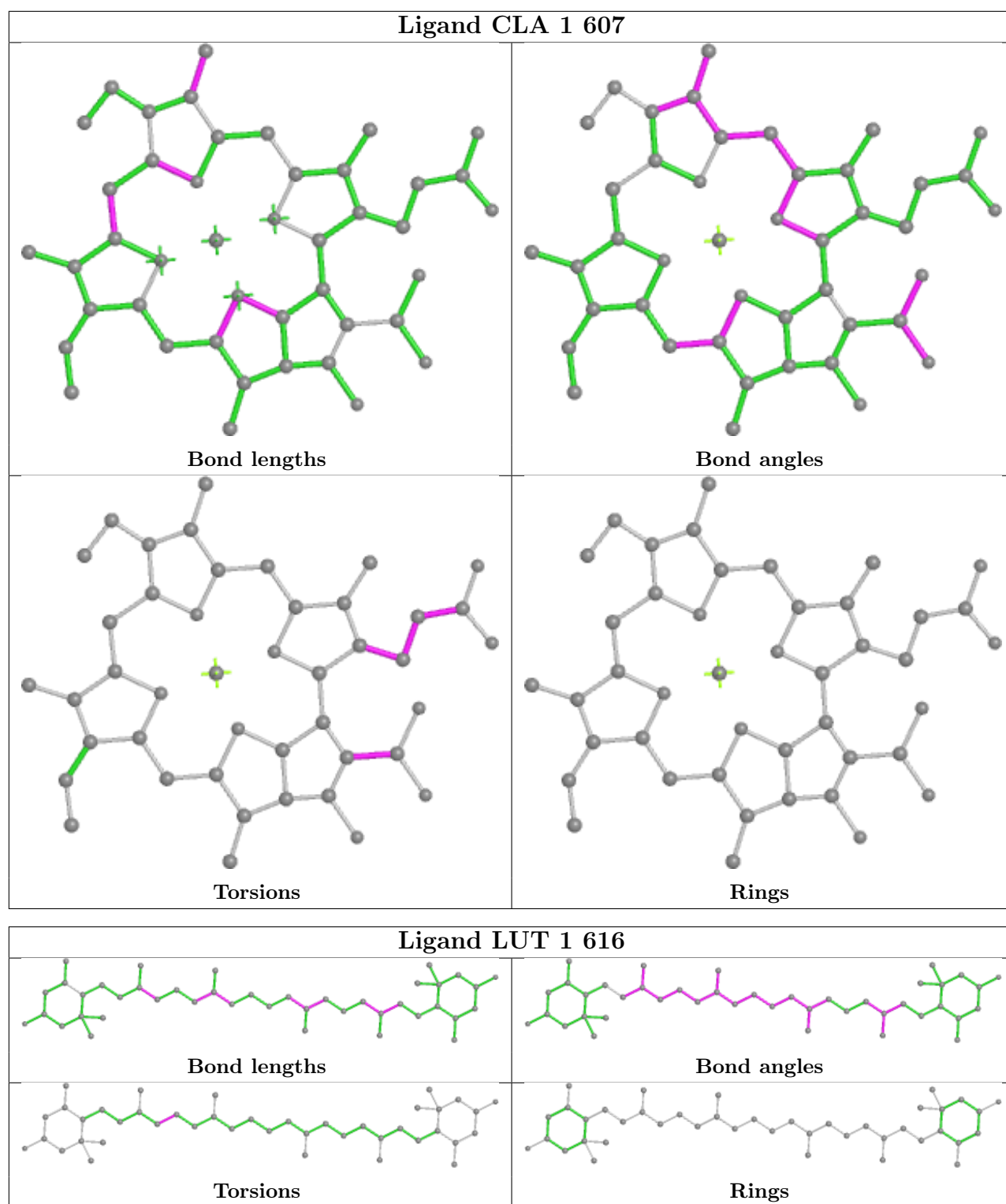


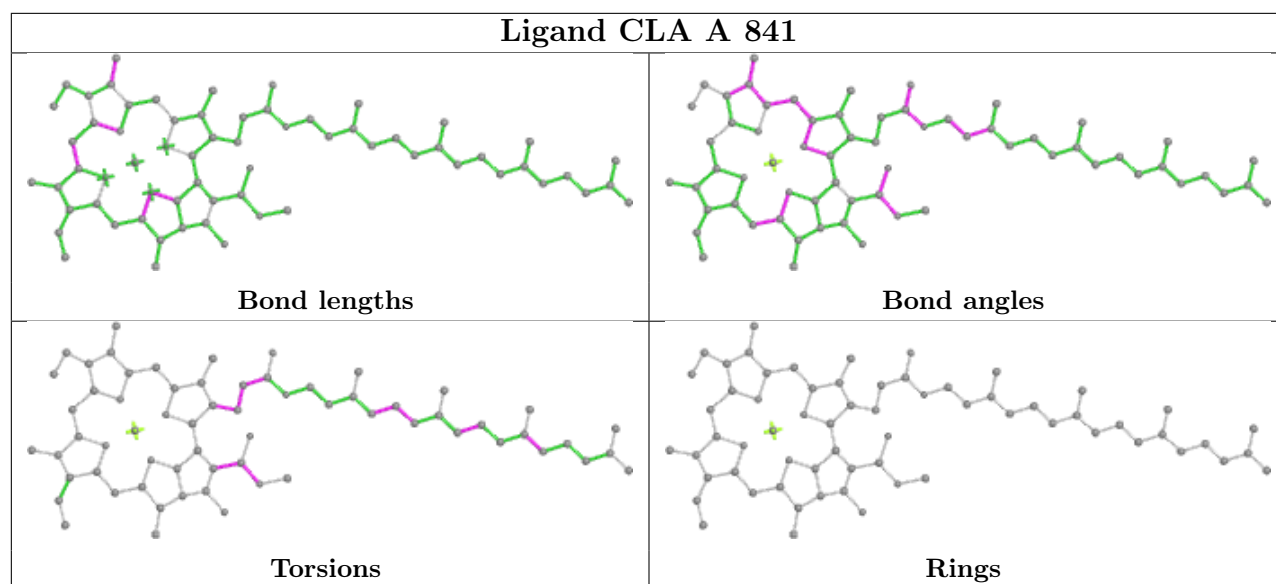
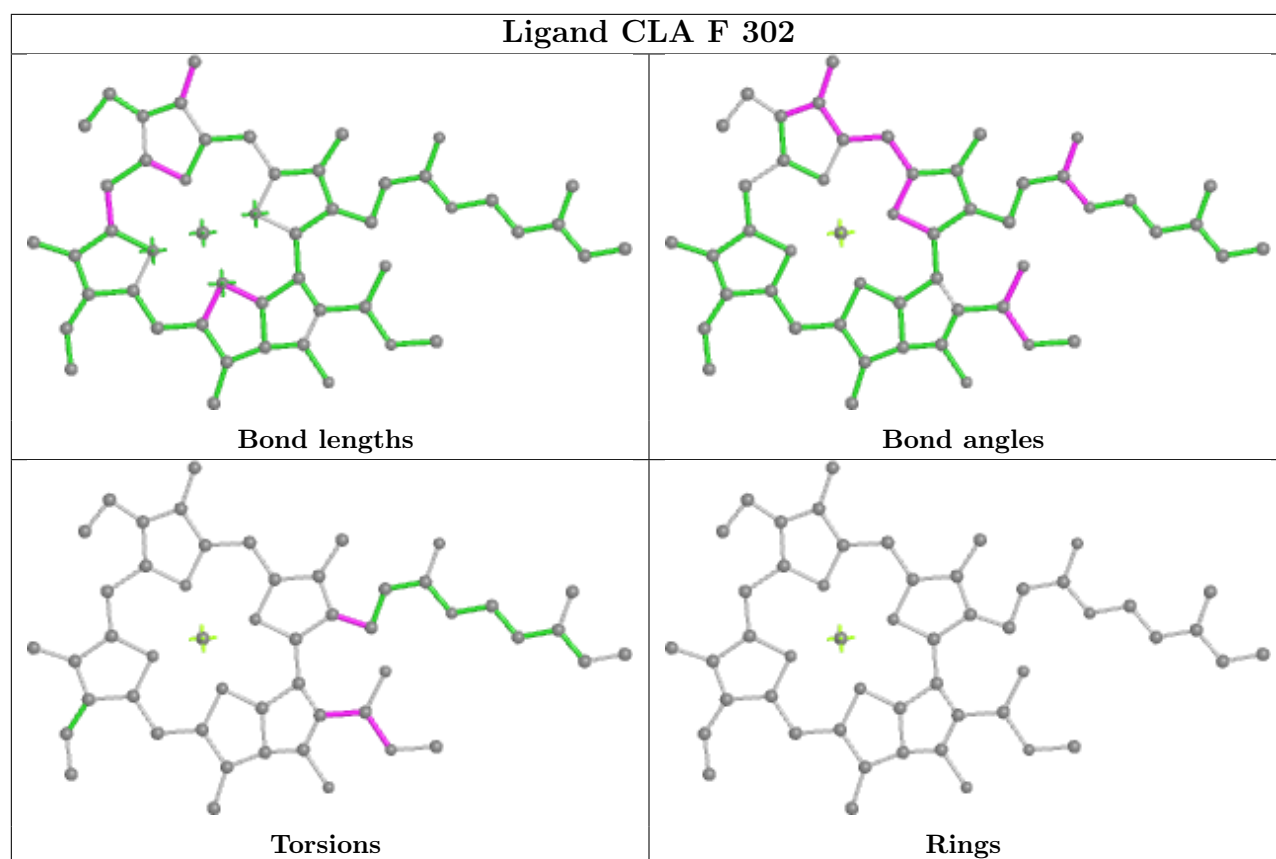


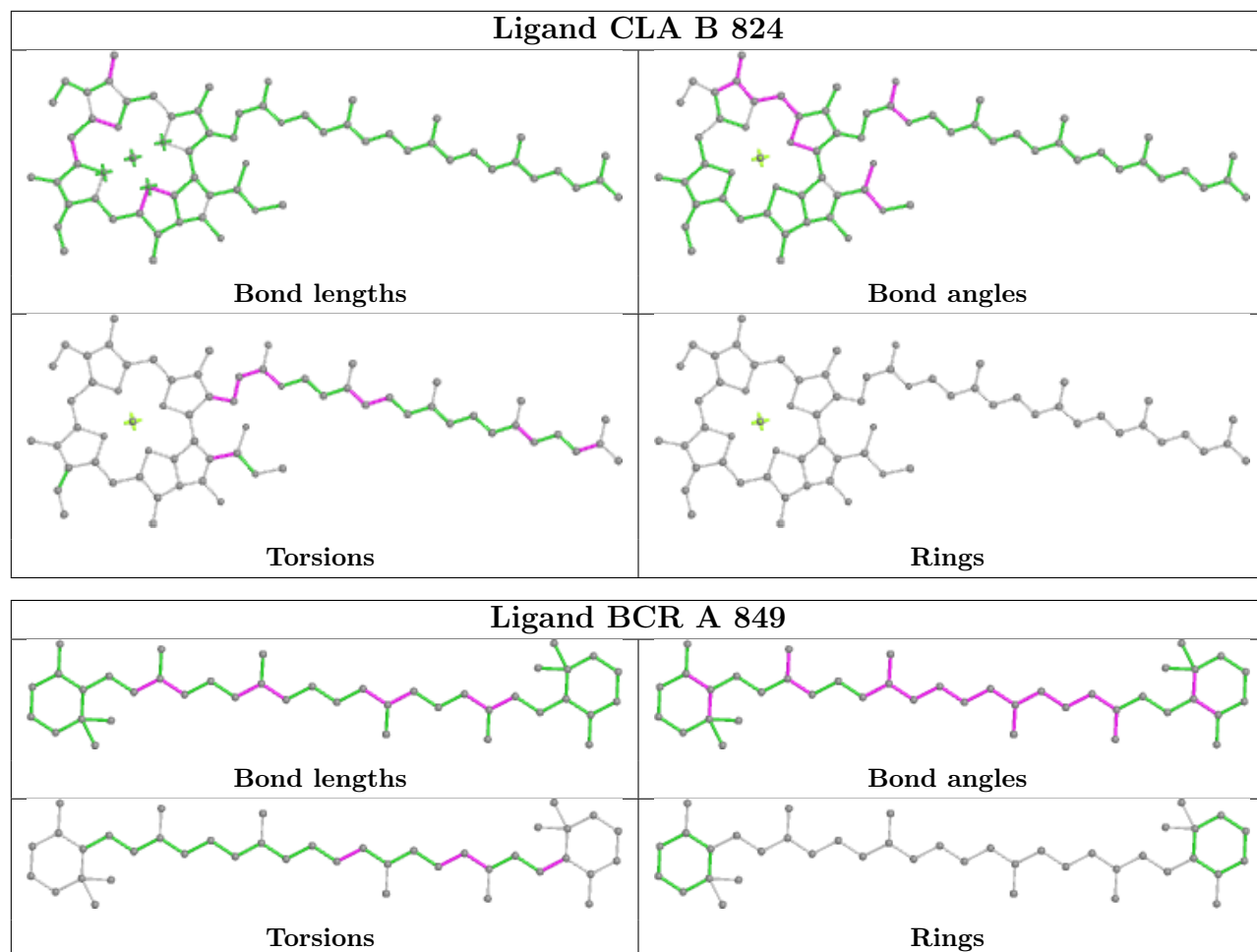


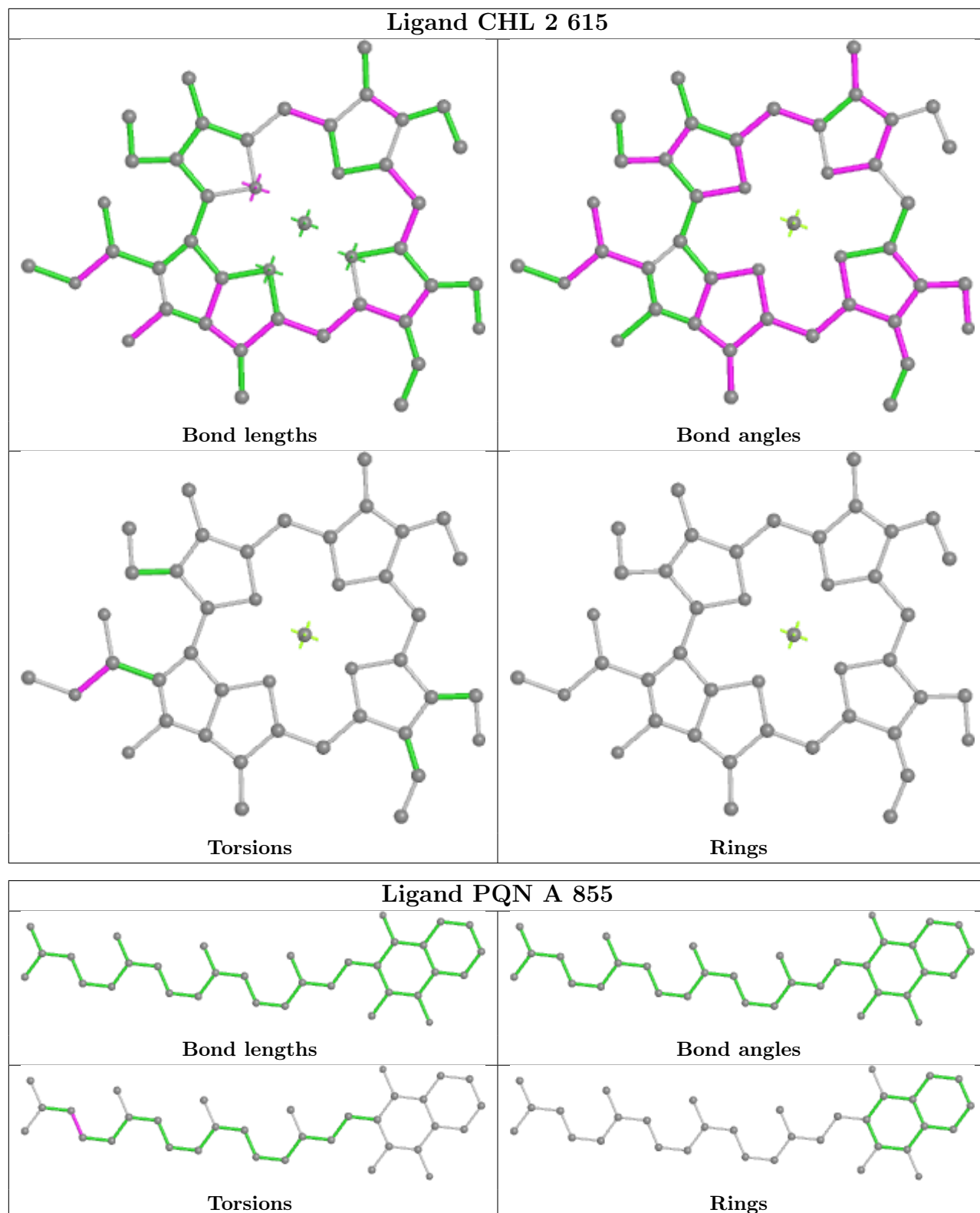


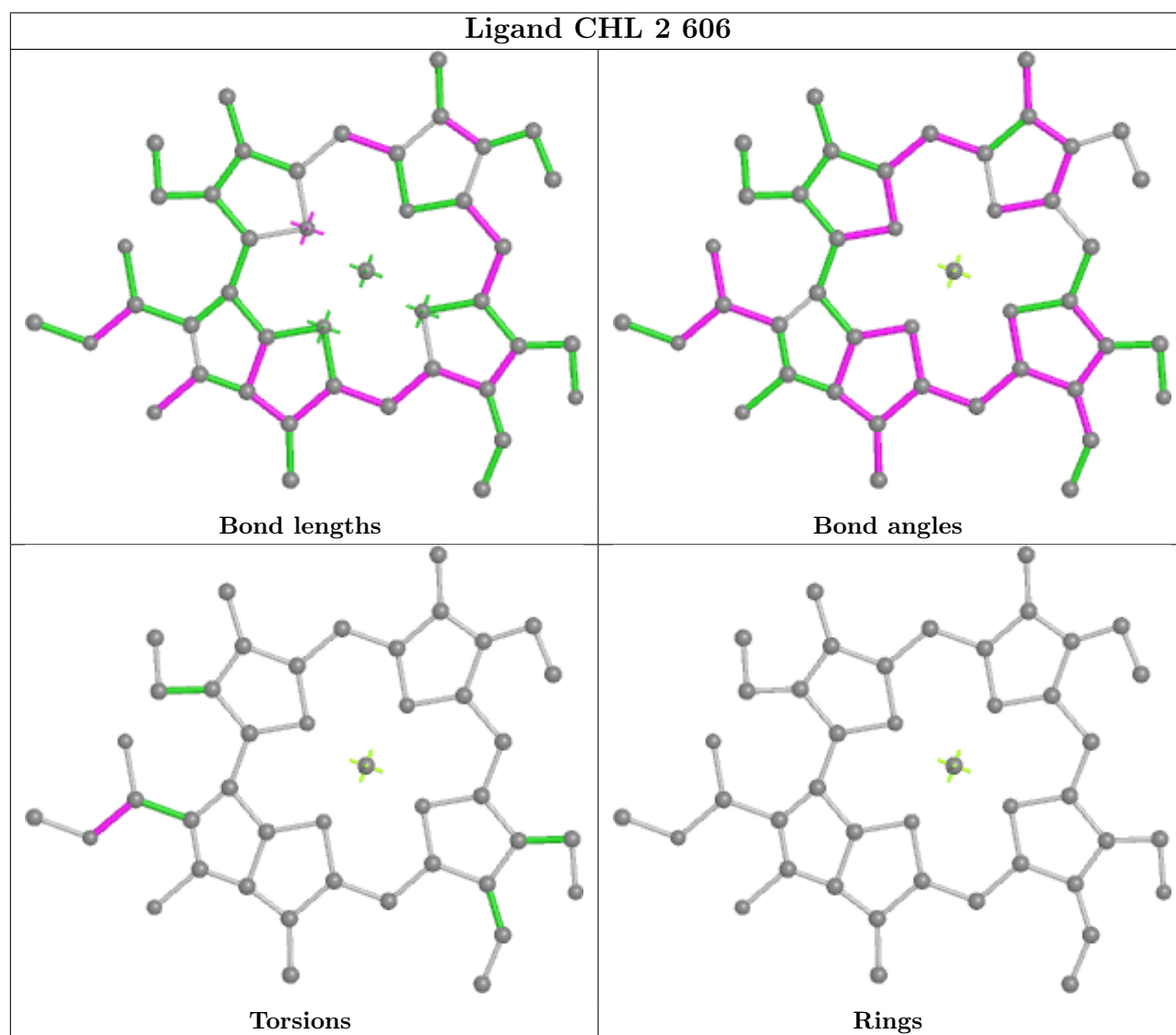
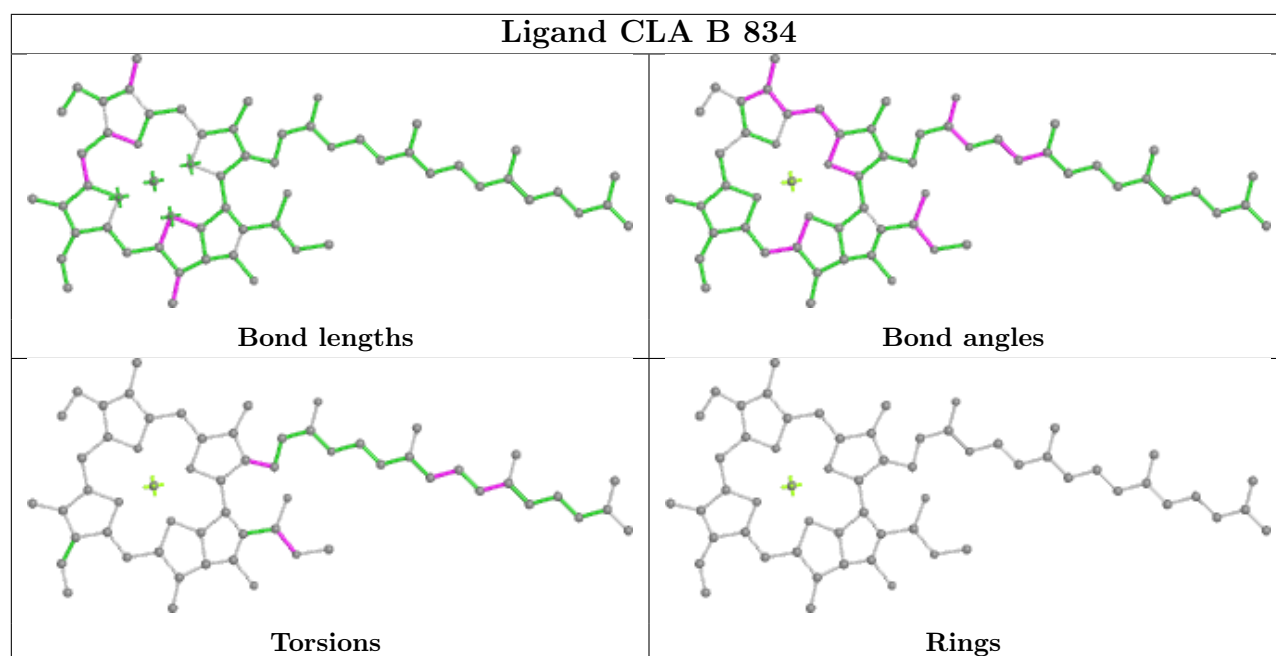


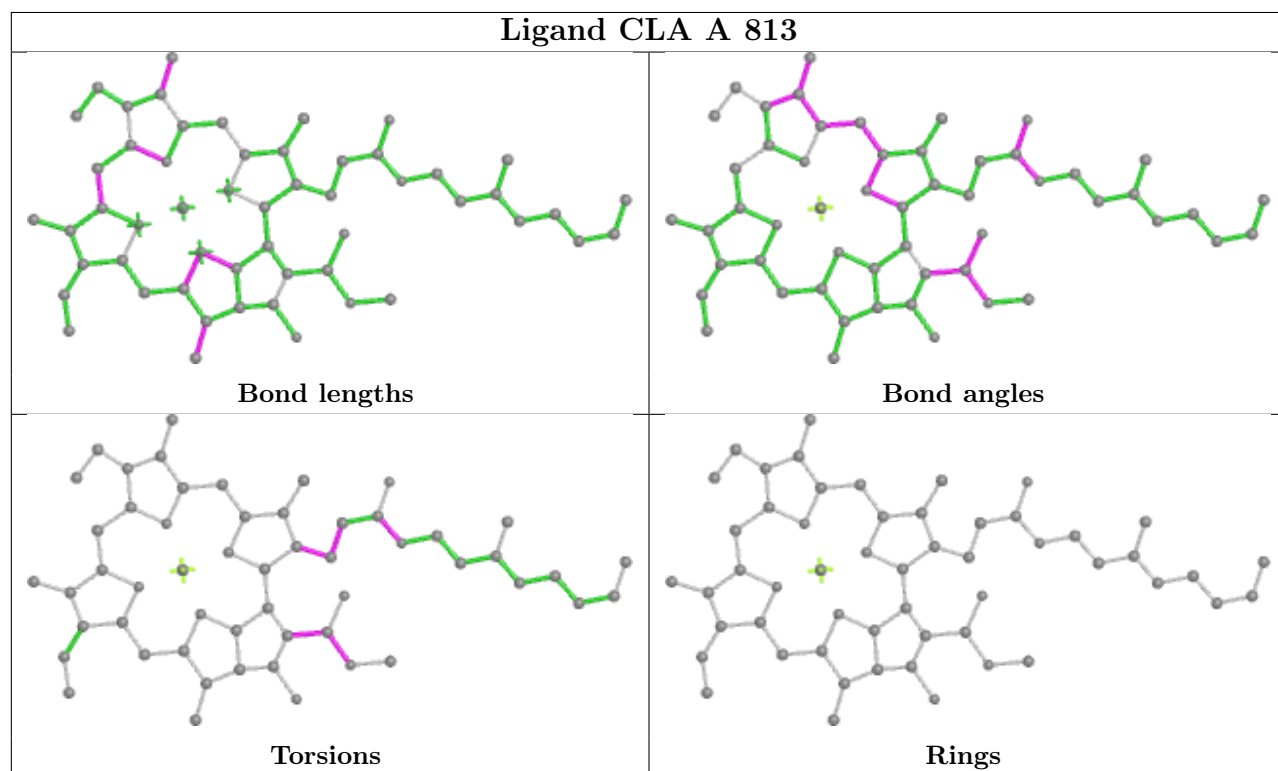
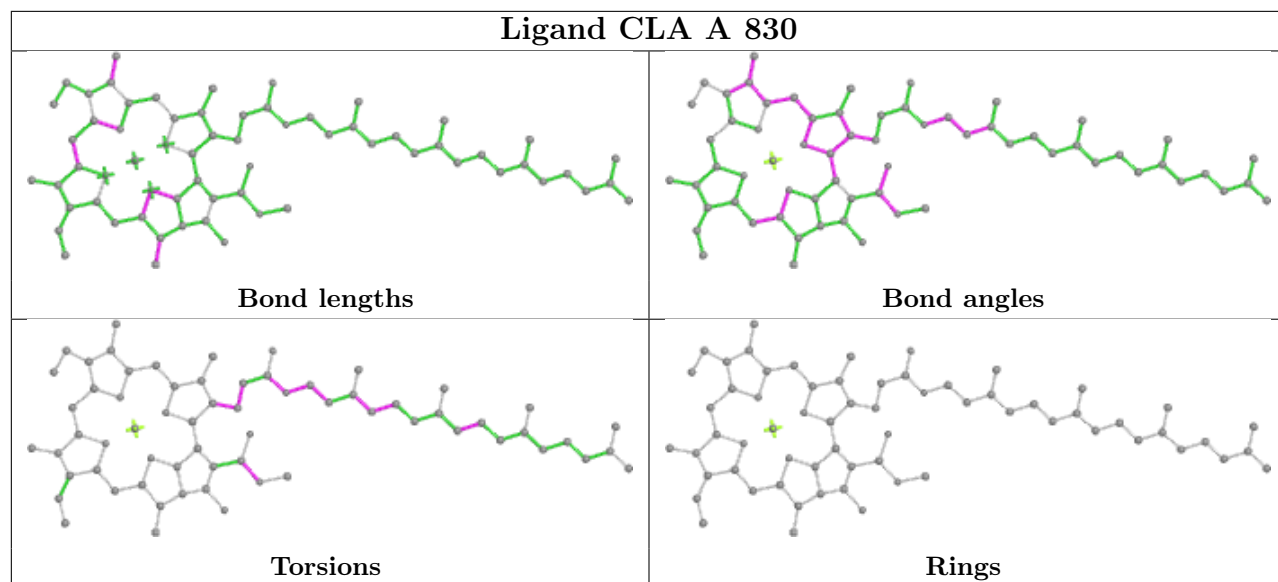


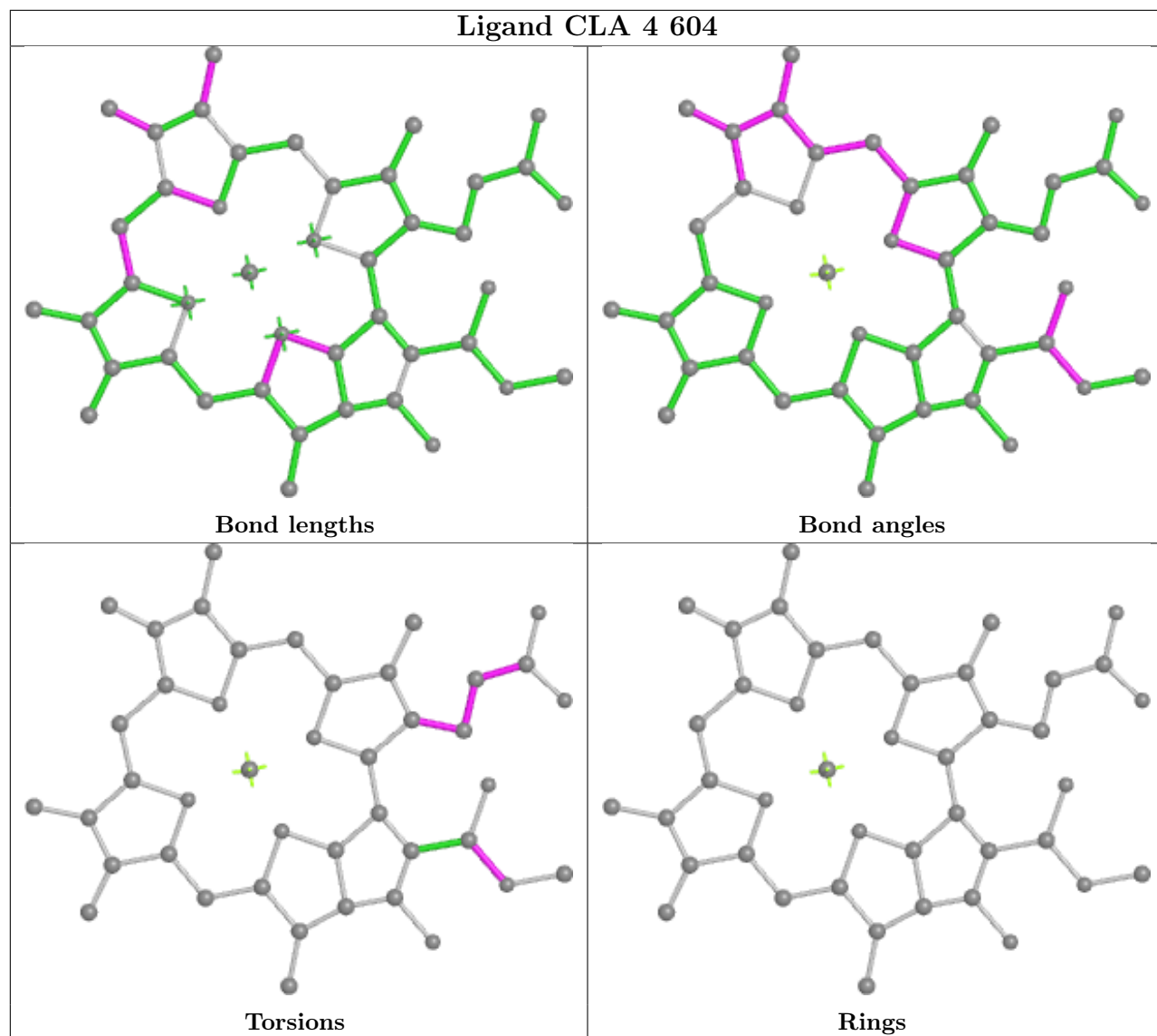


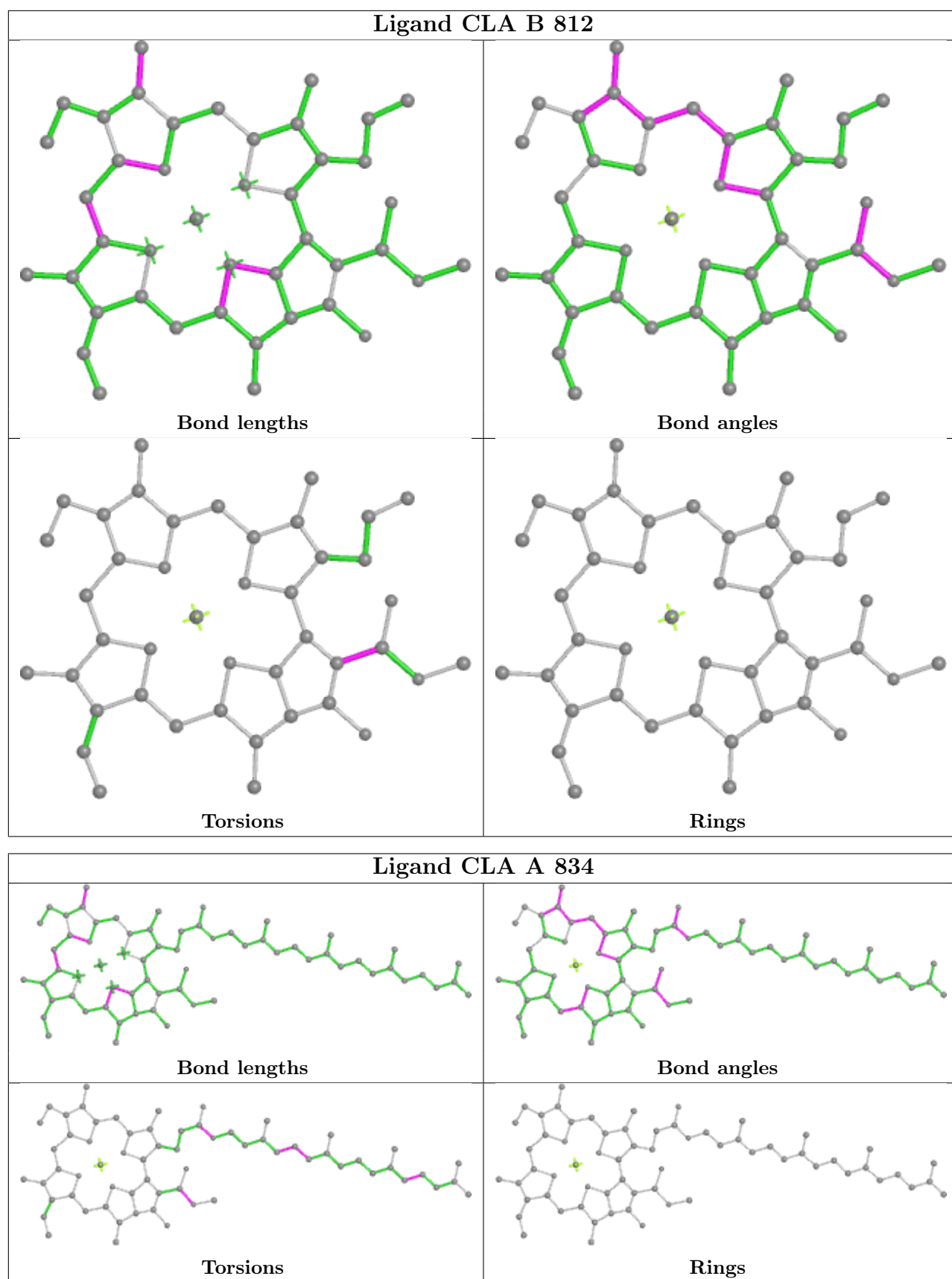


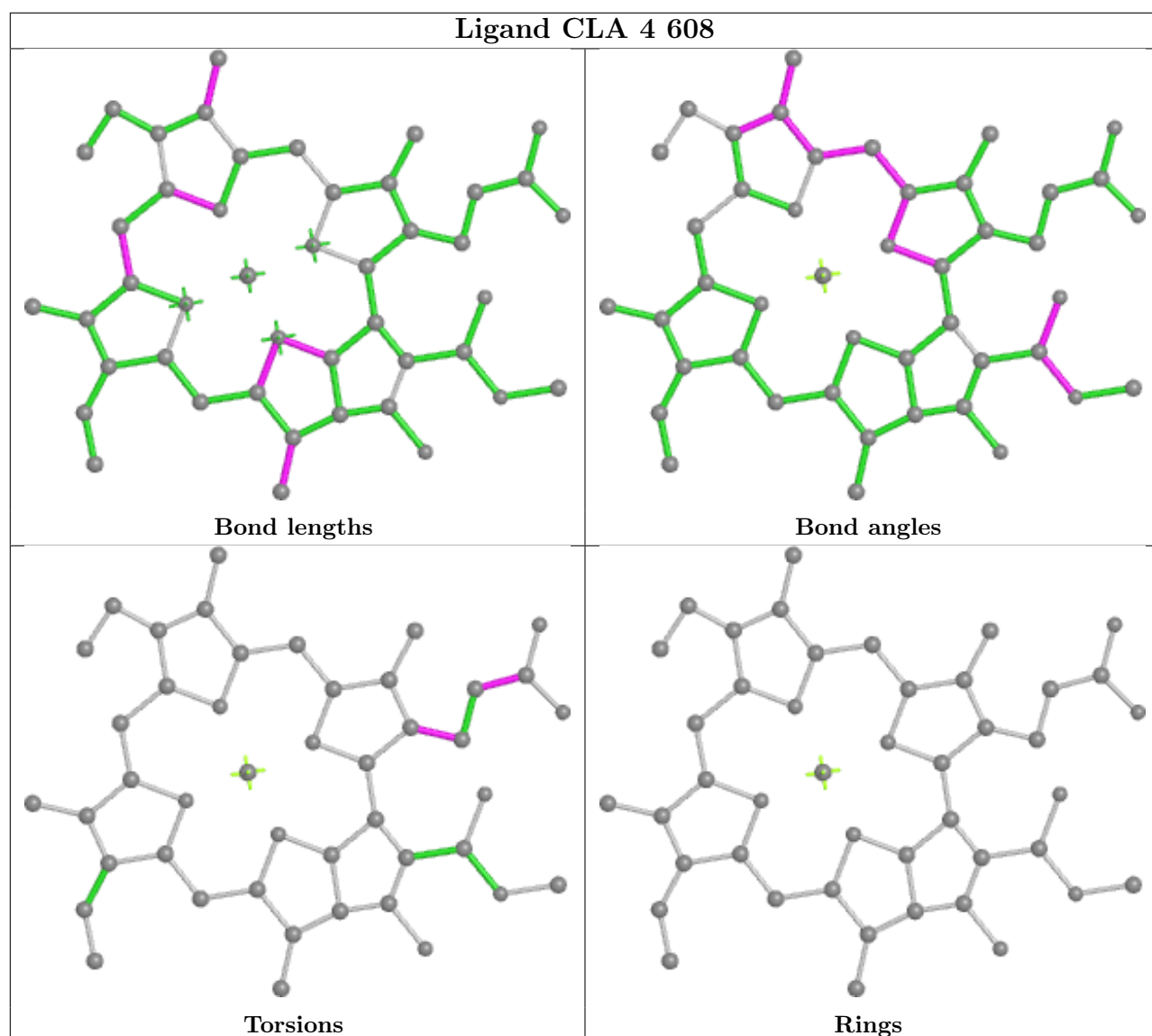


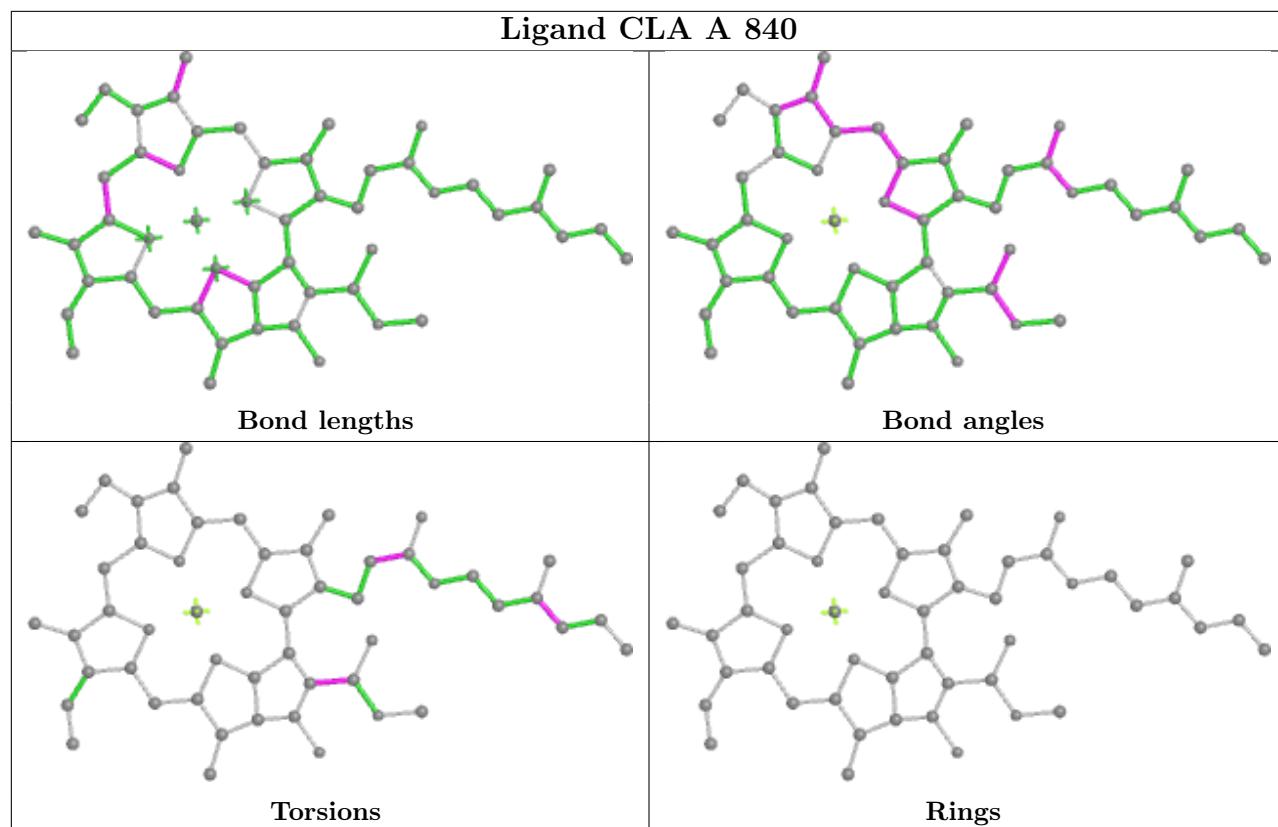


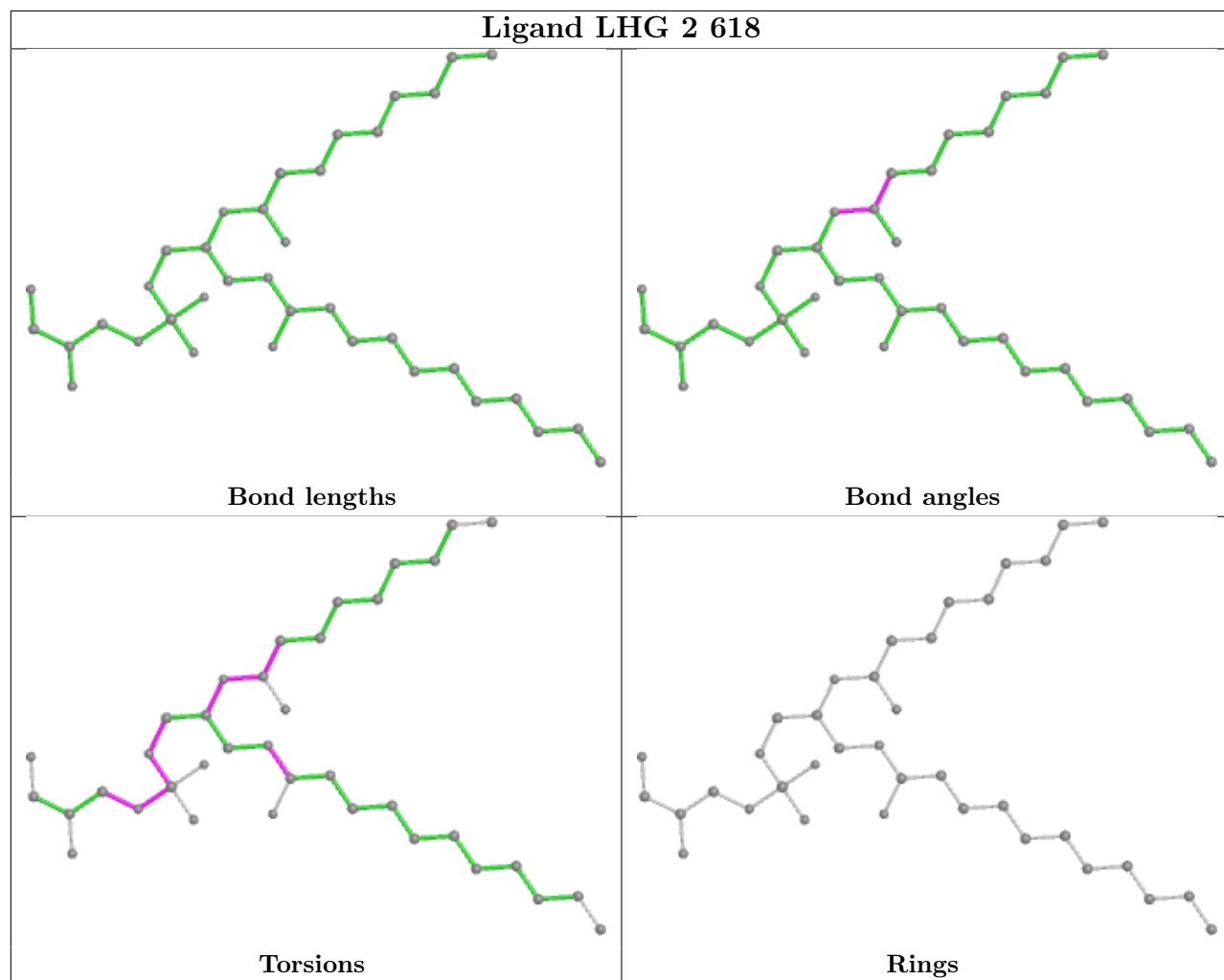


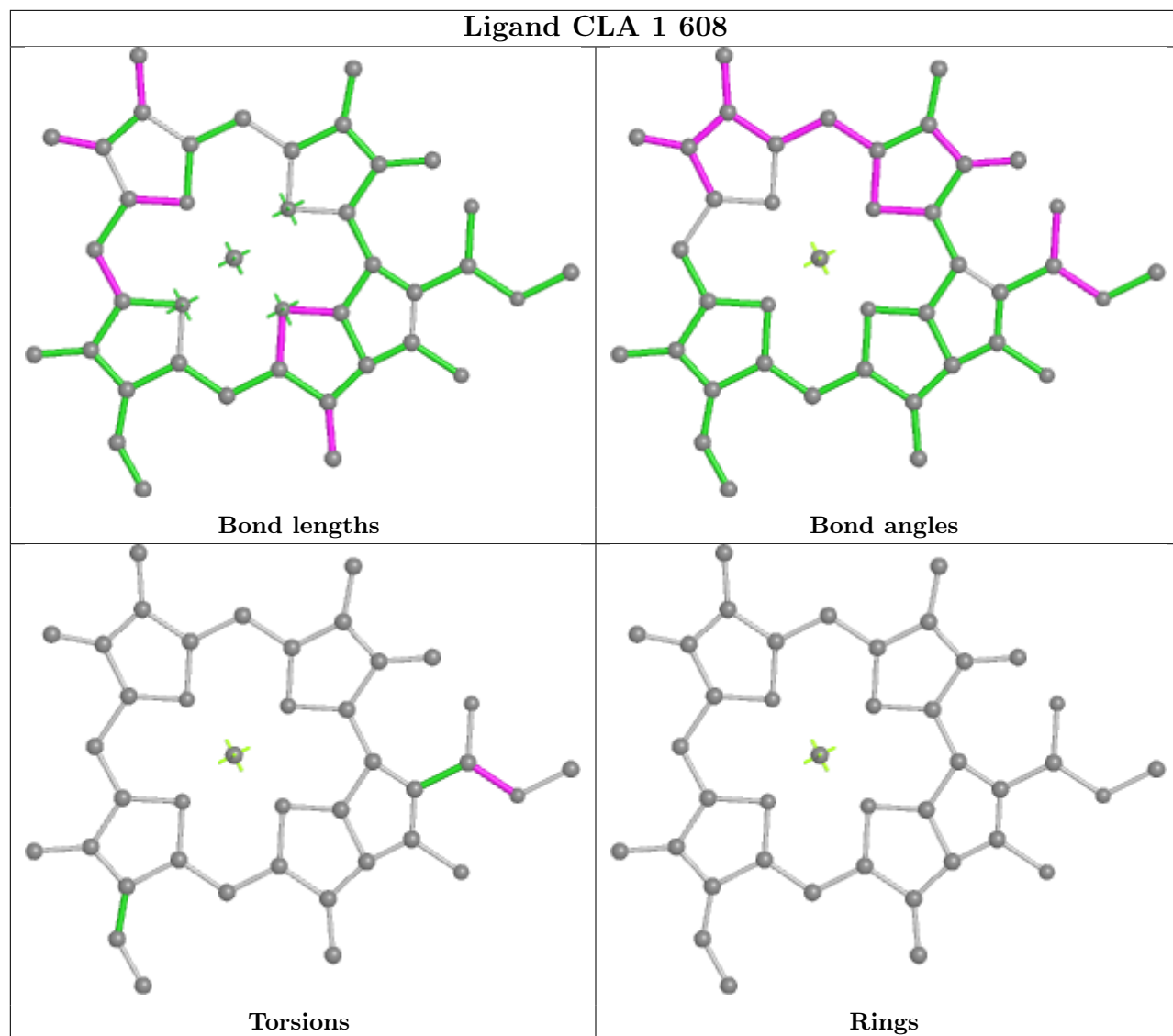


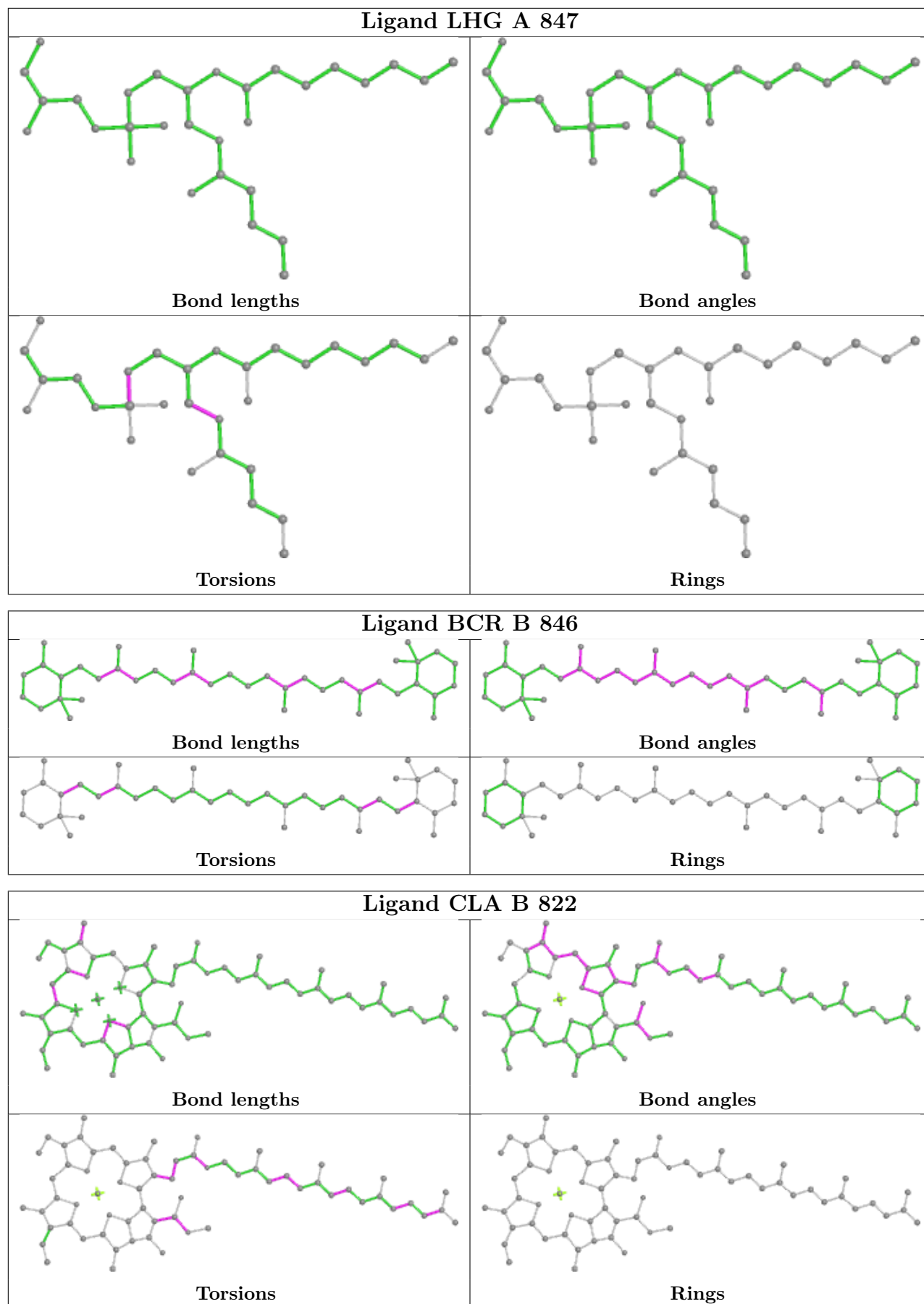


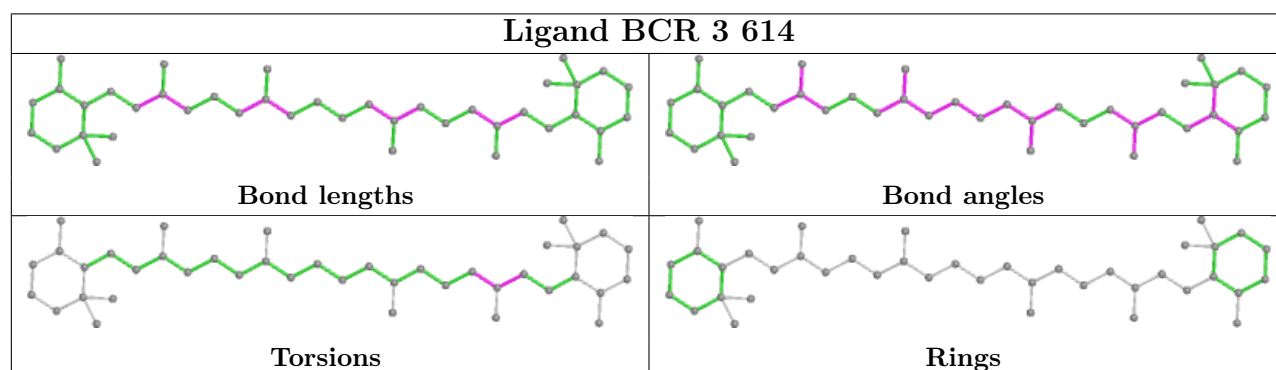
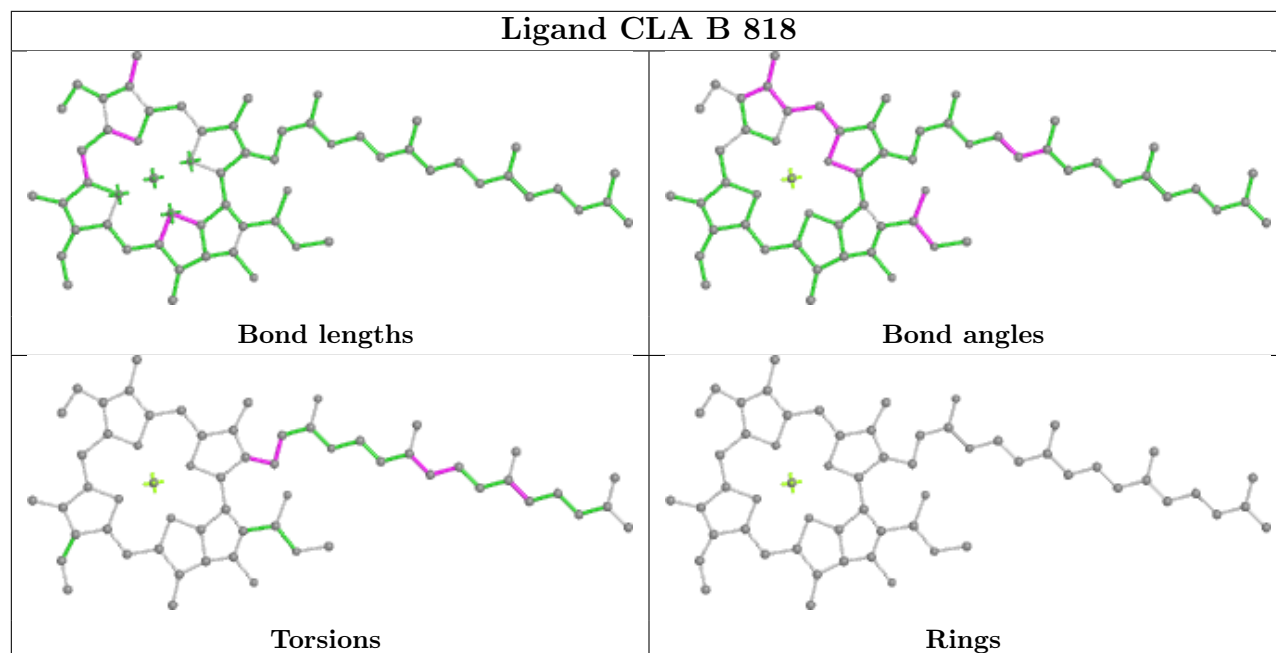
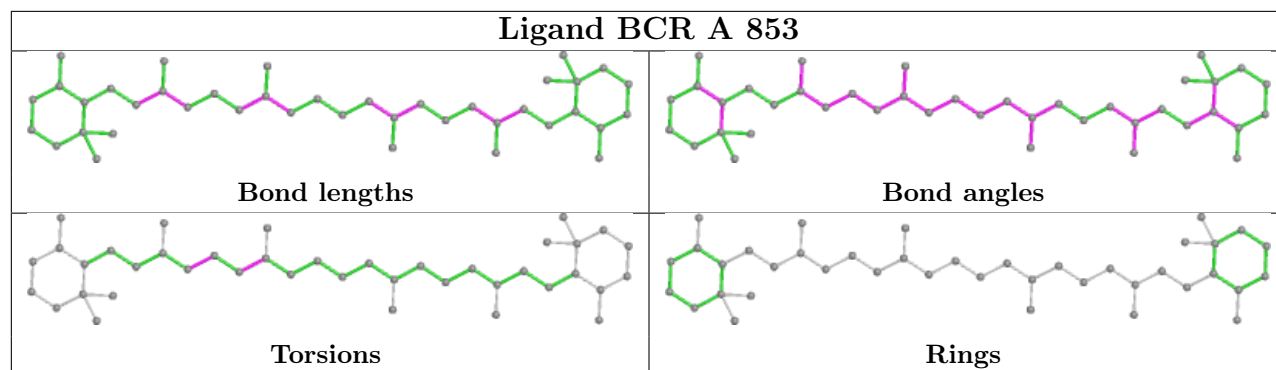


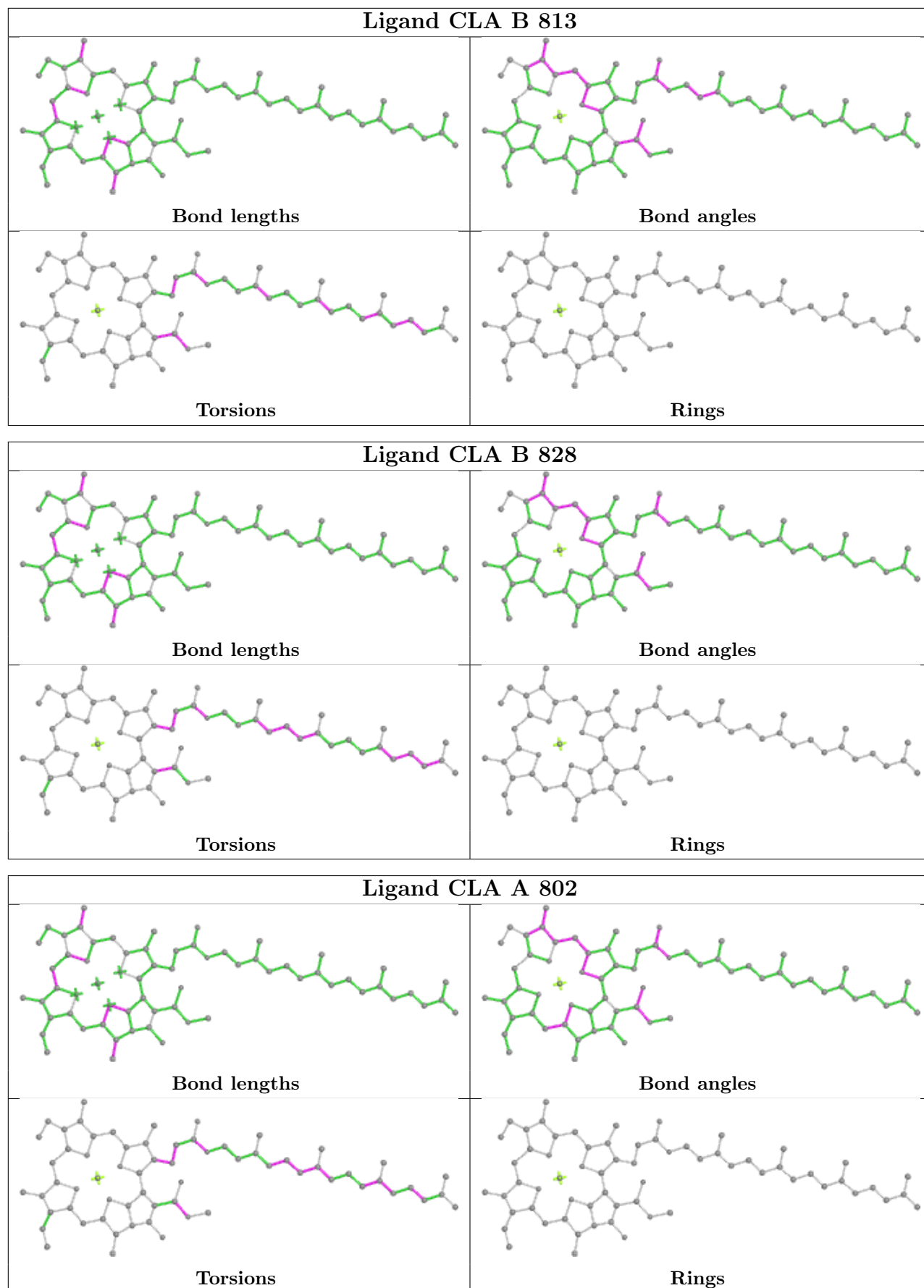


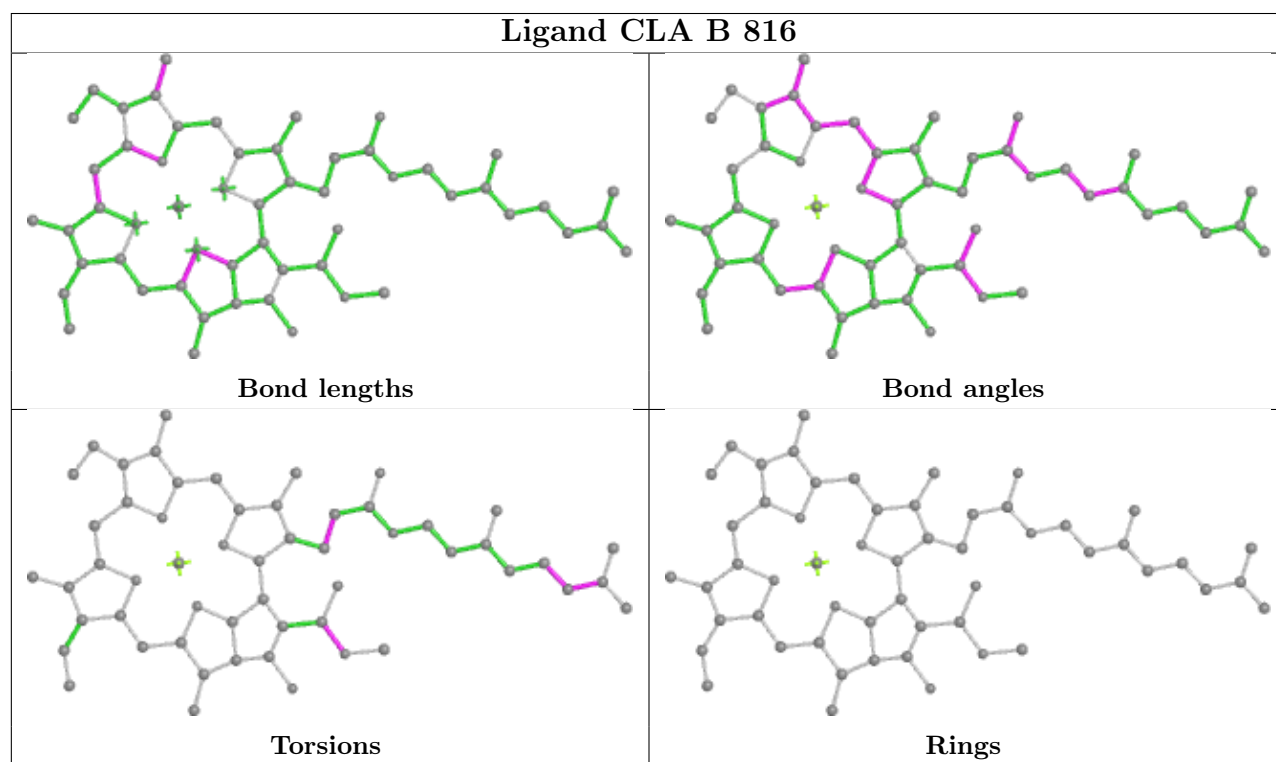
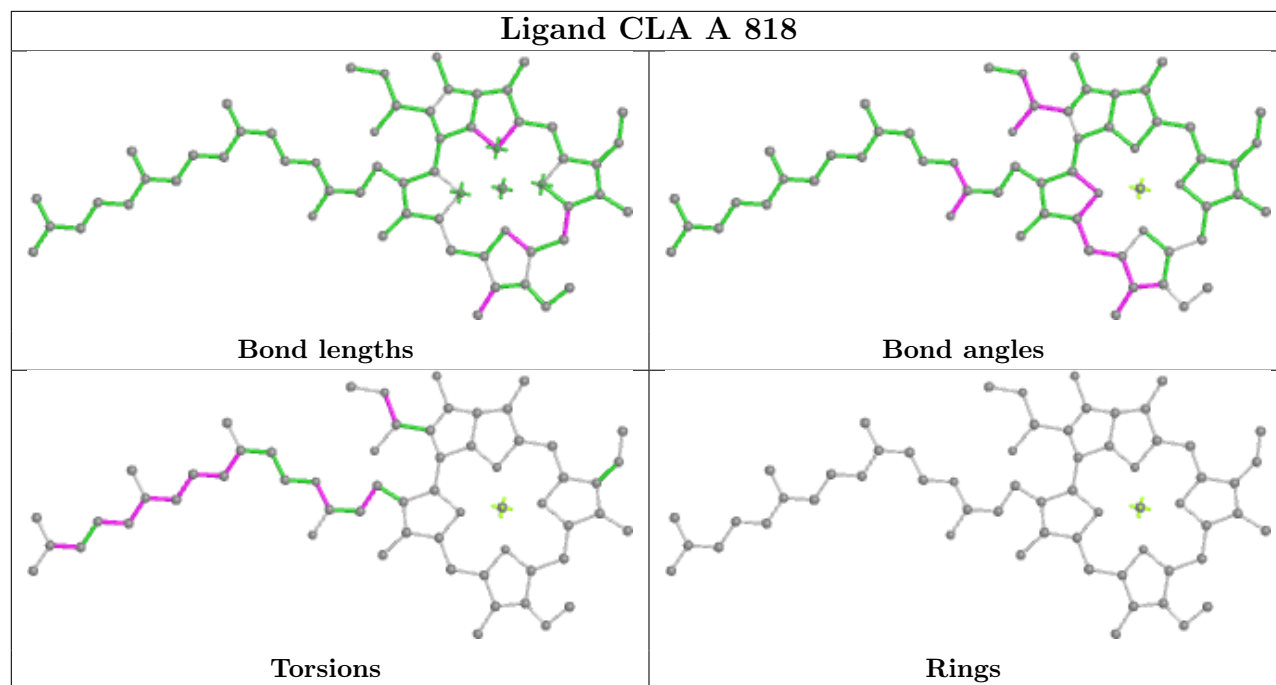


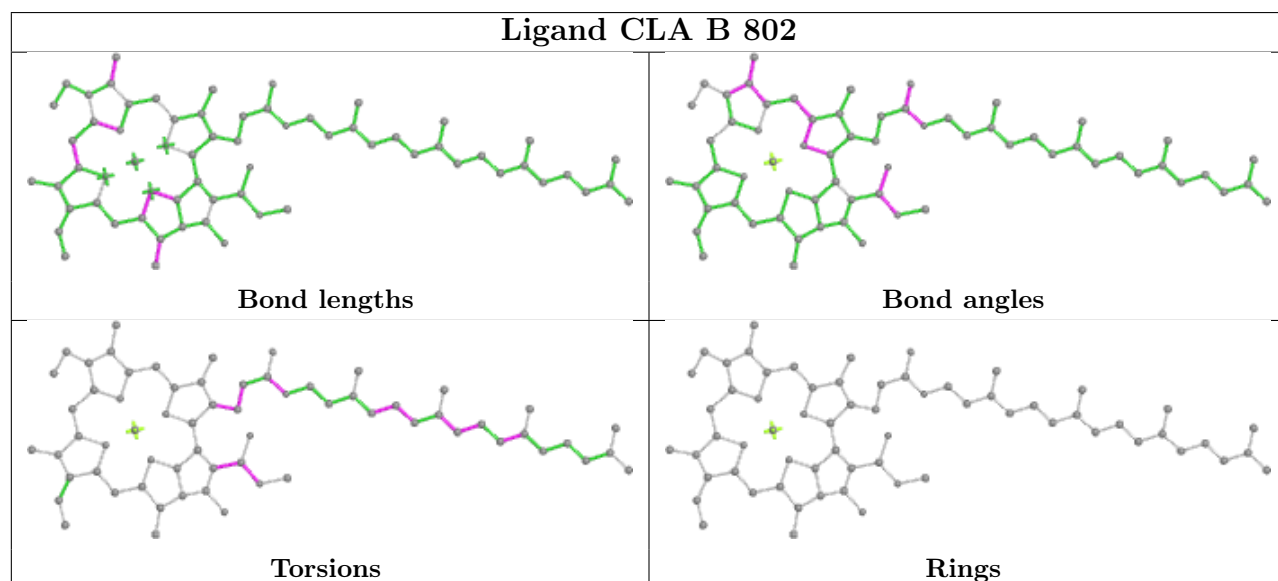
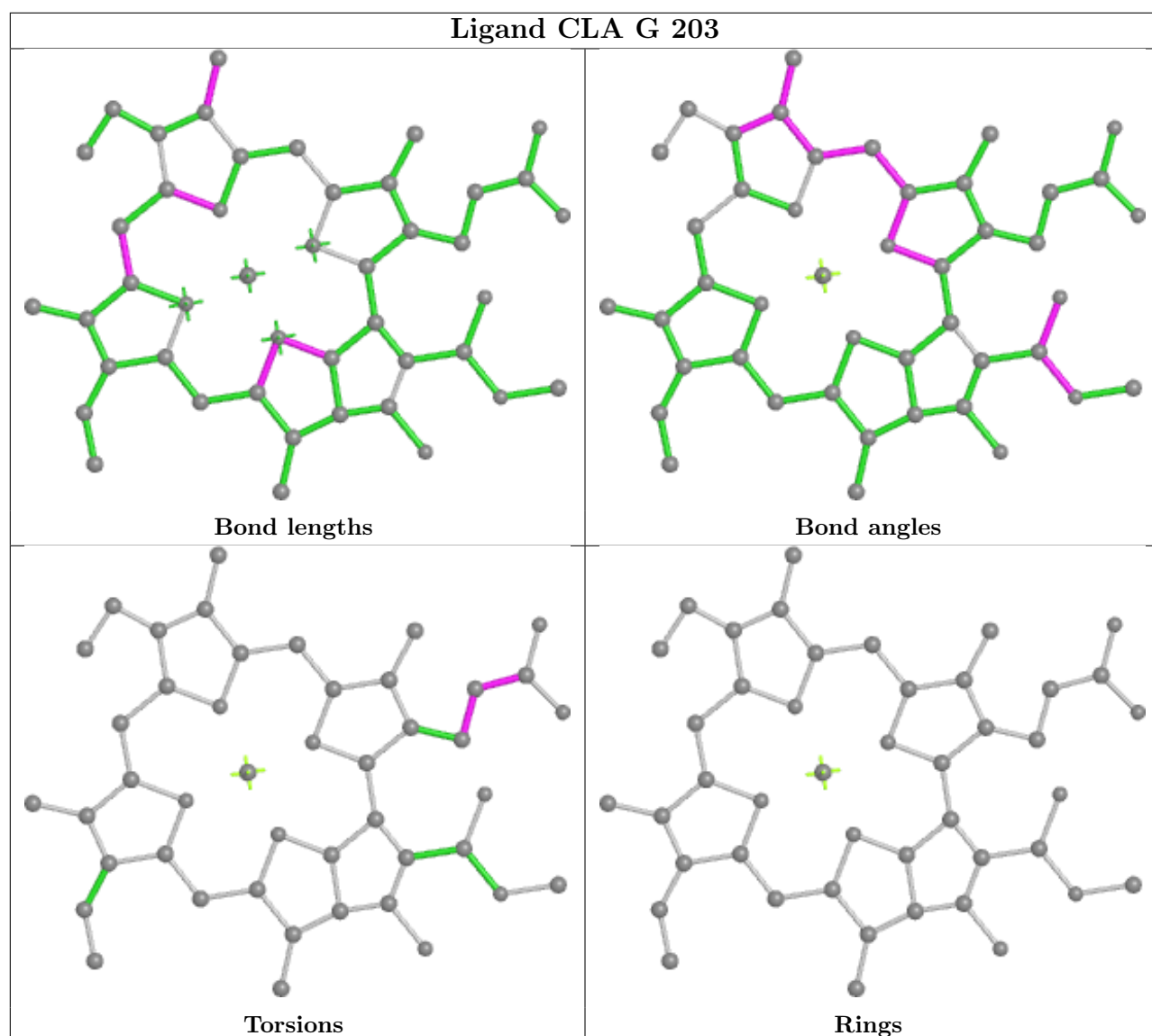


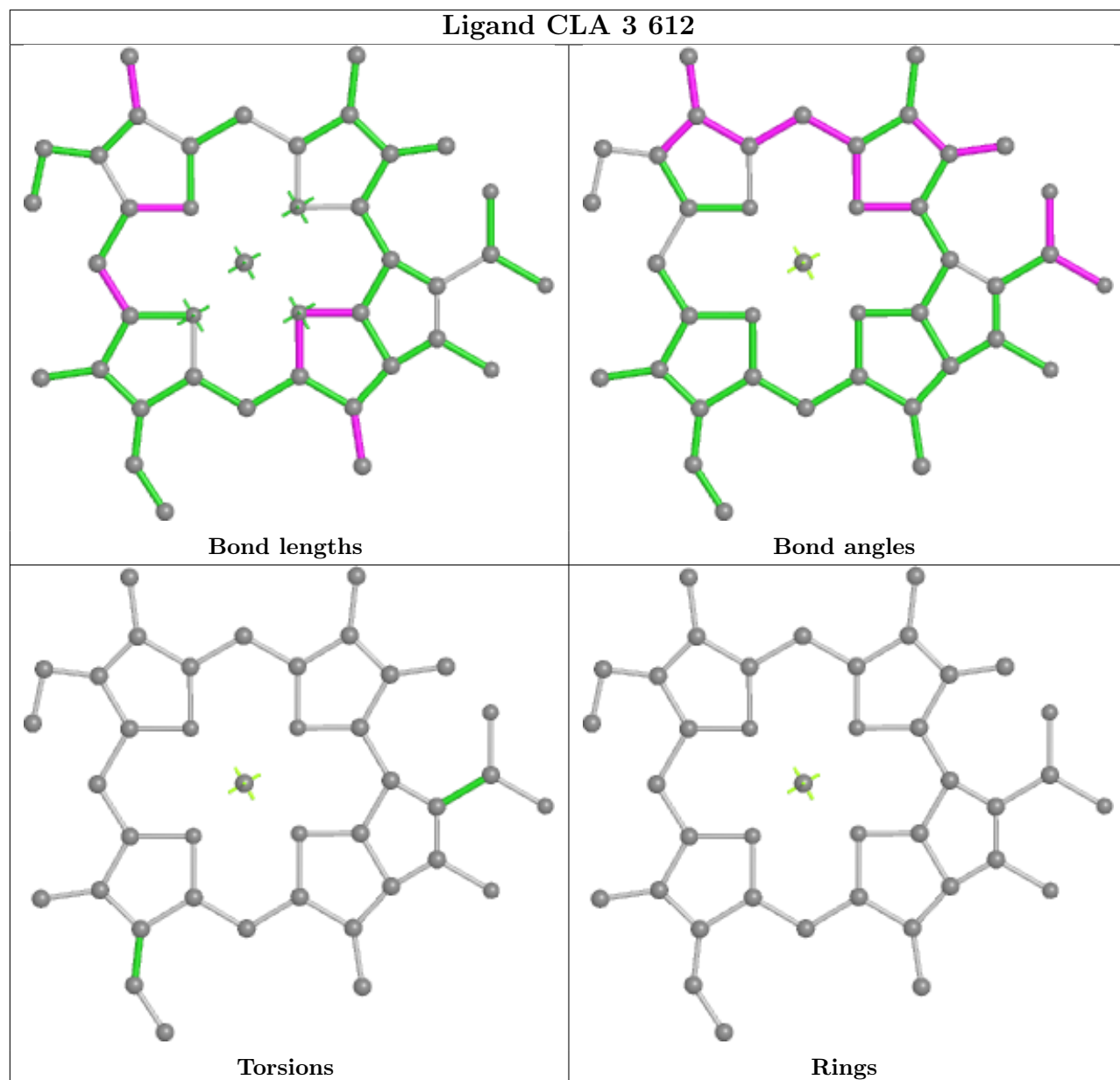


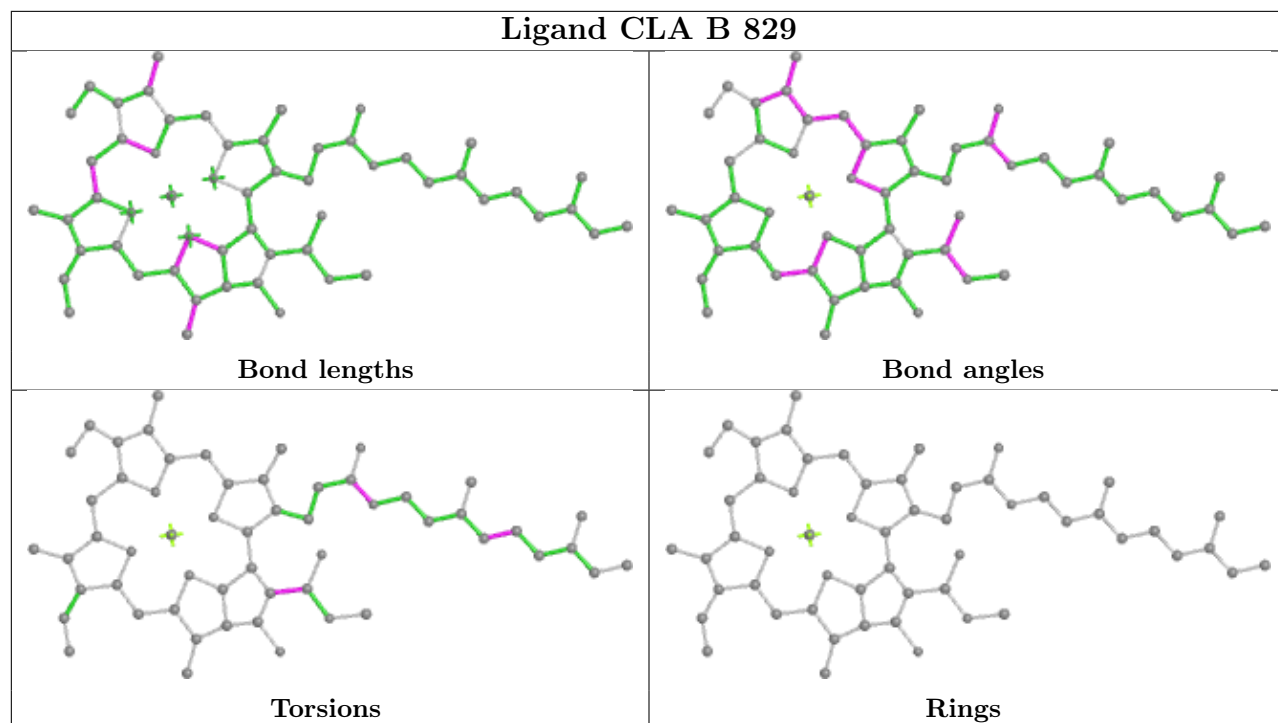


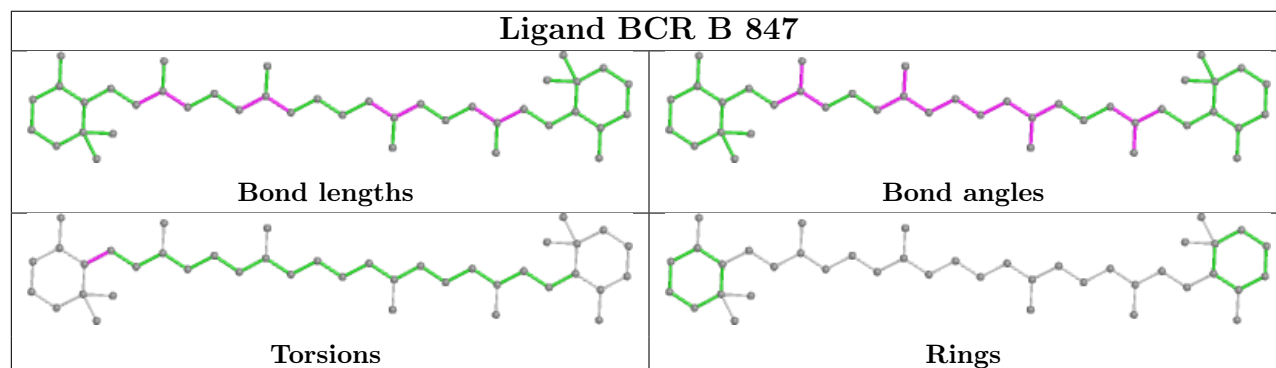
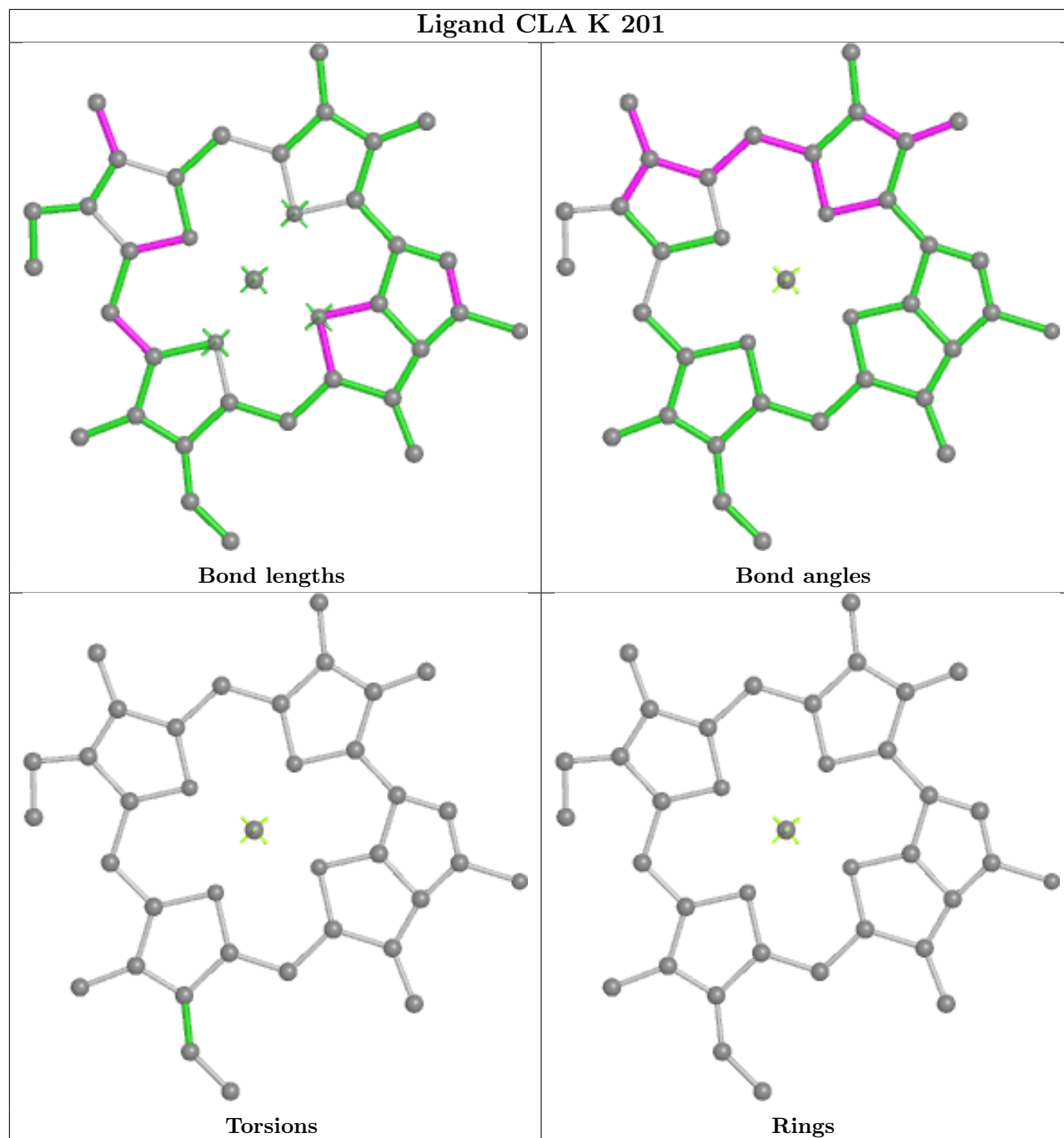


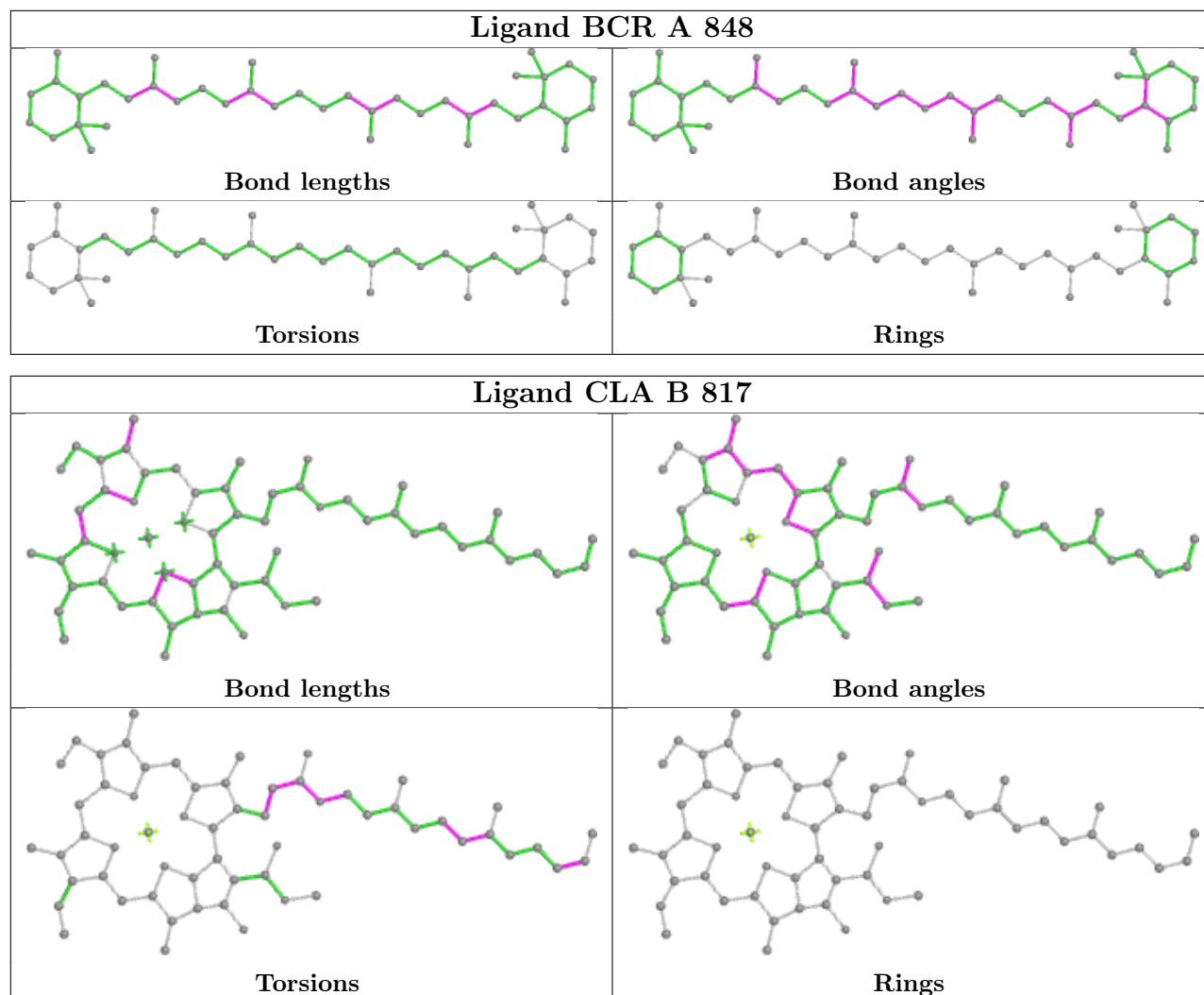


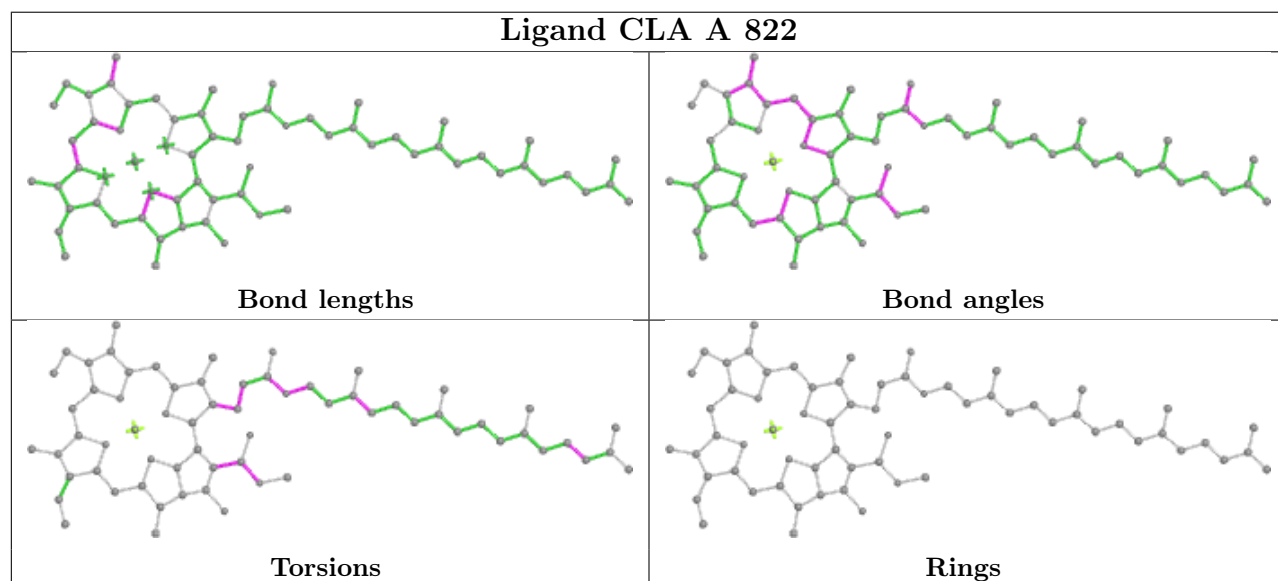
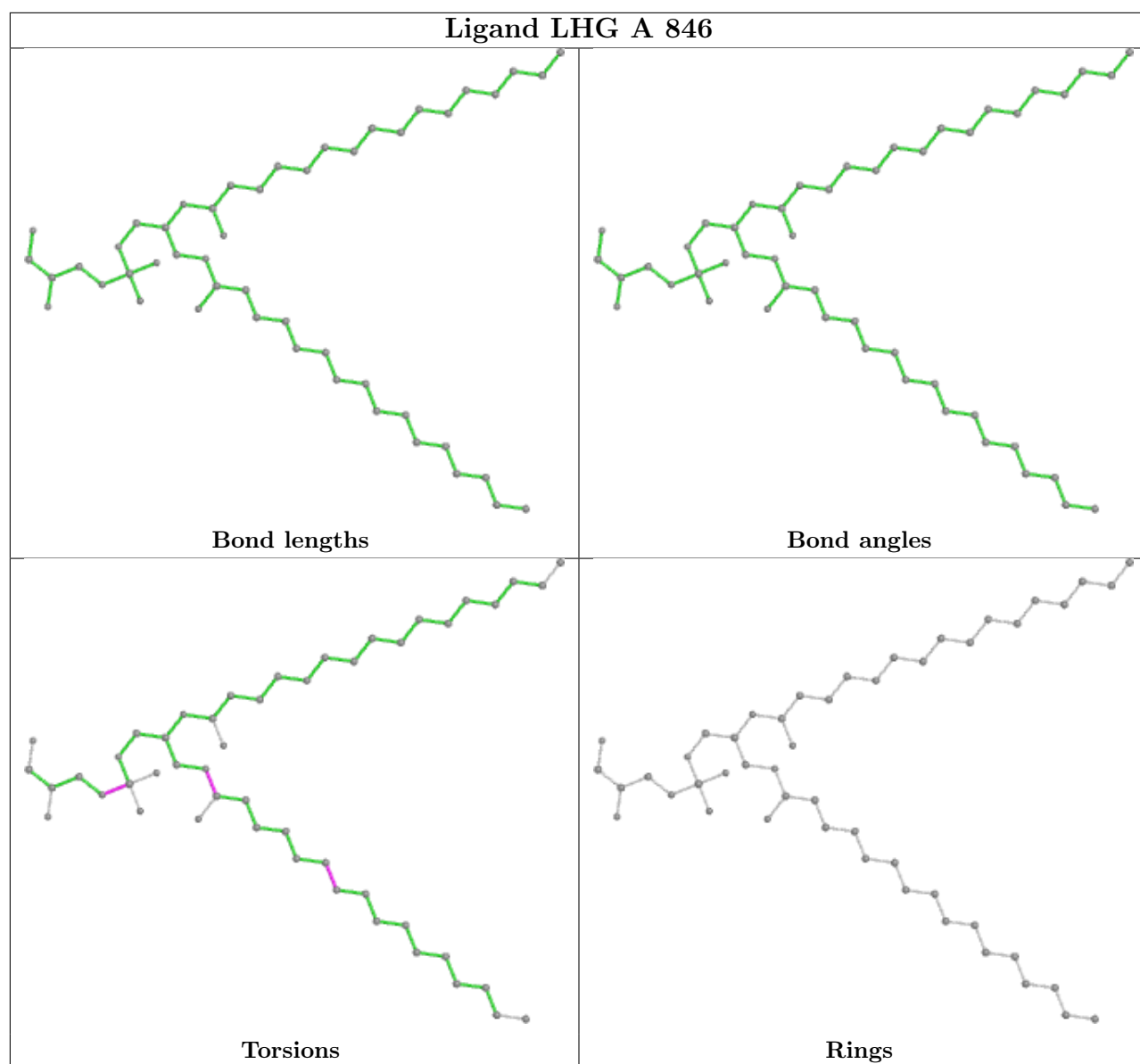


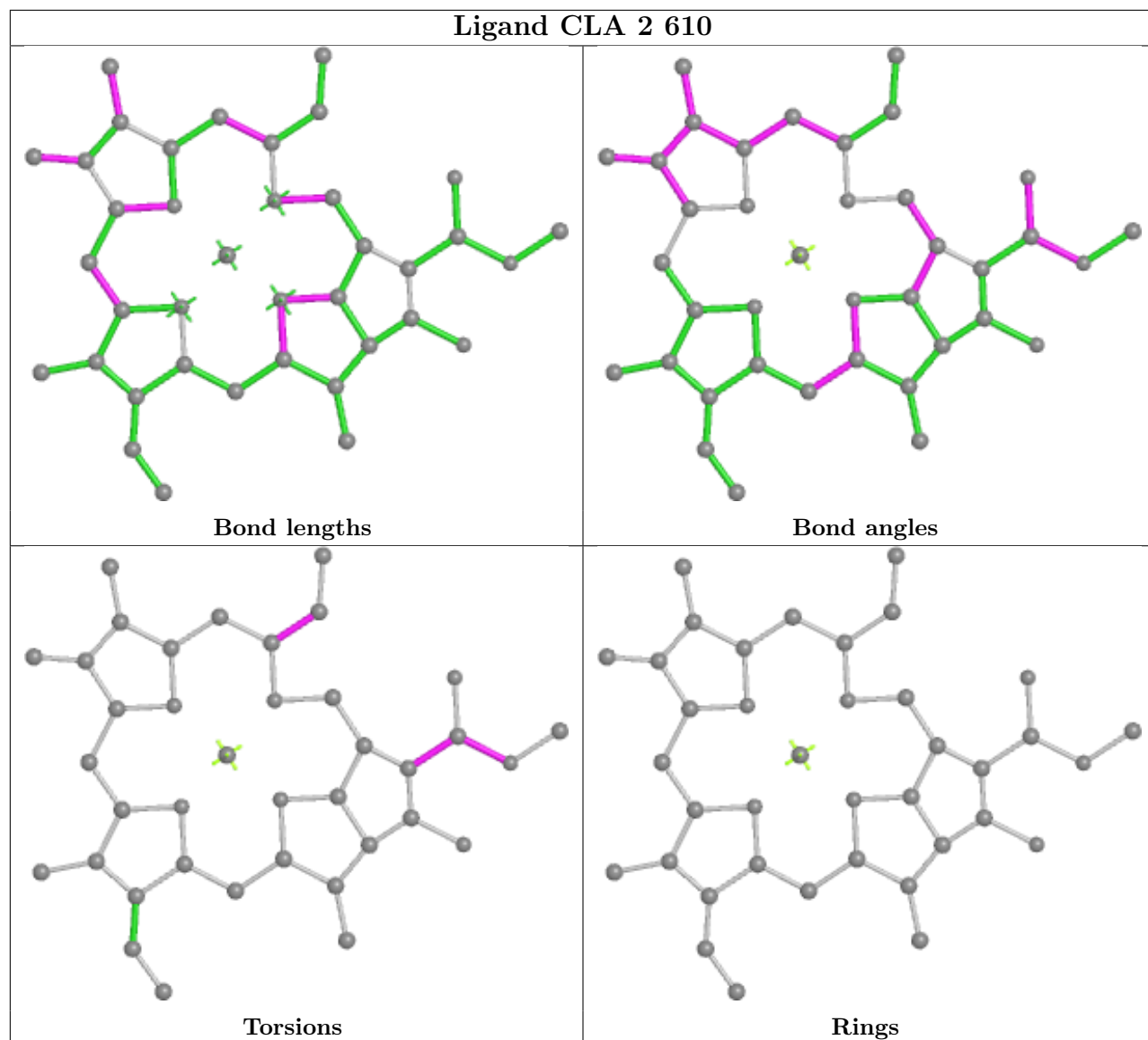


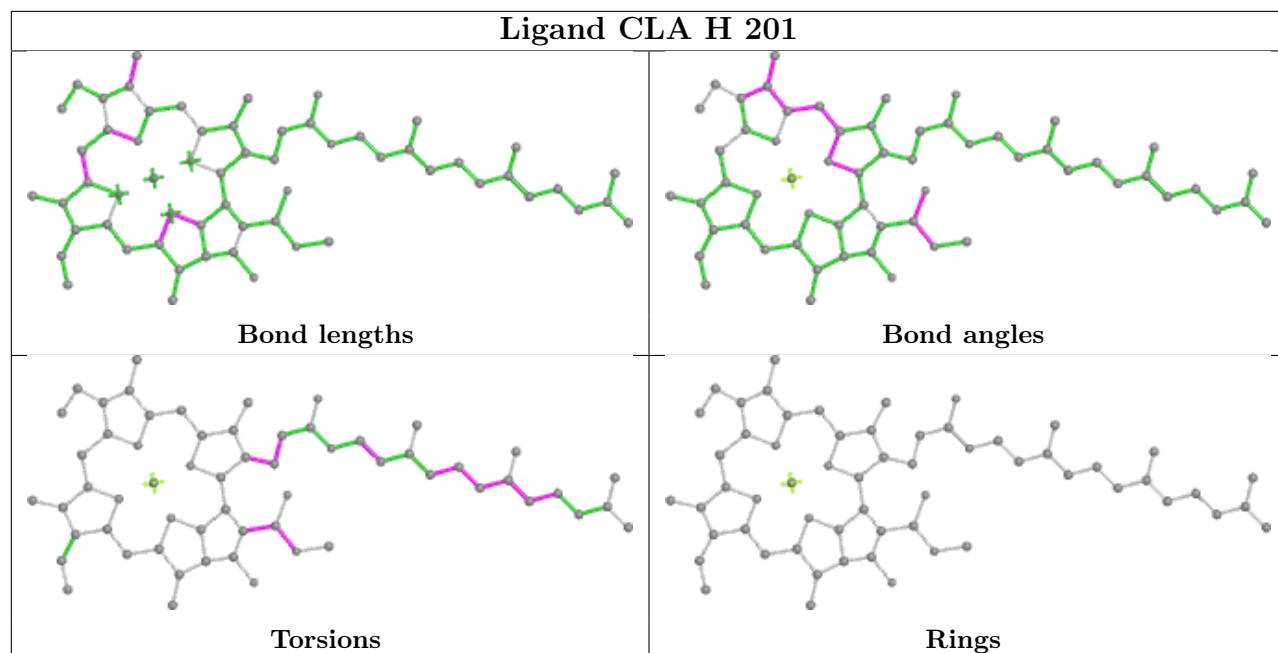


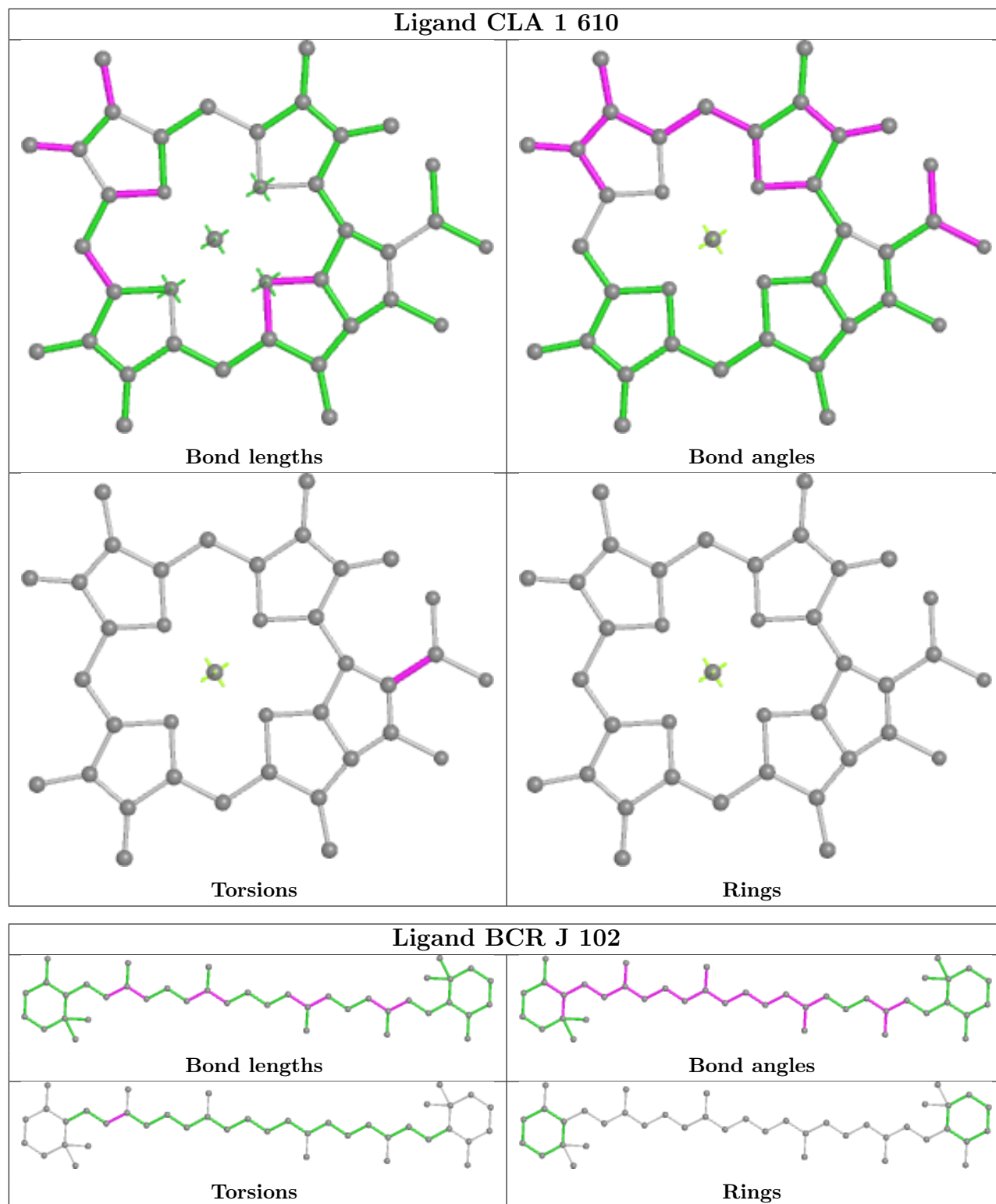


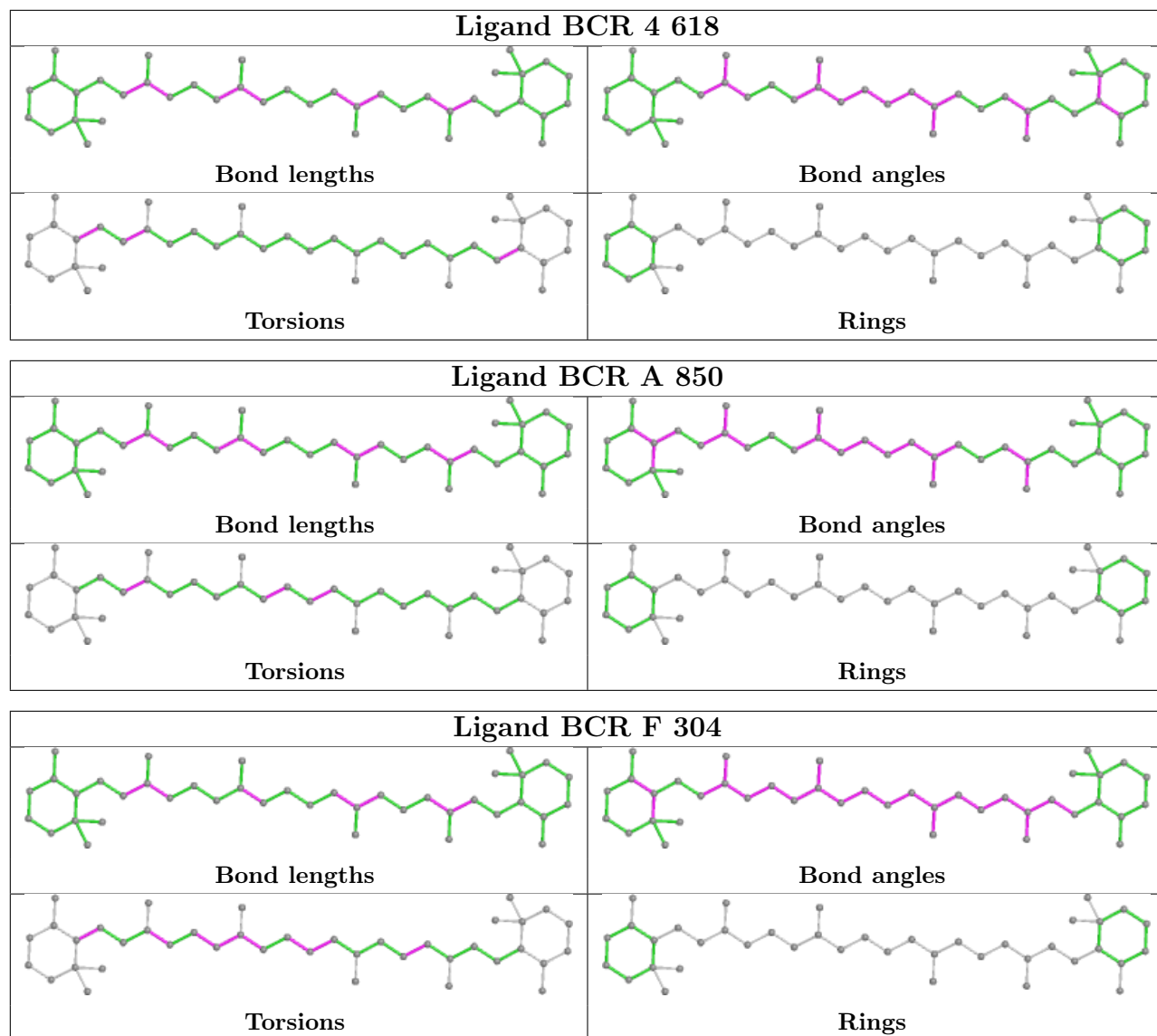


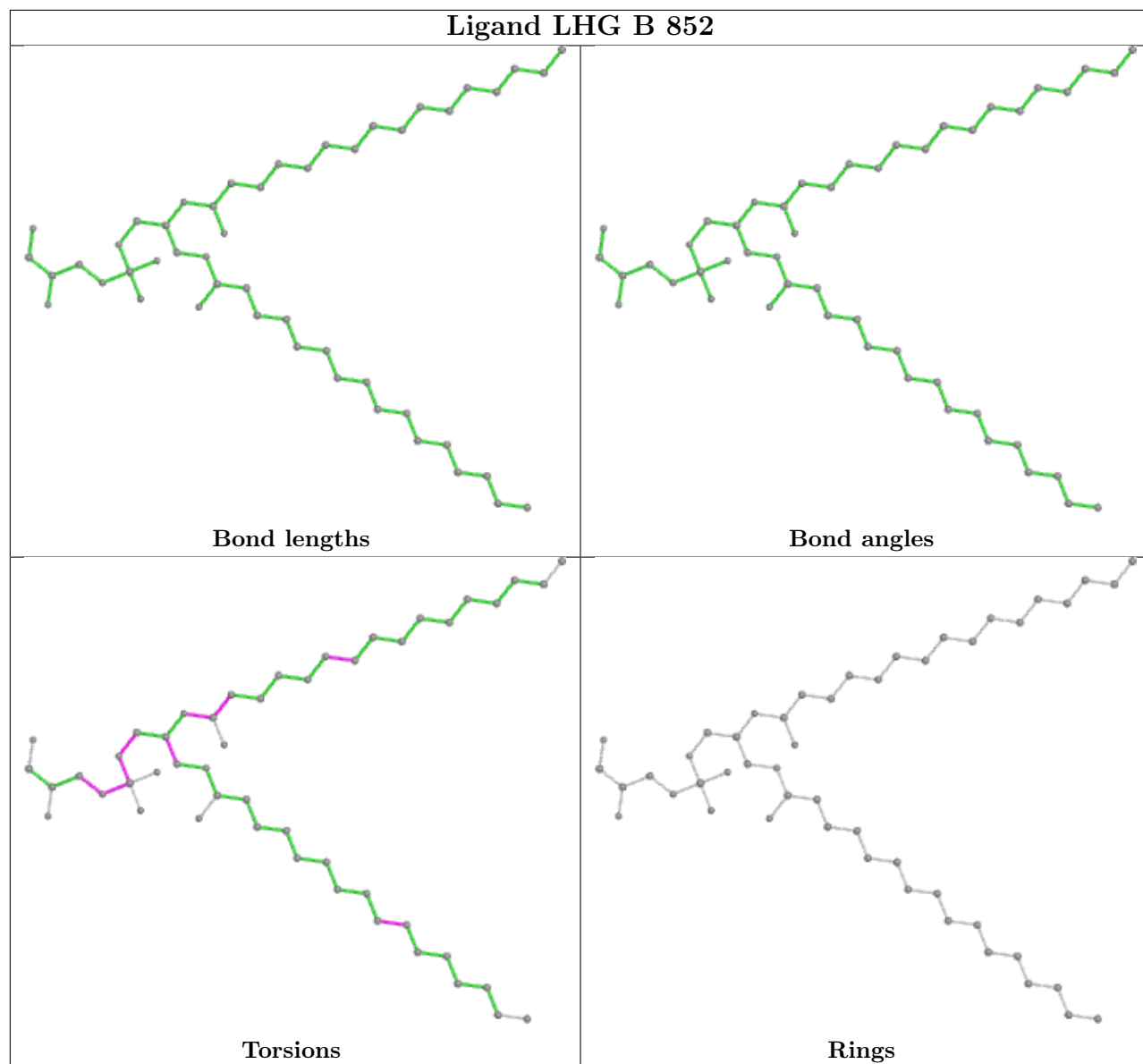


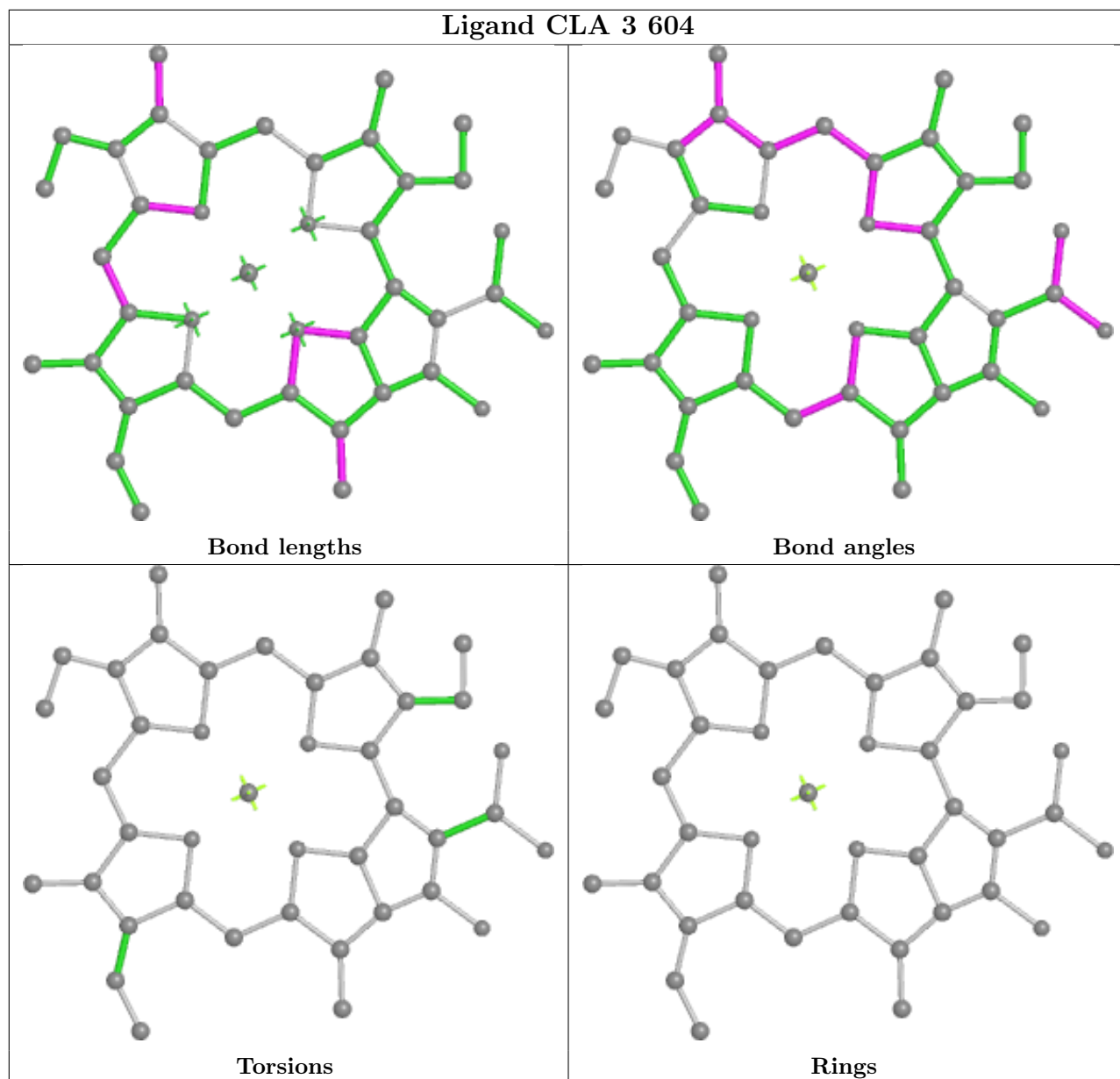


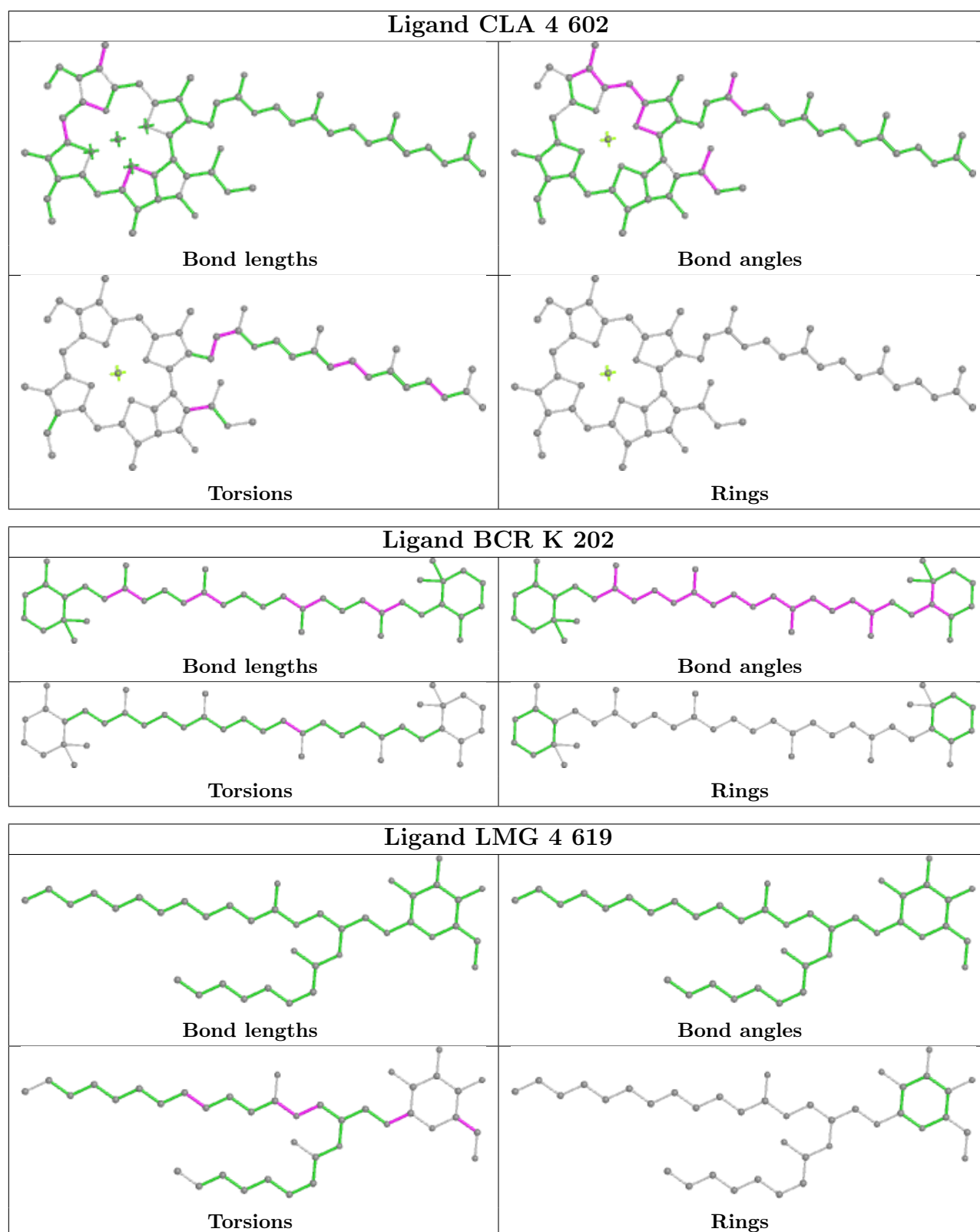


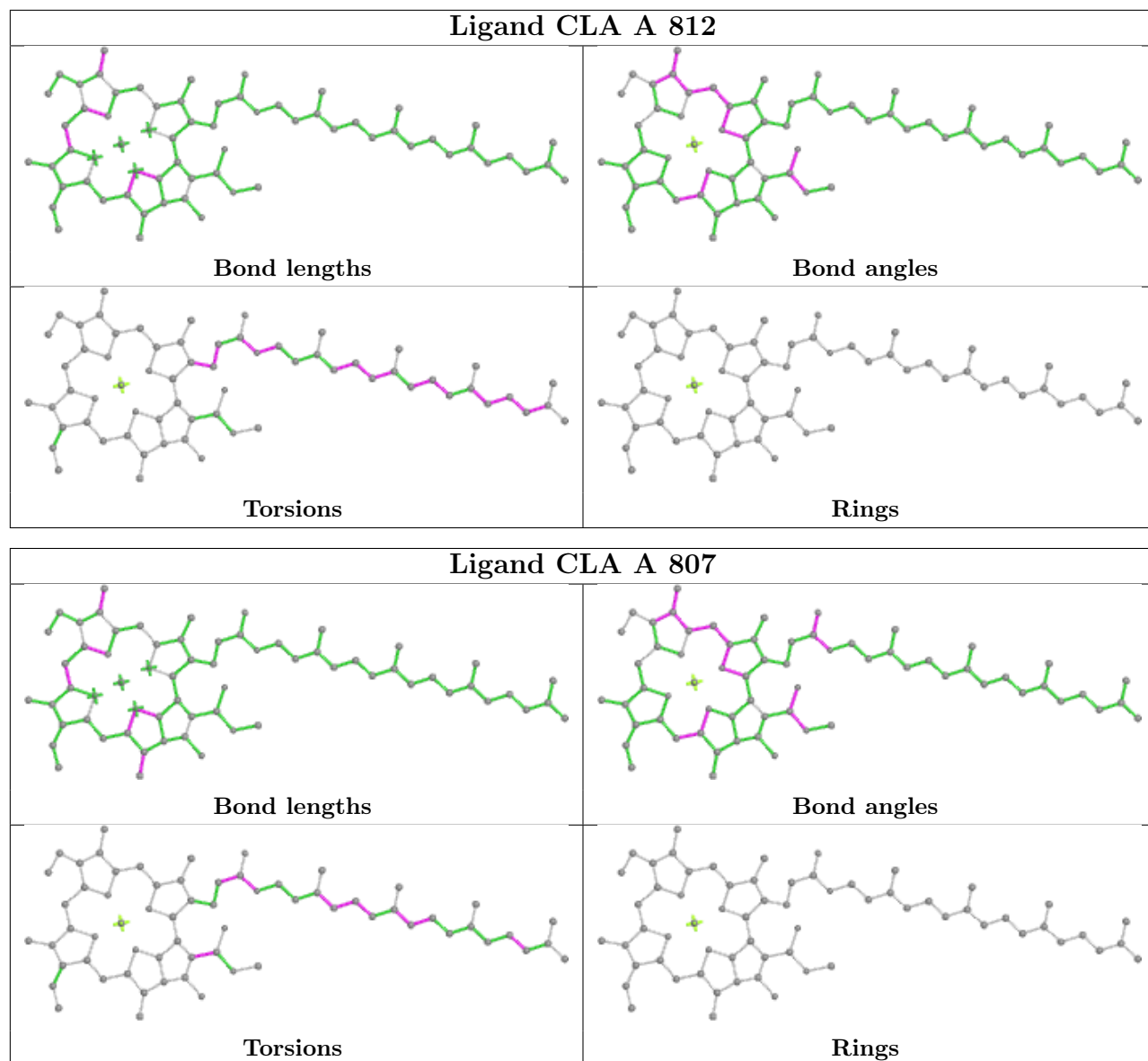


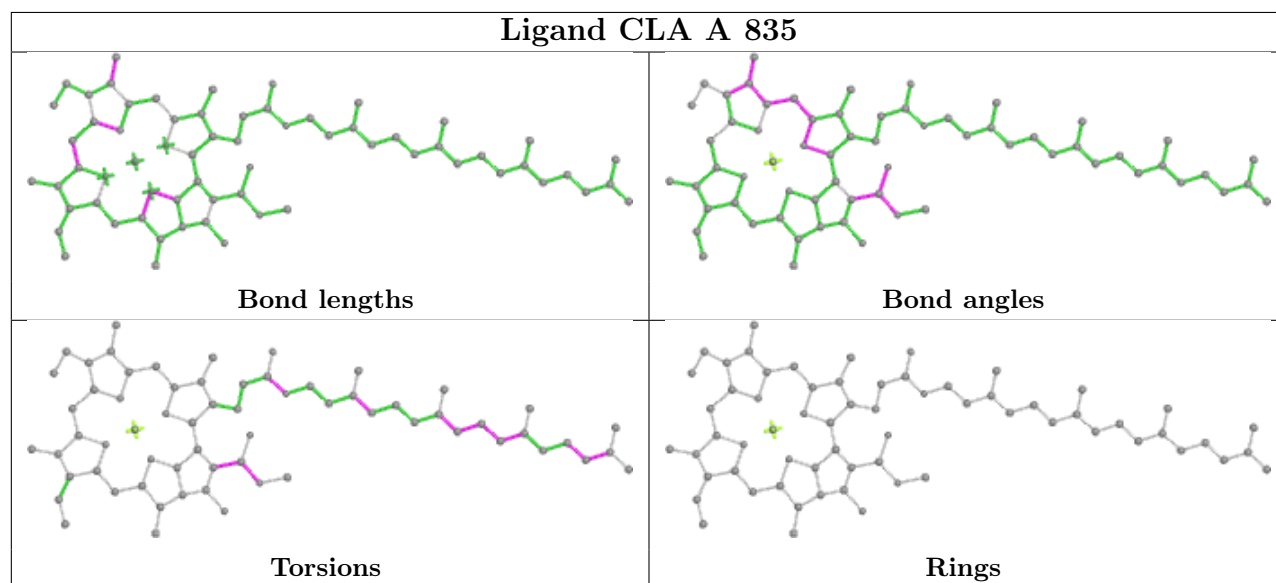
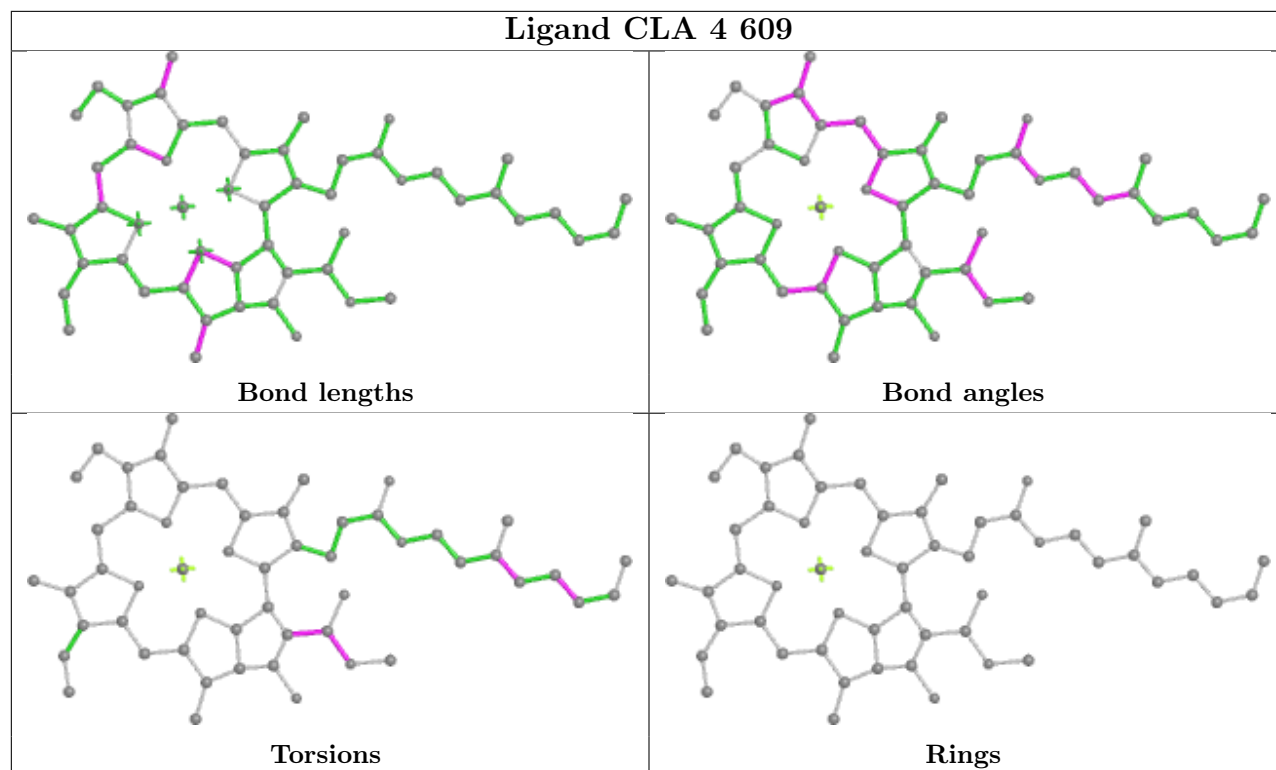


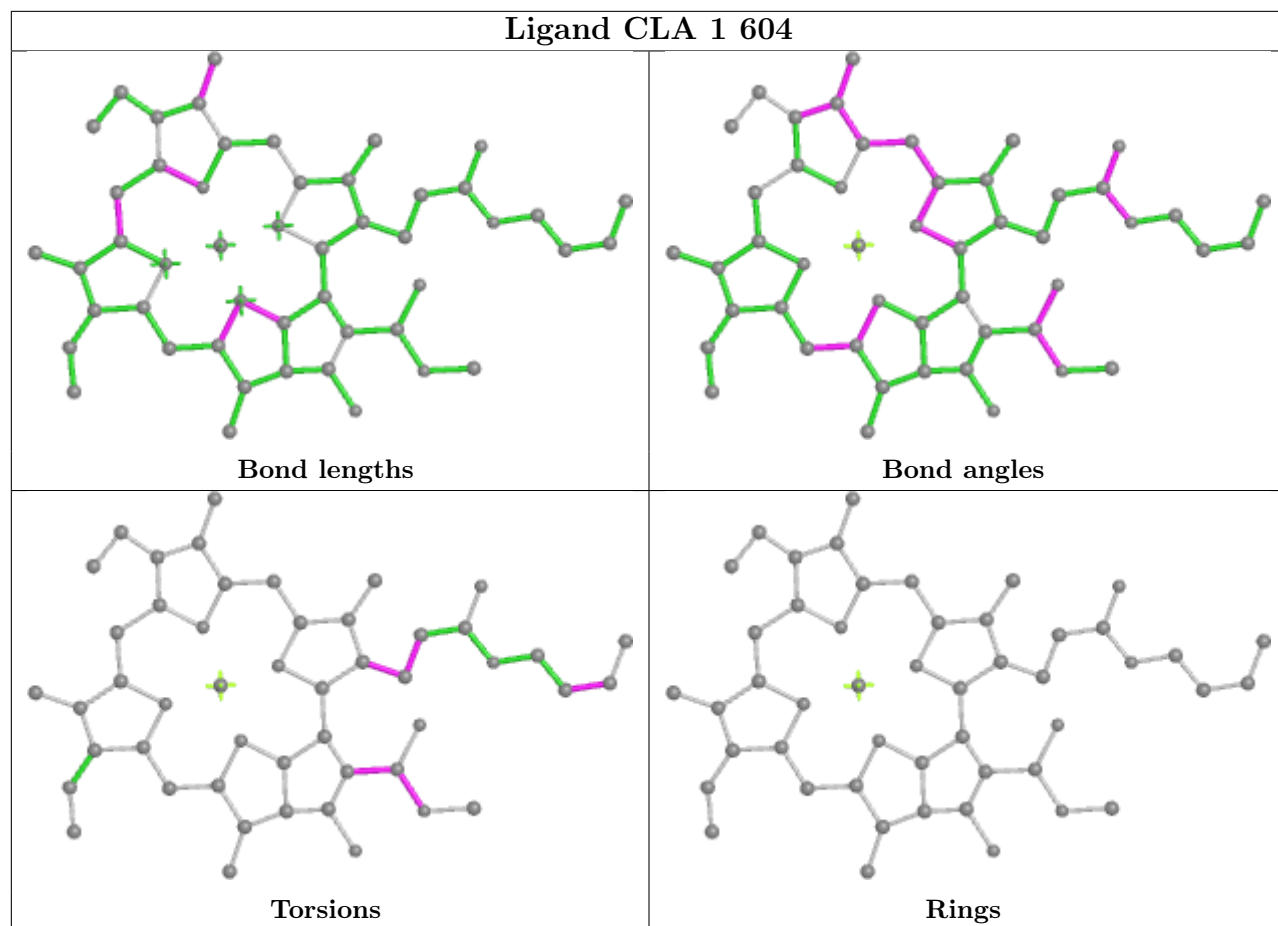


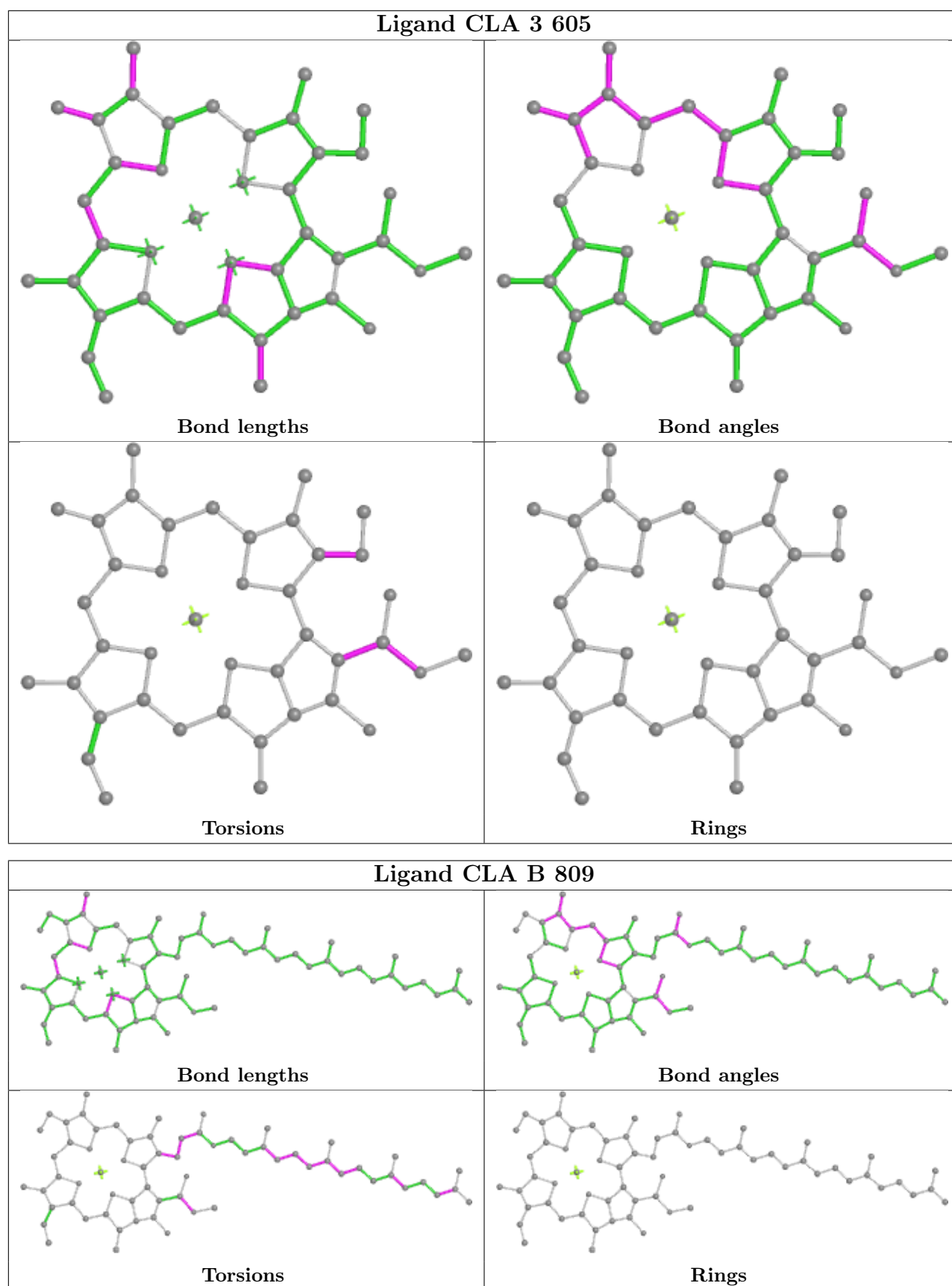


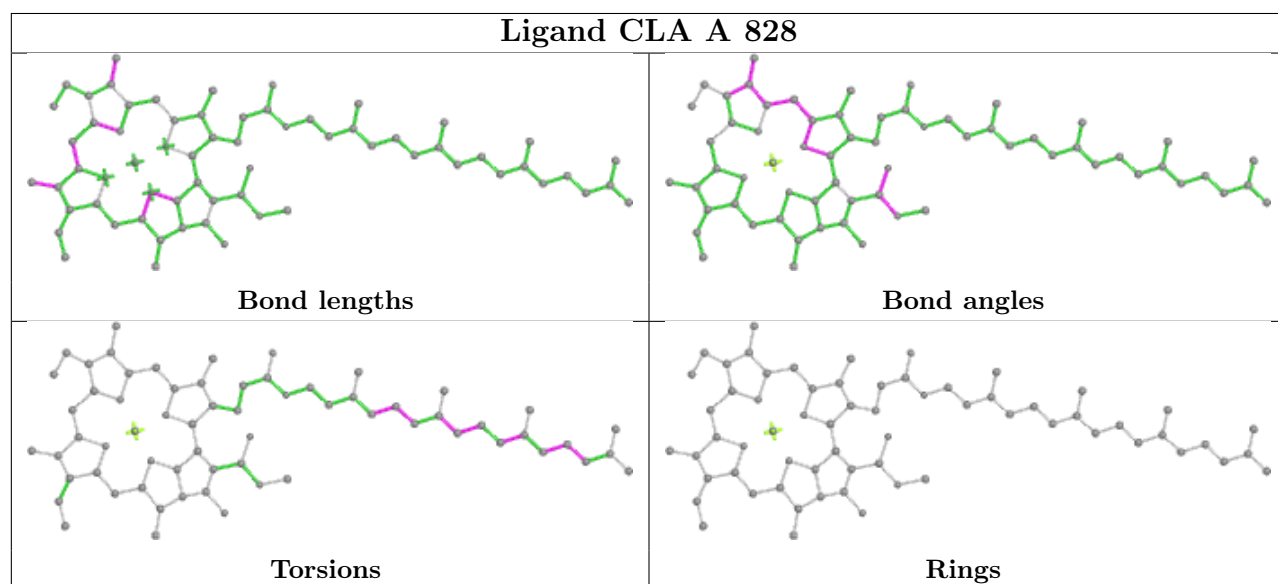
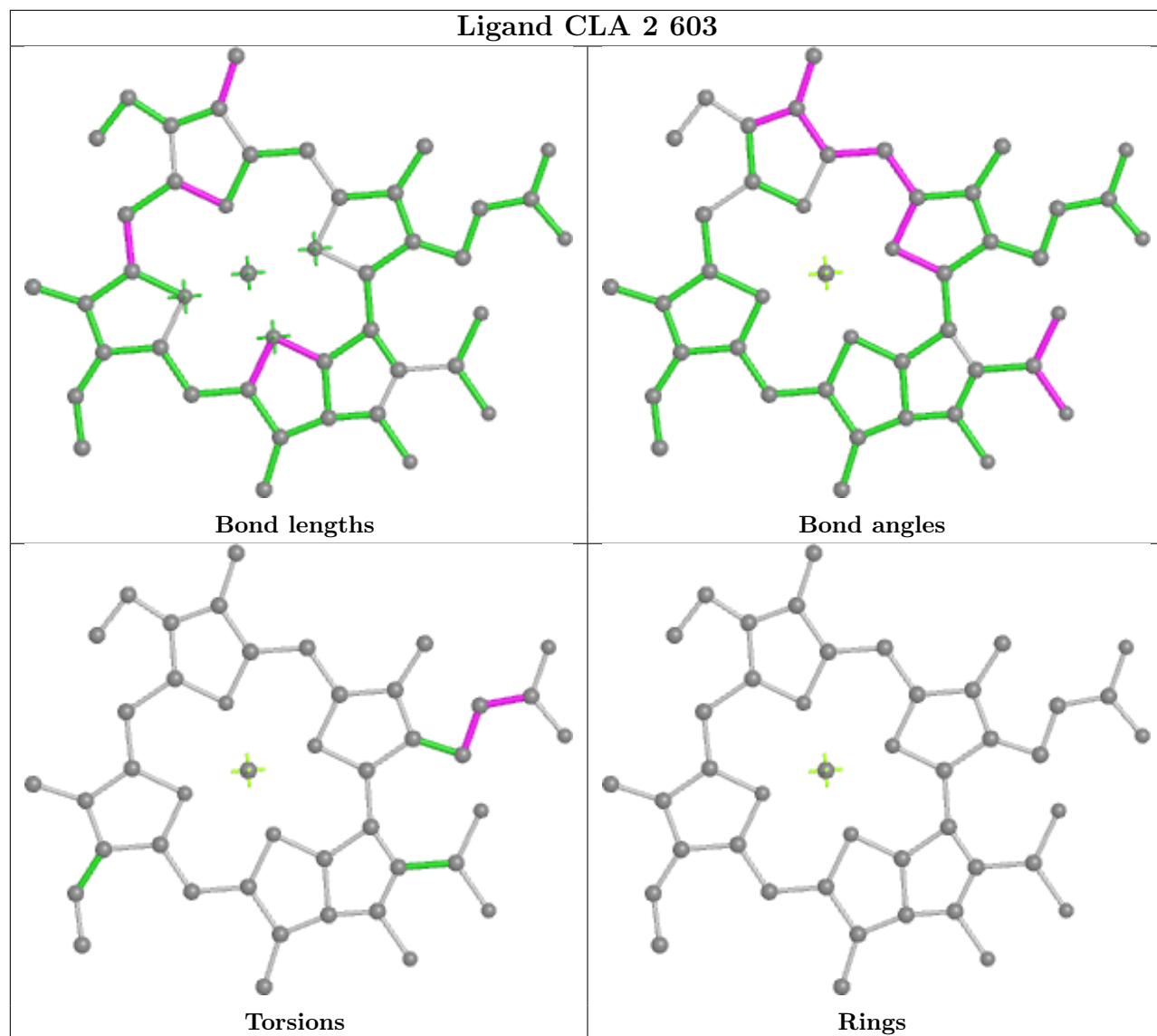


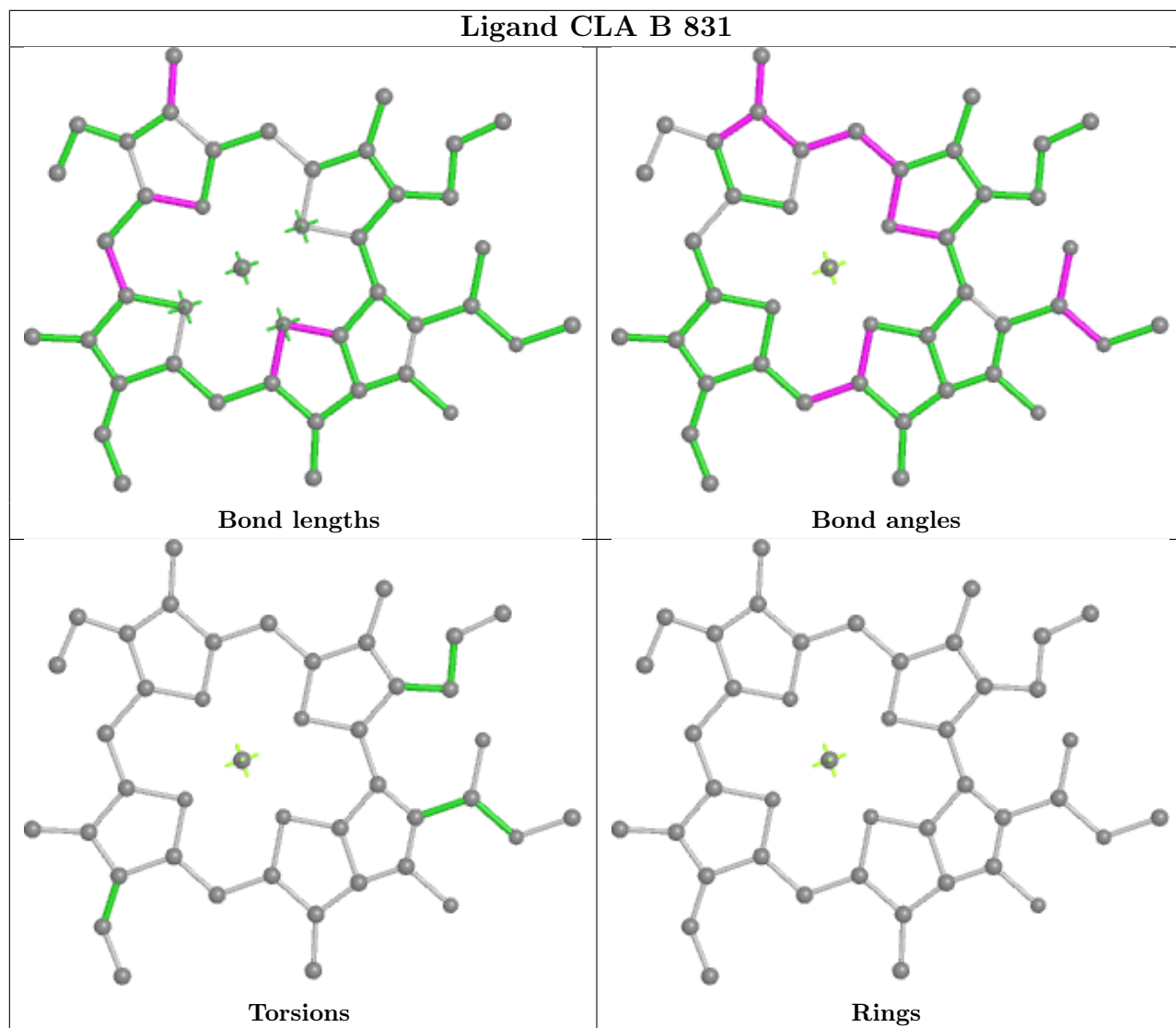


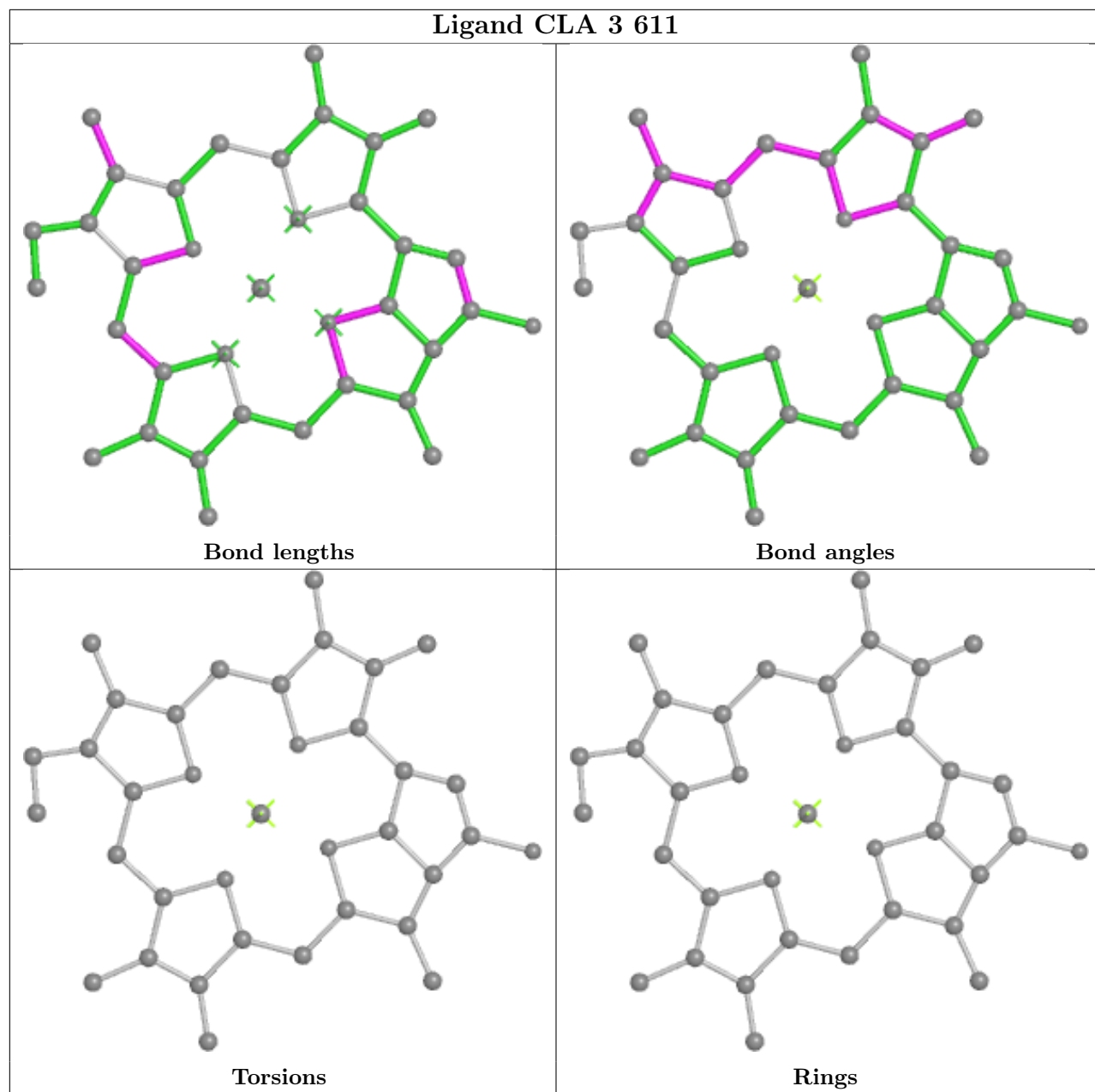


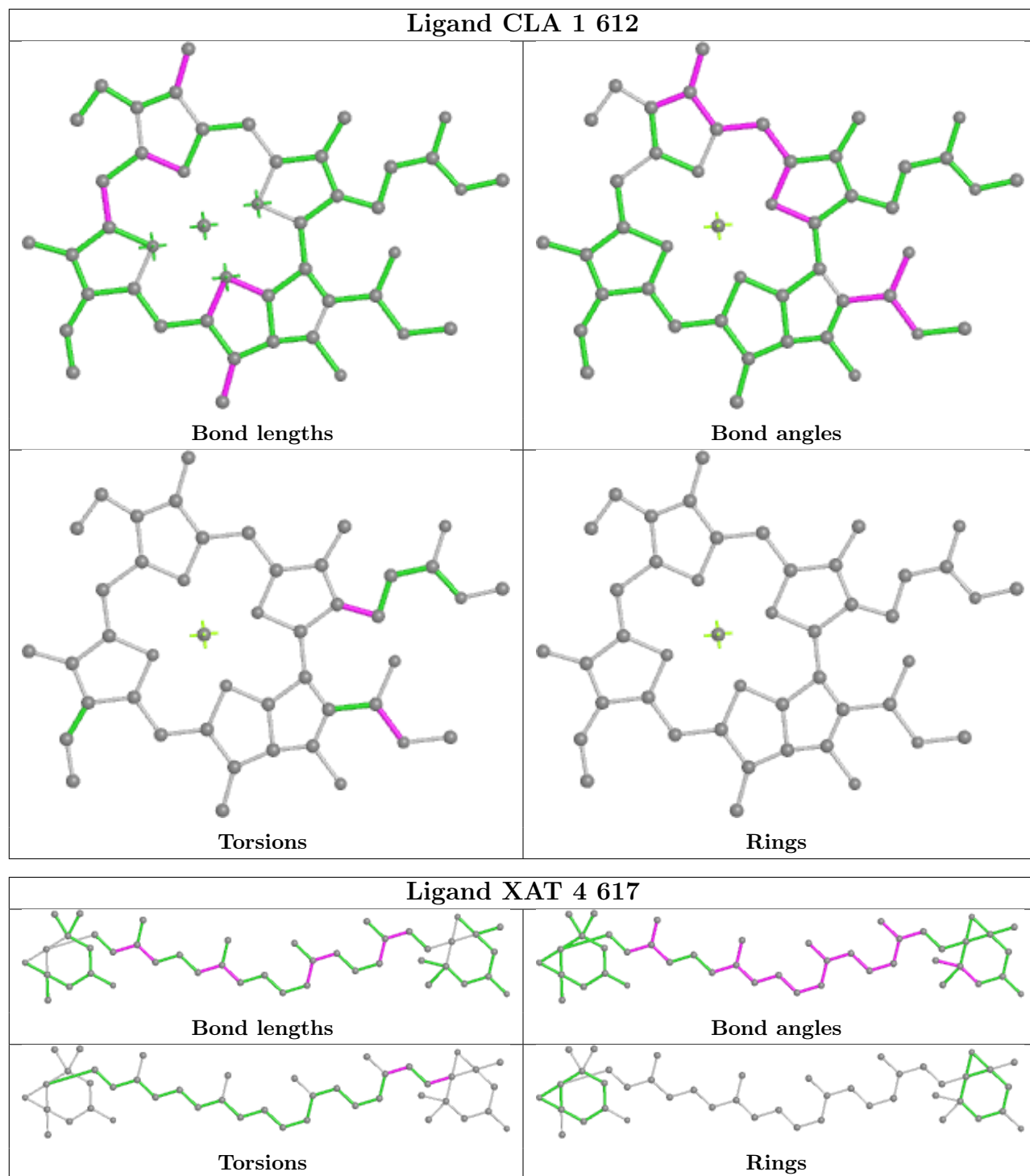


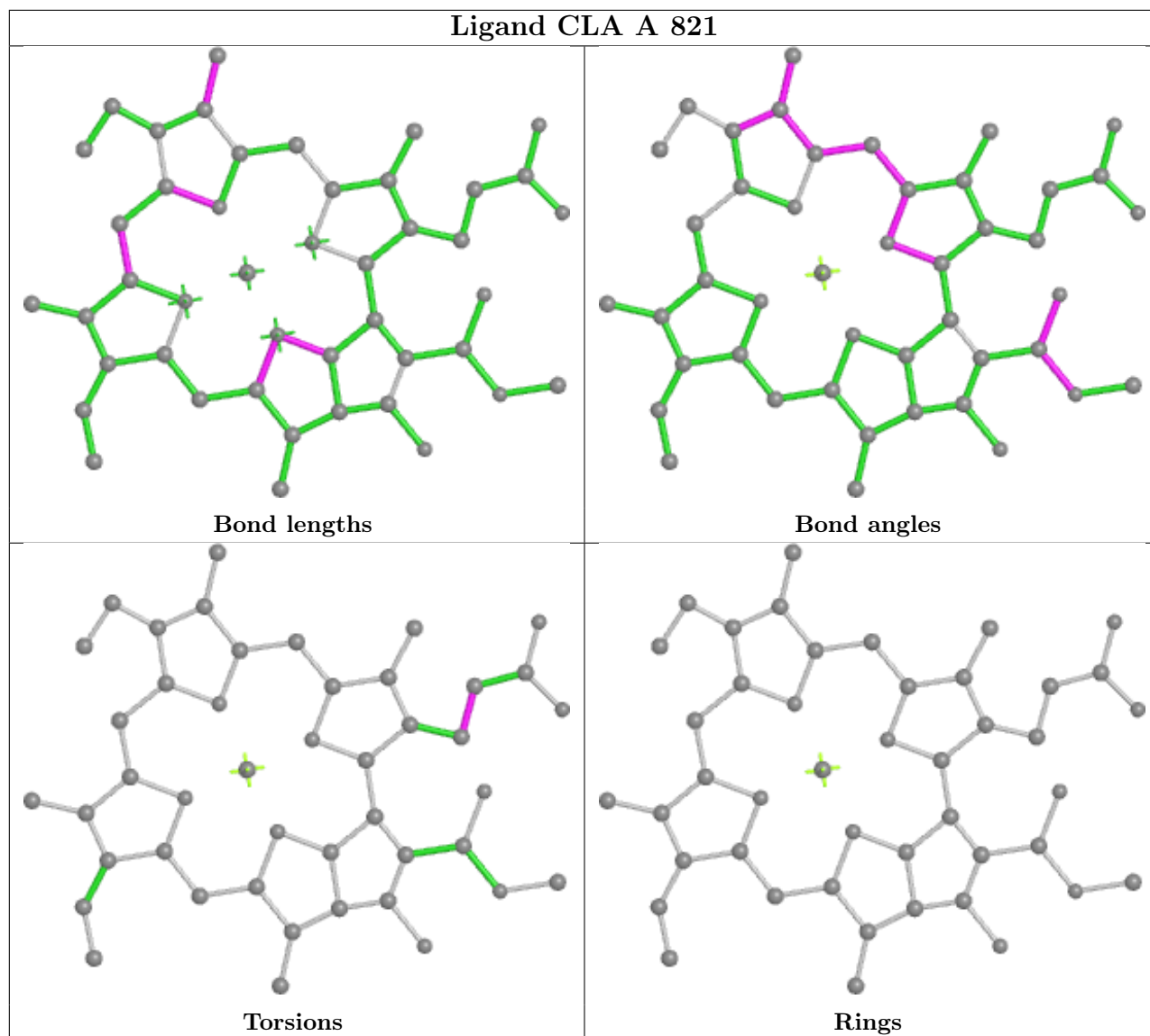
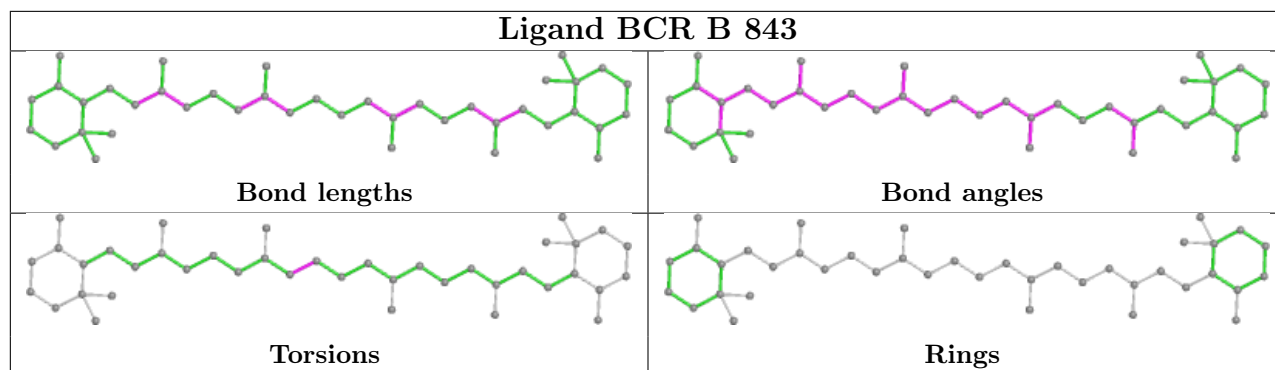


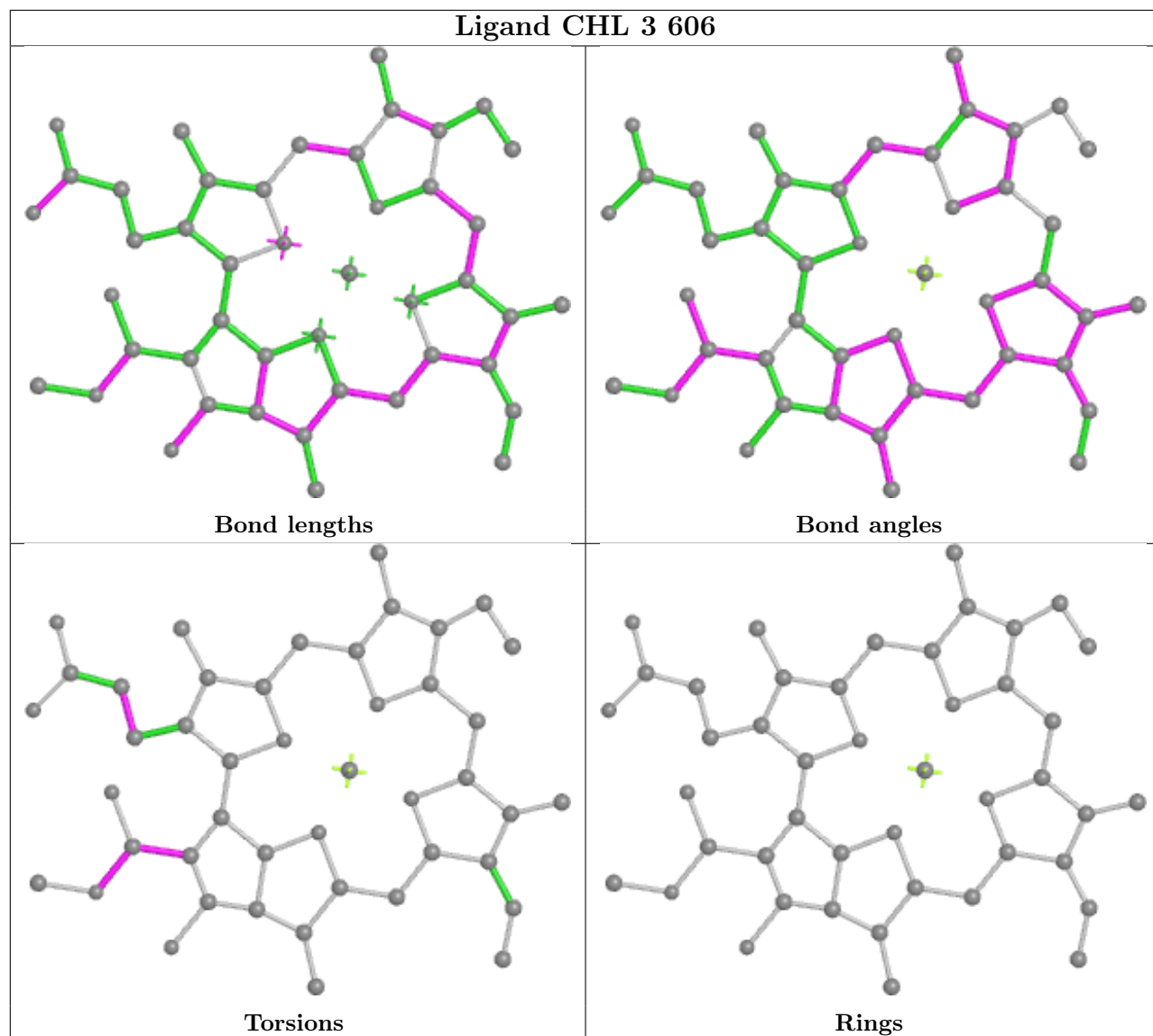


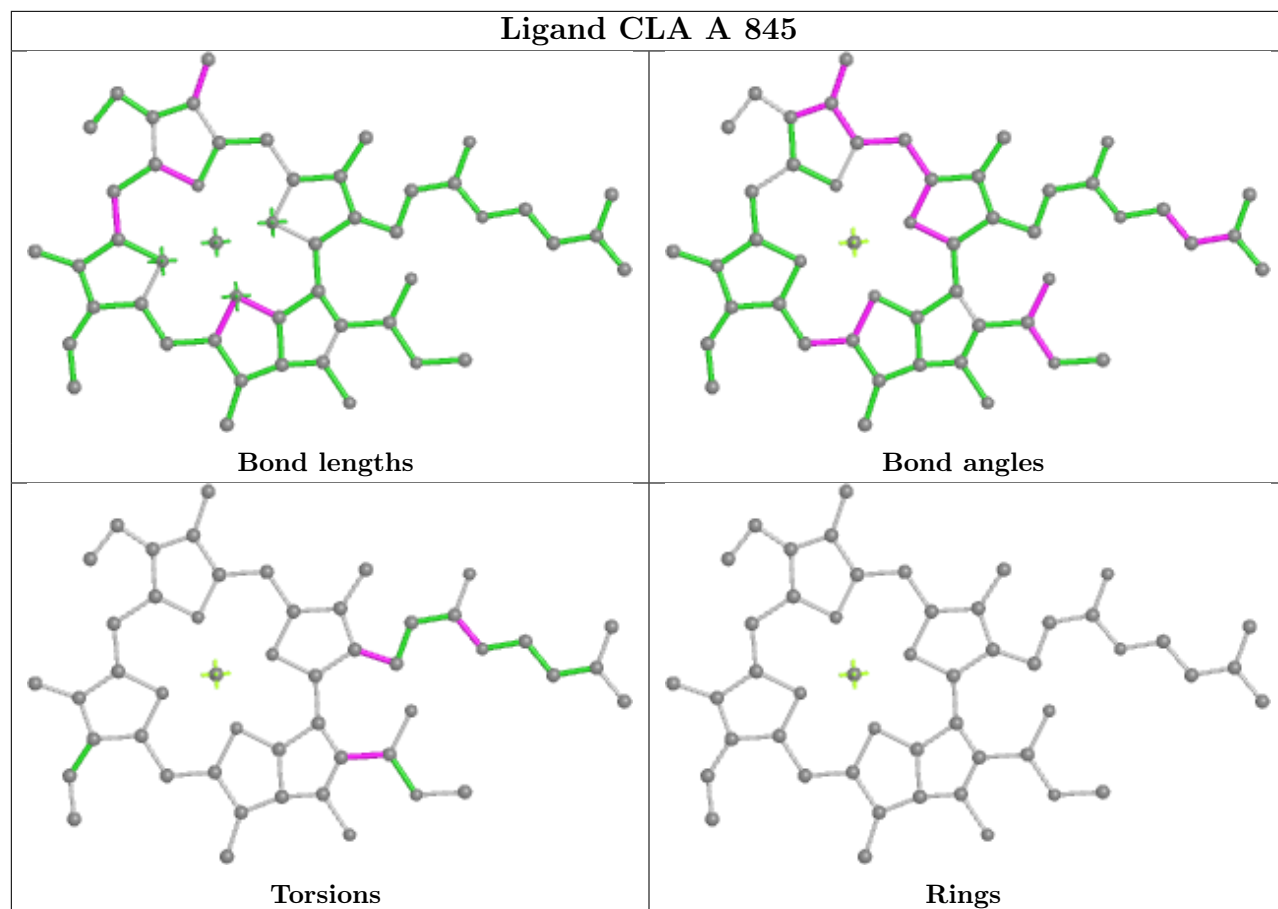


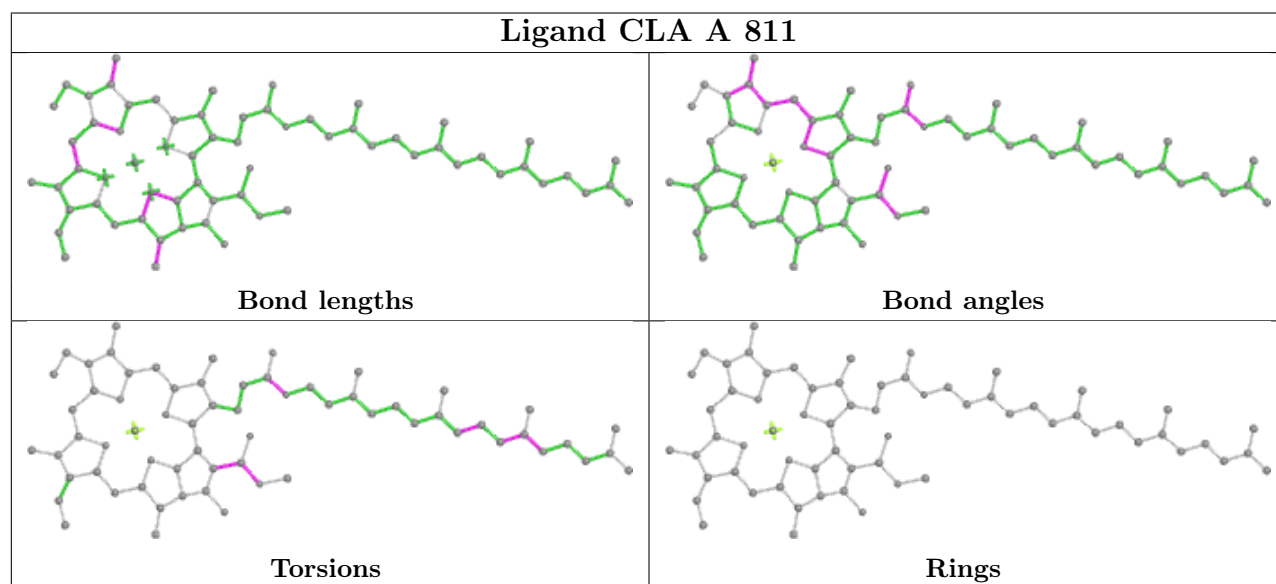
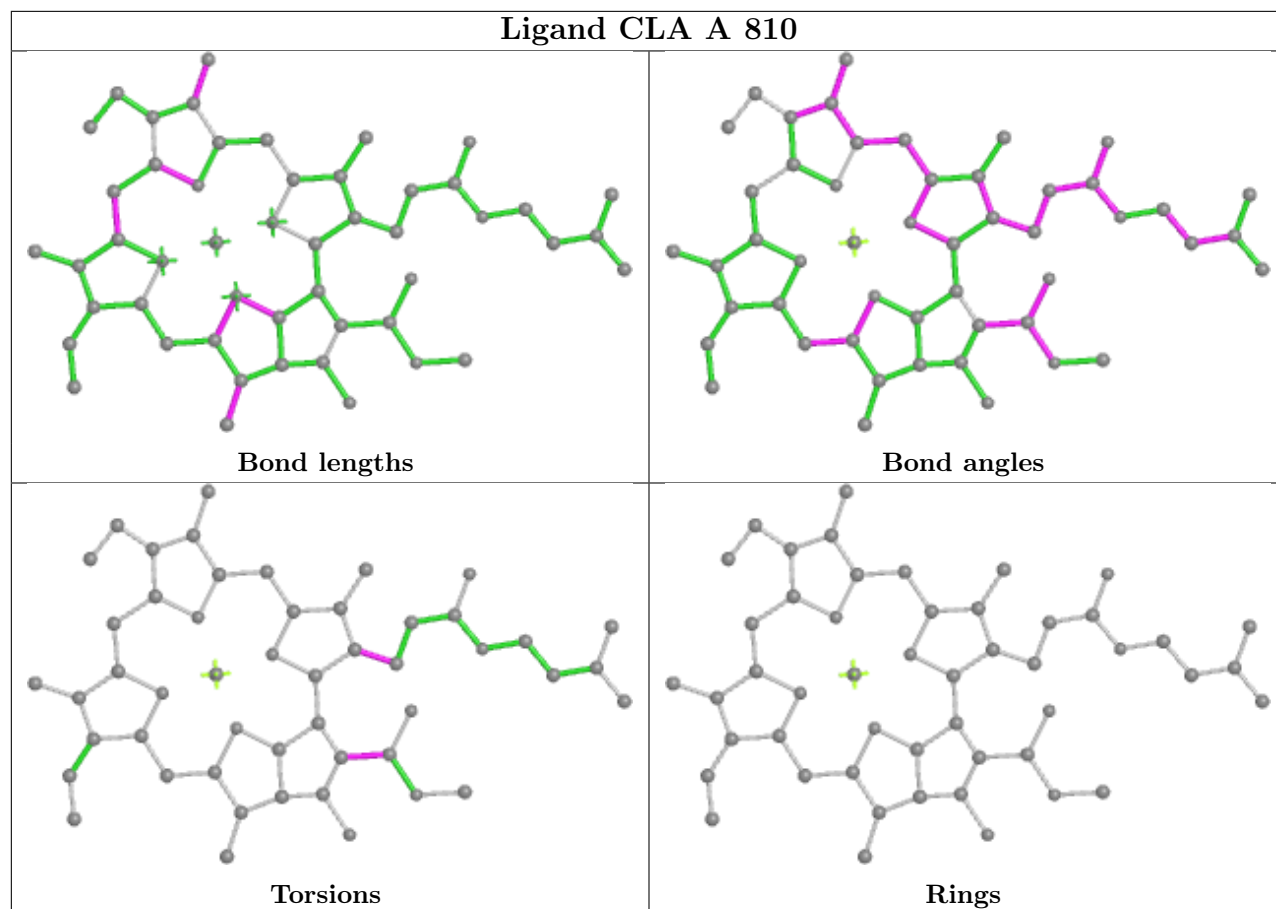


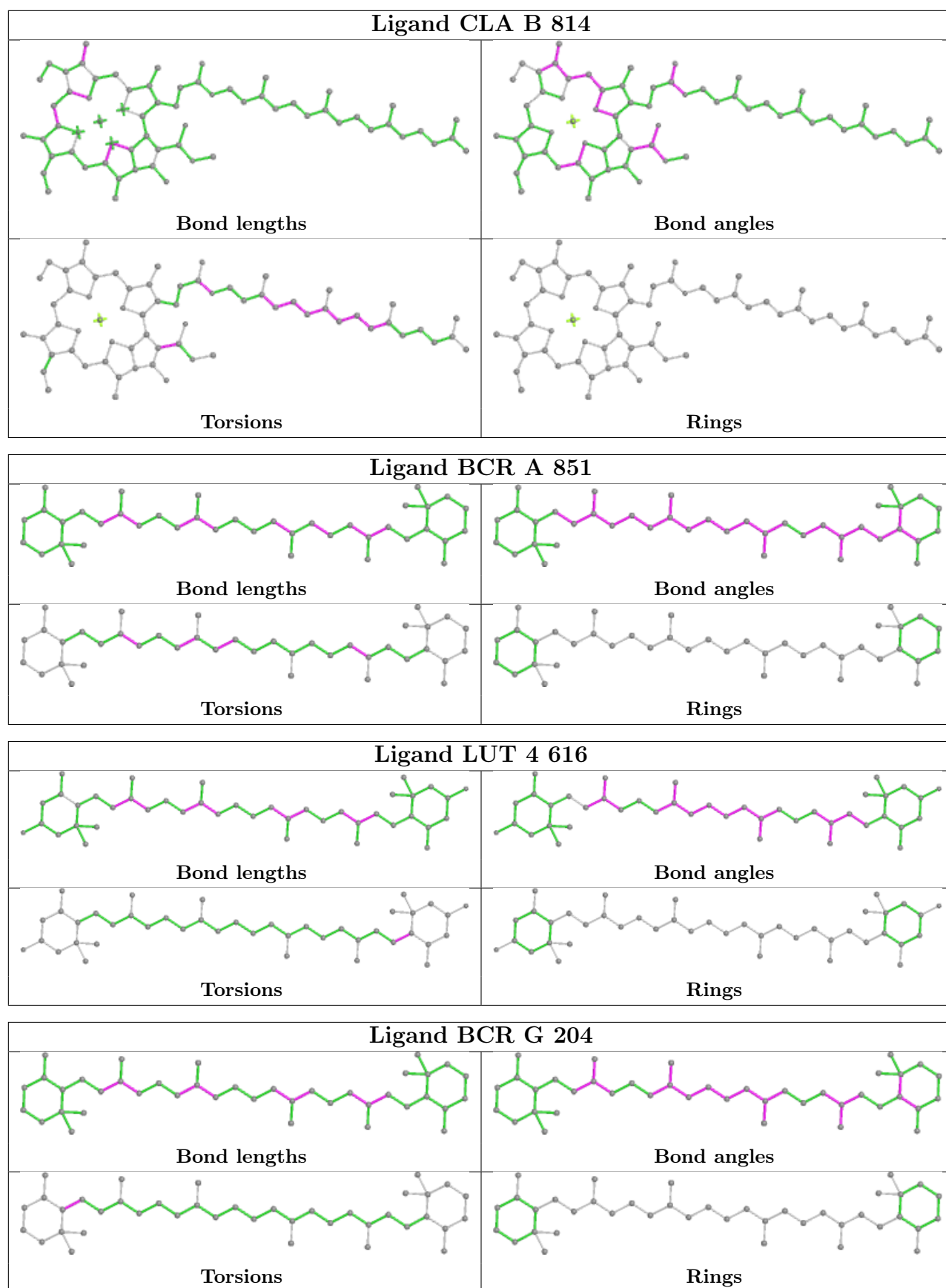


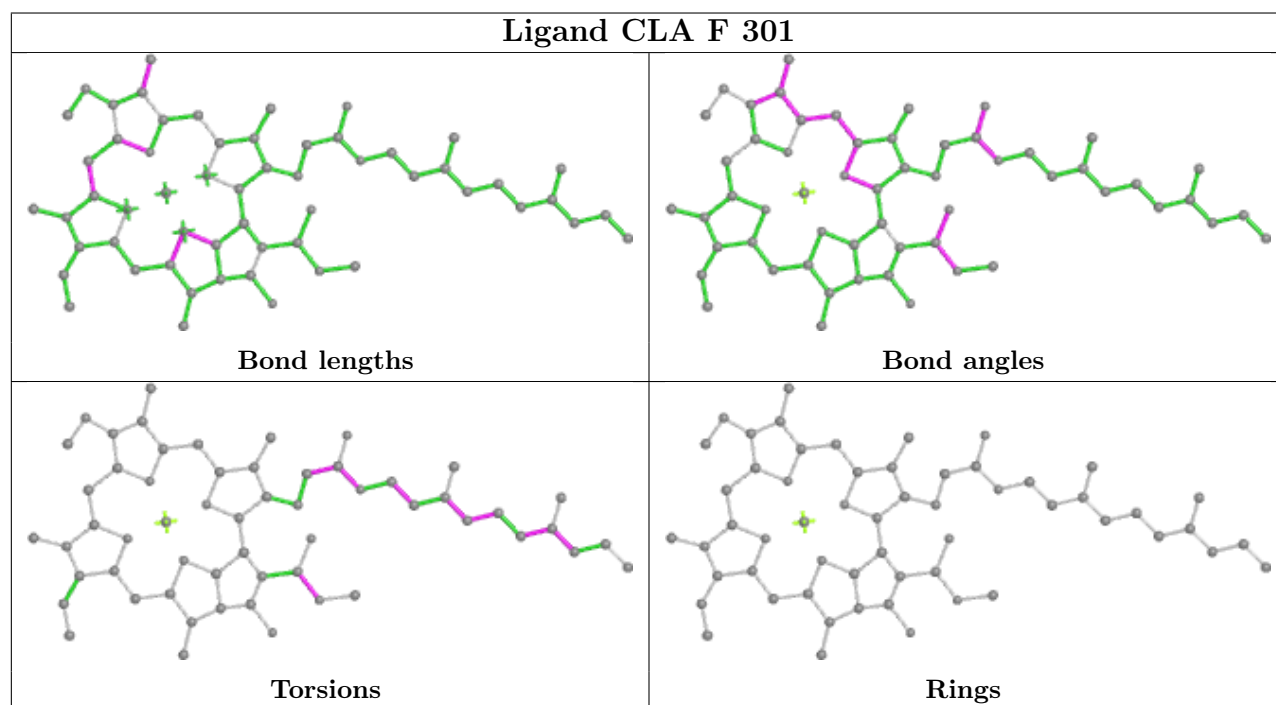
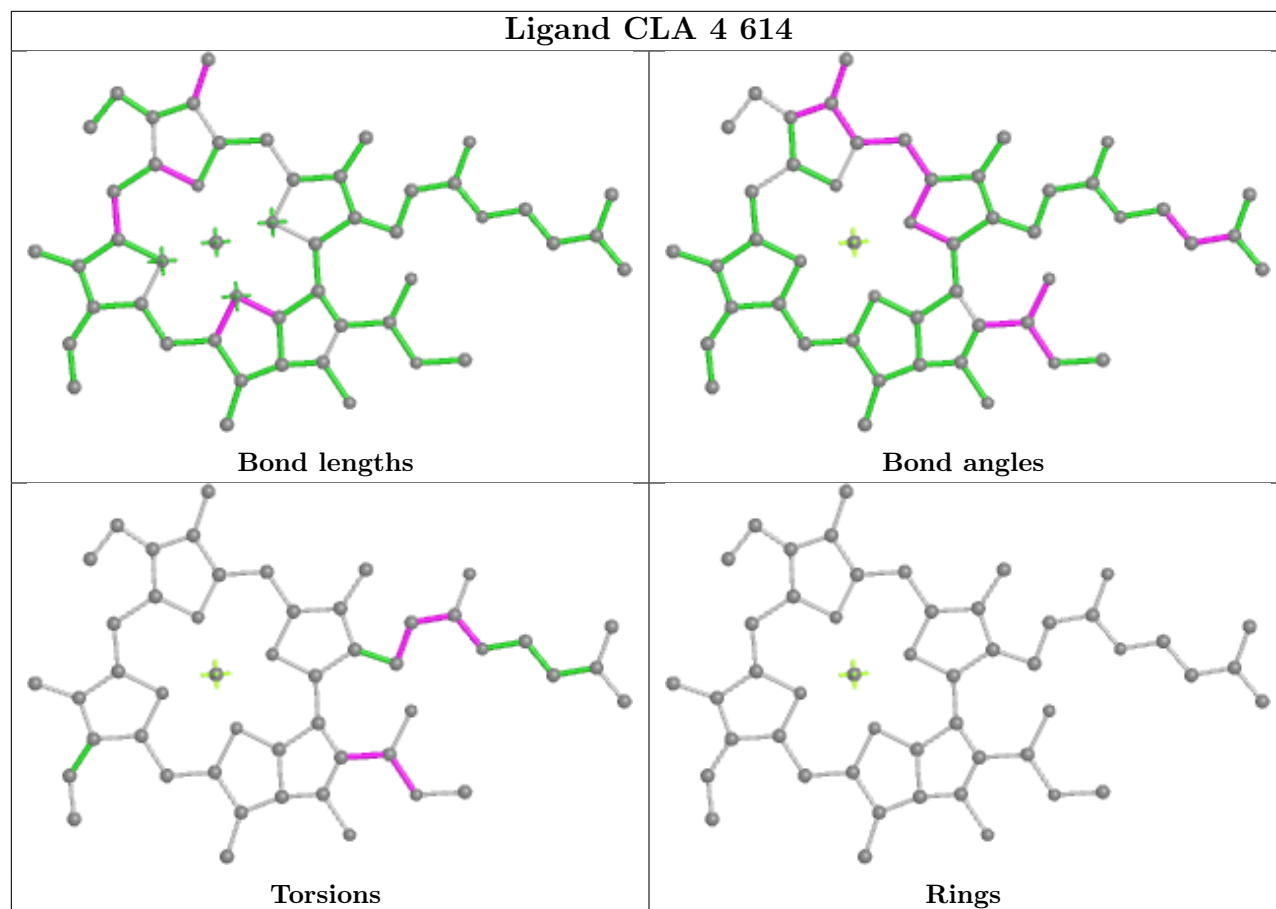


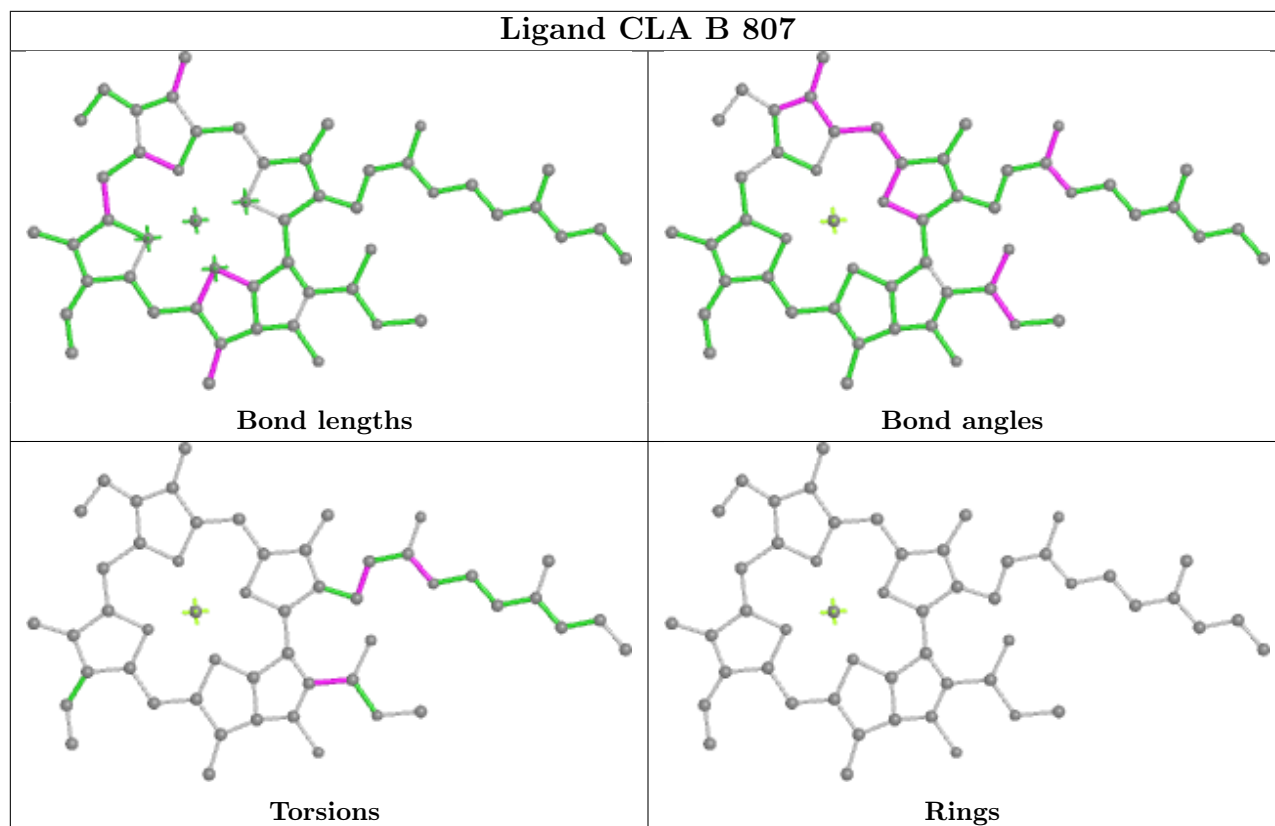
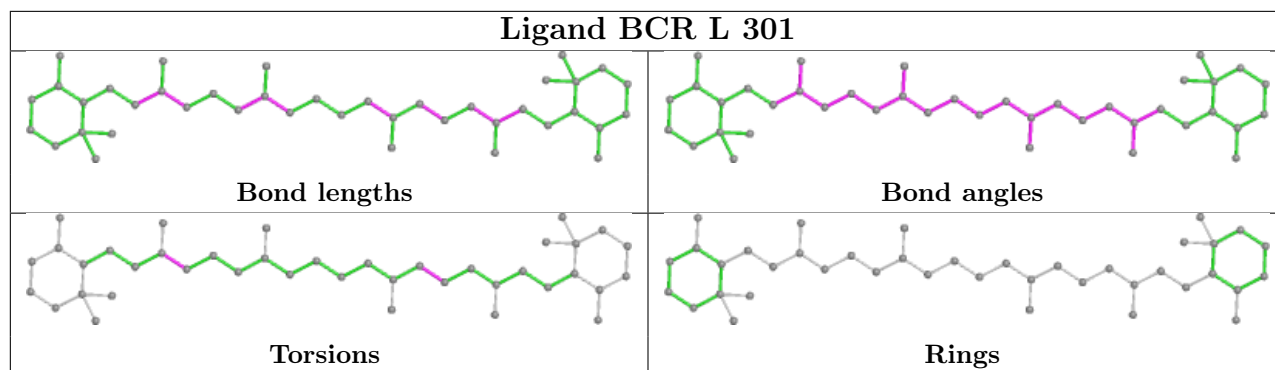


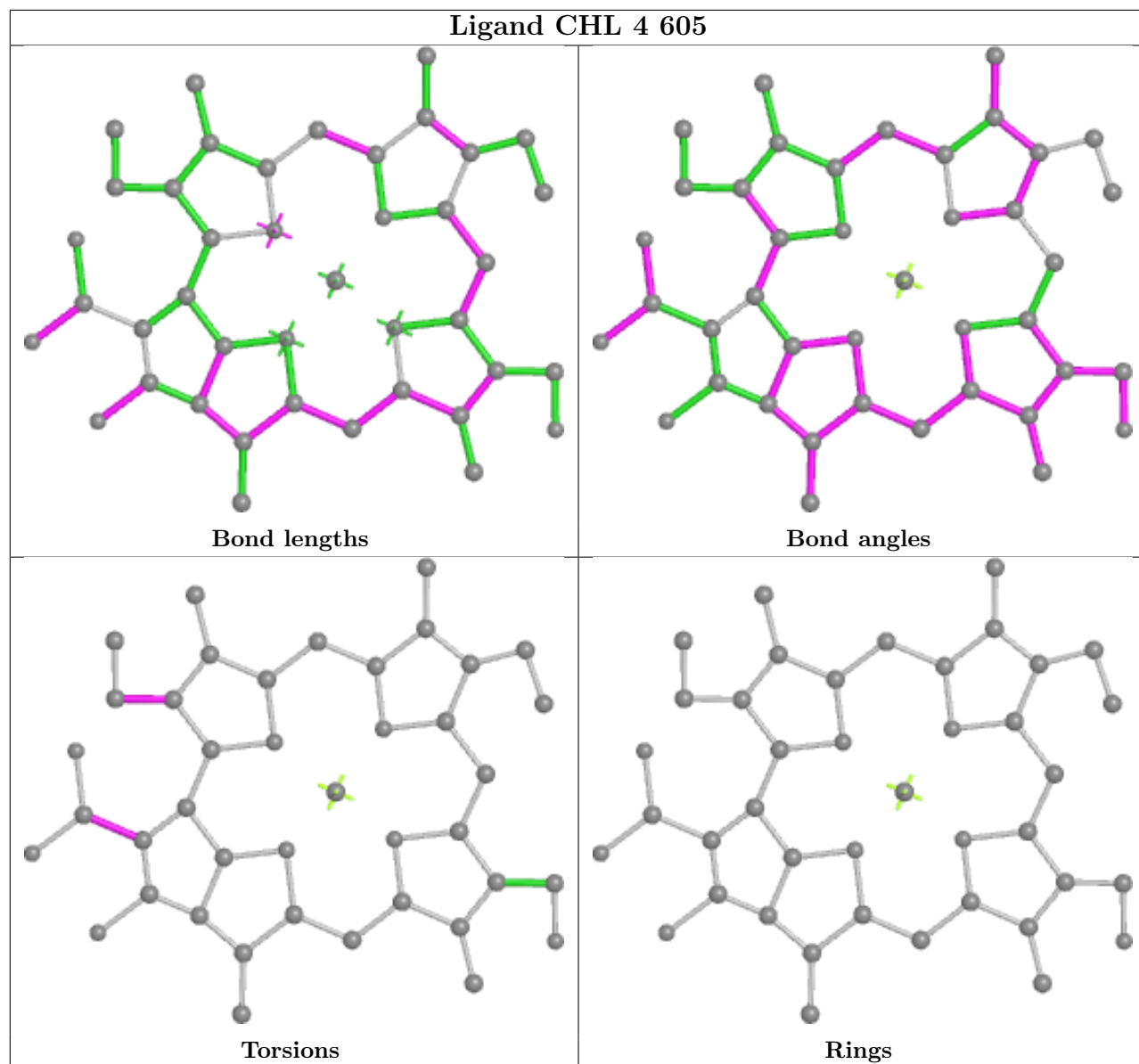


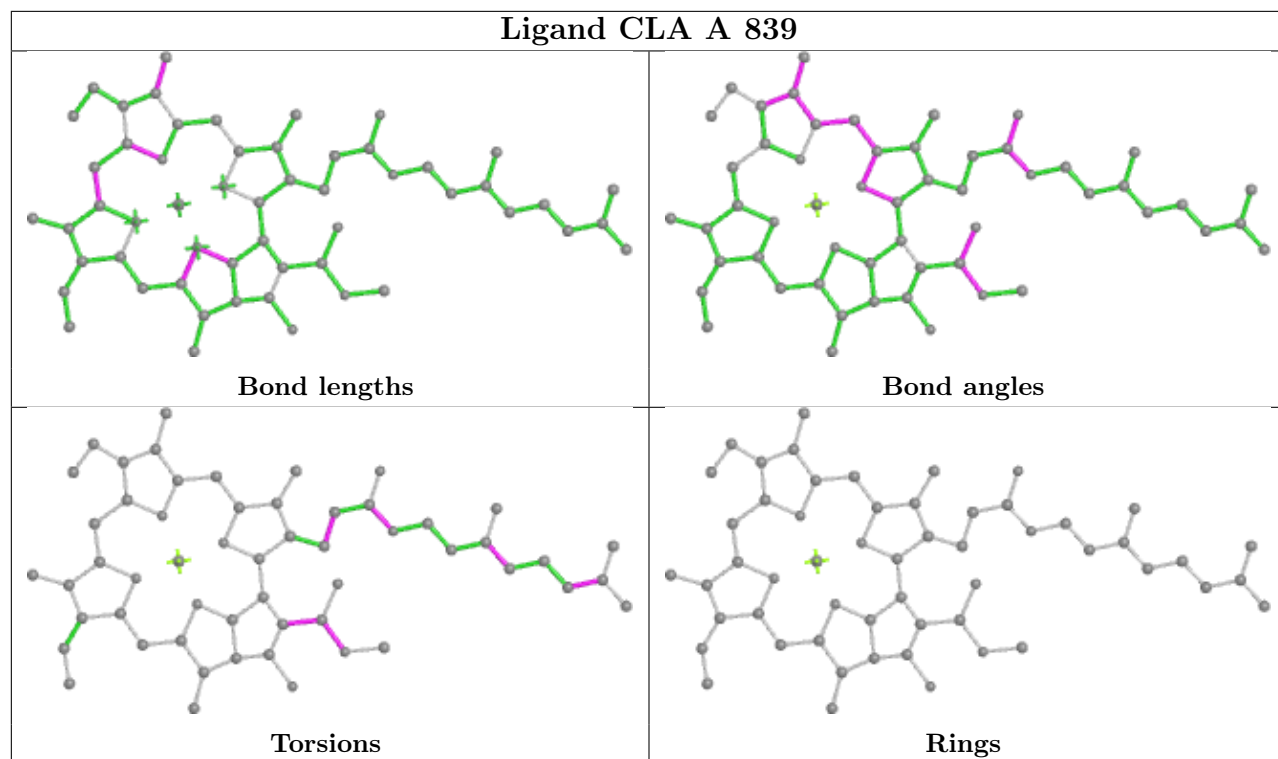


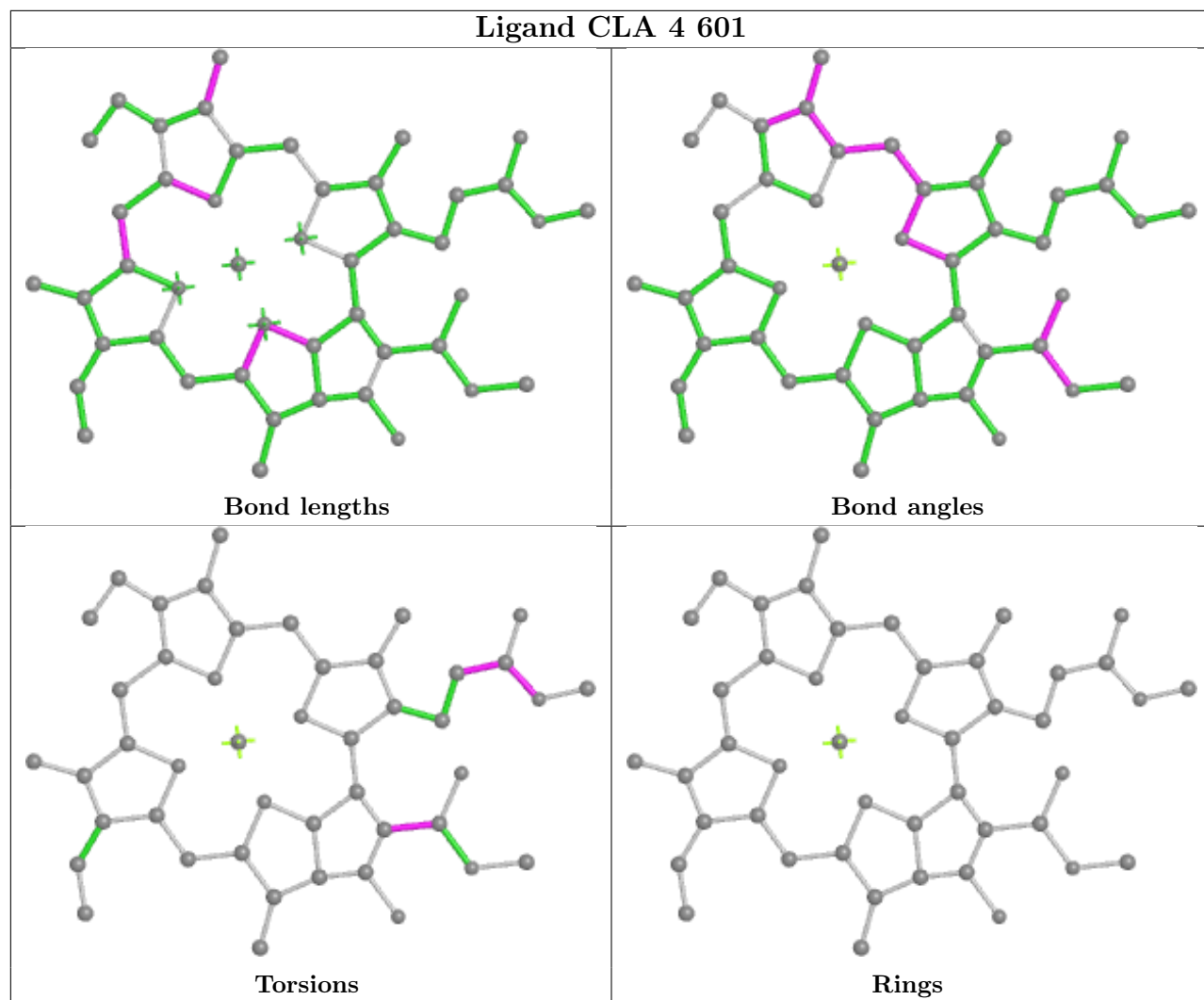


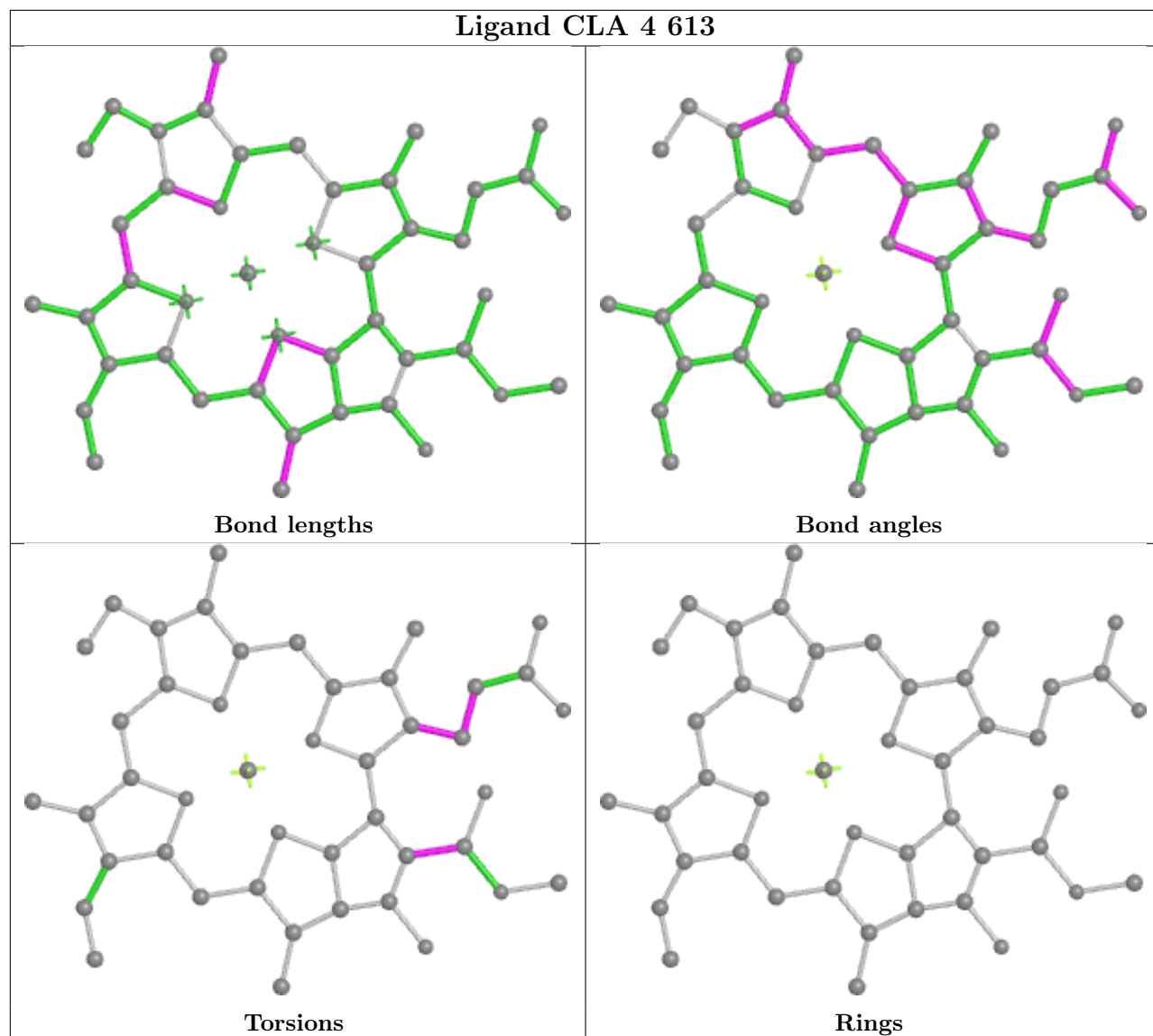


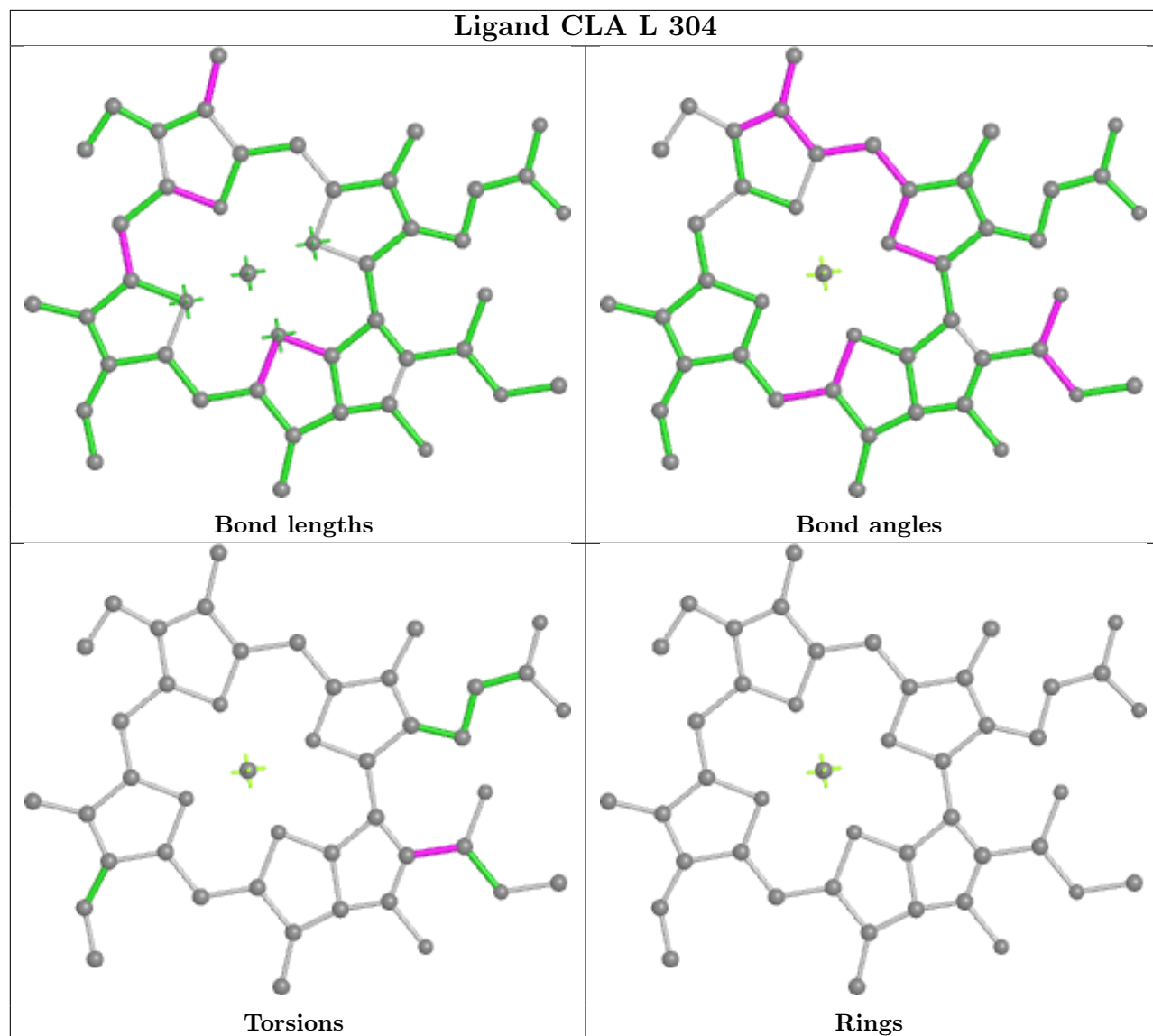


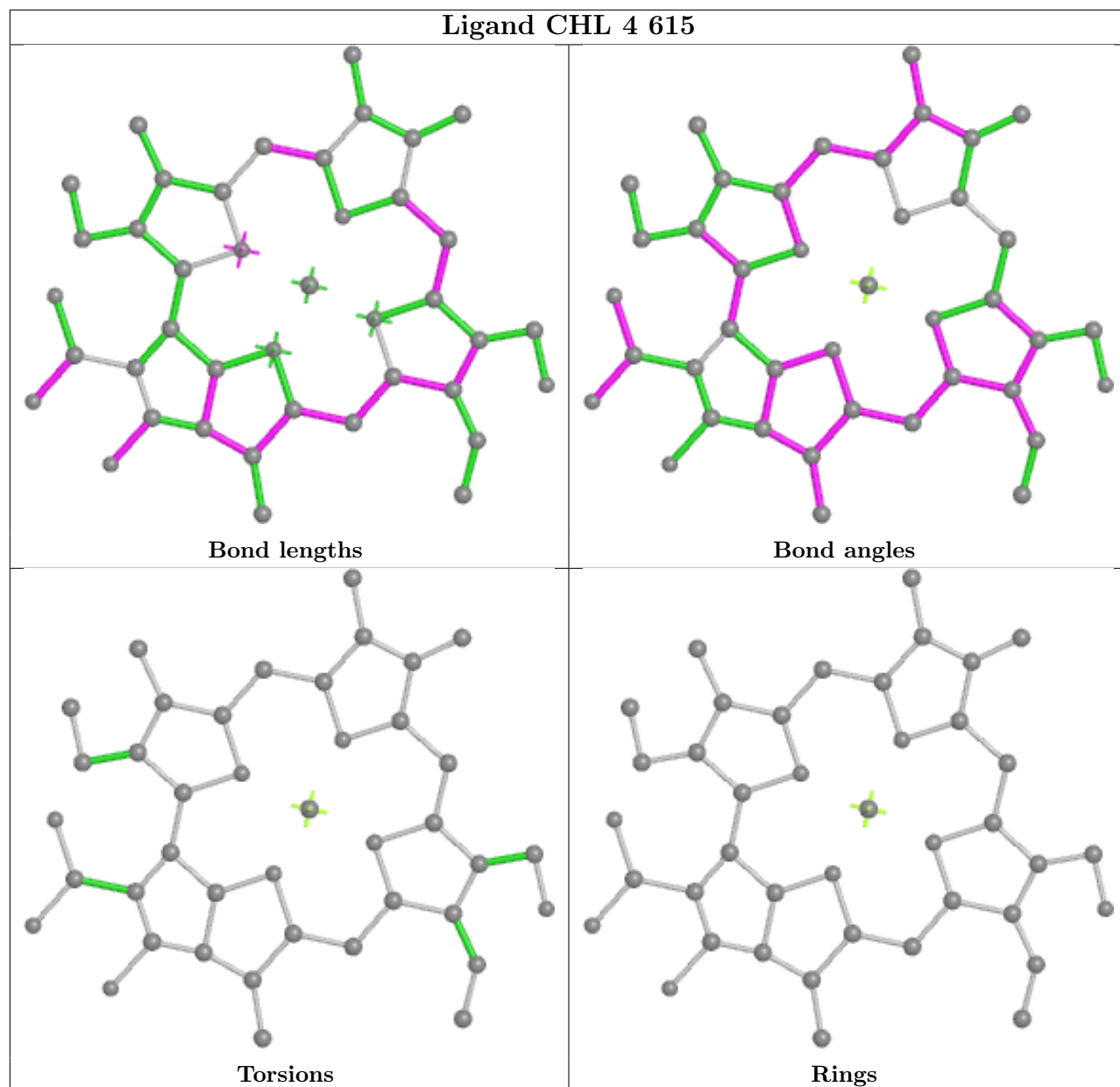


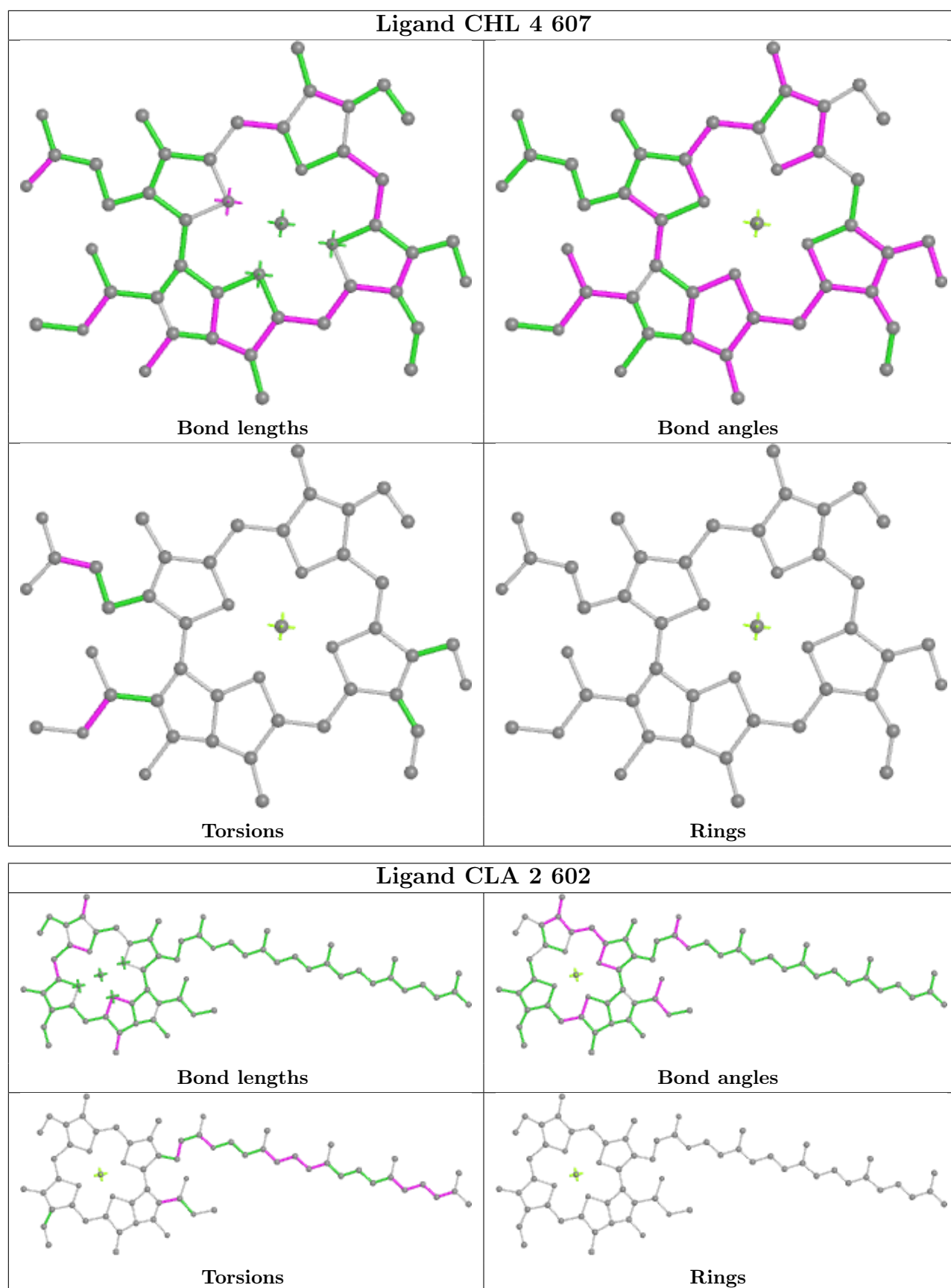


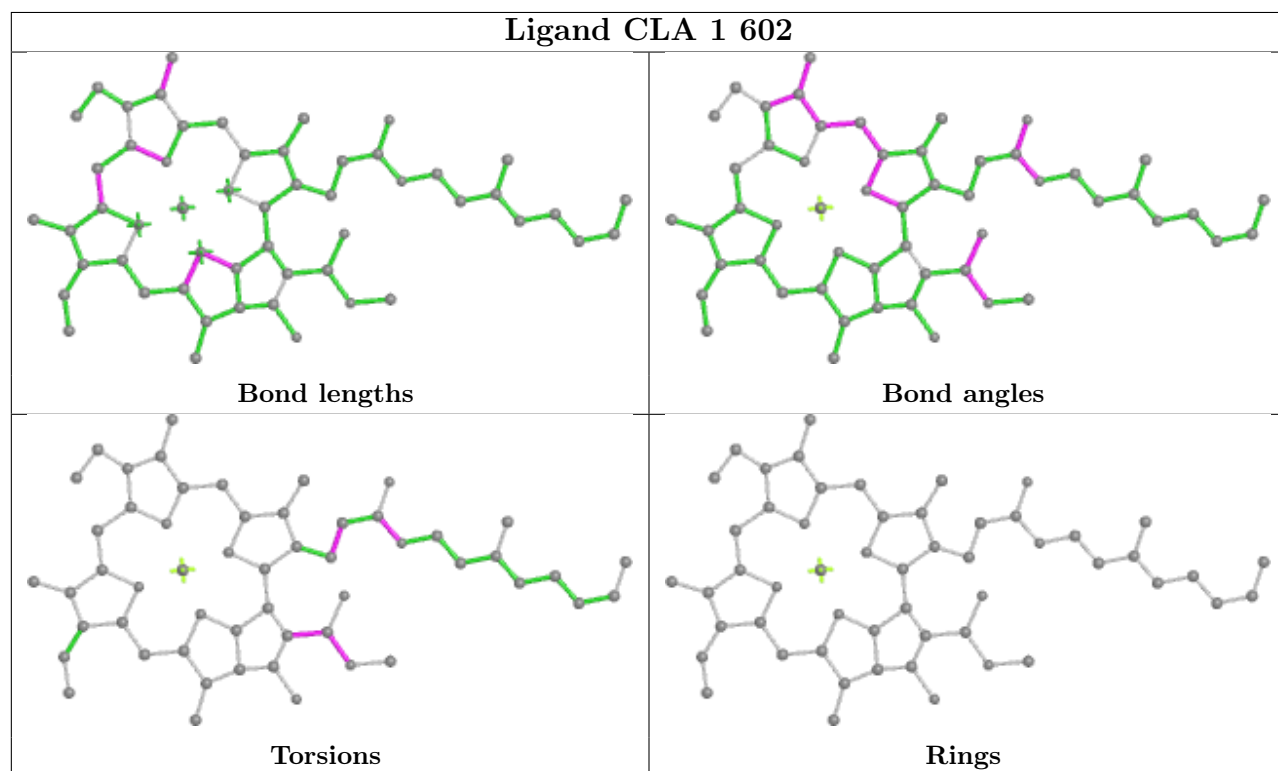
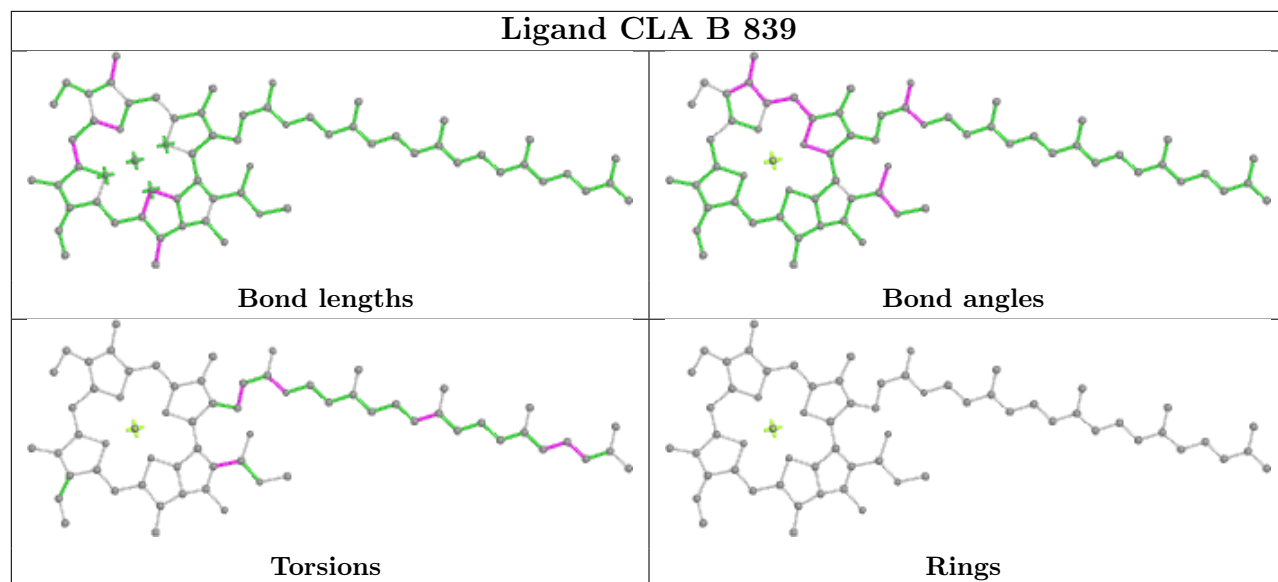


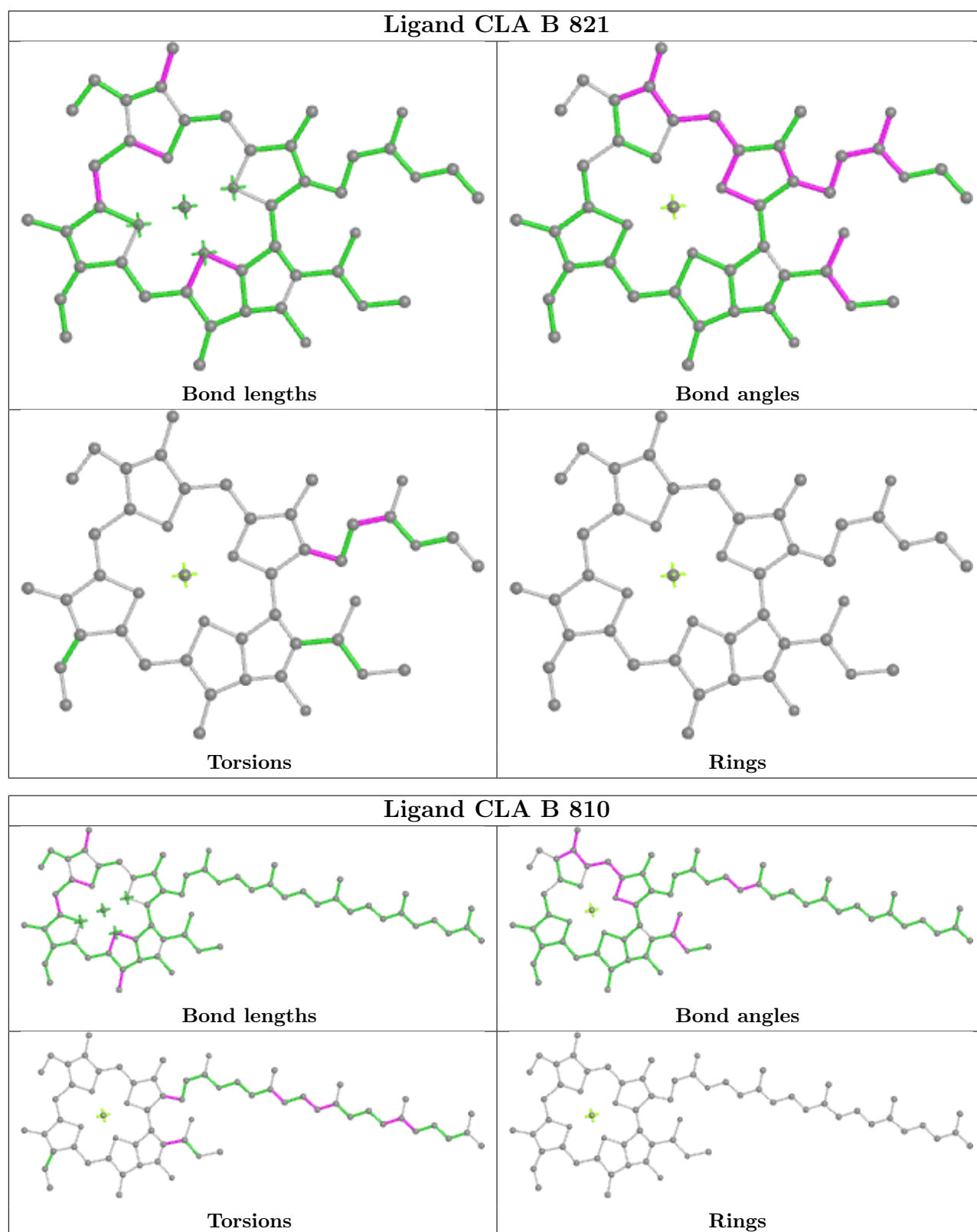


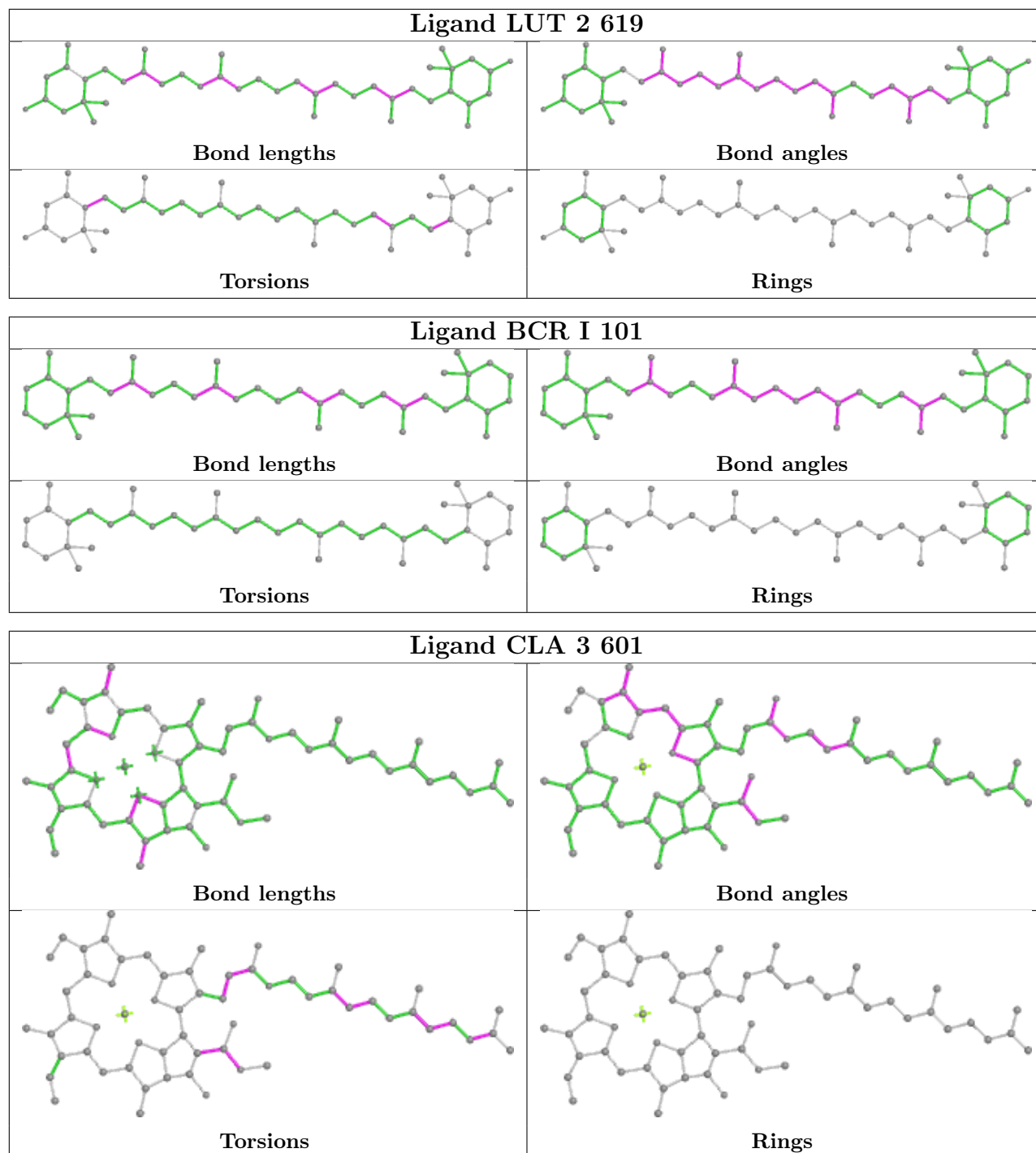


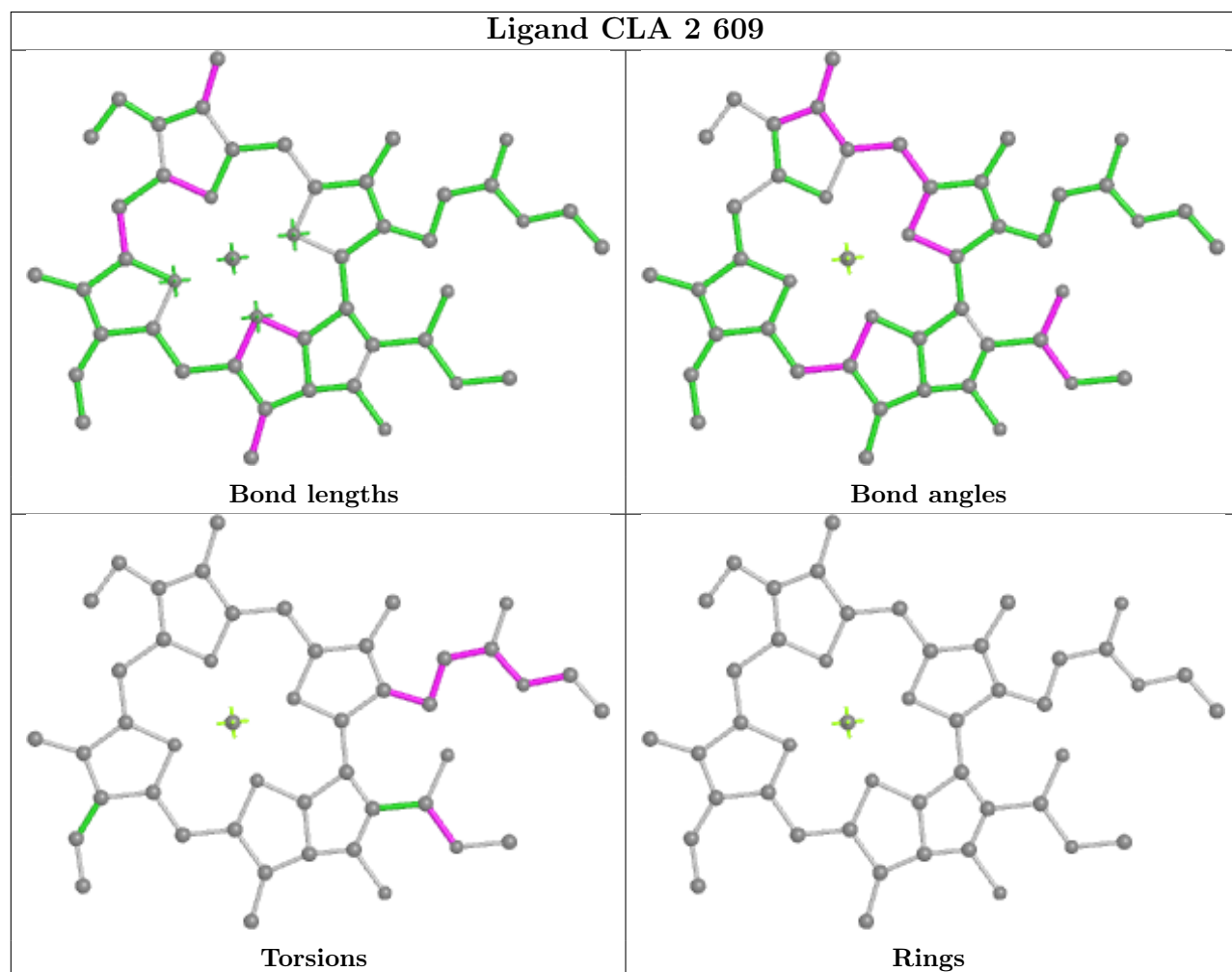
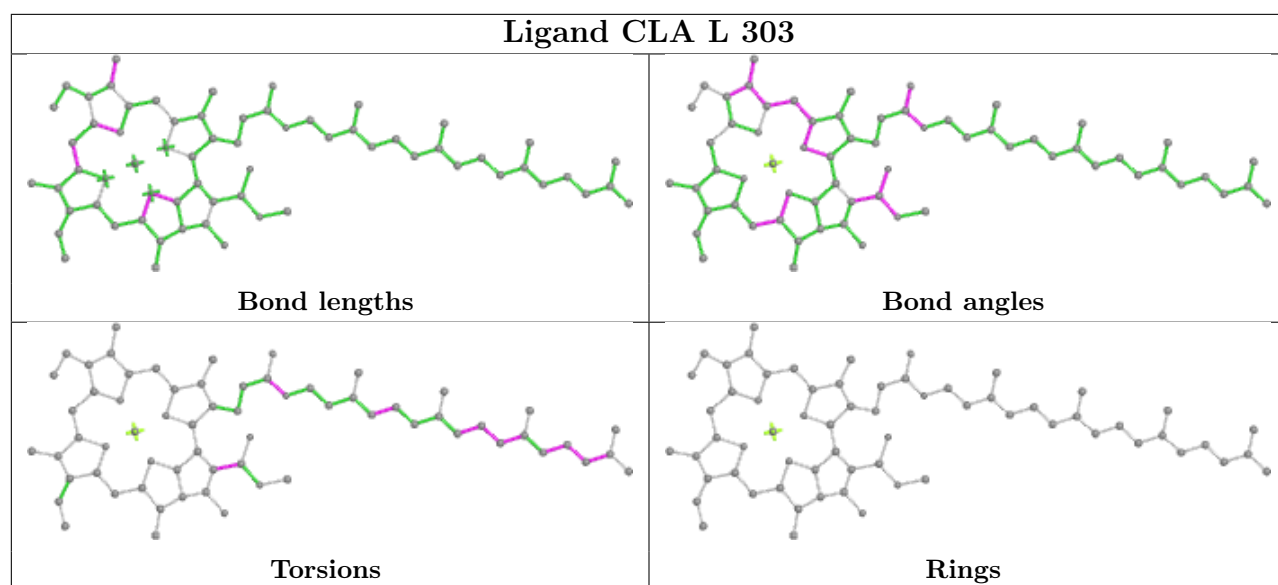


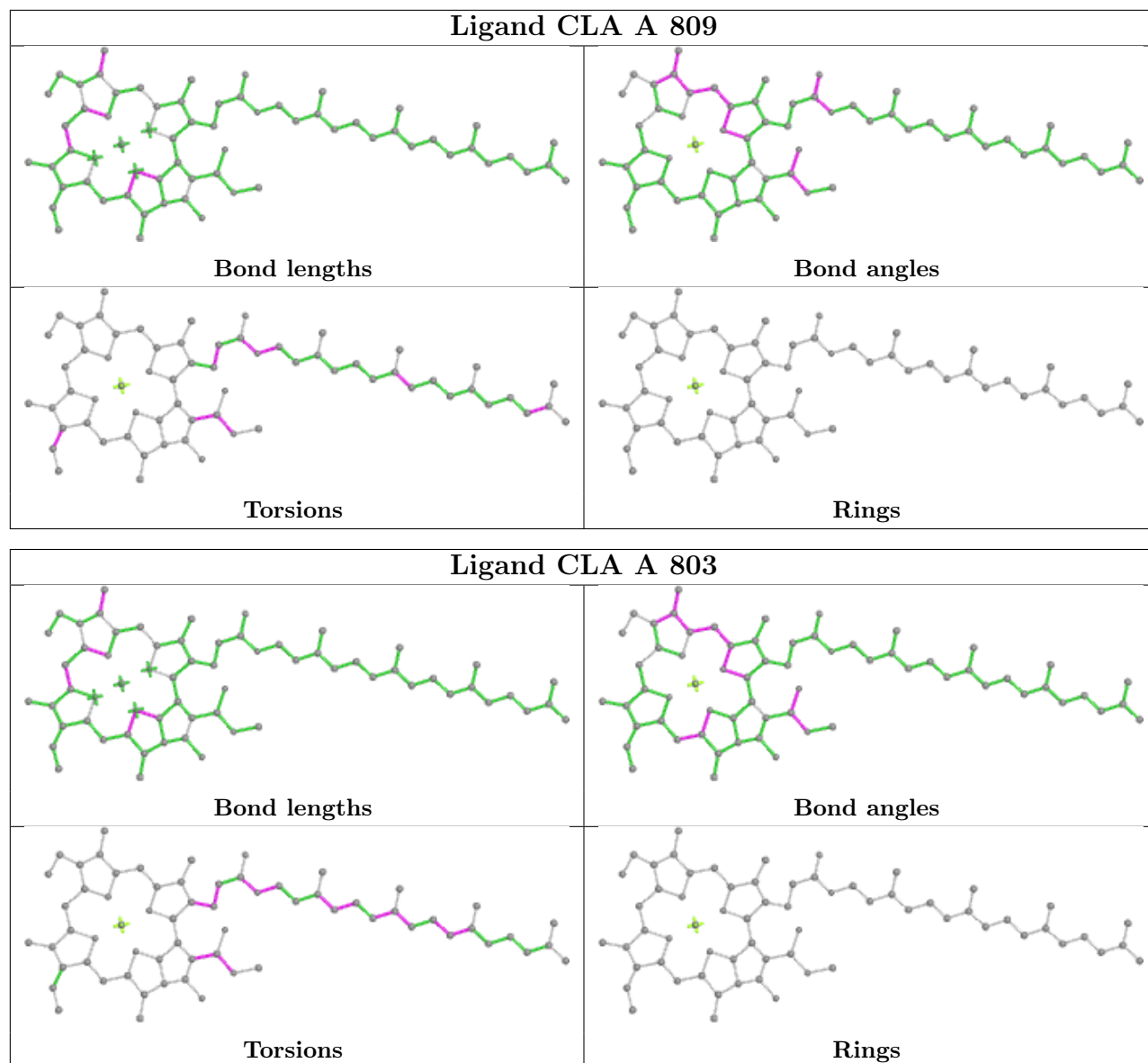


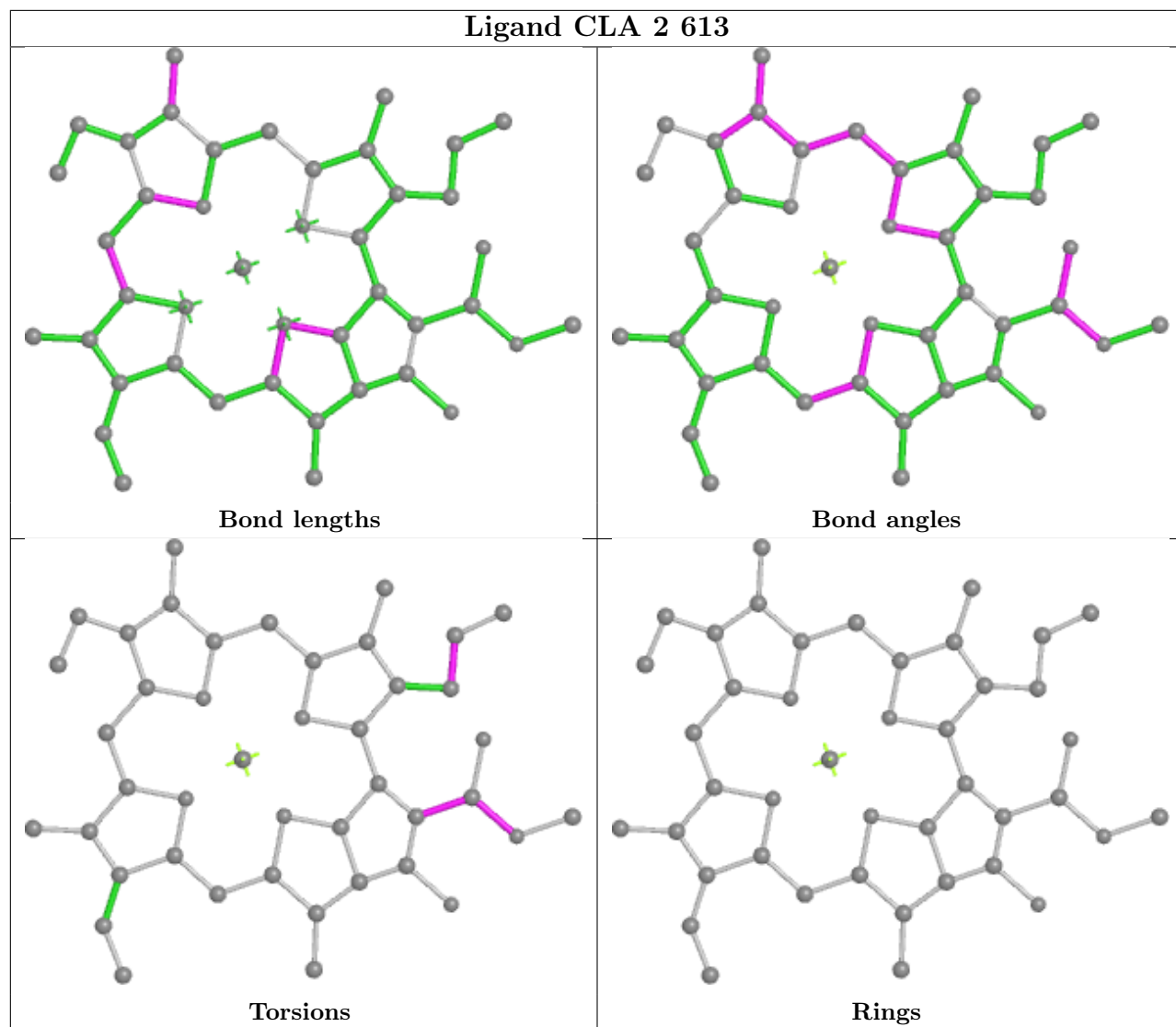


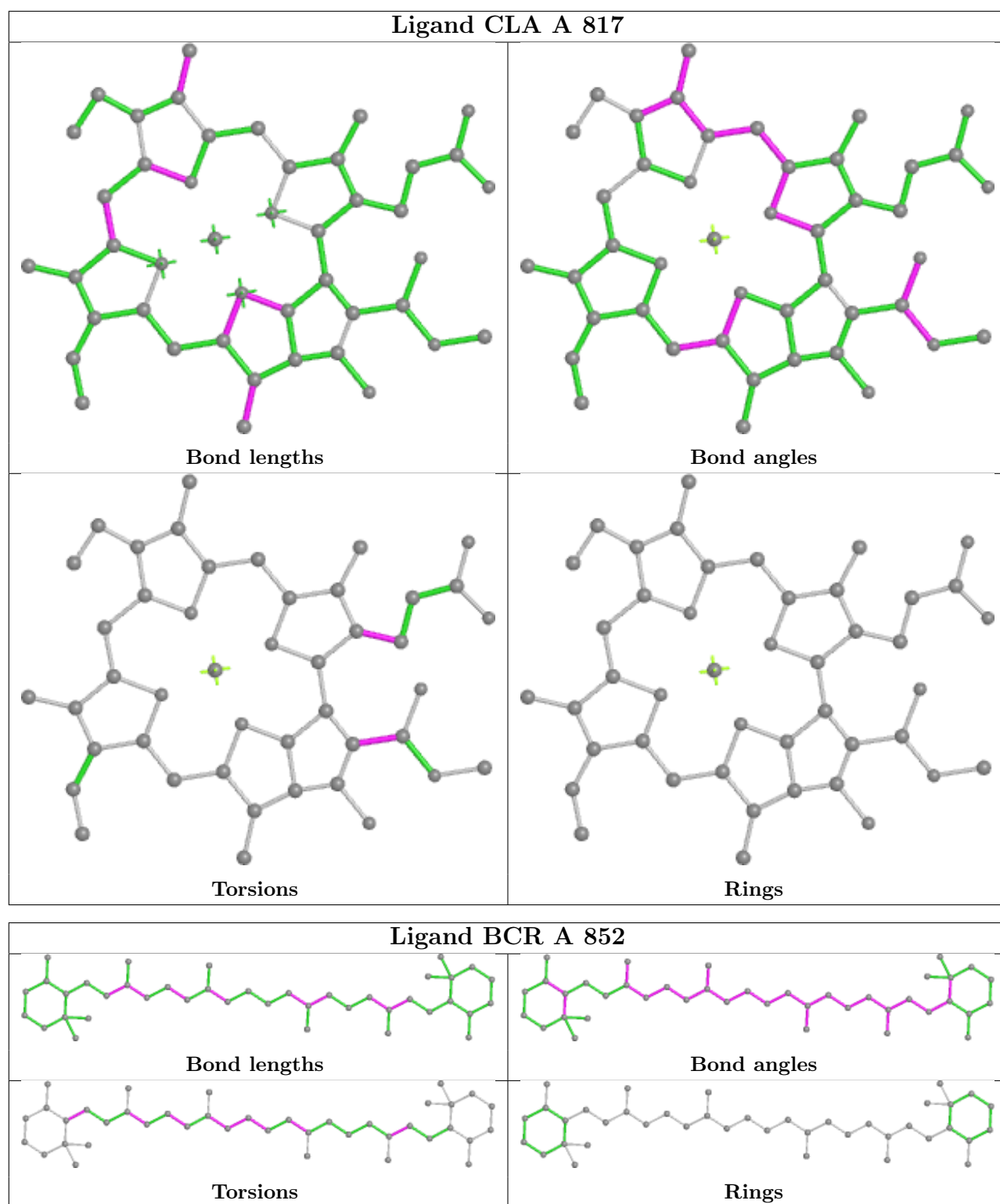


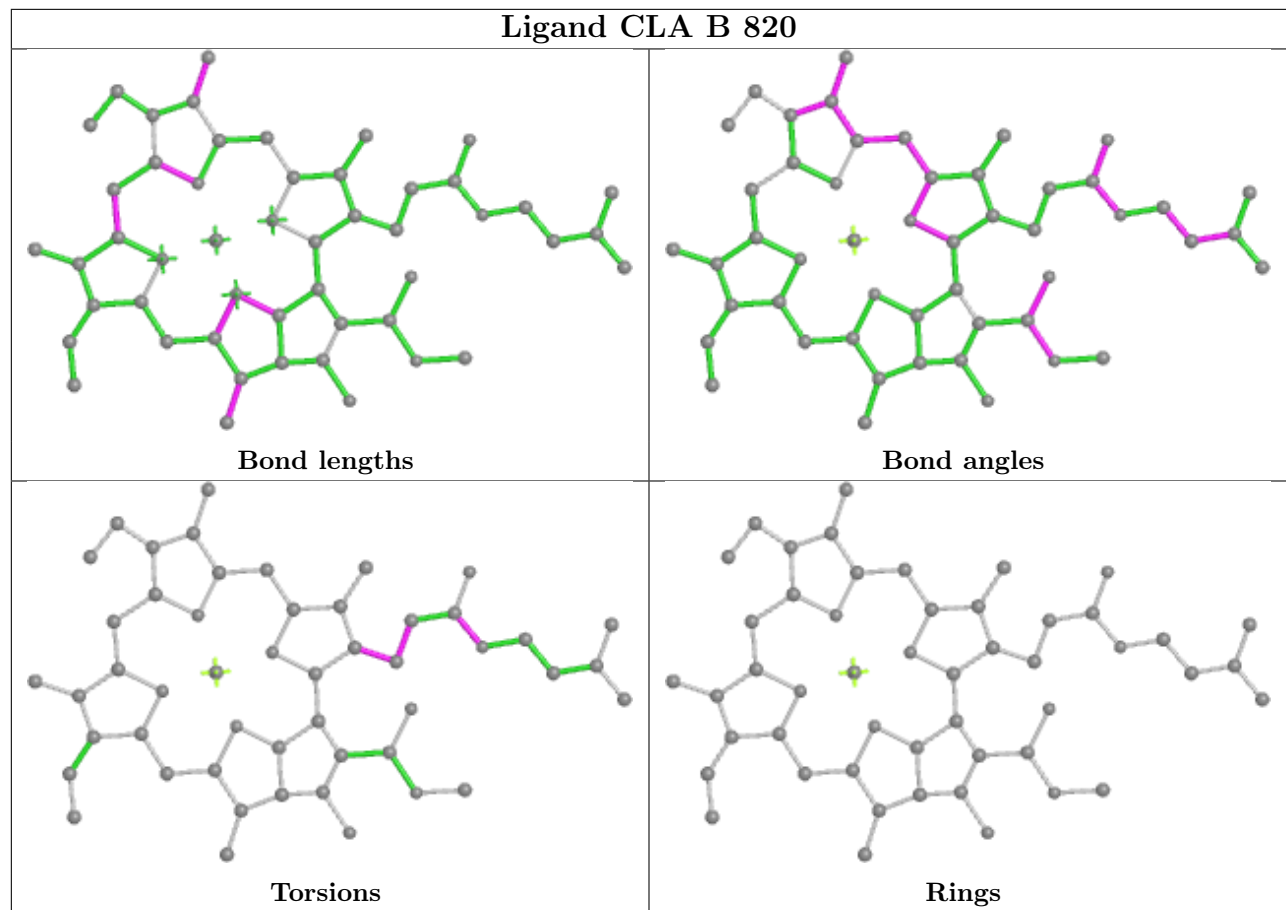


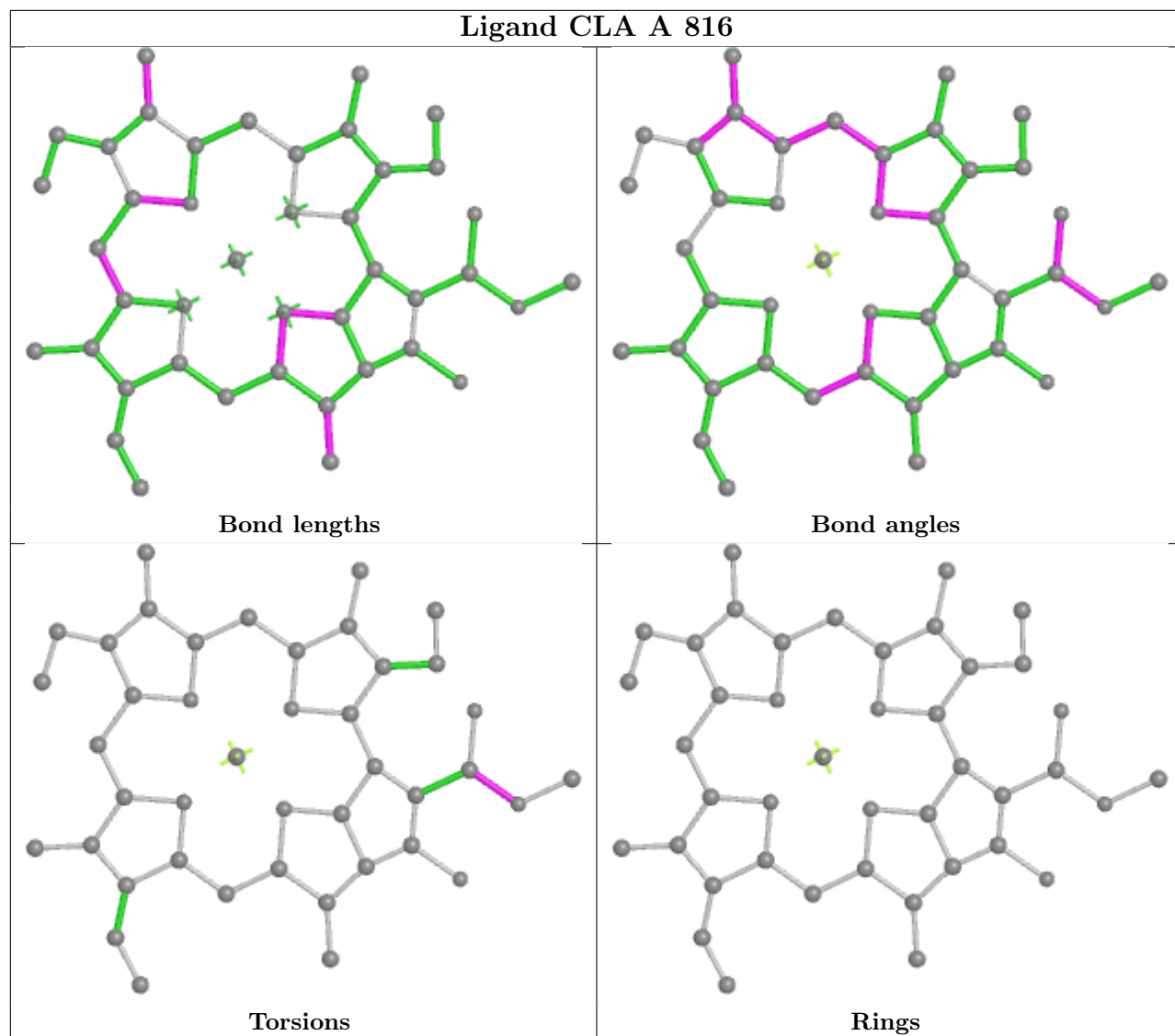


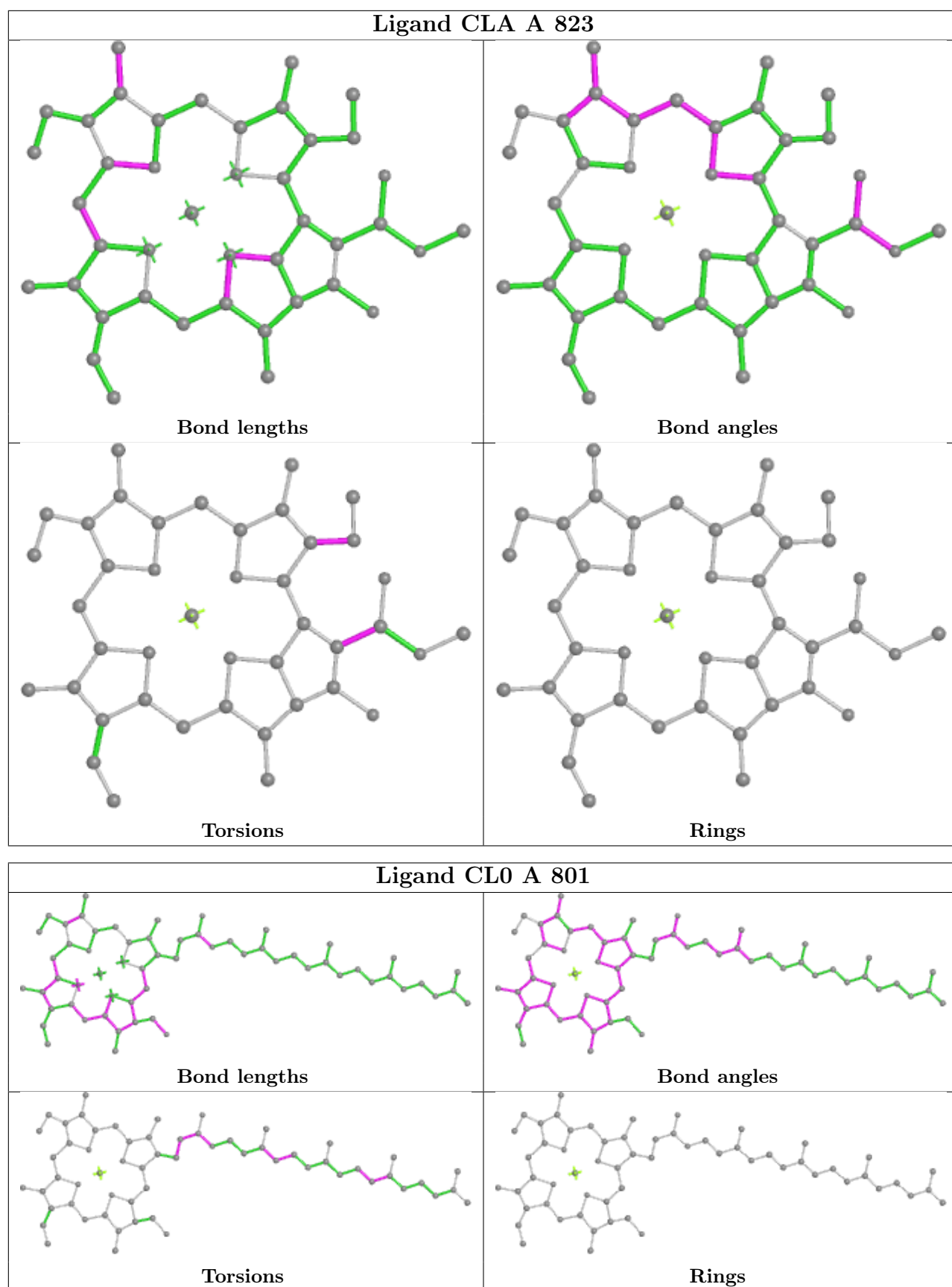


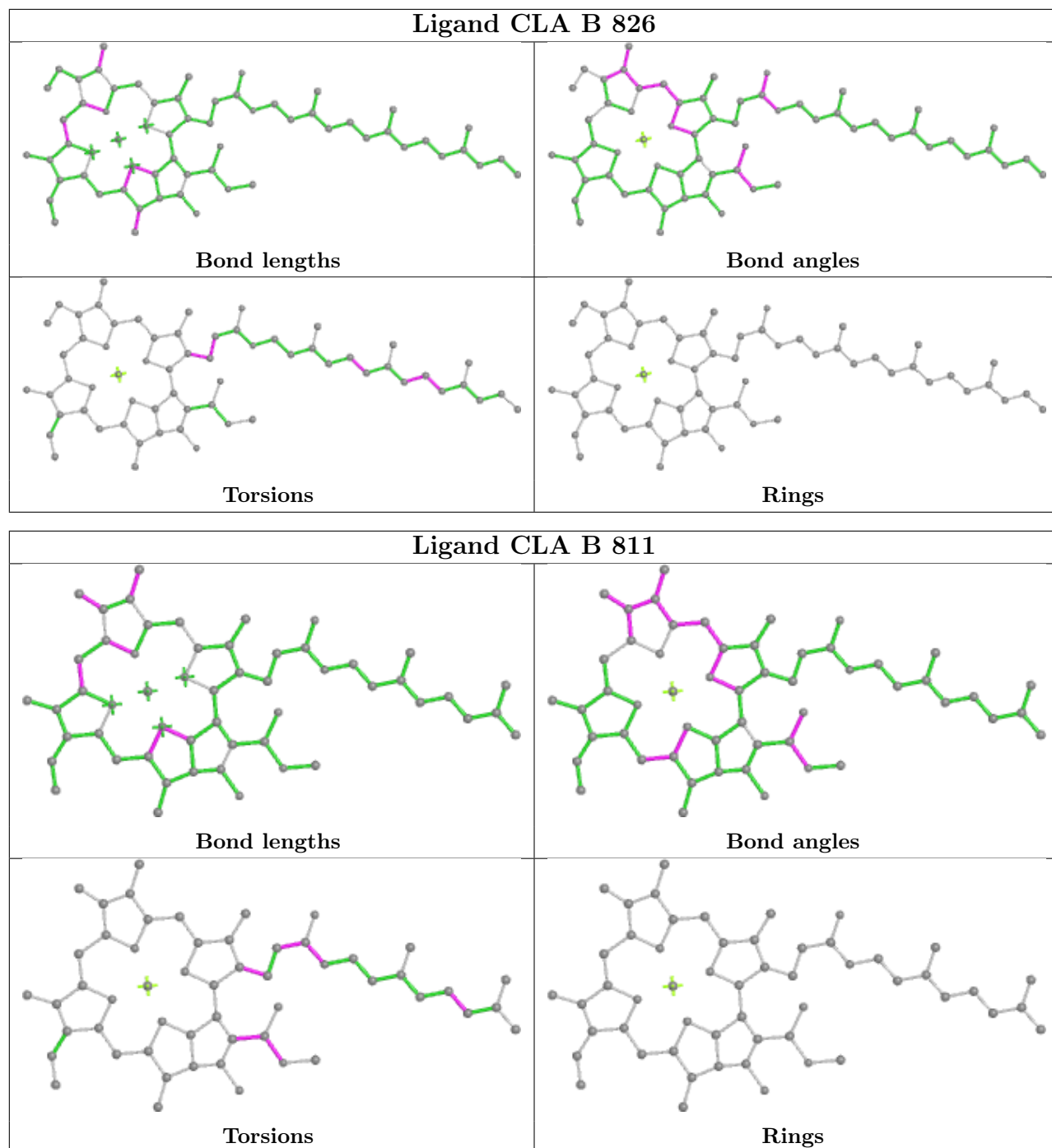


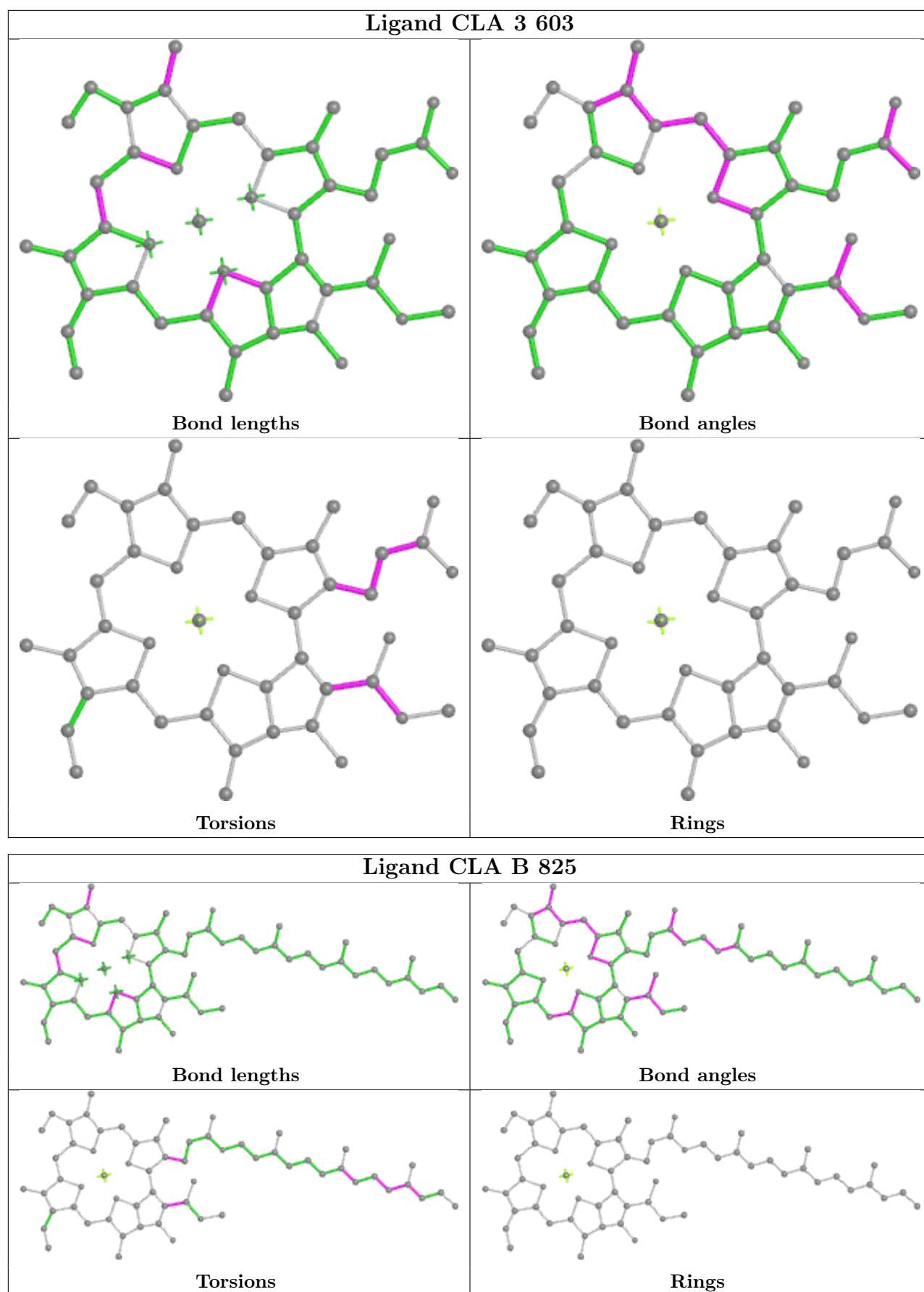


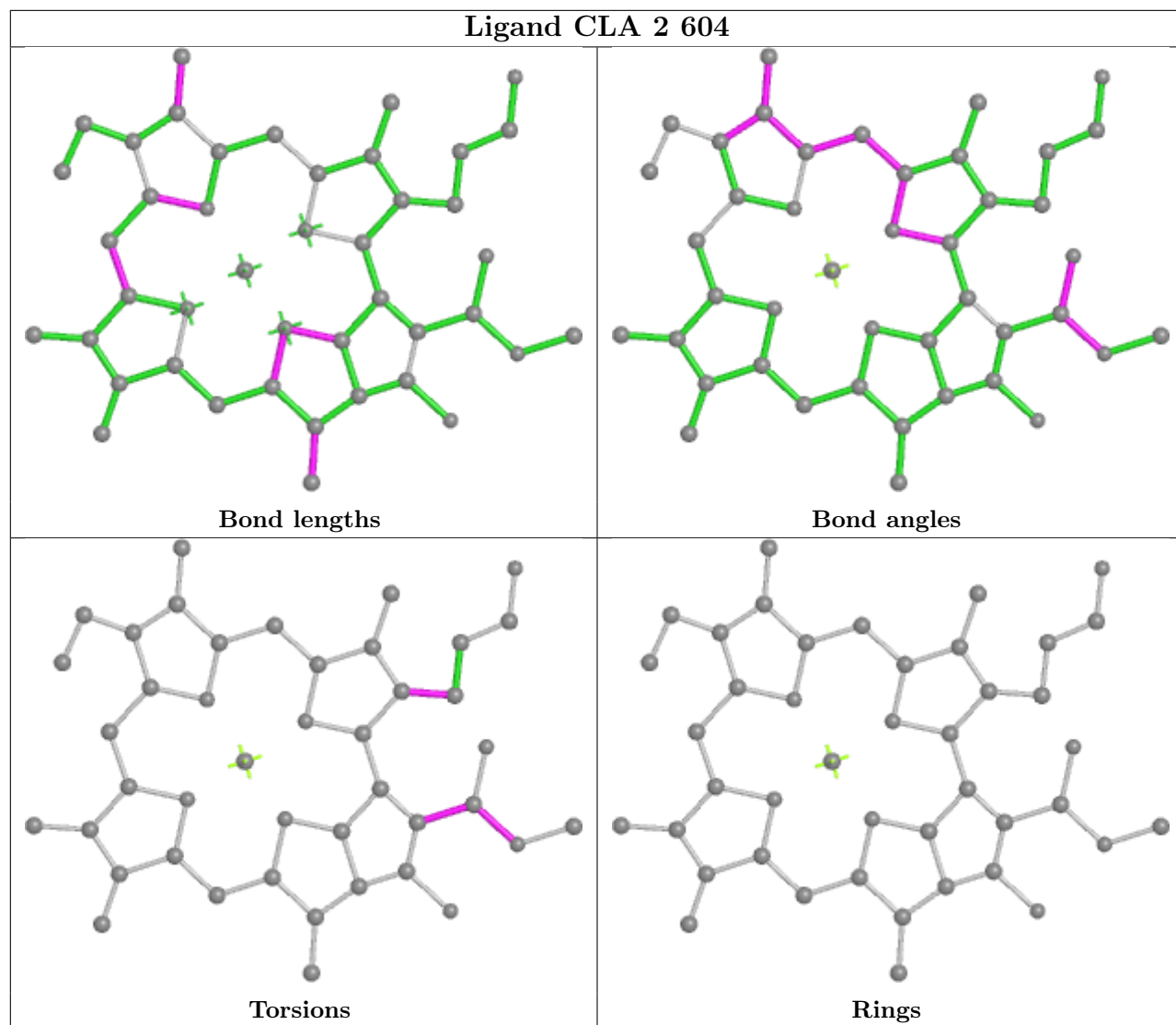


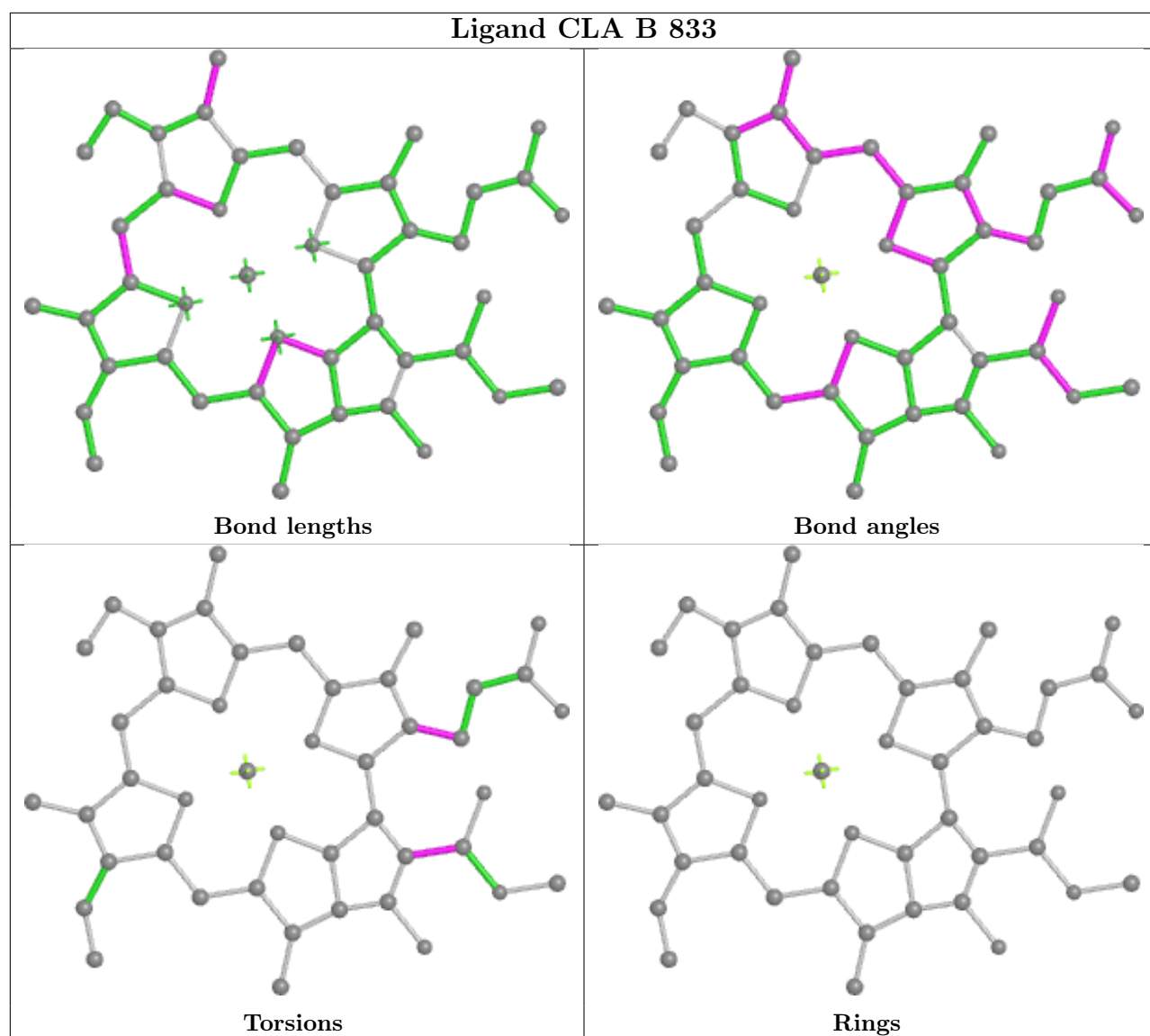


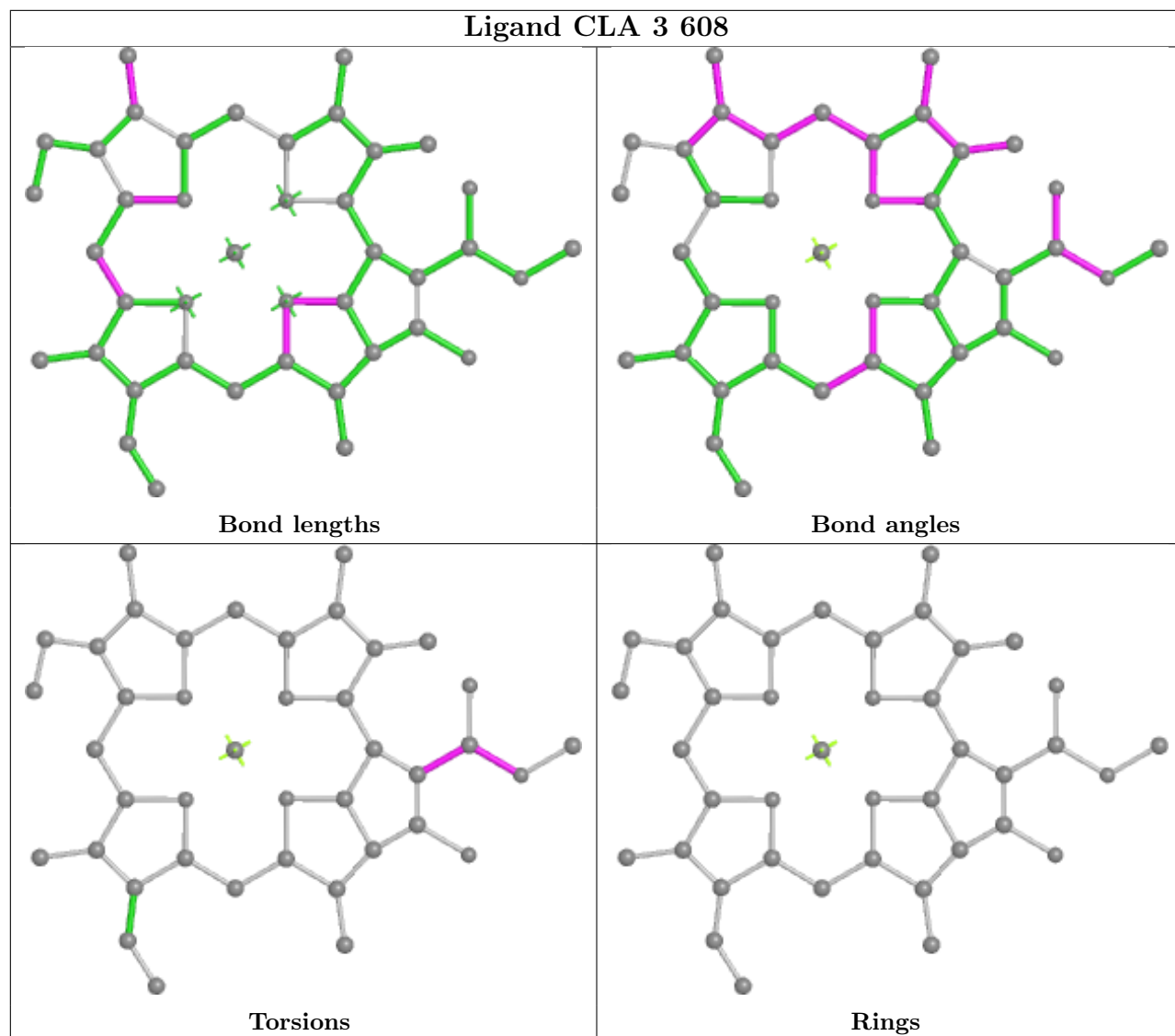


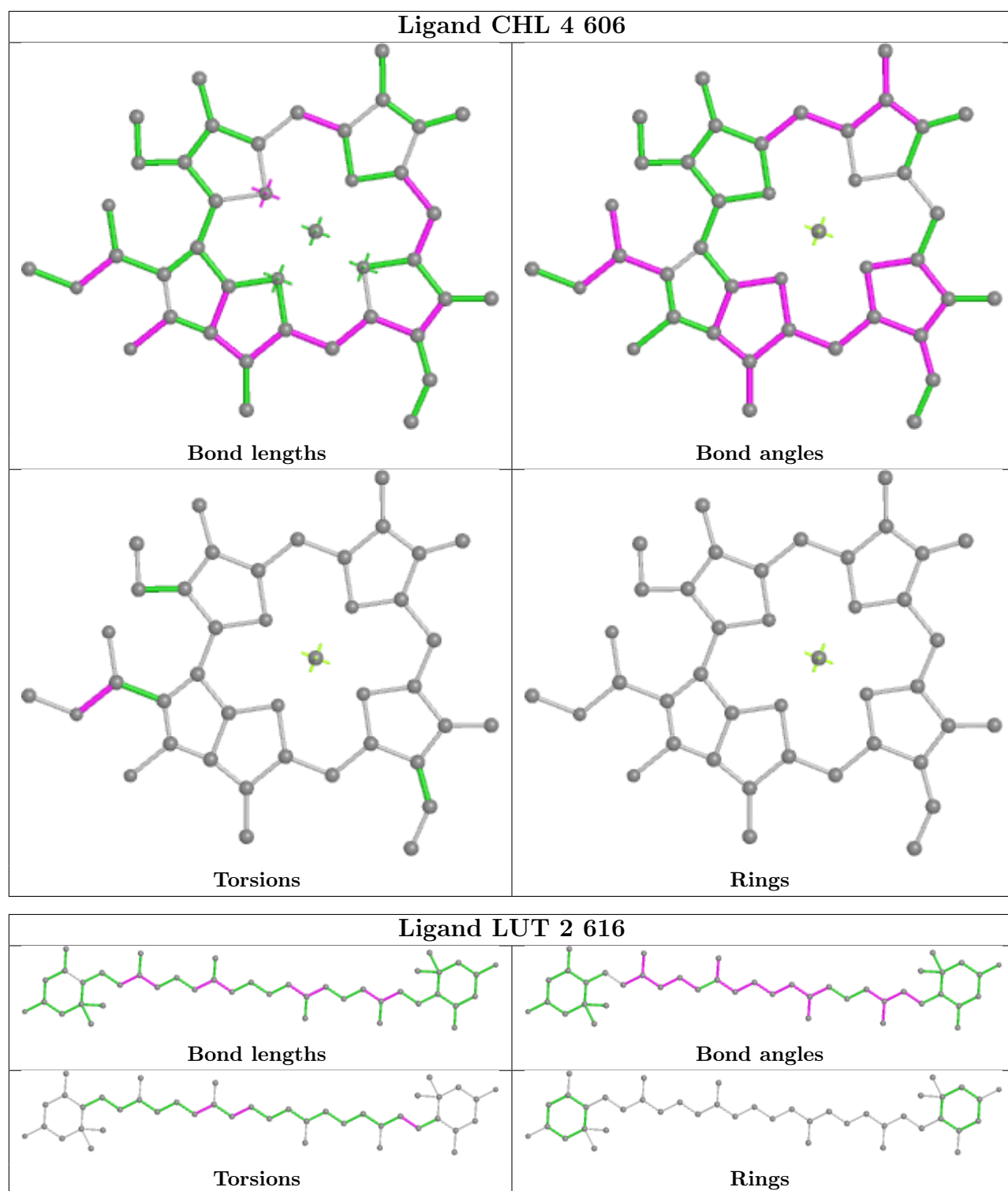


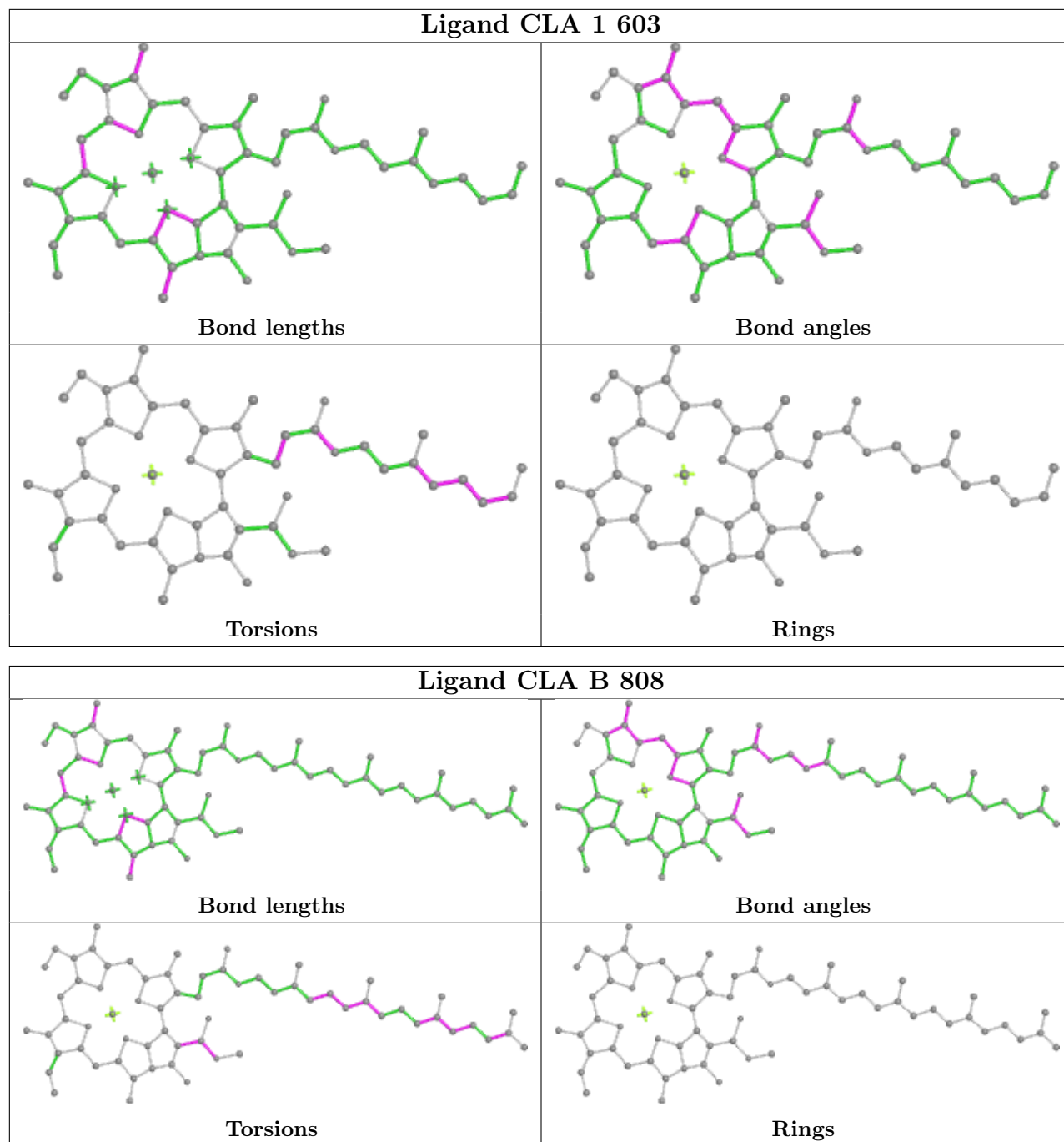


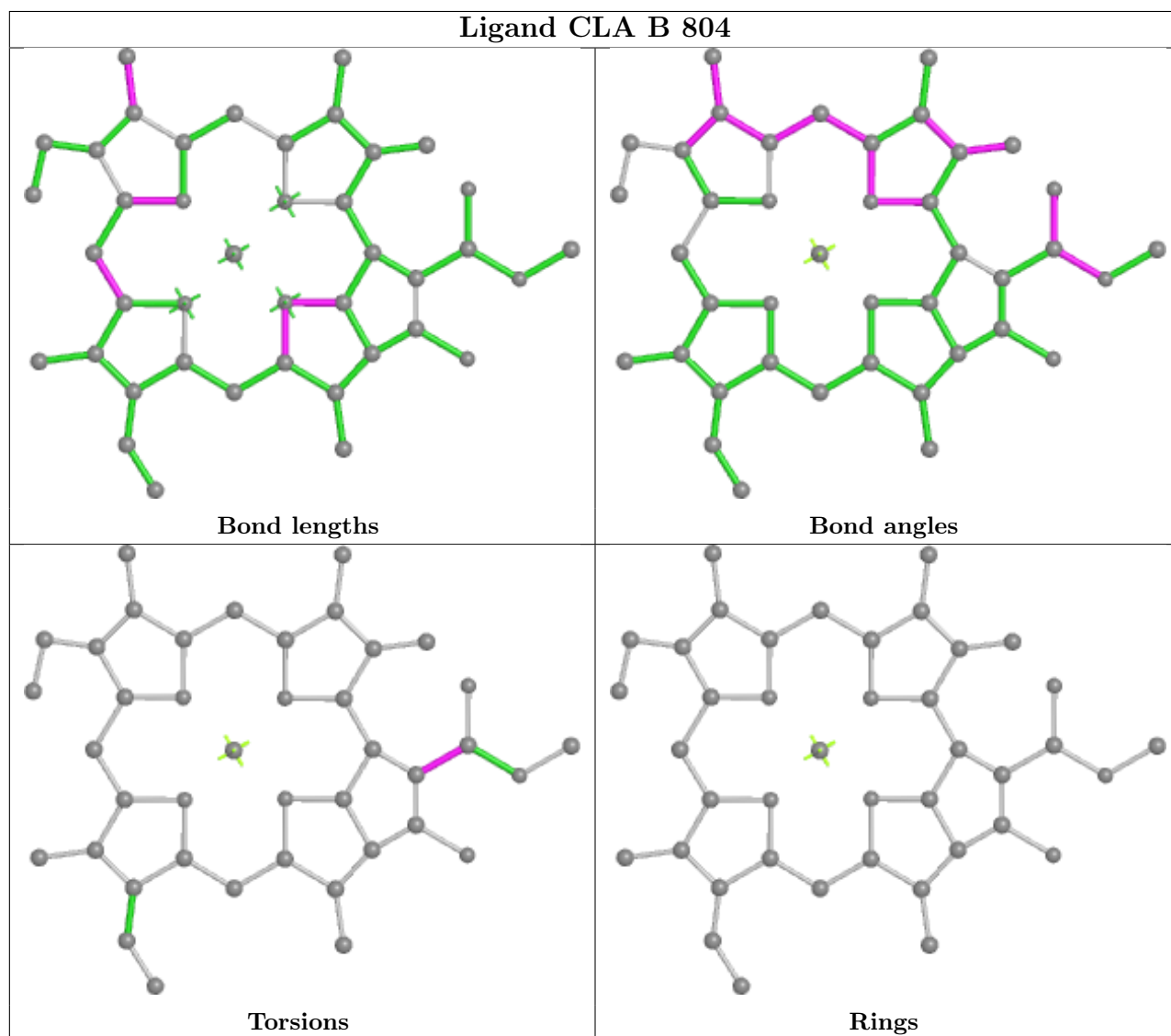
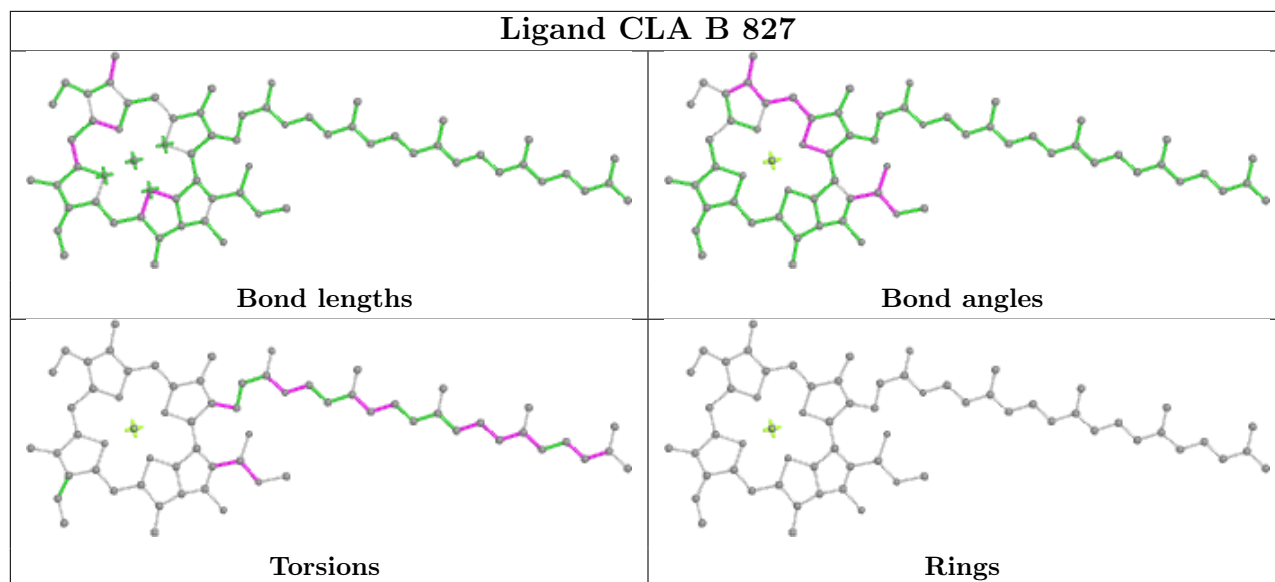


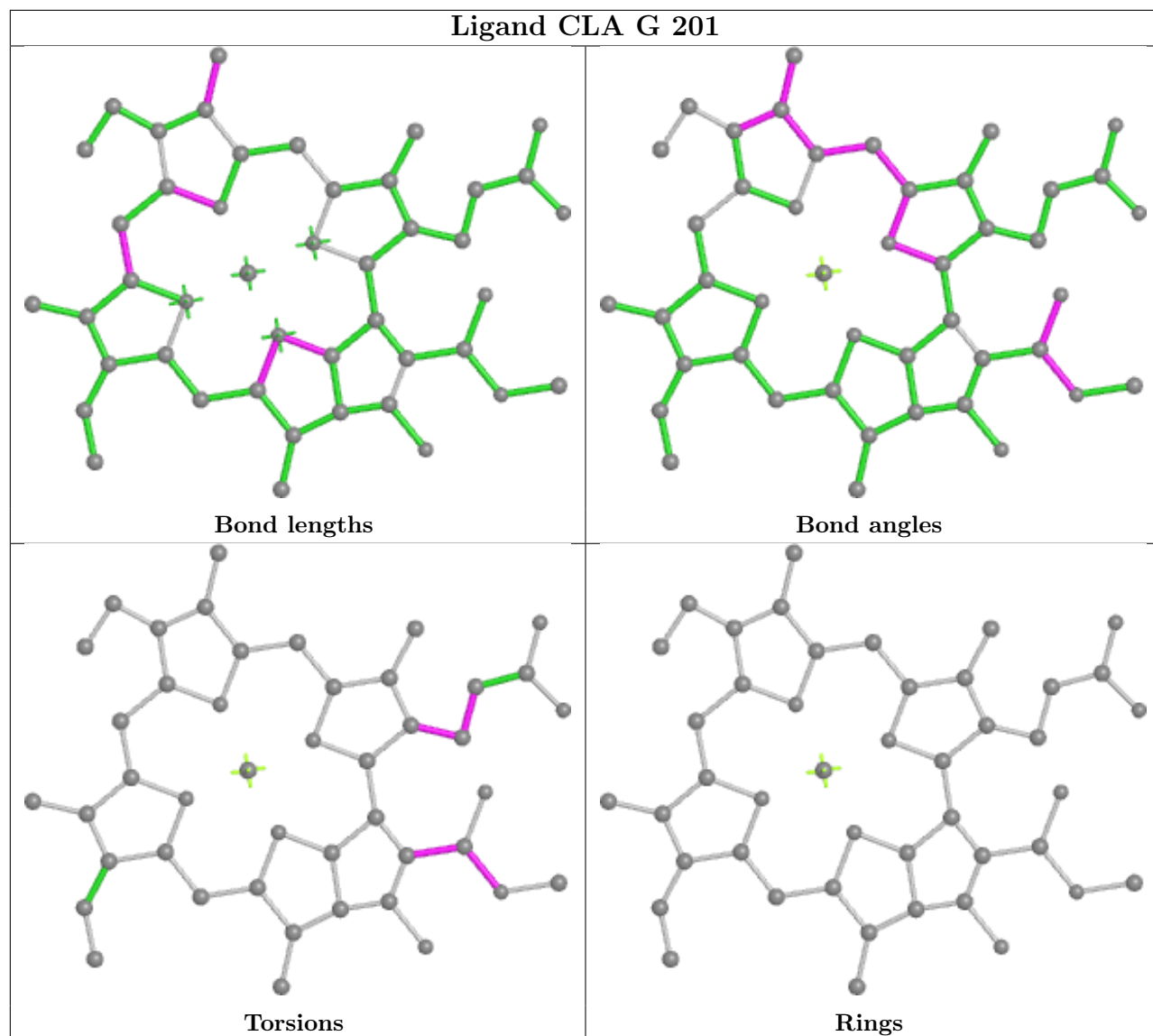


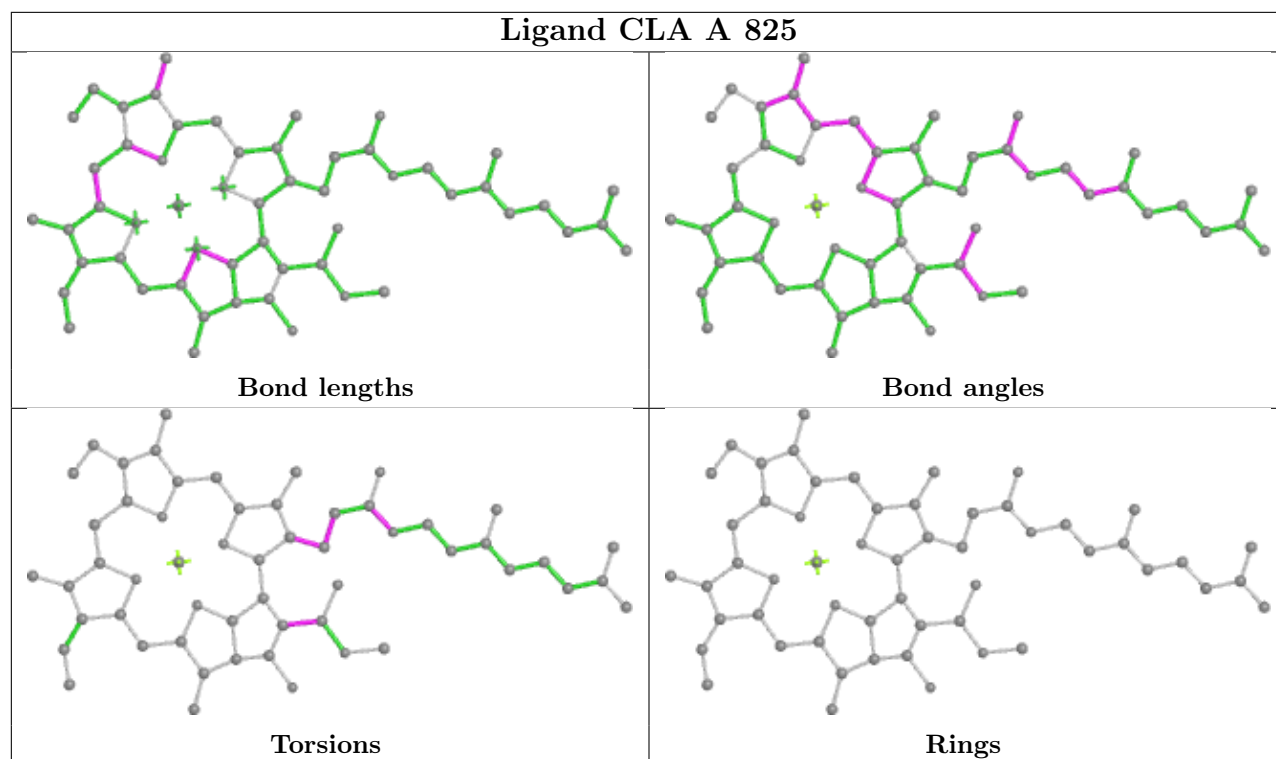
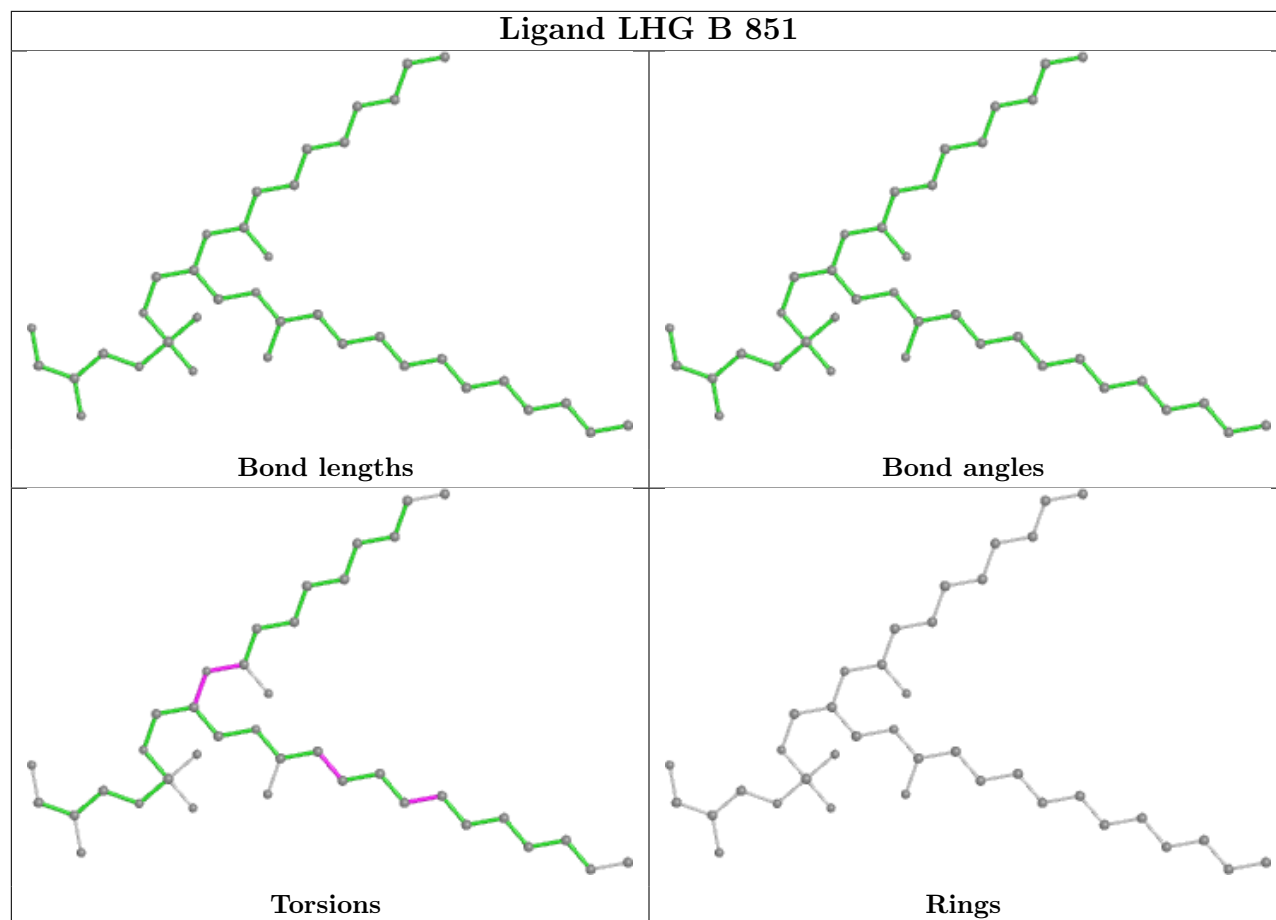


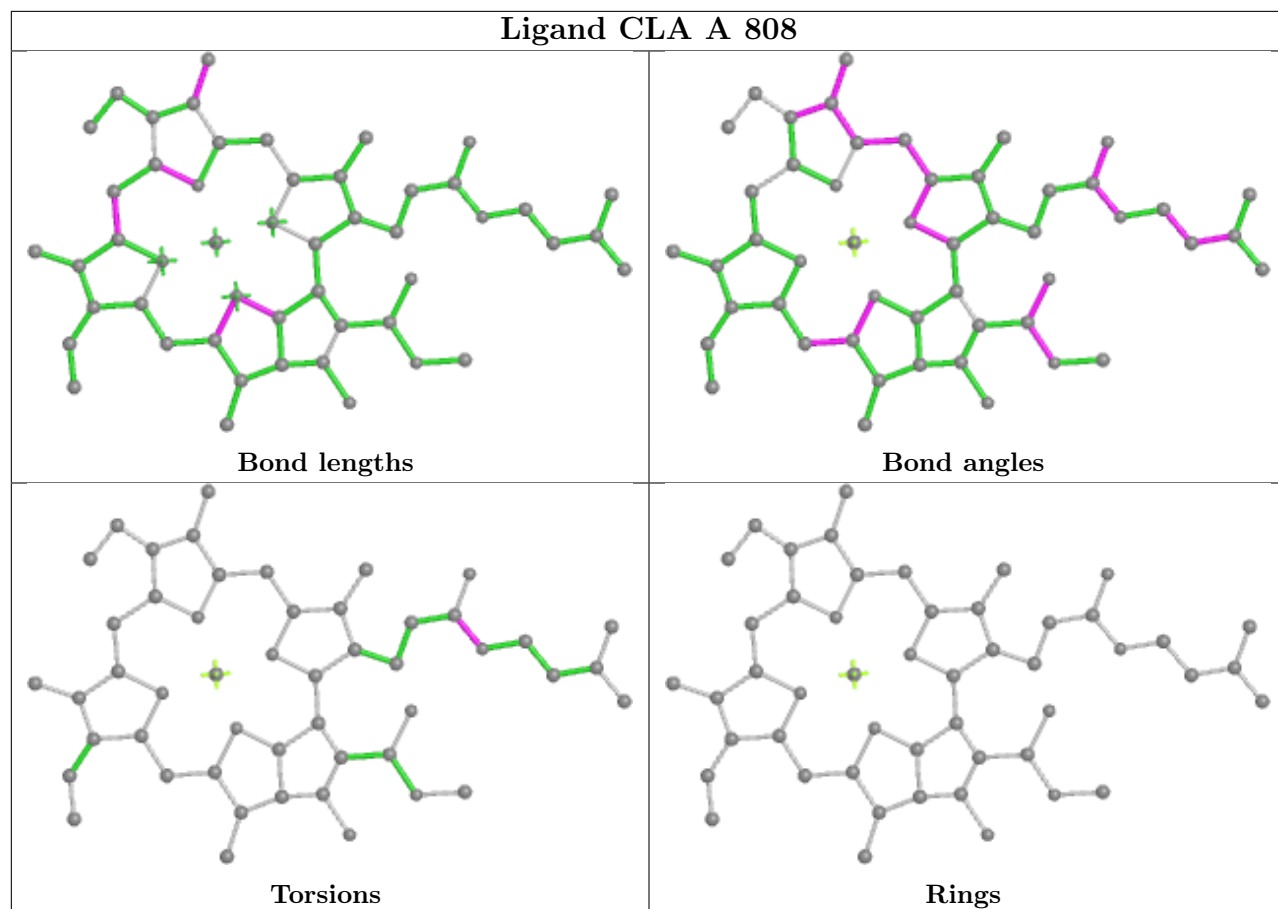


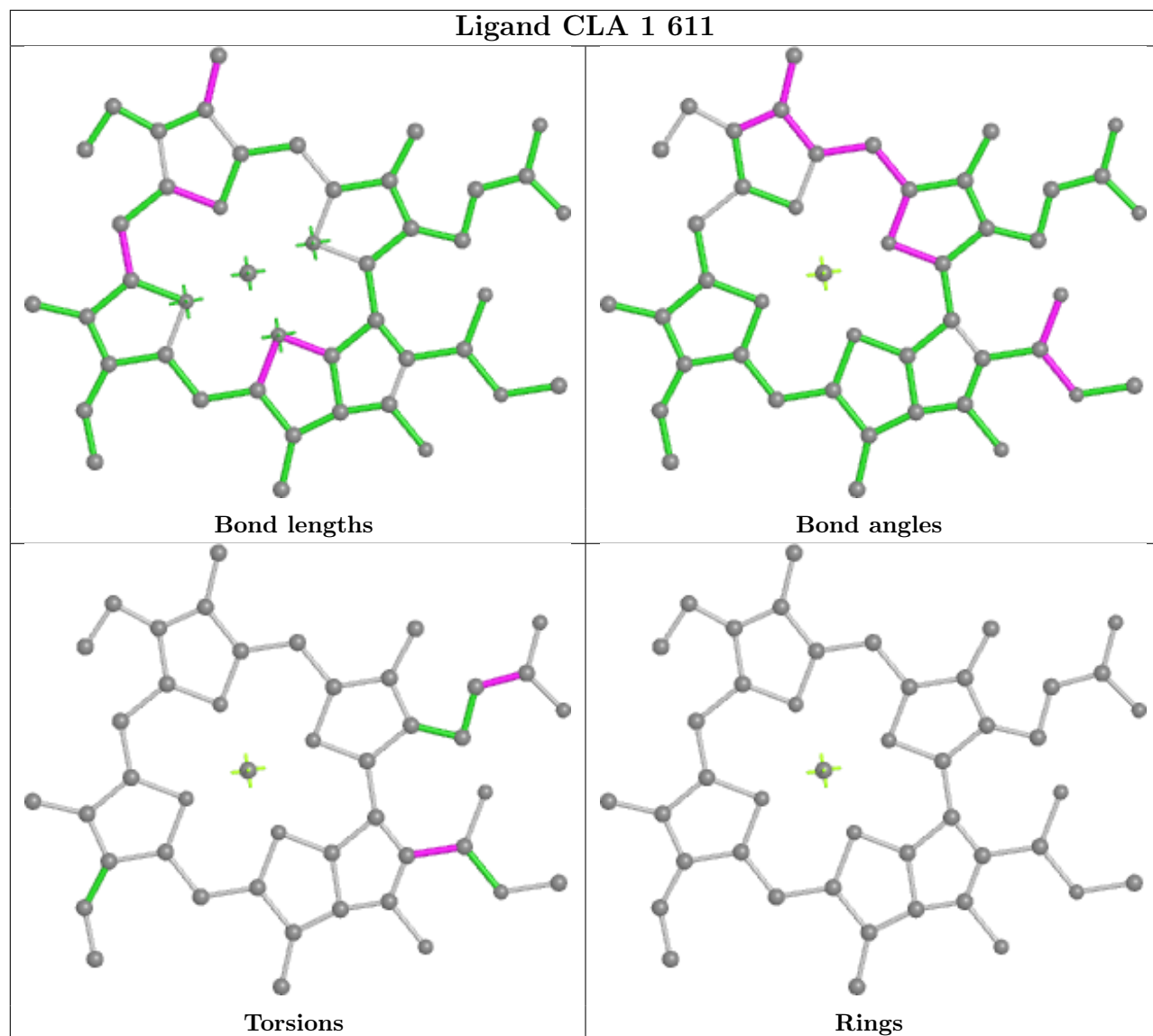


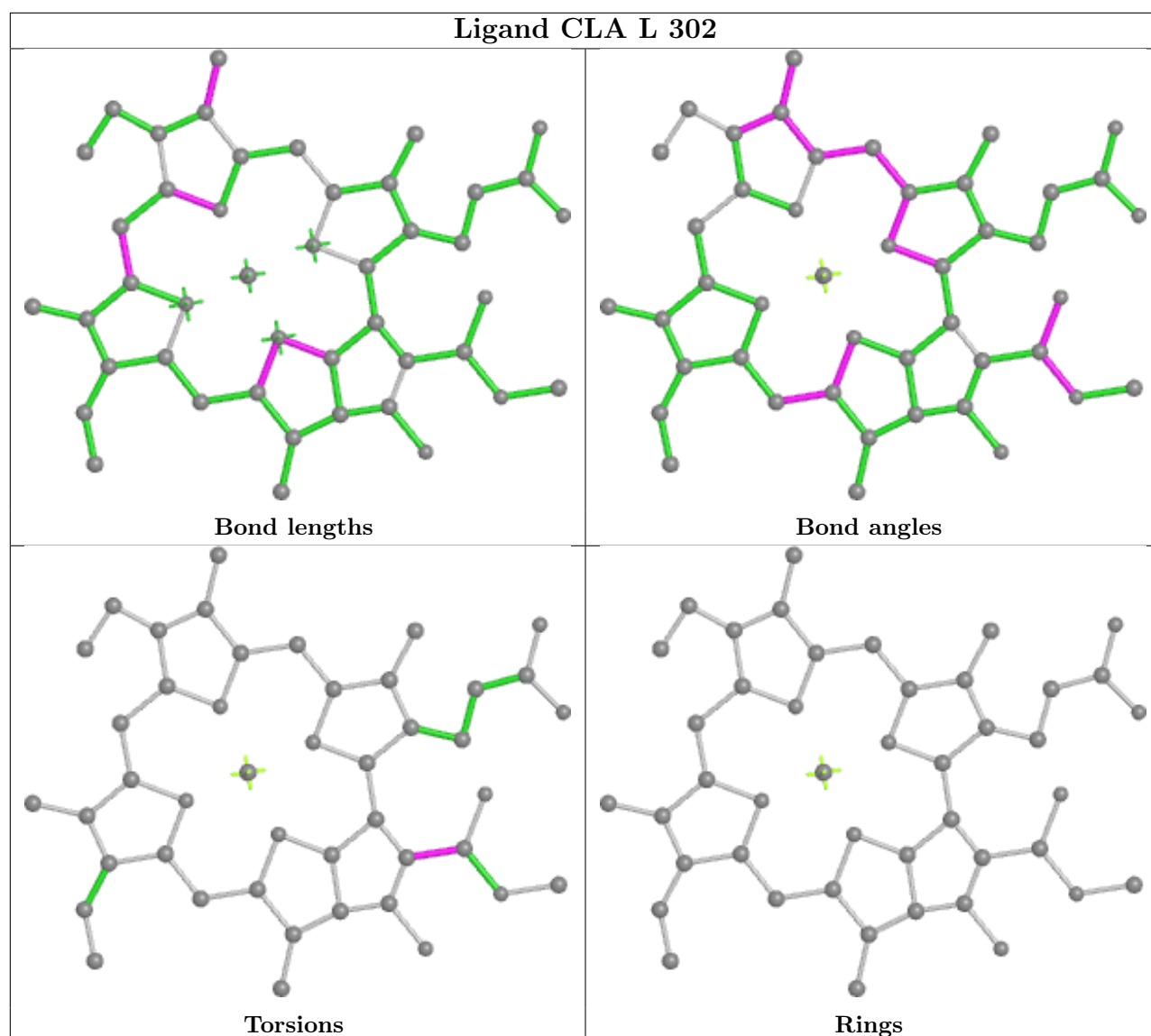












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

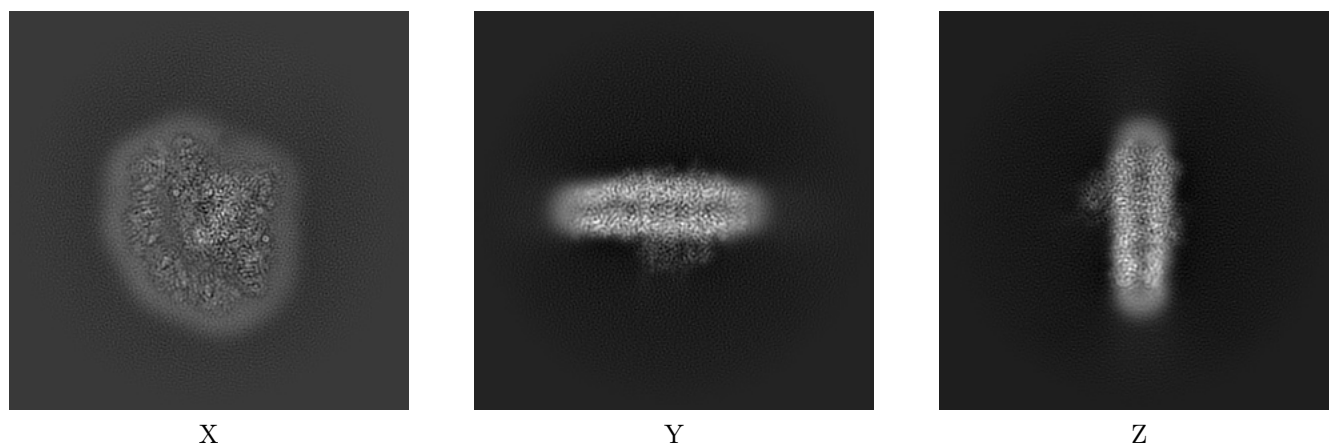
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36037. 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](#)

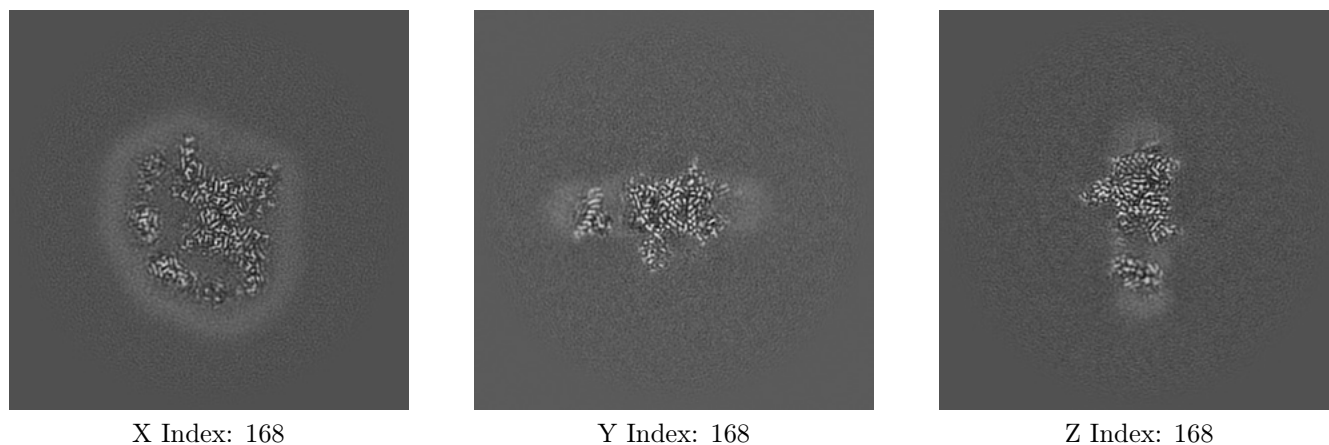
6.1.1 Primary map



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

6.2 Central slices [i](#)

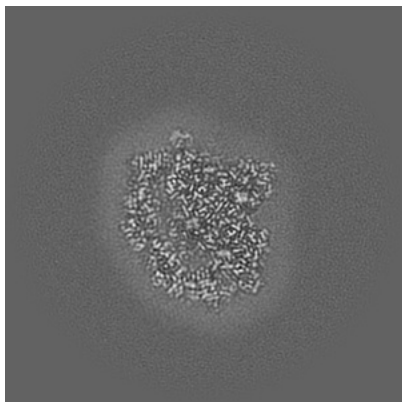
6.2.1 Primary map



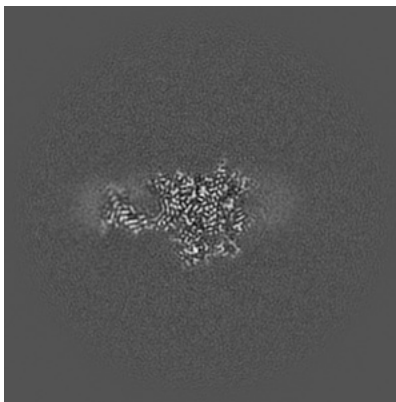
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

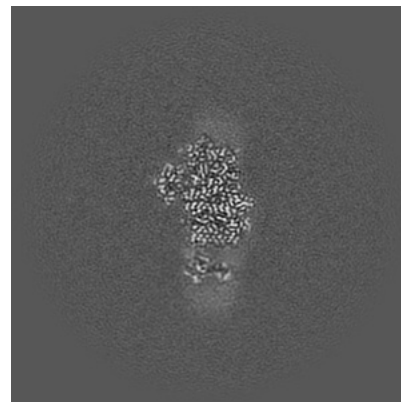
6.3.1 Primary map



X Index: 157



Y Index: 174

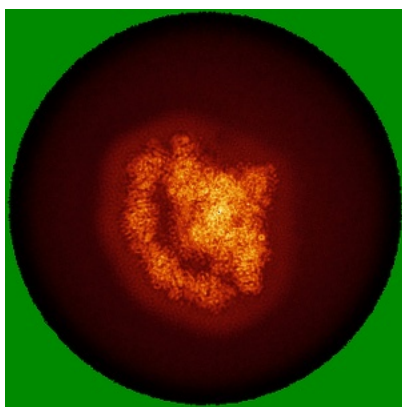


Z Index: 182

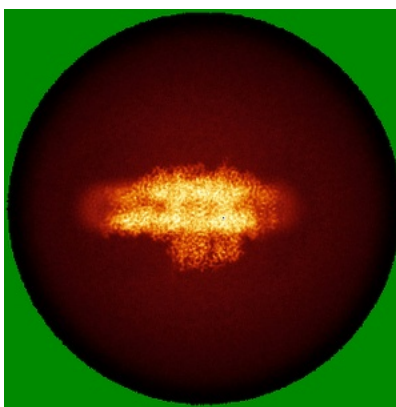
The images above show the largest variance slices of the map in three orthogonal directions.

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

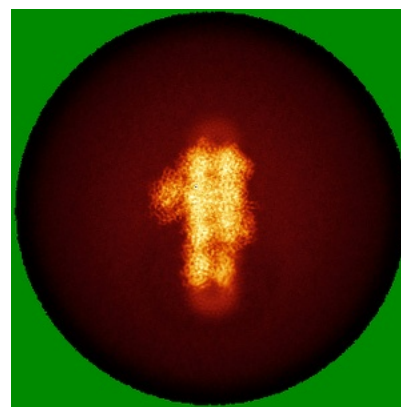
6.4.1 Primary map



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 3.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

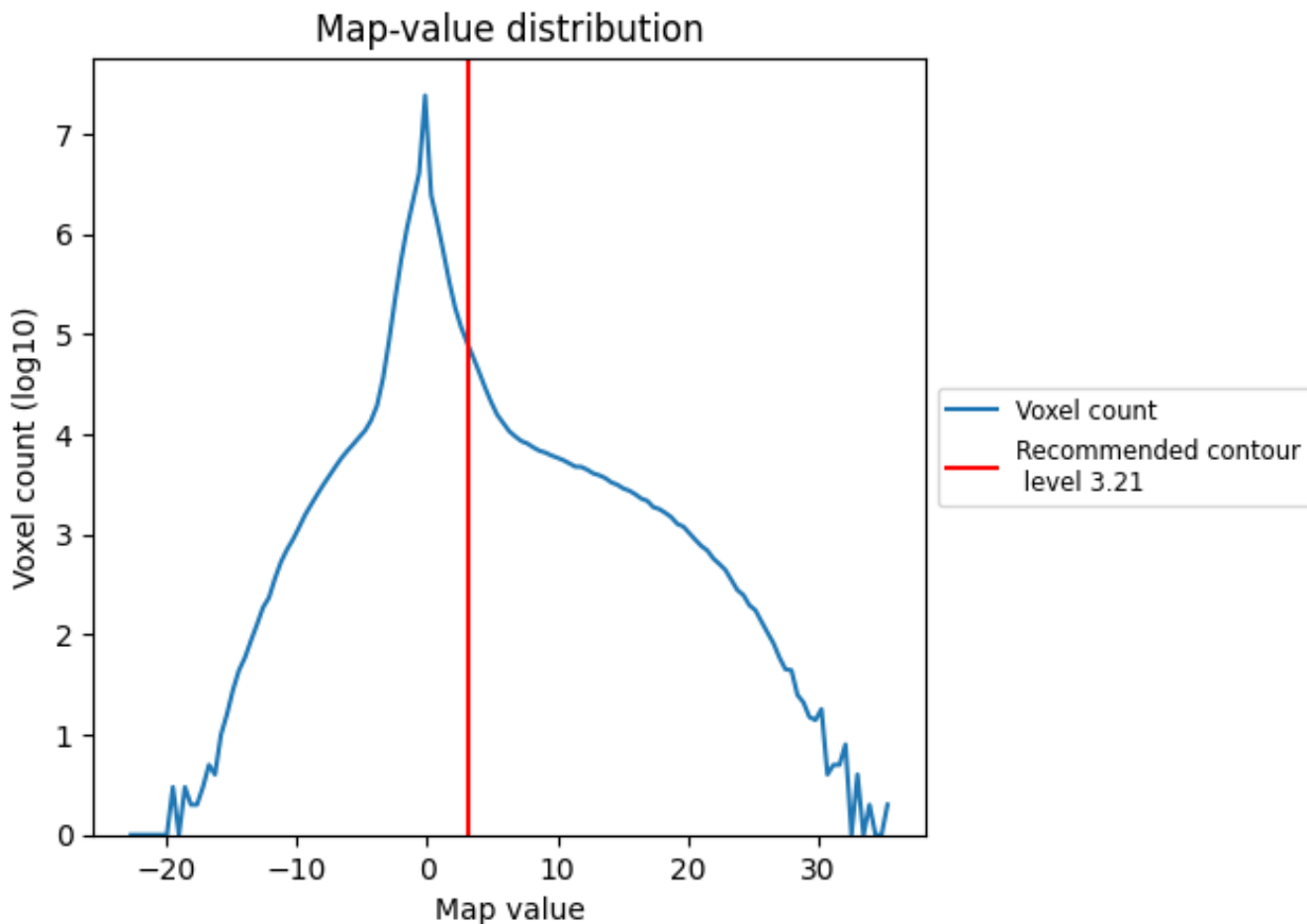
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

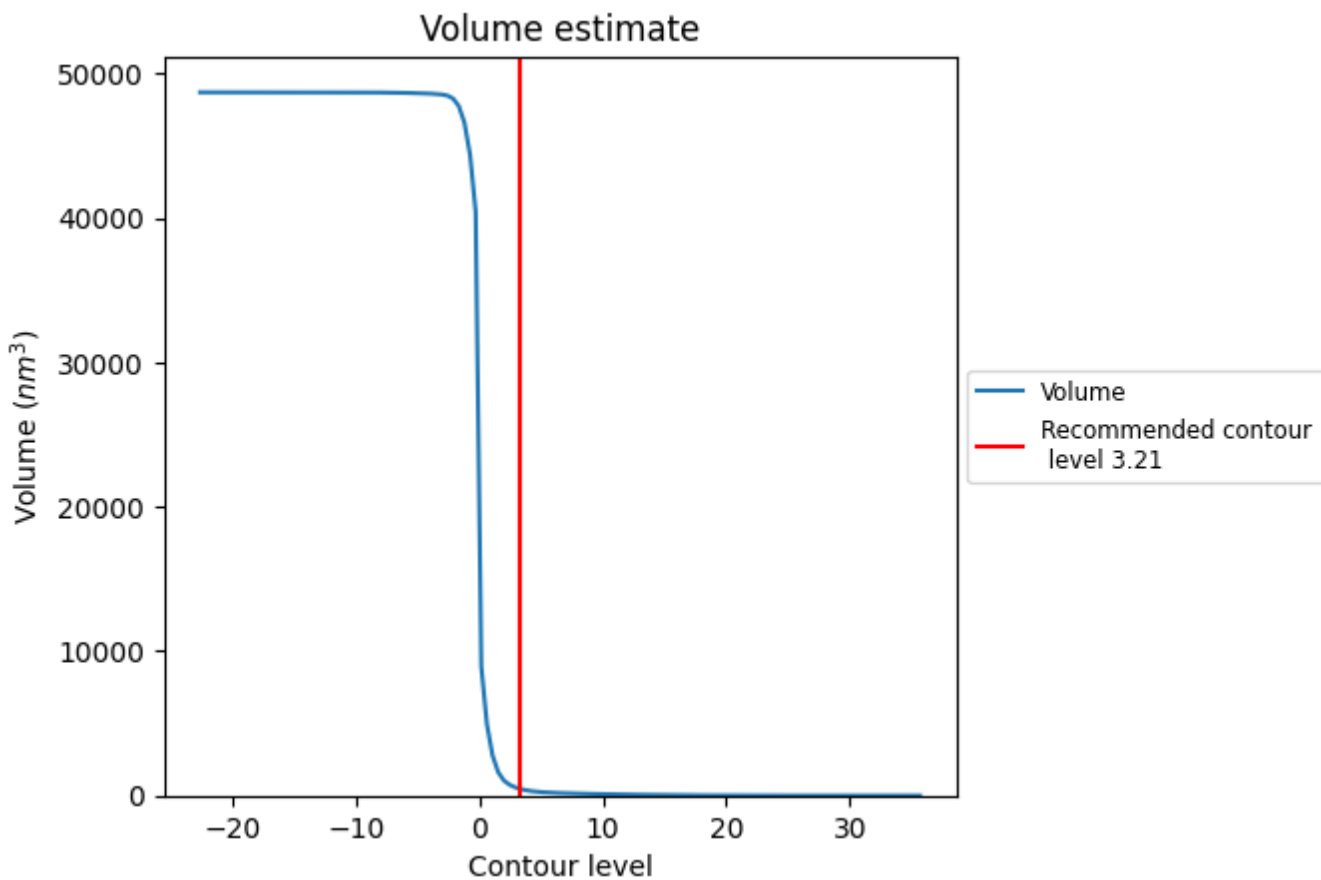
This section contains the results of statistical analysis of the map.

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.

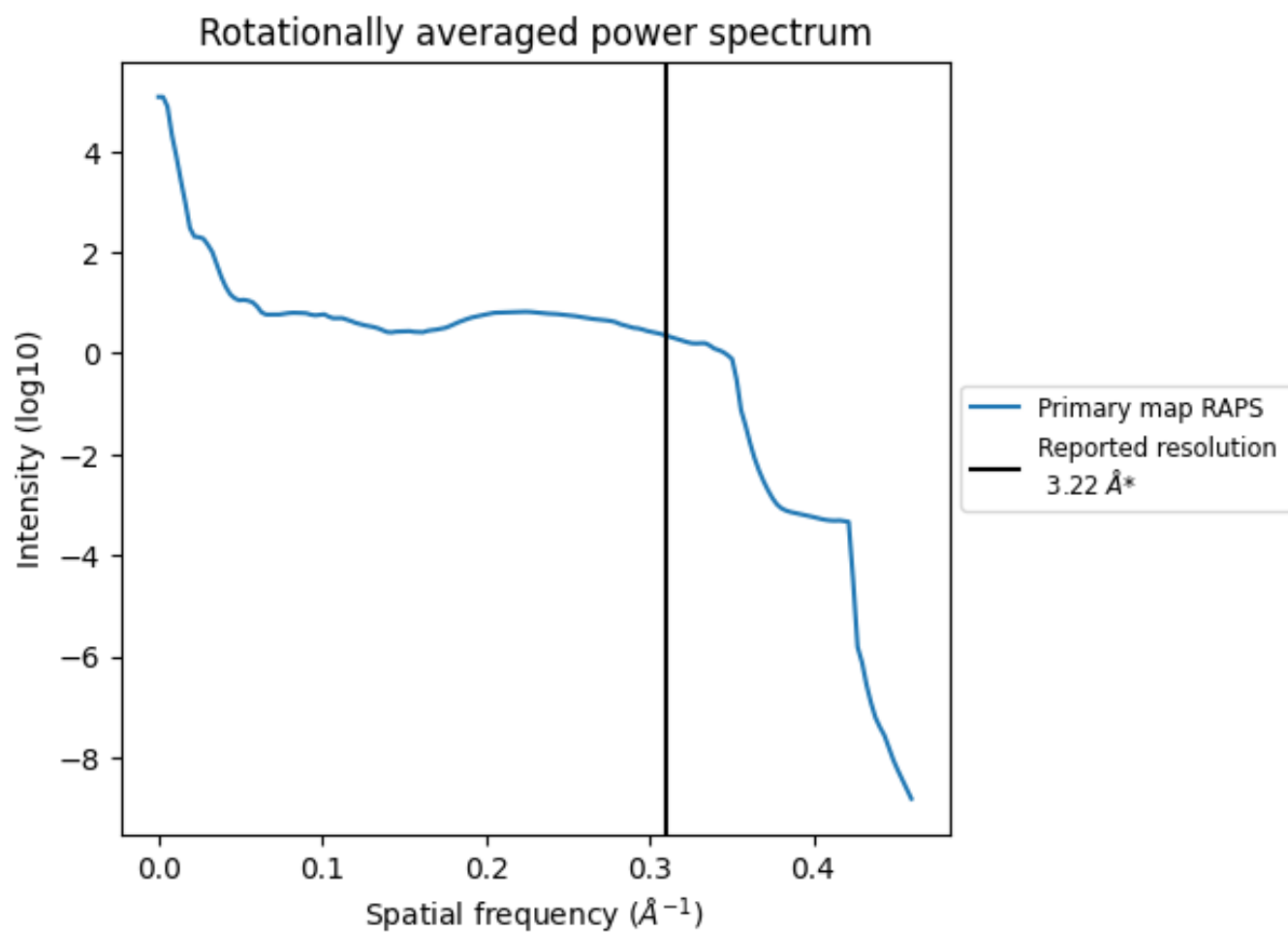
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm^3 ; this corresponds to an approximate mass of 442 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 0.311\AA^{-1}

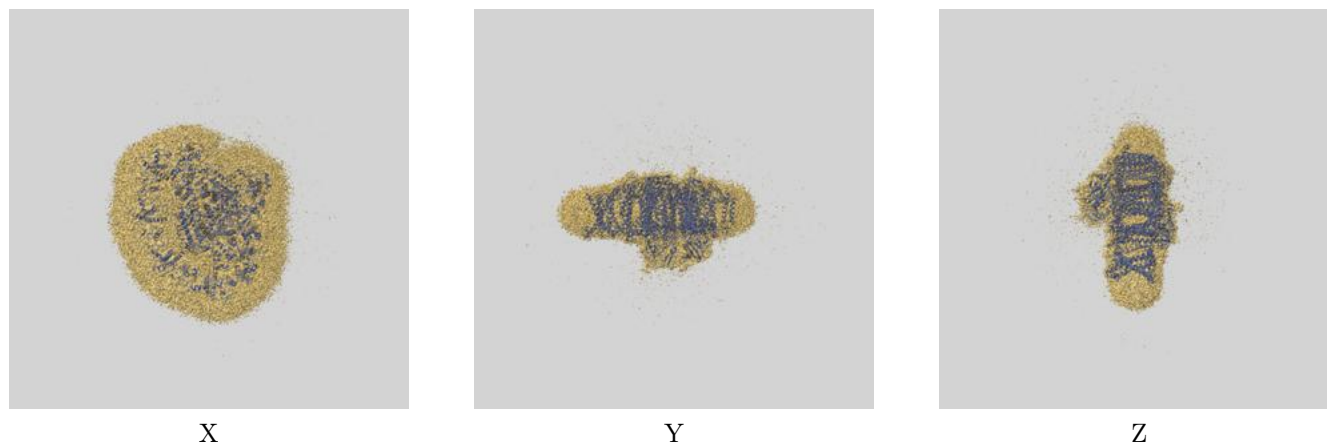
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

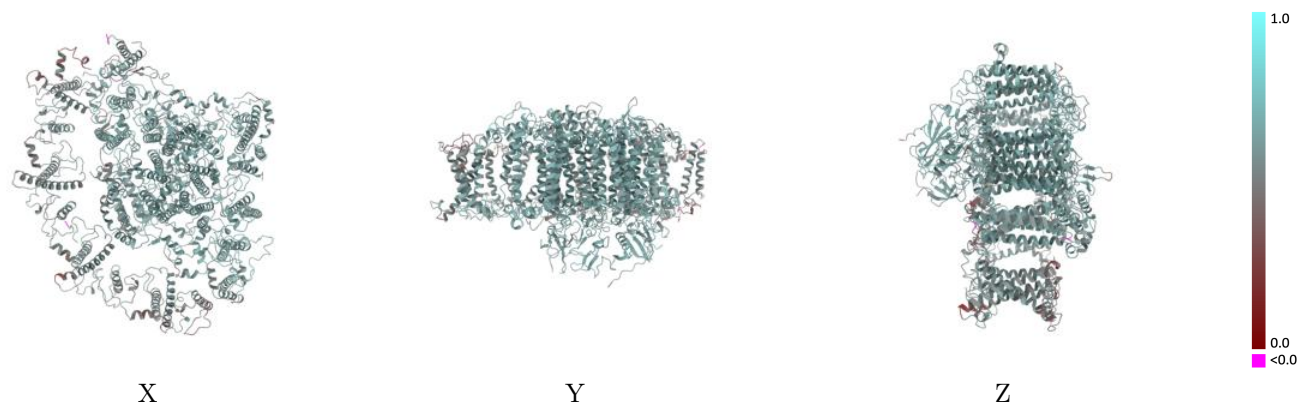
This section contains information regarding the fit between EMDB map EMD-36037 and PDB model 8J7B. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



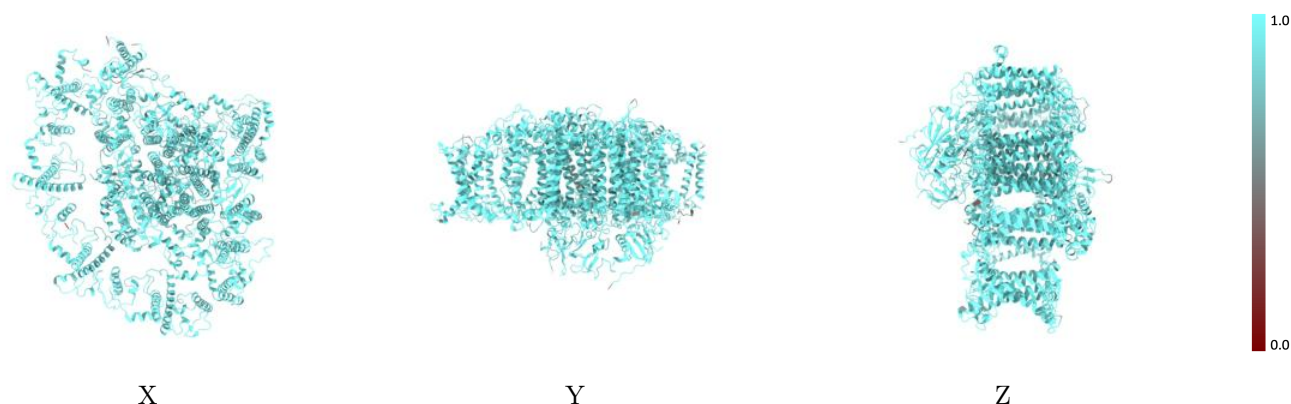
The images above show the 3D surface view of the map at the recommended contour level 3.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



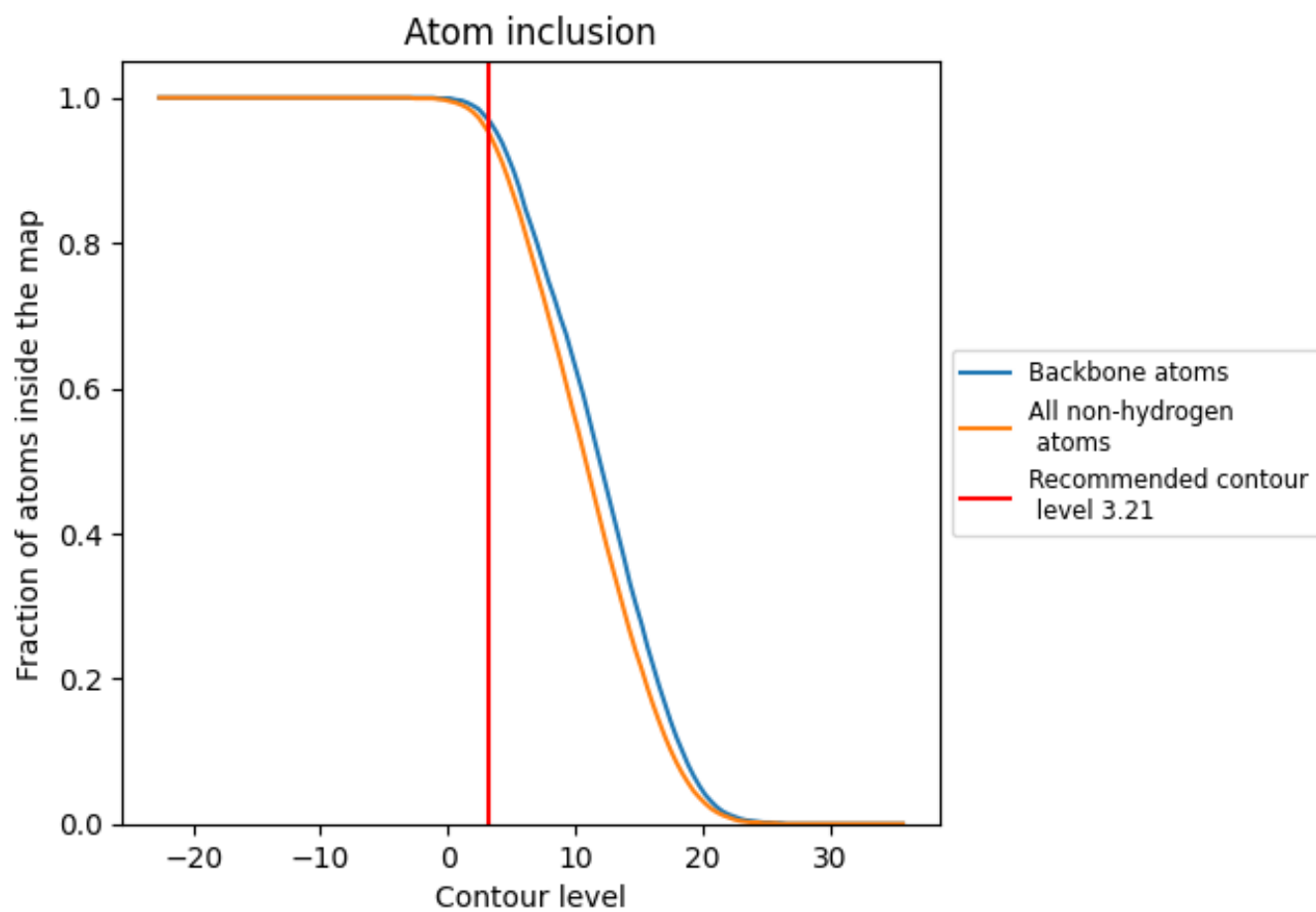
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.21).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (3.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.5760
1	 0.9220	 0.4980
2	 0.9450	 0.5180
3	 0.9450	 0.5120
4	 0.9520	 0.5350
A	 0.9570	 0.6050
B	 0.9670	 0.6150
C	 0.9810	 0.6130
D	 0.9770	 0.6080
E	 0.9760	 0.6050
F	 0.9210	 0.5690
G	 0.9520	 0.5730
H	 0.9350	 0.5650
I	 0.9790	 0.6000
J	 0.8600	 0.5340
K	 0.8620	 0.4680
L	 0.9610	 0.5960

