



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:25 AM JST

PDB ID : 6L35 / pdb_00006l35
EMDB ID : EMD-0821
Title : PSI-LHCI Supercomplex from *Physcometrella patens*
Authors : Zhao, L.; Yan, Q.J.; Qin, X.C.
Deposited on : 2019-10-09
Resolution : 3.23 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:

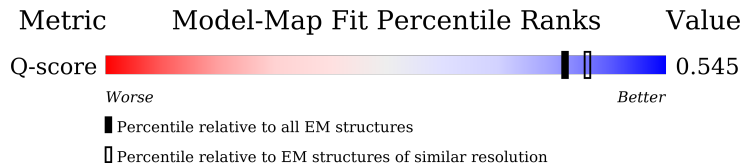
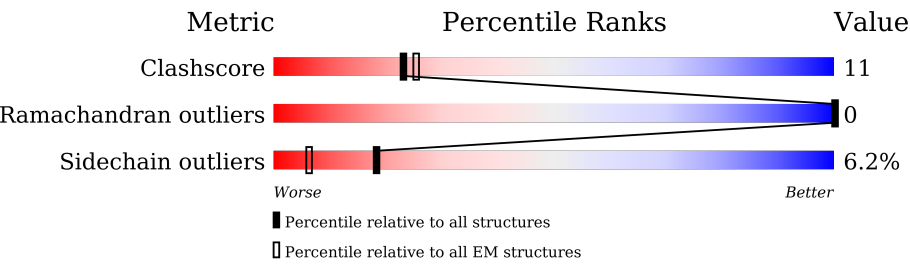
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.23 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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	A	742	78%21%
2	B	733	76%23%
3	C	80	6% 61%32%6%
4	D	141	6% 82%16%

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Mol	Chain	Length	Quality of chain
5	E	62	
6	F	159	
7	G	98	
8	H	90	
9	I	34	
10	J	41	
11	K	79	
12	L	159	
13	M	29	
14	2	210	
15	6	192	
16	3	213	
17	5	205	

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
22	SF4	C	101	-	-	X	-
22	SF4	C	102	-	-	X	-
27	XAT	2	620	-	-	X	-
27	XAT	5	620	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34822 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5837	3827	993	998	19		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3839	996	998	16		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			595	365	103	116	11		

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1104	707	196	198	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			487	309	87	91		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	159	Total	C	N	O	S	0	0
			1226	793	209	221	3		

- Molecule 7 is a protein called Predicted protein PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			693	445	117	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			550	346	96	105	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1189	781	192	214	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	29	Total	C	N	O	0	0
			214	141	34	39		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	206	Total	C	N	O	S	0	0
			1595	1039	267	285	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

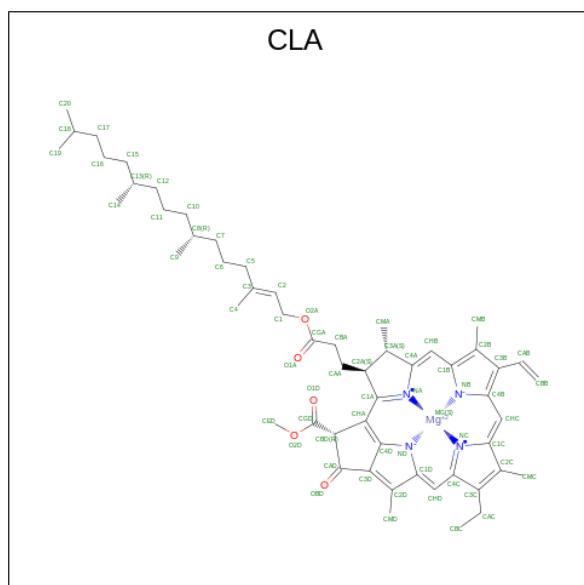
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	202	Total	C	N	O	S	0	0
			1566	1020	258	282	6		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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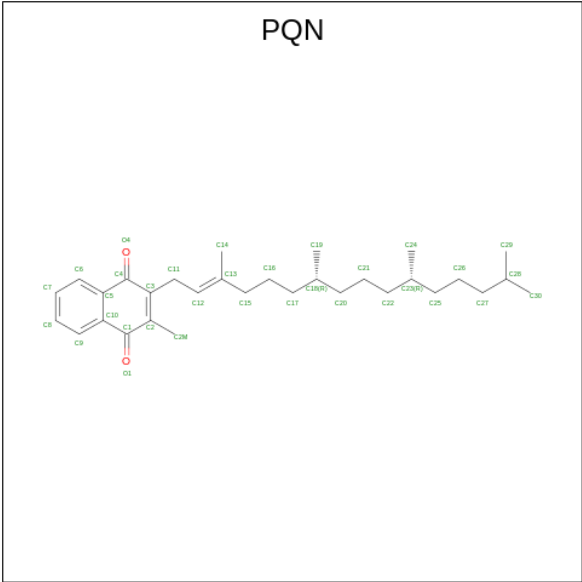
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18	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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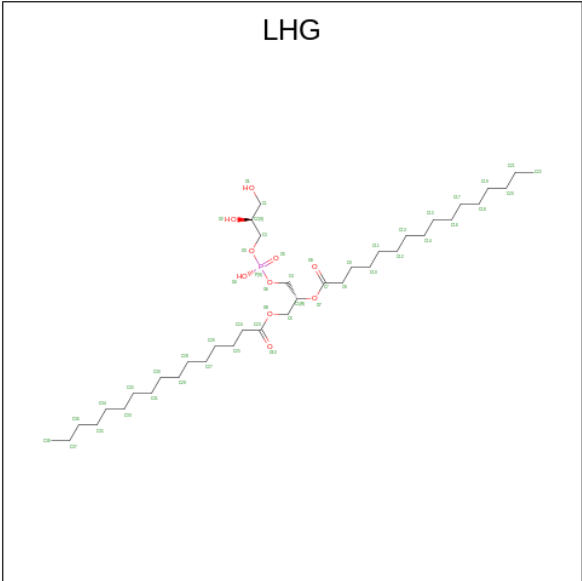
Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
18	3	1	Total	C	Mg	N	O	0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

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



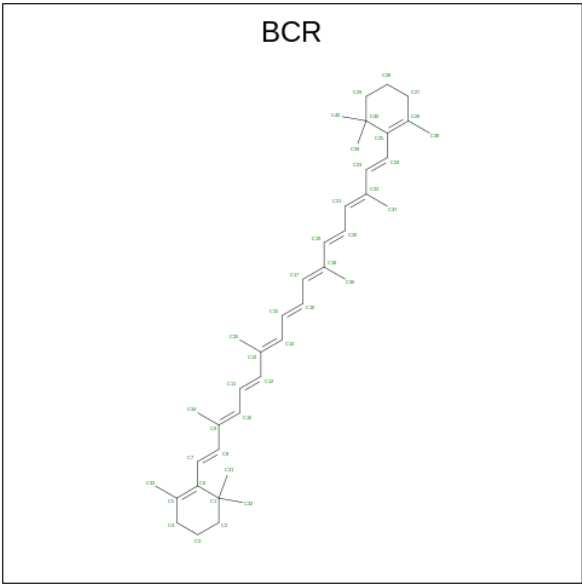
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			27	16	10	1	
20	B	1	Total	C	O	P	0
			23	12	10	1	
20	2	1	Total	C	O	P	0
			35	24	10	1	
20	6	1	Total	C	O	P	0
			28	17	10	1	
20	5	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



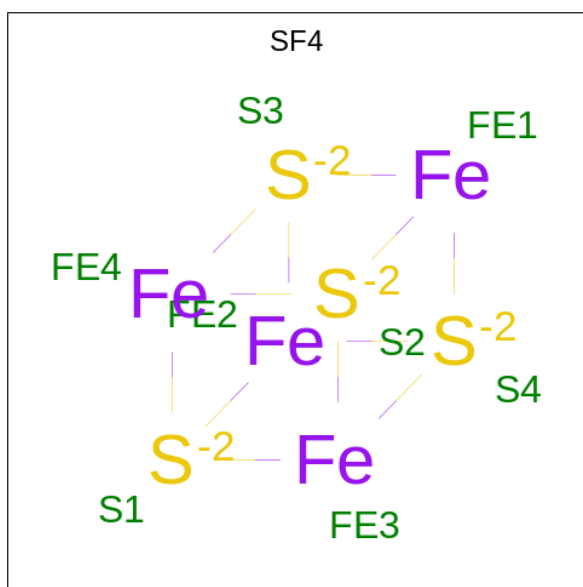
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

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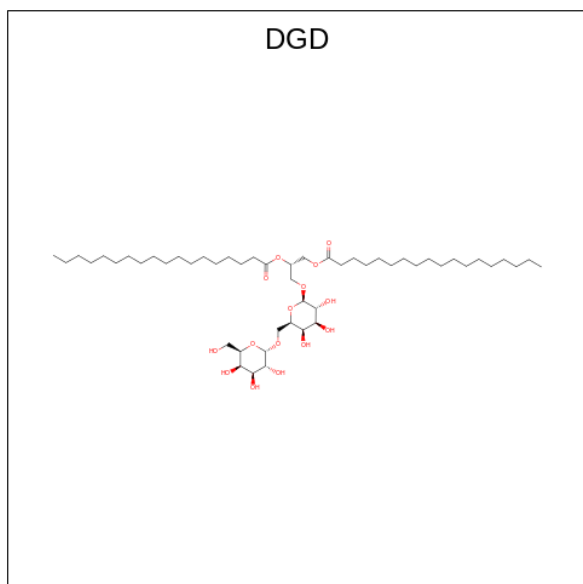
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	2	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	5	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



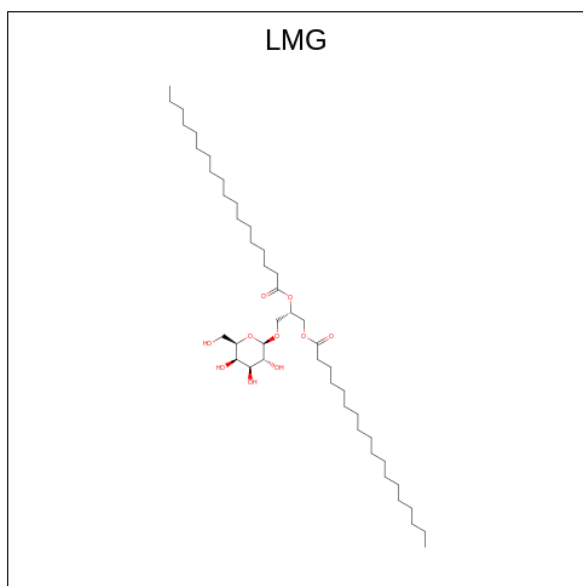
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



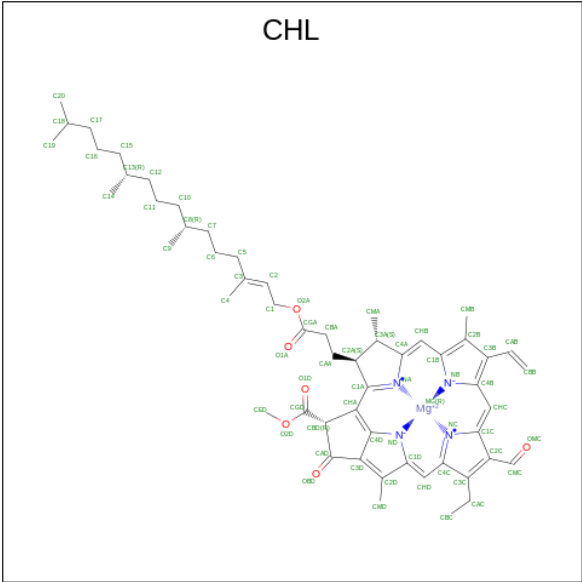
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			66	51	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



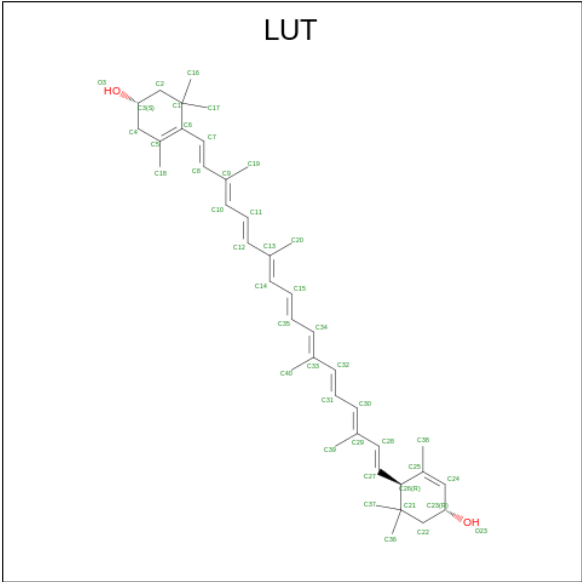
Mol	Chain	Residues	Atoms			AltConf
24	J	1	Total	C	O	0
			30	20	10	
24	2	1	Total	C	O	0
			13	7	6	
24	2	1	Total	C	O	0
			13	7	6	

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



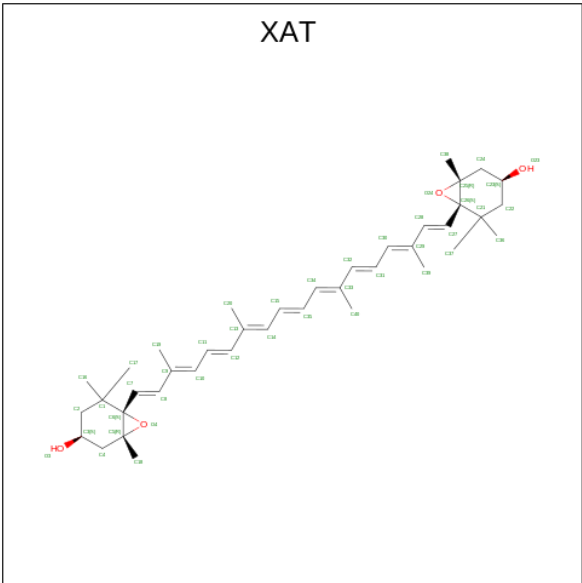
Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 45	C 34	Mg 1	N 4	O 6	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	2	1	Total 41	C 32	Mg 1	N 4	O 4	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	6	1	Total 45	C 34	Mg 1	N 4	O 6	0
25	6	1	Total 41	C 32	Mg 1	N 4	O 4	0
25	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	5	1	Total 41	C 32	Mg 1	N 4	O 4	0
25	5	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
25	5	1	Total 43	C 34	Mg 1	N 4	O 4	0

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	

- Molecule 27 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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).

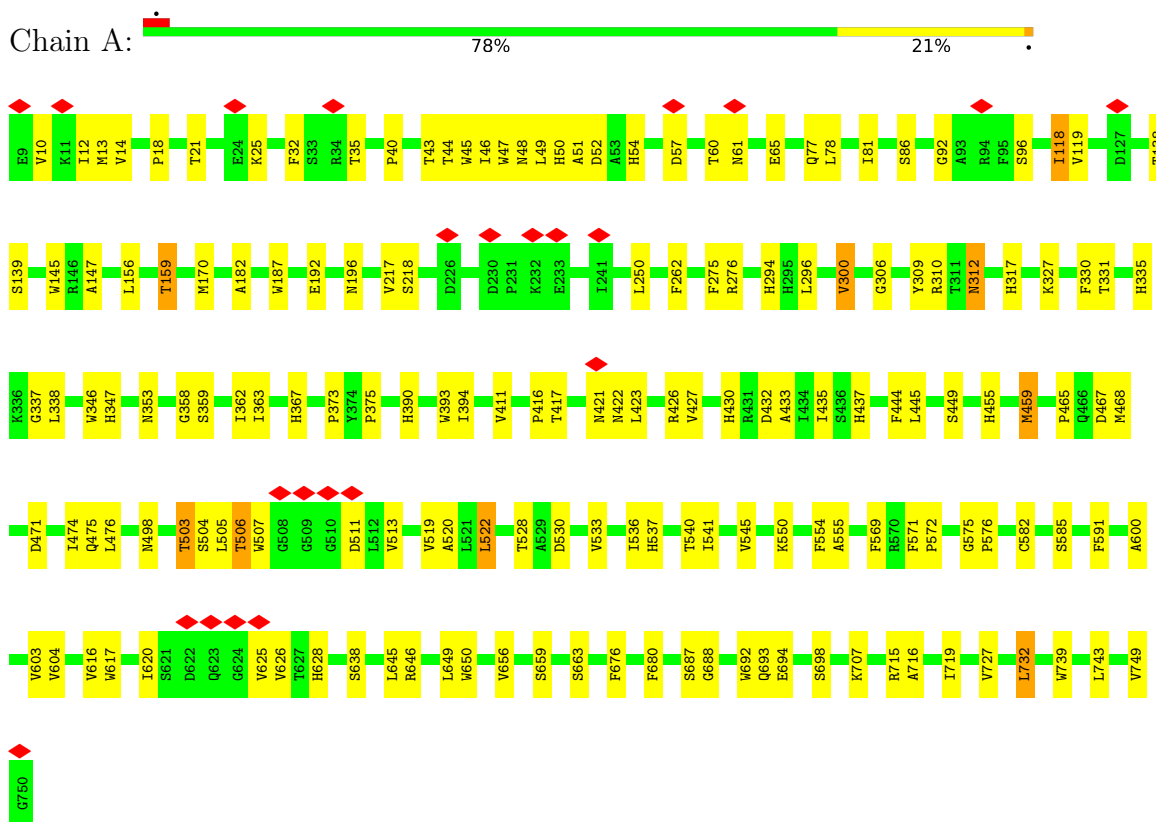


Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total 44	C 40	O 4	0
27	6	1	Total 44	C 40	O 4	0
27	3	1	Total 44	C 40	O 4	0
27	5	1	Total 44	C 40	O 4	0

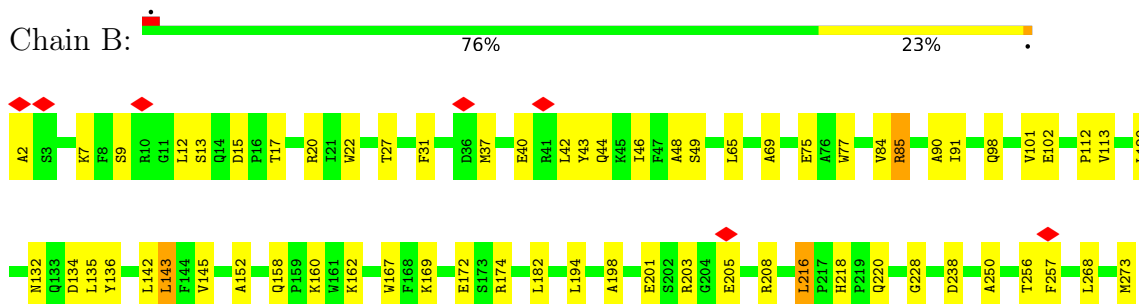
3 Residue-property plots

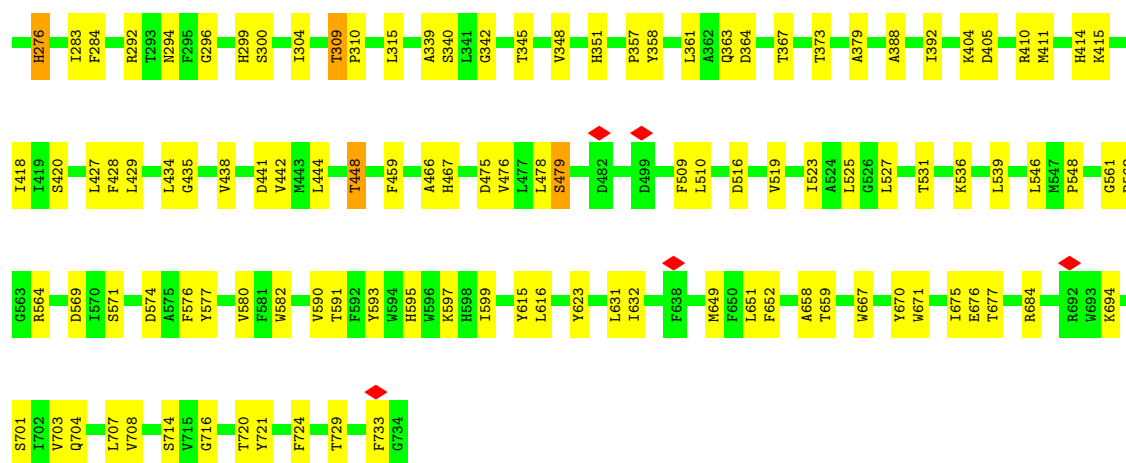
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosystem I P700 chlorophyll a apoprotein A1

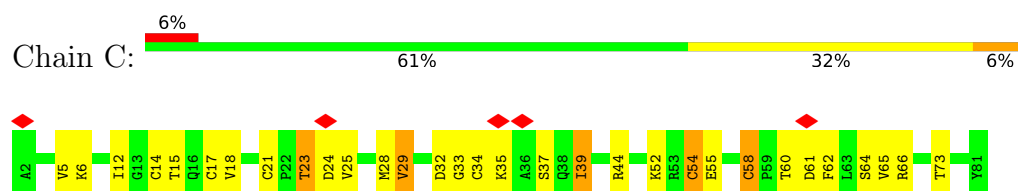


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

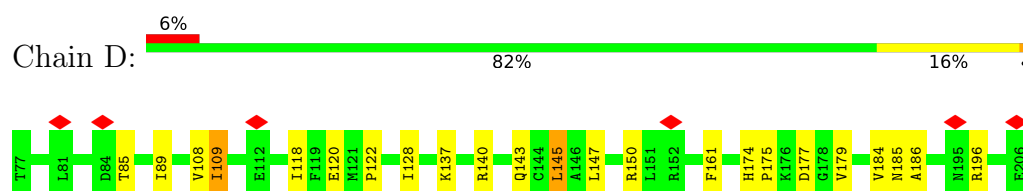




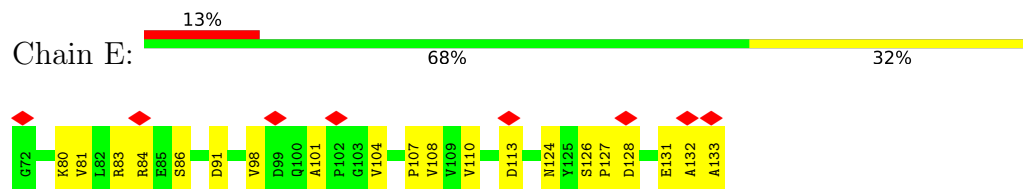
- Molecule 3: Photosystem I iron-sulfur center



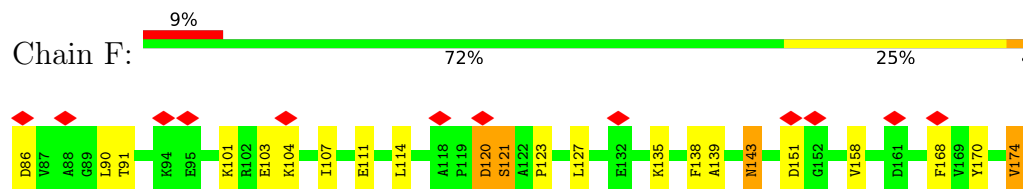
- Molecule 4: Predicted protein Psad



- Molecule 5: Psae

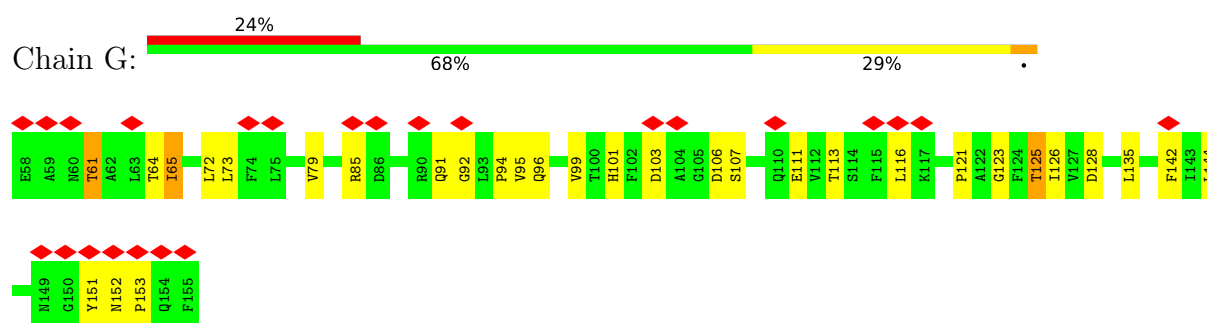


- Molecule 6: PSI-F

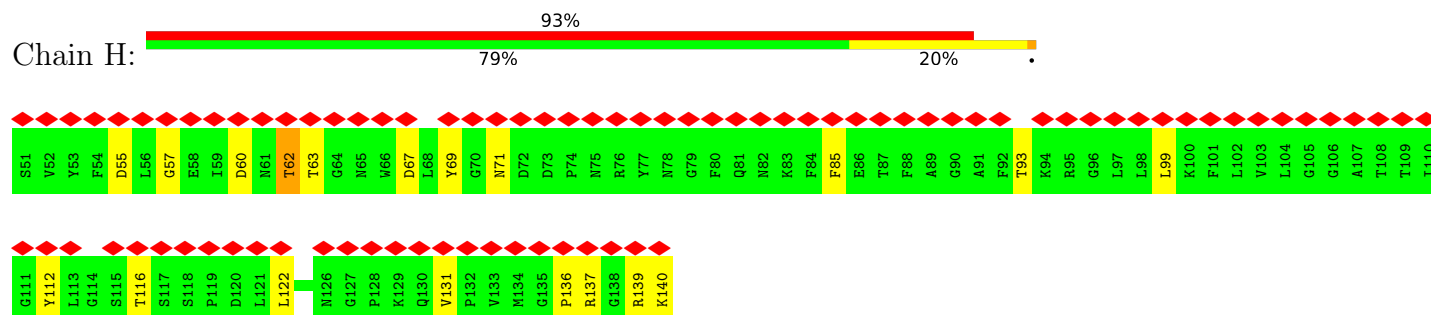


- Molecule 7: Predicted protein Psag

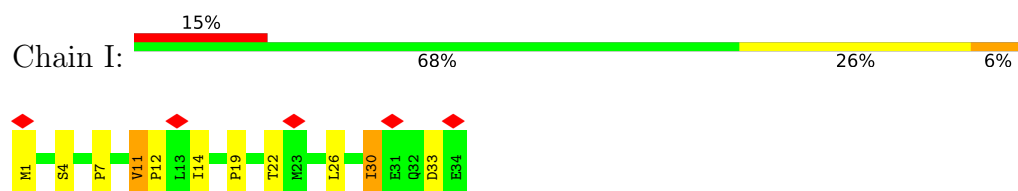




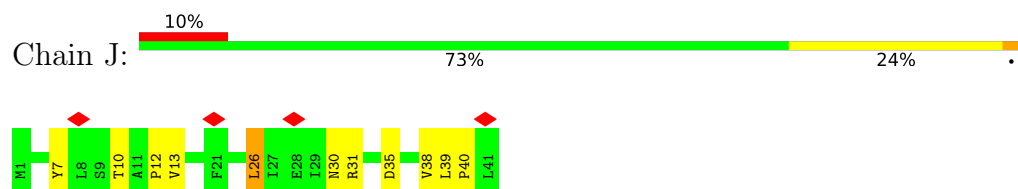
- Molecule 8: PsaH photosystem I reaction center subunit



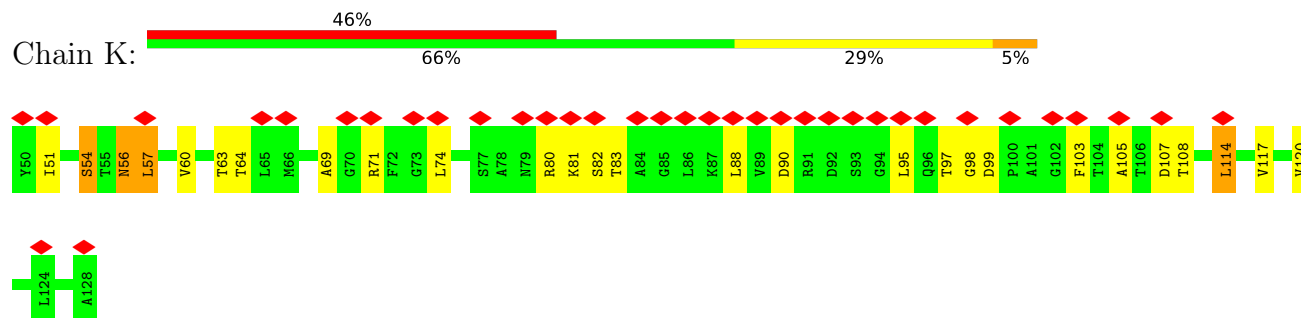
- Molecule 9: Photosystem I reaction center subunit VIII



- Molecule 10: Photosystem I reaction center subunit IX

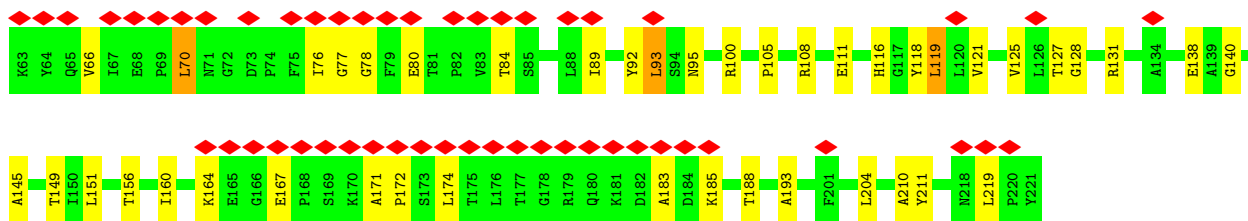


- Molecule 11: PsaK

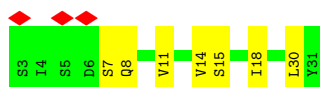
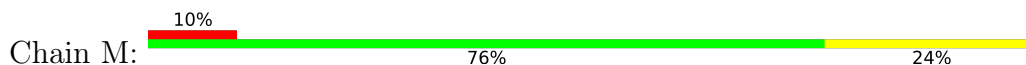


- Molecule 12: PSI subunit V

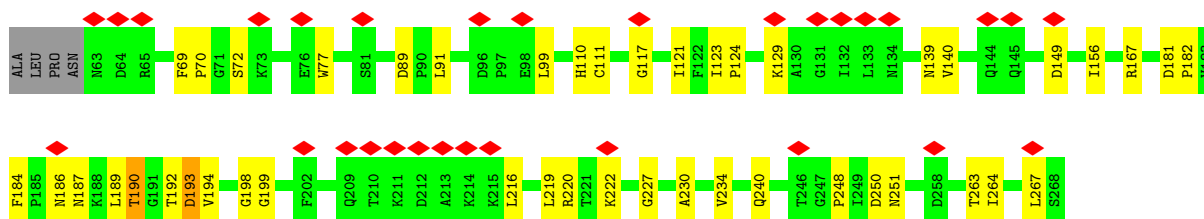
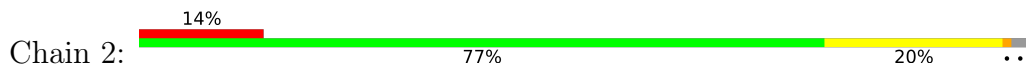




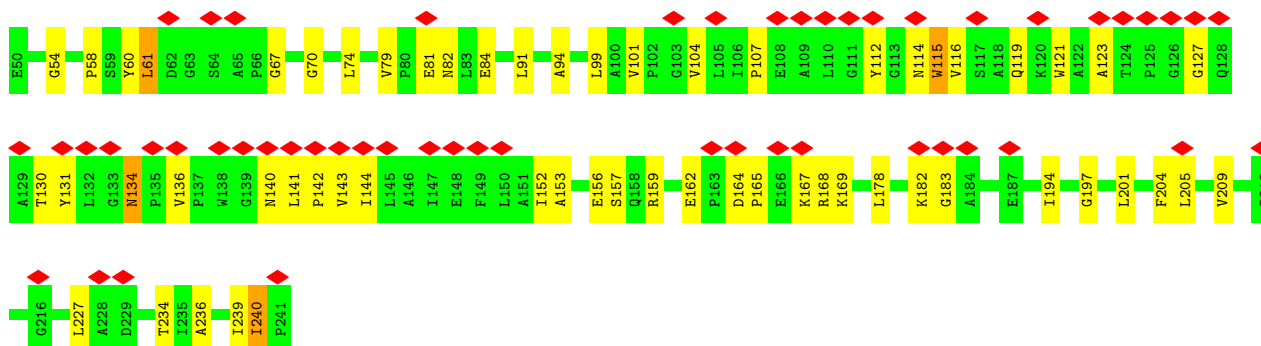
• Molecule 13: Photosystem I reaction center subunit XII



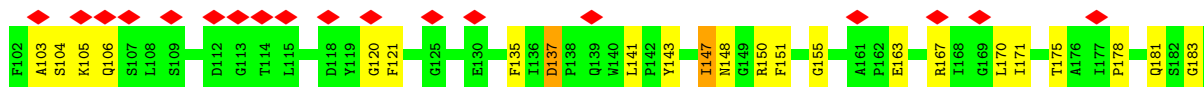
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

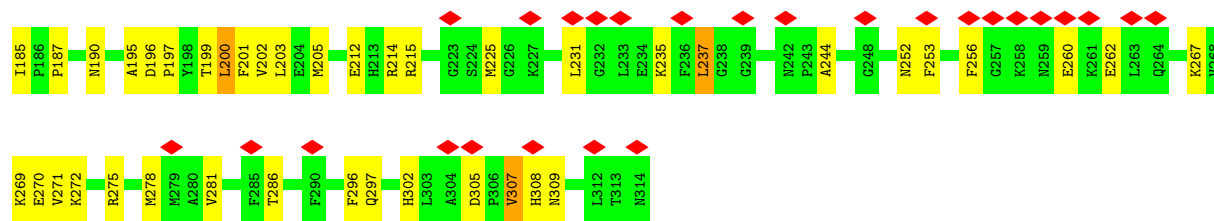


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

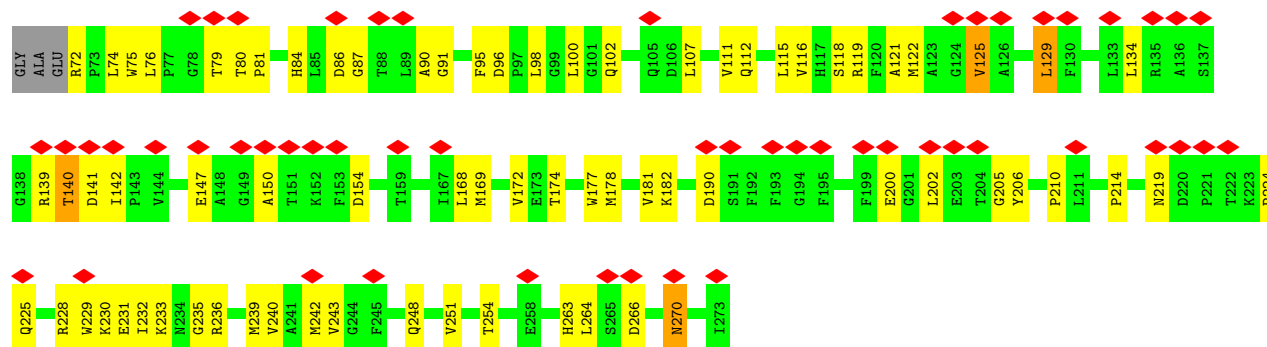


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic





- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	407.424, 407.424, 407.424	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/6032	0.30	0/8227
2	B	0.14	0/6063	0.30	0/8274
3	C	0.18	0/605	0.41	0/821
4	D	0.13	0/1132	0.36	0/1532
5	E	0.12	0/498	0.31	0/677
6	F	0.14	0/1251	0.41	2/1692 (0.1%)
7	G	0.13	0/767	0.36	0/1046
8	H	0.09	0/710	0.26	0/961
9	I	0.15	0/273	0.45	0/373
10	J	0.12	0/334	0.26	0/457
11	K	0.14	0/556	0.37	0/752
12	L	0.12	0/1222	0.31	0/1671
13	M	0.11	0/215	0.22	0/290
14	2	0.13	0/1646	0.30	0/2252
15	6	0.13	0/1522	0.32	0/2081
16	3	0.13	0/1695	0.35	0/2302
17	5	0.14	0/1614	0.37	0/2201
All	All	0.14	0/26135	0.32	2/35609 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	207	ASP	CA-C-N	6.26	124.19	120.24
6	F	207	ASP	C-N-CA	6.26	124.19	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	111	0
2	B	5849	0	5623	123	0
3	C	595	0	576	26	0
4	D	1104	0	1112	15	0
5	E	487	0	480	11	0
6	F	1226	0	1269	28	0
7	G	749	0	729	19	0
8	H	693	0	672	16	0
9	I	266	0	274	7	0
10	J	325	0	341	8	0
11	K	550	0	566	15	0
12	L	1189	0	1200	28	0
13	M	214	0	236	5	0
14	2	1595	0	1561	36	0
15	6	1473	0	1446	44	0
16	3	1644	0	1598	58	0
17	5	1566	0	1531	64	0
18	2	410	0	310	10	0
18	3	577	0	422	11	0
18	5	445	0	318	17	0
18	6	525	0	355	1	0
18	A	2421	0	2229	76	0
18	B	2093	0	1861	58	0
18	F	176	0	128	4	0
18	G	139	0	102	4	0
18	J	42	0	31	0	0
18	K	180	0	126	3	0
18	L	132	0	97	4	0
19	A	33	0	46	1	0
19	B	33	0	46	6	0
20	2	35	0	40	3	0
20	5	37	0	44	5	0
20	6	28	0	26	1	0
20	A	76	0	98	3	0
20	B	23	0	16	1	0
21	2	40	0	56	4	0
21	3	80	0	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	5	40	0	56	2	0
21	A	240	0	336	14	0
21	B	280	0	392	19	0
21	F	40	0	56	4	0
21	G	40	0	56	3	0
21	I	40	0	56	2	0
21	J	80	0	110	6	0
21	K	80	0	112	3	0
21	L	80	0	112	2	0
22	A	8	0	0	0	0
22	C	16	0	0	11	0
23	B	66	0	96	4	0
24	2	26	0	22	0	0
24	J	30	0	30	1	0
25	2	221	0	143	16	0
25	3	40	0	23	1	0
25	5	178	0	116	16	0
25	6	86	0	52	8	0
26	2	42	0	56	3	0
26	3	42	0	55	1	0
26	5	42	0	56	3	0
26	6	42	0	56	3	0
27	2	44	0	56	25	0
27	3	44	0	56	15	0
27	5	44	0	56	30	0
27	6	44	0	56	13	0
All	All	34822	0	33617	760	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (760) 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)
14:2:121:ILE:HD11	27:2:620:XAT:C17	1.25	1.61
3:C:21:CYS:SG	22:C:101:SF4:FE2	1.20	1.34
3:C:14:CYS:SG	22:C:102:SF4:S4	2.29	1.29
14:2:121:ILE:CD1	27:2:620:XAT:H173	1.68	1.22
3:C:21:CYS:SG	22:C:101:SF4:S1	2.38	1.20
14:2:121:ILE:CD1	27:2:620:XAT:C17	2.19	1.19
3:C:14:CYS:SG	22:C:102:SF4:FE3	1.33	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:CYS:SG	22:C:101:SF4:S4	2.43	1.16
25:2:606:CHL:HBB1	27:2:620:XAT:H182	1.26	1.13
3:C:14:CYS:SG	22:C:102:SF4:S2	2.47	1.12
3:C:54:CYS:SG	22:C:101:SF4:FE3	1.42	1.11
16:3:121:PHE:HE2	27:3:619:XAT:H383	1.14	1.10
14:2:121:ILE:HD11	27:2:620:XAT:H172	1.41	1.00
14:2:121:ILE:HD11	27:2:620:XAT:H173	1.02	0.98
25:2:606:CHL:CBB	27:2:620:XAT:C18	2.41	0.98
25:2:606:CHL:HBB1	27:2:620:XAT:C18	1.96	0.95
25:5:607:CHL:C3B	27:5:620:XAT:H163	1.96	0.95
14:2:121:ILE:HD11	27:2:620:XAT:H171	1.48	0.93
14:2:121:ILE:CG1	27:2:620:XAT:H173	1.97	0.92
16:3:121:PHE:CE2	27:3:619:XAT:H383	2.05	0.92
25:2:606:CHL:CBB	27:2:620:XAT:H182	1.99	0.89
3:C:58:CYS:SG	22:C:102:SF4:S2	2.73	0.87
18:2:602:CLA:O1A	27:2:620:XAT:H241	1.76	0.85
3:C:21:CYS:HG	22:C:101:SF4:FE2	0.83	0.85
1:A:416:PRO:HG3	4:D:120:GLU:HB2	1.63	0.80
12:L:70:LEU:HD13	12:L:76:ILE:HB	1.65	0.78
19:A:844:PQN:H172	21:B:801:BCR:H382	1.66	0.78
16:3:121:PHE:HE2	27:3:619:XAT:C38	1.96	0.77
17:5:118:SER:HB3	17:5:235:GLY:HA3	1.66	0.77
25:2:616:CHL:HHC	25:2:616:CHL:HBB1	1.68	0.76
1:A:196:ASN:ND2	1:A:306:GLY:O	2.19	0.75
17:5:243:VAL:HG21	27:5:620:XAT:H401	1.67	0.75
21:A:856:BCR:H312	10:J:31:ARG:HD3	1.68	0.75
17:5:121:ALA:HB2	27:5:620:XAT:H202	1.67	0.74
25:5:607:CHL:HAB	27:5:620:XAT:H161	1.69	0.74
10:J:40:PRO:HG2	21:J:103:BCR:H382	1.69	0.73
2:B:292:ARG:NH1	7:G:92:GLY:O	2.21	0.73
15:6:119:GLN:NE2	27:6:619:XAT:H21	2.04	0.72
9:I:11:VAL:HA	9:I:14:ILE:HG22	1.70	0.72
6:F:158:VAL:HG12	6:F:168:PHE:HB2	1.72	0.72
1:A:170:MET:HE1	18:A:814:CLA:H92	1.71	0.72
17:5:243:VAL:HG21	27:5:620:XAT:C40	2.20	0.71
14:2:240:GLN:HE21	14:2:251:ASN:HD22	1.37	0.71
17:5:125:VAL:HG13	17:5:129:LEU:HD23	1.72	0.71
25:2:606:CHL:HAA1	21:2:621:BCR:H402	1.72	0.70
25:5:607:CHL:CAB	27:5:620:XAT:C16	2.68	0.70
14:2:111:CYS:HB2	14:2:227:GLY:HA3	1.72	0.70
25:5:607:CHL:C3B	27:5:620:XAT:C16	2.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:607:CHL:HHC	25:2:607:CHL:HBB1	1.74	0.69
17:5:74:LEU:HD12	17:5:79:THR:HB	1.73	0.69
14:2:219:LEU:HA	14:2:222:LYS:HD2	1.75	0.68
17:5:242:MET:HE2	27:5:620:XAT:H10	1.75	0.68
18:B:819:CLA:HAA2	18:B:824:CLA:HBB1	1.75	0.68
15:6:178:LEU:HD12	26:6:617:LUT:H222	1.77	0.67
18:5:602:CLA:HMC1	27:5:620:XAT:C32	2.24	0.67
3:C:21:CYS:SG	22:C:101:SF4:S3	2.93	0.67
17:5:95:PHE:CE2	27:5:620:XAT:H383	2.29	0.67
2:B:475:ASP:HA	2:B:479:SER:HB2	1.77	0.67
20:2:622:LHG:HC42	21:3:620:BCR:HC32	1.77	0.66
16:3:231:LEU:HG	21:3:620:BCR:H323	1.77	0.66
3:C:54:CYS:SG	22:C:101:SF4:S1	2.94	0.66
17:5:243:VAL:CG2	27:5:620:XAT:H401	2.24	0.66
6:F:86:ASP:N	6:F:90:LEU:O	2.29	0.66
25:5:608:CHL:HHC	25:5:608:CHL:HBB1	1.77	0.66
2:B:694:LYS:NZ	18:B:839:CLA:O2D	2.29	0.65
25:2:606:CHL:CBB	27:2:620:XAT:H181	2.25	0.65
16:3:167:ARG:HH12	16:3:297:GLN:HE22	1.44	0.65
25:2:606:CHL:HBB2	27:2:620:XAT:C18	2.25	0.65
15:6:234:THR:HG23	15:6:236:ALA:H	1.61	0.65
16:3:212:GLU:OE2	16:3:215:ARG:NH1	2.29	0.65
2:B:42:LEU:O	2:B:46:ILE:HG12	1.97	0.65
17:5:134:LEU:HB2	17:5:139:ARG:HB3	1.78	0.64
3:C:58:CYS:SG	3:C:64:SER:OG	2.54	0.64
18:G:201:CLA:HAC2	15:6:123:ALA:HB2	1.78	0.64
15:6:201:LEU:HD22	27:6:619:XAT:C35	2.27	0.64
1:A:739:TRP:NE1	18:A:829:CLA:O1A	2.28	0.64
2:B:707:LEU:HD23	23:B:850:DGD:HA21	1.78	0.64
2:B:65:LEU:HD11	21:B:845:BCR:H271	1.78	0.64
11:K:69:ALA:O	11:K:80:ARG:NH2	2.32	0.63
1:A:118:ILE:HG23	1:A:119:VAL:HG22	1.80	0.63
15:6:156:GLU:OE1	15:6:159:ARG:NH2	2.30	0.63
15:6:162:GLU:O	15:6:168:ARG:NH2	2.32	0.63
12:L:105:PRO:HA	12:L:108:ARG:HD3	1.80	0.63
20:2:622:LHG:HC82	21:3:620:BCR:HC42	1.80	0.63
2:B:721:TYR:HB2	18:B:802:CLA:HED2	1.81	0.62
18:B:805:CLA:H93	18:B:813:CLA:H2	1.80	0.62
14:2:129:LYS:NZ	14:2:250:ASP:OD1	2.29	0.62
15:6:130:THR:HG22	15:6:131:TYR:H	1.65	0.62
25:6:607:CHL:C2B	27:6:619:XAT:H171	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:217:LYS:HA	17:5:98:LEU:HD22	1.81	0.62
1:A:57:ASP:OD2	1:A:347:HIS:NE2	2.30	0.62
18:2:602:CLA:HMC2	27:2:620:XAT:C31	2.30	0.61
16:3:150:ARG:NH1	16:3:270:GLU:OE2	2.33	0.61
17:5:95:PHE:HE2	27:5:620:XAT:H383	1.65	0.61
16:3:281:VAL:HG21	27:3:619:XAT:H12	1.83	0.61
17:5:206:TYR:HB3	18:5:610:CLA:HED2	1.83	0.61
18:A:843:CLA:H143	21:L:301:BCR:H17C	1.81	0.61
2:B:411:MET:HE2	21:B:846:BCR:H402	1.82	0.61
12:L:70:LEU:HD12	12:L:70:LEU:H	1.66	0.61
12:L:92:TYR:OH	18:L:303:CLA:O1A	2.19	0.61
2:B:201:GLU:OE1	2:B:208:ARG:NH1	2.33	0.60
18:A:843:CLA:HMD3	21:B:848:BCR:H393	1.83	0.60
18:A:834:CLA:HED3	18:A:843:CLA:H12	1.83	0.60
20:B:851:LHG:HC11	15:6:82:ASN:HD22	1.65	0.60
5:E:84:ARG:O	6:F:242:THR:OG1	2.19	0.60
16:3:281:VAL:CG1	27:3:619:XAT:H14	2.31	0.60
2:B:342:GLY:HA2	2:B:345:THR:HG22	1.83	0.60
2:B:729:THR:O	2:B:733:PHE:N	2.32	0.60
4:D:89:ILE:HB	4:D:128:ILE:HG13	1.84	0.60
15:6:84:GLU:OE2	15:6:169:LYS:NZ	2.34	0.60
1:A:327:LYS:H	18:A:845:CLA:HBC2	1.67	0.60
6:F:120:ASP:OD1	6:F:120:ASP:N	2.35	0.60
9:I:14:ILE:HD11	21:I:101:BCR:H333	1.84	0.60
3:C:15:THR:HA	3:C:28:MET:HE3	1.84	0.59
1:A:331:THR:OG1	20:A:847:LHG:O2	2.19	0.59
1:A:433:ALA:O	1:A:437:HIS:HD2	1.84	0.59
18:B:806:CLA:H151	18:B:828:CLA:HBB2	1.83	0.59
2:B:716:GLY:O	2:B:720:THR:HG22	2.03	0.59
18:5:611:CLA:HBC3	20:5:622:LHG:HC62	1.83	0.59
2:B:43:TYR:OH	2:B:169:LYS:NZ	2.35	0.58
2:B:77:TRP:HA	2:B:84:VAL:HG11	1.85	0.58
2:B:167:TRP:CZ2	18:B:813:CLA:HAC2	2.38	0.58
2:B:546:LEU:O	2:B:564:ARG:NH2	2.35	0.58
14:2:190:THR:HG23	14:2:199:GLY:HA2	1.85	0.58
15:6:201:LEU:HD22	27:6:619:XAT:C34	2.32	0.58
4:D:120:GLU:O	4:D:150:ARG:NH1	2.36	0.58
2:B:733:PHE:HE2	8:H:136:PRO:HD2	1.67	0.58
5:E:126:SER:OG	5:E:128:ASP:OD1	2.20	0.58
25:5:607:CHL:C2B	27:5:620:XAT:H163	2.33	0.58
1:A:44:THR:O	1:A:48:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LYS:HB2	2:B:539:LEU:HD13	1.84	0.58
4:D:185:ASN:ND2	4:D:186:ALA:O	2.36	0.58
16:3:178:PRO:HG2	16:3:181:GLN:HB2	1.84	0.58
1:A:14:VAL:HG21	18:A:811:CLA:HED2	1.84	0.58
2:B:85:ARG:HD3	8:H:139:ARG:HD3	1.85	0.58
2:B:684:ARG:NE	12:L:77:GLY:O	2.36	0.58
14:2:189:LEU:HD22	14:2:199:GLY:HA3	1.85	0.58
17:5:119:ARG:NH1	25:5:608:CHL:OBD	2.30	0.58
1:A:330:PHE:O	1:A:426:ARG:NH1	2.37	0.58
16:3:195:ALA:HB3	16:3:200:LEU:HD13	1.85	0.58
16:3:199:THR:HA	16:3:202:VAL:HG12	1.86	0.58
25:6:607:CHL:C2B	27:6:619:XAT:C17	2.82	0.57
1:A:676:PHE:CD1	21:A:852:BCR:H363	2.38	0.57
19:B:842:PQN:H293	23:B:850:DGD:HAE2	1.85	0.57
25:5:607:CHL:HAB	27:5:620:XAT:C16	2.31	0.57
1:A:698:SER:O	2:B:420:SER:OG	2.22	0.57
2:B:435:GLY:HA3	18:B:833:CLA:HAB	1.87	0.57
1:A:353:ASN:ND2	18:A:806:CLA:OBD	2.31	0.57
1:A:471:ASP:O	1:A:475:GLN:NE2	2.38	0.57
4:D:196:ARG:NH2	4:D:217:LEU:O	2.38	0.57
16:3:281:VAL:HG13	27:3:619:XAT:H14	1.87	0.57
1:A:118:ILE:HG12	1:A:119:VAL:HG13	1.86	0.57
2:B:142:LEU:HA	2:B:145:VAL:HG12	1.86	0.57
6:F:139:ALA:O	6:F:143:ASN:ND2	2.38	0.57
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.86	0.57
4:D:174:HIS:HB3	4:D:175:PRO:HD3	1.86	0.57
16:3:185:ILE:HG22	16:3:187:PRO:HD2	1.87	0.57
11:K:71:ARG:HH12	11:K:99:ASP:HB2	1.69	0.57
16:3:148:ASN:ND2	18:3:609:CLA:OBD	2.37	0.57
1:A:503:THR:HG23	1:A:507:TRP:HE1	1.69	0.57
18:A:854:CLA:HAB	2:B:582:TRP:CH2	2.40	0.57
19:B:842:PQN:H12	19:B:842:PQN:H2M3	1.87	0.57
1:A:12:ILE:HD12	18:A:811:CLA:HAA2	1.87	0.56
21:J:103:BCR:H311	21:J:103:BCR:H342	1.87	0.56
15:6:74:LEU:HD12	27:6:619:XAT:H221	1.86	0.56
17:5:112:GLN:HE22	17:5:205:GLY:H	1.52	0.56
1:A:687:SER:OG	1:A:692:TRP:NE1	2.36	0.56
18:A:854:CLA:H42	2:B:438:VAL:HG22	1.87	0.56
1:A:576:PRO:HD2	3:C:52:LYS:HG3	1.86	0.56
6:F:208:VAL:HG21	24:J:104:LMG:H111	1.87	0.56
14:2:193:ASP:OD1	14:2:193:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HD11	1:A:616:VAL:HA	1.88	0.56
2:B:268:LEU:HB2	2:B:273:MET:HE3	1.88	0.56
17:5:210:PRO:HA	17:5:214:PRO:HA	1.87	0.56
2:B:631:LEU:HD11	2:B:724:PHE:HA	1.88	0.55
7:G:151:TYR:HE2	18:G:201:CLA:HED2	1.70	0.55
13:M:14:VAL:O	13:M:18:ILE:HG12	2.05	0.55
16:3:286:THR:HG21	18:3:613:CLA:HAC2	1.88	0.55
1:A:600:ALA:O	1:A:604:VAL:HG23	2.06	0.55
1:A:367:HIS:ND1	18:A:819:CLA:OBD	2.39	0.55
16:3:121:PHE:CE2	27:3:619:XAT:C38	2.80	0.55
21:A:848:BCR:H383	21:K:202:BCR:HC8	1.87	0.55
2:B:351:HIS:ND1	18:B:817:CLA:OBD	2.39	0.55
18:B:803:CLA:H143	21:B:848:BCR:H362	1.89	0.55
15:6:201:LEU:HD22	27:6:619:XAT:C15	2.36	0.55
8:H:67:ASP:HB2	12:L:172:PRO:HB2	1.88	0.55
15:6:58:PRO:HD2	15:6:61:LEU:HB2	1.89	0.55
17:5:266:ASP:O	17:5:270:ASN:ND2	2.40	0.55
18:B:823:CLA:HAB	18:B:830:CLA:HMD2	1.90	0.54
1:A:617:TRP:O	1:A:628:HIS:ND1	2.31	0.54
18:B:815:CLA:HBB1	21:B:843:BCR:H382	1.90	0.54
11:K:81:LYS:NZ	11:K:82:SER:O	2.39	0.54
17:5:100:LEU:CD2	27:5:620:XAT:H373	2.37	0.54
1:A:10:VAL:HG13	18:A:813:CLA:HED3	1.89	0.54
1:A:359:SER:O	1:A:363:ILE:HG12	2.06	0.54
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.26	0.54
14:2:192:THR:OG1	14:2:193:ASP:OD1	2.24	0.54
3:C:60:THR:HG22	3:C:61:ASP:H	1.72	0.54
11:K:81:LYS:H	11:K:90:ASP:HB3	1.73	0.54
15:6:101:VAL:HG21	26:6:617:LUT:H12	1.90	0.54
17:5:121:ALA:HB2	27:5:620:XAT:C20	2.36	0.54
1:A:192:GLU:HG3	1:A:309:TYR:HB3	1.89	0.54
11:K:105:ALA:HA	18:K:201:CLA:HBA2	1.90	0.54
16:3:137:ASP:N	16:3:137:ASP:OD1	2.39	0.54
1:A:576:PRO:HD3	2:B:561:GLY:HA2	1.90	0.54
12:L:138:GLU:OE2	12:L:211:TYR:OH	2.26	0.54
25:5:607:CHL:CMB	27:5:620:XAT:H171	2.37	0.54
4:D:140:ARG:HB2	4:D:143:GLN:HG3	1.90	0.54
17:5:230:LYS:HD3	18:5:612:CLA:HBA1	1.88	0.54
14:2:167:ARG:HA	18:5:601:CLA:HED1	1.91	0.53
16:3:231:LEU:HD22	16:3:231:LEU:H	1.73	0.53
21:J:103:BCR:H371	21:J:103:BCR:H383	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:N	1:A:317:HIS:O	2.40	0.53
2:B:527:LEU:O	2:B:531:THR:HG23	2.09	0.53
6:F:107:ILE:O	6:F:111:GLU:HG2	2.08	0.53
25:2:607:CHL:CMB	27:2:620:XAT:H161	2.38	0.53
16:3:103:ALA:O	16:3:104:SER:OG	2.25	0.53
25:5:607:CHL:CMB	27:5:620:XAT:C17	2.86	0.53
2:B:364:ASP:OD1	8:H:139:ARG:NH2	2.32	0.53
15:6:182:LYS:HG3	15:6:183:GLY:H	1.73	0.53
1:A:476:LEU:HB2	1:A:528:THR:HG23	1.91	0.53
2:B:174:ARG:HB2	18:B:813:CLA:HBC3	1.89	0.53
7:G:85:ARG:NH2	7:G:123:GLY:O	2.38	0.53
9:I:1:MET:HE3	9:I:4:SER:HA	1.91	0.53
2:B:448:THR:OG1	2:B:448:THR:O	2.24	0.53
6:F:101:LYS:HA	6:F:104:LYS:HG2	1.89	0.53
12:L:185:LYS:O	12:L:188:THR:OG1	2.27	0.53
1:A:363:ILE:HD13	18:A:827:CLA:HED3	1.91	0.52
3:C:24:ASP:OD1	3:C:44:ARG:NH2	2.41	0.52
17:5:122:MET:HB3	26:5:619:LUT:H34	1.91	0.52
1:A:687:SER:OG	1:A:688:GLY:N	2.38	0.52
2:B:40:GLU:O	2:B:44:GLN:NE2	2.42	0.52
2:B:405:ASP:OD1	2:B:410:ARG:NH2	2.42	0.52
11:K:60:VAL:O	11:K:64:THR:HG23	2.09	0.52
2:B:294:ASN:HB2	7:G:111:GLU:HA	1.92	0.52
14:2:193:ASP:OD2	14:2:220:ARG:NH2	2.41	0.52
2:B:143:LEU:HD23	13:M:15:SER:HB2	1.90	0.52
4:D:108:VAL:HA	4:D:137:LYS:HA	1.90	0.52
5:E:83:ARG:HB3	5:E:86:SER:HB2	1.92	0.52
16:3:281:VAL:HG11	27:3:619:XAT:C14	2.40	0.52
2:B:363:GLN:O	8:H:137:ARG:NH2	2.43	0.52
16:3:196:ASP:OD1	16:3:197:PRO:HD2	2.10	0.52
14:2:263:THR:OG1	14:2:264:ILE:N	2.43	0.52
1:A:541:ILE:O	1:A:545:VAL:HG23	2.10	0.52
2:B:310:PRO:HD2	2:B:315:LEU:HD11	1.92	0.52
2:B:339:ALA:HB2	21:B:847:BCR:H372	1.91	0.52
18:A:802:CLA:CGA	18:A:802:CLA:H3A	2.40	0.52
2:B:15:ASP:OD1	2:B:17:THR:OG1	2.26	0.52
25:2:607:CHL:HMB3	27:2:620:XAT:C16	2.40	0.52
1:A:18:PRO:HG3	1:A:182:ALA:HB3	1.92	0.51
14:2:69:PHE:HD2	14:2:72:SER:HB2	1.75	0.51
14:2:77:TRP:NE1	14:2:89:ASP:OD2	2.41	0.51
16:3:275:ARG:HA	16:3:278:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:PHE:HE1	18:B:819:CLA:HAB	1.75	0.51
3:C:32:ASP:HA	3:C:37:SER:HA	1.92	0.51
9:I:19:PRO:HA	9:I:22:THR:HG22	1.92	0.51
18:B:814:CLA:HMA2	21:B:845:BCR:H282	1.93	0.51
18:B:833:CLA:O1A	10:J:30:ASN:ND2	2.36	0.51
18:K:203:CLA:HED2	18:K:203:CLA:H2A	1.93	0.51
1:A:60:THR:OG1	1:A:61:ASN:N	2.43	0.51
9:I:7:PRO:O	9:I:11:VAL:HG13	2.11	0.51
15:6:94:ALA:HB1	15:6:197:GLY:HA3	1.91	0.51
2:B:418:ILE:HG23	18:B:838:CLA:HBB2	1.92	0.51
18:B:825:CLA:HAA2	18:B:826:CLA:OBD	2.10	0.51
17:5:233:LYS:HD3	20:5:622:LHG:HC42	1.91	0.51
1:A:445:LEU:O	1:A:449:SER:OG	2.18	0.51
18:B:821:CLA:HMD1	21:B:843:BCR:HC7	1.92	0.51
11:K:51:ILE:O	11:K:56:ASN:ND2	2.43	0.51
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.93	0.51
10:J:7:TYR:O	10:J:10:THR:OG1	2.18	0.51
5:E:80:LYS:HB3	5:E:132:ALA:HB3	1.92	0.51
20:2:622:LHG:HC91	20:2:622:LHG:H281	1.93	0.51
16:3:269:LYS:HD3	18:3:612:CLA:HAA2	1.92	0.51
1:A:54:HIS:CD2	18:A:806:CLA:HBB2	2.46	0.50
21:L:305:BCR:H403	21:L:305:BCR:H23C	1.92	0.50
2:B:136:TYR:CZ	13:M:8:GLN:HB3	2.46	0.50
21:2:621:BCR:HC32	20:5:622:LHG:HC81	1.92	0.50
12:L:118:TYR:HD1	12:L:210:ALA:HB2	1.76	0.50
15:6:239:ILE:HG22	15:6:240:ILE:HG12	1.92	0.50
15:6:91:LEU:HD12	15:6:169:LYS:HB2	1.93	0.50
17:5:79:THR:OG1	17:5:80:THR:N	2.44	0.50
17:5:200:GLU:HB2	17:5:202:LEU:HD23	1.93	0.50
1:A:358:GLY:O	1:A:362:ILE:HG12	2.12	0.50
5:E:101:ALA:HB3	5:E:104:VAL:HG23	1.93	0.50
1:A:337:GLY:HA3	1:A:421:ASN:HD22	1.75	0.50
21:A:852:BCR:H362	18:A:854:CLA:H43	1.94	0.50
14:2:167:ARG:HH12	14:2:182:PRO:HG3	1.76	0.50
1:A:411:VAL:HG23	1:A:555:ALA:HB1	1.94	0.50
2:B:90:ALA:HA	2:B:113:VAL:HG12	1.93	0.50
2:B:276:HIS:HB2	18:B:817:CLA:C1B	2.42	0.50
17:5:91:GLY:H	17:5:229:TRP:CD1	2.30	0.50
1:A:465:PRO:HA	1:A:468:MET:HG3	1.94	0.49
1:A:571:PHE:CE1	1:A:585:SER:HB3	2.48	0.49
2:B:101:VAL:HG13	2:B:112:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5:74:LEU:HD11	17:5:81:PRO:HB3	1.94	0.49
17:5:100:LEU:HD22	27:5:620:XAT:H373	1.94	0.49
21:B:843:BCR:HC8	7:G:135:LEU:HD13	1.94	0.49
4:D:109:ILE:HG13	4:D:161:PHE:HB3	1.93	0.49
1:A:427:VAL:HA	1:A:430:HIS:CE1	2.46	0.49
1:A:656:VAL:O	1:A:659:SER:OG	2.25	0.49
4:D:161:PHE:CZ	4:D:174:HIS:HB2	2.47	0.49
15:6:61:LEU:HD12	15:6:70:GLY:HA2	1.93	0.49
16:3:267:LYS:O	16:3:271:VAL:HG13	2.11	0.49
2:B:388:ALA:O	2:B:392:ILE:HG13	2.12	0.49
9:I:11:VAL:HG22	9:I:12:PRO:HD3	1.93	0.49
16:3:302:HIS:CG	18:3:613:CLA:HAA2	2.47	0.49
1:A:40:PRO:HG3	6:F:204:ILE:HD13	1.95	0.49
1:A:732:LEU:HD12	18:A:842:CLA:HMA3	1.94	0.49
18:B:814:CLA:C1B	21:B:845:BCR:H20C	2.42	0.49
17:5:225:GLN:O	17:5:229:TRP:HB2	2.13	0.49
2:B:300:SER:HB3	7:G:91:GLN:HB2	1.93	0.49
3:C:55:GLU:OE1	3:C:66:ARG:NH1	2.45	0.49
12:L:171:ALA:HB3	12:L:183:ALA:HB1	1.94	0.49
15:6:164:ASP:HB3	15:6:167:LYS:HB2	1.93	0.49
12:L:121:VAL:HG11	12:L:210:ALA:HB1	1.94	0.49
2:B:256:THR:OG1	2:B:257:PHE:N	2.46	0.49
17:5:84:HIS:NE2	17:5:96:ASP:OD2	2.46	0.49
17:5:86:ASP:OD1	17:5:87:GLY:N	2.43	0.49
17:5:264:LEU:HD21	18:5:614:CLA:HMC2	1.94	0.49
17:5:140:THR:HG22	17:5:141:ASP:H	1.78	0.49
7:G:125:THR:OG1	7:G:126:ILE:N	2.46	0.48
25:6:607:CHL:HHC	25:6:607:CHL:HBB1	1.94	0.48
16:3:121:PHE:CE2	27:3:619:XAT:H242	2.48	0.48
6:F:114:LEU:HA	6:F:127:LEU:HD13	1.95	0.48
18:5:613:CLA:O2D	18:5:613:CLA:H2A	2.13	0.48
1:A:43:THR:HG22	1:A:715:ARG:H	1.77	0.48
2:B:292:ARG:HH21	2:B:296:GLY:HA2	1.78	0.48
2:B:358:TYR:OH	18:B:828:CLA:OBD	2.24	0.48
18:B:826:CLA:H92	18:B:826:CLA:H62	1.69	0.48
17:5:224:PRO:HG2	17:5:228:ARG:HD2	1.94	0.48
1:A:537:HIS:HE1	1:A:603:VAL:HG12	1.78	0.48
2:B:733:PHE:HB3	8:H:137:ARG:HD3	1.94	0.48
15:6:67:GLY:HA3	15:6:194:ILE:HG21	1.93	0.48
1:A:422:ASN:HB3	1:A:426:ARG:HG3	1.95	0.48
2:B:9:SER:O	2:B:13:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:ARG:O	2:B:414:HIS:ND1	2.43	0.48
2:B:459:PHE:HD1	18:F:304:CLA:HMC2	1.79	0.48
18:5:602:CLA:HMC1	27:5:620:XAT:C31	2.42	0.48
2:B:292:ARG:NE	2:B:296:GLY:O	2.34	0.48
2:B:704:GLN:O	2:B:708:VAL:HG23	2.14	0.48
15:6:205:LEU:O	15:6:209:VAL:HG23	2.14	0.48
2:B:576:PHE:O	2:B:580:VAL:HG23	2.14	0.48
18:B:816:CLA:H61	7:G:142:PHE:HD1	1.77	0.48
12:L:164:LYS:HB3	12:L:167:GLU:HG2	1.96	0.48
2:B:91:ILE:HD11	2:B:112:PRO:HB2	1.96	0.48
18:5:602:CLA:CBB	27:5:620:XAT:H34	2.44	0.48
1:A:317:HIS:NE2	18:A:824:CLA:OBD	2.46	0.48
14:2:219:LEU:HD22	18:2:610:CLA:HMA1	1.94	0.48
25:2:606:CHL:HBB2	27:2:620:XAT:H181	1.92	0.47
2:B:84:VAL:HG23	8:H:140:LYS:HG2	1.96	0.47
8:H:62:THR:O	8:H:62:THR:OG1	2.29	0.47
16:3:150:ARG:NH2	16:3:244:ALA:O	2.47	0.47
1:A:444:PHE:HE2	18:A:839:CLA:HAB	1.78	0.47
1:A:537:HIS:HB3	18:A:838:CLA:HAB	1.95	0.47
18:A:819:CLA:H3A	18:A:819:CLA:HBA2	1.50	0.47
18:A:833:CLA:H3A	18:A:833:CLA:HBA2	1.55	0.47
2:B:671:TRP:O	2:B:675:ILE:HG12	2.13	0.47
18:B:815:CLA:H112	18:B:815:CLA:H91	1.68	0.47
6:F:204:ILE:HG13	6:F:205:ILE:HG12	1.95	0.47
14:2:181:ASP:OD2	14:2:187:ASN:ND2	2.47	0.47
16:3:235:LYS:HB3	16:3:237:LEU:HD11	1.96	0.47
6:F:227:GLY:O	6:F:231:SER:OG	2.24	0.47
18:A:826:CLA:H141	18:A:826:CLA:H162	1.72	0.47
18:B:816:CLA:CHD	18:B:817:CLA:HBB2	2.44	0.47
7:G:61:THR:O	7:G:65:ILE:HG23	2.14	0.47
17:5:72:ARG:NH1	17:5:86:ASP:O	2.38	0.47
17:5:236:ARG:O	17:5:240:VAL:HG22	2.14	0.47
2:B:364:ASP:OD2	2:B:367:THR:OG1	2.22	0.47
18:B:807:CLA:H2	18:B:807:CLA:H62	1.73	0.47
10:J:10:THR:HG22	10:J:12:PRO:HD2	1.97	0.47
15:6:134:ASN:OD1	15:6:134:ASN:N	2.36	0.47
25:6:601:CHL:HMA2	17:5:174:THR:HG21	1.97	0.47
1:A:646:ARG:HA	1:A:650:TRP:HB3	1.96	0.47
1:A:680:PHE:HZ	18:A:842:CLA:HBC2	1.78	0.47
2:B:182:LEU:HD13	18:B:813:CLA:HBB	1.96	0.47
18:B:839:CLA:HBB2	19:B:842:PQN:H141	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:ASP:OD2	4:D:174:HIS:ND1	2.42	0.47
15:6:60:TYR:HD2	15:6:61:LEU:HD23	1.80	0.47
15:6:60:TYR:CD2	15:6:61:LEU:HD23	2.49	0.47
16:3:141:LEU:HD13	18:3:602:CLA:H12	1.96	0.47
16:3:155:GLY:HA2	27:3:619:XAT:H181	1.97	0.47
16:3:262:GLU:OE1	16:3:262:GLU:N	2.41	0.47
18:5:613:CLA:HMA2	26:5:619:LUT:H3	1.97	0.47
1:A:511:ASP:OD1	1:A:511:ASP:N	2.48	0.47
18:A:829:CLA:H92	18:A:829:CLA:H41	1.97	0.47
6:F:210:LEU:O	6:F:214:ILE:HG13	2.15	0.47
17:5:91:GLY:H	17:5:229:TRP:NE1	2.13	0.47
18:A:829:CLA:H162	18:A:829:CLA:H202	1.70	0.47
18:A:829:CLA:H191	21:J:102:BCR:H19C	1.96	0.47
2:B:2:ALA:HA	2:B:7:LYS:HA	1.97	0.47
4:D:145:LEU:HD23	4:D:145:LEU:HA	1.78	0.47
14:2:184:PHE:O	14:2:186:ASN:N	2.42	0.47
25:6:607:CHL:C1B	27:6:619:XAT:H172	2.45	0.47
1:A:294:HIS:HE1	18:A:820:CLA:C1B	2.27	0.47
18:A:814:CLA:HAA2	18:A:826:CLA:H52	1.96	0.47
2:B:438:VAL:O	2:B:442:VAL:HG23	2.14	0.47
18:B:805:CLA:HED1	18:B:829:CLA:HBB2	1.96	0.47
12:L:111:GLU:HB2	18:L:302:CLA:HED1	1.97	0.47
25:6:607:CHL:CMB	27:6:619:XAT:H171	2.44	0.47
18:B:812:CLA:H3A	18:B:812:CLA:HBA2	1.43	0.46
18:2:610:CLA:H3A	18:2:610:CLA:HBA2	1.49	0.46
2:B:129:LEU:HD22	2:B:134:ASP:HB3	1.96	0.46
25:2:607:CHL:CMB	27:2:620:XAT:C16	2.93	0.46
16:3:183:GLY:H	16:3:190:ASN:HA	1.81	0.46
17:5:263:HIS:HA	17:5:270:ASN:CG	2.40	0.46
18:A:831:CLA:H92	18:A:831:CLA:H61	1.75	0.46
2:B:467:HIS:HD2	2:B:509:PHE:CZ	2.33	0.46
19:B:842:PQN:H242	21:B:848:BCR:H17C	1.97	0.46
8:H:71:ASN:HD22	12:L:100:ARG:HG2	1.81	0.46
11:K:107:ASP:OD1	11:K:107:ASP:N	2.48	0.46
1:A:10:VAL:O	1:A:312:ASN:ND2	2.48	0.46
18:B:828:CLA:H171	21:B:844:BCR:H352	1.97	0.46
3:C:29:VAL:HG12	3:C:39:ILE:HG22	1.96	0.46
17:5:112:GLN:NE2	17:5:205:GLY:H	2.13	0.46
18:B:840:CLA:H2A	18:B:840:CLA:O1D	2.16	0.46
8:H:60:ASP:HA	8:H:63:THR:HG22	1.97	0.46
14:2:240:GLN:HE22	26:2:619:LUT:H24	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:809:CLA:HBB1	18:A:809:CLA:HMB1	1.98	0.46
2:B:720:THR:HG23	18:B:802:CLA:O1D	2.15	0.46
3:C:33:GLY:O	5:E:104:VAL:HA	2.16	0.46
6:F:170:TYR:HB3	10:J:39:LEU:HD23	1.97	0.46
18:2:604:CLA:H2A	18:2:604:CLA:O2D	2.15	0.46
2:B:27:THR:HG23	23:B:850:DGD:HG31	1.96	0.46
6:F:135:LYS:HB2	6:F:135:LYS:HE3	1.71	0.46
17:5:231:GLU:HG3	18:5:610:CLA:C1B	2.46	0.46
1:A:275:PHE:CE2	18:A:837:CLA:HED1	2.51	0.46
2:B:203:ARG:HG3	2:B:250:ALA:HB1	1.97	0.46
15:6:201:LEU:CD2	27:6:619:XAT:C15	2.94	0.46
18:A:806:CLA:H101	18:A:814:CLA:H43	1.97	0.45
2:B:309:THR:O	2:B:309:THR:OG1	2.34	0.45
2:B:649:MET:O	2:B:652:PHE:HB3	2.16	0.45
17:5:239:MET:SD	18:5:602:CLA:HBB1	2.56	0.45
25:5:607:CHL:CAB	27:5:620:XAT:H161	2.34	0.45
4:D:122:PRO:HD3	4:D:147:LEU:HD13	1.99	0.45
6:F:212:LEU:HB3	18:F:305:CLA:HMD3	1.98	0.45
7:G:85:ARG:NH2	7:G:128:ASP:OD2	2.49	0.45
12:L:119:LEU:HD13	18:L:304:CLA:HBC2	1.99	0.45
21:2:621:BCR:H24C	21:2:621:BCR:H371	1.76	0.45
2:B:442:VAL:HG21	18:B:833:CLA:HAC2	1.98	0.45
4:D:118:ILE:HG12	4:D:128:ILE:HG22	1.99	0.45
14:2:121:ILE:CD1	27:2:620:XAT:H172	2.17	0.45
17:5:202:LEU:HG	17:5:206:TYR:HB2	1.97	0.45
1:A:335:HIS:HB3	1:A:338:LEU:HD12	1.98	0.45
1:A:536:ILE:O	1:A:540:THR:HG23	2.16	0.45
2:B:434:LEU:O	2:B:438:VAL:HG23	2.15	0.45
18:B:815:CLA:H61	18:B:815:CLA:H41	1.64	0.45
11:K:97:THR:OG1	11:K:98:GLY:N	2.50	0.45
17:5:84:HIS:ND1	17:5:102:GLN:OE1	2.49	0.45
1:A:48:ASN:HA	1:A:51:ALA:HB3	1.99	0.45
1:A:147:ALA:HB2	1:A:375:PRO:HD2	1.99	0.45
2:B:152:ALA:HB2	18:B:811:CLA:HBC2	1.99	0.45
18:B:806:CLA:H2	18:B:806:CLA:H62	1.64	0.45
14:2:230:ALA:O	14:2:234:VAL:HG12	2.17	0.45
1:A:92:GLY:HA3	1:A:145:TRP:CH2	2.51	0.45
18:A:818:CLA:H93	11:K:120:VAL:HG12	1.99	0.45
2:B:569:ASP:OD1	2:B:574:ASP:HB3	2.15	0.45
18:B:823:CLA:C4A	21:B:846:BCR:H16C	2.47	0.45
16:3:281:VAL:CG1	27:3:619:XAT:C14	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LYS:HZ1	6:F:243:VAL:HG21	1.82	0.45
18:B:818:CLA:HBA2	18:B:818:CLA:H3A	1.43	0.45
6:F:151:ASP:OD1	6:F:151:ASP:N	2.50	0.45
1:A:13:MET:HB2	1:A:187:TRP:HB2	1.99	0.45
16:3:105:LYS:HB3	16:3:120:GLY:O	2.16	0.45
1:A:646:ARG:HB3	2:B:632:ILE:HD12	1.99	0.45
2:B:75:GLU:OE2	2:B:132:ASN:ND2	2.50	0.45
2:B:345:THR:HA	2:B:348:VAL:HG12	1.99	0.45
27:6:619:XAT:H35	27:6:619:XAT:H401	1.64	0.45
26:3:618:LUT:H31	26:3:618:LUT:H391	1.87	0.45
27:5:620:XAT:H373	27:5:620:XAT:H23	1.81	0.45
1:A:575:GLY:HA2	2:B:562:PRO:HD3	1.99	0.45
18:B:809:CLA:H91	18:B:840:CLA:H12	1.98	0.45
16:3:147:ILE:HD11	18:3:609:CLA:CAD	2.47	0.45
16:3:281:VAL:HG11	27:3:619:XAT:C12	2.47	0.45
17:5:112:GLN:O	17:5:116:VAL:HG22	2.17	0.45
1:A:25:LYS:HB3	18:A:812:CLA:HAA2	2.00	0.44
21:A:856:BCR:H20C	21:A:856:BCR:H361	1.84	0.44
21:G:205:BCR:H24C	21:G:205:BCR:H371	1.78	0.44
8:H:55:ASP:OD1	8:H:57:GLY:N	2.44	0.44
16:3:163:GLU:CD	16:3:296:PHE:HB3	2.42	0.44
1:A:147:ALA:HB1	18:A:820:CLA:HED1	1.98	0.44
1:A:693:GLN:HE22	1:A:715:ARG:HA	1.82	0.44
18:A:826:CLA:H62	18:A:826:CLA:H2	1.60	0.44
18:A:835:CLA:O2D	18:A:835:CLA:H2A	2.17	0.44
7:G:99:VAL:HG22	7:G:103:ASP:HB2	1.99	0.44
11:K:74:LEU:HD23	11:K:74:LEU:HA	1.76	0.44
18:2:604:CLA:HMB3	18:2:604:CLA:HBB1	1.99	0.44
1:A:40:PRO:HB3	1:A:45:TRP:CE3	2.53	0.44
18:A:827:CLA:HAB	21:A:851:BCR:H311	1.99	0.44
18:B:821:CLA:H3A	18:B:822:CLA:H42	1.99	0.44
12:L:138:GLU:N	12:L:138:GLU:OE1	2.50	0.44
1:A:467:ASP:HB3	18:A:835:CLA:HED3	2.00	0.44
2:B:65:LEU:HD12	2:B:142:LEU:HD12	1.99	0.44
2:B:158:GLN:O	2:B:162:LYS:HG3	2.18	0.44
2:B:516:ASP:OD2	2:B:597:LYS:NZ	2.43	0.44
5:E:81:VAL:HG12	5:E:83:ARG:H	1.82	0.44
21:F:302:BCR:H20C	21:F:302:BCR:H361	1.84	0.44
15:6:140:ASN:HB3	15:6:143:VAL:HG22	2.00	0.44
17:5:125:VAL:HG23	17:5:242:MET:HG2	1.99	0.44
1:A:156:LEU:O	1:A:159:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:HIS:O	1:A:394:ILE:HG12	2.18	0.44
8:H:69:TYR:OH	12:L:84:THR:O	2.36	0.44
27:5:620:XAT:H401	27:5:620:XAT:H35	1.78	0.44
27:5:620:XAT:H31	27:5:620:XAT:H391	1.85	0.44
1:A:52:ASP:OD2	20:A:846:LHG:O2	2.25	0.44
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.98	0.44
3:C:12:ILE:HG21	5:E:124:ASN:HD21	1.83	0.44
14:2:123:ILE:HB	14:2:124:PRO:HD3	2.00	0.44
25:5:607:CHL:HHC	25:5:607:CHL:HBB1	1.99	0.44
18:A:809:CLA:H3A	18:A:809:CLA:HBA2	1.35	0.44
18:A:820:CLA:H3A	18:A:820:CLA:HBA2	1.38	0.44
18:A:824:CLA:O1D	18:A:824:CLA:H2A	2.18	0.44
2:B:441:ASP:OD2	2:B:615:TYR:HB2	2.18	0.44
16:3:214:ARG:HH21	16:3:237:LEU:HD13	1.82	0.44
16:3:281:VAL:HG11	27:3:619:XAT:H14	1.98	0.44
17:5:169:MET:HE3	17:5:169:MET:HB3	1.93	0.44
1:A:694:GLU:OE1	2:B:536:LYS:NZ	2.47	0.44
21:A:848:BCR:H362	21:A:849:BCR:H21C	2.00	0.44
2:B:519:VAL:HG11	2:B:593:TYR:HB2	2.00	0.44
6:F:174:VAL:O	6:F:178:ILE:HG13	2.18	0.44
14:2:70:PRO:HB2	16:3:225:MET:HE1	1.99	0.44
25:3:608:CHL:HHC	25:3:608:CHL:HBB1	1.99	0.44
17:5:147:GLU:HA	17:5:150:ALA:HB3	2.00	0.44
17:5:202:LEU:HD12	17:5:228:ARG:NH2	2.33	0.44
1:A:44:THR:HG23	1:A:715:ARG:HB2	1.99	0.43
18:A:801:CLA:H162	18:A:801:CLA:H122	1.73	0.43
18:A:831:CLA:H62	18:A:831:CLA:H41	1.82	0.43
18:A:833:CLA:HMB1	18:A:843:CLA:HAA2	1.99	0.43
2:B:48:ALA:HB3	13:M:30:LEU:HD21	2.00	0.43
9:I:26:LEU:O	9:I:30:ILE:HG12	2.18	0.43
15:6:107:PRO:O	15:6:112:TYR:N	2.50	0.43
1:A:346:TRP:HB3	18:A:806:CLA:HAC1	2.00	0.43
21:A:852:BCR:H20C	21:A:852:BCR:H361	1.73	0.43
21:A:856:BCR:H11C	21:A:856:BCR:H341	1.91	0.43
18:B:809:CLA:H121	18:B:809:CLA:H161	1.77	0.43
15:6:152:ILE:HG21	18:6:609:CLA:HMC3	2.00	0.43
25:6:601:CHL:HMC	20:6:620:LHG:HC41	2.00	0.43
16:3:201:PHE:O	16:3:205:MET:HG2	2.17	0.43
18:A:827:CLA:HAA2	18:A:828:CLA:OBD	2.18	0.43
18:A:841:CLA:HED3	18:A:841:CLA:H2A	2.00	0.43
21:A:848:BCR:H20C	21:A:848:BCR:H361	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:619:LUT:H15	26:2:619:LUT:H201	1.67	0.43
16:3:214:ARG:NH1	16:3:225:MET:SD	2.91	0.43
1:A:294:HIS:HB2	18:A:819:CLA:C1B	2.48	0.43
2:B:357:PRO:HG3	18:B:818:CLA:HBA1	2.00	0.43
18:B:827:CLA:H3A	18:B:827:CLA:HBA2	1.43	0.43
12:L:145:ALA:O	12:L:149:THR:HG22	2.17	0.43
16:3:231:LEU:HD23	21:3:620:BCR:HC8	2.00	0.43
1:A:550:LYS:HD3	2:B:670:TYR:CE1	2.54	0.43
21:G:205:BCR:H20C	21:G:205:BCR:H361	1.82	0.43
11:K:82:SER:OG	11:K:83:THR:N	2.50	0.43
12:L:70:LEU:HD11	12:L:78:GLY:N	2.33	0.43
16:3:305:ASP:O	16:3:309:ASN:HB2	2.19	0.43
25:5:607:CHL:HMB1	27:5:620:XAT:H171	2.00	0.43
1:A:147:ALA:O	1:A:218:SER:OG	2.37	0.43
18:A:809:CLA:CHC	18:A:810:CLA:HMD2	2.49	0.43
18:B:826:CLA:H112	18:B:826:CLA:H71	1.73	0.43
15:6:54:GLY:HA3	17:5:178:MET:HE2	1.99	0.43
15:6:165:PRO:HA	15:6:168:ARG:HB3	2.01	0.43
1:A:572:PRO:HB3	1:A:719:ILE:HB	1.99	0.43
18:A:832:CLA:HAB	18:A:840:CLA:HBB2	2.01	0.43
2:B:516:ASP:OD2	2:B:593:TYR:OH	2.28	0.43
3:C:23:THR:HB	3:C:25:VAL:HG23	2.00	0.43
8:H:93:THR:O	12:L:193:ALA:HB1	2.19	0.43
13:M:7:SER:O	13:M:11:VAL:HG23	2.19	0.43
17:5:91:GLY:HA3	17:5:232:ILE:HD11	2.01	0.43
17:5:219:ASN:OD1	17:5:219:ASN:N	2.47	0.43
1:A:411:VAL:HG11	1:A:569:PHE:HB2	2.00	0.43
18:A:841:CLA:HAA2	18:B:831:CLA:HMB1	2.01	0.43
18:B:835:CLA:HBA2	18:B:835:CLA:H3A	1.67	0.43
5:E:108:VAL:O	5:E:124:ASN:HA	2.18	0.43
18:G:204:CLA:H3A	18:G:204:CLA:HBA1	1.76	0.43
2:B:404:LYS:HA	2:B:404:LYS:HD2	1.81	0.43
2:B:658:ALA:HB3	18:B:803:CLA:HBB2	2.01	0.43
18:B:840:CLA:H2	19:B:842:PQN:H252	2.00	0.43
6:F:219:LEU:HD23	6:F:220:THR:HG23	2.01	0.43
21:I:101:BCR:H20C	21:I:101:BCR:H361	1.83	0.43
12:L:156:THR:O	12:L:160:ILE:HG13	2.18	0.43
14:2:117:GLY:HA3	27:2:620:XAT:H8	2.00	0.43
21:B:843:BCR:H15C	21:B:843:BCR:H351	1.87	0.43
6:F:103:GLU:HG3	6:F:138:PHE:CG	2.54	0.43
17:5:263:HIS:ND1	18:5:613:CLA:HAA2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG21	1:A:743:LEU:HD21	2.00	0.42
18:A:827:CLA:H51	18:A:838:CLA:H2	2.00	0.42
2:B:428:PHE:CZ	21:J:103:BCR:HC21	2.54	0.42
2:B:595:HIS:ND1	2:B:623:TYR:OH	2.48	0.42
18:B:808:CLA:O1A	18:B:827:CLA:HBD	2.18	0.42
21:B:848:BCR:H20C	21:B:848:BCR:H361	1.81	0.42
11:K:114:LEU:HD23	11:K:114:LEU:HA	1.87	0.42
15:6:141:LEU:HB3	15:6:142:PRO:HD3	2.01	0.42
16:3:272:LYS:HB3	18:3:611:CLA:O1D	2.19	0.42
1:A:645:LEU:HD22	2:B:651:LEU:HD21	2.00	0.42
18:A:812:CLA:H62	18:A:812:CLA:H92	1.86	0.42
2:B:345:THR:HG23	2:B:379:ALA:HB2	2.00	0.42
6:F:190:LEU:HD11	18:F:301:CLA:HMD1	2.00	0.42
15:6:114:ASN:C	15:6:116:VAL:H	2.27	0.42
16:3:183:GLY:HA3	18:3:606:CLA:HBC1	2.01	0.42
17:5:154:ASP:OD1	17:5:154:ASP:N	2.51	0.42
25:5:607:CHL:HMB3	27:5:620:XAT:C17	2.48	0.42
1:A:65:GLU:N	1:A:65:GLU:OE1	2.53	0.42
1:A:707:LYS:HE2	6:F:236:GLU:HG2	2.01	0.42
2:B:194:LEU:HA	2:B:198:ALA:HB3	2.00	0.42
18:2:602:CLA:H3A	18:2:602:CLA:HBA2	1.46	0.42
17:5:177:TRP:O	17:5:181:VAL:HG12	2.19	0.42
12:L:70:LEU:HA	12:L:80:GLU:HG3	2.02	0.42
12:L:125:VAL:HG22	12:L:140:GLY:HA3	2.02	0.42
27:2:620:XAT:H15	27:2:620:XAT:H201	1.83	0.42
25:5:607:CHL:CAB	27:5:620:XAT:H163	2.38	0.42
18:A:814:CLA:H111	18:A:814:CLA:H91	1.80	0.42
18:A:814:CLA:H61	18:A:814:CLA:H101	1.76	0.42
18:B:831:CLA:C1B	21:F:302:BCR:H11C	2.50	0.42
7:G:152:ASN:N	7:G:153:PRO:HD3	2.35	0.42
8:H:69:TYR:CZ	12:L:93:LEU:HD13	2.54	0.42
15:6:121:TRP:HB2	15:6:127:GLY:HA3	2.01	0.42
17:5:214:PRO:HD2	26:5:619:LUT:H23	2.00	0.42
1:A:504:SER:OG	1:A:506:THR:OG1	2.32	0.42
18:A:854:CLA:H11	2:B:616:LEU:HD23	2.02	0.42
2:B:160:LYS:HB2	2:B:160:LYS:HE3	1.80	0.42
7:G:61:THR:HA	7:G:64:THR:HG22	2.02	0.42
12:L:128:GLY:H	12:L:131:ARG:HB3	1.84	0.42
14:2:117:GLY:CA	27:2:620:XAT:H8	2.50	0.42
15:6:99:LEU:HD23	15:6:99:LEU:HA	1.91	0.42
16:3:278:MET:HG2	27:3:619:XAT:C15	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:619:XAT:H15	27:3:619:XAT:H201	1.77	0.42
18:5:602:CLA:HBB2	27:5:620:XAT:H34	2.01	0.42
18:B:821:CLA:CMD	21:B:843:BCR:HC7	2.50	0.42
14:2:140:VAL:HG12	25:2:607:CHL:HED2	2.00	0.42
25:6:607:CHL:HBB1	25:6:607:CHL:CHC	2.50	0.42
1:A:139:SER:OG	18:A:809:CLA:OBD	2.38	0.42
1:A:513:VAL:HG23	1:A:520:ALA:HB3	2.02	0.42
2:B:228:GLY:HA3	7:G:144:LEU:HD13	2.01	0.42
5:E:107:PRO:HD2	5:E:127:PRO:HD3	2.01	0.42
12:L:95:ASN:HB3	18:L:302:CLA:HAC1	2.01	0.42
15:6:141:LEU:HA	15:6:144:ILE:HG22	2.02	0.42
15:6:144:ILE:HA	15:6:144:ILE:HD12	1.82	0.42
26:6:617:LUT:H15	26:6:617:LUT:H201	1.83	0.42
18:A:854:CLA:H142	18:A:854:CLA:H112	1.81	0.42
2:B:98:GLN:O	2:B:102:GLU:HG2	2.19	0.42
2:B:466:ALA:HA	2:B:476:VAL:O	2.20	0.42
2:B:548:PRO:HD2	3:C:62:PHE:CE1	2.54	0.42
11:K:117:VAL:HG22	21:K:207:BCR:H313	2.01	0.42
16:3:272:LYS:HB3	18:3:611:CLA:CGD	2.49	0.42
17:5:90:ALA:HA	17:5:229:TRP:CD1	2.55	0.42
17:5:178:MET:HE1	17:5:182:LYS:HE2	2.02	0.42
1:A:262:PHE:HA	18:K:204:CLA:HBC3	2.02	0.42
18:A:805:CLA:HAA1	18:A:812:CLA:H2	2.02	0.42
7:G:144:LEU:HD23	7:G:144:LEU:HA	1.88	0.42
15:6:115:TRP:O	15:6:119:GLN:NE2	2.53	0.42
16:3:151:PHE:CE1	18:3:609:CLA:HBC3	2.55	0.42
21:3:620:BCR:H371	21:3:620:BCR:H24C	1.81	0.42
27:5:620:XAT:H30	27:5:620:XAT:H27	1.70	0.42
21:5:621:BCR:H24C	21:5:621:BCR:H371	1.84	0.42
18:A:830:CLA:H161	18:A:830:CLA:H192	1.81	0.41
2:B:31:PHE:O	2:B:37:MET:HG3	2.20	0.41
2:B:172:GLU:HG3	7:G:94:PRO:HB3	2.02	0.41
2:B:429:LEU:HB3	2:B:525:LEU:HB2	2.02	0.41
16:3:307:VAL:HG13	16:3:308:HIS:CD2	2.55	0.41
21:5:621:BCR:H15C	21:5:621:BCR:H351	1.93	0.41
18:A:826:CLA:H192	18:A:826:CLA:H161	1.89	0.41
2:B:616:LEU:HD12	2:B:616:LEU:HA	1.80	0.41
2:B:733:PHE:CE2	8:H:136:PRO:HD2	2.52	0.41
6:F:176:LEU:HD23	6:F:176:LEU:HA	1.90	0.41
6:F:221:TRP:CG	6:F:222:PRO:HD3	2.55	0.41
7:G:113:THR:HA	7:G:116:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:248:PRO:O	26:2:619:LUT:O23	2.28	0.41
15:6:227:LEU:HD13	15:6:227:LEU:HA	1.89	0.41
21:3:622:BCR:H361	21:3:622:BCR:H20C	1.82	0.41
17:5:107:LEU:O	17:5:111:VAL:HG23	2.19	0.41
1:A:435:ILE:HG13	1:A:554:PHE:HE1	1.85	0.41
18:A:829:CLA:H72	18:A:829:CLA:H111	1.60	0.41
2:B:523:ILE:HG12	2:B:590:VAL:HG22	2.03	0.41
18:B:813:CLA:H62	18:B:818:CLA:HBC3	2.02	0.41
18:B:831:CLA:C1C	21:F:302:BCR:H15C	2.51	0.41
10:J:39:LEU:HD13	21:J:103:BCR:H20C	2.01	0.41
14:2:198:GLY:N	18:2:610:CLA:OBD	2.52	0.41
27:2:620:XAT:H35	27:2:620:XAT:H401	1.85	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.91	0.41
1:A:373:PRO:HG3	18:A:820:CLA:HBA1	2.02	0.41
3:C:34:CYS:SG	3:C:35:LYS:N	2.90	0.41
8:H:112:TYR:O	8:H:116:THR:OG1	2.38	0.41
21:3:622:BCR:H403	21:3:622:BCR:H371	2.01	0.41
17:5:75:TRP:CE2	17:5:76:LEU:HD22	2.55	0.41
17:5:125:VAL:HG13	17:5:129:LEU:CD2	2.46	0.41
17:5:129:LEU:HD13	17:5:129:LEU:HA	1.79	0.41
1:A:138:THR:O	1:A:138:THR:OG1	2.38	0.41
18:B:813:CLA:H102	18:B:813:CLA:H61	1.79	0.41
6:F:158:VAL:O	6:F:158:VAL:HG23	2.21	0.41
15:6:153:ALA:O	15:6:157:SER:OG	2.29	0.41
17:5:263:HIS:HA	17:5:270:ASN:OD1	2.21	0.41
1:A:591:PHE:CE1	1:A:727:VAL:HB	2.55	0.41
21:A:849:BCR:H11C	21:A:849:BCR:H341	1.95	0.41
2:B:373:THR:HG23	2:B:591:THR:HG21	2.03	0.41
2:B:694:LYS:HE2	2:B:694:LYS:HB2	1.72	0.41
3:C:6:LYS:HE3	4:D:215:TYR:HD1	1.85	0.41
5:E:131:GLU:OE2	5:E:133:ALA:N	2.53	0.41
21:F:302:BCR:H24C	21:F:302:BCR:H371	1.88	0.41
11:K:54:SER:HA	11:K:57:LEU:HB2	2.03	0.41
16:3:143:TYR:O	16:3:147:ILE:HG23	2.21	0.41
16:3:260:GLU:N	16:3:260:GLU:OE2	2.53	0.41
17:5:115:LEU:HD23	17:5:115:LEU:HA	1.92	0.41
1:A:455:HIS:CD2	1:A:455:HIS:C	2.99	0.41
1:A:498:ASN:HB2	18:A:837:CLA:HED2	2.01	0.41
1:A:530:ASP:HA	1:A:533:VAL:HG12	2.02	0.41
1:A:582:CYS:HB3	2:B:667:TRP:HE3	1.86	0.41
1:A:693:GLN:NE2	1:A:716:ALA:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:850:BCR:H15C	21:A:850:BCR:H351	1.89	0.41
16:3:106:GLN:OE1	16:3:106:GLN:N	2.48	0.41
1:A:32:PHE:HZ	1:A:49:LEU:HD12	1.86	0.41
1:A:77:GLN:NE2	1:A:81:ILE:HG13	2.36	0.41
1:A:474:ILE:H	1:A:474:ILE:HG13	1.58	0.41
1:A:537:HIS:CE1	1:A:603:VAL:HG12	2.55	0.41
18:A:811:CLA:H2A	18:A:811:CLA:HED3	2.02	0.41
18:A:812:CLA:H152	18:A:812:CLA:H18	1.69	0.41
2:B:429:LEU:HD11	18:B:837:CLA:HMB1	2.03	0.41
19:B:842:PQN:C29	23:B:850:DGD:HAE2	2.51	0.41
12:L:116:HIS:HA	12:L:119:LEU:HD23	2.03	0.41
21:2:621:BCR:H20C	21:2:621:BCR:H361	1.91	0.41
1:A:46:ILE:O	1:A:50:HIS:ND1	2.45	0.41
1:A:393:TRP:CD1	18:A:829:CLA:HAB	2.55	0.41
18:A:835:CLA:H161	18:A:835:CLA:H141	1.83	0.41
21:A:856:BCR:H371	21:A:856:BCR:H24C	1.82	0.41
2:B:268:LEU:HD12	2:B:357:PRO:HA	2.02	0.41
2:B:510:LEU:HD12	2:B:510:LEU:H	1.86	0.41
21:G:205:BCR:H11C	21:G:205:BCR:H341	1.94	0.41
16:3:170:LEU:HG	16:3:171:ILE:HD13	2.03	0.41
16:3:302:HIS:CD2	18:3:613:CLA:HAA2	2.56	0.41
1:A:296:LEU:O	1:A:300:VAL:HG12	2.21	0.41
18:A:821:CLA:HBB1	21:K:202:BCR:H14C	2.03	0.41
7:G:96:GLN:HG2	7:G:101:HIS:ND1	2.36	0.41
7:G:121:PRO:HG2	18:G:204:CLA:HBC2	2.02	0.41
10:J:26:LEU:HD13	10:J:26:LEU:HA	1.92	0.41
12:L:204:LEU:HD13	12:L:204:LEU:HA	1.90	0.41
25:2:607:CHL:HMB3	27:2:620:XAT:H161	2.03	0.41
18:2:613:CLA:HBB	18:2:614:CLA:HBC3	2.02	0.41
15:6:204:PHE:CZ	27:6:619:XAT:H10	2.56	0.41
1:A:47:TRP:HE1	18:F:301:CLA:CBB	2.34	0.40
1:A:455:HIS:CD2	1:A:459:MET:HG2	2.56	0.40
20:A:847:LHG:H242	20:A:847:LHG:H112	2.03	0.40
18:B:813:CLA:HMA2	21:B:844:BCR:H362	2.02	0.40
6:F:121:SER:HB2	6:F:123:PRO:HD2	2.03	0.40
25:2:606:CHL:HBA1	25:2:606:CHL:H3A	1.69	0.40
25:5:608:CHL:HBB1	25:5:608:CHL:CHC	2.49	0.40
1:A:426:ARG:O	1:A:430:HIS:ND1	2.53	0.40
2:B:216:LEU:HD13	2:B:218:HIS:O	2.21	0.40
14:2:156:ILE:HG12	18:5:614:CLA:HAA2	2.02	0.40
17:5:230:LYS:HA	18:5:611:CLA:HED3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:802:CLA:HBA2	2:B:427:LEU:HD23	2.03	0.40
18:A:814:CLA:HBB1	18:A:814:CLA:HMB3	2.04	0.40
18:A:854:CLA:H41	18:A:854:CLA:H62	1.64	0.40
21:B:801:BCR:H11C	21:B:801:BCR:H341	1.99	0.40
18:B:809:CLA:H92	18:B:809:CLA:H62	1.94	0.40
14:2:263:THR:HG21	16:3:199:THR:HB	2.03	0.40
18:5:601:CLA:HBB1	20:5:622:LHG:H262	2.03	0.40
21:A:852:BCR:H15C	21:A:852:BCR:H351	1.89	0.40
15:6:114:ASN:O	15:6:115:TRP:CD1	2.75	0.40
27:6:619:XAT:H15	27:6:619:XAT:H201	1.93	0.40
21:3:622:BCR:H15C	21:3:622:BCR:H351	1.95	0.40
18:A:839:CLA:H11	18:A:839:CLA:H51	1.92	0.40
18:2:614:CLA:HAA2	16:3:203:LEU:HB2	2.03	0.40
15:6:104:VAL:HG23	15:6:115:TRP:CB	2.52	0.40
20:5:622:LHG:H281	20:5:622:LHG:H102	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	700 (95%)	40 (5%)	0	100	100
2	B	731/733 (100%)	696 (95%)	35 (5%)	0	100	100
3	C	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
5	E	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
6	F	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
7	G	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
8	H	88/90 (98%)	84 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
12	L	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
13	M	27/29 (93%)	27 (100%)	0	0	100	100
14	2	204/210 (97%)	192 (94%)	12 (6%)	0	100	100
15	6	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
16	3	211/213 (99%)	195 (92%)	16 (8%)	0	100	100
17	5	200/205 (98%)	173 (86%)	27 (14%)	0	100	100
All	All	3226/3267 (99%)	3013 (93%)	213 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	575 (95%)	28 (5%)	24	55
2	B	595/595 (100%)	569 (96%)	26 (4%)	25	55
3	C	67/67 (100%)	57 (85%)	10 (15%)	3	14
4	D	115/115 (100%)	109 (95%)	6 (5%)	21	51
5	E	52/52 (100%)	48 (92%)	4 (8%)	12	39
6	F	128/129 (99%)	118 (92%)	10 (8%)	11	38
7	G	78/78 (100%)	69 (88%)	9 (12%)	5	23
8	H	72/73 (99%)	67 (93%)	5 (7%)	14	43
9	I	30/30 (100%)	27 (90%)	3 (10%)	7	28
10	J	35/35 (100%)	31 (89%)	4 (11%)	5	23
11	K	56/57 (98%)	47 (84%)	9 (16%)	2	11
12	L	121/122 (99%)	112 (93%)	9 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	24/24 (100%)	24 (100%)	0	100	100
14	2	164/167 (98%)	154 (94%)	10 (6%)	17	47
15	6	148/148 (100%)	141 (95%)	7 (5%)	23	54
16	3	166/166 (100%)	156 (94%)	10 (6%)	17	47
17	5	162/164 (99%)	151 (93%)	11 (7%)	14	43
All	All	2616/2625 (100%)	2455 (94%)	161 (6%)	18	46

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	35	THR
1	A	86	SER
1	A	96	SER
1	A	118	ILE
1	A	159	THR
1	A	217	VAL
1	A	250	LEU
1	A	276	ARG
1	A	300	VAL
1	A	312	ASN
1	A	417	THR
1	A	423	LEU
1	A	432	ASP
1	A	459	MET
1	A	503	THR
1	A	505	LEU
1	A	506	THR
1	A	519	VAL
1	A	522	LEU
1	A	620	ILE
1	A	625	VAL
1	A	626	VAL
1	A	638	SER
1	A	649	LEU
1	A	663	SER
1	A	732	LEU
1	A	749	VAL
2	B	12	LEU
2	B	49	SER

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Mol	Chain	Res	Type
2	B	85	ARG
2	B	143	LEU
2	B	205	GLU
2	B	216	LEU
2	B	220	GLN
2	B	238	ASP
2	B	276	HIS
2	B	283	ILE
2	B	309	THR
2	B	340	SER
2	B	361	LEU
2	B	444	LEU
2	B	448	THR
2	B	478	LEU
2	B	479	SER
2	B	571	SER
2	B	577	TYR
2	B	599	ILE
2	B	659	THR
2	B	676	GLU
2	B	677	THR
2	B	701	SER
2	B	703	VAL
2	B	714	SER
3	C	5	VAL
3	C	17	CYS
3	C	18	VAL
3	C	23	THR
3	C	29	VAL
3	C	39	ILE
3	C	54	CYS
3	C	58	CYS
3	C	65	VAL
3	C	73	THR
4	D	85	THR
4	D	109	ILE
4	D	145	LEU
4	D	177	ASP
4	D	179	VAL
4	D	184	VAL
5	E	91	ASP
5	E	98	VAL

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Mol	Chain	Res	Type
5	E	110	VAL
5	E	113	ASP
6	F	91	THR
6	F	120	ASP
6	F	121	SER
6	F	143	ASN
6	F	174	VAL
6	F	193	VAL
6	F	219	LEU
6	F	223	VAL
6	F	240	ASN
6	F	243	VAL
7	G	61	THR
7	G	65	ILE
7	G	72	LEU
7	G	73	LEU
7	G	79	VAL
7	G	95	VAL
7	G	106	ASP
7	G	107	SER
7	G	125	THR
8	H	62	THR
8	H	85	PHE
8	H	99	LEU
8	H	122	LEU
8	H	131	VAL
9	I	11	VAL
9	I	30	ILE
9	I	33	ASP
10	J	13	VAL
10	J	26	LEU
10	J	35	ASP
10	J	38	VAL
11	K	54	SER
11	K	56	ASN
11	K	57	LEU
11	K	63	THR
11	K	88	LEU
11	K	95	LEU
11	K	103	PHE
11	K	108	THR
11	K	114	LEU

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Mol	Chain	Res	Type
12	L	66	VAL
12	L	70	LEU
12	L	89	ILE
12	L	93	LEU
12	L	119	LEU
12	L	127	THR
12	L	151	LEU
12	L	174	LEU
12	L	219	LEU
14	2	91	LEU
14	2	99	LEU
14	2	110	HIS
14	2	139	ASN
14	2	149	ASP
14	2	190	THR
14	2	193	ASP
14	2	194	VAL
14	2	216	LEU
14	2	267	LEU
15	6	61	LEU
15	6	79	VAL
15	6	81	GLU
15	6	115	TRP
15	6	134	ASN
15	6	136	VAL
15	6	240	ILE
16	3	135	PHE
16	3	137	ASP
16	3	147	ILE
16	3	175	THR
16	3	200	LEU
16	3	237	LEU
16	3	252	ASN
16	3	253	PHE
16	3	256	PHE
16	3	307	VAL
17	5	125	VAL
17	5	129	LEU
17	5	140	THR
17	5	142	ILE
17	5	168	LEU
17	5	172	VAL

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Mol	Chain	Res	Type
17	5	190	ASP
17	5	248	GLN
17	5	251	VAL
17	5	254	THR
17	5	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	107	HIS
1	A	179	HIS
1	A	197	HIS
1	A	214	GLN
1	A	391	HIS
1	A	421	ASN
1	A	437	HIS
1	A	477	GLN
1	A	498	ASN
1	A	693	GLN
2	B	53	GLN
2	B	132	ASN
2	B	156	HIS
2	B	218	HIS
2	B	242	HIS
2	B	294	ASN
2	B	308	HIS
2	B	363	GLN
2	B	374	HIS
2	B	432	HIS
2	B	467	HIS
2	B	610	ASN
2	B	627	ASN
2	B	682	HIS
3	C	3	HIS
4	D	102	GLN
4	D	167	ASN
5	E	90	ASN
5	E	124	ASN
6	F	105	GLN
6	F	128	ASN
7	G	137	HIS

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Mol	Chain	Res	Type
7	G	149	ASN
7	G	152	ASN
8	H	75	ASN
8	H	81	GLN
8	H	126	ASN
8	H	130	GLN
10	J	2	GLN
12	L	65	GLN
12	L	95	ASN
14	2	145	GLN
14	2	187	ASN
14	2	226	ASN
14	2	251	ASN
14	2	261	HIS
15	6	82	ASN
15	6	119	GLN
16	3	148	ASN
16	3	213	HIS
16	3	297	GLN
16	3	298	ASN
16	3	308	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

205 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	3	613	-	57,62,73	1.39	8 (14%)	68,100,113	1.36	7 (10%)
18	CLA	A	820	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
18	CLA	3	603	-	59,63,73	1.36	9 (15%)	71,101,113	1.32	5 (7%)
18	CLA	5	611	-	41,45,73	2.55	11 (26%)	47,76,113	1.33	7 (14%)
18	CLA	K	201	11	50,54,73	1.51	5 (10%)	60,90,113	1.45	5 (8%)
18	CLA	K	206	11	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
18	CLA	5	601	17	49,53,73	1.49	8 (16%)	59,89,113	1.44	6 (10%)
18	CLA	G	201	-	49,53,73	1.49	6 (12%)	59,89,113	1.42	5 (8%)
18	CLA	2	609	14	59,63,73	1.35	9 (15%)	71,101,113	1.34	6 (8%)
18	CLA	A	801	-	69,73,73	1.25	9 (13%)	83,113,113	1.24	5 (6%)
18	CLA	A	835	1	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
18	CLA	6	616	15	47,51,73	1.60	8 (17%)	60,87,113	1.55	6 (10%)
18	CLA	3	614	-	43,48,73	1.56	9 (20%)	51,83,113	1.49	5 (9%)
20	LHG	A	847	18	26,26,48	0.83	1 (3%)	29,32,54	1.35	3 (10%)
18	CLA	B	819	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	7 (11%)
18	CLA	3	602	16	64,68,73	1.30	8 (12%)	77,107,113	1.32	6 (7%)
25	CHL	6	601	15	48,53,74	2.35	19 (39%)	53,89,114	3.00	20 (37%)
21	BCR	I	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
18	CLA	F	303	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	7 (11%)
25	CHL	5	608	-	55,59,74	2.15	18 (32%)	62,96,114	2.91	23 (37%)
18	CLA	B	838	-	51,55,73	1.43	8 (15%)	61,91,113	1.42	6 (9%)
18	CLA	G	203	7	54,58,73	1.42	9 (16%)	65,95,113	1.39	7 (10%)
18	CLA	A	837	1	49,53,73	1.48	8 (16%)	59,89,113	1.45	8 (13%)
18	CLA	B	807	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
18	CLA	B	815	2	64,68,73	1.30	10 (15%)	77,107,113	1.32	5 (6%)
20	LHG	6	620	15,18	27,27,48	0.80	1 (3%)	30,33,54	1.25	2 (6%)
18	CLA	6	608	-	47,52,73	1.52	9 (19%)	56,88,113	1.44	5 (8%)
18	CLA	B	818	2	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
18	CLA	B	824	-	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
18	CLA	B	837	2	50,54,73	1.45	10 (20%)	60,90,113	1.45	7 (11%)
20	LHG	B	851	18	22,22,48	0.83	0	25,28,54	1.20	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	F	301	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	5 (8%)
18	CLA	B	820	2	47,51,73	1.47	8 (17%)	56,86,113	1.48	5 (8%)
18	CLA	5	610	-	59,63,73	1.36	9 (15%)	71,101,113	1.35	7 (9%)
21	BCR	K	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
18	CLA	6	602	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
21	BCR	L	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	9 (16%)
18	CLA	B	804	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	5 (8%)
18	CLA	B	809	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
18	CLA	A	826	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
18	CLA	L	302	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
18	CLA	L	304	-	46,50,73	1.50	8 (17%)	55,85,113	1.49	6 (10%)
18	CLA	6	614	-	41,46,73	1.66	8 (19%)	52,81,113	1.51	9 (17%)
18	CLA	A	812	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
18	CLA	3	610	-	45,49,73	1.51	9 (20%)	54,84,113	1.50	6 (11%)
18	CLA	L	303	-	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
18	CLA	K	203	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
21	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	5 (8%)
21	BCR	3	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
18	CLA	5	604	-	47,51,73	1.49	7 (14%)	55,86,113	1.47	6 (10%)
24	LMG	2	617	-	13,13,55	1.01	0	18,18,63	1.55	4 (22%)
18	CLA	B	826	2	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
18	CLA	A	810	1	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
18	CLA	A	825	1	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
18	CLA	B	823	2	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
20	LHG	5	622	-	36,36,48	0.72	1 (2%)	39,42,54	1.25	4 (10%)
18	CLA	A	811	1	49,53,73	1.48	9 (18%)	59,89,113	1.46	7 (11%)
18	CLA	A	815	1	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
24	LMG	J	104	-	30,30,55	0.94	0	38,38,63	1.27	5 (13%)
26	LUT	2	619	-	42,43,43	7.18	25 (59%)	51,60,60	4.12	21 (41%)
18	CLA	B	833	-	49,53,73	1.48	9 (18%)	59,89,113	1.49	9 (15%)
18	CLA	A	829	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
18	CLA	3	606	-	44,49,73	1.55	9 (20%)	52,84,113	1.45	5 (9%)
22	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	B	816	2	57,62,73	1.38	9 (15%)	68,100,113	1.33	5 (7%)
18	CLA	B	828	-	69,73,73	1.25	9 (13%)	83,113,113	1.22	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	F	304	-	45,49,73	1.52	8 (17%)	54,84,113	1.53	5 (9%)
18	CLA	K	204	-	48,52,73	1.56	9 (18%)	61,88,113	1.53	6 (9%)
18	CLA	B	830	2	49,53,73	1.49	9 (18%)	59,89,113	1.47	7 (11%)
18	CLA	G	204	7	47,52,73	1.52	9 (19%)	56,88,113	1.43	6 (10%)
19	PQN	A	844	-	34,34,34	0.39	0	42,45,45	0.47	0
18	CLA	A	809	1	49,53,73	1.47	9 (18%)	59,89,113	1.48	8 (13%)
18	CLA	B	802	-	57,61,73	1.37	10 (17%)	68,98,113	1.30	6 (8%)
18	CLA	6	610	15	46,51,73	1.53	9 (19%)	55,87,113	1.43	5 (9%)
20	LHG	A	846	-	48,48,48	0.64	1 (2%)	51,54,54	1.27	6 (11%)
25	CHL	5	606	-	45,49,74	2.29	17 (37%)	54,84,114	3.22	23 (42%)
25	CHL	5	607	-	47,51,74	2.41	18 (38%)	52,86,114	3.03	23 (44%)
26	LUT	3	618	16	42,43,43	7.26	24 (57%)	51,60,60	3.85	22 (43%)
18	CLA	B	811	2	58,62,73	1.43	10 (17%)	73,100,113	1.39	7 (9%)
18	CLA	5	603	-	47,52,73	1.52	9 (19%)	56,88,113	1.43	5 (8%)
25	CHL	2	607	-	47,51,74	2.34	18 (38%)	52,86,114	3.06	23 (44%)
18	CLA	A	827	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	8 (9%)
25	CHL	2	608	-	44,49,74	2.40	19 (43%)	48,84,114	3.09	21 (43%)
18	CLA	6	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.43	7 (11%)
18	CLA	B	836	-	64,68,73	1.30	9 (14%)	77,107,113	1.32	7 (9%)
18	CLA	A	814	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	9 (10%)
20	LHG	2	622	18,14	34,34,48	0.72	0	37,40,54	1.27	4 (10%)
18	CLA	A	830	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	4 (4%)
25	CHL	2	601	14	49,53,74	2.38	19 (38%)	58,89,114	3.01	25 (43%)
18	CLA	A	841	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
18	CLA	6	609	-	44,48,73	1.60	10 (22%)	56,83,113	1.57	8 (14%)
21	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	4 (7%)
18	CLA	A	854	-	69,73,73	1.24	8 (11%)	83,113,113	1.25	7 (8%)
18	CLA	A	819	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
18	CLA	B	827	-	49,53,73	1.47	9 (18%)	59,89,113	1.41	7 (11%)
18	CLA	B	812	2	49,53,73	1.48	8 (16%)	59,89,113	1.47	5 (8%)
18	CLA	A	824	1	55,59,73	1.40	9 (16%)	66,96,113	1.41	4 (6%)
18	CLA	2	612	-	45,49,73	1.54	9 (20%)	54,84,113	1.49	6 (11%)
26	LUT	5	619	-	42,43,43	7.28	26 (61%)	51,60,60	3.85	19 (37%)
18	CLA	5	613	17	49,53,73	1.49	9 (18%)	59,89,113	1.49	6 (10%)
18	CLA	B	805	2	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.27	6 (7%)
27	XAT	5	620	-	39,47,47	1.03	3 (7%)	54,74,74	2.76	21 (38%)
21	BCR	K	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	6 (10%)
18	CLA	A	839	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)
21	BCR	A	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
24	LMG	2	618	-	13,13,55	1.07	0	18,18,63	1.54	4 (22%)
18	CLA	2	611	20	45,50,73	1.53	8 (17%)	56,85,113	1.46	5 (8%)
19	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.45	0
26	LUT	6	617	-	42,43,43	7.20	25 (59%)	51,60,60	3.87	19 (37%)
18	CLA	6	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
21	BCR	B	801	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	A	802	-	49,53,73	1.46	9 (18%)	59,89,113	1.47	6 (10%)
18	CLA	F	305	-	49,53,73	1.48	8 (16%)	59,89,113	1.42	5 (8%)
18	CLA	6	611	20	41,46,73	1.67	10 (24%)	52,81,113	1.57	7 (13%)
18	CLA	B	835	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
18	CLA	B	806	2	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
21	BCR	G	205	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
21	BCR	A	856	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	7 (12%)
22	SF4	A	853	1,2	0,12,12	-	-	-	-	-
18	CLA	2	602	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	5 (8%)
18	CLA	A	805	1	59,63,73	1.33	9 (15%)	71,101,113	1.41	8 (11%)
18	CLA	5	612	-	48,52,73	1.51	9 (18%)	58,88,113	1.46	6 (10%)
18	CLA	A	842	1	47,52,73	1.50	9 (19%)	56,88,113	1.43	6 (10%)
18	CLA	A	833	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	7 (11%)
25	CHL	3	608	-	43,48,74	2.38	18 (41%)	51,83,114	2.99	22 (43%)
18	CLA	B	803	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
18	CLA	A	836	1	54,58,73	1.41	9 (16%)	65,95,113	1.41	6 (9%)
18	CLA	B	829	2	49,53,73	1.50	9 (18%)	59,89,113	1.50	7 (11%)
18	CLA	6	603	-	59,63,73	1.35	8 (13%)	71,101,113	1.38	7 (9%)
21	BCR	2	621	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
18	CLA	A	804	1	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
21	BCR	3	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
18	CLA	3	612	-	47,51,73	1.51	6 (12%)	56,86,113	1.43	5 (8%)
18	CLA	2	604	-	54,58,73	1.39	8 (14%)	65,95,113	1.47	7 (10%)
18	CLA	A	823	1	48,52,73	1.50	8 (16%)	58,88,113	1.50	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	834	-	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
18	CLA	6	606	-	43,48,73	1.54	9 (20%)	52,82,113	1.59	7 (13%)
27	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.74	20 (37%)
18	CLA	2	614	-	46,50,73	1.51	9 (19%)	55,85,113	1.45	5 (9%)
18	CLA	3	611	-	43,48,73	1.57	8 (18%)	51,83,113	1.51	6 (11%)
21	BCR	F	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
25	CHL	2	616	-	50,54,74	2.31	17 (34%)	56,90,114	3.02	21 (37%)
18	CLA	A	803	-	69,73,73	1.25	8 (11%)	83,113,113	1.21	5 (6%)
18	CLA	2	610	14	49,53,73	1.43	8 (16%)	59,89,113	1.45	6 (10%)
25	CHL	6	607	15	44,49,74	2.49	19 (43%)	48,84,114	3.04	22 (45%)
21	BCR	B	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	B	841	20	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
18	CLA	B	831	2	53,57,73	1.42	9 (16%)	62,93,113	1.40	4 (6%)
23	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	1.44	11 (13%)
18	CLA	3	617	-	43,48,73	1.55	8 (18%)	51,83,113	1.50	7 (13%)
21	BCR	L	301	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
18	CLA	5	609	17	47,51,73	1.49	8 (17%)	55,86,113	1.44	7 (12%)
18	CLA	5	602	-	49,53,73	1.50	9 (18%)	59,89,113	1.39	6 (10%)
18	CLA	B	814	2	47,52,73	1.51	9 (19%)	56,88,113	1.46	5 (8%)
21	BCR	J	103	2	41,41,41	1.15	3 (7%)	56,56,56	1.30	7 (12%)
18	CLA	A	807	1	47,52,73	1.51	9 (19%)	56,88,113	1.43	5 (8%)
18	CLA	5	614	-	47,51,73	1.50	8 (17%)	56,86,113	1.44	5 (8%)
21	BCR	B	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
21	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
21	BCR	5	621	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
18	CLA	A	838	-	55,59,73	1.41	8 (14%)	66,96,113	1.38	7 (10%)
18	CLA	A	843	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
18	CLA	B	840	2	69,73,73	1.24	9 (13%)	83,113,113	1.32	4 (4%)
21	BCR	A	852	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	6 (10%)
21	BCR	J	102	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	6 (10%)
27	XAT	6	619	-	39,47,47	0.98	2 (5%)	54,74,74	3.10	21 (38%)
18	CLA	2	603	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
18	CLA	B	813	2	69,73,73	1.24	9 (13%)	83,113,113	1.35	10 (12%)
18	CLA	B	817	2	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
18	CLA	J	101	-	46,50,73	1.51	8 (17%)	55,85,113	1.45	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	615	-	41,44,73	1.60	9 (21%)	49,77,113	1.43	4 (8%)
21	BCR	A	850	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	6 (10%)
18	CLA	B	821	2	50,54,73	1.46	8 (16%)	60,90,113	1.41	6 (10%)
21	BCR	B	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
18	CLA	3	607	16	43,48,73	1.61	10 (23%)	54,83,113	1.52	7 (12%)
18	CLA	B	808	-	54,58,73	1.39	10 (18%)	65,95,113	1.44	8 (12%)
18	CLA	3	604	-	45,50,73	1.62	10 (22%)	57,86,113	1.51	7 (12%)
18	CLA	A	828	1	50,54,73	1.45	10 (20%)	60,90,113	1.39	4 (6%)
18	CLA	A	806	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
18	CLA	A	813	-	58,62,73	1.36	8 (13%)	69,99,113	1.37	5 (7%)
18	CLA	B	810	2	50,54,73	1.46	8 (16%)	60,90,113	1.41	4 (6%)
25	CHL	5	615	17	47,51,74	2.28	17 (36%)	52,86,114	3.13	23 (44%)
25	CHL	2	606	14	50,54,74	2.25	16 (32%)	56,90,114	3.15	21 (37%)
18	CLA	2	613	14	49,53,73	1.49	8 (16%)	59,89,113	1.43	6 (10%)
27	XAT	2	620	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	22 (40%)
18	CLA	B	822	-	59,63,73	1.35	9 (15%)	71,101,113	1.38	7 (9%)
18	CLA	A	821	1	48,52,73	1.51	9 (18%)	58,88,113	1.47	6 (10%)
18	CLA	3	609	-	49,53,73	1.47	9 (18%)	59,89,113	1.45	4 (6%)
18	CLA	A	822	-	47,51,73	1.58	10 (21%)	60,87,113	1.53	7 (11%)
18	CLA	A	832	1	45,49,73	1.50	9 (20%)	54,84,113	1.55	8 (14%)
18	CLA	A	840	-	49,53,73	1.48	9 (18%)	59,89,113	1.41	5 (8%)
18	CLA	B	839	-	44,49,73	1.53	9 (20%)	52,84,113	1.47	5 (9%)
21	BCR	B	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	A	818	1	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)
22	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	A	817	-	43,48,73	1.54	8 (18%)	51,83,113	1.50	6 (11%)
18	CLA	A	831	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
18	CLA	B	832	2	49,53,73	1.47	8 (16%)	59,89,113	1.48	9 (15%)
18	CLA	6	613	15	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
21	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.26	9 (16%)
18	CLA	A	845	20	56,60,73	1.39	8 (14%)	67,97,113	1.41	6 (8%)
18	CLA	A	808	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	7 (11%)
18	CLA	A	834	1	69,73,73	1.26	9 (13%)	83,113,113	1.26	5 (6%)
18	CLA	A	816	-	46,50,73	1.49	8 (17%)	55,85,113	1.49	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	613	-	-	9/25/101/115	-
18	CLA	A	820	-	-	4/15/91/115	-
18	CLA	3	603	-	-	8/27/103/115	-
18	CLA	5	611	-	-	5/10/70/115	-
18	CLA	K	201	11	-	9/17/93/115	-
18	CLA	K	206	11	-	7/15/91/115	-
18	CLA	5	601	17	-	4/15/91/115	-
18	CLA	G	201	-	-	5/15/91/115	-
18	CLA	2	609	14	-	11/27/103/115	-
18	CLA	A	801	-	-	8/39/115/115	-
18	CLA	A	835	1	-	9/39/115/115	-
18	CLA	6	616	15	-	4/11/87/115	-
18	CLA	3	614	-	-	3/8/84/115	-
20	LHG	A	847	18	-	19/31/31/53	-
18	CLA	B	819	-	-	3/15/91/115	-
18	CLA	3	602	16	-	9/33/109/115	-
25	CHL	6	601	15	-	3/15/91/117	-
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
18	CLA	F	303	-	-	6/15/91/115	-
25	CHL	5	608	-	-	8/23/99/117	-
18	CLA	B	838	-	-	2/18/94/115	-
18	CLA	G	203	7	-	9/21/97/115	-
18	CLA	A	837	1	-	4/15/91/115	-
18	CLA	B	807	2	-	12/39/115/115	-
18	CLA	B	815	2	-	13/33/109/115	-
20	LHG	6	620	15,18	-	17/32/32/53	-
18	CLA	6	608	-	-	5/13/89/115	-
18	CLA	B	818	2	-	4/15/91/115	-
18	CLA	B	824	-	-	4/15/91/115	-
18	CLA	B	837	2	-	6/17/93/115	-
20	LHG	B	851	18	-	10/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	301	-	-	5/15/91/115	-
18	CLA	B	820	2	-	1/13/89/115	-
18	CLA	5	610	-	-	5/27/103/115	-
21	BCR	K	202	-	-	8/29/63/63	0/2/2/2
18	CLA	6	602	-	-	7/15/91/115	-
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
18	CLA	B	804	2	-	5/15/91/115	-
18	CLA	B	809	-	-	9/39/115/115	-
18	CLA	A	826	-	-	12/39/115/115	-
18	CLA	L	302	-	-	2/15/91/115	-
18	CLA	L	304	-	-	2/12/88/115	-
18	CLA	6	614	-	-	2/4/80/115	-
18	CLA	A	812	-	-	13/39/115/115	-
18	CLA	3	610	-	-	3/10/86/115	-
18	CLA	L	303	-	-	2/15/91/115	-
18	CLA	K	203	-	-	6/15/91/115	-
21	BCR	B	845	-	-	19/29/63/63	0/2/2/2
21	BCR	3	622	-	-	10/29/63/63	0/2/2/2
18	CLA	5	604	-	-	5/11/88/115	-
24	LMG	2	617	-	-	4/4/24/70	0/1/1/1
18	CLA	B	826	2	-	12/39/115/115	-
18	CLA	A	810	1	-	6/15/91/115	-
18	CLA	A	825	1	-	11/27/103/115	-
18	CLA	B	823	2	-	5/15/91/115	-
20	LHG	5	622	-	-	19/41/41/53	-
18	CLA	A	811	1	-	2/15/91/115	-
18	CLA	A	815	1	-	7/15/91/115	-
24	LMG	J	104	-	-	12/25/45/70	0/1/1/1
26	LUT	2	619	-	-	7/29/67/67	0/2/2/2
18	CLA	B	833	-	-	8/15/91/115	-
18	CLA	A	829	-	-	20/39/115/115	-
18	CLA	3	606	-	-	0/10/86/115	-
22	SF4	C	102	3	-	-	0/6/5/5
18	CLA	B	816	2	-	5/25/101/115	-
18	CLA	B	828	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	304	-	-	2/10/86/115	-
18	CLA	K	204	-	-	5/13/89/115	-
18	CLA	B	830	2	-	1/15/91/115	-
18	CLA	G	204	7	-	6/13/89/115	-
19	PQN	A	844	-	-	8/23/43/43	0/2/2/2
18	CLA	A	809	1	-	5/15/91/115	-
18	CLA	B	802	-	-	4/25/101/115	-
18	CLA	6	610	15	-	1/11/87/115	-
20	LHG	A	846	-	-	24/53/53/53	-
25	CHL	5	606	-	-	2/10/86/117	-
25	CHL	5	607	-	-	4/14/90/117	-
26	LUT	3	618	16	-	7/29/67/67	0/2/2/2
18	CLA	B	811	2	-	9/25/101/115	-
18	CLA	5	603	-	-	6/13/89/115	-
25	CHL	2	607	-	-	3/14/90/117	-
18	CLA	A	827	-	-	12/39/115/115	-
25	CHL	2	608	-	-	3/10/86/117	-
18	CLA	6	604	-	-	10/20/96/115	-
18	CLA	B	836	-	-	7/33/109/115	-
18	CLA	A	814	-	-	16/39/115/115	-
20	LHG	2	622	18,14	-	23/39/39/53	-
18	CLA	A	830	-	-	5/39/115/115	-
25	CHL	2	601	14	-	8/15/91/117	-
18	CLA	A	841	-	-	15/39/115/115	-
18	CLA	6	609	-	-	3/8/84/115	-
21	BCR	A	848	-	-	6/29/63/63	0/2/2/2
18	CLA	A	854	-	-	15/39/115/115	-
18	CLA	A	819	-	-	6/15/91/115	-
18	CLA	B	827	-	-	5/15/91/115	-
18	CLA	B	812	2	-	3/15/91/115	-
18	CLA	A	824	1	-	11/23/99/115	-
18	CLA	2	612	-	-	2/10/86/115	-
26	LUT	5	619	-	-	8/29/67/67	0/2/2/2
18	CLA	5	613	17	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	805	2	-	11/39/115/115	-
18	CLA	B	825	-	-	11/39/115/115	-
27	XAT	5	620	-	-	3/31/93/93	0/4/4/4
21	BCR	K	207	-	-	11/29/63/63	0/2/2/2
18	CLA	A	839	-	-	15/39/115/115	-
21	BCR	A	849	-	-	8/29/63/63	0/2/2/2
24	LMG	2	618	-	-	2/4/24/70	0/1/1/1
18	CLA	2	611	20	-	0/9/85/115	-
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
26	LUT	6	617	-	-	12/29/67/67	0/2/2/2
18	CLA	6	612	-	-	4/15/91/115	-
21	BCR	B	801	-	-	7/29/63/63	0/2/2/2
18	CLA	A	802	-	-	7/15/91/115	-
18	CLA	F	305	-	-	7/15/91/115	-
18	CLA	6	611	20	-	1/4/80/115	-
18	CLA	B	835	-	-	8/15/91/115	-
18	CLA	B	806	2	-	19/39/115/115	-
21	BCR	G	205	-	-	5/29/63/63	0/2/2/2
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
22	SF4	A	853	1,2	-	-	0/6/5/5
18	CLA	2	602	-	-	6/15/91/115	-
18	CLA	A	805	1	-	10/27/103/115	-
18	CLA	5	612	-	-	7/13/89/115	-
18	CLA	A	842	1	-	5/13/89/115	-
18	CLA	A	833	-	-	7/15/91/115	-
25	CHL	3	608	-	-	2/8/84/117	-
18	CLA	B	803	-	-	10/39/115/115	-
18	CLA	A	836	1	-	0/21/97/115	-
18	CLA	B	829	2	-	0/15/91/115	-
18	CLA	6	603	-	-	14/27/103/115	-
21	BCR	2	621	-	-	8/29/63/63	0/2/2/2
18	CLA	A	804	1	-	9/39/115/115	-
21	BCR	3	620	-	-	9/29/63/63	0/2/2/2
18	CLA	3	612	-	-	3/13/89/115	-
18	CLA	2	604	-	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	823	1	-	5/13/89/115	-
18	CLA	B	834	-	-	6/15/91/115	-
18	CLA	6	606	-	-	5/10/82/115	-
27	XAT	3	619	-	-	0/31/93/93	0/4/4/4
18	CLA	2	614	-	-	4/12/88/115	-
18	CLA	3	611	-	-	4/8/84/115	-
21	BCR	F	302	-	-	14/29/63/63	0/2/2/2
25	CHL	2	616	-	-	6/17/93/117	-
18	CLA	A	803	-	-	7/39/115/115	-
18	CLA	2	610	14	-	4/15/91/115	-
25	CHL	6	607	15	-	2/10/86/117	-
21	BCR	B	846	-	-	17/29/63/63	0/2/2/2
18	CLA	B	841	20	-	16/39/115/115	-
18	CLA	B	831	2	-	7/20/96/115	-
23	DGD	B	850	-	-	29/55/95/95	0/2/2/2
18	CLA	3	617	-	-	2/8/84/115	-
21	BCR	L	301	-	-	10/29/63/63	0/2/2/2
18	CLA	5	609	17	-	6/11/87/115	-
18	CLA	5	602	-	-	5/15/91/115	-
18	CLA	B	814	2	-	1/13/89/115	-
21	BCR	J	103	2	-	23/29/63/63	0/2/2/2
18	CLA	A	807	1	-	4/13/89/115	-
18	CLA	5	614	-	-	7/13/89/115	-
21	BCR	B	844	-	-	6/29/63/63	0/2/2/2
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2
21	BCR	5	621	-	-	9/29/63/63	0/2/2/2
18	CLA	A	838	-	-	5/23/99/115	-
18	CLA	A	843	-	-	12/39/115/115	-
18	CLA	B	840	2	-	14/39/115/115	-
21	BCR	A	852	-	-	11/29/63/63	0/2/2/2
21	BCR	J	102	-	-	9/29/63/63	0/2/2/2
27	XAT	6	619	-	-	1/31/93/93	0/4/4/4
18	CLA	2	603	-	-	7/15/91/115	-
18	CLA	B	813	2	-	16/39/115/115	-
18	CLA	B	817	2	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	J	101	-	-	7/12/88/115	-
18	CLA	3	615	-	-	2/2/74/115	-
21	BCR	A	850	-	-	3/29/63/63	0/2/2/2
18	CLA	B	821	2	-	9/17/93/115	-
21	BCR	B	848	-	-	13/29/63/63	0/2/2/2
18	CLA	3	607	16	-	1/8/84/115	-
18	CLA	B	808	-	-	4/21/97/115	-
18	CLA	3	604	-	-	0/9/85/115	-
18	CLA	A	828	1	-	7/17/93/115	-
18	CLA	A	806	1	-	14/39/115/115	-
18	CLA	A	813	-	-	3/26/102/115	-
18	CLA	B	810	2	-	11/17/93/115	-
25	CHL	5	615	17	-	3/14/90/117	-
25	CHL	2	606	14	-	5/17/93/117	-
18	CLA	2	613	14	-	8/15/91/115	-
27	XAT	2	620	-	-	3/31/93/93	0/4/4/4
18	CLA	B	822	-	-	8/27/103/115	-
18	CLA	A	821	1	-	8/13/89/115	-
18	CLA	3	609	-	-	1/15/91/115	-
18	CLA	A	822	-	-	2/11/87/115	-
18	CLA	A	832	1	-	6/10/86/115	-
18	CLA	A	840	-	-	6/15/91/115	-
18	CLA	B	839	-	-	2/10/86/115	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	A	818	1	-	18/39/115/115	-
22	SF4	C	101	3	-	-	0/6/5/5
18	CLA	A	817	-	-	0/8/84/115	-
18	CLA	A	831	-	-	14/39/115/115	-
18	CLA	B	832	2	-	6/15/91/115	-
18	CLA	6	613	15	-	9/15/91/115	-
21	BCR	A	851	-	-	9/29/63/63	0/2/2/2
18	CLA	A	845	20	-	12/24/100/115	-
18	CLA	A	808	-	-	3/15/91/115	-
18	CLA	A	834	1	-	14/39/115/115	-
18	CLA	A	816	-	-	4/12/88/115	-

All (1645) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	LUT	C34-C33	20.14	1.62	1.35
26	3	618	LUT	C34-C33	19.98	1.62	1.35
26	2	619	LUT	C34-C33	19.80	1.62	1.35
26	6	617	LUT	C34-C33	19.76	1.62	1.35
26	5	619	LUT	C14-C13	16.75	1.58	1.35
26	2	619	LUT	C14-C13	16.50	1.57	1.35
26	3	618	LUT	C24-C25	16.50	1.53	1.33
26	3	618	LUT	C14-C13	16.48	1.57	1.35
26	3	618	LUT	C10-C9	16.46	1.57	1.35
26	5	619	LUT	C24-C25	16.45	1.53	1.33
26	6	617	LUT	C14-C13	16.40	1.57	1.35
26	5	619	LUT	C10-C9	16.40	1.57	1.35
26	6	617	LUT	C24-C25	16.38	1.53	1.33
26	2	619	LUT	C24-C25	16.23	1.53	1.33
26	2	619	LUT	C10-C9	16.22	1.57	1.35
26	6	617	LUT	C10-C9	16.15	1.57	1.35
26	5	619	LUT	C30-C29	15.72	1.56	1.35
26	3	618	LUT	C30-C29	15.70	1.56	1.35
26	2	619	LUT	C30-C29	15.50	1.56	1.35
26	6	617	LUT	C30-C29	15.48	1.56	1.35
18	5	611	CLA	C1A-NA	12.34	1.40	1.29
26	6	617	LUT	C5-C6	11.69	1.54	1.34
26	3	618	LUT	C5-C6	11.59	1.54	1.34
26	5	619	LUT	C5-C6	11.52	1.54	1.34
26	2	619	LUT	C5-C6	10.90	1.53	1.34
26	5	619	LUT	C28-C27	10.63	1.57	1.32
26	3	618	LUT	C28-C27	10.61	1.57	1.32
26	2	619	LUT	C28-C27	10.55	1.57	1.32
26	6	617	LUT	C28-C27	10.52	1.57	1.32
26	3	618	LUT	C11-C12	9.25	1.58	1.34
26	5	619	LUT	C11-C12	9.21	1.58	1.34
26	2	619	LUT	C11-C12	9.08	1.58	1.34
26	6	617	LUT	C11-C12	9.03	1.57	1.34
26	5	619	LUT	C35-C15	8.95	1.59	1.36
26	3	618	LUT	C35-C15	8.87	1.59	1.36
26	2	619	LUT	C35-C15	8.80	1.58	1.36
26	6	617	LUT	C35-C15	8.76	1.58	1.36
26	5	619	LUT	C31-C32	8.13	1.55	1.34
26	3	618	LUT	C31-C32	8.13	1.55	1.34
26	2	619	LUT	C31-C32	8.04	1.55	1.34
26	6	617	LUT	C31-C32	8.01	1.55	1.34
26	3	618	LUT	C8-C7	7.73	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	LUT	C8-C7	7.68	1.56	1.33
26	2	619	LUT	C8-C7	7.63	1.56	1.33
26	6	617	LUT	C8-C7	7.58	1.56	1.33
26	6	617	LUT	C12-C13	-6.14	1.32	1.45
26	2	619	LUT	C12-C13	-6.05	1.32	1.45
26	5	619	LUT	C12-C13	-6.00	1.33	1.45
26	6	617	LUT	C32-C33	-6.00	1.33	1.45
26	2	619	LUT	C32-C33	-5.99	1.33	1.45
26	5	619	LUT	C32-C33	-5.86	1.33	1.45
26	3	618	LUT	C32-C33	-5.83	1.33	1.45
26	3	618	LUT	C12-C13	-5.76	1.33	1.45
25	5	607	CHL	O2D-CGD	5.19	1.45	1.33
25	5	615	CHL	O2D-CGD	5.19	1.45	1.33
25	2	616	CHL	O2D-CGD	5.16	1.45	1.33
25	2	607	CHL	O2D-CGD	5.14	1.45	1.33
25	2	606	CHL	O2D-CGD	5.12	1.45	1.33
25	5	606	CHL	O2D-CGD	5.11	1.45	1.33
25	2	601	CHL	O2D-CGD	5.09	1.45	1.33
25	5	608	CHL	O2D-CGD	5.05	1.45	1.33
25	5	607	CHL	CHC-C1C	4.91	1.48	1.38
25	6	607	CHL	C2C-C3C	4.87	1.47	1.36
25	6	607	CHL	CHD-C1D	4.87	1.47	1.38
25	6	607	CHL	CHC-C1C	4.84	1.48	1.38
25	5	607	CHL	C2C-C3C	4.83	1.47	1.36
25	6	607	CHL	C3D-C4D	-4.82	1.33	1.44
25	2	601	CHL	C2C-C3C	4.81	1.47	1.36
25	2	608	CHL	C3D-C4D	-4.79	1.33	1.44
25	6	601	CHL	C3D-C4D	-4.78	1.33	1.44
25	2	608	CHL	CHC-C1C	4.78	1.48	1.38
25	3	608	CHL	C3D-C4D	-4.77	1.33	1.44
25	5	607	CHL	C3D-C4D	-4.77	1.33	1.44
25	5	607	CHL	CHD-C1D	4.75	1.47	1.38
25	2	607	CHL	C3D-C4D	-4.75	1.33	1.44
25	2	601	CHL	C3D-C4D	-4.73	1.33	1.44
25	2	601	CHL	CHC-C1C	4.72	1.48	1.38
25	5	615	CHL	C3D-C4D	-4.70	1.33	1.44
25	2	607	CHL	C2C-C3C	4.68	1.46	1.36
25	5	608	CHL	C3D-C4D	-4.68	1.33	1.44
25	2	607	CHL	CHD-C1D	4.66	1.47	1.38
25	2	616	CHL	C3D-C4D	-4.65	1.33	1.44
25	6	607	CHL	O2D-CGD	4.65	1.45	1.30
25	2	608	CHL	O2D-CGD	4.64	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	601	CHL	C2C-C3C	4.64	1.46	1.36
25	6	601	CHL	CHC-C1C	4.63	1.47	1.38
25	5	606	CHL	C3D-C4D	-4.63	1.33	1.44
25	2	601	CHL	CHD-C1D	4.63	1.47	1.38
25	5	606	CHL	C2C-C3C	4.62	1.46	1.37
25	2	606	CHL	C3D-C4D	-4.61	1.33	1.44
25	2	607	CHL	CHC-C1C	4.60	1.47	1.38
25	3	608	CHL	O2D-CGD	4.60	1.45	1.30
25	3	608	CHL	C3C-C2C	4.59	1.46	1.36
25	2	608	CHL	C2C-C3C	4.57	1.46	1.36
25	5	615	CHL	C2C-C3C	4.57	1.46	1.36
25	6	601	CHL	O2D-CGD	4.56	1.45	1.30
25	2	616	CHL	C2C-C3C	4.55	1.46	1.36
25	2	608	CHL	CHD-C1D	4.55	1.47	1.38
25	2	606	CHL	C2C-C3C	4.54	1.46	1.36
25	6	601	CHL	O2A-CGA	4.52	1.45	1.30
25	2	616	CHL	CHC-C1C	4.52	1.47	1.38
25	6	601	CHL	CHD-C1D	4.52	1.47	1.38
25	5	615	CHL	CHC-C1C	4.51	1.47	1.38
25	2	616	CHL	CHD-C1D	4.51	1.47	1.38
25	2	601	CHL	O2A-CGA	4.48	1.45	1.30
25	5	608	CHL	C2C-C3C	4.48	1.46	1.36
25	2	616	CHL	O2A-CGA	4.47	1.45	1.30
25	2	606	CHL	O2A-CGA	4.45	1.45	1.30
25	5	606	CHL	CHD-C1D	4.44	1.47	1.38
25	5	606	CHL	CHC-C1C	4.44	1.47	1.38
25	5	608	CHL	CHC-C1C	4.43	1.47	1.38
25	5	615	CHL	CHD-C1D	4.42	1.47	1.38
25	2	606	CHL	CHC-C1C	4.38	1.47	1.38
25	3	608	CHL	CHD-C1D	4.37	1.46	1.38
25	3	608	CHL	CHC-C1C	4.31	1.47	1.38
25	5	607	CHL	CHD-C4C	4.30	1.49	1.39
25	2	606	CHL	CHD-C1D	4.28	1.46	1.38
25	5	608	CHL	O2A-CGA	4.25	1.45	1.33
25	6	607	CHL	CHD-C4C	4.23	1.48	1.39
18	K	201	CLA	C1D-ND	4.22	1.43	1.37
25	2	601	CHL	CHD-C4C	4.17	1.48	1.39
25	5	608	CHL	CHD-C1D	4.17	1.46	1.38
26	6	617	LUT	C28-C29	-4.16	1.37	1.45
26	2	619	LUT	C8-C9	-4.16	1.37	1.45
25	2	607	CHL	CHD-C4C	4.13	1.48	1.39
25	2	608	CHL	CHD-C4C	4.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	617	LUT	C8-C9	-4.13	1.37	1.45
26	5	619	LUT	C11-C10	4.11	1.56	1.43
26	3	618	LUT	C11-C10	4.10	1.56	1.43
26	2	619	LUT	C28-C29	-4.09	1.37	1.45
26	5	619	LUT	C28-C29	-4.09	1.37	1.45
25	6	601	CHL	CHD-C4C	4.09	1.48	1.39
26	2	619	LUT	C11-C10	4.08	1.56	1.43
26	3	618	LUT	C28-C29	-4.07	1.37	1.45
26	5	619	LUT	C8-C9	-4.07	1.37	1.45
25	2	616	CHL	CHD-C4C	4.05	1.48	1.39
26	3	618	LUT	C8-C9	-4.04	1.37	1.45
25	3	608	CHL	CHD-C4C	4.03	1.48	1.39
25	5	615	CHL	CHD-C4C	4.01	1.48	1.39
26	6	617	LUT	C11-C10	4.00	1.55	1.43
25	5	606	CHL	CHD-C4C	3.98	1.48	1.39
18	3	611	CLA	C1D-ND	3.95	1.42	1.37
18	6	616	CLA	C1D-ND	3.94	1.42	1.37
18	B	805	CLA	C1D-ND	3.92	1.42	1.37
25	5	607	CHL	CHC-C4B	3.91	1.48	1.39
25	2	606	CHL	CHD-C4C	3.90	1.48	1.39
25	6	607	CHL	CHC-C4B	3.90	1.48	1.39
18	A	801	CLA	C1D-ND	3.89	1.42	1.37
18	3	604	CLA	C1D-ND	3.89	1.42	1.37
18	5	610	CLA	C1D-ND	3.88	1.42	1.37
18	5	614	CLA	C1D-ND	3.87	1.42	1.37
18	6	609	CLA	C1D-ND	3.86	1.42	1.37
18	3	612	CLA	C1D-ND	3.86	1.42	1.37
18	3	613	CLA	C1D-ND	3.86	1.42	1.37
18	3	615	CLA	C1D-ND	3.85	1.42	1.37
18	K	206	CLA	C1D-ND	3.85	1.42	1.37
25	2	607	CHL	CHC-C4B	3.85	1.48	1.39
25	5	608	CHL	CHD-C4C	3.84	1.48	1.39
18	6	614	CLA	C1D-ND	3.84	1.42	1.37
18	2	612	CLA	C1D-ND	3.84	1.42	1.37
18	5	613	CLA	C1D-ND	3.84	1.42	1.37
18	A	825	CLA	C1D-ND	3.84	1.42	1.37
18	B	822	CLA	C1D-ND	3.83	1.42	1.37
18	K	204	CLA	C1D-ND	3.82	1.42	1.37
18	3	606	CLA	C1D-ND	3.81	1.42	1.37
18	B	830	CLA	C1D-ND	3.81	1.42	1.37
18	5	611	CLA	C1D-ND	3.81	1.42	1.37
18	3	602	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	201	CLA	C1D-ND	3.81	1.42	1.37
18	5	609	CLA	C1D-ND	3.80	1.42	1.37
18	B	806	CLA	C1D-ND	3.80	1.42	1.37
18	A	816	CLA	C1D-ND	3.80	1.42	1.37
18	6	604	CLA	C1D-ND	3.80	1.42	1.37
18	A	821	CLA	C1D-ND	3.79	1.42	1.37
18	K	203	CLA	C1D-ND	3.79	1.42	1.37
18	6	603	CLA	C1D-ND	3.79	1.42	1.37
18	G	204	CLA	C1D-ND	3.79	1.42	1.37
18	B	821	CLA	C1D-ND	3.78	1.42	1.37
18	J	101	CLA	C1D-ND	3.78	1.42	1.37
18	5	612	CLA	C1D-ND	3.78	1.42	1.37
18	2	604	CLA	C1D-ND	3.78	1.42	1.37
18	3	610	CLA	C1D-ND	3.78	1.42	1.37
18	A	835	CLA	C1D-ND	3.78	1.42	1.37
21	5	621	BCR	C1-C6	-3.78	1.48	1.53
18	2	611	CLA	C1D-ND	3.78	1.42	1.37
18	5	604	CLA	C1D-ND	3.77	1.42	1.37
18	B	812	CLA	C1D-ND	3.77	1.42	1.37
18	6	606	CLA	C1D-ND	3.77	1.42	1.37
18	B	802	CLA	C1D-ND	3.77	1.42	1.37
18	6	610	CLA	C1D-ND	3.77	1.42	1.37
18	5	602	CLA	C1D-ND	3.77	1.42	1.37
18	A	845	CLA	C1D-ND	3.77	1.42	1.37
25	5	607	CHL	OBD-CAD	3.76	1.29	1.22
18	A	815	CLA	C1D-ND	3.76	1.42	1.37
18	G	203	CLA	C1D-ND	3.76	1.42	1.37
18	F	304	CLA	C1D-ND	3.76	1.42	1.37
18	3	603	CLA	C1D-ND	3.76	1.42	1.37
18	2	609	CLA	C1D-ND	3.76	1.42	1.37
18	B	827	CLA	C1D-ND	3.76	1.42	1.37
18	A	808	CLA	C1D-ND	3.76	1.42	1.37
18	B	817	CLA	C1D-ND	3.75	1.42	1.37
18	B	824	CLA	C1D-ND	3.75	1.42	1.37
18	A	832	CLA	C1D-ND	3.75	1.42	1.37
18	B	835	CLA	C1D-ND	3.75	1.42	1.37
18	L	302	CLA	C1D-ND	3.75	1.42	1.37
18	6	608	CLA	C1D-ND	3.75	1.42	1.37
18	B	837	CLA	C1D-ND	3.75	1.42	1.37
18	L	304	CLA	C1D-ND	3.74	1.42	1.37
18	A	843	CLA	C1D-ND	3.74	1.42	1.37
18	B	811	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	837	CLA	C1D-ND	3.74	1.42	1.37
18	A	834	CLA	C1D-ND	3.74	1.42	1.37
18	B	834	CLA	C1D-ND	3.73	1.42	1.37
18	6	612	CLA	C1D-ND	3.73	1.42	1.37
18	B	829	CLA	C1D-ND	3.73	1.42	1.37
18	A	838	CLA	C1D-ND	3.73	1.42	1.37
18	A	826	CLA	C1D-ND	3.73	1.42	1.37
18	B	836	CLA	C1D-ND	3.73	1.42	1.37
18	2	613	CLA	C1D-ND	3.73	1.42	1.37
18	A	811	CLA	C1D-ND	3.73	1.42	1.37
18	A	828	CLA	C1D-ND	3.73	1.42	1.37
18	B	841	CLA	C1D-ND	3.73	1.42	1.37
18	A	806	CLA	C1D-ND	3.73	1.42	1.37
18	A	822	CLA	C1D-ND	3.72	1.42	1.37
18	A	841	CLA	C1D-ND	3.72	1.42	1.37
25	2	606	CHL	OBD-CAD	3.72	1.28	1.22
18	5	603	CLA	C1D-ND	3.72	1.42	1.37
18	L	303	CLA	C1D-ND	3.72	1.42	1.37
18	5	601	CLA	C1D-ND	3.72	1.42	1.37
18	A	831	CLA	C1D-ND	3.71	1.42	1.37
18	6	602	CLA	C1D-ND	3.71	1.42	1.37
18	A	804	CLA	C1D-ND	3.71	1.42	1.37
18	B	807	CLA	C1D-ND	3.71	1.42	1.37
18	3	609	CLA	C1D-ND	3.71	1.42	1.37
18	B	818	CLA	C1D-ND	3.71	1.42	1.37
18	2	614	CLA	C1D-ND	3.71	1.42	1.37
18	A	824	CLA	C1D-ND	3.71	1.42	1.37
18	B	816	CLA	C1D-ND	3.70	1.42	1.37
18	3	614	CLA	C1D-ND	3.70	1.42	1.37
18	A	814	CLA	C1D-ND	3.70	1.42	1.37
18	6	611	CLA	C1D-ND	3.70	1.42	1.37
18	3	617	CLA	C1D-ND	3.70	1.42	1.37
18	A	818	CLA	C1D-ND	3.70	1.42	1.37
25	5	615	CHL	OBD-CAD	3.70	1.28	1.22
25	6	607	CHL	CHB-C1B	3.70	1.47	1.39
18	A	812	CLA	C1D-ND	3.70	1.42	1.37
18	A	810	CLA	C1D-ND	3.70	1.42	1.37
18	A	817	CLA	C1D-ND	3.70	1.42	1.37
18	B	814	CLA	C1D-ND	3.69	1.42	1.37
18	A	833	CLA	C1D-ND	3.69	1.42	1.37
18	B	819	CLA	C1D-ND	3.69	1.42	1.37
18	B	838	CLA	C1D-ND	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	C1D-ND	3.69	1.42	1.37
18	F	305	CLA	C1D-ND	3.69	1.42	1.37
18	F	301	CLA	C1D-ND	3.69	1.42	1.37
18	B	839	CLA	C1D-ND	3.69	1.42	1.37
25	2	616	CHL	CHC-C4B	3.69	1.47	1.39
18	A	840	CLA	C1D-ND	3.68	1.42	1.37
18	2	603	CLA	C1D-ND	3.68	1.42	1.37
18	A	836	CLA	C1D-ND	3.68	1.42	1.37
18	B	804	CLA	C1D-ND	3.68	1.42	1.37
25	2	608	CHL	CHC-C4B	3.68	1.47	1.39
25	2	601	CHL	CHC-C4B	3.68	1.47	1.39
18	B	803	CLA	C1D-ND	3.68	1.42	1.37
18	2	602	CLA	C1D-ND	3.68	1.42	1.37
18	B	831	CLA	C1D-ND	3.68	1.42	1.37
18	A	809	CLA	C1D-ND	3.67	1.42	1.37
18	3	607	CLA	C1D-ND	3.67	1.42	1.37
25	2	616	CHL	OBD-CAD	3.67	1.28	1.22
25	5	606	CHL	OBD-CAD	3.67	1.28	1.22
18	B	810	CLA	C1D-ND	3.67	1.42	1.37
18	A	854	CLA	C1D-ND	3.67	1.42	1.37
18	B	808	CLA	C1D-ND	3.67	1.42	1.37
18	B	833	CLA	C1D-ND	3.67	1.42	1.37
25	6	607	CHL	OBD-CAD	3.67	1.28	1.22
25	5	607	CHL	CHB-C1B	3.67	1.47	1.39
18	A	820	CLA	C1D-ND	3.67	1.42	1.37
18	B	820	CLA	C1D-ND	3.67	1.42	1.37
25	6	601	CHL	OBD-CAD	3.67	1.28	1.22
18	A	807	CLA	C1D-ND	3.66	1.42	1.37
18	K	201	CLA	C4B-NB	3.66	1.42	1.37
25	2	601	CHL	OBD-CAD	3.66	1.28	1.22
18	A	839	CLA	C1D-ND	3.66	1.42	1.37
26	2	619	LUT	C26-C27	3.66	1.55	1.50
18	B	815	CLA	C1D-ND	3.65	1.42	1.37
18	A	813	CLA	C1D-ND	3.65	1.42	1.37
18	B	825	CLA	C1D-ND	3.65	1.42	1.37
18	6	613	CLA	C1D-ND	3.65	1.42	1.37
18	A	829	CLA	C1D-ND	3.64	1.42	1.37
18	A	803	CLA	C1D-ND	3.64	1.42	1.37
18	A	827	CLA	C1D-ND	3.64	1.42	1.37
18	B	826	CLA	C1D-ND	3.64	1.42	1.37
18	A	842	CLA	C1D-ND	3.63	1.42	1.37
18	B	823	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	615	CHL	CHC-C4B	3.62	1.47	1.39
18	B	828	CLA	C1D-ND	3.62	1.42	1.37
18	A	830	CLA	C1D-ND	3.62	1.42	1.37
25	5	608	CHL	CHC-C4B	3.62	1.47	1.39
18	A	823	CLA	C1D-ND	3.62	1.42	1.37
25	6	601	CHL	CHC-C4B	3.62	1.47	1.39
25	2	601	CHL	CHB-C1B	3.62	1.47	1.39
18	B	813	CLA	C1D-ND	3.61	1.42	1.37
18	A	819	CLA	C1D-ND	3.61	1.42	1.37
18	B	840	CLA	C1D-ND	3.61	1.42	1.37
25	2	607	CHL	OBD-CAD	3.60	1.28	1.22
26	5	619	LUT	C26-C27	3.60	1.55	1.50
25	3	608	CHL	OBD-CAD	3.58	1.28	1.22
18	B	832	CLA	C1D-ND	3.58	1.42	1.37
25	3	608	CHL	CHC-C4B	3.58	1.47	1.39
21	A	852	BCR	C1-C6	-3.58	1.48	1.53
18	B	809	CLA	C1D-ND	3.58	1.42	1.37
18	A	805	CLA	C1D-ND	3.57	1.42	1.37
21	A	849	BCR	C1-C6	-3.57	1.48	1.53
21	B	848	BCR	C1-C6	-3.56	1.48	1.53
25	5	606	CHL	CHC-C4B	3.55	1.47	1.39
25	5	608	CHL	OBD-CAD	3.54	1.28	1.22
25	2	606	CHL	CHC-C4B	3.54	1.47	1.39
25	2	608	CHL	OBD-CAD	3.53	1.28	1.22
21	B	843	BCR	C1-C6	-3.53	1.48	1.53
21	A	850	BCR	C1-C6	-3.53	1.48	1.53
21	A	851	BCR	C30-C25	-3.53	1.48	1.53
25	3	608	CHL	CHB-C1B	3.52	1.47	1.39
18	A	802	CLA	C1D-ND	3.52	1.42	1.37
21	J	102	BCR	C30-C25	-3.51	1.48	1.53
25	2	608	CHL	C3A-C2A	-3.51	1.51	1.54
21	K	202	BCR	C1-C6	-3.51	1.48	1.53
21	B	847	BCR	C1-C6	-3.51	1.48	1.53
21	G	205	BCR	C1-C6	-3.51	1.48	1.53
18	2	610	CLA	C1D-ND	3.50	1.42	1.37
25	3	608	CHL	C3A-C2A	-3.49	1.51	1.54
25	2	607	CHL	CHB-C1B	3.49	1.47	1.39
21	B	801	BCR	C1-C6	-3.48	1.49	1.53
18	3	612	CLA	C4B-NB	3.48	1.42	1.37
18	K	201	CLA	C1B-C2B	3.47	1.51	1.43
21	L	301	BCR	C1-C6	-3.45	1.49	1.53
21	B	845	BCR	C1-C6	-3.45	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	602	CLA	C4B-NB	3.45	1.42	1.37
21	B	846	BCR	C1-C6	-3.44	1.49	1.53
25	2	608	CHL	CHB-C1B	3.44	1.47	1.39
18	6	616	CLA	C4B-NB	3.44	1.42	1.37
25	2	616	CHL	CHB-C1B	3.43	1.47	1.39
21	2	621	BCR	C1-C6	-3.42	1.49	1.53
26	3	618	LUT	C26-C27	3.42	1.55	1.50
18	2	612	CLA	C4B-NB	3.41	1.42	1.37
26	6	617	LUT	C26-C27	3.41	1.55	1.50
21	L	305	BCR	C1-C6	-3.41	1.49	1.53
25	5	608	CHL	CHB-C1B	3.40	1.47	1.39
18	6	613	CLA	C4B-NB	3.39	1.42	1.37
18	6	611	CLA	C4B-NB	3.38	1.41	1.37
18	B	834	CLA	C4B-NB	3.38	1.41	1.37
25	5	615	CHL	CHB-C1B	3.38	1.47	1.39
26	5	619	LUT	C15-C14	3.36	1.53	1.43
18	A	837	CLA	C4B-NB	3.36	1.41	1.37
18	K	206	CLA	C4B-NB	3.36	1.41	1.37
18	3	613	CLA	C4B-NB	3.36	1.41	1.37
21	B	843	BCR	C30-C25	-3.36	1.49	1.53
18	A	840	CLA	C4B-NB	3.36	1.41	1.37
18	G	201	CLA	C4B-NB	3.36	1.41	1.37
18	5	614	CLA	C4B-NB	3.35	1.41	1.37
25	5	606	CHL	CHB-C1B	3.35	1.46	1.39
18	A	812	CLA	C4B-NB	3.35	1.41	1.37
18	K	203	CLA	C4B-NB	3.34	1.41	1.37
18	L	302	CLA	C4B-NB	3.34	1.41	1.37
18	F	305	CLA	C4B-NB	3.34	1.41	1.37
25	6	601	CHL	CHB-C1B	3.34	1.46	1.39
21	B	845	BCR	C30-C25	-3.34	1.49	1.53
18	A	810	CLA	C4B-NB	3.34	1.41	1.37
18	5	601	CLA	C4B-NB	3.33	1.41	1.37
18	6	612	CLA	C4B-NB	3.33	1.41	1.37
18	B	824	CLA	C4B-NB	3.33	1.41	1.37
18	B	829	CLA	C4B-NB	3.33	1.41	1.37
18	5	612	CLA	C4B-NB	3.33	1.41	1.37
18	B	835	CLA	C4B-NB	3.33	1.41	1.37
21	K	207	BCR	C1-C6	-3.33	1.49	1.53
18	A	831	CLA	C4B-NB	3.33	1.41	1.37
26	3	618	LUT	C15-C14	3.32	1.53	1.43
18	3	611	CLA	C4B-NB	3.32	1.41	1.37
18	B	837	CLA	C4B-NB	3.32	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	603	CLA	C4B-NB	3.32	1.41	1.37
18	5	613	CLA	C4B-NB	3.32	1.41	1.37
18	2	613	CLA	C4B-NB	3.31	1.41	1.37
18	3	615	CLA	C4B-NB	3.31	1.41	1.37
21	A	851	BCR	C1-C6	-3.31	1.49	1.53
18	A	824	CLA	C4B-NB	3.31	1.41	1.37
18	3	607	CLA	C4B-NB	3.31	1.41	1.37
18	J	101	CLA	C4B-NB	3.31	1.41	1.37
18	3	614	CLA	C4B-NB	3.31	1.41	1.37
21	B	846	BCR	C30-C25	-3.31	1.49	1.53
21	2	621	BCR	C30-C25	-3.30	1.49	1.53
18	B	818	CLA	C4B-NB	3.30	1.41	1.37
18	3	617	CLA	C4B-NB	3.30	1.41	1.37
18	A	833	CLA	C4B-NB	3.30	1.41	1.37
18	B	811	CLA	C4B-NB	3.30	1.41	1.37
18	G	203	CLA	C4B-NB	3.30	1.41	1.37
18	A	803	CLA	C4B-NB	3.30	1.41	1.37
18	A	836	CLA	C4B-NB	3.30	1.41	1.37
18	2	614	CLA	C4B-NB	3.30	1.41	1.37
18	6	614	CLA	C4B-NB	3.29	1.41	1.37
18	A	819	CLA	C4B-NB	3.29	1.41	1.37
18	B	841	CLA	C4B-NB	3.29	1.41	1.37
18	6	608	CLA	C4B-NB	3.29	1.41	1.37
18	B	815	CLA	C4B-NB	3.29	1.41	1.37
18	B	828	CLA	C4B-NB	3.28	1.41	1.37
18	6	606	CLA	C4B-NB	3.28	1.41	1.37
18	A	845	CLA	C4B-NB	3.28	1.41	1.37
18	B	805	CLA	C4B-NB	3.27	1.41	1.37
18	G	204	CLA	C4B-NB	3.27	1.41	1.37
21	J	103	BCR	C1-C6	-3.27	1.49	1.53
25	5	607	CHL	C3D-C2D	3.27	1.48	1.39
18	5	611	CLA	C4B-NB	3.27	1.41	1.37
26	2	619	LUT	C15-C14	3.26	1.53	1.43
18	A	842	CLA	C4B-NB	3.26	1.41	1.37
18	B	821	CLA	C4B-NB	3.26	1.41	1.37
18	B	838	CLA	C4B-NB	3.26	1.41	1.37
18	2	603	CLA	C4B-NB	3.26	1.41	1.37
18	2	611	CLA	C4B-NB	3.26	1.41	1.37
21	F	302	BCR	C1-C6	-3.26	1.49	1.53
18	A	825	CLA	C4B-NB	3.26	1.41	1.37
18	B	840	CLA	C4B-NB	3.25	1.41	1.37
18	A	834	CLA	C4B-NB	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	304	CLA	C4B-NB	3.25	1.41	1.37
18	A	820	CLA	C4B-NB	3.25	1.41	1.37
18	6	604	CLA	C4B-NB	3.25	1.41	1.37
18	B	831	CLA	C4B-NB	3.24	1.41	1.37
18	A	843	CLA	C4B-NB	3.24	1.41	1.37
18	F	303	CLA	C4B-NB	3.24	1.41	1.37
18	A	811	CLA	C4B-NB	3.23	1.41	1.37
21	A	856	BCR	C1-C6	-3.23	1.49	1.53
18	A	838	CLA	C4B-NB	3.23	1.41	1.37
18	B	809	CLA	C4B-NB	3.23	1.41	1.37
26	6	617	LUT	C15-C14	3.23	1.53	1.43
18	6	609	CLA	C4B-NB	3.23	1.41	1.37
18	3	604	CLA	C4B-NB	3.23	1.41	1.37
18	F	304	CLA	C4B-NB	3.22	1.41	1.37
18	5	610	CLA	C4B-NB	3.22	1.41	1.37
25	2	606	CHL	CHB-C1B	3.22	1.46	1.39
21	A	849	BCR	C30-C25	-3.22	1.49	1.53
18	B	812	CLA	C4B-NB	3.21	1.41	1.37
18	B	839	CLA	C4B-NB	3.21	1.41	1.37
18	5	603	CLA	C4B-NB	3.21	1.41	1.37
18	B	804	CLA	C4B-NB	3.21	1.41	1.37
18	B	816	CLA	C4B-NB	3.21	1.41	1.37
21	A	848	BCR	C1-C6	-3.21	1.49	1.53
18	A	821	CLA	C4B-NB	3.21	1.41	1.37
18	B	832	CLA	C4B-NB	3.21	1.41	1.37
18	3	606	CLA	C4B-NB	3.20	1.41	1.37
18	6	603	CLA	C4B-NB	3.20	1.41	1.37
18	B	808	CLA	C4B-NB	3.20	1.41	1.37
18	5	609	CLA	C4B-NB	3.20	1.41	1.37
18	B	819	CLA	C4B-NB	3.20	1.41	1.37
21	J	102	BCR	C1-C6	-3.20	1.49	1.53
18	B	814	CLA	C4B-NB	3.20	1.41	1.37
18	A	808	CLA	C4B-NB	3.19	1.41	1.37
18	3	610	CLA	C4B-NB	3.19	1.41	1.37
18	B	830	CLA	C4B-NB	3.19	1.41	1.37
18	A	823	CLA	C4B-NB	3.19	1.41	1.37
18	B	833	CLA	C4B-NB	3.18	1.41	1.37
18	2	604	CLA	C4B-NB	3.18	1.41	1.37
18	2	602	CLA	C4B-NB	3.18	1.41	1.37
18	F	301	CLA	C4B-NB	3.18	1.41	1.37
18	A	818	CLA	C4B-NB	3.18	1.41	1.37
18	A	822	CLA	C4B-NB	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	822	CLA	C4B-NB	3.18	1.41	1.37
18	A	835	CLA	C4B-NB	3.18	1.41	1.37
18	B	810	CLA	C4B-NB	3.18	1.41	1.37
18	A	832	CLA	C4B-NB	3.17	1.41	1.37
18	B	807	CLA	C4B-NB	3.17	1.41	1.37
18	5	604	CLA	C4B-NB	3.17	1.41	1.37
21	3	620	BCR	C1-C6	-3.17	1.49	1.53
18	A	827	CLA	C4B-NB	3.17	1.41	1.37
21	I	101	BCR	C1-C6	-3.17	1.49	1.53
18	K	204	CLA	C4B-NB	3.16	1.41	1.37
18	A	841	CLA	C4B-NB	3.16	1.41	1.37
18	A	822	CLA	CAB-C3B	-3.16	1.44	1.50
25	6	607	CHL	C3D-C2D	3.16	1.47	1.39
18	5	611	CLA	CAB-C3B	-3.15	1.44	1.50
18	B	817	CLA	C4B-NB	3.15	1.41	1.37
18	3	602	CLA	C4B-NB	3.15	1.41	1.37
18	B	825	CLA	C4B-NB	3.15	1.41	1.37
26	5	619	LUT	C7-C6	3.15	1.56	1.45
18	A	807	CLA	C4B-NB	3.15	1.41	1.37
25	2	601	CHL	C3D-C2D	3.14	1.47	1.39
21	A	852	BCR	C30-C25	-3.14	1.49	1.53
18	3	609	CLA	C4B-NB	3.14	1.41	1.37
18	B	803	CLA	C4D-ND	-3.13	1.33	1.37
18	B	802	CLA	C4B-NB	3.13	1.41	1.37
18	L	303	CLA	C4B-NB	3.13	1.41	1.37
18	A	827	CLA	C4D-ND	-3.13	1.33	1.37
18	6	611	CLA	CAB-C3B	-3.13	1.44	1.50
18	B	806	CLA	C4B-NB	3.13	1.41	1.37
18	K	204	CLA	CAB-C3B	-3.12	1.44	1.50
18	A	815	CLA	C4B-NB	3.12	1.41	1.37
18	2	609	CLA	C4B-NB	3.12	1.41	1.37
18	A	806	CLA	C4B-NB	3.12	1.41	1.37
18	A	817	CLA	C4B-NB	3.12	1.41	1.37
18	B	820	CLA	C4B-NB	3.12	1.41	1.37
18	B	827	CLA	C4B-NB	3.12	1.41	1.37
18	6	610	CLA	C4B-NB	3.12	1.41	1.37
18	A	806	CLA	C4D-ND	-3.11	1.33	1.37
18	6	602	CLA	C4B-NB	3.11	1.41	1.37
18	A	804	CLA	C4B-NB	3.11	1.41	1.37
18	A	813	CLA	C4B-NB	3.11	1.41	1.37
18	B	832	CLA	C4D-ND	-3.11	1.33	1.37
21	K	207	BCR	C30-C25	-3.11	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	609	CLA	CAB-C3B	-3.11	1.44	1.50
18	5	603	CLA	C4D-ND	-3.10	1.33	1.37
26	3	618	LUT	C7-C6	3.10	1.56	1.45
18	A	816	CLA	C4B-NB	3.10	1.41	1.37
18	A	828	CLA	C4D-ND	-3.10	1.33	1.37
18	A	839	CLA	C4B-NB	3.10	1.41	1.37
18	5	611	CLA	C4D-ND	-3.10	1.33	1.37
18	B	826	CLA	C4D-ND	-3.10	1.33	1.37
18	B	811	CLA	CAB-C3B	-3.09	1.44	1.50
18	3	607	CLA	CAB-C3B	-3.09	1.44	1.50
18	A	838	CLA	C4D-ND	-3.09	1.33	1.37
18	3	612	CLA	C3B-C4B	3.09	1.50	1.42
18	A	830	CLA	C4B-NB	3.09	1.41	1.37
18	6	616	CLA	CAB-C3B	-3.09	1.44	1.50
18	A	802	CLA	C4B-NB	3.09	1.41	1.37
18	A	854	CLA	C4B-NB	3.08	1.41	1.37
18	2	603	CLA	C4D-ND	-3.08	1.33	1.37
25	2	607	CHL	C1D-C2D	3.08	1.51	1.45
18	L	303	CLA	C4D-ND	-3.08	1.33	1.37
18	B	823	CLA	C4D-ND	-3.08	1.33	1.37
18	B	836	CLA	C4B-NB	3.08	1.41	1.37
18	3	604	CLA	CAB-C3B	-3.07	1.44	1.50
21	A	856	BCR	C30-C25	-3.07	1.49	1.53
18	B	803	CLA	C4B-NB	3.07	1.41	1.37
18	B	819	CLA	C4D-ND	-3.07	1.33	1.37
25	5	607	CHL	C1D-C2D	3.07	1.51	1.45
18	B	838	CLA	C4D-ND	-3.07	1.33	1.37
18	B	825	CLA	C4D-ND	-3.07	1.33	1.37
18	B	823	CLA	C4B-NB	3.07	1.41	1.37
26	6	617	LUT	C7-C6	3.07	1.56	1.45
21	L	301	BCR	C30-C25	-3.06	1.49	1.53
18	B	836	CLA	C4D-ND	-3.06	1.33	1.37
25	2	607	CHL	C3D-C2D	3.06	1.47	1.39
18	A	839	CLA	C4D-ND	-3.06	1.33	1.37
21	3	622	BCR	C1-C6	-3.06	1.49	1.53
26	3	618	LUT	C23-C24	3.06	1.54	1.50
18	B	806	CLA	C4D-ND	-3.06	1.33	1.37
18	B	826	CLA	C4B-NB	3.06	1.41	1.37
18	6	602	CLA	C4D-ND	-3.06	1.33	1.37
18	6	614	CLA	CAB-C3B	-3.05	1.44	1.50
18	A	814	CLA	C4D-ND	-3.05	1.33	1.37
18	A	828	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	608	CHL	C1D-C2D	3.05	1.51	1.45
21	B	801	BCR	C30-C25	-3.05	1.49	1.53
18	A	819	CLA	C4D-ND	-3.05	1.33	1.37
18	A	803	CLA	C4D-ND	-3.05	1.33	1.37
21	B	844	BCR	C1-C6	-3.04	1.49	1.53
18	A	823	CLA	C3B-C4B	3.04	1.49	1.42
18	A	826	CLA	C4B-NB	3.04	1.41	1.37
25	2	601	CHL	C1D-C2D	3.04	1.51	1.45
18	B	839	CLA	C4D-ND	-3.04	1.33	1.37
21	A	850	BCR	C30-C25	-3.04	1.49	1.53
18	B	827	CLA	C4D-ND	-3.04	1.33	1.37
18	3	602	CLA	C4D-ND	-3.04	1.33	1.37
18	A	833	CLA	C4D-ND	-3.04	1.33	1.37
18	A	801	CLA	C4B-NB	3.04	1.41	1.37
18	A	830	CLA	C4D-ND	-3.04	1.33	1.37
25	6	601	CHL	C3D-C2D	3.04	1.47	1.39
18	A	809	CLA	C4B-NB	3.03	1.41	1.37
21	B	844	BCR	C30-C25	-3.03	1.49	1.53
18	K	204	CLA	C4D-ND	-3.03	1.33	1.37
18	B	813	CLA	C4D-ND	-3.03	1.33	1.37
18	B	814	CLA	C4D-ND	-3.03	1.33	1.37
18	A	807	CLA	C4D-ND	-3.02	1.33	1.37
18	2	610	CLA	C3B-C4B	3.02	1.49	1.42
18	B	818	CLA	C4D-ND	-3.02	1.33	1.37
18	2	614	CLA	C4D-ND	-3.02	1.33	1.37
25	5	615	CHL	C1D-C2D	3.02	1.51	1.45
25	6	607	CHL	C1D-C2D	3.02	1.51	1.45
18	B	817	CLA	C4D-ND	-3.02	1.33	1.37
18	B	805	CLA	C3B-C4B	3.02	1.49	1.42
18	A	813	CLA	C4D-ND	-3.01	1.33	1.37
18	2	602	CLA	C4D-ND	-3.01	1.33	1.37
18	A	842	CLA	C4D-ND	-3.01	1.33	1.37
18	2	613	CLA	C4D-ND	-3.01	1.33	1.37
18	3	606	CLA	C4D-ND	-3.01	1.33	1.37
18	A	808	CLA	C4D-ND	-3.01	1.33	1.37
18	5	601	CLA	C4D-ND	-3.01	1.33	1.37
18	2	612	CLA	C4D-ND	-3.01	1.33	1.37
18	A	804	CLA	C4D-ND	-3.01	1.33	1.37
25	2	616	CHL	C3D-C2D	3.01	1.47	1.39
18	A	829	CLA	C4B-NB	3.01	1.41	1.37
18	A	812	CLA	C4D-ND	-3.00	1.33	1.37
18	G	201	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	203	CLA	C4D-ND	-3.00	1.33	1.37
18	A	814	CLA	C4B-NB	3.00	1.41	1.37
18	F	304	CLA	C4D-ND	-3.00	1.33	1.37
18	A	837	CLA	C4D-ND	-3.00	1.33	1.37
18	2	609	CLA	C4D-ND	-2.99	1.33	1.37
18	3	615	CLA	C4D-ND	-2.99	1.33	1.37
18	A	836	CLA	C4D-ND	-2.99	1.33	1.37
18	B	841	CLA	C4D-ND	-2.99	1.33	1.37
18	A	834	CLA	C4D-ND	-2.99	1.33	1.37
18	A	817	CLA	C4D-ND	-2.99	1.33	1.37
18	A	831	CLA	C4D-ND	-2.99	1.33	1.37
18	A	805	CLA	C4B-NB	2.99	1.41	1.37
18	A	815	CLA	C4D-ND	-2.99	1.33	1.37
18	A	820	CLA	C4D-ND	-2.99	1.33	1.37
18	B	830	CLA	C4D-ND	-2.99	1.33	1.37
18	B	807	CLA	C4D-ND	-2.98	1.33	1.37
18	A	837	CLA	C3B-C4B	2.98	1.49	1.42
25	3	608	CHL	C1D-C2D	2.98	1.51	1.45
18	G	201	CLA	C3B-C4B	2.98	1.49	1.42
18	A	801	CLA	C4D-ND	-2.98	1.33	1.37
25	6	601	CHL	C1D-C2D	2.98	1.51	1.45
21	3	622	BCR	C30-C25	-2.98	1.49	1.53
25	5	606	CHL	C1D-C2D	2.98	1.51	1.45
26	2	619	LUT	C7-C6	2.98	1.55	1.45
18	5	613	CLA	C3B-C4B	2.98	1.49	1.42
18	B	833	CLA	C4D-ND	-2.98	1.33	1.37
25	2	608	CHL	C3D-C2D	2.97	1.47	1.39
25	5	615	CHL	C3D-C2D	2.97	1.47	1.39
18	A	842	CLA	C3B-C4B	2.97	1.49	1.42
18	6	604	CLA	C4D-ND	-2.97	1.33	1.37
18	B	835	CLA	C4D-ND	-2.97	1.33	1.37
18	2	611	CLA	C4D-ND	-2.97	1.33	1.37
18	B	831	CLA	C4D-ND	-2.97	1.33	1.37
18	A	822	CLA	C4D-ND	-2.97	1.33	1.37
21	F	302	BCR	C30-C25	-2.97	1.49	1.53
25	6	607	CHL	C3A-C2A	-2.97	1.51	1.54
21	I	101	BCR	C30-C25	-2.97	1.49	1.53
18	5	601	CLA	C3B-C4B	2.97	1.49	1.42
18	B	810	CLA	C4D-ND	-2.97	1.33	1.37
18	A	802	CLA	C4D-ND	-2.97	1.33	1.37
18	B	805	CLA	C4D-ND	-2.97	1.33	1.37
18	5	610	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	812	CLA	C4D-ND	-2.97	1.33	1.37
18	B	828	CLA	C4D-ND	-2.97	1.33	1.37
18	A	829	CLA	C4D-ND	-2.97	1.33	1.37
18	A	811	CLA	C4D-ND	-2.96	1.33	1.37
18	B	816	CLA	C4D-ND	-2.96	1.33	1.37
18	5	612	CLA	C3B-C4B	2.96	1.49	1.42
18	A	810	CLA	C4D-ND	-2.96	1.33	1.37
18	6	609	CLA	C4D-ND	-2.96	1.33	1.37
18	B	837	CLA	C3B-C4B	2.96	1.49	1.42
18	5	604	CLA	C3B-C4B	2.96	1.49	1.42
18	6	603	CLA	C4D-ND	-2.96	1.33	1.37
18	A	805	CLA	C4D-ND	-2.96	1.33	1.37
18	5	602	CLA	C4D-ND	-2.95	1.33	1.37
18	B	834	CLA	C3B-C4B	2.95	1.49	1.42
18	G	203	CLA	C3B-C4B	2.95	1.49	1.42
18	3	604	CLA	C4D-ND	-2.95	1.33	1.37
21	B	847	BCR	C30-C25	-2.95	1.49	1.53
18	2	604	CLA	C3B-C4B	2.95	1.49	1.42
18	A	840	CLA	C4D-ND	-2.95	1.33	1.37
18	2	611	CLA	C3B-C4B	2.95	1.49	1.42
18	B	813	CLA	C4B-NB	2.95	1.41	1.37
18	2	610	CLA	C4B-NB	2.95	1.41	1.37
18	A	826	CLA	C4D-ND	-2.95	1.33	1.37
18	J	101	CLA	C4D-ND	-2.95	1.33	1.37
25	2	616	CHL	C1D-C2D	2.95	1.51	1.45
18	5	602	CLA	C3B-C4B	2.94	1.49	1.42
18	3	611	CLA	C3B-C4B	2.94	1.49	1.42
18	6	608	CLA	C3B-C4B	2.94	1.49	1.42
18	B	840	CLA	C4D-ND	-2.94	1.33	1.37
25	5	606	CHL	C3D-C2D	2.94	1.47	1.39
18	A	805	CLA	C3B-C4B	2.94	1.49	1.42
18	6	613	CLA	C4D-ND	-2.94	1.33	1.37
18	B	810	CLA	C3B-C4B	2.94	1.49	1.42
18	B	802	CLA	C4D-ND	-2.94	1.33	1.37
18	J	101	CLA	C3B-C4B	2.94	1.49	1.42
18	B	837	CLA	C4D-ND	-2.94	1.33	1.37
18	G	204	CLA	C4D-ND	-2.94	1.33	1.37
18	B	821	CLA	C4D-ND	-2.94	1.33	1.37
18	A	821	CLA	C3B-C4B	2.93	1.49	1.42
18	3	614	CLA	C4D-ND	-2.93	1.33	1.37
18	5	610	CLA	C3B-C4B	2.93	1.49	1.42
18	A	841	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	843	CLA	C4D-ND	-2.93	1.33	1.37
18	F	301	CLA	C4D-ND	-2.93	1.33	1.37
18	3	610	CLA	C4D-ND	-2.93	1.33	1.37
18	A	825	CLA	C3B-C4B	2.93	1.49	1.42
18	6	606	CLA	C3B-C4B	2.93	1.49	1.42
18	A	823	CLA	C4D-ND	-2.93	1.33	1.37
26	3	618	LUT	C18-C5	2.93	1.55	1.50
18	L	304	CLA	C4D-ND	-2.93	1.33	1.37
18	6	610	CLA	C4D-ND	-2.92	1.33	1.37
18	A	818	CLA	C4D-ND	-2.92	1.33	1.37
18	B	834	CLA	C4D-ND	-2.92	1.33	1.37
18	3	607	CLA	C4D-ND	-2.92	1.33	1.37
18	B	808	CLA	C3B-C4B	2.92	1.49	1.42
26	5	619	LUT	C18-C5	2.92	1.55	1.50
25	2	606	CHL	C1D-C2D	2.92	1.51	1.45
18	A	809	CLA	C4D-ND	-2.92	1.33	1.37
18	3	617	CLA	C3B-C4B	2.92	1.49	1.42
18	B	820	CLA	C4D-ND	-2.92	1.33	1.37
18	3	613	CLA	C4D-ND	-2.92	1.33	1.37
18	F	303	CLA	C4D-ND	-2.91	1.33	1.37
18	A	816	CLA	C4D-ND	-2.91	1.33	1.37
18	2	613	CLA	C3B-C4B	2.91	1.49	1.42
18	B	811	CLA	C4D-ND	-2.91	1.33	1.37
18	6	608	CLA	C4D-ND	-2.91	1.33	1.37
25	5	607	CHL	MG-NA	-2.91	1.99	2.06
18	2	614	CLA	C3B-C4B	2.91	1.49	1.42
18	B	815	CLA	C4D-ND	-2.91	1.33	1.37
18	3	612	CLA	C4D-ND	-2.91	1.33	1.37
25	3	608	CHL	C3D-C2D	2.91	1.47	1.39
18	B	836	CLA	C3B-C4B	2.91	1.49	1.42
18	A	821	CLA	C4D-ND	-2.91	1.33	1.37
18	A	832	CLA	C4D-ND	-2.91	1.33	1.37
18	6	611	CLA	C4D-ND	-2.91	1.33	1.37
18	A	825	CLA	C4D-ND	-2.90	1.33	1.37
18	A	833	CLA	C3B-C4B	2.90	1.49	1.42
18	A	845	CLA	C3B-C4B	2.90	1.49	1.42
18	B	809	CLA	C4D-ND	-2.90	1.33	1.37
18	F	305	CLA	C4D-ND	-2.90	1.33	1.37
18	K	203	CLA	C4D-ND	-2.90	1.33	1.37
18	B	841	CLA	C3B-C4B	2.90	1.49	1.42
18	B	808	CLA	C4D-ND	-2.90	1.33	1.37
18	6	612	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	613	CLA	C3B-C4B	2.90	1.49	1.42
18	5	612	CLA	C4D-ND	-2.90	1.33	1.37
18	L	302	CLA	C4D-ND	-2.89	1.33	1.37
18	5	604	CLA	C4D-ND	-2.89	1.33	1.37
18	B	822	CLA	C4D-ND	-2.89	1.33	1.37
18	2	612	CLA	C3B-C4B	2.89	1.49	1.42
18	6	612	CLA	C3B-C4B	2.89	1.49	1.42
18	3	603	CLA	C4D-ND	-2.89	1.33	1.37
18	K	203	CLA	C3B-C4B	2.89	1.49	1.42
18	A	817	CLA	C3B-C4B	2.89	1.49	1.42
18	A	808	CLA	C3B-C4B	2.89	1.49	1.42
18	F	303	CLA	C3B-C4B	2.89	1.49	1.42
18	B	828	CLA	C3B-C4B	2.89	1.49	1.42
18	A	845	CLA	C4D-ND	-2.89	1.33	1.37
18	B	818	CLA	C3B-C4B	2.89	1.49	1.42
18	3	611	CLA	C4D-ND	-2.88	1.33	1.37
21	G	205	BCR	C30-C25	-2.88	1.49	1.53
18	3	615	CLA	C3B-C4B	2.88	1.49	1.42
18	5	614	CLA	C3B-C4B	2.88	1.49	1.42
18	3	614	CLA	C3B-C4B	2.88	1.49	1.42
18	A	811	CLA	C3B-C4B	2.88	1.49	1.42
18	A	812	CLA	C3B-C4B	2.88	1.49	1.42
18	3	610	CLA	C3B-C4B	2.88	1.49	1.42
18	A	836	CLA	C3B-C4B	2.88	1.49	1.42
18	B	804	CLA	C4D-ND	-2.87	1.33	1.37
18	K	206	CLA	C4D-ND	-2.87	1.33	1.37
18	B	840	CLA	C3B-C4B	2.87	1.49	1.42
18	L	304	CLA	C3B-C4B	2.87	1.49	1.42
18	3	609	CLA	C3B-C4B	2.87	1.49	1.42
18	5	614	CLA	C4D-ND	-2.87	1.33	1.37
18	A	827	CLA	C3B-C4B	2.87	1.49	1.42
18	B	833	CLA	C3B-C4B	2.87	1.49	1.42
18	A	818	CLA	C3B-C4B	2.87	1.49	1.42
18	5	609	CLA	C3B-C4B	2.87	1.49	1.42
18	5	609	CLA	C4D-ND	-2.87	1.33	1.37
18	A	809	CLA	C3B-C4B	2.87	1.49	1.42
18	A	826	CLA	C3B-C4B	2.87	1.49	1.42
18	A	814	CLA	C3B-C4B	2.87	1.49	1.42
18	3	617	CLA	C4D-ND	-2.86	1.33	1.37
21	K	202	BCR	C30-C25	-2.86	1.49	1.53
18	A	840	CLA	C3B-C4B	2.86	1.49	1.42
18	3	613	CLA	C3B-C4B	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	614	CLA	C4D-ND	-2.86	1.33	1.37
18	F	305	CLA	C3B-C4B	2.86	1.49	1.42
18	B	829	CLA	C4D-ND	-2.86	1.33	1.37
18	A	854	CLA	C4D-ND	-2.85	1.33	1.37
18	B	824	CLA	C4D-ND	-2.85	1.33	1.37
18	B	824	CLA	C3B-C4B	2.85	1.49	1.42
21	5	621	BCR	C30-C25	-2.85	1.49	1.53
18	B	803	CLA	C3B-C4B	2.85	1.49	1.42
18	A	834	CLA	C3B-C4B	2.85	1.49	1.42
18	B	821	CLA	C3B-C4B	2.85	1.49	1.42
26	2	619	LUT	C18-C5	2.85	1.55	1.50
21	3	620	BCR	C30-C25	-2.85	1.49	1.53
18	L	302	CLA	C3B-C4B	2.85	1.49	1.42
18	A	835	CLA	C4D-ND	-2.85	1.33	1.37
18	B	817	CLA	C3B-C4B	2.85	1.49	1.42
18	A	832	CLA	C3B-C4B	2.85	1.49	1.42
25	5	608	CHL	C3D-C2D	2.85	1.46	1.39
18	K	206	CLA	C3B-C4B	2.84	1.49	1.42
26	6	617	LUT	C23-C24	2.84	1.54	1.50
18	F	301	CLA	C3B-C4B	2.84	1.49	1.42
18	B	813	CLA	C3B-C4B	2.84	1.49	1.42
18	A	824	CLA	C3B-C4B	2.84	1.49	1.42
18	A	838	CLA	C3B-C4B	2.84	1.49	1.42
18	2	609	CLA	C3B-C4B	2.84	1.49	1.42
18	A	843	CLA	C3B-C4B	2.84	1.49	1.42
18	A	803	CLA	C3B-C4B	2.84	1.49	1.42
18	A	841	CLA	C3B-C4B	2.83	1.49	1.42
18	A	854	CLA	C3B-C4B	2.83	1.49	1.42
18	5	603	CLA	C3B-C4B	2.83	1.49	1.42
18	A	804	CLA	C3B-C4B	2.83	1.49	1.42
25	2	606	CHL	C3D-C2D	2.83	1.46	1.39
18	A	820	CLA	C3B-C4B	2.83	1.49	1.42
18	5	613	CLA	C4D-ND	-2.83	1.33	1.37
18	B	815	CLA	C3B-C4B	2.83	1.49	1.42
18	6	610	CLA	C3B-C4B	2.83	1.49	1.42
18	B	830	CLA	C3B-C4B	2.83	1.49	1.42
18	B	839	CLA	C3B-C4B	2.83	1.49	1.42
18	6	602	CLA	C3B-C4B	2.83	1.49	1.42
26	6	617	LUT	C18-C5	2.82	1.55	1.50
18	A	801	CLA	C3B-C4B	2.82	1.49	1.42
18	A	815	CLA	C3B-C4B	2.82	1.49	1.42
18	A	828	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	603	CLA	C3B-C4B	2.82	1.49	1.42
25	2	616	CHL	C3B-C4B	2.82	1.49	1.42
18	B	835	CLA	C3B-C4B	2.82	1.49	1.42
18	B	816	CLA	C3B-C4B	2.82	1.49	1.42
18	B	823	CLA	C3B-C4B	2.81	1.49	1.42
18	A	806	CLA	C3B-C4B	2.81	1.49	1.42
25	6	607	CHL	C3B-C4B	2.81	1.49	1.42
18	B	806	CLA	C3B-C4B	2.81	1.49	1.42
18	B	804	CLA	C3B-C4B	2.81	1.49	1.42
18	3	609	CLA	C4D-ND	-2.81	1.33	1.37
18	B	809	CLA	C3B-C4B	2.81	1.49	1.42
18	B	812	CLA	C3B-C4B	2.81	1.49	1.42
18	A	816	CLA	C3B-C4B	2.81	1.49	1.42
18	2	603	CLA	C3B-C4B	2.81	1.49	1.42
18	6	604	CLA	C3B-C4B	2.80	1.49	1.42
18	B	822	CLA	C3B-C4B	2.80	1.49	1.42
18	3	606	CLA	C3B-C4B	2.80	1.49	1.42
18	3	602	CLA	C3B-C4B	2.80	1.49	1.42
18	A	831	CLA	C3B-C4B	2.80	1.49	1.42
18	B	814	CLA	C3B-C4B	2.80	1.49	1.42
18	A	824	CLA	C4D-ND	-2.80	1.33	1.37
18	F	304	CLA	C3B-C4B	2.80	1.49	1.42
18	B	807	CLA	C3B-C4B	2.80	1.49	1.42
18	B	831	CLA	C3B-C4B	2.80	1.49	1.42
18	6	616	CLA	C4D-ND	-2.79	1.33	1.37
25	6	607	CHL	MG-NA	-2.79	1.99	2.06
21	A	848	BCR	C30-C25	-2.79	1.49	1.53
18	2	602	CLA	C3B-C4B	2.79	1.49	1.42
18	B	825	CLA	C3B-C4B	2.79	1.49	1.42
18	B	827	CLA	C3B-C4B	2.79	1.49	1.42
18	A	829	CLA	C3B-C4B	2.79	1.49	1.42
18	A	819	CLA	C3B-C4B	2.78	1.49	1.42
18	A	810	CLA	C3B-C4B	2.77	1.49	1.42
18	A	839	CLA	C3B-C4B	2.77	1.49	1.42
18	B	819	CLA	C3B-C4B	2.77	1.49	1.42
18	A	807	CLA	C3B-C4B	2.77	1.49	1.42
18	B	820	CLA	C3B-C4B	2.76	1.49	1.42
18	6	603	CLA	C3B-C4B	2.76	1.49	1.42
18	A	830	CLA	C3B-C4B	2.76	1.49	1.42
25	5	608	CHL	C3B-C4B	2.76	1.49	1.42
18	B	832	CLA	C3B-C4B	2.76	1.49	1.42
18	B	829	CLA	C3B-C4B	2.75	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	LUT	C31-C30	2.75	1.52	1.43
18	2	604	CLA	C4D-ND	-2.75	1.33	1.37
26	3	618	LUT	C31-C30	2.75	1.52	1.43
18	B	838	CLA	C3B-C4B	2.75	1.49	1.42
25	2	607	CHL	C3B-C4B	2.75	1.49	1.42
18	G	204	CLA	C3B-C4B	2.74	1.49	1.42
18	A	835	CLA	C3B-C4B	2.74	1.49	1.42
18	A	802	CLA	C3B-C4B	2.74	1.49	1.42
18	B	826	CLA	C3B-C4B	2.74	1.49	1.42
26	5	619	LUT	C23-C24	2.73	1.54	1.50
26	2	619	LUT	C23-C24	2.73	1.54	1.50
18	L	302	CLA	C1B-C2B	2.73	1.49	1.43
18	A	813	CLA	C3B-C4B	2.73	1.49	1.42
18	L	303	CLA	C3B-C4B	2.72	1.49	1.42
18	K	204	CLA	C1B-C2B	2.72	1.49	1.43
26	5	619	LUT	C19-C9	2.72	1.56	1.50
26	6	617	LUT	C19-C9	2.71	1.56	1.50
18	2	610	CLA	C4D-ND	-2.70	1.34	1.37
18	5	614	CLA	C1B-C2B	2.70	1.49	1.43
26	2	619	LUT	C19-C9	2.70	1.56	1.50
25	2	601	CHL	MG-NA	-2.70	1.99	2.06
25	5	607	CHL	C3B-C4B	2.70	1.49	1.42
26	3	618	LUT	C19-C9	2.69	1.56	1.50
18	3	614	CLA	C1B-C2B	2.69	1.49	1.43
21	B	848	BCR	C30-C25	-2.69	1.50	1.53
18	K	206	CLA	C1B-C2B	2.69	1.49	1.43
18	B	802	CLA	C3B-C4B	2.69	1.49	1.42
21	J	103	BCR	C30-C25	-2.69	1.50	1.53
26	2	619	LUT	C31-C30	2.68	1.51	1.43
18	B	811	CLA	C1B-C2B	2.68	1.49	1.43
18	G	201	CLA	C1B-C2B	2.68	1.49	1.43
18	A	817	CLA	C1B-C2B	2.68	1.49	1.43
18	B	807	CLA	C1B-C2B	2.68	1.49	1.43
18	6	611	CLA	C4B-C3B	2.66	1.49	1.43
18	3	604	CLA	C4B-C3B	2.66	1.49	1.43
18	6	609	CLA	C1B-C2B	2.66	1.49	1.43
18	B	812	CLA	C1B-C2B	2.66	1.49	1.43
18	5	604	CLA	C1B-C2B	2.66	1.49	1.43
18	6	616	CLA	C1B-C2B	2.66	1.49	1.43
25	2	607	CHL	MG-NA	-2.66	2.00	2.06
21	L	305	BCR	C30-C25	-2.66	1.50	1.53
25	5	608	CHL	C1D-C2D	2.66	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	603	CLA	C1B-C2B	2.66	1.49	1.43
18	3	602	CLA	C1B-C2B	2.66	1.49	1.43
26	6	617	LUT	C31-C30	2.65	1.51	1.43
18	3	612	CLA	C1B-C2B	2.65	1.49	1.43
18	5	611	CLA	C1B-C2B	2.65	1.49	1.43
18	A	815	CLA	C1B-C2B	2.65	1.49	1.43
18	F	304	CLA	C1B-C2B	2.65	1.49	1.43
18	B	811	CLA	C4B-C3B	2.65	1.49	1.43
18	2	602	CLA	C1B-C2B	2.65	1.49	1.43
18	A	845	CLA	C1B-C2B	2.64	1.49	1.43
18	K	203	CLA	C1B-C2B	2.64	1.49	1.43
18	B	827	CLA	C1B-C2B	2.64	1.49	1.43
18	3	603	CLA	C1B-C2B	2.64	1.49	1.43
18	3	610	CLA	C1B-C2B	2.64	1.49	1.43
18	3	611	CLA	C1B-C2B	2.64	1.49	1.43
18	B	814	CLA	C1B-C2B	2.64	1.49	1.43
18	3	613	CLA	C1B-C2B	2.63	1.49	1.43
18	B	825	CLA	C1B-C2B	2.63	1.49	1.43
18	3	615	CLA	C1B-C2B	2.63	1.49	1.43
25	3	608	CHL	C3B-C4B	2.63	1.48	1.42
18	6	614	CLA	C4B-C3B	2.63	1.49	1.43
18	5	610	CLA	C1B-C2B	2.63	1.49	1.43
18	6	611	CLA	C1B-C2B	2.62	1.49	1.43
18	2	603	CLA	C1B-C2B	2.62	1.49	1.43
18	3	604	CLA	C1B-C2B	2.62	1.49	1.43
18	6	606	CLA	C4D-ND	-2.62	1.34	1.37
18	B	831	CLA	C1B-C2B	2.62	1.49	1.43
18	B	832	CLA	C1B-C2B	2.62	1.49	1.43
18	B	802	CLA	C1B-C2B	2.62	1.49	1.43
18	A	813	CLA	C1B-C2B	2.62	1.49	1.43
18	A	818	CLA	C1B-C2B	2.62	1.49	1.43
18	3	607	CLA	C4B-C3B	2.62	1.49	1.43
18	A	836	CLA	C1B-C2B	2.61	1.49	1.43
18	A	812	CLA	C1B-C2B	2.61	1.49	1.43
18	L	303	CLA	C1B-C2B	2.61	1.49	1.43
25	6	601	CHL	C3B-C4B	2.61	1.48	1.42
18	6	616	CLA	C4B-C3B	2.61	1.49	1.43
18	5	601	CLA	C1B-C2B	2.61	1.49	1.43
18	B	810	CLA	C1B-C2B	2.61	1.49	1.43
18	A	824	CLA	C1B-C2B	2.61	1.49	1.43
18	6	613	CLA	C1B-C2B	2.61	1.49	1.43
18	6	614	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	801	CLA	C1B-C2B	2.60	1.49	1.43
18	3	607	CLA	C1B-C2B	2.60	1.49	1.43
18	J	101	CLA	C1B-C2B	2.60	1.49	1.43
18	2	614	CLA	C1B-C2B	2.60	1.49	1.43
25	2	601	CHL	C1B-C2B	2.60	1.49	1.43
18	B	815	CLA	C1B-C2B	2.60	1.49	1.43
18	5	602	CLA	C1B-C2B	2.60	1.49	1.43
18	A	830	CLA	C1B-C2B	2.60	1.49	1.43
18	6	608	CLA	C1B-C2B	2.59	1.49	1.43
18	5	611	CLA	C4B-C3B	2.59	1.49	1.43
18	B	806	CLA	C1B-C2B	2.59	1.49	1.43
18	A	816	CLA	C1B-C2B	2.59	1.49	1.43
18	6	612	CLA	C1B-C2B	2.59	1.49	1.43
18	5	603	CLA	C1B-C2B	2.59	1.49	1.43
18	A	822	CLA	C4B-C3B	2.59	1.49	1.43
18	L	304	CLA	C1B-C2B	2.59	1.49	1.43
18	2	604	CLA	C1B-C2B	2.59	1.49	1.43
18	6	604	CLA	C1B-C2B	2.59	1.49	1.43
18	6	606	CLA	C1B-C2B	2.59	1.49	1.43
18	3	606	CLA	C1B-C2B	2.59	1.49	1.43
18	A	804	CLA	C1B-C2B	2.59	1.49	1.43
18	B	804	CLA	C1B-C2B	2.58	1.49	1.43
18	B	822	CLA	C1B-C2B	2.58	1.49	1.43
18	B	821	CLA	C1B-C2B	2.58	1.49	1.43
18	A	821	CLA	C1B-C2B	2.58	1.49	1.43
25	5	615	CHL	C3B-C4B	2.58	1.48	1.42
18	5	609	CLA	C1B-C2B	2.58	1.49	1.43
18	A	809	CLA	C1B-C2B	2.58	1.49	1.43
18	K	204	CLA	C4B-C3B	2.58	1.49	1.43
18	B	817	CLA	C1B-C2B	2.58	1.49	1.43
18	A	842	CLA	C1B-C2B	2.57	1.49	1.43
25	2	608	CHL	C3B-C4B	2.57	1.48	1.42
18	A	808	CLA	C1B-C2B	2.57	1.49	1.43
18	2	609	CLA	C1B-C2B	2.57	1.49	1.43
18	2	611	CLA	C1B-C2B	2.57	1.49	1.43
18	B	834	CLA	C1B-C2B	2.57	1.49	1.43
18	F	305	CLA	C1B-C2B	2.57	1.49	1.43
18	2	613	CLA	C1B-C2B	2.57	1.49	1.43
18	A	828	CLA	C1B-C2B	2.57	1.49	1.43
18	A	825	CLA	C1B-C2B	2.57	1.49	1.43
18	B	835	CLA	C1B-C2B	2.57	1.49	1.43
18	B	809	CLA	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	612	CLA	C1B-C2B	2.57	1.49	1.43
18	6	609	CLA	C4B-C3B	2.57	1.49	1.43
18	A	822	CLA	C1B-C2B	2.56	1.49	1.43
18	3	609	CLA	C1B-C2B	2.56	1.49	1.43
18	F	301	CLA	C1B-C2B	2.56	1.49	1.43
18	A	841	CLA	C1B-C2B	2.56	1.49	1.43
18	6	602	CLA	C1B-C2B	2.56	1.49	1.43
18	A	829	CLA	C1B-C2B	2.56	1.49	1.43
18	A	834	CLA	C1B-C2B	2.56	1.49	1.43
18	6	610	CLA	C1B-C2B	2.55	1.49	1.43
25	5	607	CHL	C1B-C2B	2.55	1.49	1.43
18	5	613	CLA	C1B-C2B	2.55	1.49	1.43
18	G	204	CLA	C1B-C2B	2.55	1.49	1.43
18	B	841	CLA	C1B-C2B	2.55	1.49	1.43
18	5	612	CLA	C1B-C2B	2.55	1.49	1.43
18	3	617	CLA	C1B-C2B	2.55	1.49	1.43
18	B	826	CLA	C1B-C2B	2.55	1.49	1.43
18	A	854	CLA	C1B-C2B	2.55	1.49	1.43
18	F	303	CLA	C1B-C2B	2.55	1.49	1.43
18	K	201	CLA	C4D-ND	-2.55	1.34	1.37
18	A	810	CLA	C1B-C2B	2.54	1.49	1.43
25	6	607	CHL	C1B-C2B	2.54	1.49	1.43
25	2	606	CHL	C3B-C4B	2.54	1.48	1.42
18	A	819	CLA	C1B-C2B	2.54	1.49	1.43
18	B	816	CLA	C1B-C2B	2.54	1.49	1.43
18	A	807	CLA	C1B-C2B	2.54	1.49	1.43
18	G	203	CLA	C1B-C2B	2.53	1.49	1.43
18	B	820	CLA	C1B-C2B	2.53	1.49	1.43
25	5	606	CHL	C1B-C2B	2.53	1.49	1.43
18	A	843	CLA	C1B-C2B	2.53	1.49	1.43
18	B	823	CLA	C1B-C2B	2.53	1.49	1.43
18	A	835	CLA	C1B-C2B	2.53	1.49	1.43
18	A	838	CLA	C1B-C2B	2.53	1.49	1.43
18	A	814	CLA	C1B-C2B	2.52	1.49	1.43
18	A	833	CLA	C1B-C2B	2.52	1.49	1.43
18	A	839	CLA	C1B-C2B	2.52	1.49	1.43
18	B	836	CLA	C1B-C2B	2.52	1.49	1.43
25	3	608	CHL	C1B-C2B	2.52	1.49	1.43
23	B	850	DGD	O2G-C2G	-2.52	1.40	1.46
18	B	840	CLA	C1B-C2B	2.52	1.49	1.43
18	A	832	CLA	C1B-C2B	2.52	1.49	1.43
18	B	837	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	811	CLA	C1B-C2B	2.51	1.49	1.43
18	A	837	CLA	C1B-C2B	2.51	1.49	1.43
18	B	803	CLA	C1B-C2B	2.51	1.49	1.43
18	B	839	CLA	C1B-C2B	2.50	1.49	1.43
18	B	830	CLA	C1B-C2B	2.50	1.49	1.43
18	A	805	CLA	C1B-C2B	2.50	1.49	1.43
18	B	838	CLA	C1B-C2B	2.50	1.49	1.43
25	2	607	CHL	C1B-C2B	2.49	1.49	1.43
18	A	806	CLA	C1B-C2B	2.49	1.49	1.43
25	6	601	CHL	MG-NA	-2.49	2.00	2.06
18	A	803	CLA	C1B-C2B	2.49	1.49	1.43
18	A	820	CLA	C1B-C2B	2.49	1.49	1.43
25	2	616	CHL	C1B-C2B	2.49	1.49	1.43
25	5	615	CHL	C1B-C2B	2.48	1.49	1.43
23	B	850	DGD	O1G-C1G	-2.48	1.39	1.45
18	B	813	CLA	C1B-C2B	2.48	1.49	1.43
18	A	827	CLA	C1B-C2B	2.48	1.49	1.43
18	A	823	CLA	C1B-C2B	2.48	1.49	1.43
25	2	606	CHL	C1B-C2B	2.47	1.49	1.43
18	B	818	CLA	C1B-C2B	2.47	1.49	1.43
18	B	828	CLA	C1B-C2B	2.47	1.49	1.43
18	A	826	CLA	C1B-C2B	2.47	1.49	1.43
18	B	819	CLA	C1B-C2B	2.47	1.49	1.43
18	K	201	CLA	C3B-C4B	2.46	1.48	1.42
18	B	824	CLA	C1B-C2B	2.46	1.49	1.43
18	A	840	CLA	C1B-C2B	2.46	1.49	1.43
18	B	805	CLA	C1B-C2B	2.46	1.49	1.43
26	6	617	LUT	C39-C29	2.45	1.55	1.50
25	6	601	CHL	C1B-C2B	2.44	1.49	1.43
25	6	607	CHL	C4C-C3C	2.44	1.49	1.45
27	3	619	XAT	O4-C5	-2.44	1.42	1.46
18	B	808	CLA	C1B-C2B	2.43	1.49	1.43
18	A	831	CLA	C1B-C2B	2.43	1.49	1.43
18	B	829	CLA	CMB-C2B	-2.43	1.45	1.50
18	B	829	CLA	C1B-C2B	2.42	1.48	1.43
25	3	608	CHL	MG-NA	-2.41	2.00	2.06
25	2	608	CHL	MG-NA	-2.41	2.00	2.06
26	5	619	LUT	C39-C29	2.40	1.55	1.50
18	A	802	CLA	C1B-C2B	2.40	1.48	1.43
26	2	619	LUT	C39-C29	2.40	1.55	1.50
26	3	618	LUT	C39-C29	2.39	1.55	1.50
25	2	607	CHL	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	616	CHL	MG-NA	-2.39	2.00	2.06
20	5	622	LHG	O7-C5	-2.38	1.40	1.46
25	5	608	CHL	C1B-C2B	2.38	1.48	1.43
25	6	607	CHL	C1B-NB	-2.37	1.34	1.37
25	5	615	CHL	C4C-C3C	2.37	1.49	1.45
18	A	823	CLA	CHC-C1C	2.37	1.43	1.38
25	2	616	CHL	C4C-C3C	2.36	1.49	1.45
25	2	601	CHL	C4B-NB	-2.36	1.34	1.37
18	B	833	CLA	C1B-C2B	2.36	1.48	1.43
20	A	846	LHG	O7-C5	-2.36	1.40	1.46
27	3	619	XAT	O24-C25	-2.35	1.42	1.46
25	2	608	CHL	C1B-C2B	2.34	1.48	1.43
27	2	620	XAT	O24-C25	-2.34	1.42	1.46
18	2	610	CLA	MG-NB	-2.34	2.01	2.05
25	6	601	CHL	C4B-NB	-2.33	1.34	1.37
25	5	607	CHL	C4C-C3C	2.33	1.49	1.45
25	5	606	CHL	C4C-C3C	2.33	1.49	1.44
25	5	607	CHL	C1B-NB	-2.31	1.34	1.37
25	6	607	CHL	C4B-NB	-2.30	1.35	1.37
25	6	601	CHL	C1B-NB	-2.30	1.35	1.37
25	5	607	CHL	C4B-NB	-2.30	1.35	1.37
18	A	807	CLA	MG-NB	-2.30	2.01	2.05
18	A	811	CLA	CHC-C1C	2.29	1.43	1.38
18	5	610	CLA	CHC-C1C	2.29	1.43	1.38
25	2	607	CHL	C1B-NB	-2.28	1.35	1.37
18	B	836	CLA	CHC-C1C	2.28	1.43	1.38
18	6	611	CLA	CHC-C1C	2.28	1.43	1.38
18	A	833	CLA	CHC-C1C	2.27	1.43	1.38
18	F	305	CLA	CMD-C2D	-2.27	1.46	1.50
25	2	608	CHL	C4C-C3C	2.27	1.49	1.45
18	A	827	CLA	CHC-C1C	2.27	1.43	1.38
25	5	608	CHL	C1B-NB	-2.27	1.35	1.37
18	2	611	CLA	CHC-C1C	2.27	1.43	1.38
21	J	103	BCR	C33-C5	-2.27	1.47	1.50
18	5	609	CLA	CHC-C1C	2.26	1.43	1.38
20	6	620	LHG	O7-C5	-2.26	1.40	1.46
18	A	806	CLA	MG-NB	-2.26	2.01	2.05
27	5	620	XAT	C22-C21	-2.26	1.51	1.54
18	3	617	CLA	CHC-C1C	2.26	1.43	1.38
18	A	812	CLA	CHC-C1C	2.25	1.43	1.38
27	5	620	XAT	O24-C25	-2.24	1.43	1.46
25	6	601	CHL	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	CMB-C2B	-2.24	1.46	1.50
18	G	204	CLA	CHC-C1C	2.24	1.43	1.38
18	F	301	CLA	CHC-C1C	2.24	1.43	1.38
18	3	610	CLA	CHC-C1C	2.24	1.43	1.38
18	B	829	CLA	CMD-C2D	-2.24	1.46	1.50
18	A	831	CLA	CMB-C2B	-2.23	1.46	1.50
18	B	804	CLA	CHC-C1C	2.23	1.43	1.38
25	2	601	CHL	C1B-NB	-2.23	1.35	1.37
18	A	820	CLA	CHC-C1C	2.23	1.43	1.38
18	6	614	CLA	CHC-C1C	2.23	1.43	1.38
25	5	607	CHL	C1D-ND	-2.23	1.35	1.37
18	A	808	CLA	CHC-C1C	2.23	1.43	1.38
18	F	303	CLA	CHC-C1C	2.23	1.43	1.38
18	A	836	CLA	CHC-C1C	2.22	1.43	1.38
18	B	826	CLA	MG-NB	-2.22	2.01	2.05
25	2	606	CHL	C4C-C3C	2.22	1.48	1.45
18	5	602	CLA	CHC-C1C	2.22	1.43	1.38
18	A	805	CLA	CHC-C1C	2.22	1.43	1.38
18	B	824	CLA	CHC-C1C	2.22	1.43	1.38
18	5	614	CLA	CHC-C1C	2.22	1.43	1.38
18	A	825	CLA	CHC-C1C	2.22	1.43	1.38
18	A	854	CLA	CHC-C1C	2.22	1.43	1.38
18	A	802	CLA	CHC-C1C	2.22	1.43	1.38
18	5	611	CLA	CHC-C1C	2.22	1.43	1.38
18	6	616	CLA	CHC-C1C	2.22	1.43	1.38
18	B	823	CLA	MG-NB	-2.22	2.01	2.05
18	L	302	CLA	CHC-C1C	2.22	1.43	1.38
18	B	806	CLA	CHC-C1C	2.21	1.43	1.38
18	B	839	CLA	CHC-C1C	2.21	1.43	1.38
25	5	606	CHL	MG-NA	-2.21	2.01	2.06
18	A	822	CLA	CHC-C1C	2.21	1.43	1.38
18	3	607	CLA	CHC-C1C	2.21	1.43	1.38
25	6	607	CHL	C1D-ND	-2.21	1.35	1.37
18	5	612	CLA	CHC-C1C	2.21	1.43	1.38
18	5	604	CLA	CHC-C1C	2.21	1.43	1.38
18	A	806	CLA	CHC-C1C	2.21	1.43	1.38
25	2	607	CHL	C4B-NB	-2.21	1.35	1.37
18	A	828	CLA	CHC-C1C	2.21	1.43	1.38
18	B	831	CLA	MG-NB	-2.20	2.01	2.05
18	A	809	CLA	CHC-C1C	2.20	1.43	1.38
18	2	602	CLA	CHC-C1C	2.20	1.43	1.38
18	2	604	CLA	CHC-C1C	2.20	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	612	CLA	CHC-C1C	2.20	1.43	1.38
18	B	819	CLA	CMB-C2B	-2.20	1.46	1.50
18	B	803	CLA	CMC-C2C	-2.20	1.46	1.50
25	3	608	CHL	C1B-NB	-2.20	1.35	1.37
18	B	811	CLA	CHC-C1C	2.20	1.43	1.38
18	B	818	CLA	CMB-C2B	-2.20	1.46	1.50
18	A	828	CLA	MG-NB	-2.20	2.01	2.05
18	A	829	CLA	CHC-C1C	2.20	1.43	1.38
18	B	829	CLA	MG-NB	-2.20	2.01	2.05
18	A	838	CLA	MG-NB	-2.19	2.01	2.05
18	A	804	CLA	MG-NB	-2.19	2.01	2.05
18	B	816	CLA	CHC-C1C	2.19	1.43	1.38
18	F	304	CLA	MG-NB	-2.19	2.01	2.05
18	A	824	CLA	CHC-C1C	2.19	1.43	1.38
25	5	615	CHL	MG-NA	-2.19	2.01	2.06
18	A	807	CLA	CHC-C1C	2.19	1.43	1.38
18	B	814	CLA	CHC-C1C	2.19	1.43	1.38
18	B	837	CLA	CHC-C1C	2.19	1.43	1.38
18	B	823	CLA	CHC-C1C	2.19	1.43	1.38
18	K	203	CLA	CHC-C1C	2.19	1.43	1.38
18	A	839	CLA	MG-NB	-2.19	2.01	2.05
18	5	611	CLA	MG-NB	-2.19	2.01	2.05
18	B	807	CLA	MG-NB	-2.19	2.01	2.05
18	B	841	CLA	MG-NB	-2.19	2.01	2.05
18	6	602	CLA	MG-NB	-2.19	2.01	2.05
18	2	614	CLA	CHC-C1C	2.19	1.43	1.38
18	B	830	CLA	CHC-C1C	2.19	1.43	1.38
18	B	834	CLA	CHC-C1C	2.19	1.43	1.38
18	3	612	CLA	CHC-C1C	2.19	1.43	1.38
18	B	833	CLA	MG-NB	-2.19	2.01	2.05
18	B	819	CLA	MG-NB	-2.18	2.01	2.05
18	A	834	CLA	MG-NB	-2.18	2.01	2.05
25	2	601	CHL	C4C-C3C	2.18	1.48	1.45
18	B	833	CLA	CHC-C1C	2.18	1.43	1.38
18	B	820	CLA	CHC-C1C	2.18	1.43	1.38
18	2	610	CLA	CHC-C1C	2.18	1.43	1.38
18	A	826	CLA	MG-NB	-2.18	2.01	2.05
25	2	601	CHL	C4B-C3B	2.18	1.48	1.43
18	3	609	CLA	CHC-C1C	2.18	1.43	1.38
18	6	602	CLA	CHC-C1C	2.18	1.43	1.38
18	A	832	CLA	CHC-C1C	2.18	1.43	1.38
18	6	604	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	814	CLA	MG-NB	-2.18	2.01	2.05
18	B	814	CLA	MG-NB	-2.18	2.01	2.05
18	5	601	CLA	CHC-C1C	2.18	1.42	1.38
18	A	819	CLA	CHC-C1C	2.18	1.42	1.38
18	A	832	CLA	MG-NB	-2.18	2.01	2.05
20	A	847	LHG	O7-C5	-2.18	1.41	1.46
25	2	616	CHL	C1B-NB	-2.18	1.35	1.37
18	A	829	CLA	MG-NB	-2.17	2.01	2.05
18	A	817	CLA	CHC-C1C	2.17	1.42	1.38
25	5	606	CHL	C4B-C3B	2.17	1.48	1.43
18	A	801	CLA	MG-NB	-2.17	2.01	2.05
18	A	820	CLA	MG-NB	-2.17	2.01	2.05
18	B	830	CLA	MG-NB	-2.17	2.01	2.05
18	2	609	CLA	CHC-C1C	2.17	1.42	1.38
18	6	613	CLA	CHC-C1C	2.17	1.42	1.38
18	B	832	CLA	MG-NB	-2.17	2.01	2.05
18	B	839	CLA	CMD-C2D	-2.17	1.46	1.50
18	A	841	CLA	CHC-C1C	2.17	1.42	1.38
18	L	304	CLA	CHC-C1C	2.17	1.42	1.38
18	A	843	CLA	CMB-C2B	-2.17	1.46	1.50
18	A	843	CLA	CMD-C2D	-2.17	1.46	1.50
18	B	812	CLA	CHC-C1C	2.17	1.42	1.38
18	6	612	CLA	CHC-C1C	2.17	1.42	1.38
18	A	821	CLA	CHC-C1C	2.16	1.42	1.38
18	B	824	CLA	CMD-C2D	-2.16	1.46	1.50
18	B	832	CLA	CHC-C1C	2.16	1.42	1.38
18	B	824	CLA	MG-NB	-2.16	2.01	2.05
18	A	819	CLA	MG-NB	-2.16	2.01	2.05
18	B	838	CLA	CHC-C1C	2.16	1.42	1.38
18	A	815	CLA	CHC-C1C	2.16	1.42	1.38
18	A	831	CLA	MG-NB	-2.16	2.01	2.05
18	B	822	CLA	CHC-C1C	2.16	1.42	1.38
18	F	305	CLA	MG-NB	-2.16	2.01	2.05
18	6	610	CLA	CHC-C1C	2.16	1.42	1.38
18	B	816	CLA	MG-NB	-2.16	2.01	2.05
18	3	615	CLA	CHC-C1C	2.16	1.42	1.38
18	3	606	CLA	MG-NB	-2.16	2.01	2.05
18	B	815	CLA	CHC-C1C	2.16	1.42	1.38
18	2	613	CLA	CHC-C1C	2.16	1.42	1.38
18	B	828	CLA	CHC-C1C	2.16	1.42	1.38
18	A	803	CLA	MG-NB	-2.16	2.01	2.05
25	2	608	CHL	C1B-NB	-2.16	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	840	CLA	CHC-C1C	2.16	1.42	1.38
18	B	811	CLA	MG-NB	-2.16	2.01	2.05
18	A	840	CLA	MG-NB	-2.16	2.01	2.05
18	B	841	CLA	CHC-C1C	2.16	1.42	1.38
18	6	608	CLA	CHC-C1C	2.16	1.42	1.38
18	A	813	CLA	MG-NB	-2.16	2.01	2.05
18	B	828	CLA	CMD-C2D	-2.16	1.46	1.50
18	A	841	CLA	MG-NB	-2.15	2.01	2.05
18	F	304	CLA	CHC-C1C	2.15	1.42	1.38
18	A	824	CLA	MG-NB	-2.15	2.01	2.05
18	A	824	CLA	CMD-C2D	-2.15	1.46	1.50
18	B	831	CLA	CHC-C1C	2.15	1.42	1.38
25	5	608	CHL	MG-NA	-2.15	2.01	2.06
18	B	813	CLA	CHC-C1C	2.15	1.42	1.38
18	3	602	CLA	MG-NB	-2.15	2.01	2.05
18	A	818	CLA	CHC-C1C	2.15	1.42	1.38
18	6	609	CLA	CHC-C1C	2.15	1.42	1.38
18	A	827	CLA	MG-NB	-2.15	2.01	2.05
18	B	822	CLA	MG-NB	-2.15	2.01	2.05
18	B	827	CLA	CHC-C1C	2.15	1.42	1.38
18	J	101	CLA	CHC-C1C	2.15	1.42	1.38
18	K	206	CLA	CHC-C1C	2.15	1.42	1.38
25	2	601	CHL	C1D-ND	-2.15	1.35	1.37
18	A	827	CLA	CMD-C2D	-2.15	1.46	1.50
18	A	810	CLA	MG-NB	-2.15	2.01	2.05
27	5	620	XAT	O4-C5	-2.15	1.43	1.46
18	A	816	CLA	CHC-C1C	2.15	1.42	1.38
18	G	204	CLA	MG-NB	-2.15	2.01	2.05
18	A	815	CLA	MG-NB	-2.15	2.01	2.05
18	B	803	CLA	CHC-C1C	2.15	1.42	1.38
18	A	838	CLA	CHC-C1C	2.14	1.42	1.38
18	B	834	CLA	CMB-C2B	-2.14	1.46	1.50
18	A	830	CLA	MG-NB	-2.14	2.01	2.05
25	5	608	CHL	C1D-ND	-2.14	1.35	1.37
18	A	839	CLA	CHC-C1C	2.14	1.42	1.38
18	B	821	CLA	MG-NB	-2.14	2.01	2.05
18	A	822	CLA	CMB-C2B	-2.14	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.14	1.46	1.50
18	L	303	CLA	CHC-C1C	2.14	1.42	1.38
18	3	604	CLA	CHC-C1C	2.14	1.42	1.38
18	A	814	CLA	CHC-C1C	2.14	1.42	1.38
18	A	823	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	610	CLA	MG-NB	-2.14	2.01	2.05
18	B	813	CLA	MG-NB	-2.14	2.01	2.05
18	B	835	CLA	MG-NB	-2.14	2.01	2.05
18	B	839	CLA	MG-NB	-2.14	2.01	2.05
18	5	613	CLA	CHC-C1C	2.14	1.42	1.38
18	A	804	CLA	CHC-C1C	2.14	1.42	1.38
18	A	842	CLA	CHC-C1C	2.14	1.42	1.38
18	A	821	CLA	MG-NB	-2.14	2.01	2.05
18	B	810	CLA	MG-NB	-2.14	2.01	2.05
18	B	808	CLA	CHC-C1C	2.14	1.42	1.38
18	A	833	CLA	MG-NB	-2.14	2.01	2.05
18	B	802	CLA	MG-NB	-2.14	2.01	2.05
18	G	201	CLA	CHC-C1C	2.14	1.42	1.38
18	B	825	CLA	MG-NB	-2.14	2.01	2.05
18	B	836	CLA	MG-NB	-2.14	2.01	2.05
18	B	815	CLA	MG-NB	-2.14	2.01	2.05
18	3	614	CLA	CHC-C1C	2.14	1.42	1.38
27	6	619	XAT	O4-C5	-2.13	1.43	1.46
18	B	802	CLA	CHC-C1C	2.13	1.42	1.38
18	A	835	CLA	MG-NB	-2.13	2.01	2.05
18	3	602	CLA	CHC-C1C	2.13	1.42	1.38
18	3	606	CLA	CHC-C1C	2.13	1.42	1.38
26	2	619	LUT	C38-C25	2.13	1.54	1.50
18	B	823	CLA	CMD-C2D	-2.13	1.46	1.50
18	6	610	CLA	MG-NB	-2.13	2.01	2.05
18	F	301	CLA	MG-NB	-2.13	2.01	2.05
18	6	608	CLA	MG-NB	-2.13	2.01	2.05
18	A	835	CLA	CHC-C1C	2.13	1.42	1.38
18	A	810	CLA	CHC-C1C	2.13	1.42	1.38
18	B	825	CLA	CHC-C1C	2.13	1.42	1.38
18	B	820	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	840	CLA	MG-NB	-2.13	2.01	2.05
18	A	813	CLA	CHC-C1C	2.13	1.42	1.38
18	A	836	CLA	MG-NB	-2.13	2.01	2.05
18	A	825	CLA	MG-NB	-2.13	2.01	2.05
18	B	817	CLA	MG-NB	-2.13	2.01	2.05
18	A	801	CLA	CHC-C1C	2.13	1.42	1.38
18	A	820	CLA	CMB-C2B	-2.13	1.46	1.50
18	A	816	CLA	MG-NB	-2.12	2.01	2.05
18	B	803	CLA	MG-NB	-2.12	2.01	2.05
18	A	845	CLA	CHC-C1C	2.12	1.42	1.38
18	K	204	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	611	CLA	CHC-C1C	2.12	1.42	1.38
18	A	803	CLA	CHC-C1C	2.12	1.42	1.38
18	A	840	CLA	CHC-C1C	2.12	1.42	1.38
18	3	603	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	826	CLA	CHC-C1C	2.12	1.42	1.38
18	B	805	CLA	CHC-C1C	2.12	1.42	1.38
18	B	828	CLA	MG-NB	-2.12	2.01	2.05
25	3	608	CHL	C4C-C3C	2.12	1.48	1.45
18	6	603	CLA	CHC-C1C	2.12	1.42	1.38
18	A	802	CLA	MG-NB	-2.12	2.01	2.05
18	A	810	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	822	CLA	MG-NB	-2.12	2.01	2.05
18	5	602	CLA	CMB-C2B	-2.12	1.46	1.50
18	B	806	CLA	MG-NB	-2.12	2.01	2.05
18	B	828	CLA	CMB-C2B	-2.12	1.46	1.50
18	F	303	CLA	MG-NB	-2.12	2.01	2.05
18	6	603	CLA	MG-NB	-2.12	2.01	2.05
18	6	604	CLA	MG-NB	-2.12	2.01	2.05
18	6	608	CLA	CMD-C2D	-2.12	1.46	1.50
27	6	619	XAT	O24-C25	-2.12	1.43	1.46
18	L	303	CLA	MG-NB	-2.12	2.01	2.05
18	6	606	CLA	CHC-C1C	2.12	1.42	1.38
18	B	838	CLA	MG-NB	-2.12	2.01	2.05
18	B	809	CLA	MG-NB	-2.12	2.01	2.05
18	B	820	CLA	MG-NB	-2.12	2.01	2.05
18	L	304	CLA	MG-NB	-2.12	2.01	2.05
18	B	835	CLA	CHC-C1C	2.11	1.42	1.38
18	5	601	CLA	MG-NB	-2.11	2.01	2.05
18	6	613	CLA	MG-NB	-2.11	2.01	2.05
18	A	802	CLA	CMB-C2B	-2.11	1.46	1.50
18	3	614	CLA	MG-NB	-2.11	2.01	2.05
18	B	807	CLA	CHC-C1C	2.11	1.42	1.38
18	A	807	CLA	CMD-C2D	-2.11	1.46	1.50
18	A	812	CLA	CMD-C2D	-2.11	1.46	1.50
18	3	617	CLA	MG-NB	-2.11	2.01	2.05
18	6	604	CLA	CMB-C2B	-2.11	1.46	1.50
18	A	808	CLA	MG-NB	-2.11	2.01	2.05
18	3	613	CLA	CHC-C1C	2.11	1.42	1.38
18	A	837	CLA	CHC-C1C	2.11	1.42	1.38
18	3	606	CLA	CMB-C2B	-2.11	1.46	1.50
18	A	830	CLA	CHC-C1C	2.11	1.42	1.38
18	B	819	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	305	CLA	CHC-C1C	2.11	1.42	1.38
18	B	824	CLA	CMB-C2B	-2.11	1.46	1.50
18	B	810	CLA	CHC-C1C	2.11	1.42	1.38
18	B	826	CLA	CHC-C1C	2.11	1.42	1.38
18	A	837	CLA	MG-NB	-2.11	2.01	2.05
18	3	610	CLA	MG-NB	-2.11	2.01	2.05
18	A	822	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	840	CLA	CMB-C2B	-2.11	1.46	1.50
18	A	809	CLA	MG-NB	-2.11	2.01	2.05
18	5	610	CLA	CMD-C2D	-2.10	1.46	1.50
26	6	617	LUT	C38-C25	2.10	1.54	1.50
18	A	854	CLA	MG-NB	-2.10	2.01	2.05
25	6	601	CHL	C1D-ND	-2.10	1.35	1.37
18	B	837	CLA	CMB-C2B	-2.10	1.46	1.50
18	2	611	CLA	MG-NB	-2.10	2.01	2.05
18	B	818	CLA	MG-NB	-2.10	2.01	2.05
18	2	603	CLA	CHC-C1C	2.10	1.42	1.38
18	A	843	CLA	MG-NB	-2.10	2.01	2.05
18	2	603	CLA	MG-NB	-2.10	2.01	2.05
18	B	818	CLA	CHC-C1C	2.10	1.42	1.38
18	6	611	CLA	MG-NB	-2.10	2.01	2.05
18	B	817	CLA	CHC-C1C	2.10	1.42	1.38
18	B	808	CLA	CMB-C2B	-2.10	1.46	1.50
18	3	615	CLA	MG-NB	-2.10	2.01	2.05
18	3	603	CLA	CHC-C1C	2.10	1.42	1.38
18	5	603	CLA	MG-NB	-2.10	2.01	2.05
18	A	811	CLA	MG-NB	-2.10	2.01	2.05
18	A	818	CLA	MG-NB	-2.10	2.01	2.05
18	3	606	CLA	CMD-C2D	-2.10	1.46	1.50
18	2	602	CLA	MG-NB	-2.10	2.01	2.05
18	2	613	CLA	MG-NB	-2.10	2.01	2.05
18	A	818	CLA	CMC-C2C	-2.09	1.46	1.50
18	6	609	CLA	MG-NB	-2.09	2.01	2.05
18	5	609	CLA	MG-NB	-2.09	2.01	2.05
18	6	610	CLA	CMD-C2D	-2.09	1.46	1.50
18	G	203	CLA	CHC-C1C	2.09	1.42	1.38
18	B	829	CLA	CHC-C1C	2.09	1.42	1.38
18	A	842	CLA	MG-NB	-2.09	2.01	2.05
18	J	101	CLA	MG-NB	-2.09	2.01	2.05
18	B	821	CLA	CHC-C1C	2.09	1.42	1.38
18	B	802	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	831	CLA	CHC-C1C	2.09	1.42	1.38
18	A	843	CLA	CHC-C1C	2.09	1.42	1.38
18	B	830	CLA	CMB-C2B	-2.09	1.46	1.50
18	5	614	CLA	CMD-C2D	-2.09	1.46	1.50
18	3	613	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	836	CLA	CMB-C2B	-2.09	1.46	1.50
18	A	813	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	809	CLA	CMB-C2B	-2.08	1.46	1.50
18	5	603	CLA	CHC-C1C	2.08	1.42	1.38
18	B	839	CLA	CMB-C2B	-2.08	1.46	1.50
18	5	614	CLA	MG-NB	-2.08	2.01	2.05
18	B	823	CLA	CMC-C2C	-2.08	1.46	1.50
18	B	830	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	814	CLA	CMC-C2C	-2.08	1.46	1.50
18	G	203	CLA	MG-NB	-2.08	2.01	2.05
18	B	808	CLA	CMD-C2D	-2.08	1.46	1.50
18	5	602	CLA	MG-NB	-2.08	2.01	2.05
18	A	840	CLA	CMD-C2D	-2.08	1.46	1.50
18	6	612	CLA	MG-NB	-2.08	2.01	2.05
18	B	813	CLA	CMC-C2C	-2.08	1.46	1.50
18	3	613	CLA	MG-NB	-2.08	2.01	2.05
18	B	817	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	819	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	816	CLA	CMD-C2D	-2.08	1.46	1.50
18	L	304	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	806	CLA	CMD-C2D	-2.08	1.46	1.50
18	2	609	CLA	CMD-C2D	-2.08	1.46	1.50
18	3	603	CLA	MG-NB	-2.07	2.01	2.05
25	2	606	CHL	MG-NA	-2.07	2.01	2.06
18	B	806	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	612	CLA	MG-NB	-2.07	2.01	2.05
18	2	614	CLA	MG-NB	-2.07	2.01	2.05
18	2	613	CLA	CMB-C2B	-2.07	1.46	1.50
18	2	612	CLA	CMB-C2B	-2.07	1.46	1.50
18	3	603	CLA	CMB-C2B	-2.07	1.46	1.50
18	K	206	CLA	MG-NB	-2.07	2.01	2.05
18	B	804	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	603	CLA	CMD-C2D	-2.07	1.46	1.50
18	3	609	CLA	MG-NB	-2.07	2.01	2.05
18	B	837	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	825	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	817	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	CMB-C2B	-2.07	1.46	1.50
18	5	612	CLA	CMB-C2B	-2.07	1.46	1.50
18	3	607	CLA	MG-NB	-2.07	2.01	2.05
18	5	612	CLA	MG-NB	-2.07	2.01	2.05
18	A	809	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	834	CLA	CHC-C1C	2.07	1.42	1.38
18	A	821	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	836	CLA	CMD-C2D	-2.07	1.46	1.50
18	5	613	CLA	MG-NB	-2.07	2.01	2.05
25	5	606	CHL	C4B-NB	-2.07	1.35	1.37
18	B	837	CLA	MG-NB	-2.07	2.01	2.05
18	B	807	CLA	CMB-C2B	-2.07	1.46	1.50
18	5	602	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	805	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	818	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	802	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	840	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	840	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	845	CLA	CMB-C2B	-2.06	1.46	1.50
18	5	611	CLA	CMB-C2B	-2.06	1.46	1.50
18	6	614	CLA	MG-NB	-2.06	2.01	2.05
18	A	830	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	827	CLA	MG-NB	-2.06	2.01	2.05
18	K	203	CLA	MG-NB	-2.06	2.01	2.05
18	A	854	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	802	CLA	CMC-C2C	-2.06	1.46	1.50
18	L	302	CLA	CMD-C2D	-2.06	1.46	1.50
18	2	604	CLA	CMD-C2D	-2.06	1.46	1.50
18	L	302	CLA	MG-NB	-2.06	2.01	2.05
25	5	606	CHL	C1B-NB	-2.06	1.35	1.37
18	B	803	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	808	CLA	CMC-C2C	-2.06	1.46	1.50
18	B	822	CLA	CMB-C2B	-2.06	1.46	1.50
18	6	613	CLA	CMD-C2D	-2.06	1.46	1.50
18	5	603	CLA	CMD-C2D	-2.06	1.46	1.50
18	6	609	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	812	CLA	MG-NB	-2.06	2.01	2.05
18	A	814	CLA	CMD-C2D	-2.06	1.46	1.50
18	6	611	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	808	CLA	MG-NB	-2.06	2.01	2.05
18	3	617	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	837	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	805	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	815	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	820	CLA	CMD-C2D	-2.06	1.46	1.50
18	F	301	CLA	CMD-C2D	-2.05	1.46	1.50
18	5	611	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	831	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	602	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	838	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	603	CLA	CMD-C2D	-2.05	1.46	1.50
18	5	603	CLA	CMB-C2B	-2.05	1.46	1.50
18	3	615	CLA	CBD-CAD	2.05	1.56	1.51
18	A	807	CLA	CMB-C2B	-2.05	1.46	1.50
18	F	303	CLA	CMB-C2B	-2.05	1.46	1.50
18	G	204	CLA	CMB-C2B	-2.05	1.46	1.50
18	2	614	CLA	CMD-C2D	-2.05	1.46	1.50
18	6	606	CLA	CMD-C2D	-2.05	1.46	1.50
26	5	619	LUT	C38-C25	2.05	1.54	1.50
18	A	845	CLA	MG-NB	-2.05	2.01	2.05
18	3	611	CLA	MG-NB	-2.05	2.01	2.05
18	A	818	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	826	CLA	CMD-C2D	-2.05	1.46	1.50
18	3	604	CLA	MG-NB	-2.05	2.01	2.05
18	B	805	CLA	CMB-C2B	-2.05	1.46	1.50
18	3	604	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	612	CLA	CMD-C2D	-2.05	1.46	1.50
25	3	608	CHL	C4B-NB	-2.05	1.35	1.37
18	B	838	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	812	CLA	MG-NB	-2.05	2.01	2.05
25	2	608	CHL	C1D-ND	-2.05	1.35	1.37
18	A	801	CLA	CMB-C2B	-2.05	1.46	1.50
18	K	204	CLA	MG-NB	-2.05	2.01	2.05
18	A	804	CLA	CMD-C2D	-2.05	1.46	1.50
18	2	609	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	830	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	835	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	828	CLA	CMC-C2C	-2.05	1.46	1.50
18	2	602	CLA	CMD-C2D	-2.05	1.46	1.50
18	G	203	CLA	CMB-C2B	-2.04	1.46	1.50
18	2	603	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	831	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	805	CLA	MG-NB	-2.04	2.01	2.05
18	B	834	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	608	CHL	C4B-NB	-2.04	1.35	1.37
18	A	828	CLA	CMD-C2D	-2.04	1.46	1.50
18	3	609	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	825	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	841	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	834	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	821	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	803	CLA	CMD-C2D	-2.04	1.46	1.50
18	2	612	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	805	CLA	MG-NB	-2.04	2.01	2.05
18	A	812	CLA	CMB-C2B	-2.04	1.46	1.50
18	G	204	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	809	CLA	CHC-C1C	2.04	1.42	1.38
18	2	604	CLA	MG-NB	-2.04	2.01	2.05
18	L	303	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	811	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	811	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	814	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	831	CLA	CMD-C2D	-2.04	1.46	1.50
18	6	611	CLA	CMD-C2D	-2.04	1.46	1.50
25	2	607	CHL	C1D-ND	-2.04	1.35	1.37
18	A	819	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	821	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	826	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	824	CLA	CMB-C2B	-2.04	1.46	1.50
18	6	602	CLA	CMB-C2B	-2.04	1.46	1.50
25	5	608	CHL	C4C-C3C	2.04	1.48	1.45
18	B	841	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	801	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	826	CLA	CMD-C2D	-2.03	1.46	1.50
25	5	615	CHL	C1B-NB	-2.03	1.35	1.37
18	A	819	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	607	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	811	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	804	CLA	MG-NB	-2.03	2.01	2.05
18	2	609	CLA	MG-NB	-2.03	2.01	2.05
18	B	807	CLA	CMD-C2D	-2.03	1.46	1.50
18	K	206	CLA	CMB-C2B	-2.03	1.46	1.50
18	6	609	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	815	CLA	CMB-C2B	-2.03	1.46	1.50
18	3	610	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	620	XAT	O4-C5	-2.03	1.43	1.46
18	A	841	CLA	CMB-C2B	-2.03	1.46	1.50
18	6	616	CLA	MG-NB	-2.03	2.01	2.05
18	B	812	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	826	CLA	CMC-C2C	-2.03	1.46	1.50
18	2	610	CLA	C1B-C2B	2.03	1.48	1.43
18	2	611	CLA	CMD-C2D	-2.03	1.46	1.50
18	6	612	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	825	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	822	CLA	CMD-C2D	-2.03	1.46	1.50
18	5	613	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	835	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	832	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	835	CLA	CMB-C2B	-2.03	1.46	1.50
18	6	610	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	811	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	825	CLA	CMD-C2D	-2.03	1.46	1.50
18	K	203	CLA	CMB-C2B	-2.03	1.46	1.50
18	2	614	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	828	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	834	CLA	MG-NB	-2.02	2.01	2.05
18	3	602	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	842	CLA	CMD-C2D	-2.02	1.46	1.50
18	K	206	CLA	CMD-C2D	-2.02	1.46	1.50
18	5	610	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	815	CLA	CMD-C2D	-2.02	1.46	1.50
18	5	601	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	823	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	832	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	833	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	816	CLA	CMB-C2B	-2.02	1.46	1.50
18	3	604	CLA	CMD-C2D	-2.02	1.46	1.50
18	5	604	CLA	MG-NB	-2.02	2.01	2.05
18	B	814	CLA	CMD-C2D	-2.02	1.46	1.50
18	3	607	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	834	CLA	CMD-C2D	-2.02	1.46	1.50
18	K	203	CLA	CMD-C2D	-2.02	1.46	1.50
18	6	608	CLA	CMB-C2B	-2.02	1.46	1.50
26	5	619	LUT	C40-C33	2.02	1.55	1.50
18	A	829	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	842	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	602	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.02	1.46	1.50
18	2	610	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	835	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	841	CLA	CMD-C2D	-2.01	1.46	1.50
18	6	613	CLA	CMB-C2B	-2.01	1.46	1.50
18	5	609	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	808	CLA	CMD-C2D	-2.01	1.46	1.50
18	F	304	CLA	CMD-C2D	-2.01	1.46	1.50
18	6	606	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	829	CLA	CMB-C2B	-2.01	1.46	1.50
25	5	615	CHL	C1D-ND	-2.01	1.35	1.37
18	A	806	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	835	CLA	CMD-C2D	-2.01	1.46	1.50
18	3	614	CLA	CMB-C2B	-2.01	1.46	1.50
18	6	604	CLA	CMD-C2D	-2.01	1.46	1.50
18	3	609	CLA	CMD-C2D	-2.01	1.46	1.50
18	3	615	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	819	CLA	CMC-C2C	-2.01	1.46	1.50
18	J	101	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	841	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	809	CLA	CMD-C2D	-2.01	1.46	1.50
18	3	614	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	817	CLA	CMD-C2D	-2.01	1.46	1.50
18	G	203	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	804	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	825	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	802	CLA	CMB-C2B	-2.01	1.46	1.50
18	B	815	CLA	CMC-C2C	-2.01	1.46	1.50
18	6	606	CLA	MG-NB	-2.01	2.01	2.05
18	B	827	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	832	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	837	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	817	CLA	CMD-C2D	-2.01	1.46	1.50
18	F	301	CLA	CMB-C2B	-2.01	1.46	1.50
18	B	827	CLA	CMD-C2D	-2.00	1.46	1.50
18	5	612	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	809	CLA	CMB-C2B	-2.00	1.46	1.50
18	B	836	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	808	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	839	CLA	CMB-C2B	-2.00	1.46	1.50
18	K	204	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	805	CLA	CMC-C2C	-2.00	1.46	1.50
18	A	826	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	829	CLA	CMC-C2C	-2.00	1.46	1.50
18	5	613	CLA	CMD-C2D	-2.00	1.46	1.50
18	B	836	CLA	CMD-C2D	-2.00	1.46	1.50
18	3	610	CLA	CMC-C2C	-2.00	1.46	1.50
18	3	611	CLA	CMD-C2D	-2.00	1.46	1.50

All (1520) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	619	LUT	C18-C5-C6	-14.02	108.78	124.53
26	5	619	LUT	C18-C5-C6	-12.36	110.65	124.53
26	6	617	LUT	C18-C5-C6	-12.10	110.94	124.53
26	2	619	LUT	C15-C14-C13	-11.96	110.24	127.31
26	3	618	LUT	C18-C5-C6	-11.81	111.26	124.53
26	3	618	LUT	C15-C14-C13	-11.59	110.77	127.31
26	2	619	LUT	C11-C10-C9	-11.19	111.34	127.31
26	5	619	LUT	C15-C14-C13	-10.86	111.82	127.31
26	6	617	LUT	C15-C14-C13	-10.76	111.96	127.31
27	6	619	XAT	O24-C25-C24	10.74	121.45	113.38
25	2	606	CHL	C2B-C1B-NB	10.10	117.00	110.23
26	3	618	LUT	C11-C10-C9	-10.09	112.90	127.31
26	6	617	LUT	C11-C10-C9	-9.89	113.19	127.31
27	2	620	XAT	C18-C5-C6	-9.89	105.69	122.26
26	5	619	LUT	C31-C30-C29	-9.85	113.26	127.31
26	6	617	LUT	C31-C30-C29	-9.74	113.40	127.31
27	2	620	XAT	O24-C25-C24	9.73	120.69	113.38
26	5	619	LUT	C11-C10-C9	-9.60	113.62	127.31
25	5	606	CHL	C2B-C1B-NB	9.53	116.62	110.23
26	3	618	LUT	C31-C30-C29	-9.37	113.93	127.31
27	2	620	XAT	O4-C5-C18	9.33	126.23	115.06
25	6	601	CHL	C2B-C1B-NB	9.32	116.48	110.23
25	5	615	CHL	C2B-C1B-NB	9.32	116.48	110.23
25	2	616	CHL	C2B-C1B-NB	9.25	116.44	110.23
25	5	608	CHL	C2B-C1B-NB	9.15	116.37	110.23
25	2	608	CHL	C2B-C1B-NB	8.90	116.20	110.23
25	3	608	CHL	C2B-C1B-NB	8.85	116.16	110.23
25	2	607	CHL	C2B-C1B-NB	8.64	116.02	110.23
25	2	606	CHL	CMD-C2D-C1D	8.40	139.52	124.71
25	2	601	CHL	C2B-C1B-NB	8.33	115.82	110.23
25	5	606	CHL	CMD-C2D-C1D	8.30	139.33	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	619	LUT	C31-C30-C29	-8.29	115.48	127.31
25	3	608	CHL	CMD-C2D-C1D	8.29	139.32	124.71
25	2	608	CHL	CMD-C2D-C1D	8.26	139.26	124.71
25	5	615	CHL	CMD-C2D-C1D	8.24	139.24	124.71
25	2	616	CHL	CMD-C2D-C1D	8.22	139.19	124.71
25	2	607	CHL	CMD-C2D-C1D	8.14	139.05	124.71
25	6	601	CHL	CMD-C2D-C1D	8.11	139.01	124.71
25	5	608	CHL	CMD-C2D-C1D	8.09	138.97	124.71
25	6	607	CHL	C2B-C1B-NB	8.08	115.65	110.23
25	5	607	CHL	C2B-C1B-NB	8.07	115.64	110.23
25	2	601	CHL	CMD-C2D-C1D	8.05	138.90	124.71
25	6	607	CHL	CMD-C2D-C1D	8.05	138.89	124.71
25	5	607	CHL	CMD-C2D-C1D	7.93	138.68	124.71
27	5	620	XAT	O24-C25-C24	7.76	119.21	113.38
25	2	606	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
25	2	601	CHL	CHD-C1D-ND	-7.44	117.62	124.45
25	5	607	CHL	CHD-C1D-ND	-7.36	117.69	124.45
25	5	615	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
25	2	607	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
25	6	607	CHL	CHD-C1D-ND	-7.22	117.82	124.45
25	5	606	CHL	C2C-C3C-C4C	-7.21	101.13	106.49
25	5	608	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
27	6	619	XAT	C26-C27-C28	-7.18	110.80	125.99
25	6	601	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
25	6	607	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
18	K	201	CLA	C4A-NA-C1A	7.12	109.91	106.71
18	A	845	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	B	804	CLA	C4A-NA-C1A	7.09	109.89	106.71
25	2	616	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
25	2	608	CHL	C2C-C3C-C4C	-7.06	101.45	106.49
25	2	607	CHL	CHD-C1D-ND	-7.03	117.99	124.45
27	5	620	XAT	C18-C5-C6	-7.03	110.48	122.26
26	5	619	LUT	C38-C25-C24	-7.03	108.52	123.56
27	5	620	XAT	C27-C28-C29	-7.03	114.62	125.53
18	3	611	CLA	C4A-NA-C1A	6.99	109.85	106.71
26	6	617	LUT	C38-C25-C24	-6.96	108.68	123.56
26	2	619	LUT	C38-C25-C24	-6.95	108.69	123.56
27	3	619	XAT	C38-C25-C26	-6.91	110.68	122.26
18	2	604	CLA	C4A-NA-C1A	6.90	109.81	106.71
25	2	601	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
25	5	607	CHL	C2C-C3C-C4C	-6.88	101.58	106.49
25	5	606	CHL	C1B-C2B-C3B	-6.88	100.50	107.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	204	CLA	C4A-NA-C1A	6.87	109.80	106.71
25	2	608	CHL	CHD-C1D-ND	-6.86	118.15	124.45
25	6	601	CHL	CHD-C1D-ND	-6.85	118.16	124.45
18	B	803	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	5	613	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	A	839	CLA	C4A-NA-C1A	6.81	109.77	106.71
18	A	810	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	B	837	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	F	304	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	A	805	CLA	C4A-NA-C1A	6.78	109.75	106.71
18	5	604	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	L	303	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	A	818	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	B	808	CLA	C4A-NA-C1A	6.72	109.73	106.71
25	3	608	CHL	CHD-C1D-ND	-6.72	118.28	124.45
18	A	831	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	A	819	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	826	CLA	C4A-NA-C1A	6.68	109.71	106.71
25	2	601	CHL	C1B-C2B-C3B	-6.68	100.69	107.03
18	6	603	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	A	816	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	A	830	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	L	302	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	A	822	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	A	841	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	B	812	CLA	C4A-NA-C1A	6.65	109.70	106.71
18	K	203	CLA	C4A-NA-C1A	6.65	109.70	106.71
18	A	804	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	6	613	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	G	201	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	3	612	CLA	C4A-NA-C1A	6.63	109.69	106.71
26	3	618	LUT	C38-C25-C24	-6.62	109.40	123.56
18	B	822	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	814	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	A	812	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	3	607	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	B	832	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	5	614	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	A	802	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	B	815	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	A	835	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	3	602	CLA	C4A-NA-C1A	6.58	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	615	CHL	CHD-C1D-ND	-6.57	118.41	124.45
18	6	612	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	819	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	2	614	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	K	206	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	B	807	CLA	C4A-NA-C1A	6.56	109.65	106.71
18	2	602	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	6	616	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	A	842	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	A	823	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	B	831	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	B	820	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	5	612	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	3	603	CLA	C4A-NA-C1A	6.53	109.64	106.71
25	2	616	CHL	CHD-C1D-ND	-6.53	118.46	124.45
18	2	613	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	A	832	CLA	C4A-NA-C1A	6.51	109.64	106.71
18	B	825	CLA	C4A-NA-C1A	6.51	109.64	106.71
18	B	818	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	B	834	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	F	303	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	2	603	CLA	C4A-NA-C1A	6.51	109.63	106.71
27	3	619	XAT	C18-C5-C6	-6.50	111.36	122.26
18	L	304	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	6	608	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	B	829	CLA	C4A-NA-C1A	6.49	109.63	106.71
18	A	817	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	A	813	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	B	806	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	A	815	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	3	609	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	5	609	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	A	824	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	A	836	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	F	305	CLA	C4A-NA-C1A	6.48	109.62	106.71
27	5	620	XAT	O4-C5-C4	6.47	118.24	113.38
18	A	808	CLA	C4A-NA-C1A	6.47	109.61	106.71
26	2	619	LUT	C1-C6-C5	-6.47	113.50	122.61
18	A	837	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	A	807	CLA	C4A-NA-C1A	6.46	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	835	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	F	301	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	3	614	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	3	606	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	B	839	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	6	609	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	5	601	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	5	606	CHL	CHD-C1D-ND	-6.41	118.56	124.45
18	A	829	CLA	C4A-NA-C1A	6.41	109.59	106.71
18	B	830	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	B	810	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	6	604	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	5	603	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	B	805	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	B	827	CLA	C4A-NA-C1A	6.40	109.58	106.71
25	2	606	CHL	CHD-C1D-ND	-6.40	118.58	124.45
18	G	204	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	6	606	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	2	612	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	B	821	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	A	834	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	2	609	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	5	610	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	2	611	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	A	806	CLA	C4A-NA-C1A	6.36	109.56	106.71
27	6	619	XAT	C35-C34-C33	-6.36	118.24	127.31
18	A	833	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	B	809	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	B	840	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	3	613	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	A	826	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	3	610	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	A	838	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	B	823	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	G	203	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	J	101	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	B	824	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	A	811	CLA	C4A-NA-C1A	6.29	109.54	106.71
18	A	814	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	B	838	CLA	C4A-NA-C1A	6.28	109.53	106.71
18	A	828	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	6	610	CLA	C4A-NA-C1A	6.27	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	608	CHL	CHD-C1D-ND	-6.27	118.69	124.45
18	A	821	CLA	C4A-NA-C1A	6.27	109.52	106.71
18	6	611	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	6	602	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	A	843	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	A	840	CLA	C4A-NA-C1A	6.25	109.52	106.71
18	3	604	CLA	C4A-NA-C1A	6.24	109.51	106.71
18	B	816	CLA	C4A-NA-C1A	6.24	109.51	106.71
18	A	827	CLA	C4A-NA-C1A	6.23	109.51	106.71
18	B	841	CLA	C4A-NA-C1A	6.23	109.51	106.71
18	3	617	CLA	C4A-NA-C1A	6.22	109.50	106.71
18	B	802	CLA	C4A-NA-C1A	6.22	109.50	106.71
18	B	811	CLA	C4A-NA-C1A	6.21	109.50	106.71
18	3	615	CLA	C4A-NA-C1A	6.21	109.50	106.71
18	5	602	CLA	C4A-NA-C1A	6.20	109.49	106.71
18	B	836	CLA	C4A-NA-C1A	6.18	109.49	106.71
27	6	619	XAT	C18-C5-C6	-6.15	111.95	122.26
18	B	828	CLA	C4A-NA-C1A	6.14	109.47	106.71
18	A	825	CLA	C4A-NA-C1A	6.13	109.46	106.71
27	6	619	XAT	C6-C7-C8	-6.13	113.04	125.99
18	A	801	CLA	C4A-NA-C1A	6.11	109.45	106.71
26	5	619	LUT	C8-C7-C6	-6.11	110.04	127.20
18	A	820	CLA	C4A-NA-C1A	6.10	109.45	106.71
27	3	619	XAT	C6-C7-C8	-6.09	113.11	125.99
26	2	619	LUT	C7-C6-C5	-6.06	106.77	121.46
18	B	813	CLA	C4A-NA-C1A	6.06	109.43	106.71
27	6	619	XAT	C38-C25-C26	-6.01	112.19	122.26
18	A	854	CLA	C4A-NA-C1A	5.93	109.37	106.71
18	B	833	CLA	C4A-NA-C1A	5.91	109.36	106.71
27	2	620	XAT	C38-C25-C26	-5.83	112.49	122.26
26	6	617	LUT	C35-C15-C14	-5.82	111.55	123.47
18	2	610	CLA	C4A-NA-C1A	5.77	109.30	106.71
18	6	614	CLA	C4A-NA-C1A	5.77	109.30	106.71
25	5	607	CHL	CHB-C1B-NB	-5.69	118.23	124.26
26	3	618	LUT	C1-C6-C5	-5.68	114.61	122.61
18	A	803	CLA	C4A-NA-C1A	5.64	109.24	106.71
26	3	618	LUT	C8-C7-C6	-5.63	111.39	127.20
25	2	606	CHL	C3B-C2B-C1B	-5.52	100.50	107.16
25	6	601	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
25	5	606	CHL	C3B-C4B-NB	5.44	113.88	110.23
27	2	620	XAT	C26-C27-C28	-5.44	114.50	125.99
26	5	619	LUT	C1-C6-C5	-5.42	114.98	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	619	XAT	O4-C5-C18	5.42	121.55	115.06
25	5	615	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
27	3	619	XAT	O24-C25-C24	5.27	117.34	113.38
26	2	619	LUT	C8-C7-C6	-5.25	112.45	127.20
25	5	607	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
25	2	606	CHL	C3C-C4C-NC	5.21	116.41	110.57
25	2	607	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
25	2	608	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
25	2	616	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
26	6	617	LUT	C8-C7-C6	-5.18	112.66	127.20
25	6	607	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
26	6	617	LUT	C35-C34-C33	-5.14	119.97	127.31
25	2	601	CHL	O2D-CGD-CBD	5.14	120.40	111.27
25	2	616	CHL	O2D-CGD-CBD	5.12	120.37	111.27
25	6	607	CHL	CHB-C1B-NB	-5.12	118.84	124.26
26	6	617	LUT	C7-C6-C5	-5.10	109.11	121.46
25	5	608	CHL	C3C-C4C-NC	5.08	116.27	110.57
25	3	608	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
25	5	606	CHL	O2D-CGD-CBD	5.08	120.29	111.27
25	5	606	CHL	C3C-C4C-NC	5.04	116.07	110.57
26	2	619	LUT	C30-C31-C32	-5.03	107.51	123.22
25	2	607	CHL	O2D-CGD-CBD	4.99	120.13	111.27
26	3	618	LUT	C35-C15-C14	-4.94	113.36	123.47
25	5	608	CHL	C3B-C2B-C1B	-4.90	101.25	107.16
26	2	619	LUT	C7-C8-C9	-4.86	118.89	126.23
25	2	601	CHL	CHB-C1B-NB	-4.85	119.12	124.26
25	5	615	CHL	C3C-C4C-NC	4.85	116.01	110.57
25	2	607	CHL	CHB-C1B-NB	-4.84	119.13	124.26
27	5	620	XAT	O4-C5-C18	4.83	120.85	115.06
26	5	619	LUT	C35-C15-C14	-4.75	113.75	123.47
27	3	619	XAT	O24-C25-C38	4.70	120.69	115.06
27	6	619	XAT	O4-C5-C18	4.70	120.68	115.06
27	5	620	XAT	C35-C34-C33	-4.66	120.66	127.31
25	3	608	CHL	C2C-C1C-NC	4.66	114.34	109.97
25	5	607	CHL	O2D-CGD-CBD	4.65	119.54	111.27
25	2	606	CHL	C3D-C2D-C1D	-4.64	99.49	105.83
25	5	608	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
25	5	615	CHL	O2D-CGD-CBD	4.60	119.45	111.27
26	2	619	LUT	C35-C15-C14	-4.59	114.08	123.47
25	3	608	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
27	6	619	XAT	O4-C5-C4	4.54	116.79	113.38
25	2	616	CHL	C3C-C4C-NC	4.53	115.65	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	606	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
25	5	615	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
25	2	616	CHL	C3D-C2D-C1D	-4.50	99.70	105.83
25	2	616	CHL	CHB-C1B-NB	-4.49	119.50	124.26
25	3	608	CHL	C3C-C4C-NC	4.48	115.60	110.57
25	2	608	CHL	C3D-C2D-C1D	-4.47	99.73	105.83
25	6	601	CHL	C3C-C4C-NC	4.47	115.58	110.57
25	2	601	CHL	C3B-C4B-NB	4.46	113.22	110.23
25	6	601	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
25	2	608	CHL	C3C-C4C-NC	4.40	115.51	110.57
27	3	619	XAT	C26-C27-C28	-4.39	116.70	125.99
25	2	601	CHL	C3D-C2D-C1D	-4.37	99.86	105.83
27	3	619	XAT	C18-C5-C4	4.37	119.19	114.28
27	5	620	XAT	C6-C7-C8	-4.35	116.79	125.99
25	2	606	CHL	O2D-CGD-CBD	4.35	119.00	111.27
25	6	601	CHL	CHB-C1B-NB	-4.34	119.66	124.26
25	2	607	CHL	C3D-C2D-C1D	-4.34	99.90	105.83
26	6	617	LUT	C10-C11-C12	-4.33	109.71	123.22
25	5	607	CHL	C3D-C2D-C1D	-4.33	99.93	105.83
25	3	608	CHL	CHB-C1B-NB	-4.31	119.69	124.26
26	5	619	LUT	C35-C34-C33	-4.31	121.16	127.31
25	2	606	CHL	CHD-C4C-C3C	-4.31	118.51	124.84
25	2	607	CHL	C3C-C4C-NC	4.30	115.39	110.57
26	6	617	LUT	C30-C31-C32	-4.29	109.82	123.22
20	2	622	LHG	O4-P-O5	4.28	133.39	112.24
20	6	620	LHG	O4-P-O5	4.26	133.31	112.24
25	5	608	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
25	5	607	CHL	C4A-NA-C1A	4.22	108.60	106.71
26	6	617	LUT	C7-C8-C9	-4.22	119.86	126.23
20	A	846	LHG	O4-P-O5	4.21	133.06	112.24
25	5	608	CHL	O2D-CGD-CBD	4.20	118.74	111.27
20	A	847	LHG	O4-P-O5	4.19	132.94	112.24
20	B	851	LHG	O4-P-O5	4.18	132.91	112.24
20	5	622	LHG	O4-P-O5	4.18	132.89	112.24
26	5	619	LUT	C7-C6-C5	-4.17	111.36	121.46
25	2	601	CHL	C3C-C4C-NC	4.15	115.22	110.57
26	3	618	LUT	C30-C31-C32	-4.13	110.32	123.22
26	3	618	LUT	C35-C34-C33	-4.13	121.42	127.31
25	2	606	CHL	C2D-C1D-ND	4.09	113.12	110.10
26	3	618	LUT	C7-C6-C5	-4.08	111.58	121.46
27	3	619	XAT	C15-C14-C13	-4.07	121.51	127.31
27	2	620	XAT	C35-C34-C33	-4.06	121.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	607	CHL	C3C-C4C-NC	4.03	115.09	110.57
25	2	608	CHL	CHB-C1B-NB	-4.03	119.99	124.26
25	6	607	CHL	C3D-C2D-C1D	-4.01	100.36	105.83
26	6	617	LUT	C1-C6-C5	-3.99	117.00	122.61
23	B	850	DGD	O3G-C3G-C2G	-3.96	101.33	110.90
26	5	619	LUT	C30-C31-C32	-3.95	110.90	123.22
25	5	606	CHL	CHB-C1B-NB	-3.94	120.09	124.26
27	3	619	XAT	C5-C4-C3	-3.93	104.97	112.75
25	5	608	CHL	C2D-C1D-ND	3.93	113.00	110.10
25	5	607	CHL	C3C-C4C-NC	3.88	114.92	110.57
27	2	620	XAT	C7-C8-C9	-3.87	119.52	125.53
27	2	620	XAT	C18-C5-C4	3.87	118.63	114.28
25	2	606	CHL	C1D-ND-C4D	-3.86	103.59	106.33
25	5	608	CHL	CHB-C1B-NB	-3.86	120.17	124.26
27	5	620	XAT	C24-C23-C22	-3.86	103.33	110.77
27	6	619	XAT	C5-C4-C3	-3.82	105.20	112.75
27	5	620	XAT	C31-C30-C29	-3.81	121.87	127.31
25	5	615	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
27	3	619	XAT	C24-C23-C22	-3.79	103.45	110.77
25	5	606	CHL	CHD-C4C-C3C	-3.78	119.07	124.98
25	2	616	CHL	CAC-C3C-C4C	3.76	129.69	124.81
25	2	606	CHL	C3B-C4B-NB	3.75	114.00	110.52
27	6	619	XAT	C18-C5-C4	3.75	118.50	114.28
27	3	619	XAT	C38-C25-C24	3.74	118.49	114.28
21	K	207	BCR	C2-C1-C6	3.72	116.21	110.48
18	5	611	CLA	C3B-C4B-NB	-3.70	107.75	110.23
18	6	606	CLA	CBD-CHA-C1A	3.69	132.85	128.50
21	A	848	BCR	C2-C1-C6	3.68	116.15	110.48
25	5	615	CHL	CHB-C1B-NB	-3.68	120.36	124.26
26	3	618	LUT	C7-C8-C9	-3.67	120.68	126.23
21	A	856	BCR	C2-C1-C6	3.67	116.13	110.48
26	5	619	LUT	C10-C11-C12	-3.67	111.78	123.22
25	5	615	CHL	CAC-C3C-C4C	3.64	129.53	124.81
18	6	611	CLA	C3B-C4B-NB	-3.63	107.80	110.23
25	6	607	CHL	CHC-C4B-NB	-3.62	120.42	124.26
27	6	619	XAT	C28-C29-C30	-3.61	113.40	118.94
25	5	606	CHL	C2D-C1D-ND	3.61	112.76	110.10
25	2	607	CHL	CAC-C3C-C4C	3.61	129.49	124.81
27	2	620	XAT	C5-C4-C3	-3.59	105.64	112.75
25	3	608	CHL	C4C-C3C-C2C	-3.59	101.67	106.90
27	5	620	XAT	C35-C15-C14	-3.58	116.14	123.47
25	3	608	CHL	CHD-C4C-C3C	-3.58	119.58	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	601	CHL	CHD-C4C-C3C	-3.58	119.58	124.84
27	5	620	XAT	C38-C25-C26	-3.54	116.32	122.26
27	2	620	XAT	C4-C3-C2	-3.54	103.93	110.77
18	6	616	CLA	C3B-C4B-NB	-3.54	107.86	110.23
25	5	608	CHL	C1-C2-C3	-3.53	121.03	126.75
25	6	607	CHL	CAC-C3C-C4C	3.53	129.38	124.81
25	2	616	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
25	2	608	CHL	CAC-C3C-C4C	3.51	129.36	124.81
25	5	615	CHL	C2D-C1D-ND	3.50	112.68	110.10
25	2	608	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
18	B	811	CLA	C3B-C4B-NB	-3.48	107.90	110.23
18	B	840	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
18	3	604	CLA	C3B-C4B-NB	-3.48	107.90	110.23
26	2	619	LUT	C4-C5-C6	-3.45	113.15	120.85
27	2	620	XAT	C30-C31-C32	-3.44	112.47	123.22
25	3	608	CHL	C2D-C1D-ND	3.44	112.64	110.10
25	2	606	CHL	CAC-C3C-C4C	3.44	129.27	124.81
27	6	619	XAT	C38-C25-C24	3.43	118.14	114.28
25	2	606	CHL	C3D-C4D-ND	3.43	115.78	110.24
25	2	606	CHL	CHB-C1B-NB	-3.42	120.64	124.26
18	5	613	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
26	2	619	LUT	C15-C35-C34	-3.42	116.48	123.47
27	6	619	XAT	C10-C11-C12	-3.41	112.58	123.22
18	6	606	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
25	5	615	CHL	C3B-C4B-NB	3.40	113.67	110.52
27	2	620	XAT	C11-C10-C9	-3.40	122.46	127.31
26	2	619	LUT	C10-C11-C12	-3.40	112.62	123.22
25	3	608	CHL	C3D-C4D-ND	3.39	115.72	110.24
25	3	608	CHL	C3B-C4B-NB	3.39	113.66	110.52
25	5	615	CHL	C3D-C4D-ND	3.39	115.71	110.24
18	A	822	CLA	C3B-C4B-NB	-3.38	107.96	110.23
25	5	606	CHL	C3D-C4D-ND	3.38	115.71	110.24
18	A	831	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
25	5	608	CHL	C3B-C4B-NB	3.37	113.64	110.52
25	6	601	CHL	C3D-C4D-ND	3.34	115.65	110.24
18	A	824	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
25	5	606	CHL	C1D-ND-C4D	-3.34	103.96	106.33
18	6	609	CLA	C3B-C4B-NB	-3.34	107.99	110.23
25	2	616	CHL	C2D-C1D-ND	3.34	112.56	110.10
25	2	608	CHL	C3D-C4D-ND	3.34	115.63	110.24
18	A	835	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
25	2	607	CHL	C3D-C4D-ND	3.31	115.58	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	602	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
18	3	607	CLA	C3B-C4B-NB	-3.30	108.02	110.23
25	5	608	CHL	C1D-ND-C4D	-3.29	104.00	106.33
18	A	805	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
24	2	618	LMG	O6-C1-O1	-3.28	103.36	110.97
25	2	601	CHL	C3D-C4D-ND	3.27	115.53	110.24
24	2	617	LMG	O6-C1-O1	-3.26	103.41	110.97
18	6	616	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
25	5	607	CHL	CHC-C4B-NB	-3.25	120.81	124.26
18	B	837	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
18	B	824	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
18	B	832	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
26	3	618	LUT	C18-C5-C4	-3.25	108.34	114.36
18	3	609	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
18	A	820	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
25	2	616	CHL	C3B-C4B-NB	3.22	113.50	110.52
25	2	607	CHL	CHC-C4B-NB	-3.22	120.85	124.26
25	2	601	CHL	CHD-C4C-C3C	-3.21	120.12	124.84
20	A	847	LHG	O8-C23-C24	3.21	119.79	111.38
18	K	204	CLA	C3B-C4B-NB	-3.20	108.09	110.23
26	5	619	LUT	C18-C5-C4	-3.20	108.43	114.36
25	3	608	CHL	C1D-ND-C4D	-3.20	104.06	106.33
27	6	619	XAT	C35-C15-C14	-3.19	116.93	123.47
18	A	821	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
18	2	604	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
25	6	607	CHL	C4A-NA-C1A	3.19	108.14	106.71
26	5	619	LUT	C2-C3-C4	3.19	114.67	110.30
25	6	607	CHL	C3D-C4D-ND	3.19	115.39	110.24
18	B	838	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
25	5	615	CHL	C1D-ND-C4D	-3.18	104.08	106.33
25	6	601	CHL	C3B-C4B-NB	3.18	113.46	110.52
25	5	608	CHL	C3D-C4D-ND	3.18	115.38	110.24
18	B	825	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
18	A	818	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
25	2	616	CHL	C3D-C4D-ND	3.17	115.37	110.24
25	2	608	CHL	C2D-C1D-ND	3.17	112.44	110.10
27	6	619	XAT	C4-C3-C2	-3.17	104.65	110.77
18	B	822	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
26	6	617	LUT	C18-C5-C4	-3.15	108.52	114.36
21	B	847	BCR	C15-C16-C17	-3.15	117.03	123.47
18	B	817	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	B	850	DGD	O5D-C6D-C5D	-3.14	103.23	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	601	CHL	C2D-C1D-ND	3.14	112.42	110.10
18	B	820	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
18	B	826	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
18	B	808	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
18	6	604	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
18	A	840	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	B	807	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
18	A	804	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
26	6	617	LUT	C21-C26-C27	-3.11	108.77	112.70
18	A	837	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	3	608	CHL	CMB-C2B-C1B	3.09	130.08	125.37
25	2	607	CHL	CHD-C4C-C3C	-3.09	120.30	124.84
23	B	850	DGD	O6D-C1D-O3G	-3.09	102.66	109.97
18	B	805	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
26	2	619	LUT	C35-C34-C33	-3.09	122.91	127.31
27	3	619	XAT	C4-C3-C2	-3.08	104.82	110.77
18	2	610	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
18	5	601	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
18	B	824	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	B	811	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
18	A	825	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	A	809	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
25	5	607	CHL	CAC-C3C-C4C	3.06	128.78	124.81
18	B	804	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
21	K	202	BCR	C24-C23-C22	-3.05	121.62	126.23
26	3	618	LUT	C4-C5-C6	-3.05	114.06	120.85
27	3	619	XAT	O4-C5-C4	3.04	115.67	113.38
25	6	601	CHL	CAC-C3C-C4C	3.04	128.76	124.81
18	A	823	CLA	C3B-C4B-NB	-3.04	107.69	110.52
21	J	103	BCR	C7-C8-C9	-3.04	121.64	126.23
26	5	619	LUT	C4-C5-C6	-3.04	114.08	120.85
25	2	606	CHL	CMB-C2B-C1B	3.04	129.99	125.37
18	A	823	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
27	5	620	XAT	O24-C25-C38	3.03	118.69	115.06
18	B	839	CLA	C3B-C4B-NB	-3.03	107.70	110.52
18	A	832	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	J	102	BCR	C15-C16-C17	-3.03	117.27	123.47
18	3	602	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
18	B	808	CLA	C3B-C4B-NB	-3.03	107.71	110.52
18	A	802	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
18	A	811	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
18	B	810	CLA	O2D-CGD-O1D	-3.02	117.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	854	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	B	841	CLA	C3B-C4B-NB	-3.01	107.72	110.52
25	5	607	CHL	C3D-C4D-ND	3.01	115.11	110.24
18	5	602	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	2	606	CHL	CHB-C4A-NA	3.01	128.67	124.51
18	B	829	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
27	2	620	XAT	C15-C14-C13	-3.00	123.03	127.31
21	K	207	BCR	C15-C16-C17	-3.00	117.33	123.47
18	B	827	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
27	6	619	XAT	C30-C31-C32	-3.00	113.86	123.22
18	B	830	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
18	A	803	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
18	A	827	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
18	B	816	CLA	C3B-C4B-NB	-2.99	107.74	110.52
18	L	304	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
18	A	828	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
18	B	841	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
26	3	618	LUT	C2-C3-C4	2.99	114.39	110.30
18	A	842	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	6	607	CHL	CMD-C2D-C3D	-2.99	120.74	127.61
18	B	818	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
18	B	815	CLA	C3B-C4B-NB	-2.98	107.75	110.52
18	A	839	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	J	101	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	A	838	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	6	604	CLA	C3B-C4B-NB	-2.97	107.76	110.52
18	2	602	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	5	614	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	2	609	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	B	813	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
18	B	828	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
18	A	838	CLA	C3B-C4B-NB	-2.96	107.77	110.52
18	K	203	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	B	833	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	2	619	LUT	C18-C5-C4	-2.96	108.88	114.36
18	5	610	CLA	C3B-C4B-NB	-2.95	107.77	110.52
18	A	821	CLA	C3B-C4B-NB	-2.95	107.78	110.52
18	A	819	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	B	815	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	2	611	CLA	C3B-C4B-NB	-2.95	107.78	110.52
26	3	618	LUT	C20-C13-C14	-2.95	118.79	122.92
18	A	813	CLA	O2D-CGD-O1D	-2.95	118.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	619	LUT	C7-C8-C9	-2.95	121.78	126.23
18	B	817	CLA	C3B-C4B-NB	-2.95	107.78	110.52
18	A	816	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
18	A	814	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
18	B	805	CLA	C3B-C4B-NB	-2.94	107.78	110.52
18	B	835	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
25	5	608	CHL	CAC-C3C-C4C	2.94	128.63	124.81
18	B	823	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	5	606	CHL	CMB-C2B-C1B	2.94	129.85	125.37
21	J	102	BCR	C7-C8-C9	-2.94	121.80	126.23
18	B	812	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	L	302	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	A	825	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	B	834	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	A	836	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
25	2	608	CHL	CMB-C2B-C1B	2.93	129.82	125.37
18	6	608	CLA	C3B-C4B-NB	-2.92	107.81	110.52
18	B	821	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
18	A	834	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
18	A	812	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	B	837	CLA	C3B-C4B-NB	-2.91	107.81	110.52
18	A	833	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	A	805	CLA	CHB-C4A-NA	2.91	128.54	124.51
25	2	616	CHL	CHC-C4B-NB	-2.91	121.17	124.26
18	K	201	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	A	812	CLA	C3B-C4B-NB	-2.91	107.81	110.52
18	5	612	CLA	C3B-C4B-NB	-2.91	107.82	110.52
18	2	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	5	620	XAT	C4-C3-C2	-2.91	105.16	110.77
18	L	303	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
18	K	201	CLA	CHC-C4B-NB	2.90	127.33	124.26
25	3	608	CHL	CAC-C3C-C4C	2.90	128.57	124.81
18	2	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	2	601	CHL	C4A-NA-C1A	2.90	108.01	106.71
18	A	826	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	2	608	CHL	C3B-C4B-NB	2.89	113.20	110.52
18	A	801	CLA	C3B-C4B-NB	-2.89	107.83	110.52
18	2	612	CLA	C3B-C4B-NB	-2.89	107.83	110.52
25	2	601	CHL	CAC-C3C-C4C	2.89	128.56	124.81
18	A	841	CLA	C3B-C4B-NB	-2.89	107.84	110.52
18	6	613	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	B	831	CLA	O2D-CGD-O1D	-2.89	118.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	808	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	2	613	CLA	C3B-C4B-NB	-2.88	107.84	110.52
25	2	601	CHL	CMB-C2B-C1B	2.88	129.76	125.37
18	A	806	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	2	606	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
18	F	301	CLA	C3B-C4B-NB	-2.88	107.84	110.52
27	2	620	XAT	C6-C7-C8	-2.88	119.91	125.99
25	2	616	CHL	CMB-C2B-C1B	2.88	129.75	125.37
18	A	807	CLA	C3B-C4B-NB	-2.88	107.85	110.52
18	A	811	CLA	C3B-C4B-NB	-2.87	107.85	110.52
25	2	608	CHL	CMD-C2D-C3D	-2.87	121.00	127.61
25	5	606	CHL	CMD-C2D-C3D	-2.87	121.00	127.61
18	A	810	CLA	C3B-C4B-NB	-2.87	107.85	110.52
18	5	601	CLA	C3B-C4B-NB	-2.87	107.86	110.52
18	B	840	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	J	101	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	B	803	CLA	C3B-C4B-NB	-2.86	107.86	110.52
25	2	608	CHL	C1D-ND-C4D	-2.86	104.30	106.33
21	5	621	BCR	C33-C5-C6	-2.86	121.32	124.53
25	3	608	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
25	2	607	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
18	6	614	CLA	C3B-C4B-NB	-2.86	108.32	110.23
18	K	206	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
18	3	612	CLA	C3B-C4B-NB	-2.85	107.87	110.52
21	5	621	BCR	C15-C16-C17	-2.85	117.64	123.47
18	A	822	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	2	620	XAT	C35-C15-C14	-2.85	117.64	123.47
21	A	851	BCR	C24-C23-C22	-2.85	121.93	126.23
18	3	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	6	613	CLA	C3B-C4B-NB	-2.85	107.88	110.52
25	2	601	CHL	C2D-C1D-ND	2.84	112.20	110.10
18	2	611	CLA	CBD-CHA-C1A	2.84	131.98	127.43
18	G	201	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	5	615	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
18	B	809	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
18	F	303	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
18	5	613	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	B	836	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
18	F	304	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	5	607	CHL	CMB-C2B-C1B	2.83	129.68	125.37
25	2	616	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
25	5	608	CHL	O2A-CGA-CBA	2.83	120.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	819	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	A	836	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	5	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	F	305	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	2	614	CLA	C3B-C4B-NB	-2.81	107.90	110.52
18	2	614	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	5	612	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	5	615	CHL	CMB-C2B-C1B	2.81	129.65	125.37
25	2	607	CHL	CMB-C2B-C1B	2.81	129.65	125.37
18	F	301	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	A	832	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	A	824	CLA	C3B-C4B-NB	-2.80	107.91	110.52
18	A	801	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	6	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	B	850	DGD	CDB-CCB-CBB	-2.80	100.21	114.42
18	L	303	CLA	C3B-C4B-NB	-2.80	107.92	110.52
18	5	613	CLA	O2D-CGD-CBD	2.80	116.24	111.27
18	A	828	CLA	C3B-C4B-NB	-2.80	107.92	110.52
21	K	202	BCR	C15-C14-C13	-2.80	123.32	127.31
18	A	829	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	F	304	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	2	607	CHL	C3B-C4B-NB	2.80	113.11	110.52
18	A	802	CLA	C3B-C4B-NB	-2.79	107.92	110.52
18	A	804	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	A	830	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
18	6	614	CLA	O2D-CGD-O1D	-2.79	117.77	124.09
21	K	202	BCR	C15-C16-C17	-2.78	117.77	123.47
18	5	604	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
18	B	826	CLA	C3B-C4B-NB	-2.78	107.93	110.52
27	6	619	XAT	C15-C14-C13	-2.78	123.34	127.31
25	2	616	CHL	C1D-ND-C4D	-2.78	104.36	106.33
18	B	813	CLA	CAC-C3C-C4C	2.78	128.42	124.81
18	6	609	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	6	601	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
18	6	603	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	5	603	CLA	C3B-C4B-NB	-2.78	107.94	110.52
18	K	204	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	6	601	CHL	CMB-C2B-C1B	2.78	129.60	125.37
18	A	843	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	2	613	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
18	F	303	CLA	C3B-C4B-NB	-2.77	107.94	110.52
18	3	614	CLA	C3B-C4B-NB	-2.77	107.94	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	607	CHL	C2D-C1D-ND	2.77	112.15	110.10
25	2	601	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
18	A	842	CLA	O2D-CGD-O1D	-2.77	117.80	124.09
18	5	611	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
18	B	819	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	6	602	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	6	612	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	K	203	CLA	C3B-C4B-NB	-2.76	107.96	110.52
18	B	828	CLA	C3B-C4B-NB	-2.76	107.96	110.52
18	A	806	CLA	C3B-C4B-NB	-2.75	107.96	110.52
18	2	610	CLA	CHB-C1B-NB	2.75	127.16	124.26
18	A	815	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
18	A	815	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	A	810	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
18	B	834	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	B	810	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	G	204	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	3	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	A	834	CLA	C3B-C4B-NB	-2.74	107.97	110.52
21	B	847	BCR	C15-C14-C13	-2.74	123.40	127.31
18	A	841	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
18	3	617	CLA	O2D-CGD-O1D	-2.73	117.88	124.09
18	B	806	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	B	818	CLA	C3B-C4B-NB	-2.73	107.98	110.52
25	6	601	CHL	C1D-ND-C4D	-2.73	104.39	106.33
18	B	803	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	K	206	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	2	604	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	B	804	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	A	845	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	3	613	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	G	203	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
18	3	611	CLA	CHB-C4A-NA	2.73	128.28	124.51
18	B	806	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	2	603	CLA	C3B-C4B-NB	-2.72	108.00	110.52
21	A	852	BCR	C33-C5-C6	-2.72	121.48	124.53
24	J	104	LMG	O6-C1-O1	-2.71	103.55	109.97
18	G	203	CLA	C1-C2-C3	-2.71	122.36	126.75
25	5	608	CHL	CMB-C2B-C1B	2.71	129.50	125.37
18	3	617	CLA	C3B-C4B-NB	-2.71	108.00	110.52
21	B	843	BCR	C27-C26-C25	2.71	126.66	122.73
25	5	607	CHL	CMD-C2D-C3D	-2.71	121.39	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	102	BCR	C15-C14-C13	-2.71	123.45	127.31
21	A	852	BCR	C15-C16-C17	-2.71	117.93	123.47
27	3	619	XAT	C30-C31-C32	-2.70	114.78	123.22
25	2	606	CHL	C2A-C1A-CHA	-2.70	119.13	123.86
18	B	832	CLA	C3B-C4B-NB	-2.70	108.01	110.52
18	B	823	CLA	C3B-C4B-NB	-2.70	108.01	110.52
21	L	305	BCR	C15-C16-C17	-2.70	117.94	123.47
21	2	621	BCR	C24-C23-C22	-2.70	122.16	126.23
18	B	830	CLA	C3B-C4B-NB	-2.70	108.01	110.52
18	3	602	CLA	C3B-C4B-NB	-2.69	108.02	110.52
20	5	622	LHG	O8-C23-C24	2.69	120.35	111.91
18	A	827	CLA	C3B-C4B-NB	-2.69	108.02	110.52
18	B	822	CLA	C3B-C4B-NB	-2.69	108.02	110.52
21	2	621	BCR	C15-C16-C17	-2.68	117.98	123.47
18	B	814	CLA	C3B-C4B-NB	-2.68	108.03	110.52
20	6	620	LHG	O8-C23-C24	2.68	120.32	111.91
27	3	619	XAT	C19-C9-C8	2.68	122.30	118.08
18	B	804	CLA	CHB-C4A-NA	2.68	128.22	124.51
21	5	621	BCR	C15-C14-C13	-2.68	123.49	127.31
18	6	608	CLA	O2D-CGD-O1D	-2.68	118.01	124.09
18	A	835	CLA	O2D-CGD-CBD	2.68	116.03	111.27
18	5	611	CLA	C1A-CHA-C4D	-2.68	121.97	125.72
18	A	845	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	6	607	CHL	CMB-C2B-C1B	2.67	129.44	125.37
18	3	603	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	5	607	CHL	CHD-C4C-C3C	-2.67	120.92	124.84
18	A	813	CLA	C3B-C4B-NB	-2.67	108.04	110.52
18	A	843	CLA	C3B-C4B-NB	-2.67	108.04	110.52
25	5	606	CHL	CAC-C3C-C4C	2.67	129.10	125.04
25	5	608	CHL	CMD-C2D-C3D	-2.66	121.48	127.61
18	3	615	CLA	C3B-C4B-NB	-2.66	108.04	110.52
25	6	607	CHL	CHD-C4C-C3C	-2.66	120.93	124.84
27	5	620	XAT	C15-C14-C13	-2.66	123.51	127.31
21	B	845	BCR	C27-C26-C25	2.66	126.59	122.73
18	3	614	CLA	CAA-C2A-C3A	-2.66	109.90	116.10
18	B	802	CLA	C3B-C4B-NB	-2.66	108.05	110.52
18	B	821	CLA	C3B-C4B-NB	-2.65	108.05	110.52
21	L	301	BCR	C15-C16-C17	-2.65	118.04	123.47
18	A	831	CLA	C3B-C4B-NB	-2.65	108.05	110.52
25	5	608	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
21	3	620	BCR	C3-C4-C5	-2.65	109.34	114.08
21	A	851	BCR	C27-C26-C25	2.65	126.57	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	201	CLA	C2B-C1B-NB	-2.65	108.46	110.23
18	B	812	CLA	CHB-C4A-NA	2.65	128.17	124.51
21	J	102	BCR	C27-C26-C25	2.64	126.57	122.73
18	B	836	CLA	C3B-C4B-NB	-2.64	108.06	110.52
18	A	841	CLA	C1-C2-C3	-2.64	121.47	126.04
18	F	304	CLA	CAA-C2A-C3A	-2.64	109.93	116.10
18	A	832	CLA	CAA-C2A-C3A	-2.64	109.93	116.10
21	B	846	BCR	C24-C23-C22	-2.64	122.24	126.23
18	A	845	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	5	607	CHL	O2D-CGD-O1D	-2.64	118.68	123.84
18	B	824	CLA	O2D-CGD-CBD	2.64	115.96	111.27
18	2	602	CLA	C3B-C4B-NB	-2.64	108.07	110.52
21	K	207	BCR	C15-C14-C13	-2.63	123.55	127.31
26	3	618	LUT	C10-C11-C12	-2.63	115.00	123.22
18	B	813	CLA	C3B-C4B-NB	-2.63	108.07	110.52
18	A	833	CLA	C3B-C4B-NB	-2.63	108.07	110.52
18	3	607	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
18	6	606	CLA	C3B-C4B-NB	-2.63	108.07	110.52
18	5	612	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	5	602	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	A	835	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	837	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	B	829	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	L	304	CLA	CHB-C4A-NA	2.63	128.14	124.51
18	B	816	CLA	O2D-CGD-O1D	-2.63	118.13	124.09
21	A	849	BCR	C15-C16-C17	-2.62	118.10	123.47
25	2	606	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
18	3	610	CLA	C3B-C4B-NB	-2.62	108.08	110.52
21	J	103	BCR	C33-C5-C6	-2.62	121.59	124.53
18	A	840	CLA	C3B-C4B-NB	-2.62	108.09	110.52
21	F	302	BCR	C15-C16-C17	-2.62	118.12	123.47
21	L	301	BCR	C33-C5-C6	-2.61	121.59	124.53
18	3	613	CLA	O2D-CGD-O1D	-2.61	118.16	124.09
18	5	613	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	6	611	CLA	CAA-C2A-C3A	-2.61	110.01	116.10
26	2	619	LUT	C11-C12-C13	-2.61	119.09	126.42
21	L	305	BCR	C33-C5-C6	-2.61	121.60	124.53
21	3	620	BCR	C2-C1-C6	2.61	114.50	110.48
26	6	617	LUT	C1-C6-C7	-2.61	108.40	115.78
18	A	814	CLA	C3B-C4B-NB	-2.61	108.10	110.52
18	3	606	CLA	C3B-C4B-NB	-2.61	108.10	110.52
20	2	622	LHG	O8-C23-C24	2.60	120.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	833	CLA	CHB-C1B-NB	2.60	127.01	124.26
27	2	620	XAT	O24-C25-C38	2.60	118.17	115.06
18	A	817	CLA	C3B-C4B-NB	-2.60	108.11	110.52
21	L	305	BCR	C28-C27-C26	-2.60	109.44	114.08
18	6	610	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	B	820	CLA	C3B-C4B-NB	-2.59	108.11	110.52
21	B	846	BCR	C27-C26-C25	2.59	126.50	122.73
26	5	619	LUT	C21-C26-C27	-2.59	109.42	112.70
18	B	802	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	B	805	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	F	305	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	B	824	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	L	302	CLA	C3B-C4B-NB	-2.59	108.12	110.52
21	A	856	BCR	C15-C16-C17	-2.59	118.18	123.47
21	3	622	BCR	C24-C23-C22	-2.58	122.33	126.23
21	B	848	BCR	C33-C5-C6	-2.58	121.63	124.53
21	J	102	BCR	C24-C23-C22	-2.58	122.33	126.23
27	3	619	XAT	C31-C30-C29	-2.58	123.62	127.31
18	3	604	CLA	O2D-CGD-O1D	-2.58	118.23	124.09
18	A	817	CLA	CAA-C2A-C3A	-2.58	110.08	116.10
18	A	823	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	6	611	CLA	O2D-CGD-O1D	-2.58	118.23	124.09
18	A	802	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	B	814	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
21	K	207	BCR	C24-C23-C22	-2.58	122.34	126.23
27	2	620	XAT	C20-C13-C12	2.58	122.14	118.08
18	6	612	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	A	829	CLA	C1-C2-C3	-2.57	121.59	126.04
18	A	822	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	A	809	CLA	C3B-C4B-NB	-2.57	108.13	110.52
18	B	813	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	A	805	CLA	O2D-CGD-CBD	2.57	115.84	111.27
18	B	831	CLA	C3B-C4B-NB	-2.57	108.13	110.52
18	B	839	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	5	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	A	830	CLA	C3B-C4B-NB	-2.56	108.14	110.52
20	A	846	LHG	C11-C10-C9	-2.56	101.41	114.42
18	A	839	CLA	C3B-C4B-NB	-2.56	108.14	110.52
18	B	833	CLA	C3B-C4B-NB	-2.56	108.14	110.52
23	B	850	DGD	C3G-C2G-C1G	-2.56	105.73	111.79
18	A	804	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	A	846	LHG	O8-C23-C24	2.56	119.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	606	CLA	O2D-CGD-CBD	2.56	115.82	111.27
18	A	818	CLA	C3B-C4B-NB	-2.56	108.14	110.52
18	2	609	CLA	CHB-C4A-NA	2.56	128.05	124.51
27	2	620	XAT	C39-C29-C28	2.56	122.11	118.08
18	K	204	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	K	207	BCR	C3-C4-C5	-2.56	109.51	114.08
21	A	851	BCR	C33-C5-C6	-2.55	121.66	124.53
18	3	609	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	803	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	3	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	A	814	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	A	831	CLA	O2D-CGD-CBD	2.55	115.80	111.27
21	B	848	BCR	C7-C8-C9	-2.55	122.39	126.23
18	6	603	CLA	C3B-C4B-NB	-2.55	108.15	110.52
21	G	205	BCR	C24-C23-C22	-2.55	122.39	126.23
18	A	854	CLA	C1-C2-C3	-2.54	121.65	126.04
18	B	806	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	3	611	CLA	C3B-C4B-NB	-2.54	108.16	110.52
21	A	851	BCR	C15-C16-C17	-2.54	118.27	123.47
18	B	808	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
18	A	833	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	B	820	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	5	609	CLA	C3B-C4B-NB	-2.54	108.16	110.52
18	B	826	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	B	834	CLA	CHB-C4A-NA	2.54	128.02	124.51
27	5	620	XAT	C10-C11-C12	-2.54	115.31	123.22
25	6	601	CHL	CHC-C4B-NB	-2.54	121.57	124.26
18	A	805	CLA	C3B-C4B-NB	-2.54	108.16	110.52
18	5	614	CLA	C3B-C4B-NB	-2.54	108.16	110.52
25	5	615	CHL	C2A-C1A-CHA	-2.53	119.43	123.86
18	A	817	CLA	O2D-CGD-O1D	-2.53	118.34	124.09
21	B	801	BCR	C33-C5-C6	-2.53	121.68	124.53
18	A	817	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	3	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	I	101	BCR	C15-C16-C17	-2.53	118.29	123.47
18	A	818	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	A	826	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	6	609	CLA	CAB-C3B-C2B	2.53	130.15	123.59
21	G	205	BCR	C33-C5-C6	-2.53	121.69	124.53
18	A	836	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	3	622	BCR	C15-C14-C13	-2.52	123.71	127.31
21	B	843	BCR	C33-C5-C6	-2.52	121.70	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	201	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	B	848	BCR	C28-C27-C26	-2.52	109.58	114.08
18	6	614	CLA	CAB-C3B-C2B	2.52	130.12	123.59
18	B	817	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	L	304	CLA	C3B-C4B-NB	-2.52	108.18	110.52
21	B	843	BCR	C24-C23-C22	-2.52	122.43	126.23
18	G	204	CLA	O2D-CGD-O1D	-2.52	118.38	124.09
18	B	837	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	3	613	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	2	612	CLA	CAA-C2A-C3A	-2.51	110.24	116.10
18	A	806	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	A	809	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	A	829	CLA	C3B-C4B-NB	-2.51	108.19	110.52
18	3	606	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
18	B	840	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	5	609	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	L	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	A	807	CLA	O2D-CGD-O1D	-2.50	118.40	124.09
18	A	835	CLA	C3B-C4B-NB	-2.50	108.19	110.52
18	3	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	815	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	808	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	A	825	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	G	203	CLA	C3B-C4B-NB	-2.49	108.20	110.52
18	A	810	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	L	301	BCR	C15-C14-C13	-2.49	123.75	127.31
21	A	850	BCR	C33-C5-C6	-2.49	121.73	124.53
21	K	202	BCR	C33-C5-C6	-2.49	121.73	124.53
18	2	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	2	603	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	2	621	BCR	C27-C26-C25	2.49	126.35	122.73
18	G	201	CLA	C3B-C4B-NB	-2.49	108.20	110.52
18	K	206	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	6	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	A	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	B	830	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	3	618	LUT	C15-C35-C34	-2.49	118.38	123.47
18	3	609	CLA	C3B-C4B-NB	-2.49	108.21	110.52
18	A	832	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	6	616	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	6	614	CLA	CMB-C2B-C3B	2.49	130.03	123.59
18	A	841	CLA	CHB-C4A-NA	2.48	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	843	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	K	203	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	G	203	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	B	812	CLA	C3B-C4B-NB	-2.48	108.21	110.52
18	F	304	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	2	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	2	620	XAT	C24-C23-C22	-2.48	105.98	110.77
18	A	831	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	B	841	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	6	608	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	3	606	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	A	820	CLA	C3B-C4B-NB	-2.48	108.21	110.52
18	A	821	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	6	610	CLA	O2D-CGD-O1D	-2.48	118.46	124.09
18	B	838	CLA	C3B-C4B-NB	-2.48	108.22	110.52
18	B	822	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	B	807	CLA	C1-C2-C3	-2.48	121.76	126.04
18	5	603	CLA	O2D-CGD-O1D	-2.48	118.46	124.09
18	5	610	CLA	C1-C2-C3	-2.48	121.76	126.04
18	A	824	CLA	CHB-C4A-NA	2.48	127.94	124.51
21	B	843	BCR	C15-C16-C17	-2.48	118.40	123.47
18	6	616	CLA	CAB-C3B-C2B	2.48	130.01	123.59
18	B	829	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	6	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	5	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	5	601	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	6	604	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	3	608	CHL	CHC-C4B-NB	-2.47	121.64	124.26
18	K	204	CLA	CAB-C3B-C2B	2.47	129.99	123.59
20	A	847	LHG	C11-C10-C9	-2.47	101.88	114.42
18	5	603	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	2	616	CHL	C1C-C2C-C3C	-2.47	105.16	107.11
18	3	614	CLA	O2D-CGD-O1D	-2.47	118.49	124.09
18	G	204	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	K	201	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	6	603	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	B	810	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	3	619	XAT	C35-C34-C33	-2.46	123.80	127.31
18	3	607	CLA	CAB-C3B-C2B	2.46	129.96	123.59
18	2	610	CLA	C3B-C4B-NB	-2.46	108.23	110.52
18	A	812	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	2	609	CLA	C3B-C4B-NB	-2.46	108.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	301	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	J	101	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	2	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	A	828	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	B	839	CLA	O2D-CGD-O1D	-2.46	118.51	124.09
18	5	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
21	A	848	BCR	C3-C4-C5	-2.45	109.70	114.08
18	6	609	CLA	CHB-C4A-NA	2.45	127.90	124.51
18	3	607	CLA	CMB-C2B-C3B	2.45	129.93	123.59
18	A	839	CLA	CHB-C4A-NA	2.45	127.90	124.51
18	6	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	A	856	BCR	C15-C14-C13	-2.45	123.82	127.31
21	3	622	BCR	C11-C10-C9	-2.44	123.82	127.31
18	5	611	CLA	CAB-C3B-C2B	2.44	129.92	123.59
25	2	616	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
25	5	606	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
21	A	856	BCR	C24-C23-C22	-2.44	122.54	126.23
18	L	302	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	2	604	CLA	O2D-CGD-CBD	2.44	115.61	111.27
18	3	610	CLA	CAA-C2A-C3A	-2.44	110.41	116.10
18	A	816	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	A	827	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	3	604	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	5	615	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
25	5	607	CHL	C2D-C1D-ND	2.44	111.90	110.10
21	F	302	BCR	C27-C26-C25	2.43	126.26	122.73
18	3	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	F	303	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	6	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	B	811	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	B	814	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	B	847	BCR	C27-C26-C25	2.42	126.25	122.73
18	B	818	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	5	606	CHL	OMC-CMC-C2C	-2.42	120.21	125.69
18	3	617	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	B	819	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	A	819	CLA	C3B-C4B-NB	-2.42	108.27	110.52
18	5	611	CLA	CMB-C2B-C3B	2.42	129.86	123.59
25	5	608	CHL	C5-C3-C4	2.42	119.94	114.60
20	5	622	LHG	C11-C10-C9	-2.42	102.15	114.42
21	L	301	BCR	C27-C26-C25	2.42	126.24	122.73
18	A	826	CLA	C3B-C4B-NB	-2.42	108.27	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	611	CLA	CMB-C2B-C3B	2.42	129.85	123.59
25	6	607	CHL	CHD-C1D-C2D	2.42	130.55	125.48
20	2	622	LHG	C11-C10-C9	-2.42	102.16	114.42
21	B	843	BCR	C15-C14-C13	-2.41	123.86	127.31
18	A	807	CLA	CHB-C4A-NA	2.41	127.85	124.51
21	B	801	BCR	C27-C26-C25	2.41	126.23	122.73
18	B	816	CLA	CHB-C4A-NA	2.41	127.85	124.51
18	A	814	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
18	A	842	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	2	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
21	B	844	BCR	C15-C16-C17	-2.41	118.54	123.47
18	A	808	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	2	604	CLA	C3B-C4B-NB	-2.41	108.28	110.52
21	B	846	BCR	C33-C5-C6	-2.40	121.83	124.53
27	6	619	XAT	C39-C29-C28	2.40	121.86	118.08
21	A	856	BCR	C11-C10-C9	-2.40	123.88	127.31
18	A	822	CLA	CAB-C3B-C2B	2.40	129.81	123.59
18	B	836	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	A	834	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	2	607	CHL	C1D-ND-C4D	-2.40	104.63	106.33
18	6	613	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	6	609	CLA	CMB-C2B-C3B	2.40	129.81	123.59
18	B	825	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	3	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	B	848	BCR	C35-C13-C14	-2.40	119.56	122.92
18	B	831	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	A	856	BCR	C3-C4-C5	-2.39	109.80	114.08
18	B	807	CLA	C3B-C4B-NB	-2.39	108.30	110.52
18	A	813	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	K	207	BCR	C27-C26-C25	2.39	126.20	122.73
21	G	205	BCR	C15-C16-C17	-2.39	118.58	123.47
21	B	845	BCR	C24-C23-C22	-2.39	122.63	126.23
18	6	616	CLA	CMB-C2B-C3B	2.39	129.78	123.59
18	B	808	CLA	C1-C2-C3	-2.39	122.89	126.75
25	5	607	CHL	C3B-C4B-NB	2.39	112.73	110.52
21	A	852	BCR	C27-C26-C25	2.39	126.19	122.73
26	2	619	LUT	C20-C13-C14	-2.39	119.58	122.92
18	A	838	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	F	305	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	A	830	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	B	811	CLA	CAB-C3B-C2B	2.38	129.76	123.59
18	B	835	CLA	C3B-C4B-NB	-2.38	108.31	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	847	BCR	C11-C10-C9	-2.38	123.91	127.31
18	3	604	CLA	CAB-C3B-C2B	2.38	129.76	123.59
21	5	621	BCR	C27-C26-C25	2.38	126.19	122.73
21	A	856	BCR	C27-C26-C25	2.38	126.19	122.73
18	6	609	CLA	CAA-C2A-C3A	-2.38	110.55	116.10
25	5	606	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
18	B	821	CLA	CHB-C4A-NA	2.38	127.80	124.51
18	B	823	CLA	CHB-C4A-NA	2.37	127.80	124.51
27	5	620	XAT	C18-C5-C4	2.37	116.95	114.28
18	5	609	CLA	CMB-C2B-C1B	-2.37	121.75	125.37
18	5	604	CLA	C3B-C4B-NB	-2.37	108.31	110.52
21	F	302	BCR	C33-C5-C6	-2.37	121.86	124.53
18	B	838	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	A	849	BCR	C33-C5-C6	-2.37	121.87	124.53
18	6	611	CLA	CAB-C3B-C2B	2.37	129.73	123.59
18	3	603	CLA	CHB-C4A-NA	2.37	127.78	124.51
18	A	819	CLA	CHB-C4A-NA	2.37	127.78	124.51
18	B	833	CLA	CHB-C4A-NA	2.37	127.78	124.51
21	L	305	BCR	C15-C14-C13	-2.36	123.94	127.31
18	K	204	CLA	CMB-C2B-C3B	2.36	129.70	123.59
18	B	833	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
18	B	807	CLA	CHB-C4A-NA	2.35	127.77	124.51
18	A	833	CLA	CMB-C2B-C1B	-2.35	121.78	125.37
27	5	620	XAT	C30-C31-C32	-2.35	115.88	123.22
21	A	849	BCR	C15-C14-C13	-2.35	123.95	127.31
25	5	608	CHL	CHC-C4B-NB	-2.35	121.77	124.26
18	A	837	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	B	832	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	5	607	CHL	CHD-C1D-C2D	2.35	130.41	125.48
18	2	604	CLA	C1-C2-C3	-2.35	122.95	126.75
23	B	850	DGD	CFB-CEB-CDB	-2.35	102.51	114.42
18	5	610	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
27	2	620	XAT	C28-C29-C30	-2.35	115.34	118.94
18	3	604	CLA	CMB-C2B-C3B	2.34	129.67	123.59
25	6	607	CHL	C3B-C4B-NB	2.34	112.69	110.52
18	B	811	CLA	CMB-C2B-C3B	2.34	129.66	123.59
25	2	601	CHL	C1C-C2C-C3C	-2.34	105.25	107.11
21	A	850	BCR	C27-C26-C25	2.34	126.13	122.73
25	2	601	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
21	B	845	BCR	C33-C5-C6	-2.34	121.90	124.53
18	3	615	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	A	846	LHG	C20-C19-C18	-2.34	102.55	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	606	CHL	CMB-C2B-C3B	2.34	129.65	123.59
18	3	617	CLA	CAA-C2A-C3A	-2.34	110.64	116.10
18	2	612	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	A	831	CLA	CHB-C1B-NB	2.34	126.73	124.26
18	A	811	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	2	601	CHL	CHC-C4B-NB	-2.33	121.79	124.26
21	A	848	BCR	C27-C26-C25	2.33	126.12	122.73
18	A	822	CLA	CMB-C2B-C3B	2.33	129.62	123.59
25	2	607	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
18	3	610	CLA	CMA-C3A-C2A	-2.32	110.67	116.10
24	2	617	LMG	O1-C1-C2	-2.32	105.42	108.15
21	G	205	BCR	C27-C26-C25	2.32	126.10	122.73
21	A	851	BCR	C15-C14-C13	-2.32	124.00	127.31
25	2	608	CHL	CHC-C4B-NB	-2.32	121.80	124.26
18	2	604	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
25	5	607	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
25	6	601	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
18	A	816	CLA	C3B-C4B-NB	-2.32	108.36	110.52
24	2	618	LMG	O3-C3-C2	-2.32	104.99	110.35
18	B	805	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
23	B	850	DGD	C3D-C4D-C5D	-2.32	106.11	110.24
21	B	844	BCR	C33-C5-C6	-2.32	121.93	124.53
18	A	809	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
21	2	621	BCR	C15-C14-C13	-2.31	124.01	127.31
21	K	202	BCR	C27-C26-C25	2.31	126.09	122.73
27	3	619	XAT	C25-C24-C23	-2.31	108.18	112.75
18	A	841	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
18	B	819	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	B	829	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	B	809	CLA	CHB-C4A-NA	2.31	127.70	124.51
18	A	808	CLA	C3B-C4B-NB	-2.31	108.38	110.52
18	B	809	CLA	C3B-C4B-NB	-2.30	108.38	110.52
25	2	601	CHL	CMB-C2B-C3B	2.30	129.56	123.59
20	A	846	LHG	C18-C17-C16	-2.30	102.74	114.42
21	B	845	BCR	C15-C16-C17	-2.30	118.76	123.47
18	A	840	CLA	CHB-C4A-NA	2.30	127.69	124.51
18	3	615	CLA	CAA-C2A-C3A	-2.30	110.73	116.10
21	2	621	BCR	C33-C5-C6	-2.30	121.95	124.53
21	B	801	BCR	C24-C23-C22	-2.30	122.77	126.23
18	B	836	CLA	CHD-C1D-ND	-2.29	122.34	124.45
18	A	816	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
25	3	608	CHL	CBC-CAC-C3C	-2.29	106.11	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	825	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
18	A	820	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	6	617	LUT	C11-C12-C13	-2.29	119.98	126.42
26	3	618	LUT	C20-C13-C12	2.29	121.69	118.08
27	6	619	XAT	C24-C23-C22	-2.29	106.36	110.77
18	2	610	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
18	B	830	CLA	CHB-C1B-NB	2.28	126.67	124.26
18	B	827	CLA	CHB-C4A-NA	2.28	127.66	124.51
18	A	818	CLA	O2D-CGD-CBD	2.28	115.32	111.27
25	2	601	CHL	C1D-ND-C4D	-2.28	104.72	106.33
18	L	303	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	6	614	CLA	CAA-C2A-C3A	-2.28	110.78	116.10
18	6	614	CLA	CMA-C3A-C2A	-2.28	110.78	116.10
21	J	103	BCR	C15-C14-C13	-2.28	124.06	127.31
21	F	302	BCR	C24-C23-C22	-2.28	122.79	126.23
18	3	613	CLA	C1-C2-C3	-2.27	122.11	126.04
24	J	104	LMG	O3-C3-C2	-2.27	105.10	110.35
21	J	103	BCR	C28-C27-C26	-2.27	110.03	114.08
21	3	622	BCR	C15-C16-C17	-2.27	118.83	123.47
21	A	849	BCR	C27-C26-C25	2.27	126.02	122.73
18	B	808	CLA	O2D-CGD-CBD	2.27	115.30	111.27
18	B	826	CLA	O2D-CGD-CBD	2.27	115.29	111.27
21	2	621	BCR	C11-C10-C9	-2.27	124.08	127.31
18	A	805	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
18	3	611	CLA	CAA-C2A-C3A	-2.26	110.82	116.10
18	A	823	CLA	CHB-C1B-NB	2.26	126.64	124.26
27	5	620	XAT	C19-C9-C8	2.26	121.63	118.08
21	A	850	BCR	C24-C23-C22	-2.26	122.83	126.23
18	B	836	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
25	6	607	CHL	O2D-CGD-O1D	-2.25	118.98	124.09
18	B	835	CLA	CHB-C4A-NA	2.25	127.62	124.51
26	2	619	LUT	C2-C3-C4	2.25	113.38	110.30
25	6	601	CHL	O2D-CGD-O1D	-2.25	118.98	124.09
18	B	803	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
21	B	847	BCR	C33-C5-C6	-2.25	122.01	124.53
18	3	603	CLA	C3B-C4B-NB	-2.24	108.43	110.52
18	A	843	CLA	CHD-C1D-ND	-2.24	122.39	124.45
26	5	619	LUT	C11-C12-C13	-2.24	120.12	126.42
27	5	620	XAT	O24-C25-C26	-2.24	57.10	58.96
18	A	836	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	2	601	CHL	CHD-C1D-C2D	2.24	130.18	125.48
18	5	602	CLA	CHB-C4A-NA	2.24	127.61	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	845	BCR	C15-C14-C13	-2.24	124.12	127.31
21	A	848	BCR	C24-C23-C22	-2.24	122.86	126.23
21	J	103	BCR	C15-C16-C17	-2.24	118.89	123.47
25	2	607	CHL	C4A-NA-C1A	2.24	107.71	106.71
21	3	620	BCR	C15-C16-C17	-2.24	118.89	123.47
18	3	611	CLA	O2D-CGD-O1D	-2.23	119.02	124.09
18	B	825	CLA	C3B-C4B-NB	-2.23	108.44	110.52
27	5	620	XAT	C20-C13-C12	2.23	121.59	118.08
26	6	617	LUT	C15-C35-C34	-2.23	118.90	123.47
18	B	828	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
21	B	844	BCR	C27-C26-C25	2.23	125.96	122.73
18	A	811	CLA	CHD-C1D-ND	-2.22	122.41	124.45
18	B	832	CLA	CHD-C1D-ND	-2.22	122.41	124.45
25	5	606	CHL	C2A-C1A-CHA	-2.22	119.98	123.86
18	A	829	CLA	CHB-C4A-NA	2.22	127.58	124.51
18	B	804	CLA	O2D-CGD-CBD	2.22	115.21	111.27
21	5	621	BCR	C11-C10-C9	-2.22	124.15	127.31
18	A	809	CLA	O2D-CGD-CBD	2.21	115.20	111.27
18	B	839	CLA	CHB-C1B-NB	2.21	126.60	124.26
18	B	814	CLA	CHD-C1D-ND	-2.21	122.42	124.45
18	A	806	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
18	A	854	CLA	C3B-C4B-NB	-2.21	108.46	110.52
18	B	802	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
21	G	205	BCR	C7-C8-C9	-2.21	122.89	126.23
18	A	837	CLA	CHB-C1B-NB	2.21	126.60	124.26
18	B	813	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
21	3	622	BCR	C33-C5-C6	-2.21	122.05	124.53
18	A	816	CLA	CHD-C1D-ND	-2.21	122.42	124.45
21	B	844	BCR	C15-C14-C13	-2.21	124.16	127.31
21	I	101	BCR	C33-C5-C6	-2.21	122.05	124.53
21	A	851	BCR	C2-C1-C6	2.21	113.88	110.48
21	3	620	BCR	C28-C27-C26	-2.21	110.14	114.08
25	2	608	CHL	O2D-CGD-O1D	-2.21	119.08	124.09
18	A	811	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
18	2	611	CLA	CHB-C1B-NB	2.20	126.58	124.26
25	5	615	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
18	B	822	CLA	C1-C2-C3	-2.20	122.24	126.04
20	2	622	LHG	C27-C26-C25	-2.20	103.27	114.42
18	A	825	CLA	CHB-C1B-NB	2.20	126.58	124.26
18	G	201	CLA	CHD-C1D-ND	-2.20	122.44	124.45
18	5	604	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
18	A	845	CLA	O2A-CGA-O1A	-2.19	118.05	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	606	CLA	C2A-C1A-CHA	2.19	126.11	122.71
21	B	843	BCR	C7-C8-C9	-2.19	122.92	126.23
21	J	103	BCR	C3-C4-C5	-2.19	110.16	114.08
18	B	841	CLA	CHB-C1B-NB	2.19	126.58	124.26
18	B	813	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	2	618	LMG	O1-C1-C2	-2.19	105.58	108.15
18	A	833	CLA	CHD-C1D-ND	-2.19	122.44	124.45
21	L	301	BCR	C2-C1-C6	2.19	113.85	110.48
25	6	607	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
21	A	852	BCR	C7-C8-C9	-2.19	122.93	126.23
18	A	808	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
18	A	812	CLA	CHD-C1D-ND	-2.19	122.44	124.45
18	A	829	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
21	I	101	BCR	C15-C14-C13	-2.18	124.19	127.31
18	B	828	CLA	CHB-C4A-NA	2.18	127.53	124.51
18	A	833	CLA	CHB-C1B-NB	2.18	126.56	124.26
18	G	203	CLA	CHB-C1B-NB	2.18	126.56	124.26
18	B	827	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
18	2	609	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	2	617	LMG	O3-C3-C2	-2.18	105.31	110.35
23	B	850	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
18	B	816	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	B	802	CLA	CHB-C4A-NA	2.17	127.52	124.51
18	B	834	CLA	CHD-C1D-ND	-2.17	122.46	124.45
18	B	838	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
18	B	841	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
21	3	620	BCR	C24-C23-C22	-2.17	122.95	126.23
18	B	809	CLA	CHD-C1D-ND	-2.17	122.46	124.45
18	B	837	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	6	614	CLA	CHB-C4A-NA	2.17	127.52	124.51
18	B	819	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	F	302	BCR	C15-C14-C13	-2.17	124.22	127.31
18	A	823	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
25	5	607	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
18	A	831	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
18	A	837	CLA	O2D-CGD-CBD	2.17	115.12	111.27
20	5	622	LHG	C27-C26-C25	-2.16	103.44	114.42
25	2	607	CHL	OMC-CMC-C2C	-2.16	120.80	125.69
25	6	607	CHL	OMC-CMC-C2C	-2.16	120.80	125.69
18	B	836	CLA	CHB-C1B-NB	2.16	126.55	124.26
18	5	614	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	B	846	BCR	C15-C14-C13	-2.16	124.22	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	620	XAT	O4-C5-C6	-2.16	57.17	58.96
18	B	824	CLA	CHB-C1B-NB	2.16	126.54	124.26
18	A	803	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
18	A	826	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
18	2	613	CLA	CHB-C1B-NB	2.16	126.54	124.26
18	B	841	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	A	849	BCR	C24-C23-C22	-2.16	122.97	126.23
25	3	608	CHL	O2D-CGD-O1D	-2.16	119.19	124.09
21	3	622	BCR	C27-C26-C25	2.16	125.86	122.73
20	A	846	LHG	C27-C26-C25	-2.16	103.47	114.42
18	L	304	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
18	A	838	CLA	CHB-C1B-NB	2.15	126.54	124.26
18	B	806	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	A	801	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
18	A	811	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	A	827	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
18	A	804	CLA	O2D-CGD-CBD	2.15	115.09	111.27
18	B	807	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	B	837	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	5	611	CLA	CHB-C1B-NB	2.15	126.53	124.26
21	L	305	BCR	C2-C1-C6	2.15	113.79	110.48
18	B	825	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	A	850	BCR	C11-C10-C9	-2.15	124.24	127.31
18	6	602	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	B	821	CLA	CHD-C1D-ND	-2.15	122.48	124.45
27	3	619	XAT	C10-C11-C12	-2.14	116.53	123.22
18	6	613	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
21	3	620	BCR	C8-C7-C6	-2.14	121.19	127.20
18	B	813	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	A	838	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	3	602	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	J	102	BCR	C2-C1-C6	2.14	113.78	110.48
26	2	619	LUT	C40-C33-C32	2.14	121.45	118.08
18	A	832	CLA	CMA-C3A-C2A	-2.14	111.10	116.10
18	B	826	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	A	803	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	5	609	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	5	601	CLA	CHB-C1B-NB	2.14	126.52	124.26
18	A	820	CLA	CHD-C1D-ND	-2.13	122.49	124.45
18	A	832	CLA	CHD-C1D-ND	-2.13	122.49	124.45
18	A	802	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
18	2	602	CLA	CHD-C1D-ND	-2.13	122.49	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	854	CLA	CHB-C4A-NA	2.13	127.46	124.51
18	A	815	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	A	821	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	J	101	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	3	604	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	5	610	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	B	832	CLA	O2D-CGD-CBD	2.12	115.04	111.27
25	2	607	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
18	A	813	CLA	CHB-C1B-NB	2.12	126.50	124.26
26	2	619	LUT	C39-C29-C28	2.12	121.42	118.08
18	6	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	3	607	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	A	838	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	B	818	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	5	615	CHL	CHB-C4A-NA	2.12	127.44	124.51
21	L	305	BCR	C24-C23-C22	-2.12	123.04	126.23
18	B	812	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	A	840	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	A	851	BCR	C38-C26-C25	-2.12	122.15	124.53
21	L	305	BCR	C29-C30-C25	2.11	113.74	110.48
18	A	822	CLA	CHB-C1B-NB	2.11	126.50	124.26
18	A	814	CLA	CMB-C2B-C3B	2.11	131.71	126.59
18	A	826	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	B	813	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	2	612	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	819	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
18	A	829	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
18	G	204	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	5	602	CLA	CHD-C1D-ND	-2.11	122.51	124.45
18	3	613	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	842	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
18	A	839	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
18	B	807	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
18	A	839	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	827	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
18	A	801	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	6	617	LUT	C31-C32-C33	-2.10	120.50	126.42
18	B	802	CLA	C1-C2-C3	-2.10	122.41	126.04
18	A	806	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	6	612	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	B	809	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	F	303	CLA	O2A-CGA-O1A	-2.10	118.07	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	604	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	2	610	CLA	CHB-C4A-NA	2.10	127.41	124.51
18	6	613	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	F	303	CLA	CHD-C1D-ND	-2.10	122.53	124.45
21	F	302	BCR	C11-C10-C9	-2.10	124.32	127.31
18	B	832	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
18	A	805	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	B	811	CLA	CHD-C1D-ND	-2.09	122.53	124.45
21	L	305	BCR	C7-C8-C9	-2.09	123.07	126.23
18	A	827	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	B	806	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
18	A	839	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	B	841	CLA	C1-C2-C3	-2.09	122.43	126.04
24	J	104	LMG	O2-C2-C1	-2.09	104.97	110.05
18	B	827	CLA	C3B-C4B-NB	-2.09	108.58	110.52
25	2	606	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
25	2	607	CHL	CHD-C1D-C2D	2.09	129.86	125.48
21	B	848	BCR	C29-C30-C25	2.09	113.69	110.48
18	A	808	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
21	B	848	BCR	C15-C14-C13	-2.09	124.33	127.31
25	2	616	CHL	OMC-CMC-C2C	-2.09	120.97	125.69
18	6	614	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	5	604	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	A	806	CLA	CHB-C1B-NB	2.08	126.46	124.26
26	3	618	LUT	C1-C6-C7	-2.08	109.89	115.78
18	A	810	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
18	B	821	CLA	CHB-C1B-NB	2.08	126.46	124.26
21	G	205	BCR	C15-C14-C13	-2.08	124.34	127.31
18	6	603	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	B	824	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
25	5	615	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
18	A	839	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
18	6	604	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
18	A	835	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	A	814	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	2	608	CHL	C1C-C2C-C3C	-2.08	105.47	107.11
18	B	808	CLA	CHB-C1B-NB	2.08	126.45	124.26
18	B	835	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	6	602	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	6	607	CHL	C2D-C1D-ND	2.07	111.63	110.10
18	B	833	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
18	B	817	CLA	CHB-C1B-NB	2.07	126.45	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	828	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	5	613	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	B	833	CLA	CHD-C1D-ND	-2.07	122.55	124.45
24	2	617	LMG	O2-C2-C1	-2.07	105.02	110.05
18	B	806	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	A	808	CLA	CHD-C1D-ND	-2.07	122.56	124.45
18	A	825	CLA	CHD-C1D-ND	-2.07	122.56	124.45
18	A	812	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
18	B	815	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
18	B	830	CLA	CHD-C1D-ND	-2.07	122.56	124.45
18	B	833	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
18	A	814	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
18	6	610	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
21	B	843	BCR	C38-C26-C25	-2.06	122.21	124.53
18	A	854	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	B	847	BCR	C7-C8-C9	-2.06	123.12	126.23
18	3	611	CLA	C2A-C1A-CHA	2.06	127.45	123.85
18	5	609	CLA	CMB-C2B-C3B	2.06	131.57	126.59
21	J	103	BCR	C24-C23-C22	-2.06	123.12	126.23
25	5	608	CHL	OMC-CMC-C2C	-2.06	121.04	125.69
18	A	803	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
18	A	807	CLA	CHB-C1B-NB	2.06	126.43	124.26
18	A	836	CLA	CHB-C1B-NB	2.06	126.43	124.26
18	A	818	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
18	B	832	CLA	CHB-C1B-NB	2.06	126.43	124.26
18	3	613	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	A	843	CLA	C1-C2-C3	-2.05	122.49	126.04
21	B	846	BCR	C15-C16-C17	-2.05	119.27	123.47
18	B	805	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	F	305	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	5	612	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	B	829	CLA	C2D-C1D-ND	-2.05	108.59	110.10
18	5	603	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	A	814	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	2	603	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	A	815	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
25	6	601	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
18	2	614	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	A	850	BCR	C7-C8-C9	-2.05	123.14	126.23
18	A	812	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	6	608	CLA	CHB-C1B-NB	2.05	126.42	124.26
18	B	829	CLA	CMB-C2B-C1B	-2.05	122.25	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	826	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	3	608	CHL	C1C-C2C-C3C	-2.05	104.81	106.96
25	5	607	CHL	C4D-CHA-C1A	-2.05	118.76	121.25
21	B	801	BCR	C15-C16-C17	-2.04	119.29	123.47
21	A	850	BCR	C15-C16-C17	-2.04	119.29	123.47
18	B	838	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	L	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	B	822	CLA	CHB-C1B-NB	2.04	126.42	124.26
18	5	612	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
21	L	305	BCR	C11-C10-C9	-2.04	124.40	127.31
18	A	841	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	2	608	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
18	3	617	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
26	5	619	LUT	C17-C1-C6	-2.04	106.99	110.30
26	3	618	LUT	C21-C26-C27	-2.04	110.12	112.70
25	3	608	CHL	CAA-C2A-C3A	-2.04	111.34	116.10
18	A	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	B	813	CLA	C1-C2-C3	-2.04	122.52	126.04
18	G	204	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	842	CLA	CHB-C1B-NB	2.04	126.41	124.26
18	6	603	CLA	CHB-C1B-NB	2.04	126.41	124.26
21	A	851	BCR	C37-C22-C21	-2.04	120.07	122.92
21	K	202	BCR	C35-C13-C14	-2.04	120.07	122.92
18	A	804	CLA	C1-C2-C3	-2.04	122.52	126.04
18	B	837	CLA	O2D-CGD-CBD	2.03	114.88	111.27
18	A	804	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	B	850	DGD	C5B-C4B-C3B	-2.03	104.10	114.42
18	3	617	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	2	601	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
25	6	607	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
18	A	802	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	A	832	CLA	CHB-C1B-NB	2.03	126.41	124.26
24	2	618	LMG	C1-C2-C3	-2.03	105.77	110.00
18	A	854	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	5	602	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
18	A	845	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	A	835	CLA	C1-C2-C3	-2.03	122.54	126.04
18	3	612	CLA	CHB-C1B-NB	2.03	126.40	124.26
27	2	620	XAT	C10-C11-C12	-2.03	116.89	123.22
18	B	819	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
18	A	818	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
18	A	805	CLA	CMB-C2B-C3B	2.02	131.49	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	837	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
21	A	851	BCR	C8-C7-C6	-2.02	121.52	127.20
18	6	603	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	J	104	LMG	O1-C7-C8	-2.02	106.02	110.90
18	K	203	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
18	B	830	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
18	G	203	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	A	819	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
21	A	852	BCR	C24-C23-C22	-2.02	123.18	126.23
18	6	609	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	5	611	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	A	837	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	A	841	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	L	302	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	B	850	DGD	O3E-C3E-C2E	-2.02	105.69	110.35
18	A	804	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	J	104	LMG	C1-C2-C3	-2.02	105.80	110.00
27	6	619	XAT	O24-C25-C26	-2.02	57.29	58.96
18	2	609	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	2	601	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
21	B	848	BCR	C15-C16-C17	-2.02	119.35	123.47
21	I	101	BCR	C28-C27-C26	-2.02	110.48	114.08
18	B	805	CLA	O2D-CGD-CBD	2.01	114.85	111.27
18	5	601	CLA	CHD-C1D-ND	-2.01	122.60	124.45
18	F	303	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	3	602	CLA	O2D-CGD-CBD	2.01	114.84	111.27
18	K	206	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
18	A	834	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	A	843	CLA	C2D-C1D-ND	-2.01	108.62	110.10
21	L	301	BCR	C24-C23-C22	-2.01	123.20	126.23
18	B	822	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
21	A	852	BCR	C15-C14-C13	-2.01	124.44	127.31
18	3	603	CLA	CHB-C1B-NB	2.01	126.39	124.26
25	5	615	CHL	CHC-C4B-NB	-2.01	122.13	124.26
21	B	846	BCR	C38-C26-C25	-2.01	122.27	124.53
27	2	620	XAT	C20-C13-C14	-2.01	120.11	122.92
18	B	818	CLA	CHB-C1B-NB	2.01	126.38	124.26
18	3	606	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	5	606	CHL	C4B-C3B-C2B	-2.01	105.12	107.03
18	2	613	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
18	A	829	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	6	619	XAT	C19-C9-C8	2.01	121.24	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	825	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	B	820	CLA	CHB-C1B-NB	2.01	126.38	124.26
18	A	821	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
18	6	612	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
25	2	608	CHL	CAA-C2A-C3A	-2.00	111.42	116.10
18	A	820	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	A	843	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	B	827	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	A	809	CLA	CMB-C2B-C3B	2.00	131.44	126.59
18	A	816	CLA	CMB-C2B-C3B	2.00	131.44	126.59
23	B	850	DGD	CAB-C9B-C8B	-2.00	104.25	114.42
18	A	809	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
18	B	827	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
18	B	832	CLA	CHC-C4B-NB	2.00	126.38	124.26
18	F	301	CLA	CHB-C1B-NB	2.00	126.38	124.26
26	3	618	LUT	C17-C1-C6	-2.00	107.05	110.30
21	A	849	BCR	C11-C10-C9	-2.00	124.45	127.31
18	A	817	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	5	609	CLA	CHB-C1B-NB	2.00	126.38	124.26

There are no chirality outliers.

All (1481) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	CHA-CBD-CGD-O1D
18	A	805	CLA	CHA-CBD-CGD-O2D
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	809	CLA	C1A-C2A-CAA-CBA
18	A	809	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C2B-C3B-CAB-CBB
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	816	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	A	816	CLA	CHA-CBD-CGD-O2D
18	A	818	CLA	CHA-CBD-CGD-O1D
18	A	818	CLA	CHA-CBD-CGD-O2D
18	A	818	CLA	C4-C3-C5-C6
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	821	CLA	CHA-CBD-CGD-O1D
18	A	821	CLA	CHA-CBD-CGD-O2D
18	A	821	CLA	CAD-CBD-CGD-O1D
18	A	821	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	C2A-CAA-CBA-CGA
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	824	CLA	CAD-CBD-CGD-O1D
18	A	824	CLA	CAD-CBD-CGD-O2D
18	A	825	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	826	CLA	CHA-CBD-CGD-O1D
18	A	826	CLA	CHA-CBD-CGD-O2D
18	A	826	CLA	C6-C7-C8-C9
18	A	827	CLA	C3A-C2A-CAA-CBA
18	A	828	CLA	CHA-CBD-CGD-O1D
18	A	828	CLA	CHA-CBD-CGD-O2D
18	A	828	CLA	CAD-CBD-CGD-O1D
18	A	828	CLA	CAD-CBD-CGD-O2D
18	A	829	CLA	C1A-C2A-CAA-CBA
18	A	829	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	832	CLA	CHA-CBD-CGD-O1D
18	A	832	CLA	CHA-CBD-CGD-O2D
18	A	832	CLA	CAD-CBD-CGD-O1D
18	A	833	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	C2B-C3B-CAB-CBB
18	A	843	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	CHA-CBD-CGD-O1D
18	A	845	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	845	CLA	CAD-CBD-CGD-O1D
18	A	854	CLA	CHA-CBD-CGD-O1D
18	A	854	CLA	CHA-CBD-CGD-O2D
18	A	854	CLA	CAD-CBD-CGD-O1D
18	A	854	CLA	CAD-CBD-CGD-O2D
18	A	854	CLA	C2-C3-C5-C6
18	A	854	CLA	C4-C3-C5-C6
18	B	802	CLA	CHA-CBD-CGD-O1D
18	B	802	CLA	CHA-CBD-CGD-O2D
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	806	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	CHA-CBD-CGD-O1D
18	B	813	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O1D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	815	CLA	C2-C3-C5-C6
18	B	815	CLA	C4-C3-C5-C6
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	C2-C3-C5-C6
18	B	822	CLA	C4-C3-C5-C6
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C2-C3-C5-C6
18	B	826	CLA	C4-C3-C5-C6
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	C2A-CAA-CBA-CGA
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	834	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	CHA-CBD-CGD-O1D
18	B	837	CLA	CHA-CBD-CGD-O2D
18	B	839	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	841	CLA	C14-C13-C15-C16
18	F	301	CLA	CBD-CGD-O2D-CED
18	G	204	CLA	C2B-C3B-CAB-CBB
18	G	204	CLA	C4B-C3B-CAB-CBB
18	J	101	CLA	C3A-C2A-CAA-CBA
18	K	201	CLA	C4B-C3B-CAB-CBB
18	K	203	CLA	C2B-C3B-CAB-CBB
18	K	203	CLA	C4B-C3B-CAB-CBB
18	K	206	CLA	CBD-CGD-O2D-CED
18	2	602	CLA	C1A-C2A-CAA-CBA
18	2	602	CLA	C3A-C2A-CAA-CBA
18	2	603	CLA	CBD-CGD-O2D-CED
18	2	604	CLA	C1A-C2A-CAA-CBA
18	2	604	CLA	C3A-C2A-CAA-CBA
18	2	609	CLA	C1A-C2A-CAA-CBA
18	2	609	CLA	C3A-C2A-CAA-CBA
18	2	610	CLA	C3A-C2A-CAA-CBA
18	2	610	CLA	CBD-CGD-O2D-CED
18	2	614	CLA	CBD-CGD-O2D-CED
18	6	603	CLA	C2-C3-C5-C6
18	6	603	CLA	C4-C3-C5-C6
18	6	604	CLA	C1A-C2A-CAA-CBA
18	6	609	CLA	CBD-CGD-O2D-CED
18	6	611	CLA	CHA-CBD-CGD-O2D
18	6	613	CLA	C1A-C2A-CAA-CBA
18	6	613	CLA	C3A-C2A-CAA-CBA
18	6	616	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	CHA-CBD-CGD-O1D
18	3	602	CLA	CHA-CBD-CGD-O2D
18	3	607	CLA	C3A-C2A-CAA-CBA
18	3	610	CLA	CBD-CGD-O2D-CED
18	3	612	CLA	CBD-CGD-O2D-CED
18	5	604	CLA	CHA-CBD-CGD-O1D
18	5	604	CLA	CHA-CBD-CGD-O2D
18	5	604	CLA	CBD-CGD-O2D-CED
18	5	609	CLA	C1A-C2A-CAA-CBA
18	5	609	CLA	C3A-C2A-CAA-CBA
18	5	609	CLA	CHA-CBD-CGD-O2D
18	5	609	CLA	CAD-CBD-CGD-O2D
18	5	610	CLA	C2B-C3B-CAB-CBB
18	5	610	CLA	C4B-C3B-CAB-CBB
18	5	611	CLA	CMA-C3A-C4A-NA

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Mol	Chain	Res	Type	Atoms
18	5	611	CLA	CBD-CGD-O2D-CED
18	5	614	CLA	CAD-CBD-CGD-O1D
18	5	614	CLA	CAD-CBD-CGD-O2D
18	5	614	CLA	CBD-CGD-O2D-CED
19	A	844	PQN	C12-C13-C15-C16
19	A	844	PQN	C14-C13-C15-C16
19	A	844	PQN	C24-C23-C25-C26
20	A	846	LHG	C4-O6-P-O5
20	A	846	LHG	O7-C5-C6-O8
20	A	847	LHG	C3-O3-P-O4
20	A	847	LHG	C3-O3-P-O5
20	A	847	LHG	C4-O6-P-O5
20	A	847	LHG	O7-C5-C6-O8
20	B	851	LHG	C1-C2-C3-O3
20	B	851	LHG	C4-O6-P-O5
20	B	851	LHG	O9-C7-O7-C5
20	B	851	LHG	C8-C7-O7-C5
20	2	622	LHG	C1-C2-C3-O3
20	2	622	LHG	C3-O3-P-O5
20	2	622	LHG	C4-O6-P-O3
20	2	622	LHG	C4-O6-P-O4
20	2	622	LHG	C4-O6-P-O5
20	6	620	LHG	O1-C1-C2-O2
20	6	620	LHG	O1-C1-C2-C3
20	6	620	LHG	C3-O3-P-O4
20	6	620	LHG	C3-O3-P-O6
20	6	620	LHG	C4-O6-P-O3
20	6	620	LHG	C4-O6-P-O4
20	5	622	LHG	C1-C2-C3-O3
20	5	622	LHG	C4-O6-P-O4
21	A	849	BCR	C7-C8-C9-C34
21	A	851	BCR	C7-C8-C9-C34
21	A	851	BCR	C37-C22-C23-C24
21	A	851	BCR	C22-C23-C24-C25
21	A	851	BCR	C23-C24-C25-C30
21	A	852	BCR	C1-C6-C7-C8
21	A	852	BCR	C7-C8-C9-C10
21	A	852	BCR	C7-C8-C9-C34
21	A	852	BCR	C21-C22-C23-C24
21	A	852	BCR	C37-C22-C23-C24
21	A	856	BCR	C23-C24-C25-C30
21	B	801	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	B	801	BCR	C7-C8-C9-C34
21	B	843	BCR	C7-C8-C9-C34
21	B	843	BCR	C37-C22-C23-C24
21	B	844	BCR	C7-C8-C9-C34
21	B	844	BCR	C21-C22-C23-C24
21	B	845	BCR	C14-C15-C16-C17
21	B	845	BCR	C16-C17-C18-C36
21	B	845	BCR	C17-C18-C19-C20
21	B	845	BCR	C18-C19-C20-C21
21	B	845	BCR	C21-C22-C23-C24
21	B	845	BCR	C37-C22-C23-C24
21	B	846	BCR	C7-C8-C9-C34
21	B	846	BCR	C13-C14-C15-C16
21	B	846	BCR	C14-C15-C16-C17
21	B	846	BCR	C16-C17-C18-C19
21	B	846	BCR	C16-C17-C18-C36
21	B	846	BCR	C36-C18-C19-C20
21	B	846	BCR	C18-C19-C20-C21
21	B	846	BCR	C20-C21-C22-C37
21	B	846	BCR	C22-C23-C24-C25
21	B	847	BCR	C23-C24-C25-C30
21	B	848	BCR	C1-C6-C7-C8
21	B	848	BCR	C7-C8-C9-C10
21	B	848	BCR	C11-C10-C9-C8
21	B	848	BCR	C11-C10-C9-C34
21	B	848	BCR	C10-C11-C12-C13
21	B	848	BCR	C11-C12-C13-C35
21	F	302	BCR	C10-C11-C12-C13
21	F	302	BCR	C11-C12-C13-C35
21	F	302	BCR	C14-C15-C16-C17
21	F	302	BCR	C16-C17-C18-C36
21	G	205	BCR	C23-C24-C25-C30
21	I	101	BCR	C14-C15-C16-C17
21	J	102	BCR	C6-C7-C8-C9
21	J	103	BCR	C1-C6-C7-C8
21	J	103	BCR	C6-C7-C8-C9
21	J	103	BCR	C11-C10-C9-C8
21	J	103	BCR	C11-C12-C13-C14
21	J	103	BCR	C11-C12-C13-C35
21	J	103	BCR	C14-C15-C16-C17
21	J	103	BCR	C18-C19-C20-C21
21	J	103	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	J	103	BCR	C20-C21-C22-C37
21	J	103	BCR	C22-C23-C24-C25
21	K	202	BCR	C7-C8-C9-C34
21	K	207	BCR	C6-C7-C8-C9
21	K	207	BCR	C18-C19-C20-C21
21	K	207	BCR	C21-C22-C23-C24
21	K	207	BCR	C22-C23-C24-C25
21	L	301	BCR	C1-C6-C7-C8
21	L	305	BCR	C7-C8-C9-C34
21	L	305	BCR	C21-C22-C23-C24
21	L	305	BCR	C37-C22-C23-C24
21	L	305	BCR	C22-C23-C24-C25
21	L	305	BCR	C23-C24-C25-C26
21	L	305	BCR	C23-C24-C25-C30
21	3	620	BCR	C6-C7-C8-C9
21	3	620	BCR	C7-C8-C9-C10
21	3	620	BCR	C7-C8-C9-C34
21	3	620	BCR	C20-C21-C22-C23
21	3	620	BCR	C20-C21-C22-C37
21	3	620	BCR	C23-C24-C25-C30
21	3	622	BCR	C6-C7-C8-C9
21	3	622	BCR	C7-C8-C9-C10
21	3	622	BCR	C7-C8-C9-C34
21	3	622	BCR	C22-C23-C24-C25
21	5	621	BCR	C20-C21-C22-C37
21	5	621	BCR	C23-C24-C25-C30
23	B	850	DGD	O1B-C1B-O2G-C2G
24	J	104	LMG	O6-C1-O1-C7
24	2	617	LMG	C2-C1-O1-C7
24	2	617	LMG	O6-C1-O1-C7
25	2	616	CHL	CHA-CBD-CGD-O1D
25	2	616	CHL	CHA-CBD-CGD-O2D
25	5	606	CHL	C1C-C2C-CMC-OMC
25	5	608	CHL	C2A-CAA-CBA-CGA
26	2	619	LUT	C5-C6-C7-C8
26	2	619	LUT	C7-C8-C9-C10
26	2	619	LUT	C7-C8-C9-C19
26	6	617	LUT	C6-C7-C8-C9
26	6	617	LUT	C11-C10-C9-C8
26	6	617	LUT	C11-C10-C9-C19
26	6	617	LUT	C10-C11-C12-C13
26	6	617	LUT	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	3	618	LUT	C5-C6-C7-C8
26	3	618	LUT	C11-C10-C9-C8
26	3	618	LUT	C11-C10-C9-C19
26	3	618	LUT	C10-C11-C12-C13
26	3	618	LUT	C12-C13-C14-C15
26	3	618	LUT	C20-C13-C14-C15
26	3	618	LUT	C26-C27-C28-C29
26	5	619	LUT	C5-C6-C7-C8
26	5	619	LUT	C12-C13-C14-C15
26	5	619	LUT	C20-C13-C14-C15
26	5	619	LUT	C14-C15-C35-C34
27	2	620	XAT	O4-C6-C7-C8
18	F	303	CLA	O1D-CGD-O2D-CED
18	2	603	CLA	O1D-CGD-O2D-CED
18	6	606	CLA	O1D-CGD-O2D-CED
18	6	609	CLA	O1D-CGD-O2D-CED
18	A	801	CLA	O1D-CGD-O2D-CED
18	B	811	CLA	O1D-CGD-O2D-CED
18	5	604	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	812	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	F	303	CLA	CBD-CGD-O2D-CED
18	K	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	CBD-CGD-O2D-CED
18	2	613	CLA	CBD-CGD-O2D-CED
18	6	603	CLA	CBD-CGD-O2D-CED
18	6	606	CLA	CBD-CGD-O2D-CED
18	6	613	CLA	CBD-CGD-O2D-CED
18	3	603	CLA	CBD-CGD-O2D-CED
18	5	613	CLA	CBD-CGD-O2D-CED
25	5	608	CHL	CBD-CGD-O2D-CED
20	6	620	LHG	O10-C23-O8-C6
24	J	104	LMG	O10-C28-O8-C9
18	B	821	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1D-CGD-O2D-CED
18	K	206	CLA	O1D-CGD-O2D-CED
18	6	616	CLA	O1D-CGD-O2D-CED
18	3	603	CLA	O1D-CGD-O2D-CED
18	B	821	CLA	CBA-CGA-O2A-C1
18	B	834	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	3	610	CLA	O1D-CGD-O2D-CED
18	5	611	CLA	O1D-CGD-O2D-CED
20	6	620	LHG	C24-C23-O8-C6
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	841	CLA	CBD-CGD-O2D-CED
18	A	854	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	CBD-CGD-O2D-CED
18	2	602	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	824	CLA	O1A-CGA-O2A-C1
18	A	845	CLA	O1A-CGA-O2A-C1
18	3	603	CLA	O1A-CGA-O2A-C1
20	5	622	LHG	O10-C23-O8-C6
18	B	810	CLA	O1A-CGA-O2A-C1
18	B	806	CLA	O1D-CGD-O2D-CED
18	3	612	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
18	2	610	CLA	O1D-CGD-O2D-CED
18	2	614	CLA	O1D-CGD-O2D-CED
18	5	614	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	CBD-CGD-O2D-CED
18	G	203	CLA	CBD-CGD-O2D-CED
25	2	601	CHL	CBD-CGD-O2D-CED
25	5	615	CHL	CBD-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	6	613	CLA	O1D-CGD-O2D-CED
18	A	805	CLA	C3-C5-C6-C7
18	A	818	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	A	843	CLA	C3-C5-C6-C7
18	B	815	CLA	C3-C5-C6-C7
18	B	826	CLA	C3-C5-C6-C7
19	A	844	PQN	C13-C15-C16-C17
18	A	806	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	CBA-CGA-O2A-C1
18	A	824	CLA	CBA-CGA-O2A-C1
18	A	845	CLA	CBA-CGA-O2A-C1
18	3	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	5	622	LHG	C24-C23-O8-C6
23	B	850	DGD	C2B-C1B-O2G-C2G
18	2	613	CLA	O1D-CGD-O2D-CED
18	5	613	CLA	O1D-CGD-O2D-CED
18	K	204	CLA	O1D-CGD-O2D-CED
18	A	839	CLA	C4-C3-C5-C6
18	A	839	CLA	C2-C3-C5-C6
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CBD-CGD-O2D-CED
25	2	606	CHL	CBD-CGD-O2D-CED
18	A	824	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C2A-CAA-CBA-CGA
18	B	835	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	C2A-CAA-CBA-CGA
18	6	616	CLA	C2A-CAA-CBA-CGA
18	A	801	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	CBA-CGA-O2A-C1
18	B	815	CLA	CBA-CGA-O2A-C1
18	6	604	CLA	CBA-CGA-O2A-C1
18	A	831	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	O1D-CGD-O2D-CED
18	K	201	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1A-CGA-O2A-C1
18	6	604	CLA	O1A-CGA-O2A-C1
25	5	608	CHL	O1D-CGD-O2D-CED
21	B	845	BCR	C13-C14-C15-C16
21	B	845	BCR	C15-C16-C17-C18
21	B	846	BCR	C19-C20-C21-C22
18	A	803	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	CBD-CGD-O2D-CED
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	CBD-CGD-O2D-CED
25	2	616	CHL	CBD-CGD-O2D-CED
20	2	622	LHG	O2-C2-C3-O3
20	5	622	LHG	O2-C2-C3-O3
18	A	826	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	B	842	PQN	C13-C15-C16-C17
18	A	829	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	O1A-CGA-O2A-C1
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	839	CLA	O1A-CGA-O2A-C1
24	J	104	LMG	O6-C5-C6-O5
18	A	802	CLA	O1D-CGD-O2D-CED
25	5	607	CHL	CBD-CGD-O2D-CED
18	B	811	CLA	O1A-CGA-O2A-C1
18	A	839	CLA	CBD-CGD-O2D-CED
18	B	804	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	C3-C5-C6-C7
18	A	854	CLA	C3-C5-C6-C7
18	B	809	CLA	C3-C5-C6-C7
24	J	104	LMG	C29-C28-O8-C9
18	A	822	CLA	O1D-CGD-O2D-CED
18	A	845	CLA	C3-C5-C6-C7
18	B	840	CLA	C4-C3-C5-C6
18	A	818	CLA	C2-C3-C5-C6
18	B	840	CLA	C2-C3-C5-C6
18	F	305	CLA	C2A-CAA-CBA-CGA
18	6	603	CLA	O1D-CGD-O2D-CED
18	B	815	CLA	O1A-CGA-O2A-C1
18	G	203	CLA	CBA-CGA-O2A-C1
20	2	622	LHG	C23-C24-C25-C26
18	A	812	CLA	O1D-CGD-O2D-CED
18	B	819	CLA	O1D-CGD-O2D-CED
18	A	854	CLA	O1D-CGD-O2D-CED
18	K	203	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	C3-C5-C6-C7
18	B	807	CLA	C3-C5-C6-C7
18	B	831	CLA	CBA-CGA-O2A-C1
18	A	815	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	O1D-CGD-O2D-CED
18	2	602	CLA	O1D-CGD-O2D-CED
21	B	846	BCR	C15-C16-C17-C18
21	B	848	BCR	C9-C10-C11-C12
21	F	302	BCR	C9-C10-C11-C12
21	F	302	BCR	C13-C14-C15-C16
21	J	102	BCR	C9-C10-C11-C12
20	A	846	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
18	B	806	CLA	C15-C16-C17-C18
18	B	813	CLA	C5-C6-C7-C8
20	B	851	LHG	O2-C2-C3-O3
23	B	850	DGD	C2E-C1E-O5D-C6D
24	J	104	LMG	C2-C1-O1-C7
18	B	828	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C14-C13-C15-C16
18	A	827	CLA	C6-C7-C8-C9
18	A	839	CLA	C14-C13-C15-C16
18	A	841	CLA	C6-C7-C8-C9
18	A	841	CLA	C14-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C9
18	B	813	CLA	O1D-CGD-O2D-CED
18	G	201	CLA	O1D-CGD-O2D-CED
18	F	304	CLA	CBD-CGD-O2D-CED
21	B	844	BCR	C37-C22-C23-C24
21	B	845	BCR	C7-C8-C9-C34
21	J	102	BCR	C11-C12-C13-C35
21	J	103	BCR	C37-C22-C23-C24
21	K	207	BCR	C11-C12-C13-C35
21	3	622	BCR	C37-C22-C23-C24
27	2	620	XAT	C7-C8-C9-C19
21	A	851	BCR	C21-C22-C23-C24
21	B	848	BCR	C11-C12-C13-C14
21	3	622	BCR	C21-C22-C23-C24
27	2	620	XAT	C7-C8-C9-C10
27	5	620	XAT	C27-C28-C29-C30
23	B	850	DGD	C1A-C2A-C3A-C4A
24	2	618	LMG	O6-C5-C6-O5
18	A	841	CLA	O1D-CGD-O2D-CED
18	A	843	CLA	CBA-CGA-O2A-C1
18	A	818	CLA	C10-C11-C12-C13
18	A	829	CLA	C13-C15-C16-C17
18	A	835	CLA	C5-C6-C7-C8
18	A	841	CLA	C5-C6-C7-C8
18	B	803	CLA	C10-C11-C12-C13
18	B	825	CLA	C13-C15-C16-C17
18	B	840	CLA	C15-C16-C17-C18
20	A	846	LHG	C28-C29-C30-C31
18	A	831	CLA	C5-C6-C7-C8
20	A	846	LHG	C23-C24-C25-C26
20	A	847	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	6	620	LHG	C23-C24-C25-C26
18	6	602	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	C15-C16-C17-C18
18	A	814	CLA	O1D-CGD-O2D-CED
18	A	843	CLA	C2-C1-O2A-CGA
18	B	825	CLA	C10-C11-C12-C13
18	B	826	CLA	C5-C6-C7-C8
24	J	104	LMG	C28-C29-C30-C31
18	A	808	CLA	CBD-CGD-O2D-CED
18	A	828	CLA	CBA-CGA-O2A-C1
18	B	813	CLA	C15-C16-C17-C18
18	A	826	CLA	C11-C10-C8-C7
18	B	831	CLA	O1A-CGA-O2A-C1
21	J	103	BCR	C9-C10-C11-C12
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	825	CLA	C2A-CAA-CBA-CGA
18	G	201	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	O1D-CGD-O2D-CED
25	5	615	CHL	O1D-CGD-O2D-CED
18	A	834	CLA	C5-C6-C7-C8
18	B	815	CLA	C8-C10-C11-C12
18	2	609	CLA	C5-C6-C7-C8
21	A	849	BCR	C6-C7-C8-C9
18	B	827	CLA	CBD-CGD-O2D-CED
23	B	850	DGD	O6E-C1E-O5D-C6D
21	G	205	BCR	C10-C11-C12-C13
21	J	103	BCR	C10-C11-C12-C13
26	2	619	LUT	C10-C11-C12-C13
26	5	619	LUT	C30-C31-C32-C33
23	B	850	DGD	O6E-C5E-C6E-O5E
24	2	617	LMG	C4-C5-C6-O5
18	B	840	CLA	C13-C15-C16-C17
18	B	828	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	C8-C10-C11-C12
18	B	807	CLA	C10-C11-C12-C13
18	A	829	CLA	O1D-CGD-O2D-CED
24	J	104	LMG	C4-C5-C6-O5
18	A	843	CLA	O1A-CGA-O2A-C1
18	G	203	CLA	O1A-CGA-O2A-C1
25	2	606	CHL	O1D-CGD-O2D-CED
18	B	807	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A	844	PQN	C18-C20-C21-C22
20	A	847	LHG	C3-O3-P-O6
20	A	847	LHG	C4-O6-P-O3
20	5	622	LHG	C4-O6-P-O3
20	2	622	LHG	C7-C8-C9-C10
18	6	603	CLA	CBA-CGA-O2A-C1
25	2	601	CHL	O1D-CGD-O2D-CED
18	B	820	CLA	C2A-CAA-CBA-CGA
18	3	613	CLA	C4-C3-C5-C6
18	A	839	CLA	C13-C15-C16-C17
18	A	854	CLA	C2A-CAA-CBA-CGA
18	B	804	CLA	C2A-CAA-CBA-CGA
18	K	201	CLA	C2A-CAA-CBA-CGA
18	6	603	CLA	C6-C7-C8-C10
21	J	103	BCR	C15-C16-C17-C18
26	2	619	LUT	C9-C10-C11-C12
18	B	811	CLA	C5-C6-C7-C8
21	A	852	BCR	C16-C17-C18-C36
21	A	852	BCR	C20-C21-C22-C37
21	B	845	BCR	C20-C21-C22-C37
21	I	101	BCR	C20-C21-C22-C37
21	J	103	BCR	C16-C17-C18-C36
21	K	207	BCR	C16-C17-C18-C36
21	L	301	BCR	C16-C17-C18-C36
21	L	301	BCR	C20-C21-C22-C37
21	2	621	BCR	C20-C21-C22-C37
21	5	621	BCR	C16-C17-C18-C36
26	2	619	LUT	C11-C10-C9-C19
26	6	617	LUT	C39-C29-C30-C31
26	6	617	LUT	C40-C33-C34-C35
18	3	613	CLA	C3-C5-C6-C7
18	A	824	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	C16-C17-C18-C20
18	A	825	CLA	C6-C7-C8-C10
18	A	831	CLA	O1D-CGD-O2D-CED
20	5	622	LHG	C5-C4-O6-P
20	5	622	LHG	C23-C24-C25-C26
21	A	852	BCR	C16-C17-C18-C19
21	B	845	BCR	C16-C17-C18-C19
21	B	845	BCR	C20-C21-C22-C23
21	B	846	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	F	302	BCR	C16-C17-C18-C19
21	J	102	BCR	C11-C10-C9-C8
21	J	103	BCR	C16-C17-C18-C19
21	L	301	BCR	C11-C10-C9-C8
21	5	621	BCR	C20-C21-C22-C23
26	2	619	LUT	C11-C10-C9-C8
26	6	617	LUT	C28-C29-C30-C31
26	6	617	LUT	C32-C33-C34-C35
23	B	850	DGD	C9A-CAA-CBA-CCA
18	2	609	CLA	C6-C7-C8-C10
18	3	613	CLA	C6-C7-C8-C9
18	B	835	CLA	O1D-CGD-O2D-CED
20	A	846	LHG	C13-C14-C15-C16
18	3	613	CLA	C2-C3-C5-C6
18	A	804	CLA	C11-C10-C8-C9
18	A	841	CLA	C11-C10-C8-C9
18	B	806	CLA	C11-C10-C8-C9
18	B	809	CLA	C11-C10-C8-C9
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	838	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C2A-CAA-CBA-CGA
25	2	601	CHL	C2A-CAA-CBA-CGA
25	6	601	CHL	C2A-CAA-CBA-CGA
18	6	603	CLA	O1A-CGA-O2A-C1
27	5	620	XAT	C27-C28-C29-C39
23	B	850	DGD	C4B-C5B-C6B-C7B
20	A	847	LHG	O1-C1-C2-C3
20	5	622	LHG	O1-C1-C2-C3
21	F	302	BCR	C11-C12-C13-C14
21	J	103	BCR	C21-C22-C23-C24
21	L	305	BCR	C7-C8-C9-C10
20	A	846	LHG	C9-C10-C11-C12
20	6	620	LHG	C7-C8-C9-C10
18	B	816	CLA	C4B-C3B-CAB-CBB
18	B	824	CLA	C4B-C3B-CAB-CBB
18	F	301	CLA	C4B-C3B-CAB-CBB
18	K	206	CLA	C4B-C3B-CAB-CBB
18	L	303	CLA	C4B-C3B-CAB-CBB
18	6	604	CLA	C4B-C3B-CAB-CBB
25	2	608	CHL	C4B-C3B-CAB-CBB
18	A	814	CLA	C16-C17-C18-C19
18	K	201	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	823	CLA	CBD-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
20	5	622	LHG	C11-C10-C9-C8
23	B	850	DGD	CAB-CBB-CCB-CDB
18	A	803	CLA	O1D-CGD-O2D-CED
25	2	616	CHL	O1D-CGD-O2D-CED
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	807	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	C3A-C2A-CAA-CBA
18	A	838	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	5	612	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	O1D-CGD-O2D-CED
18	3	613	CLA	C6-C7-C8-C10
18	2	609	CLA	C4-C3-C5-C6
25	5	607	CHL	O1D-CGD-O2D-CED
18	A	826	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	C6-C7-C8-C9
18	A	812	CLA	C2B-C3B-CAB-CBB
18	A	841	CLA	C2B-C3B-CAB-CBB
18	B	816	CLA	C2B-C3B-CAB-CBB
18	B	824	CLA	C2B-C3B-CAB-CBB
18	B	839	CLA	C2B-C3B-CAB-CBB
18	F	301	CLA	C2B-C3B-CAB-CBB
18	K	201	CLA	C2B-C3B-CAB-CBB
18	K	206	CLA	C2B-C3B-CAB-CBB
18	L	303	CLA	C2B-C3B-CAB-CBB
18	6	604	CLA	C2B-C3B-CAB-CBB
25	2	608	CHL	C2B-C3B-CAB-CBB
18	A	806	CLA	C2-C1-O2A-CGA
18	A	829	CLA	C2-C1-O2A-CGA
18	B	809	CLA	C10-C11-C12-C13
18	B	836	CLA	C5-C6-C7-C8
21	A	848	BCR	C23-C24-C25-C26
21	A	848	BCR	C23-C24-C25-C30
21	A	851	BCR	C23-C24-C25-C26
21	A	852	BCR	C5-C6-C7-C8
21	A	856	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	A	856	BCR	C23-C24-C25-C26
21	B	846	BCR	C23-C24-C25-C26
21	B	846	BCR	C23-C24-C25-C30
21	B	847	BCR	C23-C24-C25-C26
21	B	848	BCR	C5-C6-C7-C8
21	B	848	BCR	C23-C24-C25-C26
21	B	848	BCR	C23-C24-C25-C30
21	G	205	BCR	C23-C24-C25-C26
21	J	103	BCR	C5-C6-C7-C8
21	J	103	BCR	C23-C24-C25-C26
21	J	103	BCR	C23-C24-C25-C30
21	K	207	BCR	C23-C24-C25-C30
21	L	301	BCR	C5-C6-C7-C8
21	L	305	BCR	C5-C6-C7-C8
21	3	620	BCR	C23-C24-C25-C26
21	5	621	BCR	C1-C6-C7-C8
21	5	621	BCR	C5-C6-C7-C8
21	5	621	BCR	C23-C24-C25-C26
26	6	617	LUT	C5-C6-C7-C8
19	A	844	PQN	C15-C16-C17-C18
24	2	617	LMG	O6-C5-C6-O5
23	B	850	DGD	CBA-CCA-CDA-CEA
18	A	804	CLA	C11-C10-C8-C7
18	A	827	CLA	C6-C7-C8-C10
18	A	831	CLA	C11-C10-C8-C7
18	A	831	CLA	C12-C13-C15-C16
18	A	841	CLA	C6-C7-C8-C10
18	A	841	CLA	C12-C13-C15-C16
18	B	805	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C10-C8-C7
18	B	809	CLA	C11-C10-C8-C7
18	B	809	CLA	C12-C13-C15-C16
18	B	815	CLA	C6-C7-C8-C10
18	B	825	CLA	C11-C10-C8-C7
18	2	609	CLA	C2-C3-C5-C6
19	B	842	PQN	C22-C23-C25-C26
18	A	814	CLA	C5-C6-C7-C8
18	A	829	CLA	C10-C11-C12-C13
20	A	847	LHG	C24-C23-O8-C6
18	A	803	CLA	C2A-CAA-CBA-CGA
18	B	803	CLA	C2A-CAA-CBA-CGA
18	2	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	6	613	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C5-C6-C7-C8
23	B	850	DGD	CAA-CBA-CCA-CDA
23	B	850	DGD	O6D-C1D-O3G-C3G
18	A	843	CLA	C5-C6-C7-C8
18	A	839	CLA	O1D-CGD-O2D-CED
20	A	846	LHG	C32-C33-C34-C35
20	A	846	LHG	C8-C7-O7-C5
20	2	622	LHG	C8-C7-O7-C5
21	L	301	BCR	C10-C11-C12-C13
18	B	813	CLA	C13-C15-C16-C17
18	A	812	CLA	C16-C17-C18-C19
18	6	603	CLA	C6-C7-C8-C9
18	A	826	CLA	C11-C10-C8-C9
18	A	827	CLA	C11-C12-C13-C14
18	A	831	CLA	C11-C10-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	B	815	CLA	C6-C7-C8-C9
18	3	602	CLA	C11-C10-C8-C9
18	B	804	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	C2A-CAA-CBA-CGA
18	G	204	CLA	C2A-CAA-CBA-CGA
18	6	602	CLA	C2A-CAA-CBA-CGA
21	2	621	BCR	C11-C12-C13-C35
21	A	848	BCR	C21-C22-C23-C24
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	807	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	827	CLA	C1A-C2A-CAA-CBA
18	A	834	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C1A-C2A-CAA-CBA
18	A	845	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	2	610	CLA	C1A-C2A-CAA-CBA
18	6	610	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C1A-C2A-CAA-CBA
18	5	612	CLA	C1A-C2A-CAA-CBA
18	A	814	CLA	C16-C17-C18-C20
18	2	609	CLA	C6-C7-C8-C9
18	A	835	CLA	C13-C15-C16-C17
18	5	611	CLA	CMA-C3A-C4A-CHB
18	B	841	CLA	C13-C15-C16-C17
18	B	807	CLA	C4-C3-C5-C6
20	A	846	LHG	C4-C5-C6-O8
20	5	622	LHG	C24-C25-C26-C27
18	A	815	CLA	O1D-CGD-O2D-CED
18	F	304	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	CAA-CBA-CGA-O2A
20	5	622	LHG	O1-C1-C2-O2
20	2	622	LHG	C11-C12-C13-C14
20	2	622	LHG	C27-C28-C29-C30
21	J	102	BCR	C11-C10-C9-C34
21	J	103	BCR	C11-C10-C9-C34
21	L	305	BCR	C16-C17-C18-C36
18	A	835	CLA	C4-C3-C5-C6
18	B	825	CLA	C4-C3-C5-C6
18	B	836	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	C2A-CAA-CBA-CGA
18	A	828	CLA	O1A-CGA-O2A-C1
19	B	842	PQN	C20-C21-C22-C23
20	6	620	LHG	C24-C25-C26-C27
18	B	809	CLA	C13-C15-C16-C17
18	A	808	CLA	O1D-CGD-O2D-CED
21	B	848	BCR	C12-C13-C14-C15
23	B	850	DGD	C2A-C3A-C4A-C5A
18	A	812	CLA	C11-C12-C13-C15
18	A	814	CLA	C6-C7-C8-C10
18	A	827	CLA	C11-C12-C13-C15
18	A	829	CLA	C6-C7-C8-C10
18	A	829	CLA	C11-C12-C13-C15
18	A	839	CLA	C12-C13-C15-C16
18	A	843	CLA	C6-C7-C8-C10
18	B	805	CLA	C11-C12-C13-C15
18	B	825	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	841	CLA	C12-C13-C15-C16
19	A	844	PQN	C22-C23-C25-C26
18	A	812	CLA	C11-C12-C13-C14
18	A	829	CLA	C11-C12-C13-C14
18	B	803	CLA	C11-C10-C8-C9
18	B	805	CLA	C6-C7-C8-C9
18	B	806	CLA	C11-C12-C13-C14
18	B	826	CLA	C11-C12-C13-C14
18	B	836	CLA	C11-C10-C8-C9
18	B	841	CLA	C11-C12-C13-C14
18	A	805	CLA	C6-C7-C8-C10
21	B	846	BCR	C7-C8-C9-C10
21	K	202	BCR	C7-C8-C9-C10
24	J	104	LMG	C30-C31-C32-C33
18	A	819	CLA	CBD-CGD-O2D-CED
18	A	812	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	A	838	CLA	C4B-C3B-CAB-CBB
18	A	841	CLA	C4B-C3B-CAB-CBB
18	B	837	CLA	C4B-C3B-CAB-CBB
18	2	603	CLA	C4B-C3B-CAB-CBB
18	2	612	CLA	C4B-C3B-CAB-CBB
18	3	603	CLA	C4B-C3B-CAB-CBB
20	6	620	LHG	O6-C4-C5-C6
20	6	620	LHG	C11-C10-C9-C8
18	A	835	CLA	C2-C3-C5-C6
20	A	846	LHG	O9-C7-O7-C5
23	B	850	DGD	C9B-CAB-CBB-CCB
18	B	811	CLA	C6-C7-C8-C9
20	A	846	LHG	C27-C28-C29-C30
18	B	841	CLA	O1A-CGA-O2A-C1
18	B	828	CLA	C3A-C2A-CAA-CBA
18	6	604	CLA	C3A-C2A-CAA-CBA
23	B	850	DGD	CCA-CDA-CEA-CFA
20	B	851	LHG	C4-C5-C6-O8
20	2	622	LHG	C4-C5-C6-O8
23	B	850	DGD	O1G-C1G-C2G-C3G
23	B	850	DGD	C4E-C5E-C6E-O5E
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	807	CLA	C2-C3-C5-C6
18	B	827	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	6	602	CLA	O1D-CGD-O2D-CED
20	2	622	LHG	C12-C13-C14-C15
25	5	606	CHL	C3C-C2C-CMC-OMC
18	B	823	CLA	O1D-CGD-O2D-CED
20	B	851	LHG	C24-C23-O8-C6
18	6	608	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C15-C16-C17-C18
19	A	844	PQN	C25-C26-C27-C28
18	A	825	CLA	C2B-C3B-CAB-CBB
18	A	838	CLA	C2B-C3B-CAB-CBB
18	3	603	CLA	C2B-C3B-CAB-CBB
23	B	850	DGD	C6B-C7B-C8B-C9B
18	A	805	CLA	C6-C7-C8-C9
18	A	854	CLA	C2-C1-O2A-CGA
18	B	806	CLA	C2-C1-O2A-CGA
18	B	815	CLA	C2-C1-O2A-CGA
18	A	826	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C11-C10-C8-C9
18	A	818	CLA	C14-C13-C15-C16
18	A	834	CLA	C6-C7-C8-C9
18	B	813	CLA	C11-C12-C13-C14
18	B	825	CLA	C6-C7-C8-C9
18	B	826	CLA	C6-C7-C8-C9
19	B	842	PQN	C16-C17-C18-C19
18	B	813	CLA	C2C-C3C-CAC-CBC
18	A	829	CLA	C15-C16-C17-C18
18	B	807	CLA	C2A-CAA-CBA-CGA
25	2	607	CHL	CBD-CGD-O2D-CED
21	A	848	BCR	C1-C6-C7-C8
21	A	848	BCR	C5-C6-C7-C8
21	A	849	BCR	C1-C6-C7-C8
21	A	849	BCR	C5-C6-C7-C8
21	A	850	BCR	C1-C6-C7-C8
21	A	850	BCR	C5-C6-C7-C8
21	A	851	BCR	C1-C6-C7-C8
21	A	851	BCR	C5-C6-C7-C8
21	A	856	BCR	C5-C6-C7-C8
21	B	801	BCR	C1-C6-C7-C8
21	B	801	BCR	C5-C6-C7-C8
21	B	801	BCR	C23-C24-C25-C26
21	B	843	BCR	C1-C6-C7-C8
21	B	843	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	B	843	BCR	C23-C24-C25-C26
21	B	843	BCR	C23-C24-C25-C30
21	B	844	BCR	C1-C6-C7-C8
21	B	844	BCR	C5-C6-C7-C8
21	B	845	BCR	C1-C6-C7-C8
21	B	845	BCR	C5-C6-C7-C8
21	B	845	BCR	C23-C24-C25-C26
21	B	845	BCR	C23-C24-C25-C30
21	B	846	BCR	C1-C6-C7-C8
21	B	846	BCR	C5-C6-C7-C8
21	G	205	BCR	C1-C6-C7-C8
21	G	205	BCR	C5-C6-C7-C8
21	K	202	BCR	C1-C6-C7-C8
21	K	202	BCR	C5-C6-C7-C8
21	K	202	BCR	C23-C24-C25-C26
21	K	207	BCR	C1-C6-C7-C8
21	K	207	BCR	C5-C6-C7-C8
21	K	207	BCR	C23-C24-C25-C26
21	L	301	BCR	C23-C24-C25-C26
21	L	305	BCR	C1-C6-C7-C8
21	2	621	BCR	C1-C6-C7-C8
21	2	621	BCR	C5-C6-C7-C8
21	2	621	BCR	C23-C24-C25-C26
21	2	621	BCR	C23-C24-C25-C30
21	3	622	BCR	C23-C24-C25-C26
21	3	622	BCR	C23-C24-C25-C30
18	A	834	CLA	C8-C10-C11-C12
18	A	816	CLA	C1A-C2A-CAA-CBA
18	J	101	CLA	C1A-C2A-CAA-CBA
21	A	849	BCR	C7-C8-C9-C10
21	B	843	BCR	C21-C22-C23-C24
21	J	102	BCR	C7-C8-C9-C10
25	5	607	CHL	C1A-C2A-CAA-CBA
18	B	811	CLA	C6-C7-C8-C10
18	B	807	CLA	C5-C6-C7-C8
20	A	847	LHG	O2-C2-C3-O3
18	K	201	CLA	O1A-CGA-O2A-C1
18	A	818	CLA	C6-C7-C8-C10
18	A	818	CLA	C12-C13-C15-C16
18	A	826	CLA	C6-C7-C8-C10
18	A	827	CLA	C12-C13-C15-C16
18	A	834	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	A	839	CLA	C6-C7-C8-C10
18	B	803	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C12-C13-C15
18	B	806	CLA	C12-C13-C15-C16
18	B	807	CLA	C12-C13-C15-C16
18	B	825	CLA	C6-C7-C8-C10
18	B	826	CLA	C11-C12-C13-C15
18	B	841	CLA	C11-C12-C13-C15
18	3	602	CLA	C6-C7-C8-C10
19	B	842	PQN	C21-C22-C23-C25
21	J	103	BCR	C13-C14-C15-C16
18	2	604	CLA	CBA-CGA-O2A-C1
21	A	856	BCR	C20-C21-C22-C37
21	B	843	BCR	C20-C21-C22-C37
21	B	844	BCR	C20-C21-C22-C37
21	B	845	BCR	C35-C13-C14-C15
21	K	202	BCR	C20-C21-C22-C37
21	3	620	BCR	C16-C17-C18-C36
26	5	619	LUT	C11-C10-C9-C19
18	A	806	CLA	C3-C5-C6-C7
18	B	822	CLA	C3-C5-C6-C7
18	B	822	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	808	CLA	CAD-CBD-CGD-O2D
18	A	810	CLA	CAD-CBD-CGD-O2D
18	A	813	CLA	CAD-CBD-CGD-O2D
18	A	819	CLA	CAD-CBD-CGD-O2D
18	A	829	CLA	CAD-CBD-CGD-O2D
18	A	832	CLA	CAD-CBD-CGD-O2D
18	A	845	CLA	CAD-CBD-CGD-O2D
18	B	819	CLA	CAD-CBD-CGD-O2D
18	B	830	CLA	CAD-CBD-CGD-O2D
18	B	832	CLA	CAD-CBD-CGD-O2D
18	B	836	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	2	604	CLA	CAD-CBD-CGD-O2D
18	2	613	CLA	CAD-CBD-CGD-O2D
18	6	606	CLA	CAD-CBD-CGD-O2D
18	6	609	CLA	CAD-CBD-CGD-O2D
18	5	610	CLA	CAD-CBD-CGD-O2D
18	5	612	CLA	CAD-CBD-CGD-O2D
20	B	851	LHG	C6-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
21	A	849	BCR	C22-C23-C24-C25
21	2	621	BCR	C6-C7-C8-C9
18	A	825	CLA	CBA-CGA-O2A-C1
20	A	847	LHG	C4-C5-C6-O8
20	2	622	LHG	C2-C3-O3-P
18	2	604	CLA	O1A-CGA-O2A-C1
18	B	832	CLA	C2A-CAA-CBA-CGA
18	B	806	CLA	C16-C17-C18-C19
24	J	104	LMG	O9-C10-O7-C8
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	814	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	805	CLA	CHA-CBD-CGD-O1D
18	B	805	CLA	CHA-CBD-CGD-O2D
18	B	810	CLA	CHA-CBD-CGD-O1D
18	B	810	CLA	CHA-CBD-CGD-O2D
18	B	815	CLA	CHA-CBD-CGD-O1D
18	B	815	CLA	CHA-CBD-CGD-O2D
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	826	CLA	CHA-CBD-CGD-O1D
18	B	826	CLA	CHA-CBD-CGD-O2D
18	J	101	CLA	CHA-CBD-CGD-O1D
18	J	101	CLA	CHA-CBD-CGD-O2D
18	5	614	CLA	CHA-CBD-CGD-O1D
24	J	104	LMG	C29-C30-C31-C32
21	B	845	BCR	C11-C10-C9-C8
23	B	850	DGD	C2D-C1D-O3G-C3G
20	2	622	LHG	O7-C5-C6-O8
23	B	850	DGD	O1G-C1G-C2G-O2G
18	B	833	CLA	CBD-CGD-O2D-CED
20	5	622	LHG	C28-C29-C30-C31
18	A	819	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	C15-C16-C17-C18
18	A	829	CLA	C5-C6-C7-C8
21	A	851	BCR	C11-C12-C13-C35
21	K	207	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	2	622	LHG	O1-C1-C2-C3
20	2	622	LHG	C24-C25-C26-C27
18	A	814	CLA	C1A-C2A-CAA-CBA
18	B	813	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	6	614	CLA	CHA-CBD-CGD-O2D
18	5	610	CLA	C1A-C2A-CAA-CBA
25	2	608	CHL	CHA-CBD-CGD-O2D
25	5	608	CHL	C1A-C2A-CAA-CBA
25	2	607	CHL	O1D-CGD-O2D-CED
18	A	825	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	C4B-C3B-CAB-CBB
18	A	824	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	C4B-C3B-CAB-CBB
18	A	840	CLA	C4B-C3B-CAB-CBB
18	A	842	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	C4B-C3B-CAB-CBB
18	B	808	CLA	C4B-C3B-CAB-CBB
18	B	810	CLA	C4B-C3B-CAB-CBB
18	B	815	CLA	C4B-C3B-CAB-CBB
18	B	817	CLA	C4B-C3B-CAB-CBB
18	B	818	CLA	C4B-C3B-CAB-CBB
18	B	821	CLA	C4B-C3B-CAB-CBB
18	B	828	CLA	C4B-C3B-CAB-CBB
18	B	840	CLA	C4B-C3B-CAB-CBB
18	B	841	CLA	C4B-C3B-CAB-CBB
18	F	303	CLA	C4B-C3B-CAB-CBB
18	F	305	CLA	C4B-C3B-CAB-CBB
18	G	203	CLA	C4B-C3B-CAB-CBB
18	J	101	CLA	C4B-C3B-CAB-CBB
18	2	613	CLA	C4B-C3B-CAB-CBB
18	2	614	CLA	C4B-C3B-CAB-CBB
18	6	608	CLA	C4B-C3B-CAB-CBB
18	6	612	CLA	C4B-C3B-CAB-CBB
18	6	613	CLA	C4B-C3B-CAB-CBB
18	3	611	CLA	C4B-C3B-CAB-CBB
18	3	613	CLA	C4B-C3B-CAB-CBB
18	3	614	CLA	C4B-C3B-CAB-CBB
18	3	615	CLA	C4B-C3B-CAB-CBB
18	5	601	CLA	C4B-C3B-CAB-CBB
18	5	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	5	603	CLA	C4B-C3B-CAB-CBB
18	5	612	CLA	C4B-C3B-CAB-CBB
18	5	613	CLA	C4B-C3B-CAB-CBB
20	A	847	LHG	C4-O6-P-O4
20	5	622	LHG	C3-O3-P-O4
18	A	827	CLA	C16-C17-C18-C20
18	A	805	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	O6-C4-C5-C6
20	A	847	LHG	O6-C4-C5-C6
20	A	846	LHG	C24-C25-C26-C27
18	B	802	CLA	CAA-CBA-CGA-O2A
18	3	613	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	C16-C17-C18-C19
18	A	814	CLA	CAD-CBD-CGD-O1D
18	A	815	CLA	CAD-CBD-CGD-O1D
18	A	816	CLA	CAD-CBD-CGD-O1D
18	A	826	CLA	CAD-CBD-CGD-O1D
18	A	834	CLA	CAD-CBD-CGD-O1D
18	B	817	CLA	CAD-CBD-CGD-O1D
18	B	821	CLA	CAD-CBD-CGD-O1D
18	B	837	CLA	CAD-CBD-CGD-O1D
18	B	840	CLA	CAD-CBD-CGD-O1D
18	J	101	CLA	CAD-CBD-CGD-O1D
18	6	616	CLA	CAD-CBD-CGD-O1D
18	5	604	CLA	CAD-CBD-CGD-O1D
25	5	607	CHL	CAD-CBD-CGD-O1D
18	A	831	CLA	C16-C17-C18-C20
18	B	807	CLA	C11-C10-C8-C7
18	B	840	CLA	C6-C7-C8-C10
18	3	611	CLA	CAD-CBD-CGD-O2D
20	A	846	LHG	O6-C4-C5-O7
20	A	847	LHG	O6-C4-C5-O7
20	6	620	LHG	O6-C4-C5-O7
25	3	608	CHL	CAD-CBD-CGD-O2D
18	B	816	CLA	C2A-CAA-CBA-CGA
18	B	811	CLA	C3-C5-C6-C7
18	3	617	CLA	CAD-CBD-CGD-O1D
20	B	851	LHG	O7-C5-C6-O8
23	B	850	DGD	C6A-C7A-C8A-C9A
18	A	831	CLA	C15-C16-C17-C18
21	B	801	BCR	C14-C15-C16-C17
18	A	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	818	CLA	C6-C7-C8-C9
18	A	827	CLA	C14-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C9
18	A	839	CLA	C6-C7-C8-C9
18	A	843	CLA	C6-C7-C8-C9
18	B	806	CLA	C14-C13-C15-C16
18	B	807	CLA	C14-C13-C15-C16
18	3	602	CLA	C6-C7-C8-C9
21	B	848	BCR	C6-C7-C8-C9
20	A	846	LHG	C11-C12-C13-C14
18	B	841	CLA	C3-C5-C6-C7
21	F	302	BCR	C15-C16-C17-C18
20	5	622	LHG	C12-C13-C14-C15
18	A	806	CLA	C16-C17-C18-C20
21	5	621	BCR	C7-C8-C9-C10
18	A	821	CLA	C2B-C3B-CAB-CBB
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C2B-C3B-CAB-CBB
18	A	842	CLA	C2B-C3B-CAB-CBB
18	A	845	CLA	C2B-C3B-CAB-CBB
18	B	815	CLA	C2B-C3B-CAB-CBB
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	837	CLA	C2B-C3B-CAB-CBB
18	2	603	CLA	C2B-C3B-CAB-CBB
18	2	612	CLA	C2B-C3B-CAB-CBB
18	2	614	CLA	C2B-C3B-CAB-CBB
18	6	608	CLA	C2B-C3B-CAB-CBB
18	6	612	CLA	C2B-C3B-CAB-CBB
18	3	611	CLA	C2B-C3B-CAB-CBB
18	3	614	CLA	C2B-C3B-CAB-CBB
18	3	615	CLA	C2B-C3B-CAB-CBB
18	5	602	CLA	C2B-C3B-CAB-CBB
18	5	612	CLA	C2B-C3B-CAB-CBB
18	5	613	CLA	C2B-C3B-CAB-CBB
26	6	617	LUT	C20-C13-C14-C15
18	A	829	CLA	C16-C17-C18-C20
18	B	831	CLA	C1-C2-C3-C4
18	6	604	CLA	C1-C2-C3-C4
18	B	833	CLA	O1D-CGD-O2D-CED
23	B	850	DGD	C4D-C5D-C6D-O5D
18	A	829	CLA	CAA-CBA-CGA-O2A
20	2	622	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C2A-CAA-CBA-CGA
18	K	206	CLA	C2A-CAA-CBA-CGA
18	5	613	CLA	C2A-CAA-CBA-CGA
18	A	805	CLA	C2-C1-O2A-CGA
18	B	803	CLA	C2-C1-O2A-CGA
18	B	826	CLA	C2-C1-O2A-CGA
20	6	620	LHG	C2-C3-O3-P
20	2	622	LHG	O6-C4-C5-O7
20	5	622	LHG	O6-C4-C5-O7
21	B	801	BCR	C23-C24-C25-C30
21	F	302	BCR	C23-C24-C25-C26
21	F	302	BCR	C23-C24-C25-C30
21	K	202	BCR	C23-C24-C25-C30
21	L	301	BCR	C23-C24-C25-C30
18	A	826	CLA	CAA-CBA-CGA-O2A
18	3	602	CLA	C2A-CAA-CBA-CGA
20	A	846	LHG	C3-O3-P-O6
20	B	851	LHG	C4-O6-P-O3
20	2	622	LHG	C3-O3-P-O6
20	A	846	LHG	C25-C26-C27-C28
18	B	822	CLA	C6-C7-C8-C10
23	B	850	DGD	CCB-CDB-CEB-CFB
18	A	818	CLA	C11-C10-C8-C7
18	A	830	CLA	C11-C12-C13-C15
18	A	841	CLA	C11-C10-C8-C7
18	3	602	CLA	C11-C10-C8-C7
19	B	842	PQN	C16-C17-C18-C20
18	B	805	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
19	B	842	PQN	C21-C22-C23-C24
21	5	621	BCR	C9-C10-C11-C12
18	B	840	CLA	CAA-CBA-CGA-O1A
18	A	827	CLA	C16-C17-C18-C19
18	A	831	CLA	C4-C3-C5-C6
18	6	603	CLA	C4B-C3B-CAB-CBB
18	6	606	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C2A-CAA-CBA-CGA
21	K	202	BCR	C13-C14-C15-C16
20	5	622	LHG	O6-C4-C5-C6
18	A	814	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	5	609	CLA	CAA-CBA-CGA-O2A
18	6	613	CLA	CAA-CBA-CGA-O1A
18	6	613	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O1A
18	A	827	CLA	C2-C1-O2A-CGA
18	B	805	CLA	C2A-CAA-CBA-CGA
18	5	602	CLA	C2A-CAA-CBA-CGA
20	A	847	LHG	O10-C23-C24-C25
25	2	606	CHL	C2A-CAA-CBA-CGA
20	5	622	LHG	C27-C28-C29-C30
18	A	814	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	C3A-C2A-CAA-CBA
18	B	841	CLA	C3A-C2A-CAA-CBA
25	6	601	CHL	CAA-CBA-CGA-O2A
18	A	854	CLA	C11-C12-C13-C14
18	B	807	CLA	C11-C10-C8-C9
18	B	828	CLA	C14-C13-C15-C16
19	B	842	PQN	C26-C27-C28-C30
18	B	832	CLA	CAA-CBA-CGA-O2A
21	A	848	BCR	C20-C21-C22-C37
21	A	852	BCR	C11-C10-C9-C34
18	B	833	CLA	CAA-CBA-CGA-O2A
18	K	203	CLA	CAA-CBA-CGA-O1A
18	A	829	CLA	C16-C17-C18-C19
20	6	620	LHG	O2-C2-C3-O3
18	B	822	CLA	O1D-CGD-O2D-CED
21	A	856	BCR	C7-C8-C9-C34
25	2	616	CHL	CAA-CBA-CGA-O1A
20	A	846	LHG	C31-C32-C33-C34
21	L	301	BCR	C21-C22-C23-C24
18	A	840	CLA	CAA-CBA-CGA-O1A
23	B	850	DGD	O6D-C5D-C6D-O5D
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	C1A-C2A-CAA-CBA
18	B	831	CLA	C1A-C2A-CAA-CBA
18	5	614	CLA	C1A-C2A-CAA-CBA
18	A	854	CLA	C6-C7-C8-C10
18	B	826	CLA	C11-C10-C8-C7
18	B	836	CLA	C11-C10-C8-C7
18	A	839	CLA	C15-C16-C17-C18
25	6	601	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	2	607	CHL	C3C-C2C-CMC-OMC
25	5	615	CHL	C3C-C2C-CMC-OMC
18	A	833	CLA	CAA-CBA-CGA-O1A
18	B	833	CLA	CAA-CBA-CGA-O1A
18	B	834	CLA	CAA-CBA-CGA-O1A
18	B	834	CLA	CAA-CBA-CGA-O2A
18	5	603	CLA	CAA-CBA-CGA-O1A
18	A	814	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	C2A-CAA-CBA-CGA
18	A	839	CLA	C2A-CAA-CBA-CGA
18	L	302	CLA	C2A-CAA-CBA-CGA
18	2	604	CLA	C2A-CAA-CBA-CGA
18	B	831	CLA	O2A-C1-C2-C3
25	5	608	CHL	CBA-CGA-O2A-C1
18	A	831	CLA	C13-C15-C16-C17
18	5	612	CLA	CAA-CBA-CGA-O1A
25	2	601	CHL	CAA-CBA-CGA-O2A
18	3	613	CLA	C5-C6-C7-C8
18	B	841	CLA	CBD-CGD-O2D-CED
18	A	815	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	A	840	CLA	C2B-C3B-CAB-CBB
18	B	808	CLA	C2B-C3B-CAB-CBB
18	B	810	CLA	C2B-C3B-CAB-CBB
18	B	818	CLA	C2B-C3B-CAB-CBB
18	B	821	CLA	C2B-C3B-CAB-CBB
18	B	828	CLA	C2B-C3B-CAB-CBB
18	B	840	CLA	C2B-C3B-CAB-CBB
18	B	841	CLA	C2B-C3B-CAB-CBB
18	F	303	CLA	C2B-C3B-CAB-CBB
18	F	305	CLA	C2B-C3B-CAB-CBB
18	G	203	CLA	C2B-C3B-CAB-CBB
18	J	101	CLA	C2B-C3B-CAB-CBB
18	2	613	CLA	C2B-C3B-CAB-CBB
18	6	606	CLA	C2B-C3B-CAB-CBB
18	6	613	CLA	C2B-C3B-CAB-CBB
18	3	613	CLA	C2B-C3B-CAB-CBB
18	5	601	CLA	C2B-C3B-CAB-CBB
18	5	603	CLA	C2B-C3B-CAB-CBB
25	2	601	CHL	CAA-CBA-CGA-O1A
18	B	806	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	A	852	BCR	C11-C10-C9-C8
18	A	833	CLA	CAA-CBA-CGA-O2A
18	B	835	CLA	CAA-CBA-CGA-O1A
25	2	616	CHL	CAA-CBA-CGA-O2A
24	J	104	LMG	O1-C7-C8-O7
18	A	801	CLA	C5-C6-C7-C8
21	A	856	BCR	C19-C20-C21-C22
26	6	617	LUT	C9-C10-C11-C12
27	6	619	XAT	C29-C30-C31-C32
18	2	603	CLA	CAA-CBA-CGA-O1A
18	A	834	CLA	C10-C11-C12-C13
18	G	204	CLA	CAA-CBA-CGA-O2A
18	B	841	CLA	O1D-CGD-O2D-CED
18	A	804	CLA	C2-C1-O2A-CGA
18	A	825	CLA	C2-C1-O2A-CGA
18	6	603	CLA	C2-C1-O2A-CGA
21	B	843	BCR	C18-C19-C20-C21
26	5	619	LUT	C10-C11-C12-C13
18	A	840	CLA	CAA-CBA-CGA-O2A
18	5	609	CLA	CAA-CBA-CGA-O1A
18	5	612	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	C11-C12-C13-C14
25	5	608	CHL	O1A-CGA-O2A-C1
20	A	846	LHG	C17-C18-C19-C20
18	K	203	CLA	CAA-CBA-CGA-O2A
18	A	801	CLA	CAA-CBA-CGA-O2A
23	B	850	DGD	C8A-C9A-CAA-CBA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	B	827	CLA	C2A-CAA-CBA-CGA
21	A	849	BCR	C23-C24-C25-C30
21	A	850	BCR	C23-C24-C25-C30
21	F	302	BCR	C1-C6-C7-C8
21	I	101	BCR	C1-C6-C7-C8
21	J	102	BCR	C23-C24-C25-C30
21	3	620	BCR	C1-C6-C7-C8
21	3	622	BCR	C1-C6-C7-C8
21	3	622	BCR	C5-C6-C7-C8
18	A	842	CLA	CAA-CBA-CGA-O2A
18	2	603	CLA	CAA-CBA-CGA-O2A
18	B	813	CLA	C8-C10-C11-C12
18	L	304	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	B	835	CLA	CAA-CBA-CGA-O2A
18	K	206	CLA	CAA-CBA-CGA-O2A
18	6	612	CLA	CAA-CBA-CGA-O2A
18	5	603	CLA	CAA-CBA-CGA-O2A
18	K	206	CLA	CAA-CBA-CGA-O1A
18	A	828	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C3-C5-C6-C7
18	A	801	CLA	C4B-C3B-CAB-CBB
18	A	815	CLA	C4B-C3B-CAB-CBB
18	B	802	CLA	C4B-C3B-CAB-CBB
18	A	801	CLA	C6-C7-C8-C10
18	A	803	CLA	C12-C13-C15-C16
18	A	823	CLA	CAA-CBA-CGA-O2A
20	A	847	LHG	O1-C1-C2-O2
20	2	622	LHG	O1-C1-C2-O2
21	2	621	BCR	C19-C20-C21-C22
24	2	618	LMG	C4-C5-C6-O5
23	B	850	DGD	CEB-CFB-CGB-CHB
18	B	813	CLA	CAA-CBA-CGA-O2A
18	A	810	CLA	CAA-CBA-CGA-O1A
18	G	204	CLA	CAA-CBA-CGA-O1A
18	2	613	CLA	CAA-CBA-CGA-O2A
18	6	612	CLA	CAA-CBA-CGA-O1A
18	5	602	CLA	CAA-CBA-CGA-O2A
21	B	845	BCR	C11-C10-C9-C34
21	L	301	BCR	C11-C10-C9-C34
20	5	622	LHG	O7-C7-C8-C9
18	A	818	CLA	C11-C10-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	C3A-C2A-CAA-CBA
20	A	847	LHG	O10-C23-O8-C6
18	A	823	CLA	CAA-CBA-CGA-O1A
18	A	820	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	833	CLA	CAD-CBD-CGD-O2D
18	B	811	CLA	CAD-CBD-CGD-O2D
18	B	812	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	2	602	CLA	CAD-CBD-CGD-O2D
18	2	603	CLA	CAD-CBD-CGD-O2D
18	3	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	3	610	CLA	CAD-CBD-CGD-O2D
18	5	611	CLA	CAD-CBD-CGD-O2D
18	F	303	CLA	CAA-CBA-CGA-O2A
18	6	602	CLA	CAA-CBA-CGA-O2A
18	6	608	CLA	CAA-CBA-CGA-O2A
18	2	609	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O1A
20	A	846	LHG	O8-C23-C24-C25
21	J	103	BCR	C7-C8-C9-C10
27	5	620	XAT	O24-C26-C27-C28
25	5	608	CHL	CAA-CBA-CGA-O2A
18	6	608	CLA	CAA-CBA-CGA-O1A
20	A	846	LHG	C16-C17-C18-C19
18	A	806	CLA	O2A-C1-C2-C3
18	A	801	CLA	C16-C17-C18-C20
20	2	622	LHG	O9-C7-O7-C5
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	CHA-CBD-CGD-O1D
18	B	808	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	CHA-CBD-CGD-O1D
18	B	841	CLA	CHA-CBD-CGD-O1D
18	F	305	CLA	CHA-CBD-CGD-O1D
18	F	305	CLA	CHA-CBD-CGD-O2D
18	G	203	CLA	CHA-CBD-CGD-O1D
18	G	203	CLA	CHA-CBD-CGD-O2D
18	K	201	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	L	302	CLA	CHA-CBD-CGD-O1D
18	6	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	6	603	CLA	CHA-CBD-CGD-O1D
18	5	613	CLA	CHA-CBD-CGD-O1D
18	5	613	CLA	CHA-CBD-CGD-O2D
18	5	614	CLA	CHA-CBD-CGD-O2D
25	2	601	CHL	CHA-CBD-CGD-O1D
25	2	601	CHL	CHA-CBD-CGD-O2D
26	5	619	LUT	C29-C30-C31-C32
18	A	821	CLA	CAA-CBA-CGA-O2A
18	F	303	CLA	CAA-CBA-CGA-O1A
18	A	814	CLA	CAA-CBA-CGA-O2A
18	B	806	CLA	CAA-CBA-CGA-O2A
23	B	850	DGD	O2G-C2G-C3G-O3G
18	F	305	CLA	CAA-CBA-CGA-O1A
18	A	845	CLA	CAA-CBA-CGA-O2A
18	6	604	CLA	O1D-CGD-O2D-CED
20	2	622	LHG	C28-C29-C30-C31
18	A	839	CLA	C5-C6-C7-C8
18	B	806	CLA	CBA-CGA-O2A-C1
18	6	604	CLA	CBD-CGD-O2D-CED
20	A	847	LHG	C10-C11-C12-C13
18	B	806	CLA	C2-C3-C5-C6
18	B	828	CLA	C11-C10-C8-C9
18	K	204	CLA	C4C-C3C-CAC-CBC
18	2	613	CLA	CAA-CBA-CGA-O1A
18	5	602	CLA	CAA-CBA-CGA-O1A
18	B	813	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	O1A-CGA-O2A-C1
20	6	620	LHG	C8-C7-O7-C5
18	5	610	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	CAA-CBA-CGA-O1A
18	B	837	CLA	CBA-CGA-O2A-C1
18	G	201	CLA	CAA-CBA-CGA-O1A
18	6	602	CLA	CAA-CBA-CGA-O1A
25	2	606	CHL	CAA-CBA-CGA-O2A
18	2	609	CLA	CBA-CGA-O2A-C1
18	A	807	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	C1A-C2A-CAA-CBA
18	A	854	CLA	C1A-C2A-CAA-CBA
18	B	814	CLA	CHA-CBD-CGD-O2D
18	B	838	CLA	C1A-C2A-CAA-CBA
18	B	841	CLA	C1A-C2A-CAA-CBA
18	K	201	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	3	611	CLA	CHA-CBD-CGD-O2D
18	5	603	CLA	CHA-CBD-CGD-O2D
25	2	601	CHL	C1A-C2A-CAA-CBA
25	6	607	CHL	CHA-CBD-CGD-O2D
18	3	602	CLA	C11-C12-C13-C15
18	A	854	CLA	C13-C15-C16-C17
18	B	840	CLA	C2-C1-O2A-CGA
18	A	812	CLA	C5-C6-C7-C8
20	A	846	LHG	O10-C23-C24-C25
18	A	802	CLA	CAA-CBA-CGA-O2A
18	A	820	CLA	C2A-CAA-CBA-CGA
18	B	825	CLA	C16-C17-C18-C19
25	5	608	CHL	CAA-CBA-CGA-O1A
18	A	843	CLA	C10-C11-C12-C13
18	B	826	CLA	C13-C15-C16-C17
18	A	831	CLA	C2-C3-C5-C6
21	F	302	BCR	C6-C7-C8-C9
21	I	101	BCR	C6-C7-C8-C9
18	2	609	CLA	O1A-CGA-O2A-C1
18	B	834	CLA	C4B-C3B-CAB-CBB
18	3	612	CLA	C4B-C3B-CAB-CBB
20	A	846	LHG	C3-O3-P-O5
23	B	850	DGD	CEA-CFA-CGA-CHA
18	2	609	CLA	CAA-CBA-CGA-O1A
18	A	813	CLA	CAA-CBA-CGA-O2A
21	J	102	BCR	C16-C17-C18-C36
21	A	849	BCR	C23-C24-C25-C26
21	F	302	BCR	C5-C6-C7-C8
21	I	101	BCR	C5-C6-C7-C8
18	B	828	CLA	C5-C6-C7-C8
18	A	806	CLA	CAA-CBA-CGA-O2A
18	F	305	CLA	CAA-CBA-CGA-O2A
18	A	814	CLA	CAA-CBA-CGA-O1A
18	5	601	CLA	CAA-CBA-CGA-O2A
24	J	104	LMG	C10-C11-C12-C13
18	A	831	CLA	CAD-CBD-CGD-O1D
18	B	803	CLA	CAD-CBD-CGD-O1D
18	B	835	CLA	CAD-CBD-CGD-O1D
18	B	838	CLA	CAD-CBD-CGD-O1D
18	B	841	CLA	CAD-CBD-CGD-O1D
18	2	602	CLA	CAD-CBD-CGD-O1D
18	2	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	6	602	CLA	CAD-CBD-CGD-O1D
18	6	603	CLA	CAD-CBD-CGD-O1D
18	6	604	CLA	CAD-CBD-CGD-O1D
18	B	806	CLA	CAA-CBA-CGA-O1A
18	6	603	CLA	CAA-CBA-CGA-O2A
19	B	842	PQN	C19-C18-C20-C21
18	A	833	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CAA-CBA-CGA-O2A
18	B	816	CLA	CAA-CBA-CGA-O2A
18	G	201	CLA	CAA-CBA-CGA-O2A
25	2	606	CHL	CAA-CBA-CGA-O1A
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	C10-C11-C12-C13
18	5	601	CLA	CAA-CBA-CGA-O1A
18	A	845	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	C4-C3-C5-C6
18	A	807	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	C11-C12-C13-C15
18	B	828	CLA	C11-C10-C8-C7
18	G	204	CLA	CAD-CBD-CGD-O2D
18	6	614	CLA	CHA-CBD-CGD-O1D
18	3	614	CLA	CHA-CBD-CGD-O1D
18	3	617	CLA	CAD-CBD-CGD-O2D
18	5	603	CLA	CHA-CBD-CGD-O1D
25	6	607	CHL	CAD-CBD-CGD-O2D
25	3	608	CHL	CHA-CBD-CGD-O1D
18	A	824	CLA	CAA-CBA-CGA-O1A
23	B	850	DGD	O1B-C1B-C2B-C3B
18	3	602	CLA	CAA-CBA-CGA-O2A
20	A	847	LHG	O8-C23-C24-C25
21	J	102	BCR	C11-C12-C13-C14
18	A	802	CLA	CAA-CBA-CGA-O1A
18	B	816	CLA	CAA-CBA-CGA-O1A
18	A	835	CLA	CAA-CBA-CGA-O2A
18	6	603	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

151 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	613	CLA	3	0
18	A	820	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	5	611	CLA	2	0
18	K	201	CLA	1	0
18	5	601	CLA	2	0
18	G	201	CLA	2	0
18	A	801	CLA	1	0
18	A	835	CLA	3	0
20	A	847	LHG	2	0
18	B	819	CLA	2	0
18	3	602	CLA	1	0
25	6	601	CHL	2	0
21	I	101	BCR	2	0
25	5	608	CHL	3	0
18	B	838	CLA	1	0
18	A	837	CLA	2	0
18	B	807	CLA	1	0
18	B	815	CLA	3	0
20	6	620	LHG	1	0
18	B	818	CLA	3	0
18	B	824	CLA	1	0
18	B	837	CLA	1	0
20	B	851	LHG	1	0
18	F	301	CLA	2	0
18	5	610	CLA	2	0
21	K	202	BCR	2	0
21	L	305	BCR	1	0
18	B	809	CLA	3	0
18	A	826	CLA	4	0
18	L	302	CLA	2	0
18	L	304	CLA	1	0
18	A	812	CLA	4	0
18	L	303	CLA	1	0
18	K	203	CLA	1	0
21	B	845	BCR	3	0
21	3	622	BCR	3	0
18	B	826	CLA	3	0
18	A	810	CLA	1	0
18	B	823	CLA	2	0
20	5	622	LHG	5	0
18	A	811	CLA	3	0
24	J	104	LMG	1	0
26	2	619	LUT	3	0
18	B	833	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	829	CLA	6	0
18	3	606	CLA	1	0
22	C	102	SF4	4	0
18	B	816	CLA	2	0
18	B	828	CLA	3	0
18	F	304	CLA	1	0
18	K	204	CLA	1	0
18	B	830	CLA	1	0
18	G	204	CLA	2	0
19	A	844	PQN	1	0
18	A	809	CLA	4	0
18	B	802	CLA	2	0
20	A	846	LHG	1	0
25	5	607	CHL	13	0
26	3	618	LUT	1	0
18	B	811	CLA	1	0
25	2	607	CHL	6	0
18	A	827	CLA	4	0
18	A	814	CLA	6	0
20	2	622	LHG	3	0
18	A	830	CLA	1	0
18	A	841	CLA	2	0
18	6	609	CLA	1	0
21	A	848	BCR	3	0
18	A	854	CLA	6	0
18	A	819	CLA	3	0
18	B	827	CLA	2	0
18	B	812	CLA	1	0
18	A	824	CLA	2	0
26	5	619	LUT	3	0
18	5	613	CLA	3	0
18	B	805	CLA	2	0
18	B	825	CLA	1	0
27	5	620	XAT	30	0
21	K	207	BCR	1	0
18	A	839	CLA	2	0
21	A	849	BCR	2	0
19	B	842	PQN	6	0
26	6	617	LUT	3	0
21	B	801	BCR	2	0
18	A	802	CLA	2	0
18	F	305	CLA	1	0

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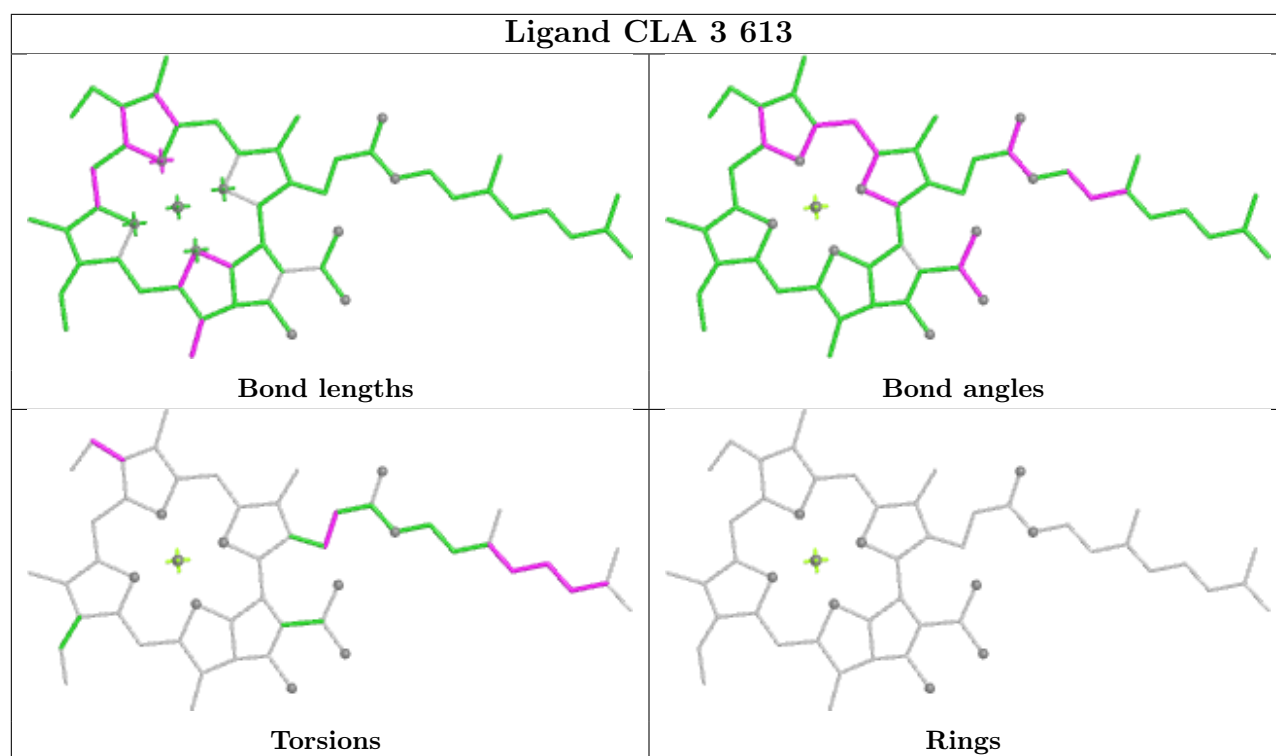
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	835	CLA	1	0
18	B	806	CLA	2	0
21	G	205	BCR	3	0
21	A	856	BCR	4	0
18	2	602	CLA	3	0
18	A	805	CLA	1	0
18	5	612	CLA	1	0
18	A	842	CLA	2	0
18	A	833	CLA	2	0
25	3	608	CHL	1	0
18	B	803	CLA	2	0
18	B	829	CLA	1	0
21	2	621	BCR	4	0
21	3	620	BCR	5	0
18	3	612	CLA	1	0
18	2	604	CLA	2	0
27	3	619	XAT	15	0
18	2	614	CLA	2	0
18	3	611	CLA	2	0
21	F	302	BCR	4	0
25	2	616	CHL	1	0
18	2	610	CLA	3	0
25	6	607	CHL	6	0
21	B	846	BCR	2	0
18	B	831	CLA	3	0
23	B	850	DGD	4	0
21	L	301	BCR	1	0
18	5	602	CLA	5	0
18	B	814	CLA	2	0
21	J	103	BCR	5	0
18	5	614	CLA	2	0
21	B	844	BCR	2	0
21	B	843	BCR	5	0
21	5	621	BCR	2	0
18	A	838	CLA	2	0
18	A	843	CLA	4	0
18	B	840	CLA	3	0
21	A	852	BCR	4	0
21	J	102	BCR	1	0
27	6	619	XAT	13	0
18	B	813	CLA	7	0
18	B	817	CLA	3	0

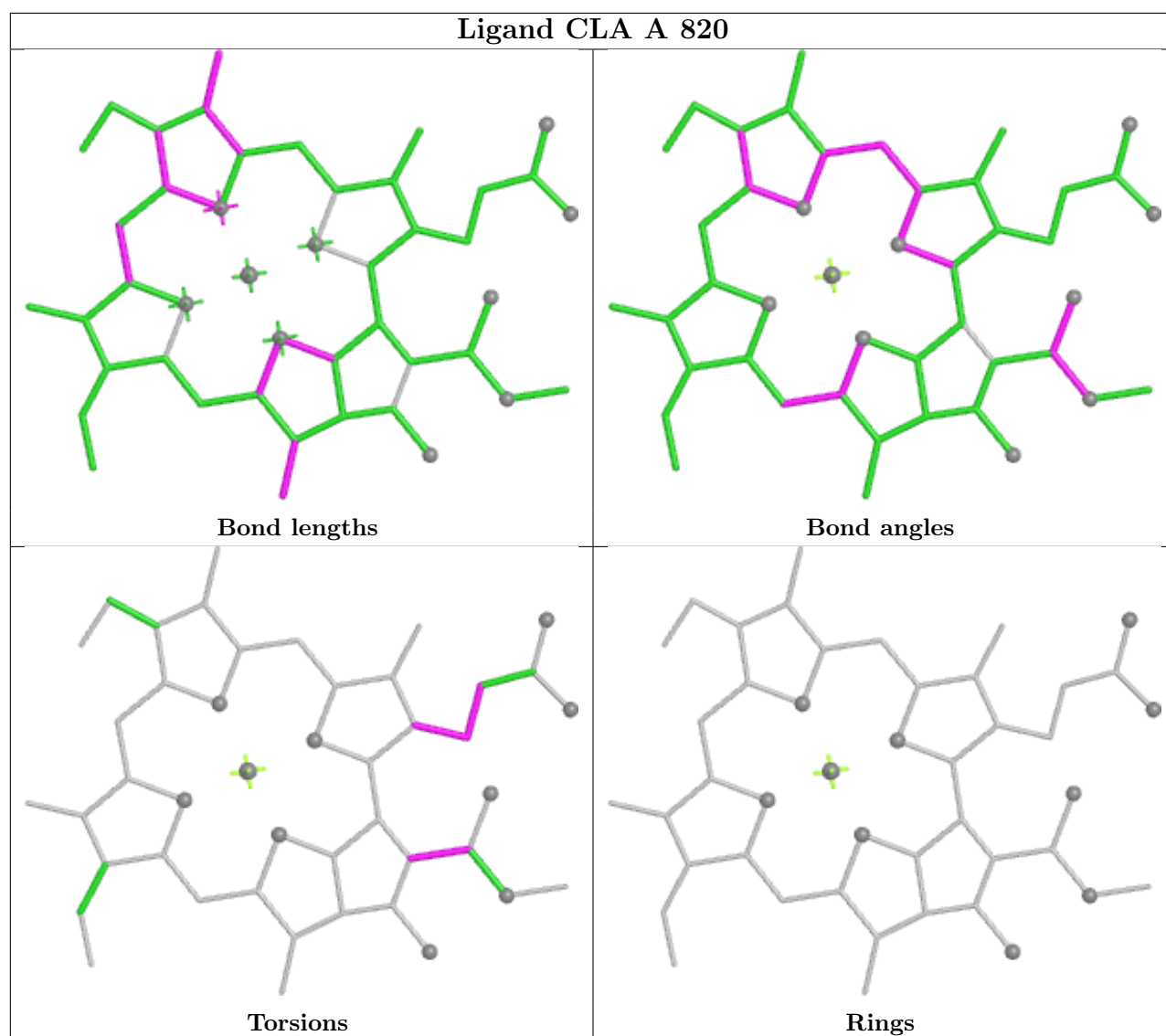
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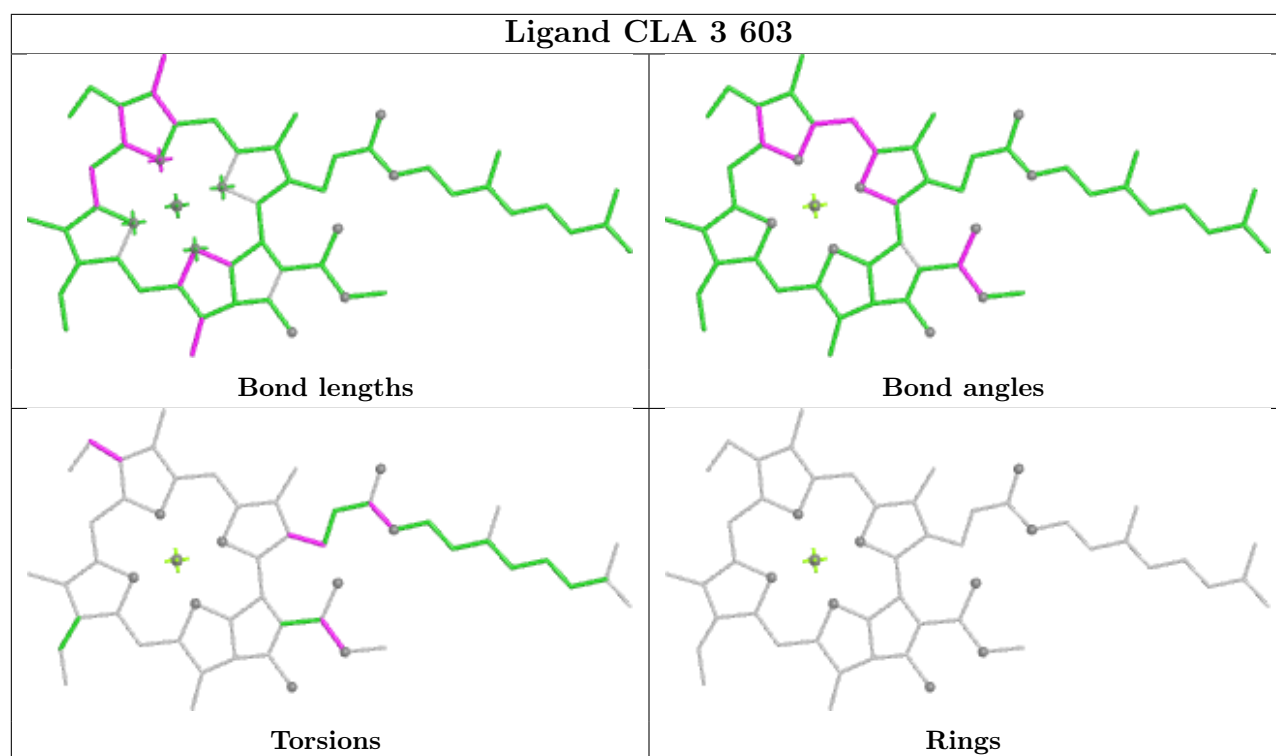
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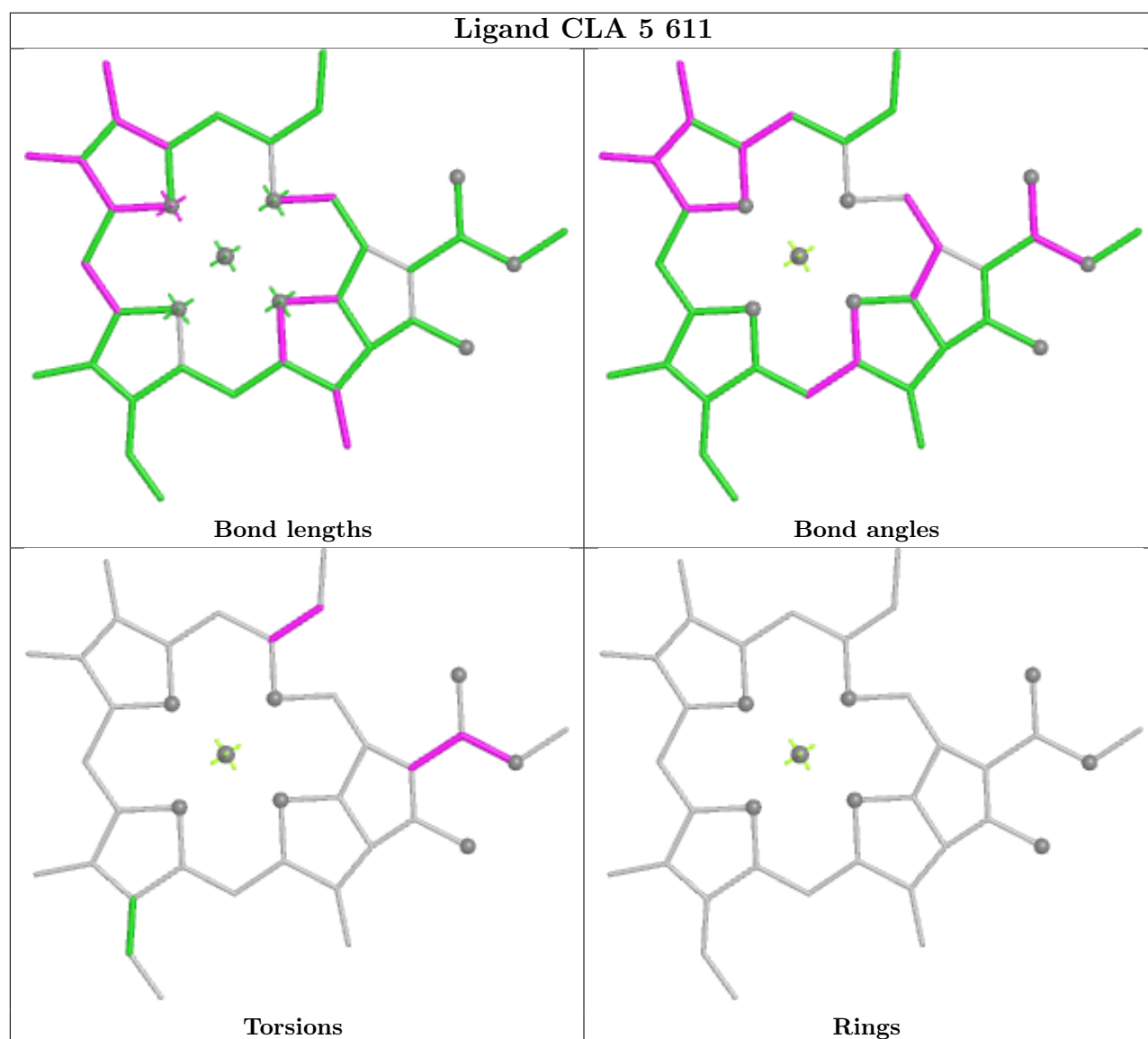
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	850	BCR	1	0
18	B	821	CLA	3	0
21	B	848	BCR	4	0
18	B	808	CLA	1	0
18	A	828	CLA	1	0
18	A	806	CLA	4	0
18	A	813	CLA	1	0
25	2	606	CHL	9	0
18	2	613	CLA	1	0
27	2	620	XAT	25	0
18	B	822	CLA	1	0
18	A	821	CLA	1	0
18	3	609	CLA	3	0
18	A	832	CLA	1	0
18	A	840	CLA	1	0
18	B	839	CLA	2	0
21	B	847	BCR	1	0
18	A	818	CLA	1	0
22	C	101	SF4	7	0
18	A	831	CLA	2	0
21	A	851	BCR	1	0
18	A	845	CLA	1	0
18	A	834	CLA	1	0

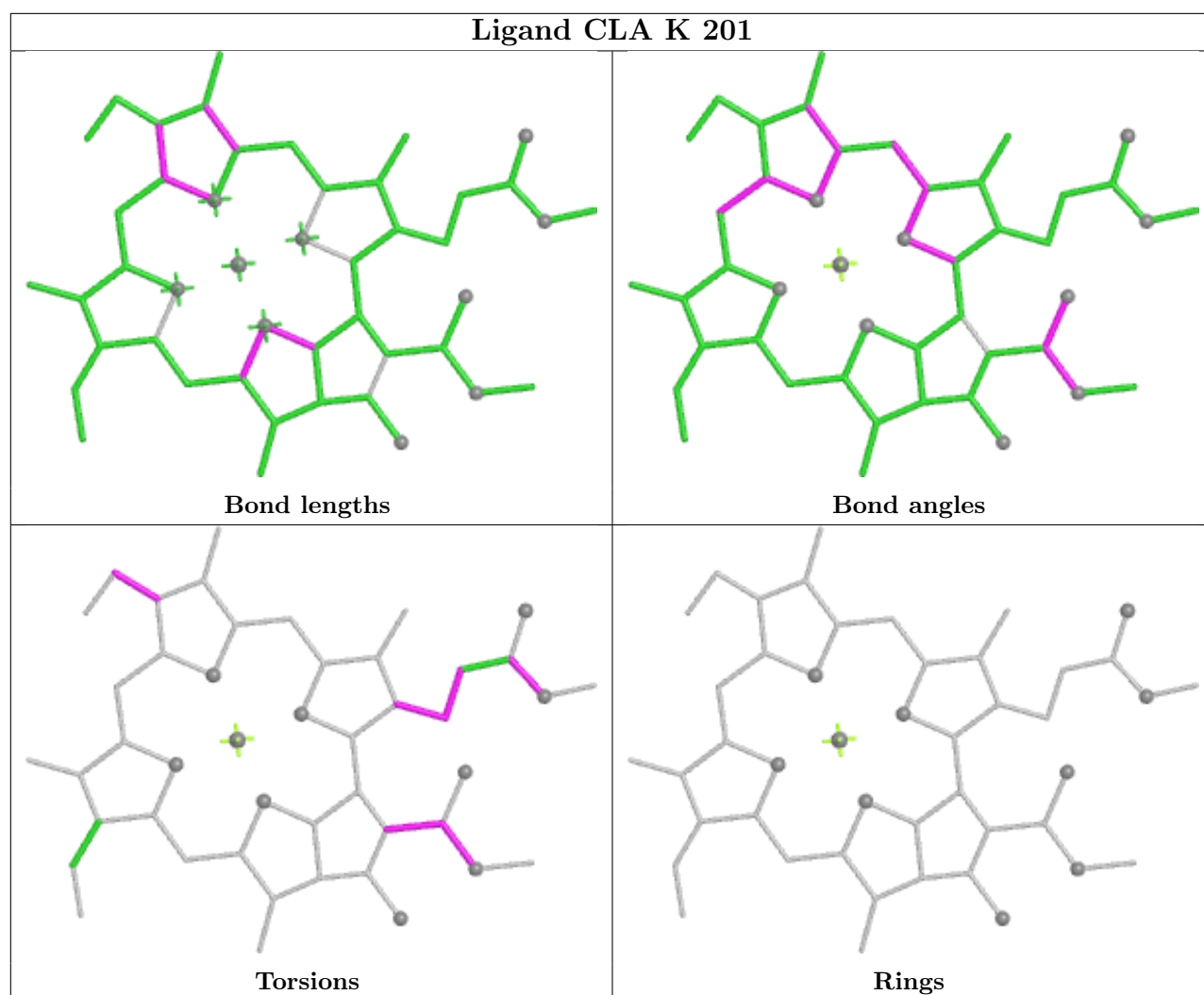
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

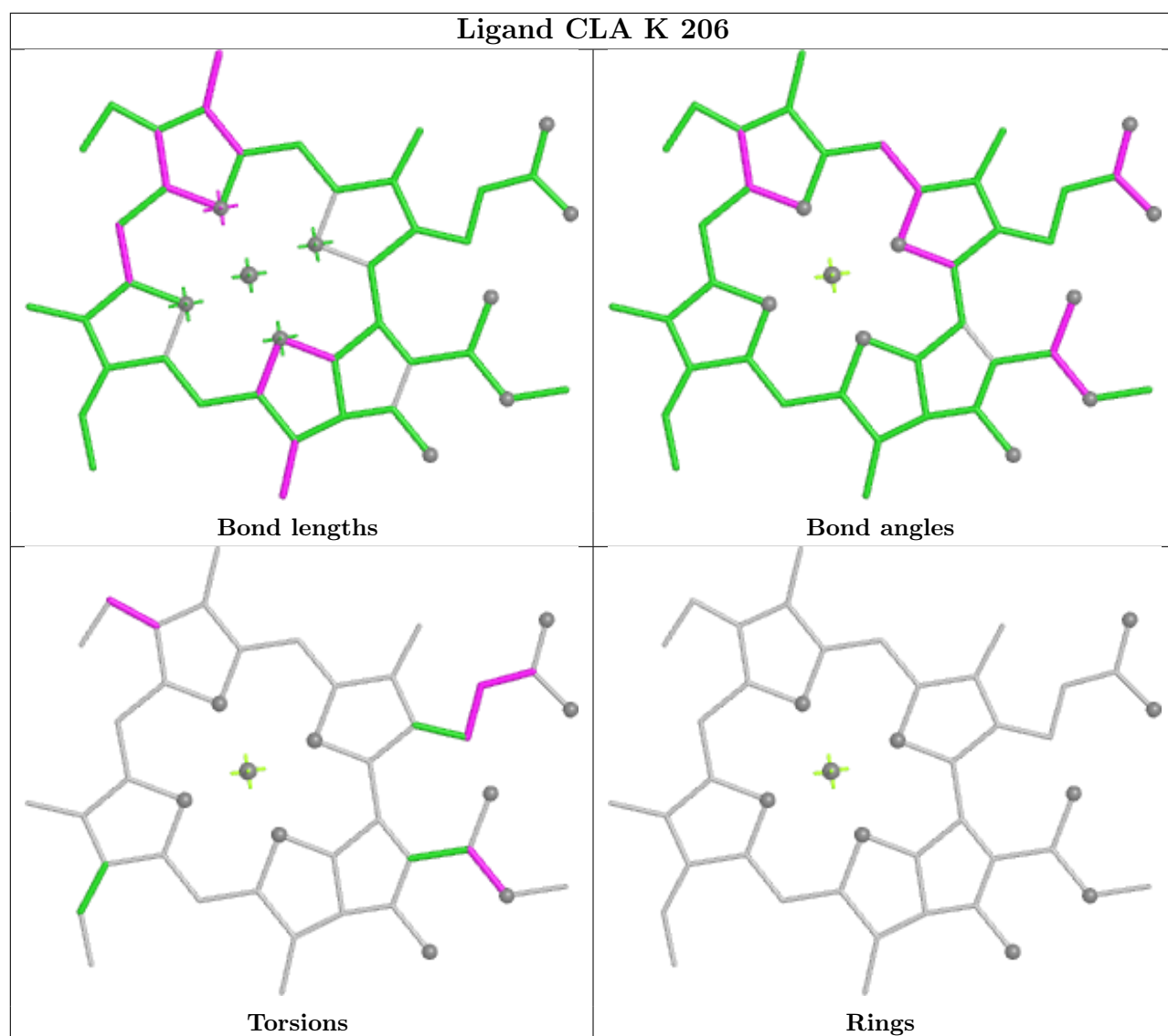




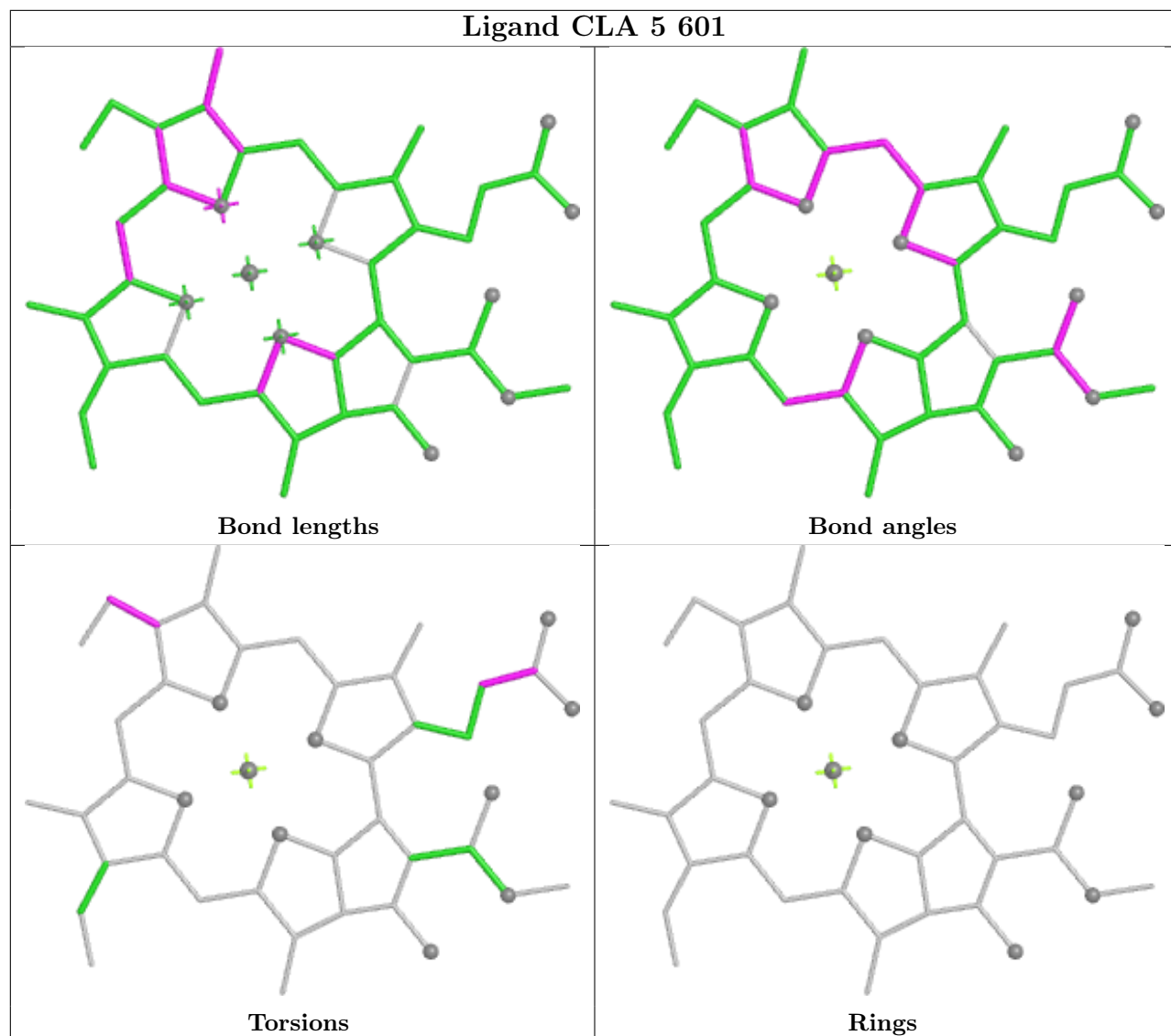


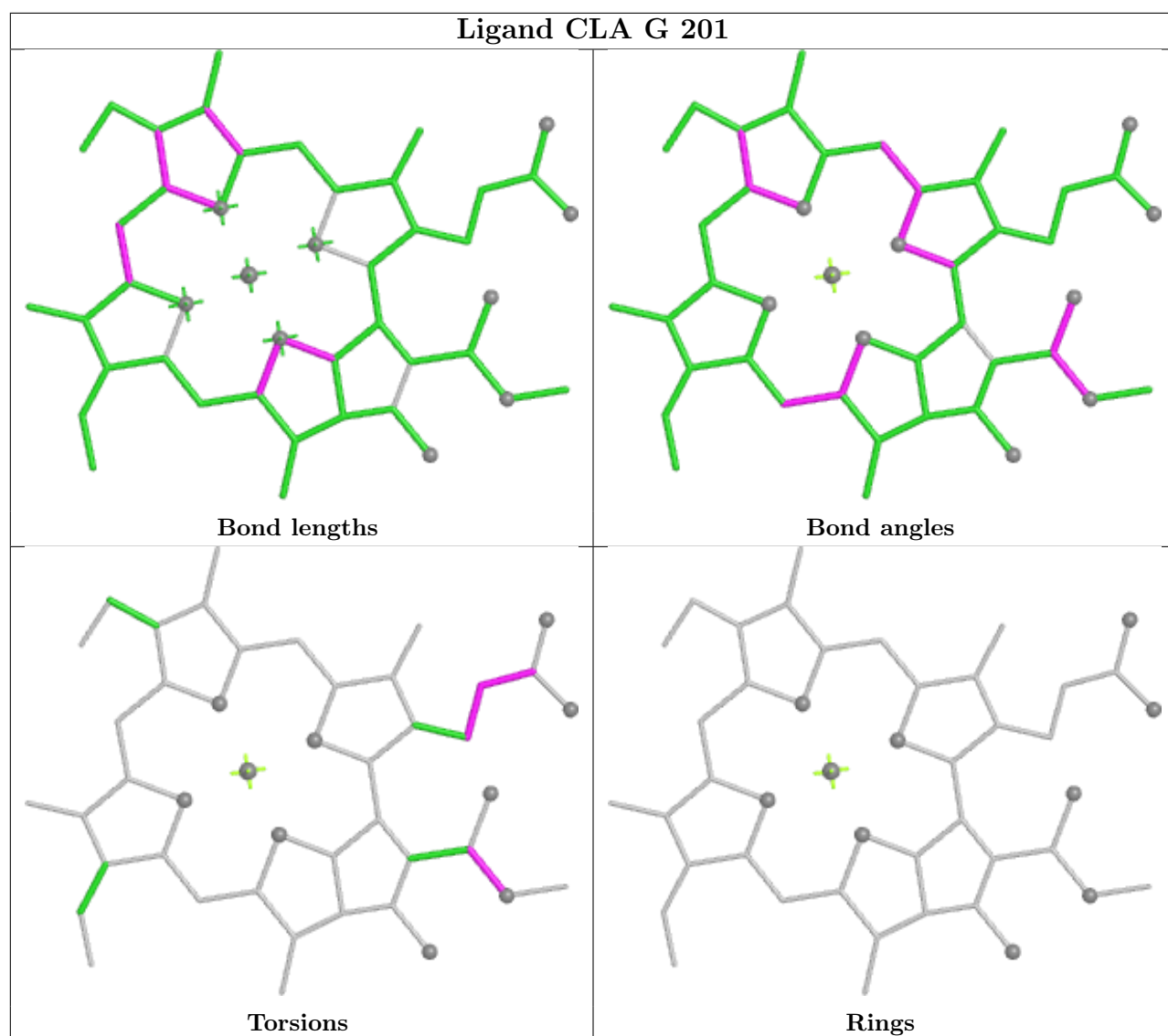


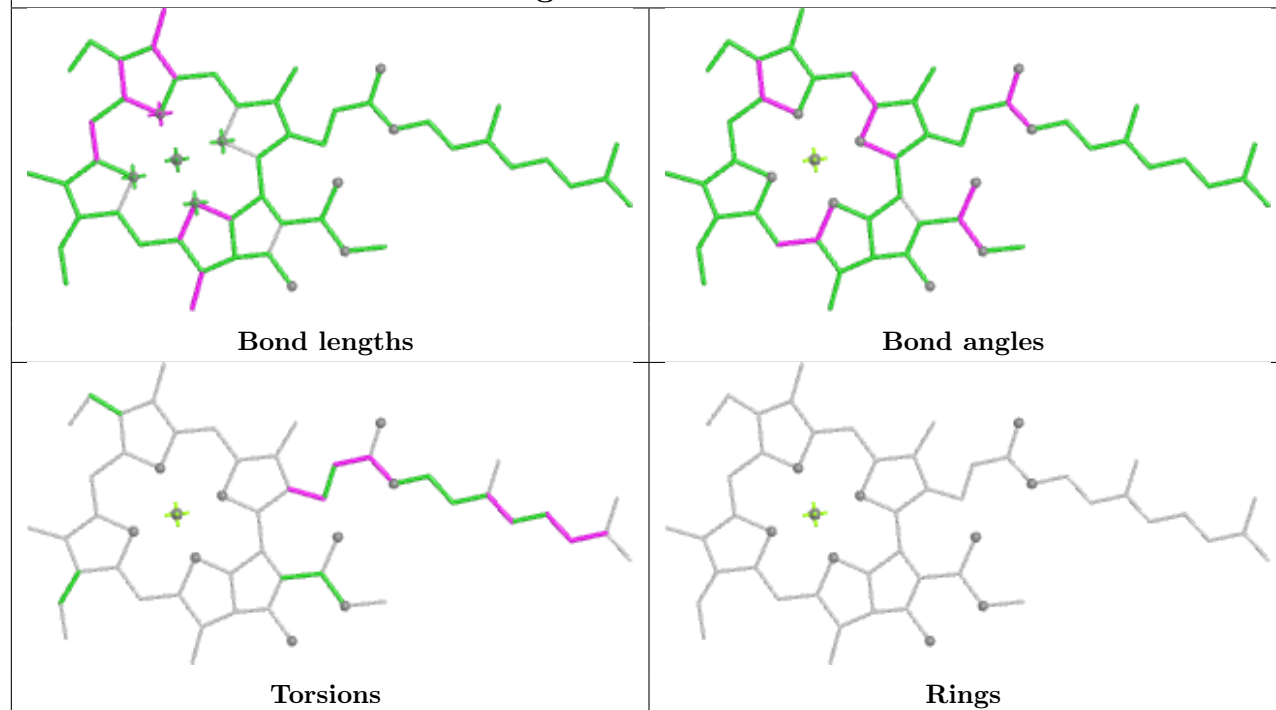
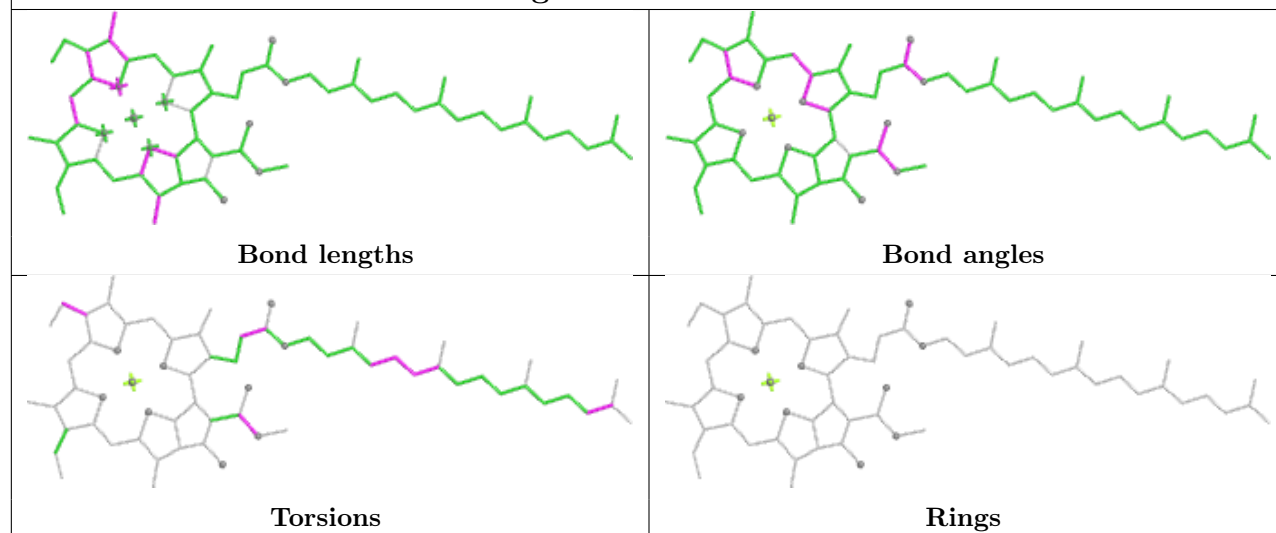




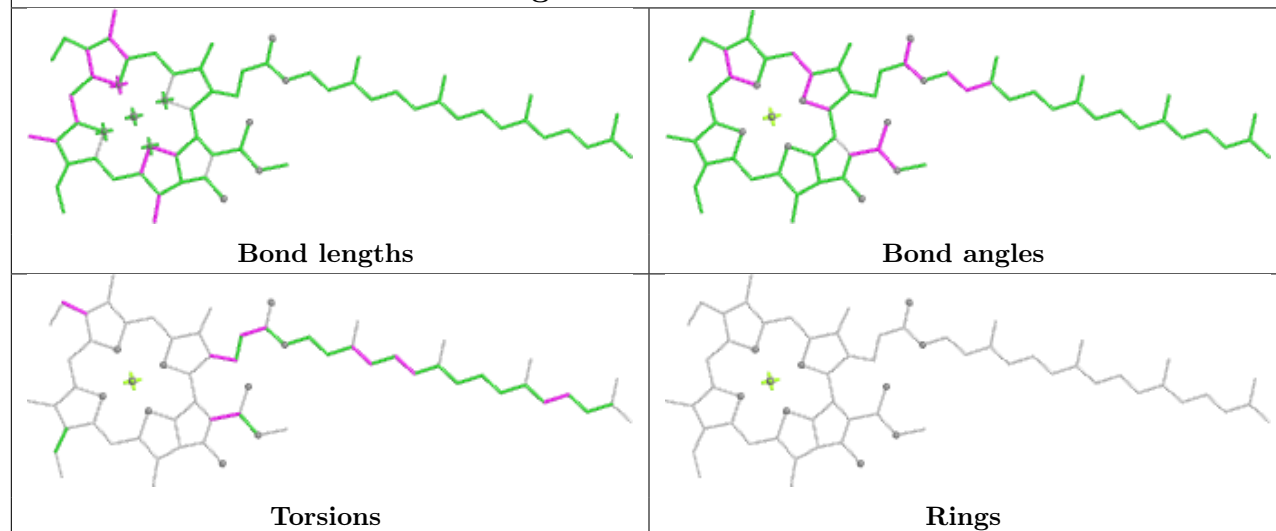
Ligand CLA 5 601



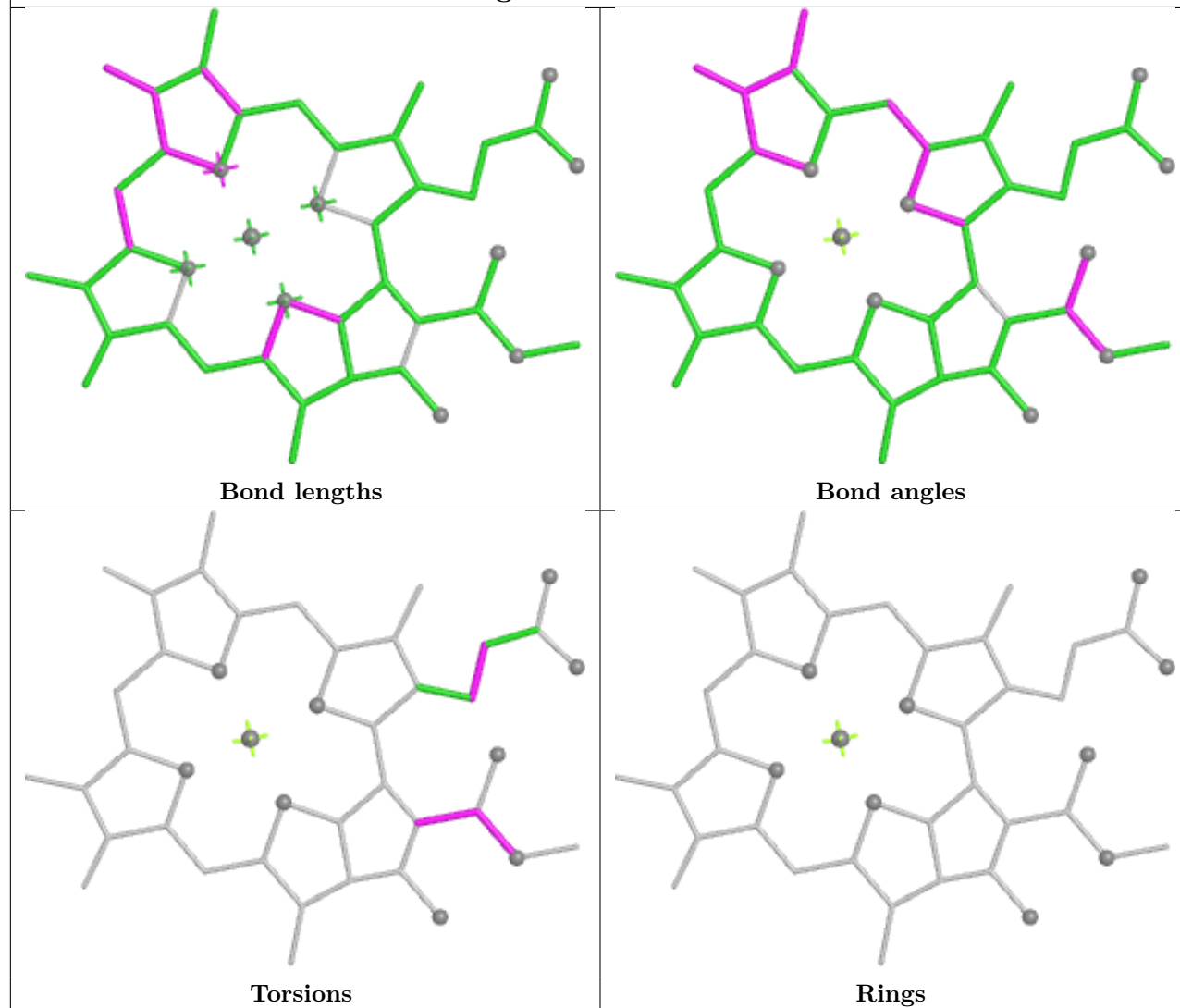


Ligand CLA 2 609**Ligand CLA A 801**

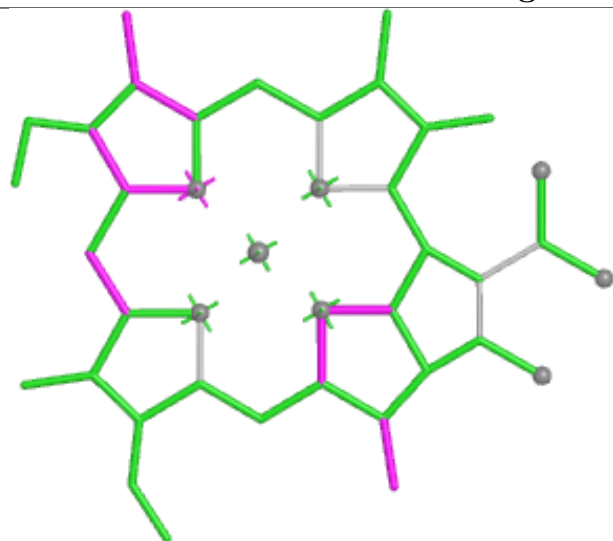
Ligand CLA A 835



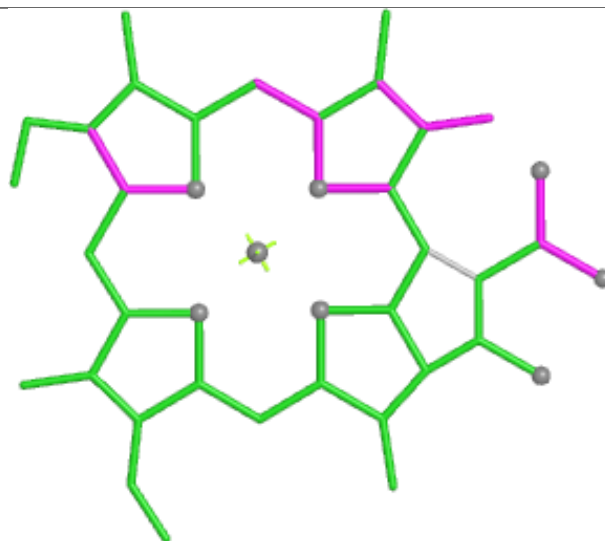
Ligand CLA 6 616



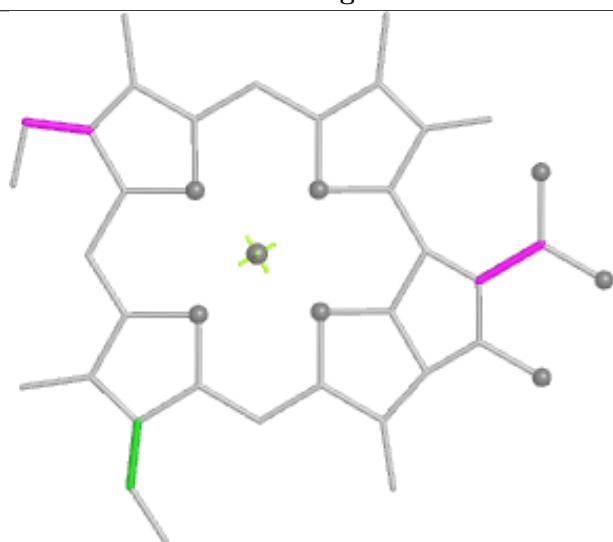
Ligand CLA 3 614



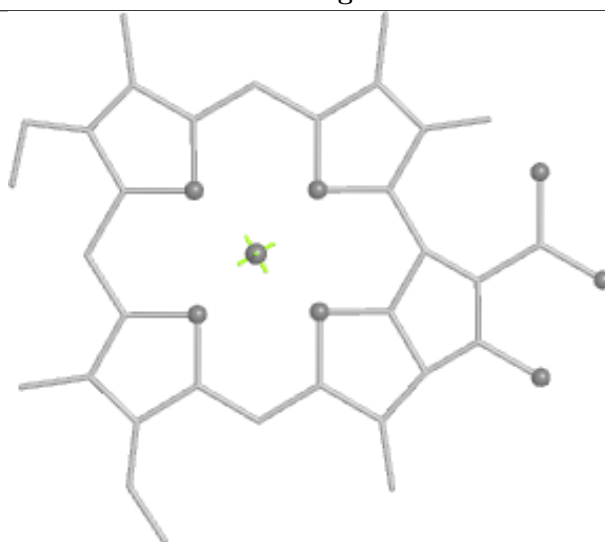
Bond lengths



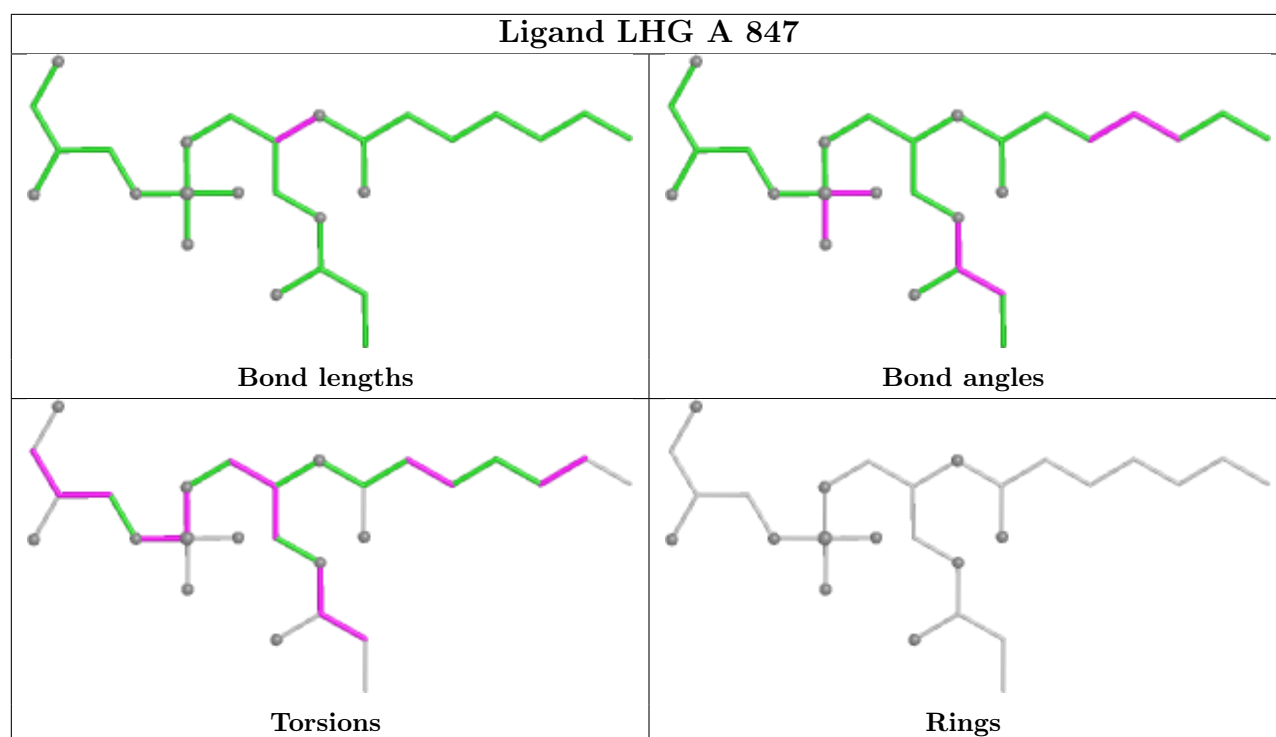
Bond angles



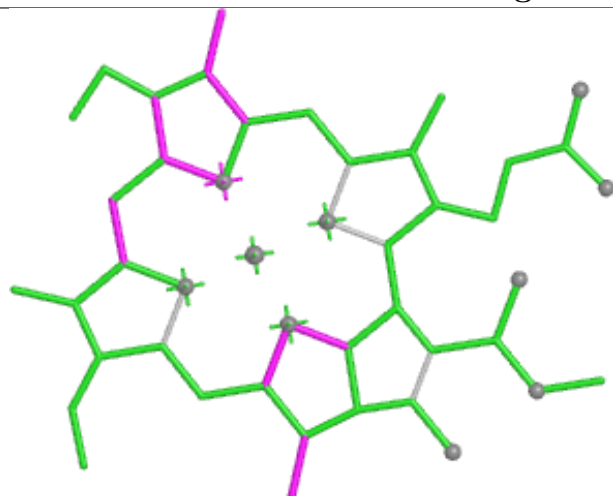
Torsions



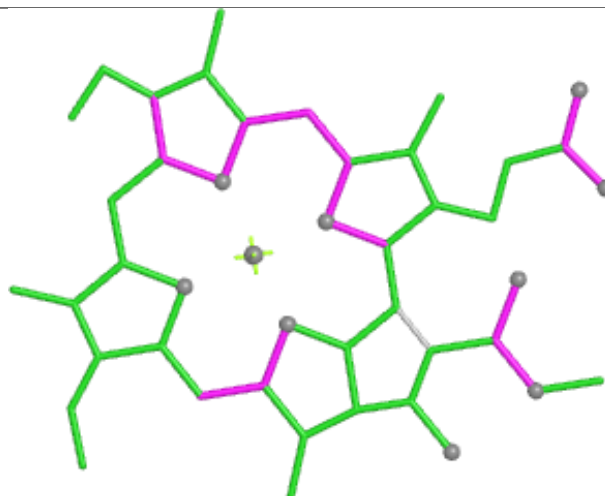
Rings



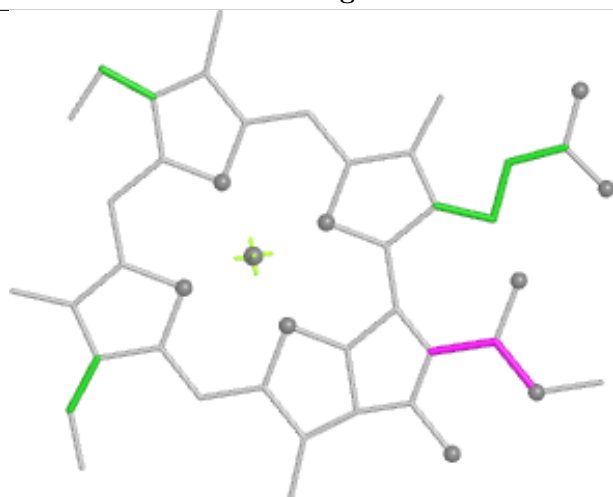
Ligand CLA B 819



Bond lengths



Bond angles

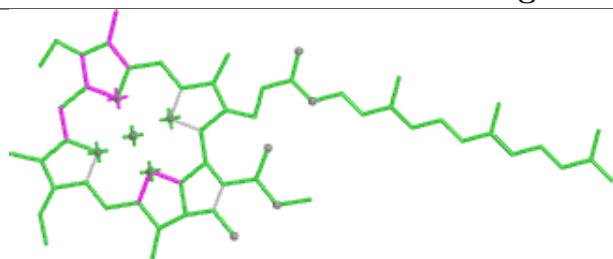


Torsions

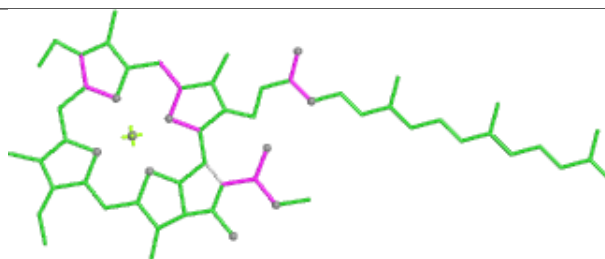


Rings

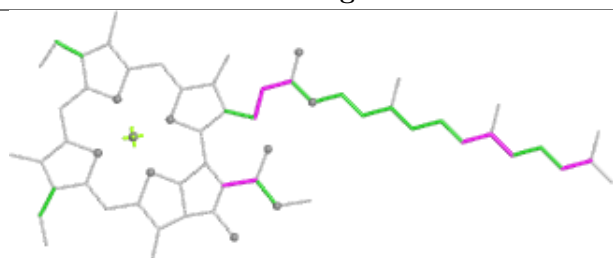
Ligand CLA 3 602



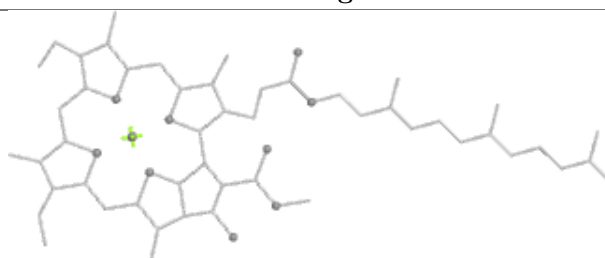
Bond lengths



Bond angles

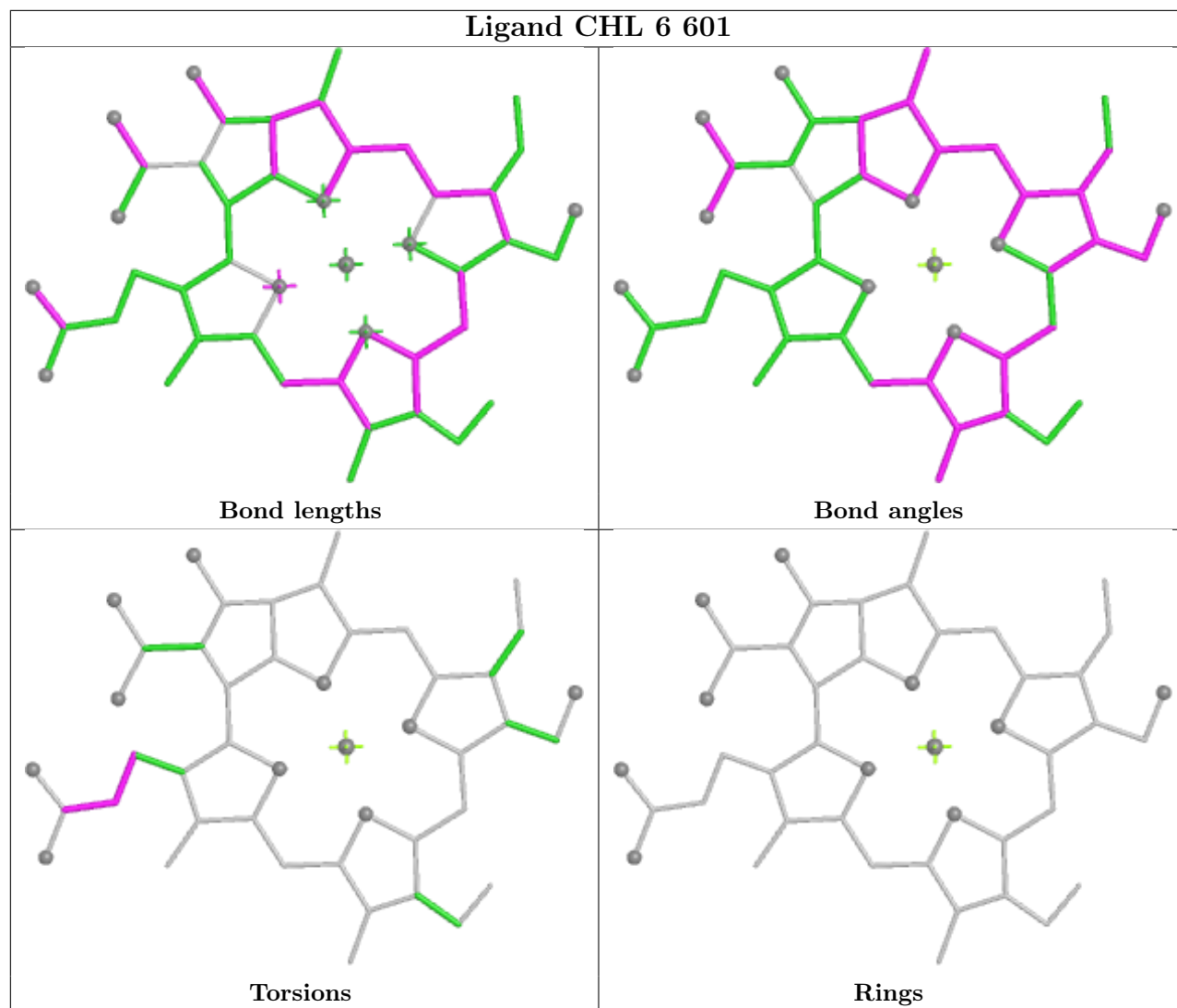


Torsions

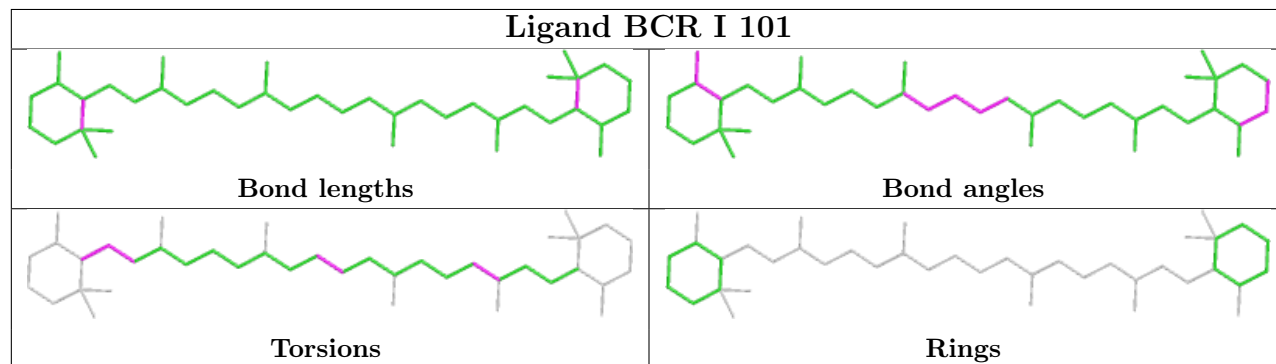


Rings

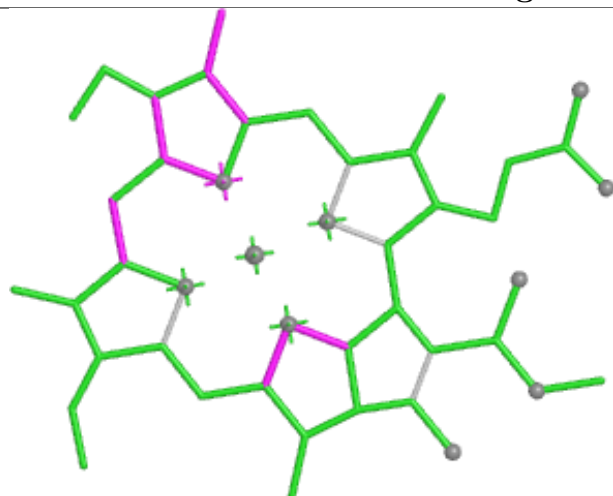
Ligand CHL 6 601



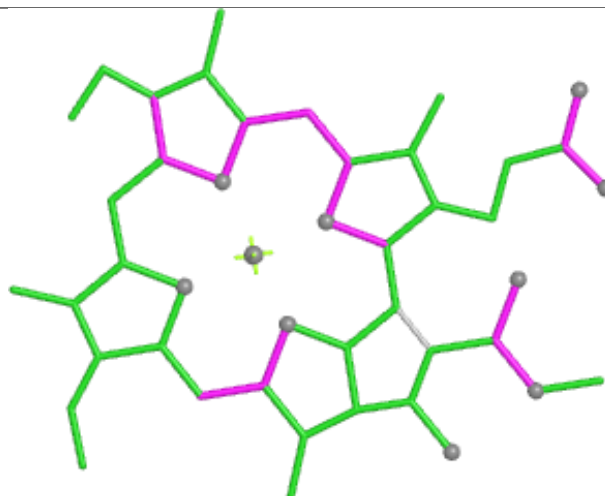
Ligand BCR I 101



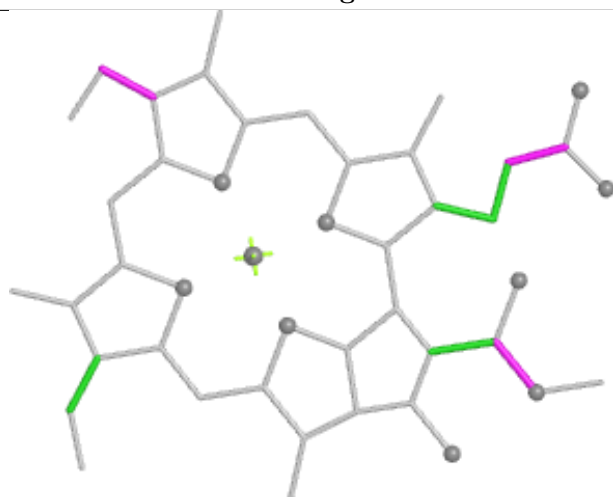
Ligand CLA F 303



Bond lengths



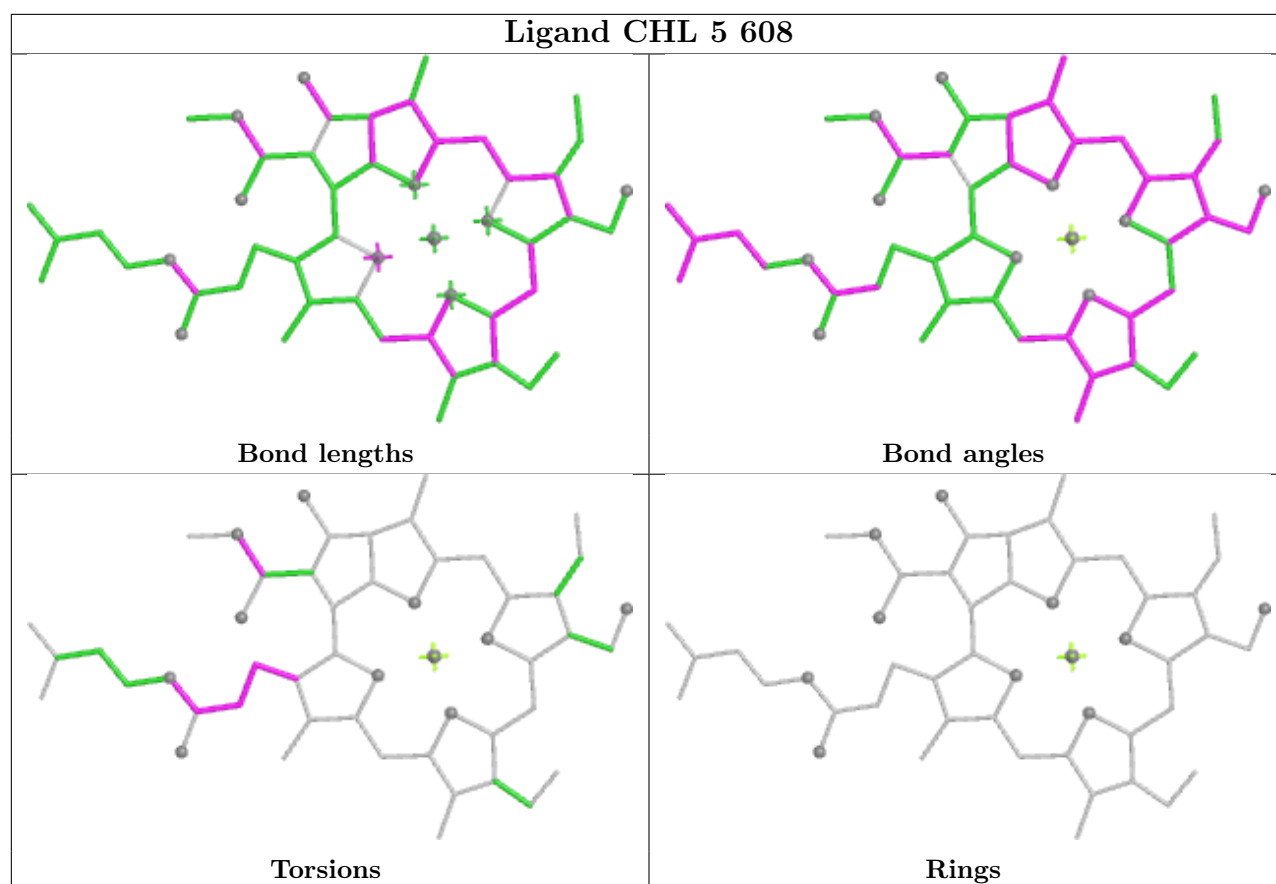
Bond angles



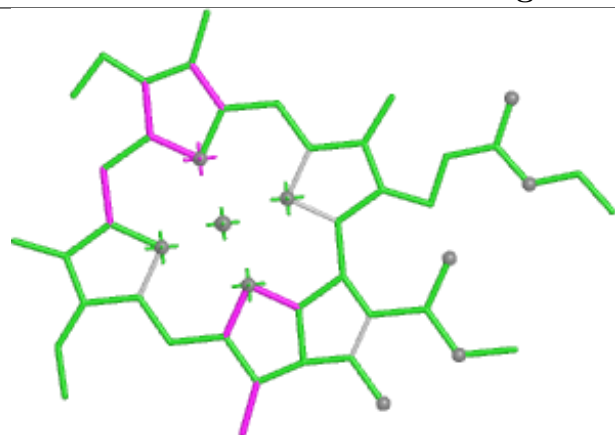
Torsions



Rings



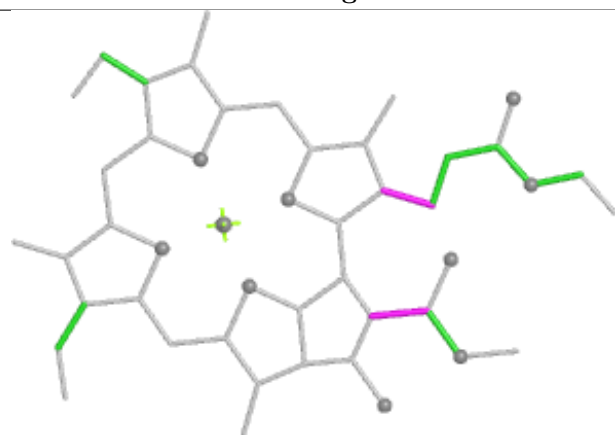
Ligand CLA B 838



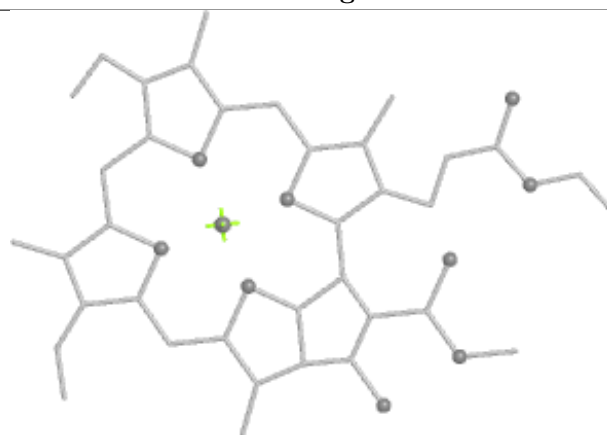
Bond lengths



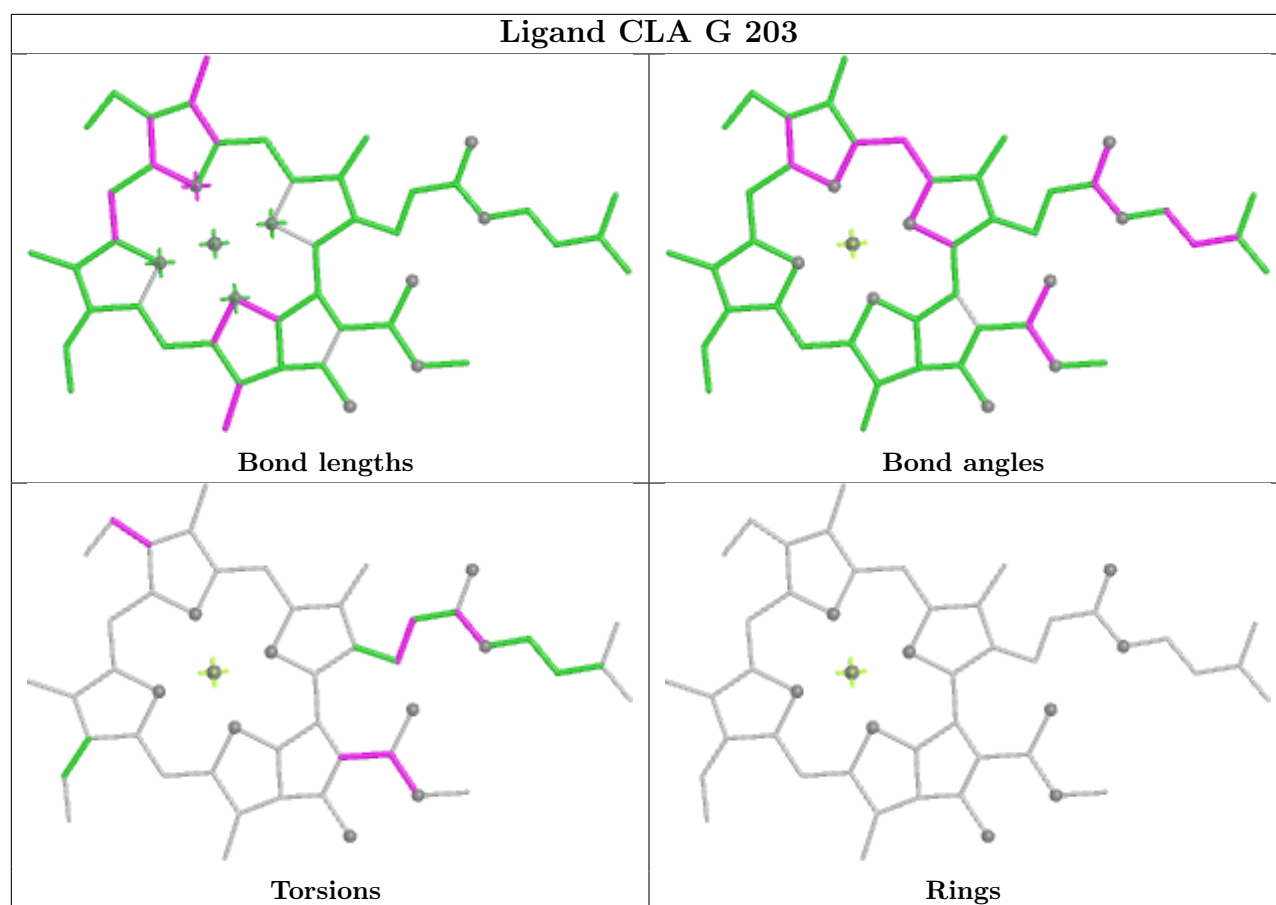
Bond angles



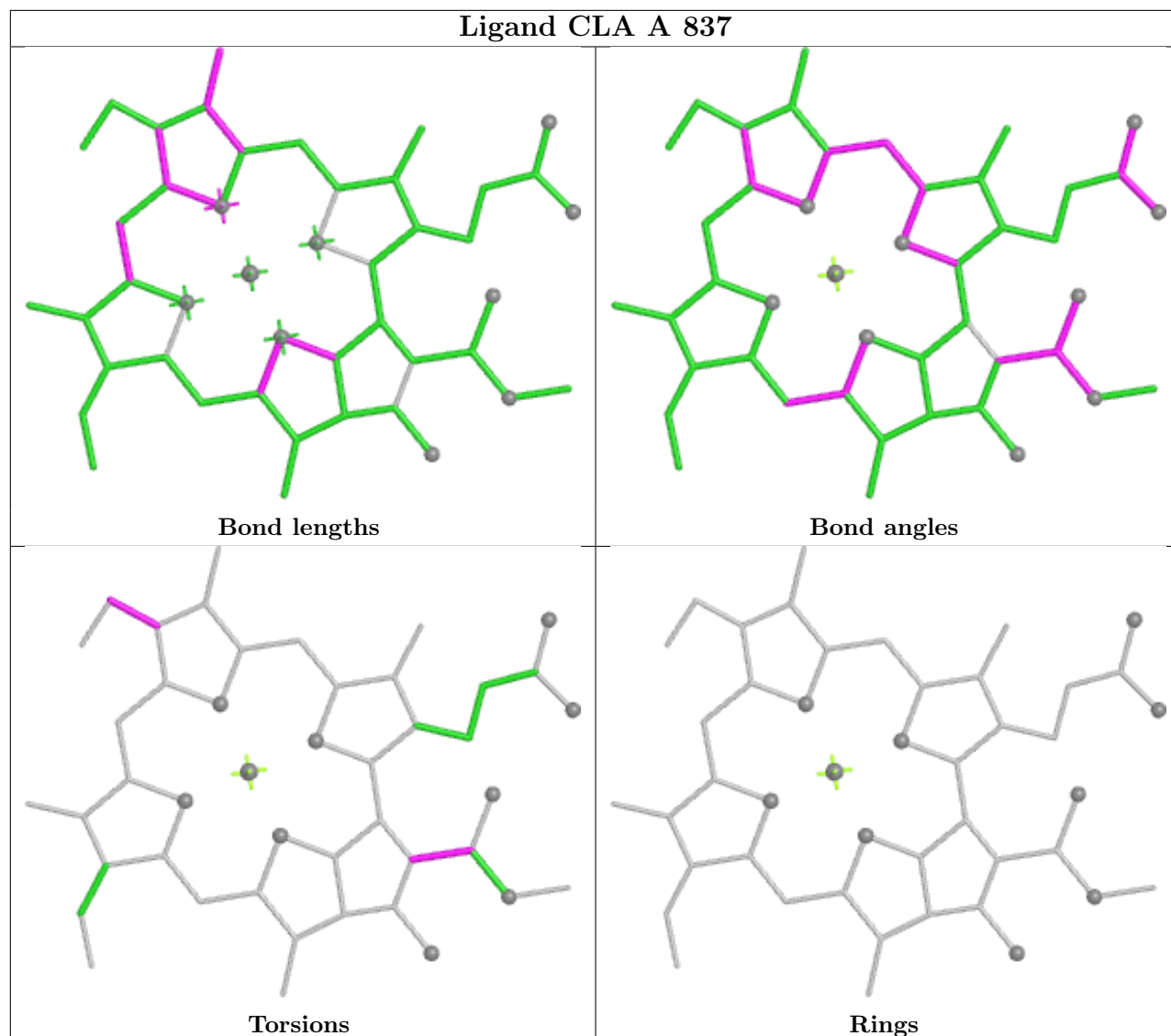
Torsions



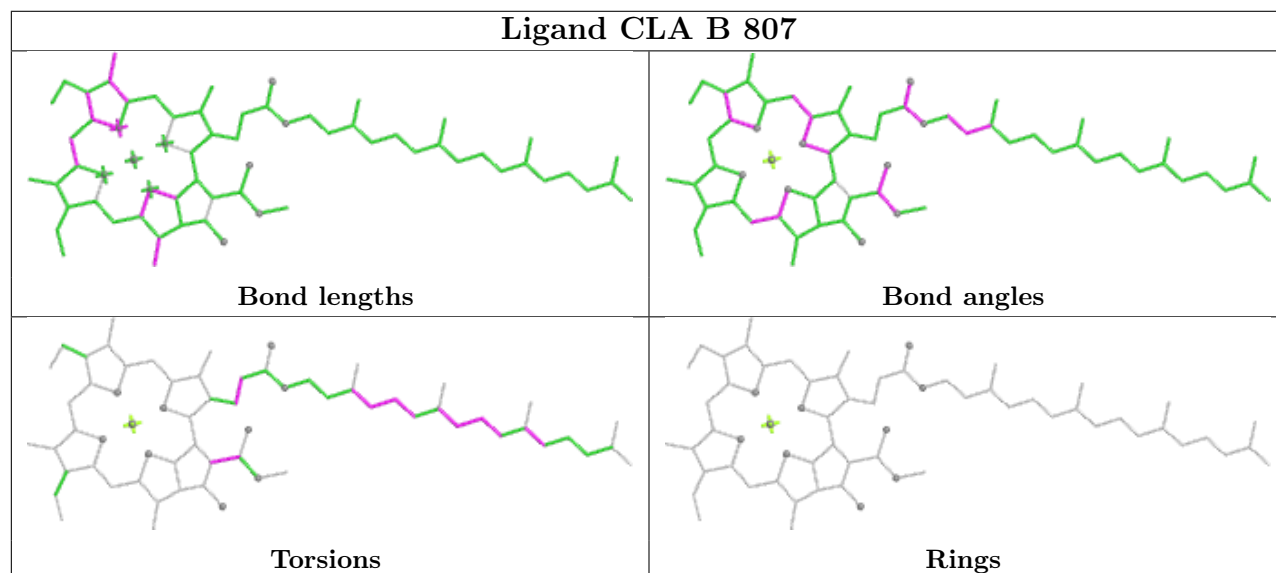
Rings



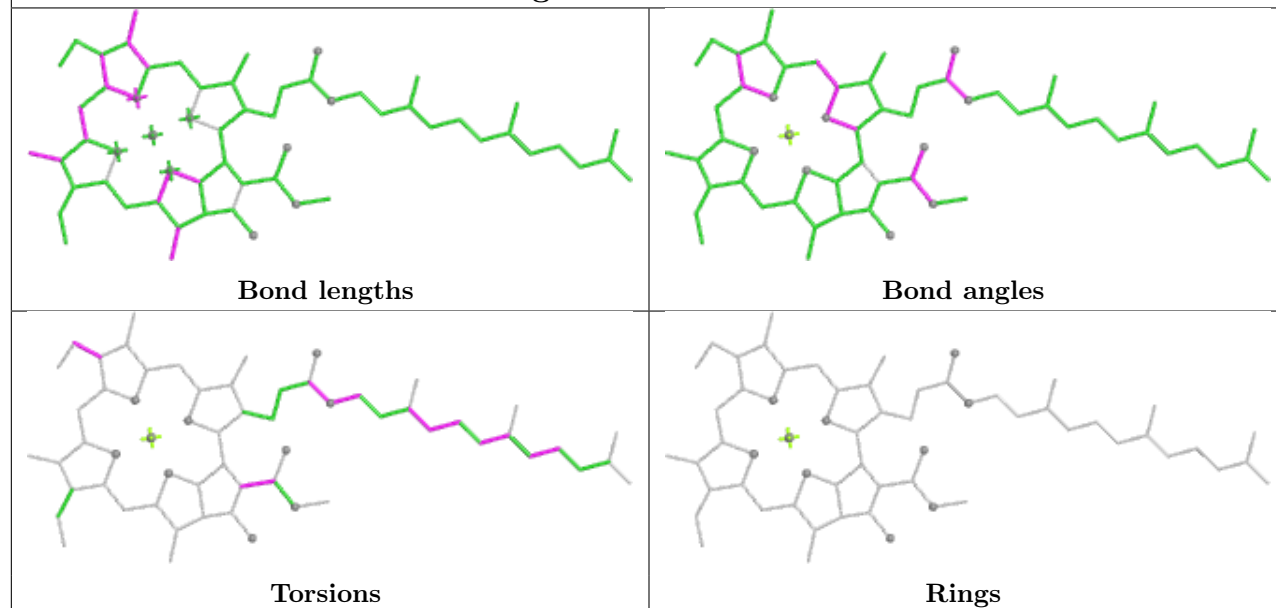
Ligand CLA A 837



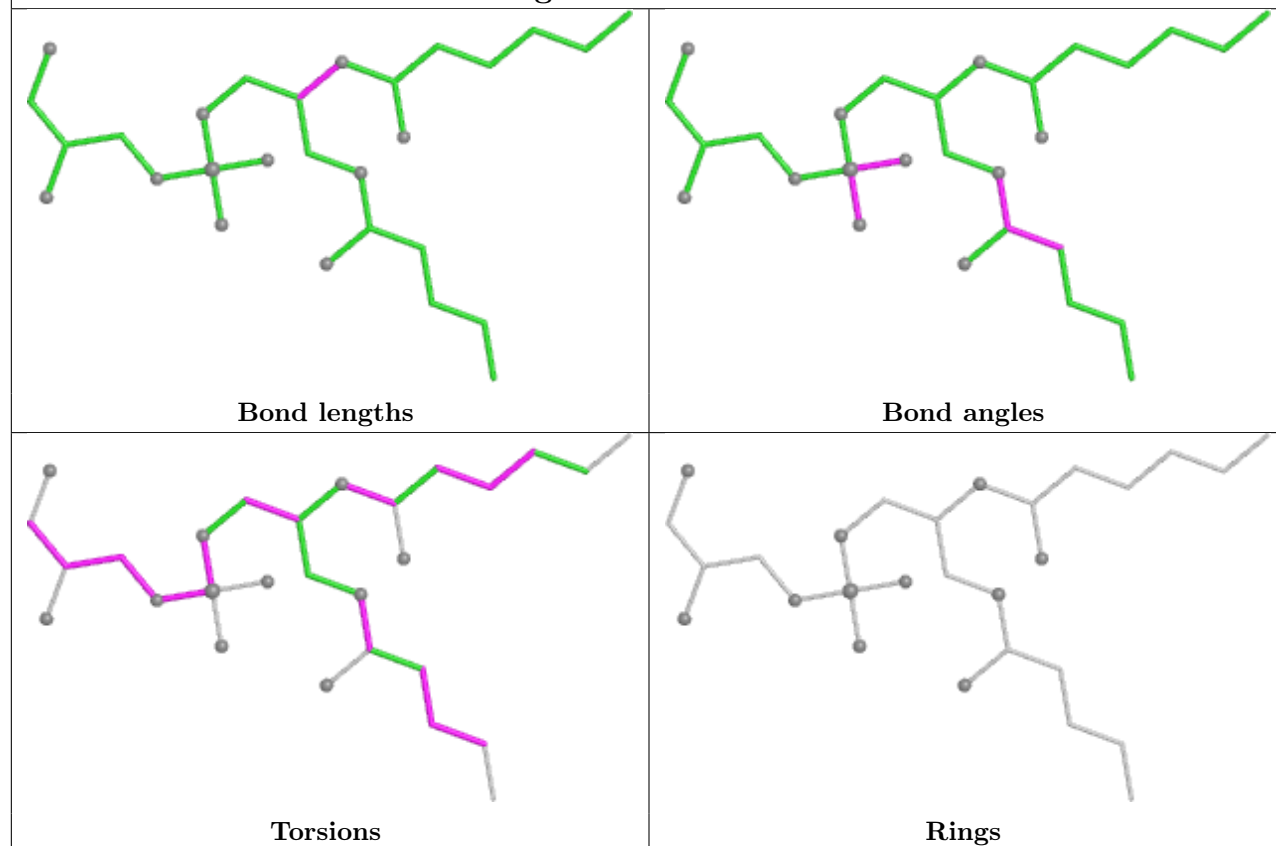
Ligand CLA B 807



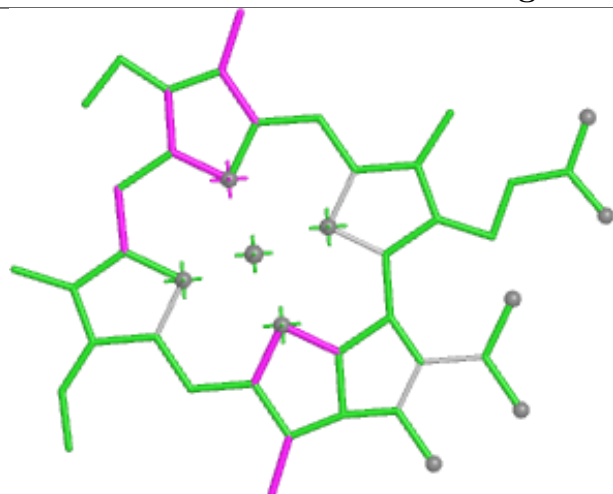
Ligand CLA B 815



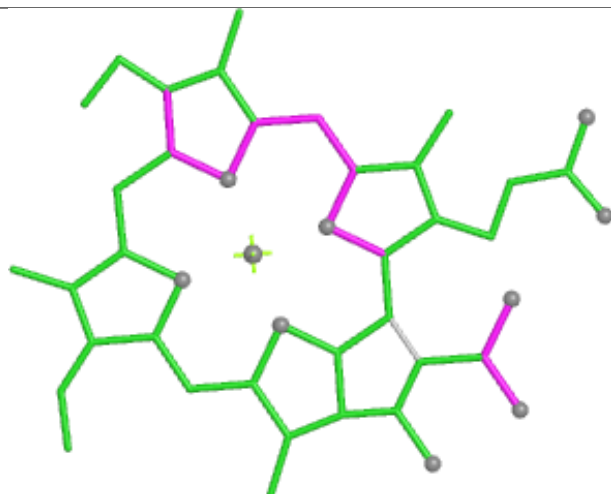
Ligand LHG 6 620



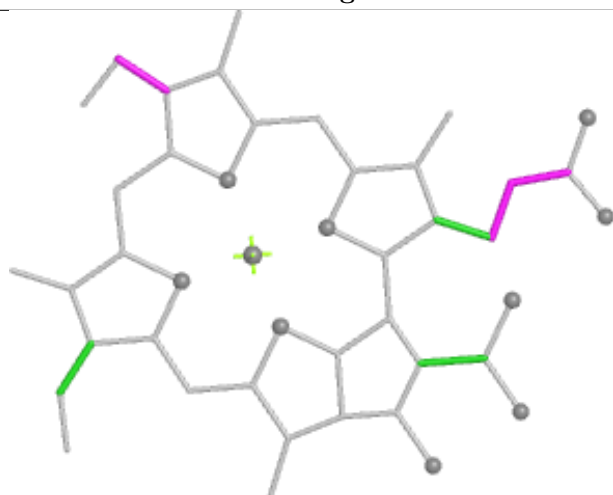
Ligand CLA 6 608



Bond lengths



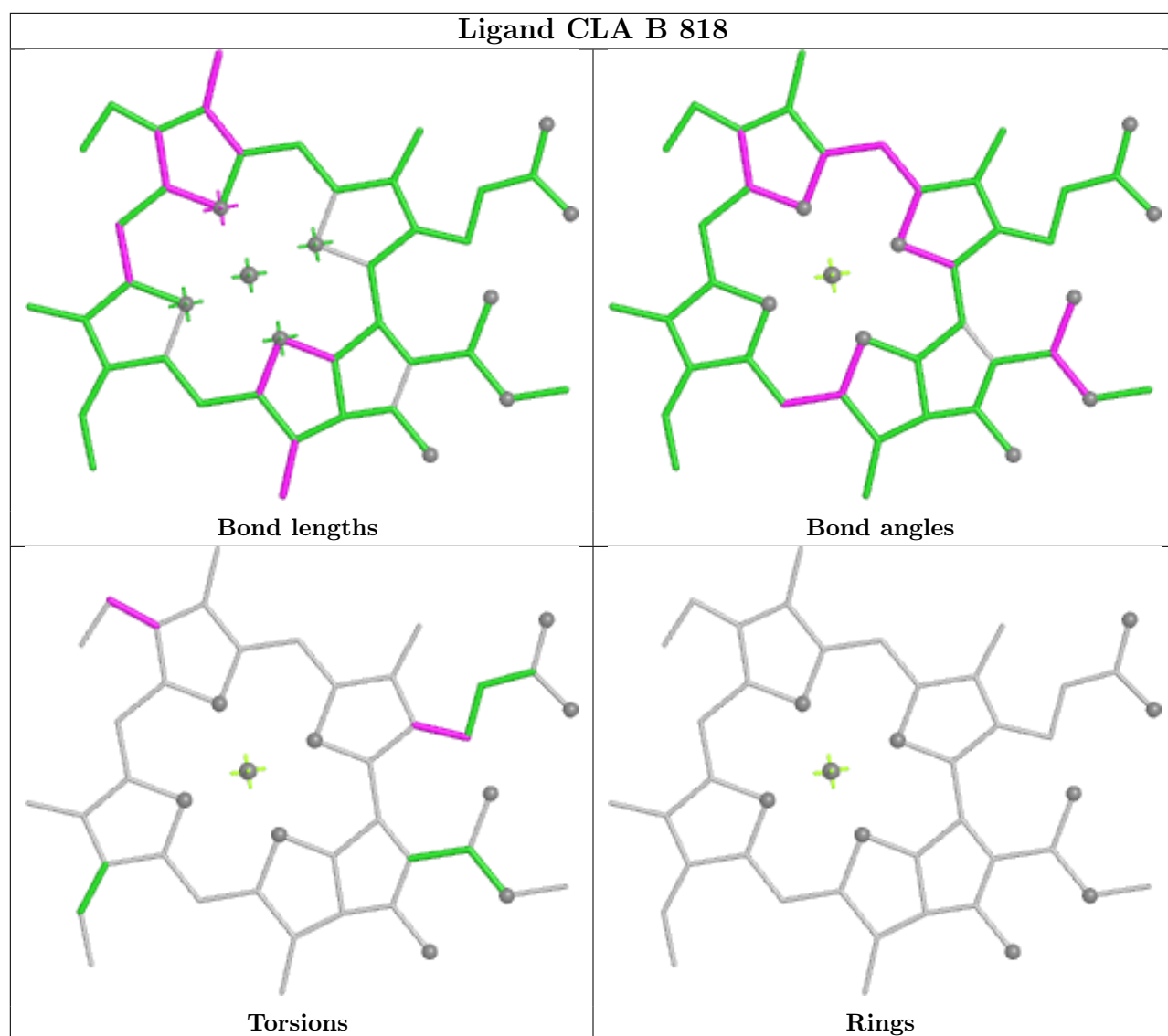
Bond angles

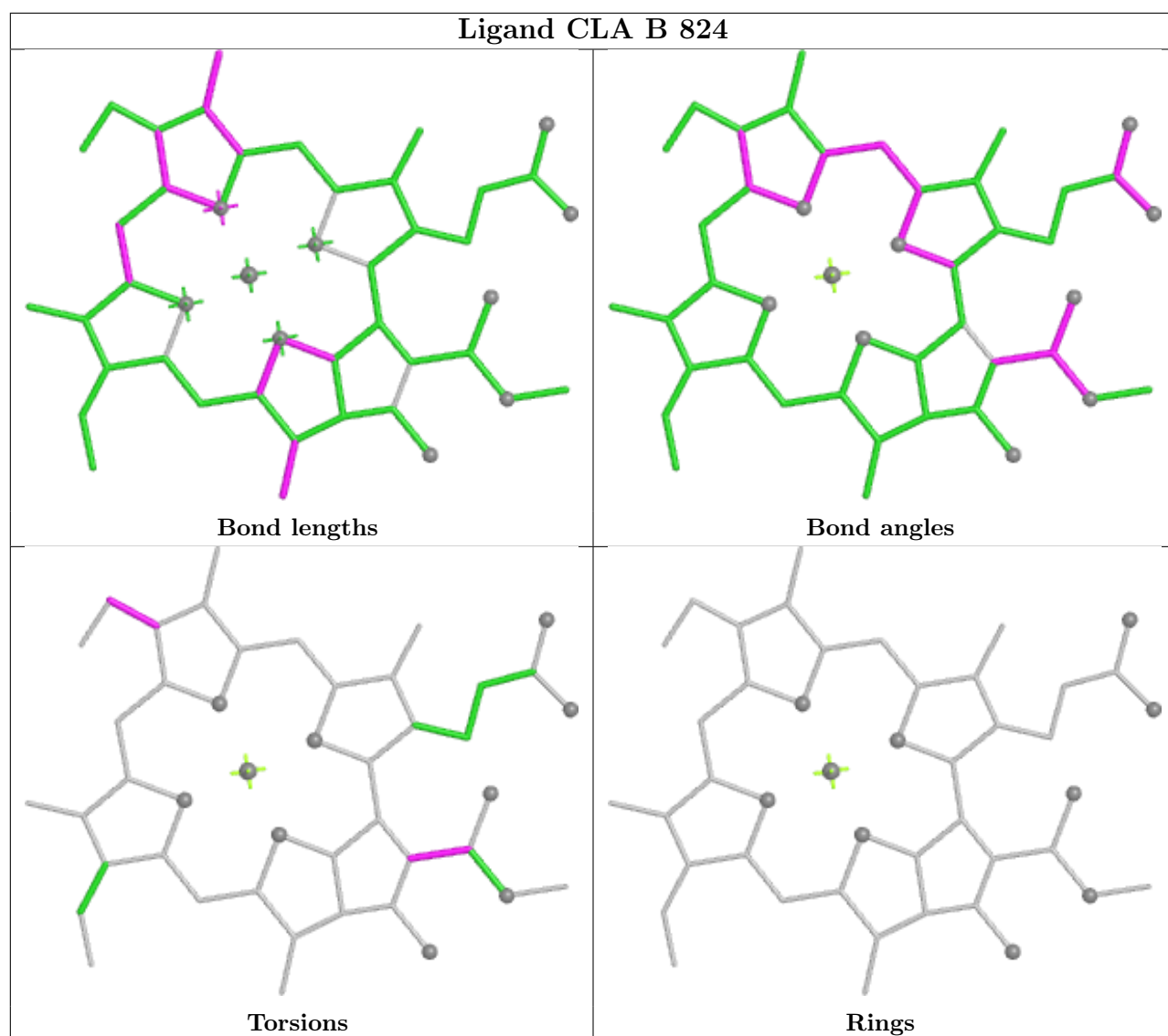


Torsions

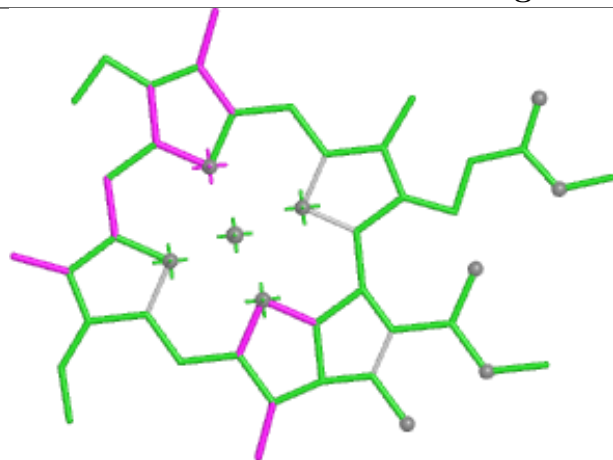


Rings

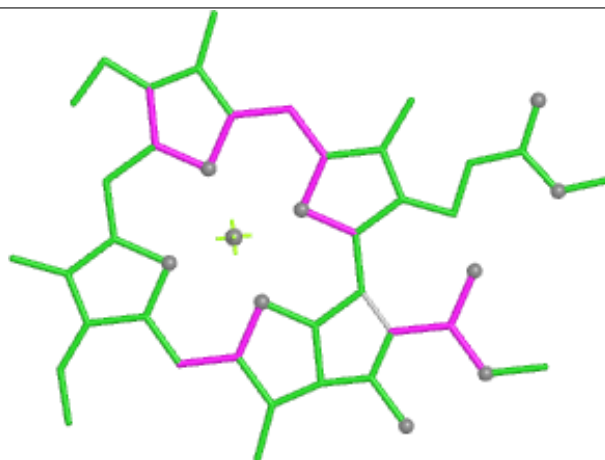




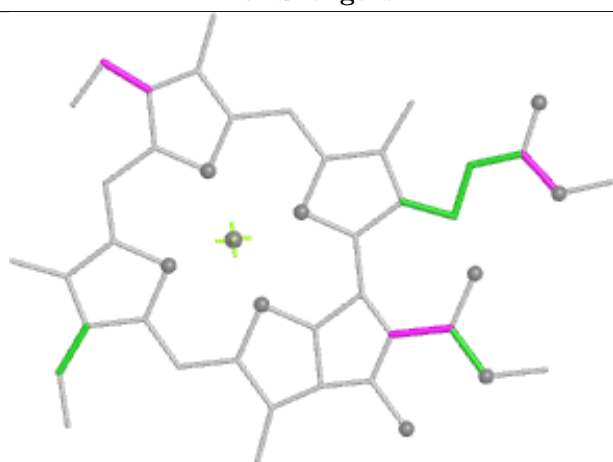
Ligand CLA B 837



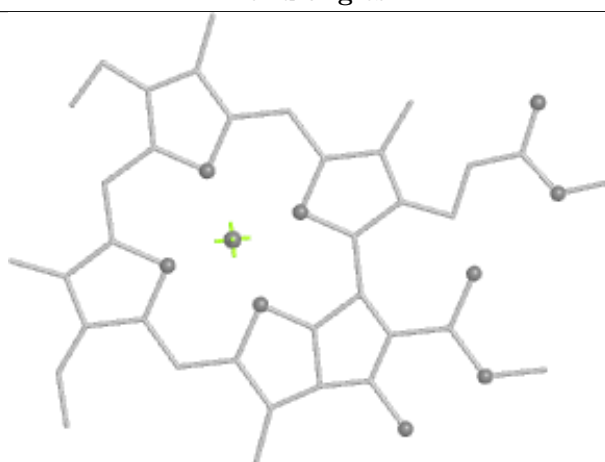
Bond lengths



Bond angles

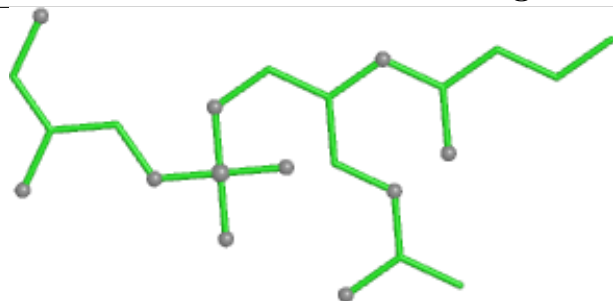


Torsions

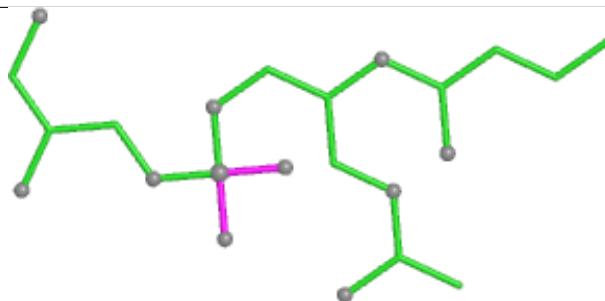


Rings

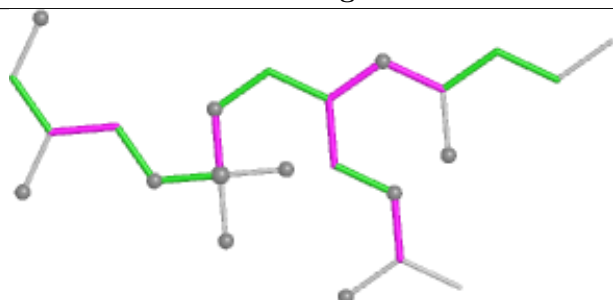
Ligand LHG B 851



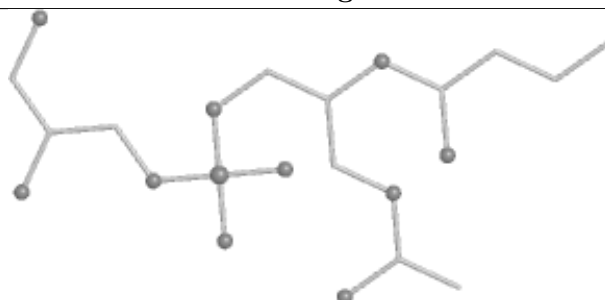
Bond lengths



Bond angles

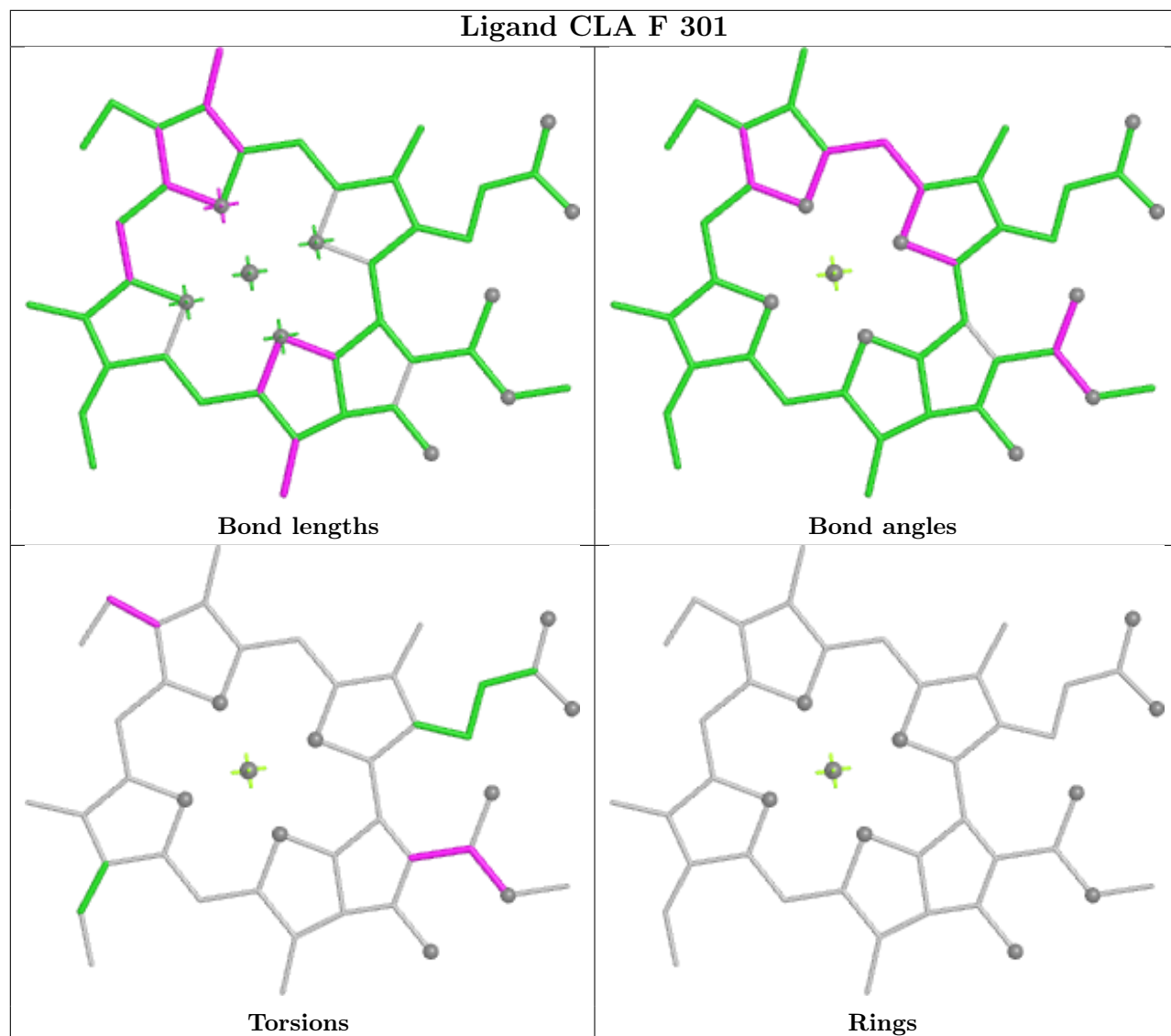


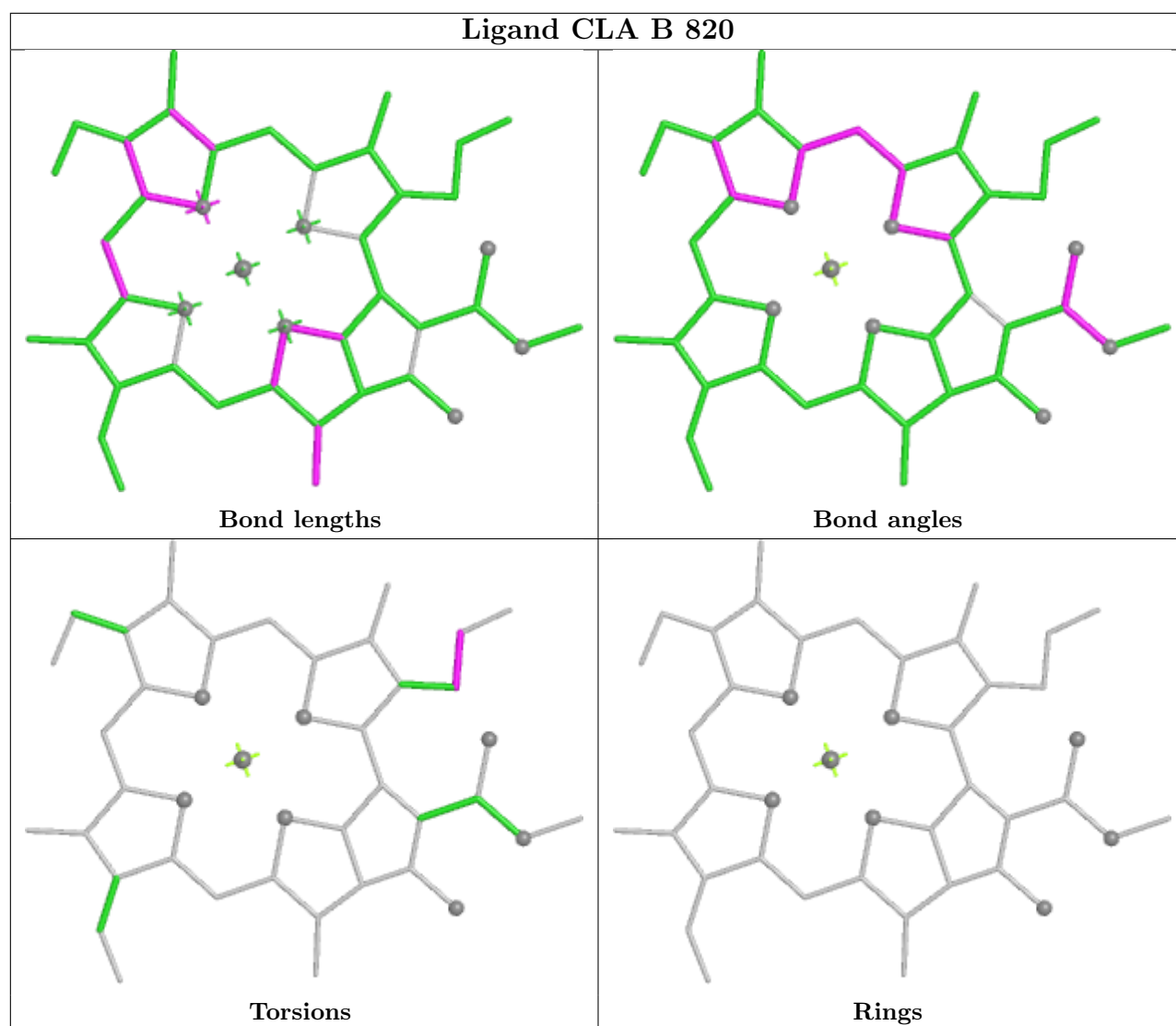
Torsions

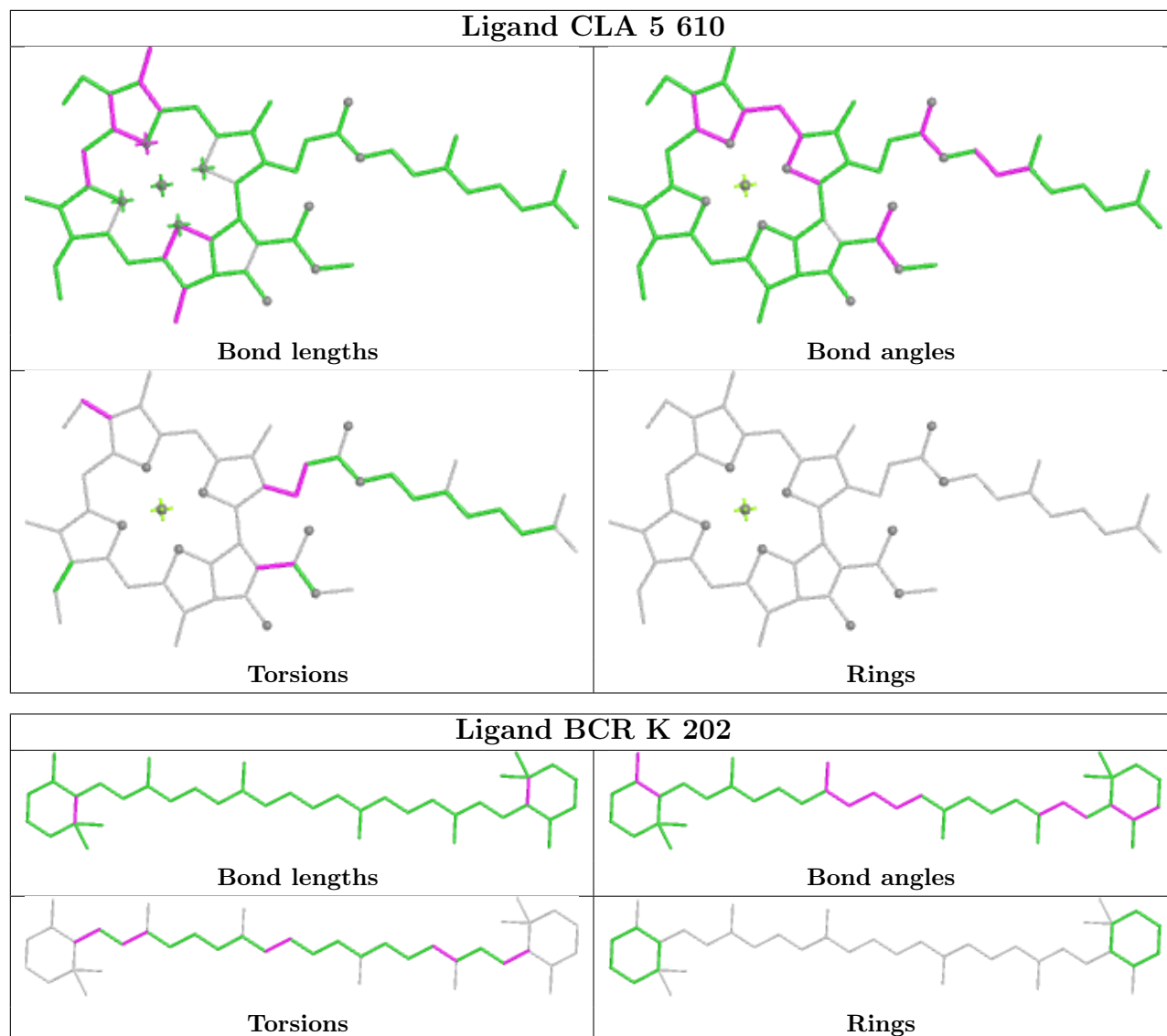


Rings

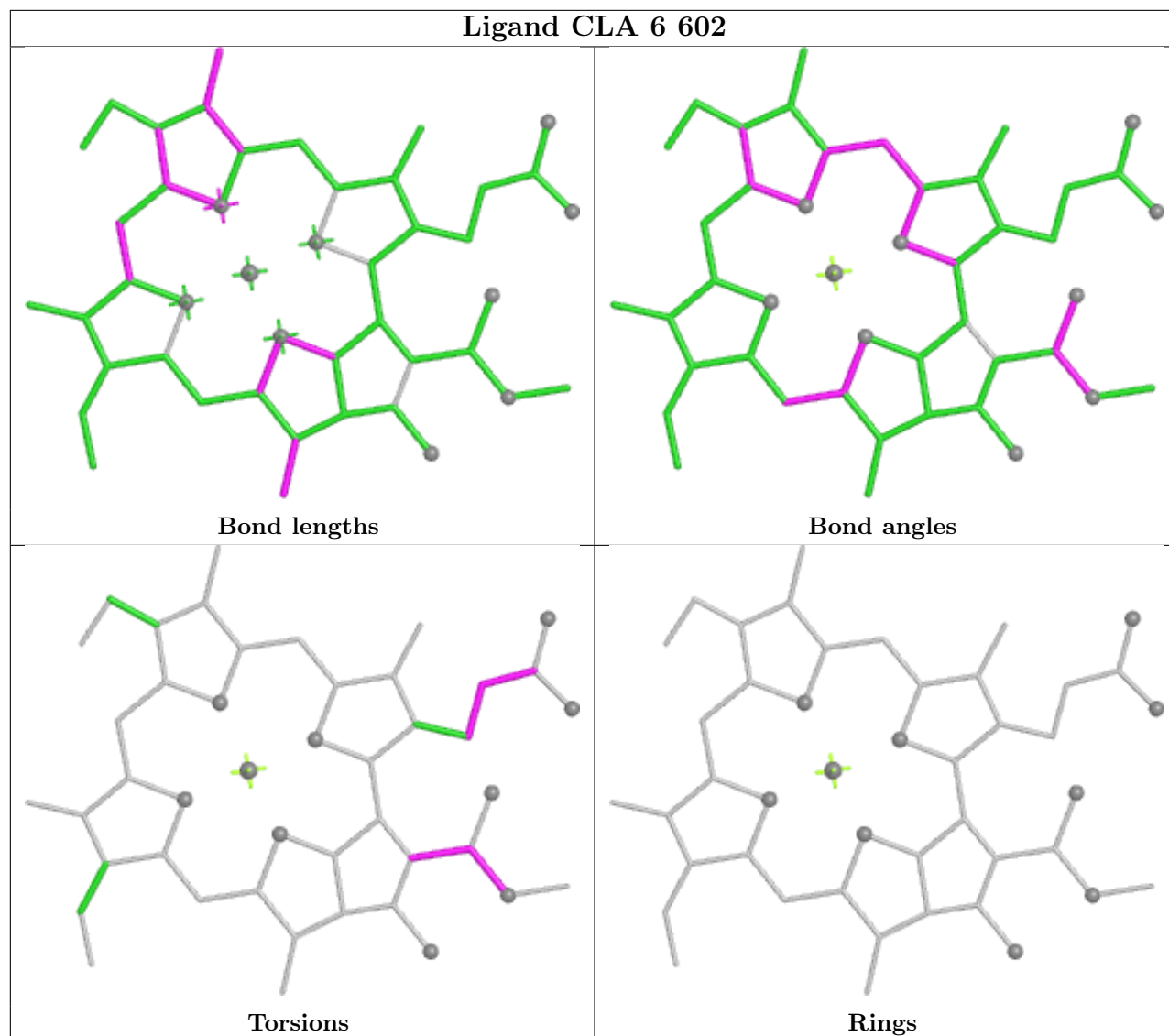
Ligand CLA F 301



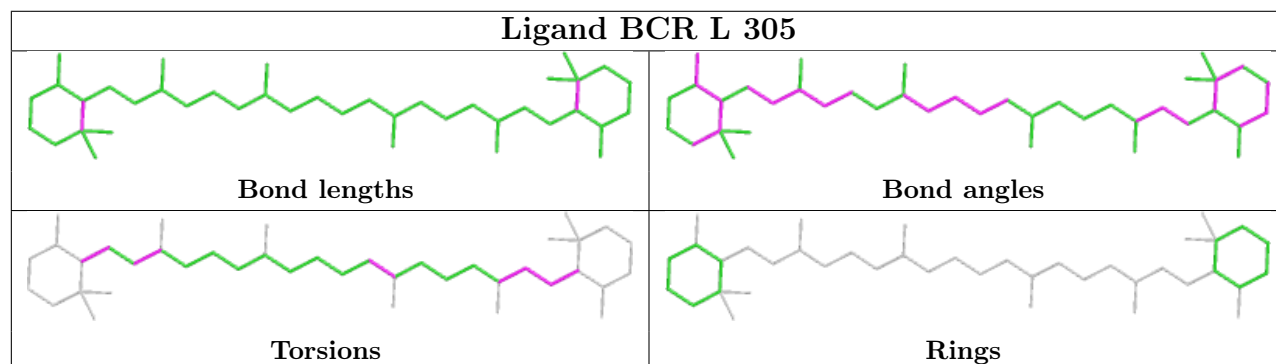


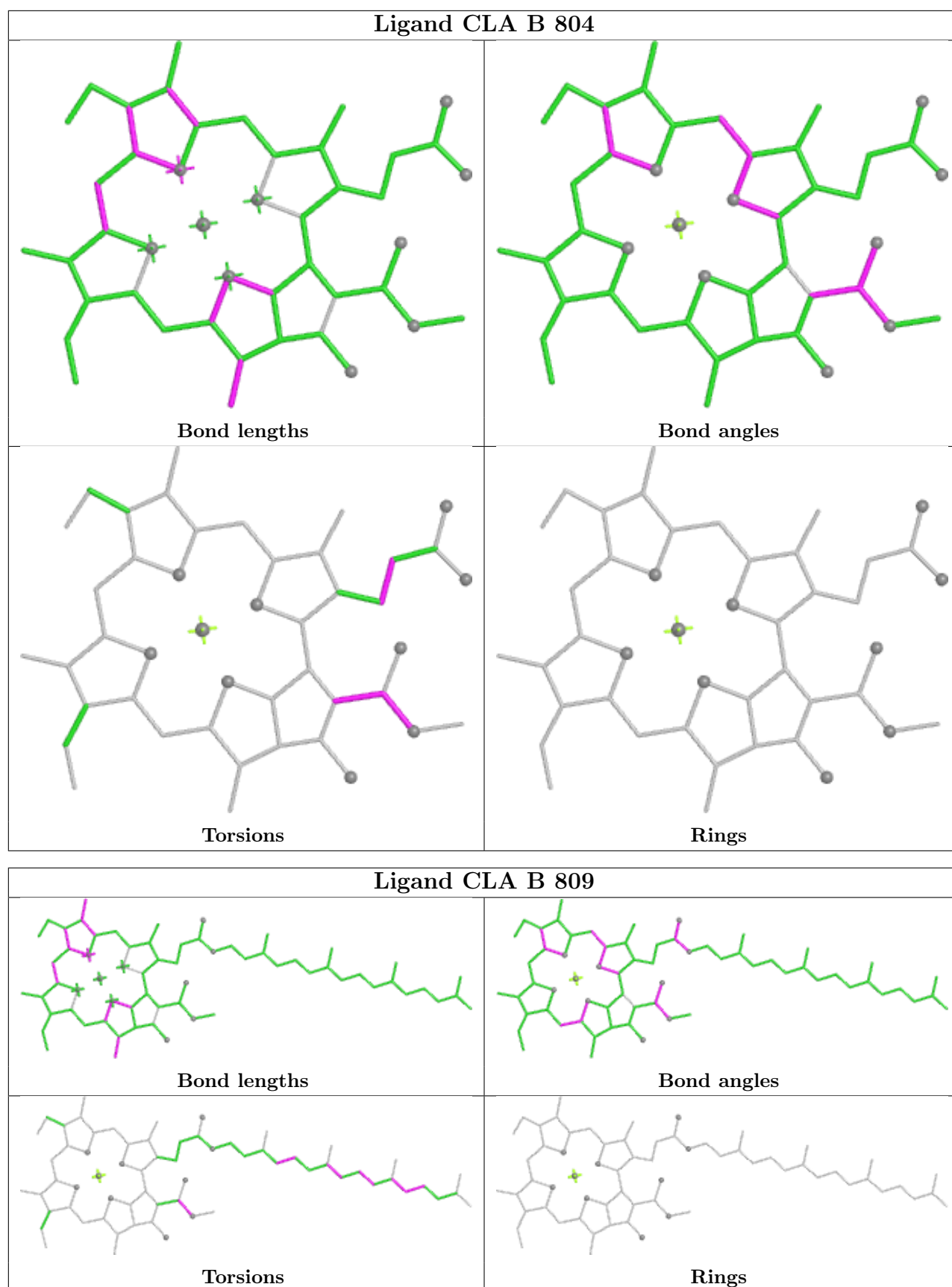


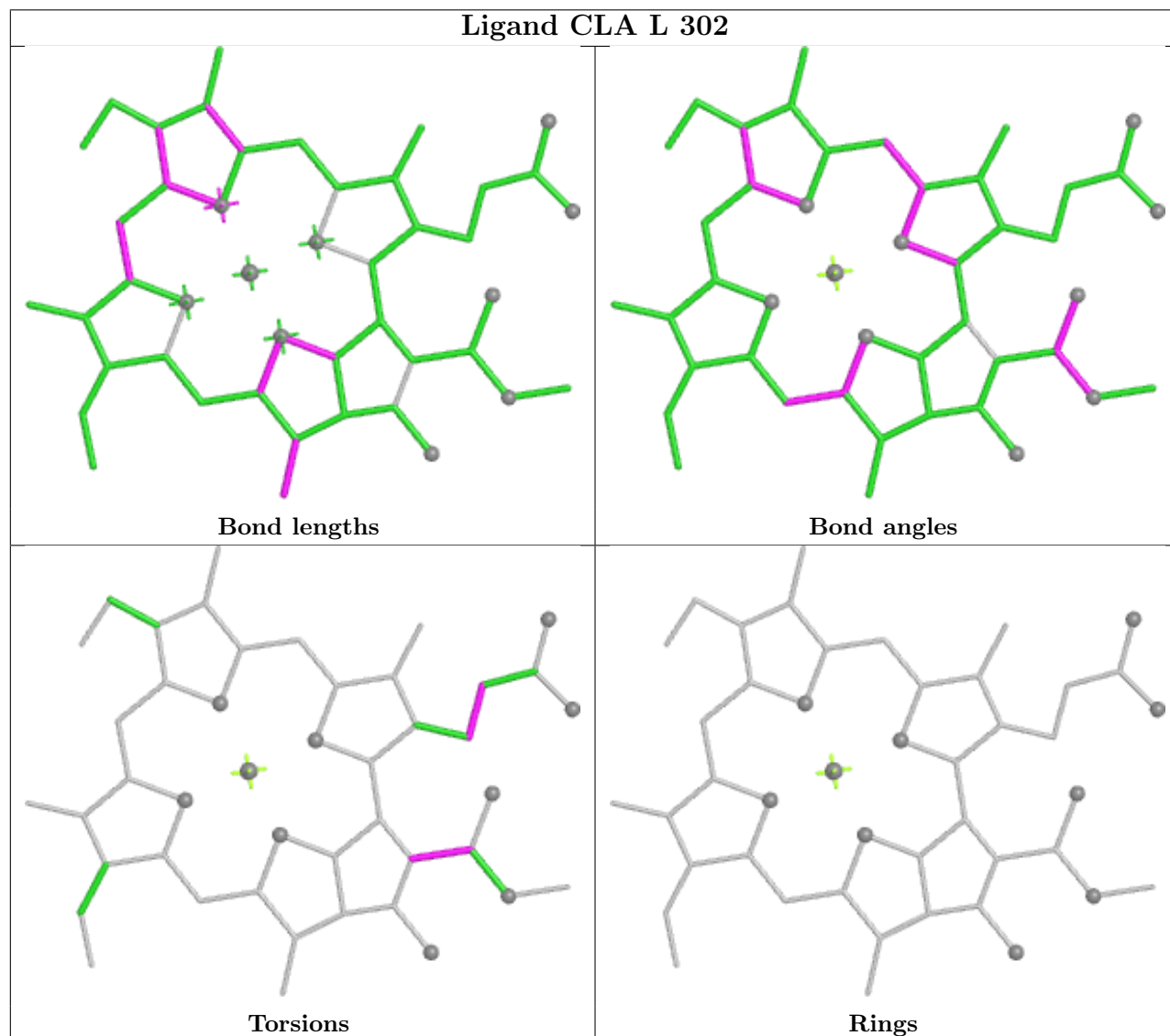
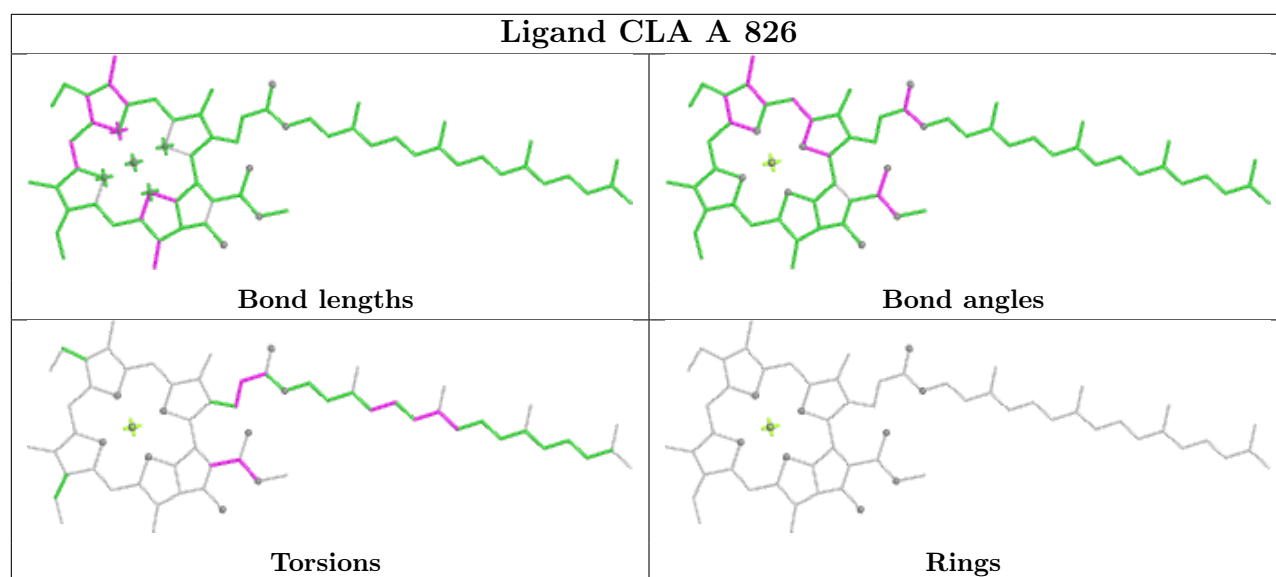
Ligand CLA 6 602

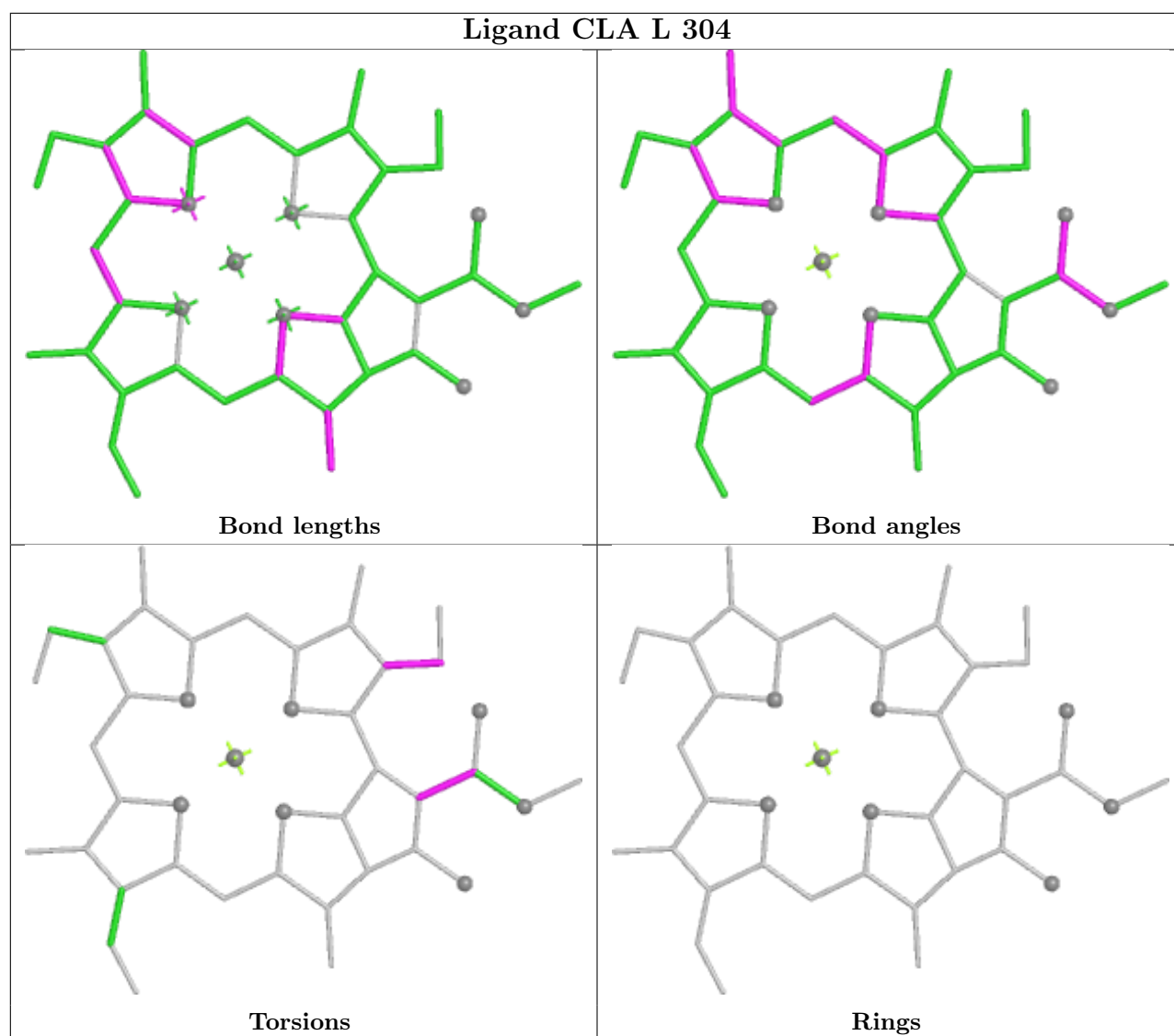


Ligand BCR L 305

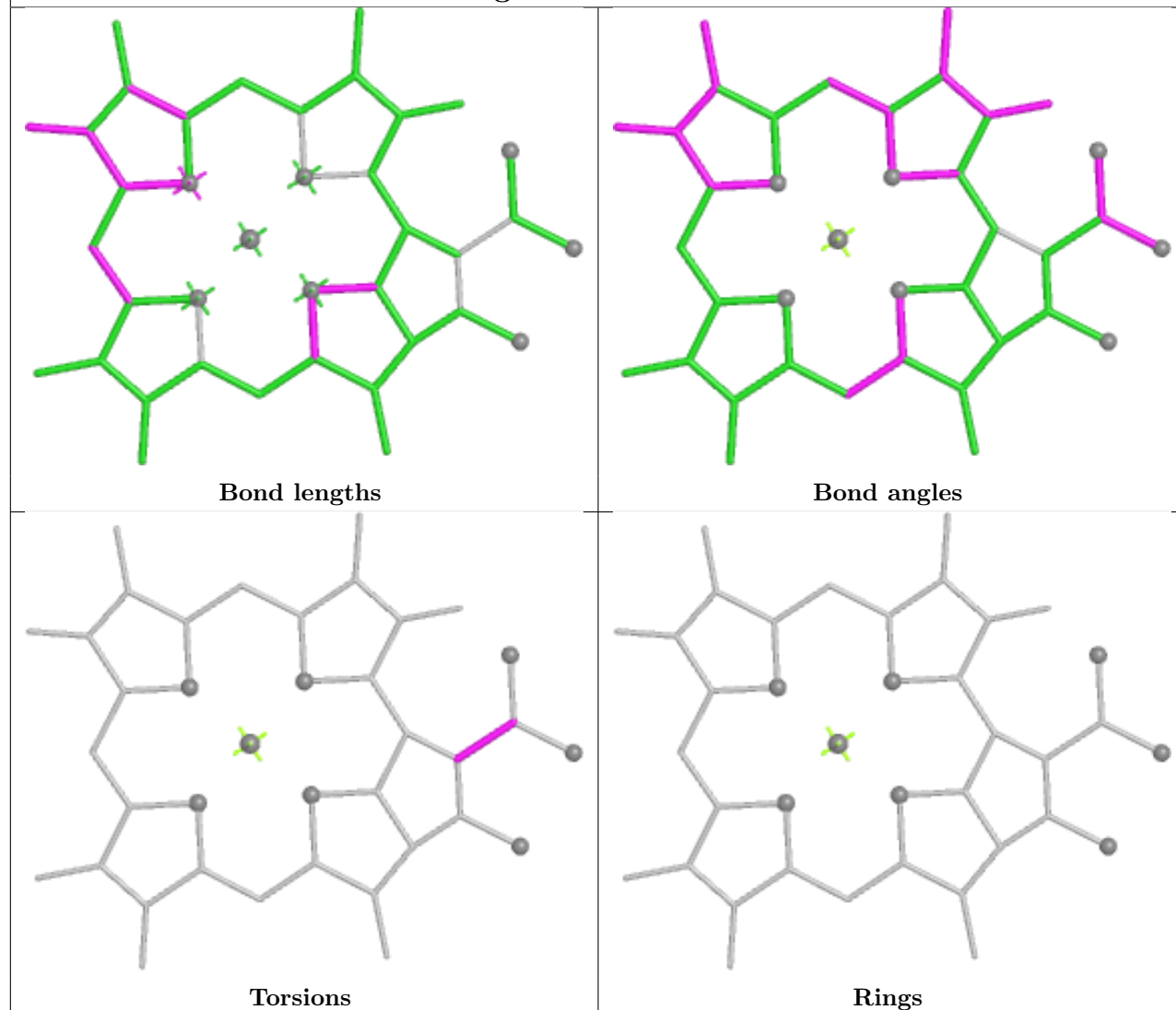




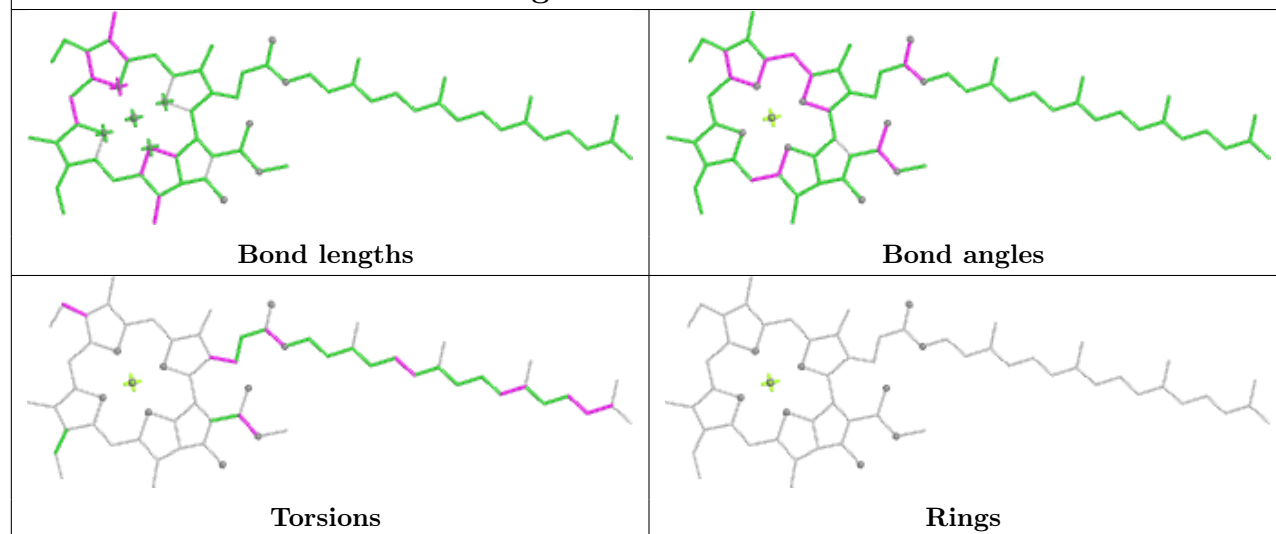




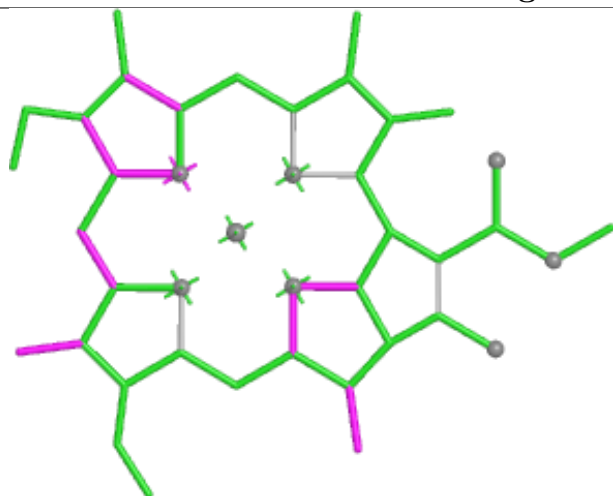
Ligand CLA 6 614



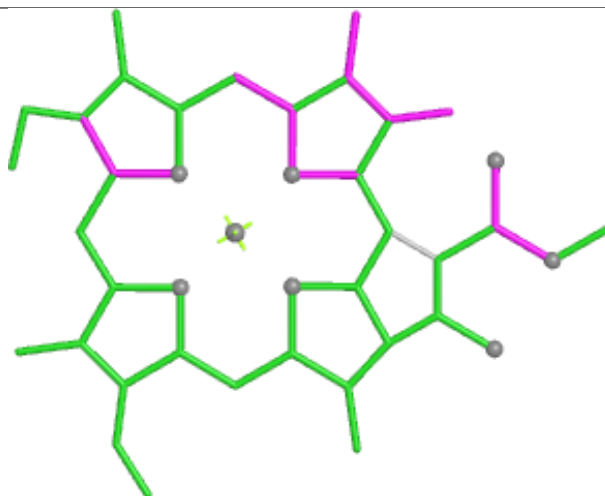
Ligand CLA A 812



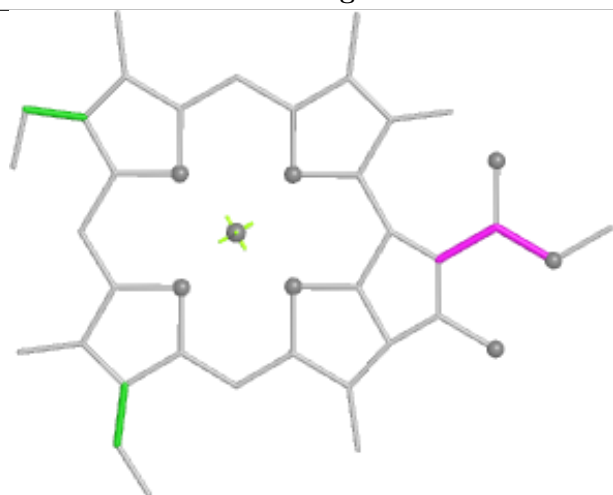
Ligand CLA 3 610



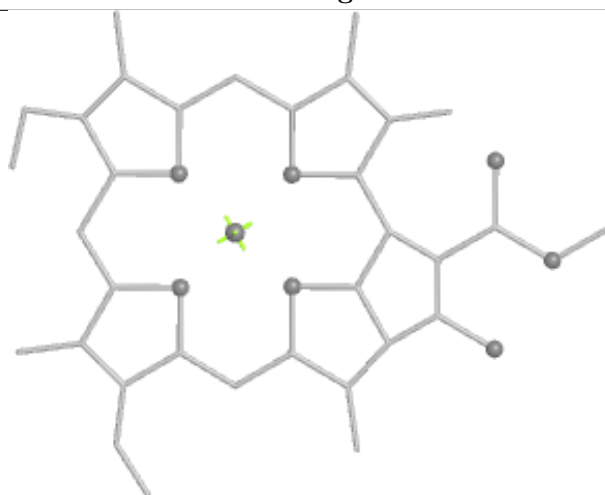
Bond lengths



Bond angles

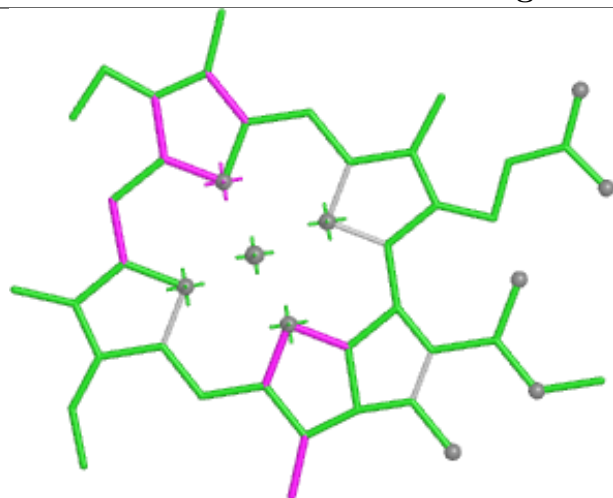


Torsions

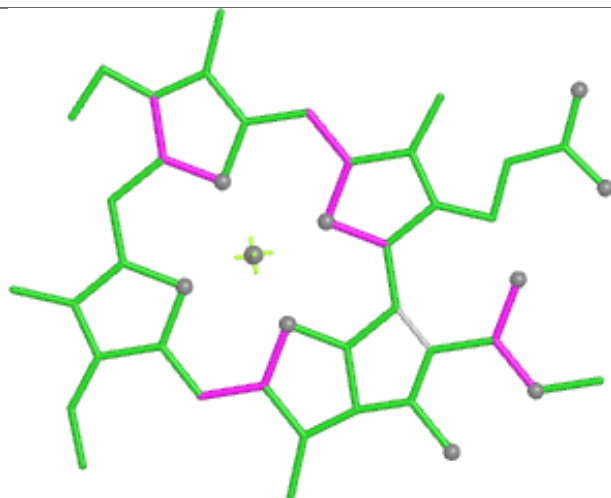


Rings

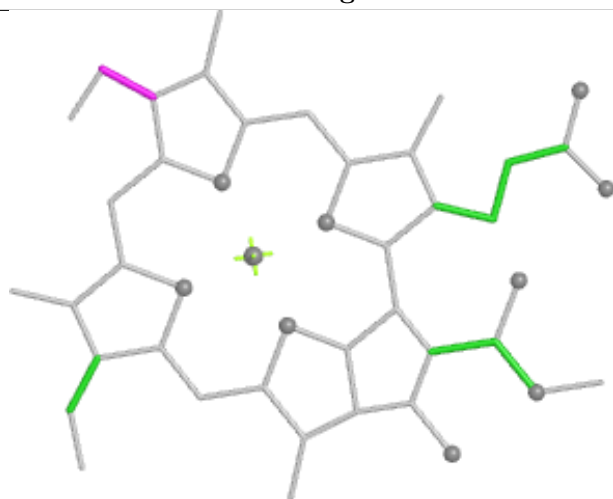
Ligand CLA L 303



Bond lengths



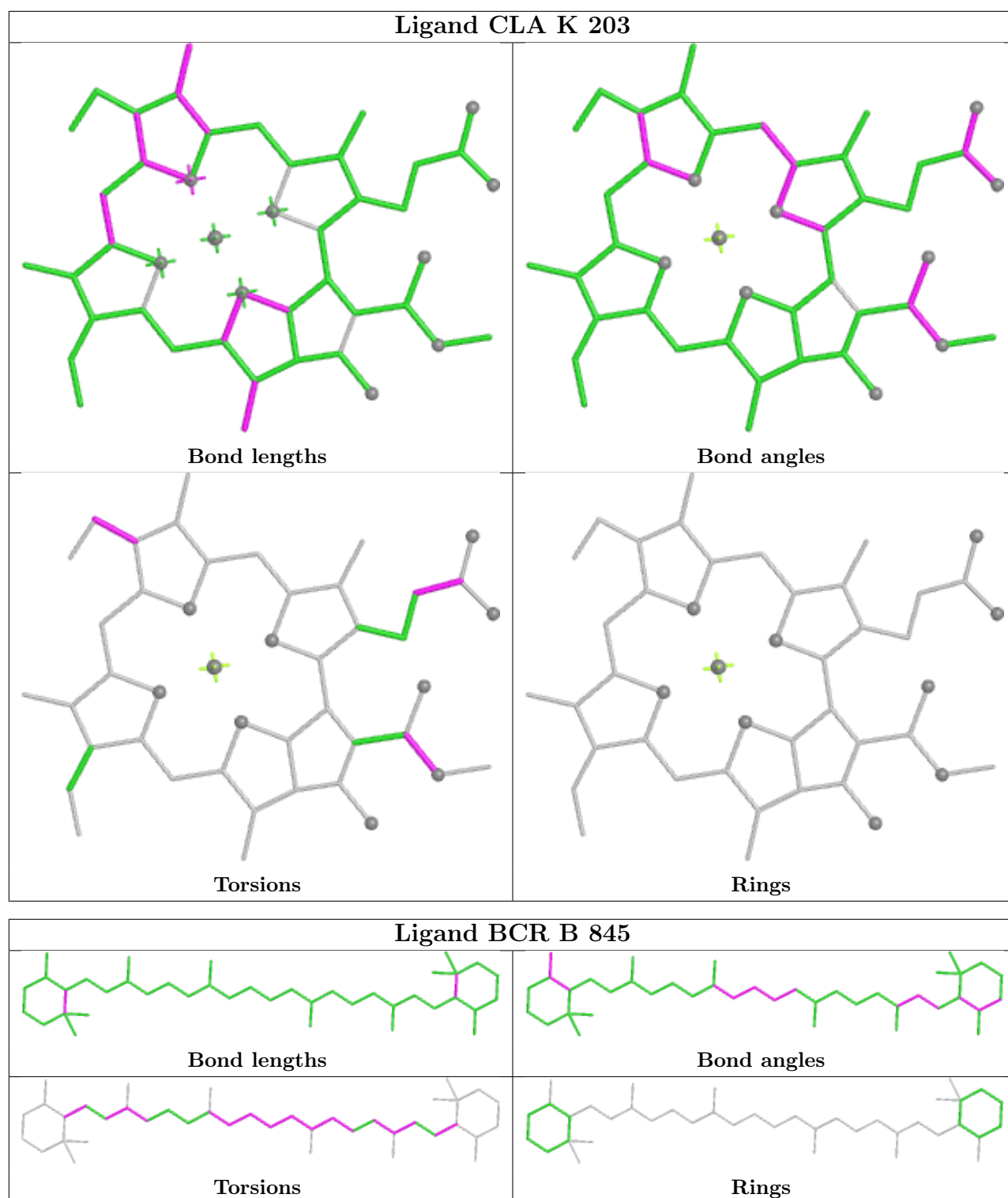
Bond angles



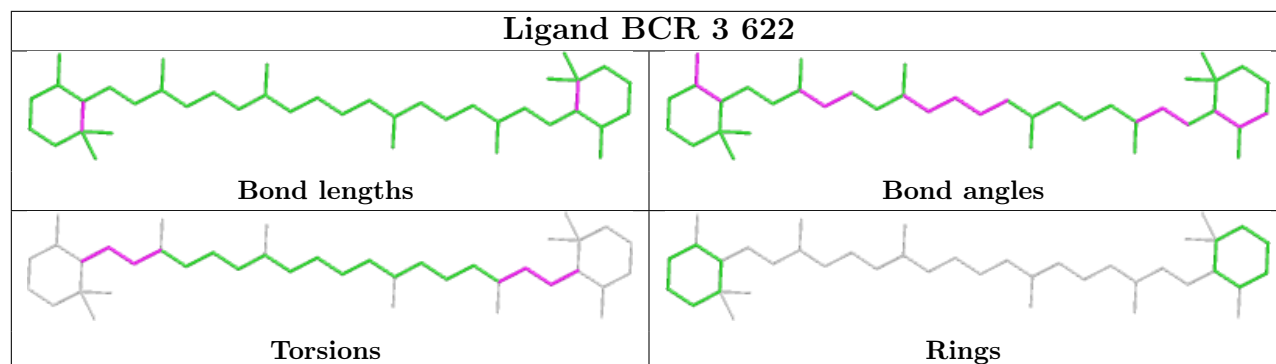
Torsions



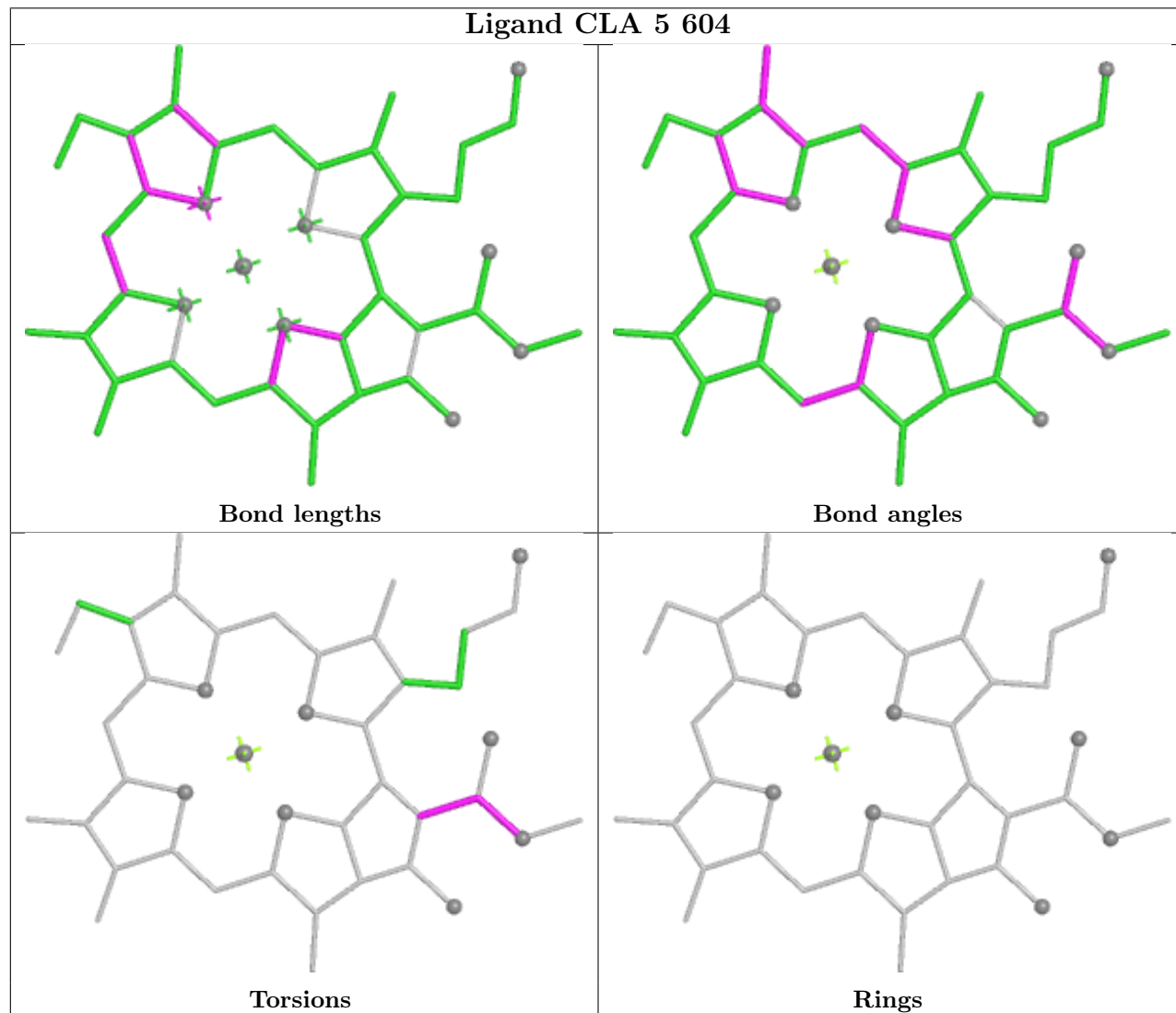
Rings

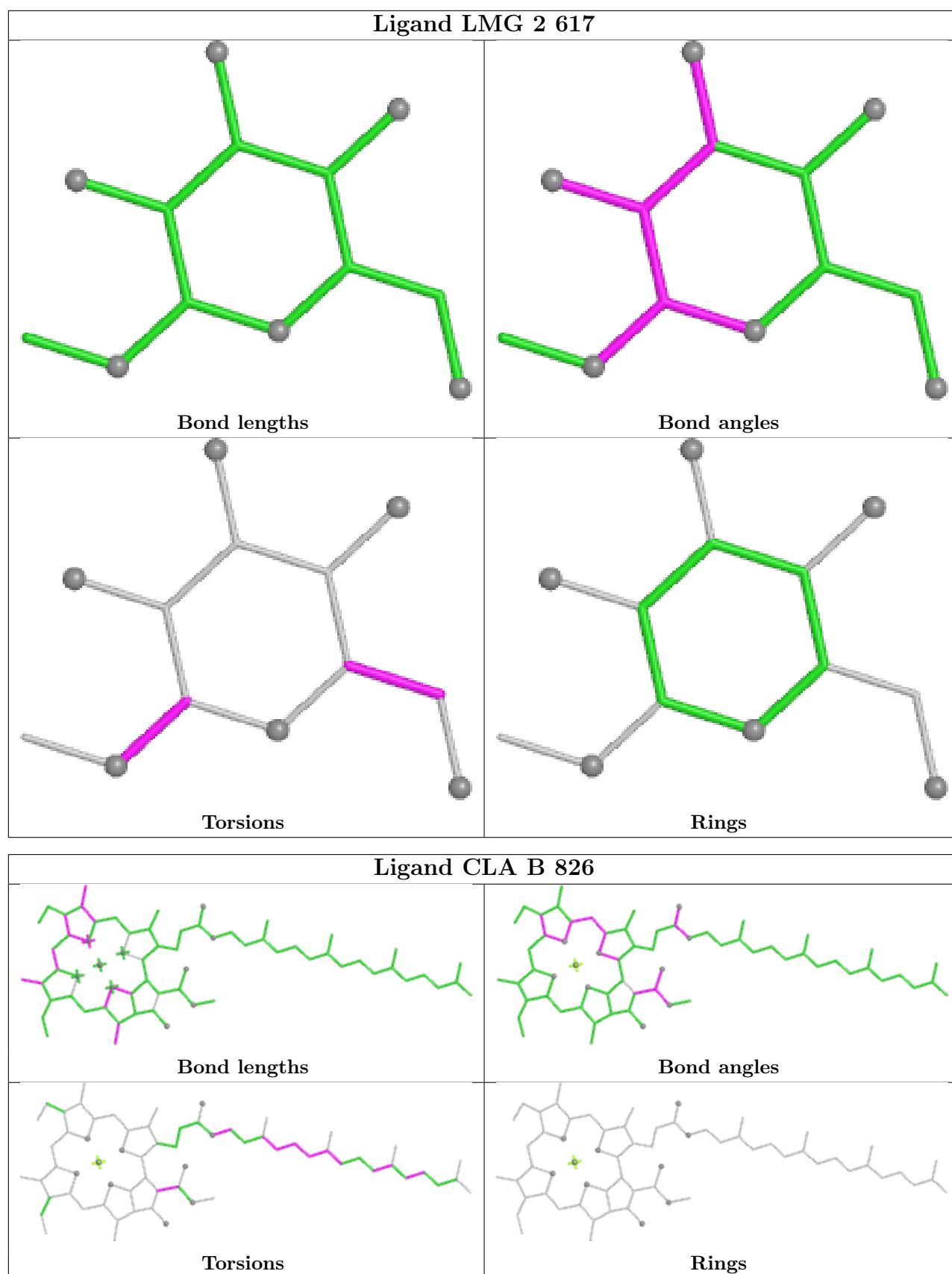


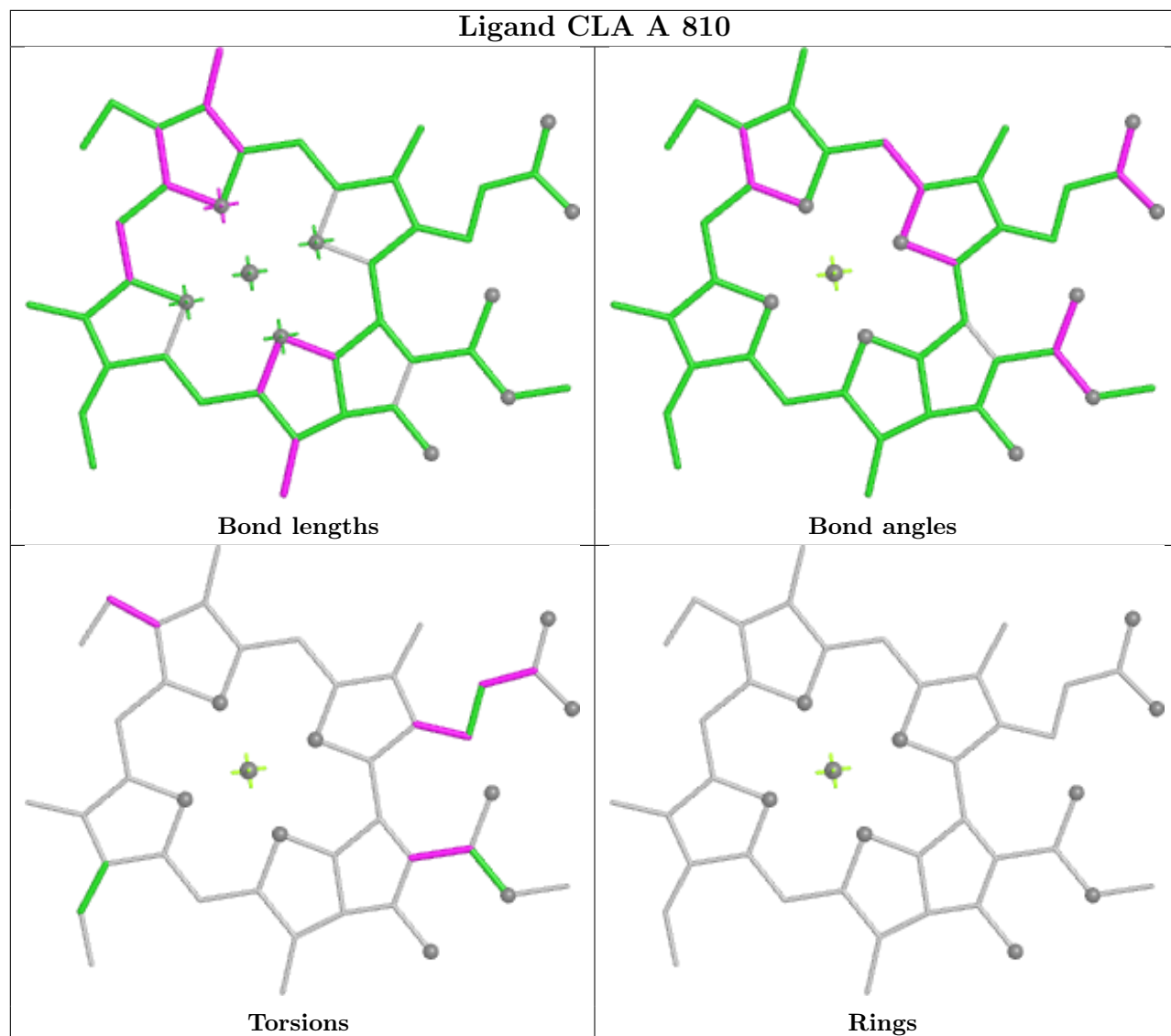
Ligand BCR 3 622

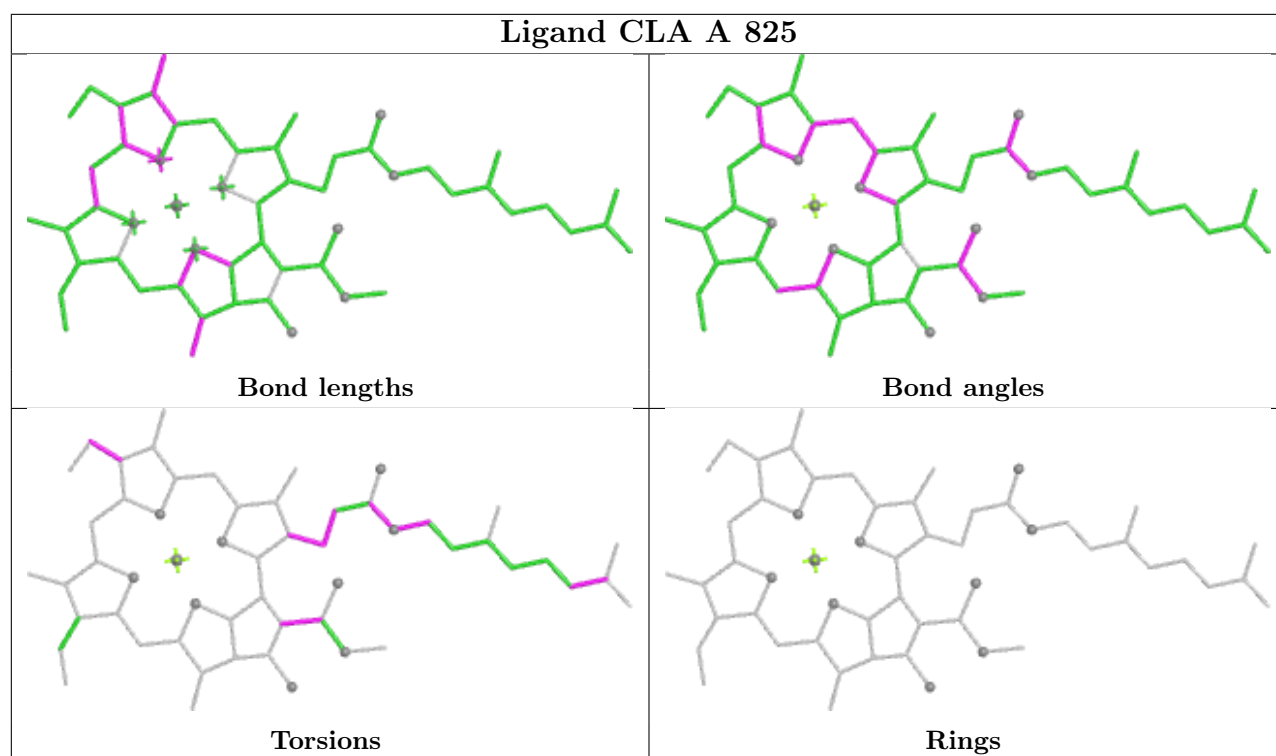


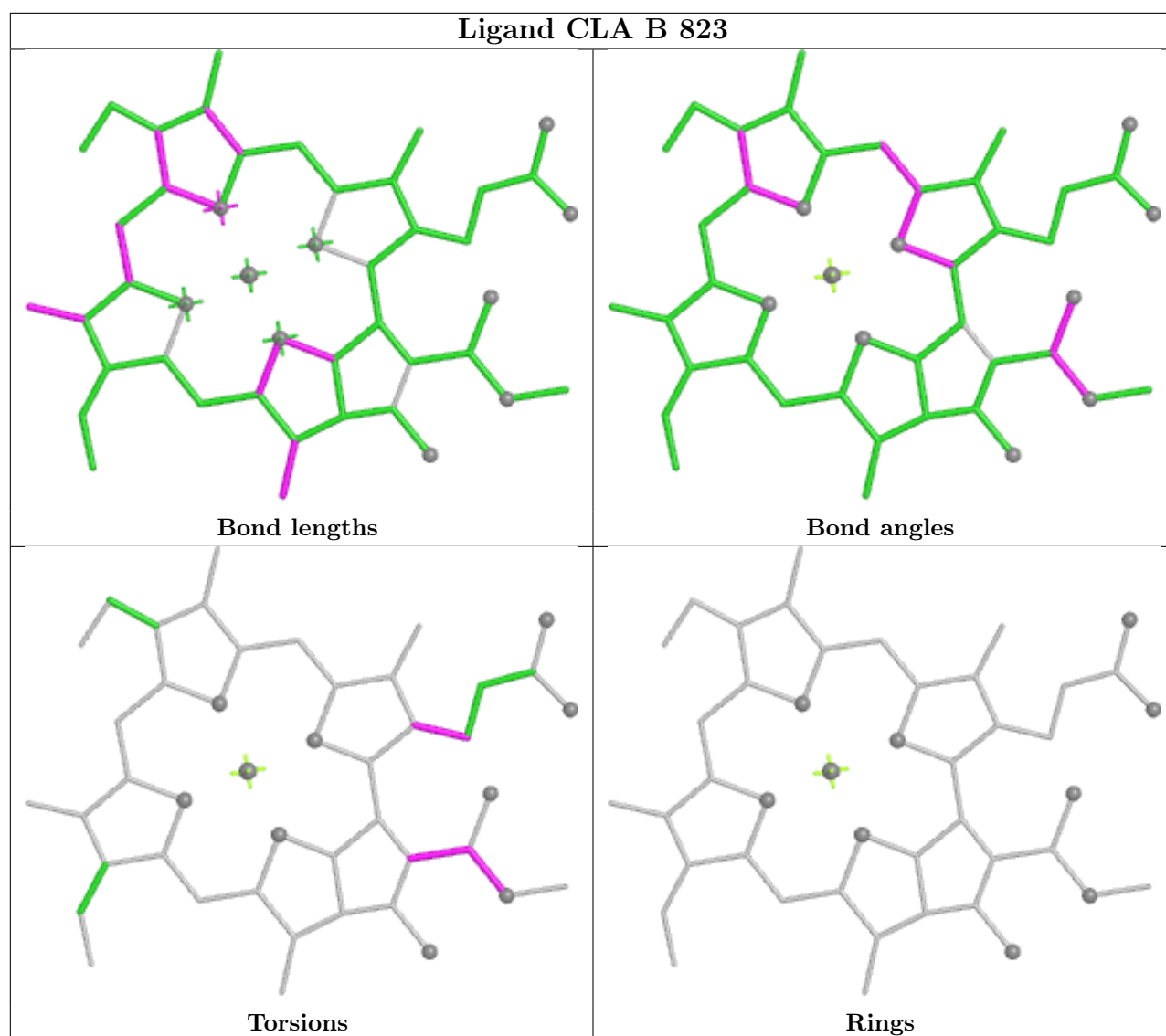
Ligand CLA 5 604

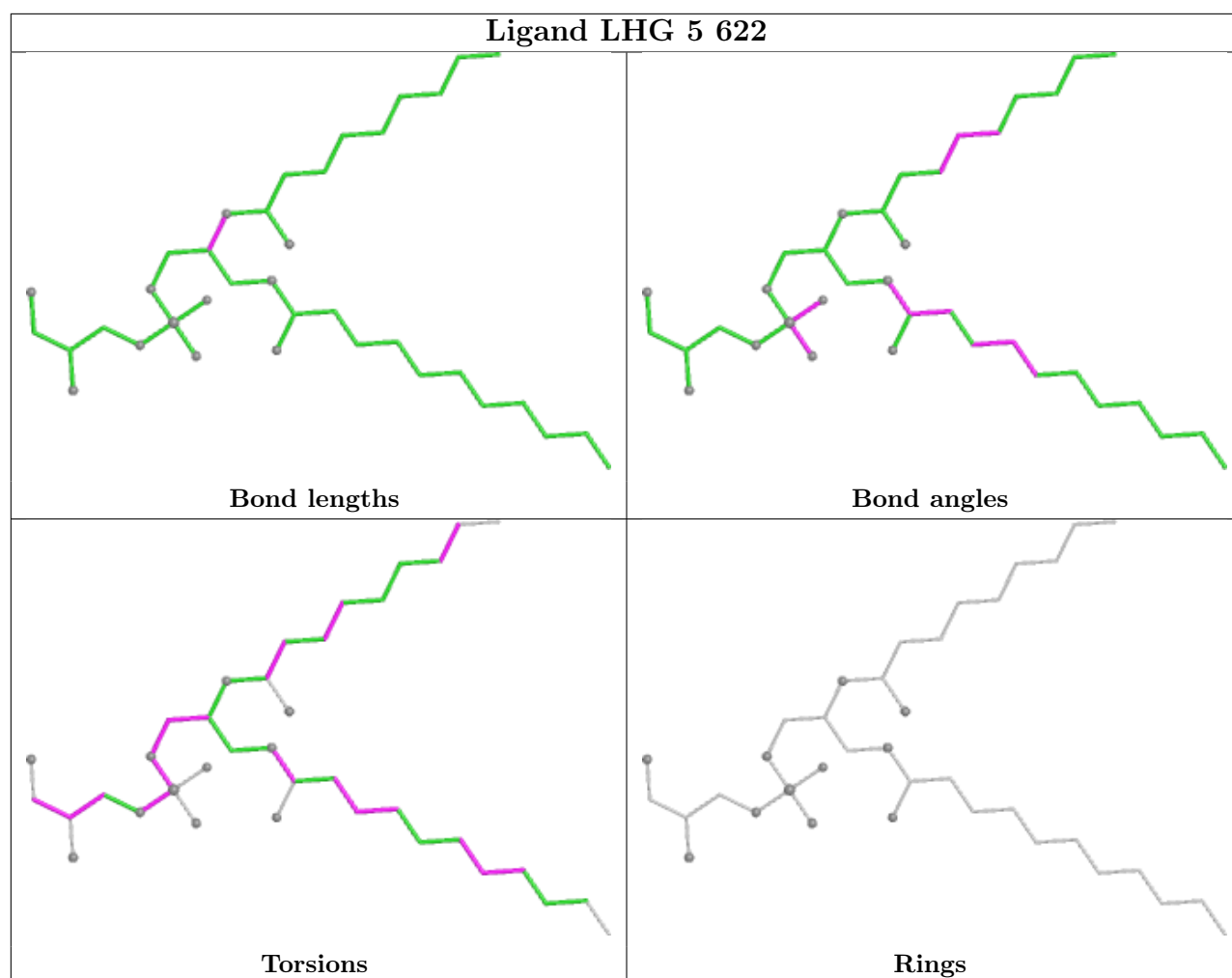


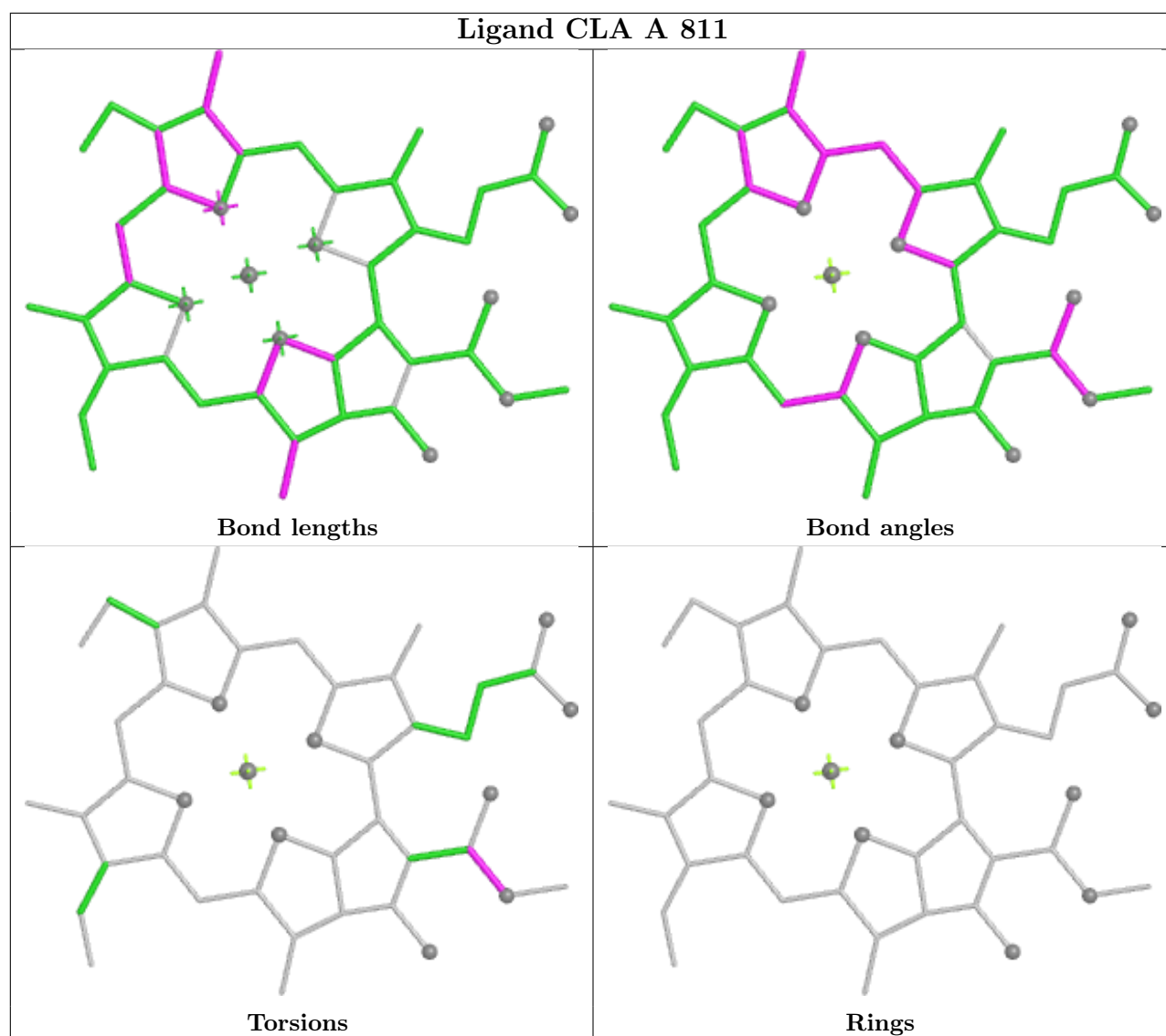


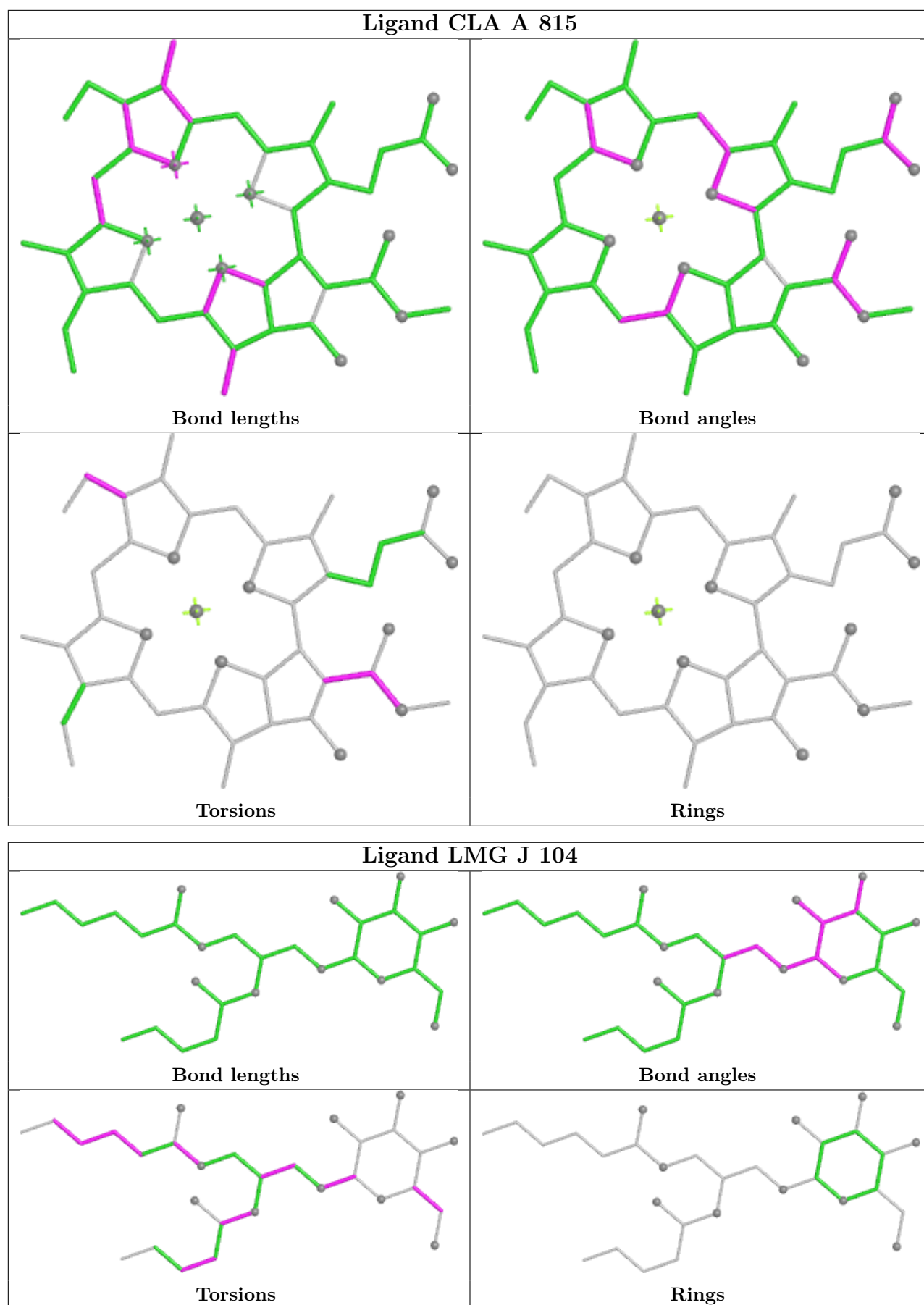




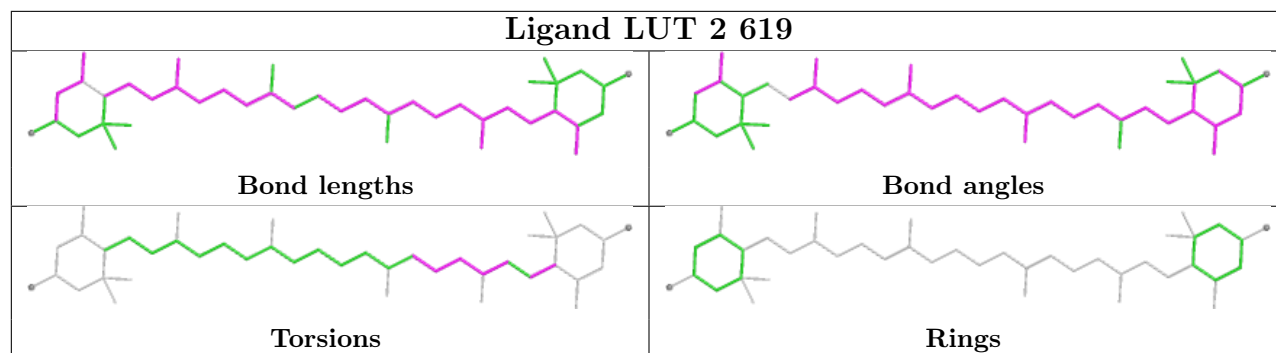




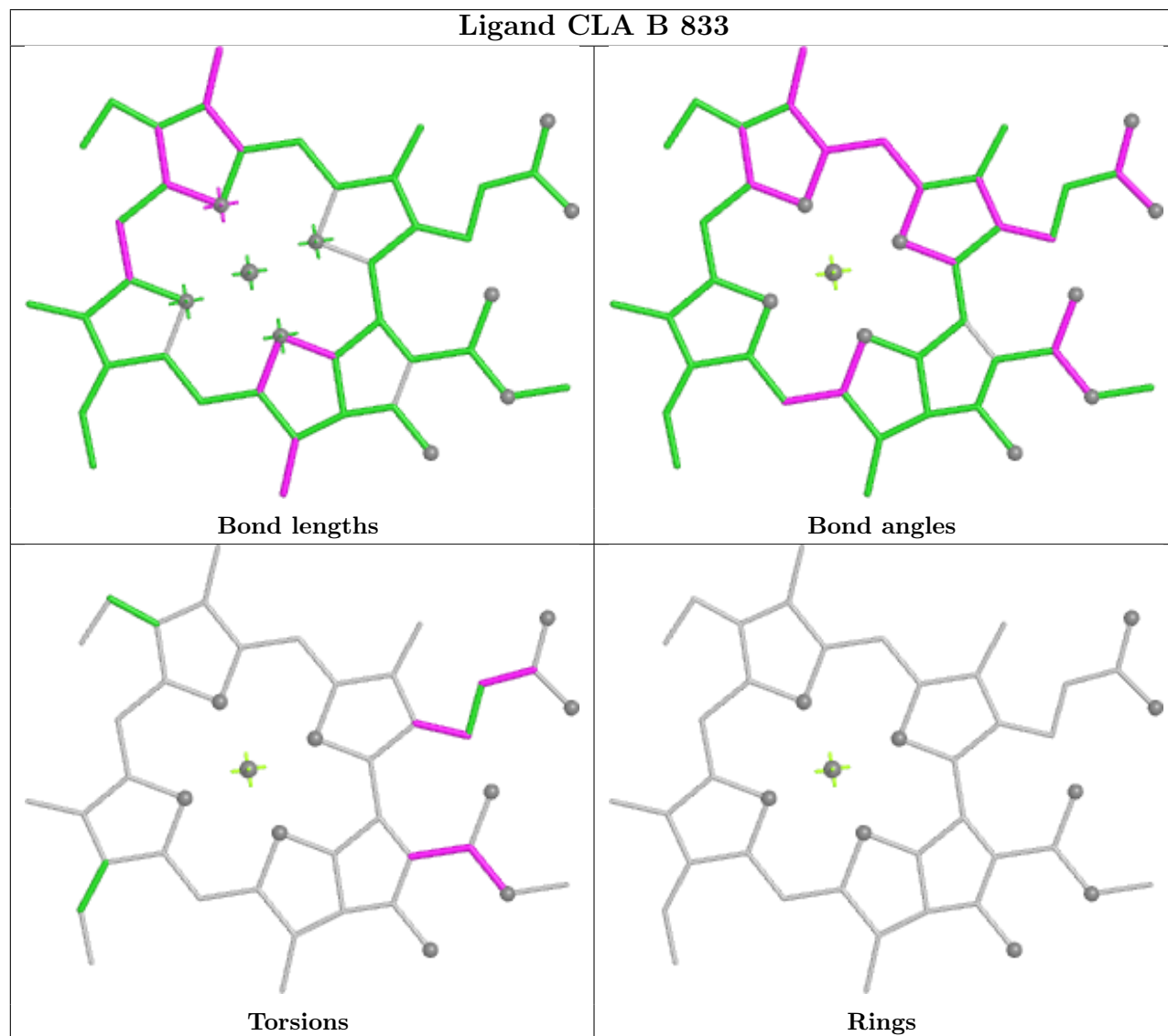


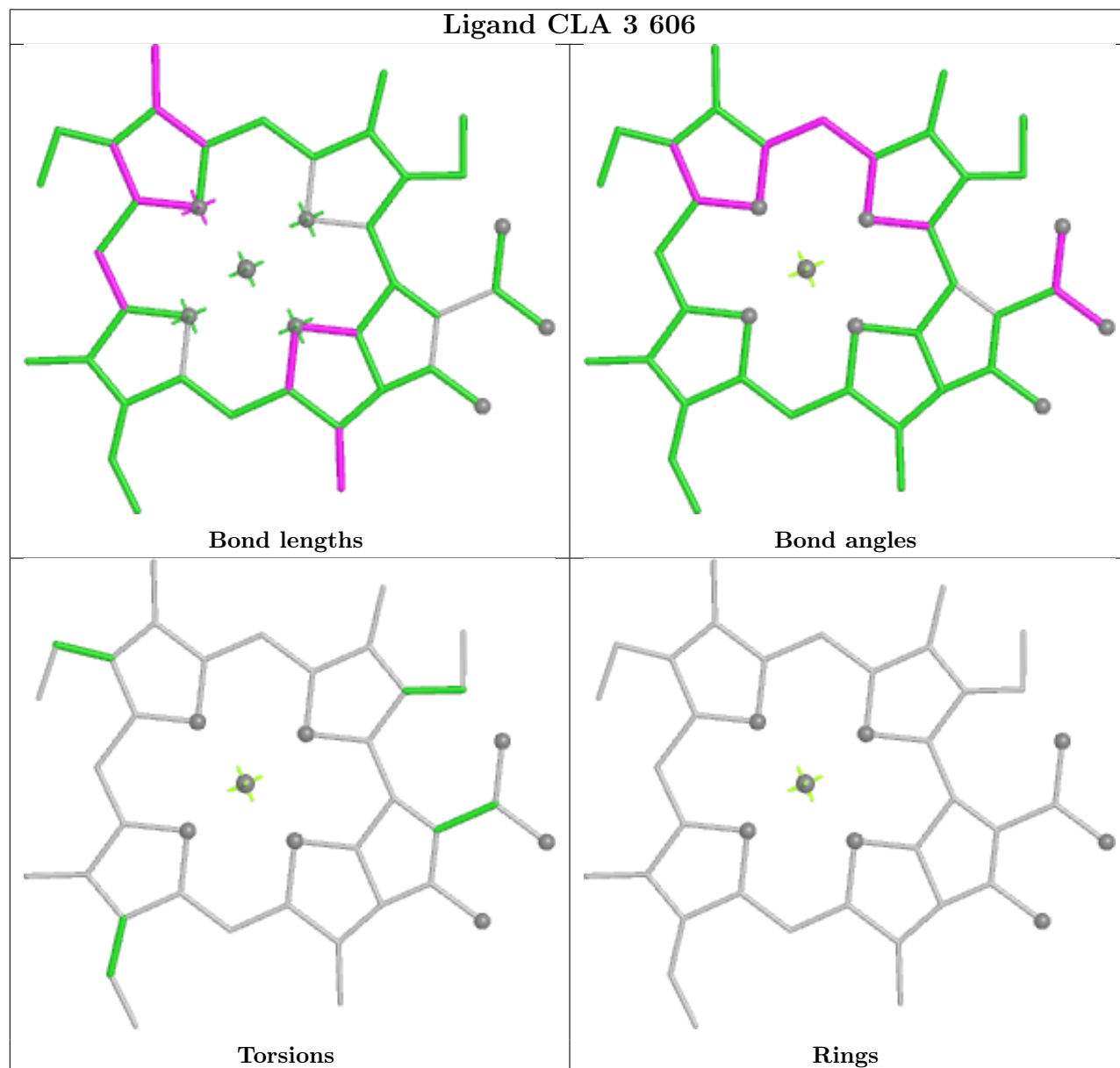
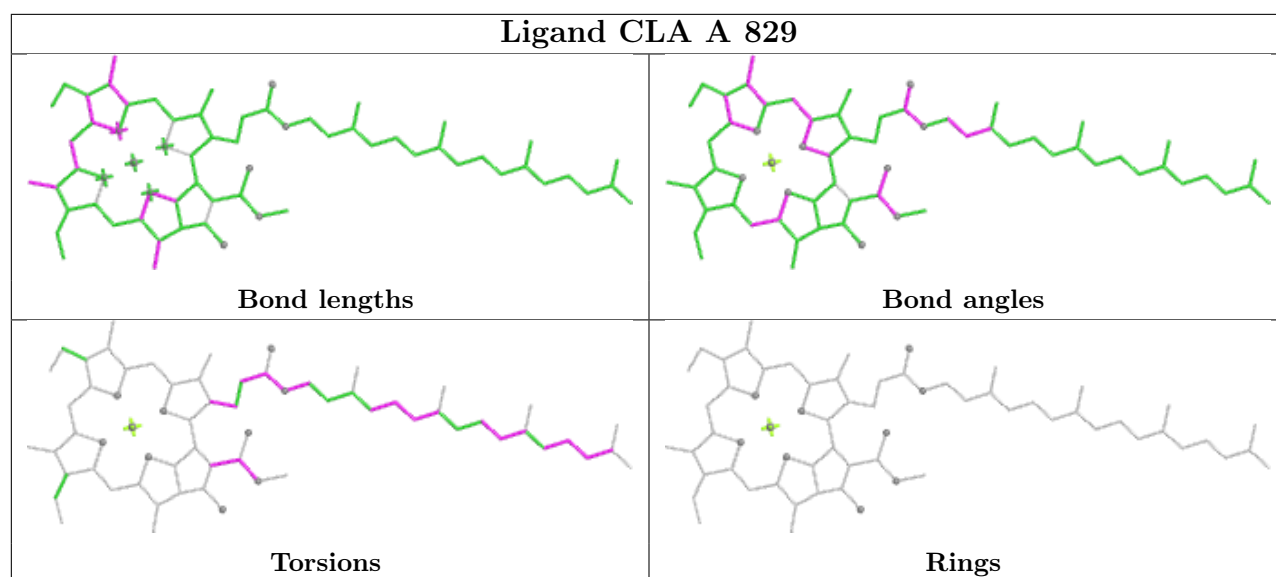


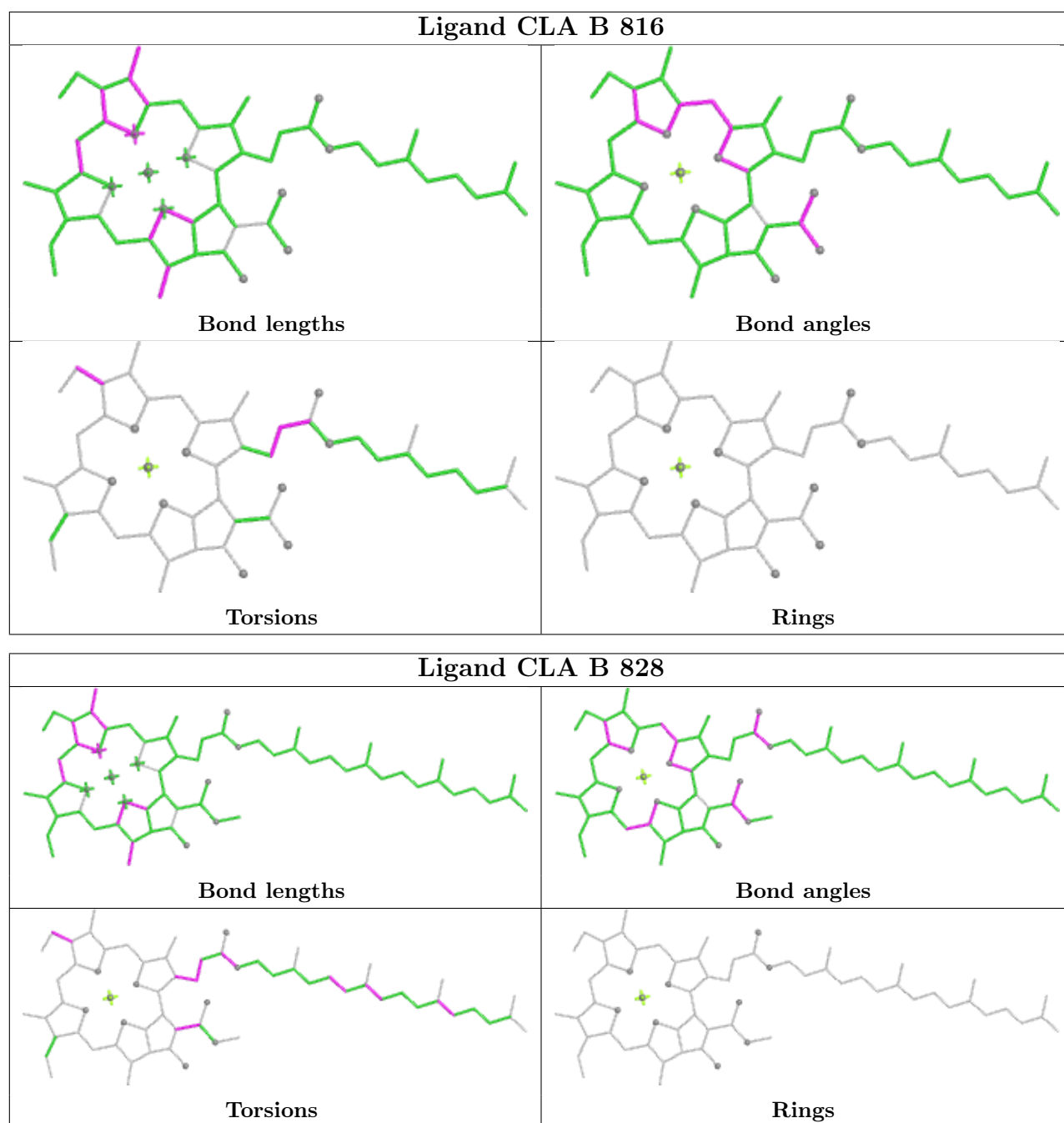
Ligand LUT 2 619



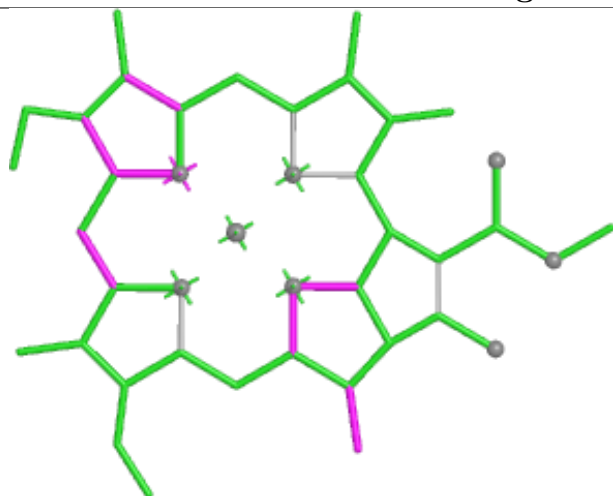
Ligand CLA B 833



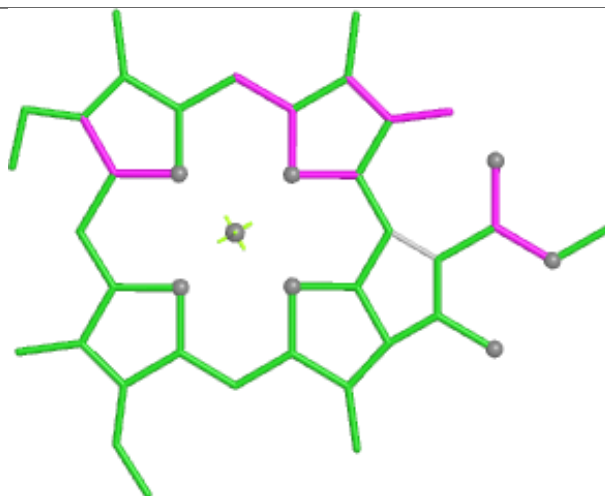




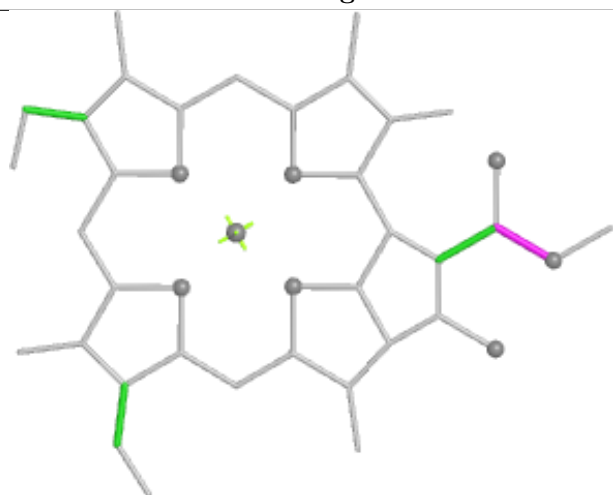
Ligand CLA F 304



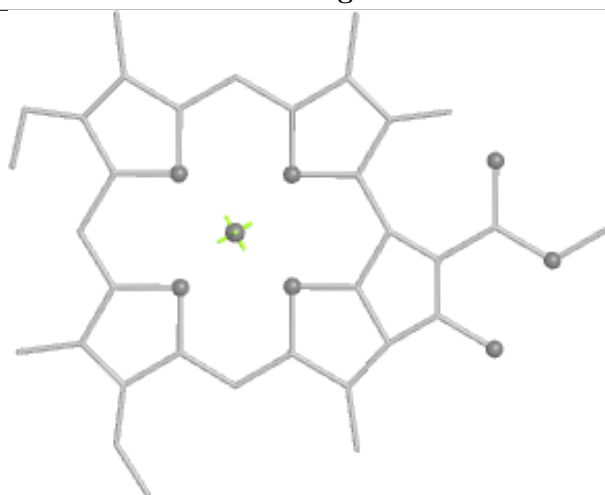
Bond lengths



Bond angles

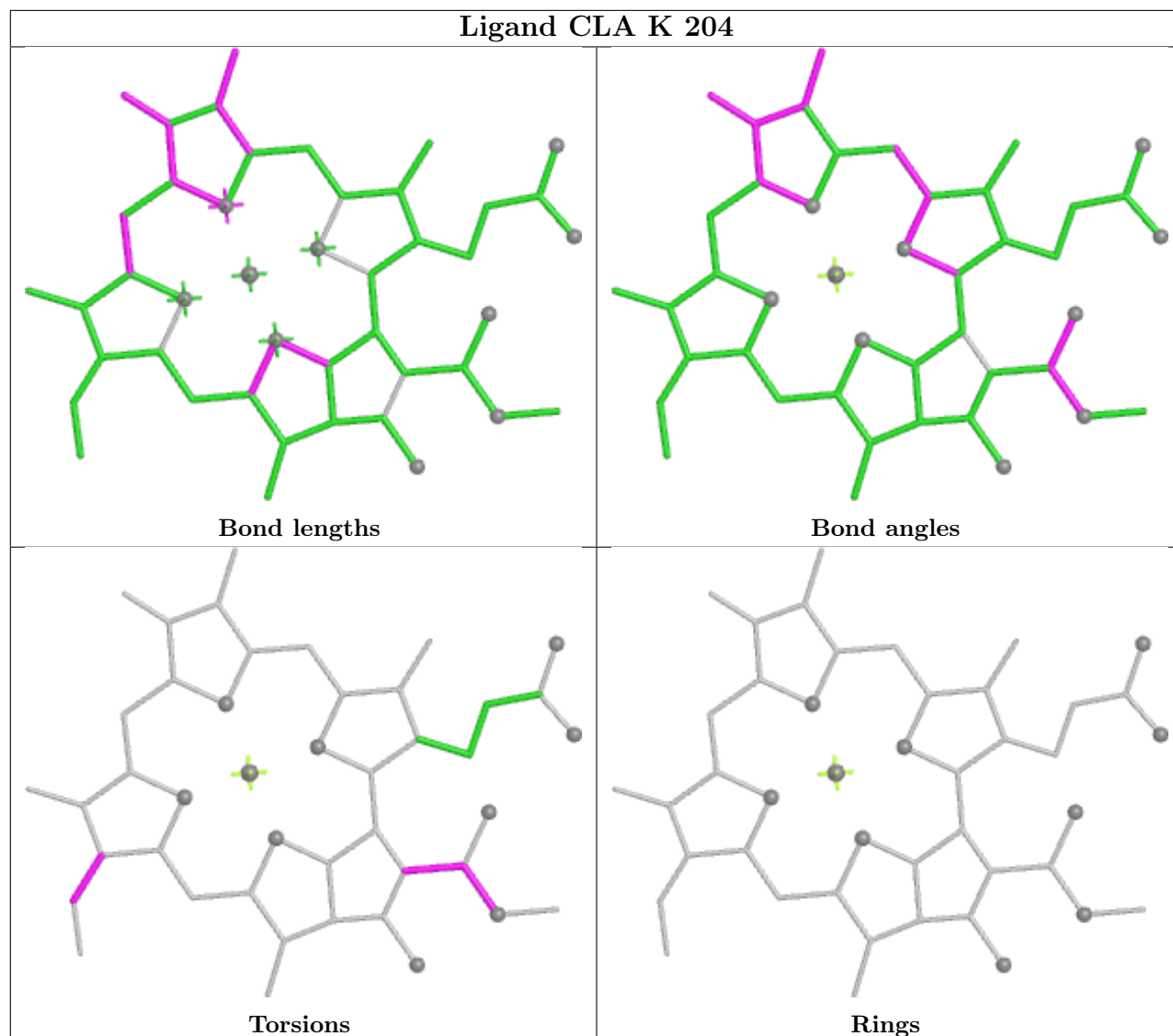


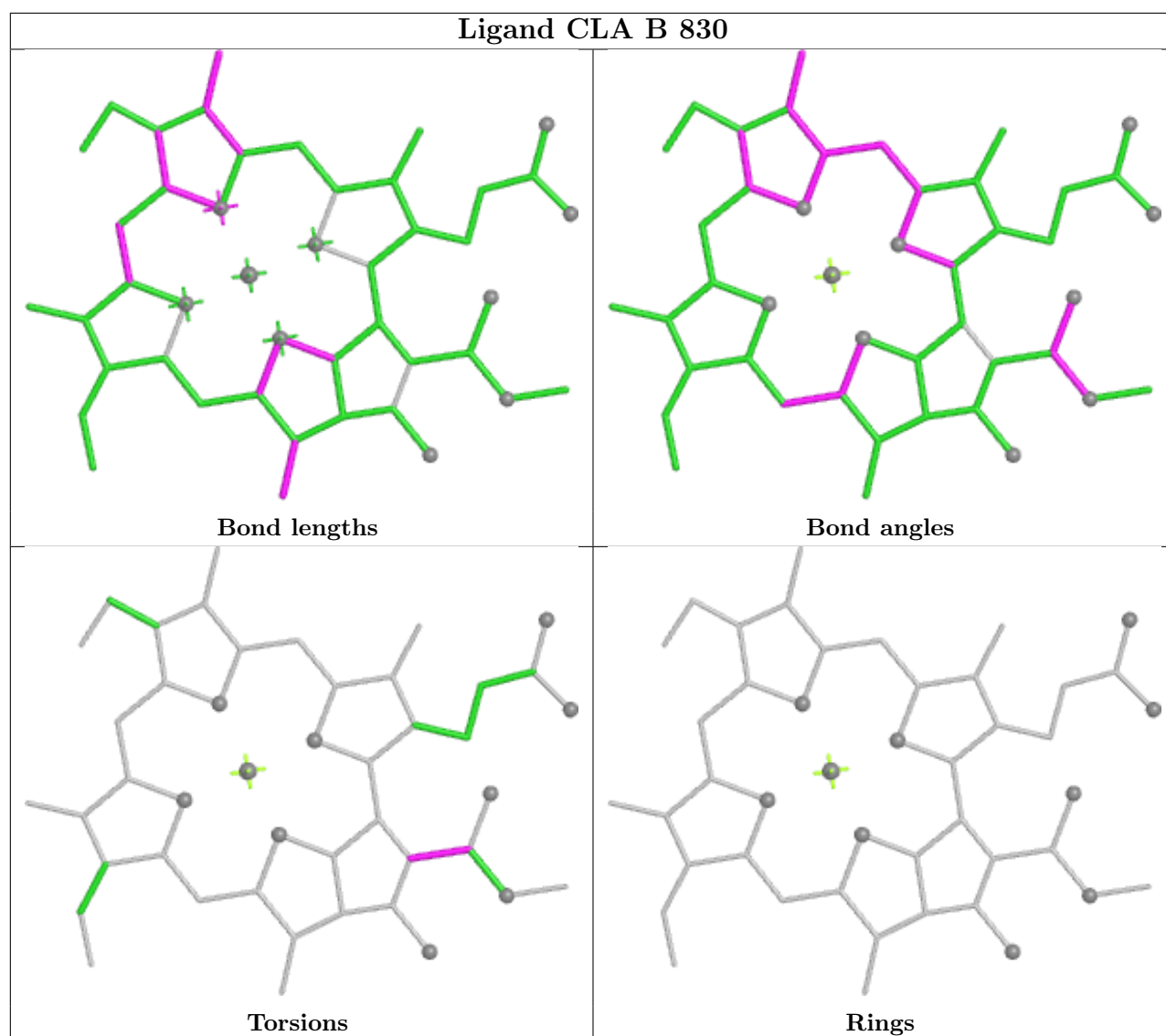
Torsions

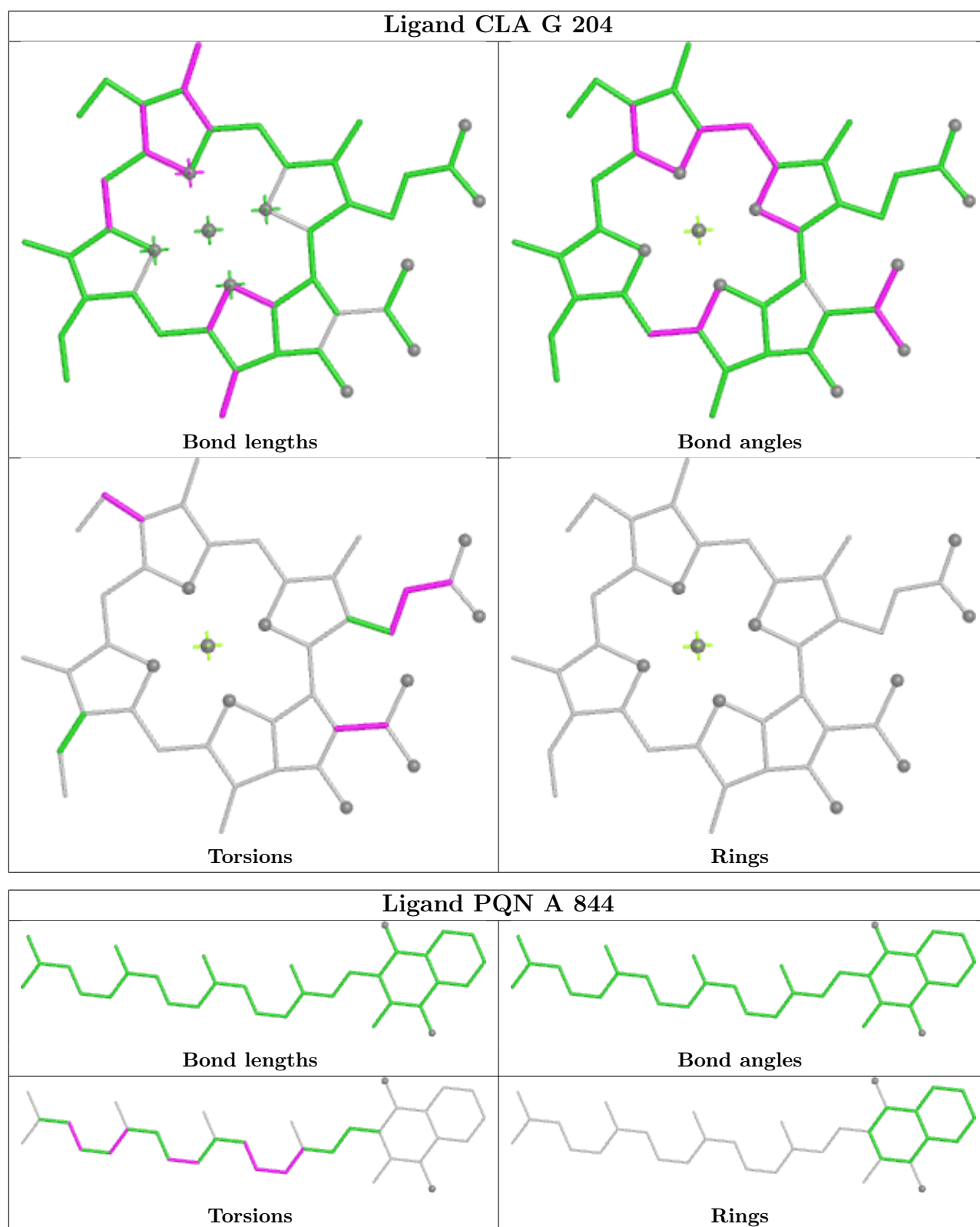


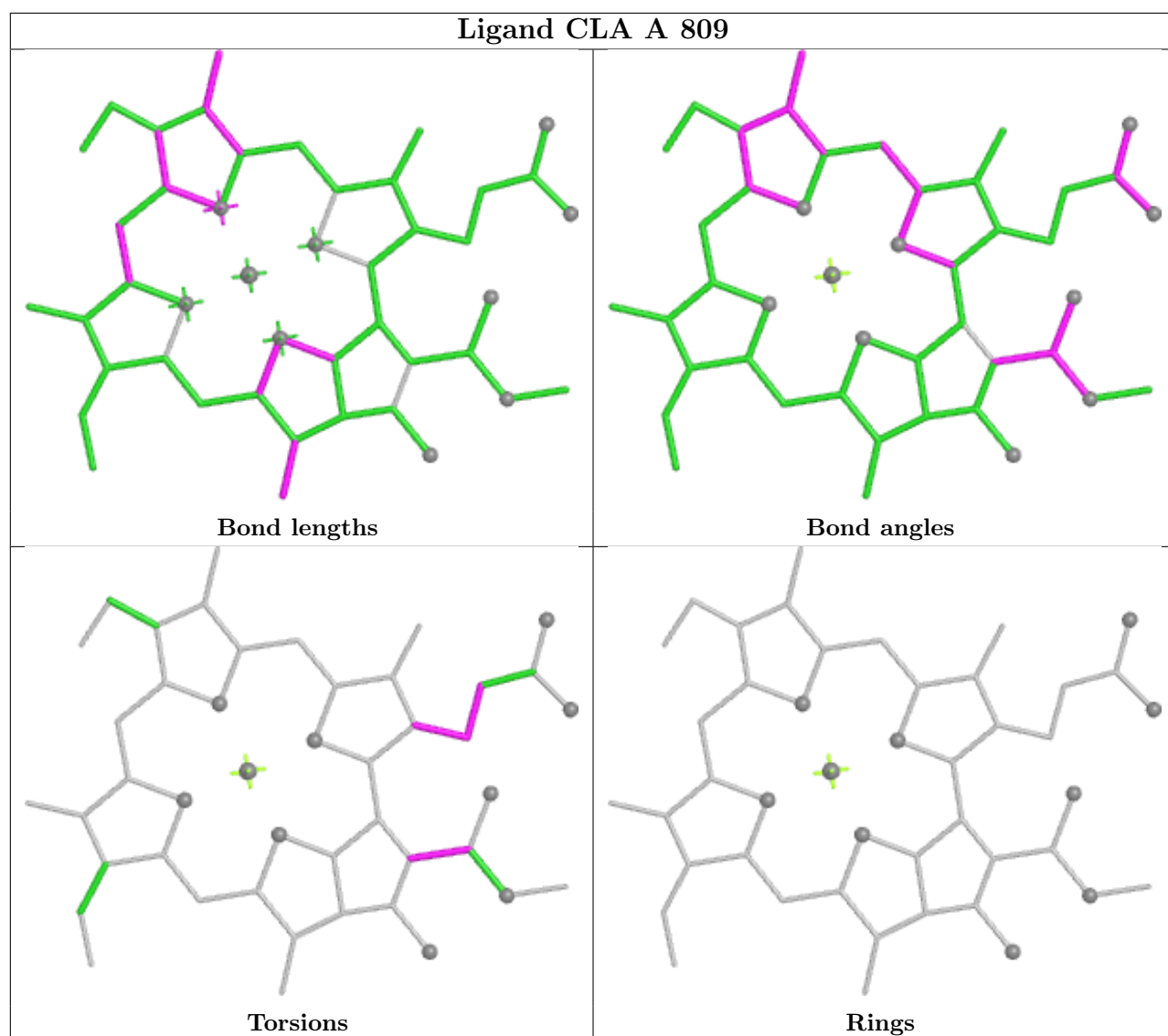
Rings

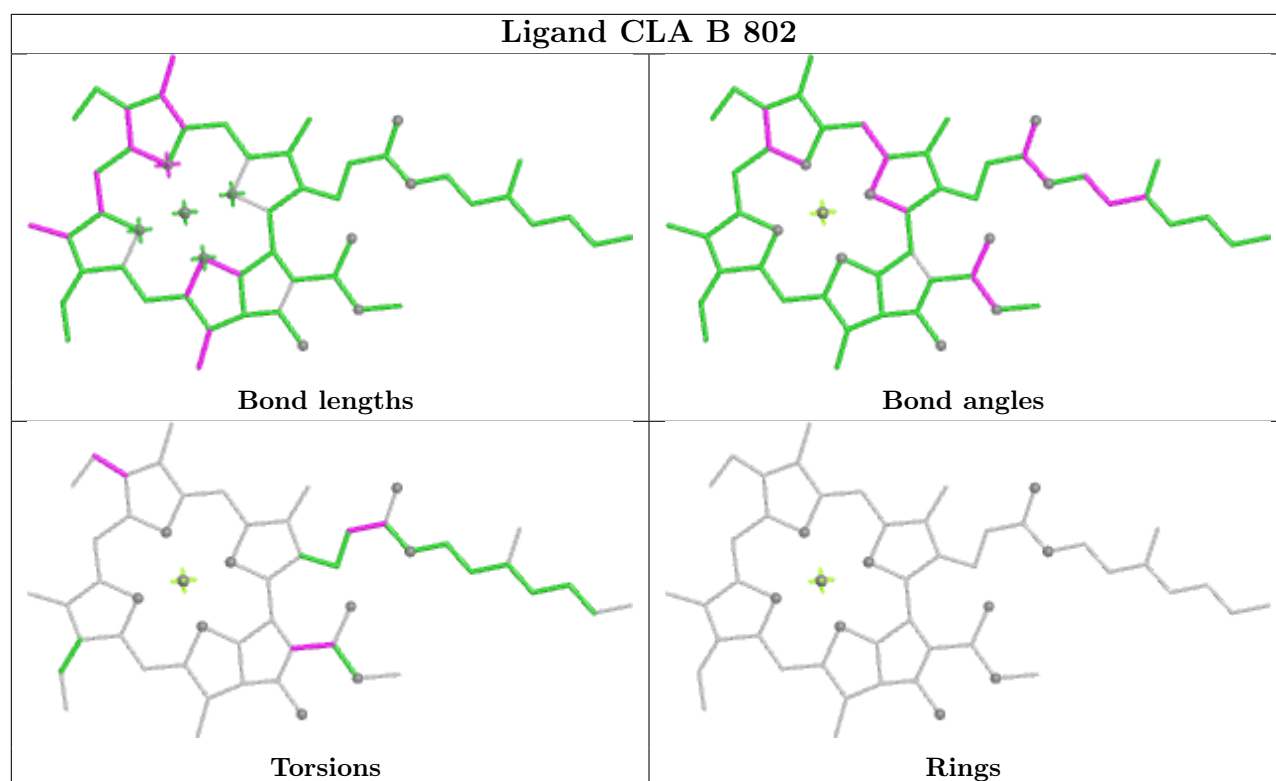
Ligand CLA K 204



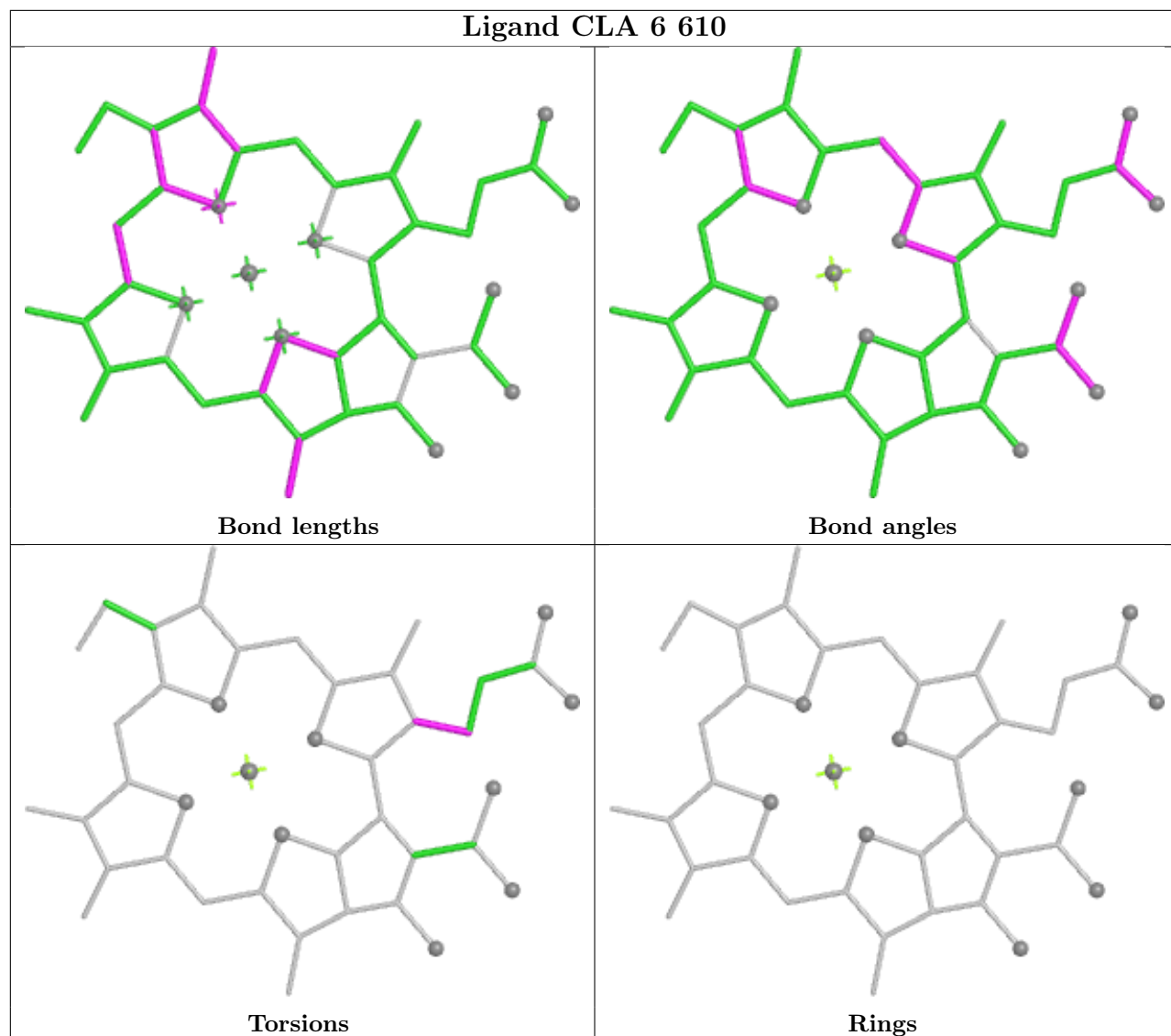


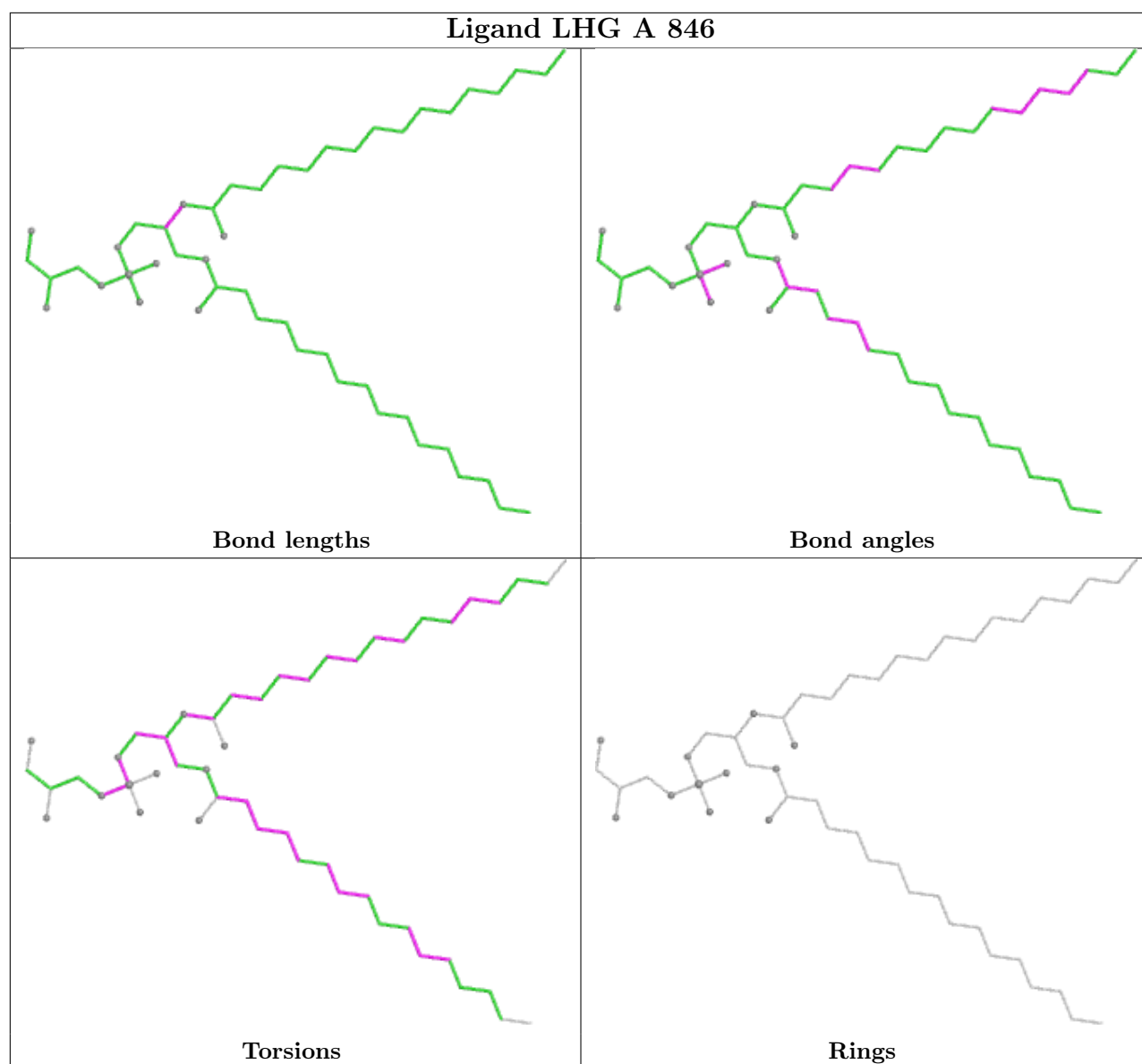




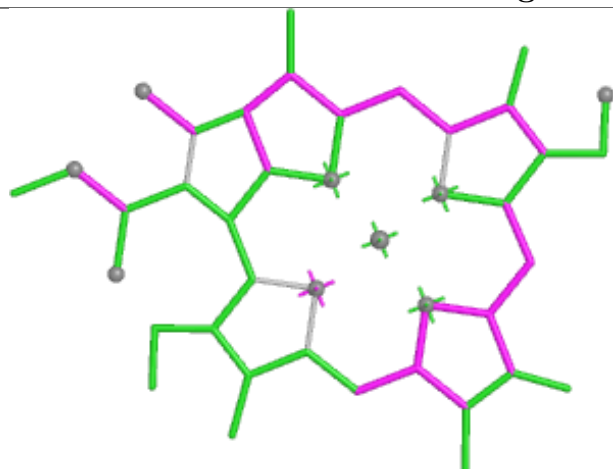


Ligand CLA 6 610

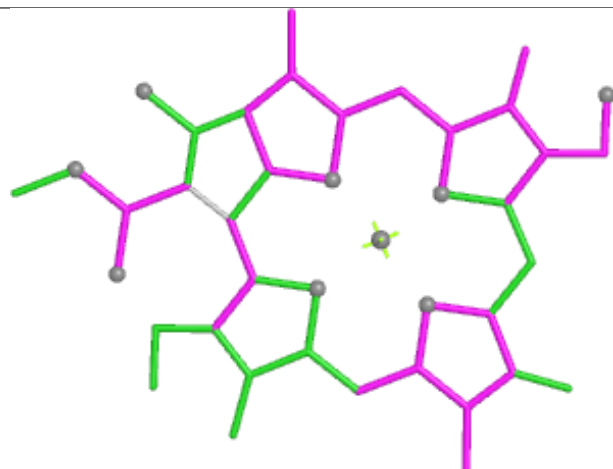




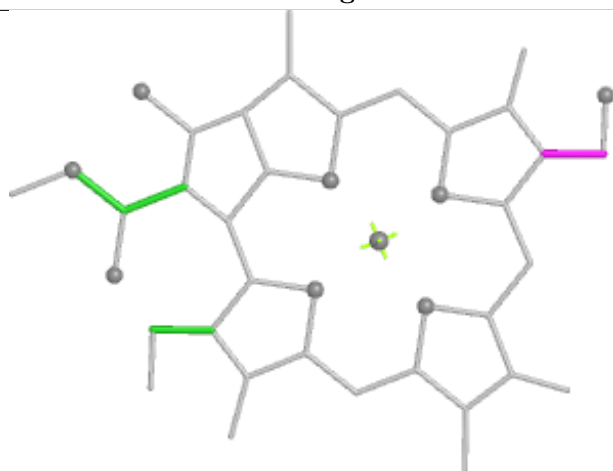
Ligand CHL 5 606



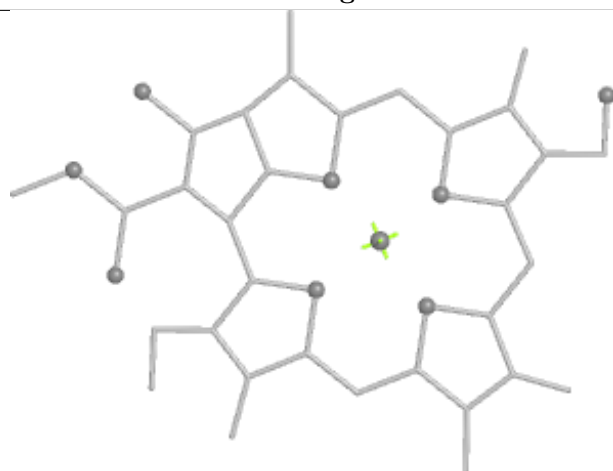
Bond lengths



Bond angles

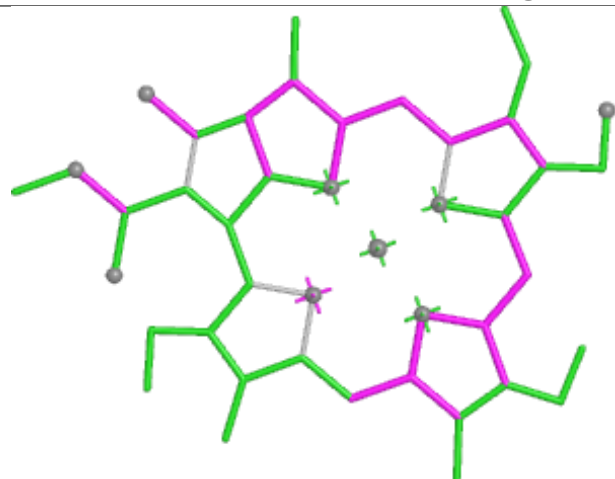


Torsions

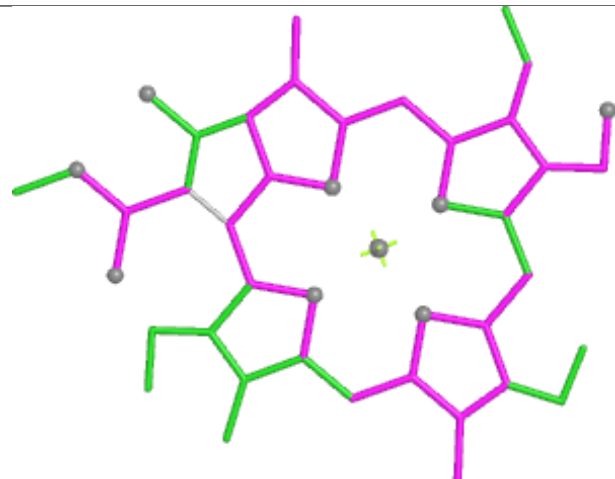


Rings

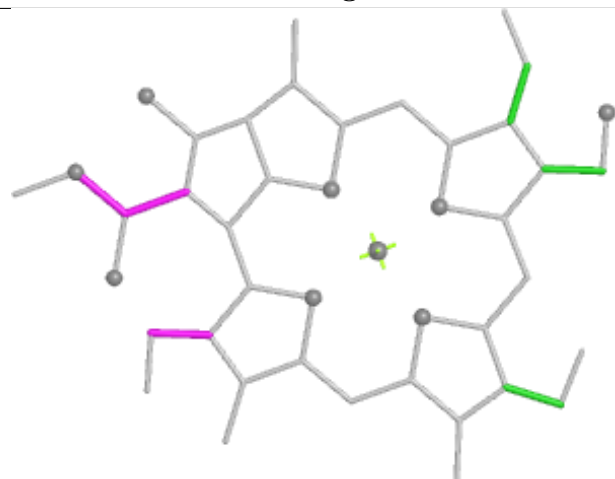
Ligand CHL 5 607



Bond lengths



Bond angles



Torsions



Rings

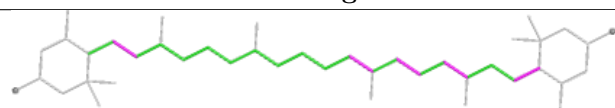
Ligand LUT 3 618



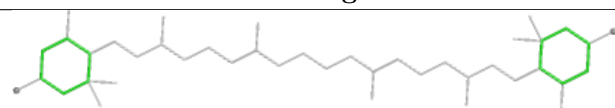
Bond lengths



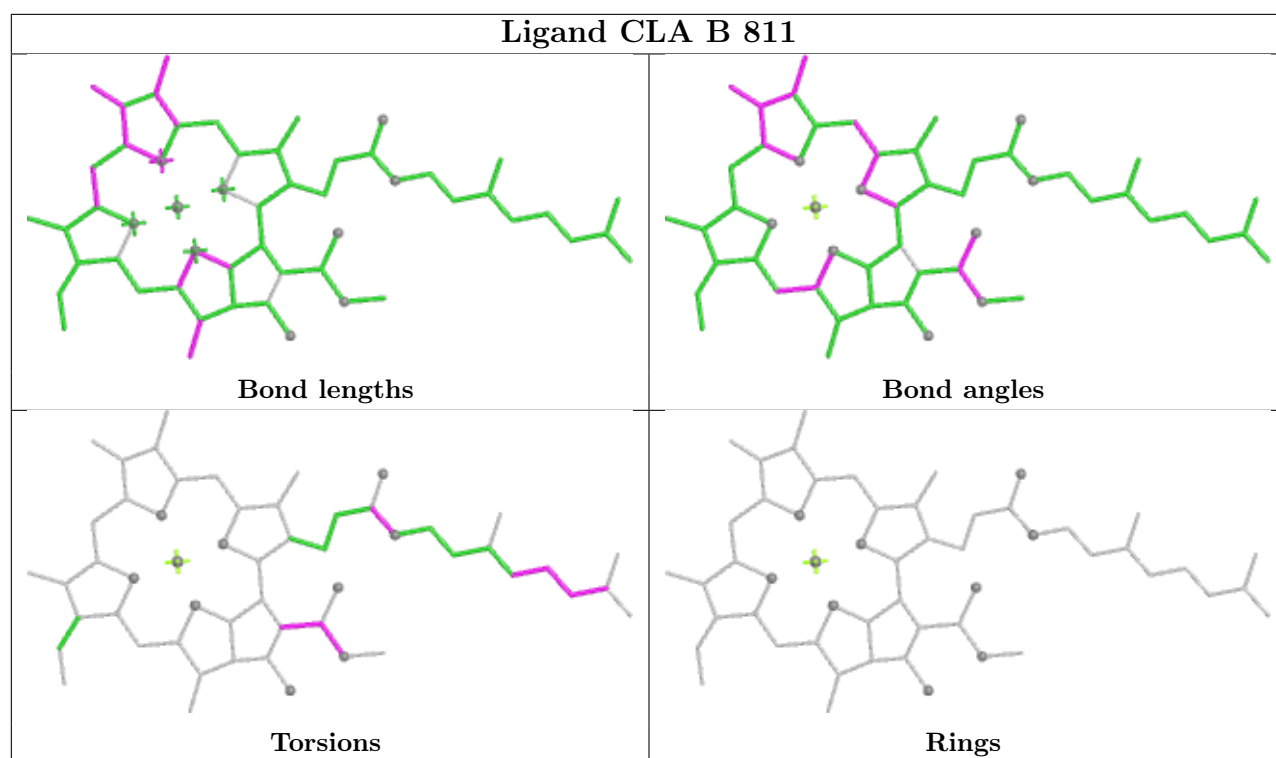
Bond angles



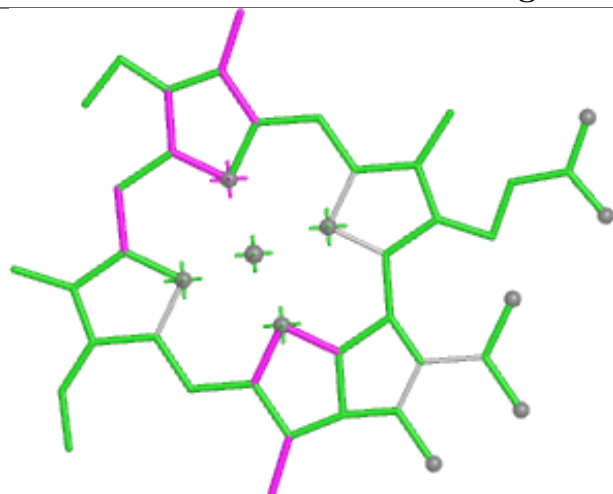
Torsions



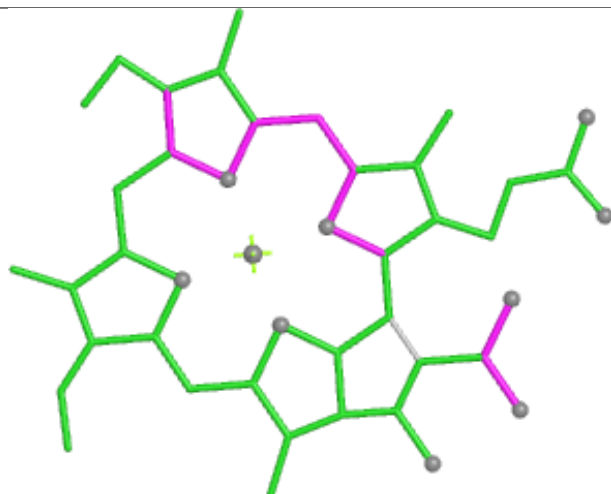
Rings



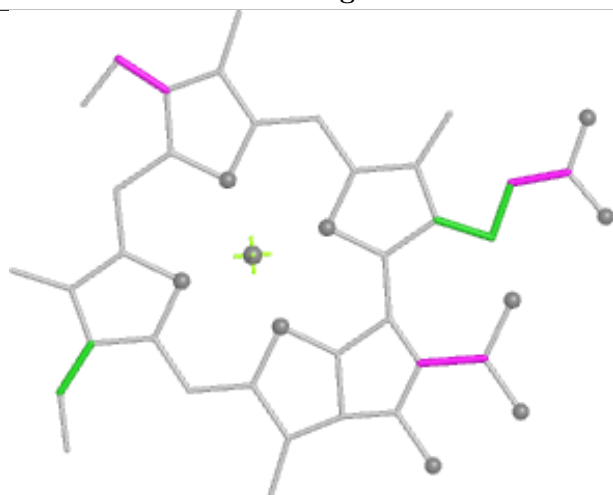
Ligand CLA 5 603



Bond lengths



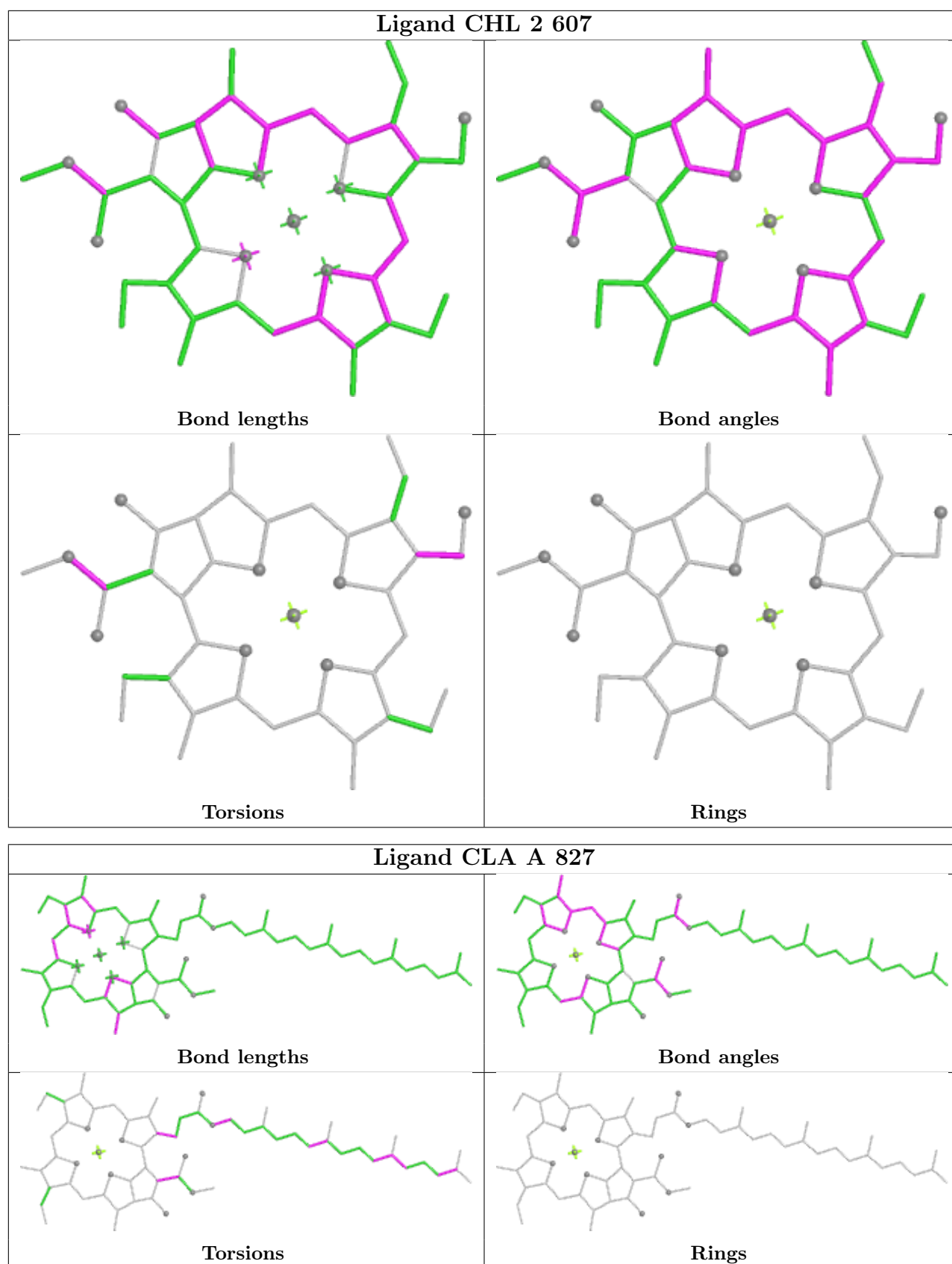
Bond angles

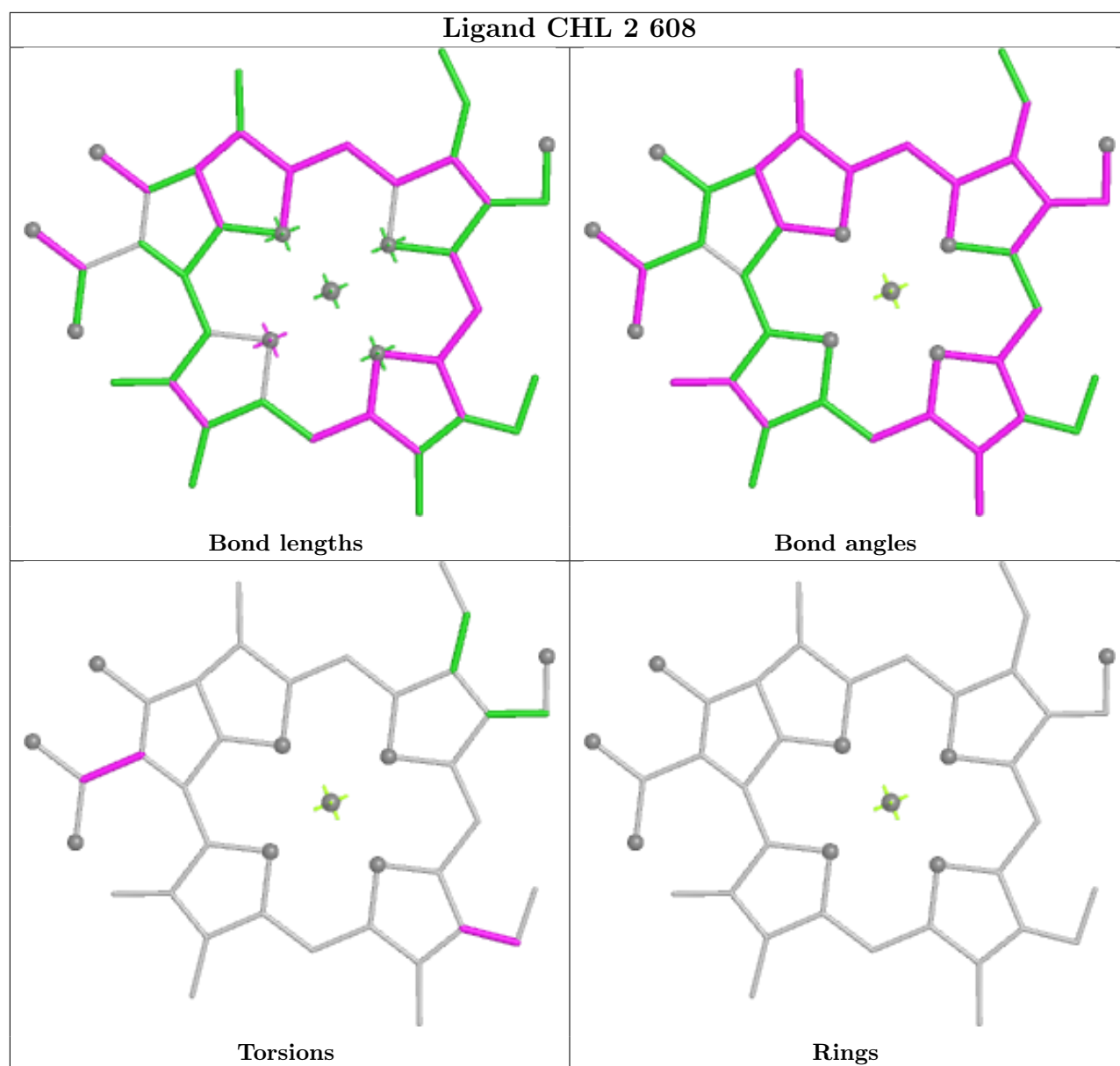


Torsions

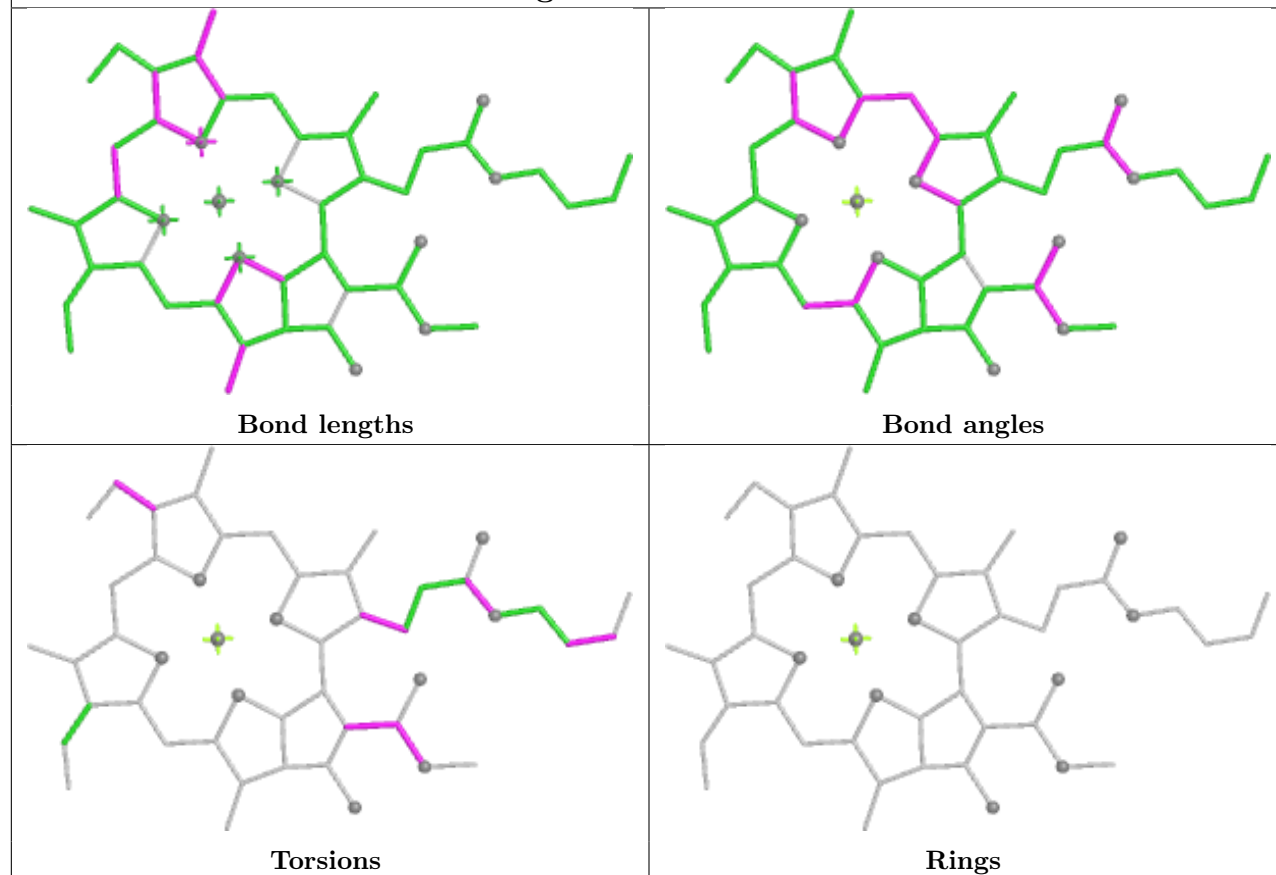


Rings

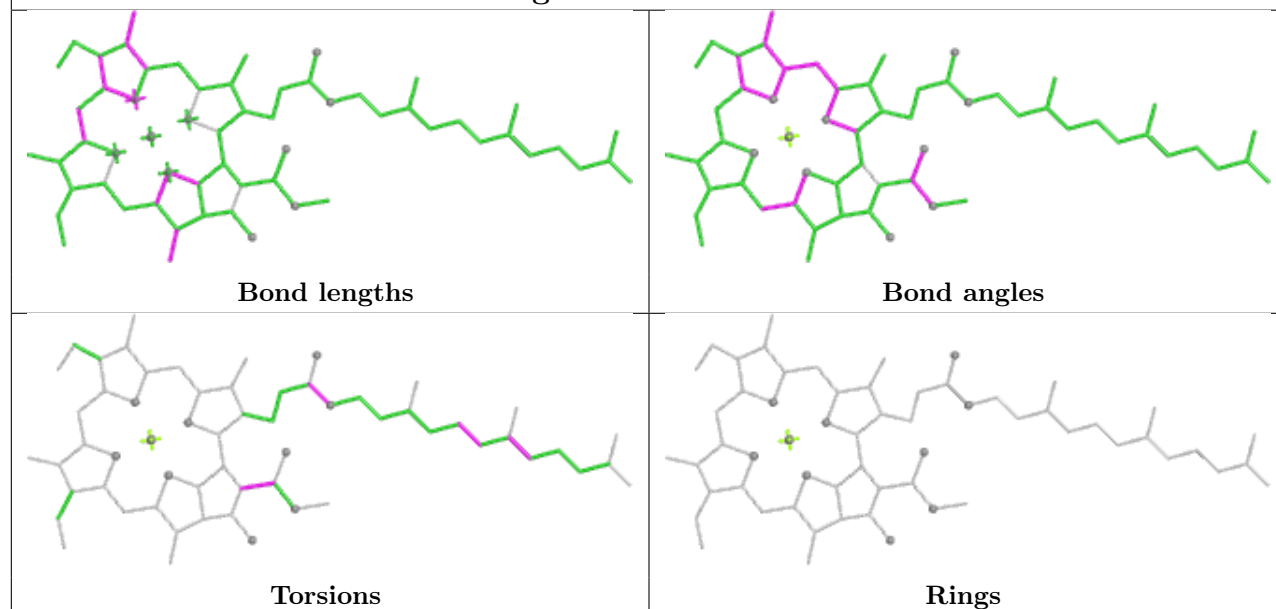


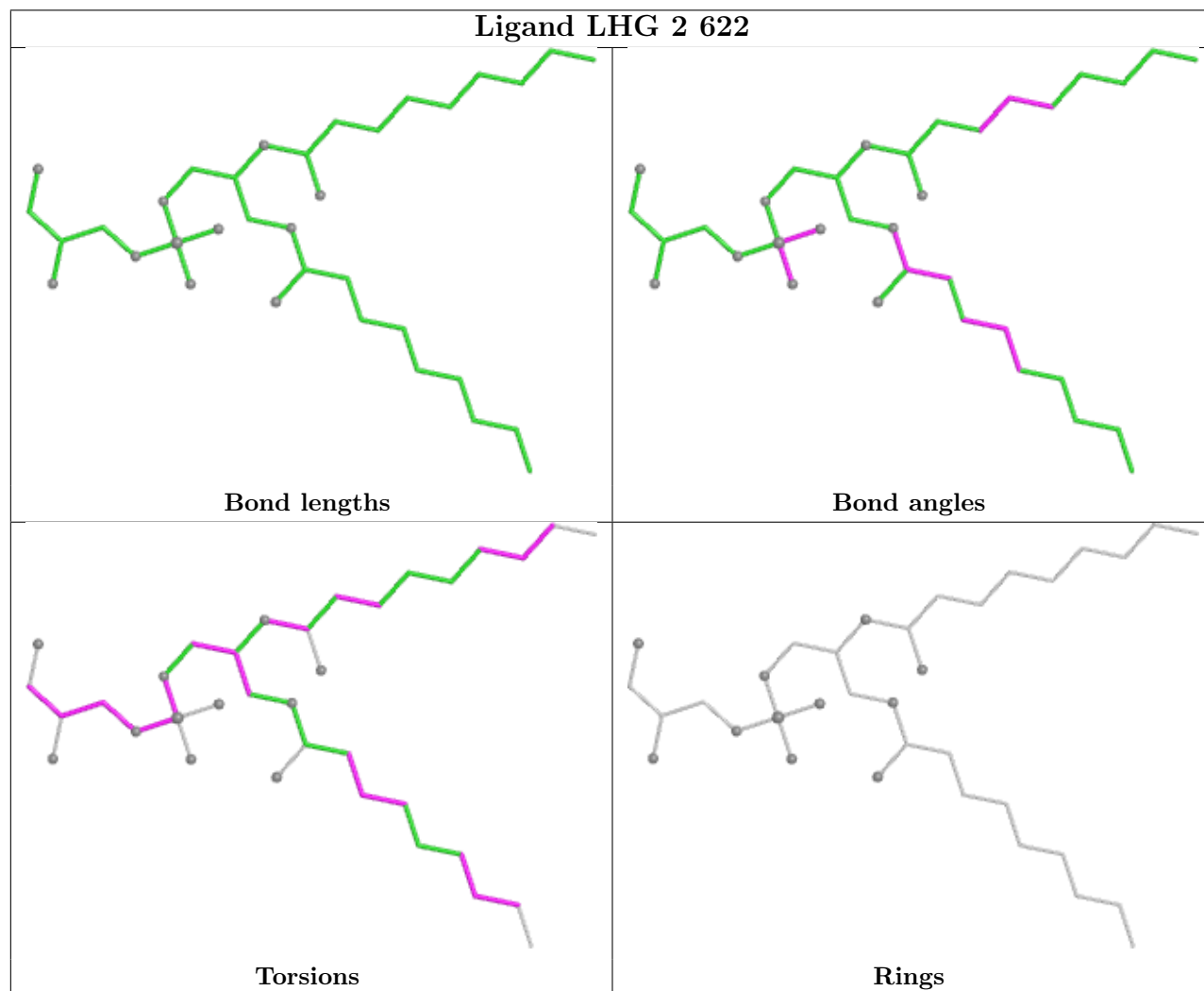
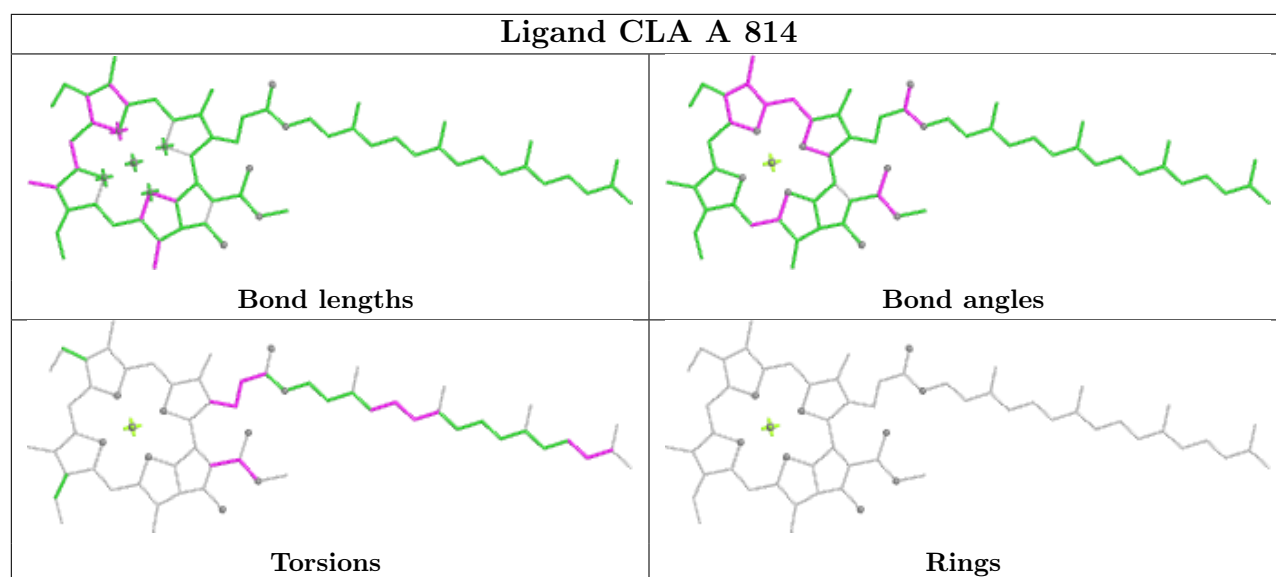


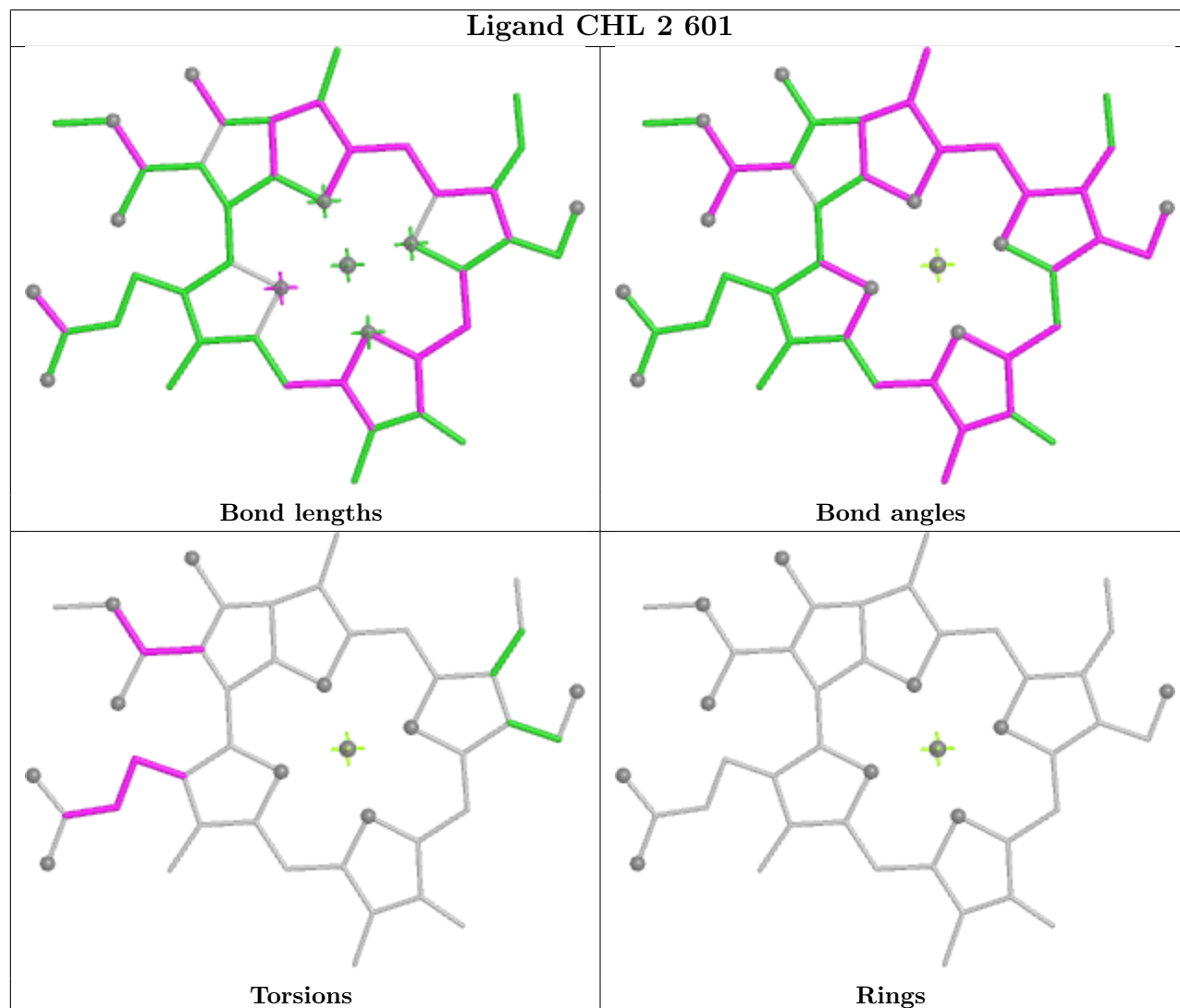
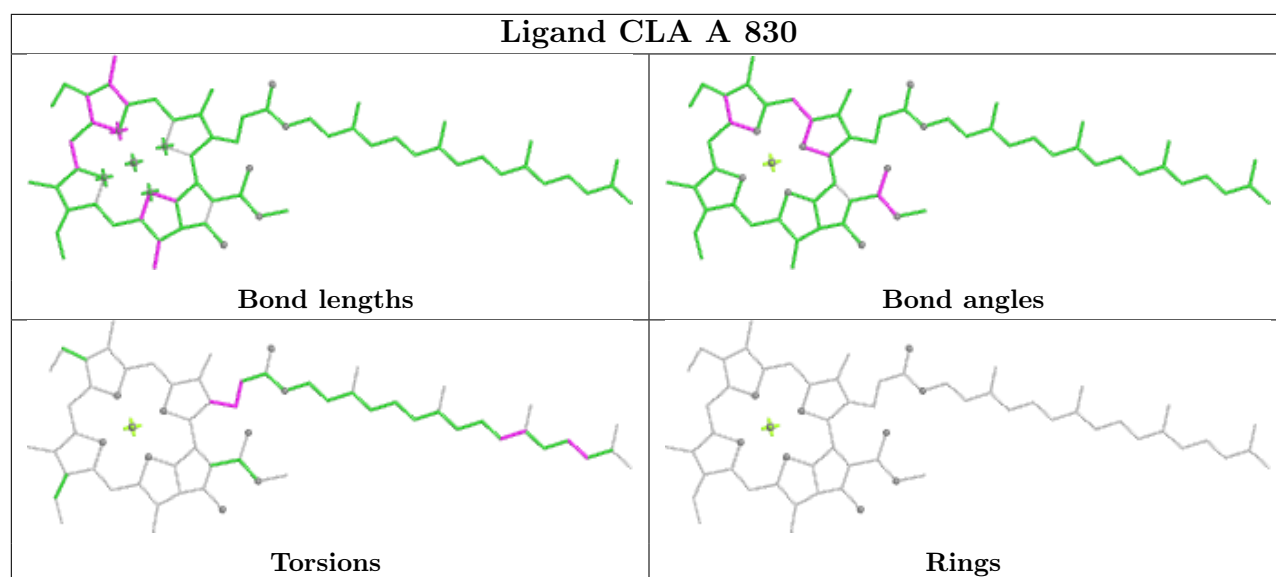
Ligand CLA 6 604



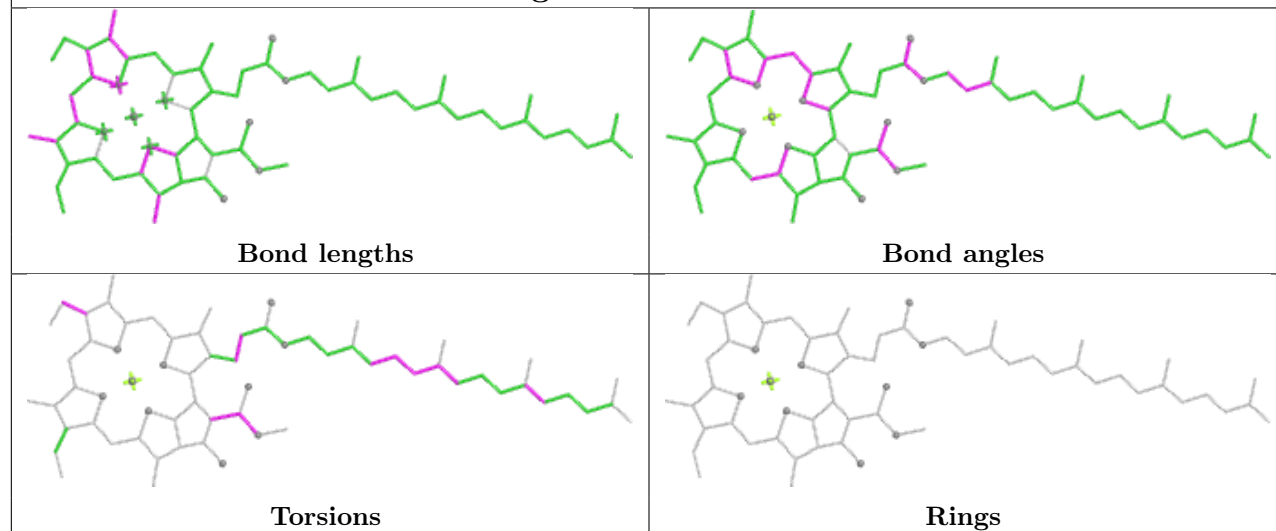
Ligand CLA B 836



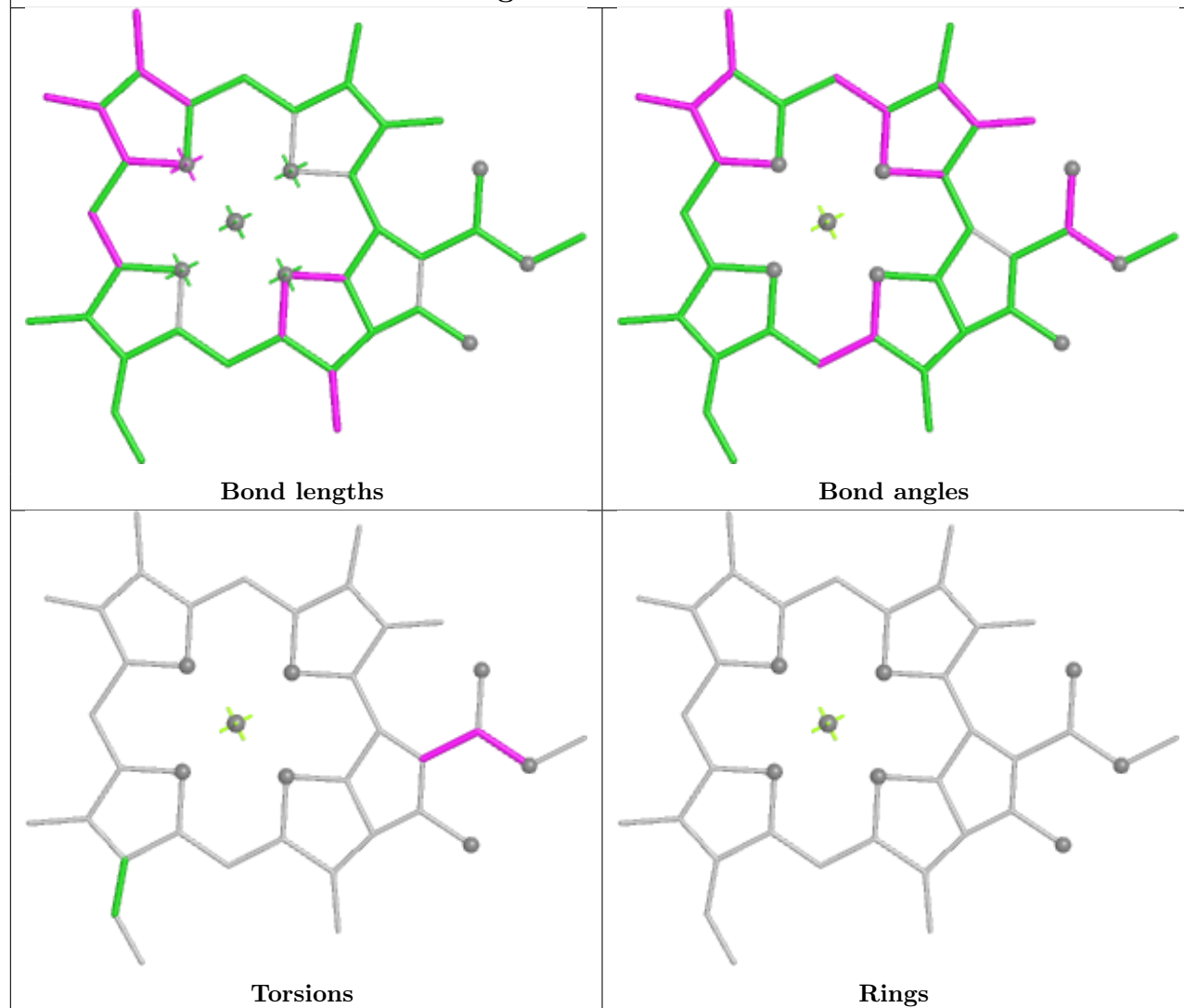


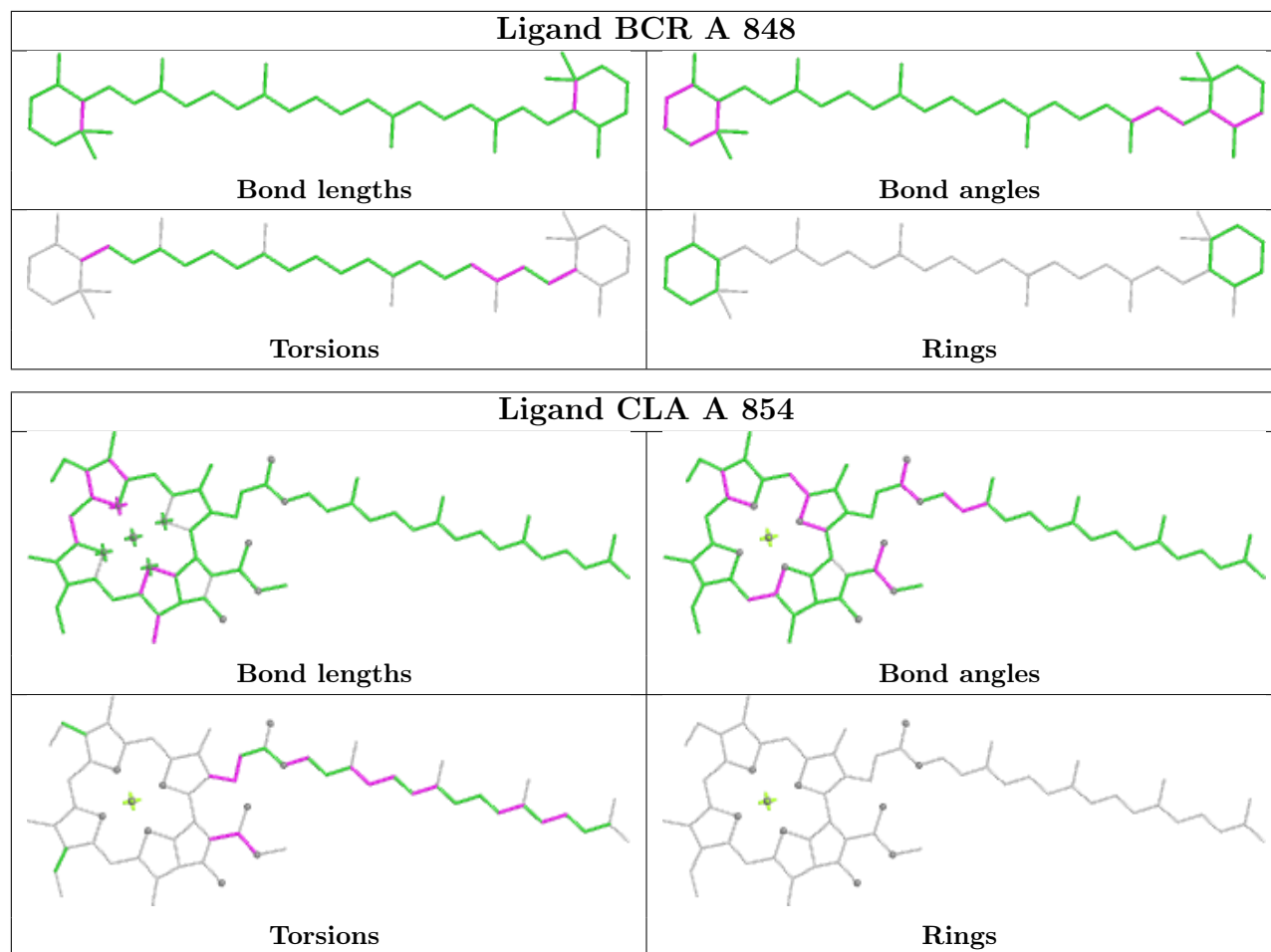


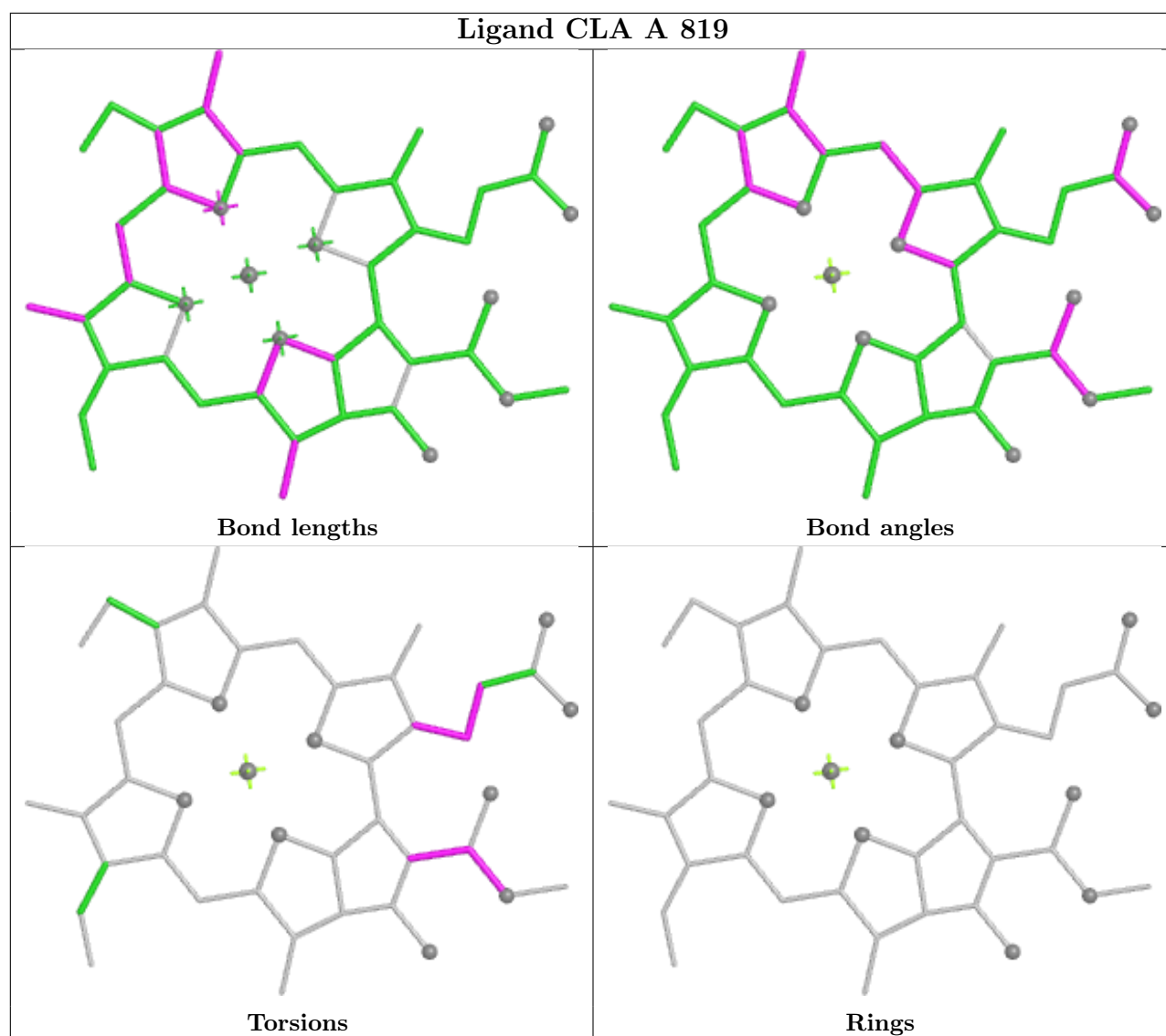
Ligand CLA A 841

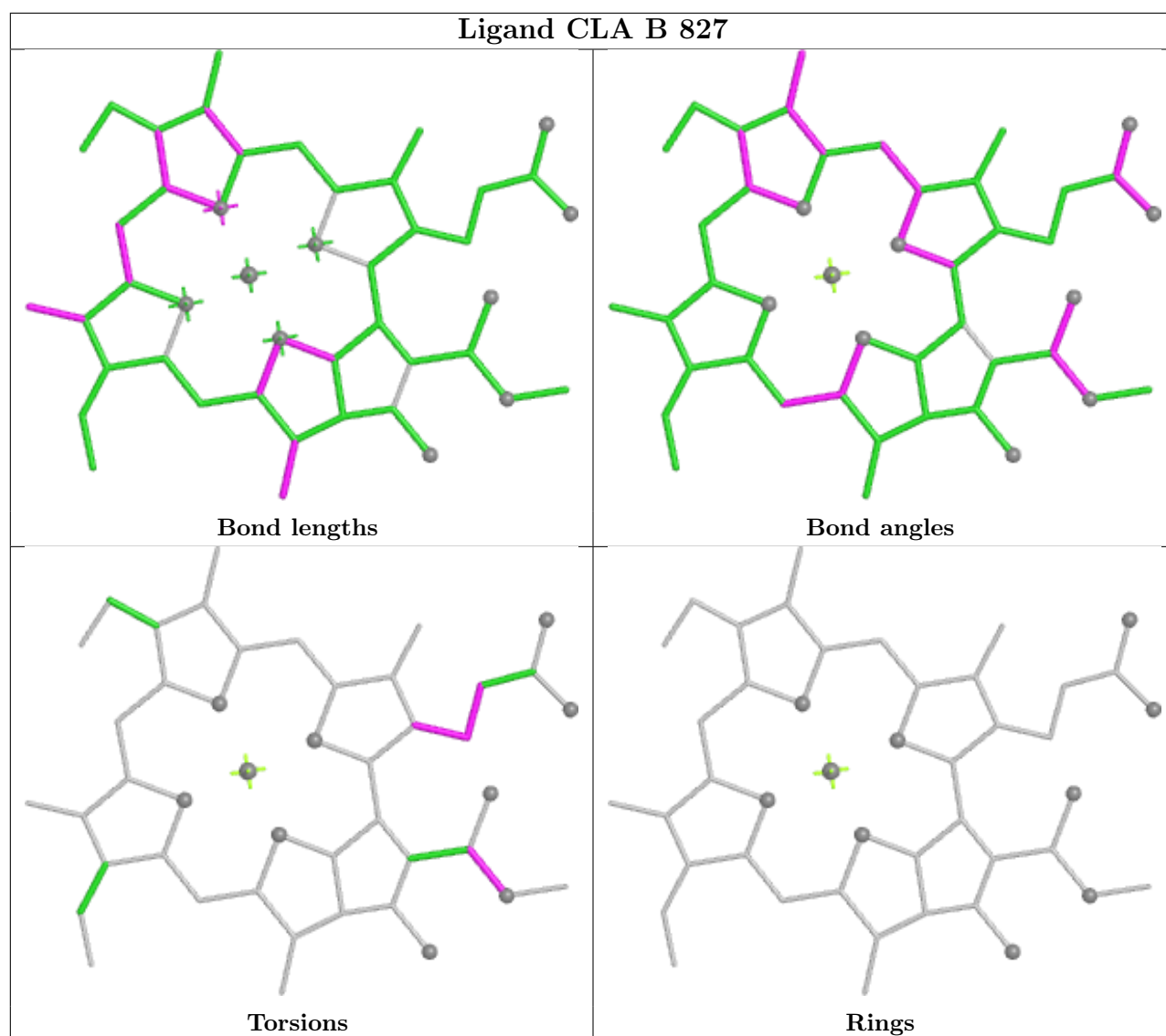


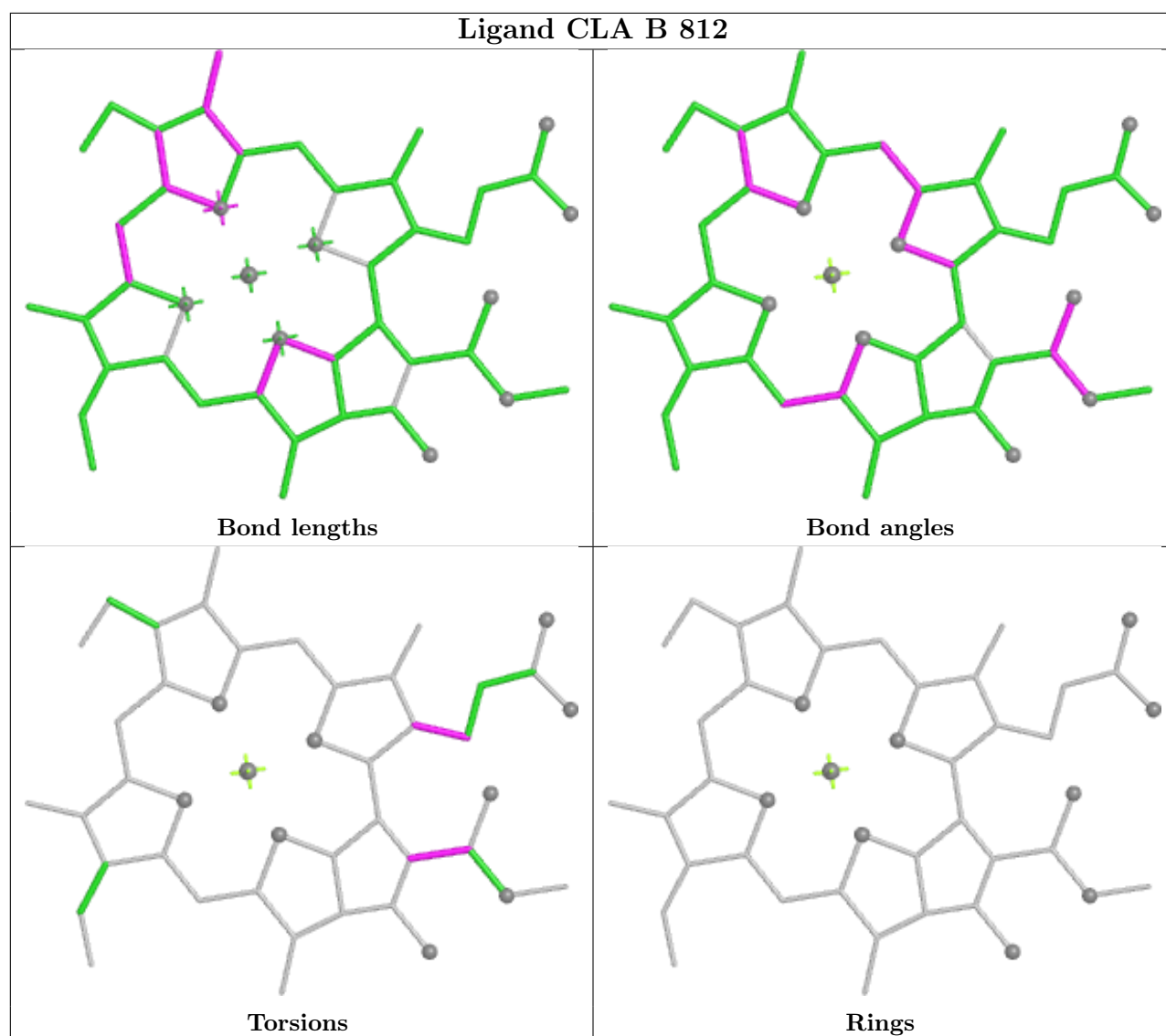
Ligand CLA 6 609

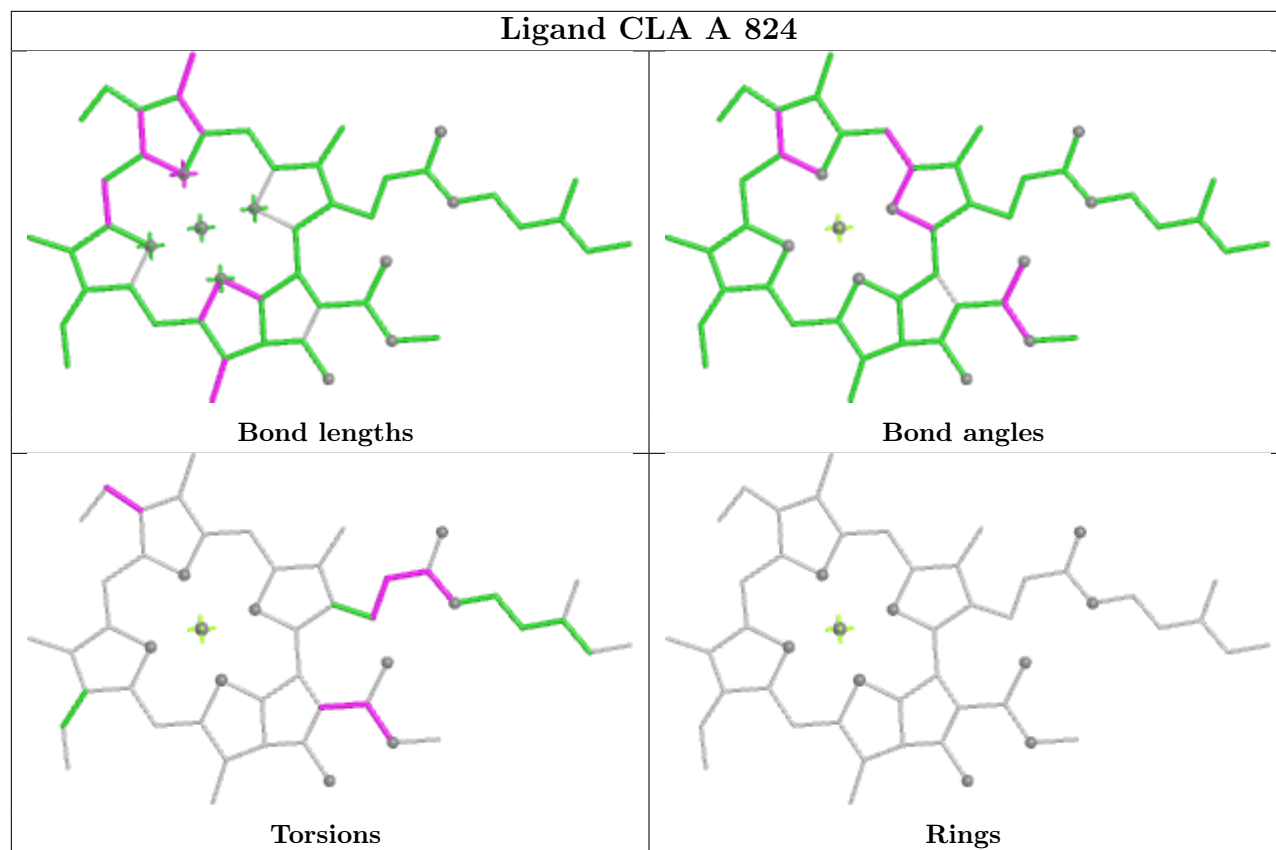




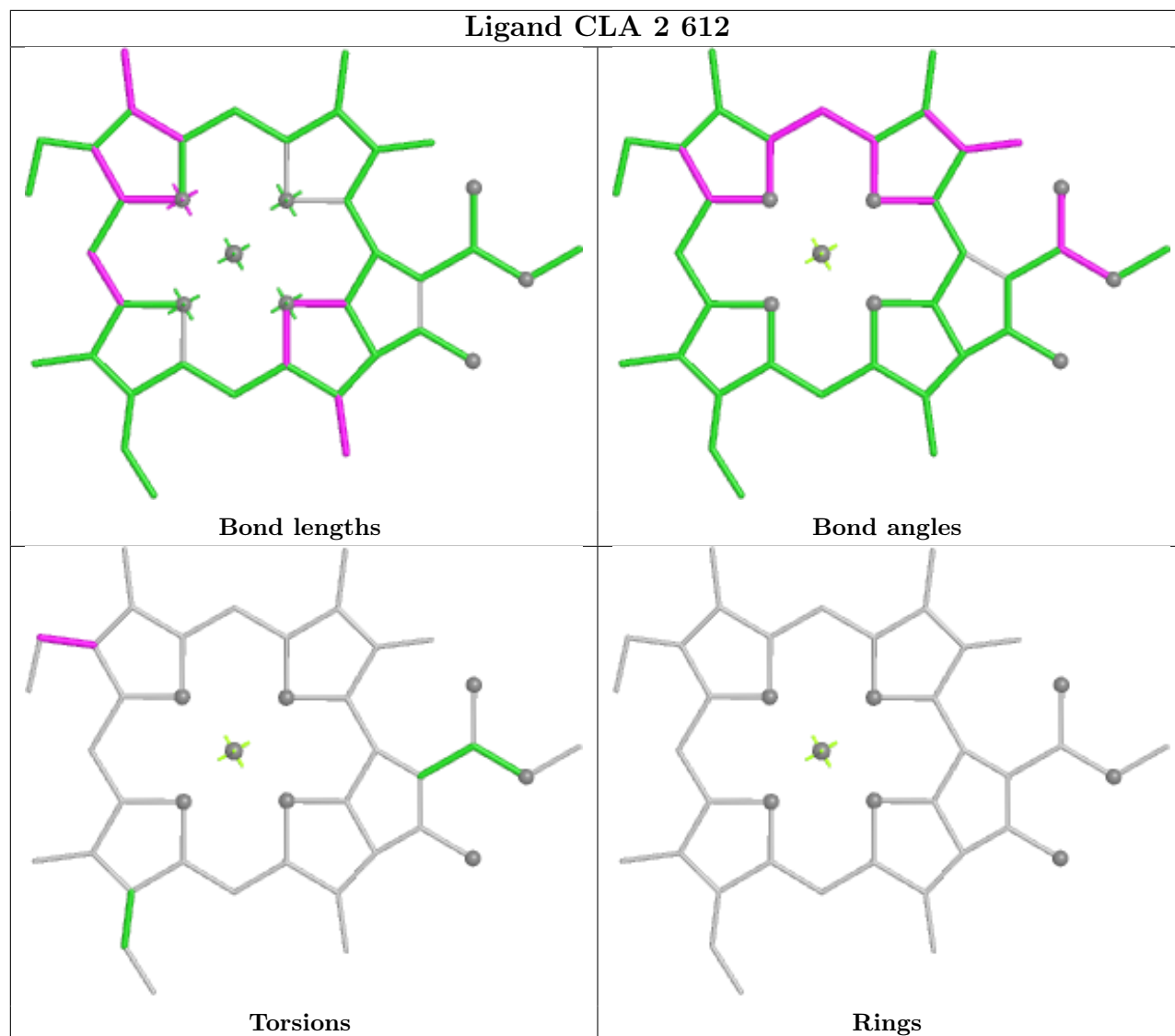




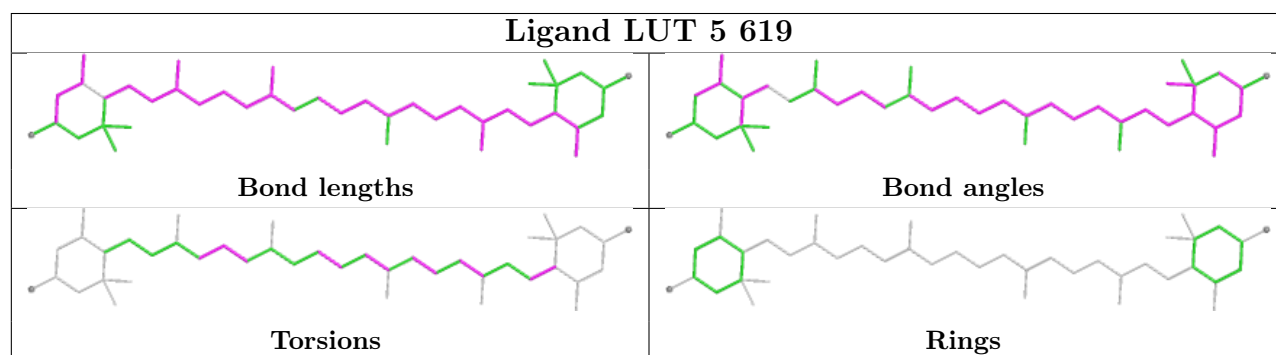




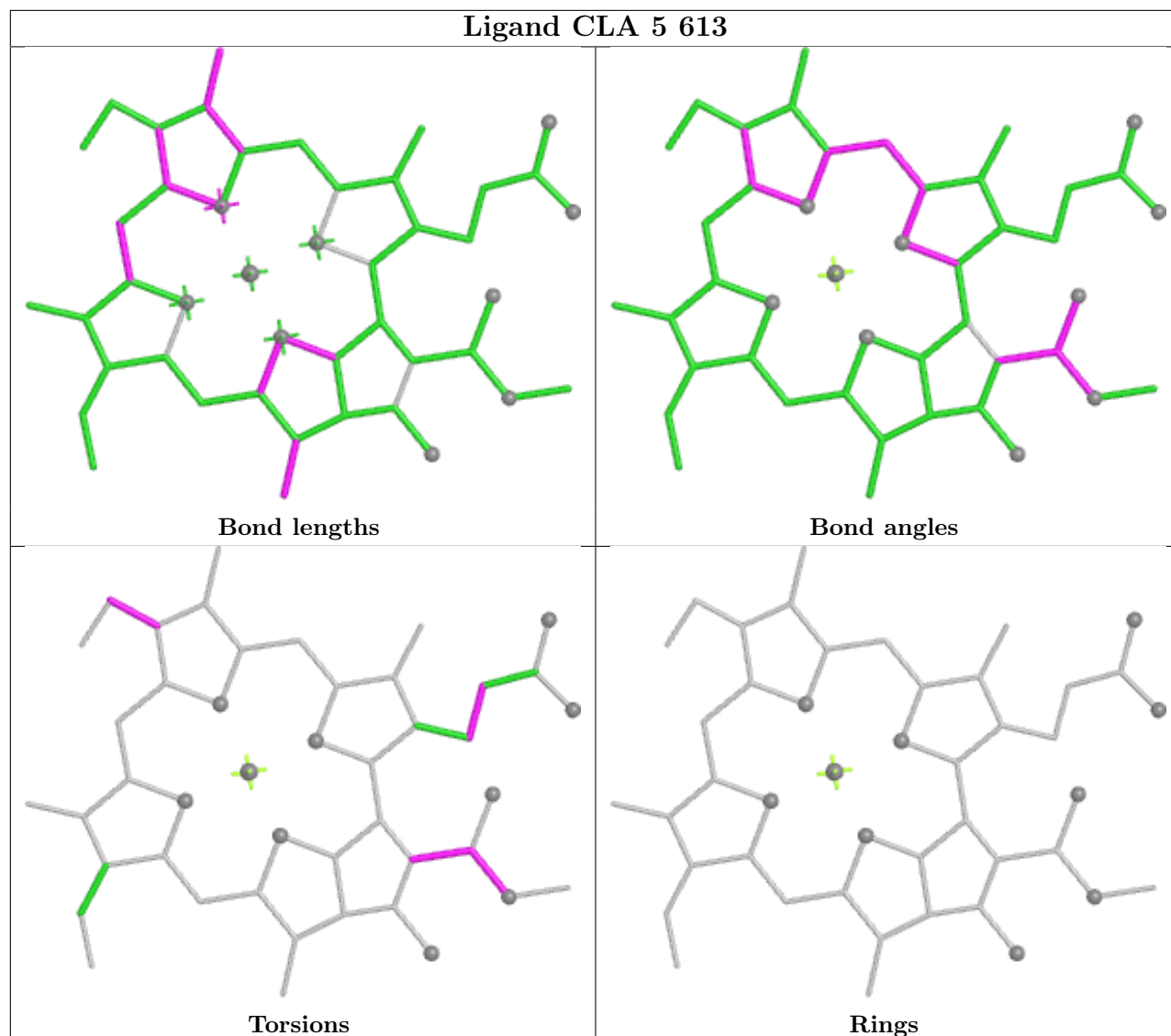
Ligand CLA 2 612



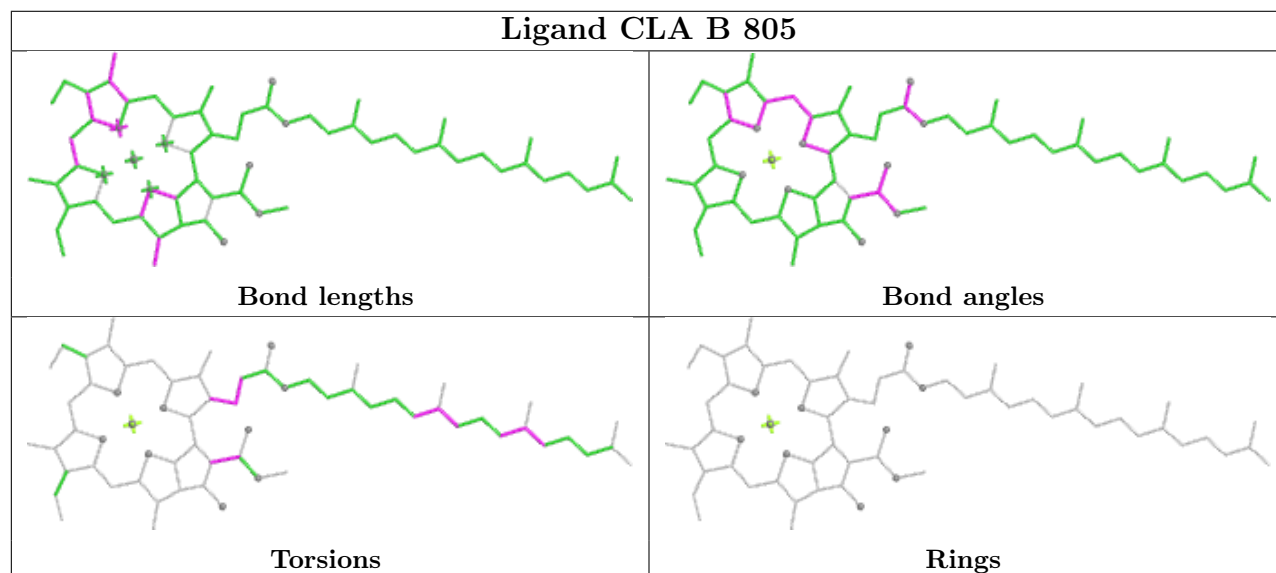
Ligand LUT 5 619

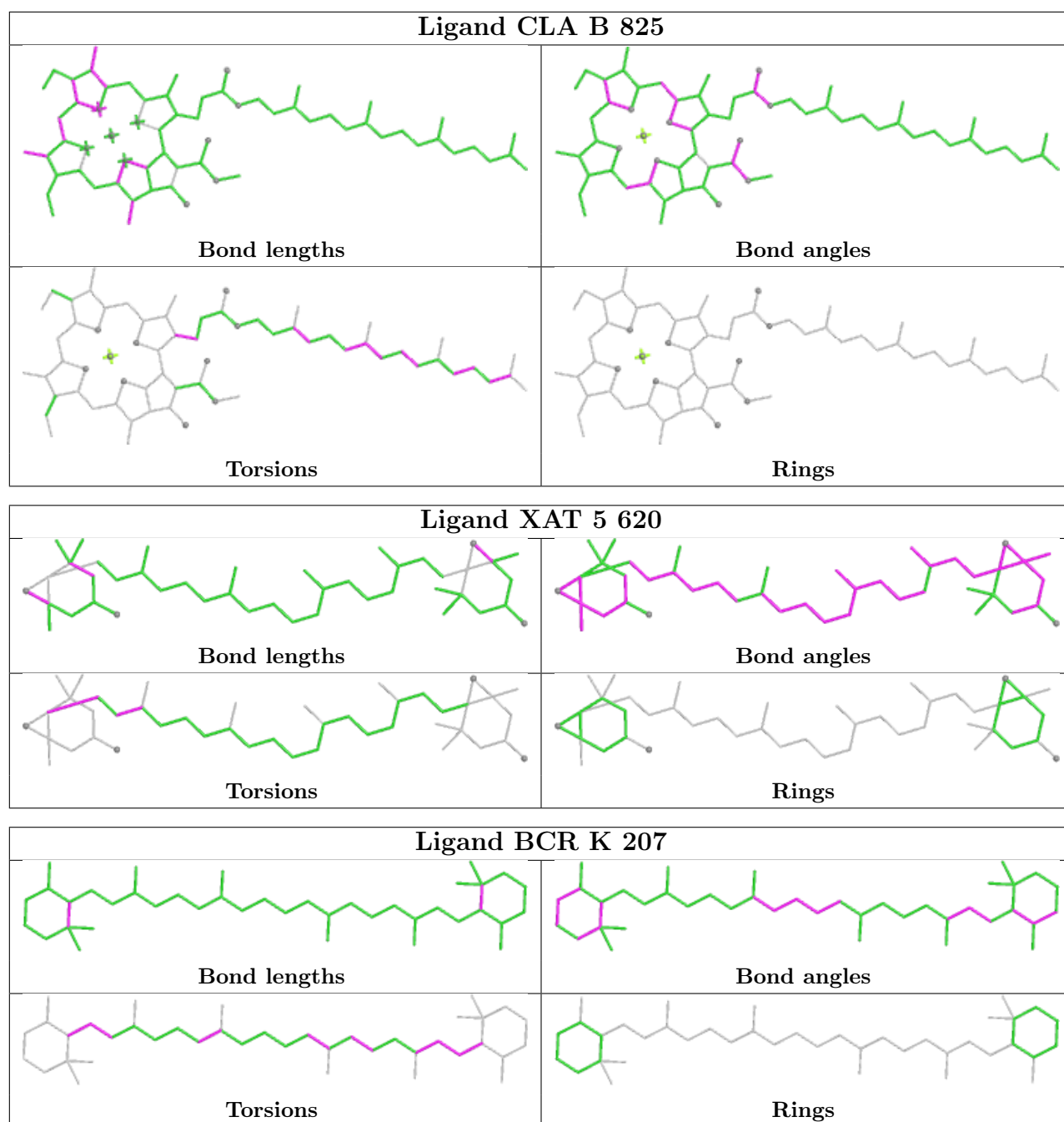


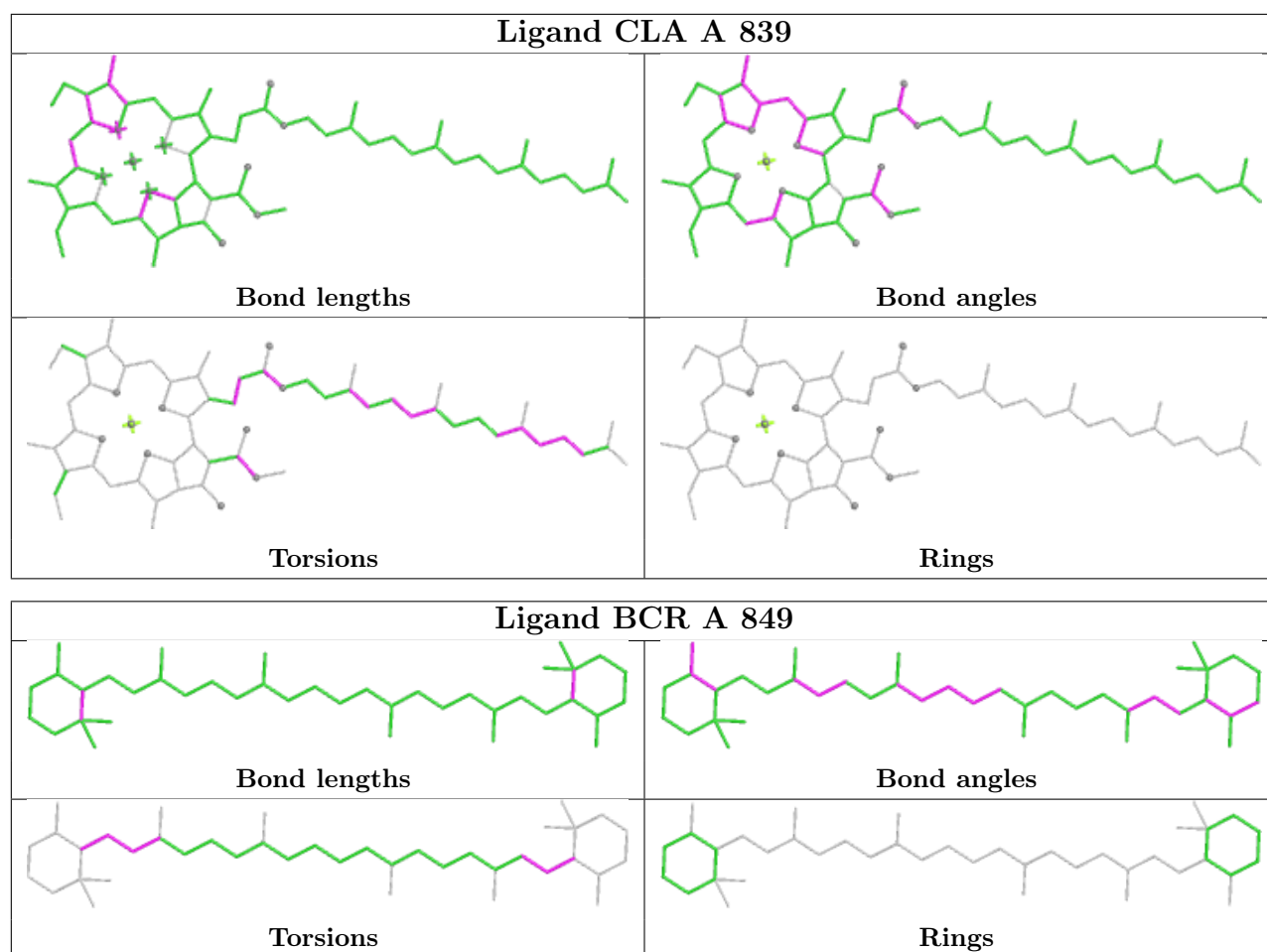
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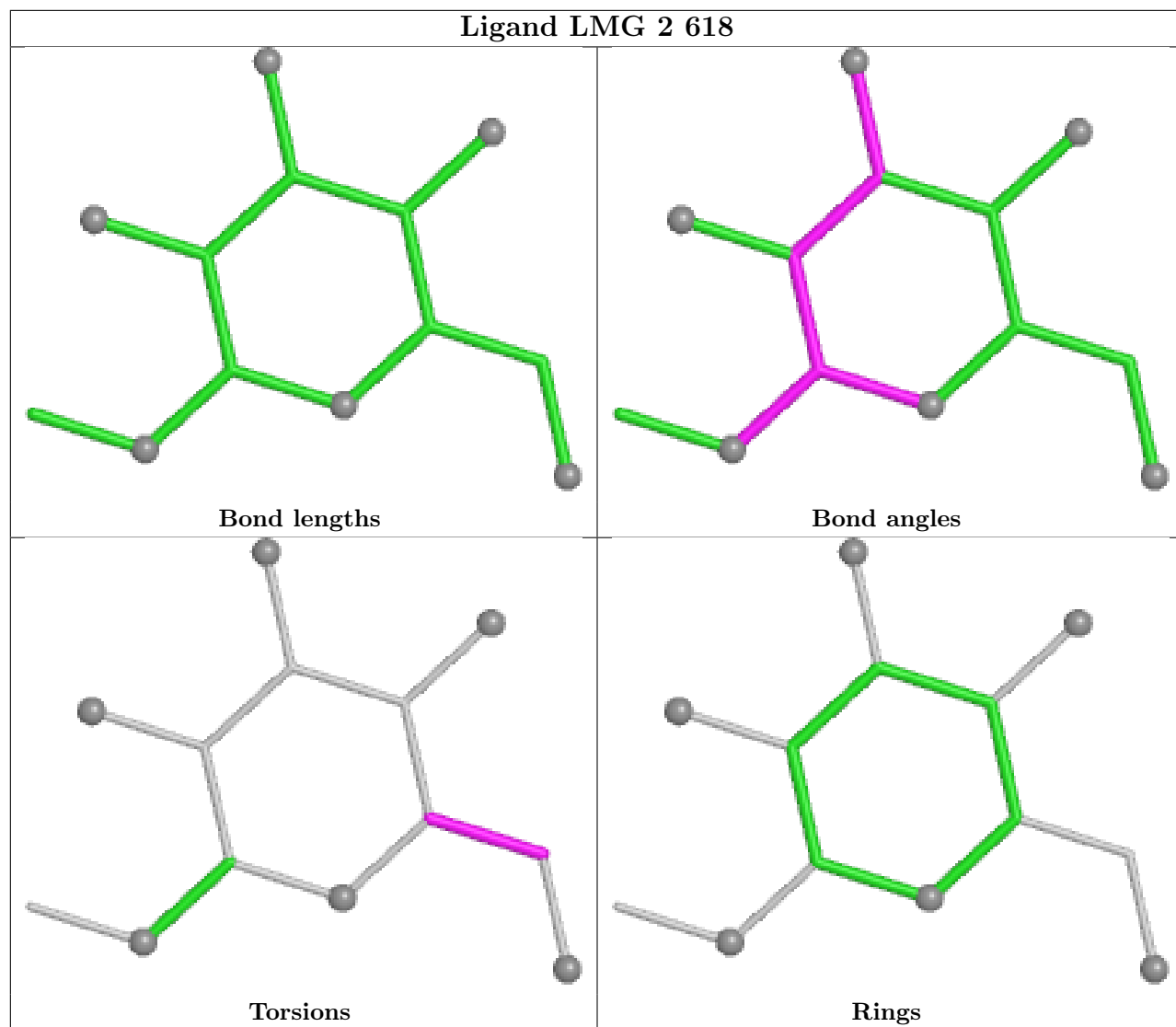


Ligand CLA B 805

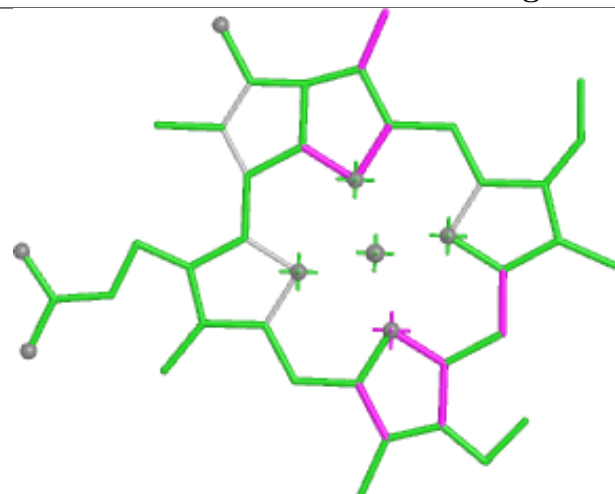




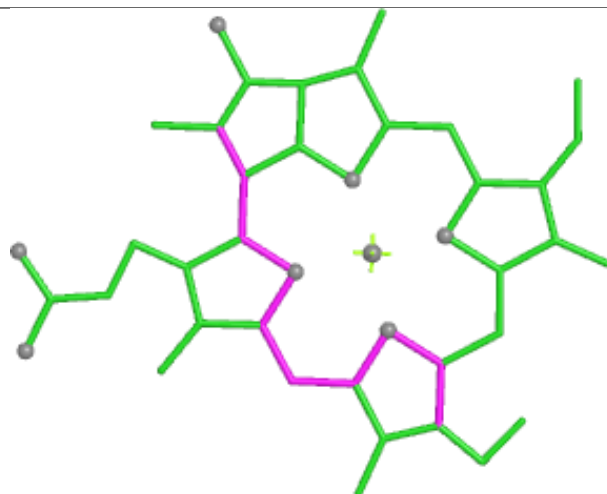




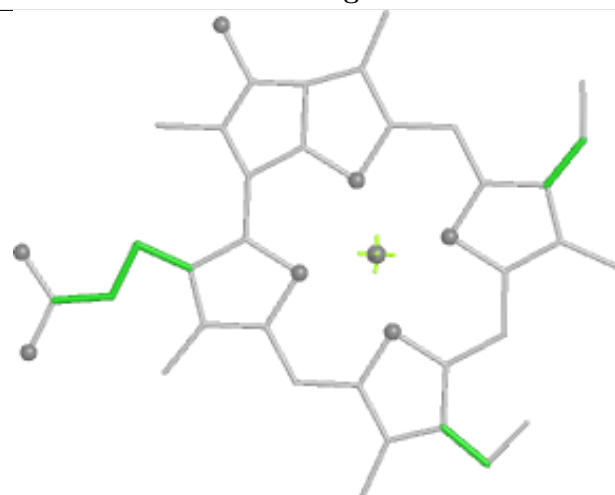
Ligand CLA 2 611



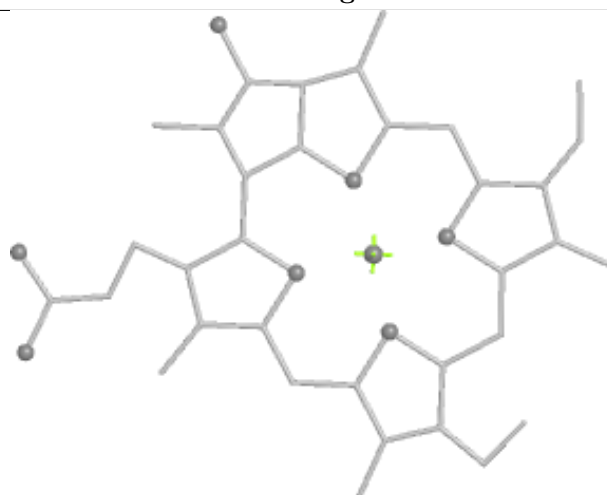
Bond lengths



Bond angles

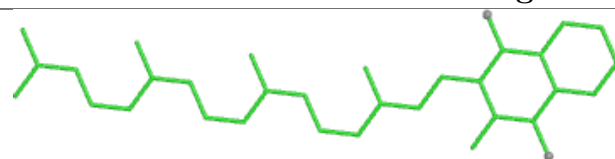


Torsions

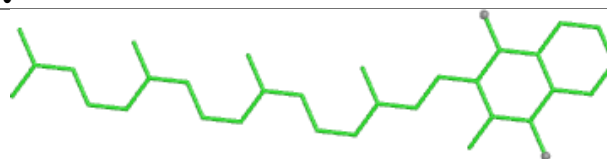


Rings

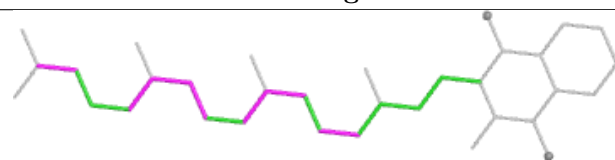
Ligand PQN B 842



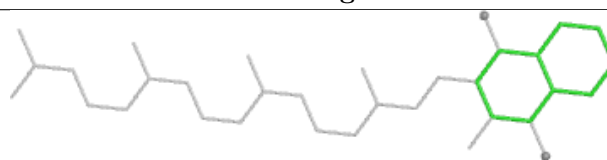
Bond lengths



Bond angles

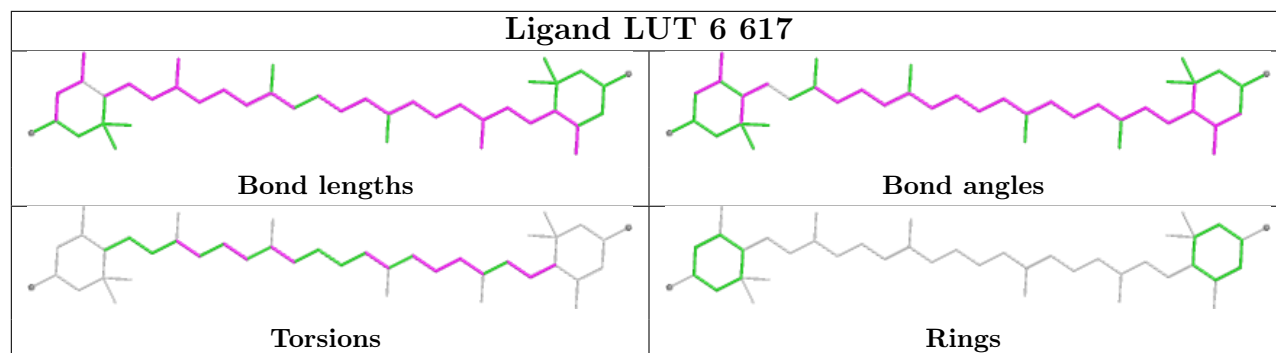


Torsions

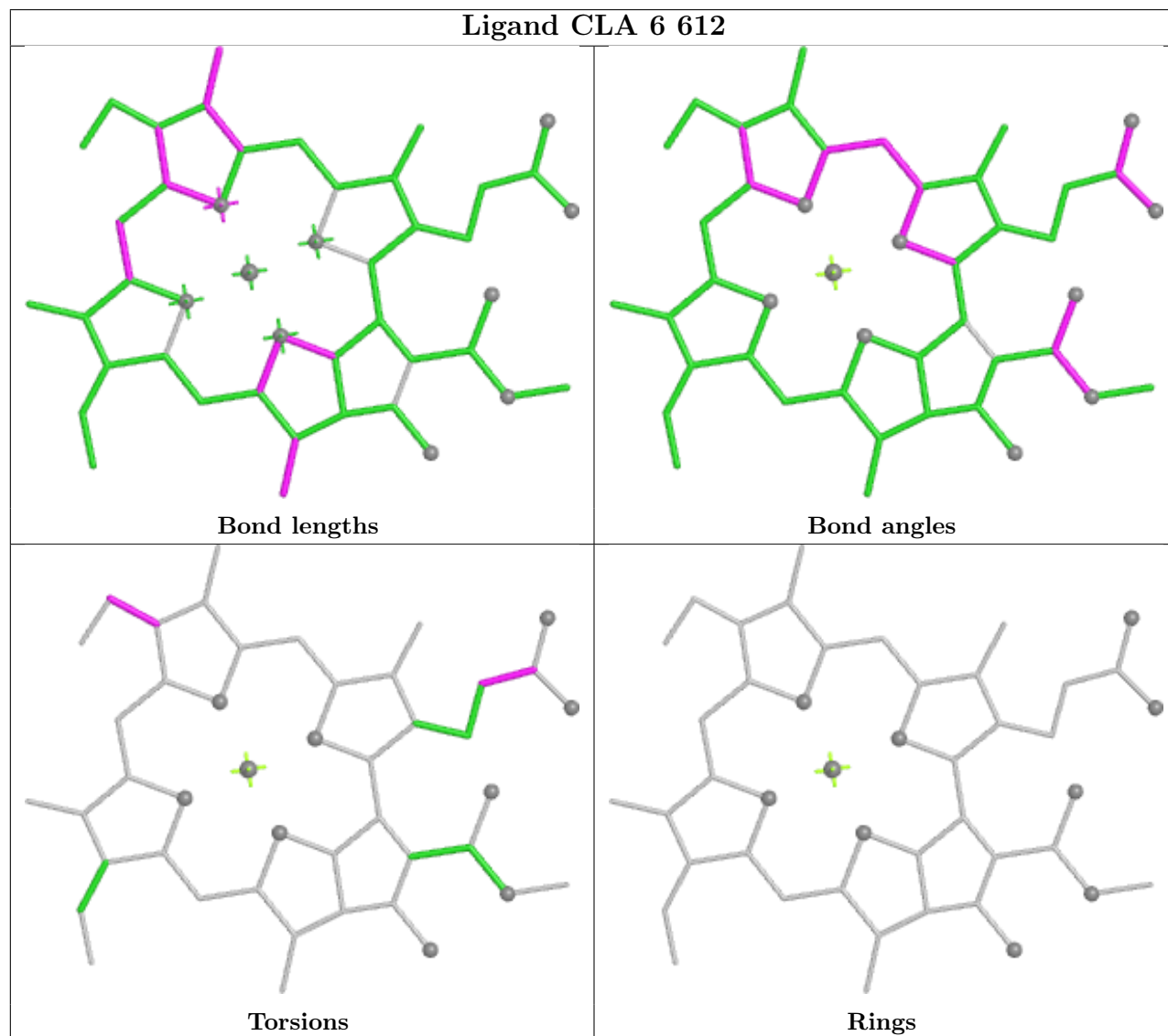


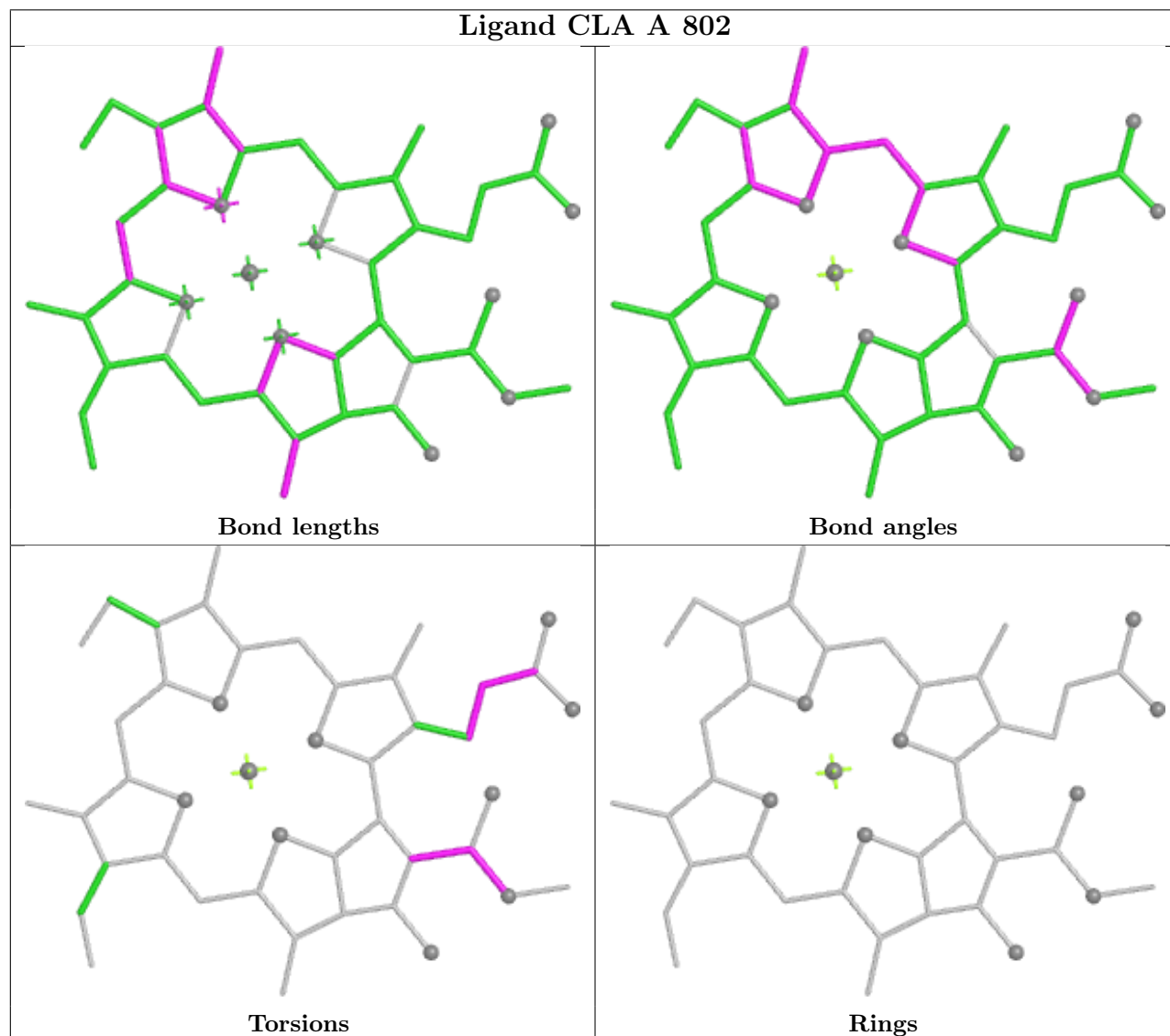
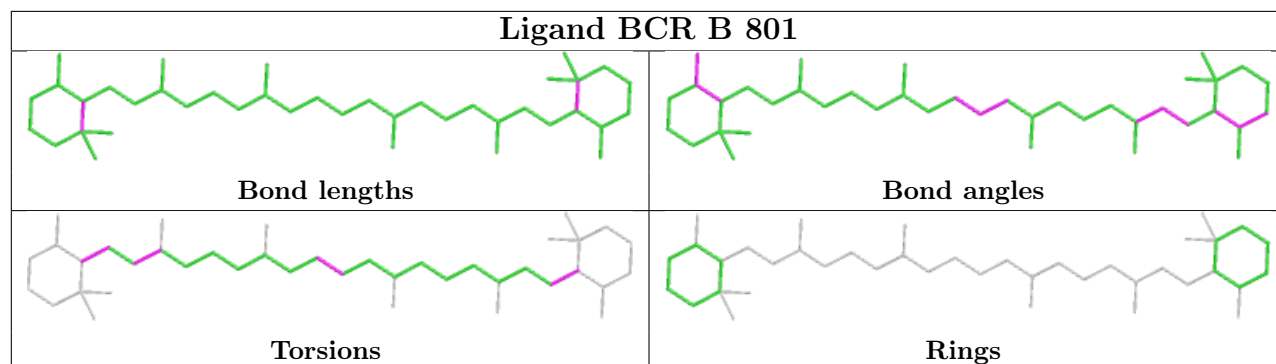
Rings

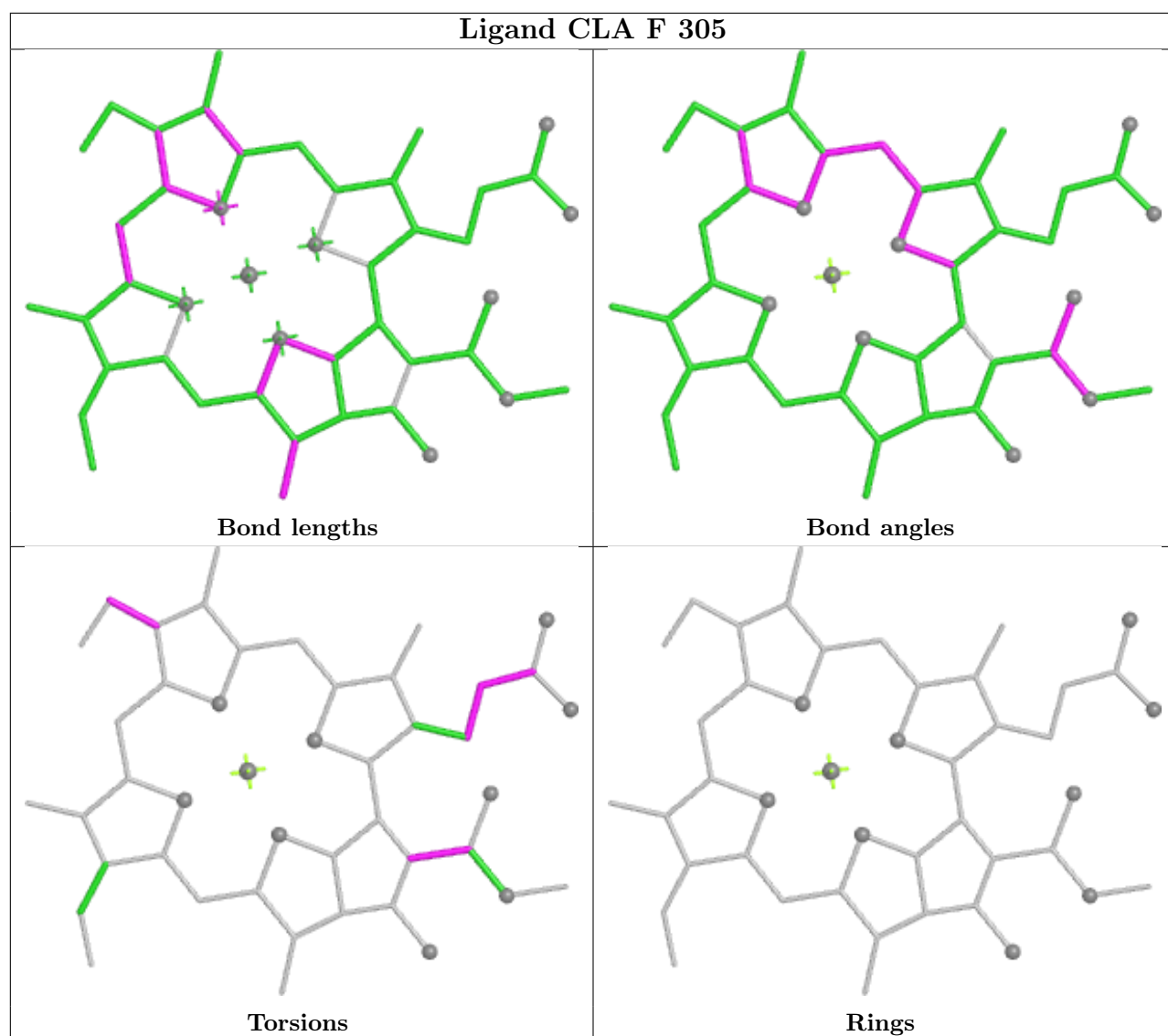
Ligand LUT 6 617



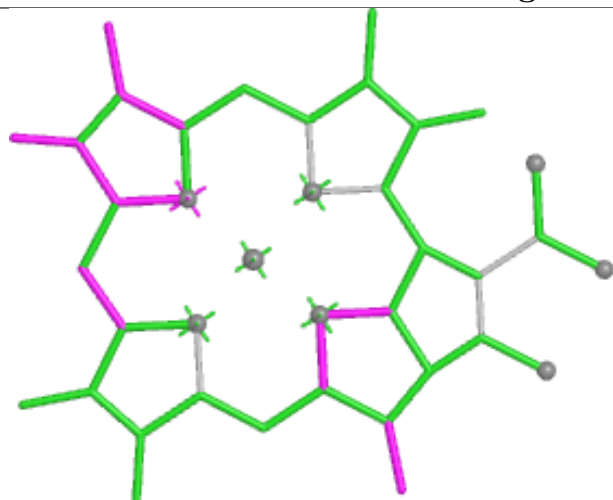
Ligand CLA 6 612



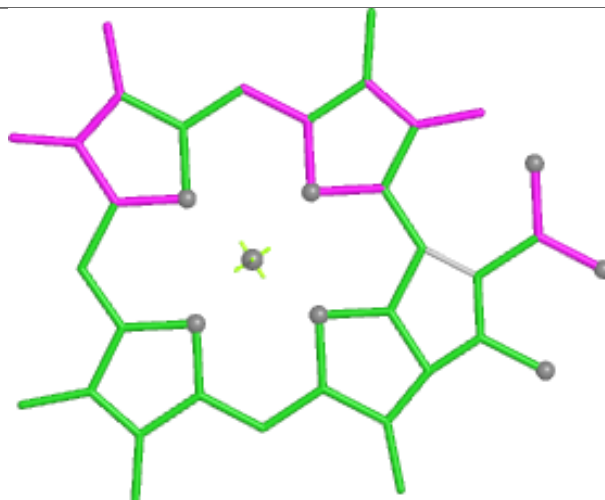




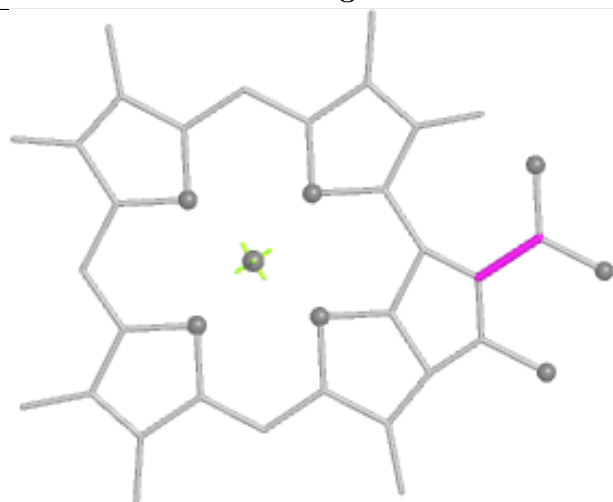
Ligand CLA 6 611



Bond lengths



Bond angles

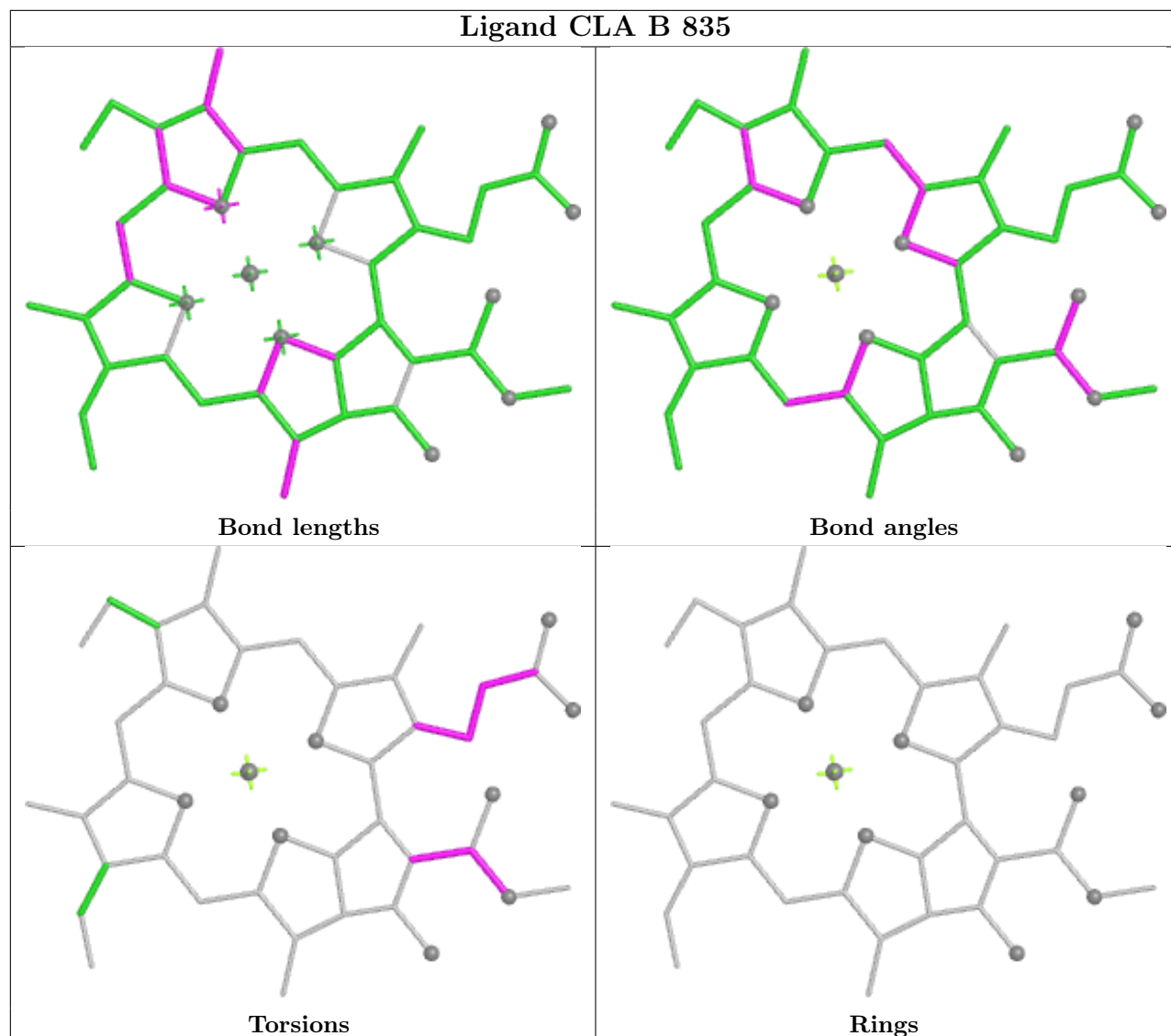


Torsions

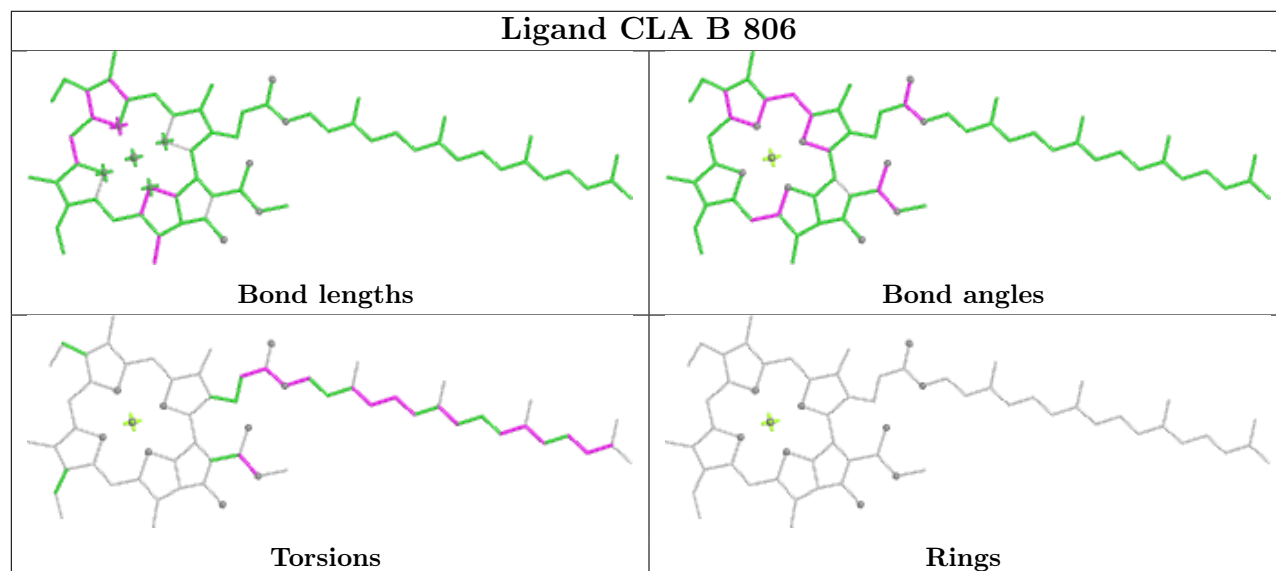


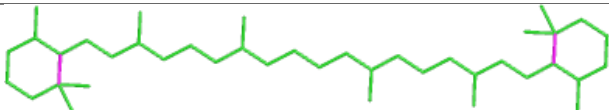
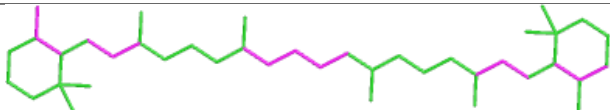
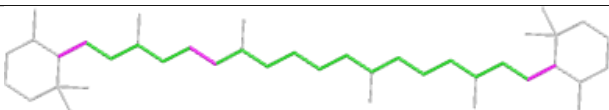
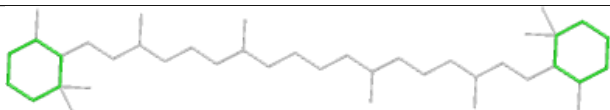
Rings

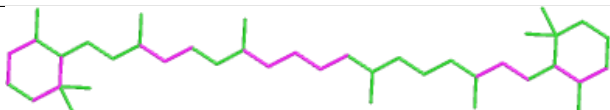
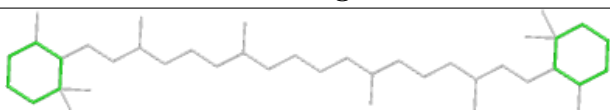
Ligand CLA B 835

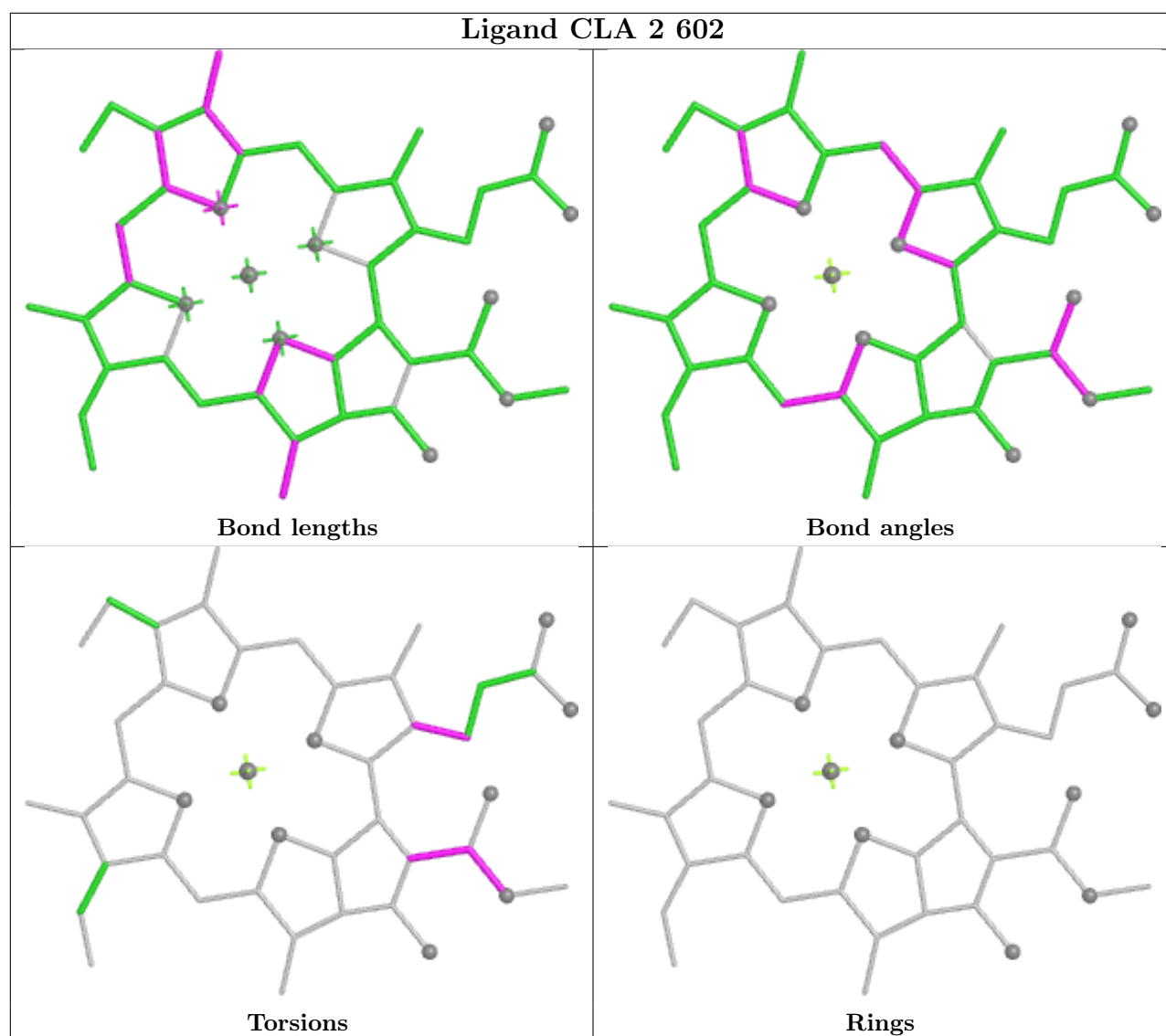


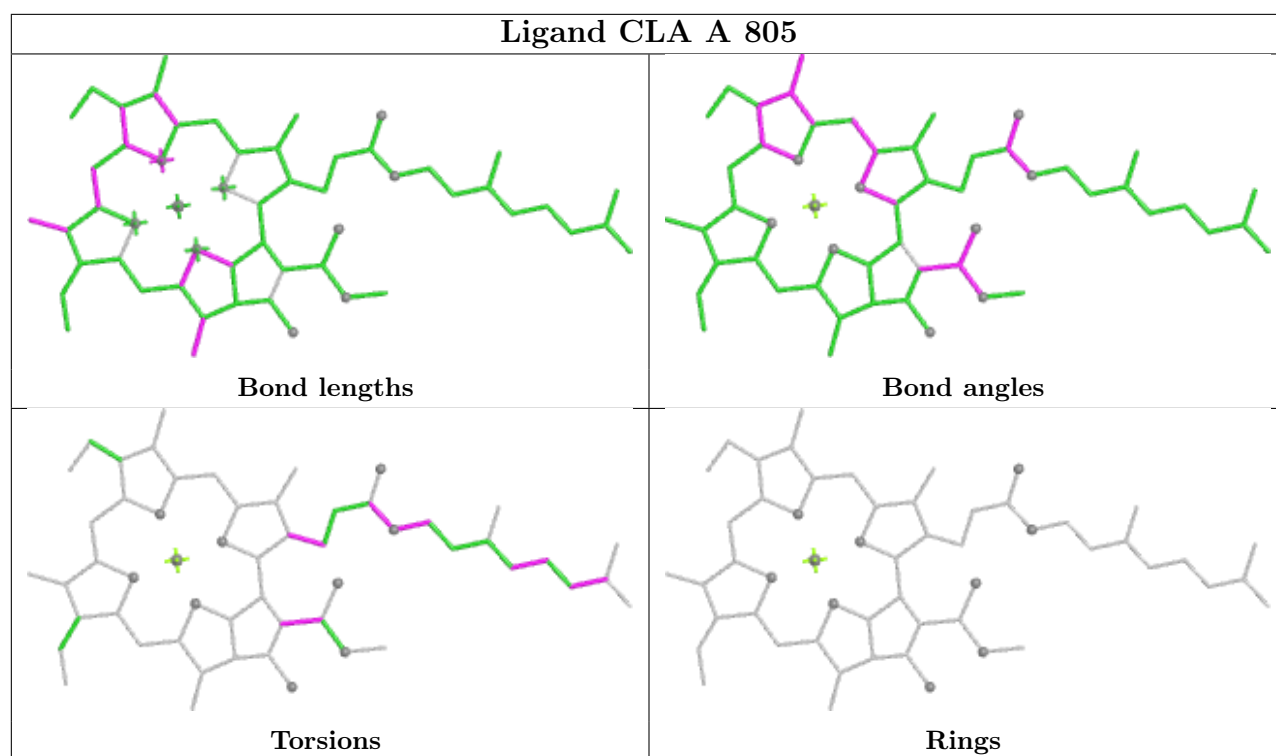
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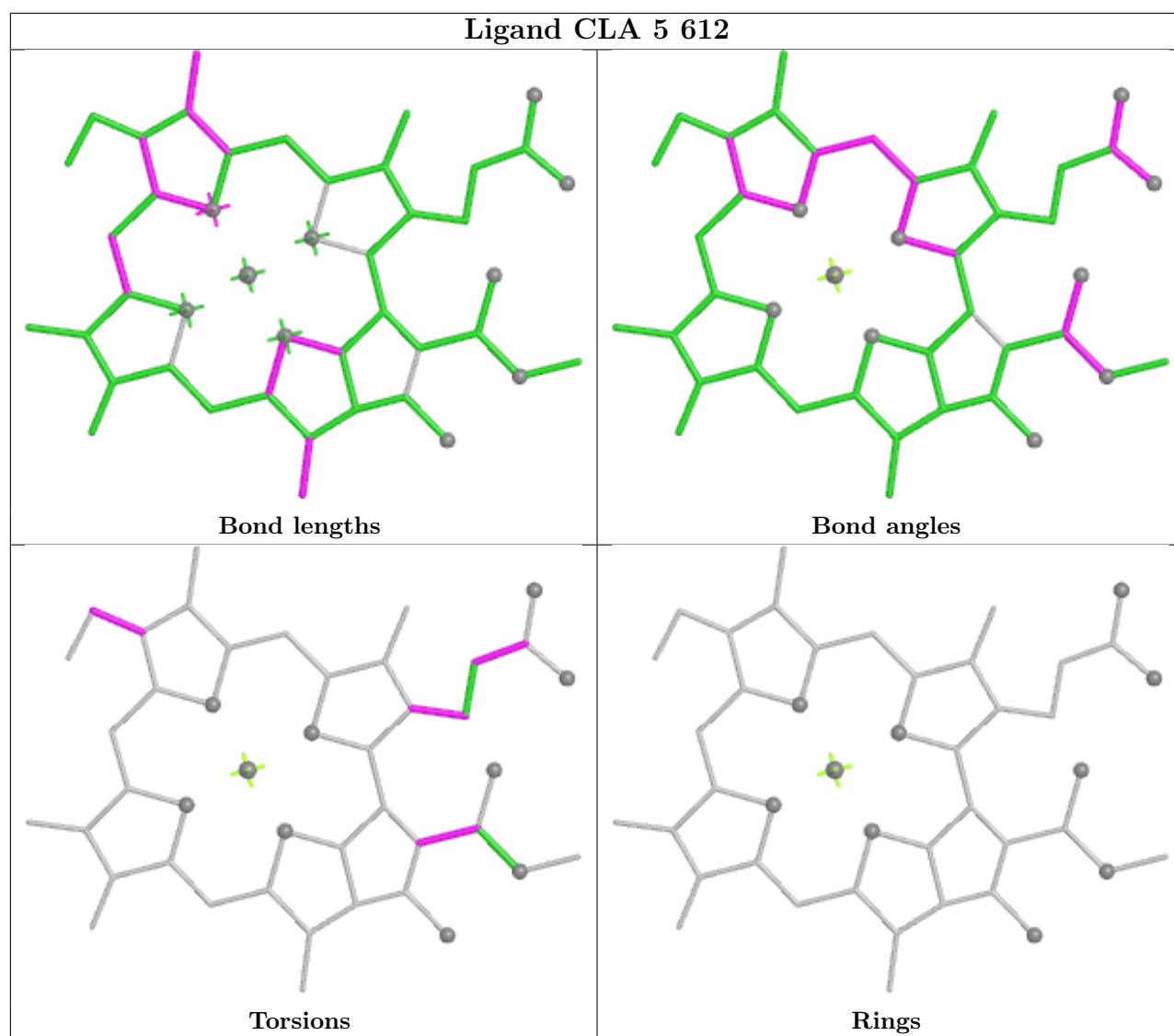


Ligand BCR G 205	
	Bond lengths
	Bond angles
	Torsions
	Rings

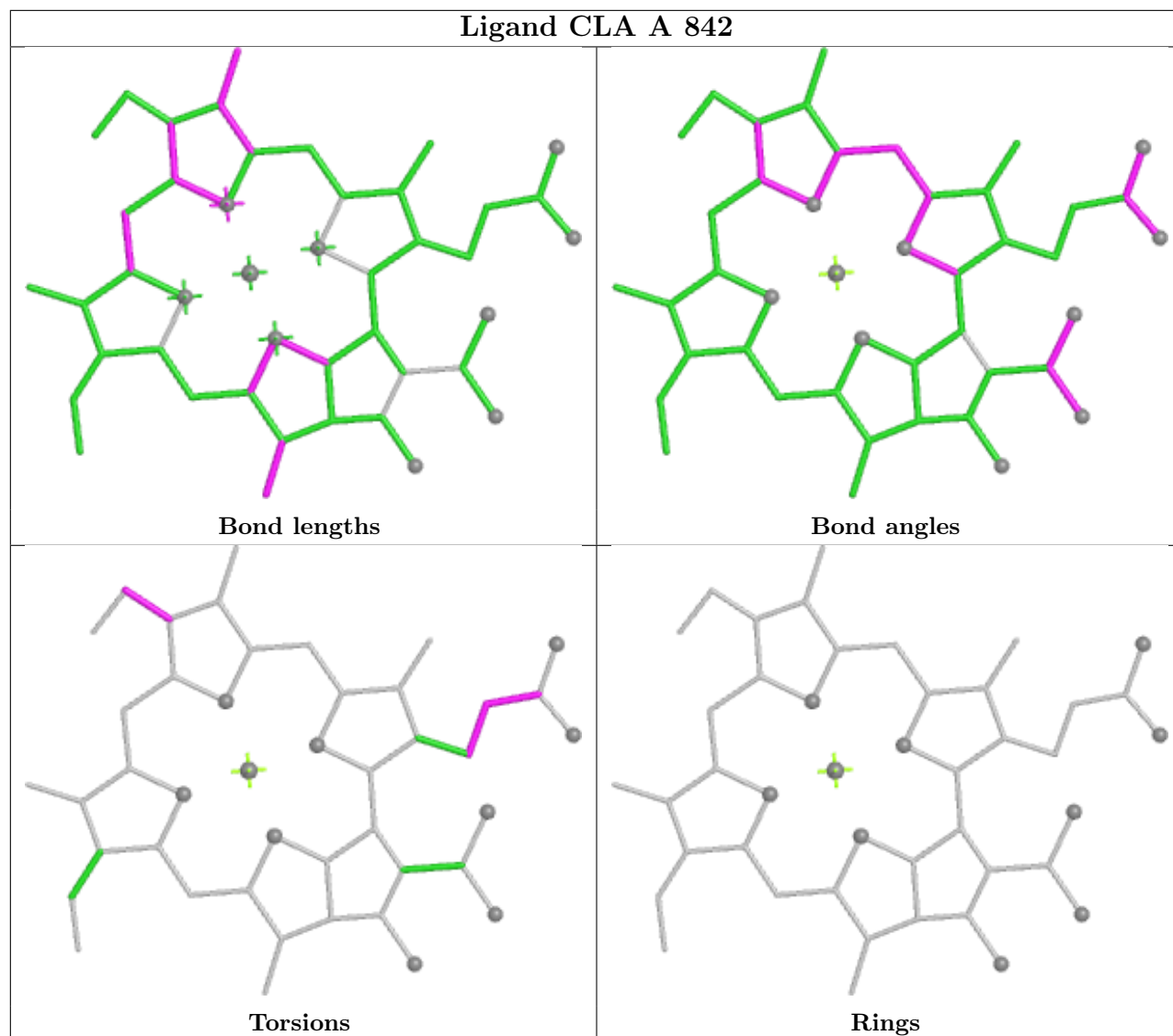
Ligand BCR A 856	
	Bond lengths
	Bond angles
	Torsions
	Rings

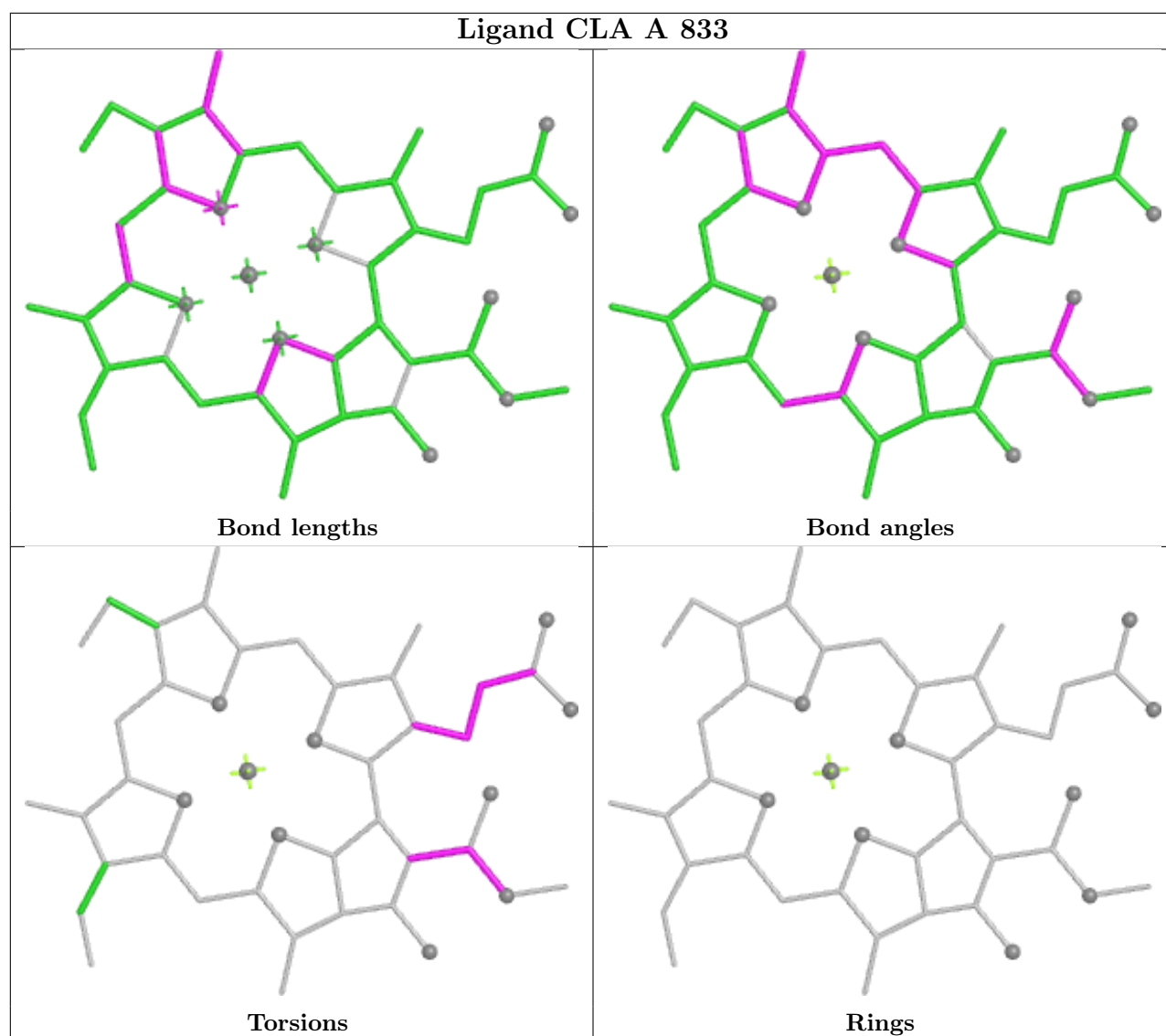




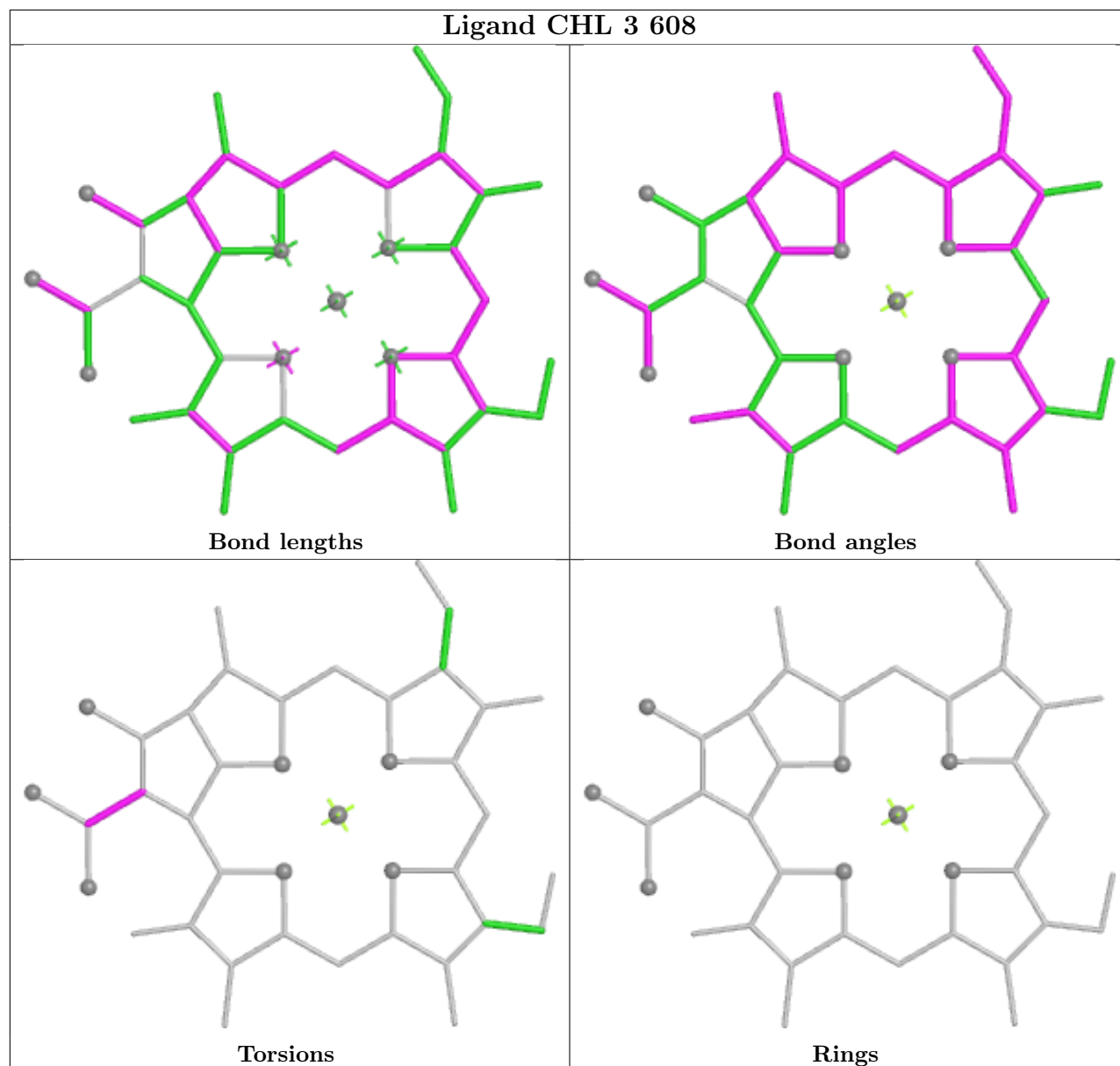


Ligand CLA A 842

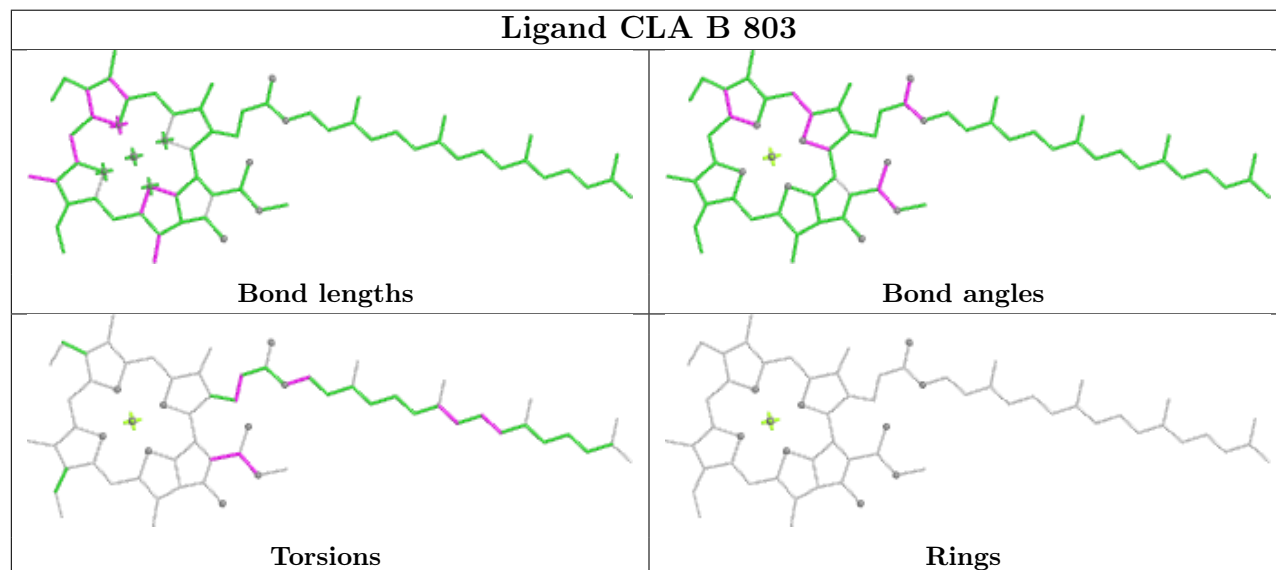


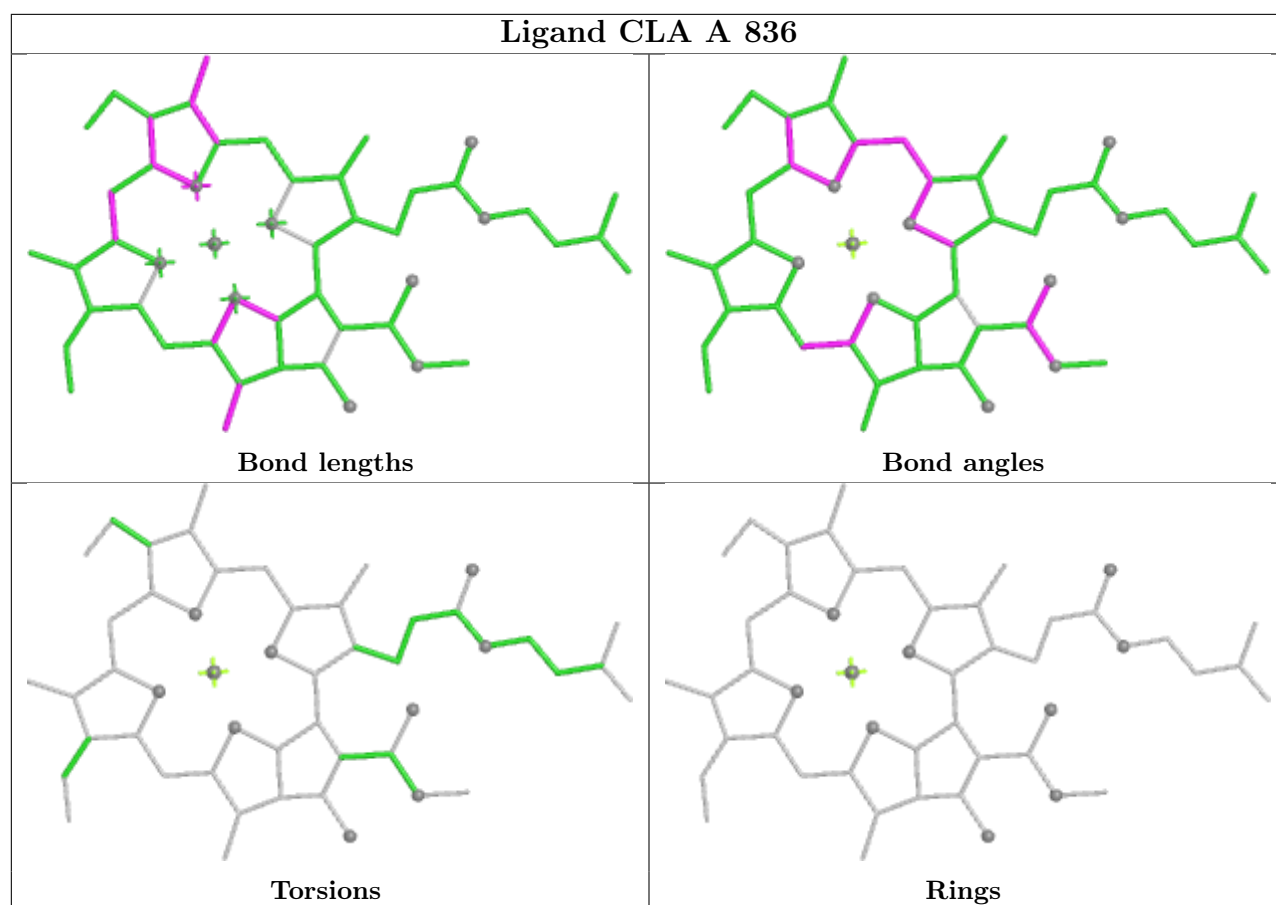


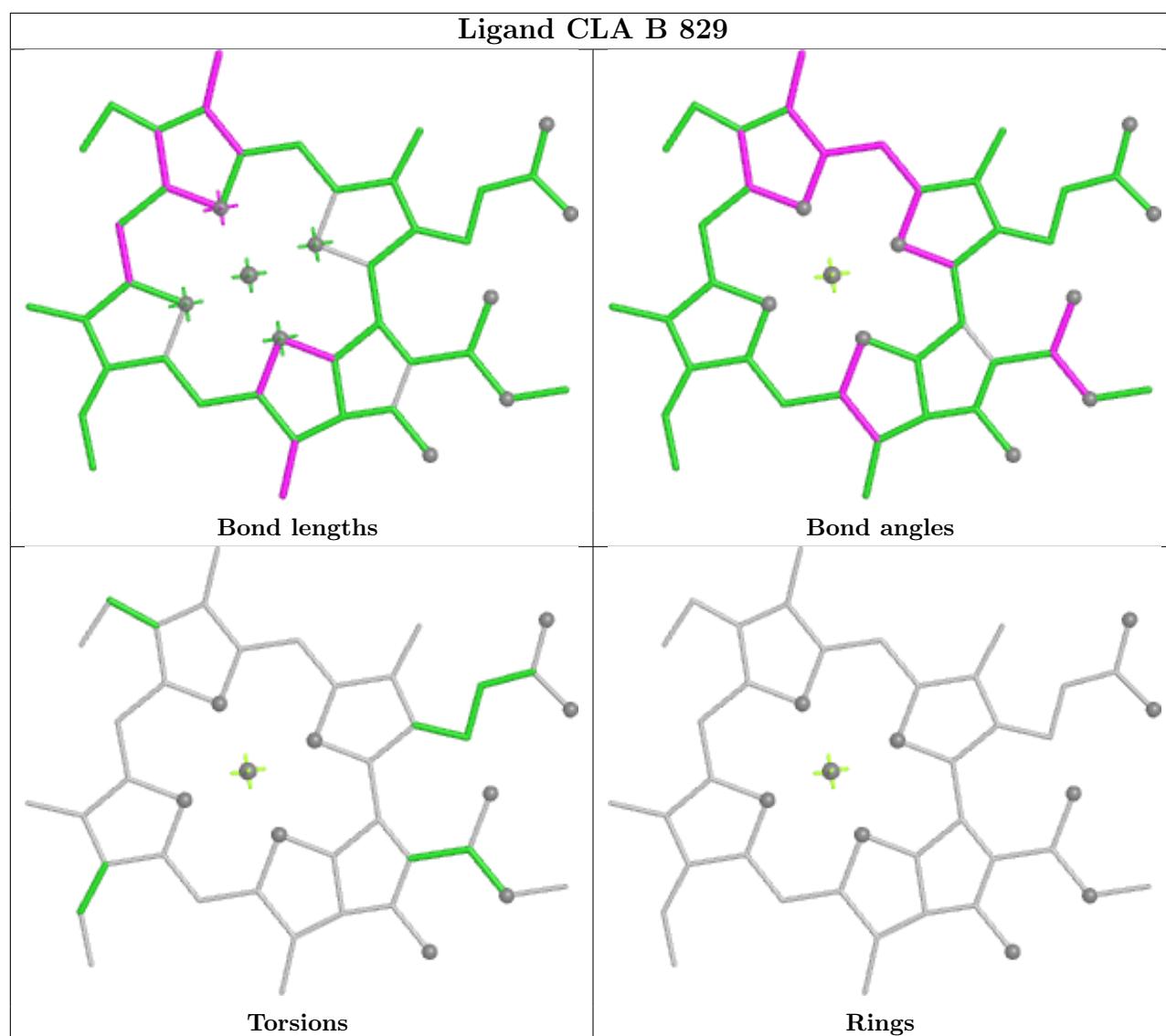
Ligand CHL 3 608



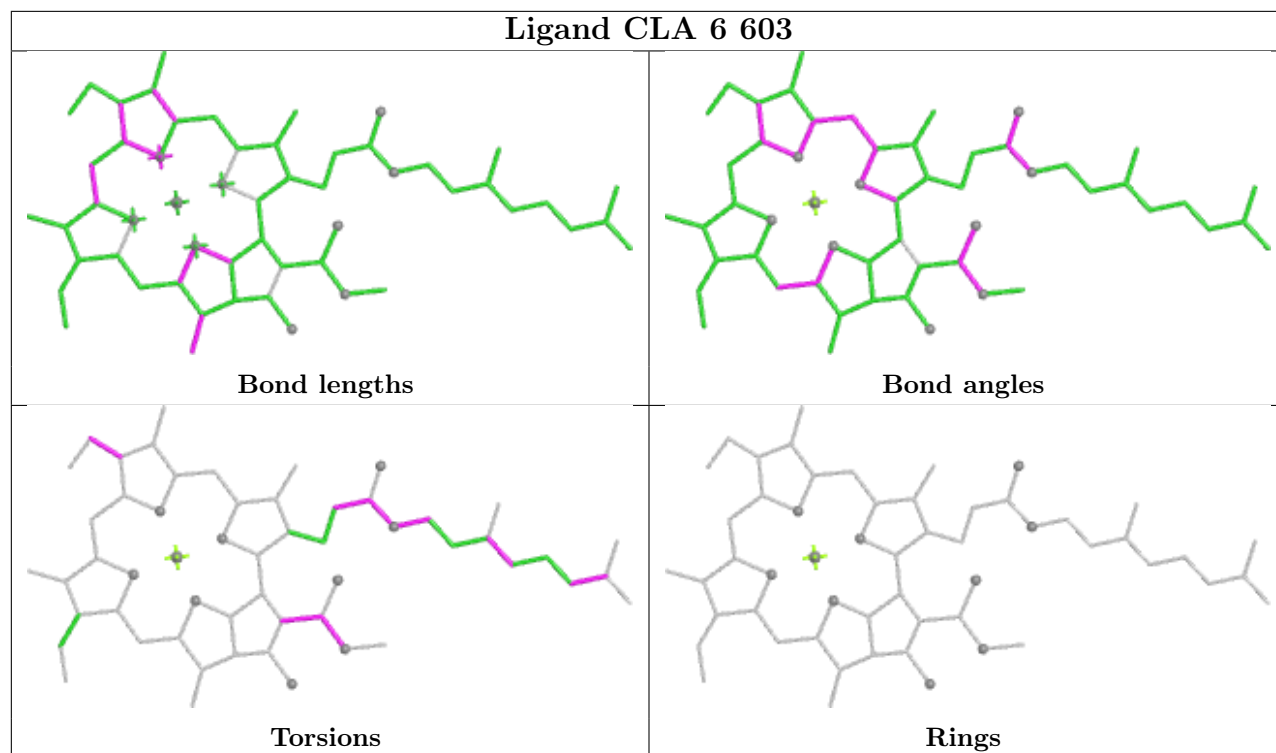
Ligand CLA B 803



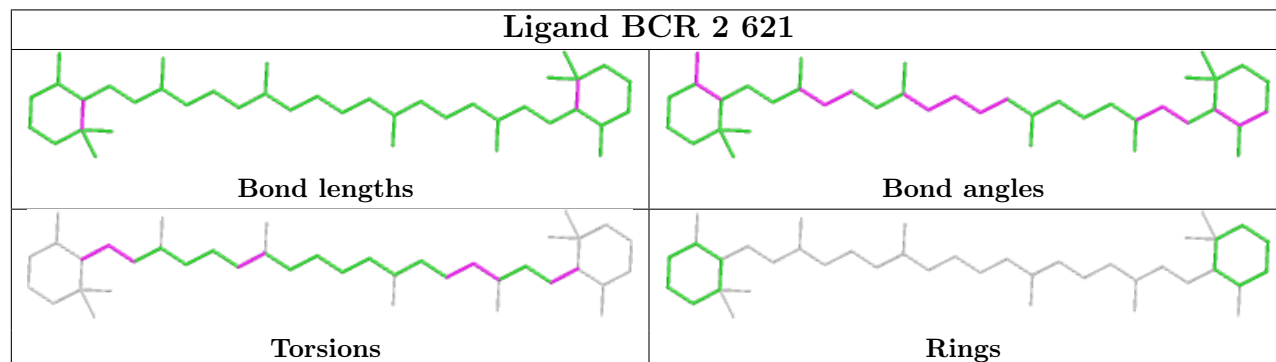




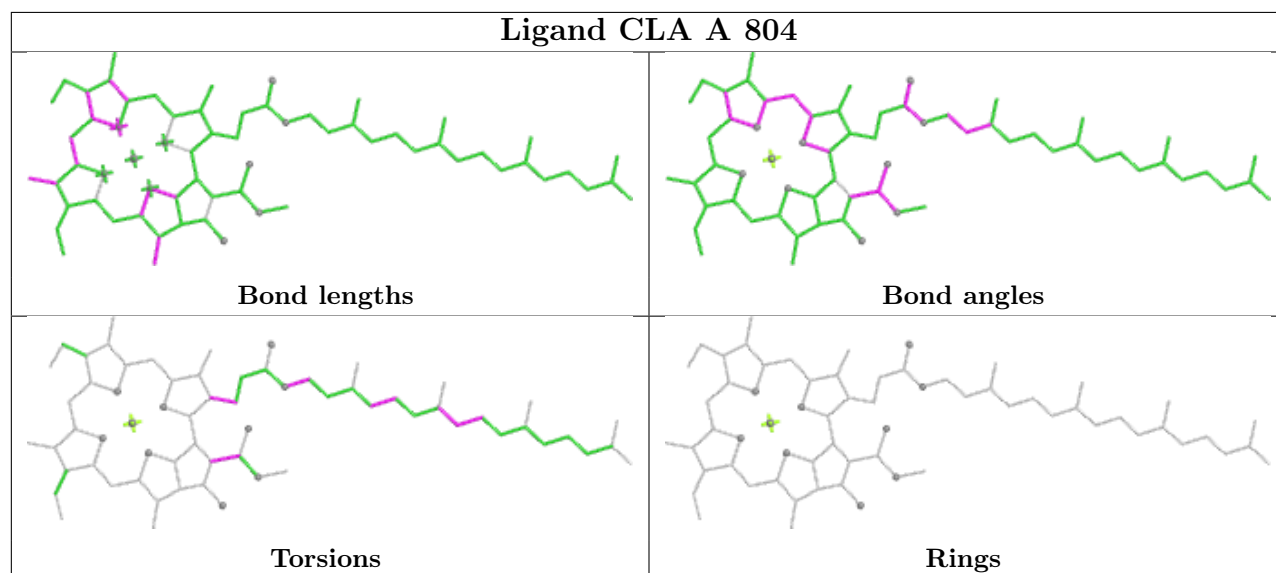
Ligand CLA 6 603

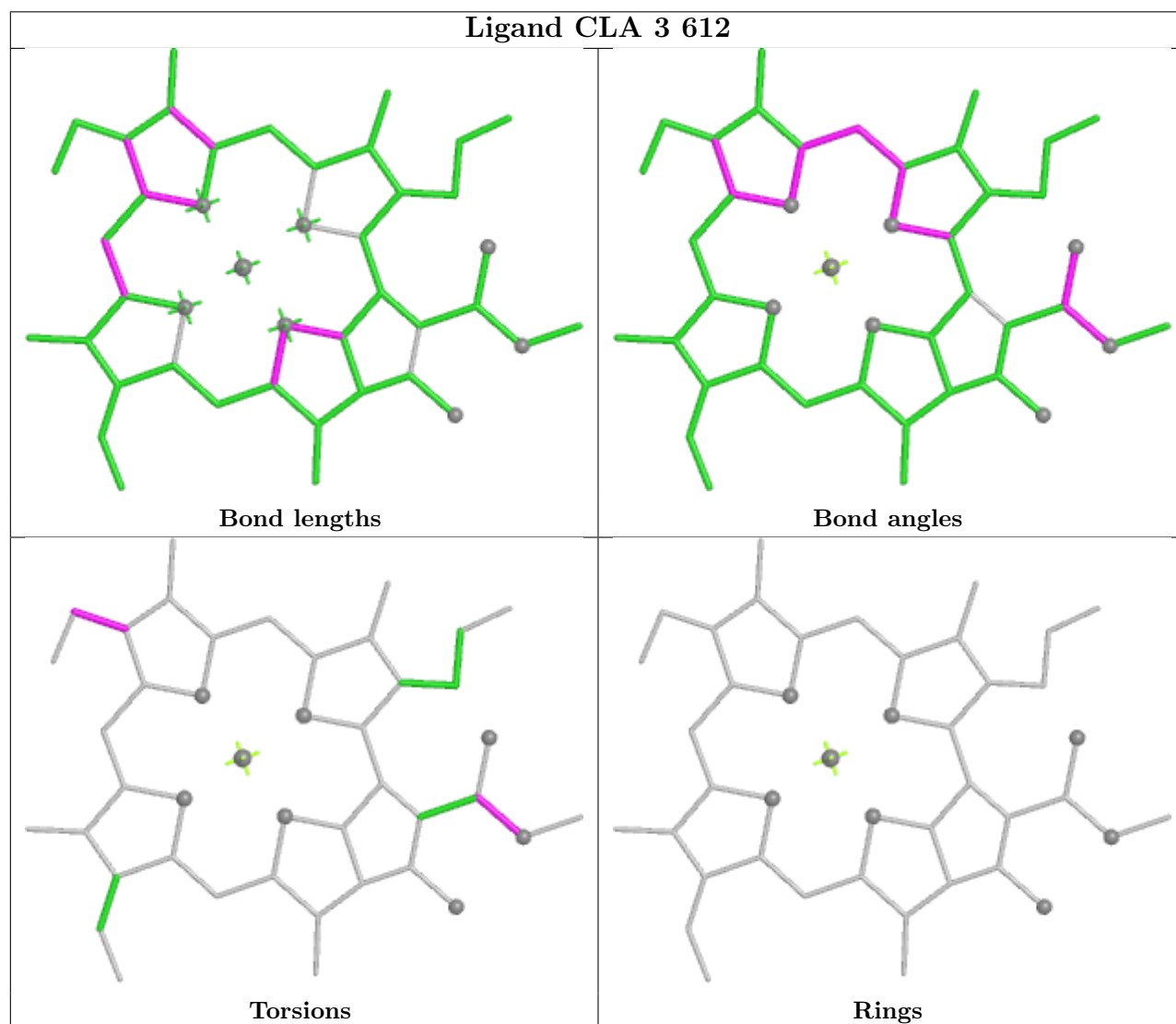
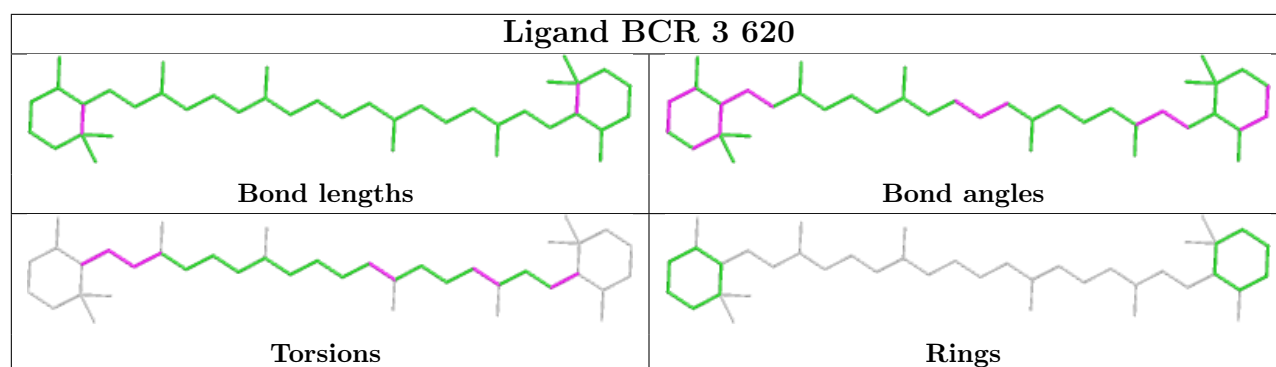


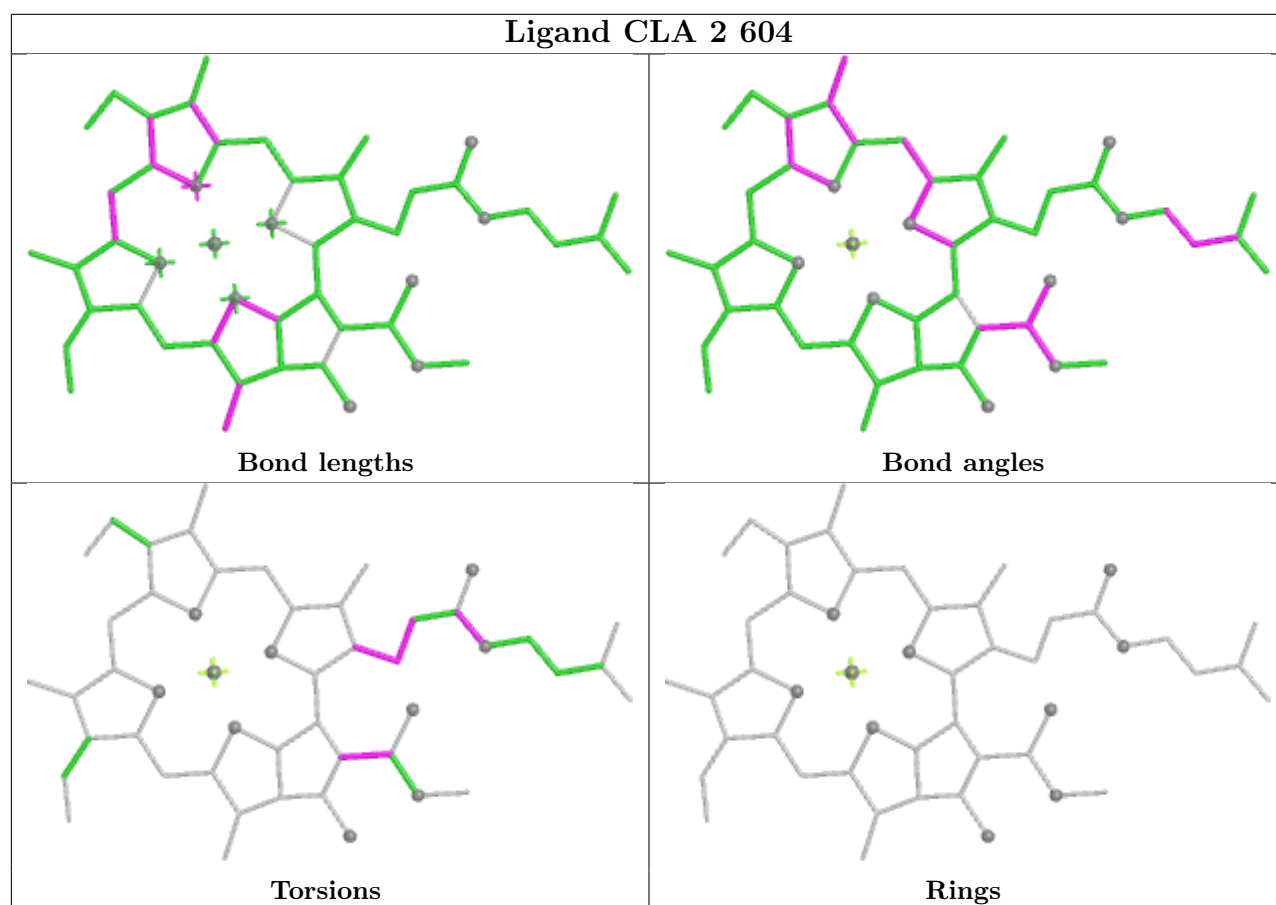
Ligand BCR 2 621

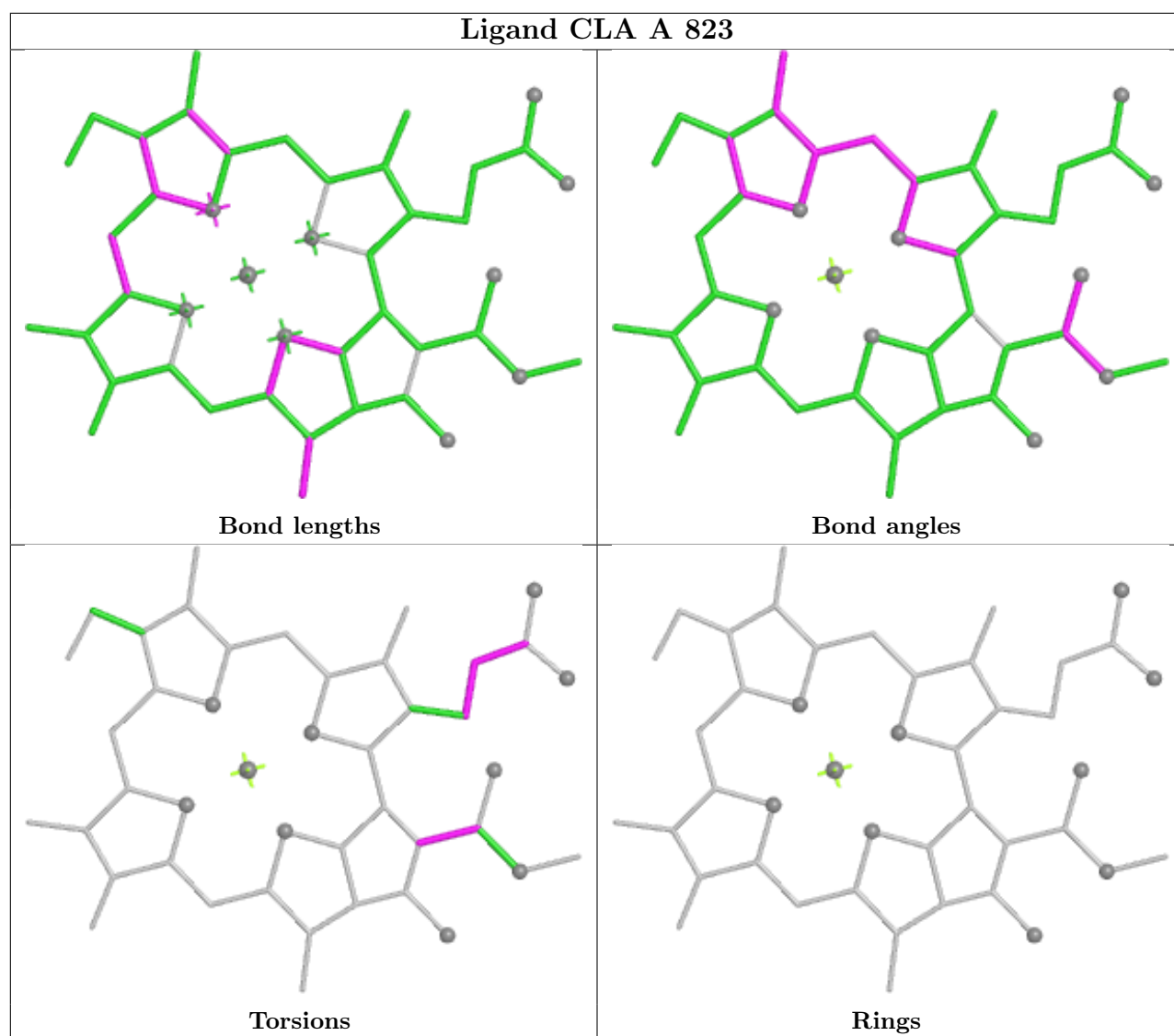


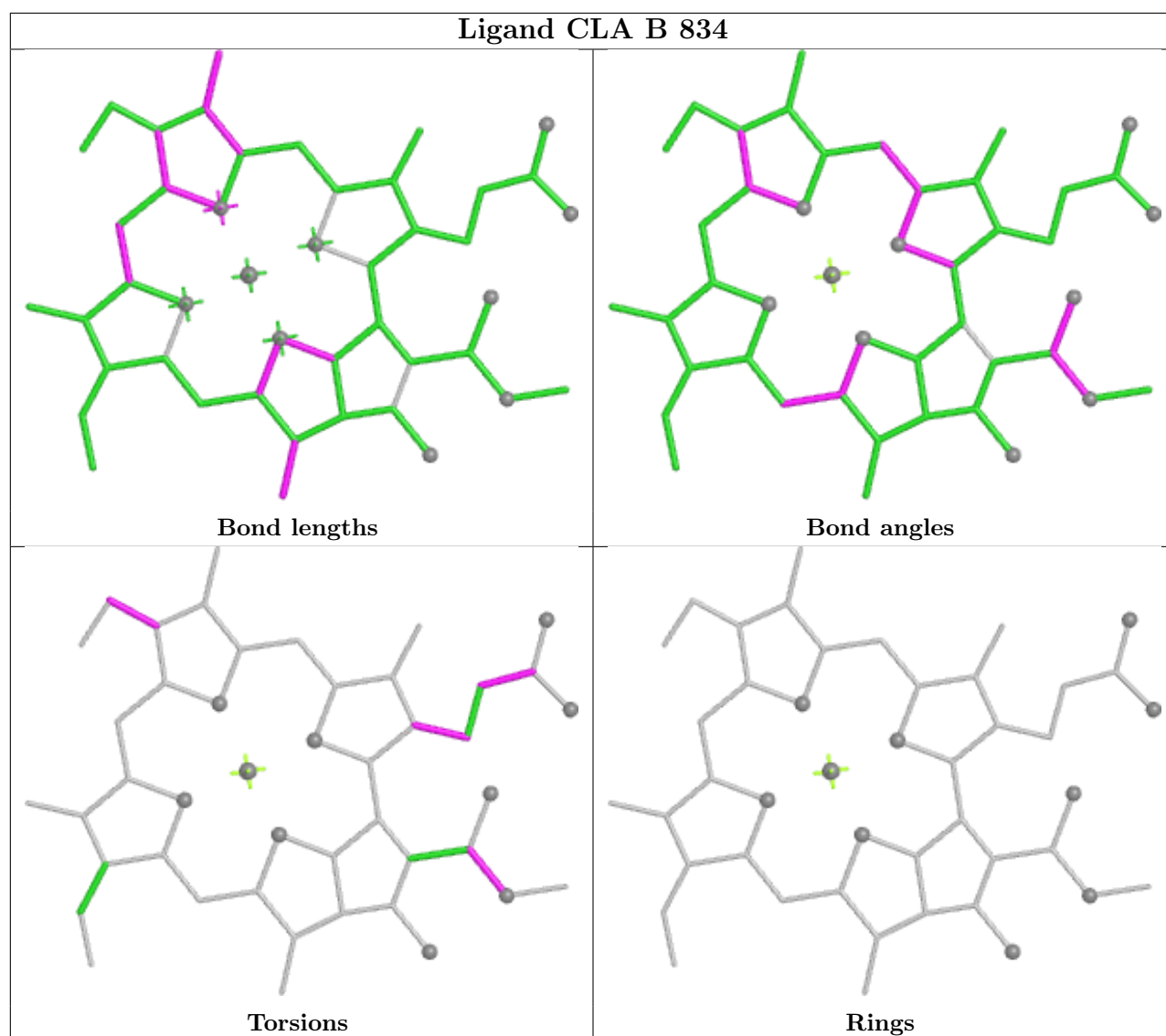
Ligand CLA A 804



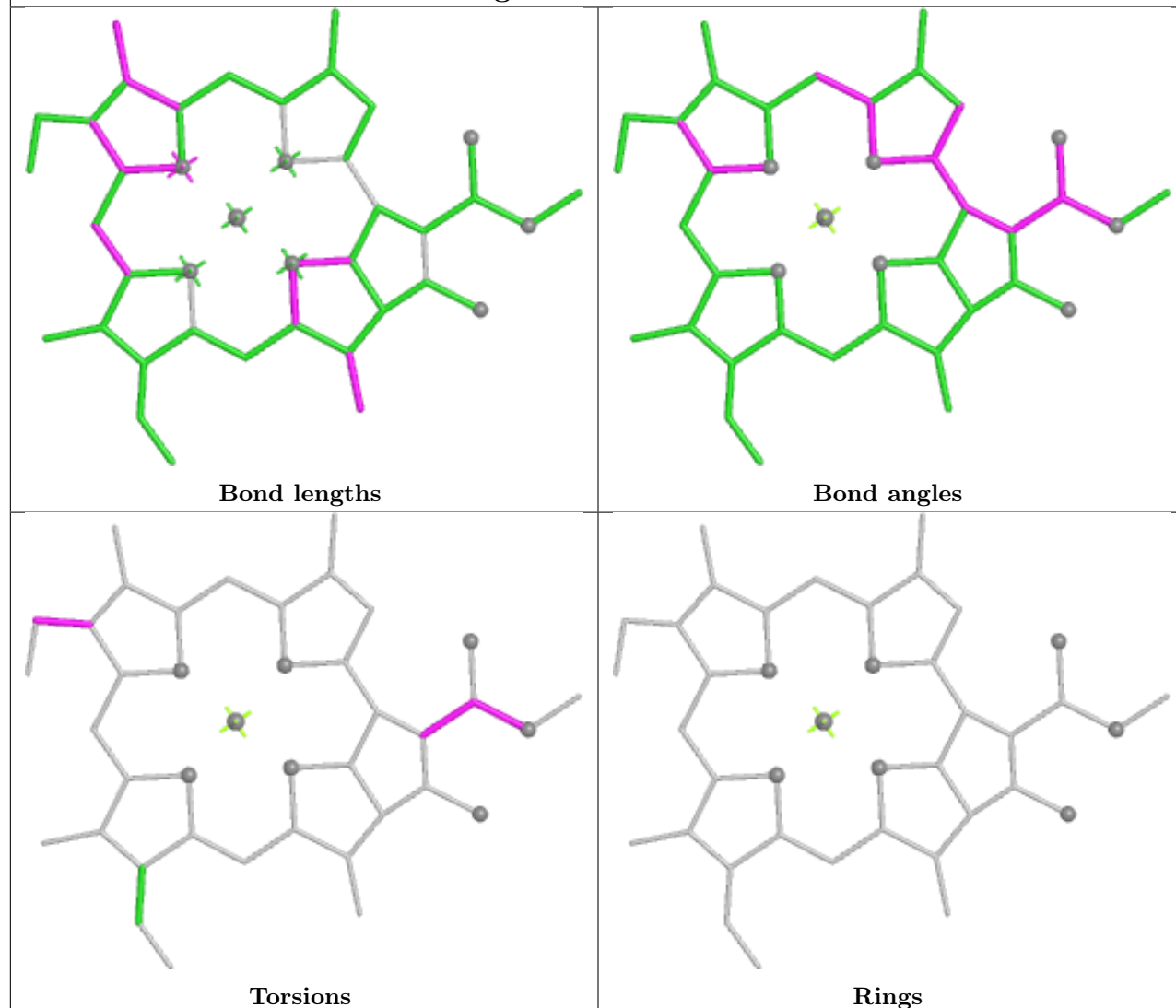




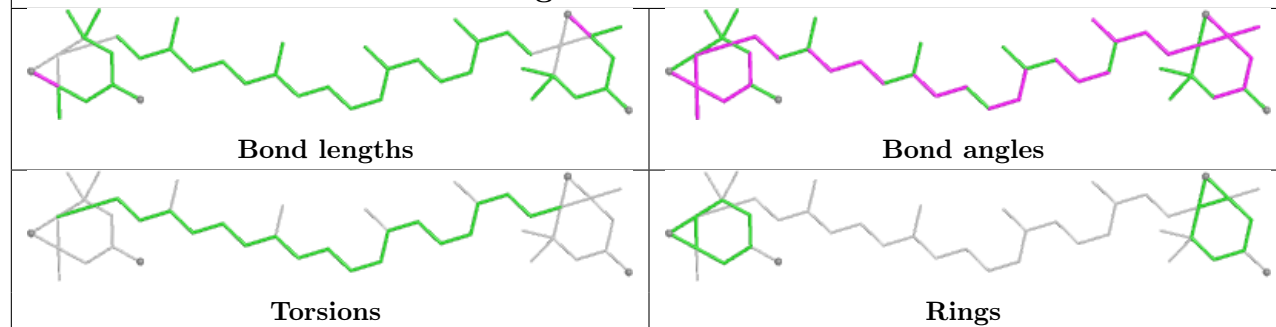


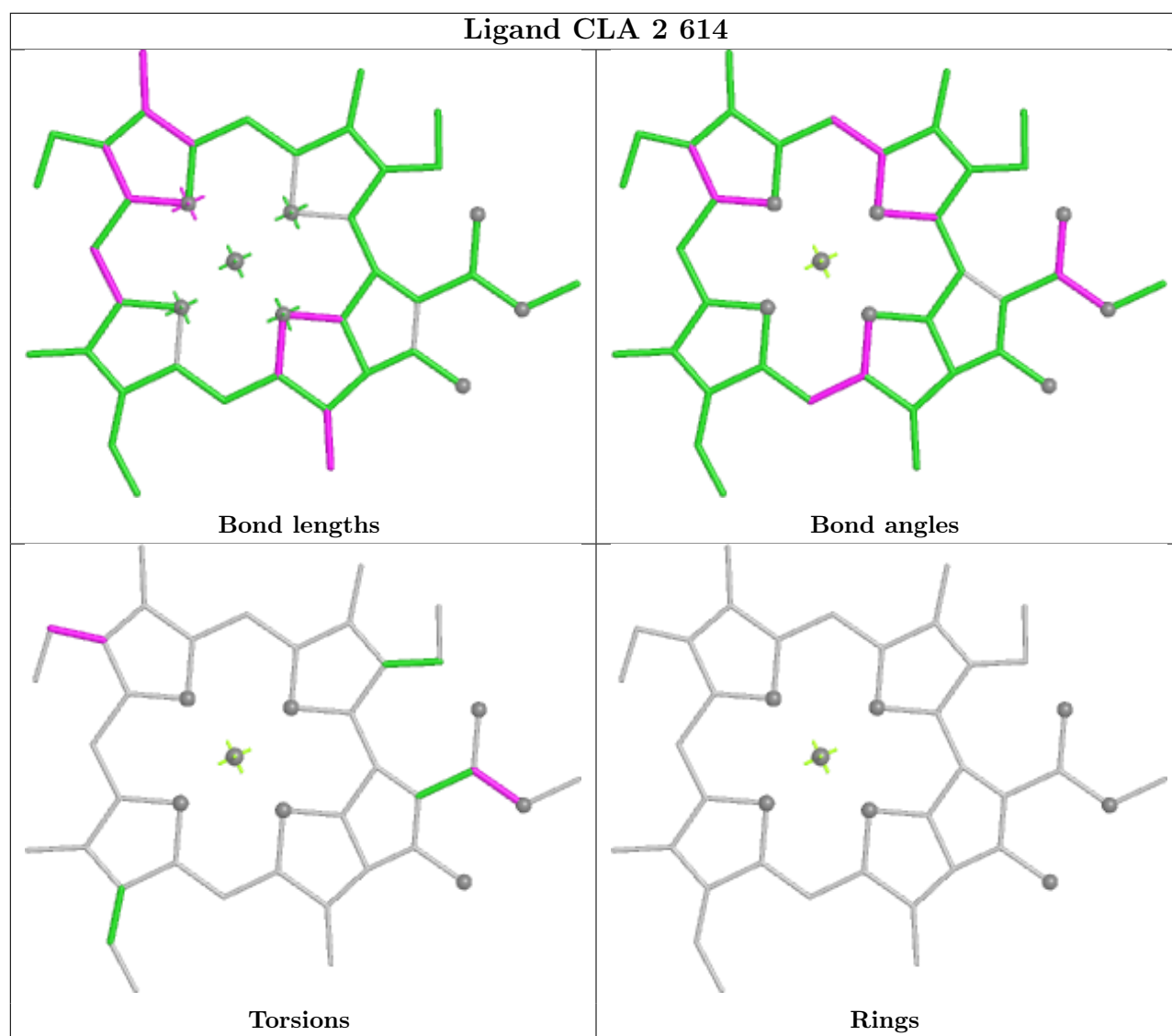


Ligand CLA 6 606

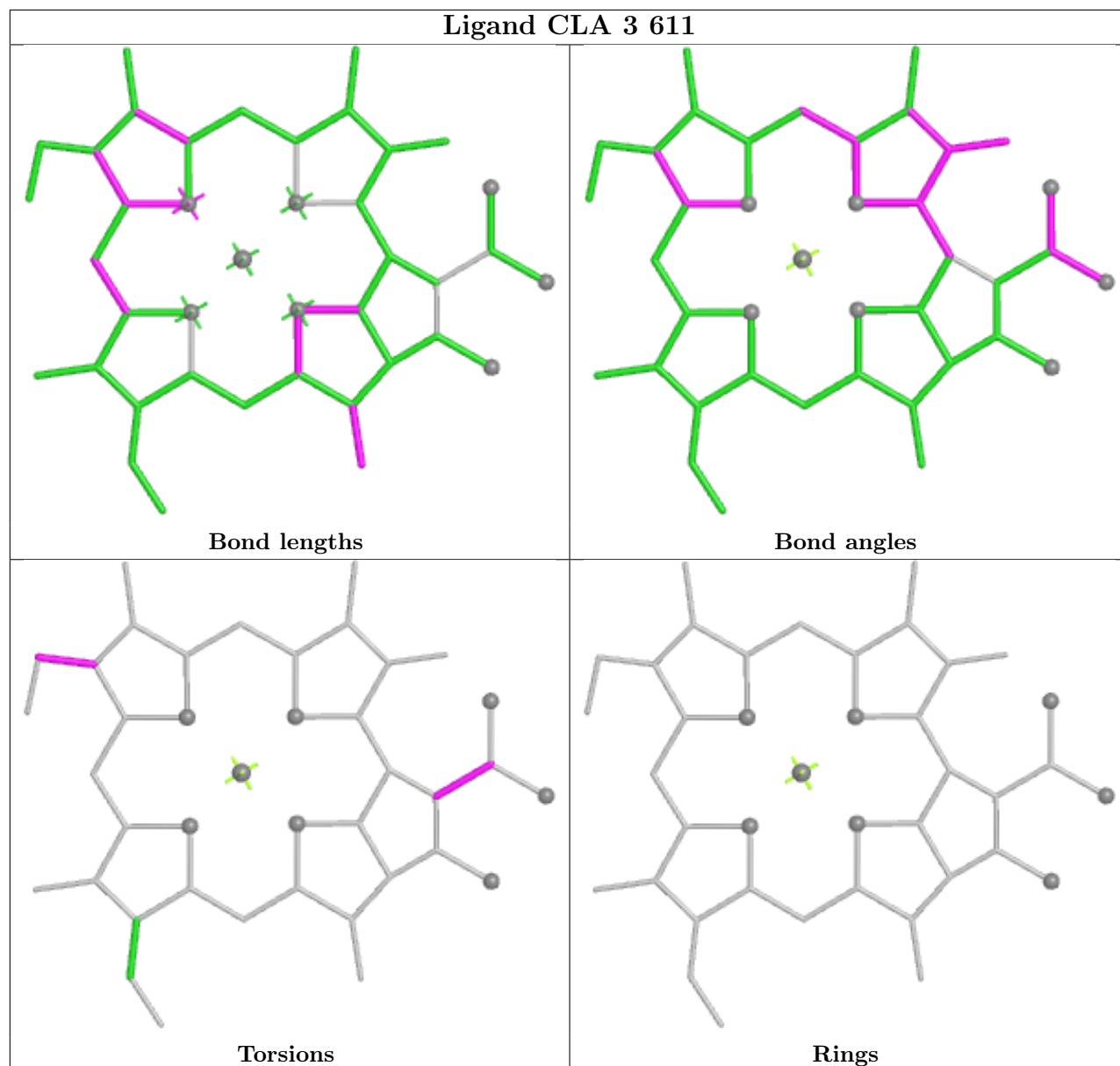


Ligand XAT 3 619

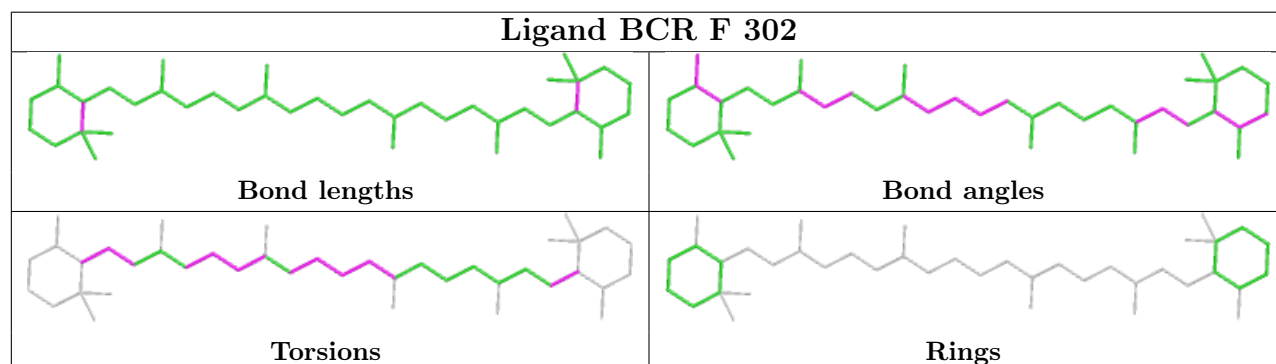


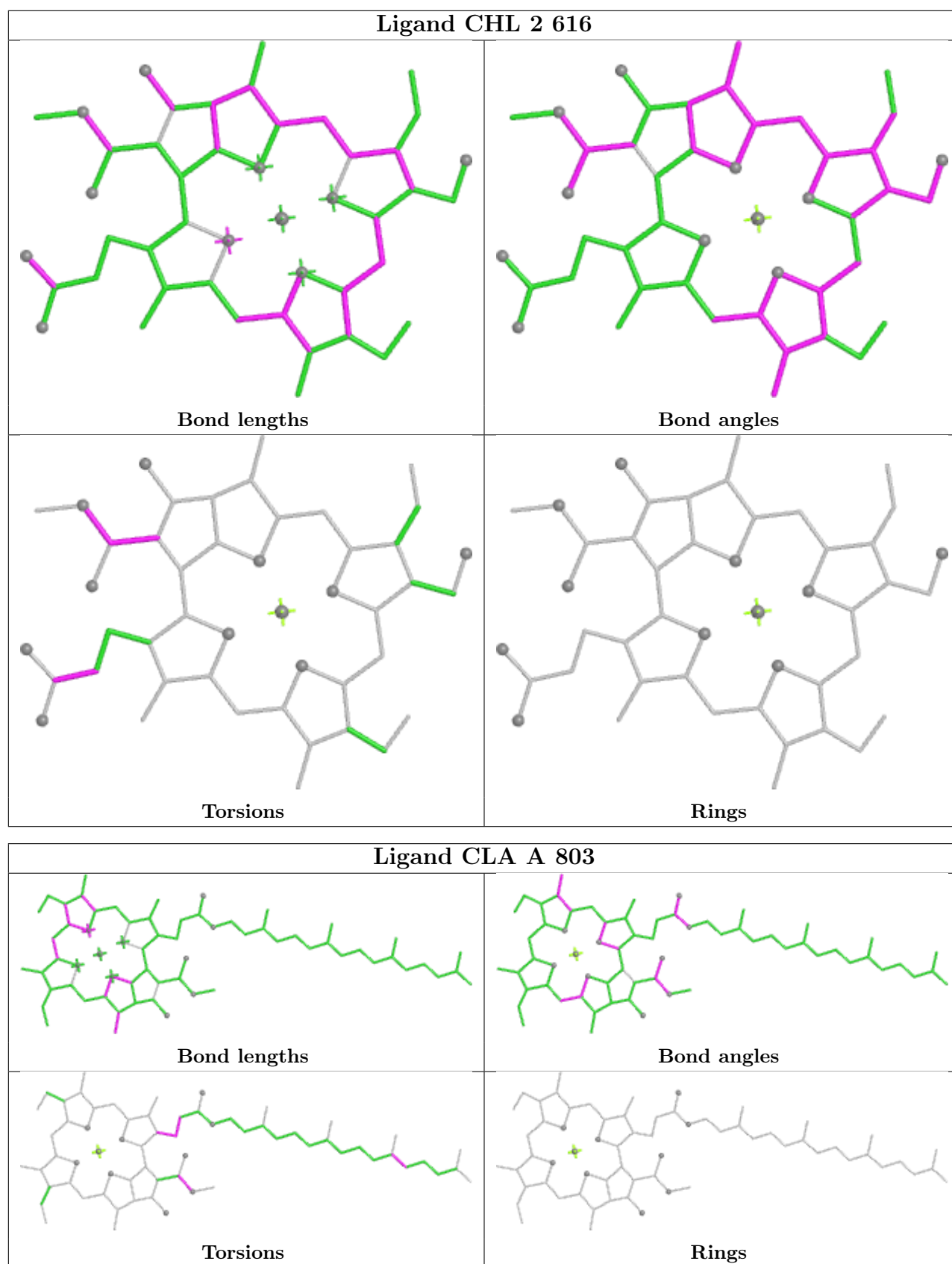


Ligand CLA 3 611

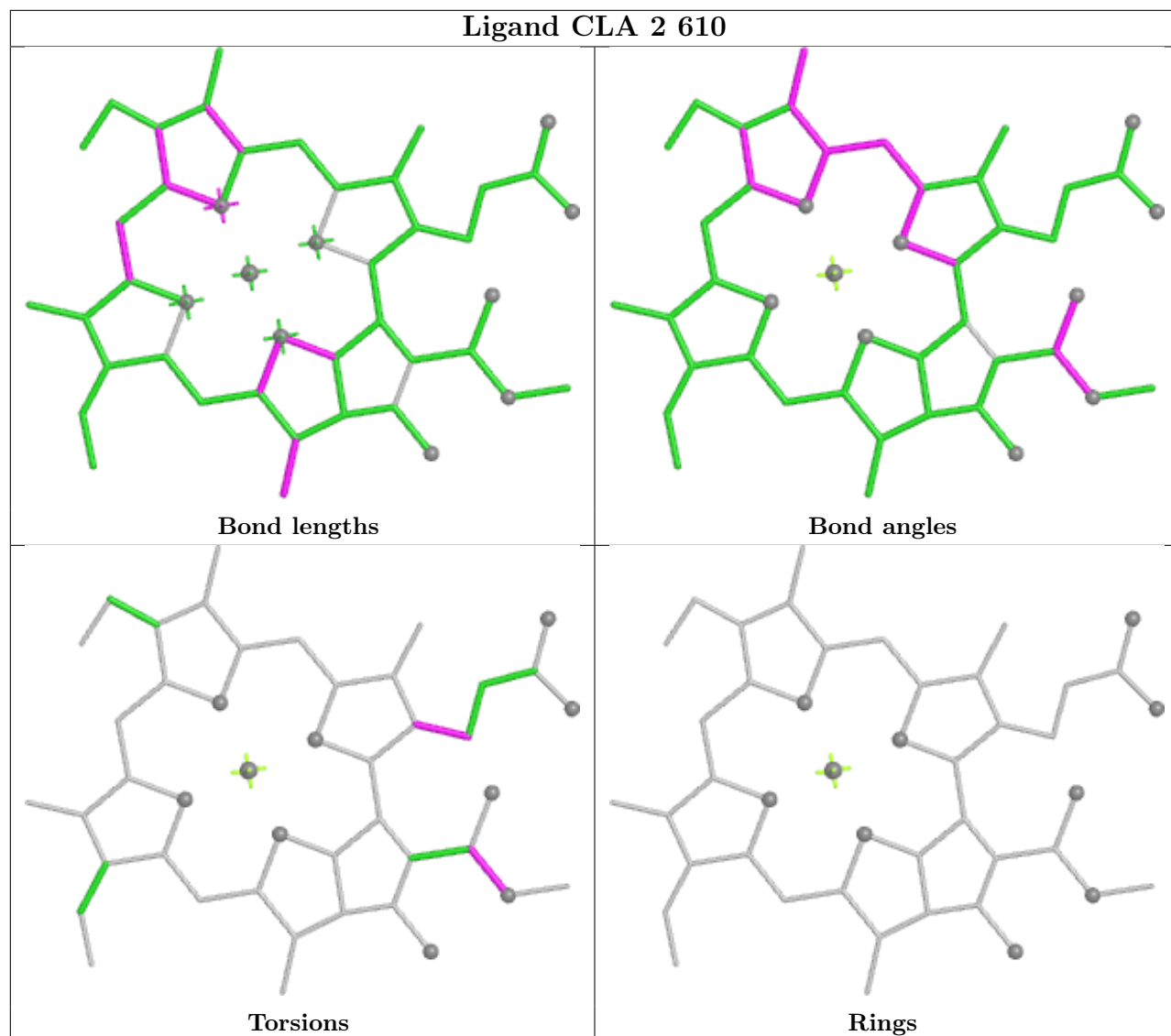


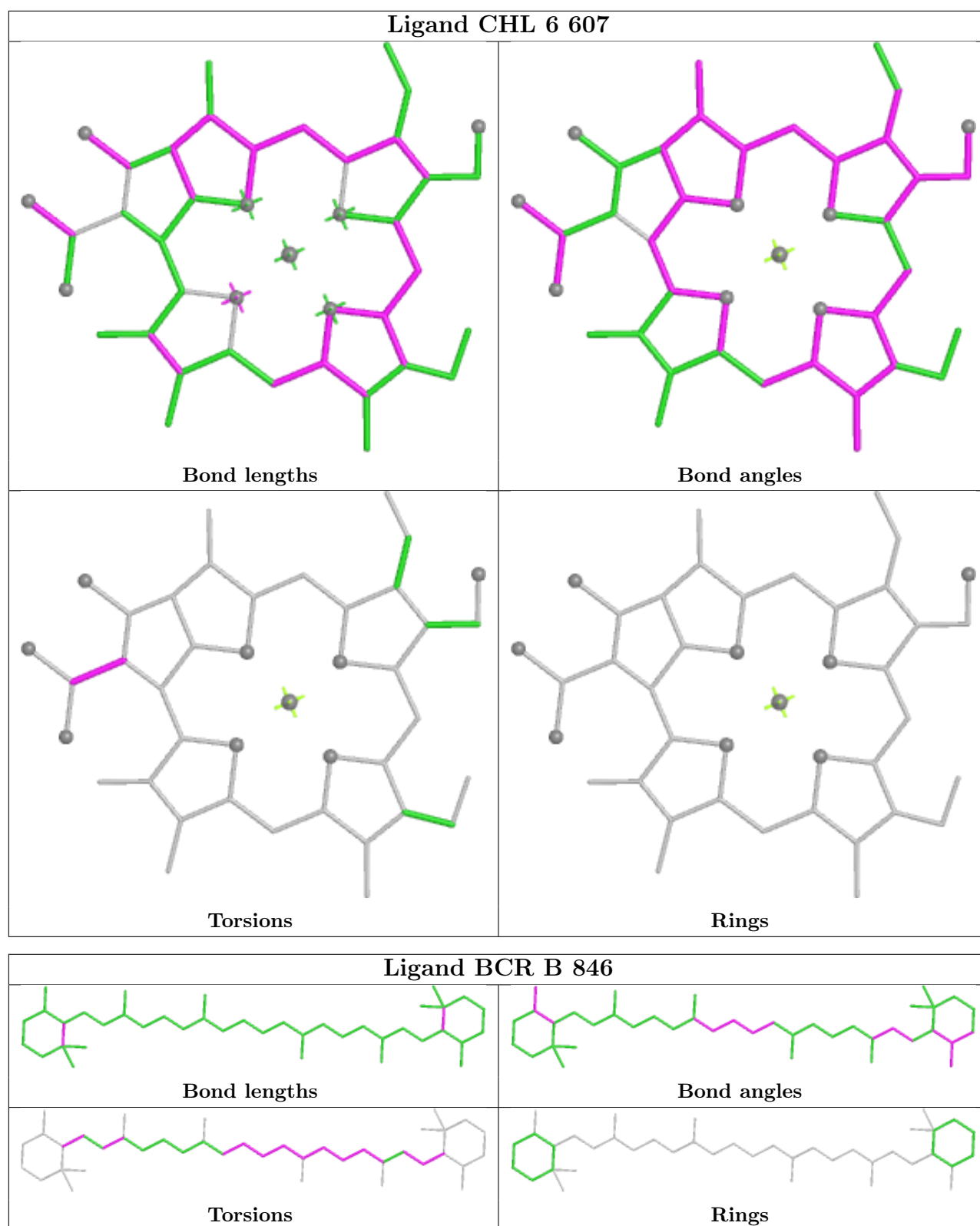
Ligand BCR F 302

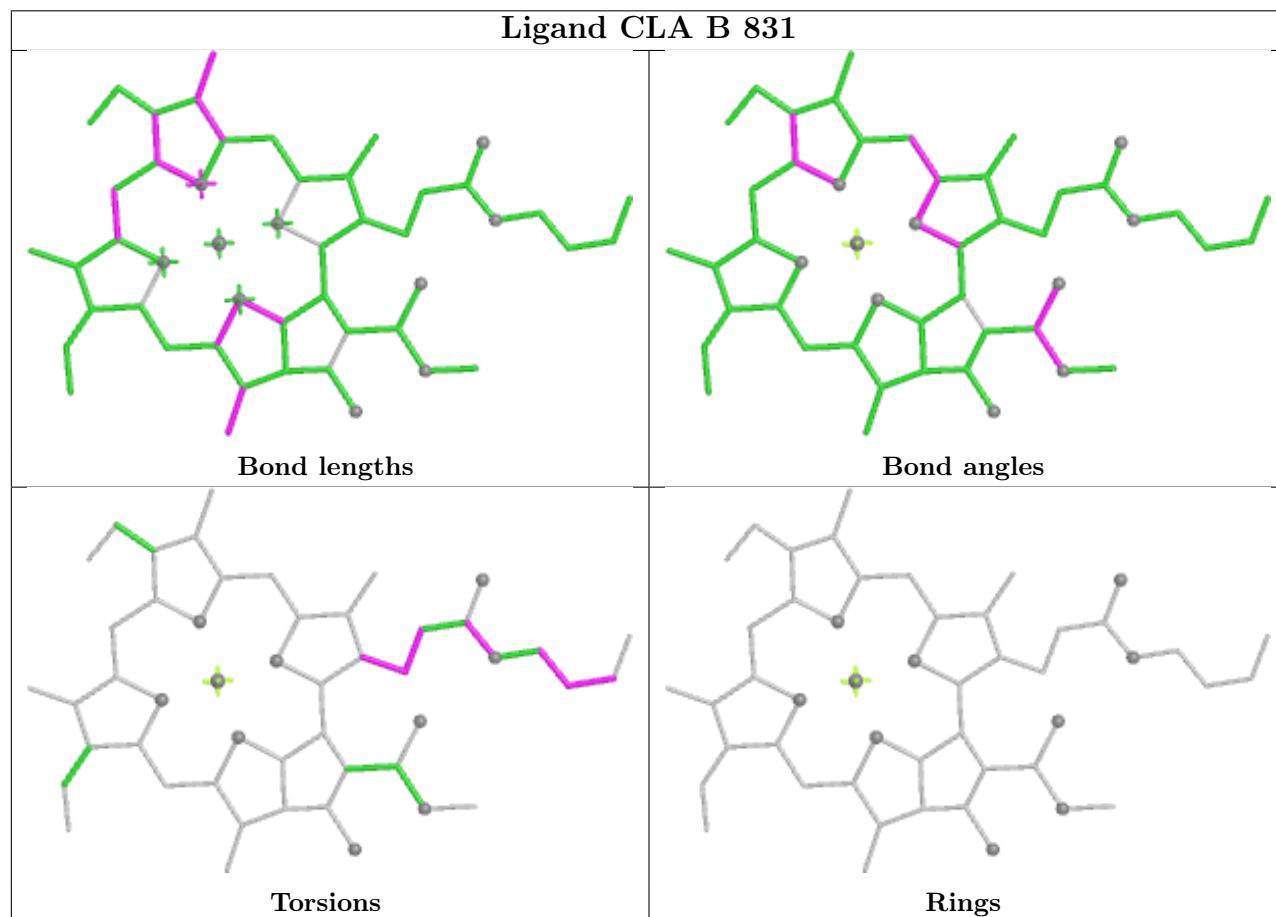
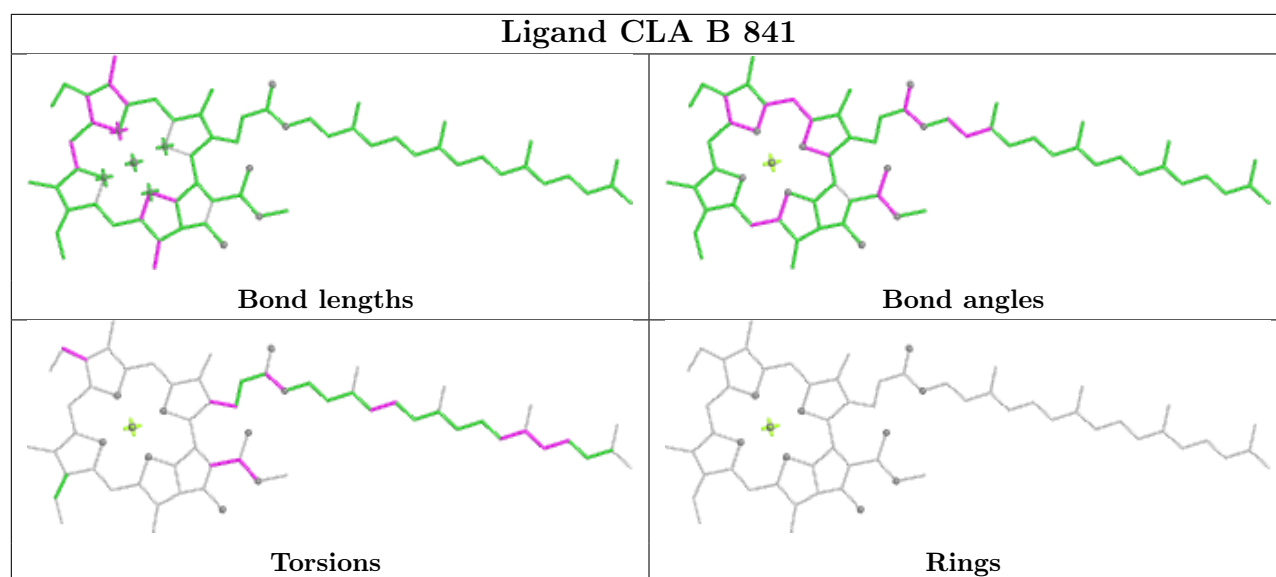


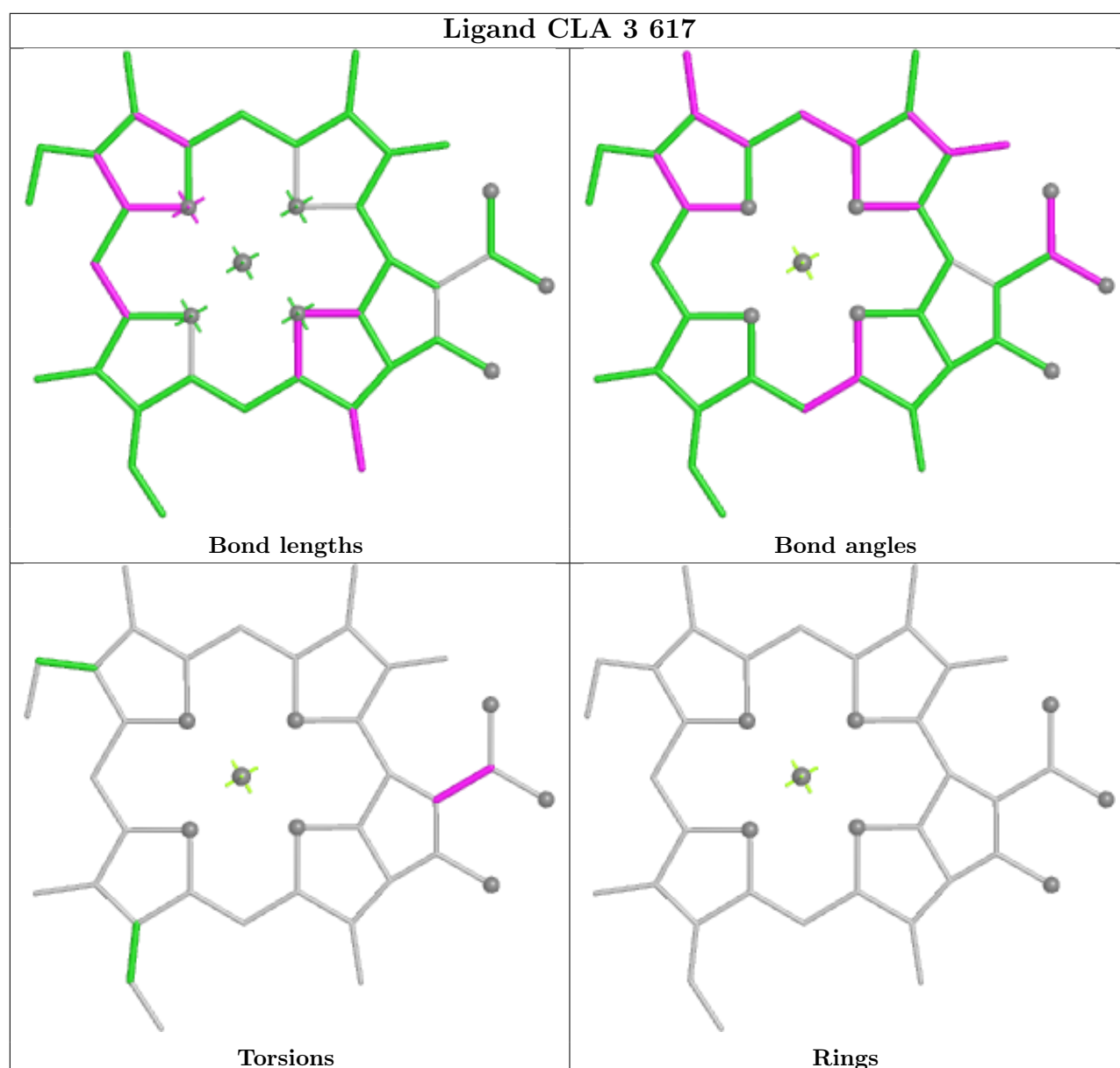
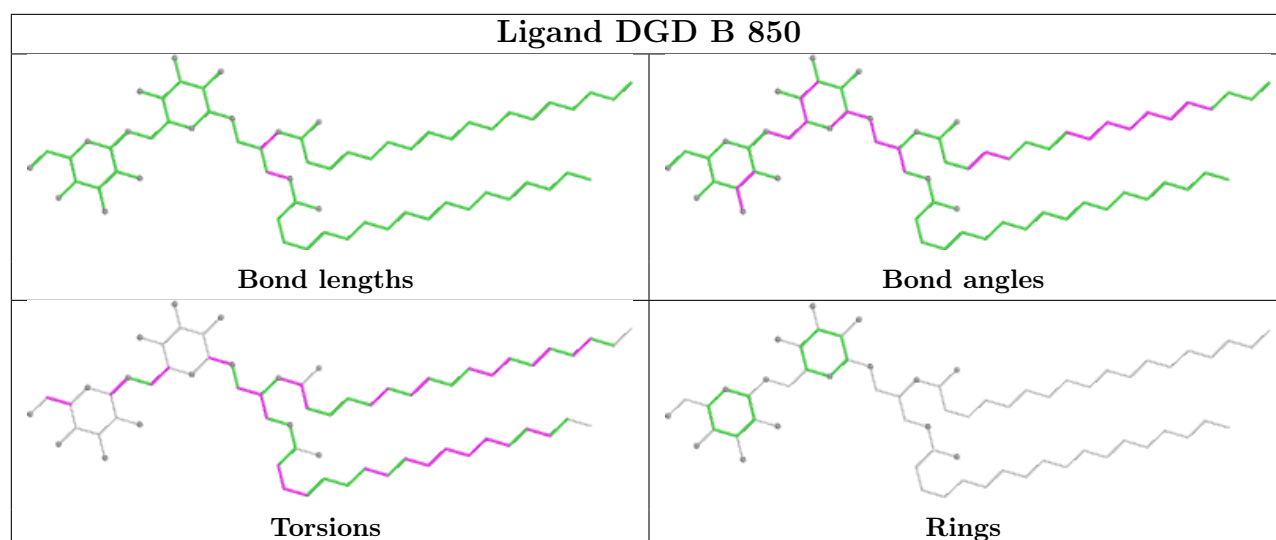


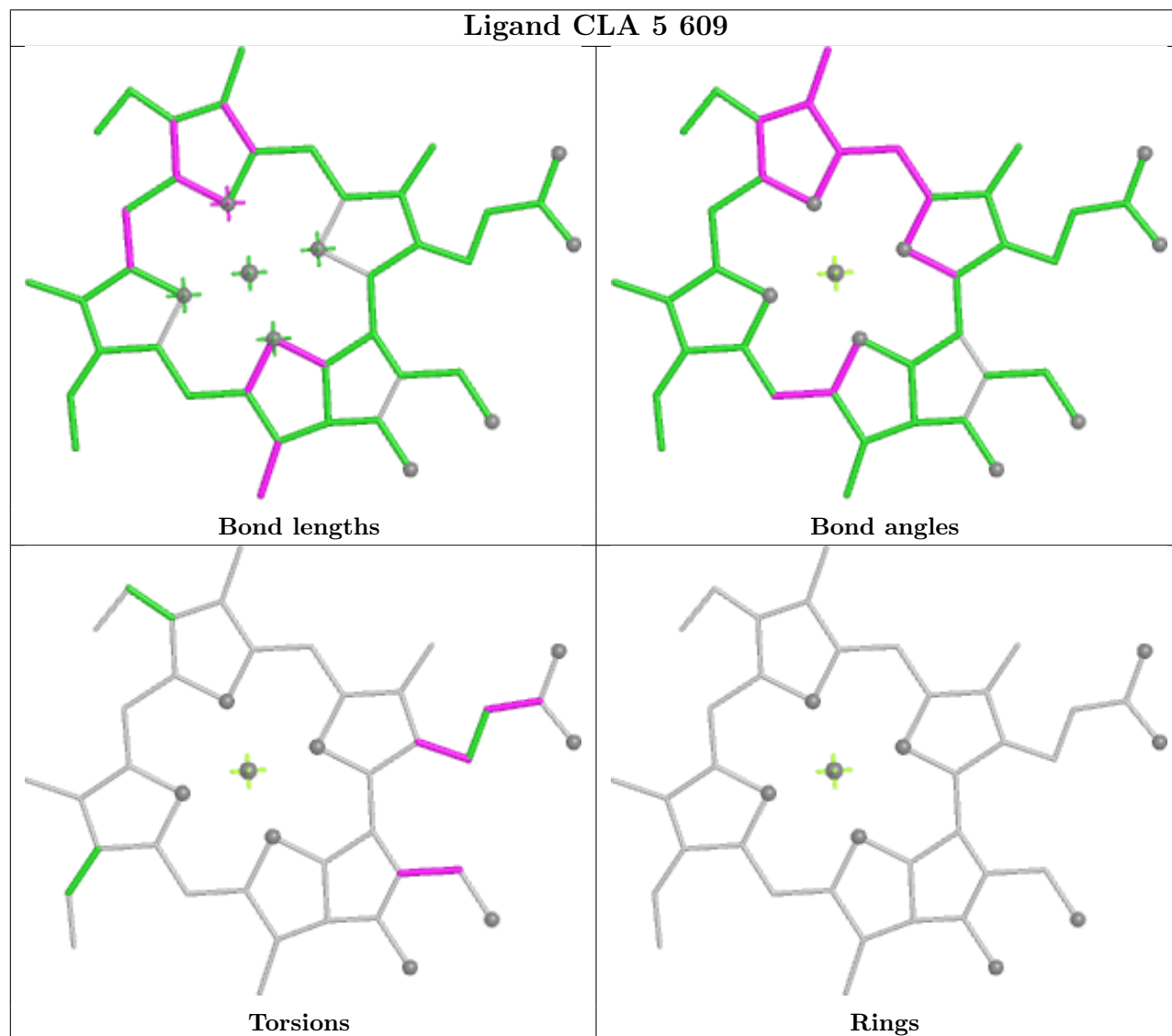
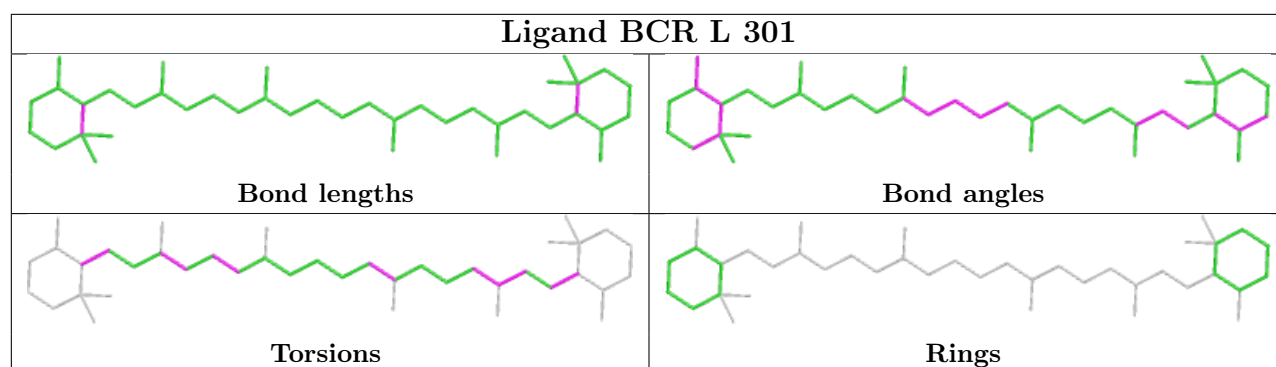
Ligand CLA 2 610



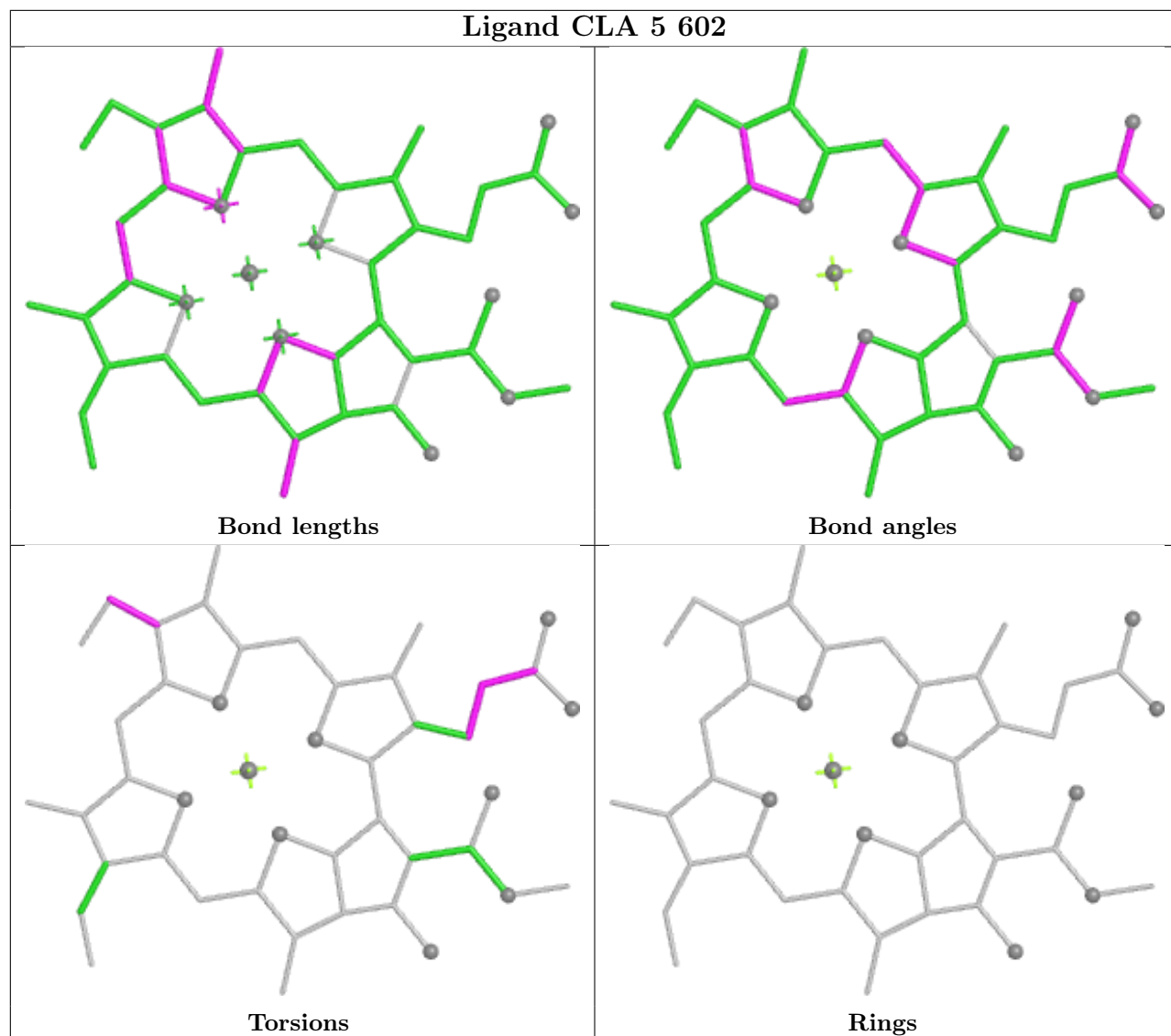




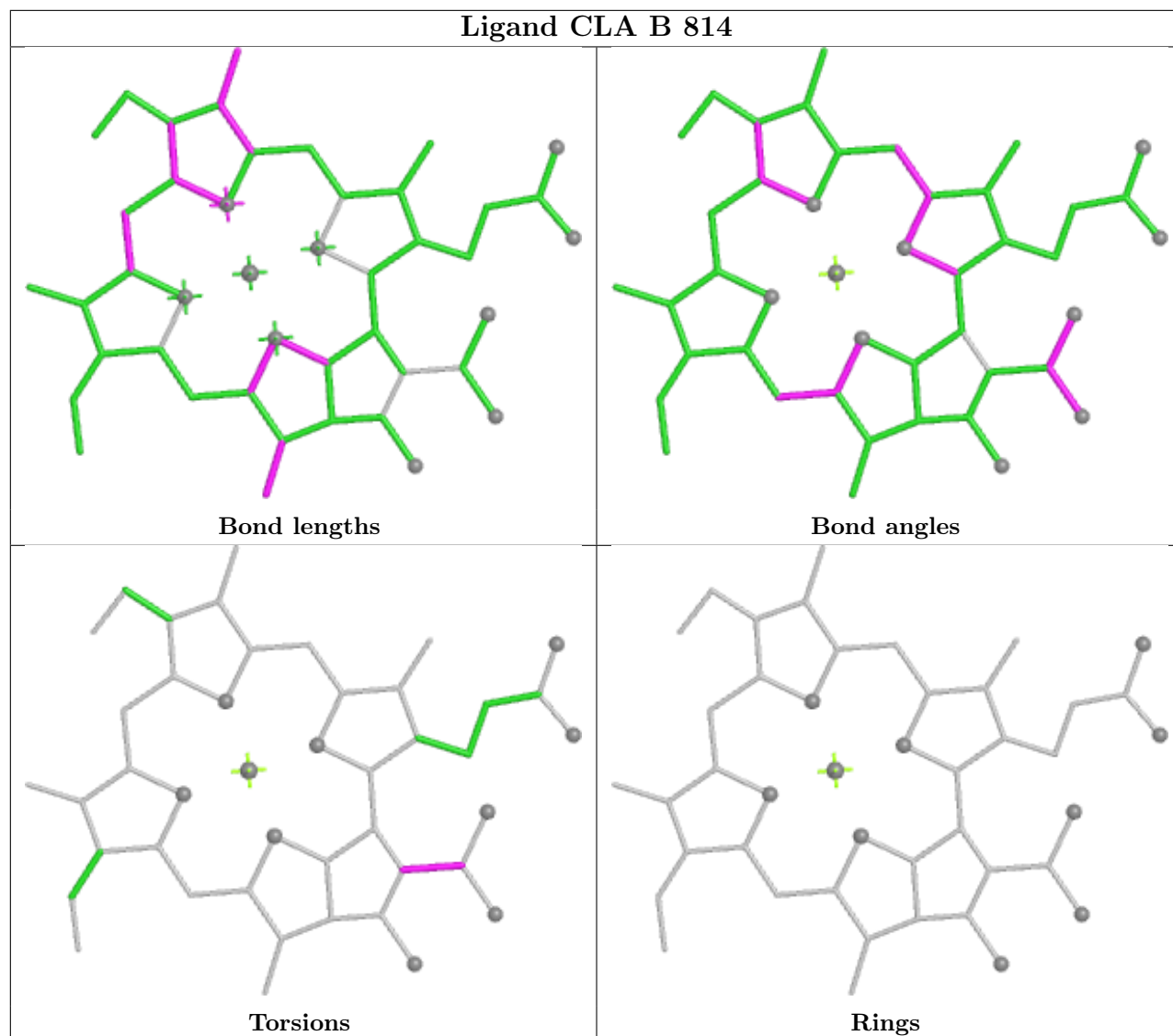




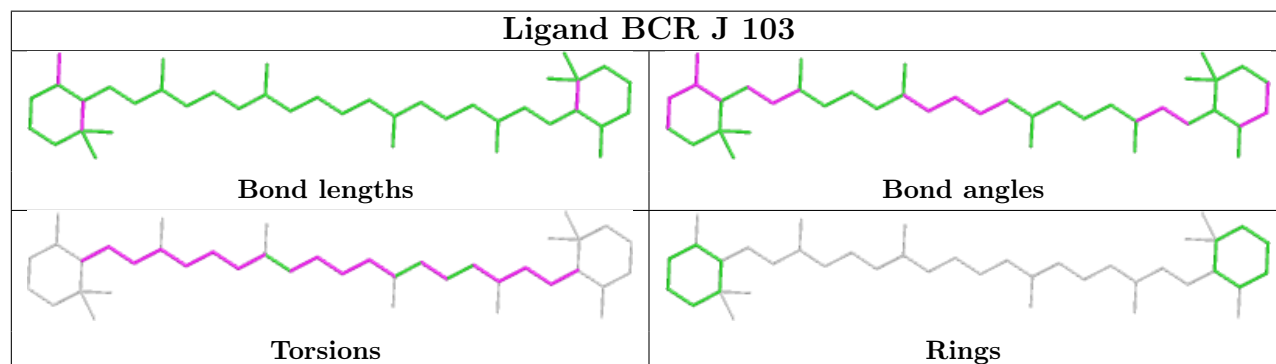
Ligand CLA 5 602



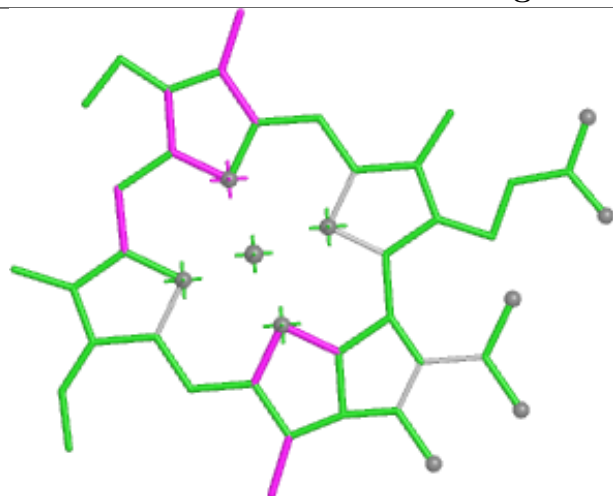
Ligand CLA B 814



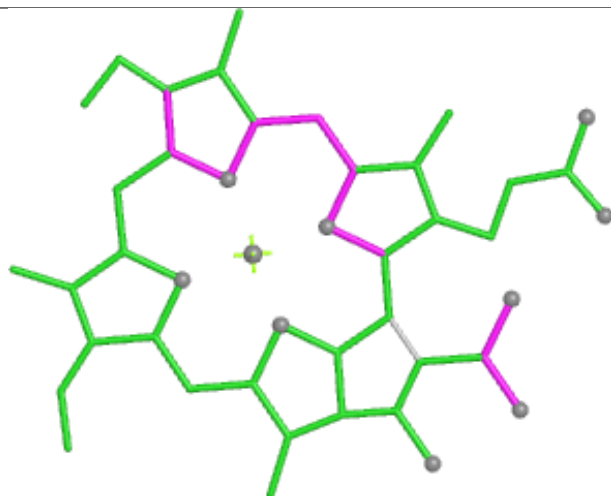
Ligand BCR J 103



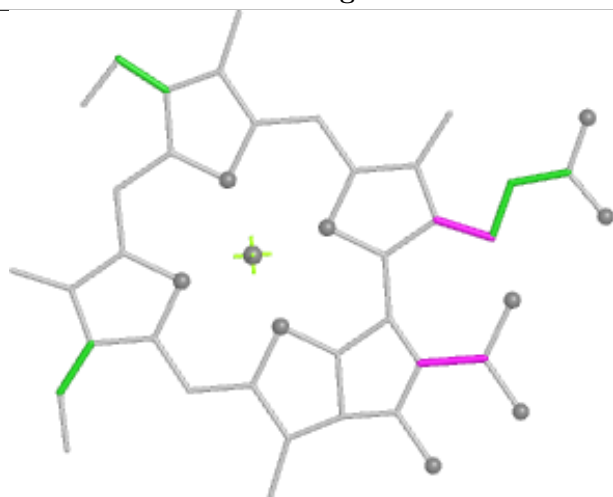
Ligand CLA A 807



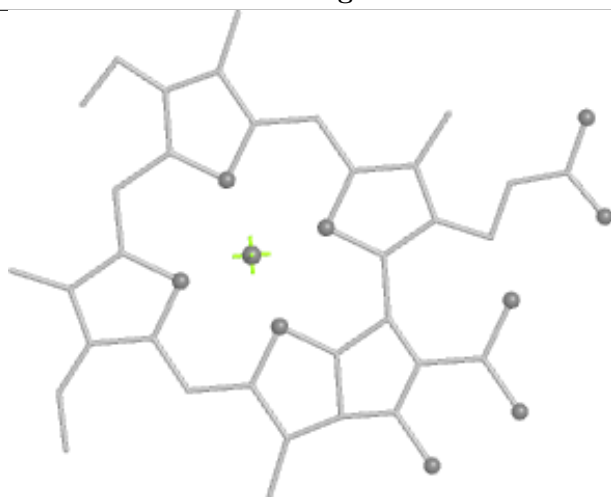
Bond lengths



Bond angles

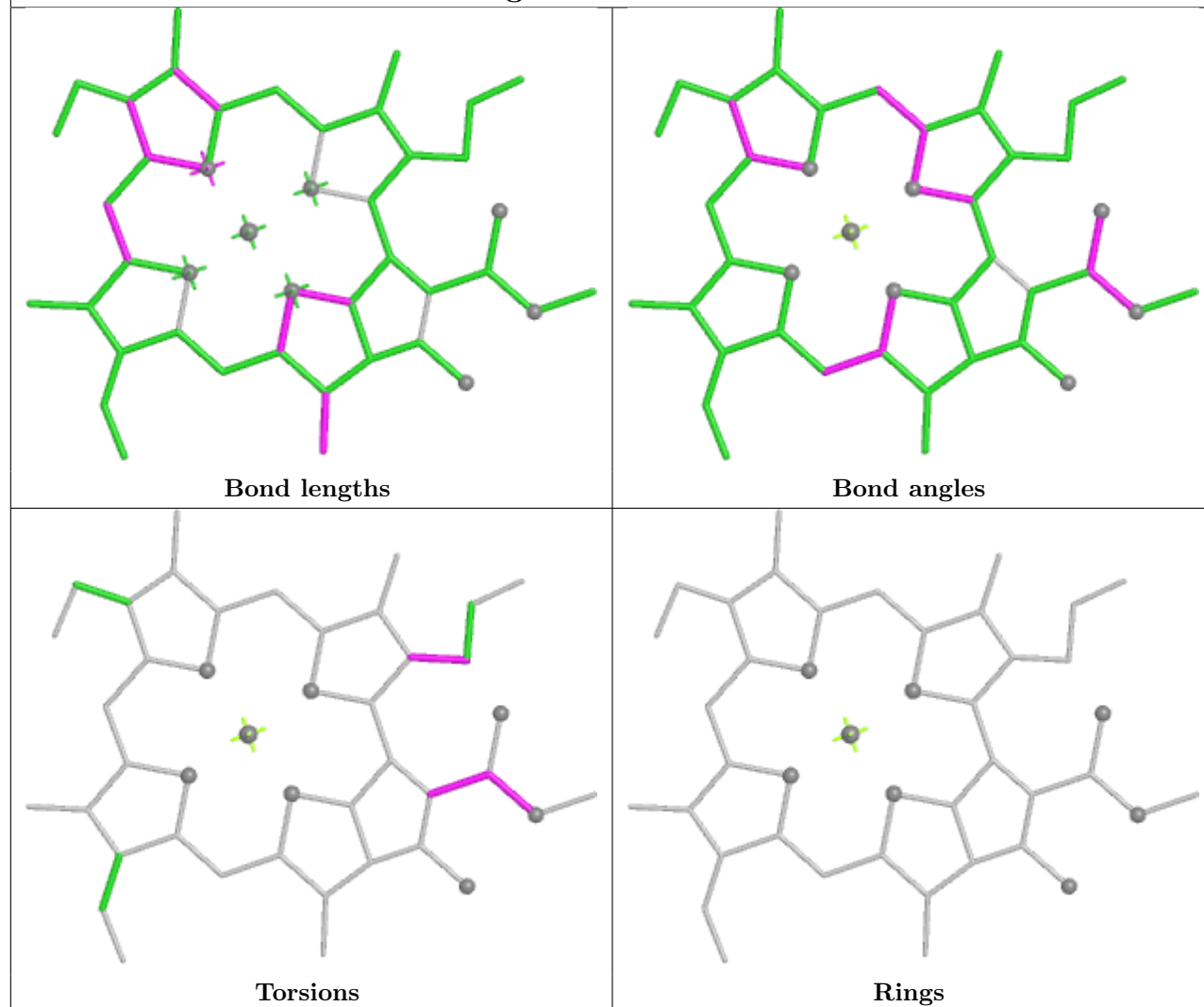


Torsions

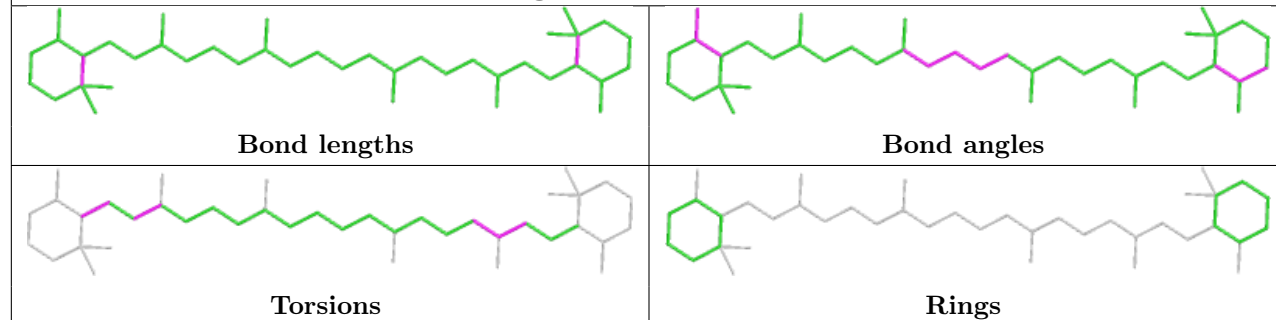


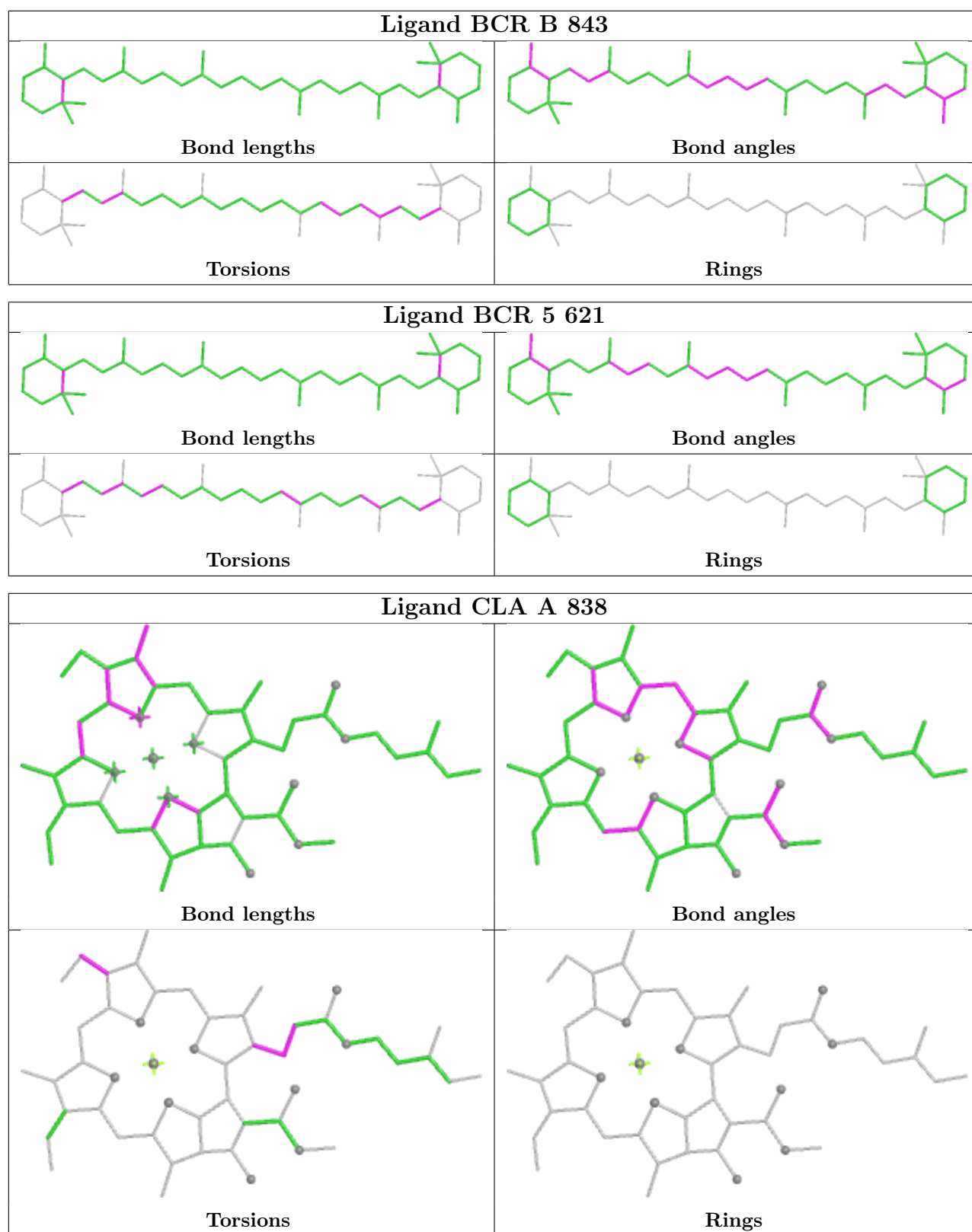
Rings

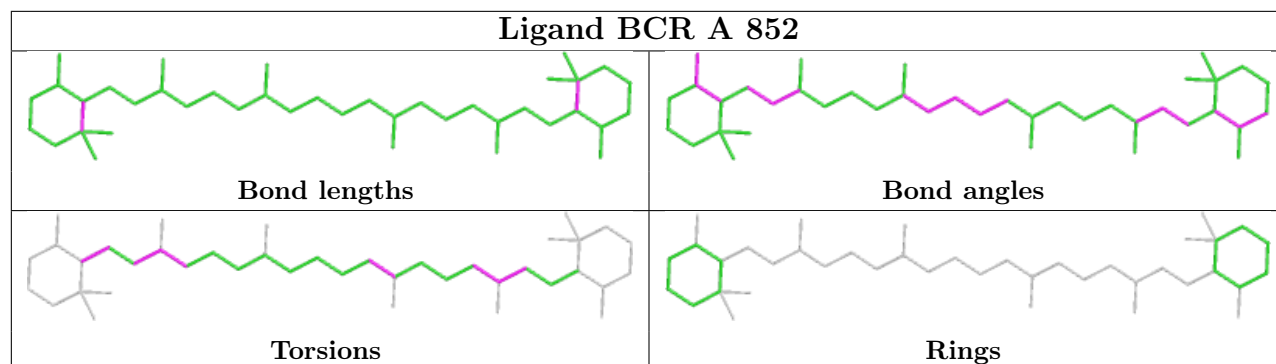
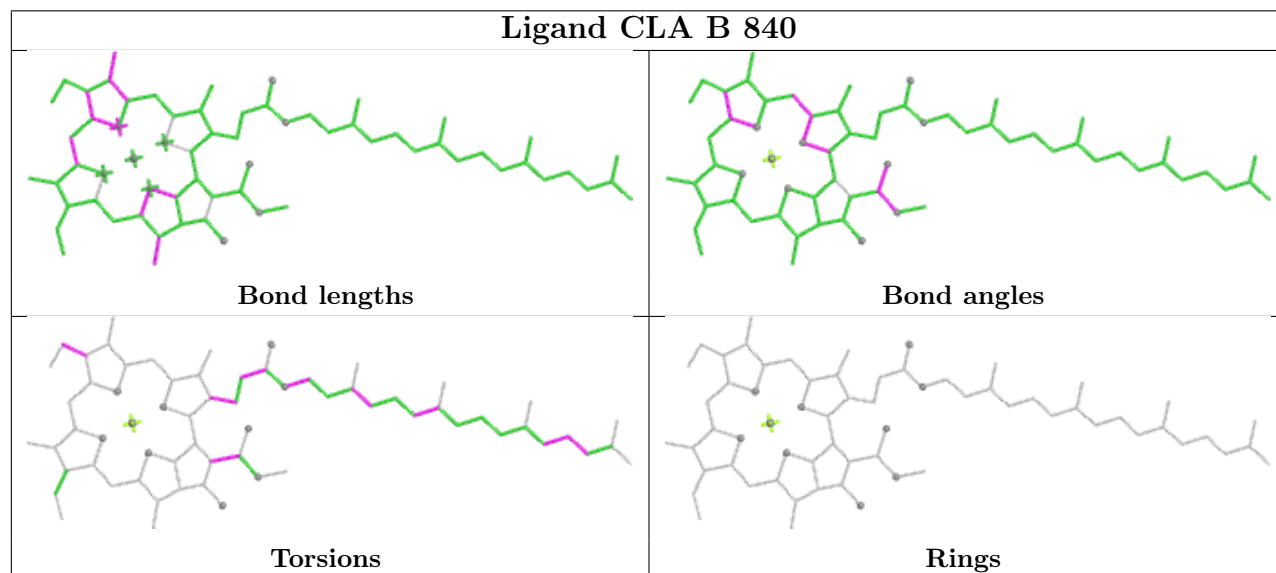
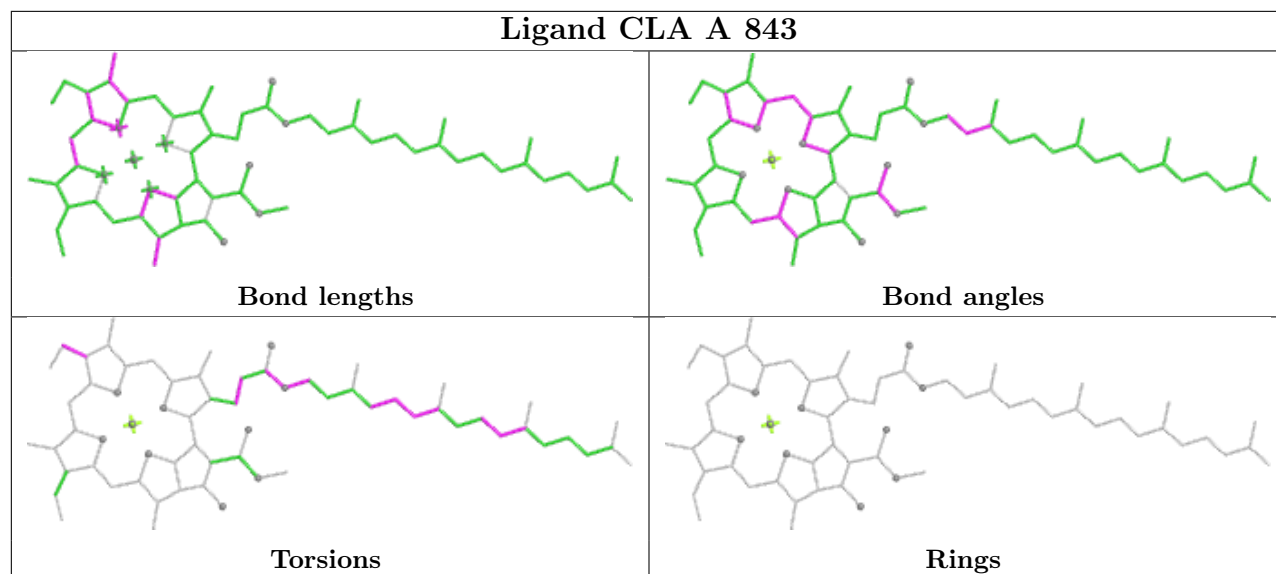
Ligand CLA 5 614

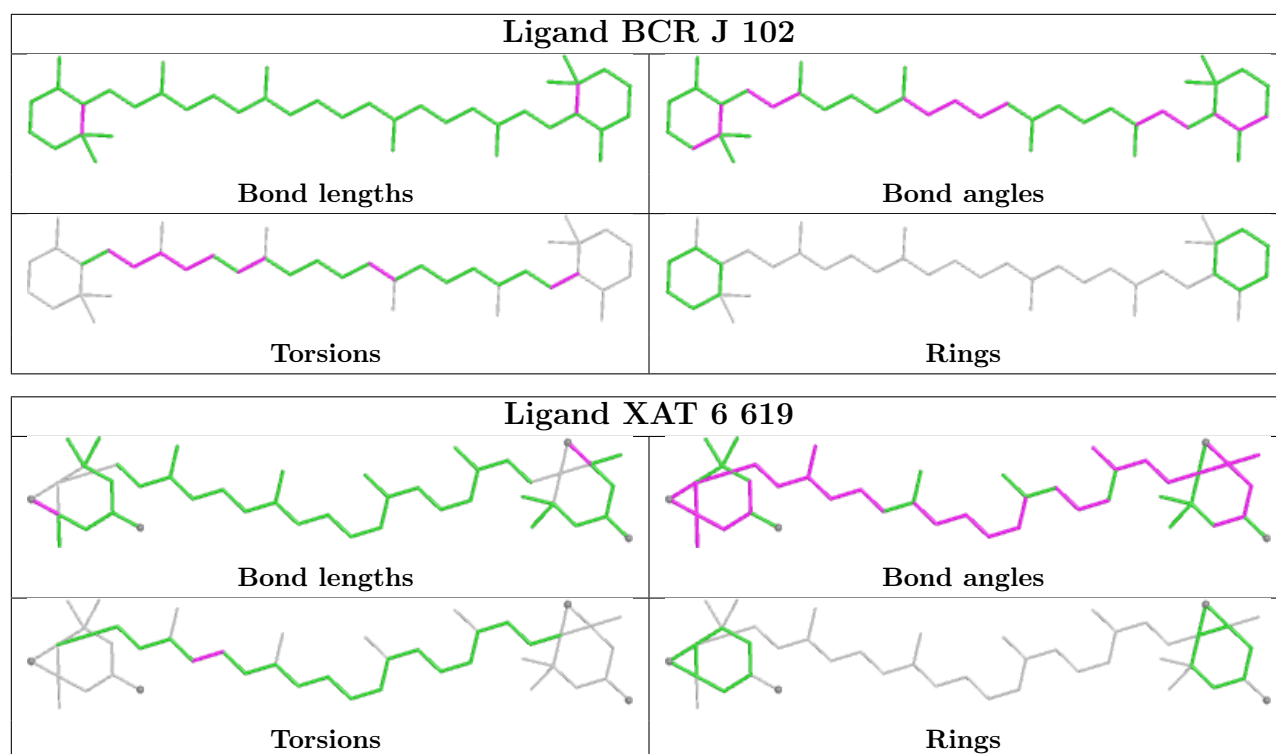


Ligand BCR B 844

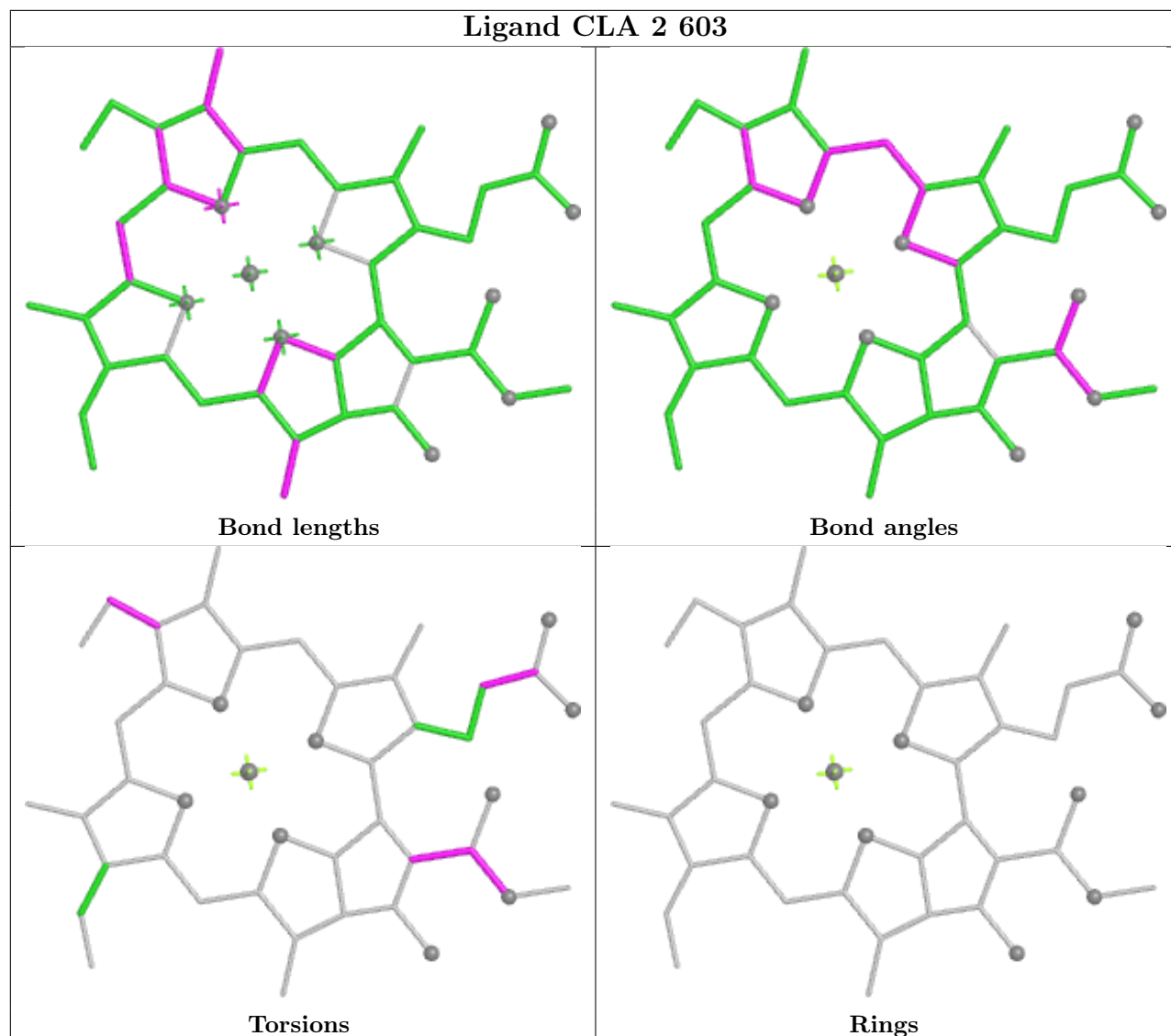




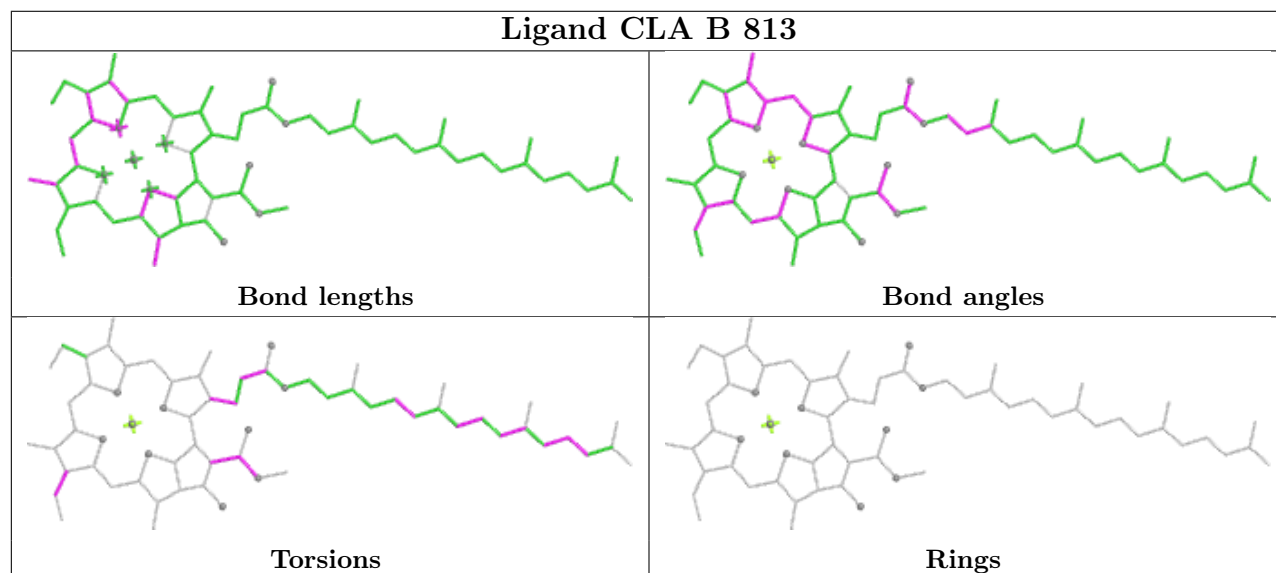


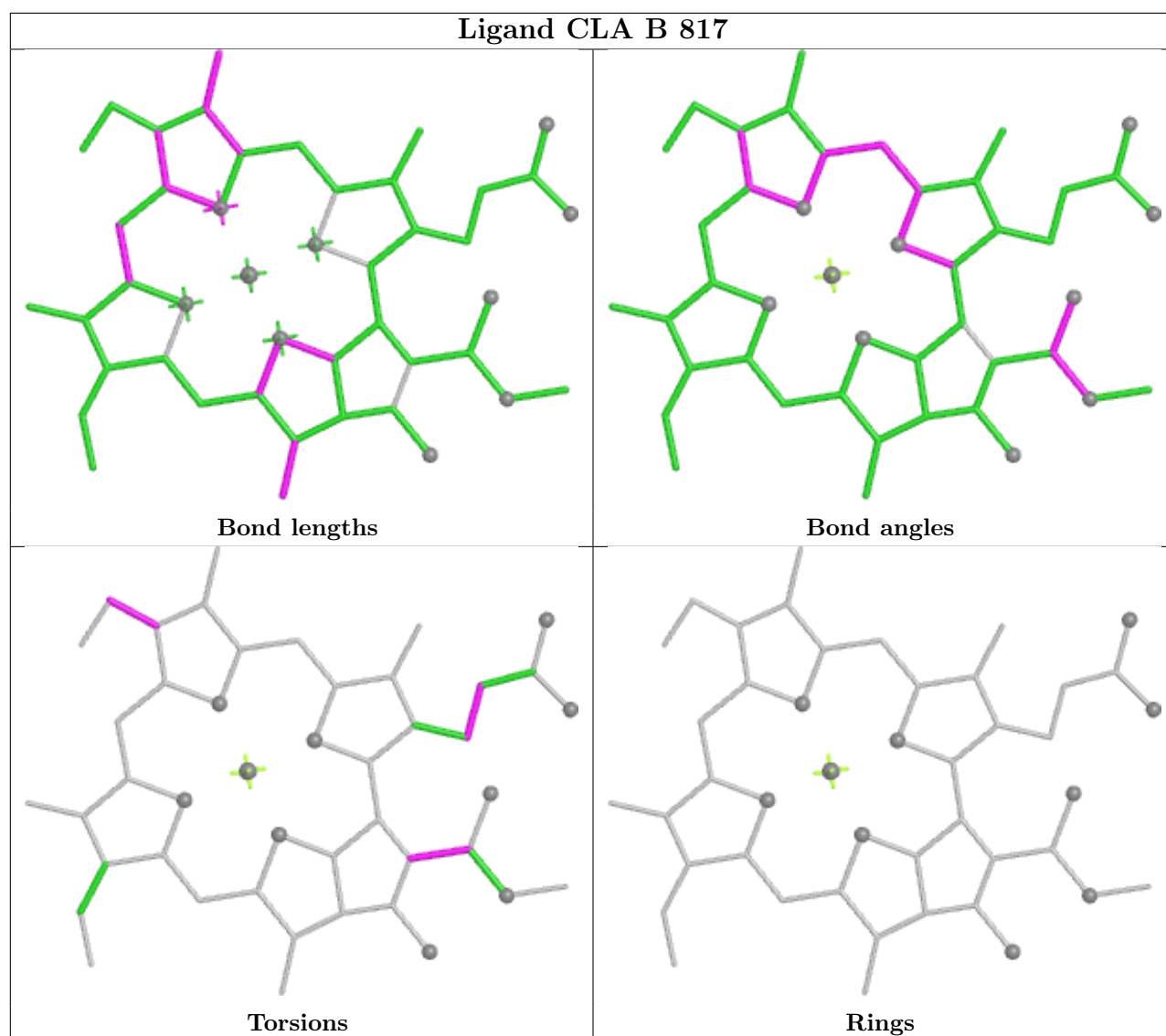


Ligand CLA 2 603

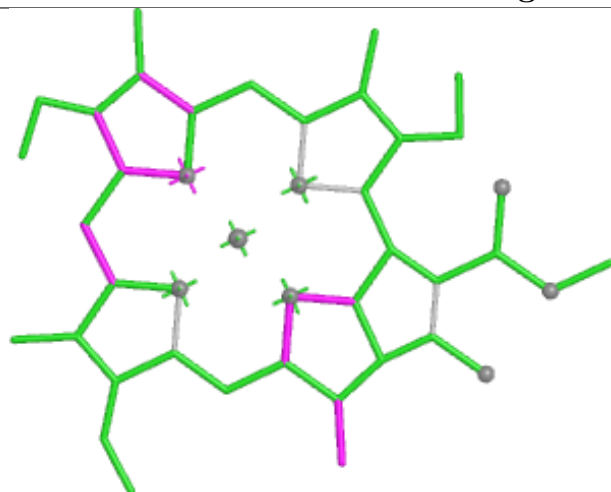


Ligand CLA B 813

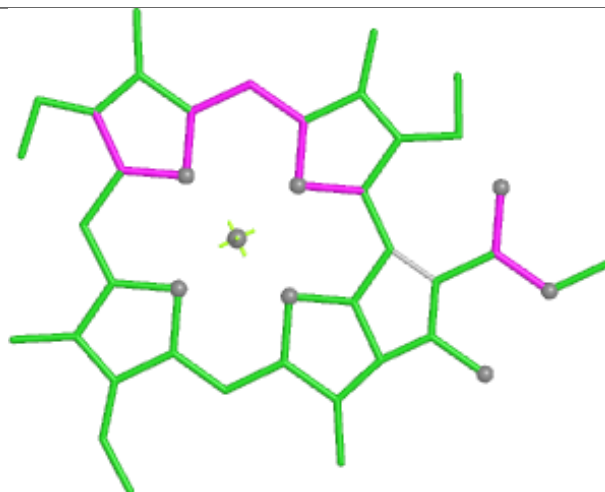




Ligand CLA J 101



Bond lengths



Bond angles

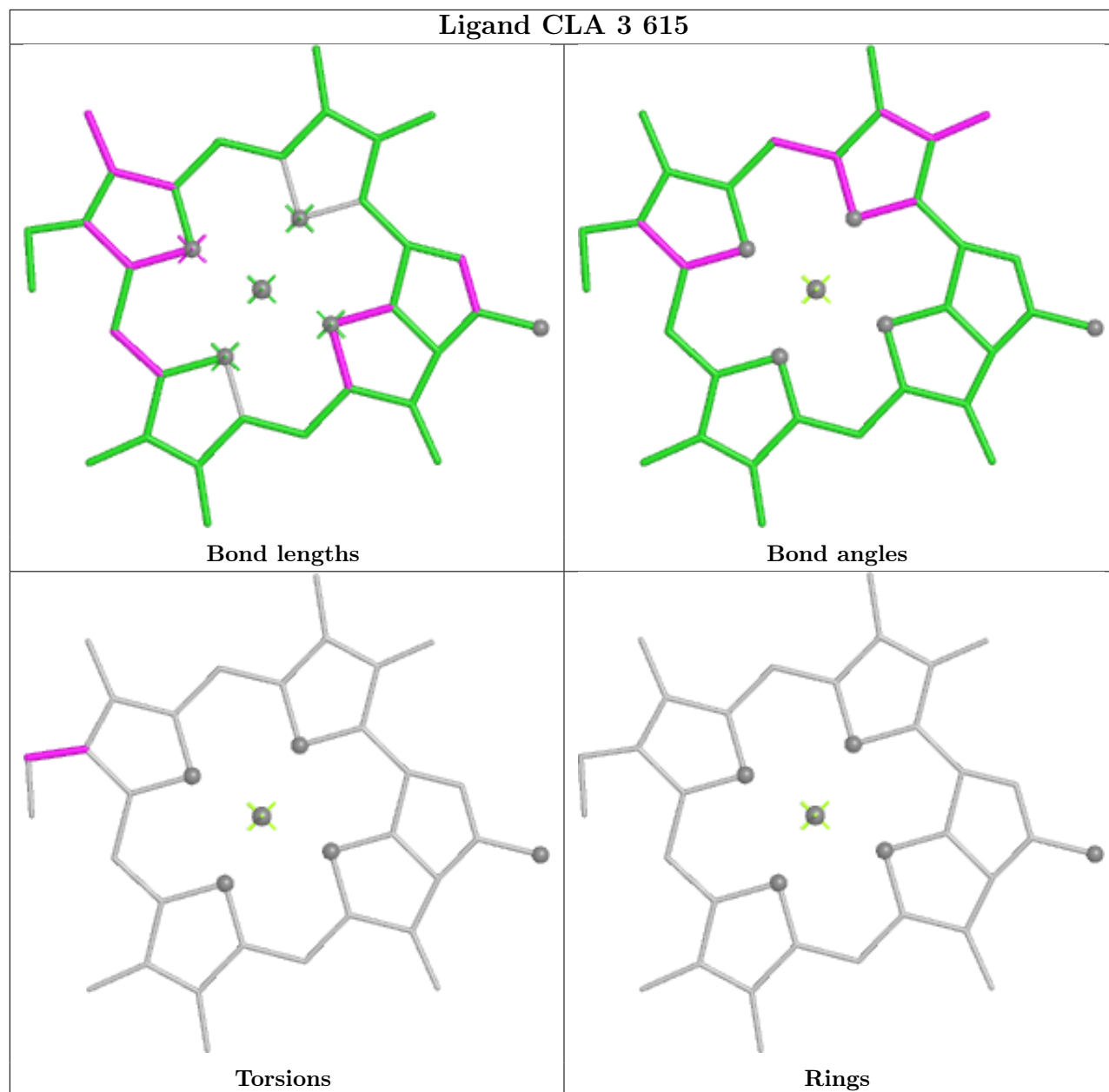


Torsions

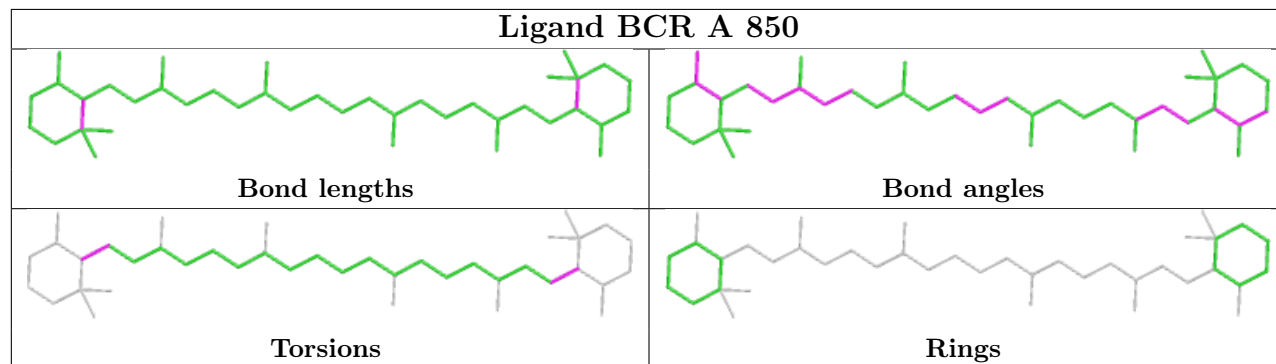


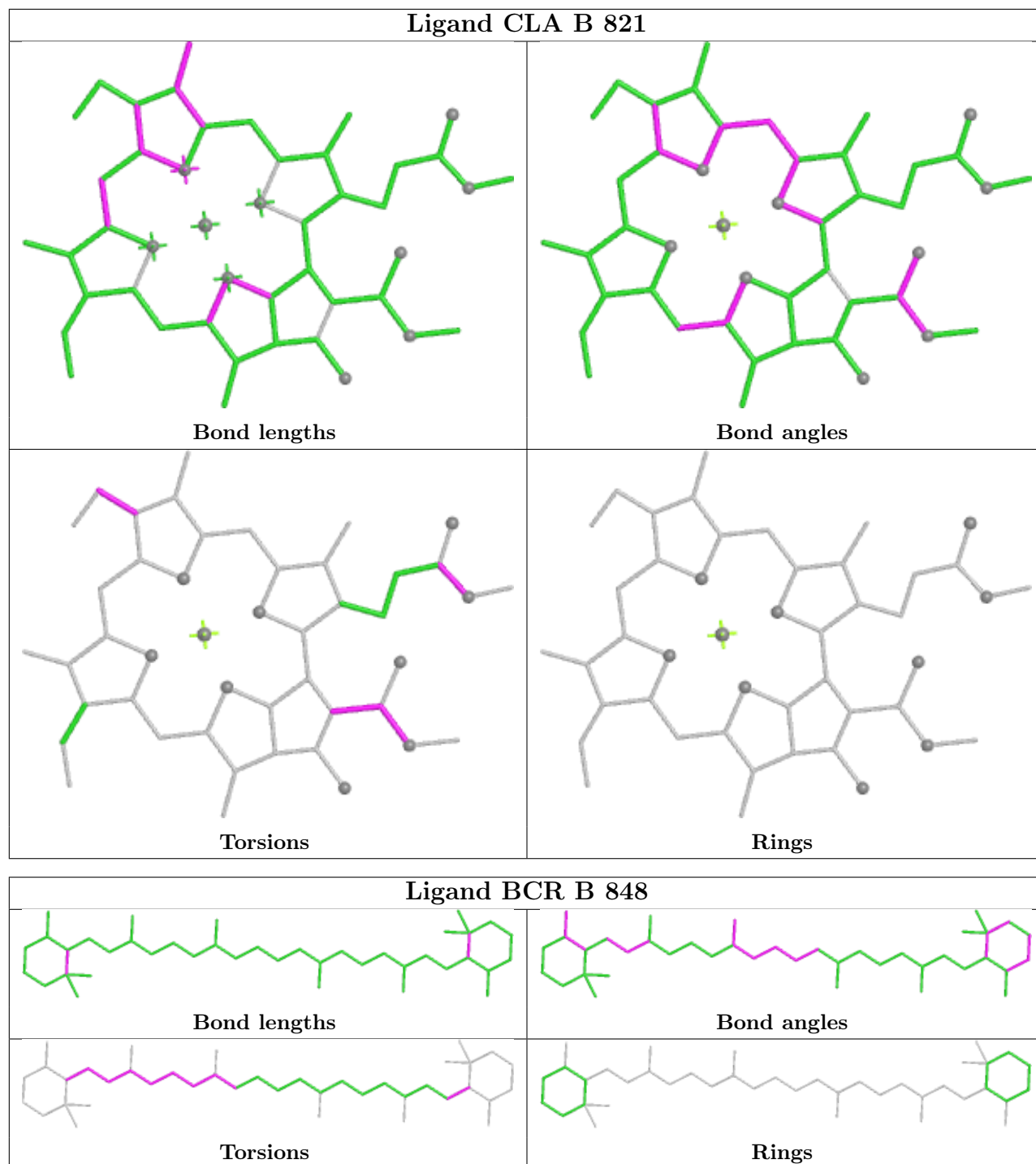
Rings

Ligand CLA 3 615

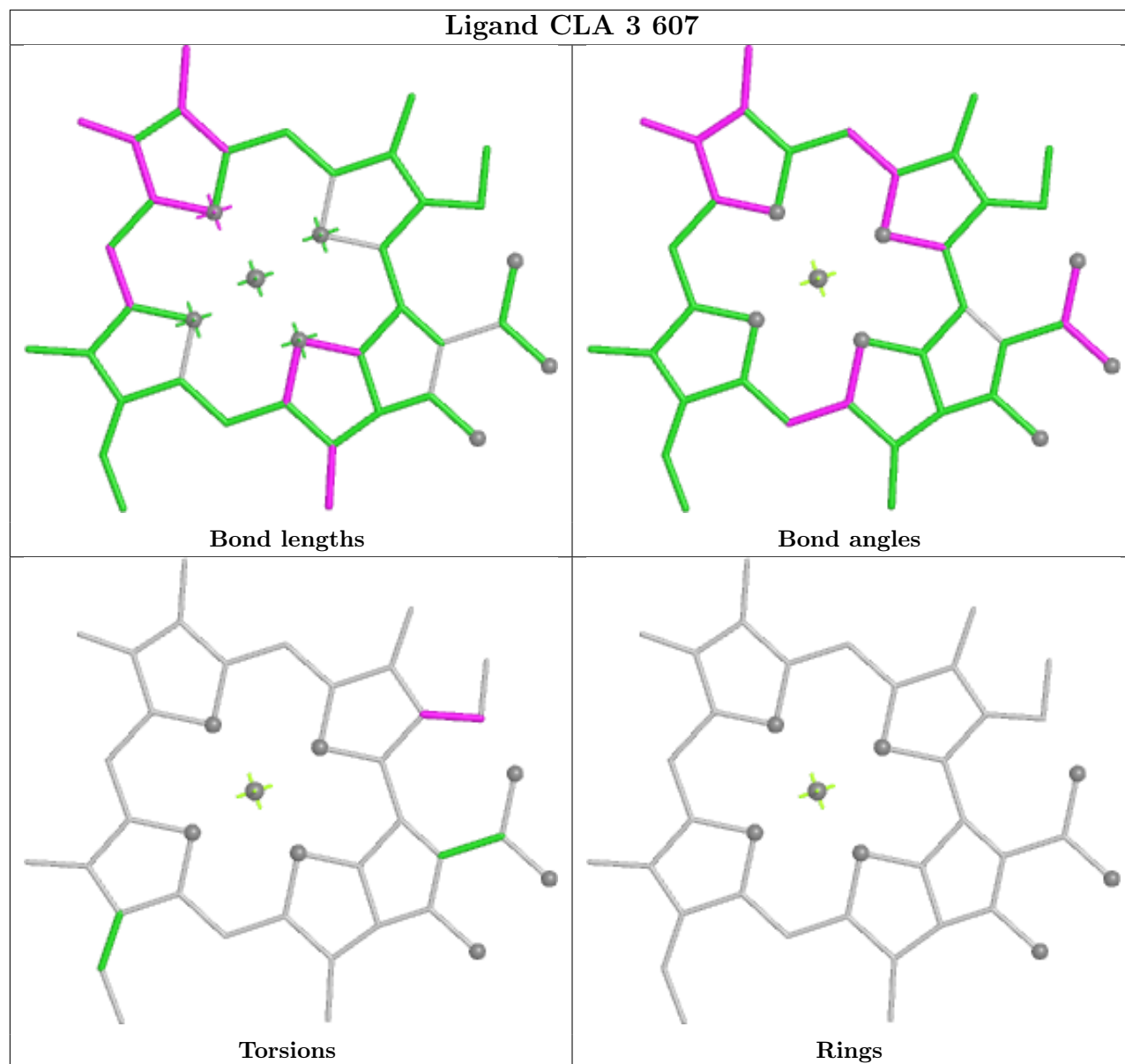


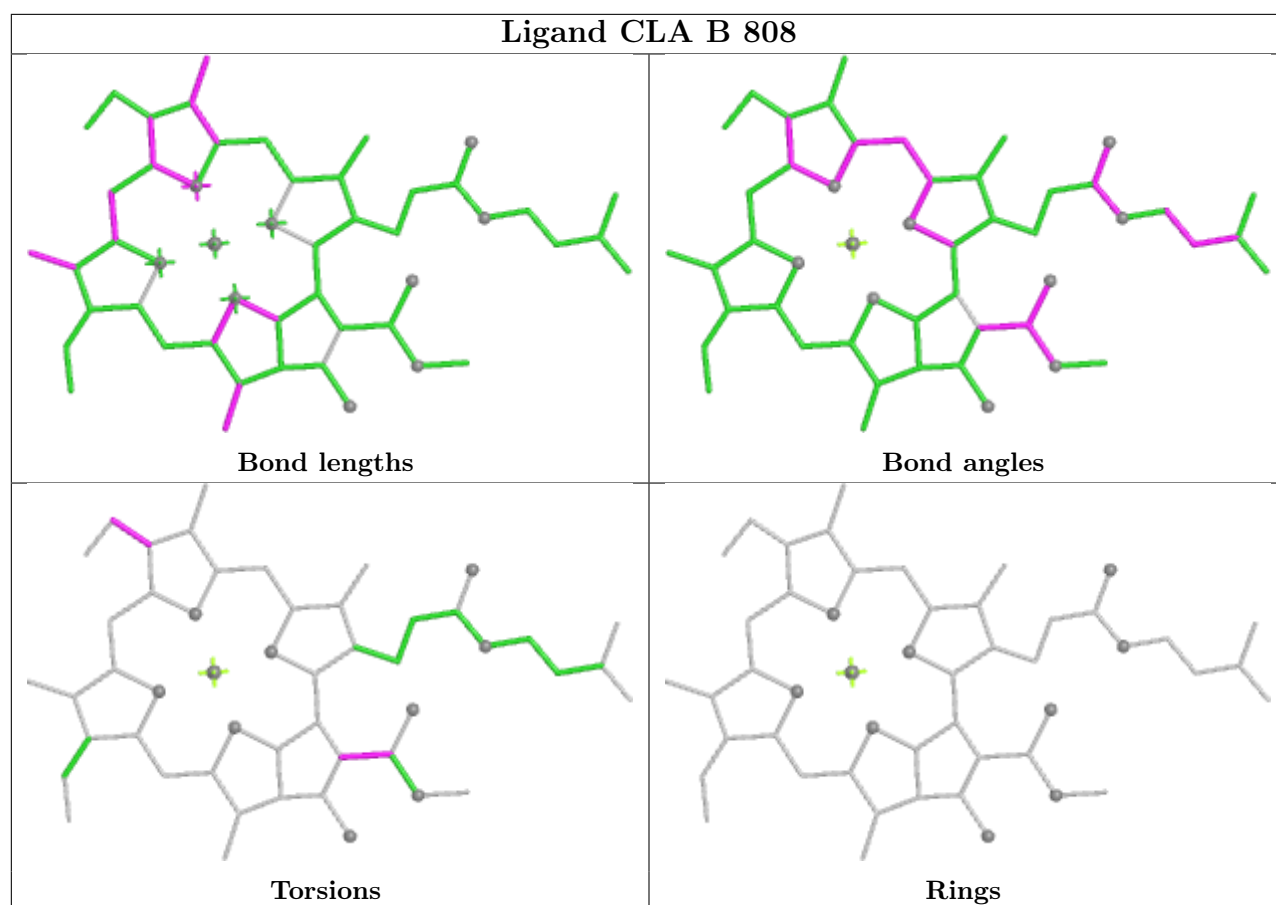
Ligand BCR A 850



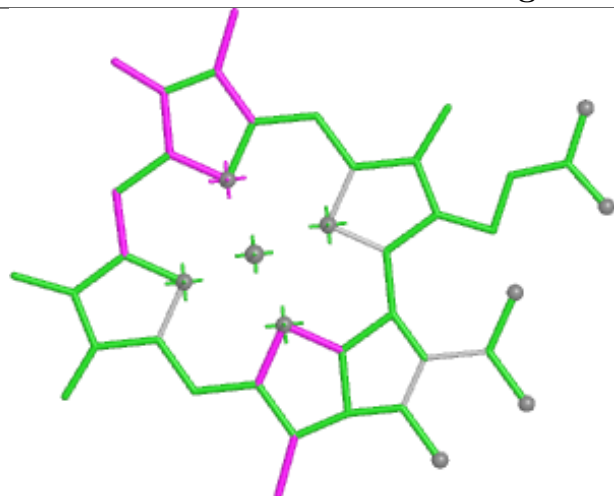


Ligand CLA 3 607

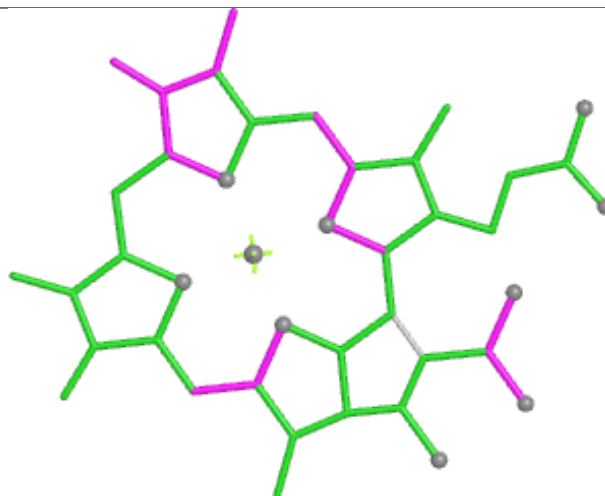




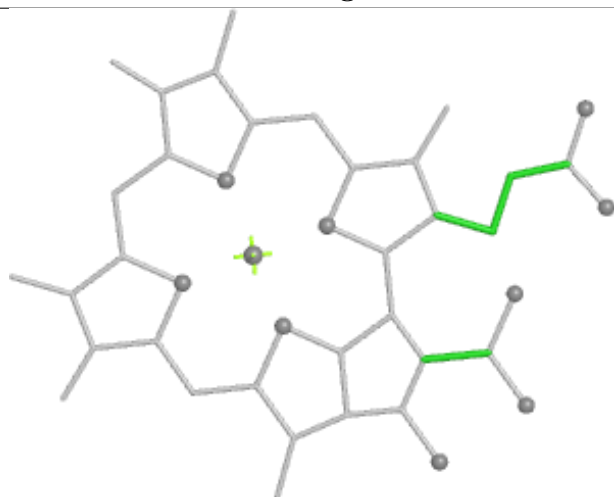
Ligand CLA 3 604



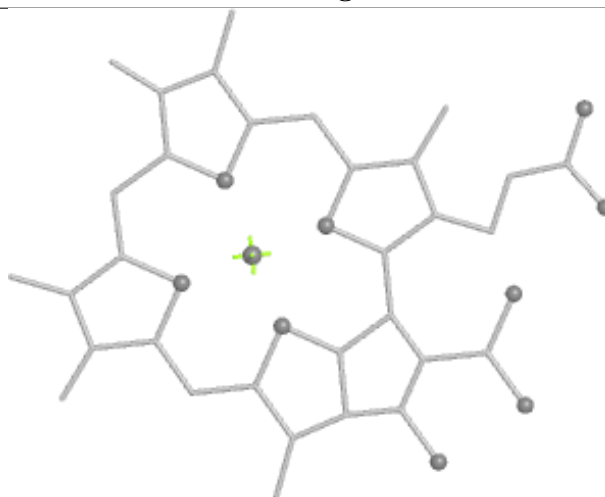
Bond lengths



Bond angles

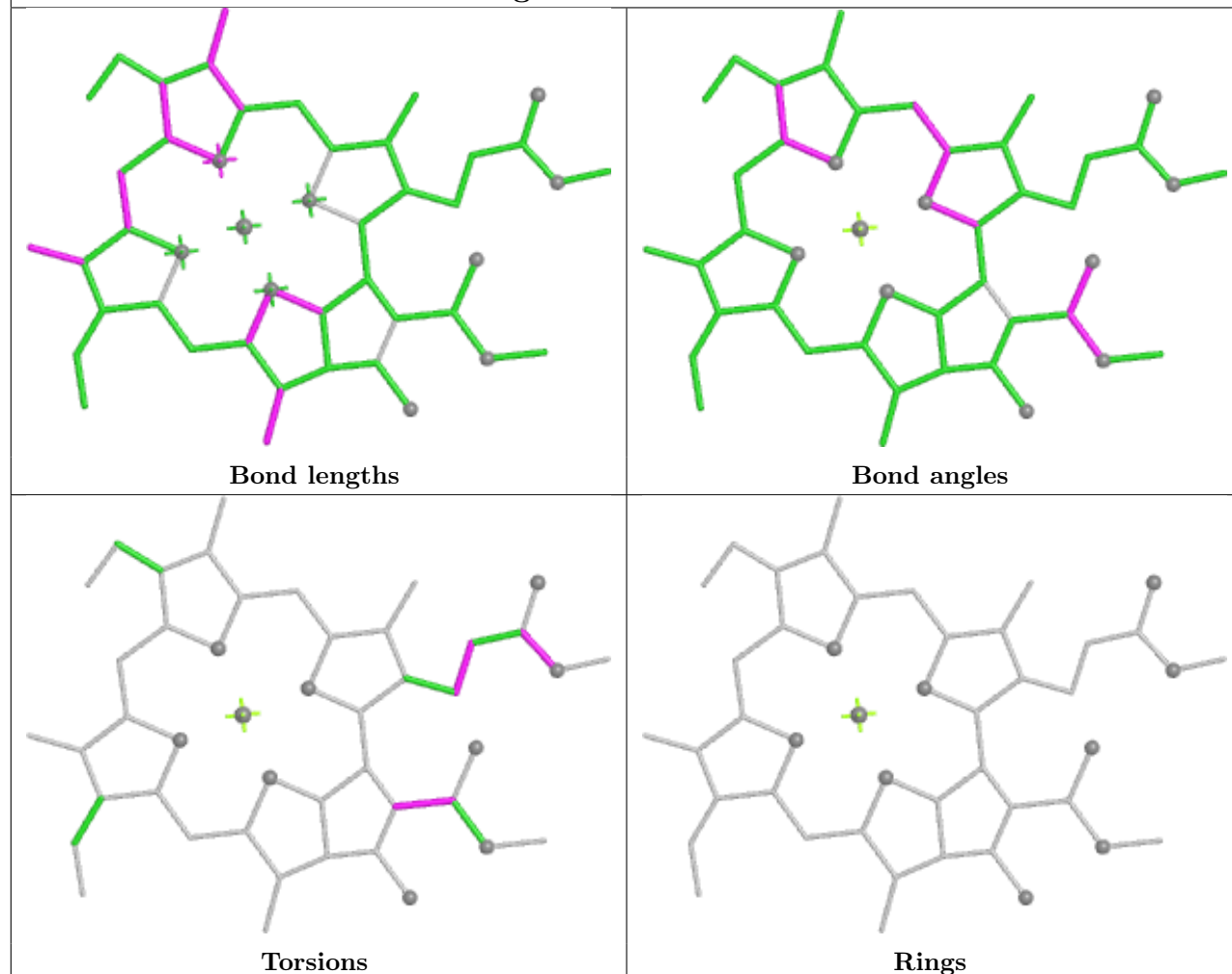


Torsions

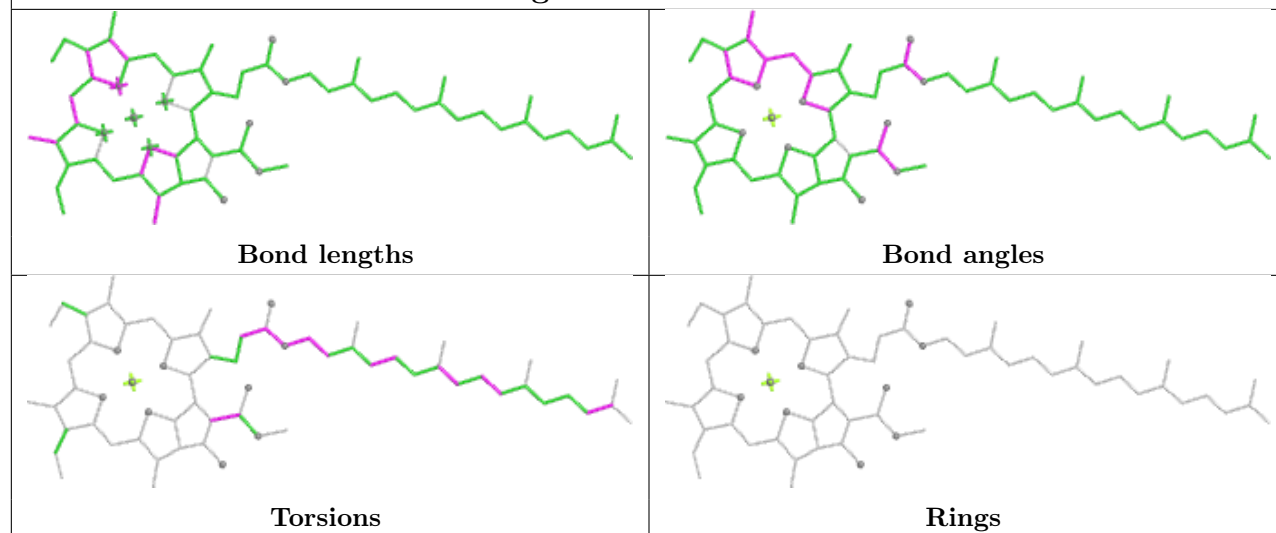


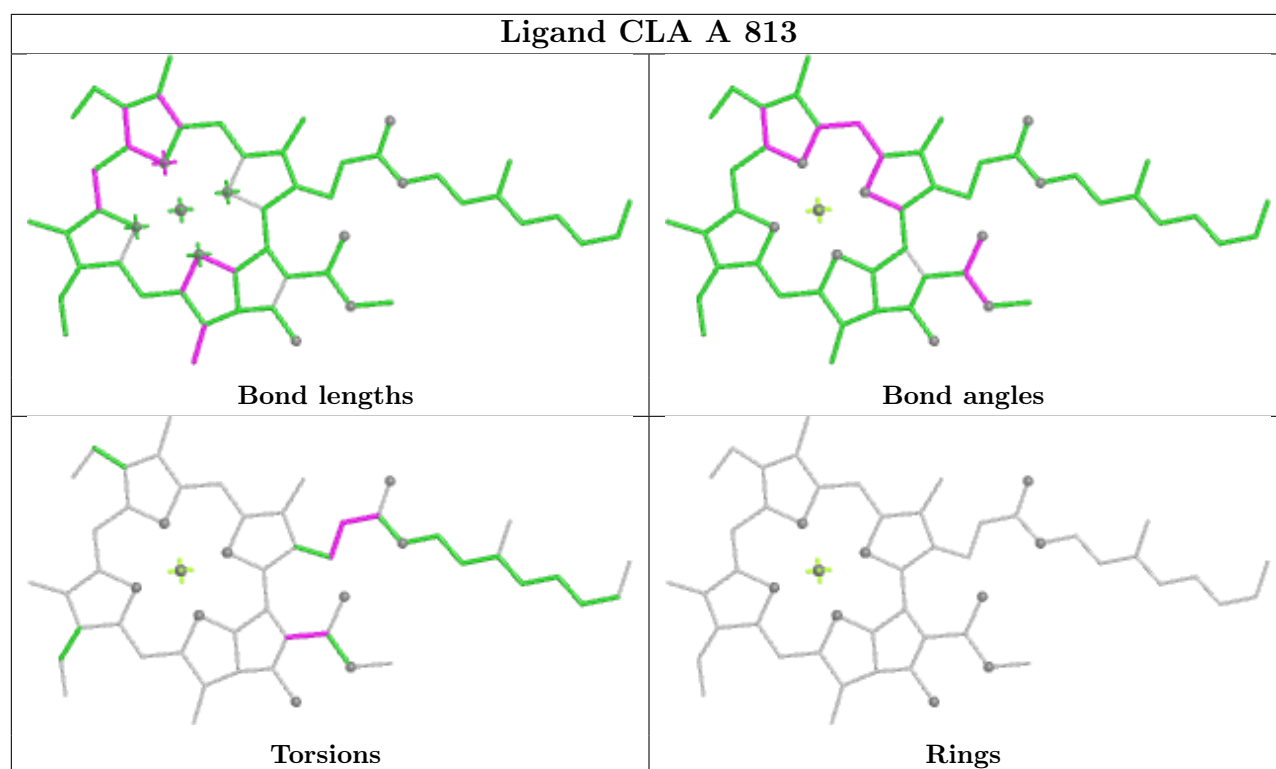
Rings

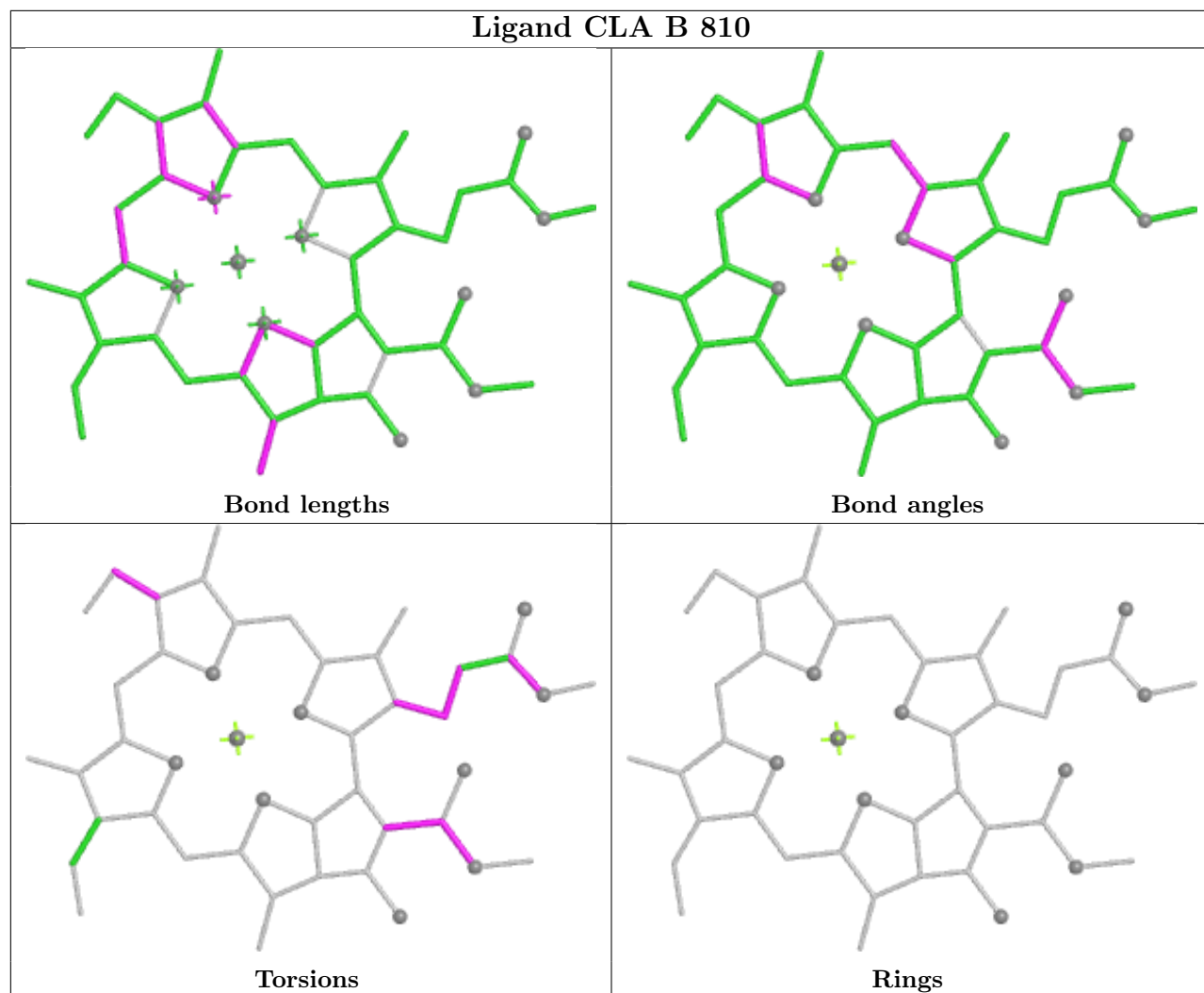
Ligand CLA A 828



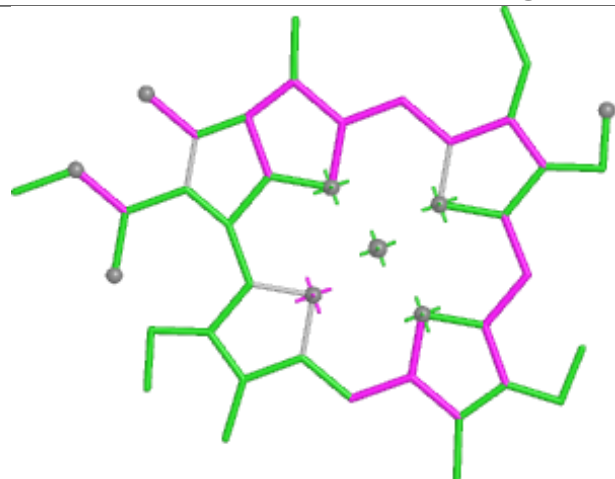
Ligand CLA A 806



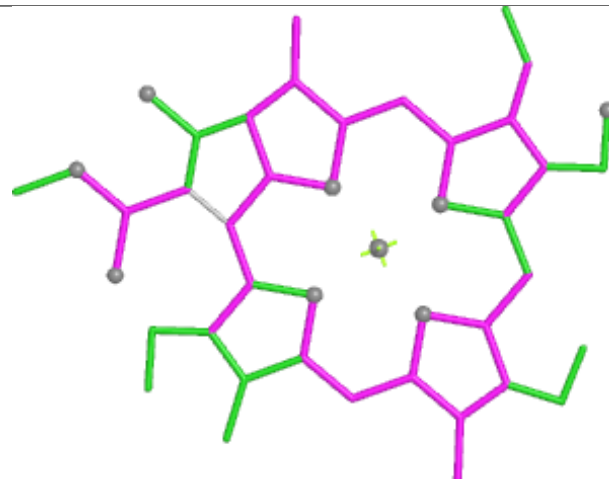




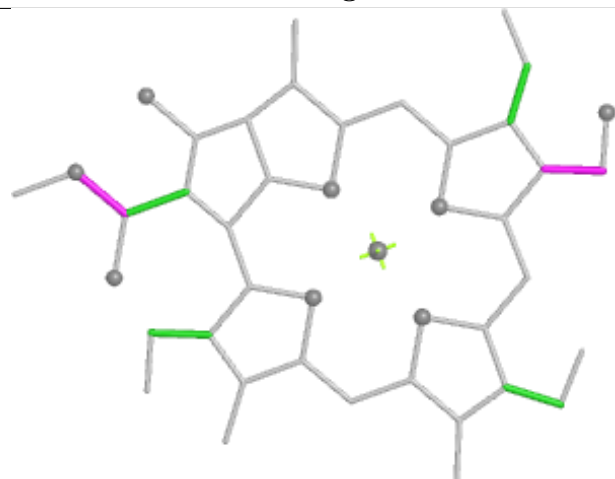
Ligand CHL 5 615



Bond lengths



Bond angles

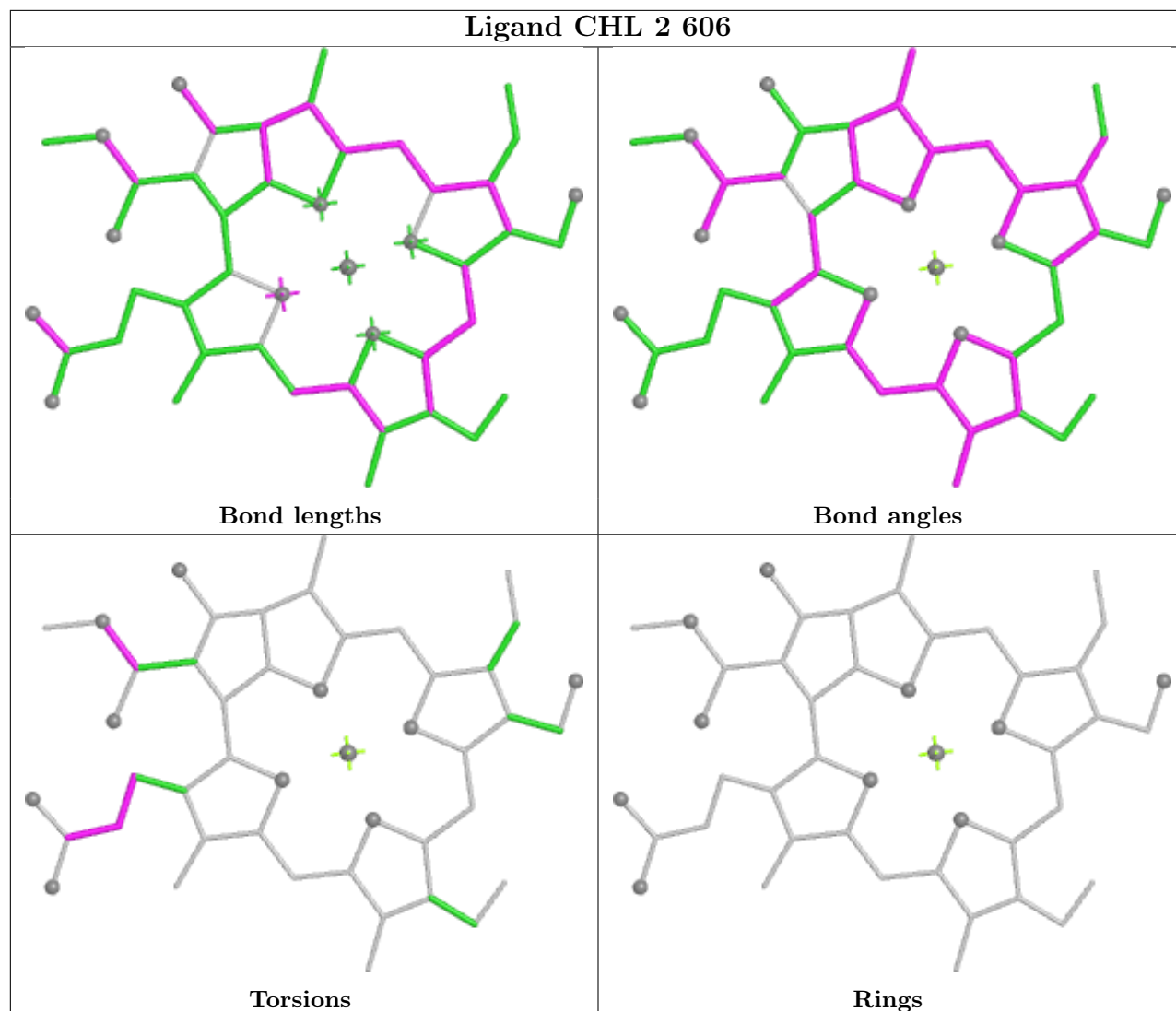


Torsions

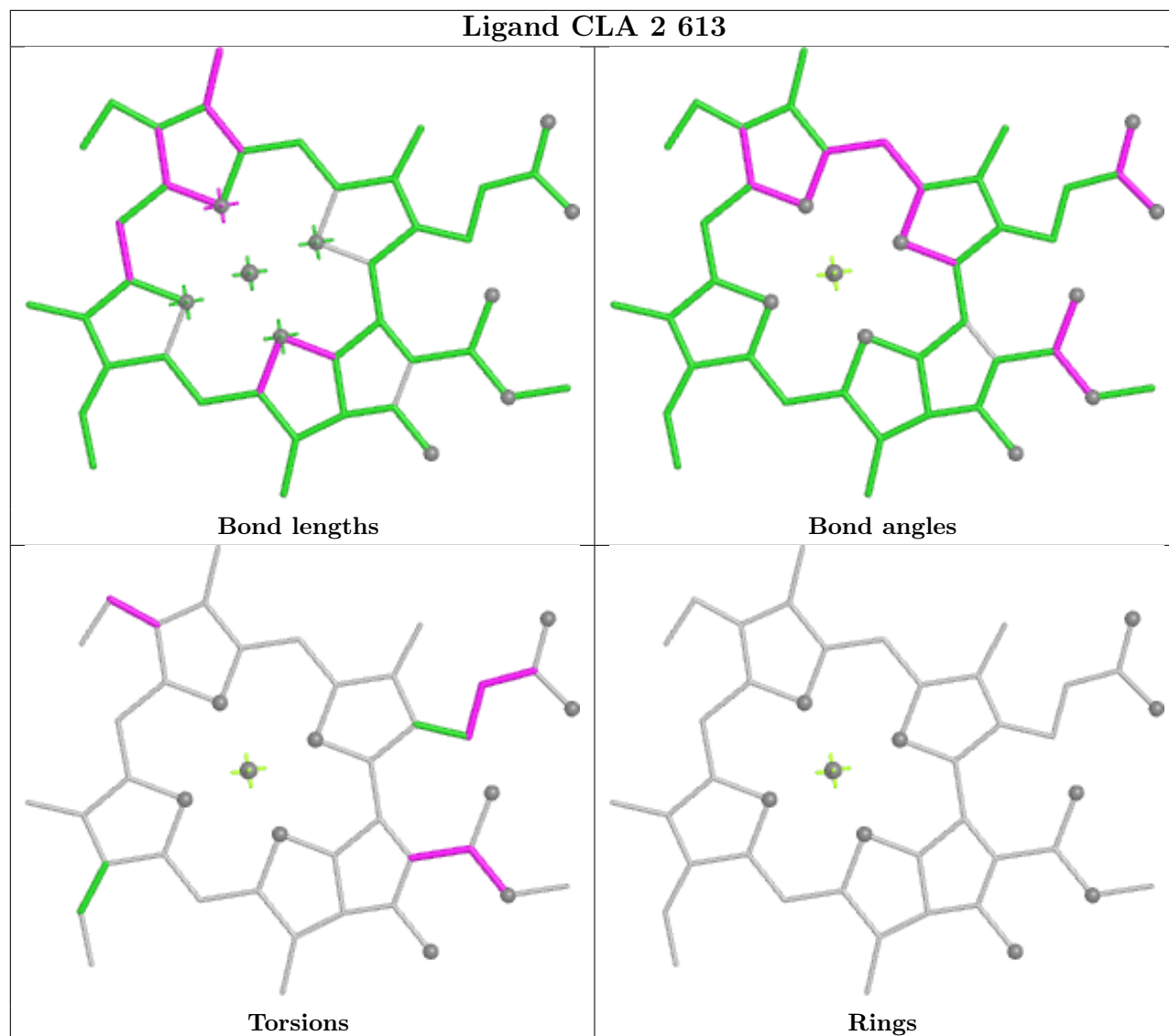


Rings

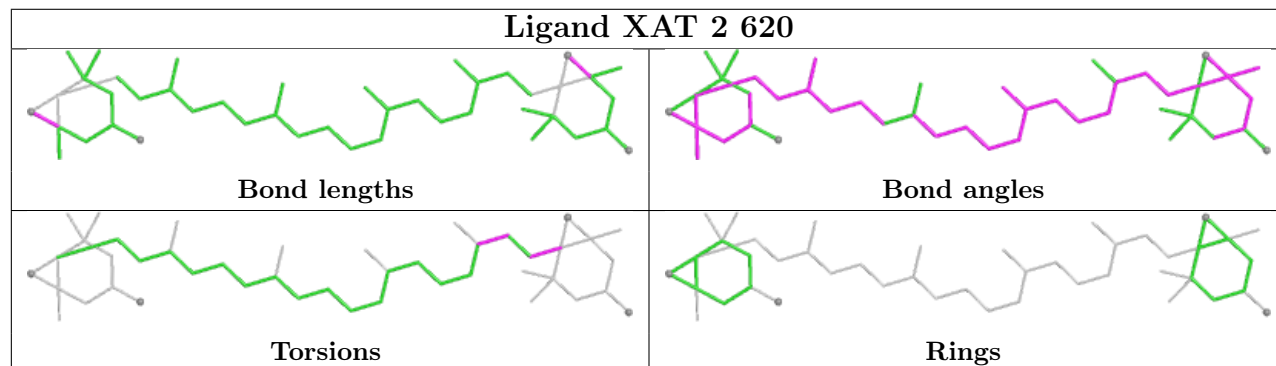
Ligand CHL 2 606

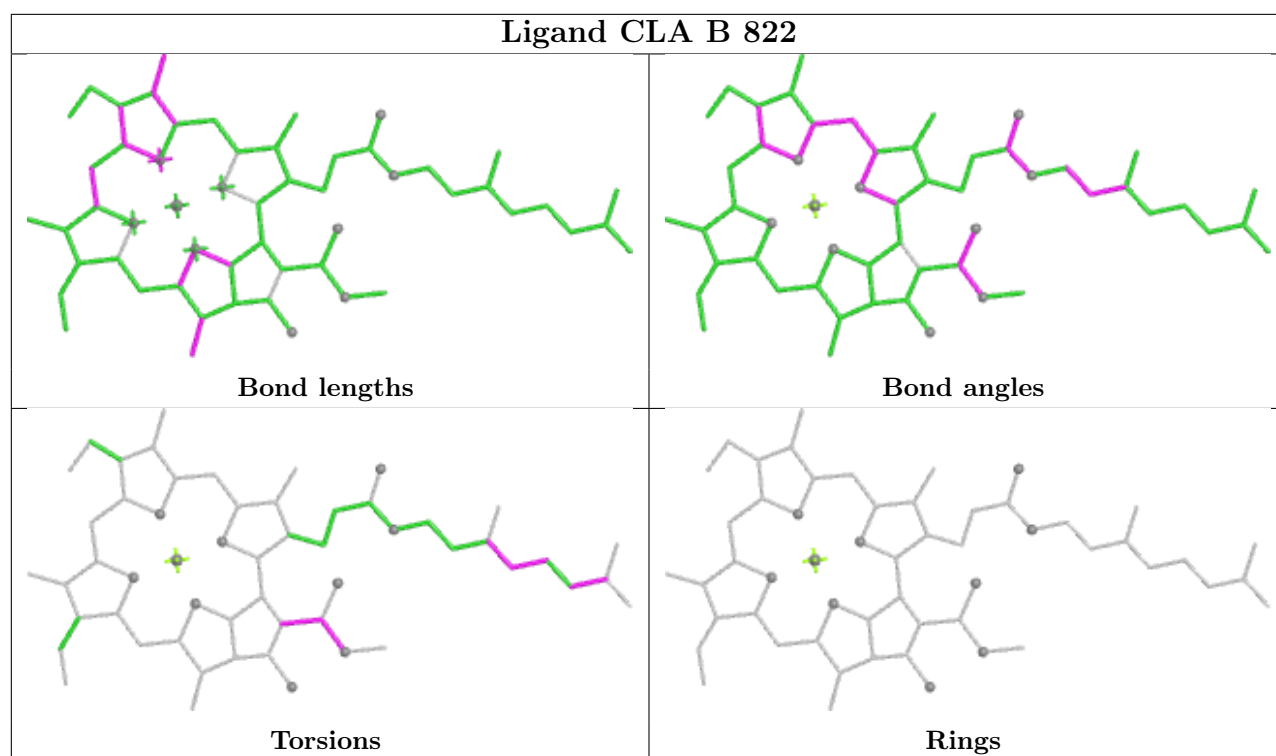


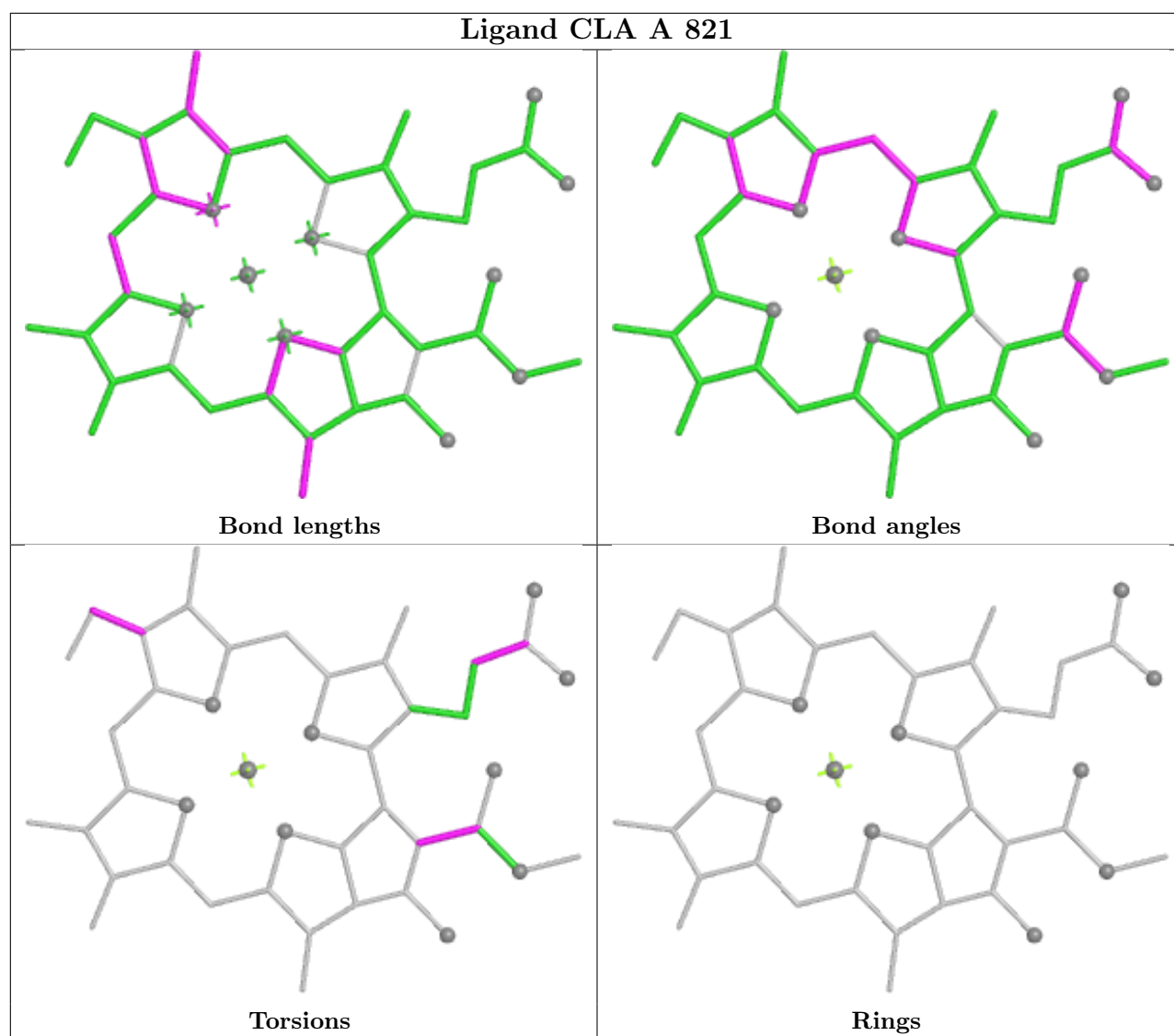
Ligand CLA 2 613

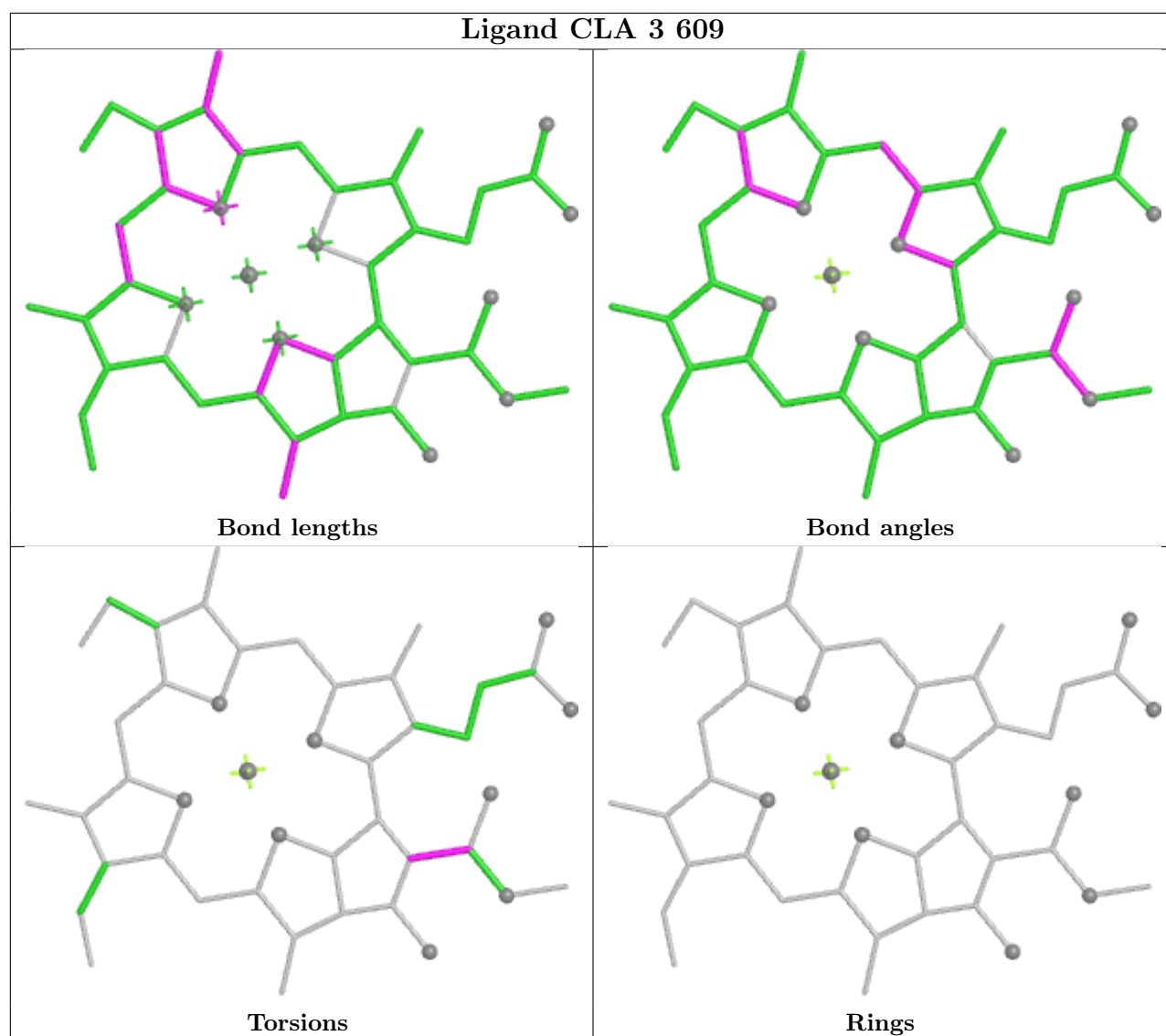


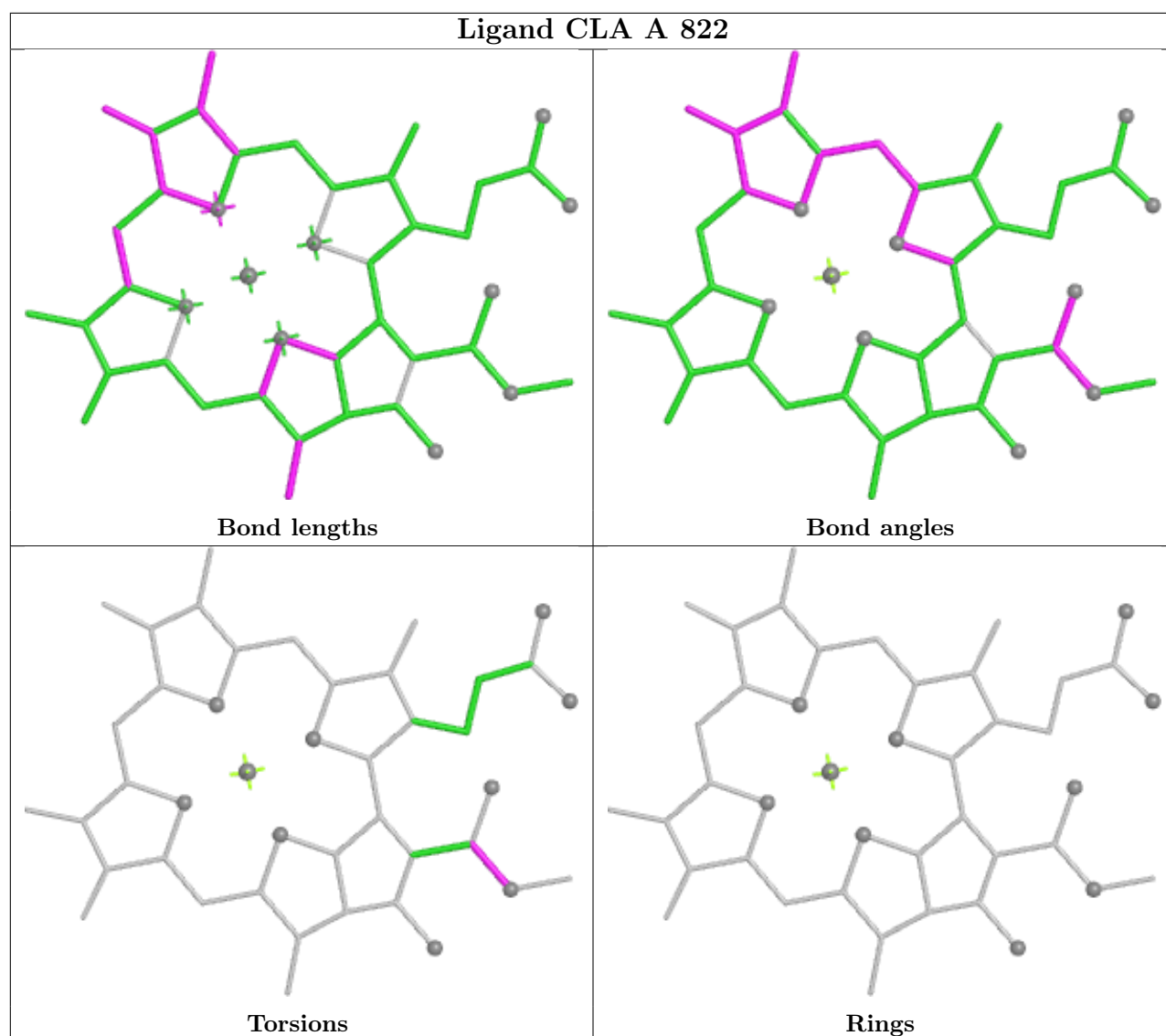
Ligand XAT 2 620

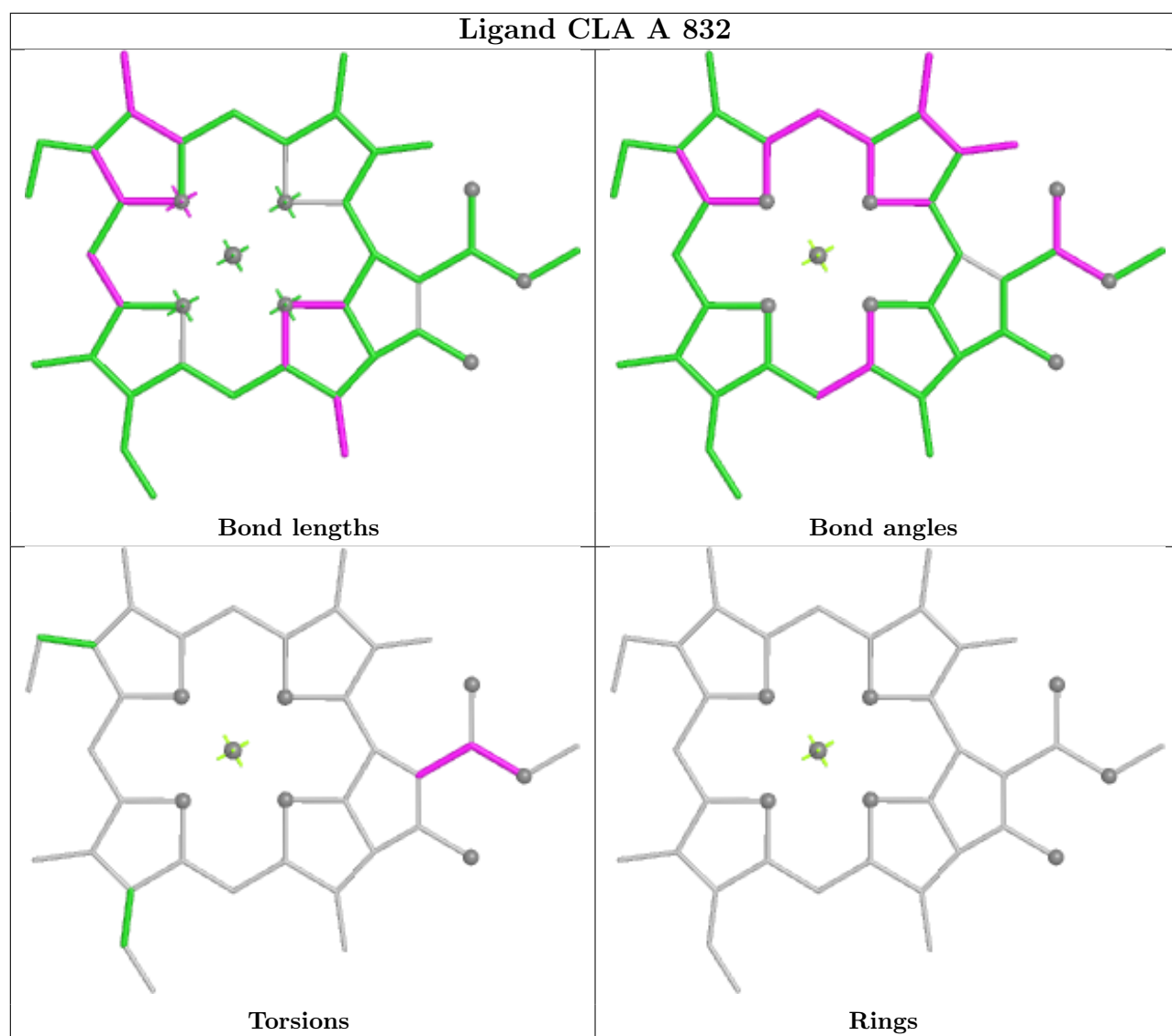


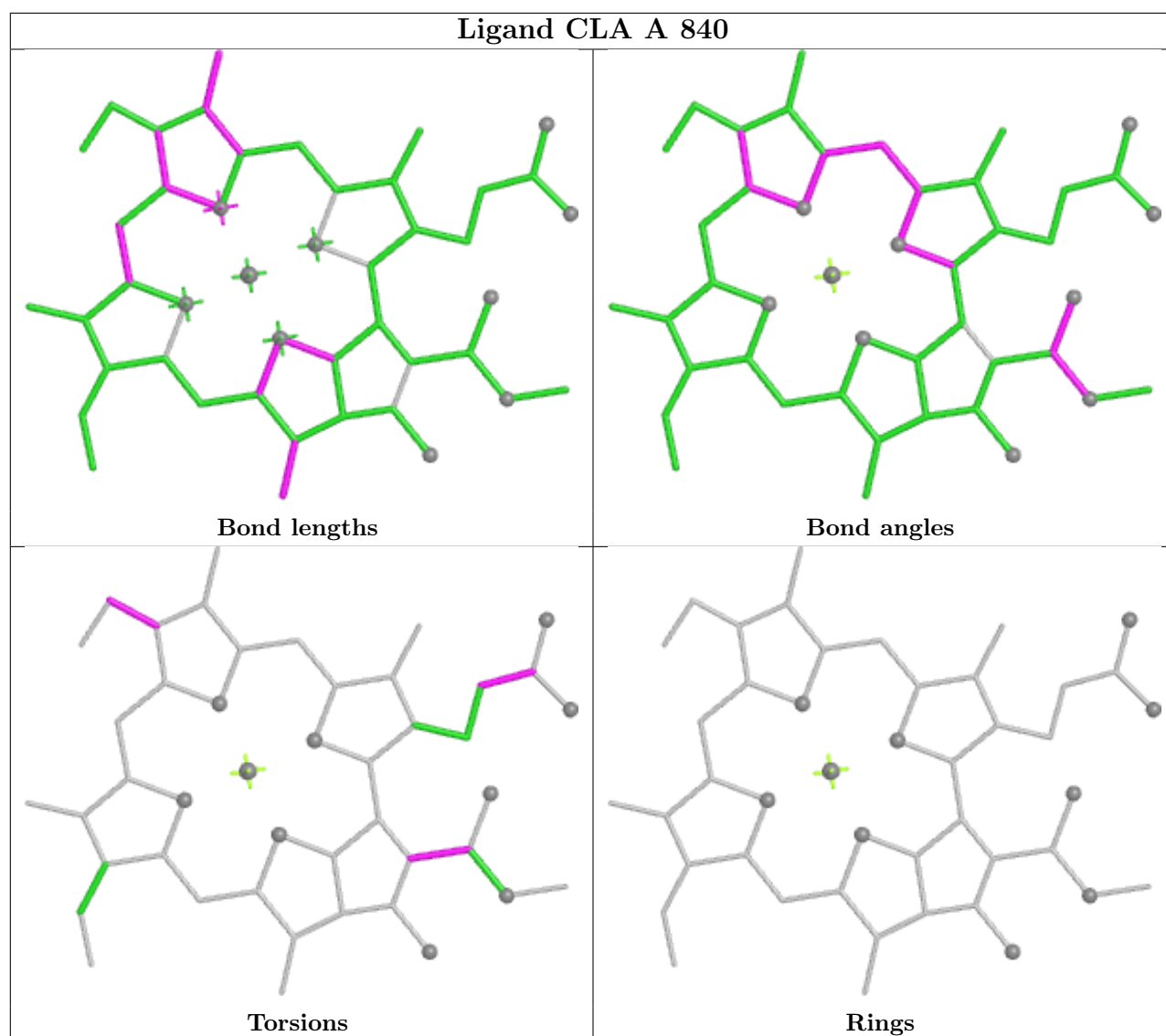




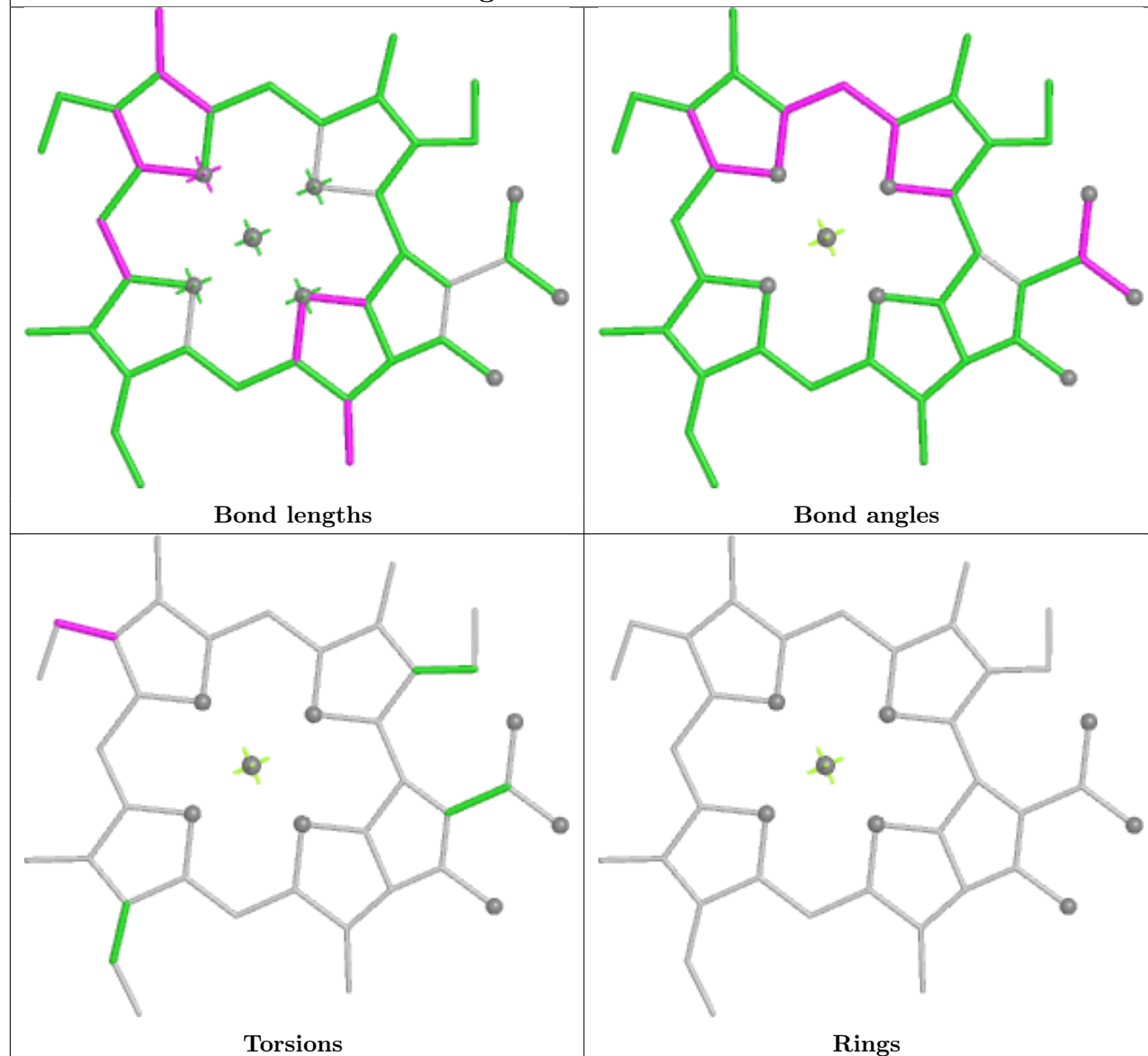




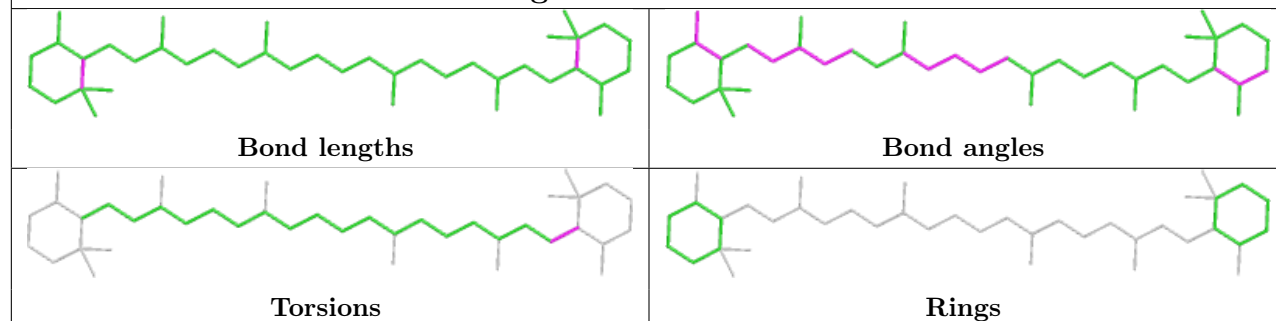


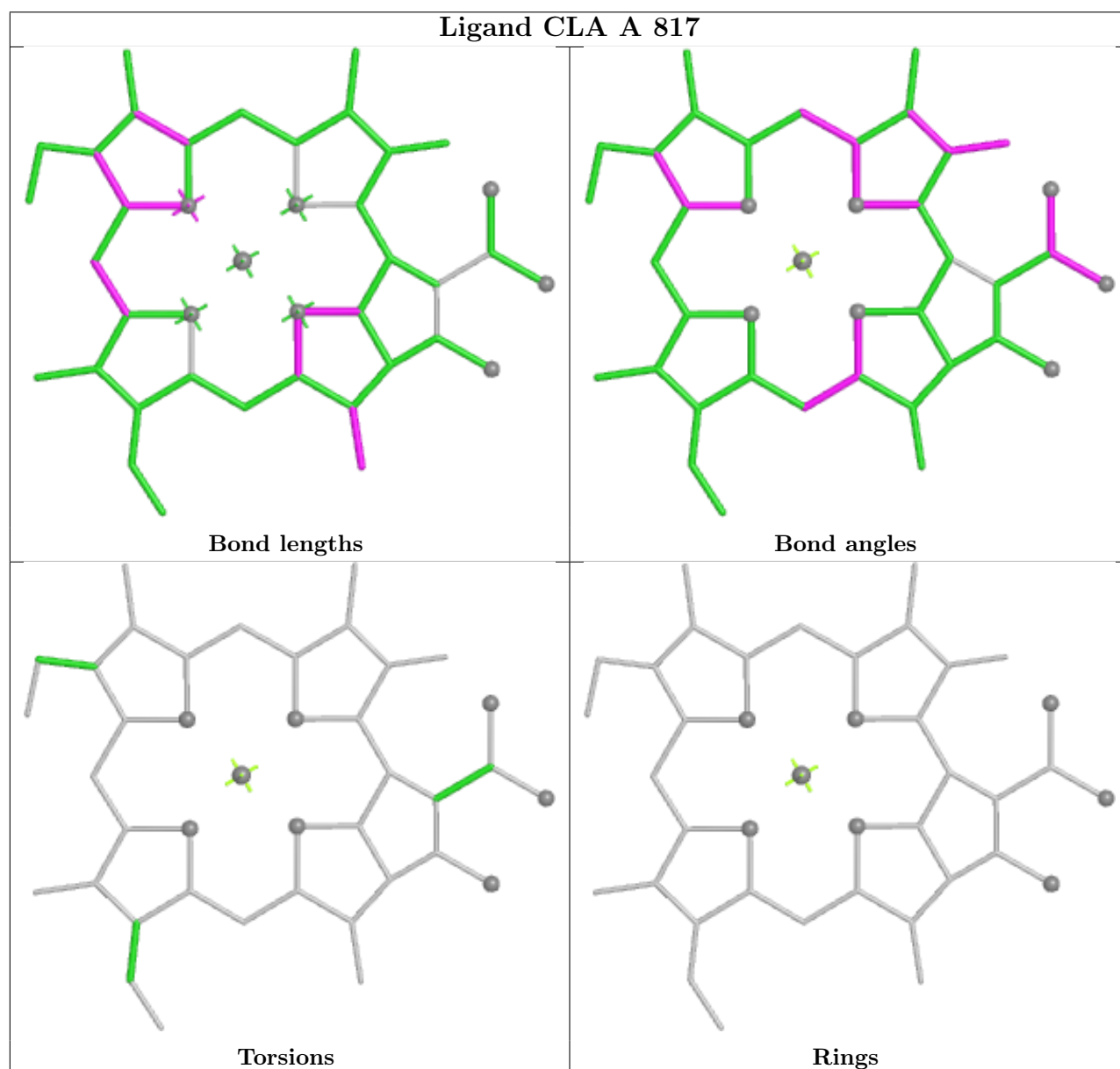
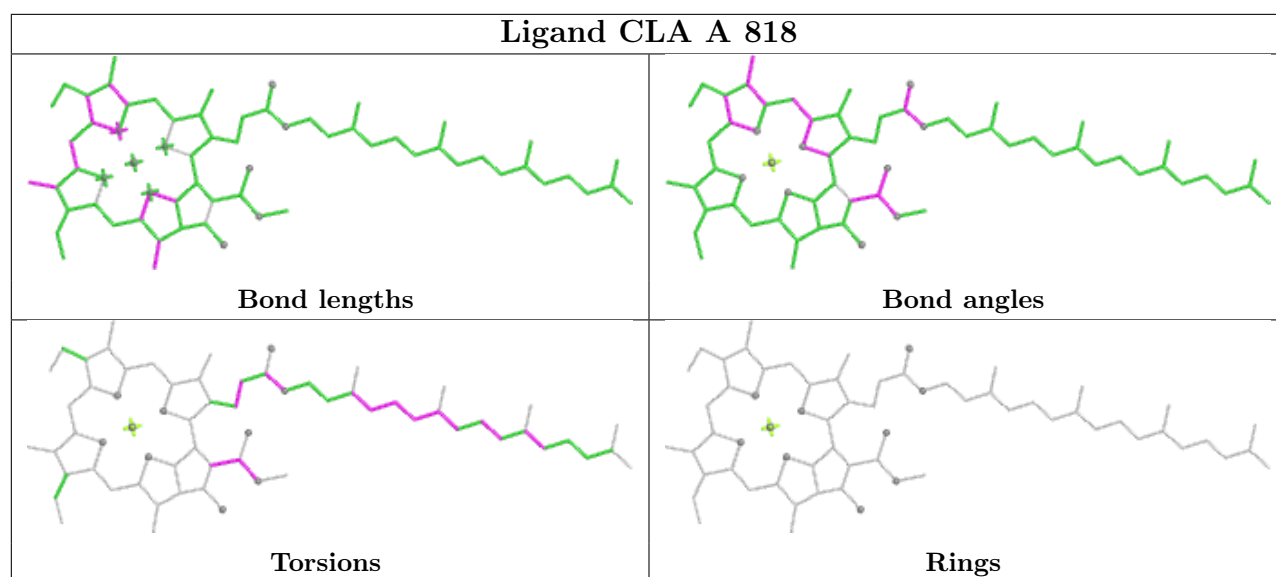


Ligand CLA B 839

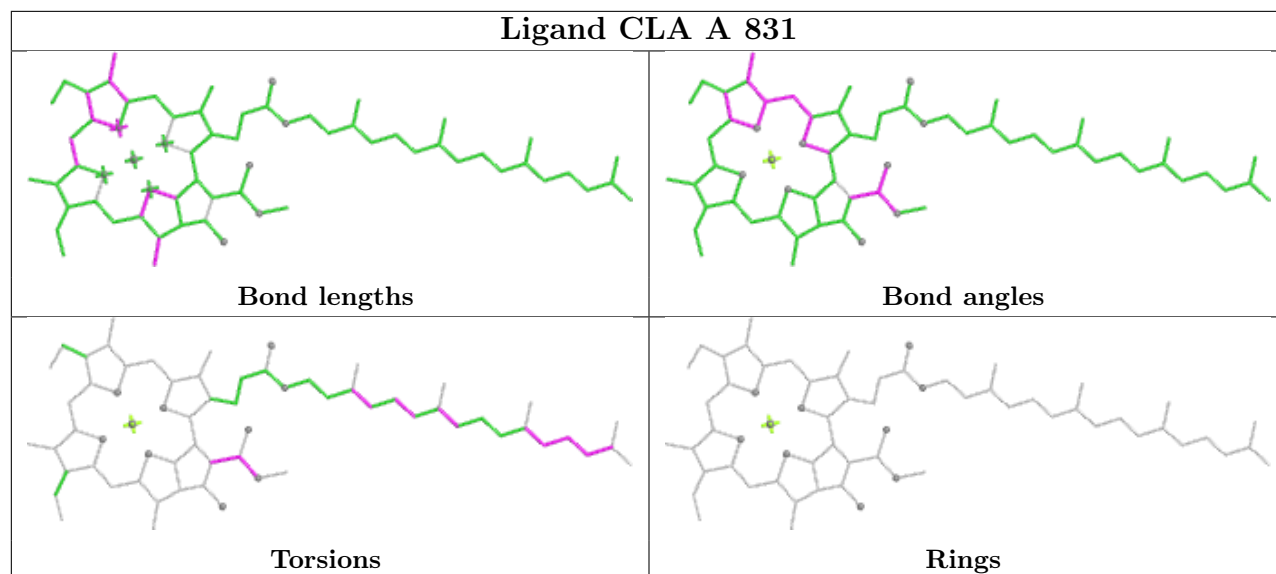


Ligand BCR B 847

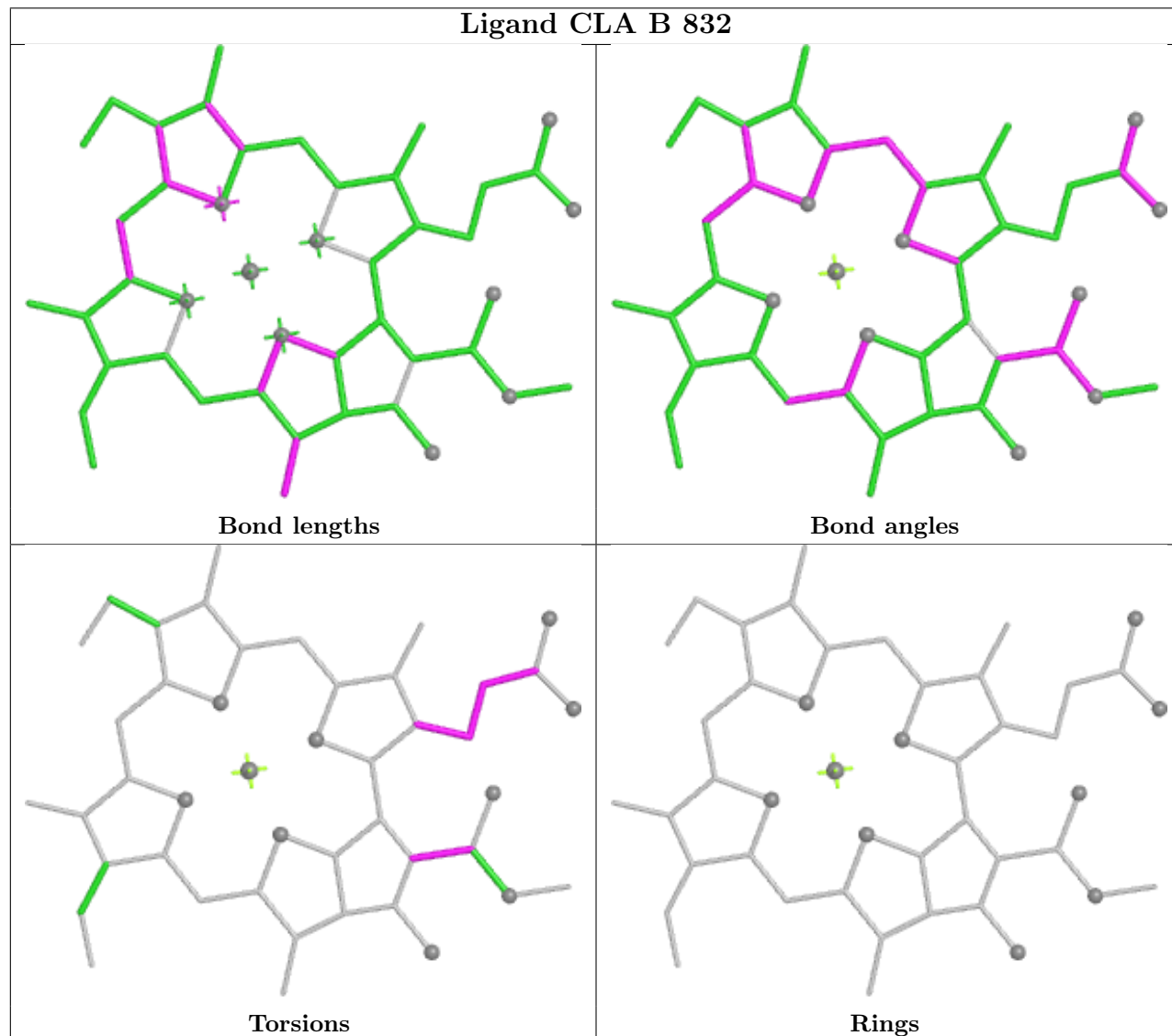




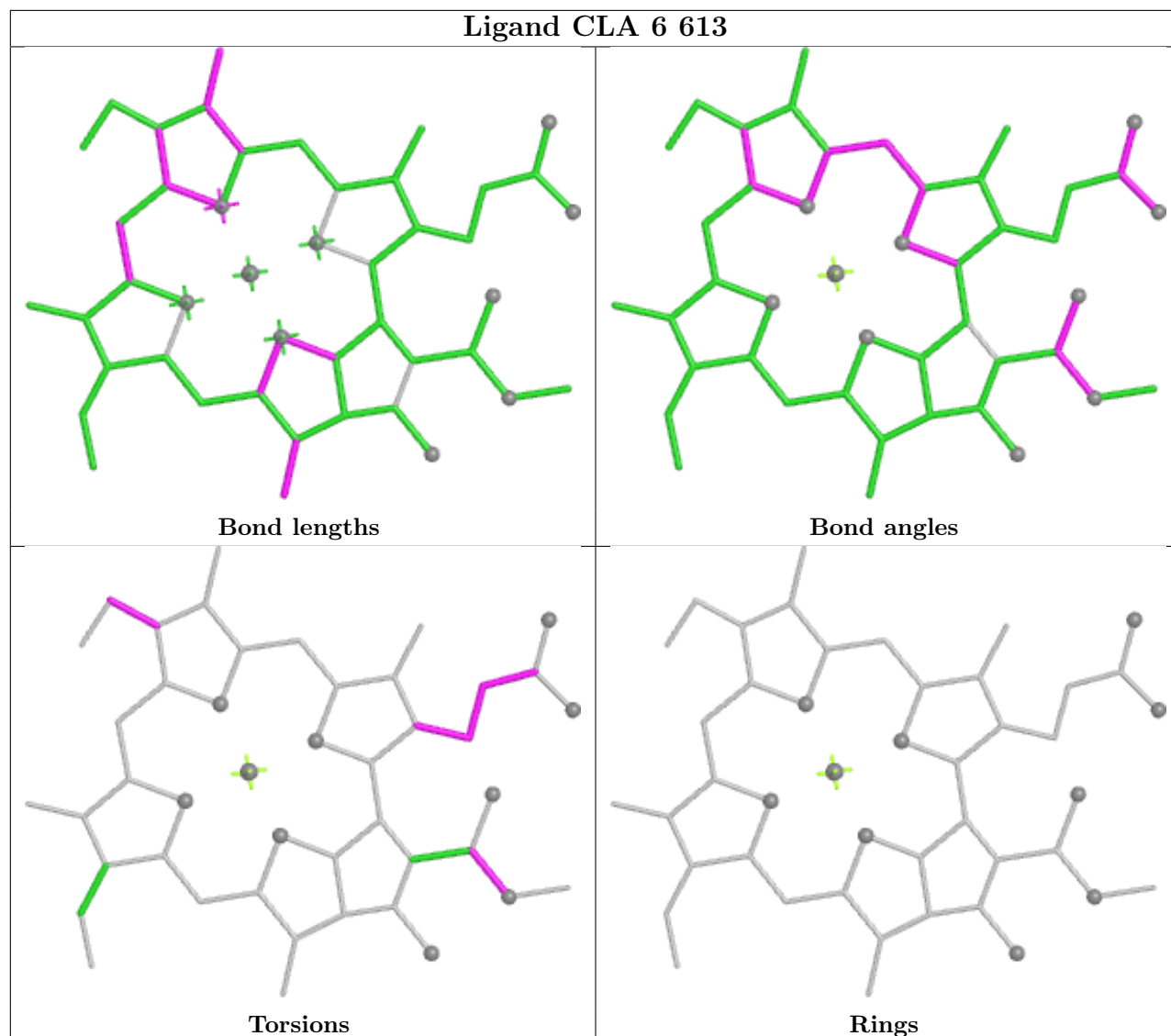
Ligand CLA A 831



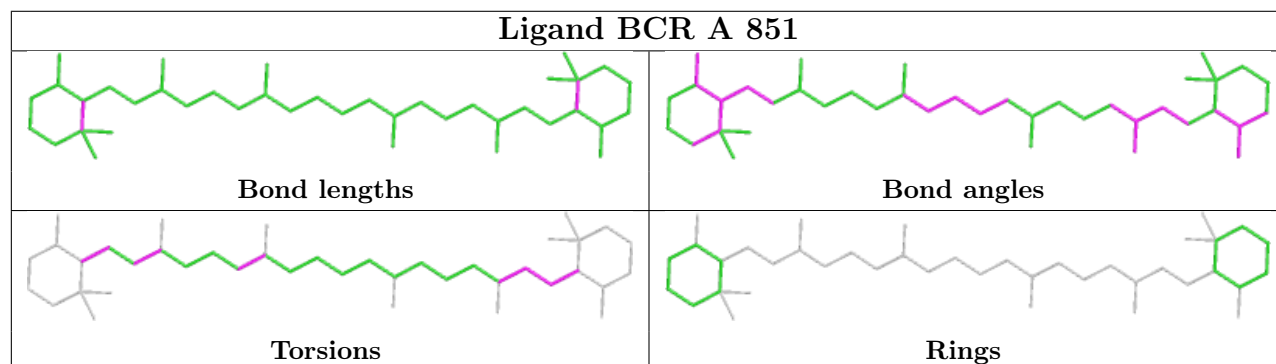
Ligand CLA B 832

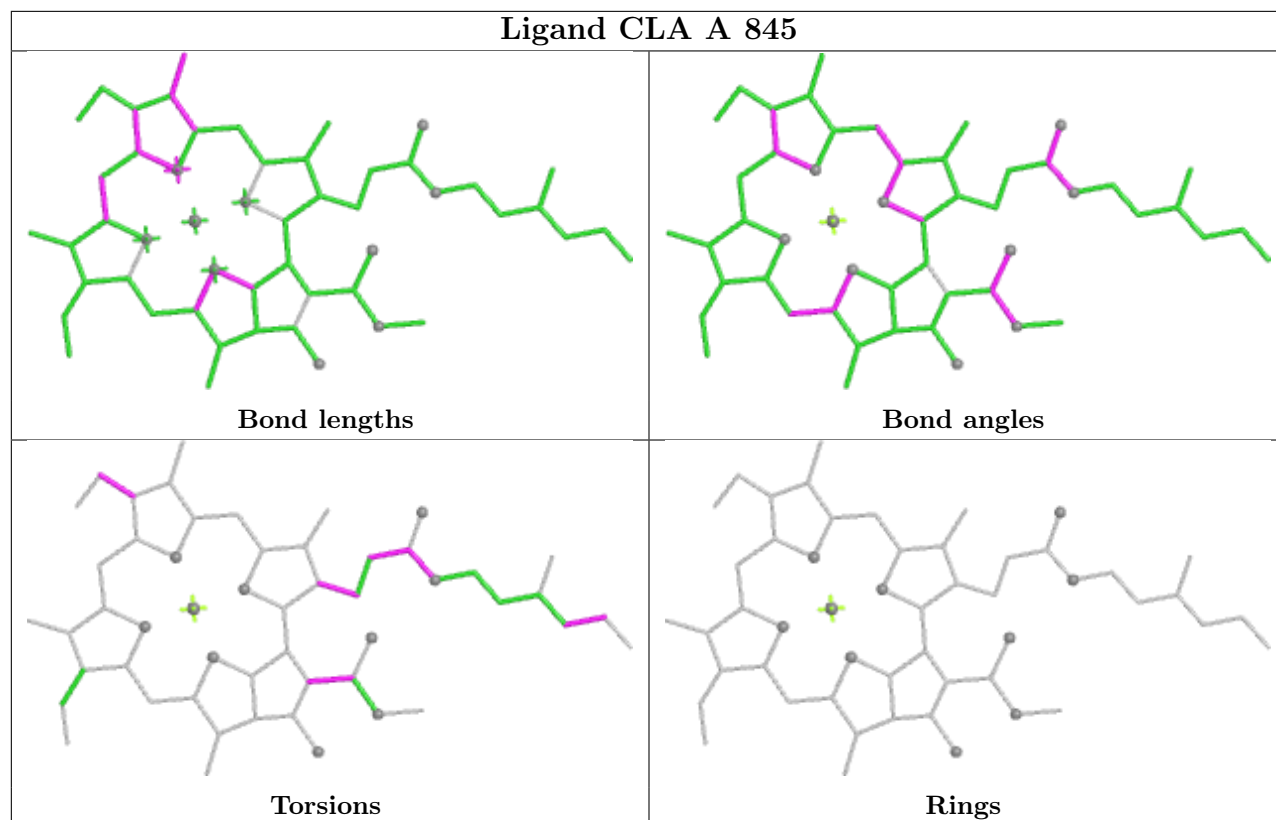


Ligand CLA 6 613

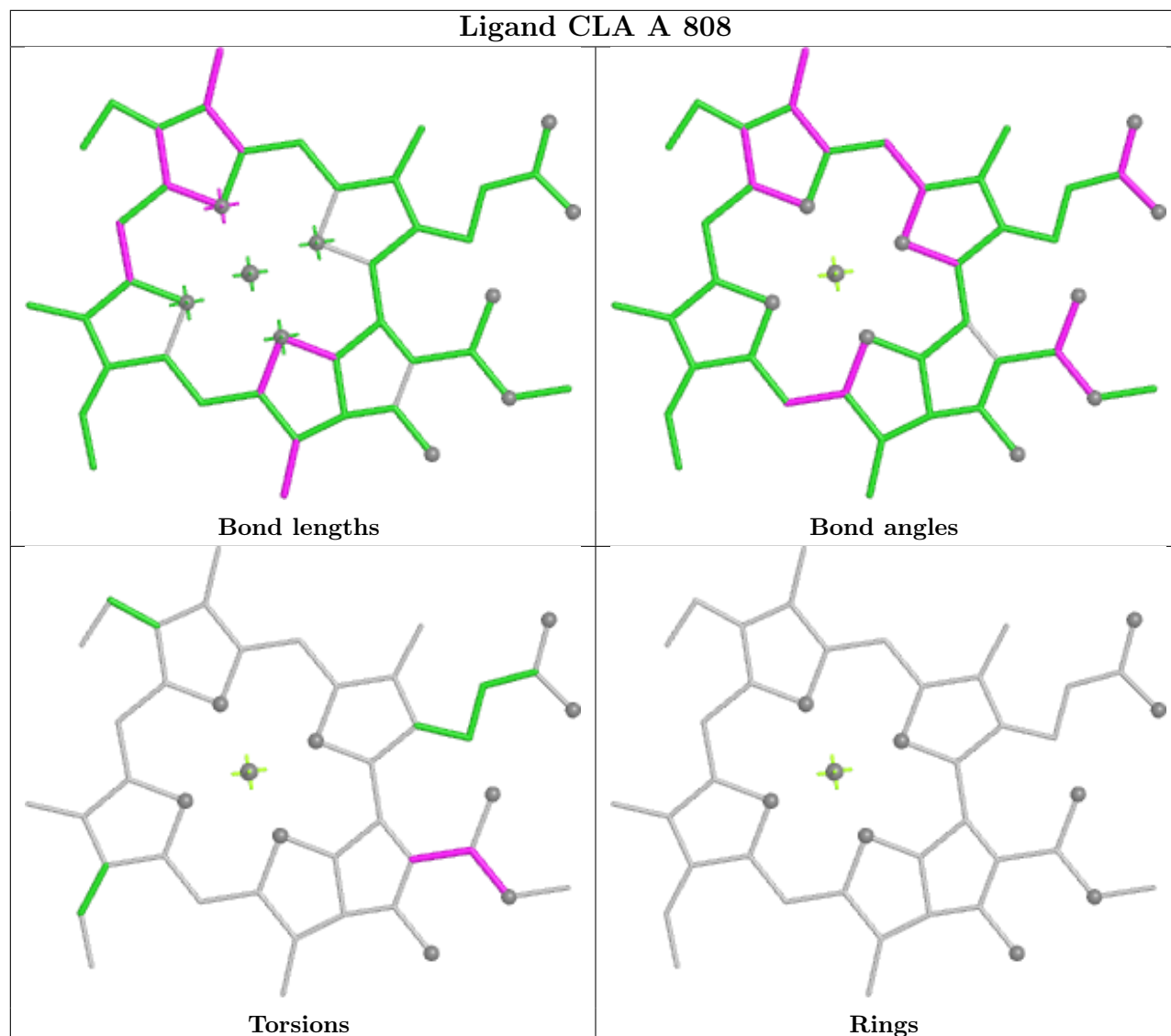


Ligand BCR A 851

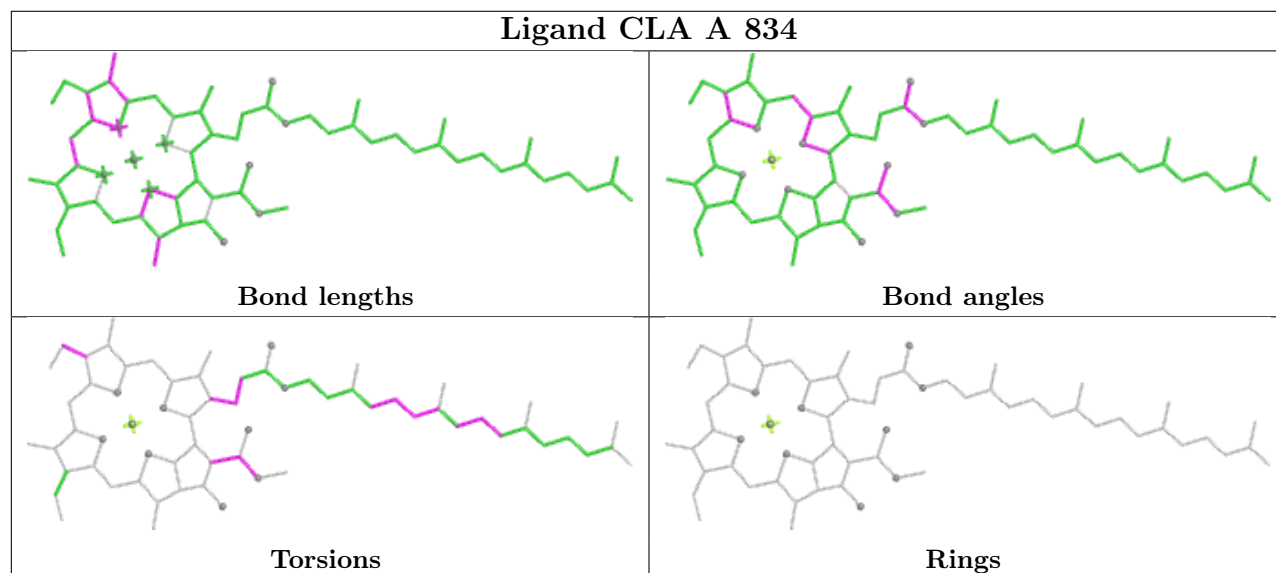


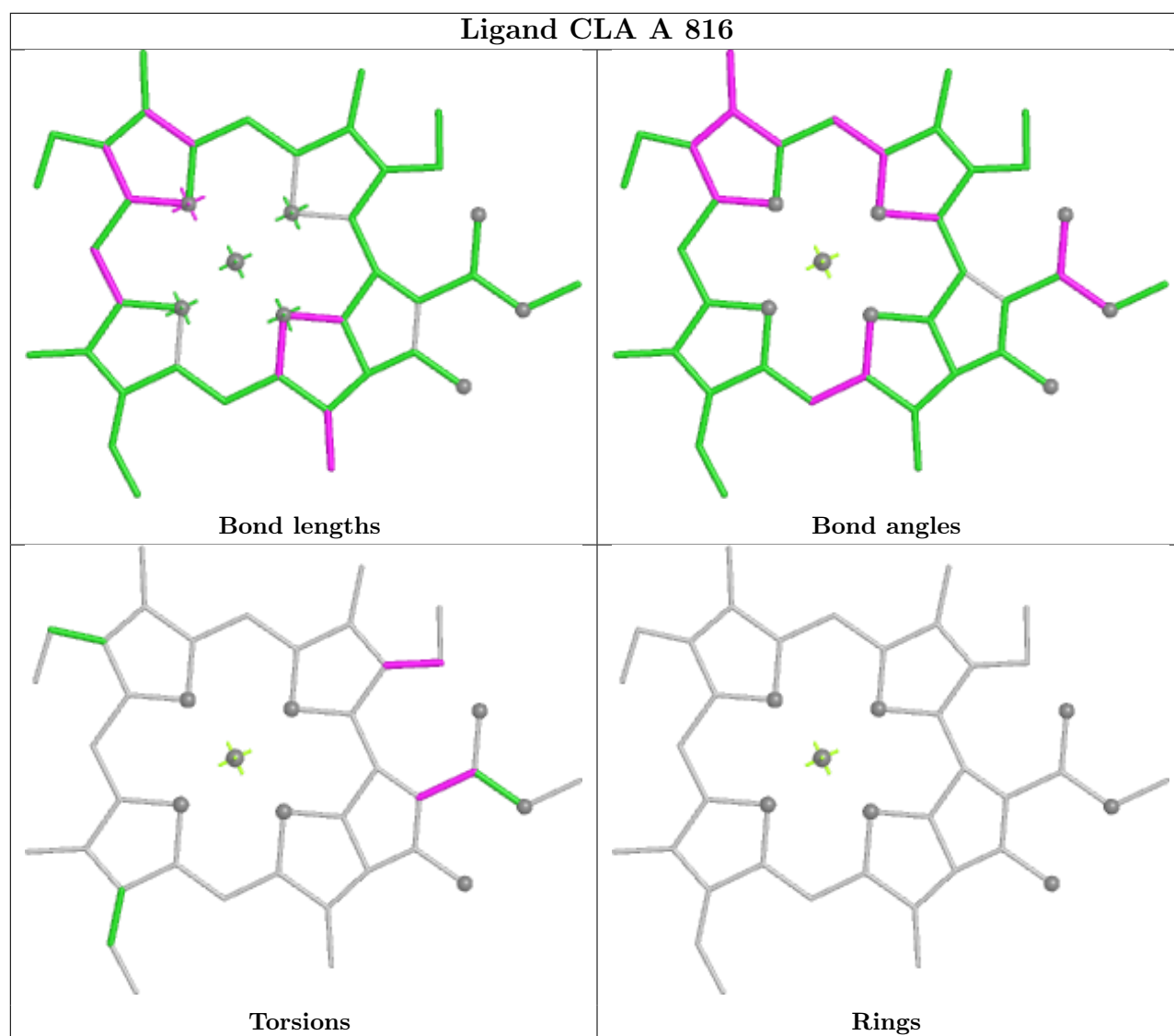


Ligand CLA A 808



Ligand CLA A 834





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.

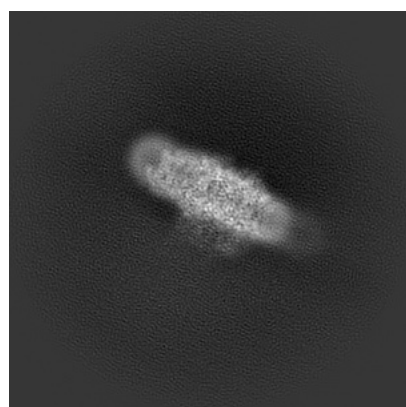
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0821. These allow visual inspection of the internal detail of the map and identification of artifacts.

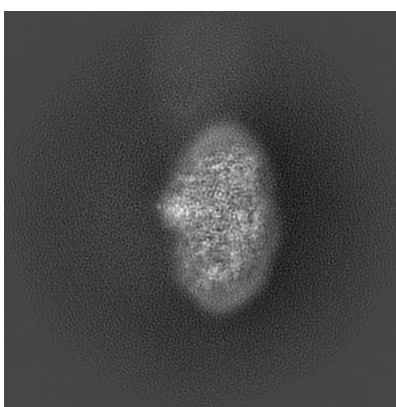
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

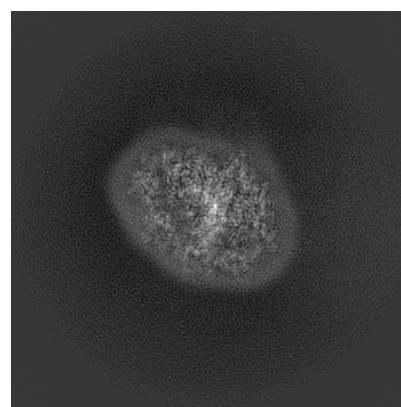
6.1.1 Primary map



X



Y

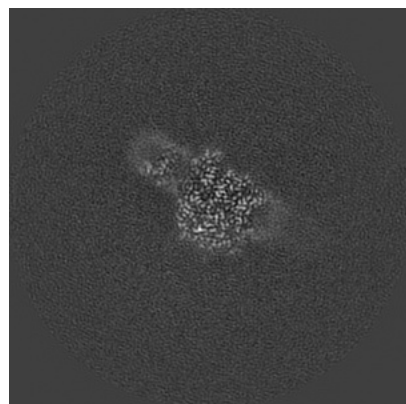


Z

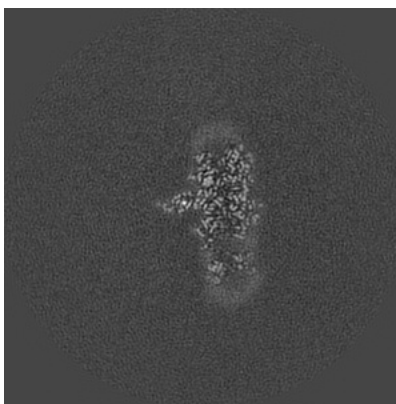
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

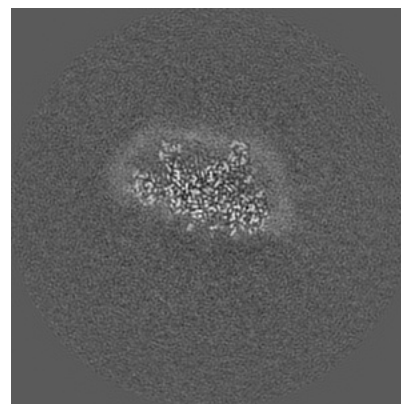
6.2.1 Primary map



X Index: 192



Y Index: 192

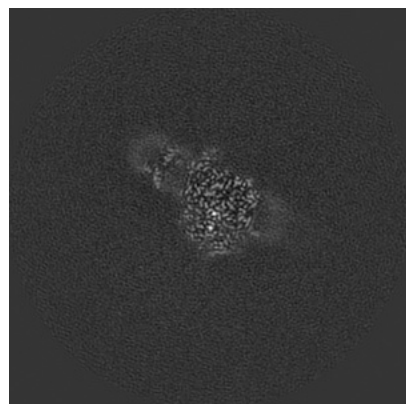


Z Index: 192

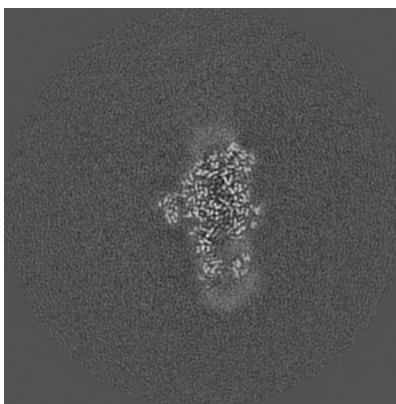
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

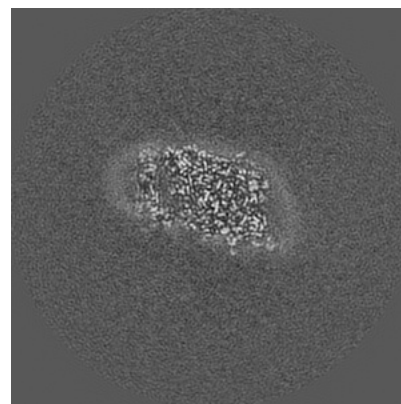
6.3.1 Primary map



X Index: 196



Y Index: 200

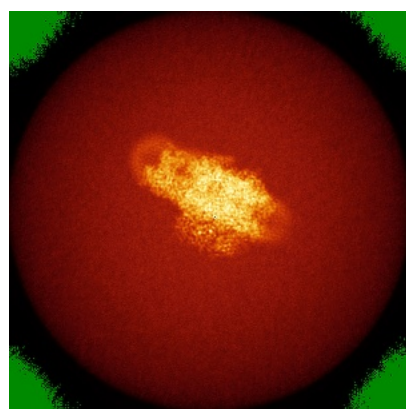


Z Index: 204

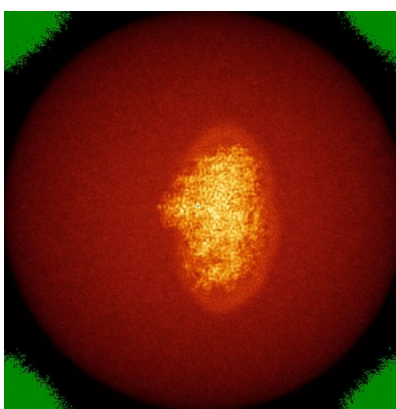
The images above show the largest variance slices of the map in three orthogonal directions.

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

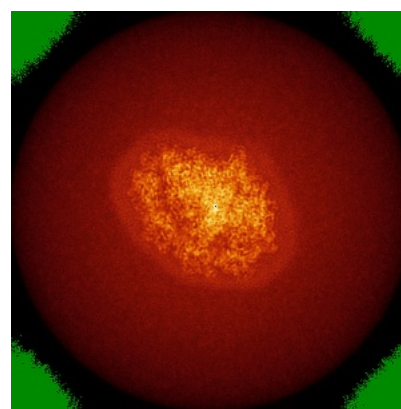
6.4.1 Primary map



X



Y

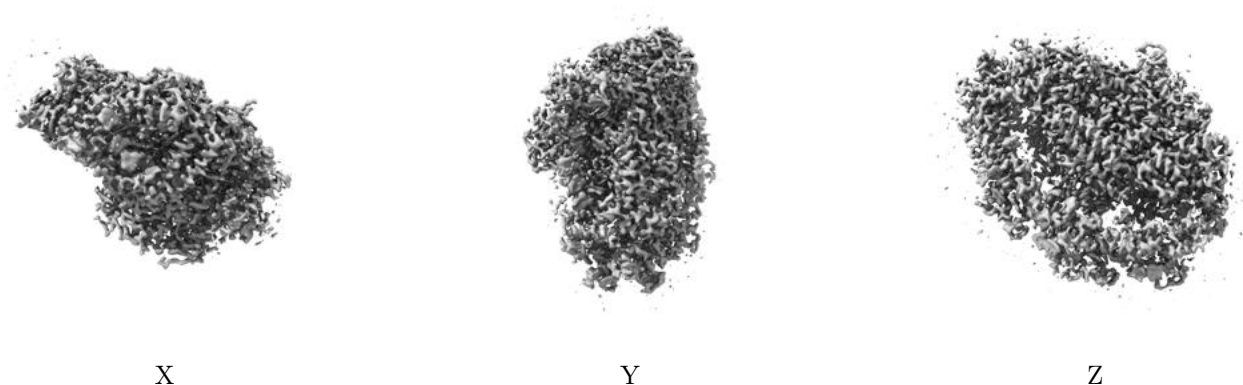


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

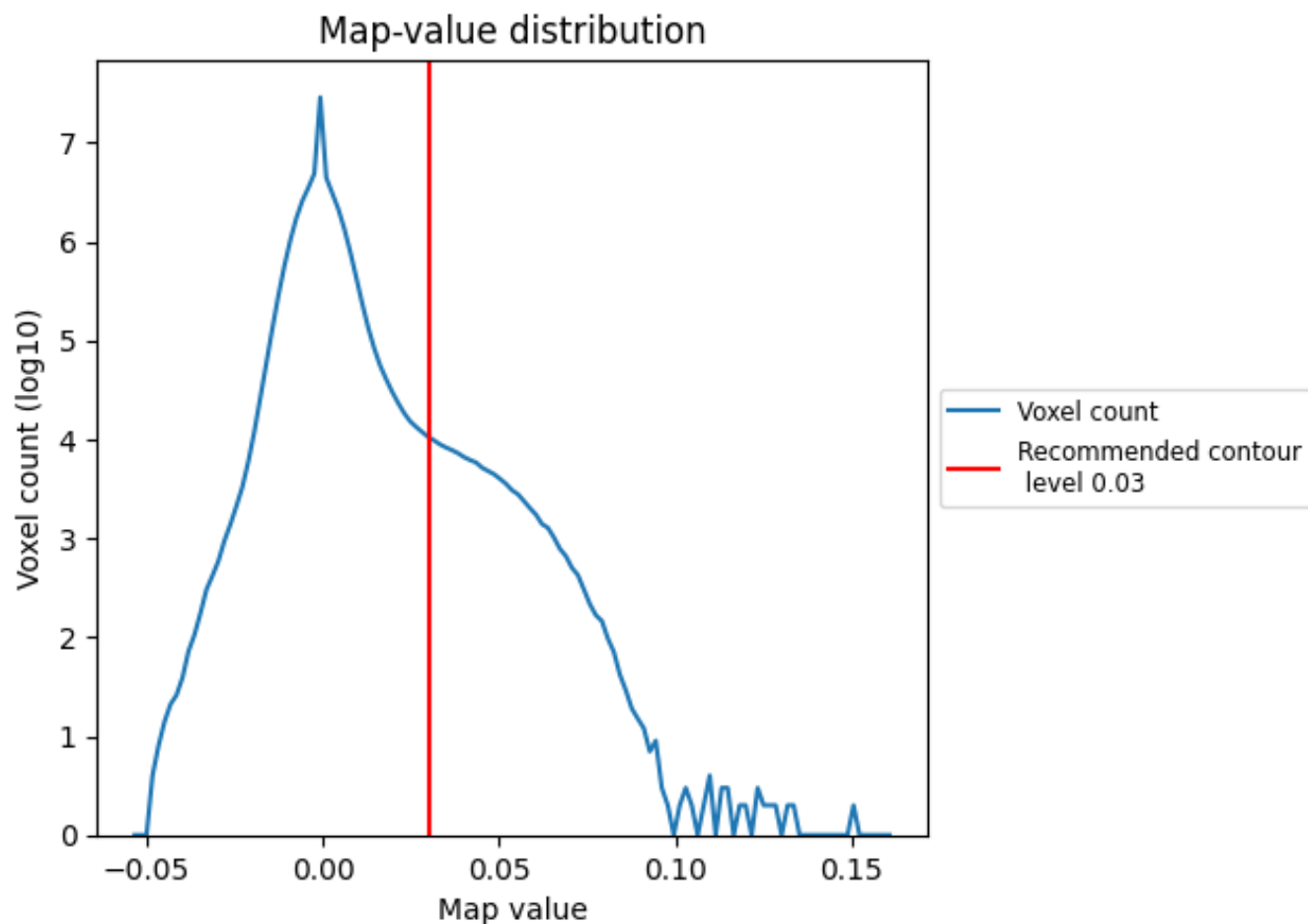
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

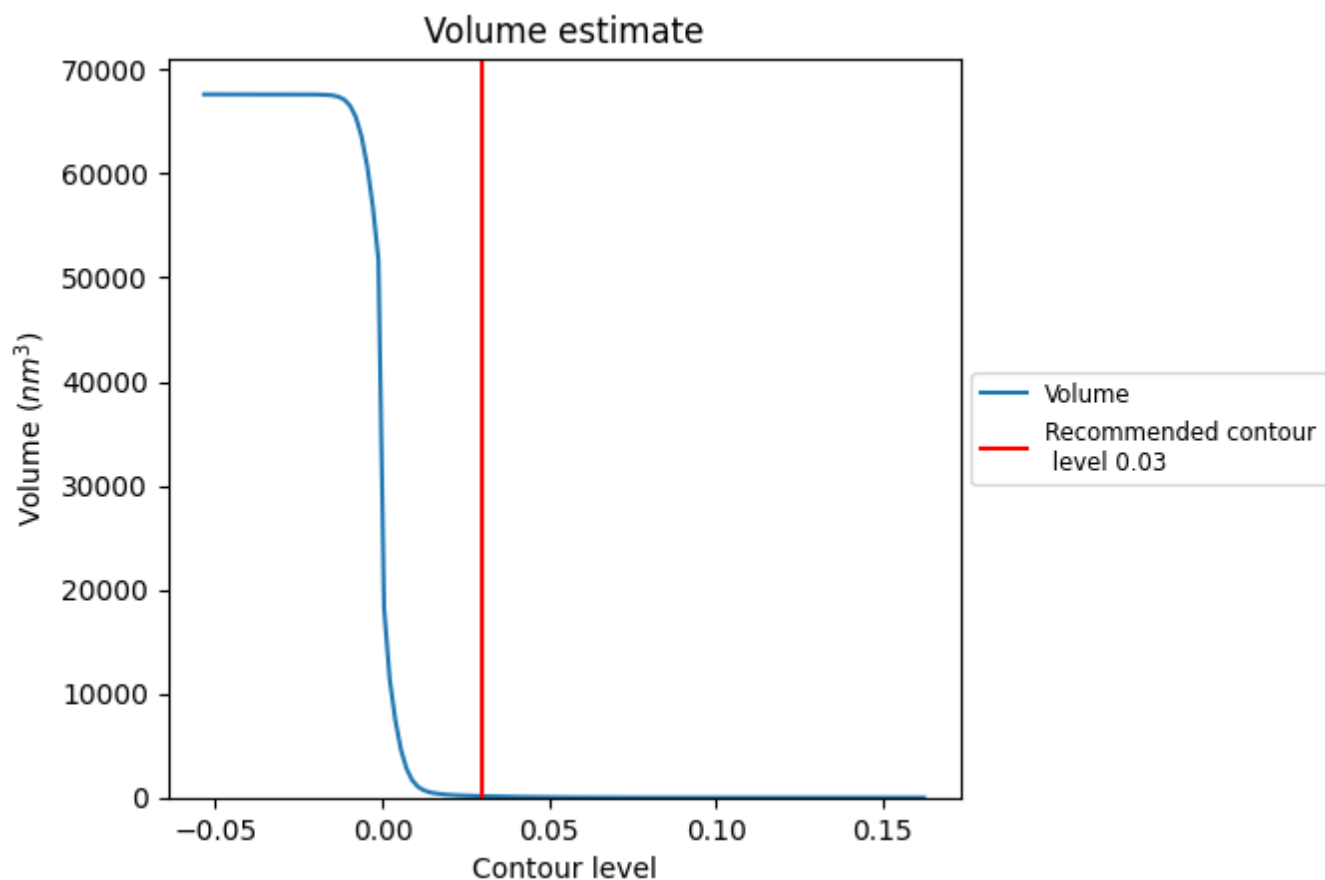
This section contains the results of statistical analysis of the map.

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.

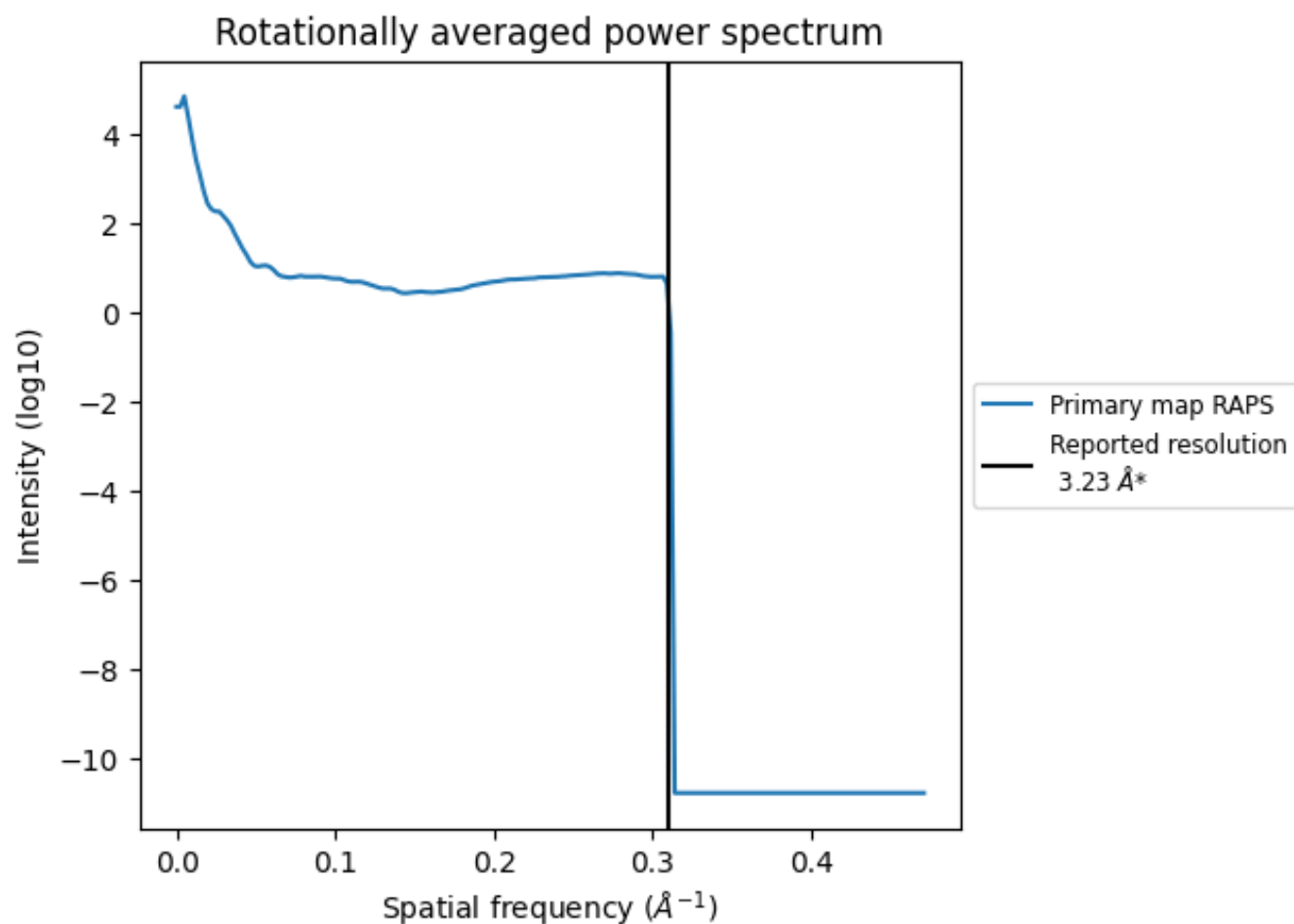
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

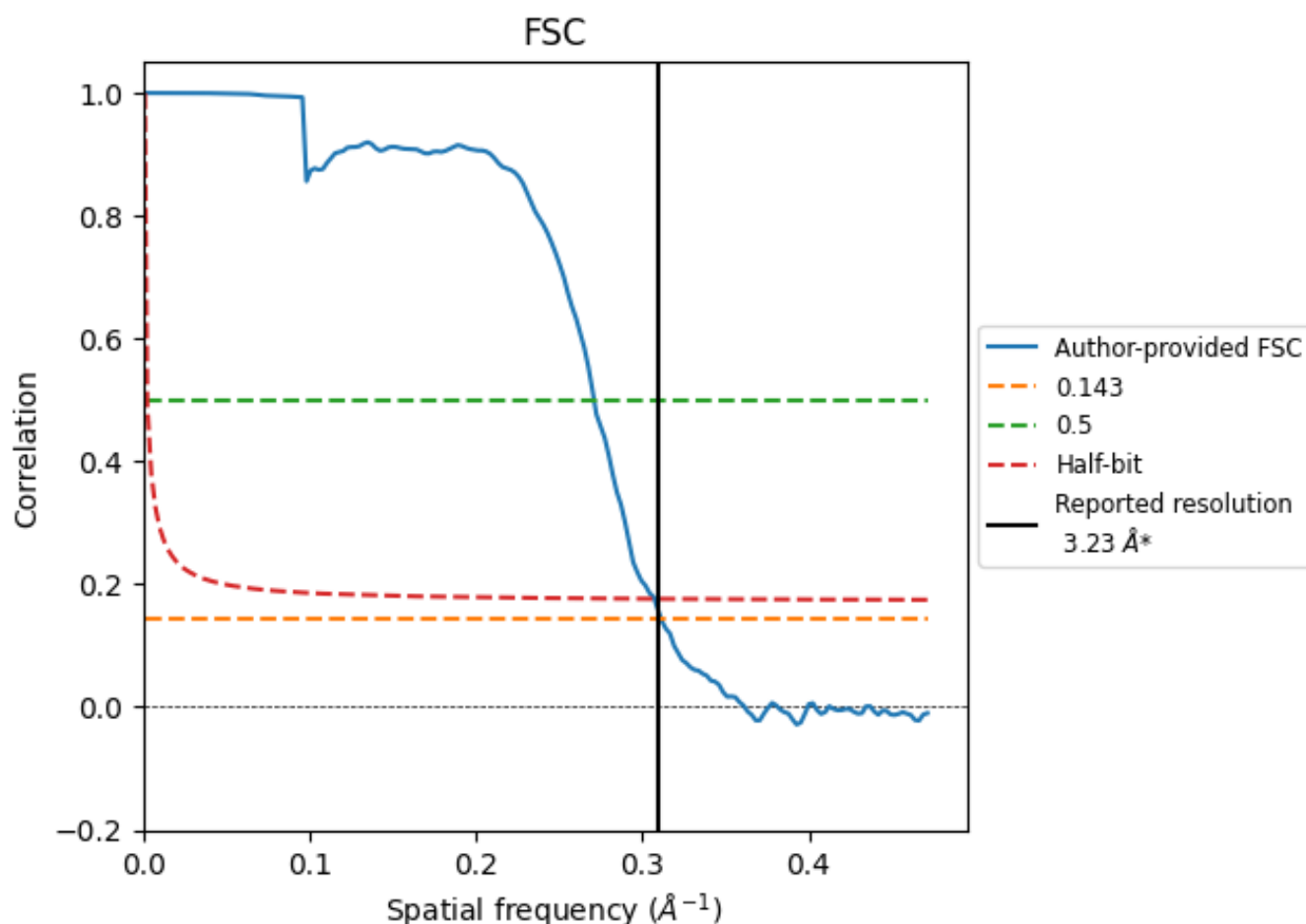


*Reported resolution corresponds to spatial frequency of 0.310 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.310 Å⁻¹

8.2 Resolution estimates [i](#)

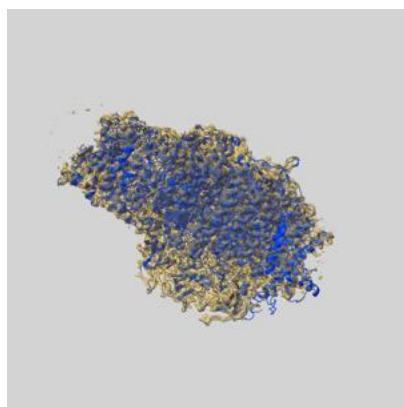
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.21	3.69	3.26
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

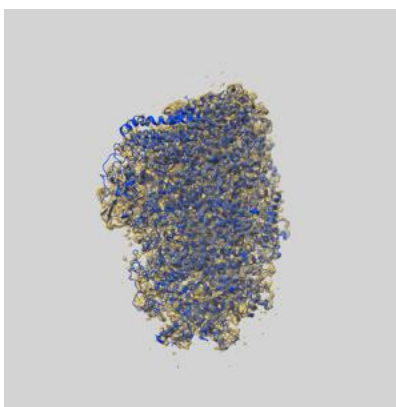
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0821 and PDB model 6L35. Per-residue inclusion information can be found in section 3 on page 22.

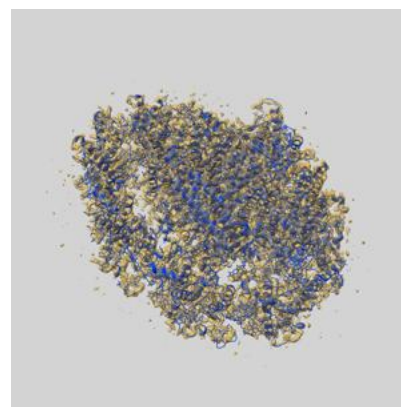
9.1 Map-model overlay [i](#)



X



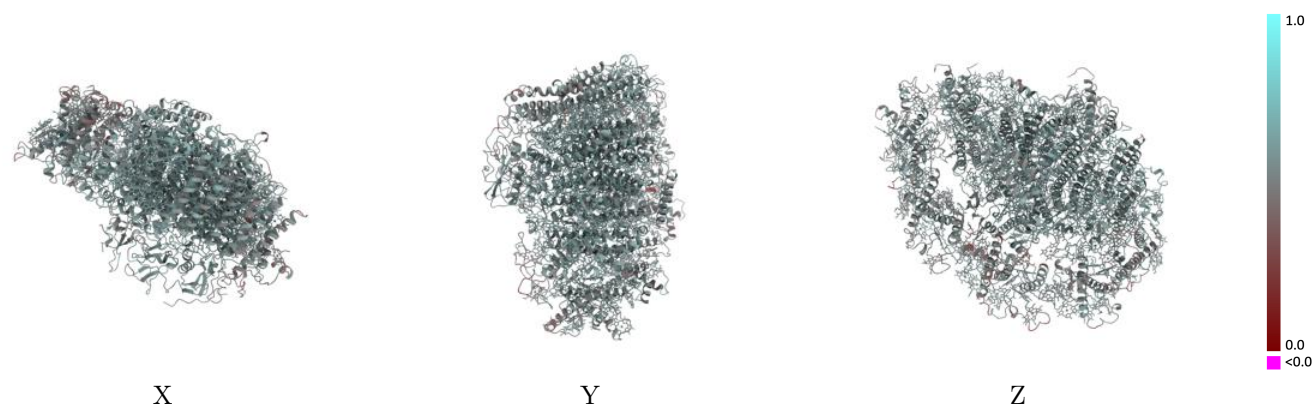
Y



Z

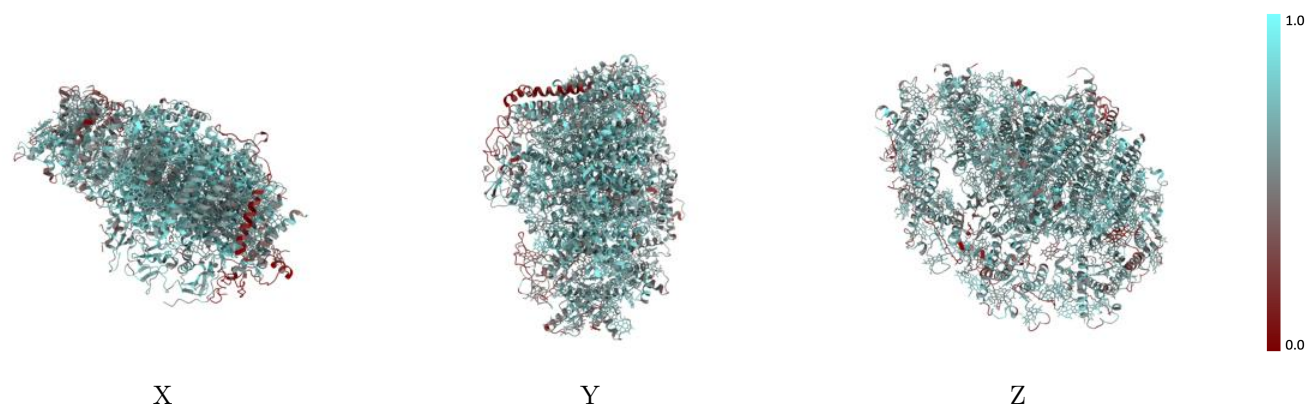
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



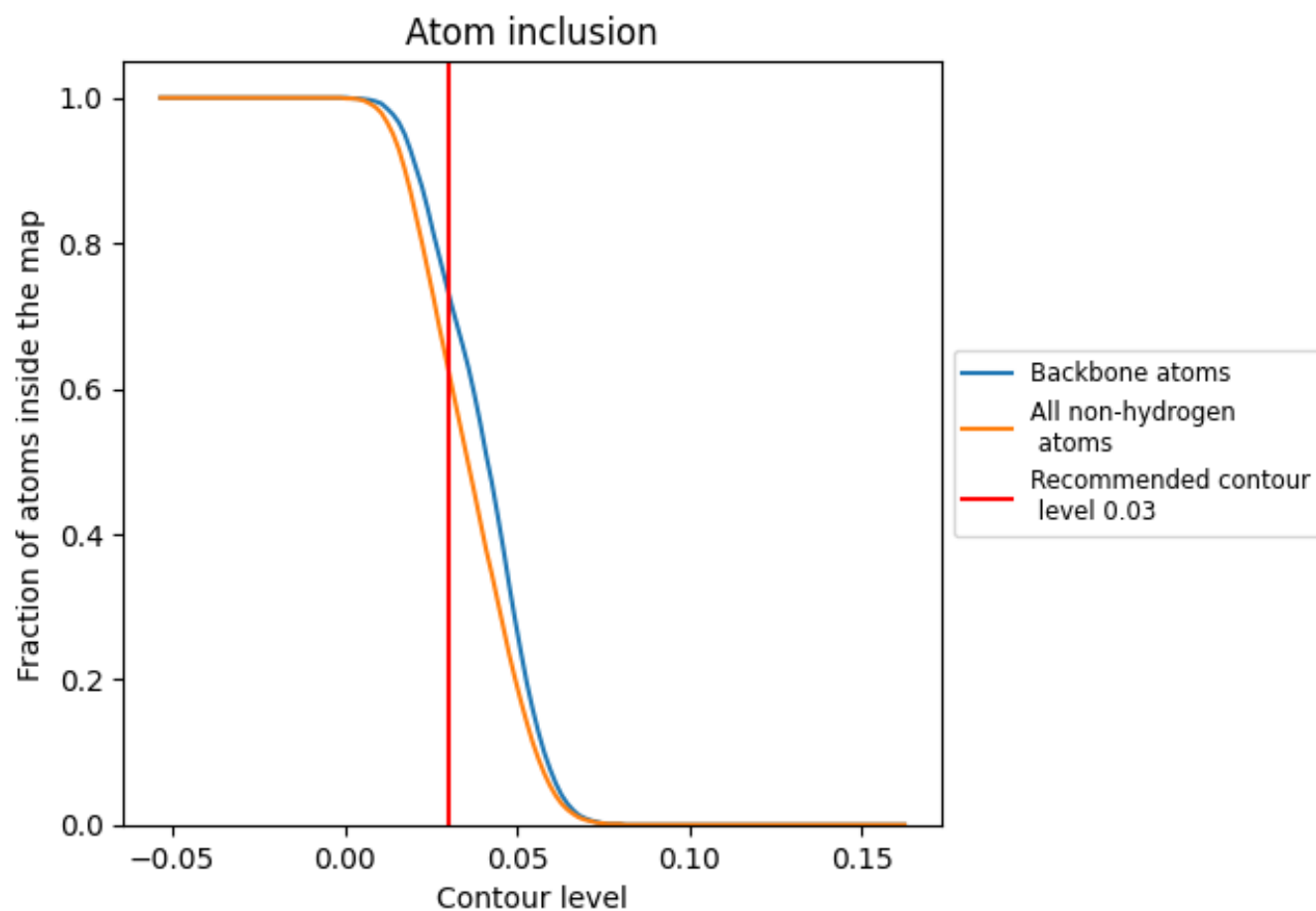
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.5450
2	0.5840	0.5210
3	0.5710	0.5210
5	0.5620	0.4890
6	0.5770	0.5130
A	0.7030	0.5700
B	0.7100	0.5730
C	0.7400	0.5450
D	0.6350	0.5460
E	0.6670	0.5550
F	0.6180	0.5420
G	0.5080	0.5190
H	0.1310	0.4850
I	0.5560	0.5500
J	0.5630	0.5490
K	0.4190	0.5040
L	0.4850	0.5170
M	0.6070	0.5250

1.0

0.0

<0.0