



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 02:49 pm BST

PDB ID : 8ASP  
EMDB ID : EMD-15621  
Title : RCII/PSI complex, focused refinement of PSI  
Authors : Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.;  
Sazanov, L.A.; Komenda, J.  
Deposited on : 2022-08-20  
Resolution : 2.90 Å (reported)  
Based on initial models : 5OY0, 2XBG, 6WJ6

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

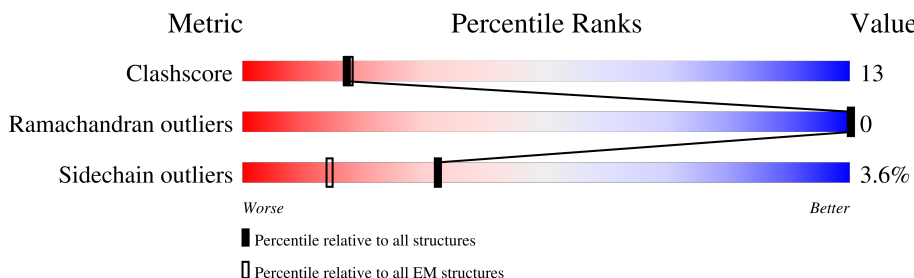
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	a	751	97% ..
2	b	731	98% .
3	c	81	95% . .
4	d	141	96% . .
5	e	74	86% 7% 7%
6	f	165	82% . 14%
7	i	40	8% 95% 5%
8	j	40	95% 5%

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Mol	Chain	Length	Quality of chain
9	k	88	
10	l	157	
11	m	31	

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
12	CL0	a	801	X	-	-	-
13	CLA	a	802	X	-	-	-
13	CLA	a	803	X	-	-	-
13	CLA	a	804	X	-	-	-
13	CLA	a	805	X	-	-	-
13	CLA	a	806	X	-	-	-
13	CLA	a	807	X	-	-	-
13	CLA	a	808	X	-	-	-
13	CLA	a	809	X	-	-	-
13	CLA	a	810	X	-	-	-
13	CLA	a	811	X	-	-	-
13	CLA	a	812	X	-	-	-
13	CLA	a	813	X	-	-	-
13	CLA	a	814	X	-	-	-
13	CLA	a	815	X	-	-	-
13	CLA	a	816	X	-	-	-
13	CLA	a	817	X	-	-	-
13	CLA	a	818	X	-	-	-
13	CLA	a	819	X	-	-	-
13	CLA	a	820	X	-	-	-
13	CLA	a	821	X	-	-	-
13	CLA	a	822	X	-	-	-
13	CLA	a	823	X	-	-	-
13	CLA	a	824	X	-	-	-
13	CLA	a	825	X	-	-	-
13	CLA	a	826	X	-	-	-
13	CLA	a	827	X	-	-	-
13	CLA	a	828	X	-	-	-
13	CLA	a	829	X	-	-	-
13	CLA	a	830	X	-	-	-
13	CLA	a	831	X	-	-	-
13	CLA	a	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	a	833	X	-	-	-
13	CLA	a	834	X	-	-	-
13	CLA	a	835	X	-	-	-
13	CLA	a	836	X	-	-	-
13	CLA	a	837	X	-	-	-
13	CLA	a	838	X	-	-	-
13	CLA	a	839	X	-	-	-
13	CLA	a	840	X	-	-	-
13	CLA	a	841	X	-	-	-
13	CLA	a	842	X	-	-	-
13	CLA	a	854	X	-	-	-
13	CLA	a	855	X	-	-	-
13	CLA	b	801	X	-	-	-
13	CLA	b	803	X	-	-	-
13	CLA	b	804	X	-	-	-
13	CLA	b	805	X	-	-	-
13	CLA	b	806	X	-	-	-
13	CLA	b	807	X	-	-	-
13	CLA	b	808	X	-	-	-
13	CLA	b	809	X	-	-	-
13	CLA	b	810	X	-	-	-
13	CLA	b	811	X	-	-	-
13	CLA	b	812	X	-	-	-
13	CLA	b	813	X	-	-	-
13	CLA	b	814	X	-	-	-
13	CLA	b	815	X	-	-	-
13	CLA	b	816	X	-	-	-
13	CLA	b	817	X	-	-	-
13	CLA	b	818	X	-	-	-
13	CLA	b	819	X	-	-	-
13	CLA	b	820	X	-	-	-
13	CLA	b	821	X	-	-	-
13	CLA	b	822	X	-	-	-
13	CLA	b	823	X	-	-	-
13	CLA	b	824	X	-	-	-
13	CLA	b	825	X	-	-	-
13	CLA	b	826	X	-	-	-
13	CLA	b	827	X	-	-	-
13	CLA	b	828	X	-	-	-
13	CLA	b	829	X	-	-	-
13	CLA	b	830	X	-	-	-
13	CLA	b	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	b	832	X	-	-	-
13	CLA	b	833	X	-	-	-
13	CLA	b	834	X	-	-	-
13	CLA	b	835	X	-	-	-
13	CLA	b	836	X	-	-	-
13	CLA	b	837	X	-	-	-
13	CLA	b	838	X	-	-	-
13	CLA	b	839	X	-	-	-
13	CLA	b	840	X	-	-	-
13	CLA	b	841	X	-	-	-
13	CLA	b	842	X	-	-	-
13	CLA	f	201	X	-	-	-
13	CLA	f	203	X	-	-	-
13	CLA	f	204	X	-	-	-
13	CLA	j	103	X	-	-	-
13	CLA	j	104	X	-	-	-
13	CLA	k	4002	X	-	-	-
13	CLA	k	4003	X	-	-	-
13	CLA	k	4004	X	-	-	-
13	CLA	l	1501	X	-	-	-
13	CLA	l	1502	X	-	-	-
13	CLA	l	1503	X	-	-	-

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 24596 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	740	Total	C	N	O	S	0	0
			5786	3791	982	986	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

- 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
			600	369	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	69	Total	C	N	O	0	0
			538	337	95	106		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	142	Total	C	N	O	S	0	0
			1108	715	184	204	5		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			319	215	47	54	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	77	Total	C	N	O	S	0	0
			535	350	89	92	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	87	GLY	-	expression tag	UNP P72712
k	88	VAL	-	expression tag	UNP P72712

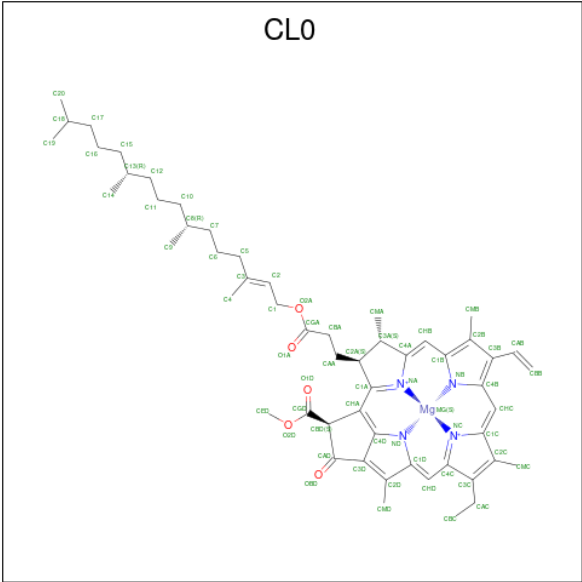
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1069	697	173	197	2		

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

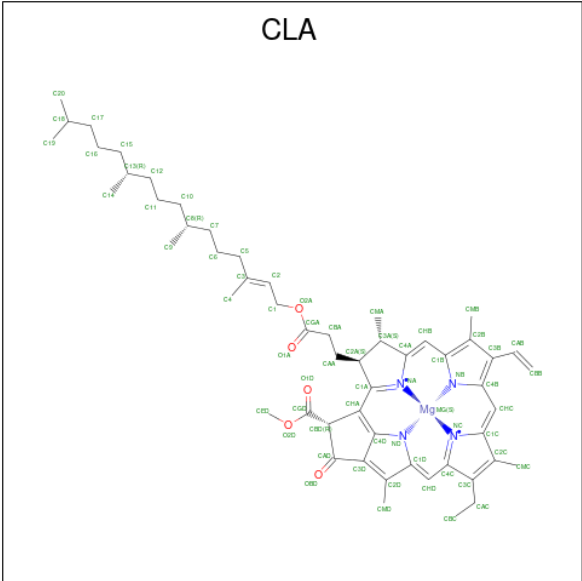
Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

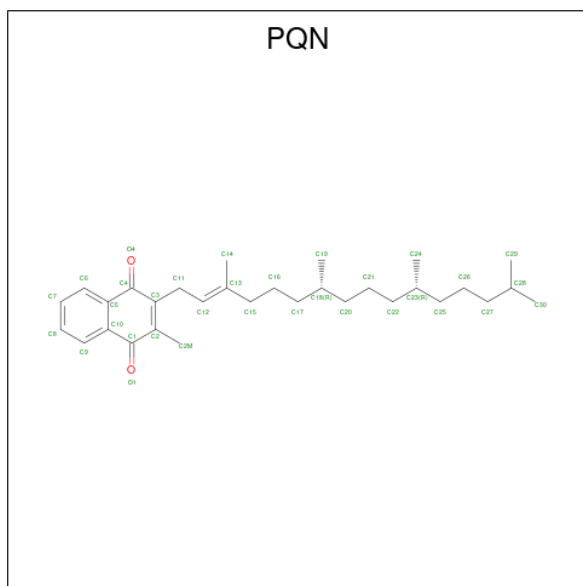
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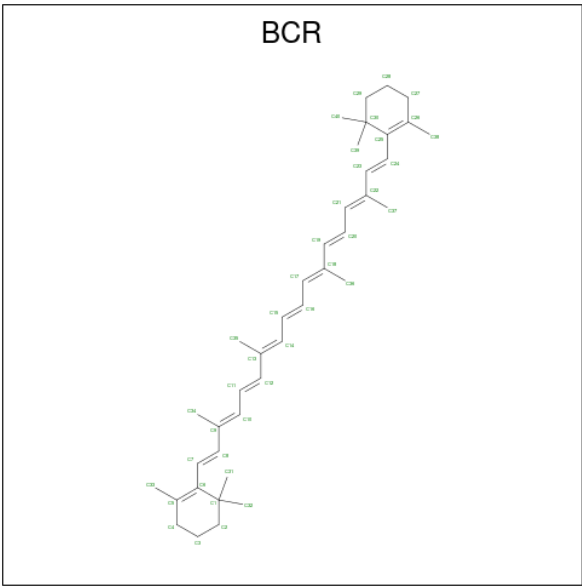
Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



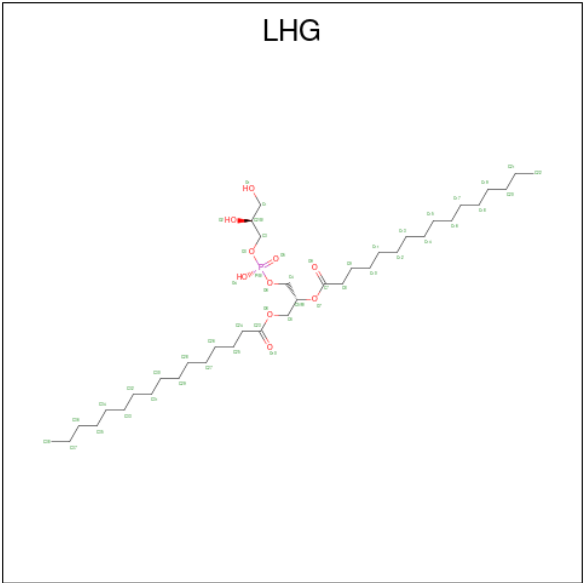
Mol	Chain	Residues	Atoms		AltConf
15	a	1	Total	C	0
			40	40	
15	a	1	Total	C	0
			40	40	
15	a	1	Total	C	0
			40	40	
15	a	1	Total	C	0
			40	40	
15	a	1	Total	C	0
			25	25	
15	b	1	Total	C	0
			40	40	
15	b	1	Total	C	0
			40	40	
15	b	1	Total	C	0
			40	40	
15	b	1	Total	C	0
			40	40	
15	f	1	Total	C	0
			40	40	
15	i	1	Total	C	0
			40	40	
15	i	1	Total	C	0
			40	40	

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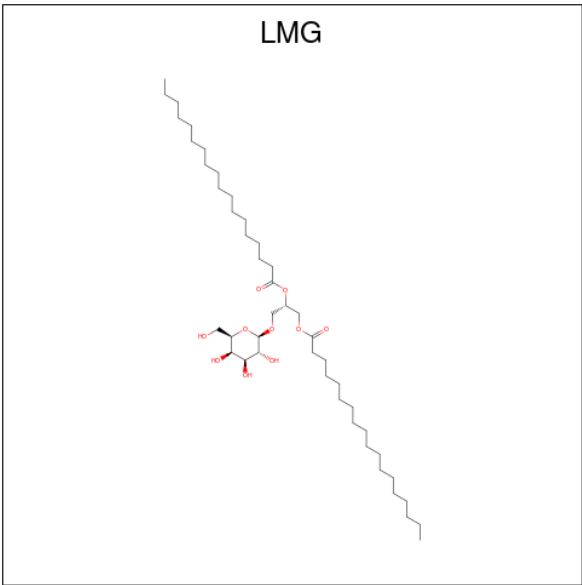
Mol	Chain	Residues	Atoms		AltConf
15	j	1	Total	C	0
			40	40	
15	j	1	Total	C	0
			40	40	
15	k	1	Total	C	0
			40	40	
15	k	1	Total	C	0
			40	40	

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



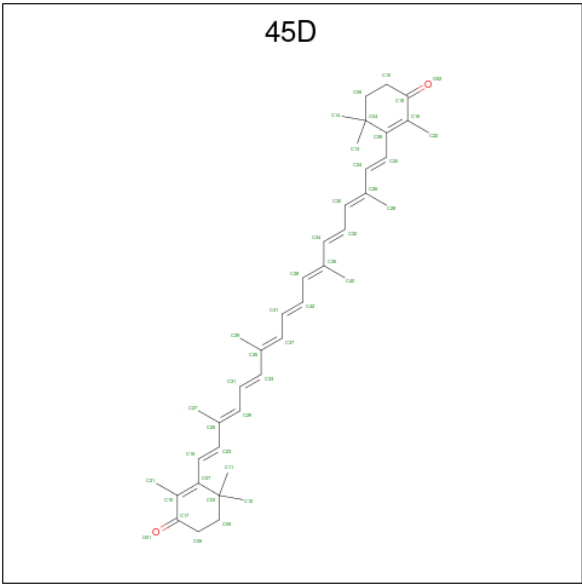
Mol	Chain	Residues	Atoms				AltConf
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	b	1	Total	C	O	P	0
			38	27	10	1	
16	f	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



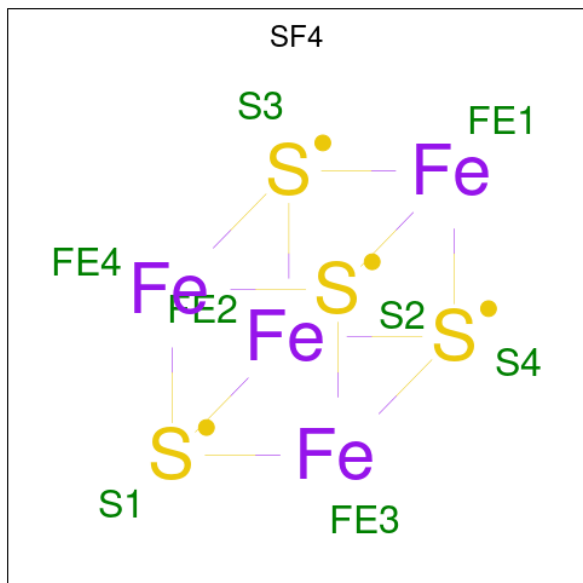
Mol	Chain	Residues	Atoms			AltConf
17	a	1	Total	C	O	0
			50	40	10	
17	a	1	Total	C	O	0
			40	30	10	
17	b	1	Total	C	O	0
			55	45	10	
17	b	1	Total	C	O	0
			55	45	10	

- Molecule 18 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>).



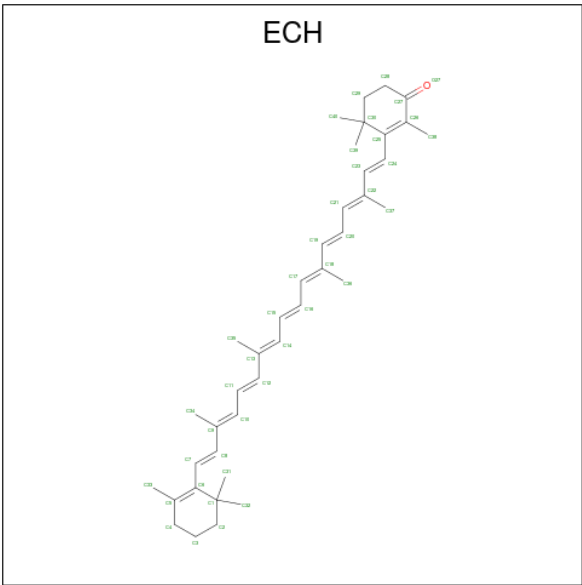
Mol	Chain	Residues	Atoms			AltConf
18	a	1	Total	C	O	0
			42	40	2	

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



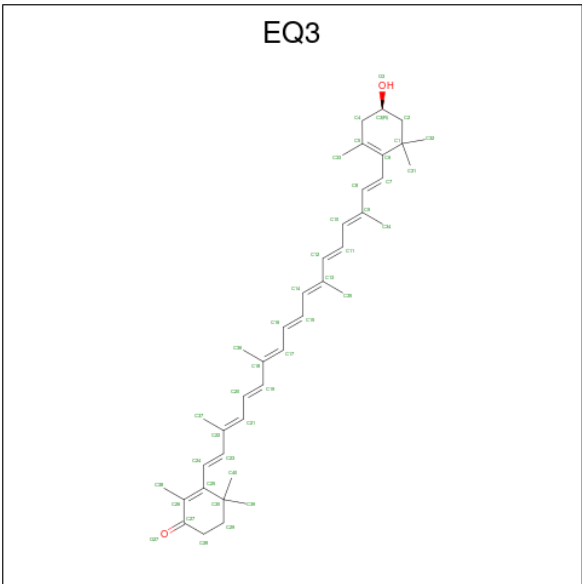
Mol	Chain	Residues	Atoms			AltConf
19	b	1	Total	Fe	S	0
			8	4	4	
19	c	1	Total	Fe	S	0
			8	4	4	
19	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 20 is beta,beta-caroten-4-one (three-letter code: ECH) (formula:  $\text{C}_{40}\text{H}_{54}\text{O}$ ).



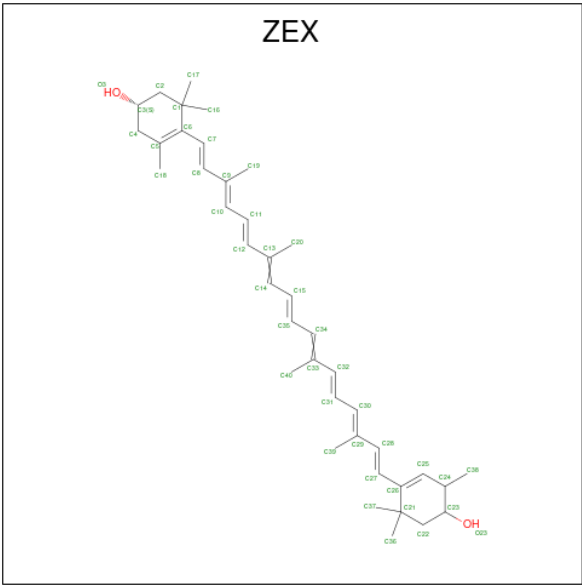
Mol	Chain	Residues	Atoms			AltConf
20	b	1	Total	C	O	0
			41	40	1	
20	m	1	Total	C	O	0
			41	40	1	

- Molecule 21 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>).



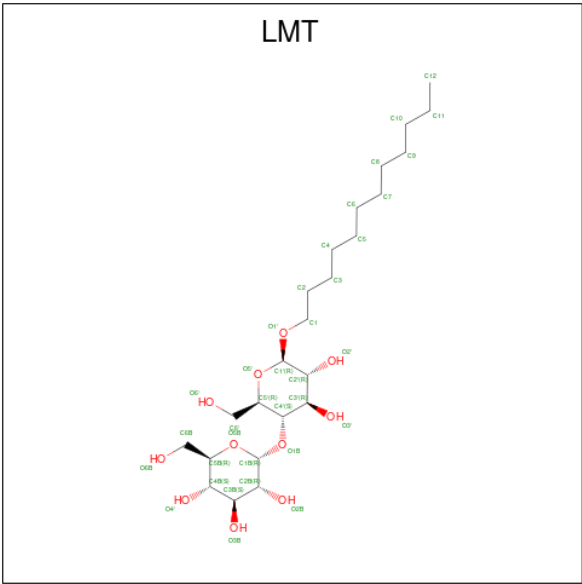
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
22	b	1	Total	C	O	0
			42	40	2	
22	f	1	Total	C	O	0
			42	40	2	

- Molecule 23 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
23	j	1	Total	C	O	0
			35	24	11	



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

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:  97%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  98%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  95%




- Molecule 4: Photosystem I reaction center subunit II

Chain d:  96%

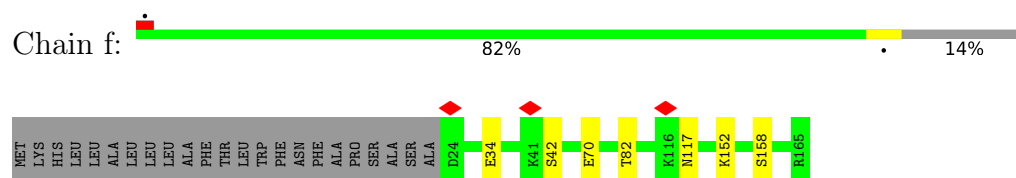


- Molecule 5: Photosystem I reaction center subunit IV

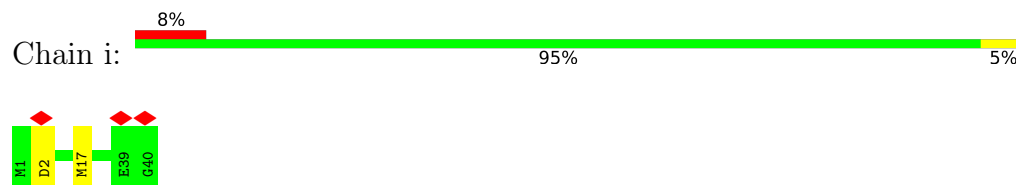
Chain e:  86% 7% 7%



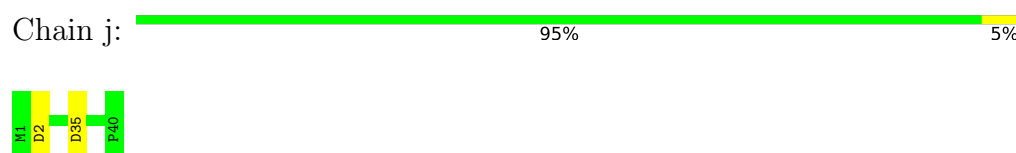
- Molecule 6: Photosystem I reaction center subunit III



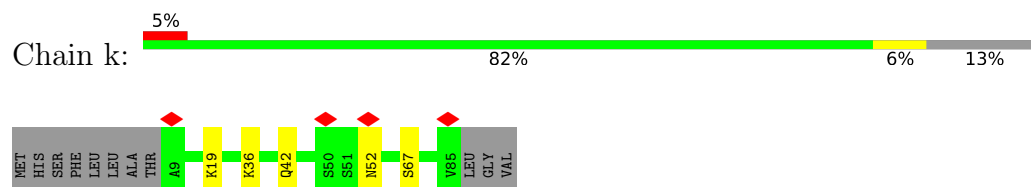
- Molecule 7: Photosystem I reaction center subunit VIII



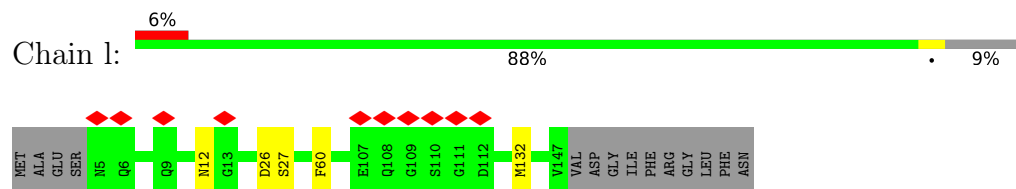
- Molecule 8: Photosystem I reaction center subunit IX



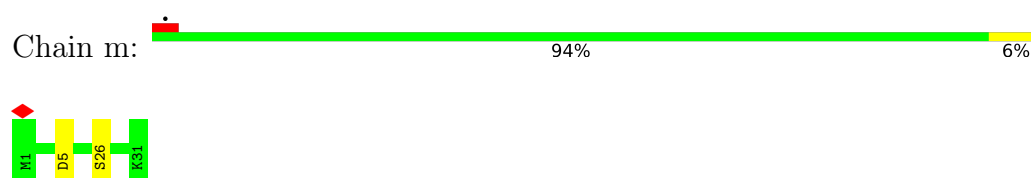
- Molecule 9: Photosystem I reaction center subunit PsaK 1



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.526	Depositor
Minimum map value	-0.118	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, ECH, SF4, EQ3, PQN, ZEX, CL0, LHG, CLA, LMG, LMT, 45D

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	0.26	0/5984	0.43	0/8158
2	b	0.26	0/5981	0.43	1/8178 (0.0%)
3	c	0.25	0/610	0.51	0/826
4	d	0.26	0/1111	0.49	0/1497
5	e	0.28	0/547	0.58	0/741
6	f	0.28	0/1138	0.49	0/1546
7	i	0.27	0/322	0.45	0/438
8	j	0.25	0/328	0.45	0/443
9	k	0.26	0/546	0.50	0/741
10	l	0.27	0/1097	0.49	0/1493
11	m	0.27	0/241	0.50	0/326
All	All	0.26	0/17905	0.46	1/24387 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	b	659	MET	CA-CB-CG	5.75	123.08	113.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5786	0	5640	0	0
2	b	5770	0	5547	0	0
3	c	600	0	581	0	0
4	d	1087	0	1082	0	0
5	e	538	0	514	0	0
6	f	1108	0	1100	0	0
7	i	311	0	304	0	0
8	j	319	0	328	0	0
9	k	535	0	559	0	0
10	l	1069	0	1044	0	0
11	m	238	0	260	0	0
12	a	65	0	72	0	0
13	a	2637	0	2754	0	0
13	b	2475	0	2528	0	0
13	f	160	0	144	0	0
13	j	101	0	82	0	0
13	k	156	0	138	0	0
13	l	167	0	154	0	0
14	a	33	0	46	0	0
14	b	33	0	46	0	0
15	a	185	0	257	0	0
15	b	200	0	280	0	0
15	f	40	0	56	0	0
15	i	80	0	112	0	0
15	j	80	0	112	0	0
15	k	80	0	112	0	0
16	a	147	0	222	0	0
16	b	38	0	49	0	0
16	f	49	0	74	0	0
17	a	90	0	123	0	0
17	b	110	0	172	0	0
18	a	42	0	52	0	0
19	b	8	0	0	0	0
19	c	16	0	0	0	0
20	b	41	0	54	0	0
20	m	41	0	54	0	0
21	b	42	0	0	0	0
22	b	42	0	56	0	0
22	f	42	0	56	0	0
23	j	35	0	45	0	0
All	All	24596	0	24809	0	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 13.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	738/751 (98%)	717 (97%)	21 (3%)	0	100	100
2	b	727/731 (100%)	705 (97%)	22 (3%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	d	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
5	e	67/74 (90%)	65 (97%)	2 (3%)	0	100	100
6	f	140/165 (85%)	139 (99%)	1 (1%)	0	100	100
7	i	38/40 (95%)	38 (100%)	0	0	100	100
8	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
9	k	75/88 (85%)	70 (93%)	5 (7%)	0	100	100
10	l	141/157 (90%)	136 (96%)	5 (4%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	2208/2299 (96%)	2144 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	592/603 (98%)	577 (98%)	15 (2%)	42	75
2	b	582/583 (100%)	568 (98%)	14 (2%)	44	76
3	c	68/69 (99%)	65 (96%)	3 (4%)	24	57
4	d	114/116 (98%)	110 (96%)	4 (4%)	31	66
5	e	57/60 (95%)	52 (91%)	5 (9%)	8	26
6	f	119/137 (87%)	112 (94%)	7 (6%)	16	45
7	i	32/32 (100%)	30 (94%)	2 (6%)	15	42
8	j	35/35 (100%)	33 (94%)	2 (6%)	17	47
9	k	54/63 (86%)	49 (91%)	5 (9%)	7	23
10	l	107/118 (91%)	102 (95%)	5 (5%)	22	55
11	m	25/25 (100%)	23 (92%)	2 (8%)	10	30
All	All	1785/1841 (97%)	1721 (96%)	64 (4%)	32	65

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	59	ASP
1	a	186	LYS
1	a	196	MET
1	a	249	MET
1	a	256	PHE
1	a	277	PHE
1	a	292	ASP
1	a	363	THR
1	a	365	ILE
1	a	434	ASP
1	a	449	PHE
1	a	459	ASP
1	a	522	MET
1	a	537	ILE
1	a	545	THR
2	b	257	PHE
2	b	300	SER
2	b	343	THR
2	b	391	PHE
2	b	392	PHE
2	b	409	MET
2	b	439	ASP
2	b	476	LEU

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Mol	Chain	Res	Type
2	b	500	SER
2	b	517	HIS
2	b	527	THR
2	b	533	LYS
2	b	573	PHE
2	b	574	TYR
3	c	28	MET
3	c	69	LEU
3	c	76	SER
4	d	10	LYS
4	d	107	LYS
4	d	115	GLN
4	d	134	SER
5	e	7	ASP
5	e	27	SER
5	e	34	LEU
5	e	54	SER
5	e	63	GLU
6	f	34	GLU
6	f	42	SER
6	f	70	GLU
6	f	82	THR
6	f	117	ASN
6	f	152	LYS
6	f	158	SER
7	i	2	ASP
7	i	17	MET
8	j	2	ASP
8	j	35	ASP
9	k	19	LYS
9	k	36	LYS
9	k	42	GLN
9	k	52	ASN
9	k	67	SER
10	l	12	ASN
10	l	26	ASP
10	l	27	SER
10	l	60	PHE
10	l	132	MET
11	m	5	ASP
11	m	26	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such



sidechains are listed below:

Mol	Chain	Res	Type
4	d	7	GLN
6	f	121	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

134 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	$\# Z  > 2$
13	CLA	b	820	-	60,68,73	1.53	6 (10%)	70,107,113	1.39	7 (10%)
13	CLA	a	831	-	56,64,73	1.59	6 (10%)	65,102,113	1.46	8 (12%)
13	CLA	b	834	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
13	CLA	b	839	-	50,58,73	1.72	6 (12%)	58,95,113	1.52	7 (12%)
17	LMG	a	852	-	40,40,55	0.83	0	48,48,63	1.24	4 (8%)
13	CLA	a	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
13	CLA	j	103	8	55,63,73	1.62	5 (9%)	64,101,113	1.41	7 (10%)
19	SF4	c	101	3	0,12,12	-	-	-	-	-
13	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	b	849	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	5 (8%)
14	PQN	b	843	-	34,34,34	0.39	0	42,45,45	0.38	0
15	BCR	k	4001	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	k	4004	9	45,53,73	1.77	5 (11%)	52,89,113	1.70	9 (17%)
13	CLA	a	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
16	LHG	a	851	13	48,48,48	0.59	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	b	825	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	b	823	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	6 (11%)
13	CLA	a	821	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
13	CLA	a	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.33	9 (11%)
12	CL0	a	801	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	7 (9%)
13	CLA	b	803	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
13	CLA	a	820	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	6 (7%)
13	CLA	a	805	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	8 (10%)
13	CLA	b	801	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	7 (9%)
13	CLA	a	839	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
13	CLA	a	836	1	55,63,73	1.61	6 (10%)	64,101,113	1.47	8 (12%)
13	CLA	a	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
15	BCR	k	4005	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	a	808	1	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
13	CLA	a	812	-	52,60,73	1.68	6 (11%)	60,97,113	1.50	9 (15%)
13	CLA	b	835	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	b	840	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	9 (11%)
13	CLA	a	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	8 (10%)
13	CLA	a	823	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
16	LHG	f	206	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
23	LMT	j	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	2 (4%)
13	CLA	a	810	-	53,61,73	1.62	7 (13%)	61,98,113	1.51	8 (13%)
13	CLA	b	811	-	56,64,73	1.64	6 (10%)	65,102,113	1.41	7 (10%)
13	CLA	b	814	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
15	BCR	a	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
15	BCR	b	845	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	4 (7%)
13	CLA	a	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
13	CLA	l	1503	-	52,60,73	1.64	6 (11%)	60,97,113	1.55	7 (11%)
13	CLA	a	815	-	46,54,73	1.71	6 (13%)	53,90,113	1.60	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	b	817	-	56,64,73	1.55	6 (10%)	65,102,113	1.49	8 (12%)
22	ZEX	b	854	-	42,43,43	1.67	8 (19%)	55,60,60	1.61	12 (21%)
15	BCR	a	848	-	25,25,41	1.16	1 (4%)	33,33,56	1.30	5 (15%)
14	PQN	a	843	-	34,34,34	0.38	0	42,45,45	0.40	0
13	CLA	a	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
15	BCR	b	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	a	854	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	7 (9%)
13	CLA	a	822	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	7 (9%)
13	CLA	a	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	7 (9%)
13	CLA	a	835	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	9 (11%)
13	CLA	a	809	1	51,59,73	1.65	6 (11%)	59,96,113	1.61	7 (11%)
17	LMG	b	852	-	55,55,55	0.78	1 (1%)	63,63,63	1.33	9 (14%)
17	LMG	a	850	-	50,50,55	0.78	0	58,58,63	1.31	7 (12%)
13	CLA	b	819	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
13	CLA	a	803	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	8 (10%)
13	CLA	a	855	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	6 (7%)
13	CLA	b	827	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
13	CLA	b	816	-	55,63,73	1.62	6 (10%)	64,101,113	1.42	8 (12%)
13	CLA	a	818	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	7 (9%)
13	CLA	f	204	6	45,53,73	1.80	5 (11%)	52,89,113	1.58	6 (11%)
17	LMG	b	850	-	55,55,55	0.70	0	63,63,63	1.38	8 (12%)
13	CLA	b	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.34	7 (9%)
15	BCR	a	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	5 (8%)
15	BCR	a	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	b	831	-	51,59,73	1.69	5 (9%)	59,96,113	1.49	8 (13%)
15	BCR	b	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	7 (12%)
18	45D	a	856	-	43,43,43	1.73	10 (23%)	54,60,60	1.61	10 (18%)
13	CLA	b	805	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	9 (11%)
13	CLA	a	837	-	51,59,73	1.63	6 (11%)	59,96,113	1.56	7 (11%)
13	CLA	b	826	-	55,63,73	1.59	6 (10%)	64,101,113	1.49	8 (12%)
13	CLA	f	201	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
13	CLA	b	821	-	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
22	ZEX	f	205	-	42,43,43	1.67	8 (19%)	55,60,60	1.59	11 (20%)
13	CLA	l	1502	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
19	SF4	c	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	b	838	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
21	EQ3	b	853	-	43,43,43	1.66	9 (20%)	56,60,60	1.54	11 (19%)
13	CLA	b	808	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
20	ECH	m	101	-	42,42,42	1.79	9 (21%)	55,58,58	1.86	13 (23%)
13	CLA	b	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
16	LHG	a	853	-	48,48,48	0.60	0	51,54,54	1.26	6 (11%)
13	CLA	a	824	-	60,68,73	1.52	6 (10%)	70,107,113	1.47	7 (10%)
13	CLA	b	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.54	7 (12%)
13	CLA	a	817	-	65,73,73	1.46	5 (7%)	76,113,113	1.38	8 (10%)
13	CLA	b	829	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	6 (7%)
13	CLA	k	4002	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	b	815	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	b	812	-	56,64,73	1.58	6 (10%)	65,102,113	1.49	6 (9%)
13	CLA	b	842	16	46,54,73	1.74	5 (10%)	53,90,113	1.58	6 (11%)
13	CLA	b	824	-	57,65,73	1.59	6 (10%)	66,103,113	1.47	8 (12%)
13	CLA	a	816	-	46,54,73	1.75	5 (10%)	53,90,113	1.59	6 (11%)
13	CLA	a	838	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
13	CLA	b	810	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
13	CLA	b	822	-	60,68,73	1.54	5 (8%)	70,107,113	1.44	6 (8%)
13	CLA	j	104	-	46,54,73	1.76	6 (13%)	53,90,113	1.49	6 (11%)
13	CLA	a	819	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	9 (11%)
15	BCR	a	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	8 (14%)
13	CLA	a	832	-	60,68,73	1.53	6 (10%)	70,107,113	1.44	9 (12%)
13	CLA	k	4003	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
16	LHG	a	849	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	b	804	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	9 (11%)
15	BCR	j	105	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
13	CLA	a	814	-	47,55,73	1.73	5 (10%)	54,91,113	1.61	8 (14%)
13	CLA	b	807	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
15	BCR	i	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	b	813	-	50,58,73	1.68	6 (12%)	58,95,113	1.52	8 (13%)
13	CLA	b	830	-	65,73,73	1.45	6 (9%)	76,113,113	1.52	8 (10%)
15	BCR	b	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.16	5 (8%)
13	CLA	b	841	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	7 (9%)
13	CLA	a	804	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	b	806	-	65,73,73	1.46	6 (9%)	76,113,113	1.47	7 (9%)
13	CLA	a	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.50	9 (11%)
13	CLA	b	832	-	50,58,73	1.66	6 (12%)	58,95,113	1.55	9 (15%)
16	LHG	b	851	13	37,37,48	0.69	1 (2%)	40,43,54	1.20	3 (7%)
13	CLA	b	809	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
20	ECH	b	846	-	42,42,42	1.74	8 (19%)	55,58,58	2.33	14 (25%)
13	CLA	a	841	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	9 (11%)
13	CLA	a	840	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
13	CLA	f	203	-	50,58,73	1.71	5 (10%)	58,95,113	1.52	8 (13%)
15	BCR	i	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
15	BCR	f	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
15	BCR	j	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	a	811	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
13	CLA	b	818	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	8 (10%)
19	SF4	b	802	2,1	0,12,12	-	-	-	-	-
13	CLA	a	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
13	CLA	a	842	16	45,53,73	1.76	5 (11%)	52,89,113	1.62	7 (13%)
13	CLA	l	1501	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
13	CLA	a	827	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
13	CLA	b	837	-	52,60,73	1.63	6 (11%)	60,97,113	1.59	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	820	-	1/1/14/20	7/31/109/115	-
13	CLA	a	831	-	1/1/13/20	10/27/105/115	-
13	CLA	b	834	-	1/1/15/20	14/37/115/115	-
13	CLA	b	839	-	1/1/12/20	5/19/97/115	-
17	LMG	a	852	-	-	19/35/55/70	0/1/1/1
13	CLA	a	826	-	1/1/15/20	9/37/115/115	-
13	CLA	j	103	8	1/1/13/20	9/25/103/115	-
19	SF4	c	101	3	-	-	0/6/5/5
13	CLA	a	828	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	b	849	-	-	14/29/63/63	0/2/2/2
14	PQN	b	843	-	-	1/23/43/43	0/2/2/2
15	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	k	4004	9	1/1/11/20	6/13/91/115	-
13	CLA	a	806	-	1/1/15/20	12/37/115/115	-
16	LHG	a	851	13	-	19/53/53/53	-
13	CLA	b	825	-	1/1/15/20	14/37/115/115	-
13	CLA	b	823	-	1/1/11/20	4/15/93/115	-
13	CLA	a	821	-	1/1/15/20	13/37/115/115	-
13	CLA	a	833	-	1/1/15/20	16/37/115/115	-
12	CL0	a	801	-	3/3/20/25	8/37/135/135	-
13	CLA	b	803	-	1/1/15/20	18/37/115/115	-
13	CLA	a	820	-	1/1/15/20	24/37/115/115	-
13	CLA	a	805	-	1/1/15/20	11/37/115/115	-
13	CLA	b	801	-	1/1/15/20	14/37/115/115	-
13	CLA	a	839	-	1/1/15/20	19/37/115/115	-
13	CLA	a	836	1	1/1/13/20	8/25/103/115	-
13	CLA	a	807	-	1/1/15/20	16/37/115/115	-
15	BCR	k	4005	-	-	4/29/63/63	0/2/2/2
13	CLA	a	808	1	1/1/15/20	13/37/115/115	-
13	CLA	a	812	-	1/1/12/20	8/22/100/115	-
13	CLA	b	835	-	1/1/15/20	19/37/115/115	-
13	CLA	b	840	-	1/1/15/20	16/37/115/115	-
13	CLA	a	825	-	1/1/15/20	13/37/115/115	-
13	CLA	a	823	-	1/1/15/20	18/37/115/115	-
16	LHG	f	206	-	-	20/53/53/53	-
23	LMT	j	102	-	-	15/21/61/61	0/2/2/2
13	CLA	a	810	-	1/1/12/20	10/23/101/115	-
13	CLA	b	811	-	1/1/13/20	9/27/105/115	-
13	CLA	b	814	-	1/1/15/20	16/37/115/115	-
15	BCR	a	847	-	-	10/29/63/63	0/2/2/2
15	BCR	b	845	-	-	5/29/63/63	0/2/2/2
13	CLA	a	834	-	1/1/15/20	15/37/115/115	-
13	CLA	l	1503	-	1/1/12/20	6/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	815	-	1/1/11/20	5/15/93/115	-
13	CLA	b	817	-	1/1/13/20	9/27/105/115	-
22	ZEX	b	854	-	-	3/29/67/67	0/2/2/2
15	BCR	a	848	-	-	8/18/35/63	0/1/1/2
14	PQN	a	843	-	-	1/23/43/43	0/2/2/2
13	CLA	a	829	-	1/1/15/20	15/37/115/115	-
15	BCR	b	847	-	-	6/29/63/63	0/2/2/2
13	CLA	a	854	-	1/1/15/20	6/37/115/115	-
13	CLA	a	822	-	1/1/15/20	13/37/115/115	-
13	CLA	a	802	-	1/1/15/20	10/37/115/115	-
13	CLA	a	835	-	1/1/15/20	13/37/115/115	-
13	CLA	a	809	1	1/1/12/20	4/21/99/115	-
17	LMG	b	852	-	-	22/50/70/70	0/1/1/1
17	LMG	a	850	-	-	27/45/65/70	0/1/1/1
13	CLA	b	819	-	1/1/15/20	15/37/115/115	-
13	CLA	a	803	-	1/1/15/20	6/37/115/115	-
13	CLA	a	855	-	1/1/15/20	17/37/115/115	-
13	CLA	b	827	-	1/1/15/20	7/37/115/115	-
13	CLA	b	816	-	1/1/13/20	12/25/103/115	-
13	CLA	a	818	-	1/1/15/20	23/37/115/115	-
13	CLA	f	204	6	1/1/11/20	5/13/91/115	-
17	LMG	b	850	-	-	24/50/70/70	0/1/1/1
13	CLA	b	833	-	1/1/15/20	15/37/115/115	-
15	BCR	a	844	-	-	6/29/63/63	0/2/2/2
15	BCR	a	845	-	-	6/29/63/63	0/2/2/2
13	CLA	b	831	-	1/1/12/20	9/21/99/115	-
15	BCR	b	844	-	-	11/29/63/63	0/2/2/2
18	45D	a	856	-	-	4/29/69/69	0/2/2/2
13	CLA	b	805	-	1/1/15/20	12/37/115/115	-
13	CLA	a	837	-	1/1/12/20	5/21/99/115	-
13	CLA	b	826	-	1/1/13/20	6/25/103/115	-
13	CLA	f	201	-	1/1/15/20	18/37/115/115	-
13	CLA	b	821	-	1/1/15/20	11/37/115/115	-
22	ZEX	f	205	-	-	6/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	l	1502	-	1/1/15/20	13/37/115/115	-
19	SF4	c	102	3	-	-	0/6/5/5
13	CLA	b	838	-	1/1/15/20	15/37/115/115	-
21	EQ3	b	853	-	-	2/29/68/68	0/2/2/2
13	CLA	b	808	-	1/1/15/20	15/37/115/115	-
20	ECH	m	101	-	-	6/29/66/66	0/2/2/2
13	CLA	b	828	-	1/1/15/20	15/37/115/115	-
16	LHG	a	853	-	-	30/53/53/53	-
13	CLA	a	824	-	1/1/14/20	11/31/109/115	-
13	CLA	b	836	-	1/1/12/20	9/19/97/115	-
13	CLA	a	817	-	1/1/15/20	12/37/115/115	-
13	CLA	b	829	-	1/1/15/20	10/37/115/115	-
13	CLA	k	4002	-	1/1/15/20	12/37/115/115	-
13	CLA	b	815	-	1/1/15/20	10/37/115/115	-
13	CLA	b	812	-	1/1/13/20	7/27/105/115	-
13	CLA	b	842	16	1/1/11/20	9/15/93/115	-
13	CLA	b	824	-	1/1/13/20	12/28/106/115	-
13	CLA	a	816	-	1/1/11/20	7/15/93/115	-
13	CLA	a	838	-	1/1/15/20	15/37/115/115	-
13	CLA	b	810	2	1/1/15/20	13/37/115/115	-
13	CLA	b	822	-	1/1/14/20	16/31/109/115	-
13	CLA	j	104	-	1/1/11/20	8/15/93/115	-
13	CLA	a	819	-	1/1/15/20	15/37/115/115	-
15	BCR	a	846	-	-	6/29/63/63	0/2/2/2
13	CLA	a	832	-	1/1/14/20	14/31/109/115	-
13	CLA	k	4003	-	1/1/11/20	9/15/93/115	-
16	LHG	a	849	-	-	31/53/53/53	-
13	CLA	b	804	-	1/1/15/20	18/37/115/115	-
15	BCR	j	105	-	-	5/29/63/63	0/2/2/2
13	CLA	a	814	-	1/1/11/20	11/16/94/115	-
13	CLA	b	807	-	1/1/15/20	14/37/115/115	-
15	BCR	i	102	-	-	11/29/63/63	0/2/2/2
13	CLA	b	813	-	1/1/12/20	7/19/97/115	-
13	CLA	b	830	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	b	848	-	-	8/29/63/63	0/2/2/2
13	CLA	b	841	-	1/1/15/20	16/37/115/115	-
13	CLA	a	804	-	1/1/15/20	12/37/115/115	-
13	CLA	b	806	-	1/1/15/20	12/37/115/115	-
13	CLA	a	830	-	1/1/15/20	12/37/115/115	-
13	CLA	b	832	-	1/1/12/20	5/19/97/115	-
16	LHG	b	851	13	-	25/42/42/53	-
13	CLA	b	809	-	1/1/15/20	5/37/115/115	-
20	ECH	b	846	-	-	10/29/66/66	0/2/2/2
13	CLA	a	841	-	1/1/15/20	13/37/115/115	-
13	CLA	a	840	-	1/1/15/20	18/37/115/115	-
13	CLA	f	203	-	1/1/12/20	4/19/97/115	-
15	BCR	i	101	-	-	7/29/63/63	0/2/2/2
15	BCR	f	202	-	-	8/29/63/63	0/2/2/2
15	BCR	j	101	-	-	6/29/63/63	0/2/2/2
13	CLA	a	811	-	1/1/15/20	15/37/115/115	-
13	CLA	b	818	-	1/1/15/20	7/37/115/115	-
19	SF4	b	802	2,1	-	-	0/6/5/5
13	CLA	a	813	-	1/1/15/20	13/37/115/115	-
13	CLA	a	842	16	1/1/11/20	6/13/91/115	-
13	CLA	l	1501	-	1/1/12/20	10/19/97/115	-
13	CLA	a	827	-	1/1/15/20	16/37/115/115	-
13	CLA	b	837	-	1/1/12/20	6/22/100/115	-

All (662) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	811	CLA	C4B-NB	7.94	1.42	1.35
13	b	823	CLA	C4B-NB	7.88	1.42	1.35
13	a	804	CLA	C4B-NB	7.73	1.42	1.35
13	b	839	CLA	C4B-NB	7.72	1.42	1.35
13	b	805	CLA	C4B-NB	7.67	1.42	1.35
13	a	839	CLA	C4B-NB	7.66	1.42	1.35
13	b	841	CLA	C4B-NB	7.65	1.42	1.35
13	b	833	CLA	C4B-NB	7.64	1.42	1.35
13	a	833	CLA	C4B-NB	7.59	1.42	1.35
13	b	803	CLA	C4B-NB	7.56	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	1501	CLA	C4B-NB	7.56	1.41	1.35
13	f	204	CLA	C4B-NB	7.54	1.41	1.35
13	a	820	CLA	C4B-NB	7.51	1.41	1.35
13	a	841	CLA	C4B-NB	7.50	1.41	1.35
13	b	801	CLA	C4B-NB	7.50	1.41	1.35
13	b	831	CLA	C4B-NB	7.50	1.41	1.35
13	b	816	CLA	C4B-NB	7.49	1.41	1.35
13	a	814	CLA	C4B-NB	7.48	1.41	1.35
13	b	824	CLA	C4B-NB	7.46	1.41	1.35
13	a	812	CLA	C4B-NB	7.46	1.41	1.35
13	j	104	CLA	C4B-NB	7.46	1.41	1.35
13	b	836	CLA	C4B-NB	7.46	1.41	1.35
13	a	823	CLA	C4B-NB	7.46	1.41	1.35
13	f	203	CLA	C4B-NB	7.44	1.41	1.35
13	j	103	CLA	C4B-NB	7.44	1.41	1.35
13	b	813	CLA	C4B-NB	7.43	1.41	1.35
13	a	803	CLA	C4B-NB	7.43	1.41	1.35
13	a	854	CLA	C4B-NB	7.42	1.41	1.35
13	a	838	CLA	C4B-NB	7.41	1.41	1.35
13	a	818	CLA	C4B-NB	7.40	1.41	1.35
13	b	822	CLA	C4B-NB	7.40	1.41	1.35
13	l	1502	CLA	C4B-NB	7.40	1.41	1.35
13	k	4003	CLA	C4B-NB	7.39	1.41	1.35
13	a	840	CLA	C4B-NB	7.39	1.41	1.35
13	b	821	CLA	C4B-NB	7.37	1.41	1.35
13	a	836	CLA	C4B-NB	7.37	1.41	1.35
13	b	827	CLA	C4B-NB	7.36	1.41	1.35
13	b	840	CLA	C4B-NB	7.36	1.41	1.35
13	b	828	CLA	C4B-NB	7.36	1.41	1.35
13	f	201	CLA	C4B-NB	7.36	1.41	1.35
13	b	810	CLA	C4B-NB	7.34	1.41	1.35
13	a	816	CLA	C4B-NB	7.33	1.41	1.35
13	a	806	CLA	C4B-NB	7.33	1.41	1.35
13	a	831	CLA	C4B-NB	7.33	1.41	1.35
13	a	819	CLA	C4B-NB	7.31	1.41	1.35
13	a	807	CLA	C4B-NB	7.30	1.41	1.35
13	b	834	CLA	C4B-NB	7.29	1.41	1.35
13	a	829	CLA	C4B-NB	7.29	1.41	1.35
13	b	807	CLA	C4B-NB	7.29	1.41	1.35
13	b	842	CLA	C4B-NB	7.29	1.41	1.35
13	k	4004	CLA	C4B-NB	7.29	1.41	1.35
13	k	4002	CLA	C4B-NB	7.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	814	CLA	C4B-NB	7.29	1.41	1.35
13	b	838	CLA	C4B-NB	7.29	1.41	1.35
13	l	1503	CLA	C4B-NB	7.28	1.41	1.35
13	a	835	CLA	C4B-NB	7.27	1.41	1.35
13	a	828	CLA	C4B-NB	7.27	1.41	1.35
12	a	801	CL0	C4B-NB	7.27	1.41	1.35
13	b	819	CLA	C4B-NB	7.27	1.41	1.35
13	b	809	CLA	C4B-NB	7.26	1.41	1.35
13	a	809	CLA	C4B-NB	7.26	1.41	1.35
13	b	812	CLA	C4B-NB	7.25	1.41	1.35
13	a	855	CLA	C4B-NB	7.25	1.41	1.35
13	a	830	CLA	C4B-NB	7.25	1.41	1.35
13	a	817	CLA	C4B-NB	7.24	1.41	1.35
13	a	810	CLA	C4B-NB	7.23	1.41	1.35
13	a	808	CLA	C4B-NB	7.23	1.41	1.35
13	a	822	CLA	C4B-NB	7.23	1.41	1.35
13	a	834	CLA	C4B-NB	7.22	1.41	1.35
13	a	805	CLA	C4B-NB	7.21	1.41	1.35
13	a	811	CLA	C4B-NB	7.21	1.41	1.35
13	a	842	CLA	C4B-NB	7.21	1.41	1.35
13	b	808	CLA	C4B-NB	7.21	1.41	1.35
13	a	825	CLA	C4B-NB	7.21	1.41	1.35
13	b	830	CLA	C4B-NB	7.20	1.41	1.35
13	b	815	CLA	C4B-NB	7.19	1.41	1.35
13	a	832	CLA	C4B-NB	7.19	1.41	1.35
13	b	817	CLA	C4B-NB	7.19	1.41	1.35
13	b	832	CLA	C4B-NB	7.19	1.41	1.35
13	a	802	CLA	C4B-NB	7.19	1.41	1.35
13	a	826	CLA	C4B-NB	7.18	1.41	1.35
13	b	825	CLA	C4B-NB	7.15	1.41	1.35
13	a	813	CLA	C4B-NB	7.14	1.41	1.35
13	b	829	CLA	C4B-NB	7.14	1.41	1.35
13	a	815	CLA	C4B-NB	7.14	1.41	1.35
13	b	818	CLA	C4B-NB	7.14	1.41	1.35
13	b	837	CLA	C4B-NB	7.13	1.41	1.35
13	a	821	CLA	C4B-NB	7.12	1.41	1.35
13	b	806	CLA	C4B-NB	7.12	1.41	1.35
13	b	804	CLA	C4B-NB	7.12	1.41	1.35
13	b	835	CLA	C4B-NB	7.11	1.41	1.35
13	b	820	CLA	C4B-NB	7.11	1.41	1.35
13	b	826	CLA	C4B-NB	7.10	1.41	1.35
13	a	827	CLA	C4B-NB	7.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	824	CLA	C4B-NB	7.09	1.41	1.35
13	a	837	CLA	C4B-NB	6.98	1.41	1.35
20	m	101	ECH	C14-C13	4.10	1.41	1.35
20	m	101	ECH	C17-C18	4.10	1.41	1.35
20	m	101	ECH	C21-C22	4.10	1.41	1.35
13	b	818	CLA	C1D-ND	4.07	1.42	1.37
20	m	101	ECH	C10-C9	4.04	1.41	1.35
20	b	846	ECH	C21-C22	4.02	1.41	1.35
13	a	828	CLA	C1D-ND	4.02	1.42	1.37
22	f	205	ZEX	C34-C33	4.00	1.41	1.35
22	f	205	ZEX	C30-C29	3.98	1.41	1.35
20	b	846	ECH	C17-C18	3.97	1.41	1.35
13	b	814	CLA	C1D-ND	3.94	1.42	1.37
20	b	846	ECH	C10-C9	3.93	1.41	1.35
13	b	828	CLA	C1D-ND	3.92	1.42	1.37
22	b	854	ZEX	C30-C29	3.92	1.41	1.35
13	b	835	CLA	C1D-ND	3.91	1.42	1.37
18	a	856	45D	C37-C35	3.91	1.41	1.35
13	a	836	CLA	C1D-ND	3.91	1.42	1.37
13	a	816	CLA	C1D-ND	3.91	1.42	1.37
22	f	205	ZEX	C14-C13	3.90	1.41	1.35
13	l	1501	CLA	C1D-ND	3.90	1.42	1.37
18	a	856	45D	C38-C36	3.89	1.40	1.35
13	a	824	CLA	C1D-ND	3.89	1.42	1.37
13	b	831	CLA	C1D-ND	3.89	1.42	1.37
13	a	834	CLA	C1D-ND	3.88	1.42	1.37
22	b	854	ZEX	C14-C13	3.88	1.40	1.35
20	b	846	ECH	C14-C13	3.88	1.40	1.35
13	a	839	CLA	C1D-ND	3.88	1.42	1.37
13	a	818	CLA	C1D-ND	3.87	1.42	1.37
13	f	203	CLA	C1D-ND	3.87	1.42	1.37
13	a	802	CLA	C1D-ND	3.86	1.42	1.37
22	b	854	ZEX	C34-C33	3.86	1.40	1.35
13	k	4003	CLA	C1D-ND	3.86	1.42	1.37
13	j	103	CLA	C1D-ND	3.85	1.42	1.37
13	a	813	CLA	C1D-ND	3.85	1.42	1.37
13	b	822	CLA	C1D-ND	3.84	1.42	1.37
13	b	821	CLA	C1D-ND	3.84	1.42	1.37
13	b	827	CLA	C1D-ND	3.84	1.42	1.37
22	f	205	ZEX	C10-C9	3.84	1.40	1.35
13	b	803	CLA	C1D-ND	3.83	1.42	1.37
13	j	104	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	819	CLA	C1D-ND	3.82	1.42	1.37
13	b	837	CLA	C1D-ND	3.82	1.42	1.37
13	a	825	CLA	C1D-ND	3.82	1.42	1.37
13	b	811	CLA	C1D-ND	3.81	1.42	1.37
13	f	204	CLA	C1D-ND	3.81	1.42	1.37
13	k	4002	CLA	C1D-ND	3.81	1.42	1.37
18	a	856	45D	C30-C26	3.81	1.40	1.35
13	a	837	CLA	C1D-ND	3.81	1.42	1.37
13	a	833	CLA	C1D-ND	3.81	1.42	1.37
13	a	820	CLA	C1D-ND	3.81	1.42	1.37
18	a	856	45D	C29-C25	3.80	1.40	1.35
12	a	801	CL0	C1D-ND	3.80	1.42	1.37
13	a	838	CLA	C1D-ND	3.80	1.42	1.37
13	b	801	CLA	C1D-ND	3.80	1.42	1.37
13	b	808	CLA	C1D-ND	3.80	1.42	1.37
13	a	821	CLA	C1D-ND	3.80	1.42	1.37
13	a	827	CLA	C1D-ND	3.80	1.42	1.37
13	a	841	CLA	C1D-ND	3.80	1.42	1.37
13	a	840	CLA	C1D-ND	3.79	1.42	1.37
13	b	842	CLA	C1D-ND	3.79	1.42	1.37
13	a	812	CLA	C1D-ND	3.79	1.42	1.37
13	a	855	CLA	C1D-ND	3.79	1.42	1.37
13	b	807	CLA	C1D-ND	3.79	1.42	1.37
13	b	834	CLA	C1D-ND	3.79	1.42	1.37
13	a	823	CLA	C1D-ND	3.79	1.42	1.37
13	b	824	CLA	C1D-ND	3.79	1.42	1.37
13	f	201	CLA	C1D-ND	3.79	1.42	1.37
13	b	815	CLA	C1D-ND	3.79	1.42	1.37
13	b	817	CLA	C1D-ND	3.79	1.42	1.37
13	b	836	CLA	C1D-ND	3.78	1.42	1.37
13	a	835	CLA	C1D-ND	3.78	1.42	1.37
13	b	839	CLA	C1D-ND	3.78	1.42	1.37
13	a	817	CLA	C1D-ND	3.78	1.42	1.37
13	a	805	CLA	C1D-ND	3.78	1.42	1.37
13	b	838	CLA	C1D-ND	3.78	1.42	1.37
13	b	806	CLA	C1D-ND	3.77	1.42	1.37
13	a	822	CLA	C1D-ND	3.77	1.42	1.37
13	b	810	CLA	C1D-ND	3.77	1.42	1.37
13	b	820	CLA	C1D-ND	3.77	1.42	1.37
13	l	1503	CLA	C1D-ND	3.76	1.42	1.37
13	a	814	CLA	C1D-ND	3.76	1.42	1.37
13	a	809	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	810	CLA	C1D-ND	3.76	1.42	1.37
13	a	811	CLA	C1D-ND	3.76	1.42	1.37
13	b	825	CLA	C1D-ND	3.75	1.42	1.37
13	a	815	CLA	C1D-ND	3.75	1.42	1.37
13	a	804	CLA	C1D-ND	3.75	1.42	1.37
13	b	826	CLA	C1D-ND	3.75	1.42	1.37
13	a	842	CLA	C1D-ND	3.74	1.42	1.37
13	b	833	CLA	C1D-ND	3.74	1.42	1.37
13	a	803	CLA	C1D-ND	3.73	1.42	1.37
13	a	806	CLA	C1D-ND	3.73	1.42	1.37
13	a	830	CLA	C1D-ND	3.73	1.42	1.37
13	a	832	CLA	C1D-ND	3.73	1.42	1.37
13	b	832	CLA	C1D-ND	3.73	1.42	1.37
13	b	823	CLA	C1D-ND	3.73	1.42	1.37
13	a	807	CLA	C1D-ND	3.72	1.42	1.37
21	b	853	EQ3	C21-C22	3.71	1.40	1.35
13	b	805	CLA	C1D-ND	3.71	1.42	1.37
21	b	853	EQ3	C17-C18	3.71	1.40	1.35
15	b	844	BCR	C1-C6	-3.70	1.48	1.53
13	b	830	CLA	C1D-ND	3.70	1.42	1.37
13	b	840	CLA	C1D-ND	3.70	1.42	1.37
22	b	854	ZEX	C10-C9	3.70	1.40	1.35
13	b	841	CLA	C1D-ND	3.70	1.42	1.37
13	a	808	CLA	C1D-ND	3.70	1.42	1.37
13	a	829	CLA	C1D-ND	3.70	1.42	1.37
13	b	812	CLA	C1D-ND	3.69	1.42	1.37
13	a	819	CLA	C1D-ND	3.69	1.42	1.37
13	a	854	CLA	C1D-ND	3.69	1.42	1.37
13	b	816	CLA	C1D-ND	3.67	1.42	1.37
15	j	105	BCR	C1-C6	-3.67	1.48	1.53
13	k	4004	CLA	C1D-ND	3.67	1.42	1.37
13	b	813	CLA	C1D-ND	3.67	1.42	1.37
13	b	804	CLA	C1D-ND	3.66	1.42	1.37
13	b	829	CLA	C1D-ND	3.66	1.42	1.37
15	k	4001	BCR	C1-C6	-3.66	1.48	1.53
15	a	847	BCR	C1-C6	-3.65	1.48	1.53
13	a	831	CLA	C1D-ND	3.65	1.42	1.37
21	b	853	EQ3	C14-C13	3.64	1.40	1.35
13	b	809	CLA	C1D-ND	3.62	1.42	1.37
13	a	826	CLA	C1D-ND	3.56	1.42	1.37
21	b	853	EQ3	C10-C9	3.54	1.40	1.35
15	j	101	BCR	C1-C6	-3.54	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	1502	CLA	C1D-ND	3.53	1.42	1.37
15	a	846	BCR	C1-C6	-3.53	1.48	1.53
20	m	101	ECH	C25-C26	3.49	1.40	1.35
15	a	844	BCR	C1-C6	-3.48	1.49	1.53
15	a	848	BCR	C1-C6	-3.46	1.49	1.53
15	a	845	BCR	C1-C6	-3.46	1.49	1.53
15	f	202	BCR	C1-C6	-3.41	1.49	1.53
15	b	848	BCR	C30-C25	-3.37	1.49	1.53
15	b	845	BCR	C1-C6	-3.36	1.49	1.53
15	b	849	BCR	C1-C6	-3.32	1.49	1.53
13	b	805	CLA	CHC-C1C	3.29	1.43	1.35
15	a	844	BCR	C30-C25	-3.29	1.49	1.53
13	a	804	CLA	CHC-C1C	3.28	1.43	1.35
15	b	844	BCR	C30-C25	-3.27	1.49	1.53
15	j	105	BCR	C30-C25	-3.24	1.49	1.53
15	i	101	BCR	C30-C25	-3.22	1.49	1.53
15	i	102	BCR	C1-C6	-3.19	1.49	1.53
15	b	847	BCR	C1-C6	-3.18	1.49	1.53
13	a	808	CLA	CHC-C1C	3.18	1.43	1.35
15	i	101	BCR	C1-C6	-3.17	1.49	1.53
13	b	824	CLA	CHC-C1C	3.17	1.43	1.35
13	b	826	CLA	CHC-C1C	3.17	1.43	1.35
13	b	809	CLA	C4D-ND	-3.17	1.33	1.37
13	b	814	CLA	CHC-C1C	3.16	1.43	1.35
13	j	104	CLA	CHC-C1C	3.16	1.43	1.35
15	k	4005	BCR	C1-C6	-3.16	1.49	1.53
13	a	802	CLA	CHC-C1C	3.15	1.43	1.35
13	a	806	CLA	CHC-C1C	3.15	1.43	1.35
13	b	821	CLA	CHC-C1C	3.15	1.43	1.35
13	b	840	CLA	CHC-C1C	3.15	1.43	1.35
13	a	832	CLA	CHC-C1C	3.15	1.43	1.35
13	b	832	CLA	CHC-C1C	3.14	1.43	1.35
13	b	833	CLA	CHC-C1C	3.14	1.43	1.35
13	a	810	CLA	CHC-C1C	3.14	1.43	1.35
13	a	814	CLA	CHC-C1C	3.14	1.43	1.35
13	b	806	CLA	CHC-C1C	3.13	1.43	1.35
13	a	826	CLA	CHC-C1C	3.13	1.43	1.35
15	k	4001	BCR	C30-C25	-3.13	1.49	1.53
15	b	848	BCR	C1-C6	-3.13	1.49	1.53
13	b	825	CLA	CHC-C1C	3.13	1.43	1.35
13	a	828	CLA	CHC-C1C	3.13	1.43	1.35
15	b	849	BCR	C30-C25	-3.13	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	204	CLA	CHC-C1C	3.13	1.43	1.35
13	b	823	CLA	CHC-C1C	3.13	1.43	1.35
13	b	807	CLA	CHC-C1C	3.12	1.43	1.35
13	b	820	CLA	CHC-C1C	3.12	1.43	1.35
13	a	854	CLA	C4D-ND	-3.12	1.33	1.37
13	b	807	CLA	C4D-ND	-3.12	1.33	1.37
15	f	202	BCR	C30-C25	-3.12	1.49	1.53
13	j	103	CLA	CHC-C1C	3.12	1.43	1.35
13	a	838	CLA	CHC-C1C	3.12	1.43	1.35
13	f	201	CLA	CHC-C1C	3.12	1.43	1.35
13	b	835	CLA	CHC-C1C	3.11	1.42	1.35
15	j	101	BCR	C30-C25	-3.11	1.49	1.53
13	b	801	CLA	CHC-C1C	3.11	1.42	1.35
13	b	806	CLA	C4D-ND	-3.11	1.33	1.37
13	l	1501	CLA	CHC-C1C	3.11	1.42	1.35
13	a	835	CLA	CHC-C1C	3.11	1.42	1.35
13	a	807	CLA	CHC-C1C	3.11	1.42	1.35
13	b	815	CLA	CHC-C1C	3.11	1.42	1.35
13	a	818	CLA	CHC-C1C	3.11	1.42	1.35
13	k	4002	CLA	CHC-C1C	3.11	1.42	1.35
13	a	822	CLA	CHC-C1C	3.11	1.42	1.35
13	a	813	CLA	CHC-C1C	3.11	1.42	1.35
13	a	841	CLA	CHC-C1C	3.11	1.42	1.35
13	b	812	CLA	C4D-ND	-3.11	1.33	1.37
13	a	842	CLA	CHC-C1C	3.11	1.42	1.35
13	a	809	CLA	CHC-C1C	3.11	1.42	1.35
13	b	842	CLA	CHC-C1C	3.11	1.42	1.35
13	a	827	CLA	CHC-C1C	3.10	1.42	1.35
13	b	837	CLA	CHC-C1C	3.10	1.42	1.35
13	b	803	CLA	CHC-C1C	3.10	1.42	1.35
13	a	821	CLA	CHC-C1C	3.10	1.42	1.35
13	b	827	CLA	CHC-C1C	3.10	1.42	1.35
13	b	822	CLA	CHC-C1C	3.10	1.42	1.35
13	a	811	CLA	CHC-C1C	3.10	1.42	1.35
13	a	812	CLA	CHC-C1C	3.10	1.42	1.35
13	b	839	CLA	C4D-ND	-3.10	1.33	1.37
15	b	845	BCR	C30-C25	-3.09	1.49	1.53
13	a	817	CLA	CHC-C1C	3.09	1.42	1.35
13	b	817	CLA	CHC-C1C	3.09	1.42	1.35
13	b	839	CLA	CHC-C1C	3.09	1.42	1.35
20	b	846	ECH	C23-C22	-3.09	1.39	1.45
13	b	830	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	834	CLA	CHC-C1C	3.09	1.42	1.35
13	a	829	CLA	CHC-C1C	3.09	1.42	1.35
13	a	833	CLA	CHC-C1C	3.09	1.42	1.35
13	b	836	CLA	CHC-C1C	3.09	1.42	1.35
13	b	804	CLA	CHC-C1C	3.09	1.42	1.35
13	a	806	CLA	C4D-ND	-3.09	1.33	1.37
13	a	855	CLA	CHC-C1C	3.09	1.42	1.35
13	l	1503	CLA	CHC-C1C	3.08	1.42	1.35
13	a	803	CLA	CHC-C1C	3.08	1.42	1.35
13	b	828	CLA	CHC-C1C	3.08	1.42	1.35
13	a	838	CLA	C4D-ND	-3.08	1.33	1.37
13	b	831	CLA	C4D-ND	-3.08	1.33	1.37
13	b	816	CLA	CHC-C1C	3.08	1.42	1.35
13	a	805	CLA	CHC-C1C	3.08	1.42	1.35
13	a	820	CLA	CHC-C1C	3.08	1.42	1.35
13	k	4003	CLA	CHC-C1C	3.08	1.42	1.35
13	b	812	CLA	CHC-C1C	3.08	1.42	1.35
15	a	846	BCR	C30-C25	-3.07	1.49	1.53
15	k	4005	BCR	C30-C25	-3.07	1.49	1.53
13	a	819	CLA	CHC-C1C	3.07	1.42	1.35
13	f	203	CLA	C4D-ND	-3.07	1.33	1.37
13	a	834	CLA	CHC-C1C	3.07	1.42	1.35
13	b	811	CLA	CHC-C1C	3.07	1.42	1.35
13	b	829	CLA	CHC-C1C	3.07	1.42	1.35
13	a	824	CLA	CHC-C1C	3.07	1.42	1.35
13	b	831	CLA	CHC-C1C	3.07	1.42	1.35
13	b	824	CLA	C4D-ND	-3.07	1.33	1.37
13	a	827	CLA	C4D-ND	-3.07	1.33	1.37
13	a	808	CLA	C4D-ND	-3.07	1.33	1.37
13	f	203	CLA	CHC-C1C	3.06	1.42	1.35
13	a	803	CLA	C4D-ND	-3.06	1.33	1.37
13	a	815	CLA	CHC-C1C	3.06	1.42	1.35
13	b	820	CLA	C4D-ND	-3.06	1.33	1.37
13	b	840	CLA	C4D-ND	-3.06	1.33	1.37
13	a	837	CLA	C4D-ND	-3.06	1.33	1.37
13	a	816	CLA	CHC-C1C	3.05	1.42	1.35
13	b	838	CLA	CHC-C1C	3.05	1.42	1.35
13	b	838	CLA	C4D-ND	-3.05	1.33	1.37
13	a	840	CLA	CHC-C1C	3.05	1.42	1.35
13	b	819	CLA	CHC-C1C	3.05	1.42	1.35
13	a	819	CLA	C4D-ND	-3.05	1.33	1.37
12	a	801	CL0	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	829	CLA	C4D-ND	-3.05	1.33	1.37
13	a	831	CLA	C4D-ND	-3.04	1.33	1.37
13	b	810	CLA	CHC-C1C	3.04	1.42	1.35
13	a	830	CLA	CHC-C1C	3.04	1.42	1.35
13	b	813	CLA	CHC-C1C	3.04	1.42	1.35
13	a	831	CLA	CHC-C1C	3.04	1.42	1.35
13	k	4004	CLA	CHC-C1C	3.03	1.42	1.35
13	a	836	CLA	CHC-C1C	3.03	1.42	1.35
13	b	809	CLA	CHC-C1C	3.03	1.42	1.35
13	b	811	CLA	C4D-ND	-3.03	1.33	1.37
13	b	826	CLA	C4D-ND	-3.03	1.33	1.37
13	a	823	CLA	CHC-C1C	3.03	1.42	1.35
13	l	1502	CLA	CHC-C1C	3.03	1.42	1.35
13	b	827	CLA	C4D-ND	-3.02	1.33	1.37
13	b	835	CLA	C4D-ND	-3.02	1.33	1.37
13	a	854	CLA	CHC-C1C	3.02	1.42	1.35
13	b	842	CLA	C4D-ND	-3.01	1.33	1.37
13	a	825	CLA	CHC-C1C	3.01	1.42	1.35
13	a	809	CLA	C4D-ND	-3.01	1.33	1.37
13	a	807	CLA	C4D-ND	-3.01	1.33	1.37
13	b	808	CLA	C4D-ND	-3.00	1.33	1.37
13	l	1503	CLA	C4D-ND	-3.00	1.33	1.37
13	a	804	CLA	C4D-ND	-3.00	1.33	1.37
13	a	821	CLA	C4D-ND	-3.00	1.33	1.37
13	a	826	CLA	C4D-ND	-3.00	1.33	1.37
13	b	808	CLA	CHC-C1C	3.00	1.42	1.35
13	a	839	CLA	CHC-C1C	2.99	1.42	1.35
15	b	847	BCR	C30-C25	-2.99	1.49	1.53
13	b	813	CLA	C4D-ND	-2.99	1.33	1.37
13	b	825	CLA	C4D-ND	-2.98	1.33	1.37
13	b	801	CLA	C4D-ND	-2.98	1.33	1.37
18	a	856	45D	C24-C26	-2.98	1.39	1.45
13	a	805	CLA	C4D-ND	-2.98	1.33	1.37
13	a	855	CLA	C4D-ND	-2.98	1.33	1.37
13	b	833	CLA	C4D-ND	-2.98	1.33	1.37
13	b	841	CLA	C4D-ND	-2.98	1.33	1.37
13	a	822	CLA	C4D-ND	-2.98	1.33	1.37
13	b	821	CLA	C4D-ND	-2.98	1.33	1.37
13	a	836	CLA	C4D-ND	-2.97	1.33	1.37
13	b	805	CLA	C4D-ND	-2.97	1.33	1.37
13	b	818	CLA	CHC-C1C	2.97	1.42	1.35
13	a	829	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	834	CLA	C4D-ND	-2.97	1.33	1.37
13	b	832	CLA	C4D-ND	-2.97	1.33	1.37
21	b	853	EQ3	C23-C22	-2.96	1.39	1.45
13	b	841	CLA	CHC-C1C	2.96	1.42	1.35
13	b	818	CLA	C4D-ND	-2.96	1.33	1.37
13	a	841	CLA	C4D-ND	-2.96	1.33	1.37
13	b	810	CLA	C4D-ND	-2.96	1.33	1.37
13	a	835	CLA	C4D-ND	-2.96	1.33	1.37
13	a	837	CLA	CHC-C1C	2.96	1.42	1.35
13	a	842	CLA	C4D-ND	-2.96	1.33	1.37
13	b	816	CLA	C4D-ND	-2.96	1.33	1.37
13	a	811	CLA	C4D-ND	-2.95	1.33	1.37
13	a	816	CLA	C4D-ND	-2.95	1.33	1.37
13	k	4003	CLA	C4D-ND	-2.95	1.33	1.37
13	a	814	CLA	C4D-ND	-2.94	1.33	1.37
13	a	812	CLA	C4D-ND	-2.94	1.33	1.37
12	a	801	CL0	C4D-ND	-2.94	1.33	1.37
13	a	815	CLA	C4D-ND	-2.94	1.33	1.37
13	a	839	CLA	C4D-ND	-2.94	1.33	1.37
13	b	836	CLA	C4D-ND	-2.94	1.33	1.37
15	a	845	BCR	C30-C25	-2.93	1.49	1.53
13	b	819	CLA	C4D-ND	-2.93	1.33	1.37
21	b	853	EQ3	C8-C9	-2.93	1.39	1.45
13	b	837	CLA	C4D-ND	-2.92	1.33	1.37
13	a	832	CLA	C4D-ND	-2.92	1.33	1.37
13	a	813	CLA	C4D-ND	-2.92	1.33	1.37
13	b	822	CLA	C4D-ND	-2.92	1.33	1.37
13	b	814	CLA	C4D-ND	-2.92	1.33	1.37
13	b	823	CLA	C4D-ND	-2.92	1.33	1.37
22	b	854	ZEX	C8-C9	-2.92	1.39	1.45
13	k	4002	CLA	C4D-ND	-2.91	1.33	1.37
13	a	833	CLA	C4D-ND	-2.91	1.33	1.37
18	a	856	45D	C23-C25	-2.91	1.39	1.45
13	b	803	CLA	C4D-ND	-2.91	1.33	1.37
13	l	1502	CLA	C4D-ND	-2.91	1.33	1.37
13	f	201	CLA	C4D-ND	-2.90	1.33	1.37
13	a	817	CLA	C4D-ND	-2.89	1.33	1.37
13	a	810	CLA	C4D-ND	-2.89	1.33	1.37
13	b	804	CLA	C4D-ND	-2.89	1.33	1.37
13	b	828	CLA	C4D-ND	-2.89	1.33	1.37
13	a	825	CLA	C4D-ND	-2.88	1.33	1.37
13	a	824	CLA	C4D-ND	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	818	CLA	C4D-ND	-2.88	1.33	1.37
13	b	815	CLA	C4D-ND	-2.88	1.33	1.37
13	f	204	CLA	C4D-ND	-2.88	1.33	1.37
13	b	830	CLA	C4D-ND	-2.87	1.33	1.37
13	a	830	CLA	C4D-ND	-2.87	1.33	1.37
13	j	103	CLA	C4D-ND	-2.87	1.33	1.37
13	a	840	CLA	C4D-ND	-2.87	1.33	1.37
13	a	820	CLA	C4D-ND	-2.87	1.33	1.37
13	k	4004	CLA	C4D-ND	-2.85	1.33	1.37
13	b	817	CLA	C4D-ND	-2.85	1.33	1.37
15	a	847	BCR	C30-C25	-2.84	1.49	1.53
20	m	101	ECH	C23-C22	-2.81	1.39	1.45
13	a	823	CLA	C4D-ND	-2.81	1.33	1.37
13	j	104	CLA	C4D-ND	-2.80	1.33	1.37
22	f	205	ZEX	C8-C9	-2.80	1.39	1.45
13	a	834	CLA	C4D-ND	-2.79	1.33	1.37
22	b	854	ZEX	C28-C29	-2.76	1.40	1.45
13	a	802	CLA	C4D-ND	-2.76	1.33	1.37
13	a	828	CLA	C4D-ND	-2.75	1.33	1.37
20	b	846	ECH	C8-C9	-2.74	1.40	1.45
22	f	205	ZEX	C28-C29	-2.72	1.40	1.45
20	m	101	ECH	C8-C9	-2.72	1.40	1.45
13	b	841	CLA	CMB-C2B	-2.71	1.46	1.51
13	l	1501	CLA	C4D-ND	-2.70	1.34	1.37
18	a	856	45D	C08-C16	2.68	1.39	1.35
23	j	102	LMT	O3'-C3'	-2.63	1.36	1.43
15	i	102	BCR	C30-C25	-2.60	1.50	1.53
13	a	830	CLA	CMB-C2B	-2.59	1.46	1.51
13	b	816	CLA	CMB-C2B	-2.58	1.46	1.51
13	b	830	CLA	CMB-C2B	-2.56	1.46	1.51
13	a	812	CLA	CMB-C2B	-2.55	1.46	1.51
13	b	813	CLA	CMB-C2B	-2.54	1.46	1.51
13	b	836	CLA	CMB-C2B	-2.52	1.46	1.51
13	a	833	CLA	CMB-C2B	-2.52	1.46	1.51
13	a	819	CLA	CMB-C2B	-2.52	1.46	1.51
13	a	821	CLA	CMB-C2B	-2.51	1.46	1.51
13	a	835	CLA	CMB-C2B	-2.51	1.46	1.51
13	b	818	CLA	CMB-C2B	-2.51	1.46	1.51
13	a	841	CLA	CMB-C2B	-2.50	1.46	1.51
13	b	810	CLA	CMB-C2B	-2.49	1.46	1.51
13	a	855	CLA	CMB-C2B	-2.49	1.46	1.51
13	b	809	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	831	CLA	CMB-C2B	-2.48	1.46	1.51
13	b	820	CLA	CMB-C2B	-2.48	1.46	1.51
13	a	818	CLA	CMB-C2B	-2.47	1.46	1.51
12	a	801	CL0	CMB-C2B	-2.47	1.46	1.51
13	l	1502	CLA	CMB-C2B	-2.47	1.46	1.51
21	b	853	EQ3	C25-C26	2.47	1.39	1.35
13	b	839	CLA	CMB-C2B	-2.47	1.46	1.51
13	b	803	CLA	CMB-C2B	-2.47	1.46	1.51
13	a	803	CLA	CMB-C2B	-2.47	1.46	1.51
13	f	201	CLA	CMB-C2B	-2.47	1.46	1.51
13	b	821	CLA	CMB-C2B	-2.46	1.46	1.51
13	b	819	CLA	CMB-C2B	-2.46	1.46	1.51
13	a	834	CLA	CMB-C2B	-2.46	1.46	1.51
13	k	4003	CLA	CMB-C2B	-2.46	1.46	1.51
13	a	823	CLA	CMB-C2B	-2.46	1.46	1.51
13	a	816	CLA	CMB-C2B	-2.45	1.46	1.51
13	b	840	CLA	CMB-C2B	-2.45	1.46	1.51
21	b	853	EQ3	C19-C18	-2.45	1.40	1.45
13	a	802	CLA	CMB-C2B	-2.45	1.46	1.51
13	b	834	CLA	CMB-C2B	-2.44	1.46	1.51
13	b	826	CLA	CMB-C2B	-2.44	1.46	1.51
20	b	846	ECH	C19-C18	-2.44	1.40	1.45
13	b	833	CLA	CMB-C2B	-2.44	1.46	1.51
13	a	804	CLA	CMB-C2B	-2.44	1.46	1.51
13	b	807	CLA	CMB-C2B	-2.44	1.46	1.51
13	a	827	CLA	CMB-C2B	-2.44	1.46	1.51
13	a	826	CLA	CMB-C2B	-2.44	1.46	1.51
13	b	831	CLA	CMB-C2B	-2.43	1.46	1.51
13	a	838	CLA	CMB-C2B	-2.43	1.46	1.51
13	a	840	CLA	CMB-C2B	-2.43	1.46	1.51
13	a	825	CLA	CMB-C2B	-2.43	1.46	1.51
13	b	824	CLA	CMB-C2B	-2.43	1.46	1.51
13	b	825	CLA	CMB-C2B	-2.43	1.46	1.51
13	a	837	CLA	CMB-C2B	-2.43	1.46	1.51
20	b	846	ECH	C12-C13	-2.43	1.40	1.45
13	a	854	CLA	CMB-C2B	-2.43	1.46	1.51
13	a	820	CLA	CMB-C2B	-2.43	1.46	1.51
13	b	808	CLA	CMB-C2B	-2.42	1.46	1.51
13	a	808	CLA	CMB-C2B	-2.42	1.46	1.51
13	a	817	CLA	CMB-C2B	-2.42	1.46	1.51
13	b	838	CLA	CMB-C2B	-2.42	1.46	1.51
13	b	814	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	823	CLA	CMB-C2B	-2.42	1.46	1.51
13	a	839	CLA	CMB-C2B	-2.42	1.46	1.51
13	b	832	CLA	CMB-C2B	-2.42	1.46	1.51
13	b	811	CLA	CMB-C2B	-2.41	1.46	1.51
13	k	4002	CLA	CMB-C2B	-2.41	1.46	1.51
13	b	835	CLA	CMB-C2B	-2.41	1.46	1.51
13	a	832	CLA	CMB-C2B	-2.41	1.46	1.51
21	b	853	EQ3	C12-C13	-2.41	1.40	1.45
13	a	806	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	854	ZEX	C32-C33	-2.41	1.40	1.45
13	f	204	CLA	CMB-C2B	-2.41	1.46	1.51
13	b	806	CLA	CMB-C2B	-2.40	1.46	1.51
13	a	836	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	854	ZEX	C12-C13	-2.40	1.40	1.45
13	a	822	CLA	CMB-C2B	-2.40	1.46	1.51
13	b	805	CLA	CMB-C2B	-2.40	1.46	1.51
13	a	842	CLA	CMB-C2B	-2.40	1.46	1.51
18	a	856	45D	C33-C35	-2.40	1.40	1.45
13	a	824	CLA	CMB-C2B	-2.40	1.46	1.51
13	b	804	CLA	CMB-C2B	-2.39	1.46	1.51
13	b	842	CLA	CMB-C2B	-2.39	1.46	1.51
13	f	203	CLA	CMB-C2B	-2.39	1.46	1.51
13	a	814	CLA	CMB-C2B	-2.39	1.46	1.51
13	b	801	CLA	CMB-C2B	-2.39	1.46	1.51
13	a	813	CLA	CMB-C2B	-2.39	1.46	1.51
23	j	102	LMT	O2B-C2B	-2.39	1.37	1.43
13	b	822	CLA	CMB-C2B	-2.38	1.46	1.51
13	b	837	CLA	CMB-C2B	-2.38	1.46	1.51
13	b	815	CLA	CMB-C2B	-2.38	1.46	1.51
13	b	812	CLA	CMB-C2B	-2.38	1.46	1.51
13	a	811	CLA	CMB-C2B	-2.38	1.46	1.51
13	l	1501	CLA	CMB-C2B	-2.37	1.46	1.51
13	a	815	CLA	CMB-C2B	-2.37	1.46	1.51
13	j	104	CLA	CMB-C2B	-2.37	1.46	1.51
13	a	805	CLA	CMB-C2B	-2.37	1.46	1.51
13	j	103	CLA	CMB-C2B	-2.37	1.46	1.51
13	b	817	CLA	CMB-C2B	-2.36	1.46	1.51
13	k	4004	CLA	CMB-C2B	-2.36	1.46	1.51
13	a	809	CLA	CMB-C2B	-2.36	1.46	1.51
16	a	849	LHG	O7-C5	-2.36	1.40	1.46
13	l	1503	CLA	CMB-C2B	-2.36	1.46	1.51
13	a	828	CLA	CMB-C2B	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	829	CLA	CMB-C2B	-2.36	1.46	1.51
13	a	807	CLA	CMB-C2B	-2.36	1.46	1.51
13	b	828	CLA	CMB-C2B	-2.35	1.46	1.51
13	b	829	CLA	CMB-C2B	-2.35	1.46	1.51
13	a	810	CLA	CMB-C2B	-2.34	1.46	1.51
13	b	827	CLA	CMB-C2B	-2.33	1.46	1.51
22	f	205	ZEX	C12-C13	-2.33	1.40	1.45
18	a	856	45D	C34-C36	-2.31	1.41	1.45
23	j	102	LMT	O3B-C3B	-2.29	1.37	1.43
23	j	102	LMT	O2'-C2'	-2.26	1.37	1.43
13	b	830	CLA	CMD-C2D	-2.26	1.46	1.50
20	m	101	ECH	C12-C13	-2.24	1.41	1.45
13	b	804	CLA	CMC-C2C	-2.23	1.46	1.50
22	f	205	ZEX	C32-C33	-2.21	1.41	1.45
13	a	809	CLA	CMD-C2D	-2.21	1.46	1.50
16	b	851	LHG	O7-C5	-2.20	1.41	1.46
13	a	827	CLA	CMC-C2C	-2.17	1.46	1.50
23	j	102	LMT	O4'-C4B	-2.16	1.37	1.43
13	b	829	CLA	CMD-C2D	-2.14	1.46	1.50
16	f	206	LHG	O7-C5	-2.14	1.41	1.46
13	b	824	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	831	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	827	CLA	CMC-C2C	-2.13	1.46	1.50
13	b	833	CLA	C3B-C2B	-2.12	1.37	1.40
20	m	101	ECH	C19-C18	-2.12	1.41	1.45
18	a	856	45D	C07-C15	2.12	1.38	1.35
13	a	802	CLA	CMC-C2C	-2.12	1.46	1.50
13	b	809	CLA	CMD-C2D	-2.11	1.46	1.50
13	a	805	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	815	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	809	CLA	CMC-C2C	-2.09	1.46	1.50
13	a	826	CLA	CMD-C2D	-2.09	1.46	1.50
13	b	810	CLA	CMD-C2D	-2.08	1.46	1.50
13	b	841	CLA	C3B-C2B	-2.08	1.37	1.40
16	a	851	LHG	O7-C5	-2.08	1.41	1.46
17	b	852	LMG	O7-C8	-2.08	1.41	1.46
13	b	803	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	830	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	837	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	201	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	829	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	813	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	841	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	816	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	806	CLA	CMD-C2D	-2.05	1.46	1.50
13	b	814	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	839	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	823	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	838	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	807	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	824	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	833	CLA	C3B-C2B	-2.04	1.37	1.40
12	a	801	CL0	CMD-C2D	-2.04	1.46	1.50
13	a	833	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	813	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	821	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	841	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	811	CLA	CMD-C2D	-2.04	1.46	1.50
13	k	4003	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	818	CLA	C3B-C2B	-2.03	1.37	1.40
13	b	812	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	832	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	818	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	825	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	832	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	808	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	836	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	820	CLA	CMD-C2D	-2.03	1.46	1.50
13	l	1502	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	802	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	808	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	826	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	820	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	817	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	840	CLA	CMD-C2D	-2.02	1.46	1.50
13	k	4002	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	838	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	835	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	803	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	833	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	835	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	811	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	812	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	818	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	823	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	819	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	825	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	813	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	839	CLA	C3B-C2B	-2.02	1.37	1.40
13	a	828	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	834	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	810	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	805	CLA	CMC-C2C	-2.01	1.46	1.50
13	l	1503	CLA	CMD-C2D	-2.01	1.46	1.50
13	b	837	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	854	CLA	CMD-C2D	-2.01	1.46	1.50
13	j	104	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	815	CLA	CMD-C2D	-2.01	1.46	1.50
13	b	827	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	827	CLA	CMD-C2D	-2.00	1.46	1.50
13	b	828	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	818	CLA	CMC-C2C	-2.00	1.46	1.50
13	b	819	CLA	CMD-C2D	-2.00	1.46	1.50
13	a	803	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	810	CLA	CMC-C2C	-2.00	1.46	1.50
13	l	1502	CLA	CMC-C2C	-2.00	1.46	1.50

All (948) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	846	ECH	C15-C16-C17	8.45	140.79	123.47
13	a	840	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	a	805	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	l	1502	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	b	806	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	b	838	CLA	C4A-NA-C1A	7.03	109.87	106.71
13	a	823	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	b	830	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	a	839	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	a	809	CLA	C4A-NA-C1A	6.98	109.85	106.71
13	a	825	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	a	837	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	a	817	CLA	C4A-NA-C1A	6.94	109.83	106.71
13	b	822	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	a	807	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	k	4004	CLA	C4A-NA-C1A	6.88	109.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	841	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	a	816	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	b	840	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	b	828	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	a	818	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	a	855	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	a	815	CLA	C4A-NA-C1A	6.83	109.78	106.71
13	b	808	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	b	823	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	l	1503	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	b	842	CLA	C4A-NA-C1A	6.80	109.76	106.71
13	f	201	CLA	C4A-NA-C1A	6.78	109.76	106.71
13	b	817	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	a	834	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	a	841	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	b	812	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	a	820	CLA	C4A-NA-C1A	6.76	109.75	106.71
13	a	835	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	a	806	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	a	824	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	b	835	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	a	828	CLA	C4A-NA-C1A	6.69	109.71	106.71
13	a	822	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	a	813	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	b	809	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	l	1501	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	a	827	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	a	838	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	b	839	CLA	C4A-NA-C1A	6.65	109.70	106.71
13	b	810	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	b	813	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	b	834	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	f	204	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	a	814	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	b	805	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	a	836	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	a	832	CLA	C4A-NA-C1A	6.58	109.67	106.71
13	b	825	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	a	831	CLA	C4A-NA-C1A	6.56	109.65	106.71
13	k	4002	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	b	836	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	b	814	CLA	C4A-NA-C1A	6.53	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	808	CLA	C4A-NA-C1A	6.51	109.63	106.71
13	a	803	CLA	C4A-NA-C1A	6.51	109.63	106.71
12	a	801	CL0	C4A-NA-C1A	6.51	109.63	106.71
13	b	811	CLA	C4A-NA-C1A	6.50	109.63	106.71
13	b	824	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	b	807	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	j	103	CLA	C4A-NA-C1A	6.47	109.61	106.71
13	a	811	CLA	C4A-NA-C1A	6.45	109.60	106.71
13	k	4003	CLA	C4A-NA-C1A	6.45	109.60	106.71
13	b	815	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	b	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	a	829	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	a	842	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	b	833	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	a	826	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	b	826	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	b	837	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	a	802	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	a	812	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	b	818	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	a	830	CLA	C4A-NA-C1A	6.38	109.57	106.71
13	a	821	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	b	821	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	b	827	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	b	831	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	b	819	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	a	804	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	b	816	CLA	C4A-NA-C1A	6.31	109.54	106.71
13	b	832	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	f	203	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	b	801	CLA	C4A-NA-C1A	6.17	109.48	106.71
13	a	833	CLA	C4A-NA-C1A	6.16	109.47	106.71
13	j	104	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	b	829	CLA	C4A-NA-C1A	6.05	109.42	106.71
13	a	810	CLA	C4A-NA-C1A	5.99	109.40	106.71
13	a	854	CLA	C4A-NA-C1A	5.84	109.33	106.71
13	a	819	CLA	C4A-NA-C1A	5.76	109.30	106.71
13	b	803	CLA	C4A-NA-C1A	5.49	109.17	106.71
13	b	804	CLA	C4A-NA-C1A	5.43	109.15	106.71
18	a	856	45D	C42-C41-C37	5.15	134.03	123.47
20	b	846	ECH	C12-C13-C14	5.02	126.65	118.94
20	m	101	ECH	C15-C16-C17	4.79	133.30	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	846	ECH	C19-C18-C17	4.71	126.17	118.94
22	f	205	ZEX	C35-C15-C14	4.48	132.64	123.47
20	b	846	ECH	C35-C13-C14	-4.44	116.70	122.92
13	b	830	CLA	CMB-C2B-C1B	-4.35	121.77	128.46
20	b	846	ECH	C36-C18-C17	-4.28	116.93	122.92
20	m	101	ECH	C37-C22-C21	-4.26	116.96	122.92
13	a	822	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
13	b	829	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
16	a	851	LHG	O4-P-O5	4.23	133.17	112.24
16	a	849	LHG	O4-P-O5	4.23	133.14	112.24
13	a	809	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
13	a	807	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
13	b	832	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
16	f	206	LHG	O4-P-O5	4.21	133.04	112.24
16	b	851	LHG	O4-P-O5	4.20	133.01	112.24
16	a	853	LHG	O4-P-O5	4.20	132.98	112.24
22	f	205	ZEX	C19-C9-C10	-4.19	117.05	122.92
13	b	837	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
13	b	801	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
13	b	806	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
22	f	205	ZEX	C39-C29-C30	-4.13	117.13	122.92
13	a	813	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
20	b	846	ECH	C24-C23-C22	-4.12	120.01	126.23
20	b	846	ECH	C1-C6-C5	-4.12	116.82	122.61
13	a	805	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
13	a	854	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
13	b	817	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
18	a	856	45D	C28-C26-C30	-4.10	117.18	122.92
13	a	815	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
13	a	821	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
22	b	854	ZEX	C19-C9-C10	-4.07	117.22	122.92
13	a	830	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
22	b	854	ZEX	C39-C29-C30	-4.07	117.23	122.92
13	a	819	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
20	m	101	ECH	C34-C9-C10	-4.06	117.23	122.92
13	a	828	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
13	a	814	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
13	l	1503	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
13	a	808	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
18	a	856	45D	C27-C25-C29	-4.02	117.29	122.92
13	a	855	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
13	b	827	CLA	CMB-C2B-C1B	-3.97	122.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	824	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
13	b	826	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
13	a	825	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
13	b	814	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
13	b	810	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
13	b	815	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
13	a	829	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
13	b	834	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
13	a	806	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
13	a	811	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
13	a	804	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
21	b	853	EQ3	C34-C9-C10	-3.86	117.52	122.92
13	a	802	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
21	b	853	EQ3	C37-C22-C21	-3.83	117.56	122.92
13	b	828	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
20	m	101	ECH	C23-C22-C21	3.82	124.80	118.94
13	a	810	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
13	b	805	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
20	m	101	ECH	C36-C18-C17	-3.79	117.61	122.92
13	l	1501	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
13	b	836	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
13	a	832	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
20	b	846	ECH	C34-C9-C10	-3.75	117.67	122.92
13	a	816	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
13	b	807	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
13	b	819	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
13	b	825	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
13	a	824	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
20	m	101	ECH	C19-C18-C17	3.73	124.66	118.94
13	a	837	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
13	k	4002	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
13	a	842	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
20	m	101	ECH	C1-C6-C5	-3.68	117.42	122.61
13	a	836	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
13	b	835	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
20	b	846	ECH	C10-C11-C12	3.67	134.68	123.22
13	b	829	CLA	CMB-C2B-C3B	3.67	131.55	124.68
13	b	842	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
13	b	822	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
13	b	801	CLA	CMB-C2B-C3B	3.64	131.50	124.68
20	b	846	ECH	C37-C22-C21	-3.63	117.84	122.92
13	a	822	CLA	CMB-C2B-C3B	3.61	131.44	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	854	CLA	CMB-C2B-C3B	3.61	131.43	124.68
13	a	809	CLA	CMB-C2B-C3B	3.60	131.42	124.68
22	b	854	ZEX	C35-C15-C14	3.60	130.84	123.47
13	a	828	CLA	CMB-C2B-C3B	3.59	131.39	124.68
13	b	830	CLA	CMB-C2B-C3B	3.58	131.38	124.68
13	a	807	CLA	CMB-C2B-C3B	3.58	131.38	124.68
13	b	832	CLA	CMB-C2B-C3B	3.58	131.38	124.68
13	b	838	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
13	b	837	CLA	CMB-C2B-C3B	3.57	131.36	124.68
13	b	804	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
13	j	104	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
13	b	812	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
13	a	830	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
13	b	831	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
13	b	820	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
13	k	4004	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
13	a	818	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
13	a	834	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
13	a	831	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
13	b	806	CLA	CMB-C2B-C3B	3.49	131.20	124.68
13	a	820	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
20	b	846	ECH	C15-C14-C13	3.48	132.28	127.31
13	a	817	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
13	a	826	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
13	a	815	CLA	CMB-C2B-C3B	3.48	131.19	124.68
13	b	817	CLA	CMB-C2B-C3B	3.48	131.19	124.68
13	a	813	CLA	CMB-C2B-C3B	3.47	131.17	124.68
13	a	805	CLA	CMB-C2B-C3B	3.47	131.17	124.68
13	f	203	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
13	b	811	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
13	a	808	CLA	CMB-C2B-C3B	3.45	131.13	124.68
13	b	814	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
13	a	840	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
13	l	1503	CLA	CMB-C2B-C3B	3.43	131.10	124.68
13	a	812	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
13	b	827	CLA	CMB-C2B-C3B	3.41	131.06	124.68
13	a	830	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
21	b	853	EQ3	C15-C16-C17	3.41	130.46	123.47
13	a	819	CLA	CMB-C2B-C3B	3.40	131.03	124.68
13	a	821	CLA	CMB-C2B-C3B	3.39	131.03	124.68
13	b	808	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	a	827	CLA	CMB-C2B-C1B	-3.38	123.26	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	1502	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
13	j	103	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
13	b	803	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
13	a	803	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
13	f	204	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
13	a	814	CLA	CMB-C2B-C3B	3.35	130.95	124.68
13	b	809	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
13	a	813	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
13	a	829	CLA	CMB-C2B-C3B	3.34	130.93	124.68
13	b	828	CLA	CMB-C2B-C3B	3.34	130.93	124.68
13	b	826	CLA	CMB-C2B-C3B	3.33	130.92	124.68
13	a	830	CLA	CMB-C2B-C3B	3.33	130.91	124.68
13	b	823	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
13	b	815	CLA	CMB-C2B-C3B	3.33	130.90	124.68
22	f	205	ZEX	C40-C33-C34	-3.32	118.28	122.92
13	b	830	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
13	b	813	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
13	b	840	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
13	a	810	CLA	CMB-C2B-C3B	3.30	130.85	124.68
21	b	853	EQ3	C35-C13-C14	-3.30	118.30	122.92
13	a	811	CLA	CMB-C2B-C3B	3.30	130.85	124.68
13	b	839	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
13	b	814	CLA	CMB-C2B-C3B	3.29	130.83	124.68
13	k	4004	CLA	CAC-C3C-C4C	3.29	129.07	124.81
15	b	847	BCR	C15-C16-C17	-3.28	116.75	123.47
13	a	806	CLA	CMB-C2B-C3B	3.28	130.82	124.68
20	m	101	ECH	C35-C13-C14	-3.28	118.33	122.92
13	b	824	CLA	CMB-C2B-C3B	3.28	130.81	124.68
13	a	825	CLA	CMB-C2B-C3B	3.28	130.81	124.68
13	b	816	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
13	b	821	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
13	a	814	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
13	k	4003	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
13	a	839	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
13	a	855	CLA	CMB-C2B-C3B	3.26	130.77	124.68
13	b	825	CLA	CMB-C2B-C3B	3.24	130.75	124.68
13	a	832	CLA	CMB-C2B-C3B	3.24	130.74	124.68
13	a	833	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
13	b	841	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
13	a	838	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
13	b	834	CLA	CMB-C2B-C3B	3.22	130.71	124.68
22	b	854	ZEX	C20-C13-C14	-3.22	118.42	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	854	ZEX	C27-C26-C25	-3.21	117.65	122.84
13	l	1501	CLA	CMB-C2B-C3B	3.21	130.69	124.68
13	a	824	CLA	CMB-C2B-C3B	3.21	130.69	124.68
13	b	837	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
13	a	831	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
13	b	833	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
21	b	853	EQ3	C16-C15-C14	3.19	130.01	123.47
13	a	804	CLA	CMB-C2B-C3B	3.19	130.64	124.68
13	a	834	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
13	a	835	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
13	a	823	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
13	a	842	CLA	CMB-C2B-C3B	3.18	130.63	124.68
13	b	805	CLA	CMB-C2B-C3B	3.18	130.63	124.68
13	a	837	CLA	CMB-C2B-C3B	3.18	130.63	124.68
13	a	825	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
13	a	836	CLA	CMB-C2B-C3B	3.17	130.62	124.68
13	b	819	CLA	CMB-C2B-C3B	3.17	130.62	124.68
21	b	853	EQ3	C36-C18-C17	-3.17	118.48	122.92
13	a	823	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
22	b	854	ZEX	C15-C35-C34	3.17	129.97	123.47
13	a	802	CLA	CMB-C2B-C3B	3.17	130.60	124.68
13	a	841	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
22	b	854	ZEX	C40-C33-C34	-3.16	118.49	122.92
13	b	810	CLA	CMB-C2B-C3B	3.16	130.59	124.68
13	f	201	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
13	a	816	CLA	CMB-C2B-C3B	3.15	130.57	124.68
13	b	835	CLA	CMB-C2B-C3B	3.14	130.55	124.68
13	b	842	CLA	CMB-C2B-C3B	3.11	130.51	124.68
22	f	205	ZEX	C20-C13-C14	-3.11	118.57	122.92
13	b	804	CLA	CMB-C2B-C3B	3.11	130.50	124.68
13	b	807	CLA	CMB-C2B-C3B	3.11	130.49	124.68
13	b	834	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
13	k	4002	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
13	k	4002	CLA	CMB-C2B-C3B	3.09	130.47	124.68
13	b	803	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
13	b	836	CLA	CMB-C2B-C3B	3.09	130.45	124.68
12	a	801	CL0	CMB-C2B-C1B	-3.09	123.72	128.46
13	a	818	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
13	b	822	CLA	CMB-C2B-C3B	3.07	130.42	124.68
13	b	812	CLA	CMB-C2B-C3B	3.07	130.42	124.68
13	b	838	CLA	CMB-C2B-C3B	3.07	130.41	124.68
13	b	820	CLA	CMB-C2B-C3B	3.06	130.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	846	ECH	C30-C25-C24	3.06	124.43	115.78
13	a	807	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
13	a	804	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	a	837	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	a	834	CLA	CMB-C2B-C3B	3.04	130.37	124.68
13	a	854	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
13	k	4004	CLA	CMB-C2B-C3B	3.02	130.32	124.68
13	j	104	CLA	CMB-C2B-C3B	3.01	130.32	124.68
13	b	805	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	a	802	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	b	818	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
13	a	818	CLA	CMB-C2B-C3B	3.01	130.31	124.68
13	b	804	CLA	CAC-C3C-C4C	3.00	128.71	124.81
22	f	205	ZEX	C15-C35-C34	3.00	129.62	123.47
13	a	808	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
13	a	826	CLA	CMB-C2B-C3B	3.00	130.29	124.68
13	b	808	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
18	a	856	45D	C40-C36-C38	-2.99	118.73	122.92
12	a	801	CL0	O2D-CGD-O1D	-2.99	117.99	123.84
13	b	803	CLA	CAA-CBA-CGA	-2.99	104.52	113.25
13	b	825	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	b	817	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
13	a	803	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
13	b	830	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	a	846	BCR	C15-C16-C17	-2.95	117.43	123.47
20	m	101	ECH	C16-C15-C14	2.94	129.50	123.47
13	b	818	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
13	b	801	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
13	b	838	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
22	f	205	ZEX	C32-C33-C34	2.93	123.44	118.94
13	a	838	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
18	a	856	45D	C39-C35-C37	-2.92	118.83	122.92
13	b	809	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
13	a	817	CLA	CMB-C2B-C3B	2.92	130.14	124.68
13	a	840	CLA	CMB-C2B-C3B	2.92	130.13	124.68
13	a	823	CLA	CHB-C4A-NA	2.92	128.54	124.51
13	a	839	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	f	203	CLA	CMB-C2B-C3B	2.91	130.13	124.68
20	m	101	ECH	C12-C13-C14	2.91	123.41	118.94
13	f	204	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	k	4004	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	a	819	CLA	O2D-CGD-O1D	-2.91	118.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	804	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
15	j	101	BCR	C15-C16-C17	-2.90	117.53	123.47
13	b	813	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
13	a	824	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	a	812	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	b	815	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	b	822	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
13	a	833	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	b	816	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	a	828	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	805	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	836	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	817	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
13	b	831	CLA	CMB-C2B-C3B	2.88	130.07	124.68
13	b	808	CLA	CMB-C2B-C3B	2.88	130.07	124.68
13	a	820	CLA	CMB-C2B-C3B	2.88	130.06	124.68
13	a	827	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	a	820	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	b	844	BCR	C33-C5-C6	-2.87	121.31	124.53
13	b	841	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	b	823	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	f	203	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	a	830	CLA	CHB-C4A-NA	2.86	128.47	124.51
13	a	831	CLA	CMB-C2B-C3B	2.86	130.03	124.68
15	a	847	BCR	C33-C5-C6	-2.86	121.32	124.53
13	b	821	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	a	826	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	a	842	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
21	b	853	EQ3	C12-C13-C14	2.85	123.32	118.94
13	b	839	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	b	829	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	l	1501	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	a	846	BCR	C15-C14-C13	-2.85	123.24	127.31
13	l	1502	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	b	803	CLA	CMB-C2B-C3B	2.85	130.01	124.68
13	b	811	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	b	819	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	b	806	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	a	827	CLA	CMB-C2B-C3B	2.84	129.99	124.68
13	a	840	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	b	801	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	b	840	CLA	O2D-CGD-O1D	-2.83	118.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	828	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	b	824	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	b	826	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	l	1502	CLA	CMB-C2B-C3B	2.82	129.95	124.68
13	a	854	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
13	a	835	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	b	842	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	a	830	CLA	O2D-CGD-CBD	2.81	116.27	111.27
13	l	1503	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	a	832	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	k	4003	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	b	814	CLA	O2D-CGD-CBD	2.81	116.26	111.27
23	j	102	LMT	C1'-O5'-C5'	-2.81	108.18	113.69
13	a	811	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	b	827	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	b	844	BCR	C15-C16-C17	-2.80	117.73	123.47
13	a	810	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
13	b	839	CLA	CMB-C2B-C3B	2.80	129.92	124.68
15	b	847	BCR	C15-C14-C13	-2.80	123.32	127.31
13	b	833	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	a	816	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	b	809	CLA	CMB-C2B-C3B	2.79	129.90	124.68
13	b	812	CLA	CHB-C4A-NA	2.78	128.36	124.51
13	a	809	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
13	f	204	CLA	CMB-C2B-C3B	2.78	129.88	124.68
13	b	831	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	b	836	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
13	f	201	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	b	854	ZEX	C12-C13-C14	2.77	123.19	118.94
13	a	841	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	a	815	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	j	104	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	b	812	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	b	850	LMG	O6-C1-O1	-2.76	103.43	109.97
20	b	846	ECH	C37-C22-C23	2.75	122.42	118.08
13	a	810	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	j	103	CLA	CMB-C2B-C3B	2.75	129.82	124.68
13	a	855	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	a	834	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	b	840	CLA	CMB-C2B-C3B	2.74	129.81	124.68
13	a	822	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
13	b	818	CLA	CHB-C4A-NA	2.73	128.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	810	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	f	205	ZEX	C27-C26-C25	-2.73	118.44	122.84
13	b	821	CLA	CMB-C2B-C3B	2.72	129.78	124.68
13	a	835	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	a	806	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	a	812	CLA	CMB-C2B-C3B	2.72	129.76	124.68
13	b	803	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
13	b	832	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	b	835	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	k	4001	BCR	C15-C14-C13	-2.71	123.44	127.31
13	a	835	CLA	CMB-C2B-C3B	2.71	129.74	124.68
13	a	805	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	k	4003	CLA	CMB-C2B-C3B	2.70	129.73	124.68
16	a	851	LHG	O8-C23-C24	2.70	120.38	111.91
13	a	833	CLA	CMB-C2B-C3B	2.69	129.72	124.68
13	j	103	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	a	810	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	b	830	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
13	b	806	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	j	105	BCR	C33-C5-C6	-2.69	121.51	124.53
15	b	844	BCR	C24-C23-C22	-2.68	122.19	126.23
18	a	856	45D	C03-C07-C19	2.68	123.35	115.78
13	a	803	CLA	CMB-C2B-C3B	2.67	129.68	124.68
13	b	820	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
13	a	813	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	k	4005	BCR	C15-C16-C17	-2.66	118.02	123.47
13	a	838	CLA	CMB-C2B-C3B	2.66	129.66	124.68
13	a	809	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	b	813	CLA	CMB-C2B-C3B	2.66	129.65	124.68
13	a	828	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
15	b	845	BCR	C33-C5-C6	-2.65	121.55	124.53
13	a	829	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
13	a	825	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	f	205	ZEX	C28-C29-C30	2.65	123.00	118.94
15	j	101	BCR	C15-C14-C13	-2.64	123.54	127.31
15	j	105	BCR	C15-C16-C17	-2.64	118.06	123.47
13	a	841	CLA	CMB-C2B-C3B	2.64	129.62	124.68
13	a	823	CLA	CMB-C2B-C3B	2.64	129.62	124.68
13	a	820	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	a	850	LMG	O6-C1-O1	-2.64	103.72	109.97
13	l	1501	CLA	C1-C2-C3	-2.64	122.49	126.75
13	b	825	CLA	CHB-C4A-NA	2.63	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	f	205	ZEX	C12-C13-C14	2.63	122.98	118.94
13	a	833	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
13	a	819	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
13	f	201	CLA	CMB-C2B-C3B	2.62	129.58	124.68
13	b	833	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	a	810	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
13	b	839	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
13	a	837	CLA	CHB-C4A-NA	2.62	128.14	124.51
15	a	848	BCR	C15-C16-C17	-2.62	118.11	123.47
16	a	853	LHG	O8-C23-C24	2.62	120.12	111.91
22	b	854	ZEX	C32-C33-C34	2.62	122.96	118.94
13	b	816	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	b	833	CLA	CMB-C2B-C3B	2.61	129.57	124.68
13	a	821	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	l	1502	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	a	824	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	l	1503	CLA	CHB-C4A-NA	2.60	128.11	124.51
16	f	206	LHG	O8-C23-C24	2.60	120.07	111.91
13	a	818	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	b	837	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	a	840	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	b	807	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
13	a	839	CLA	CHB-C4A-NA	2.59	128.10	124.51
21	b	853	EQ3	C37-C22-C23	2.59	122.16	118.08
13	f	204	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	k	4003	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	b	841	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
13	a	839	CLA	CMB-C2B-C3B	2.59	129.52	124.68
13	b	811	CLA	CMB-C2B-C3B	2.59	129.52	124.68
13	b	836	CLA	C1-C2-C3	-2.58	122.57	126.75
13	b	818	CLA	CMB-C2B-C3B	2.58	129.51	124.68
15	k	4001	BCR	C27-C26-C25	2.58	126.48	122.73
13	b	821	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	f	203	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
13	b	842	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	a	816	CLA	CHB-C4A-NA	2.58	128.07	124.51
13	b	823	CLA	CHB-C4A-NA	2.58	128.07	124.51
13	k	4004	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	b	807	CLA	CHB-C4A-NA	2.56	128.06	124.51
13	k	4002	CLA	CHB-C4A-NA	2.56	128.06	124.51
13	a	832	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	a	842	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	823	CLA	CMB-C2B-C3B	2.56	129.47	124.68
21	b	853	EQ3	C19-C18-C17	2.56	122.87	118.94
13	a	817	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	b	814	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	b	853	EQ3	C24-C23-C22	2.56	130.10	126.23
13	b	816	CLA	CMB-C2B-C3B	2.56	129.46	124.68
20	m	101	ECH	C21-C20-C19	2.56	131.19	123.22
15	k	4001	BCR	C11-C10-C9	-2.56	123.66	127.31
13	a	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	a	849	LHG	O8-C23-C24	2.55	119.91	111.91
15	b	847	BCR	C2-C1-C6	2.55	114.41	110.48
12	a	801	CL0	CMB-C2B-C3B	2.55	129.45	124.68
16	b	851	LHG	O8-C23-C24	2.55	119.91	111.91
15	b	844	BCR	C27-C26-C25	2.55	126.43	122.73
13	b	835	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	a	807	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	a	821	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	b	840	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	b	801	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
13	a	842	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
13	f	201	CLA	CHB-C4A-NA	2.53	128.02	124.51
15	b	845	BCR	C15-C16-C17	-2.53	118.29	123.47
13	j	103	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
13	b	829	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
17	a	852	LMG	O6-C1-O1	-2.52	104.00	109.97
13	a	808	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	l	1501	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	a	841	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	b	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	b	850	LMG	O1-C7-C8	-2.51	104.84	110.90
13	b	809	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
13	a	815	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	b	808	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
13	a	827	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	a	801	CL0	C1B-CHB-C4A	-2.50	125.16	130.12
13	a	840	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	k	4001	BCR	C33-C5-C6	-2.50	121.72	124.53
22	b	854	ZEX	C39-C29-C28	2.50	122.02	118.08
13	b	815	CLA	CHB-C4A-NA	2.50	127.97	124.51
15	i	102	BCR	C2-C1-C6	2.50	114.32	110.48
13	a	811	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	a	855	CLA	CHB-C4A-NA	2.49	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	806	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
13	a	817	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
15	i	101	BCR	C15-C16-C17	-2.48	118.39	123.47
13	b	833	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
13	a	822	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	b	828	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
15	a	848	BCR	C33-C5-C6	-2.48	121.75	124.53
13	a	830	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	b	805	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	a	831	CLA	O2D-CGD-CBD	2.48	115.67	111.27
13	f	203	CLA	C1-C2-C3	-2.48	122.75	126.75
15	j	101	BCR	C33-C5-C6	-2.48	121.75	124.53
13	b	838	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
13	b	840	CLA	C1-C2-C3	-2.47	121.76	126.04
13	a	838	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	b	827	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
15	j	105	BCR	C27-C26-C25	2.47	126.31	122.73
13	a	836	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
13	a	826	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
15	b	844	BCR	C15-C14-C13	-2.46	123.79	127.31
13	b	841	CLA	CMB-C2B-C3B	2.46	129.28	124.68
13	b	813	CLA	CHB-C4A-NA	2.46	127.92	124.51
15	a	844	BCR	C33-C5-C6	-2.46	121.77	124.53
13	b	828	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	a	848	BCR	C15-C14-C13	-2.46	123.80	127.31
15	k	4005	BCR	C2-C1-C6	2.46	114.26	110.48
13	b	832	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	a	845	BCR	C33-C5-C6	-2.46	121.77	124.53
13	b	822	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	b	848	BCR	C27-C26-C25	2.45	126.29	122.73
13	b	804	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
16	a	849	LHG	C11-C10-C9	-2.45	101.99	114.42
16	a	851	LHG	C20-C19-C18	-2.45	102.00	114.42
13	b	813	CLA	C1-C2-C3	-2.45	122.80	126.75
15	a	846	BCR	C33-C5-C6	-2.44	121.78	124.53
13	b	835	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
17	b	852	LMG	C1-O6-C5	-2.44	108.89	113.69
12	a	801	CL0	CAA-CBA-CGA	-2.44	106.12	113.25
13	b	820	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	a	808	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	k	4005	BCR	C15-C14-C13	-2.44	123.83	127.31
15	b	847	BCR	C27-C26-C25	2.44	126.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	821	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	b	810	CLA	CHB-C4A-NA	2.44	127.88	124.51
15	k	4005	BCR	C27-C26-C25	2.44	126.27	122.73
15	j	101	BCR	C27-C26-C25	2.43	126.26	122.73
16	a	851	LHG	C11-C10-C9	-2.43	102.08	114.42
13	a	834	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
13	b	826	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	b	850	LMG	O1-C1-C2	-2.43	104.51	108.30
16	a	853	LHG	C11-C10-C9	-2.43	102.11	114.42
13	a	829	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	b	841	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	a	847	BCR	C15-C16-C17	-2.42	118.51	123.47
13	a	828	CLA	CHD-C1D-ND	-2.42	122.23	124.45
15	a	845	BCR	C15-C16-C17	-2.42	118.51	123.47
13	a	813	CLA	O2D-CGD-CBD	2.42	115.57	111.27
13	a	835	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
13	b	819	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
15	a	845	BCR	C28-C27-C26	-2.42	109.76	114.08
17	a	850	LMG	C40-C39-C38	-2.42	102.16	114.42
13	a	828	CLA	CHB-C4A-NA	2.42	127.85	124.51
13	b	817	CLA	CHB-C4A-NA	2.42	127.85	124.51
13	b	839	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	b	818	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
21	b	853	EQ3	C34-C9-C8	2.41	121.88	118.08
13	a	834	CLA	O2D-CGD-CBD	2.41	115.55	111.27
13	a	803	CLA	CHB-C4A-NA	2.41	127.84	124.51
13	a	812	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
13	a	826	CLA	CHB-C4A-NA	2.40	127.84	124.51
13	b	811	CLA	CHB-C4A-NA	2.40	127.84	124.51
13	b	829	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	a	844	BCR	C27-C26-C25	2.40	126.22	122.73
13	a	802	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	b	838	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	a	814	CLA	CHB-C4A-NA	2.40	127.83	124.51
16	f	206	LHG	C20-C19-C18	-2.40	102.25	114.42
13	b	838	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	b	849	BCR	C27-C26-C25	2.40	126.21	122.73
13	a	812	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	a	823	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
13	b	812	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
16	a	849	LHG	C20-C19-C18	-2.40	102.26	114.42
13	b	809	CLA	O2A-CGA-O1A	-2.39	117.55	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	854	ZEX	C27-C28-C29	2.39	129.85	126.23
13	a	839	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
13	b	824	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	b	804	CLA	CHD-C1D-ND	-2.39	122.26	124.45
13	b	809	CLA	CHB-C4A-NA	2.39	127.81	124.51
13	a	818	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
15	f	202	BCR	C27-C26-C25	2.38	126.19	122.73
13	b	826	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
13	b	808	CLA	CHB-C4A-NA	2.38	127.81	124.51
13	a	827	CLA	C1-C2-C3	-2.38	121.92	126.04
13	b	831	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
13	a	841	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	a	824	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	b	834	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	a	822	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	b	836	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	b	852	LMG	C40-C39-C38	-2.37	102.39	114.42
13	b	816	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	b	837	CLA	C1-C2-C3	-2.37	121.94	126.04
18	a	856	45D	C33-C35-C37	2.37	122.58	118.94
13	a	829	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	b	832	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	a	836	CLA	CHB-C4A-NA	2.37	127.78	124.51
16	a	853	LHG	C20-C19-C18	-2.37	102.42	114.42
13	b	827	CLA	CHB-C4A-NA	2.37	127.78	124.51
16	f	206	LHG	C11-C10-C9	-2.36	102.42	114.42
13	b	837	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
13	a	811	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
13	b	830	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
13	a	802	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
13	b	808	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
13	b	821	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
15	k	4001	BCR	C24-C23-C22	-2.36	122.67	126.23
13	j	104	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
13	a	831	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
13	b	824	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
13	j	103	CLA	CHB-C4A-NA	2.35	127.76	124.51
13	b	803	CLA	C1-C2-C3	-2.35	121.98	126.04
13	a	838	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
13	b	819	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	a	805	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
15	j	105	BCR	C24-C23-C22	-2.34	122.70	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	850	LMG	C40-C39-C38	-2.34	102.54	114.42
13	a	825	CLA	O2D-CGD-CBD	2.34	115.43	111.27
13	a	804	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	a	837	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	b	848	BCR	C2-C1-C6	2.34	114.08	110.48
13	a	802	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
13	b	836	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
15	i	101	BCR	C27-C26-C25	2.33	126.12	122.73
13	k	4003	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
13	a	832	CLA	C1-C2-C3	-2.33	122.01	126.04
13	b	825	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
18	a	856	45D	C34-C36-C38	2.33	122.51	118.94
13	b	837	CLA	O2D-CGD-CBD	2.33	115.40	111.27
13	a	831	CLA	CHB-C4A-NA	2.33	127.73	124.51
13	b	813	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
15	i	102	BCR	C33-C5-C6	-2.33	121.92	124.53
13	b	805	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
13	a	819	CLA	CHB-C4A-NA	2.32	127.73	124.51
13	a	854	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
15	a	846	BCR	C27-C26-C25	2.32	126.10	122.73
13	a	803	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
13	b	834	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
22	f	205	ZEX	C8-C9-C10	2.32	122.50	118.94
13	a	807	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
13	a	817	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
13	b	821	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
17	b	850	LMG	C38-C37-C36	-2.31	102.67	114.42
15	j	105	BCR	C15-C14-C13	-2.31	124.01	127.31
13	l	1501	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
15	a	844	BCR	C24-C23-C22	-2.31	122.74	126.23
13	b	817	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
17	b	852	LMG	C38-C37-C36	-2.31	102.70	114.42
13	a	815	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
13	f	204	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
13	j	104	CLA	CHB-C4A-NA	2.31	127.70	124.51
15	b	849	BCR	C33-C5-C6	-2.30	121.94	124.53
18	a	856	45D	C24-C26-C30	2.30	122.47	118.94
13	l	1503	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
13	b	807	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
20	m	101	ECH	C24-C23-C22	2.30	129.71	126.23
13	b	840	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
13	b	804	CLA	CHB-C4A-NA	2.29	127.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	833	CLA	CHB-C4A-NA	2.29	127.68	124.51
20	m	101	ECH	C8-C9-C10	2.29	122.45	118.94
13	a	812	CLA	C1-C2-C3	-2.29	122.08	126.04
13	b	817	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
13	b	807	CLA	C1-C2-C3	-2.29	122.09	126.04
13	b	815	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
13	a	832	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
12	a	801	CL0	CHB-C4A-NA	2.28	127.67	124.51
17	b	850	LMG	O3-C3-C2	-2.28	105.08	110.35
13	l	1502	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
15	k	4001	BCR	C15-C16-C17	-2.28	118.80	123.47
13	b	824	CLA	C1-C2-C3	-2.28	122.10	126.04
13	b	815	CLA	C1-C2-C3	-2.28	122.11	126.04
13	b	835	CLA	CHD-C1D-ND	-2.27	122.36	124.45
13	b	810	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
13	a	804	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
17	b	852	LMG	O6-C1-O1	-2.27	104.61	109.97
13	a	827	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
13	b	823	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
15	i	102	BCR	C15-C14-C13	-2.26	124.08	127.31
13	b	824	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
13	a	804	CLA	CHD-C1D-ND	-2.26	122.38	124.45
13	b	837	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
13	a	835	CLA	CHD-C1D-ND	-2.26	122.38	124.45
13	b	828	CLA	CHD-C1D-ND	-2.26	122.38	124.45
13	a	825	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	f	202	BCR	C24-C23-C22	-2.26	122.82	126.23
13	a	813	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
13	a	819	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
15	a	847	BCR	C15-C14-C13	-2.25	124.09	127.31
13	b	818	CLA	CHD-C1D-ND	-2.25	122.39	124.45
15	a	846	BCR	C11-C10-C9	-2.25	124.10	127.31
13	b	842	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
17	b	852	LMG	C42-C41-C40	-2.25	103.01	114.42
16	a	853	LHG	C27-C26-C25	-2.25	103.02	114.42
15	i	102	BCR	C15-C16-C17	-2.25	118.88	123.47
13	a	806	CLA	CHD-C1D-ND	-2.24	122.39	124.45
15	a	844	BCR	C15-C16-C17	-2.24	118.88	123.47
15	b	849	BCR	C15-C14-C13	-2.24	124.12	127.31
17	b	850	LMG	C42-C41-C40	-2.24	103.07	114.42
13	a	813	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
13	b	814	CLA	C1B-CHB-C4A	-2.23	125.69	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	f	201	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
16	a	851	LHG	C18-C17-C16	-2.23	103.09	114.42
13	a	803	CLA	CHD-C1D-ND	-2.23	122.40	124.45
13	b	831	CLA	CHB-C4A-NA	2.23	127.60	124.51
13	b	840	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
13	a	809	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
15	b	845	BCR	C15-C14-C13	-2.23	124.13	127.31
15	b	848	BCR	C15-C16-C17	-2.22	118.92	123.47
13	a	855	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
16	a	851	LHG	C27-C26-C25	-2.22	103.16	114.42
13	a	808	CLA	CHD-C1D-ND	-2.22	122.42	124.45
13	a	806	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
13	b	822	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
13	b	839	CLA	C1-C2-C3	-2.21	123.17	126.75
13	b	805	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
13	a	826	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
13	a	809	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
13	a	816	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
17	b	850	LMG	O2-C2-C1	-2.21	104.68	110.05
13	b	805	CLA	CHD-C1D-ND	-2.21	122.43	124.45
17	a	850	LMG	C38-C37-C36	-2.21	103.23	114.42
16	a	849	LHG	C18-C17-C16	-2.20	103.23	114.42
13	f	203	CLA	CHB-C4A-NA	2.20	127.56	124.51
13	b	832	CLA	C1-C2-C3	-2.20	123.19	126.75
13	a	840	CLA	CHD-C1D-ND	-2.20	122.43	124.45
17	a	852	LMG	O3-C3-C2	-2.20	105.25	110.35
13	a	840	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	b	845	BCR	C27-C26-C25	2.20	125.93	122.73
17	a	850	LMG	C42-C41-C40	-2.20	103.26	114.42
13	a	814	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
13	b	817	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	a	828	CLA	C1-C2-C3	-2.19	122.25	126.04
15	i	101	BCR	C33-C5-C6	-2.19	122.06	124.53
13	b	831	CLA	C1-C2-C3	-2.19	122.25	126.04
15	b	849	BCR	C15-C16-C17	-2.19	118.99	123.47
22	b	854	ZEX	C8-C9-C10	2.19	122.30	118.94
13	b	830	CLA	O2D-CGD-CBD	2.19	115.15	111.27
13	b	811	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
13	b	833	CLA	CHD-C1D-ND	-2.18	122.45	124.45
13	b	827	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
15	f	202	BCR	C33-C5-C6	-2.18	122.08	124.53
13	a	826	CLA	C1-C2-C3	-2.18	122.28	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	850	LMG	O3-C3-C2	-2.18	105.32	110.35
16	b	851	LHG	C27-C26-C25	-2.17	103.40	114.42
15	i	102	BCR	C28-C27-C26	-2.17	110.20	114.08
13	a	803	CLA	C1-C2-C3	-2.17	122.29	126.04
16	a	849	LHG	C27-C26-C25	-2.17	103.40	114.42
16	a	853	LHG	C18-C17-C16	-2.17	103.41	114.42
13	a	842	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	b	826	CLA	CHD-C1D-ND	-2.17	122.46	124.45
15	a	847	BCR	C27-C26-C25	2.16	125.87	122.73
13	a	822	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	a	823	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
17	b	852	LMG	O2-C2-C1	-2.16	104.80	110.05
13	b	838	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	a	814	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	k	4002	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
13	k	4004	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
15	b	844	BCR	C11-C10-C9	-2.16	124.23	127.31
13	b	834	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
15	a	848	BCR	C7-C8-C9	-2.15	122.98	126.23
13	b	801	CLA	CHB-C4A-NA	2.15	127.49	124.51
16	f	206	LHG	C18-C17-C16	-2.15	103.50	114.42
13	a	821	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	f	203	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	a	812	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	a	825	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	a	805	CLA	C1-C2-C3	-2.14	122.34	126.04
15	b	848	BCR	C33-C5-C6	-2.14	122.12	124.53
15	j	101	BCR	C11-C10-C9	-2.14	124.26	127.31
15	b	849	BCR	C24-C23-C22	-2.13	123.01	126.23
13	a	820	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
13	b	807	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
15	a	846	BCR	C24-C23-C22	-2.13	123.02	126.23
16	f	206	LHG	C27-C26-C25	-2.13	103.63	114.42
15	a	845	BCR	C8-C7-C6	-2.13	121.23	127.20
13	b	826	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
13	a	833	CLA	C1-C2-C3	-2.12	122.37	126.04
17	b	852	LMG	O1-C7-C8	-2.12	105.77	110.90
13	a	814	CLA	O2D-CGD-CBD	2.12	115.04	111.27
13	a	823	CLA	CBA-CAA-C2A	2.12	120.11	113.86
17	a	850	LMG	O1-C7-C8	-2.12	105.79	110.90
20	b	846	ECH	C34-C9-C8	2.11	121.41	118.08
13	b	810	CLA	C1-C2-C3	-2.11	122.39	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	819	CLA	C1-C2-C3	-2.11	122.40	126.04
15	i	101	BCR	C15-C14-C13	-2.11	124.30	127.31
15	i	101	BCR	C8-C7-C6	-2.11	121.28	127.20
15	f	202	BCR	C8-C7-C6	-2.11	121.29	127.20
13	a	854	CLA	CHD-C1D-ND	-2.10	122.52	124.45
15	a	848	BCR	C11-C10-C9	-2.10	124.31	127.31
18	a	856	45D	C41-C42-C38	2.10	127.77	123.47
13	a	829	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	a	823	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	b	818	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	a	841	CLA	C1-C2-C3	-2.10	122.42	126.04
17	a	850	LMG	O2-C2-C1	-2.09	104.96	110.05
15	k	4005	BCR	C33-C5-C6	-2.09	122.18	124.53
13	a	838	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
13	a	819	CLA	CHD-C1D-ND	-2.09	122.53	124.45
13	b	820	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	a	847	BCR	C24-C23-C22	-2.09	123.08	126.23
13	a	835	CLA	C1-C2-C3	-2.09	122.43	126.04
13	a	836	CLA	C1-C2-C3	-2.09	122.43	126.04
13	a	835	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
13	b	816	CLA	CHD-C1D-ND	-2.08	122.54	124.45
13	l	1503	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
15	b	847	BCR	C33-C5-C6	-2.08	122.19	124.53
15	k	4005	BCR	C24-C23-C22	-2.08	123.10	126.23
13	b	832	CLA	CHD-C1D-ND	-2.08	122.55	124.45
13	a	836	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	b	831	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	k	4004	CLA	CAC-C3C-C2C	-2.08	123.98	127.53
15	j	101	BCR	C24-C23-C22	-2.08	123.10	126.23
13	a	812	CLA	CHD-C1D-ND	-2.07	122.55	124.45
17	a	852	LMG	O2-C2-C1	-2.07	105.01	110.05
15	i	102	BCR	C11-C10-C9	-2.07	124.36	127.31
13	b	806	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
15	a	846	BCR	C7-C8-C9	-2.07	123.11	126.23
13	a	817	CLA	CHD-C1D-ND	-2.07	122.56	124.45
13	k	4002	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
15	f	202	BCR	C16-C15-C14	-2.06	119.25	123.47
13	b	841	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	b	844	BCR	C38-C26-C25	-2.06	122.21	124.53
13	a	830	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	a	832	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	a	838	CLA	CHD-C1D-ND	-2.06	122.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	819	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	a	841	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	l	1502	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	a	845	BCR	C24-C23-C22	-2.06	123.13	126.23
15	a	847	BCR	C8-C7-C6	-2.05	121.43	127.20
13	a	807	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	b	848	BCR	C15-C14-C13	-2.05	124.39	127.31
13	a	833	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	k	4004	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	b	805	CLA	C1-C2-C3	-2.05	122.51	126.04
13	a	827	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	a	831	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	b	832	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	a	811	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	b	828	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	a	844	BCR	C15-C14-C13	-2.04	124.39	127.31
17	b	852	LMG	O3-C3-C2	-2.04	105.63	110.35
23	j	102	LMT	O5B-C5B-C4B	2.04	113.39	109.69
13	b	811	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
13	a	832	CLA	CHD-C1D-ND	-2.03	122.58	124.45
13	b	804	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	a	821	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
15	a	846	BCR	C35-C13-C14	-2.03	120.08	122.92
13	a	808	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	a	810	CLA	C2A-C1A-CHA	2.03	127.41	123.86
17	a	852	LMG	O1-C7-C8	-2.03	106.00	110.90
13	l	1501	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	j	105	BCR	C8-C7-C6	-2.03	121.51	127.20
15	i	102	BCR	C27-C26-C25	2.02	125.67	122.73
13	b	819	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
13	b	825	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
13	f	201	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
13	j	103	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	a	837	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	b	816	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	b	813	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
13	a	833	CLA	CHD-C1D-ND	-2.01	122.60	124.45
13	k	4003	CLA	CHD-C1D-ND	-2.01	122.60	124.45
13	a	824	CLA	CHD-C1D-ND	-2.01	122.60	124.45
17	b	852	LMG	O7-C10-O9	-2.01	118.84	123.70
15	b	847	BCR	C11-C10-C9	-2.01	124.44	127.31
15	f	202	BCR	C15-C16-C17	-2.01	119.36	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	840	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	a	845	BCR	C15-C14-C13	-2.01	124.44	127.31
13	a	841	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
13	b	808	CLA	CHD-C1D-ND	-2.00	122.61	124.45
13	a	818	CLA	CAA-CBA-CGA	-2.00	107.41	113.25
13	b	810	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
13	a	805	CLA	CHD-C1D-ND	-2.00	122.62	124.45
13	b	834	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (98) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	a	801	CL0	ND
12	a	801	CL0	NA
12	a	801	CL0	NC
13	a	802	CLA	ND
13	a	803	CLA	ND
13	a	804	CLA	ND
13	a	805	CLA	ND
13	a	806	CLA	ND
13	a	807	CLA	ND
13	a	808	CLA	ND
13	a	809	CLA	ND
13	a	810	CLA	ND
13	a	811	CLA	ND
13	a	812	CLA	ND
13	a	813	CLA	ND
13	a	814	CLA	ND
13	a	815	CLA	ND
13	a	816	CLA	ND
13	a	817	CLA	ND
13	a	818	CLA	ND
13	a	819	CLA	ND
13	a	820	CLA	ND
13	a	821	CLA	ND
13	a	822	CLA	ND
13	a	823	CLA	ND
13	a	824	CLA	ND
13	a	825	CLA	ND
13	a	826	CLA	ND
13	a	827	CLA	ND
13	a	828	CLA	ND

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Mol	Chain	Res	Type	Atom
13	a	829	CLA	ND
13	a	830	CLA	ND
13	a	831	CLA	ND
13	a	832	CLA	ND
13	a	833	CLA	ND
13	a	834	CLA	ND
13	a	835	CLA	ND
13	a	836	CLA	ND
13	a	837	CLA	ND
13	a	838	CLA	ND
13	a	839	CLA	ND
13	a	840	CLA	ND
13	a	841	CLA	ND
13	a	842	CLA	ND
13	a	854	CLA	ND
13	a	855	CLA	ND
13	b	801	CLA	ND
13	b	803	CLA	ND
13	b	804	CLA	ND
13	b	805	CLA	ND
13	b	806	CLA	ND
13	b	807	CLA	ND
13	b	808	CLA	ND
13	b	809	CLA	ND
13	b	810	CLA	ND
13	b	811	CLA	ND
13	b	812	CLA	ND
13	b	813	CLA	ND
13	b	814	CLA	ND
13	b	815	CLA	ND
13	b	816	CLA	ND
13	b	817	CLA	ND
13	b	818	CLA	ND
13	b	819	CLA	ND
13	b	820	CLA	ND
13	b	821	CLA	ND
13	b	822	CLA	ND
13	b	823	CLA	ND
13	b	824	CLA	ND
13	b	825	CLA	ND
13	b	826	CLA	ND
13	b	827	CLA	ND

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Mol	Chain	Res	Type	Atom
13	b	828	CLA	ND
13	b	829	CLA	ND
13	b	830	CLA	ND
13	b	831	CLA	ND
13	b	832	CLA	ND
13	b	833	CLA	ND
13	b	834	CLA	ND
13	b	835	CLA	ND
13	b	836	CLA	ND
13	b	837	CLA	ND
13	b	838	CLA	ND
13	b	839	CLA	ND
13	b	840	CLA	ND
13	b	841	CLA	ND
13	b	842	CLA	ND
13	f	201	CLA	ND
13	f	203	CLA	ND
13	f	204	CLA	ND
13	j	103	CLA	ND
13	j	104	CLA	ND
13	k	4002	CLA	ND
13	k	4003	CLA	ND
13	k	4004	CLA	ND
13	l	1501	CLA	ND
13	l	1502	CLA	ND
13	l	1503	CLA	ND

All (1505) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	a	802	CLA	CBA-CGA-O2A-C1
13	a	802	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	CHA-CBD-CGD-O1D
13	a	805	CLA	C3A-C2A-CAA-CBA
13	a	806	CLA	C2-C3-C5-C6
13	a	806	CLA	C4-C3-C5-C6
13	a	808	CLA	C1A-C2A-CAA-CBA
13	a	808	CLA	C3A-C2A-CAA-CBA
13	a	810	CLA	C2A-CAA-CBA-CGA
13	a	810	CLA	CHA-CBD-CGD-O1D
13	a	810	CLA	CHA-CBD-CGD-O2D
13	a	812	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	a	814	CLA	C3A-C2A-CAA-CBA
13	a	814	CLA	CHA-CBD-CGD-O1D
13	a	814	CLA	CHA-CBD-CGD-O2D
13	a	815	CLA	CBD-CGD-O2D-CED
13	a	816	CLA	C1A-C2A-CAA-CBA
13	a	816	CLA	C3A-C2A-CAA-CBA
13	a	816	CLA	CBA-CGA-O2A-C1
13	a	817	CLA	C1A-C2A-CAA-CBA
13	a	818	CLA	C1A-C2A-CAA-CBA
13	a	818	CLA	C3A-C2A-CAA-CBA
13	a	818	CLA	CBD-CGD-O2D-CED
13	a	819	CLA	C1A-C2A-CAA-CBA
13	a	819	CLA	C3A-C2A-CAA-CBA
13	a	819	CLA	CHA-CBD-CGD-O1D
13	a	819	CLA	CHA-CBD-CGD-O2D
13	a	820	CLA	C1A-C2A-CAA-CBA
13	a	820	CLA	C3A-C2A-CAA-CBA
13	a	820	CLA	C2-C1-O2A-CGA
13	a	822	CLA	C1A-C2A-CAA-CBA
13	a	822	CLA	C3A-C2A-CAA-CBA
13	a	823	CLA	C1A-C2A-CAA-CBA
13	a	824	CLA	CHA-CBD-CGD-O1D
13	a	824	CLA	CHA-CBD-CGD-O2D
13	a	826	CLA	C3A-C2A-CAA-CBA
13	a	828	CLA	C1A-C2A-CAA-CBA
13	a	831	CLA	C3A-C2A-CAA-CBA
13	a	832	CLA	C1A-C2A-CAA-CBA
13	a	832	CLA	C3A-C2A-CAA-CBA
13	a	834	CLA	C1A-C2A-CAA-CBA
13	a	835	CLA	C2-C3-C5-C6
13	a	835	CLA	C4-C3-C5-C6
13	a	835	CLA	C6-C7-C8-C9
13	a	836	CLA	CHA-CBD-CGD-O1D
13	a	836	CLA	CHA-CBD-CGD-O2D
13	a	838	CLA	C1A-C2A-CAA-CBA
13	a	838	CLA	C3A-C2A-CAA-CBA
13	a	838	CLA	CHA-CBD-CGD-O1D
13	a	838	CLA	CHA-CBD-CGD-O2D
13	a	840	CLA	C1A-C2A-CAA-CBA
13	a	840	CLA	C3A-C2A-CAA-CBA
13	a	842	CLA	CHA-CBD-CGD-O1D
13	a	855	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	a	855	CLA	C3A-C2A-CAA-CBA
13	a	855	CLA	C4-C3-C5-C6
13	b	801	CLA	CBD-CGD-O2D-CED
13	b	801	CLA	C2-C3-C5-C6
13	b	801	CLA	C4-C3-C5-C6
13	b	803	CLA	C1A-C2A-CAA-CBA
13	b	803	CLA	C3A-C2A-CAA-CBA
13	b	803	CLA	CHA-CBD-CGD-O1D
13	b	803	CLA	CHA-CBD-CGD-O2D
13	b	803	CLA	C2-C3-C5-C6
13	b	803	CLA	C4-C3-C5-C6
13	b	804	CLA	CHA-CBD-CGD-O1D
13	b	804	CLA	CHA-CBD-CGD-O2D
13	b	804	CLA	CBD-CGD-O2D-CED
13	b	804	CLA	O1D-CGD-O2D-CED
13	b	805	CLA	C2A-CAA-CBA-CGA
13	b	807	CLA	C14-C13-C15-C16
13	b	808	CLA	C1A-C2A-CAA-CBA
13	b	808	CLA	C3A-C2A-CAA-CBA
13	b	808	CLA	C2-C3-C5-C6
13	b	808	CLA	C4-C3-C5-C6
13	b	808	CLA	C6-C7-C8-C9
13	b	810	CLA	C2A-CAA-CBA-CGA
13	b	810	CLA	CBD-CGD-O2D-CED
13	b	812	CLA	C1A-C2A-CAA-CBA
13	b	813	CLA	C1A-C2A-CAA-CBA
13	b	816	CLA	C1A-C2A-CAA-CBA
13	b	816	CLA	CBD-CGD-O2D-CED
13	b	816	CLA	C2-C3-C5-C6
13	b	816	CLA	C4-C3-C5-C6
13	b	817	CLA	C1A-C2A-CAA-CBA
13	b	818	CLA	C11-C10-C8-C9
13	b	819	CLA	C1A-C2A-CAA-CBA
13	b	819	CLA	C3A-C2A-CAA-CBA
13	b	821	CLA	C1A-C2A-CAA-CBA
13	b	821	CLA	C3A-C2A-CAA-CBA
13	b	822	CLA	C1A-C2A-CAA-CBA
13	b	822	CLA	C3A-C2A-CAA-CBA
13	b	823	CLA	C1A-C2A-CAA-CBA
13	b	823	CLA	C3A-C2A-CAA-CBA
13	b	823	CLA	CBA-CGA-O2A-C1
13	b	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	824	CLA	C1A-C2A-CAA-CBA
13	b	824	CLA	C3A-C2A-CAA-CBA
13	b	825	CLA	C1A-C2A-CAA-CBA
13	b	826	CLA	C3A-C2A-CAA-CBA
13	b	828	CLA	C1A-C2A-CAA-CBA
13	b	828	CLA	C3A-C2A-CAA-CBA
13	b	830	CLA	C1A-C2A-CAA-CBA
13	b	830	CLA	C3A-C2A-CAA-CBA
13	b	831	CLA	C1A-C2A-CAA-CBA
13	b	831	CLA	C3A-C2A-CAA-CBA
13	b	831	CLA	CBD-CGD-O2D-CED
13	b	831	CLA	O1D-CGD-O2D-CED
13	b	834	CLA	C1A-C2A-CAA-CBA
13	b	834	CLA	C3A-C2A-CAA-CBA
13	b	834	CLA	CBA-CGA-O2A-C1
13	b	834	CLA	O1A-CGA-O2A-C1
13	b	834	CLA	CHA-CBD-CGD-O1D
13	b	834	CLA	CHA-CBD-CGD-O2D
13	b	835	CLA	C1A-C2A-CAA-CBA
13	b	835	CLA	C3A-C2A-CAA-CBA
13	b	836	CLA	C1A-C2A-CAA-CBA
13	b	836	CLA	C3A-C2A-CAA-CBA
13	b	838	CLA	C1A-C2A-CAA-CBA
13	b	838	CLA	C3A-C2A-CAA-CBA
13	b	839	CLA	C1A-C2A-CAA-CBA
13	b	839	CLA	C3A-C2A-CAA-CBA
13	b	840	CLA	C1A-C2A-CAA-CBA
13	b	841	CLA	CHA-CBD-CGD-O1D
13	b	841	CLA	CHA-CBD-CGD-O2D
13	b	842	CLA	C1A-C2A-CAA-CBA
13	b	842	CLA	C3A-C2A-CAA-CBA
13	b	842	CLA	CAD-CBD-CGD-O1D
13	b	842	CLA	CAD-CBD-CGD-O2D
13	f	201	CLA	CHA-CBD-CGD-O1D
13	f	201	CLA	CHA-CBD-CGD-O2D
13	j	103	CLA	C1A-C2A-CAA-CBA
13	j	104	CLA	CBA-CGA-O2A-C1
13	j	104	CLA	CHA-CBD-CGD-O1D
13	j	104	CLA	CHA-CBD-CGD-O2D
13	k	4003	CLA	C3A-C2A-CAA-CBA
13	k	4003	CLA	CBA-CGA-O2A-C1
13	k	4003	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	k	4003	CLA	CHA-CBD-CGD-O1D
13	k	4003	CLA	CHA-CBD-CGD-O2D
13	l	1501	CLA	C1A-C2A-CAA-CBA
13	l	1501	CLA	C3A-C2A-CAA-CBA
13	l	1502	CLA	C1A-C2A-CAA-CBA
13	l	1502	CLA	CHA-CBD-CGD-O1D
13	l	1502	CLA	CHA-CBD-CGD-O2D
15	a	844	BCR	C1-C6-C7-C8
15	a	844	BCR	C7-C8-C9-C34
15	a	845	BCR	C1-C6-C7-C8
15	a	847	BCR	C1-C6-C7-C8
15	a	847	BCR	C7-C8-C9-C34
15	a	847	BCR	C20-C21-C22-C37
15	a	847	BCR	C21-C22-C23-C24
15	a	847	BCR	C37-C22-C23-C24
15	a	847	BCR	C23-C24-C25-C30
15	a	848	BCR	C9-C10-C11-C12
15	a	848	BCR	C11-C12-C13-C35
15	b	844	BCR	C7-C8-C9-C10
15	b	844	BCR	C7-C8-C9-C34
15	b	844	BCR	C21-C22-C23-C24
15	b	844	BCR	C37-C22-C23-C24
15	b	844	BCR	C22-C23-C24-C25
15	b	845	BCR	C1-C6-C7-C8
15	b	847	BCR	C21-C22-C23-C24
15	b	847	BCR	C22-C23-C24-C25
15	b	848	BCR	C10-C11-C12-C13
15	b	848	BCR	C11-C12-C13-C35
15	b	848	BCR	C20-C21-C22-C37
15	b	849	BCR	C6-C7-C8-C9
15	b	849	BCR	C11-C10-C9-C8
15	b	849	BCR	C11-C12-C13-C35
15	b	849	BCR	C16-C17-C18-C36
15	b	849	BCR	C21-C22-C23-C24
15	b	849	BCR	C37-C22-C23-C24
15	f	202	BCR	C7-C8-C9-C10
15	f	202	BCR	C37-C22-C23-C24
15	i	101	BCR	C21-C22-C23-C24
15	i	102	BCR	C7-C8-C9-C10
15	i	102	BCR	C7-C8-C9-C34
15	i	102	BCR	C37-C22-C23-C24
15	j	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	j	105	BCR	C23-C24-C25-C30
15	k	4001	BCR	C7-C8-C9-C34
16	a	849	LHG	O2-C2-C3-O3
16	a	849	LHG	C3-O3-P-O5
16	a	849	LHG	O10-C23-O8-C6
16	a	849	LHG	C24-C23-O8-C6
16	a	853	LHG	O9-C7-O7-C5
16	a	853	LHG	C8-C7-O7-C5
16	b	851	LHG	O1-C1-C2-C3
16	b	851	LHG	C3-O3-P-O4
16	b	851	LHG	C3-O3-P-O6
16	f	206	LHG	O9-C7-O7-C5
16	f	206	LHG	O10-C23-O8-C6
17	a	850	LMG	O6-C1-O1-C7
17	a	850	LMG	O9-C10-O7-C8
17	a	850	LMG	C11-C10-O7-C8
17	a	852	LMG	C2-C1-O1-C7
17	a	852	LMG	O6-C1-O1-C7
17	a	852	LMG	O9-C10-O7-C8
17	a	852	LMG	C11-C10-O7-C8
20	b	846	ECH	C21-C22-C23-C24
20	b	846	ECH	C37-C22-C23-C24
20	m	101	ECH	C21-C22-C23-C24
20	m	101	ECH	C37-C22-C23-C24
23	j	102	LMT	C2'-C1'-O1'-C1
23	j	102	LMT	O5'-C1'-O1'-C1
13	b	803	CLA	O1D-CGD-O2D-CED
13	b	816	CLA	O1D-CGD-O2D-CED
13	a	805	CLA	CBD-CGD-O2D-CED
13	a	810	CLA	CBD-CGD-O2D-CED
13	a	813	CLA	CBD-CGD-O2D-CED
13	a	820	CLA	CBD-CGD-O2D-CED
13	b	803	CLA	CBD-CGD-O2D-CED
13	b	821	CLA	CBD-CGD-O2D-CED
13	b	822	CLA	CBD-CGD-O2D-CED
13	b	824	CLA	CBD-CGD-O2D-CED
13	b	835	CLA	CBD-CGD-O2D-CED
13	b	837	CLA	CBD-CGD-O2D-CED
13	f	201	CLA	CBD-CGD-O2D-CED
13	j	103	CLA	CBD-CGD-O2D-CED
13	k	4004	CLA	CBD-CGD-O2D-CED
13	l	1501	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	812	CLA	O1A-CGA-O2A-C1
13	a	819	CLA	O1A-CGA-O2A-C1
13	b	806	CLA	O1A-CGA-O2A-C1
13	b	807	CLA	O1A-CGA-O2A-C1
13	b	839	CLA	O1A-CGA-O2A-C1
13	b	840	CLA	O1A-CGA-O2A-C1
13	l	1501	CLA	O1A-CGA-O2A-C1
17	a	850	LMG	O10-C28-O8-C9
13	j	104	CLA	O1A-CGA-O2A-C1
13	a	810	CLA	O1D-CGD-O2D-CED
13	a	815	CLA	O1D-CGD-O2D-CED
13	b	801	CLA	O1D-CGD-O2D-CED
13	k	4004	CLA	O1D-CGD-O2D-CED
13	a	815	CLA	CBA-CGA-O2A-C1
13	a	818	CLA	O1D-CGD-O2D-CED
13	a	820	CLA	O1D-CGD-O2D-CED
13	f	201	CLA	O1D-CGD-O2D-CED
13	a	812	CLA	CBA-CGA-O2A-C1
13	a	819	CLA	CBA-CGA-O2A-C1
13	b	807	CLA	CBA-CGA-O2A-C1
13	b	839	CLA	CBA-CGA-O2A-C1
17	a	850	LMG	C29-C28-O8-C9
13	a	809	CLA	CBD-CGD-O2D-CED
13	a	822	CLA	CBD-CGD-O2D-CED
13	a	827	CLA	CBD-CGD-O2D-CED
13	b	830	CLA	CBD-CGD-O2D-CED
13	b	834	CLA	CBD-CGD-O2D-CED
13	b	836	CLA	CBD-CGD-O2D-CED
13	b	841	CLA	CBD-CGD-O2D-CED
13	a	820	CLA	O1A-CGA-O2A-C1
13	a	824	CLA	O1A-CGA-O2A-C1
13	a	831	CLA	O1A-CGA-O2A-C1
13	a	834	CLA	O1A-CGA-O2A-C1
13	a	854	CLA	O1A-CGA-O2A-C1
13	b	801	CLA	O1A-CGA-O2A-C1
13	b	804	CLA	O1A-CGA-O2A-C1
13	b	813	CLA	O1A-CGA-O2A-C1
13	b	818	CLA	O1A-CGA-O2A-C1
13	b	822	CLA	O1A-CGA-O2A-C1
13	b	825	CLA	O1A-CGA-O2A-C1
13	b	828	CLA	O1A-CGA-O2A-C1
13	b	836	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	837	CLA	O1A-CGA-O2A-C1
13	f	203	CLA	O1A-CGA-O2A-C1
13	l	1502	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	O10-C23-O8-C6
13	a	816	CLA	O1A-CGA-O2A-C1
13	b	810	CLA	O1D-CGD-O2D-CED
13	l	1501	CLA	O1D-CGD-O2D-CED
13	a	802	CLA	C3-C5-C6-C7
13	a	817	CLA	C3-C5-C6-C7
13	a	825	CLA	C3-C5-C6-C7
13	a	835	CLA	C3-C5-C6-C7
13	a	855	CLA	C3-C5-C6-C7
13	b	805	CLA	C3-C5-C6-C7
13	b	838	CLA	C3-C5-C6-C7
13	a	829	CLA	CBA-CGA-O2A-C1
13	a	834	CLA	CBA-CGA-O2A-C1
13	b	801	CLA	CBA-CGA-O2A-C1
13	b	803	CLA	CBA-CGA-O2A-C1
13	b	806	CLA	CBA-CGA-O2A-C1
13	b	808	CLA	CBA-CGA-O2A-C1
13	b	813	CLA	CBA-CGA-O2A-C1
13	b	822	CLA	CBA-CGA-O2A-C1
13	b	833	CLA	CBA-CGA-O2A-C1
13	b	838	CLA	CBA-CGA-O2A-C1
13	b	840	CLA	CBA-CGA-O2A-C1
13	j	103	CLA	CBA-CGA-O2A-C1
13	l	1501	CLA	CBA-CGA-O2A-C1
16	f	206	LHG	C8-C7-O7-C5
13	a	824	CLA	CBD-CGD-O2D-CED
13	b	804	CLA	C2C-C3C-CAC-CBC
13	a	830	CLA	C4-C3-C5-C6
13	b	810	CLA	C4-C3-C5-C6
13	f	201	CLA	C4-C3-C5-C6
13	a	855	CLA	C2-C3-C5-C6
13	a	808	CLA	C2A-CAA-CBA-CGA
13	a	814	CLA	C2A-CAA-CBA-CGA
13	a	815	CLA	C2A-CAA-CBA-CGA
13	a	836	CLA	C2A-CAA-CBA-CGA
13	b	818	CLA	C2A-CAA-CBA-CGA
13	b	829	CLA	C2A-CAA-CBA-CGA
13	b	832	CLA	C2A-CAA-CBA-CGA
13	b	833	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	b	842	CLA	C2A-CAA-CBA-CGA
13	k	4003	CLA	C2A-CAA-CBA-CGA
13	a	811	CLA	O1A-CGA-O2A-C1
13	a	815	CLA	O1A-CGA-O2A-C1
13	a	830	CLA	C3-C5-C6-C7
13	a	839	CLA	C3-C5-C6-C7
13	a	840	CLA	C3-C5-C6-C7
13	b	801	CLA	C3-C5-C6-C7
13	a	811	CLA	CBA-CGA-O2A-C1
13	a	818	CLA	CBA-CGA-O2A-C1
13	a	820	CLA	CBA-CGA-O2A-C1
13	a	824	CLA	CBA-CGA-O2A-C1
13	a	827	CLA	CBA-CGA-O2A-C1
13	a	831	CLA	CBA-CGA-O2A-C1
13	a	838	CLA	CBA-CGA-O2A-C1
13	a	841	CLA	CBA-CGA-O2A-C1
13	a	854	CLA	CBA-CGA-O2A-C1
13	a	855	CLA	CBA-CGA-O2A-C1
13	b	804	CLA	CBA-CGA-O2A-C1
13	b	814	CLA	CBA-CGA-O2A-C1
13	b	817	CLA	CBA-CGA-O2A-C1
13	b	818	CLA	CBA-CGA-O2A-C1
13	b	825	CLA	CBA-CGA-O2A-C1
13	b	828	CLA	CBA-CGA-O2A-C1
13	b	831	CLA	CBA-CGA-O2A-C1
13	b	835	CLA	CBA-CGA-O2A-C1
13	b	836	CLA	CBA-CGA-O2A-C1
13	b	837	CLA	CBA-CGA-O2A-C1
13	f	201	CLA	CBA-CGA-O2A-C1
13	f	203	CLA	CBA-CGA-O2A-C1
13	k	4002	CLA	CBA-CGA-O2A-C1
13	l	1502	CLA	CBA-CGA-O2A-C1
16	a	853	LHG	C24-C23-O8-C6
16	f	206	LHG	C24-C23-O8-C6
23	j	102	LMT	C4'-C5'-C6'-O6'
13	b	821	CLA	O1D-CGD-O2D-CED
13	b	837	CLA	O1D-CGD-O2D-CED
13	a	805	CLA	O1D-CGD-O2D-CED
13	j	103	CLA	O1D-CGD-O2D-CED
13	a	818	CLA	O1A-CGA-O2A-C1
13	a	822	CLA	O1A-CGA-O2A-C1
13	a	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	829	CLA	O1A-CGA-O2A-C1
13	a	841	CLA	O1A-CGA-O2A-C1
13	b	803	CLA	O1A-CGA-O2A-C1
13	b	808	CLA	O1A-CGA-O2A-C1
13	b	830	CLA	O1A-CGA-O2A-C1
13	b	832	CLA	O1A-CGA-O2A-C1
13	b	833	CLA	O1A-CGA-O2A-C1
13	b	835	CLA	O1A-CGA-O2A-C1
13	b	838	CLA	O1A-CGA-O2A-C1
13	j	103	CLA	O1A-CGA-O2A-C1
13	k	4002	CLA	O1A-CGA-O2A-C1
13	a	806	CLA	CBD-CGD-O2D-CED
13	a	833	CLA	CBD-CGD-O2D-CED
13	b	814	CLA	CBD-CGD-O2D-CED
13	b	828	CLA	CBD-CGD-O2D-CED
13	b	840	CLA	CBD-CGD-O2D-CED
13	b	822	CLA	O1D-CGD-O2D-CED
16	b	851	LHG	O2-C2-C3-O3
13	k	4002	CLA	C3-C5-C6-C7
13	a	803	CLA	CBA-CGA-O2A-C1
13	a	821	CLA	CBA-CGA-O2A-C1
13	a	822	CLA	CBA-CGA-O2A-C1
13	a	823	CLA	CBA-CGA-O2A-C1
13	a	832	CLA	CBA-CGA-O2A-C1
13	b	812	CLA	CBA-CGA-O2A-C1
13	b	816	CLA	CBA-CGA-O2A-C1
13	b	829	CLA	CBA-CGA-O2A-C1
13	b	830	CLA	CBA-CGA-O2A-C1
13	b	832	CLA	CBA-CGA-O2A-C1
17	b	852	LMG	C29-C28-O8-C9
12	a	801	CL0	O1A-CGA-O2A-C1
13	a	823	CLA	O1A-CGA-O2A-C1
13	a	838	CLA	O1A-CGA-O2A-C1
13	a	855	CLA	O1A-CGA-O2A-C1
13	b	812	CLA	O1A-CGA-O2A-C1
13	b	824	CLA	O1D-CGD-O2D-CED
13	b	835	CLA	O1D-CGD-O2D-CED
13	a	814	CLA	CBD-CGD-O2D-CED
13	f	203	CLA	CBD-CGD-O2D-CED
16	a	851	LHG	C29-C30-C31-C32
13	b	816	CLA	O1A-CGA-O2A-C1
13	f	201	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	813	CLA	O1D-CGD-O2D-CED
13	a	834	CLA	CBD-CGD-O2D-CED
13	j	104	CLA	CBD-CGD-O2D-CED
13	a	823	CLA	C3-C5-C6-C7
13	b	814	CLA	C3-C5-C6-C7
12	a	801	CL0	CBA-CGA-O2A-C1
17	b	850	LMG	C4-C5-C6-O5
17	b	852	LMG	C4-C5-C6-O5
13	a	832	CLA	O1A-CGA-O2A-C1
13	b	817	CLA	O1A-CGA-O2A-C1
13	b	831	CLA	O1A-CGA-O2A-C1
16	b	851	LHG	C32-C33-C34-C35
17	b	850	LMG	O6-C5-C6-O5
13	b	830	CLA	C4-C3-C5-C6
13	b	838	CLA	C4-C3-C5-C6
13	a	830	CLA	C2-C3-C5-C6
13	b	830	CLA	C2-C3-C5-C6
13	b	838	CLA	C2-C3-C5-C6
13	a	820	CLA	C2A-CAA-CBA-CGA
13	a	827	CLA	C2A-CAA-CBA-CGA
23	j	102	LMT	O5'-C5'-C6'-O6'
13	a	803	CLA	O1A-CGA-O2A-C1
13	a	821	CLA	O1A-CGA-O2A-C1
13	b	814	CLA	O1A-CGA-O2A-C1
13	b	829	CLA	O1A-CGA-O2A-C1
17	b	852	LMG	O10-C28-O8-C9
13	a	804	CLA	CBA-CGA-O2A-C1
13	a	825	CLA	CBA-CGA-O2A-C1
13	a	830	CLA	CBA-CGA-O2A-C1
13	b	842	CLA	CBA-CGA-O2A-C1
13	a	822	CLA	O1D-CGD-O2D-CED
13	a	816	CLA	CBD-CGD-O2D-CED
13	k	4004	CLA	C2C-C3C-CAC-CBC
16	a	849	LHG	C1-C2-C3-O3
17	b	852	LMG	O6-C5-C6-O5
13	a	804	CLA	O1A-CGA-O2A-C1
13	a	830	CLA	O1A-CGA-O2A-C1
13	b	810	CLA	O1A-CGA-O2A-C1
13	a	807	CLA	CBA-CGA-O2A-C1
13	a	808	CLA	CBA-CGA-O2A-C1
13	a	835	CLA	CBA-CGA-O2A-C1
13	a	836	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	840	CLA	CBA-CGA-O2A-C1
13	b	810	CLA	CBA-CGA-O2A-C1
23	j	102	LMT	C4B-C5B-C6B-O6B
13	a	813	CLA	C13-C15-C16-C17
13	a	828	CLA	C10-C11-C12-C13
13	b	834	CLA	C15-C16-C17-C18
13	k	4002	CLA	C5-C6-C7-C8
17	a	850	LMG	C2-C1-O1-C7
17	b	850	LMG	O7-C8-C9-O8
13	a	836	CLA	O1A-CGA-O2A-C1
13	a	840	CLA	O1A-CGA-O2A-C1
13	b	810	CLA	C2-C3-C5-C6
13	f	201	CLA	C2-C3-C5-C6
13	a	807	CLA	C11-C10-C8-C9
13	a	808	CLA	C11-C12-C13-C14
13	a	817	CLA	C11-C10-C8-C9
13	a	818	CLA	C6-C7-C8-C9
13	a	818	CLA	C11-C10-C8-C9
13	a	820	CLA	C11-C10-C8-C9
13	a	825	CLA	C14-C13-C15-C16
13	a	834	CLA	C6-C7-C8-C9
13	a	838	CLA	C11-C10-C8-C9
13	a	841	CLA	C11-C12-C13-C14
13	b	801	CLA	C11-C10-C8-C9
13	b	805	CLA	C14-C13-C15-C16
13	b	820	CLA	C11-C10-C8-C9
13	b	830	CLA	C11-C12-C13-C14
13	a	827	CLA	O1D-CGD-O2D-CED
13	b	830	CLA	O1D-CGD-O2D-CED
13	a	807	CLA	C2A-CAA-CBA-CGA
13	l	1503	CLA	C2A-CAA-CBA-CGA
15	a	845	BCR	C37-C22-C23-C24
15	b	845	BCR	C37-C22-C23-C24
15	f	202	BCR	C7-C8-C9-C34
15	k	4001	BCR	C37-C22-C23-C24
15	i	102	BCR	C21-C22-C23-C24
17	b	852	LMG	C28-C29-C30-C31
13	a	835	CLA	O1A-CGA-O2A-C1
13	a	818	CLA	C8-C10-C11-C12
13	a	827	CLA	C8-C10-C11-C12
13	l	1503	CLA	CBA-CGA-O2A-C1
17	b	850	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
13	a	811	CLA	C13-C15-C16-C17
13	a	813	CLA	C15-C16-C17-C18
13	a	841	CLA	C10-C11-C12-C13
13	b	827	CLA	C8-C10-C11-C12
13	b	833	CLA	C10-C11-C12-C13
13	b	834	CLA	C5-C6-C7-C8
13	b	840	CLA	C10-C11-C12-C13
14	a	843	PQN	C18-C20-C21-C22
13	a	809	CLA	O1D-CGD-O2D-CED
17	a	852	LMG	O6-C5-C6-O5
13	a	807	CLA	C13-C15-C16-C17
13	a	832	CLA	C10-C11-C12-C13
13	a	839	CLA	C15-C16-C17-C18
13	b	804	CLA	C10-C11-C12-C13
13	b	805	CLA	C10-C11-C12-C13
13	b	806	CLA	C13-C15-C16-C17
13	b	807	CLA	C5-C6-C7-C8
13	b	808	CLA	C5-C6-C7-C8
13	b	811	CLA	C5-C6-C7-C8
13	b	841	CLA	C15-C16-C17-C18
16	a	849	LHG	O1-C1-C2-O2
16	a	853	LHG	C23-C24-C25-C26
16	b	851	LHG	C23-C24-C25-C26
17	a	852	LMG	C28-C29-C30-C31
13	b	804	CLA	C4C-C3C-CAC-CBC
16	a	853	LHG	C28-C29-C30-C31
13	b	841	CLA	O1D-CGD-O2D-CED
13	a	822	CLA	C13-C15-C16-C17
13	b	828	CLA	C8-C10-C11-C12
13	b	834	CLA	O1D-CGD-O2D-CED
13	b	836	CLA	O1D-CGD-O2D-CED
13	a	854	CLA	C2-C1-O2A-CGA
13	b	822	CLA	C2-C1-O2A-CGA
13	a	818	CLA	C13-C15-C16-C17
13	a	819	CLA	C15-C16-C17-C18
13	b	827	CLA	C5-C6-C7-C8
13	a	808	CLA	O1A-CGA-O2A-C1
16	a	851	LHG	C7-C8-C9-C10
16	f	206	LHG	C23-C24-C25-C26
17	a	850	LMG	C10-C11-C12-C13
13	a	811	CLA	C5-C6-C7-C8
13	a	820	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	a	808	CLA	C6-C7-C8-C10
13	a	808	CLA	C11-C12-C13-C15
13	a	833	CLA	C11-C12-C13-C15
13	a	838	CLA	C11-C10-C8-C7
13	b	807	CLA	C11-C10-C8-C7
13	b	807	CLA	C12-C13-C15-C16
13	b	825	CLA	C11-C10-C8-C7
13	b	825	CLA	C11-C12-C13-C15
13	b	833	CLA	C6-C7-C8-C10
13	b	819	CLA	C3-C5-C6-C7
13	a	807	CLA	O1A-CGA-O2A-C1
13	a	827	CLA	C10-C11-C12-C13
13	a	829	CLA	C5-C6-C7-C8
23	j	102	LMT	O5B-C5B-C6B-O6B
15	b	844	BCR	C18-C19-C20-C21
15	b	849	BCR	C10-C11-C12-C13
16	a	851	LHG	O2-C2-C3-O3
16	f	206	LHG	O2-C2-C3-O3
13	a	804	CLA	C13-C15-C16-C17
13	b	835	CLA	C13-C15-C16-C17
13	a	825	CLA	O1A-CGA-O2A-C1
13	a	818	CLA	C5-C6-C7-C8
13	b	803	CLA	C5-C6-C7-C8
13	b	814	CLA	C5-C6-C7-C8
13	b	830	CLA	C5-C6-C7-C8
13	k	4002	CLA	C13-C15-C16-C17
13	l	1503	CLA	O1A-CGA-O2A-C1
13	k	4004	CLA	C4C-C3C-CAC-CBC
13	a	821	CLA	C8-C10-C11-C12
13	a	823	CLA	C5-C6-C7-C8
13	a	855	CLA	C13-C15-C16-C17
13	b	807	CLA	C13-C15-C16-C17
13	b	814	CLA	C13-C15-C16-C17
16	a	851	LHG	C4-O6-P-O3
13	a	824	CLA	O1D-CGD-O2D-CED
22	b	854	ZEX	C25-C26-C27-C28
16	a	851	LHG	C23-C24-C25-C26
16	a	851	LHG	C1-C2-C3-O3
16	b	851	LHG	C1-C2-C3-O3
16	f	206	LHG	C1-C2-C3-O3
13	a	821	CLA	C10-C11-C12-C13
13	b	801	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	a	836	CLA	C6-C7-C8-C9
17	b	850	LMG	C28-C29-C30-C31
13	b	842	CLA	O1A-CGA-O2A-C1
16	f	206	LHG	C11-C12-C13-C14
23	j	102	LMT	O5B-C1B-O1B-C4'
17	a	852	LMG	C30-C31-C32-C33
15	b	847	BCR	C20-C21-C22-C37
15	b	849	BCR	C20-C21-C22-C37
15	i	101	BCR	C16-C17-C18-C36
15	i	101	BCR	C20-C21-C22-C37
15	k	4005	BCR	C16-C17-C18-C36
16	a	853	LHG	C12-C13-C14-C15
13	a	824	CLA	C11-C12-C13-C15
13	a	829	CLA	C16-C17-C18-C19
13	b	841	CLA	C16-C17-C18-C20
17	b	852	LMG	C17-C18-C19-C20
17	b	850	LMG	C32-C33-C34-C35
17	b	852	LMG	C14-C15-C16-C17
17	b	852	LMG	C18-C19-C20-C21
16	a	849	LHG	C24-C25-C26-C27
16	a	851	LHG	C28-C29-C30-C31
17	b	852	LMG	C34-C35-C36-C37
13	b	809	CLA	C3-C5-C6-C7
15	a	847	BCR	C20-C21-C22-C23
15	b	849	BCR	C16-C17-C18-C19
17	b	850	LMG	C30-C31-C32-C33
17	b	850	LMG	C33-C34-C35-C36
13	a	833	CLA	O1D-CGD-O2D-CED
13	b	814	CLA	C4-C3-C5-C6
16	a	851	LHG	C27-C28-C29-C30
16	a	851	LHG	C32-C33-C34-C35
13	a	805	CLA	C11-C12-C13-C14
13	a	826	CLA	C11-C10-C8-C9
13	a	829	CLA	C11-C12-C13-C14
13	f	201	CLA	C11-C12-C13-C14
16	f	206	LHG	C7-C8-C9-C10
17	a	850	LMG	C38-C39-C40-C41
17	a	852	LMG	C32-C33-C34-C35
17	b	850	LMG	C34-C35-C36-C37
13	a	834	CLA	C5-C6-C7-C8
13	a	839	CLA	C10-C11-C12-C13
13	b	810	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	b	821	CLA	C5-C6-C7-C8
13	a	804	CLA	C2A-CAA-CBA-CGA
13	j	104	CLA	C2A-CAA-CBA-CGA
15	b	845	BCR	C36-C18-C19-C20
16	a	853	LHG	C16-C17-C18-C19
17	b	850	LMG	C39-C40-C41-C42
16	a	849	LHG	O1-C1-C2-C3
13	b	829	CLA	C8-C10-C11-C12
16	a	849	LHG	C23-C24-C25-C26
23	j	102	LMT	C11-C10-C9-C8
13	a	824	CLA	C11-C12-C13-C14
13	a	829	CLA	C16-C17-C18-C20
13	a	833	CLA	C16-C17-C18-C20
13	b	825	CLA	C13-C15-C16-C17
16	a	849	LHG	C29-C30-C31-C32
16	a	849	LHG	C34-C35-C36-C37
17	b	850	LMG	C16-C17-C18-C19
17	b	852	LMG	C30-C31-C32-C33
16	f	206	LHG	C28-C29-C30-C31
17	a	850	LMG	C16-C17-C18-C19
17	a	852	LMG	C33-C34-C35-C36
17	b	850	LMG	C37-C38-C39-C40
16	a	851	LHG	C24-C25-C26-C27
16	b	851	LHG	C24-C25-C26-C27
13	b	828	CLA	O1D-CGD-O2D-CED
13	b	840	CLA	O1D-CGD-O2D-CED
13	a	823	CLA	C3A-C2A-CAA-CBA
13	a	827	CLA	C3A-C2A-CAA-CBA
13	a	837	CLA	C3A-C2A-CAA-CBA
13	a	842	CLA	C3A-C2A-CAA-CBA
13	b	806	CLA	C3A-C2A-CAA-CBA
13	b	812	CLA	C3A-C2A-CAA-CBA
13	b	817	CLA	C3A-C2A-CAA-CBA
13	b	825	CLA	C3A-C2A-CAA-CBA
13	j	103	CLA	C3A-C2A-CAA-CBA
13	b	812	CLA	C5-C6-C7-C8
16	a	853	LHG	C29-C30-C31-C32
16	a	853	LHG	C32-C33-C34-C35
16	b	851	LHG	C28-C29-C30-C31
17	a	850	LMG	C36-C37-C38-C39
13	a	806	CLA	O1D-CGD-O2D-CED
13	b	807	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
16	a	853	LHG	C30-C31-C32-C33
17	b	852	LMG	C32-C33-C34-C35
17	b	852	LMG	C16-C17-C18-C19
13	a	855	CLA	O2A-C1-C2-C3
15	f	202	BCR	C14-C15-C16-C17
13	a	807	CLA	C8-C10-C11-C12
13	b	806	CLA	C4-C3-C5-C6
13	b	833	CLA	C4-C3-C5-C6
13	a	839	CLA	CBA-CGA-O2A-C1
13	a	819	CLA	C2-C3-C5-C6
13	b	806	CLA	C2-C3-C5-C6
17	a	852	LMG	C31-C32-C33-C34
13	b	814	CLA	C2A-CAA-CBA-CGA
16	b	851	LHG	O1-C1-C2-O2
13	a	820	CLA	C13-C15-C16-C17
13	b	841	CLA	C16-C17-C18-C19
17	a	850	LMG	C17-C18-C19-C20
13	a	813	CLA	CBA-CGA-O2A-C1
17	a	852	LMG	C13-C14-C15-C16
12	a	801	CL0	C2-C1-O2A-CGA
13	a	818	CLA	C2-C1-O2A-CGA
13	a	823	CLA	C2-C1-O2A-CGA
13	a	829	CLA	C2-C1-O2A-CGA
13	a	838	CLA	C2-C1-O2A-CGA
13	b	804	CLA	C2-C1-O2A-CGA
13	l	1502	CLA	C2-C1-O2A-CGA
13	a	823	CLA	C8-C10-C11-C12
13	b	807	CLA	C15-C16-C17-C18
13	b	840	CLA	C8-C10-C11-C12
16	a	851	LHG	C11-C12-C13-C14
16	a	853	LHG	C7-C8-C9-C10
13	a	818	CLA	C3-C5-C6-C7
13	b	834	CLA	C3-C5-C6-C7
15	a	844	BCR	C5-C6-C7-C8
15	a	845	BCR	C5-C6-C7-C8
15	a	847	BCR	C5-C6-C7-C8
15	a	847	BCR	C23-C24-C25-C26
15	b	844	BCR	C1-C6-C7-C8
15	b	844	BCR	C5-C6-C7-C8
15	b	844	BCR	C23-C24-C25-C26
15	b	844	BCR	C23-C24-C25-C30
15	b	845	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	i	102	BCR	C23-C24-C25-C26
15	i	102	BCR	C23-C24-C25-C30
15	j	101	BCR	C5-C6-C7-C8
15	j	105	BCR	C1-C6-C7-C8
15	j	105	BCR	C5-C6-C7-C8
15	k	4005	BCR	C23-C24-C25-C30
20	b	846	ECH	C1-C6-C7-C8
20	b	846	ECH	C5-C6-C7-C8
20	m	101	ECH	C5-C6-C7-C8
13	b	814	CLA	O1D-CGD-O2D-CED
13	b	826	CLA	CBA-CGA-O2A-C1
13	a	817	CLA	C10-C11-C12-C13
13	b	805	CLA	C15-C16-C17-C18
16	a	853	LHG	C11-C10-C9-C8
23	j	102	LMT	C7-C8-C9-C10
13	a	836	CLA	C5-C6-C7-C8
13	a	839	CLA	C8-C10-C11-C12
16	b	851	LHG	C26-C27-C28-C29
13	a	819	CLA	C4-C3-C5-C6
13	a	805	CLA	C11-C12-C13-C15
13	a	813	CLA	C6-C7-C8-C10
13	a	817	CLA	C11-C10-C8-C7
13	a	820	CLA	C2-C3-C5-C6
13	a	826	CLA	C11-C10-C8-C7
13	a	827	CLA	C2-C3-C5-C6
13	a	829	CLA	C11-C12-C13-C15
13	a	835	CLA	C11-C12-C13-C15
13	b	814	CLA	C2-C3-C5-C6
13	b	833	CLA	C2-C3-C5-C6
13	b	841	CLA	C11-C12-C13-C15
13	f	201	CLA	C11-C12-C13-C15
13	a	807	CLA	C3-C5-C6-C7
13	a	813	CLA	O1A-CGA-O2A-C1
13	a	839	CLA	O1A-CGA-O2A-C1
13	a	828	CLA	C15-C16-C17-C18
13	a	840	CLA	C15-C16-C17-C18
13	a	832	CLA	CBD-CGD-O2D-CED
13	a	839	CLA	CBD-CGD-O2D-CED
13	a	814	CLA	CBA-CGA-O2A-C1
13	a	833	CLA	CBA-CGA-O2A-C1
13	b	828	CLA	C2A-CAA-CBA-CGA
13	l	1501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	a	803	CLA	C15-C16-C17-C18
13	a	834	CLA	O1D-CGD-O2D-CED
16	a	849	LHG	C11-C12-C13-C14
16	a	849	LHG	C32-C33-C34-C35
13	a	821	CLA	C16-C17-C18-C20
13	k	4002	CLA	C16-C17-C18-C19
13	b	815	CLA	C15-C16-C17-C18
13	a	814	CLA	O1D-CGD-O2D-CED
13	f	203	CLA	O1D-CGD-O2D-CED
16	a	849	LHG	C15-C16-C17-C18
16	a	849	LHG	C26-C27-C28-C29
16	a	849	LHG	C8-C7-O7-C5
17	b	852	LMG	C11-C10-O7-C8
15	i	102	BCR	C18-C19-C20-C21
16	f	206	LHG	C24-C25-C26-C27
13	b	805	CLA	C13-C15-C16-C17
13	b	833	CLA	CBD-CGD-O2D-CED
16	f	206	LHG	C32-C33-C34-C35
13	b	820	CLA	C3-C5-C6-C7
17	a	850	LMG	O7-C8-C9-O8
13	a	836	CLA	C6-C7-C8-C10
13	j	104	CLA	O1D-CGD-O2D-CED
13	a	820	CLA	C4-C3-C5-C6
13	a	827	CLA	C4-C3-C5-C6
13	a	811	CLA	C14-C13-C15-C16
13	a	823	CLA	C14-C13-C15-C16
13	a	829	CLA	C14-C13-C15-C16
13	a	835	CLA	C11-C12-C13-C14
13	a	840	CLA	C11-C12-C13-C14
13	b	819	CLA	C11-C10-C8-C9
13	b	819	CLA	C14-C13-C15-C16
13	b	824	CLA	C11-C10-C8-C9
13	b	833	CLA	C6-C7-C8-C9
13	b	841	CLA	C11-C12-C13-C14
13	b	808	CLA	C3-C5-C6-C7
13	a	830	CLA	C2A-CAA-CBA-CGA
13	b	835	CLA	C2A-CAA-CBA-CGA
13	b	826	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	C1A-C2A-CAA-CBA
13	a	805	CLA	C1A-C2A-CAA-CBA
13	a	807	CLA	C1A-C2A-CAA-CBA
13	a	809	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	a	810	CLA	C1A-C2A-CAA-CBA
13	a	814	CLA	C1A-C2A-CAA-CBA
13	a	826	CLA	C1A-C2A-CAA-CBA
13	a	827	CLA	C1A-C2A-CAA-CBA
13	a	831	CLA	C1A-C2A-CAA-CBA
13	a	837	CLA	C1A-C2A-CAA-CBA
13	a	841	CLA	C1A-C2A-CAA-CBA
13	a	842	CLA	C1A-C2A-CAA-CBA
13	b	826	CLA	C1A-C2A-CAA-CBA
13	k	4003	CLA	C1A-C2A-CAA-CBA
13	k	4004	CLA	C1A-C2A-CAA-CBA
13	a	821	CLA	C16-C17-C18-C19
13	b	807	CLA	C16-C17-C18-C19
13	b	825	CLA	C5-C6-C7-C8
12	a	801	CL0	C3-C5-C6-C7
13	a	841	CLA	C3-C5-C6-C7
13	b	811	CLA	C3-C5-C6-C7
13	a	803	CLA	C5-C6-C7-C8
13	a	825	CLA	C13-C15-C16-C17
13	a	816	CLA	O1D-CGD-O2D-CED
16	b	851	LHG	C33-C34-C35-C36
13	a	818	CLA	C16-C17-C18-C20
22	f	205	ZEX	C25-C26-C27-C28
17	a	850	LMG	C32-C33-C34-C35
16	a	849	LHG	C28-C29-C30-C31
16	a	853	LHG	C34-C35-C36-C37
13	b	804	CLA	C2A-CAA-CBA-CGA
13	a	833	CLA	C16-C17-C18-C19
16	b	851	LHG	C30-C31-C32-C33
13	b	826	CLA	C6-C7-C8-C10
13	a	814	CLA	O1A-CGA-O2A-C1
15	b	849	BCR	C11-C10-C9-C34
15	f	202	BCR	C35-C13-C14-C15
15	i	102	BCR	C20-C21-C22-C37
13	a	833	CLA	C4-C3-C5-C6
13	b	815	CLA	C4-C3-C5-C6
13	b	815	CLA	C2-C3-C5-C6
13	a	837	CLA	CBA-CGA-O2A-C1
13	b	811	CLA	CBA-CGA-O2A-C1
13	k	4003	CLA	CBD-CGD-O2D-CED
13	a	841	CLA	C5-C6-C7-C8
13	l	1502	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	a	849	LHG	C30-C31-C32-C33
13	a	802	CLA	C2A-CAA-CBA-CGA
13	b	824	CLA	C2A-CAA-CBA-CGA
13	a	805	CLA	C5-C6-C7-C8
13	a	855	CLA	C5-C6-C7-C8
13	b	801	CLA	C5-C6-C7-C8
13	a	822	CLA	C2-C1-O2A-CGA
13	a	824	CLA	C2-C1-O2A-CGA
13	a	825	CLA	C2-C1-O2A-CGA
13	a	855	CLA	C2-C1-O2A-CGA
13	b	803	CLA	C2-C1-O2A-CGA
13	b	808	CLA	C2-C1-O2A-CGA
13	b	825	CLA	C2-C1-O2A-CGA
13	b	838	CLA	C2-C1-O2A-CGA
16	a	849	LHG	C18-C19-C20-C21
17	a	850	LMG	C29-C30-C31-C32
17	b	852	LMG	C13-C14-C15-C16
13	a	829	CLA	C15-C16-C17-C18
13	a	833	CLA	O1A-CGA-O2A-C1
16	b	851	LHG	O6-C4-C5-O7
13	a	818	CLA	C16-C17-C18-C19
12	a	801	CL0	C5-C6-C7-C8
13	b	809	CLA	C5-C6-C7-C8
17	b	852	LMG	C2-C1-O1-C7
13	k	4002	CLA	C15-C16-C17-C18
13	a	806	CLA	C12-C13-C15-C16
13	a	807	CLA	C11-C12-C13-C15
13	a	811	CLA	C12-C13-C15-C16
13	a	820	CLA	C6-C7-C8-C10
13	a	820	CLA	C11-C12-C13-C15
13	a	821	CLA	C11-C12-C13-C15
13	a	823	CLA	C11-C12-C13-C15
13	a	823	CLA	C12-C13-C15-C16
13	a	829	CLA	C12-C13-C15-C16
13	a	833	CLA	C2-C3-C5-C6
13	a	833	CLA	C11-C10-C8-C7
13	a	834	CLA	C6-C7-C8-C10
13	a	839	CLA	C12-C13-C15-C16
13	a	841	CLA	C11-C12-C13-C15
13	b	801	CLA	C6-C7-C8-C10
13	b	803	CLA	C11-C10-C8-C7
13	b	804	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	b	805	CLA	C12-C13-C15-C16
13	b	814	CLA	C11-C12-C13-C15
13	b	815	CLA	C11-C10-C8-C7
13	b	815	CLA	C12-C13-C15-C16
13	b	819	CLA	C11-C10-C8-C7
13	b	819	CLA	C12-C13-C15-C16
13	b	824	CLA	C11-C10-C8-C7
13	b	828	CLA	C11-C12-C13-C15
13	b	835	CLA	C11-C10-C8-C7
13	b	835	CLA	C11-C12-C13-C15
13	b	838	CLA	C6-C7-C8-C10
13	b	840	CLA	C6-C7-C8-C10
13	f	201	CLA	C6-C7-C8-C10
13	k	4002	CLA	C12-C13-C15-C16
13	l	1502	CLA	C11-C12-C13-C15
16	f	206	LHG	C29-C30-C31-C32
13	a	806	CLA	C6-C7-C8-C9
13	a	806	CLA	C11-C12-C13-C14
13	a	806	CLA	C14-C13-C15-C16
13	a	807	CLA	C11-C12-C13-C14
13	a	808	CLA	C6-C7-C8-C9
13	a	811	CLA	C11-C12-C13-C14
13	a	813	CLA	C11-C12-C13-C14
13	a	817	CLA	C11-C12-C13-C14
13	a	819	CLA	C14-C13-C15-C16
13	a	820	CLA	C11-C12-C13-C14
13	a	822	CLA	C11-C10-C8-C9
13	a	830	CLA	C6-C7-C8-C9
13	a	833	CLA	C11-C10-C8-C9
13	a	839	CLA	C14-C13-C15-C16
13	a	841	CLA	C6-C7-C8-C9
13	b	801	CLA	C6-C7-C8-C9
13	b	803	CLA	C11-C10-C8-C9
13	b	803	CLA	C11-C12-C13-C14
13	b	804	CLA	C11-C10-C8-C9
13	b	815	CLA	C14-C13-C15-C16
13	b	825	CLA	C6-C7-C8-C9
13	b	825	CLA	C11-C10-C8-C9
13	b	828	CLA	C11-C12-C13-C14
13	b	833	CLA	C11-C10-C8-C9
13	b	834	CLA	C11-C10-C8-C9
13	b	835	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	b	835	CLA	C11-C12-C13-C14
13	b	838	CLA	C6-C7-C8-C9
13	f	201	CLA	C6-C7-C8-C9
13	k	4002	CLA	C6-C7-C8-C9
13	k	4002	CLA	C14-C13-C15-C16
13	l	1502	CLA	C11-C12-C13-C14
13	a	839	CLA	C5-C6-C7-C8
13	a	819	CLA	C16-C17-C18-C20
13	a	820	CLA	C16-C17-C18-C20
13	b	826	CLA	C6-C7-C8-C9
15	b	845	BCR	C21-C22-C23-C24
15	b	849	BCR	C11-C12-C13-C14
13	b	816	CLA	C3-C5-C6-C7
13	a	841	CLA	C8-C10-C11-C12
13	b	819	CLA	C13-C15-C16-C17
17	a	850	LMG	C15-C16-C17-C18
17	b	852	LMG	C33-C34-C35-C36
16	a	853	LHG	O6-C4-C5-C6
16	b	851	LHG	O6-C4-C5-C6
13	a	812	CLA	C4-C3-C5-C6
13	a	807	CLA	C16-C17-C18-C20
13	a	855	CLA	C16-C17-C18-C20
13	a	804	CLA	C3A-C2A-CAA-CBA
13	a	807	CLA	C3A-C2A-CAA-CBA
13	a	810	CLA	C3A-C2A-CAA-CBA
13	a	811	CLA	C3A-C2A-CAA-CBA
13	a	812	CLA	C3A-C2A-CAA-CBA
13	a	817	CLA	C3A-C2A-CAA-CBA
13	a	828	CLA	C3A-C2A-CAA-CBA
13	b	813	CLA	C3A-C2A-CAA-CBA
13	b	840	CLA	C3A-C2A-CAA-CBA
13	l	1502	CLA	C3A-C2A-CAA-CBA
17	a	850	LMG	C12-C13-C14-C15
13	a	810	CLA	CBA-CGA-O2A-C1
17	b	850	LMG	C7-C8-C9-O8
13	b	811	CLA	O1A-CGA-O2A-C1
13	b	804	CLA	O2A-C1-C2-C3
13	b	841	CLA	C10-C11-C12-C13
17	b	852	LMG	C41-C42-C43-C44
13	b	829	CLA	CBD-CGD-O2D-CED
13	f	201	CLA	C15-C16-C17-C18
13	a	837	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	821	CLA	C2A-CAA-CBA-CGA
13	a	805	CLA	C10-C11-C12-C13
13	a	820	CLA	C16-C17-C18-C19
17	a	850	LMG	C11-C12-C13-C14
16	a	849	LHG	O7-C5-C6-O8
13	b	821	CLA	C15-C16-C17-C18
16	f	206	LHG	C30-C31-C32-C33
13	a	817	CLA	C2-C1-O2A-CGA
13	a	825	CLA	C11-C12-C13-C14
13	a	827	CLA	C14-C13-C15-C16
13	a	833	CLA	C11-C12-C13-C14
13	a	835	CLA	C14-C13-C15-C16
13	b	805	CLA	C6-C7-C8-C9
13	b	807	CLA	C11-C10-C8-C9
13	b	815	CLA	C6-C7-C8-C9
13	b	825	CLA	C11-C12-C13-C14
13	b	835	CLA	C14-C13-C15-C16
13	a	820	CLA	C8-C10-C11-C12
22	b	854	ZEX	C21-C26-C27-C28
22	f	205	ZEX	C21-C26-C27-C28
13	a	803	CLA	C2A-CAA-CBA-CGA
13	b	831	CLA	C2A-CAA-CBA-CGA
13	a	819	CLA	C16-C17-C18-C19
13	a	831	CLA	C3-C5-C6-C7
15	a	845	BCR	C23-C24-C25-C26
15	a	845	BCR	C23-C24-C25-C30
15	a	846	BCR	C1-C6-C7-C8
15	a	846	BCR	C5-C6-C7-C8
15	a	848	BCR	C1-C6-C7-C8
15	a	848	BCR	C5-C6-C7-C8
15	b	847	BCR	C23-C24-C25-C26
15	b	847	BCR	C23-C24-C25-C30
15	i	102	BCR	C1-C6-C7-C8
15	i	102	BCR	C5-C6-C7-C8
15	j	105	BCR	C23-C24-C25-C26
15	k	4001	BCR	C1-C6-C7-C8
15	k	4001	BCR	C5-C6-C7-C8
13	b	807	CLA	C10-C11-C12-C13
17	a	850	LMG	C19-C20-C21-C22
17	b	850	LMG	C15-C16-C17-C18
16	a	853	LHG	C33-C34-C35-C36
13	a	839	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	a	848	BCR	C11-C12-C13-C14
15	a	848	BCR	C16-C17-C18-C36
15	b	848	BCR	C21-C22-C23-C24
13	a	808	CLA	C10-C11-C12-C13
13	b	822	CLA	C11-C12-C13-C15
13	k	4002	CLA	C16-C17-C18-C20
14	b	843	PQN	C13-C15-C16-C17
13	a	832	CLA	O1D-CGD-O2D-CED
17	b	850	LMG	O10-C28-O8-C9
17	b	850	LMG	C38-C39-C40-C41
17	b	852	LMG	C37-C38-C39-C40
13	a	806	CLA	C11-C12-C13-C15
13	a	818	CLA	C11-C10-C8-C7
13	a	819	CLA	C12-C13-C15-C16
13	a	822	CLA	C11-C10-C8-C7
13	a	825	CLA	C11-C12-C13-C15
13	a	826	CLA	C12-C13-C15-C16
13	a	827	CLA	C11-C10-C8-C7
13	a	827	CLA	C12-C13-C15-C16
13	a	830	CLA	C6-C7-C8-C10
13	a	835	CLA	C6-C7-C8-C10
13	a	841	CLA	C6-C7-C8-C10
13	b	801	CLA	C11-C10-C8-C7
13	b	806	CLA	C12-C13-C15-C16
13	b	808	CLA	C6-C7-C8-C10
13	b	815	CLA	C6-C7-C8-C10
13	b	818	CLA	C11-C10-C8-C7
13	b	825	CLA	C6-C7-C8-C10
13	b	833	CLA	C11-C10-C8-C7
13	b	835	CLA	C12-C13-C15-C16
13	k	4002	CLA	C6-C7-C8-C10
13	a	855	CLA	C16-C17-C18-C19
17	b	850	LMG	C41-C42-C43-C44
13	b	838	CLA	C5-C6-C7-C8
13	a	823	CLA	C13-C15-C16-C17
15	a	845	BCR	C20-C21-C22-C37
15	a	846	BCR	C16-C17-C18-C36
13	b	803	CLA	C3-C5-C6-C7
13	b	807	CLA	C3-C5-C6-C7
13	a	804	CLA	C16-C17-C18-C20
13	a	807	CLA	C16-C17-C18-C19
13	f	201	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	b	805	CLA	CBA-CGA-O2A-C1
17	b	850	LMG	C31-C32-C33-C34
13	a	808	CLA	C15-C16-C17-C18
13	b	819	CLA	C10-C11-C12-C13
13	a	810	CLA	O1A-CGA-O2A-C1
13	a	808	CLA	CAD-CBD-CGD-O2D
13	a	825	CLA	CAD-CBD-CGD-O2D
13	b	813	CLA	CAD-CBD-CGD-O2D
13	b	817	CLA	CAD-CBD-CGD-O2D
13	b	819	CLA	CAD-CBD-CGD-O2D
13	b	830	CLA	CAD-CBD-CGD-O2D
13	b	833	CLA	CAD-CBD-CGD-O2D
13	b	839	CLA	CAD-CBD-CGD-O2D
16	a	853	LHG	C6-C5-O7-C7
15	a	846	BCR	C22-C23-C24-C25
15	b	844	BCR	C6-C7-C8-C9
15	i	102	BCR	C22-C23-C24-C25
15	j	105	BCR	C6-C7-C8-C9
13	b	824	CLA	CBA-CGA-O2A-C1
17	b	852	LMG	O1-C7-C8-C9
16	a	853	LHG	O6-C4-C5-O7
13	a	802	CLA	C10-C11-C12-C13
13	a	838	CLA	C8-C10-C11-C12
13	a	838	CLA	C10-C11-C12-C13
16	a	851	LHG	C10-C11-C12-C13
13	f	204	CLA	C2A-CAA-CBA-CGA
13	f	201	CLA	C8-C10-C11-C12
23	j	102	LMT	C3-C4-C5-C6
13	b	833	CLA	O1D-CGD-O2D-CED
13	a	804	CLA	CHA-CBD-CGD-O2D
13	a	822	CLA	CHA-CBD-CGD-O1D
13	a	834	CLA	CHA-CBD-CGD-O1D
13	a	834	CLA	CHA-CBD-CGD-O2D
13	a	839	CLA	CHA-CBD-CGD-O1D
13	a	839	CLA	CHA-CBD-CGD-O2D
13	b	806	CLA	CHA-CBD-CGD-O1D
13	b	806	CLA	CHA-CBD-CGD-O2D
13	b	822	CLA	CHA-CBD-CGD-O1D
13	b	837	CLA	CHA-CBD-CGD-O1D
13	b	837	CLA	CHA-CBD-CGD-O2D
13	f	204	CLA	CHA-CBD-CGD-O1D
13	l	1501	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	l	1501	CLA	CHA-CBD-CGD-O2D
15	a	846	BCR	C12-C13-C14-C15
16	a	853	LHG	C24-C25-C26-C27
13	b	828	CLA	C4-C3-C5-C6
13	a	827	CLA	C11-C10-C8-C9
13	a	833	CLA	C14-C13-C15-C16
13	f	201	CLA	C3-C5-C6-C7
13	a	816	CLA	C2A-CAA-CBA-CGA
13	k	4004	CLA	C2A-CAA-CBA-CGA
13	b	809	CLA	C10-C11-C12-C13
13	k	4003	CLA	O1D-CGD-O2D-CED
15	j	101	BCR	C21-C22-C23-C24
13	a	806	CLA	C3-C5-C6-C7
16	a	853	LHG	C13-C14-C15-C16
13	a	811	CLA	C1A-C2A-CAA-CBA
13	b	806	CLA	C1A-C2A-CAA-CBA
13	b	841	CLA	C1A-C2A-CAA-CBA
13	j	104	CLA	C1A-C2A-CAA-CBA
13	a	840	CLA	C2-C1-O2A-CGA
13	b	828	CLA	C2-C1-O2A-CGA
13	a	839	CLA	C4-C3-C5-C6
23	j	102	LMT	O1'-C1-C2-C3
13	b	805	CLA	O1A-CGA-O2A-C1
16	a	851	LHG	C4-O6-P-O5
16	b	851	LHG	C3-O3-P-O5
16	f	206	LHG	C3-O3-P-O4
13	a	840	CLA	C16-C17-C18-C19
13	b	821	CLA	C16-C17-C18-C20
13	b	822	CLA	C11-C12-C13-C14
13	a	825	CLA	C5-C6-C7-C8
12	a	801	CL0	CBD-CGD-O2D-CED
17	a	850	LMG	C18-C19-C20-C21
13	a	832	CLA	C3-C5-C6-C7
13	b	810	CLA	C3-C5-C6-C7
17	b	852	LMG	C42-C43-C44-C45
13	a	818	CLA	CAD-CBD-CGD-O1D
13	a	822	CLA	CAD-CBD-CGD-O1D
13	a	823	CLA	CAD-CBD-CGD-O1D
13	b	831	CLA	C2-C3-C5-C6
13	b	828	CLA	C10-C11-C12-C13
17	a	850	LMG	C37-C38-C39-C40
13	a	807	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	a	824	CLA	C6-C7-C8-C10
13	a	825	CLA	C12-C13-C15-C16
13	a	828	CLA	C11-C12-C13-C15
13	a	832	CLA	C11-C10-C8-C7
13	a	833	CLA	C12-C13-C15-C16
13	a	838	CLA	C11-C12-C13-C15
13	a	840	CLA	C6-C7-C8-C10
13	a	855	CLA	C11-C12-C13-C15
13	b	810	CLA	C11-C10-C8-C7
13	b	814	CLA	C12-C13-C15-C16
13	b	820	CLA	C11-C10-C8-C7
13	b	829	CLA	C11-C12-C13-C15
13	b	832	CLA	C3A-C2A-CAA-CBA
13	b	833	CLA	C12-C13-C15-C16
13	b	841	CLA	C12-C13-C15-C16
17	b	850	LMG	C42-C43-C44-C45
13	a	854	CLA	C5-C6-C7-C8
16	b	851	LHG	C8-C7-O7-C5
13	b	824	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	C27-C28-C29-C30
13	a	841	CLA	C2A-CAA-CBA-CGA
13	b	829	CLA	O1D-CGD-O2D-CED
17	a	850	LMG	C42-C43-C44-C45
23	j	102	LMT	C6-C7-C8-C9
17	a	852	LMG	C4-C5-C6-O5
17	a	850	LMG	C7-C8-C9-O8
17	b	852	LMG	O1-C7-C8-O7
17	a	850	LMG	C41-C42-C43-C44
13	b	811	CLA	CAA-CBA-CGA-O2A
17	a	850	LMG	C34-C35-C36-C37
13	a	817	CLA	C14-C13-C15-C16
13	a	823	CLA	C11-C10-C8-C9
13	a	826	CLA	C14-C13-C15-C16
13	a	840	CLA	C6-C7-C8-C9
13	b	806	CLA	C14-C13-C15-C16
20	b	846	ECH	C22-C23-C24-C25
16	a	851	LHG	C15-C16-C17-C18
13	a	804	CLA	C16-C17-C18-C19
13	f	201	CLA	C16-C17-C18-C19
13	b	828	CLA	C2-C3-C5-C6
13	b	819	CLA	C8-C10-C11-C12
13	a	832	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	b	811	CLA	C2A-CAA-CBA-CGA
13	b	816	CLA	C2A-CAA-CBA-CGA
13	a	834	CLA	C2-C1-O2A-CGA
13	b	811	CLA	C2-C1-O2A-CGA
13	b	817	CLA	C2-C1-O2A-CGA
13	l	1501	CLA	C2-C1-O2A-CGA
16	a	853	LHG	C10-C11-C12-C13
15	b	849	BCR	C15-C16-C17-C18
15	a	844	BCR	C23-C24-C25-C30
15	f	202	BCR	C1-C6-C7-C8
15	f	202	BCR	C5-C6-C7-C8
15	i	101	BCR	C1-C6-C7-C8
15	j	101	BCR	C23-C24-C25-C26
15	j	101	BCR	C23-C24-C25-C30
15	k	4005	BCR	C23-C24-C25-C26
20	m	101	ECH	C1-C6-C7-C8
20	m	101	ECH	C23-C24-C25-C26
13	b	815	CLA	C8-C10-C11-C12
17	b	850	LMG	C17-C18-C19-C20
13	a	813	CLA	C2A-CAA-CBA-CGA
16	a	849	LHG	C3-O3-P-O6
16	a	851	LHG	C3-O3-P-O6
16	a	853	LHG	C3-O3-P-O6
16	b	851	LHG	C4-O6-P-O3
16	f	206	LHG	C3-O3-P-O6
16	a	851	LHG	C31-C32-C33-C34
13	b	835	CLA	C4-C3-C5-C6
13	a	811	CLA	C11-C12-C13-C15
13	a	813	CLA	C11-C12-C13-C15
13	b	803	CLA	C11-C12-C13-C15
13	b	805	CLA	C6-C7-C8-C10
13	a	821	CLA	C11-C12-C13-C14
13	a	832	CLA	C11-C10-C8-C9
13	a	838	CLA	C11-C12-C13-C14
13	b	814	CLA	C6-C7-C8-C9
13	b	814	CLA	C14-C13-C15-C16
15	b	849	BCR	C13-C14-C15-C16
13	a	840	CLA	C16-C17-C18-C20
12	a	801	CL0	C2A-CAA-CBA-CGA
13	a	837	CLA	C2A-CAA-CBA-CGA
13	b	810	CLA	C5-C6-C7-C8
17	a	852	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	b	821	CLA	C16-C17-C18-C19
13	b	827	CLA	CBA-CGA-O2A-C1
16	a	853	LHG	C14-C15-C16-C17
15	k	4001	BCR	C7-C8-C9-C10
13	a	812	CLA	C2-C3-C5-C6
23	j	102	LMT	C5'-C4'-O1B-C1B
16	a	853	LHG	C25-C26-C27-C28
13	b	827	CLA	O1A-CGA-O2A-C1
13	b	813	CLA	C2A-CAA-CBA-CGA
15	b	848	BCR	C9-C10-C11-C12
13	a	828	CLA	CBD-CGD-O2D-CED
16	f	206	LHG	C26-C27-C28-C29
13	a	840	CLA	CBD-CGD-O2D-CED
16	b	851	LHG	C7-C8-C9-C10
13	b	829	CLA	C16-C17-C18-C19
13	a	818	CLA	C4-C3-C5-C6
13	a	828	CLA	C4-C3-C5-C6
16	a	849	LHG	C12-C13-C14-C15
16	b	851	LHG	C27-C28-C29-C30
16	a	849	LHG	C35-C36-C37-C38
17	b	850	LMG	C35-C36-C37-C38
12	a	801	CL0	O1D-CGD-O2D-CED
13	a	811	CLA	C2A-CAA-CBA-CGA
13	a	812	CLA	C2A-CAA-CBA-CGA
13	a	831	CLA	C2A-CAA-CBA-CGA
13	a	854	CLA	C2A-CAA-CBA-CGA
13	a	830	CLA	C3A-C2A-CAA-CBA
13	a	834	CLA	C3A-C2A-CAA-CBA
13	b	820	CLA	C3A-C2A-CAA-CBA
13	a	823	CLA	C16-C17-C18-C20
13	b	841	CLA	C2C-C3C-CAC-CBC
16	a	849	LHG	C33-C34-C35-C36
13	a	804	CLA	C11-C10-C8-C9
13	a	813	CLA	C6-C7-C8-C9
13	a	819	CLA	C11-C12-C13-C14
13	a	854	CLA	C14-C13-C15-C16
13	a	855	CLA	C11-C12-C13-C14
13	b	804	CLA	C6-C7-C8-C9
13	b	804	CLA	C11-C12-C13-C14
13	b	819	CLA	C6-C7-C8-C9
13	b	825	CLA	C14-C13-C15-C16
13	b	838	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	b	840	CLA	C14-C13-C15-C16
13	a	834	CLA	C16-C17-C18-C19
17	a	850	LMG	C30-C31-C32-C33
18	a	856	45D	C28-C26-C30-C32
18	a	856	45D	C39-C35-C37-C41
20	b	846	ECH	C11-C10-C9-C34
20	b	846	ECH	C35-C13-C14-C15
21	b	853	EQ3	C11-C10-C9-C34
22	f	205	ZEX	C20-C13-C14-C15
23	j	102	LMT	C1-C2-C3-C4
16	f	206	LHG	C14-C15-C16-C17
13	b	835	CLA	C5-C6-C7-C8
13	b	820	CLA	CBD-CGD-O2D-CED
13	b	832	CLA	C1A-C2A-CAA-CBA
13	a	813	CLA	C11-C10-C8-C7
13	a	818	CLA	C11-C12-C13-C15
13	a	855	CLA	C6-C7-C8-C10
13	b	818	CLA	C11-C12-C13-C15
13	b	821	CLA	C6-C7-C8-C10
13	b	827	CLA	C11-C12-C13-C15
13	a	838	CLA	C13-C15-C16-C17
13	b	809	CLA	CBA-CGA-O2A-C1
17	a	852	LMG	C14-C15-C16-C17
13	b	836	CLA	C2A-CAA-CBA-CGA
13	a	804	CLA	C5-C6-C7-C8
16	a	849	LHG	O9-C7-O7-C5
13	a	833	CLA	C13-C15-C16-C17
13	a	817	CLA	CBA-CGA-O2A-C1
16	b	851	LHG	C29-C30-C31-C32
13	b	835	CLA	C2-C3-C5-C6
13	b	822	CLA	C10-C11-C12-C13
15	i	101	BCR	C16-C17-C18-C19
18	a	856	45D	C24-C26-C30-C32
18	a	856	45D	C33-C35-C37-C41
20	b	846	ECH	C11-C10-C9-C8
20	b	846	ECH	C12-C13-C14-C15
21	b	853	EQ3	C11-C10-C9-C8
22	f	205	ZEX	C12-C13-C14-C15
16	b	851	LHG	C24-C23-O8-C6
17	a	852	LMG	C29-C28-O8-C9
15	a	848	BCR	C13-C14-C15-C16
15	j	101	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	b	840	CLA	C5-C6-C7-C8
13	b	841	CLA	C4-C3-C5-C6
13	a	828	CLA	O1D-CGD-O2D-CED
13	a	817	CLA	O1A-CGA-O2A-C1
13	b	820	CLA	O1D-CGD-O2D-CED
13	b	840	CLA	C11-C12-C13-C14
13	b	803	CLA	C8-C10-C11-C12
13	b	818	CLA	C15-C16-C17-C18
13	a	828	CLA	C2A-CAA-CBA-CGA
13	a	839	CLA	C2A-CAA-CBA-CGA
13	b	830	CLA	C2A-CAA-CBA-CGA
15	a	846	BCR	C23-C24-C25-C30
15	b	847	BCR	C1-C6-C7-C8
15	b	848	BCR	C1-C6-C7-C8
15	b	848	BCR	C23-C24-C25-C30
15	b	849	BCR	C23-C24-C25-C30
15	f	202	BCR	C23-C24-C25-C30
15	i	101	BCR	C5-C6-C7-C8
15	i	101	BCR	C23-C24-C25-C30
15	k	4001	BCR	C23-C24-C25-C30
15	k	4005	BCR	C1-C6-C7-C8
20	b	846	ECH	C23-C24-C25-C26
20	m	101	ECH	C23-C24-C25-C30
13	b	807	CLA	C4-C3-C5-C6
15	a	844	BCR	C21-C22-C23-C24
13	a	842	CLA	CAA-CBA-CGA-O2A
13	a	821	CLA	C3-C5-C6-C7
13	l	1502	CLA	C10-C11-C12-C13
13	a	808	CLA	C8-C10-C11-C12
13	a	805	CLA	CAA-CBA-CGA-O2A
13	l	1503	CLA	CAA-CBA-CGA-O2A
13	f	204	CLA	CAA-CBA-CGA-O2A
13	a	840	CLA	O1D-CGD-O2D-CED
16	a	851	LHG	O6-C4-C5-C6
13	b	821	CLA	C4-C3-C5-C6
13	a	817	CLA	C12-C13-C15-C16
13	a	819	CLA	C11-C12-C13-C15
13	a	835	CLA	C12-C13-C15-C16
13	a	839	CLA	C16-C17-C18-C19
13	b	815	CLA	C16-C17-C18-C20
17	a	852	LMG	C15-C16-C17-C18
16	a	853	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
13	b	804	CLA	C8-C10-C11-C12
13	b	812	CLA	CAA-CBA-CGA-O2A
16	a	849	LHG	C27-C28-C29-C30
13	a	832	CLA	C4-C3-C5-C6
13	a	834	CLA	C4-C3-C5-C6
13	b	819	CLA	C5-C6-C7-C8
13	a	839	CLA	C2-C3-C5-C6
17	a	850	LMG	C14-C15-C16-C17
13	a	813	CLA	C11-C10-C8-C9
13	a	824	CLA	C6-C7-C8-C9
13	a	828	CLA	C11-C12-C13-C14
13	b	805	CLA	C11-C10-C8-C9
13	b	810	CLA	C11-C10-C8-C9
13	b	822	CLA	C11-C10-C8-C9
13	b	833	CLA	C14-C13-C15-C16
13	b	835	CLA	C6-C7-C8-C9
13	b	841	CLA	C14-C13-C15-C16
13	a	802	CLA	C3A-C2A-CAA-CBA
13	b	811	CLA	C3A-C2A-CAA-CBA
13	a	811	CLA	C8-C10-C11-C12
17	b	850	LMG	C36-C37-C38-C39
13	a	803	CLA	CAD-CBD-CGD-O2D
13	a	807	CLA	CAD-CBD-CGD-O2D
13	a	811	CLA	CAD-CBD-CGD-O2D
13	a	812	CLA	CAD-CBD-CGD-O2D
13	a	826	CLA	CAD-CBD-CGD-O2D
13	a	830	CLA	CAD-CBD-CGD-O2D
13	a	833	CLA	CAD-CBD-CGD-O2D
13	a	841	CLA	CAD-CBD-CGD-O2D
13	b	835	CLA	CAD-CBD-CGD-O2D
13	j	103	CLA	CAD-CBD-CGD-O2D
13	l	1503	CLA	CAD-CBD-CGD-O2D
13	b	819	CLA	CBA-CGA-O2A-C1
13	b	834	CLA	C2-C1-O2A-CGA
13	a	806	CLA	CAA-CBA-CGA-O2A
13	a	839	CLA	CAA-CBA-CGA-O2A
13	j	103	CLA	CAA-CBA-CGA-O2A
13	b	804	CLA	C4-C3-C5-C6
13	a	842	CLA	CAA-CBA-CGA-O1A
13	f	204	CLA	CAA-CBA-CGA-O1A
17	b	850	LMG	C18-C19-C20-C21
15	a	847	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	a	848	BCR	C7-C8-C9-C10
16	a	849	LHG	C4-C5-C6-O8
16	a	853	LHG	C4-C5-C6-O8
13	a	818	CLA	C15-C16-C17-C18
13	a	830	CLA	CAA-CBA-CGA-O2A
13	a	831	CLA	CAA-CBA-CGA-O2A
13	b	836	CLA	CAA-CBA-CGA-O2A
13	a	802	CLA	O2A-C1-C2-C3
13	a	807	CLA	O2A-C1-C2-C3
13	a	818	CLA	O2A-C1-C2-C3
13	a	820	CLA	O2A-C1-C2-C3
13	a	823	CLA	O2A-C1-C2-C3
13	b	808	CLA	O2A-C1-C2-C3
13	b	817	CLA	O2A-C1-C2-C3
13	b	828	CLA	O2A-C1-C2-C3
13	b	838	CLA	O2A-C1-C2-C3
13	l	1503	CLA	O2A-C1-C2-C3
13	b	819	CLA	O1A-CGA-O2A-C1
13	a	825	CLA	C15-C16-C17-C18
13	a	811	CLA	CAA-CBA-CGA-O2A
13	b	809	CLA	O1A-CGA-O2A-C1
13	a	802	CLA	CHA-CBD-CGD-O1D
13	a	802	CLA	CHA-CBD-CGD-O2D
13	a	805	CLA	CHA-CBD-CGD-O1D
13	a	805	CLA	CHA-CBD-CGD-O2D
13	a	822	CLA	CHA-CBD-CGD-O2D
13	a	829	CLA	CHA-CBD-CGD-O1D
13	a	829	CLA	CHA-CBD-CGD-O2D
13	a	840	CLA	CHA-CBD-CGD-O1D
13	a	840	CLA	CHA-CBD-CGD-O2D
13	a	842	CLA	CHA-CBD-CGD-O2D
13	b	808	CLA	CHA-CBD-CGD-O1D
13	b	808	CLA	CHA-CBD-CGD-O2D
13	b	822	CLA	CHA-CBD-CGD-O2D
13	b	824	CLA	CHA-CBD-CGD-O2D
13	b	838	CLA	CHA-CBD-CGD-O1D
13	b	838	CLA	CHA-CBD-CGD-O2D
13	b	842	CLA	CHA-CBD-CGD-O1D
13	b	842	CLA	CHA-CBD-CGD-O2D
13	f	204	CLA	CHA-CBD-CGD-O2D
13	a	832	CLA	CAA-CBA-CGA-O2A
17	a	852	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	a	820	CLA	CAA-CBA-CGA-O2A
13	a	829	CLA	CAA-CBA-CGA-O2A
13	b	830	CLA	CAA-CBA-CGA-O2A
13	a	840	CLA	C5-C6-C7-C8
17	a	852	LMG	C10-C11-C12-C13
13	b	817	CLA	CAA-CBA-CGA-O2A
13	a	821	CLA	C2-C3-C5-C6
13	a	834	CLA	C2-C3-C5-C6
13	b	824	CLA	C2-C3-C5-C6
13	a	838	CLA	C16-C17-C18-C20
17	a	850	LMG	C31-C32-C33-C34
16	f	206	LHG	C25-C26-C27-C28
13	a	818	CLA	C11-C12-C13-C14
13	a	820	CLA	C6-C7-C8-C9
13	a	855	CLA	C6-C7-C8-C9
13	b	827	CLA	C11-C12-C13-C14
13	b	829	CLA	C11-C12-C13-C14
16	a	853	LHG	C9-C10-C11-C12
16	a	849	LHG	C11-C10-C9-C8
17	b	850	LMG	O7-C10-C11-C12
16	b	851	LHG	C25-C26-C27-C28
13	a	831	CLA	C2C-C3C-CAC-CBC
13	a	831	CLA	C4C-C3C-CAC-CBC
22	f	205	ZEX	C27-C28-C29-C39
13	b	836	CLA	CAA-CBA-CGA-O1A
13	b	829	CLA	C16-C17-C18-C20
16	a	851	LHG	O1-C1-C2-C3
13	b	812	CLA	CAA-CBA-CGA-O1A
15	b	848	BCR	C11-C12-C13-C14
22	f	205	ZEX	C27-C28-C29-C30
13	a	802	CLA	C1A-C2A-CAA-CBA
13	b	811	CLA	C1A-C2A-CAA-CBA
13	b	820	CLA	C1A-C2A-CAA-CBA
13	b	827	CLA	C1A-C2A-CAA-CBA
16	a	849	LHG	O9-C7-C8-C9
13	a	839	CLA	CAA-CBA-CGA-O1A
13	j	103	CLA	CAA-CBA-CGA-O1A
13	a	806	CLA	CAA-CBA-CGA-O1A
13	a	827	CLA	C13-C15-C16-C17
16	a	853	LHG	C11-C12-C13-C14
16	a	851	LHG	C3-O3-P-O5
16	a	853	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
16	b	851	LHG	C4-O6-P-O5
13	a	811	CLA	CAA-CBA-CGA-O1A
13	a	832	CLA	CAA-CBA-CGA-O1A
16	f	206	LHG	O10-C23-C24-C25
15	a	844	BCR	C23-C24-C25-C26
15	k	4001	BCR	C23-C24-C25-C26
22	b	854	ZEX	C1-C6-C7-C8
13	a	829	CLA	CAA-CBA-CGA-O1A
13	a	826	CLA	C15-C16-C17-C18
13	f	201	CLA	C13-C15-C16-C17
13	a	809	CLA	CAA-CBA-CGA-O2A
13	b	808	CLA	CAA-CBA-CGA-O2A
13	l	1502	CLA	CAA-CBA-CGA-O2A
13	b	821	CLA	C13-C15-C16-C17
13	a	830	CLA	CAA-CBA-CGA-O1A
13	a	825	CLA	CAD-CBD-CGD-O1D
13	a	840	CLA	CAD-CBD-CGD-O1D
13	b	830	CLA	CAD-CBD-CGD-O1D
13	a	831	CLA	CAA-CBA-CGA-O1A
13	b	841	CLA	C4C-C3C-CAC-CBC
17	b	852	LMG	C31-C32-C33-C34
13	a	823	CLA	C11-C12-C13-C14
13	b	814	CLA	C11-C12-C13-C14
13	b	840	CLA	C6-C7-C8-C9
16	b	851	LHG	C11-C10-C9-C8
13	b	801	CLA	C15-C16-C17-C18
13	a	810	CLA	CAA-CBA-CGA-O2A
13	a	823	CLA	CAA-CBA-CGA-O2A
13	b	822	CLA	CAA-CBA-CGA-O2A
13	a	828	CLA	CAA-CBA-CGA-O2A
13	b	816	CLA	CAA-CBA-CGA-O2A
16	a	849	LHG	O7-C7-C8-C9
16	a	849	LHG	O8-C23-C24-C25
13	b	824	CLA	C4-C3-C5-C6
13	a	818	CLA	C2-C3-C5-C6
13	a	820	CLA	C11-C10-C8-C7
13	a	821	CLA	C12-C13-C15-C16
13	a	828	CLA	C2-C3-C5-C6
13	b	810	CLA	C6-C7-C8-C10
13	b	816	CLA	C3A-C2A-CAA-CBA
13	b	830	CLA	C11-C12-C13-C15
13	b	840	CLA	C11-C12-C13-C15

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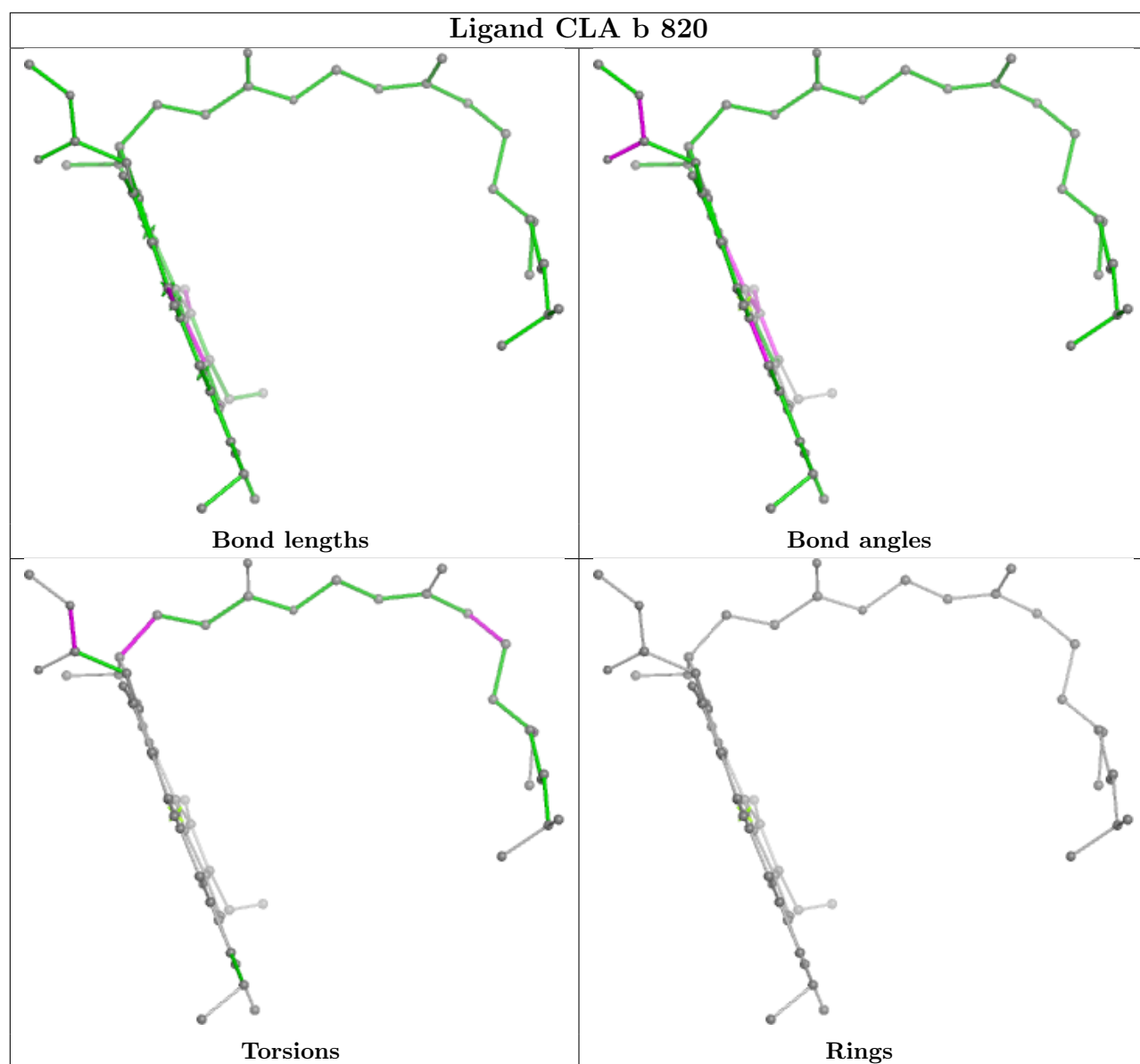
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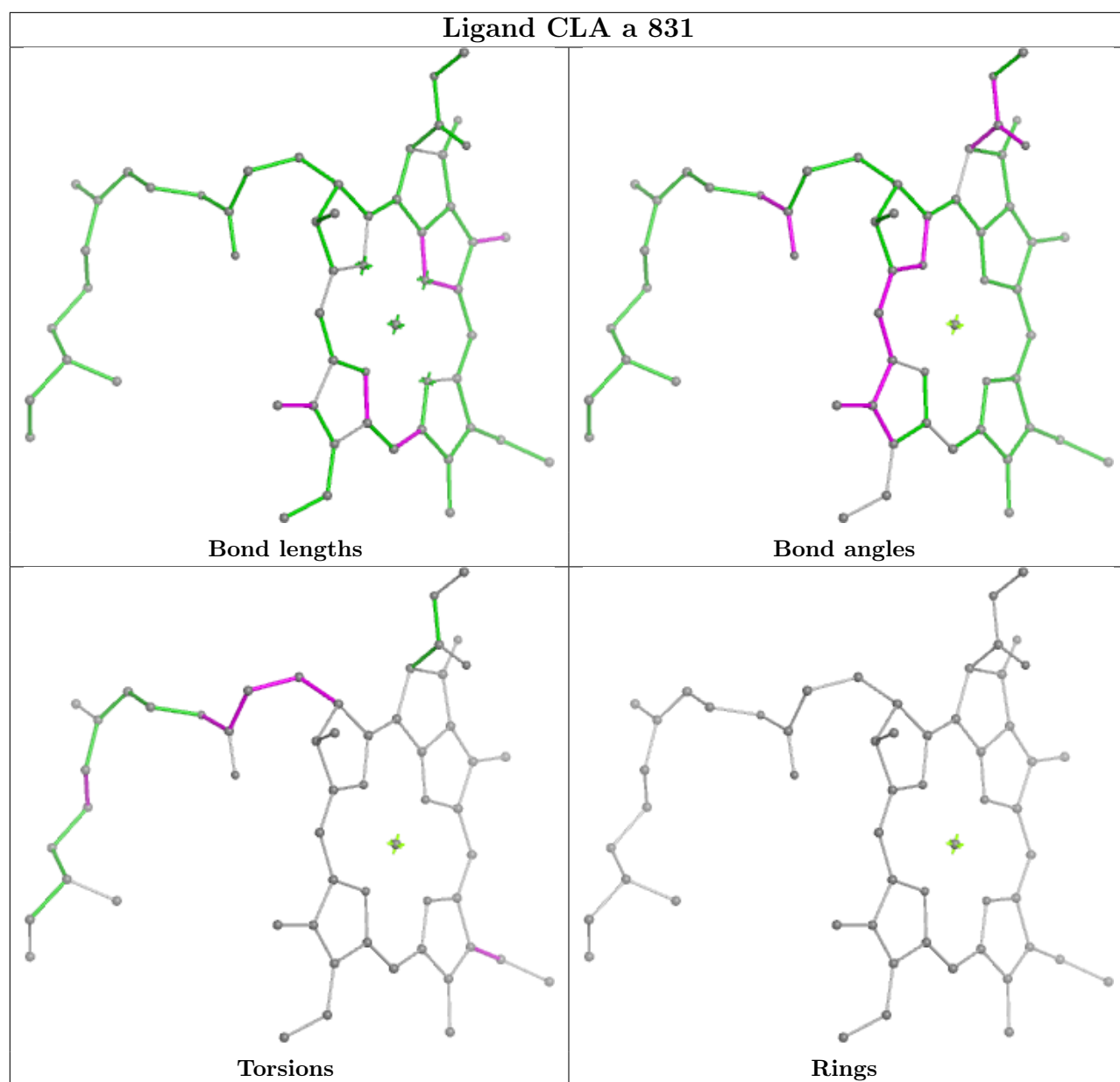
Mol	Chain	Res	Type	Atoms
13	a	814	CLA	CAA-CBA-CGA-O2A
13	a	835	CLA	CAA-CBA-CGA-O2A
13	b	831	CLA	CAA-CBA-CGA-O2A
15	k	4001	BCR	C21-C22-C23-C24
13	a	814	CLA	CAA-CBA-CGA-O1A
13	a	820	CLA	CAA-CBA-CGA-O1A
13	a	835	CLA	CAA-CBA-CGA-O1A
13	b	830	CLA	CAA-CBA-CGA-O1A
23	j	102	LMT	C2-C1-O1'-C1'
13	b	813	CLA	CAA-CBA-CGA-O2A
13	b	834	CLA	CAA-CBA-CGA-O2A
13	b	840	CLA	CAA-CBA-CGA-O2A
13	b	814	CLA	C8-C10-C11-C12
13	b	822	CLA	C5-C6-C7-C8
13	a	826	CLA	O1A-CGA-O2A-C1
13	b	817	CLA	CAA-CBA-CGA-O1A
13	b	822	CLA	CAA-CBA-CGA-O1A
13	l	1502	CLA	CAA-CBA-CGA-O1A
13	b	816	CLA	C5-C6-C7-C8
13	b	840	CLA	CAA-CBA-CGA-O1A
17	a	852	LMG	O9-C10-C11-C12
13	a	821	CLA	C4-C3-C5-C6
13	b	806	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

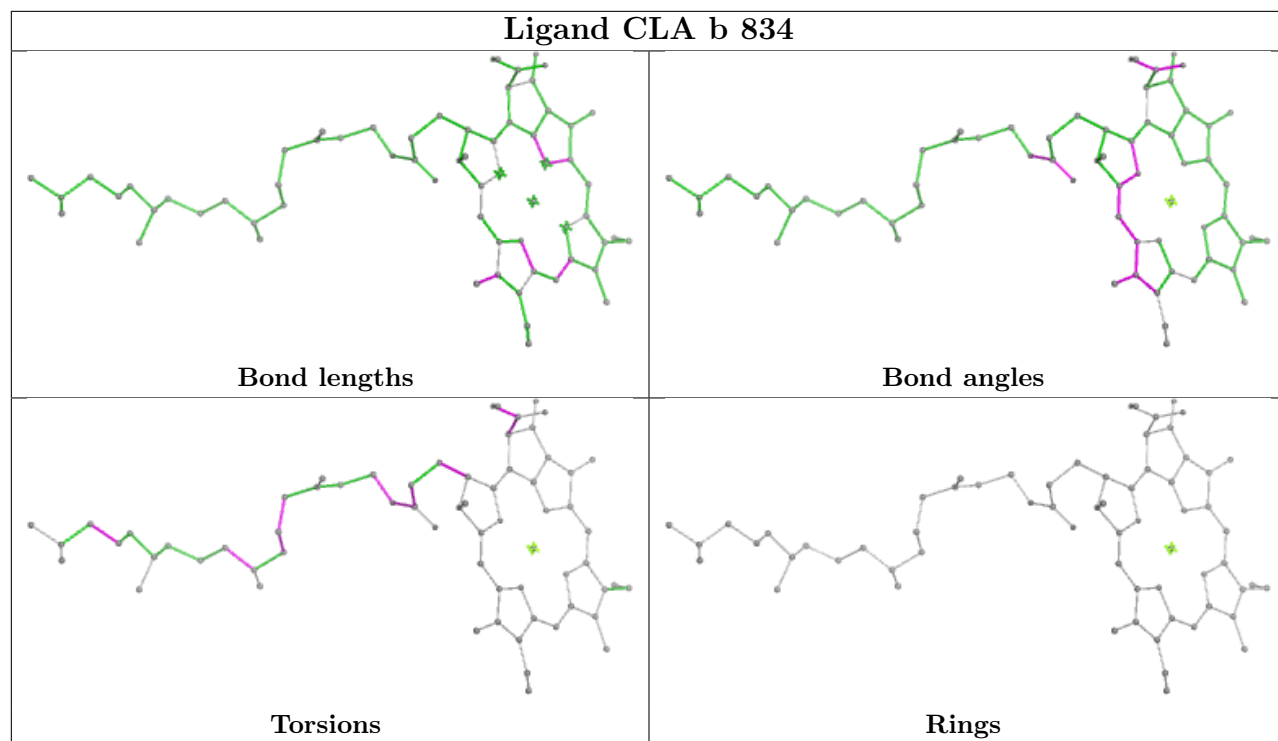
No monomer is involved in short contacts.

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.

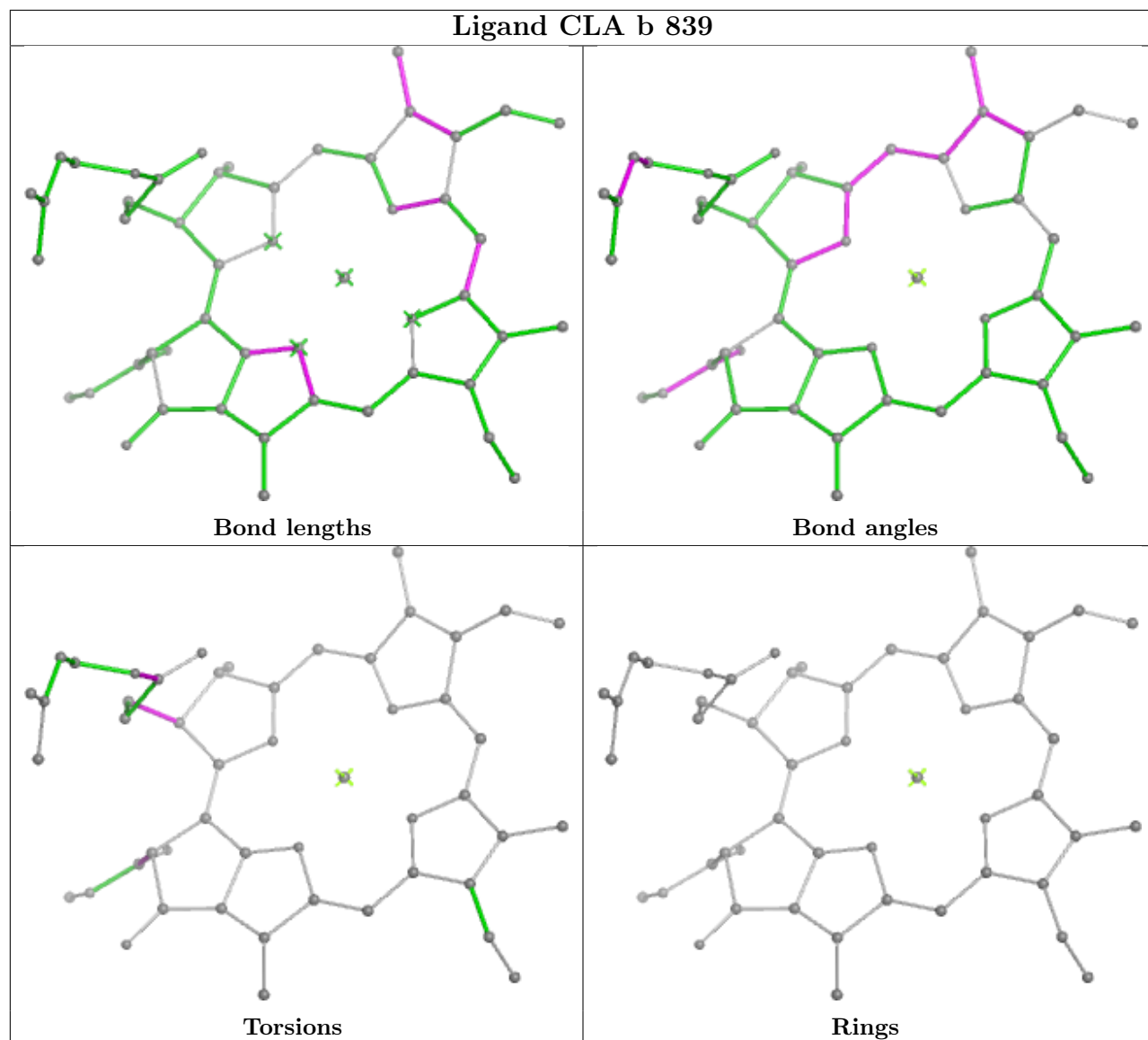


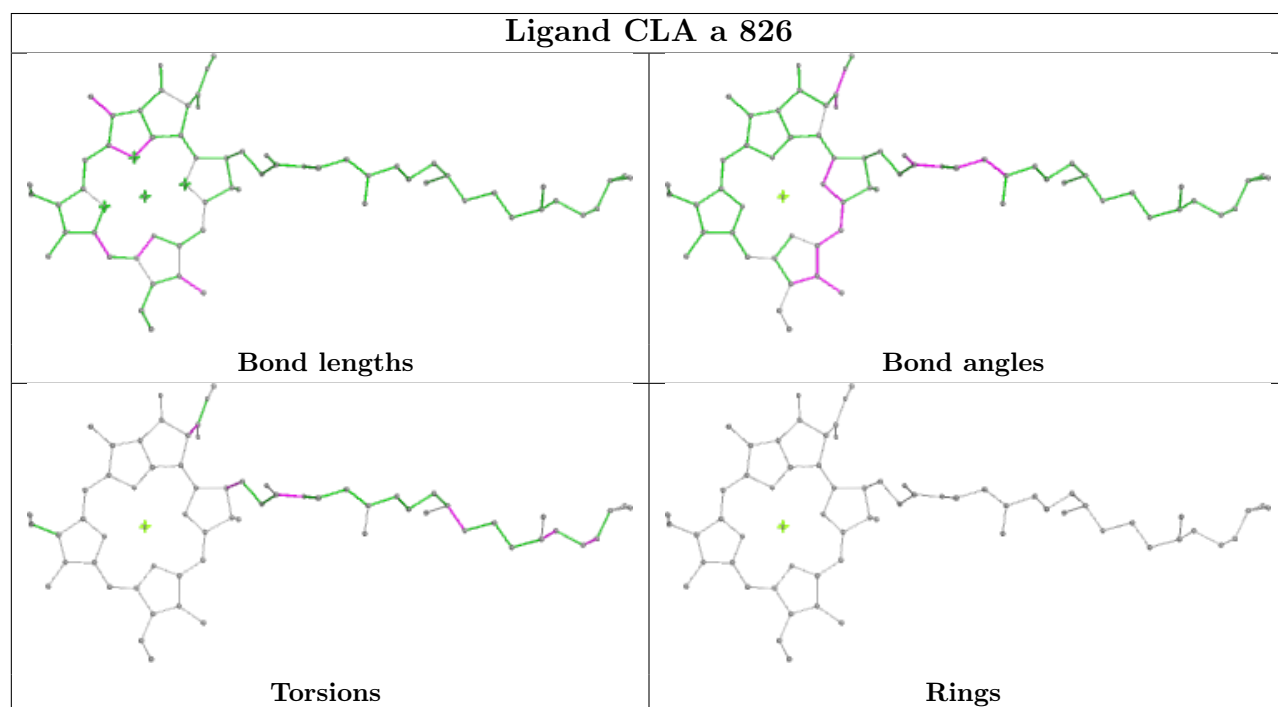
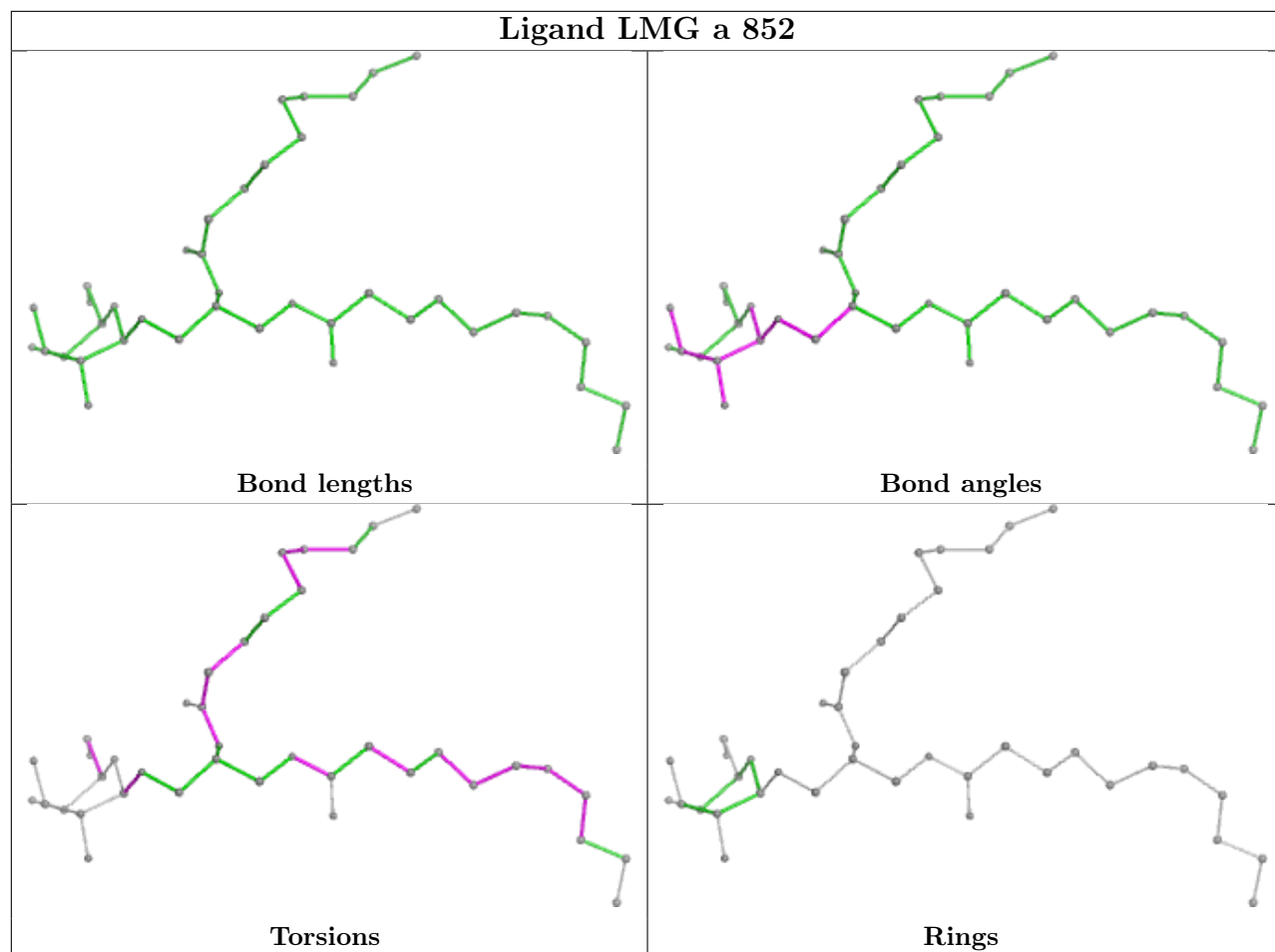




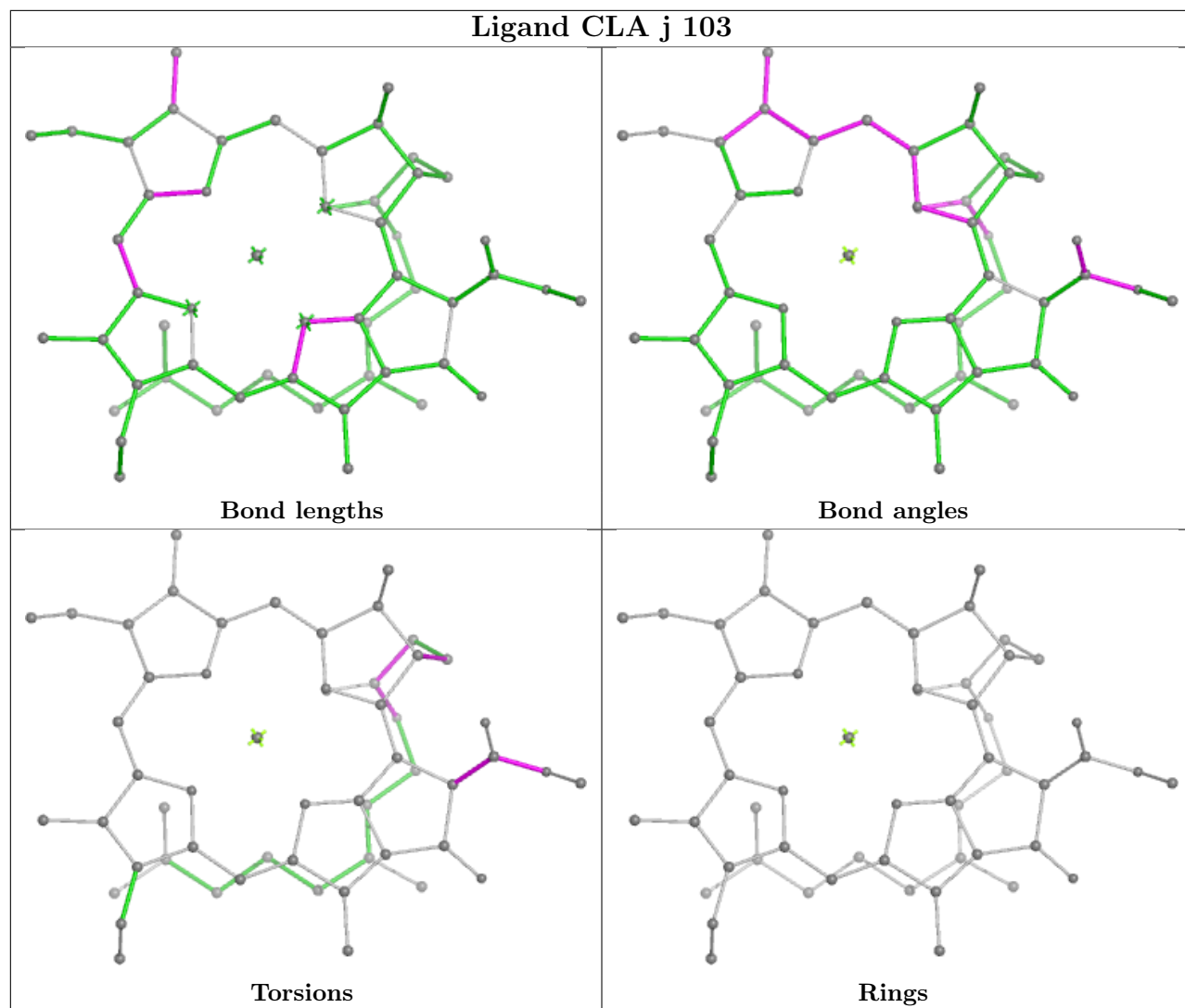


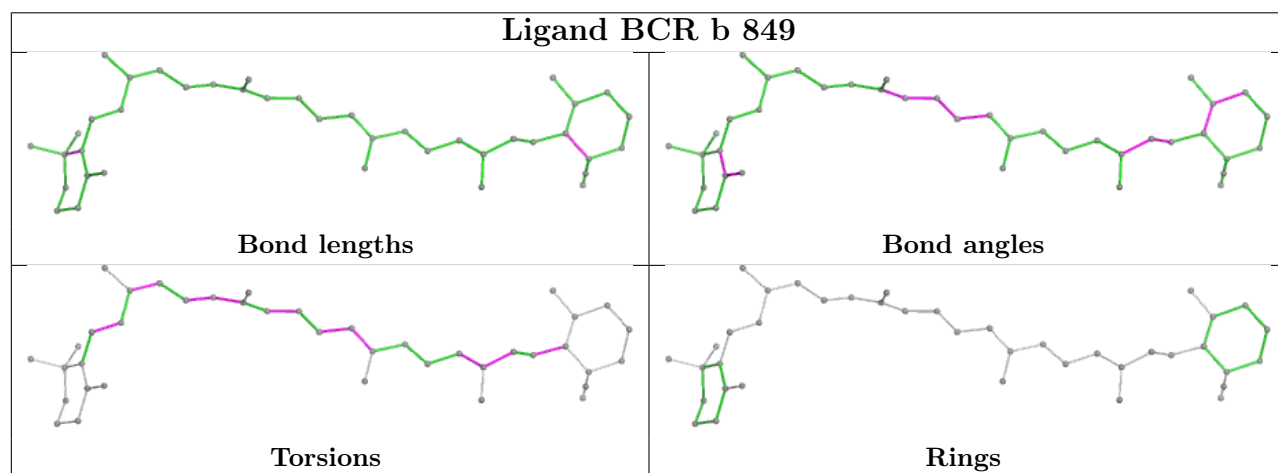
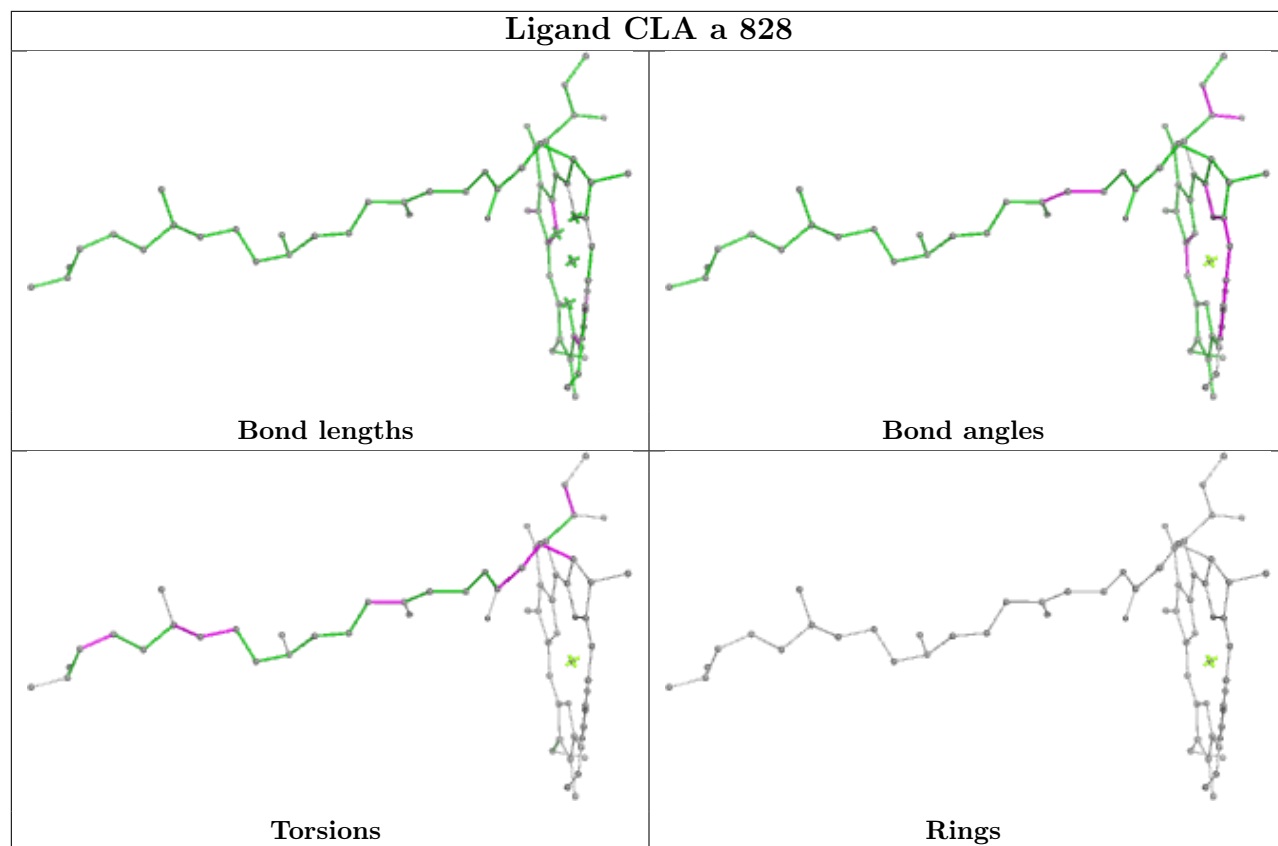
## Ligand CLA b 839

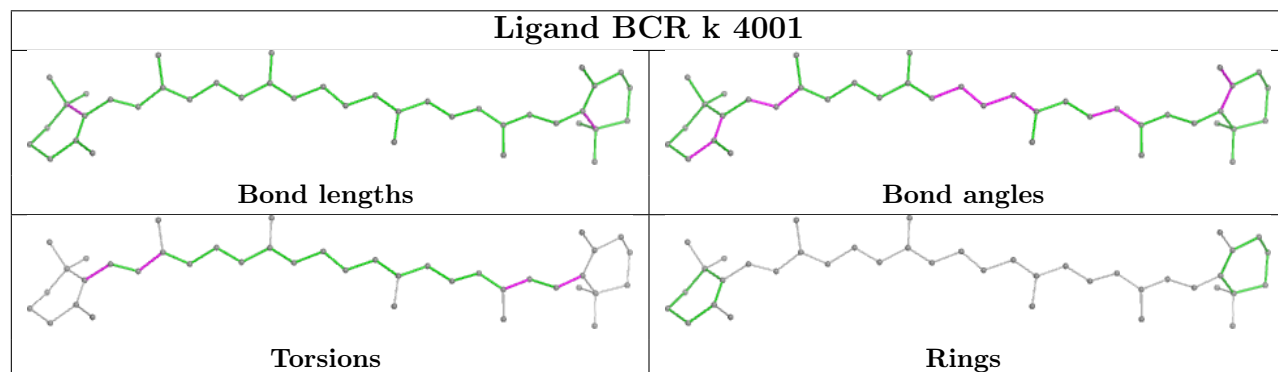
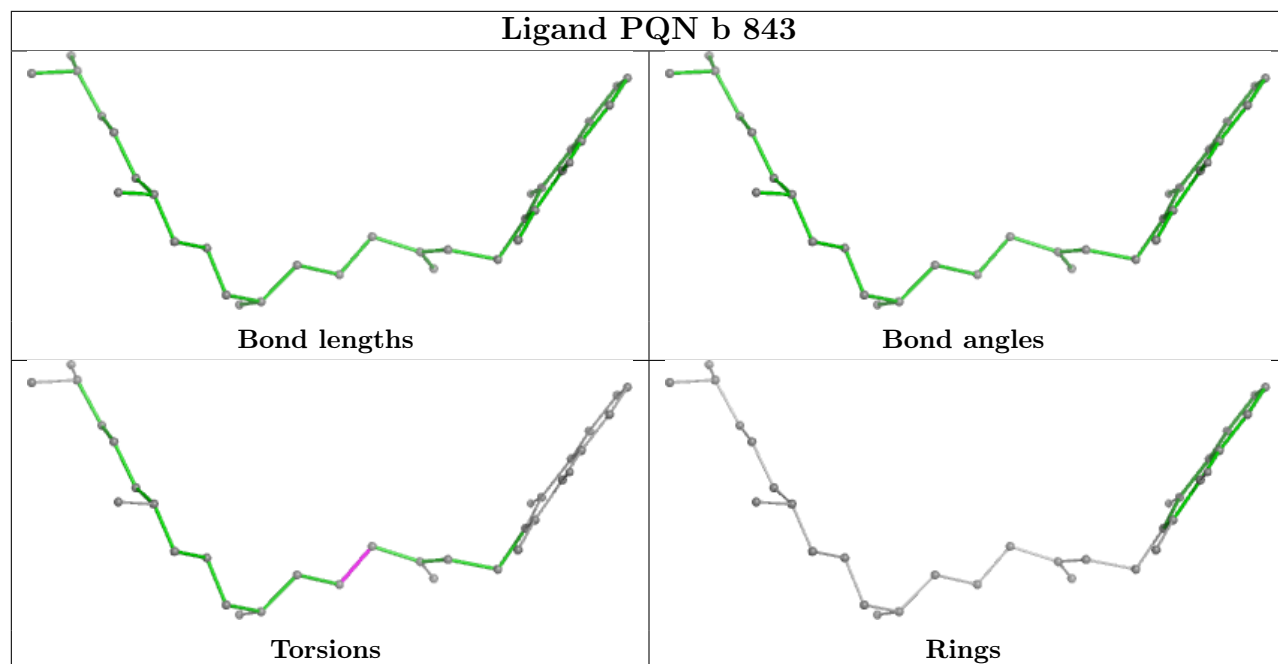


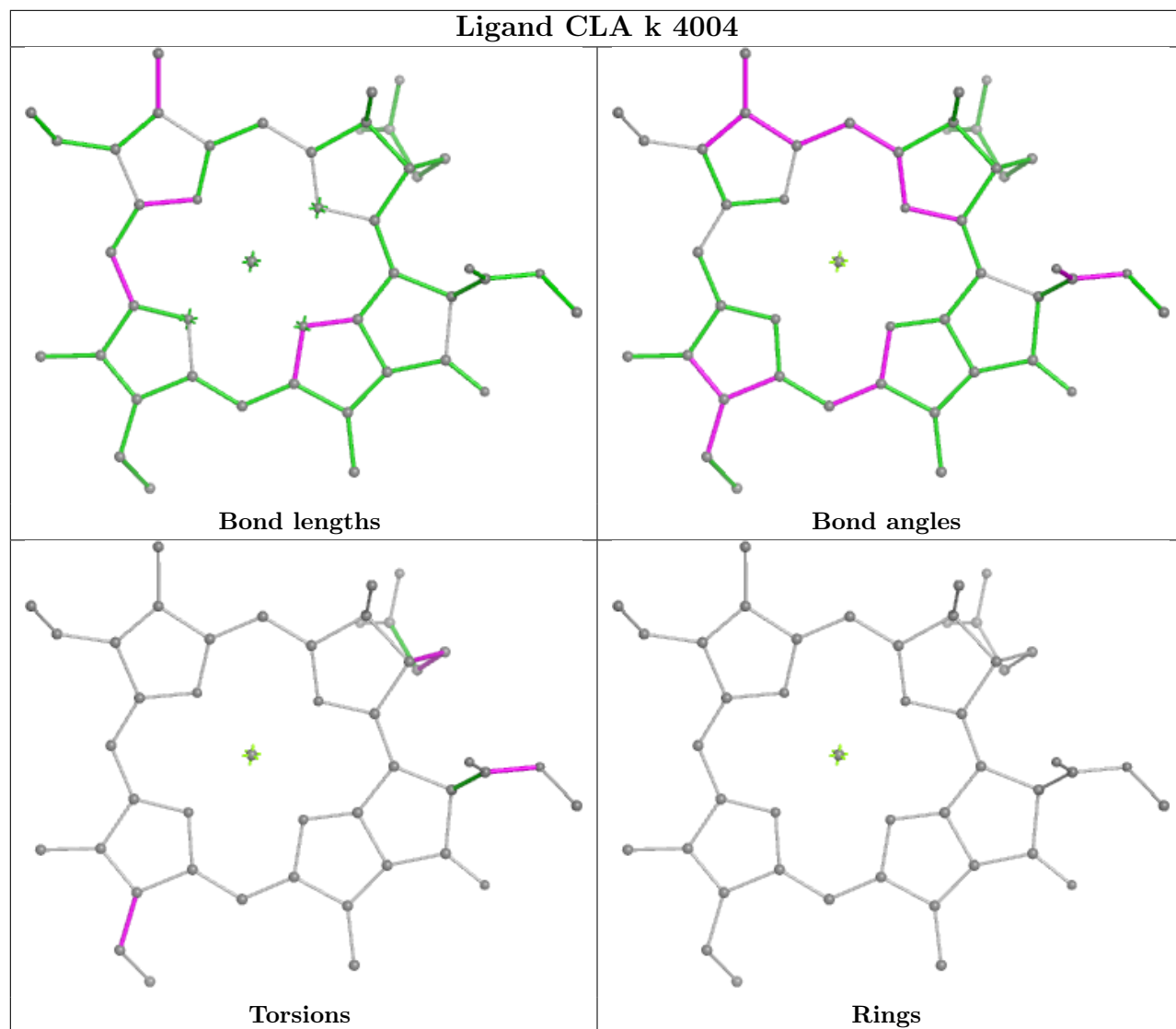


## Ligand CLA j 103

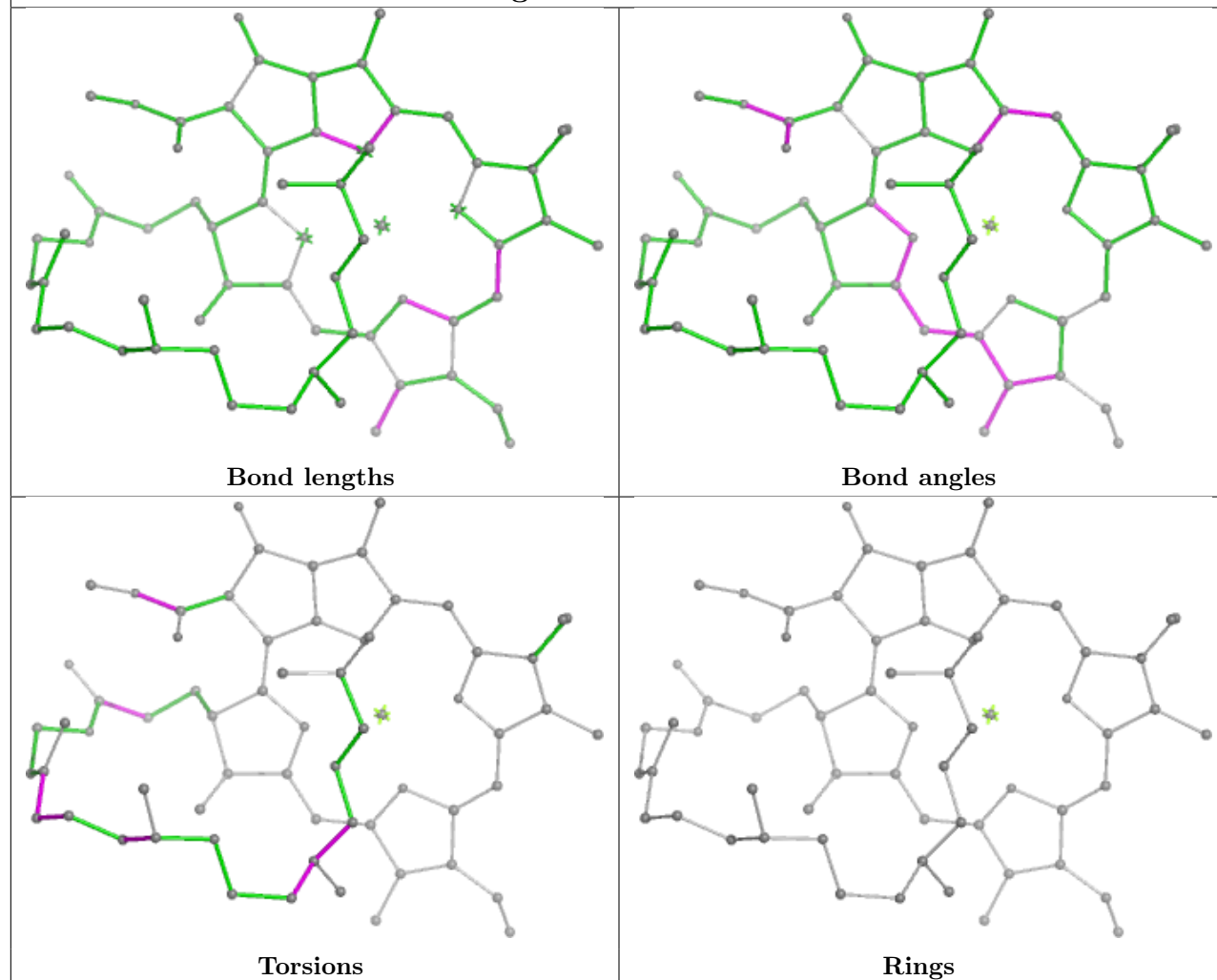




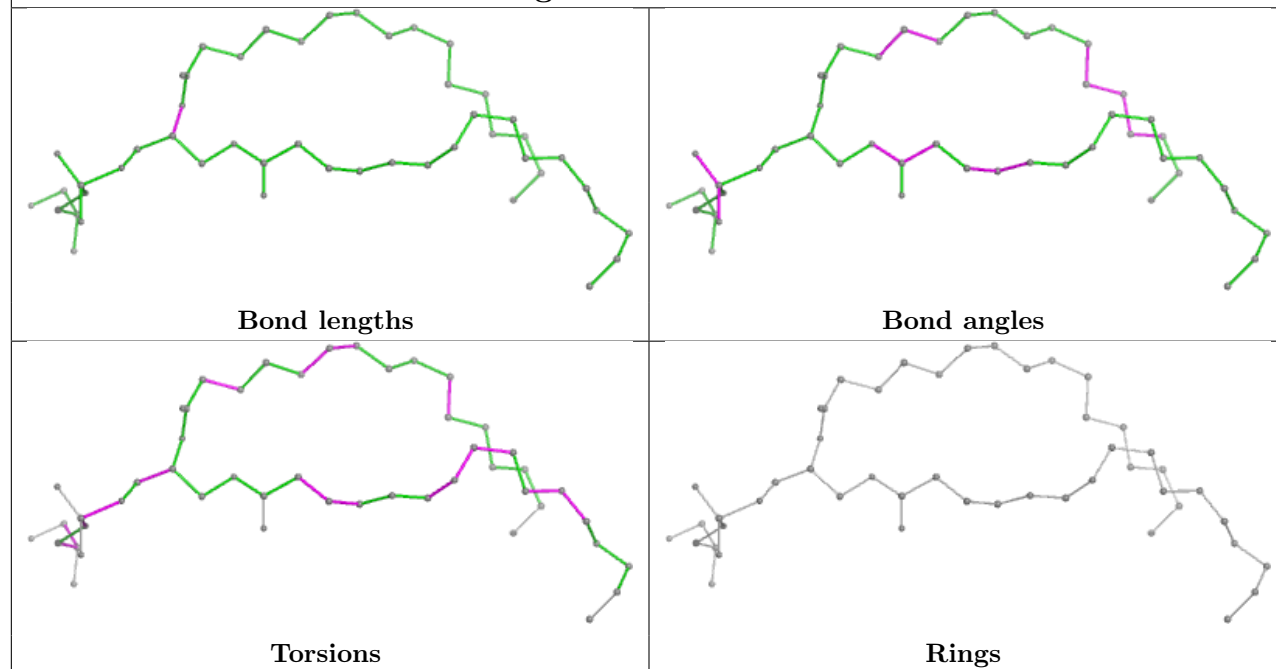




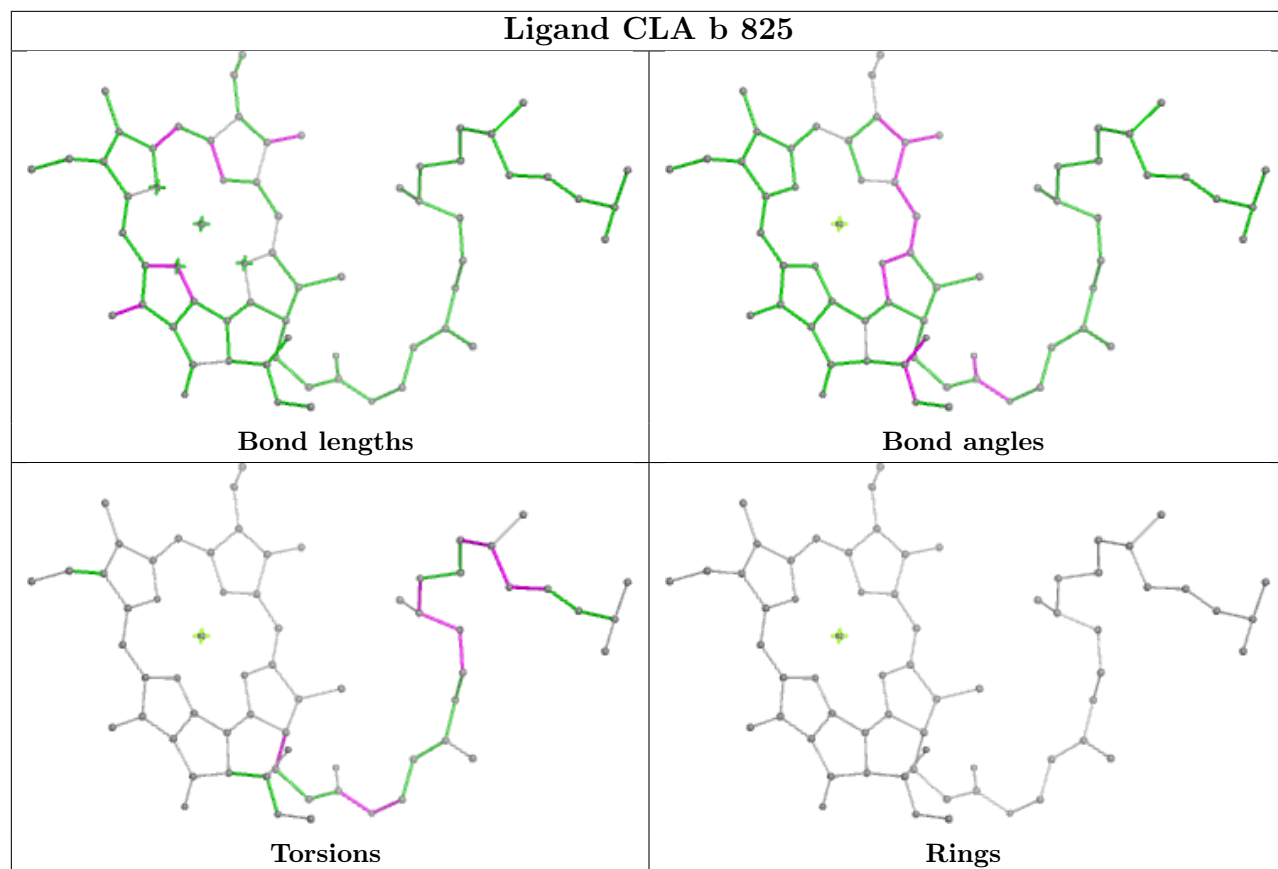
## Ligand CLA a 806



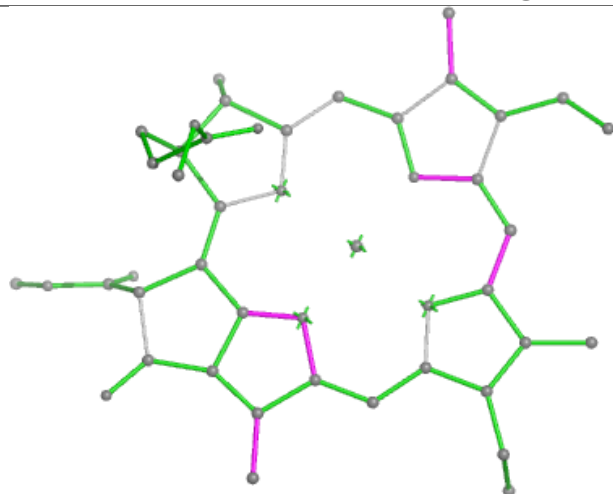
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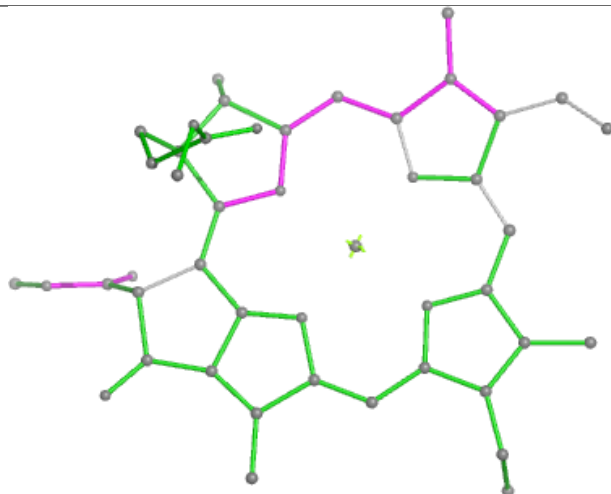




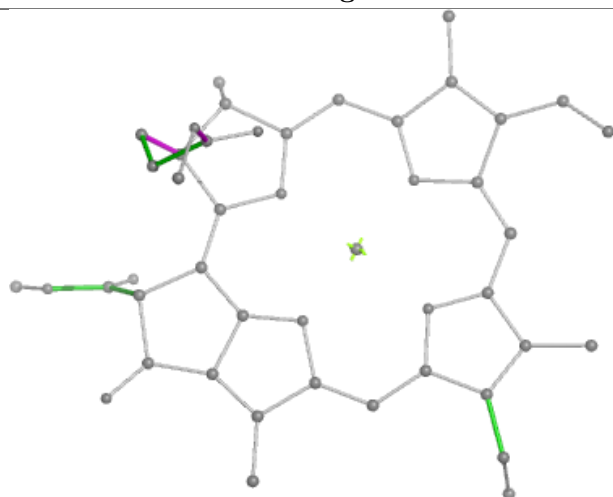
## Ligand CLA b 823



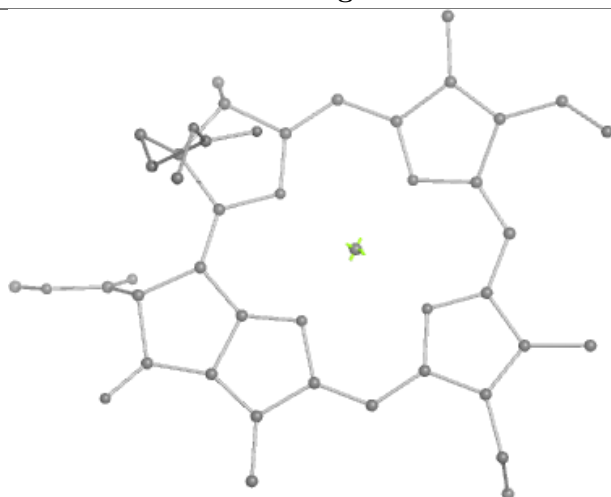
Bond lengths



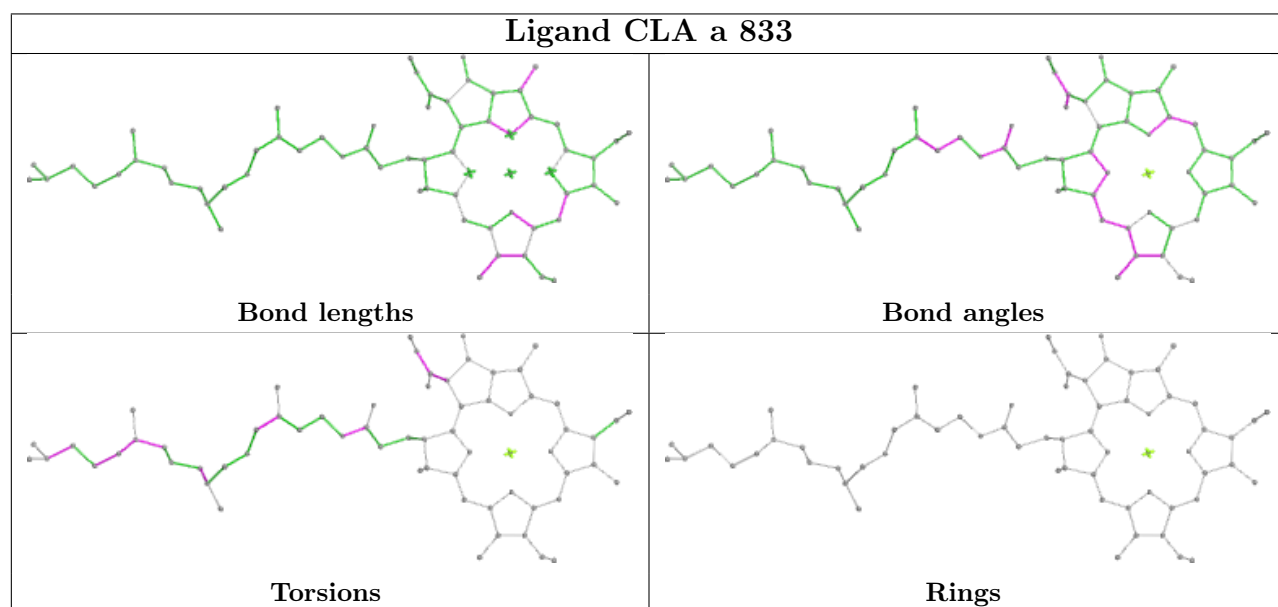
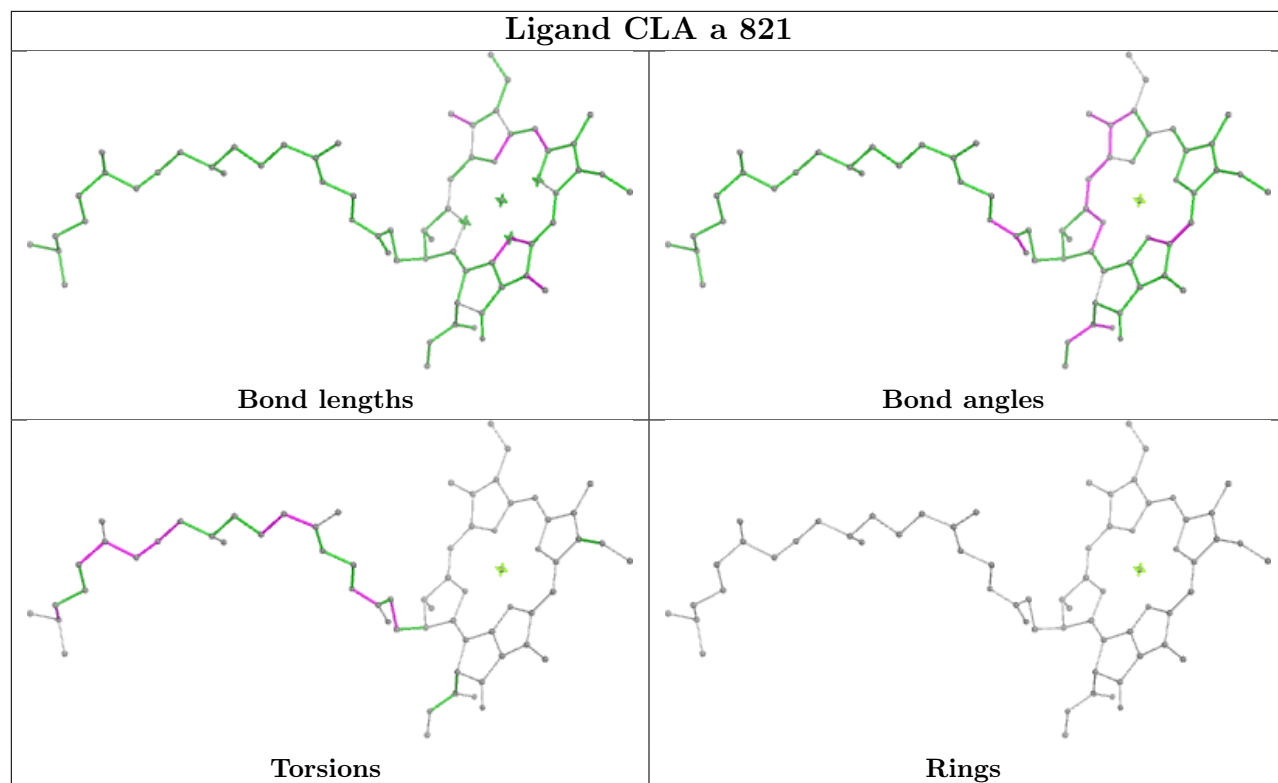
Bond angles

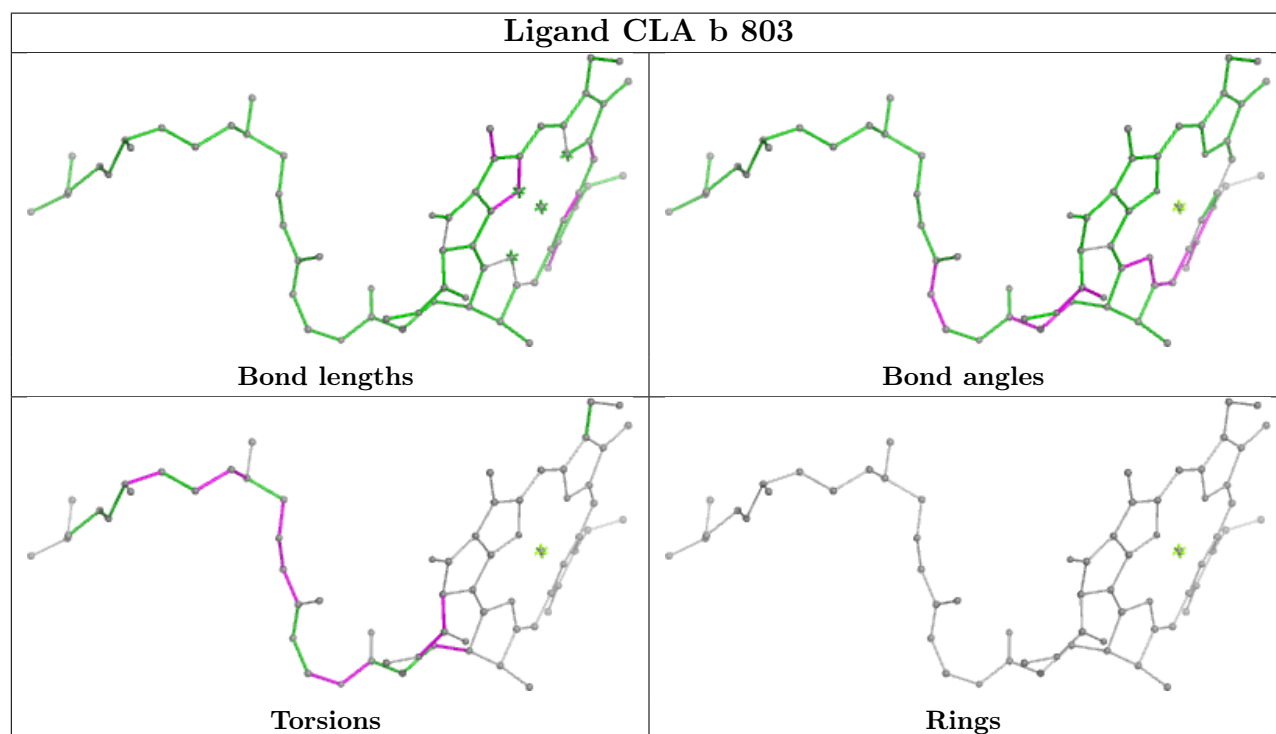
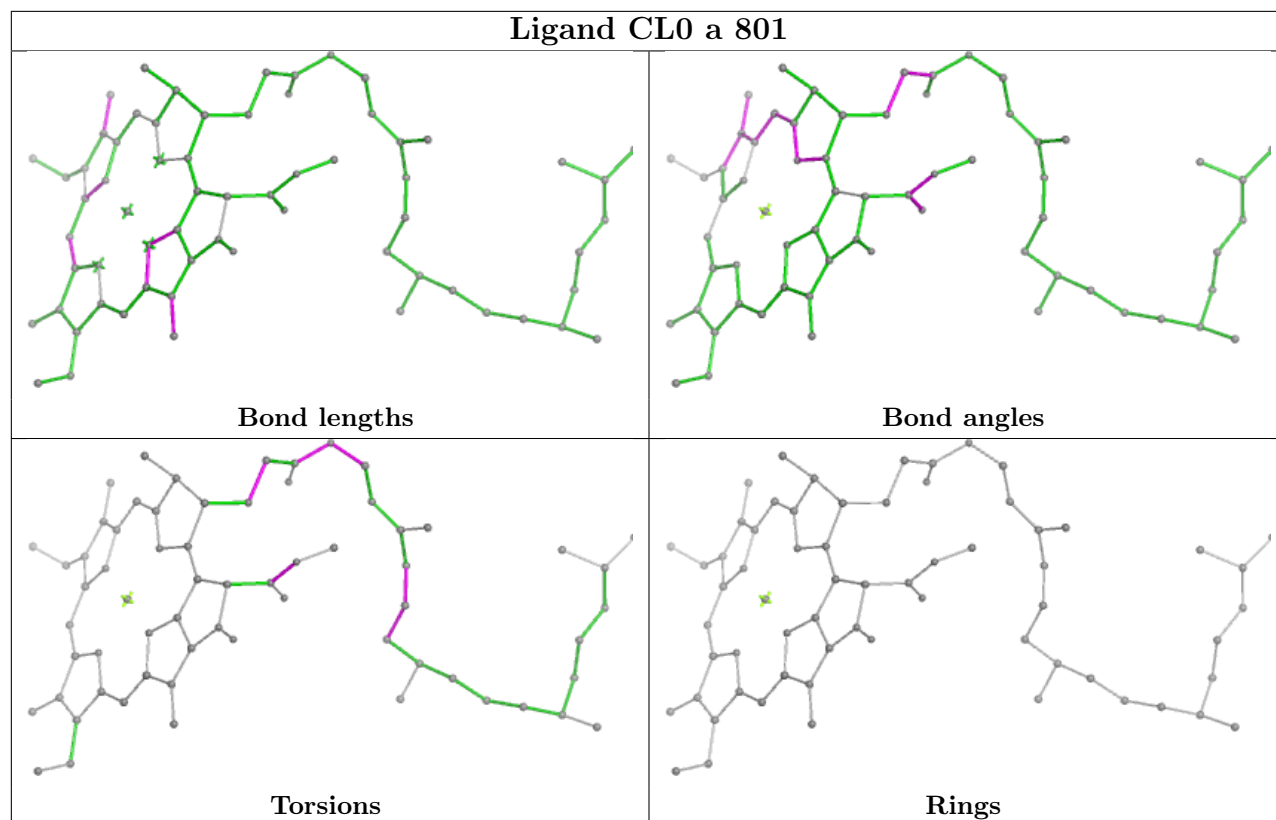


Torsions

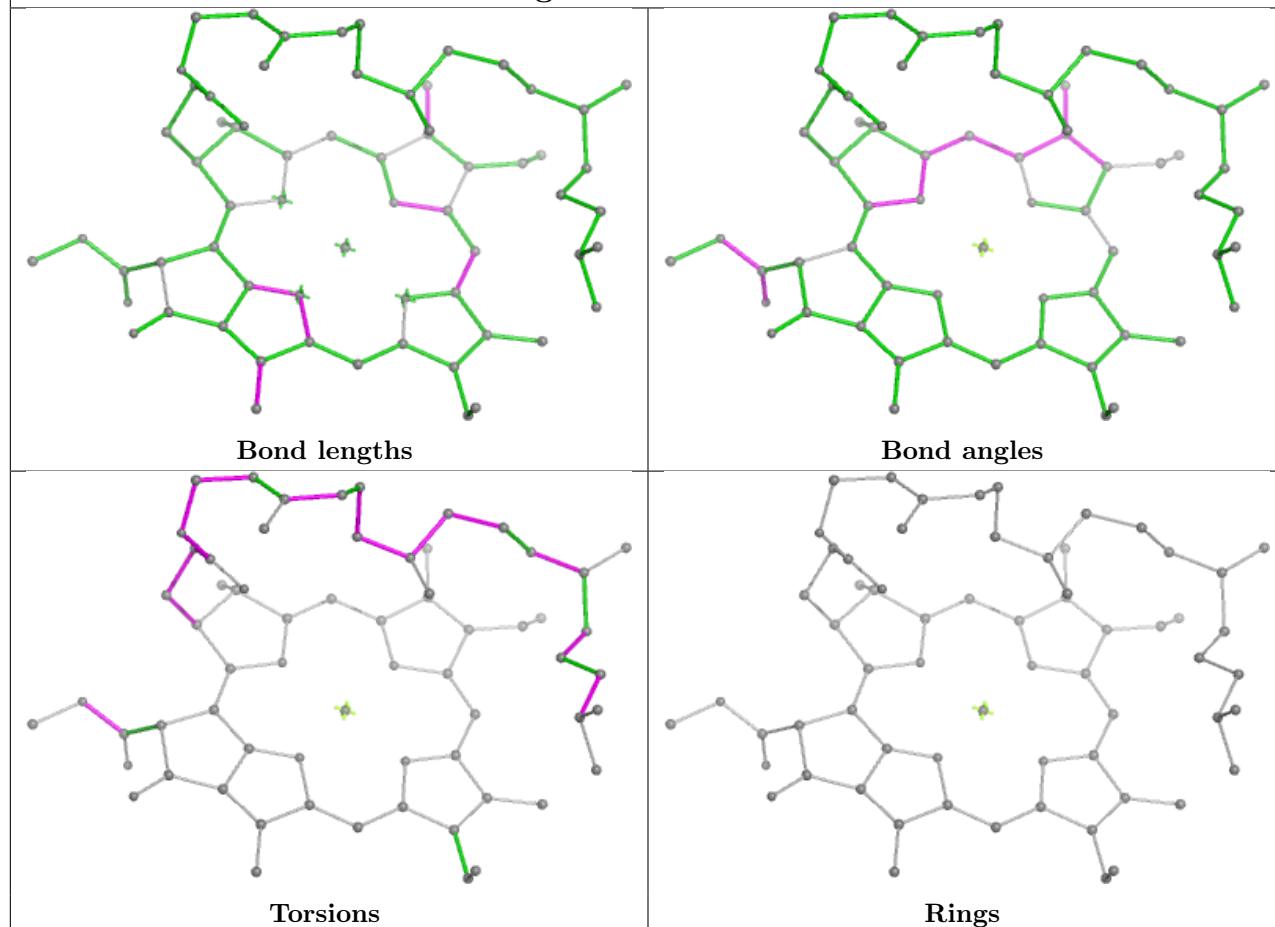


Rings

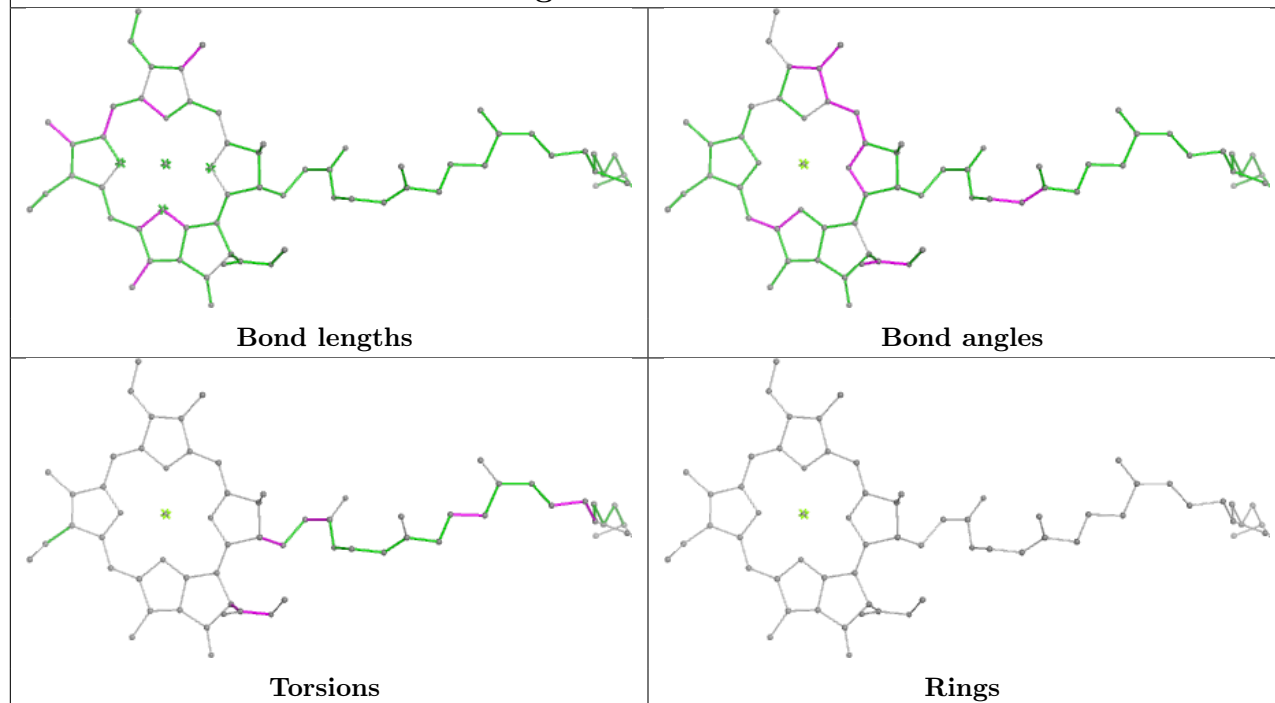


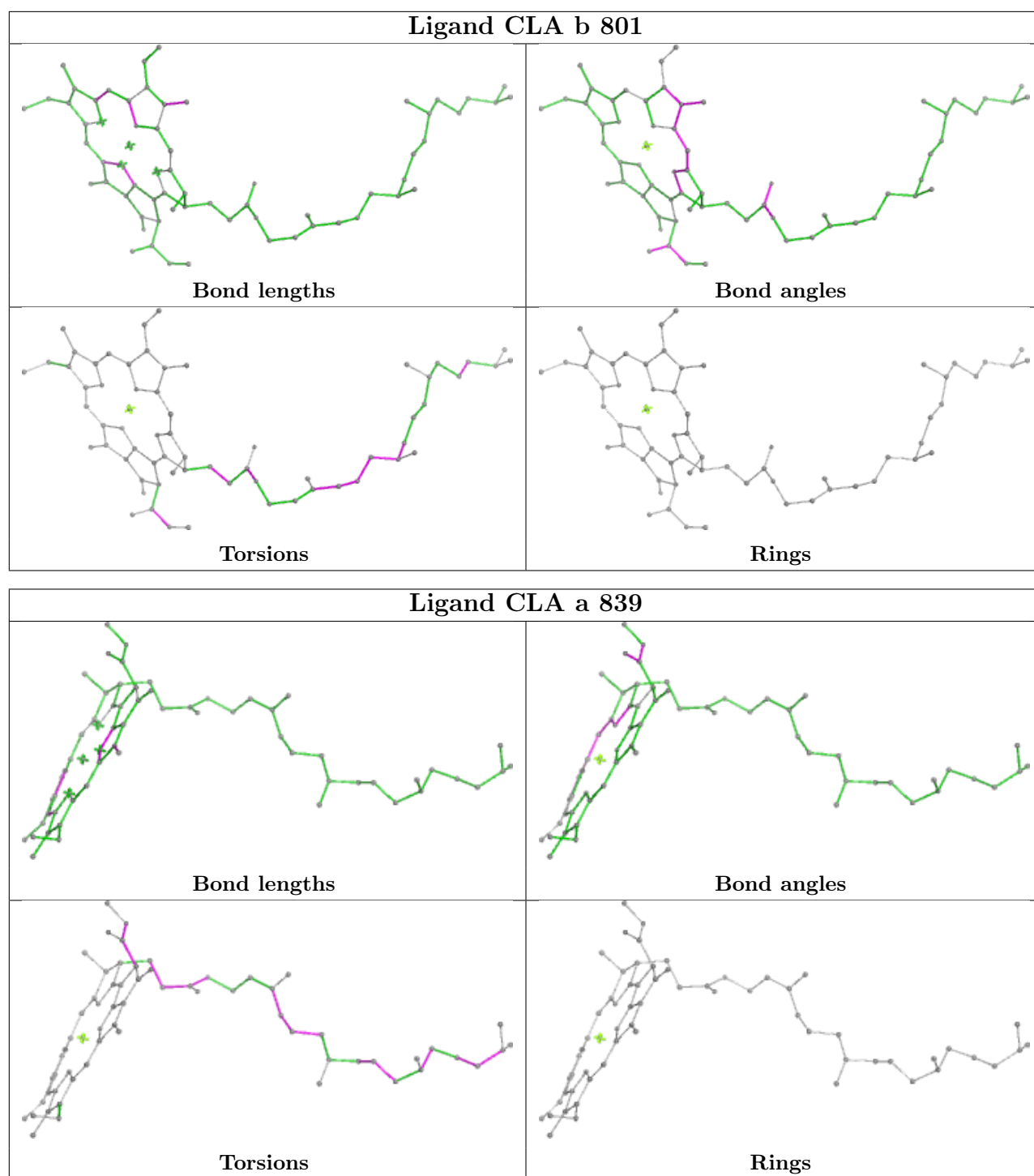


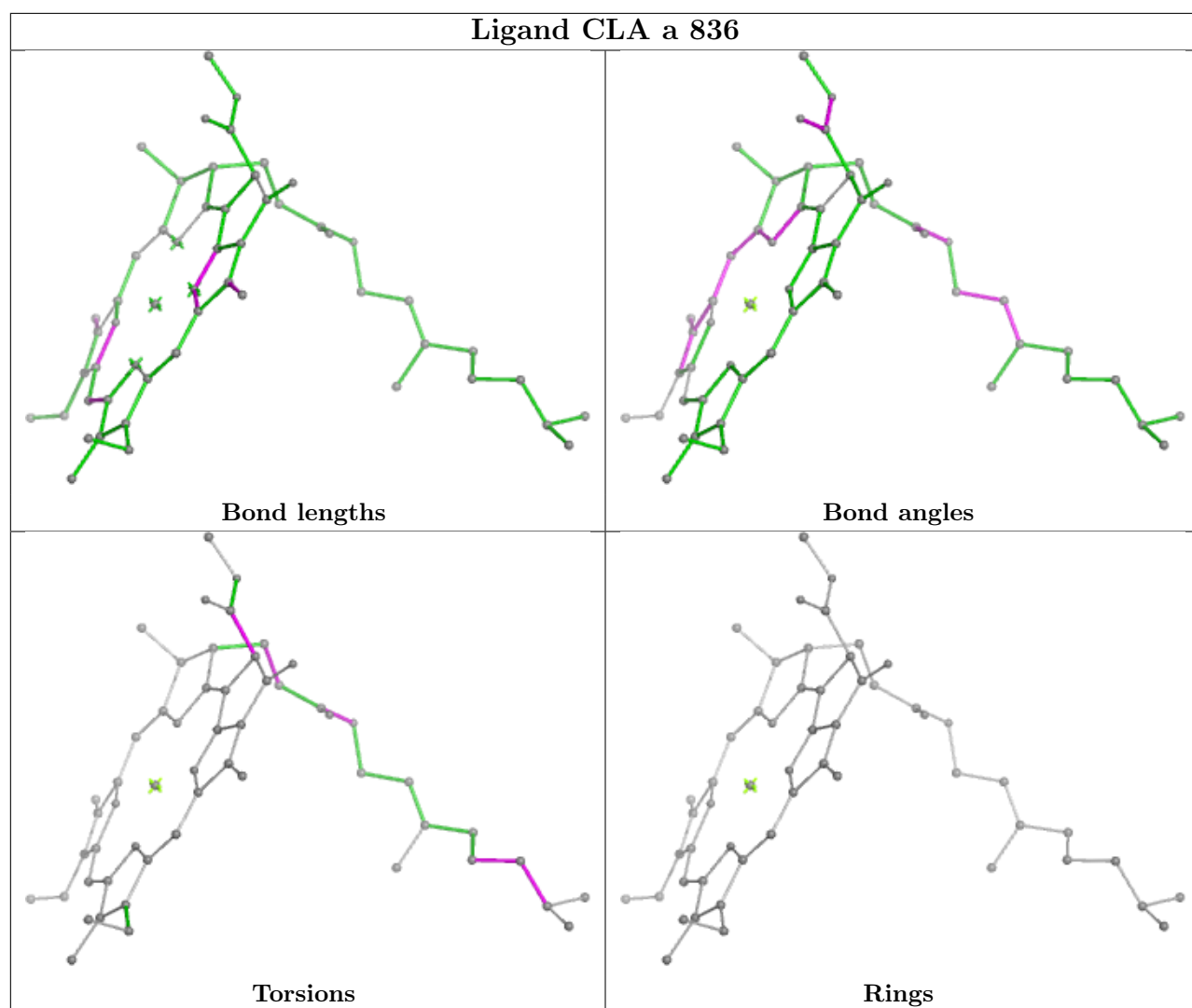
## Ligand CLA a 820

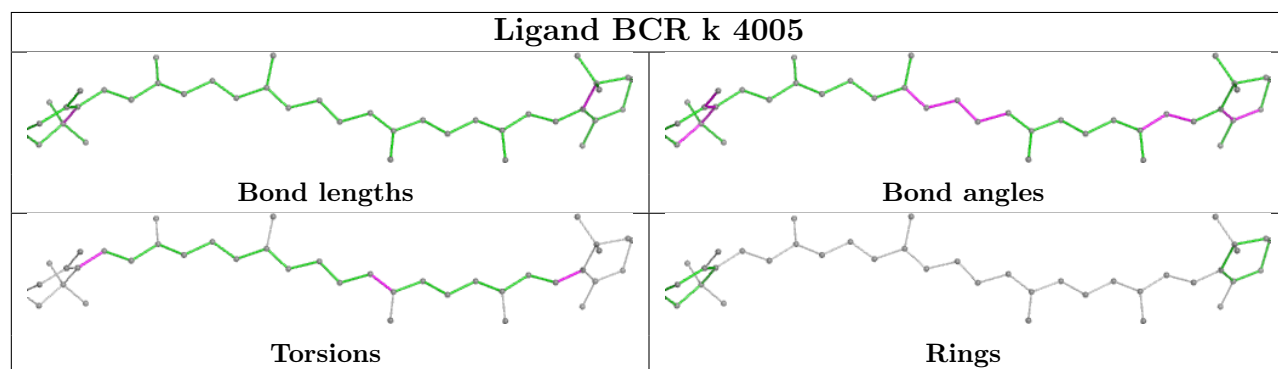
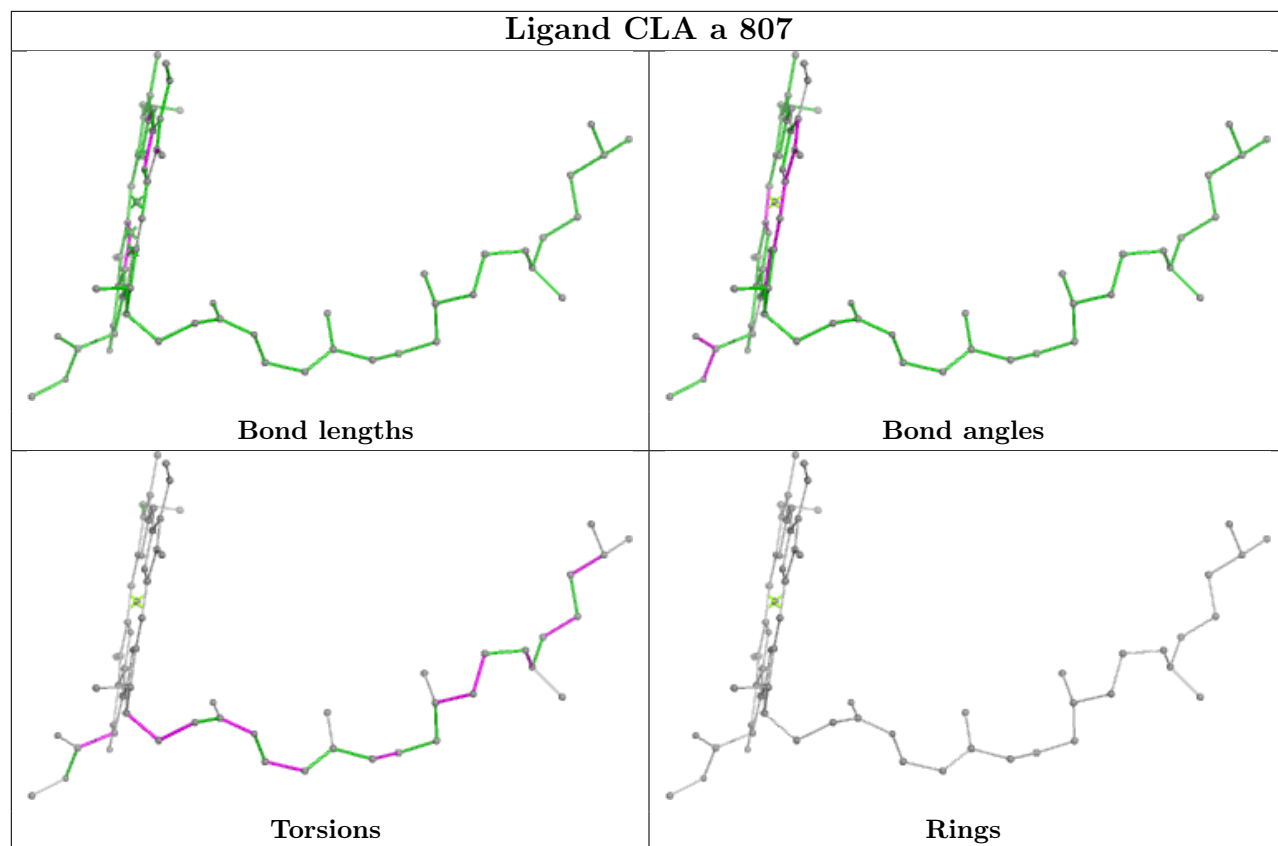


## Ligand CLA a 805

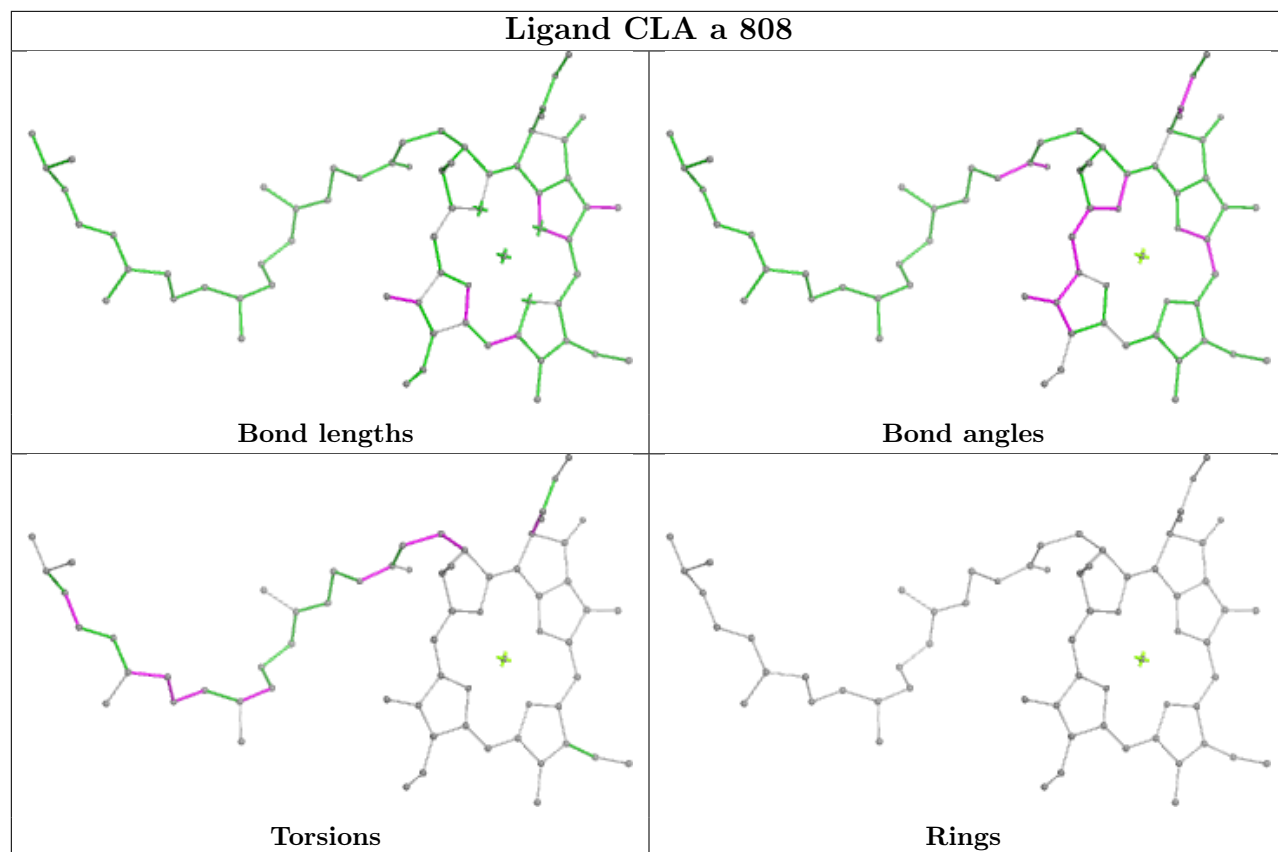




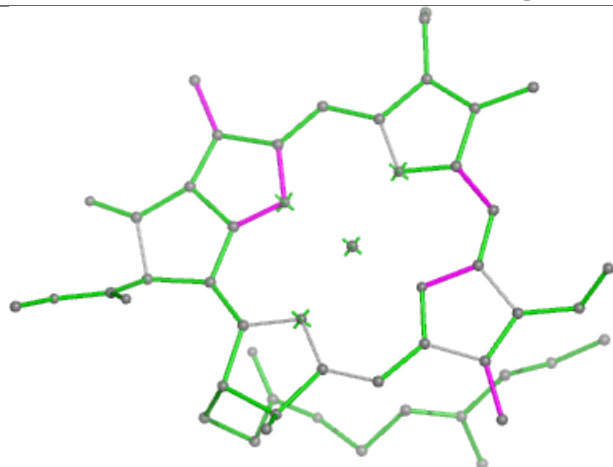




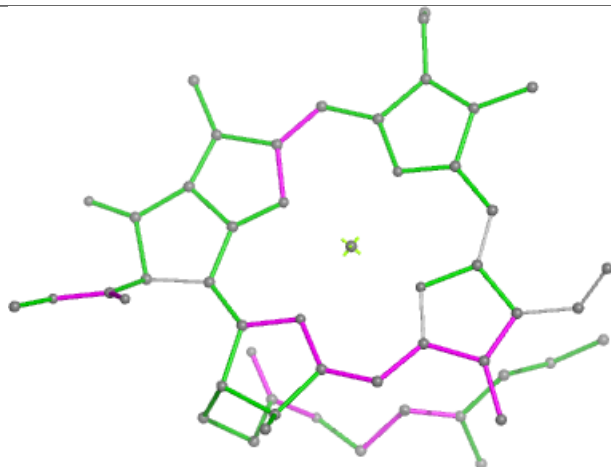




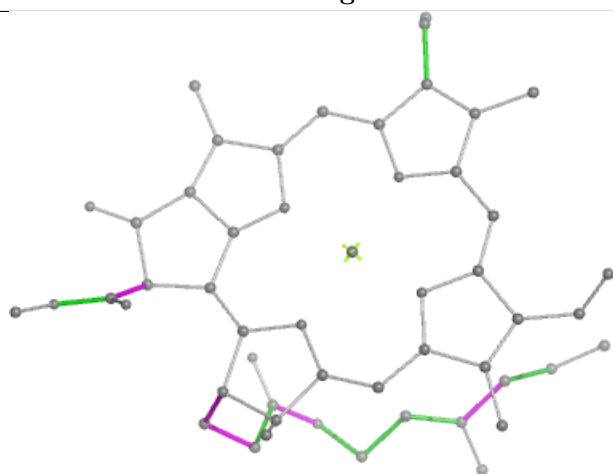
## Ligand CLA a 812



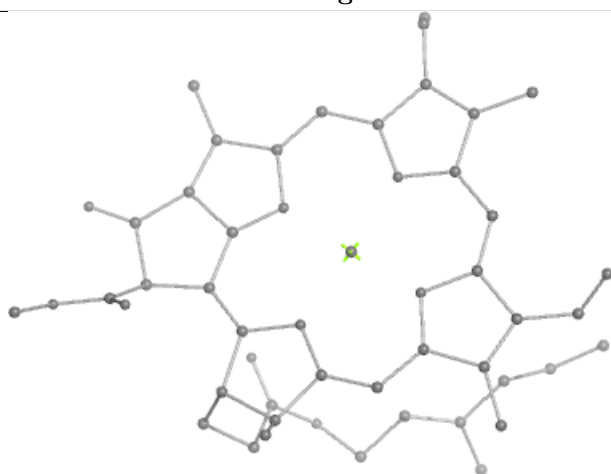
Bond lengths



Bond angles

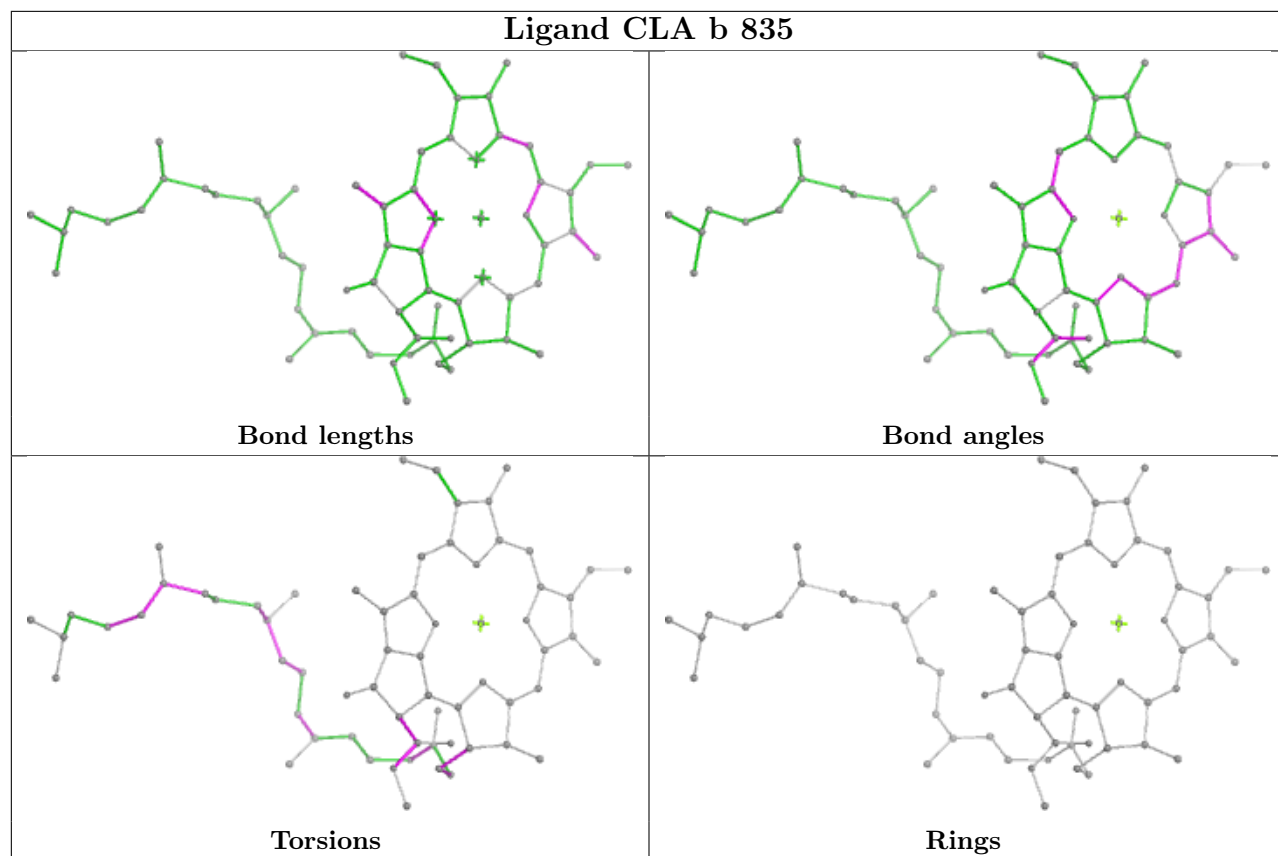


Torsions

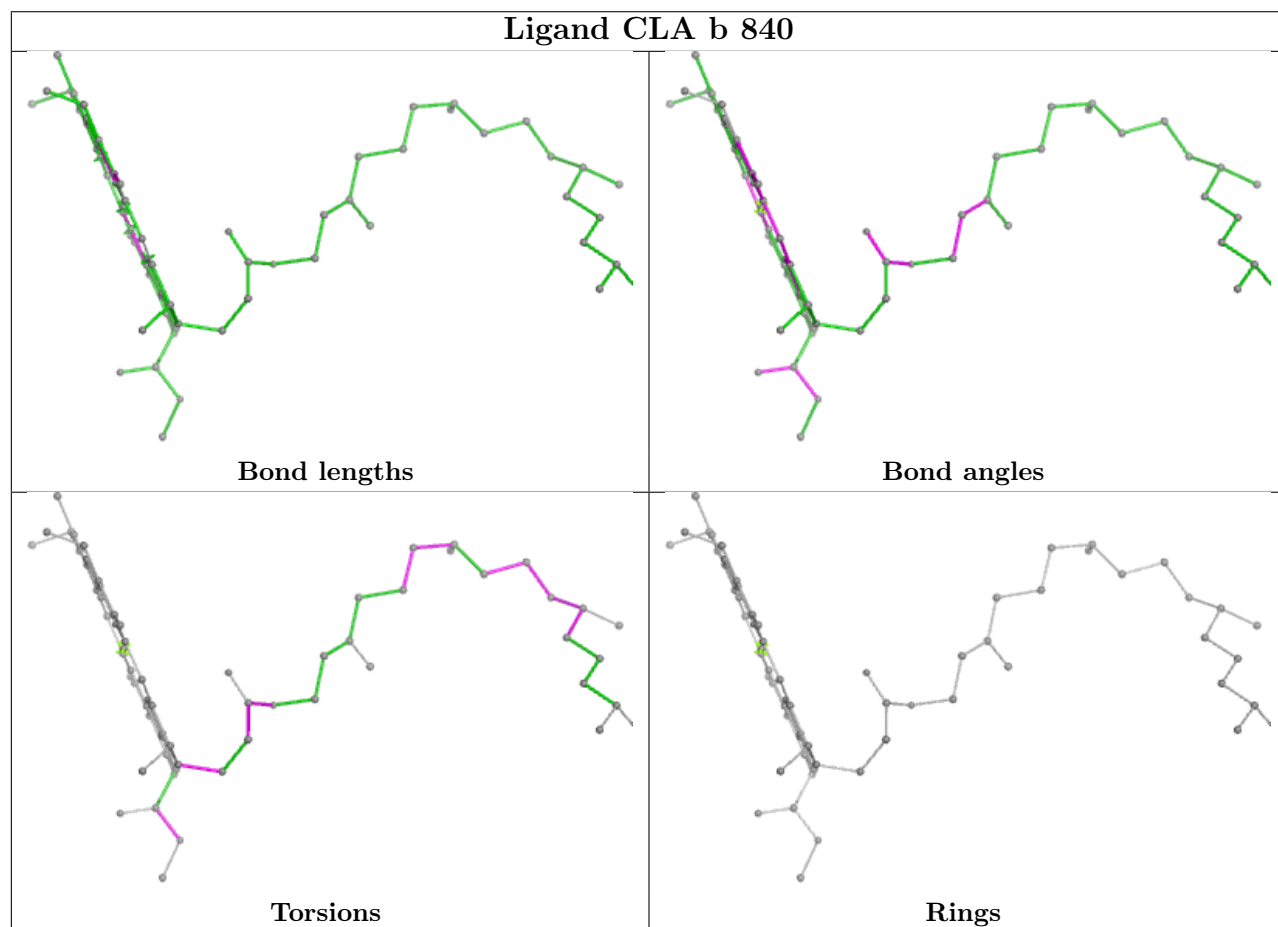


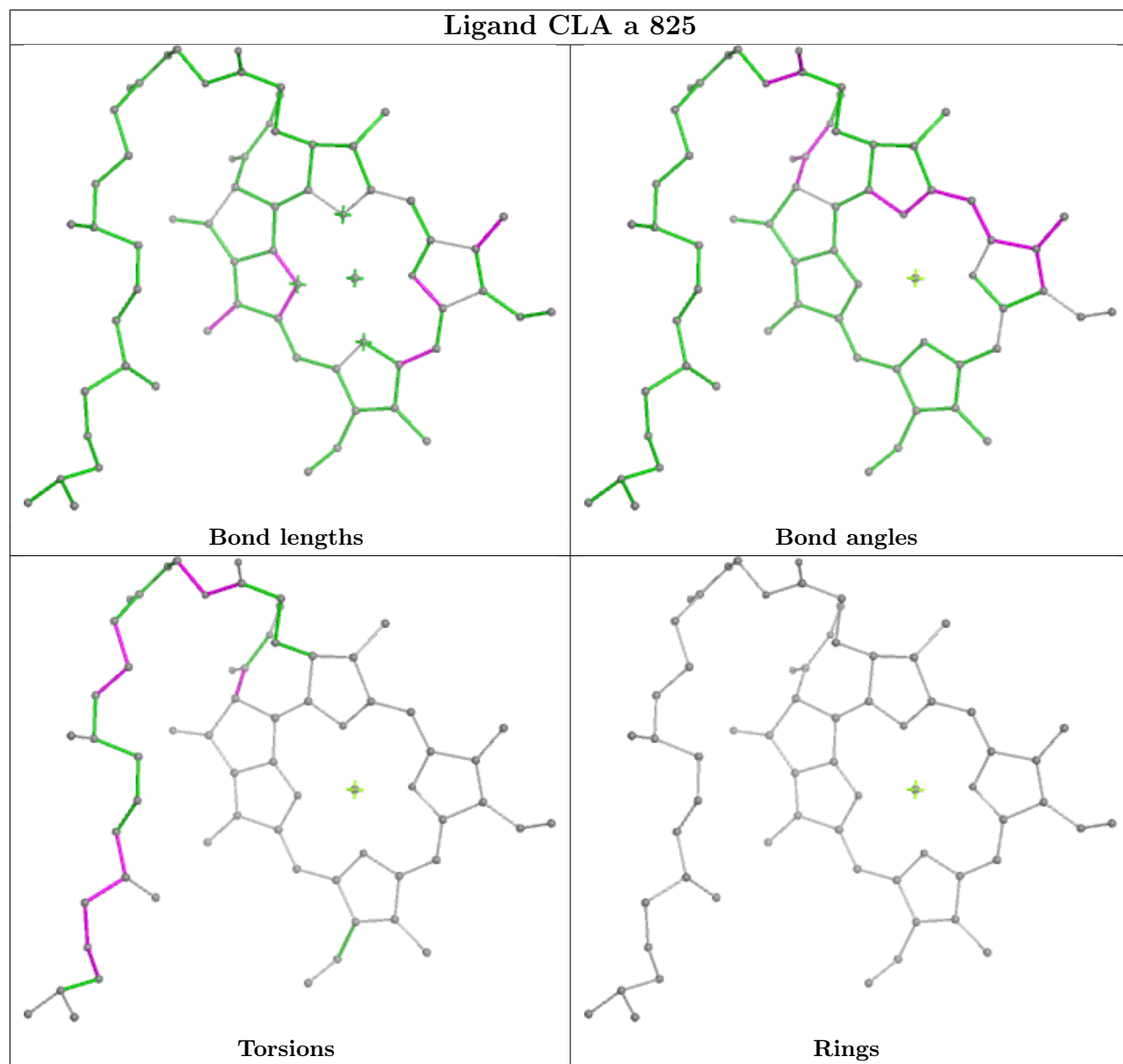
Rings

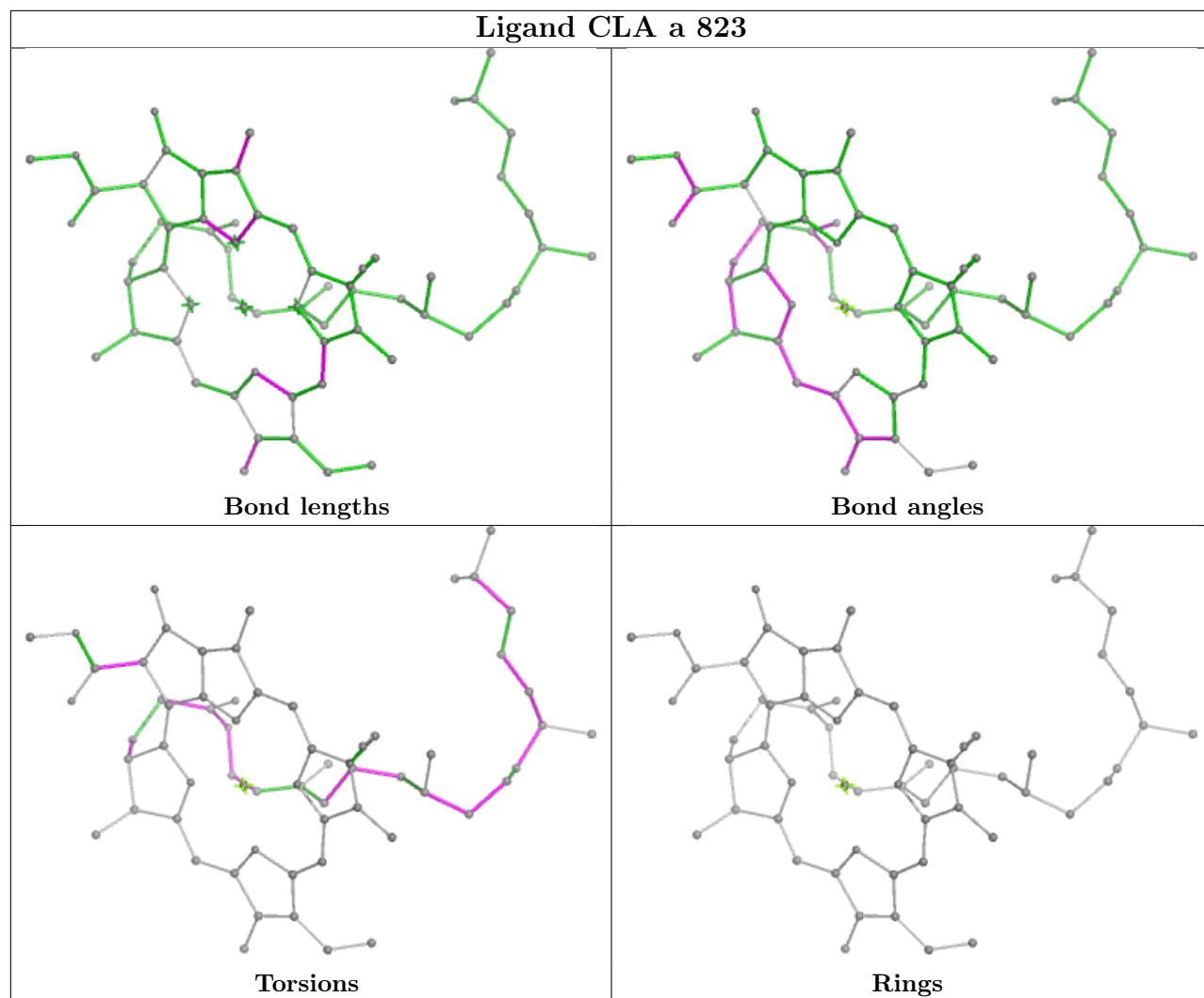
## Ligand CLA b 835



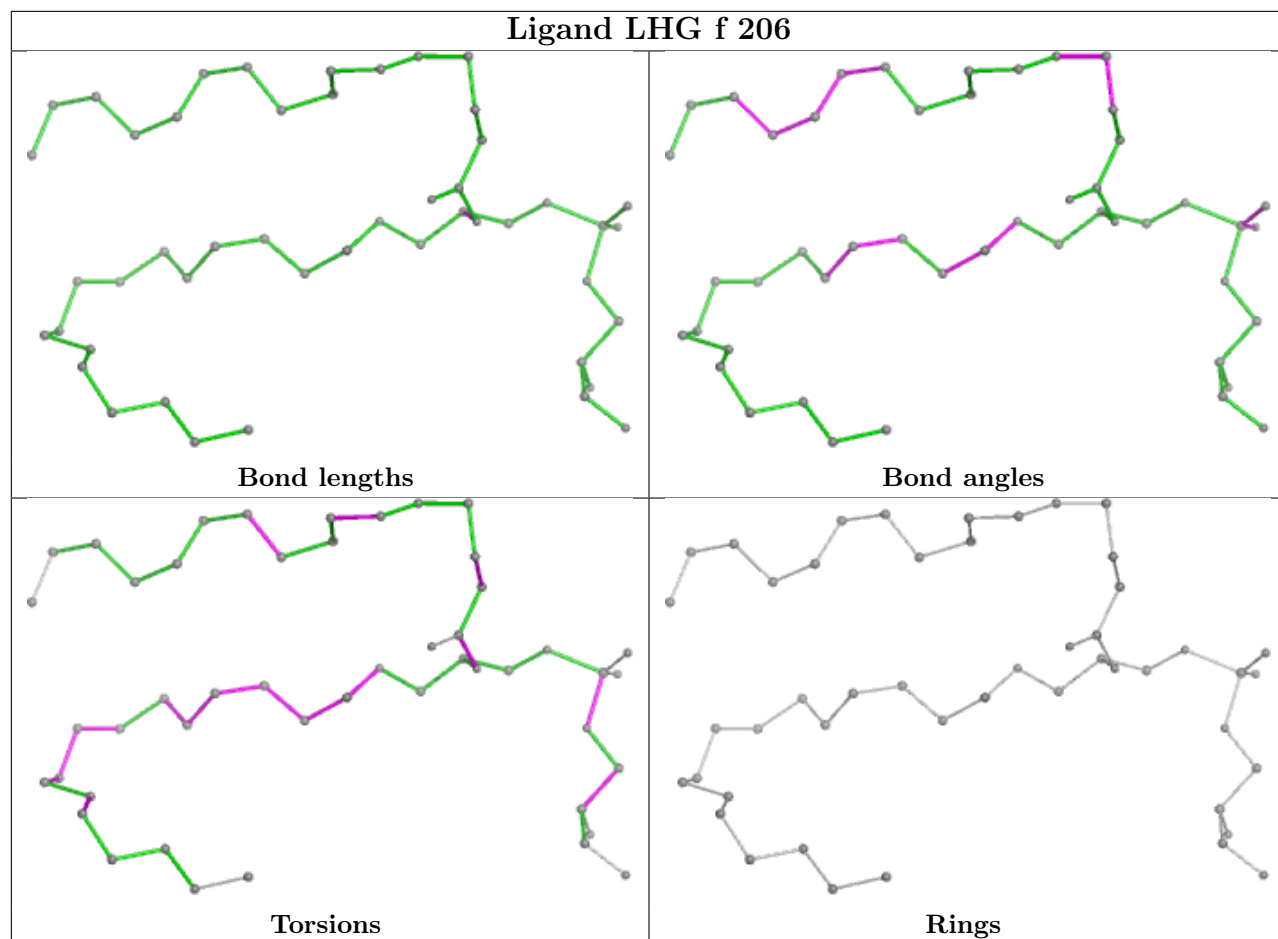
## Ligand CLA b 840



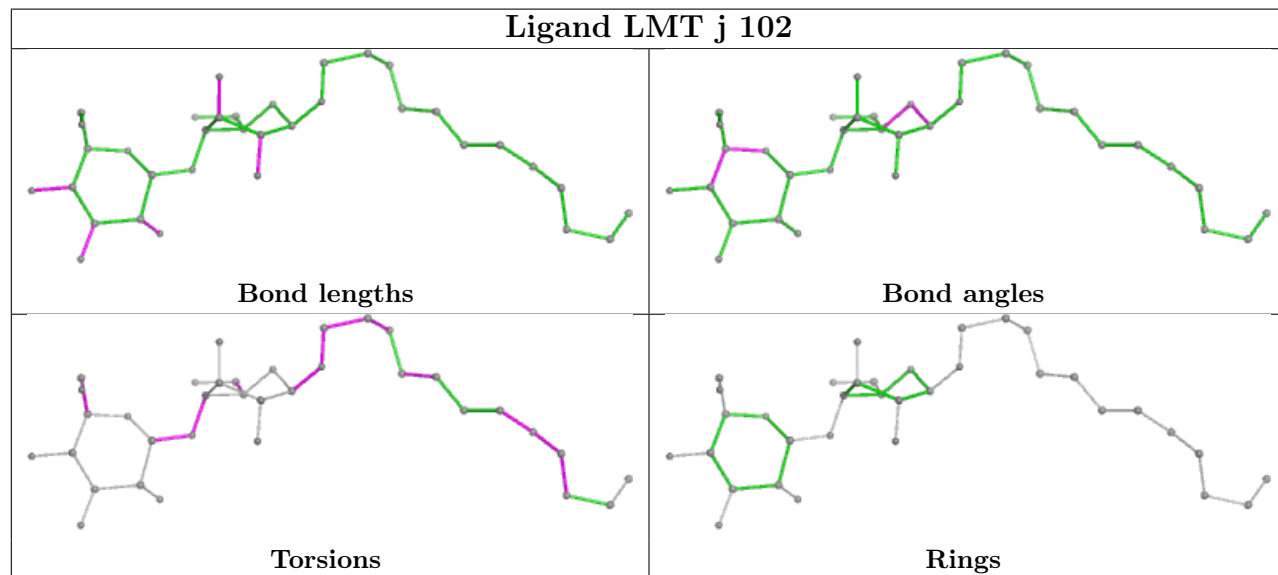


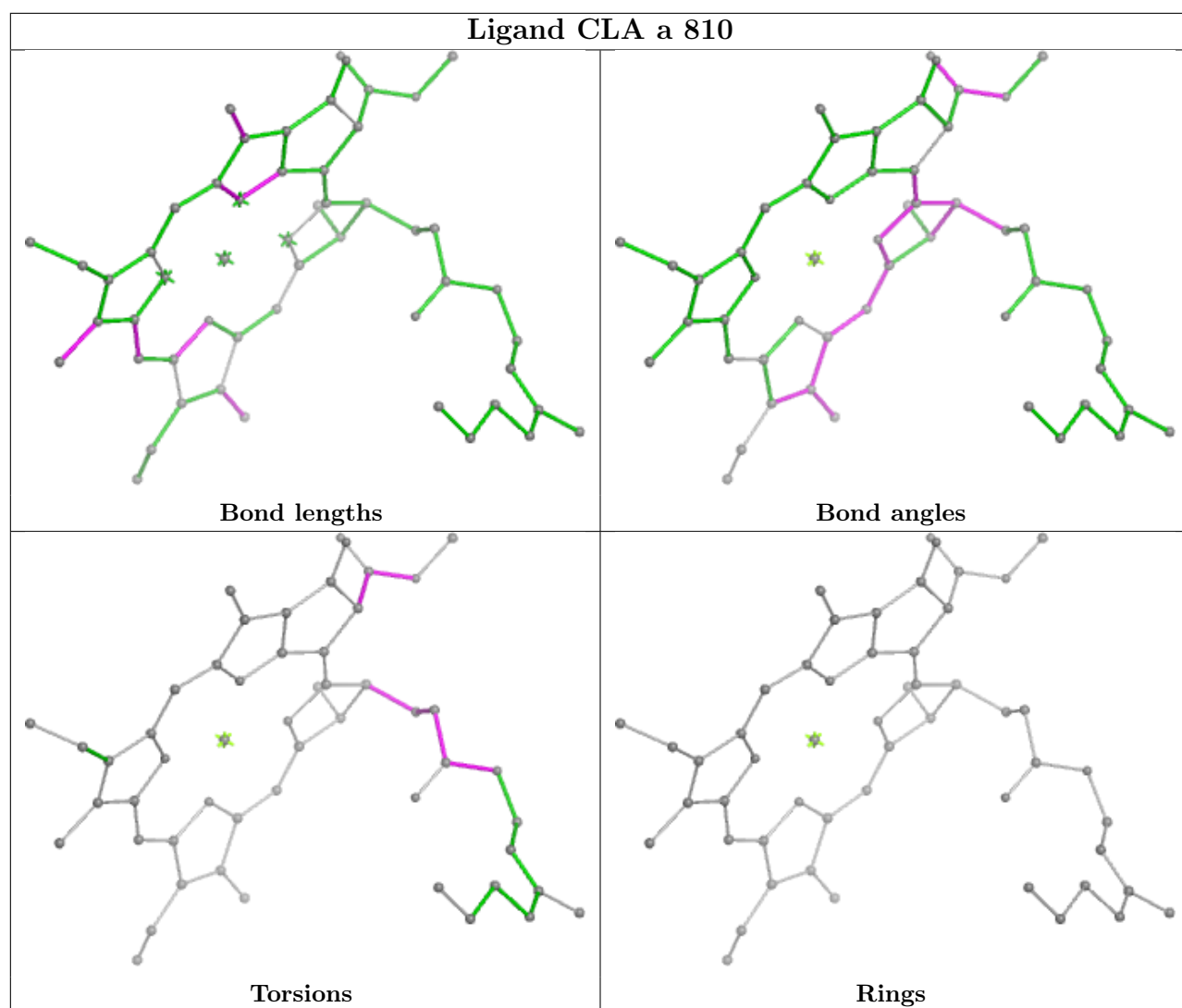


## Ligand LHG f 206

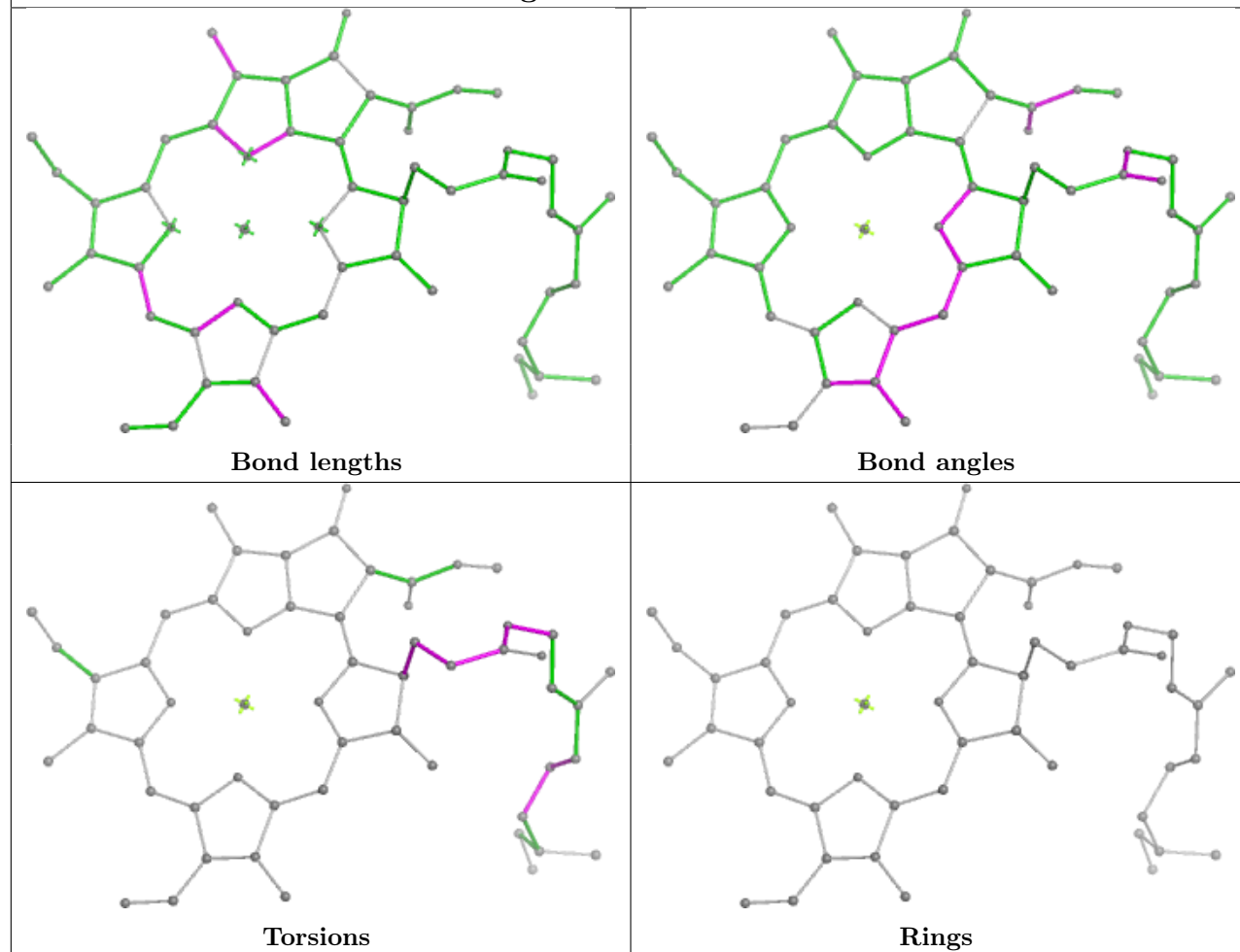


## Ligand LMT j 102

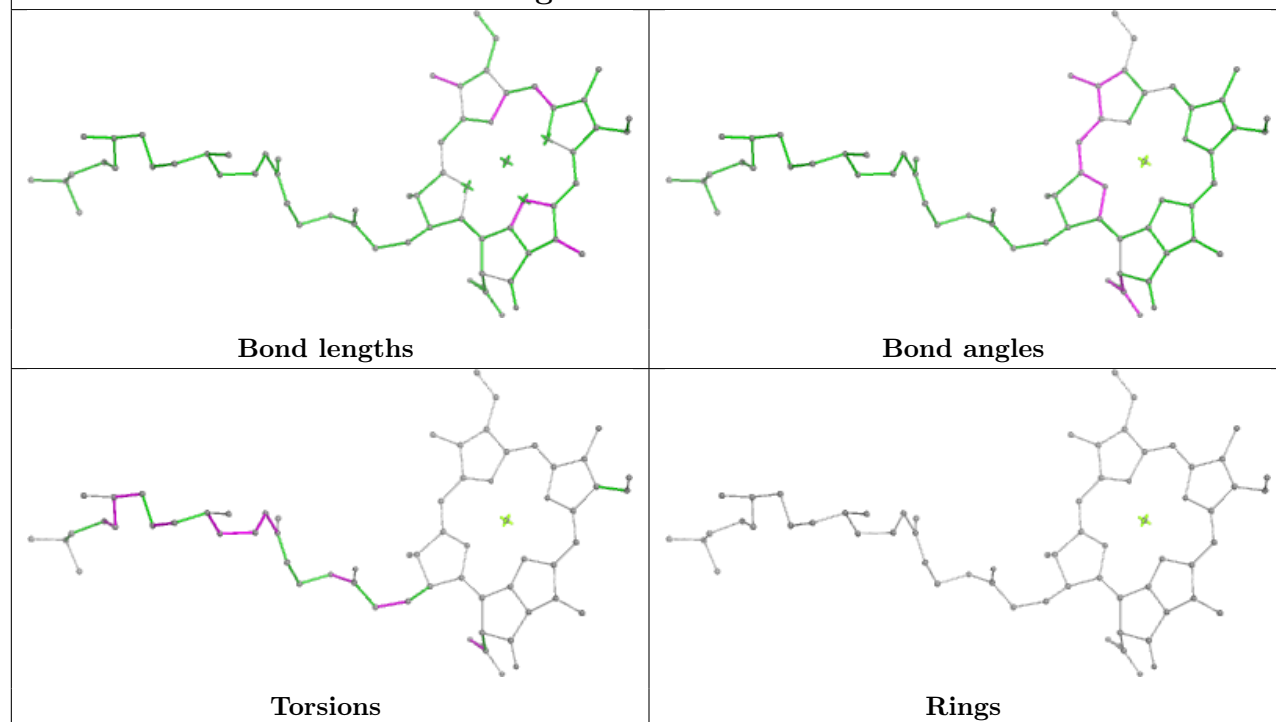




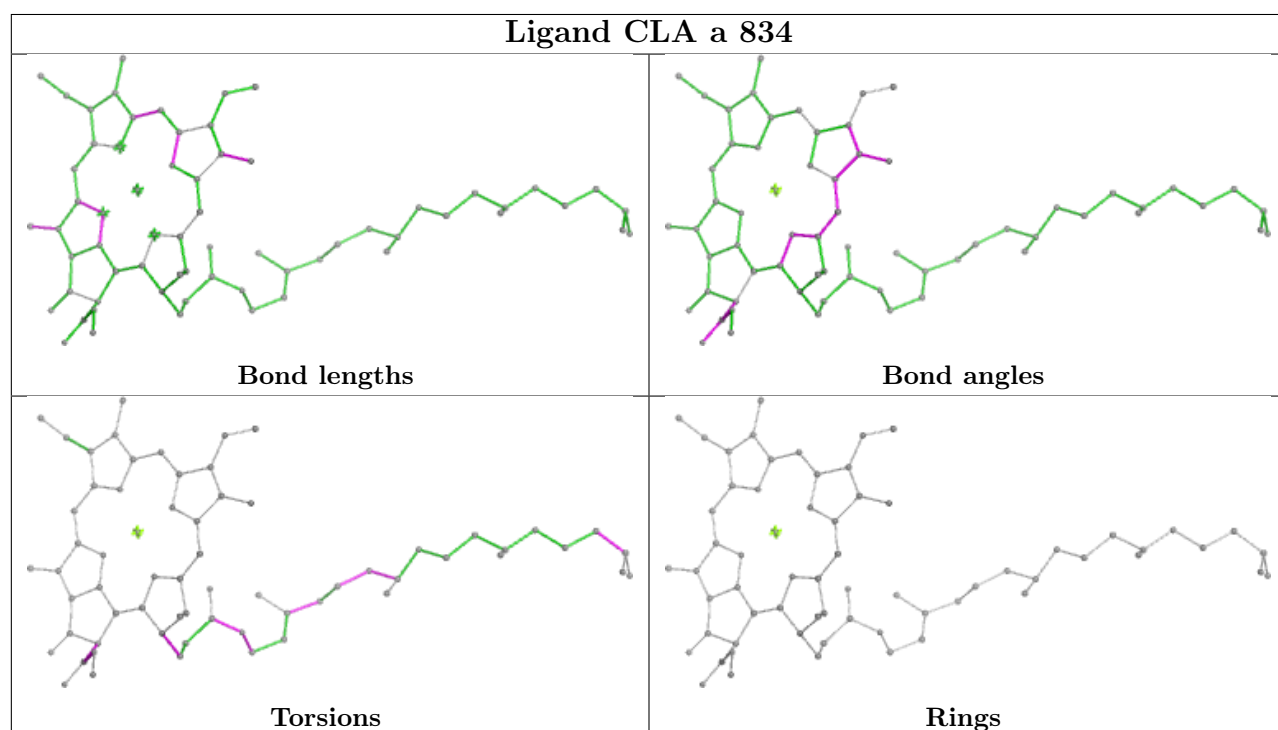
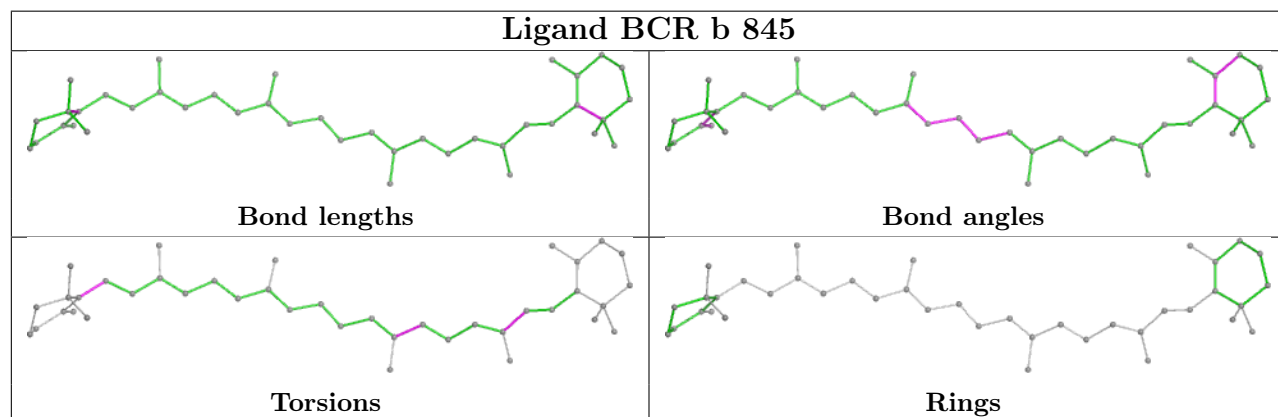
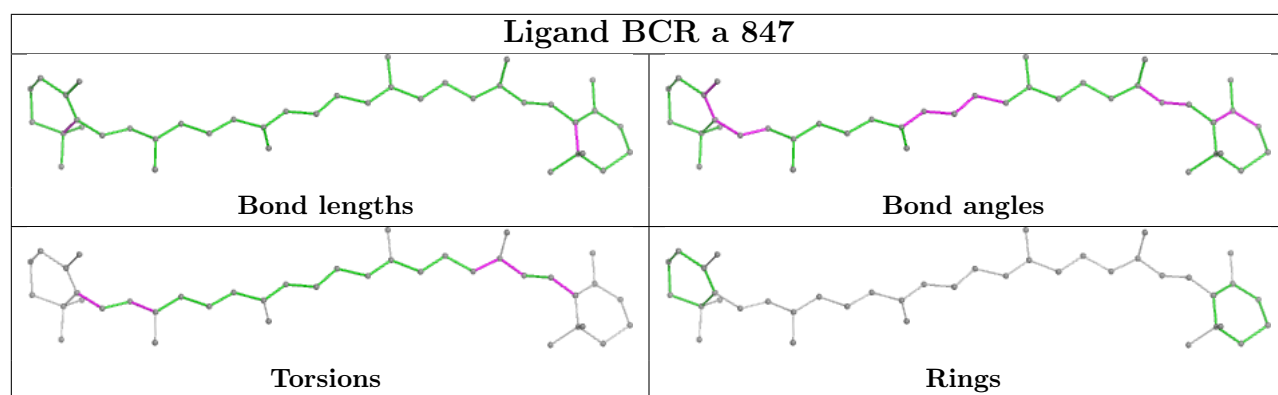
## Ligand CLA b 811

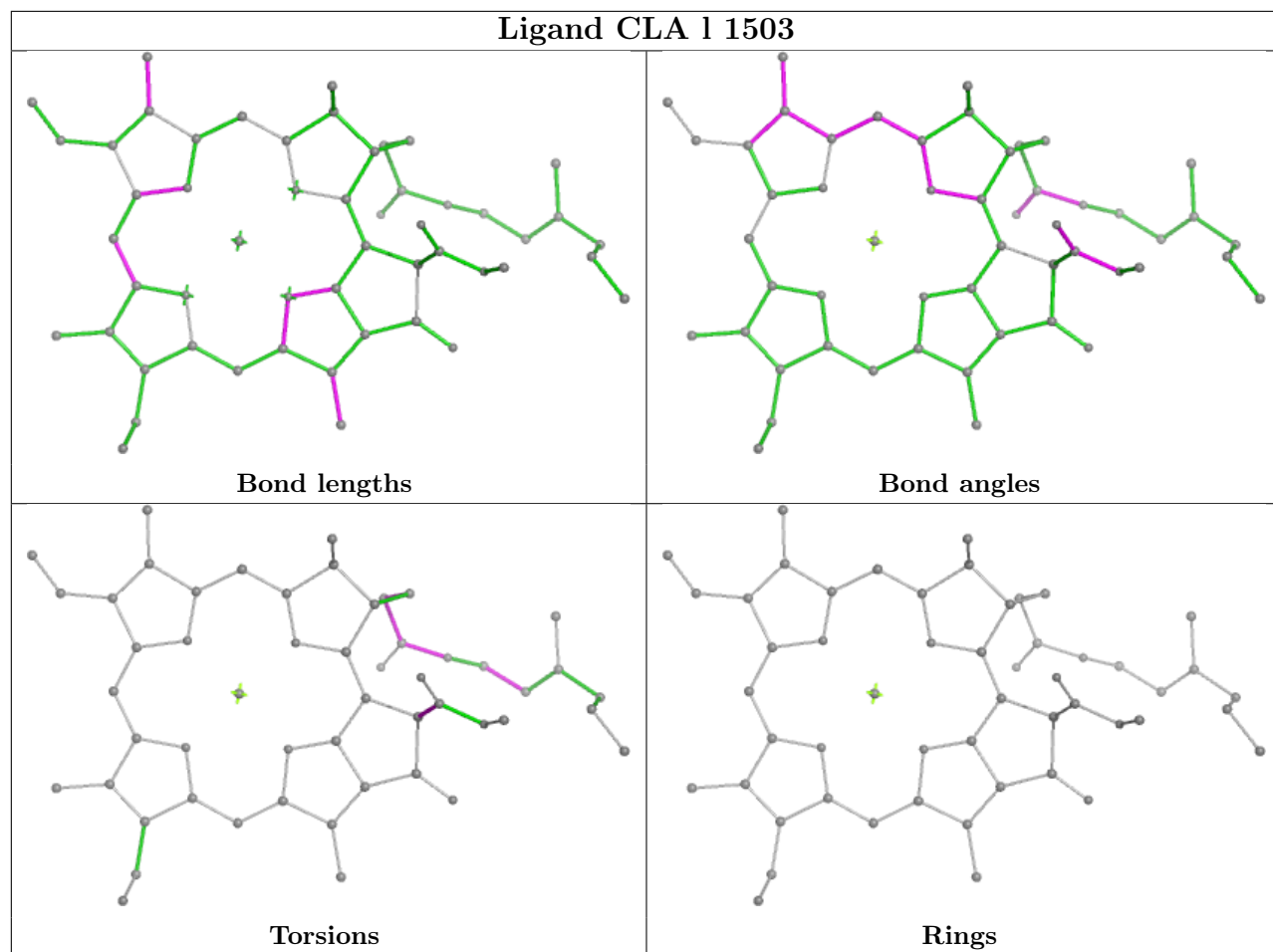


## Ligand CLA b 814

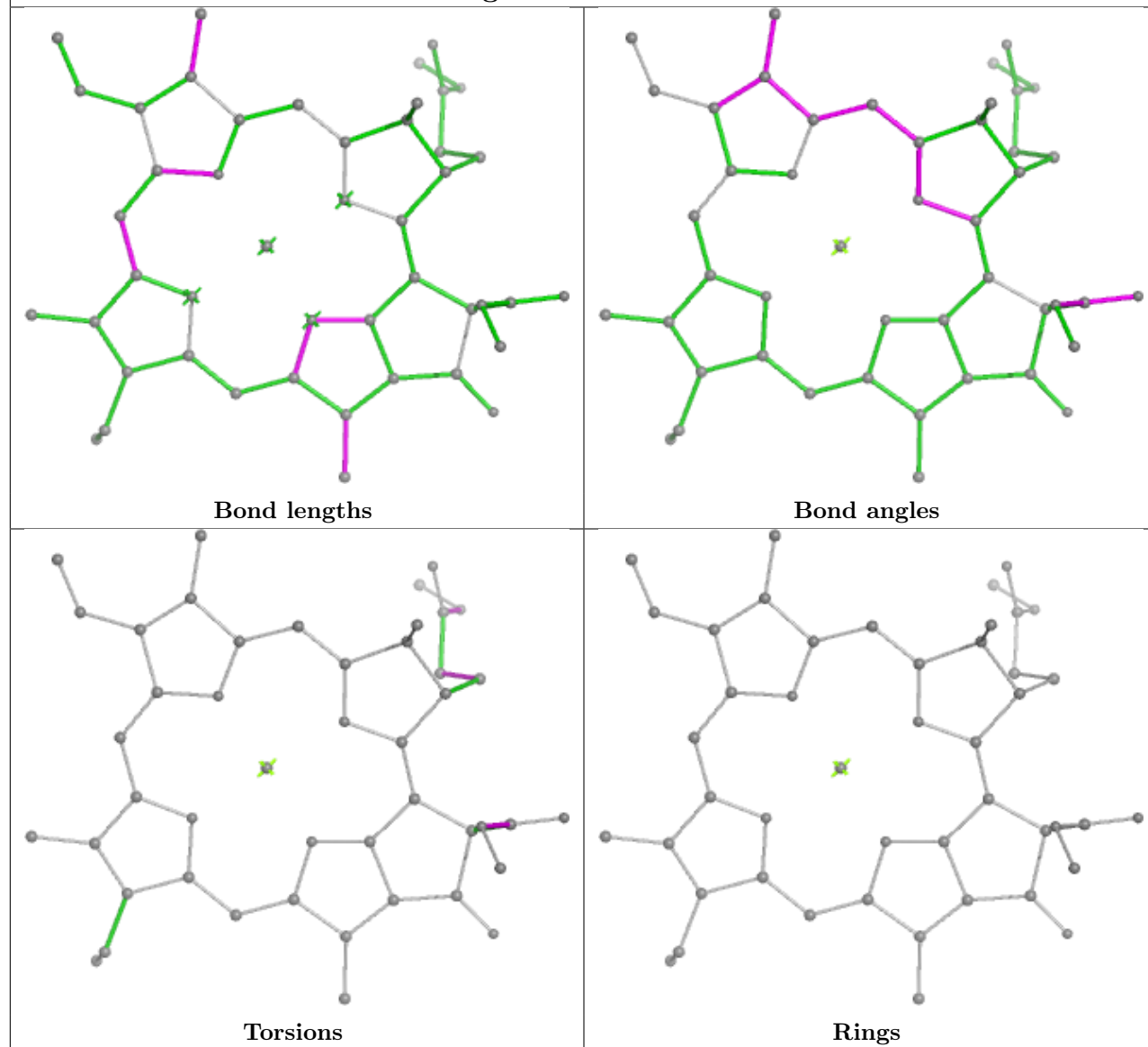




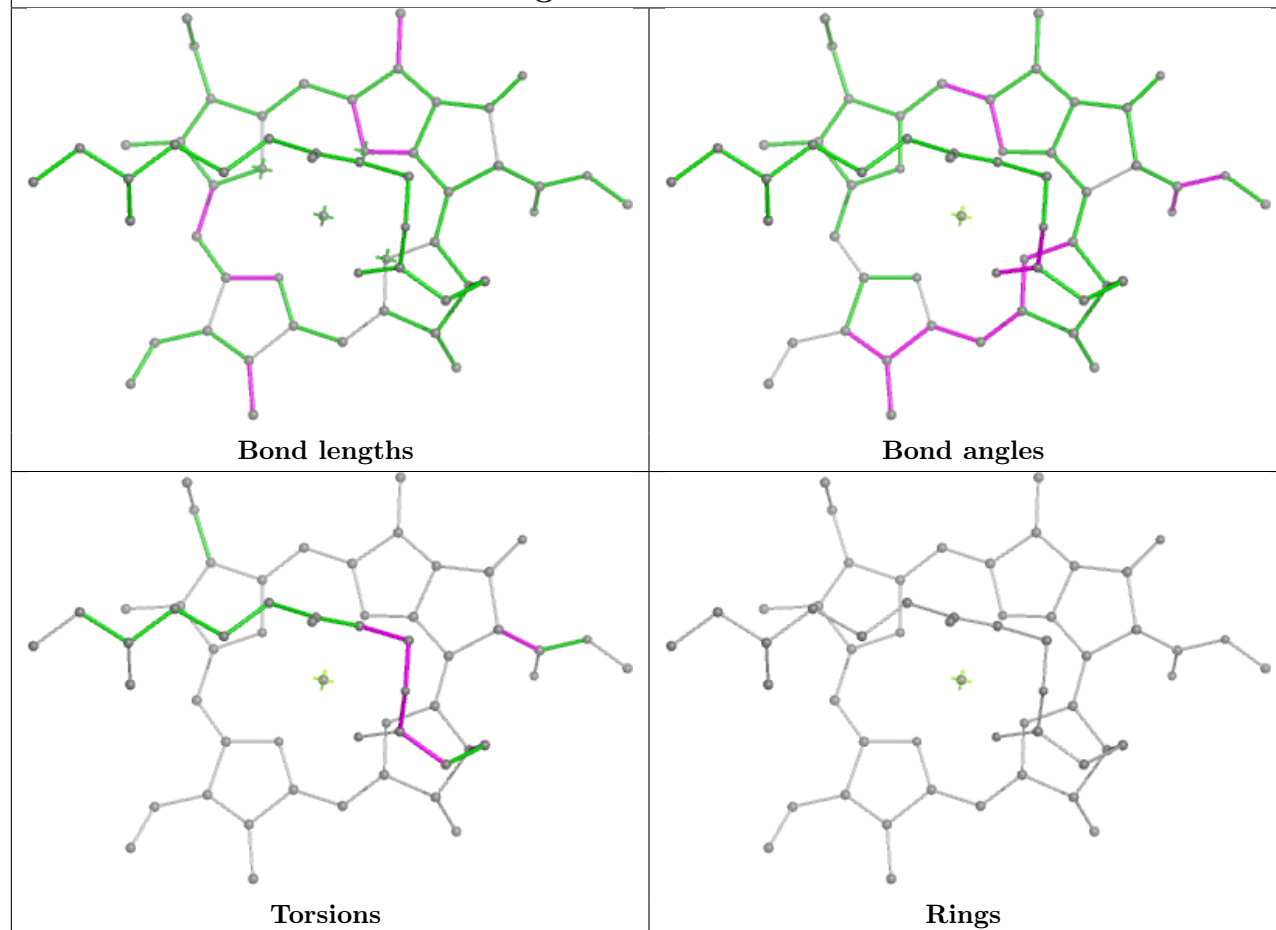




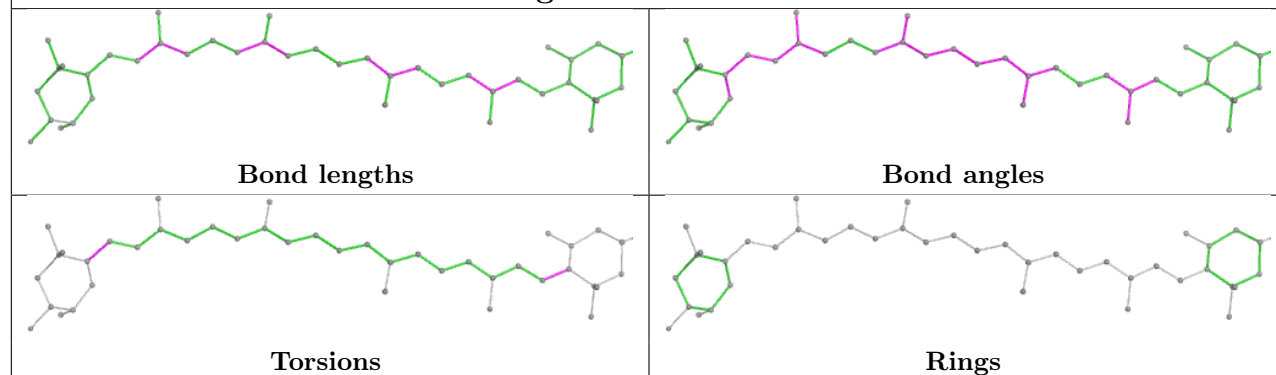
## Ligand CLA a 815

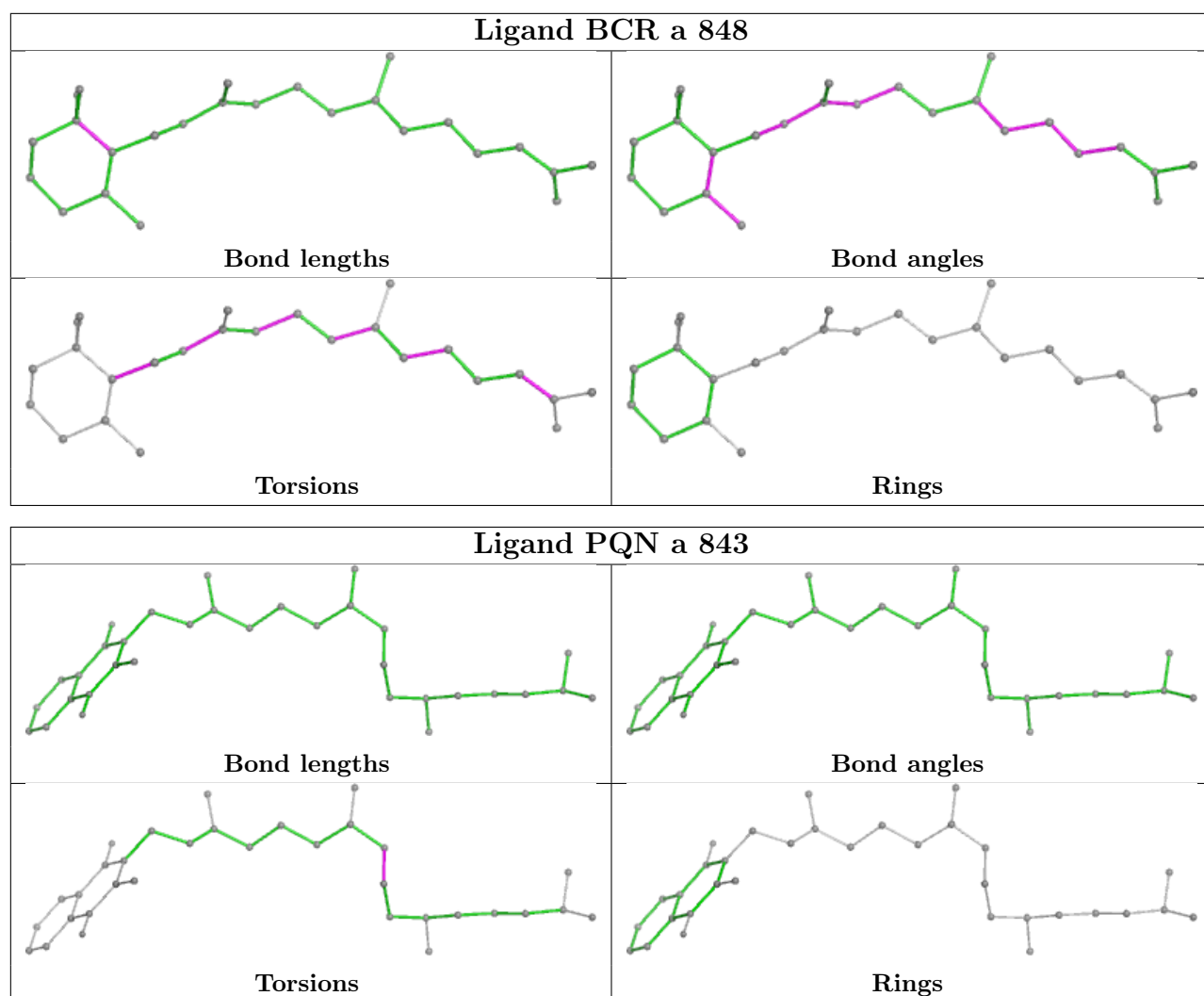


## Ligand CLA b 817

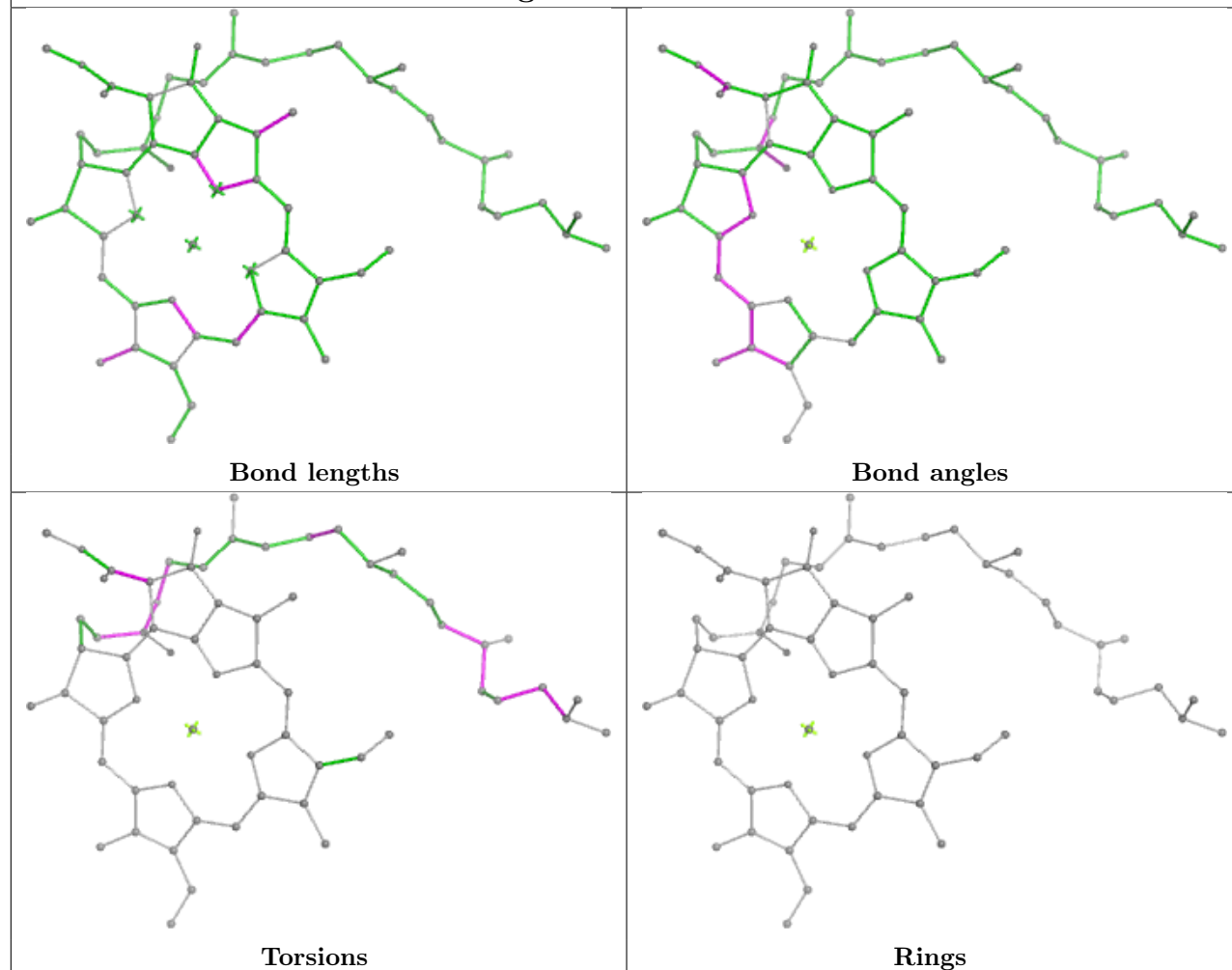


## Ligand ZEX b 854

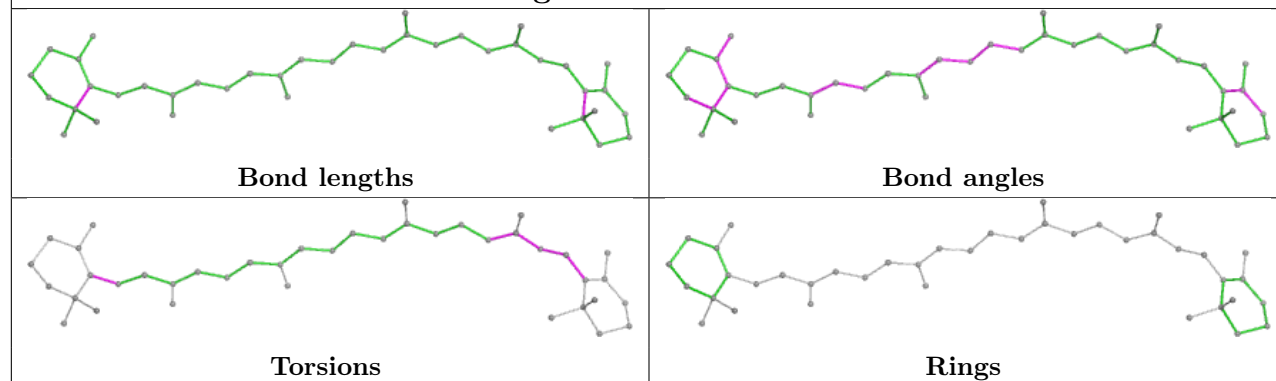


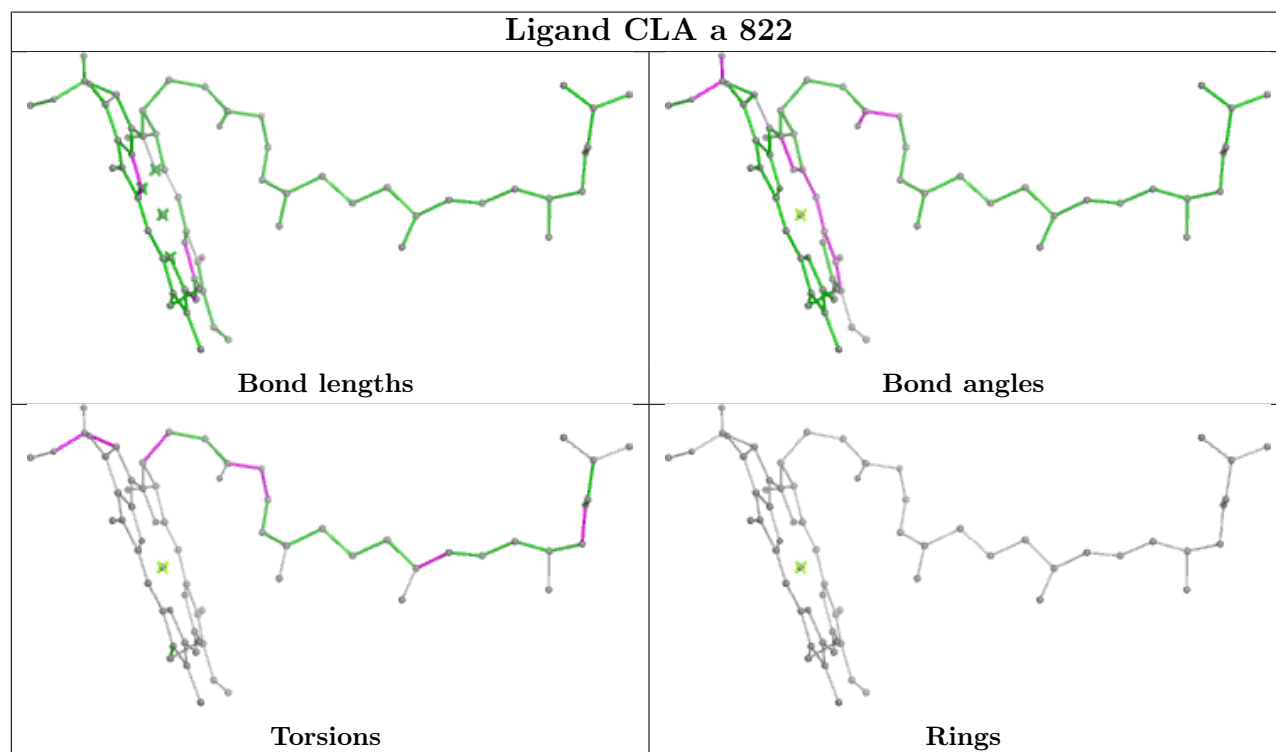
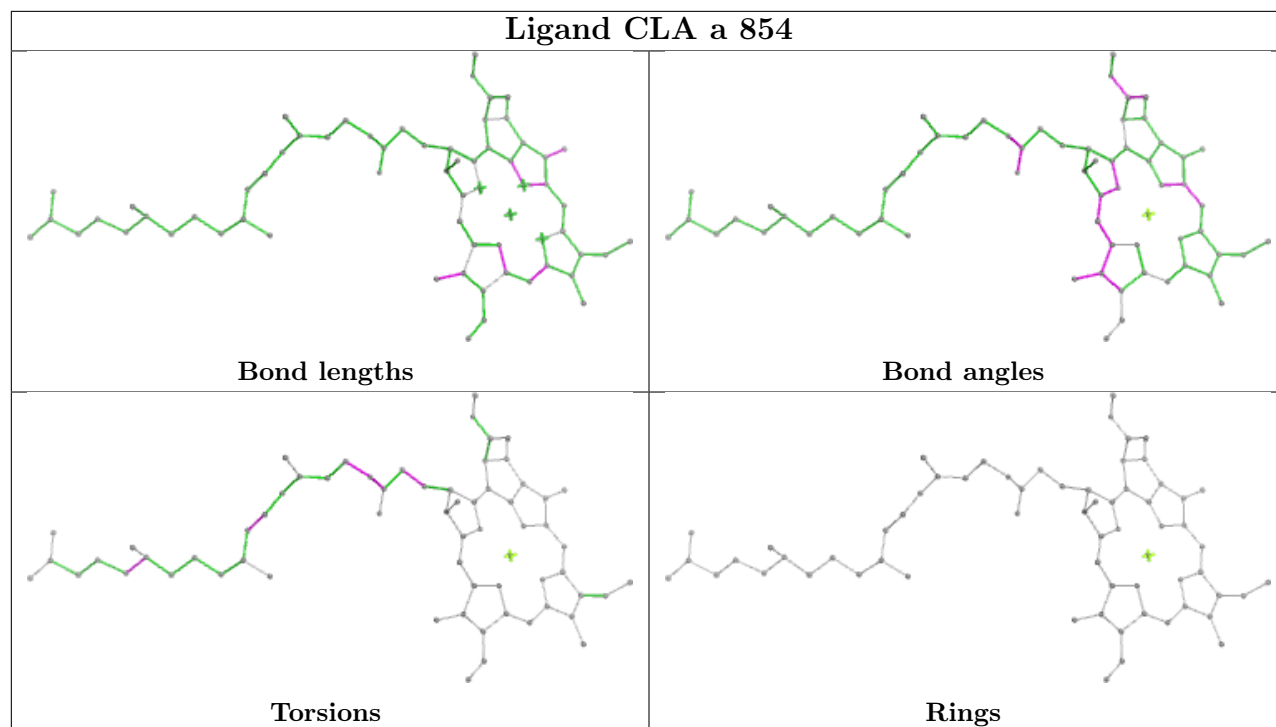


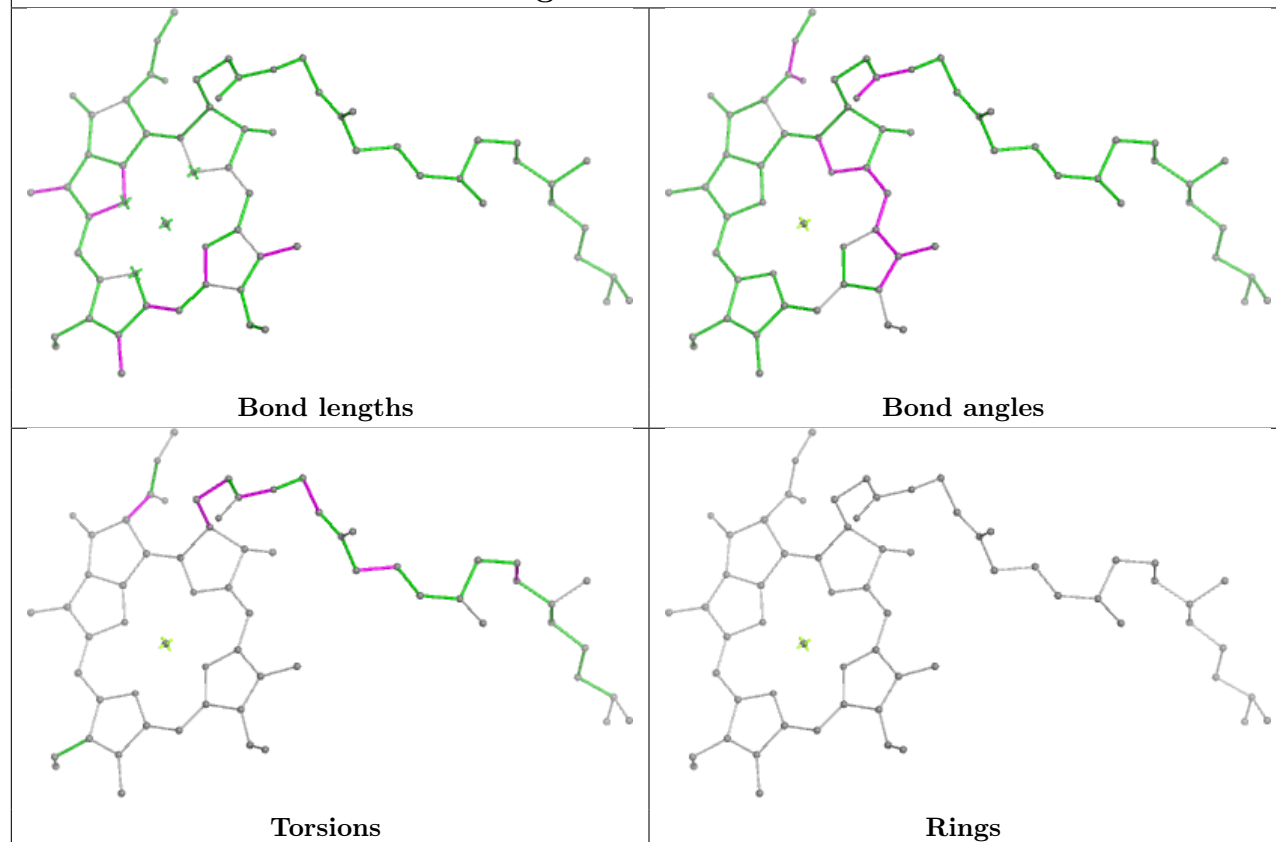
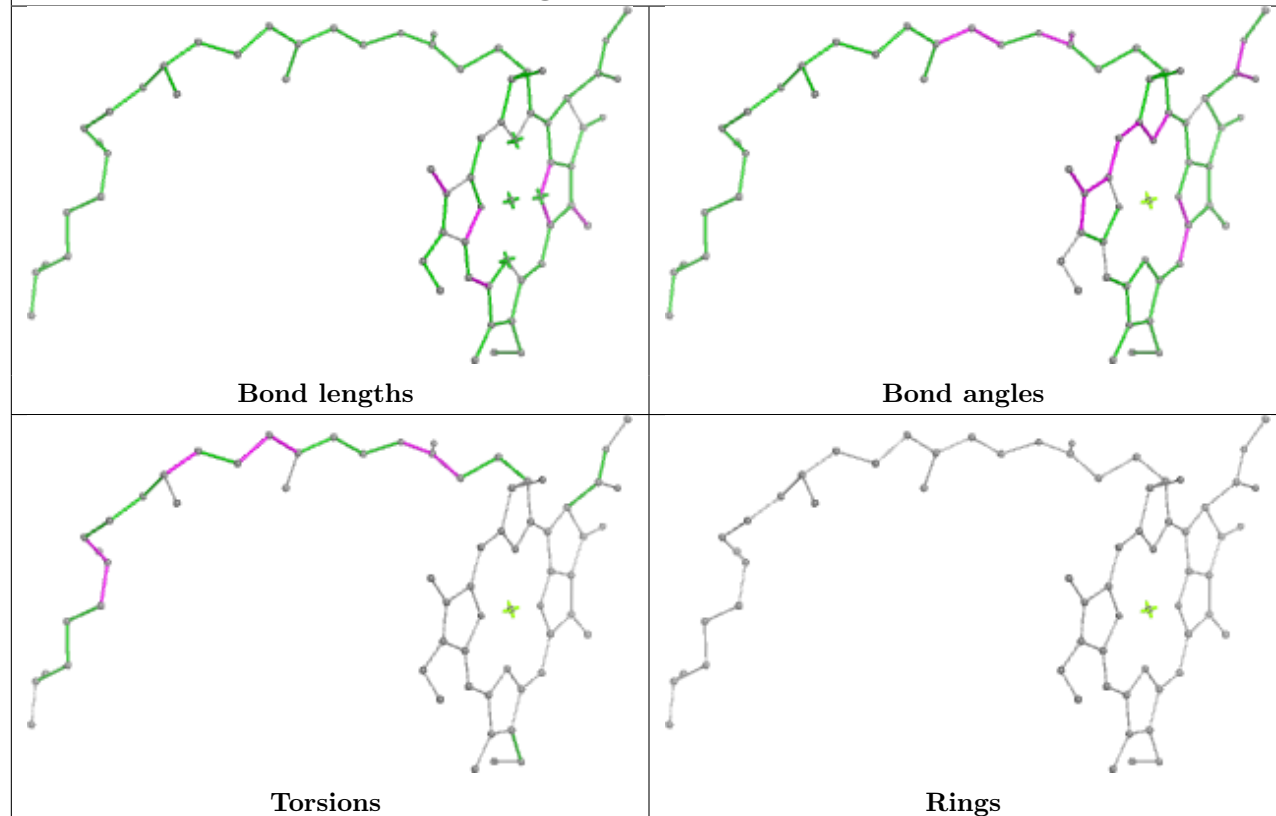
## Ligand CLA a 829



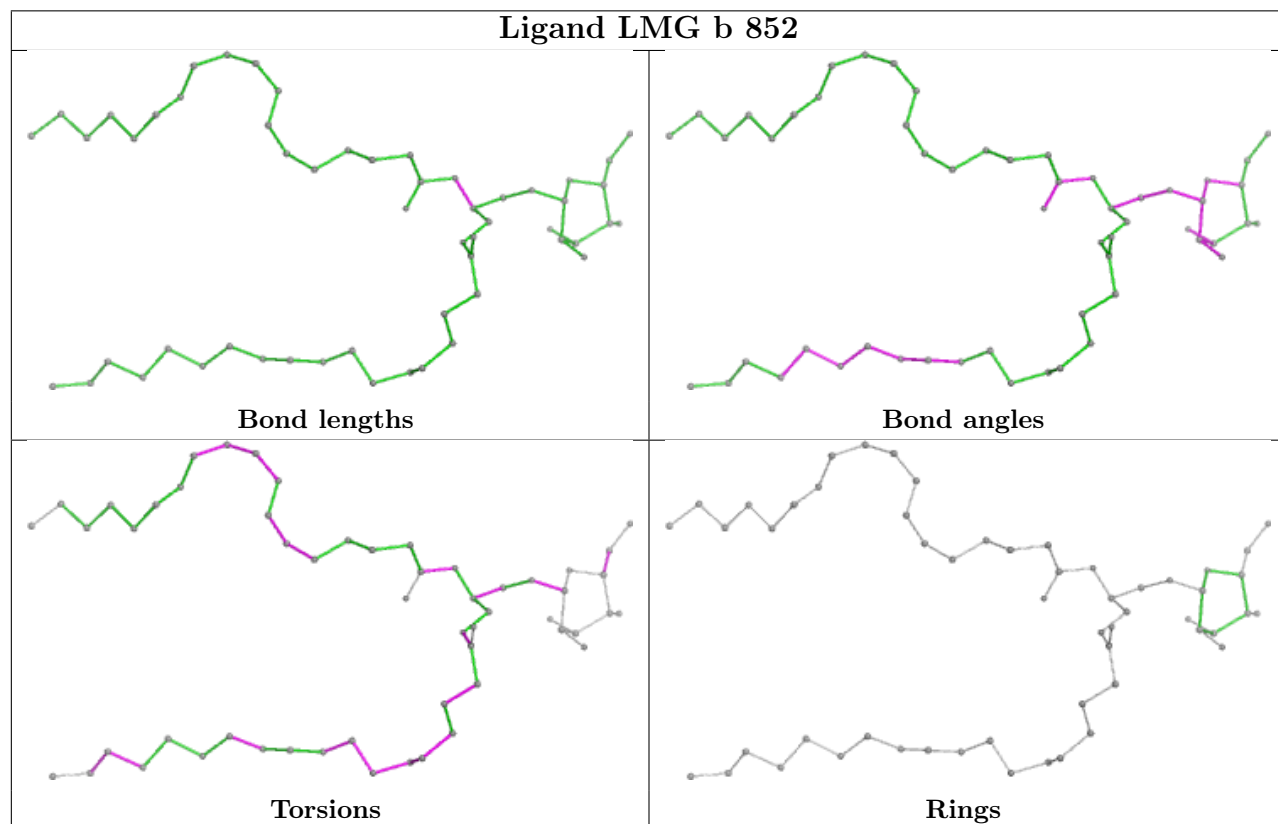
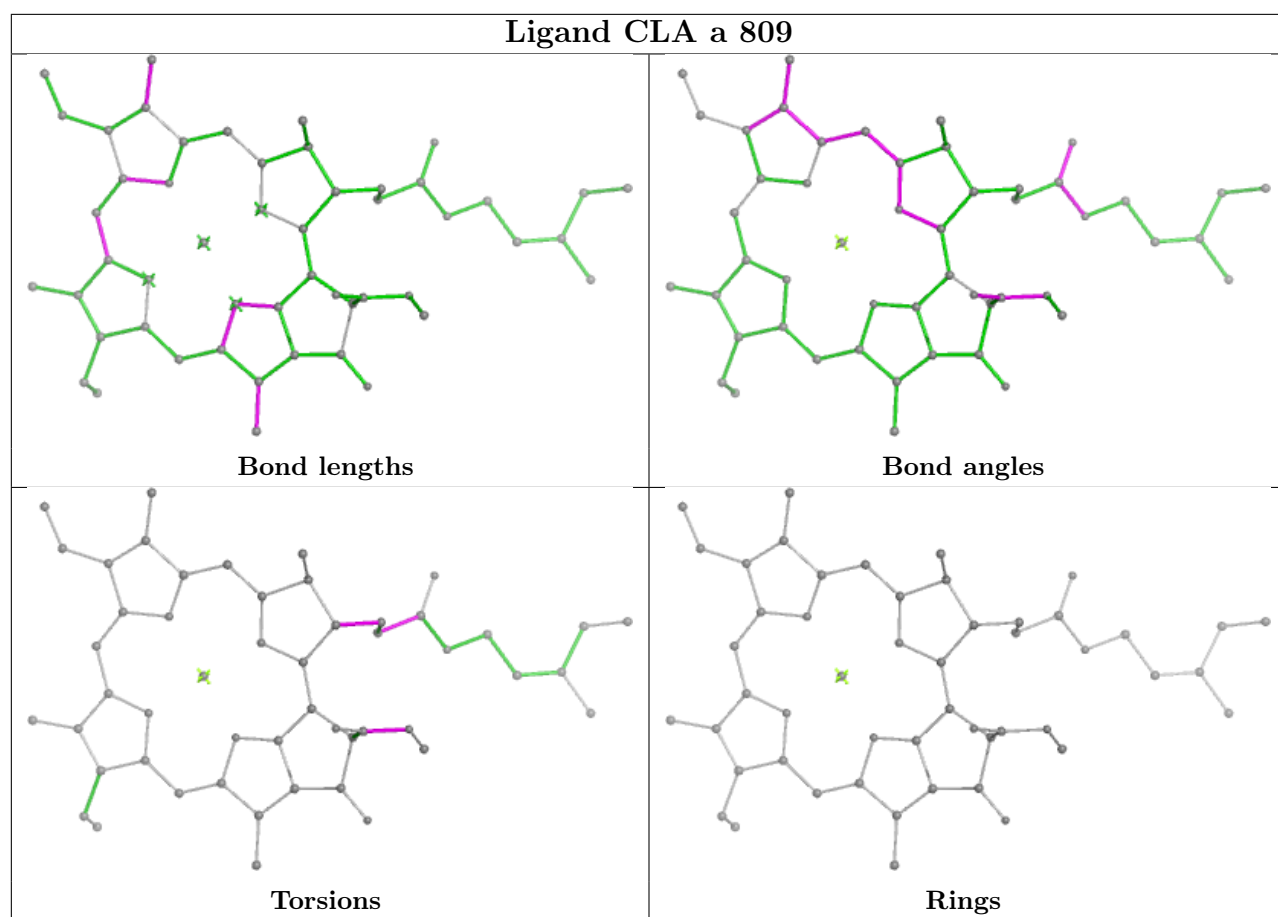
## Ligand BCR b 847

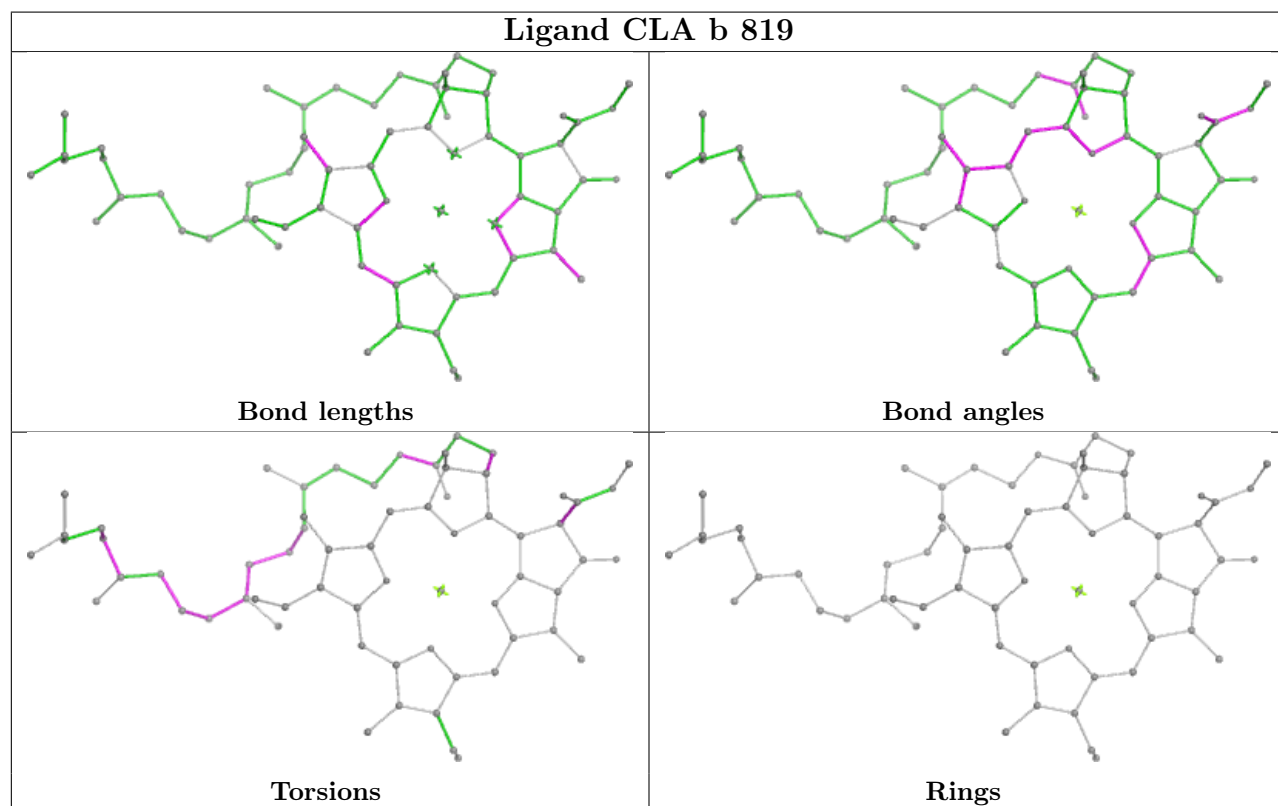
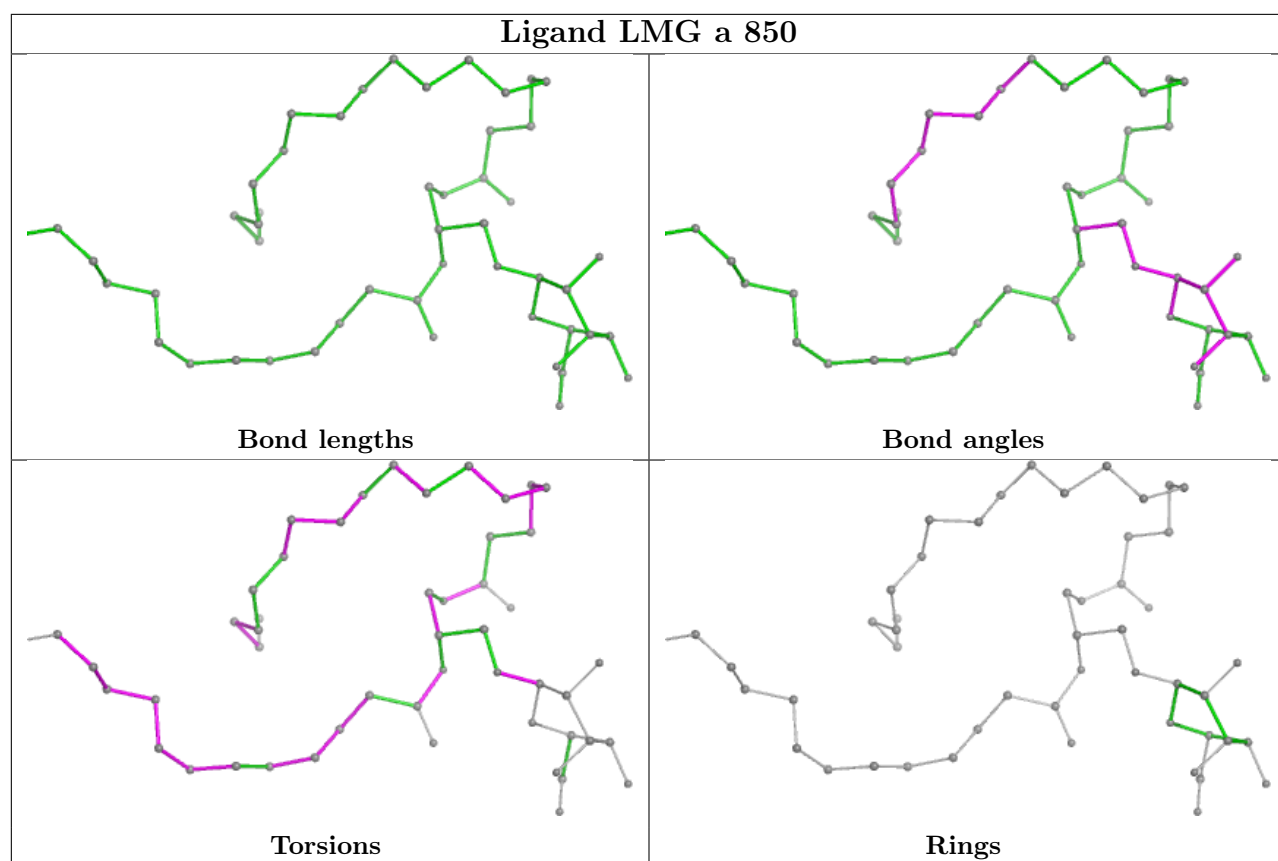


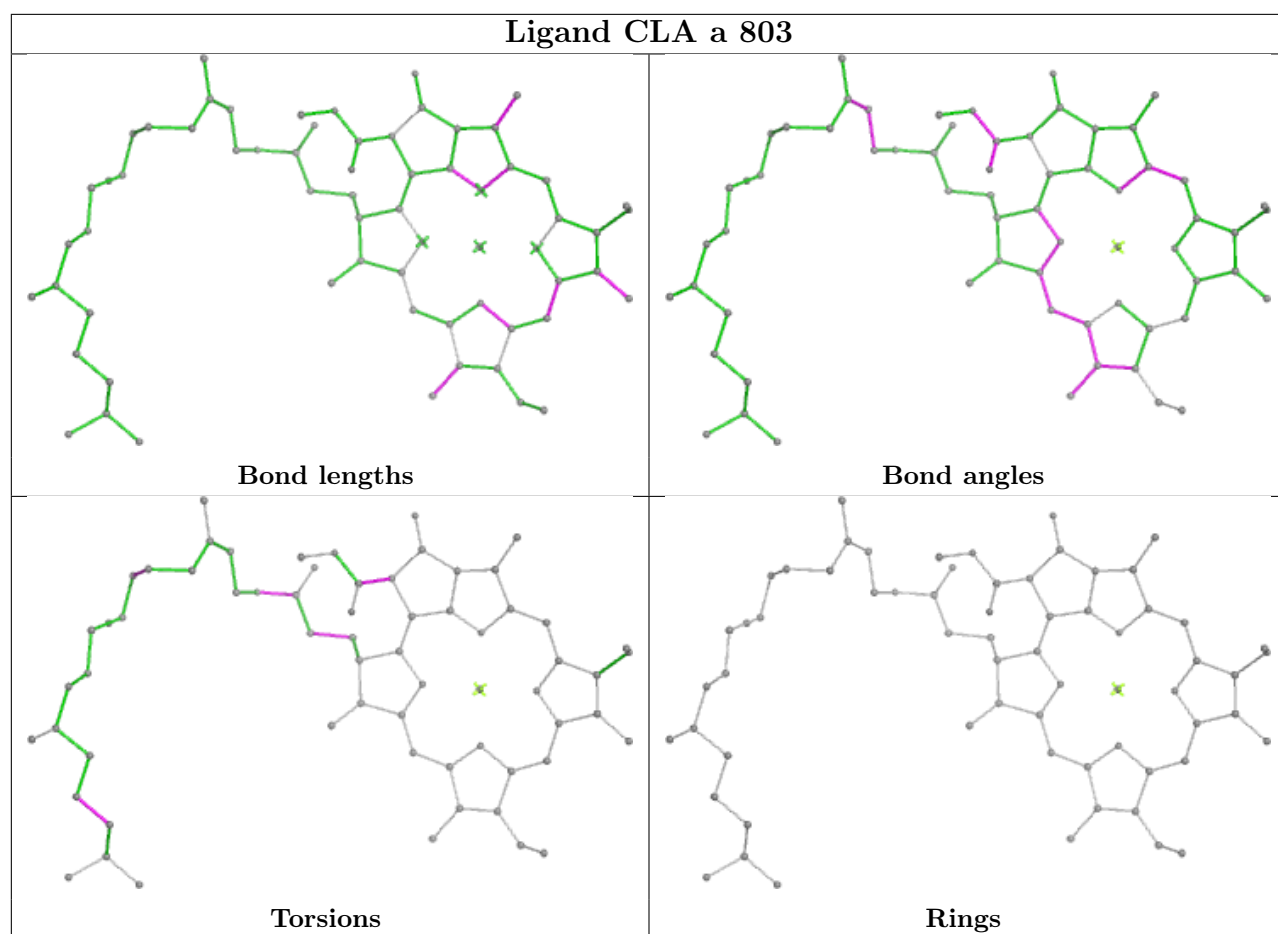


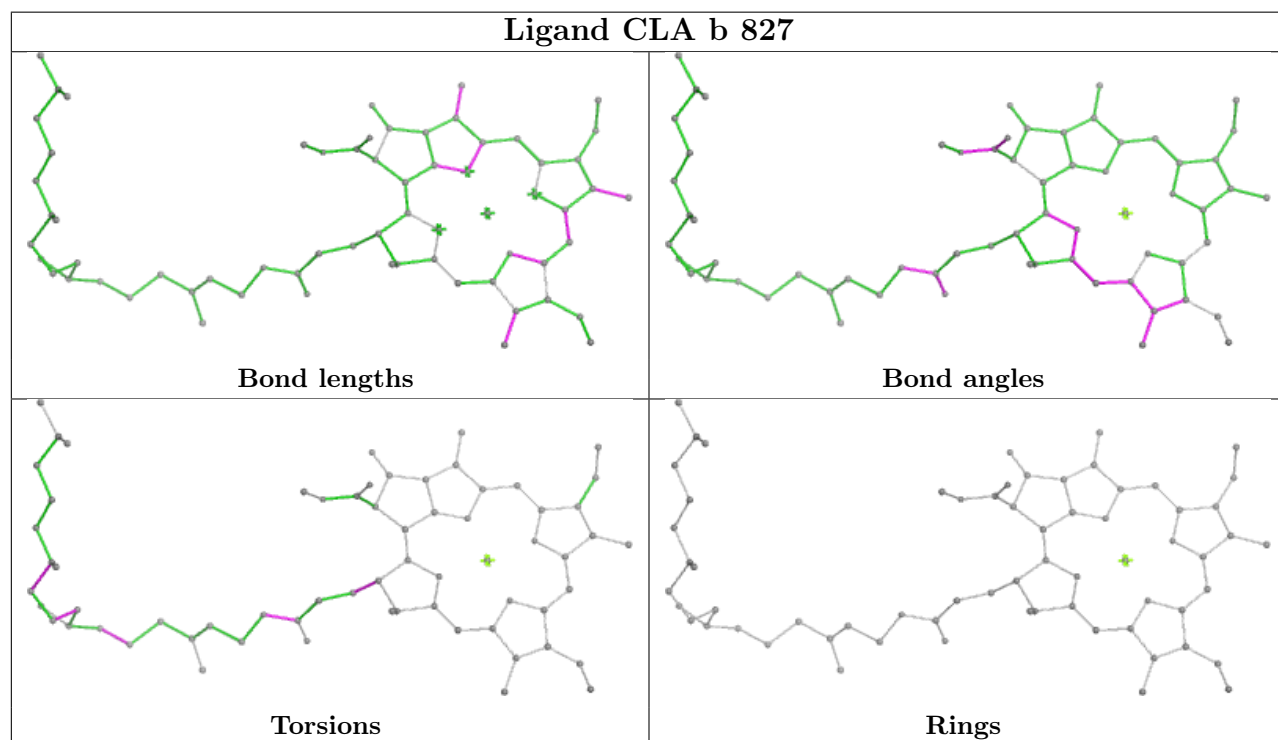
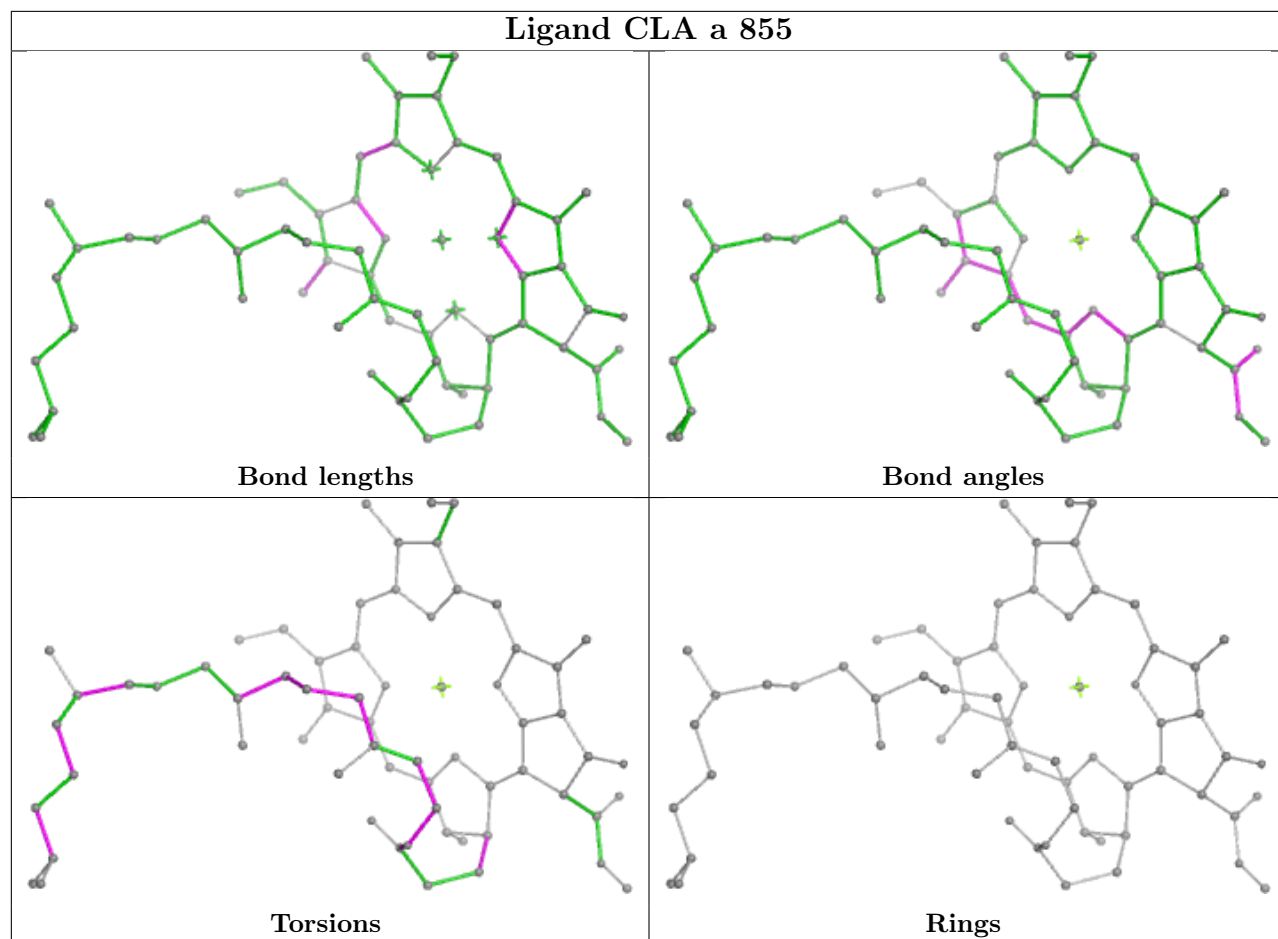
**Ligand CLA a 802****Ligand CLA a 835**

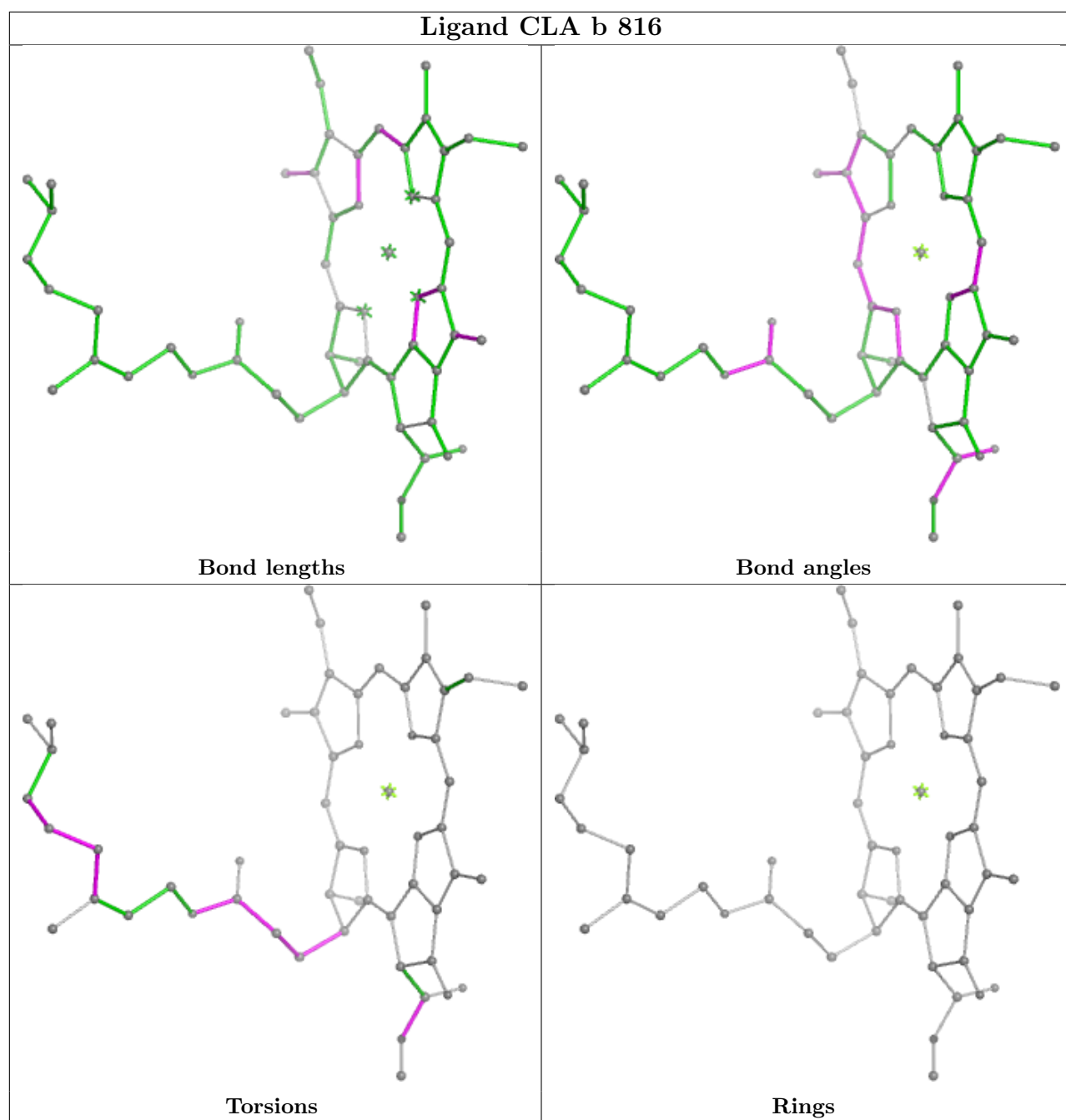


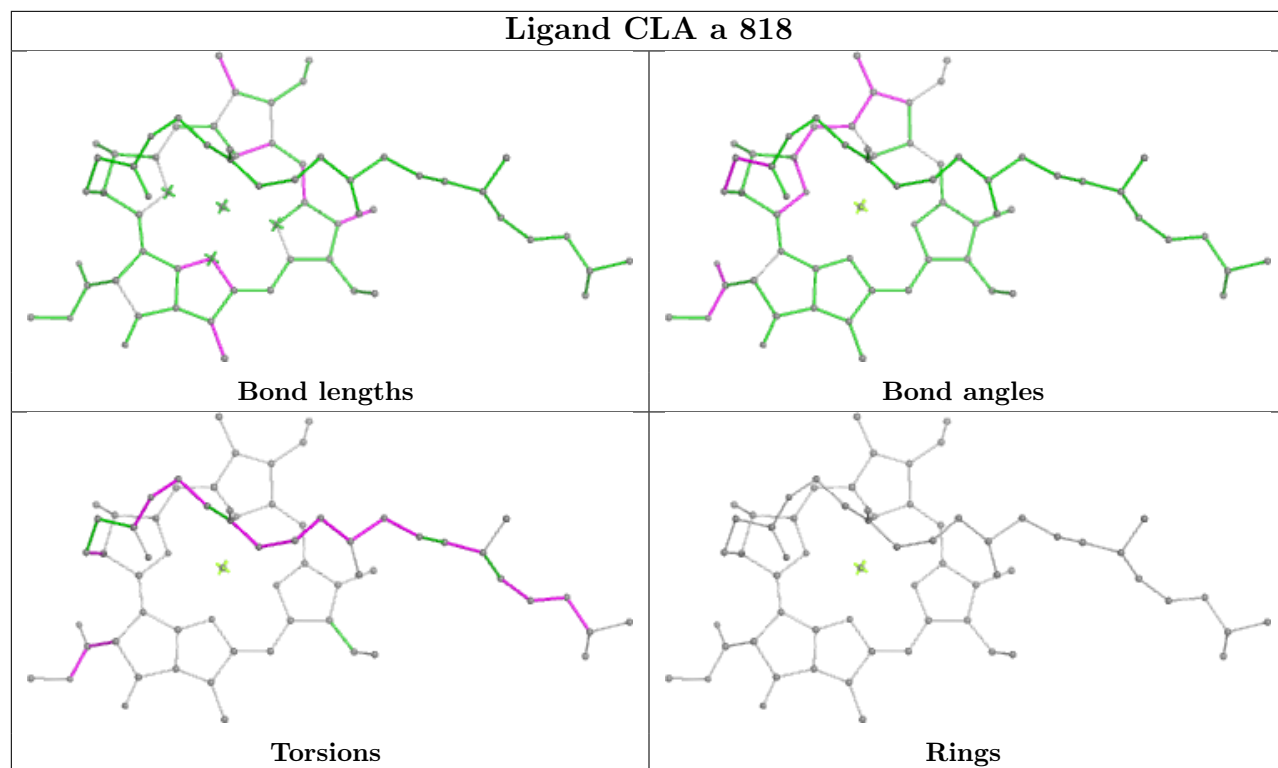


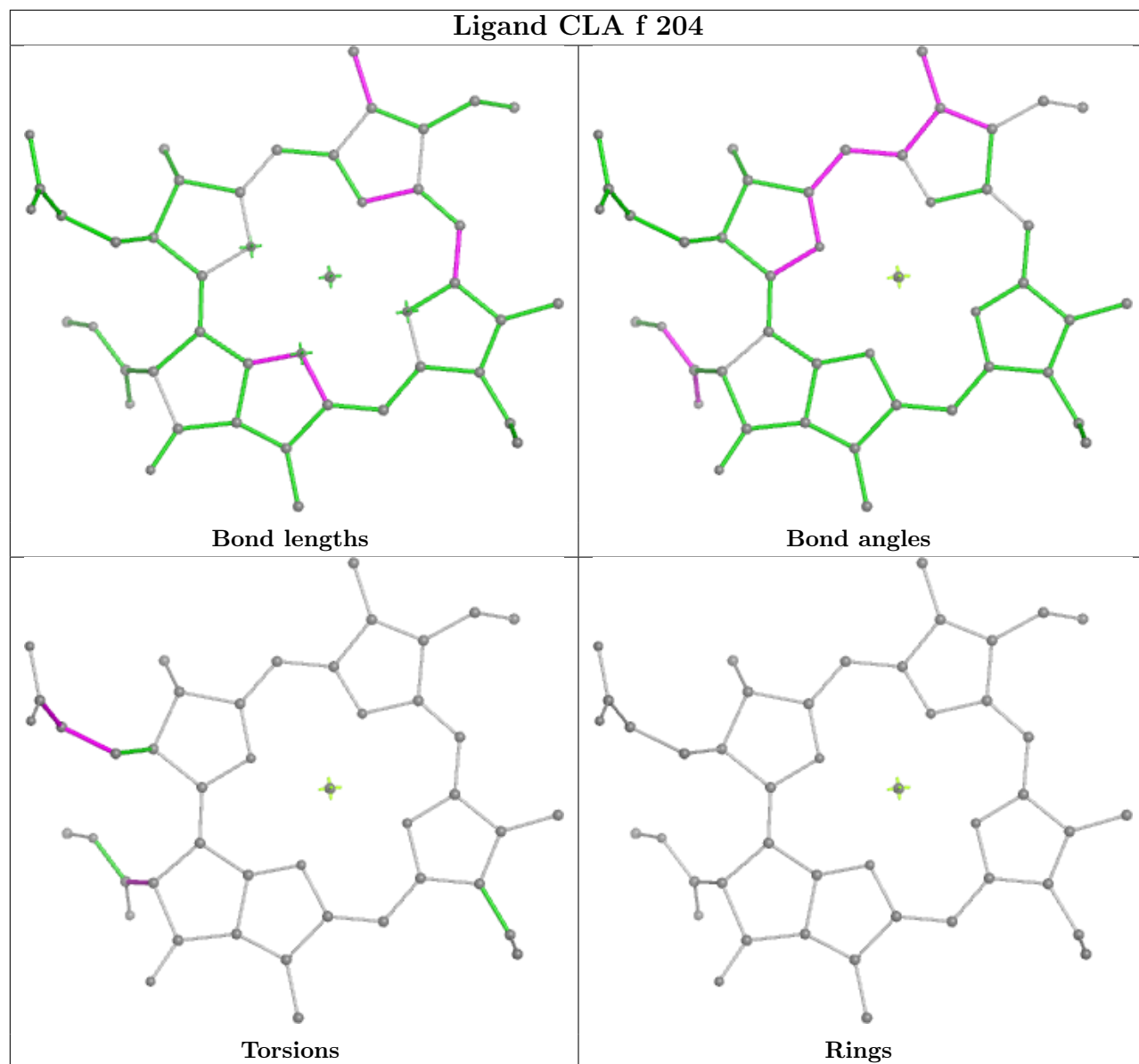


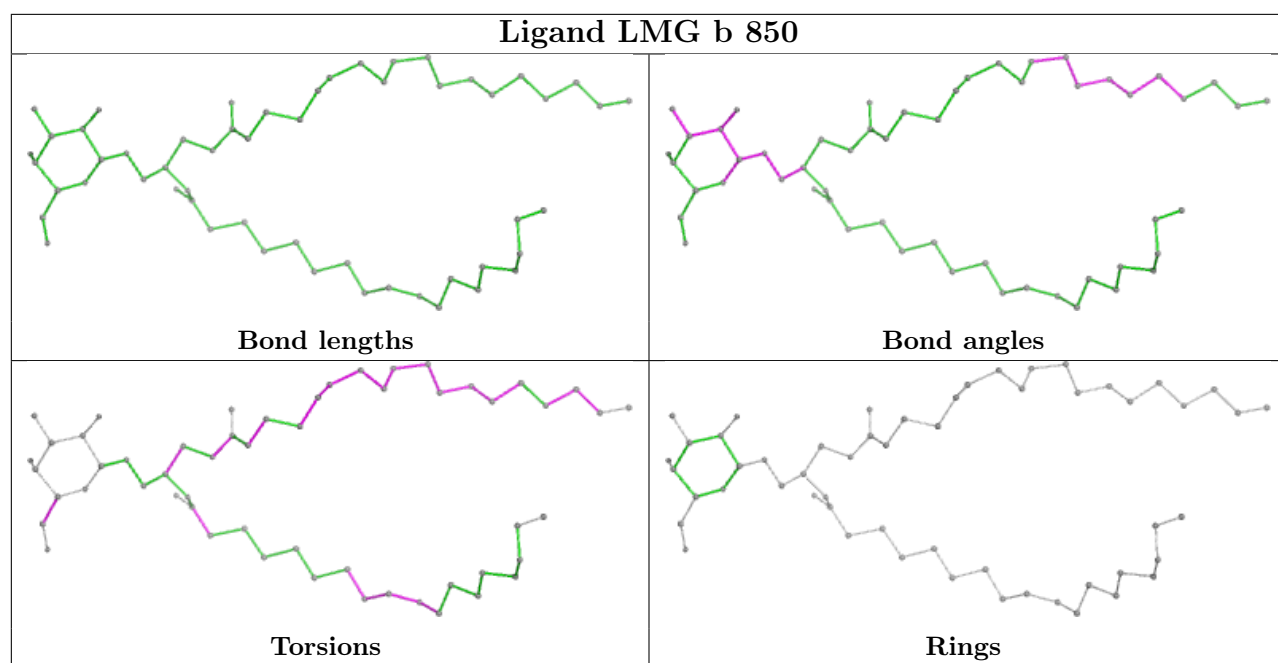






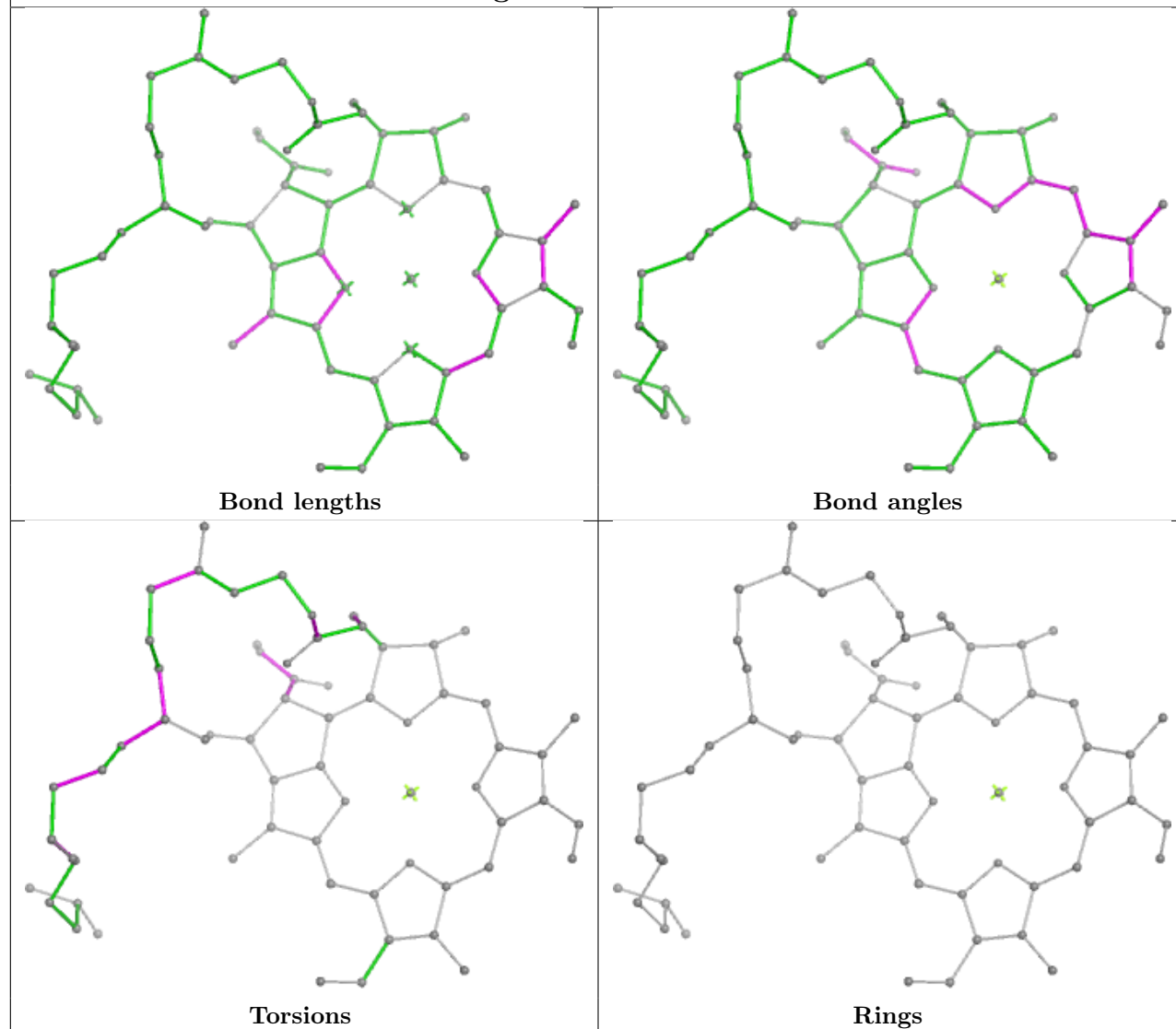




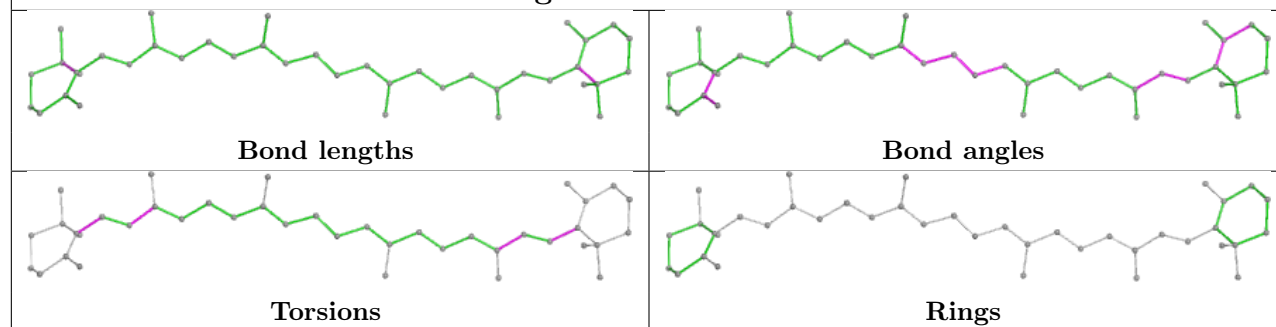


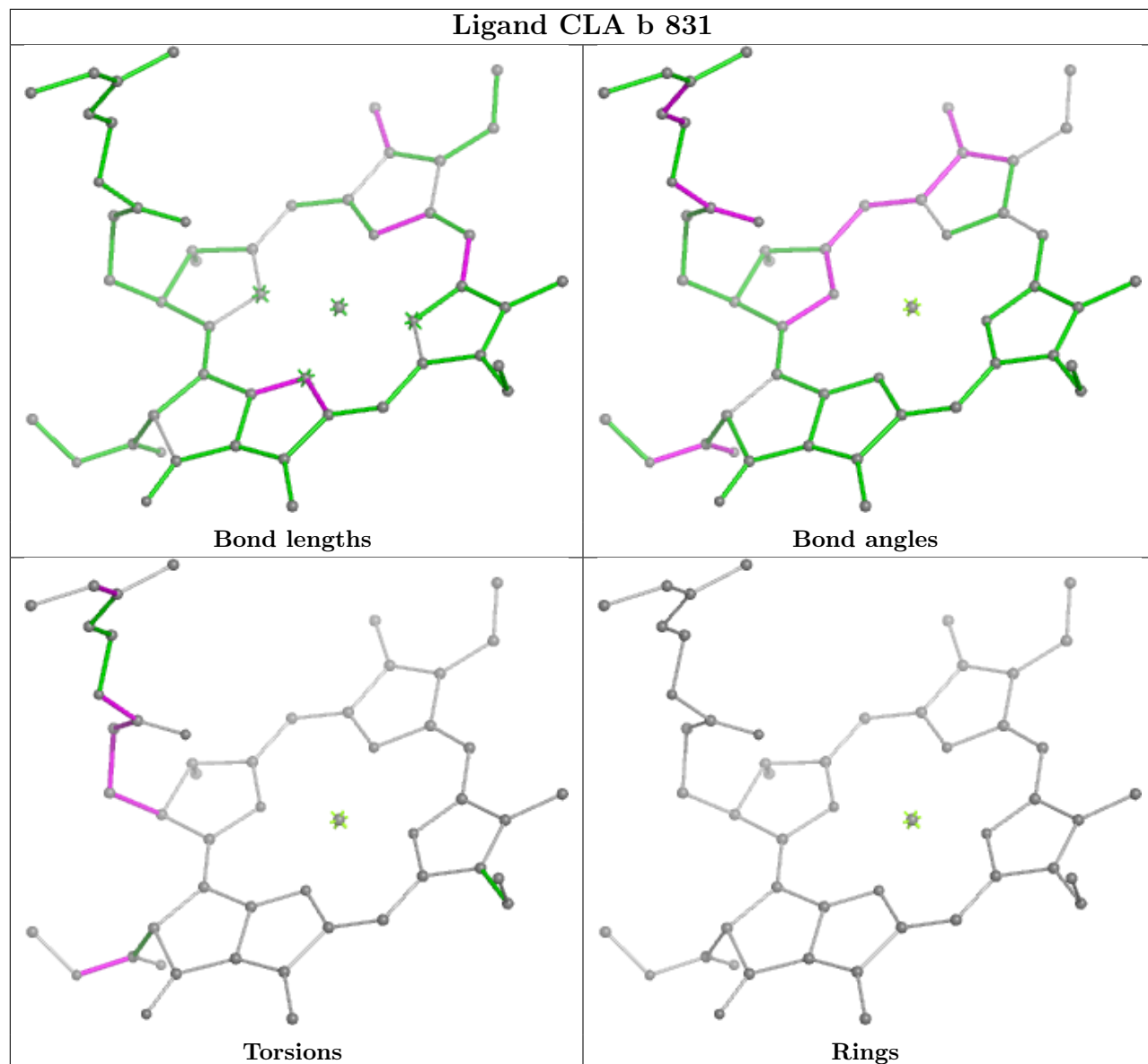
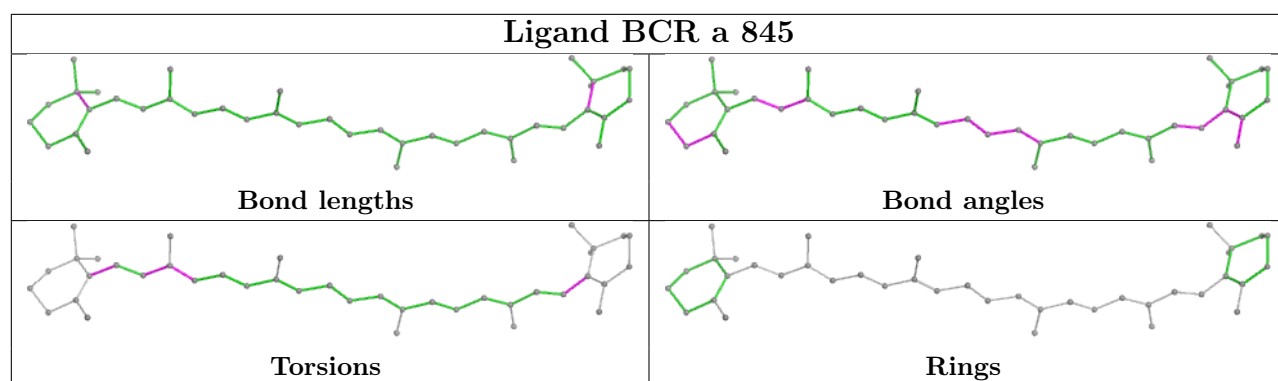


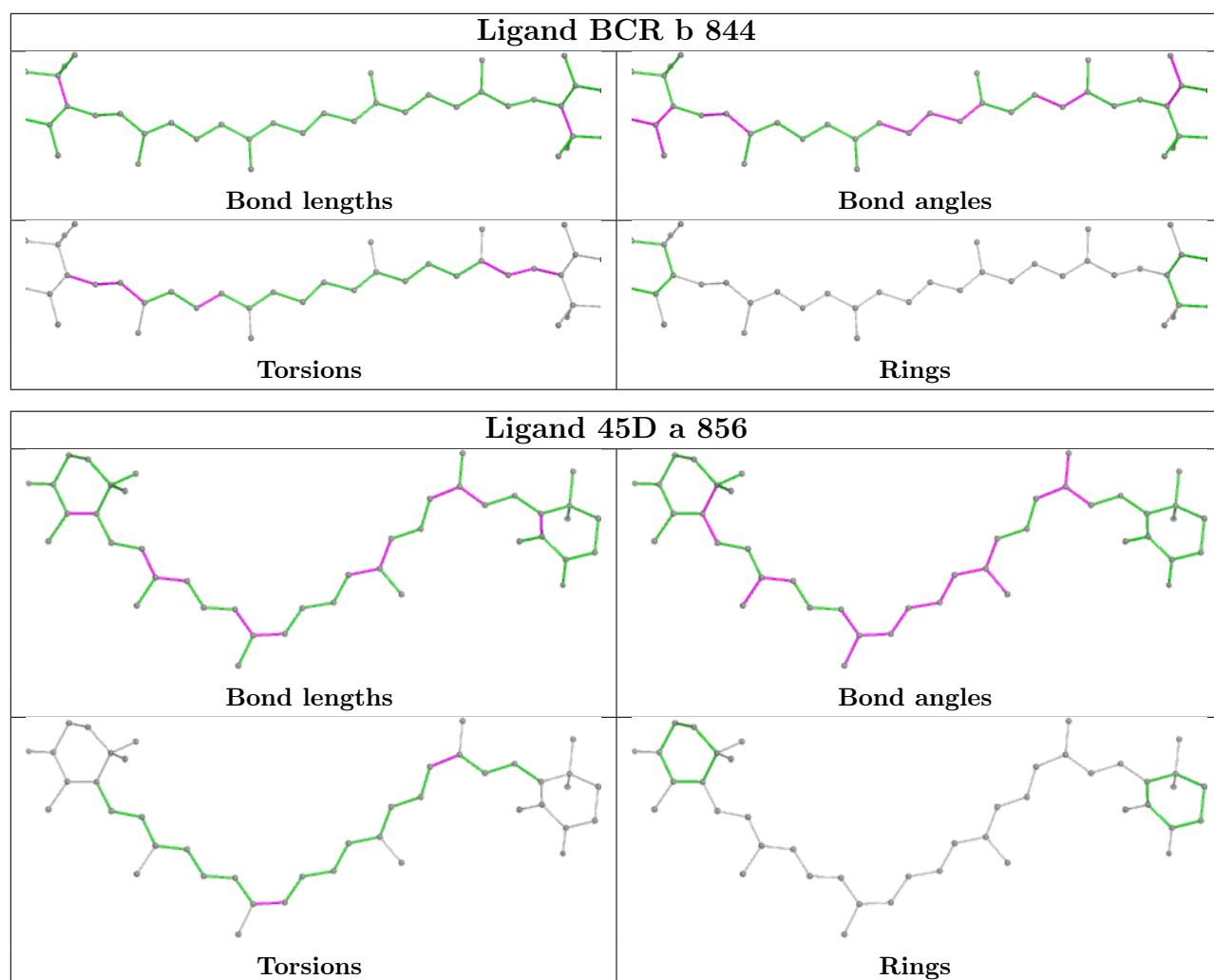
## Ligand CLA b 833

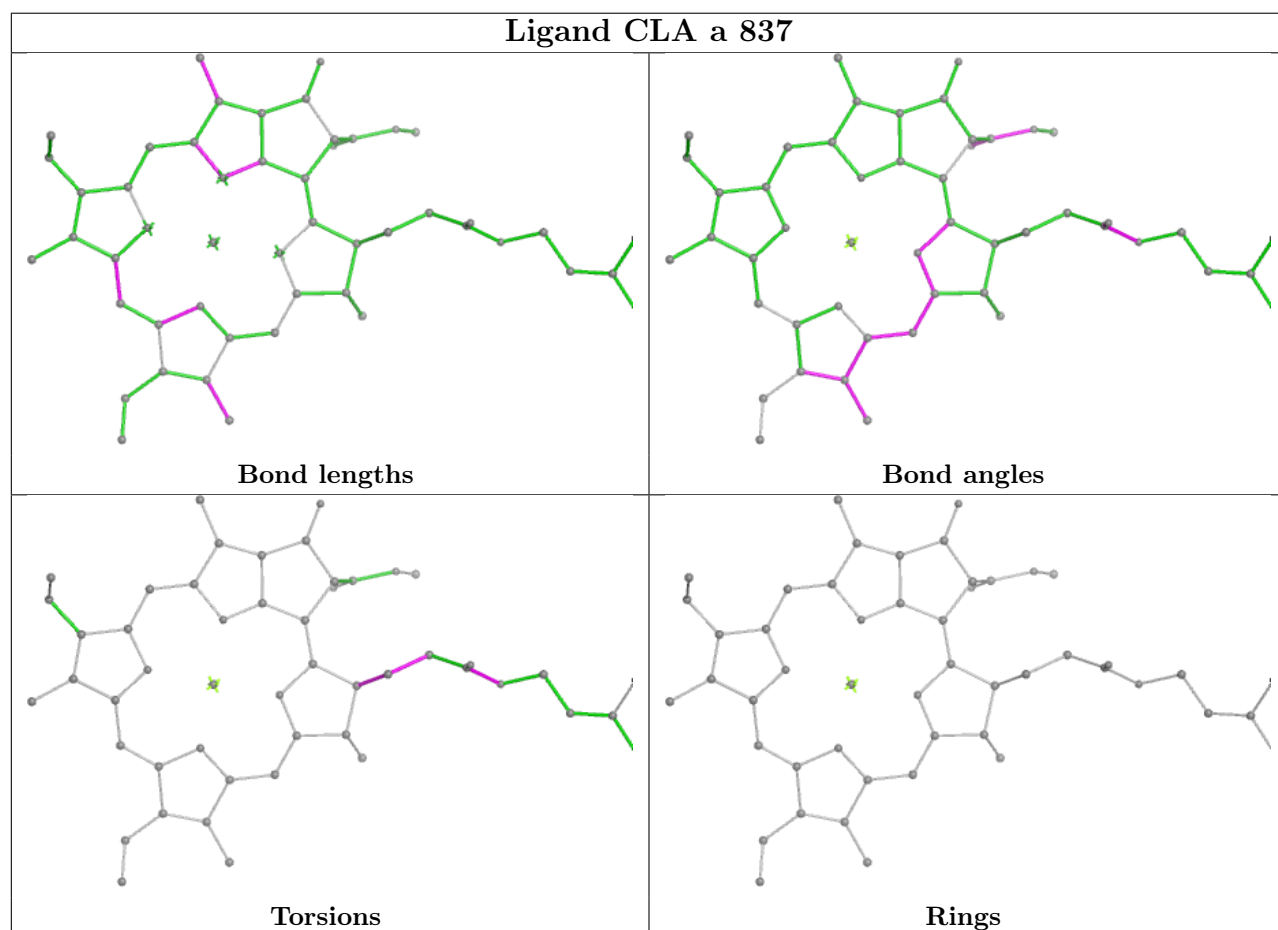
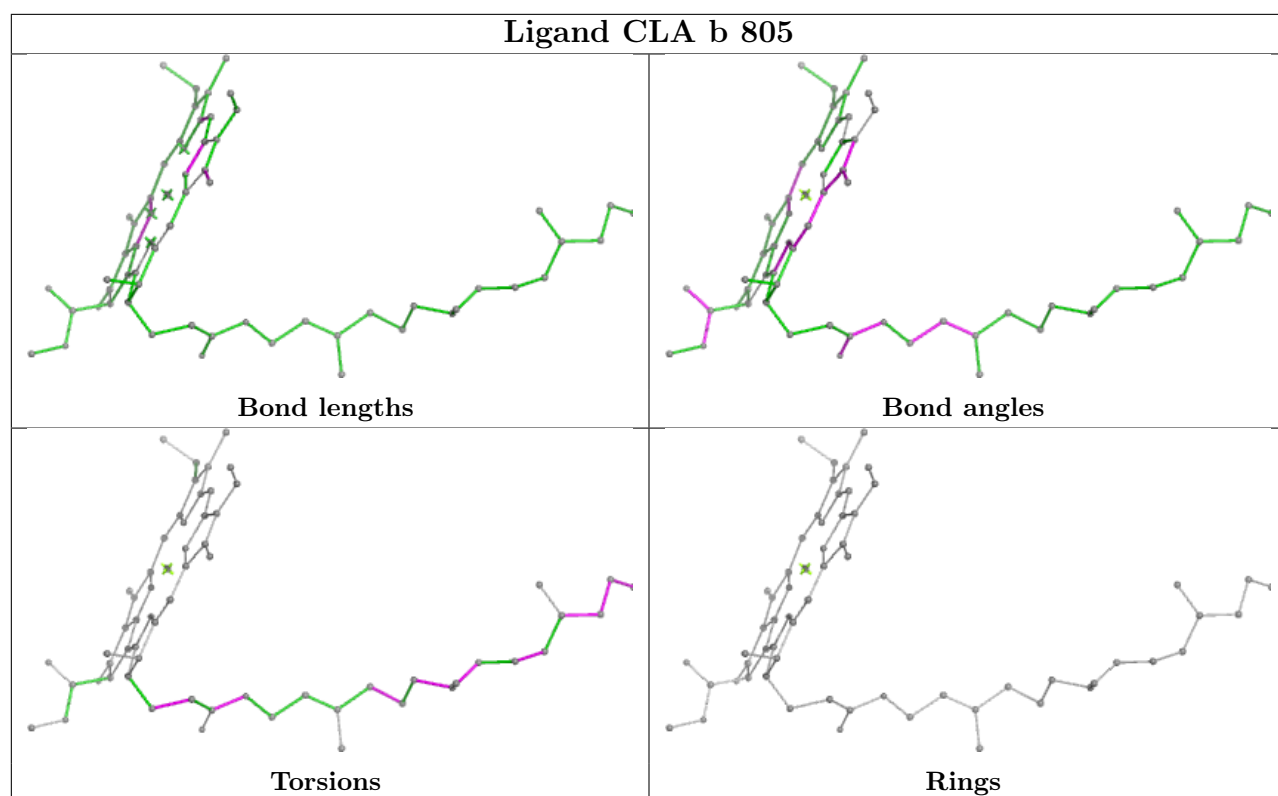


## Ligand BCR a 844

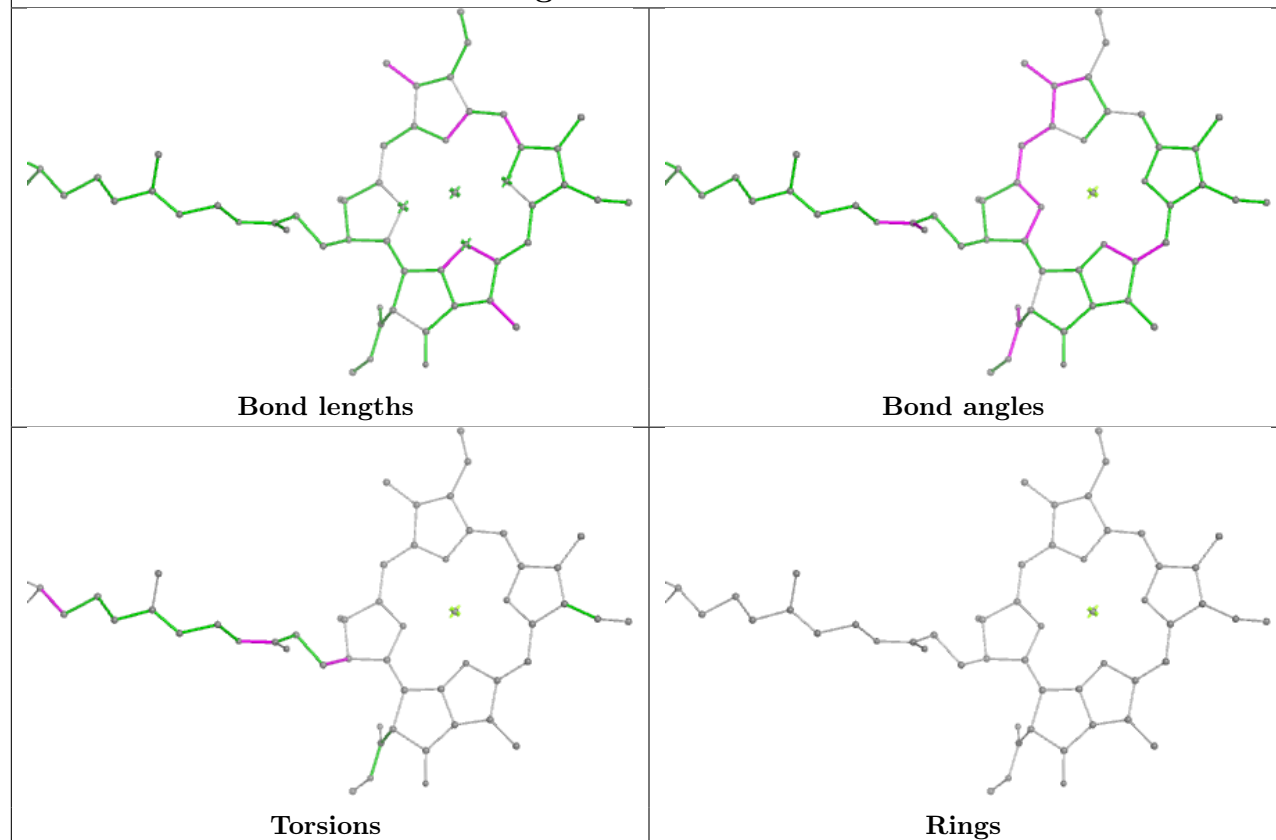




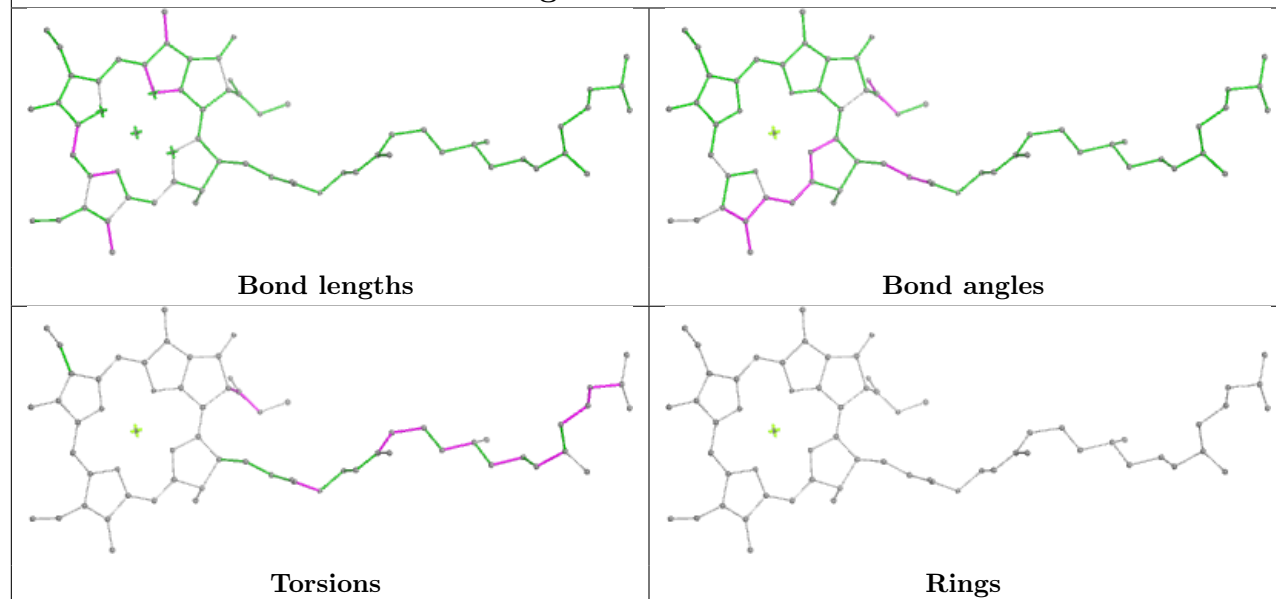




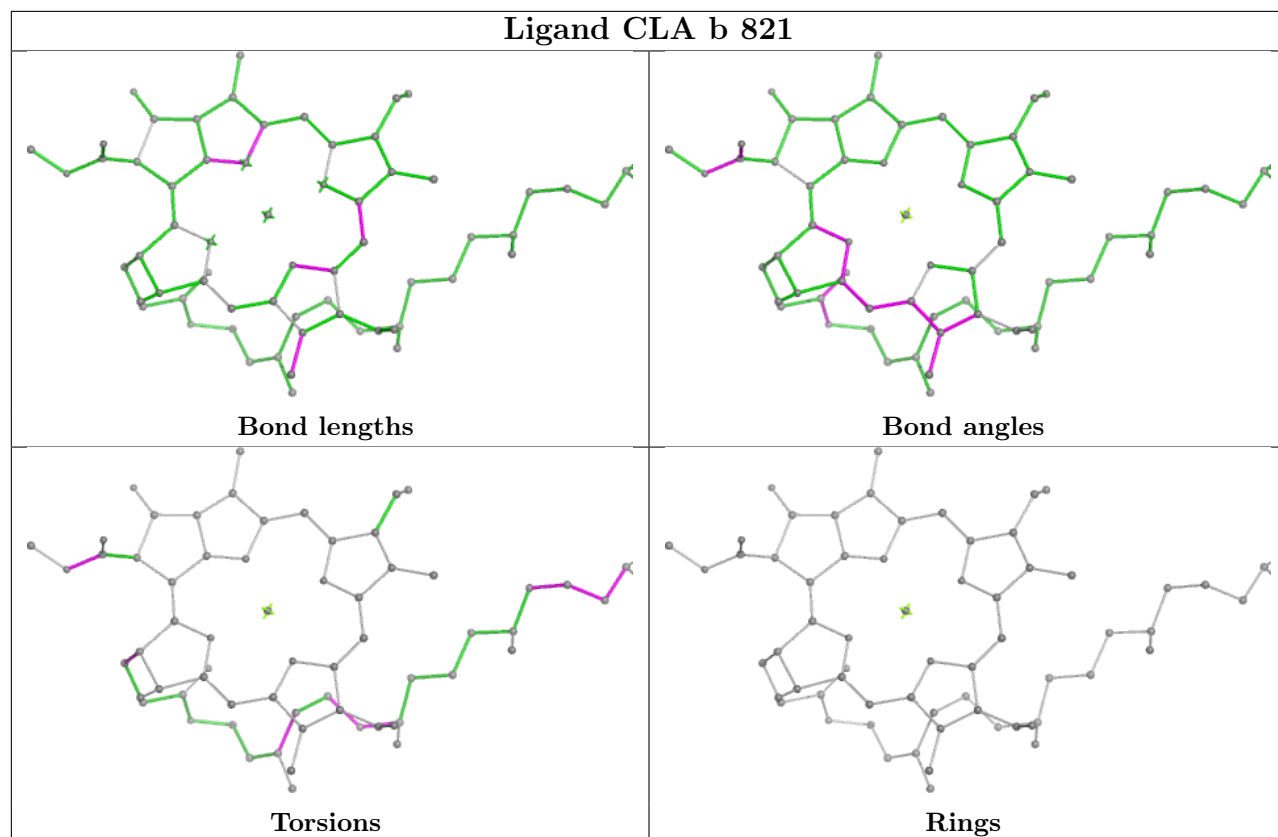
## Ligand CLA b 826



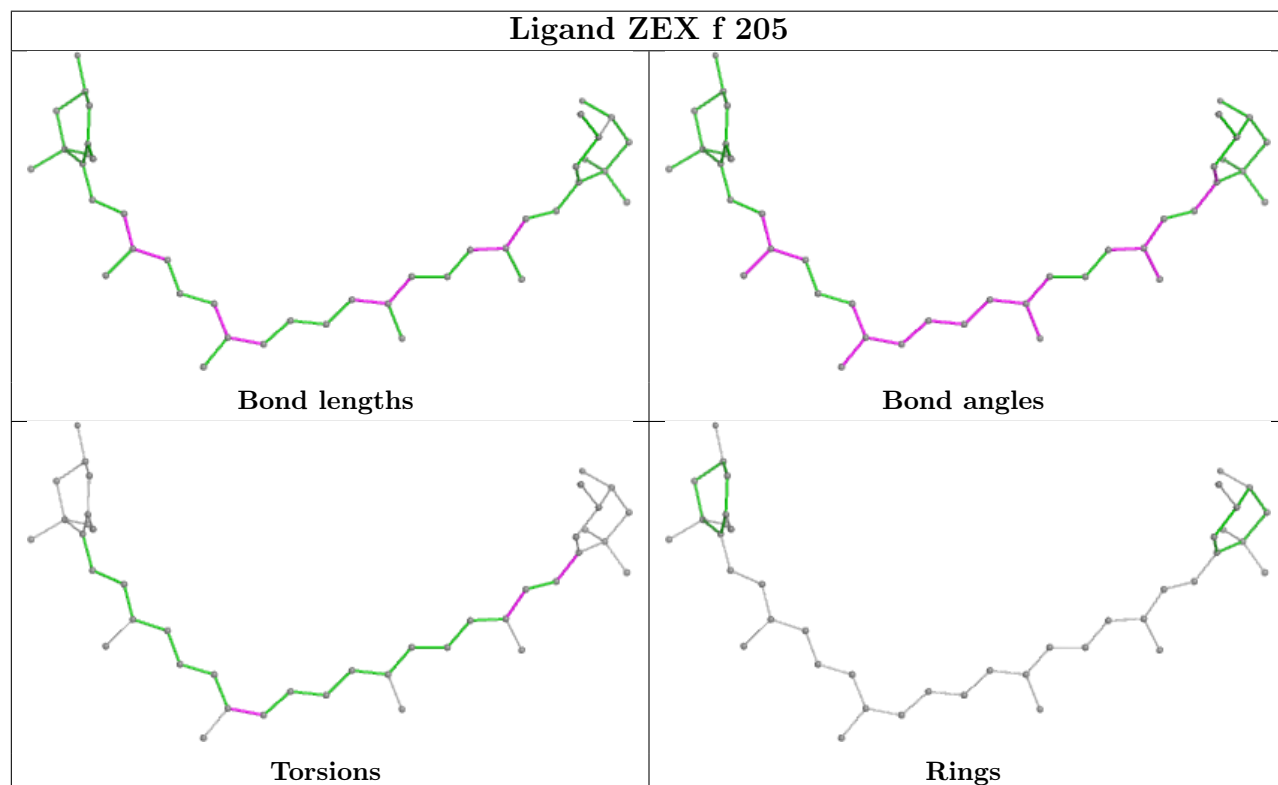
## Ligand CLA f 201



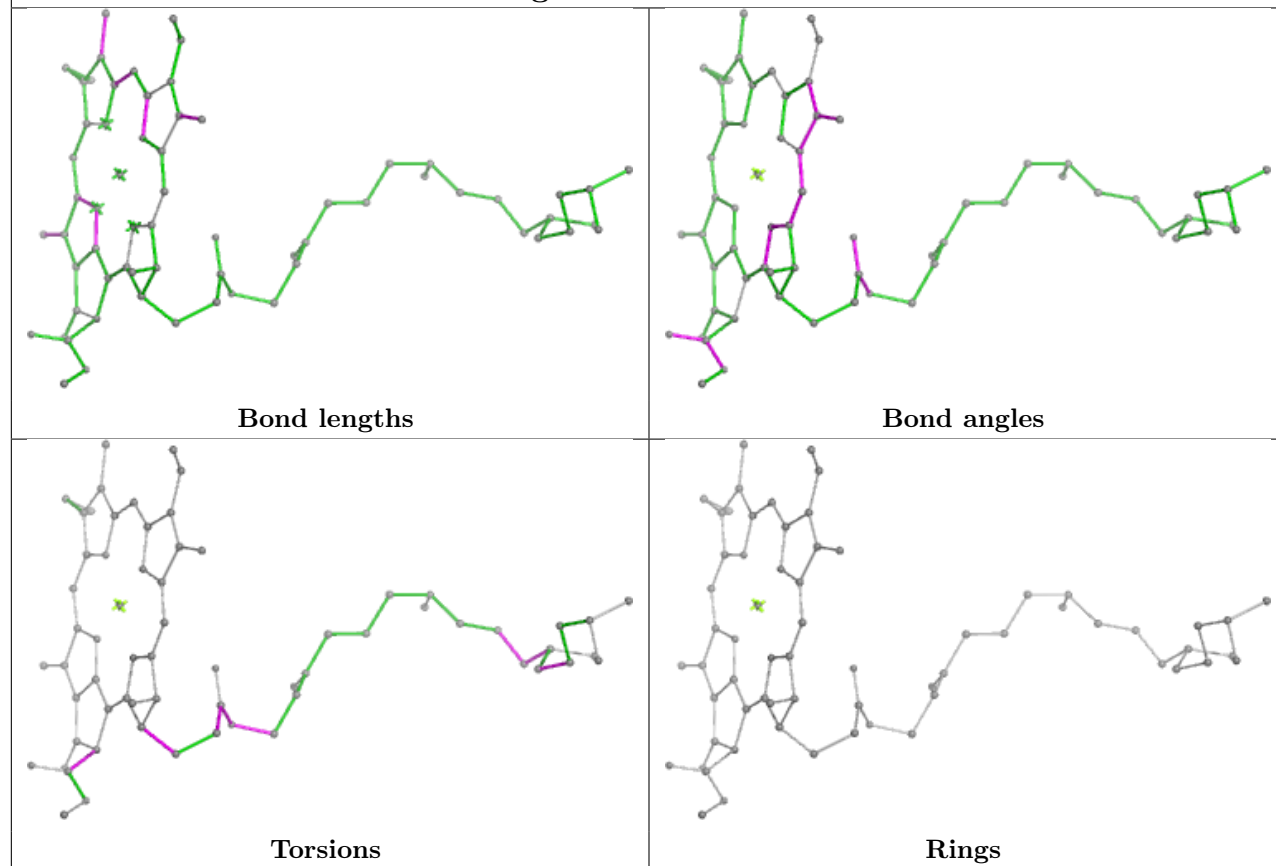
## Ligand CLA b 821



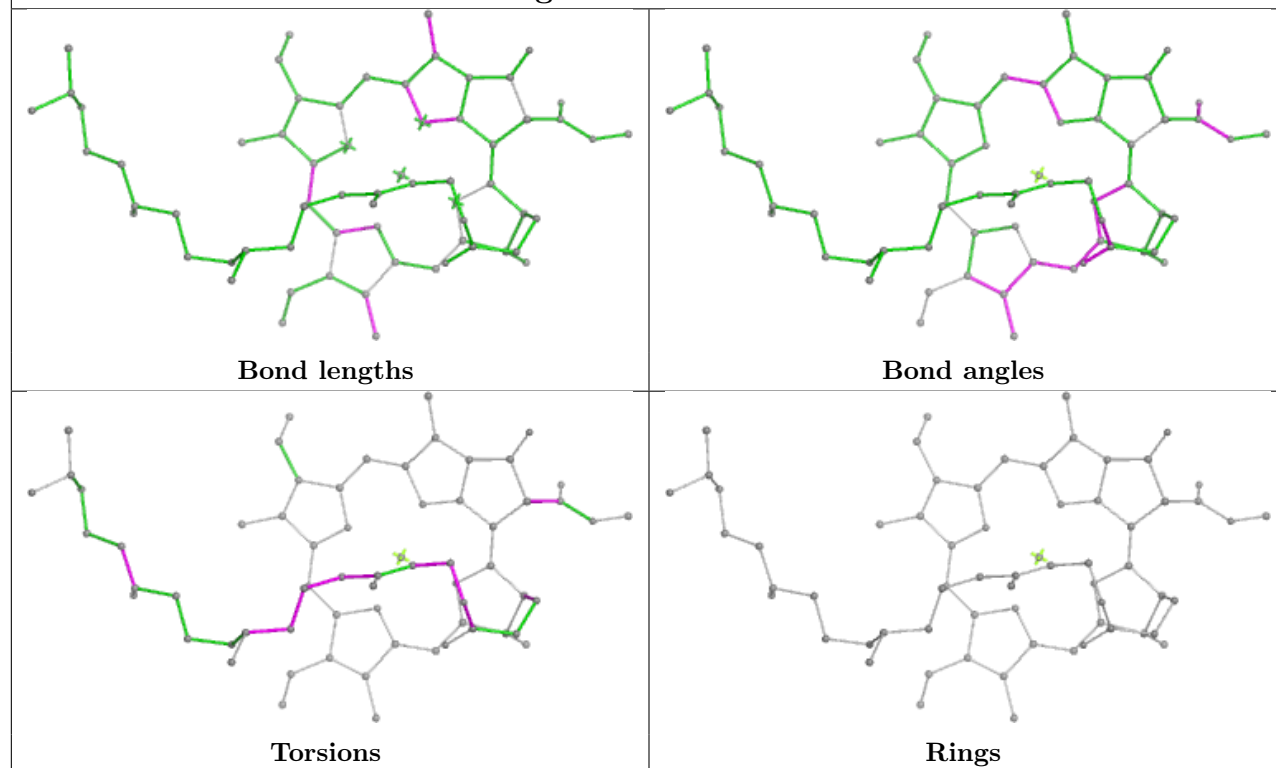
## Ligand ZEX f 205

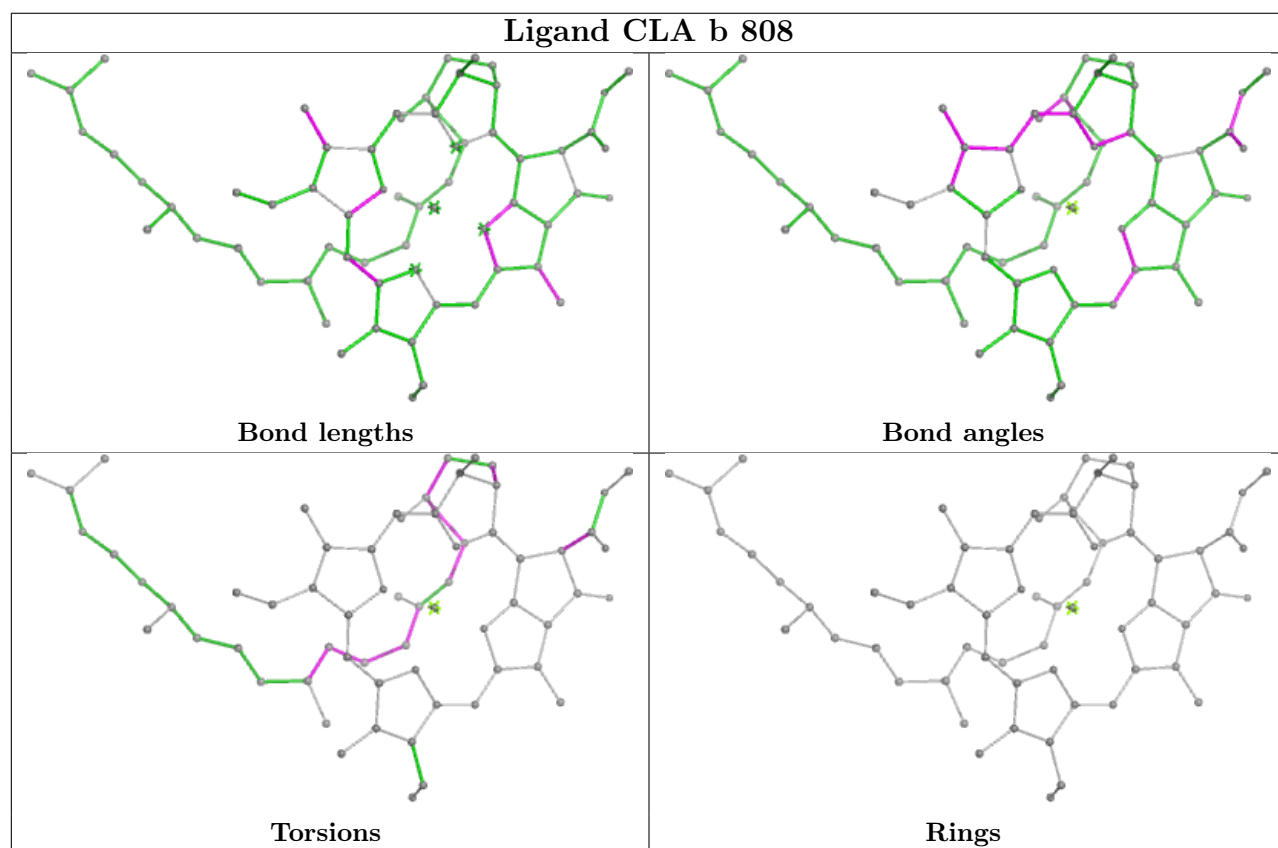
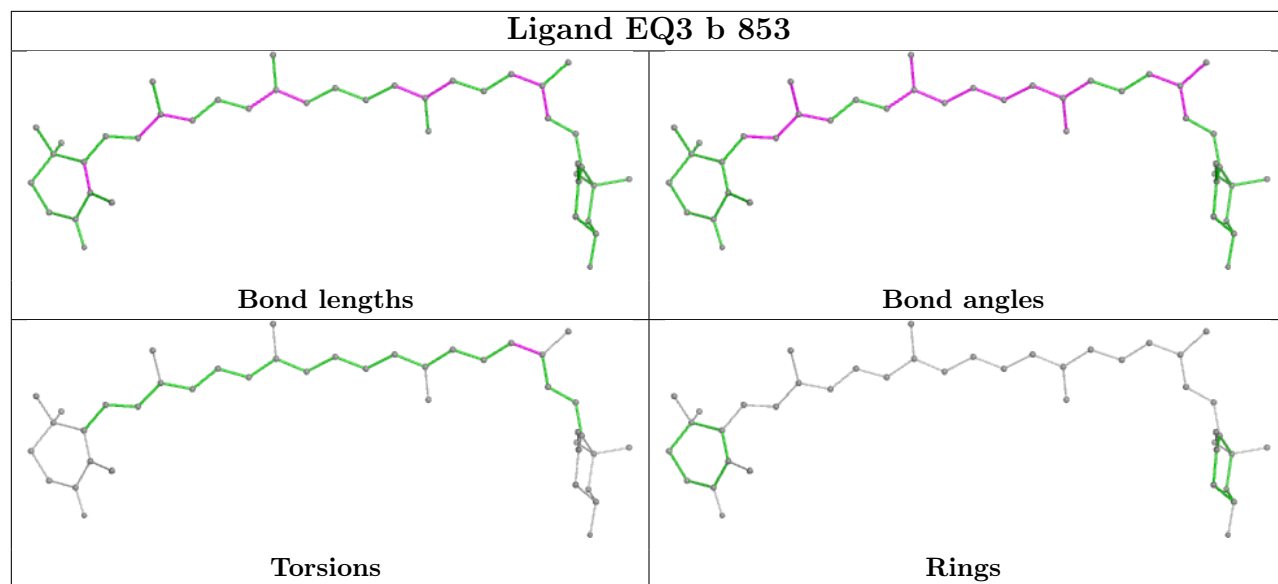


## Ligand CLA l 1502

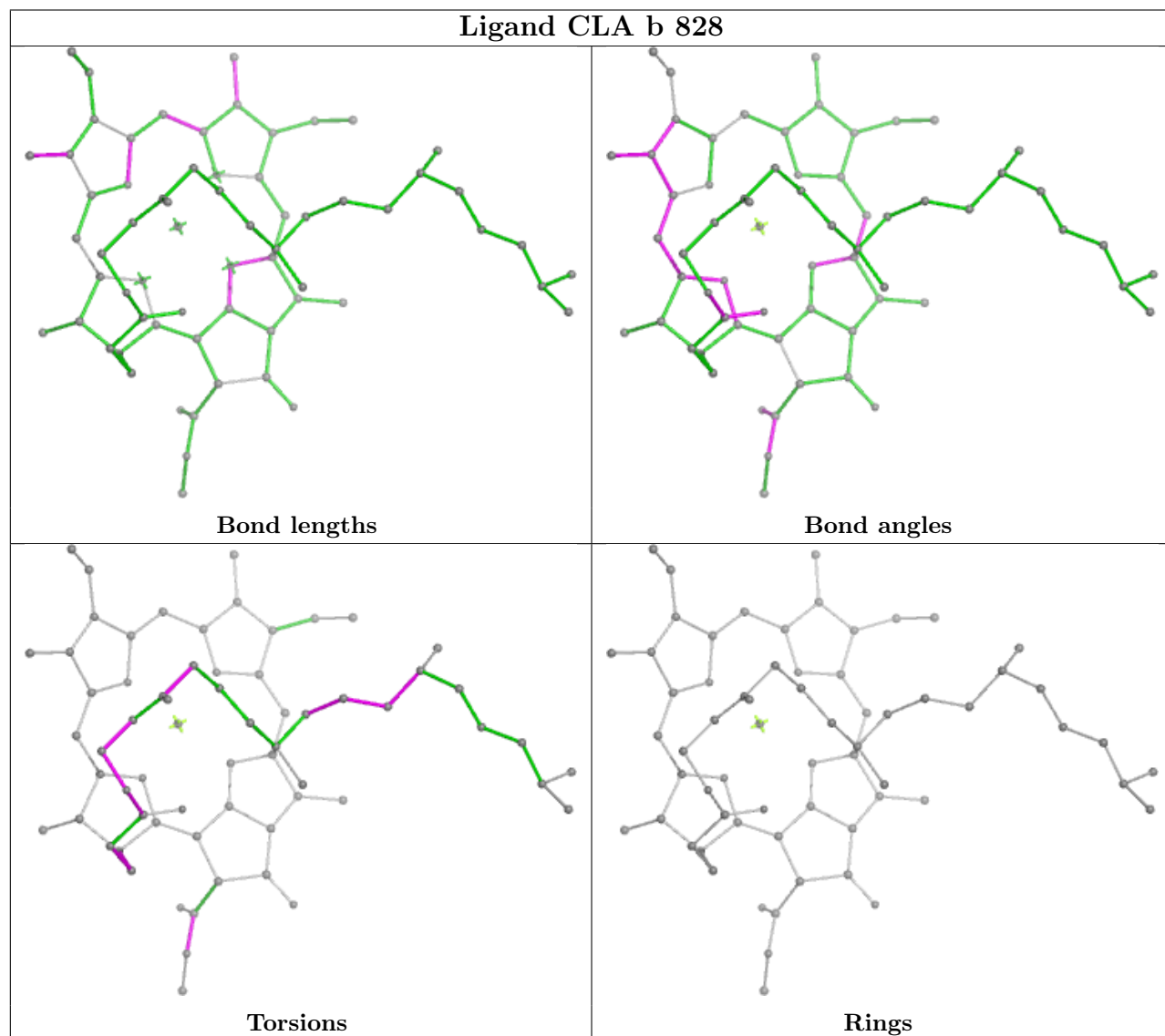
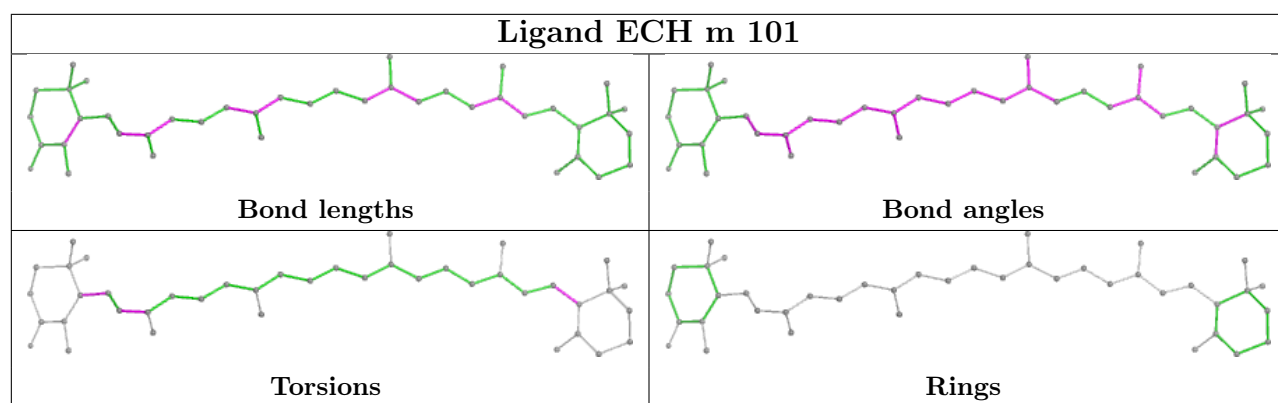


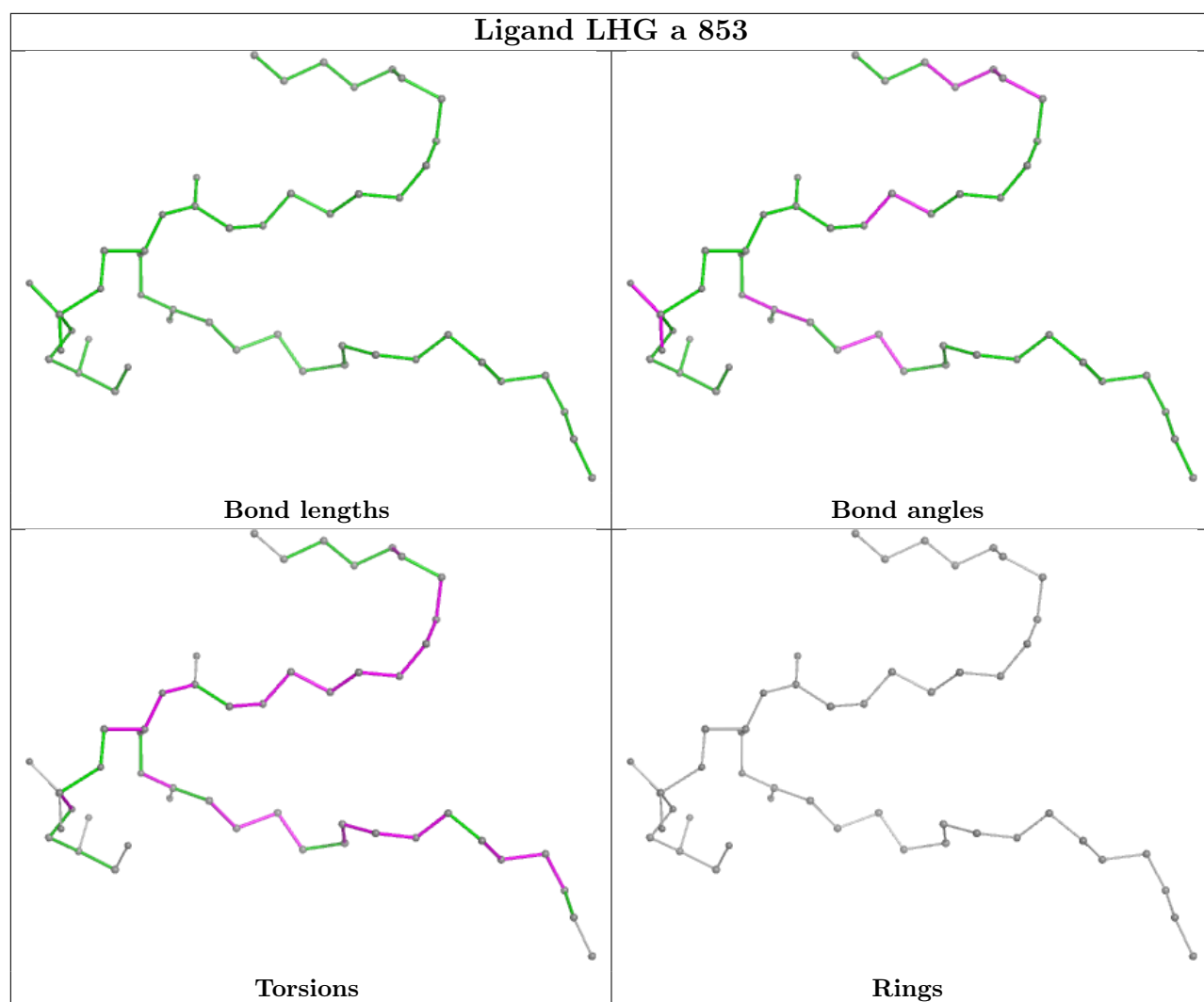
## Ligand CLA b 838



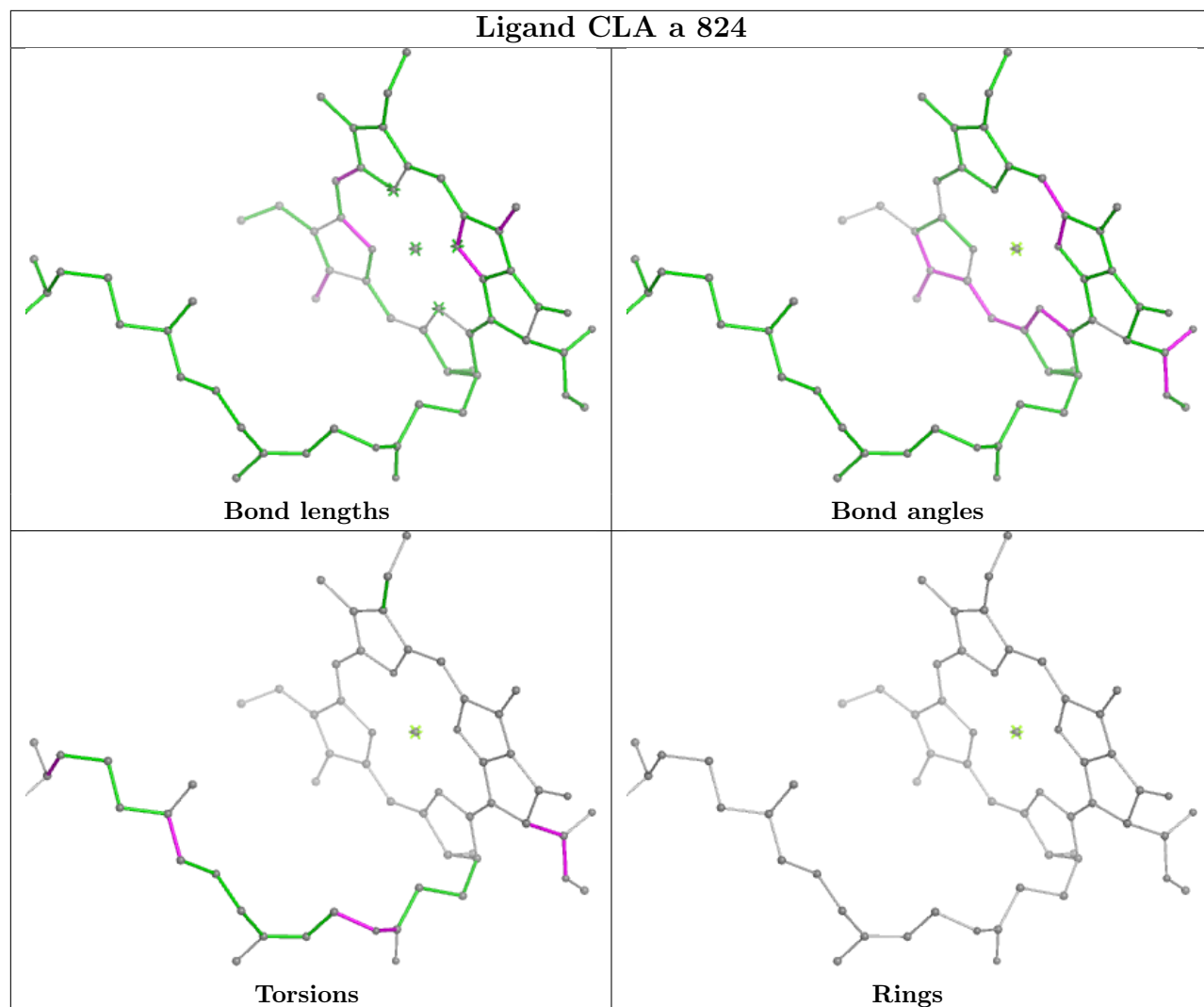




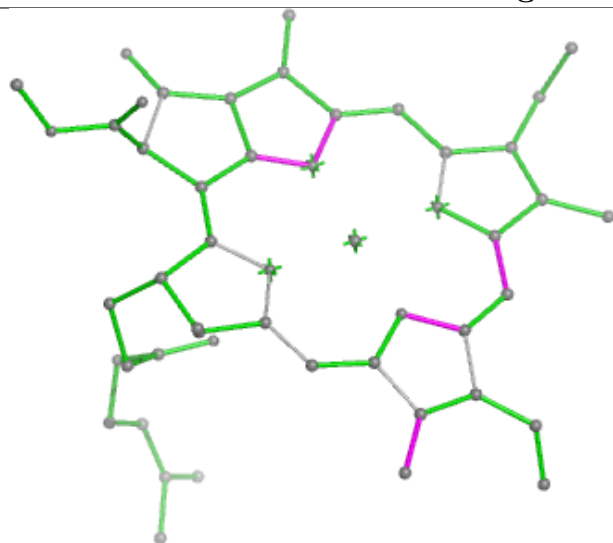




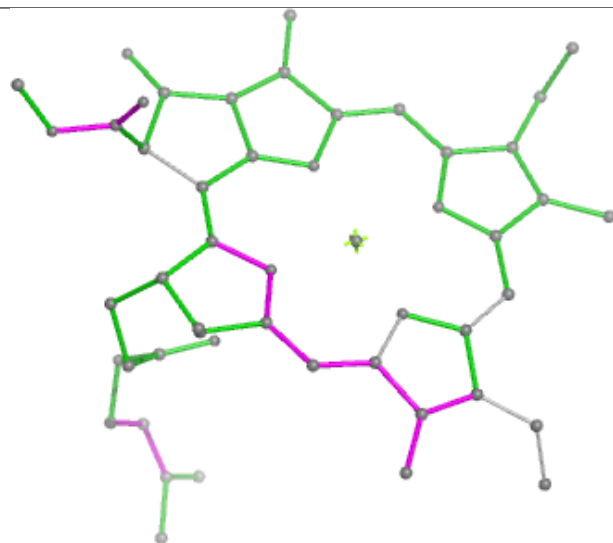
## Ligand CLA a 824



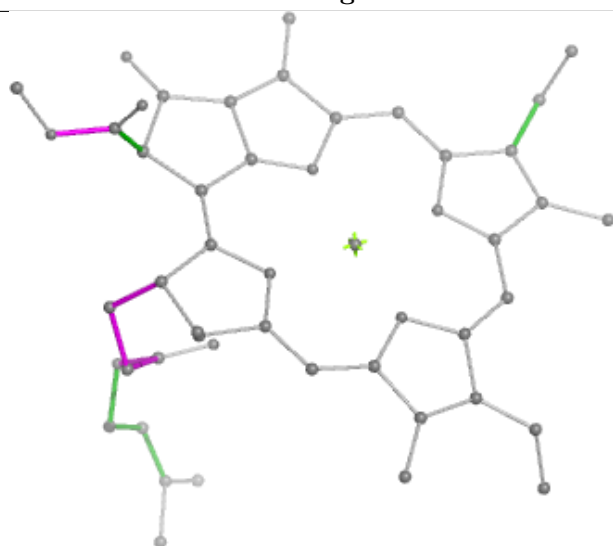
## Ligand CLA b 836



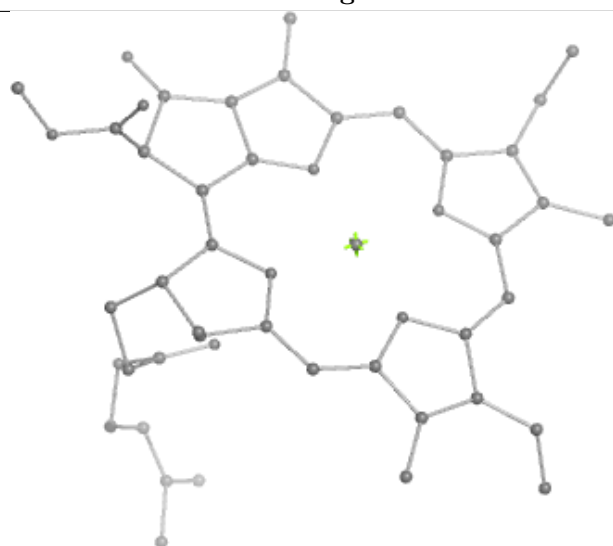
Bond lengths



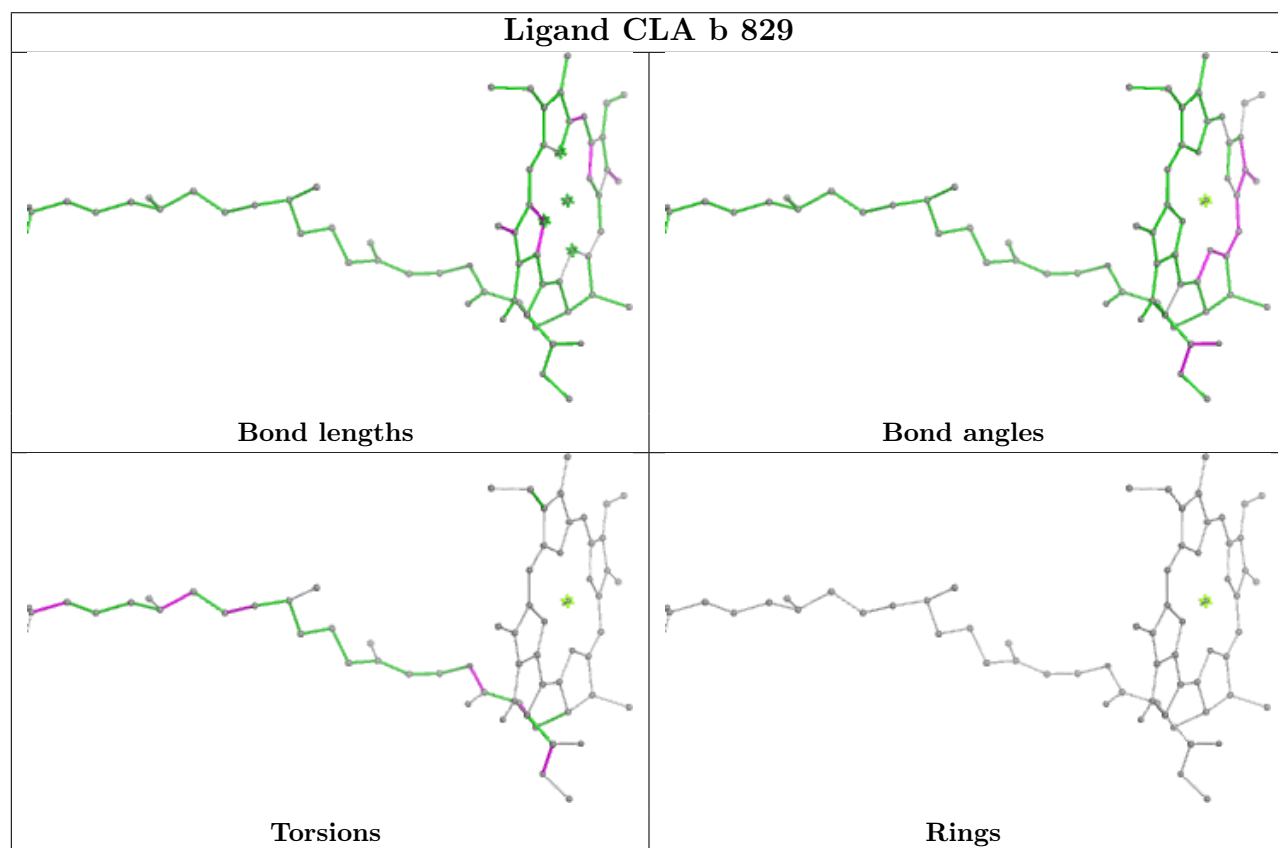
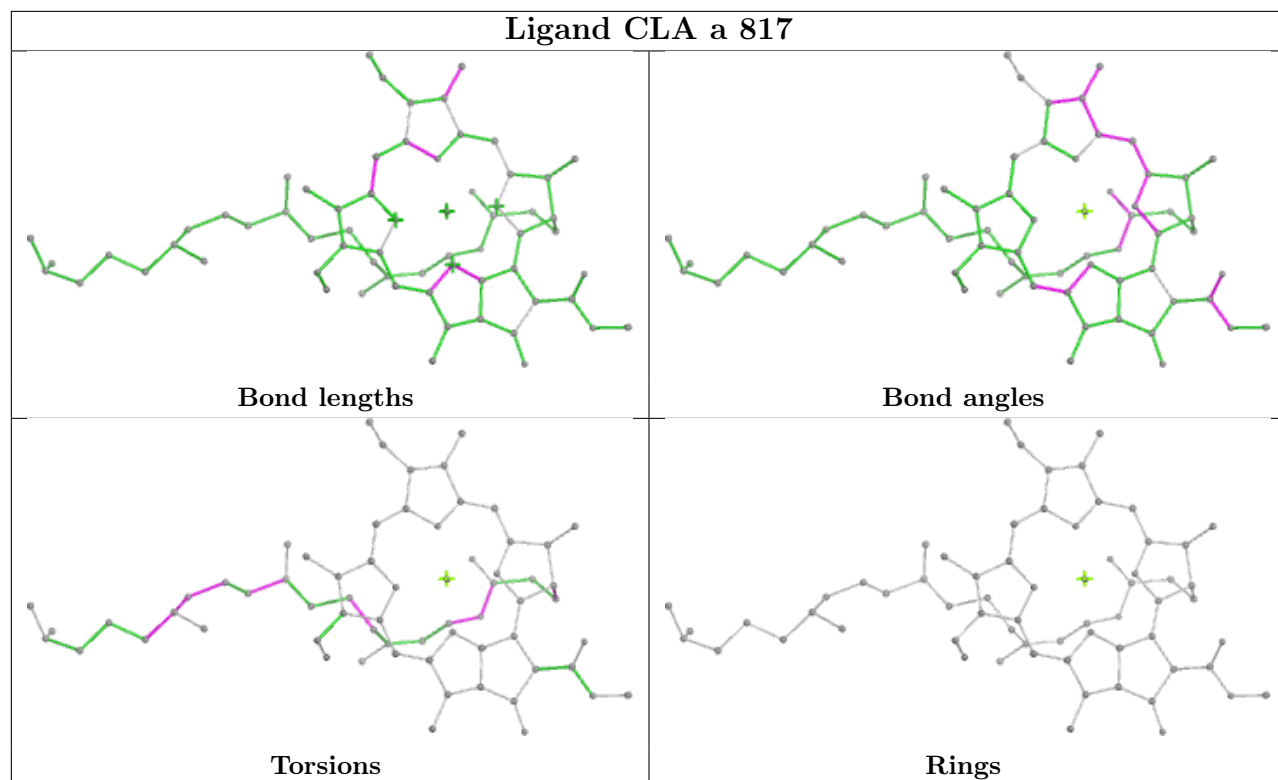
Bond angles

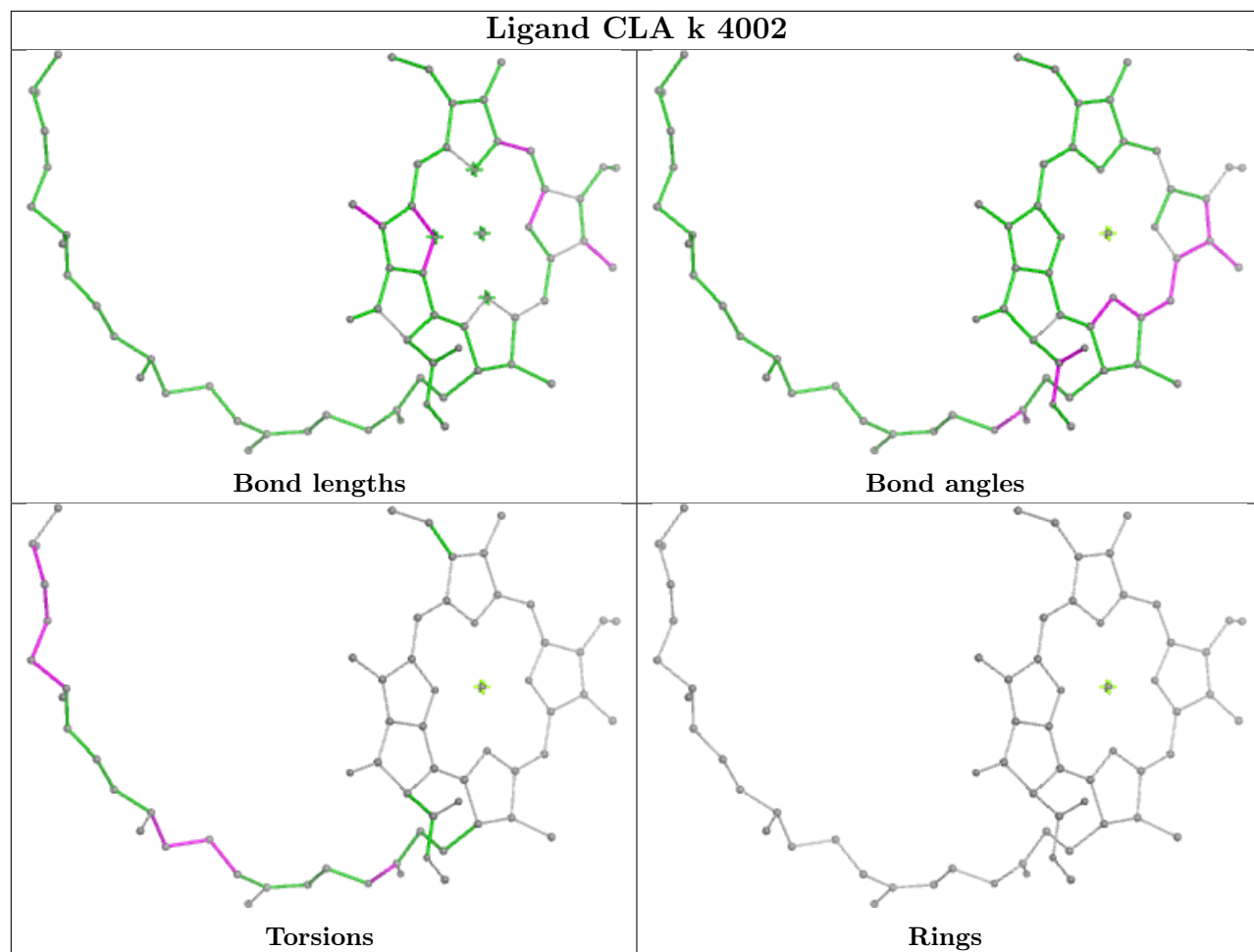


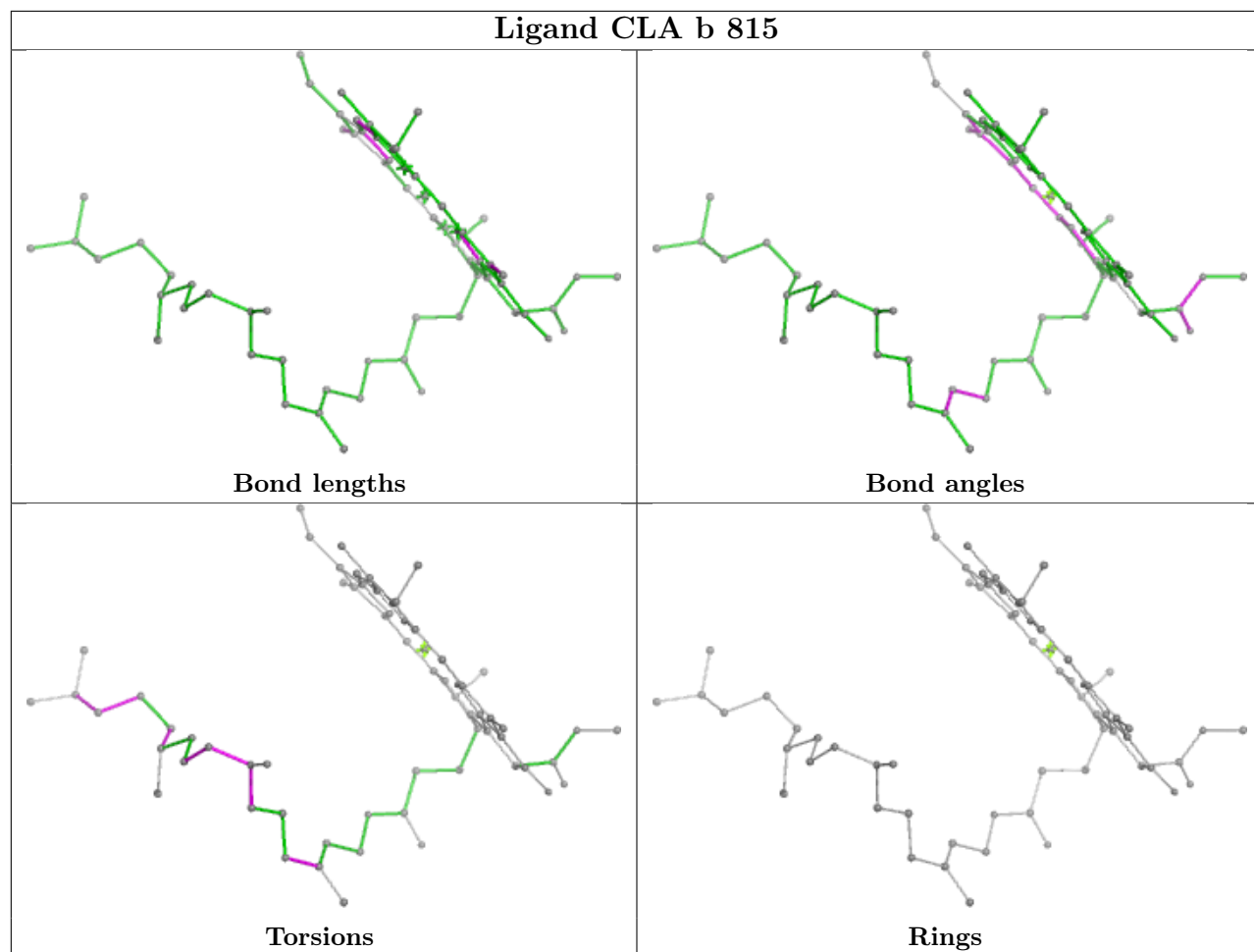
Torsions

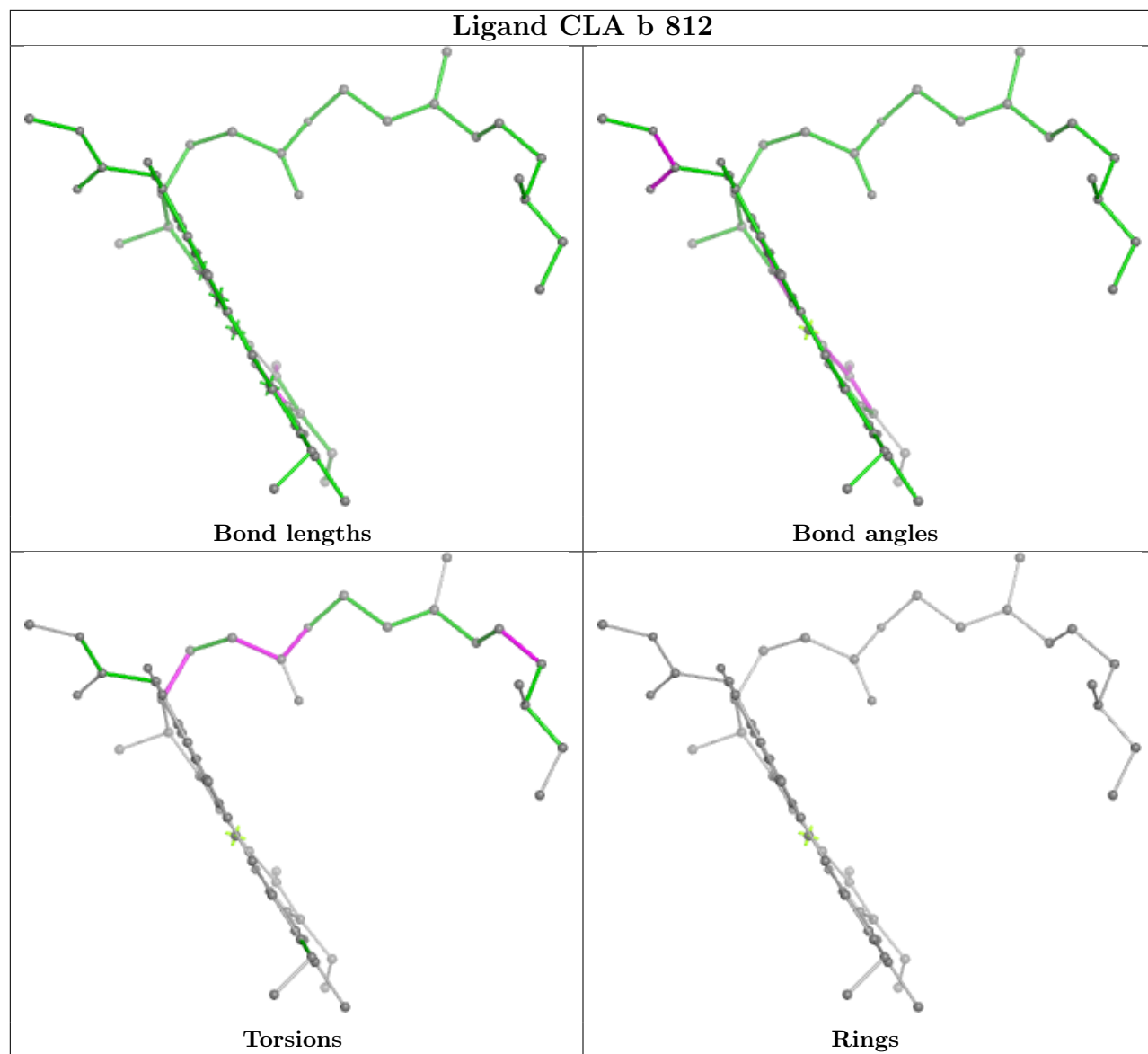


Rings

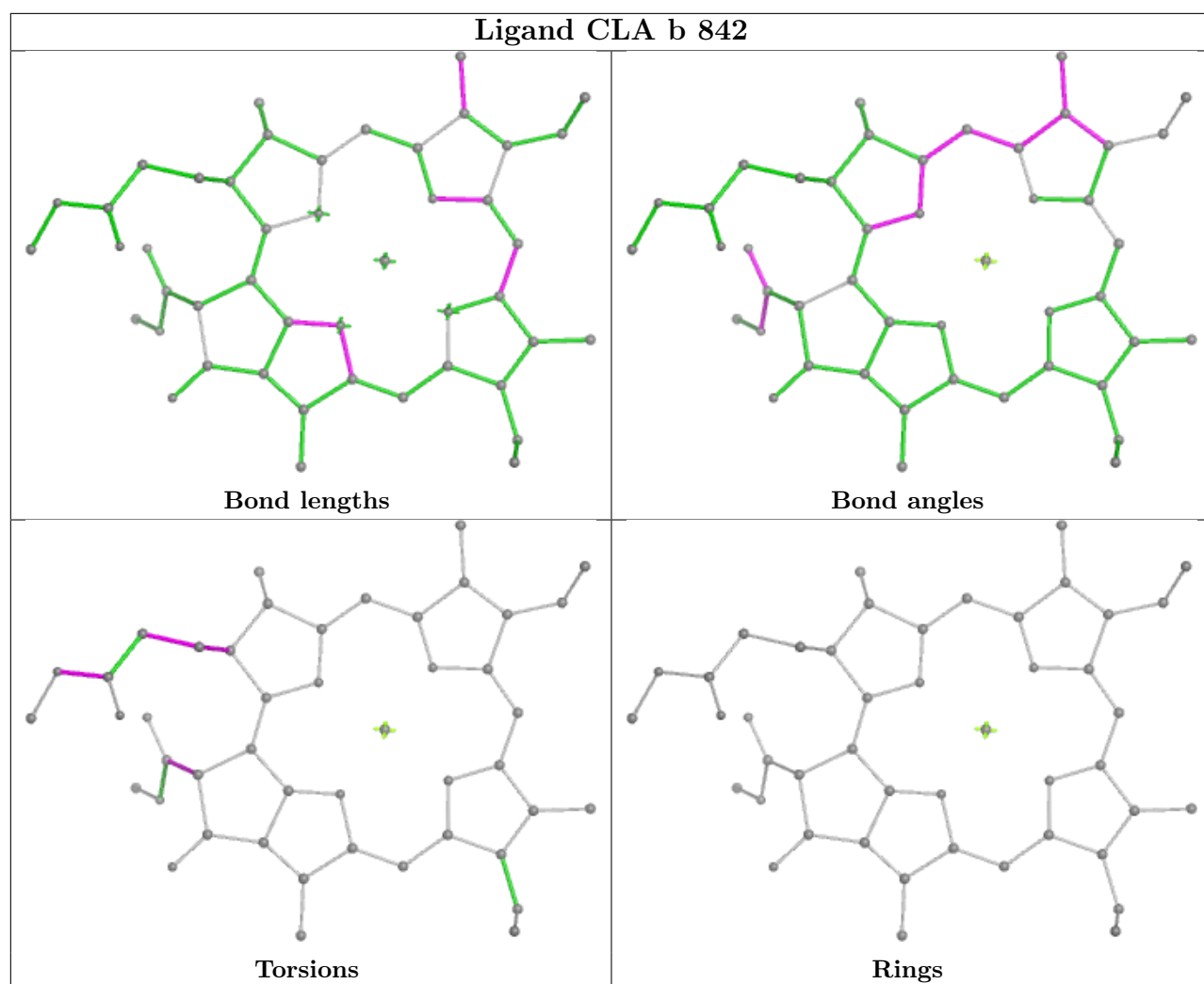


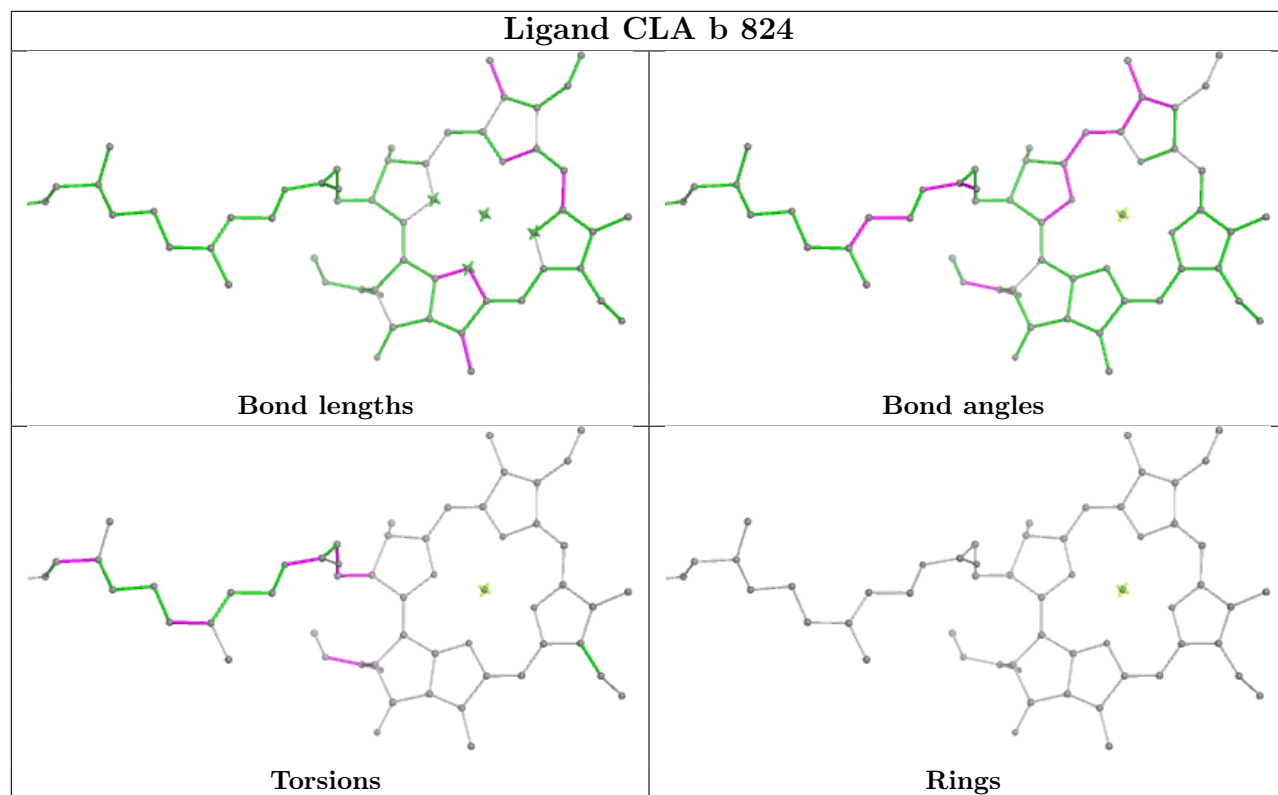




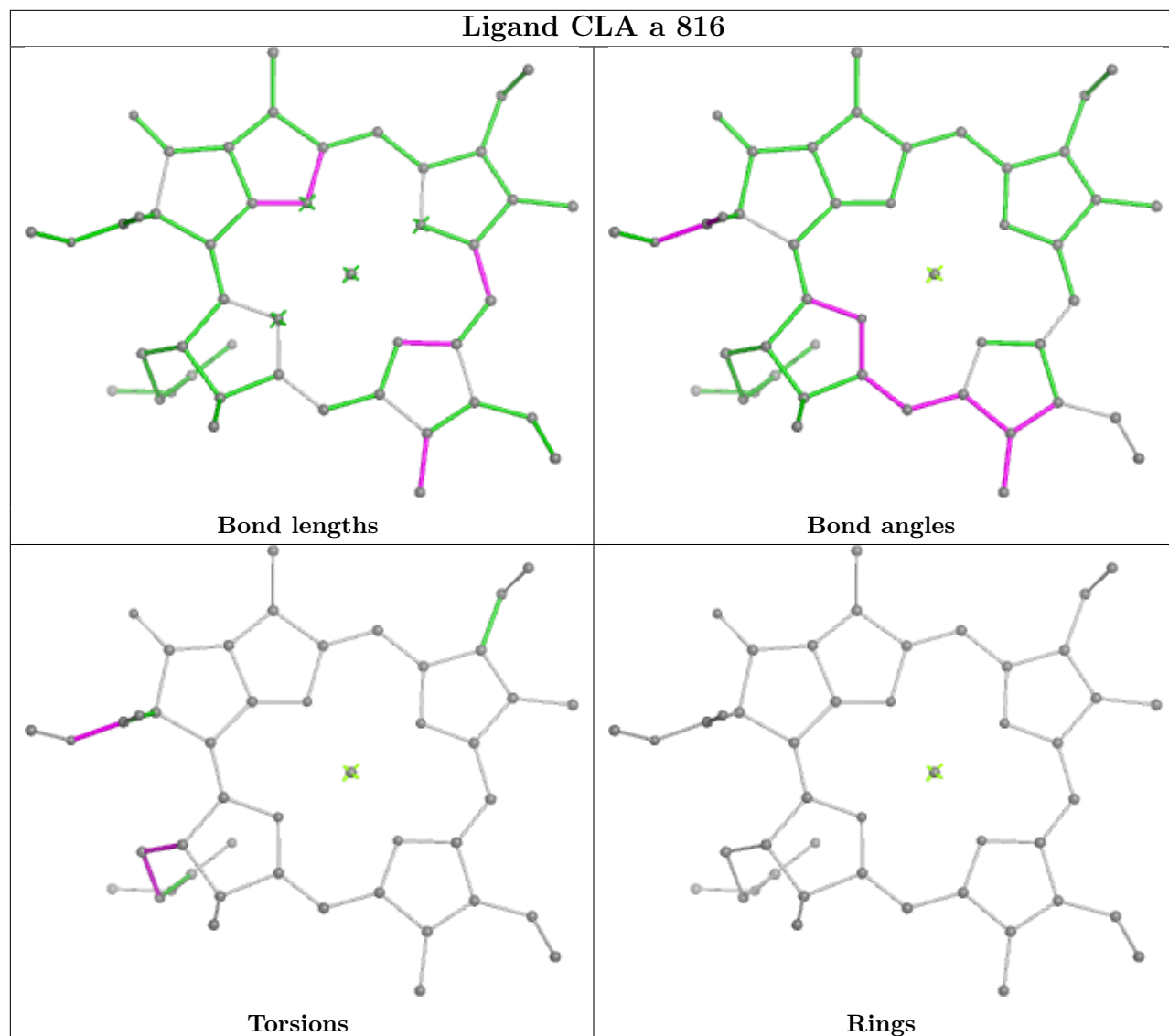


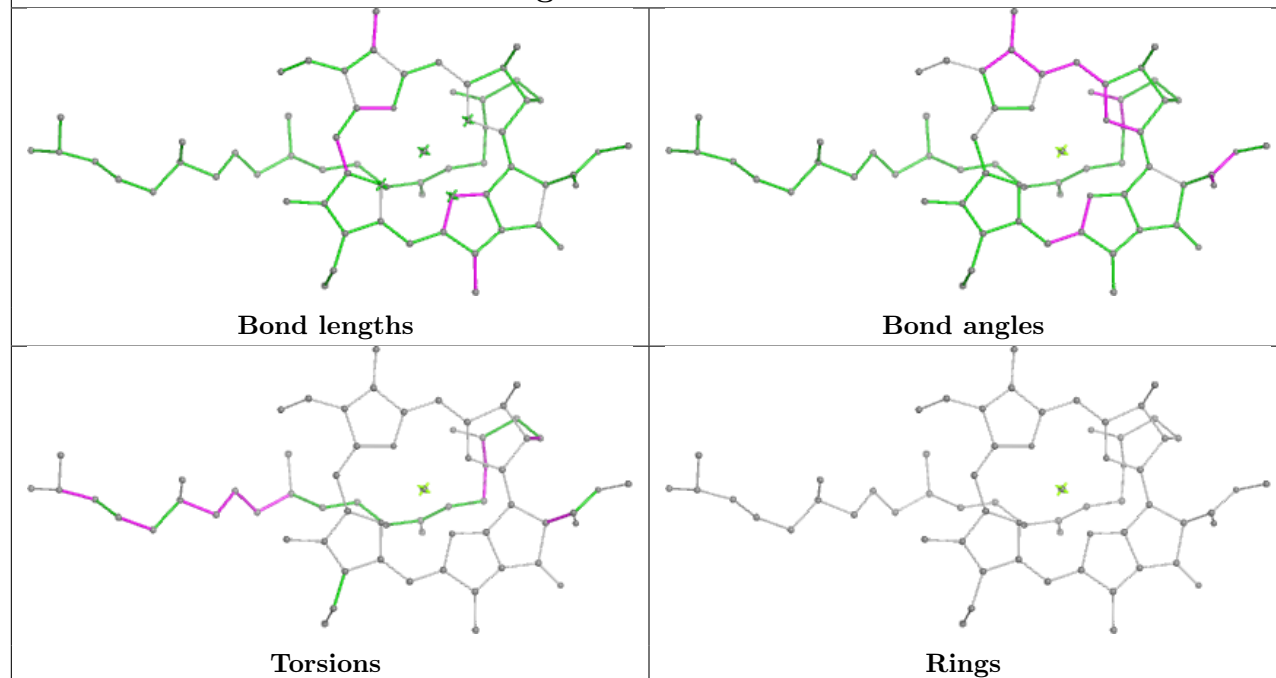
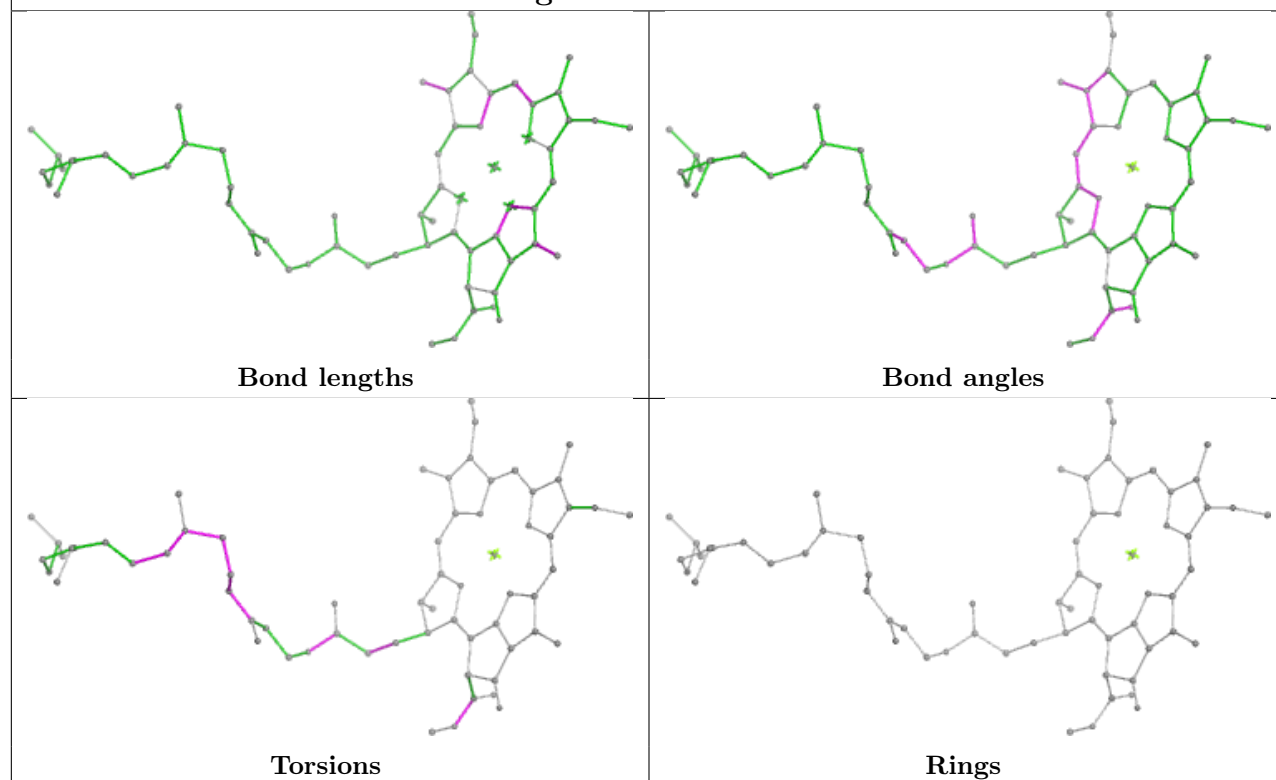




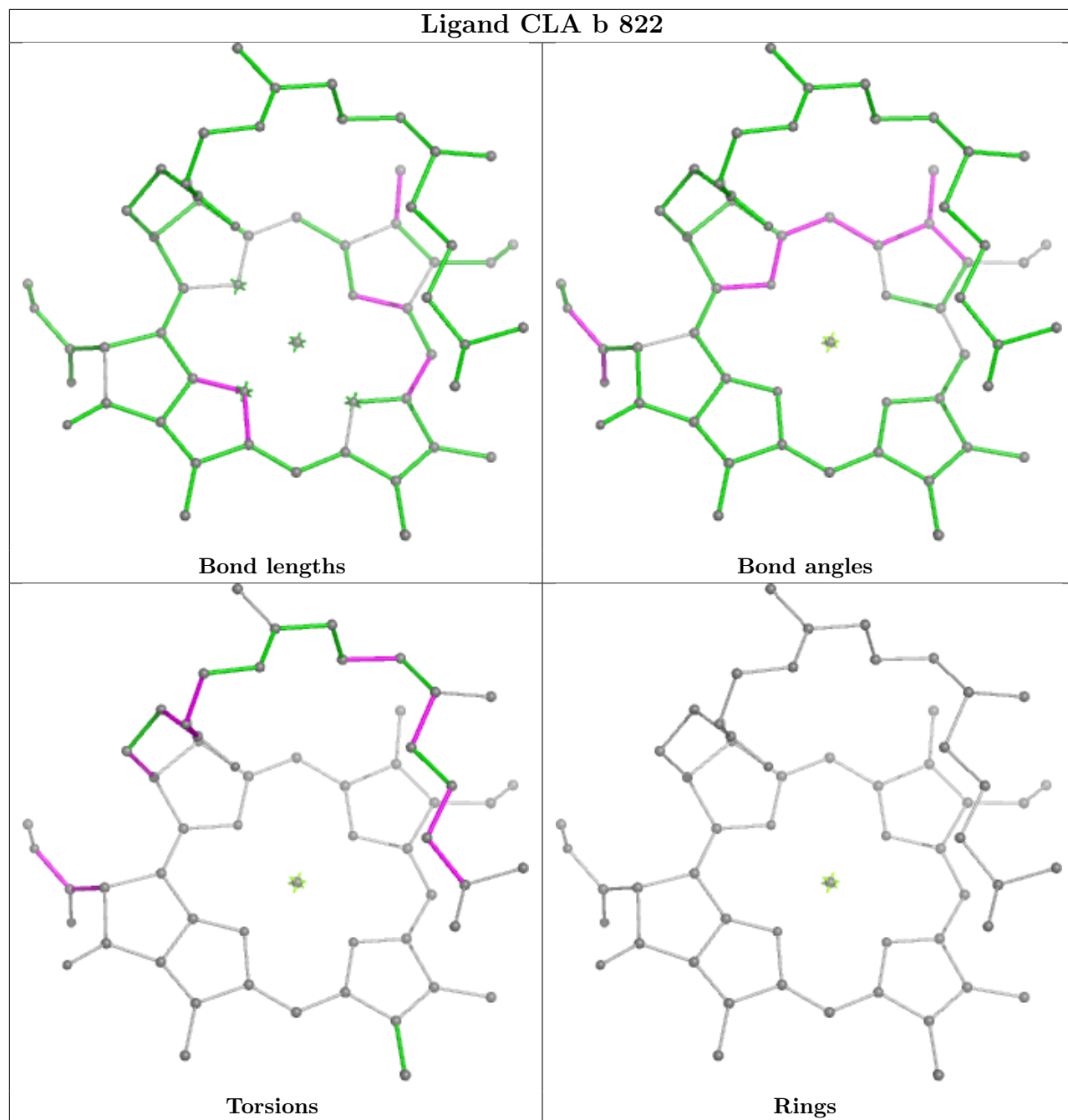


## Ligand CLA a 816

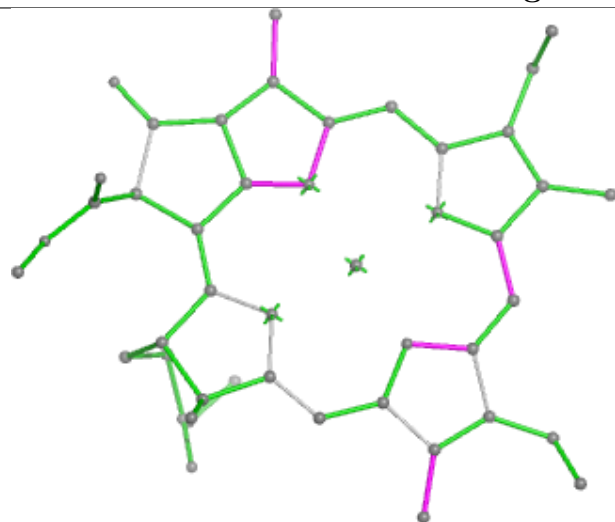


**Ligand CLA a 838****Ligand CLA b 810**

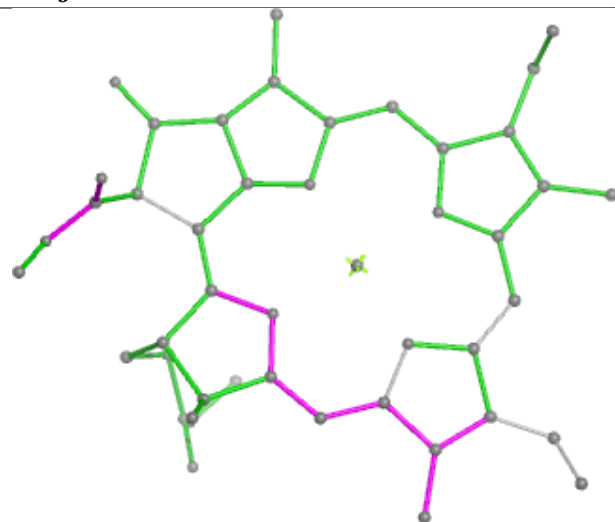
## Ligand CLA b 822



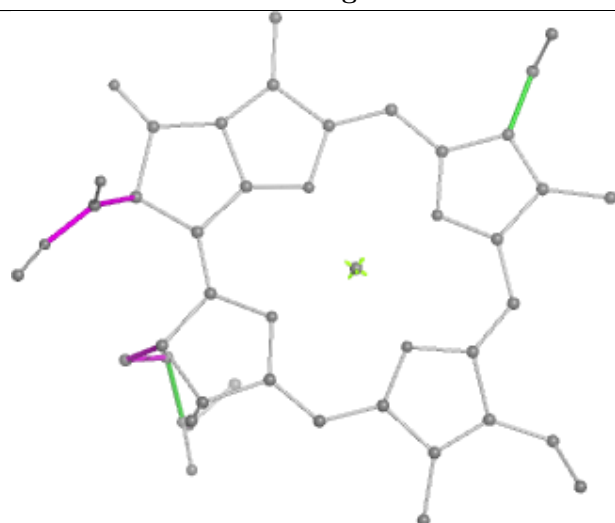
## Ligand CLA j 104



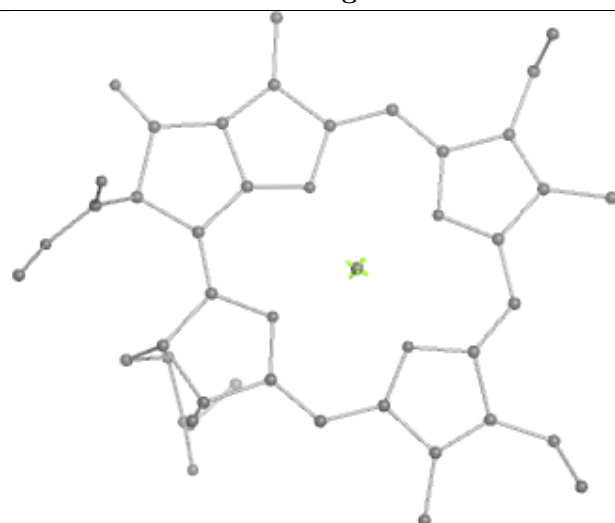
Bond lengths



Bond angles

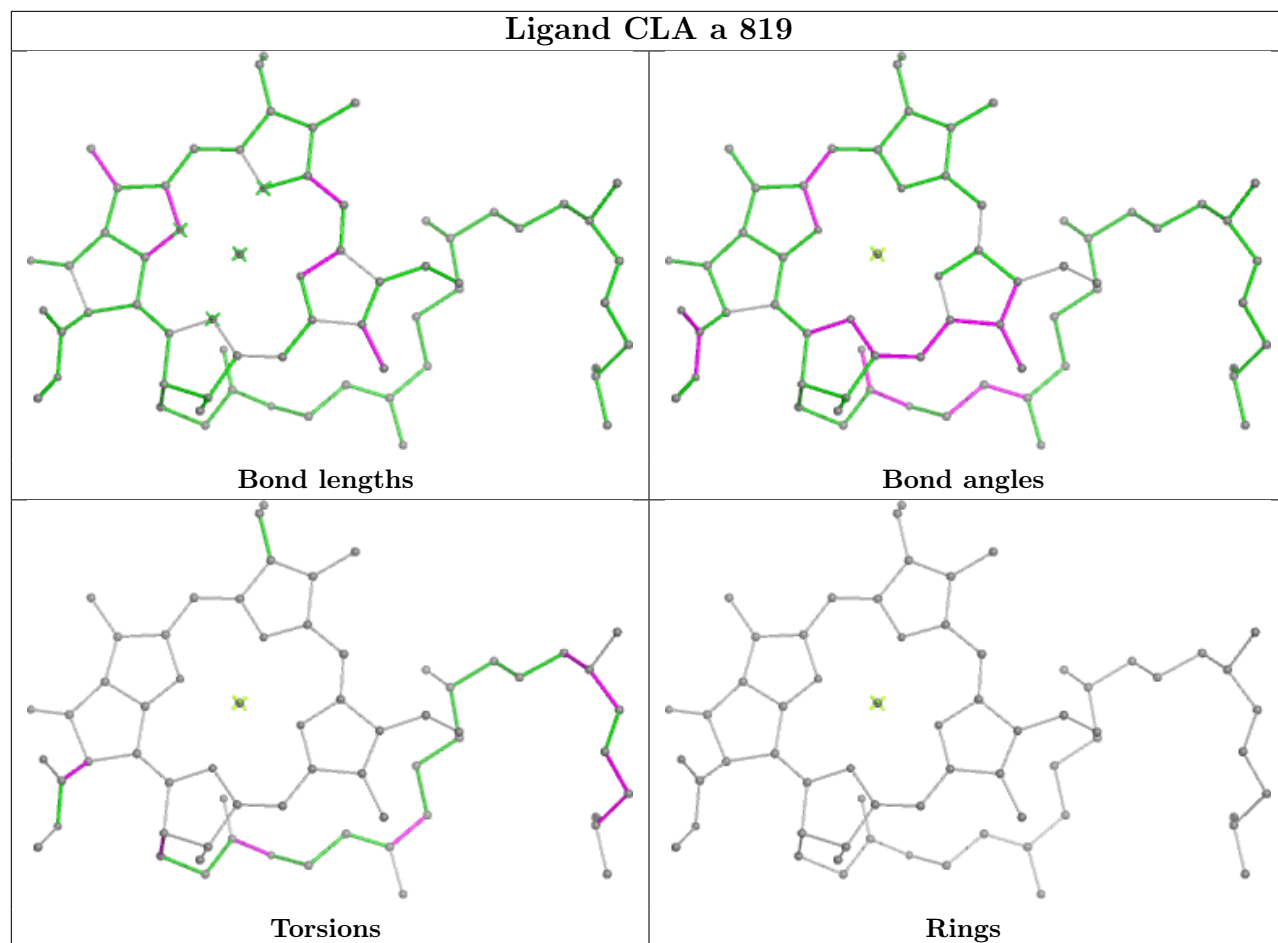


Torsions

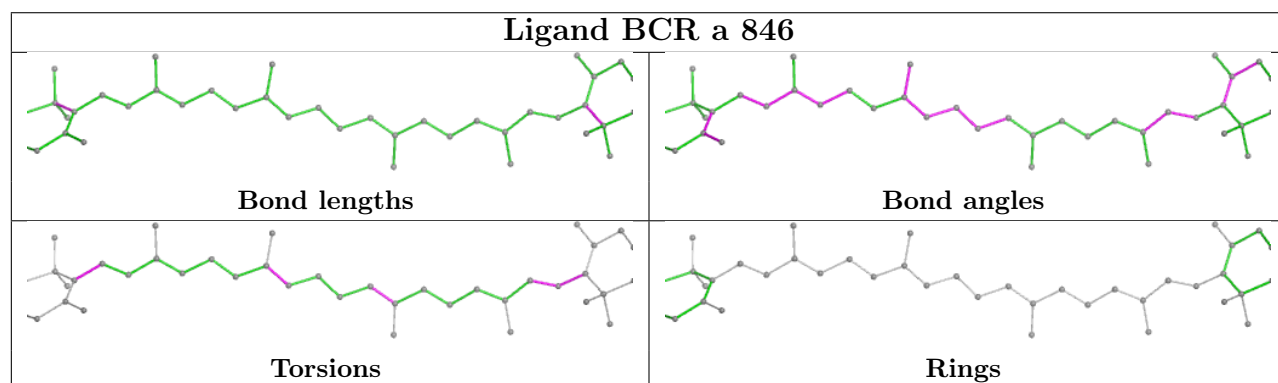


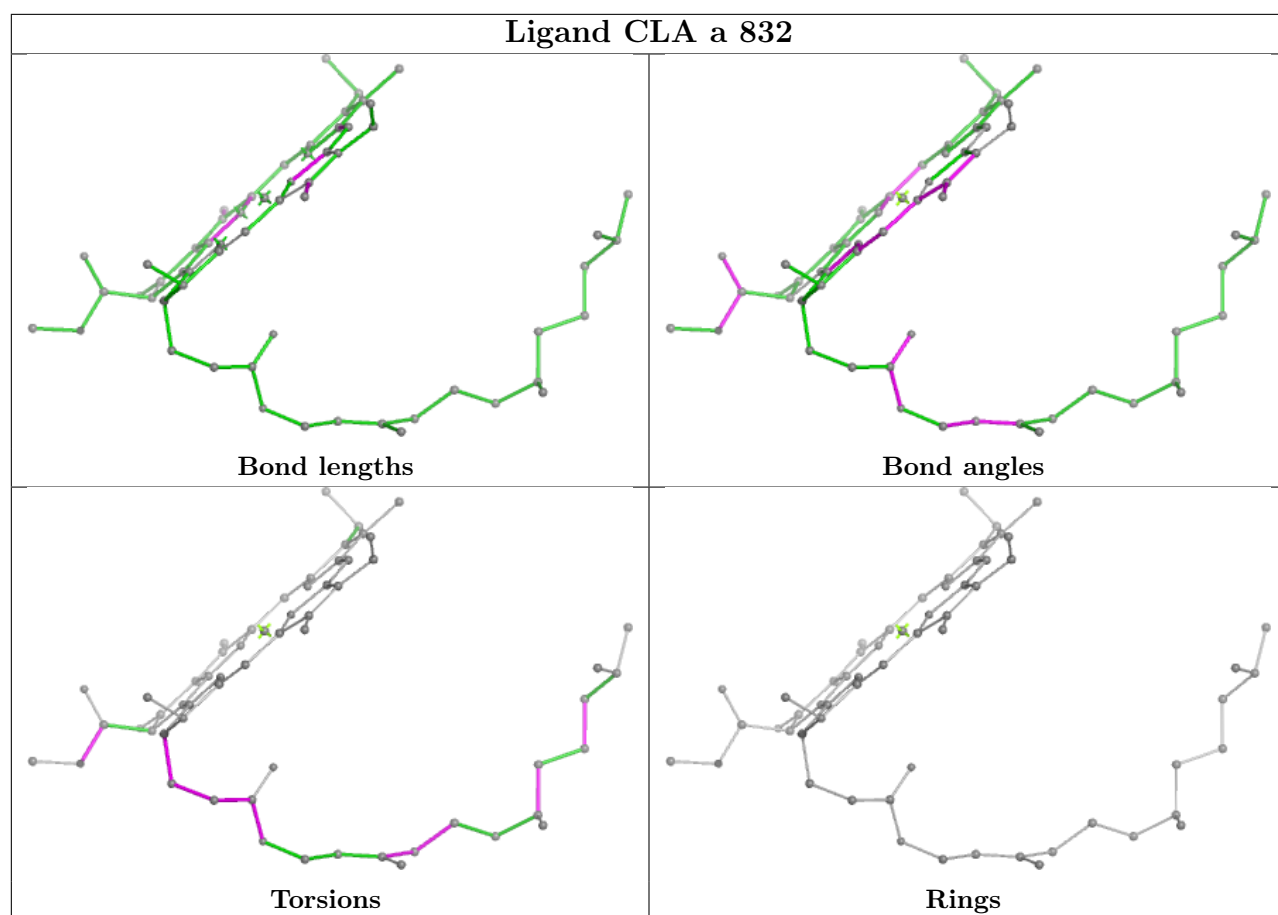
Rings

## Ligand CLA a 819

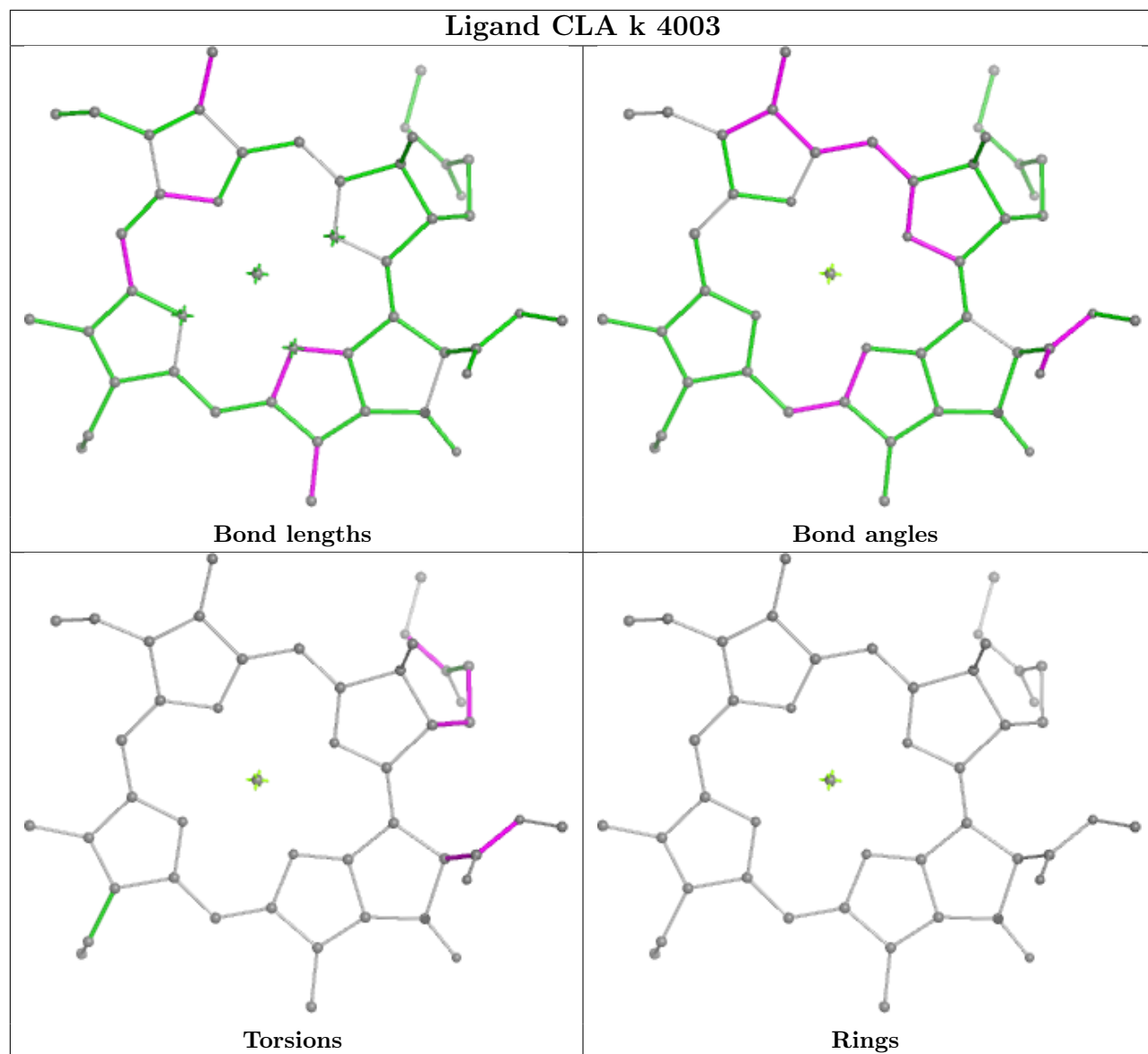


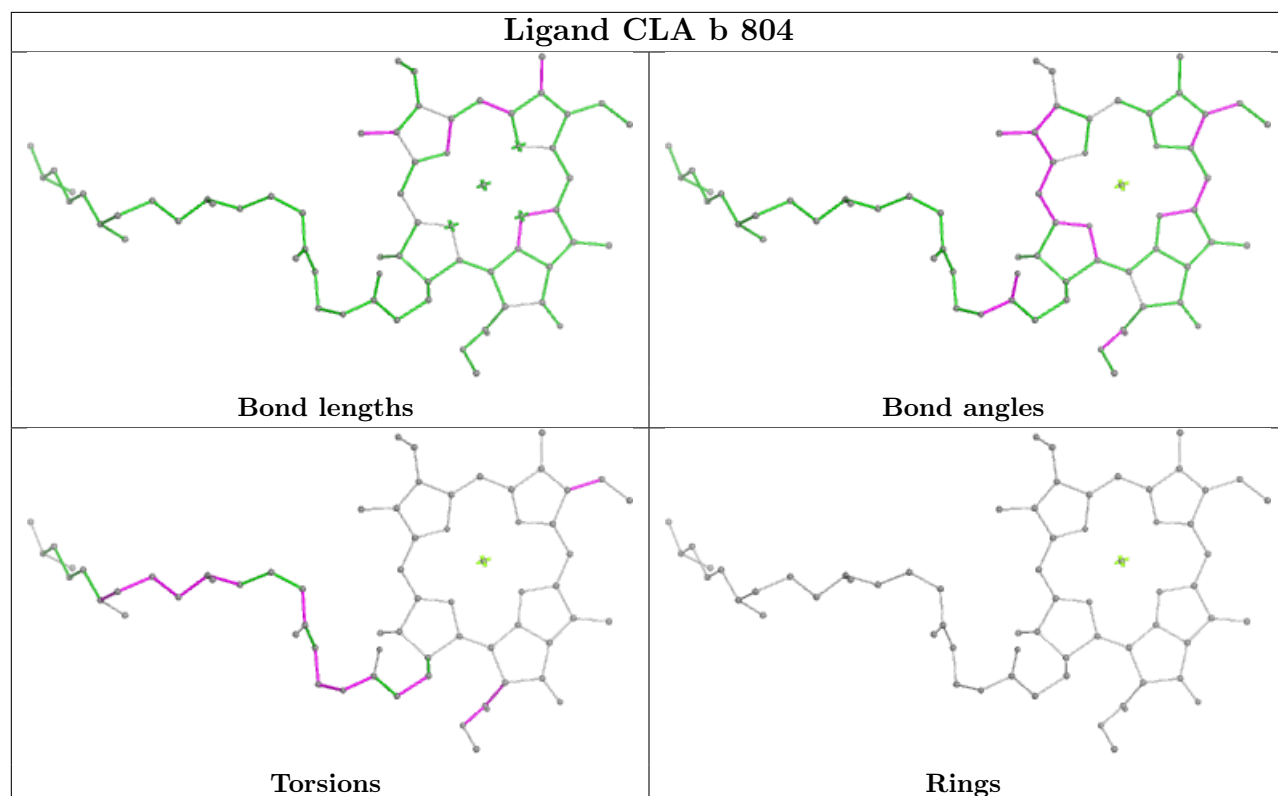
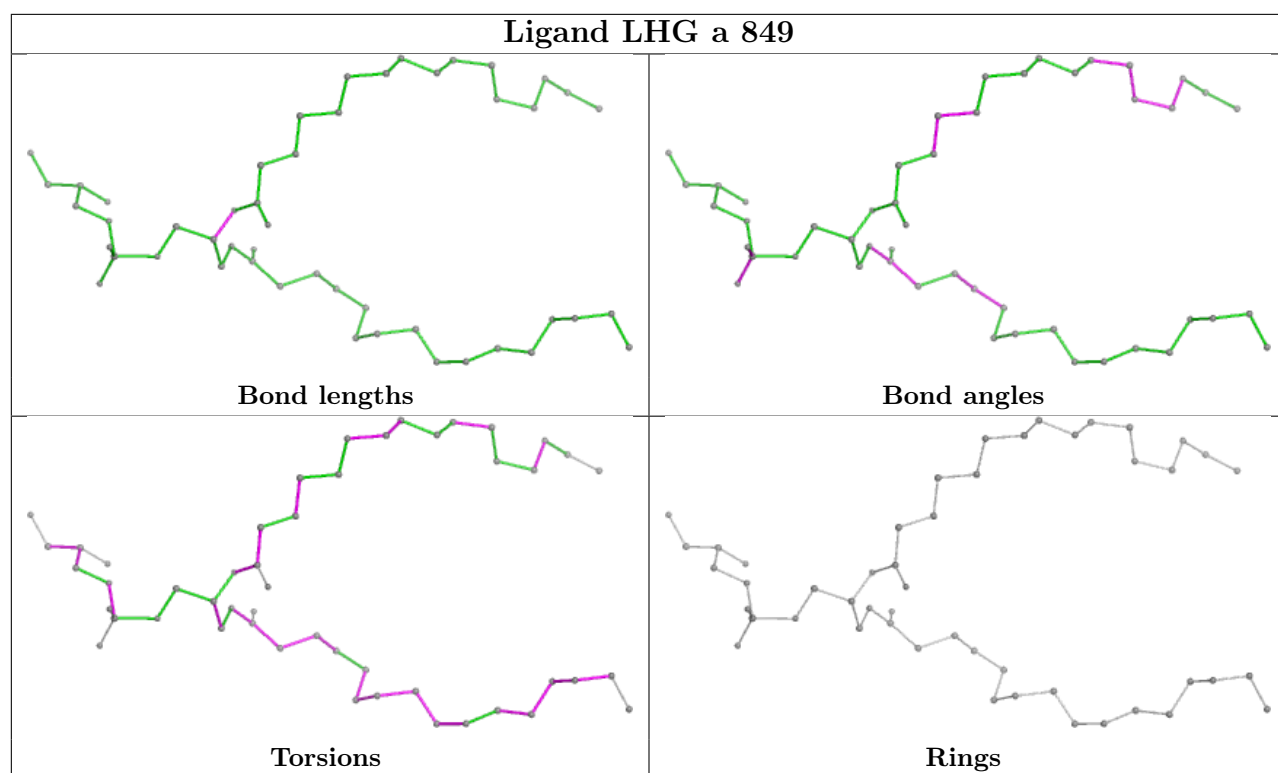
## Ligand BCR a 846

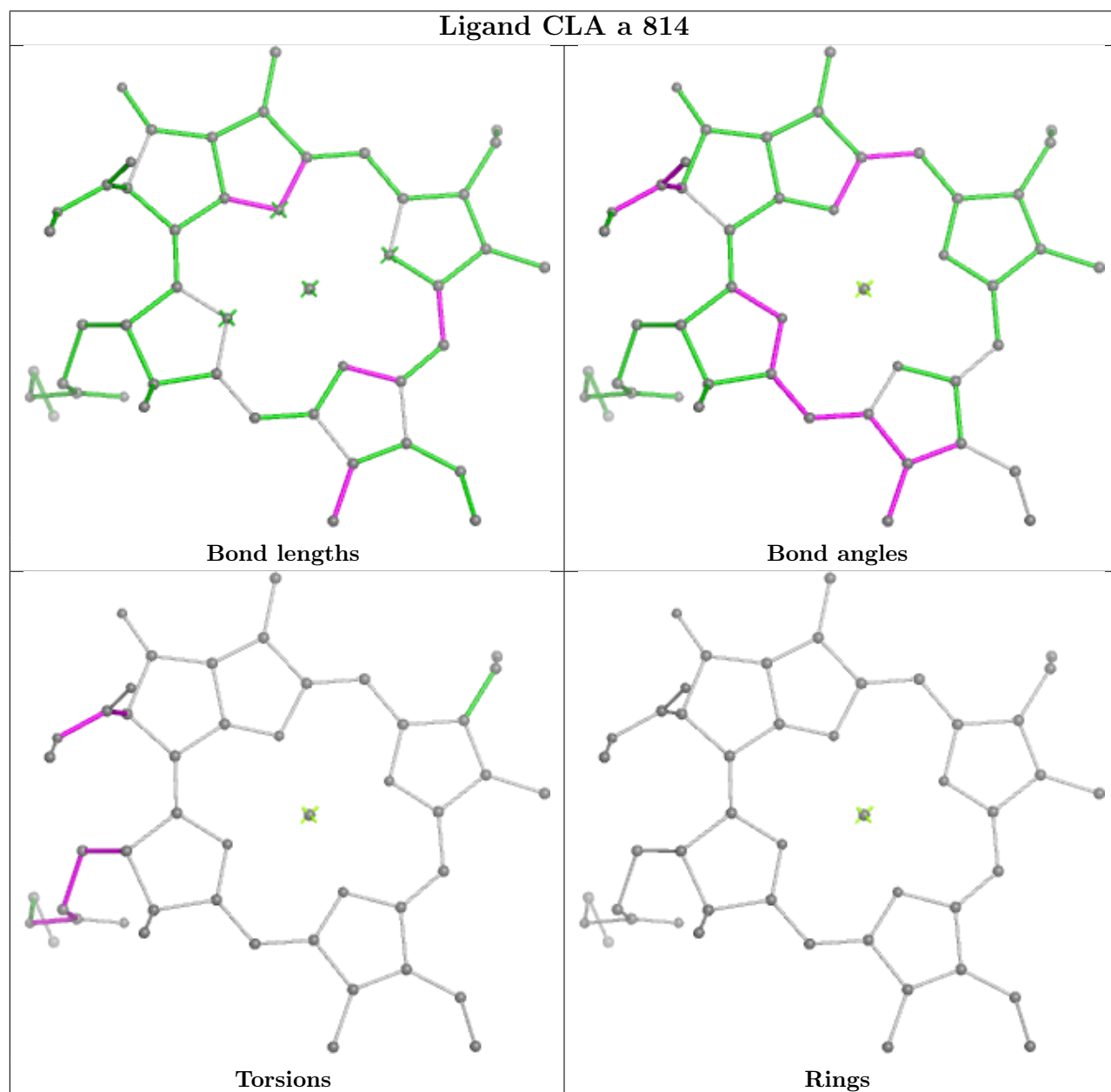
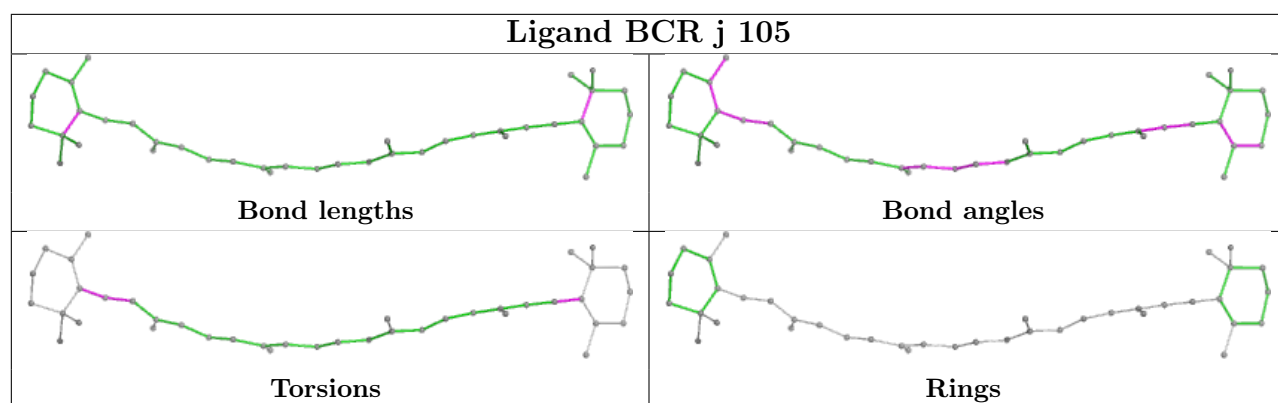




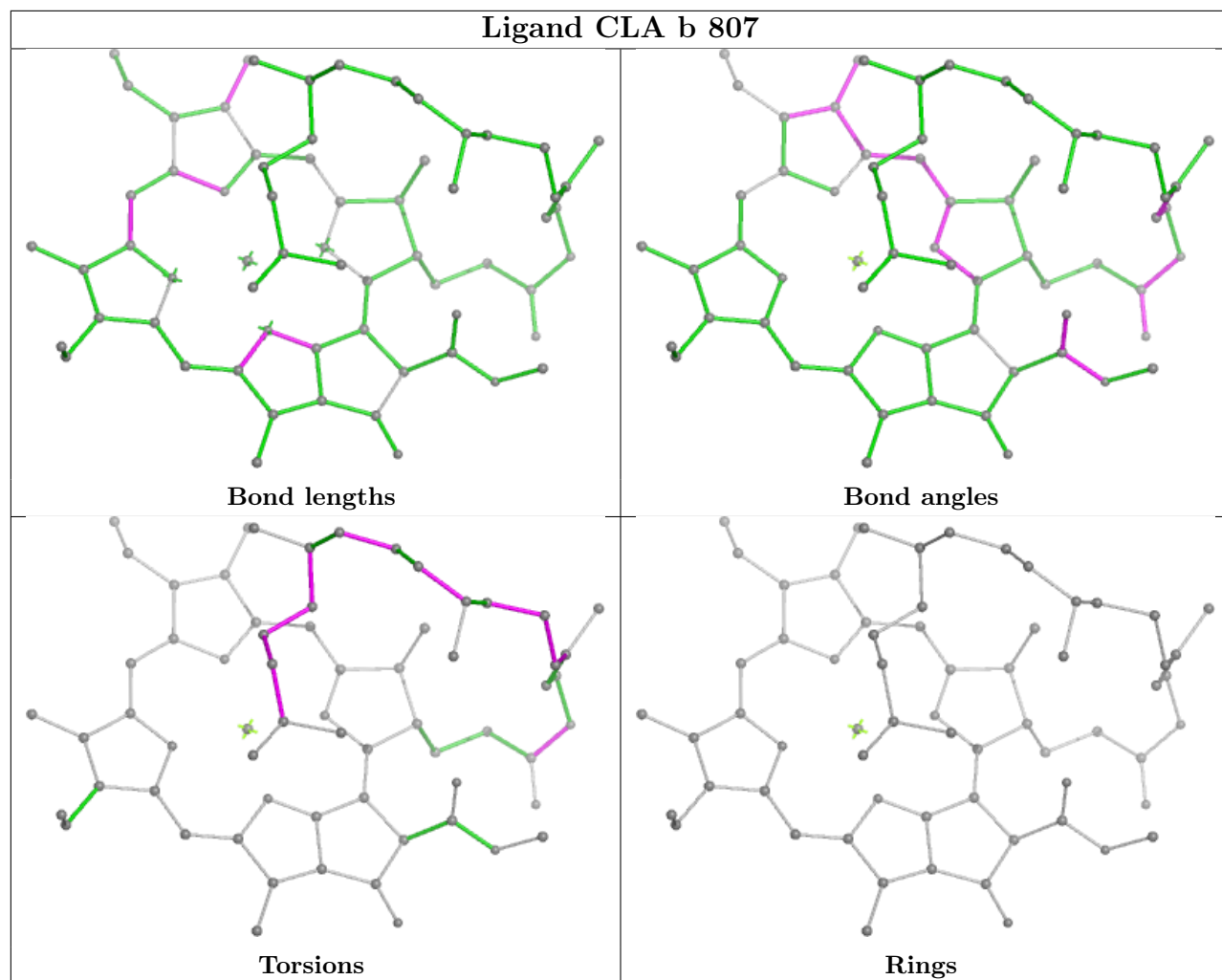




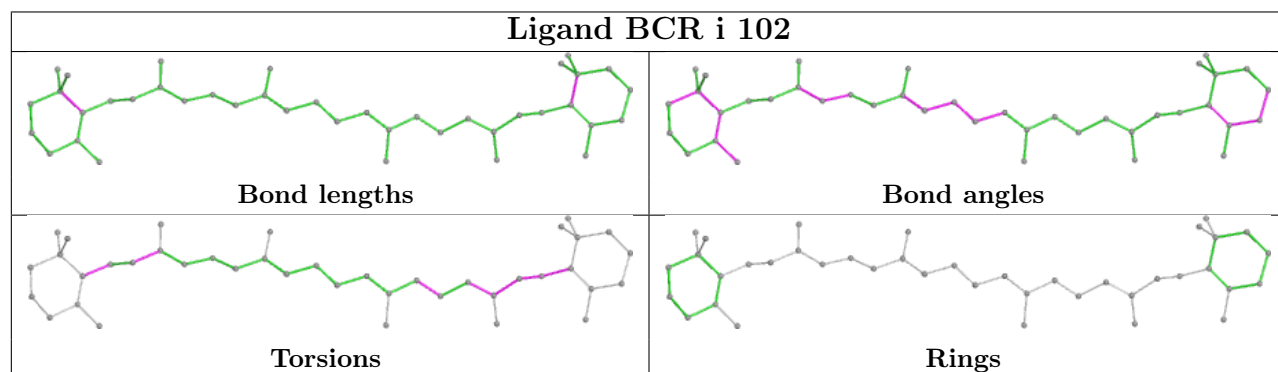




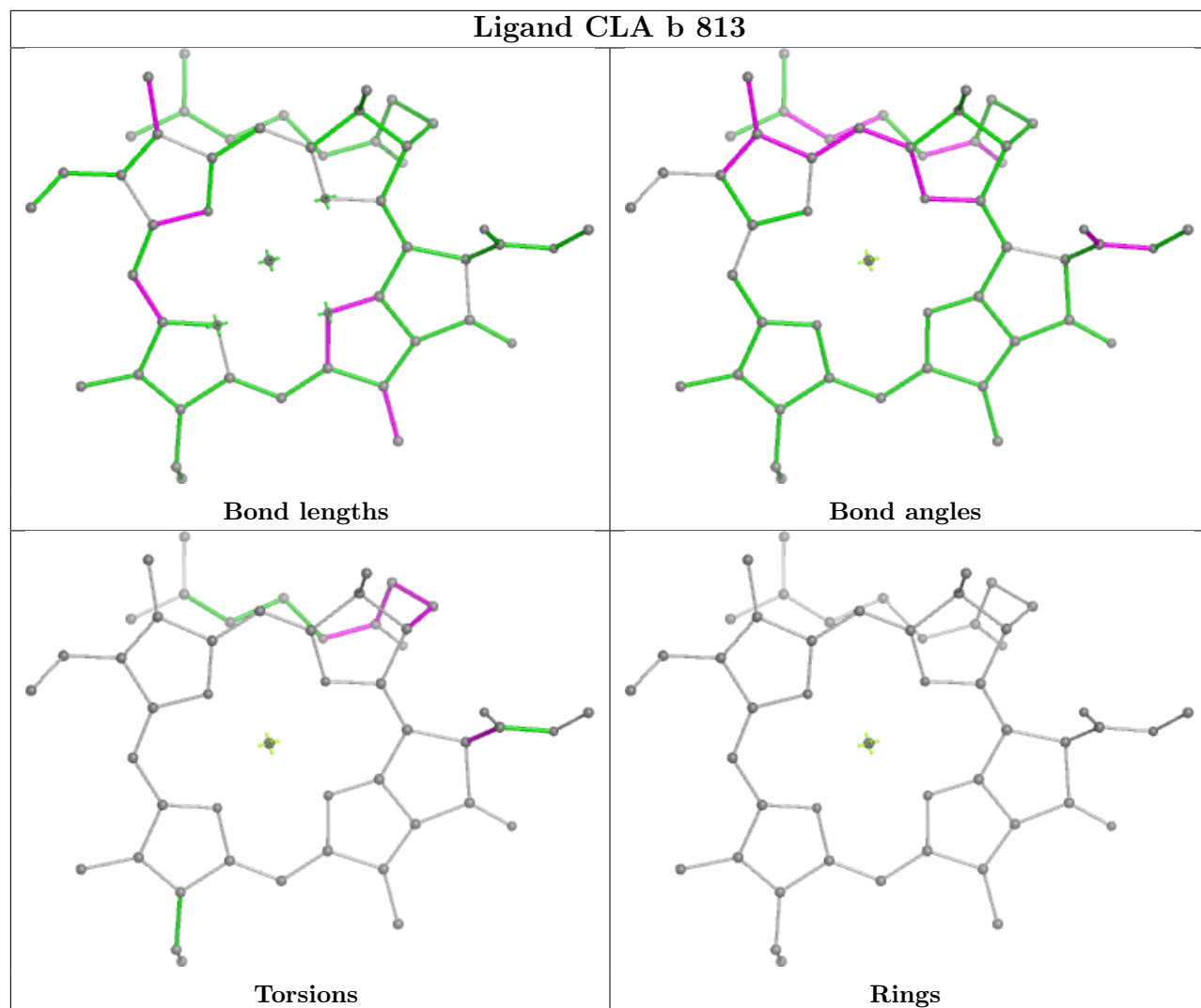
## Ligand CLA b 807

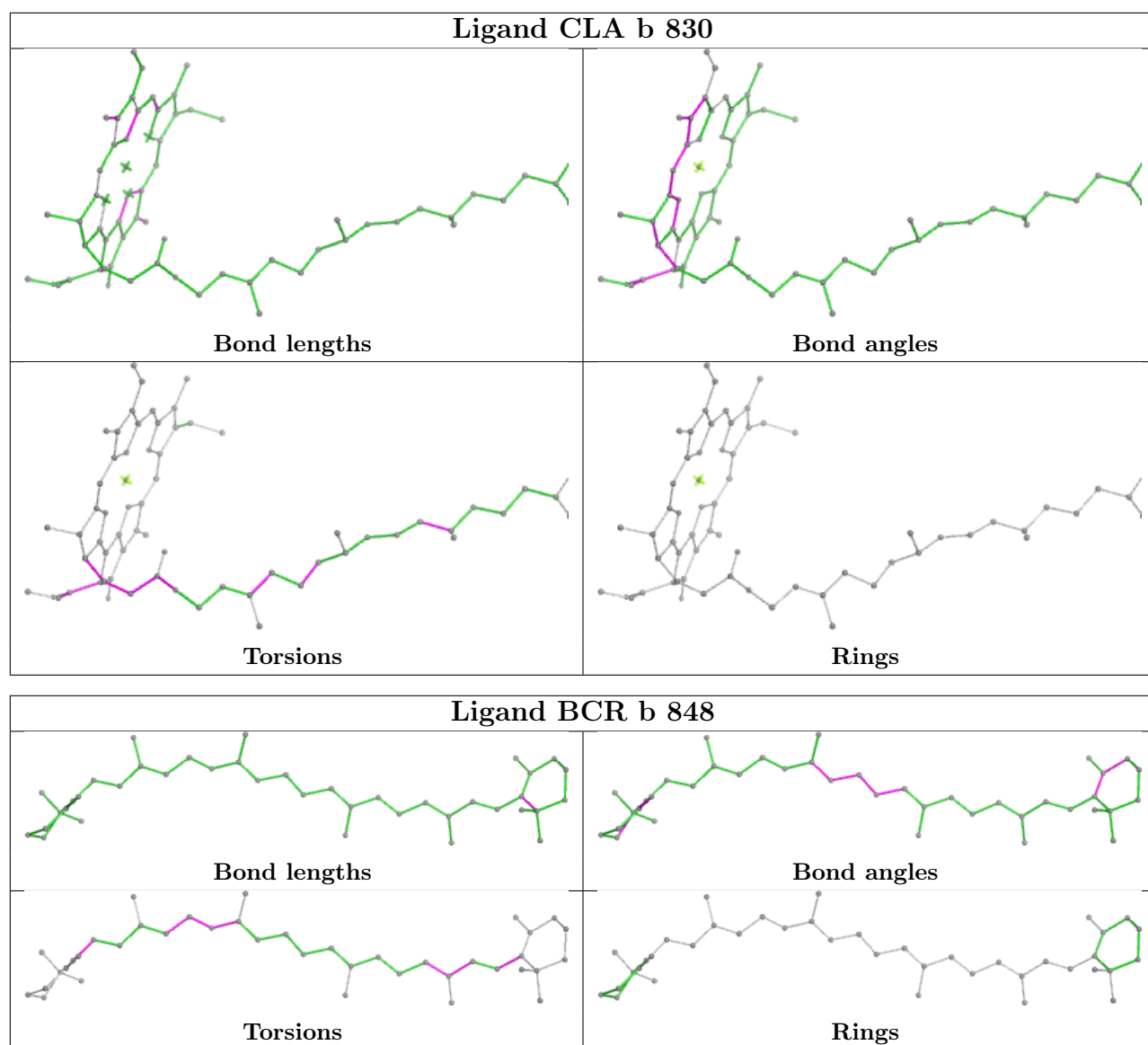


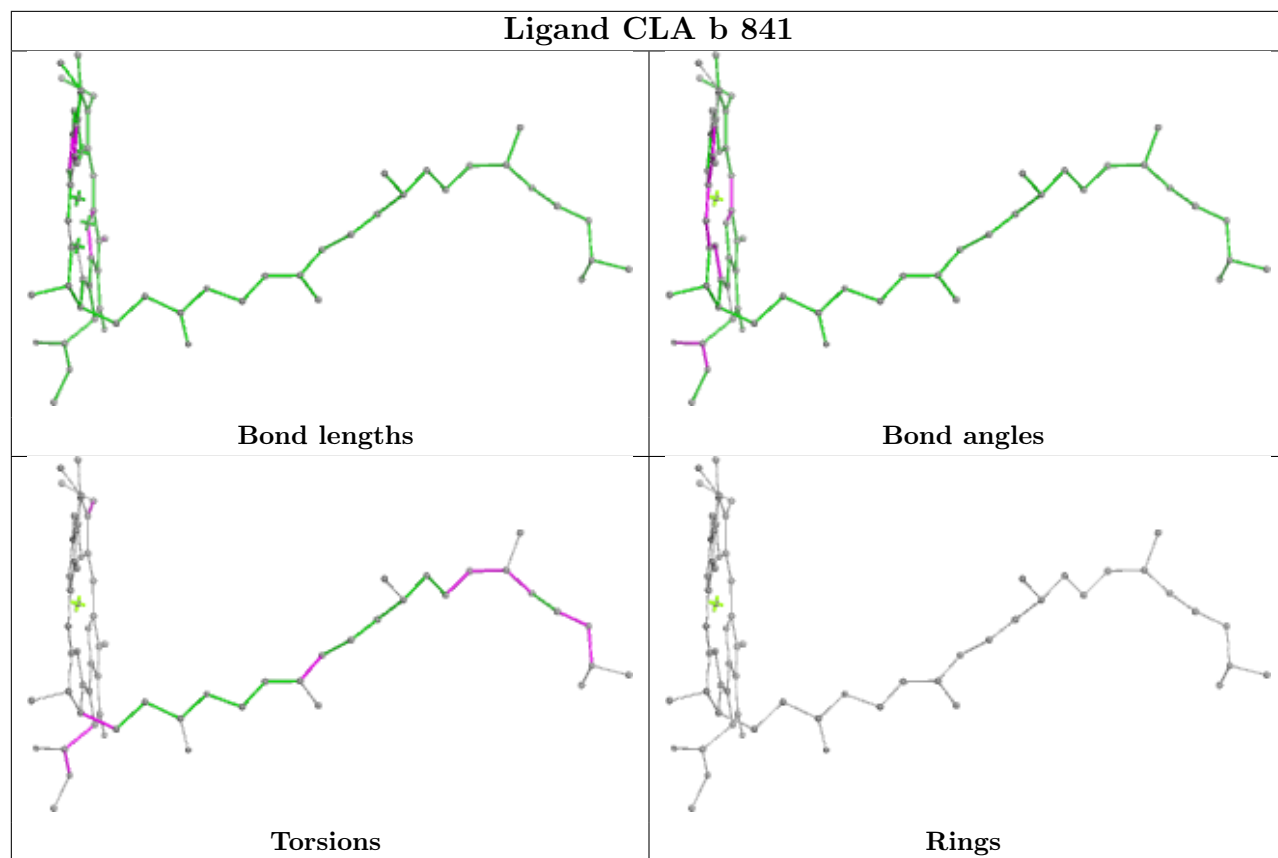
## Ligand BCR i 102

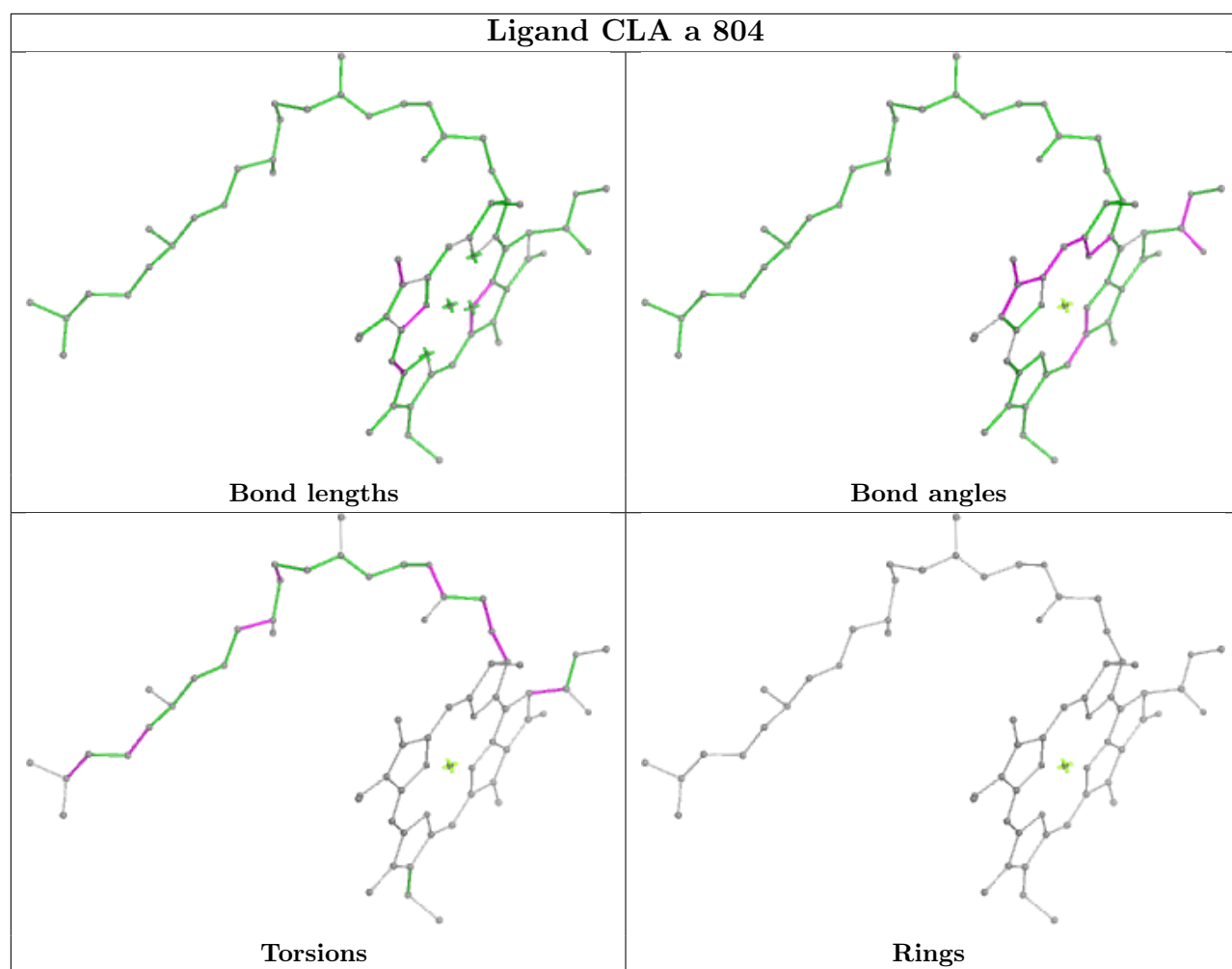


## Ligand CLA b 813



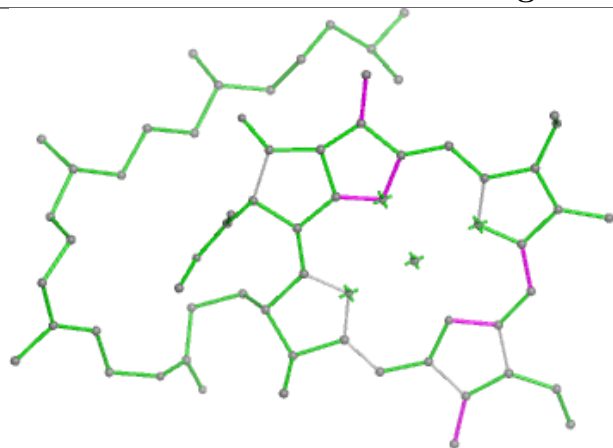




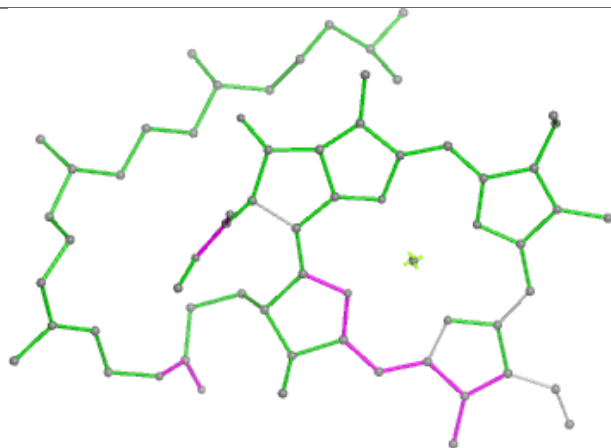




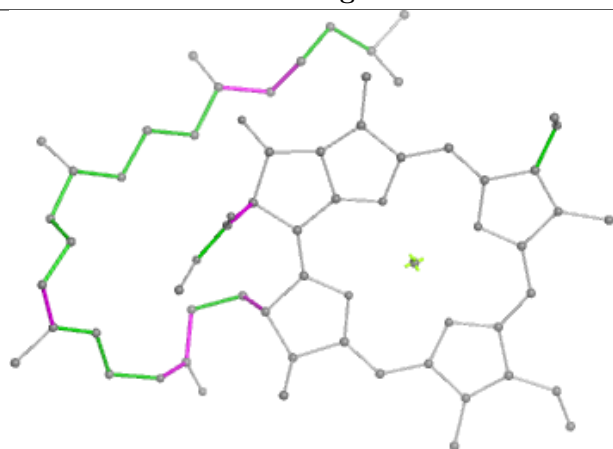
## Ligand CLA b 806



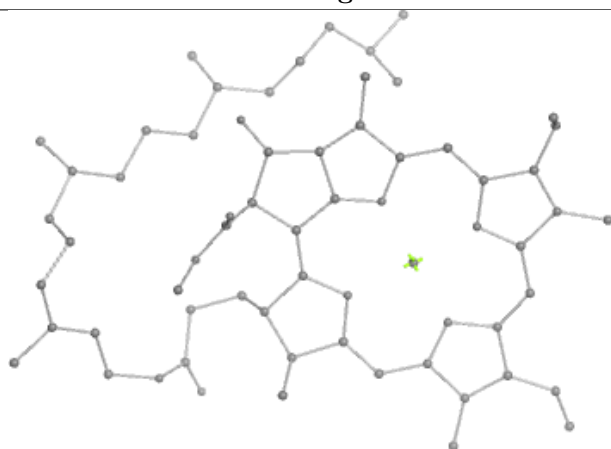
Bond lengths



Bond angles

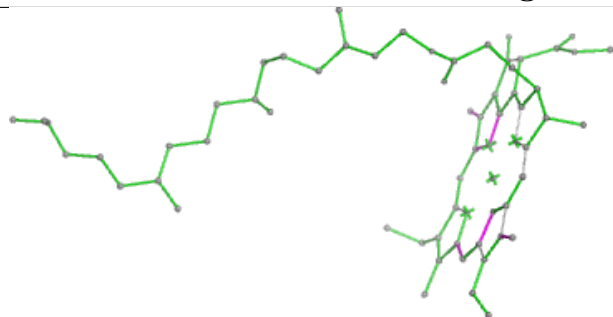


Torsions

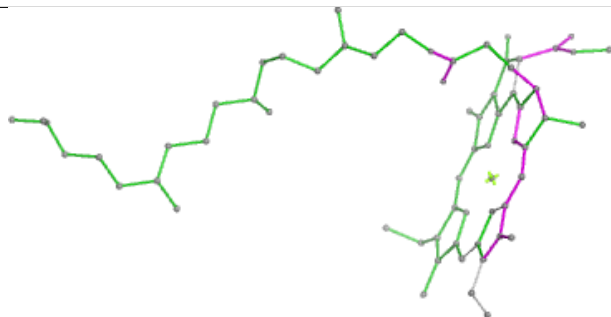


Rings

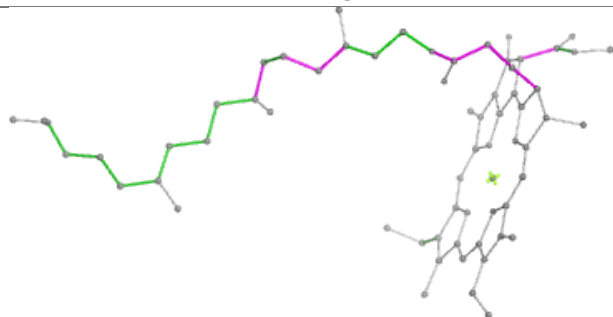
## Ligand CLA a 830



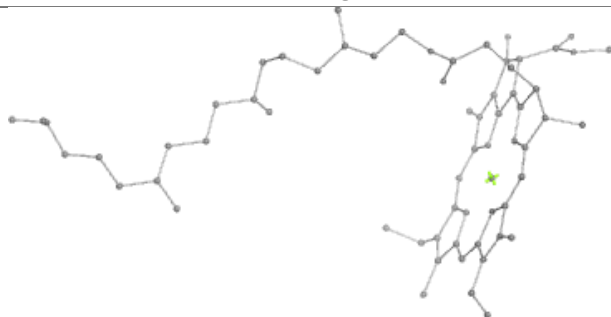
Bond lengths



Bond angles

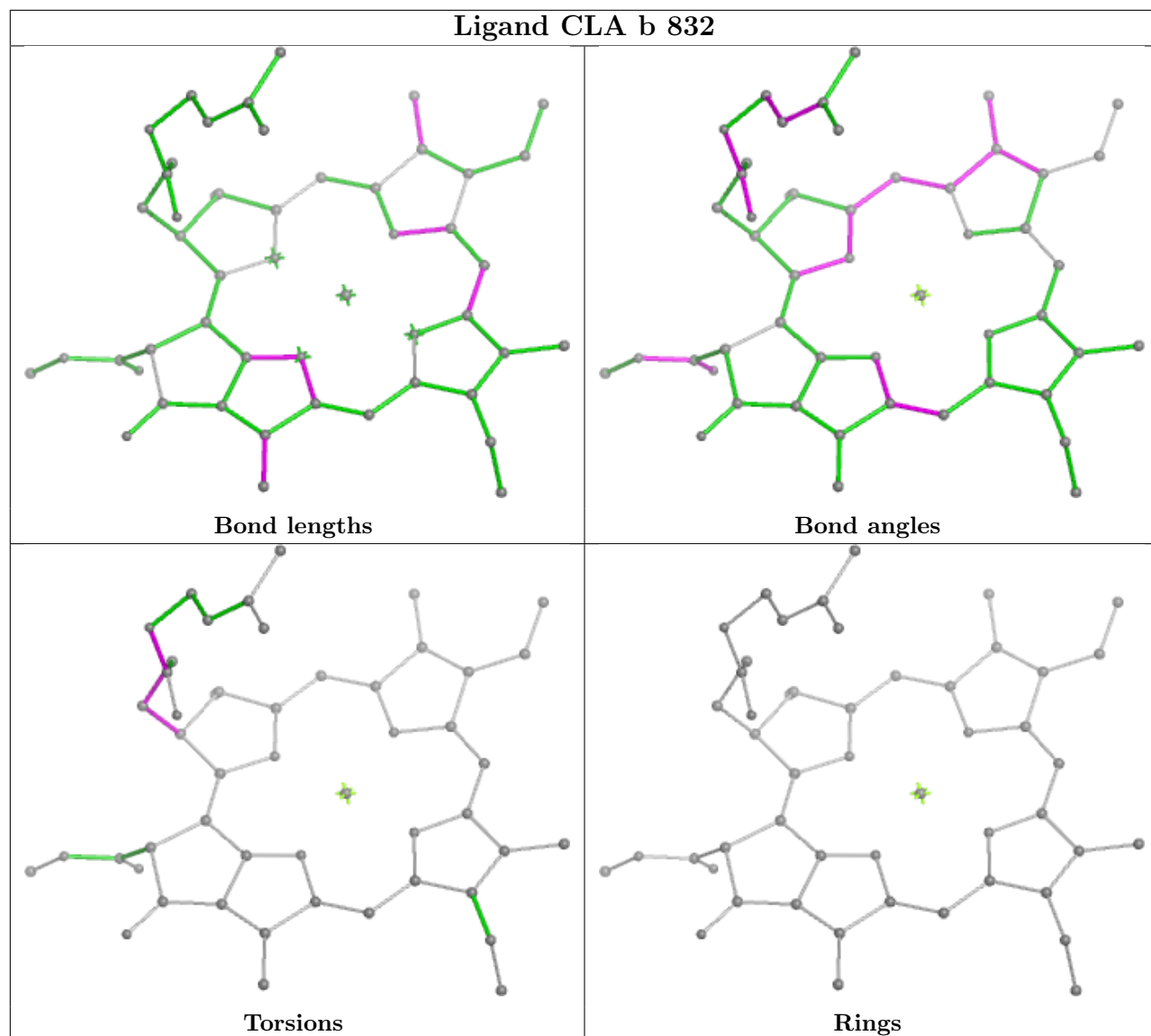


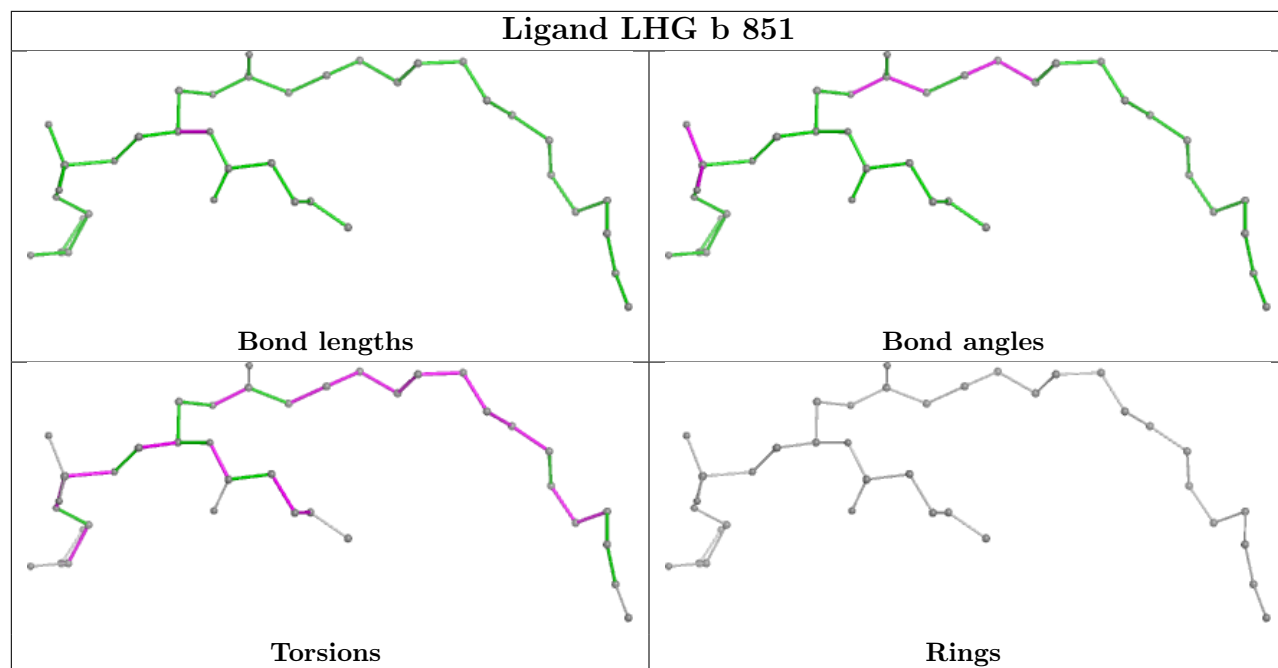
Torsions



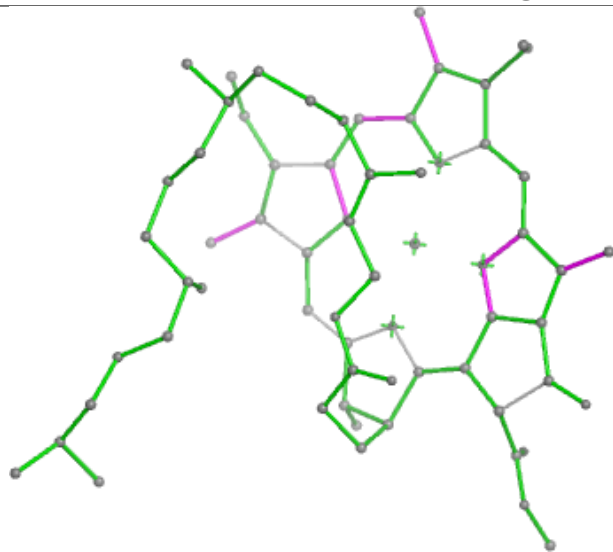
Rings

## Ligand CLA b 832

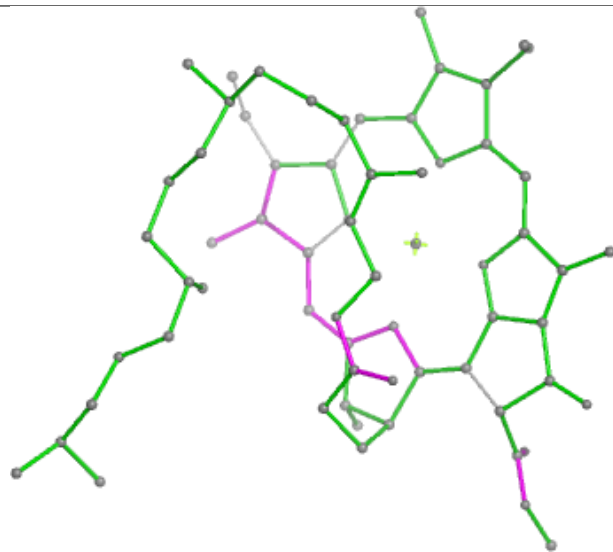




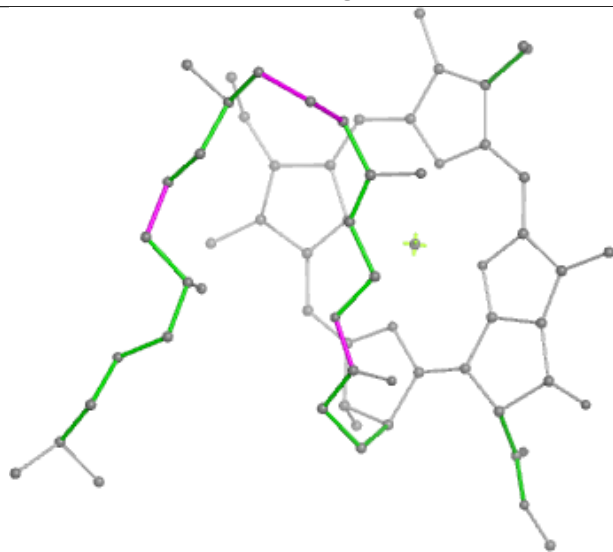
## Ligand CLA b 809



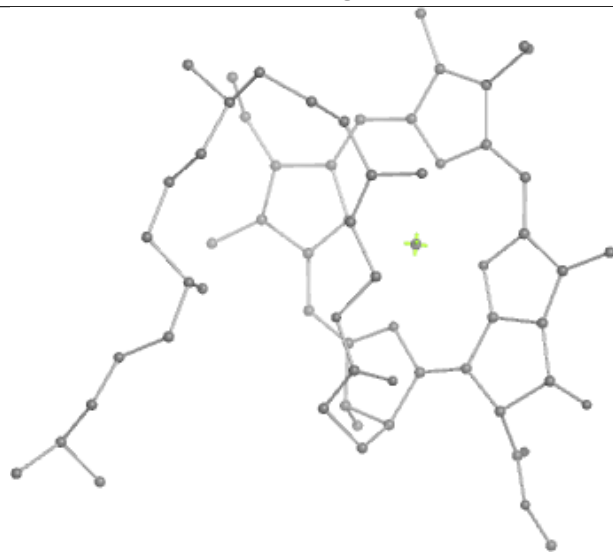
Bond lengths



Bond angles

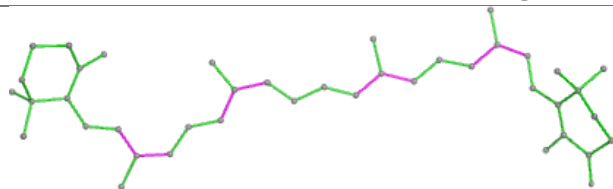


Torsions

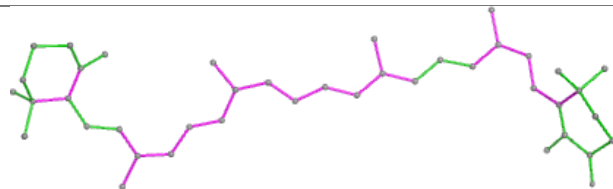


Rings

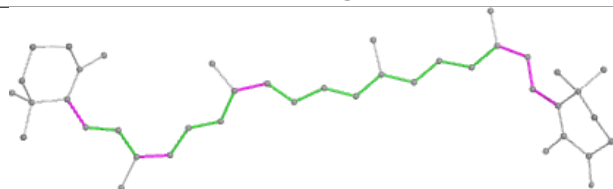
## Ligand ECH b 846



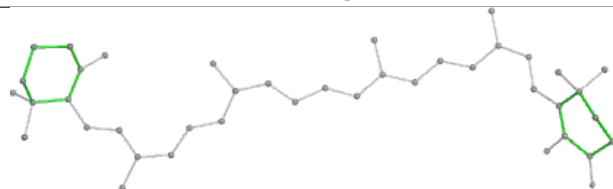
Bond lengths



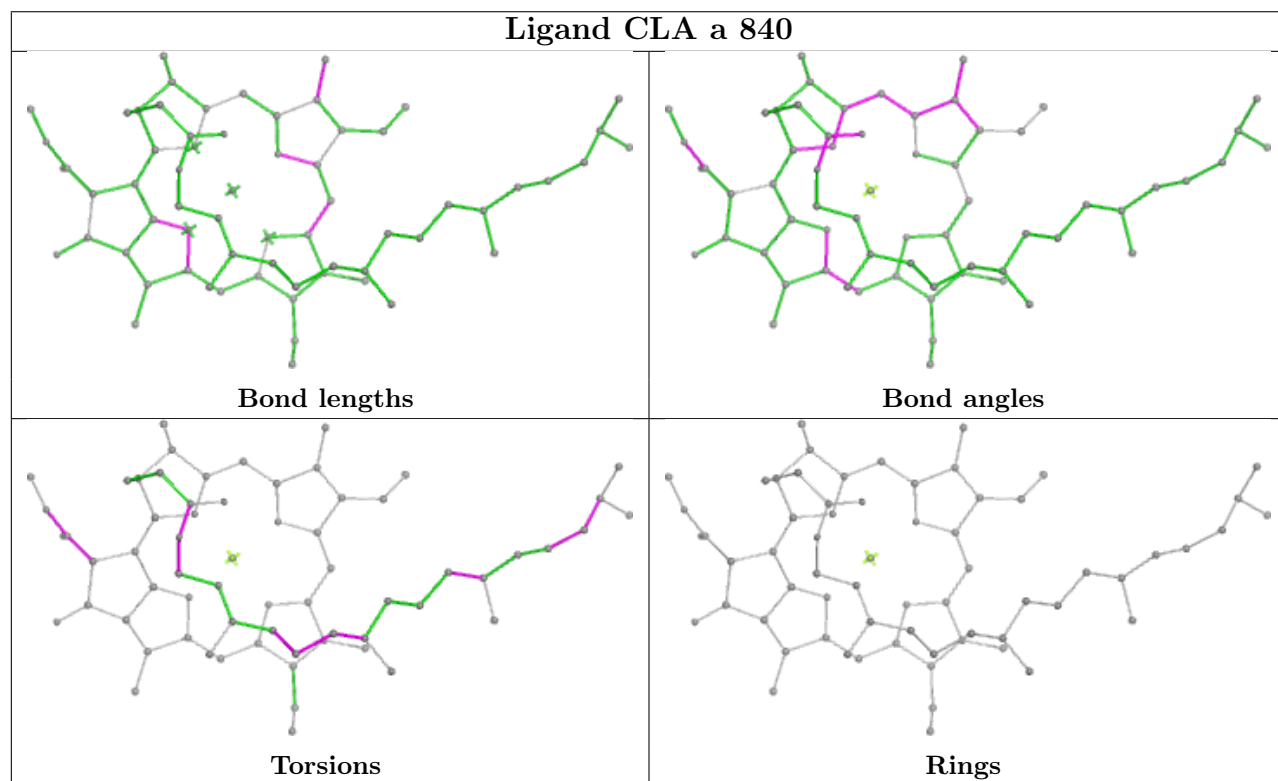
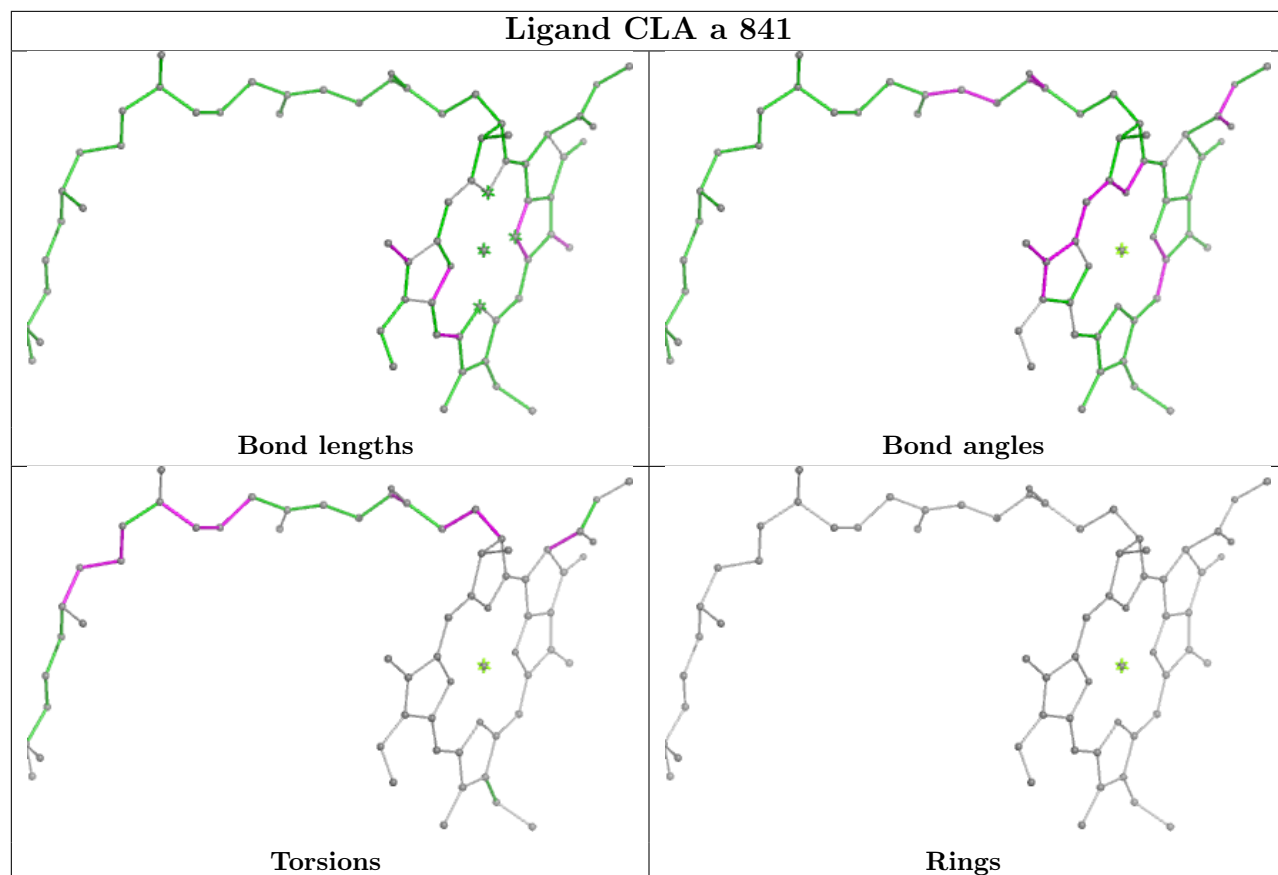
Bond angles



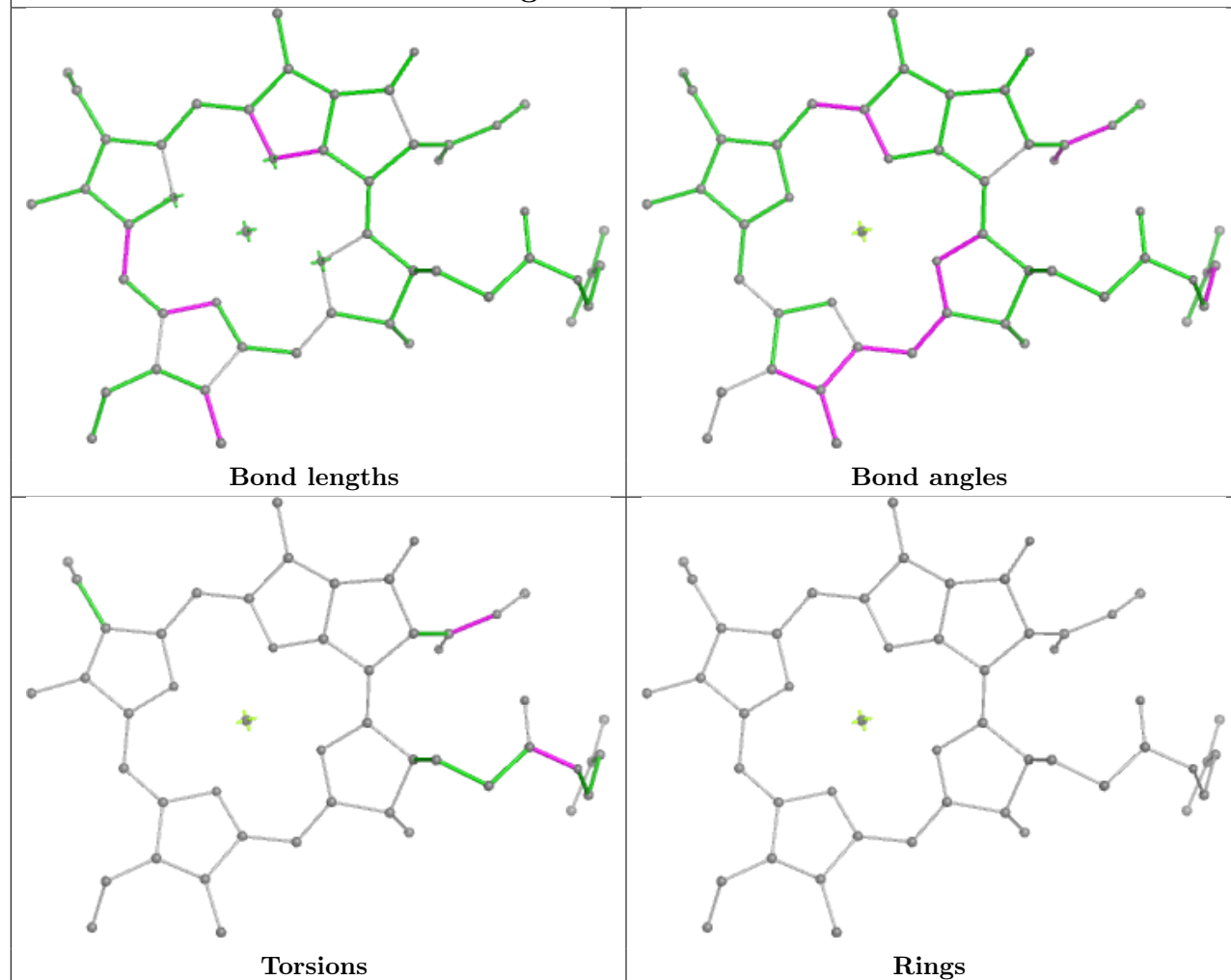
Torsions



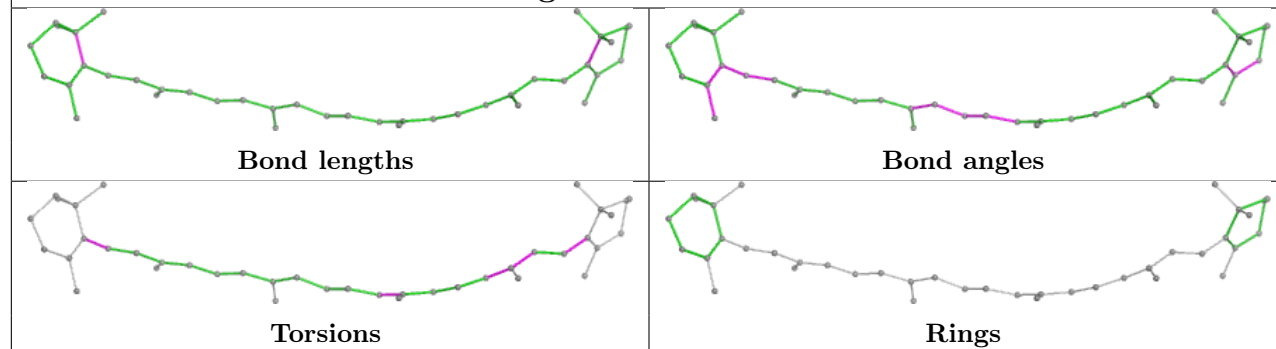
Rings

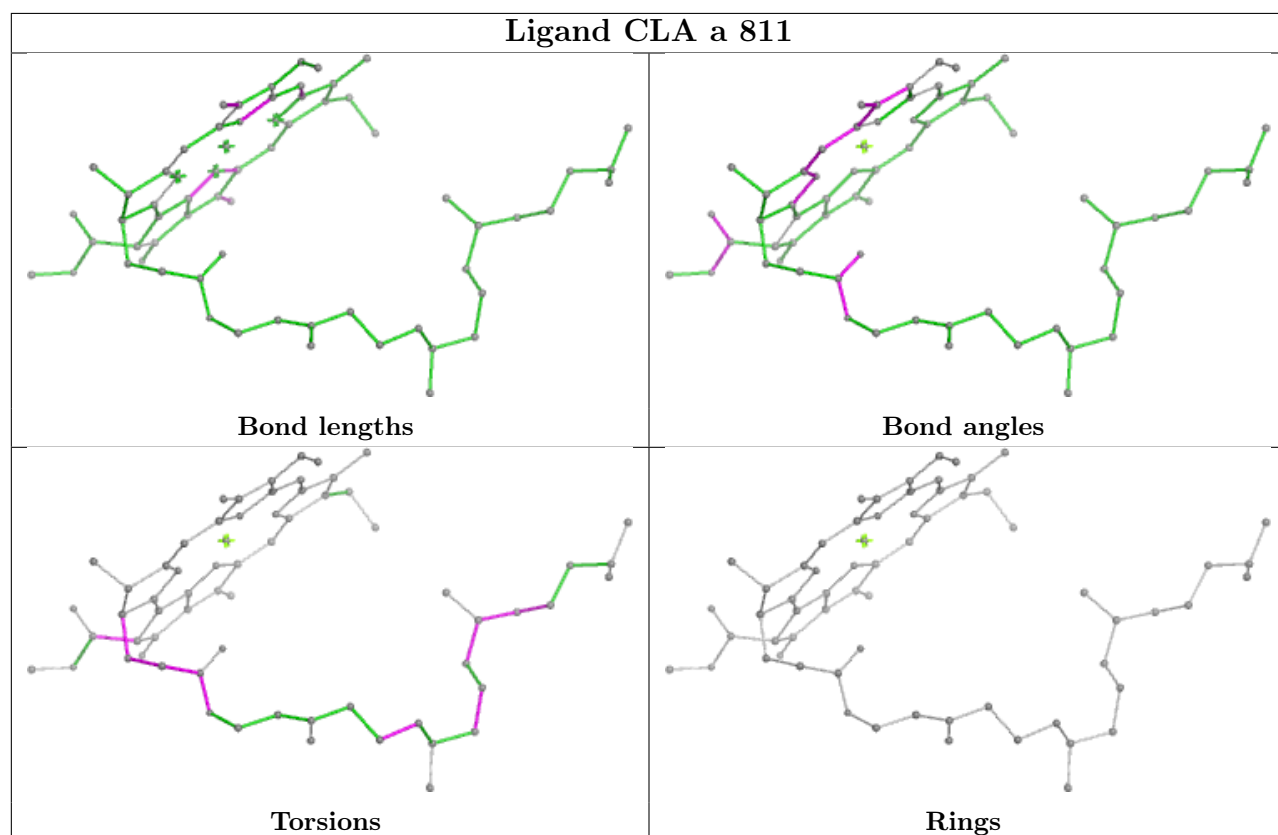
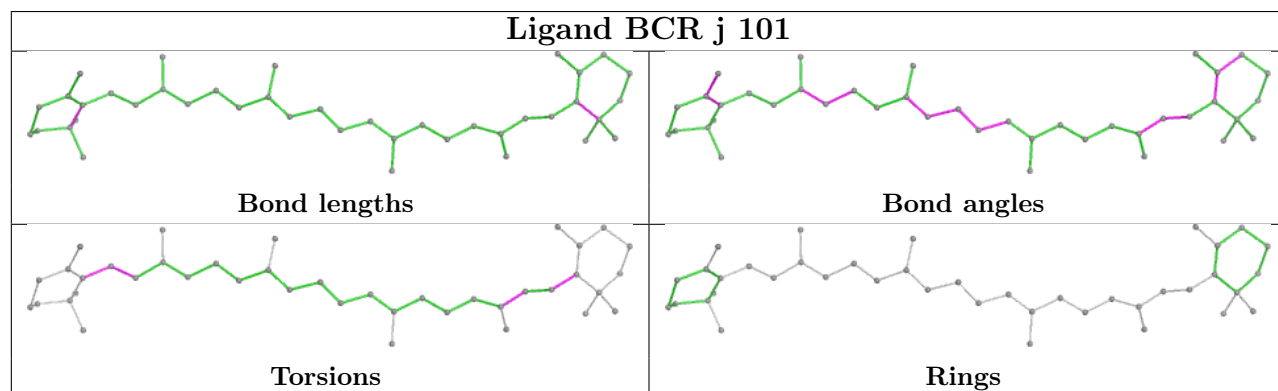
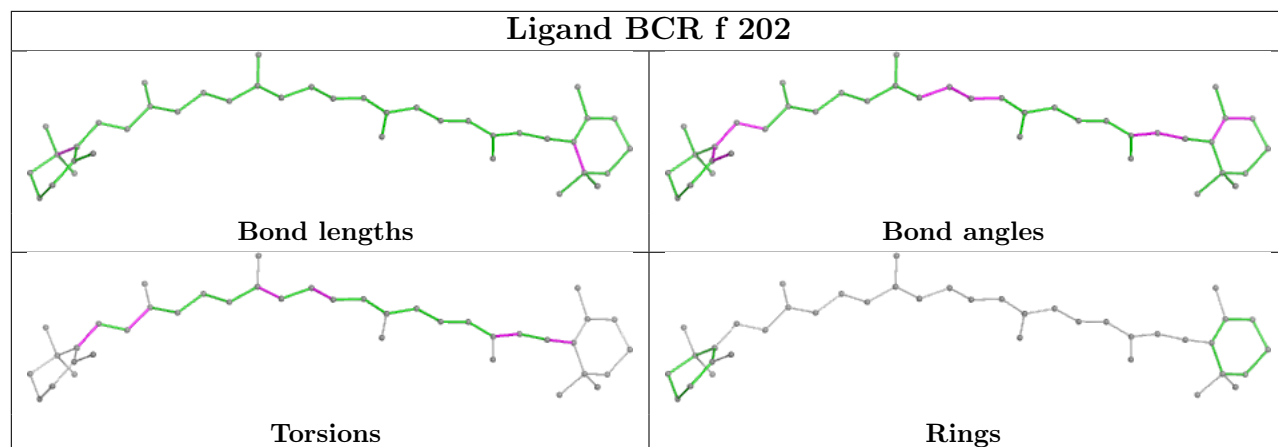


## Ligand CLA f 203

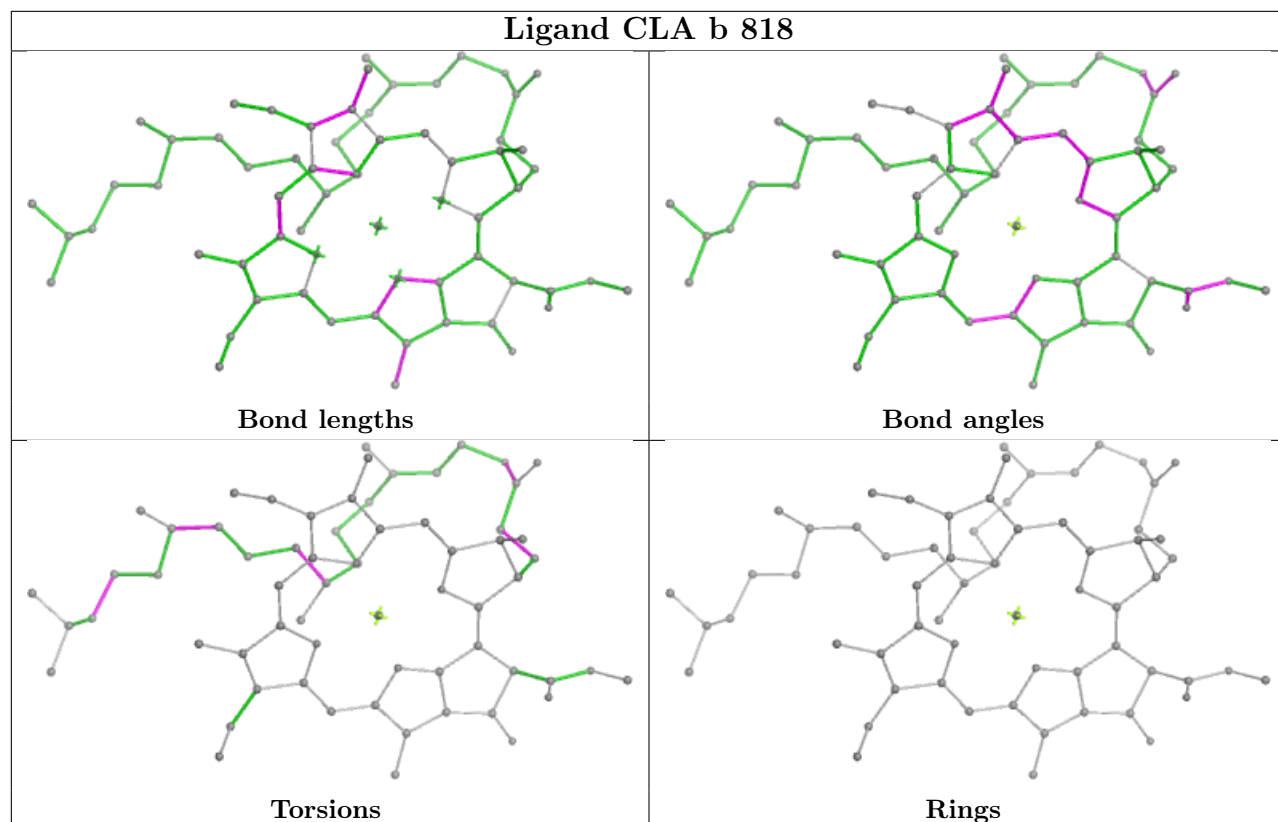


## Ligand BCR i 101

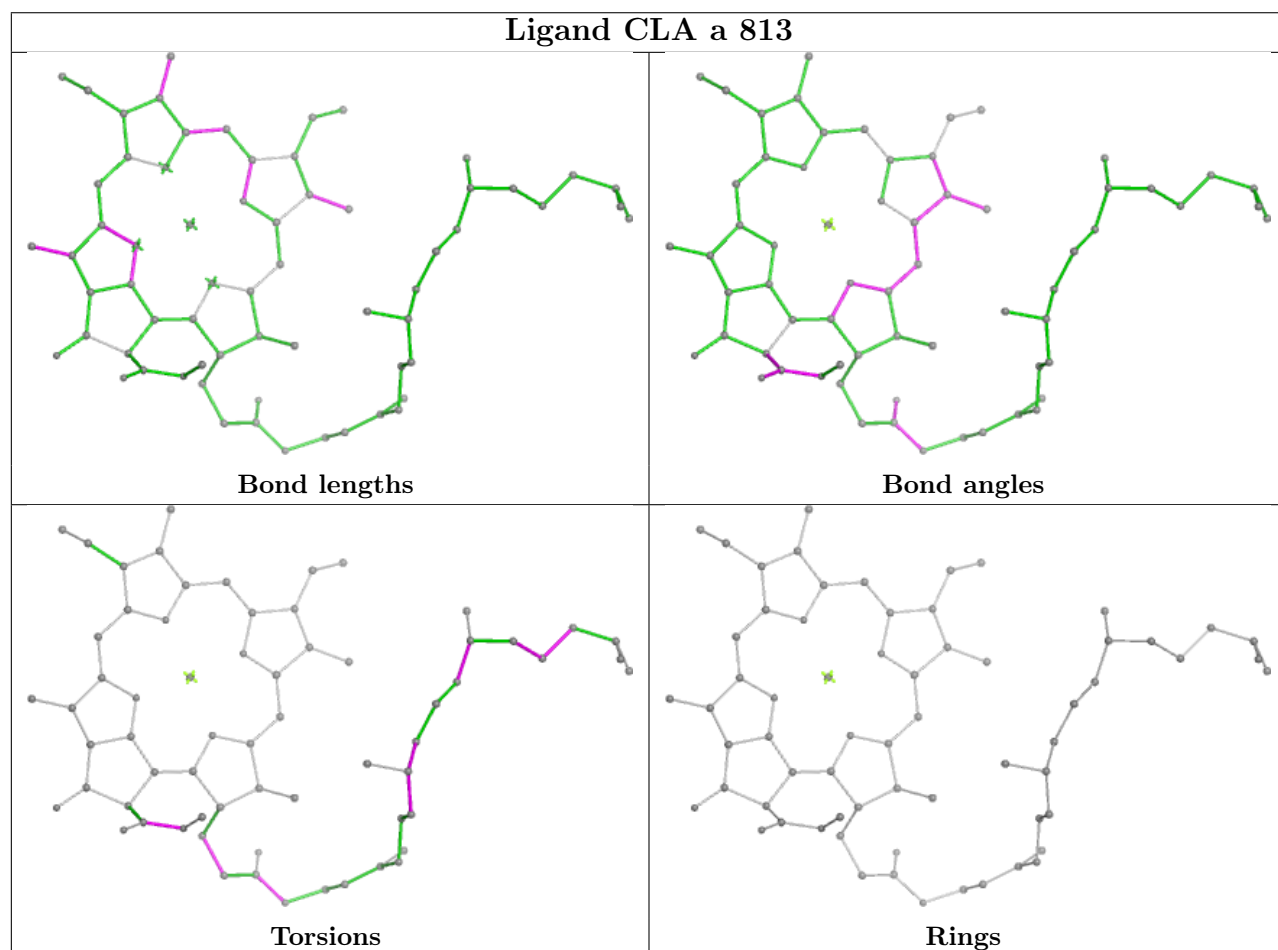




## Ligand CLA b 818

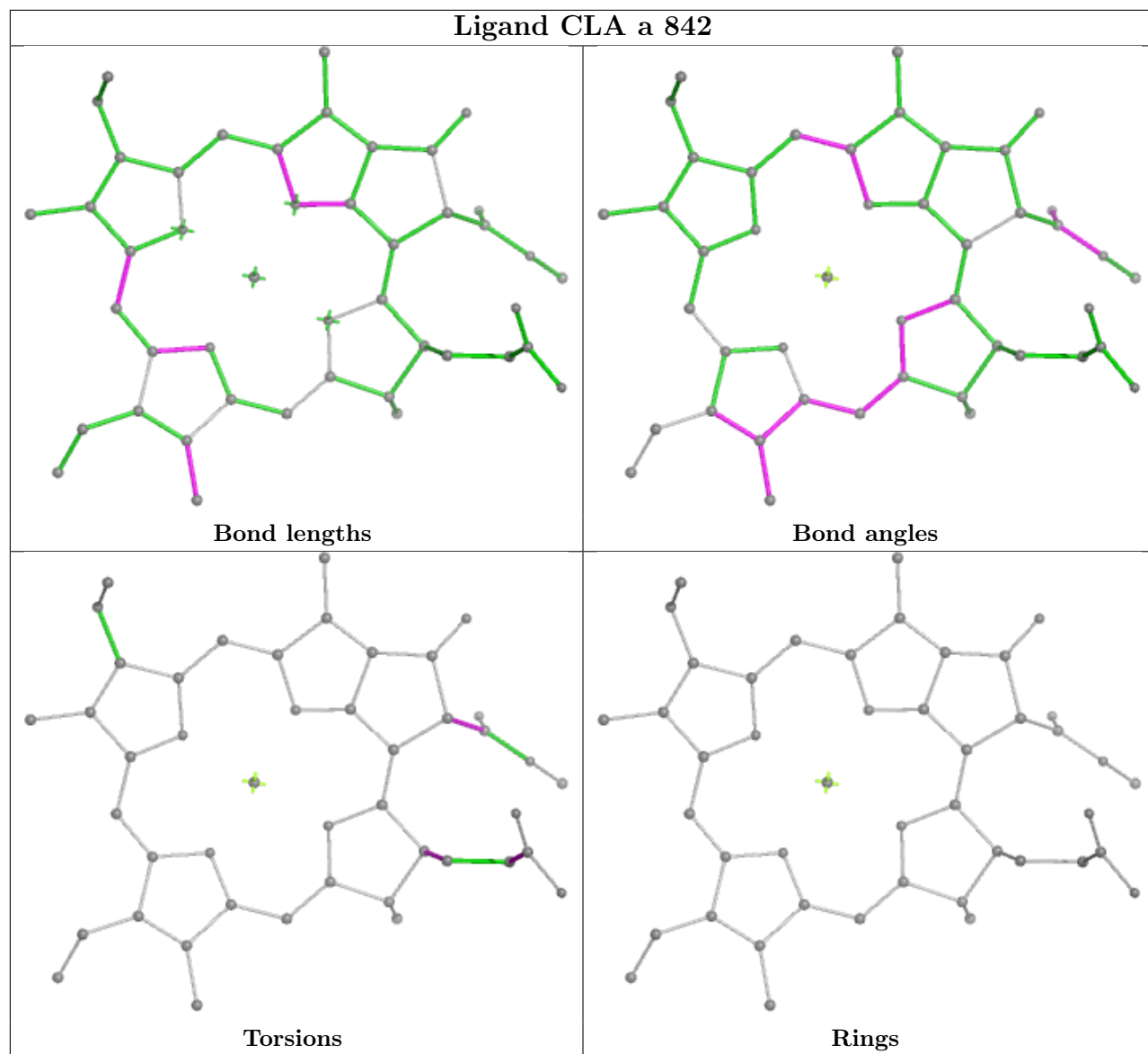


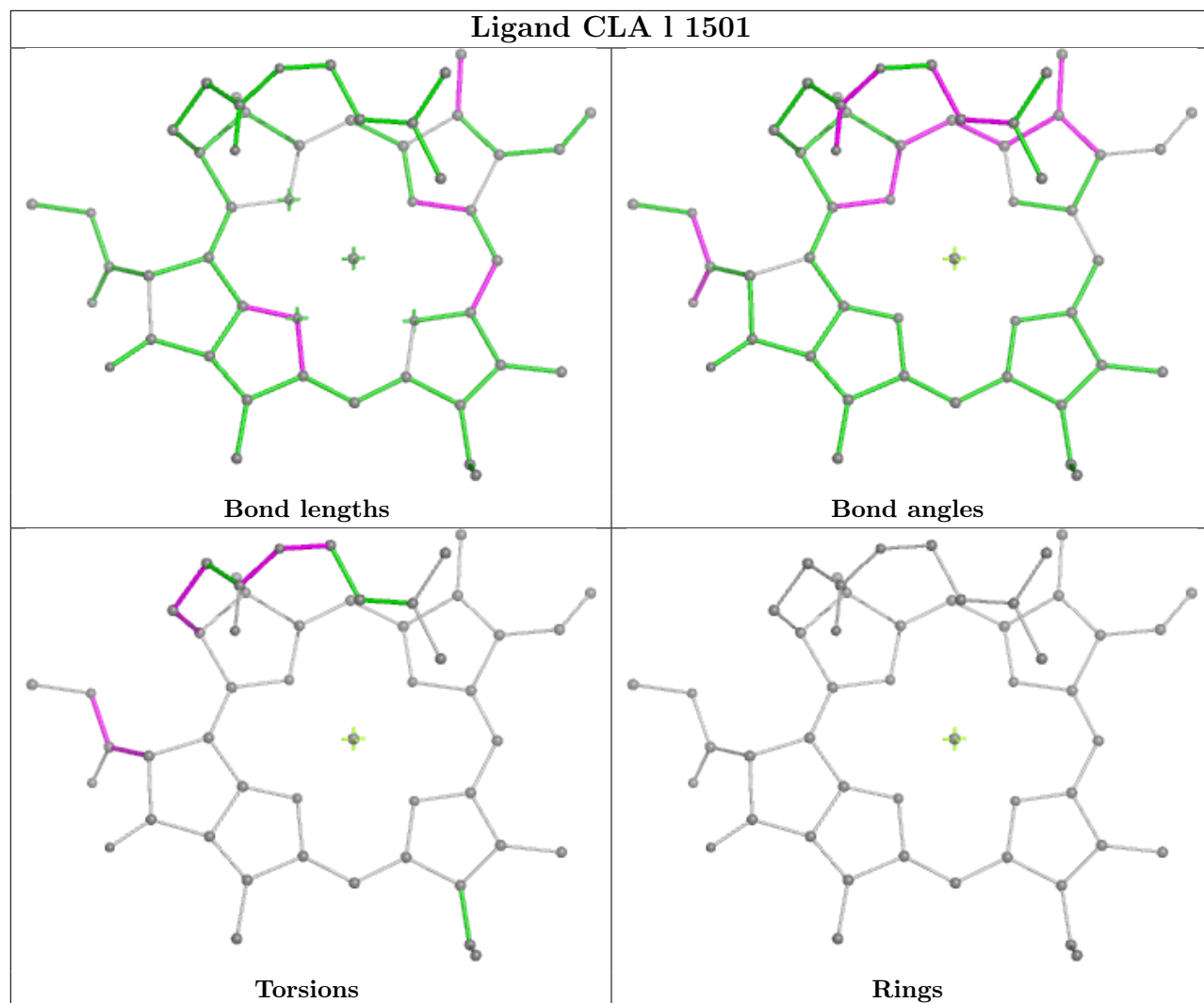
## Ligand CLA a 813



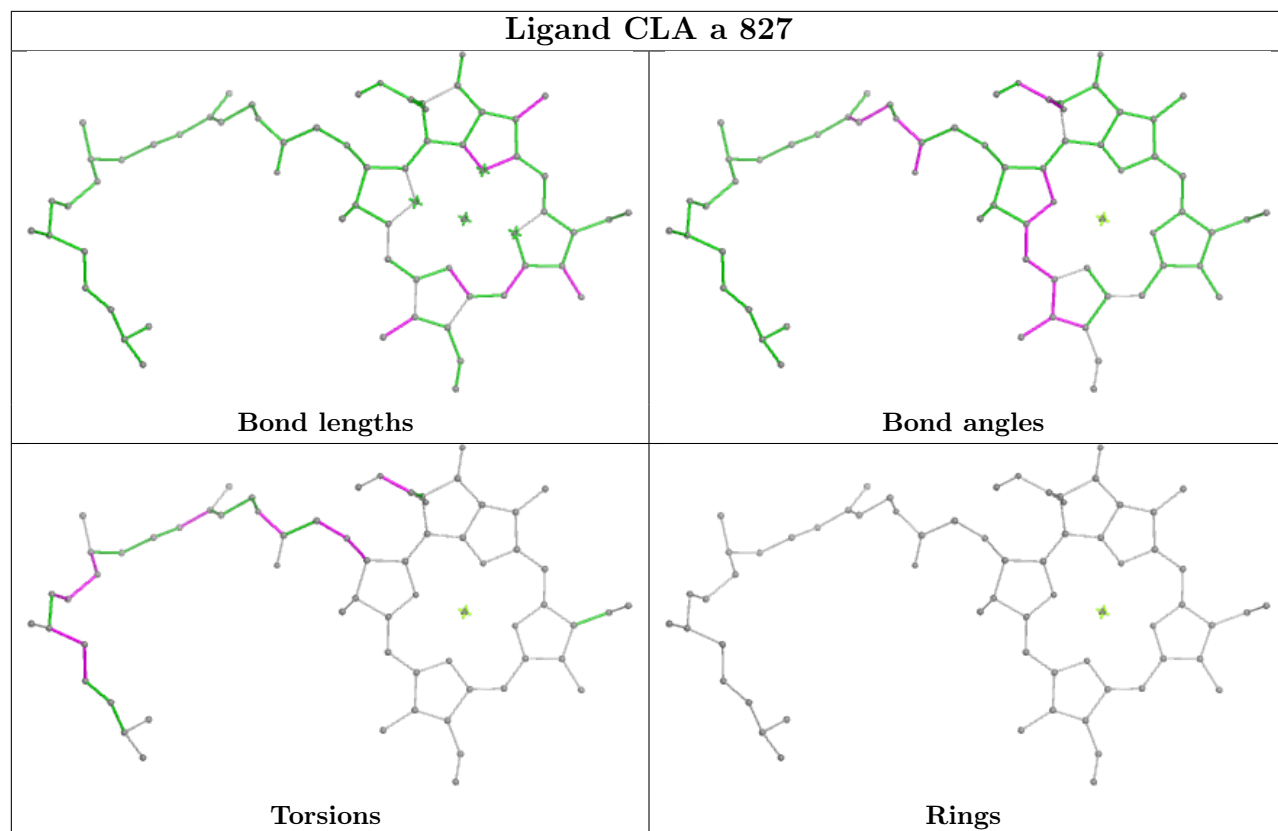


## Ligand CLA a 842

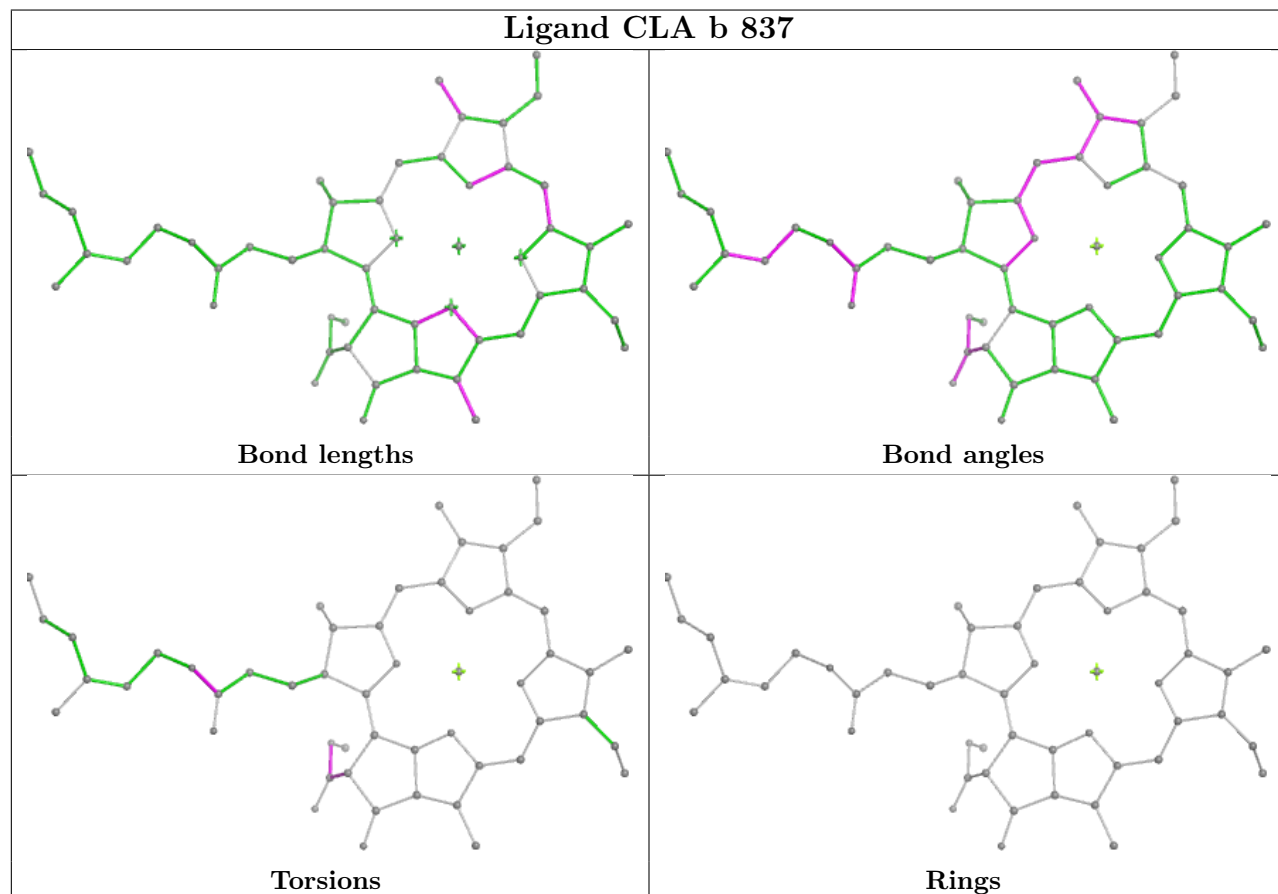




## Ligand CLA a 827



## Ligand CLA b 837



## 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.

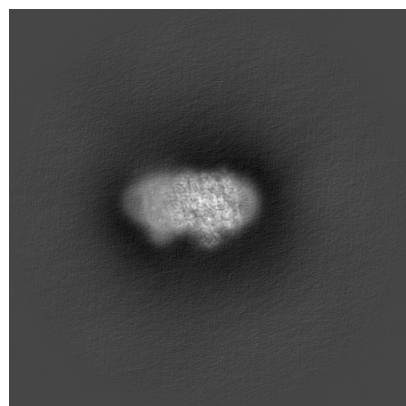
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15621. These allow visual inspection of the internal detail of the map and identification of artifacts.

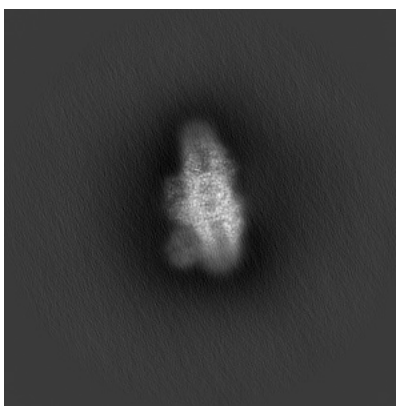
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

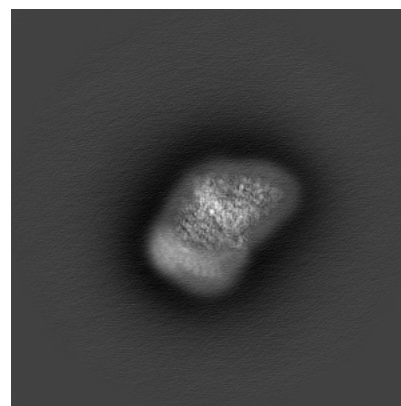
#### 6.1.1 Primary map



X

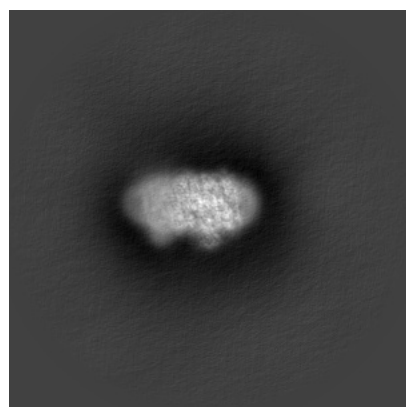


Y

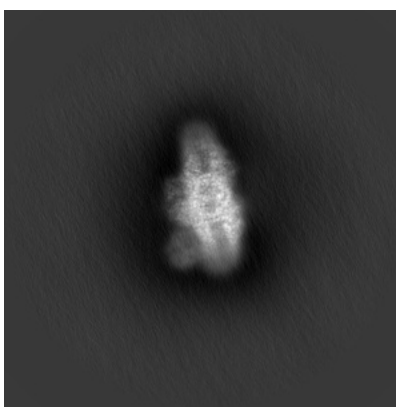


Z

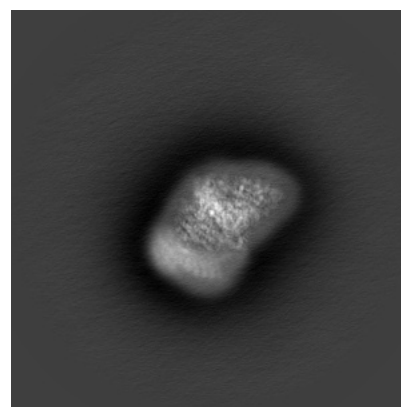
#### 6.1.2 Raw map



X



Y

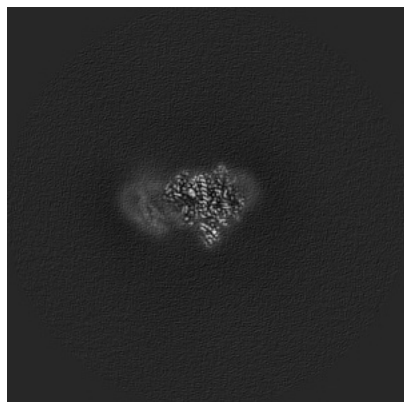


Z

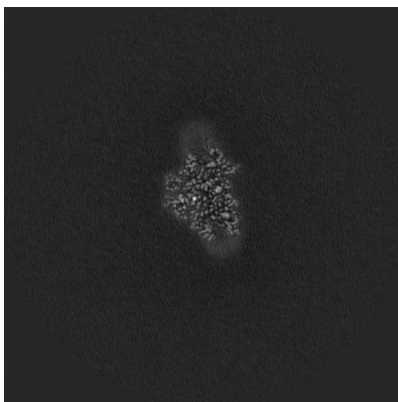
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

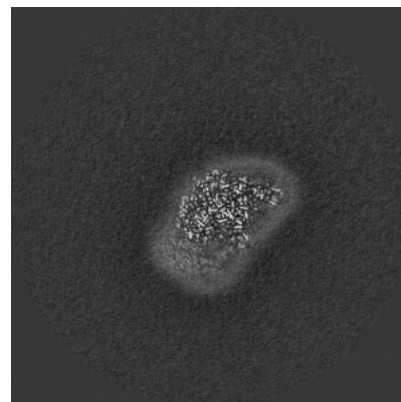
### 6.2.1 Primary map



X Index: 200

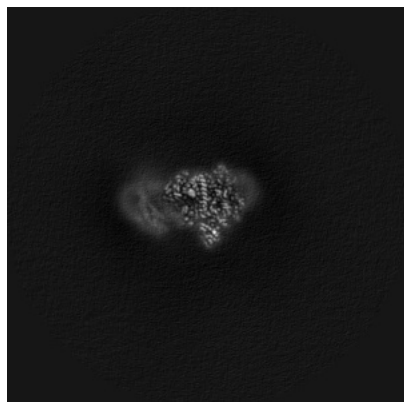


Y Index: 200

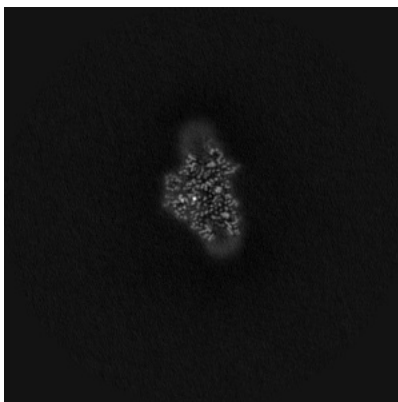


Z Index: 200

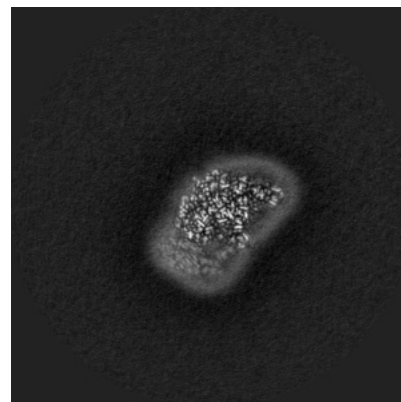
### 6.2.2 Raw map



X Index: 200



Y Index: 200

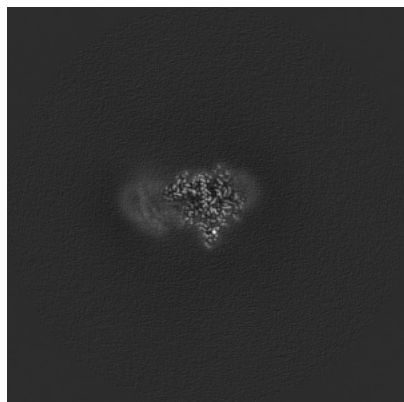


Z Index: 200

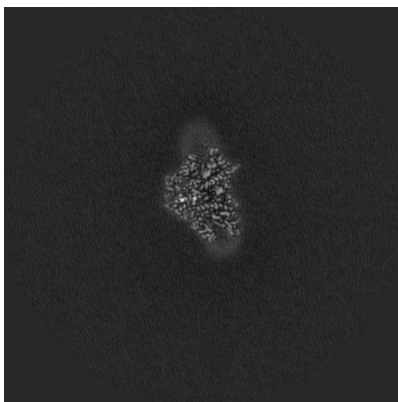
The images above show central slices of the map in three orthogonal directions.

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

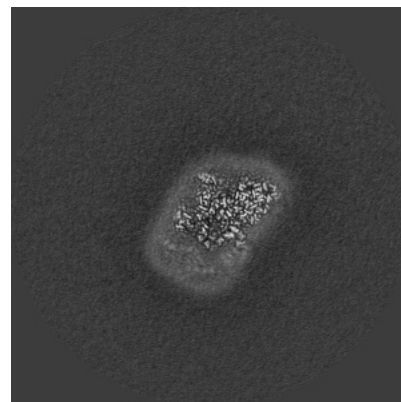
### 6.3.1 Primary map



X Index: 201

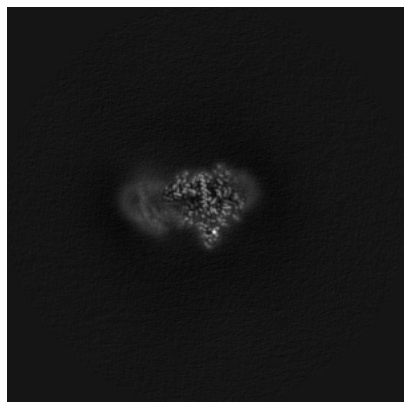


Y Index: 199

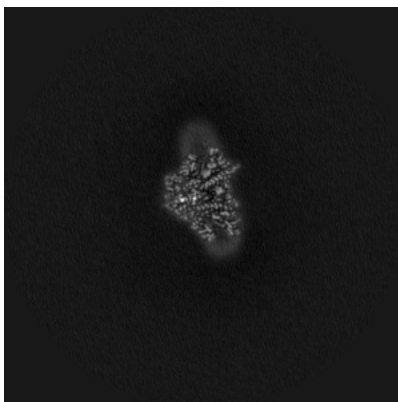


Z Index: 209

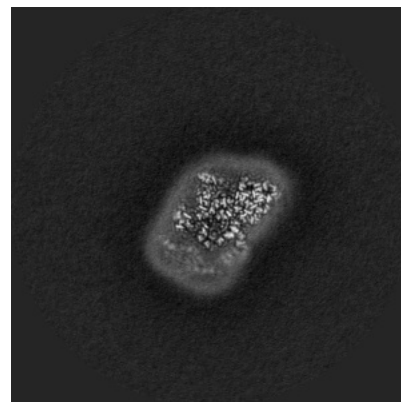
### 6.3.2 Raw map



X Index: 201



Y Index: 199

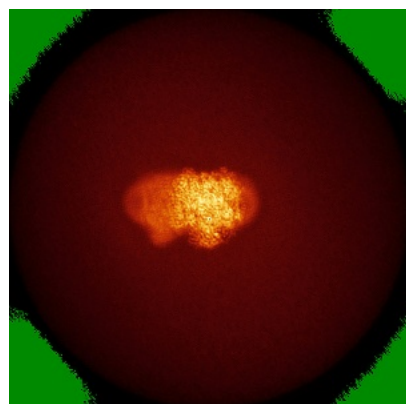


Z Index: 209

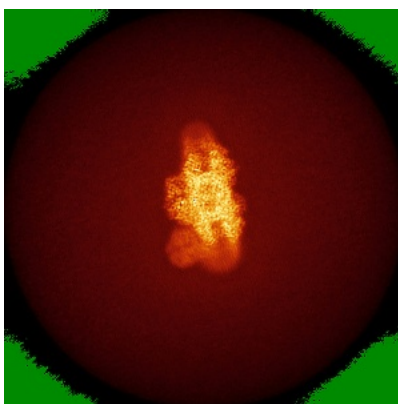
The images above show the largest variance slices of the map in three orthogonal directions.

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

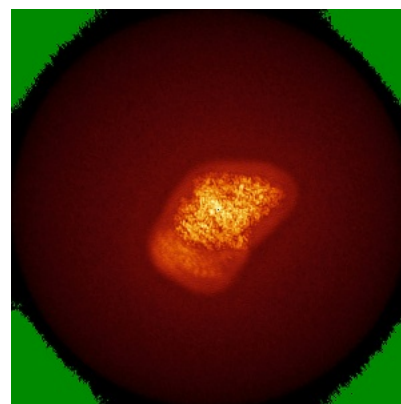
### 6.4.1 Primary map



X

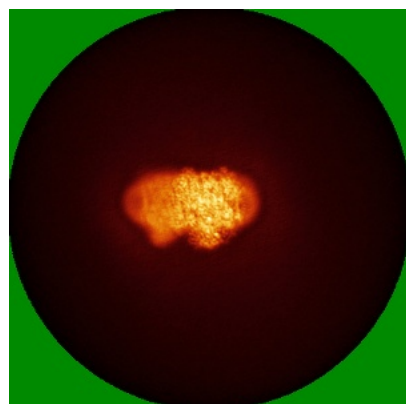


Y

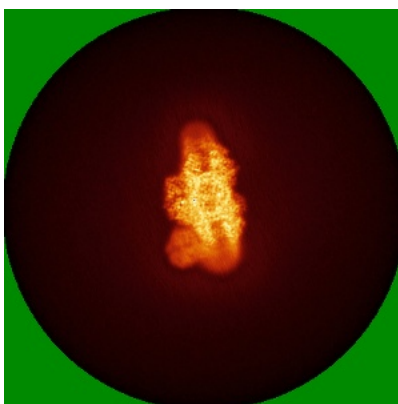


Z

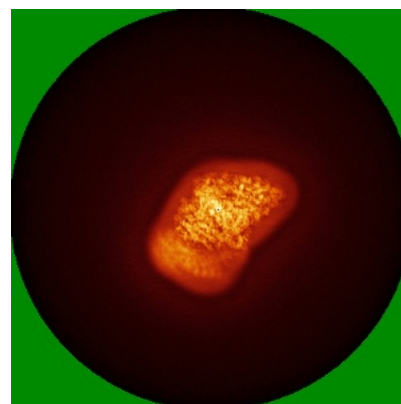
### 6.4.2 Raw map



X



Y



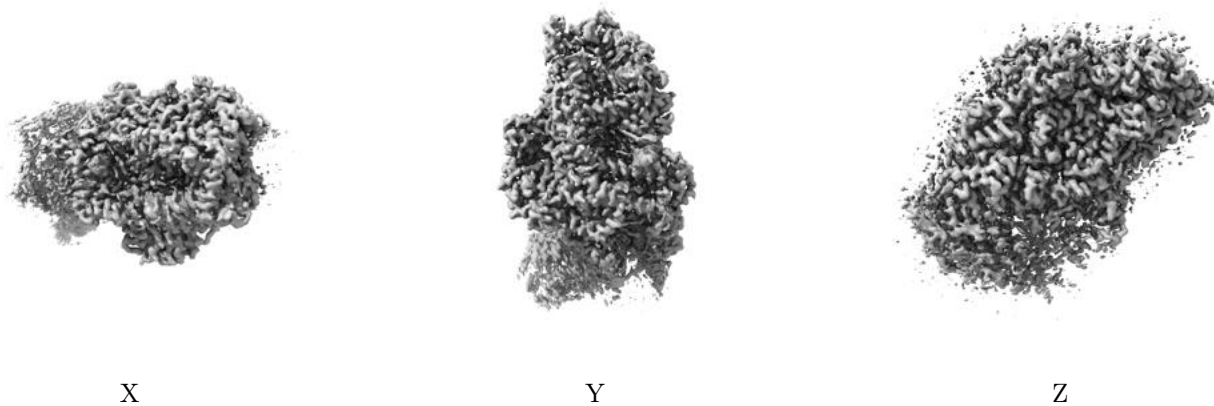
Z

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.



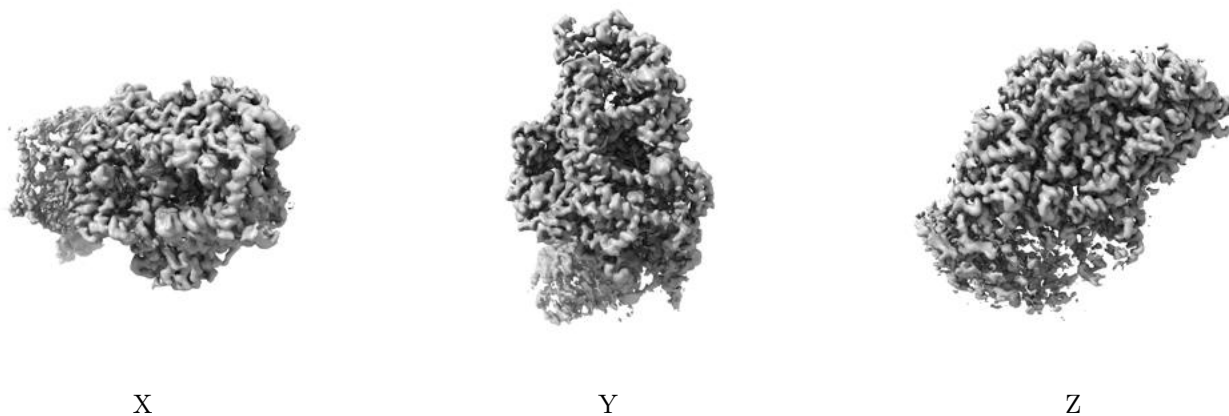
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

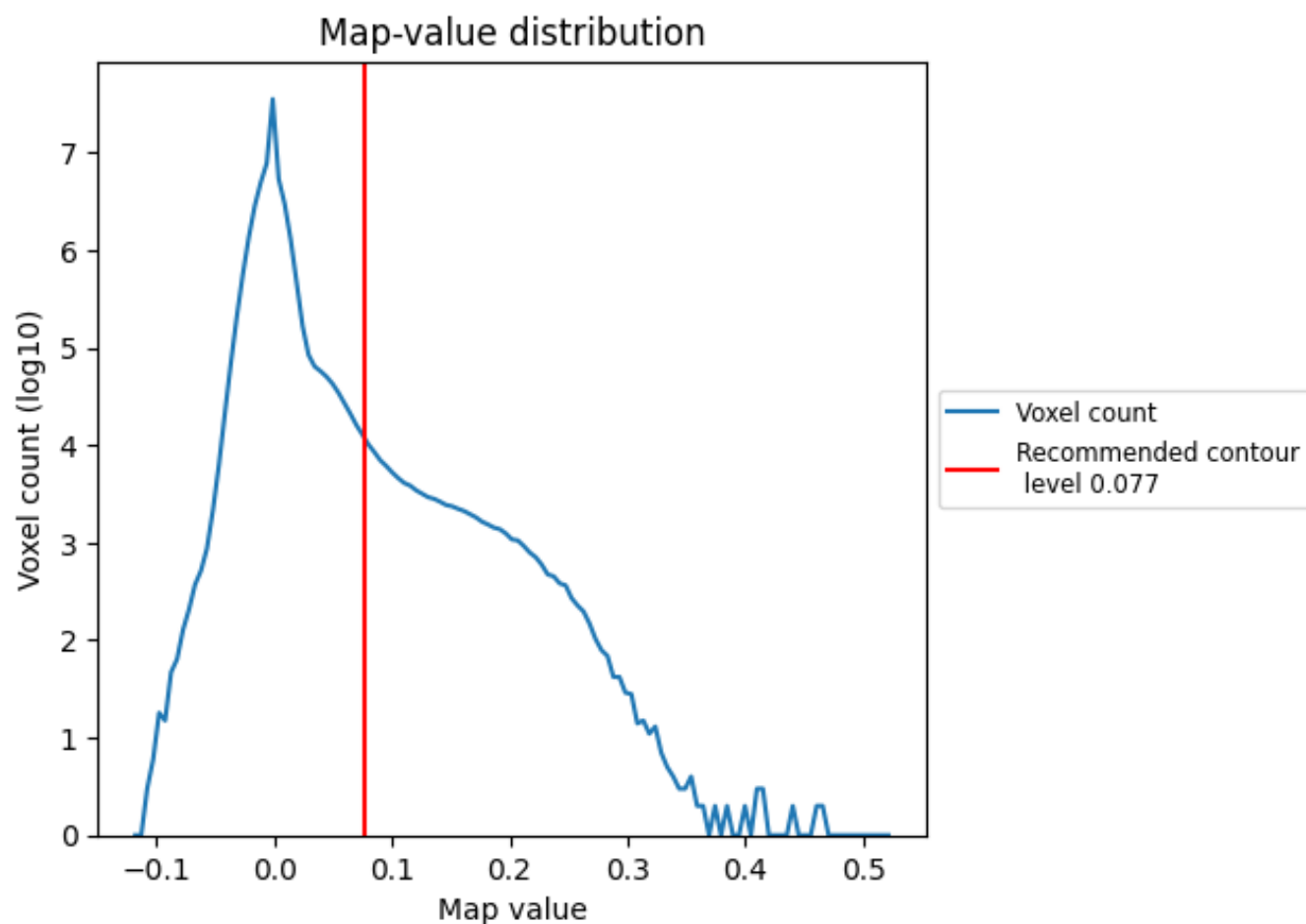
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

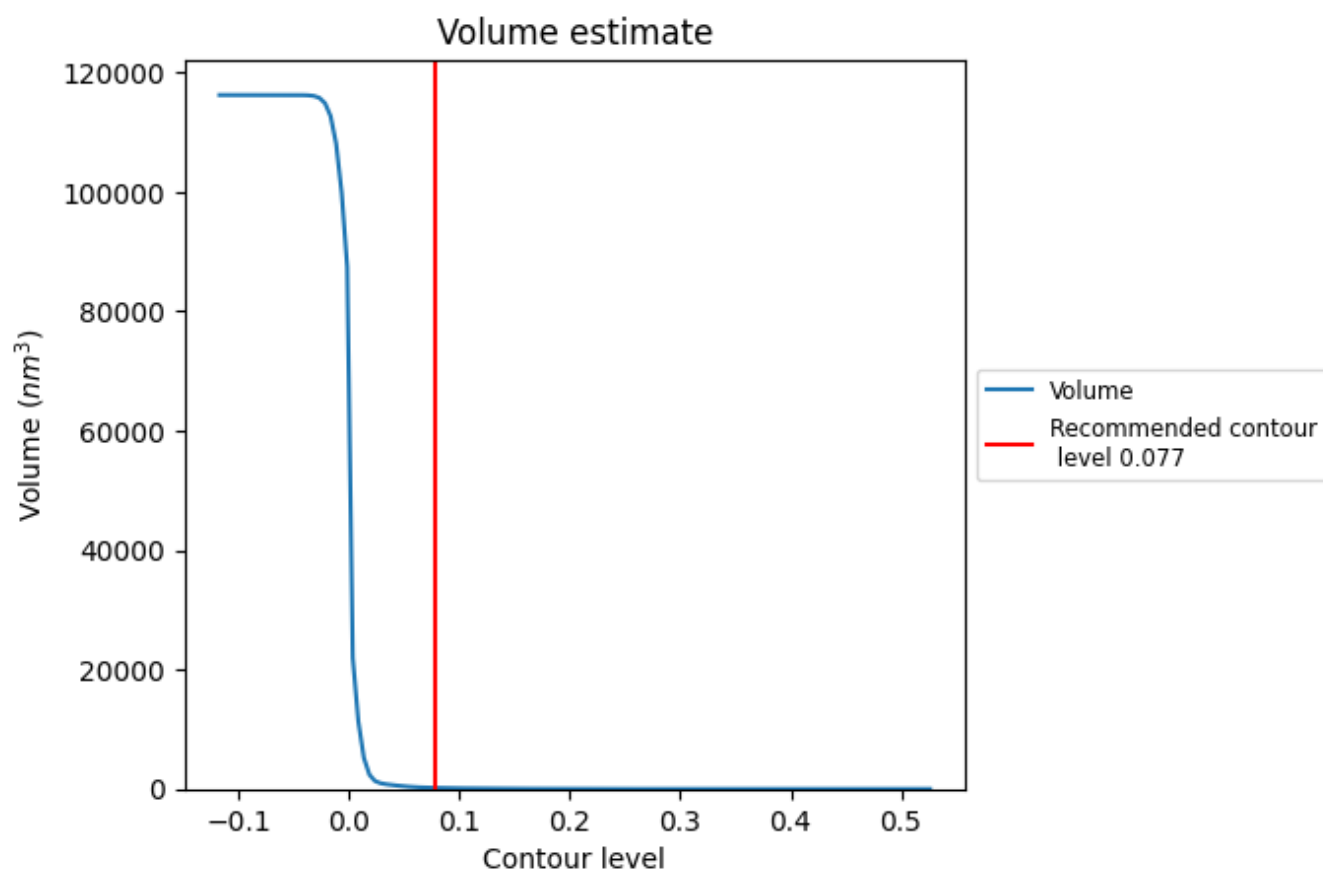
This section contains the results of statistical analysis of the map.

### 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.

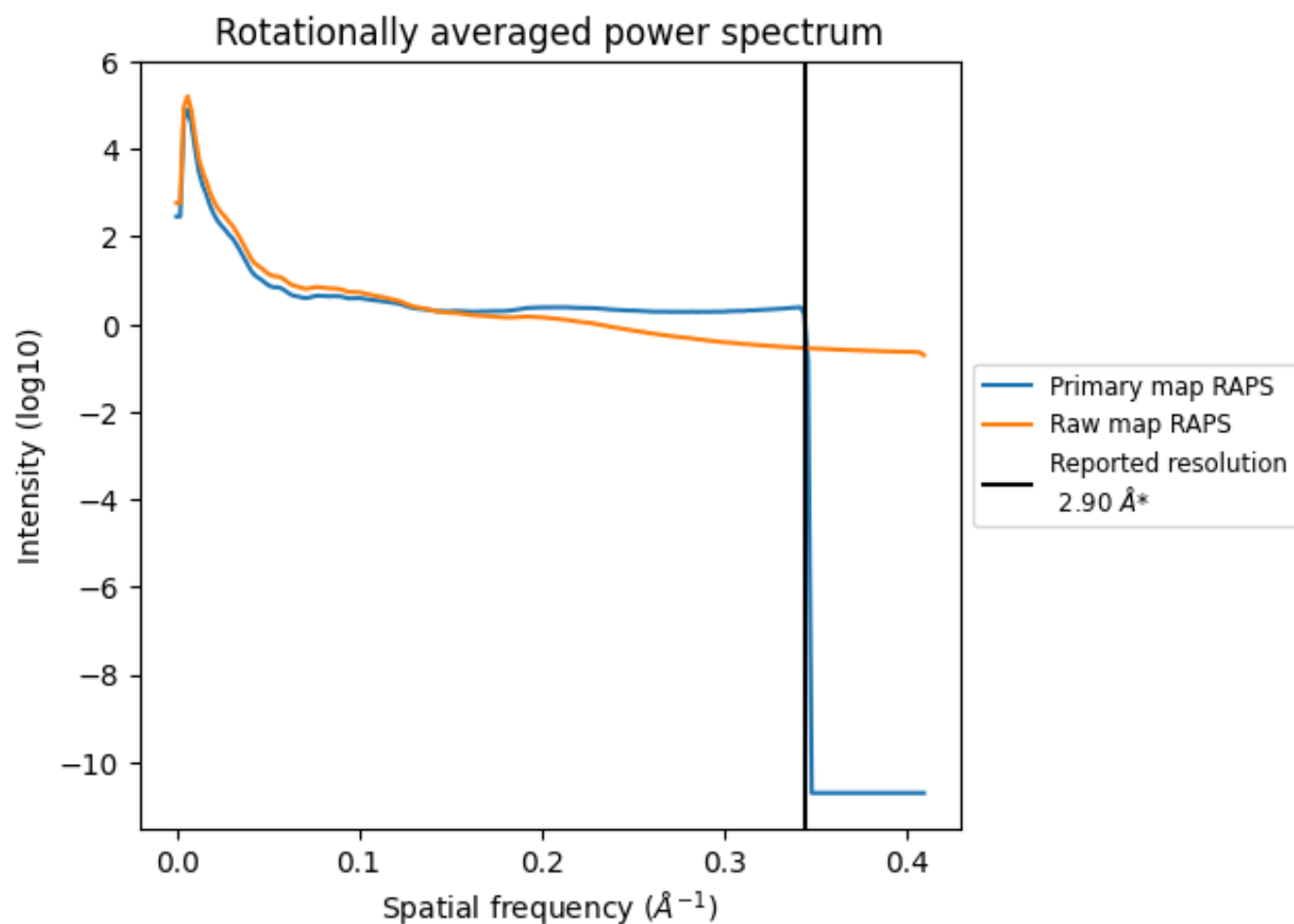
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm<sup>3</sup>; this corresponds to an approximate mass of 165 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 ⓘ

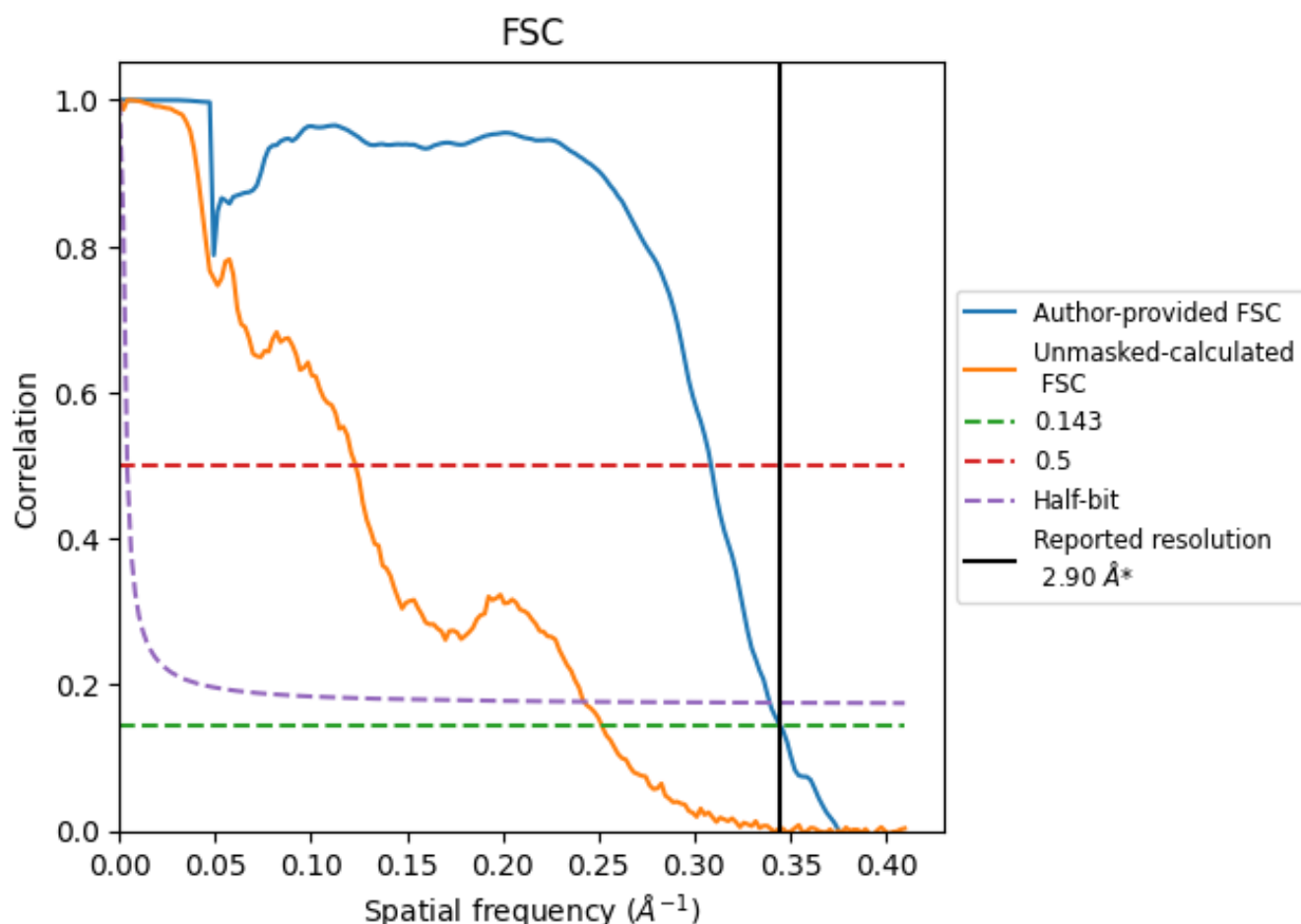


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

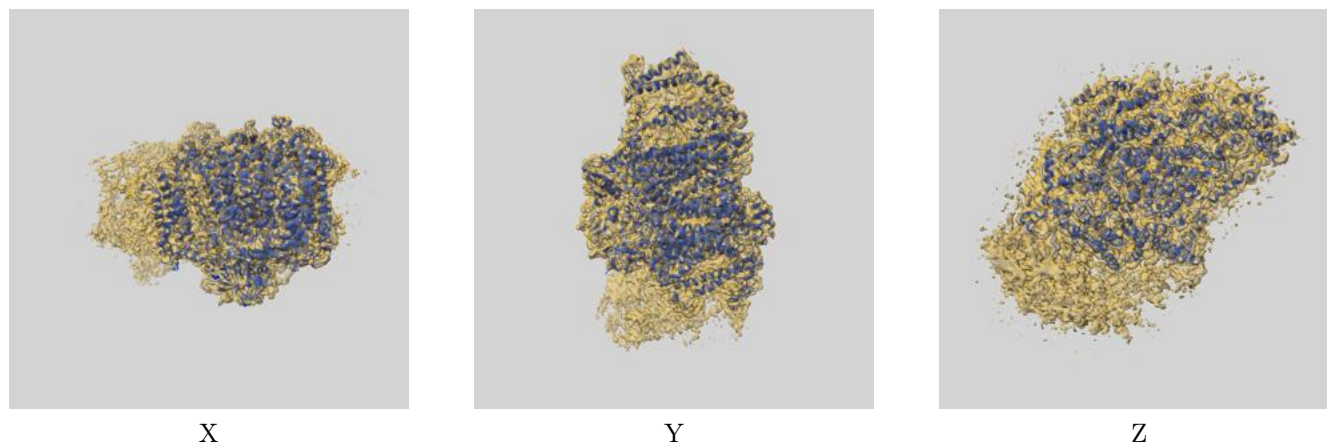
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.24	2.95
Unmasked-calculated*	3.97	8.12	4.13

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 2.9 by more than 10 %

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

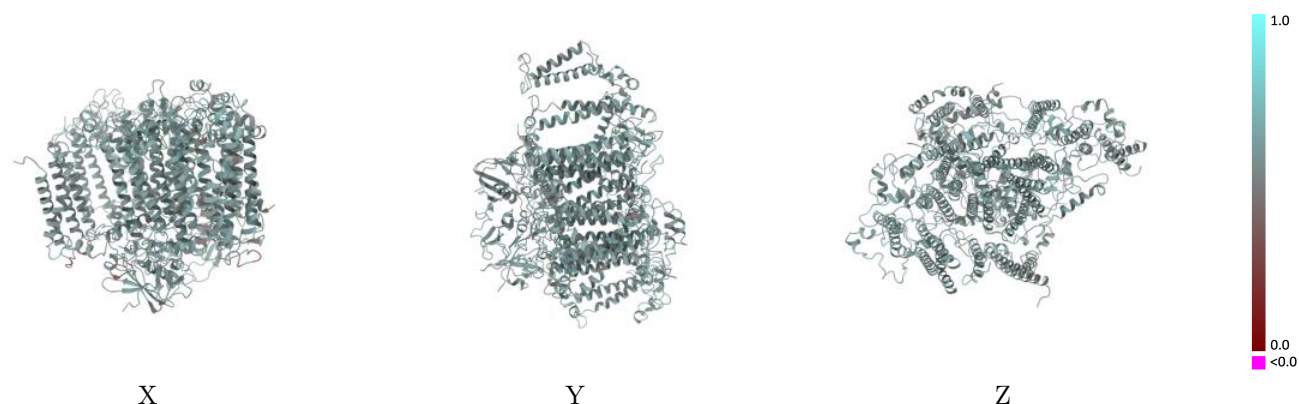
This section contains information regarding the fit between EMDB map EMD-15621 and PDB model 8ASP. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

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



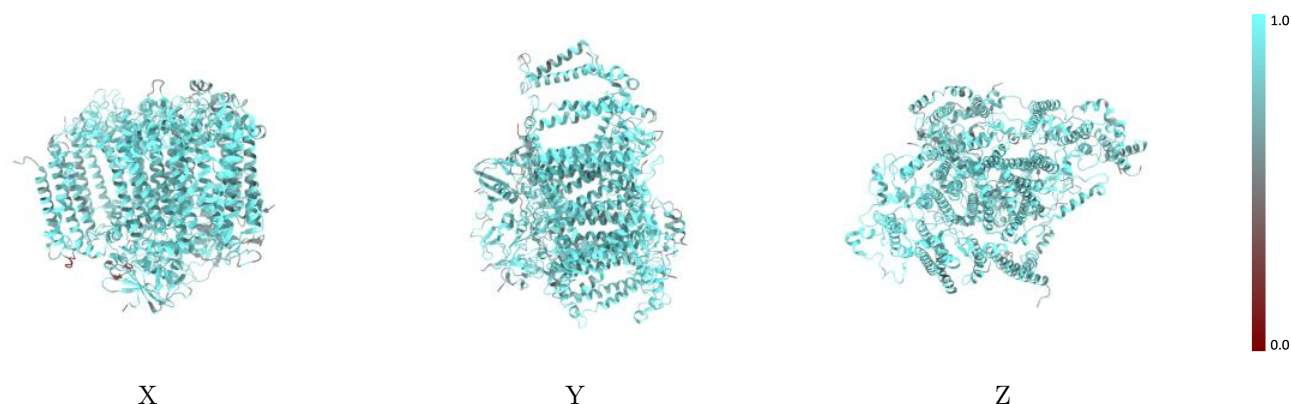
The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

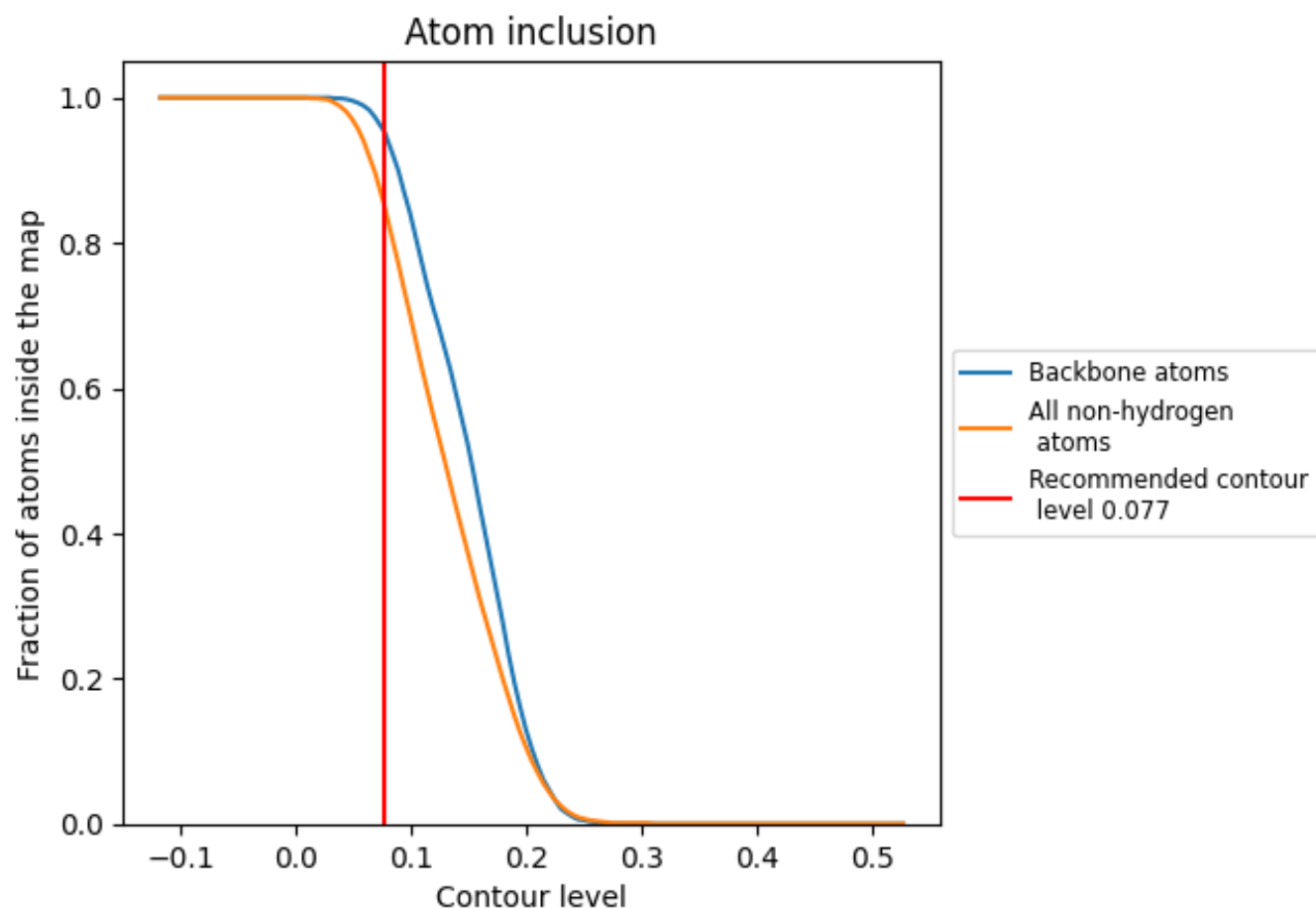
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.077).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8490	<div><div></div></div> 0.5710
a	<div><div></div></div> 0.8670	<div><div></div></div> 0.5810
b	<div><div></div></div> 0.8770	<div><div></div></div> 0.5800
c	<div><div></div></div> 0.9450	<div><div></div></div> 0.5740
d	<div><div></div></div> 0.8630	<div><div></div></div> 0.5670
e	<div><div></div></div> 0.8160	<div><div></div></div> 0.5560
f	<div><div></div></div> 0.7640	<div><div></div></div> 0.5490
i	<div><div></div></div> 0.8350	<div><div></div></div> 0.5750
j	<div><div></div></div> 0.6760	<div><div></div></div> 0.5200
k	<div><div></div></div> 0.7140	<div><div></div></div> 0.5370
l	<div><div></div></div> 0.7420	<div><div></div></div> 0.5220
m	<div><div></div></div> 0.7970	<div><div></div></div> 0.5590

1.0

0.0

<0.0