



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 06:21 pm BST

PDB ID : 8AM5  
EMDB ID : EMD-15522  
Title : RCII/PSI complex, class 3  
Authors : Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.;  
Sazanov, L.A.; Komenda, J.  
Deposited on : 2022-08-02  
Resolution : 3.10 Å (reported)  
Based on initial models : 2XBG, 6WJ6, 5OY0

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

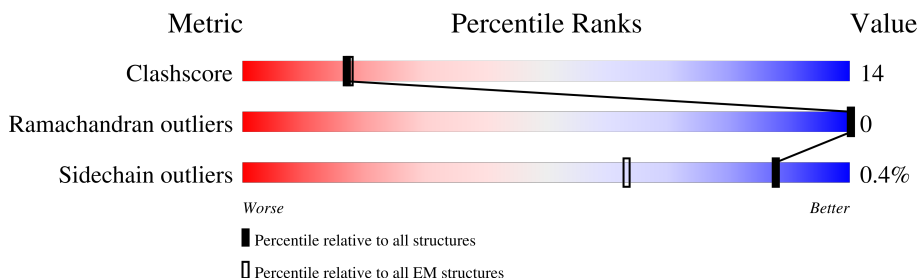
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.



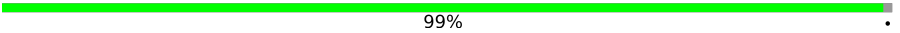
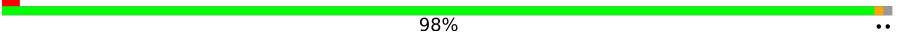


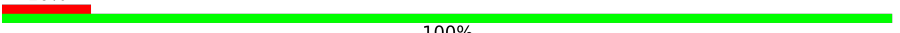
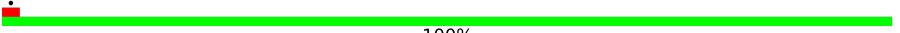



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	344	<div> <div>12%</div> <div>67%</div> <div>17%</div> <div>16%</div> </div>
2	D	336	<div> <div>34%</div> <div>63%</div> <div>19%</div> <div>17%</div> </div>
3	E	81	<div> <div>25%</div> <div>35%</div> <div>11%</div> <div>54%</div> </div>
4	F	44	<div> <div>43%</div> <div>41%</div> <div>23%</div> <div>36%</div> </div>
5	I	38	<div> <div>26%</div> <div>53%</div> <div>21%</div> <div>•</div> <div>24%</div> </div>
6	S	342	<div> <div>34%</div> <div>63%</div> <div>25%</div> <div>11%</div> </div>
7	a	751	<div> <div>•</div> <div>99%</div> <div>•</div> </div>
8	b	731	<div> <div>99%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	c	81	
10	d	141	
11	e	74	
12	f	165	
13	i	40	
14	j	40	
15	k	86	
16	l	157	
17	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
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	A	407	X	-	-	-
19	CLA	D	402	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	838	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	843	X	-	-	-
19	CLA	a	856	X	-	-	-
19	CLA	a	857	X	-	-	-
19	CLA	a	860	X	-	-	-
19	CLA	b	801	X	-	-	-
19	CLA	b	802	X	-	-	-
19	CLA	b	803	X	-	-	-
19	CLA	b	804	X	-	-	-
19	CLA	b	805	X	-	-	-
19	CLA	b	806	X	-	-	-
19	CLA	b	807	X	-	-	-
19	CLA	b	808	X	-	-	-
19	CLA	b	809	X	-	-	-
19	CLA	b	810	X	-	-	-
19	CLA	b	811	X	-	-	-
19	CLA	b	812	X	-	-	-
19	CLA	b	813	X	-	-	-
19	CLA	b	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	815	X	-	-	-
19	CLA	b	816	X	-	-	-
19	CLA	b	817	X	-	-	-
19	CLA	b	818	X	-	-	-
19	CLA	b	819	X	-	-	-
19	CLA	b	820	X	-	-	-
19	CLA	b	821	X	-	-	-
19	CLA	b	822	X	-	-	-
19	CLA	b	823	X	-	-	-
19	CLA	b	824	X	-	-	-
19	CLA	b	825	X	-	-	-
19	CLA	b	826	X	-	-	-
19	CLA	b	827	X	-	-	-
19	CLA	b	828	X	-	-	-
19	CLA	b	829	X	-	-	-
19	CLA	b	830	X	-	-	-
19	CLA	b	831	X	-	-	-
19	CLA	b	832	X	-	-	-
19	CLA	b	833	X	-	-	-
19	CLA	b	834	X	-	-	-
19	CLA	b	835	X	-	-	-
19	CLA	b	836	X	-	-	-
19	CLA	b	837	X	-	-	-
19	CLA	b	838	X	-	-	-
19	CLA	b	839	X	-	-	-
19	CLA	b	840	X	-	-	-
19	CLA	f	201	X	-	-	-
19	CLA	f	203	X	-	-	-
19	CLA	f	204	X	-	-	-
19	CLA	j	103	X	-	-	-
19	CLA	j	104	X	-	-	-
19	CLA	k	101	X	-	-	-
19	CLA	k	102	X	-	-	-
19	CLA	l	202	X	-	-	-
19	CLA	l	203	X	-	-	-
19	CLA	l	204	X	-	-	-
23	CL0	a	801	X	-	-	-

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 32746 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 II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	290	Total	C	N	O	S	0	0
			2256	1484	367	390	15		

- Molecule 2 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	278	Total	C	N	O	S	0	0
			2188	1465	351	360	12		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	initiating methionine	UNP P09192
D	-4	HIS	-	expression tag	UNP P09192
D	-3	HIS	-	expression tag	UNP P09192
D	-2	HIS	-	expression tag	UNP P09192
D	-1	HIS	-	expression tag	UNP P09192
D	0	HIS	-	expression tag	UNP P09192
D	1	HIS	-	expression tag	UNP P09192

- Molecule 3 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	37	Total	C	N	O	S	0	0
			301	206	44	50	1		

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	28	Total	C	N	O	S	0	0
			222	149	39	33	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	29	Total	C	N	O	0	0
			229	159	33	37		

- Molecule 6 is a protein called Photosystem II assembly lipoprotein Ycf48.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	303	Total	C	N	O	S	0	0
			2328	1481	393	451	3		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	741	Total	C	N	O	S	0	0
			5795	3797	984	987	27		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

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

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

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

- Molecule 12 is a protein called Photosystem I reaction center subunit III.

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

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

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

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

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

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	75	Total	C	N	O	S	0	0
			524	343	87	90	4		

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

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

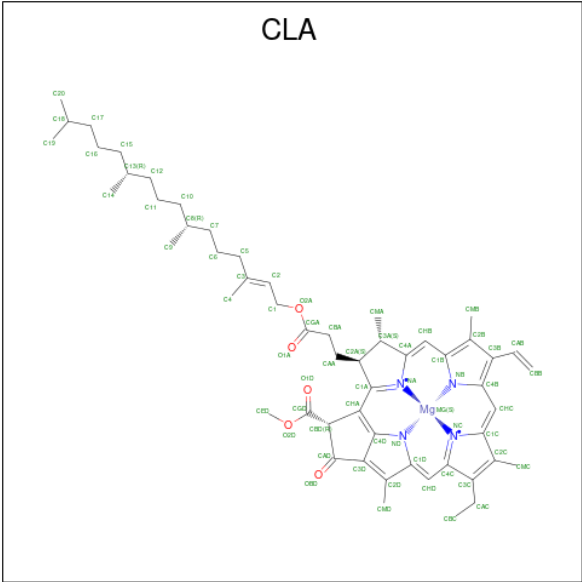
- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 18 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	

- Molecule 19 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
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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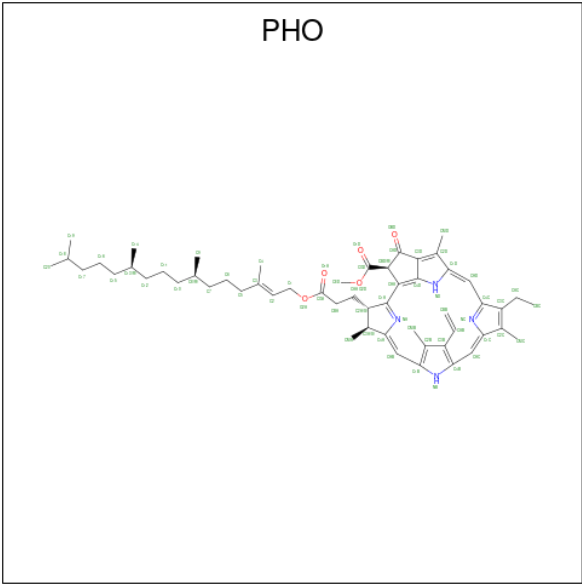
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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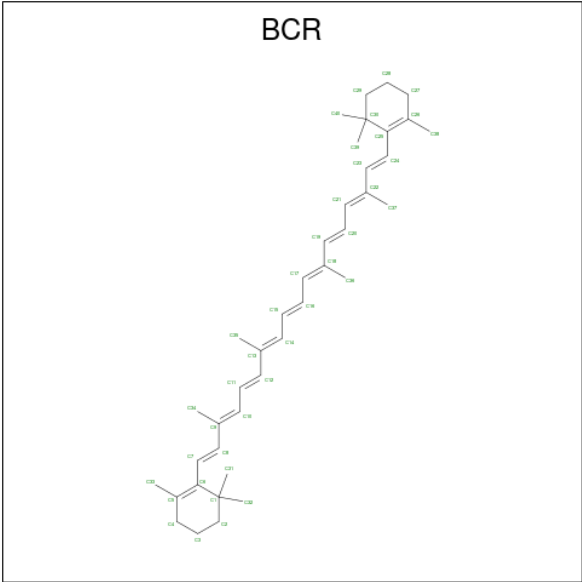
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 20 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	N	O	0
			64	55	4	5	
20	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



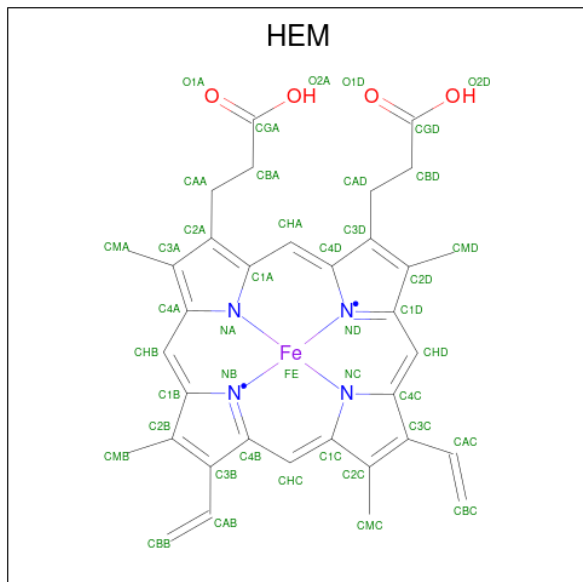
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			25	25	
21	a	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	f	1	Total	C	0
			40	40	

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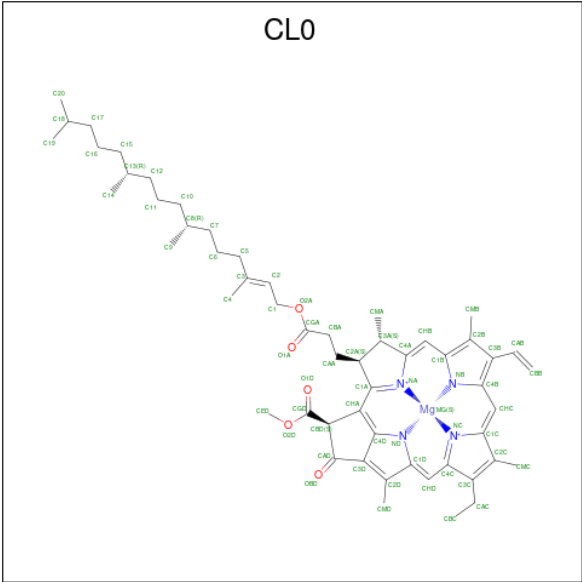
Mol	Chain	Residues	Atoms	AltConf
21	i	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0

- Molecule 22 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



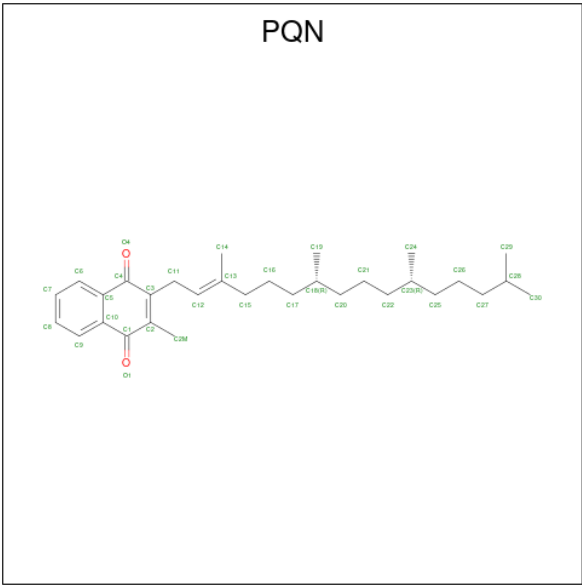
Mol	Chain	Residues	Atoms	AltConf
22	E	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 23 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



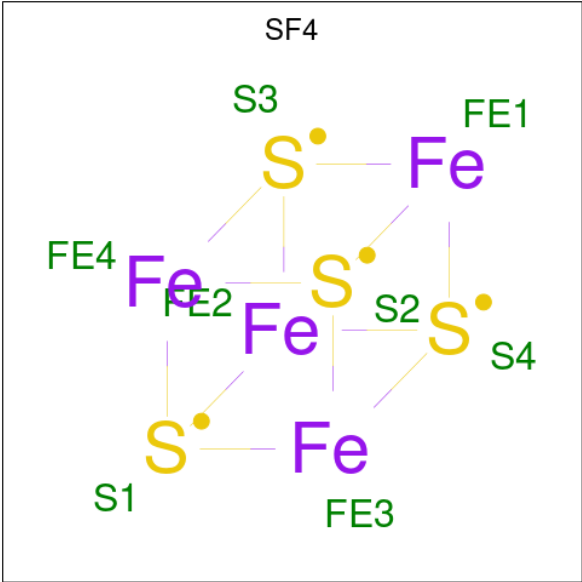
Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 24 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



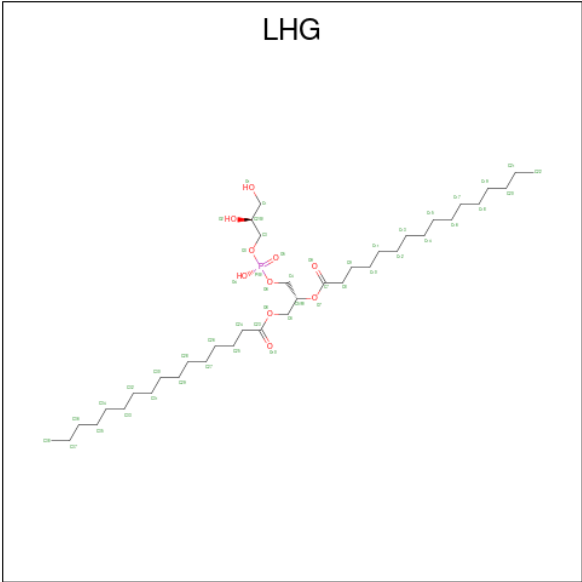
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			33	31	2	
24	b	1	Total	C	O	0
			33	31	2	

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



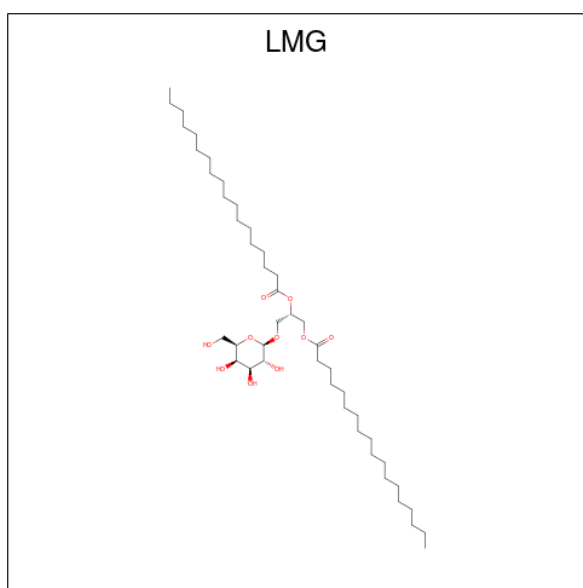
Mol	Chain	Residues	Atoms			AltConf
25	a	1	Total	Fe	S	0
			8	4	4	
25	c	1	Total	Fe	S	0
			8	4	4	
25	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



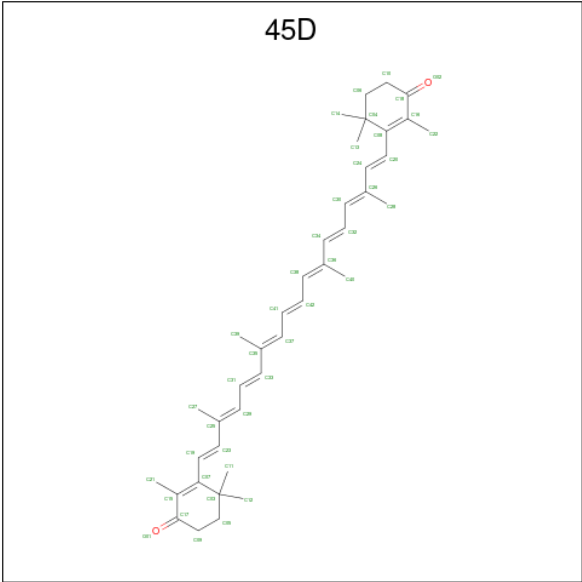
Mol	Chain	Residues	Atoms				AltConf
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			38	27	10	1	
26	f	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



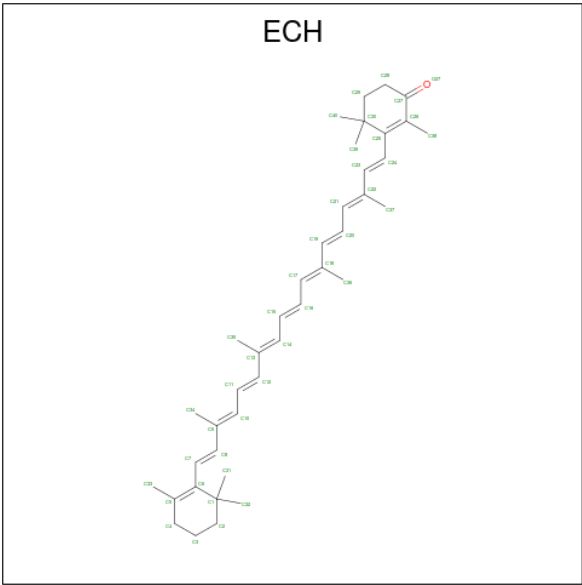
Mol	Chain	Residues	Atoms			AltConf
27	a	1	Total	C	O	0
			40	30	10	
27	b	1	Total	C	O	0
			55	45	10	
27	b	1	Total	C	O	0
			55	45	10	
27	l	1	Total	C	O	0
			50	40	10	

- Molecule 28 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula:  $C_{40}H_{52}O_2$ ).



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

- Molecule 29 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C<sub>40</sub>H<sub>54</sub>O).

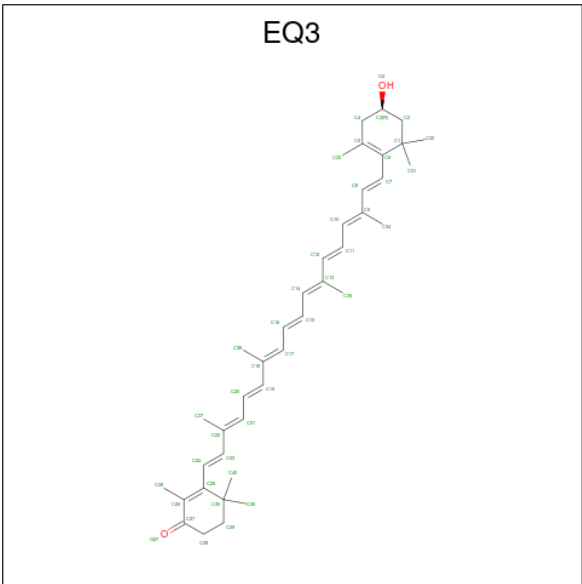


Mol	Chain	Residues	Atoms			AltConf
29	b	1	Total	C	O	0
			41	40	1	
29	m	1	Total	C	O	0
			41	40	1	

- Molecule 30 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula:

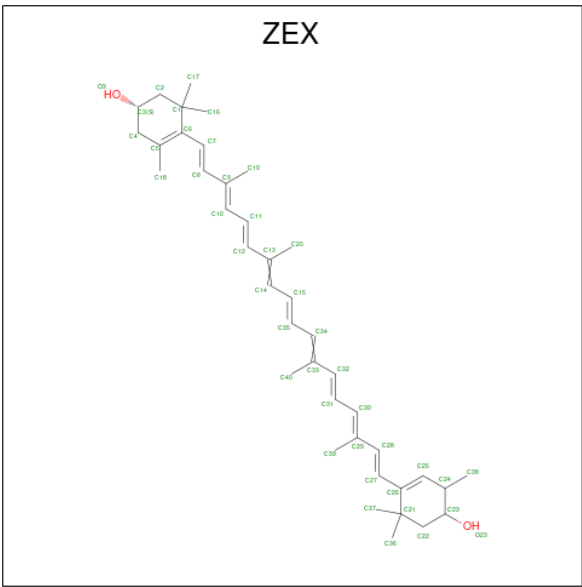


C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>).



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

- Molecule 31 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>).



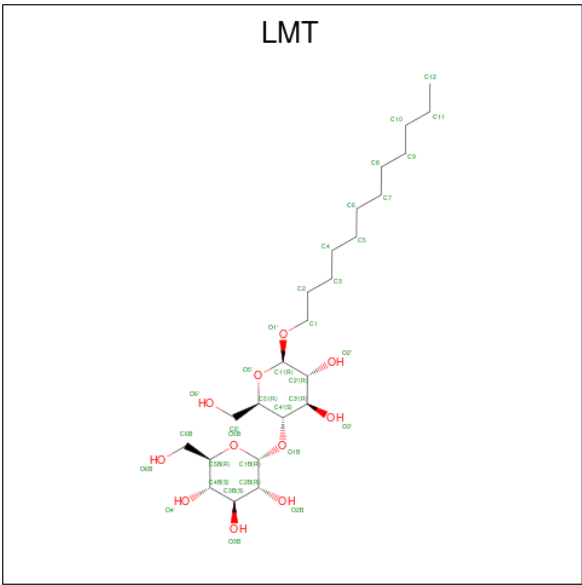
Mol	Chain	Residues	Atoms			AltConf
31	b	1	Total	C	O	0
			42	40	2	

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

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).

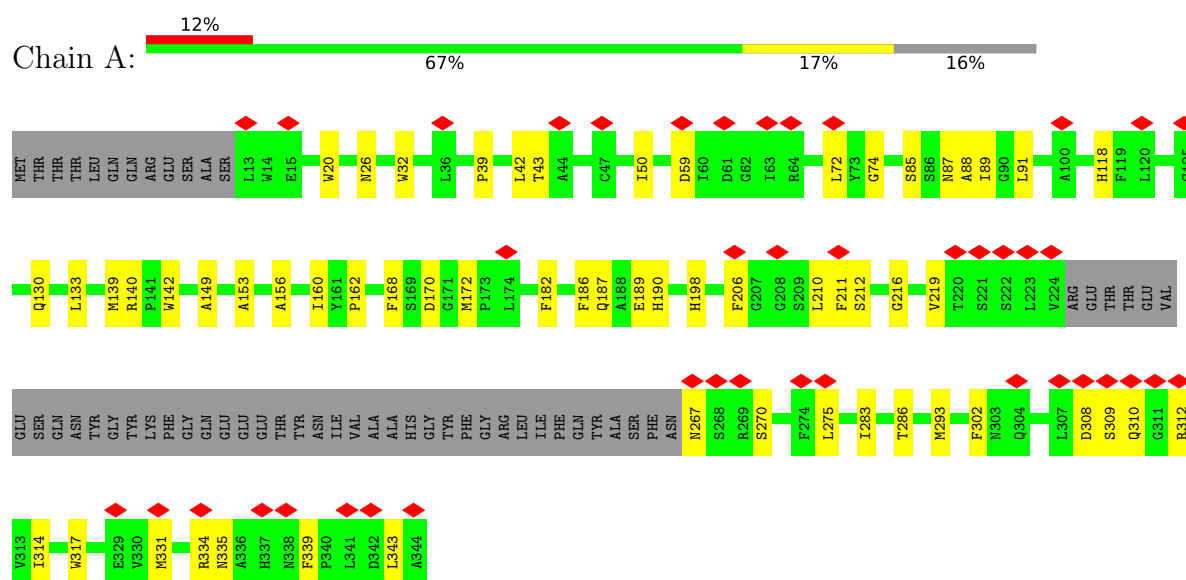


Mol	Chain	Residues	Atoms			AltConf
32	j	1	Total	C	O	0
			35	24	11	

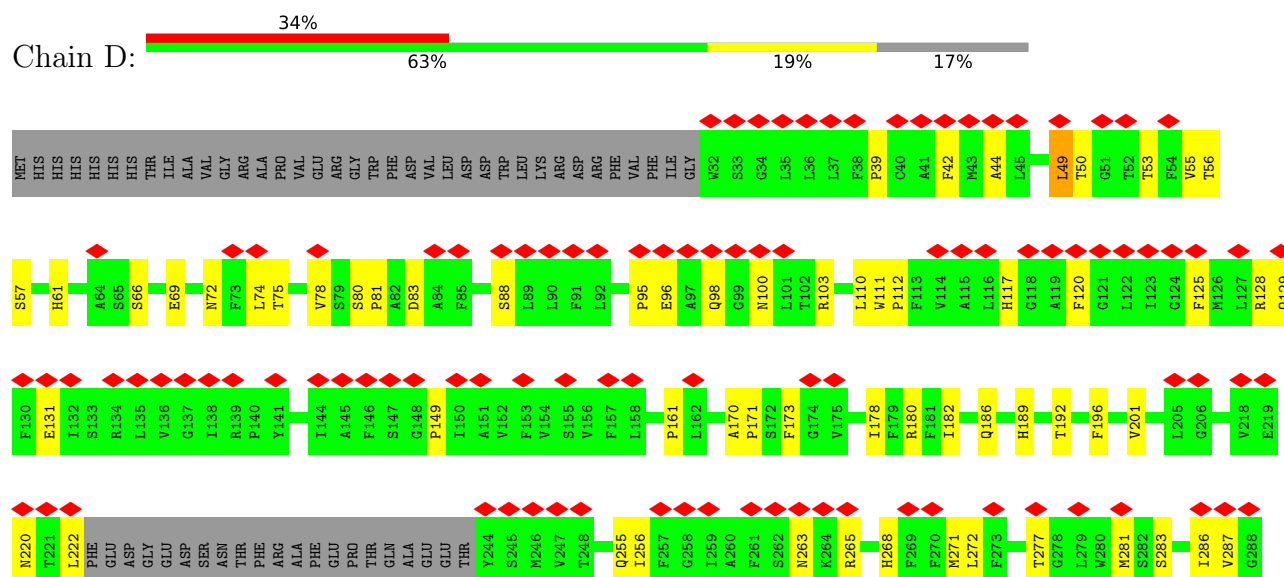
### 3 Residue-property plots [i](#)

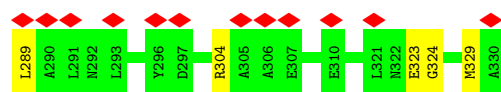
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 II protein D1 2

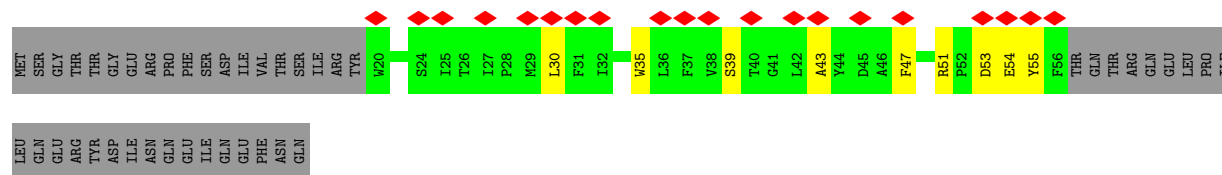
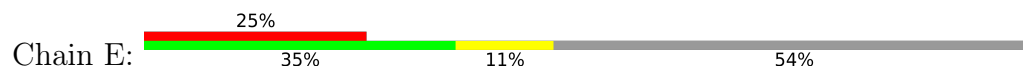


#### • Molecule 2: Photosystem II D2 protein

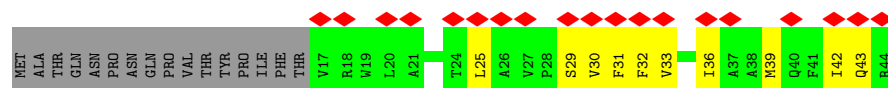




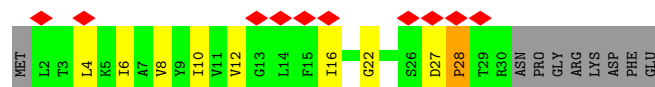
• Molecule 3: Cytochrome b559 subunit alpha



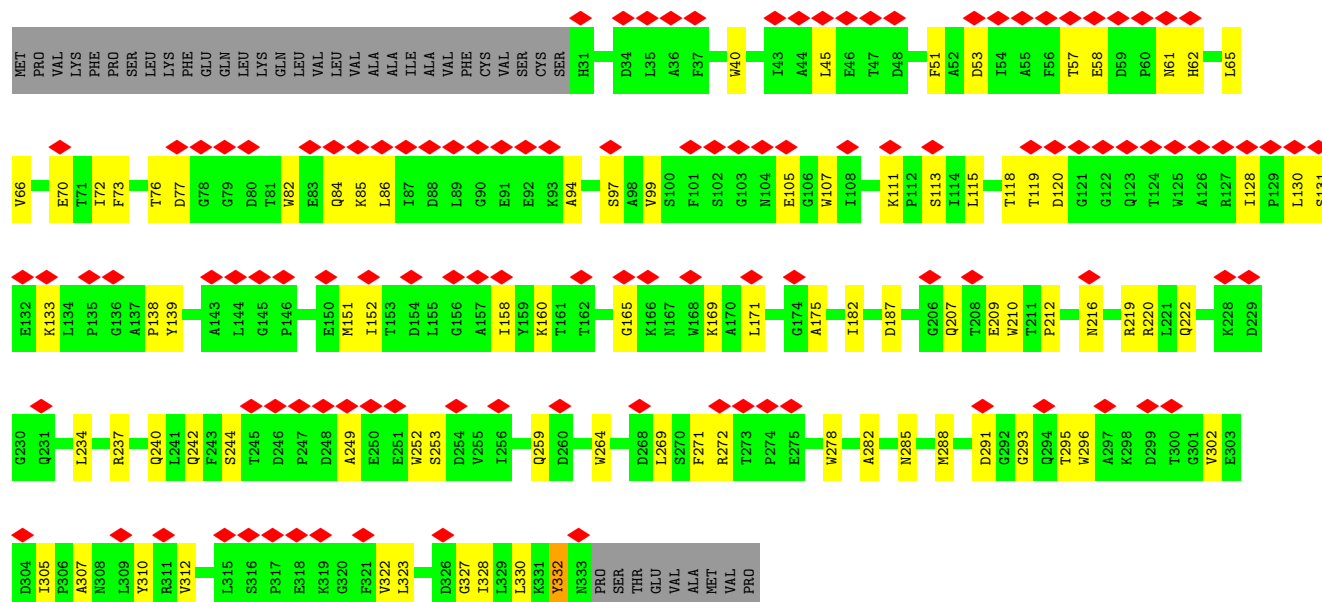
• Molecule 4: Cytochrome b559 subunit beta



• Molecule 5: Photosystem II reaction center protein I

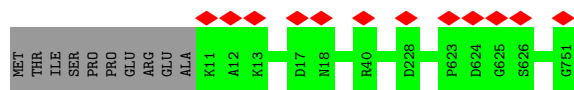


• Molecule 6: Photosystem II assembly lipoprotein Ycf48



- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:  99%



- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  99%



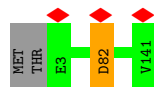
- Molecule 9: Photosystem I iron-sulfur center

Chain c:  99%



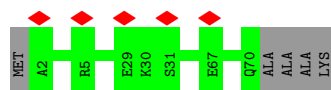
- Molecule 10: Photosystem I reaction center subunit II

Chain d:  98%




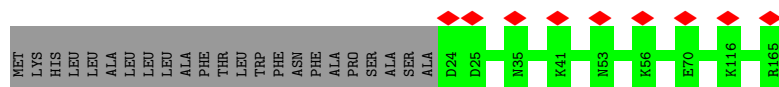
- Molecule 11: Photosystem I reaction center subunit IV

Chain e:  7%



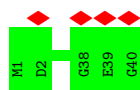
- Molecule 12: Photosystem I reaction center subunit III

Chain f:  5%



- Molecule 13: Photosystem I reaction center subunit VIII

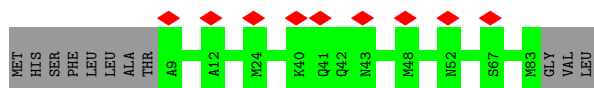
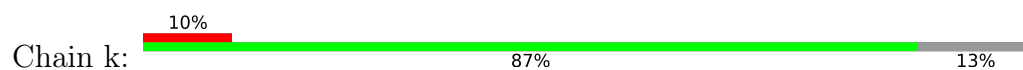
Chain i:  10%



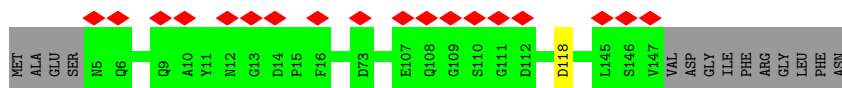
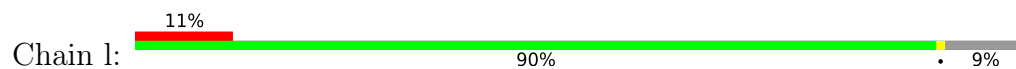
- Molecule 14: Photosystem I reaction center subunit IX



- Molecule 15: Photosystem I reaction center subunit PsaK 1



- Molecule 16: Photosystem I reaction center subunit XI



- Molecule 17: 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	0.510	Depositor
Minimum map value	-0.104	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0845	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: PQN, BCR, EQ3, FE2, SF4, CL0, LHG, LMG, ZEX, PHO, LMT, ECH, CLA, 45D, HEM

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	0/2330	0.43	0/3180
2	D	0.26	0/2266	0.46	0/3086
3	E	0.26	0/314	0.40	0/431
4	F	0.27	0/228	0.53	0/309
5	I	0.31	0/234	0.65	1/317 (0.3%)
6	S	0.25	0/2390	0.49	0/3258
7	a	0.27	0/5993	0.43	0/8169
8	b	0.27	0/5981	0.43	0/8178
9	c	0.28	0/610	0.51	0/826
10	d	0.28	0/1111	0.51	1/1497 (0.1%)
11	e	0.28	0/547	0.52	0/741
12	f	0.26	0/1138	0.47	0/1546
13	i	0.28	0/322	0.44	0/438
14	j	0.27	0/328	0.48	0/443
15	k	0.26	0/535	0.47	0/726
16	l	0.27	0/1097	0.44	0/1493
17	m	0.26	0/241	0.42	0/326
All	All	0.27	0/25665	0.45	2/34964 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	28	PRO	CA-N-CD	-6.63	102.22	111.50
10	d	82	ASP	CB-CG-OD2	5.22	123.00	118.30

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	2256	0	2181	57	0
2	D	2188	0	2129	51	0
3	E	301	0	287	7	0
4	F	222	0	230	7	0
5	I	229	0	247	7	0
6	S	2328	0	2227	62	0
7	a	5795	0	5653	0	0
8	b	5770	0	5547	0	0
9	c	600	0	581	0	0
10	d	1087	0	1082	0	0
11	e	538	0	514	0	0
12	f	1108	0	1100	0	0
13	i	311	0	304	0	0
14	j	319	0	328	0	0
15	k	524	0	547	0	0
16	l	1069	0	1044	0	0
17	m	238	0	260	0	0
18	A	1	0	0	0	0
19	A	226	0	216	20	0
19	D	101	0	82	12	0
19	a	2811	0	2986	0	0
19	b	2410	0	2456	0	0
19	f	165	0	150	0	0
19	j	101	0	82	0	0
19	k	91	0	66	0	0
19	l	167	0	154	0	0
20	A	64	0	74	5	0
20	D	64	0	74	3	0
21	A	40	0	56	6	0
21	a	265	0	369	0	0
21	b	200	0	280	0	0
21	f	40	0	56	0	0
21	i	80	0	112	0	0
21	j	40	0	56	0	0
21	k	40	0	56	0	0
21	l	40	0	56	0	0
22	E	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	65	0	72	0	0
24	a	33	0	46	0	0
24	b	33	0	46	0	0
25	a	8	0	0	0	0
25	c	16	0	0	0	0
26	a	147	0	222	0	0
26	b	38	0	49	0	0
26	f	49	0	74	0	0
27	a	40	0	50	0	0
27	b	110	0	172	0	0
27	l	50	0	73	0	0
28	a	42	0	52	0	0
29	b	41	0	54	0	0
29	m	41	0	54	0	0
30	b	42	0	0	0	0
31	b	42	0	56	0	0
31	f	42	0	56	0	0
32	j	35	0	45	0	0
All	All	32746	0	32793	184	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 14.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:GLN:HB2	19:D:402:CLA:HBC1	1.59	0.83
6:S:322:VAL:HB	6:S:330:LEU:HB2	1.67	0.76
1:A:211:PHE:HB3	1:A:275:LEU:HD13	1.72	0.71
6:S:113:SER:HB3	6:S:130:LEU:HD12	1.75	0.68
20:D:401:PHO:HAB	19:D:402:CLA:H11	1.76	0.68
4:F:29:SER:O	4:F:33:VAL:HG23	1.93	0.68
2:D:161:PRO:HB3	2:D:170:ALA:HB2	1.76	0.67
2:D:78:VAL:HB	2:D:173:PHE:HB2	1.78	0.64
1:A:334:ARG:HG3	1:A:335:ASN:H	1.63	0.63
19:A:403:CLA:HAB	19:D:402:CLA:H72	1.80	0.63
1:A:39:PRO:HB2	19:A:405:CLA:HAB	1.81	0.63
22:E:101:HEM:HBC2	22:E:101:HEM:HHD	1.81	0.63
19:A:405:CLA:HAC1	21:A:406:BCR:H14C	1.81	0.62
6:S:40:TRP:HB3	6:S:330:LEU:HD22	1.80	0.62
6:S:291:ASP:OD2	6:S:295:THR:OG1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:PHE:O	2:D:129:GLN:NE2	2.33	0.60
5:I:8:VAL:O	5:I:12:VAL:HG22	2.01	0.60
6:S:51:PHE:HB3	6:S:323:LEU:HD23	1.84	0.59
1:A:343:LEU:HD13	6:S:131:SER:HB3	1.84	0.59
6:S:97:SER:OG	6:S:111:LYS:NZ	2.32	0.59
1:A:317:TRP:HZ3	2:D:180:ARG:HD2	1.68	0.58
6:S:207:GLN:HG2	6:S:209:GLU:H	1.68	0.58
6:S:272:ARG:HE	6:S:332:TYR:HE2	1.51	0.58
1:A:343:LEU:HD21	6:S:133:LYS:HB2	1.83	0.58
2:D:61:HIS:HE2	2:D:80:SER:HG	1.49	0.58
5:I:4:LEU:O	5:I:8:VAL:HG23	2.03	0.58
1:A:87:ASN:ND2	6:S:222:GLN:OE1	2.37	0.58
1:A:308:ASP:OD1	1:A:312:ARG:N	2.36	0.58
1:A:50:ILE:HG21	21:A:406:BCR:H23C	1.85	0.58
22:E:101:HEM:HBB2	22:E:101:HEM:HMB2	1.86	0.57
3:E:53:ASP:OD1	3:E:54:GLU:N	2.37	0.57
6:S:139:TYR:HE2	6:S:182:ILE:H	1.52	0.57
3:E:30:LEU:HD23	4:F:30:VAL:HG23	1.87	0.56
2:D:83:ASP:N	2:D:83:ASP:OD1	2.36	0.56
1:A:59:ASP:OD2	6:S:310:TYR:OH	2.22	0.55
2:D:98:GLN:OE1	2:D:103:ARG:NH1	2.40	0.55
1:A:216:GLY:HA3	2:D:272:LEU:HB2	1.89	0.55
20:A:404:PHO:H172	19:A:407:CLA:H143	1.89	0.55
5:I:12:VAL:O	5:I:16:ILE:HG23	2.06	0.55
1:A:189:GLU:OE2	6:S:220:ARG:NE	2.40	0.54
2:D:61:HIS:NE2	2:D:80:SER:OG	2.36	0.54
6:S:85:LYS:NZ	6:S:86:LEU:O	2.37	0.54
2:D:69:GLU:OE2	3:E:55:TYR:OH	2.26	0.54
6:S:139:TYR:HD2	6:S:182:ILE:HD12	1.73	0.54
2:D:55:VAL:HG21	2:D:110:LEU:HD22	1.90	0.53
6:S:128:ILE:HD13	6:S:165:GLY:HA3	1.90	0.53
2:D:192:THR:HG23	19:D:402:CLA:HBC2	1.90	0.53
6:S:138:PRO:HB3	6:S:151:MET:SD	2.48	0.53
4:F:32:PHE:O	4:F:36:ILE:HG12	2.09	0.53
2:D:100:ASN:HB3	2:D:103:ARG:HB2	1.91	0.52
6:S:282:ALA:O	6:S:285:ASN:ND2	2.36	0.52
1:A:42:LEU:HB3	21:A:406:BCR:H353	1.91	0.52
1:A:302:PHE:HE2	2:D:74:LEU:HD12	1.74	0.52
4:F:25:LEU:HD23	4:F:25:LEU:H	1.75	0.52
6:S:307:ALA:HB2	6:S:328:ILE:HD12	1.92	0.52
1:A:310:GLN:HE21	1:A:312:ARG:HH21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLY:HA3	2:D:304:ARG:HH12	1.76	0.51
6:S:66:VAL:HG12	6:S:72:ILE:HG22	1.93	0.51
1:A:142:TRP:HB2	2:D:220:ASN:OD1	2.10	0.51
6:S:62:HIS:HA	6:S:76:THR:HA	1.92	0.51
6:S:105:GLU:HG3	6:S:119:THR:HG22	1.93	0.51
2:D:263:ASN:HB3	2:D:265:ARG:HG3	1.93	0.50
1:A:219:VAL:HG21	2:D:268:HIS:CD2	2.47	0.50
19:A:407:CLA:H2A	19:A:407:CLA:HED3	1.92	0.50
2:D:88:SER:OG	2:D:96:GLU:OE2	2.28	0.50
2:D:111:TRP:HB3	2:D:112:PRO:HD3	1.94	0.50
1:A:309:SER:OG	1:A:310:GLN:OE1	2.29	0.50
1:A:133:LEU:HD23	2:D:256:ILE:HG12	1.94	0.50
3:E:30:LEU:HG	4:F:31:PHE:HA	1.94	0.50
6:S:57:THR:OG1	6:S:61:ASN:ND2	2.45	0.49
6:S:259:GLN:OE1	6:S:264:TRP:HB2	2.13	0.49
2:D:149:PRO:HB3	19:D:402:CLA:H62	1.95	0.48
6:S:70:GLU:OE2	6:S:94:ALA:N	2.45	0.48
1:A:149:ALA:HB1	1:A:283:ILE:HB	1.96	0.48
6:S:53:ASP:HB3	6:S:99:VAL:HG12	1.95	0.48
6:S:302:VAL:HB	6:S:305:ILE:HD12	1.95	0.48
2:D:323:GLU:OE1	2:D:323:GLU:N	2.47	0.47
6:S:293:GLY:HA2	6:S:296:TRP:CZ2	2.49	0.47
1:A:308:ASP:HB3	1:A:314:ILE:HD11	1.96	0.47
6:S:278:TRP:CE2	6:S:288:MET:HG3	2.48	0.47
1:A:334:ARG:HH12	6:S:212:PRO:HG3	1.79	0.47
1:A:140:ARG:HH12	2:D:222:LEU:HB2	1.79	0.47
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.97	0.47
1:A:339:PHE:CZ	6:S:175:ALA:HB2	2.50	0.47
20:A:404:PHO:H18	19:A:407:CLA:HBB1	1.96	0.47
2:D:44:ALA:HB2	2:D:117:HIS:HB3	1.96	0.47
5:I:27:ASP:HB2	5:I:28:PRO:HD2	1.97	0.47
6:S:107:TRP:HE3	6:S:115:LEU:HD21	1.80	0.47
6:S:160:LYS:N	6:S:169:LYS:O	2.43	0.47
2:D:120:PHE:N	2:D:120:PHE:CD1	2.82	0.47
6:S:160:LYS:HB2	6:S:171:LEU:HD11	1.97	0.47
1:A:187:GLN:HB2	19:A:402:CLA:HAC2	1.95	0.47
20:A:404:PHO:H13	20:A:404:PHO:H102	1.61	0.47
2:D:201:VAL:HG22	19:D:402:CLA:C1B	2.46	0.46
2:D:277:THR:O	2:D:281:MET:HG2	2.15	0.46
1:A:212:SER:OG	2:D:271:MET:HB2	2.16	0.46
2:D:39:PRO:O	2:D:42:PHE:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD13	1:A:168:PHE:CE2	2.50	0.46
1:A:339:PHE:HZ	6:S:175:ALA:HB2	1.81	0.46
19:D:403:CLA:HBA1	19:D:403:CLA:H3A	1.50	0.46
1:A:198:HIS:HE1	19:A:402:CLA:NB	2.13	0.46
2:D:111:TRP:NE1	2:D:171:PRO:O	2.44	0.46
6:S:115:LEU:HD22	6:S:128:ILE:HD12	1.98	0.46
1:A:88:ALA:HB1	6:S:282:ALA:HB2	1.98	0.46
6:S:187:ASP:OD1	6:S:187:ASP:N	2.35	0.45
1:A:186:PHE:O	1:A:190:HIS:HB2	2.17	0.45
1:A:283:ILE:HA	1:A:286:THR:HG22	1.98	0.45
6:S:244:SER:HB2	6:S:249:ALA:HB1	1.98	0.45
2:D:196:PHE:HB3	2:D:281:MET:O	2.17	0.45
1:A:20:TRP:O	1:A:26:ASN:ND2	2.44	0.45
1:A:153:ALA:HB1	19:A:402:CLA:HED1	1.98	0.45
20:A:404:PHO:H152	19:A:407:CLA:H151	1.99	0.45
1:A:334:ARG:NH1	6:S:212:PRO:HG3	2.32	0.45
1:A:210:LEU:HD12	20:D:401:PHO:NC	2.32	0.45
21:A:406:BCR:H15C	21:A:406:BCR:H351	1.87	0.45
2:D:49:LEU:H	2:D:49:LEU:HD12	1.82	0.45
22:E:101:HEM:HBC2	22:E:101:HEM:CHD	2.47	0.45
1:A:156:ALA:HA	1:A:160:ILE:HB	1.98	0.45
2:D:55:VAL:O	2:D:66:SER:HB2	2.17	0.44
4:F:42:ILE:HD12	4:F:43:GLN:HG3	1.99	0.44
1:A:331:MET:HB3	2:D:324:GLY:HA3	1.99	0.44
5:I:6:ILE:O	5:I:10:ILE:HG23	2.18	0.44
1:A:85:SER:HB3	1:A:89:ILE:HD12	2.00	0.44
19:A:402:CLA:HMB2	19:D:402:CLA:HMB2	1.98	0.44
4:F:36:ILE:O	4:F:39:MET:HB2	2.17	0.44
6:S:72:ILE:HG13	6:S:85:LYS:HB3	1.99	0.44
1:A:206:PHE:CD2	20:D:401:PHO:HBB2	2.53	0.44
6:S:152:ILE:HG12	6:S:158:ILE:HD12	2.00	0.44
1:A:334:ARG:CG	1:A:335:ASN:H	2.31	0.43
1:A:118:HIS:HE1	19:A:405:CLA:C4D	2.31	0.43
6:S:219:ARG:HD2	6:S:240:GLN:HG3	2.00	0.43
2:D:81:PRO:HG3	2:D:112:PRO:HD3	2.00	0.43
2:D:120:PHE:N	2:D:120:PHE:HD1	2.15	0.43
6:S:242:GLN:NE2	6:S:253:SER:O	2.39	0.43
6:S:160:LYS:O	6:S:169:LYS:N	2.50	0.43
19:D:402:CLA:H62	19:D:402:CLA:H41	1.75	0.43
19:A:405:CLA:H2	5:I:12:VAL:HG21	2.00	0.43
2:D:72:ASN:N	2:D:75:THR:OG1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:TRP:O	3:E:39:SER:OG	2.27	0.43
1:A:89:ILE:HG12	6:S:264:TRP:HZ3	1.84	0.42
1:A:87:ASN:HD21	6:S:237:ARG:NE	2.17	0.42
2:D:286:ILE:HD13	2:D:289:LEU:HD12	2.00	0.42
6:S:65:LEU:HD23	6:S:82:TRP:CH2	2.54	0.42
1:A:32:TRP:CD2	5:I:22:GLY:HA3	2.54	0.42
1:A:172:MET:HG3	1:A:182:PHE:CD2	2.55	0.42
21:A:406:BCR:H11C	21:A:406:BCR:H341	1.93	0.42
2:D:182:ILE:HA	19:D:402:CLA:HMD2	2.01	0.42
6:S:118:THR:OG1	6:S:120:ASP:OD1	2.24	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.90	0.42
6:S:216:ASN:OD1	6:S:252:TRP:NE1	2.52	0.42
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.02	0.42
19:A:403:CLA:HBA2	19:A:403:CLA:H3A	1.45	0.42
19:A:403:CLA:CHC	19:D:402:CLA:H2	2.50	0.42
6:S:312:VAL:HG22	6:S:322:VAL:HG22	2.01	0.42
1:A:186:PHE:CE1	1:A:293:MET:HG2	2.55	0.41
2:D:189:HIS:ND1	2:D:289:LEU:HD22	2.35	0.41
3:E:43:ALA:O	3:E:47:PHE:HD1	2.03	0.41
3:E:51:ARG:HB2	3:E:53:ASP:OD1	2.20	0.41
6:S:269:LEU:HD21	6:S:271:PHE:HE1	1.85	0.41
1:A:170:ASP:OD1	6:S:220:ARG:NH2	2.53	0.41
6:S:73:PHE:CZ	6:S:84:GLN:HB2	2.55	0.41
2:D:128:ARG:O	2:D:131:GLU:HG3	2.20	0.41
2:D:329:MET:SD	2:D:329:MET:N	2.93	0.41
1:A:335:ASN:ND2	6:S:210:TRP:H	2.18	0.41
6:S:57:THR:OG1	6:S:58:GLU:N	2.53	0.41
20:A:404:PHO:HMB3	19:A:407:CLA:H71	2.01	0.41
6:S:151:MET:HE2	6:S:151:MET:HA	2.03	0.41
1:A:139:MET:HE3	1:A:139:MET:HB3	1.95	0.41
1:A:212:SER:OG	2:D:271:MET:O	2.36	0.41
19:A:407:CLA:H92	19:A:407:CLA:H62	1.78	0.41
2:D:201:VAL:HG22	19:D:402:CLA:C2B	2.50	0.41
19:A:402:CLA:H203	19:A:402:CLA:H161	1.83	0.41
2:D:56:THR:OG1	2:D:57:SER:N	2.54	0.41
2:D:95:PRO:O	2:D:98:GLN:NE2	2.54	0.41
19:A:405:CLA:HBA2	19:A:405:CLA:H3A	1.27	0.40
6:S:77:ASP:OD1	6:S:77:ASP:N	2.42	0.40
6:S:45:LEU:N	6:S:327:GLY:O	2.54	0.40
6:S:234:LEU:HG	6:S:242:GLN:HB3	2.02	0.40
1:A:331:MET:SD	1:A:331:MET:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:THR:HA	2:D:53:THR:HG22	2.04	0.40
19:A:403:CLA:HBC3	2:D:178:ILE:HG23	2.02	0.40
2:D:283:SER:O	2:D:287:VAL:HG23	2.22	0.40
6:S:58:GLU:HB2	6:S:61:ASN:HB2	2.03	0.40
1:A:43:THR:HG23	21:A:406:BCR:H362	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/344 (83%)	278 (97%)	8 (3%)	0	100	100
2	D	274/336 (82%)	264 (96%)	10 (4%)	0	100	100
3	E	35/81 (43%)	33 (94%)	2 (6%)	0	100	100
4	F	26/44 (59%)	26 (100%)	0	0	100	100
5	I	27/38 (71%)	26 (96%)	1 (4%)	0	100	100
6	S	301/342 (88%)	292 (97%)	9 (3%)	0	100	100
7	a	739/751 (98%)	715 (97%)	24 (3%)	0	100	100
8	b	727/731 (100%)	707 (97%)	20 (3%)	0	100	100
9	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
10	d	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
11	e	67/74 (90%)	63 (94%)	4 (6%)	0	100	100
12	f	140/165 (85%)	135 (96%)	5 (4%)	0	100	100
13	i	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
14	j	38/40 (95%)	38 (100%)	0	0	100	100
15	k	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
16	l	141/157 (90%)	137 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	3156/3482 (91%)	3060 (97%)	96 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/283 (83%)	235 (100%)	1 (0%)	89	94
2	D	220/271 (81%)	218 (99%)	2 (1%)	75	88
3	E	31/73 (42%)	31 (100%)	0	100	100
4	F	22/37 (60%)	22 (100%)	0	100	100
5	I	26/34 (76%)	26 (100%)	0	100	100
6	S	239/279 (86%)	238 (100%)	1 (0%)	89	94
7	a	593/603 (98%)	593 (100%)	0	100	100
8	b	582/583 (100%)	578 (99%)	4 (1%)	81	90
9	c	68/69 (99%)	68 (100%)	0	100	100
10	d	114/116 (98%)	113 (99%)	1 (1%)	75	88
11	e	57/60 (95%)	57 (100%)	0	100	100
12	f	119/137 (87%)	119 (100%)	0	100	100
13	i	32/32 (100%)	32 (100%)	0	100	100
14	j	35/35 (100%)	35 (100%)	0	100	100
15	k	53/62 (86%)	53 (100%)	0	100	100
16	l	107/118 (91%)	106 (99%)	1 (1%)	75	88
17	m	25/25 (100%)	25 (100%)	0	100	100
All	All	2559/2817 (91%)	2549 (100%)	10 (0%)	88	94

All (10) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	130	GLN
2	D	49	LEU
2	D	255	GLN
6	S	332	TYR
8	b	129	MET
8	b	257	PHE
8	b	439	ASP
8	b	573	PHE
10	d	82	ASP
16	l	118	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
2	D	129	GLN
7	a	54	ASN
7	a	109	HIS
8	b	41	ASN
16	l	6	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](#)

Of 146 ligands modelled in this entry, 1 is monoatomic - leaving 145 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	BCR	b	842	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
19	CLA	a	808	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
31	ZEX	b	852	-	42,43,43	1.65	8 (19%)	55,60,60	1.58	11 (20%)
19	CLA	a	804	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	b	815	-	56,64,73	1.55	6 (10%)	65,102,113	1.51	8 (12%)
19	CLA	a	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	7 (9%)
21	BCR	b	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	5 (8%)
19	CLA	b	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
26	LHG	f	206	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
19	CLA	a	833	-	60,68,73	1.53	6 (10%)	70,107,113	1.41	9 (12%)
21	BCR	a	850	-	41,41,41	1.20	2 (4%)	56,56,56	1.26	6 (10%)
19	CLA	b	822	-	57,65,73	1.57	6 (10%)	66,103,113	1.48	8 (12%)
19	CLA	a	838	-	51,59,73	1.64	6 (11%)	59,96,113	1.52	7 (11%)
19	CLA	a	834	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	b	820	-	60,68,73	1.52	6 (10%)	70,107,113	1.42	7 (10%)
21	BCR	a	859	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	6 (10%)
21	BCR	b	847	-	41,41,41	1.10	2 (4%)	56,56,56	1.14	6 (10%)
19	CLA	a	837	7	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
19	CLA	b	812	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	8 (10%)
19	CLA	l	203	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	7 (9%)
19	CLA	b	823	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
19	CLA	b	832	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
19	CLA	a	810	7	51,59,73	1.64	6 (11%)	59,96,113	1.59	8 (13%)
19	CLA	a	820	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	9 (11%)
19	CLA	a	826	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
21	BCR	a	851	-	25,25,41	1.16	1 (4%)	33,33,56	1.30	3 (9%)
19	CLA	D	402	-	55,63,73	1.61	7 (12%)	64,101,113	1.48	8 (12%)
26	LHG	b	849	19	37,37,48	0.71	1 (2%)	40,43,54	1.21	3 (7%)
19	CLA	a	836	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
19	CLA	l	202	-	50,58,73	1.70	5 (10%)	58,95,113	1.53	9 (15%)
19	CLA	b	816	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	b	833	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
19	CLA	a	841	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
19	CLA	b	829	-	51,59,73	1.68	6 (11%)	59,96,113	1.51	8 (13%)
19	CLA	b	818	-	60,68,73	1.51	6 (10%)	70,107,113	1.39	6 (8%)
19	CLA	a	805	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	6 (7%)
19	CLA	a	811	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	8 (13%)
19	CLA	k	101	-	46,54,73	1.75	6 (13%)	53,90,113	1.46	6 (11%)
25	SF4	c	101	9	0,12,12	-	-	-		
21	BCR	k	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	6 (10%)
19	CLA	a	842	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	6 (7%)
21	BCR	a	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	7 (12%)
27	LMG	b	850	-	55,55,55	0.78	1 (1%)	63,63,63	1.34	9 (14%)
29	ECH	m	101	-	42,42,42	1.78	9 (21%)	55,58,58	1.85	13 (23%)
19	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	8 (10%)
24	PQN	b	841	-	34,34,34	0.38	0	42,45,45	0.39	0
29	ECH	b	844	-	42,42,42	1.73	8 (19%)	55,58,58	2.37	16 (29%)
19	CLA	b	836	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	8 (10%)
19	CLA	a	835	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	8 (10%)
19	CLA	b	819	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	7 (9%)
26	LHG	a	853	19	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
19	CLA	a	831	-	65,73,73	1.46	7 (10%)	76,113,113	1.51	9 (11%)
21	BCR	j	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
19	CLA	b	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
27	LMG	l	201	-	50,50,55	0.73	0	58,58,63	1.34	7 (12%)
19	CLA	b	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	6 (7%)
19	CLA	A	403	-	46,54,73	1.75	6 (13%)	53,90,113	1.54	7 (13%)
19	CLA	b	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	8 (10%)
30	EQ3	b	851	-	43,43,43	1.66	9 (20%)	56,60,60	1.55	11 (19%)
25	SF4	c	102	9	0,12,12	-	-	-		
25	SF4	a	845	8,7	0,12,12	-	-	-		
19	CLA	a	824	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	9 (11%)
19	CLA	a	806	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	7 (9%)
20	PHO	A	404	-	51,69,69	1.01	4 (7%)	47,99,99	1.09	5 (10%)
19	CLA	a	829	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
19	CLA	b	839	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	b	809	-	56,64,73	1.63	6 (10%)	65,102,113	1.41	7 (10%)
19	CLA	b	838	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
19	CLA	a	803	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
24	PQN	a	844	-	34,34,34	0.37	0	42,45,45	0.40	0
19	CLA	b	830	-	50,58,73	1.65	6 (12%)	58,95,113	1.57	8 (13%)
19	CLA	b	801	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	7 (9%)
19	CLA	a	813	-	60,68,73	1.55	8 (13%)	70,107,113	1.39	8 (11%)
19	CLA	A	407	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
19	CLA	j	104	-	46,54,73	1.77	6 (13%)	53,90,113	1.53	7 (13%)
19	CLA	b	811	-	50,58,73	1.68	6 (12%)	58,95,113	1.52	7 (12%)
21	BCR	f	202	-	41,41,41	1.17	2 (4%)	56,56,56	1.20	5 (8%)
19	CLA	a	818	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	7 (9%)
26	LHG	a	855	-	48,48,48	0.60	1 (2%)	51,54,54	1.27	6 (11%)
19	CLA	b	810	-	56,64,73	1.58	6 (10%)	65,102,113	1.47	6 (9%)
19	CLA	b	834	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	7 (12%)
19	CLA	D	403	-	46,54,73	1.75	5 (10%)	53,90,113	1.57	6 (11%)
19	CLA	a	814	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
21	BCR	a	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	6 (10%)
20	PHO	D	401	-	51,69,69	1.03	6 (11%)	47,99,99	1.14	5 (10%)
19	CLA	b	821	-	46,54,73	1.76	7 (15%)	53,90,113	1.56	6 (11%)
19	CLA	a	812	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
21	BCR	A	406	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	a	821	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
19	CLA	b	813	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
21	BCR	a	847	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	5 (8%)
21	BCR	l	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	4 (7%)
19	CLA	j	103	14	55,63,73	1.63	5 (9%)	64,101,113	1.45	7 (10%)
19	CLA	a	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.34	6 (7%)
19	CLA	a	825	-	60,68,73	1.52	6 (10%)	70,107,113	1.43	7 (10%)
19	CLA	a	807	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
27	LMG	b	848	-	55,55,55	0.70	1 (1%)	63,63,63	1.40	8 (12%)
19	CLA	f	203	-	50,58,73	1.69	6 (12%)	58,95,113	1.53	8 (13%)
23	CL0	a	801	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
19	CLA	f	201	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	a	817	-	46,54,73	1.72	6 (13%)	53,90,113	1.58	6 (11%)
19	CLA	a	856	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
21	BCR	b	843	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	6 (10%)
19	CLA	a	832	-	56,64,73	1.59	6 (10%)	65,102,113	1.44	8 (12%)
19	CLA	b	805	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	8 (10%)
19	CLA	b	827	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	f	204	12	50,58,73	1.70	5 (10%)	58,95,113	1.52	8 (13%)
21	BCR	i	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.21	5 (8%)
32	LMT	j	102	-	36,36,36	1.18	6 (16%)	47,47,47	0.95	2 (4%)
19	CLA	A	402	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	6 (7%)
19	CLA	a	809	7	65,73,73	1.44	6 (9%)	76,113,113	1.43	9 (11%)
19	CLA	b	814	-	55,63,73	1.59	8 (14%)	64,101,113	1.46	7 (10%)
19	CLA	k	102	15	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
19	CLA	b	825	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
19	CLA	b	835	-	52,60,73	1.61	7 (13%)	60,97,113	1.56	9 (15%)
26	LHG	a	852	-	48,48,48	0.62	1 (2%)	51,54,54	1.29	6 (11%)
27	LMG	a	854	-	40,40,55	0.82	0	48,48,63	1.29	5 (10%)
19	CLA	b	840	26	46,54,73	1.73	5 (10%)	53,90,113	1.56	6 (11%)
28	45D	a	858	-	43,43,43	1.70	9 (20%)	54,60,60	1.63	11 (20%)
19	CLA	b	817	-	65,73,73	1.45	6 (9%)	76,113,113	1.37	6 (7%)
19	CLA	a	857	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	6 (7%)
19	CLA	b	824	-	55,63,73	1.57	6 (10%)	64,101,113	1.53	7 (10%)
19	CLA	b	831	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	7 (9%)
19	CLA	a	840	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	6 (7%)
21	BCR	b	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	4 (7%)
19	CLA	a	815	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	9 (11%)
31	ZEX	f	205	-	42,43,43	1.66	8 (19%)	55,60,60	1.56	11 (20%)
21	BCR	a	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	7 (12%)
19	CLA	a	823	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	7 (9%)
19	CLA	b	803	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	8 (10%)
19	CLA	a	816	-	46,54,73	1.73	7 (15%)	53,90,113	1.59	6 (11%)
19	CLA	a	860	-	65,73,73	1.46	5 (7%)	76,113,113	1.37	8 (10%)
19	CLA	b	806	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
19	CLA	b	804	-	65,73,73	1.44	6 (9%)	76,113,113	1.45	8 (10%)
19	CLA	b	837	-	50,58,73	1.71	7 (14%)	58,95,113	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	a	843	26	56,64,73	1.57	7 (12%)	65,102,113	1.50	8 (12%)
19	CLA	b	808	8	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
19	CLA	a	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
21	BCR	i	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
22	HEM	E	101	4,3	41,50,50	1.54	5 (12%)	45,82,82	1.28	5 (11%)
19	CLA	a	822	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)
19	CLA	l	204	-	52,60,73	1.63	6 (11%)	60,97,113	1.51	7 (11%)
19	CLA	A	405	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	9 (15%)
19	CLA	a	819	-	65,73,73	1.48	8 (12%)	76,113,113	1.39	6 (7%)

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
21	BCR	b	842	-	-	11/29/63/63	0/2/2/2
19	CLA	a	808	-	1/1/15/20	14/37/115/115	-
31	ZEX	b	852	-	-	3/29/67/67	0/2/2/2
19	CLA	a	804	-	1/1/15/20	10/37/115/115	-
19	CLA	b	815	-	1/1/13/20	8/27/105/115	-
19	CLA	a	828	-	1/1/15/20	16/37/115/115	-
21	BCR	b	845	-	-	5/29/63/63	0/2/2/2
19	CLA	b	802	-	1/1/15/20	15/37/115/115	-
26	LHG	f	206	-	-	30/53/53/53	-
19	CLA	a	833	-	1/1/14/20	13/31/109/115	-
21	BCR	a	850	-	-	10/29/63/63	0/2/2/2
19	CLA	b	822	-	1/1/13/20	15/28/106/115	-
19	CLA	a	838	-	1/1/12/20	5/21/99/115	-
19	CLA	a	834	-	1/1/15/20	12/37/115/115	-
19	CLA	b	820	-	1/1/14/20	11/31/109/115	-
21	BCR	a	859	-	-	6/29/63/63	0/2/2/2
21	BCR	b	847	-	-	15/29/63/63	0/2/2/2
19	CLA	a	837	7	1/1/15/20	13/37/115/115	-
19	CLA	b	812	-	1/1/15/20	15/37/115/115	-
19	CLA	l	203	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	823	-	1/1/15/20	13/37/115/115	-
19	CLA	b	832	-	1/1/15/20	18/37/115/115	-
19	CLA	a	810	7	1/1/12/20	3/21/99/115	-
19	CLA	a	820	-	1/1/15/20	14/37/115/115	-
19	CLA	a	826	-	1/1/15/20	13/37/115/115	-
21	BCR	a	851	-	-	7/18/35/63	0/1/1/2
19	CLA	D	402	-	1/1/13/20	13/25/103/115	-
26	LHG	b	849	19	-	20/42/42/53	-
19	CLA	a	836	-	1/1/15/20	11/37/115/115	-
19	CLA	l	202	-	1/1/12/20	10/19/97/115	-
19	CLA	b	816	-	1/1/15/20	9/37/115/115	-
19	CLA	b	833	-	1/1/15/20	19/37/115/115	-
19	CLA	a	841	-	1/1/15/20	13/37/115/115	-
19	CLA	b	829	-	1/1/12/20	6/21/99/115	-
19	CLA	b	818	-	1/1/14/20	6/31/109/115	-
19	CLA	a	805	-	1/1/15/20	11/37/115/115	-
19	CLA	a	811	-	1/1/12/20	6/19/97/115	-
19	CLA	k	101	-	1/1/11/20	11/15/93/115	-
25	SF4	c	101	9	-	-	0/6/5/5
21	BCR	k	103	-	-	8/29/63/63	0/2/2/2
19	CLA	a	842	-	1/1/15/20	12/37/115/115	-
21	BCR	a	849	-	-	6/29/63/63	0/2/2/2
27	LMG	b	850	-	-	24/50/70/70	0/1/1/1
29	ECH	m	101	-	-	6/29/66/66	0/2/2/2
19	CLA	a	839	-	1/1/15/20	12/37/115/115	-
24	PQN	b	841	-	-	0/23/43/43	0/2/2/2
29	ECH	b	844	-	-	10/29/66/66	0/2/2/2
19	CLA	b	836	-	1/1/15/20	17/37/115/115	-
19	CLA	a	835	-	1/1/15/20	15/37/115/115	-
19	CLA	b	819	-	1/1/15/20	10/37/115/115	-
26	LHG	a	853	19	-	23/53/53/53	-
19	CLA	a	831	-	1/1/15/20	16/37/115/115	-
21	BCR	j	101	-	-	7/29/63/63	0/2/2/2
19	CLA	b	826	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	l	201	-	-	25/45/65/70	0/1/1/1
19	CLA	b	828	-	1/1/15/20	16/37/115/115	-
19	CLA	A	403	-	1/1/11/20	10/15/93/115	-
19	CLA	b	807	-	1/1/15/20	8/37/115/115	-
30	EQ3	b	851	-	-	3/29/68/68	0/2/2/2
25	SF4	c	102	9	-	-	0/6/5/5
25	SF4	a	845	8,7	-	-	0/6/5/5
19	CLA	a	824	-	1/1/15/20	16/37/115/115	-
19	CLA	a	806	-	1/1/15/20	11/37/115/115	-
20	PHO	A	404	-	-	11/37/103/103	0/5/6/6
19	CLA	a	829	-	1/1/15/20	10/37/115/115	-
19	CLA	b	839	-	1/1/15/20	10/37/115/115	-
19	CLA	b	809	-	1/1/13/20	8/27/105/115	-
19	CLA	b	838	-	1/1/15/20	12/37/115/115	-
19	CLA	a	803	-	1/1/15/20	10/37/115/115	-
24	PQN	a	844	-	-	1/23/43/43	0/2/2/2
19	CLA	b	830	-	1/1/12/20	5/19/97/115	-
19	CLA	b	801	-	1/1/15/20	16/37/115/115	-
19	CLA	a	813	-	1/1/14/20	14/31/109/115	-
19	CLA	A	407	-	1/1/15/20	15/37/115/115	-
19	CLA	j	104	-	1/1/11/20	7/15/93/115	-
19	CLA	b	811	-	1/1/12/20	6/19/97/115	-
21	BCR	f	202	-	-	10/29/63/63	0/2/2/2
19	CLA	a	818	-	1/1/15/20	14/37/115/115	-
26	LHG	a	855	-	-	20/53/53/53	-
19	CLA	b	810	-	1/1/13/20	8/27/105/115	-
19	CLA	b	834	-	1/1/12/20	8/19/97/115	-
19	CLA	D	403	-	1/1/11/20	6/15/93/115	-
19	CLA	a	814	-	-	11/37/115/115	-
21	BCR	a	848	-	-	6/29/63/63	0/2/2/2
20	PHO	D	401	-	-	10/37/103/103	0/5/6/6
19	CLA	b	821	-	1/1/11/20	5/15/93/115	-
19	CLA	a	812	-	1/1/15/20	13/37/115/115	-
21	BCR	A	406	-	-	9/29/63/63	0/2/2/2
19	CLA	a	821	-	1/1/15/20	22/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	827	-	1/1/15/20	7/37/115/115	-
19	CLA	b	813	-	1/1/15/20	12/37/115/115	-
21	BCR	a	847	-	-	6/29/63/63	0/2/2/2
21	BCR	l	205	-	-	10/29/63/63	0/2/2/2
19	CLA	j	103	14	1/1/13/20	11/25/103/115	-
19	CLA	a	830	-	1/1/15/20	19/37/115/115	-
19	CLA	a	825	-	1/1/14/20	11/31/109/115	-
19	CLA	a	807	-	1/1/15/20	10/37/115/115	-
27	LMG	b	848	-	-	22/50/70/70	0/1/1/1
19	CLA	f	203	-	1/1/12/20	3/19/97/115	-
23	CL0	a	801	-	3/3/20/25	10/37/135/135	-
19	CLA	f	201	-	1/1/15/20	15/37/115/115	-
19	CLA	a	817	-	1/1/11/20	5/15/93/115	-
19	CLA	a	856	-	1/1/15/20	5/37/115/115	-
21	BCR	b	843	-	-	6/29/63/63	0/2/2/2
19	CLA	a	832	-	1/1/13/20	10/27/105/115	-
19	CLA	b	805	-	1/1/15/20	16/37/115/115	-
19	CLA	b	827	-	1/1/15/20	10/37/115/115	-
19	CLA	f	204	12	1/1/12/20	5/19/97/115	-
21	BCR	i	101	-	-	7/29/63/63	0/2/2/2
32	LMT	j	102	-	-	5/21/61/61	0/2/2/2
19	CLA	A	402	-	1/1/15/20	10/37/115/115	-
19	CLA	a	809	7	1/1/15/20	14/37/115/115	-
19	CLA	b	814	-	1/1/13/20	12/25/103/115	-
19	CLA	k	102	15	1/1/11/20	4/13/91/115	-
19	CLA	b	825	-	1/1/15/20	5/37/115/115	-
19	CLA	b	835	-	1/1/12/20	6/22/100/115	-
26	LHG	a	852	-	-	25/53/53/53	-
27	LMG	a	854	-	-	18/35/55/70	0/1/1/1
19	CLA	b	840	26	1/1/11/20	9/15/93/115	-
28	45D	a	858	-	-	4/29/69/69	0/2/2/2
19	CLA	b	817	-	1/1/15/20	13/37/115/115	-
19	CLA	a	857	-	1/1/15/20	19/37/115/115	-
19	CLA	b	824	-	1/1/13/20	6/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	831	-	1/1/15/20	13/37/115/115	-
19	CLA	a	840	-	1/1/15/20	18/37/115/115	-
21	BCR	b	846	-	-	7/29/63/63	0/2/2/2
19	CLA	a	815	-	1/1/15/20	17/37/115/115	-
31	ZEX	f	205	-	-	4/29/67/67	0/2/2/2
21	BCR	a	846	-	-	8/29/63/63	0/2/2/2
19	CLA	a	823	-	1/1/15/20	15/37/115/115	-
19	CLA	b	803	-	1/1/15/20	13/37/115/115	-
19	CLA	a	816	-	1/1/11/20	7/15/93/115	-
19	CLA	a	860	-	1/1/15/20	14/37/115/115	-
19	CLA	b	806	-	1/1/15/20	15/37/115/115	-
19	CLA	b	804	-	1/1/15/20	15/37/115/115	-
19	CLA	b	837	-	1/1/12/20	4/19/97/115	-
19	CLA	a	843	26	1/1/13/20	10/27/105/115	-
19	CLA	b	808	8	1/1/15/20	9/37/115/115	-
19	CLA	a	802	-	1/1/15/20	13/37/115/115	-
21	BCR	i	102	-	-	12/29/63/63	0/2/2/2
22	HEM	E	101	4,3	-	1/12/54/54	-
19	CLA	a	822	-	1/1/15/20	10/37/115/115	-
19	CLA	l	204	-	1/1/12/20	8/22/100/115	-
19	CLA	A	405	-	1/1/12/20	7/19/97/115	-
19	CLA	a	819	-	1/1/15/20	18/37/115/115	-

All (758) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	809	CLA	C4B-NB	7.74	1.42	1.35
19	b	821	CLA	C4B-NB	7.74	1.42	1.35
19	j	103	CLA	C4B-NB	7.70	1.42	1.35
19	b	839	CLA	C4B-NB	7.62	1.42	1.35
19	b	837	CLA	C4B-NB	7.58	1.42	1.35
19	f	204	CLA	C4B-NB	7.52	1.41	1.35
19	l	202	CLA	C4B-NB	7.51	1.41	1.35
19	a	840	CLA	C4B-NB	7.50	1.41	1.35
19	D	402	CLA	C4B-NB	7.49	1.41	1.35
19	A	405	CLA	C4B-NB	7.46	1.41	1.35
19	a	803	CLA	C4B-NB	7.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	102	CLA	C4B-NB	7.46	1.41	1.35
19	j	104	CLA	C4B-NB	7.45	1.41	1.35
19	a	821	CLA	C4B-NB	7.44	1.41	1.35
19	f	203	CLA	C4B-NB	7.44	1.41	1.35
19	a	802	CLA	C4B-NB	7.44	1.41	1.35
19	k	101	CLA	C4B-NB	7.43	1.41	1.35
19	b	831	CLA	C4B-NB	7.42	1.41	1.35
19	a	824	CLA	C4B-NB	7.42	1.41	1.35
19	b	811	CLA	C4B-NB	7.38	1.41	1.35
19	D	403	CLA	C4B-NB	7.37	1.41	1.35
19	A	403	CLA	C4B-NB	7.36	1.41	1.35
19	a	804	CLA	C4B-NB	7.34	1.41	1.35
19	a	813	CLA	C4B-NB	7.34	1.41	1.35
19	f	201	CLA	C4B-NB	7.33	1.41	1.35
19	a	841	CLA	C4B-NB	7.32	1.41	1.35
19	a	822	CLA	C4B-NB	7.31	1.41	1.35
19	l	203	CLA	C4B-NB	7.31	1.41	1.35
19	b	801	CLA	C4B-NB	7.31	1.41	1.35
19	a	805	CLA	C4B-NB	7.30	1.41	1.35
19	a	816	CLA	C4B-NB	7.30	1.41	1.35
19	a	837	CLA	C4B-NB	7.29	1.41	1.35
19	b	828	CLA	C4B-NB	7.29	1.41	1.35
19	b	808	CLA	C4B-NB	7.28	1.41	1.35
19	b	819	CLA	C4B-NB	7.27	1.41	1.35
19	a	832	CLA	C4B-NB	7.27	1.41	1.35
19	a	836	CLA	C4B-NB	7.27	1.41	1.35
19	a	857	CLA	C4B-NB	7.27	1.41	1.35
19	a	827	CLA	C4B-NB	7.26	1.41	1.35
19	b	810	CLA	C4B-NB	7.26	1.41	1.35
19	a	860	CLA	C4B-NB	7.26	1.41	1.35
19	a	815	CLA	C4B-NB	7.26	1.41	1.35
19	a	819	CLA	C4B-NB	7.25	1.41	1.35
19	A	402	CLA	C4B-NB	7.25	1.41	1.35
23	a	801	CL0	C4B-NB	7.24	1.41	1.35
19	a	808	CLA	C4B-NB	7.24	1.41	1.35
19	a	810	CLA	C4B-NB	7.24	1.41	1.35
19	a	812	CLA	C4B-NB	7.23	1.41	1.35
19	A	407	CLA	C4B-NB	7.23	1.41	1.35
19	b	803	CLA	C4B-NB	7.22	1.41	1.35
19	a	842	CLA	C4B-NB	7.22	1.41	1.35
19	b	829	CLA	C4B-NB	7.22	1.41	1.35
19	b	840	CLA	C4B-NB	7.21	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	835	CLA	C4B-NB	7.21	1.41	1.35
19	a	811	CLA	C4B-NB	7.20	1.41	1.35
19	a	829	CLA	C4B-NB	7.20	1.41	1.35
19	l	204	CLA	C4B-NB	7.19	1.41	1.35
19	b	834	CLA	C4B-NB	7.19	1.41	1.35
19	a	806	CLA	C4B-NB	7.18	1.41	1.35
19	a	818	CLA	C4B-NB	7.18	1.41	1.35
19	a	833	CLA	C4B-NB	7.18	1.41	1.35
19	b	802	CLA	C4B-NB	7.18	1.41	1.35
19	b	807	CLA	C4B-NB	7.18	1.41	1.35
19	b	826	CLA	C4B-NB	7.17	1.41	1.35
19	a	830	CLA	C4B-NB	7.16	1.41	1.35
19	b	813	CLA	C4B-NB	7.16	1.41	1.35
19	a	820	CLA	C4B-NB	7.16	1.41	1.35
19	b	833	CLA	C4B-NB	7.16	1.41	1.35
19	a	831	CLA	C4B-NB	7.15	1.41	1.35
19	a	823	CLA	C4B-NB	7.15	1.41	1.35
19	a	843	CLA	C4B-NB	7.15	1.41	1.35
19	b	812	CLA	C4B-NB	7.14	1.41	1.35
19	b	823	CLA	C4B-NB	7.13	1.41	1.35
19	a	839	CLA	C4B-NB	7.13	1.41	1.35
19	b	822	CLA	C4B-NB	7.13	1.41	1.35
19	b	814	CLA	C4B-NB	7.12	1.41	1.35
19	b	820	CLA	C4B-NB	7.11	1.41	1.35
19	b	832	CLA	C4B-NB	7.11	1.41	1.35
19	a	856	CLA	C4B-NB	7.10	1.41	1.35
19	a	834	CLA	C4B-NB	7.09	1.41	1.35
19	b	838	CLA	C4B-NB	7.09	1.41	1.35
19	a	807	CLA	C4B-NB	7.09	1.41	1.35
19	b	830	CLA	C4B-NB	7.09	1.41	1.35
19	b	825	CLA	C4B-NB	7.08	1.41	1.35
19	b	815	CLA	C4B-NB	7.08	1.41	1.35
19	a	826	CLA	C4B-NB	7.07	1.41	1.35
19	b	817	CLA	C4B-NB	7.07	1.41	1.35
19	a	817	CLA	C4B-NB	7.06	1.41	1.35
19	b	816	CLA	C4B-NB	7.05	1.41	1.35
19	b	805	CLA	C4B-NB	7.04	1.41	1.35
19	b	836	CLA	C4B-NB	7.04	1.41	1.35
19	a	825	CLA	C4B-NB	7.03	1.41	1.35
19	b	827	CLA	C4B-NB	7.01	1.41	1.35
19	b	824	CLA	C4B-NB	6.98	1.41	1.35
19	b	804	CLA	C4B-NB	6.96	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	838	CLA	C4B-NB	6.96	1.41	1.35
19	a	809	CLA	C4B-NB	6.95	1.41	1.35
19	a	814	CLA	C4B-NB	6.94	1.41	1.35
19	b	835	CLA	C4B-NB	6.93	1.41	1.35
19	b	818	CLA	C4B-NB	6.93	1.41	1.35
19	b	806	CLA	C4B-NB	6.91	1.41	1.35
19	a	828	CLA	C4B-NB	6.90	1.41	1.35
22	E	101	HEM	C3C-C2C	-4.69	1.33	1.40
29	b	844	ECH	C21-C22	4.09	1.41	1.35
29	m	101	ECH	C14-C13	4.09	1.41	1.35
29	m	101	ECH	C21-C22	4.05	1.41	1.35
29	m	101	ECH	C17-C18	4.00	1.41	1.35
29	m	101	ECH	C10-C9	3.99	1.41	1.35
29	b	844	ECH	C17-C18	3.94	1.41	1.35
29	b	844	ECH	C10-C9	3.91	1.41	1.35
19	j	104	CLA	C1D-ND	3.90	1.42	1.37
19	a	814	CLA	C1D-ND	3.87	1.42	1.37
19	b	816	CLA	C1D-ND	3.86	1.42	1.37
19	k	101	CLA	C1D-ND	3.86	1.42	1.37
19	l	202	CLA	C1D-ND	3.86	1.42	1.37
31	f	205	ZEX	C30-C29	3.84	1.40	1.35
19	j	103	CLA	C1D-ND	3.83	1.42	1.37
19	D	403	CLA	C1D-ND	3.83	1.42	1.37
19	a	829	CLA	C1D-ND	3.81	1.42	1.37
29	b	844	ECH	C14-C13	3.80	1.40	1.35
19	A	403	CLA	C1D-ND	3.79	1.42	1.37
19	a	840	CLA	C1D-ND	3.79	1.42	1.37
19	b	809	CLA	C1D-ND	3.79	1.42	1.37
31	b	852	ZEX	C14-C13	3.78	1.40	1.35
19	A	405	CLA	C1D-ND	3.77	1.42	1.37
19	k	102	CLA	C1D-ND	3.76	1.42	1.37
19	b	829	CLA	C1D-ND	3.75	1.42	1.37
19	A	407	CLA	C1D-ND	3.74	1.42	1.37
19	a	819	CLA	C1D-ND	3.74	1.42	1.37
19	a	841	CLA	C1D-ND	3.74	1.42	1.37
19	b	812	CLA	C1D-ND	3.73	1.42	1.37
19	f	203	CLA	C1D-ND	3.73	1.42	1.37
19	a	837	CLA	C1D-ND	3.73	1.42	1.37
21	a	850	BCR	C1-C6	-3.72	1.48	1.53
19	a	817	CLA	C1D-ND	3.72	1.42	1.37
31	b	852	ZEX	C34-C33	3.72	1.40	1.35
31	f	205	ZEX	C34-C33	3.72	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	E	101	HEM	C3C-CAC	3.72	1.55	1.47
19	a	824	CLA	C1D-ND	3.71	1.42	1.37
31	b	852	ZEX	C30-C29	3.70	1.40	1.35
21	b	842	BCR	C1-C6	-3.70	1.48	1.53
19	a	825	CLA	C1D-ND	3.70	1.42	1.37
19	a	802	CLA	C1D-ND	3.70	1.42	1.37
19	a	842	CLA	C1D-ND	3.70	1.42	1.37
31	f	205	ZEX	C10-C9	3.70	1.40	1.35
31	f	205	ZEX	C14-C13	3.69	1.40	1.35
19	l	204	CLA	C1D-ND	3.69	1.42	1.37
19	b	826	CLA	C1D-ND	3.69	1.42	1.37
19	a	860	CLA	C1D-ND	3.69	1.42	1.37
19	f	204	CLA	C1D-ND	3.69	1.42	1.37
19	a	813	CLA	C1D-ND	3.69	1.42	1.37
19	a	821	CLA	C1D-ND	3.68	1.42	1.37
19	a	812	CLA	C1D-ND	3.68	1.42	1.37
19	a	822	CLA	C1D-ND	3.68	1.42	1.37
19	b	808	CLA	C1D-ND	3.67	1.42	1.37
19	a	823	CLA	C1D-ND	3.67	1.42	1.37
19	f	201	CLA	C1D-ND	3.67	1.42	1.37
19	b	815	CLA	C1D-ND	3.67	1.42	1.37
19	b	832	CLA	C1D-ND	3.67	1.42	1.37
28	a	858	45D	C37-C35	3.67	1.40	1.35
19	a	818	CLA	C1D-ND	3.67	1.42	1.37
19	b	801	CLA	C1D-ND	3.66	1.42	1.37
19	b	837	CLA	C1D-ND	3.66	1.42	1.37
19	a	803	CLA	C1D-ND	3.66	1.42	1.37
19	b	820	CLA	C1D-ND	3.66	1.42	1.37
19	a	838	CLA	C1D-ND	3.65	1.42	1.37
19	b	840	CLA	C1D-ND	3.65	1.42	1.37
19	b	835	CLA	C1D-ND	3.64	1.42	1.37
19	a	804	CLA	C1D-ND	3.64	1.42	1.37
19	a	839	CLA	C1D-ND	3.64	1.42	1.37
19	b	813	CLA	C1D-ND	3.64	1.42	1.37
19	b	831	CLA	C1D-ND	3.64	1.42	1.37
19	b	811	CLA	C1D-ND	3.63	1.42	1.37
19	b	825	CLA	C1D-ND	3.63	1.42	1.37
19	b	839	CLA	C1D-ND	3.63	1.42	1.37
19	b	806	CLA	C1D-ND	3.63	1.42	1.37
19	b	803	CLA	C1D-ND	3.63	1.42	1.37
19	a	828	CLA	C1D-ND	3.62	1.42	1.37
19	b	807	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	858	45D	C38-C36	3.62	1.40	1.35
19	b	836	CLA	C1D-ND	3.62	1.42	1.37
28	a	858	45D	C29-C25	3.62	1.40	1.35
19	A	402	CLA	C1D-ND	3.62	1.42	1.37
19	b	823	CLA	C1D-ND	3.61	1.42	1.37
19	a	835	CLA	C1D-ND	3.61	1.42	1.37
19	a	833	CLA	C1D-ND	3.61	1.42	1.37
19	b	804	CLA	C1D-ND	3.61	1.42	1.37
21	a	859	BCR	C1-C6	-3.61	1.48	1.53
31	b	852	ZEX	C10-C9	3.61	1.40	1.35
21	a	846	BCR	C1-C6	-3.61	1.48	1.53
21	f	202	BCR	C1-C6	-3.61	1.48	1.53
19	a	857	CLA	C1D-ND	3.60	1.42	1.37
21	a	849	BCR	C1-C6	-3.60	1.48	1.53
19	b	821	CLA	C1D-ND	3.60	1.42	1.37
19	a	806	CLA	C1D-ND	3.59	1.42	1.37
19	a	815	CLA	C1D-ND	3.59	1.42	1.37
19	b	817	CLA	C1D-ND	3.59	1.42	1.37
19	b	833	CLA	C1D-ND	3.59	1.42	1.37
19	D	402	CLA	C1D-ND	3.59	1.42	1.37
19	b	834	CLA	C1D-ND	3.58	1.42	1.37
19	a	831	CLA	C1D-ND	3.58	1.42	1.37
30	b	851	EQ3	C21-C22	3.58	1.40	1.35
19	a	811	CLA	C1D-ND	3.58	1.42	1.37
19	a	807	CLA	C1D-ND	3.58	1.42	1.37
19	b	818	CLA	C1D-ND	3.58	1.42	1.37
23	a	801	CL0	C1D-ND	3.57	1.42	1.37
19	a	809	CLA	C1D-ND	3.57	1.42	1.37
19	a	826	CLA	C1D-ND	3.57	1.42	1.37
19	b	830	CLA	C1D-ND	3.57	1.42	1.37
21	j	101	BCR	C1-C6	-3.57	1.48	1.53
19	a	843	CLA	C1D-ND	3.57	1.42	1.37
19	b	819	CLA	C1D-ND	3.56	1.42	1.37
19	a	808	CLA	C1D-ND	3.56	1.42	1.37
19	b	810	CLA	C1D-ND	3.56	1.42	1.37
19	a	816	CLA	C1D-ND	3.56	1.42	1.37
21	a	847	BCR	C1-C6	-3.55	1.48	1.53
19	a	820	CLA	C1D-ND	3.55	1.42	1.37
19	a	827	CLA	C1D-ND	3.55	1.42	1.37
19	b	822	CLA	C1D-ND	3.55	1.42	1.37
19	b	824	CLA	C1D-ND	3.55	1.42	1.37
19	a	834	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	848	BCR	C1-C6	-3.54	1.48	1.53
19	l	203	CLA	C1D-ND	3.54	1.42	1.37
19	b	838	CLA	C1D-ND	3.54	1.42	1.37
19	a	856	CLA	C1D-ND	3.54	1.42	1.37
30	b	851	EQ3	C17-C18	3.54	1.40	1.35
19	b	814	CLA	C1D-ND	3.52	1.42	1.37
28	a	858	45D	C30-C26	3.51	1.40	1.35
19	b	828	CLA	C1D-ND	3.51	1.42	1.37
19	a	810	CLA	C1D-ND	3.51	1.42	1.37
30	b	851	EQ3	C10-C9	3.49	1.40	1.35
21	A	406	BCR	C1-C6	-3.49	1.49	1.53
30	b	851	EQ3	C14-C13	3.48	1.40	1.35
19	a	805	CLA	C1D-ND	3.47	1.42	1.37
19	b	805	CLA	C1D-ND	3.47	1.42	1.37
21	l	205	BCR	C1-C6	-3.47	1.49	1.53
19	a	836	CLA	C1D-ND	3.45	1.42	1.37
19	a	830	CLA	C1D-ND	3.45	1.42	1.37
21	a	851	BCR	C1-C6	-3.45	1.49	1.53
19	b	802	CLA	C1D-ND	3.44	1.42	1.37
19	a	832	CLA	C1D-ND	3.43	1.42	1.37
19	b	827	CLA	C1D-ND	3.43	1.42	1.37
21	b	843	BCR	C1-C6	-3.38	1.49	1.53
19	b	829	CLA	C4D-ND	-3.37	1.33	1.37
21	a	847	BCR	C30-C25	-3.36	1.49	1.53
29	m	101	ECH	C25-C26	3.35	1.40	1.35
21	b	846	BCR	C30-C25	-3.32	1.49	1.53
21	a	859	BCR	C30-C25	-3.32	1.49	1.53
21	b	842	BCR	C30-C25	-3.31	1.49	1.53
19	a	832	CLA	C4D-ND	-3.28	1.33	1.37
21	A	406	BCR	C30-C25	-3.28	1.49	1.53
21	i	101	BCR	C30-C25	-3.27	1.49	1.53
21	k	103	BCR	C1-C6	-3.26	1.49	1.53
19	a	805	CLA	CHC-C1C	3.24	1.43	1.35
19	j	104	CLA	CHC-C1C	3.24	1.43	1.35
19	b	807	CLA	C4D-ND	-3.24	1.33	1.37
19	a	803	CLA	CHC-C1C	3.23	1.43	1.35
19	b	804	CLA	C4D-ND	-3.23	1.33	1.37
21	b	843	BCR	C30-C25	-3.22	1.49	1.53
19	a	809	CLA	C4D-ND	-3.22	1.33	1.37
21	b	845	BCR	C1-C6	-3.22	1.49	1.53
21	i	102	BCR	C1-C6	-3.21	1.49	1.53
19	a	839	CLA	C4D-ND	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	836	CLA	C4D-ND	-3.21	1.33	1.37
21	b	847	BCR	C30-C25	-3.20	1.49	1.53
19	a	838	CLA	C4D-ND	-3.20	1.33	1.37
21	b	846	BCR	C1-C6	-3.20	1.49	1.53
19	a	856	CLA	C4D-ND	-3.19	1.33	1.37
19	b	805	CLA	C4D-ND	-3.19	1.33	1.37
19	b	802	CLA	CHC-C1C	3.19	1.43	1.35
19	b	837	CLA	C4D-ND	-3.19	1.33	1.37
21	i	101	BCR	C1-C6	-3.18	1.49	1.53
19	a	828	CLA	C4D-ND	-3.17	1.33	1.37
19	b	806	CLA	C4D-ND	-3.17	1.33	1.37
21	k	103	BCR	C30-C25	-3.17	1.49	1.53
19	a	827	CLA	C4D-ND	-3.16	1.33	1.37
21	a	849	BCR	C30-C25	-3.16	1.49	1.53
19	b	825	CLA	C4D-ND	-3.16	1.33	1.37
19	D	403	CLA	CHC-C1C	3.15	1.43	1.35
19	b	824	CLA	C4D-ND	-3.15	1.33	1.37
19	a	805	CLA	C4D-ND	-3.15	1.33	1.37
19	a	815	CLA	CHC-C1C	3.15	1.43	1.35
19	b	827	CLA	C4D-ND	-3.14	1.33	1.37
21	b	847	BCR	C1-C6	-3.14	1.49	1.53
19	b	831	CLA	CHC-C1C	3.14	1.43	1.35
19	b	838	CLA	C4D-ND	-3.14	1.33	1.37
19	a	806	CLA	C4D-ND	-3.14	1.33	1.37
19	b	803	CLA	CHC-C1C	3.14	1.43	1.35
19	b	813	CLA	C4D-ND	-3.14	1.33	1.37
19	a	837	CLA	CHC-C1C	3.13	1.43	1.35
19	b	810	CLA	C4D-ND	-3.13	1.33	1.37
19	a	808	CLA	CHC-C1C	3.13	1.43	1.35
19	l	202	CLA	CHC-C1C	3.13	1.43	1.35
19	a	820	CLA	C4D-ND	-3.13	1.33	1.37
19	b	833	CLA	C4D-ND	-3.13	1.33	1.37
19	b	812	CLA	CHC-C1C	3.13	1.43	1.35
19	b	840	CLA	CHC-C1C	3.13	1.43	1.35
19	b	821	CLA	C4D-ND	-3.13	1.33	1.37
19	b	814	CLA	C4D-ND	-3.13	1.33	1.37
19	a	811	CLA	CHC-C1C	3.13	1.43	1.35
19	b	830	CLA	CHC-C1C	3.13	1.43	1.35
19	k	102	CLA	CHC-C1C	3.13	1.43	1.35
19	a	825	CLA	C4D-ND	-3.13	1.33	1.37
19	b	822	CLA	C4D-ND	-3.12	1.33	1.37
19	a	843	CLA	CHC-C1C	3.12	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	828	CLA	CHC-C1C	3.12	1.43	1.35
21	a	850	BCR	C30-C25	-3.12	1.49	1.53
19	b	825	CLA	CHC-C1C	3.12	1.43	1.35
19	b	823	CLA	CHC-C1C	3.12	1.43	1.35
19	f	204	CLA	CHC-C1C	3.11	1.43	1.35
19	f	201	CLA	CHC-C1C	3.11	1.42	1.35
19	a	802	CLA	CHC-C1C	3.11	1.42	1.35
19	a	830	CLA	CHC-C1C	3.11	1.42	1.35
29	b	844	ECH	C23-C22	-3.11	1.39	1.45
19	a	809	CLA	CHC-C1C	3.11	1.42	1.35
19	b	839	CLA	C4D-ND	-3.11	1.33	1.37
21	f	202	BCR	C30-C25	-3.11	1.49	1.53
19	a	810	CLA	C4D-ND	-3.11	1.33	1.37
19	b	817	CLA	C4D-ND	-3.11	1.33	1.37
19	a	822	CLA	C4D-ND	-3.11	1.33	1.37
19	a	826	CLA	CHC-C1C	3.10	1.42	1.35
19	a	836	CLA	CHC-C1C	3.10	1.42	1.35
28	a	858	45D	C24-C26	-3.10	1.39	1.45
19	b	818	CLA	C4D-ND	-3.10	1.33	1.37
19	A	402	CLA	C4D-ND	-3.10	1.33	1.37
19	a	816	CLA	CHC-C1C	3.10	1.42	1.35
19	b	822	CLA	CHC-C1C	3.10	1.42	1.35
19	a	807	CLA	C4D-ND	-3.10	1.33	1.37
19	b	809	CLA	C4D-ND	-3.10	1.33	1.37
19	a	822	CLA	CHC-C1C	3.09	1.42	1.35
19	f	203	CLA	CHC-C1C	3.09	1.42	1.35
19	b	801	CLA	CHC-C1C	3.09	1.42	1.35
19	a	816	CLA	C4D-ND	-3.09	1.33	1.37
19	a	842	CLA	C4D-ND	-3.09	1.33	1.37
19	b	827	CLA	CHC-C1C	3.09	1.42	1.35
19	b	802	CLA	C4D-ND	-3.09	1.33	1.37
19	b	826	CLA	C4D-ND	-3.09	1.33	1.37
19	l	204	CLA	C4D-ND	-3.09	1.33	1.37
19	a	802	CLA	C4D-ND	-3.09	1.33	1.37
19	a	815	CLA	C4D-ND	-3.09	1.33	1.37
19	b	838	CLA	CHC-C1C	3.08	1.42	1.35
19	a	823	CLA	C4D-ND	-3.08	1.33	1.37
19	b	813	CLA	CHC-C1C	3.08	1.42	1.35
19	j	103	CLA	CHC-C1C	3.08	1.42	1.35
19	b	820	CLA	C4D-ND	-3.08	1.33	1.37
19	l	204	CLA	CHC-C1C	3.08	1.42	1.35
19	a	827	CLA	CHC-C1C	3.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	843	CLA	C4D-ND	-3.08	1.33	1.37
19	a	804	CLA	CHC-C1C	3.08	1.42	1.35
19	a	823	CLA	CHC-C1C	3.08	1.42	1.35
19	a	814	CLA	C4D-ND	-3.08	1.33	1.37
19	a	813	CLA	CHC-C1C	3.08	1.42	1.35
19	b	824	CLA	CHC-C1C	3.08	1.42	1.35
19	A	403	CLA	CHC-C1C	3.08	1.42	1.35
19	a	821	CLA	CHC-C1C	3.08	1.42	1.35
19	a	830	CLA	C4D-ND	-3.08	1.33	1.37
19	a	842	CLA	CHC-C1C	3.07	1.42	1.35
19	b	821	CLA	CHC-C1C	3.07	1.42	1.35
19	a	824	CLA	CHC-C1C	3.07	1.42	1.35
19	b	818	CLA	CHC-C1C	3.07	1.42	1.35
19	a	857	CLA	C4D-ND	-3.07	1.33	1.37
19	A	405	CLA	CHC-C1C	3.07	1.42	1.35
19	a	813	CLA	C4D-ND	-3.07	1.33	1.37
19	A	407	CLA	CHC-C1C	3.07	1.42	1.35
19	b	828	CLA	CHC-C1C	3.07	1.42	1.35
19	b	820	CLA	CHC-C1C	3.07	1.42	1.35
19	b	837	CLA	CHC-C1C	3.07	1.42	1.35
19	a	819	CLA	CHC-C1C	3.07	1.42	1.35
19	b	815	CLA	CHC-C1C	3.06	1.42	1.35
19	b	835	CLA	CHC-C1C	3.06	1.42	1.35
19	b	835	CLA	C4D-ND	-3.06	1.33	1.37
19	b	819	CLA	CHC-C1C	3.06	1.42	1.35
19	a	833	CLA	C4D-ND	-3.06	1.33	1.37
19	b	833	CLA	CHC-C1C	3.06	1.42	1.35
19	a	834	CLA	C4D-ND	-3.06	1.33	1.37
19	b	823	CLA	C4D-ND	-3.06	1.33	1.37
19	a	812	CLA	C4D-ND	-3.06	1.33	1.37
19	a	810	CLA	CHC-C1C	3.06	1.42	1.35
19	D	402	CLA	C4D-ND	-3.06	1.33	1.37
19	b	811	CLA	C4D-ND	-3.06	1.33	1.37
19	b	826	CLA	CHC-C1C	3.05	1.42	1.35
19	b	829	CLA	CHC-C1C	3.05	1.42	1.35
19	a	808	CLA	C4D-ND	-3.05	1.33	1.37
19	l	203	CLA	CHC-C1C	3.05	1.42	1.35
23	a	801	CL0	C4D-ND	-3.05	1.33	1.37
19	b	808	CLA	CHC-C1C	3.05	1.42	1.35
21	b	845	BCR	C30-C25	-3.05	1.49	1.53
19	b	809	CLA	CHC-C1C	3.05	1.42	1.35
19	a	824	CLA	C4D-ND	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	804	CLA	C4D-ND	-3.05	1.33	1.37
19	a	833	CLA	CHC-C1C	3.05	1.42	1.35
19	k	101	CLA	CHC-C1C	3.05	1.42	1.35
19	a	821	CLA	C4D-ND	-3.05	1.33	1.37
19	a	839	CLA	CHC-C1C	3.05	1.42	1.35
21	a	846	BCR	C30-C25	-3.04	1.49	1.53
19	b	830	CLA	C4D-ND	-3.04	1.33	1.37
19	b	832	CLA	CHC-C1C	3.04	1.42	1.35
19	a	841	CLA	C4D-ND	-3.04	1.33	1.37
19	a	829	CLA	CHC-C1C	3.04	1.42	1.35
19	a	817	CLA	C4D-ND	-3.04	1.33	1.37
19	b	816	CLA	C4D-ND	-3.04	1.33	1.37
19	b	832	CLA	C4D-ND	-3.04	1.33	1.37
19	b	840	CLA	C4D-ND	-3.04	1.33	1.37
19	a	820	CLA	CHC-C1C	3.04	1.42	1.35
19	a	832	CLA	CHC-C1C	3.04	1.42	1.35
19	a	831	CLA	C4D-ND	-3.03	1.33	1.37
19	f	203	CLA	C4D-ND	-3.03	1.33	1.37
19	a	857	CLA	CHC-C1C	3.03	1.42	1.35
19	a	840	CLA	C4D-ND	-3.03	1.33	1.37
19	b	808	CLA	C4D-ND	-3.03	1.33	1.37
19	b	819	CLA	C4D-ND	-3.03	1.33	1.37
19	a	812	CLA	CHC-C1C	3.03	1.42	1.35
19	a	860	CLA	CHC-C1C	3.03	1.42	1.35
19	b	804	CLA	CHC-C1C	3.03	1.42	1.35
19	b	831	CLA	C4D-ND	-3.03	1.33	1.37
19	a	806	CLA	CHC-C1C	3.03	1.42	1.35
19	b	801	CLA	C4D-ND	-3.03	1.33	1.37
19	b	828	CLA	C4D-ND	-3.03	1.33	1.37
19	b	807	CLA	CHC-C1C	3.03	1.42	1.35
19	A	407	CLA	C4D-ND	-3.02	1.33	1.37
19	b	805	CLA	CHC-C1C	3.02	1.42	1.35
21	j	101	BCR	C30-C25	-3.02	1.49	1.53
30	b	851	EQ3	C23-C22	-3.02	1.39	1.45
19	a	856	CLA	CHC-C1C	3.02	1.42	1.35
23	a	801	CL0	CHC-C1C	3.02	1.42	1.35
19	a	807	CLA	CHC-C1C	3.02	1.42	1.35
19	a	819	CLA	C4D-ND	-3.02	1.33	1.37
19	a	831	CLA	CHC-C1C	3.01	1.42	1.35
19	a	838	CLA	CHC-C1C	3.01	1.42	1.35
19	a	817	CLA	CHC-C1C	3.01	1.42	1.35
19	a	825	CLA	CHC-C1C	3.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	858	45D	C23-C25	-3.01	1.39	1.45
22	E	101	HEM	CAB-C3B	3.01	1.55	1.47
19	D	402	CLA	CHC-C1C	3.01	1.42	1.35
19	a	811	CLA	C4D-ND	-3.01	1.33	1.37
19	b	803	CLA	C4D-ND	-3.01	1.33	1.37
19	b	834	CLA	CHC-C1C	3.00	1.42	1.35
19	b	814	CLA	CHC-C1C	3.00	1.42	1.35
19	a	818	CLA	CHC-C1C	3.00	1.42	1.35
31	f	205	ZEX	C8-C9	-3.00	1.39	1.45
19	b	812	CLA	C4D-ND	-3.00	1.33	1.37
19	A	405	CLA	C4D-ND	-2.99	1.33	1.37
19	b	834	CLA	C4D-ND	-2.99	1.33	1.37
19	a	841	CLA	CHC-C1C	2.99	1.42	1.35
19	a	835	CLA	CHC-C1C	2.99	1.42	1.35
19	a	836	CLA	C4D-ND	-2.99	1.33	1.37
19	A	402	CLA	CHC-C1C	2.99	1.42	1.35
19	a	840	CLA	CHC-C1C	2.99	1.42	1.35
19	a	837	CLA	C4D-ND	-2.99	1.33	1.37
19	b	815	CLA	C4D-ND	-2.99	1.33	1.37
19	b	836	CLA	CHC-C1C	2.99	1.42	1.35
19	a	829	CLA	C4D-ND	-2.98	1.33	1.37
19	f	201	CLA	C4D-ND	-2.98	1.33	1.37
19	b	810	CLA	CHC-C1C	2.98	1.42	1.35
21	a	848	BCR	C30-C25	-2.98	1.49	1.53
19	a	834	CLA	CHC-C1C	2.98	1.42	1.35
19	b	817	CLA	CHC-C1C	2.98	1.42	1.35
19	b	811	CLA	CHC-C1C	2.98	1.42	1.35
31	b	852	ZEX	C8-C9	-2.97	1.39	1.45
19	a	835	CLA	C4D-ND	-2.97	1.33	1.37
19	A	403	CLA	C4D-ND	-2.96	1.33	1.37
19	a	814	CLA	CHC-C1C	2.96	1.42	1.35
19	j	104	CLA	C4D-ND	-2.95	1.33	1.37
19	a	860	CLA	C4D-ND	-2.95	1.33	1.37
19	a	826	CLA	C4D-ND	-2.94	1.33	1.37
30	b	851	EQ3	C25-C26	2.94	1.39	1.35
19	f	204	CLA	C4D-ND	-2.94	1.33	1.37
19	l	203	CLA	C4D-ND	-2.94	1.33	1.37
19	b	839	CLA	CHC-C1C	2.94	1.42	1.35
19	D	403	CLA	C4D-ND	-2.94	1.33	1.37
31	f	205	ZEX	C28-C29	-2.93	1.39	1.45
19	b	806	CLA	CHC-C1C	2.93	1.42	1.35
19	k	102	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	851	EQ3	C8-C9	-2.92	1.39	1.45
19	a	818	CLA	C4D-ND	-2.91	1.33	1.37
19	j	103	CLA	C4D-ND	-2.89	1.33	1.37
29	m	101	ECH	C23-C22	-2.88	1.39	1.45
21	l	205	BCR	C30-C25	-2.87	1.49	1.53
19	b	816	CLA	CHC-C1C	2.83	1.42	1.35
31	b	852	ZEX	C28-C29	-2.83	1.39	1.45
19	l	202	CLA	C4D-ND	-2.80	1.33	1.37
29	m	101	ECH	C8-C9	-2.80	1.39	1.45
19	b	839	CLA	CMB-C2B	-2.79	1.45	1.51
29	b	844	ECH	C8-C9	-2.79	1.39	1.45
19	k	101	CLA	C4D-ND	-2.77	1.33	1.37
19	a	803	CLA	C4D-ND	-2.72	1.33	1.37
28	a	858	45D	C08-C16	2.71	1.39	1.35
20	D	401	PHO	CAC-C3C	-2.70	1.47	1.52
20	A	404	PHO	CAC-C3C	-2.68	1.47	1.52
32	j	102	LMT	O3'-C3'	-2.68	1.36	1.43
19	b	834	CLA	CMB-C2B	-2.65	1.46	1.51
21	i	102	BCR	C30-C25	-2.65	1.50	1.53
19	b	828	CLA	CMB-C2B	-2.65	1.46	1.51
19	a	831	CLA	CMB-C2B	-2.64	1.46	1.51
19	b	808	CLA	CMB-C2B	-2.64	1.46	1.51
19	a	857	CLA	CMB-C2B	-2.63	1.46	1.51
19	a	836	CLA	CMB-C2B	-2.61	1.46	1.51
19	a	819	CLA	CMB-C2B	-2.60	1.46	1.51
23	a	801	CL0	CMB-C2B	-2.59	1.46	1.51
19	a	822	CLA	CMB-C2B	-2.58	1.46	1.51
19	b	814	CLA	CMB-C2B	-2.58	1.46	1.51
19	a	832	CLA	CMB-C2B	-2.57	1.46	1.51
19	a	821	CLA	CMB-C2B	-2.57	1.46	1.51
19	a	820	CLA	CMB-C2B	-2.56	1.46	1.51
19	a	834	CLA	CMB-C2B	-2.55	1.46	1.51
19	a	842	CLA	CMB-C2B	-2.55	1.46	1.51
19	f	201	CLA	CMB-C2B	-2.55	1.46	1.51
19	a	804	CLA	CMB-C2B	-2.55	1.46	1.51
30	b	851	EQ3	C19-C18	-2.54	1.40	1.45
19	b	837	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	818	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	839	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	840	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	801	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	822	CLA	CMB-C2B	-2.53	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	831	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	811	CLA	CMB-C2B	-2.52	1.46	1.51
19	a	835	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	818	CLA	CMB-C2B	-2.52	1.46	1.51
19	a	828	CLA	CMB-C2B	-2.52	1.46	1.51
19	a	813	CLA	CMB-C2B	-2.52	1.46	1.51
19	a	841	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	836	CLA	CMB-C2B	-2.51	1.46	1.51
19	b	817	CLA	CMB-C2B	-2.51	1.46	1.51
19	b	829	CLA	CMB-C2B	-2.51	1.46	1.51
19	a	824	CLA	CMB-C2B	-2.51	1.46	1.51
19	a	833	CLA	CMB-C2B	-2.51	1.46	1.51
32	j	102	LMT	O2'-C2'	-2.51	1.37	1.43
19	b	806	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	805	CLA	CMB-C2B	-2.50	1.46	1.51
29	b	844	ECH	C19-C18	-2.50	1.40	1.45
19	b	838	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	806	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	816	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	819	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	809	CLA	CMB-C2B	-2.49	1.46	1.51
19	f	204	CLA	CMB-C2B	-2.49	1.46	1.51
29	b	844	ECH	C12-C13	-2.49	1.40	1.45
19	b	807	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	821	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	823	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	813	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	832	CLA	CMB-C2B	-2.49	1.46	1.51
30	b	851	EQ3	C12-C13	-2.48	1.40	1.45
19	b	833	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	825	CLA	CMB-C2B	-2.48	1.46	1.51
19	b	824	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	817	CLA	CMB-C2B	-2.48	1.46	1.51
31	b	852	ZEX	C12-C13	-2.48	1.40	1.45
19	a	838	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	807	CLA	CMB-C2B	-2.48	1.46	1.51
19	j	103	CLA	CMB-C2B	-2.47	1.46	1.51
19	b	827	CLA	CMB-C2B	-2.47	1.46	1.51
19	a	829	CLA	CMB-C2B	-2.47	1.46	1.51
19	l	203	CLA	CMB-C2B	-2.47	1.46	1.51
19	b	805	CLA	CMB-C2B	-2.47	1.46	1.51
19	a	826	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	815	CLA	CMB-C2B	-2.47	1.46	1.51
19	a	803	CLA	CMB-C2B	-2.47	1.46	1.51
19	a	843	CLA	CMB-C2B	-2.47	1.46	1.51
32	j	102	LMT	O2B-C2B	-2.46	1.37	1.43
19	A	407	CLA	CMB-C2B	-2.46	1.46	1.51
19	a	860	CLA	CMB-C2B	-2.46	1.46	1.51
19	a	812	CLA	CMB-C2B	-2.46	1.46	1.51
19	a	856	CLA	CMB-C2B	-2.46	1.46	1.51
28	a	858	45D	C34-C36	-2.46	1.40	1.45
31	f	205	ZEX	C12-C13	-2.46	1.40	1.45
19	a	815	CLA	CMB-C2B	-2.45	1.46	1.51
19	a	827	CLA	CMB-C2B	-2.45	1.46	1.51
19	l	202	CLA	CMB-C2B	-2.45	1.46	1.51
19	b	803	CLA	CMB-C2B	-2.45	1.46	1.51
19	b	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	k	102	CLA	CMB-C2B	-2.44	1.46	1.51
19	l	204	CLA	CMB-C2B	-2.44	1.46	1.51
19	f	203	CLA	CMB-C2B	-2.44	1.46	1.51
19	a	802	CLA	CMB-C2B	-2.44	1.46	1.51
19	b	825	CLA	CMB-C2B	-2.44	1.46	1.51
19	b	810	CLA	CMB-C2B	-2.44	1.46	1.51
19	a	830	CLA	CMB-C2B	-2.43	1.46	1.51
19	k	101	CLA	CMB-C2B	-2.43	1.46	1.51
19	D	402	CLA	CMB-C2B	-2.43	1.46	1.51
26	a	852	LHG	O7-C5	-2.42	1.40	1.46
19	A	403	CLA	CMB-C2B	-2.42	1.46	1.51
19	A	402	CLA	CMB-C2B	-2.42	1.46	1.51
19	b	840	CLA	CMB-C2B	-2.42	1.46	1.51
19	a	808	CLA	CMB-C2B	-2.42	1.46	1.51
19	b	802	CLA	CMB-C2B	-2.42	1.46	1.51
19	b	804	CLA	CMB-C2B	-2.42	1.46	1.51
19	a	810	CLA	CMB-C2B	-2.41	1.46	1.51
28	a	858	45D	C33-C35	-2.41	1.40	1.45
19	a	837	CLA	CMB-C2B	-2.41	1.46	1.51
19	A	405	CLA	CMB-C2B	-2.41	1.46	1.51
19	D	403	CLA	CMB-C2B	-2.41	1.46	1.51
19	a	816	CLA	CMB-C2B	-2.41	1.46	1.51
19	a	814	CLA	CMB-C2B	-2.41	1.46	1.51
19	b	820	CLA	CMB-C2B	-2.41	1.46	1.51
19	b	826	CLA	CMB-C2B	-2.41	1.46	1.51
19	b	835	CLA	CMB-C2B	-2.40	1.46	1.51
19	a	811	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	852	ZEX	C32-C33	-2.39	1.40	1.45
19	b	830	CLA	CMB-C2B	-2.39	1.46	1.51
19	b	839	CLA	C3B-C2B	-2.38	1.37	1.40
19	a	823	CLA	CMB-C2B	-2.38	1.46	1.51
31	f	205	ZEX	C32-C33	-2.37	1.40	1.45
19	b	812	CLA	CMB-C2B	-2.37	1.46	1.51
19	j	104	CLA	CMB-C2B	-2.34	1.46	1.51
32	j	102	LMT	O3B-C3B	-2.31	1.37	1.43
26	b	849	LHG	O7-C5	-2.31	1.40	1.46
29	m	101	ECH	C12-C13	-2.30	1.41	1.45
19	b	828	CLA	CMD-C2D	-2.29	1.45	1.50
19	b	822	CLA	CMD-C2D	-2.26	1.46	1.50
19	a	810	CLA	CMD-C2D	-2.25	1.46	1.50
19	b	801	CLA	CMD-C2D	-2.21	1.46	1.50
27	b	850	LMG	O7-C8	-2.20	1.41	1.46
19	b	823	CLA	CMD-C2D	-2.20	1.46	1.50
19	a	836	CLA	CMD-C2D	-2.19	1.46	1.50
19	b	802	CLA	CMC-C2C	-2.18	1.46	1.50
19	b	827	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	806	CLA	CMD-C2D	-2.17	1.46	1.50
19	a	828	CLA	CMC-C2C	-2.17	1.46	1.50
19	a	806	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	830	CLA	CMD-C2D	-2.15	1.46	1.50
29	m	101	ECH	C19-C18	-2.15	1.41	1.45
19	a	826	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	809	CLA	CMD-C2D	-2.14	1.46	1.50
19	b	813	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	809	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	824	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	838	CLA	CMD-C2D	-2.12	1.46	1.50
19	A	402	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	837	CLA	C3B-C2B	-2.12	1.37	1.40
19	a	825	CLA	CMD-C2D	-2.12	1.46	1.50
19	f	201	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	834	CLA	CMD-C2D	-2.11	1.46	1.50
19	b	835	CLA	CMD-C2D	-2.11	1.46	1.50
19	b	804	CLA	CMD-C2D	-2.11	1.46	1.50
19	b	811	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	831	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	804	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	404	PHO	CMD-C2D	-2.11	1.46	1.51
19	a	819	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	807	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	832	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	805	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	825	CLA	CMC-C2C	-2.10	1.46	1.50
19	a	820	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	815	CLA	CMD-C2D	-2.10	1.46	1.50
32	j	102	LMT	O4'-C4B	-2.10	1.38	1.43
19	l	203	CLA	CMD-C2D	-2.09	1.46	1.50
20	D	401	PHO	CMC-C2C	-2.09	1.46	1.51
19	b	833	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	404	PHO	CMC-C2C	-2.09	1.46	1.51
19	b	837	CLA	CMD-C2D	-2.09	1.46	1.50
19	b	807	CLA	CMC-C2C	-2.09	1.46	1.50
19	a	816	CLA	CMD-C2D	-2.09	1.46	1.50
19	b	808	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	827	CLA	CMD-C2D	-2.09	1.46	1.50
19	b	826	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	838	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	840	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	814	CLA	CMC-C2C	-2.08	1.46	1.50
19	a	835	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	817	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	803	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	820	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	818	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	833	CLA	CMD-C2D	-2.08	1.46	1.50
19	D	402	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	819	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	802	CLA	CMD-C2D	-2.08	1.46	1.50
26	a	855	LHG	O7-C5	-2.08	1.41	1.46
19	b	814	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	824	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	836	CLA	CMD-C2D	-2.07	1.46	1.50
27	b	848	LMG	O7-C8	-2.07	1.41	1.46
19	a	818	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	830	CLA	CMD-C2D	-2.07	1.46	1.50
26	a	853	LHG	O7-C5	-2.07	1.41	1.46
19	a	856	CLA	CMD-C2D	-2.07	1.46	1.50
19	a	841	CLA	CMC-C2C	-2.07	1.46	1.50
19	a	857	CLA	CMD-C2D	-2.07	1.46	1.50
19	l	203	CLA	CMC-C2C	-2.07	1.46	1.50
19	b	832	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	807	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	829	CLA	CMD-C2D	-2.06	1.46	1.50
19	b	815	CLA	CMD-C2D	-2.06	1.46	1.50
19	b	823	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	808	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	803	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	837	CLA	CMD-C2D	-2.06	1.46	1.50
19	f	203	CLA	CMD-C2D	-2.06	1.46	1.50
19	D	402	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	828	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	812	CLA	CMD-C2D	-2.05	1.46	1.50
20	D	401	PHO	C3B-C2B	-2.05	1.37	1.40
19	b	832	CLA	CMC-C2C	-2.05	1.46	1.50
19	b	821	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	805	CLA	CMC-C2C	-2.05	1.46	1.50
19	a	841	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	825	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	829	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	839	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	834	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	814	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	817	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	404	PHO	CMB-C2B	-2.04	1.46	1.51
19	a	843	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	819	CLA	CMC-C2C	-2.04	1.46	1.50
23	a	801	CL0	CMD-C2D	-2.04	1.46	1.50
22	E	101	HEM	FE-NB	2.04	2.07	1.96
19	b	839	CLA	CMD-C2D	-2.04	1.46	1.50
19	k	101	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	842	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	821	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	812	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	840	CLA	C3B-C2B	-2.04	1.37	1.40
19	a	813	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	856	CLA	CMC-C2C	-2.04	1.46	1.50
21	a	859	BCR	C33-C5	-2.04	1.47	1.50
19	a	806	CLA	CMC-C2C	-2.03	1.46	1.50
19	A	402	CLA	CMC-C2C	-2.03	1.46	1.50
22	E	101	HEM	CMB-C2B	2.03	1.55	1.50
19	a	803	CLA	CMD-C2D	-2.03	1.46	1.50
19	b	831	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	813	CLA	C3B-C2B	-2.03	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	810	CLA	CMD-C2D	-2.03	1.46	1.50
20	D	401	PHO	CMB-C2B	-2.03	1.46	1.51
19	b	805	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	843	CLA	CMD-C2D	-2.03	1.46	1.50
19	b	814	CLA	C3B-C2B	-2.03	1.37	1.40
19	a	811	CLA	CMD-C2D	-2.02	1.46	1.50
19	k	102	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	831	CLA	C3B-C2B	-2.02	1.37	1.40
32	j	102	LMT	O1'-C1'	-2.02	1.36	1.40
19	a	804	CLA	CMC-C2C	-2.02	1.46	1.50
20	D	401	PHO	CMD-C2D	-2.02	1.46	1.51
19	A	403	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	812	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	816	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	818	CLA	CMC-C2C	-2.01	1.46	1.50
19	j	104	CLA	CMD-C2D	-2.01	1.46	1.50
19	b	835	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	826	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	813	CLA	CMD-C2D	-2.01	1.46	1.50
19	b	816	CLA	CMD-C2D	-2.01	1.46	1.50
19	b	821	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	827	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	821	CLA	CMC-C2C	-2.01	1.46	1.50
19	A	405	CLA	CMD-C2D	-2.01	1.46	1.50
19	a	822	CLA	CMD-C2D	-2.01	1.46	1.50
19	a	819	CLA	C3B-CAB	-2.00	1.43	1.47
19	l	204	CLA	CMD-C2D	-2.00	1.46	1.50
19	A	407	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	805	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	801	CLA	CMC-C2C	-2.00	1.46	1.50
19	a	831	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	814	CLA	CMC-C2C	-2.00	1.46	1.50
20	D	401	PHO	C3B-CAB	-2.00	1.43	1.47

All (1003) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	844	ECH	C15-C16-C17	8.39	140.66	123.47
19	a	806	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	a	842	CLA	C4A-NA-C1A	7.09	109.89	106.71
19	a	841	CLA	C4A-NA-C1A	7.05	109.88	106.71
19	a	818	CLA	C4A-NA-C1A	7.04	109.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	836	CLA	C4A-NA-C1A	7.03	109.87	106.71
19	a	835	CLA	C4A-NA-C1A	7.00	109.86	106.71
19	b	815	CLA	C4A-NA-C1A	6.98	109.84	106.71
19	j	103	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	b	828	CLA	C4A-NA-C1A	6.89	109.80	106.71
19	b	839	CLA	C4A-NA-C1A	6.88	109.80	106.71
19	a	810	CLA	C4A-NA-C1A	6.87	109.79	106.71
19	a	823	CLA	C4A-NA-C1A	6.86	109.79	106.71
19	a	840	CLA	C4A-NA-C1A	6.86	109.79	106.71
19	D	402	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	l	203	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	a	832	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	b	806	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	a	817	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	b	816	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	D	403	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	b	826	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	b	834	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	a	801	CL0	C4A-NA-C1A	6.71	109.72	106.71
19	b	837	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	b	821	CLA	C4A-NA-C1A	6.69	109.72	106.71
19	b	832	CLA	C4A-NA-C1A	6.69	109.72	106.71
19	l	204	CLA	C4A-NA-C1A	6.69	109.71	106.71
19	a	824	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	a	814	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	a	834	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	b	824	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	a	826	CLA	C4A-NA-C1A	6.66	109.70	106.71
19	b	805	CLA	C4A-NA-C1A	6.66	109.70	106.71
19	b	838	CLA	C4A-NA-C1A	6.66	109.70	106.71
19	a	808	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	b	833	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	a	831	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	b	811	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	b	804	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	a	837	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A	407	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	a	819	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	b	802	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	f	201	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	a	857	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	A	403	CLA	C4A-NA-C1A	6.58	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	816	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	a	804	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	a	821	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	a	807	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	a	860	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	b	810	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	a	829	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	b	813	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	b	803	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	b	808	CLA	C4A-NA-C1A	6.51	109.64	106.71
19	a	838	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	b	840	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	b	817	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	a	809	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	b	820	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	a	839	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	f	203	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	a	813	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	A	405	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	a	828	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	b	822	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	a	827	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	a	815	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	b	818	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	b	807	CLA	C4A-NA-C1A	6.38	109.58	106.71
19	a	836	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	a	825	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	b	831	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	b	823	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	b	819	CLA	C4A-NA-C1A	6.31	109.54	106.71
19	f	204	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	A	402	CLA	C4A-NA-C1A	6.29	109.53	106.71
19	b	825	CLA	C4A-NA-C1A	6.29	109.53	106.71
19	a	811	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	a	843	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	a	802	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	a	805	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	k	102	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	b	829	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	l	202	CLA	C4A-NA-C1A	6.24	109.51	106.71
19	b	812	CLA	C4A-NA-C1A	6.23	109.51	106.71
19	a	812	CLA	C4A-NA-C1A	6.21	109.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	833	CLA	C4A-NA-C1A	6.18	109.48	106.71
19	b	809	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	a	830	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	b	814	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	a	820	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	j	104	CLA	C4A-NA-C1A	6.09	109.44	106.71
19	b	830	CLA	C4A-NA-C1A	6.03	109.42	106.71
19	a	822	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	a	803	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	b	827	CLA	C4A-NA-C1A	5.87	109.35	106.71
19	k	101	CLA	C4A-NA-C1A	5.82	109.32	106.71
19	a	856	CLA	C4A-NA-C1A	5.79	109.31	106.71
19	b	835	CLA	C4A-NA-C1A	5.71	109.27	106.71
19	b	801	CLA	C4A-NA-C1A	5.51	109.18	106.71
28	a	858	45D	C42-C41-C37	5.28	134.28	123.47
29	b	844	ECH	C12-C13-C14	4.97	126.57	118.94
29	b	844	ECH	C19-C18-C17	4.84	126.37	118.94
19	b	830	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
19	b	835	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
29	b	844	ECH	C24-C23-C22	-4.45	119.51	126.23
29	b	844	ECH	C35-C13-C14	-4.43	116.71	122.92
19	a	809	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
29	b	844	ECH	C36-C18-C17	-4.39	116.77	122.92
29	m	101	ECH	C37-C22-C21	-4.34	116.84	122.92
19	a	831	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
19	a	803	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
19	a	810	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
19	a	815	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
26	a	853	LHG	O4-P-O5	4.25	133.24	112.24
19	a	822	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
29	b	844	ECH	C1-C6-C5	-4.24	116.64	122.61
19	b	824	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
19	a	811	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
26	a	852	LHG	O4-P-O5	4.23	133.14	112.24
29	m	101	ECH	C15-C16-C17	4.22	132.12	123.47
19	a	816	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
26	a	855	LHG	O4-P-O5	4.21	133.04	112.24
19	a	814	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
19	b	804	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
31	b	852	ZEX	C39-C29-C30	-4.20	117.04	122.92
19	a	823	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
26	f	206	LHG	O4-P-O5	4.19	132.96	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	820	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
19	b	815	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
19	a	826	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
19	b	813	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
31	f	205	ZEX	C35-C15-C14	4.18	132.04	123.47
26	b	849	LHG	O4-P-O5	4.17	132.84	112.24
28	a	858	45D	C28-C26-C30	-4.15	117.11	122.92
19	a	802	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
19	a	806	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
19	b	812	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
31	f	205	ZEX	C19-C9-C10	-4.09	117.20	122.92
19	a	830	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
31	b	852	ZEX	C19-C9-C10	-4.08	117.21	122.92
19	a	807	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
19	b	827	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
29	m	101	ECH	C34-C9-C10	-4.06	117.24	122.92
19	b	826	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
19	a	856	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
19	b	834	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
28	a	858	45D	C27-C25-C29	-4.04	117.26	122.92
19	b	832	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
19	a	843	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
19	b	802	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
31	f	205	ZEX	C39-C29-C30	-4.01	117.31	122.92
19	a	805	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
29	m	101	ECH	C1-C6-C5	-3.97	117.02	122.61
30	b	851	EQ3	C34-C9-C10	-3.96	117.37	122.92
19	a	837	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
19	b	833	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
29	m	101	ECH	C23-C22-C21	3.94	124.98	118.94
19	b	840	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
19	a	812	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
19	b	823	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
19	l	202	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
19	b	817	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	a	829	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	b	805	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
19	b	835	CLA	CMB-C2B-C3B	3.85	131.89	124.68
19	b	830	CLA	CMB-C2B-C3B	3.83	131.85	124.68
19	b	828	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
19	a	819	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
19	a	817	CLA	CMB-C2B-C1B	-3.82	122.59	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	825	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
19	b	820	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
19	l	204	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
19	a	838	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
19	b	822	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
29	b	844	ECH	C10-C11-C12	3.78	135.00	123.22
19	f	203	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
19	D	402	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
19	j	104	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	A	407	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	b	803	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	b	808	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
19	A	402	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
30	b	851	EQ3	C37-C22-C21	-3.71	117.73	122.92
19	k	102	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
19	a	809	CLA	CMB-C2B-C3B	3.70	131.59	124.68
29	b	844	ECH	C34-C9-C10	-3.69	117.75	122.92
19	a	833	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
19	a	828	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
19	b	829	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
19	a	808	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
19	A	405	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
29	m	101	ECH	C36-C18-C17	-3.66	117.80	122.92
19	a	860	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
19	l	203	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
19	a	825	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
19	a	810	CLA	CMB-C2B-C3B	3.62	131.46	124.68
29	b	844	ECH	C37-C22-C21	-3.62	117.85	122.92
19	a	818	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
19	b	810	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
19	b	804	CLA	CMB-C2B-C3B	3.59	131.40	124.68
19	a	856	CLA	CMB-C2B-C3B	3.59	131.39	124.68
19	a	857	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
19	a	814	CLA	CMB-C2B-C3B	3.58	131.37	124.68
19	b	818	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
19	D	403	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
19	a	802	CLA	CMB-C2B-C3B	3.57	131.35	124.68
19	a	841	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
19	b	809	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
29	m	101	ECH	C19-C18-C17	3.55	124.38	118.94
19	b	838	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
19	b	815	CLA	CMB-C2B-C3B	3.53	131.29	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	831	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
19	b	806	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
19	a	815	CLA	CMB-C2B-C3B	3.52	131.26	124.68
19	b	824	CLA	CMB-C2B-C3B	3.51	131.25	124.68
19	a	823	CLA	CMB-C2B-C3B	3.51	131.25	124.68
19	a	816	CLA	CMB-C2B-C3B	3.51	131.24	124.68
19	b	812	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
21	b	845	BCR	C15-C16-C17	-3.51	116.29	123.47
19	a	840	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
19	a	811	CLA	CMB-C2B-C3B	3.50	131.23	124.68
31	b	852	ZEX	C35-C15-C14	3.50	130.63	123.47
19	a	820	CLA	CMB-C2B-C3B	3.50	131.22	124.68
19	b	819	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
19	a	835	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
19	b	813	CLA	CMB-C2B-C3B	3.49	131.20	124.68
19	k	101	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
19	j	103	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
19	a	813	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
19	b	812	CLA	CMB-C2B-C3B	3.48	131.19	124.68
19	b	821	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
19	a	831	CLA	CMB-C2B-C3B	3.48	131.18	124.68
19	b	826	CLA	CMB-C2B-C3B	3.48	131.18	124.68
19	a	806	CLA	CMB-C2B-C3B	3.47	131.18	124.68
19	b	827	CLA	CMB-C2B-C3B	3.47	131.17	124.68
19	a	826	CLA	CMB-C2B-C3B	3.47	131.16	124.68
19	b	801	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
19	A	403	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
19	a	827	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	a	815	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
19	f	204	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
19	b	836	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
19	a	830	CLA	CMB-C2B-C3B	3.41	131.07	124.68
19	b	807	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
19	b	811	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	b	837	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	f	201	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
19	a	834	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
19	a	814	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
19	a	807	CLA	CMB-C2B-C3B	3.39	131.01	124.68
19	a	839	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	a	843	CLA	CMB-C2B-C3B	3.38	131.00	124.68
19	a	836	CLA	CMB-C2B-C1B	-3.38	123.27	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	814	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	a	829	CLA	CMB-C2B-C3B	3.37	130.98	124.68
19	a	831	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
19	a	804	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
19	b	802	CLA	CMB-C2B-C3B	3.36	130.96	124.68
19	b	832	CLA	CMB-C2B-C3B	3.34	130.93	124.68
29	b	844	ECH	C15-C14-C13	3.34	132.07	127.31
19	a	805	CLA	CMB-C2B-C3B	3.34	130.92	124.68
19	a	837	CLA	CMB-C2B-C3B	3.33	130.91	124.68
19	b	816	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	b	823	CLA	CMB-C2B-C3B	3.32	130.88	124.68
31	f	205	ZEX	C40-C33-C34	-3.30	118.30	122.92
19	b	840	CLA	CMB-C2B-C3B	3.30	130.85	124.68
19	a	821	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
19	a	822	CLA	CMB-C2B-C3B	3.29	130.84	124.68
19	a	832	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	b	831	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
30	b	851	EQ3	C35-C13-C14	-3.28	118.33	122.92
31	f	205	ZEX	C27-C26-C25	-3.28	117.54	122.84
19	b	833	CLA	CMB-C2B-C3B	3.28	130.81	124.68
19	a	824	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
30	b	851	EQ3	C24-C23-C22	3.27	131.17	126.23
19	b	835	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
19	b	825	CLA	CMB-C2B-C3B	3.26	130.78	124.68
19	a	803	CLA	CMB-C2B-C3B	3.26	130.78	124.68
19	a	812	CLA	CMB-C2B-C3B	3.26	130.78	124.68
19	b	805	CLA	CMB-C2B-C3B	3.26	130.77	124.68
19	b	804	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
30	b	851	EQ3	C16-C15-C14	3.24	130.10	123.47
29	m	101	ECH	C35-C13-C14	-3.22	118.41	122.92
19	b	839	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
19	b	834	CLA	CMB-C2B-C3B	3.22	130.70	124.68
19	j	104	CLA	CMB-C2B-C3B	3.22	130.70	124.68
19	b	820	CLA	CMB-C2B-C3B	3.22	130.70	124.68
19	a	819	CLA	CMB-C2B-C3B	3.21	130.68	124.68
19	a	838	CLA	CMB-C2B-C3B	3.20	130.67	124.68
19	b	817	CLA	CMB-C2B-C3B	3.20	130.67	124.68
31	b	852	ZEX	C40-C33-C34	-3.20	118.45	122.92
19	l	204	CLA	CMB-C2B-C3B	3.19	130.64	124.68
19	l	202	CLA	CMB-C2B-C3B	3.19	130.64	124.68
31	b	852	ZEX	C27-C26-C25	-3.18	117.70	122.84
31	b	852	ZEX	C20-C13-C14	-3.18	118.47	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	805	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
19	a	842	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
29	m	101	ECH	C16-C15-C14	3.17	129.97	123.47
31	b	852	ZEX	C15-C35-C34	3.16	129.94	123.47
19	b	828	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
19	A	407	CLA	CMB-C2B-C3B	3.16	130.58	124.68
19	A	402	CLA	CMB-C2B-C3B	3.15	130.58	124.68
19	a	817	CLA	CMB-C2B-C3B	3.15	130.57	124.68
30	b	851	EQ3	C15-C16-C17	3.14	129.91	123.47
31	f	205	ZEX	C20-C13-C14	-3.14	118.53	122.92
19	b	806	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
19	a	834	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
19	a	833	CLA	CMB-C2B-C3B	3.13	130.53	124.68
19	b	803	CLA	CMB-C2B-C3B	3.11	130.49	124.68
29	b	844	ECH	C30-C25-C24	3.10	124.56	115.78
19	f	203	CLA	CMB-C2B-C3B	3.10	130.48	124.68
19	b	836	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
19	b	822	CLA	CMB-C2B-C3B	3.10	130.47	124.68
21	b	845	BCR	C15-C14-C13	-3.10	122.89	127.31
19	a	835	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
21	k	103	BCR	C2-C1-C6	3.10	115.25	110.48
19	k	102	CLA	CMB-C2B-C3B	3.09	130.46	124.68
19	A	405	CLA	CMB-C2B-C3B	3.08	130.44	124.68
19	b	832	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	a	860	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	D	402	CLA	CMB-C2B-C3B	3.07	130.43	124.68
19	a	860	CLA	CMB-C2B-C3B	3.07	130.42	124.68
19	b	823	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	a	809	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	a	808	CLA	CMB-C2B-C3B	3.07	130.42	124.68
19	b	837	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	A	405	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	D	403	CLA	CMB-C2B-C3B	3.06	130.41	124.68
19	b	810	CLA	CMB-C2B-C3B	3.06	130.41	124.68
31	f	205	ZEX	C15-C35-C34	3.05	129.72	123.47
19	a	840	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
30	b	851	EQ3	C36-C18-C17	-3.05	118.66	122.92
19	a	825	CLA	CMB-C2B-C3B	3.04	130.37	124.68
19	b	828	CLA	CMB-C2B-C3B	3.04	130.37	124.68
19	b	801	CLA	CAA-CBA-CGA	-3.04	104.36	113.25
23	a	801	CL0	O2D-CGD-O1D	-3.04	117.89	123.84
19	a	828	CLA	CMB-C2B-C3B	3.03	130.36	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	813	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	a	832	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	b	802	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	b	818	CLA	CMB-C2B-C3B	3.02	130.34	124.68
19	l	203	CLA	CMB-C2B-C3B	3.02	130.33	124.68
19	a	821	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	b	806	CLA	CMB-C2B-C3B	3.01	130.31	124.68
19	b	829	CLA	CMB-C2B-C3B	3.01	130.30	124.68
19	b	824	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	a	836	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	a	818	CLA	CMB-C2B-C3B	2.99	130.28	124.68
19	a	838	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	a	826	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	b	838	CLA	CMB-C2B-C3B	2.99	130.27	124.68
19	a	818	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
19	a	804	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	a	841	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	b	813	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
19	b	803	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	b	839	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	b	821	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	b	827	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
30	b	851	EQ3	C37-C22-C23	2.97	122.76	118.08
19	a	829	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	b	801	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
19	a	856	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
19	b	801	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	a	801	CL0	CMB-C2B-C1B	-2.96	123.92	128.46
19	b	815	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	a	811	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	b	808	CLA	CMB-C2B-C3B	2.95	130.21	124.68
19	a	835	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	a	857	CLA	CMB-C2B-C3B	2.94	130.18	124.68
19	a	841	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	a	812	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
19	a	808	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
19	a	806	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
19	a	820	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	D	403	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	b	809	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
19	a	843	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
19	l	203	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	840	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	a	839	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
21	a	851	BCR	C15-C16-C17	-2.91	117.50	123.47
19	a	828	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	a	833	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	b	836	CLA	CMB-C2B-C3B	2.91	130.12	124.68
19	a	827	CLA	CMB-C2B-C3B	2.91	130.12	124.68
19	b	840	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	a	827	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
19	b	831	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
19	f	201	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
19	A	402	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	b	814	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	a	802	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
21	a	849	BCR	C15-C16-C17	-2.90	117.54	123.47
28	a	858	45D	C39-C35-C37	-2.89	118.87	122.92
19	b	822	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	b	825	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	l	204	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	b	820	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	a	816	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	f	204	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
28	a	858	45D	C40-C36-C38	-2.88	118.89	122.92
19	b	816	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
21	j	101	BCR	C15-C16-C17	-2.88	117.58	123.47
19	a	822	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	D	401	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
29	m	101	ECH	C12-C13-C14	2.87	123.34	118.94
19	b	810	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
19	a	802	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	A	403	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	b	807	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	a	819	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	a	834	CLA	CMB-C2B-C3B	2.86	130.03	124.68
19	b	829	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	b	834	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	a	842	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
27	l	201	LMG	O6-C1-O1	-2.84	103.24	109.97
19	b	807	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	f	204	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	k	101	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	b	833	CLA	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	403	CLA	CMB-C2B-C3B	2.84	129.99	124.68
19	A	407	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	b	805	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	b	801	CLA	CMB-C2B-C3B	2.84	129.99	124.68
19	b	811	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	a	857	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
27	b	848	LMG	O6-C1-O1	-2.83	103.28	109.97
19	a	817	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
21	b	842	BCR	C33-C5-C6	-2.82	121.36	124.53
19	l	202	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	f	205	ZEX	C32-C33-C34	2.82	123.26	118.94
19	j	103	CLA	CMB-C2B-C3B	2.82	129.95	124.68
19	b	808	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	a	823	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	a	855	LHG	O8-C23-C24	2.81	120.74	111.91
19	a	839	CLA	CMB-C2B-C3B	2.81	129.94	124.68
19	b	819	CLA	CMB-C2B-C3B	2.81	129.94	124.68
19	b	817	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	a	824	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	j	104	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	a	813	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	A	404	PHO	O1D-CGD-CBD	2.79	129.39	124.74
19	b	837	CLA	CMB-C2B-C3B	2.79	129.90	124.68
19	b	830	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	f	206	LHG	O8-C23-C24	2.79	120.65	111.91
26	b	849	LHG	O8-C23-C24	2.78	120.64	111.91
19	a	806	CLA	CHB-C4A-NA	2.77	128.35	124.51
19	a	824	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
19	a	825	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	b	819	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
21	b	845	BCR	C2-C1-C6	2.76	114.73	110.48
19	b	826	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	a	824	CLA	CHB-C4A-NA	2.76	128.32	124.51
19	a	810	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
19	k	102	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
19	a	803	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	b	838	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	b	805	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	a	854	LMG	O6-C1-O1	-2.75	103.47	109.97
19	a	856	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	a	836	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	f	201	CLA	CMB-C2B-C3B	2.73	129.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	824	CLA	CMB-C2B-C3B	2.73	129.78	124.68
19	b	809	CLA	CMB-C2B-C3B	2.73	129.78	124.68
19	b	839	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
21	a	851	BCR	C15-C14-C13	-2.73	123.42	127.31
19	a	803	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
19	a	821	CLA	CMB-C2B-C3B	2.72	129.78	124.68
19	D	402	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
30	b	851	EQ3	C12-C13-C14	2.72	123.12	118.94
19	a	837	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	E	101	HEM	C4D-ND-C1D	2.71	107.88	105.07
21	a	847	BCR	C24-C23-C22	-2.71	122.14	126.23
19	f	203	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
21	l	205	BCR	C33-C5-C6	-2.71	121.49	124.53
19	a	829	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
19	k	101	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
20	D	401	PHO	O1D-CGD-CBD	2.70	129.23	124.74
19	b	827	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
21	j	101	BCR	C15-C14-C13	-2.69	123.47	127.31
19	j	103	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
31	b	852	ZEX	C12-C13-C14	2.69	123.07	118.94
19	b	831	CLA	CMB-C2B-C3B	2.69	129.71	124.68
31	b	852	ZEX	C32-C33-C34	2.69	123.07	118.94
19	b	818	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
19	a	830	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
19	a	804	CLA	CMB-C2B-C3B	2.68	129.69	124.68
21	i	102	BCR	C2-C1-C6	2.68	114.60	110.48
19	b	807	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
19	a	835	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	b	837	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
19	a	831	CLA	CHB-C4A-NA	2.67	128.20	124.51
21	a	859	BCR	C33-C5-C6	-2.67	121.53	124.53
21	a	850	BCR	C15-C16-C17	-2.66	118.02	123.47
31	f	205	ZEX	C12-C13-C14	2.66	123.03	118.94
26	a	853	LHG	O8-C23-C24	2.66	120.26	111.91
19	b	816	CLA	CMB-C2B-C3B	2.66	129.66	124.68
21	a	849	BCR	C15-C14-C13	-2.66	123.51	127.31
19	a	803	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
19	a	807	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
19	b	823	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	a	858	45D	C24-C26-C30	2.65	123.00	118.94
21	l	205	BCR	C15-C16-C17	-2.65	118.06	123.47
21	A	406	BCR	C24-C23-C22	-2.64	122.24	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	812	CLA	O2D-CGD-CBD	2.64	115.97	111.27
19	b	814	CLA	CMB-C2B-C3B	2.64	129.62	124.68
32	j	102	LMT	C1'-O5'-C5'	-2.64	108.50	113.69
21	b	842	BCR	C24-C23-C22	-2.64	122.25	126.23
19	a	818	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	a	820	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
19	a	837	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	a	842	CLA	CMB-C2B-C3B	2.63	129.60	124.68
20	A	404	PHO	CMB-C2B-C3B	2.63	129.60	124.68
19	D	403	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	a	821	CLA	CHB-C4A-NA	2.63	128.14	124.51
19	j	103	CLA	CHB-C4A-NA	2.63	128.14	124.51
20	A	404	PHO	O2D-CGD-O1D	-2.62	118.71	123.84
19	b	816	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	a	826	CLA	CHB-C4A-NA	2.62	128.14	124.51
21	a	850	BCR	C33-C5-C6	-2.62	121.59	124.53
19	a	840	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
21	k	103	BCR	C15-C14-C13	-2.61	123.58	127.31
19	b	838	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	b	821	CLA	CMB-C2B-C3B	2.61	129.56	124.68
19	b	811	CLA	C1-C2-C3	-2.60	122.54	126.75
19	a	831	CLA	O2D-CGD-CBD	2.60	115.89	111.27
19	b	806	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
21	a	846	BCR	C24-C23-C22	-2.59	122.32	126.23
19	f	204	CLA	C1-C2-C3	-2.59	122.56	126.75
28	a	858	45D	C03-C07-C19	2.59	123.10	115.78
21	a	850	BCR	C15-C14-C13	-2.59	123.62	127.31
29	b	844	ECH	C37-C22-C23	2.58	122.14	118.08
19	b	811	CLA	CMB-C2B-C3B	2.58	129.50	124.68
19	a	832	CLA	CMB-C2B-C3B	2.58	129.50	124.68
21	i	102	BCR	C28-C27-C26	-2.57	109.49	114.08
20	D	401	PHO	CMB-C2B-C3B	2.57	129.48	124.68
19	b	818	CLA	CHB-C4A-NA	2.56	128.06	124.51
19	b	804	CLA	CHB-C4A-NA	2.56	128.06	124.51
21	k	103	BCR	C15-C16-C17	-2.56	118.23	123.47
29	m	101	ECH	C21-C20-C19	2.55	131.19	123.22
21	a	849	BCR	C24-C23-C22	-2.55	122.38	126.23
19	a	860	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	836	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	b	831	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	a	823	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	l	203	CLA	CHB-C4A-NA	2.55	128.03	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	841	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
19	a	814	CLA	O2D-CGD-CBD	2.54	115.79	111.27
19	b	838	CLA	C1-C2-C3	-2.54	121.65	126.04
19	a	840	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	k	101	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	a	804	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	b	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	f	201	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	a	859	BCR	C15-C16-C17	-2.53	118.29	123.47
21	A	406	BCR	C27-C26-C25	2.53	126.40	122.73
19	b	815	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	a	848	BCR	C33-C5-C6	-2.53	121.69	124.53
19	a	814	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	A	402	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
21	b	843	BCR	C33-C5-C6	-2.53	121.69	124.53
19	b	828	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	a	818	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
19	b	832	CLA	CHB-C4A-NA	2.53	128.00	124.51
19	A	407	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	a	853	LHG	C11-C10-C9	-2.52	101.61	114.42
19	b	814	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	A	406	BCR	C33-C5-C6	-2.52	121.70	124.53
19	f	203	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
21	j	101	BCR	C33-C5-C6	-2.52	121.70	124.53
26	a	855	LHG	C11-C10-C9	-2.52	101.64	114.42
21	l	205	BCR	C27-C26-C25	2.52	126.39	122.73
19	a	819	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	a	843	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
21	b	847	BCR	C27-C26-C25	2.51	126.38	122.73
29	b	844	ECH	C34-C9-C8	2.51	122.03	118.08
21	a	846	BCR	C33-C5-C6	-2.51	121.71	124.53
19	b	822	CLA	C1-C2-C3	-2.51	121.70	126.04
19	a	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	a	842	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	f	203	CLA	C1-C2-C3	-2.50	122.70	126.75
19	a	813	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
21	b	845	BCR	C11-C10-C9	-2.50	123.74	127.31
19	f	204	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	b	836	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	b	818	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	l	204	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	b	826	CLA	C1B-CHB-C4A	-2.50	125.17	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	837	CLA	C1-C2-C3	-2.49	122.73	126.75
19	b	810	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	a	843	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	i	102	BCR	C15-C16-C17	-2.49	118.38	123.47
19	a	824	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	b	842	BCR	C15-C16-C17	-2.48	118.39	123.47
21	a	851	BCR	C33-C5-C6	-2.48	121.74	124.53
19	b	834	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	a	813	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	b	802	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	a	807	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	a	838	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	b	804	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
19	b	827	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	b	817	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
19	b	813	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	b	829	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
19	a	829	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	b	840	CLA	CHB-C4A-NA	2.47	127.92	124.51
27	l	201	LMG	C38-C37-C36	-2.46	101.92	114.42
19	b	822	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	A	405	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	a	817	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	a	834	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	a	801	CL0	CMB-C2B-C3B	2.46	129.27	124.68
21	a	859	BCR	C27-C26-C25	2.45	126.30	122.73
19	a	816	CLA	CHB-C4A-NA	2.45	127.91	124.51
21	a	859	BCR	C24-C23-C22	-2.45	122.53	126.23
27	a	854	LMG	O1-C7-C8	-2.45	104.98	110.90
19	b	812	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	b	833	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	A	403	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	a	803	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
19	l	202	CLA	C1-C2-C3	-2.45	122.79	126.75
21	b	846	BCR	C27-C26-C25	2.45	126.28	122.73
21	i	102	BCR	C7-C8-C9	-2.44	122.54	126.23
19	a	857	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	b	842	BCR	C11-C10-C9	-2.44	123.83	127.31
19	a	825	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	a	828	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	a	812	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	k	102	CLA	CHB-C4A-NA	2.44	127.89	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	834	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	a	827	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	b	823	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	b	830	CLA	C1-C2-C3	-2.44	122.81	126.75
19	a	812	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	a	830	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	b	830	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
26	a	852	LHG	O8-C23-C24	2.44	119.55	111.91
19	b	802	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
21	b	842	BCR	C27-C26-C25	2.43	126.27	122.73
19	a	836	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	a	837	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	b	811	CLA	CHB-C4A-NA	2.43	127.88	124.51
26	a	852	LHG	C11-C10-C9	-2.43	102.08	114.42
19	a	811	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	a	811	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	l	202	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
19	j	103	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
19	a	833	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	a	841	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	b	845	BCR	C27-C26-C25	2.43	126.25	122.73
19	b	835	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
29	m	101	ECH	C24-C23-C22	2.42	129.90	126.23
19	A	402	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	b	822	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
19	a	835	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
19	b	803	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	b	820	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	a	849	BCR	C33-C5-C6	-2.42	121.81	124.53
19	a	831	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
19	a	836	CLA	C1-C2-C3	-2.42	121.86	126.04
19	a	809	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	a	801	CL0	C1B-CHB-C4A	-2.42	125.32	130.12
26	f	206	LHG	C11-C10-C9	-2.42	102.14	114.42
19	a	809	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	b	819	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	b	835	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	a	801	CL0	CHB-C4A-NA	2.42	127.85	124.51
19	b	808	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	b	833	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	a	852	LHG	C20-C19-C18	-2.41	102.17	114.42
27	b	850	LMG	C40-C39-C38	-2.41	102.18	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	814	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	b	816	CLA	C1-C2-C3	-2.41	121.88	126.04
19	b	825	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	b	824	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	b	805	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
27	b	848	LMG	C40-C39-C38	-2.40	102.23	114.42
19	a	823	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	a	839	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	a	808	CLA	CHB-C4A-NA	2.40	127.83	124.51
27	b	850	LMG	C1-O6-C5	-2.40	108.98	113.69
19	A	405	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	b	815	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	b	810	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	a	850	BCR	C27-C26-C25	2.39	126.20	122.73
19	a	825	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	a	819	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
27	b	848	LMG	C38-C37-C36	-2.39	102.30	114.42
21	b	846	BCR	C2-C1-C6	2.39	114.16	110.48
21	i	101	BCR	C27-C26-C25	2.39	126.20	122.73
19	a	805	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	b	850	LMG	C38-C37-C36	-2.39	102.31	114.42
19	b	838	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
19	b	821	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
19	b	807	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
19	k	102	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	a	847	BCR	C27-C26-C25	2.38	126.19	122.73
21	i	101	BCR	C15-C16-C17	-2.38	118.60	123.47
19	D	403	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	j	104	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	a	855	LHG	C20-C19-C18	-2.38	102.35	114.42
19	j	104	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	a	815	CLA	O2D-CGD-CBD	2.38	115.49	111.27
19	a	827	CLA	CHB-C4A-NA	2.37	127.80	124.51
19	b	839	CLA	CMB-C2B-C3B	2.37	129.12	124.68
19	b	830	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	f	206	LHG	C20-C19-C18	-2.37	102.39	114.42
30	b	851	EQ3	C19-C18-C17	2.37	122.58	118.94
19	a	805	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	b	816	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	a	802	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
19	b	813	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	b	831	CLA	C1B-CHB-C4A	-2.36	125.44	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	846	BCR	C15-C14-C13	-2.36	123.94	127.31
19	f	204	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	a	821	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	b	819	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
21	f	202	BCR	C33-C5-C6	-2.36	121.88	124.53
27	b	850	LMG	O6-C1-O1	-2.36	104.39	109.97
19	a	820	CLA	CHB-C4A-NA	2.36	127.77	124.51
19	a	839	CLA	CHB-C4A-NA	2.36	127.77	124.51
19	b	806	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
21	a	849	BCR	C27-C26-C25	2.36	126.15	122.73
19	a	842	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
21	b	843	BCR	C15-C16-C17	-2.35	118.66	123.47
19	b	819	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	b	835	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
21	k	103	BCR	C27-C26-C25	2.35	126.14	122.73
21	a	848	BCR	C27-C26-C25	2.35	126.14	122.73
19	A	407	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	a	838	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	b	834	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	f	201	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	b	825	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	k	101	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	a	847	BCR	C33-C5-C6	-2.34	121.90	124.53
19	b	820	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	l	202	CLA	CHB-C4A-NA	2.34	127.75	124.51
26	a	853	LHG	C20-C19-C18	-2.34	102.55	114.42
19	a	833	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	D	402	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	b	826	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	a	806	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	f	202	BCR	C27-C26-C25	2.33	126.11	122.73
19	b	839	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	l	204	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
19	b	806	CLA	CHB-C4A-NA	2.32	127.73	124.51
21	a	846	BCR	C15-C16-C17	-2.32	118.72	123.47
22	E	101	HEM	C1B-NB-C4B	2.32	107.47	105.07
27	b	848	LMG	O3-C3-C2	-2.32	104.98	110.35
19	A	403	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	a	832	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
28	a	858	45D	C33-C35-C37	2.32	122.50	118.94
19	a	815	CLA	CHB-C4A-NA	2.32	127.71	124.51
19	b	808	CLA	C1B-CHB-C4A	-2.32	125.53	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	801	CL0	CAA-CBA-CGA	-2.31	106.49	113.25
19	b	815	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
21	b	847	BCR	C33-C5-C6	-2.31	121.93	124.53
19	a	815	CLA	C1-C2-C3	-2.31	122.05	126.04
19	a	811	CLA	C1-C2-C3	-2.31	123.01	126.75
27	l	201	LMG	O3-C3-C2	-2.31	105.01	110.35
19	b	832	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	a	835	CLA	C1-C2-C3	-2.31	122.05	126.04
19	a	810	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	b	828	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	a	857	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	b	836	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	a	828	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	b	803	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	l	203	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	a	820	CLA	C1-C2-C3	-2.30	122.07	126.04
27	b	850	LMG	C42-C41-C40	-2.30	102.75	114.42
26	f	206	LHG	C27-C26-C25	-2.30	102.76	114.42
19	b	807	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	b	809	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	b	840	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
19	f	203	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	a	804	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
21	b	843	BCR	C27-C26-C25	2.29	126.06	122.73
26	a	853	LHG	C27-C26-C25	-2.29	102.79	114.42
21	i	102	BCR	C33-C5-C6	-2.29	121.96	124.53
19	a	816	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	b	834	CLA	C1-C2-C3	-2.29	123.05	126.75
19	b	824	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
30	b	851	EQ3	C34-C9-C8	2.28	121.67	118.08
19	b	811	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	A	405	CLA	C1-C2-C3	-2.28	123.07	126.75
29	b	844	ECH	C7-C8-C9	2.27	129.67	126.23
19	a	828	CLA	C1-C2-C3	-2.27	122.11	126.04
19	b	836	CLA	CHB-C4A-NA	2.27	127.66	124.51
19	a	835	CLA	O2D-CGD-CBD	2.27	115.31	111.27
19	b	817	CLA	CHB-C4A-NA	2.27	127.65	124.51
27	a	854	LMG	O3-C3-C2	-2.27	105.10	110.35
21	f	202	BCR	C24-C23-C22	-2.27	122.81	126.23
21	b	843	BCR	C15-C14-C13	-2.27	124.07	127.31
31	b	852	ZEX	C8-C9-C10	2.27	122.42	118.94
19	a	818	CLA	C1B-CHB-C4A	-2.26	125.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	809	CLA	CHB-C4A-NA	2.26	127.64	124.51
32	j	102	LMT	C3'-C4'-C5'	-2.26	105.74	110.93
21	A	406	BCR	C15-C14-C13	-2.26	124.08	127.31
21	a	847	BCR	C15-C16-C17	-2.26	118.85	123.47
20	D	401	PHO	CMC-C2C-C3C	2.26	129.20	124.94
19	a	829	CLA	CHD-C1D-ND	-2.26	122.38	124.45
19	a	822	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
19	a	814	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	i	102	BCR	C29-C30-C25	2.25	113.95	110.48
19	b	835	CLA	O2D-CGD-CBD	2.25	115.27	111.27
19	D	402	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
27	a	854	LMG	O2-C2-C1	-2.25	104.58	110.05
21	b	842	BCR	C15-C14-C13	-2.25	124.11	127.31
19	a	808	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
19	a	827	CLA	CHD-C1D-ND	-2.24	122.39	124.45
27	b	848	LMG	O1-C7-C8	-2.24	105.49	110.90
19	a	809	CLA	CHD-C1D-ND	-2.24	122.39	124.45
21	l	205	BCR	C15-C14-C13	-2.24	124.11	127.31
19	a	826	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
19	b	837	CLA	CHB-C4A-NA	2.23	127.60	124.51
21	b	843	BCR	C24-C23-C22	-2.23	122.86	126.23
21	A	406	BCR	C15-C16-C17	-2.23	118.90	123.47
27	l	201	LMG	C40-C39-C38	-2.23	103.10	114.42
19	D	402	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
19	b	822	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
19	a	817	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
27	l	201	LMG	O1-C7-C8	-2.23	105.52	110.90
27	b	848	LMG	C42-C41-C40	-2.23	103.12	114.42
19	a	807	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	b	805	CLA	C1-C2-C3	-2.22	122.19	126.04
27	b	848	LMG	O2-C2-C1	-2.22	104.64	110.05
19	b	812	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
19	a	806	CLA	C1-C2-C3	-2.22	122.20	126.04
21	f	202	BCR	C15-C16-C17	-2.22	118.93	123.47
21	j	101	BCR	C27-C26-C25	2.22	125.95	122.73
21	a	848	BCR	C16-C15-C14	-2.22	118.93	123.47
19	a	826	CLA	O2D-CGD-CBD	2.22	115.21	111.27
19	a	832	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	a	820	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
19	a	814	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
19	a	809	CLA	C1-C2-C3	-2.21	122.22	126.04
21	a	846	BCR	C27-C26-C25	2.21	125.94	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	849	BCR	C11-C10-C9	-2.21	124.16	127.31
19	a	830	CLA	CHB-C4A-NA	2.20	127.56	124.51
27	b	848	LMG	O1-C1-C2	-2.20	104.87	108.30
21	a	846	BCR	C11-C10-C9	-2.20	124.17	127.31
19	b	825	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
19	a	839	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	a	852	LHG	C18-C17-C16	-2.19	103.29	114.42
19	a	824	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	f	206	LHG	C18-C17-C16	-2.19	103.30	114.42
26	a	855	LHG	C27-C26-C25	-2.19	103.31	114.42
26	a	852	LHG	C27-C26-C25	-2.19	103.32	114.42
19	b	829	CLA	CHB-C4A-NA	2.18	127.53	124.51
31	f	205	ZEX	C28-C29-C30	2.18	122.29	118.94
19	b	804	CLA	O2D-CGD-CBD	2.18	115.14	111.27
19	a	860	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
21	b	842	BCR	C7-C8-C9	-2.18	122.94	126.23
28	a	858	45D	C23-C25-C29	2.18	122.28	118.94
19	b	824	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
19	a	802	CLA	C1-C2-C3	-2.18	122.28	126.04
21	b	843	BCR	C11-C10-C9	-2.18	124.20	127.31
19	a	833	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	b	814	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
26	b	849	LHG	C27-C26-C25	-2.17	103.39	114.42
21	a	859	BCR	C15-C14-C13	-2.17	124.21	127.31
19	b	803	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	a	856	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	D	402	CLA	CHD-C1D-ND	-2.17	122.46	124.45
27	b	850	LMG	O2-C2-C1	-2.17	104.79	110.05
19	b	801	CLA	C1-C2-C3	-2.16	122.30	126.04
19	a	802	CLA	CHB-C4A-NA	2.16	127.50	124.51
19	b	816	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	a	815	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
27	a	854	LMG	O1-C1-C2	-2.16	104.93	108.30
31	f	205	ZEX	C8-C9-C10	2.16	122.25	118.94
19	a	843	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
19	b	838	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
27	b	850	LMG	O1-C7-C8	-2.16	105.70	110.90
19	b	838	CLA	CHD-C1D-ND	-2.15	122.47	124.45
28	a	858	45D	C34-C36-C38	2.15	122.24	118.94
19	a	841	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	f	202	BCR	C8-C7-C6	-2.15	121.17	127.20
29	m	101	ECH	C8-C9-C10	2.15	122.23	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	855	LHG	C18-C17-C16	-2.15	103.53	114.42
19	a	833	CLA	C1-C2-C3	-2.14	122.34	126.04
21	a	849	BCR	C7-C8-C9	-2.14	123.00	126.23
31	b	852	ZEX	C39-C29-C28	2.13	121.44	118.08
26	a	853	LHG	C18-C17-C16	-2.13	103.60	114.42
19	a	836	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
19	j	103	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
21	a	850	BCR	C24-C23-C22	-2.13	123.02	126.23
19	a	827	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	a	807	CLA	CHD-C1D-ND	-2.13	122.50	124.45
21	a	847	BCR	C15-C14-C13	-2.13	124.28	127.31
21	A	406	BCR	C11-C10-C9	-2.12	124.28	127.31
19	a	826	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
21	b	846	BCR	C16-C15-C14	-2.12	119.13	123.47
21	b	847	BCR	C15-C14-C13	-2.12	124.29	127.31
21	i	102	BCR	C15-C14-C13	-2.12	124.29	127.31
21	b	847	BCR	C24-C23-C22	-2.12	123.03	126.23
27	l	201	LMG	C42-C41-C40	-2.11	103.69	114.42
19	a	810	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	a	837	CLA	CHD-C1D-ND	-2.11	122.51	124.45
20	A	404	PHO	CMC-C2C-C3C	2.11	128.92	124.94
21	i	101	BCR	C33-C5-C6	-2.11	122.16	124.53
19	A	405	CLA	CHD-C1D-ND	-2.10	122.52	124.45
27	b	850	LMG	O3-C3-C2	-2.10	105.48	110.35
19	b	836	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	a	841	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	a	860	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
21	b	846	BCR	C33-C5-C6	-2.10	122.17	124.53
19	a	821	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
19	b	820	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	E	101	HEM	CBA-CAA-C2A	-2.10	109.04	112.62
21	b	847	BCR	C15-C16-C17	-2.09	119.18	123.47
19	b	815	CLA	CHD-C1D-ND	-2.09	122.53	124.45
21	k	103	BCR	C24-C23-C22	-2.09	123.08	126.23
19	l	204	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	b	839	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	a	809	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	E	101	HEM	C4C-CHD-C1D	2.09	125.31	122.56
21	j	101	BCR	C11-C10-C9	-2.08	124.34	127.31
19	b	832	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	a	838	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
21	a	846	BCR	C7-C8-C9	-2.08	123.09	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	811	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	l	202	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	a	822	CLA	CHB-C4A-NA	2.07	127.38	124.51
19	a	815	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	f	203	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
19	f	204	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
19	b	808	CLA	C1-C2-C3	-2.07	122.47	126.04
19	a	804	CLA	CHD-C1D-ND	-2.07	122.56	124.45
21	a	859	BCR	C38-C26-C25	-2.07	122.21	124.53
19	l	203	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
19	a	810	CLA	C1-C2-C3	-2.06	122.47	126.04
19	b	833	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	b	805	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	a	820	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	a	832	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	b	832	CLA	C1-C2-C3	-2.06	122.48	126.04
22	E	101	HEM	CAD-CBD-CGD	-2.06	109.17	113.60
21	b	847	BCR	C2-C1-C6	2.06	113.65	110.48
19	b	803	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	b	830	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	a	834	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	b	802	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
29	b	844	ECH	C21-C20-C19	2.05	129.63	123.22
19	b	829	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	b	835	CLA	C1-C2-C3	-2.05	122.50	126.04
19	b	826	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	829	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	816	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	b	813	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
21	i	101	BCR	C2-C1-C6	2.04	113.62	110.48
19	a	823	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	a	833	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	a	824	CLA	C1-C2-C3	-2.04	122.52	126.04
21	i	101	BCR	C16-C15-C14	-2.04	119.30	123.47
19	a	831	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	b	823	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	b	807	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	j	104	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	a	858	45D	C10-C06-C04	-2.04	109.91	113.18
19	b	826	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	a	813	CLA	CHD-C1D-ND	-2.03	122.59	124.45
27	l	201	LMG	O2-C2-C1	-2.03	105.12	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	843	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	b	812	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	A	404	PHO	O2A-CGA-O1A	-2.03	118.48	123.59
19	a	839	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	a	808	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
21	a	848	BCR	C8-C7-C6	-2.02	121.52	127.20
19	b	831	CLA	CHD-C1D-ND	-2.02	122.59	124.45
19	b	804	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	l	202	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	A	405	CLA	O2D-CGD-CBD	2.02	114.86	111.27
21	j	101	BCR	C24-C23-C22	-2.02	123.19	126.23
19	a	856	CLA	O1D-CGD-CBD	2.02	128.61	124.48
20	D	401	PHO	O2A-CGA-O1A	-2.02	118.50	123.59
21	a	848	BCR	C15-C14-C13	-2.02	124.43	127.31
19	b	813	CLA	CHD-C1D-ND	-2.02	122.60	124.45
21	k	103	BCR	C35-C13-C14	-2.01	120.10	122.92
19	b	809	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
19	b	833	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
19	a	860	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	b	827	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	b	850	LMG	O7-C10-O9	-2.01	118.84	123.70
19	a	803	CLA	O1D-CGD-CBD	2.01	128.59	124.48
19	b	813	CLA	C1-C2-C3	-2.01	122.57	126.04
21	a	850	BCR	C8-C7-C6	-2.01	121.56	127.20
23	a	801	CL0	O2A-CGA-O1A	-2.01	118.53	123.59
21	a	848	BCR	C15-C16-C17	-2.01	119.36	123.47
19	a	812	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
19	a	832	CLA	CHD-C1D-ND	-2.00	122.61	124.45
19	A	403	CLA	CHD-C1D-ND	-2.00	122.61	124.45
19	a	808	CLA	CHD-C1D-ND	-2.00	122.61	124.45
19	a	813	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	a	825	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (103) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	402	CLA	ND
19	A	403	CLA	ND
19	A	405	CLA	ND
19	A	407	CLA	ND
19	D	402	CLA	ND
19	D	403	CLA	ND

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Mol	Chain	Res	Type	Atom
19	a	802	CLA	ND
19	a	803	CLA	ND
19	a	804	CLA	ND
19	a	805	CLA	ND
19	a	806	CLA	ND
19	a	807	CLA	ND
19	a	808	CLA	ND
19	a	809	CLA	ND
19	a	810	CLA	ND
19	a	811	CLA	ND
19	a	812	CLA	ND
19	a	813	CLA	ND
19	a	815	CLA	ND
19	a	816	CLA	ND
19	a	817	CLA	ND
19	a	818	CLA	ND
19	a	819	CLA	ND
19	a	820	CLA	ND
19	a	821	CLA	ND
19	a	822	CLA	ND
19	a	823	CLA	ND
19	a	824	CLA	ND
19	a	825	CLA	ND
19	a	826	CLA	ND
19	a	827	CLA	ND
19	a	828	CLA	ND
19	a	829	CLA	ND
19	a	830	CLA	ND
19	a	831	CLA	ND
19	a	832	CLA	ND
19	a	833	CLA	ND
19	a	834	CLA	ND
19	a	835	CLA	ND
19	a	836	CLA	ND
19	a	837	CLA	ND
19	a	838	CLA	ND
19	a	839	CLA	ND
19	a	840	CLA	ND
19	a	841	CLA	ND
19	a	842	CLA	ND
19	a	843	CLA	ND
19	a	856	CLA	ND

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Mol	Chain	Res	Type	Atom
19	a	857	CLA	ND
19	a	860	CLA	ND
19	b	801	CLA	ND
19	b	802	CLA	ND
19	b	803	CLA	ND
19	b	804	CLA	ND
19	b	805	CLA	ND
19	b	806	CLA	ND
19	b	807	CLA	ND
19	b	808	CLA	ND
19	b	809	CLA	ND
19	b	810	CLA	ND
19	b	811	CLA	ND
19	b	812	CLA	ND
19	b	813	CLA	ND
19	b	814	CLA	ND
19	b	815	CLA	ND
19	b	816	CLA	ND
19	b	817	CLA	ND
19	b	818	CLA	ND
19	b	819	CLA	ND
19	b	820	CLA	ND
19	b	821	CLA	ND
19	b	822	CLA	ND
19	b	823	CLA	ND
19	b	824	CLA	ND
19	b	825	CLA	ND
19	b	826	CLA	ND
19	b	827	CLA	ND
19	b	828	CLA	ND
19	b	829	CLA	ND
19	b	830	CLA	ND
19	b	831	CLA	ND
19	b	832	CLA	ND
19	b	833	CLA	ND
19	b	834	CLA	ND
19	b	835	CLA	ND
19	b	836	CLA	ND
19	b	837	CLA	ND
19	b	838	CLA	ND
19	b	839	CLA	ND
19	b	840	CLA	ND

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Mol	Chain	Res	Type	Atom
19	f	201	CLA	ND
19	f	203	CLA	ND
19	f	204	CLA	ND
19	j	103	CLA	ND
19	j	104	CLA	ND
19	k	101	CLA	ND
19	k	102	CLA	ND
19	l	202	CLA	ND
19	l	203	CLA	ND
19	l	204	CLA	ND
23	a	801	CL0	NA
23	a	801	CL0	ND
23	a	801	CL0	NC

All (1568) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	C1A-C2A-CAA-CBA
19	A	403	CLA	C3A-C2A-CAA-CBA
19	A	403	CLA	CHA-CBD-CGD-O1D
19	A	403	CLA	CHA-CBD-CGD-O2D
19	A	405	CLA	C1A-C2A-CAA-CBA
19	A	405	CLA	C3A-C2A-CAA-CBA
19	D	402	CLA	C1A-C2A-CAA-CBA
19	D	402	CLA	C3A-C2A-CAA-CBA
19	D	402	CLA	CBD-CGD-O2D-CED
19	D	403	CLA	C1A-C2A-CAA-CBA
19	D	403	CLA	C3A-C2A-CAA-CBA
19	a	802	CLA	O1A-CGA-O2A-C1
19	a	802	CLA	CBD-CGD-O2D-CED
19	a	803	CLA	CBA-CGA-O2A-C1
19	a	803	CLA	O1A-CGA-O2A-C1
19	a	805	CLA	C1A-C2A-CAA-CBA
19	a	806	CLA	C3A-C2A-CAA-CBA
19	a	807	CLA	C2-C3-C5-C6
19	a	807	CLA	C4-C3-C5-C6
19	a	808	CLA	C1A-C2A-CAA-CBA
19	a	808	CLA	C3A-C2A-CAA-CBA
19	a	809	CLA	C1A-C2A-CAA-CBA
19	a	809	CLA	C3A-C2A-CAA-CBA
19	a	809	CLA	C6-C7-C8-C10
19	a	811	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	a	811	CLA	O1D-CGD-O2D-CED
19	a	813	CLA	C1A-C2A-CAA-CBA
19	a	813	CLA	C3A-C2A-CAA-CBA
19	a	815	CLA	C1A-C2A-CAA-CBA
19	a	815	CLA	C3A-C2A-CAA-CBA
19	a	815	CLA	CHA-CBD-CGD-O1D
19	a	816	CLA	CBA-CGA-O2A-C1
19	a	817	CLA	C1A-C2A-CAA-CBA
19	a	817	CLA	C3A-C2A-CAA-CBA
19	a	817	CLA	CBA-CGA-O2A-C1
19	a	818	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C3A-C2A-CAA-CBA
19	a	819	CLA	C11-C10-C8-C9
19	a	820	CLA	C1A-C2A-CAA-CBA
19	a	820	CLA	C3A-C2A-CAA-CBA
19	a	820	CLA	CHA-CBD-CGD-O1D
19	a	820	CLA	CHA-CBD-CGD-O2D
19	a	821	CLA	C1A-C2A-CAA-CBA
19	a	821	CLA	C3A-C2A-CAA-CBA
19	a	821	CLA	C2-C1-O2A-CGA
19	a	821	CLA	CBD-CGD-O2D-CED
19	a	822	CLA	C2A-CAA-CBA-CGA
19	a	823	CLA	C1A-C2A-CAA-CBA
19	a	823	CLA	C3A-C2A-CAA-CBA
19	a	825	CLA	CHA-CBD-CGD-O1D
19	a	825	CLA	CHA-CBD-CGD-O2D
19	a	826	CLA	CAD-CBD-CGD-O2D
19	a	827	CLA	C3A-C2A-CAA-CBA
19	a	828	CLA	C1A-C2A-CAA-CBA
19	a	829	CLA	C1A-C2A-CAA-CBA
19	a	829	CLA	C3A-C2A-CAA-CBA
19	a	830	CLA	CHA-CBD-CGD-O1D
19	a	830	CLA	CHA-CBD-CGD-O2D
19	a	832	CLA	C1A-C2A-CAA-CBA
19	a	832	CLA	C3A-C2A-CAA-CBA
19	a	833	CLA	C1A-C2A-CAA-CBA
19	a	833	CLA	C3A-C2A-CAA-CBA
19	a	835	CLA	C1A-C2A-CAA-CBA
19	a	835	CLA	C6-C7-C8-C9
19	a	836	CLA	C2-C3-C5-C6
19	a	836	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	a	837	CLA	C2A-CAA-CBA-CGA
19	a	837	CLA	CHA-CBD-CGD-O1D
19	a	837	CLA	CHA-CBD-CGD-O2D
19	a	837	CLA	C4-C3-C5-C6
19	a	838	CLA	C1A-C2A-CAA-CBA
19	a	838	CLA	C3A-C2A-CAA-CBA
19	a	839	CLA	C1A-C2A-CAA-CBA
19	a	839	CLA	C3A-C2A-CAA-CBA
19	a	841	CLA	C1A-C2A-CAA-CBA
19	a	841	CLA	C3A-C2A-CAA-CBA
19	a	857	CLA	C1A-C2A-CAA-CBA
19	a	857	CLA	C3A-C2A-CAA-CBA
19	a	857	CLA	CHA-CBD-CGD-O1D
19	a	857	CLA	CHA-CBD-CGD-O2D
19	a	857	CLA	C4-C3-C5-C6
19	a	860	CLA	CHA-CBD-CGD-O1D
19	a	860	CLA	CHA-CBD-CGD-O2D
19	b	801	CLA	CHA-CBD-CGD-O1D
19	b	801	CLA	CHA-CBD-CGD-O2D
19	b	802	CLA	CHA-CBD-CGD-O1D
19	b	802	CLA	CHA-CBD-CGD-O2D
19	b	802	CLA	CBD-CGD-O2D-CED
19	b	806	CLA	C1A-C2A-CAA-CBA
19	b	806	CLA	C3A-C2A-CAA-CBA
19	b	806	CLA	C2-C3-C5-C6
19	b	806	CLA	C4-C3-C5-C6
19	b	810	CLA	C1A-C2A-CAA-CBA
19	b	810	CLA	C3A-C2A-CAA-CBA
19	b	811	CLA	C1A-C2A-CAA-CBA
19	b	811	CLA	C3A-C2A-CAA-CBA
19	b	814	CLA	C1A-C2A-CAA-CBA
19	b	814	CLA	CBD-CGD-O2D-CED
19	b	814	CLA	C2-C3-C5-C6
19	b	814	CLA	C4-C3-C5-C6
19	b	815	CLA	C1A-C2A-CAA-CBA
19	b	815	CLA	C3A-C2A-CAA-CBA
19	b	817	CLA	C1A-C2A-CAA-CBA
19	b	817	CLA	C3A-C2A-CAA-CBA
19	b	819	CLA	C1A-C2A-CAA-CBA
19	b	819	CLA	C3A-C2A-CAA-CBA
19	b	820	CLA	C1A-C2A-CAA-CBA
19	b	820	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	b	821	CLA	C1A-C2A-CAA-CBA
19	b	821	CLA	CBA-CGA-O2A-C1
19	b	821	CLA	O1A-CGA-O2A-C1
19	b	822	CLA	C1A-C2A-CAA-CBA
19	b	822	CLA	C3A-C2A-CAA-CBA
19	b	822	CLA	CHA-CBD-CGD-O1D
19	b	822	CLA	CHA-CBD-CGD-O2D
19	b	823	CLA	C1A-C2A-CAA-CBA
19	b	823	CLA	C11-C10-C8-C7
19	b	824	CLA	C1A-C2A-CAA-CBA
19	b	824	CLA	C3A-C2A-CAA-CBA
19	b	826	CLA	C1A-C2A-CAA-CBA
19	b	826	CLA	C3A-C2A-CAA-CBA
19	b	828	CLA	C1A-C2A-CAA-CBA
19	b	828	CLA	C3A-C2A-CAA-CBA
19	b	828	CLA	C4-C3-C5-C6
19	b	829	CLA	CBD-CGD-O2D-CED
19	b	832	CLA	C1A-C2A-CAA-CBA
19	b	832	CLA	C3A-C2A-CAA-CBA
19	b	832	CLA	CHA-CBD-CGD-O1D
19	b	832	CLA	CHA-CBD-CGD-O2D
19	b	833	CLA	C1A-C2A-CAA-CBA
19	b	833	CLA	C3A-C2A-CAA-CBA
19	b	834	CLA	C1A-C2A-CAA-CBA
19	b	834	CLA	C3A-C2A-CAA-CBA
19	b	836	CLA	C1A-C2A-CAA-CBA
19	b	836	CLA	C3A-C2A-CAA-CBA
19	b	836	CLA	CHA-CBD-CGD-O1D
19	b	836	CLA	CHA-CBD-CGD-O2D
19	b	836	CLA	C4-C3-C5-C6
19	b	837	CLA	C1A-C2A-CAA-CBA
19	b	837	CLA	C3A-C2A-CAA-CBA
19	b	838	CLA	C1A-C2A-CAA-CBA
19	b	840	CLA	C1A-C2A-CAA-CBA
19	b	840	CLA	C3A-C2A-CAA-CBA
19	b	840	CLA	CAD-CBD-CGD-O1D
19	b	840	CLA	CAD-CBD-CGD-O2D
19	f	201	CLA	CBD-CGD-O2D-CED
19	f	201	CLA	C2-C3-C5-C6
19	f	201	CLA	C4-C3-C5-C6
19	j	103	CLA	C1A-C2A-CAA-CBA
19	j	103	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	j	104	CLA	CBA-CGA-O2A-C1
19	k	101	CLA	C3A-C2A-CAA-CBA
19	k	101	CLA	CBA-CGA-O2A-C1
19	k	101	CLA	CHA-CBD-CGD-O1D
19	k	101	CLA	CHA-CBD-CGD-O2D
19	k	101	CLA	CBD-CGD-O2D-CED
19	l	202	CLA	C1A-C2A-CAA-CBA
19	l	202	CLA	C3A-C2A-CAA-CBA
19	l	202	CLA	CHA-CBD-CGD-O1D
19	l	202	CLA	CHA-CBD-CGD-O2D
19	l	203	CLA	C1A-C2A-CAA-CBA
19	l	203	CLA	CHA-CBD-CGD-O1D
19	l	203	CLA	CHA-CBD-CGD-O2D
20	D	401	PHO	CBD-CGD-O2D-CED
21	A	406	BCR	C6-C7-C8-C9
21	A	406	BCR	C22-C23-C24-C25
21	a	846	BCR	C7-C8-C9-C10
21	a	846	BCR	C7-C8-C9-C34
21	a	847	BCR	C7-C8-C9-C34
21	a	847	BCR	C11-C12-C13-C35
21	a	848	BCR	C1-C6-C7-C8
21	a	848	BCR	C37-C22-C23-C24
21	a	849	BCR	C21-C22-C23-C24
21	a	850	BCR	C7-C8-C9-C34
21	a	850	BCR	C21-C22-C23-C24
21	a	850	BCR	C23-C24-C25-C30
21	a	859	BCR	C6-C7-C8-C9
21	a	859	BCR	C23-C24-C25-C30
21	b	842	BCR	C6-C7-C8-C9
21	b	842	BCR	C7-C8-C9-C10
21	b	842	BCR	C7-C8-C9-C34
21	b	842	BCR	C18-C19-C20-C21
21	b	842	BCR	C21-C22-C23-C24
21	b	842	BCR	C37-C22-C23-C24
21	b	842	BCR	C22-C23-C24-C25
21	b	842	BCR	C23-C24-C25-C30
21	b	843	BCR	C1-C6-C7-C8
21	b	843	BCR	C21-C22-C23-C24
21	b	845	BCR	C22-C23-C24-C25
21	b	846	BCR	C20-C21-C22-C37
21	b	846	BCR	C21-C22-C23-C24
21	b	847	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	b	847	BCR	C10-C11-C12-C13
21	b	847	BCR	C11-C12-C13-C14
21	b	847	BCR	C11-C12-C13-C35
21	b	847	BCR	C16-C17-C18-C36
21	b	847	BCR	C21-C22-C23-C24
21	b	847	BCR	C37-C22-C23-C24
21	f	202	BCR	C7-C8-C9-C10
21	f	202	BCR	C37-C22-C23-C24
21	i	101	BCR	C20-C21-C22-C37
21	i	101	BCR	C21-C22-C23-C24
21	i	102	BCR	C7-C8-C9-C34
21	i	102	BCR	C21-C22-C23-C24
21	i	102	BCR	C37-C22-C23-C24
21	i	102	BCR	C23-C24-C25-C26
21	i	102	BCR	C23-C24-C25-C30
21	j	101	BCR	C1-C6-C7-C8
21	j	101	BCR	C21-C22-C23-C24
21	l	205	BCR	C7-C8-C9-C10
26	a	852	LHG	O1-C1-C2-C3
26	a	852	LHG	C3-O3-P-O4
26	a	852	LHG	C3-O3-P-O6
26	a	853	LHG	C3-O3-P-O5
26	a	855	LHG	C4-O6-P-O5
26	a	855	LHG	O9-C7-O7-C5
26	b	849	LHG	O1-C1-C2-C3
26	b	849	LHG	C3-O3-P-O5
26	b	849	LHG	C4-O6-P-O5
26	f	206	LHG	O2-C2-C3-O3
26	f	206	LHG	C2-C3-O3-P
26	f	206	LHG	C3-O3-P-O4
26	f	206	LHG	C4-O6-P-O5
27	l	201	LMG	O6-C1-O1-C7
27	l	201	LMG	O9-C10-O7-C8
27	l	201	LMG	C11-C10-O7-C8
29	b	844	ECH	C21-C22-C23-C24
29	b	844	ECH	C37-C22-C23-C24
29	m	101	ECH	C21-C22-C23-C24
29	m	101	ECH	C37-C22-C23-C24
19	a	821	CLA	O1D-CGD-O2D-CED
19	b	801	CLA	O1D-CGD-O2D-CED
19	b	808	CLA	O1D-CGD-O2D-CED
19	b	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	b	834	CLA	O1D-CGD-O2D-CED
19	k	101	CLA	O1D-CGD-O2D-CED
19	a	802	CLA	O1D-CGD-O2D-CED
19	b	802	CLA	O1D-CGD-O2D-CED
19	a	806	CLA	CBD-CGD-O2D-CED
19	a	814	CLA	CBD-CGD-O2D-CED
19	a	819	CLA	CBD-CGD-O2D-CED
19	a	829	CLA	CBD-CGD-O2D-CED
19	a	841	CLA	CBD-CGD-O2D-CED
19	b	801	CLA	CBD-CGD-O2D-CED
19	b	808	CLA	CBD-CGD-O2D-CED
19	b	813	CLA	CBD-CGD-O2D-CED
19	b	819	CLA	CBD-CGD-O2D-CED
19	b	820	CLA	CBD-CGD-O2D-CED
19	b	826	CLA	CBD-CGD-O2D-CED
19	b	827	CLA	CBD-CGD-O2D-CED
19	b	834	CLA	CBD-CGD-O2D-CED
19	j	104	CLA	CBD-CGD-O2D-CED
19	k	102	CLA	CBD-CGD-O2D-CED
19	a	843	CLA	O1A-CGA-O2A-C1
19	b	805	CLA	O1A-CGA-O2A-C1
19	b	820	CLA	O1A-CGA-O2A-C1
19	b	826	CLA	O1A-CGA-O2A-C1
19	b	832	CLA	O1A-CGA-O2A-C1
19	b	837	CLA	O1A-CGA-O2A-C1
26	a	852	LHG	O10-C23-O8-C6
19	a	816	CLA	O1A-CGA-O2A-C1
19	j	104	CLA	O1A-CGA-O2A-C1
19	b	827	CLA	O1D-CGD-O2D-CED
19	D	402	CLA	O1D-CGD-O2D-CED
19	a	841	CLA	O1D-CGD-O2D-CED
19	b	814	CLA	O1D-CGD-O2D-CED
19	f	201	CLA	O1D-CGD-O2D-CED
19	j	103	CLA	O1D-CGD-O2D-CED
19	k	102	CLA	O1D-CGD-O2D-CED
19	a	843	CLA	CBA-CGA-O2A-C1
19	b	805	CLA	CBA-CGA-O2A-C1
19	b	832	CLA	CBA-CGA-O2A-C1
19	b	837	CLA	CBA-CGA-O2A-C1
19	l	203	CLA	CBA-CGA-O2A-C1
19	A	402	CLA	CBD-CGD-O2D-CED
19	A	403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	407	CLA	CBD-CGD-O2D-CED
19	b	805	CLA	CBD-CGD-O2D-CED
19	b	812	CLA	CBD-CGD-O2D-CED
19	b	835	CLA	CBD-CGD-O2D-CED
19	a	811	CLA	O1A-CGA-O2A-C1
19	a	813	CLA	O1A-CGA-O2A-C1
19	a	820	CLA	O1A-CGA-O2A-C1
19	a	832	CLA	O1A-CGA-O2A-C1
19	a	835	CLA	O1A-CGA-O2A-C1
19	a	856	CLA	O1A-CGA-O2A-C1
19	b	804	CLA	O1A-CGA-O2A-C1
19	b	810	CLA	O1A-CGA-O2A-C1
19	b	811	CLA	O1A-CGA-O2A-C1
19	b	823	CLA	O1A-CGA-O2A-C1
19	b	828	CLA	O1A-CGA-O2A-C1
19	b	829	CLA	O1A-CGA-O2A-C1
19	b	833	CLA	O1A-CGA-O2A-C1
19	b	834	CLA	O1A-CGA-O2A-C1
19	b	835	CLA	O1A-CGA-O2A-C1
19	b	838	CLA	O1A-CGA-O2A-C1
19	f	203	CLA	O1A-CGA-O2A-C1
19	l	202	CLA	O1A-CGA-O2A-C1
19	l	203	CLA	O1A-CGA-O2A-C1
26	f	206	LHG	O10-C23-O8-C6
27	a	854	LMG	O10-C28-O8-C9
27	b	850	LMG	O10-C28-O8-C9
27	l	201	LMG	O10-C28-O8-C9
19	a	817	CLA	O1A-CGA-O2A-C1
19	k	101	CLA	O1A-CGA-O2A-C1
19	b	819	CLA	O1D-CGD-O2D-CED
19	a	816	CLA	CBD-CGD-O2D-CED
19	b	822	CLA	CBD-CGD-O2D-CED
19	b	833	CLA	CBD-CGD-O2D-CED
20	D	401	PHO	O1D-CGD-O2D-CED
26	f	206	LHG	O9-C7-O7-C5
19	a	824	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	O1A-CGA-O2A-C1
19	A	403	CLA	O1A-CGA-O2A-C1
19	b	840	CLA	O1A-CGA-O2A-C1
19	a	803	CLA	C3-C5-C6-C7
19	a	818	CLA	C3-C5-C6-C7
19	a	824	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	a	836	CLA	C3-C5-C6-C7
19	a	840	CLA	C3-C5-C6-C7
19	a	841	CLA	C3-C5-C6-C7
19	a	843	CLA	C3-C5-C6-C7
19	b	812	CLA	C3-C5-C6-C7
19	b	836	CLA	C3-C5-C6-C7
19	A	402	CLA	CBA-CGA-O2A-C1
19	A	405	CLA	CBA-CGA-O2A-C1
19	a	802	CLA	CBA-CGA-O2A-C1
19	a	819	CLA	CBA-CGA-O2A-C1
19	a	820	CLA	CBA-CGA-O2A-C1
19	a	832	CLA	CBA-CGA-O2A-C1
19	a	835	CLA	CBA-CGA-O2A-C1
19	a	839	CLA	CBA-CGA-O2A-C1
19	a	857	CLA	CBA-CGA-O2A-C1
19	a	860	CLA	CBA-CGA-O2A-C1
19	b	806	CLA	CBA-CGA-O2A-C1
19	b	811	CLA	CBA-CGA-O2A-C1
19	b	820	CLA	CBA-CGA-O2A-C1
19	b	826	CLA	CBA-CGA-O2A-C1
19	b	828	CLA	CBA-CGA-O2A-C1
19	b	829	CLA	CBA-CGA-O2A-C1
19	b	835	CLA	CBA-CGA-O2A-C1
19	j	103	CLA	CBA-CGA-O2A-C1
19	l	202	CLA	CBA-CGA-O2A-C1
26	a	852	LHG	C24-C23-O8-C6
26	f	206	LHG	C24-C23-O8-C6
26	a	855	LHG	C8-C7-O7-C5
19	b	813	CLA	O1D-CGD-O2D-CED
19	b	826	CLA	O1D-CGD-O2D-CED
19	a	828	CLA	CBD-CGD-O2D-CED
19	A	403	CLA	CBA-CGA-O2A-C1
19	b	840	CLA	CBA-CGA-O2A-C1
19	a	802	CLA	C4-C3-C5-C6
19	b	808	CLA	C4-C3-C5-C6
19	a	802	CLA	C2-C3-C5-C6
19	a	837	CLA	C2-C3-C5-C6
19	a	857	CLA	C2-C3-C5-C6
19	b	828	CLA	C2-C3-C5-C6
19	b	836	CLA	C2-C3-C5-C6
19	b	828	CLA	CBD-CGD-O2D-CED
19	b	832	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	405	CLA	C2A-CAA-CBA-CGA
19	a	821	CLA	C2A-CAA-CBA-CGA
19	b	808	CLA	C2A-CAA-CBA-CGA
19	b	827	CLA	C2A-CAA-CBA-CGA
19	b	830	CLA	C2A-CAA-CBA-CGA
19	b	831	CLA	C2A-CAA-CBA-CGA
19	b	840	CLA	C2A-CAA-CBA-CGA
19	l	202	CLA	C2A-CAA-CBA-CGA
20	A	404	PHO	C2A-CAA-CBA-CGA
19	b	801	CLA	O1A-CGA-O2A-C1
19	a	802	CLA	C3-C5-C6-C7
19	a	831	CLA	C3-C5-C6-C7
19	a	832	CLA	C3-C5-C6-C7
19	a	857	CLA	C3-C5-C6-C7
19	a	860	CLA	C3-C5-C6-C7
20	D	401	PHO	C3-C5-C6-C7
19	a	808	CLA	CBA-CGA-O2A-C1
19	a	811	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	CBA-CGA-O2A-C1
19	a	842	CLA	CBA-CGA-O2A-C1
19	a	856	CLA	CBA-CGA-O2A-C1
19	b	801	CLA	CBA-CGA-O2A-C1
19	b	802	CLA	CBA-CGA-O2A-C1
19	b	804	CLA	CBA-CGA-O2A-C1
19	b	810	CLA	CBA-CGA-O2A-C1
19	b	815	CLA	CBA-CGA-O2A-C1
19	b	823	CLA	CBA-CGA-O2A-C1
19	b	830	CLA	CBA-CGA-O2A-C1
19	b	831	CLA	CBA-CGA-O2A-C1
19	b	833	CLA	CBA-CGA-O2A-C1
19	b	834	CLA	CBA-CGA-O2A-C1
19	b	836	CLA	CBA-CGA-O2A-C1
19	b	838	CLA	CBA-CGA-O2A-C1
19	f	203	CLA	CBA-CGA-O2A-C1
20	A	404	PHO	CBA-CGA-O2A-C1
27	a	854	LMG	C29-C28-O8-C9
27	b	850	LMG	C29-C28-O8-C9
27	l	201	LMG	C29-C28-O8-C9
27	b	850	LMG	O6-C5-C6-O5
19	a	819	CLA	O1D-CGD-O2D-CED
19	b	804	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	l	204	CLA	CBD-CGD-O2D-CED
19	a	806	CLA	O1D-CGD-O2D-CED
19	b	820	CLA	O1D-CGD-O2D-CED
19	A	402	CLA	O1A-CGA-O2A-C1
19	A	405	CLA	O1A-CGA-O2A-C1
19	a	808	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	O1A-CGA-O2A-C1
19	a	815	CLA	O1A-CGA-O2A-C1
19	a	819	CLA	O1A-CGA-O2A-C1
19	a	821	CLA	O1A-CGA-O2A-C1
19	a	825	CLA	O1A-CGA-O2A-C1
19	a	828	CLA	O1A-CGA-O2A-C1
19	a	839	CLA	O1A-CGA-O2A-C1
19	a	860	CLA	O1A-CGA-O2A-C1
19	b	806	CLA	O1A-CGA-O2A-C1
19	b	816	CLA	O1A-CGA-O2A-C1
19	b	830	CLA	O1A-CGA-O2A-C1
19	b	831	CLA	O1A-CGA-O2A-C1
19	f	201	CLA	O1A-CGA-O2A-C1
19	j	103	CLA	O1A-CGA-O2A-C1
20	A	404	PHO	O1A-CGA-O2A-C1
23	a	801	CL0	O1A-CGA-O2A-C1
19	j	104	CLA	O1D-CGD-O2D-CED
19	a	805	CLA	CBD-CGD-O2D-CED
19	a	815	CLA	CBD-CGD-O2D-CED
19	a	831	CLA	CBD-CGD-O2D-CED
19	a	840	CLA	CBD-CGD-O2D-CED
19	a	813	CLA	C3-C5-C6-C7
19	b	803	CLA	C3-C5-C6-C7
19	a	804	CLA	CBA-CGA-O2A-C1
19	a	809	CLA	CBA-CGA-O2A-C1
19	a	812	CLA	CBA-CGA-O2A-C1
19	a	815	CLA	CBA-CGA-O2A-C1
19	a	823	CLA	CBA-CGA-O2A-C1
19	a	824	CLA	CBA-CGA-O2A-C1
19	a	828	CLA	CBA-CGA-O2A-C1
19	a	833	CLA	CBA-CGA-O2A-C1
19	b	808	CLA	CBA-CGA-O2A-C1
19	b	812	CLA	CBA-CGA-O2A-C1
23	a	801	CL0	CBA-CGA-O2A-C1
19	a	823	CLA	O1A-CGA-O2A-C1
19	a	857	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	b	815	CLA	O1A-CGA-O2A-C1
19	b	836	CLA	O1A-CGA-O2A-C1
19	a	823	CLA	CBD-CGD-O2D-CED
19	a	826	CLA	C3-C5-C6-C7
19	a	821	CLA	CBA-CGA-O2A-C1
19	a	825	CLA	CBA-CGA-O2A-C1
19	b	816	CLA	CBA-CGA-O2A-C1
19	f	201	CLA	CBA-CGA-O2A-C1
32	j	102	LMT	O5'-C5'-C6'-O6'
27	a	854	LMG	C4-C5-C6-O5
27	b	850	LMG	C4-C5-C6-O5
19	a	804	CLA	O1A-CGA-O2A-C1
19	a	830	CLA	O1A-CGA-O2A-C1
19	a	833	CLA	O1A-CGA-O2A-C1
19	a	842	CLA	O1A-CGA-O2A-C1
19	b	812	CLA	O1A-CGA-O2A-C1
26	a	853	LHG	C29-C30-C31-C32
27	b	848	LMG	O6-C5-C6-O5
19	a	809	CLA	C2A-CAA-CBA-CGA
19	b	816	CLA	C2A-CAA-CBA-CGA
19	j	104	CLA	C2A-CAA-CBA-CGA
19	l	204	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	O1D-CGD-O2D-CED
19	a	809	CLA	O1A-CGA-O2A-C1
19	a	841	CLA	O1A-CGA-O2A-C1
19	b	808	CLA	O1A-CGA-O2A-C1
19	a	819	CLA	C3-C5-C6-C7
19	a	837	CLA	CBA-CGA-O2A-C1
19	a	841	CLA	CBA-CGA-O2A-C1
19	f	204	CLA	CBA-CGA-O2A-C1
26	b	849	LHG	C32-C33-C34-C35
19	a	829	CLA	O1D-CGD-O2D-CED
19	A	407	CLA	O1D-CGD-O2D-CED
19	b	835	CLA	O1D-CGD-O2D-CED
19	b	803	CLA	CBD-CGD-O2D-CED
19	b	836	CLA	CBD-CGD-O2D-CED
19	A	402	CLA	O1D-CGD-O2D-CED
26	f	206	LHG	C1-C2-C3-O3
27	a	854	LMG	O6-C5-C6-O5
19	a	837	CLA	O1A-CGA-O2A-C1
19	b	827	CLA	O1A-CGA-O2A-C1
19	f	204	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	805	CLA	CBA-CGA-O2A-C1
19	a	822	CLA	CBA-CGA-O2A-C1
19	a	826	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	CBA-CGA-O2A-C1
19	a	836	CLA	CBA-CGA-O2A-C1
19	b	824	CLA	CBA-CGA-O2A-C1
19	b	827	CLA	CBA-CGA-O2A-C1
19	a	804	CLA	C15-C16-C17-C18
19	a	805	CLA	O1A-CGA-O2A-C1
27	b	848	LMG	C4-C5-C6-O5
19	a	819	CLA	C8-C10-C11-C12
19	a	835	CLA	C5-C6-C7-C8
19	a	840	CLA	C8-C10-C11-C12
19	a	842	CLA	C10-C11-C12-C13
19	a	857	CLA	C13-C15-C16-C17
26	a	853	LHG	O2-C2-C3-O3
26	a	852	LHG	O7-C5-C6-O8
26	a	853	LHG	O7-C5-C6-O8
19	a	831	CLA	O1A-CGA-O2A-C1
19	b	808	CLA	C2-C3-C5-C6
19	a	807	CLA	C6-C7-C8-C9
19	a	808	CLA	C11-C10-C8-C9
19	a	809	CLA	C11-C12-C13-C14
19	a	836	CLA	C6-C7-C8-C9
19	a	836	CLA	C14-C13-C15-C16
19	a	839	CLA	C11-C10-C8-C9
19	a	842	CLA	C11-C12-C13-C14
19	b	801	CLA	C11-C12-C13-C14
19	b	803	CLA	C11-C12-C13-C14
19	b	805	CLA	C14-C13-C15-C16
19	b	806	CLA	C6-C7-C8-C9
19	b	816	CLA	C11-C10-C8-C9
19	b	817	CLA	C6-C7-C8-C9
19	b	818	CLA	C11-C10-C8-C9
19	b	828	CLA	C11-C12-C13-C14
19	b	832	CLA	C14-C13-C15-C16
19	A	403	CLA	O1D-CGD-O2D-CED
19	a	815	CLA	C8-C10-C11-C12
19	a	802	CLA	C2A-CAA-CBA-CGA
19	a	815	CLA	C2A-CAA-CBA-CGA
19	a	816	CLA	C2A-CAA-CBA-CGA
21	A	406	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
21	f	202	BCR	C7-C8-C9-C34
21	k	103	BCR	C11-C12-C13-C35
21	l	205	BCR	C11-C12-C13-C35
21	i	102	BCR	C7-C8-C9-C10
19	a	826	CLA	O1A-CGA-O2A-C1
19	b	826	CLA	C8-C10-C11-C12
20	D	401	PHO	C15-C16-C17-C18
19	b	814	CLA	CBA-CGA-O2A-C1
22	E	101	HEM	C2A-CAA-CBA-CGA
19	a	814	CLA	C15-C16-C17-C18
19	a	829	CLA	C15-C16-C17-C18
19	a	840	CLA	C15-C16-C17-C18
19	a	860	CLA	C13-C15-C16-C17
19	b	802	CLA	C15-C16-C17-C18
19	b	805	CLA	C5-C6-C7-C8
24	a	844	PQN	C18-C20-C21-C22
26	a	853	LHG	C7-C8-C9-C10
26	a	853	LHG	C23-C24-C25-C26
26	b	849	LHG	C23-C24-C25-C26
26	f	206	LHG	C7-C8-C9-C10
21	f	202	BCR	C14-C15-C16-C17
19	a	814	CLA	C13-C15-C16-C17
19	a	815	CLA	C5-C6-C7-C8
19	a	822	CLA	C8-C10-C11-C12
19	b	802	CLA	C10-C11-C12-C13
19	b	803	CLA	C10-C11-C12-C13
19	b	809	CLA	C5-C6-C7-C8
19	b	825	CLA	C8-C10-C11-C12
19	b	828	CLA	C5-C6-C7-C8
19	b	832	CLA	C5-C6-C7-C8
19	b	805	CLA	O1D-CGD-O2D-CED
26	a	855	LHG	C23-C24-C25-C26
27	b	848	LMG	C28-C29-C30-C31
19	a	834	CLA	C13-C15-C16-C17
19	a	841	CLA	C15-C16-C17-C18
19	b	804	CLA	C13-C15-C16-C17
19	b	806	CLA	C5-C6-C7-C8
19	a	824	CLA	C2-C1-O2A-CGA
19	a	856	CLA	C2-C1-O2A-CGA
19	b	820	CLA	C2-C1-O2A-CGA
19	a	802	CLA	C15-C16-C17-C18
19	a	805	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	b	832	CLA	C8-C10-C11-C12
26	a	852	LHG	C23-C24-C25-C26
19	D	403	CLA	CBD-CGD-O2D-CED
19	b	809	CLA	CBD-CGD-O2D-CED
19	b	825	CLA	C5-C6-C7-C8
19	a	812	CLA	C11-C12-C13-C15
19	a	813	CLA	C11-C10-C8-C7
19	a	814	CLA	C6-C7-C8-C10
19	a	821	CLA	C6-C7-C8-C10
19	a	827	CLA	C11-C10-C8-C7
19	a	834	CLA	C11-C12-C13-C15
19	a	837	CLA	C6-C7-C8-C10
19	b	813	CLA	C11-C10-C8-C7
19	b	823	CLA	C11-C12-C13-C15
19	b	838	CLA	C11-C12-C13-C15
19	b	824	CLA	O1A-CGA-O2A-C1
21	a	851	BCR	C9-C10-C11-C12
21	b	847	BCR	C13-C14-C15-C16
19	a	804	CLA	C2A-CAA-CBA-CGA
19	a	842	CLA	C2A-CAA-CBA-CGA
19	b	803	CLA	C2A-CAA-CBA-CGA
19	a	816	CLA	O1D-CGD-O2D-CED
19	b	812	CLA	O1D-CGD-O2D-CED
19	a	823	CLA	C13-C15-C16-C17
19	b	823	CLA	C13-C15-C16-C17
19	b	827	CLA	C8-C10-C11-C12
32	j	102	LMT	C4'-C5'-C6'-O6'
19	a	822	CLA	O1A-CGA-O2A-C1
20	A	404	PHO	C8-C10-C11-C12
21	a	846	BCR	C18-C19-C20-C21
21	a	850	BCR	C18-C19-C20-C21
21	b	843	BCR	C18-C19-C20-C21
21	i	102	BCR	C10-C11-C12-C13
21	i	102	BCR	C18-C19-C20-C21
20	A	404	PHO	C3-C5-C6-C7
19	a	808	CLA	C13-C15-C16-C17
19	a	828	CLA	C10-C11-C12-C13
19	a	837	CLA	C8-C10-C11-C12
19	b	808	CLA	C8-C10-C11-C12
19	b	813	CLA	C15-C16-C17-C18
19	b	831	CLA	C10-C11-C12-C13
19	a	836	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	860	CLA	C5-C6-C7-C8
19	b	822	CLA	O1D-CGD-O2D-CED
19	b	833	CLA	O1D-CGD-O2D-CED
19	b	814	CLA	O1A-CGA-O2A-C1
19	a	821	CLA	C5-C6-C7-C8
19	b	819	CLA	C5-C6-C7-C8
19	b	838	CLA	C10-C11-C12-C13
26	b	849	LHG	C3-O3-P-O6
26	f	206	LHG	C3-O3-P-O6
26	f	206	LHG	C4-O6-P-O3
19	A	407	CLA	CBA-CGA-O2A-C1
19	b	822	CLA	CBA-CGA-O2A-C1
19	a	828	CLA	O1D-CGD-O2D-CED
19	b	828	CLA	O1D-CGD-O2D-CED
31	b	852	ZEX	C25-C26-C27-C28
31	f	205	ZEX	C25-C26-C27-C28
26	a	853	LHG	C1-C2-C3-O3
19	D	403	CLA	C2A-CAA-CBA-CGA
19	a	828	CLA	C2A-CAA-CBA-CGA
19	b	812	CLA	C2A-CAA-CBA-CGA
19	b	805	CLA	C16-C17-C18-C20
19	b	839	CLA	C16-C17-C18-C20
19	b	803	CLA	CBA-CGA-O2A-C1
26	a	852	LHG	C24-C25-C26-C27
27	b	848	LMG	C37-C38-C39-C40
19	a	812	CLA	C13-C15-C16-C17
19	a	820	CLA	C15-C16-C17-C18
21	a	847	BCR	C20-C21-C22-C37
21	a	850	BCR	C20-C21-C22-C37
21	b	847	BCR	C11-C10-C9-C34
21	i	102	BCR	C20-C21-C22-C37
21	k	103	BCR	C16-C17-C18-C36
21	l	205	BCR	C35-C13-C14-C15
27	a	854	LMG	C32-C33-C34-C35
27	l	201	LMG	C32-C33-C34-C35
19	a	804	CLA	C16-C17-C18-C19
23	a	801	CL0	C16-C17-C18-C19
19	a	838	CLA	CBA-CGA-O2A-C1
26	a	853	LHG	C27-C28-C29-C30
26	a	853	LHG	C28-C29-C30-C31
27	b	850	LMG	C18-C19-C20-C21
19	l	204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	b	826	CLA	C10-C11-C12-C13
26	b	849	LHG	C27-C28-C29-C30
26	f	206	LHG	C27-C28-C29-C30
27	b	848	LMG	C16-C17-C18-C19
27	b	848	LMG	C33-C34-C35-C36
27	b	850	LMG	C17-C18-C19-C20
19	a	831	CLA	O1D-CGD-O2D-CED
19	b	832	CLA	O1D-CGD-O2D-CED
19	a	808	CLA	C8-C10-C11-C12
26	a	853	LHG	C32-C33-C34-C35
19	a	830	CLA	C3-C5-C6-C7
26	a	855	LHG	C7-C8-C9-C10
21	b	847	BCR	C16-C17-C18-C19
27	b	848	LMG	C34-C35-C36-C37
19	a	804	CLA	C10-C11-C12-C13
19	A	407	CLA	O1A-CGA-O2A-C1
19	a	830	CLA	C16-C17-C18-C20
19	f	201	CLA	C16-C17-C18-C20
19	a	805	CLA	O1D-CGD-O2D-CED
19	b	804	CLA	O1D-CGD-O2D-CED
19	b	804	CLA	C4-C3-C5-C6
19	b	812	CLA	C2-C3-C5-C6
19	a	806	CLA	C11-C12-C13-C14
19	a	809	CLA	C6-C7-C8-C9
19	a	818	CLA	C11-C10-C8-C9
19	a	826	CLA	C14-C13-C15-C16
19	b	804	CLA	C6-C7-C8-C9
19	b	817	CLA	C14-C13-C15-C16
19	b	818	CLA	C6-C7-C8-C9
27	b	848	LMG	C32-C33-C34-C35
27	b	850	LMG	C13-C14-C15-C16
27	b	850	LMG	C30-C31-C32-C33
27	l	201	LMG	C18-C19-C20-C21
19	a	803	CLA	C10-C11-C12-C13
19	a	822	CLA	C10-C11-C12-C13
19	a	805	CLA	C2A-CAA-CBA-CGA
19	a	811	CLA	C2A-CAA-CBA-CGA
19	a	825	CLA	C2A-CAA-CBA-CGA
19	b	829	CLA	C2A-CAA-CBA-CGA
26	b	849	LHG	C30-C31-C32-C33
26	a	853	LHG	O1-C1-C2-C3
26	f	206	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	b	817	CLA	C3-C5-C6-C7
26	b	849	LHG	C24-C25-C26-C27
26	a	855	LHG	C32-C33-C34-C35
27	l	201	LMG	C17-C18-C19-C20
19	a	825	CLA	C11-C12-C13-C14
19	a	825	CLA	C11-C12-C13-C15
26	a	855	LHG	C16-C17-C18-C19
26	f	206	LHG	C31-C32-C33-C34
19	a	828	CLA	C8-C10-C11-C12
19	b	813	CLA	C3-C5-C6-C7
23	a	801	CL0	C3-C5-C6-C7
19	l	204	CLA	CBA-CGA-O2A-C1
27	b	848	LMG	C30-C31-C32-C33
19	a	840	CLA	O1D-CGD-O2D-CED
19	a	805	CLA	C3A-C2A-CAA-CBA
19	a	818	CLA	C3A-C2A-CAA-CBA
19	a	828	CLA	C3A-C2A-CAA-CBA
19	a	835	CLA	C3A-C2A-CAA-CBA
19	a	843	CLA	C3A-C2A-CAA-CBA
19	b	814	CLA	C3A-C2A-CAA-CBA
19	b	821	CLA	C3A-C2A-CAA-CBA
19	b	823	CLA	C3A-C2A-CAA-CBA
19	b	838	CLA	C3A-C2A-CAA-CBA
19	j	103	CLA	C3A-C2A-CAA-CBA
19	l	203	CLA	C3A-C2A-CAA-CBA
32	j	102	LMT	C2-C1-O1'-C1'
19	b	839	CLA	C16-C17-C18-C19
26	a	852	LHG	C29-C30-C31-C32
21	a	851	BCR	C14-C15-C16-C17
21	i	101	BCR	C14-C15-C16-C17
19	b	809	CLA	C3-C5-C6-C7
19	a	833	CLA	C10-C11-C12-C13
19	a	830	CLA	C4-C3-C5-C6
19	a	828	CLA	C2-C3-C5-C6
19	b	804	CLA	C2-C3-C5-C6
26	a	852	LHG	C26-C27-C28-C29
26	a	852	LHG	O1-C1-C2-O2
26	b	849	LHG	O1-C1-C2-O2
27	b	850	LMG	C16-C17-C18-C19
19	a	830	CLA	C16-C17-C18-C19
19	a	833	CLA	C11-C12-C13-C15
26	f	206	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	a	852	LHG	C11-C10-C9-C8
19	b	803	CLA	O1A-CGA-O2A-C1
19	b	822	CLA	O1A-CGA-O2A-C1
19	a	811	CLA	C2-C1-O2A-CGA
19	a	830	CLA	C2-C1-O2A-CGA
19	a	841	CLA	C2-C1-O2A-CGA
19	b	801	CLA	C2-C1-O2A-CGA
19	b	802	CLA	C2-C1-O2A-CGA
19	b	806	CLA	C2-C1-O2A-CGA
19	l	203	CLA	C2-C1-O2A-CGA
19	b	812	CLA	C13-C15-C16-C17
31	b	852	ZEX	C21-C26-C27-C28
31	f	205	ZEX	C21-C26-C27-C28
19	a	838	CLA	O1A-CGA-O2A-C1
21	A	406	BCR	C1-C6-C7-C8
21	a	848	BCR	C5-C6-C7-C8
21	a	850	BCR	C1-C6-C7-C8
21	a	850	BCR	C5-C6-C7-C8
21	a	850	BCR	C23-C24-C25-C26
21	a	851	BCR	C1-C6-C7-C8
21	a	859	BCR	C1-C6-C7-C8
21	a	859	BCR	C5-C6-C7-C8
21	a	859	BCR	C23-C24-C25-C26
21	b	842	BCR	C1-C6-C7-C8
21	b	842	BCR	C5-C6-C7-C8
21	b	842	BCR	C23-C24-C25-C26
21	b	843	BCR	C5-C6-C7-C8
21	j	101	BCR	C5-C6-C7-C8
21	l	205	BCR	C1-C6-C7-C8
21	l	205	BCR	C5-C6-C7-C8
21	l	205	BCR	C23-C24-C25-C26
21	l	205	BCR	C23-C24-C25-C30
29	b	844	ECH	C1-C6-C7-C8
29	b	844	ECH	C5-C6-C7-C8
29	m	101	ECH	C5-C6-C7-C8
29	m	101	ECH	C23-C24-C25-C26
30	b	851	EQ3	C23-C24-C25-C26
19	b	809	CLA	CBA-CGA-O2A-C1
27	b	850	LMG	C14-C15-C16-C17
19	b	817	CLA	C10-C11-C12-C13
19	b	812	CLA	C4-C3-C5-C6
19	a	815	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	407	CLA	C11-C12-C13-C15
19	a	806	CLA	C11-C12-C13-C15
19	a	812	CLA	C12-C13-C15-C16
19	a	836	CLA	C11-C12-C13-C15
19	a	842	CLA	C11-C12-C13-C15
19	b	801	CLA	C11-C12-C13-C15
19	b	804	CLA	C6-C7-C8-C10
19	b	805	CLA	C12-C13-C15-C16
19	b	816	CLA	C11-C12-C13-C15
19	b	817	CLA	C12-C13-C15-C16
19	b	833	CLA	C11-C12-C13-C15
19	l	204	CLA	O1A-CGA-O2A-C1
26	a	852	LHG	C15-C16-C17-C18
19	a	856	CLA	C5-C6-C7-C8
19	f	201	CLA	C16-C17-C18-C19
19	a	823	CLA	O1D-CGD-O2D-CED
19	a	814	CLA	CBA-CGA-O2A-C1
19	a	803	CLA	C2A-CAA-CBA-CGA
19	a	831	CLA	C2A-CAA-CBA-CGA
19	b	826	CLA	C2A-CAA-CBA-CGA
19	f	201	CLA	C15-C16-C17-C18
27	b	850	LMG	C34-C35-C36-C37
27	l	201	LMG	C31-C32-C33-C34
19	a	824	CLA	C5-C6-C7-C8
19	a	842	CLA	C8-C10-C11-C12
27	a	854	LMG	C15-C16-C17-C18
26	f	206	LHG	C8-C7-O7-C5
19	a	834	CLA	CBD-CGD-O2D-CED
26	f	206	LHG	C23-C24-C25-C26
27	l	201	LMG	C2-C1-O1-C7
19	b	805	CLA	C16-C17-C18-C19
23	a	801	CL0	C16-C17-C18-C20
19	b	802	CLA	C8-C10-C11-C12
19	a	824	CLA	C4-C3-C5-C6
19	a	828	CLA	C4-C3-C5-C6
19	A	407	CLA	C11-C12-C13-C14
19	a	808	CLA	C11-C12-C13-C14
19	a	812	CLA	C11-C12-C13-C14
19	a	812	CLA	C14-C13-C15-C16
19	a	814	CLA	C11-C12-C13-C14
19	a	827	CLA	C11-C10-C8-C9
19	a	837	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	a	837	CLA	C11-C10-C8-C9
19	b	817	CLA	C11-C10-C8-C9
19	b	823	CLA	C11-C10-C8-C9
19	b	833	CLA	C11-C12-C13-C14
19	b	836	CLA	C6-C7-C8-C9
19	b	838	CLA	C11-C12-C13-C14
26	a	852	LHG	C18-C19-C20-C21
26	f	206	LHG	C34-C35-C36-C37
19	b	814	CLA	C3-C5-C6-C7
19	f	201	CLA	C3-C5-C6-C7
19	b	811	CLA	C2A-CAA-CBA-CGA
21	b	843	BCR	C37-C22-C23-C24
27	l	201	LMG	C15-C16-C17-C18
19	b	809	CLA	O1A-CGA-O2A-C1
19	A	407	CLA	C1A-C2A-CAA-CBA
19	a	806	CLA	C1A-C2A-CAA-CBA
19	a	824	CLA	C1A-C2A-CAA-CBA
19	a	827	CLA	C1A-C2A-CAA-CBA
19	a	842	CLA	C1A-C2A-CAA-CBA
19	a	843	CLA	C1A-C2A-CAA-CBA
19	b	839	CLA	C1A-C2A-CAA-CBA
19	k	101	CLA	C1A-C2A-CAA-CBA
27	l	201	LMG	O6-C5-C6-O5
19	a	833	CLA	C11-C12-C13-C14
26	a	852	LHG	C8-C7-O7-C5
26	b	849	LHG	C8-C7-O7-C5
27	a	854	LMG	C11-C10-O7-C8
19	a	824	CLA	C8-C10-C11-C12
19	a	813	CLA	C8-C10-C11-C12
19	a	841	CLA	C5-C6-C7-C8
26	b	849	LHG	O6-C4-C5-C6
19	b	803	CLA	O1D-CGD-O2D-CED
19	b	836	CLA	O1D-CGD-O2D-CED
26	b	849	LHG	C33-C34-C35-C36
19	a	804	CLA	C16-C17-C18-C20
27	b	850	LMG	C41-C42-C43-C44
27	a	854	LMG	C30-C31-C32-C33
27	b	848	LMG	C31-C32-C33-C34
26	f	206	LHG	C11-C12-C13-C14
19	b	806	CLA	C3-C5-C6-C7
26	a	855	LHG	C4-C5-C6-O8
27	a	854	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	l	201	LMG	O1-C7-C8-C9
19	a	814	CLA	O1A-CGA-O2A-C1
26	a	853	LHG	C24-C25-C26-C27
27	l	201	LMG	C42-C43-C44-C45
20	A	404	PHO	C5-C6-C7-C8
27	a	854	LMG	C16-C17-C18-C19
21	k	103	BCR	C20-C21-C22-C37
19	b	833	CLA	C4-C3-C5-C6
19	D	403	CLA	O1D-CGD-O2D-CED
19	a	840	CLA	CBA-CGA-O2A-C1
19	b	805	CLA	C13-C15-C16-C17
19	b	817	CLA	C13-C15-C16-C17
26	f	206	LHG	C35-C36-C37-C38
26	f	206	LHG	C6-C5-O7-C7
19	b	822	CLA	C2A-CAA-CBA-CGA
19	a	815	CLA	C13-C15-C16-C17
19	a	839	CLA	C2-C1-O2A-CGA
19	a	857	CLA	C2-C1-O2A-CGA
19	b	823	CLA	C2-C1-O2A-CGA
19	b	836	CLA	C2-C1-O2A-CGA
23	a	801	CL0	C2-C1-O2A-CGA
26	a	853	LHG	C19-C20-C21-C22
19	b	809	CLA	O1D-CGD-O2D-CED
26	a	855	LHG	C11-C10-C9-C8
19	a	820	CLA	C16-C17-C18-C20
19	a	821	CLA	C13-C15-C16-C17
27	l	201	LMG	C37-C38-C39-C40
19	b	820	CLA	C10-C11-C12-C13
21	b	846	BCR	C20-C21-C22-C23
27	b	850	LMG	C2-C1-O1-C7
27	b	848	LMG	O7-C8-C9-O8
27	l	201	LMG	O1-C7-C8-O7
19	a	840	CLA	O1A-CGA-O2A-C1
19	A	402	CLA	C6-C7-C8-C10
19	a	808	CLA	C11-C12-C13-C15
19	a	809	CLA	C11-C12-C13-C15
19	a	814	CLA	C11-C12-C13-C15
19	a	820	CLA	C12-C13-C15-C16
19	a	822	CLA	C11-C12-C13-C15
19	a	822	CLA	C12-C13-C15-C16
19	a	823	CLA	C11-C10-C8-C7
19	a	825	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	a	830	CLA	C2-C3-C5-C6
19	a	830	CLA	C11-C12-C13-C15
19	a	830	CLA	C12-C13-C15-C16
19	a	837	CLA	C11-C10-C8-C7
19	a	842	CLA	C6-C7-C8-C10
19	a	857	CLA	C6-C7-C8-C10
19	b	801	CLA	C11-C10-C8-C7
19	b	804	CLA	C12-C13-C15-C16
19	b	806	CLA	C6-C7-C8-C10
19	b	813	CLA	C6-C7-C8-C10
19	b	817	CLA	C11-C10-C8-C7
19	b	831	CLA	C6-C7-C8-C10
19	b	833	CLA	C2-C3-C5-C6
19	b	833	CLA	C11-C10-C8-C7
19	b	836	CLA	C6-C7-C8-C10
19	b	838	CLA	C6-C7-C8-C10
19	l	203	CLA	C11-C12-C13-C15
19	A	402	CLA	C6-C7-C8-C9
19	a	804	CLA	C11-C10-C8-C9
19	a	807	CLA	C11-C12-C13-C14
19	a	815	CLA	C6-C7-C8-C9
19	a	820	CLA	C14-C13-C15-C16
19	a	821	CLA	C11-C12-C13-C14
19	a	824	CLA	C6-C7-C8-C9
19	a	825	CLA	C6-C7-C8-C9
19	a	828	CLA	C11-C10-C8-C9
19	a	830	CLA	C14-C13-C15-C16
19	a	831	CLA	C6-C7-C8-C9
19	a	836	CLA	C11-C12-C13-C14
19	a	840	CLA	C14-C13-C15-C16
19	a	842	CLA	C6-C7-C8-C9
19	b	804	CLA	C14-C13-C15-C16
19	b	813	CLA	C6-C7-C8-C9
19	b	823	CLA	C6-C7-C8-C9
19	b	831	CLA	C6-C7-C8-C9
19	b	831	CLA	C11-C10-C8-C9
19	b	833	CLA	C11-C10-C8-C9
19	l	203	CLA	C11-C12-C13-C14
19	l	203	CLA	C10-C11-C12-C13
19	k	101	CLA	C2A-CAA-CBA-CGA
21	a	851	BCR	C11-C12-C13-C35
19	a	842	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	a	857	CLA	C5-C6-C7-C8
26	a	852	LHG	C32-C33-C34-C35
27	b	848	LMG	C17-C18-C19-C20
19	a	806	CLA	C10-C11-C12-C13
19	b	801	CLA	C4-C3-C5-C6
19	b	801	CLA	C5-C6-C7-C8
19	b	805	CLA	C3-C5-C6-C7
19	a	820	CLA	C16-C17-C18-C19
20	A	404	PHO	C10-C11-C12-C13
19	a	803	CLA	C3A-C2A-CAA-CBA
23	a	801	CL0	C3A-C2A-CAA-CBA
19	b	816	CLA	C15-C16-C17-C18
19	a	839	CLA	C13-C15-C16-C17
27	b	848	LMG	C29-C28-O8-C9
26	a	852	LHG	C4-C5-C6-O8
26	a	853	LHG	C4-C5-C6-O8
27	a	854	LMG	C33-C34-C35-C36
19	a	857	CLA	O2A-C1-C2-C3
19	b	802	CLA	O2A-C1-C2-C3
27	b	848	LMG	C36-C37-C38-C39
27	b	850	LMG	C32-C33-C34-C35
19	b	805	CLA	C15-C16-C17-C18
19	a	829	CLA	C10-C11-C12-C13
19	D	402	CLA	CBA-CGA-O2A-C1
19	b	819	CLA	C15-C16-C17-C18
27	b	848	LMG	C42-C43-C44-C45
19	b	823	CLA	C5-C6-C7-C8
19	a	818	CLA	C2-C1-O2A-CGA
19	a	802	CLA	C6-C7-C8-C9
19	a	823	CLA	C11-C12-C13-C14
19	a	824	CLA	C11-C10-C8-C9
19	a	828	CLA	C14-C13-C15-C16
19	a	830	CLA	C11-C12-C13-C14
19	a	833	CLA	C11-C10-C8-C9
19	a	843	CLA	C6-C7-C8-C9
19	b	801	CLA	C11-C10-C8-C9
19	b	802	CLA	C11-C10-C8-C9
19	b	813	CLA	C14-C13-C15-C16
19	b	826	CLA	C11-C12-C13-C14
19	b	833	CLA	C6-C7-C8-C9
19	b	833	CLA	C14-C13-C15-C16
19	a	830	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	406	BCR	C5-C6-C7-C8
21	A	406	BCR	C23-C24-C25-C30
21	a	846	BCR	C1-C6-C7-C8
21	a	847	BCR	C1-C6-C7-C8
21	a	847	BCR	C5-C6-C7-C8
21	a	848	BCR	C23-C24-C25-C30
21	a	849	BCR	C1-C6-C7-C8
21	a	849	BCR	C5-C6-C7-C8
21	a	851	BCR	C5-C6-C7-C8
21	b	845	BCR	C23-C24-C25-C26
21	b	845	BCR	C23-C24-C25-C30
21	f	202	BCR	C1-C6-C7-C8
21	f	202	BCR	C5-C6-C7-C8
21	i	102	BCR	C5-C6-C7-C8
21	k	103	BCR	C23-C24-C25-C26
21	k	103	BCR	C23-C24-C25-C30
29	m	101	ECH	C1-C6-C7-C8
26	b	849	LHG	C26-C27-C28-C29
27	l	201	LMG	C30-C31-C32-C33
21	a	846	BCR	C21-C22-C23-C24
21	a	851	BCR	C16-C17-C18-C36
19	a	806	CLA	C5-C6-C7-C8
26	a	852	LHG	C30-C31-C32-C33
26	a	855	LHG	C14-C15-C16-C17
26	a	855	LHG	C31-C32-C33-C34
26	f	206	LHG	C30-C31-C32-C33
19	b	807	CLA	C3-C5-C6-C7
27	b	848	LMG	C38-C39-C40-C41
27	b	848	LMG	C18-C19-C20-C21
27	l	201	LMG	C19-C20-C21-C22
19	b	813	CLA	C8-C10-C11-C12
19	a	802	CLA	C6-C7-C8-C10
19	a	804	CLA	C11-C10-C8-C7
19	a	807	CLA	C11-C12-C13-C15
19	a	807	CLA	C12-C13-C15-C16
19	a	815	CLA	C6-C7-C8-C10
19	a	819	CLA	C11-C10-C8-C7
19	a	821	CLA	C11-C12-C13-C15
19	a	826	CLA	C11-C12-C13-C15
19	a	828	CLA	C11-C10-C8-C7
19	a	828	CLA	C12-C13-C15-C16
19	a	831	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	a	833	CLA	C11-C10-C8-C7
19	a	835	CLA	C6-C7-C8-C10
19	a	836	CLA	C6-C7-C8-C10
19	a	836	CLA	C12-C13-C15-C16
19	a	839	CLA	C11-C10-C8-C7
19	a	840	CLA	C12-C13-C15-C16
19	a	843	CLA	C6-C7-C8-C10
19	a	860	CLA	C6-C7-C8-C10
19	b	802	CLA	C11-C10-C8-C7
19	b	812	CLA	C12-C13-C15-C16
19	b	818	CLA	C6-C7-C8-C10
19	b	823	CLA	C6-C7-C8-C10
19	b	826	CLA	C11-C12-C13-C15
19	b	827	CLA	C11-C12-C13-C15
19	b	828	CLA	C11-C12-C13-C15
19	b	831	CLA	C11-C10-C8-C7
19	b	831	CLA	C12-C13-C15-C16
19	b	833	CLA	C12-C13-C15-C16
19	b	832	CLA	C3-C5-C6-C7
27	l	201	LMG	C14-C15-C16-C17
19	A	407	CLA	C5-C6-C7-C8
21	l	205	BCR	C9-C10-C11-C12
27	b	848	LMG	C21-C22-C23-C24
19	a	834	CLA	O1D-CGD-O2D-CED
19	b	812	CLA	C5-C6-C7-C8
19	a	817	CLA	C2A-CAA-CBA-CGA
23	a	801	CL0	C2A-CAA-CBA-CGA
26	a	852	LHG	C11-C12-C13-C14
19	A	402	CLA	C15-C16-C17-C18
21	A	406	BCR	C20-C21-C22-C37
21	b	847	BCR	C20-C21-C22-C37
21	f	202	BCR	C35-C13-C14-C15
21	f	202	BCR	C20-C21-C22-C37
19	b	839	CLA	CBD-CGD-O2D-CED
19	a	857	CLA	C16-C17-C18-C20
19	a	834	CLA	CBA-CGA-O2A-C1
19	a	819	CLA	C5-C6-C7-C8
19	a	819	CLA	C13-C15-C16-C17
19	A	405	CLA	CAD-CBD-CGD-O2D
19	a	809	CLA	CAD-CBD-CGD-O2D
19	a	812	CLA	CAD-CBD-CGD-O2D
19	a	827	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	a	831	CLA	CAD-CBD-CGD-O2D
19	a	835	CLA	CAD-CBD-CGD-O2D
19	b	805	CLA	CAD-CBD-CGD-O2D
19	b	810	CLA	CAD-CBD-CGD-O2D
19	b	831	CLA	CAD-CBD-CGD-O2D
19	j	103	CLA	CAD-CBD-CGD-O2D
19	a	813	CLA	C5-C6-C7-C8
21	b	847	BCR	C6-C7-C8-C9
21	b	847	BCR	C22-C23-C24-C25
19	D	402	CLA	C4-C3-C5-C6
19	a	831	CLA	C4-C3-C5-C6
19	a	813	CLA	C11-C12-C13-C15
19	a	826	CLA	C13-C15-C16-C17
19	a	830	CLA	C5-C6-C7-C8
19	a	837	CLA	C5-C6-C7-C8
27	b	850	LMG	O1-C7-C8-C9
19	a	818	CLA	C15-C16-C17-C18
19	a	805	CLA	CHA-CBD-CGD-O1D
19	a	805	CLA	CHA-CBD-CGD-O2D
19	a	815	CLA	CHA-CBD-CGD-O2D
19	a	816	CLA	CHA-CBD-CGD-O1D
19	a	816	CLA	CHA-CBD-CGD-O2D
19	a	823	CLA	CHA-CBD-CGD-O1D
19	a	823	CLA	CHA-CBD-CGD-O2D
19	a	840	CLA	CHA-CBD-CGD-O1D
19	b	828	CLA	CHA-CBD-CGD-O1D
19	b	828	CLA	CHA-CBD-CGD-O2D
19	b	835	CLA	CHA-CBD-CGD-O1D
19	b	835	CLA	CHA-CBD-CGD-O2D
19	f	201	CLA	CHA-CBD-CGD-O1D
19	f	201	CLA	CHA-CBD-CGD-O2D
27	l	201	LMG	C40-C41-C42-C43
26	f	206	LHG	C29-C30-C31-C32
26	a	855	LHG	O7-C5-C6-O8
26	f	206	LHG	O7-C5-C6-O8
27	a	854	LMG	O1-C7-C8-O7
27	b	850	LMG	C42-C43-C44-C45
19	b	838	CLA	C8-C10-C11-C12
19	D	402	CLA	O1A-CGA-O2A-C1
26	a	853	LHG	C24-C23-O8-C6
19	A	407	CLA	C11-C10-C8-C9
19	a	807	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	a	818	CLA	C14-C13-C15-C16
19	b	823	CLA	C11-C12-C13-C14
19	b	839	CLA	C11-C12-C13-C14
19	a	834	CLA	O1A-CGA-O2A-C1
27	l	201	LMG	C12-C13-C14-C15
26	a	853	LHG	C34-C35-C36-C37
19	a	860	CLA	C15-C16-C17-C18
19	b	839	CLA	C10-C11-C12-C13
21	b	845	BCR	C21-C22-C23-C24
26	a	852	LHG	C28-C29-C30-C31
19	a	803	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C2-C1-O2A-CGA
19	a	843	CLA	C2-C1-O2A-CGA
19	l	202	CLA	C2-C1-O2A-CGA
20	D	401	PHO	CBA-CGA-O2A-C1
26	a	855	LHG	C4-O6-P-O3
19	b	826	CLA	C4-C3-C5-C6
19	a	808	CLA	C3-C5-C6-C7
26	b	849	LHG	C3-O3-P-O4
26	f	206	LHG	C4-O6-P-O4
19	a	841	CLA	C13-C15-C16-C17
19	b	817	CLA	C5-C6-C7-C8
19	l	203	CLA	C13-C15-C16-C17
19	b	836	CLA	C5-C6-C7-C8
19	b	802	CLA	C2A-CAA-CBA-CGA
26	a	855	LHG	C33-C34-C35-C36
26	f	206	LHG	C33-C34-C35-C36
32	j	102	LMT	C4-C5-C6-C7
19	a	808	CLA	C16-C17-C18-C20
27	b	848	LMG	C39-C40-C41-C42
19	D	403	CLA	CAD-CBD-CGD-O1D
19	a	823	CLA	CAD-CBD-CGD-O1D
19	a	834	CLA	CAD-CBD-CGD-O1D
19	b	825	CLA	CBA-CGA-O2A-C1
19	b	822	CLA	C4-C3-C5-C6
19	A	407	CLA	C11-C10-C8-C7
19	a	815	CLA	C11-C12-C13-C15
19	a	818	CLA	C11-C10-C8-C7
19	a	819	CLA	C12-C13-C15-C16
19	a	824	CLA	C3A-C2A-CAA-CBA
19	a	824	CLA	C2-C3-C5-C6
19	a	839	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	a	841	CLA	C6-C7-C8-C10
19	a	857	CLA	C11-C12-C13-C15
19	a	860	CLA	C11-C12-C13-C15
19	b	804	CLA	C3A-C2A-CAA-CBA
19	b	813	CLA	C12-C13-C15-C16
19	b	816	CLA	C11-C10-C8-C7
26	b	849	LHG	O6-C4-C5-O7
27	b	850	LMG	C28-C29-C30-C31
20	D	401	PHO	O1A-CGA-O2A-C1
26	f	206	LHG	C4-C5-C6-O8
26	a	852	LHG	C12-C13-C14-C15
19	b	833	CLA	C13-C15-C16-C17
19	b	814	CLA	C2C-C3C-CAC-CBC
19	b	806	CLA	C15-C16-C17-C18
19	b	839	CLA	O1D-CGD-O2D-CED
19	b	807	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	C6-C7-C8-C9
19	a	814	CLA	C6-C7-C8-C9
19	a	826	CLA	C11-C12-C13-C14
19	a	834	CLA	C11-C12-C13-C14
19	a	860	CLA	C6-C7-C8-C9
19	b	803	CLA	C14-C13-C15-C16
19	b	812	CLA	C14-C13-C15-C16
19	b	827	CLA	C11-C12-C13-C14
19	b	831	CLA	C14-C13-C15-C16
19	b	832	CLA	C11-C10-C8-C9
20	A	404	PHO	C11-C12-C13-C14
21	a	848	BCR	C6-C7-C8-C9
21	a	849	BCR	C22-C23-C24-C25
21	l	205	BCR	C22-C23-C24-C25
29	b	844	ECH	C22-C23-C24-C25
19	b	828	CLA	C3-C5-C6-C7
19	b	825	CLA	O1A-CGA-O2A-C1
26	f	206	LHG	O1-C1-C2-O2
21	j	101	BCR	C37-C22-C23-C24
19	a	807	CLA	C3-C5-C6-C7
19	a	857	CLA	C16-C17-C18-C19
21	a	851	BCR	C11-C12-C13-C14
27	b	850	LMG	C19-C20-C21-C22
27	b	850	LMG	C39-C40-C41-C42
26	a	853	LHG	C30-C31-C32-C33
19	a	809	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	a	840	CLA	C4-C3-C5-C6
19	b	826	CLA	C2-C3-C5-C6
19	b	809	CLA	C2A-CAA-CBA-CGA
19	k	102	CLA	C2A-CAA-CBA-CGA
19	a	826	CLA	C2-C1-O2A-CGA
19	b	833	CLA	C2-C1-O2A-CGA
19	b	802	CLA	C2C-C3C-CAC-CBC
26	a	853	LHG	C11-C10-C9-C8
19	b	828	CLA	C10-C11-C12-C13
26	a	852	LHG	C34-C35-C36-C37
19	a	802	CLA	C5-C6-C7-C8
19	a	832	CLA	C4-C3-C5-C6
21	A	406	BCR	C23-C24-C25-C26
21	a	846	BCR	C5-C6-C7-C8
21	a	848	BCR	C23-C24-C25-C26
21	i	101	BCR	C1-C6-C7-C8
21	i	101	BCR	C5-C6-C7-C8
21	i	102	BCR	C1-C6-C7-C8
21	j	101	BCR	C23-C24-C25-C26
21	j	101	BCR	C23-C24-C25-C30
19	f	201	CLA	C13-C15-C16-C17
19	a	833	CLA	C8-C10-C11-C12
19	A	402	CLA	C2A-CAA-CBA-CGA
27	b	850	LMG	O1-C7-C8-O7
26	a	853	LHG	C3-O3-P-O6
26	b	849	LHG	C4-O6-P-O3
19	a	803	CLA	C16-C17-C18-C19
20	D	401	PHO	CHA-CBD-CGD-O1D
20	D	401	PHO	CHA-CBD-CGD-O2D
19	a	818	CLA	C12-C13-C15-C16
19	b	805	CLA	C11-C12-C13-C15
19	b	822	CLA	C11-C10-C8-C7
20	A	404	PHO	C11-C12-C13-C15
26	a	855	LHG	C28-C29-C30-C31
19	a	815	CLA	C11-C12-C13-C14
19	a	821	CLA	C6-C7-C8-C9
19	a	822	CLA	C11-C12-C13-C14
19	a	823	CLA	C11-C10-C8-C9
19	a	839	CLA	C11-C12-C13-C14
19	a	841	CLA	C6-C7-C8-C9
19	a	857	CLA	C6-C7-C8-C9
19	b	822	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	i	102	BCR	C9-C10-C11-C12
19	a	808	CLA	C16-C17-C18-C19
19	a	818	CLA	C16-C17-C18-C20
19	a	835	CLA	C16-C17-C18-C19
19	b	820	CLA	C11-C12-C13-C15
19	a	812	CLA	C2A-CAA-CBA-CGA
21	k	103	BCR	C7-C8-C9-C34
19	b	838	CLA	C5-C6-C7-C8
19	b	801	CLA	C2-C3-C5-C6
19	b	822	CLA	C2-C3-C5-C6
26	a	853	LHG	C12-C13-C14-C15
19	a	809	CLA	C15-C16-C17-C18
21	A	406	BCR	C19-C20-C21-C22
21	b	843	BCR	C19-C20-C21-C22
19	b	808	CLA	C3-C5-C6-C7
19	b	827	CLA	C10-C11-C12-C13
19	a	810	CLA	CBD-CGD-O2D-CED
19	b	807	CLA	O1A-CGA-O2A-C1
19	b	833	CLA	C5-C6-C7-C8
27	b	848	LMG	C35-C36-C37-C38
19	a	823	CLA	C2-C1-O2A-CGA
19	a	818	CLA	CBA-CGA-O2A-C1
19	a	812	CLA	C3A-C2A-CAA-CBA
19	a	831	CLA	C3A-C2A-CAA-CBA
19	b	818	CLA	C3A-C2A-CAA-CBA
19	b	830	CLA	C3A-C2A-CAA-CBA
20	A	404	PHO	C3A-C2A-CAA-CBA
19	a	802	CLA	C11-C10-C8-C9
19	b	812	CLA	C6-C7-C8-C9
19	b	813	CLA	C11-C10-C8-C9
19	b	825	CLA	C14-C13-C15-C16
19	a	830	CLA	C13-C15-C16-C17
21	a	849	BCR	C20-C21-C22-C37
28	a	858	45D	C28-C26-C30-C32
28	a	858	45D	C39-C35-C37-C41
29	b	844	ECH	C11-C10-C9-C34
29	b	844	ECH	C35-C13-C14-C15
31	f	205	ZEX	C20-C13-C14-C15
27	l	201	LMG	C28-C29-C30-C31
19	D	402	CLA	C2A-CAA-CBA-CGA
19	A	402	CLA	O2A-C1-C2-C3
19	a	819	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	a	850	BCR	C37-C22-C23-C24
19	j	103	CLA	C4-C3-C5-C6
19	b	804	CLA	C1A-C2A-CAA-CBA
19	b	830	CLA	C1A-C2A-CAA-CBA
23	a	801	CL0	C1A-C2A-CAA-CBA
19	b	809	CLA	CAA-CBA-CGA-O2A
19	a	834	CLA	C6-C7-C8-C10
19	b	803	CLA	C6-C7-C8-C10
19	b	816	CLA	C6-C7-C8-C10
19	b	818	CLA	C11-C10-C8-C7
19	b	832	CLA	C12-C13-C15-C16
19	b	839	CLA	C11-C12-C13-C15
23	a	801	CL0	C5-C6-C7-C8
27	a	854	LMG	C11-C12-C13-C14
26	b	849	LHG	C28-C29-C30-C31
19	a	826	CLA	C15-C16-C17-C18
19	b	827	CLA	C16-C17-C18-C19
19	a	838	CLA	C2A-CAA-CBA-CGA
19	a	856	CLA	C2A-CAA-CBA-CGA
26	f	206	LHG	C32-C33-C34-C35
19	b	803	CLA	C8-C10-C11-C12
19	a	835	CLA	C8-C10-C11-C12
19	j	103	CLA	C2-C3-C5-C6
20	D	401	PHO	C10-C11-C12-C13
20	D	401	PHO	C13-C15-C16-C17
28	a	858	45D	C24-C26-C30-C32
28	a	858	45D	C33-C35-C37-C41
29	b	844	ECH	C11-C10-C9-C8
29	b	844	ECH	C12-C13-C14-C15
31	f	205	ZEX	C12-C13-C14-C15
19	a	810	CLA	O1D-CGD-O2D-CED
19	a	819	CLA	C16-C17-C18-C20
19	a	834	CLA	C4-C3-C5-C6
26	a	855	LHG	C26-C27-C28-C29
19	b	815	CLA	C2-C1-O2A-CGA
19	f	201	CLA	C2-C1-O2A-CGA
19	a	820	CLA	C2-C3-C5-C6
19	a	818	CLA	O1A-CGA-O2A-C1
19	b	831	CLA	C15-C16-C17-C18
19	a	813	CLA	C11-C10-C8-C9
20	A	404	PHO	C1A-C2A-CAA-CBA
26	a	855	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
19	f	204	CLA	C2A-CAA-CBA-CGA
21	a	846	BCR	C23-C24-C25-C26
21	a	846	BCR	C23-C24-C25-C30
21	a	847	BCR	C23-C24-C25-C30
21	a	849	BCR	C23-C24-C25-C30
21	b	845	BCR	C1-C6-C7-C8
21	b	846	BCR	C23-C24-C25-C30
21	b	847	BCR	C1-C6-C7-C8
21	f	202	BCR	C23-C24-C25-C30
21	i	101	BCR	C23-C24-C25-C30
21	k	103	BCR	C1-C6-C7-C8
29	b	844	ECH	C23-C24-C25-C26
29	m	101	ECH	C23-C24-C25-C30
31	b	852	ZEX	C1-C6-C7-C8
27	a	854	LMG	C7-C8-C9-O8
21	a	859	BCR	C19-C20-C21-C22
19	b	819	CLA	C4-C3-C5-C6
21	a	850	BCR	C14-C15-C16-C17
27	l	201	LMG	C8-C7-O1-C1
19	a	860	CLA	C16-C17-C18-C19
19	b	836	CLA	C10-C11-C12-C13
19	l	202	CLA	O1D-CGD-O2D-CED
19	a	840	CLA	C2A-CAA-CBA-CGA
19	a	843	CLA	C2A-CAA-CBA-CGA
19	b	819	CLA	C3-C5-C6-C7
19	b	832	CLA	C16-C17-C18-C20
26	a	855	LHG	C13-C14-C15-C16
27	b	850	LMG	C40-C41-C42-C43
19	l	204	CLA	CAA-CBA-CGA-O2A
19	a	820	CLA	C4-C3-C5-C6
19	b	805	CLA	C4-C3-C5-C6
26	a	855	LHG	O2-C2-C3-O3
19	D	402	CLA	C2-C3-C5-C6
19	a	824	CLA	C11-C10-C8-C7
19	a	831	CLA	C2-C3-C5-C6
19	b	805	CLA	C11-C10-C8-C7
19	a	805	CLA	C13-C15-C16-C17
21	i	101	BCR	C13-C14-C15-C16
19	D	402	CLA	CAA-CBA-CGA-O2A
26	a	852	LHG	O8-C23-C24-C25
19	a	821	CLA	C16-C17-C18-C20
26	a	853	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	j	101	BCR	C20-C21-C22-C37
21	l	205	BCR	C16-C17-C18-C36
26	a	853	LHG	C17-C18-C19-C20
30	b	851	EQ3	C11-C10-C9-C34
26	f	206	LHG	O7-C7-C8-C9
19	l	202	CLA	CBD-CGD-O2D-CED
19	b	810	CLA	C4-C3-C5-C6
19	a	832	CLA	C2-C3-C5-C6
26	a	852	LHG	C33-C34-C35-C36
19	a	818	CLA	C16-C17-C18-C19
19	a	819	CLA	C14-C13-C15-C16
19	a	821	CLA	C11-C10-C8-C9
19	a	857	CLA	C11-C12-C13-C14
19	a	860	CLA	C11-C12-C13-C14
19	b	819	CLA	C13-C15-C16-C17
19	a	822	CLA	C3A-C2A-CAA-CBA
19	b	801	CLA	C3A-C2A-CAA-CBA
19	a	832	CLA	CAA-CBA-CGA-O2A
19	a	813	CLA	CAD-CBD-CGD-O2D
19	a	818	CLA	CAD-CBD-CGD-O2D
19	a	824	CLA	CAD-CBD-CGD-O2D
19	a	840	CLA	CAD-CBD-CGD-O2D
19	a	842	CLA	CAD-CBD-CGD-O2D
19	b	807	CLA	CAD-CBD-CGD-O2D
19	b	815	CLA	CAD-CBD-CGD-O2D
19	b	821	CLA	CAD-CBD-CGD-O2D
19	b	826	CLA	CAD-CBD-CGD-O2D
19	b	838	CLA	CAD-CBD-CGD-O2D
19	f	203	CLA	CAD-CBD-CGD-O2D
19	l	204	CLA	CAD-CBD-CGD-O2D
19	a	835	CLA	C16-C17-C18-C20
19	a	825	CLA	C5-C6-C7-C8
19	a	814	CLA	C2A-CAA-CBA-CGA
27	a	854	LMG	O9-C10-O7-C8
19	a	835	CLA	C2-C1-O2A-CGA
19	a	812	CLA	CAA-CBA-CGA-O2A
19	a	824	CLA	CAA-CBA-CGA-O2A
19	b	810	CLA	CAA-CBA-CGA-O2A
26	a	852	LHG	O7-C7-C8-C9
19	a	840	CLA	C10-C11-C12-C13
19	a	833	CLA	CAA-CBA-CGA-O2A
19	b	834	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	b	848	LMG	C7-C8-C9-O8
19	b	807	CLA	C10-C11-C12-C13
19	a	831	CLA	CAA-CBA-CGA-O2A
19	a	840	CLA	CAA-CBA-CGA-O2A
19	A	407	CLA	O2A-C1-C2-C3
19	a	823	CLA	O2A-C1-C2-C3
19	b	812	CLA	O2A-C1-C2-C3
19	b	815	CLA	O2A-C1-C2-C3
19	b	826	CLA	O2A-C1-C2-C3
19	b	836	CLA	O2A-C1-C2-C3
19	l	204	CLA	O2A-C1-C2-C3
19	a	808	CLA	C2A-CAA-CBA-CGA
19	a	832	CLA	C2A-CAA-CBA-CGA
19	b	831	CLA	C3-C5-C6-C7
19	A	407	CLA	CHA-CBD-CGD-O1D
19	A	407	CLA	CHA-CBD-CGD-O2D
19	D	402	CLA	CHA-CBD-CGD-O1D
19	D	402	CLA	CHA-CBD-CGD-O2D
19	a	803	CLA	CHA-CBD-CGD-O1D
19	a	803	CLA	CHA-CBD-CGD-O2D
19	a	806	CLA	CHA-CBD-CGD-O1D
19	a	806	CLA	CHA-CBD-CGD-O2D
19	a	821	CLA	CHA-CBD-CGD-O1D
19	a	821	CLA	CHA-CBD-CGD-O2D
19	a	829	CLA	CHA-CBD-CGD-O2D
19	a	839	CLA	CHA-CBD-CGD-O2D
19	a	840	CLA	CHA-CBD-CGD-O2D
19	b	840	CLA	CHA-CBD-CGD-O1D
19	b	840	CLA	CHA-CBD-CGD-O2D
19	f	204	CLA	CHA-CBD-CGD-O1D
19	f	204	CLA	CHA-CBD-CGD-O2D
19	j	104	CLA	CHA-CBD-CGD-O1D
19	j	104	CLA	CHA-CBD-CGD-O2D
30	b	851	EQ3	C11-C10-C9-C8
26	b	849	LHG	C35-C36-C37-C38
32	j	102	LMT	C5-C6-C7-C8
19	b	807	CLA	C16-C17-C18-C20
19	A	407	CLA	CAA-CBA-CGA-O2A
19	a	830	CLA	CAA-CBA-CGA-O2A
19	b	806	CLA	CAA-CBA-CGA-O2A
19	a	809	CLA	C3-C5-C6-C7
19	A	403	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	a	835	CLA	CAA-CBA-CGA-O2A
19	b	814	CLA	CAA-CBA-CGA-O2A
19	b	832	CLA	C2A-CAA-CBA-CGA
19	a	819	CLA	C16-C17-C18-C19
26	a	855	LHG	C29-C30-C31-C32
27	a	854	LMG	O7-C10-C11-C12
26	b	849	LHG	C29-C30-C31-C32
19	a	827	CLA	C12-C13-C15-C16
19	a	840	CLA	C2-C3-C5-C6
19	a	813	CLA	C11-C12-C13-C14
19	a	828	CLA	C15-C16-C17-C18
19	a	834	CLA	C11-C10-C8-C9
19	b	803	CLA	C6-C7-C8-C9
19	b	838	CLA	C6-C7-C8-C9
19	b	839	CLA	C15-C16-C17-C18
27	b	850	LMG	C38-C39-C40-C41
19	a	807	CLA	CAA-CBA-CGA-O2A
19	j	103	CLA	CAA-CBA-CGA-O2A
19	l	203	CLA	CAA-CBA-CGA-O2A
19	a	829	CLA	C2A-CAA-CBA-CGA
19	a	840	CLA	CAA-CBA-CGA-O1A
27	b	848	LMG	O7-C10-C11-C12
27	b	850	LMG	C37-C38-C39-C40
19	D	402	CLA	CAA-CBA-CGA-O1A
19	b	832	CLA	C16-C17-C18-C19
19	a	821	CLA	CAA-CBA-CGA-O2A
19	a	812	CLA	C1A-C2A-CAA-CBA
19	b	801	CLA	C1A-C2A-CAA-CBA
19	b	818	CLA	C1A-C2A-CAA-CBA
19	k	102	CLA	C1A-C2A-CAA-CBA
19	a	812	CLA	CAA-CBA-CGA-O1A
19	a	824	CLA	CAA-CBA-CGA-O1A
27	a	854	LMG	O10-C28-C29-C30
19	b	839	CLA	C2-C1-O2A-CGA
19	k	101	CLA	CAA-CBA-CGA-O2A
27	a	854	LMG	O8-C28-C29-C30
19	b	814	CLA	CAA-CBA-CGA-O1A
19	b	834	CLA	CAA-CBA-CGA-O1A
27	b	850	LMG	O10-C28-C29-C30
19	a	835	CLA	CAA-CBA-CGA-O1A
27	l	201	LMG	C39-C40-C41-C42
19	a	809	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	a	853	LHG	C4-O6-P-O5
19	a	821	CLA	C16-C17-C18-C19
19	A	407	CLA	CAA-CBA-CGA-O1A
19	b	810	CLA	CAA-CBA-CGA-O1A
19	j	103	CLA	CAA-CBA-CGA-O1A
21	b	846	BCR	C1-C6-C7-C8
21	b	846	BCR	C23-C24-C25-C26
21	f	202	BCR	C23-C24-C25-C26
19	a	832	CLA	CAA-CBA-CGA-O1A
19	a	833	CLA	CAA-CBA-CGA-O1A
19	b	815	CLA	CAA-CBA-CGA-O2A
19	b	828	CLA	CAA-CBA-CGA-O2A
19	b	807	CLA	C16-C17-C18-C19
27	l	201	LMG	C38-C39-C40-C41
21	b	846	BCR	C10-C11-C12-C13
19	a	807	CLA	CAA-CBA-CGA-O1A
19	a	830	CLA	CAA-CBA-CGA-O1A
19	a	804	CLA	C5-C6-C7-C8
19	b	811	CLA	CAA-CBA-CGA-O2A
19	a	831	CLA	CAA-CBA-CGA-O1A
19	a	826	CLA	CAD-CBD-CGD-O1D
19	a	831	CLA	CAD-CBD-CGD-O1D
19	a	835	CLA	CAD-CBD-CGD-O1D
19	A	403	CLA	CAA-CBA-CGA-O1A
19	a	839	CLA	CAA-CBA-CGA-O2A
19	b	804	CLA	CAA-CBA-CGA-O2A
19	a	822	CLA	C13-C15-C16-C17
19	a	831	CLA	C10-C11-C12-C13
19	b	832	CLA	C10-C11-C12-C13
19	A	402	CLA	C11-C10-C8-C9
19	a	820	CLA	C11-C12-C13-C14
19	a	827	CLA	C14-C13-C15-C16
19	a	829	CLA	C11-C12-C13-C14
19	b	822	CLA	C3-C5-C6-C7
19	b	806	CLA	C16-C17-C18-C20
19	a	833	CLA	C2A-CAA-CBA-CGA
19	b	833	CLA	C2A-CAA-CBA-CGA
19	a	843	CLA	CAA-CBA-CGA-O2A
19	b	824	CLA	CAA-CBA-CGA-O2A
19	a	808	CLA	C5-C6-C7-C8
19	b	817	CLA	C8-C10-C11-C12
19	k	101	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	b	807	CLA	O1D-CGD-O2D-CED
19	a	826	CLA	C5-C6-C7-C8
19	a	813	CLA	C6-C7-C8-C10
19	a	826	CLA	C6-C7-C8-C10
19	a	829	CLA	C11-C12-C13-C15
19	a	834	CLA	C11-C10-C8-C7
19	b	803	CLA	C11-C12-C13-C15
19	b	817	CLA	C6-C7-C8-C10
19	b	819	CLA	C6-C7-C8-C10
19	f	201	CLA	C6-C7-C8-C10
19	b	820	CLA	CAA-CBA-CGA-O1A
19	b	820	CLA	CAA-CBA-CGA-O2A
19	b	822	CLA	CAA-CBA-CGA-O2A
19	b	804	CLA	CAA-CBA-CGA-O1A
19	b	824	CLA	CAA-CBA-CGA-O1A
21	b	847	BCR	C15-C16-C17-C18
21	k	103	BCR	C15-C16-C17-C18
19	a	860	CLA	C16-C17-C18-C20
19	a	810	CLA	CAA-CBA-CGA-O2A
19	b	829	CLA	CAA-CBA-CGA-O2A
19	b	813	CLA	C13-C15-C16-C17
19	a	821	CLA	CAA-CBA-CGA-O1A
19	l	203	CLA	CAA-CBA-CGA-O1A
19	a	821	CLA	C8-C10-C11-C12
19	a	806	CLA	CAA-CBA-CGA-O2A
19	a	815	CLA	C15-C16-C17-C18
19	b	812	CLA	C8-C10-C11-C12
19	b	806	CLA	CAA-CBA-CGA-O1A
19	a	825	CLA	C10-C11-C12-C13
19	b	816	CLA	C4-C3-C5-C6
19	A	405	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

10 monomers are involved in 40 short contacts:

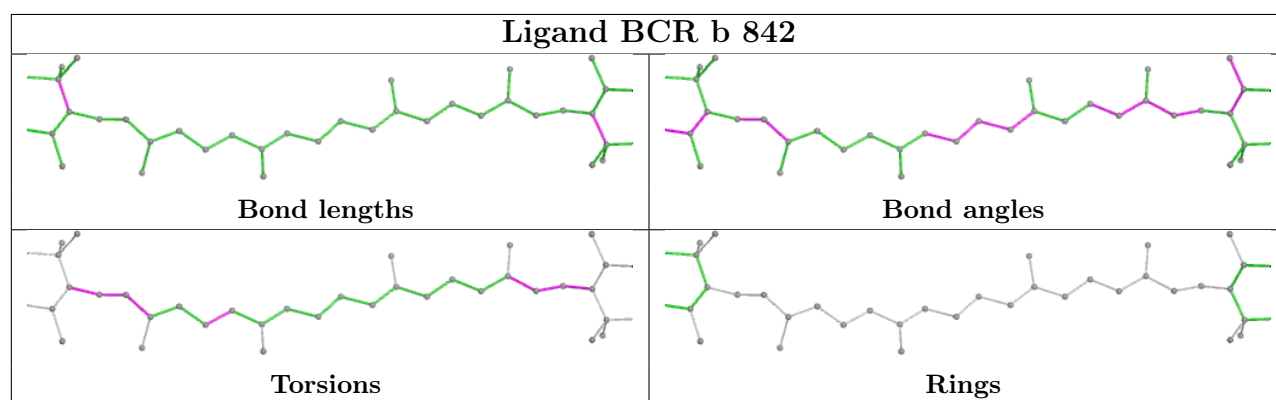
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	D	402	CLA	11	0
19	A	403	CLA	4	0
20	A	404	PHO	5	0
19	A	407	CLA	6	0
19	D	403	CLA	1	0
20	D	401	PHO	3	0

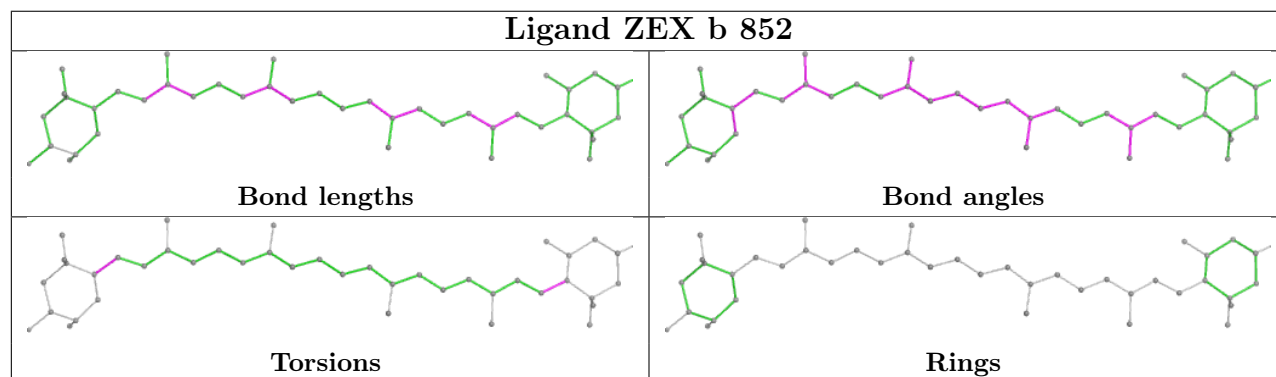
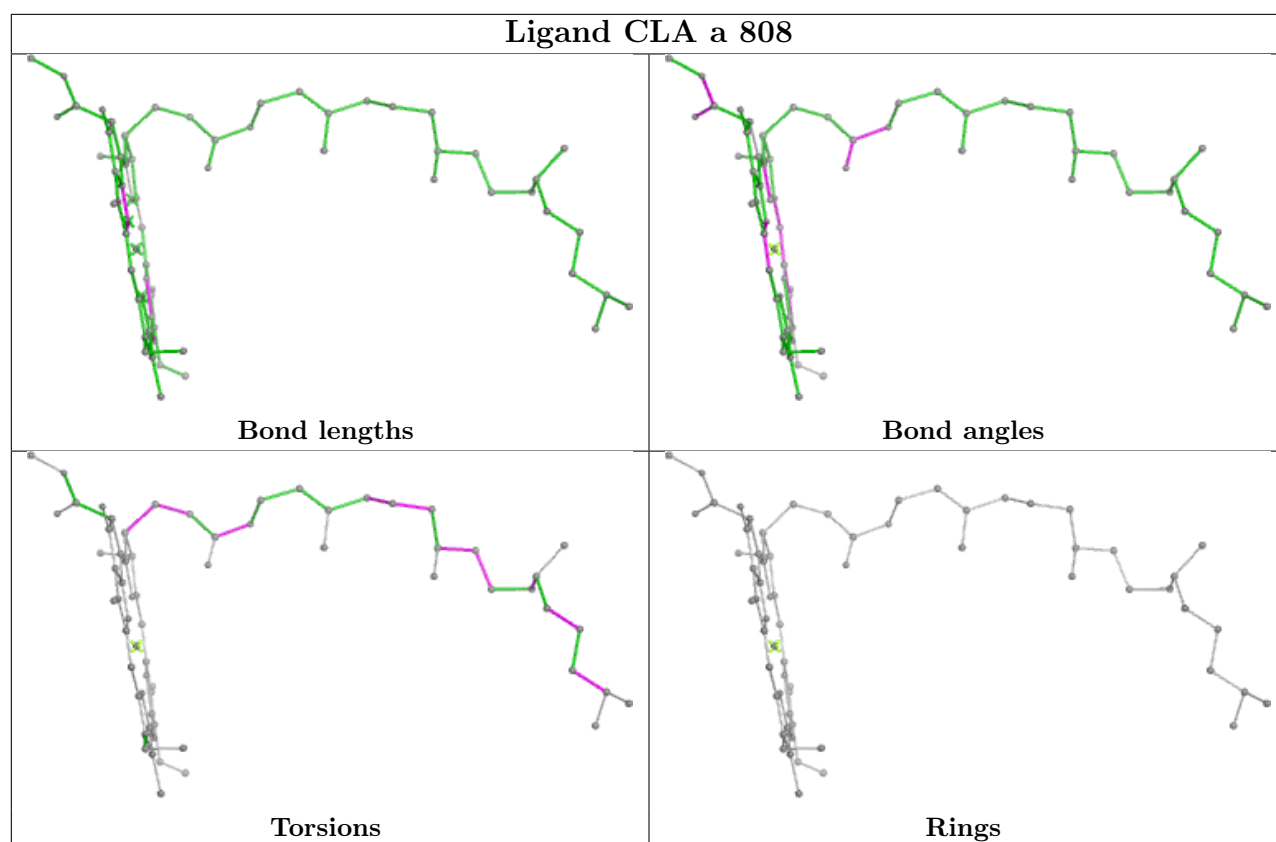
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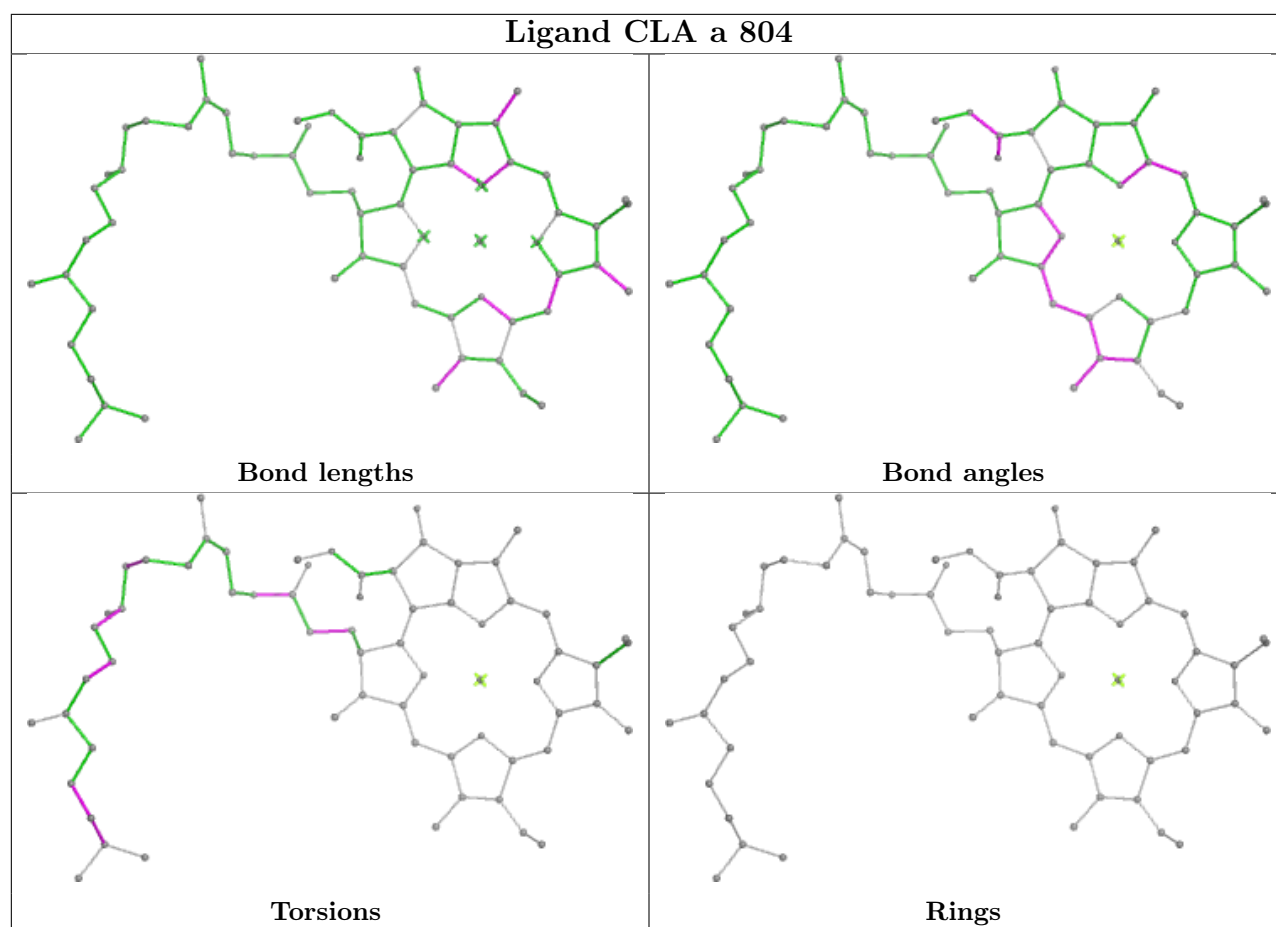
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	406	BCR	6	0
19	A	402	CLA	5	0
22	E	101	HEM	3	0
19	A	405	CLA	5	0

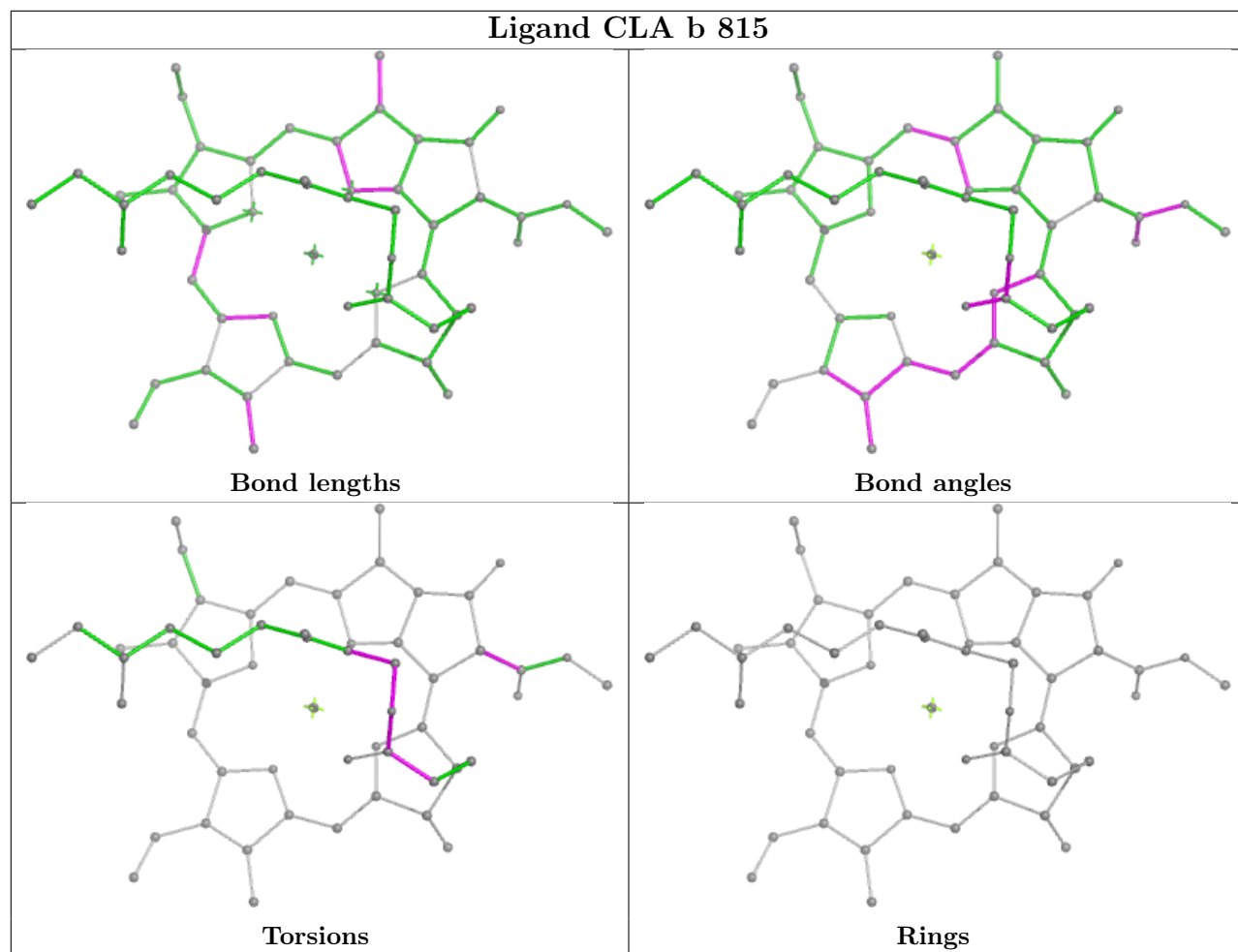
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



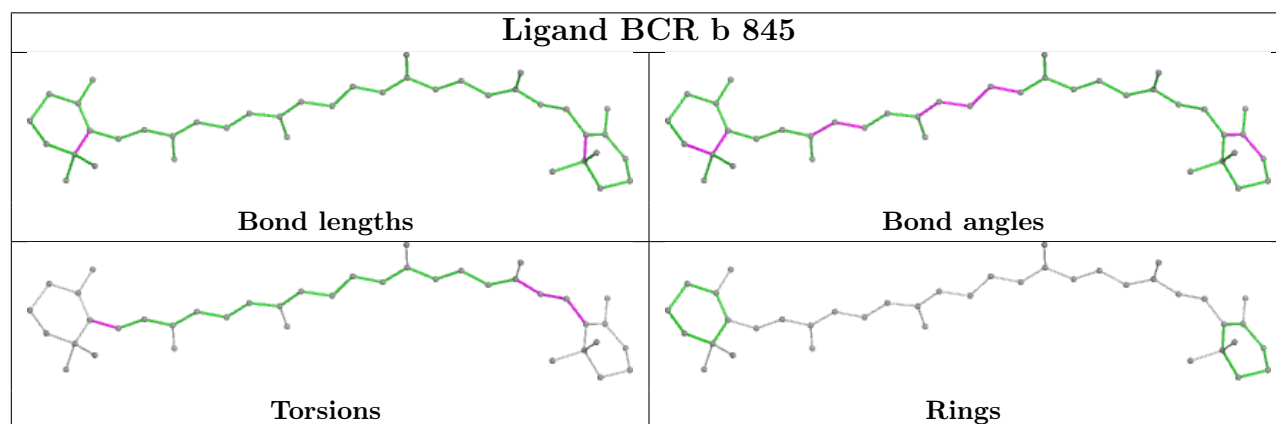
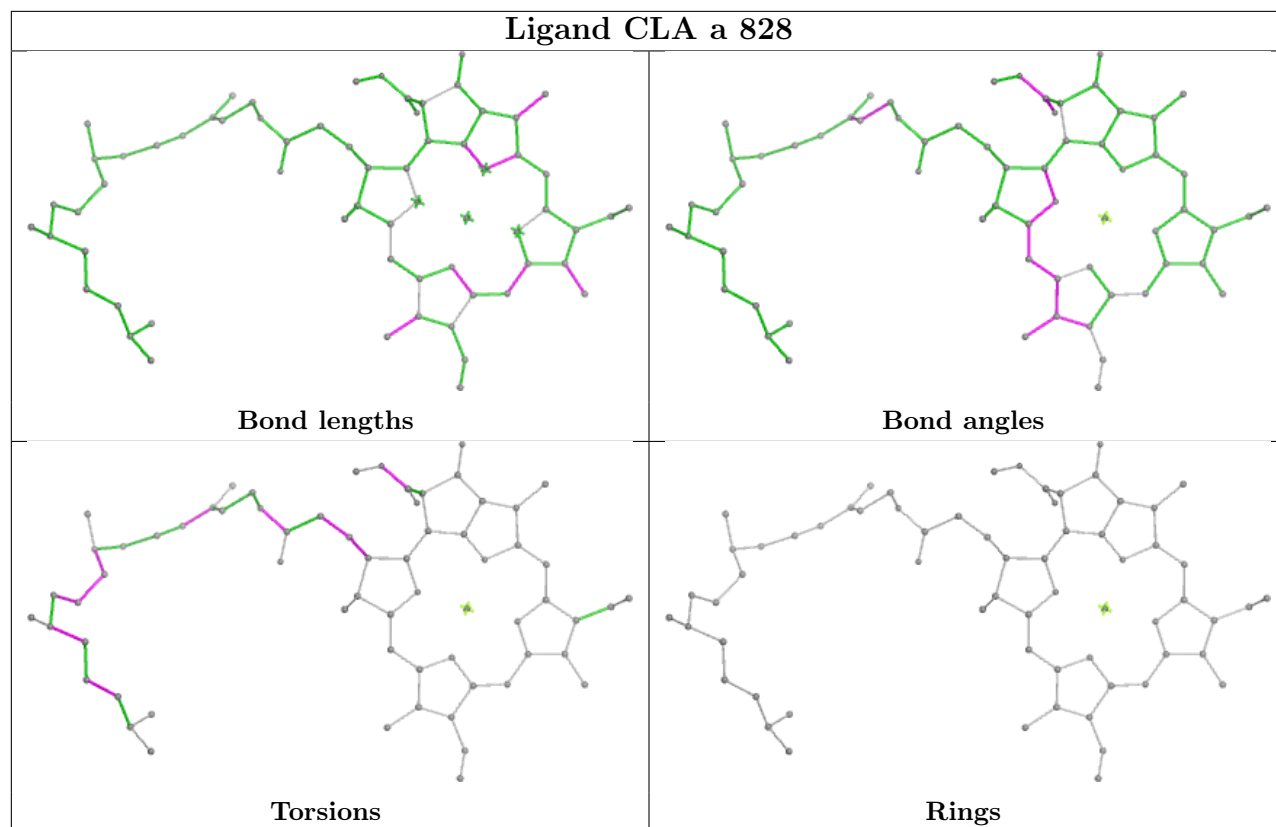


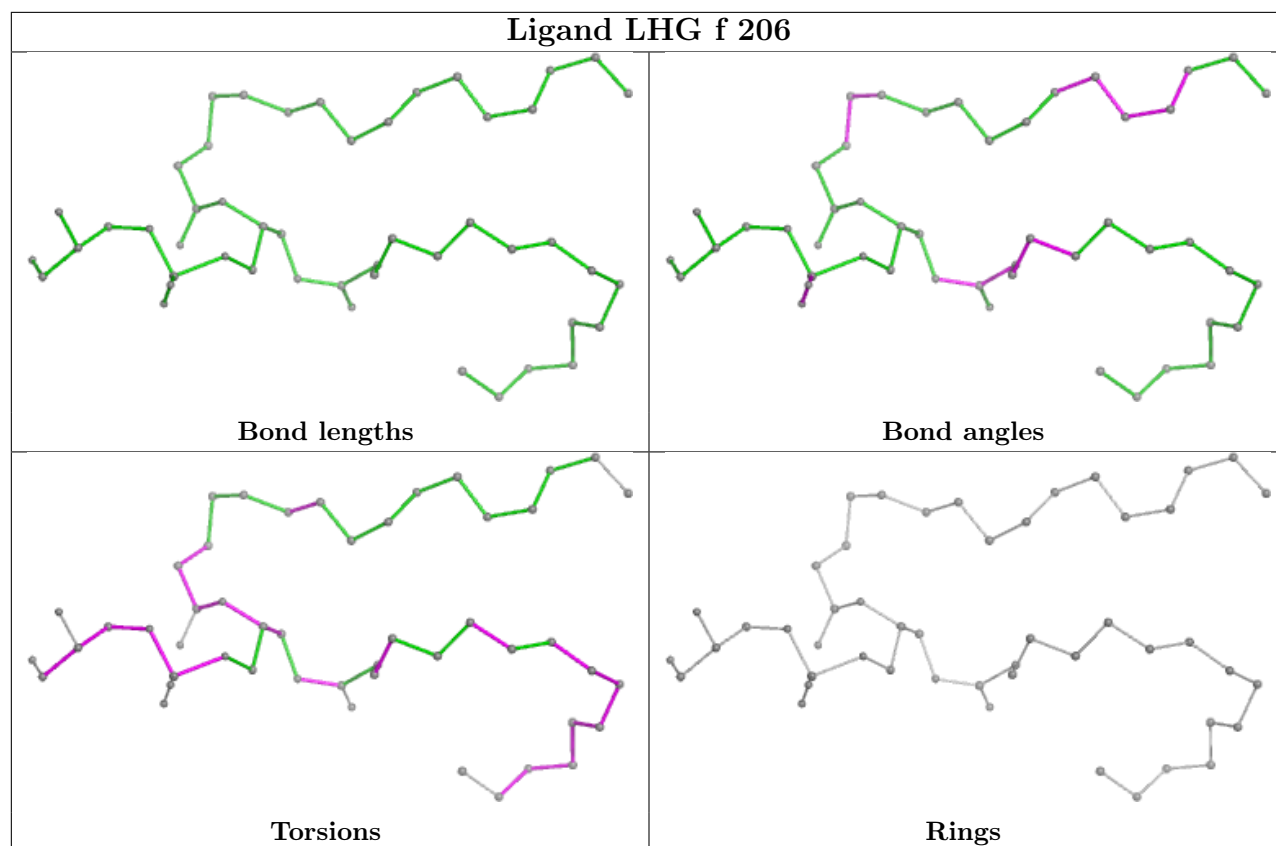
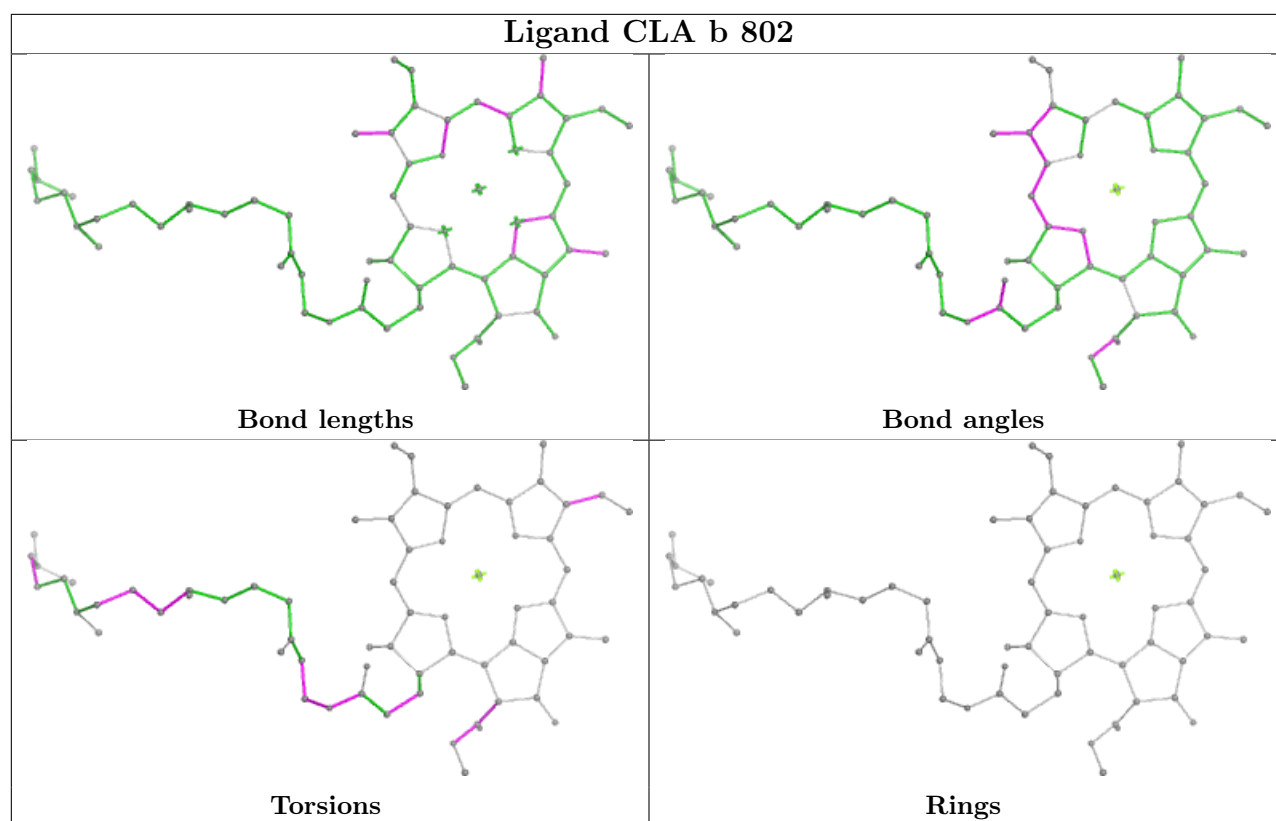


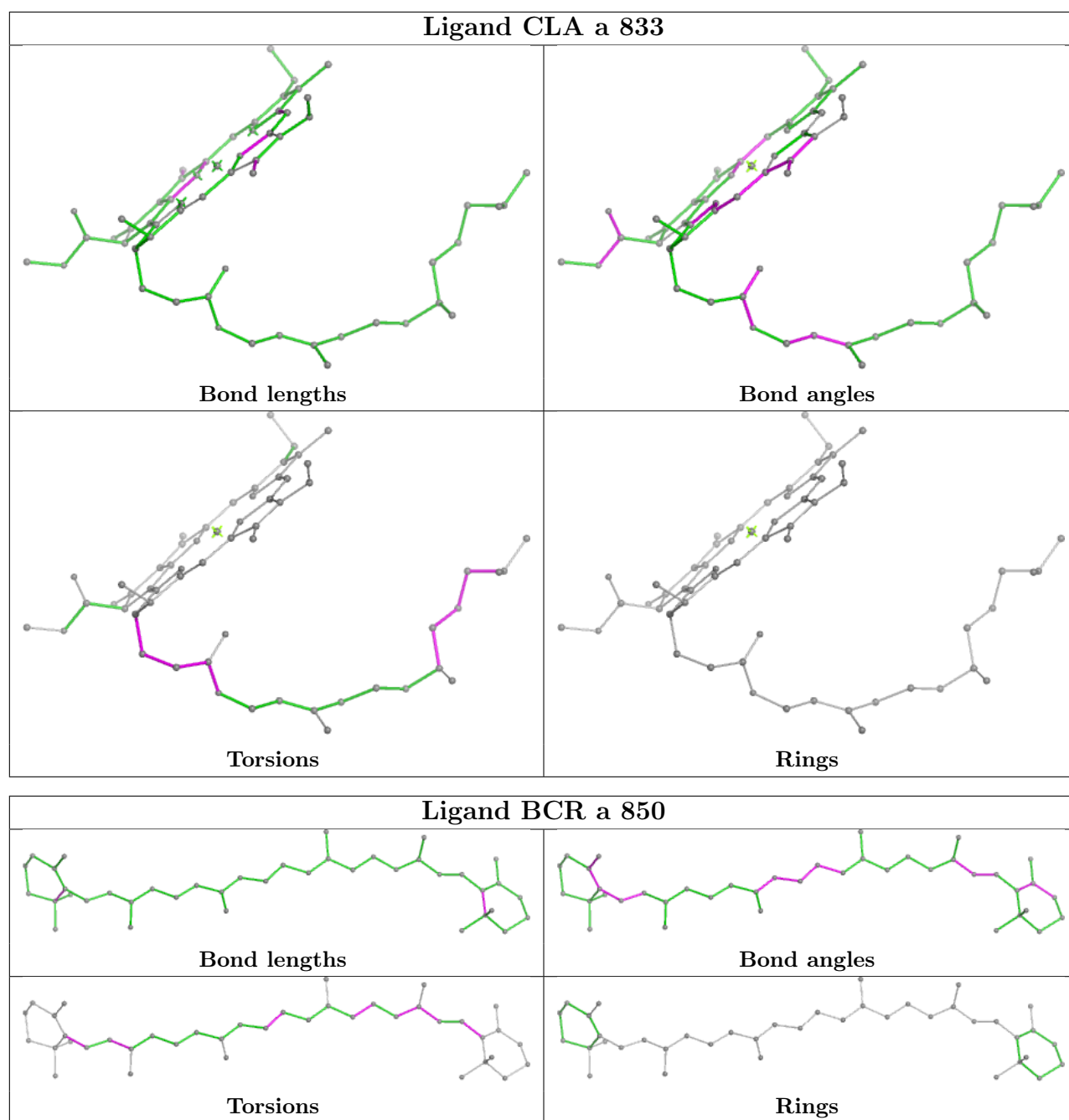
## Ligand CLA b 815

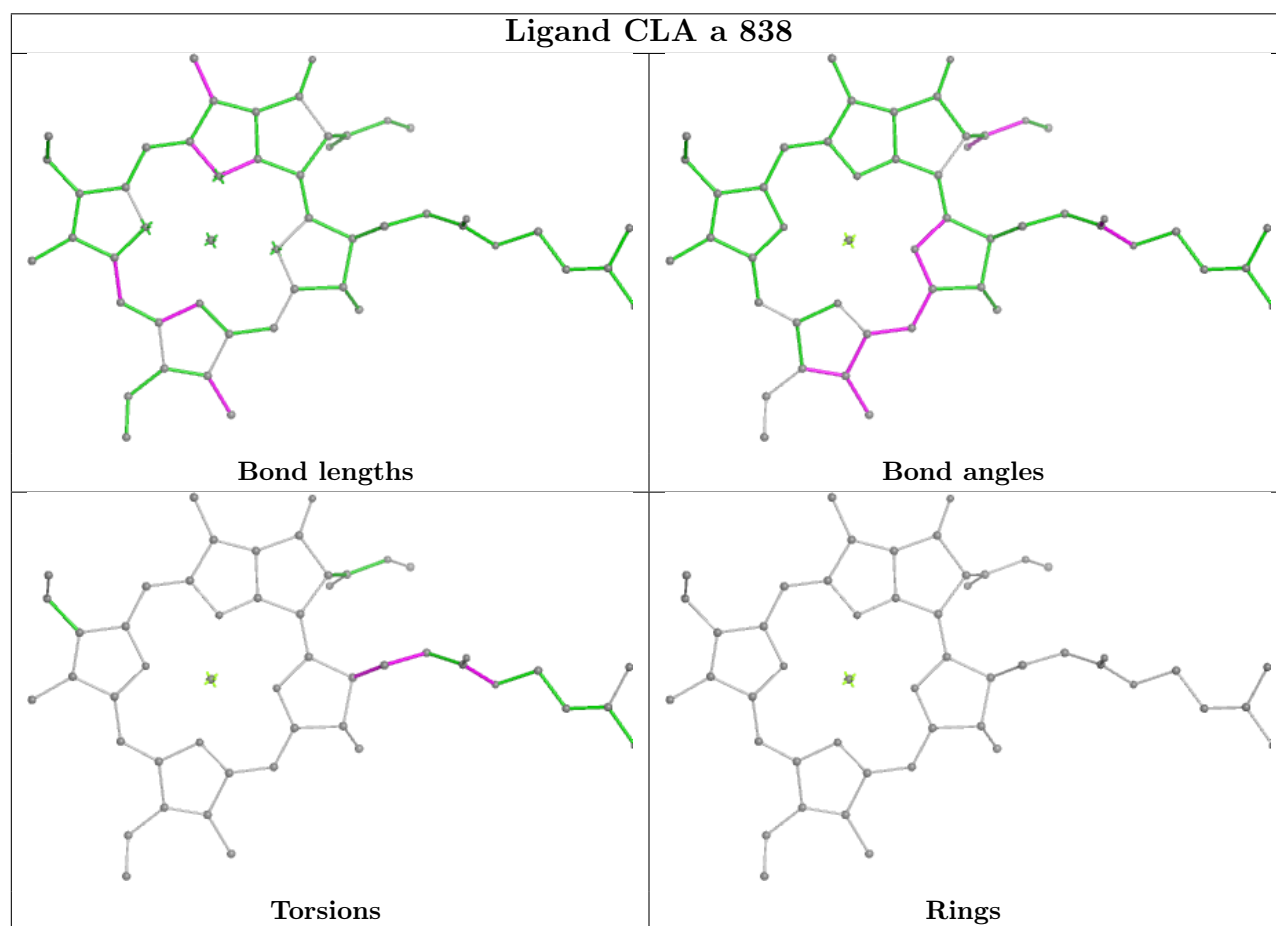
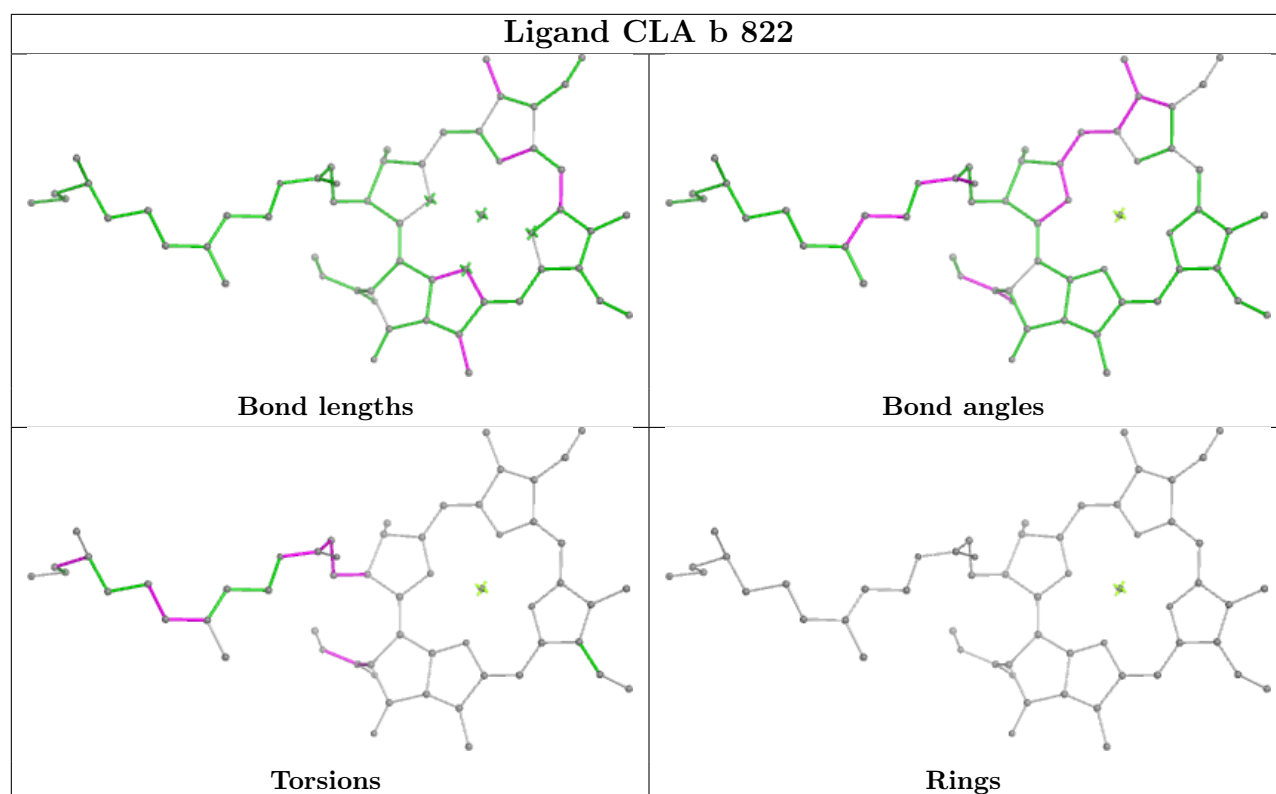


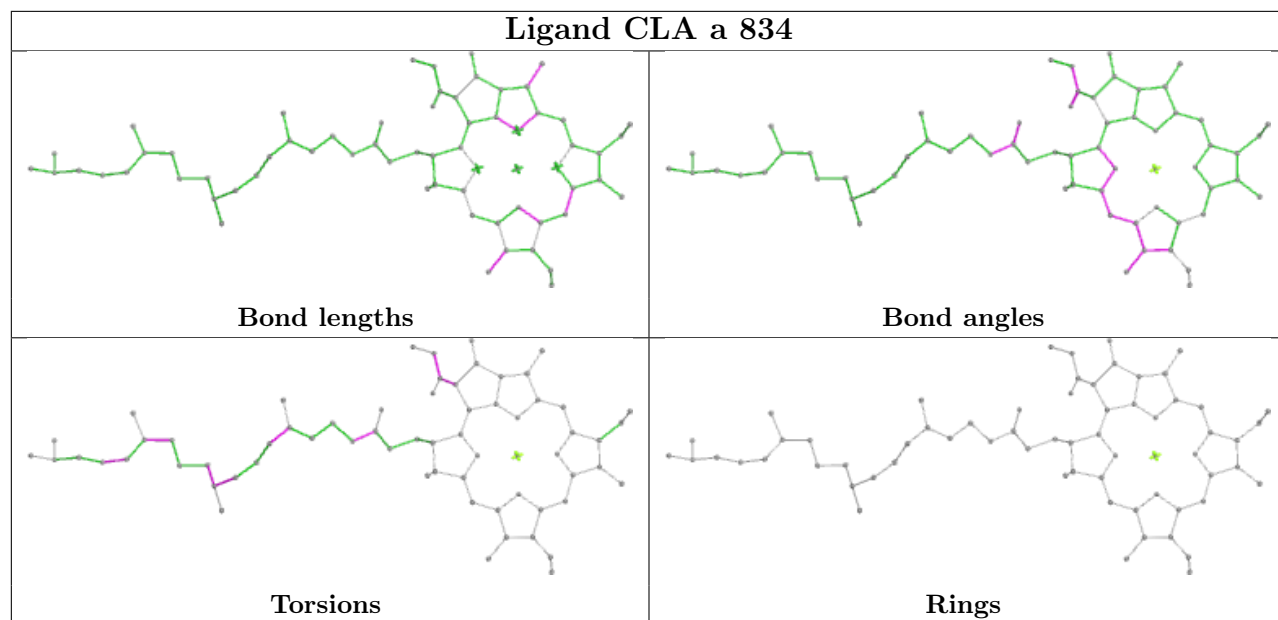




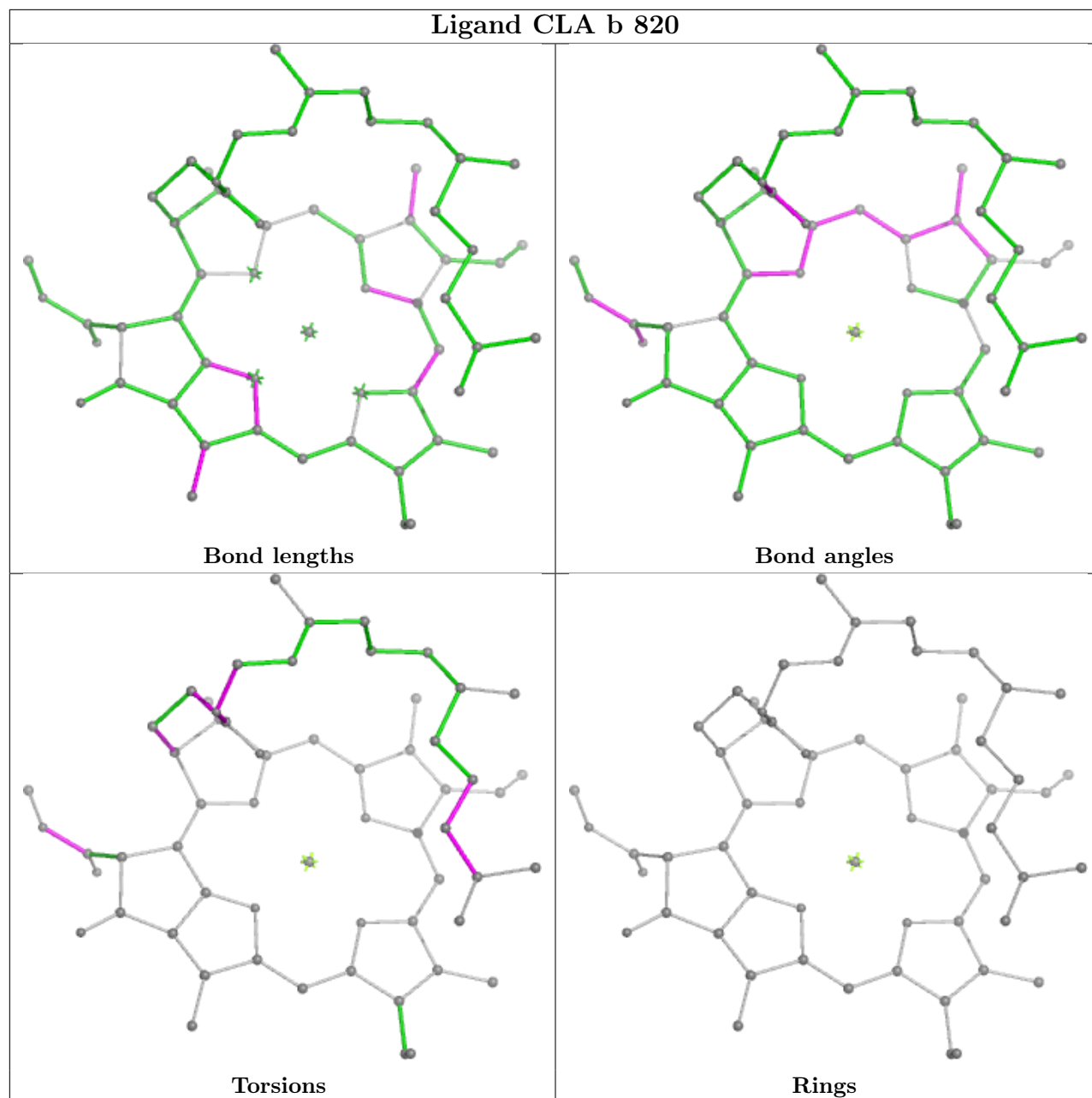




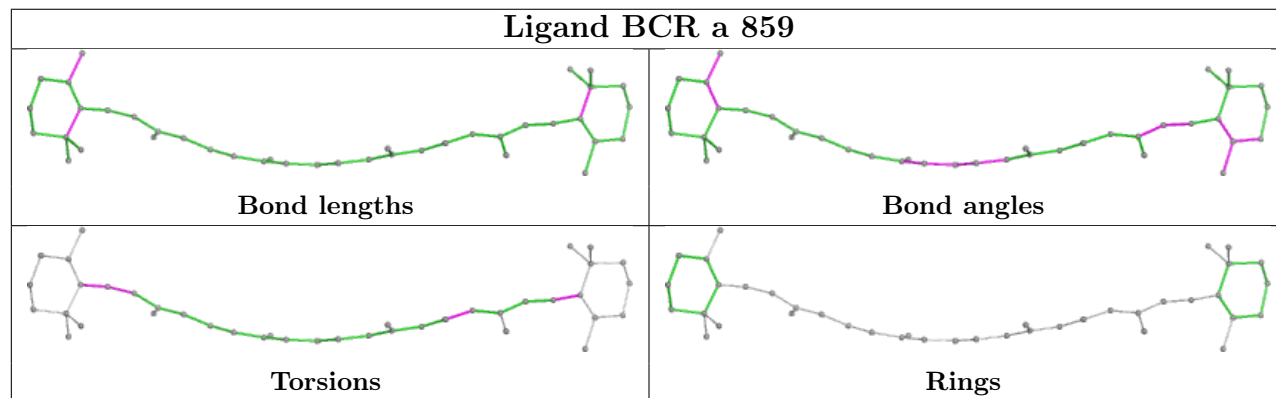


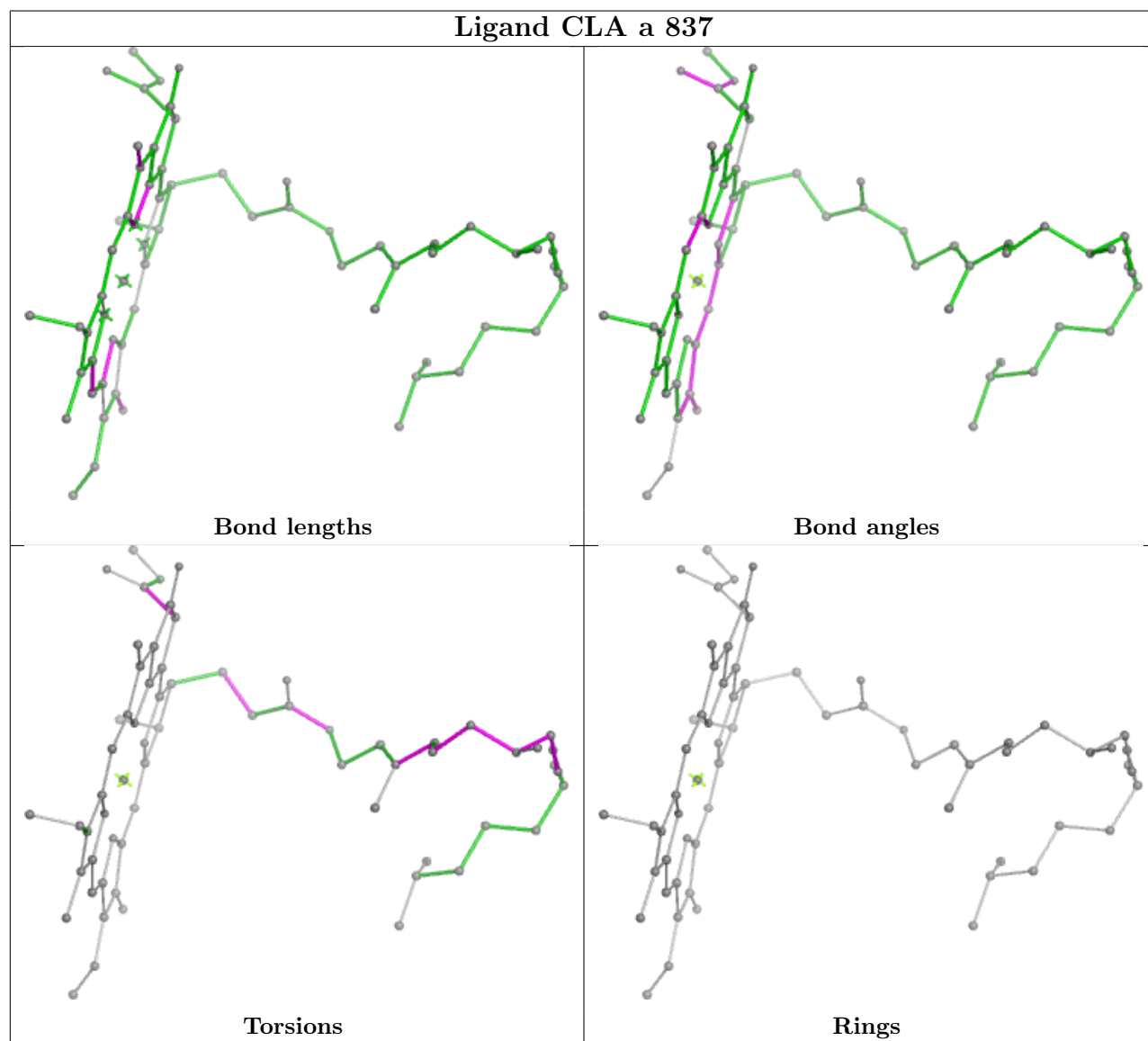
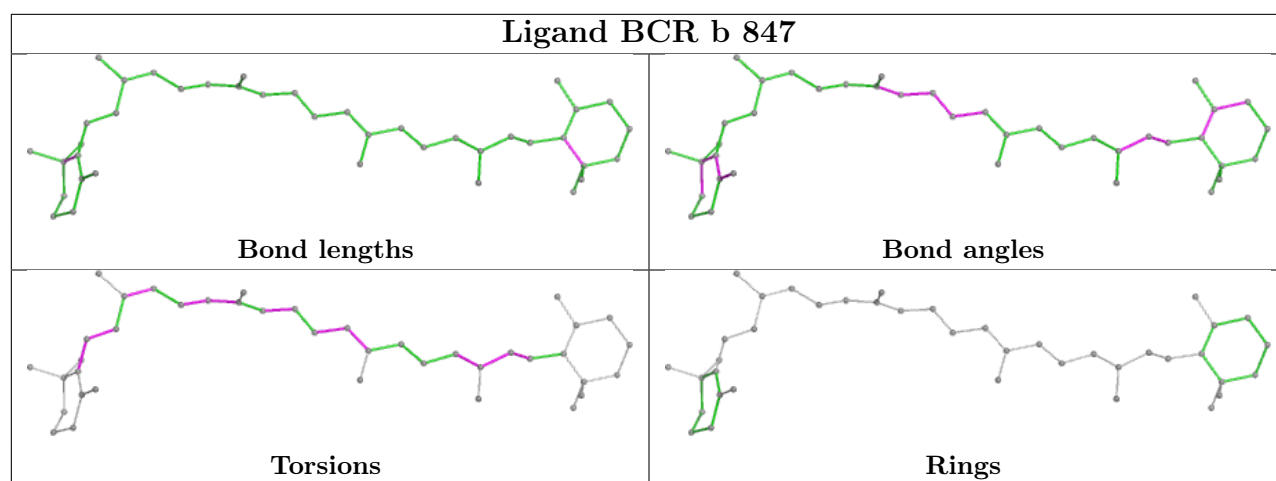


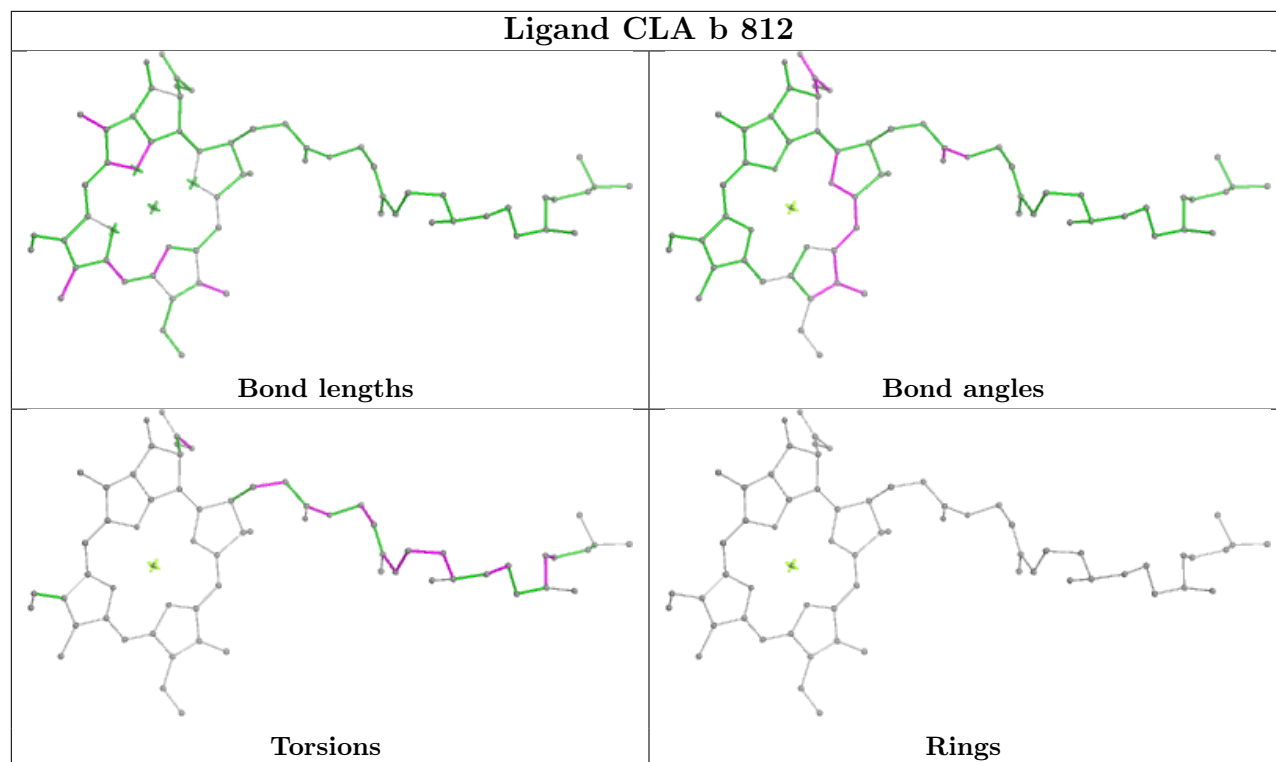
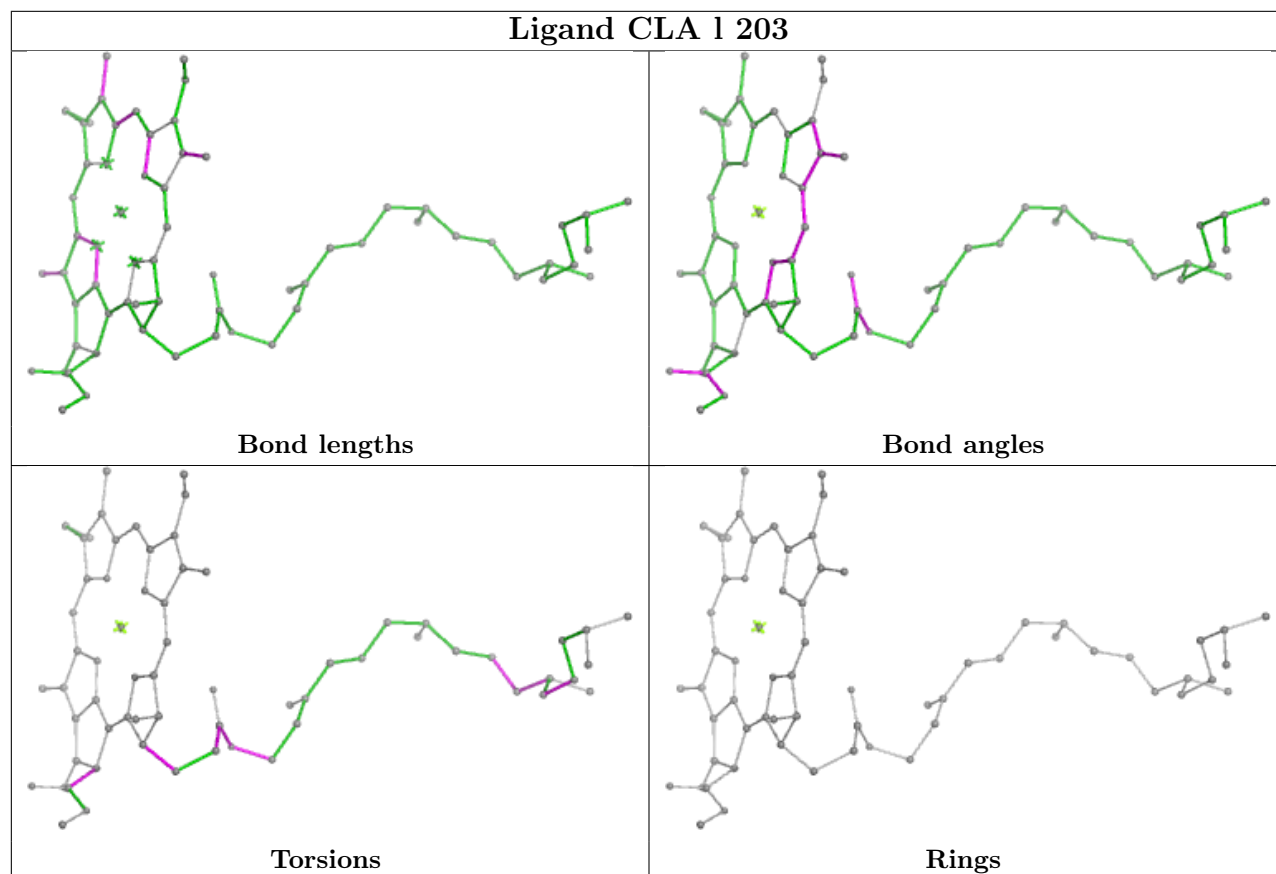
## Ligand CLA b 820



## Ligand BCR a 859

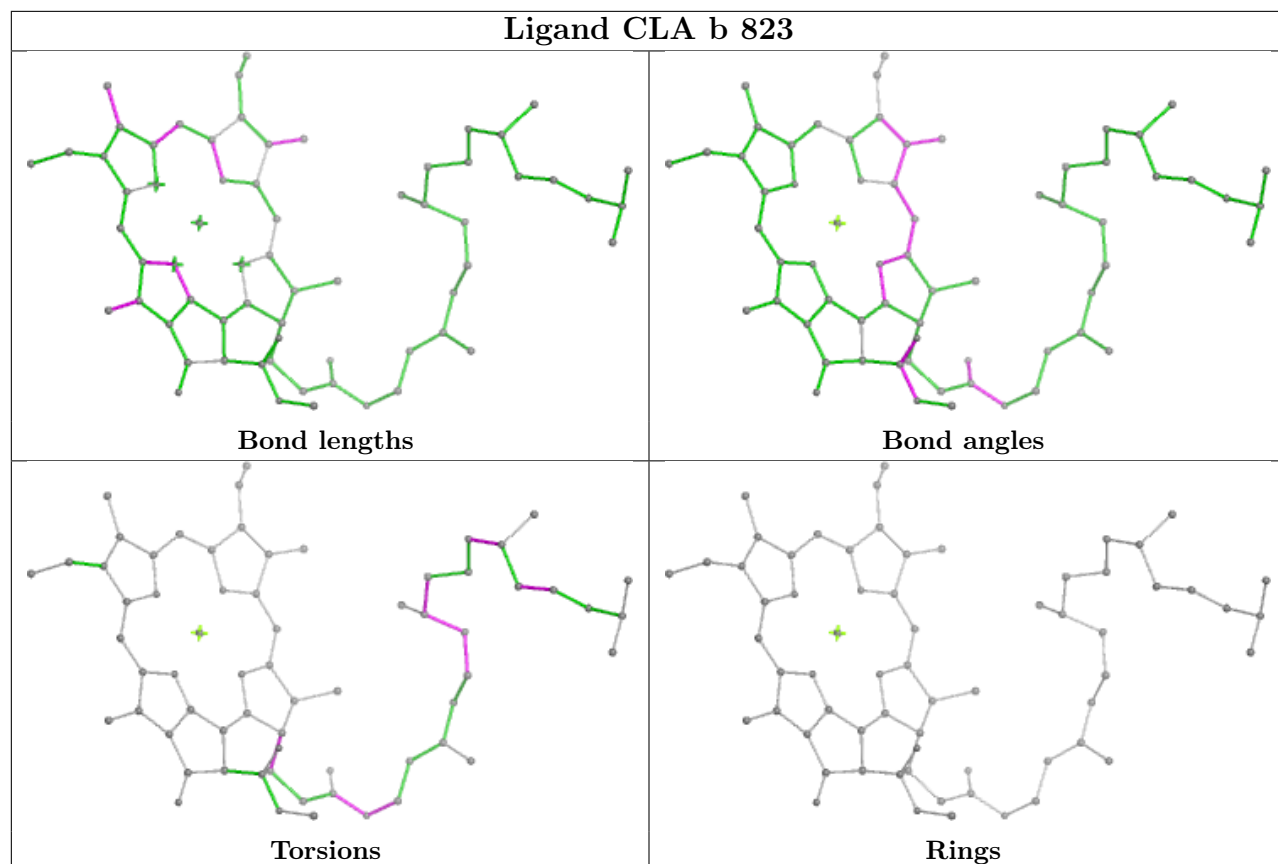




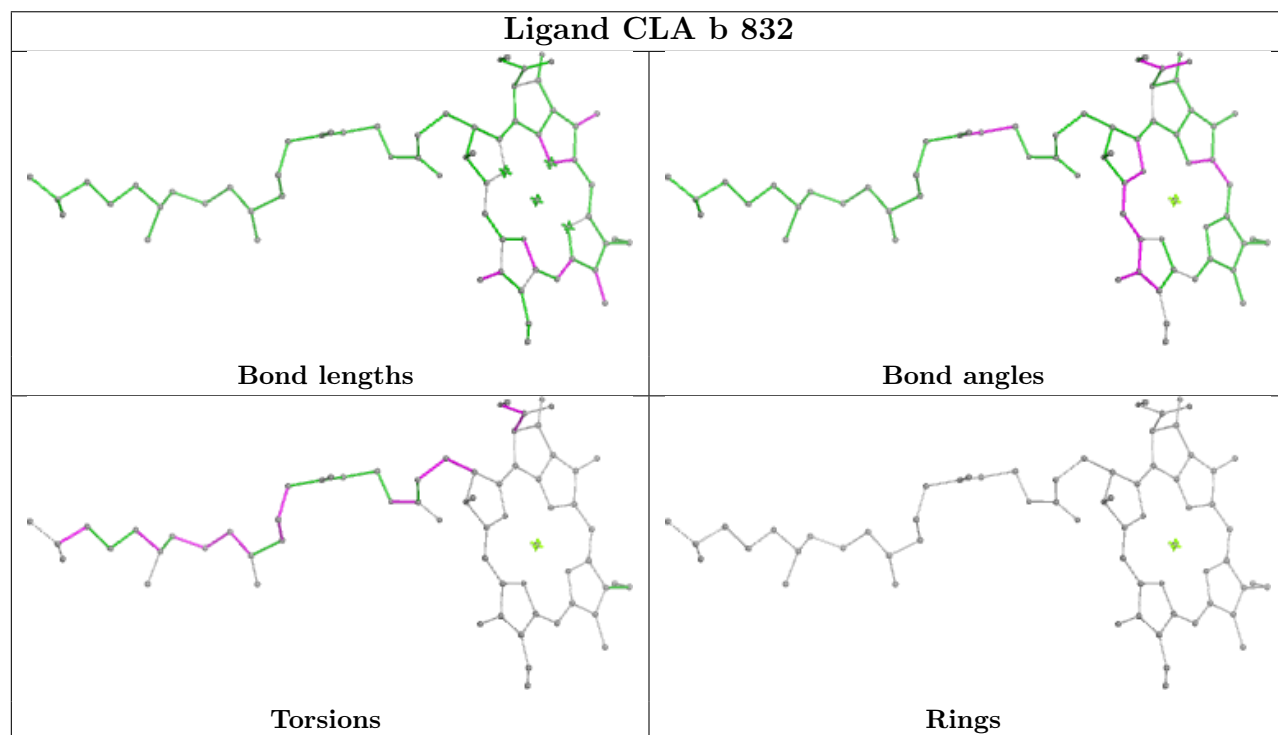
**Ligand CLA b 812****Ligand CLA l 203**

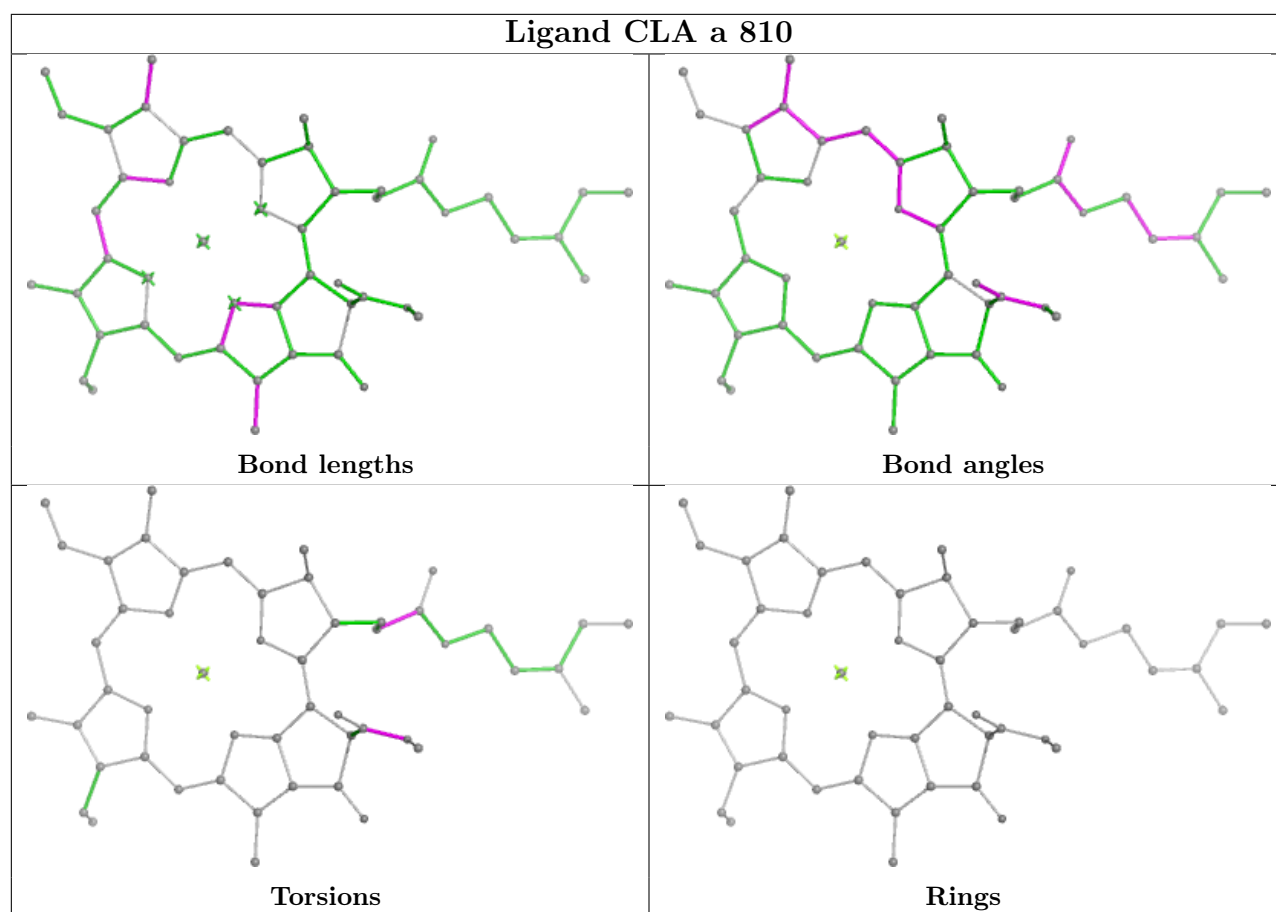


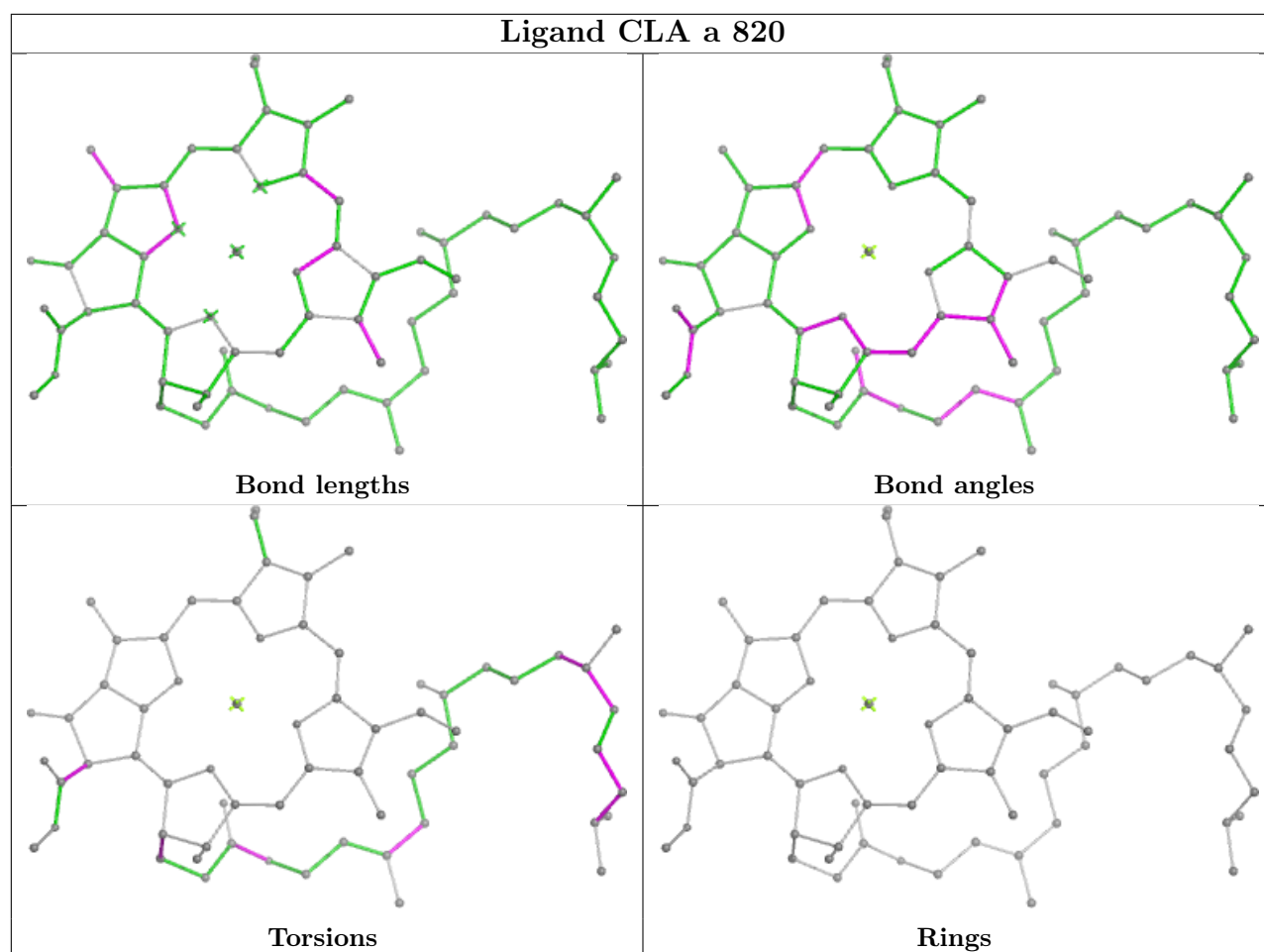
## Ligand CLA b 823



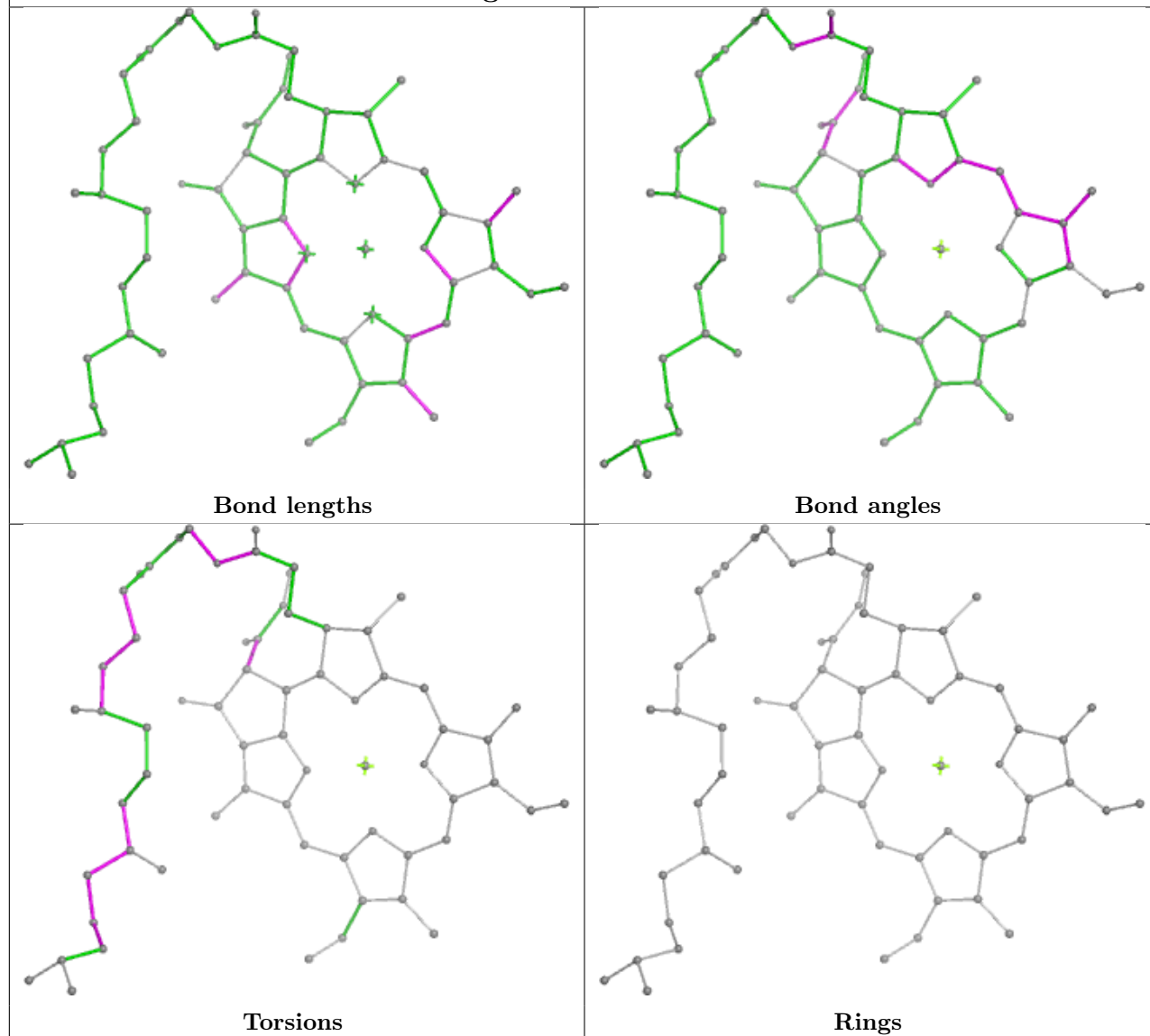
## Ligand CLA b 832



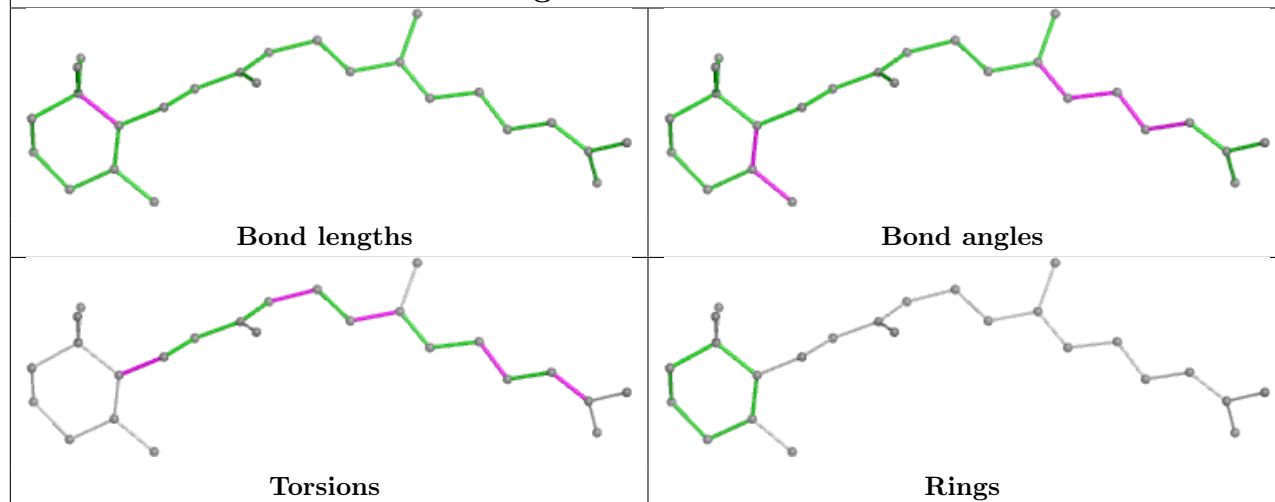


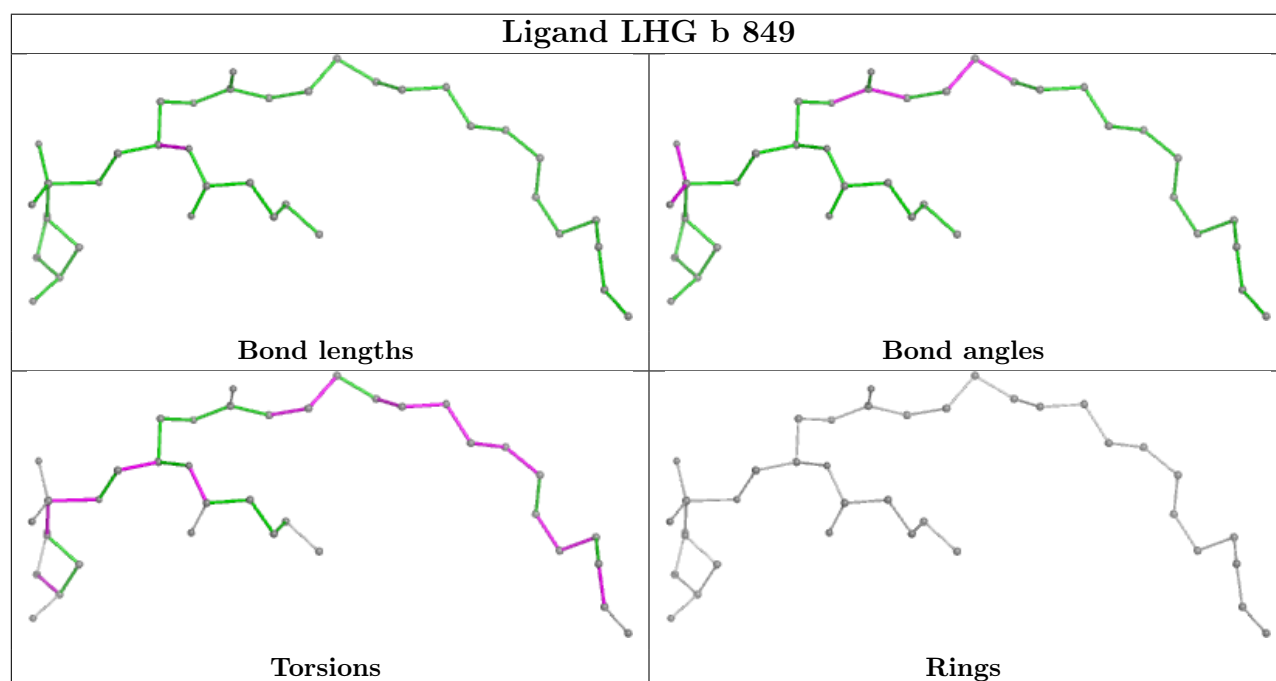
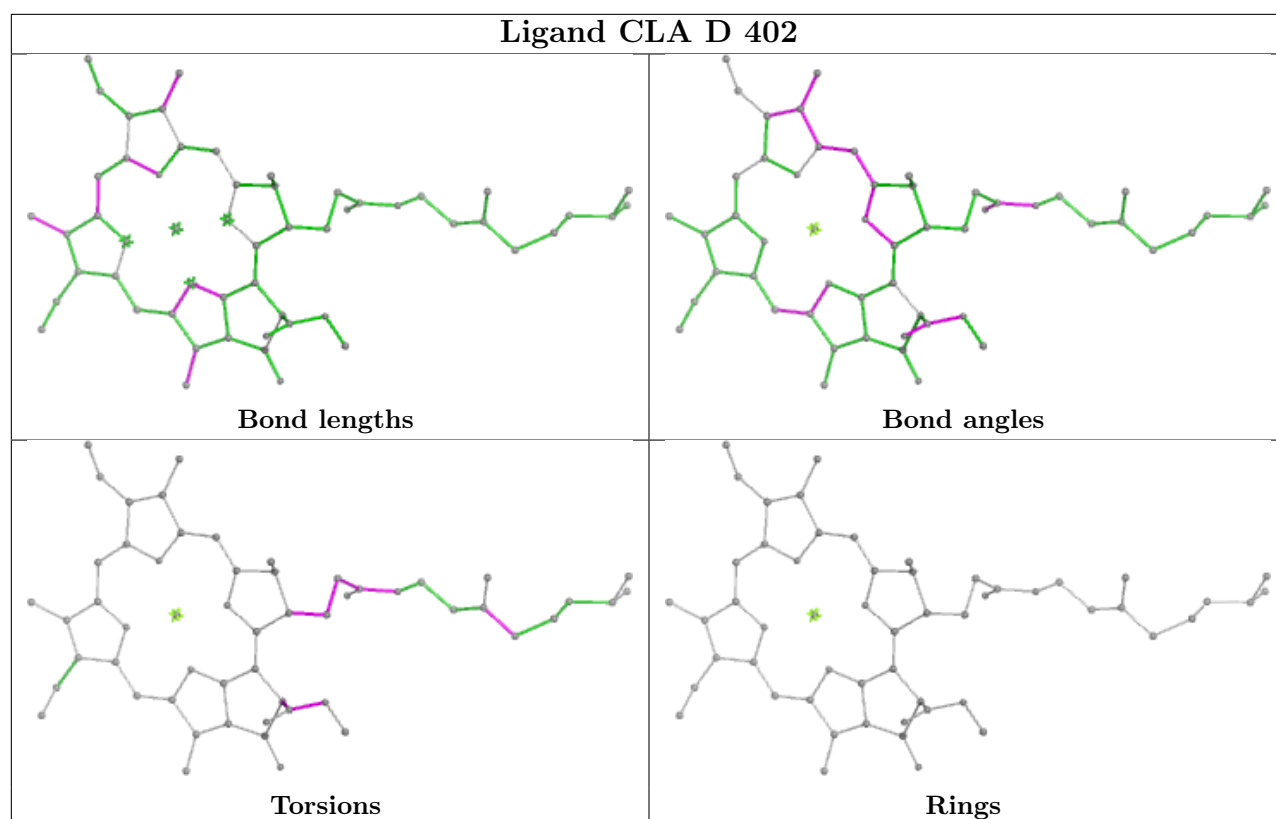


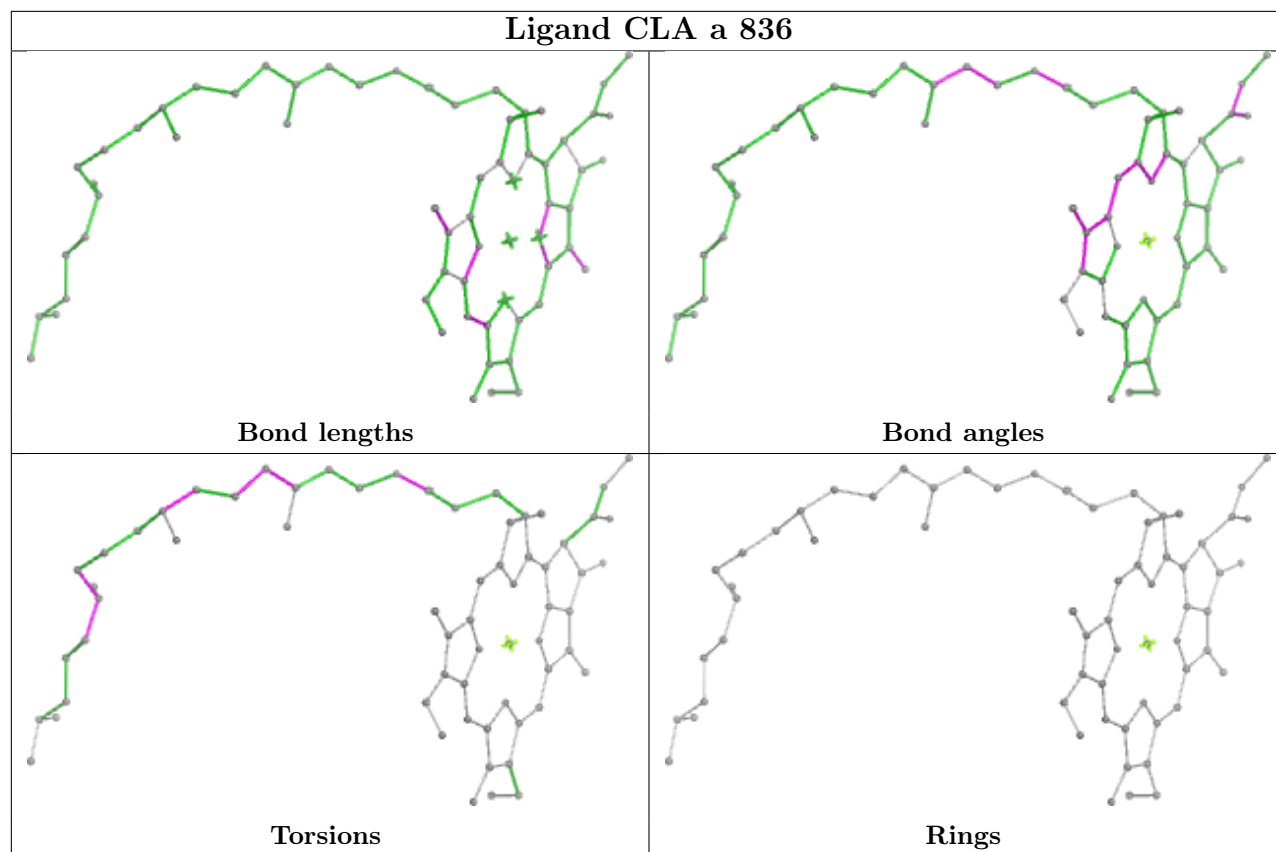
## Ligand CLA a 826

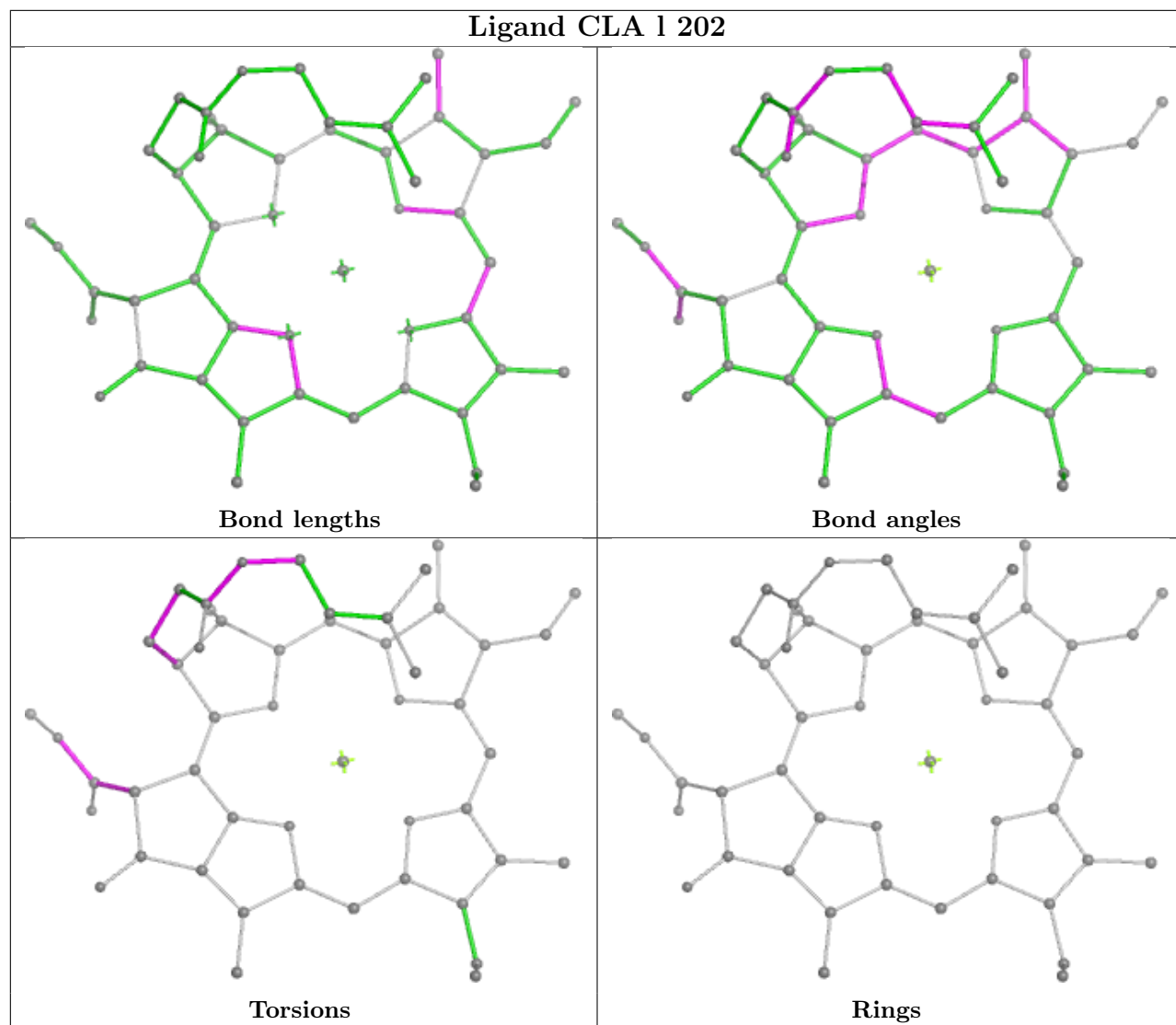


## Ligand BCR a 851

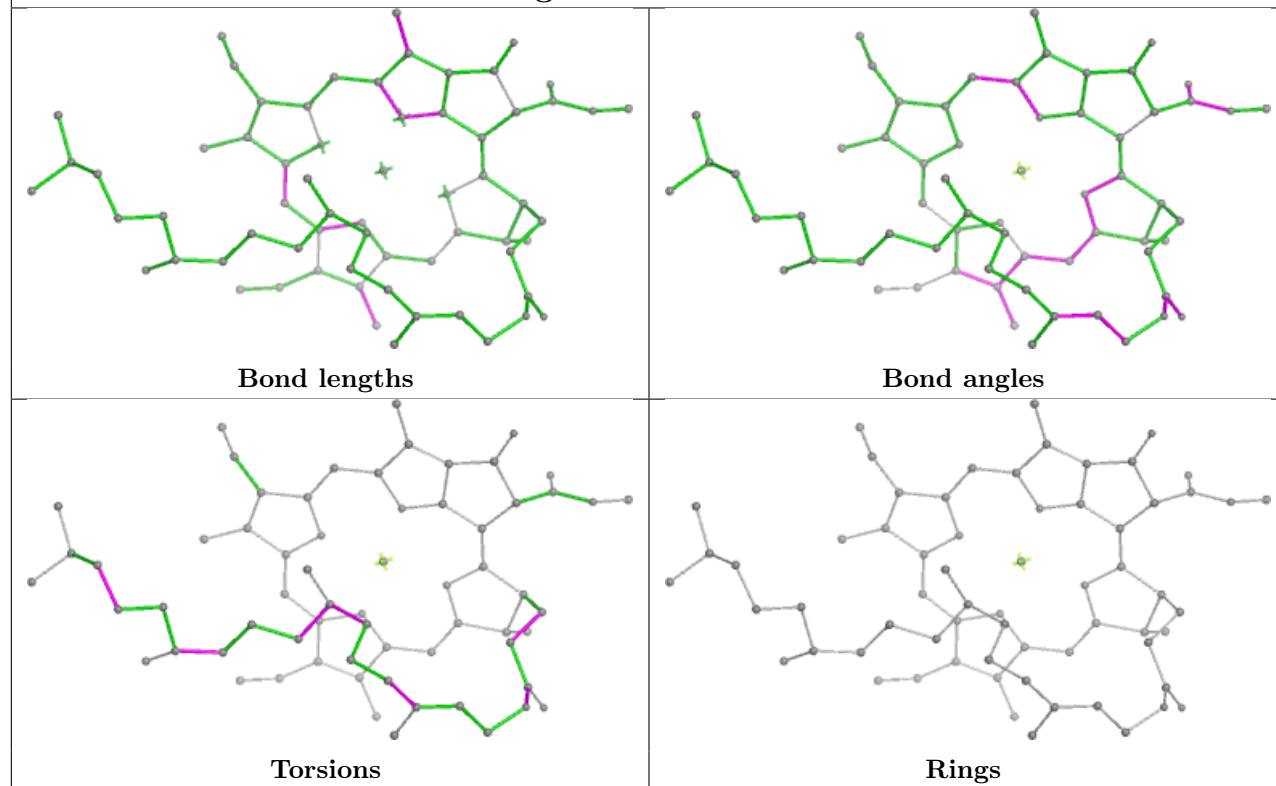




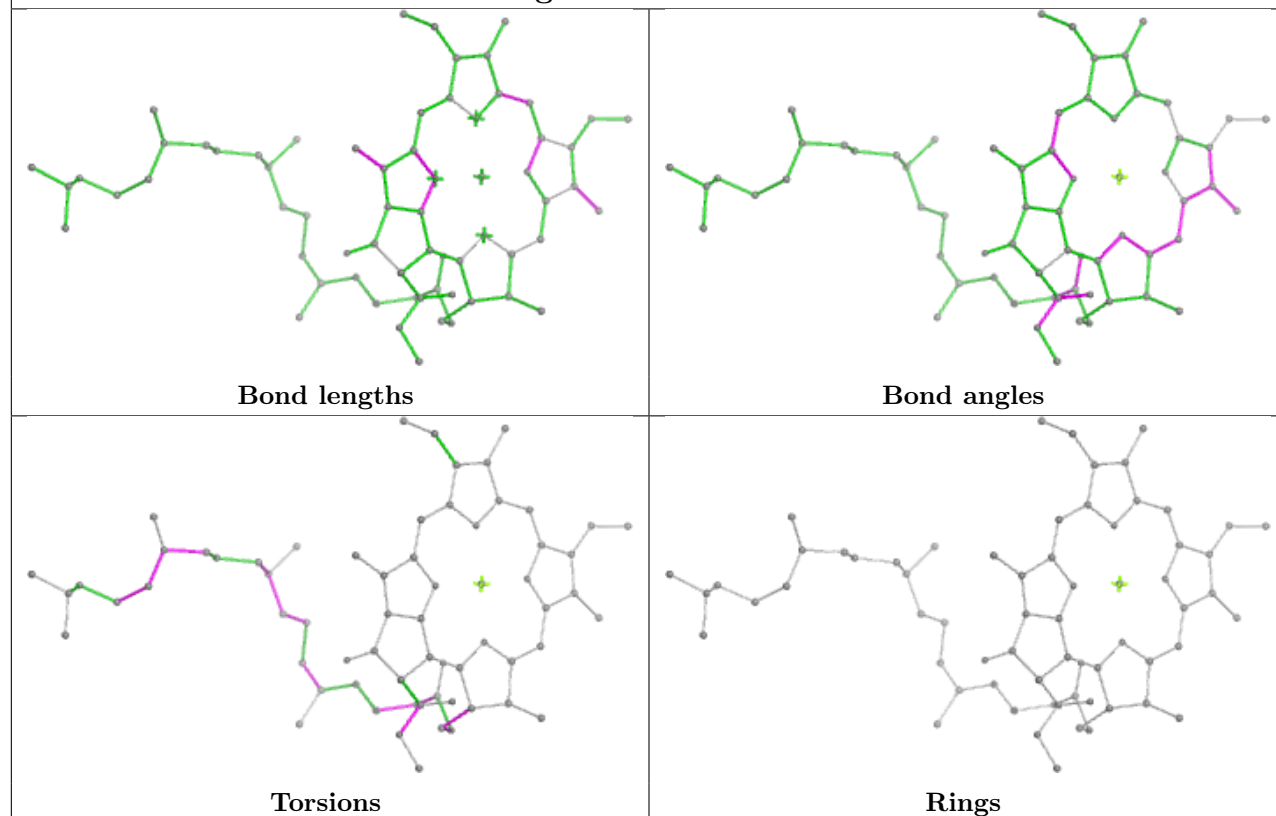




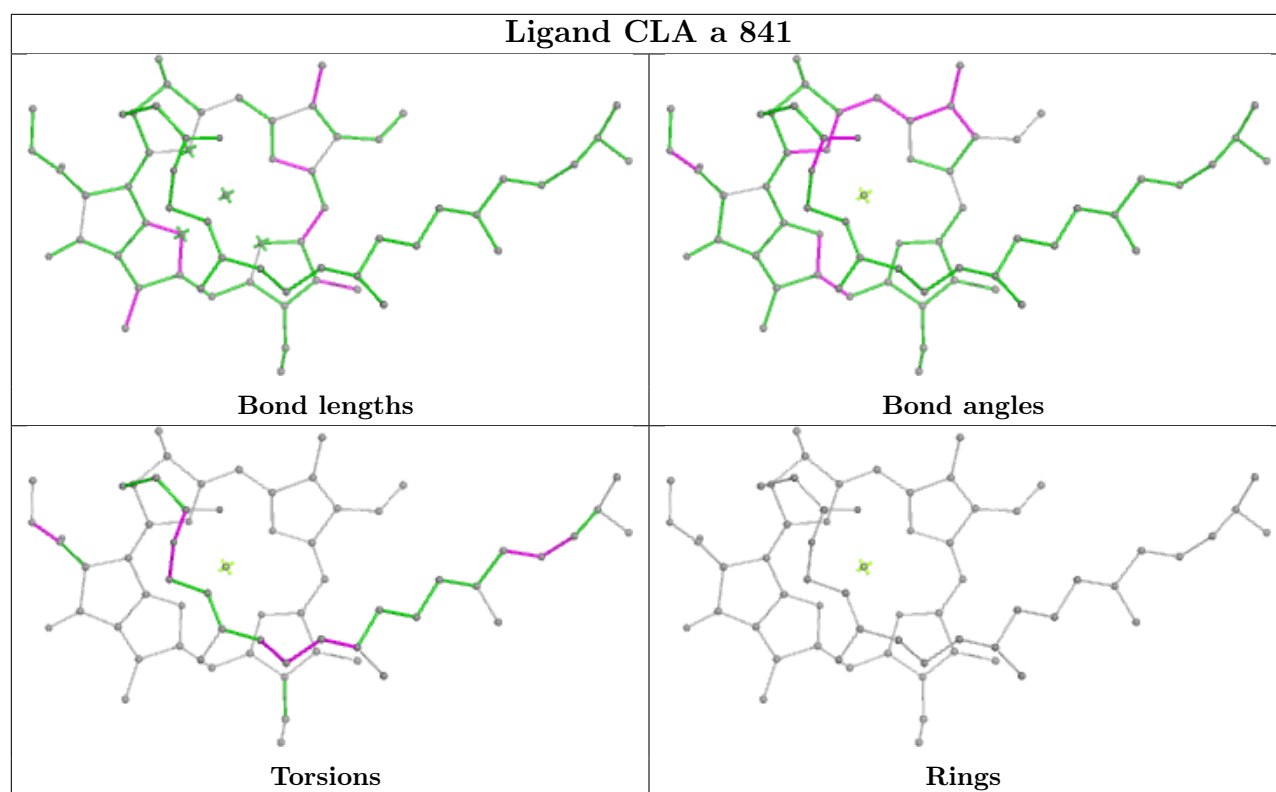
## Ligand CLA b 816

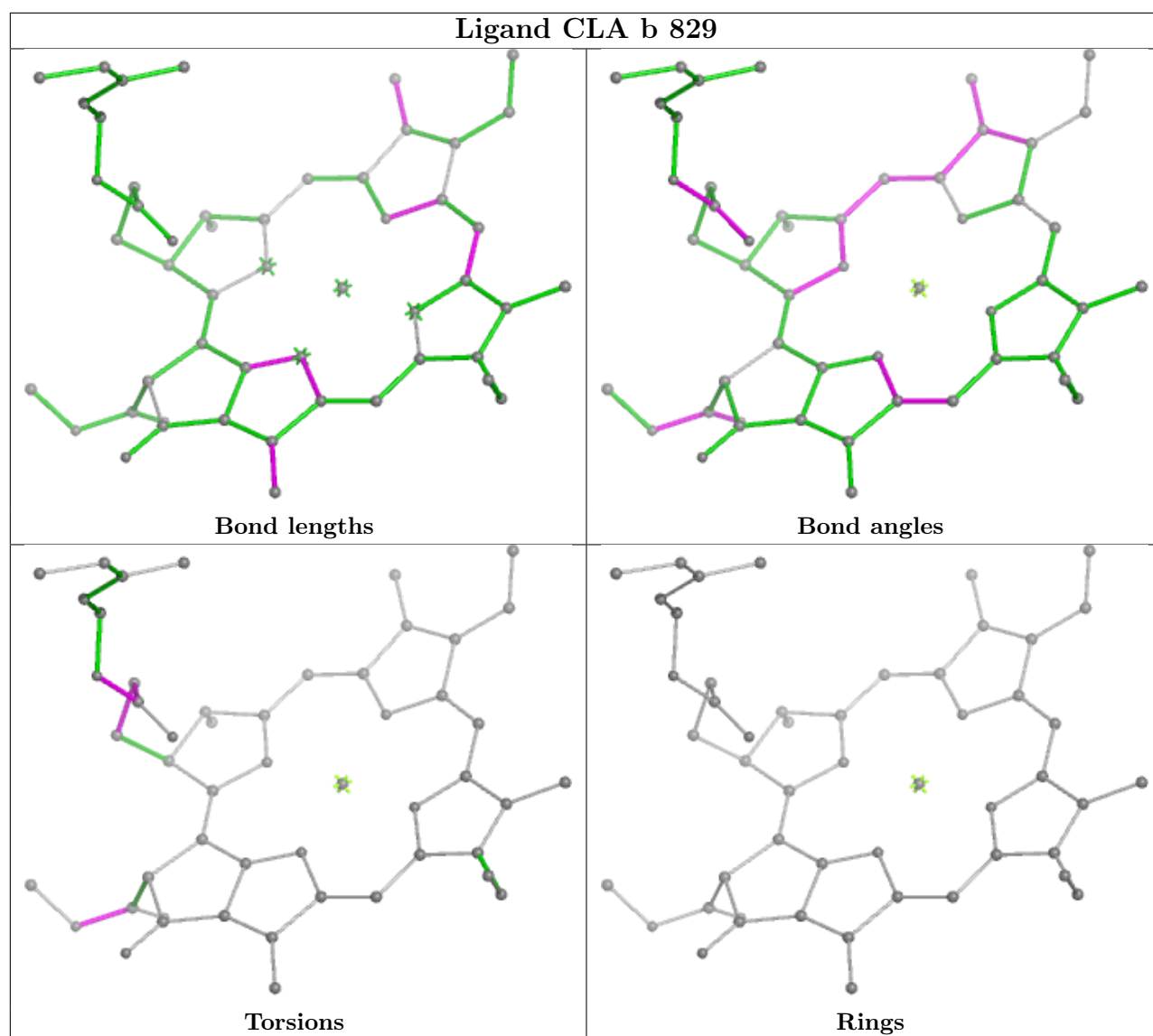


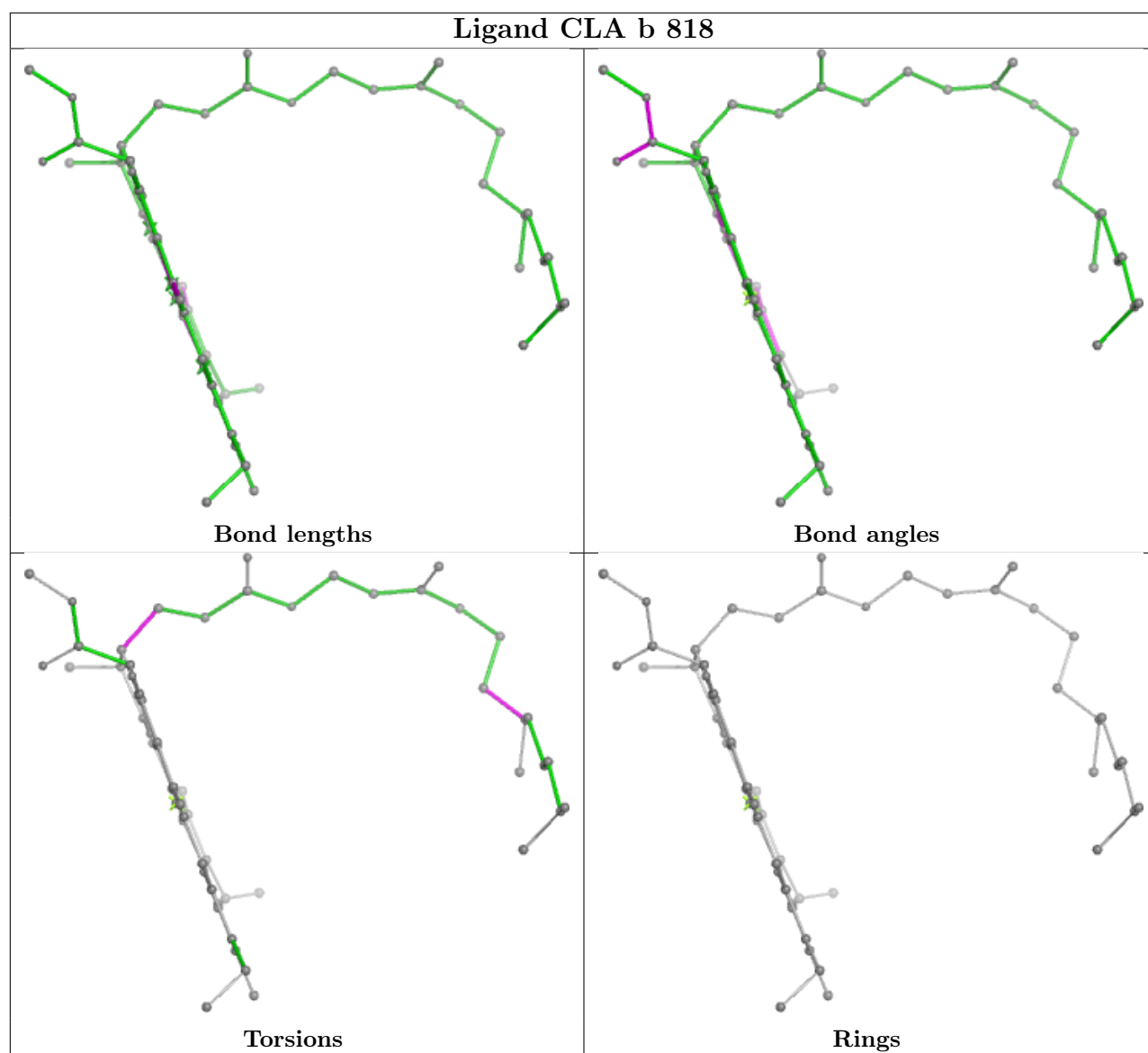
## Ligand CLA b 833

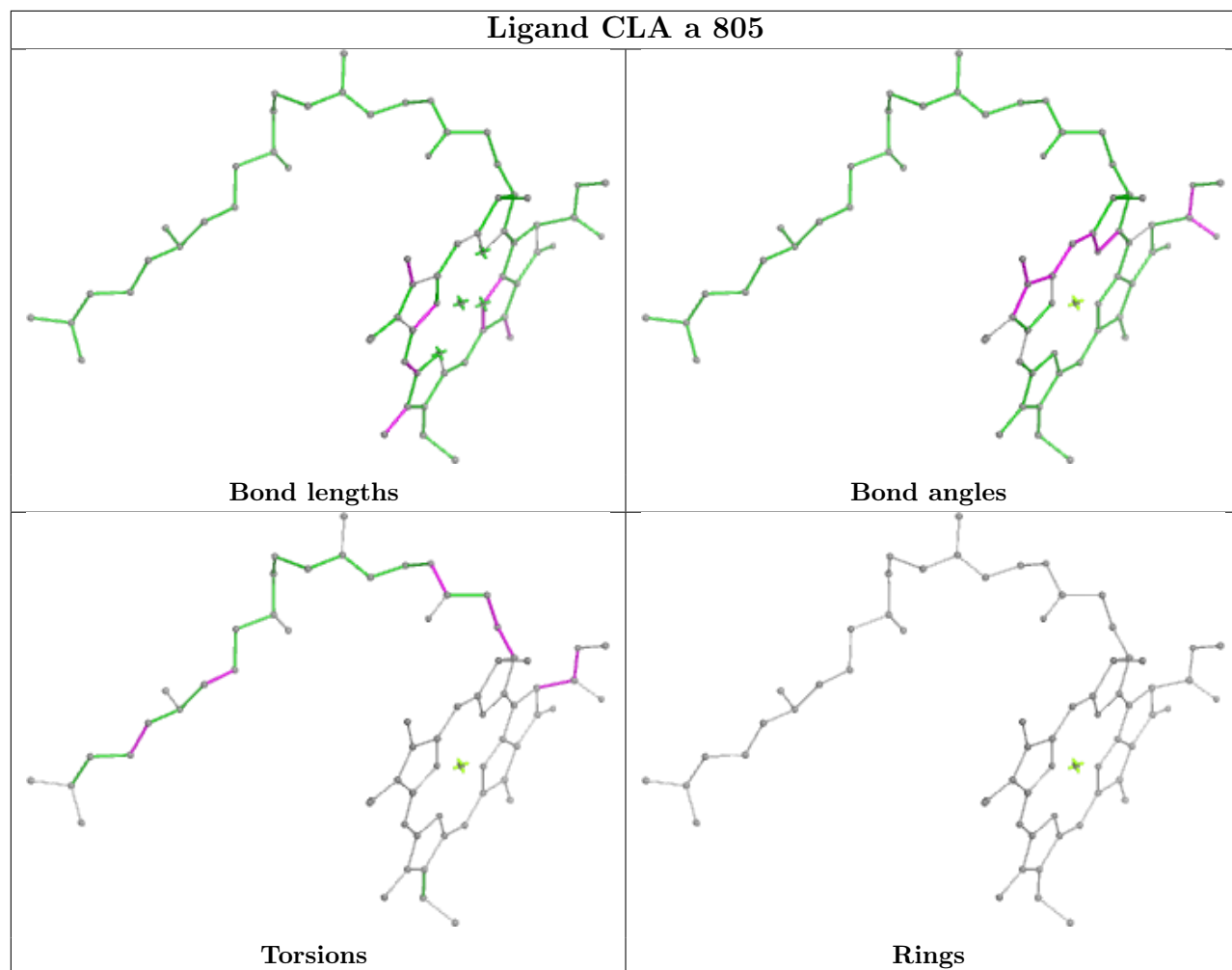




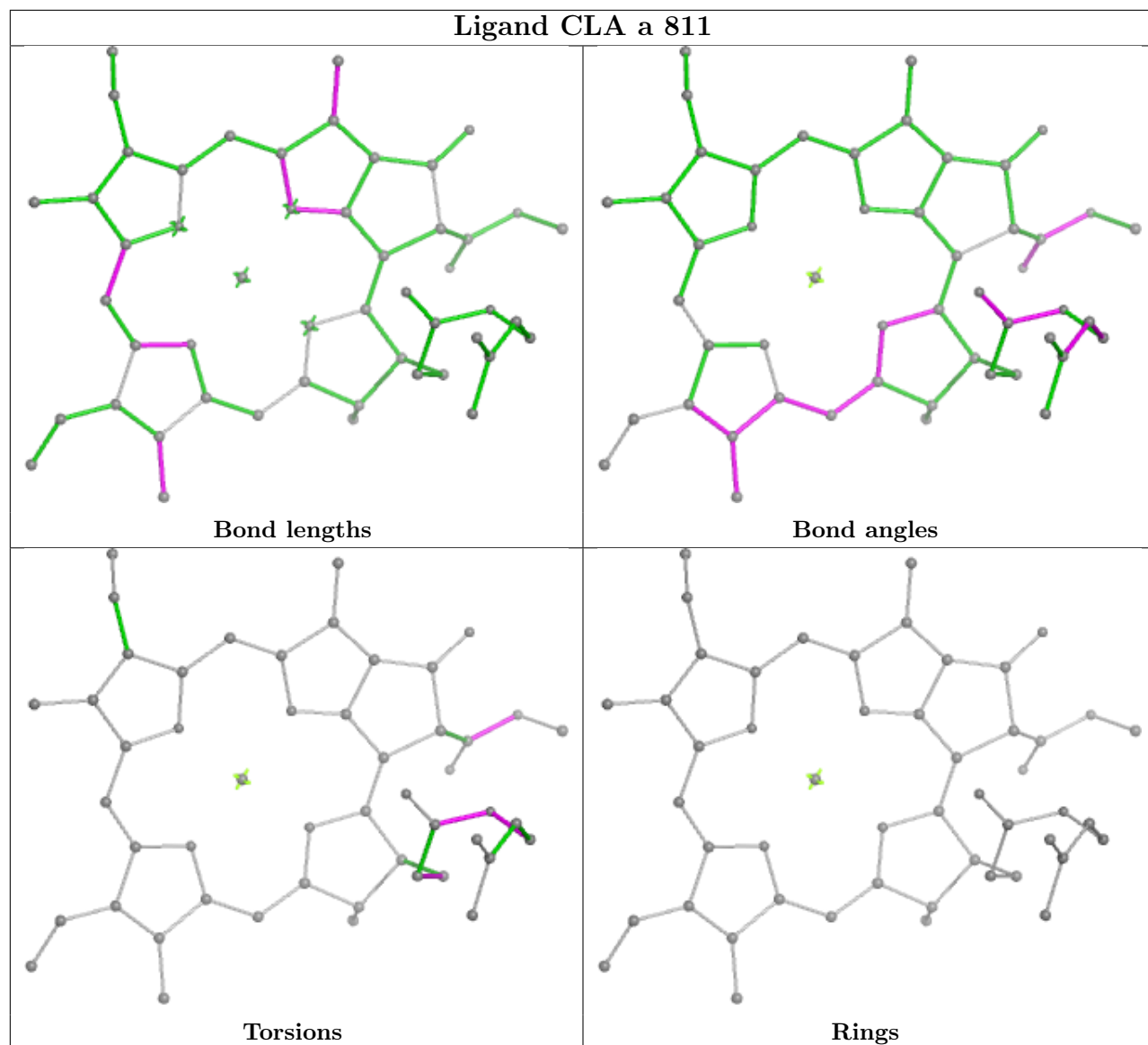




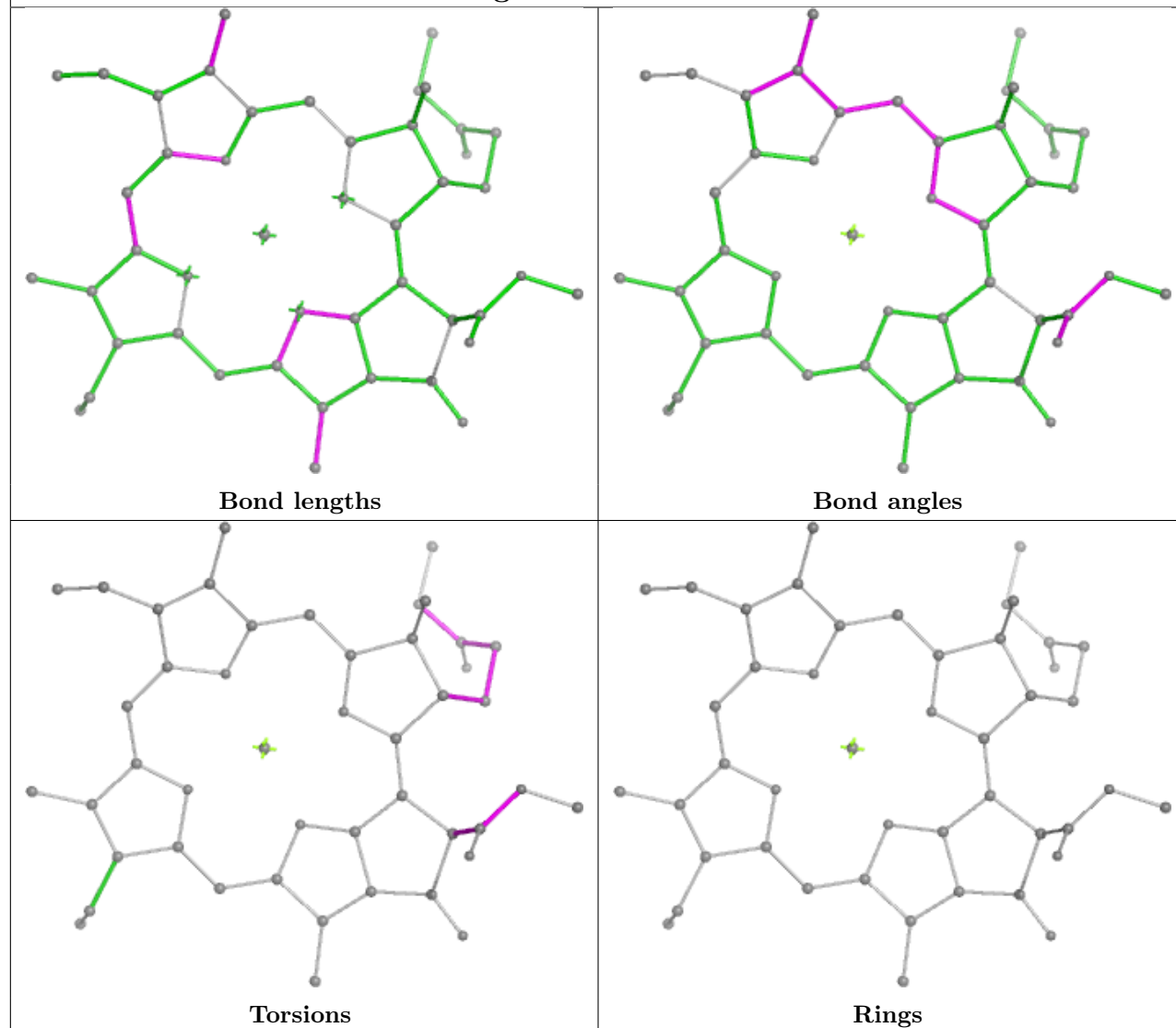




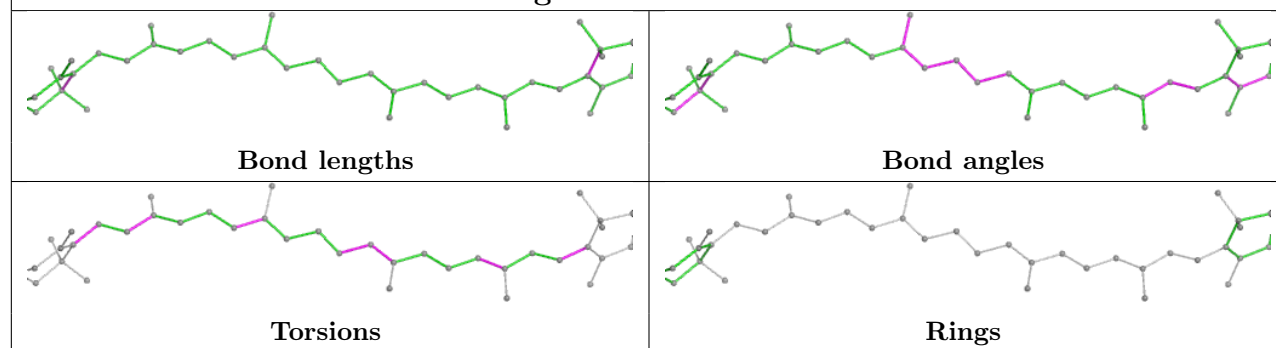
## Ligand CLA a 811

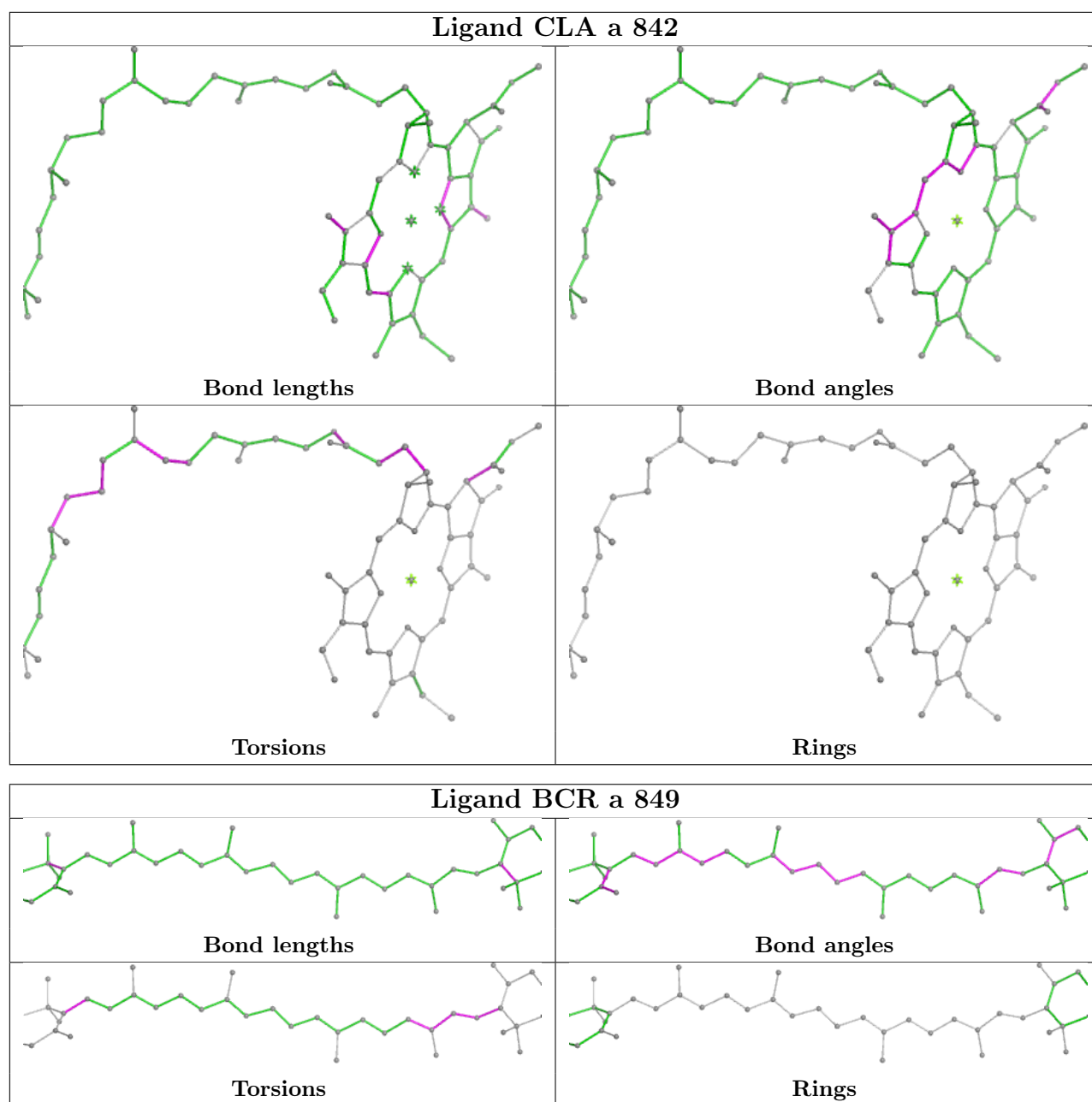


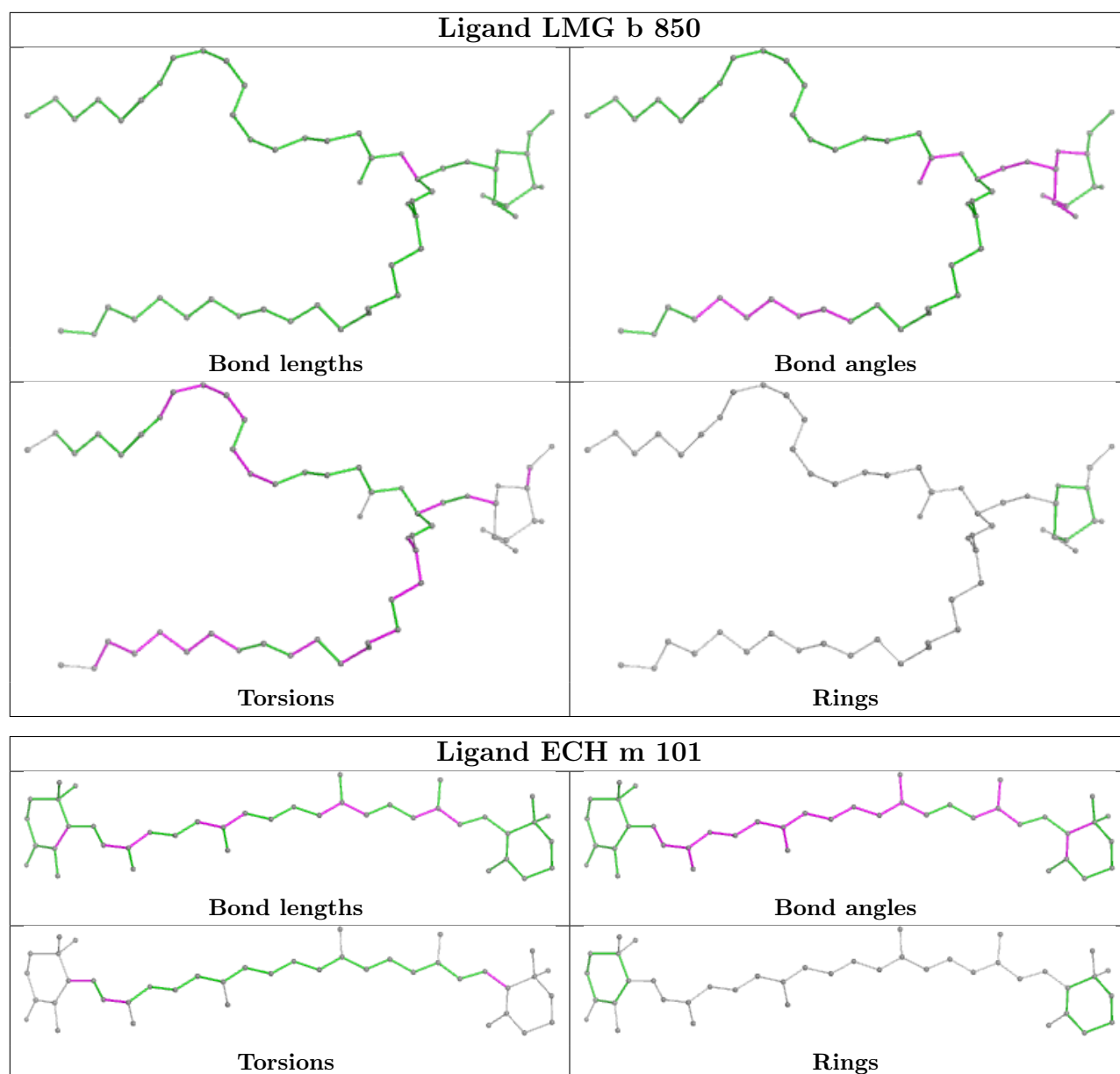
## Ligand CLA k 101



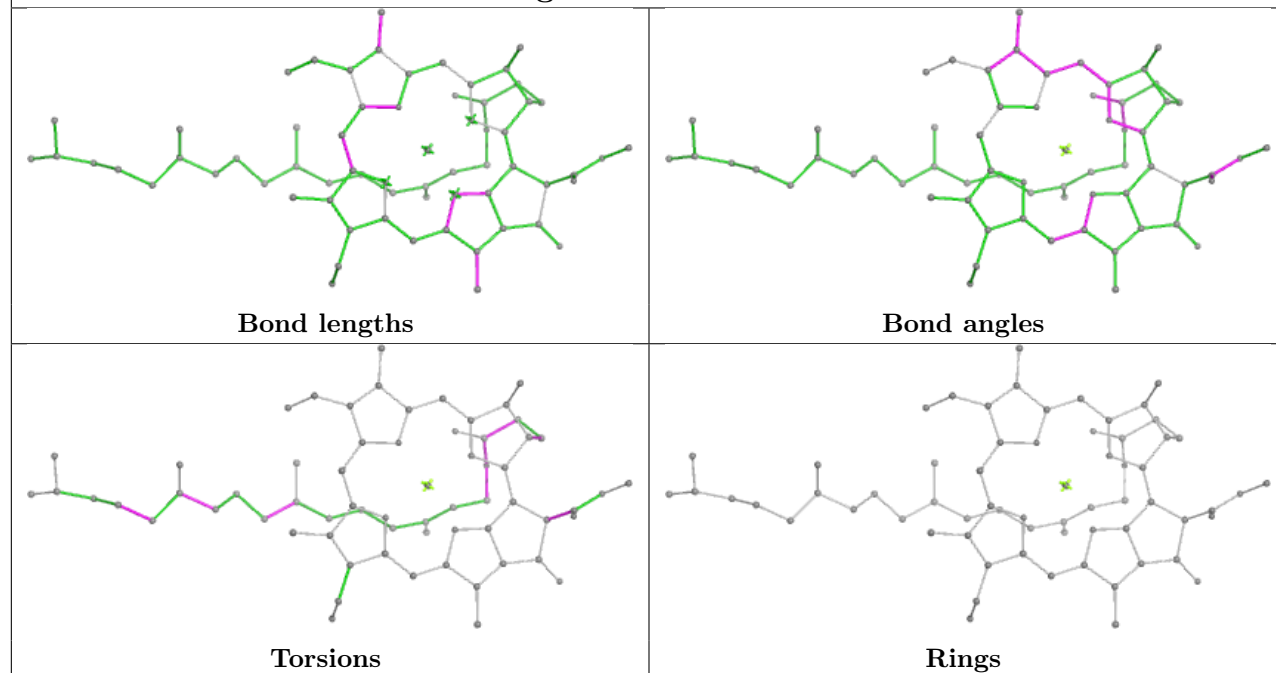
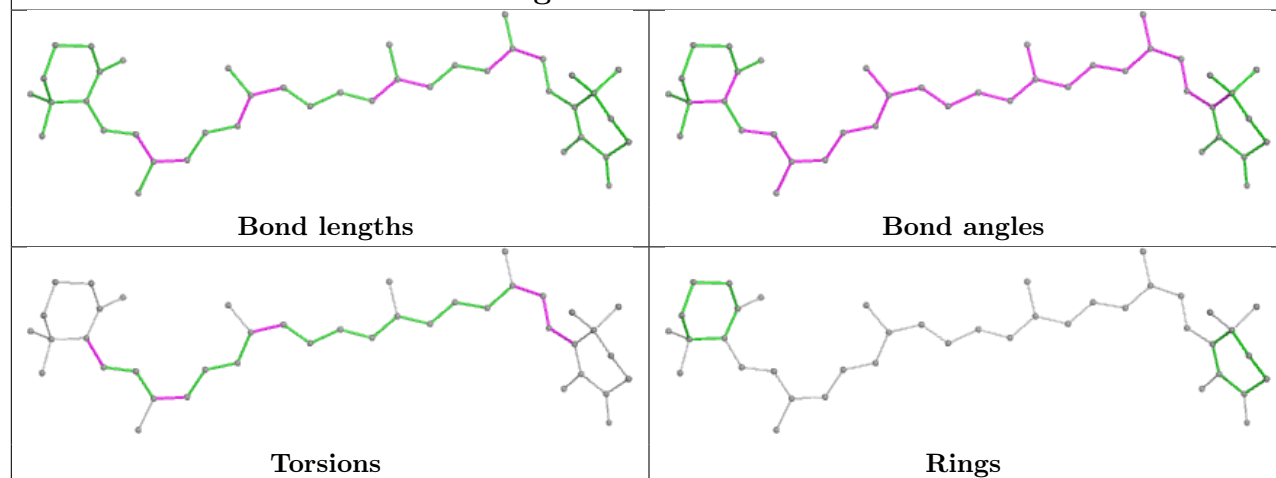
## Ligand BCR k 103



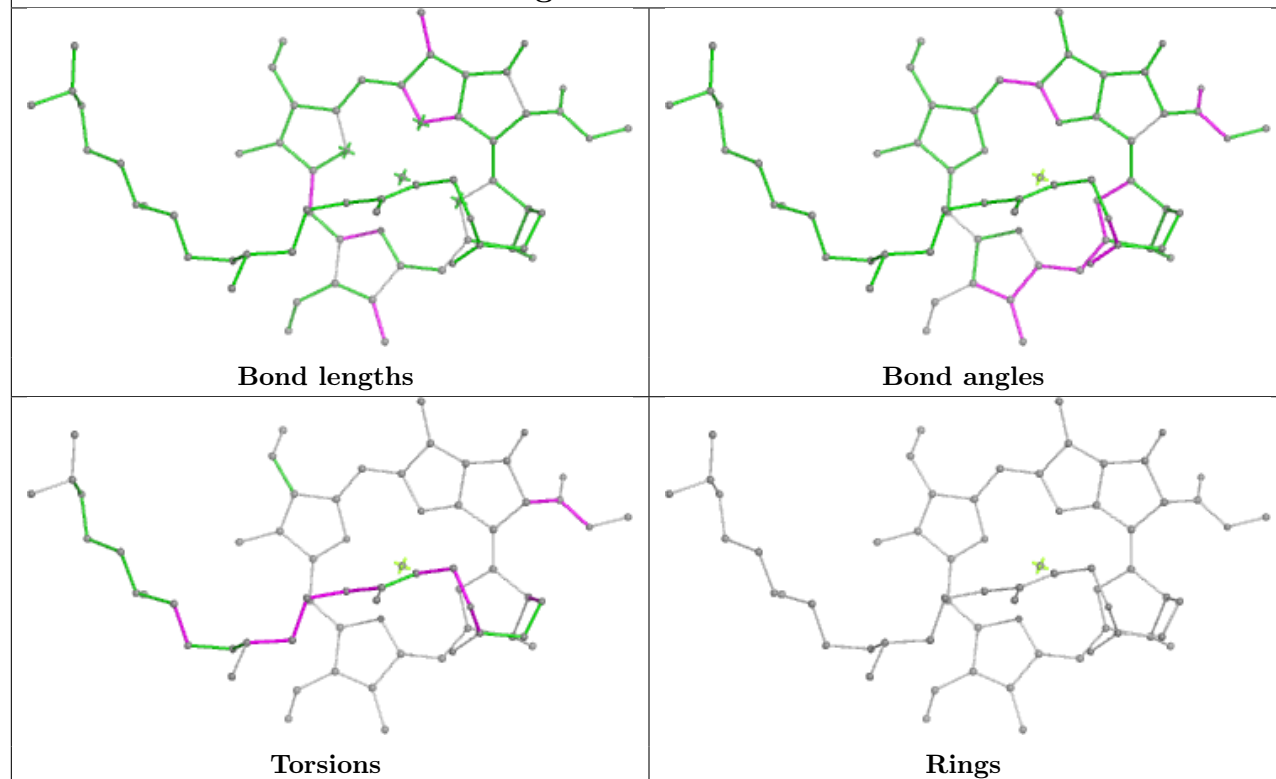




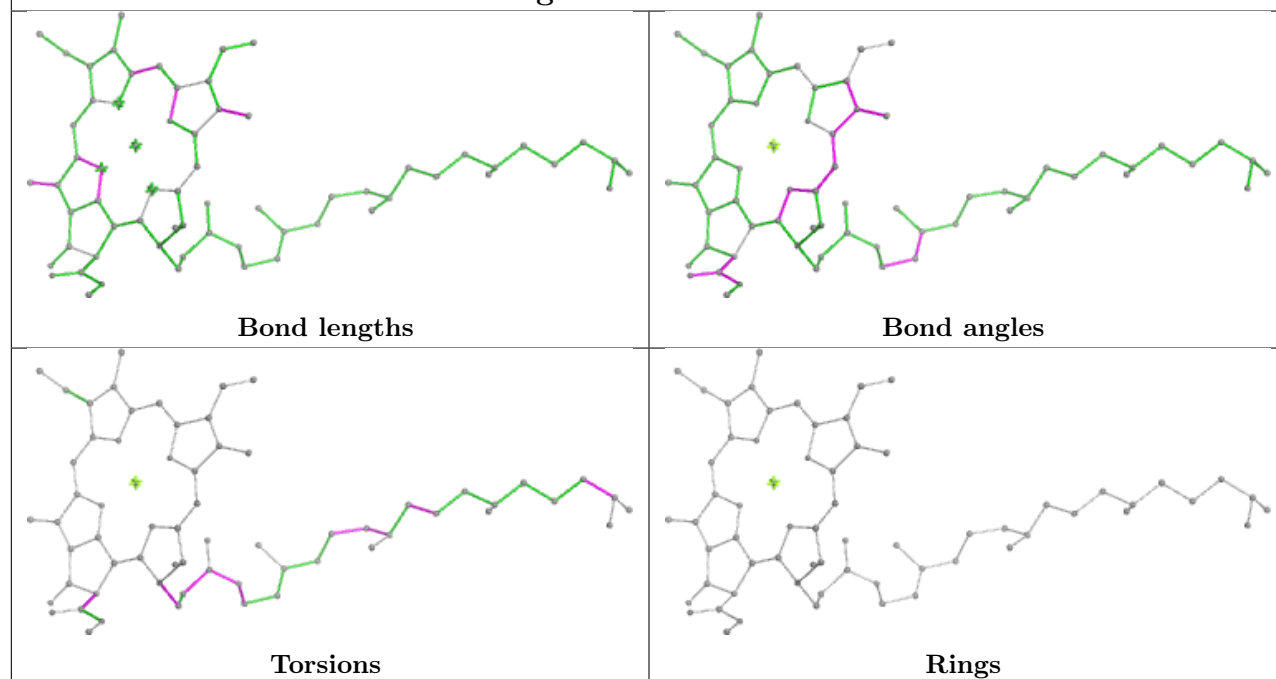


**Ligand CLA a 839****Ligand ECH b 844**

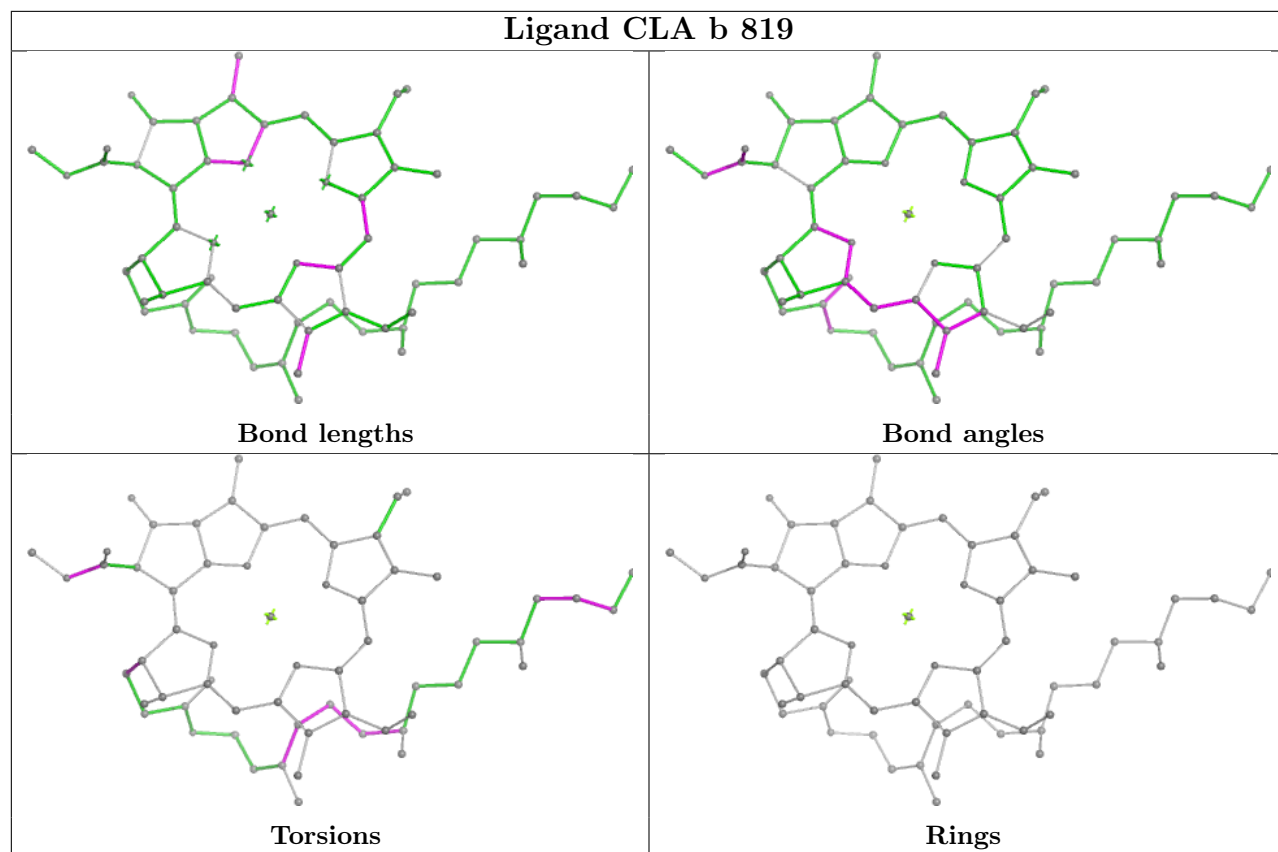
## Ligand CLA b 836



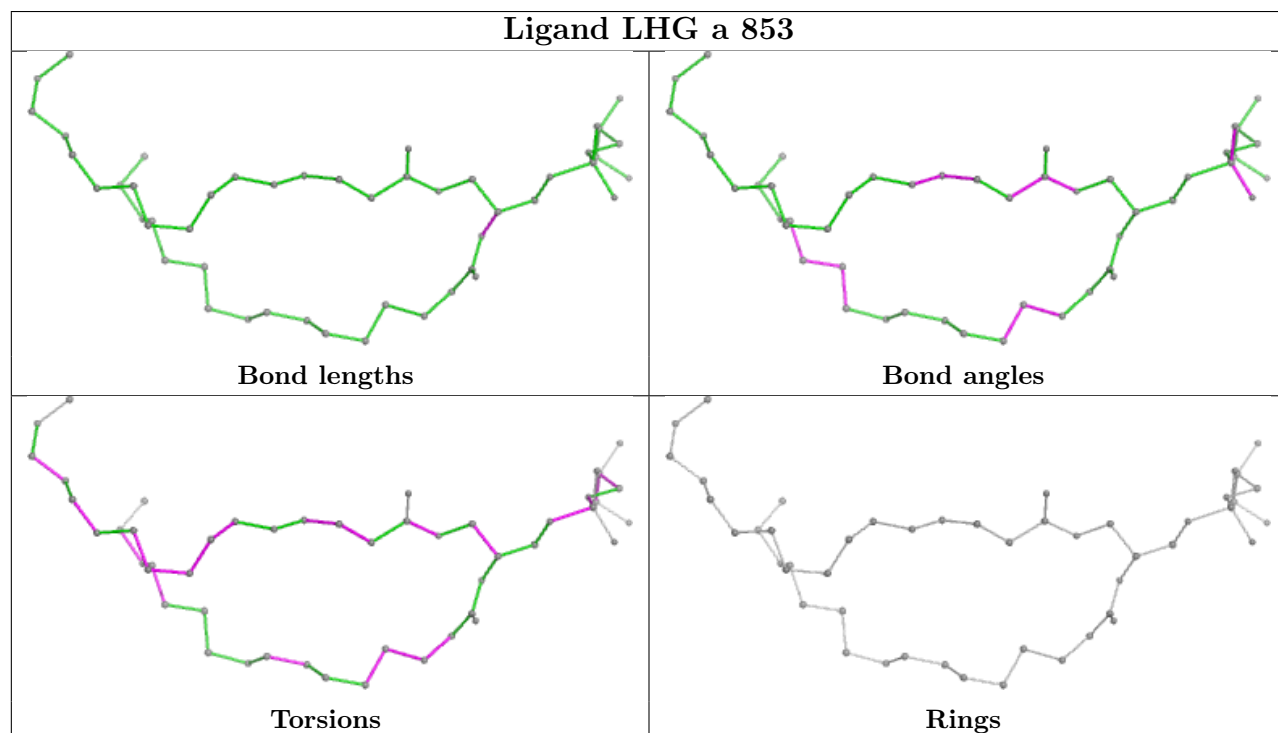
## Ligand CLA a 835

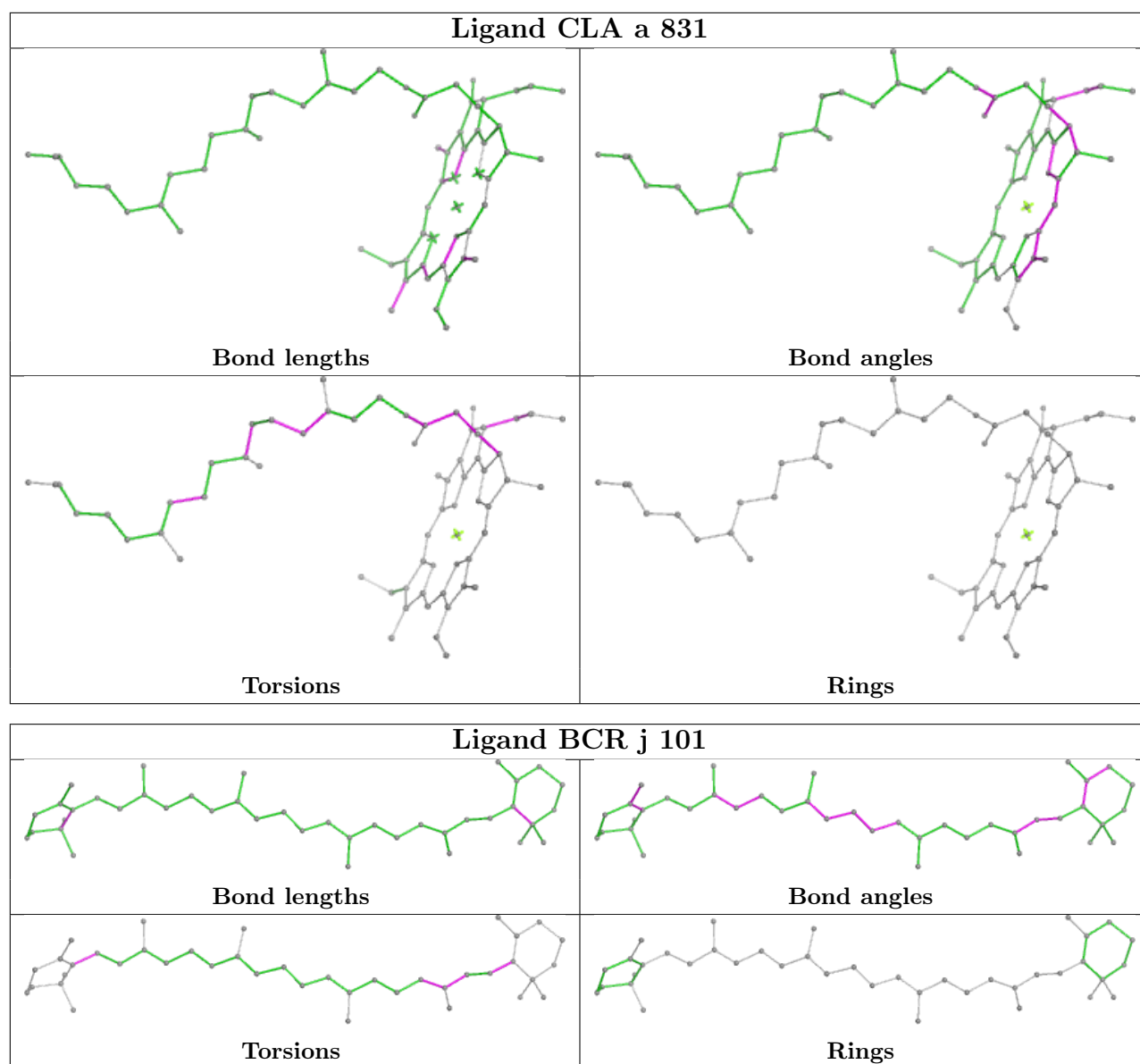


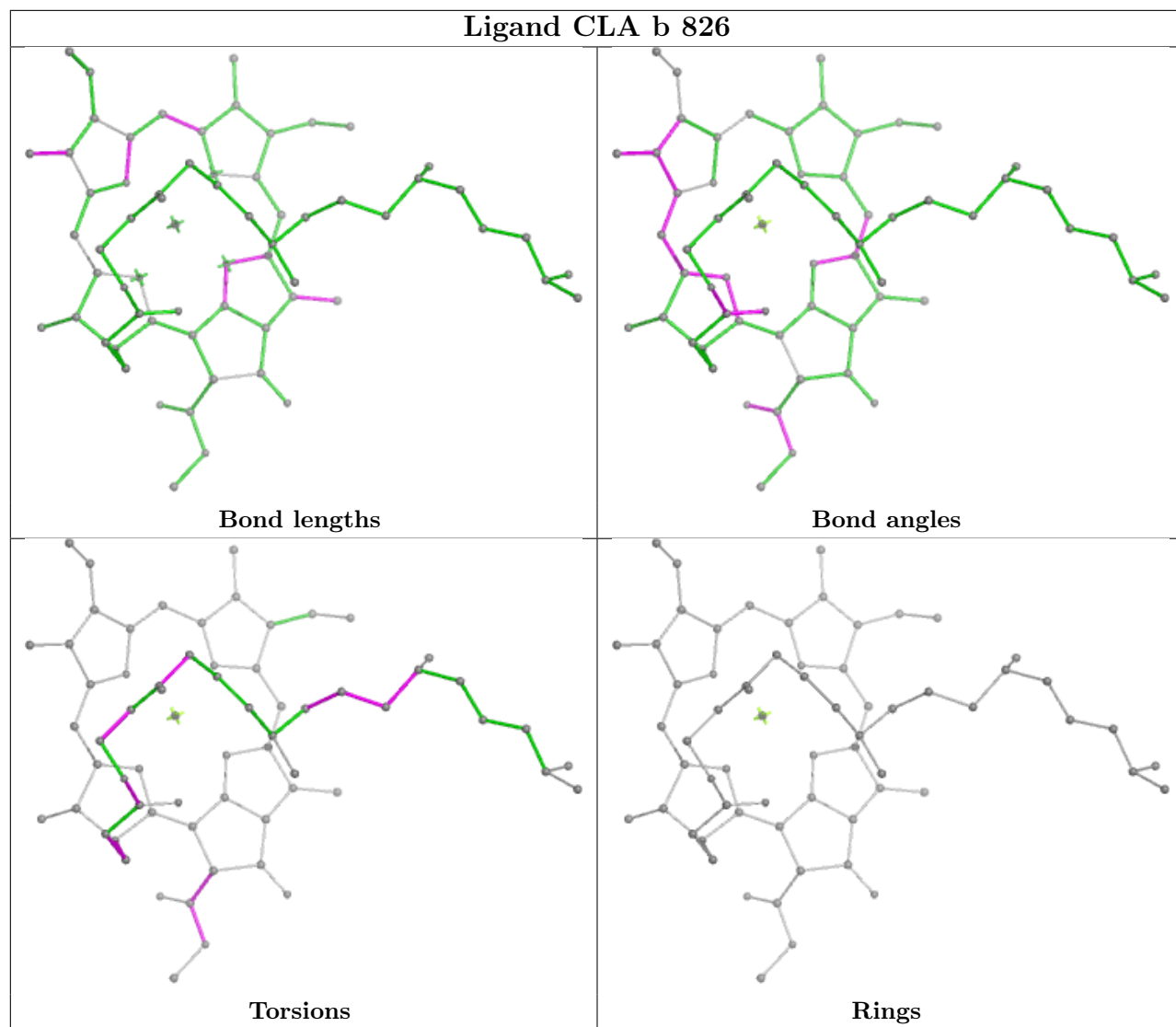
## Ligand CLA b 819

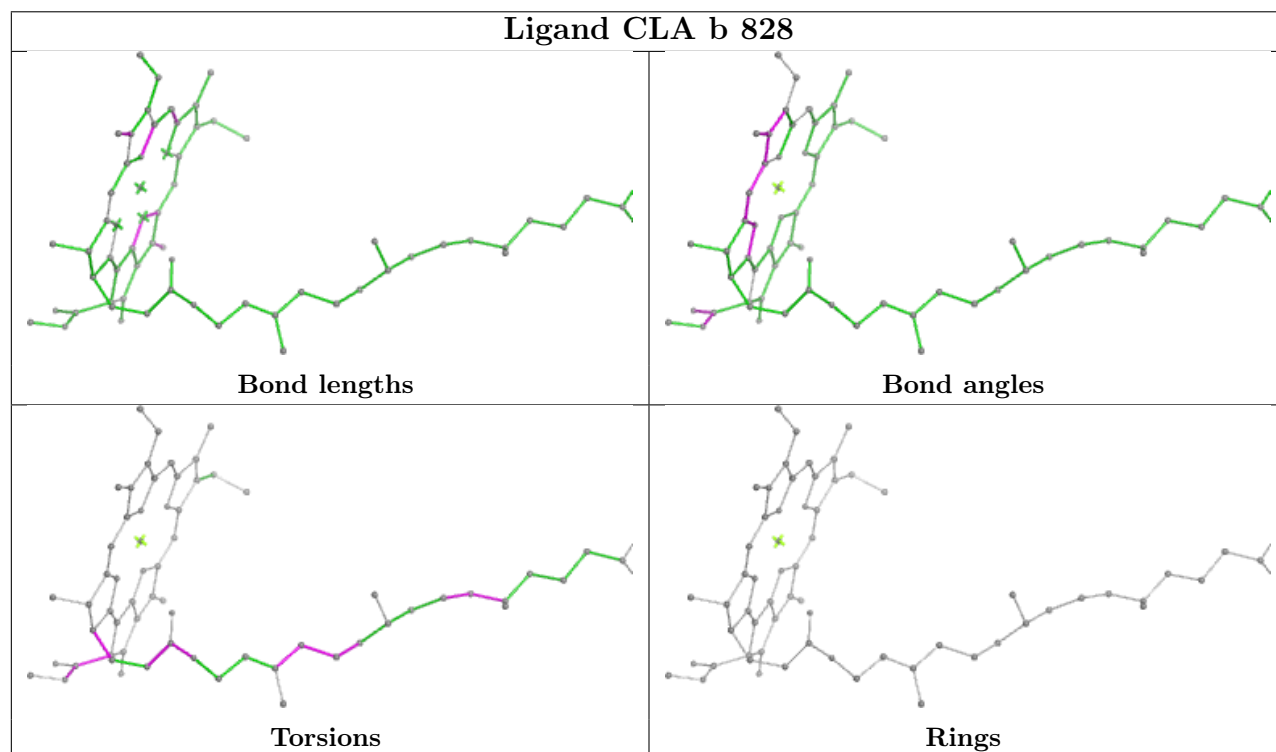
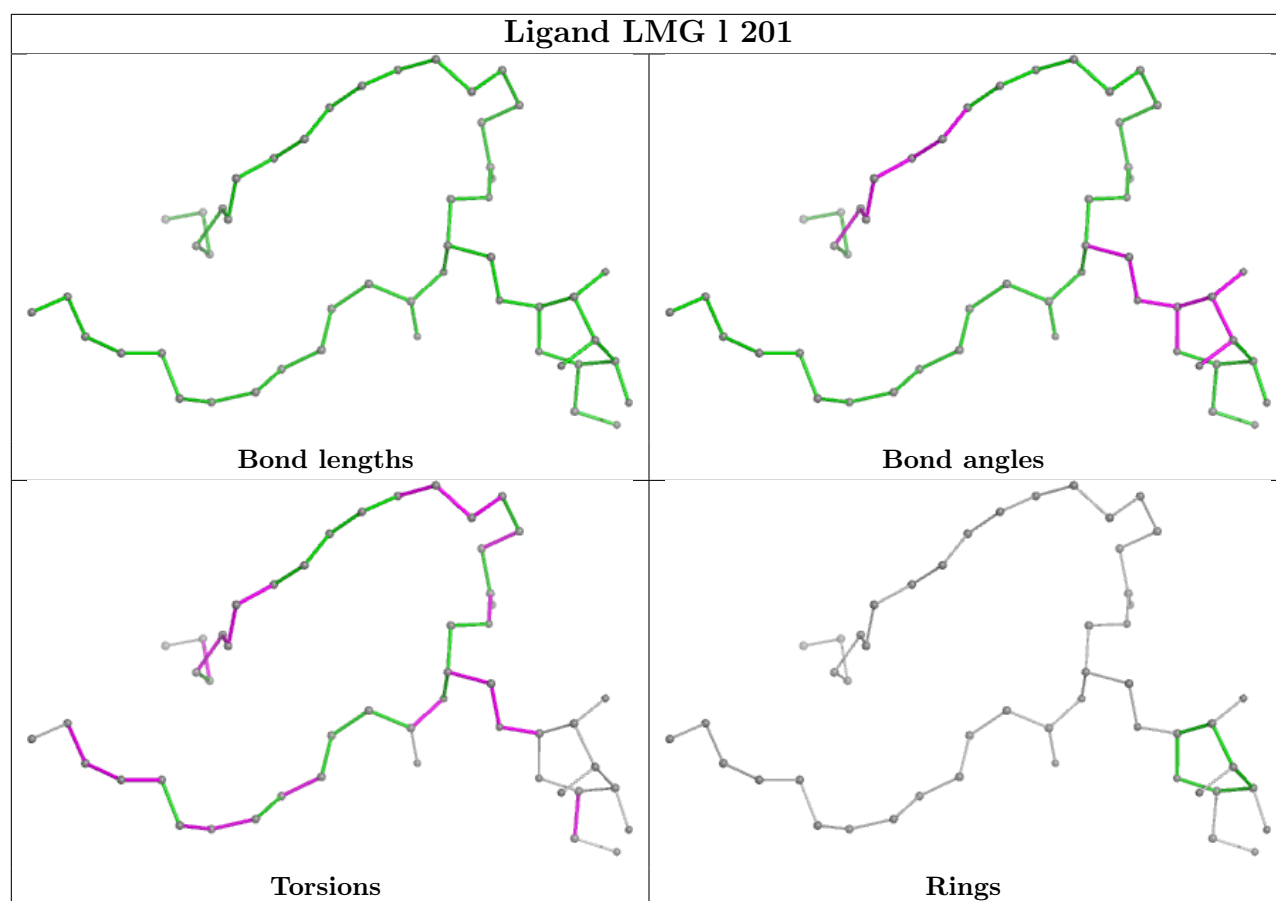


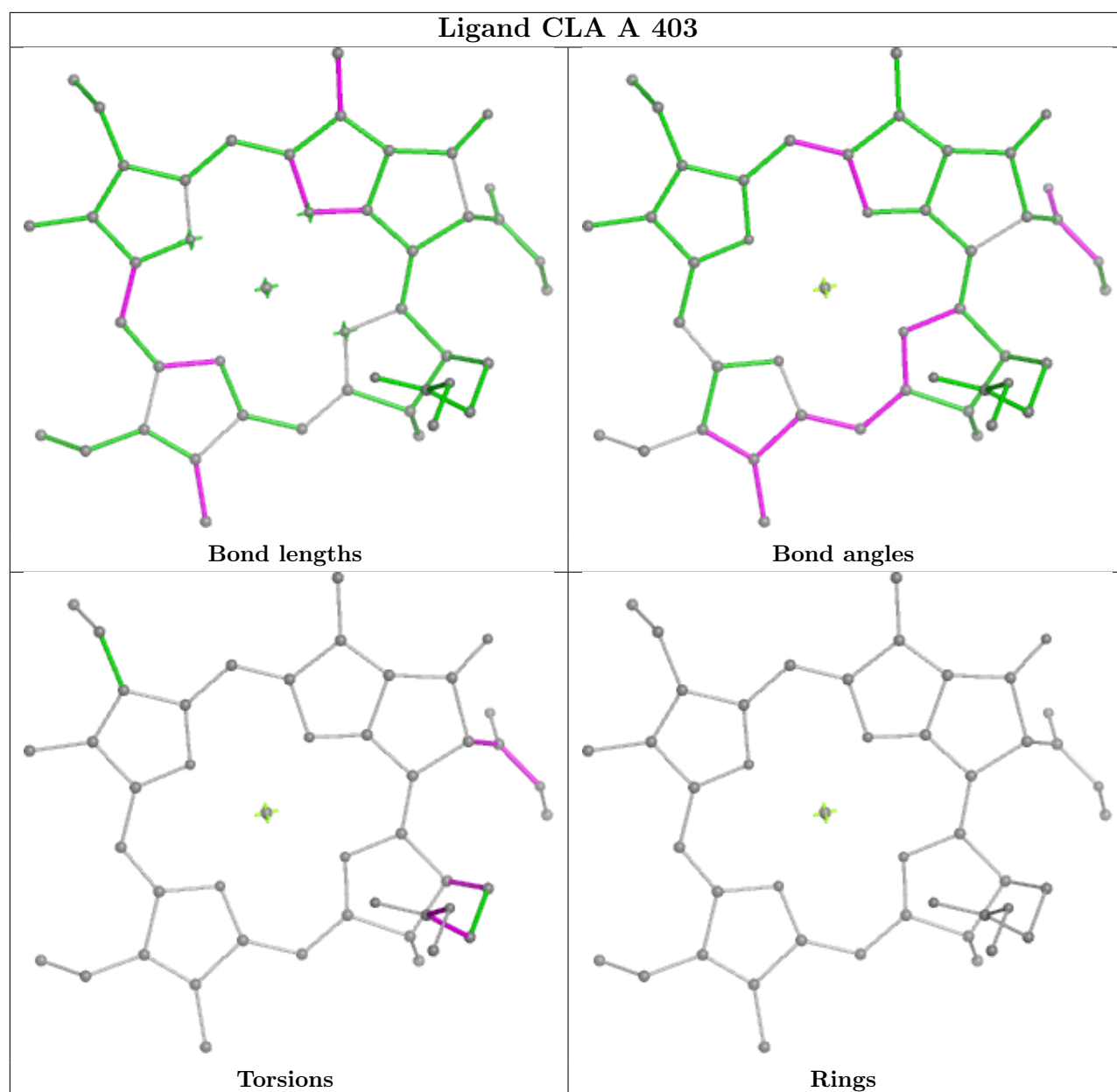
## Ligand LHG a 853



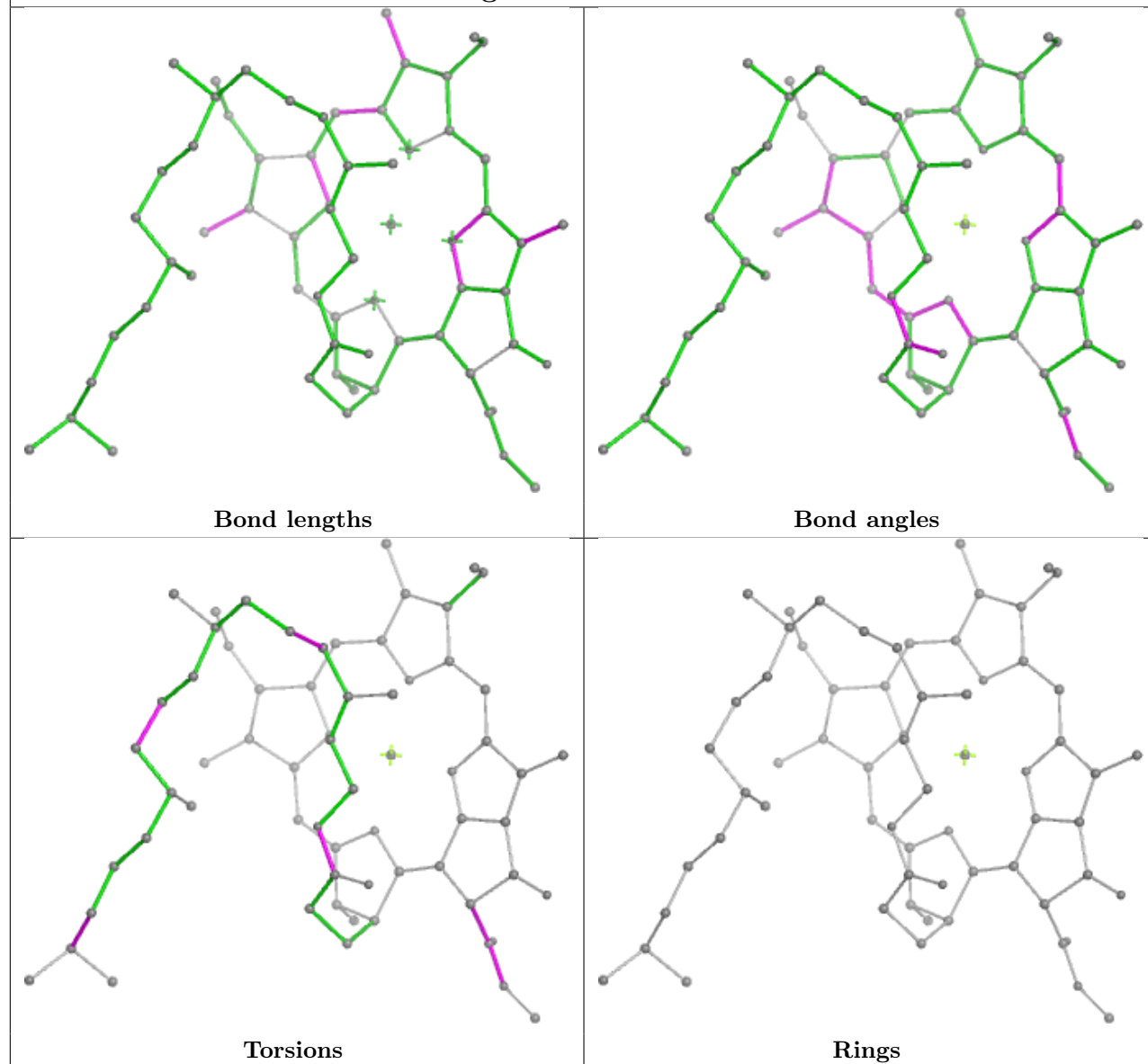




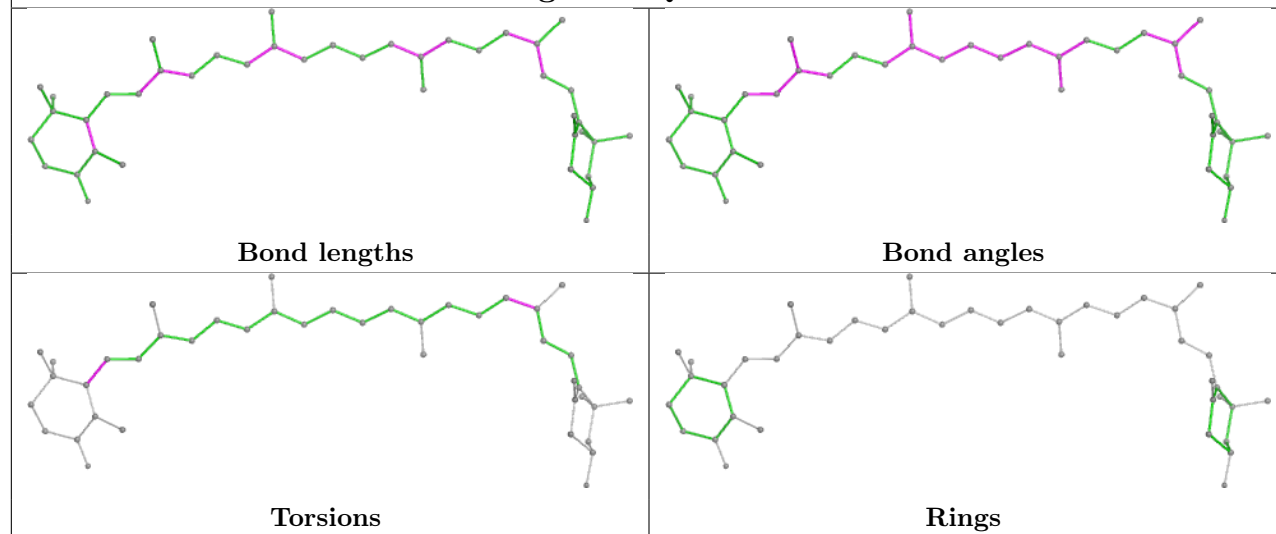




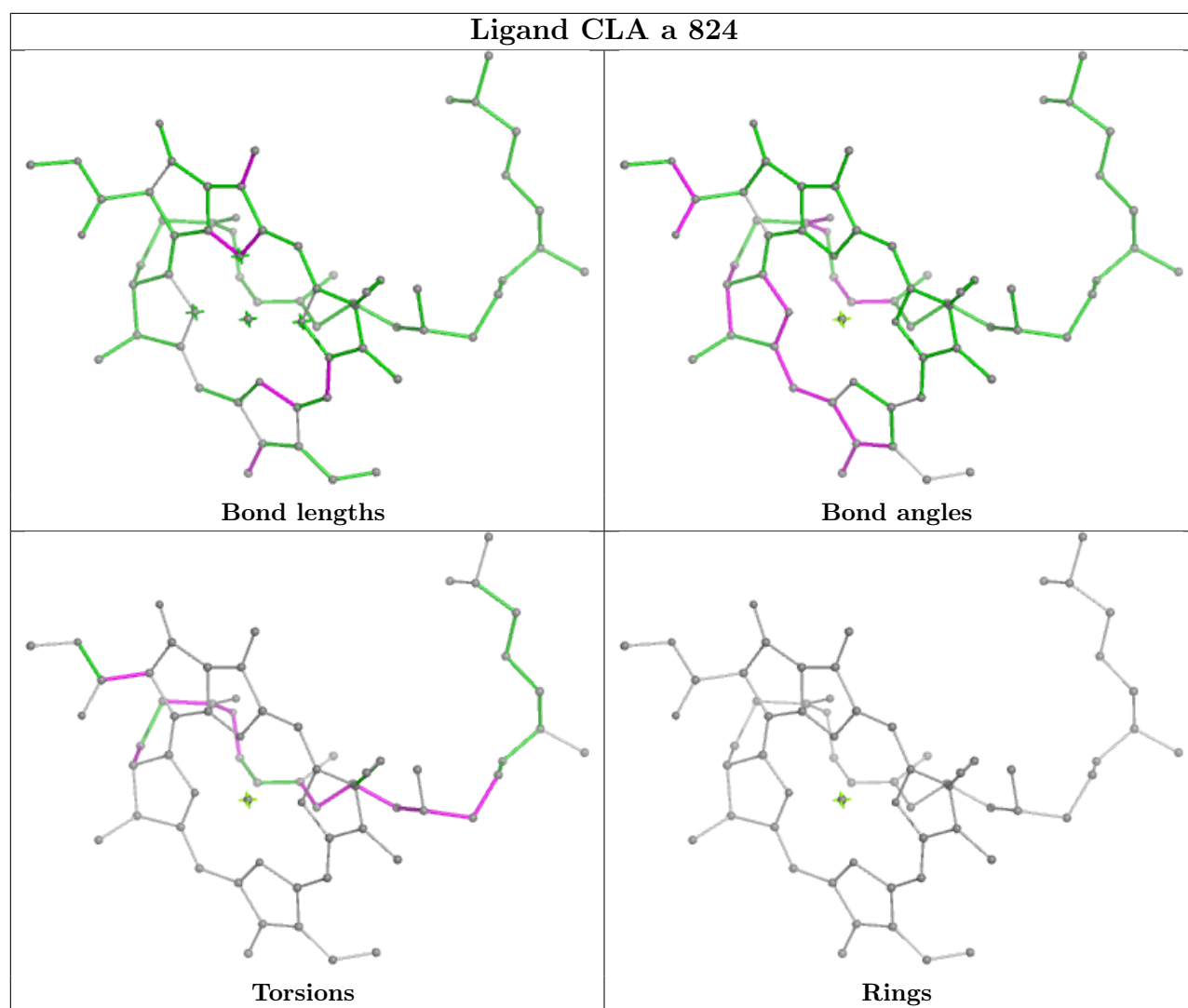
## Ligand CLA b 807

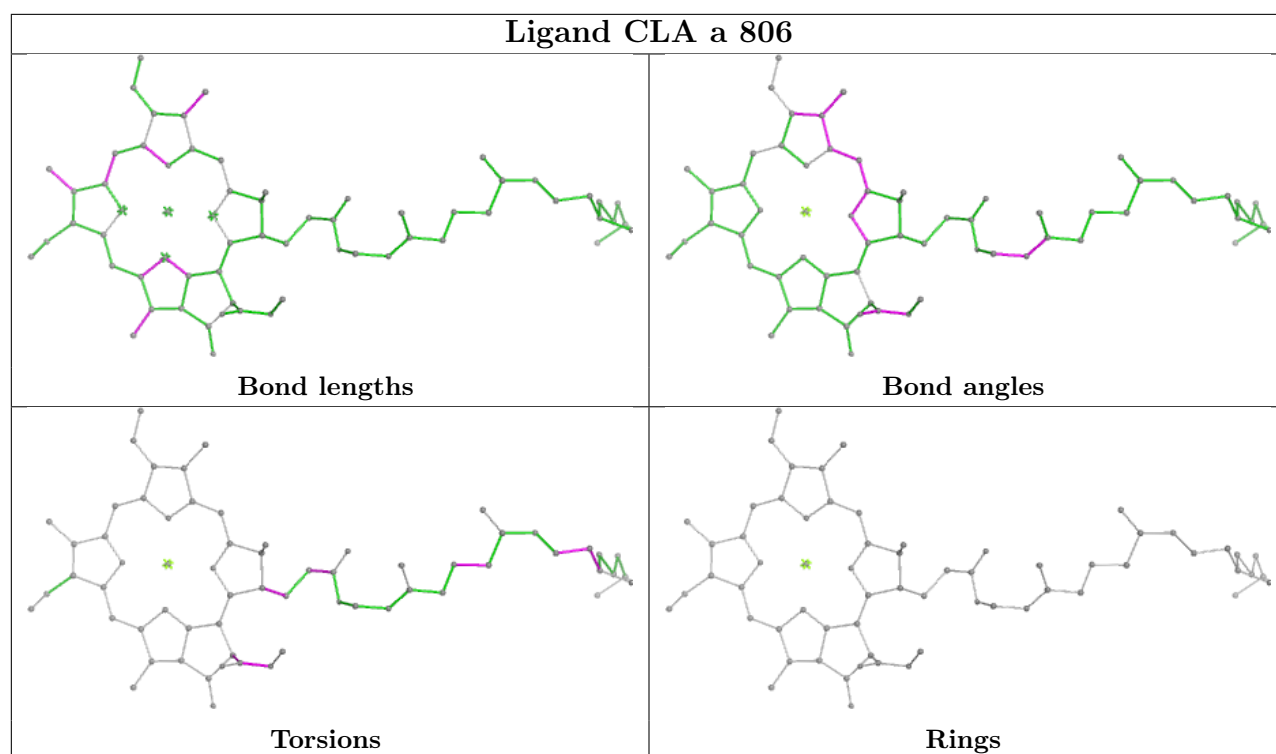


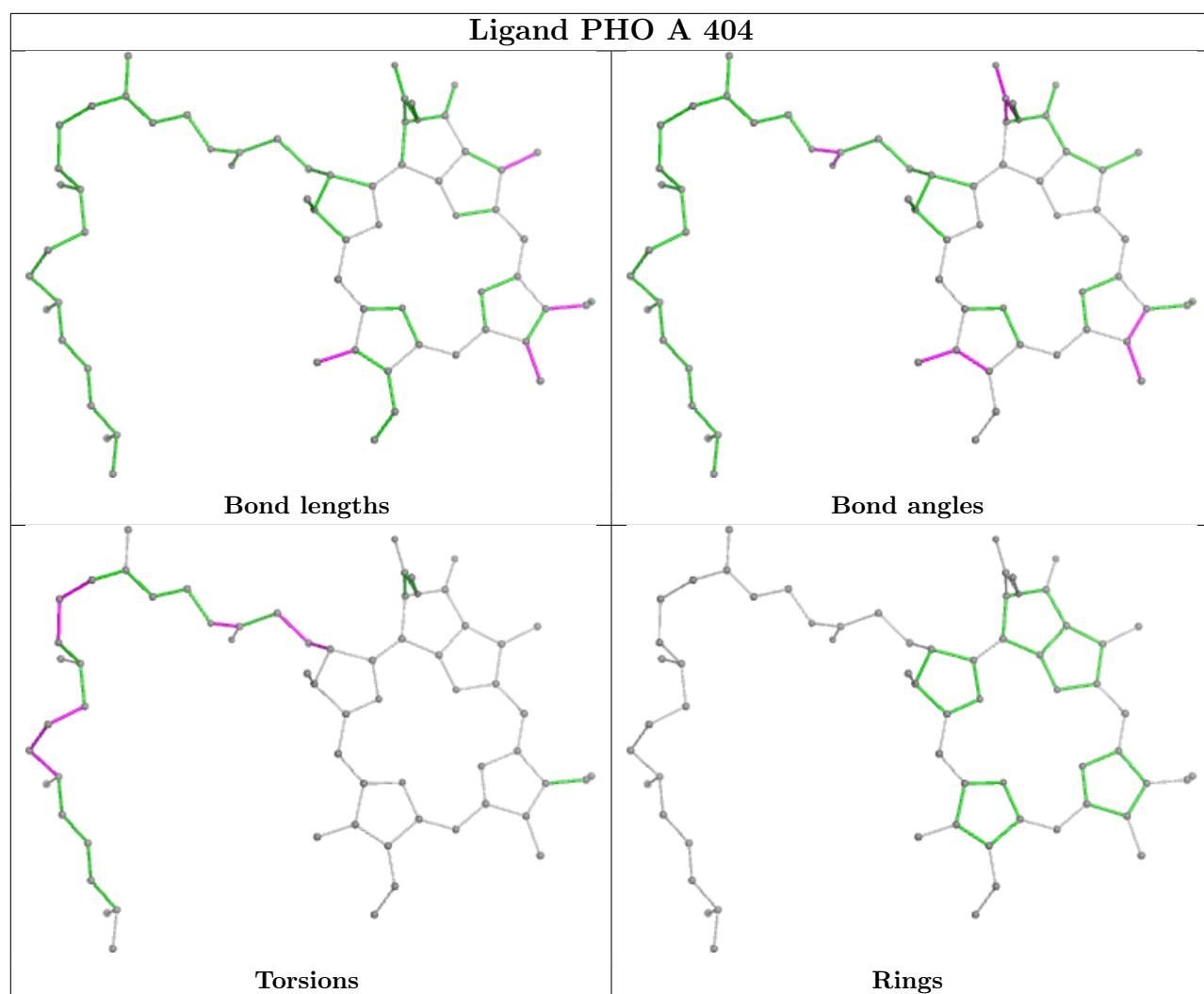
## Ligand EQ3 b 851

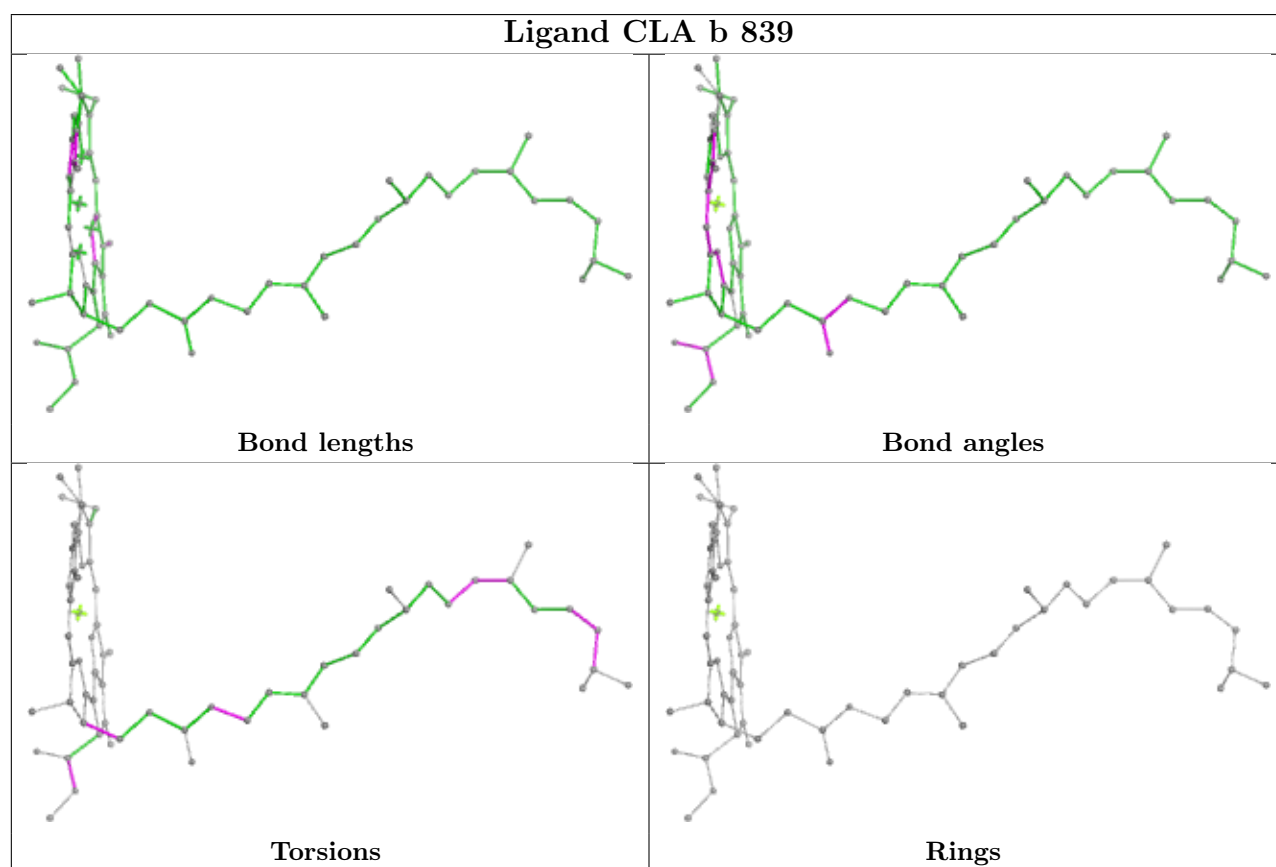
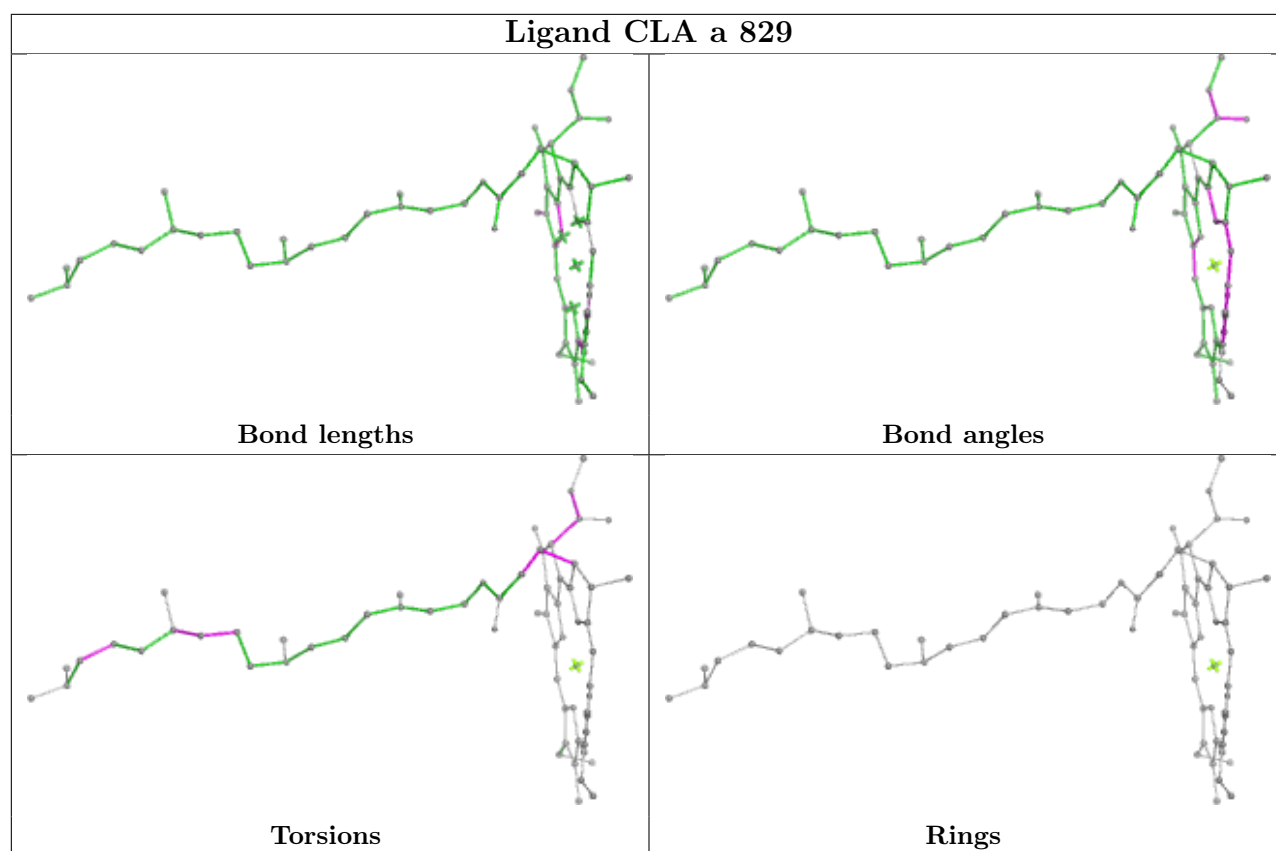




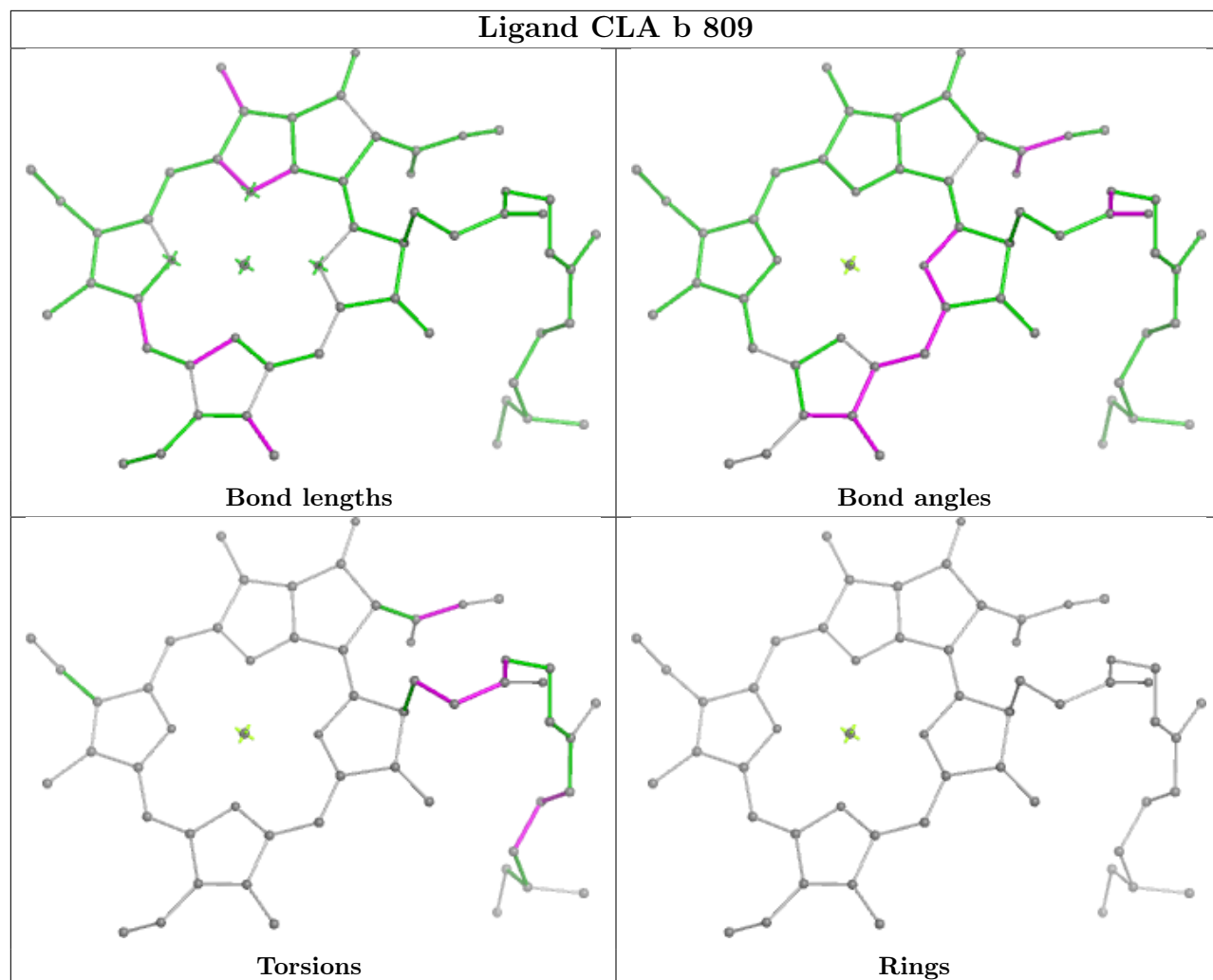




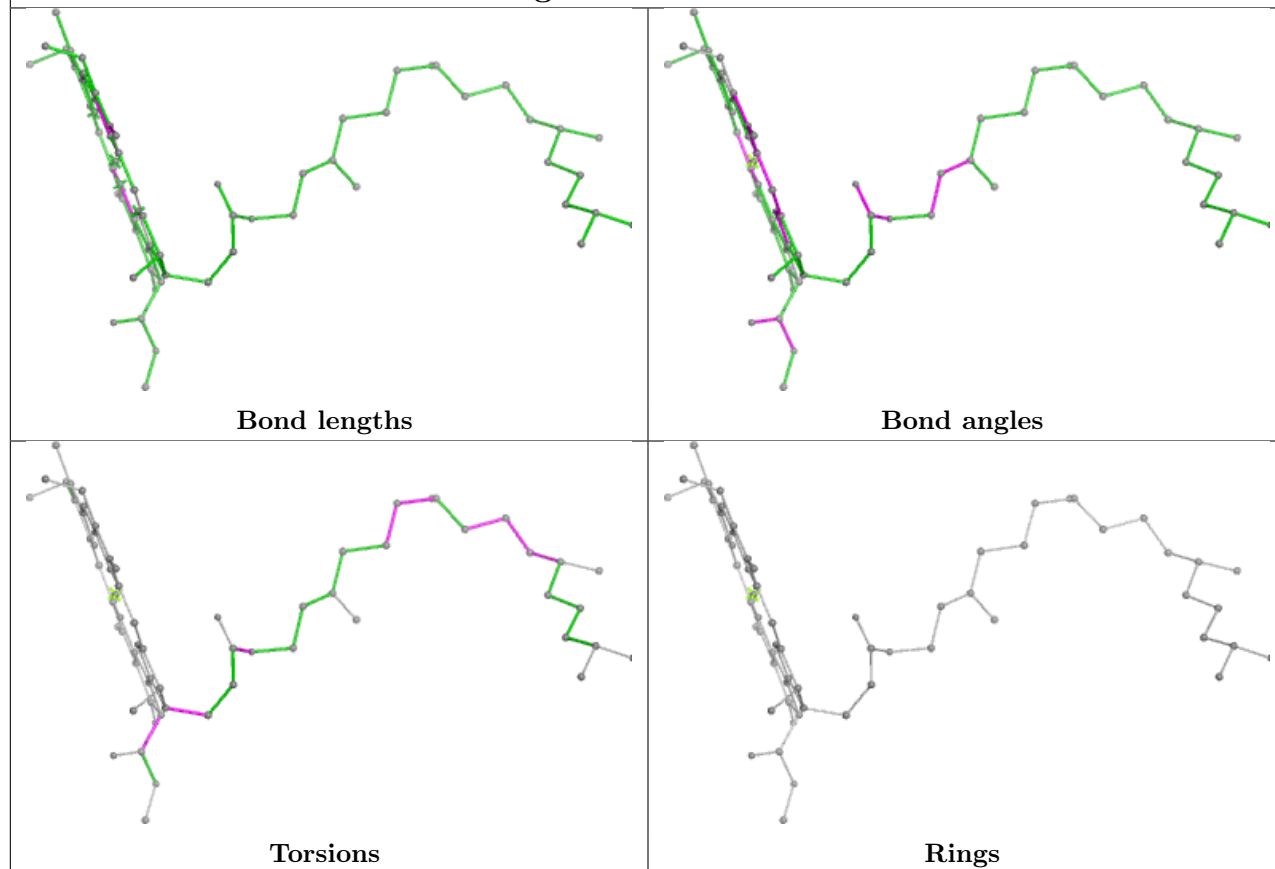




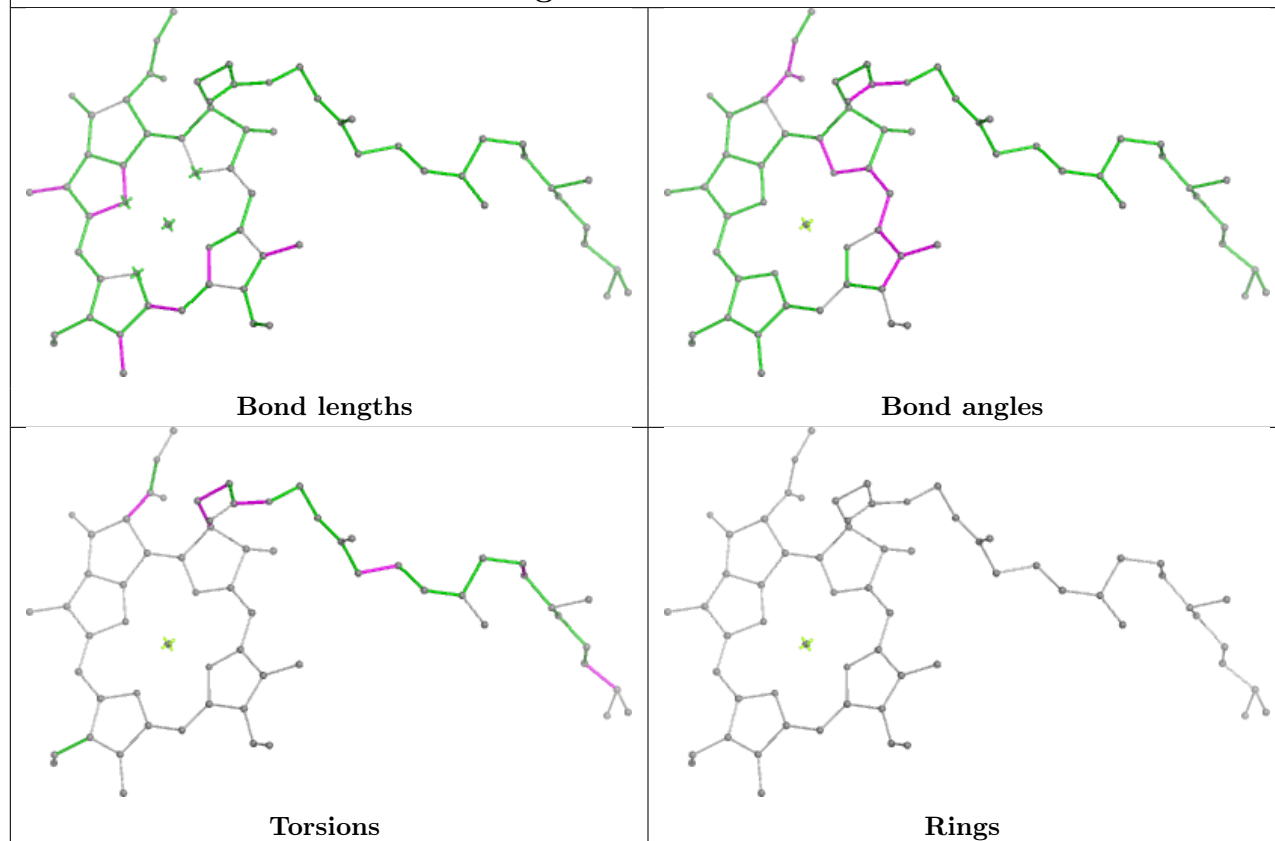
## Ligand CLA b 809



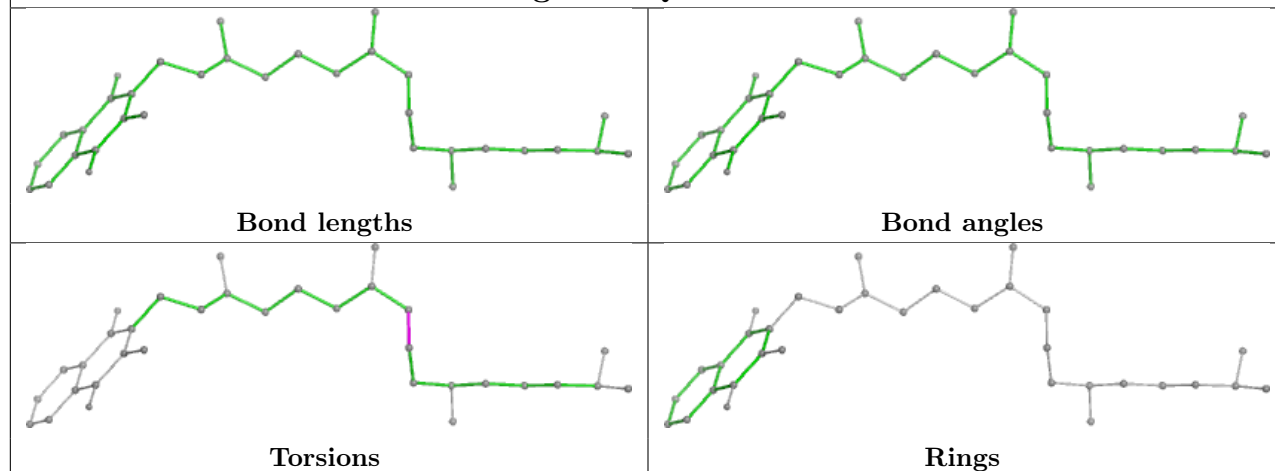
## Ligand CLA b 838



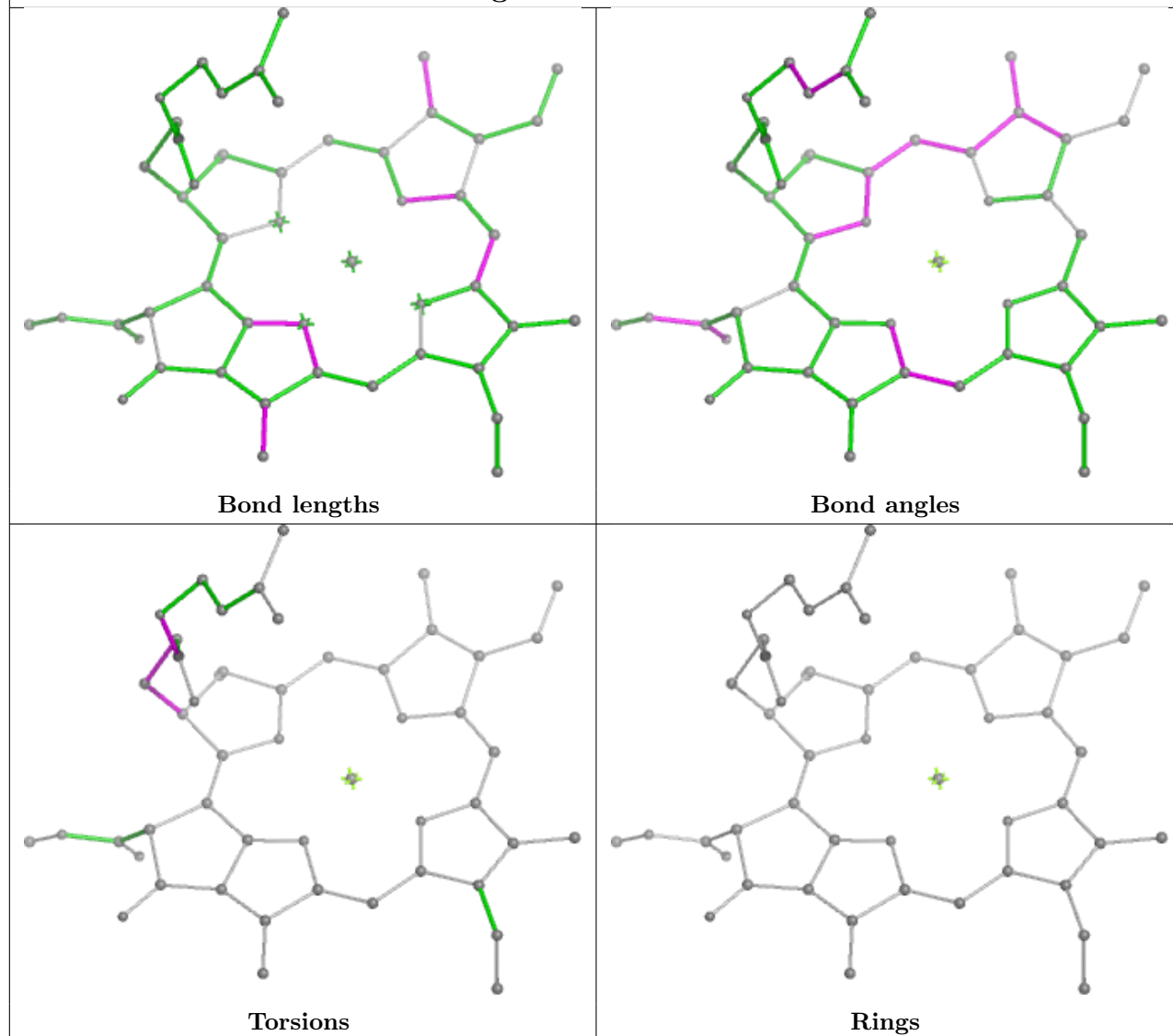
## Ligand CLA a 803

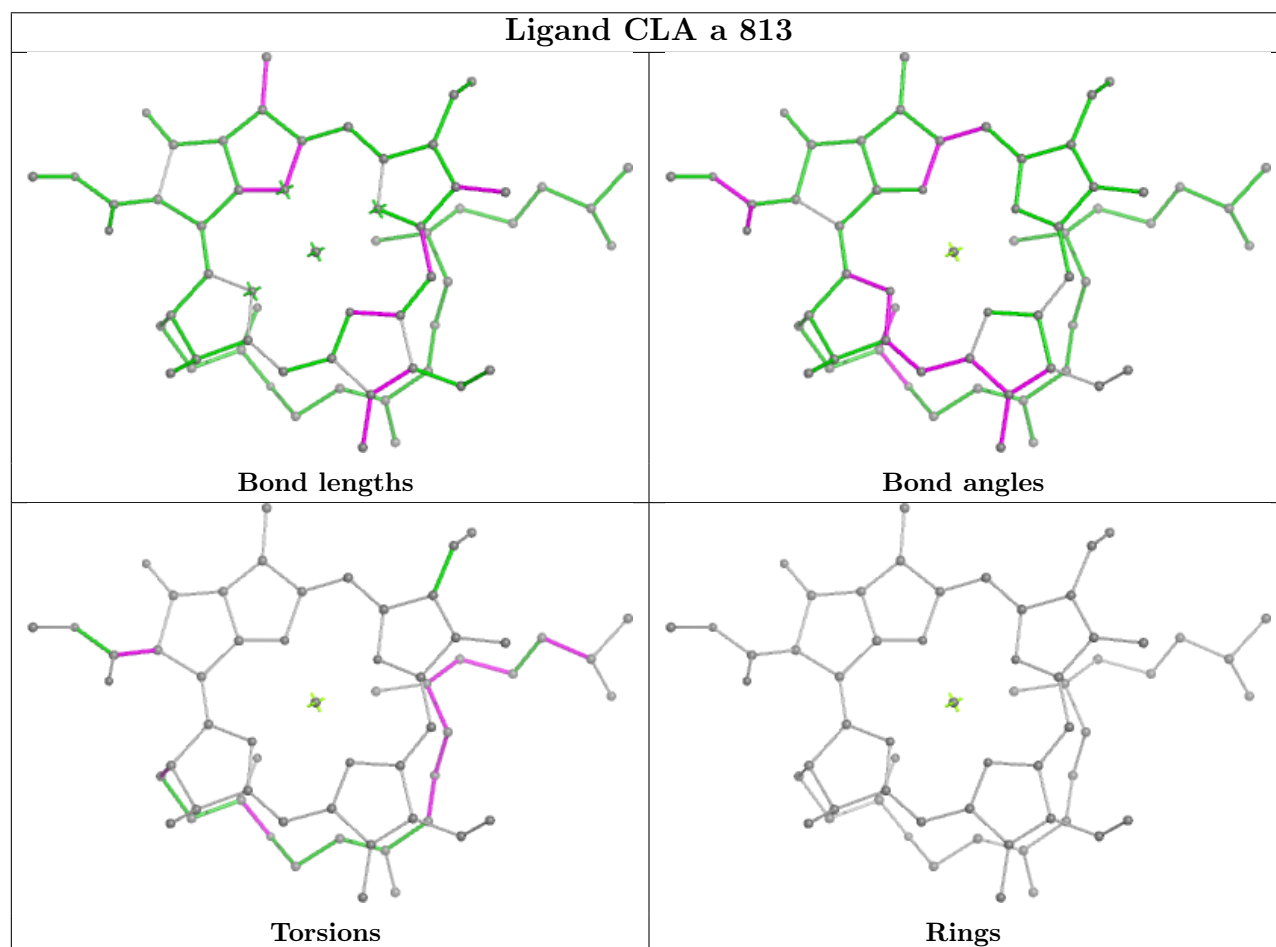
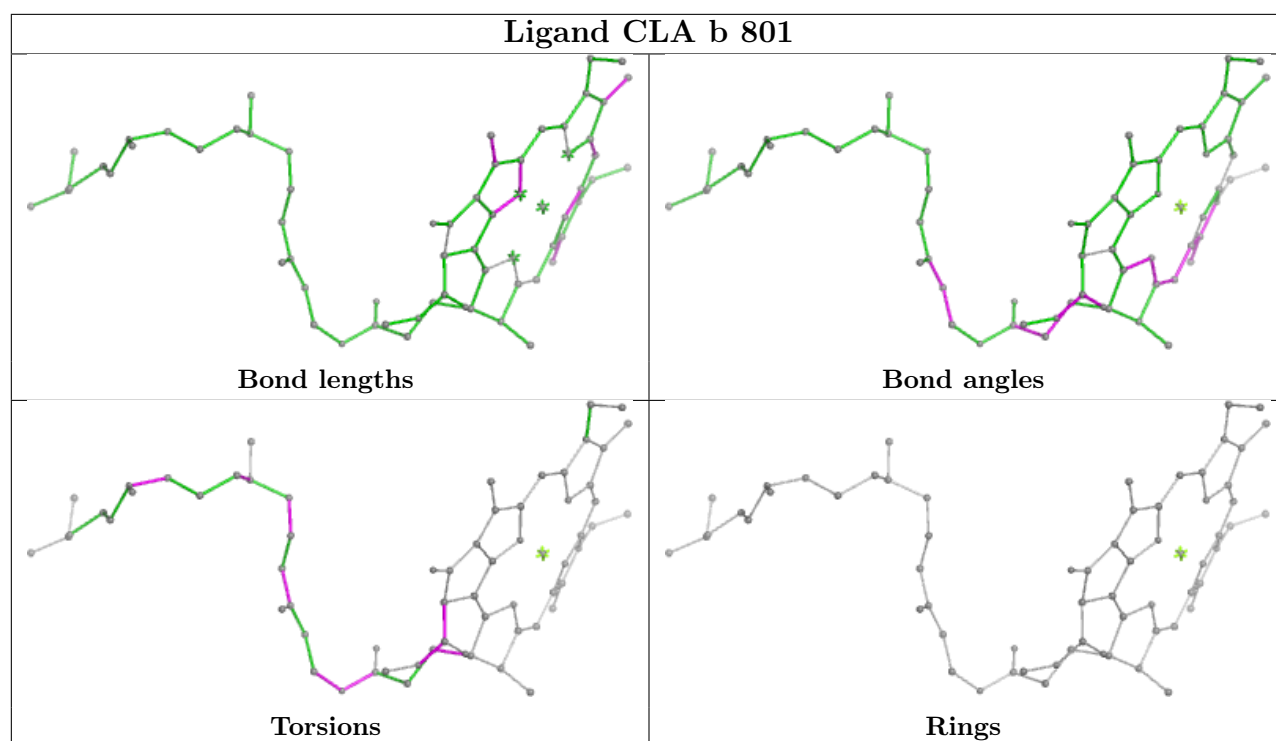


## Ligand PQN a 844

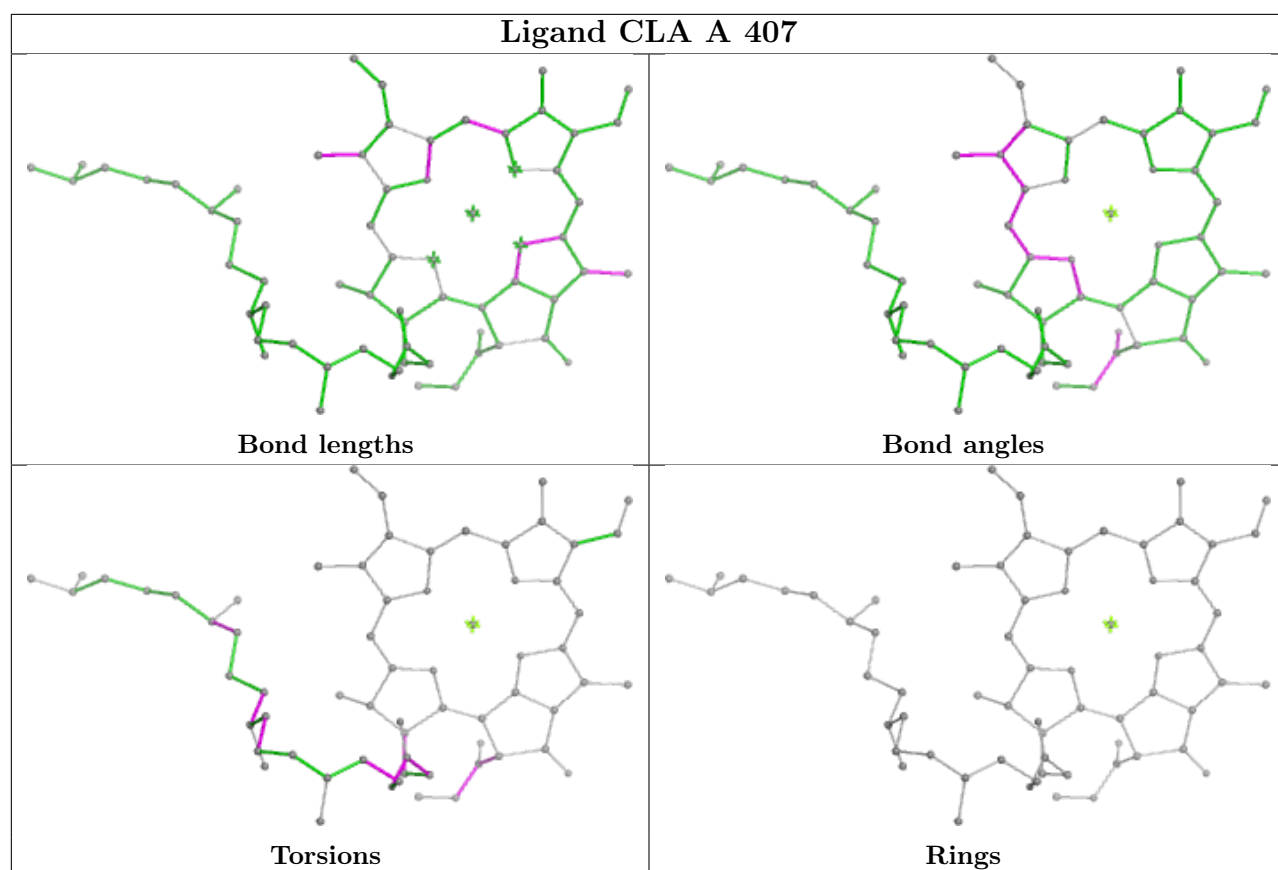


## Ligand CLA b 830

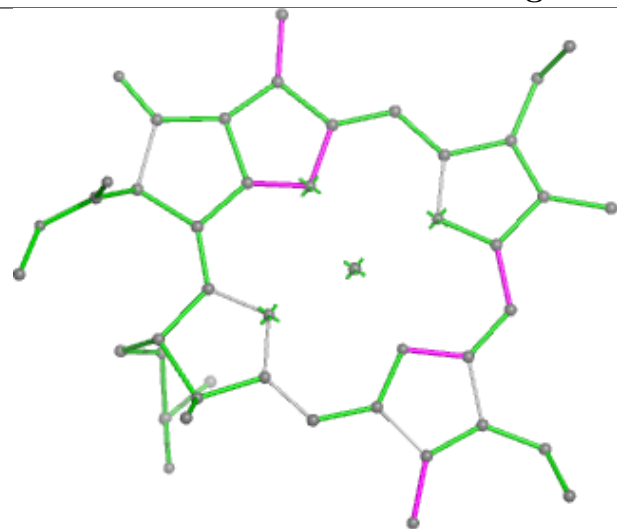




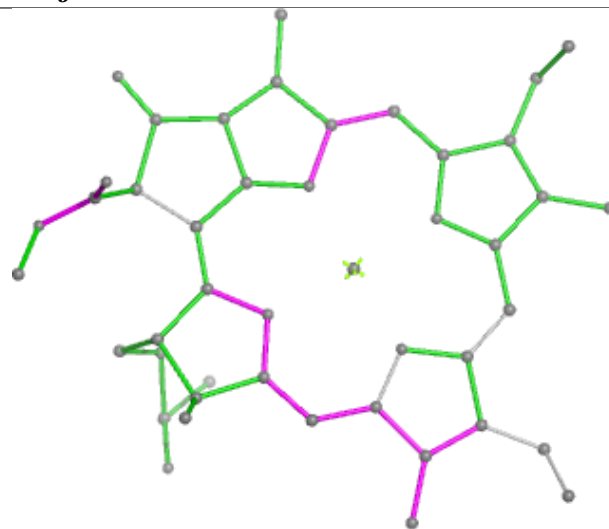




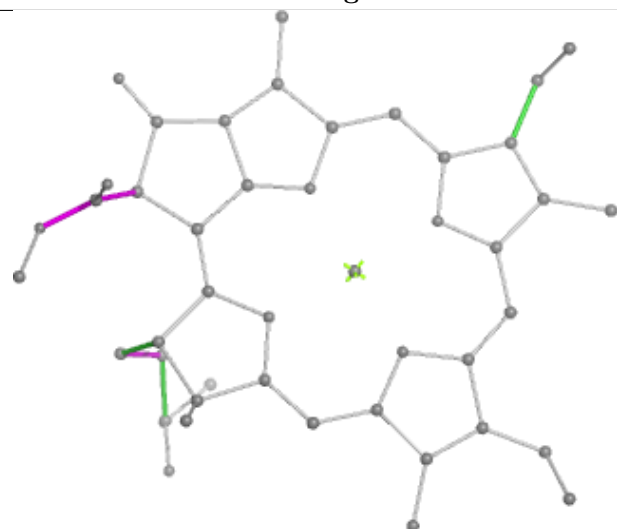
## Ligand CLA j 104



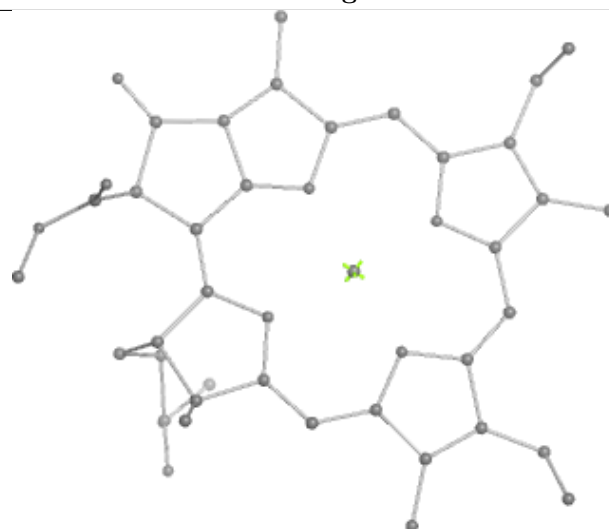
Bond lengths



Bond angles

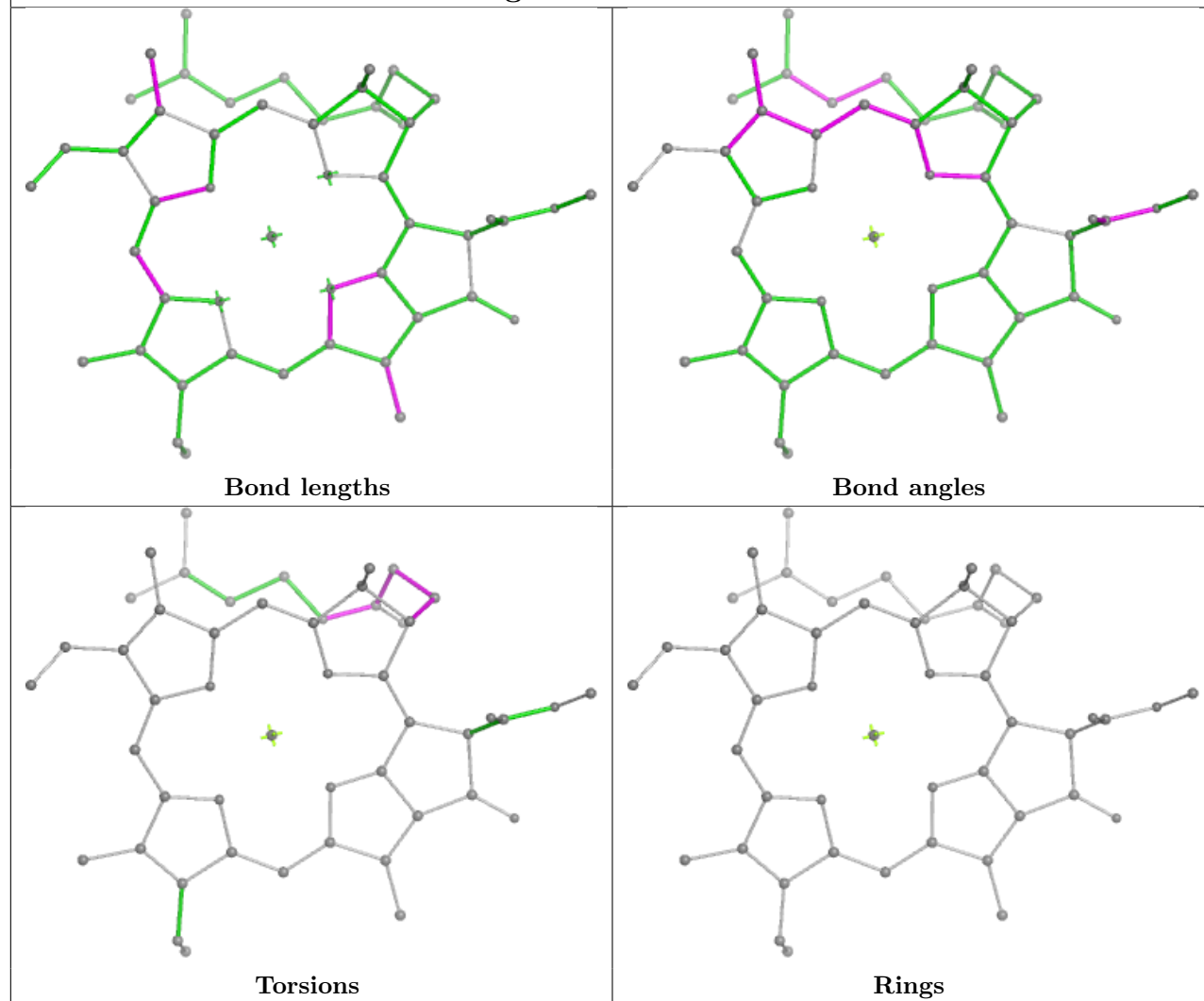


Torsions

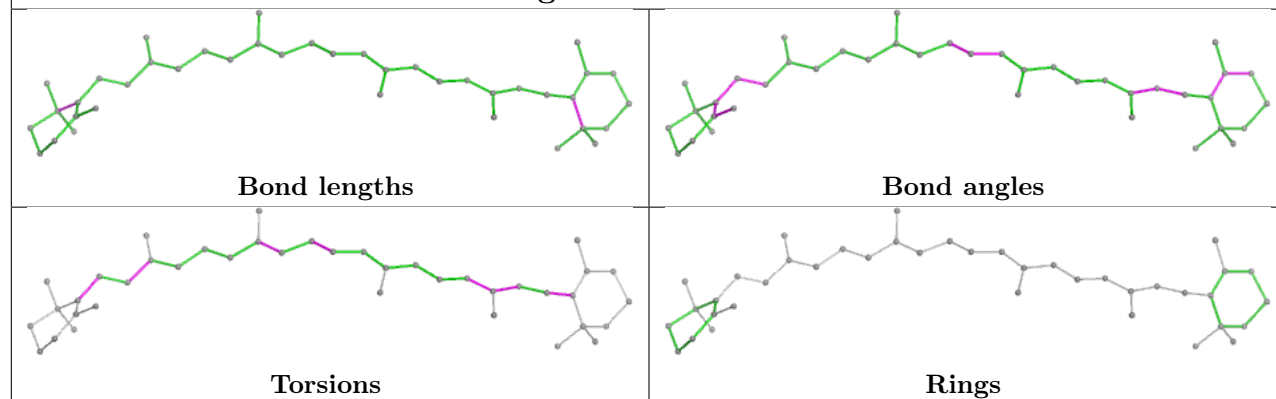


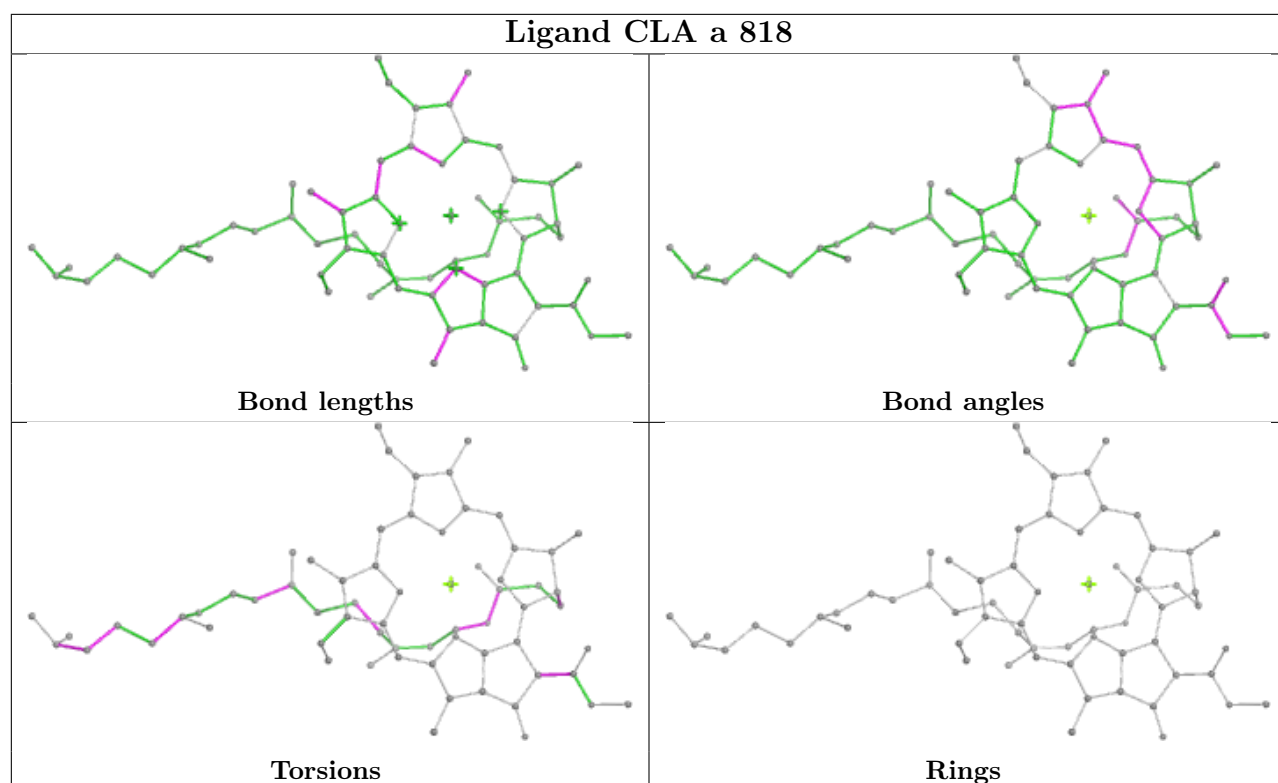
Rings

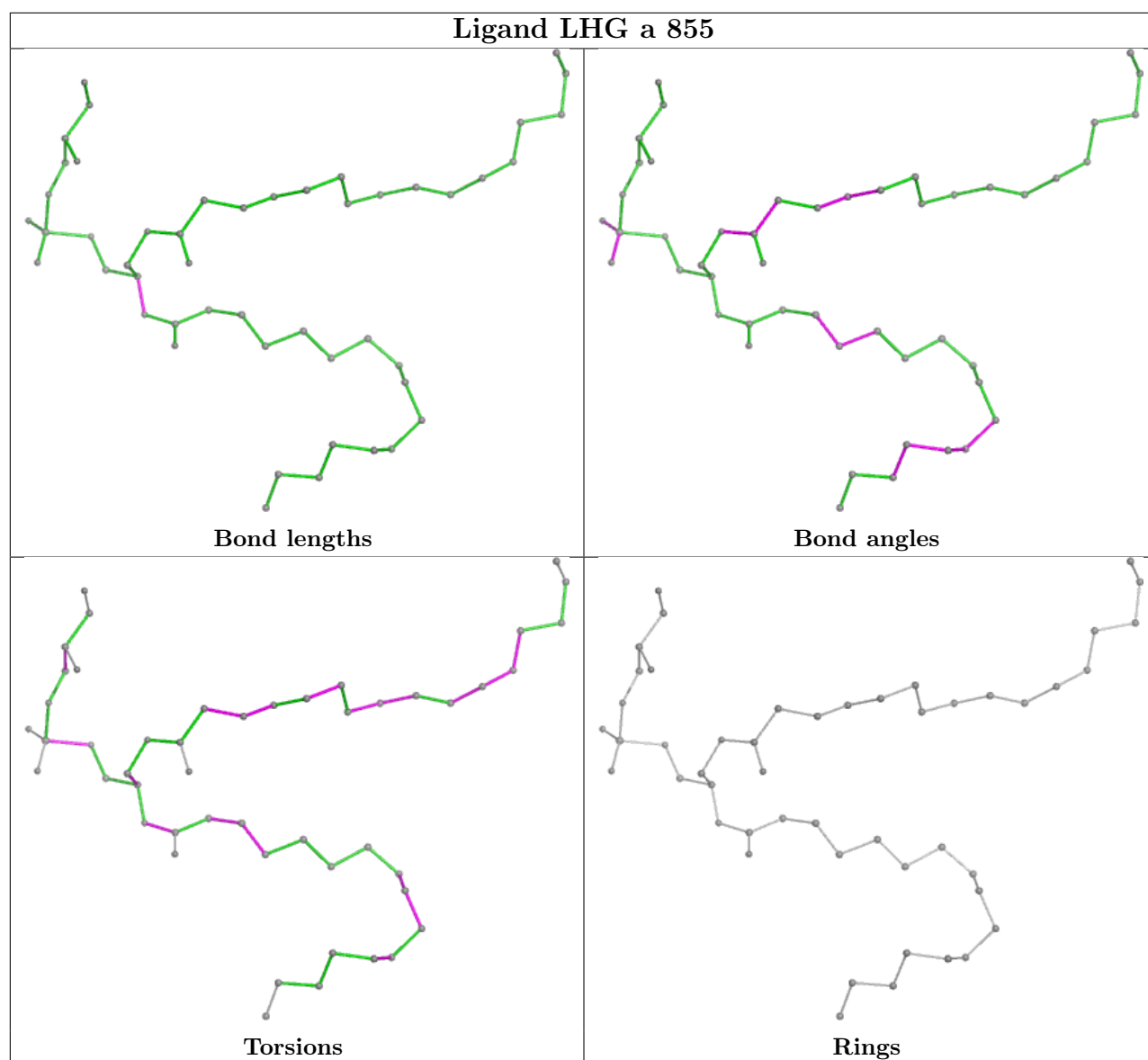
## Ligand CLA b 811

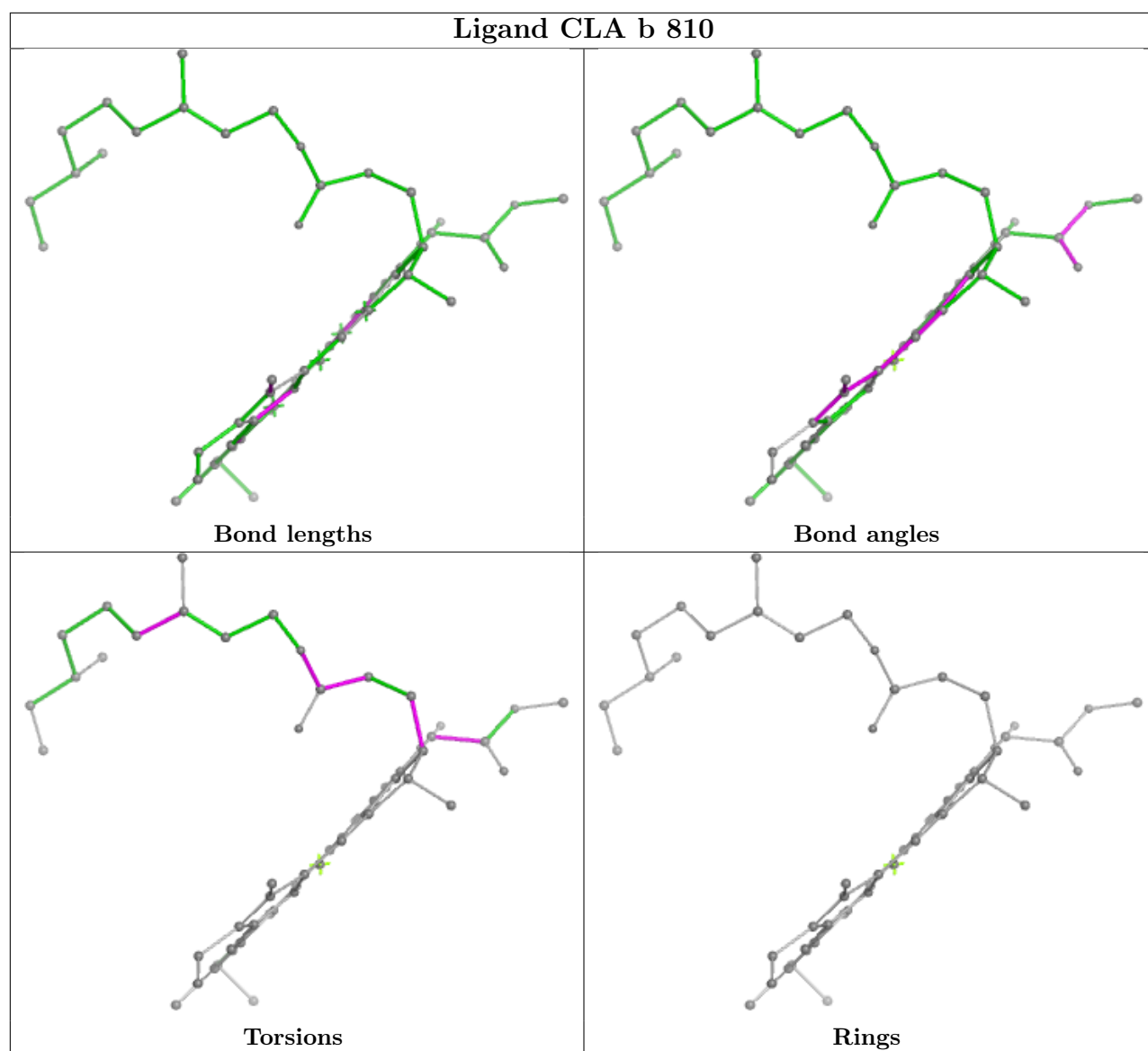


## Ligand BCR f 202

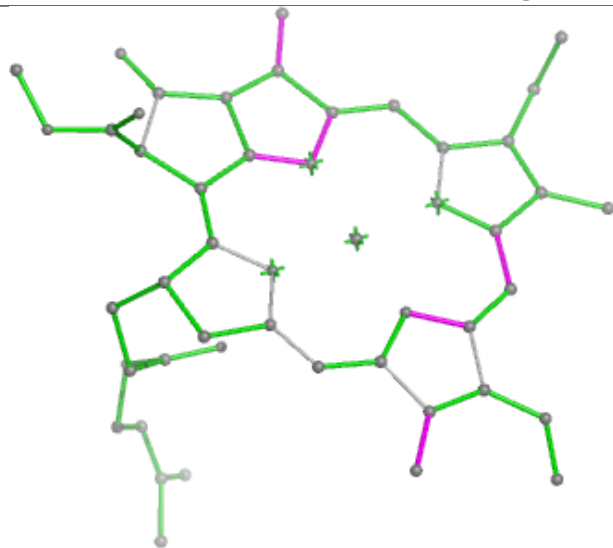




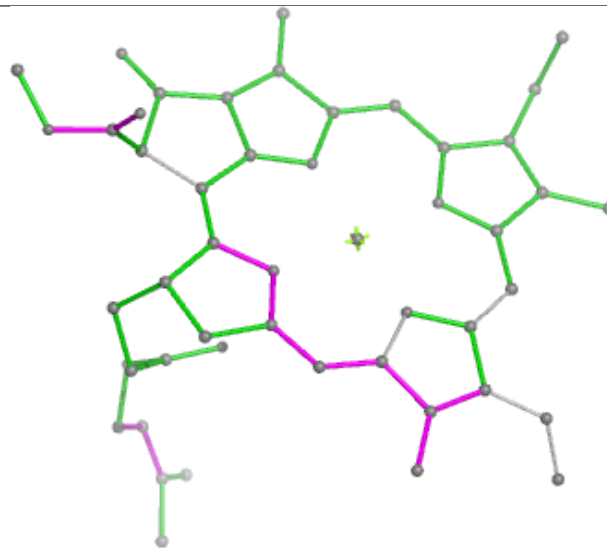




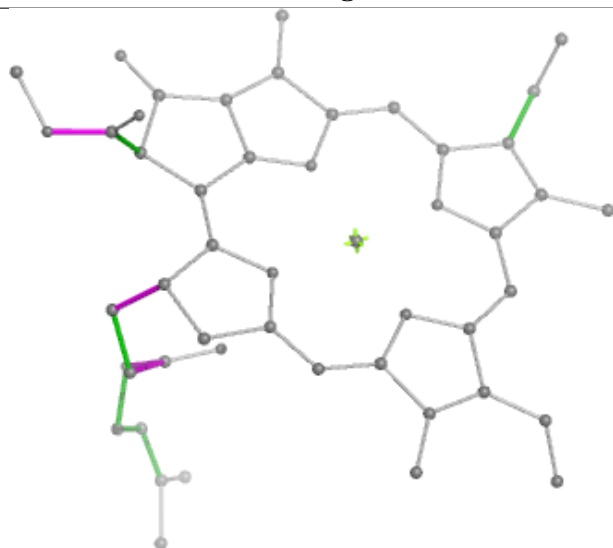
## Ligand CLA b 834



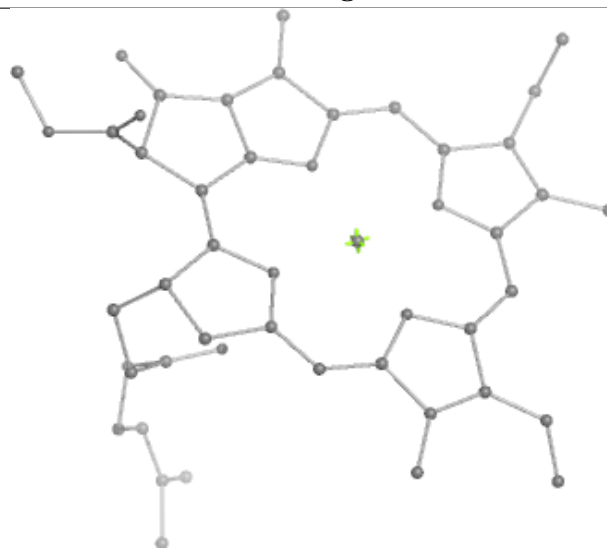
Bond lengths



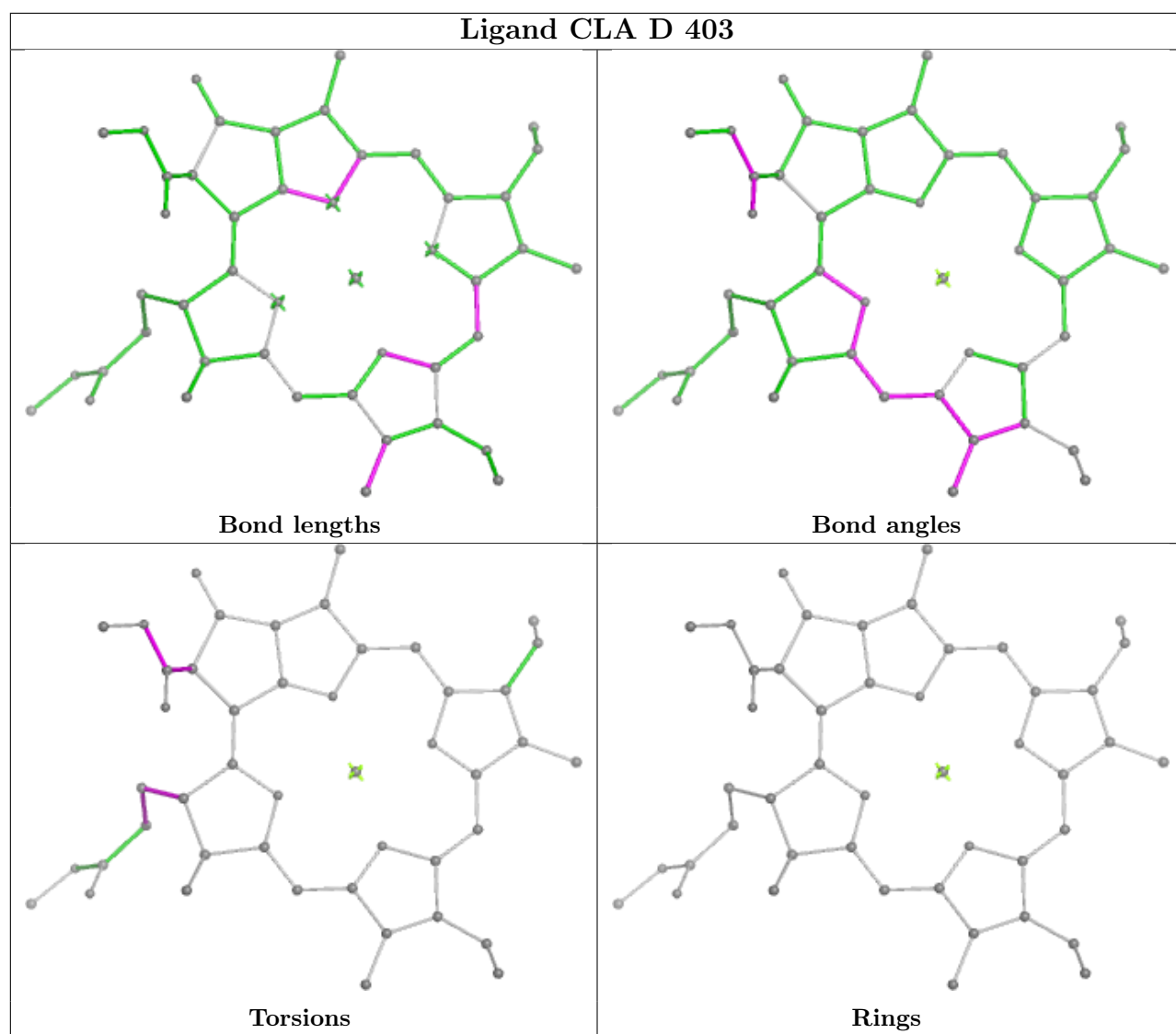
Bond angles



Torsions

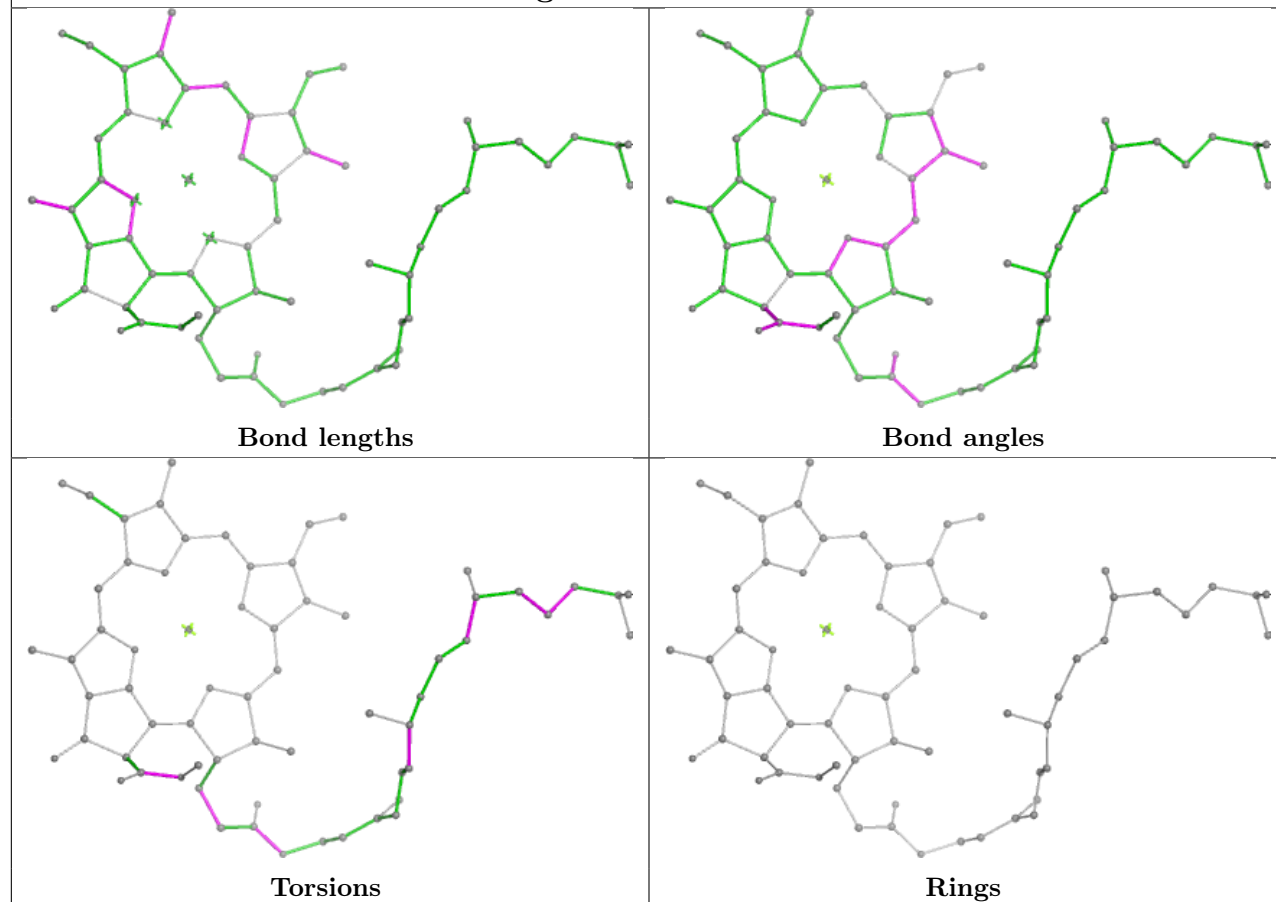


Rings

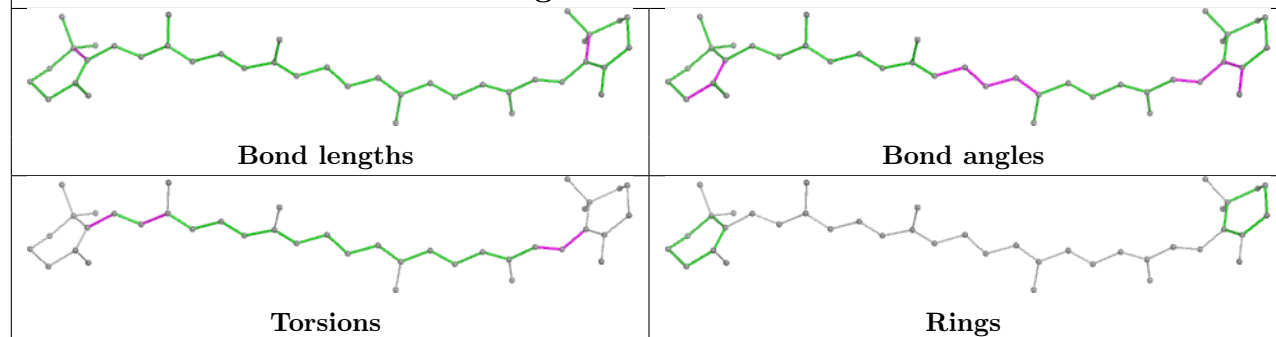


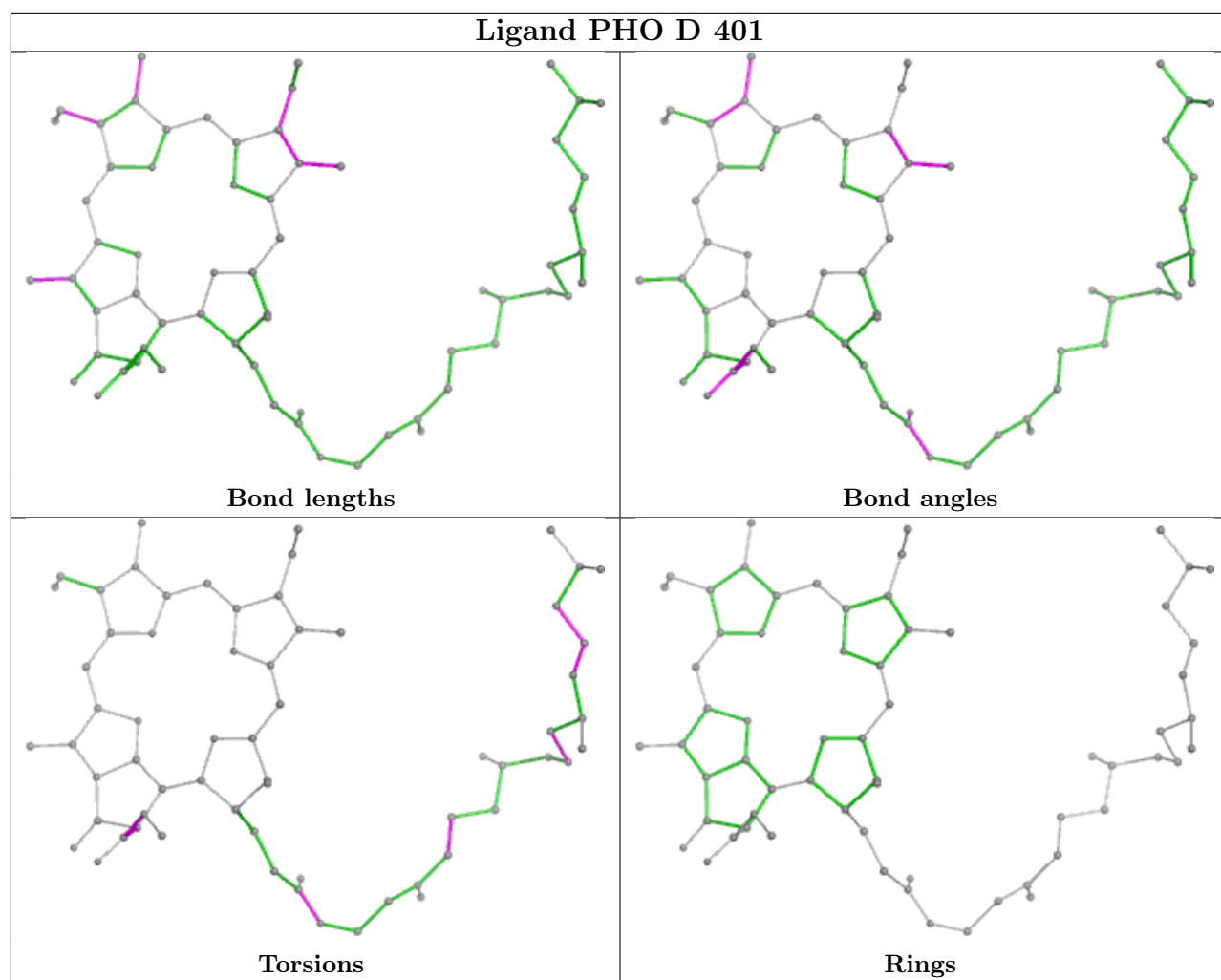


## Ligand CLA a 814

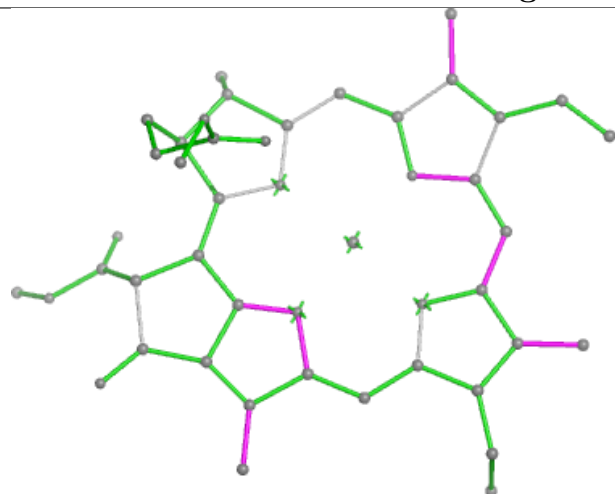


## Ligand BCR a 848

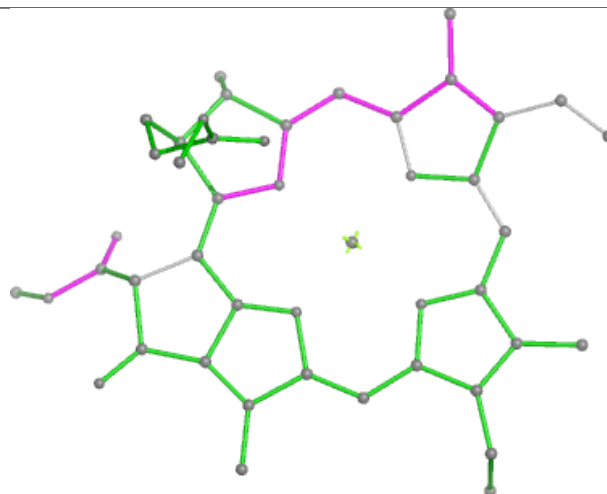




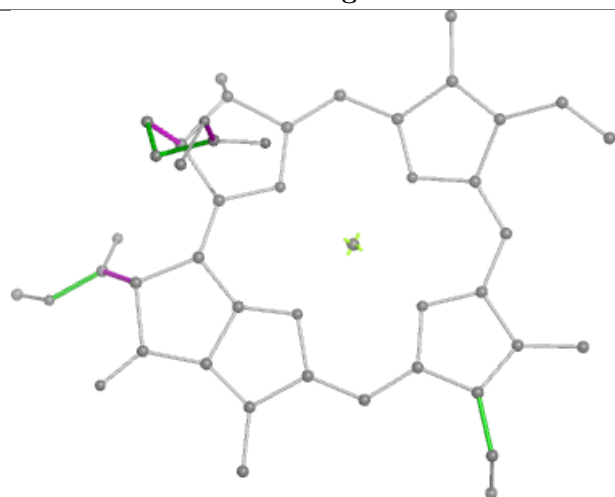
## Ligand CLA b 821



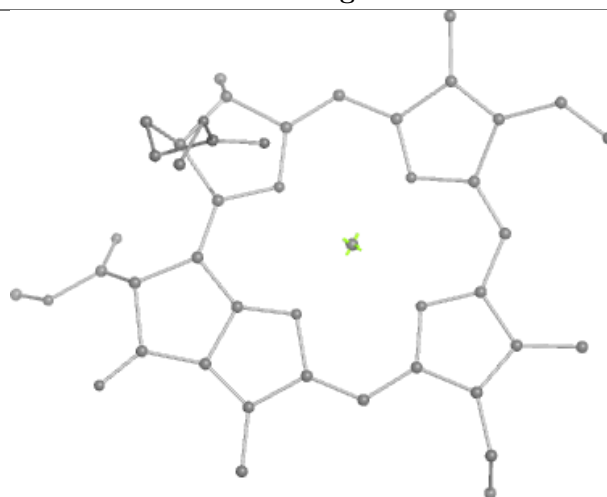
Bond lengths



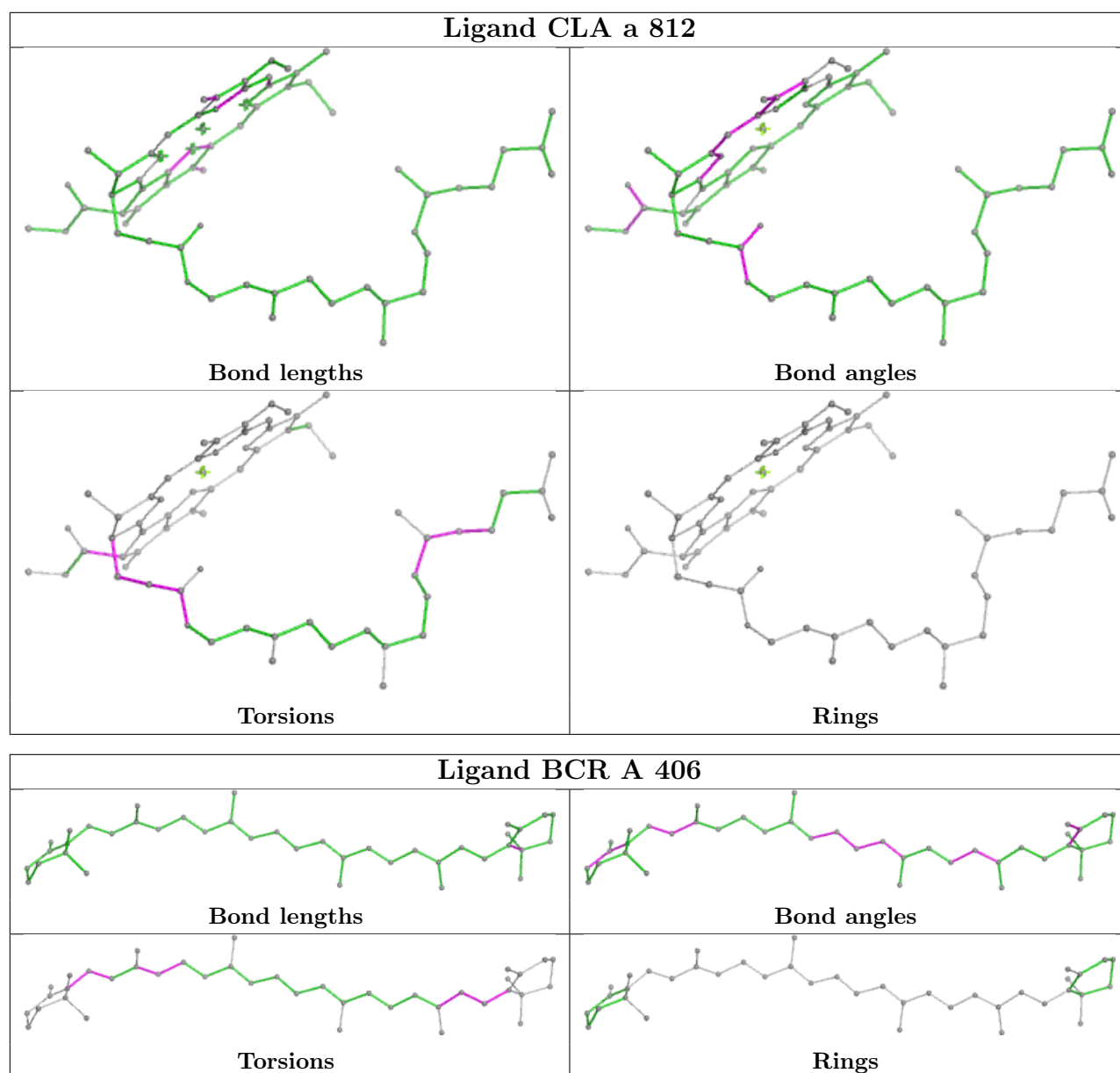
Bond angles



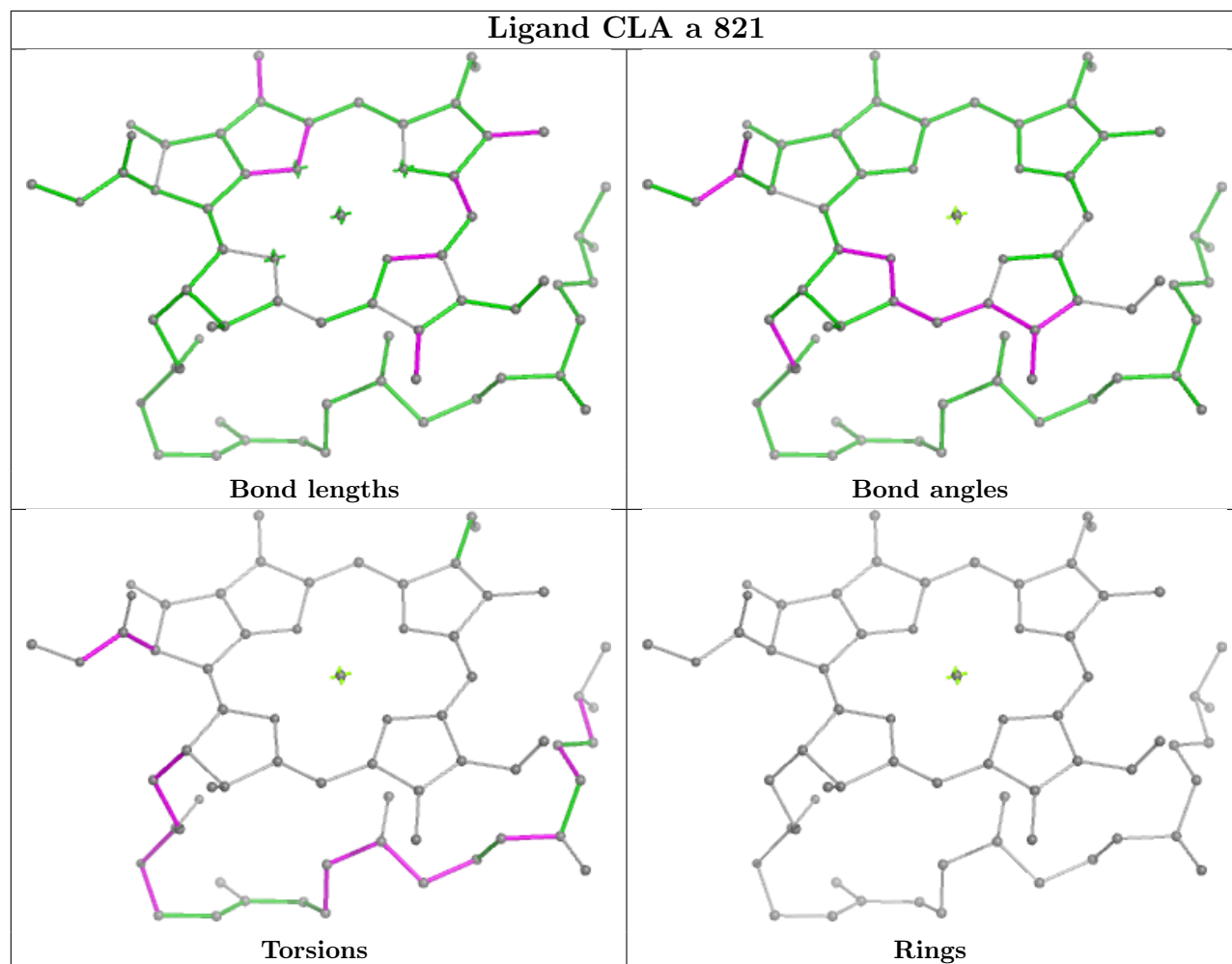
Torsions



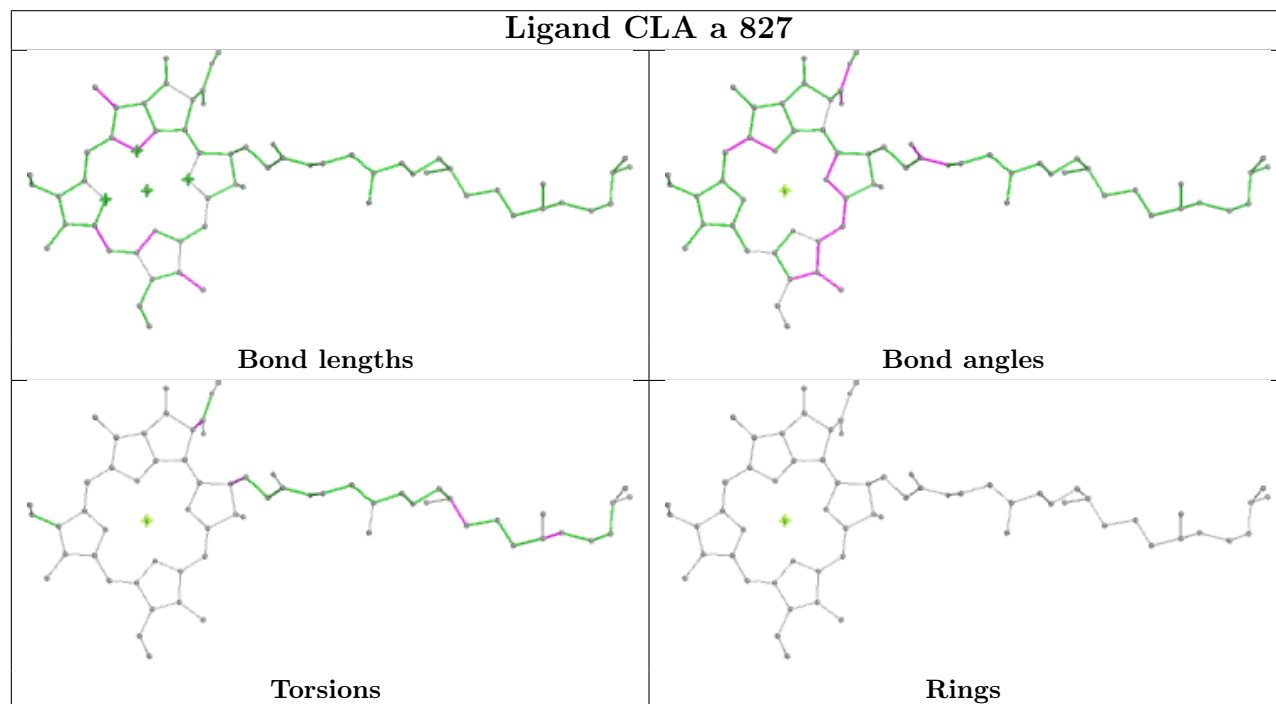
Rings



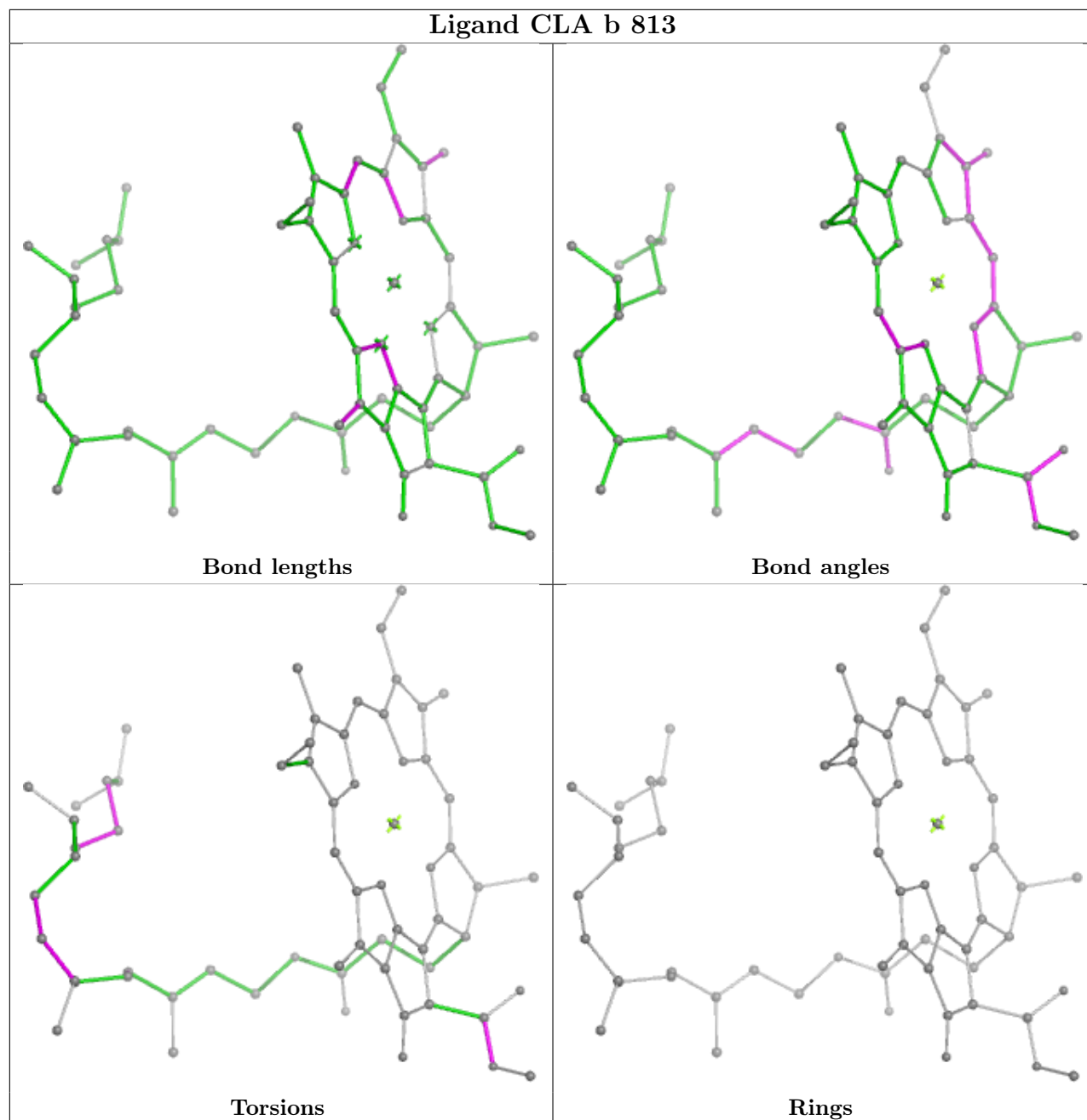
## Ligand CLA a 821



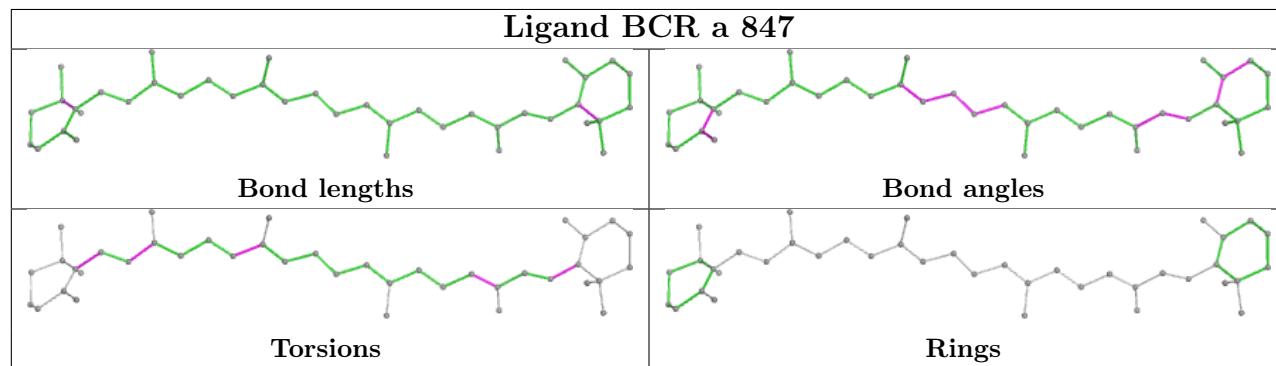
## Ligand CLA a 827



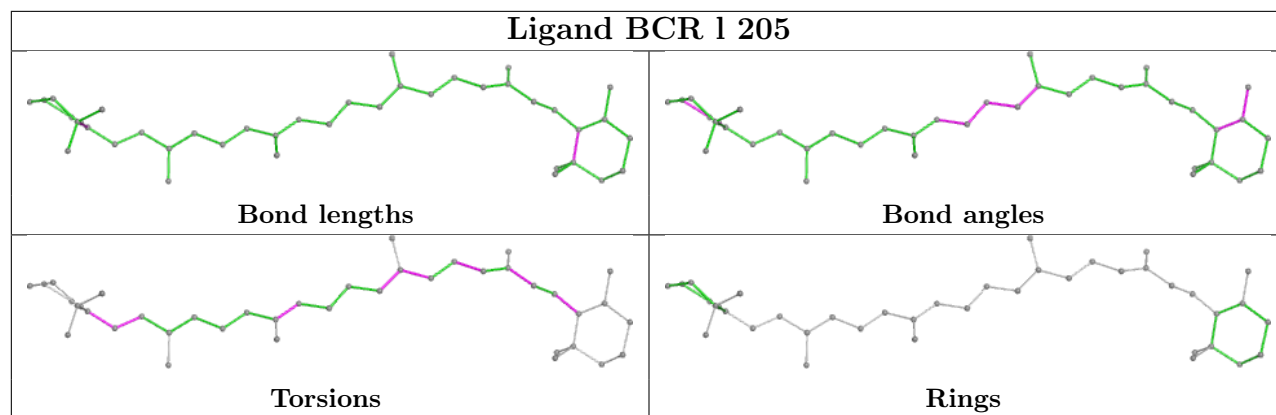
## Ligand CLA b 813



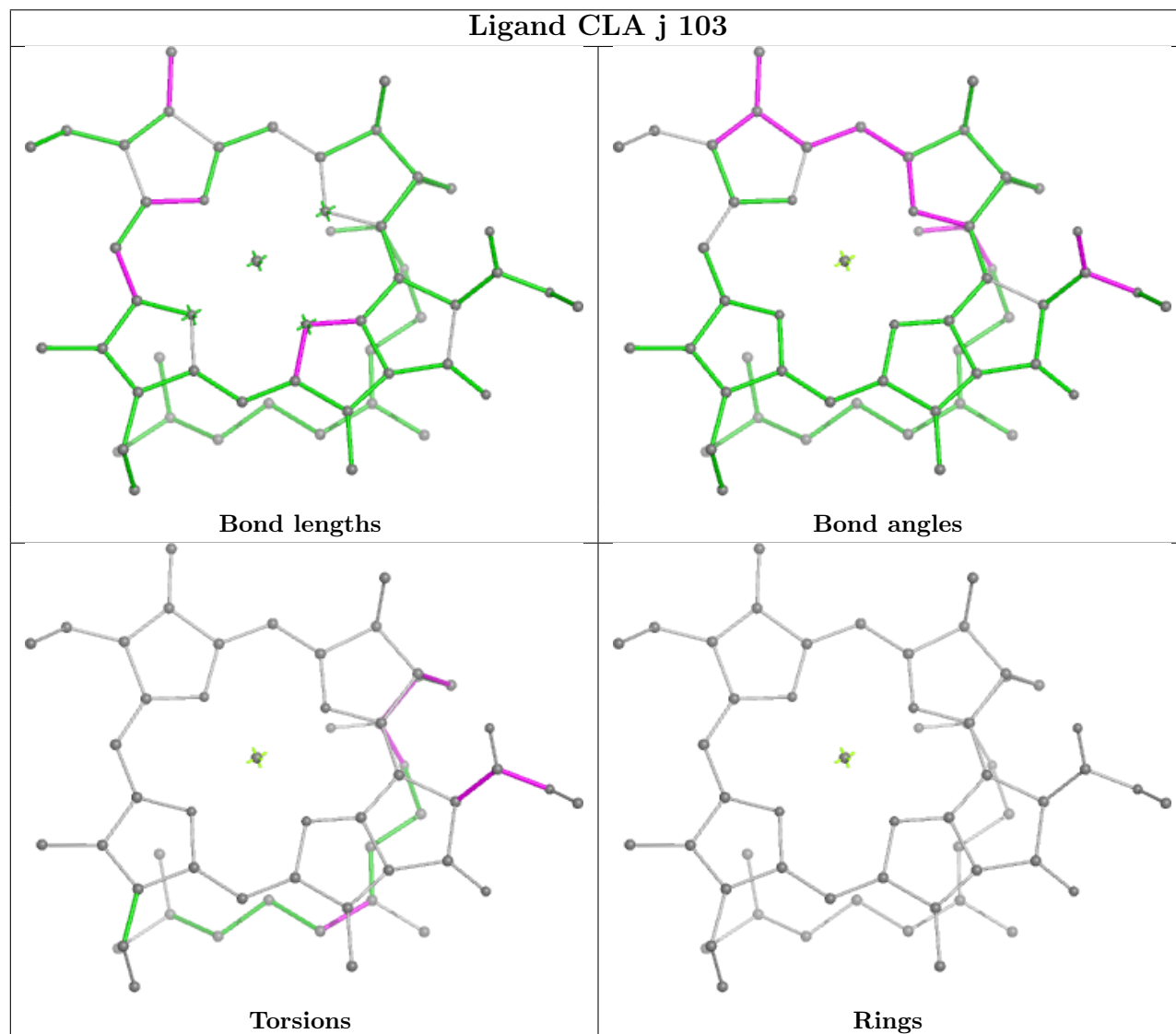
## Ligand BCR a 847



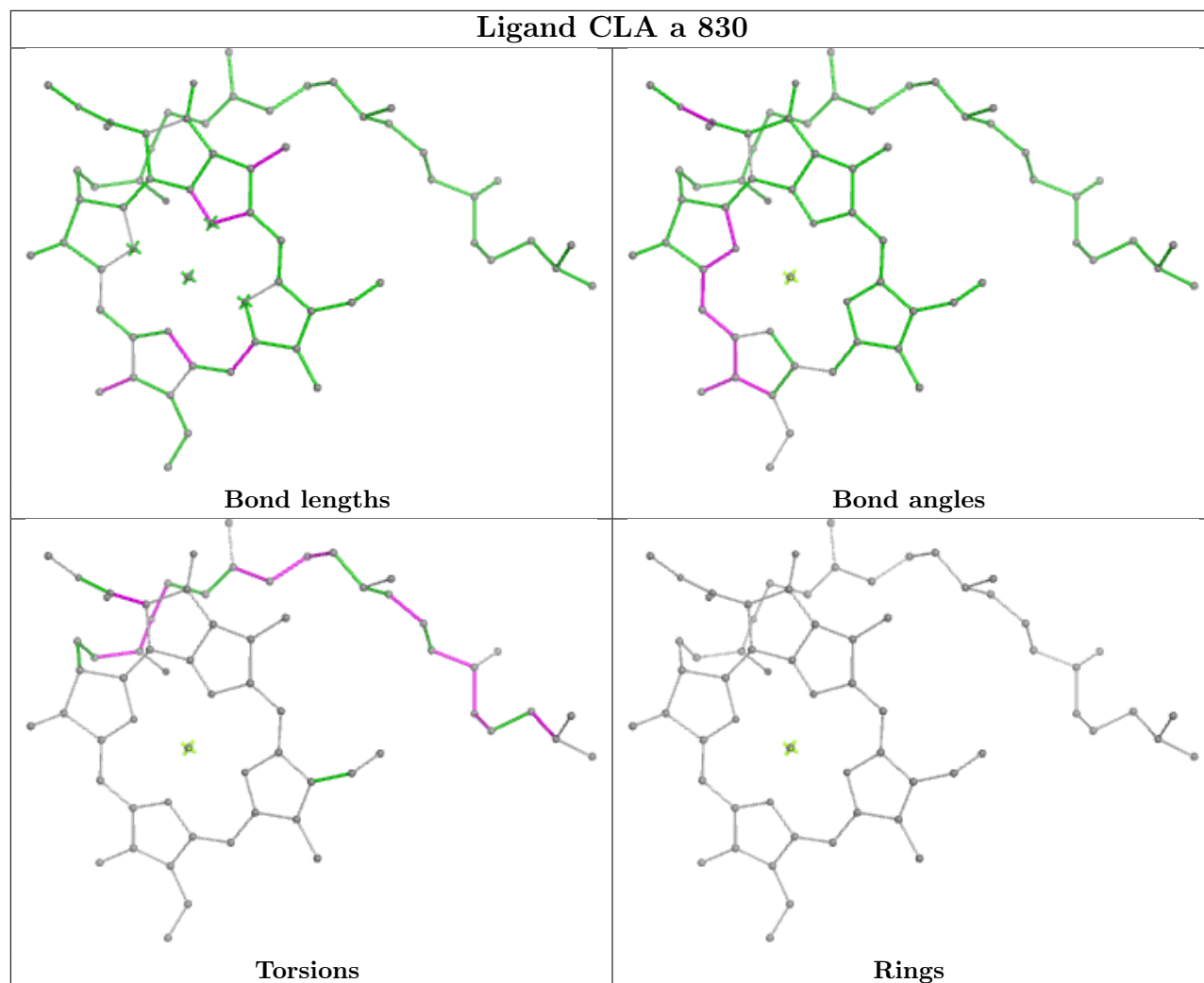
## Ligand BCR 1 205



## Ligand CLA j 103

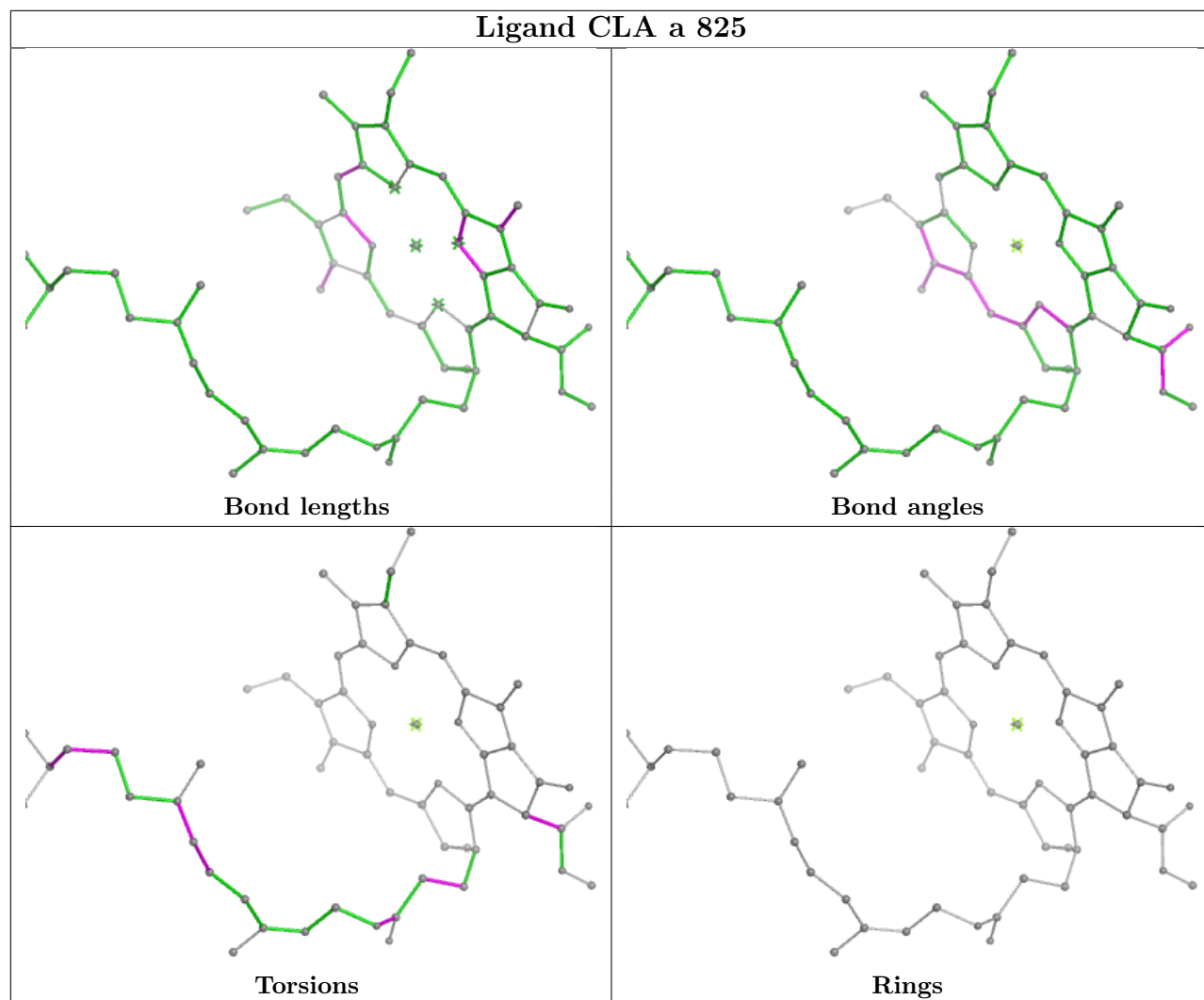


## Ligand CLA a 830

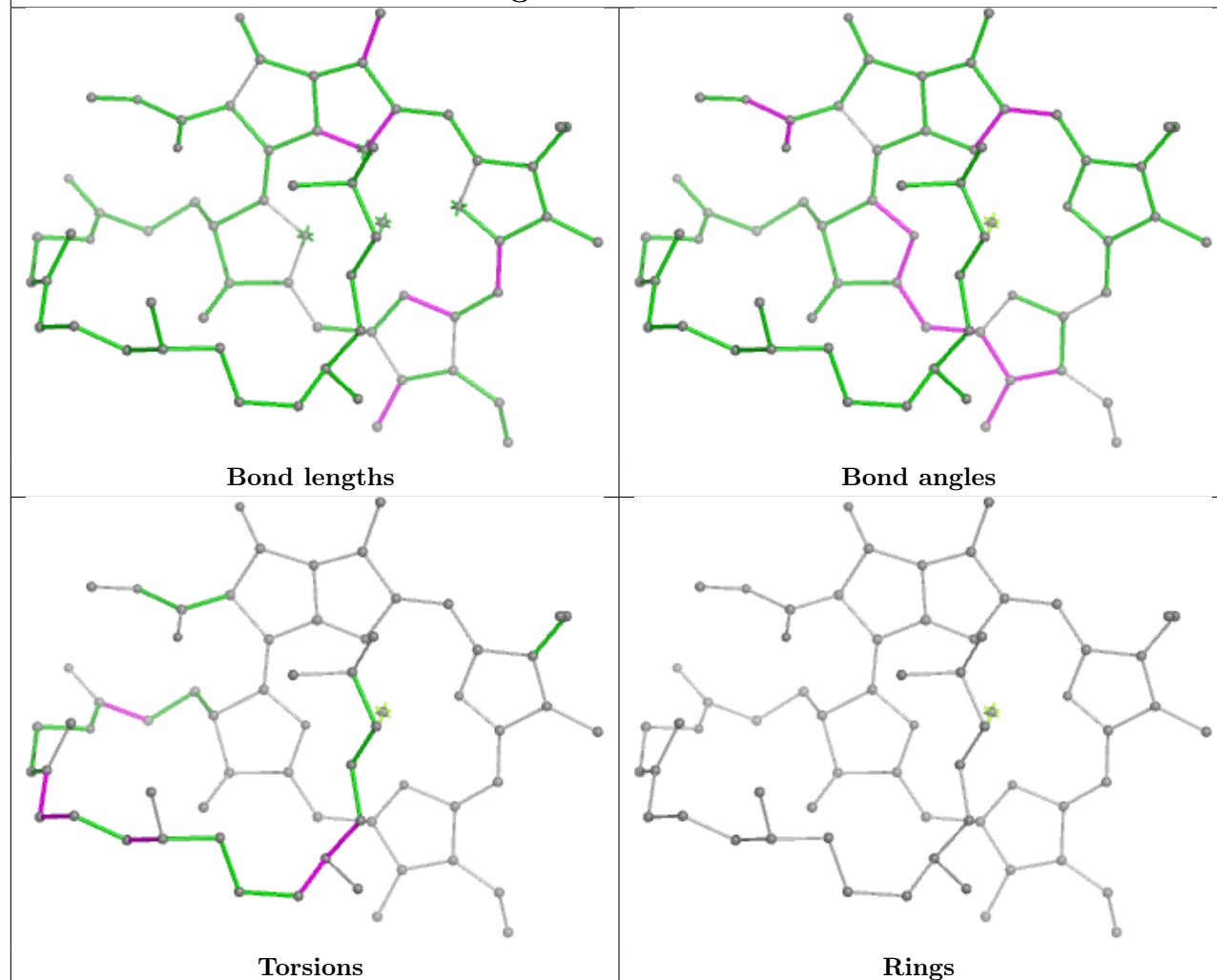




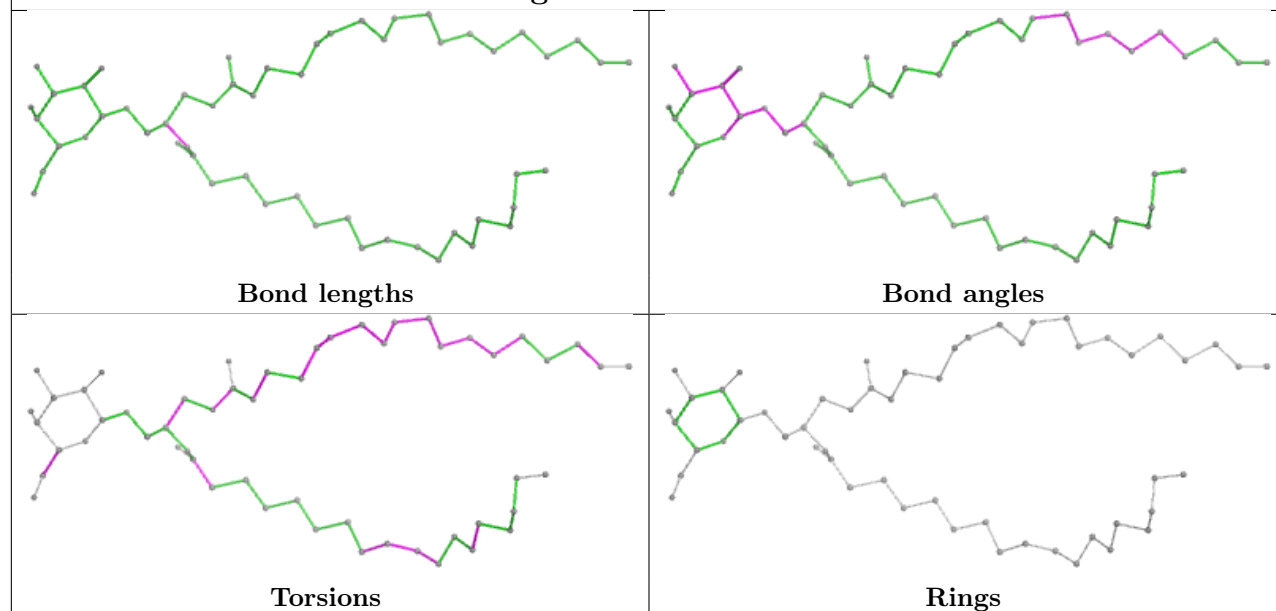
## Ligand CLA a 825



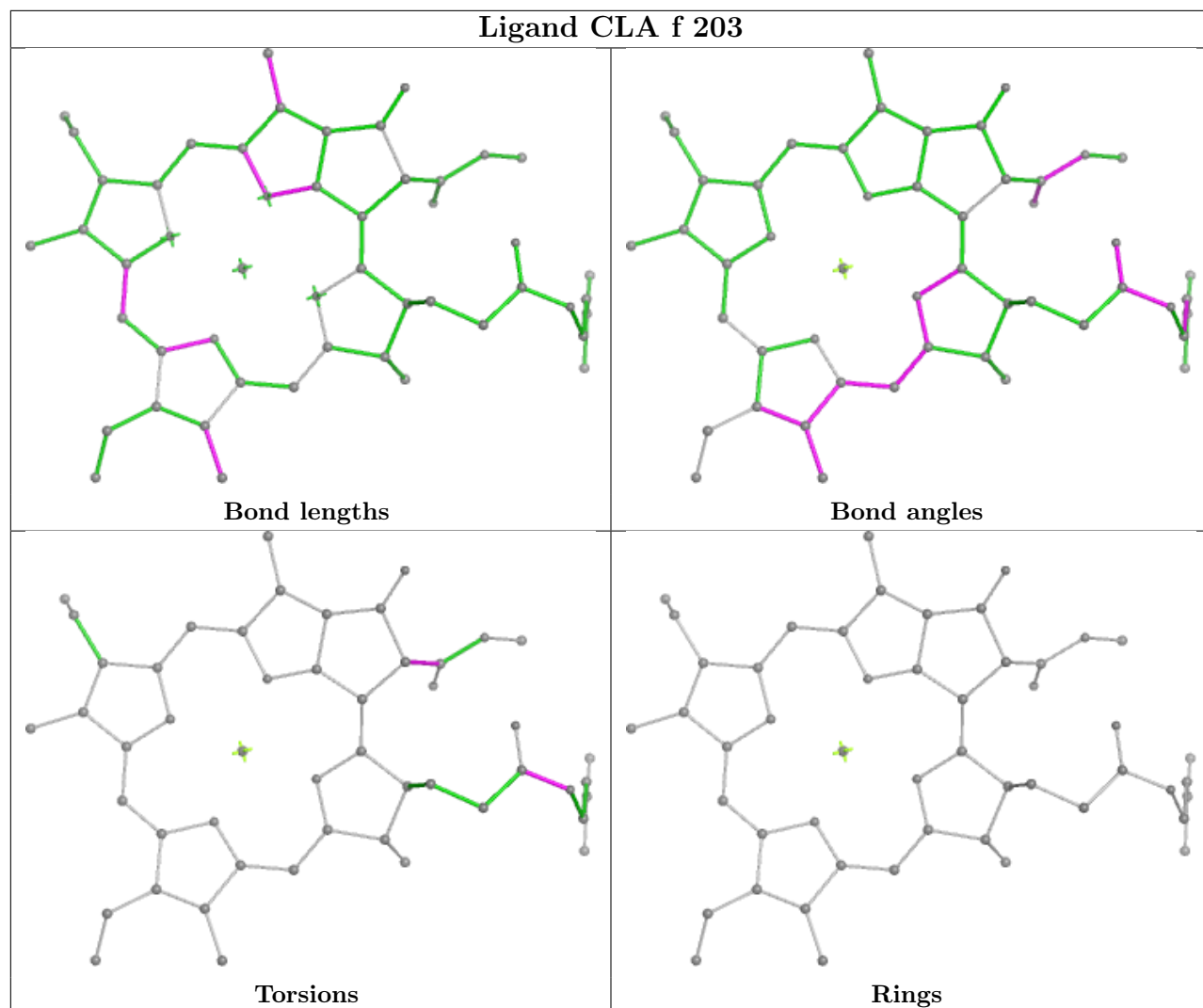
## Ligand CLA a 807

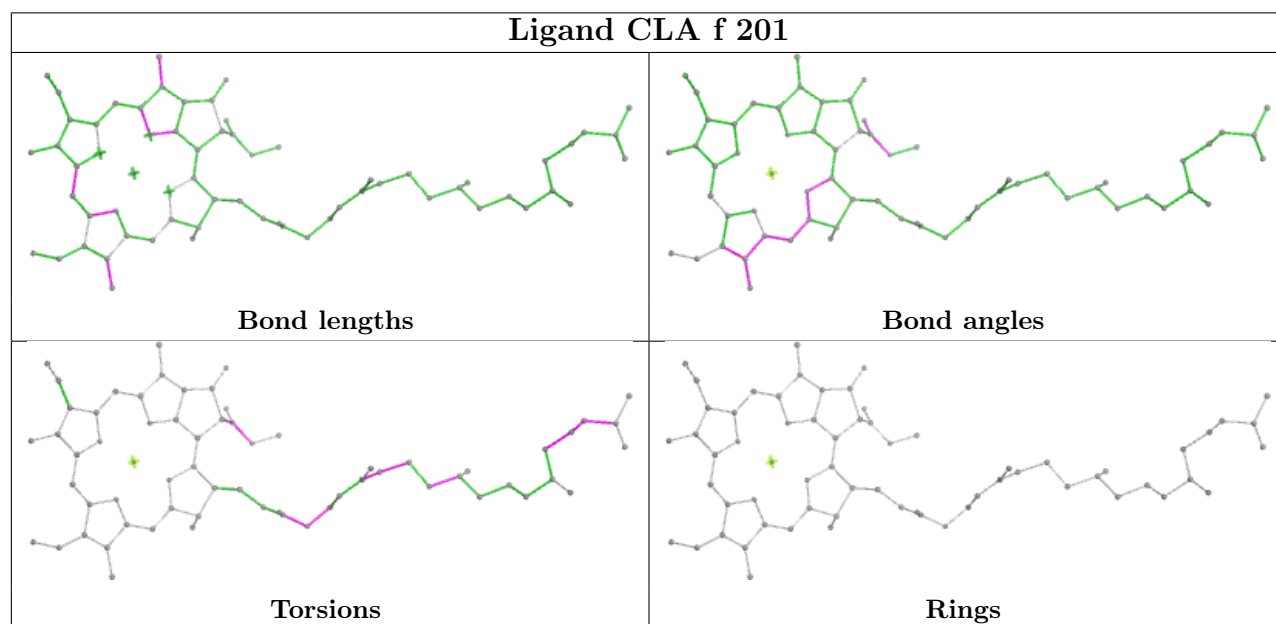
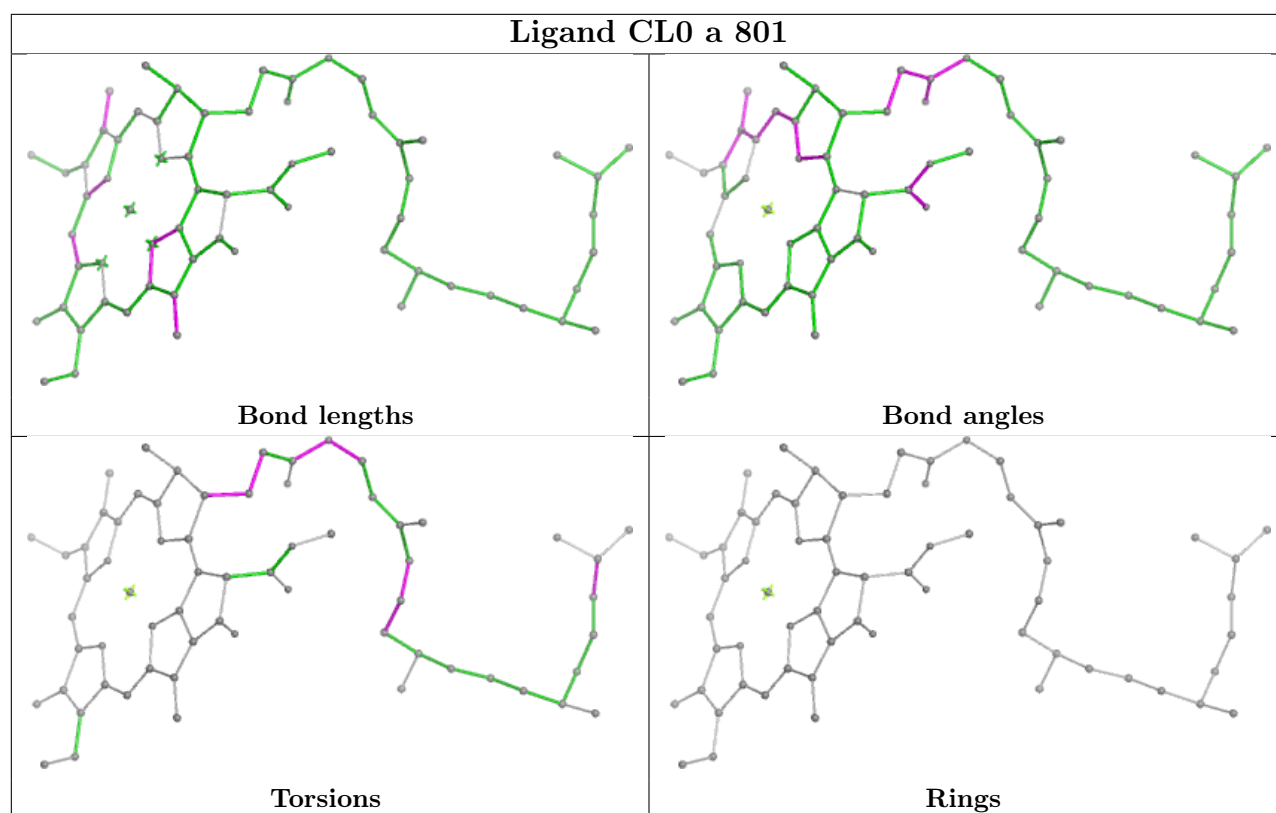


## Ligand LMG b 848

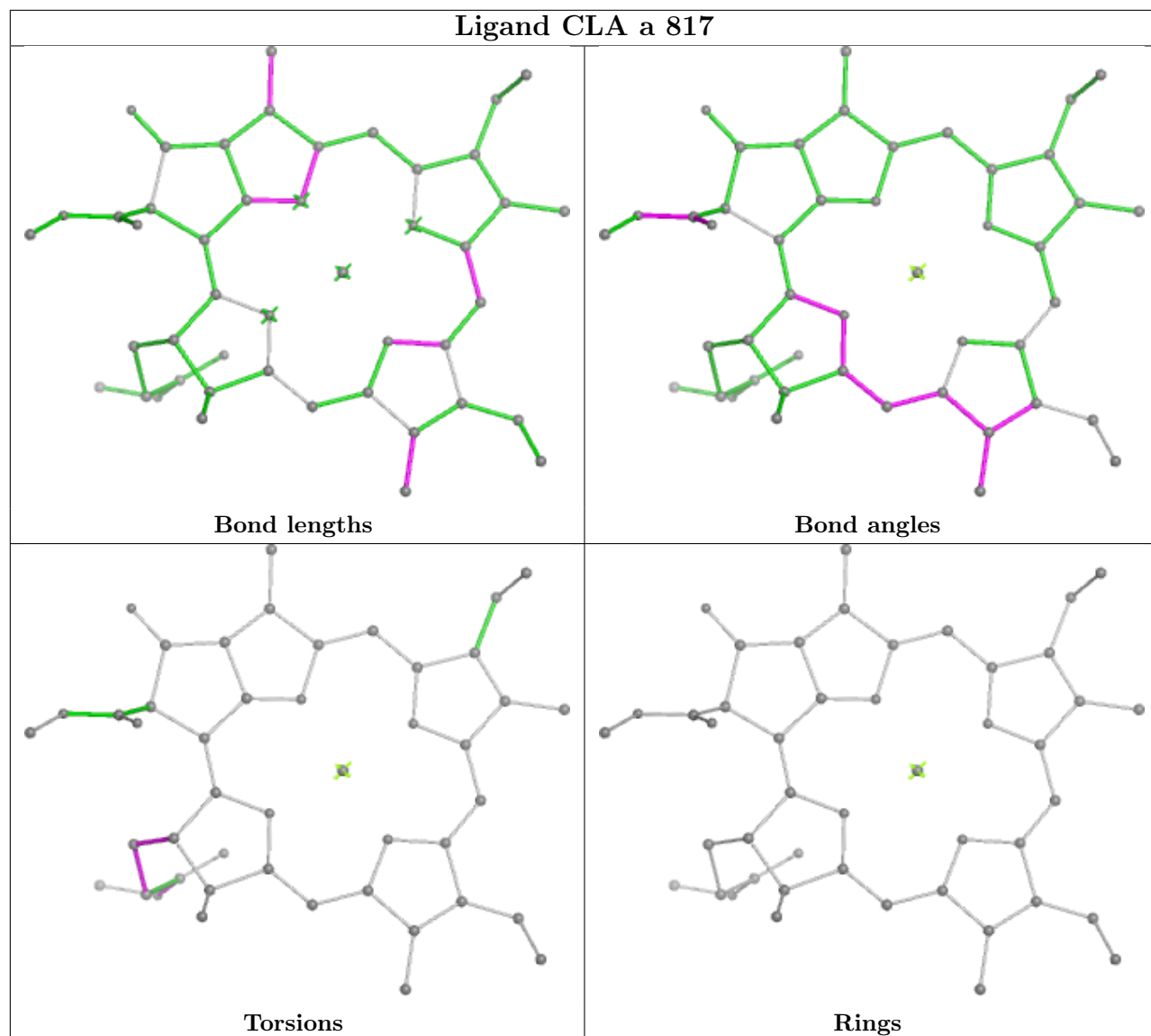


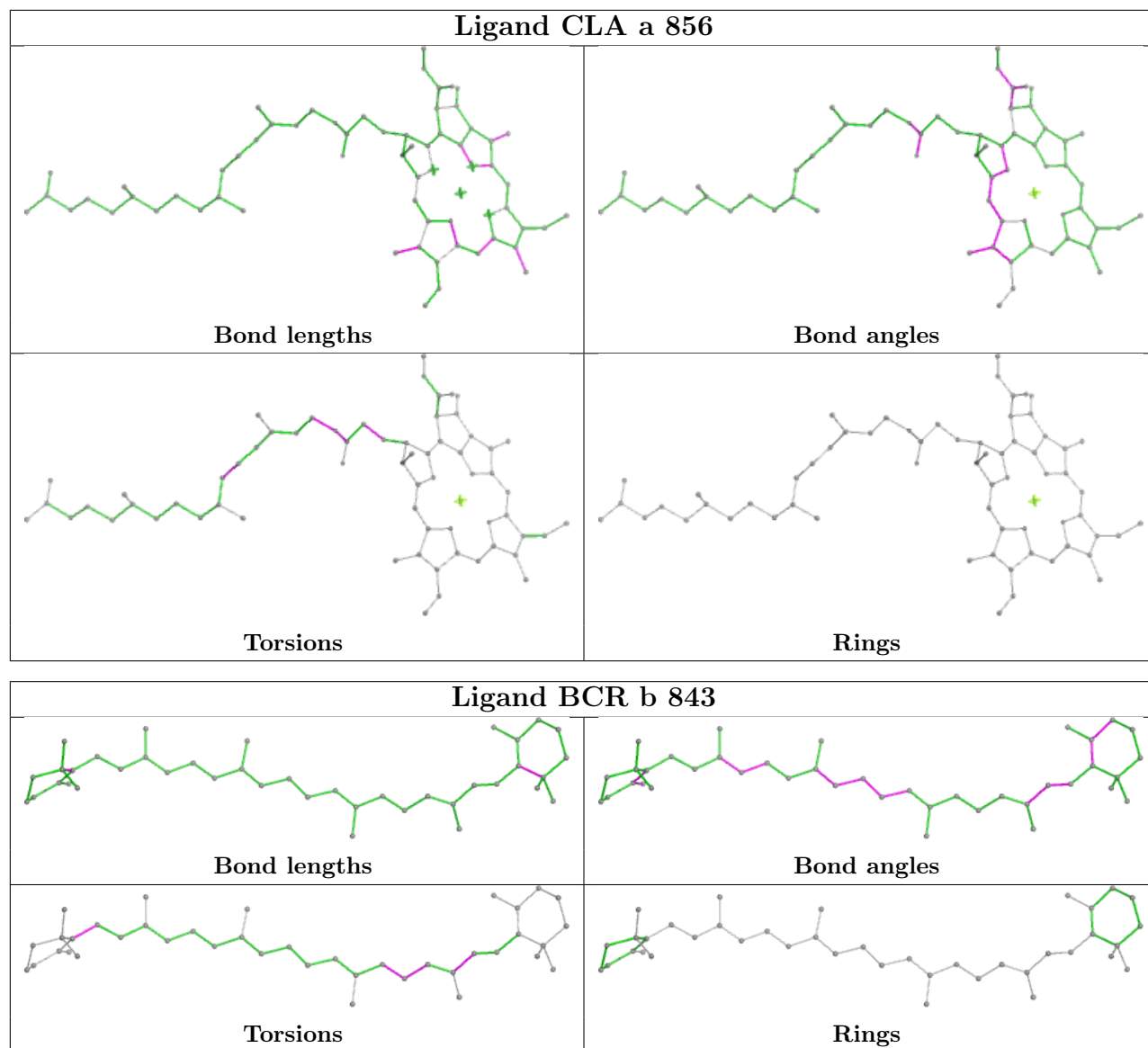
## Ligand CLA f 203

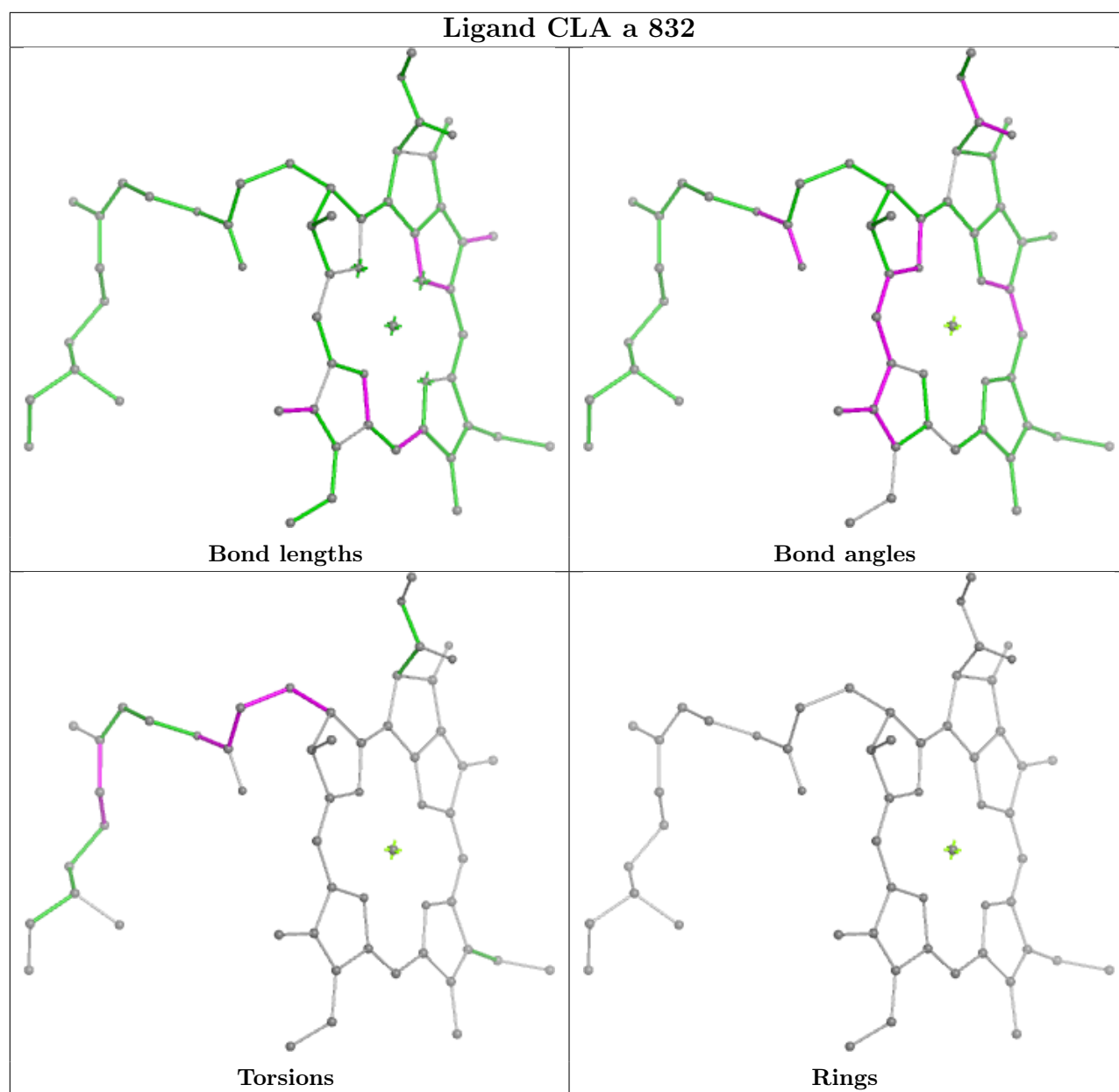




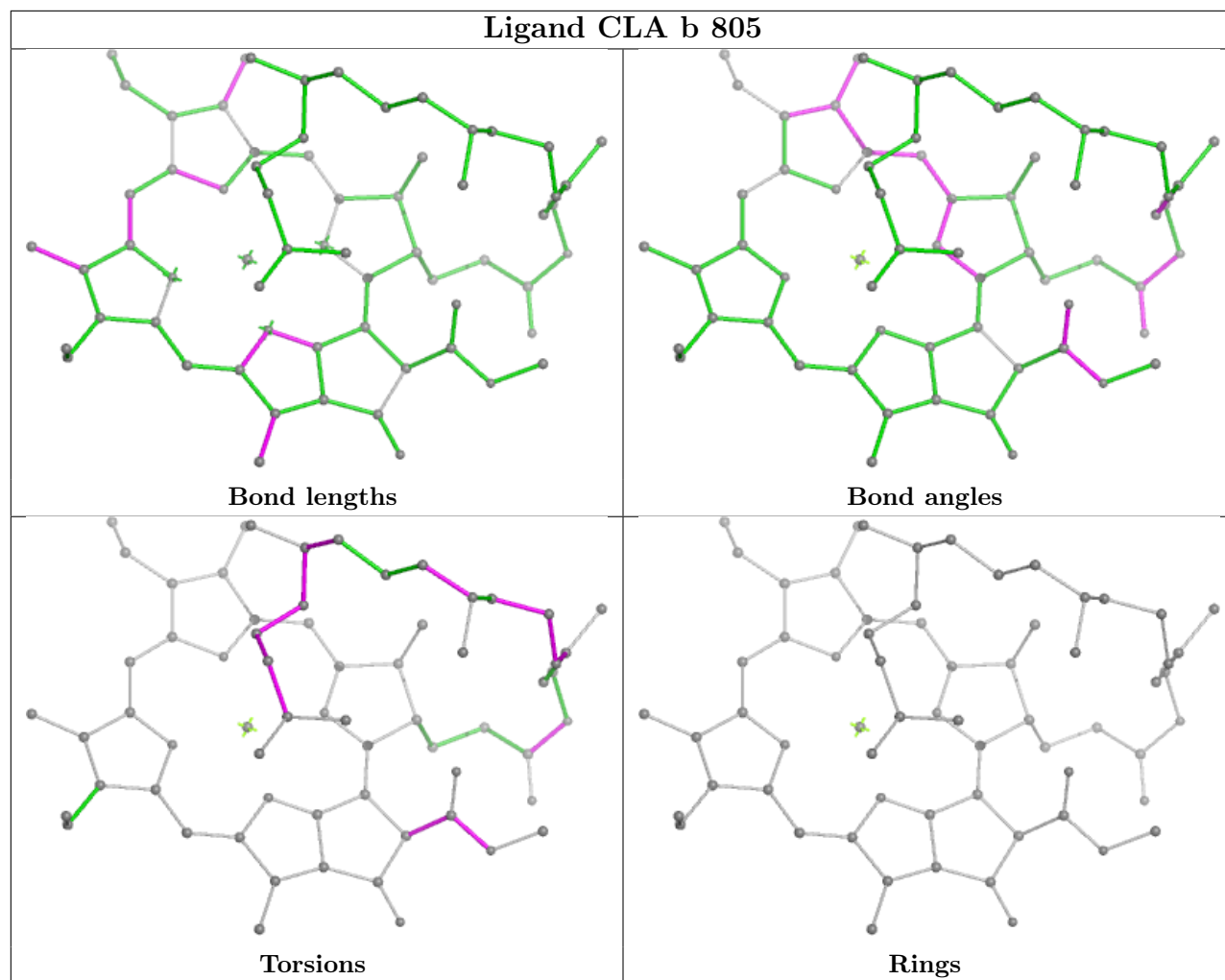
## Ligand CLA a 817



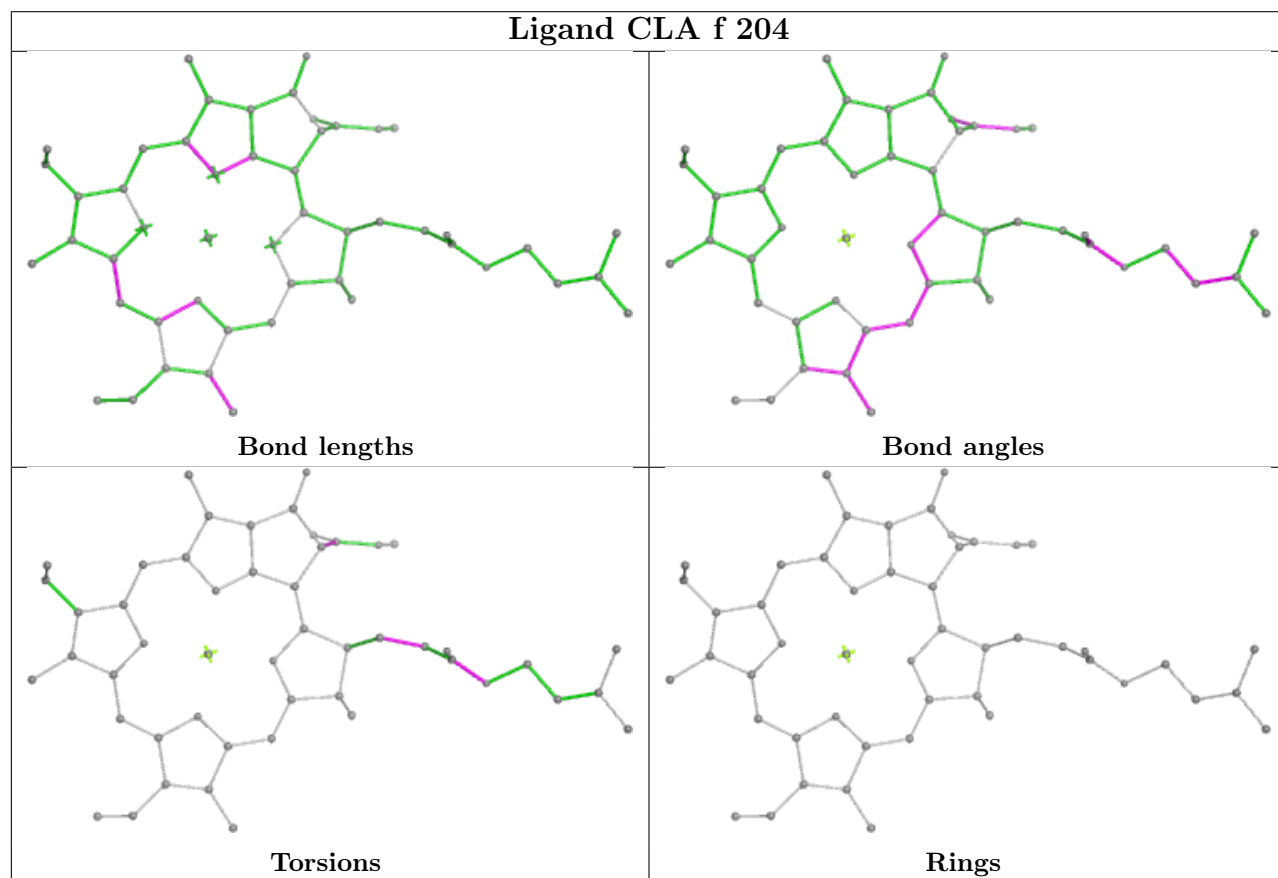
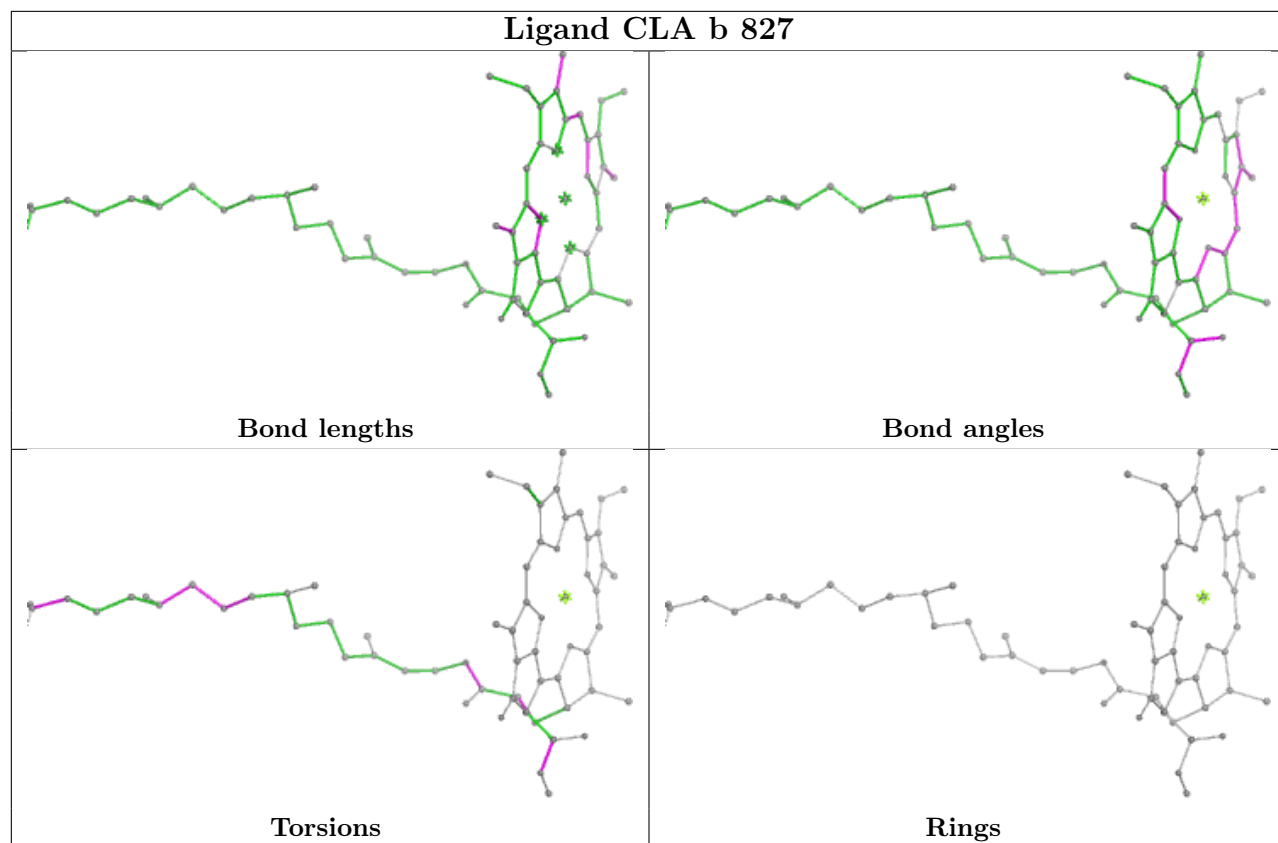


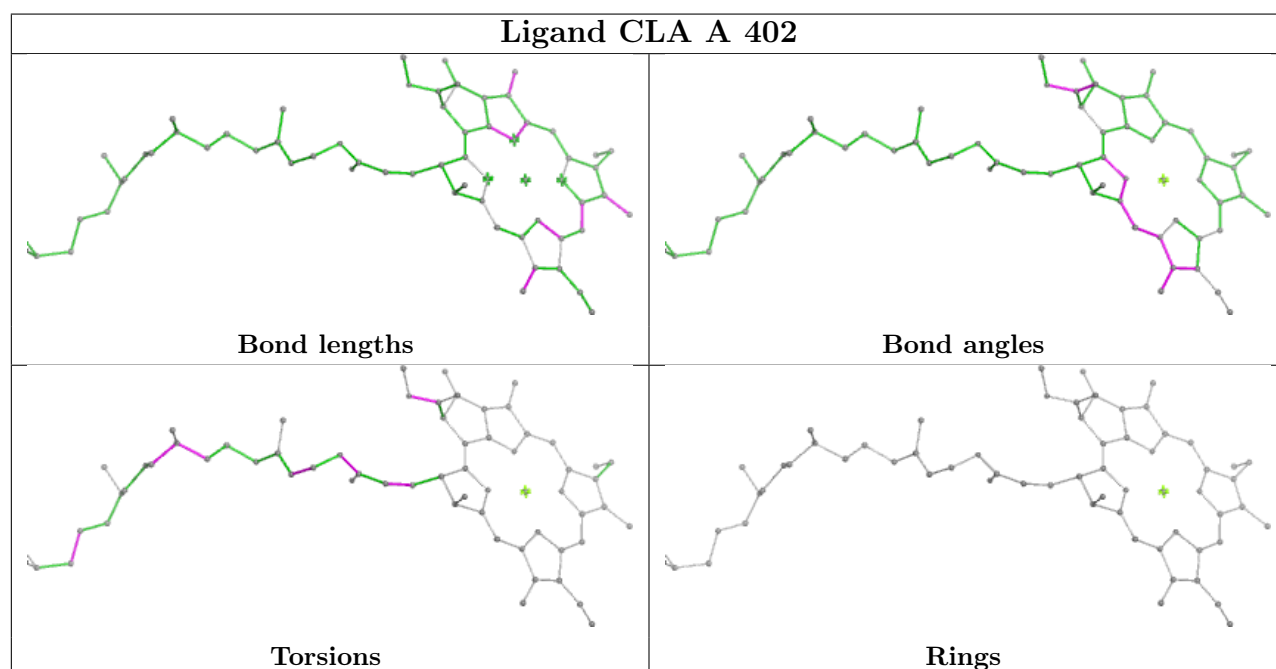
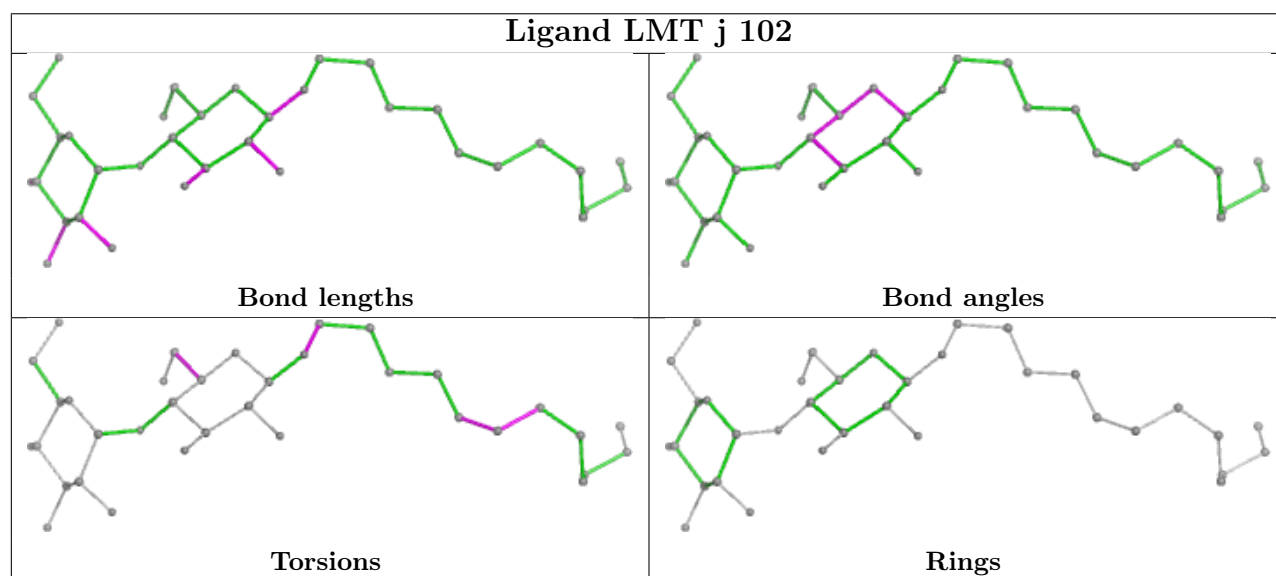
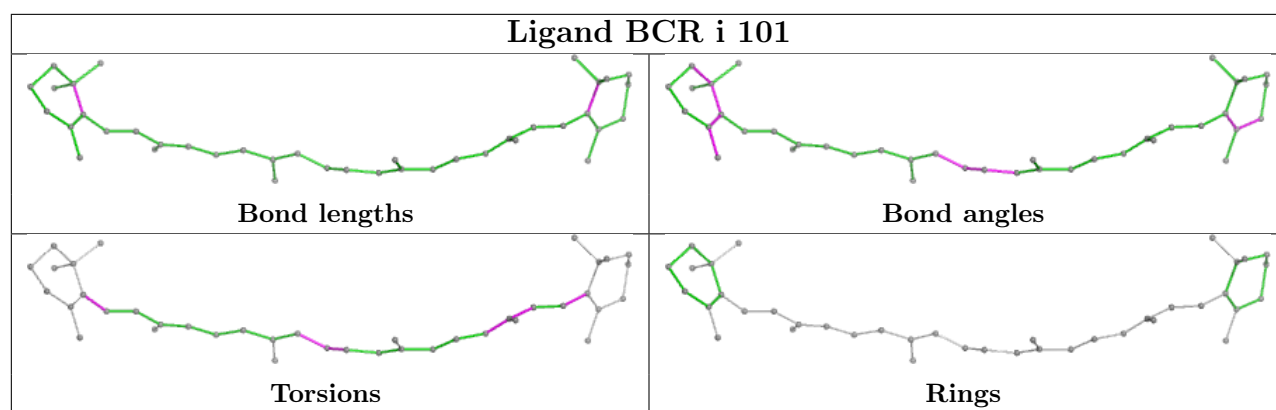


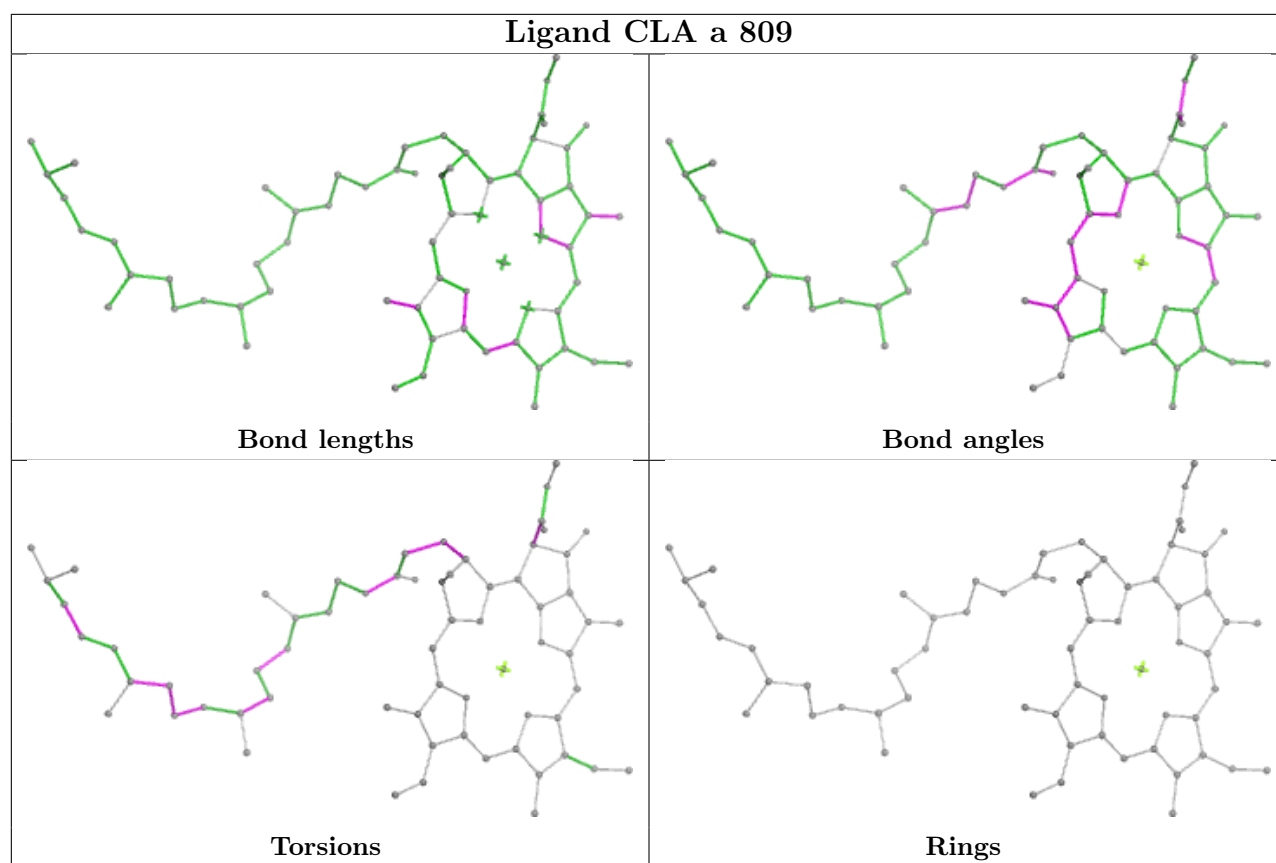
## Ligand CLA b 805

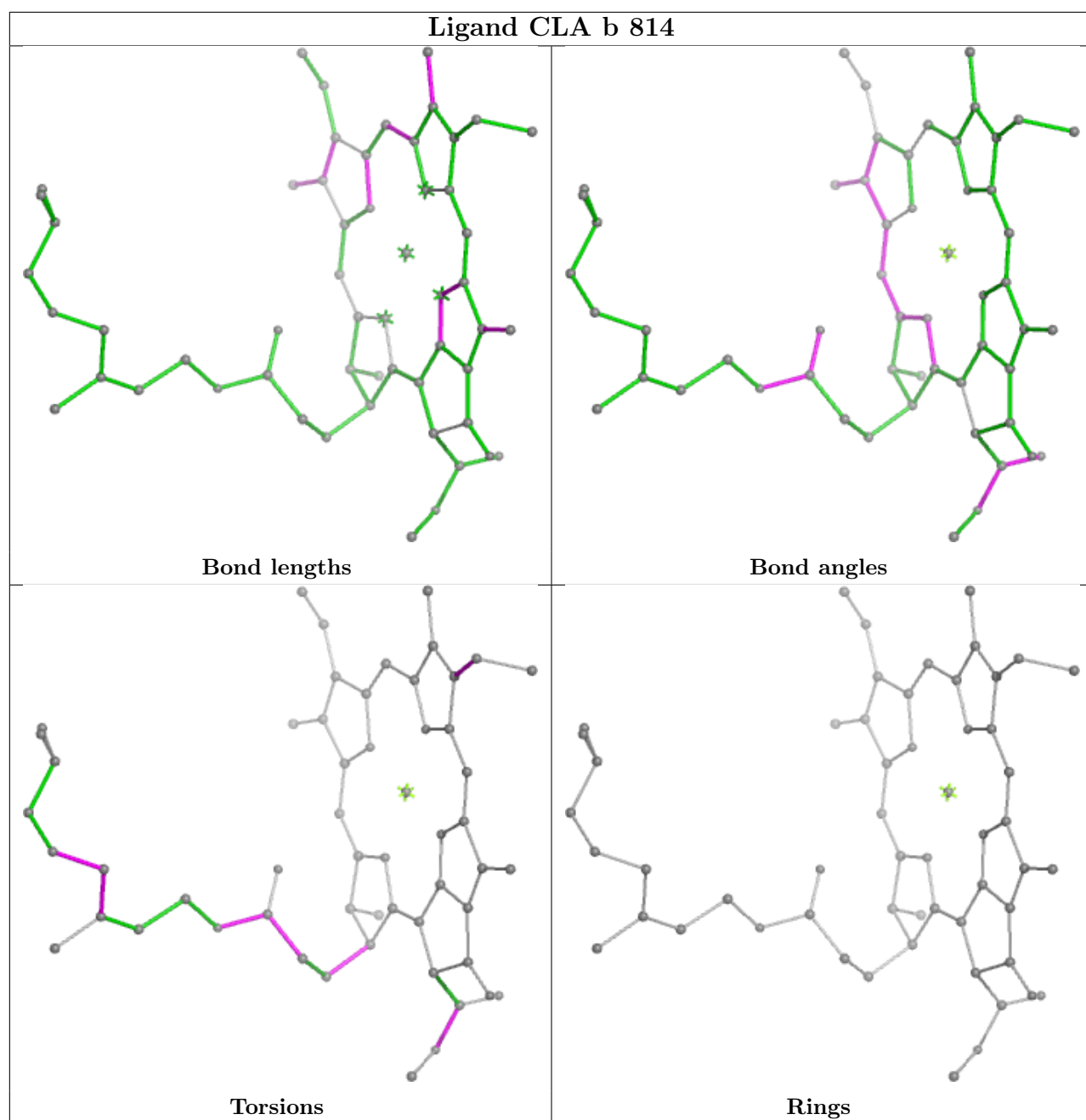




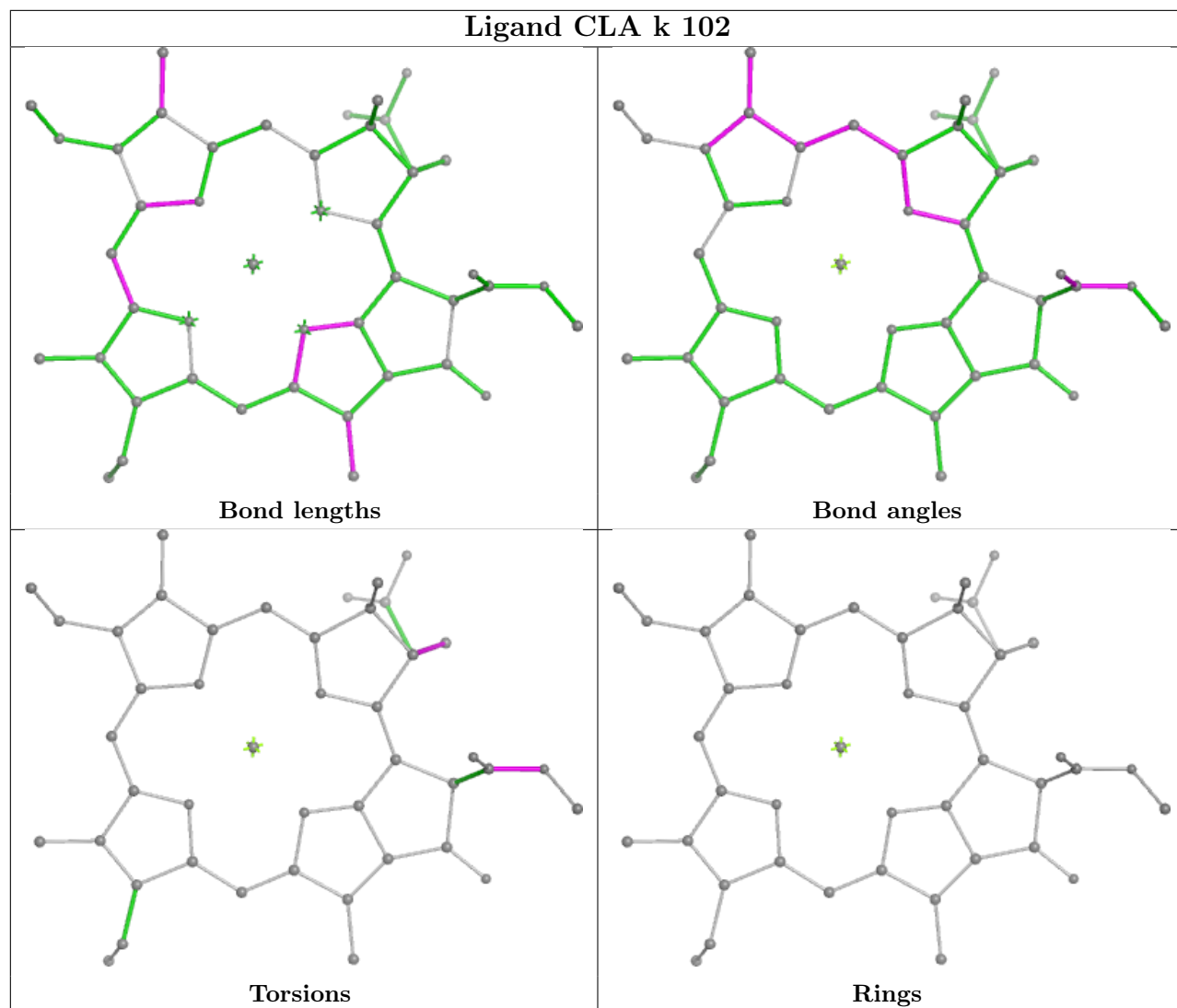


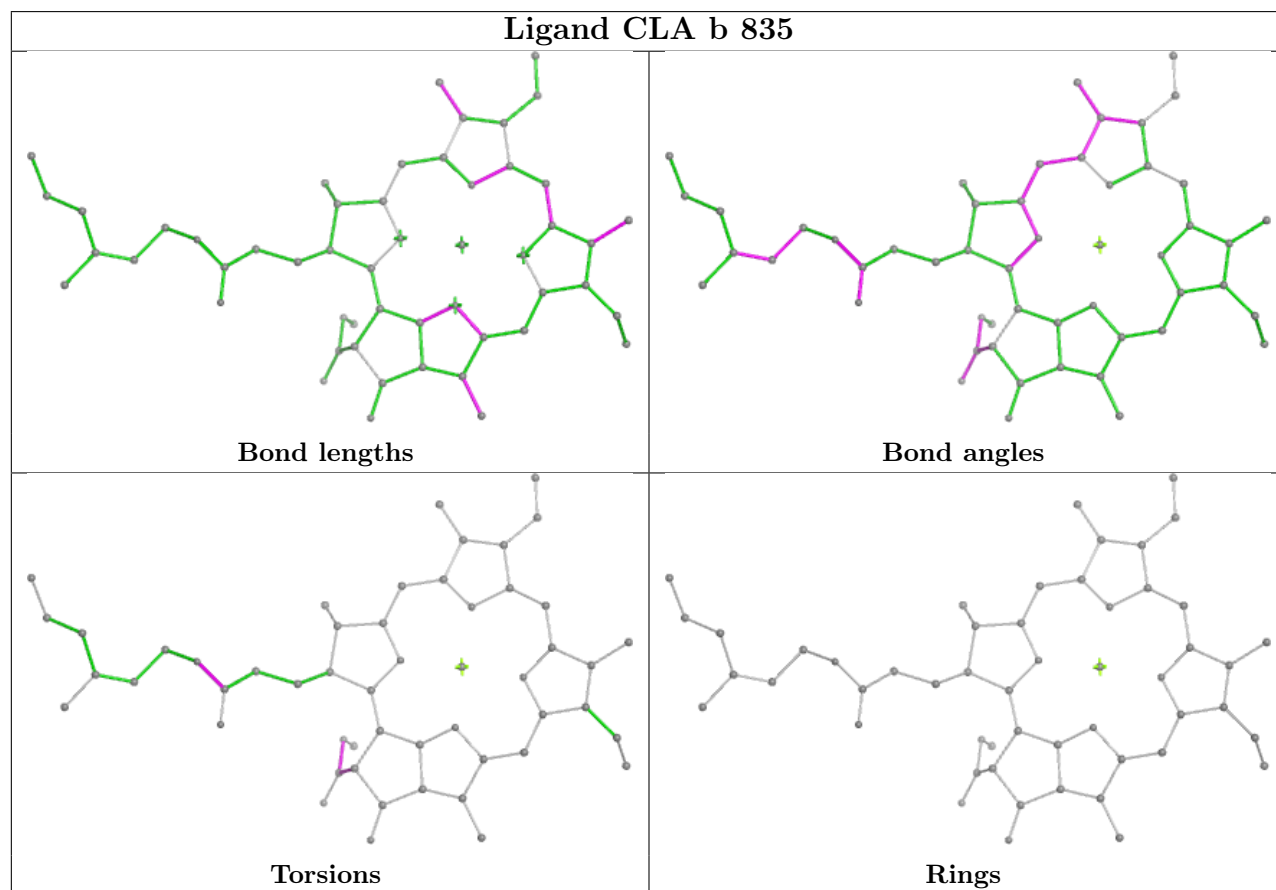
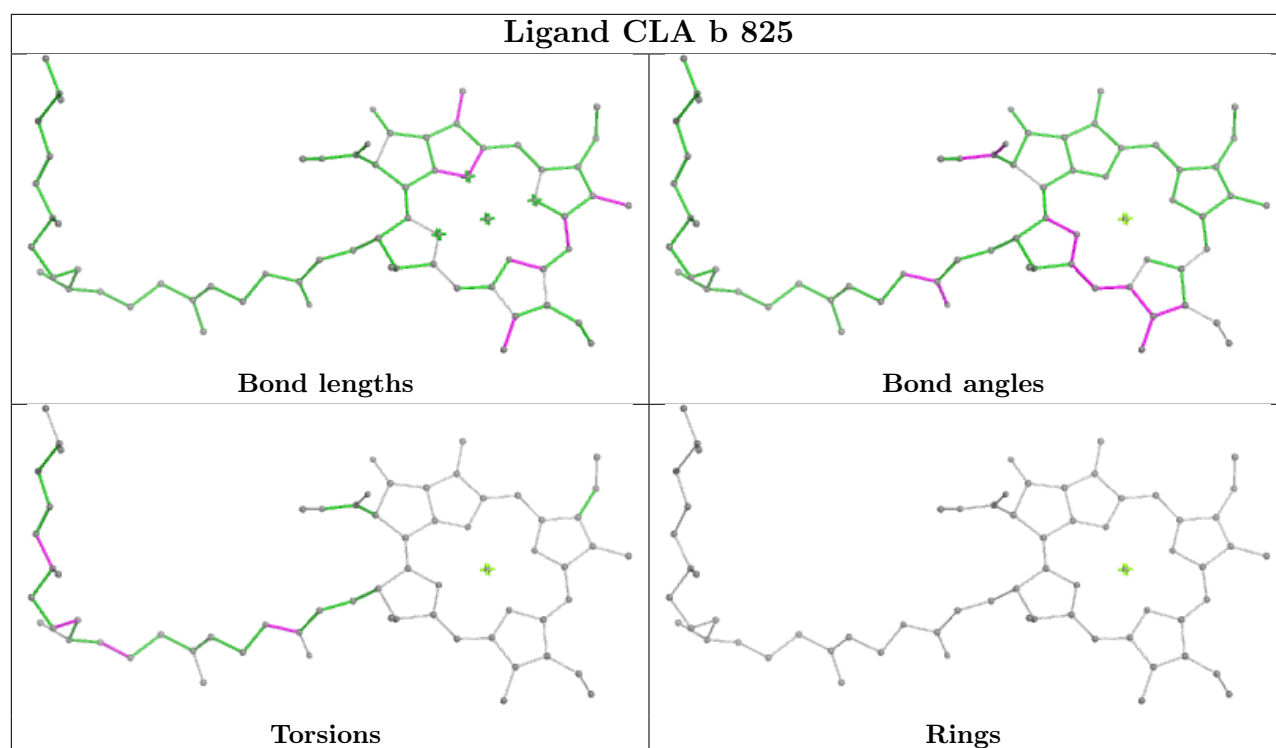


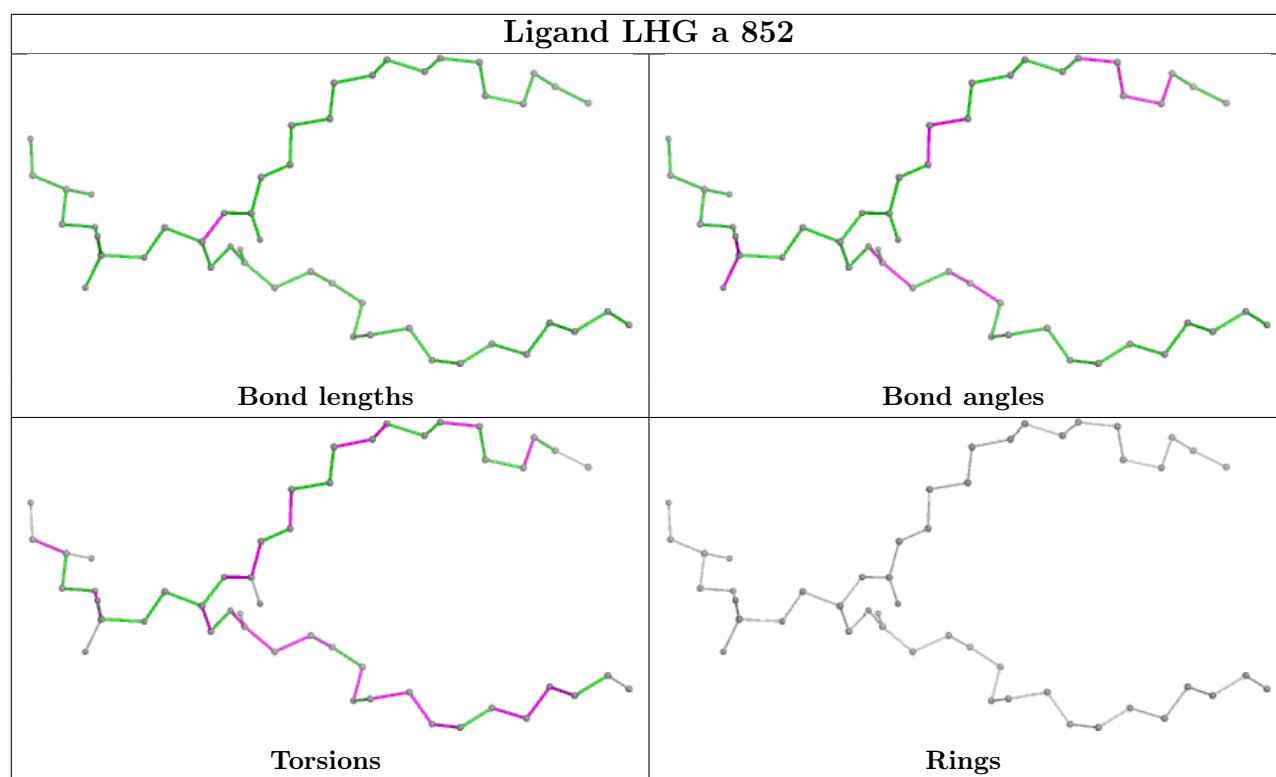


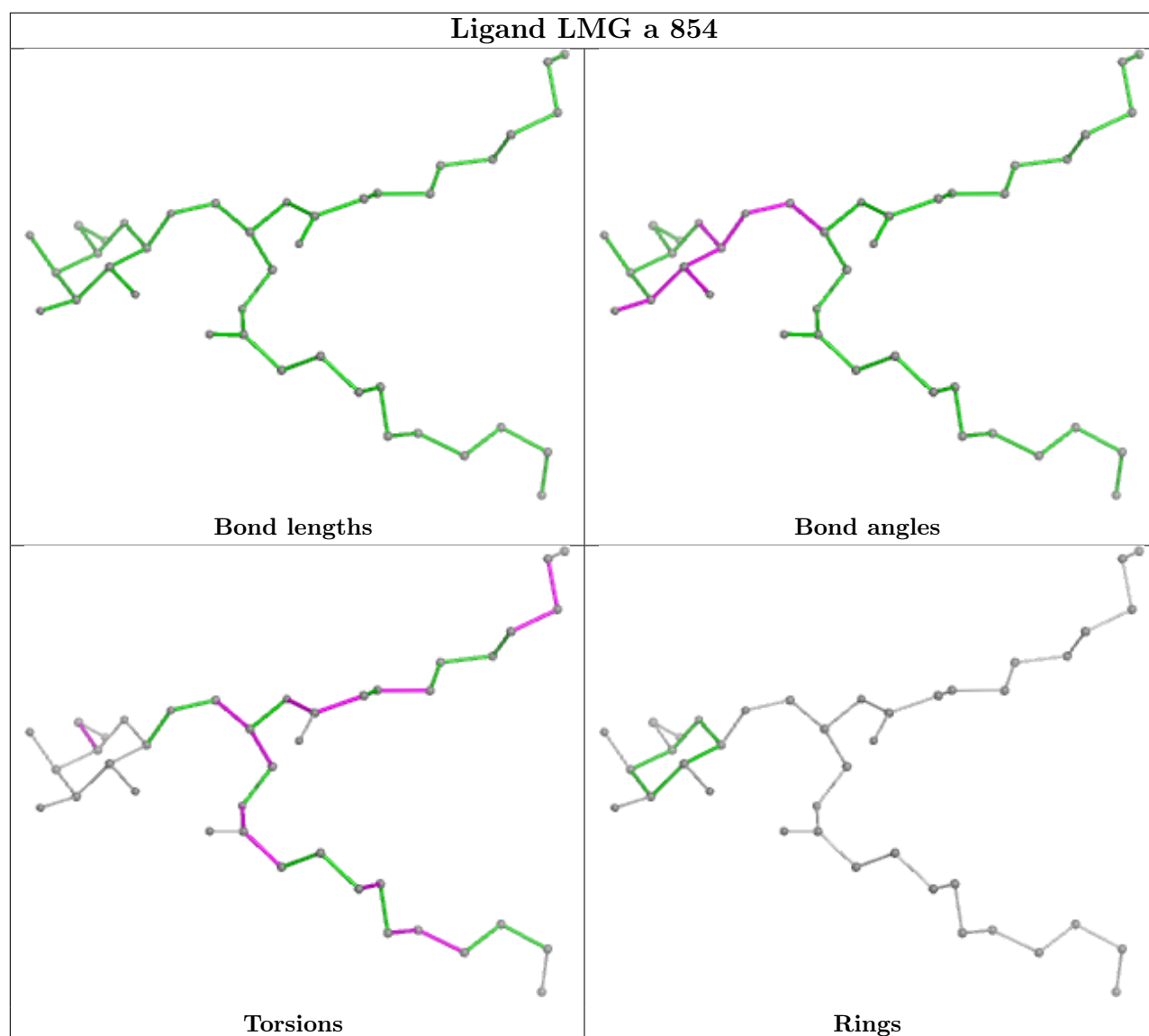


## Ligand CLA k 102



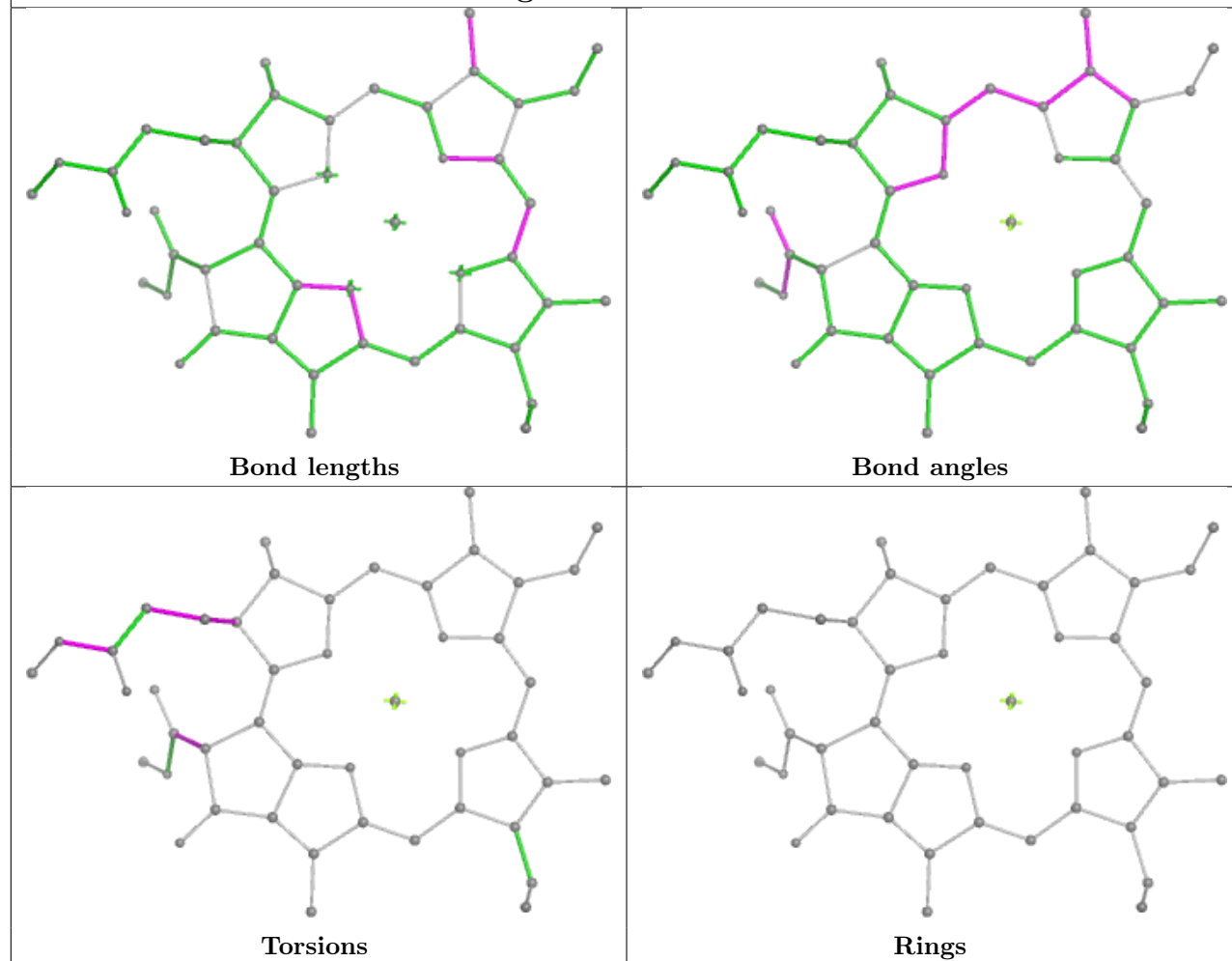




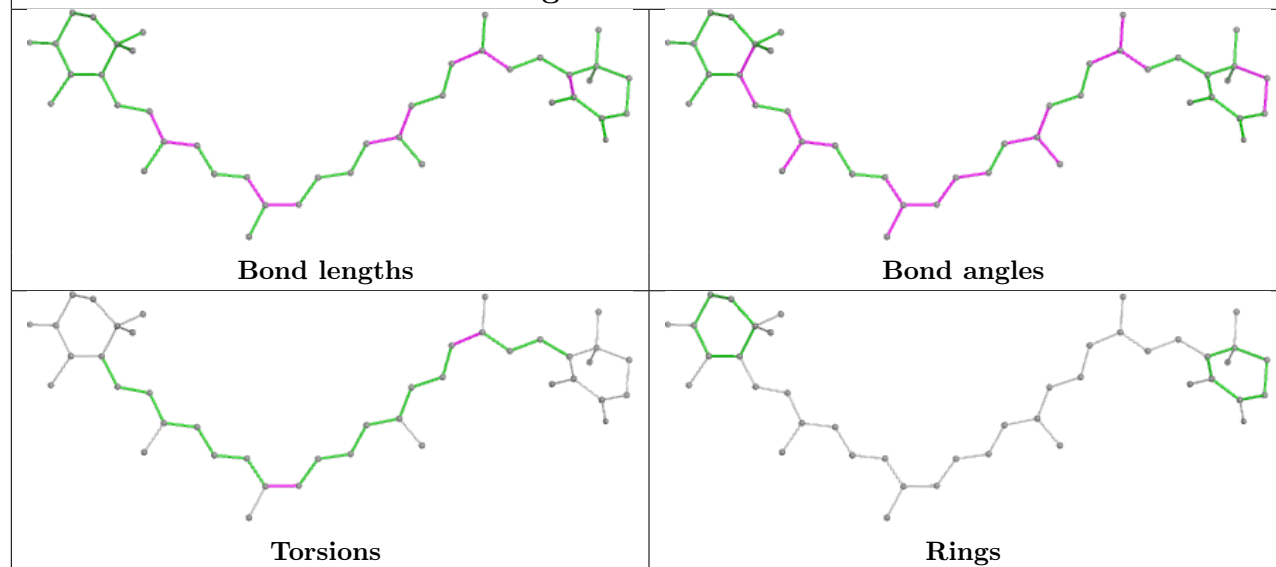


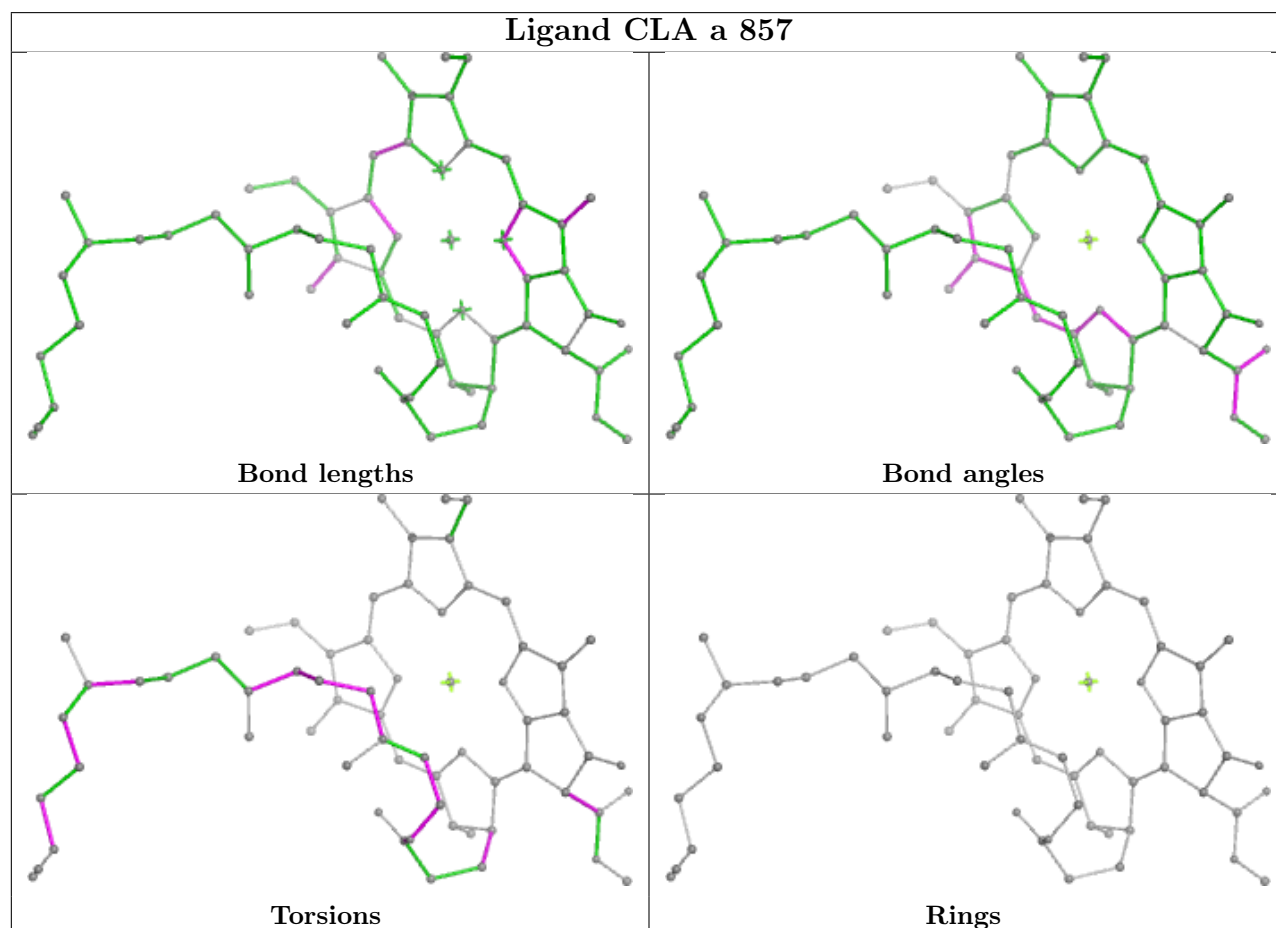
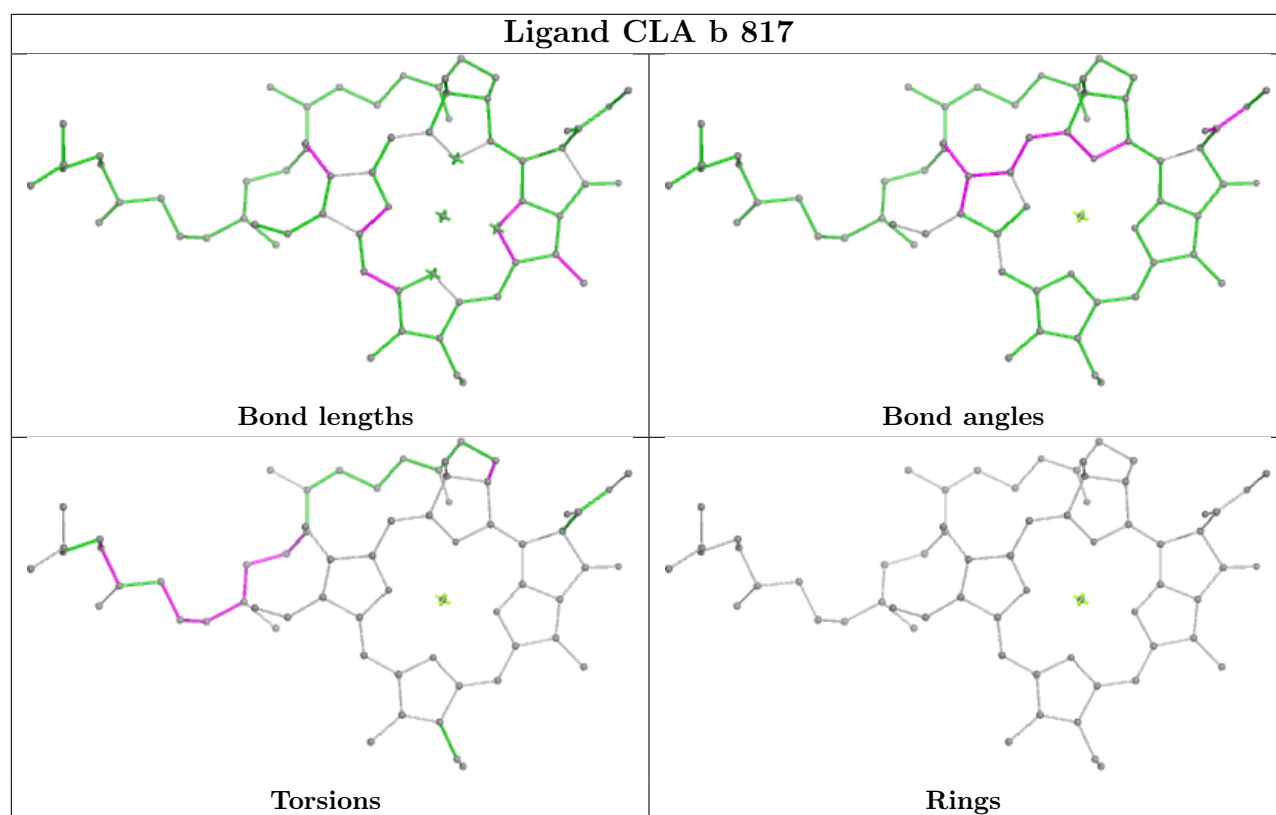


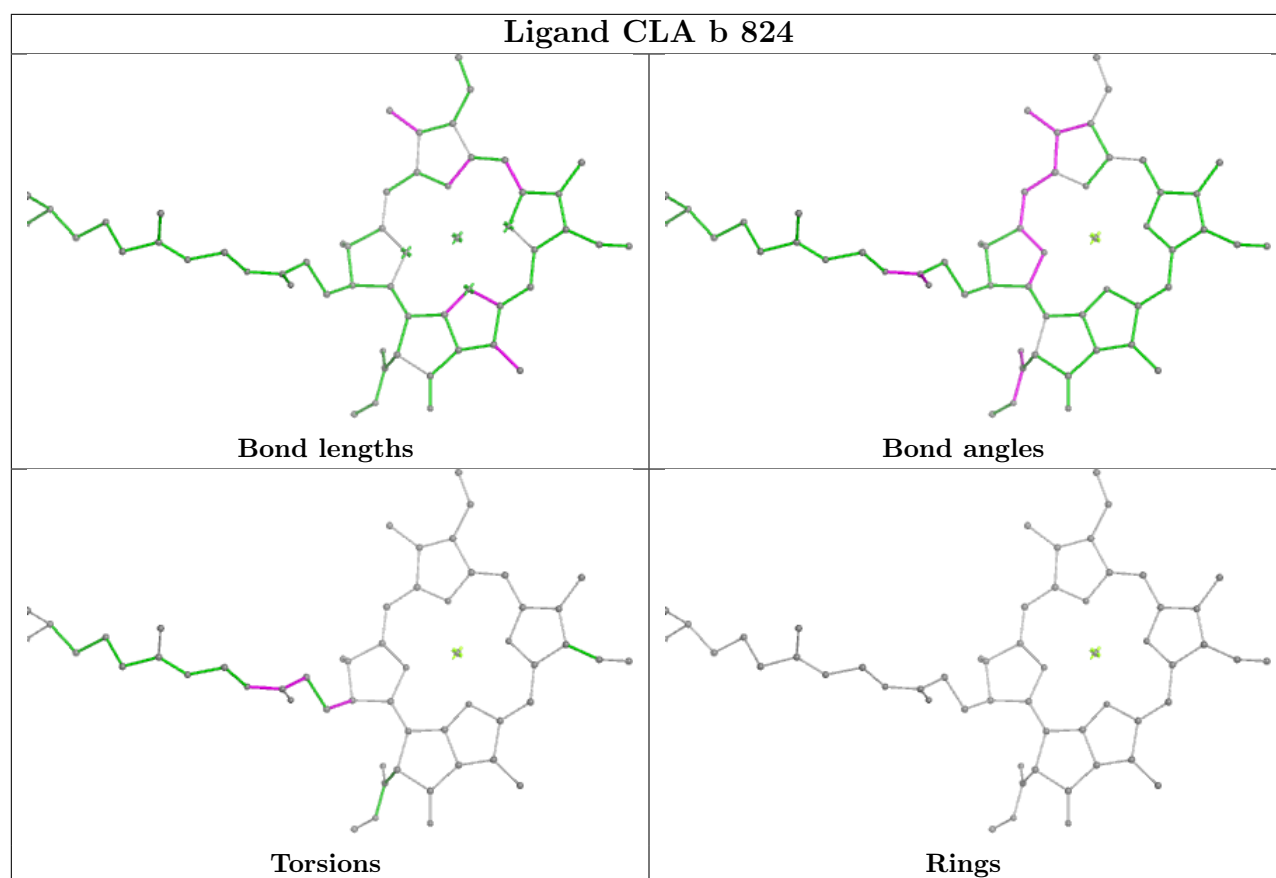
## Ligand CLA b 840



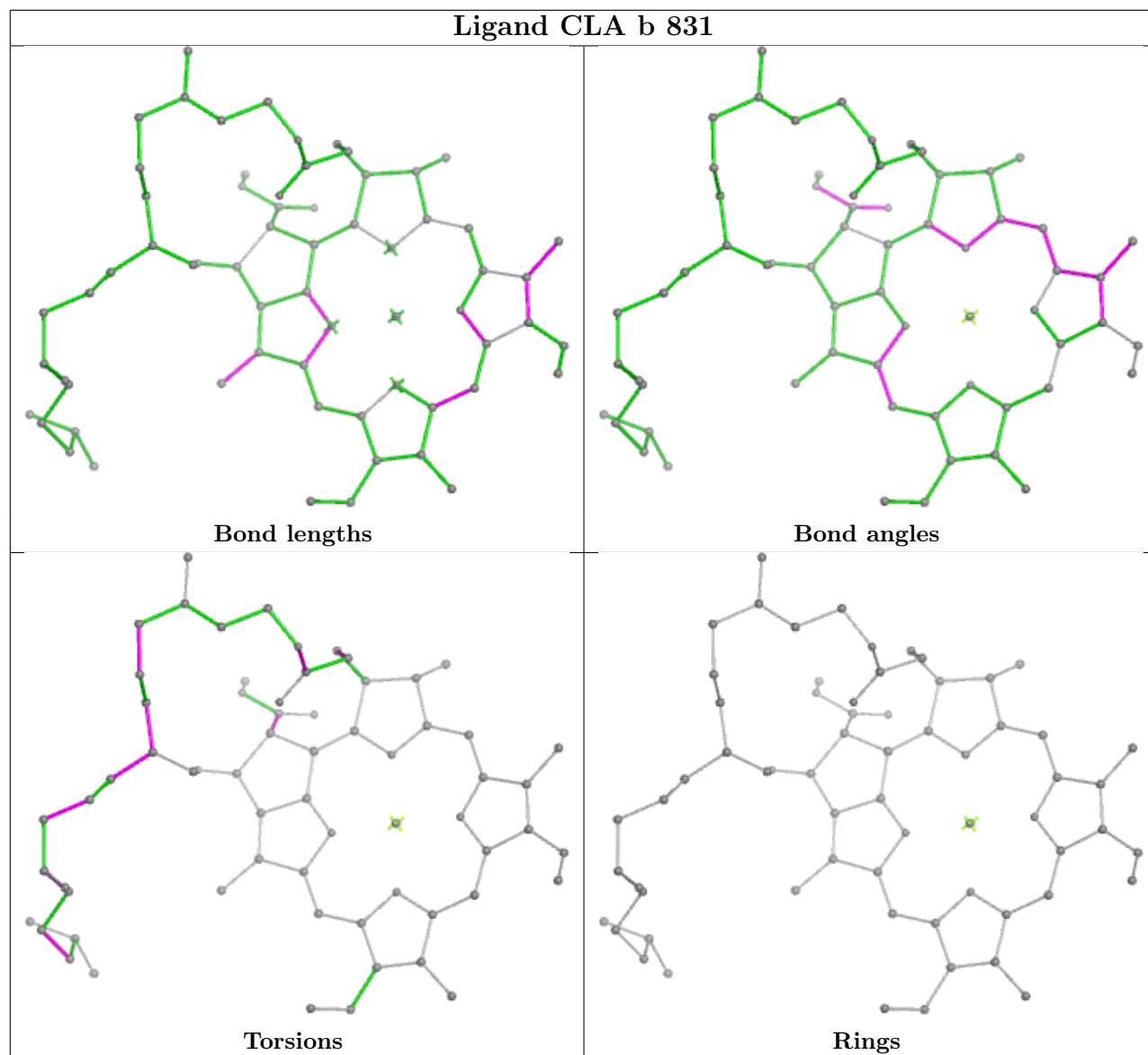
## Ligand 45D a 858

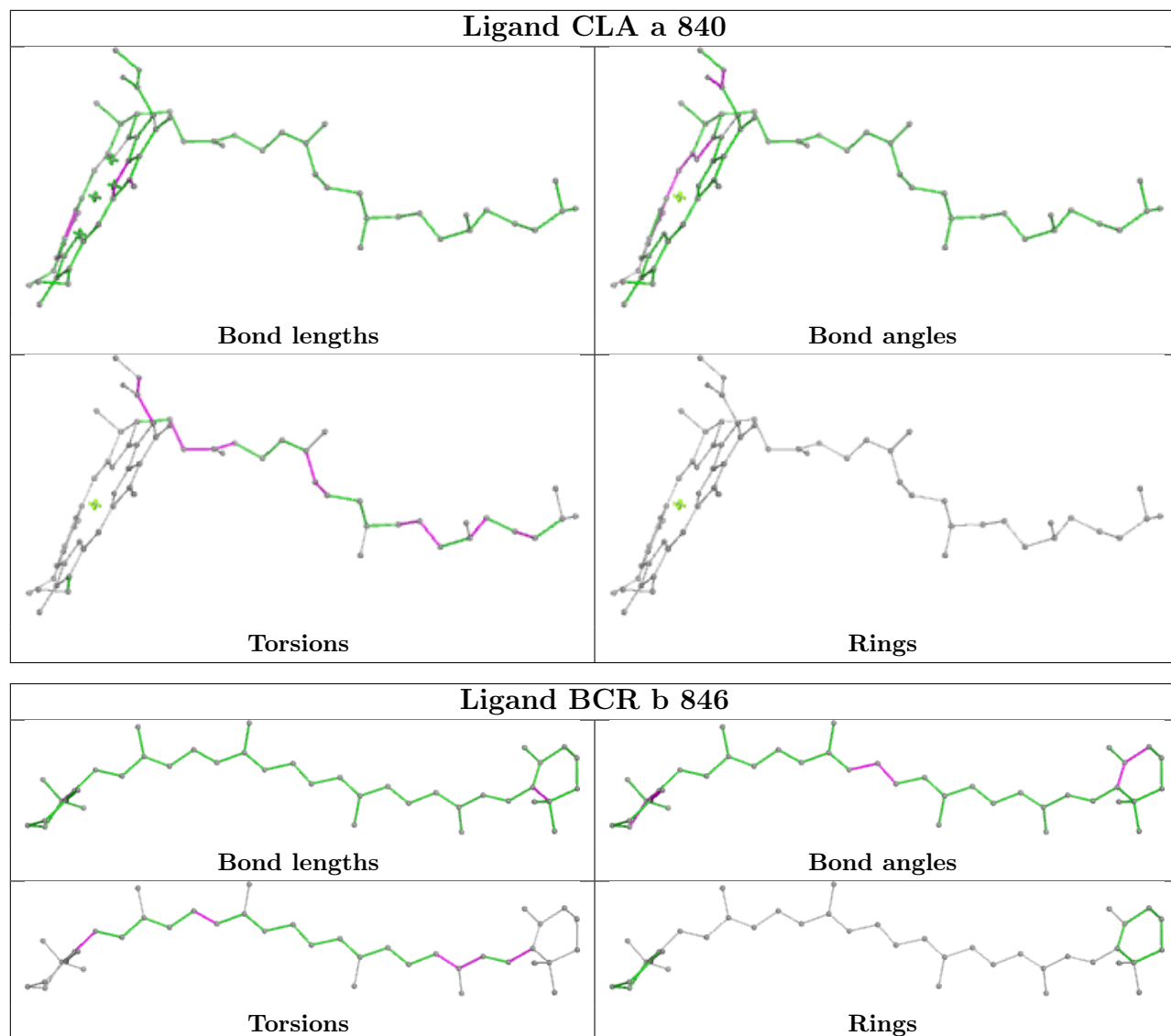


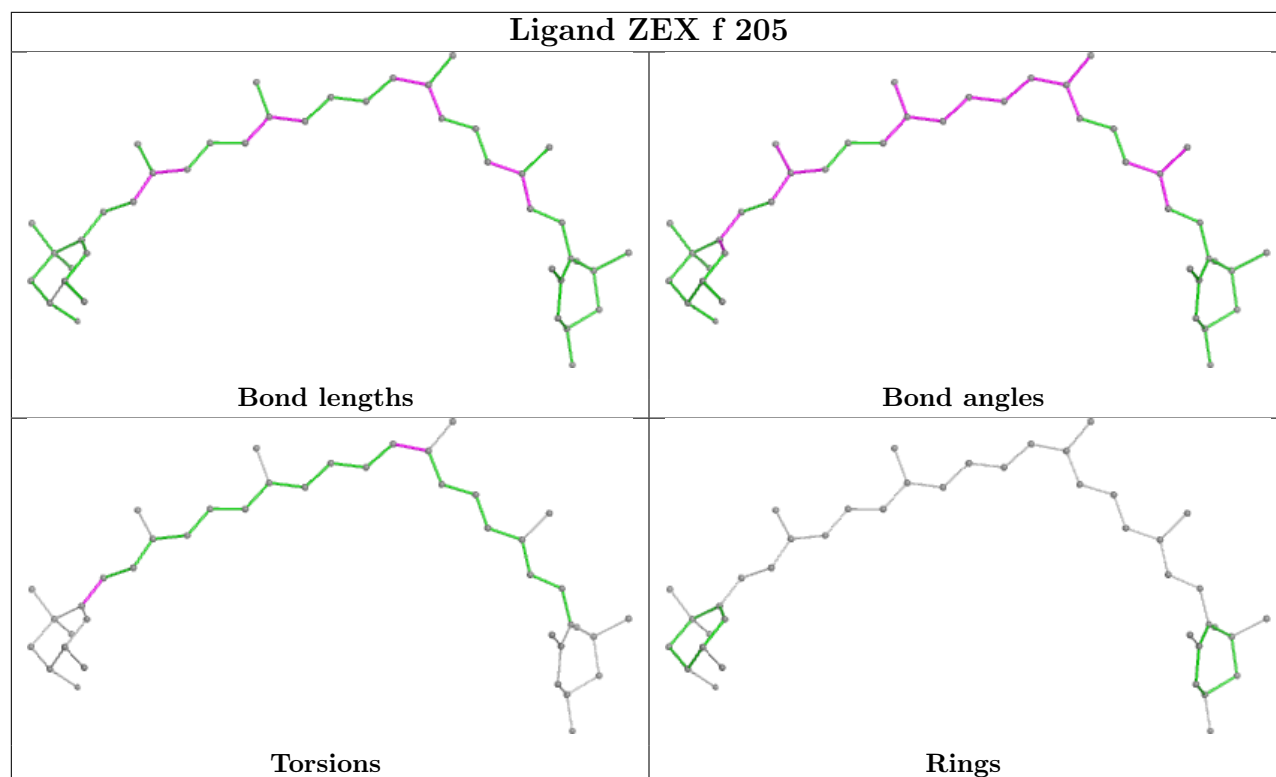
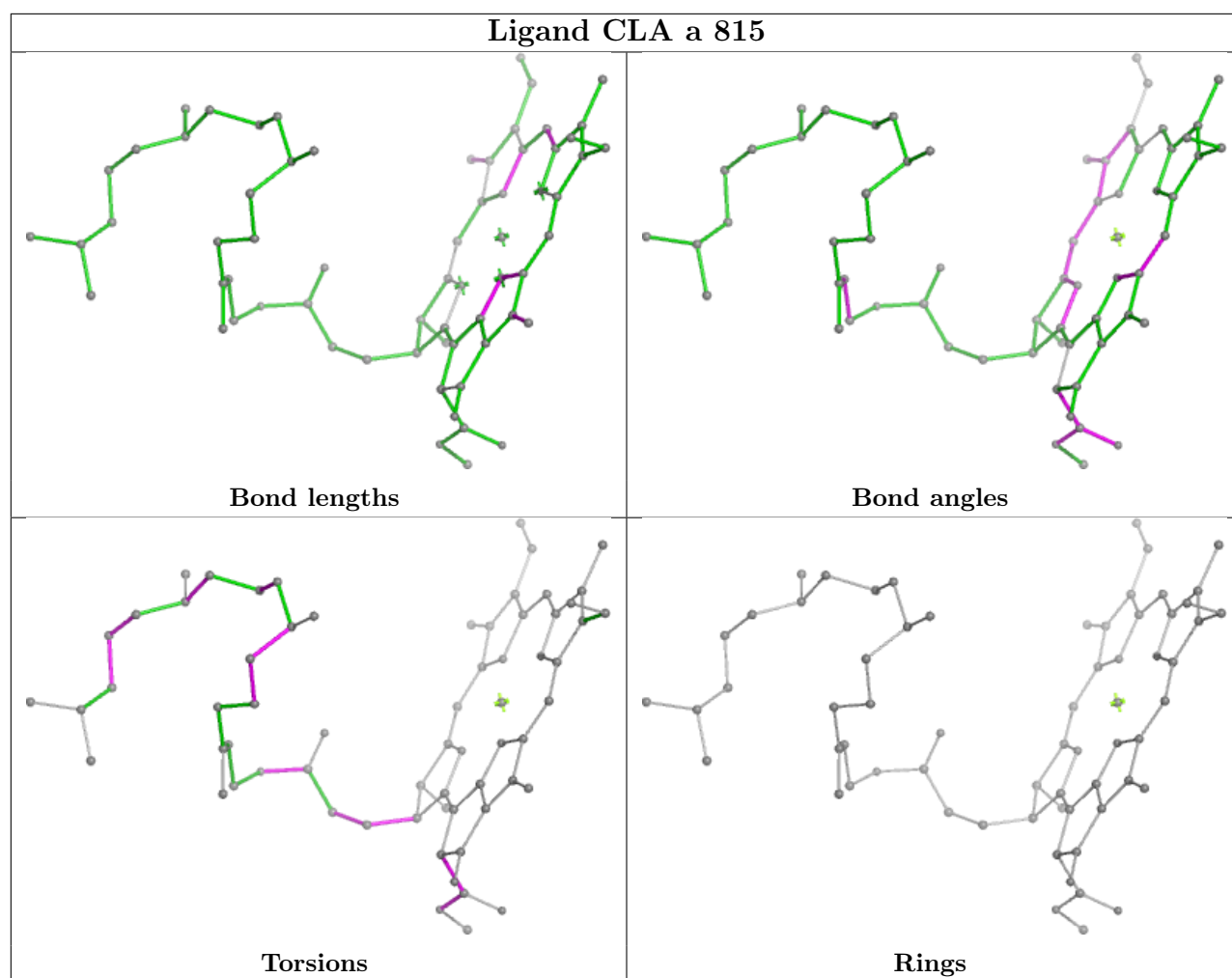


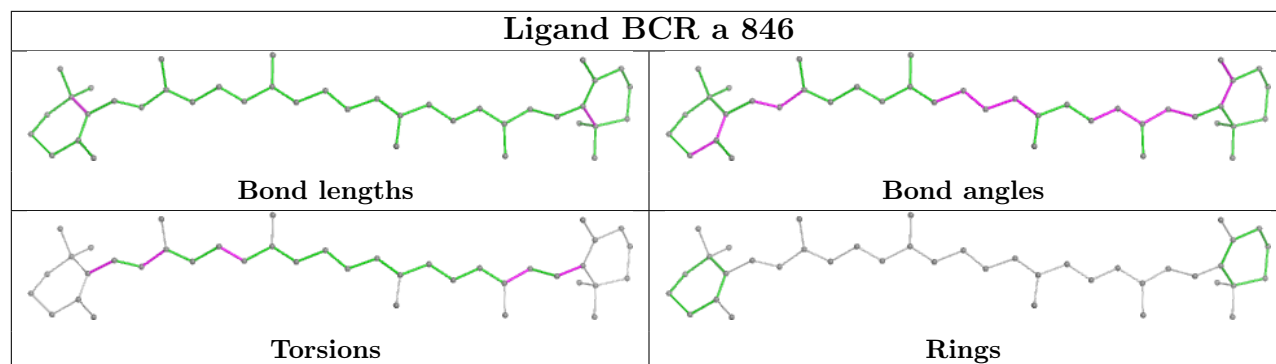
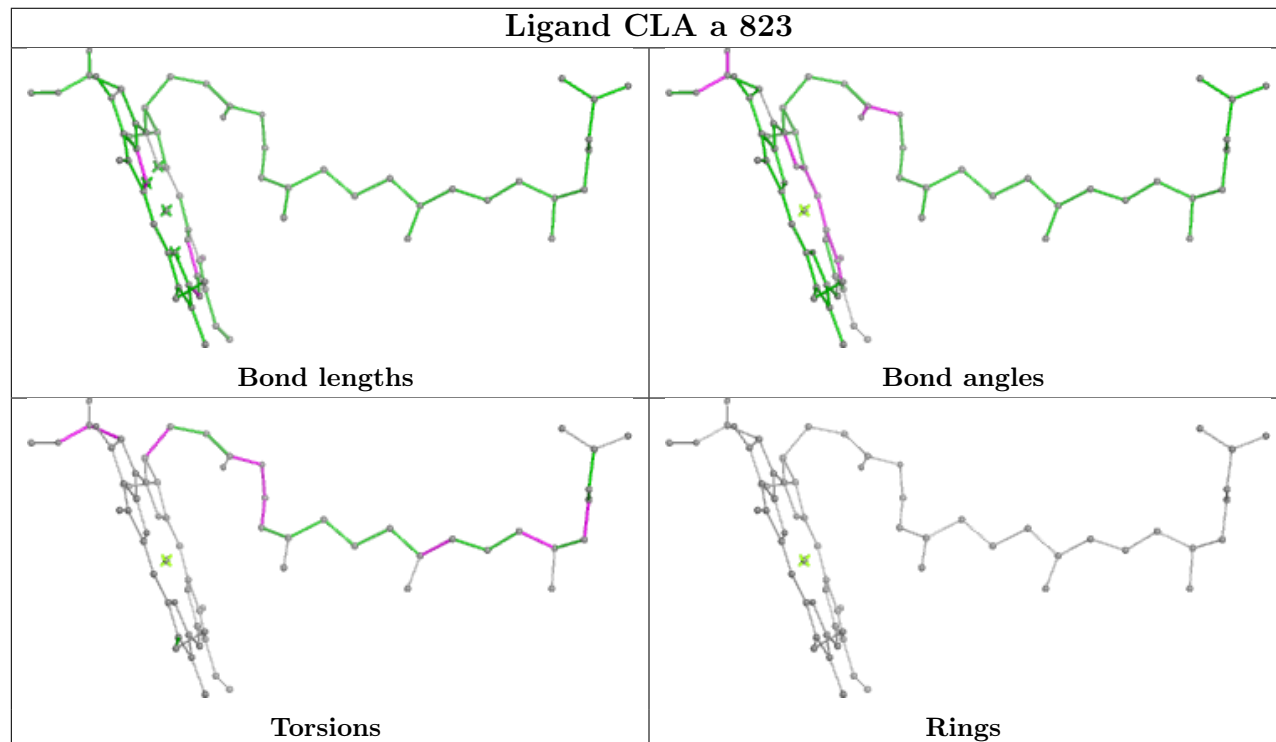


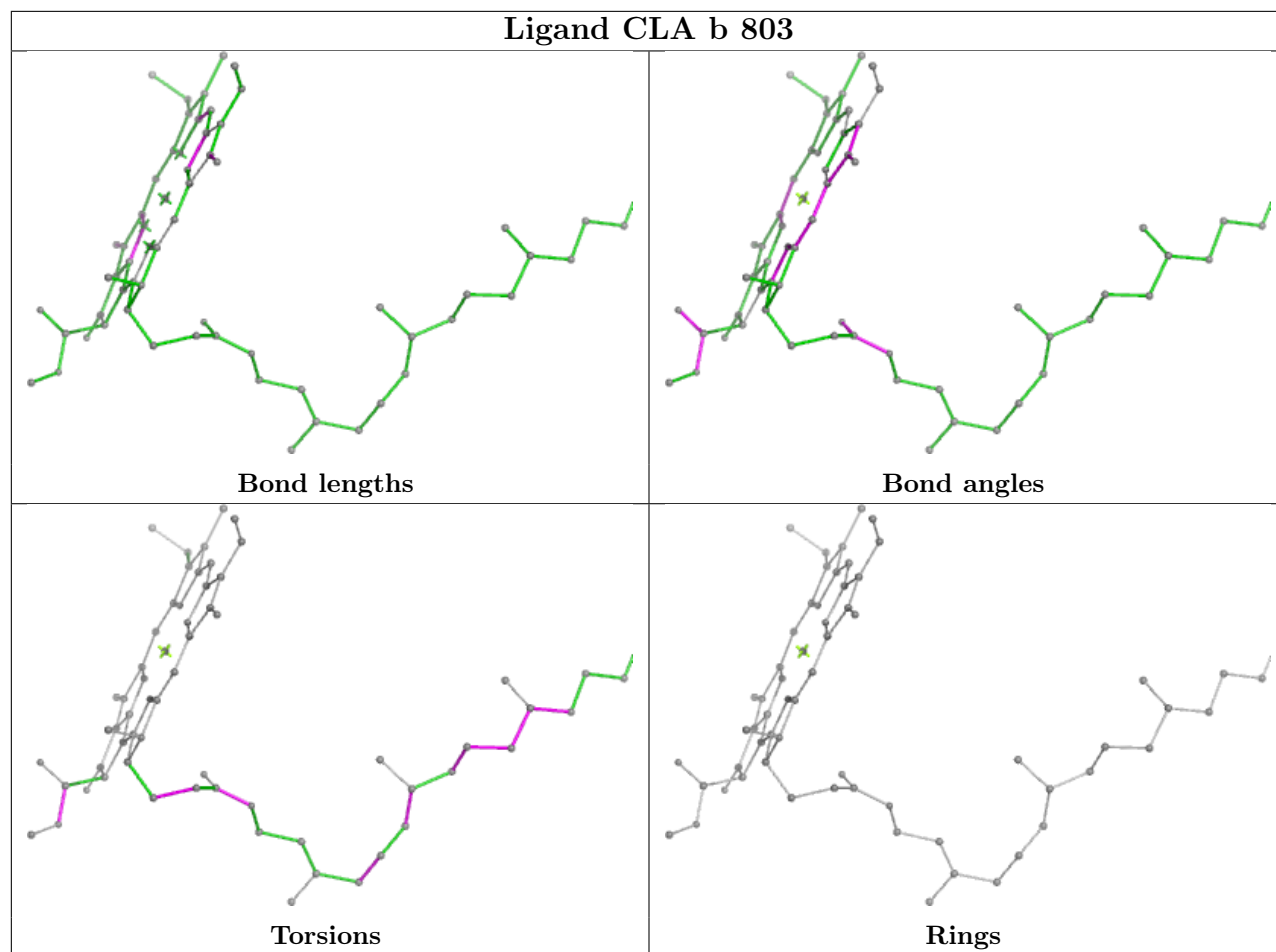
## Ligand CLA b 831





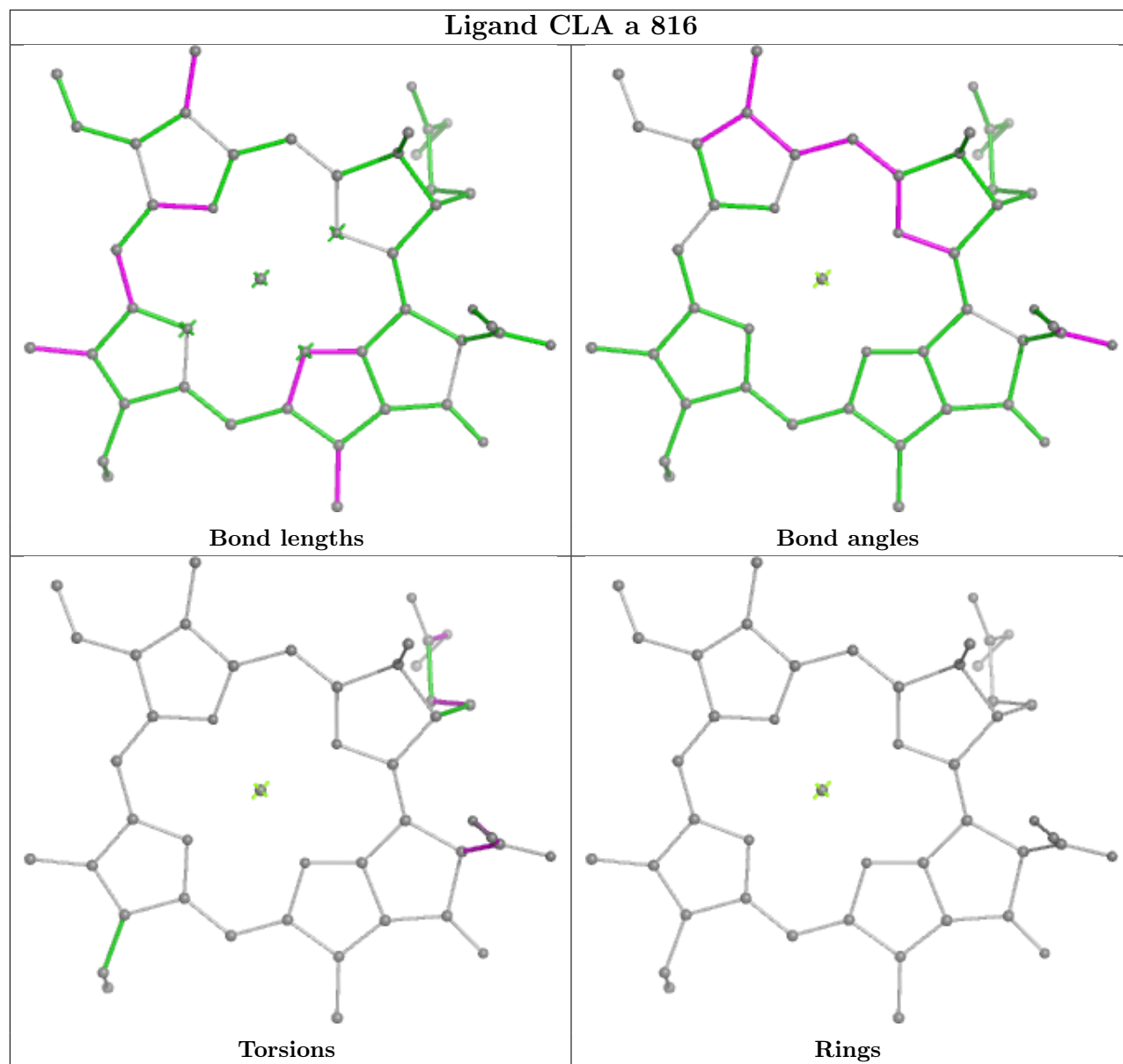


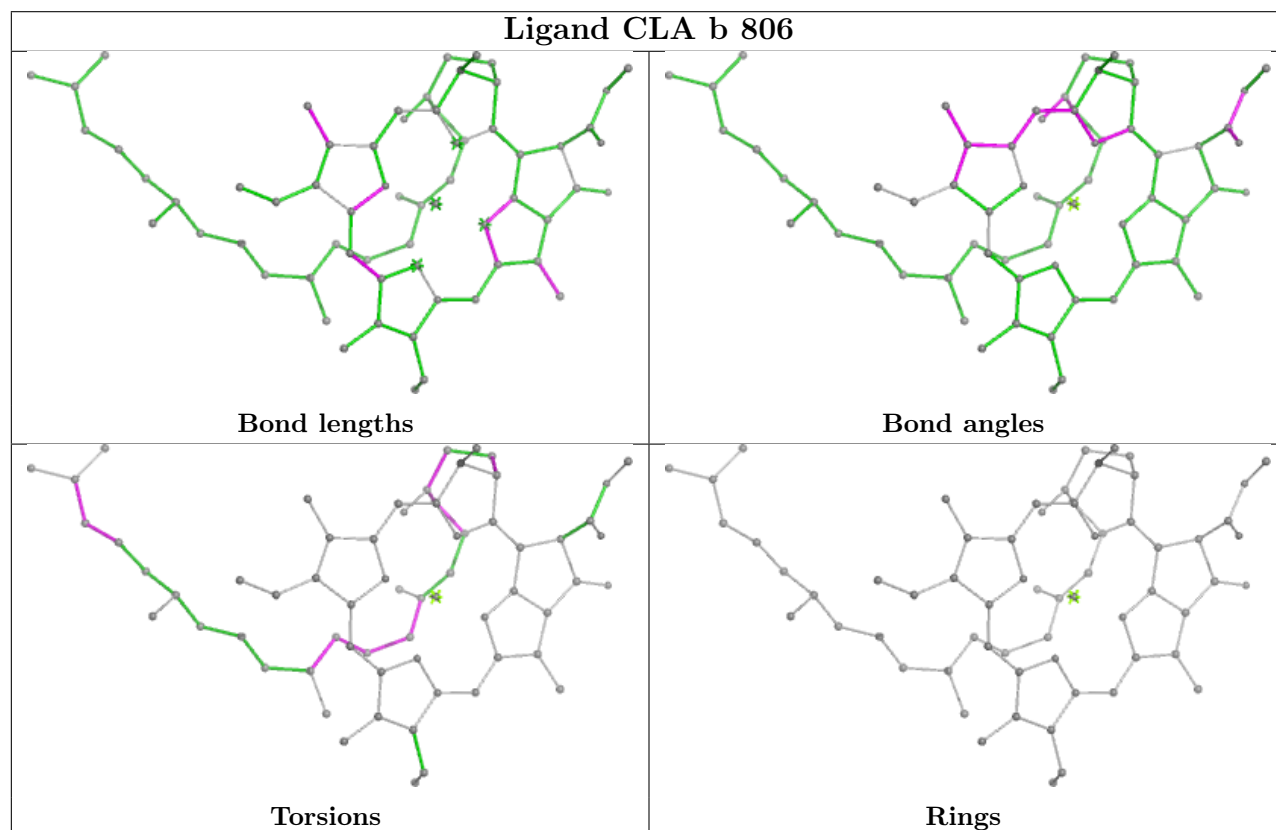
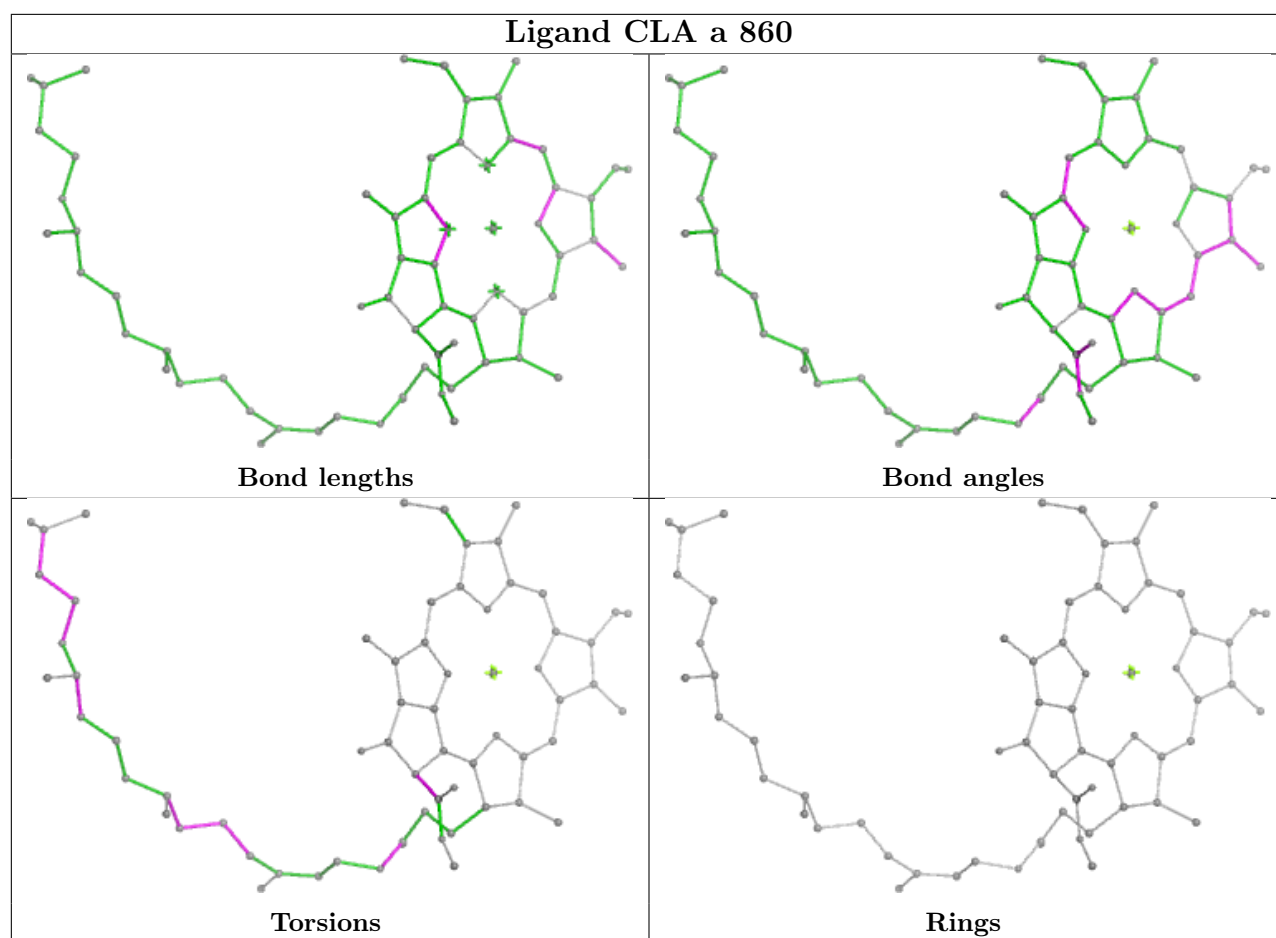
**Ligand BCR a 846****Ligand CLA a 823**



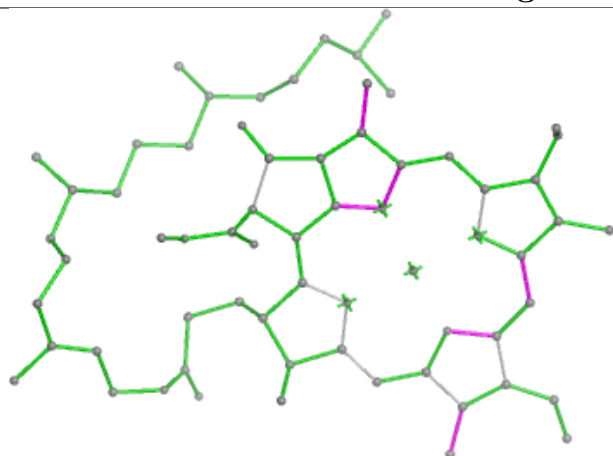


## Ligand CLA a 816

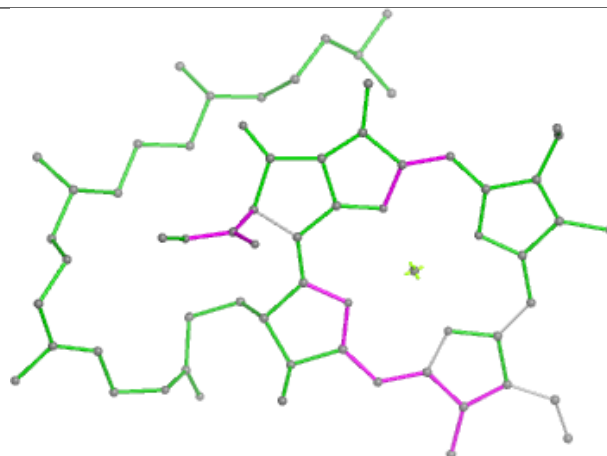




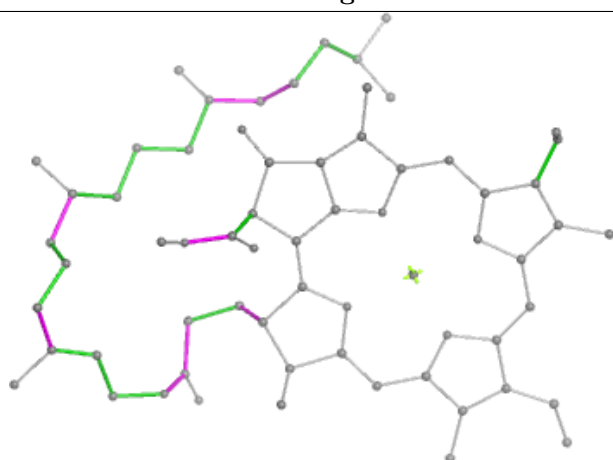
## Ligand CLA b 804



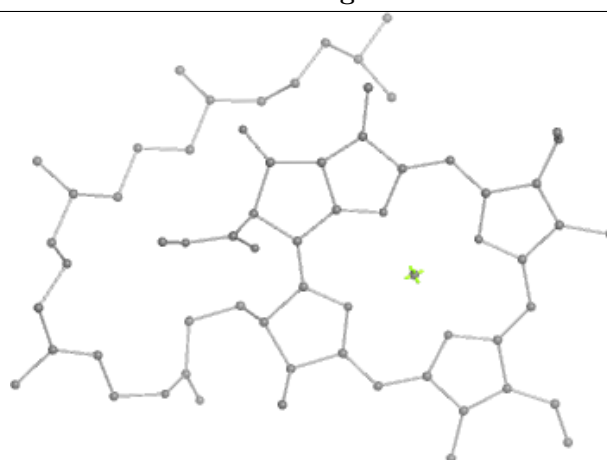
Bond lengths



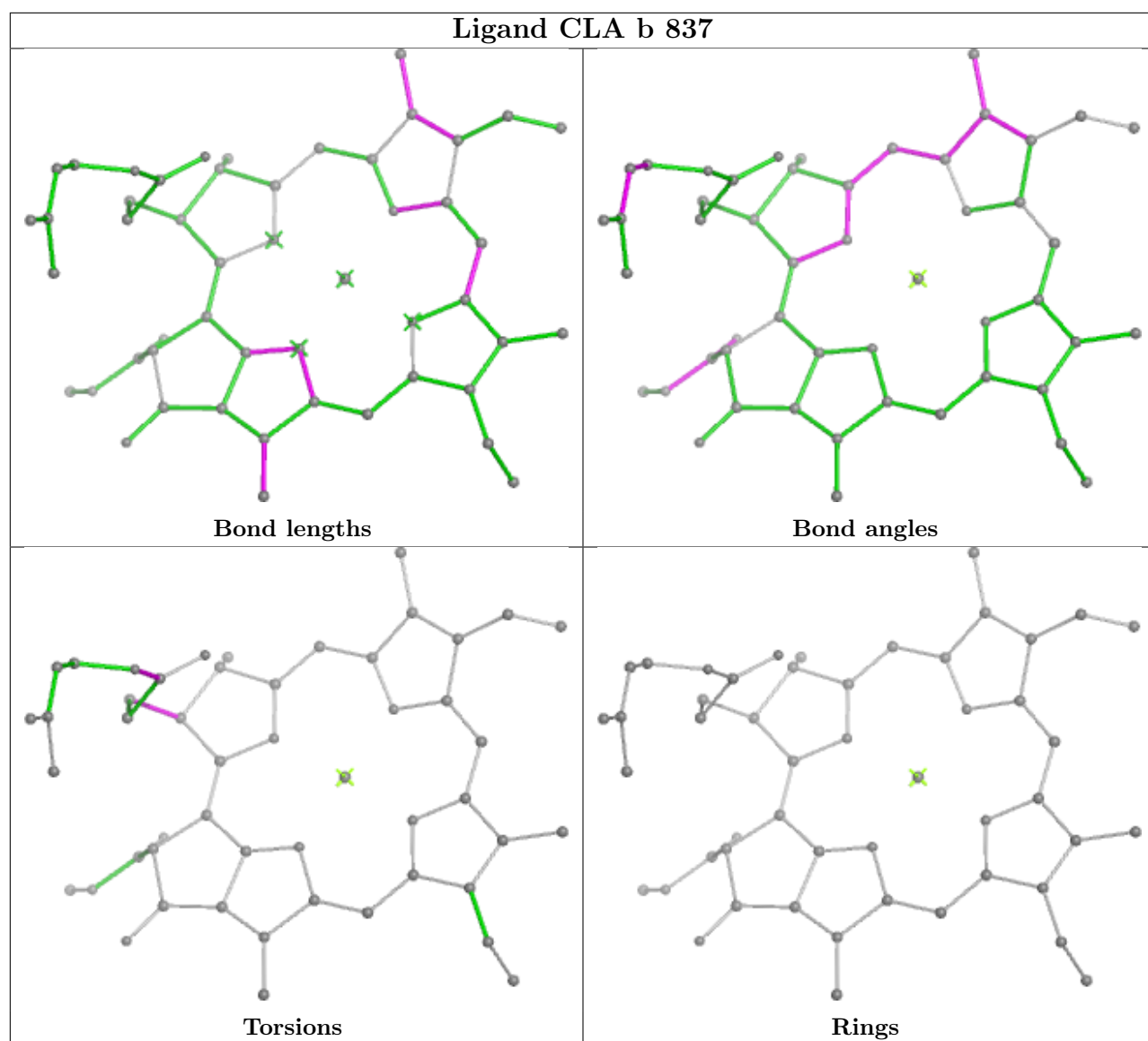
Bond angles



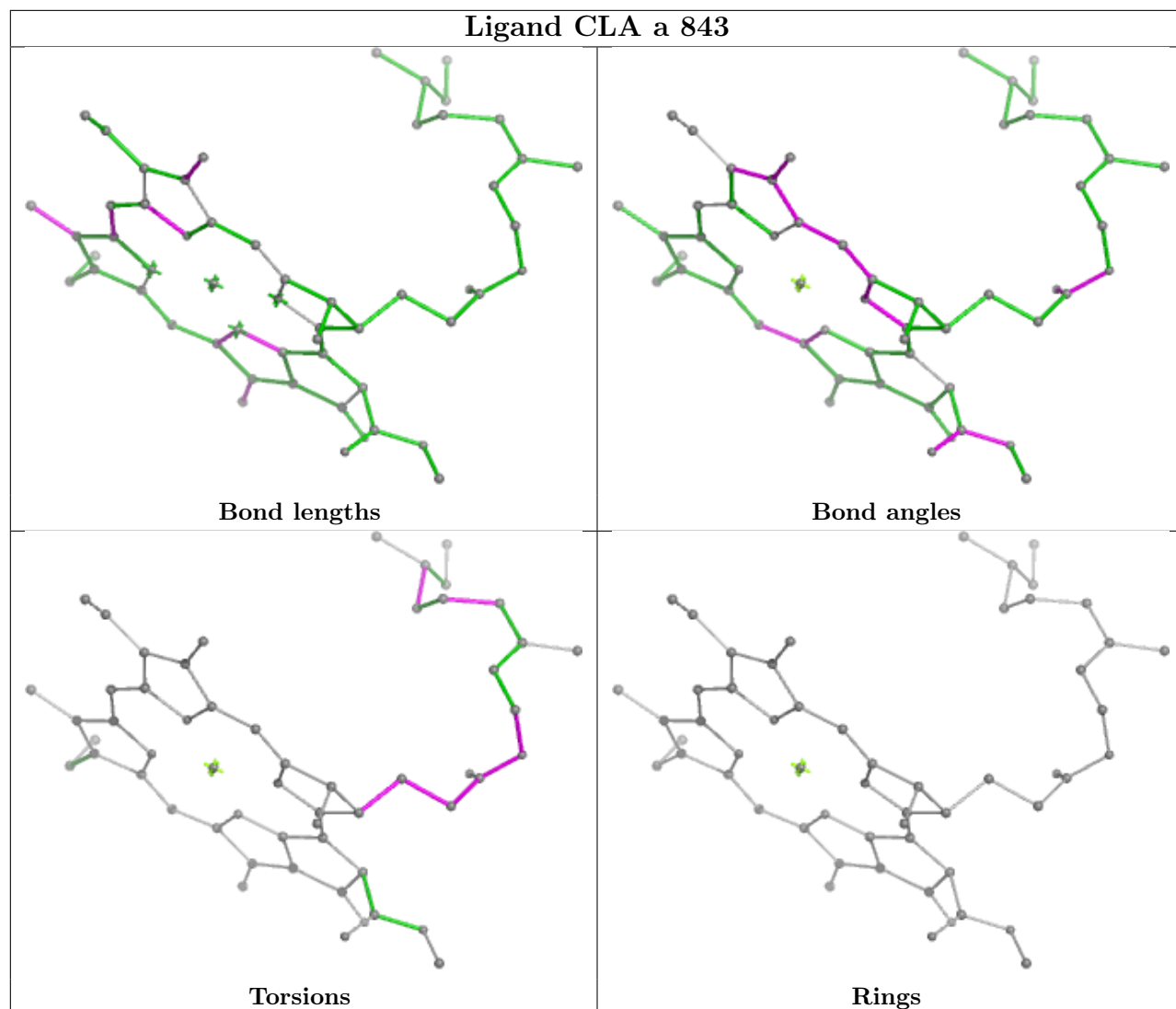
Torsions

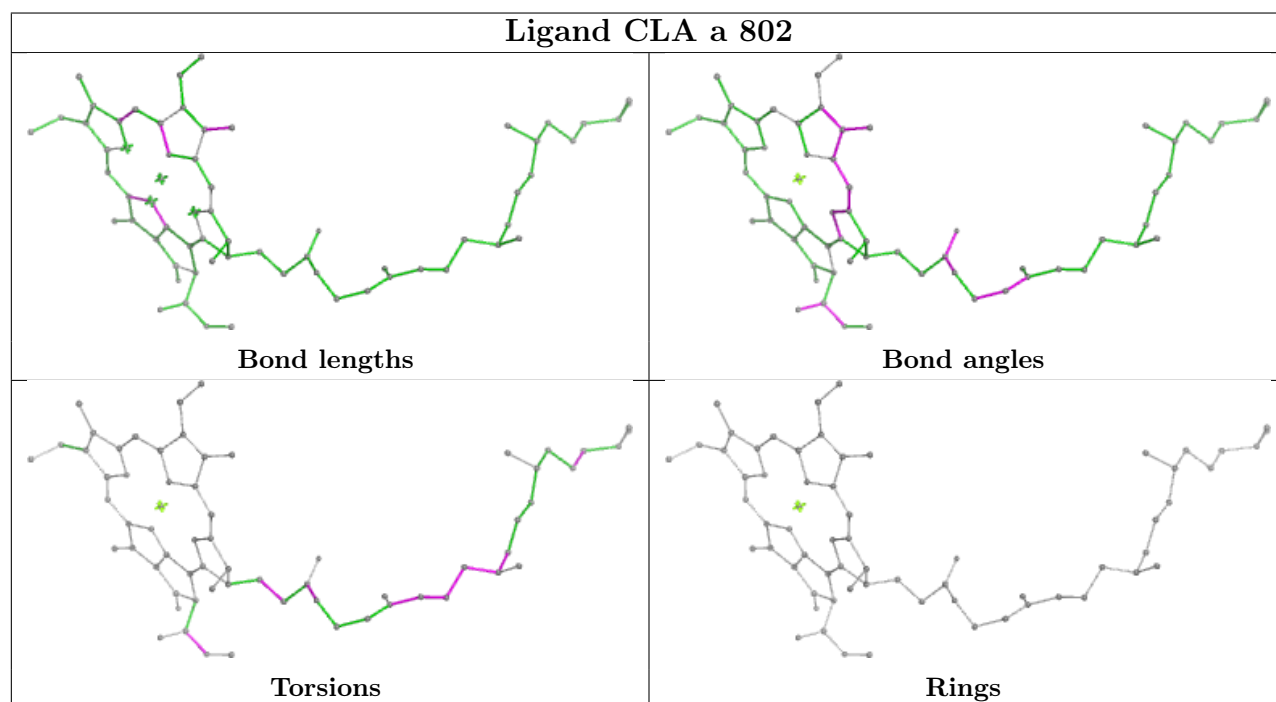
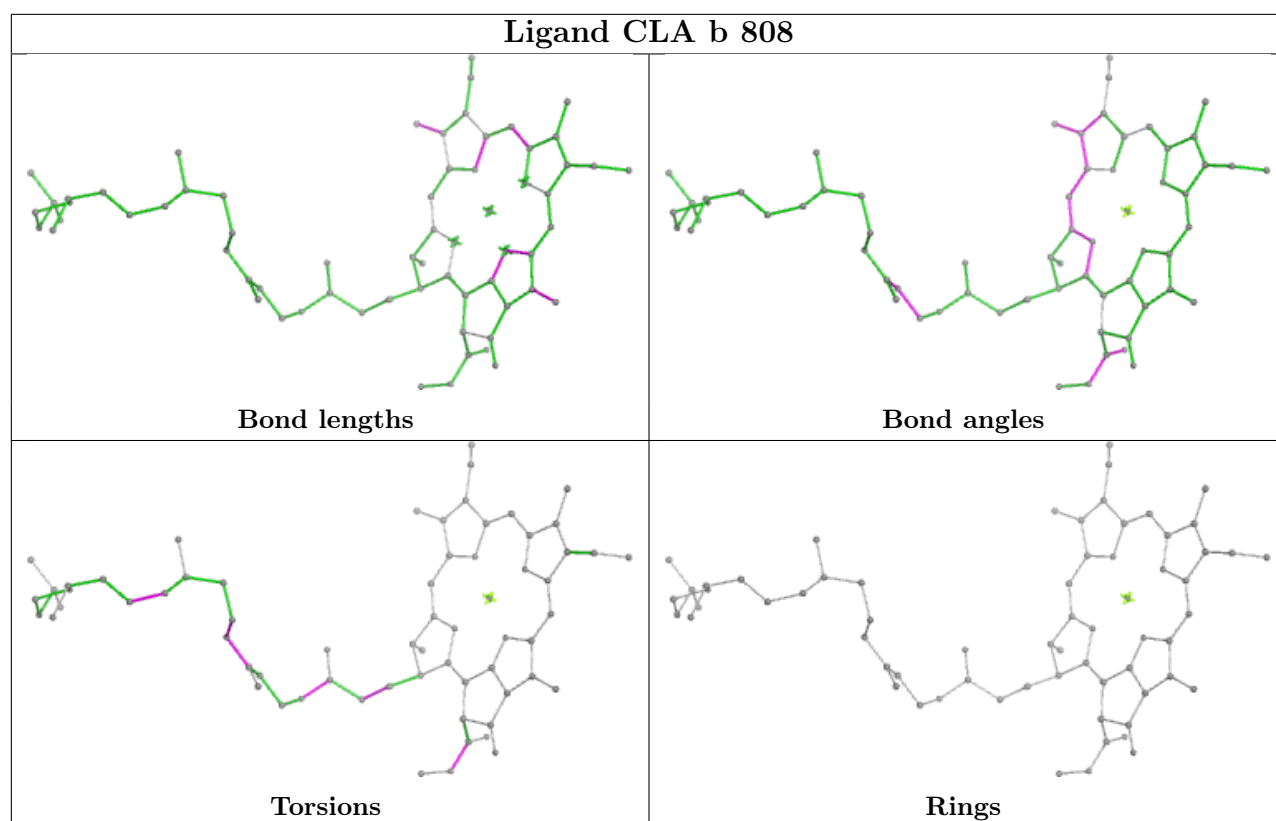


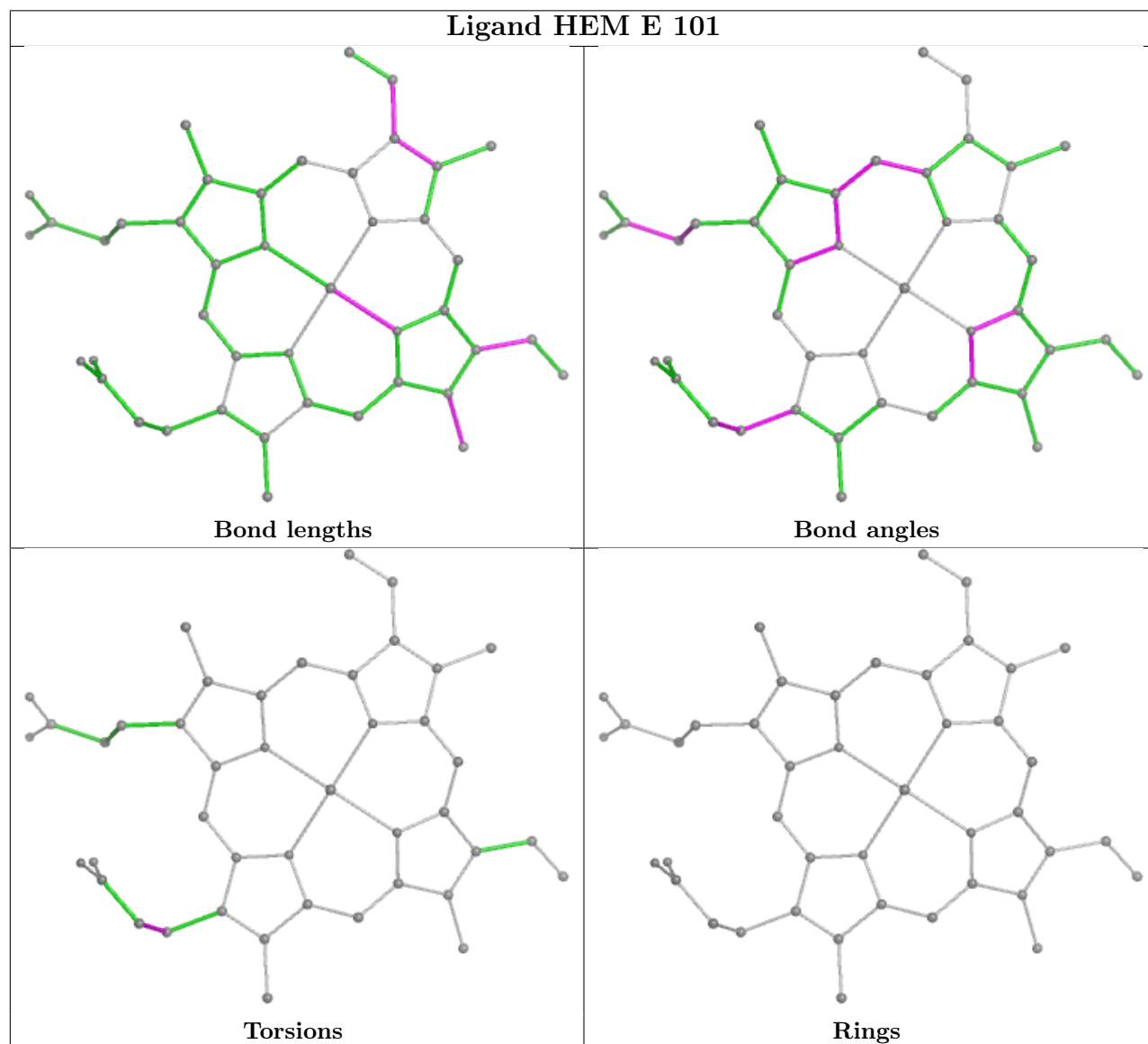
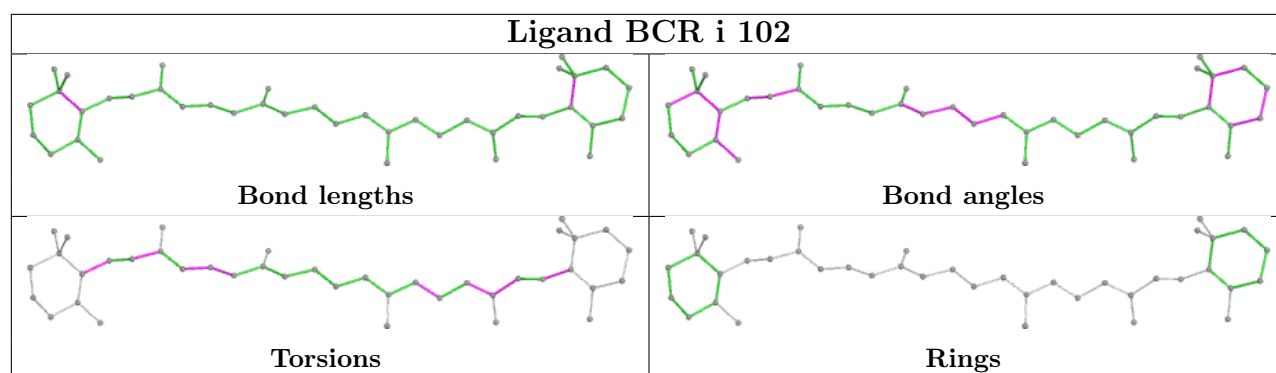
Rings

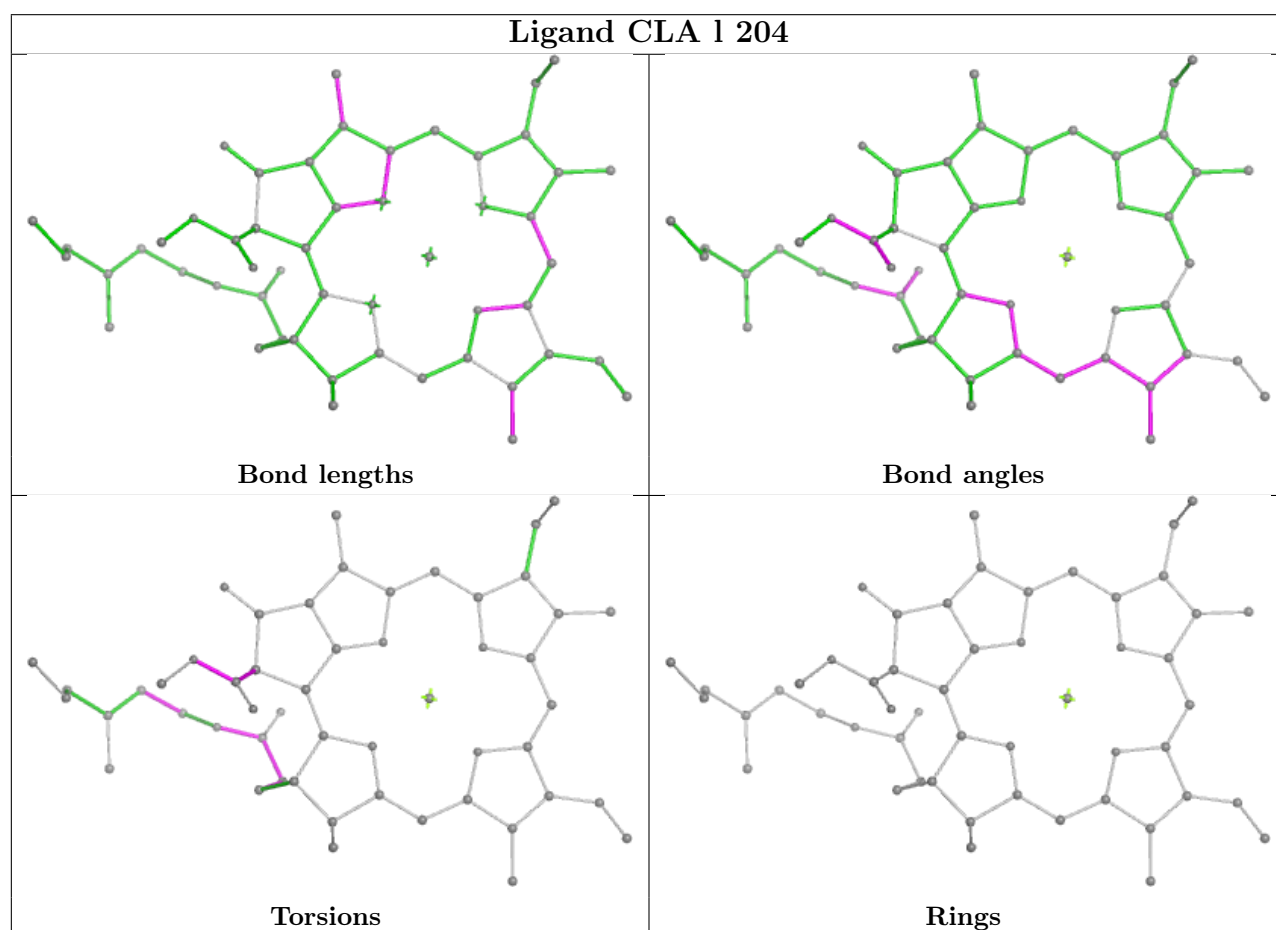
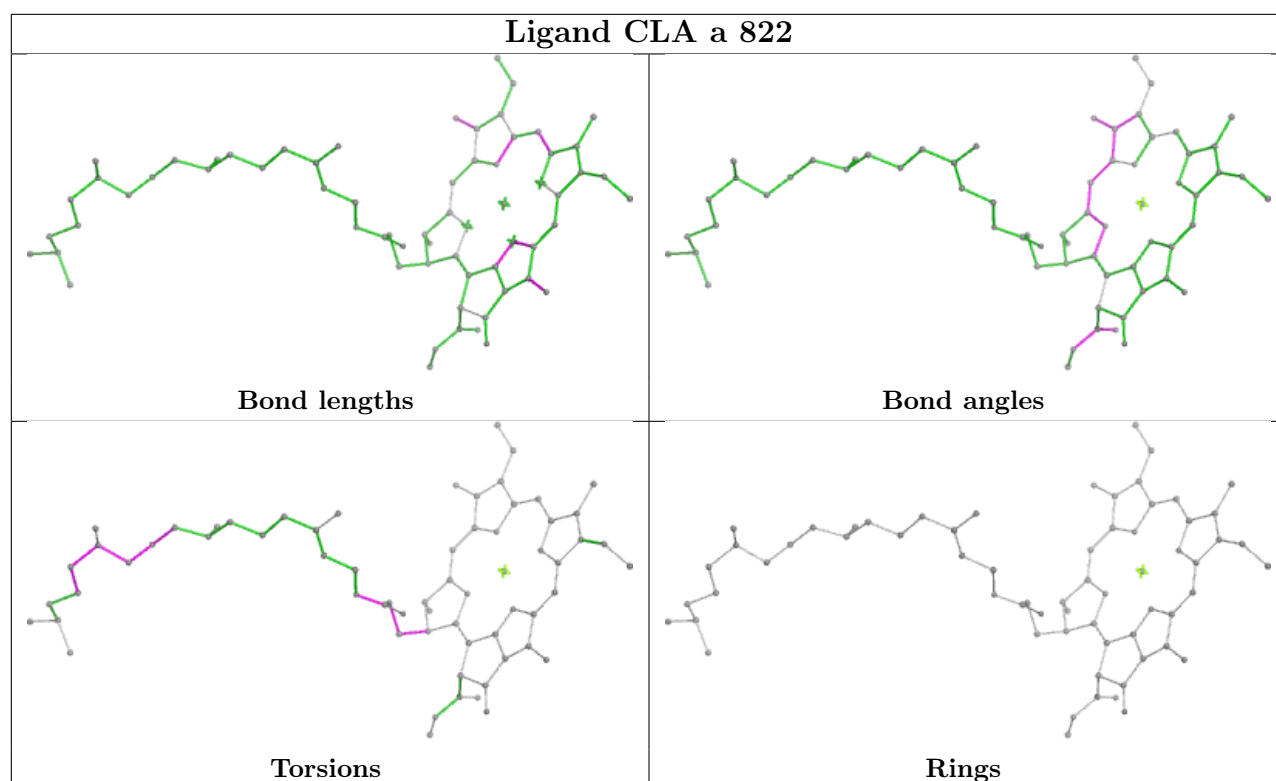


## Ligand CLA a 843

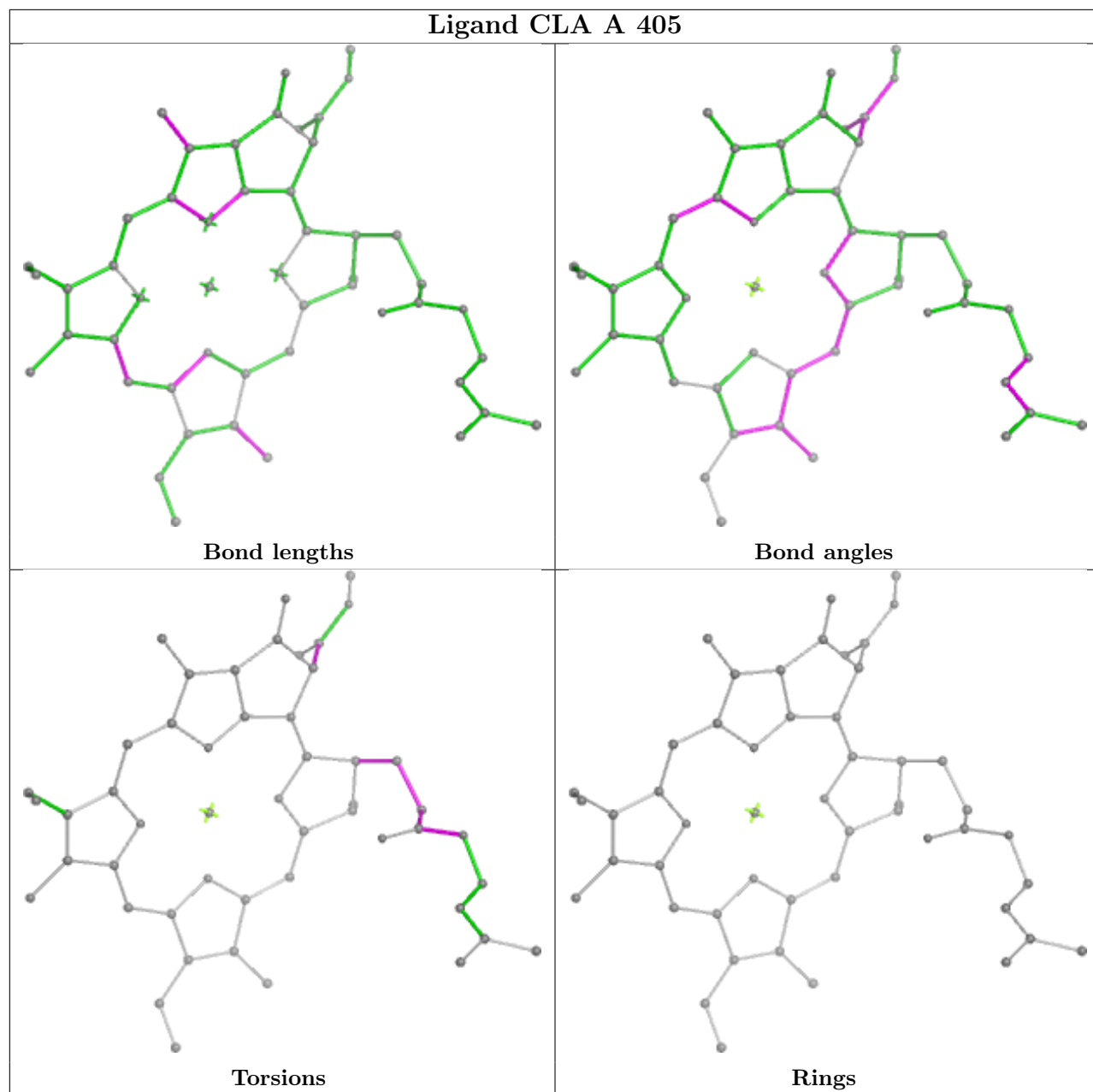


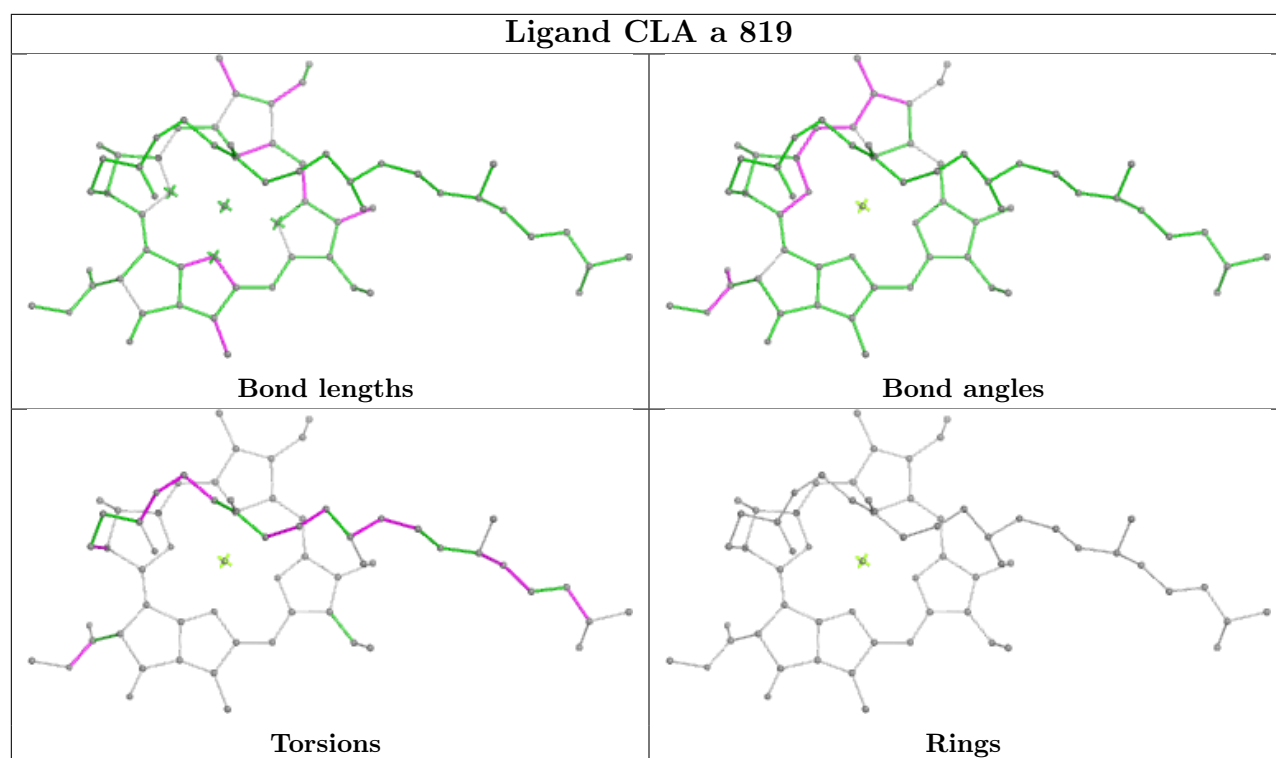












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

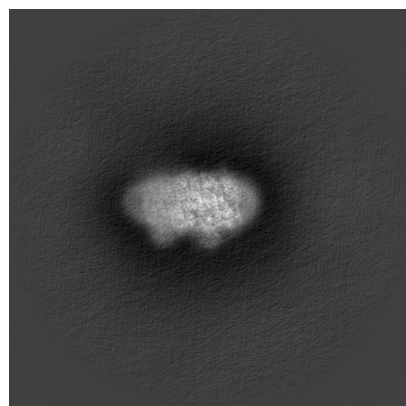
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15522. These allow visual inspection of the internal detail of the map and identification of artifacts.

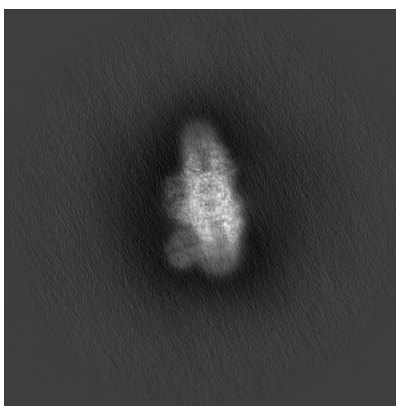
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

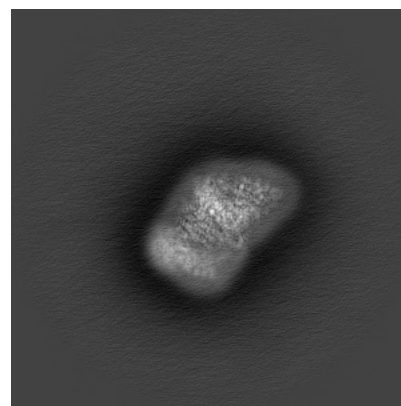
#### 6.1.1 Primary map



X

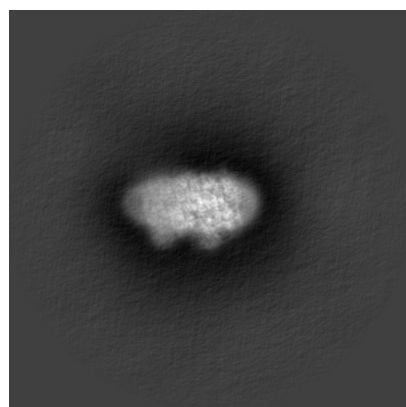


Y

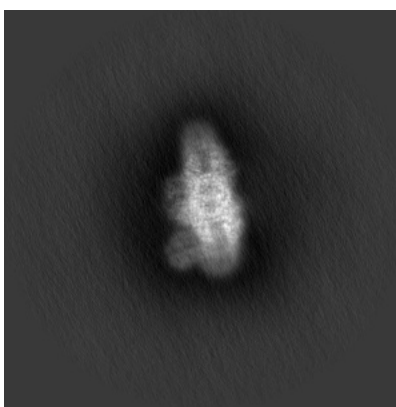


Z

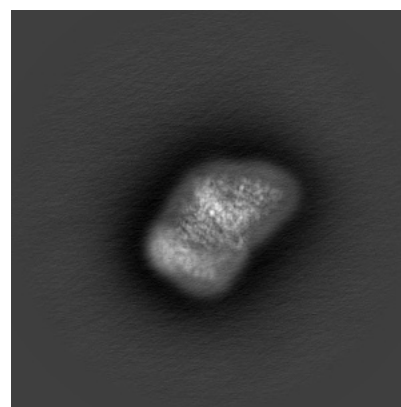
#### 6.1.2 Raw map



X



Y

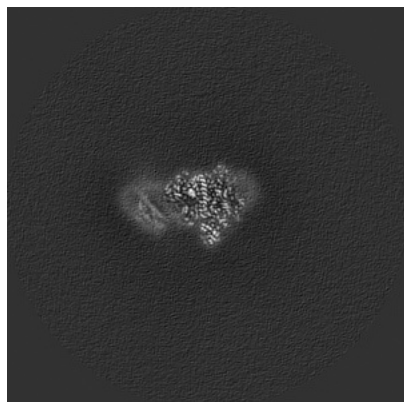


Z

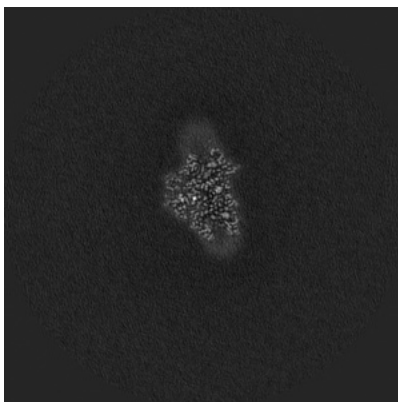
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

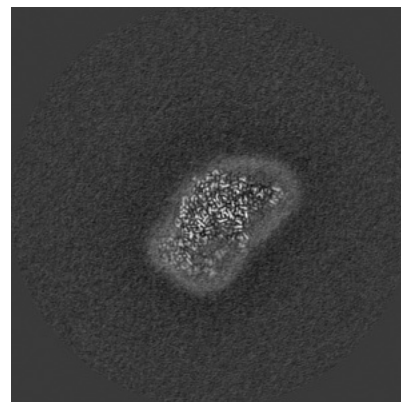
### 6.2.1 Primary map



X Index: 200

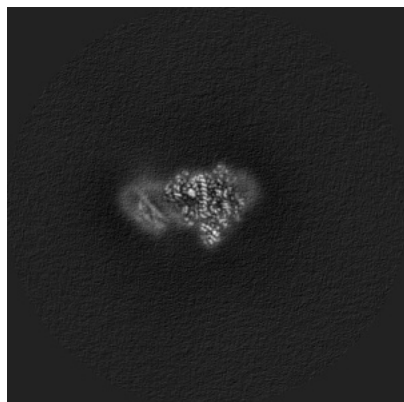


Y Index: 200

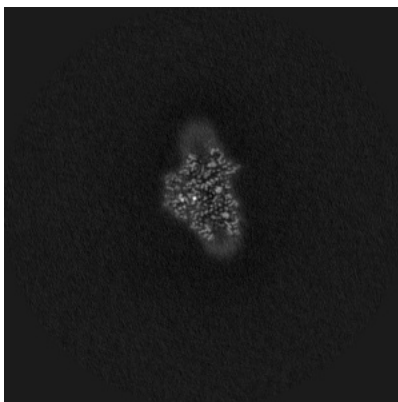


Z Index: 200

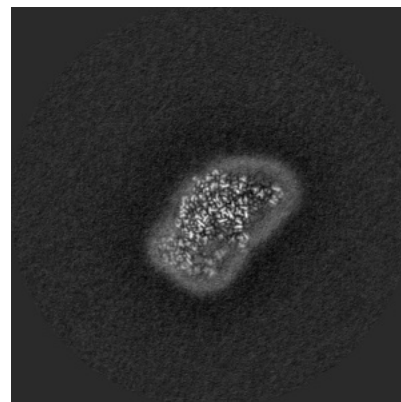
### 6.2.2 Raw map



X Index: 200



Y Index: 200

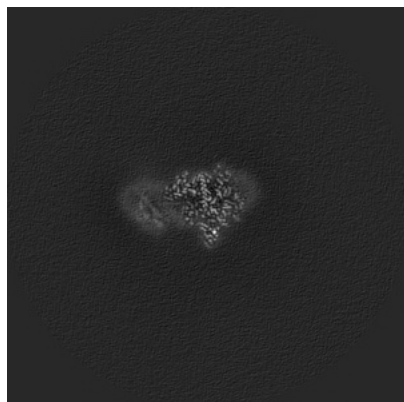


Z Index: 200

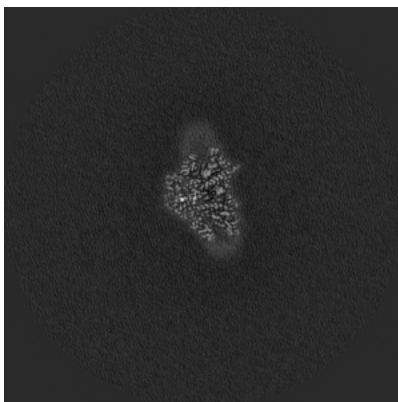
The images above show central slices of the map in three orthogonal directions.

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

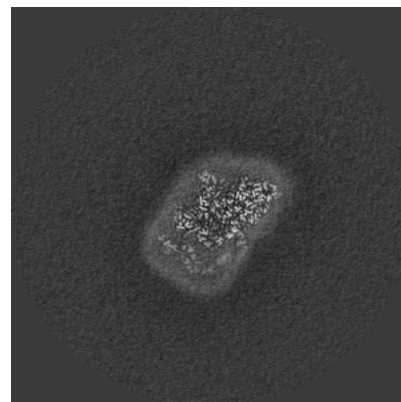
### 6.3.1 Primary map



X Index: 201

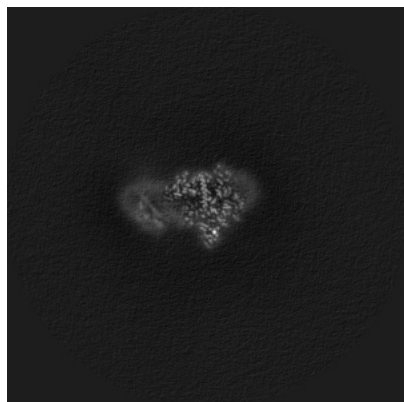


Y Index: 199

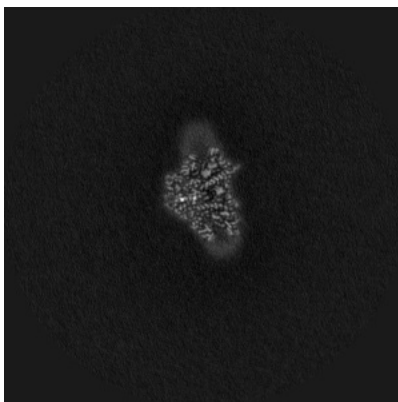


Z Index: 210

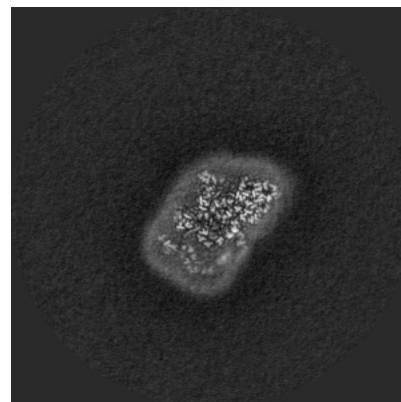
### 6.3.2 Raw map



X Index: 201



Y Index: 199

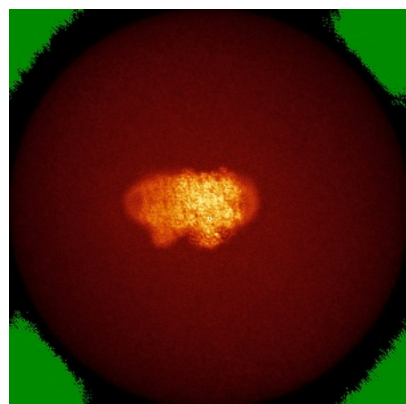


Z Index: 210

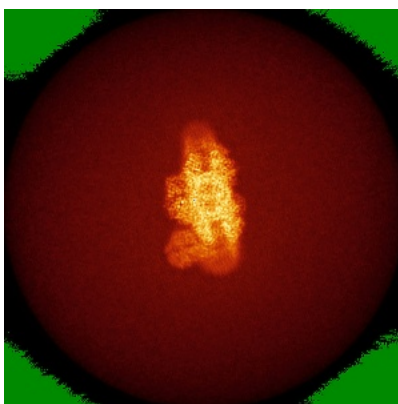
The images above show the largest variance slices of the map in three orthogonal directions.

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

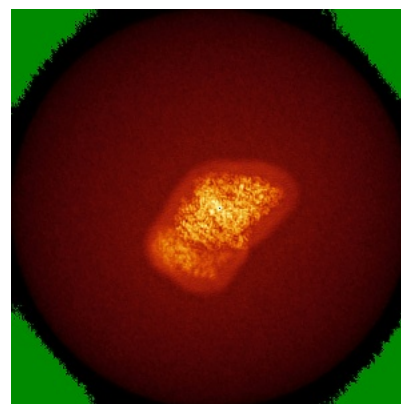
### 6.4.1 Primary map



X

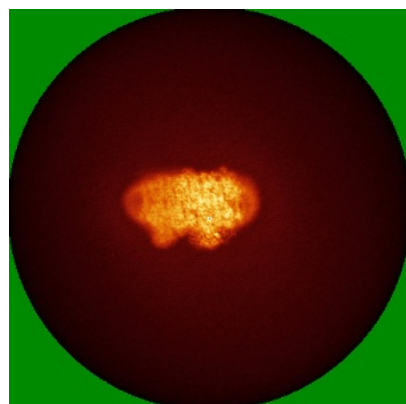


Y

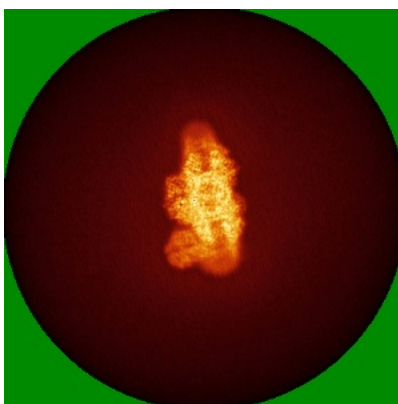


Z

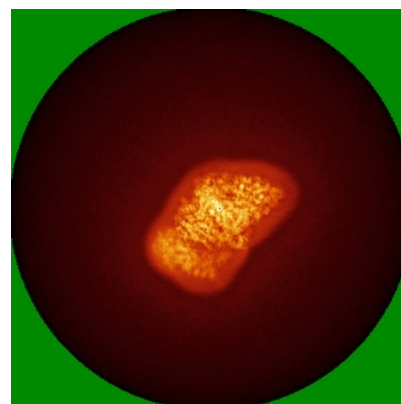
### 6.4.2 Raw map



X



Y



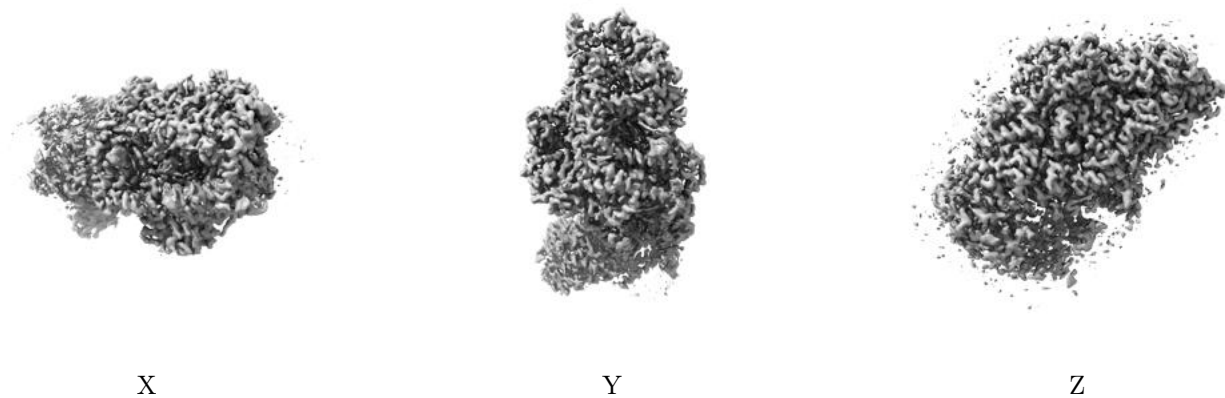
Z

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.



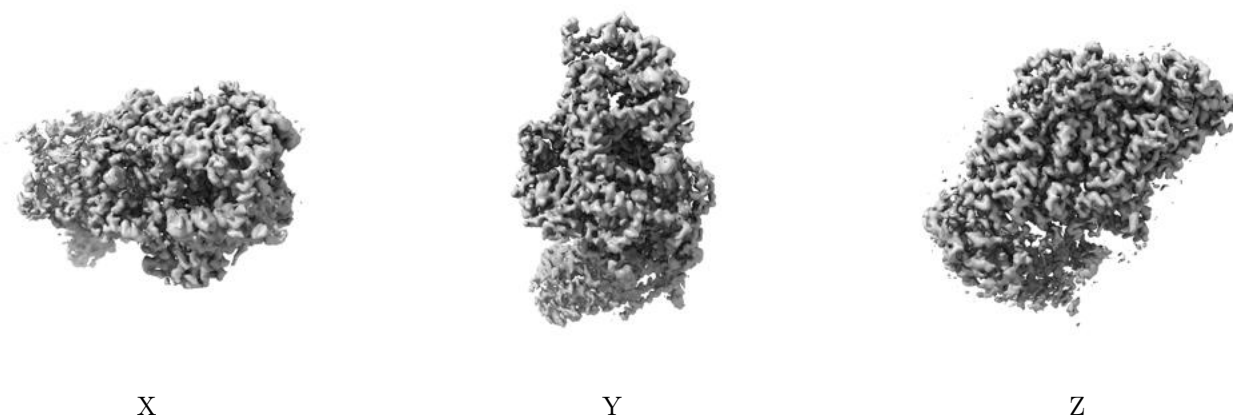
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0845. 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.

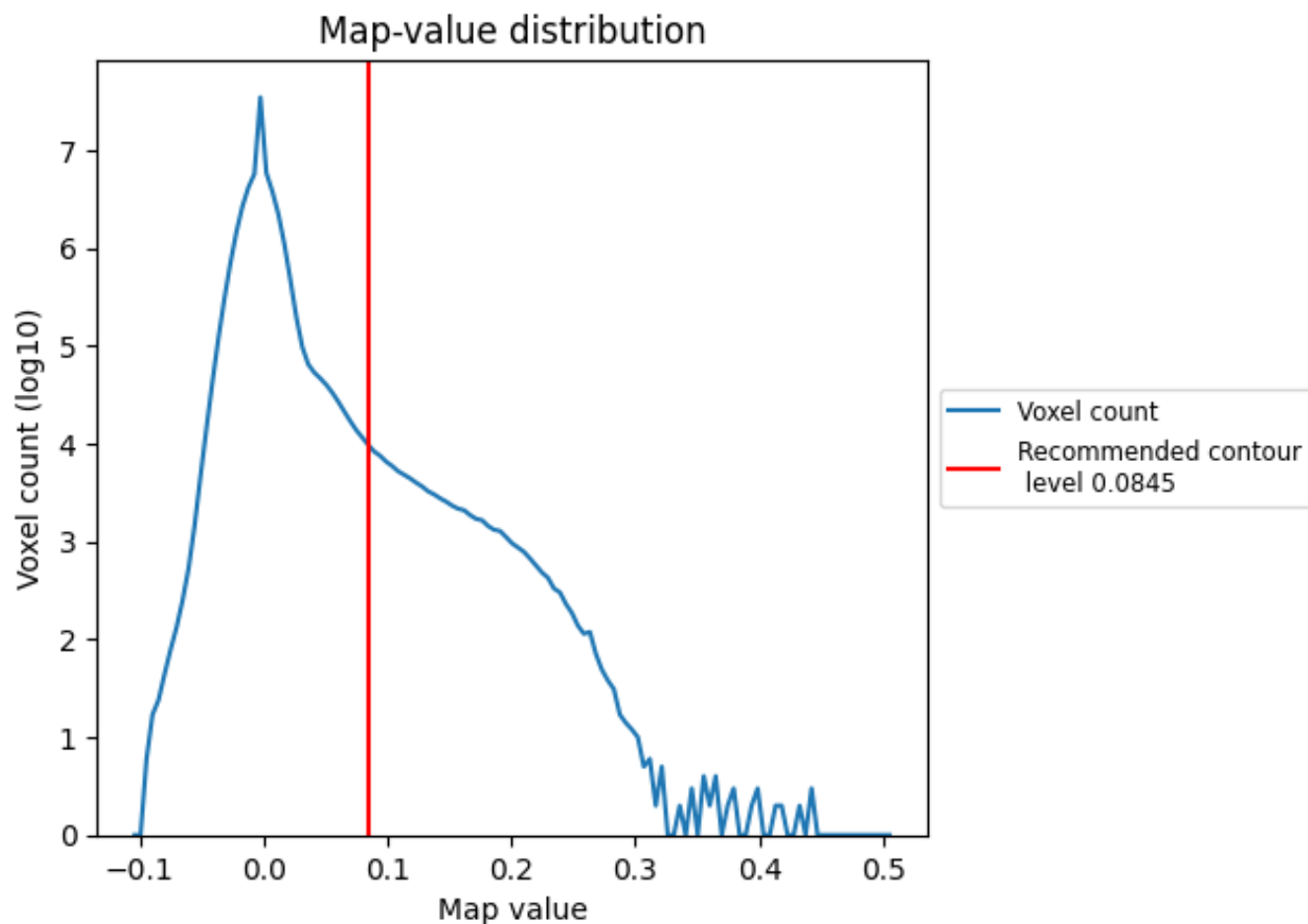
## 6.6 Mask visualisation [i](#)

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.

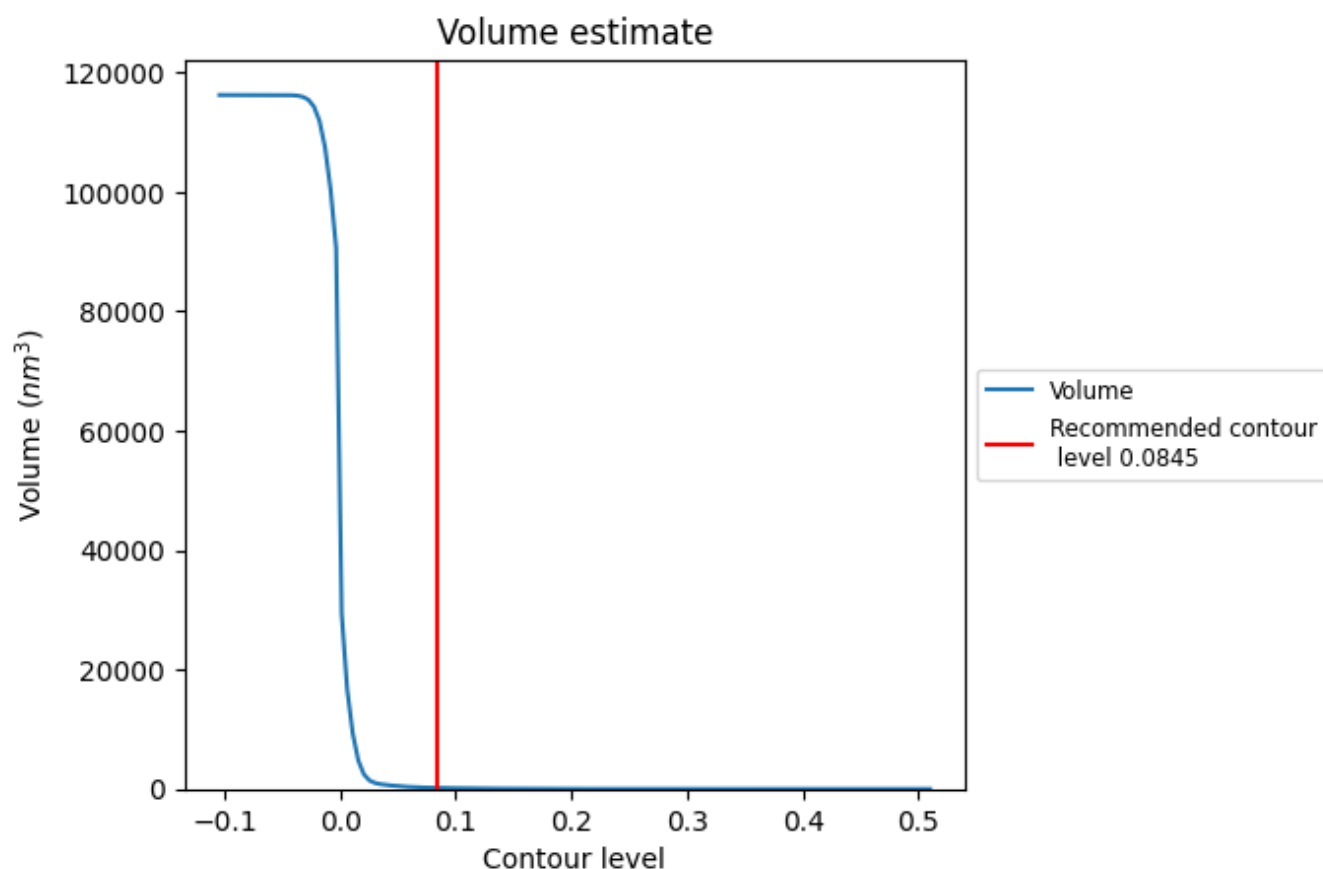
### 7.1 Map-value distribution [i](#)



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.



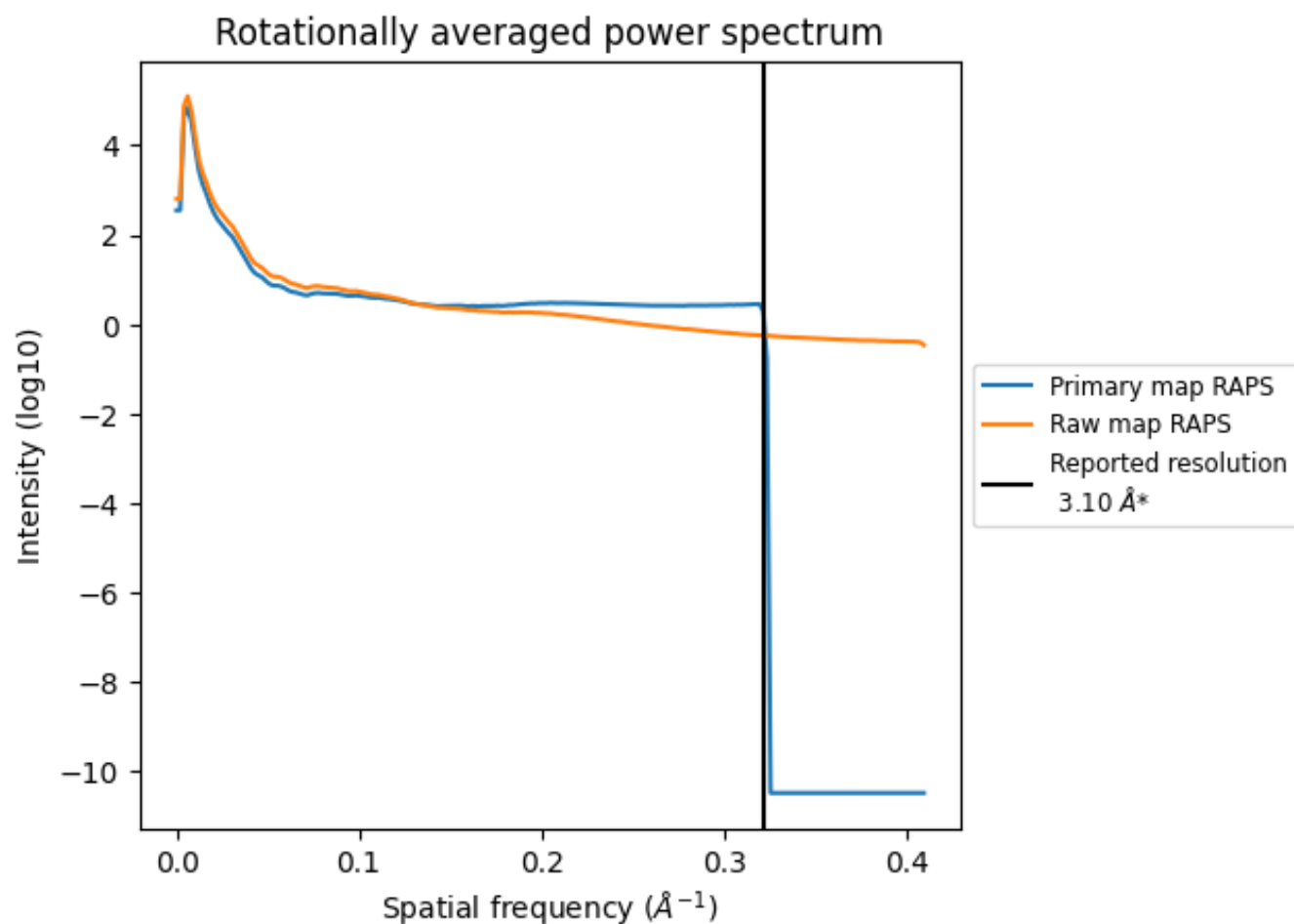
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173  $\text{nm}^3$ ; this corresponds to an approximate mass of 156 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 ⓘ

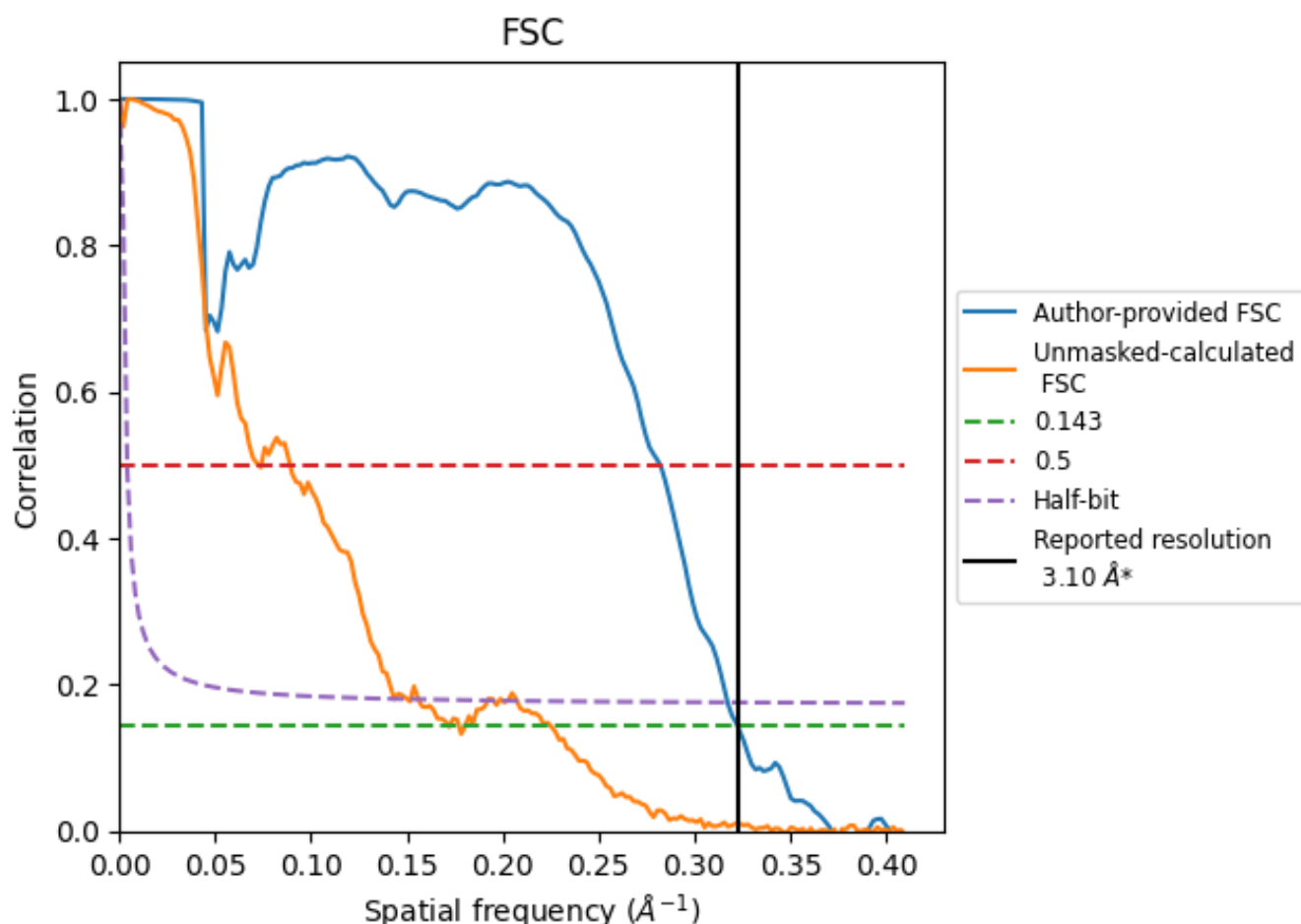


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

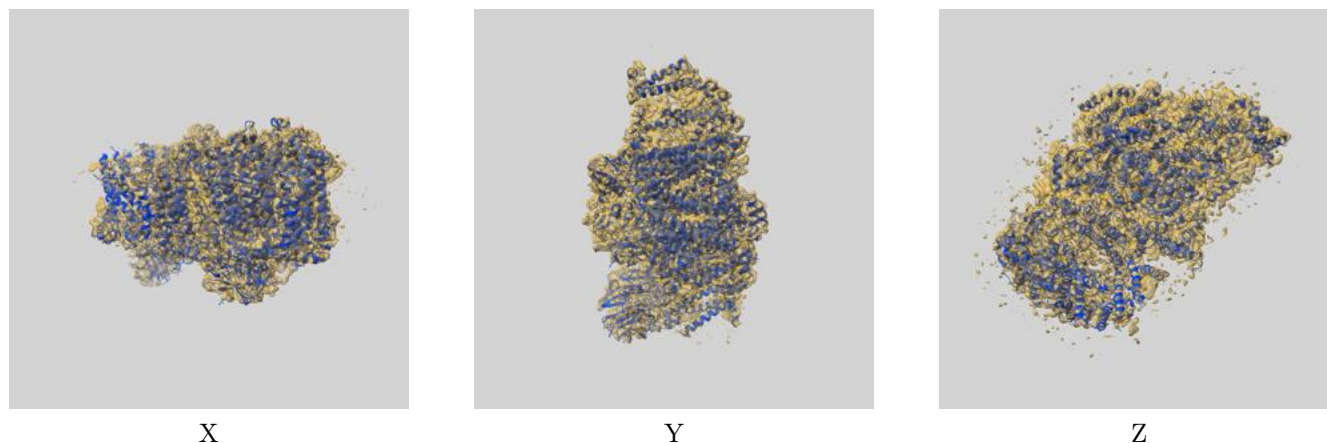
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.55	3.15
Unmasked-calculated*	5.82	13.79	6.97

\*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 5.82 differs from the reported value 3.1 by more than 10 %

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

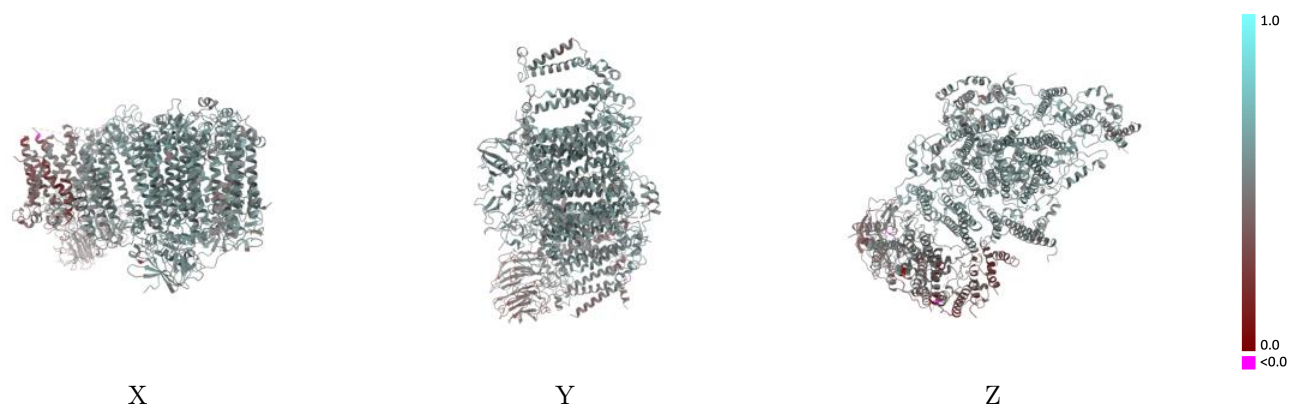
This section contains information regarding the fit between EMDB map EMD-15522 and PDB model 8AM5. Per-residue inclusion information can be found in section 3 on page 23.

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



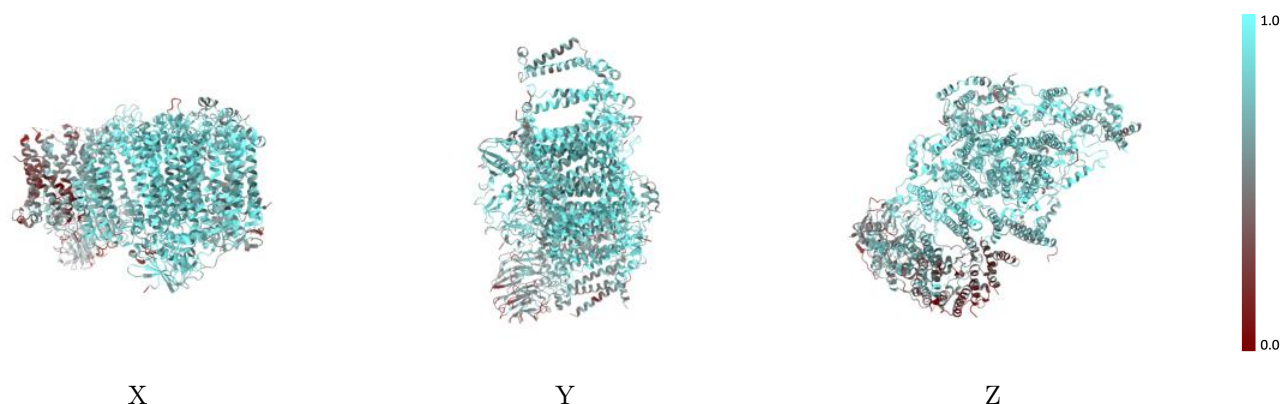
The images above show the 3D surface view of the map at the recommended contour level 0.0845 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



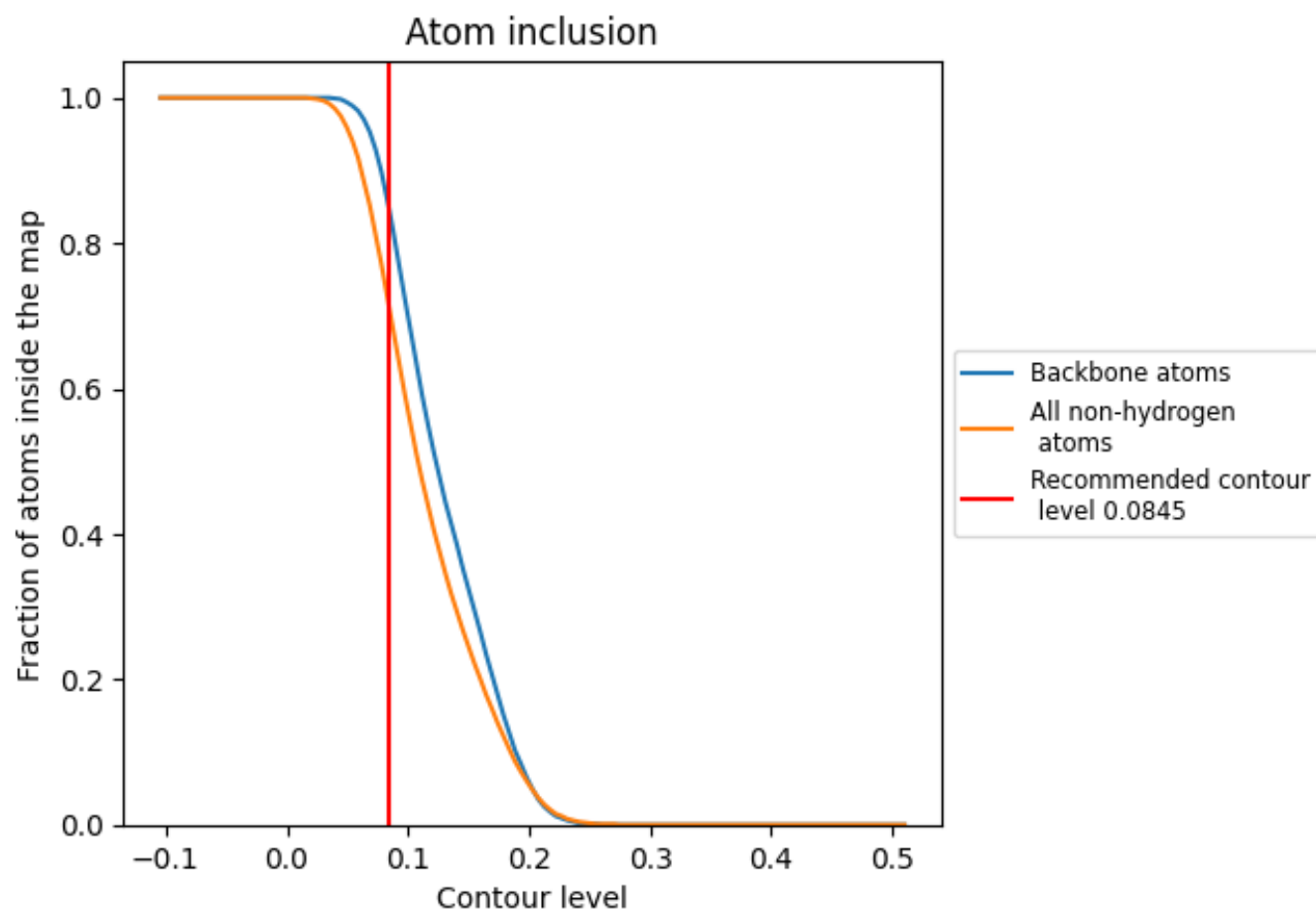
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0845).





































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.0845) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.5200
A	 0.6090	 0.4720
D	 0.4770	 0.4120
E	 0.4100	 0.3530
F	 0.3460	 0.3150
I	 0.4820	 0.4130
S	 0.4850	 0.4110
a	 0.7970	 0.5600
b	 0.8220	 0.5610
c	 0.8970	 0.5540
d	 0.7830	 0.5440
e	 0.7480	 0.5360
f	 0.6720	 0.5250
i	 0.7080	 0.5450
j	 0.5850	 0.5060
k	 0.5770	 0.4970
l	 0.6190	 0.4990
m	 0.6920	 0.5460

