



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 02:38 PM JST

PDB ID : 8ZET
EMDB ID : EMD-60044
Title : Tp-PSI-FCPI-S in Thalassiosira pseudonana
Authors : Feng, Y.; Li, Z.; Shen, J.R.; Wang, W.
Deposited on : 2024-05-06
Resolution : 3.20 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

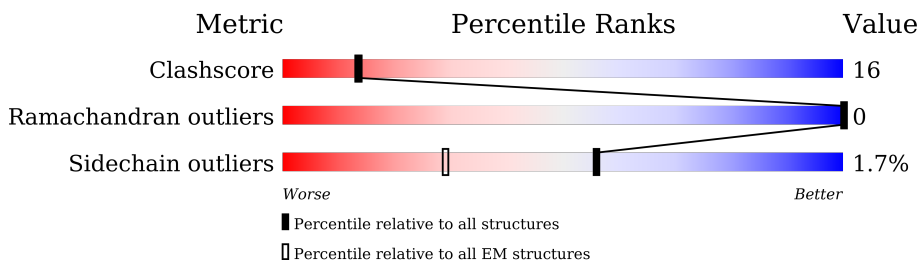
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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.




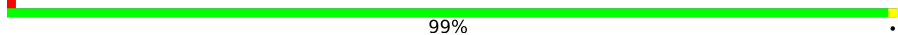
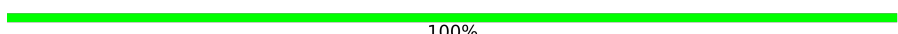
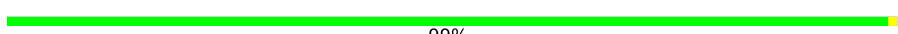


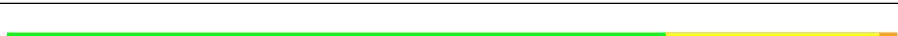
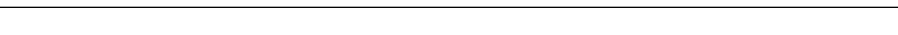
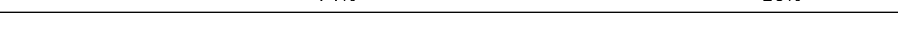
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	743	99%
2	b	732	99%
3	c	80	100%
4	d	132	98%
5	e	62	95% 5%
6	f	160	99%
7	g	131	97%
8	i	33	100%

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Mol	Chain	Length	Quality of chain
9	j	40	 92% 8%
10	l	146	 99%
11	m	29	 100%
12	r	89	 99%
13	B	165	 68% 27% 5%
14	C	170	 67% 32%
15	D	164	 74% 24%
16	E	185	 74% 26%
17	H	168	 72% 28%

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
18	CLA	B	306	X	-	-	-
18	CLA	B	307	X	-	-	-
18	CLA	B	308	X	-	-	-
18	CLA	B	309	X	-	-	-
18	CLA	B	310	X	-	-	-
18	CLA	B	311	X	-	-	-
18	CLA	B	312	X	-	-	-
18	CLA	B	314	X	-	-	-
18	CLA	C	306	X	-	-	-
18	CLA	C	307	X	-	-	-
18	CLA	C	309	X	-	-	-
18	CLA	C	310	X	-	-	-
18	CLA	C	311	X	-	-	-
18	CLA	C	312	X	-	-	-
18	CLA	C	314	X	-	-	-
18	CLA	C	315	X	-	-	-
18	CLA	C	316	X	-	-	-
18	CLA	C	317	X	-	-	-
18	CLA	C	318	X	-	-	-
18	CLA	D	207	X	-	-	-
18	CLA	D	208	X	-	-	-
18	CLA	D	209	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	D	210	X	-	-	-
18	CLA	D	211	X	-	-	-
18	CLA	D	212	X	-	-	-
18	CLA	D	213	X	-	-	-
18	CLA	D	214	X	-	-	-
18	CLA	D	215	X	-	-	-
18	CLA	D	216	X	-	-	-
18	CLA	D	217	X	-	-	-
18	CLA	E	309	X	-	-	-
18	CLA	E	310	X	-	-	-
18	CLA	E	311	X	-	-	-
18	CLA	E	312	X	-	-	-
18	CLA	E	313	X	-	-	-
18	CLA	E	314	X	-	-	-
18	CLA	E	315	X	-	-	-
18	CLA	E	316	X	-	-	-
18	CLA	H	305	X	-	-	-
18	CLA	H	306	X	-	-	-
18	CLA	H	307	X	-	-	-
18	CLA	H	308	X	-	-	-
18	CLA	H	309	X	-	-	-
18	CLA	H	310	X	-	-	-
18	CLA	H	311	X	-	-	-
18	CLA	H	313	X	-	-	-
18	CLA	H	314	X	-	-	-
18	CLA	H	315	X	-	-	-
18	CLA	a	801	X	-	-	-
18	CLA	a	802	X	-	-	-
18	CLA	a	803	X	-	-	-
18	CLA	a	804	X	-	-	-
18	CLA	a	805	X	-	-	-
18	CLA	a	806	X	-	-	-
18	CLA	a	807	X	-	-	-
18	CLA	a	808	X	-	-	-
18	CLA	a	809	X	-	-	-
18	CLA	a	810	X	-	-	-
18	CLA	a	811	X	-	-	-
18	CLA	a	812	X	-	-	-
18	CLA	a	813	X	-	-	-
18	CLA	a	814	X	-	-	-
18	CLA	a	815	X	-	-	-
18	CLA	a	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	a	817	X	-	-	-
18	CLA	a	818	X	-	-	-
18	CLA	a	819	X	-	-	-
18	CLA	a	820	X	-	-	-
18	CLA	a	821	X	-	-	-
18	CLA	a	822	X	-	-	-
18	CLA	a	823	X	-	-	-
18	CLA	a	824	X	-	-	-
18	CLA	a	825	X	-	-	-
18	CLA	a	826	X	-	-	-
18	CLA	a	827	X	-	-	-
18	CLA	a	828	X	-	-	-
18	CLA	a	830	X	-	-	-
18	CLA	a	836	X	-	-	-
18	CLA	a	837	X	-	-	-
18	CLA	a	838	X	-	-	-
18	CLA	a	839	X	-	-	-
18	CLA	a	840	X	-	-	-
18	CLA	a	841	X	-	-	-
18	CLA	a	842	X	-	-	-
18	CLA	a	843	X	-	-	-
18	CLA	a	844	X	-	-	-
18	CLA	a	846	X	-	-	-
18	CLA	a	847	X	-	-	-
18	CLA	a	848	X	-	-	-
18	CLA	a	853	X	-	-	-
18	CLA	a	854	X	-	-	-
18	CLA	a	855	X	-	-	-
18	CLA	b	801	X	-	-	-
18	CLA	b	803	X	-	-	-
18	CLA	b	804	X	-	-	-
18	CLA	b	805	X	-	-	-
18	CLA	b	806	X	-	-	-
18	CLA	b	807	X	-	-	-
18	CLA	b	808	X	-	-	-
18	CLA	b	809	X	-	-	-
18	CLA	b	810	X	-	-	-
18	CLA	b	811	X	-	-	-
18	CLA	b	812	X	-	-	-
18	CLA	b	813	X	-	-	-
18	CLA	b	814	X	-	-	-
18	CLA	b	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	b	816	X	-	-	-
18	CLA	b	817	X	-	-	-
18	CLA	b	818	X	-	-	-
18	CLA	b	819	X	-	-	-
18	CLA	b	820	X	-	-	-
18	CLA	b	821	X	-	-	-
18	CLA	b	822	X	-	-	-
18	CLA	b	823	X	-	-	-
18	CLA	b	824	X	-	-	-
18	CLA	b	825	X	-	-	-
18	CLA	b	826	X	-	-	-
18	CLA	b	827	X	-	-	-
18	CLA	b	828	X	-	-	-
18	CLA	b	829	X	-	-	-
18	CLA	b	830	X	-	-	-
18	CLA	b	837	X	-	-	-
18	CLA	b	838	X	-	-	-
18	CLA	b	840	X	-	-	-
18	CLA	b	841	X	-	-	-
18	CLA	b	842	X	-	-	-
18	CLA	b	843	X	-	-	-
18	CLA	b	844	X	-	-	-
18	CLA	b	845	X	-	-	-
18	CLA	b	846	X	-	-	-
18	CLA	b	848	X	-	-	-
18	CLA	b	849	X	-	-	-
18	CLA	b	850	X	-	-	-
18	CLA	f	202	X	-	-	-
18	CLA	f	203	X	-	-	-
18	CLA	f	204	X	-	-	-
18	CLA	i	101	X	-	-	-
18	CLA	j	104	X	-	-	-
18	CLA	l	202	X	-	-	-
18	CLA	l	203	X	-	-	-
18	CLA	l	205	X	-	-	-
18	CLA	r	202	X	-	-	-

2 Entry composition i

There are 29 unique types of molecules in this entry. The entry contains 36577 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	743	Total	C	N	O	S	0	0
			5852	3822	992	1009	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	732	Total	C	N	O	S	0	0
			5824	3827	982	996	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	132	Total	C	N	O	S	0	0
			1040	665	177	195	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	62	Total	C	N	O	S	0	0
			503	317	89	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	160	Total	C	N	O	S	0	0
			1242	795	211	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	131	981	619	154	204	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	33	256	177	34	44	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	j	40	332	224	48	57	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	146	1095	722	178	193	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	m	29	220	147	33	38	2	0	0

- Molecule 12 is a protein called Tp-PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	r	89	683	443	112	121	7	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B	165	1285	833	204	240	8	0	0

- Molecule 14 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	170	1302	841	213	240	8	0	0

- Molecule 15 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	D	164	1271	819	208	234	10	0	0

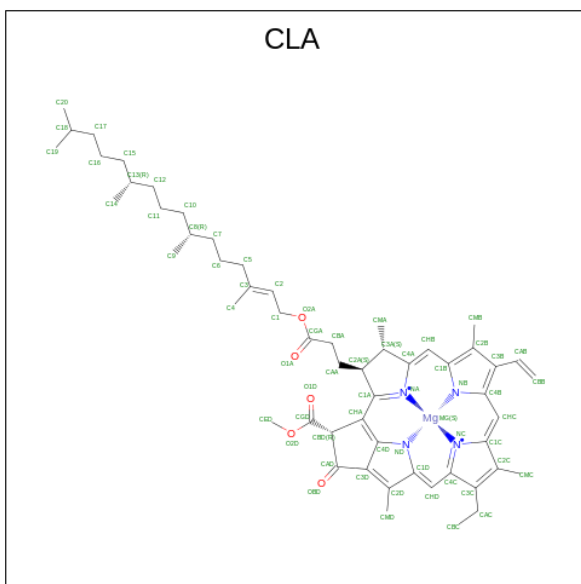
- Molecule 16 is a protein called Tp-RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	E	185	1413	902	235	262	14	0	0

- Molecule 17 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H	168	1300	834	214	242	10	0	0

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	55	45	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	62	52	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	50	40	1	4	5	0
18	a	1	45	35	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	45	35	1	4	5	0
18	a	1	49	39	1	4	5	0
18	a	1	51	41	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	a	1	45	35	1	4	5	0
18	a	1	51	41	1	4	5	0
18	a	1	60	50	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	52	42	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	60	50	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	65	55	1	4	5	0
18	a	1	56	46	1	4	5	0
18	a	1	55	45	1	4	5	0
18	a	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	b	1	65	55	1	4	5	0
18	b	1	58	48	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	45	35	1	4	5	0
18	b	1	60	50	1	4	5	0
18	b	1	47	37	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	60	50	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	61	51	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	62	52	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	54	44	1	4	5	0
18	b	1	65	55	1	4	5	0
18	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	f	1	65	55	1	4	5	0
18	f	1	65	55	1	4	5	0
18	f	1	45	35	1	4	5	0
18	i	1	60	50	1	4	5	0
18	j	1	41	33	1	4	3	0
18	l	1	49	39	1	4	5	0
18	l	1	65	55	1	4	5	0
18	l	1	45	35	1	4	5	0
18	r	1	45	35	1	4	5	0
18	B	1	57	49	1	4	3	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	46	36	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	41	33	1	4	3	0
18	C	1	45	35	1	4	5	0
18	C	1	65	55	1	4	5	0
18	C	1	62	52	1	4	5	0
18	C	1	46	36	1	4	5	0

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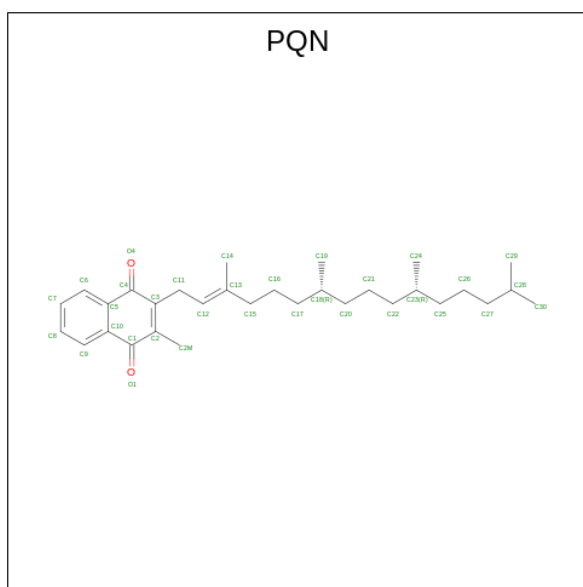
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	C	1	60	50	1	4	5	0
18	C	1	61	51	1	4	5	0
18	C	1	41	33	1	4	3	0
18	C	1	42	34	1	4	3	0
18	C	1	41	33	1	4	3	0
18	C	1	42	34	1	4	3	0
18	C	1	42	34	1	4	3	0
18	D	1	61	51	1	4	5	0
18	D	1	65	55	1	4	5	0
18	D	1	49	39	1	4	5	0
18	D	1	56	46	1	4	5	0
18	D	1	46	36	1	4	5	0
18	D	1	42	34	1	4	3	0
18	D	1	65	55	1	4	5	0
18	D	1	56	46	1	4	5	0
18	D	1	41	33	1	4	3	0
18	D	1	46	36	1	4	5	0
18	D	1	41	33	1	4	3	0
18	E	1	65	55	1	4	5	0
18	E	1	65	55	1	4	5	0
18	E	1	46	36	1	4	5	0

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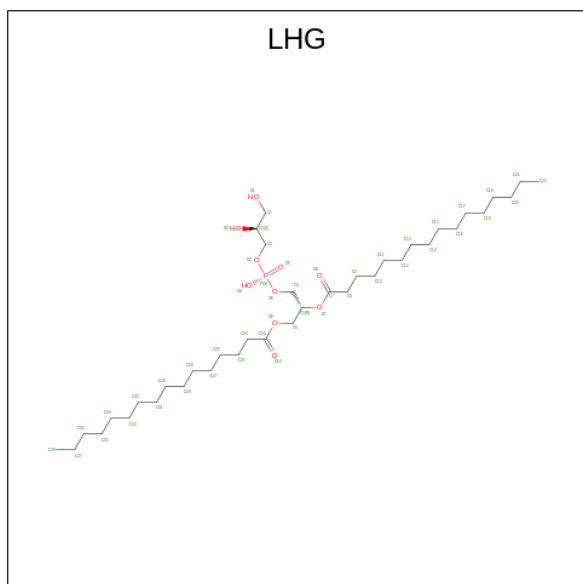
Mol	Chain	Residues	Atoms					AltConf
18	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



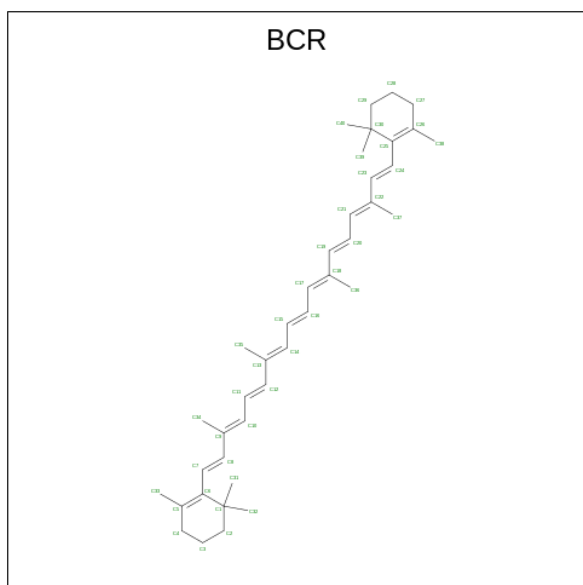
Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	a	1	Total 27	C 16	O 10	P 1	0
20	a	1	Total 33	C 22	O 10	P 1	0
20	b	1	Total 49	C 38	O 10	P 1	0
20	j	1	Total 49	C 38	O 10	P 1	0
20	B	1	Total 42	C 31	O 10	P 1	0
20	D	1	Total 49	C 38	O 10	P 1	0
20	E	1	Total 49	C 38	O 10	P 1	0
20	E	1	Total 42	C 31	O 10	P 1	0
20	H	1	Total 35	C 24	O 10	P 1	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



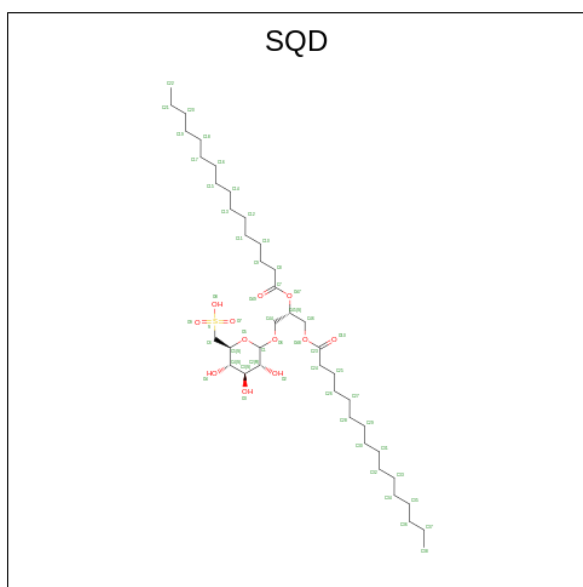
Mol	Chain	Residues	Atoms		AltConf
21	a	1	Total 40	C 40	0
21	a	1	Total 40	C 40	0

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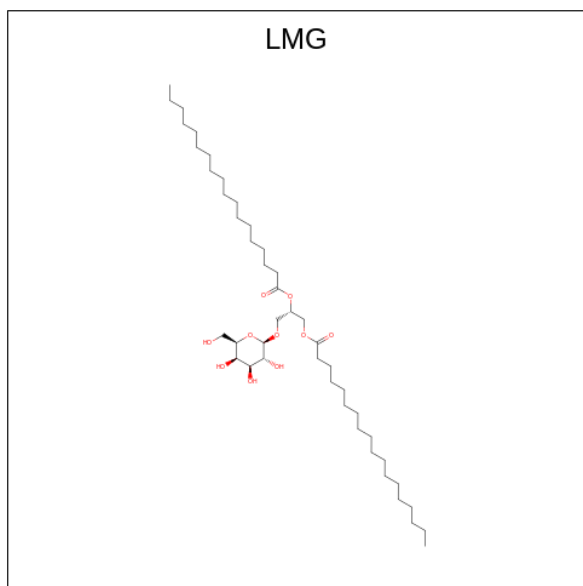
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	m	1	Total C 40 40	0
21	r	1	Total C 40 40	0
21	E	1	Total C 40 40	0
21	E	1	Total C 40 40	0

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
22	a	1	33	23	9	1	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



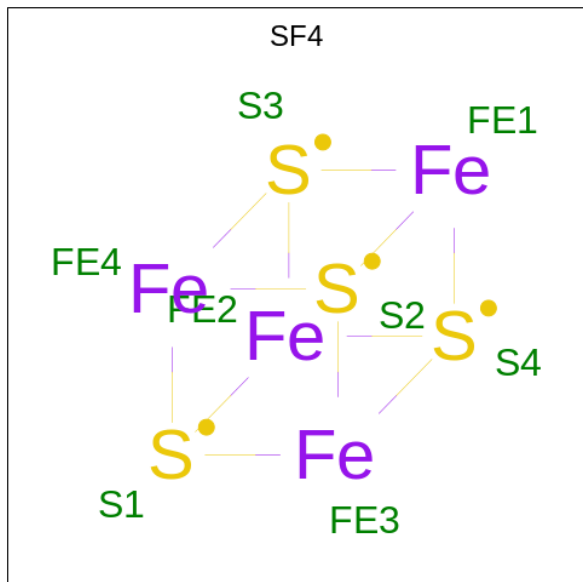
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	a	1	33	23	10	0
23	j	1	37	27	10	0

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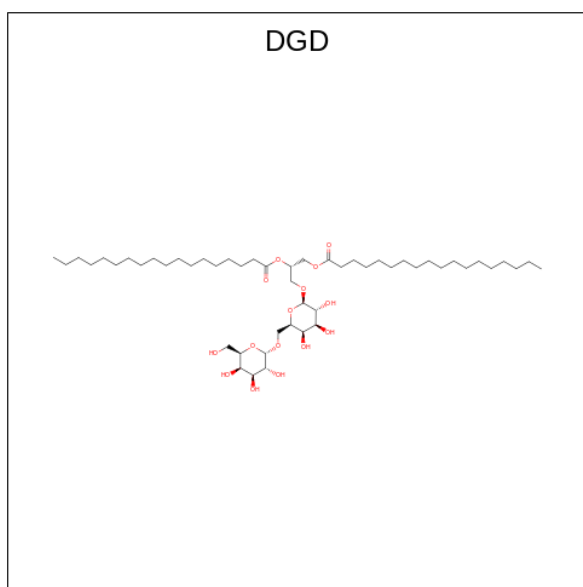
Mol	Chain	Residues	Atoms			AltConf
23	l	1	Total	C	O	0
			40	30	10	
23	C	1	Total	C	O	0
			31	21	10	
23	C	1	Total	C	O	0
			44	34	10	
23	D	1	Total	C	O	0
			46	36	10	
23	E	1	Total	C	O	0
			43	33	10	

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



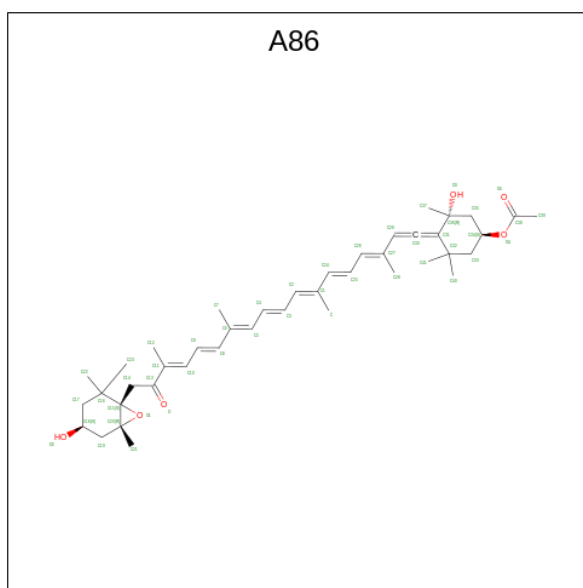
Mol	Chain	Residues	Atoms			AltConf
24	b	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	b	1	60	45	15	0

- Molecule 26 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



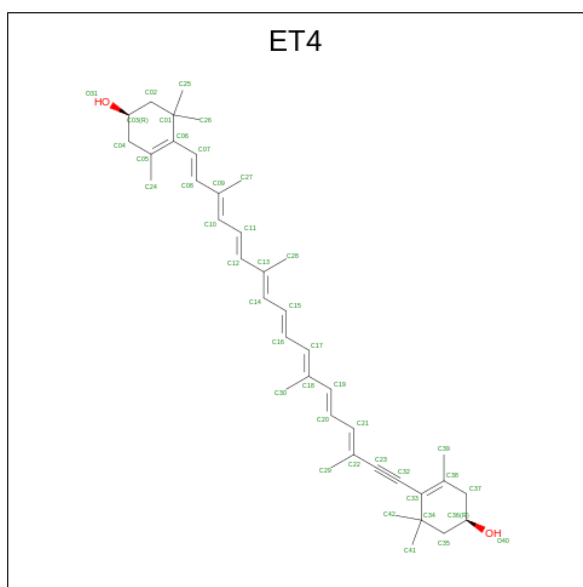
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	b	1	48	42	6	0
26	m	1	48	42	6	0

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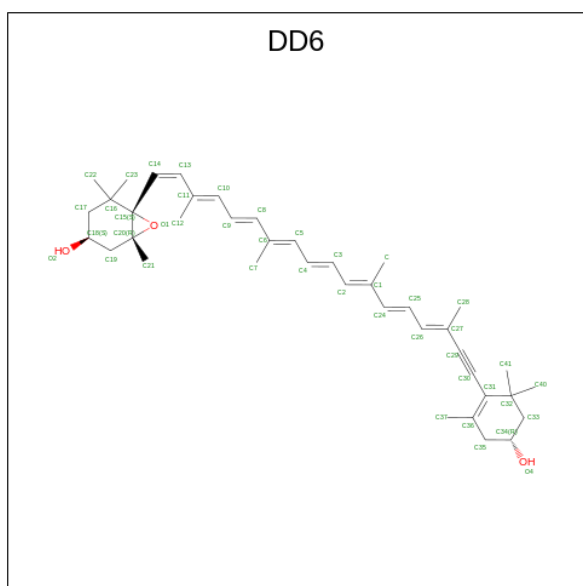
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	r	1	48	42	6	0
26	B	1	48	42	6	0
26	B	1	48	42	6	0
26	B	1	48	42	6	0
26	B	1	48	42	6	0
26	C	1	48	42	6	0
26	C	1	48	42	6	0
26	C	1	48	42	6	0
26	D	1	48	42	6	0
26	D	1	48	42	6	0
26	D	1	48	42	6	0
26	E	1	48	42	6	0
26	H	1	48	42	6	0
26	H	1	48	42	6	0
26	H	1	48	42	6	0

- Molecule 27 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (three-letter code: ET4) (formula: C₄₀H₅₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



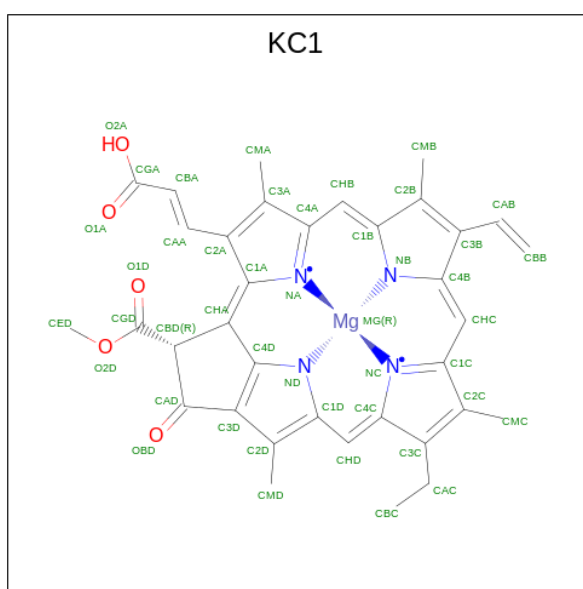
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	40	3	
28	C	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	H	1	Total	C	O	0
			43	40	3	

- Molecule 29 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

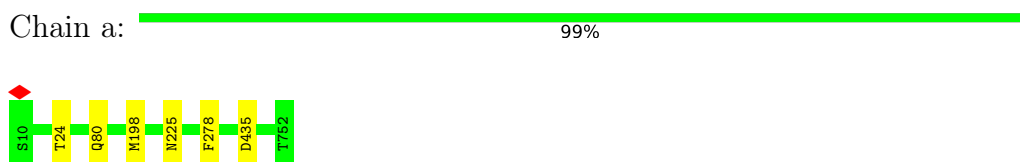


Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

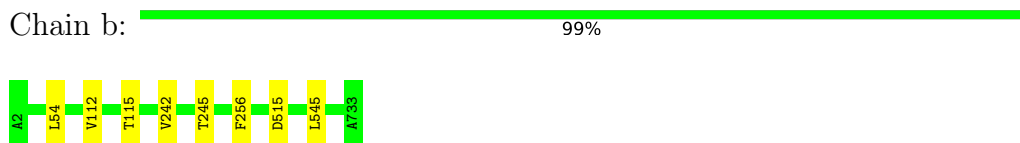
3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

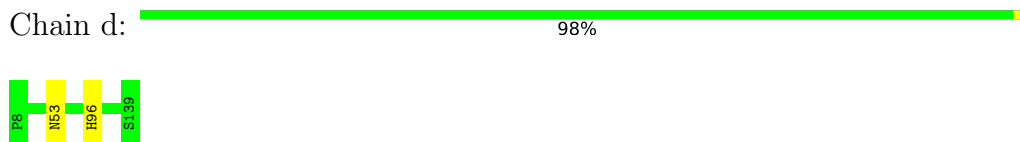


- Molecule 3: Photosystem I iron-sulfur center

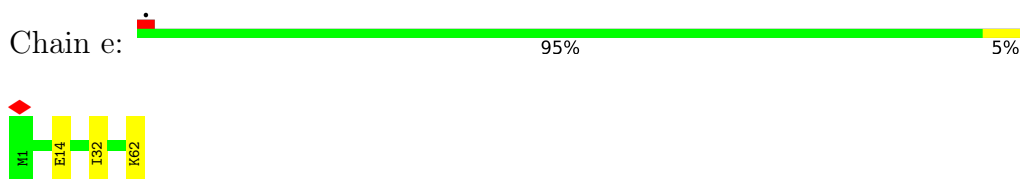


There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I reaction center subunit II



- Molecule 5: Photosystem I reaction center subunit IV



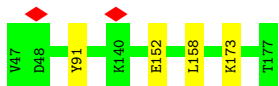
- Molecule 6: Photosystem I reaction center subunit III

Chain f:  99%



- Molecule 7: Photosystem I reaction center subunit Psa29

Chain g:  97%

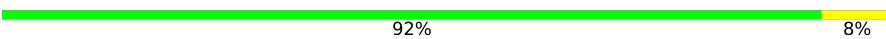


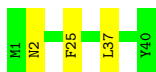
- Molecule 8: Photosystem I reaction center subunit VIII

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit IX

Chain j:  92%



- Molecule 10: Photosystem I reaction center subunit XI

Chain l:  99%



- Molecule 11: Photosystem I reaction center subunit XII

Chain m:  100%

There are no outlier residues recorded for this chain.

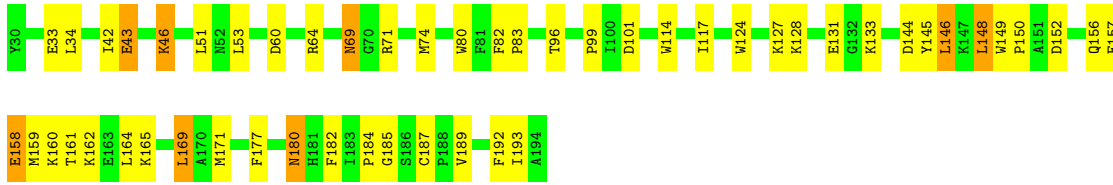
- Molecule 12: Tp-PsaR

Chain r:  99%



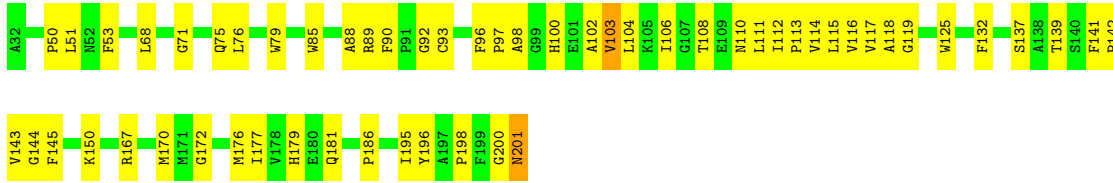
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain B:  68%



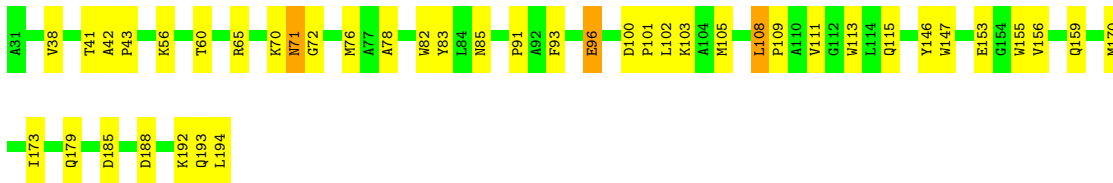
- Molecule 14: Fucoxanthin chl a/c light-harvesting protein, major type

Chain C: 67% 32%



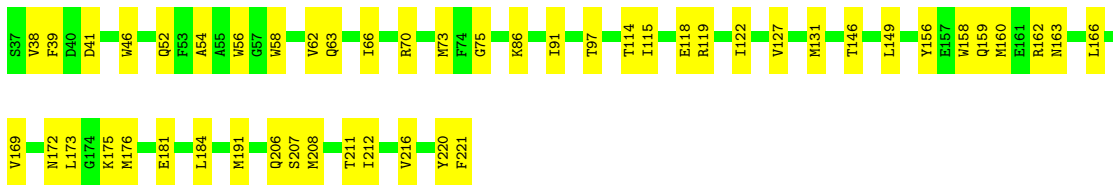
- Molecule 15: Pt17531-like protein

Chain D: 74% 24%



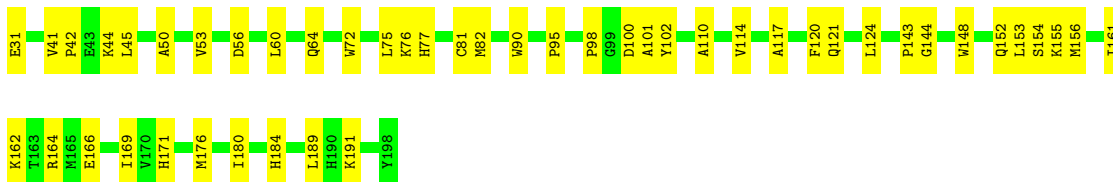
- Molecule 16: Tp-RedCAP

Chain E: 74% 26%



- Molecule 17: Fucoxanthin chl a/c light-harvesting protein

Chain H: 72% 28%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.370	Depositor
Minimum map value	-0.381	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ET4, PQN, LHG, SQD, DD6, KC1, BCR, DGD, LMG, CLA, A86, SF4

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	0.34	0/6049	0.41	0/8234
2	b	0.34	0/6034	0.41	0/8236
3	c	0.33	0/609	0.44	0/826
4	d	0.32	0/1067	0.41	0/1441
5	e	0.31	0/511	0.41	0/690
6	f	0.33	0/1271	0.42	0/1727
7	g	0.30	0/1003	0.41	0/1354
8	i	0.33	0/264	0.40	0/360
9	j	0.34	0/342	0.50	0/463
10	l	0.35	0/1123	0.44	0/1523
11	m	0.35	0/222	0.38	0/300
12	r	0.31	0/704	0.38	0/957
13	B	0.34	0/1324	0.39	0/1804
14	C	0.33	0/1339	0.40	0/1813
15	D	0.32	0/1304	0.39	0/1771
16	E	0.33	0/1450	0.40	0/1974
17	H	0.33	0/1334	0.41	0/1809
All	All	0.33	0/25950	0.41	0/35282

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	d	96	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5852	0	5682	0	0
2	b	5824	0	5643	0	0
3	c	599	0	582	0	0
4	d	1040	0	1027	0	0
5	e	503	0	500	0	0
6	f	1242	0	1239	0	0
7	g	981	0	922	0	0
8	i	256	0	259	0	0
9	j	332	0	331	0	0
10	l	1095	0	1116	0	0
11	m	220	0	241	0	0
12	r	683	0	675	0	0
13	B	1285	0	1239	66	0
14	C	1302	0	1243	70	0
15	D	1271	0	1227	33	0
16	E	1413	0	1365	41	0
17	H	1300	0	1262	44	0
18	B	469	0	479	39	0
18	C	547	0	472	64	0
18	D	568	0	501	37	0
18	E	462	0	454	23	0
18	H	587	0	583	56	0
18	a	2671	0	2759	0	0
18	b	2492	0	2569	0	0
18	f	175	0	177	0	0
18	i	60	0	59	0	0
18	j	41	0	29	0	0
18	l	159	0	144	0	0
18	r	45	0	33	0	0
19	a	33	0	46	0	0
19	b	33	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	42	0	54	2	0
20	D	49	0	74	6	0
20	E	91	0	131	2	0
20	H	35	0	43	0	0
20	a	109	0	134	0	0
20	b	49	0	74	0	0
20	j	49	0	74	0	0
21	E	80	0	112	5	0
21	a	200	0	280	0	0
21	b	160	0	224	0	0
21	f	80	0	112	0	0
21	i	80	0	112	0	0
21	j	80	0	112	0	0
21	l	80	0	112	0	0
21	m	40	0	56	0	0
21	r	40	0	56	0	0
22	a	33	0	39	0	0
23	C	75	0	88	2	0
23	D	46	0	61	0	0
23	E	43	0	55	3	0
23	a	33	0	33	0	0
23	j	37	0	42	0	0
23	l	40	0	49	0	0
24	b	8	0	0	0	0
24	c	16	0	0	0	0
25	b	60	0	81	0	0
26	B	192	0	0	8	0
26	C	144	0	0	5	0
26	D	144	0	0	6	0
26	E	48	0	0	0	0
26	H	144	0	0	14	0
26	b	48	0	0	0	0
26	m	48	0	0	0	0
26	r	48	0	0	0	0
27	l	42	0	0	0	0
28	B	43	0	0	1	0
28	C	43	0	0	1	0
28	D	43	0	0	2	0
28	E	172	0	0	2	0
28	H	43	0	0	3	0
29	B	45	0	0	5	0
29	C	90	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	H	45	0	0	1	0
All	All	36577	0	35112	398	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 16.

All (398) 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)
26:H:302:A86:C1	18:H:309:CLA:HMD2	1.45	1.46
26:H:302:A86:C2	18:H:309:CLA:HMD2	1.73	1.17
26:H:302:A86:C1	18:H:309:CLA:CMD	2.27	1.12
13:B:165:LYS:HB3	18:B:306:CLA:HMD3	1.32	1.06
26:H:302:A86:C	18:H:309:CLA:HMD2	1.87	1.03
13:B:165:LYS:HB3	18:B:306:CLA:CMD	1.88	1.02
26:H:302:A86:C	18:H:309:CLA:C1D	2.40	0.98
26:H:302:A86:C	18:H:309:CLA:C2D	2.43	0.95
14:C:144:GLY:H	18:C:316:CLA:HBC2	1.32	0.92
26:H:302:A86:C	18:H:309:CLA:CHD	2.49	0.90
26:B:301:A86:C22	18:B:306:CLA:HAC2	2.04	0.88
26:H:302:A86:C	18:H:309:CLA:CMD	2.51	0.87
18:B:314:CLA:HMB1	18:B:314:CLA:HBB1	1.60	0.83
16:E:75:GLY:HA3	28:E:304:DD6:C22	2.10	0.81
18:C:317:CLA:HBC2	18:C:317:CLA:HHD	1.61	0.81
14:C:97:PRO:HG2	14:C:102:ALA:HA	1.62	0.79
18:C:307:CLA:HMB1	18:C:307:CLA:HBB1	1.65	0.79
14:C:142:PRO:HG2	18:C:316:CLA:CAA	2.14	0.78
14:C:144:GLY:N	18:C:316:CLA:HBC2	1.99	0.77
17:H:42:PRO:HG3	17:H:56:ASP:HB3	1.67	0.77
17:H:180:ILE:HD12	18:H:306:CLA:H203	1.68	0.75
18:H:306:CLA:HBB1	18:H:306:CLA:HMB1	1.69	0.75
13:B:169:LEU:HD11	18:B:306:CLA:CBC	2.17	0.74
17:H:176:MET:HE3	18:H:306:CLA:HMC3	1.68	0.74
26:C:305:A86:C41	26:C:305:A86:C37	2.66	0.73
26:C:305:A86:C41	18:C:312:CLA:O1A	2.36	0.73
16:E:208:MET:HE3	18:E:316:CLA:H3A	1.70	0.73
13:B:165:LYS:CB	18:B:306:CLA:CMD	2.65	0.73
14:C:198:PRO:HG2	18:C:318:CLA:HAA1	1.72	0.71
13:B:171:MET:HE1	18:B:307:CLA:HAB	1.73	0.70
26:B:301:A86:C22	18:B:306:CLA:CAC	2.70	0.70
21:E:306:BCR:H10C	18:E:309:CLA:HBC2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:305:A86:C37	26:C:305:A86:O4	2.42	0.67
14:C:172:GLY:O	14:C:176:MET:HG3	1.95	0.67
26:D:203:A86:C2	18:D:215:CLA:HBC2	2.26	0.66
14:C:88:ALA:CB	18:C:317:CLA:HMD3	2.26	0.66
18:H:313:CLA:HBB1	18:H:313:CLA:HMB1	1.78	0.65
18:H:314:CLA:O1D	18:H:314:CLA:HBA2	1.96	0.65
13:B:165:LYS:CB	18:B:306:CLA:HMD1	2.25	0.65
18:H:307:CLA:HBB1	18:H:307:CLA:HMB1	1.77	0.65
14:C:145:PHE:HA	18:C:312:CLA:HBA1	1.78	0.65
16:E:115:ILE:HD11	16:E:119:ARG:HG2	1.78	0.65
20:B:315:LHG:HC11	20:B:315:LHG:HC41	1.77	0.64
18:B:306:CLA:CAD	29:B:313:KC1:OBD	2.45	0.64
13:B:169:LEU:HD11	18:B:306:CLA:HBC2	1.79	0.64
17:H:153:LEU:HA	17:H:156:MET:SD	2.37	0.63
14:C:113:PRO:O	14:C:116:VAL:HG22	1.98	0.63
17:H:60:LEU:HD23	18:H:306:CLA:H42	1.81	0.63
14:C:195:ILE:HG22	18:C:318:CLA:HAC1	1.80	0.63
13:B:165:LYS:HB3	18:B:306:CLA:HMD1	1.79	0.63
26:C:305:A86:C29	18:C:312:CLA:H72	2.30	0.62
17:H:98:PRO:HB2	26:H:302:A86:C41	2.29	0.62
26:B:302:A86:C2	18:B:309:CLA:H12	2.30	0.62
26:D:203:A86:C25	18:D:215:CLA:HMD2	2.29	0.62
16:E:70:ARG:HA	16:E:73:MET:HE3	1.81	0.62
17:H:82:MET:SD	18:H:311:CLA:HMC3	2.39	0.62
14:C:88:ALA:HB2	18:C:317:CLA:HMD3	1.82	0.61
14:C:170:MET:HE3	18:C:307:CLA:HMC3	1.82	0.61
16:E:175:LYS:HD3	16:E:181:GLU:HG2	1.81	0.61
13:B:169:LEU:HD11	18:B:306:CLA:HBC1	1.81	0.61
15:D:82:TRP:CE2	15:D:101:PRO:HG2	2.36	0.61
15:D:102:LEU:O	15:D:105:MET:HG2	2.00	0.61
18:C:312:CLA:HBD	18:C:316:CLA:CBC	2.31	0.60
15:D:83:TYR:O	18:D:216:CLA:HBA1	2.01	0.60
18:D:208:CLA:H51	18:D:209:CLA:H12	1.83	0.60
15:D:108:LEU:HD11	18:D:210:CLA:HAA2	1.83	0.60
18:B:311:CLA:H13	18:E:312:CLA:H93	1.82	0.60
18:D:209:CLA:HMA2	18:D:209:CLA:H11	1.83	0.60
18:C:312:CLA:HBD	18:C:316:CLA:HBC1	1.82	0.60
18:D:208:CLA:H52	18:D:208:CLA:HMB2	1.84	0.60
18:B:307:CLA:H41	18:B:308:CLA:H43	1.82	0.59
13:B:149:TRP:HZ3	18:B:312:CLA:HMA2	1.68	0.59
18:B:306:CLA:C3D	29:B:313:KC1:OBD	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:85:TRP:CE2	14:C:186:PRO:HG3	2.38	0.59
15:D:193:GLN:O	15:D:194:LEU:C	2.40	0.59
26:D:203:A86:C1	18:D:215:CLA:HBC2	2.33	0.59
17:H:110:ALA:O	17:H:114:VAL:HG23	2.03	0.58
14:C:51:LEU:HB2	14:C:53:PHE:CE2	2.38	0.58
14:C:53:PHE:CD2	18:C:307:CLA:H11	2.38	0.58
20:D:201:LHG:H102	18:D:214:CLA:H42	1.85	0.58
16:E:146:THR:H	16:E:159:GLN:HE22	1.51	0.58
14:C:200:GLY:O	14:C:201:ASN:C	2.42	0.57
16:E:173:LEU:HD12	16:E:176:MET:SD	2.43	0.57
14:C:195:ILE:HG23	18:C:317:CLA:HBC3	1.86	0.57
18:C:309:CLA:C1A	18:C:309:CLA:CGA	2.81	0.57
17:H:72:TRP:CE2	17:H:143:PRO:HA	2.39	0.57
26:H:302:A86:C2	18:H:309:CLA:CMD	2.63	0.57
15:D:70:LYS:HD2	18:D:212:CLA:C3D	2.35	0.57
13:B:146:LEU:HB3	13:B:148:LEU:HG	1.87	0.56
15:D:194:LEU:HD13	18:D:217:CLA:CHB	2.35	0.56
26:H:302:A86:C1	18:H:309:CLA:C2D	2.80	0.56
16:E:208:MET:HE1	23:E:318:LMG:HC91	1.88	0.56
18:D:208:CLA:H41	18:D:209:CLA:H12	1.87	0.55
18:H:305:CLA:HBC1	18:H:313:CLA:H203	1.87	0.55
13:B:74:MET:HE3	18:B:312:CLA:HMC3	1.88	0.55
18:H:305:CLA:HBC3	18:H:305:CLA:HMC1	1.88	0.55
15:D:111:VAL:O	15:D:115:GLN:HG3	2.06	0.55
20:D:201:LHG:H321	18:D:214:CLA:CMA	2.36	0.55
26:H:302:A86:C7	18:H:309:CLA:HBC1	2.36	0.55
14:C:177:ILE:O	14:C:181:GLN:HG2	2.07	0.55
14:C:143:VAL:HG12	18:C:316:CLA:C1C	2.36	0.54
20:D:201:LHG:H102	18:D:214:CLA:C4	2.38	0.54
14:C:141:PHE:CZ	18:C:316:CLA:HBB1	2.42	0.54
13:B:82:PHE:HZ	14:C:198:PRO:HG3	1.72	0.54
13:B:171:MET:CE	18:B:307:CLA:HAB	2.38	0.54
15:D:173:ILE:HG21	28:D:205:DD6:C24	2.37	0.54
17:H:184:HIS:HB2	18:H:313:CLA:HBC3	1.90	0.54
13:B:148:LEU:HD12	13:B:148:LEU:H	1.72	0.54
13:B:51:LEU:HB2	13:B:53:LEU:HD13	1.88	0.54
13:B:114:TRP:O	13:B:117:ILE:HG22	2.08	0.54
14:C:50:PRO:HB2	14:C:51:LEU:HD22	1.89	0.53
14:C:198:PRO:CG	18:C:318:CLA:H3A	2.39	0.53
29:C:308:KC1:OBD	18:C:311:CLA:HBD	2.09	0.53
13:B:128:LYS:HD2	13:B:133:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:108:LEU:HD23	15:D:109:PRO:HD2	1.88	0.53
18:H:311:CLA:CGA	18:H:311:CLA:C3A	2.87	0.53
15:D:82:TRP:CD2	15:D:101:PRO:HG2	2.43	0.53
17:H:90:TRP:CD1	18:H:308:CLA:HMD3	2.44	0.53
13:B:80:TRP:CE2	13:B:99:PRO:HG2	2.44	0.53
16:E:97:THR:HB	16:E:114:THR:OG1	2.08	0.53
15:D:71:ASN:ND2	18:D:212:CLA:HMD1	2.24	0.53
16:E:207:SER:HA	23:E:318:LMG:HC3	1.91	0.53
18:E:312:CLA:HED2	18:E:313:CLA:HMD2	1.90	0.53
14:C:71:GLY:O	14:C:75:GLN:HG3	2.09	0.53
14:C:106:ILE:HG21	14:C:111:LEU:HD21	1.91	0.53
15:D:188:ASP:OD2	18:D:216:CLA:ND	2.42	0.53
18:D:210:CLA:HBB1	18:D:210:CLA:HMB1	1.90	0.53
18:H:307:CLA:CBB	18:H:314:CLA:HMB1	2.39	0.52
18:B:311:CLA:H171	18:E:312:CLA:H71	1.92	0.52
14:C:167:ARG:HA	14:C:170:MET:HE3	1.92	0.52
17:H:53:VAL:HG22	18:H:306:CLA:HMD1	1.92	0.52
13:B:145:TYR:CD2	13:B:146:LEU:HD13	2.45	0.52
18:B:306:CLA:H43	29:B:313:KC1:O1D	2.10	0.52
13:B:157:GLU:HA	13:B:160:LYS:HE2	1.92	0.52
18:D:208:CLA:H201	18:D:215:CLA:HBC3	1.92	0.52
16:E:66:ILE:HD13	16:E:184:LEU:HD13	1.92	0.52
17:H:153:LEU:HD11	17:H:161:ILE:HG23	1.92	0.52
14:C:198:PRO:CG	18:C:318:CLA:HAA1	2.40	0.51
17:H:180:ILE:HG22	18:H:313:CLA:HBC2	1.92	0.51
14:C:79:TRP:CD2	18:C:309:CLA:HBC2	2.45	0.51
13:B:165:LYS:HB2	18:B:306:CLA:HMD1	1.91	0.51
18:C:317:CLA:NB	18:C:318:CLA:HMD3	2.24	0.51
16:E:172:ASN:HD21	16:E:181:GLU:HG2	1.74	0.51
28:B:303:DD6:C9	18:B:307:CLA:HMC2	2.41	0.51
14:C:79:TRP:HE1	18:C:317:CLA:C4B	2.24	0.51
14:C:150:LYS:NZ	14:C:150:LYS:HB2	2.25	0.51
17:H:81:CYS:SG	28:H:303:DD6:C5	2.99	0.51
13:B:182:PHE:O	13:B:184:PRO:HD3	2.11	0.51
14:C:89:ARG:NH2	14:C:98:ALA:HB2	2.25	0.51
16:E:63:GLN:HG2	16:E:163:ASN:HD21	1.76	0.51
14:C:88:ALA:HB1	18:C:317:CLA:HMD3	1.93	0.51
18:H:311:CLA:CGA	18:H:311:CLA:H3A	2.40	0.51
13:B:69:ASN:HD22	13:B:69:ASN:N	2.09	0.50
16:E:56:TRP:HB2	16:E:58:TRP:CD1	2.46	0.50
14:C:102:ALA:O	14:C:106:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:119:GLY:HA3	18:C:311:CLA:HAB	1.94	0.50
14:C:114:VAL:O	14:C:117:VAL:HG12	2.11	0.50
15:D:179:GLN:HG2	15:D:185:ASP:O	2.11	0.50
16:E:63:GLN:HG2	16:E:163:ASN:ND2	2.26	0.50
16:E:118:GLU:O	16:E:122:ILE:HG12	2.11	0.50
16:E:169:VAL:HG13	18:E:309:CLA:HMD1	1.92	0.50
17:H:100:ASP:O	17:H:101:ALA:HB3	2.11	0.50
18:B:311:CLA:HBA1	20:B:315:LHG:H261	1.91	0.50
13:B:158:GLU:OE2	13:B:162:LYS:HD2	2.12	0.50
18:D:208:CLA:CGA	18:D:208:CLA:H3A	2.42	0.50
16:E:38:VAL:HG23	16:E:41:ASP:H	1.76	0.50
16:E:156:TYR:O	16:E:160:MET:HG2	2.12	0.50
13:B:114:TRP:HE1	26:B:302:A86:C9	2.25	0.49
18:D:217:CLA:HBC2	18:D:217:CLA:HHD	1.93	0.49
13:B:69:ASN:ND2	18:B:311:CLA:HMD1	2.27	0.49
26:D:203:A86:C24	18:D:215:CLA:HBC2	2.42	0.49
17:H:152:GLN:HB3	17:H:164:ARG:HH12	1.76	0.49
13:B:46:LYS:NZ	13:B:46:LYS:H	2.11	0.49
14:C:139:THR:HG21	14:C:141:PHE:CZ	2.47	0.49
15:D:38:VAL:HG23	15:D:65:ARG:HH12	1.77	0.49
13:B:148:LEU:HD11	26:B:304:A86:C17	2.43	0.49
16:E:169:VAL:HG22	18:E:309:CLA:OBD	2.12	0.49
26:B:302:A86:C27	18:C:318:CLA:HBB2	2.43	0.49
17:H:184:HIS:CB	18:H:313:CLA:HBC3	2.42	0.49
28:H:303:DD6:C24	18:H:306:CLA:HAB	2.43	0.49
13:B:157:GLU:O	13:B:161:THR:HG23	2.12	0.49
14:C:137:SER:HA	14:C:143:VAL:HG23	1.95	0.48
15:D:41:THR:HG23	15:D:43:PRO:HD2	1.95	0.48
13:B:158:GLU:O	13:B:162:LYS:HG3	2.13	0.48
15:D:93:PHE:O	15:D:96:GLU:HB2	2.13	0.48
26:H:302:A86:C24	18:H:309:CLA:CMD	2.91	0.48
14:C:195:ILE:HG22	18:C:318:CLA:CAC	2.44	0.48
18:C:309:CLA:H111	18:C:309:CLA:H72	1.63	0.48
20:D:201:LHG:H321	18:D:214:CLA:HMA2	1.95	0.48
14:C:93:CYS:SG	18:C:310:CLA:HBB1	2.53	0.48
13:B:180:ASN:OD1	13:B:189:VAL:HG12	2.13	0.48
13:B:82:PHE:HB3	13:B:83:PRO:HD3	1.96	0.48
18:C:317:CLA:HBB1	18:C:318:CLA:HBC3	1.96	0.48
26:D:204:A86:C3	18:D:211:CLA:HMD2	2.44	0.47
16:E:38:VAL:O	16:E:39:PHE:HB2	2.14	0.47
13:B:156:GLN:O	13:B:160:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:108:THR:O	14:C:112:ILE:HG12	2.14	0.47
17:H:114:VAL:HG21	18:H:308:CLA:HAA2	1.96	0.47
14:C:141:PHE:CE2	18:C:316:CLA:HBB1	2.50	0.47
16:E:216:VAL:HG21	16:E:220:TYR:CE2	2.49	0.47
13:B:33:GLU:H	13:B:33:GLU:CD	2.18	0.47
26:B:302:A86:C40	18:C:318:CLA:HMC2	2.45	0.47
18:C:306:CLA:HMA3	23:C:319:LMG:HC4	1.95	0.47
28:H:303:DD6:C13	28:H:303:DD6:C21	2.92	0.47
13:B:124:TRP:CZ2	13:B:128:LYS:HE2	2.49	0.47
16:E:206:GLN:NE2	16:E:211:THR:HG22	2.29	0.47
18:H:310:CLA:HMB1	18:H:310:CLA:HBB1	1.96	0.47
13:B:192:PHE:CE1	13:B:193:ILE:HG13	2.49	0.47
14:C:96:PHE:CD1	14:C:96:PHE:N	2.81	0.47
16:E:73:MET:HE3	18:E:313:CLA:HMC3	1.97	0.47
16:E:149:LEU:HD13	16:E:160:MET:SD	2.54	0.47
26:H:302:A86:C	18:H:309:CLA:HHD	2.39	0.47
18:D:208:CLA:H91	18:D:208:CLA:H112	1.51	0.47
18:H:314:CLA:HMB1	18:H:314:CLA:HBB1	1.95	0.47
13:B:60:ASP:O	13:B:64:ARG:HG3	2.14	0.47
29:C:308:KC1:CED	18:C:311:CLA:H51	2.45	0.47
18:D:207:CLA:H61	18:D:207:CLA:H41	1.51	0.47
13:B:144:ASP:OD1	13:B:148:LEU:HD12	2.15	0.47
18:B:311:CLA:H62	18:B:311:CLA:H41	1.54	0.47
14:C:179:HIS:HE1	18:C:314:CLA:NA	2.12	0.47
17:H:171:HIS:CE1	18:H:305:CLA:HMD1	2.50	0.47
15:D:71:ASN:HD22	15:D:71:ASN:N	2.12	0.46
18:H:311:CLA:C2B	18:H:311:CLA:H43	2.44	0.46
16:E:172:ASN:HD21	16:E:181:GLU:CG	2.28	0.46
17:H:75:LEU:HD13	17:H:144:GLY:HA3	1.96	0.46
13:B:177:PHE:CE1	13:B:193:ILE:HG21	2.50	0.46
18:D:208:CLA:H52	18:D:208:CLA:CMB	2.46	0.46
14:C:119:GLY:CA	18:C:311:CLA:HAB	2.45	0.46
17:H:180:ILE:HD12	18:H:306:CLA:C20	2.43	0.46
13:B:43:GLU:H	13:B:43:GLU:HG2	1.38	0.46
13:B:159:MET:HG3	18:B:312:CLA:HMA1	1.96	0.46
14:C:106:ILE:HG13	14:C:110:ASN:OD1	2.15	0.46
18:D:216:CLA:H3A	18:D:216:CLA:HBA2	1.58	0.46
13:B:152:ASP:O	13:B:156:GLN:HG3	2.16	0.46
14:C:167:ARG:HA	14:C:170:MET:CE	2.45	0.46
18:C:314:CLA:HHD	18:C:314:CLA:HBC2	1.96	0.46
18:D:215:CLA:HED3	18:D:215:CLA:H2A	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:72:TRP:NE1	17:H:143:PRO:HA	2.31	0.46
13:B:46:LYS:HD2	13:B:46:LYS:C	2.36	0.46
20:D:201:LHG:H331	20:D:201:LHG:H301	1.58	0.46
18:D:207:CLA:H111	18:D:207:CLA:H91	1.42	0.46
16:E:39:PHE:HD1	18:E:309:CLA:HBA2	1.80	0.46
21:E:306:BCR:H24C	21:E:306:BCR:H371	1.76	0.46
18:E:312:CLA:CBB	18:E:316:CLA:HBC2	2.46	0.46
18:E:316:CLA:HBA1	23:E:318:LMG:O2	2.16	0.46
18:H:311:CLA:H3A	18:H:311:CLA:HBA2	1.75	0.46
14:C:125:TRP:CZ3	14:C:141:PHE:HE2	2.34	0.45
13:B:127:LYS:O	13:B:131:GLU:HG3	2.17	0.45
16:E:62:VAL:O	16:E:66:ILE:HG12	2.16	0.45
17:H:102:TYR:HA	18:H:308:CLA:HED2	1.98	0.45
13:B:124:TRP:CH2	13:B:128:LYS:HE2	2.51	0.45
13:B:152:ASP:OD1	13:B:152:ASP:N	2.50	0.45
14:C:118:ALA:CB	18:C:311:CLA:HMC3	2.47	0.45
14:C:132:PHE:HZ	18:C:312:CLA:HED2	1.81	0.45
14:C:198:PRO:HD2	18:C:318:CLA:HAA1	1.97	0.45
17:H:82:MET:HE1	17:H:171:HIS:HB3	1.99	0.45
18:H:311:CLA:H102	18:H:311:CLA:H62	1.50	0.45
18:C:312:CLA:H111	18:C:312:CLA:H142	1.68	0.45
17:H:42:PRO:HG2	17:H:45:LEU:HG	1.98	0.45
29:B:313:KC1:CHC	29:B:313:KC1:CBB	2.94	0.45
23:C:319:LMG:H111	23:C:319:LMG:H142	1.67	0.45
20:E:301:LHG:H371	20:E:301:LHG:H342	1.48	0.45
17:H:148:TRP:N	17:H:148:TRP:CD1	2.84	0.45
17:H:189:LEU:HB2	17:H:191:LYS:HG2	1.98	0.45
14:C:198:PRO:CD	18:C:318:CLA:HAA1	2.46	0.45
18:C:309:CLA:H102	18:C:309:CLA:H13	1.75	0.45
16:E:46:TRP:HZ3	16:E:54:ALA:HB2	1.82	0.45
17:H:162:LYS:O	17:H:166:GLU:HG3	2.16	0.45
16:E:70:ARG:HA	16:E:73:MET:CE	2.46	0.44
18:H:308:CLA:H91	18:H:308:CLA:H111	1.60	0.44
13:B:149:TRP:CE3	18:B:312:CLA:HAA2	2.52	0.44
26:D:204:A86:C2	18:D:211:CLA:HMD2	2.47	0.44
17:H:120:PHE:CZ	17:H:124:LEU:HD11	2.51	0.44
14:C:117:VAL:HG11	28:C:303:DD6:C5	2.46	0.44
16:E:172:ASN:ND2	16:E:181:GLU:HG2	2.32	0.44
18:E:312:CLA:H112	18:E:312:CLA:H142	1.71	0.44
18:E:316:CLA:HMB1	18:E:316:CLA:HBB1	1.98	0.44
15:D:78:ALA:HB1	28:D:205:DD6:C37	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:158:GLU:HG3	13:B:159:MET:N	2.32	0.44
15:D:146:TYR:HD2	15:D:147:TRP:CE2	2.36	0.44
14:C:112:ILE:N	14:C:113:PRO:HD2	2.32	0.44
14:C:179:HIS:CE1	18:C:314:CLA:NA	2.86	0.44
15:D:72:GLY:O	15:D:76:MET:HG3	2.18	0.44
18:D:208:CLA:H92	18:D:208:CLA:H61	1.54	0.44
13:B:71:ARG:HA	13:B:74:MET:CE	2.47	0.44
17:H:166:GLU:O	17:H:169:ILE:HG22	2.17	0.44
18:D:217:CLA:H2A	18:D:217:CLA:HED2	2.00	0.44
13:B:187:CYS:SG	18:B:314:CLA:C4B	3.06	0.43
18:E:315:CLA:H62	18:E:315:CLA:H92	1.84	0.43
18:E:316:CLA:H3A	18:E:316:CLA:HBA2	1.79	0.43
17:H:77:HIS:CE1	18:H:310:CLA:HMD1	2.53	0.43
13:B:34:LEU:HB3	18:B:307:CLA:HED3	2.00	0.43
18:B:312:CLA:HBA2	18:B:312:CLA:H3A	1.45	0.43
18:C:309:CLA:H2A	18:C:309:CLA:O2D	2.18	0.43
18:D:207:CLA:H71	18:D:214:CLA:C1D	2.48	0.43
13:B:128:LYS:HD3	13:B:128:LYS:HA	1.74	0.43
29:C:308:KC1:CAD	18:C:311:CLA:HBD	2.48	0.43
15:D:100:ASP:HB3	15:D:103:LYS:HD3	1.99	0.43
13:B:149:TRP:CE3	13:B:150:PRO:HD2	2.53	0.43
13:B:159:MET:HG3	18:B:312:CLA:CMA	2.48	0.43
18:B:306:CLA:HBA2	18:B:306:CLA:H3A	1.16	0.43
18:E:311:CLA:O1A	18:E:312:CLA:H203	2.19	0.43
13:B:42:ILE:HG13	18:B:306:CLA:HMA3	2.00	0.43
21:E:306:BCR:H20C	21:E:306:BCR:H361	1.77	0.43
14:C:106:ILE:HG13	14:C:110:ASN:HD21	1.83	0.43
21:E:305:BCR:H11C	21:E:305:BCR:H341	1.83	0.43
14:C:115:LEU:HD22	14:C:115:LEU:H	1.84	0.43
17:H:76:LYS:HD2	18:H:310:CLA:C3D	2.49	0.43
17:H:102:TYR:CE1	17:H:114:VAL:HG13	2.54	0.43
16:E:91:ILE:HD13	16:E:118:GLU:HG3	2.00	0.43
16:E:166:LEU:HD11	16:E:181:GLU:HA	2.01	0.43
13:B:46:LYS:H	13:B:46:LYS:HZ2	1.66	0.43
15:D:153:GLU:O	15:D:156:VAL:HG22	2.19	0.43
15:D:170:MET:O	15:D:173:ILE:HG22	2.19	0.43
17:H:31:GLU:O	17:H:41:VAL:HG12	2.18	0.43
18:H:313:CLA:H93	18:H:313:CLA:H61	1.83	0.43
18:C:312:CLA:H3A	18:C:312:CLA:HBA2	1.54	0.42
18:C:315:CLA:HED2	18:C:315:CLA:H2A	2.01	0.42
18:E:310:CLA:HBB2	18:E:316:CLA:HAB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:91:PRO:HD2	18:D:210:CLA:HMD1	2.00	0.42
16:E:52:GLN:CD	16:E:52:GLN:H	2.22	0.42
14:C:112:ILE:O	14:C:116:VAL:HG13	2.20	0.42
18:C:312:CLA:HAA1	18:C:316:CLA:HBC1	2.00	0.42
15:D:192:LYS:NZ	18:D:216:CLA:OBD	2.51	0.42
18:E:312:CLA:HBA1	18:E:312:CLA:H3A	1.67	0.42
18:H:307:CLA:H41	18:H:307:CLA:H62	1.39	0.42
29:C:308:KC1:C2D	18:C:311:CLA:H62	2.49	0.42
15:D:155:TRP:O	15:D:159:GLN:HG3	2.19	0.42
17:H:53:VAL:CG2	18:H:306:CLA:HMD1	2.48	0.42
13:B:180:ASN:HD22	13:B:184:PRO:HA	1.85	0.42
14:C:196:TYR:CD2	14:C:198:PRO:HD3	2.54	0.42
26:C:304:A86:C24	18:C:307:CLA:HAB	2.49	0.42
15:D:153:GLU:HA	15:D:156:VAL:HG22	2.00	0.42
28:E:307:DD6:C10	28:E:307:DD6:C7	2.98	0.42
17:H:154:SER:CB	17:H:155:LYS:HD3	2.49	0.42
18:H:308:CLA:CGA	18:H:308:CLA:C1A	2.97	0.42
13:B:96:THR:HG21	13:B:101:ASP:HB2	2.00	0.42
14:C:201:ASN:C	14:C:201:ASN:HD22	2.22	0.42
15:D:41:THR:OG1	15:D:42:ALA:N	2.52	0.42
15:D:56:LYS:HD2	15:D:60:THR:HG21	2.01	0.42
15:D:105:MET:HA	15:D:113:TRP:HZ2	1.85	0.42
18:B:309:CLA:H41	18:B:309:CLA:H61	1.78	0.42
14:C:142:PRO:HB2	18:C:316:CLA:CHA	2.49	0.42
14:C:76:LEU:HD11	18:C:312:CLA:HBC1	2.01	0.41
18:C:310:CLA:O1D	18:C:310:CLA:H2A	2.20	0.41
16:E:158:TRP:HZ3	16:E:162:ARG:HH21	1.66	0.41
21:E:306:BCR:H15C	21:E:306:BCR:H351	1.83	0.41
18:H:313:CLA:H143	18:H:313:CLA:H161	1.65	0.41
13:B:69:ASN:HD22	13:B:69:ASN:H	1.67	0.41
14:C:100:HIS:HE1	14:C:104:LEU:HD21	1.85	0.41
14:C:103:VAL:CG2	18:C:315:CLA:HAB	2.50	0.41
18:C:307:CLA:H193	18:C:307:CLA:H161	1.73	0.41
18:C:309:CLA:H161	18:C:309:CLA:H141	1.75	0.41
18:D:209:CLA:O1A	18:D:209:CLA:H2A	2.19	0.41
16:E:39:PHE:CD1	18:E:309:CLA:HBA2	2.56	0.41
14:C:90:PHE:CD2	18:C:310:CLA:HMC3	2.55	0.41
18:E:315:CLA:H3A	18:E:315:CLA:H12	2.02	0.41
17:H:50:ALA:HB1	17:H:166:GLU:HG2	2.02	0.41
20:D:201:LHG:H142	20:D:201:LHG:H111	1.47	0.41
14:C:195:ILE:CG2	18:C:317:CLA:HBC3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:315:CLA:H91	18:E:315:CLA:H112	1.84	0.41
17:H:117:ALA:O	17:H:121:GLN:HG3	2.21	0.41
18:H:306:CLA:CGA	18:H:306:CLA:H3A	2.50	0.41
13:B:71:ARG:HA	13:B:74:MET:HE2	2.02	0.41
20:E:301:LHG:H191	20:E:301:LHG:H222	1.81	0.41
17:H:90:TRP:CZ2	17:H:95:PRO:HD2	2.54	0.41
13:B:180:ASN:ND2	13:B:185:GLY:H	2.18	0.41
16:E:86:LYS:HE3	16:E:221:PHE:HE1	1.85	0.41
17:H:44:LYS:HE2	17:H:64:GLN:O	2.21	0.41
17:H:120:PHE:O	17:H:124:LEU:HD13	2.20	0.41
13:B:146:LEU:HD23	13:B:148:LEU:HD21	2.02	0.41
14:C:112:ILE:HA	14:C:115:LEU:HD23	2.02	0.41
13:B:145:TYR:HD2	13:B:146:LEU:HD13	1.85	0.41
13:B:149:TRP:CZ3	18:B:312:CLA:HMA2	2.53	0.41
13:B:169:LEU:HD22	26:B:304:A86:C28	2.51	0.41
18:C:318:CLA:CB D	18:C:318:CLA:HAA2	2.51	0.41
18:D:208:CLA:H161	18:D:208:CLA:H141	1.62	0.41
17:H:155:LYS:HE2	17:H:155:LYS:HB2	1.70	0.41
18:H:306:CLA:H61	18:H:306:CLA:H92	1.77	0.41
18:H:310:CLA:H62	18:H:310:CLA:H41	1.48	0.41
14:C:125:TRP:CZ3	14:C:141:PHE:CE2	3.08	0.41
15:D:42:ALA:N	15:D:43:PRO:HD2	2.37	0.41
16:E:191:MET:HE3	18:E:309:CLA:HMC3	2.03	0.41
18:E:312:CLA:HED3	18:E:313:CLA:HBC2	2.03	0.41
14:C:112:ILE:N	14:C:113:PRO:CD	2.84	0.40
16:E:208:MET:O	16:E:212:ILE:HG13	2.21	0.40
17:H:152:GLN:HG3	18:H:311:CLA:H12	2.01	0.40
18:H:305:CLA:H62	18:H:305:CLA:C1B	2.51	0.40
18:H:305:CLA:HBA2	18:H:305:CLA:H3A	1.18	0.40
29:H:312:KC1:CGD	29:H:312:KC1:CAA	2.98	0.40
15:D:65:ARG:HD3	15:D:65:ARG:O	2.21	0.40
16:E:91:ILE:CD1	16:E:118:GLU:HG3	2.52	0.40
16:E:127:VAL:O	16:E:131:MET:HG2	2.21	0.40
18:H:314:CLA:H61	18:H:314:CLA:H41	1.79	0.40
18:B:308:CLA:HMD2	18:B:311:CLA:C1D	2.51	0.40
14:C:92:GLY:HA3	18:C:310:CLA:C4A	2.51	0.40
18:B:312:CLA:H43	29:B:313:KC1:O1A	2.22	0.40
14:C:106:ILE:HG13	14:C:110:ASN:ND2	2.36	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	741/743 (100%)	723 (98%)	18 (2%)	0	100	100
2	b	730/732 (100%)	713 (98%)	17 (2%)	0	100	100
3	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	d	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
5	e	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
6	f	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
7	g	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
8	i	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
10	l	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
11	m	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	r	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
13	B	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
14	C	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
15	D	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
16	E	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
17	H	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
All	All	3195/3229 (99%)	3103 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	603/603 (100%)	597 (99%)	6 (1%)	73	87
2	b	597/597 (100%)	589 (99%)	8 (1%)	65	83
3	c	69/69 (100%)	69 (100%)	0	100	100
4	d	111/111 (100%)	110 (99%)	1 (1%)	75	89
5	e	55/55 (100%)	52 (94%)	3 (6%)	18	51
6	f	132/132 (100%)	130 (98%)	2 (2%)	60	81
7	g	98/98 (100%)	94 (96%)	4 (4%)	26	59
8	i	28/28 (100%)	28 (100%)	0	100	100
9	j	36/36 (100%)	33 (92%)	3 (8%)	9	35
10	l	113/113 (100%)	112 (99%)	1 (1%)	75	89
11	m	22/22 (100%)	22 (100%)	0	100	100
12	r	72/72 (100%)	71 (99%)	1 (1%)	62	82
13	B	133/133 (100%)	124 (93%)	9 (7%)	13	43
14	C	129/130 (99%)	126 (98%)	3 (2%)	45	72
15	D	128/128 (100%)	124 (97%)	4 (3%)	35	66
16	E	144/144 (100%)	144 (100%)	0	100	100
17	H	136/136 (100%)	136 (100%)	0	100	100
All	All	2606/2607 (100%)	2561 (98%)	45 (2%)	56	78

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	24	THR
1	a	80	GLN
1	a	198	MET
1	a	225	ASN
1	a	278	PHE
1	a	435	ASP
2	b	54	LEU
2	b	112	VAL
2	b	115	THR
2	b	242	VAL
2	b	245	THR
2	b	256	PHE

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Mol	Chain	Res	Type
2	b	515	ASP
2	b	545	LEU
4	d	53	ASN
5	e	14	GLU
5	e	32	ILE
5	e	62	LYS
6	f	139	SER
6	f	178	GLU
7	g	91	TYR
7	g	152	GLU
7	g	158	LEU
7	g	173	LYS
9	j	2	ASN
9	j	25	PHE
9	j	37	LEU
10	l	105	LYS
12	r	113	TYR
13	B	43	GLU
13	B	46	LYS
13	B	69	ASN
13	B	146	LEU
13	B	148	LEU
13	B	158	GLU
13	B	164	LEU
13	B	169	LEU
13	B	180	ASN
14	C	68	LEU
14	C	103	VAL
14	C	201	ASN
15	D	71	ASN
15	D	85	ASN
15	D	96	GLU
15	D	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	12	ASN
1	a	14	GLN
1	a	134	ASN
1	a	321	ASN
1	a	421	ASN

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Mol	Chain	Res	Type
1	a	478	GLN
1	a	489	ASN
1	a	501	ASN
2	b	10	GLN
2	b	34	HIS
2	b	89	HIS
2	b	113	ASN
2	b	330	HIS
2	b	451	GLN
2	b	472	GLN
2	b	474	ASN
2	b	626	ASN
2	b	688	ASN
4	d	53	ASN
4	d	114	ASN
6	f	55	GLN
6	f	171	ASN
9	j	2	ASN
10	l	9	ASN
10	l	33	ASN
13	B	52	ASN
13	B	69	ASN
13	B	181	HIS
14	C	52	ASN
14	C	201	ASN
15	D	71	ASN
15	D	85	ASN
15	D	179	GLN
16	E	213	ASN
17	H	91	GLN
17	H	185	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

217 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	SQD	a	849	-	31,32,54	3.14	8 (25%)	34,36,65	2.91	9 (26%)
18	CLA	H	315	17	45,53,73	1.76	5 (11%)	52,89,113	1.62	6 (11%)
18	CLA	a	830	20	52,60,73	1.67	7 (13%)	60,97,113	1.51	7 (11%)
18	CLA	b	817	2	60,68,73	1.55	7 (11%)	70,107,113	1.41	7 (10%)
18	CLA	j	104	9	41,49,73	1.84	6 (14%)	47,84,113	1.68	7 (14%)
18	CLA	b	838	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	a	807	1	65,73,73	1.47	11 (16%)	76,113,113	1.56	11 (14%)
18	CLA	a	806	1	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
28	DD6	E	304	-	39,45,45	2.53	8 (20%)	52,67,67	3.42	16 (30%)
26	A86	B	305	-	44,50,50	1.49	7 (15%)	51,76,76	3.13	26 (50%)
21	BCR	l	204	-	41,41,41	0.86	0	56,56,56	2.07	15 (26%)
25	DGD	b	834	-	61,61,67	0.85	2 (3%)	75,75,81	1.10	4 (5%)
24	SF4	c	102	3	0,12,12	-	-	-	-	-
18	CLA	b	850	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
18	CLA	b	844	2	62,70,73	1.50	6 (9%)	72,109,113	1.45	7 (9%)
21	BCR	i	102	-	41,41,41	0.75	0	56,56,56	1.94	17 (30%)
23	LMG	l	207	-	40,40,55	1.22	4 (10%)	48,48,63	1.76	4 (8%)
18	CLA	a	813	1	65,73,73	1.45	10 (15%)	76,113,113	1.56	12 (15%)
20	LHG	D	201	-	48,48,48	1.08	4 (8%)	51,54,54	1.03	2 (3%)
26	A86	D	203	-	44,50,50	1.34	4 (9%)	51,76,76	3.58	21 (41%)
18	CLA	D	212	15	42,50,73	1.79	6 (14%)	48,85,113	1.59	6 (12%)
27	ET4	l	206	-	41,43,43	1.45	7 (17%)	54,60,60	2.28	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	b	810	2	65,73,73	1.48	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	a	804	18,1	55,63,73	1.64	7 (12%)	64,101,113	1.49	8 (12%)
21	BCR	E	305	-	41,41,41	0.70	0	56,56,56	1.87	17 (30%)
18	CLA	f	204	6	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
18	CLA	r	202	12	45,53,73	1.77	5 (11%)	52,89,113	1.57	8 (15%)
18	CLA	C	312	14	61,69,73	1.52	10 (16%)	71,108,113	1.47	7 (9%)
18	CLA	b	811	2	60,68,73	1.49	10 (16%)	70,107,113	1.51	8 (11%)
18	CLA	a	844	1	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
18	CLA	a	853	1	55,63,73	1.61	6 (10%)	64,101,113	1.49	9 (14%)
20	LHG	B	315	-	41,41,48	0.98	2 (4%)	44,47,54	1.08	3 (6%)
18	CLA	C	310	14	46,54,73	1.66	8 (17%)	53,90,113	1.56	7 (13%)
18	CLA	a	822	1	50,58,73	1.68	6 (12%)	58,95,113	1.55	7 (12%)
20	LHG	E	301	-	48,48,48	1.11	6 (12%)	51,54,54	1.04	3 (5%)
18	CLA	a	810	1	65,73,73	1.46	7 (10%)	76,113,113	1.39	7 (9%)
18	CLA	l	205	-	45,53,73	1.75	6 (13%)	52,89,113	1.62	6 (11%)
18	CLA	b	840	2	61,69,73	1.52	7 (11%)	71,108,113	1.46	8 (11%)
18	CLA	B	312	13	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)
18	CLA	C	309	-	62,70,73	1.49	10 (16%)	72,109,113	1.59	10 (13%)
18	CLA	H	310	-	60,68,73	1.46	10 (16%)	70,107,113	1.59	9 (12%)
21	BCR	f	205	-	41,41,41	0.72	0	56,56,56	1.96	16 (28%)
21	BCR	m	101	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
18	CLA	a	825	1	60,68,73	1.55	11 (18%)	70,107,113	1.54	9 (12%)
18	CLA	b	843	2	65,73,73	1.45	10 (15%)	76,113,113	1.46	8 (10%)
23	LMG	E	318	-	43,43,55	2.06	7 (16%)	51,51,63	1.98	7 (13%)
20	LHG	a	835	-	32,32,48	1.28	5 (15%)	35,38,54	1.17	2 (5%)
28	DD6	E	308	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
26	A86	E	302	-	44,50,50	1.45	6 (13%)	51,76,76	2.82	23 (45%)
28	DD6	B	303	-	39,45,45	2.32	7 (17%)	52,67,67	2.91	20 (38%)
18	CLA	C	306	23	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
18	CLA	b	812	2	59,67,73	1.53	5 (8%)	68,105,113	1.46	7 (10%)
23	LMG	a	851	-	33,33,55	1.62	5 (15%)	41,41,63	3.61	8 (19%)
19	PQN	b	831	-	34,34,34	1.58	2 (5%)	42,45,45	1.17	3 (7%)
18	CLA	a	814	1	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	f	202	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
18	CLA	b	824	-	65,73,73	1.48	10 (15%)	76,113,113	1.57	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	b	836	-	41,41,41	0.74	0	56,56,56	2.00	18 (32%)
18	CLA	b	826	2	60,68,73	1.51	6 (10%)	70,107,113	1.53	7 (10%)
18	CLA	C	315	14	42,50,73	1.83	5 (11%)	48,85,113	1.60	6 (12%)
18	CLA	E	314	16	45,53,73	1.76	11 (24%)	52,89,113	1.62	9 (17%)
18	CLA	a	824	1	51,59,73	1.63	6 (11%)	59,96,113	1.58	7 (11%)
18	CLA	a	854	-	65,73,73	1.45	11 (16%)	76,113,113	1.54	10 (13%)
18	CLA	H	306	17	65,73,73	1.43	11 (16%)	76,113,113	1.40	9 (11%)
18	CLA	H	314	17	65,73,73	1.44	11 (16%)	76,113,113	1.50	10 (13%)
18	CLA	D	217	-	41,49,73	1.80	6 (14%)	47,84,113	1.64	8 (17%)
18	CLA	b	814	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
26	A86	H	304	-	44,50,50	1.46	5 (11%)	51,76,76	2.89	24 (47%)
18	CLA	b	848	2	54,62,73	1.61	6 (11%)	62,99,113	1.44	6 (9%)
18	CLA	i	101	-	60,68,73	1.55	6 (10%)	70,107,113	1.43	10 (14%)
18	CLA	b	842	2	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
21	BCR	j	105	-	41,41,41	0.72	0	56,56,56	2.09	13 (23%)
18	CLA	a	811	1	50,58,73	1.64	6 (12%)	58,95,113	1.60	7 (12%)
18	CLA	a	823	1	45,53,73	1.78	6 (13%)	52,89,113	1.60	6 (11%)
18	CLA	b	813	2	55,63,73	1.62	7 (12%)	64,101,113	1.49	6 (9%)
26	A86	B	301	-	44,50,50	1.30	4 (9%)	51,76,76	2.80	18 (35%)
18	CLA	a	828	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	C	311	14	60,68,73	1.54	9 (15%)	70,107,113	1.45	9 (12%)
18	CLA	a	848	1	56,64,73	1.59	6 (10%)	65,102,113	1.45	6 (9%)
18	CLA	b	849	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	B	310	13	46,54,73	1.77	6 (13%)	53,90,113	1.54	6 (11%)
18	CLA	a	803	1	65,73,73	1.44	11 (16%)	76,113,113	1.59	10 (13%)
20	LHG	H	316	-	34,34,48	1.12	3 (8%)	37,40,54	0.97	2 (5%)
26	A86	D	204	-	44,50,50	1.54	8 (18%)	51,76,76	3.73	22 (43%)
21	BCR	b	839	-	41,41,41	1.01	2 (4%)	56,56,56	2.04	21 (37%)
28	DD6	E	307	-	39,45,45	2.13	3 (7%)	52,67,67	3.02	23 (44%)
18	CLA	b	829	2	65,73,73	1.47	10 (15%)	76,113,113	1.51	11 (14%)
18	CLA	a	820	1	65,73,73	1.48	6 (9%)	76,113,113	1.41	8 (10%)
18	CLA	a	847	1	65,73,73	1.48	7 (10%)	76,113,113	1.39	6 (7%)
18	CLA	E	313	16	55,63,73	1.59	6 (10%)	64,101,113	1.52	8 (12%)
20	LHG	a	832	18	26,26,48	1.29	5 (19%)	29,32,54	1.19	2 (6%)
28	DD6	E	303	-	39,45,45	1.99	2 (5%)	52,67,67	1.91	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	b	823	2	58,66,73	1.56	6 (10%)	67,104,113	1.48	8 (11%)
21	BCR	a	834	-	41,41,41	0.73	0	56,56,56	1.97	14 (25%)
18	CLA	b	818	2	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
24	SF4	c	101	3	0,12,12	-	-	-	-	-
23	LMG	C	319	18	44,44,55	1.32	7 (15%)	52,52,63	1.86	4 (7%)
18	CLA	b	804	2	45,53,73	1.74	11 (24%)	52,89,113	1.69	8 (15%)
18	CLA	l	203	10	65,73,73	1.45	11 (16%)	76,113,113	1.56	10 (13%)
18	CLA	C	317	-	42,50,73	1.81	10 (23%)	48,85,113	1.69	8 (16%)
18	CLA	D	216	15	46,54,73	1.71	10 (21%)	53,90,113	1.54	7 (13%)
23	LMG	D	202	-	46,46,55	1.84	7 (15%)	54,54,63	1.36	5 (9%)
26	A86	b	847	-	44,50,50	1.41	6 (13%)	51,76,76	2.22	13 (25%)
24	SF4	b	802	2	0,12,12	-	-	-	-	-
18	CLA	B	306	13	58,65,73	1.54	10 (17%)	67,102,113	1.39	5 (7%)
18	CLA	D	214	15	56,64,73	1.60	7 (12%)	65,102,113	1.52	7 (10%)
18	CLA	H	313	17	65,73,73	1.46	11 (16%)	76,113,113	1.53	9 (11%)
18	CLA	E	312	16	65,73,73	1.47	11 (16%)	76,113,113	1.45	9 (11%)
18	CLA	a	837	1	60,68,73	1.53	12 (20%)	70,107,113	1.62	10 (14%)
18	CLA	D	210	-	56,64,73	1.57	10 (17%)	65,102,113	1.55	9 (13%)
18	CLA	a	855	1	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)
18	CLA	H	307	17	65,73,73	1.43	11 (16%)	76,113,113	1.62	13 (17%)
21	BCR	r	201	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
18	CLA	b	837	2	60,68,73	1.52	10 (16%)	70,107,113	1.55	8 (11%)
26	A86	m	102	-	44,50,50	1.36	4 (9%)	51,76,76	3.28	25 (49%)
18	CLA	b	815	2	46,54,73	1.73	6 (13%)	53,90,113	1.62	6 (11%)
26	A86	C	304	-	44,50,50	1.44	5 (11%)	51,76,76	2.68	16 (31%)
21	BCR	b	833	-	41,41,41	0.71	0	56,56,56	3.25	21 (37%)
20	LHG	E	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.20	4 (9%)
18	CLA	b	827	2	47,55,73	1.76	8 (17%)	54,91,113	1.57	7 (12%)
18	CLA	b	846	2	65,73,73	1.47	7 (10%)	76,113,113	1.34	7 (9%)
18	CLA	B	308	13	65,73,73	1.47	7 (10%)	76,113,113	1.39	7 (9%)
18	CLA	a	826	1	65,73,73	1.53	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	a	839	1	65,73,73	1.44	6 (9%)	76,113,113	1.42	7 (9%)
18	CLA	a	840	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	9 (11%)
18	CLA	b	830	20	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
18	CLA	f	203	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	a	809	18,1	62,70,73	1.50	6 (9%)	72,109,113	1.39	6 (8%)
18	CLA	a	836	1	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	b	801	-	65,73,73	1.49	12 (18%)	76,113,113	1.58	8 (10%)
20	LHG	b	835	18	48,48,48	1.09	3 (6%)	51,54,54	1.03	3 (5%)
26	A86	B	302	-	44,50,50	1.62	9 (20%)	51,76,76	3.40	23 (45%)
18	CLA	H	309	17	46,54,73	1.75	6 (13%)	53,90,113	1.57	6 (11%)
18	CLA	a	841	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
18	CLA	a	843	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	7 (9%)
18	CLA	a	805	1	65,73,73	1.46	7 (10%)	76,113,113	1.46	6 (7%)
18	CLA	C	307	14	65,73,73	1.45	10 (15%)	76,113,113	1.45	9 (11%)
18	CLA	B	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.42	6 (7%)
18	CLA	D	213	15	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
18	CLA	a	821	1	65,73,73	1.50	7 (10%)	76,113,113	1.39	8 (10%)
26	A86	D	206	-	44,50,50	1.46	6 (13%)	51,76,76	3.10	21 (41%)
20	LHG	a	831	-	48,48,48	1.11	3 (6%)	51,54,54	1.00	3 (5%)
18	CLA	a	842	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	9 (11%)
18	CLA	a	817	1	49,57,73	1.68	6 (12%)	55,93,113	1.58	7 (12%)
18	CLA	B	311	13	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
21	BCR	i	103	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
21	BCR	E	306	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
18	CLA	b	819	2	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
29	KC1	B	313	-	48,53,53	1.72	8 (16%)	55,89,89	1.99	10 (18%)
18	CLA	b	806	2	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
26	A86	C	302	-	44,50,50	1.50	6 (13%)	51,76,76	2.99	22 (43%)
18	CLA	a	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
18	CLA	a	812	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	6 (11%)
21	BCR	a	852	-	41,41,41	0.71	0	56,56,56	2.16	19 (33%)
21	BCR	j	101	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
18	CLA	b	841	2	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
18	CLA	b	803	2	65,73,73	1.45	12 (18%)	76,113,113	1.41	9 (11%)
18	CLA	a	819	1	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
18	CLA	H	308	17	65,73,73	1.45	10 (15%)	76,113,113	1.50	9 (11%)
21	BCR	a	850	-	41,41,41	1.03	2 (4%)	56,56,56	1.82	13 (23%)
21	BCR	l	201	-	41,41,41	1.00	2 (4%)	56,56,56	2.04	16 (28%)
18	CLA	H	305	-	54,62,73	1.60	10 (18%)	62,99,113	1.60	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	b	808	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	H	311	17	57,65,73	1.54	10 (17%)	66,103,113	1.49	7 (10%)
21	BCR	a	833	-	41,41,41	0.93	1 (2%)	56,56,56	1.92	20 (35%)
18	CLA	a	815	1	65,73,73	1.48	6 (9%)	76,113,113	1.39	9 (11%)
18	CLA	b	820	2	65,73,73	1.44	11 (16%)	76,113,113	1.58	9 (11%)
18	CLA	C	316	14	41,49,73	1.81	11 (26%)	47,84,113	1.69	9 (19%)
18	CLA	E	309	16	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	E	316	-	56,64,73	1.56	6 (10%)	65,102,113	1.51	6 (9%)
29	KC1	C	308	14	48,53,53	1.51	7 (14%)	55,89,89	1.92	10 (18%)
18	CLA	b	821	2	50,58,73	1.69	6 (12%)	58,95,113	1.49	8 (13%)
18	CLA	a	827	1	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
18	CLA	C	314	14	41,49,73	1.80	10 (24%)	47,84,113	1.63	8 (17%)
28	DD6	C	303	-	39,45,45	2.20	5 (12%)	52,67,67	2.32	18 (34%)
29	KC1	C	313	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
18	CLA	B	307	13	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
18	CLA	b	825	-	45,53,73	1.81	6 (13%)	52,89,113	1.58	7 (13%)
18	CLA	b	845	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	a	816	1	45,53,73	1.81	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	b	807	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
18	CLA	D	215	-	41,49,73	1.84	5 (12%)	47,84,113	1.66	7 (14%)
20	LHG	j	102	-	48,48,48	1.11	6 (12%)	51,54,54	0.91	2 (3%)
23	LMG	j	103	-	37,37,55	1.59	5 (13%)	45,45,63	3.61	8 (17%)
26	A86	H	302	-	44,50,50	1.61	8 (18%)	51,76,76	3.41	23 (45%)
26	A86	C	305	-	44,50,50	1.53	7 (15%)	51,76,76	3.11	24 (47%)
18	CLA	a	801	1	65,73,73	1.53	11 (16%)	76,113,113	1.44	10 (13%)
26	A86	B	304	-	44,50,50	1.52	7 (15%)	51,76,76	2.80	18 (35%)
18	CLA	l	202	10	49,57,73	1.66	10 (20%)	55,93,113	1.62	8 (14%)
18	CLA	C	318	14	42,50,73	1.77	10 (23%)	48,85,113	1.59	6 (12%)
18	CLA	E	311	16	46,54,73	1.76	6 (13%)	53,90,113	1.52	7 (13%)
21	BCR	b	832	-	41,41,41	0.70	0	56,56,56	1.92	14 (25%)
21	BCR	f	201	-	41,41,41	0.94	1 (2%)	56,56,56	1.94	18 (32%)
26	A86	r	203	-	44,50,50	1.50	7 (15%)	51,76,76	3.78	27 (52%)
26	A86	H	301	-	44,50,50	1.51	8 (18%)	51,76,76	3.17	24 (47%)
18	CLA	b	822	2	65,73,73	1.47	6 (9%)	76,113,113	1.45	6 (7%)
18	CLA	b	805	2	65,73,73	1.49	6 (9%)	76,113,113	1.46	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	KC1	H	312	17	48,53,53	1.82	8 (16%)	55,89,89	1.96	11 (20%)
19	PQN	a	829	-	34,34,34	1.59	2 (5%)	42,45,45	1.07	2 (4%)
18	CLA	D	208	15	65,73,73	1.48	10 (15%)	76,113,113	1.52	11 (14%)
18	CLA	D	209	15	49,57,73	1.71	7 (14%)	55,93,113	1.56	7 (12%)
28	DD6	H	303	-	39,45,45	2.48	11 (28%)	52,67,67	2.56	20 (38%)
18	CLA	D	207	-	61,69,73	1.53	10 (16%)	71,108,113	1.48	8 (11%)
18	CLA	a	818	1	51,59,73	1.63	11 (21%)	59,96,113	1.69	7 (11%)
18	CLA	a	808	1	65,73,73	1.49	8 (12%)	76,113,113	1.37	7 (9%)
18	CLA	E	315	16	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	b	816	2	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
18	CLA	a	846	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	a	838	1	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
23	LMG	C	301	-	31,31,55	1.61	6 (19%)	39,39,63	3.02	7 (17%)
18	CLA	D	211	15	46,54,73	1.76	7 (15%)	53,90,113	1.55	6 (11%)
18	CLA	b	809	2	55,63,73	1.64	6 (10%)	64,101,113	1.48	6 (9%)
28	DD6	D	205	-	39,45,45	2.22	6 (15%)	52,67,67	3.22	26 (50%)
21	BCR	a	845	-	41,41,41	0.98	2 (4%)	56,56,56	1.94	20 (35%)
18	CLA	E	310	16	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
18	CLA	B	314	13	41,49,73	1.83	10 (24%)	47,84,113	1.62	8 (17%)
18	CLA	b	828	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)

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
22	SQD	a	849	-	-	18/33/33/69	-
18	CLA	H	315	17	1/1/11/20	4/13/91/115	-
18	CLA	a	830	20	1/1/12/20	6/22/100/115	-
18	CLA	b	817	2	1/1/14/20	17/31/109/115	-
18	CLA	j	104	9	1/1/10/20	2/8/86/115	-
18	CLA	b	838	-	1/1/15/20	5/37/115/115	-
18	CLA	a	807	1	1/1/15/20	9/37/115/115	-
18	CLA	a	806	1	1/1/15/20	13/37/115/115	-
28	DD6	E	304	-	-	6/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	A86	B	305	-	-	4/34/90/90	0/3/3/3
21	BCR	l	204	-	-	8/29/63/63	0/2/2/2
25	DGD	b	834	-	-	27/49/89/95	0/2/2/2
24	SF4	c	102	3	-	-	0/6/5/5
18	CLA	b	850	2	1/1/15/20	12/37/115/115	-
18	CLA	b	844	2	1/1/14/20	10/34/112/115	-
21	BCR	i	102	-	-	0/29/63/63	0/2/2/2
23	LMG	l	207	-	-	16/35/55/70	0/1/1/1
18	CLA	a	813	1	1/1/15/20	24/37/115/115	-
20	LHG	D	201	-	-	32/53/53/53	-
26	A86	D	203	-	-	9/34/90/90	0/3/3/3
18	CLA	D	212	15	1/1/10/20	1/10/88/115	-
27	ET4	l	206	-	-	3/25/67/67	0/2/2/2
18	CLA	b	810	2	1/1/15/20	10/37/115/115	-
18	CLA	a	804	18,1	1/1/13/20	6/25/103/115	-
21	BCR	E	305	-	-	2/29/63/63	0/2/2/2
18	CLA	f	204	6	1/1/11/20	3/13/91/115	-
18	CLA	r	202	12	1/1/11/20	12/13/91/115	-
18	CLA	C	312	14	1/1/14/20	10/33/111/115	-
18	CLA	b	811	2	1/1/14/20	9/31/109/115	-
18	CLA	a	844	1	1/1/15/20	17/37/115/115	-
18	CLA	a	853	1	1/1/13/20	10/25/103/115	-
20	LHG	B	315	-	-	25/46/46/53	-
18	CLA	C	310	14	1/1/11/20	6/15/93/115	-
18	CLA	a	822	1	1/1/12/20	5/19/97/115	-
20	LHG	E	301	-	-	35/53/53/53	-
18	CLA	a	810	1	1/1/15/20	7/37/115/115	-
18	CLA	l	205	-	1/1/11/20	4/13/91/115	-
18	CLA	b	840	2	1/1/14/20	10/33/111/115	-
18	CLA	B	312	13	1/1/15/20	11/37/115/115	-
18	CLA	C	309	-	1/1/14/20	12/34/112/115	-
18	CLA	H	310	-	1/1/14/20	9/31/109/115	-
21	BCR	f	205	-	-	2/29/63/63	0/2/2/2
21	BCR	m	101	-	-	7/29/63/63	0/2/2/2
18	CLA	a	825	1	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	843	2	1/1/15/20	17/37/115/115	-
23	LMG	E	318	-	-	21/38/58/70	0/1/1/1
20	LHG	a	835	-	-	20/36/36/53	-
28	DD6	E	308	-	-	1/26/80/80	0/3/3/3
26	A86	E	302	-	-	5/34/90/90	0/3/3/3
28	DD6	B	303	-	-	0/26/80/80	0/3/3/3
18	CLA	C	306	23	1/1/11/20	4/13/91/115	-
18	CLA	b	812	2	1/1/13/20	9/30/108/115	-
23	LMG	a	851	-	-	16/28/48/70	0/1/1/1
19	PQN	b	831	-	-	3/23/43/43	0/2/2/2
18	CLA	a	814	1	1/1/15/20	7/37/115/115	-
18	CLA	f	202	-	1/1/15/20	10/37/115/115	-
18	CLA	b	824	-	1/1/15/20	17/37/115/115	-
21	BCR	b	836	-	-	5/29/63/63	0/2/2/2
18	CLA	b	826	2	1/1/14/20	8/31/109/115	-
18	CLA	C	315	14	1/1/10/20	4/10/88/115	-
18	CLA	E	314	16	1/1/11/20	3/13/91/115	-
18	CLA	a	824	1	1/1/12/20	10/21/99/115	-
18	CLA	a	854	-	1/1/15/20	16/37/115/115	-
18	CLA	H	306	17	1/1/15/20	12/37/115/115	-
18	CLA	H	314	17	1/1/15/20	15/37/115/115	-
18	CLA	D	217	-	1/1/10/20	5/8/86/115	-
18	CLA	b	814	-	1/1/15/20	11/37/115/115	-
26	A86	H	304	-	-	4/34/90/90	0/3/3/3
18	CLA	b	848	2	1/1/12/20	8/24/102/115	-
18	CLA	i	101	-	1/1/14/20	11/31/109/115	-
18	CLA	b	842	2	1/1/15/20	14/37/115/115	-
21	BCR	j	105	-	-	5/29/63/63	0/2/2/2
18	CLA	a	811	1	1/1/12/20	8/19/97/115	-
18	CLA	a	823	1	1/1/11/20	9/13/91/115	-
18	CLA	b	813	2	1/1/13/20	12/25/103/115	-
26	A86	B	301	-	-	12/34/90/90	0/3/3/3
18	CLA	a	828	1	1/1/15/20	11/37/115/115	-
18	CLA	C	311	14	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	848	1	1/1/13/20	9/27/105/115	-
18	CLA	b	849	-	1/1/15/20	14/37/115/115	-
18	CLA	B	310	13	1/1/11/20	5/15/93/115	-
18	CLA	a	803	1	1/1/15/20	13/37/115/115	-
20	LHG	H	316	-	-	19/38/38/53	-
26	A86	D	204	-	-	4/34/90/90	0/3/3/3
21	BCR	b	839	-	-	6/29/63/63	0/2/2/2
28	DD6	E	307	-	-	10/26/80/80	0/3/3/3
18	CLA	b	829	2	1/1/15/20	14/37/115/115	-
18	CLA	a	820	1	1/1/15/20	8/37/115/115	-
18	CLA	a	847	1	1/1/15/20	13/37/115/115	-
18	CLA	E	313	16	1/1/13/20	9/25/103/115	-
20	LHG	a	832	18	-	12/31/31/53	-
28	DD6	E	303	-	-	3/26/80/80	0/3/3/3
18	CLA	b	823	2	1/1/13/20	11/29/107/115	-
21	BCR	a	834	-	-	4/29/63/63	0/2/2/2
18	CLA	b	818	2	1/1/15/20	9/37/115/115	-
24	SF4	c	101	3	-	-	0/6/5/5
23	LMG	C	319	18	-	19/39/59/70	0/1/1/1
18	CLA	b	804	2	1/1/11/20	3/13/91/115	-
18	CLA	l	203	10	1/1/15/20	16/37/115/115	-
18	CLA	C	317	-	1/1/10/20	8/10/88/115	-
18	CLA	D	216	15	1/1/11/20	5/15/93/115	-
23	LMG	D	202	-	-	17/41/61/70	0/1/1/1
26	A86	b	847	-	-	17/34/90/90	0/3/3/3
24	SF4	b	802	2	-	-	0/6/5/5
18	CLA	B	306	13	1/1/12/20	17/27/101/115	-
18	CLA	D	214	15	1/1/13/20	9/27/105/115	-
18	CLA	H	313	17	1/1/15/20	18/37/115/115	-
18	CLA	E	312	16	1/1/15/20	11/37/115/115	-
18	CLA	a	837	1	1/1/14/20	14/31/109/115	-
18	CLA	D	210	-	1/1/13/20	6/27/105/115	-
18	CLA	a	855	1	1/1/15/20	14/37/115/115	-
18	CLA	H	307	17	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	r	201	-	-	4/29/63/63	0/2/2/2
18	CLA	b	837	2	1/1/14/20	14/31/109/115	-
26	A86	m	102	-	-	7/34/90/90	0/3/3/3
18	CLA	b	815	2	1/1/11/20	5/15/93/115	-
26	A86	C	304	-	-	3/34/90/90	0/3/3/3
21	BCR	b	833	-	-	6/29/63/63	0/2/2/2
20	LHG	E	317	-	-	6/46/46/53	-
18	CLA	b	827	2	1/1/11/20	5/16/94/115	-
18	CLA	b	846	2	1/1/15/20	12/37/115/115	-
18	CLA	B	308	13	1/1/15/20	11/37/115/115	-
18	CLA	a	826	1	1/1/15/20	12/37/115/115	-
18	CLA	a	839	1	1/1/15/20	9/37/115/115	-
18	CLA	a	840	-	1/1/15/20	13/37/115/115	-
18	CLA	b	830	20	1/1/15/20	7/37/115/115	-
18	CLA	f	203	-	1/1/15/20	10/37/115/115	-
18	CLA	a	809	18,1	1/1/14/20	12/34/112/115	-
18	CLA	a	836	1	1/1/15/20	13/37/115/115	-
18	CLA	b	801	-	1/1/15/20	9/37/115/115	-
20	LHG	b	835	18	-	32/53/53/53	-
26	A86	B	302	-	-	5/34/90/90	0/3/3/3
18	CLA	H	309	17	1/1/11/20	8/15/93/115	-
18	CLA	a	841	-	1/1/15/20	21/37/115/115	-
18	CLA	a	843	-	1/1/15/20	12/37/115/115	-
18	CLA	a	805	1	1/1/15/20	15/37/115/115	-
18	CLA	C	307	14	1/1/15/20	8/37/115/115	-
18	CLA	B	309	-	1/1/15/20	12/37/115/115	-
18	CLA	D	213	15	1/1/15/20	8/37/115/115	-
18	CLA	a	821	1	1/1/15/20	10/37/115/115	-
26	A86	D	206	-	-	6/34/90/90	0/3/3/3
20	LHG	a	831	-	-	26/53/53/53	-
18	CLA	a	842	-	1/1/15/20	10/37/115/115	-
18	CLA	a	817	1	1/1/11/20	10/18/96/115	-
18	CLA	B	311	13	1/1/15/20	11/37/115/115	-
21	BCR	i	103	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	E	306	-	-	0/29/63/63	0/2/2/2
18	CLA	b	819	2	1/1/15/20	14/37/115/115	-
29	KC1	B	313	-	-	8/15/71/71	-
18	CLA	b	806	2	1/1/15/20	17/37/115/115	-
26	A86	C	302	-	-	5/34/90/90	0/3/3/3
18	CLA	a	802	-	1/1/15/20	10/37/115/115	-
18	CLA	a	812	-	1/1/11/20	4/13/91/115	-
21	BCR	a	852	-	-	8/29/63/63	0/2/2/2
21	BCR	j	101	-	-	4/29/63/63	0/2/2/2
18	CLA	b	841	2	1/1/15/20	9/37/115/115	-
18	CLA	b	803	2	1/1/15/20	16/37/115/115	-
18	CLA	a	819	1	1/1/15/20	4/37/115/115	-
18	CLA	H	308	17	1/1/15/20	10/37/115/115	-
21	BCR	a	850	-	-	4/29/63/63	0/2/2/2
21	BCR	l	201	-	-	6/29/63/63	0/2/2/2
18	CLA	H	305	-	1/1/12/20	10/24/102/115	-
18	CLA	b	808	2	1/1/15/20	10/37/115/115	-
18	CLA	H	311	17	1/1/13/20	8/28/106/115	-
21	BCR	a	833	-	-	0/29/63/63	0/2/2/2
18	CLA	a	815	1	1/1/15/20	15/37/115/115	-
18	CLA	b	820	2	1/1/15/20	17/37/115/115	-
18	CLA	C	316	14	1/1/10/20	3/8/86/115	-
18	CLA	E	309	16	1/1/15/20	14/37/115/115	-
18	CLA	E	316	-	1/1/13/20	7/27/105/115	-
29	KC1	C	308	14	-	7/15/71/71	-
18	CLA	b	821	2	1/1/12/20	8/19/97/115	-
18	CLA	a	827	1	1/1/15/20	10/37/115/115	-
18	CLA	C	314	14	1/1/10/20	4/8/86/115	-
28	DD6	C	303	-	-	5/26/80/80	0/3/3/3
29	KC1	C	313	-	-	7/15/71/71	-
18	CLA	B	307	13	1/1/15/20	7/37/115/115	-
18	CLA	b	825	-	1/1/11/20	4/13/91/115	-
18	CLA	b	845	-	1/1/15/20	12/37/115/115	-
18	CLA	a	816	1	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	807	2	1/1/15/20	10/37/115/115	-
18	CLA	D	215	-	1/1/10/20	2/8/86/115	-
20	LHG	j	102	-	-	20/53/53/53	-
23	LMG	j	103	-	-	16/32/52/70	0/1/1/1
26	A86	H	302	-	-	5/34/90/90	0/3/3/3
26	A86	C	305	-	-	4/34/90/90	0/3/3/3
18	CLA	a	801	1	1/1/15/20	15/37/115/115	-
26	A86	B	304	-	-	3/34/90/90	0/3/3/3
18	CLA	l	202	10	1/1/11/20	8/18/96/115	-
18	CLA	C	318	14	1/1/10/20	5/10/88/115	-
18	CLA	E	311	16	1/1/11/20	6/15/93/115	-
21	BCR	b	832	-	-	0/29/63/63	0/2/2/2
21	BCR	f	201	-	-	9/29/63/63	0/2/2/2
26	A86	r	203	-	-	6/34/90/90	0/3/3/3
26	A86	H	301	-	-	5/34/90/90	0/3/3/3
18	CLA	b	822	2	1/1/15/20	18/37/115/115	-
18	CLA	b	805	2	1/1/15/20	13/37/115/115	-
29	KC1	H	312	17	-	9/15/71/71	-
19	PQN	a	829	-	-	2/23/43/43	0/2/2/2
18	CLA	D	208	15	1/1/15/20	13/37/115/115	-
18	CLA	D	209	15	1/1/11/20	9/18/96/115	-
28	DD6	H	303	-	-	3/26/80/80	0/3/3/3
18	CLA	D	207	-	1/1/14/20	10/33/111/115	-
18	CLA	a	818	1	1/1/12/20	5/21/99/115	-
18	CLA	a	808	1	1/1/15/20	10/37/115/115	-
18	CLA	E	315	16	1/1/15/20	10/37/115/115	-
18	CLA	b	816	2	1/1/13/20	3/25/103/115	-
18	CLA	a	846	-	1/1/15/20	8/37/115/115	-
18	CLA	a	838	1	1/1/15/20	12/37/115/115	-
23	LMG	C	301	-	-	14/26/46/70	0/1/1/1
18	CLA	D	211	15	1/1/11/20	9/15/93/115	-
18	CLA	b	809	2	1/1/13/20	3/25/103/115	-
28	DD6	D	205	-	-	3/26/80/80	0/3/3/3
21	BCR	a	845	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	E	310	16	1/1/15/20	12/37/115/115	-
18	CLA	B	314	13	1/1/10/20	2/8/86/115	-
18	CLA	b	828	-	1/1/15/20	9/37/115/115	-

All (1371) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	849	SQD	C6-S	-12.47	1.59	1.77
23	E	318	LMG	O2-C2	-10.74	1.17	1.43
23	D	202	LMG	O2-C2	-9.35	1.21	1.43
28	H	303	DD6	C29-C27	-9.22	1.24	1.42
28	C	303	DD6	C29-C27	-9.14	1.25	1.42
28	E	304	DD6	C29-C27	-9.03	1.25	1.42
28	E	307	DD6	C29-C27	-8.85	1.25	1.42
28	E	303	DD6	C29-C27	-8.58	1.26	1.42
28	E	308	DD6	C29-C27	-8.57	1.26	1.42
28	E	307	DD6	C30-C31	-8.31	1.25	1.42
28	E	304	DD6	C30-C31	-8.28	1.25	1.42
28	C	303	DD6	C30-C31	-8.26	1.25	1.42
28	B	303	DD6	C29-C27	-8.21	1.26	1.42
28	D	205	DD6	C29-C27	-7.91	1.27	1.42
18	a	826	CLA	C4B-NB	7.86	1.42	1.35
28	B	303	DD6	C30-C31	-7.83	1.26	1.42
28	H	303	DD6	C30-C31	-7.82	1.26	1.42
19	a	829	PQN	C3-C2	7.72	1.49	1.35
28	E	303	DD6	C30-C31	-7.71	1.26	1.42
18	a	804	CLA	C4B-NB	7.71	1.42	1.35
28	E	308	DD6	C30-C31	-7.69	1.26	1.42
18	b	827	CLA	C4B-NB	7.66	1.42	1.35
18	a	816	CLA	C4B-NB	7.64	1.42	1.35
18	b	825	CLA	C4B-NB	7.62	1.42	1.35
19	b	831	PQN	C3-C2	7.57	1.49	1.35
18	b	841	CLA	C4B-NB	7.56	1.42	1.35
29	H	312	KC1	C4D-CHA	-7.55	1.35	1.45
18	B	311	CLA	C4B-NB	7.55	1.41	1.35
18	a	838	CLA	C4B-NB	7.54	1.41	1.35
18	b	809	CLA	C4B-NB	7.51	1.41	1.35
18	b	821	CLA	C4B-NB	7.50	1.41	1.35
18	j	104	CLA	C4B-NB	7.50	1.41	1.35
18	b	822	CLA	C4B-NB	7.49	1.41	1.35
18	D	209	CLA	C4B-NB	7.48	1.41	1.35
18	b	805	CLA	C4B-NB	7.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	310	CLA	C4B-NB	7.47	1.41	1.35
18	C	306	CLA	C4B-NB	7.46	1.41	1.35
18	C	315	CLA	C4B-NB	7.46	1.41	1.35
18	b	816	CLA	C4B-NB	7.46	1.41	1.35
18	D	215	CLA	C4B-NB	7.45	1.41	1.35
18	a	812	CLA	C4B-NB	7.45	1.41	1.35
18	a	821	CLA	C4B-NB	7.45	1.41	1.35
18	b	806	CLA	C4B-NB	7.44	1.41	1.35
18	a	820	CLA	C4B-NB	7.43	1.41	1.35
18	a	823	CLA	C4B-NB	7.43	1.41	1.35
18	a	830	CLA	C4B-NB	7.42	1.41	1.35
18	H	309	CLA	C4B-NB	7.42	1.41	1.35
18	D	214	CLA	C4B-NB	7.41	1.41	1.35
18	a	828	CLA	C4B-NB	7.41	1.41	1.35
18	a	814	CLA	C4B-NB	7.40	1.41	1.35
18	E	310	CLA	C4B-NB	7.39	1.41	1.35
18	a	827	CLA	C4B-NB	7.39	1.41	1.35
18	b	814	CLA	C4B-NB	7.38	1.41	1.35
18	a	808	CLA	C4B-NB	7.38	1.41	1.35
18	b	828	CLA	C4B-NB	7.38	1.41	1.35
18	a	805	CLA	C4B-NB	7.38	1.41	1.35
18	a	853	CLA	C4B-NB	7.38	1.41	1.35
18	b	844	CLA	C4B-NB	7.38	1.41	1.35
18	b	850	CLA	C4B-NB	7.37	1.41	1.35
18	b	823	CLA	C4B-NB	7.37	1.41	1.35
18	a	847	CLA	C4B-NB	7.37	1.41	1.35
18	E	311	CLA	C4B-NB	7.36	1.41	1.35
18	b	840	CLA	C4B-NB	7.36	1.41	1.35
18	b	817	CLA	C4B-NB	7.35	1.41	1.35
18	b	810	CLA	C4B-NB	7.35	1.41	1.35
18	a	815	CLA	C4B-NB	7.34	1.41	1.35
18	b	849	CLA	C4B-NB	7.33	1.41	1.35
18	i	101	CLA	C4B-NB	7.33	1.41	1.35
18	b	807	CLA	C4B-NB	7.33	1.41	1.35
18	b	845	CLA	C4B-NB	7.32	1.41	1.35
18	f	203	CLA	C4B-NB	7.31	1.41	1.35
18	f	204	CLA	C4B-NB	7.31	1.41	1.35
18	D	211	CLA	C4B-NB	7.31	1.41	1.35
18	E	315	CLA	C4B-NB	7.30	1.41	1.35
18	a	810	CLA	C4B-NB	7.30	1.41	1.35
18	a	822	CLA	C4B-NB	7.30	1.41	1.35
18	D	213	CLA	C4B-NB	7.30	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	844	CLA	C4B-NB	7.29	1.41	1.35
29	B	313	KC1	C4D-CHA	-7.28	1.36	1.45
18	E	309	CLA	C4B-NB	7.28	1.41	1.35
18	b	830	CLA	C4B-NB	7.27	1.41	1.35
18	f	202	CLA	C4B-NB	7.27	1.41	1.35
18	r	202	CLA	C4B-NB	7.27	1.41	1.35
18	H	315	CLA	C4B-NB	7.26	1.41	1.35
18	B	307	CLA	C4B-NB	7.26	1.41	1.35
18	E	316	CLA	C4B-NB	7.26	1.41	1.35
18	a	848	CLA	C4B-NB	7.25	1.41	1.35
18	b	848	CLA	C4B-NB	7.25	1.41	1.35
18	b	819	CLA	C4B-NB	7.25	1.41	1.35
18	a	809	CLA	C4B-NB	7.24	1.41	1.35
18	D	212	CLA	C4B-NB	7.24	1.41	1.35
18	b	808	CLA	C4B-NB	7.23	1.41	1.35
18	b	818	CLA	C4B-NB	7.22	1.41	1.35
18	a	843	CLA	C4B-NB	7.21	1.41	1.35
18	l	205	CLA	C4B-NB	7.21	1.41	1.35
18	b	815	CLA	C4B-NB	7.21	1.41	1.35
18	a	802	CLA	C4B-NB	7.20	1.41	1.35
18	b	812	CLA	C4B-NB	7.19	1.41	1.35
18	b	846	CLA	C4B-NB	7.19	1.41	1.35
18	a	817	CLA	C4B-NB	7.18	1.41	1.35
18	E	313	CLA	C4B-NB	7.18	1.41	1.35
18	b	813	CLA	C4B-NB	7.17	1.41	1.35
18	a	855	CLA	C4B-NB	7.16	1.41	1.35
18	a	836	CLA	C4B-NB	7.16	1.41	1.35
18	B	308	CLA	C4B-NB	7.15	1.41	1.35
18	b	842	CLA	C4B-NB	7.15	1.41	1.35
18	a	819	CLA	C4B-NB	7.15	1.41	1.35
18	B	312	CLA	C4B-NB	7.15	1.41	1.35
18	b	838	CLA	C4B-NB	7.12	1.41	1.35
18	b	826	CLA	C4B-NB	7.11	1.41	1.35
18	B	309	CLA	C4B-NB	7.09	1.41	1.35
18	a	806	CLA	C4B-NB	7.08	1.41	1.35
18	a	824	CLA	C4B-NB	7.06	1.41	1.35
18	a	839	CLA	C4B-NB	7.05	1.41	1.35
18	a	846	CLA	C4B-NB	7.03	1.41	1.35
18	B	306	CLA	C4B-NB	7.01	1.41	1.35
18	a	811	CLA	C4B-NB	6.99	1.41	1.35
28	D	205	DD6	C30-C31	-6.99	1.27	1.42
18	D	217	CLA	C4B-NB	6.88	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	314	CLA	C4B-NB	6.85	1.41	1.35
22	a	849	SQD	O9-S	6.75	1.64	1.45
29	C	313	KC1	C4D-CHA	-6.72	1.36	1.45
18	C	311	CLA	C4B-NB	6.69	1.41	1.35
18	H	305	CLA	C4B-NB	6.63	1.41	1.35
18	C	316	CLA	C4B-NB	6.53	1.41	1.35
29	C	308	KC1	C4D-CHA	-6.52	1.36	1.45
18	a	825	CLA	C4B-NB	6.50	1.41	1.35
18	C	309	CLA	C4B-NB	6.43	1.40	1.35
18	E	314	CLA	C4B-NB	6.42	1.40	1.35
18	D	207	CLA	C4B-NB	6.40	1.40	1.35
18	C	314	CLA	C4B-NB	6.40	1.40	1.35
18	H	308	CLA	C4B-NB	6.40	1.40	1.35
18	H	313	CLA	C4B-NB	6.34	1.40	1.35
18	C	310	CLA	C4B-NB	6.32	1.40	1.35
18	D	210	CLA	C4B-NB	6.26	1.40	1.35
18	D	208	CLA	C4B-NB	6.21	1.40	1.35
18	a	841	CLA	C4B-NB	6.21	1.40	1.35
18	D	216	CLA	C4B-NB	6.20	1.40	1.35
18	C	312	CLA	C4B-NB	6.20	1.40	1.35
18	b	801	CLA	C4B-NB	6.18	1.40	1.35
18	a	840	CLA	C4B-NB	6.15	1.40	1.35
22	a	849	SQD	O47-C45	-6.13	1.39	1.46
18	a	813	CLA	C4B-NB	6.10	1.40	1.35
18	C	318	CLA	C4B-NB	6.05	1.40	1.35
18	H	314	CLA	C4B-NB	6.04	1.40	1.35
18	l	202	CLA	C4B-NB	6.02	1.40	1.35
18	b	843	CLA	C4B-NB	6.00	1.40	1.35
18	b	837	CLA	C4B-NB	5.98	1.40	1.35
18	b	829	CLA	C4B-NB	5.96	1.40	1.35
23	j	103	LMG	O2-C2	-5.96	1.28	1.43
23	a	851	LMG	O2-C2	-5.94	1.29	1.43
18	a	818	CLA	C4B-NB	5.91	1.40	1.35
18	a	807	CLA	C4B-NB	5.88	1.40	1.35
18	b	824	CLA	C4B-NB	5.86	1.40	1.35
18	l	203	CLA	C4B-NB	5.84	1.40	1.35
18	H	311	CLA	C4B-NB	5.81	1.40	1.35
18	b	804	CLA	C4B-NB	5.78	1.40	1.35
18	H	307	CLA	C4B-NB	5.73	1.40	1.35
18	C	307	CLA	C4B-NB	5.70	1.40	1.35
18	H	310	CLA	C4B-NB	5.68	1.40	1.35
18	a	842	CLA	C4B-NB	5.68	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	803	CLA	C4B-NB	5.67	1.40	1.35
18	b	820	CLA	C4B-NB	5.62	1.40	1.35
18	a	801	CLA	C4B-NB	5.61	1.40	1.35
18	a	837	CLA	C4B-NB	5.59	1.40	1.35
18	E	312	CLA	C4B-NB	5.54	1.40	1.35
18	b	811	CLA	C4B-NB	5.54	1.40	1.35
18	H	306	CLA	C4B-NB	5.47	1.40	1.35
18	a	854	CLA	C4B-NB	5.46	1.40	1.35
18	C	317	CLA	C4B-NB	5.43	1.40	1.35
29	H	312	KC1	MG-NB	-5.15	1.95	2.05
18	b	803	CLA	C4B-NB	5.07	1.39	1.35
29	B	313	KC1	MG-NB	-5.04	1.95	2.05
26	b	847	A86	O4-C38	4.99	1.46	1.35
22	a	849	SQD	O8-S	4.96	1.65	1.47
23	C	301	LMG	O2-C2	4.83	1.54	1.43
26	B	301	A86	O4-C38	4.82	1.46	1.35
18	C	317	CLA	C4D-ND	-4.77	1.31	1.37
18	a	801	CLA	C4D-ND	-4.74	1.31	1.37
29	C	308	KC1	MG-NB	-4.72	1.96	2.05
26	m	102	A86	O4-C38	4.71	1.45	1.35
19	a	829	PQN	C10-C5	4.71	1.48	1.40
19	b	831	PQN	C10-C5	4.69	1.48	1.40
26	E	302	A86	O4-C38	4.68	1.45	1.35
29	C	313	KC1	MG-NB	-4.62	1.96	2.05
26	C	305	A86	O4-C38	4.52	1.45	1.35
26	D	203	A86	O4-C38	4.51	1.45	1.35
26	H	301	A86	O4-C38	4.50	1.45	1.35
26	H	304	A86	O4-C38	4.47	1.45	1.35
26	D	204	A86	O4-C38	4.41	1.45	1.35
26	B	304	A86	O4-C38	4.32	1.45	1.35
22	a	849	SQD	O49-C7	4.32	1.40	1.22
26	C	302	A86	C30-C29	-4.24	1.24	1.32
26	D	206	A86	O4-C38	4.24	1.44	1.35
26	C	302	A86	O4-C38	4.22	1.44	1.35
20	B	315	LHG	O8-C23	4.20	1.45	1.33
20	E	317	LHG	O8-C23	4.19	1.45	1.33
18	b	824	CLA	C4D-ND	-4.16	1.32	1.37
18	b	804	CLA	C4D-ND	-4.14	1.32	1.37
25	b	834	DGD	O1G-C1A	4.14	1.45	1.33
18	H	306	CLA	C4D-ND	-4.13	1.32	1.37
26	H	302	A86	O4-C38	4.13	1.44	1.35
26	B	302	A86	C30-C29	-4.13	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	302	A86	O4-C38	4.11	1.44	1.35
27	l	206	ET4	C08-C07	4.10	1.45	1.33
18	l	203	CLA	C4D-ND	-4.10	1.32	1.37
26	C	304	A86	C30-C29	-4.09	1.25	1.32
26	r	203	A86	C30-C29	-4.09	1.25	1.32
26	H	302	A86	C30-C29	-4.07	1.25	1.32
20	E	317	LHG	O7-C7	4.07	1.45	1.34
18	a	837	CLA	C4D-ND	-4.07	1.32	1.37
26	E	302	A86	C30-C29	-4.06	1.25	1.32
18	a	818	CLA	C4D-ND	-4.05	1.32	1.37
26	C	304	A86	O4-C38	4.05	1.44	1.35
18	b	811	CLA	C4D-ND	-4.04	1.32	1.37
26	D	204	A86	C30-C29	-4.03	1.25	1.32
18	b	837	CLA	C4D-ND	-4.03	1.32	1.37
26	r	203	A86	O4-C38	4.02	1.44	1.35
18	b	842	CLA	C1D-ND	4.02	1.42	1.37
18	H	314	CLA	C4D-ND	-4.02	1.32	1.37
26	B	305	A86	O4-C38	4.01	1.44	1.35
18	a	807	CLA	C4D-ND	-4.01	1.32	1.37
18	C	307	CLA	C4D-ND	-4.01	1.32	1.37
18	a	826	CLA	C1D-ND	4.00	1.42	1.37
26	H	301	A86	C30-C29	-3.99	1.25	1.32
18	D	207	CLA	C4D-ND	-3.99	1.32	1.37
18	a	840	CLA	C4D-ND	-3.98	1.32	1.37
18	a	814	CLA	C1D-ND	3.97	1.42	1.37
18	a	844	CLA	C1D-ND	3.97	1.42	1.37
18	b	843	CLA	C4D-ND	-3.96	1.32	1.37
26	D	206	A86	C30-C29	-3.95	1.25	1.32
25	b	834	DGD	O2G-C1B	3.95	1.45	1.34
26	C	305	A86	C30-C29	-3.95	1.25	1.32
18	a	838	CLA	C1D-ND	3.94	1.42	1.37
18	H	311	CLA	C4D-ND	-3.94	1.32	1.37
18	a	854	CLA	C4D-ND	-3.93	1.32	1.37
18	b	818	CLA	C1D-ND	3.93	1.42	1.37
18	D	211	CLA	C1D-ND	3.93	1.42	1.37
18	E	312	CLA	C4D-ND	-3.93	1.32	1.37
18	b	841	CLA	C1D-ND	3.92	1.42	1.37
18	b	820	CLA	C4D-ND	-3.92	1.32	1.37
18	D	216	CLA	C4D-ND	-3.91	1.32	1.37
18	a	821	CLA	C1D-ND	3.91	1.42	1.37
18	D	208	CLA	C4D-ND	-3.91	1.32	1.37
26	B	305	A86	C30-C29	-3.91	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	803	CLA	C4D-ND	-3.89	1.32	1.37
18	C	318	CLA	C4D-ND	-3.89	1.32	1.37
18	b	809	CLA	C1D-ND	3.88	1.42	1.37
26	H	304	A86	C30-C29	-3.88	1.25	1.32
18	l	202	CLA	C4D-ND	-3.87	1.32	1.37
26	B	304	A86	C30-C29	-3.86	1.25	1.32
18	E	313	CLA	C1D-ND	3.86	1.42	1.37
18	b	813	CLA	C1D-ND	3.86	1.42	1.37
18	b	825	CLA	C1D-ND	3.86	1.42	1.37
18	a	817	CLA	C1D-ND	3.86	1.42	1.37
18	b	815	CLA	C1D-ND	3.85	1.42	1.37
18	C	311	CLA	C4D-ND	-3.85	1.32	1.37
18	a	812	CLA	C1D-ND	3.84	1.42	1.37
28	E	304	DD6	C21-C20	-3.84	1.45	1.51
18	b	829	CLA	C4D-ND	-3.84	1.32	1.37
20	B	315	LHG	O7-C7	3.84	1.45	1.34
18	C	315	CLA	C1D-ND	3.84	1.42	1.37
18	a	841	CLA	C4D-ND	-3.83	1.32	1.37
18	f	204	CLA	C1D-ND	3.83	1.42	1.37
18	a	813	CLA	C4D-ND	-3.83	1.32	1.37
18	a	848	CLA	C1D-ND	3.83	1.42	1.37
18	D	209	CLA	C1D-ND	3.83	1.42	1.37
18	b	805	CLA	C1D-ND	3.82	1.42	1.37
18	C	312	CLA	C4D-ND	-3.82	1.32	1.37
29	H	312	KC1	C4B-NB	-3.81	1.33	1.37
18	b	803	CLA	C4D-ND	-3.81	1.32	1.37
18	a	853	CLA	C1D-ND	3.80	1.42	1.37
18	H	307	CLA	C4D-ND	-3.79	1.32	1.37
18	D	215	CLA	C1D-ND	3.79	1.42	1.37
18	a	830	CLA	C1D-ND	3.79	1.42	1.37
18	B	308	CLA	C1D-ND	3.79	1.42	1.37
18	b	817	CLA	C1D-ND	3.79	1.42	1.37
18	b	838	CLA	C1D-ND	3.79	1.42	1.37
18	C	306	CLA	C1D-ND	3.79	1.42	1.37
18	D	214	CLA	C1D-ND	3.79	1.42	1.37
18	a	825	CLA	C4D-ND	-3.79	1.32	1.37
18	b	812	CLA	C1D-ND	3.79	1.42	1.37
18	B	312	CLA	C1D-ND	3.78	1.42	1.37
18	a	819	CLA	C1D-ND	3.78	1.42	1.37
18	C	314	CLA	C4D-ND	-3.78	1.32	1.37
18	a	824	CLA	C1D-ND	3.78	1.42	1.37
18	a	842	CLA	C4D-ND	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	816	CLA	C1D-ND	3.77	1.42	1.37
18	a	806	CLA	C1D-ND	3.76	1.42	1.37
18	E	311	CLA	C1D-ND	3.76	1.42	1.37
18	H	309	CLA	C1D-ND	3.76	1.42	1.37
28	B	303	DD6	C-C1	-3.76	1.43	1.50
18	a	811	CLA	C1D-ND	3.76	1.42	1.37
18	B	310	CLA	C1D-ND	3.75	1.42	1.37
18	b	807	CLA	C1D-ND	3.75	1.42	1.37
18	H	313	CLA	C4D-ND	-3.75	1.32	1.37
18	b	806	CLA	C1D-ND	3.75	1.42	1.37
18	b	827	CLA	C1D-ND	3.75	1.42	1.37
18	a	823	CLA	C1D-ND	3.74	1.42	1.37
18	b	810	CLA	C1D-ND	3.74	1.42	1.37
18	E	310	CLA	C1D-ND	3.74	1.42	1.37
18	b	850	CLA	C1D-ND	3.74	1.42	1.37
18	b	846	CLA	C1D-ND	3.74	1.42	1.37
18	E	309	CLA	C1D-ND	3.73	1.42	1.37
18	a	827	CLA	C1D-ND	3.73	1.42	1.37
18	r	202	CLA	C1D-ND	3.73	1.42	1.37
18	b	814	CLA	C1D-ND	3.73	1.42	1.37
18	b	823	CLA	C1D-ND	3.73	1.42	1.37
18	b	801	CLA	C4D-ND	-3.72	1.32	1.37
18	a	822	CLA	C1D-ND	3.72	1.42	1.37
18	H	305	CLA	C4D-ND	-3.72	1.32	1.37
18	E	315	CLA	C1D-ND	3.72	1.42	1.37
18	a	828	CLA	C1D-ND	3.72	1.42	1.37
18	b	826	CLA	C1D-ND	3.72	1.42	1.37
18	H	315	CLA	C1D-ND	3.72	1.42	1.37
18	b	819	CLA	C1D-ND	3.71	1.42	1.37
18	a	809	CLA	C1D-ND	3.71	1.42	1.37
18	l	205	CLA	C1D-ND	3.71	1.42	1.37
18	B	307	CLA	C1D-ND	3.70	1.42	1.37
18	j	104	CLA	C1D-ND	3.70	1.42	1.37
18	D	213	CLA	C1D-ND	3.70	1.42	1.37
26	b	847	A86	C30-C29	-3.69	1.25	1.32
18	i	101	CLA	C1D-ND	3.68	1.42	1.37
18	a	843	CLA	C1D-ND	3.68	1.42	1.37
18	a	847	CLA	C1D-ND	3.68	1.42	1.37
18	b	849	CLA	C1D-ND	3.67	1.42	1.37
18	a	810	CLA	C1D-ND	3.67	1.42	1.37
18	B	309	CLA	C1D-ND	3.67	1.42	1.37
18	a	808	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	828	CLA	C1D-ND	3.67	1.42	1.37
18	E	314	CLA	C4D-ND	-3.67	1.32	1.37
18	b	845	CLA	C1D-ND	3.67	1.42	1.37
18	b	816	CLA	C1D-ND	3.66	1.42	1.37
23	C	319	LMG	O2-C2	-3.66	1.34	1.43
18	b	840	CLA	C1D-ND	3.66	1.42	1.37
18	a	855	CLA	C1D-ND	3.66	1.42	1.37
18	D	212	CLA	C1D-ND	3.66	1.42	1.37
28	H	303	DD6	C-C1	-3.65	1.43	1.50
18	a	804	CLA	C1D-ND	3.65	1.42	1.37
18	a	815	CLA	C1D-ND	3.65	1.42	1.37
18	a	805	CLA	C1D-ND	3.64	1.42	1.37
18	b	844	CLA	C1D-ND	3.64	1.42	1.37
18	a	846	CLA	C1D-ND	3.64	1.42	1.37
18	b	808	CLA	C1D-ND	3.64	1.42	1.37
18	f	203	CLA	C1D-ND	3.63	1.42	1.37
18	D	210	CLA	C4D-ND	-3.63	1.32	1.37
18	b	830	CLA	C1D-ND	3.63	1.42	1.37
18	B	314	CLA	C4D-ND	-3.61	1.32	1.37
18	H	310	CLA	C4D-ND	-3.61	1.32	1.37
18	a	820	CLA	C1D-ND	3.60	1.42	1.37
18	b	822	CLA	C1D-ND	3.60	1.42	1.37
18	b	848	CLA	C1D-ND	3.60	1.42	1.37
18	f	202	CLA	C1D-ND	3.59	1.42	1.37
18	a	836	CLA	C1D-ND	3.58	1.42	1.37
26	D	203	A86	O1-C20	-3.58	1.41	1.46
18	D	217	CLA	C4D-ND	-3.57	1.32	1.37
18	a	839	CLA	C1D-ND	3.57	1.42	1.37
18	B	311	CLA	C1D-ND	3.55	1.42	1.37
18	b	821	CLA	C1D-ND	3.53	1.42	1.37
18	E	316	CLA	C1D-ND	3.53	1.42	1.37
18	C	310	CLA	C4D-ND	-3.52	1.32	1.37
23	D	202	LMG	O6-C1	3.51	1.50	1.41
18	a	802	CLA	C1D-ND	3.50	1.42	1.37
28	E	304	DD6	C19-C18	-3.50	1.47	1.52
26	B	301	A86	C30-C29	-3.49	1.26	1.32
18	C	316	CLA	C4D-ND	-3.47	1.32	1.37
26	D	203	A86	C30-C29	-3.46	1.26	1.32
18	H	308	CLA	C4D-ND	-3.46	1.32	1.37
18	C	309	CLA	C4D-ND	-3.45	1.33	1.37
23	j	103	LMG	O6-C1	3.43	1.50	1.41
29	H	312	KC1	CBA-CGA	-3.41	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	217	CLA	C1D-ND	3.41	1.42	1.37
26	B	302	A86	O1-C20	-3.41	1.41	1.46
23	l	207	LMG	O6-C1	3.40	1.50	1.41
29	B	313	KC1	C4B-NB	-3.37	1.33	1.37
18	a	804	CLA	CHC-C1C	3.34	1.43	1.35
18	B	314	CLA	C1D-ND	3.34	1.41	1.37
26	D	206	A86	O1-C20	-3.33	1.41	1.46
18	b	813	CLA	C4D-ND	-3.32	1.33	1.37
18	B	306	CLA	C4D-ND	-3.31	1.33	1.37
28	E	304	DD6	C36-C31	-3.31	1.31	1.34
26	m	102	A86	C30-C29	-3.29	1.26	1.32
18	b	801	CLA	CMB-C2B	-3.29	1.44	1.51
26	C	302	A86	O1-C20	-3.28	1.41	1.46
23	E	318	LMG	O6-C1	3.26	1.50	1.41
26	H	302	A86	C32-C31	-3.25	1.49	1.54
18	D	213	CLA	CHC-C1C	3.25	1.43	1.35
18	C	310	CLA	C1D-ND	3.23	1.41	1.37
29	H	312	KC1	C1B-NB	-3.22	1.33	1.37
18	a	815	CLA	CHC-C1C	3.21	1.43	1.35
18	a	853	CLA	CHC-C1C	3.21	1.43	1.35
18	b	841	CLA	CHC-C1C	3.21	1.43	1.35
18	E	309	CLA	CHC-C1C	3.21	1.43	1.35
18	b	814	CLA	CHC-C1C	3.20	1.43	1.35
26	H	302	A86	O1-C20	-3.19	1.41	1.46
28	D	205	DD6	C36-C31	-3.19	1.31	1.34
18	D	210	CLA	C1D-ND	3.19	1.41	1.37
26	B	302	A86	C32-C31	-3.19	1.49	1.54
29	B	313	KC1	CBA-CGA	-3.18	1.41	1.48
18	a	802	CLA	C4D-ND	-3.18	1.33	1.37
18	b	828	CLA	CHC-C1C	3.17	1.43	1.35
18	C	316	CLA	C1D-ND	3.17	1.41	1.37
18	i	101	CLA	CHC-C1C	3.17	1.43	1.35
18	a	838	CLA	CHC-C1C	3.17	1.43	1.35
18	C	315	CLA	CHC-C1C	3.16	1.43	1.35
18	b	826	CLA	CHC-C1C	3.16	1.43	1.35
18	H	305	CLA	C1D-ND	3.15	1.41	1.37
18	B	307	CLA	CHC-C1C	3.15	1.43	1.35
18	l	205	CLA	CHC-C1C	3.15	1.43	1.35
26	C	305	A86	C32-C31	-3.15	1.49	1.54
26	B	304	A86	O1-C20	-3.15	1.41	1.46
18	a	855	CLA	CHC-C1C	3.14	1.43	1.35
18	D	212	CLA	CHC-C1C	3.14	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	j	104	CLA	CHC-C1C	3.14	1.43	1.35
23	C	301	LMG	O6-C1	3.14	1.49	1.41
18	l	202	CLA	CMB-C2B	-3.14	1.45	1.51
18	E	315	CLA	CHC-C1C	3.14	1.43	1.35
18	b	822	CLA	CHC-C1C	3.13	1.43	1.35
18	a	825	CLA	CMB-C2B	-3.13	1.45	1.51
18	a	846	CLA	CHC-C1C	3.13	1.43	1.35
29	H	312	KC1	C4A-C3A	-3.13	1.38	1.44
18	B	310	CLA	CHC-C1C	3.13	1.43	1.35
18	b	806	CLA	C4D-ND	-3.13	1.33	1.37
26	B	305	A86	C32-C31	-3.13	1.49	1.54
18	a	819	CLA	C4D-ND	-3.12	1.33	1.37
18	C	306	CLA	CHC-C1C	3.12	1.43	1.35
18	a	822	CLA	CHC-C1C	3.12	1.43	1.35
18	b	812	CLA	CHC-C1C	3.12	1.43	1.35
18	a	854	CLA	CMB-C2B	-3.11	1.45	1.51
18	b	810	CLA	CHC-C1C	3.11	1.42	1.35
18	b	809	CLA	CHC-C1C	3.11	1.42	1.35
18	r	202	CLA	C4D-ND	-3.11	1.33	1.37
18	a	819	CLA	CHC-C1C	3.11	1.42	1.35
18	b	817	CLA	CHC-C1C	3.11	1.42	1.35
18	E	313	CLA	CHC-C1C	3.11	1.42	1.35
18	r	202	CLA	CHC-C1C	3.11	1.42	1.35
18	D	211	CLA	CHC-C1C	3.11	1.42	1.35
18	a	846	CLA	C4D-ND	-3.11	1.33	1.37
18	a	810	CLA	CHC-C1C	3.11	1.42	1.35
18	a	806	CLA	CHC-C1C	3.10	1.42	1.35
18	b	807	CLA	CHC-C1C	3.10	1.42	1.35
18	a	823	CLA	CHC-C1C	3.10	1.42	1.35
18	b	805	CLA	CHC-C1C	3.10	1.42	1.35
18	b	818	CLA	CHC-C1C	3.10	1.42	1.35
18	a	824	CLA	CHC-C1C	3.10	1.42	1.35
18	b	830	CLA	CHC-C1C	3.10	1.42	1.35
18	a	802	CLA	CHC-C1C	3.10	1.42	1.35
18	a	830	CLA	CHC-C1C	3.10	1.42	1.35
18	a	839	CLA	CHC-C1C	3.10	1.42	1.35
18	H	309	CLA	CHC-C1C	3.09	1.42	1.35
18	C	307	CLA	C1D-ND	3.09	1.41	1.37
18	b	850	CLA	CHC-C1C	3.09	1.42	1.35
18	f	202	CLA	CHC-C1C	3.09	1.42	1.35
18	B	308	CLA	CHC-C1C	3.09	1.42	1.35
18	a	843	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	847	CLA	CHC-C1C	3.09	1.42	1.35
18	E	310	CLA	CHC-C1C	3.09	1.42	1.35
18	b	803	CLA	C3B-C2B	-3.09	1.36	1.40
18	a	828	CLA	CHC-C1C	3.09	1.42	1.35
18	a	816	CLA	CHC-C1C	3.08	1.42	1.35
18	a	826	CLA	CHC-C1C	3.08	1.42	1.35
20	D	201	LHG	C26-C25	-3.08	1.34	1.51
18	b	815	CLA	CHC-C1C	3.08	1.42	1.35
18	b	820	CLA	CMB-C2B	-3.08	1.45	1.51
18	H	315	CLA	CHC-C1C	3.08	1.42	1.35
18	D	214	CLA	CHC-C1C	3.08	1.42	1.35
18	H	308	CLA	C1D-ND	3.08	1.41	1.37
18	a	814	CLA	CHC-C1C	3.08	1.42	1.35
18	a	812	CLA	CHC-C1C	3.08	1.42	1.35
18	b	848	CLA	CHC-C1C	3.08	1.42	1.35
18	b	826	CLA	C4D-ND	-3.08	1.33	1.37
18	b	849	CLA	CHC-C1C	3.08	1.42	1.35
18	b	817	CLA	C4D-ND	-3.08	1.33	1.37
18	b	838	CLA	CHC-C1C	3.08	1.42	1.35
18	a	836	CLA	CHC-C1C	3.08	1.42	1.35
29	B	313	KC1	C1B-NB	-3.07	1.34	1.37
18	b	842	CLA	CHC-C1C	3.07	1.42	1.35
18	f	204	CLA	CHC-C1C	3.07	1.42	1.35
18	b	823	CLA	CHC-C1C	3.07	1.42	1.35
18	B	311	CLA	CHC-C1C	3.07	1.42	1.35
18	a	827	CLA	CHC-C1C	3.07	1.42	1.35
18	b	844	CLA	CHC-C1C	3.07	1.42	1.35
18	b	825	CLA	CHC-C1C	3.07	1.42	1.35
18	b	846	CLA	CHC-C1C	3.07	1.42	1.35
18	b	846	CLA	C4D-ND	-3.07	1.33	1.37
18	E	311	CLA	CHC-C1C	3.07	1.42	1.35
18	b	819	CLA	CHC-C1C	3.06	1.42	1.35
18	b	837	CLA	CMB-C2B	-3.06	1.45	1.51
18	a	840	CLA	CMB-C2B	-3.06	1.45	1.51
23	C	301	LMG	O8-C28	3.06	1.42	1.33
18	B	312	CLA	CHC-C1C	3.06	1.42	1.35
18	D	215	CLA	CHC-C1C	3.06	1.42	1.35
18	B	307	CLA	C4D-ND	-3.06	1.33	1.37
18	b	827	CLA	CHC-C1C	3.06	1.42	1.35
18	a	825	CLA	C3B-C2B	-3.06	1.36	1.40
18	D	209	CLA	CHC-C1C	3.06	1.42	1.35
18	C	314	CLA	C1D-ND	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	848	CLA	CHC-C1C	3.05	1.42	1.35
26	H	304	A86	O1-C20	-3.05	1.41	1.46
18	B	312	CLA	C4D-ND	-3.05	1.33	1.37
18	a	809	CLA	CHC-C1C	3.05	1.42	1.35
18	b	845	CLA	CHC-C1C	3.05	1.42	1.35
18	C	309	CLA	C1D-ND	3.05	1.41	1.37
26	m	102	A86	O1-C20	-3.05	1.41	1.46
18	B	306	CLA	C1D-ND	3.05	1.41	1.37
18	a	817	CLA	CHC-C1C	3.05	1.42	1.35
18	C	311	CLA	C1D-ND	3.04	1.41	1.37
18	b	829	CLA	CMB-C2B	-3.04	1.45	1.51
23	E	318	LMG	O1-C1	-3.04	1.35	1.40
18	a	837	CLA	CMB-C2B	-3.04	1.45	1.51
18	a	808	CLA	C4D-ND	-3.04	1.33	1.37
18	b	806	CLA	CHC-C1C	3.04	1.42	1.35
18	l	202	CLA	C1D-ND	3.03	1.41	1.37
18	a	844	CLA	CHC-C1C	3.03	1.42	1.35
18	b	821	CLA	CHC-C1C	3.03	1.42	1.35
18	b	807	CLA	C4D-ND	-3.03	1.33	1.37
18	a	821	CLA	CHC-C1C	3.03	1.42	1.35
18	b	843	CLA	CMB-C2B	-3.03	1.45	1.51
18	a	808	CLA	CHC-C1C	3.03	1.42	1.35
26	B	305	A86	O1-C20	-3.03	1.41	1.46
18	D	214	CLA	C4D-ND	-3.02	1.33	1.37
18	b	822	CLA	C4D-ND	-3.02	1.33	1.37
26	C	304	A86	O1-C20	-3.02	1.41	1.46
18	b	819	CLA	C4D-ND	-3.02	1.33	1.37
18	b	845	CLA	C4D-ND	-3.02	1.33	1.37
18	a	806	CLA	C4D-ND	-3.01	1.33	1.37
18	f	202	CLA	C4D-ND	-3.01	1.33	1.37
18	H	309	CLA	C4D-ND	-3.01	1.33	1.37
18	D	213	CLA	C4D-ND	-3.01	1.33	1.37
18	D	216	CLA	C1D-ND	3.01	1.41	1.37
18	a	811	CLA	CHC-C1C	3.01	1.42	1.35
18	b	849	CLA	C4D-ND	-3.01	1.33	1.37
18	E	316	CLA	CHC-C1C	3.01	1.42	1.35
18	l	203	CLA	CMB-C2B	-3.01	1.45	1.51
18	C	312	CLA	CHC-C1C	3.00	1.42	1.35
18	a	812	CLA	C4D-ND	-3.00	1.33	1.37
18	b	840	CLA	CHC-C1C	3.00	1.42	1.35
18	b	814	CLA	C4D-ND	-3.00	1.33	1.37
18	b	816	CLA	CHC-C1C	3.00	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	815	CLA	C4D-ND	-2.99	1.33	1.37
18	i	101	CLA	C4D-ND	-2.99	1.33	1.37
18	a	817	CLA	C4D-ND	-2.99	1.33	1.37
18	b	809	CLA	C4D-ND	-2.99	1.33	1.37
18	H	307	CLA	C1D-ND	2.99	1.41	1.37
20	b	835	LHG	O8-C6	-2.99	1.38	1.45
18	B	309	CLA	CHC-C1C	2.99	1.42	1.35
18	E	314	CLA	CHC-C1C	2.99	1.42	1.35
18	D	208	CLA	CHC-C1C	2.99	1.42	1.35
28	B	303	DD6	O1-C20	-2.99	1.41	1.46
18	a	801	CLA	C1D-ND	2.99	1.41	1.37
18	C	314	CLA	CHC-C1C	2.98	1.42	1.35
18	b	830	CLA	C4D-ND	-2.98	1.33	1.37
18	b	804	CLA	CMB-C2B	-2.98	1.45	1.51
18	b	825	CLA	C4D-ND	-2.98	1.33	1.37
18	f	203	CLA	CHC-C1C	2.98	1.42	1.35
18	a	816	CLA	C4D-ND	-2.98	1.33	1.37
18	b	808	CLA	CHC-C1C	2.98	1.42	1.35
18	a	842	CLA	CMB-C2B	-2.98	1.45	1.51
18	a	805	CLA	CHC-C1C	2.98	1.42	1.35
18	B	314	CLA	CHC-C1C	2.98	1.42	1.35
18	D	209	CLA	C4D-ND	-2.98	1.33	1.37
18	b	801	CLA	C3B-C2B	-2.98	1.36	1.40
26	H	301	A86	O1-C20	-2.98	1.41	1.46
18	C	316	CLA	CHC-C1C	2.97	1.42	1.35
18	C	306	CLA	C4D-ND	-2.97	1.33	1.37
18	a	827	CLA	C4D-ND	-2.97	1.33	1.37
26	C	305	A86	O1-C20	-2.97	1.41	1.46
18	D	210	CLA	CMB-C2B	-2.97	1.45	1.51
18	D	211	CLA	C4D-ND	-2.97	1.33	1.37
18	E	309	CLA	C4D-ND	-2.97	1.33	1.37
18	a	839	CLA	C4D-ND	-2.97	1.33	1.37
26	B	302	A86	C2-C1	-2.97	1.31	1.35
18	b	850	CLA	C4D-ND	-2.97	1.33	1.37
18	B	310	CLA	C4D-ND	-2.97	1.33	1.37
28	H	303	DD6	O1-C20	-2.96	1.42	1.46
18	a	807	CLA	CMB-C2B	-2.96	1.45	1.51
18	a	820	CLA	CHC-C1C	2.96	1.42	1.35
28	E	304	DD6	O1-C20	-2.96	1.42	1.46
18	b	827	CLA	C4D-ND	-2.96	1.33	1.37
18	a	801	CLA	CMB-C2B	-2.96	1.45	1.51
18	a	841	CLA	CMB-C2B	-2.95	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	202	LMG	O8-C28	2.95	1.42	1.33
18	a	824	CLA	C4D-ND	-2.95	1.33	1.37
18	C	311	CLA	CHC-C1C	2.95	1.42	1.35
18	a	830	CLA	C4D-ND	-2.95	1.33	1.37
18	f	204	CLA	C4D-ND	-2.95	1.33	1.37
18	a	844	CLA	C4D-ND	-2.94	1.33	1.37
18	a	842	CLA	C1D-ND	2.94	1.41	1.37
18	a	805	CLA	C4D-ND	-2.94	1.33	1.37
18	a	843	CLA	C4D-ND	-2.94	1.33	1.37
18	C	312	CLA	C1D-ND	2.94	1.41	1.37
18	B	309	CLA	C4D-ND	-2.94	1.33	1.37
18	B	311	CLA	C4D-ND	-2.94	1.33	1.37
18	D	207	CLA	CHC-C1C	2.94	1.42	1.35
18	E	312	CLA	C1D-ND	2.93	1.41	1.37
18	b	805	CLA	C4D-ND	-2.93	1.33	1.37
18	b	813	CLA	CHC-C1C	2.93	1.42	1.35
18	H	311	CLA	CHC-C1C	2.93	1.42	1.35
18	C	312	CLA	CMB-C2B	-2.93	1.45	1.51
26	H	302	A86	C2-C1	-2.93	1.31	1.35
29	C	313	KC1	CBA-CGA	-2.93	1.41	1.48
18	a	841	CLA	CHC-C1C	2.93	1.42	1.35
18	a	847	CLA	C4D-ND	-2.93	1.33	1.37
22	a	849	SQD	O47-C7	2.92	1.39	1.33
18	b	824	CLA	CMB-C2B	-2.92	1.45	1.51
18	E	312	CLA	CHC-C1C	2.92	1.42	1.35
26	H	301	A86	C32-C31	-2.92	1.49	1.54
20	E	301	LHG	C26-C25	-2.92	1.35	1.51
18	D	208	CLA	CMB-C2B	-2.92	1.45	1.51
18	E	313	CLA	C4D-ND	-2.92	1.33	1.37
18	a	813	CLA	C1D-ND	2.92	1.41	1.37
18	E	315	CLA	C4D-ND	-2.91	1.33	1.37
18	a	821	CLA	C4D-ND	-2.91	1.33	1.37
18	H	306	CLA	CMB-C2B	-2.91	1.45	1.51
18	b	828	CLA	C4D-ND	-2.91	1.33	1.37
18	a	811	CLA	C4D-ND	-2.91	1.33	1.37
18	b	811	CLA	CMB-C2B	-2.91	1.45	1.51
18	E	310	CLA	C4D-ND	-2.91	1.33	1.37
18	b	818	CLA	C4D-ND	-2.90	1.33	1.37
18	E	316	CLA	C4D-ND	-2.90	1.33	1.37
26	H	304	A86	C32-C31	-2.90	1.49	1.54
18	H	305	CLA	CHC-C1C	2.90	1.42	1.35
18	C	317	CLA	CMB-C2B	-2.90	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	831	LHG	C26-C25	-2.90	1.35	1.51
18	b	838	CLA	C4D-ND	-2.90	1.33	1.37
18	C	311	CLA	CMB-C2B	-2.90	1.45	1.51
18	l	205	CLA	C4D-ND	-2.90	1.33	1.37
18	H	314	CLA	CMB-C2B	-2.90	1.45	1.51
18	a	803	CLA	CMB-C2B	-2.89	1.45	1.51
18	a	855	CLA	C4D-ND	-2.89	1.33	1.37
23	l	207	LMG	O8-C28	2.89	1.41	1.33
18	a	826	CLA	C4D-ND	-2.89	1.33	1.37
18	l	202	CLA	CHC-C1C	2.89	1.42	1.35
18	E	312	CLA	CMB-C2B	-2.89	1.45	1.51
18	C	312	CLA	C3B-C2B	-2.89	1.36	1.40
18	a	813	CLA	CHC-C1C	2.89	1.42	1.35
18	a	823	CLA	C4D-ND	-2.89	1.33	1.37
18	a	836	CLA	C4D-ND	-2.88	1.33	1.37
20	b	835	LHG	C26-C25	-2.88	1.35	1.51
18	a	840	CLA	C1D-ND	2.88	1.41	1.37
18	b	837	CLA	CHC-C1C	2.88	1.42	1.35
18	a	804	CLA	C4D-ND	-2.88	1.33	1.37
18	H	315	CLA	C4D-ND	-2.88	1.33	1.37
18	a	822	CLA	C4D-ND	-2.88	1.33	1.37
18	D	207	CLA	CMB-C2B	-2.88	1.45	1.51
18	C	307	CLA	CHC-C1C	2.88	1.42	1.35
18	a	814	CLA	C4D-ND	-2.88	1.33	1.37
18	j	104	CLA	C4D-ND	-2.88	1.33	1.37
18	b	803	CLA	CMB-C2B	-2.88	1.45	1.51
18	a	818	CLA	CMB-C2B	-2.87	1.45	1.51
18	b	821	CLA	C4D-ND	-2.87	1.33	1.37
18	a	807	CLA	C1D-ND	2.87	1.41	1.37
18	B	308	CLA	C4D-ND	-2.87	1.33	1.37
18	f	203	CLA	C4D-ND	-2.87	1.33	1.37
26	r	203	A86	O1-C20	-2.87	1.42	1.46
28	B	303	DD6	C17-C16	-2.87	1.50	1.54
18	b	842	CLA	C4D-ND	-2.87	1.33	1.37
26	E	302	A86	O1-C20	-2.87	1.42	1.46
18	D	216	CLA	CHC-C1C	2.87	1.42	1.35
18	b	848	CLA	C4D-ND	-2.87	1.33	1.37
18	b	844	CLA	C4D-ND	-2.87	1.33	1.37
18	b	808	CLA	C4D-ND	-2.87	1.33	1.37
20	a	835	LHG	C26-C25	-2.87	1.35	1.51
18	b	840	CLA	C4D-ND	-2.86	1.33	1.37
18	H	307	CLA	CMB-C2B	-2.86	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	313	CLA	CHC-C1C	2.86	1.42	1.35
18	C	315	CLA	C4D-ND	-2.86	1.33	1.37
18	a	809	CLA	C4D-ND	-2.86	1.33	1.37
18	b	837	CLA	C1D-ND	2.86	1.41	1.37
28	D	205	DD6	O1-C20	-2.86	1.42	1.46
18	D	217	CLA	CHC-C1C	2.86	1.42	1.35
26	D	204	A86	O1-C20	-2.86	1.42	1.46
18	a	801	CLA	C3B-C2B	-2.85	1.36	1.40
18	b	812	CLA	C4D-ND	-2.85	1.33	1.37
18	a	810	CLA	C4D-ND	-2.85	1.33	1.37
18	E	311	CLA	C4D-ND	-2.85	1.33	1.37
18	C	318	CLA	CHC-C1C	2.85	1.42	1.35
18	C	309	CLA	CMB-C2B	-2.84	1.45	1.51
18	a	828	CLA	C4D-ND	-2.84	1.33	1.37
29	B	313	KC1	C4A-C3A	-2.84	1.39	1.44
18	b	829	CLA	C1D-ND	2.84	1.41	1.37
23	a	851	LMG	O6-C1	2.84	1.49	1.41
18	b	823	CLA	C4D-ND	-2.84	1.33	1.37
23	C	319	LMG	O1-C1	-2.84	1.35	1.40
18	a	853	CLA	C4D-ND	-2.83	1.33	1.37
18	a	815	CLA	C4D-ND	-2.83	1.33	1.37
23	D	202	LMG	O1-C1	-2.83	1.35	1.40
18	D	208	CLA	C3B-C2B	-2.82	1.36	1.40
18	b	804	CLA	C1D-ND	2.82	1.41	1.37
18	a	841	CLA	C1D-ND	2.82	1.41	1.37
18	D	210	CLA	CHC-C1C	2.82	1.42	1.35
28	D	205	DD6	C17-C16	-2.82	1.50	1.54
26	H	302	A86	C-C1	-2.82	1.45	1.50
18	a	820	CLA	C4D-ND	-2.82	1.33	1.37
20	j	102	LHG	C26-C25	-2.82	1.35	1.51
18	a	840	CLA	CHC-C1C	2.81	1.42	1.35
18	a	848	CLA	C4D-ND	-2.81	1.33	1.37
18	D	215	CLA	C4D-ND	-2.81	1.33	1.37
18	b	841	CLA	C4D-ND	-2.81	1.33	1.37
18	C	318	CLA	CMB-C2B	-2.81	1.45	1.51
18	a	803	CLA	C1D-ND	2.81	1.41	1.37
18	D	216	CLA	CMB-C2B	-2.80	1.45	1.51
18	D	212	CLA	C4D-ND	-2.80	1.33	1.37
18	C	310	CLA	CHC-C1C	2.80	1.42	1.35
18	b	804	CLA	CHC-C1C	2.80	1.42	1.35
26	D	204	A86	C32-C31	-2.80	1.49	1.54
18	b	829	CLA	C3B-C2B	-2.80	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	838	CLA	C4D-ND	-2.80	1.33	1.37
18	a	840	CLA	C3B-C2B	-2.79	1.36	1.40
18	b	843	CLA	CHC-C1C	2.79	1.42	1.35
18	B	306	CLA	CHC-C1C	2.79	1.42	1.35
18	b	810	CLA	C4D-ND	-2.79	1.33	1.37
18	H	308	CLA	CMB-C2B	-2.78	1.45	1.51
26	B	302	A86	C-C1	-2.78	1.45	1.50
18	C	309	CLA	CHC-C1C	2.78	1.42	1.35
29	C	313	KC1	C4B-NB	-2.78	1.34	1.37
18	E	314	CLA	C1D-ND	2.78	1.41	1.37
18	b	820	CLA	C1D-ND	2.77	1.41	1.37
23	j	103	LMG	O8-C28	2.77	1.41	1.33
18	C	314	CLA	CMB-C2B	-2.77	1.45	1.51
18	E	314	CLA	CMB-C2B	-2.77	1.45	1.51
18	H	305	CLA	CMB-C2B	-2.77	1.45	1.51
18	a	807	CLA	CHC-C1C	2.77	1.42	1.35
18	b	824	CLA	CMD-C2D	-2.77	1.44	1.50
18	C	317	CLA	CHC-C1C	2.77	1.42	1.35
18	C	307	CLA	CMB-C2B	-2.76	1.45	1.51
20	a	831	LHG	O8-C6	-2.76	1.38	1.45
18	H	306	CLA	CHC-C1C	2.76	1.42	1.35
27	l	206	ET4	C37-C38	-2.76	1.46	1.51
28	C	303	DD6	C36-C31	-2.76	1.31	1.34
28	D	205	DD6	C-C1	-2.76	1.45	1.50
18	a	820	CLA	CMB-C2B	-2.75	1.45	1.51
23	D	202	LMG	O7-C8	-2.75	1.39	1.46
29	C	308	KC1	CBA-CGA	-2.74	1.42	1.48
18	H	313	CLA	CMB-C2B	-2.74	1.45	1.51
21	a	850	BCR	C30-C25	-2.73	1.50	1.53
18	a	854	CLA	CHC-C1C	2.73	1.42	1.35
18	a	825	CLA	CHC-C1C	2.73	1.42	1.35
18	b	820	CLA	CMD-C2D	-2.73	1.45	1.50
18	a	813	CLA	CMB-C2B	-2.73	1.46	1.51
18	H	313	CLA	C1D-ND	2.73	1.41	1.37
18	b	824	CLA	C1D-ND	2.73	1.41	1.37
18	H	311	CLA	C1D-ND	2.72	1.41	1.37
18	b	816	CLA	C4D-ND	-2.72	1.33	1.37
18	b	803	CLA	C3B-CAB	-2.72	1.42	1.47
18	H	314	CLA	C1D-ND	2.72	1.41	1.37
18	b	801	CLA	CHC-C1C	2.72	1.41	1.35
18	b	811	CLA	CHC-C1C	2.71	1.41	1.35
18	C	316	CLA	CMB-C2B	-2.71	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	207	CLA	C1D-ND	2.71	1.41	1.37
18	H	311	CLA	CMB-C2B	-2.71	1.46	1.51
18	D	208	CLA	C1D-ND	2.71	1.41	1.37
18	C	318	CLA	C3B-C2B	-2.70	1.36	1.40
18	H	310	CLA	CMB-C2B	-2.70	1.46	1.51
18	b	843	CLA	C1D-ND	2.69	1.41	1.37
18	b	837	CLA	C3B-C2B	-2.69	1.36	1.40
18	B	314	CLA	CMB-C2B	-2.69	1.46	1.51
18	H	306	CLA	C1D-ND	2.69	1.41	1.37
18	a	801	CLA	CHC-C1C	2.69	1.41	1.35
18	b	808	CLA	CMB-C2B	-2.69	1.46	1.51
18	b	811	CLA	C3B-C2B	-2.69	1.36	1.40
28	H	303	DD6	C36-C31	-2.68	1.31	1.34
18	a	837	CLA	C1D-ND	2.68	1.41	1.37
18	l	203	CLA	CHC-C1C	2.68	1.41	1.35
18	a	818	CLA	CHC-C1C	2.68	1.41	1.35
18	H	308	CLA	CHC-C1C	2.67	1.41	1.35
18	a	837	CLA	CHC-C1C	2.67	1.41	1.35
18	b	803	CLA	MG-ND	-2.67	2.00	2.05
18	H	310	CLA	C1D-ND	2.67	1.41	1.37
18	b	829	CLA	CHC-C1C	2.67	1.41	1.35
18	a	818	CLA	C1D-ND	2.67	1.41	1.37
18	a	854	CLA	C3B-C2B	-2.66	1.36	1.40
18	b	824	CLA	CHC-C1C	2.66	1.41	1.35
18	E	314	CLA	C3B-C2B	-2.66	1.36	1.40
26	C	302	A86	C32-C31	-2.66	1.50	1.54
18	a	837	CLA	C3B-C2B	-2.66	1.36	1.40
23	C	319	LMG	O6-C1	2.65	1.48	1.41
18	C	317	CLA	C3B-CAB	-2.65	1.42	1.47
18	E	312	CLA	C3B-C2B	-2.64	1.36	1.40
18	C	318	CLA	CMD-C2D	-2.64	1.45	1.50
18	b	803	CLA	C1D-ND	2.64	1.41	1.37
29	C	308	KC1	C4B-NB	-2.64	1.34	1.37
18	b	849	CLA	CMB-C2B	-2.64	1.46	1.51
18	b	801	CLA	C1D-ND	2.64	1.41	1.37
21	a	850	BCR	C1-C6	-2.64	1.50	1.53
23	C	319	LMG	O8-C28	2.64	1.41	1.33
20	D	201	LHG	O8-C6	-2.64	1.39	1.45
18	b	803	CLA	CMD-C2D	-2.63	1.45	1.50
18	a	803	CLA	CHC-C1C	2.63	1.41	1.35
18	C	317	CLA	CMD-C2D	-2.63	1.45	1.50
26	D	204	A86	C2-C1	-2.63	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	828	CLA	CMB-C2B	-2.62	1.46	1.51
18	b	804	CLA	C3B-C2B	-2.61	1.36	1.40
18	a	842	CLA	CHC-C1C	2.61	1.41	1.35
23	j	103	LMG	O7-C8	-2.61	1.40	1.46
20	H	316	LHG	O8-C6	-2.60	1.39	1.45
18	H	308	CLA	C3B-C2B	-2.60	1.36	1.40
18	a	801	CLA	CMD-C2D	-2.60	1.45	1.50
18	b	811	CLA	CMC-C2C	-2.60	1.45	1.50
18	b	811	CLA	C1D-ND	2.60	1.41	1.37
18	C	318	CLA	C3B-CAB	-2.60	1.42	1.47
18	b	820	CLA	C3B-C2B	-2.59	1.36	1.40
21	b	839	BCR	C30-C25	-2.59	1.50	1.53
18	b	820	CLA	CHC-C1C	2.59	1.41	1.35
18	B	306	CLA	CMB-C2B	-2.59	1.46	1.51
18	H	310	CLA	CHC-C1C	2.59	1.41	1.35
23	E	318	LMG	O8-C28	2.59	1.40	1.33
18	l	202	CLA	CMD-C2D	-2.58	1.45	1.50
18	a	815	CLA	CMB-C2B	-2.58	1.46	1.51
18	E	312	CLA	CMD-C2D	-2.58	1.45	1.50
18	b	813	CLA	CMB-C2B	-2.58	1.46	1.51
18	a	807	CLA	C3B-C2B	-2.58	1.36	1.40
18	D	207	CLA	C3B-C2B	-2.58	1.36	1.40
18	a	841	CLA	CMD-C2D	-2.58	1.45	1.50
18	b	829	CLA	CMD-C2D	-2.58	1.45	1.50
18	C	318	CLA	C1D-ND	2.58	1.41	1.37
18	a	825	CLA	C1D-ND	2.57	1.40	1.37
18	a	837	CLA	CMD-C2D	-2.57	1.45	1.50
18	C	317	CLA	C3B-C2B	-2.56	1.36	1.40
18	H	314	CLA	CHC-C1C	2.56	1.41	1.35
18	a	837	CLA	CMC-C2C	-2.56	1.45	1.50
18	b	816	CLA	CMB-C2B	-2.56	1.46	1.51
26	C	302	A86	C13-C11	-2.56	1.44	1.49
18	D	212	CLA	CMB-C2B	-2.56	1.46	1.51
18	a	812	CLA	CMB-C2B	-2.56	1.46	1.51
26	D	203	A86	C13-C11	-2.55	1.44	1.49
18	E	312	CLA	C3B-CAB	-2.55	1.42	1.47
18	a	801	CLA	C3B-CAB	-2.55	1.42	1.47
18	E	315	CLA	CMB-C2B	-2.55	1.46	1.51
18	H	307	CLA	CHC-C1C	2.55	1.41	1.35
18	b	820	CLA	C3B-CAB	-2.55	1.42	1.47
18	C	317	CLA	C1D-ND	2.54	1.40	1.37
18	a	854	CLA	C3B-CAB	-2.54	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	208	CLA	CMC-C2C	-2.54	1.45	1.50
26	E	302	A86	C32-C31	-2.54	1.50	1.54
18	b	829	CLA	CMC-C2C	-2.54	1.45	1.50
18	B	306	CLA	CBD-CAD	2.54	1.57	1.51
26	D	204	A86	C13-C11	-2.54	1.44	1.49
18	D	217	CLA	CMB-C2B	-2.53	1.46	1.51
18	b	801	CLA	CMC-C2C	-2.53	1.45	1.50
18	a	813	CLA	C3B-C2B	-2.53	1.36	1.40
18	a	839	CLA	CMB-C2B	-2.53	1.46	1.51
18	a	818	CLA	CMD-C2D	-2.53	1.45	1.50
18	C	310	CLA	CMB-C2B	-2.53	1.46	1.51
18	a	802	CLA	CMB-C2B	-2.53	1.46	1.51
18	a	819	CLA	CMB-C2B	-2.53	1.46	1.51
18	b	814	CLA	CMB-C2B	-2.52	1.46	1.51
18	b	824	CLA	CMC-C2C	-2.52	1.45	1.50
18	l	203	CLA	C3B-C2B	-2.52	1.36	1.40
18	E	310	CLA	CMB-C2B	-2.52	1.46	1.51
20	E	301	LHG	O8-C6	-2.52	1.39	1.45
26	B	304	A86	C32-C31	-2.52	1.50	1.54
20	a	835	LHG	O8-C6	-2.52	1.39	1.45
26	C	304	A86	C13-C11	-2.52	1.44	1.49
18	b	812	CLA	CMB-C2B	-2.52	1.46	1.51
18	H	311	CLA	CMC-C2C	-2.51	1.45	1.50
18	C	317	CLA	MG-ND	-2.51	2.00	2.05
18	b	842	CLA	CMB-C2B	-2.51	1.46	1.51
18	a	840	CLA	CMD-C2D	-2.51	1.45	1.50
18	a	842	CLA	CMD-C2D	-2.51	1.45	1.50
26	b	847	A86	C32-C31	-2.51	1.50	1.54
18	B	311	CLA	CMB-C2B	-2.51	1.46	1.51
18	H	310	CLA	CMD-C2D	-2.51	1.45	1.50
20	a	831	LHG	O7-C5	-2.51	1.40	1.46
18	b	827	CLA	CMB-C2B	-2.51	1.46	1.51
18	H	306	CLA	C3B-C2B	-2.51	1.36	1.40
18	a	837	CLA	MG-ND	-2.51	2.00	2.05
18	b	825	CLA	CMB-C2B	-2.51	1.46	1.51
29	C	308	KC1	C1B-NB	-2.50	1.34	1.37
18	a	822	CLA	CMB-C2B	-2.50	1.46	1.51
18	E	312	CLA	MG-ND	-2.50	2.00	2.05
21	b	839	BCR	C1-C6	-2.50	1.50	1.53
18	a	814	CLA	CMB-C2B	-2.50	1.46	1.51
18	b	809	CLA	CMB-C2B	-2.49	1.46	1.51
18	a	848	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	805	CLA	CMB-C2B	-2.49	1.46	1.51
26	r	203	A86	C32-C31	-2.49	1.50	1.54
26	b	847	A86	O1-C20	-2.49	1.42	1.46
18	b	805	CLA	CMB-C2B	-2.49	1.46	1.51
18	H	309	CLA	CMB-C2B	-2.49	1.46	1.51
18	b	823	CLA	CMB-C2B	-2.49	1.46	1.51
18	a	840	CLA	CMC-C2C	-2.49	1.45	1.50
18	b	843	CLA	CMD-C2D	-2.49	1.45	1.50
18	b	846	CLA	CMB-C2B	-2.49	1.46	1.51
28	E	304	DD6	C-C1	-2.49	1.45	1.50
18	a	821	CLA	CMB-C2B	-2.49	1.46	1.51
18	b	811	CLA	CMD-C2D	-2.49	1.45	1.50
18	a	826	CLA	CMB-C2B	-2.49	1.46	1.51
23	E	318	LMG	O7-C8	-2.49	1.40	1.46
18	C	311	CLA	C3B-C2B	-2.48	1.36	1.40
18	B	307	CLA	CMB-C2B	-2.48	1.46	1.51
18	C	314	CLA	CMD-C2D	-2.48	1.45	1.50
18	H	306	CLA	C3B-CAB	-2.48	1.42	1.47
18	a	830	CLA	CMB-C2B	-2.48	1.46	1.51
18	l	202	CLA	C3B-C2B	-2.48	1.36	1.40
18	b	844	CLA	CMB-C2B	-2.48	1.46	1.51
18	a	807	CLA	CAA-C2A	-2.48	1.49	1.54
18	B	309	CLA	CMB-C2B	-2.48	1.46	1.51
18	b	803	CLA	CHC-C1C	2.48	1.41	1.35
18	a	854	CLA	CMC-C2C	-2.47	1.45	1.50
18	H	311	CLA	C3B-CAB	-2.47	1.42	1.47
18	b	819	CLA	CMB-C2B	-2.47	1.46	1.51
18	H	311	CLA	CMD-C2D	-2.47	1.45	1.50
18	a	806	CLA	CMB-C2B	-2.47	1.46	1.51
18	b	821	CLA	CMB-C2B	-2.47	1.46	1.51
18	b	848	CLA	CMB-C2B	-2.47	1.46	1.51
18	E	313	CLA	CMB-C2B	-2.47	1.46	1.51
18	b	845	CLA	CMB-C2B	-2.47	1.46	1.51
26	C	304	A86	C32-C31	-2.47	1.50	1.54
18	a	816	CLA	CMB-C2B	-2.47	1.46	1.51
18	C	309	CLA	C3B-C2B	-2.47	1.36	1.40
18	a	846	CLA	CMB-C2B	-2.47	1.46	1.51
18	a	803	CLA	C3B-C2B	-2.46	1.36	1.40
18	b	838	CLA	CMB-C2B	-2.46	1.46	1.51
18	E	309	CLA	CMB-C2B	-2.46	1.46	1.51
18	f	204	CLA	CMB-C2B	-2.46	1.46	1.51
18	D	214	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	840	CLA	CMB-C2B	-2.46	1.46	1.51
18	a	813	CLA	CMD-C2D	-2.46	1.45	1.50
18	a	841	CLA	CMC-C2C	-2.46	1.45	1.50
18	b	843	CLA	C3B-C2B	-2.46	1.37	1.40
18	D	215	CLA	CMB-C2B	-2.46	1.46	1.51
18	H	308	CLA	CMD-C2D	-2.46	1.45	1.50
18	i	101	CLA	CMB-C2B	-2.46	1.46	1.51
18	b	810	CLA	CMB-C2B	-2.46	1.46	1.51
18	D	209	CLA	CMB-C2B	-2.46	1.46	1.51
18	l	203	CLA	C1D-ND	2.46	1.40	1.37
18	a	853	CLA	CMB-C2B	-2.46	1.46	1.51
18	a	825	CLA	CMD-C2D	-2.46	1.45	1.50
23	l	207	LMG	O7-C8	-2.46	1.40	1.46
18	a	841	CLA	C3B-C2B	-2.46	1.37	1.40
18	C	306	CLA	CMB-C2B	-2.45	1.46	1.51
18	D	216	CLA	CMD-C2D	-2.45	1.45	1.50
18	H	307	CLA	CMC-C2C	-2.45	1.45	1.50
18	E	311	CLA	CMB-C2B	-2.45	1.46	1.51
18	b	811	CLA	C3B-CAB	-2.45	1.42	1.47
18	a	808	CLA	CMB-C2B	-2.45	1.46	1.51
18	b	818	CLA	CMB-C2B	-2.45	1.46	1.51
18	a	807	CLA	CMD-C2D	-2.45	1.45	1.50
18	D	208	CLA	CMD-C2D	-2.45	1.45	1.50
18	C	316	CLA	C3B-C2B	-2.45	1.37	1.40
18	b	837	CLA	CMD-C2D	-2.44	1.45	1.50
18	b	803	CLA	CMC-C2C	-2.44	1.45	1.50
18	a	803	CLA	CMD-C2D	-2.44	1.45	1.50
18	H	311	CLA	C3B-C2B	-2.44	1.37	1.40
18	a	823	CLA	CMB-C2B	-2.44	1.46	1.51
18	D	213	CLA	CMB-C2B	-2.44	1.46	1.51
20	E	301	LHG	O7-C5	-2.44	1.40	1.46
18	a	809	CLA	CMB-C2B	-2.44	1.46	1.51
23	C	301	LMG	O7-C10	2.44	1.41	1.34
18	r	202	CLA	CMB-C2B	-2.44	1.46	1.51
18	D	211	CLA	CMB-C2B	-2.44	1.46	1.51
23	a	851	LMG	O8-C28	2.44	1.40	1.33
18	a	801	CLA	MG-ND	-2.44	2.01	2.05
18	D	216	CLA	CMC-C2C	-2.43	1.45	1.50
18	a	844	CLA	CMB-C2B	-2.43	1.46	1.51
18	b	850	CLA	CMB-C2B	-2.43	1.46	1.51
28	H	303	DD6	C35-C36	-2.43	1.47	1.51
18	a	817	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	312	CLA	CMB-C2B	-2.43	1.46	1.51
18	a	810	CLA	CMB-C2B	-2.43	1.46	1.51
18	j	104	CLA	CMB-C2B	-2.43	1.46	1.51
18	a	840	CLA	MG-ND	-2.43	2.01	2.05
18	a	803	CLA	CMC-C2C	-2.43	1.45	1.50
18	l	203	CLA	CMD-C2D	-2.43	1.45	1.50
27	l	206	ET4	C19-C18	2.43	1.51	1.45
18	a	811	CLA	CMB-C2B	-2.43	1.46	1.51
18	C	316	CLA	CMD-C2D	-2.43	1.45	1.50
29	C	313	KC1	C4A-C3A	-2.43	1.39	1.44
18	a	847	CLA	CMB-C2B	-2.43	1.46	1.51
18	b	817	CLA	CMB-C2B	-2.43	1.46	1.51
18	C	309	CLA	CMD-C2D	-2.43	1.45	1.50
18	C	307	CLA	C3B-CAB	-2.42	1.43	1.47
18	b	801	CLA	CMD-C2D	-2.42	1.45	1.50
18	a	827	CLA	CMB-C2B	-2.42	1.46	1.51
18	a	824	CLA	CMB-C2B	-2.42	1.46	1.51
18	b	806	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	308	CLA	CMB-C2B	-2.42	1.46	1.51
18	b	843	CLA	CMC-C2C	-2.42	1.45	1.50
26	B	301	A86	O1-C20	-2.42	1.42	1.46
18	b	815	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	310	CLA	CMB-C2B	-2.42	1.46	1.51
26	D	206	A86	C32-C31	-2.42	1.50	1.54
20	b	835	LHG	O7-C5	-2.42	1.40	1.46
18	a	854	CLA	C1D-ND	2.42	1.40	1.37
23	C	319	LMG	O7-C10	2.42	1.41	1.34
18	a	813	CLA	CMC-C2C	-2.42	1.45	1.50
18	H	307	CLA	CMD-C2D	-2.42	1.45	1.50
18	b	830	CLA	CMB-C2B	-2.42	1.46	1.51
18	E	314	CLA	CMD-C2D	-2.42	1.45	1.50
18	a	828	CLA	CMB-C2B	-2.42	1.46	1.51
26	b	847	A86	C17-C16	-2.41	1.50	1.54
18	f	203	CLA	CMB-C2B	-2.41	1.46	1.51
20	a	835	LHG	O7-C5	-2.41	1.40	1.46
18	l	203	CLA	CMC-C2C	-2.41	1.45	1.50
18	D	207	CLA	CMD-C2D	-2.41	1.45	1.50
18	b	826	CLA	CMB-C2B	-2.41	1.46	1.51
18	a	855	CLA	CMB-C2B	-2.41	1.46	1.51
18	b	801	CLA	C3B-CAB	-2.41	1.43	1.47
18	a	804	CLA	CMB-C2B	-2.41	1.46	1.51
18	D	207	CLA	C3B-CAB	-2.41	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	315	CLA	CMB-C2B	-2.41	1.46	1.51
18	D	208	CLA	C3B-CAB	-2.41	1.43	1.47
18	l	205	CLA	CMB-C2B	-2.41	1.46	1.51
18	D	210	CLA	C3B-C2B	-2.41	1.37	1.40
18	C	314	CLA	C3B-C2B	-2.40	1.37	1.40
18	D	216	CLA	C3B-C2B	-2.40	1.37	1.40
23	C	319	LMG	O7-C8	-2.40	1.40	1.46
28	E	304	DD6	C17-C16	-2.40	1.50	1.54
21	a	833	BCR	C1-C6	-2.40	1.50	1.53
18	a	825	CLA	CMC-C2C	-2.40	1.45	1.50
18	l	202	CLA	CMC-C2C	-2.40	1.45	1.50
18	H	305	CLA	CMD-C2D	-2.40	1.45	1.50
18	H	306	CLA	CMD-C2D	-2.40	1.45	1.50
18	a	837	CLA	C3B-CAB	-2.40	1.43	1.47
18	b	804	CLA	CMC-C2C	-2.40	1.45	1.50
21	l	201	BCR	C30-C25	-2.39	1.50	1.53
28	H	303	DD6	C17-C16	-2.39	1.50	1.54
18	D	210	CLA	CMD-C2D	-2.39	1.45	1.50
18	b	813	CLA	CMC-C2C	-2.39	1.45	1.50
18	b	824	CLA	MG-ND	-2.39	2.01	2.05
18	l	202	CLA	MG-ND	-2.39	2.01	2.05
18	a	807	CLA	CMC-C2C	-2.39	1.45	1.50
18	C	312	CLA	C3B-CAB	-2.39	1.43	1.47
18	b	807	CLA	CMB-C2B	-2.39	1.46	1.51
18	C	315	CLA	CMB-C2B	-2.39	1.46	1.51
18	a	842	CLA	MG-ND	-2.39	2.01	2.05
18	b	801	CLA	MG-ND	-2.39	2.01	2.05
18	H	310	CLA	CMC-C2C	-2.38	1.45	1.50
18	a	854	CLA	CMD-C2D	-2.38	1.45	1.50
18	a	840	CLA	C3B-CAB	-2.38	1.43	1.47
18	H	313	CLA	C3B-C2B	-2.38	1.37	1.40
18	C	316	CLA	C3B-CAB	-2.38	1.43	1.47
18	a	836	CLA	CMB-C2B	-2.38	1.46	1.51
18	a	838	CLA	CMB-C2B	-2.38	1.46	1.51
21	a	845	BCR	C30-C25	-2.38	1.50	1.53
18	C	307	CLA	CMC-C2C	-2.38	1.45	1.50
28	H	303	DD6	C21-C20	-2.38	1.48	1.51
18	f	202	CLA	CMB-C2B	-2.38	1.46	1.51
18	b	804	CLA	CMD-C2D	-2.38	1.45	1.50
18	b	841	CLA	CMB-C2B	-2.38	1.46	1.51
26	D	204	A86	C17-C16	-2.38	1.50	1.54
18	a	841	CLA	MG-ND	-2.37	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	837	CLA	CMC-C2C	-2.37	1.45	1.50
20	a	832	LHG	O8-C6	-2.37	1.39	1.45
18	l	203	CLA	C3B-CAB	-2.37	1.43	1.47
18	H	314	CLA	CMC-C2C	-2.37	1.45	1.50
22	a	849	SQD	O48-C23	2.37	1.40	1.33
18	H	314	CLA	CMD-C2D	-2.37	1.45	1.50
18	a	843	CLA	CMB-C2B	-2.37	1.46	1.51
18	D	210	CLA	C3B-CAB	-2.37	1.43	1.47
28	H	303	DD6	C19-C18	-2.37	1.48	1.52
18	C	312	CLA	CMD-C2D	-2.37	1.45	1.50
23	a	851	LMG	O7-C10	2.36	1.41	1.34
18	H	307	CLA	C3B-CAB	-2.36	1.43	1.47
26	B	304	A86	C-C1	-2.36	1.46	1.50
18	a	818	CLA	CMC-C2C	-2.36	1.45	1.50
18	b	843	CLA	MG-ND	-2.36	2.01	2.05
18	E	316	CLA	CMB-C2B	-2.35	1.46	1.51
18	a	813	CLA	C3B-CAB	-2.35	1.43	1.47
26	H	302	A86	C17-C16	-2.35	1.50	1.54
18	E	312	CLA	CMC-C2C	-2.35	1.45	1.50
18	H	310	CLA	MG-ND	-2.35	2.01	2.05
20	a	835	LHG	O7-C7	2.35	1.40	1.35
18	H	308	CLA	CMC-C2C	-2.34	1.45	1.50
18	B	314	CLA	MG-ND	-2.34	2.01	2.05
29	C	313	KC1	C1B-NB	-2.34	1.34	1.37
18	C	309	CLA	CMC-C2C	-2.34	1.45	1.50
26	b	847	A86	C13-C11	-2.34	1.45	1.49
20	j	102	LHG	O8-C23	2.34	1.40	1.33
18	D	207	CLA	CMC-C2C	-2.34	1.45	1.50
18	b	824	CLA	C3B-C2B	-2.34	1.37	1.40
20	a	835	LHG	O8-C23	2.33	1.40	1.33
26	H	301	A86	C2-C1	-2.33	1.32	1.35
29	C	313	KC1	CHD-C4C	2.33	1.40	1.35
18	a	818	CLA	MG-ND	-2.33	2.01	2.05
18	a	854	CLA	MG-ND	-2.33	2.01	2.05
18	a	803	CLA	C3B-CAB	-2.33	1.43	1.47
18	b	822	CLA	CMB-C2B	-2.33	1.46	1.51
18	b	837	CLA	C3B-CAB	-2.33	1.43	1.47
26	r	203	A86	C-C1	-2.32	1.46	1.50
18	a	842	CLA	C3B-CAB	-2.32	1.43	1.47
20	H	316	LHG	O7-C7	2.32	1.40	1.34
26	C	305	A86	C17-C16	-2.32	1.50	1.54
18	H	308	CLA	C3B-CAB	-2.32	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	301	LMG	O7-C8	-2.32	1.40	1.46
20	a	832	LHG	O7-C7	2.32	1.40	1.34
18	a	801	CLA	CMC-C2C	-2.32	1.45	1.50
20	j	102	LHG	O7-C7	2.32	1.40	1.34
18	C	309	CLA	C3B-CAB	-2.31	1.43	1.47
20	j	102	LHG	O8-C6	-2.31	1.39	1.45
18	H	307	CLA	C3B-C2B	-2.31	1.37	1.40
18	b	824	CLA	C3B-CAB	-2.31	1.43	1.47
18	B	310	CLA	CMD-C2D	-2.31	1.45	1.50
26	B	302	A86	C17-C16	-2.30	1.50	1.54
21	a	845	BCR	C1-C6	-2.30	1.50	1.53
26	C	305	A86	C13-C11	-2.30	1.45	1.49
18	E	314	CLA	C3B-CAB	-2.29	1.43	1.47
20	D	201	LHG	O7-C5	-2.29	1.40	1.46
18	H	313	CLA	CMD-C2D	-2.29	1.45	1.50
18	D	210	CLA	CMC-C2C	-2.29	1.45	1.50
18	b	829	CLA	C3B-CAB	-2.29	1.43	1.47
18	C	314	CLA	CMC-C2C	-2.29	1.45	1.50
18	C	314	CLA	C3B-CAB	-2.29	1.43	1.47
28	B	303	DD6	C36-C31	-2.29	1.32	1.34
20	a	832	LHG	O8-C23	2.29	1.40	1.33
18	C	307	CLA	MG-ND	-2.29	2.01	2.05
18	C	312	CLA	CMC-C2C	-2.28	1.46	1.50
29	H	312	KC1	C1B-C2B	-2.28	1.40	1.45
18	D	207	CLA	MG-ND	-2.28	2.01	2.05
18	a	842	CLA	CMC-C2C	-2.28	1.46	1.50
18	H	314	CLA	C3B-CAB	-2.27	1.43	1.47
29	C	308	KC1	CHD-C4C	2.27	1.40	1.35
18	C	318	CLA	MG-ND	-2.27	2.01	2.05
18	H	311	CLA	MG-ND	-2.27	2.01	2.05
18	D	216	CLA	C3B-CAB	-2.27	1.43	1.47
18	b	811	CLA	MG-ND	-2.27	2.01	2.05
29	B	313	KC1	C1B-C2B	-2.27	1.40	1.45
18	a	818	CLA	C3B-CAB	-2.27	1.43	1.47
18	a	825	CLA	C3B-CAB	-2.27	1.43	1.47
18	C	307	CLA	C3B-C2B	-2.26	1.37	1.40
18	b	849	CLA	CMD-C2D	-2.26	1.46	1.50
27	l	206	ET4	C04-C05	-2.26	1.47	1.51
18	E	312	CLA	CAA-C2A	-2.26	1.49	1.54
18	b	837	CLA	MG-ND	-2.26	2.01	2.05
18	H	306	CLA	MG-ND	-2.26	2.01	2.05
20	a	832	LHG	O7-C5	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	E	314	CLA	CMC-C2C	-2.25	1.46	1.50
21	l	201	BCR	C1-C6	-2.25	1.50	1.53
18	H	310	CLA	C3B-CAB	-2.25	1.43	1.47
21	f	201	BCR	C1-C6	-2.25	1.50	1.53
28	E	307	DD6	C36-C31	-2.25	1.32	1.34
18	C	316	CLA	CMC-C2C	-2.25	1.46	1.50
18	H	314	CLA	MG-ND	-2.25	2.01	2.05
18	H	313	CLA	CMC-C2C	-2.25	1.46	1.50
18	B	314	CLA	C3B-CAB	-2.25	1.43	1.47
23	C	301	LMG	O1-C1	-2.24	1.36	1.40
18	a	842	CLA	C3B-C2B	-2.24	1.37	1.40
18	a	808	CLA	CMD-C2D	-2.24	1.46	1.50
18	H	306	CLA	CMC-C2C	-2.24	1.46	1.50
18	b	804	CLA	MG-ND	-2.24	2.01	2.05
18	C	311	CLA	C3B-CAB	-2.24	1.43	1.47
18	a	841	CLA	C3B-CAB	-2.24	1.43	1.47
18	b	804	CLA	C3B-CAB	-2.23	1.43	1.47
18	E	316	CLA	CMD-C2D	-2.23	1.46	1.50
18	b	821	CLA	CMD-C2D	-2.23	1.46	1.50
18	H	308	CLA	MG-ND	-2.23	2.01	2.05
18	b	803	CLA	C4B-CHC	-2.23	1.34	1.41
18	H	307	CLA	MG-ND	-2.23	2.01	2.05
18	b	848	CLA	CMD-C2D	-2.23	1.46	1.50
18	C	311	CLA	CMC-C2C	-2.22	1.46	1.50
26	B	301	A86	C13-C11	-2.22	1.45	1.49
18	a	821	CLA	C3B-C2B	-2.21	1.37	1.40
18	E	309	CLA	CMC-C2C	-2.21	1.46	1.50
18	a	836	CLA	CMD-C2D	-2.20	1.46	1.50
18	a	830	CLA	CMC-C2C	-2.20	1.46	1.50
18	C	307	CLA	CMD-C2D	-2.20	1.46	1.50
18	b	820	CLA	C4B-CHC	-2.20	1.34	1.41
29	B	313	KC1	CHD-C4C	2.19	1.40	1.35
18	a	820	CLA	CMD-C2D	-2.19	1.46	1.50
18	C	311	CLA	CMD-C2D	-2.19	1.46	1.50
18	C	317	CLA	CMC-C2C	-2.18	1.46	1.50
18	a	825	CLA	MG-ND	-2.18	2.01	2.05
18	b	820	CLA	CMC-C2C	-2.18	1.46	1.50
23	j	103	LMG	O7-C10	2.18	1.40	1.34
18	H	313	CLA	C3B-CAB	-2.18	1.43	1.47
18	H	313	CLA	MG-ND	-2.18	2.01	2.05
18	H	310	CLA	C4B-CHC	-2.18	1.34	1.41
18	a	807	CLA	C3B-CAB	-2.17	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	E	314	CLA	MG-ND	-2.17	2.01	2.05
18	a	805	CLA	CMD-C2D	-2.17	1.46	1.50
18	H	305	CLA	CMC-C2C	-2.17	1.46	1.50
18	a	818	CLA	C3B-C2B	-2.16	1.37	1.40
18	b	843	CLA	C3B-CAB	-2.16	1.43	1.47
23	C	319	LMG	C3-C2	-2.16	1.46	1.52
18	B	314	CLA	CMD-C2D	-2.16	1.46	1.50
29	C	308	KC1	C4A-C3A	-2.16	1.40	1.44
26	H	301	A86	C-C1	-2.16	1.46	1.50
26	B	304	A86	C2-C1	-2.16	1.32	1.35
26	B	302	A86	O1-C15	-2.16	1.41	1.45
18	a	807	CLA	MG-ND	-2.16	2.01	2.05
20	j	102	LHG	O7-C5	-2.15	1.41	1.46
18	b	810	CLA	CMD-C2D	-2.15	1.46	1.50
18	l	205	CLA	CMD-C2D	-2.15	1.46	1.50
18	B	306	CLA	MG-ND	-2.15	2.01	2.05
18	D	217	CLA	CMD-C2D	-2.15	1.46	1.50
18	a	837	CLA	CAA-C2A	-2.15	1.50	1.54
26	C	302	A86	O1-C15	-2.14	1.41	1.45
18	C	310	CLA	CMD-C2D	-2.14	1.46	1.50
20	E	301	LHG	O7-C7	2.14	1.40	1.34
18	D	216	CLA	MG-ND	-2.14	2.01	2.05
18	D	208	CLA	MG-ND	-2.14	2.01	2.05
18	l	203	CLA	MG-ND	-2.14	2.01	2.05
18	b	840	CLA	CMC-C2C	-2.14	1.46	1.50
18	B	309	CLA	CMD-C2D	-2.14	1.46	1.50
18	B	314	CLA	CMC-C2C	-2.14	1.46	1.50
18	C	309	CLA	MG-ND	-2.13	2.01	2.05
18	b	803	CLA	CAA-C2A	-2.13	1.50	1.54
18	H	305	CLA	C3B-C2B	-2.13	1.37	1.40
18	b	820	CLA	MG-ND	-2.13	2.01	2.05
27	l	206	ET4	C35-C36	-2.13	1.49	1.52
23	a	851	LMG	O7-C8	-2.13	1.41	1.46
18	b	829	CLA	MG-ND	-2.13	2.01	2.05
18	C	318	CLA	CMC-C2C	-2.13	1.46	1.50
18	a	803	CLA	CAA-C2A	-2.13	1.50	1.54
20	E	301	LHG	P-O6	2.13	1.67	1.59
18	a	822	CLA	CMD-C2D	-2.13	1.46	1.50
26	D	206	A86	O4-C34	-2.12	1.41	1.46
18	C	314	CLA	MG-ND	-2.12	2.01	2.05
18	E	311	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	308	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	E	310	CLA	CMD-C2D	-2.12	1.46	1.50
18	C	310	CLA	CMC-C2C	-2.12	1.46	1.50
26	r	203	A86	O4-C34	-2.12	1.41	1.46
18	D	210	CLA	MG-ND	-2.12	2.01	2.05
28	H	303	DD6	C40-C32	-2.12	1.49	1.53
18	D	212	CLA	CMD-C2D	-2.12	1.46	1.50
18	b	845	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	302	A86	C26-C27	-2.12	1.33	1.35
18	a	809	CLA	CMD-C2D	-2.12	1.46	1.50
18	b	840	CLA	CMD-C2D	-2.11	1.46	1.50
18	D	213	CLA	CMC-C2C	-2.11	1.46	1.50
18	H	313	CLA	CAA-C2A	-2.11	1.50	1.54
26	D	206	A86	O1-C15	-2.11	1.42	1.45
22	a	849	SQD	O48-C46	-2.11	1.40	1.45
18	b	804	CLA	CAA-C2A	-2.11	1.50	1.54
18	a	819	CLA	CMC-C2C	-2.11	1.46	1.50
18	a	803	CLA	MG-ND	-2.11	2.01	2.05
27	l	206	ET4	C12-C13	2.11	1.50	1.45
18	b	819	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	306	CLA	CMC-C2C	-2.10	1.46	1.50
18	a	855	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	311	CLA	CMD-C2D	-2.10	1.46	1.50
20	E	301	LHG	O8-C23	2.10	1.39	1.33
18	H	314	CLA	C4B-CHC	-2.10	1.35	1.41
18	B	314	CLA	C3B-C2B	-2.09	1.37	1.40
18	a	844	CLA	CMD-C2D	-2.09	1.46	1.50
23	E	318	LMG	O1-C7	-2.09	1.39	1.43
26	B	304	A86	C5-C6	-2.09	1.33	1.35
20	j	102	LHG	P-O6	2.09	1.67	1.59
18	a	802	CLA	CMD-C2D	-2.09	1.46	1.50
18	b	805	CLA	CMD-C2D	-2.09	1.46	1.50
28	C	303	DD6	C17-C16	-2.09	1.51	1.54
18	a	843	CLA	CMD-C2D	-2.09	1.46	1.50
18	b	830	CLA	CMD-C2D	-2.09	1.46	1.50
18	D	214	CLA	CMC-C2C	-2.09	1.46	1.50
18	D	209	CLA	CMD-C2D	-2.09	1.46	1.50
18	b	816	CLA	CMD-C2D	-2.09	1.46	1.50
18	b	838	CLA	CMD-C2D	-2.09	1.46	1.50
28	E	308	DD6	O1-C20	-2.09	1.43	1.46
18	a	815	CLA	CMD-C2D	-2.09	1.46	1.50
18	b	828	CLA	CMD-C2D	-2.09	1.46	1.50
18	H	314	CLA	C3B-C2B	-2.09	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	801	CLA	CAA-C2A	-2.09	1.50	1.54
18	b	810	CLA	CMC-C2C	-2.08	1.46	1.50
26	E	302	A86	C13-C11	-2.08	1.45	1.49
18	f	202	CLA	CMD-C2D	-2.08	1.46	1.50
18	H	305	CLA	MG-ND	-2.08	2.01	2.05
20	H	316	LHG	P-O6	2.08	1.67	1.59
26	D	204	A86	C-C1	-2.08	1.46	1.50
18	a	817	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	306	CLA	CMD-C2D	-2.08	1.46	1.50
18	a	837	CLA	C4B-CHC	-2.08	1.35	1.41
18	b	841	CLA	CMD-C2D	-2.08	1.46	1.50
18	H	305	CLA	C3B-CAB	-2.08	1.43	1.47
26	B	305	A86	C-C1	-2.08	1.46	1.50
18	a	804	CLA	CMD-C2D	-2.07	1.46	1.50
18	j	104	CLA	CMD-C2D	-2.07	1.46	1.50
23	E	318	LMG	O7-C10	2.07	1.40	1.34
18	i	101	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	307	CLA	CMC-C2C	-2.07	1.46	1.50
18	b	827	CLA	C3B-C2B	-2.07	1.37	1.40
18	a	816	CLA	CMD-C2D	-2.07	1.46	1.50
18	a	847	CLA	CMD-C2D	-2.07	1.46	1.50
18	E	314	CLA	CAA-C2A	-2.07	1.50	1.54
28	H	303	DD6	C41-C32	-2.07	1.49	1.53
18	D	211	CLA	CMC-C2C	-2.07	1.46	1.50
18	b	807	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	853	CLA	CMD-C2D	-2.06	1.46	1.50
18	b	844	CLA	CMD-C2D	-2.06	1.46	1.50
18	f	204	CLA	CMD-C2D	-2.06	1.46	1.50
18	b	818	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	808	CLA	CMC-C2C	-2.06	1.46	1.50
18	b	846	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	305	A86	C17-C16	-2.06	1.51	1.54
26	H	302	A86	C26-C27	-2.06	1.33	1.35
18	b	815	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	814	CLA	CMD-C2D	-2.06	1.46	1.50
20	D	201	LHG	O7-C7	2.06	1.40	1.34
18	D	209	CLA	CMC-C2C	-2.05	1.46	1.50
18	a	806	CLA	CMD-C2D	-2.05	1.46	1.50
20	a	832	LHG	P-O6	2.05	1.67	1.59
18	a	826	CLA	C3B-C2B	-2.05	1.37	1.40
18	b	813	CLA	CMD-C2D	-2.05	1.46	1.50
18	C	310	CLA	C3B-C2B	-2.05	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	825	CLA	CAC-C3C	-2.05	1.45	1.51
18	b	817	CLA	CMC-C2C	-2.05	1.46	1.50
18	E	313	CLA	CMD-C2D	-2.05	1.46	1.50
18	a	842	CLA	C4B-CHC	-2.05	1.35	1.41
18	b	814	CLA	CMD-C2D	-2.05	1.46	1.50
18	a	824	CLA	CMD-C2D	-2.05	1.46	1.50
18	a	813	CLA	MG-ND	-2.05	2.01	2.05
18	b	822	CLA	CMD-C2D	-2.04	1.46	1.50
18	a	838	CLA	CMD-C2D	-2.04	1.46	1.50
18	b	801	CLA	C4B-CHC	-2.04	1.35	1.41
18	b	850	CLA	CMD-C2D	-2.04	1.46	1.50
18	a	854	CLA	C4B-CHC	-2.04	1.35	1.41
28	C	303	DD6	C2-C1	-2.04	1.33	1.35
18	a	812	CLA	CMD-C2D	-2.04	1.46	1.50
18	a	810	CLA	CMD-C2D	-2.04	1.46	1.50
18	E	309	CLA	CMD-C2D	-2.04	1.46	1.50
26	H	301	A86	O1-C15	-2.04	1.42	1.45
18	a	848	CLA	CMD-C2D	-2.04	1.46	1.50
18	D	213	CLA	CMD-C2D	-2.04	1.46	1.50
26	m	102	A86	C32-C31	-2.03	1.51	1.54
29	H	312	KC1	CHD-C4C	2.03	1.40	1.35
18	b	825	CLA	CMD-C2D	-2.03	1.46	1.50
26	r	203	A86	O1-C15	-2.03	1.42	1.45
18	D	211	CLA	CMD-C2D	-2.03	1.46	1.50
18	l	203	CLA	C4B-CHC	-2.03	1.35	1.41
18	f	203	CLA	CMD-C2D	-2.03	1.46	1.50
28	B	303	DD6	C33-C34	-2.03	1.49	1.52
18	b	801	CLA	CAC-C3C	-2.03	1.45	1.51
18	H	309	CLA	CMD-C2D	-2.03	1.46	1.50
18	b	817	CLA	CMD-C2D	-2.03	1.46	1.50
26	H	301	A86	C13-C11	-2.02	1.45	1.49
18	a	847	CLA	CMC-C2C	-2.02	1.46	1.50
23	l	207	LMG	O7-C10	2.02	1.40	1.34
18	a	819	CLA	CMD-C2D	-2.02	1.46	1.50
26	E	302	A86	C17-C16	-2.02	1.51	1.54
23	D	202	LMG	O1-C7	-2.02	1.40	1.43
18	b	827	CLA	CMD-C2D	-2.02	1.46	1.50
18	b	827	CLA	CMC-C2C	-2.02	1.46	1.50
18	a	818	CLA	C4B-CHC	-2.02	1.35	1.41
18	a	804	CLA	CMC-C2C	-2.02	1.46	1.50
18	b	809	CLA	CMD-C2D	-2.02	1.46	1.50
18	b	808	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	214	CLA	CMD-C2D	-2.02	1.46	1.50
18	a	839	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	306	CLA	C3B-C2B	-2.02	1.37	1.40
18	b	838	CLA	CMC-C2C	-2.02	1.46	1.50
26	H	304	A86	C13-C11	-2.02	1.45	1.49
18	a	805	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	308	CLA	CMC-C2C	-2.01	1.46	1.50
18	a	821	CLA	CMC-C2C	-2.01	1.46	1.50
18	a	828	CLA	CMD-C2D	-2.01	1.46	1.50
18	a	811	CLA	CMD-C2D	-2.01	1.46	1.50
18	H	307	CLA	C4B-CHC	-2.01	1.35	1.41
18	b	806	CLA	CMC-C2C	-2.01	1.46	1.50
18	C	312	CLA	MG-ND	-2.01	2.01	2.05
18	C	316	CLA	MG-ND	-2.01	2.01	2.05
27	l	206	ET4	C41-C34	-2.01	1.49	1.53
18	a	808	CLA	C3B-C2B	-2.01	1.37	1.40
18	b	849	CLA	C3B-C2B	-2.01	1.37	1.40
18	a	823	CLA	CMD-C2D	-2.01	1.46	1.50
18	C	306	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	307	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	305	A86	O1-C15	-2.01	1.42	1.45
26	B	305	A86	O4-C34	-2.00	1.41	1.46
18	H	306	CLA	CAC-C3C	-2.00	1.46	1.51
18	a	830	CLA	CMD-C2D	-2.00	1.46	1.50
18	b	826	CLA	CMD-C2D	-2.00	1.46	1.50
18	a	846	CLA	CMD-C2D	-2.00	1.46	1.50
18	b	818	CLA	CMC-C2C	-2.00	1.46	1.50
18	b	823	CLA	CMD-C2D	-2.00	1.46	1.50
18	E	315	CLA	CMD-C2D	-2.00	1.46	1.50
18	l	202	CLA	C3B-CAB	-2.00	1.43	1.47
18	b	846	CLA	CMC-C2C	-2.00	1.46	1.50
23	D	202	LMG	O7-C10	2.00	1.40	1.34
18	a	810	CLA	CMC-C2C	-2.00	1.46	1.50
18	C	316	CLA	CAC-C3C	-2.00	1.46	1.51

All (2085) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	103	LMG	O2-C2-C1	-21.31	58.28	110.05
23	a	851	LMG	O2-C2-C1	-18.81	64.35	110.05
28	E	304	DD6	C21-C20-C15	-16.18	95.14	122.26
26	r	203	A86	O1-C20-C19	-15.79	101.52	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	301	LMG	O2-C2-C1	15.25	147.09	110.05
21	b	833	BCR	C32-C1-C6	-14.13	87.39	110.30
26	D	203	A86	O1-C20-C19	-13.62	103.15	113.38
26	D	204	A86	C3-C4-C5	-12.10	98.69	123.47
26	C	304	A86	O1-C20-C19	-11.97	104.39	113.38
26	H	302	A86	O1-C20-C19	-11.90	104.45	113.38
26	B	302	A86	O1-C20-C19	-11.81	104.51	113.38
28	B	303	DD6	C21-C20-C15	-11.37	103.21	122.26
26	D	203	A86	C25-C26-C27	-11.19	111.34	127.31
26	D	206	A86	O1-C20-C19	-10.92	105.18	113.38
22	a	849	SQD	O47-C7-O49	-10.68	111.97	125.57
28	D	205	DD6	C21-C20-C15	-10.68	104.36	122.26
23	C	319	LMG	O2-C2-C3	-10.39	86.32	110.35
26	C	305	A86	O1-C20-C19	-10.38	105.59	113.38
26	H	301	A86	O1-C20-C19	-10.33	105.62	113.38
26	m	102	A86	O1-C20-C19	-9.97	105.89	113.38
26	H	304	A86	O1-C20-C19	-9.88	105.96	113.38
26	H	302	A86	C3-C4-C5	-9.59	103.83	123.47
26	B	302	A86	C3-C4-C5	-9.56	103.90	123.47
23	l	207	LMG	O2-C2-C1	9.38	132.83	110.05
26	C	305	A86	C3-C4-C5	-9.38	104.26	123.47
28	E	307	DD6	C14-C13-C11	-9.36	111.01	125.53
26	E	302	A86	O1-C20-C19	-9.24	106.44	113.38
26	B	301	A86	O1-C20-C19	-9.18	106.49	113.38
26	B	304	A86	C3-C4-C5	-9.06	104.92	123.47
26	D	204	A86	C4-C3-C2	9.04	141.98	123.47
26	m	102	A86	C24-C1-C2	9.02	132.78	118.94
28	E	304	DD6	O1-C20-C19	8.82	120.00	113.38
28	E	307	DD6	C3-C2-C1	-8.74	114.84	127.31
21	b	833	BCR	C32-C1-C31	-8.62	82.06	108.53
26	C	302	A86	C3-C4-C5	-8.56	105.93	123.47
26	C	302	A86	O1-C20-C19	-8.47	107.02	113.38
23	E	318	LMG	O2-C2-C3	-8.35	91.04	110.35
26	B	305	A86	C3-C4-C5	-8.27	106.54	123.47
26	B	302	A86	C4-C3-C2	8.20	140.27	123.47
26	H	302	A86	C4-C3-C2	8.18	140.22	123.47
26	D	204	A86	O1-C20-C19	-8.14	107.27	113.38
28	B	303	DD6	C21-C20-C19	8.12	123.42	114.28
26	D	204	A86	C3-C2-C1	8.09	138.85	127.31
26	B	305	A86	O1-C20-C19	-8.06	107.33	113.38
26	H	301	A86	C3-C4-C5	-8.05	106.97	123.47
28	D	205	DD6	C8-C6-C5	7.89	131.05	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	E	318	LMG	O2-C2-C1	-7.79	91.13	110.05
18	b	805	CLA	C4A-NA-C1A	7.63	110.14	106.71
26	D	203	A86	O1-C15-C14	-7.55	98.05	113.21
26	H	304	A86	C3-C4-C5	-7.53	108.05	123.47
18	a	854	CLA	C4A-NA-C1A	7.52	110.09	106.71
18	b	829	CLA	C4A-NA-C1A	7.42	110.04	106.71
26	E	302	A86	C3-C4-C5	-7.41	108.30	123.47
18	H	305	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	H	310	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	a	837	CLA	C4A-NA-C1A	7.39	110.03	106.71
18	a	805	CLA	C4A-NA-C1A	7.34	110.01	106.71
18	b	820	CLA	C4A-NA-C1A	7.34	110.01	106.71
18	a	807	CLA	C4A-NA-C1A	7.30	109.99	106.71
18	a	826	CLA	C4A-NA-C1A	7.29	109.98	106.71
18	D	210	CLA	C4A-NA-C1A	7.28	109.98	106.71
18	b	824	CLA	C4A-NA-C1A	7.27	109.97	106.71
26	D	204	A86	C4-C5-C6	7.19	137.57	127.31
18	b	803	CLA	C4A-NA-C1A	7.17	109.93	106.71
18	a	827	CLA	C4A-NA-C1A	7.16	109.93	106.71
18	a	803	CLA	C4A-NA-C1A	7.16	109.92	106.71
28	H	303	DD6	C24-C1-C2	7.15	129.91	118.94
18	C	309	CLA	C4A-NA-C1A	7.13	109.91	106.71
29	B	313	KC1	CHB-C1B-NB	7.13	131.01	124.45
18	E	313	CLA	C4A-NA-C1A	7.12	109.91	106.71
18	a	818	CLA	C4A-NA-C1A	7.11	109.90	106.71
26	B	301	A86	C25-C26-C27	-7.10	117.18	127.31
28	D	205	DD6	O1-C20-C21	7.07	123.53	115.06
18	b	840	CLA	C4A-NA-C1A	7.06	109.88	106.71
18	b	822	CLA	C4A-NA-C1A	7.05	109.88	106.71
26	D	204	A86	O1-C20-C21	-7.05	106.61	115.06
29	H	312	KC1	CHB-C1B-NB	7.04	130.93	124.45
18	b	815	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	a	849	SQD	O8-S-C6	7.01	117.10	105.77
18	a	824	CLA	C4A-NA-C1A	7.00	109.85	106.71
18	b	844	CLA	C4A-NA-C1A	7.00	109.85	106.71
18	b	827	CLA	C4A-NA-C1A	6.99	109.85	106.71
18	B	309	CLA	C4A-NA-C1A	6.98	109.85	106.71
18	H	307	CLA	C4A-NA-C1A	6.98	109.84	106.71
18	a	839	CLA	C4A-NA-C1A	6.98	109.84	106.71
18	b	804	CLA	C4A-NA-C1A	6.97	109.84	106.71
18	b	838	CLA	C4A-NA-C1A	6.96	109.83	106.71
26	r	203	A86	C34-O4-C38	-6.96	104.93	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	820	CLA	C4A-NA-C1A	6.96	109.83	106.71
18	b	850	CLA	C4A-NA-C1A	6.95	109.83	106.71
18	H	313	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	a	811	CLA	C4A-NA-C1A	6.90	109.81	106.71
18	a	822	CLA	C4A-NA-C1A	6.89	109.81	106.71
18	b	809	CLA	C4A-NA-C1A	6.89	109.80	106.71
18	C	317	CLA	C4A-NA-C1A	6.87	109.79	106.71
18	b	816	CLA	C4A-NA-C1A	6.86	109.79	106.71
26	B	302	A86	C3-C2-C1	6.85	137.09	127.31
18	a	819	CLA	C4A-NA-C1A	6.82	109.77	106.71
26	H	302	A86	C3-C2-C1	6.82	137.04	127.31
18	b	849	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	a	812	CLA	C4A-NA-C1A	6.80	109.77	106.71
23	a	851	LMG	O1-C1-C2	6.79	118.90	108.30
18	D	214	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	H	315	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	H	308	CLA	C4A-NA-C1A	6.77	109.75	106.71
26	H	301	A86	C4-C3-C2	6.76	137.32	123.47
26	B	305	A86	C41-C32-C31	-6.75	104.43	110.47
18	b	817	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	B	310	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	j	104	CLA	C4A-NA-C1A	6.74	109.74	106.71
18	b	813	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	b	833	BCR	C31-C1-C6	6.73	121.21	110.30
18	a	808	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	a	813	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	C	306	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	b	842	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	B	312	CLA	C4A-NA-C1A	6.69	109.71	106.71
18	B	308	CLA	C4A-NA-C1A	6.68	109.71	106.71
26	C	304	A86	C3-C2-C1	-6.68	117.77	127.31
18	a	825	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	E	316	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	a	843	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	a	814	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	B	306	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	b	811	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	D	211	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	B	307	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	E	310	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	a	840	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	b	845	CLA	C4A-NA-C1A	6.63	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	830	CLA	C4A-NA-C1A	6.63	109.69	106.71
26	b	847	A86	C3-C2-C1	-6.62	117.86	127.31
18	b	818	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	H	311	CLA	C4A-NA-C1A	6.62	109.68	106.71
26	B	304	A86	C4-C3-C2	6.62	137.03	123.47
18	b	810	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	b	843	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	a	817	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	b	823	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	f	202	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	a	816	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	C	310	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	a	828	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	a	838	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	D	209	CLA	C4A-NA-C1A	6.58	109.66	106.71
28	H	303	DD6	C21-C20-C19	6.58	121.68	114.28
18	l	203	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	a	836	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	b	808	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	a	823	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	f	204	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	a	806	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	b	830	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	a	844	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	b	812	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	E	312	CLA	C4A-NA-C1A	6.49	109.62	106.71
26	D	206	A86	C4-C3-C2	6.49	136.77	123.47
18	b	807	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	C	301	LMG	O2-C2-C3	-6.49	95.35	110.35
18	C	318	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	a	855	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	b	825	CLA	C4A-NA-C1A	6.48	109.62	106.71
26	D	206	A86	C3-C4-C5	-6.48	110.20	123.47
26	D	206	A86	C3-C2-C1	6.48	136.56	127.31
18	a	821	CLA	C4A-NA-C1A	6.47	109.62	106.71
29	C	308	KC1	CHB-C1B-NB	6.47	130.40	124.45
18	B	311	CLA	C4A-NA-C1A	6.47	109.61	106.71
18	b	806	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	a	810	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	b	821	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	D	213	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	b	814	CLA	C4A-NA-C1A	6.45	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	208	CLA	C4A-NA-C1A	6.45	109.60	106.71
18	b	841	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	b	801	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	C	307	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	b	837	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	b	819	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	C	315	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	H	309	CLA	C4A-NA-C1A	6.42	109.59	106.71
29	C	313	KC1	CHB-C1B-NB	6.41	130.35	124.45
18	a	853	CLA	C4A-NA-C1A	6.41	109.59	106.71
18	C	311	CLA	C4A-NA-C1A	6.41	109.59	106.71
29	C	308	KC1	CHC-C4B-NB	6.40	130.34	124.45
23	a	851	LMG	O6-C1-O1	-6.40	94.82	109.97
18	a	801	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	E	309	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	a	809	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	D	212	CLA	C4A-NA-C1A	6.38	109.58	106.71
26	B	305	A86	C4-C3-C2	6.38	136.55	123.47
26	B	301	A86	C3-C2-C1	-6.38	118.20	127.31
18	a	847	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	a	846	CLA	C4A-NA-C1A	6.37	109.57	106.71
28	B	303	DD6	C24-C1-C2	6.36	128.70	118.94
29	H	312	KC1	CHC-C4B-NB	6.35	130.29	124.45
18	D	215	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	r	202	CLA	C4A-NA-C1A	6.34	109.56	106.71
26	r	203	A86	C25-C24-C1	-6.32	108.66	126.42
26	r	203	A86	O1-C15-C14	-6.32	100.53	113.21
18	a	804	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	l	205	CLA	C4A-NA-C1A	6.32	109.55	106.71
26	C	305	A86	C4-C3-C2	6.30	136.38	123.47
18	C	312	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	b	848	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	a	848	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	E	314	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	E	311	CLA	C4A-NA-C1A	6.25	109.52	106.71
28	E	307	DD6	C24-C1-C2	6.23	128.50	118.94
18	a	802	CLA	C4A-NA-C1A	6.22	109.50	106.71
18	f	203	CLA	C4A-NA-C1A	6.22	109.50	106.71
26	r	203	A86	C3-C4-C5	-6.22	110.74	123.47
18	E	315	CLA	C4A-NA-C1A	6.21	109.50	106.71
18	b	826	CLA	C4A-NA-C1A	6.19	109.49	106.71
26	D	204	A86	C8-C6-C5	6.19	128.44	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	l	202	CLA	C4A-NA-C1A	6.18	109.49	106.71
18	b	828	CLA	C4A-NA-C1A	6.18	109.48	106.71
18	i	101	CLA	C4A-NA-C1A	6.17	109.48	106.71
18	D	217	CLA	C4A-NA-C1A	6.15	109.47	106.71
21	b	836	BCR	C16-C17-C18	-6.14	118.55	127.31
28	D	205	DD6	C21-C20-C19	6.13	121.18	114.28
18	b	846	CLA	C4A-NA-C1A	6.13	109.46	106.71
28	E	304	DD6	C4-C5-C6	-6.13	118.56	127.31
21	l	201	BCR	C7-C8-C9	-6.13	116.98	126.23
21	a	852	BCR	C15-C14-C13	-6.12	118.57	127.31
28	H	303	DD6	C21-C20-C15	-6.12	112.00	122.26
26	B	304	A86	O1-C20-C19	-6.11	108.80	113.38
21	j	105	BCR	C24-C23-C22	-6.10	117.01	126.23
29	C	313	KC1	CHC-C4B-NB	6.10	130.06	124.45
18	D	207	CLA	C4A-NA-C1A	6.08	109.44	106.71
26	C	302	A86	C4-C3-C2	6.07	135.90	123.47
28	E	307	DD6	C13-C11-C10	6.06	128.25	118.94
18	a	842	CLA	C4A-NA-C1A	6.04	109.42	106.71
28	E	307	DD6	C21-C20-C19	6.02	121.06	114.28
18	D	216	CLA	C4A-NA-C1A	5.99	109.40	106.71
26	D	204	A86	C9-C8-C6	-5.96	109.67	126.42
28	H	303	DD6	C-C1-C2	-5.94	114.61	122.92
26	B	305	A86	O1-C20-C21	-5.92	107.96	115.06
18	a	815	CLA	C4A-NA-C1A	5.91	109.36	106.71
18	H	306	CLA	C4A-NA-C1A	5.91	109.36	106.71
21	m	101	BCR	C7-C8-C9	-5.91	117.31	126.23
21	l	204	BCR	C11-C10-C9	-5.91	118.88	127.31
18	a	841	CLA	C4A-NA-C1A	5.89	109.35	106.71
18	H	314	CLA	C4A-NA-C1A	5.89	109.35	106.71
18	C	316	CLA	C4A-NA-C1A	5.88	109.35	106.71
18	C	314	CLA	C4A-NA-C1A	5.86	109.34	106.71
26	H	304	A86	O1-C20-C21	-5.86	108.04	115.06
21	a	834	BCR	C24-C23-C22	-5.85	117.40	126.23
26	r	203	A86	C9-C10-C11	-5.84	109.45	126.61
26	m	102	A86	C17-C16-C15	5.81	115.09	109.16
26	B	304	A86	C17-C16-C15	5.81	115.09	109.16
28	C	303	DD6	C3-C2-C1	-5.76	119.09	127.31
21	b	839	BCR	C11-C10-C9	-5.75	119.10	127.31
26	B	302	A86	C9-C10-C11	-5.73	109.78	126.61
26	C	302	A86	C9-C10-C11	-5.71	109.82	126.61
26	H	302	A86	C9-C10-C11	-5.71	109.83	126.61
26	H	304	A86	C4-C3-C2	5.65	135.04	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	302	A86	O1-C20-C21	-5.64	108.30	115.06
18	B	314	CLA	C4A-NA-C1A	5.63	109.23	106.71
26	D	203	A86	C9-C10-C11	-5.62	110.09	126.61
29	B	313	KC1	CHC-C4B-NB	5.60	129.60	124.45
26	H	302	A86	O1-C20-C21	-5.59	108.36	115.06
26	b	847	A86	C4-C5-C6	-5.58	119.34	127.31
21	j	105	BCR	C20-C21-C22	-5.58	119.34	127.31
23	a	851	LMG	O2-C2-C3	5.57	123.23	110.35
26	m	102	A86	C7-C6-C5	-5.56	115.14	122.92
21	l	204	BCR	C28-C27-C26	-5.55	104.17	114.08
26	B	302	A86	O1-C20-C21	-5.53	108.42	115.06
26	H	301	A86	O1-C20-C21	-5.52	108.44	115.06
27	l	206	ET4	C29-C22-C23	5.51	127.76	116.84
26	D	206	A86	O1-C20-C21	-5.49	108.48	115.06
21	b	833	BCR	C11-C10-C9	-5.48	119.49	127.31
26	B	304	A86	C9-C10-C11	-5.45	110.60	126.61
21	j	101	BCR	C24-C23-C22	-5.42	118.05	126.23
22	a	849	SQD	O8-S-O7	5.42	124.51	111.27
21	E	306	BCR	C16-C17-C18	-5.41	119.59	127.31
27	l	206	ET4	C19-C18-C17	5.40	127.23	118.94
26	D	203	A86	O1-C20-C21	-5.36	108.63	115.06
26	D	206	A86	C34-O4-C38	-5.34	107.94	117.90
26	m	102	A86	C25-C24-C1	-5.34	111.42	126.42
26	B	305	A86	C9-C10-C11	-5.34	110.92	126.61
21	i	103	BCR	C24-C23-C22	-5.34	118.17	126.23
23	j	103	LMG	O6-C1-O1	-5.34	97.34	109.97
26	r	203	A86	C4-C3-C2	5.33	134.40	123.47
26	H	301	A86	C3-C2-C1	5.32	134.91	127.31
22	a	849	SQD	O8-S-O9	-5.32	98.27	111.27
21	m	101	BCR	C16-C17-C18	-5.31	119.73	127.31
26	E	302	A86	C4-C3-C2	5.31	134.35	123.47
26	D	203	A86	C17-C16-C15	5.30	114.57	109.16
21	b	833	BCR	C32-C1-C2	-5.27	87.84	108.91
26	E	302	A86	C9-C10-C11	-5.25	111.17	126.61
26	C	305	A86	C9-C10-C11	-5.22	111.26	126.61
21	b	832	BCR	C16-C17-C18	-5.22	119.86	127.31
27	l	206	ET4	C30-C18-C17	-5.22	115.62	122.92
26	m	102	A86	C-C1-C2	-5.20	115.64	122.92
28	D	205	DD6	C7-C6-C5	-5.20	115.64	122.92
28	D	205	DD6	C3-C2-C1	-5.20	119.89	127.31
26	b	847	A86	O1-C20-C21	-5.17	108.86	115.06
28	E	304	DD6	O1-C20-C21	5.16	121.24	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E	302	A86	O1-C20-C21	-5.16	108.88	115.06
21	b	833	BCR	C15-C14-C13	-5.16	119.95	127.31
26	r	203	A86	O1-C20-C21	-5.15	108.89	115.06
26	B	301	A86	O1-C15-C14	-5.12	102.93	113.21
21	j	101	BCR	C20-C21-C22	-5.11	120.02	127.31
26	r	203	A86	C17-C16-C15	5.11	114.38	109.16
21	f	205	BCR	C15-C14-C13	-5.09	120.04	127.31
21	f	201	BCR	C24-C23-C22	-5.08	118.56	126.23
21	l	201	BCR	C33-C5-C6	-5.08	118.82	124.53
26	B	301	A86	O1-C20-C21	-5.05	109.00	115.06
23	D	202	LMG	O2-C2-C1	5.04	122.28	110.05
21	b	833	BCR	C33-C5-C6	-5.02	118.90	124.53
29	B	313	KC1	O2D-CGD-CBD	5.00	120.16	111.27
28	B	303	DD6	O1-C20-C21	4.97	121.02	115.06
26	H	304	A86	C9-C10-C11	-4.97	112.00	126.61
26	B	304	A86	O1-C20-C21	-4.93	109.14	115.06
21	m	101	BCR	C3-C4-C5	-4.93	105.28	114.08
26	m	102	A86	O1-C20-C21	-4.92	109.16	115.06
21	i	103	BCR	C15-C14-C13	-4.92	120.28	127.31
21	a	834	BCR	C20-C21-C22	-4.92	120.29	127.31
26	D	204	A86	C7-C6-C5	-4.90	116.06	122.92
26	H	302	A86	O4-C38-C39	4.89	120.08	111.09
28	C	303	DD6	C4-C5-C6	-4.88	120.35	127.31
21	l	201	BCR	C38-C26-C25	-4.87	119.06	124.53
26	B	302	A86	O4-C38-C39	4.87	120.05	111.09
26	r	203	A86	C35-C34-C33	4.86	118.36	109.88
18	b	826	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
26	D	206	A86	C9-C10-C11	-4.85	112.34	126.61
28	E	304	DD6	C-C1-C2	-4.85	116.13	122.92
26	b	847	A86	O1-C20-C19	-4.85	109.74	113.38
26	C	305	A86	O4-C38-C39	4.84	120.00	111.09
28	E	307	DD6	C7-C6-C5	-4.84	116.14	122.92
27	l	206	ET4	C24-C05-C06	-4.84	119.10	124.53
26	m	102	A86	C33-C32-C31	4.81	113.89	109.21
26	H	301	A86	C33-C32-C31	4.81	113.88	109.21
22	a	849	SQD	O9-S-C6	-4.81	101.13	106.92
25	b	834	DGD	O2G-C1B-C2B	4.81	121.86	111.50
23	j	103	LMG	O1-C1-C2	4.78	115.77	108.30
21	a	852	BCR	C16-C17-C18	-4.78	120.49	127.31
29	C	308	KC1	O2D-CGD-CBD	4.77	119.75	111.27
26	H	301	A86	O4-C38-C39	4.77	119.87	111.09
28	E	303	DD6	C21-C20-C19	4.76	119.63	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	305	A86	C33-C32-C31	4.75	113.83	109.21
21	E	306	BCR	C20-C21-C22	-4.75	120.53	127.31
29	C	313	KC1	O2D-CGD-CBD	4.75	119.70	111.27
18	a	855	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
26	m	102	A86	C25-C26-C27	-4.70	120.60	127.31
26	C	302	A86	O4-C38-C39	4.70	119.74	111.09
28	D	205	DD6	C32-C31-C36	-4.67	116.05	122.63
23	j	103	LMG	O2-C2-C3	4.66	121.13	110.35
26	C	305	A86	O1-C20-C21	-4.66	109.47	115.06
21	a	850	BCR	C33-C5-C6	-4.66	119.29	124.53
21	a	852	BCR	C7-C8-C9	-4.66	119.19	126.23
21	i	102	BCR	C20-C21-C22	-4.66	120.66	127.31
26	D	204	A86	O4-C38-C39	4.65	119.65	111.09
20	a	835	LHG	O7-C7-C8	4.65	119.65	111.09
28	E	303	DD6	C9-C10-C11	-4.64	120.69	127.31
28	E	304	DD6	C24-C1-C2	4.62	126.03	118.94
21	i	102	BCR	C16-C17-C18	-4.60	120.74	127.31
21	b	839	BCR	C38-C26-C25	-4.60	119.36	124.53
26	H	304	A86	C3-C2-C1	4.60	133.87	127.31
26	B	305	A86	O4-C38-C39	4.57	119.49	111.09
21	a	834	BCR	C16-C17-C18	-4.56	120.80	127.31
26	C	304	A86	C-C1-C2	-4.56	116.54	122.92
26	D	203	A86	C8-C6-C5	-4.56	111.95	118.94
21	j	105	BCR	C16-C17-C18	-4.55	120.82	127.31
18	a	843	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
23	C	301	LMG	C3-C4-C5	4.54	118.33	110.24
28	E	303	DD6	C3-C2-C1	-4.53	120.84	127.31
26	B	301	A86	O4-C38-C39	4.53	119.42	111.09
21	a	850	BCR	C24-C23-C22	-4.53	119.39	126.23
28	E	304	DD6	C3-C2-C1	-4.52	120.86	127.31
21	E	305	BCR	C15-C14-C13	-4.52	120.86	127.31
18	b	822	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
26	E	302	A86	O4-C38-C39	4.50	119.37	111.09
28	E	307	DD6	C12-C11-C10	-4.50	116.62	122.92
18	E	316	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
18	H	314	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
18	b	814	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
26	D	203	A86	O4-C38-C39	4.47	119.31	111.09
21	a	845	BCR	C33-C5-C6	-4.46	119.52	124.53
26	m	102	A86	O4-C38-C39	4.45	119.28	111.09
28	E	308	DD6	C21-C20-C19	4.41	119.25	114.28
23	j	103	LMG	O7-C10-C11	4.41	121.01	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	f	205	BCR	C11-C10-C9	-4.41	121.01	127.31
20	E	317	LHG	O7-C7-C8	4.41	121.00	111.50
18	a	838	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
27	l	206	ET4	C27-C09-C10	-4.40	116.76	122.92
18	b	820	CLA	O2D-CGD-O1D	-4.39	115.25	123.84
26	r	203	A86	C25-C26-C27	4.38	133.56	127.31
21	m	101	BCR	C20-C21-C22	-4.37	121.07	127.31
28	C	303	DD6	C25-C26-C27	-4.37	113.89	126.58
28	H	303	DD6	C32-C31-C36	-4.36	116.47	122.63
26	B	305	A86	C35-C34-C33	4.36	117.49	109.88
18	a	803	CLA	O2D-CGD-O1D	-4.35	115.33	123.84
18	b	801	CLA	O2D-CGD-O1D	-4.35	115.33	123.84
20	b	835	LHG	O7-C7-C8	4.35	120.88	111.50
21	a	852	BCR	C20-C21-C22	-4.35	121.10	127.31
26	E	302	A86	C17-C16-C15	4.34	113.59	109.16
28	C	303	DD6	C21-C20-C19	4.34	119.16	114.28
26	H	301	A86	C9-C10-C11	-4.33	113.89	126.61
21	i	102	BCR	C24-C23-C22	-4.33	119.70	126.23
26	D	203	A86	C34-O4-C38	-4.32	109.84	117.90
21	a	834	BCR	C15-C14-C13	-4.32	121.15	127.31
28	E	303	DD6	C14-C13-C11	-4.32	118.83	125.53
21	l	204	BCR	C24-C23-C22	-4.30	119.73	126.23
28	D	205	DD6	C34-C35-C36	-4.30	103.29	111.85
23	D	202	LMG	O7-C10-C11	4.29	120.75	111.50
26	H	301	A86	C17-C16-C15	4.29	113.54	109.16
26	B	304	A86	C3-C2-C1	4.29	133.43	127.31
20	D	201	LHG	O7-C7-C8	4.29	120.74	111.50
18	b	843	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
26	H	304	A86	O4-C38-C39	4.28	118.96	111.09
26	B	304	A86	O4-C38-C39	4.28	118.96	111.09
18	a	805	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
23	C	319	LMG	O7-C10-C11	4.27	120.70	111.50
21	j	101	BCR	C15-C14-C13	-4.26	121.23	127.31
18	l	205	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
21	a	833	BCR	C28-C27-C26	-4.24	106.50	114.08
26	r	203	A86	C24-C1-C2	4.24	125.44	118.94
21	f	201	BCR	C33-C5-C6	-4.23	119.78	124.53
26	C	305	A86	C3-C2-C1	4.22	133.34	127.31
18	l	203	CLA	O2D-CGD-O1D	-4.21	115.60	123.84
21	r	201	BCR	C3-C4-C5	-4.21	106.57	114.08
18	b	824	CLA	C1-C2-C3	-4.20	118.78	126.04
18	l	202	CLA	CMB-C2B-C1B	-4.20	122.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	815	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
23	a	851	LMG	O7-C10-C11	4.19	120.54	111.50
21	f	201	BCR	C20-C21-C22	-4.19	121.33	127.31
26	D	206	A86	O4-C38-C39	4.18	118.79	111.09
18	b	837	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
26	B	305	A86	C3-C2-C1	4.17	133.26	127.31
26	C	304	A86	O1-C20-C21	-4.17	110.06	115.06
28	C	303	DD6	C3-C4-C5	-4.16	114.94	123.47
21	i	103	BCR	C11-C10-C9	-4.16	121.37	127.31
21	b	832	BCR	C20-C21-C22	-4.16	121.38	127.31
18	f	202	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
18	b	841	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
18	C	307	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
18	E	309	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
28	E	303	DD6	C4-C5-C6	-4.14	121.40	127.31
18	b	826	CLA	CMB-C2B-C3B	4.14	132.42	124.68
20	a	832	LHG	O7-C7-C8	4.14	120.42	111.50
20	E	301	LHG	O7-C7-C8	4.13	120.39	111.50
26	m	102	A86	C-C1-C24	-4.12	111.58	118.08
29	H	312	KC1	O2D-CGD-CBD	4.11	118.58	111.27
22	a	849	SQD	O9-S-O7	-4.11	99.72	113.95
21	i	103	BCR	C20-C21-C22	-4.11	121.44	127.31
26	D	206	A86	O1-C15-C14	-4.11	104.97	113.21
18	H	307	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
28	C	303	DD6	C37-C36-C35	4.11	121.96	114.36
18	a	804	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
28	H	303	DD6	C34-C35-C36	-4.10	103.68	111.85
18	a	818	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
28	E	304	DD6	O2-C18-C19	-4.10	101.66	109.80
18	b	828	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
18	a	824	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
18	b	812	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
21	E	306	BCR	C24-C23-C22	-4.08	120.07	126.23
26	b	847	A86	O4-C38-C39	4.07	118.58	111.09
18	H	313	CLA	C1-C2-C3	-4.07	119.01	126.04
26	r	203	A86	C10-C9-C8	4.06	135.88	123.22
26	C	304	A86	O4-C38-C39	4.06	118.55	111.09
21	b	833	BCR	C24-C23-C22	-4.04	120.12	126.23
21	b	833	BCR	C38-C26-C25	-4.04	119.99	124.53
21	m	101	BCR	C24-C23-C22	-4.04	120.13	126.23
28	B	303	DD6	C14-C13-C11	-4.04	119.26	125.53
21	j	101	BCR	C11-C10-C9	-4.04	121.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	205	DD6	C24-C1-C2	4.03	125.13	118.94
18	a	855	CLA	CMB-C2B-C3B	4.03	132.22	124.68
18	D	214	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
21	a	833	BCR	C16-C17-C18	-4.03	121.56	127.31
28	B	303	DD6	C-C1-C2	-4.02	117.30	122.92
21	b	832	BCR	C28-C27-C26	-4.01	106.91	114.08
18	b	801	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
26	C	302	A86	C17-C16-C15	4.01	113.25	109.16
23	C	301	LMG	O7-C10-C11	4.01	120.14	111.50
20	j	102	LHG	O7-C7-C8	4.01	120.14	111.50
21	i	103	BCR	C7-C8-C9	-4.00	120.18	126.23
18	a	811	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
18	a	820	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
18	a	841	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
26	C	304	A86	C4-C5-C6	-3.99	121.62	127.31
20	H	316	LHG	O7-C7-C8	3.97	120.06	111.50
18	b	824	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
26	H	301	A86	C41-C32-C31	-3.96	106.92	110.47
21	f	205	BCR	C7-C8-C9	-3.96	120.25	126.23
18	a	837	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
21	E	306	BCR	C15-C14-C13	-3.94	121.68	127.31
26	D	204	A86	C9-C10-C11	-3.94	115.01	126.61
26	D	206	A86	C10-C9-C8	3.94	135.53	123.22
21	b	839	BCR	C1-C6-C5	-3.94	117.06	122.61
21	l	204	BCR	C8-C9-C10	3.94	124.99	118.94
18	a	806	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
21	b	836	BCR	C3-C4-C5	-3.94	107.05	114.08
26	D	204	A86	C26-C25-C24	-3.93	110.96	123.22
19	b	831	PQN	C11-C12-C13	-3.92	120.26	126.79
26	m	102	A86	O1-C15-C14	-3.92	105.34	113.21
28	C	303	DD6	C14-C13-C11	-3.92	119.44	125.53
21	a	850	BCR	C20-C21-C22	-3.92	121.72	127.31
26	C	302	A86	C3-C2-C1	3.91	132.90	127.31
28	B	303	DD6	C37-C36-C31	-3.91	119.03	124.35
18	a	802	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
18	b	810	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
18	a	842	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	l	207	LMG	O7-C10-C11	3.91	119.92	111.50
18	a	836	CLA	CMB-C2B-C1B	-3.90	122.46	128.46
26	H	304	A86	C26-C25-C24	-3.90	111.04	123.22
26	H	302	A86	C10-C9-C8	3.90	135.38	123.22
26	B	302	A86	C10-C9-C8	3.89	135.36	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	305	A86	C10-C9-C8	3.89	135.36	123.22
28	C	303	DD6	C15-C14-C13	-3.89	117.77	125.99
18	a	827	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
29	B	313	KC1	O1D-CGD-CBD	-3.88	116.54	124.48
28	B	303	DD6	C4-C5-C6	-3.88	121.77	127.31
18	a	813	CLA	CAC-C3C-C4C	3.88	129.84	124.81
18	a	810	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
18	b	806	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
18	H	310	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
18	E	315	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
21	j	101	BCR	C16-C17-C18	-3.86	121.80	127.31
18	H	313	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
21	j	105	BCR	C15-C14-C13	-3.86	121.80	127.31
18	B	314	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
18	B	308	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
21	a	850	BCR	C16-C17-C18	-3.85	121.81	127.31
21	i	103	BCR	C16-C17-C18	-3.85	121.82	127.31
21	a	833	BCR	C15-C14-C13	-3.84	121.83	127.31
21	m	101	BCR	C4-C5-C6	-3.84	117.15	122.73
26	D	203	A86	C7-C6-C8	3.84	124.13	118.08
18	H	309	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
18	b	808	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
18	a	819	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
18	B	306	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
18	a	843	CLA	CMB-C2B-C3B	3.82	131.83	124.68
18	b	837	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
18	a	838	CLA	CMB-C2B-C3B	3.81	131.80	124.68
18	b	820	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
18	b	822	CLA	CMB-C2B-C3B	3.80	131.78	124.68
18	a	847	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
18	b	850	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
21	j	105	BCR	C28-C27-C26	-3.79	107.31	114.08
18	H	307	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
28	E	308	DD6	C4-C5-C6	-3.79	121.90	127.31
18	D	213	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
18	a	823	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
18	a	839	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
21	l	201	BCR	C15-C14-C13	-3.77	121.93	127.31
28	E	308	DD6	C3-C2-C1	-3.77	121.93	127.31
21	a	845	BCR	C38-C26-C25	-3.77	120.29	124.53
18	E	313	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
26	D	206	A86	C35-C34-C33	3.77	116.45	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	301	A86	C7-C6-C8	3.76	124.01	118.08
21	i	102	BCR	C7-C8-C9	-3.76	120.55	126.23
28	C	303	DD6	C32-C31-C36	-3.76	117.32	122.63
18	a	825	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
18	H	310	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
18	B	309	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
18	b	815	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
18	b	818	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
21	a	852	BCR	C24-C23-C22	-3.75	120.58	126.23
23	E	318	LMG	O7-C10-C11	3.74	119.57	111.50
18	a	817	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
18	a	853	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
18	C	312	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
21	j	105	BCR	C7-C8-C9	-3.73	120.59	126.23
18	l	202	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
21	E	305	BCR	C28-C27-C26	-3.73	107.41	114.08
18	r	202	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	C	302	A86	C8-C6-C5	-3.73	113.22	118.94
18	D	210	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
18	a	842	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
18	b	814	CLA	CMB-C2B-C3B	3.72	131.64	124.68
21	j	105	BCR	C11-C10-C9	-3.72	122.00	127.31
28	E	307	DD6	C25-C24-C1	-3.72	115.97	126.42
18	b	844	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
18	b	819	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
18	H	308	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
20	a	831	LHG	O7-C7-C8	3.72	119.51	111.50
18	b	845	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	E	304	DD6	C21-C20-C19	3.71	118.46	114.28
18	b	830	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
18	D	207	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
21	f	201	BCR	C1-C6-C5	-3.71	117.39	122.61
18	b	804	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
26	B	304	A86	C10-C9-C8	3.71	134.79	123.22
18	a	807	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
26	B	305	A86	C26-C25-C24	-3.70	111.66	123.22
18	a	828	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
26	D	203	A86	C10-C9-C8	3.69	134.75	123.22
28	C	303	DD6	O1-C20-C19	-3.69	110.61	113.38
18	a	854	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	B	301	A86	C4-C5-C6	-3.69	122.05	127.31
21	a	852	BCR	C11-C10-C9	-3.69	122.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	846	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
18	b	842	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
18	H	315	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	H	302	A86	C26-C25-C24	-3.68	111.73	123.22
18	b	811	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
18	H	314	CLA	CMB-C2B-C3B	3.68	131.55	124.68
28	E	308	DD6	C9-C10-C11	-3.67	122.07	127.31
21	f	205	BCR	C16-C17-C18	-3.67	122.07	127.31
18	H	306	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
18	D	217	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
21	a	833	BCR	C24-C23-C22	-3.67	120.69	126.23
26	B	302	A86	C26-C25-C24	-3.67	111.78	123.22
21	r	201	BCR	C16-C17-C18	-3.66	122.08	127.31
18	C	316	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
18	l	203	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
21	f	205	BCR	C20-C21-C22	-3.66	122.09	127.31
18	E	316	CLA	CMB-C2B-C3B	3.66	131.52	124.68
26	C	305	A86	C26-C25-C24	-3.66	111.80	123.22
18	D	208	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
18	D	209	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
21	a	852	BCR	C33-C5-C6	-3.65	120.43	124.53
18	f	203	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
18	b	843	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
18	a	848	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
18	a	803	CLA	O2D-CGD-CBD	3.64	117.74	111.27
26	C	305	A86	C34-O4-C38	-3.64	111.11	117.90
18	C	314	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
18	a	809	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
28	E	307	DD6	C4-C5-C6	-3.64	122.12	127.31
18	a	813	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
26	r	203	A86	C20-C19-C18	-3.63	105.57	112.75
18	b	807	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
18	D	212	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
18	b	805	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
21	a	834	BCR	C33-C5-C6	-3.62	120.46	124.53
18	D	215	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
26	B	301	A86	C34-O4-C38	-3.62	111.16	117.90
18	D	210	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
26	m	102	A86	C9-C10-C11	-3.62	115.98	126.61
18	a	818	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
18	E	312	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
18	H	305	CLA	CMB-C2B-C1B	-3.61	122.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	302	A86	C7-C6-C8	3.60	123.76	118.08
18	b	811	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
18	a	841	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
21	i	102	BCR	C11-C10-C9	-3.59	122.19	127.31
26	H	304	A86	C41-C32-C31	-3.59	107.26	110.47
18	a	807	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
21	j	101	BCR	C33-C5-C6	-3.58	120.51	124.53
18	a	805	CLA	CMB-C2B-C3B	3.57	131.37	124.68
18	b	817	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
21	r	201	BCR	C24-C23-C22	-3.57	120.84	126.23
28	E	304	DD6	C37-C36-C31	-3.57	119.50	124.35
18	B	312	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
21	a	852	BCR	C38-C26-C25	-3.57	120.52	124.53
18	C	315	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
21	a	850	BCR	C15-C14-C13	-3.57	122.22	127.31
18	b	813	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
28	E	304	DD6	C37-C36-C35	3.57	120.96	114.36
21	m	101	BCR	C34-C9-C10	-3.57	117.93	122.92
20	B	315	LHG	O7-C7-C8	3.56	119.17	111.50
18	H	307	CLA	CMB-C2B-C3B	3.56	131.33	124.68
18	E	309	CLA	CMB-C2B-C3B	3.56	131.33	124.68
18	D	208	CLA	C1-C2-C3	-3.55	119.90	126.04
18	l	205	CLA	CMB-C2B-C3B	3.55	131.32	124.68
26	B	304	A86	C26-C25-C24	-3.55	112.14	123.22
18	D	207	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
18	a	830	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
18	b	838	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
18	b	823	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
21	i	103	BCR	C28-C27-C26	-3.54	107.76	114.08
21	r	201	BCR	C20-C21-C22	-3.53	122.27	127.31
28	C	303	DD6	C-C1-C2	-3.53	117.97	122.92
21	j	105	BCR	C33-C5-C6	-3.53	120.56	124.53
19	a	829	PQN	C14-C13-C15	3.53	121.20	115.27
21	l	204	BCR	C3-C4-C5	-3.52	107.80	114.08
18	H	311	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
26	B	301	A86	C20-C19-C18	-3.52	105.79	112.75
18	a	824	CLA	CMB-C2B-C3B	3.52	131.26	124.68
21	b	836	BCR	C28-C27-C26	-3.52	107.80	114.08
18	a	840	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
18	b	848	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
21	a	845	BCR	C7-C8-C9	-3.51	120.93	126.23
26	C	305	A86	O1-C15-C14	-3.51	106.16	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	803	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
18	C	309	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
21	a	833	BCR	C3-C4-C5	-3.51	107.82	114.08
18	b	829	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
28	E	304	DD6	C34-C35-C36	-3.50	104.88	111.85
21	j	101	BCR	C38-C26-C25	-3.50	120.60	124.53
18	a	822	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
26	H	302	A86	C17-C16-C15	3.50	112.73	109.16
18	b	841	CLA	CMB-C2B-C3B	3.49	131.21	124.68
26	H	301	A86	C35-C34-C33	3.48	115.96	109.88
18	a	837	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
21	b	836	BCR	C7-C8-C9	-3.48	120.98	126.23
18	B	307	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
18	a	814	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	E	305	BCR	C33-C5-C6	-3.47	120.64	124.53
21	E	306	BCR	C33-C5-C6	-3.47	120.64	124.53
18	b	840	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
18	a	813	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
18	a	804	CLA	CMB-C2B-C3B	3.46	131.16	124.68
18	f	204	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
21	a	834	BCR	C38-C26-C25	-3.46	120.64	124.53
18	l	203	CLA	O2D-CGD-CBD	3.46	117.41	111.27
21	a	845	BCR	C24-C23-C22	-3.45	121.02	126.23
18	E	311	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
18	f	202	CLA	CMB-C2B-C3B	3.45	131.13	124.68
18	i	101	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
18	C	307	CLA	CMB-C2B-C3B	3.45	131.13	124.68
21	b	832	BCR	C15-C14-C13	-3.45	122.39	127.31
18	b	825	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
18	a	815	CLA	CMB-C2B-C3B	3.45	131.12	124.68
26	D	204	A86	C19-C18-C17	-3.45	104.12	110.77
18	b	812	CLA	CMB-C2B-C3B	3.44	131.12	124.68
21	b	833	BCR	C7-C8-C9	-3.44	121.03	126.23
26	H	301	A86	C7-C6-C8	3.44	123.50	118.08
18	a	844	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
26	B	305	A86	C34-O4-C38	-3.43	111.50	117.90
26	B	301	A86	C25-C24-C1	-3.43	116.77	126.42
28	E	307	DD6	O1-C20-C19	-3.43	110.80	113.38
21	E	305	BCR	C11-C10-C9	-3.42	122.42	127.31
21	j	101	BCR	C28-C27-C26	-3.42	107.96	114.08
18	b	809	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
18	j	104	CLA	CMB-C2B-C1B	-3.41	123.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	E	306	BCR	C11-C10-C9	-3.41	122.45	127.31
26	B	302	A86	C17-C16-C15	3.41	112.64	109.16
21	i	102	BCR	C15-C14-C13	-3.40	122.45	127.31
18	H	311	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	a	850	BCR	C38-C26-C25	-3.40	120.71	124.53
21	l	204	BCR	C34-C9-C10	-3.40	118.17	122.92
18	C	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
18	B	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
18	D	214	CLA	CMB-C2B-C3B	3.39	131.02	124.68
18	a	818	CLA	CMB-C2B-C3B	3.39	131.02	124.68
21	j	101	BCR	C7-C8-C9	-3.39	121.12	126.23
18	H	310	CLA	CMB-C2B-C3B	3.39	131.01	124.68
28	H	303	DD6	C3-C2-C1	-3.38	122.49	127.31
28	H	303	DD6	O1-C20-C19	-3.38	110.84	113.38
18	a	821	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
21	f	205	BCR	C28-C27-C26	-3.37	108.06	114.08
21	E	306	BCR	C38-C26-C25	-3.37	120.75	124.53
27	l	206	ET4	C01-C06-C05	-3.37	117.87	122.61
21	f	205	BCR	C24-C23-C22	-3.37	121.15	126.23
21	b	832	BCR	C3-C4-C5	-3.37	108.07	114.08
21	b	839	BCR	C34-C9-C10	-3.36	118.21	122.92
18	a	837	CLA	O2D-CGD-CBD	3.36	117.24	111.27
18	b	849	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
28	D	205	DD6	C4-C3-C2	3.36	130.35	123.47
26	H	304	A86	C7-C6-C8	3.35	123.36	118.08
26	C	305	A86	C7-C6-C8	3.35	123.36	118.08
21	a	845	BCR	C11-C10-C9	-3.35	122.52	127.31
21	b	836	BCR	C20-C21-C22	-3.35	122.53	127.31
23	C	319	LMG	O8-C28-C29	3.35	122.42	111.91
18	b	821	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
28	E	307	DD6	C20-C19-C18	-3.35	106.12	112.75
18	C	306	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
18	b	816	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
18	E	310	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
18	a	816	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
18	a	836	CLA	CMB-C2B-C3B	3.34	130.93	124.68
28	D	205	DD6	C9-C8-C6	-3.34	117.04	126.42
18	a	811	CLA	CMB-C2B-C3B	3.34	130.92	124.68
26	E	302	A86	C7-C6-C8	3.33	123.33	118.08
18	a	806	CLA	CMB-C2B-C3B	3.33	130.91	124.68
21	f	205	BCR	C33-C5-C6	-3.33	120.79	124.53
27	l	206	ET4	C07-C06-C05	-3.33	113.39	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m	102	A86	C8-C6-C5	3.33	124.05	118.94
26	H	302	A86	O1-C15-C14	-3.33	106.54	113.21
18	D	216	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
28	B	303	DD6	C15-C14-C13	-3.32	118.97	125.99
21	b	839	BCR	C24-C23-C22	-3.32	121.22	126.23
21	m	101	BCR	C2-C1-C6	3.32	115.59	110.48
18	b	846	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
18	b	824	CLA	CMB-C2B-C3B	3.31	130.88	124.68
26	C	304	A86	O1-C15-C14	-3.31	106.56	113.21
26	B	301	A86	C9-C10-C11	-3.31	116.87	126.61
21	l	204	BCR	C33-C5-C6	-3.31	120.81	124.53
18	H	306	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
27	l	206	ET4	C35-C36-C37	-3.30	105.78	110.30
18	C	310	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
18	a	812	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
26	b	847	A86	O-C13-C11	-3.30	113.86	121.15
26	B	302	A86	O1-C15-C14	-3.30	106.59	113.21
18	B	310	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
26	D	203	A86	C4-C3-C2	-3.29	116.73	123.47
18	b	843	CLA	CMB-C2B-C3B	3.29	130.83	124.68
26	B	302	A86	O-C13-C11	-3.29	113.88	121.15
20	a	832	LHG	O8-C23-C24	3.29	120.00	111.38
18	C	314	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
18	b	828	CLA	CMB-C2B-C3B	3.28	130.82	124.68
18	b	820	CLA	O2D-CGD-CBD	3.28	117.10	111.27
18	C	309	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
21	a	845	BCR	C16-C17-C18	-3.27	122.64	127.31
18	a	828	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
21	b	832	BCR	C7-C8-C9	-3.27	121.30	126.23
18	D	213	CLA	CMB-C2B-C3B	3.26	130.78	124.68
18	b	806	CLA	CMB-C2B-C3B	3.26	130.78	124.68
21	l	201	BCR	C34-C9-C10	-3.26	118.36	122.92
21	b	839	BCR	C3-C4-C5	-3.25	108.27	114.08
26	H	302	A86	O-C13-C11	-3.25	113.97	121.15
26	H	301	A86	O1-C15-C14	-3.25	106.69	113.21
28	E	307	DD6	C-C1-C24	-3.25	112.96	118.08
26	C	302	A86	O1-C15-C14	-3.25	106.69	113.21
18	D	211	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
18	a	841	CLA	CMB-C2B-C3B	3.25	130.75	124.68
18	b	810	CLA	CMB-C2B-C3B	3.25	130.75	124.68
21	b	832	BCR	C11-C10-C9	-3.25	122.68	127.31
26	E	302	A86	C26-C25-C24	-3.24	113.09	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	842	CLA	CMB-C2B-C3B	3.24	130.75	124.68
18	a	827	CLA	CMB-C2B-C3B	3.24	130.74	124.68
18	b	840	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
21	b	833	BCR	C15-C16-C17	-3.24	116.84	123.47
18	C	312	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
26	D	206	A86	C26-C25-C24	-3.24	113.12	123.22
18	H	308	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
18	B	308	CLA	CMB-C2B-C3B	3.23	130.72	124.68
26	D	203	A86	C26-C25-C24	3.23	133.30	123.22
20	E	317	LHG	C5-O7-C7	-3.23	109.84	117.79
18	a	810	CLA	CMB-C2B-C3B	3.23	130.72	124.68
18	a	820	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
18	C	316	CLA	CMB-C2B-C3B	3.23	130.72	124.68
18	C	318	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
21	b	836	BCR	C11-C10-C9	-3.22	122.71	127.31
20	B	315	LHG	O8-C23-C24	3.22	122.02	111.91
21	a	833	BCR	C7-C8-C9	-3.22	121.37	126.23
18	E	314	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
21	j	105	BCR	C38-C26-C25	-3.22	120.91	124.53
21	b	833	BCR	C2-C1-C6	3.22	115.44	110.48
26	D	204	A86	C24-C1-C2	-3.22	114.00	118.94
21	a	852	BCR	C28-C27-C26	-3.22	108.33	114.08
26	E	302	A86	C8-C6-C5	-3.22	114.01	118.94
21	i	103	BCR	C33-C5-C6	-3.21	120.92	124.53
18	H	309	CLA	CMB-C2B-C3B	3.21	130.68	124.68
21	E	306	BCR	C3-C4-C5	-3.21	108.35	114.08
18	b	819	CLA	CMB-C2B-C3B	3.21	130.68	124.68
26	C	302	A86	C34-O4-C38	-3.21	111.92	117.90
18	B	306	CLA	CMB-C2B-C3B	3.21	130.68	124.68
29	H	312	KC1	CHB-C1B-C2B	-3.20	118.76	125.48
21	b	832	BCR	C24-C23-C22	-3.20	121.39	126.23
21	b	836	BCR	C16-C15-C14	-3.20	116.92	123.47
18	a	802	CLA	CMB-C2B-C3B	3.20	130.66	124.68
18	a	826	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
18	b	827	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
28	H	303	DD6	C9-C10-C11	-3.19	122.75	127.31
21	E	305	BCR	C3-C4-C5	-3.19	108.38	114.08
20	a	831	LHG	O8-C23-C24	3.19	121.93	111.91
18	b	850	CLA	CMB-C2B-C3B	3.19	130.65	124.68
26	H	304	A86	C10-C9-C8	3.19	133.17	123.22
21	b	833	BCR	C31-C1-C2	3.19	121.67	108.91
28	D	205	DD6	C37-C36-C31	-3.19	120.02	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	839	CLA	CMB-C2B-C3B	3.18	130.64	124.68
18	E	314	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
18	b	811	CLA	CMB-C2B-C3B	3.18	130.63	124.68
18	B	309	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	b	834	DGD	C2G-O2G-C1B	-3.18	109.96	117.79
21	E	306	BCR	C7-C8-C9	-3.18	121.43	126.23
18	a	821	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
26	m	102	A86	C4-C3-C2	-3.18	116.96	123.47
18	a	819	CLA	CMB-C2B-C3B	3.18	130.62	124.68
18	a	809	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
18	a	823	CLA	CMB-C2B-C3B	3.17	130.61	124.68
18	a	847	CLA	CMB-C2B-C3B	3.17	130.60	124.68
29	C	308	KC1	C3D-CAD-CBD	-3.16	103.44	107.61
18	H	313	CLA	CMB-C2B-C3B	3.16	130.60	124.68
28	D	205	DD6	C-C1-C2	-3.16	118.49	122.92
28	H	303	DD6	C13-C11-C10	3.16	123.80	118.94
21	b	839	BCR	C8-C9-C10	3.16	123.79	118.94
18	a	837	CLA	CMB-C2B-C3B	3.16	130.59	124.68
18	a	842	CLA	O1D-CGD-CBD	3.16	130.95	124.48
28	E	307	DD6	C-C1-C2	-3.16	118.50	122.92
18	E	313	CLA	CMB-C2B-C3B	3.16	130.58	124.68
18	a	825	CLA	CMB-C2B-C1B	-3.15	123.61	128.46
21	f	201	BCR	C33-C5-C4	3.15	119.67	113.62
18	b	837	CLA	O2D-CGD-CBD	3.15	116.86	111.27
21	a	833	BCR	C38-C26-C25	-3.15	120.99	124.53
18	H	314	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
18	r	202	CLA	CMB-C2B-C3B	3.15	130.56	124.68
18	a	817	CLA	CMB-C2B-C3B	3.14	130.56	124.68
18	b	818	CLA	CMB-C2B-C3B	3.14	130.56	124.68
18	a	846	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	C	305	A86	C10-C9-C8	3.14	133.01	123.22
26	C	302	A86	C26-C25-C24	-3.14	113.43	123.22
18	b	813	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
18	E	315	CLA	CMB-C2B-C3B	3.13	130.54	124.68
18	b	830	CLA	CMB-C2B-C3B	3.13	130.54	124.68
18	a	808	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
28	E	308	DD6	O1-C20-C19	-3.13	111.03	113.38
18	H	307	CLA	O2D-CGD-CBD	3.13	116.82	111.27
18	b	815	CLA	CMB-C2B-C3B	3.12	130.52	124.68
18	D	209	CLA	CMB-C2B-C3B	3.12	130.51	124.68
18	D	208	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
18	b	823	CLA	O2D-CGD-O1D	-3.12	117.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	848	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
26	E	302	A86	C10-C9-C8	3.11	132.94	123.22
18	E	312	CLA	CMB-C2B-C3B	3.11	130.50	124.68
27	l	206	ET4	O40-C36-C35	3.11	115.98	109.80
26	D	204	A86	C-C1-C24	3.11	122.97	118.08
18	b	820	CLA	CMB-C2B-C3B	3.11	130.49	124.68
21	l	204	BCR	C38-C26-C27	3.10	119.58	113.62
18	a	828	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	a	853	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	D	215	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	f	203	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	a	804	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	b	818	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
28	E	307	DD6	C37-C36-C31	-3.10	120.14	124.35
18	b	844	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
21	m	101	BCR	C16-C15-C14	-3.09	117.15	123.47
26	H	304	A86	O1-C15-C14	-3.08	107.02	113.21
21	a	852	BCR	C11-C12-C13	-3.08	117.76	126.42
26	b	847	A86	C12-C11-C13	3.08	121.20	116.02
18	D	208	CLA	CAA-CBA-CGA	-3.08	104.25	113.25
28	B	303	DD6	C32-C33-C34	-3.08	106.69	113.64
18	b	842	CLA	CMB-C2B-C3B	3.08	130.44	124.68
18	H	306	CLA	CMB-C2B-C3B	3.08	130.44	124.68
21	f	205	BCR	C38-C26-C25	-3.08	121.07	124.53
18	b	807	CLA	CMB-C2B-C3B	3.08	130.44	124.68
18	b	845	CLA	CMB-C2B-C3B	3.07	130.43	124.68
18	a	826	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
18	a	854	CLA	CMB-C2B-C3B	3.07	130.42	124.68
28	E	303	DD6	C37-C36-C31	-3.07	120.18	124.35
18	D	216	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
18	b	837	CLA	CMB-C2B-C3B	3.06	130.41	124.68
26	C	304	A86	C17-C16-C15	3.06	112.29	109.16
20	D	201	LHG	O8-C23-C24	3.06	121.50	111.91
18	b	804	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
18	a	853	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
26	D	206	A86	C17-C16-C15	3.05	112.28	109.16
21	a	845	BCR	C15-C14-C13	-3.05	122.95	127.31
18	b	829	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
21	f	201	BCR	C3-C4-C5	-3.05	108.63	114.08
21	a	833	BCR	C38-C26-C27	3.05	119.47	113.62
18	l	202	CLA	CMB-C2B-C3B	3.05	130.38	124.68
29	B	313	KC1	CHB-C1B-C2B	-3.05	119.09	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E	302	A86	O1-C15-C14	-3.05	107.10	113.21
18	b	805	CLA	CMB-C2B-C3B	3.05	130.38	124.68
27	l	206	ET4	C16-C15-C14	3.05	129.71	123.47
18	B	310	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	B	313	KC1	C3D-CAD-CBD	-3.04	103.60	107.61
18	b	801	CLA	CMB-C2B-C3B	3.04	130.37	124.68
26	B	304	A86	C34-O4-C38	-3.04	112.24	117.90
18	b	844	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	C	302	A86	O-C13-C11	-3.03	114.44	121.15
26	B	301	A86	C28-C27-C26	-3.03	118.67	122.92
18	H	315	CLA	CMB-C2B-C3B	3.03	130.35	124.68
18	D	212	CLA	CMB-C2B-C3B	3.03	130.35	124.68
28	D	205	DD6	C7-C6-C8	-3.03	113.30	118.08
18	a	848	CLA	CMB-C2B-C3B	3.03	130.35	124.68
20	E	301	LHG	O8-C23-C24	3.03	121.41	111.91
18	b	827	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
26	C	302	A86	C10-C9-C8	3.03	132.66	123.22
18	C	317	CLA	CMB-C2B-C1B	-3.02	123.81	128.46
18	l	203	CLA	CMB-C2B-C3B	3.02	130.34	124.68
18	b	804	CLA	CMB-C2B-C3B	3.02	130.33	124.68
18	b	838	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
18	b	816	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
28	D	205	DD6	C19-C18-C17	-3.02	104.94	110.77
21	m	101	BCR	C8-C9-C10	3.02	123.57	118.94
21	l	204	BCR	C15-C14-C13	-3.02	123.00	127.31
21	i	103	BCR	C3-C4-C5	-3.02	108.69	114.08
26	b	847	A86	C7-C6-C5	-3.02	118.70	122.92
26	D	203	A86	C28-C27-C26	-3.02	118.70	122.92
18	b	805	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
18	C	315	CLA	CMB-C2B-C3B	3.01	130.32	124.68
18	a	839	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	a	809	CLA	CMB-C2B-C3B	3.01	130.32	124.68
18	D	217	CLA	CMB-C2B-C3B	3.01	130.32	124.68
23	E	318	LMG	O1-C7-C8	-3.01	103.63	110.90
26	C	302	A86	C19-C18-C17	-3.01	104.96	110.77
18	b	841	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	b	807	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	C	307	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	H	305	CLA	CMB-C2B-C3B	3.01	130.31	124.68
26	H	301	A86	C25-C26-C27	-3.01	123.02	127.31
18	a	801	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
18	a	855	CLA	O2D-CGD-O1D	-3.01	117.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	313	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
18	a	819	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	D	207	CLA	CMB-C2B-C3B	3.00	130.30	124.68
21	E	305	BCR	C7-C8-C9	-3.00	121.70	126.23
18	a	844	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
21	l	201	BCR	C3-C4-C5	-3.00	108.72	114.08
28	D	205	DD6	C33-C34-C35	-3.00	106.20	110.30
26	H	301	A86	C10-C9-C8	3.00	132.58	123.22
26	r	203	A86	O4-C38-C39	3.00	116.61	111.09
21	b	836	BCR	C33-C5-C6	-2.99	121.17	124.53
21	b	839	BCR	C30-C25-C26	-2.99	118.40	122.61
18	b	830	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
18	B	312	CLA	CMB-C2B-C3B	2.99	130.28	124.68
18	a	843	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
18	b	808	CLA	CMB-C2B-C3B	2.99	130.27	124.68
26	b	847	A86	C41-C32-C31	-2.99	107.80	110.47
26	B	305	A86	C7-C6-C8	2.99	122.78	118.08
28	D	205	DD6	C26-C25-C24	2.99	132.53	123.22
18	a	830	CLA	CMB-C2B-C3B	2.98	130.26	124.68
28	B	303	DD6	C3-C2-C1	-2.98	123.05	127.31
18	a	840	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	a	807	CLA	CMB-C2B-C3B	2.98	130.25	124.68
26	D	204	A86	C34-O4-C38	-2.98	112.35	117.90
21	l	201	BCR	C24-C23-C22	-2.97	121.75	126.23
18	B	314	CLA	CMB-C2B-C3B	2.97	130.23	124.68
26	b	847	A86	C10-C9-C8	-2.97	113.96	123.22
26	E	302	A86	C34-O4-C38	-2.96	112.37	117.90
18	C	314	CLA	CMB-C2B-C3B	2.96	130.22	124.68
18	b	822	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	b	805	CLA	CHB-C4A-NA	2.96	128.61	124.51
28	E	307	DD6	C32-C31-C36	-2.96	118.46	122.63
18	a	815	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	a	820	CLA	CMB-C2B-C3B	2.96	130.21	124.68
18	b	801	CLA	O2D-CGD-CBD	2.96	116.52	111.27
28	D	205	DD6	C41-C32-C31	-2.95	105.77	110.47
18	C	318	CLA	CMB-C2B-C3B	2.95	130.20	124.68
18	D	210	CLA	CMB-C2B-C3B	2.95	130.20	124.68
18	a	830	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
21	f	201	BCR	C28-C27-C26	-2.95	108.81	114.08
18	b	838	CLA	CMB-C2B-C3B	2.95	130.19	124.68
18	b	823	CLA	CMB-C2B-C3B	2.94	130.19	124.68
18	b	842	CLA	O2D-CGD-O1D	-2.94	118.08	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E	307	DD6	C37-C36-C35	2.94	119.81	114.36
18	b	840	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	m	101	BCR	C28-C27-C26	-2.94	108.83	114.08
18	b	850	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
18	f	204	CLA	CMB-C2B-C3B	2.94	130.18	124.68
18	B	307	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
18	D	214	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	D	202	LMG	O8-C28-C29	2.94	121.12	111.91
18	b	817	CLA	CMB-C2B-C3B	2.93	130.17	124.68
18	b	810	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
21	j	101	BCR	C3-C4-C5	-2.93	108.84	114.08
18	B	309	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	a	822	CLA	CMB-C2B-C3B	2.93	130.16	124.68
21	b	833	BCR	C20-C21-C22	-2.93	123.13	127.31
18	E	312	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
23	l	207	LMG	O8-C28-C29	2.93	121.10	111.91
26	r	203	A86	O-C13-C14	-2.93	115.71	121.66
18	b	826	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	l	201	BCR	C16-C17-C18	-2.93	123.13	127.31
18	H	315	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	b	812	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
18	i	101	CLA	C1-C2-C3	-2.93	120.98	126.04
21	r	201	BCR	C15-C14-C13	-2.92	123.14	127.31
18	j	104	CLA	CAA-C2A-C3A	-2.92	109.28	116.10
29	C	308	KC1	CHC-C4B-C3B	-2.92	120.26	125.26
18	a	836	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
18	a	816	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
18	b	809	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
18	a	806	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
21	a	845	BCR	C3-C4-C5	-2.92	108.87	114.08
18	a	824	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
21	b	839	BCR	C16-C17-C18	-2.91	123.15	127.31
21	a	845	BCR	C29-C30-C25	-2.91	106.00	110.48
18	D	211	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	C	312	CLA	CMB-C2B-C3B	2.91	130.13	124.68
18	B	311	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	B	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	a	850	BCR	C37-C22-C21	-2.91	118.85	122.92
21	f	201	BCR	C16-C17-C18	-2.91	123.16	127.31
18	a	854	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
18	b	845	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	j	103	LMG	O8-C28-C29	2.91	121.04	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	308	KC1	O1D-CGD-CBD	-2.91	118.53	124.48
18	E	316	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
18	H	305	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
18	b	848	CLA	CMB-C2B-C3B	2.90	130.11	124.68
18	a	823	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	C	301	LMG	O8-C28-C29	2.90	121.02	111.91
21	i	103	BCR	C38-C26-C25	-2.90	121.27	124.53
18	H	308	CLA	O2D-CGD-CBD	2.90	116.42	111.27
18	a	814	CLA	CMB-C2B-C3B	2.90	130.10	124.68
18	a	847	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	a	848	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	l	205	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	l	202	CLA	O2D-CGD-CBD	2.90	116.41	111.27
26	D	203	A86	C9-C8-C6	2.90	134.55	126.42
23	E	318	LMG	O8-C28-C29	2.89	120.98	111.91
18	b	846	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	a	822	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	b	828	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	a	814	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	D	210	CLA	O2D-CGD-CBD	2.88	116.39	111.27
18	a	839	CLA	CHB-C4A-NA	2.88	128.50	124.51
28	H	303	DD6	C20-C19-C18	-2.88	107.05	112.75
18	a	805	CLA	CHB-C4A-NA	2.88	128.50	124.51
26	C	305	A86	O-C13-C11	-2.88	114.78	121.15
21	a	833	BCR	C20-C21-C22	-2.88	123.20	127.31
21	b	839	BCR	C33-C5-C4	2.88	119.15	113.62
18	b	801	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
28	E	303	DD6	C21-C20-C15	-2.88	117.44	122.26
18	E	309	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
18	b	815	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
18	j	104	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	E	313	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	a	812	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	b	825	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
28	D	205	DD6	C13-C11-C10	2.87	123.35	118.94
18	H	309	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	r	203	A86	C12-C11-C10	-2.87	116.48	123.42
18	a	811	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	D	207	CLA	O2D-CGD-CBD	2.87	116.36	111.27
26	E	302	A86	C19-C18-C17	-2.87	105.23	110.77
18	a	810	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	D	215	CLA	O2D-CGD-O1D	-2.87	118.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	E	311	CLA	CMB-C2B-C3B	2.86	130.04	124.68
18	b	806	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	a	846	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	a	805	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	b	849	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	a	813	CLA	C1-C2-C3	-2.86	121.09	126.04
18	a	842	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
18	C	306	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	m	102	A86	C34-O4-C38	-2.86	112.56	117.90
23	D	202	LMG	O2-C2-C3	-2.86	103.74	110.35
18	H	311	CLA	CMB-C2B-C3B	2.86	130.03	124.68
26	H	301	A86	C40-C32-C31	-2.86	107.91	110.47
18	a	803	CLA	CMB-C2B-C3B	2.86	130.03	124.68
18	b	816	CLA	CMB-C2B-C3B	2.86	130.02	124.68
18	a	802	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
21	E	305	BCR	C16-C17-C18	-2.86	123.23	127.31
18	B	307	CLA	CMB-C2B-C3B	2.85	130.02	124.68
18	b	825	CLA	CMB-C2B-C3B	2.85	130.01	124.68
28	B	303	DD6	C26-C25-C24	-2.85	114.32	123.22
20	E	317	LHG	O8-C23-C24	2.85	120.86	111.91
18	C	311	CLA	CAA-CBA-CGA	-2.85	104.92	113.25
27	l	206	ET4	C01-C06-C07	2.85	123.83	115.78
29	H	312	KC1	CBD-CHA-C1A	2.85	134.19	128.88
18	b	838	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	f	202	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
18	D	212	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	l	201	BCR	C15-C16-C17	-2.84	117.66	123.47
28	H	303	DD6	C15-C14-C13	-2.84	119.99	125.99
18	b	819	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
21	E	305	BCR	C24-C23-C22	-2.84	121.95	126.23
21	a	833	BCR	C11-C10-C9	-2.84	123.26	127.31
18	D	216	CLA	CMB-C2B-C3B	2.84	129.98	124.68
18	C	309	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	l	204	BCR	C20-C21-C22	-2.83	123.27	127.31
18	E	315	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
18	a	844	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	H	301	A86	C19-C18-C17	-2.83	105.31	110.77
18	a	842	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
18	D	213	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	a	841	CLA	O2D-CGD-CBD	2.82	116.29	111.27
18	b	808	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	C	309	CLA	CMB-C2B-C3B	2.82	129.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	l	204	BCR	C38-C26-C25	-2.82	121.36	124.53
25	b	834	DGD	O1G-C1A-C2A	2.82	120.76	111.91
21	m	101	BCR	C10-C11-C12	-2.82	114.42	123.22
18	b	814	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	j	104	CLA	CMB-C2B-C3B	2.82	129.95	124.68
28	D	205	DD6	C25-C24-C1	2.82	134.33	126.42
28	B	303	DD6	C20-C19-C18	-2.82	107.18	112.75
18	a	840	CLA	CMB-C2B-C3B	2.81	129.94	124.68
26	H	302	A86	C12-C11-C10	-2.81	116.62	123.42
26	C	305	A86	C19-C18-C17	-2.81	105.34	110.77
21	E	306	BCR	C33-C5-C4	2.81	119.02	113.62
18	E	310	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	b	813	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	b	817	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	a	817	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	a	841	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
29	C	313	KC1	CBD-CHA-C1A	2.81	134.11	128.88
18	a	838	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
18	C	317	CLA	CMB-C2B-C3B	2.81	129.93	124.68
18	a	808	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	B	301	A86	C3-C4-C5	-2.80	117.74	123.47
18	B	308	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
28	B	303	DD6	C4-C3-C2	-2.80	117.74	123.47
26	B	304	A86	O-C13-C11	-2.80	114.97	121.15
21	a	834	BCR	C7-C8-C9	-2.80	122.01	126.23
26	m	102	A86	C10-C9-C8	2.79	131.94	123.22
18	C	318	CLA	CHB-C4A-NA	2.79	128.38	124.51
26	r	203	A86	C26-C25-C24	2.79	131.92	123.22
21	a	852	BCR	C38-C26-C27	2.79	118.97	113.62
18	a	827	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
21	b	836	BCR	C24-C23-C22	-2.78	122.03	126.23
18	C	310	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	B	302	A86	C12-C11-C10	-2.78	116.69	123.42
18	a	826	CLA	CHB-C4A-NA	2.78	128.36	124.51
18	E	311	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	f	203	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	H	304	A86	C8-C6-C5	-2.78	114.68	118.94
21	b	839	BCR	C4-C5-C6	-2.77	118.70	122.73
18	E	310	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
29	C	308	KC1	C4B-CHC-C1C	-2.77	120.07	126.06
26	B	305	A86	C17-C16-C15	2.77	111.99	109.16
18	i	101	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	r	201	BCR	C38-C26-C25	-2.77	121.42	124.53
18	i	101	CLA	CMB-C2B-C3B	2.77	129.86	124.68
18	E	313	CLA	CHB-C4A-NA	2.77	128.34	124.51
21	f	201	BCR	C1-C6-C7	2.77	123.61	115.78
18	b	809	CLA	CMB-C2B-C3B	2.77	129.86	124.68
18	B	310	CLA	CMB-C2B-C3B	2.77	129.85	124.68
18	D	215	CLA	CAA-C2A-C3A	-2.76	109.65	116.10
21	E	305	BCR	C38-C26-C25	-2.76	121.42	124.53
18	a	816	CLA	CMB-C2B-C3B	2.76	129.84	124.68
26	C	305	A86	C40-C32-C31	-2.76	108.00	110.47
18	b	827	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
26	r	203	A86	C7-C6-C8	2.76	122.42	118.08
18	b	821	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
29	H	312	KC1	O1D-CGD-CBD	-2.75	118.85	124.48
21	E	305	BCR	C33-C5-C4	2.75	118.90	113.62
18	b	837	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
26	B	305	A86	O-C13-C14	-2.75	116.07	121.66
21	i	102	BCR	C33-C5-C4	2.75	118.89	113.62
18	a	813	CLA	CMB-C2B-C3B	2.74	129.81	124.68
23	C	301	LMG	C4-C3-C2	2.74	115.61	110.82
18	a	854	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
26	C	305	A86	C8-C6-C5	-2.74	114.74	118.94
18	b	846	CLA	CMB-C2B-C3B	2.74	129.80	124.68
29	C	313	KC1	CHB-C1B-C2B	-2.74	119.74	125.48
21	a	834	BCR	C28-C27-C26	-2.74	109.19	114.08
18	b	801	CLA	C1-C2-C3	-2.73	121.31	126.04
21	a	852	BCR	C20-C19-C18	-2.73	118.73	126.42
26	C	302	A86	O4-C38-O5	-2.73	117.53	122.96
26	m	102	A86	C3-C4-C5	-2.73	117.88	123.47
28	E	308	DD6	C14-C13-C11	-2.73	121.29	125.53
21	l	201	BCR	C8-C9-C10	2.73	123.13	118.94
18	r	202	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	a	822	CLA	CHB-C4A-NA	2.73	128.29	124.51
28	E	308	DD6	C37-C36-C31	-2.73	120.64	124.35
29	H	312	KC1	C3D-CAD-CBD	-2.73	104.02	107.61
18	a	811	CLA	CHB-C4A-NA	2.73	128.28	124.51
18	D	214	CLA	CHB-C4A-NA	2.73	128.28	124.51
21	a	845	BCR	C30-C25-C26	-2.73	118.77	122.61
18	C	315	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	C	319	LMG	C1-O6-C5	-2.72	108.34	113.69
21	b	833	BCR	C11-C12-C13	-2.72	118.78	126.42
21	f	201	BCR	C7-C8-C9	-2.72	122.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	305	A86	C19-C18-C17	-2.72	105.52	110.77
18	b	821	CLA	CMB-C2B-C3B	2.72	129.76	124.68
18	b	811	CLA	O2A-CGA-O1A	-2.72	116.74	123.59
18	b	822	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	B	304	A86	C12-C11-C10	-2.71	116.86	123.42
21	b	836	BCR	C20-C19-C18	-2.71	118.80	126.42
29	C	313	KC1	CHC-C4B-C3B	-2.71	120.62	125.26
18	a	801	CLA	CMB-C2B-C3B	2.71	129.75	124.68
28	C	303	DD6	C33-C34-C35	2.71	114.02	110.30
28	E	303	DD6	C33-C34-C35	-2.71	106.59	110.30
18	a	815	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
21	b	836	BCR	C38-C26-C27	2.71	118.82	113.62
18	E	311	CLA	CHB-C4A-NA	2.71	128.25	124.51
18	a	821	CLA	CHB-C4A-NA	2.71	128.25	124.51
21	b	839	BCR	C15-C14-C13	-2.71	123.45	127.31
18	b	826	CLA	CHB-C4A-NA	2.70	128.25	124.51
21	b	839	BCR	C38-C26-C27	2.70	118.80	113.62
18	C	306	CLA	CMB-C2B-C3B	2.70	129.73	124.68
18	B	306	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
26	B	304	A86	O-C13-C14	-2.70	116.18	121.66
18	a	819	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	E	302	A86	C41-C32-C31	-2.70	108.06	110.47
26	H	302	A86	C7-C6-C8	2.70	122.33	118.08
18	a	812	CLA	CMB-C2B-C3B	2.69	129.72	124.68
26	B	302	A86	C7-C6-C8	2.69	122.32	118.08
18	D	211	CLA	CMB-C2B-C3B	2.69	129.72	124.68
18	D	209	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
18	B	312	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	C	302	A86	C41-C32-C31	-2.69	108.06	110.47
18	C	309	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
18	b	814	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	f	201	BCR	C20-C19-C18	-2.69	118.86	126.42
18	H	308	CLA	CMB-C2B-C3B	2.68	129.70	124.68
18	C	318	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
21	a	852	BCR	C3-C4-C5	-2.68	109.28	114.08
18	a	821	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
18	C	310	CLA	CMB-C2B-C3B	2.68	129.70	124.68
18	a	807	CLA	C1-C2-C3	-2.68	121.41	126.04
18	b	827	CLA	CMB-C2B-C3B	2.68	129.69	124.68
18	b	818	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	308	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	a	854	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	816	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
18	b	844	CLA	CHB-C4A-NA	2.68	128.21	124.51
28	C	303	DD6	C10-C9-C8	-2.68	114.86	123.22
18	B	311	CLA	CMB-C2B-C3B	2.67	129.68	124.68
18	a	810	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	f	204	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
18	E	314	CLA	CMB-C2B-C3B	2.67	129.66	124.68
26	b	847	A86	C-C1-C24	2.67	122.28	118.08
18	b	801	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
26	E	302	A86	O-C13-C11	-2.66	115.27	121.15
18	b	824	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
21	i	102	BCR	C33-C5-C6	-2.66	121.54	124.53
20	j	102	LHG	O8-C23-C24	2.66	120.25	111.91
23	a	851	LMG	O8-C28-C29	2.65	120.24	111.91
18	f	203	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	i	102	BCR	C3-C4-C5	-2.65	109.34	114.08
18	f	204	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	b	849	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	H	303	DD6	C4-C5-C6	-2.65	123.53	127.31
26	b	847	A86	C24-C1-C2	-2.65	114.88	118.94
21	r	201	BCR	C33-C5-C6	-2.65	121.55	124.53
18	a	843	CLA	CHB-C4A-NA	2.65	128.17	124.51
21	a	845	BCR	C38-C26-C27	2.64	118.70	113.62
18	D	209	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	B	314	CLA	CMA-C3A-C2A	-2.64	109.93	116.10
21	a	833	BCR	C8-C7-C6	-2.64	119.78	127.20
21	E	305	BCR	C20-C21-C22	-2.64	123.54	127.31
21	r	201	BCR	C11-C10-C9	-2.64	123.54	127.31
18	a	801	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
18	a	824	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	C	316	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	b	804	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	E	305	BCR	C15-C16-C17	-2.63	118.08	123.47
18	H	310	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
21	f	201	BCR	C16-C15-C14	-2.63	118.09	123.47
18	H	310	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	H	312	KC1	CHC-C4B-C3B	-2.63	120.76	125.26
18	b	810	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	a	826	CLA	CMB-C2B-C3B	2.63	129.59	124.68
18	b	811	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
19	b	831	PQN	C14-C13-C15	2.62	119.69	115.27
28	E	308	DD6	C15-C14-C13	-2.62	120.45	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	l	206	ET4	C34-C35-C36	-2.62	107.72	113.64
22	a	849	SQD	O7-S-C6	2.62	110.07	106.92
21	b	836	BCR	C33-C5-C4	2.62	118.65	113.62
18	C	316	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
18	b	843	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
21	a	845	BCR	C23-C24-C25	-2.62	119.84	127.20
21	j	105	BCR	C38-C26-C27	2.62	118.65	113.62
18	b	809	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	a	835	LHG	O8-C23-C24	2.62	120.12	111.91
28	H	303	DD6	C23-C16-C22	2.62	111.23	107.37
18	E	309	CLA	CHB-C4A-NA	2.62	128.13	124.51
29	C	308	KC1	CHB-C1B-C2B	-2.61	120.00	125.48
18	b	812	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	a	818	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	B	309	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	j	104	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	C	302	A86	C21-C20-C19	-2.60	111.35	114.28
18	a	816	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	b	813	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	b	835	LHG	O8-C23-C24	2.60	120.07	111.91
21	E	305	BCR	C21-C20-C19	-2.60	115.11	123.22
18	D	211	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	b	837	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
26	D	204	A86	C17-C16-C15	2.60	111.81	109.16
18	a	821	CLA	CMB-C2B-C3B	2.59	129.53	124.68
26	r	203	A86	C28-C27-C26	2.59	126.56	122.92
18	a	827	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	a	855	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	b	806	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	a	801	CLA	C4D-C3D-CAD	-2.59	105.04	108.10
18	a	807	CLA	CBA-CAA-C2A	-2.59	106.22	113.86
26	E	302	A86	C3-C2-C1	2.59	131.01	127.31
21	m	101	BCR	C33-C5-C4	2.59	118.59	113.62
28	B	303	DD6	C-C1-C24	-2.59	114.00	118.08
18	b	811	CLA	CHB-C4A-NA	2.59	128.09	124.51
28	C	303	DD6	C33-C32-C31	-2.59	104.37	109.62
26	D	203	A86	O1-C15-C20	-2.59	56.87	59.40
18	b	849	CLA	CMB-C2B-C3B	2.59	129.52	124.68
18	H	308	CLA	C1-C2-C3	-2.59	121.57	126.04
18	H	307	CLA	CAA-CBA-CGA	-2.59	105.70	113.25
18	D	213	CLA	CHB-C4A-NA	2.58	128.09	124.51
27	l	206	ET4	C42-C34-C33	-2.58	106.36	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	840	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
18	b	848	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	r	201	BCR	C7-C8-C9	-2.58	122.33	126.23
18	a	803	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	a	838	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
18	C	317	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
18	H	314	CLA	C1-C2-C3	-2.58	121.58	126.04
18	b	840	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
21	b	832	BCR	C38-C26-C25	-2.58	121.63	124.53
28	H	303	DD6	C12-C11-C10	-2.57	119.32	122.92
21	a	850	BCR	C30-C25-C26	-2.57	118.99	122.61
18	D	208	CLA	CMB-C2B-C3B	2.57	129.49	124.68
26	B	305	A86	C8-C6-C5	-2.57	114.99	118.94
26	C	305	A86	O4-C38-O5	-2.57	117.85	122.96
26	C	302	A86	C4-C5-C6	2.57	130.98	127.31
18	C	306	CLA	CHB-C4A-NA	2.57	128.07	124.51
28	E	308	DD6	C33-C34-C35	-2.57	106.79	110.30
18	B	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	a	814	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	C	311	CLA	CMB-C2B-C3B	2.57	129.48	124.68
26	D	203	A86	C25-C24-C1	2.56	133.62	126.42
26	r	203	A86	C21-C20-C19	-2.56	111.40	114.28
18	a	812	CLA	CHB-C4A-NA	2.56	128.06	124.51
18	b	842	CLA	CHB-C4A-NA	2.56	128.06	124.51
18	C	312	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
18	b	840	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	H	302	A86	O4-C38-O5	-2.56	117.88	122.96
26	B	302	A86	O4-C38-O5	-2.56	117.88	122.96
18	H	305	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	a	839	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
18	a	841	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
18	a	808	CLA	CMB-C2B-C3B	2.56	129.46	124.68
18	a	854	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	l	201	BCR	C21-C20-C19	-2.55	115.24	123.22
29	B	313	KC1	O2D-CGD-O1D	-2.55	118.84	123.84
18	a	847	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	f	201	BCR	C38-C26-C25	-2.55	121.66	124.53
18	H	315	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	l	202	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
26	D	203	A86	C19-C18-C17	-2.55	105.85	110.77
26	H	304	A86	C24-C1-C2	-2.55	115.03	118.94
18	a	818	CLA	C1B-CHB-C4A	-2.55	125.08	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	313	KC1	O1D-CGD-CBD	-2.54	119.28	124.48
18	a	804	CLA	CHB-C4A-NA	2.54	128.03	124.51
18	a	844	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	H	313	CLA	CHB-C4A-NA	2.54	128.02	124.51
28	D	205	DD6	C14-C13-C11	-2.54	121.59	125.53
18	a	823	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
18	b	840	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
21	b	839	BCR	C21-C20-C19	-2.53	115.31	123.22
18	D	213	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
21	l	204	BCR	C27-C26-C25	-2.53	119.06	122.73
22	a	849	SQD	O48-C23-C24	2.53	119.85	111.91
18	a	853	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	b	843	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	H	309	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	a	825	CLA	O1D-CGD-CBD	2.53	129.66	124.48
23	l	207	LMG	O2-C2-C3	-2.53	104.51	110.35
18	C	310	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
18	b	825	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	H	302	A86	C40-C32-C31	-2.52	108.21	110.47
21	a	850	BCR	C35-C13-C14	-2.52	119.39	122.92
18	l	205	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	a	808	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	D	204	A86	O4-C38-O5	-2.52	117.96	122.96
21	b	833	BCR	C8-C7-C6	-2.52	120.13	127.20
18	E	315	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	B	302	A86	C40-C32-C31	-2.52	108.22	110.47
18	b	837	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	E	302	A86	C36-C31-C32	2.52	122.19	119.70
18	D	207	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
18	b	850	CLA	CHB-C4A-NA	2.52	127.99	124.51
18	a	803	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
18	B	310	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
27	l	206	ET4	C28-C13-C14	-2.51	119.41	122.92
18	B	312	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
26	C	304	A86	C3-C4-C5	-2.51	118.33	123.47
18	l	203	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
18	B	311	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	C	309	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
18	C	311	CLA	C1B-CHB-C4A	-2.51	125.16	130.12
18	b	820	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	D	208	CLA	O2D-CGD-CBD	2.50	115.72	111.27
18	b	819	CLA	C1B-CHB-C4A	-2.50	125.16	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	317	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
18	a	836	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
18	f	202	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	b	831	PQN	C2M-C2-C3	-2.50	120.32	124.40
18	a	825	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
21	i	102	BCR	C30-C25-C26	-2.50	119.09	122.61
18	b	819	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	314	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
18	H	307	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
28	D	205	DD6	C4-C5-C6	2.50	130.87	127.31
21	E	305	BCR	C8-C7-C6	-2.49	120.19	127.20
18	E	312	CLA	CAA-CBA-CGA	-2.49	105.96	113.25
18	a	840	CLA	C11-C10-C8	-2.49	107.86	115.92
18	E	310	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
21	b	832	BCR	C38-C26-C27	2.49	118.41	113.62
18	a	823	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	H	311	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
28	E	304	DD6	C4-C3-C2	-2.49	118.37	123.47
26	C	305	A86	C4-C5-C6	2.49	130.87	127.31
18	a	806	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	l	204	BCR	C33-C5-C4	2.49	118.40	113.62
18	a	837	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	l	202	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
18	a	830	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	b	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	b	820	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
21	E	306	BCR	C38-C26-C27	2.49	118.39	113.62
18	E	310	CLA	CHB-C4A-NA	2.49	127.95	124.51
28	B	303	DD6	C9-C10-C11	-2.49	123.76	127.31
18	a	827	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
18	b	828	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
18	a	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	b	828	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	a	813	CLA	O2D-CGD-CBD	2.48	115.68	111.27
18	b	817	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	E	314	CLA	O2D-CGD-CBD	2.48	115.68	111.27
21	f	205	BCR	C38-C26-C27	2.48	118.39	113.62
18	a	828	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	b	829	CLA	C1-C2-C3	-2.48	121.75	126.04
18	b	830	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	a	817	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	l	206	ET4	C35-C34-C33	2.48	114.65	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	a	836	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	b	823	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	H	307	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	a	813	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
18	l	203	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
18	b	803	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
18	E	314	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
18	H	314	CLA	CHD-C1D-ND	-2.47	122.18	124.45
26	C	305	A86	C41-C32-C31	-2.47	108.26	110.47
18	B	311	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
18	b	803	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
26	H	301	A86	C34-O4-C38	-2.47	113.30	117.90
18	H	313	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
18	a	826	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
18	a	827	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
18	H	307	CLA	C16-C15-C13	-2.46	107.96	115.92
18	b	814	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
18	D	210	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	D	217	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	D	206	A86	C41-C32-C31	2.46	112.67	110.47
18	b	807	CLA	CHB-C4A-NA	2.46	127.91	124.51
21	f	201	BCR	C10-C11-C12	-2.46	115.55	123.22
18	H	306	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
18	E	312	CLA	CHB-C4A-NA	2.45	127.91	124.51
18	D	215	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
21	a	850	BCR	C7-C8-C9	-2.45	122.53	126.23
23	C	301	LMG	C6-C5-C4	-2.45	107.26	113.00
29	H	312	KC1	C4B-CHC-C1C	-2.45	120.77	126.06
26	C	304	A86	C24-C1-C2	2.45	122.70	118.94
21	j	101	BCR	C33-C5-C4	2.45	118.32	113.62
18	b	844	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
18	a	809	CLA	CHB-C4A-NA	2.45	127.90	124.51
18	a	802	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
18	a	804	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	b	836	BCR	C30-C25-C26	-2.44	119.17	122.61
21	b	836	BCR	C15-C14-C13	-2.44	123.82	127.31
21	a	833	BCR	C10-C11-C12	-2.44	115.59	123.22
18	b	845	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	a	848	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	C	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	a	833	BCR	C33-C5-C4	2.44	118.30	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	848	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
18	a	825	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	D	212	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	H	308	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
18	E	309	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
18	C	311	CLA	CHD-C1D-ND	-2.43	122.22	124.45
18	b	825	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	D	206	A86	C19-C18-C17	-2.43	106.08	110.77
26	E	302	A86	C12-C11-C10	-2.43	117.54	123.42
18	B	314	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
18	a	801	CLA	CBA-CAA-C2A	-2.43	106.69	113.86
18	H	309	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
18	a	838	CLA	CHD-C1D-ND	-2.43	122.22	124.45
28	H	303	DD6	C33-C32-C31	2.43	114.53	109.62
18	a	846	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	b	846	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	a	813	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	D	217	CLA	CMA-C3A-C2A	-2.42	110.45	116.10
18	b	841	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	r	201	BCR	C33-C5-C4	2.42	118.27	113.62
26	D	203	A86	O4-C38-O5	-2.42	118.15	122.96
21	E	306	BCR	C8-C7-C6	-2.42	120.41	127.20
18	b	816	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	a	822	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
21	a	833	BCR	C33-C5-C6	-2.42	121.81	124.53
23	E	318	LMG	C8-O7-C10	-2.42	111.84	117.79
29	C	313	KC1	C4B-CHC-C1C	-2.42	120.84	126.06
18	b	807	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
26	m	102	A86	C41-C32-C31	-2.42	108.31	110.47
21	a	834	BCR	C38-C26-C27	2.42	118.26	113.62
26	B	305	A86	C9-C8-C6	2.42	133.20	126.42
18	E	312	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
21	l	201	BCR	C11-C10-C9	-2.42	123.86	127.31
21	i	103	BCR	C15-C16-C17	-2.41	118.53	123.47
21	a	845	BCR	C21-C20-C19	-2.41	115.69	123.22
21	i	102	BCR	C1-C6-C5	-2.41	119.22	122.61
18	H	305	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
18	C	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	C	305	A86	C36-C31-C32	-2.41	117.30	119.70
18	C	307	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
18	a	848	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
18	H	314	CLA	C1B-CHB-C4A	-2.41	125.35	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	824	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	a	814	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
18	b	804	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
21	a	845	BCR	C20-C21-C22	-2.40	123.88	127.31
18	a	830	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	b	808	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	B	307	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
21	j	105	BCR	C20-C19-C18	-2.40	119.67	126.42
21	l	201	BCR	C10-C11-C12	-2.40	115.72	123.22
26	E	302	A86	C4-C5-C6	2.40	130.74	127.31
21	b	839	BCR	C8-C7-C6	-2.40	120.46	127.20
18	C	317	CLA	CHD-C1D-ND	-2.40	122.25	124.45
26	m	102	A86	C12-C11-C10	-2.40	117.62	123.42
21	l	204	BCR	C35-C13-C14	-2.40	119.57	122.92
18	b	841	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
18	b	824	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	C	305	A86	C21-C20-C19	-2.39	111.59	114.28
18	i	101	CLA	CHB-C4A-NA	2.39	127.82	124.51
18	H	310	CLA	O2D-CGD-CBD	2.39	115.52	111.27
18	H	307	CLA	C1-C2-C3	-2.39	121.91	126.04
18	b	826	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
18	a	801	CLA	CHB-C4A-NA	2.39	127.81	124.51
29	C	308	KC1	C2A-C3A-C4A	2.39	108.26	106.49
29	B	313	KC1	C4B-CHC-C1C	-2.39	120.91	126.06
18	r	202	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
18	C	316	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
18	D	217	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
18	b	821	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	b	812	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	f	201	BCR	C37-C22-C21	-2.38	119.58	122.92
18	b	830	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	i	101	CLA	C11-C10-C8	-2.38	108.23	115.92
18	H	306	CLA	O2D-CGD-CBD	2.38	115.50	111.27
18	E	316	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
18	b	826	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
18	b	811	CLA	O2D-CGD-CBD	2.38	115.49	111.27
18	a	837	CLA	C1-C2-C3	-2.38	121.93	126.04
21	b	836	BCR	C27-C26-C25	-2.38	119.28	122.73
28	D	205	DD6	C28-C27-C29	-2.38	112.13	116.84
18	b	829	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
18	D	215	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	H	301	A86	O4-C38-O5	-2.38	118.24	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	308	CLA	CHB-C4A-NA	2.37	127.80	124.51
21	f	205	BCR	C33-C5-C4	2.37	118.17	113.62
18	a	838	CLA	CHB-C4A-NA	2.37	127.79	124.51
18	b	820	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
28	E	308	DD6	O1-C20-C21	-2.37	112.22	115.06
18	D	209	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
21	E	306	BCR	C20-C19-C18	-2.37	119.76	126.42
26	D	206	A86	C12-C11-C10	-2.37	117.69	123.42
21	b	832	BCR	C33-C5-C6	-2.37	121.87	124.53
27	l	206	ET4	C15-C14-C13	2.37	130.69	127.31
28	D	205	DD6	C20-C19-C18	-2.37	108.07	112.75
18	E	311	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
21	i	103	BCR	C38-C26-C27	2.36	118.16	113.62
18	a	843	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
21	l	201	BCR	C33-C5-C4	2.36	118.16	113.62
18	r	202	CLA	CHB-C4A-NA	2.36	127.78	124.51
18	C	312	CLA	C1-C2-C3	-2.36	121.96	126.04
18	j	104	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	B	313	KC1	CBD-CHA-C1A	2.36	133.29	128.88
26	D	204	A86	O-C13-C11	-2.36	115.93	121.15
18	b	822	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	b	836	BCR	C38-C26-C25	-2.36	121.88	124.53
18	a	846	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
18	b	827	CLA	CHB-C4A-NA	2.36	127.77	124.51
18	a	825	CLA	CMB-C2B-C3B	2.36	129.09	124.68
21	b	839	BCR	C30-C25-C24	2.36	122.45	115.78
18	a	809	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	B	305	A86	C12-C11-C10	-2.36	117.72	123.42
18	a	808	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
18	b	806	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	r	203	A86	O-C13-C11	-2.36	115.94	121.15
18	a	842	CLA	CHB-C4A-NA	2.35	127.77	124.51
18	B	310	CLA	CHB-C4A-NA	2.35	127.77	124.51
18	a	817	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
18	C	309	CLA	C1-C2-C3	-2.35	121.97	126.04
21	a	845	BCR	C16-C15-C14	-2.35	118.66	123.47
21	b	832	BCR	C16-C15-C14	-2.35	118.66	123.47
18	B	306	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	E	314	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	C	306	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
18	H	311	CLA	O2D-CGD-CBD	2.35	115.44	111.27
21	i	102	BCR	C16-C15-C14	-2.35	118.67	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	803	CLA	C1-C2-C3	-2.35	121.99	126.04
21	E	306	BCR	C16-C15-C14	-2.34	118.67	123.47
21	i	102	BCR	C27-C26-C25	-2.34	119.33	122.73
26	B	305	A86	O1-C15-C14	-2.34	108.52	113.21
18	b	803	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
18	H	307	CLA	C2D-C1D-ND	-2.34	108.38	110.10
21	i	102	BCR	C20-C19-C18	-2.34	119.85	126.42
18	f	203	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	a	845	BCR	C33-C5-C4	2.34	118.10	113.62
26	D	204	A86	C21-C20-C19	-2.34	111.65	114.28
21	l	201	BCR	C23-C24-C25	-2.33	120.64	127.20
28	E	304	DD6	O2-C18-C17	-2.33	105.17	109.80
26	H	302	A86	O-C13-C14	-2.33	116.92	121.66
28	D	205	DD6	C9-C10-C11	-2.33	123.98	127.31
18	i	101	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	b	839	BCR	C35-C13-C14	-2.33	119.66	122.92
18	a	837	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
26	b	847	A86	C25-C26-C27	-2.33	123.99	127.31
26	H	302	A86	C19-C18-C17	-2.33	106.28	110.77
18	a	847	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	C	314	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	b	829	CLA	CHB-C4A-NA	2.33	127.73	124.51
28	H	303	DD6	C7-C6-C5	-2.33	119.67	122.92
26	B	302	A86	C-C1-C24	2.32	121.74	118.08
26	H	304	A86	O1-C15-C20	-2.32	57.13	59.40
21	j	101	BCR	C38-C26-C27	2.32	118.08	113.62
28	E	304	DD6	C7-C6-C5	-2.32	119.67	122.92
18	a	828	CLA	CHB-C4A-NA	2.32	127.72	124.51
18	b	846	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	a	852	BCR	C35-C13-C14	-2.32	119.67	122.92
18	D	212	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	a	820	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	C	304	A86	C26-C25-C24	-2.32	115.98	123.22
18	b	805	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	b	809	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	f	204	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	b	842	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	a	850	BCR	C36-C18-C17	-2.32	119.68	122.92
18	E	313	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
26	r	203	A86	O1-C15-C20	-2.31	57.14	59.40
26	H	301	A86	C26-C25-C24	-2.31	116.00	123.22
21	m	101	BCR	C20-C19-C18	-2.31	119.92	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	214	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	B	302	A86	C19-C18-C17	-2.31	106.31	110.77
18	a	816	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	a	852	BCR	C33-C5-C4	2.31	118.05	113.62
18	C	318	CLA	CHD-C1D-ND	-2.31	122.33	124.45
18	a	801	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
18	b	813	CLA	CHB-C4A-NA	2.31	127.70	124.51
26	H	302	A86	C8-C6-C5	-2.31	115.40	118.94
29	B	313	KC1	CHC-C4B-C3B	-2.31	121.31	125.26
18	b	829	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
26	C	304	A86	C10-C9-C8	-2.31	116.02	123.22
26	H	304	A86	O-C13-C11	-2.30	116.06	121.15
18	C	315	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	b	829	CLA	CMB-C2B-C3B	2.30	128.99	124.68
26	H	304	A86	C12-C11-C10	-2.30	117.86	123.42
18	H	315	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	f	205	BCR	C3-C4-C5	-2.30	109.97	114.08
18	D	216	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	a	820	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
26	m	102	A86	C19-C18-C17	-2.30	106.34	110.77
26	H	304	A86	C-C1-C24	2.30	121.70	118.08
18	D	210	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	b	836	BCR	C36-C18-C17	-2.30	119.71	122.92
26	H	302	A86	C-C1-C24	2.30	121.69	118.08
18	a	811	CLA	C1-C2-C3	-2.30	123.04	126.75
26	B	301	A86	C7-C6-C5	-2.30	119.71	122.92
26	C	305	A86	C12-C11-C10	-2.29	117.87	123.42
18	a	813	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
21	j	101	BCR	C37-C22-C21	-2.29	119.71	122.92
18	a	837	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
29	C	313	KC1	C2A-C3A-C4A	2.29	108.19	106.49
26	B	301	A86	C-C1-C2	-2.29	119.71	122.92
18	C	310	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	E	302	A86	O4-C38-O5	-2.29	118.41	122.96
18	a	855	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	b	821	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
18	E	316	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	C	308	KC1	O2D-CGD-O1D	-2.29	119.36	123.84
18	D	208	CLA	C7-C6-C5	-2.29	107.14	113.36
26	B	302	A86	O1-C15-C20	-2.28	57.17	59.40
21	E	306	BCR	C28-C27-C26	-2.28	110.00	114.08
18	a	810	CLA	C1B-CHB-C4A	-2.28	125.59	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	802	CLA	CHB-C4A-NA	2.28	127.67	124.51
18	b	845	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
18	a	820	CLA	O2D-CGD-CBD	2.28	115.32	111.27
18	E	315	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	E	307	DD6	C32-C33-C34	-2.28	108.49	113.64
18	f	202	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	b	833	BCR	C38-C26-C27	2.28	118.00	113.62
26	B	305	A86	O-C13-C11	-2.28	116.11	121.15
26	D	206	A86	O1-C15-C20	-2.28	57.17	59.40
26	H	301	A86	C21-C20-C19	-2.28	111.72	114.28
21	a	852	BCR	C12-C13-C14	2.28	122.43	118.94
18	a	844	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
21	b	832	BCR	C20-C19-C18	-2.28	120.03	126.42
21	f	205	BCR	C11-C12-C13	-2.27	120.03	126.42
26	B	302	A86	O-C13-C14	-2.27	117.04	121.66
26	C	302	A86	O1-C15-C20	-2.27	57.18	59.40
18	l	203	CLA	C11-C10-C8	-2.27	108.58	115.92
26	D	206	A86	O4-C38-O5	-2.27	118.45	122.96
18	D	207	CLA	CHB-C4A-NA	2.27	127.65	124.51
18	H	313	CLA	CBA-CAA-C2A	-2.27	107.17	113.86
28	B	303	DD6	C28-C27-C29	2.27	121.33	116.84
18	a	811	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
25	b	834	DGD	O2G-C1B-O1B	-2.27	118.23	123.70
18	C	316	CLA	C2D-C1D-ND	-2.26	108.44	110.10
21	a	834	BCR	C10-C11-C12	-2.26	116.15	123.22
21	a	845	BCR	C8-C7-C6	-2.26	120.84	127.20
18	H	308	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
26	m	102	A86	O-C13-C11	-2.26	116.16	121.15
18	a	806	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	j	105	BCR	C37-C22-C21	-2.26	119.76	122.92
29	C	313	KC1	O2D-CGD-O1D	-2.26	119.42	123.84
26	E	302	A86	C40-C32-C31	-2.26	108.45	110.47
18	a	801	CLA	C2D-C1D-ND	-2.26	108.44	110.10
18	D	216	CLA	CHB-C4A-NA	2.26	127.63	124.51
21	b	833	BCR	C35-C13-C14	-2.26	119.76	122.92
18	b	817	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
21	b	839	BCR	C23-C24-C25	-2.25	120.88	127.20
21	b	833	BCR	C33-C5-C4	2.25	117.94	113.62
21	b	836	BCR	C23-C24-C25	-2.25	120.88	127.20
21	r	201	BCR	C2-C1-C6	2.25	113.95	110.48
21	a	834	BCR	C8-C7-C6	-2.25	120.88	127.20
21	i	103	BCR	C33-C5-C4	2.25	117.94	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	303	DD6	C37-C36-C31	-2.25	121.29	124.35
26	B	304	A86	C7-C6-C8	2.25	121.62	118.08
28	E	307	DD6	C28-C27-C29	2.25	121.29	116.84
18	D	217	CLA	CHD-C1D-ND	-2.25	122.39	124.45
18	B	309	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
18	a	808	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
18	b	842	CLA	CHD-C1D-ND	-2.24	122.39	124.45
18	b	818	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
18	C	317	CLA	CHB-C4A-NA	2.24	127.61	124.51
18	l	205	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
18	H	307	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
26	C	305	A86	O1-C15-C20	-2.24	57.21	59.40
26	B	302	A86	C8-C6-C5	-2.24	115.50	118.94
18	b	823	CLA	C1-C2-C3	-2.24	122.17	126.04
21	j	101	BCR	C8-C7-C6	-2.24	120.92	127.20
26	r	203	A86	O2-C18-C19	2.24	114.25	109.80
26	D	206	A86	C7-C6-C8	2.24	121.60	118.08
18	a	825	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
21	f	205	BCR	C15-C16-C17	-2.24	118.89	123.47
18	a	844	CLA	CHD-C1D-ND	-2.24	122.40	124.45
22	a	849	SQD	C5-C6-S	2.23	120.02	113.20
18	C	312	CLA	CHB-C4A-NA	2.23	127.60	124.51
18	a	819	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
18	E	314	CLA	CHD-C1D-ND	-2.23	122.40	124.45
26	H	301	A86	C8-C6-C5	-2.23	115.52	118.94
18	C	307	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	a	834	BCR	C11-C10-C9	-2.23	124.13	127.31
18	C	307	CLA	CHB-C4A-NA	2.23	127.59	124.51
18	a	805	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	b	839	BCR	C7-C8-C9	-2.23	122.87	126.23
18	a	840	CLA	CHB-C4A-NA	2.23	127.59	124.51
18	D	217	CLA	CHB-C4A-NA	2.23	127.59	124.51
26	D	204	A86	C41-C32-C31	-2.23	108.48	110.47
21	f	201	BCR	C23-C22-C21	2.23	122.36	118.94
28	E	307	DD6	O1-C20-C21	-2.23	112.39	115.06
27	l	206	ET4	C15-C16-C17	2.23	128.03	123.47
18	a	813	CLA	C2D-C1D-ND	-2.22	108.47	110.10
18	a	854	CLA	O1D-CGD-CBD	2.22	129.03	124.48
28	C	303	DD6	C23-C16-C22	2.22	110.65	107.37
21	r	201	BCR	C10-C11-C12	-2.22	116.28	123.22
18	i	101	CLA	CHD-C1D-ND	-2.22	122.41	124.45
18	a	812	CLA	C1B-CHB-C4A	-2.22	125.72	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	303	DD6	C37-C36-C35	2.22	118.47	114.36
21	l	204	BCR	C8-C7-C6	-2.22	120.97	127.20
20	a	831	LHG	C26-C25-C24	2.22	121.17	113.19
26	C	302	A86	C12-C11-C10	-2.22	118.06	123.42
21	a	845	BCR	C10-C11-C12	-2.22	116.29	123.22
21	i	102	BCR	C4-C5-C6	-2.22	119.51	122.73
18	E	314	CLA	CAA-CBA-CGA	-2.22	106.62	112.51
18	l	203	CLA	CHB-C4A-NA	2.22	127.58	124.51
21	r	201	BCR	C16-C15-C14	-2.22	118.93	123.47
18	a	804	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	B	301	A86	C17-C16-C15	2.21	111.42	109.16
18	D	211	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
18	a	815	CLA	C1-C2-C3	-2.21	122.22	126.04
21	a	833	BCR	C27-C26-C25	-2.21	119.52	122.73
18	b	821	CLA	C1-C2-C3	-2.21	123.18	126.75
18	B	314	CLA	CAA-C2A-C3A	-2.21	110.94	116.10
26	C	304	A86	C20-C19-C18	-2.20	108.39	112.75
18	a	807	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
18	b	804	CLA	CAA-CBA-CGA	-2.20	106.66	112.51
26	r	203	A86	C-C1-C2	-2.20	119.84	122.92
18	a	803	CLA	CHD-C1D-ND	-2.20	122.43	124.45
18	b	815	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
18	b	823	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
18	b	840	CLA	O2D-CGD-CBD	2.20	115.17	111.27
28	E	307	DD6	C8-C6-C5	2.20	122.31	118.94
18	b	823	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
20	b	835	LHG	O8-C6-C5	-2.20	102.04	108.43
18	b	810	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
18	a	803	CLA	CAA-CBA-CGA	-2.19	106.84	113.25
26	C	305	A86	C35-C34-C33	2.19	113.71	109.88
26	H	302	A86	O1-C15-C20	-2.19	57.26	59.40
20	B	315	LHG	O8-C23-O10	-2.19	118.06	123.59
18	b	828	CLA	CHD-C1D-ND	-2.19	122.44	124.45
28	D	205	DD6	C33-C32-C31	2.19	114.06	109.62
26	H	304	A86	C19-C18-C17	-2.19	106.55	110.77
21	f	205	BCR	C35-C13-C14	-2.19	119.86	122.92
28	E	307	DD6	C7-C6-C8	2.19	121.52	118.08
18	a	839	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
18	a	813	CLA	CAC-C3C-C2C	-2.18	123.80	127.53
26	H	304	A86	C34-O4-C38	-2.18	113.83	117.90
21	a	833	BCR	C29-C30-C25	2.18	113.84	110.48
29	C	313	KC1	C3D-CAD-CBD	-2.18	104.74	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	808	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
26	C	304	A86	O1-C15-C20	-2.18	57.27	59.40
21	E	305	BCR	C38-C26-C27	2.17	117.79	113.62
18	b	812	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
18	a	853	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
18	H	306	CLA	CHB-C4A-NA	2.17	127.52	124.51
18	C	311	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
28	E	307	DD6	C15-C14-C13	2.17	130.59	125.99
21	r	201	BCR	C8-C7-C6	-2.17	121.10	127.20
18	D	208	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
27	l	206	ET4	C26-C01-C06	-2.17	106.78	110.30
18	E	315	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	C	311	CLA	C1-C2-C3	-2.17	122.29	126.04
18	a	842	CLA	C2D-C1D-ND	-2.17	108.51	110.10
18	f	202	CLA	C1-C2-C3	-2.17	122.30	126.04
21	a	845	BCR	C30-C25-C24	2.17	121.91	115.78
18	H	310	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
26	r	203	A86	O4-C34-C35	2.17	112.98	107.59
18	l	202	CLA	CHB-C4A-NA	2.16	127.50	124.51
18	H	307	CLA	CAA-C2A-C1A	-2.16	104.88	111.97
18	b	829	CLA	O2D-CGD-CBD	2.16	115.11	111.27
18	D	208	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
18	H	314	CLA	CHB-C4A-NA	2.16	127.50	124.51
18	a	824	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
18	b	810	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	D	203	A86	C20-C19-C18	-2.16	108.48	112.75
18	b	845	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
18	a	818	CLA	O2D-CGD-CBD	2.16	115.10	111.27
18	C	314	CLA	CHB-C4A-NA	2.16	127.49	124.51
18	D	207	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
18	a	854	CLA	CHD-C1D-ND	-2.15	122.47	124.45
18	a	846	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
18	a	802	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	D	203	A86	C3-C4-C5	-2.15	119.07	123.47
18	b	838	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
21	b	832	BCR	C36-C18-C17	-2.15	119.91	122.92
18	a	814	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	a	815	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	C	317	CLA	O2D-CGD-CBD	2.15	115.08	111.27
18	C	307	CLA	O2D-CGD-CBD	2.15	115.08	111.27
21	i	102	BCR	C38-C26-C27	2.15	117.74	113.62
21	a	833	BCR	C15-C16-C17	-2.14	119.08	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	853	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
18	b	814	CLA	CHD-C1D-ND	-2.14	122.48	124.45
18	a	836	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	a	807	CLA	O2D-CGD-CBD	2.14	115.07	111.27
26	C	304	A86	O4-C38-O5	-2.14	118.71	122.96
18	b	816	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
26	r	203	A86	C-C1-C24	-2.14	114.70	118.08
26	B	305	A86	O1-C15-C20	-2.14	57.31	59.40
28	E	308	DD6	C4-C3-C2	-2.14	119.09	123.47
21	b	833	BCR	C16-C17-C18	-2.14	124.25	127.31
18	E	309	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	b	849	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
21	b	833	BCR	C21-C20-C19	-2.14	116.55	123.22
18	b	842	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	b	804	CLA	O2D-CGD-CBD	2.14	115.06	111.27
18	b	850	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
21	a	834	BCR	C20-C19-C18	-2.13	120.42	126.42
21	l	201	BCR	C38-C26-C27	2.13	117.71	113.62
18	C	316	CLA	CAA-C2A-C3A	-2.13	111.13	116.10
18	H	311	CLA	CHB-C4A-NA	2.13	127.46	124.51
21	b	839	BCR	C33-C5-C6	-2.13	122.14	124.53
28	C	303	DD6	C25-C24-C1	-2.13	120.44	126.42
18	C	310	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	b	814	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	C	314	CLA	CAA-C2A-C3A	-2.13	111.14	116.10
29	H	312	KC1	O2D-CGD-O1D	-2.13	119.68	123.84
18	b	803	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
18	a	825	CLA	C6-C7-C8	-2.12	109.06	115.92
18	C	316	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	a	840	CLA	O2D-CGD-CBD	2.12	115.04	111.27
18	b	830	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	E	318	LMG	O3-C3-C2	-2.12	105.45	110.35
18	D	210	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
18	a	815	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
18	D	209	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
26	C	304	A86	C19-C18-C17	-2.12	106.68	110.77
18	b	841	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	E	310	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	b	827	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	a	837	CLA	CGD-CBD-CAD	-2.12	103.88	110.73
26	H	301	A86	O1-C15-C20	-2.12	57.33	59.40
18	a	804	CLA	O2A-CGA-O1A	-2.11	118.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	f	205	BCR	C23-C24-C25	-2.11	121.26	127.20
18	a	810	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	B	301	A86	O4-C38-O5	-2.11	118.77	122.96
28	H	303	DD6	O4-C34-C33	-2.11	105.61	109.80
18	b	846	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	H	314	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
26	B	302	A86	C4-C5-C6	2.11	130.32	127.31
26	H	304	A86	C17-C16-C15	2.11	111.31	109.16
18	b	825	CLA	O2A-CGA-O1A	-2.10	118.05	123.30
28	B	303	DD6	C33-C34-C35	-2.10	107.43	110.30
21	a	833	BCR	C21-C20-C19	-2.10	116.66	123.22
18	H	310	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
28	B	303	DD6	C10-C9-C8	-2.10	116.67	123.22
18	B	308	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
18	a	855	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	a	822	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	B	314	CLA	C2D-C1D-ND	-2.10	108.56	110.10
20	E	301	LHG	C26-C25-C24	2.09	120.72	113.19
23	a	851	LMG	O6-C5-C4	2.09	113.50	109.69
21	b	839	BCR	C16-C15-C14	-2.09	119.19	123.47
26	m	102	A86	O1-C15-C20	-2.09	57.35	59.40
26	B	304	A86	O1-C15-C20	-2.09	57.35	59.40
18	E	312	CLA	C11-C12-C13	-2.09	109.16	115.92
26	B	302	A86	C9-C8-C6	2.09	132.29	126.42
18	b	821	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	D	206	A86	O-C13-C11	-2.09	116.53	121.15
26	H	304	A86	O4-C38-O5	-2.09	118.81	122.96
18	a	820	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	a	824	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
21	E	306	BCR	C36-C18-C17	-2.09	120.00	122.92
18	B	308	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	m	102	A86	O-C13-C14	-2.09	117.42	121.66
18	H	306	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	B	305	A86	C-C1-C24	2.08	121.36	118.08
18	b	817	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	b	818	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	D	214	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	b	803	CLA	CBA-CAA-C2A	-2.08	107.72	113.86
28	B	303	DD6	C32-C31-C36	-2.08	119.69	122.63
18	a	807	CLA	CHB-C4A-NA	2.08	127.39	124.51
21	a	852	BCR	C36-C18-C17	-2.08	120.01	122.92
21	i	102	BCR	C8-C7-C6	-2.08	121.36	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	305	A86	C4-C5-C6	2.08	130.28	127.31
18	b	829	CLA	C11-C10-C8	-2.08	109.20	115.92
18	b	828	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	a	846	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	a	819	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	r	202	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
18	D	208	CLA	CHB-C4A-NA	2.07	127.38	124.51
18	b	838	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
28	E	307	DD6	C4-C3-C2	2.07	127.72	123.47
18	D	213	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
28	E	304	DD6	C10-C9-C8	-2.07	116.75	123.22
26	H	302	A86	C9-C8-C6	2.07	132.24	126.42
18	a	803	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	b	843	CLA	C2D-C1D-ND	-2.07	108.58	110.10
18	b	806	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	a	854	CLA	C2D-C1D-ND	-2.07	108.58	110.10
18	a	830	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	D	210	CLA	CHD-C1D-ND	-2.07	122.56	124.45
26	H	302	A86	C4-C5-C6	2.07	130.26	127.31
27	l	206	ET4	C27-C09-C08	2.07	121.33	118.08
18	f	203	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
18	H	306	CLA	CHD-C1D-ND	-2.07	122.56	124.45
21	f	201	BCR	C38-C26-C27	2.07	117.58	113.62
21	r	201	BCR	C21-C20-C19	-2.06	116.77	123.22
26	H	304	A86	O-C13-C14	-2.06	117.47	121.66
21	a	850	BCR	C23-C22-C21	2.06	122.11	118.94
18	B	307	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	a	802	CLA	C1-C2-C3	-2.06	122.48	126.04
29	H	312	KC1	CBA-CAA-C2A	-2.06	117.41	125.27
18	b	820	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
18	C	309	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
18	B	311	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	E	311	CLA	C2A-C1A-CHA	2.06	127.46	123.86
21	E	305	BCR	C36-C18-C19	2.06	121.32	118.08
18	a	814	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
18	a	807	CLA	CAA-CBA-CGA	-2.06	107.25	113.25
23	D	202	LMG	O7-C10-O9	-2.05	118.74	123.70
18	H	313	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
21	f	201	BCR	C8-C7-C6	-2.05	121.44	127.20
18	b	803	CLA	CHB-C4A-NA	2.05	127.35	124.51
18	f	202	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
18	E	312	CLA	CHD-C1D-ND	-2.05	122.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	303	DD6	C19-C18-C17	-2.05	106.82	110.77
26	H	301	A86	C12-C11-C10	-2.04	118.48	123.42
18	b	843	CLA	O1D-CGD-CBD	2.04	128.67	124.48
18	B	311	CLA	CAC-C3C-C4C	2.04	127.46	124.81
21	m	101	BCR	C38-C26-C25	-2.04	122.23	124.53
18	b	807	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	a	826	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	a	843	CLA	C2A-C1A-CHA	2.04	127.43	123.86
23	j	103	LMG	O6-C5-C6	2.04	111.51	106.44
21	E	305	BCR	C23-C24-C25	-2.04	121.47	127.20
21	a	833	BCR	C39-C30-C25	-2.04	107.00	110.30
21	a	833	BCR	C23-C24-C25	-2.03	121.49	127.20
28	C	303	DD6	C21-C20-C15	-2.03	118.85	122.26
18	b	849	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	b	845	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	E	313	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
21	a	852	BCR	C23-C24-C25	-2.03	121.50	127.20
26	m	102	A86	C28-C27-C26	-2.03	120.08	122.92
26	B	305	A86	O4-C38-O5	-2.03	118.93	122.96
21	a	845	BCR	C2-C3-C4	-2.03	106.84	111.38
26	D	206	A86	C9-C8-C6	2.03	132.11	126.42
26	B	304	A86	O4-C38-O5	-2.03	118.94	122.96
21	m	101	BCR	C36-C18-C17	-2.03	120.08	122.92
18	a	817	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
18	D	216	CLA	C2D-C1D-ND	-2.02	108.61	110.10
26	E	302	A86	O1-C15-C20	-2.02	57.42	59.40
18	a	841	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
28	E	308	DD6	C37-C36-C35	2.02	118.10	114.36
23	j	103	LMG	C6-C5-C4	-2.02	108.27	113.00
28	E	308	DD6	C34-C35-C36	-2.02	107.83	111.85
18	B	312	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	a	801	CLA	C16-C15-C13	-2.02	109.39	115.92
18	a	807	CLA	C3A-C2A-C1A	2.02	104.36	101.34
19	a	829	PQN	C11-C12-C13	-2.02	123.43	126.79
18	b	819	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	H	314	CLA	C16-C15-C13	-2.02	109.39	115.92
18	a	853	CLA	C1-C2-C3	-2.02	122.55	126.04
20	E	317	LHG	O8-C23-O10	-2.02	118.50	123.59
18	C	314	CLA	O2D-CGD-CBD	2.02	114.85	111.27
18	b	844	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	a	828	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
26	B	304	A86	C21-C20-C19	-2.01	112.01	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	852	BCR	C34-C9-C10	-2.01	120.10	122.92
20	H	316	LHG	O8-C23-C24	2.01	121.16	112.38
18	b	805	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	a	840	CLA	C6-C7-C8	-2.01	109.42	115.92
28	E	303	DD6	C12-C11-C10	-2.01	120.11	122.92
23	a	851	LMG	C3-C4-C5	2.01	113.83	110.24
18	a	853	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	a	834	BCR	C34-C9-C8	2.01	121.24	118.08
21	a	850	BCR	C8-C7-C6	-2.01	121.56	127.20
18	b	803	CLA	CMB-C2B-C3B	2.01	128.43	124.68
18	a	821	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
21	j	105	BCR	C33-C5-C4	2.00	117.47	113.62
18	i	101	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
18	l	203	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	C	307	CLA	CHD-C1D-ND	-2.00	122.61	124.45
28	E	303	DD6	C15-C14-C13	-2.00	121.76	125.99
18	C	309	CLA	O2D-CGD-CBD	2.00	114.83	111.27
18	r	202	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	D	204	A86	O1-C15-C20	-2.00	57.44	59.40
18	b	829	CLA	C16-C15-C13	-2.00	109.45	115.92
18	E	313	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	H	304	A86	C21-C20-C19	-2.00	112.03	114.28
18	a	821	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (142) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	a	801	CLA	ND
18	a	802	CLA	ND
18	a	803	CLA	ND
18	a	804	CLA	ND
18	a	805	CLA	ND
18	a	806	CLA	ND
18	a	807	CLA	ND
18	a	808	CLA	ND
18	a	809	CLA	ND
18	a	810	CLA	ND
18	a	811	CLA	ND
18	a	812	CLA	ND
18	a	813	CLA	ND
18	a	814	CLA	ND
18	a	815	CLA	ND

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Mol	Chain	Res	Type	Atom
18	a	816	CLA	ND
18	a	817	CLA	ND
18	a	818	CLA	ND
18	a	819	CLA	ND
18	a	820	CLA	ND
18	a	821	CLA	ND
18	a	822	CLA	ND
18	a	823	CLA	ND
18	a	824	CLA	ND
18	a	825	CLA	ND
18	a	826	CLA	ND
18	a	827	CLA	ND
18	a	828	CLA	ND
18	a	830	CLA	ND
18	a	836	CLA	ND
18	a	837	CLA	ND
18	a	838	CLA	ND
18	a	839	CLA	ND
18	a	840	CLA	ND
18	a	841	CLA	ND
18	a	842	CLA	ND
18	a	843	CLA	ND
18	a	844	CLA	ND
18	a	846	CLA	ND
18	a	847	CLA	ND
18	a	848	CLA	ND
18	a	853	CLA	ND
18	a	854	CLA	ND
18	a	855	CLA	ND
18	b	801	CLA	ND
18	b	803	CLA	ND
18	b	804	CLA	ND
18	b	805	CLA	ND
18	b	806	CLA	ND
18	b	807	CLA	ND
18	b	808	CLA	ND
18	b	809	CLA	ND
18	b	810	CLA	ND
18	b	811	CLA	ND
18	b	812	CLA	ND
18	b	813	CLA	ND
18	b	814	CLA	ND

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Mol	Chain	Res	Type	Atom
18	b	815	CLA	ND
18	b	816	CLA	ND
18	b	817	CLA	ND
18	b	818	CLA	ND
18	b	819	CLA	ND
18	b	820	CLA	ND
18	b	821	CLA	ND
18	b	822	CLA	ND
18	b	823	CLA	ND
18	b	824	CLA	ND
18	b	825	CLA	ND
18	b	826	CLA	ND
18	b	827	CLA	ND
18	b	828	CLA	ND
18	b	829	CLA	ND
18	b	830	CLA	ND
18	b	837	CLA	ND
18	b	838	CLA	ND
18	b	840	CLA	ND
18	b	841	CLA	ND
18	b	842	CLA	ND
18	b	843	CLA	ND
18	b	844	CLA	ND
18	b	845	CLA	ND
18	b	846	CLA	ND
18	b	848	CLA	ND
18	b	849	CLA	ND
18	b	850	CLA	ND
18	f	202	CLA	ND
18	f	203	CLA	ND
18	f	204	CLA	ND
18	i	101	CLA	ND
18	j	104	CLA	ND
18	l	202	CLA	ND
18	l	203	CLA	ND
18	l	205	CLA	ND
18	r	202	CLA	ND
18	B	306	CLA	ND
18	B	307	CLA	ND
18	B	308	CLA	ND
18	B	309	CLA	ND
18	B	310	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	311	CLA	ND
18	B	312	CLA	ND
18	B	314	CLA	ND
18	C	306	CLA	ND
18	C	307	CLA	ND
18	C	309	CLA	ND
18	C	310	CLA	ND
18	C	311	CLA	ND
18	C	312	CLA	ND
18	C	314	CLA	ND
18	C	315	CLA	ND
18	C	316	CLA	ND
18	C	317	CLA	ND
18	C	318	CLA	ND
18	D	207	CLA	ND
18	D	208	CLA	ND
18	D	209	CLA	ND
18	D	210	CLA	ND
18	D	211	CLA	ND
18	D	212	CLA	ND
18	D	213	CLA	ND
18	D	214	CLA	ND
18	D	215	CLA	ND
18	D	216	CLA	ND
18	D	217	CLA	ND
18	E	309	CLA	ND
18	E	310	CLA	ND
18	E	311	CLA	ND
18	E	312	CLA	ND
18	E	313	CLA	ND
18	E	314	CLA	ND
18	E	315	CLA	ND
18	E	316	CLA	ND
18	H	305	CLA	ND
18	H	306	CLA	ND
18	H	307	CLA	ND
18	H	308	CLA	ND
18	H	309	CLA	ND
18	H	310	CLA	ND
18	H	311	CLA	ND
18	H	313	CLA	ND
18	H	314	CLA	ND

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Mol	Chain	Res	Type	Atom
18	H	315	CLA	ND

All (2052) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	801	CLA	CBD-CGD-O2D-CED
18	a	801	CLA	O1D-CGD-O2D-CED
18	a	802	CLA	CHA-CBD-CGD-O1D
18	a	802	CLA	CHA-CBD-CGD-O2D
18	a	803	CLA	CHA-CBD-CGD-O1D
18	a	803	CLA	CHA-CBD-CGD-O2D
18	a	804	CLA	C1A-C2A-CAA-CBA
18	a	804	CLA	C3A-C2A-CAA-CBA
18	a	805	CLA	C3A-C2A-CAA-CBA
18	a	809	CLA	C2A-CAA-CBA-CGA
18	a	809	CLA	CHA-CBD-CGD-O1D
18	a	809	CLA	CHA-CBD-CGD-O2D
18	a	813	CLA	C1A-C2A-CAA-CBA
18	a	813	CLA	CHA-CBD-CGD-O1D
18	a	813	CLA	CHA-CBD-CGD-O2D
18	a	814	CLA	C3A-C2A-CAA-CBA
18	a	815	CLA	C1A-C2A-CAA-CBA
18	a	815	CLA	C3A-C2A-CAA-CBA
18	a	816	CLA	C1A-C2A-CAA-CBA
18	a	816	CLA	C3A-C2A-CAA-CBA
18	a	821	CLA	C1A-C2A-CAA-CBA
18	a	821	CLA	C3A-C2A-CAA-CBA
18	a	823	CLA	C1A-C2A-CAA-CBA
18	a	823	CLA	C3A-C2A-CAA-CBA
18	a	823	CLA	CHA-CBD-CGD-O1D
18	a	823	CLA	CHA-CBD-CGD-O2D
18	a	824	CLA	C1A-C2A-CAA-CBA
18	a	824	CLA	CHA-CBD-CGD-O1D
18	a	824	CLA	CHA-CBD-CGD-O2D
18	a	827	CLA	CHA-CBD-CGD-O1D
18	a	828	CLA	CHA-CBD-CGD-O1D
18	a	828	CLA	CHA-CBD-CGD-O2D
18	a	828	CLA	CAD-CBD-CGD-O1D
18	a	837	CLA	C1A-C2A-CAA-CBA
18	a	837	CLA	C3A-C2A-CAA-CBA
18	a	837	CLA	CHA-CBD-CGD-O2D
18	a	838	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	a	841	CLA	CHA-CBD-CGD-O1D
18	a	841	CLA	CHA-CBD-CGD-O2D
18	a	841	CLA	CAD-CBD-CGD-O1D
18	a	841	CLA	C11-C12-C13-C14
18	a	844	CLA	C1A-C2A-CAA-CBA
18	a	844	CLA	C3A-C2A-CAA-CBA
18	a	846	CLA	C1A-C2A-CAA-CBA
18	a	846	CLA	C3A-C2A-CAA-CBA
18	a	847	CLA	C2A-CAA-CBA-CGA
18	a	853	CLA	CHA-CBD-CGD-O1D
18	a	853	CLA	CHA-CBD-CGD-O2D
18	a	853	CLA	CAD-CBD-CGD-O1D
18	a	854	CLA	CBD-CGD-O2D-CED
18	a	854	CLA	C2-C3-C5-C6
18	a	854	CLA	C4-C3-C5-C6
18	b	801	CLA	C2A-CAA-CBA-CGA
18	b	803	CLA	CHA-CBD-CGD-O1D
18	b	803	CLA	CHA-CBD-CGD-O2D
18	b	803	CLA	CBD-CGD-O2D-CED
18	b	805	CLA	C3A-C2A-CAA-CBA
18	b	806	CLA	CBD-CGD-O2D-CED
18	b	809	CLA	C1A-C2A-CAA-CBA
18	b	812	CLA	O1A-CGA-O2A-C1
18	b	813	CLA	CHA-CBD-CGD-O1D
18	b	813	CLA	CHA-CBD-CGD-O2D
18	b	813	CLA	CAD-CBD-CGD-O1D
18	b	814	CLA	C1A-C2A-CAA-CBA
18	b	814	CLA	C3A-C2A-CAA-CBA
18	b	817	CLA	C1A-C2A-CAA-CBA
18	b	817	CLA	C3A-C2A-CAA-CBA
18	b	817	CLA	CHA-CBD-CGD-O1D
18	b	817	CLA	CHA-CBD-CGD-O2D
18	b	818	CLA	C1A-C2A-CAA-CBA
18	b	818	CLA	C3A-C2A-CAA-CBA
18	b	819	CLA	C1A-C2A-CAA-CBA
18	b	819	CLA	C3A-C2A-CAA-CBA
18	b	819	CLA	CHA-CBD-CGD-O1D
18	b	819	CLA	CHA-CBD-CGD-O2D
18	b	820	CLA	CHA-CBD-CGD-O2D
18	b	820	CLA	C11-C12-C13-C14
18	b	821	CLA	C1A-C2A-CAA-CBA
18	b	821	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	b	822	CLA	C1A-C2A-CAA-CBA
18	b	822	CLA	C3A-C2A-CAA-CBA
18	b	823	CLA	C1A-C2A-CAA-CBA
18	b	824	CLA	C1A-C2A-CAA-CBA
18	b	840	CLA	CHA-CBD-CGD-O2D
18	b	841	CLA	C1A-C2A-CAA-CBA
18	b	841	CLA	C3A-C2A-CAA-CBA
18	b	841	CLA	CBD-CGD-O2D-CED
18	b	843	CLA	C4-C3-C5-C6
18	b	844	CLA	C1A-C2A-CAA-CBA
18	b	845	CLA	C1A-C2A-CAA-CBA
18	b	845	CLA	C3A-C2A-CAA-CBA
18	b	849	CLA	C2-C3-C5-C6
18	b	849	CLA	C4-C3-C5-C6
18	f	202	CLA	CBD-CGD-O2D-CED
18	l	203	CLA	C2-C3-C5-C6
18	l	203	CLA	C4-C3-C5-C6
18	l	203	CLA	C11-C10-C8-C9
18	r	202	CLA	C1A-C2A-CAA-CBA
18	r	202	CLA	C3A-C2A-CAA-CBA
18	r	202	CLA	CBD-CGD-O2D-CED
18	B	306	CLA	C1A-C2A-CAA-CBA
18	B	306	CLA	C3A-C2A-CAA-CBA
18	B	309	CLA	C4-C3-C5-C6
18	B	310	CLA	CBA-CGA-O2A-C1
18	B	310	CLA	CBD-CGD-O2D-CED
18	B	310	CLA	O1D-CGD-O2D-CED
18	B	311	CLA	CBD-CGD-O2D-CED
18	B	312	CLA	C3A-C2A-CAA-CBA
18	B	314	CLA	CBD-CGD-O2D-CED
18	C	306	CLA	CHA-CBD-CGD-O1D
18	C	306	CLA	CHA-CBD-CGD-O2D
18	C	310	CLA	CBA-CGA-O2A-C1
18	C	310	CLA	CBD-CGD-O2D-CED
18	C	311	CLA	CBD-CGD-O2D-CED
18	C	312	CLA	C3A-C2A-CAA-CBA
18	C	315	CLA	C1A-C2A-CAA-CBA
18	C	316	CLA	CHA-CBD-CGD-O1D
18	C	317	CLA	C1A-C2A-CAA-CBA
18	C	317	CLA	CHA-CBD-CGD-O1D
18	C	318	CLA	C1A-C2A-CAA-CBA
18	C	318	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	D	213	CLA	C2A-CAA-CBA-CGA
18	D	215	CLA	CBD-CGD-O2D-CED
18	D	216	CLA	C1A-C2A-CAA-CBA
18	D	216	CLA	C3A-C2A-CAA-CBA
18	E	311	CLA	CBA-CGA-O2A-C1
18	E	311	CLA	O1A-CGA-O2A-C1
18	E	311	CLA	CHA-CBD-CGD-O1D
18	E	311	CLA	CHA-CBD-CGD-O2D
18	E	315	CLA	CHA-CBD-CGD-O1D
18	E	315	CLA	CHA-CBD-CGD-O2D
18	E	315	CLA	CAD-CBD-CGD-O1D
18	H	305	CLA	C1A-C2A-CAA-CBA
18	H	305	CLA	C3A-C2A-CAA-CBA
18	H	305	CLA	C2A-CAA-CBA-CGA
18	H	311	CLA	C1A-C2A-CAA-CBA
18	H	311	CLA	C3A-C2A-CAA-CBA
18	H	313	CLA	CHA-CBD-CGD-O1D
18	H	313	CLA	CHA-CBD-CGD-O2D
18	H	314	CLA	C2-C3-C5-C6
18	H	314	CLA	C4-C3-C5-C6
18	H	315	CLA	CBD-CGD-O2D-CED
18	H	315	CLA	O1D-CGD-O2D-CED
19	a	829	PQN	C12-C13-C15-C16
19	a	829	PQN	C14-C13-C15-C16
20	a	832	LHG	C3-O3-P-O4
20	a	832	LHG	C4-O6-P-O3
20	a	832	LHG	C8-C7-O7-C5
20	B	315	LHG	O1-C1-C2-C3
20	B	315	LHG	C3-O3-P-O4
20	B	315	LHG	C4-O6-P-O4
20	D	201	LHG	C3-O3-P-O4
20	D	201	LHG	C3-O3-P-O5
20	D	201	LHG	C3-O3-P-O6
20	E	301	LHG	C2-C3-O3-P
20	H	316	LHG	C4-O6-P-O3
20	H	316	LHG	C4-O6-P-O4
20	H	316	LHG	C4-O6-P-O5
20	H	316	LHG	C8-C7-O7-C5
21	a	834	BCR	C37-C22-C23-C24
21	a	845	BCR	C23-C24-C25-C26
21	a	845	BCR	C23-C24-C25-C30
21	a	850	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	a	850	BCR	C5-C6-C7-C8
21	a	852	BCR	C5-C6-C7-C8
21	b	836	BCR	C7-C8-C9-C10
21	b	836	BCR	C7-C8-C9-C34
21	b	836	BCR	C19-C20-C21-C22
21	b	836	BCR	C21-C22-C23-C24
21	b	836	BCR	C37-C22-C23-C24
21	b	839	BCR	C23-C24-C25-C26
21	b	839	BCR	C23-C24-C25-C30
21	f	201	BCR	C5-C6-C7-C8
21	f	201	BCR	C17-C18-C19-C20
21	f	201	BCR	C36-C18-C19-C20
21	f	201	BCR	C21-C22-C23-C24
21	f	201	BCR	C37-C22-C23-C24
21	i	103	BCR	C21-C22-C23-C24
21	i	103	BCR	C37-C22-C23-C24
21	j	105	BCR	C21-C22-C23-C24
21	j	105	BCR	C37-C22-C23-C24
21	l	204	BCR	C1-C6-C7-C8
21	l	204	BCR	C21-C22-C23-C24
21	l	204	BCR	C37-C22-C23-C24
21	m	101	BCR	C7-C8-C9-C10
21	m	101	BCR	C7-C8-C9-C34
22	a	849	SQD	O49-C7-O47-C45
22	a	849	SQD	O5-C5-C6-S
22	a	849	SQD	C5-C6-S-O7
23	a	851	LMG	O7-C8-C9-O8
23	j	103	LMG	O10-C28-O8-C9
23	j	103	LMG	C29-C28-O8-C9
23	l	207	LMG	O6-C1-O1-C7
23	l	207	LMG	O7-C8-C9-O8
23	l	207	LMG	C11-C10-O7-C8
23	C	301	LMG	O6-C1-O1-C7
23	D	202	LMG	C2-C1-O1-C7
23	D	202	LMG	O6-C1-O1-C7
23	E	318	LMG	O7-C8-C9-O8
26	b	847	A86	C-C1-C24-C25
26	b	847	A86	C2-C1-C24-C25
26	b	847	A86	C11-C10-C9-C8
26	m	102	A86	C39-C38-O4-C34
26	B	301	A86	C26-C27-C29-C30
26	B	301	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
26	B	302	A86	C39-C38-O4-C34
26	B	302	A86	O5-C38-O4-C34
26	B	305	A86	C1-C2-C3-C4
26	C	304	A86	C35-C34-O4-C38
26	C	305	A86	C1-C2-C3-C4
26	D	203	A86	C-C1-C24-C25
26	D	203	A86	C2-C1-C24-C25
26	D	203	A86	O5-C38-O4-C34
26	D	206	A86	C1-C2-C3-C4
26	D	206	A86	C39-C38-O4-C34
26	D	206	A86	O5-C38-O4-C34
26	E	302	A86	C1-C2-C3-C4
26	E	302	A86	C35-C34-O4-C38
26	H	301	A86	O5-C38-O4-C34
26	H	302	A86	C39-C38-O4-C34
26	H	302	A86	O5-C38-O4-C34
27	I	206	ET4	C05-C06-C07-C08
28	E	303	DD6	C10-C11-C13-C14
28	E	303	DD6	C12-C11-C13-C14
28	E	304	DD6	C13-C14-C15-C16
28	E	304	DD6	C13-C14-C15-O1
28	E	307	DD6	C13-C14-C15-C16
28	E	307	DD6	C13-C14-C15-C20
28	E	307	DD6	C13-C14-C15-O1
28	E	307	DD6	C5-C6-C8-C9
28	E	307	DD6	C7-C6-C8-C9
28	H	303	DD6	C27-C29-C30-C31
29	B	313	KC1	C2A-CAA-CBA-CGA
29	B	313	KC1	CHA-CBD-CGD-O1D
29	B	313	KC1	CBD-CGD-O2D-CED
29	C	308	KC1	C1A-C2A-CAA-CBA
29	C	308	KC1	C3A-C2A-CAA-CBA
29	C	308	KC1	C2B-C3B-CAB-CBB
29	C	308	KC1	C4B-C3B-CAB-CBB
29	C	308	KC1	C2A-CAA-CBA-CGA
29	C	308	KC1	CHA-CBD-CGD-O1D
29	C	313	KC1	C1A-C2A-CAA-CBA
29	C	313	KC1	C3A-C2A-CAA-CBA
29	C	313	KC1	C2B-C3B-CAB-CBB
29	C	313	KC1	C4B-C3B-CAB-CBB
18	a	813	CLA	C2C-C3C-CAC-CBC
26	B	301	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
26	C	302	A86	C39-C38-O4-C34
26	C	305	A86	O5-C38-O4-C34
26	D	203	A86	C39-C38-O4-C34
26	E	302	A86	C39-C38-O4-C34
26	H	301	A86	C39-C38-O4-C34
18	B	311	CLA	O1D-CGD-O2D-CED
18	B	314	CLA	O1D-CGD-O2D-CED
18	C	311	CLA	O1D-CGD-O2D-CED
18	C	314	CLA	O1D-CGD-O2D-CED
26	B	301	A86	O5-C38-O4-C34
26	C	302	A86	O5-C38-O4-C34
26	C	304	A86	C39-C38-O4-C34
26	C	305	A86	C39-C38-O4-C34
18	a	802	CLA	O1D-CGD-O2D-CED
18	b	806	CLA	O1D-CGD-O2D-CED
18	j	104	CLA	O1D-CGD-O2D-CED
18	a	802	CLA	CBD-CGD-O2D-CED
18	a	821	CLA	CBD-CGD-O2D-CED
18	a	853	CLA	CBD-CGD-O2D-CED
18	b	813	CLA	CBD-CGD-O2D-CED
18	j	104	CLA	CBD-CGD-O2D-CED
18	B	307	CLA	CBD-CGD-O2D-CED
18	B	312	CLA	CBD-CGD-O2D-CED
18	C	314	CLA	CBD-CGD-O2D-CED
18	C	315	CLA	CBD-CGD-O2D-CED
18	D	211	CLA	CBD-CGD-O2D-CED
18	D	217	CLA	CBD-CGD-O2D-CED
18	E	309	CLA	CBD-CGD-O2D-CED
18	E	315	CLA	CBD-CGD-O2D-CED
18	E	315	CLA	O1A-CGA-O2A-C1
20	j	102	LHG	O10-C23-O8-C6
18	B	310	CLA	O1A-CGA-O2A-C1
18	C	310	CLA	O1A-CGA-O2A-C1
18	b	813	CLA	O1D-CGD-O2D-CED
18	D	217	CLA	O1D-CGD-O2D-CED
18	a	813	CLA	C4C-C3C-CAC-CBC
26	H	304	A86	C39-C38-O4-C34
18	a	854	CLA	O1D-CGD-O2D-CED
18	b	803	CLA	O1D-CGD-O2D-CED
18	C	310	CLA	O1D-CGD-O2D-CED
18	D	215	CLA	O1D-CGD-O2D-CED
18	E	315	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	j	102	LHG	C24-C23-O8-C6
18	a	811	CLA	CBD-CGD-O2D-CED
18	a	828	CLA	CBD-CGD-O2D-CED
18	a	841	CLA	CBD-CGD-O2D-CED
18	a	842	CLA	CBD-CGD-O2D-CED
18	a	844	CLA	CBD-CGD-O2D-CED
18	b	815	CLA	CBD-CGD-O2D-CED
18	b	816	CLA	CBD-CGD-O2D-CED
18	b	817	CLA	CBD-CGD-O2D-CED
18	b	822	CLA	CBD-CGD-O2D-CED
18	b	830	CLA	CBD-CGD-O2D-CED
18	C	317	CLA	CBD-CGD-O2D-CED
18	C	318	CLA	CBD-CGD-O2D-CED
18	E	313	CLA	CBD-CGD-O2D-CED
18	C	317	CLA	C2C-C3C-CAC-CBC
18	a	804	CLA	O1A-CGA-O2A-C1
18	a	811	CLA	O1A-CGA-O2A-C1
18	a	813	CLA	O1A-CGA-O2A-C1
18	a	815	CLA	O1A-CGA-O2A-C1
18	a	817	CLA	O1A-CGA-O2A-C1
18	a	838	CLA	O1A-CGA-O2A-C1
18	a	839	CLA	O1A-CGA-O2A-C1
18	b	813	CLA	O1A-CGA-O2A-C1
18	b	826	CLA	O1A-CGA-O2A-C1
18	b	849	CLA	O1A-CGA-O2A-C1
18	E	313	CLA	O1A-CGA-O2A-C1
18	H	305	CLA	O1A-CGA-O2A-C1
20	a	835	LHG	O10-C23-O8-C6
23	C	319	LMG	O10-C28-O8-C9
18	f	202	CLA	O1D-CGD-O2D-CED
18	r	202	CLA	O1D-CGD-O2D-CED
26	E	302	A86	O5-C38-O4-C34
18	b	841	CLA	O1D-CGD-O2D-CED
18	a	823	CLA	CBD-CGD-O2D-CED
18	b	805	CLA	CBD-CGD-O2D-CED
18	b	837	CLA	CBD-CGD-O2D-CED
18	D	211	CLA	O1D-CGD-O2D-CED
20	a	832	LHG	O9-C7-O7-C5
20	H	316	LHG	O9-C7-O7-C5
23	l	207	LMG	O9-C10-O7-C8
26	B	305	A86	C39-C38-O4-C34
18	a	807	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	a	837	CLA	C3-C5-C6-C7
18	a	839	CLA	C3-C5-C6-C7
18	b	806	CLA	C3-C5-C6-C7
18	b	822	CLA	C3-C5-C6-C7
18	b	837	CLA	C3-C5-C6-C7
18	b	846	CLA	C3-C5-C6-C7
18	C	309	CLA	C3-C5-C6-C7
18	C	312	CLA	C3-C5-C6-C7
18	E	309	CLA	C3-C5-C6-C7
18	a	804	CLA	CBA-CGA-O2A-C1
18	a	811	CLA	CBA-CGA-O2A-C1
18	a	813	CLA	CBA-CGA-O2A-C1
18	a	817	CLA	CBA-CGA-O2A-C1
18	a	839	CLA	CBA-CGA-O2A-C1
18	b	812	CLA	CBA-CGA-O2A-C1
18	b	813	CLA	CBA-CGA-O2A-C1
18	b	826	CLA	CBA-CGA-O2A-C1
18	b	849	CLA	CBA-CGA-O2A-C1
18	H	305	CLA	CBA-CGA-O2A-C1
18	a	803	CLA	C5-C6-C7-C8
18	C	315	CLA	O1D-CGD-O2D-CED
18	C	309	CLA	CBD-CGD-O2D-CED
18	H	313	CLA	CBD-CGD-O2D-CED
18	H	314	CLA	CBD-CGD-O2D-CED
18	H	305	CLA	C2C-C3C-CAC-CBC
26	m	102	A86	O5-C38-O4-C34
29	B	313	KC1	CAA-CBA-CGA-O1A
29	B	313	KC1	CAA-CBA-CGA-O2A
26	b	847	A86	C39-C38-O4-C34
18	a	847	CLA	C4-C3-C5-C6
18	a	848	CLA	C4-C3-C5-C6
18	b	829	CLA	C4-C3-C5-C6
18	a	848	CLA	C2-C3-C5-C6
18	b	843	CLA	C2-C3-C5-C6
18	B	309	CLA	C2-C3-C5-C6
18	a	806	CLA	CBD-CGD-O2D-CED
18	a	836	CLA	CBD-CGD-O2D-CED
18	a	837	CLA	CBD-CGD-O2D-CED
18	b	850	CLA	CBD-CGD-O2D-CED
18	a	841	CLA	C2A-CAA-CBA-CGA
18	b	808	CLA	C2A-CAA-CBA-CGA
18	b	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	306	CLA	C2A-CAA-CBA-CGA
18	C	310	CLA	C2A-CAA-CBA-CGA
18	D	216	CLA	C2A-CAA-CBA-CGA
18	b	844	CLA	O1A-CGA-O2A-C1
20	a	831	LHG	C24-C25-C26-C27
20	a	835	LHG	C24-C25-C26-C27
20	b	835	LHG	C24-C25-C26-C27
20	D	201	LHG	C24-C25-C26-C27
20	E	301	LHG	C24-C25-C26-C27
23	a	851	LMG	C31-C32-C33-C34
18	a	836	CLA	C3-C5-C6-C7
18	b	840	CLA	C3-C5-C6-C7
18	D	213	CLA	C3-C5-C6-C7
18	H	307	CLA	C3-C5-C6-C7
18	H	311	CLA	C3-C5-C6-C7
18	a	803	CLA	CBA-CGA-O2A-C1
18	a	815	CLA	CBA-CGA-O2A-C1
18	a	822	CLA	CBA-CGA-O2A-C1
18	a	825	CLA	CBA-CGA-O2A-C1
18	a	838	CLA	CBA-CGA-O2A-C1
18	a	847	CLA	CBA-CGA-O2A-C1
18	a	853	CLA	CBA-CGA-O2A-C1
18	b	821	CLA	CBA-CGA-O2A-C1
18	B	308	CLA	CBA-CGA-O2A-C1
18	D	207	CLA	CBA-CGA-O2A-C1
18	E	313	CLA	CBA-CGA-O2A-C1
20	a	835	LHG	C24-C23-O8-C6
23	C	319	LMG	C29-C28-O8-C9
20	D	201	LHG	C15-C16-C17-C18
20	D	201	LHG	C30-C31-C32-C33
18	a	822	CLA	CBD-CGD-O2D-CED
18	b	826	CLA	CBD-CGD-O2D-CED
18	C	317	CLA	C4C-C3C-CAC-CBC
18	a	853	CLA	O1D-CGD-O2D-CED
18	B	307	CLA	O1D-CGD-O2D-CED
23	E	318	LMG	C4-C5-C6-O5
18	a	822	CLA	O1A-CGA-O2A-C1
18	a	847	CLA	O1A-CGA-O2A-C1
18	a	848	CLA	O1A-CGA-O2A-C1
18	b	815	CLA	CBA-CGA-O2A-C1
26	b	847	A86	C24-C25-C26-C27
26	r	203	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	r	203	A86	C24-C25-C26-C27
26	B	302	A86	C1-C2-C3-C4
26	B	304	A86	C1-C2-C3-C4
26	C	302	A86	C1-C2-C3-C4
26	H	301	A86	C1-C2-C3-C4
26	H	302	A86	C1-C2-C3-C4
26	H	304	A86	C1-C2-C3-C4
28	C	303	DD6	C1-C2-C3-C4
26	r	203	A86	C39-C38-O4-C34
26	C	304	A86	O5-C38-O4-C34
18	a	805	CLA	CBD-CGD-O2D-CED
18	a	824	CLA	CBD-CGD-O2D-CED
18	a	848	CLA	CBD-CGD-O2D-CED
18	a	855	CLA	CBD-CGD-O2D-CED
18	D	208	CLA	CBD-CGD-O2D-CED
18	a	821	CLA	O1D-CGD-O2D-CED
18	B	312	CLA	O1D-CGD-O2D-CED
20	a	835	LHG	O2-C2-C3-O3
18	a	801	CLA	C3-C5-C6-C7
18	b	814	CLA	C3-C5-C6-C7
18	a	841	CLA	CBA-CGA-O2A-C1
18	b	844	CLA	CBA-CGA-O2A-C1
18	B	311	CLA	CBA-CGA-O2A-C1
18	E	312	CLA	CBA-CGA-O2A-C1
20	b	835	LHG	C8-C7-O7-C5
26	r	203	A86	O5-C38-O4-C34
18	a	812	CLA	CBD-CGD-O2D-CED
18	b	818	CLA	CBD-CGD-O2D-CED
18	b	848	CLA	CBD-CGD-O2D-CED
20	b	835	LHG	C27-C28-C29-C30
20	D	201	LHG	C13-C14-C15-C16
18	a	803	CLA	O1A-CGA-O2A-C1
18	E	312	CLA	O1A-CGA-O2A-C1
20	D	201	LHG	C11-C12-C13-C14
23	l	207	LMG	C21-C22-C23-C24
23	C	319	LMG	C13-C14-C15-C16
20	b	835	LHG	C13-C14-C15-C16
23	C	319	LMG	C11-C12-C13-C14
18	a	847	CLA	CBD-CGD-O2D-CED
18	l	205	CLA	CBD-CGD-O2D-CED
18	B	311	CLA	C3-C5-C6-C7
18	a	848	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	E	309	CLA	O1D-CGD-O2D-CED
20	b	835	LHG	O9-C7-O7-C5
18	a	825	CLA	O1A-CGA-O2A-C1
18	a	841	CLA	O1A-CGA-O2A-C1
18	b	821	CLA	O1A-CGA-O2A-C1
18	B	311	CLA	O1A-CGA-O2A-C1
18	D	207	CLA	O1A-CGA-O2A-C1
18	b	815	CLA	O1A-CGA-O2A-C1
23	E	318	LMG	O6-C5-C6-O5
18	a	825	CLA	C4-C3-C5-C6
18	a	841	CLA	C4-C3-C5-C6
18	B	311	CLA	C4-C3-C5-C6
18	D	207	CLA	C4-C3-C5-C6
18	H	307	CLA	C4-C3-C5-C6
18	H	310	CLA	C4-C3-C5-C6
19	b	831	PQN	C14-C13-C15-C16
18	a	825	CLA	C2-C3-C5-C6
18	a	841	CLA	C2-C3-C5-C6
18	b	829	CLA	C2-C3-C5-C6
18	B	311	CLA	C2-C3-C5-C6
18	D	207	CLA	C2-C3-C5-C6
18	H	307	CLA	C2-C3-C5-C6
18	H	310	CLA	C2-C3-C5-C6
18	b	819	CLA	C2A-CAA-CBA-CGA
18	a	853	CLA	O1A-CGA-O2A-C1
18	B	308	CLA	O1A-CGA-O2A-C1
18	E	315	CLA	O1D-CGD-O2D-CED
18	b	842	CLA	CBA-CGA-O2A-C1
18	b	824	CLA	CBD-CGD-O2D-CED
18	C	312	CLA	CBD-CGD-O2D-CED
18	C	318	CLA	O1D-CGD-O2D-CED
25	b	834	DGD	O6E-C5E-C6E-O5E
18	E	313	CLA	O1D-CGD-O2D-CED
20	B	315	LHG	C8-C7-O7-C5
23	j	103	LMG	O6-C5-C6-O5
18	H	305	CLA	C4C-C3C-CAC-CBC
23	E	318	LMG	C16-C17-C18-C19
18	b	815	CLA	O1D-CGD-O2D-CED
29	H	312	KC1	O1D-CGD-O2D-CED
20	a	835	LHG	C1-C2-C3-O3
20	B	315	LHG	C1-C2-C3-O3
20	D	201	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
20	H	316	LHG	C1-C2-C3-O3
18	b	842	CLA	O1A-CGA-O2A-C1
18	b	820	CLA	C3-C5-C6-C7
18	H	313	CLA	C3-C5-C6-C7
18	b	822	CLA	O1D-CGD-O2D-CED
18	a	806	CLA	CBA-CGA-O2A-C1
18	a	824	CLA	CBA-CGA-O2A-C1
18	b	801	CLA	CBA-CGA-O2A-C1
18	E	309	CLA	CBA-CGA-O2A-C1
20	E	301	LHG	C24-C23-O8-C6
23	l	207	LMG	C29-C28-O8-C9
18	a	817	CLA	CBD-CGD-O2D-CED
23	j	103	LMG	C4-C5-C6-O5
23	C	301	LMG	C4-C5-C6-O5
26	b	847	A86	C1-C2-C3-C4
26	H	304	A86	O5-C38-O4-C34
18	a	813	CLA	C10-C11-C12-C13
20	E	301	LHG	C34-C35-C36-C37
18	a	810	CLA	C15-C16-C17-C18
18	a	813	CLA	C13-C15-C16-C17
18	a	825	CLA	C8-C10-C11-C12
18	a	840	CLA	C15-C16-C17-C18
18	a	841	CLA	C5-C6-C7-C8
20	H	316	LHG	O2-C2-C3-O3
23	l	207	LMG	C2-C1-O1-C7
18	a	824	CLA	O1A-CGA-O2A-C1
18	a	847	CLA	C2-C3-C5-C6
18	a	813	CLA	C6-C7-C8-C9
18	a	813	CLA	C11-C12-C13-C14
18	a	813	CLA	C14-C13-C15-C16
18	a	854	CLA	C6-C7-C8-C9
18	b	803	CLA	C11-C12-C13-C14
18	b	837	CLA	C11-C10-C8-C9
18	b	843	CLA	C11-C10-C8-C9
18	i	101	CLA	C11-C10-C8-C9
18	B	308	CLA	C11-C12-C13-C14
18	C	311	CLA	C11-C10-C8-C9
18	D	207	CLA	C11-C10-C8-C9
18	D	208	CLA	C11-C10-C8-C9
18	H	306	CLA	C11-C12-C13-C14
18	H	307	CLA	C6-C7-C8-C9
18	H	313	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	H	313	CLA	C14-C13-C15-C16
18	a	811	CLA	O1D-CGD-O2D-CED
18	a	828	CLA	O1D-CGD-O2D-CED
18	a	841	CLA	O1D-CGD-O2D-CED
18	a	827	CLA	CBD-CGD-O2D-CED
21	a	852	BCR	C11-C12-C13-C35
21	a	852	BCR	C36-C18-C19-C20
21	b	833	BCR	C7-C8-C9-C34
21	b	839	BCR	C7-C8-C9-C34
21	j	101	BCR	C37-C22-C23-C24
21	j	105	BCR	C36-C18-C19-C20
21	m	101	BCR	C37-C22-C23-C24
26	b	847	A86	C7-C6-C8-C9
26	B	301	A86	C-C1-C24-C25
28	C	303	DD6	C12-C11-C13-C14
28	E	304	DD6	C12-C11-C13-C14
28	H	303	DD6	C12-C11-C13-C14
21	a	834	BCR	C21-C22-C23-C24
21	a	852	BCR	C11-C12-C13-C14
21	b	839	BCR	C7-C8-C9-C10
21	j	101	BCR	C21-C22-C23-C24
21	m	101	BCR	C21-C22-C23-C24
26	b	847	A86	C5-C6-C8-C9
26	B	301	A86	C2-C1-C24-C25
28	C	303	DD6	C10-C11-C13-C14
28	E	304	DD6	C10-C11-C13-C14
28	H	303	DD6	C10-C11-C13-C14
23	C	319	LMG	C28-C29-C30-C31
23	D	202	LMG	C28-C29-C30-C31
18	b	811	CLA	C10-C11-C12-C13
18	C	311	CLA	C10-C11-C12-C13
18	H	306	CLA	C8-C10-C11-C12
18	H	313	CLA	C10-C11-C12-C13
22	a	849	SQD	C28-C29-C30-C31
29	H	312	KC1	C2C-C3C-CAC-CBC
18	H	311	CLA	C8-C10-C11-C12
18	H	314	CLA	CBA-CGA-O2A-C1
23	D	202	LMG	C29-C28-O8-C9
18	a	854	CLA	C5-C6-C7-C8
18	b	803	CLA	C10-C11-C12-C13
18	b	850	CLA	C13-C15-C16-C17
23	j	103	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	a	806	CLA	C8-C10-C11-C12
18	a	813	CLA	C8-C10-C11-C12
18	a	813	CLA	C15-C16-C17-C18
18	a	836	CLA	C8-C10-C11-C12
18	a	838	CLA	C5-C6-C7-C8
18	b	807	CLA	C10-C11-C12-C13
18	b	823	CLA	C5-C6-C7-C8
18	b	824	CLA	C13-C15-C16-C17
18	b	849	CLA	C13-C15-C16-C17
18	l	203	CLA	C8-C10-C11-C12
18	D	208	CLA	C8-C10-C11-C12
18	D	213	CLA	C8-C10-C11-C12
18	E	312	CLA	C5-C6-C7-C8
18	E	312	CLA	C15-C16-C17-C18
20	D	201	LHG	C26-C27-C28-C29
18	b	817	CLA	O1D-CGD-O2D-CED
20	B	315	LHG	O1-C1-C2-O2
22	a	849	SQD	O5-C1-O6-C44
22	a	849	SQD	O6-C1-O5-C5
20	b	835	LHG	C7-C8-C9-C10
20	B	315	LHG	C7-C8-C9-C10
23	a	851	LMG	C10-C11-C12-C13
23	l	207	LMG	C10-C11-C12-C13
18	b	823	CLA	CBD-CGD-O2D-CED
18	a	840	CLA	C13-C15-C16-C17
18	b	843	CLA	C10-C11-C12-C13
18	E	309	CLA	C5-C6-C7-C8
18	E	312	CLA	C8-C10-C11-C12
18	H	307	CLA	C8-C10-C11-C12
18	a	809	CLA	CBA-CGA-O2A-C1
18	a	855	CLA	CBA-CGA-O2A-C1
18	a	844	CLA	O1D-CGD-O2D-CED
18	b	816	CLA	O1D-CGD-O2D-CED
20	B	315	LHG	O9-C7-O7-C5
18	b	842	CLA	C5-C6-C7-C8
18	b	845	CLA	C8-C10-C11-C12
18	C	307	CLA	C13-C15-C16-C17
23	C	301	LMG	C28-C29-C30-C31
18	b	805	CLA	C15-C16-C17-C18
18	H	313	CLA	C15-C16-C17-C18
18	b	830	CLA	O1D-CGD-O2D-CED
18	a	801	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	a	854	CLA	C6-C7-C8-C10
18	a	855	CLA	C12-C13-C15-C16
18	b	801	CLA	C11-C10-C8-C7
18	b	803	CLA	C12-C13-C15-C16
18	B	306	CLA	C11-C12-C13-C15
18	C	309	CLA	C11-C10-C8-C7
18	a	806	CLA	O1A-CGA-O2A-C1
18	b	801	CLA	O1A-CGA-O2A-C1
20	E	301	LHG	O10-C23-O8-C6
23	l	207	LMG	O10-C28-O8-C9
28	C	303	DD6	C3-C4-C5-C6
18	a	823	CLA	O1D-CGD-O2D-CED
18	a	842	CLA	O1D-CGD-O2D-CED
18	b	837	CLA	O1D-CGD-O2D-CED
18	C	317	CLA	O1D-CGD-O2D-CED
18	a	801	CLA	C15-C16-C17-C18
18	a	815	CLA	C5-C6-C7-C8
18	a	827	CLA	C13-C15-C16-C17
18	a	836	CLA	C13-C15-C16-C17
18	a	841	CLA	C15-C16-C17-C18
18	a	843	CLA	C5-C6-C7-C8
18	b	820	CLA	C13-C15-C16-C17
18	b	829	CLA	C13-C15-C16-C17
18	H	307	CLA	C5-C6-C7-C8
18	H	311	CLA	C5-C6-C7-C8
18	D	216	CLA	CBA-CGA-O2A-C1
26	B	305	A86	O5-C38-O4-C34
18	E	309	CLA	O1A-CGA-O2A-C1
18	b	843	CLA	CBD-CGD-O2D-CED
18	b	811	CLA	C8-C10-C11-C12
18	b	817	CLA	C8-C10-C11-C12
20	E	301	LHG	C10-C11-C12-C13
20	B	315	LHG	O2-C2-C3-O3
18	B	306	CLA	C5-C6-C7-C8
18	D	207	CLA	C8-C10-C11-C12
18	D	213	CLA	C10-C11-C12-C13
18	E	315	CLA	C5-C6-C7-C8
18	H	306	CLA	C13-C15-C16-C17
18	H	313	CLA	C13-C15-C16-C17
18	b	817	CLA	CBA-CGA-O2A-C1
23	D	202	LMG	O10-C28-O8-C9
22	a	849	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	C	301	LMG	C11-C12-C13-C14
18	b	803	CLA	C8-C10-C11-C12
18	b	829	CLA	C5-C6-C7-C8
18	C	312	CLA	C10-C11-C12-C13
18	E	312	CLA	C10-C11-C12-C13
18	b	805	CLA	O1D-CGD-O2D-CED
18	b	827	CLA	CBD-CGD-O2D-CED
20	D	201	LHG	C8-C7-O7-C5
18	a	843	CLA	C15-C16-C17-C18
18	b	820	CLA	C8-C10-C11-C12
20	B	315	LHG	C3-O3-P-O6
20	B	315	LHG	C4-O6-P-O3
20	D	201	LHG	C4-O6-P-O3
20	E	301	LHG	C4-O6-P-O3
18	f	202	CLA	C3-C5-C6-C7
20	a	831	LHG	C11-C12-C13-C14
18	a	836	CLA	CBA-CGA-O2A-C1
18	b	808	CLA	CBA-CGA-O2A-C1
18	a	826	CLA	CBD-CGD-O2D-CED
18	b	821	CLA	CBD-CGD-O2D-CED
18	H	313	CLA	O1D-CGD-O2D-CED
20	D	201	LHG	O9-C7-O7-C5
18	b	811	CLA	CBD-CGD-O2D-CED
18	a	806	CLA	O1D-CGD-O2D-CED
18	a	855	CLA	O1A-CGA-O2A-C1
18	a	823	CLA	C2A-CAA-CBA-CGA
18	b	837	CLA	C2A-CAA-CBA-CGA
18	b	838	CLA	C2A-CAA-CBA-CGA
29	H	312	KC1	CAA-CBA-CGA-O2A
18	b	830	CLA	CBA-CGA-O2A-C1
18	f	203	CLA	CBA-CGA-O2A-C1
18	i	101	CLA	CBA-CGA-O2A-C1
18	D	213	CLA	CBA-CGA-O2A-C1
21	a	852	BCR	C9-C10-C11-C12
26	B	301	A86	C24-C25-C26-C27
28	C	303	DD6	C24-C25-C26-C27
20	b	835	LHG	C14-C15-C16-C17
20	B	315	LHG	C15-C16-C17-C18
20	E	301	LHG	C25-C26-C27-C28
18	b	850	CLA	O1D-CGD-O2D-CED
18	E	316	CLA	CBD-CGD-O2D-CED
18	a	803	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	301	LMG	O6-C5-C6-O5
20	b	835	LHG	C34-C35-C36-C37
20	j	102	LHG	C30-C31-C32-C33
20	D	201	LHG	C18-C19-C20-C21
23	j	103	LMG	C30-C31-C32-C33
23	D	202	LMG	C35-C36-C37-C38
25	b	834	DGD	C8A-C9A-CAA-CBA
18	a	809	CLA	O1A-CGA-O2A-C1
18	H	314	CLA	O1A-CGA-O2A-C1
18	a	836	CLA	O1D-CGD-O2D-CED
18	H	314	CLA	O1D-CGD-O2D-CED
29	H	312	KC1	C2A-CAA-CBA-CGA
18	a	801	CLA	C16-C17-C18-C19
18	a	825	CLA	C11-C12-C13-C14
18	b	842	CLA	C16-C17-C18-C20
20	E	301	LHG	C17-C18-C19-C20
23	C	319	LMG	C17-C18-C19-C20
23	E	318	LMG	C11-C12-C13-C14
20	H	316	LHG	C6-C5-O7-C7
18	C	309	CLA	O1D-CGD-O2D-CED
18	a	827	CLA	C15-C16-C17-C18
23	E	318	LMG	C10-C11-C12-C13
20	a	831	LHG	C11-C10-C9-C8
20	b	835	LHG	C30-C31-C32-C33
25	b	834	DGD	C6A-C7A-C8A-C9A
25	b	834	DGD	C6B-C7B-C8B-C9B
18	a	822	CLA	O1D-CGD-O2D-CED
18	b	826	CLA	O1D-CGD-O2D-CED
20	D	201	LHG	C2-C3-O3-P
20	H	316	LHG	C15-C16-C17-C18
23	l	207	LMG	C20-C21-C22-C23
23	C	319	LMG	C20-C21-C22-C23
18	a	801	CLA	C8-C10-C11-C12
20	b	835	LHG	O2-C2-C3-O3
20	D	201	LHG	O2-C2-C3-O3
20	a	831	LHG	C29-C30-C31-C32
20	b	835	LHG	C26-C27-C28-C29
20	E	301	LHG	C14-C15-C16-C17
25	b	834	DGD	CAB-CBB-CCB-CDB
25	b	834	DGD	CEB-CFB-CGB-CHB
26	b	847	A86	O5-C38-O4-C34
20	b	835	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	a	837	CLA	O1D-CGD-O2D-CED
18	l	202	CLA	C2C-C3C-CAC-CBC
20	H	316	LHG	C11-C12-C13-C14
23	C	319	LMG	C29-C30-C31-C32
18	b	845	CLA	C13-C15-C16-C17
18	a	836	CLA	O1A-CGA-O2A-C1
18	a	854	CLA	C16-C17-C18-C19
18	C	311	CLA	C11-C12-C13-C15
18	a	805	CLA	O1D-CGD-O2D-CED
18	b	846	CLA	C4-C3-C5-C6
20	a	831	LHG	C26-C27-C28-C29
20	a	831	LHG	C31-C32-C33-C34
20	j	102	LHG	C10-C11-C12-C13
23	D	202	LMG	C32-C33-C34-C35
18	a	801	CLA	C11-C12-C13-C14
18	a	807	CLA	C14-C13-C15-C16
18	a	815	CLA	C11-C12-C13-C14
18	a	847	CLA	C11-C10-C8-C9
18	b	806	CLA	C14-C13-C15-C16
18	b	843	CLA	C14-C13-C15-C16
18	E	309	CLA	C6-C7-C8-C9
20	a	831	LHG	C14-C15-C16-C17
20	a	835	LHG	C30-C31-C32-C33
20	B	315	LHG	C26-C27-C28-C29
20	D	201	LHG	C11-C10-C9-C8
23	a	851	LMG	C30-C31-C32-C33
18	a	808	CLA	C2A-CAA-CBA-CGA
18	b	811	CLA	C2A-CAA-CBA-CGA
18	b	842	CLA	C2A-CAA-CBA-CGA
18	D	209	CLA	C2A-CAA-CBA-CGA
18	D	210	CLA	C2A-CAA-CBA-CGA
21	a	850	BCR	C37-C22-C23-C24
20	b	835	LHG	C29-C30-C31-C32
20	j	102	LHG	C9-C10-C11-C12
20	B	315	LHG	C28-C29-C30-C31
20	E	301	LHG	C9-C10-C11-C12
20	b	835	LHG	O1-C1-C2-C3
21	a	850	BCR	C21-C22-C23-C24
21	b	833	BCR	C7-C8-C9-C10
23	E	318	LMG	C11-C10-O7-C8
20	E	301	LHG	C29-C30-C31-C32
23	a	851	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	834	DGD	C3A-C4A-C5A-C6A
18	l	202	CLA	CBA-CGA-O2A-C1
23	a	851	LMG	C28-C29-C30-C31
20	a	835	LHG	C31-C32-C33-C34
20	B	315	LHG	C10-C11-C12-C13
20	D	201	LHG	C10-C11-C12-C13
20	D	201	LHG	C16-C17-C18-C19
20	H	316	LHG	C13-C14-C15-C16
22	a	849	SQD	C24-C25-C26-C27
18	a	825	CLA	C11-C12-C13-C15
18	b	822	CLA	C16-C17-C18-C19
18	b	842	CLA	C16-C17-C18-C19
18	E	313	CLA	C6-C7-C8-C9
18	a	807	CLA	C5-C6-C7-C8
18	b	806	CLA	C13-C15-C16-C17
18	b	837	CLA	C10-C11-C12-C13
18	D	208	CLA	C5-C6-C7-C8
20	b	835	LHG	C10-C11-C12-C13
20	j	102	LHG	C26-C27-C28-C29
20	D	201	LHG	C28-C29-C30-C31
23	C	319	LMG	C31-C32-C33-C34
25	b	834	DGD	C7B-C8B-C9B-CAB
18	b	829	CLA	CBD-CGD-O2D-CED
18	a	824	CLA	O1D-CGD-O2D-CED
20	a	831	LHG	C13-C14-C15-C16
20	a	831	LHG	C15-C16-C17-C18
20	B	315	LHG	C11-C10-C9-C8
20	E	301	LHG	C12-C13-C14-C15
23	j	103	LMG	C14-C15-C16-C17
23	C	319	LMG	C16-C17-C18-C19
23	C	319	LMG	C30-C31-C32-C33
23	E	318	LMG	C33-C34-C35-C36
25	b	834	DGD	C3B-C4B-C5B-C6B
18	b	843	CLA	C5-C6-C7-C8
18	H	313	CLA	C5-C6-C7-C8
18	D	213	CLA	O1A-CGA-O2A-C1
18	a	848	CLA	O1D-CGD-O2D-CED
18	a	855	CLA	O1D-CGD-O2D-CED
18	a	806	CLA	C3A-C2A-CAA-CBA
18	a	824	CLA	C3A-C2A-CAA-CBA
18	a	838	CLA	C3A-C2A-CAA-CBA
18	b	808	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	b	810	CLA	C3A-C2A-CAA-CBA
18	b	824	CLA	C3A-C2A-CAA-CBA
18	b	825	CLA	C3A-C2A-CAA-CBA
18	b	844	CLA	C3A-C2A-CAA-CBA
18	f	204	CLA	C3A-C2A-CAA-CBA
18	D	209	CLA	C3A-C2A-CAA-CBA
18	D	211	CLA	C3A-C2A-CAA-CBA
18	H	314	CLA	C3A-C2A-CAA-CBA
18	a	837	CLA	C5-C6-C7-C8
25	b	834	DGD	C2G-C1G-O1G-C1A
26	D	204	A86	C1-C2-C3-C4
18	b	808	CLA	O1A-CGA-O2A-C1
18	b	817	CLA	O1A-CGA-O2A-C1
18	a	840	CLA	C16-C17-C18-C19
18	E	313	CLA	C6-C7-C8-C10
20	b	835	LHG	C4-C5-C6-O8
20	E	301	LHG	C4-C5-C6-O8
25	b	834	DGD	O1G-C1G-C2G-C3G
20	b	835	LHG	C31-C32-C33-C34
23	C	319	LMG	C12-C13-C14-C15
18	b	818	CLA	O1D-CGD-O2D-CED
23	l	207	LMG	C13-C14-C15-C16
18	a	807	CLA	C8-C10-C11-C12
18	b	837	CLA	CBA-CGA-O2A-C1
18	a	840	CLA	C2-C3-C5-C6
18	E	310	CLA	C2-C3-C5-C6
18	H	308	CLA	C2-C3-C5-C6
20	j	102	LHG	C8-C7-O7-C5
23	C	319	LMG	C11-C10-O7-C8
18	b	822	CLA	C2A-CAA-CBA-CGA
20	b	835	LHG	O1-C1-C2-O2
18	a	854	CLA	C15-C16-C17-C18
20	a	832	LHG	C9-C10-C11-C12
20	H	316	LHG	C11-C10-C9-C8
25	b	834	DGD	CDB-CEB-CFB-CGB
18	i	101	CLA	O1A-CGA-O2A-C1
18	H	308	CLA	C5-C6-C7-C8
18	a	827	CLA	C3-C5-C6-C7
18	D	208	CLA	C3-C5-C6-C7
18	b	830	CLA	O1A-CGA-O2A-C1
18	f	203	CLA	O1A-CGA-O2A-C1
18	b	849	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	b	835	LHG	C1-C2-C3-O3
22	a	849	SQD	C26-C27-C28-C29
23	E	318	LMG	C13-C14-C15-C16
20	j	102	LHG	O9-C7-O7-C5
23	E	318	LMG	O9-C10-O7-C8
18	a	841	CLA	C2-C1-O2A-CGA
20	a	831	LHG	C28-C29-C30-C31
20	E	301	LHG	C11-C12-C13-C14
20	j	102	LHG	C34-C35-C36-C37
18	a	840	CLA	C16-C17-C18-C20
21	a	834	BCR	C23-C24-C25-C26
21	a	834	BCR	C23-C24-C25-C30
21	a	852	BCR	C1-C6-C7-C8
21	b	833	BCR	C1-C6-C7-C8
21	b	833	BCR	C5-C6-C7-C8
21	f	201	BCR	C1-C6-C7-C8
21	i	103	BCR	C23-C24-C25-C26
21	i	103	BCR	C23-C24-C25-C30
21	l	201	BCR	C1-C6-C7-C8
21	l	201	BCR	C5-C6-C7-C8
21	l	204	BCR	C5-C6-C7-C8
21	l	204	BCR	C23-C24-C25-C26
21	l	204	BCR	C23-C24-C25-C30
21	r	201	BCR	C1-C6-C7-C8
21	r	201	BCR	C5-C6-C7-C8
21	E	305	BCR	C23-C24-C25-C26
21	E	305	BCR	C23-C24-C25-C30
27	l	206	ET4	C01-C06-C07-C08
18	D	217	CLA	C2C-C3C-CAC-CBC
20	j	102	LHG	C25-C26-C27-C28
18	a	844	CLA	CBA-CGA-O2A-C1
18	B	306	CLA	CBA-CGA-O2A-C1
23	a	851	LMG	C29-C28-O8-C9
18	a	807	CLA	C10-C11-C12-C13
18	b	840	CLA	C5-C6-C7-C8
18	C	312	CLA	C8-C10-C11-C12
18	H	307	CLA	C13-C15-C16-C17
18	l	202	CLA	O1A-CGA-O2A-C1
20	E	301	LHG	C7-C8-C9-C10
18	a	854	CLA	C10-C11-C12-C13
18	B	308	CLA	C10-C11-C12-C13
20	D	201	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	E	318	LMG	C30-C31-C32-C33
18	a	840	CLA	C4-C3-C5-C6
18	b	838	CLA	C4-C3-C5-C6
18	D	208	CLA	C4-C3-C5-C6
18	E	310	CLA	C4-C3-C5-C6
18	H	308	CLA	C4-C3-C5-C6
18	a	812	CLA	O1D-CGD-O2D-CED
18	a	802	CLA	C12-C13-C15-C16
18	a	815	CLA	C11-C12-C13-C15
18	a	840	CLA	C11-C10-C8-C7
18	a	847	CLA	C11-C10-C8-C7
18	b	803	CLA	C11-C12-C13-C15
18	b	806	CLA	C12-C13-C15-C16
18	b	838	CLA	C2-C3-C5-C6
18	b	842	CLA	C6-C7-C8-C10
18	b	843	CLA	C12-C13-C15-C16
18	b	845	CLA	C12-C13-C15-C16
18	b	846	CLA	C2-C3-C5-C6
18	D	208	CLA	C2-C3-C5-C6
18	D	208	CLA	C11-C12-C13-C15
18	E	309	CLA	C6-C7-C8-C10
18	E	310	CLA	C12-C13-C15-C16
18	H	311	CLA	C6-C7-C8-C10
19	b	831	PQN	C12-C13-C15-C16
18	b	837	CLA	O1A-CGA-O2A-C1
20	a	831	LHG	C33-C34-C35-C36
18	H	308	CLA	C8-C10-C11-C12
28	E	304	DD6	C24-C25-C26-C27
18	b	819	CLA	CBD-CGD-O2D-CED
18	C	311	CLA	C11-C12-C13-C14
18	b	848	CLA	O1D-CGD-O2D-CED
18	D	208	CLA	O1D-CGD-O2D-CED
29	B	313	KC1	O1D-CGD-O2D-CED
20	E	301	LHG	O9-C7-O7-C5
23	C	319	LMG	O9-C10-O7-C8
23	D	202	LMG	O9-C10-O7-C8
18	a	801	CLA	CBA-CGA-O2A-C1
18	a	818	CLA	CBA-CGA-O2A-C1
23	j	103	LMG	C31-C32-C33-C34
18	a	814	CLA	C2A-CAA-CBA-CGA
18	a	816	CLA	C2A-CAA-CBA-CGA
18	a	839	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	a	854	CLA	C2A-CAA-CBA-CGA
18	b	841	CLA	C2A-CAA-CBA-CGA
18	H	309	CLA	C2A-CAA-CBA-CGA
18	a	840	CLA	C10-C11-C12-C13
18	C	307	CLA	C15-C16-C17-C18
18	a	842	CLA	C2C-C3C-CAC-CBC
23	j	103	LMG	C11-C12-C13-C14
23	C	319	LMG	C32-C33-C34-C35
18	B	306	CLA	C12-C13-C15-C16
18	b	820	CLA	C10-C11-C12-C13
18	l	202	CLA	C4C-C3C-CAC-CBC
23	l	207	LMG	C29-C30-C31-C32
29	H	312	KC1	C2B-C3B-CAB-CBB
18	a	847	CLA	O1D-CGD-O2D-CED
20	E	301	LHG	C19-C20-C21-C22
18	b	846	CLA	CBA-CGA-O2A-C1
18	l	203	CLA	C13-C15-C16-C17
20	E	301	LHG	C8-C7-O7-C5
23	C	301	LMG	C11-C10-O7-C8
23	D	202	LMG	C11-C10-O7-C8
25	b	834	DGD	C8B-C9B-CAB-CBB
23	a	851	LMG	C4-C5-C6-O5
29	H	312	KC1	C4B-C3B-CAB-CBB
20	B	315	LHG	C24-C25-C26-C27
23	E	318	LMG	C17-C18-C19-C20
23	C	301	LMG	O9-C10-O7-C8
18	a	841	CLA	C3-C5-C6-C7
18	b	805	CLA	C3-C5-C6-C7
20	E	301	LHG	O7-C5-C6-O8
23	C	301	LMG	O7-C8-C9-O8
18	B	306	CLA	O1A-CGA-O2A-C1
23	l	207	LMG	C18-C19-C20-C21
18	a	825	CLA	C5-C6-C7-C8
18	H	314	CLA	C8-C10-C11-C12
18	b	823	CLA	C4-C3-C5-C6
18	B	312	CLA	C4-C3-C5-C6
18	b	840	CLA	C2-C3-C5-C6
20	E	301	LHG	C11-C10-C9-C8
18	a	803	CLA	C11-C10-C8-C9
18	a	809	CLA	C14-C13-C15-C16
18	a	840	CLA	C11-C10-C8-C9
18	a	843	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	a	844	CLA	C11-C12-C13-C14
18	a	855	CLA	C11-C10-C8-C9
18	b	803	CLA	C11-C10-C8-C9
18	b	803	CLA	C14-C13-C15-C16
18	b	805	CLA	C6-C7-C8-C9
18	b	822	CLA	C11-C12-C13-C14
18	b	830	CLA	C11-C12-C13-C14
18	b	850	CLA	C11-C12-C13-C14
18	B	306	CLA	C11-C12-C13-C14
18	B	308	CLA	C14-C13-C15-C16
18	D	208	CLA	C6-C7-C8-C9
18	D	214	CLA	C6-C7-C8-C9
18	E	310	CLA	C14-C13-C15-C16
18	l	205	CLA	O1D-CGD-O2D-CED
18	b	807	CLA	C2A-CAA-CBA-CGA
18	b	816	CLA	C2A-CAA-CBA-CGA
18	E	312	CLA	C2A-CAA-CBA-CGA
18	H	307	CLA	C2A-CAA-CBA-CGA
29	H	312	KC1	C4C-C3C-CAC-CBC
18	D	209	CLA	CBA-CGA-O2A-C1
21	l	204	BCR	C7-C8-C9-C34
18	b	803	CLA	C5-C6-C7-C8
18	H	306	CLA	C5-C6-C7-C8
20	E	301	LHG	C30-C31-C32-C33
21	l	204	BCR	C7-C8-C9-C10
18	a	844	CLA	O1A-CGA-O2A-C1
23	a	851	LMG	O10-C28-O8-C9
18	a	805	CLA	C1A-C2A-CAA-CBA
18	a	806	CLA	C1A-C2A-CAA-CBA
18	a	814	CLA	C1A-C2A-CAA-CBA
18	b	805	CLA	C1A-C2A-CAA-CBA
18	b	808	CLA	C1A-C2A-CAA-CBA
18	b	810	CLA	C1A-C2A-CAA-CBA
18	b	813	CLA	C1A-C2A-CAA-CBA
18	b	825	CLA	C1A-C2A-CAA-CBA
18	b	827	CLA	C1A-C2A-CAA-CBA
18	b	849	CLA	C1A-C2A-CAA-CBA
18	f	204	CLA	C1A-C2A-CAA-CBA
18	B	312	CLA	C1A-C2A-CAA-CBA
18	C	310	CLA	C1A-C2A-CAA-CBA
18	C	312	CLA	C1A-C2A-CAA-CBA
18	D	209	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	D	211	CLA	C1A-C2A-CAA-CBA
18	E	309	CLA	C1A-C2A-CAA-CBA
18	H	314	CLA	C1A-C2A-CAA-CBA
18	b	824	CLA	O1D-CGD-O2D-CED
18	C	312	CLA	O1D-CGD-O2D-CED
18	a	815	CLA	C15-C16-C17-C18
18	a	841	CLA	C8-C10-C11-C12
18	H	308	CLA	C15-C16-C17-C18
20	a	832	LHG	C3-O3-P-O6
20	E	301	LHG	C3-O3-P-O6
23	j	103	LMG	C28-C29-C30-C31
18	a	806	CLA	C3-C5-C6-C7
18	a	844	CLA	C3-C5-C6-C7
18	E	315	CLA	C3-C5-C6-C7
20	a	835	LHG	C2-C3-O3-P
18	H	306	CLA	CBA-CGA-O2A-C1
20	E	301	LHG	C27-C28-C29-C30
23	j	103	LMG	C29-C30-C31-C32
18	a	817	CLA	O1D-CGD-O2D-CED
18	b	822	CLA	C16-C17-C18-C20
18	b	817	CLA	C3-C5-C6-C7
18	l	203	CLA	C3-C5-C6-C7
25	b	834	DGD	C9B-CAB-CBB-CCB
18	b	840	CLA	C4-C3-C5-C6
18	D	213	CLA	C4-C3-C5-C6
18	C	315	CLA	C3A-C2A-CAA-CBA
18	C	317	CLA	C3A-C2A-CAA-CBA
20	a	831	LHG	C34-C35-C36-C37
20	j	102	LHG	C15-C16-C17-C18
23	E	318	LMG	C15-C16-C17-C18
18	b	819	CLA	C13-C15-C16-C17
18	B	306	CLA	C8-C10-C11-C12
20	H	316	LHG	C12-C13-C14-C15
18	a	801	CLA	O1A-CGA-O2A-C1
23	j	103	LMG	C15-C16-C17-C18
18	E	315	CLA	C2A-CAA-CBA-CGA
18	a	853	CLA	C6-C7-C8-C9
20	a	835	LHG	C4-C5-C6-O8
23	a	851	LMG	O1-C7-C8-C9
23	a	851	LMG	C7-C8-C9-O8
23	l	207	LMG	C7-C8-C9-O8
23	C	301	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	D	202	LMG	C7-C8-C9-O8
18	b	824	CLA	C10-C11-C12-C13
18	C	309	CLA	C5-C6-C7-C8
18	a	827	CLA	O1D-CGD-O2D-CED
18	b	823	CLA	O1D-CGD-O2D-CED
23	C	319	LMG	C21-C22-C23-C24
23	D	202	LMG	C30-C31-C32-C33
23	C	319	LMG	C18-C19-C20-C21
18	b	850	CLA	CAA-CBA-CGA-O2A
18	a	818	CLA	O1A-CGA-O2A-C1
20	a	831	LHG	C16-C17-C18-C19
18	D	209	CLA	O1A-CGA-O2A-C1
20	j	102	LHG	C12-C13-C14-C15
20	b	835	LHG	C19-C20-C21-C22
20	D	201	LHG	C35-C36-C37-C38
18	a	819	CLA	C4-C3-C5-C6
18	a	821	CLA	C4-C3-C5-C6
18	a	842	CLA	C4-C3-C5-C6
18	a	842	CLA	C2-C3-C5-C6
29	C	313	KC1	C2A-CAA-CBA-CGA
18	a	841	CLA	C16-C17-C18-C19
18	E	310	CLA	CBA-CGA-O2A-C1
20	B	315	LHG	C31-C32-C33-C34
18	H	309	CLA	CBD-CGD-O2D-CED
18	b	814	CLA	C2A-CAA-CBA-CGA
18	b	824	CLA	C5-C6-C7-C8
18	b	803	CLA	C3-C5-C6-C7
18	b	811	CLA	C3-C5-C6-C7
18	D	207	CLA	C3-C5-C6-C7
18	D	216	CLA	O1A-CGA-O2A-C1
18	b	819	CLA	CBA-CGA-O2A-C1
18	b	846	CLA	O1A-CGA-O2A-C1
18	b	829	CLA	C16-C17-C18-C20
18	b	843	CLA	O1D-CGD-O2D-CED
18	b	844	CLA	C5-C6-C7-C8
23	C	301	LMG	C2-C1-O1-C7
23	j	103	LMG	C17-C18-C19-C20
23	D	202	LMG	O7-C8-C9-O8
18	b	807	CLA	C5-C6-C7-C8
18	b	812	CLA	C5-C6-C7-C8
18	H	306	CLA	O1A-CGA-O2A-C1
20	E	301	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	834	DGD	C7A-C8A-C9A-CAA
18	a	809	CLA	C4-C3-C5-C6
18	H	311	CLA	C4-C3-C5-C6
18	a	802	CLA	C6-C7-C8-C10
18	a	805	CLA	C12-C13-C15-C16
18	a	806	CLA	C11-C12-C13-C15
18	a	809	CLA	C12-C13-C15-C16
18	a	813	CLA	C12-C13-C15-C16
18	a	819	CLA	C2-C3-C5-C6
18	a	826	CLA	C11-C12-C13-C15
18	a	837	CLA	C6-C7-C8-C10
18	a	843	CLA	C11-C12-C13-C15
18	a	844	CLA	C11-C12-C13-C15
18	a	854	CLA	C11-C10-C8-C7
18	a	855	CLA	C11-C10-C8-C7
18	b	803	CLA	C11-C10-C8-C7
18	b	806	CLA	C11-C12-C13-C15
18	b	807	CLA	C11-C12-C13-C15
18	b	820	CLA	C11-C10-C8-C7
18	b	820	CLA	C11-C12-C13-C15
18	b	822	CLA	C11-C12-C13-C15
18	b	830	CLA	C11-C12-C13-C15
18	b	843	CLA	C11-C10-C8-C7
18	b	850	CLA	C11-C12-C13-C15
18	f	202	CLA	C11-C10-C8-C7
18	f	203	CLA	C12-C13-C15-C16
18	l	203	CLA	C6-C7-C8-C10
18	B	308	CLA	C12-C13-C15-C16
18	D	207	CLA	C11-C10-C8-C7
18	D	214	CLA	C6-C7-C8-C10
18	H	306	CLA	C12-C13-C15-C16
18	H	307	CLA	C6-C7-C8-C10
18	H	313	CLA	C11-C10-C8-C7
18	H	313	CLA	C12-C13-C15-C16
18	a	802	CLA	C6-C7-C8-C9
18	a	805	CLA	C14-C13-C15-C16
18	a	806	CLA	C11-C12-C13-C14
18	a	808	CLA	C14-C13-C15-C16
18	a	815	CLA	C6-C7-C8-C9
18	a	826	CLA	C11-C12-C13-C14
18	a	828	CLA	C14-C13-C15-C16
18	a	837	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	a	840	CLA	C11-C12-C13-C14
18	a	842	CLA	C14-C13-C15-C16
18	a	854	CLA	C11-C10-C8-C9
18	b	806	CLA	C11-C12-C13-C14
18	b	824	CLA	C11-C12-C13-C14
18	b	842	CLA	C11-C12-C13-C14
18	b	843	CLA	C11-C12-C13-C14
18	f	202	CLA	C11-C10-C8-C9
18	f	203	CLA	C11-C12-C13-C14
18	f	203	CLA	C14-C13-C15-C16
18	D	210	CLA	C6-C7-C8-C9
18	E	310	CLA	C6-C7-C8-C9
18	H	306	CLA	C14-C13-C15-C16
18	b	849	CLA	CBD-CGD-O2D-CED
20	E	301	LHG	C16-C17-C18-C19
18	a	830	CLA	CBA-CGA-O2A-C1
18	H	307	CLA	CBA-CGA-O2A-C1
18	a	826	CLA	O1D-CGD-O2D-CED
21	b	833	BCR	C37-C22-C23-C24
18	a	853	CLA	C6-C7-C8-C10
18	H	308	CLA	C16-C17-C18-C20
18	b	811	CLA	O1D-CGD-O2D-CED
18	b	812	CLA	C11-C12-C13-C14
18	a	846	CLA	CBA-CGA-O2A-C1
18	a	854	CLA	C16-C17-C18-C20
18	b	843	CLA	C3-C5-C6-C7
18	b	827	CLA	O1D-CGD-O2D-CED
25	b	834	DGD	C2B-C3B-C4B-C5B
18	a	810	CLA	CBA-CGA-O2A-C1
18	b	840	CLA	CBA-CGA-O2A-C1
23	l	207	LMG	C14-C15-C16-C17
18	a	848	CLA	C11-C10-C8-C9
18	b	821	CLA	O1D-CGD-O2D-CED
18	H	313	CLA	C16-C17-C18-C20
18	a	847	CLA	C13-C15-C16-C17
18	b	819	CLA	C15-C16-C17-C18
22	a	849	SQD	C6-C5-O5-C1
18	a	820	CLA	CBA-CGA-O2A-C1
20	E	317	LHG	C24-C23-O8-C6
18	f	203	CLA	CBD-CGD-O2D-CED
18	a	813	CLA	C3A-C2A-CAA-CBA
18	a	839	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	b	809	CLA	C3A-C2A-CAA-CBA
18	b	823	CLA	C3A-C2A-CAA-CBA
18	l	202	CLA	C3A-C2A-CAA-CBA
20	b	835	LHG	C28-C29-C30-C31
20	E	301	LHG	C28-C29-C30-C31
26	D	203	A86	C1-C2-C3-C4
26	C	302	A86	O-C13-C14-C15
26	D	203	A86	O-C13-C14-C15
18	H	309	CLA	CBA-CGA-O2A-C1
18	E	316	CLA	O1D-CGD-O2D-CED
18	a	803	CLA	C15-C16-C17-C18
18	E	310	CLA	O1A-CGA-O2A-C1
18	H	313	CLA	C16-C17-C18-C19
18	a	821	CLA	CBA-CGA-O2A-C1
18	b	810	CLA	CBA-CGA-O2A-C1
18	H	305	CLA	C6-C7-C8-C10
20	a	835	LHG	C32-C33-C34-C35
20	D	201	LHG	C19-C20-C21-C22
19	b	831	PQN	C18-C20-C21-C22
20	H	316	LHG	C4-C5-C6-O8
20	b	835	LHG	C33-C34-C35-C36
18	b	820	CLA	O2A-C1-C2-C3
20	E	301	LHG	C15-C16-C17-C18
18	b	845	CLA	C10-C11-C12-C13
18	b	820	CLA	C4-C3-C5-C6
18	a	841	CLA	C16-C17-C18-C20
18	b	829	CLA	C16-C17-C18-C19
23	j	103	LMG	C13-C14-C15-C16
18	b	829	CLA	C2A-CAA-CBA-CGA
18	b	822	CLA	C10-C11-C12-C13
20	H	316	LHG	O6-C4-C5-O7
18	a	837	CLA	CBA-CGA-O2A-C1
18	b	820	CLA	CBA-CGA-O2A-C1
25	b	834	DGD	C2A-C1A-O1G-C1G
18	b	819	CLA	O1A-CGA-O2A-C1
18	a	801	CLA	C16-C17-C18-C20
20	a	831	LHG	C12-C13-C14-C15
18	a	802	CLA	C2C-C3C-CAC-CBC
20	E	301	LHG	C18-C19-C20-C21
22	a	849	SQD	O47-C45-C46-O48
23	a	851	LMG	O1-C7-C8-O7
18	a	806	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	a	828	CLA	C5-C6-C7-C8
18	b	818	CLA	C16-C17-C18-C19
20	a	831	LHG	C32-C33-C34-C35
23	E	318	LMG	O6-C1-O1-C7
18	a	805	CLA	C15-C16-C17-C18
18	a	820	CLA	C5-C6-C7-C8
18	a	837	CLA	C2-C1-O2A-CGA
18	b	841	CLA	C2-C1-O2A-CGA
18	b	845	CLA	C2-C1-O2A-CGA
18	D	207	CLA	C2-C1-O2A-CGA
18	a	844	CLA	C14-C13-C15-C16
18	a	846	CLA	C11-C10-C8-C9
18	a	855	CLA	C6-C7-C8-C9
18	b	807	CLA	C6-C7-C8-C9
18	b	820	CLA	C11-C10-C8-C9
18	b	824	CLA	C6-C7-C8-C9
18	H	306	CLA	C6-C7-C8-C9
18	H	314	CLA	C14-C13-C15-C16
23	D	202	LMG	C17-C18-C19-C20
18	a	825	CLA	CBD-CGD-O2D-CED
18	b	822	CLA	C15-C16-C17-C18
18	b	850	CLA	C5-C6-C7-C8
18	B	307	CLA	C15-C16-C17-C18
20	a	835	LHG	C5-C4-O6-P
20	b	835	LHG	C12-C13-C14-C15
20	j	102	LHG	C14-C15-C16-C17
18	a	843	CLA	C16-C17-C18-C19
18	H	308	CLA	C16-C17-C18-C19
21	b	839	BCR	C5-C6-C7-C8
21	r	201	BCR	C23-C24-C25-C26
21	r	201	BCR	C23-C24-C25-C30
18	a	855	CLA	C8-C10-C11-C12
21	j	105	BCR	C17-C18-C19-C20
18	b	830	CLA	C8-C10-C11-C12
18	b	850	CLA	C10-C11-C12-C13
20	a	831	LHG	C35-C36-C37-C38
18	a	830	CLA	O1A-CGA-O2A-C1
20	a	832	LHG	C10-C11-C12-C13
18	H	306	CLA	C16-C17-C18-C19
18	B	306	CLA	C14-C13-C15-C16
18	H	307	CLA	O1A-CGA-O2A-C1
18	b	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	a	808	CLA	C12-C13-C15-C16
18	a	815	CLA	C6-C7-C8-C10
18	a	819	CLA	C11-C12-C13-C15
18	a	820	CLA	C11-C12-C13-C15
18	a	821	CLA	C2-C3-C5-C6
18	a	828	CLA	C12-C13-C15-C16
18	a	836	CLA	C12-C13-C15-C16
18	a	840	CLA	C11-C12-C13-C15
18	a	841	CLA	C11-C12-C13-C15
18	a	842	CLA	C12-C13-C15-C16
18	a	844	CLA	C12-C13-C15-C16
18	a	846	CLA	C11-C10-C8-C7
18	a	855	CLA	C6-C7-C8-C10
18	b	805	CLA	C11-C10-C8-C7
18	b	812	CLA	C6-C7-C8-C10
18	b	824	CLA	C11-C12-C13-C15
18	b	842	CLA	C11-C12-C13-C15
18	b	843	CLA	C11-C12-C13-C15
18	f	202	CLA	C12-C13-C15-C16
18	f	203	CLA	C11-C12-C13-C15
18	i	101	CLA	C11-C10-C8-C7
18	B	306	CLA	C6-C7-C8-C10
18	B	308	CLA	C11-C10-C8-C7
18	B	311	CLA	C6-C7-C8-C10
18	D	208	CLA	C11-C10-C8-C7
18	D	210	CLA	C6-C7-C8-C10
18	E	309	CLA	C12-C13-C15-C16
18	E	310	CLA	C6-C7-C8-C10
18	H	313	CLA	C6-C7-C8-C10
18	H	314	CLA	C12-C13-C15-C16
21	f	201	BCR	C19-C20-C21-C22
26	B	301	A86	C11-C10-C9-C8
26	B	304	A86	C3-C4-C5-C6
25	b	834	DGD	C4B-C5B-C6B-C7B
18	a	809	CLA	C10-C11-C12-C13
18	b	804	CLA	C2A-CAA-CBA-CGA
18	b	817	CLA	C2A-CAA-CBA-CGA
18	b	845	CLA	C2A-CAA-CBA-CGA
18	b	828	CLA	C13-C15-C16-C17
18	a	843	CLA	C3-C5-C6-C7
18	a	843	CLA	C16-C17-C18-C20
18	b	818	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
18	a	854	CLA	C8-C10-C11-C12
18	b	806	CLA	CBA-CGA-O2A-C1
18	b	814	CLA	CBA-CGA-O2A-C1
20	D	201	LHG	C24-C23-O8-C6
18	a	848	CLA	C11-C10-C8-C7
18	b	828	CLA	C5-C6-C7-C8
18	a	804	CLA	CAD-CBD-CGD-O2D
18	a	808	CLA	CAD-CBD-CGD-O2D
18	a	811	CLA	CAD-CBD-CGD-O2D
18	a	814	CLA	CAD-CBD-CGD-O2D
18	a	817	CLA	CAD-CBD-CGD-O2D
18	a	818	CLA	CAD-CBD-CGD-O2D
18	a	828	CLA	CAD-CBD-CGD-O2D
18	a	841	CLA	CAD-CBD-CGD-O2D
18	a	842	CLA	CAD-CBD-CGD-O2D
18	a	843	CLA	CAD-CBD-CGD-O2D
18	a	846	CLA	CAD-CBD-CGD-O2D
18	a	847	CLA	CAD-CBD-CGD-O2D
18	a	853	CLA	CAD-CBD-CGD-O2D
18	b	827	CLA	CAD-CBD-CGD-O2D
18	b	828	CLA	CAD-CBD-CGD-O2D
18	b	837	CLA	CAD-CBD-CGD-O2D
18	b	846	CLA	CAD-CBD-CGD-O2D
18	l	202	CLA	CAD-CBD-CGD-O2D
18	B	307	CLA	CAD-CBD-CGD-O2D
18	B	312	CLA	CAD-CBD-CGD-O2D
18	C	311	CLA	CAD-CBD-CGD-O2D
18	D	211	CLA	CAD-CBD-CGD-O2D
18	E	310	CLA	CAD-CBD-CGD-O2D
18	E	314	CLA	CAD-CBD-CGD-O2D
18	E	316	CLA	CAD-CBD-CGD-O2D
18	H	309	CLA	CAD-CBD-CGD-O2D
29	H	312	KC1	CAD-CBD-CGD-O2D
18	b	843	CLA	C15-C16-C17-C18
18	C	311	CLA	C5-C6-C7-C8
18	a	807	CLA	C16-C17-C18-C20
18	b	820	CLA	C16-C17-C18-C20
18	i	101	CLA	C11-C12-C13-C14
20	a	832	LHG	C4-C5-C6-O8
23	C	301	LMG	C7-C8-C9-O8
23	E	318	LMG	O1-C7-C8-C9
23	E	318	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
18	a	846	CLA	O1A-CGA-O2A-C1
20	a	835	LHG	O6-C4-C5-O7
18	a	803	CLA	C13-C15-C16-C17
18	H	309	CLA	CAA-CBA-CGA-O2A
20	D	201	LHG	C29-C30-C31-C32
22	a	849	SQD	C31-C32-C33-C34
29	B	313	KC1	C4B-C3B-CAB-CBB
18	a	817	CLA	C2A-CAA-CBA-CGA
18	H	306	CLA	C2A-CAA-CBA-CGA
18	a	838	CLA	C16-C17-C18-C20
18	H	310	CLA	C11-C12-C13-C15
18	a	801	CLA	CHA-CBD-CGD-O1D
18	a	820	CLA	CHA-CBD-CGD-O1D
18	a	820	CLA	CHA-CBD-CGD-O2D
18	a	826	CLA	CHA-CBD-CGD-O1D
18	a	826	CLA	CHA-CBD-CGD-O2D
18	a	827	CLA	CHA-CBD-CGD-O2D
18	a	830	CLA	CHA-CBD-CGD-O1D
18	a	837	CLA	CHA-CBD-CGD-O1D
18	a	844	CLA	CHA-CBD-CGD-O1D
18	b	820	CLA	CHA-CBD-CGD-O1D
18	b	840	CLA	CHA-CBD-CGD-O1D
18	r	202	CLA	CHA-CBD-CGD-O1D
18	r	202	CLA	CHA-CBD-CGD-O2D
18	B	309	CLA	CHA-CBD-CGD-O1D
18	B	309	CLA	CHA-CBD-CGD-O2D
18	C	316	CLA	CHA-CBD-CGD-O2D
18	C	317	CLA	CHA-CBD-CGD-O2D
18	D	210	CLA	CHA-CBD-CGD-O1D
18	D	210	CLA	CHA-CBD-CGD-O2D
18	H	308	CLA	CHA-CBD-CGD-O1D
18	H	308	CLA	CHA-CBD-CGD-O2D
18	H	314	CLA	CHA-CBD-CGD-O1D
18	H	314	CLA	CHA-CBD-CGD-O2D
29	B	313	KC1	CHA-CBD-CGD-O2D
29	C	308	KC1	CHA-CBD-CGD-O2D
29	C	313	KC1	CHA-CBD-CGD-O1D
18	a	813	CLA	C3-C5-C6-C7
18	b	842	CLA	C3-C5-C6-C7
18	b	849	CLA	C3-C5-C6-C7
18	i	101	CLA	CBD-CGD-O2D-CED
18	a	810	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	a	820	CLA	O1A-CGA-O2A-C1
18	a	821	CLA	O1A-CGA-O2A-C1
18	a	837	CLA	O1A-CGA-O2A-C1
18	b	810	CLA	O1A-CGA-O2A-C1
18	b	820	CLA	O1A-CGA-O2A-C1
18	b	840	CLA	O1A-CGA-O2A-C1
20	H	316	LHG	O7-C5-C6-O8
23	E	318	LMG	O1-C7-C8-O7
20	j	102	LHG	C31-C32-C33-C34
18	b	806	CLA	O1A-CGA-O2A-C1
18	b	843	CLA	C16-C17-C18-C19
26	D	204	A86	C13-C14-C15-O1
26	H	301	A86	C13-C14-C15-O1
18	b	829	CLA	O1D-CGD-O2D-CED
18	b	849	CLA	O1D-CGD-O2D-CED
18	a	826	CLA	C3-C5-C6-C7
18	a	821	CLA	C5-C6-C7-C8
25	b	834	DGD	O1A-C1A-O1G-C1G
28	E	308	DD6	C27-C29-C30-C31
18	a	819	CLA	C11-C12-C13-C14
18	a	838	CLA	C11-C10-C8-C9
18	b	824	CLA	C11-C10-C8-C9
18	B	308	CLA	C11-C10-C8-C9
18	H	310	CLA	C11-C10-C8-C9
23	a	851	LMG	O6-C5-C6-O5
20	D	201	LHG	O10-C23-O8-C6
18	b	801	CLA	C5-C6-C7-C8
18	a	816	CLA	CBD-CGD-O2D-CED
18	D	214	CLA	C11-C10-C8-C9
20	E	317	LHG	O10-C23-O8-C6
20	D	201	LHG	C33-C34-C35-C36
18	H	309	CLA	O1D-CGD-O2D-CED
18	a	828	CLA	C1A-C2A-CAA-CBA
18	b	848	CLA	C1A-C2A-CAA-CBA
18	C	307	CLA	C16-C17-C18-C19
20	b	835	LHG	C11-C10-C9-C8
18	a	813	CLA	C2-C1-O2A-CGA
18	i	101	CLA	C2-C1-O2A-CGA
18	H	305	CLA	C2-C1-O2A-CGA
20	H	316	LHG	C14-C15-C16-C17
21	m	101	BCR	C19-C20-C21-C22
18	a	848	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	b	845	CLA	C3-C5-C6-C7
18	b	823	CLA	C2-C3-C5-C6
18	b	814	CLA	O1A-CGA-O2A-C1
20	a	832	LHG	C3-O3-P-O5
20	b	835	LHG	C3-O3-P-O4
20	B	315	LHG	C4-O6-P-O5
20	D	201	LHG	C4-O6-P-O4
20	D	201	LHG	C4-O6-P-O5
20	E	301	LHG	C3-O3-P-O5
20	E	301	LHG	C4-O6-P-O5
18	b	814	CLA	C16-C17-C18-C20
18	b	820	CLA	C16-C17-C18-C19
18	B	307	CLA	C16-C17-C18-C20
18	a	817	CLA	O2A-C1-C2-C3
18	l	202	CLA	O2A-C1-C2-C3
20	a	831	LHG	O6-C4-C5-C6
20	a	835	LHG	O6-C4-C5-C6
20	E	301	LHG	O6-C4-C5-C6
18	f	203	CLA	O1D-CGD-O2D-CED
18	C	314	CLA	C2C-C3C-CAC-CBC
18	a	827	CLA	C2A-CAA-CBA-CGA
18	a	808	CLA	C15-C16-C17-C18
18	B	312	CLA	C8-C10-C11-C12
18	b	828	CLA	C16-C17-C18-C20
18	H	306	CLA	C16-C17-C18-C20
18	a	809	CLA	CAD-CBD-CGD-O1D
18	a	824	CLA	CAD-CBD-CGD-O1D
18	a	824	CLA	C2-C3-C5-C6
18	r	202	CLA	CAD-CBD-CGD-O1D
18	B	309	CLA	CAD-CBD-CGD-O1D
18	C	316	CLA	CAD-CBD-CGD-O1D
18	H	314	CLA	CAD-CBD-CGD-O1D
18	a	836	CLA	C5-C6-C7-C8
18	a	841	CLA	C10-C11-C12-C13
20	B	315	LHG	C30-C31-C32-C33
18	b	810	CLA	C16-C17-C18-C20
18	b	817	CLA	C11-C12-C13-C15
18	a	813	CLA	C11-C12-C13-C15
18	a	814	CLA	C11-C10-C8-C7
18	a	838	CLA	C11-C10-C8-C7
18	a	838	CLA	C12-C13-C15-C16
18	b	814	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	b	824	CLA	C6-C7-C8-C10
18	B	308	CLA	C11-C12-C13-C15
18	B	309	CLA	C12-C13-C15-C16
18	B	312	CLA	C12-C13-C15-C16
18	C	309	CLA	C6-C7-C8-C10
18	H	310	CLA	C11-C10-C8-C7
20	a	831	LHG	O6-C4-C5-O7
20	E	301	LHG	O6-C4-C5-O7
20	D	201	LHG	C9-C10-C11-C12
23	C	301	LMG	C29-C30-C31-C32
22	a	849	SQD	C44-C45-C46-O48
18	D	211	CLA	CBA-CGA-O2A-C1
20	a	832	LHG	O7-C5-C6-O8
20	b	835	LHG	O7-C5-C6-O8
22	a	849	SQD	O6-C44-C45-O47
25	b	834	DGD	O1G-C1G-C2G-O2G
18	a	810	CLA	C8-C10-C11-C12
18	b	828	CLA	CBA-CGA-O2A-C1
26	b	847	A86	C13-C14-C15-C20
18	a	820	CLA	C11-C12-C13-C14
18	a	836	CLA	C14-C13-C15-C16
18	a	840	CLA	C14-C13-C15-C16
18	b	805	CLA	C11-C10-C8-C9
18	b	808	CLA	C11-C12-C13-C14
18	b	812	CLA	C6-C7-C8-C9
18	f	202	CLA	C14-C13-C15-C16
18	l	203	CLA	C6-C7-C8-C9
18	B	306	CLA	C6-C7-C8-C9
18	B	309	CLA	C6-C7-C8-C9
18	B	311	CLA	C6-C7-C8-C9
18	D	208	CLA	C14-C13-C15-C16
18	E	309	CLA	C14-C13-C15-C16
18	H	314	CLA	C6-C7-C8-C9
18	C	311	CLA	C3-C5-C6-C7
18	a	838	CLA	C16-C17-C18-C19
18	b	828	CLA	C16-C17-C18-C19
18	b	846	CLA	C15-C16-C17-C18
18	r	202	CLA	C2C-C3C-CAC-CBC
18	b	846	CLA	CAA-CBA-CGA-O2A
18	a	801	CLA	C5-C6-C7-C8
26	b	847	A86	C1-C24-C25-C26
26	m	102	A86	C6-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	r	203	A86	C6-C8-C9-C10
26	B	301	A86	C6-C8-C9-C10
26	B	302	A86	C6-C8-C9-C10
26	B	304	A86	C6-C8-C9-C10
26	B	305	A86	C6-C8-C9-C10
26	C	302	A86	C6-C8-C9-C10
26	C	305	A86	C6-C8-C9-C10
26	D	203	A86	C1-C24-C25-C26
26	D	203	A86	C6-C8-C9-C10
26	D	206	A86	C6-C8-C9-C10
26	E	302	A86	C6-C8-C9-C10
26	H	301	A86	C6-C8-C9-C10
26	H	302	A86	C6-C8-C9-C10
26	H	304	A86	C6-C8-C9-C10
28	D	205	DD6	C1-C24-C25-C26
28	E	307	DD6	C6-C8-C9-C10
23	D	202	LMG	C11-C12-C13-C14
18	B	308	CLA	C3-C5-C6-C7
18	a	813	CLA	C5-C6-C7-C8
25	b	834	DGD	C4E-C5E-C6E-O5E
18	a	809	CLA	C2-C3-C5-C6
18	B	312	CLA	C2-C3-C5-C6
18	D	213	CLA	C2-C3-C5-C6
18	a	817	CLA	C1-C2-C3-C4
18	D	209	CLA	C1-C2-C3-C4
18	H	310	CLA	C3-C5-C6-C7
20	b	835	LHG	C6-C5-O7-C7
18	a	803	CLA	C2A-CAA-CBA-CGA
18	a	825	CLA	C2A-CAA-CBA-CGA
18	C	307	CLA	C2A-CAA-CBA-CGA
18	H	308	CLA	C2A-CAA-CBA-CGA
18	b	828	CLA	O1A-CGA-O2A-C1
18	b	806	CLA	C2-C1-O2A-CGA
18	b	838	CLA	C2-C1-O2A-CGA
18	i	101	CLA	C11-C12-C13-C15
20	B	315	LHG	C9-C10-C11-C12
23	C	319	LMG	C34-C35-C36-C37
18	C	312	CLA	O1A-CGA-O2A-C1
20	E	317	LHG	O6-C4-C5-O7
18	a	825	CLA	O1D-CGD-O2D-CED
21	b	839	BCR	C1-C6-C7-C8
21	j	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	i	101	CLA	O1D-CGD-O2D-CED
20	a	835	LHG	C25-C26-C27-C28
20	b	835	LHG	C35-C36-C37-C38
18	b	808	CLA	C15-C16-C17-C18
18	D	208	CLA	C13-C15-C16-C17
18	a	844	CLA	C2A-CAA-CBA-CGA
20	a	835	LHG	O7-C5-C6-O8
23	C	301	LMG	O1-C7-C8-O7
18	a	815	CLA	C10-C11-C12-C13
18	b	811	CLA	CBA-CGA-O2A-C1
20	a	831	LHG	C3-O3-P-O6
20	a	835	LHG	C4-O6-P-O3
20	b	835	LHG	C3-O3-P-O6
20	j	102	LHG	C4-O6-P-O3
20	E	317	LHG	C3-O3-P-O6
20	a	831	LHG	C27-C28-C29-C30
23	C	301	LMG	O1-C7-C8-C9
18	a	813	CLA	C6-C7-C8-C10
18	b	805	CLA	C6-C7-C8-C10
18	b	823	CLA	C11-C10-C8-C7
23	E	318	LMG	C28-C29-C30-C31
25	b	834	DGD	CBB-CCB-CDB-CEB
18	a	814	CLA	C11-C10-C8-C9
18	a	838	CLA	C14-C13-C15-C16
18	a	855	CLA	C14-C13-C15-C16
18	b	801	CLA	C11-C10-C8-C9
18	b	807	CLA	C11-C12-C13-C14
18	b	814	CLA	C11-C12-C13-C14
18	b	845	CLA	C14-C13-C15-C16
18	B	309	CLA	C14-C13-C15-C16
18	B	312	CLA	C14-C13-C15-C16
18	C	309	CLA	C6-C7-C8-C9
18	b	846	CLA	C5-C6-C7-C8
21	j	105	BCR	C19-C20-C21-C22
18	b	814	CLA	C16-C17-C18-C19
18	B	307	CLA	C16-C17-C18-C19
18	a	816	CLA	O1D-CGD-O2D-CED
18	D	217	CLA	C4C-C3C-CAC-CBC
18	B	307	CLA	C2A-CAA-CBA-CGA
20	b	835	LHG	C5-C4-O6-P
18	b	811	CLA	O1A-CGA-O2A-C1
18	b	818	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	b	833	BCR	C21-C22-C23-C24
18	H	311	CLA	C2-C3-C5-C6
18	b	810	CLA	C16-C17-C18-C19
18	C	312	CLA	CBA-CGA-O2A-C1
18	a	826	CLA	C10-C11-C12-C13
29	H	312	KC1	CAA-CBA-CGA-O1A
25	b	834	DGD	C1B-C2B-C3B-C4B
18	f	204	CLA	C2A-CAA-CBA-CGA
21	a	852	BCR	C19-C20-C21-C22
26	B	302	A86	C3-C4-C5-C6
26	H	302	A86	C3-C4-C5-C6
20	a	831	LHG	C25-C26-C27-C28
20	H	316	LHG	O6-C4-C5-C6
20	D	201	LHG	C32-C33-C34-C35
18	a	807	CLA	C13-C15-C16-C17
18	H	309	CLA	O1A-CGA-O2A-C1
18	a	844	CLA	C4-C3-C5-C6
18	b	813	CLA	C4-C3-C5-C6
18	H	313	CLA	C4-C3-C5-C6
18	b	813	CLA	C2-C3-C5-C6
18	b	817	CLA	C2-C3-C5-C6
18	l	203	CLA	C15-C16-C17-C18
18	C	311	CLA	C2C-C3C-CAC-CBC
18	b	829	CLA	C2-C1-O2A-CGA
18	E	309	CLA	C2-C1-O2A-CGA
18	B	309	CLA	C15-C16-C17-C18
18	E	310	CLA	C10-C11-C12-C13
18	a	810	CLA	C2A-CAA-CBA-CGA
18	a	813	CLA	C2A-CAA-CBA-CGA
18	B	312	CLA	C2A-CAA-CBA-CGA
18	b	850	CLA	CAA-CBA-CGA-O1A
20	a	831	LHG	C9-C10-C11-C12
23	a	851	LMG	O9-C10-O7-C8
18	a	830	CLA	C4-C3-C5-C6
18	b	817	CLA	C4-C3-C5-C6
18	a	815	CLA	C2-C3-C5-C6
18	a	830	CLA	C2-C3-C5-C6
18	H	310	CLA	C2C-C3C-CAC-CBC
18	b	801	CLA	C6-C7-C8-C9
18	b	806	CLA	C11-C10-C8-C9
18	b	850	CLA	C6-C7-C8-C9
18	C	307	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	C	312	CLA	C6-C7-C8-C9
18	E	310	CLA	C15-C16-C17-C18
20	a	835	LHG	C23-C24-C25-C26
21	f	205	BCR	C35-C13-C14-C15
21	l	201	BCR	C11-C10-C9-C34
21	m	101	BCR	C11-C10-C9-C34
26	b	847	A86	C-C1-C2-C3
26	m	102	A86	C-C1-C2-C3
26	m	102	A86	C4-C5-C6-C7
26	D	204	A86	C4-C5-C6-C7
28	D	205	DD6	C4-C5-C6-C7
28	E	307	DD6	C9-C10-C11-C12
28	E	307	DD6	C4-C5-C6-C7
21	f	201	BCR	C7-C8-C9-C34
18	a	815	CLA	C4-C3-C5-C6
18	b	805	CLA	C4-C3-C5-C6
18	a	808	CLA	C1A-C2A-CAA-CBA
18	a	818	CLA	C1A-C2A-CAA-CBA
18	a	836	CLA	C1A-C2A-CAA-CBA
18	a	839	CLA	C1A-C2A-CAA-CBA
18	l	202	CLA	C1A-C2A-CAA-CBA
18	E	311	CLA	C1A-C2A-CAA-CBA
18	b	850	CLA	C16-C17-C18-C19
18	b	844	CLA	CBD-CGD-O2D-CED
18	a	825	CLA	C6-C7-C8-C10
18	a	826	CLA	C11-C10-C8-C7
18	b	817	CLA	C11-C10-C8-C7
18	b	826	CLA	C11-C10-C8-C7
18	b	837	CLA	C11-C10-C8-C7
18	l	203	CLA	C11-C10-C8-C7
18	C	311	CLA	C11-C10-C8-C7
18	E	312	CLA	C12-C13-C15-C16
18	a	809	CLA	C3-C5-C6-C7
18	r	202	CLA	C4C-C3C-CAC-CBC
18	b	844	CLA	C3-C5-C6-C7
18	b	821	CLA	C2A-CAA-CBA-CGA
23	E	318	LMG	C18-C19-C20-C21
18	b	829	CLA	C8-C10-C11-C12
18	b	828	CLA	C15-C16-C17-C18
25	b	834	DGD	C2A-C3A-C4A-C5A
18	b	837	CLA	C8-C10-C11-C12
18	E	312	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	j	102	LHG	C16-C17-C18-C19
23	D	202	LMG	C20-C21-C22-C23
18	b	812	CLA	C3-C5-C6-C7
25	b	834	DGD	O1B-C1B-O2G-C2G
18	l	203	CLA	C16-C17-C18-C19
18	C	311	CLA	C4C-C3C-CAC-CBC
18	b	840	CLA	O1D-CGD-O2D-CED
21	f	205	BCR	C12-C13-C14-C15
21	l	201	BCR	C11-C10-C9-C8
21	m	101	BCR	C11-C10-C9-C8
26	b	847	A86	C24-C1-C2-C3
26	m	102	A86	C24-C1-C2-C3
26	m	102	A86	C4-C5-C6-C8
26	r	203	A86	C13-C14-C15-C16
26	D	204	A86	C4-C5-C6-C8
28	D	205	DD6	C4-C5-C6-C8
28	E	307	DD6	C9-C10-C11-C13
28	E	307	DD6	C4-C5-C6-C8
18	a	840	CLA	C8-C10-C11-C12
23	j	103	LMG	O7-C8-C9-O8
18	a	814	CLA	CAA-CBA-CGA-O2A
25	b	834	DGD	C9A-CAA-CBA-CCA
28	E	304	DD6	C1-C2-C3-C4
18	a	854	CLA	C2C-C3C-CAC-CBC
20	a	831	LHG	C17-C18-C19-C20
18	b	842	CLA	C10-C11-C12-C13
26	B	301	A86	C10-C11-C13-C14
18	b	824	CLA	C2C-C3C-CAC-CBC
18	a	808	CLA	C8-C10-C11-C12
18	a	803	CLA	C2-C1-O2A-CGA
18	a	842	CLA	C2-C1-O2A-CGA
18	b	824	CLA	C2-C1-O2A-CGA
18	a	805	CLA	C2-C3-C5-C6
18	H	313	CLA	C2-C3-C5-C6
23	C	319	LMG	C15-C16-C17-C18
18	b	849	CLA	C10-C11-C12-C13
18	b	810	CLA	C6-C7-C8-C9
18	C	309	CLA	C11-C10-C8-C9
20	B	315	LHG	C23-C24-C25-C26
18	H	307	CLA	C10-C11-C12-C13
18	a	801	CLA	CAA-CBA-CGA-O2A
20	a	832	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
18	b	826	CLA	C2A-CAA-CBA-CGA
18	B	309	CLA	C2A-CAA-CBA-CGA
18	D	209	CLA	O2A-C1-C2-C3
18	C	309	CLA	C4C-C3C-CAC-CBC
21	j	101	BCR	C23-C24-C25-C30
21	l	201	BCR	C23-C24-C25-C30
23	l	207	LMG	C12-C13-C14-C15
20	B	315	LHG	C13-C14-C15-C16
18	a	837	CLA	C4-C3-C5-C6
18	b	801	CLA	C4-C3-C5-C6
18	b	803	CLA	C4-C3-C5-C6
18	b	837	CLA	C4-C3-C5-C6
21	a	852	BCR	C17-C18-C19-C20
18	H	315	CLA	CAA-CBA-CGA-O2A
23	j	103	LMG	C8-C7-O1-C1
25	b	834	DGD	C2B-C1B-O2G-C2G
23	a	851	LMG	C32-C33-C34-C35
18	H	310	CLA	C10-C11-C12-C13
18	E	314	CLA	O1D-CGD-O2D-CED
18	a	826	CLA	C2A-CAA-CBA-CGA
18	b	806	CLA	C2A-CAA-CBA-CGA
18	b	824	CLA	C2A-CAA-CBA-CGA
18	b	840	CLA	CBD-CGD-O2D-CED
18	B	306	CLA	C4-C3-C5-C6
18	B	308	CLA	C4-C3-C5-C6
18	b	848	CLA	C5-C6-C7-C8
23	E	318	LMG	C31-C32-C33-C34
18	a	803	CLA	C11-C12-C13-C15
18	b	808	CLA	C11-C12-C13-C15
18	b	810	CLA	C6-C7-C8-C10
18	b	820	CLA	C2-C3-C5-C6
18	a	843	CLA	C13-C15-C16-C17
18	D	214	CLA	O1D-CGD-O2D-CED
27	l	206	ET4	C19-C20-C21-C22
18	a	805	CLA	CAA-CBA-CGA-O2A
18	i	101	CLA	C10-C11-C12-C13
18	B	311	CLA	C13-C15-C16-C17
18	a	823	CLA	CAA-CBA-CGA-O2A
18	a	842	CLA	C4C-C3C-CAC-CBC
18	b	822	CLA	O1A-CGA-O2A-C1
23	a	851	LMG	C11-C10-O7-C8
18	C	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	b	844	CLA	O1D-CGD-O2D-CED
18	b	822	CLA	CBA-CGA-O2A-C1
18	b	824	CLA	CAA-CBA-CGA-O2A
20	a	831	LHG	C30-C31-C32-C33
18	b	842	CLA	C2-C3-C5-C6
18	D	214	CLA	CBA-CGA-O2A-C1
18	a	802	CLA	C14-C13-C15-C16
18	a	826	CLA	C11-C10-C8-C9
18	i	101	CLA	C6-C7-C8-C9
18	l	203	CLA	C11-C12-C13-C14
20	j	102	LHG	C18-C19-C20-C21
18	a	855	CLA	C3A-C2A-CAA-CBA
18	b	843	CLA	C3A-C2A-CAA-CBA
18	b	849	CLA	C3A-C2A-CAA-CBA
18	E	313	CLA	C3A-C2A-CAA-CBA
18	E	316	CLA	C3A-C2A-CAA-CBA
18	a	818	CLA	C2C-C3C-CAC-CBC
18	a	827	CLA	C5-C6-C7-C8
18	D	214	CLA	O1A-CGA-O2A-C1
20	H	316	LHG	C17-C18-C19-C20
18	a	812	CLA	CAA-CBA-CGA-O2A
18	a	806	CLA	CAD-CBD-CGD-O2D
18	a	810	CLA	CAD-CBD-CGD-O2D
18	a	825	CLA	CAD-CBD-CGD-O2D
18	a	855	CLA	CAD-CBD-CGD-O2D
18	b	805	CLA	CAD-CBD-CGD-O2D
18	b	806	CLA	CAD-CBD-CGD-O2D
18	b	813	CLA	CAD-CBD-CGD-O2D
18	b	821	CLA	CAD-CBD-CGD-O2D
18	b	825	CLA	CAD-CBD-CGD-O2D
18	b	829	CLA	CAD-CBD-CGD-O2D
18	b	843	CLA	CAD-CBD-CGD-O2D
18	b	845	CLA	CAD-CBD-CGD-O2D
18	b	850	CLA	CAD-CBD-CGD-O2D
18	f	203	CLA	CAD-CBD-CGD-O2D
18	l	205	CLA	CAD-CBD-CGD-O2D
18	C	307	CLA	CAD-CBD-CGD-O2D
18	C	318	CLA	CAD-CBD-CGD-O2D
18	D	212	CLA	CAD-CBD-CGD-O2D
18	D	217	CLA	CAD-CBD-CGD-O2D
26	b	847	A86	C28-C27-C29-C30
29	C	313	KC1	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	a	836	CLA	C15-C16-C17-C18
18	H	315	CLA	CAA-CBA-CGA-O1A
22	a	849	SQD	C25-C26-C27-C28
18	a	813	CLA	CAA-CBA-CGA-O2A
18	B	306	CLA	CAA-CBA-CGA-O2A
18	D	209	CLA	CAA-CBA-CGA-O2A
18	b	810	CLA	C15-C16-C17-C18
18	a	805	CLA	C4-C3-C5-C6
18	C	309	CLA	C4-C3-C5-C6
18	b	846	CLA	C16-C17-C18-C20
23	D	202	LMG	C10-C11-C12-C13
18	b	805	CLA	C2-C3-C5-C6
18	b	837	CLA	C2-C3-C5-C6
18	a	808	CLA	CAA-CBA-CGA-O2A
18	D	214	CLA	CBD-CGD-O2D-CED
26	b	847	A86	C12-C11-C13-O
26	B	301	A86	C12-C11-C13-O
28	E	303	DD6	C13-C14-C15-O1
18	b	806	CLA	C10-C11-C12-C13
18	b	817	CLA	CAA-CBA-CGA-O2A
18	b	844	CLA	CAA-CBA-CGA-O2A
18	D	211	CLA	CAA-CBA-CGA-O2A
20	E	317	LHG	C16-C17-C18-C19
18	a	836	CLA	O2A-C1-C2-C3
18	b	813	CLA	C2A-CAA-CBA-CGA
18	E	309	CLA	C2A-CAA-CBA-CGA
18	a	823	CLA	CAA-CBA-CGA-O1A
18	H	310	CLA	C11-C12-C13-C14
18	E	314	CLA	CBD-CGD-O2D-CED
20	a	835	LHG	C27-C28-C29-C30
18	a	801	CLA	CHA-CBD-CGD-O2D
18	a	805	CLA	CHA-CBD-CGD-O1D
18	a	811	CLA	CHA-CBD-CGD-O1D
18	a	816	CLA	CHA-CBD-CGD-O2D
18	a	821	CLA	CHA-CBD-CGD-O1D
18	a	830	CLA	CHA-CBD-CGD-O2D
18	a	839	CLA	CHA-CBD-CGD-O1D
18	a	839	CLA	CHA-CBD-CGD-O2D
18	a	843	CLA	CHA-CBD-CGD-O2D
18	a	844	CLA	CHA-CBD-CGD-O2D
18	b	804	CLA	CHA-CBD-CGD-O1D
18	b	804	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	b	807	CLA	CHA-CBD-CGD-O1D
18	b	807	CLA	CHA-CBD-CGD-O2D
18	b	812	CLA	CHA-CBD-CGD-O2D
18	b	815	CLA	CHA-CBD-CGD-O1D
18	b	822	CLA	CHA-CBD-CGD-O1D
18	b	822	CLA	CHA-CBD-CGD-O2D
18	b	823	CLA	CHA-CBD-CGD-O1D
18	b	823	CLA	CHA-CBD-CGD-O2D
18	b	838	CLA	CHA-CBD-CGD-O1D
18	b	841	CLA	CHA-CBD-CGD-O1D
18	b	841	CLA	CHA-CBD-CGD-O2D
18	b	848	CLA	CHA-CBD-CGD-O1D
18	b	848	CLA	CHA-CBD-CGD-O2D
18	f	202	CLA	CHA-CBD-CGD-O1D
18	f	202	CLA	CHA-CBD-CGD-O2D
18	l	203	CLA	CHA-CBD-CGD-O1D
18	l	203	CLA	CHA-CBD-CGD-O2D
18	B	311	CLA	CHA-CBD-CGD-O2D
18	H	307	CLA	CHA-CBD-CGD-O1D
18	H	307	CLA	CHA-CBD-CGD-O2D
18	a	817	CLA	CAA-CBA-CGA-O2A
20	B	315	LHG	O7-C7-C8-C9
18	b	801	CLA	C2-C3-C5-C6
18	a	838	CLA	C13-C15-C16-C17
20	E	317	LHG	O6-C4-C5-C6
18	C	306	CLA	CAA-CBA-CGA-O1A
18	b	807	CLA	C16-C17-C18-C19
18	a	811	CLA	CAA-CBA-CGA-O2A
22	a	849	SQD	C33-C34-C35-C36
18	a	812	CLA	CAA-CBA-CGA-O1A
18	D	211	CLA	O1A-CGA-O2A-C1
18	l	203	CLA	O1A-CGA-O2A-C1
18	b	849	CLA	CAA-CBA-CGA-O2A
20	a	831	LHG	O8-C23-C24-C25
26	b	847	A86	C13-C14-C15-O1
26	B	301	A86	C10-C11-C13-O
26	D	206	A86	C13-C14-C15-O1
18	l	203	CLA	CBA-CGA-O2A-C1
20	a	835	LHG	C29-C30-C31-C32
18	a	807	CLA	C16-C17-C18-C19
18	b	846	CLA	C13-C15-C16-C17
18	b	829	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
18	a	803	CLA	C14-C13-C15-C16
18	a	815	CLA	C11-C10-C8-C9
18	a	825	CLA	C6-C7-C8-C9
18	a	846	CLA	C14-C13-C15-C16
18	b	819	CLA	C11-C10-C8-C9
18	b	823	CLA	C11-C10-C8-C9
18	b	826	CLA	C11-C10-C8-C9
18	b	842	CLA	C6-C7-C8-C9
26	D	206	A86	C3-C4-C5-C6
23	D	202	LMG	C21-C22-C23-C24
18	D	209	CLA	CAA-CBA-CGA-O1A
18	r	202	CLA	C2A-CAA-CBA-CGA
18	E	313	CLA	C2A-CAA-CBA-CGA
18	b	824	CLA	CAA-CBA-CGA-O1A
22	a	849	SQD	O48-C23-C24-C25
18	B	306	CLA	C10-C11-C12-C13
20	D	201	LHG	C17-C18-C19-C20
18	b	848	CLA	CBA-CGA-O2A-C1
20	b	835	LHG	O10-C23-O8-C6
18	a	847	CLA	CAA-CBA-CGA-O2A
18	D	211	CLA	CAA-CBA-CGA-O1A
18	a	805	CLA	CBA-CGA-O2A-C1
18	H	307	CLA	O1D-CGD-O2D-CED
18	a	810	CLA	C1A-C2A-CAA-CBA
18	a	843	CLA	C1A-C2A-CAA-CBA
18	a	855	CLA	C1A-C2A-CAA-CBA
18	f	202	CLA	C1A-C2A-CAA-CBA
18	E	310	CLA	C1A-C2A-CAA-CBA
18	E	313	CLA	C1A-C2A-CAA-CBA
18	E	316	CLA	C1A-C2A-CAA-CBA
18	a	808	CLA	CAA-CBA-CGA-O1A
18	b	817	CLA	CAA-CBA-CGA-O1A
20	b	835	LHG	C24-C23-O8-C6
18	a	817	CLA	CAA-CBA-CGA-O1A
18	b	846	CLA	C16-C17-C18-C19
20	a	831	LHG	O10-C23-C24-C25
20	j	102	LHG	C29-C30-C31-C32
18	a	816	CLA	CAA-CBA-CGA-O2A
18	b	848	CLA	O1A-CGA-O2A-C1
18	b	808	CLA	CAA-CBA-CGA-O2A
18	C	309	CLA	C10-C11-C12-C13
18	a	808	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	a	835	LHG	C4-O6-P-O5
20	j	102	LHG	C3-O3-P-O5
20	E	301	LHG	C3-O3-P-O4
20	E	301	LHG	C4-O6-P-O4
20	B	315	LHG	O9-C7-C8-C9
18	r	202	CLA	CAA-CBA-CGA-O2A
22	a	849	SQD	O10-C23-C24-C25
18	C	309	CLA	C2C-C3C-CAC-CBC
18	E	316	CLA	C2A-CAA-CBA-CGA
18	B	306	CLA	CAA-CBA-CGA-O1A
18	f	203	CLA	C5-C6-C7-C8
18	a	811	CLA	CAA-CBA-CGA-O1A
18	a	813	CLA	CAA-CBA-CGA-O1A
18	b	844	CLA	CAA-CBA-CGA-O1A
18	H	305	CLA	O1D-CGD-O2D-CED
18	r	202	CLA	CAA-CBA-CGA-O1A
18	a	805	CLA	CAD-CBD-CGD-O1D
18	a	844	CLA	CAD-CBD-CGD-O1D
18	b	811	CLA	CAD-CBD-CGD-O1D
18	b	822	CLA	CAD-CBD-CGD-O1D
18	b	826	CLA	CAD-CBD-CGD-O1D
18	b	841	CLA	CAD-CBD-CGD-O1D
18	B	310	CLA	CAD-CBD-CGD-O1D
18	C	314	CLA	CAD-CBD-CGD-O1D
26	b	847	A86	C26-C27-C29-C30
26	D	203	A86	C26-C27-C29-C30
18	b	806	CLA	CAA-CBA-CGA-O2A
18	D	214	CLA	CAA-CBA-CGA-O2A
18	a	820	CLA	C14-C13-C15-C16
18	a	828	CLA	C6-C7-C8-C9
18	b	818	CLA	C6-C7-C8-C9
18	E	312	CLA	C11-C10-C8-C9
18	a	802	CLA	C15-C16-C17-C18
18	H	309	CLA	CAA-CBA-CGA-O1A
18	b	807	CLA	C16-C17-C18-C20
18	b	845	CLA	C16-C17-C18-C20
18	a	822	CLA	CAA-CBA-CGA-O2A
18	E	311	CLA	CAA-CBA-CGA-O2A
18	a	839	CLA	C10-C11-C12-C13
18	b	808	CLA	C13-C15-C16-C17
18	a	807	CLA	CAA-CBA-CGA-O2A
18	a	827	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	D	207	CLA	CAA-CBA-CGA-O2A
18	E	309	CLA	CAA-CBA-CGA-O2A
18	b	842	CLA	C4-C3-C5-C6
18	a	805	CLA	C6-C7-C8-C10
18	a	815	CLA	C11-C10-C8-C7
18	a	844	CLA	C2-C3-C5-C6
18	b	818	CLA	C6-C7-C8-C10
18	b	819	CLA	C11-C10-C8-C7
18	b	829	CLA	C11-C10-C8-C7
18	B	309	CLA	C6-C7-C8-C10
18	E	312	CLA	C11-C10-C8-C7
18	a	847	CLA	CAA-CBA-CGA-O1A
18	b	806	CLA	CAA-CBA-CGA-O1A
18	b	849	CLA	CAA-CBA-CGA-O1A
18	l	205	CLA	CAA-CBA-CGA-O2A
18	b	809	CLA	CAA-CBA-CGA-O2A
18	b	822	CLA	CAA-CBA-CGA-O2A
18	B	309	CLA	CAA-CBA-CGA-O2A
18	C	307	CLA	CAA-CBA-CGA-O2A
23	E	318	LMG	O7-C10-C11-C12
20	a	832	LHG	O8-C23-C24-C25
18	b	814	CLA	C13-C15-C16-C17
21	f	201	BCR	C7-C8-C9-C10
21	l	201	BCR	C21-C22-C23-C24
18	a	806	CLA	C16-C17-C18-C20
18	b	812	CLA	CAA-CBA-CGA-O2A
18	E	316	CLA	CAA-CBA-CGA-O2A
18	a	804	CLA	O1D-CGD-O2D-CED
18	b	819	CLA	C10-C11-C12-C13
18	D	210	CLA	O1A-CGA-O2A-C1
20	j	102	LHG	C17-C18-C19-C20
18	a	805	CLA	O1A-CGA-O2A-C1
18	a	826	CLA	CAA-CBA-CGA-O2A
18	b	803	CLA	CAA-CBA-CGA-O2A
18	b	827	CLA	CAA-CBA-CGA-O2A
18	D	214	CLA	CAA-CBA-CGA-O1A
18	b	825	CLA	C2A-CAA-CBA-CGA
18	C	307	CLA	CAA-CBA-CGA-O1A
18	a	843	CLA	CAA-CBA-CGA-O2A
18	b	810	CLA	CAA-CBA-CGA-O2A
18	b	837	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

68 monomers are involved in 244 short contacts:

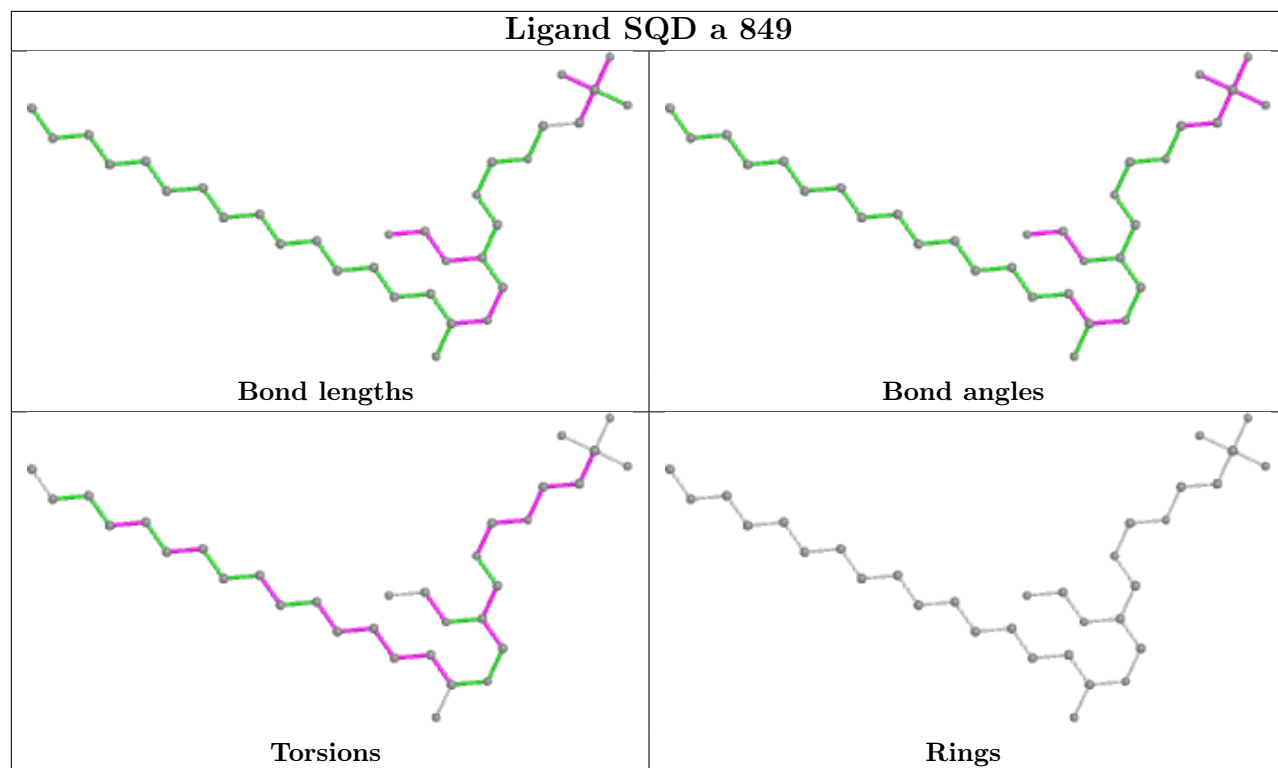
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	E	304	DD6	1	0
20	D	201	LHG	6	0
26	D	203	A86	4	0
18	D	212	CLA	2	0
21	E	305	BCR	1	0
18	C	312	CLA	10	0
20	B	315	LHG	2	0
18	C	310	CLA	4	0
20	E	301	LHG	2	0
18	B	312	CLA	8	0
18	C	309	CLA	6	0
18	H	310	CLA	4	0
23	E	318	LMG	3	0
28	B	303	DD6	1	0
18	C	306	CLA	1	0
18	C	315	CLA	2	0
18	H	306	CLA	10	0
18	H	314	CLA	4	0
18	D	217	CLA	3	0
26	B	301	A86	2	0
18	C	311	CLA	7	0
26	D	204	A86	2	0
28	E	307	DD6	1	0
18	E	313	CLA	3	0
23	C	319	LMG	2	0
18	C	317	CLA	9	0
18	D	216	CLA	4	0
18	B	306	CLA	16	0
18	D	214	CLA	5	0
18	H	313	CLA	7	0
18	E	312	CLA	8	0
18	D	210	CLA	3	0
18	H	307	CLA	3	0
26	C	304	A86	1	0
18	B	308	CLA	2	0
26	B	302	A86	4	0
18	H	309	CLA	13	0
18	C	307	CLA	5	0
18	B	309	CLA	2	0
18	B	311	CLA	6	0
21	E	306	BCR	4	0
29	B	313	KC1	5	0

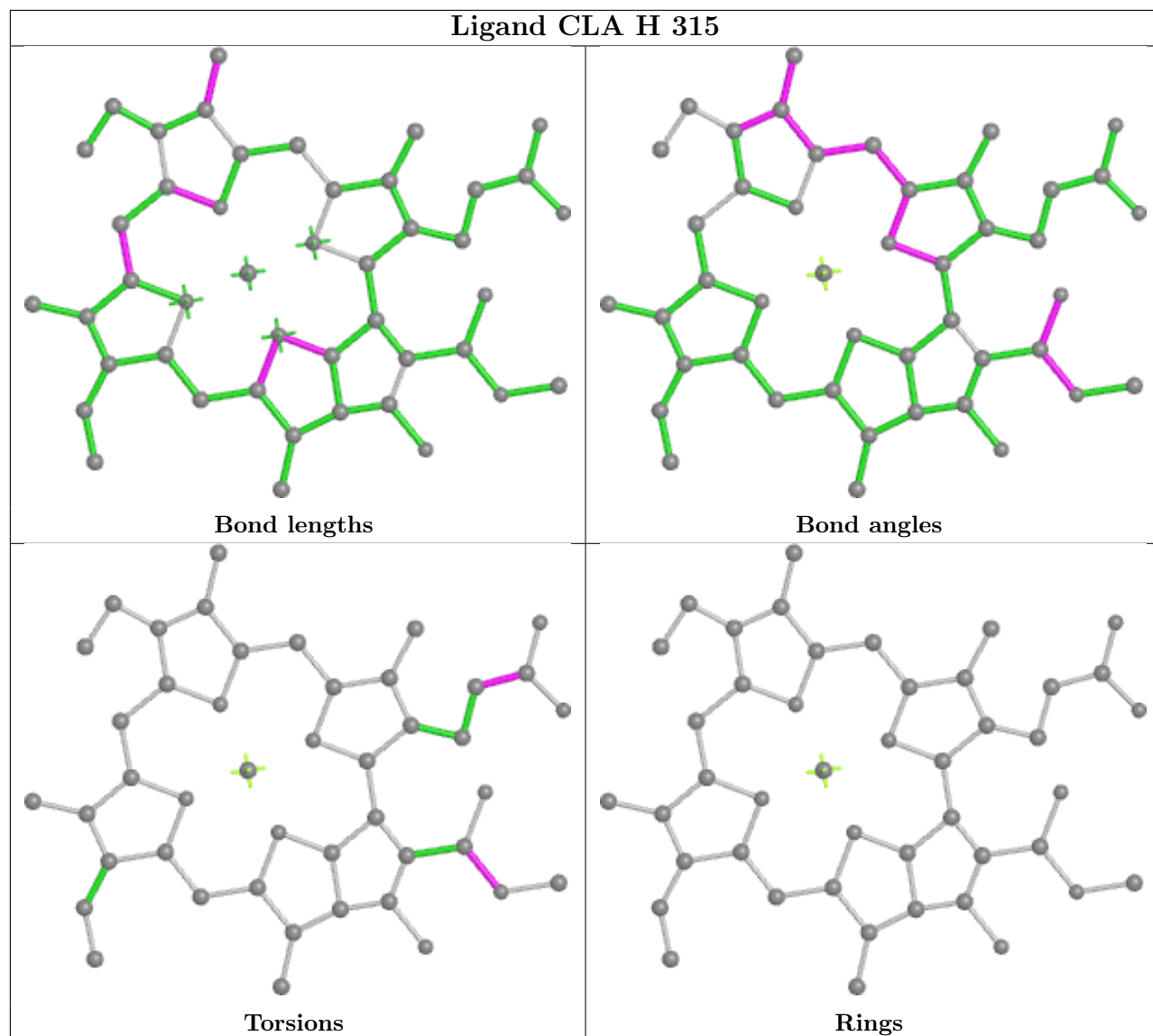
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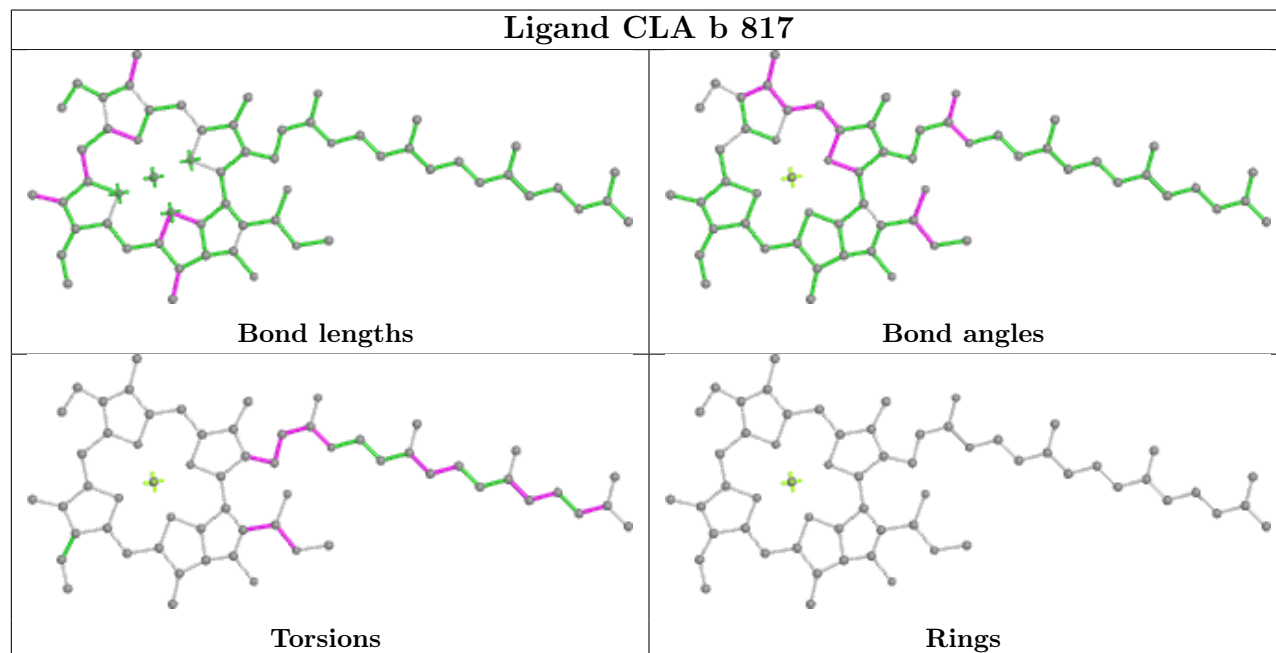
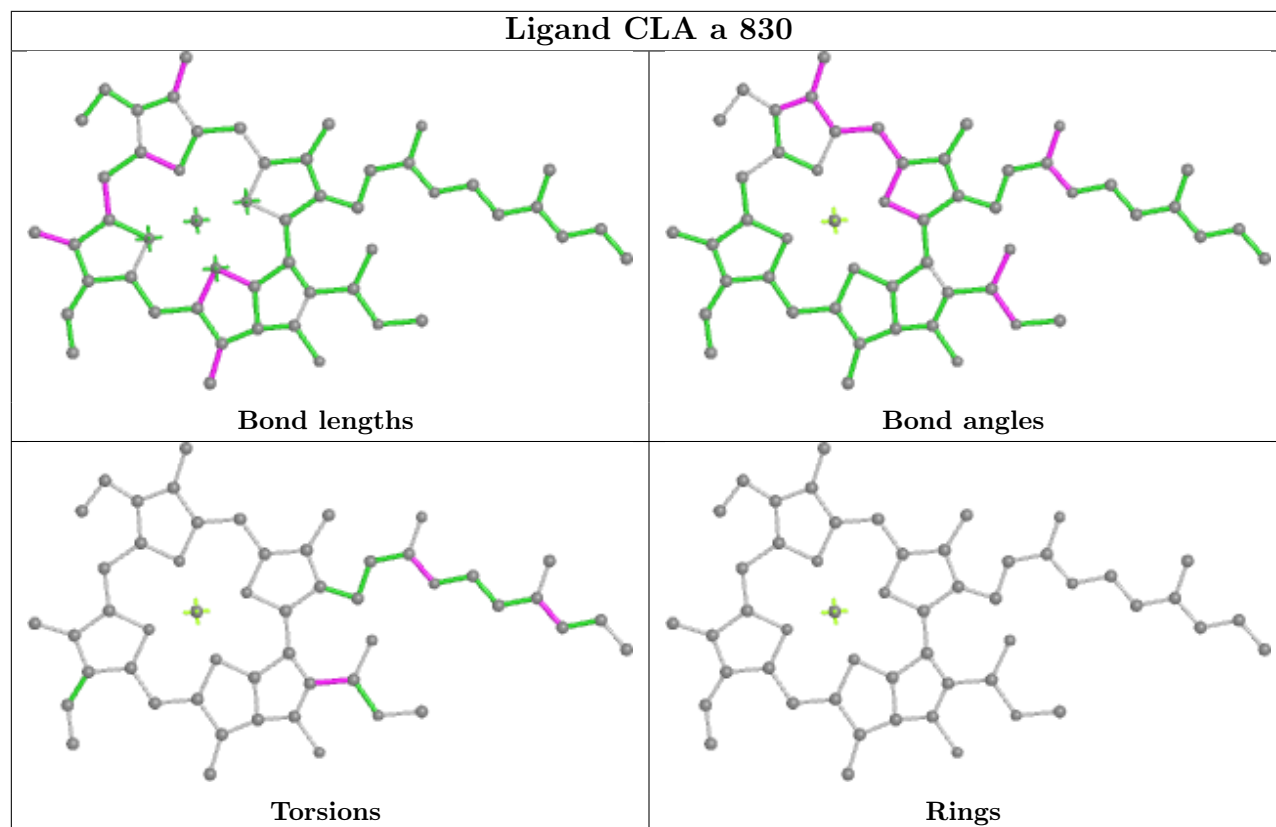
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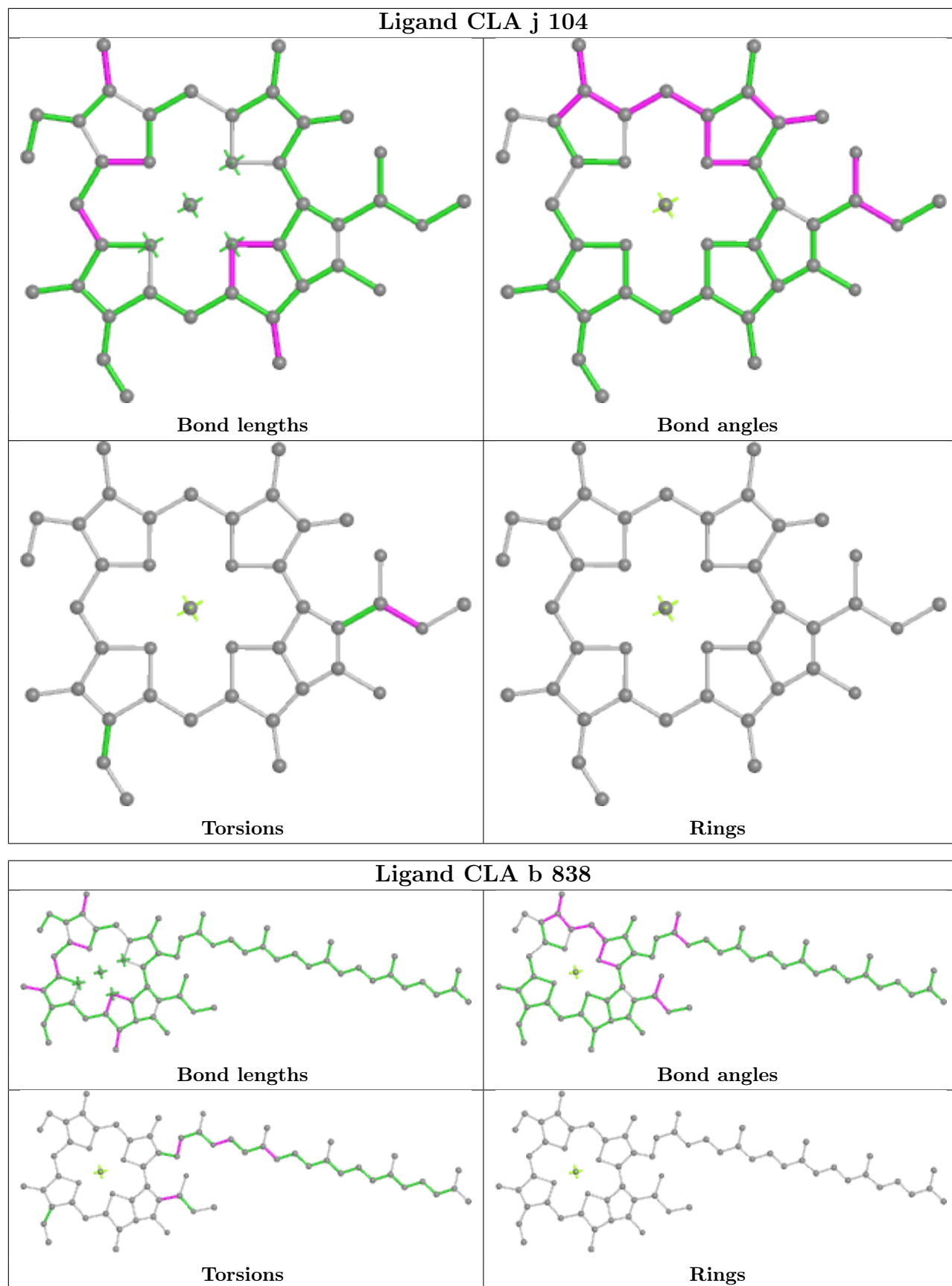
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	H	308	CLA	5	0
18	H	305	CLA	5	0
18	H	311	CLA	7	0
18	C	316	CLA	10	0
18	E	309	CLA	6	0
18	E	316	CLA	6	0
29	C	308	KC1	4	0
18	C	314	CLA	3	0
28	C	303	DD6	1	0
18	B	307	CLA	5	0
18	D	215	CLA	6	0
26	H	302	A86	14	0
26	C	305	A86	4	0
26	B	304	A86	2	0
18	C	318	CLA	12	0
18	E	311	CLA	1	0
29	H	312	KC1	1	0
18	D	208	CLA	9	0
18	D	209	CLA	4	0
28	H	303	DD6	3	0
18	D	207	CLA	3	0
18	E	315	CLA	3	0
18	D	211	CLA	2	0
28	D	205	DD6	2	0
18	E	310	CLA	1	0
18	B	314	CLA	2	0

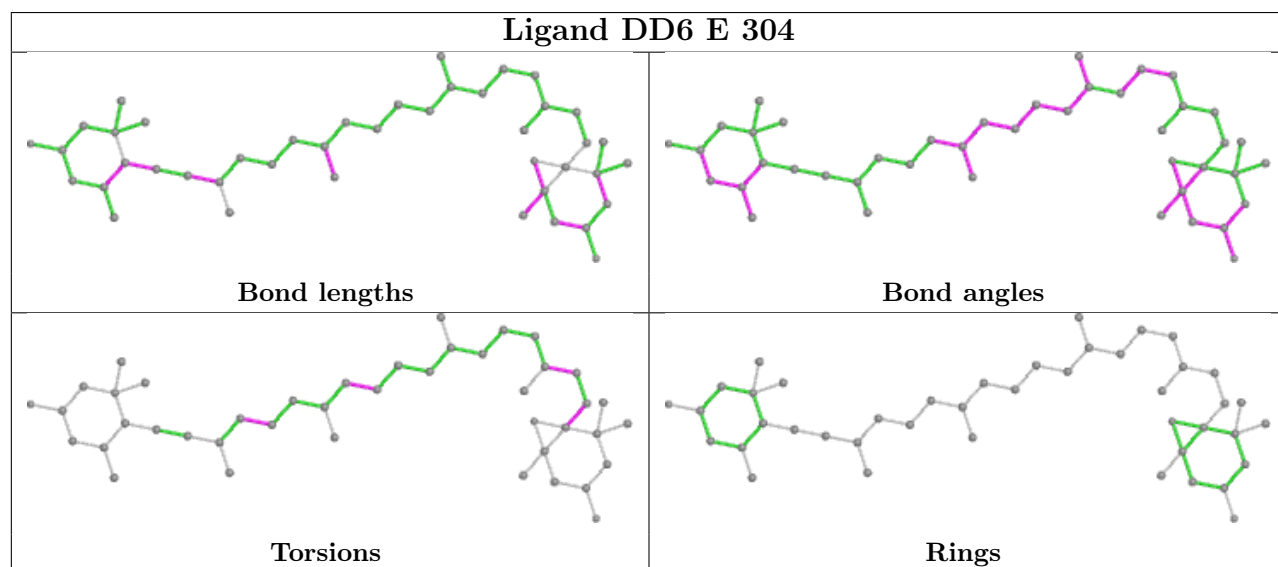
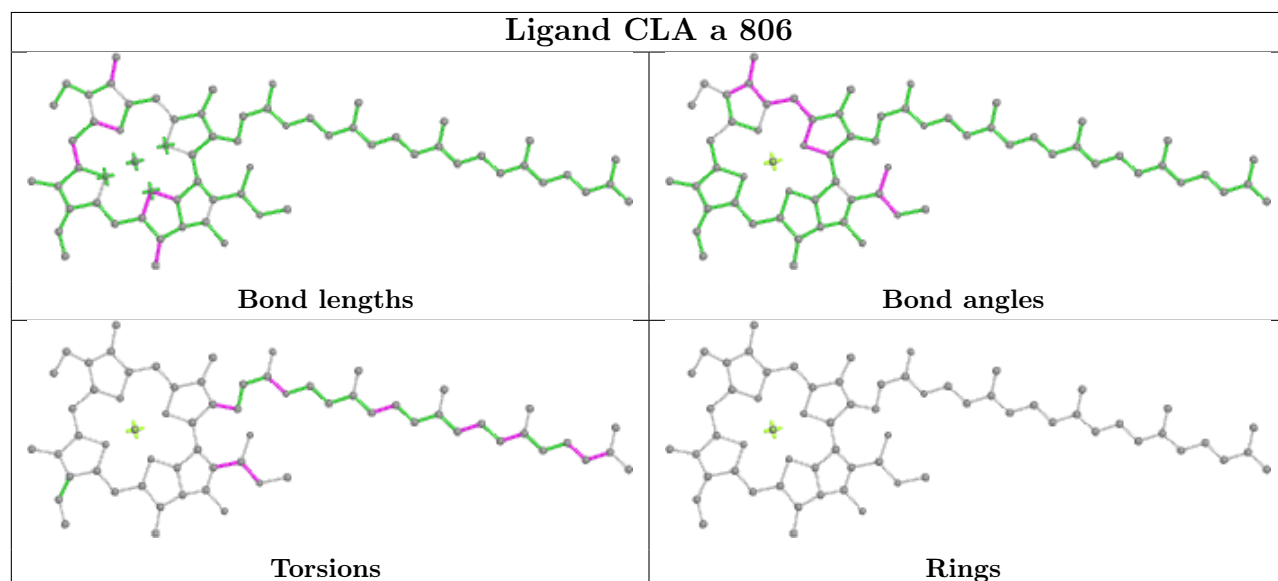
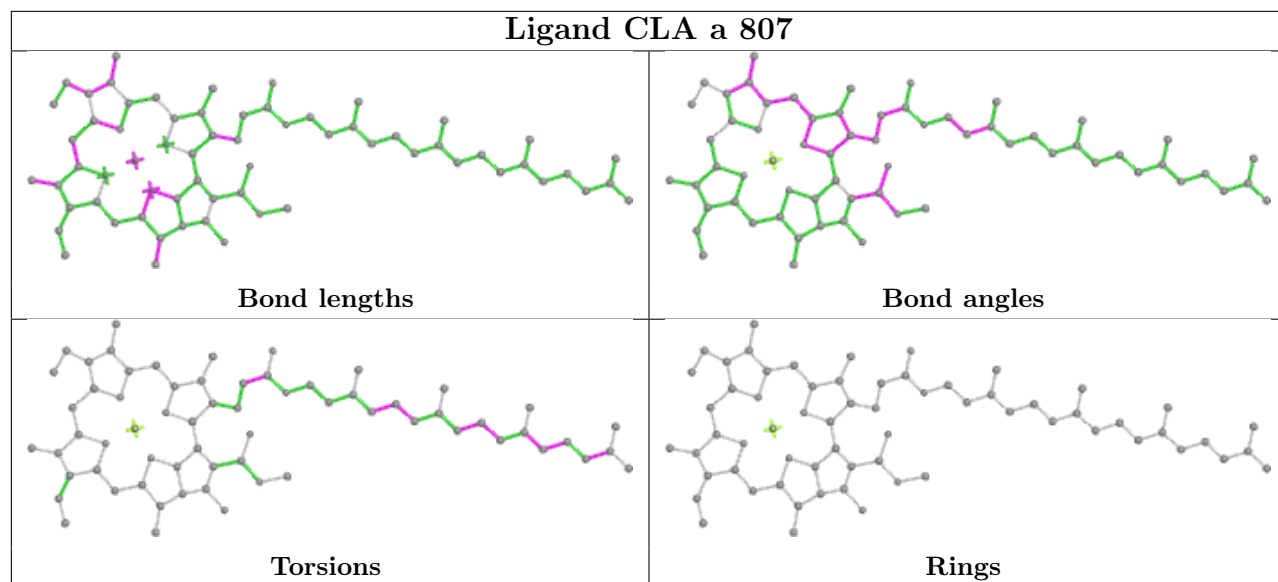
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

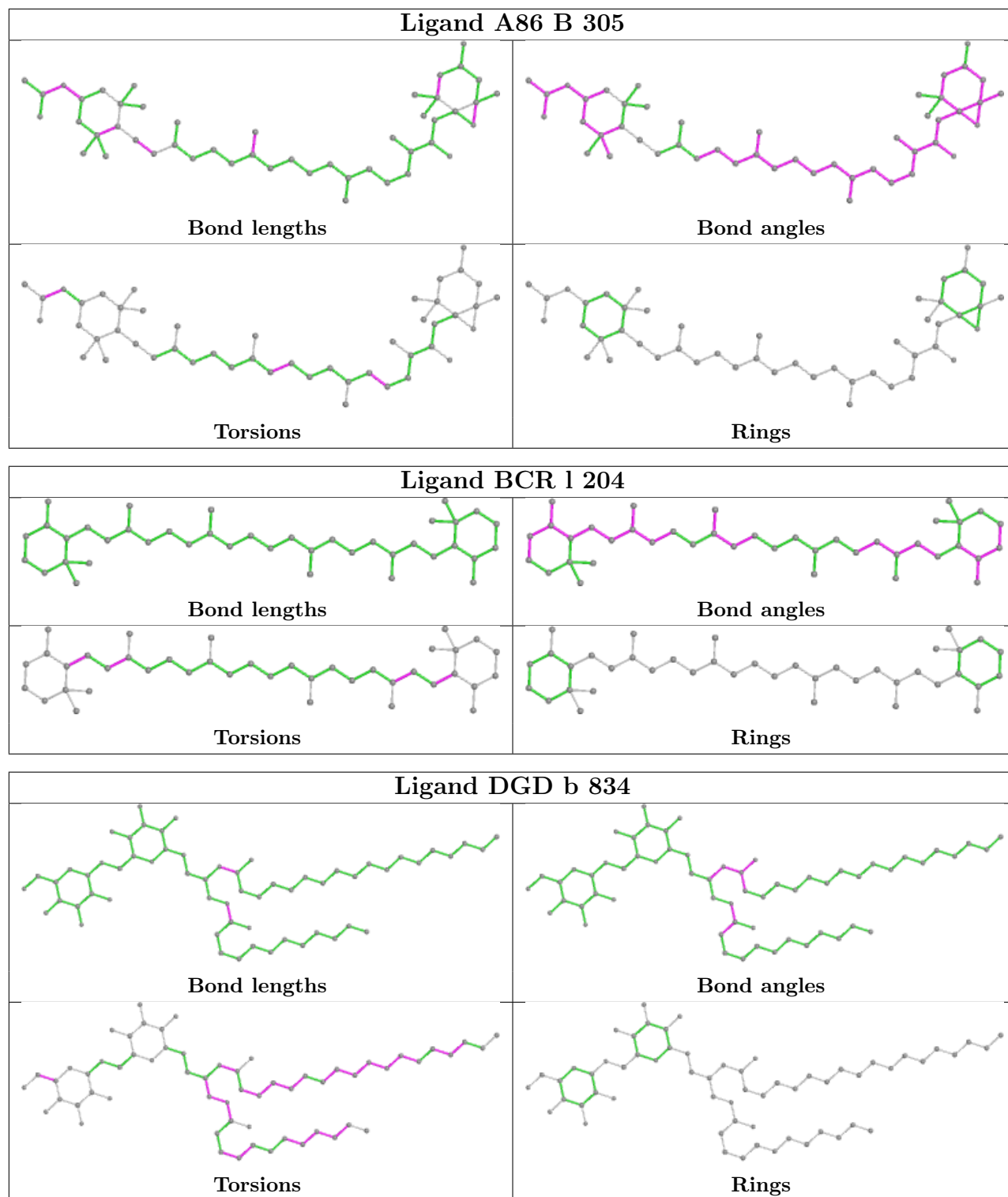


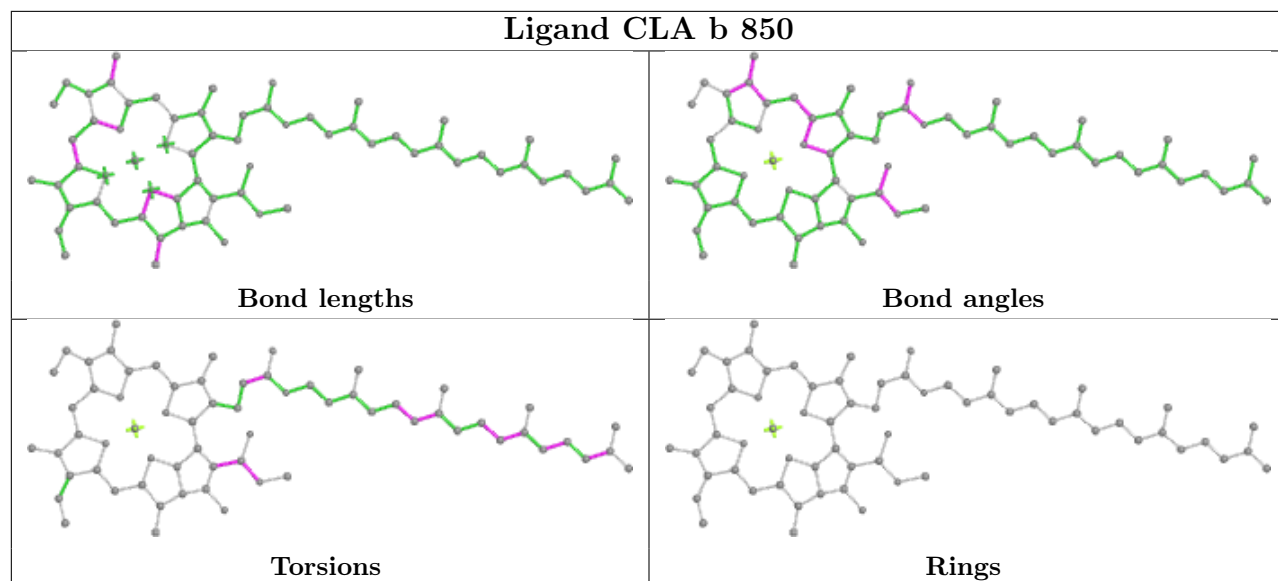
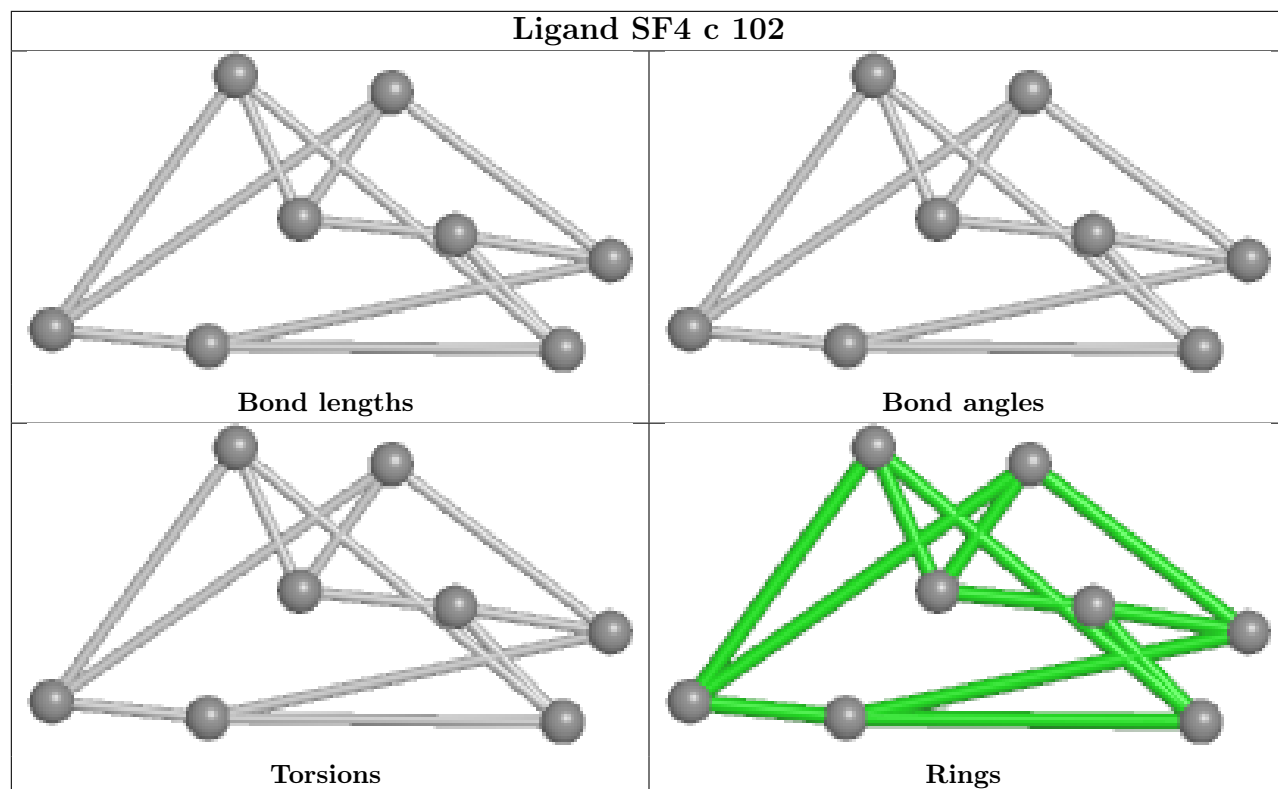


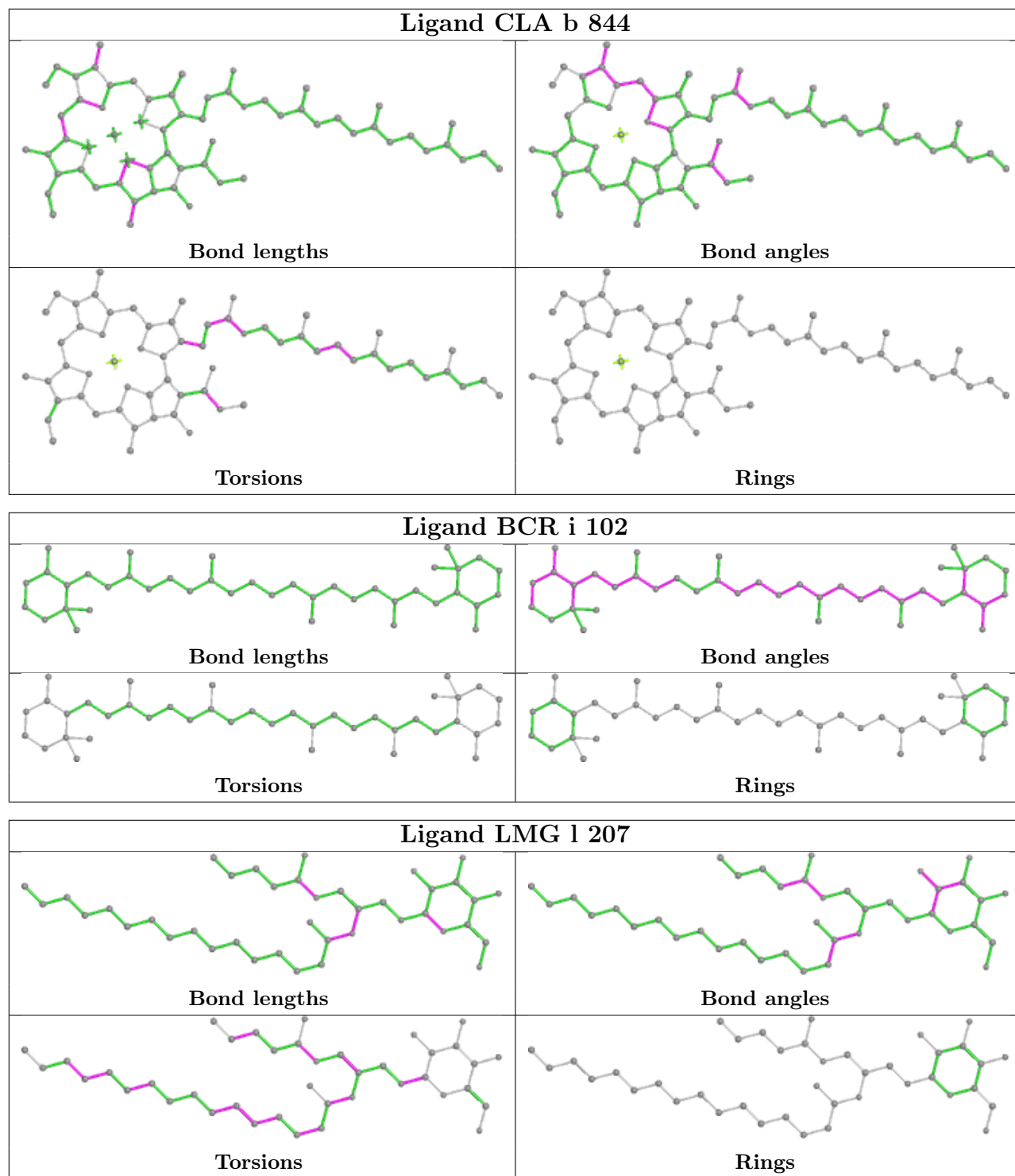


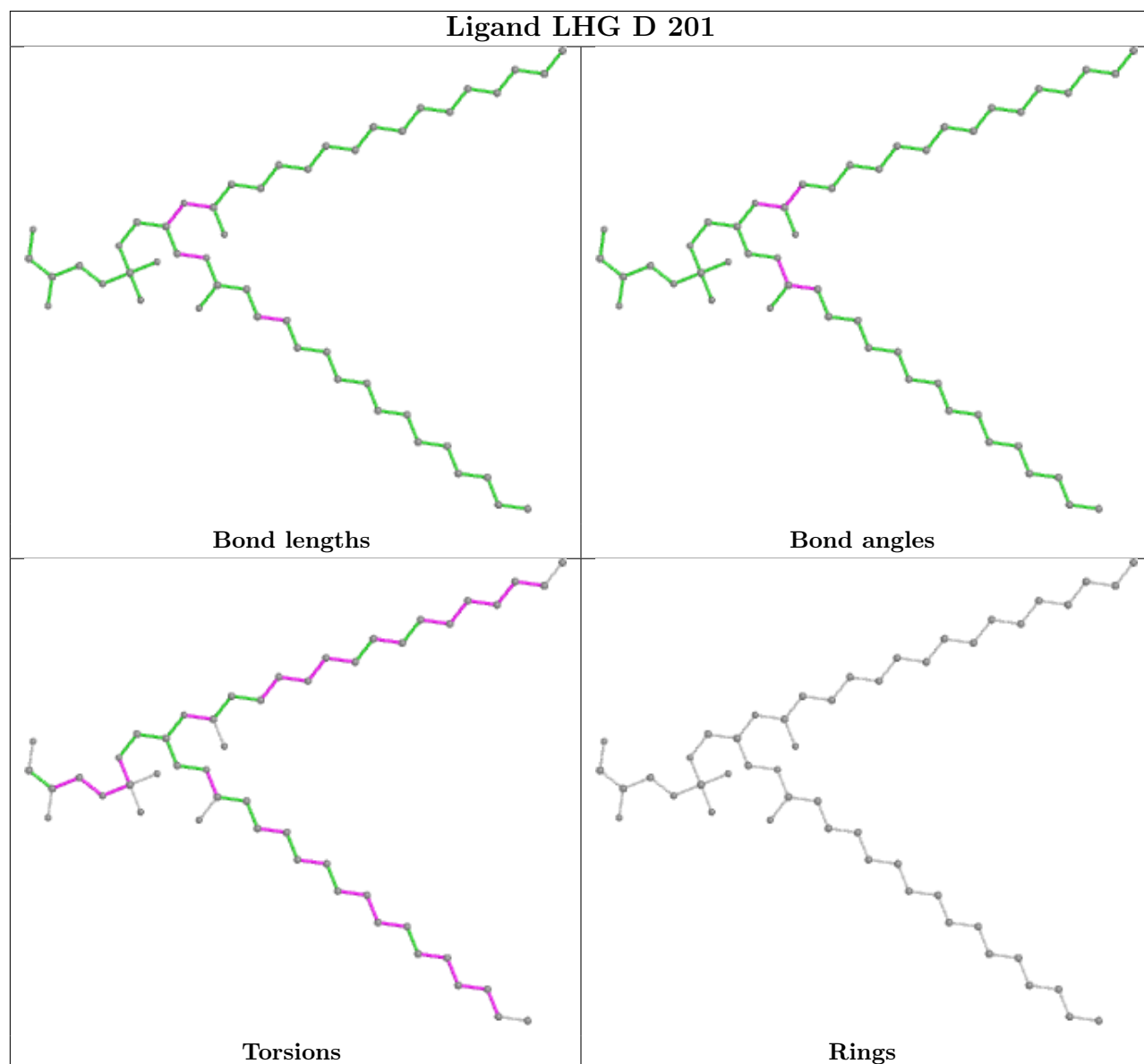
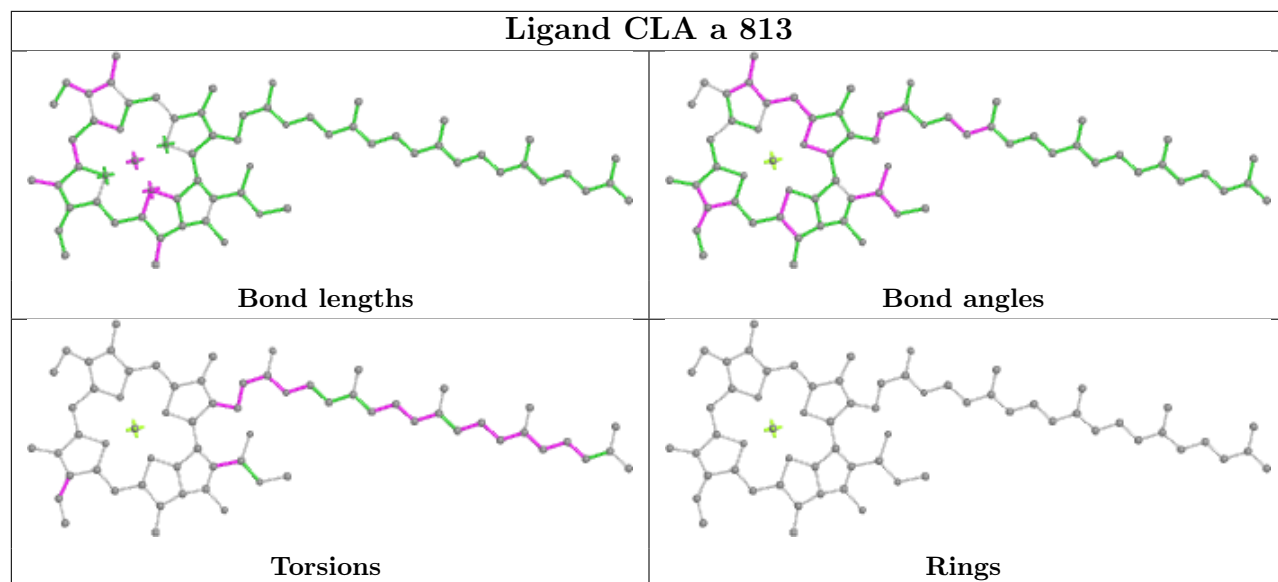


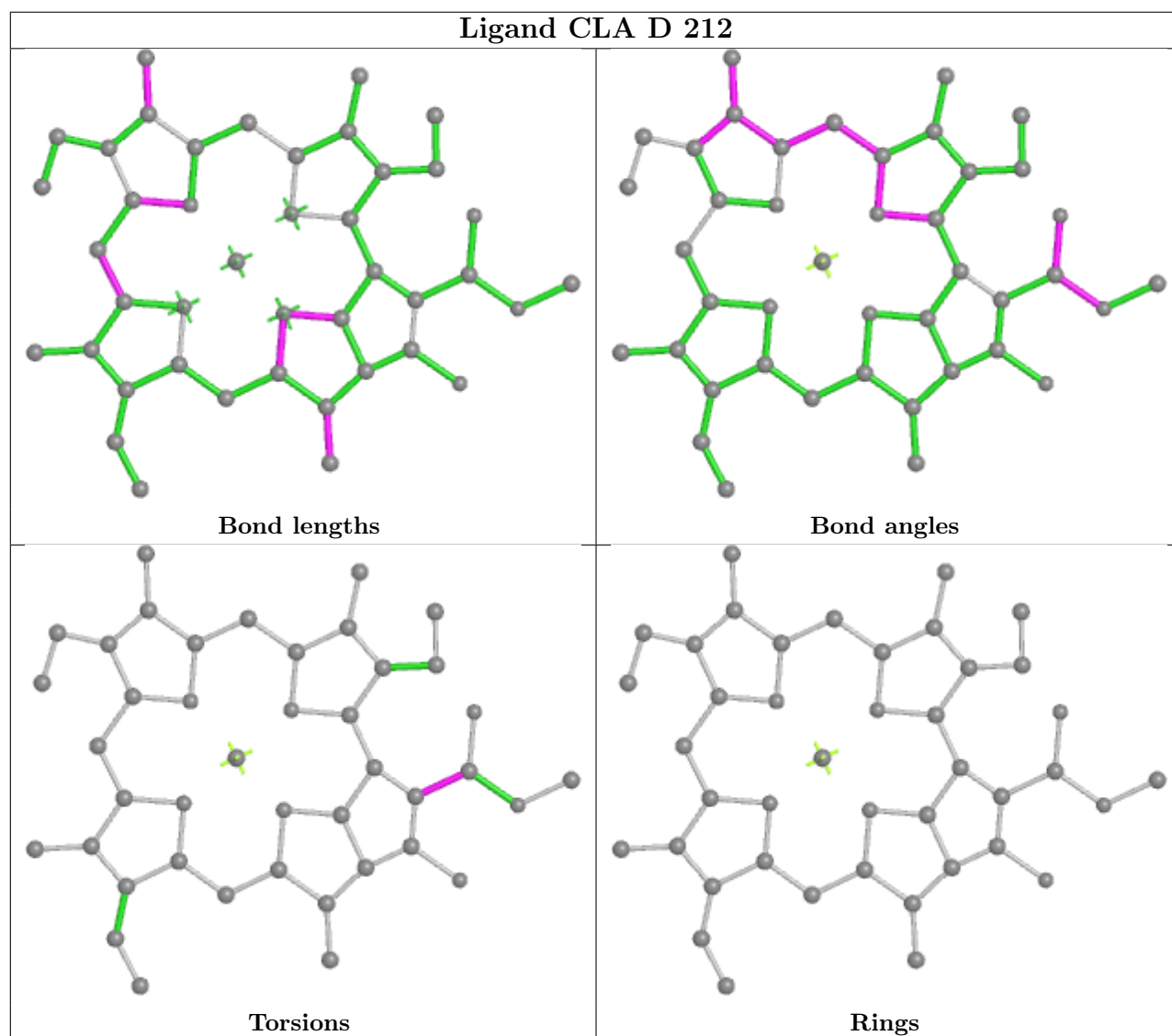
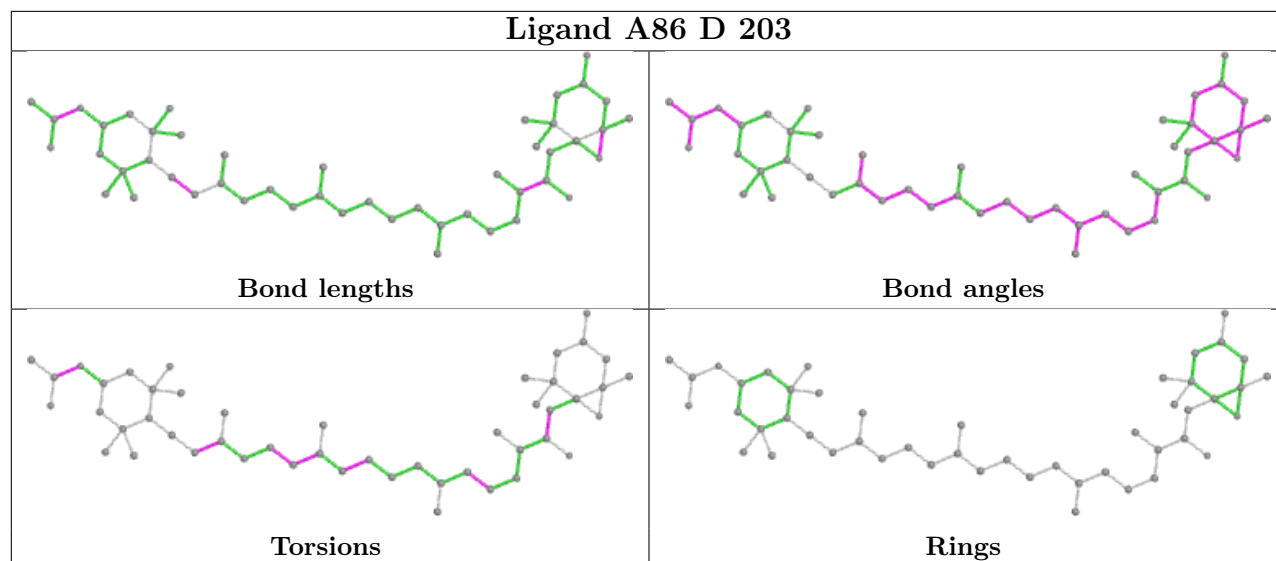


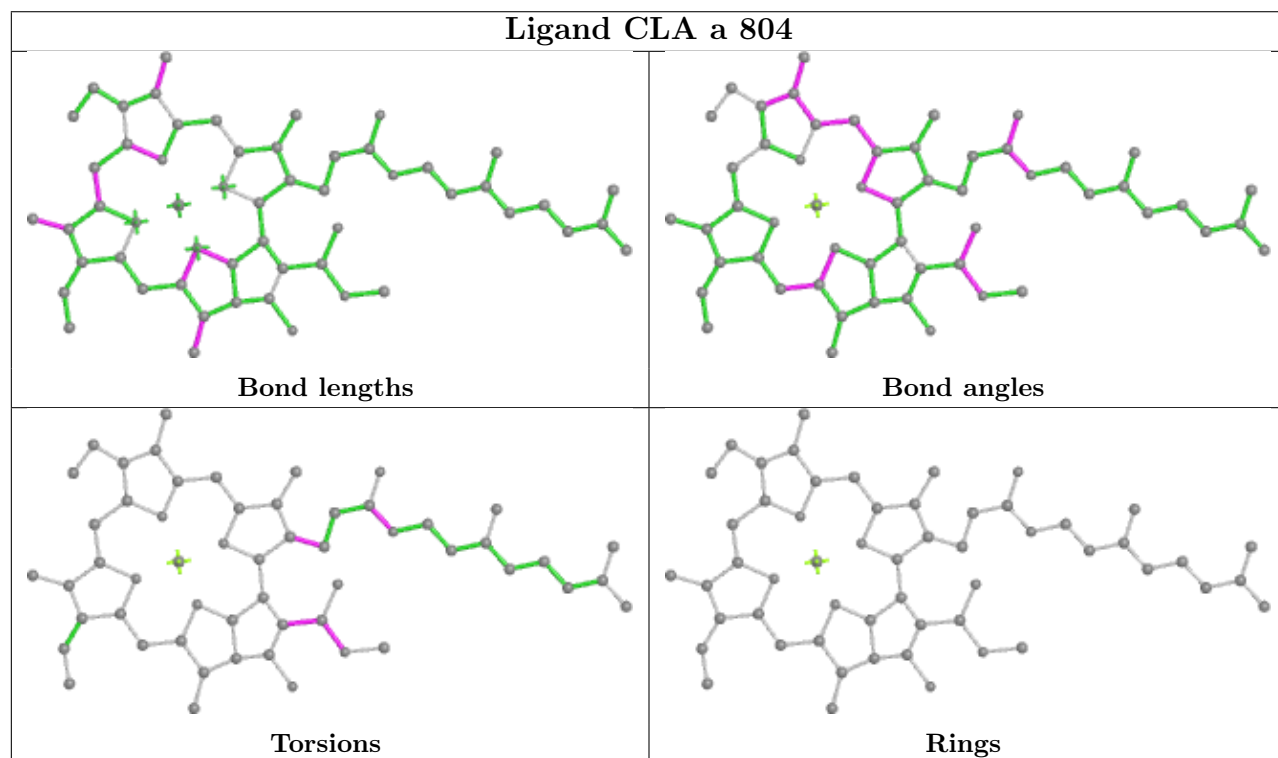
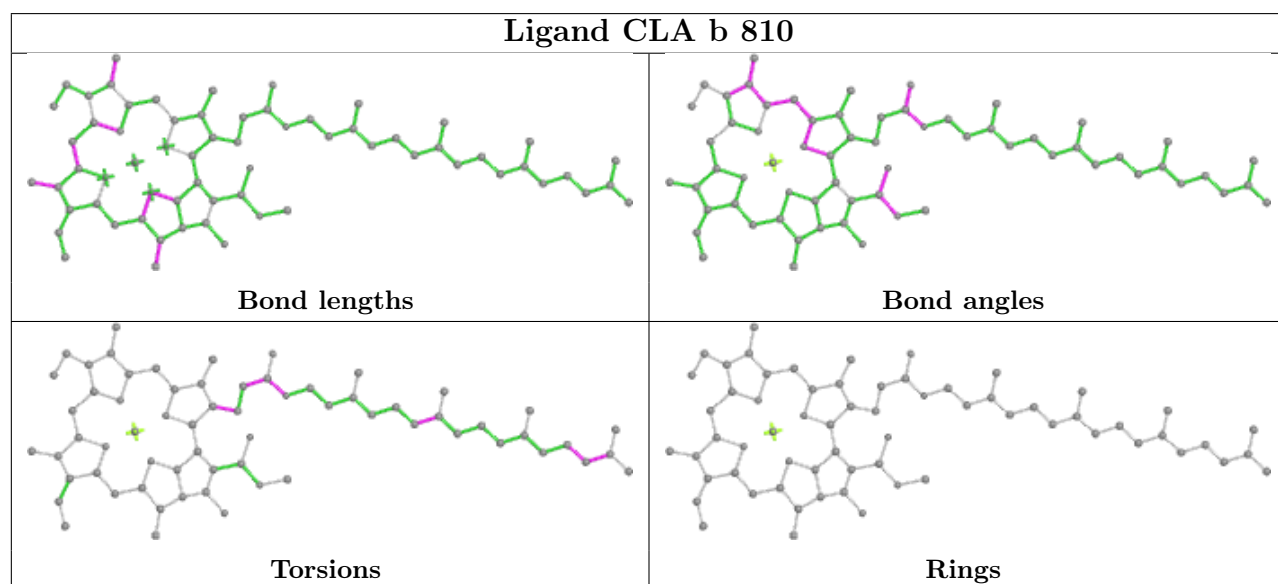
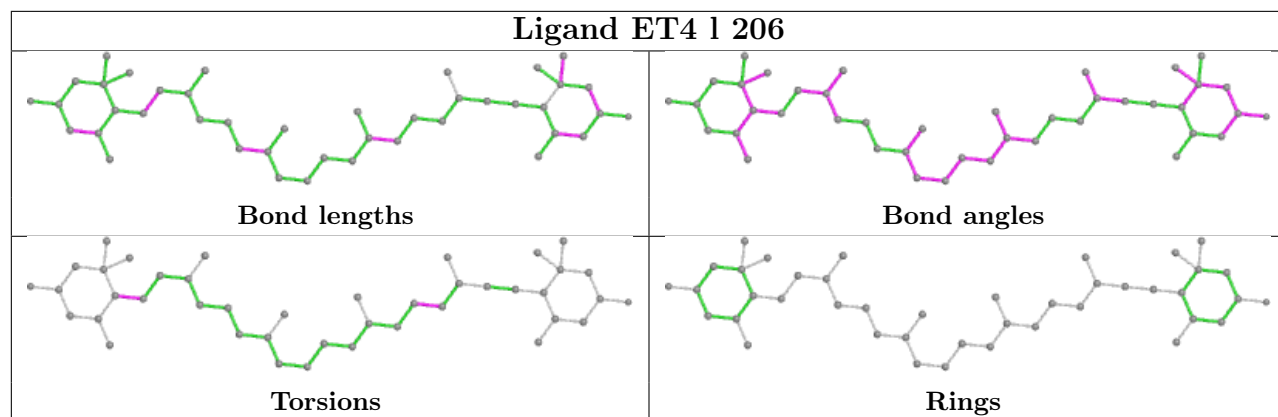


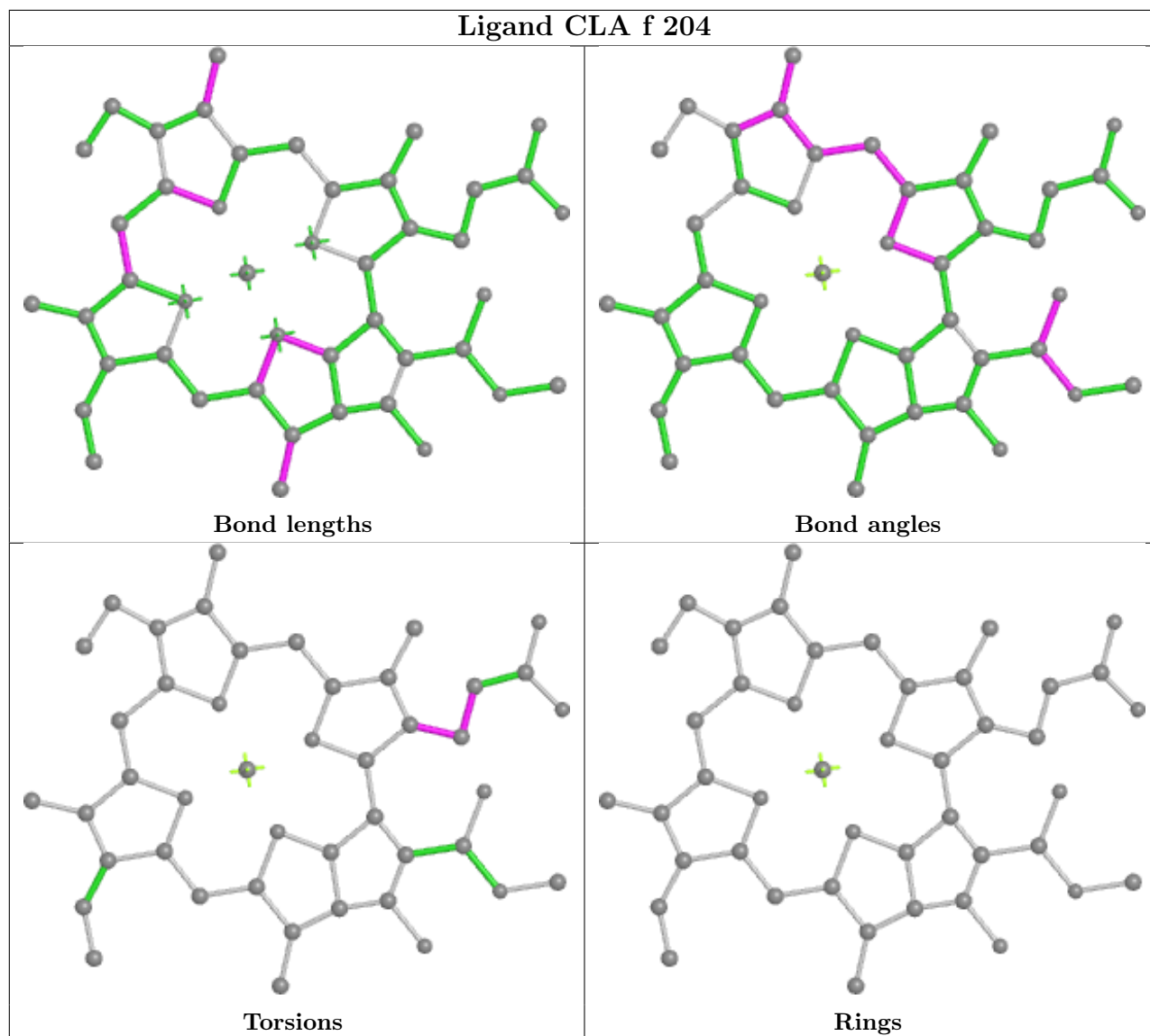
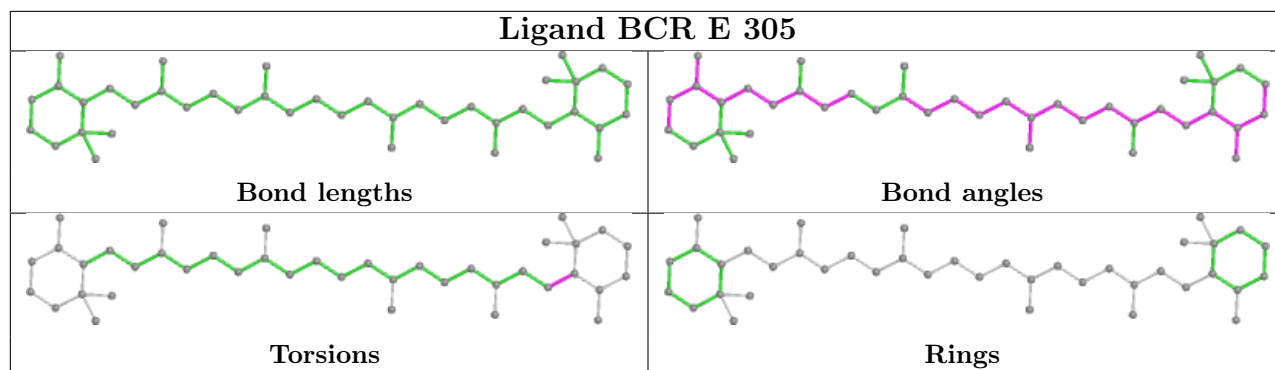


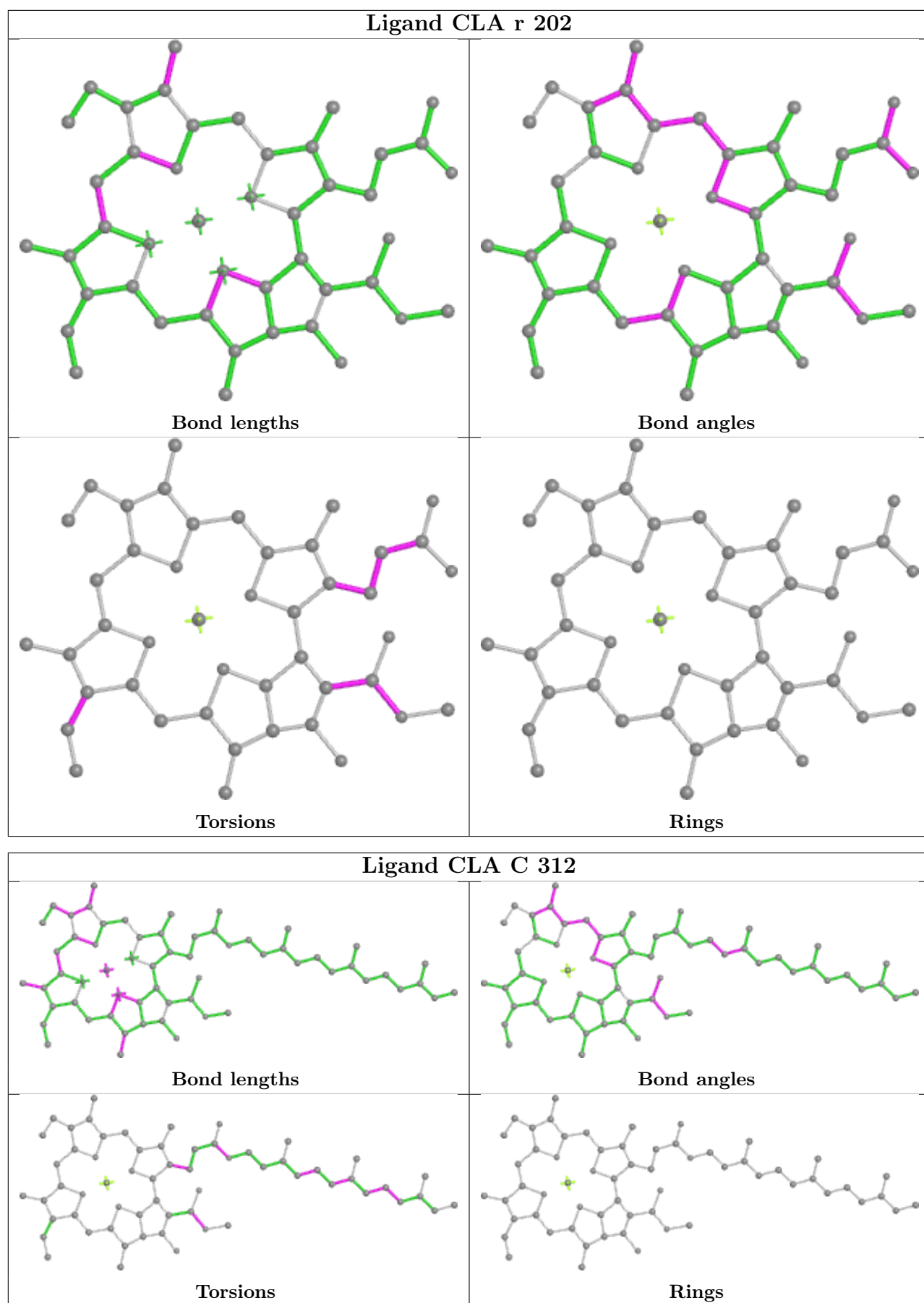


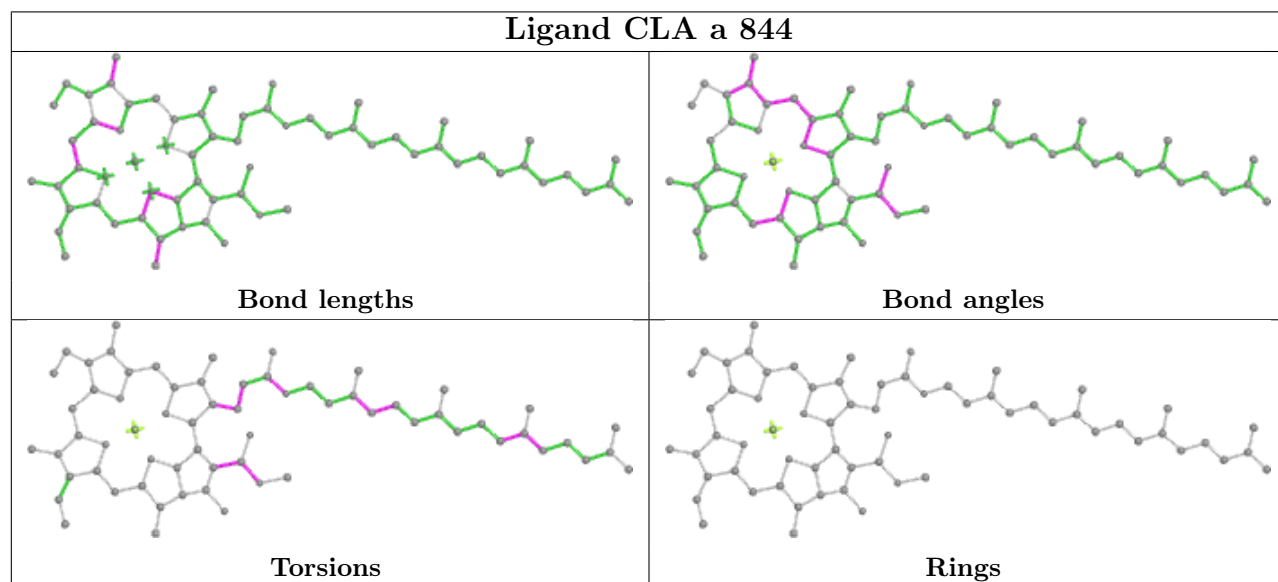
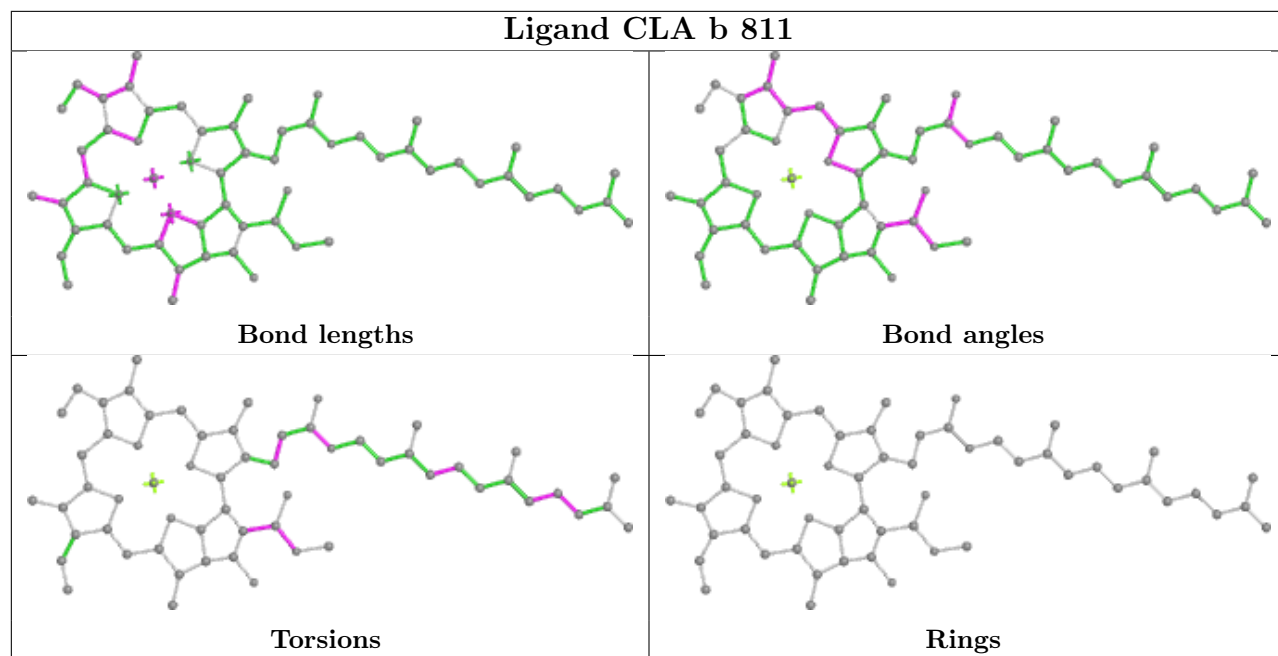


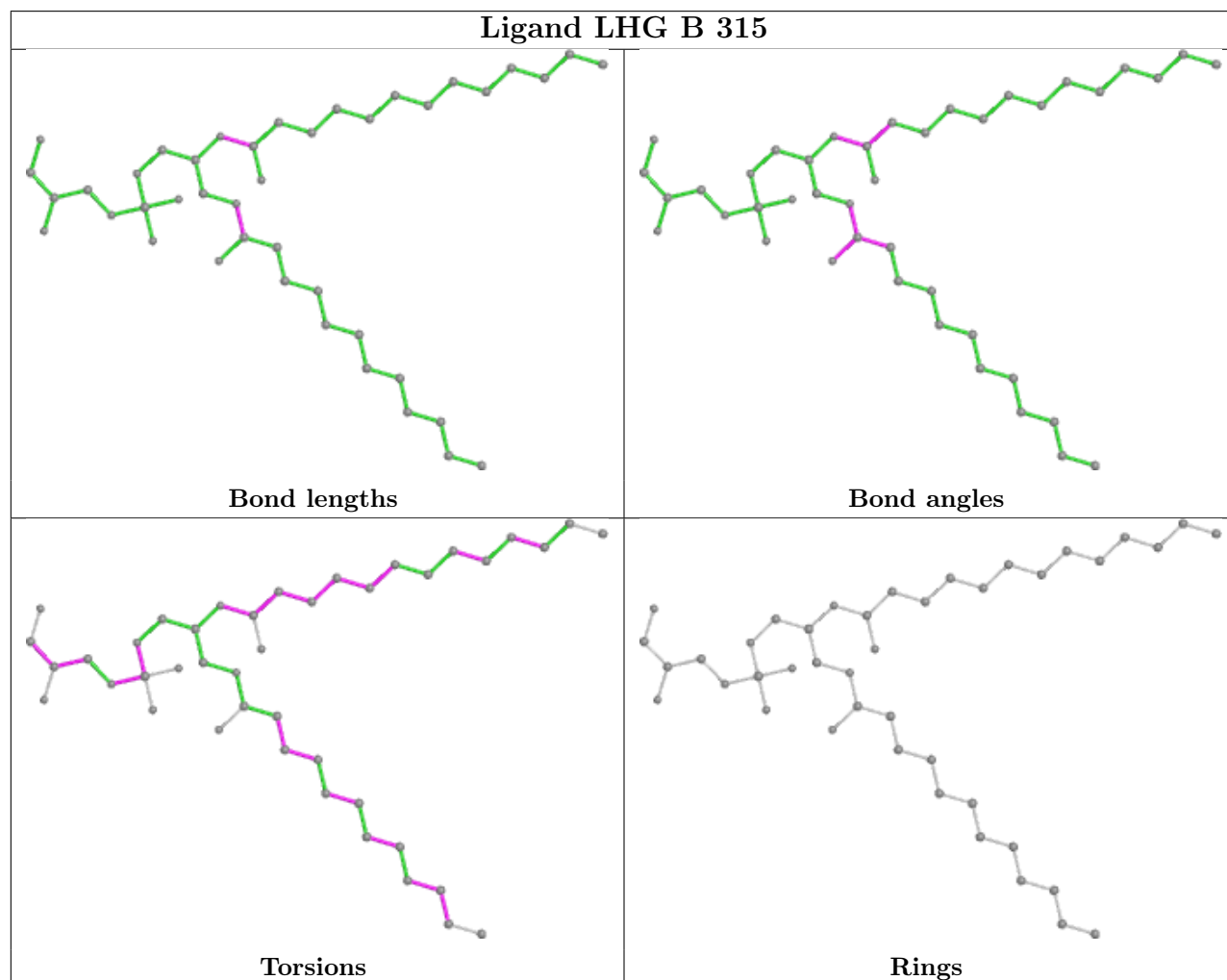
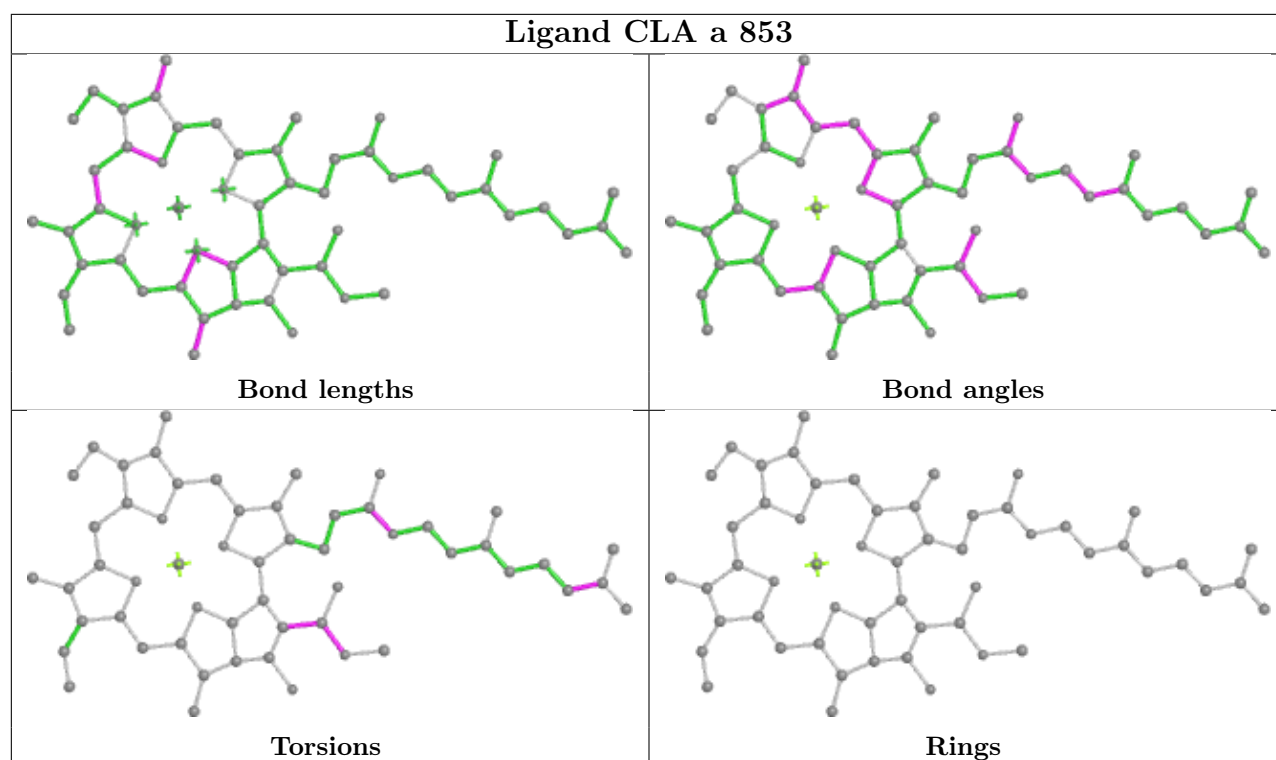


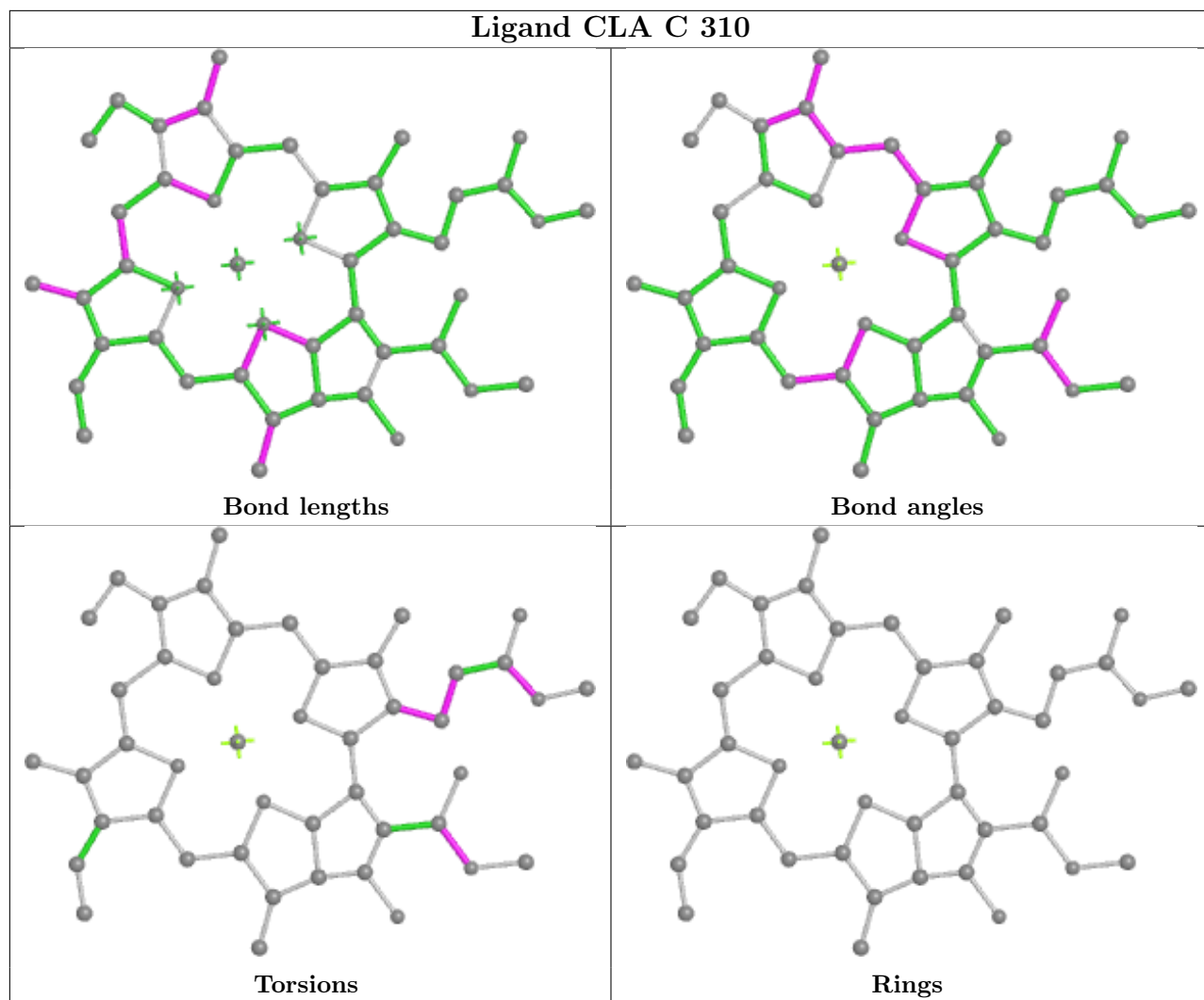


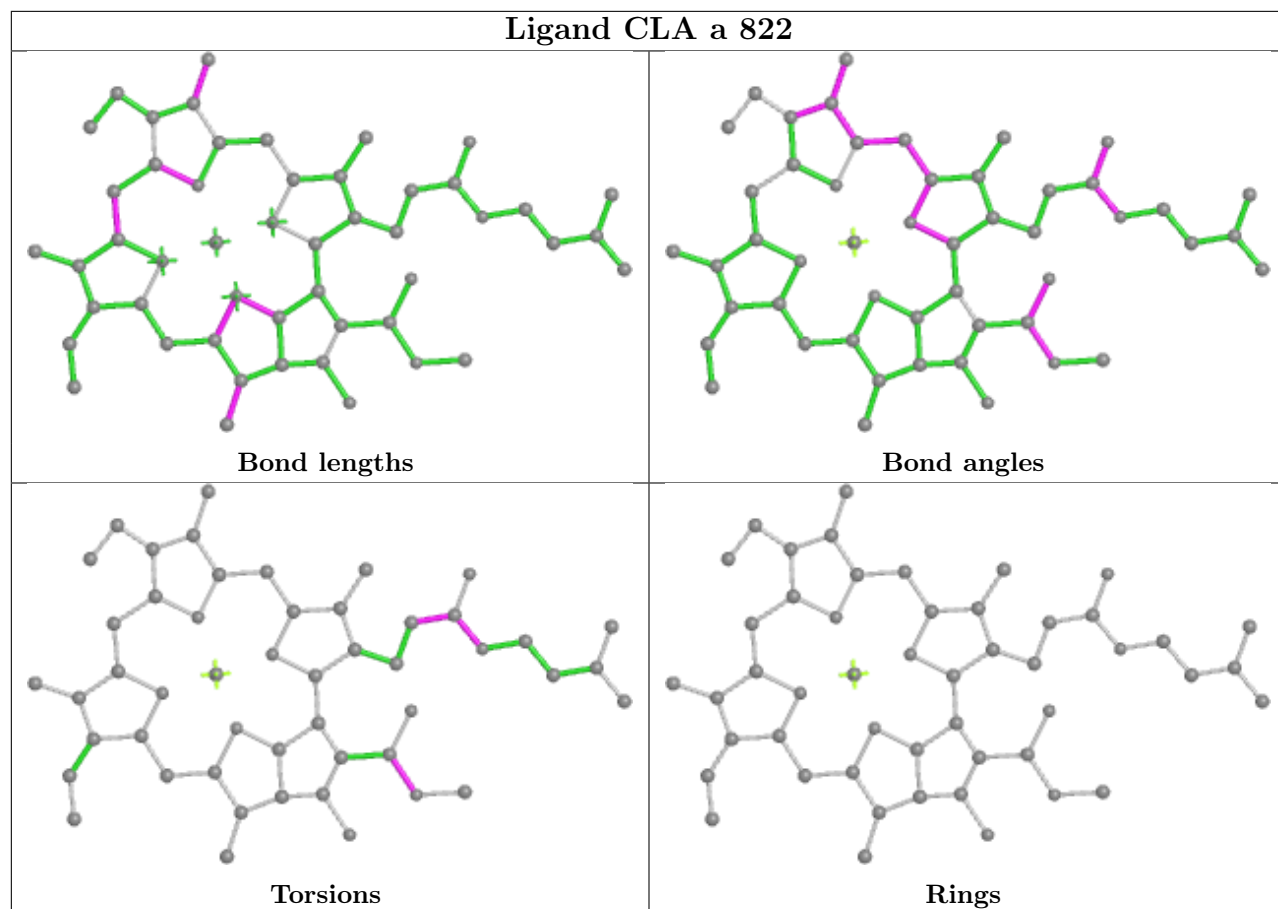


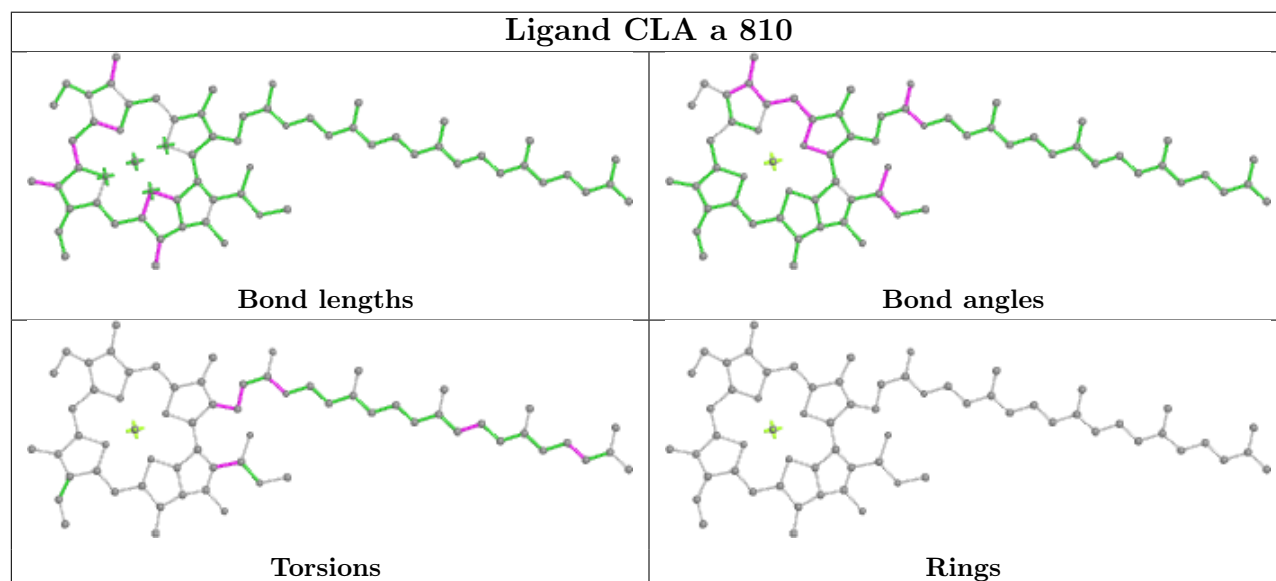
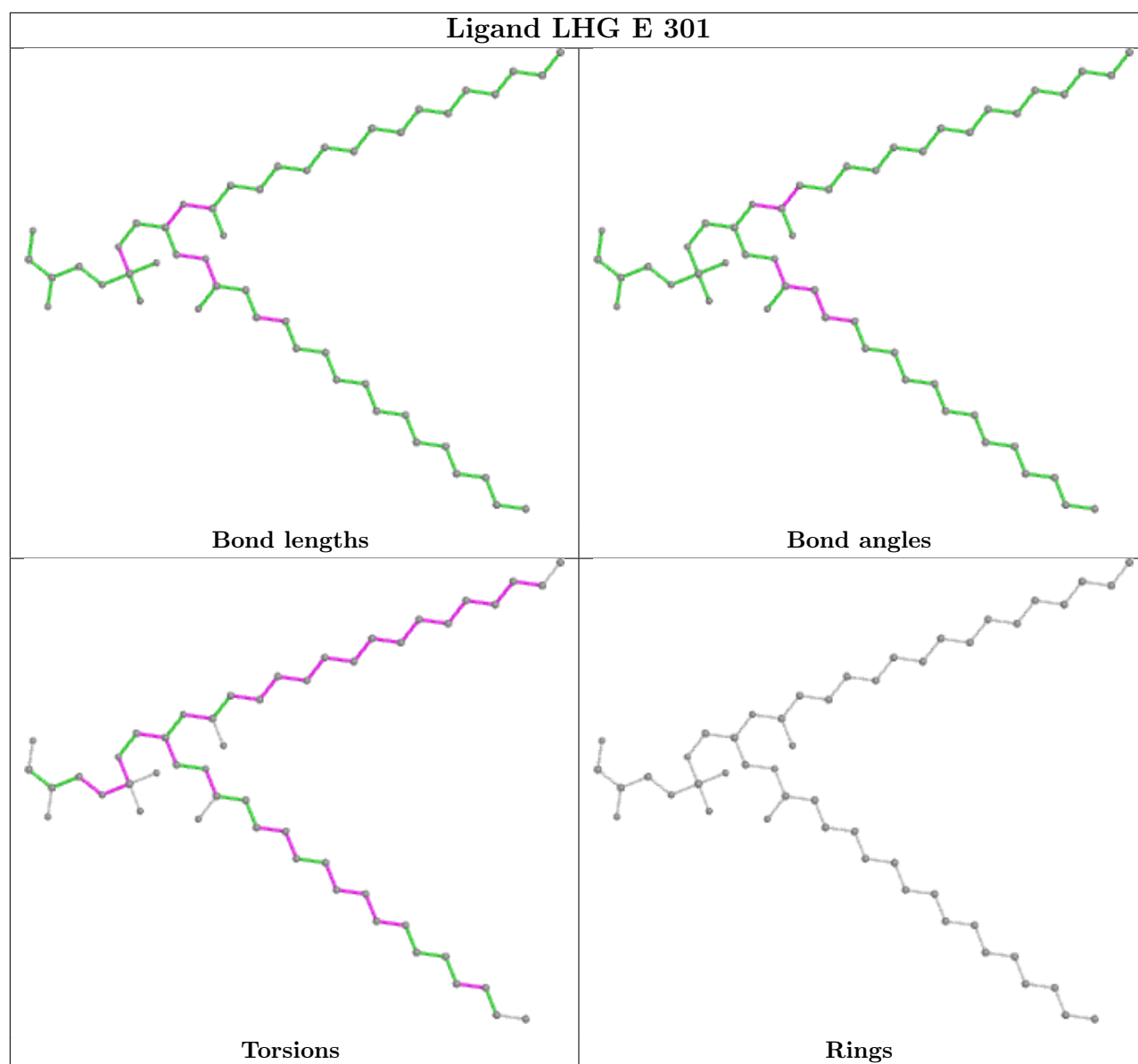


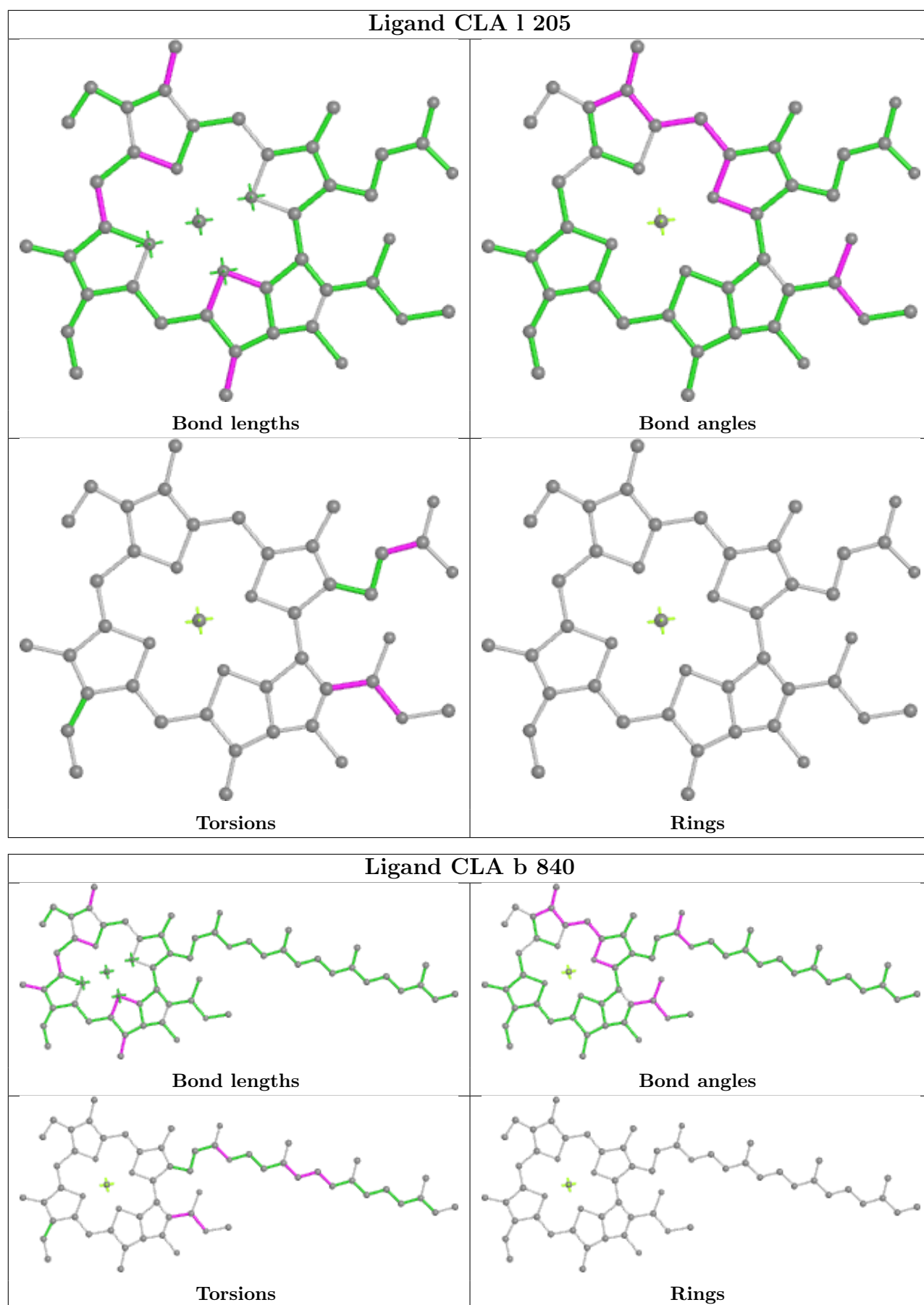


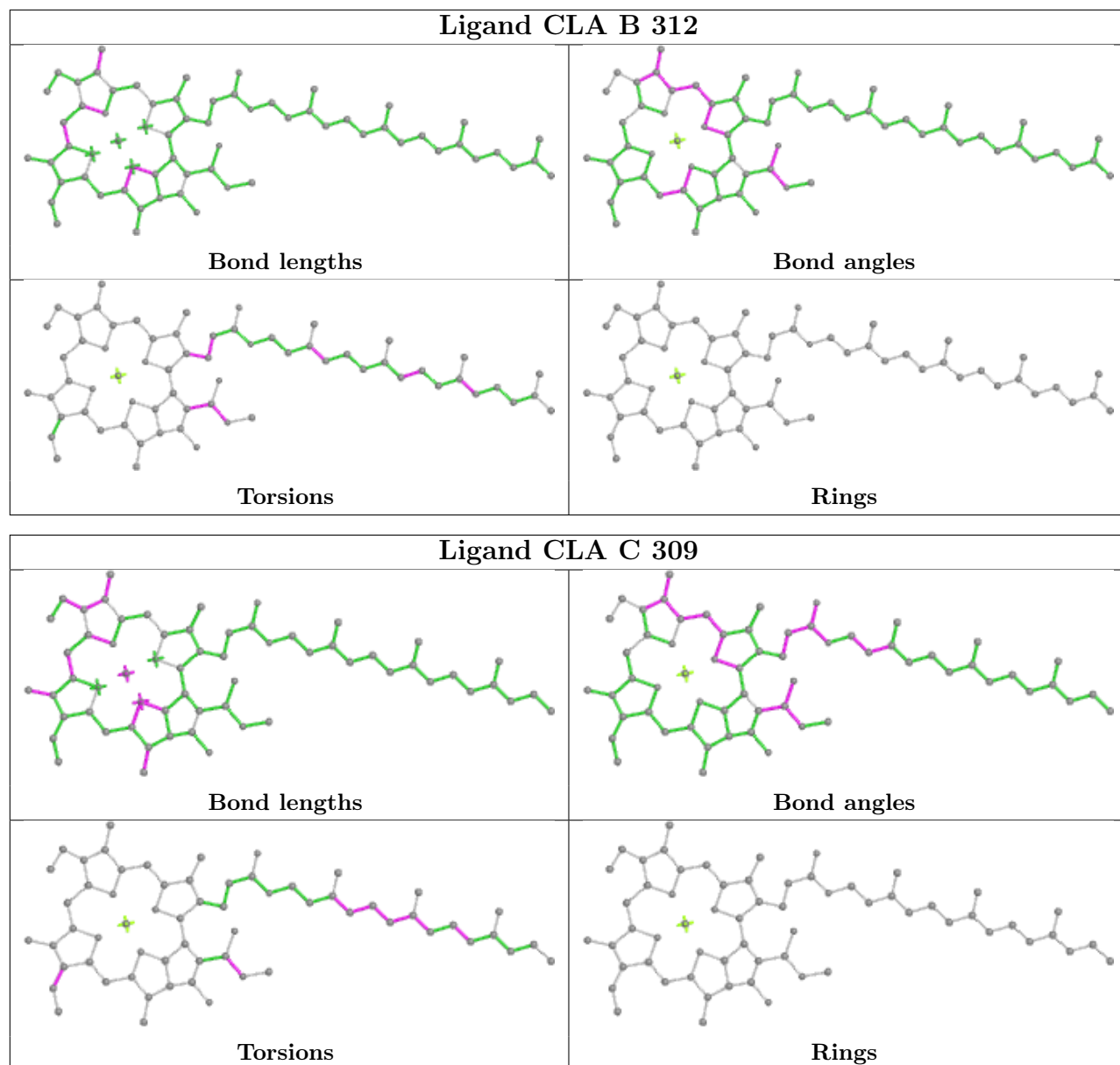


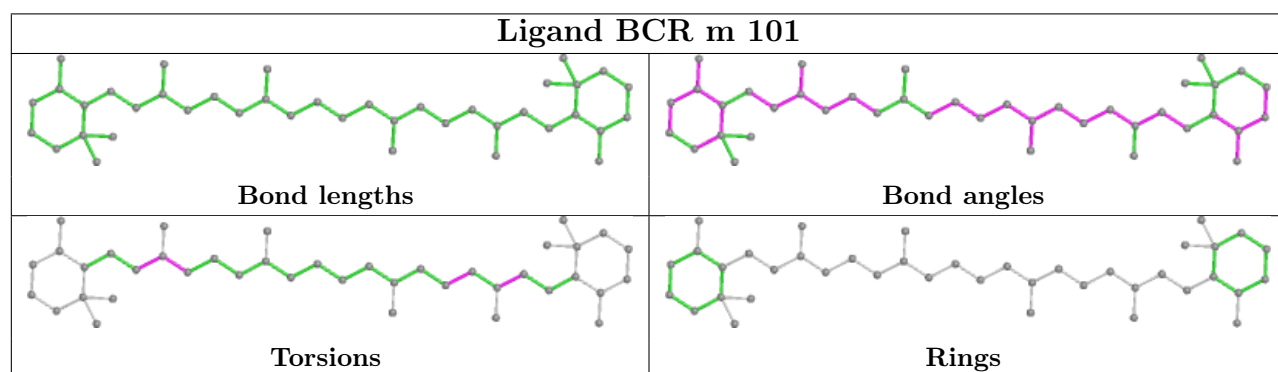
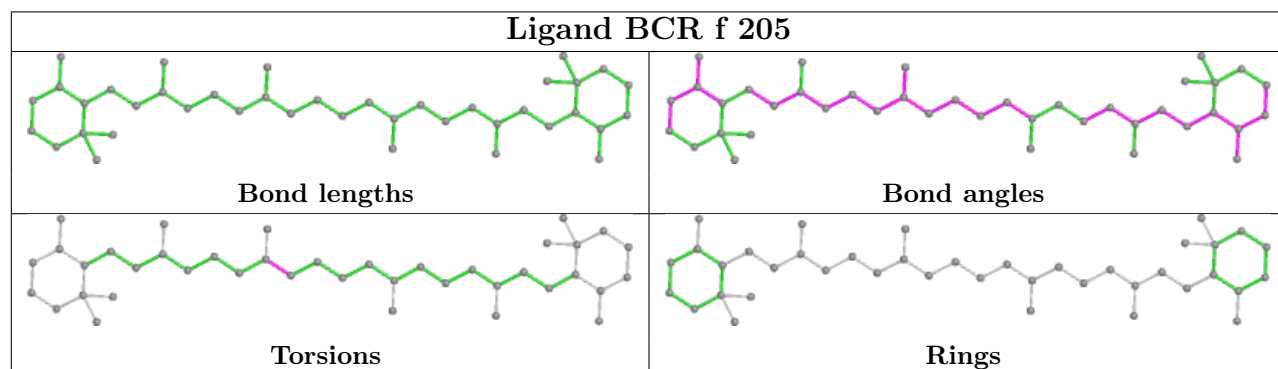
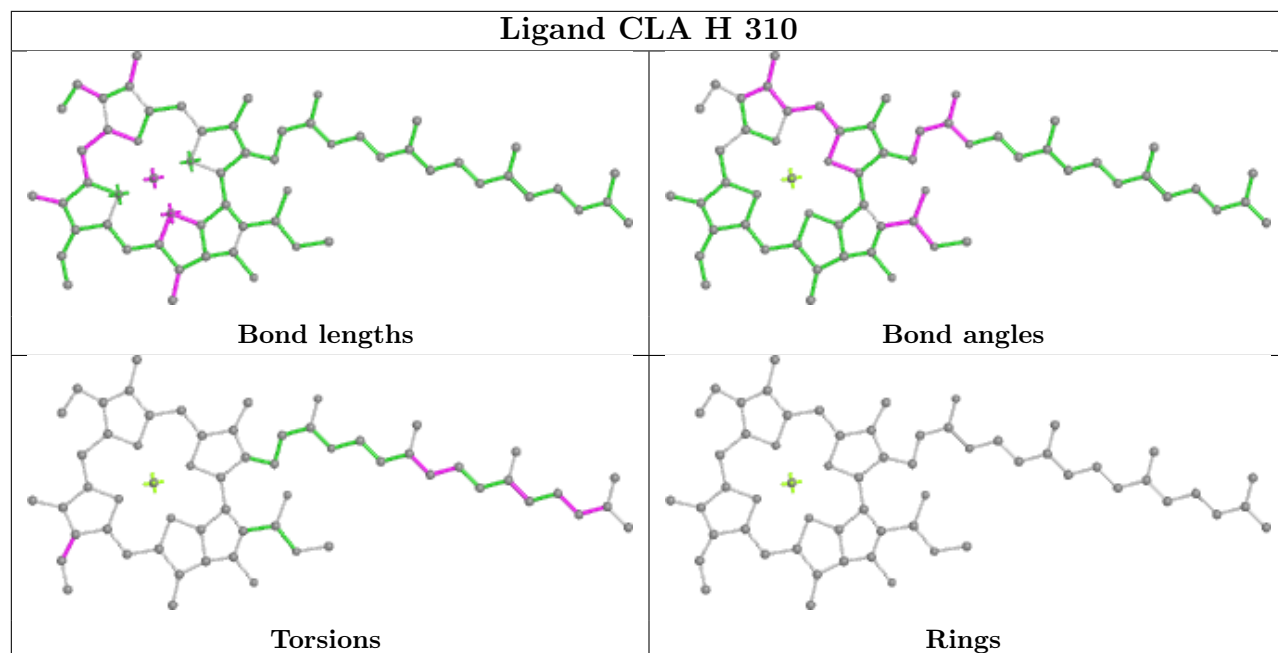


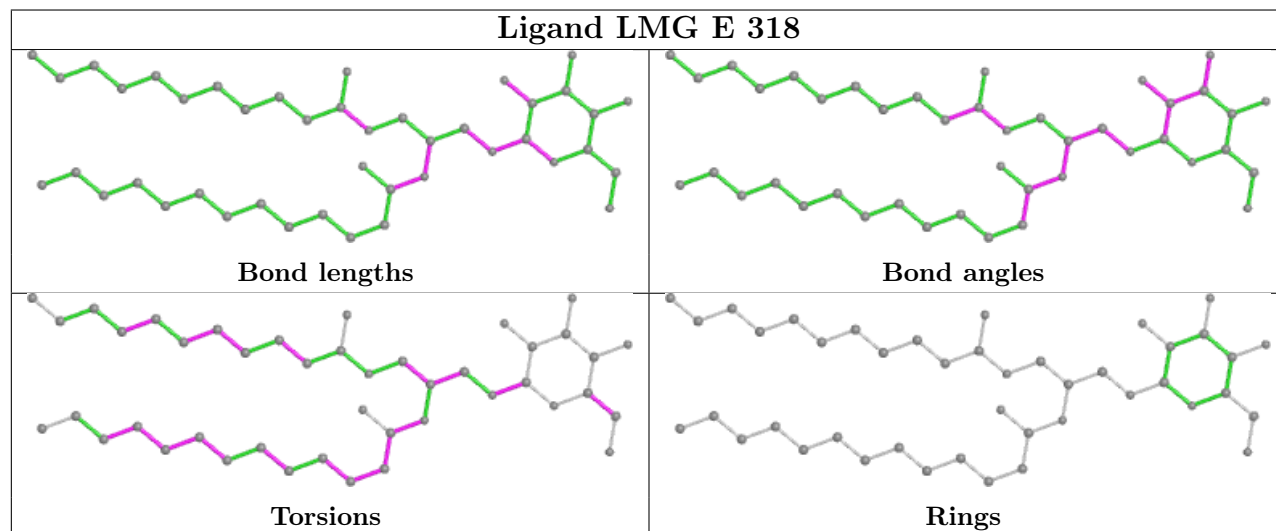
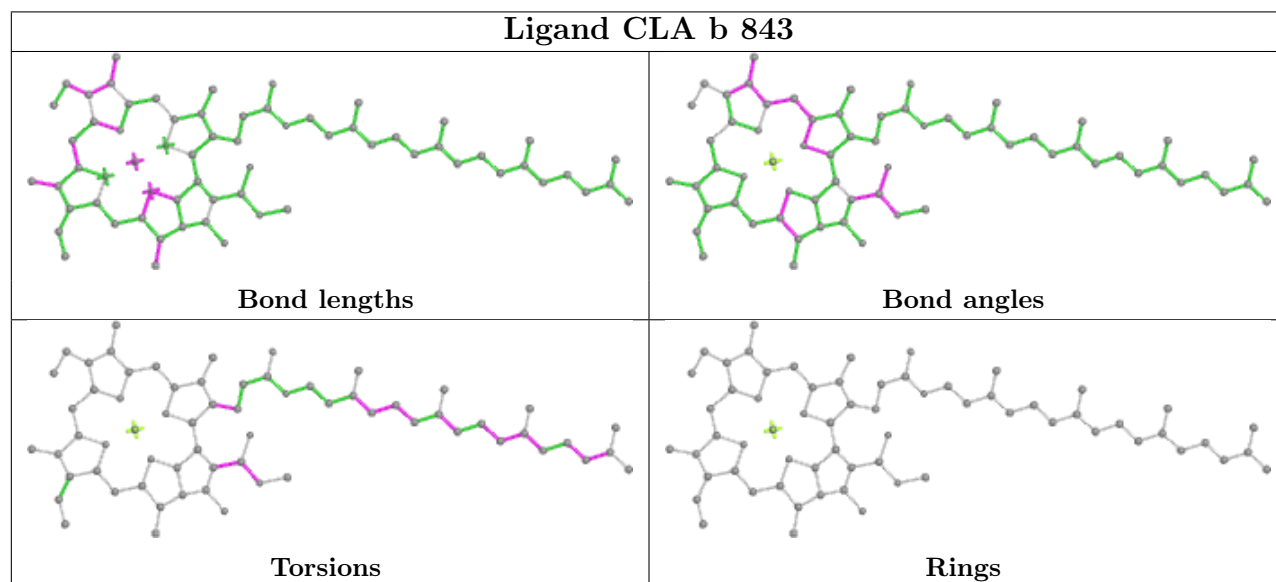
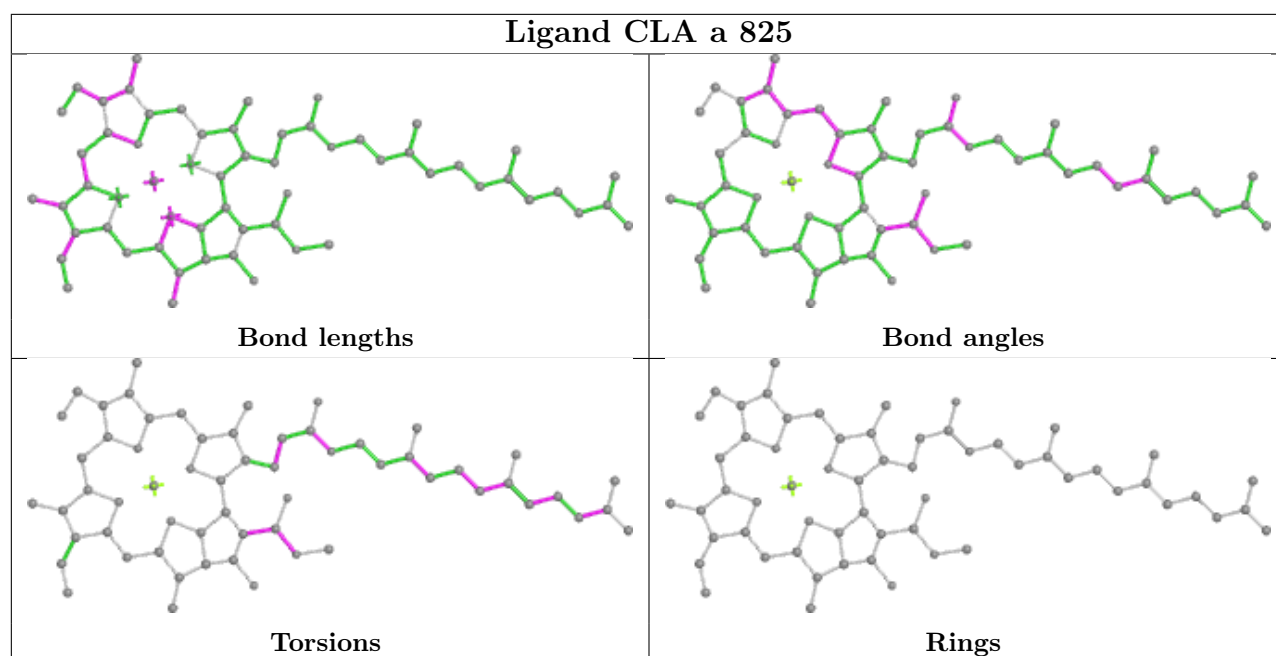


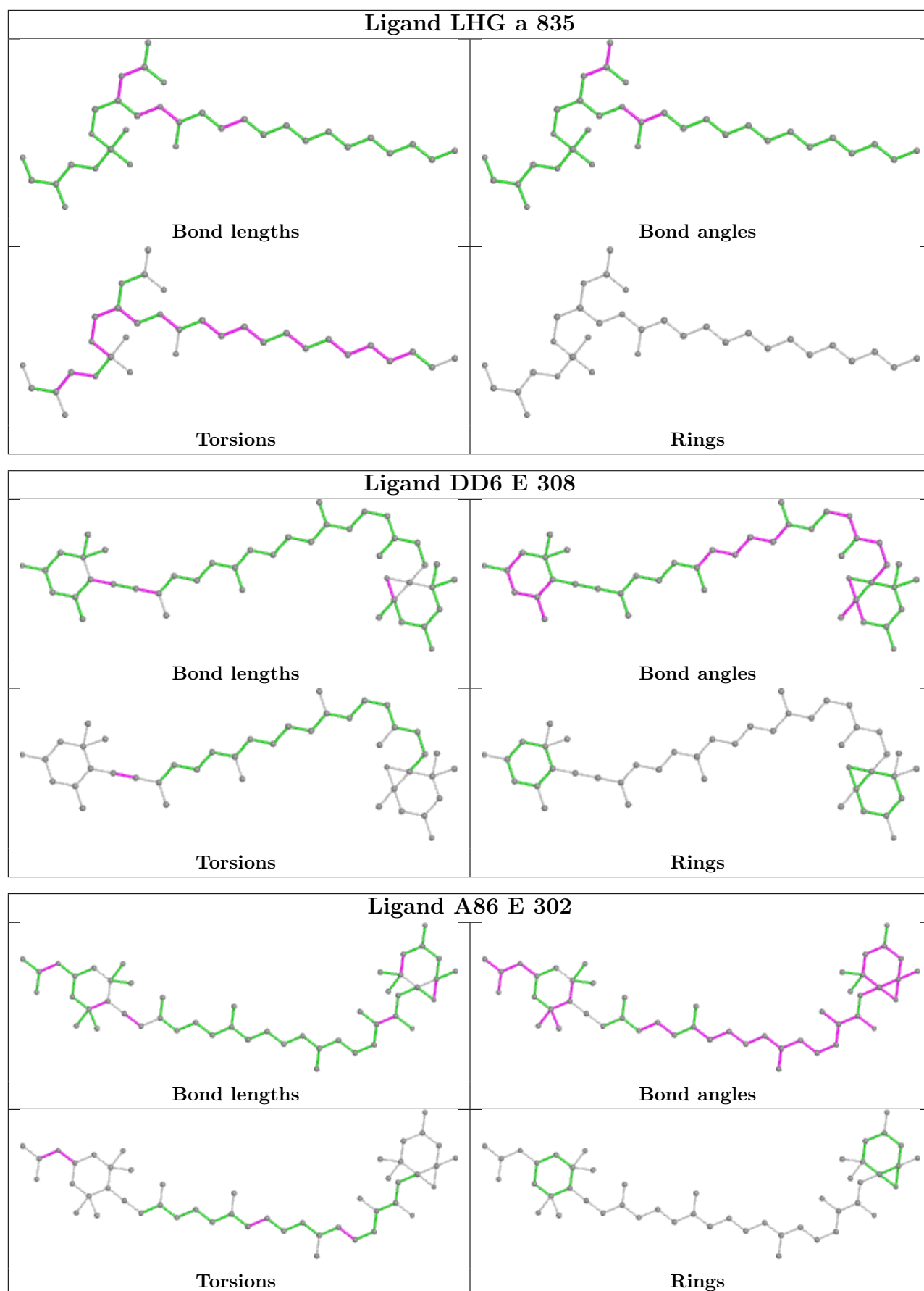


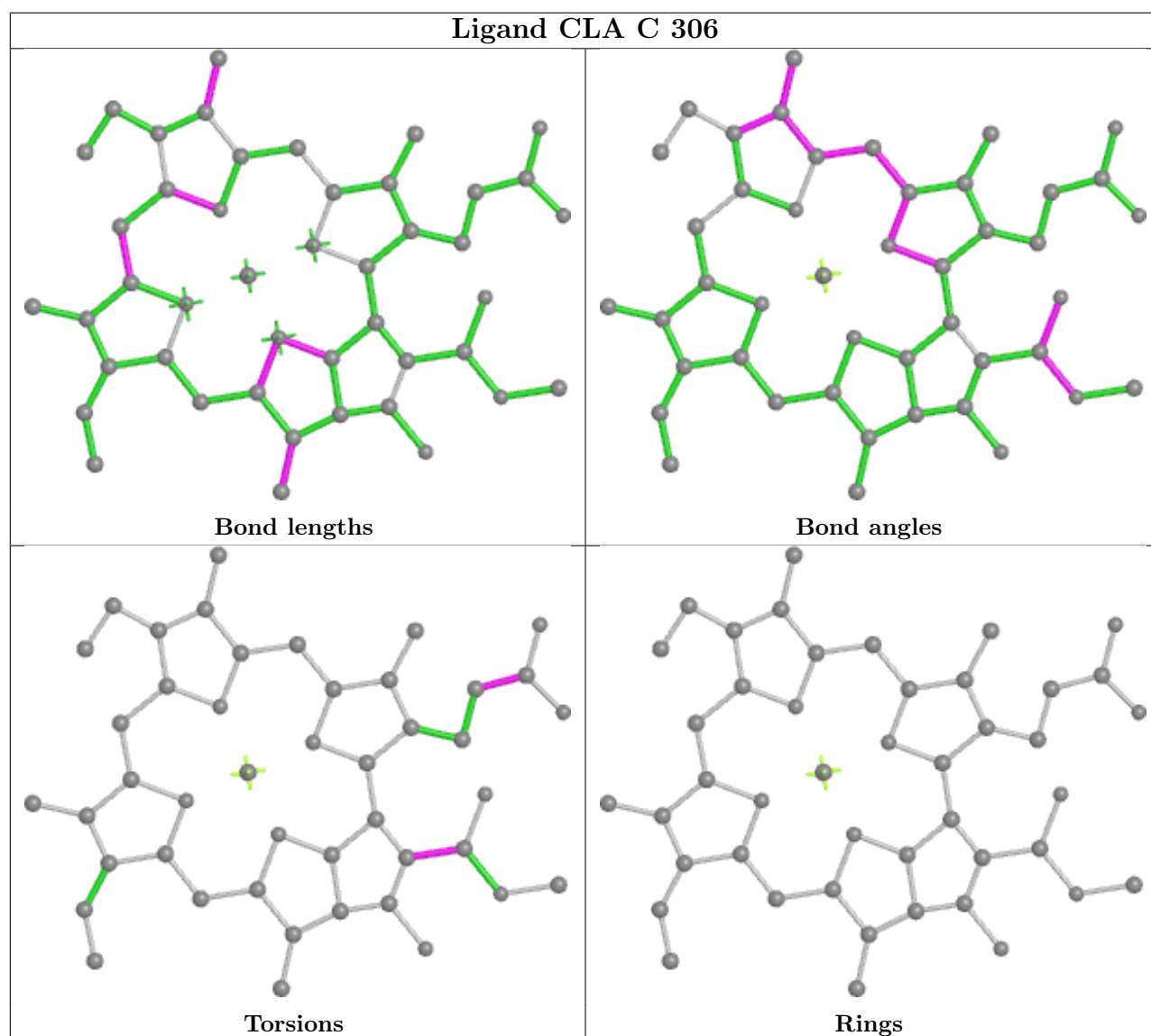
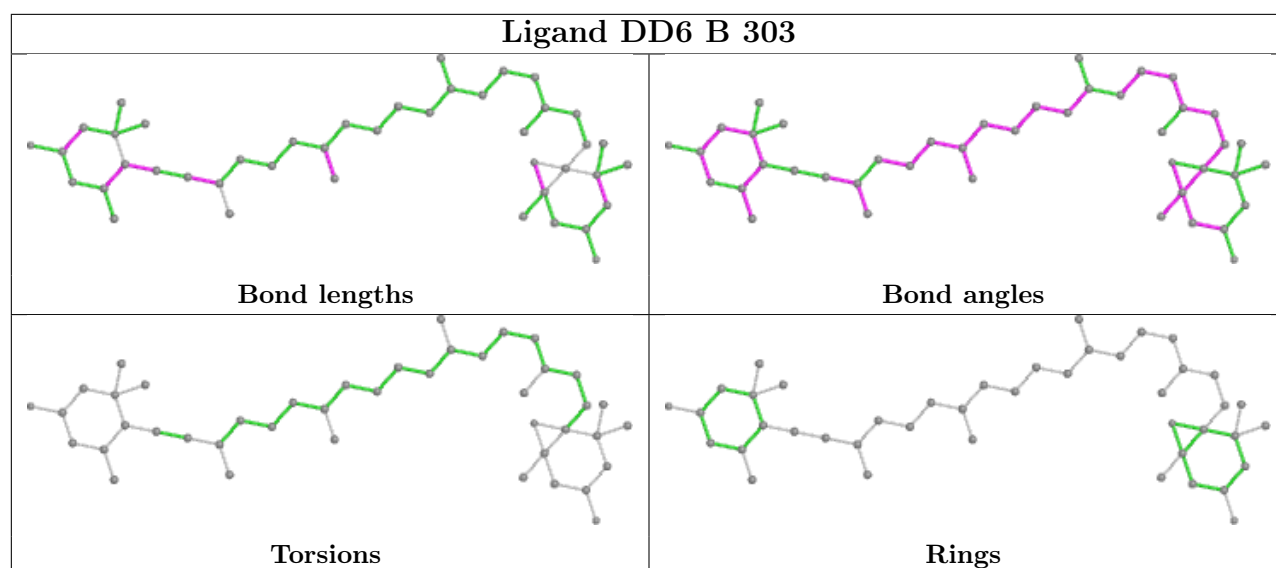


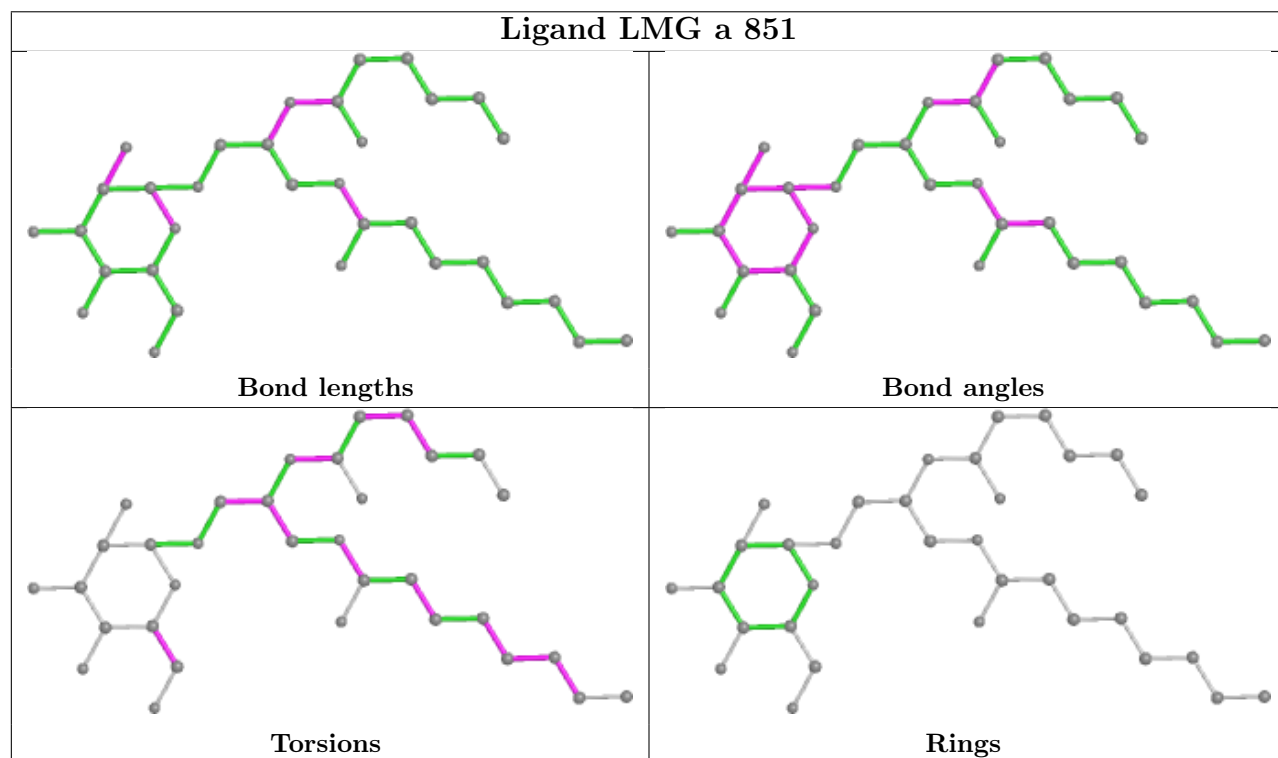
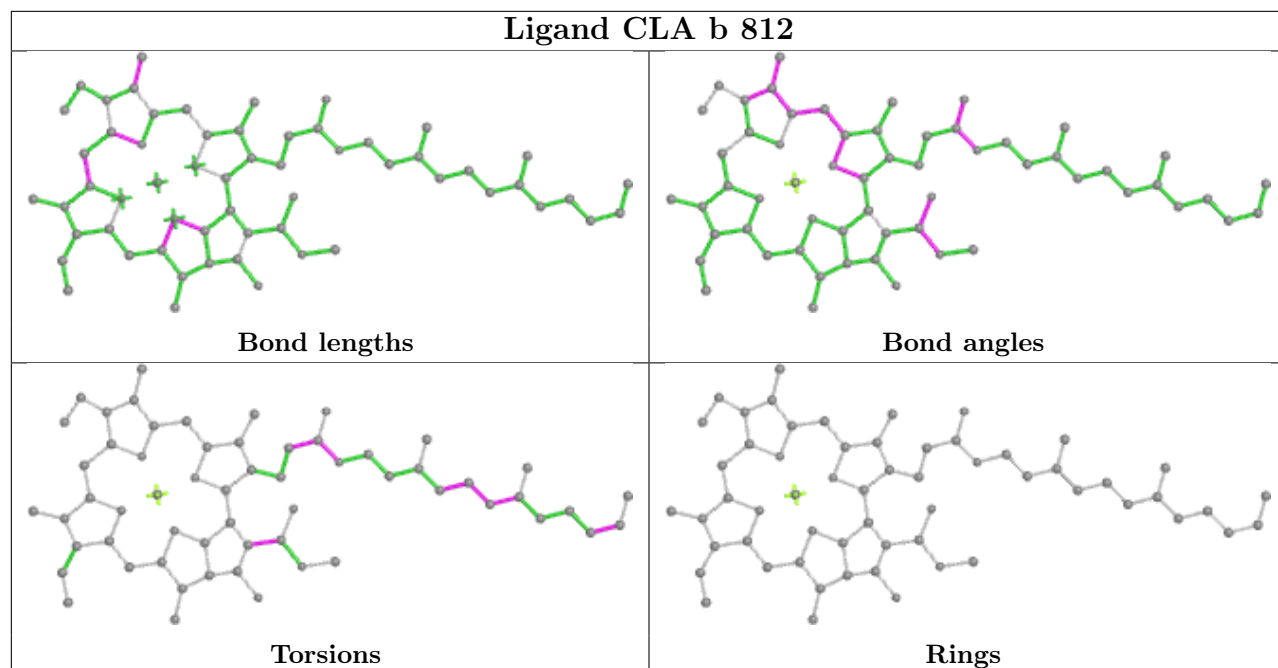


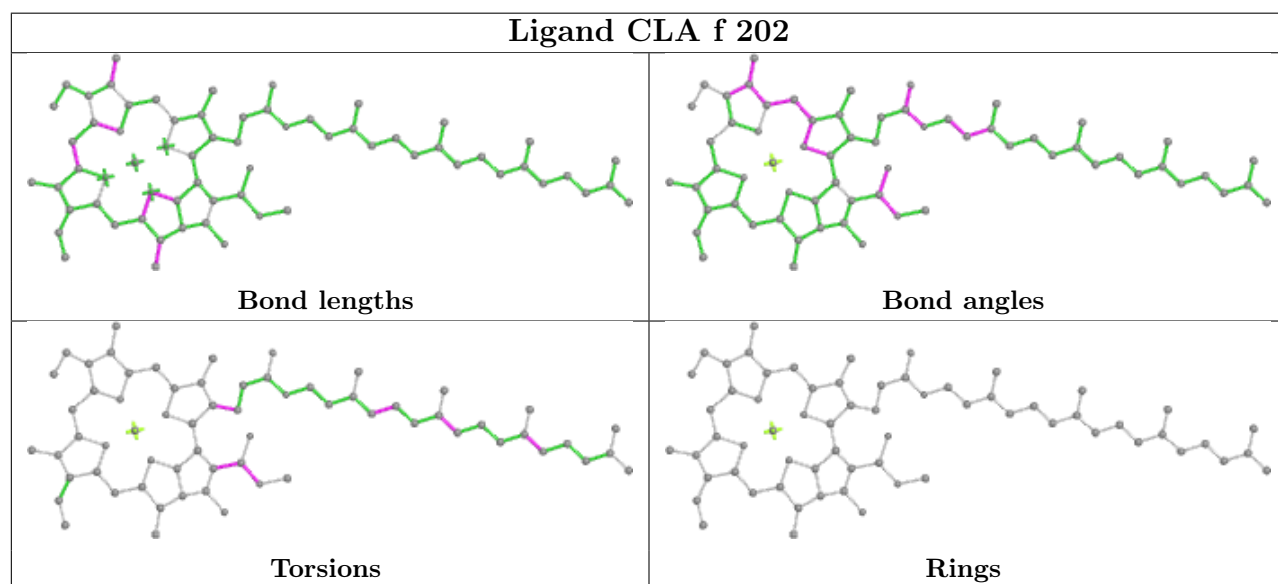
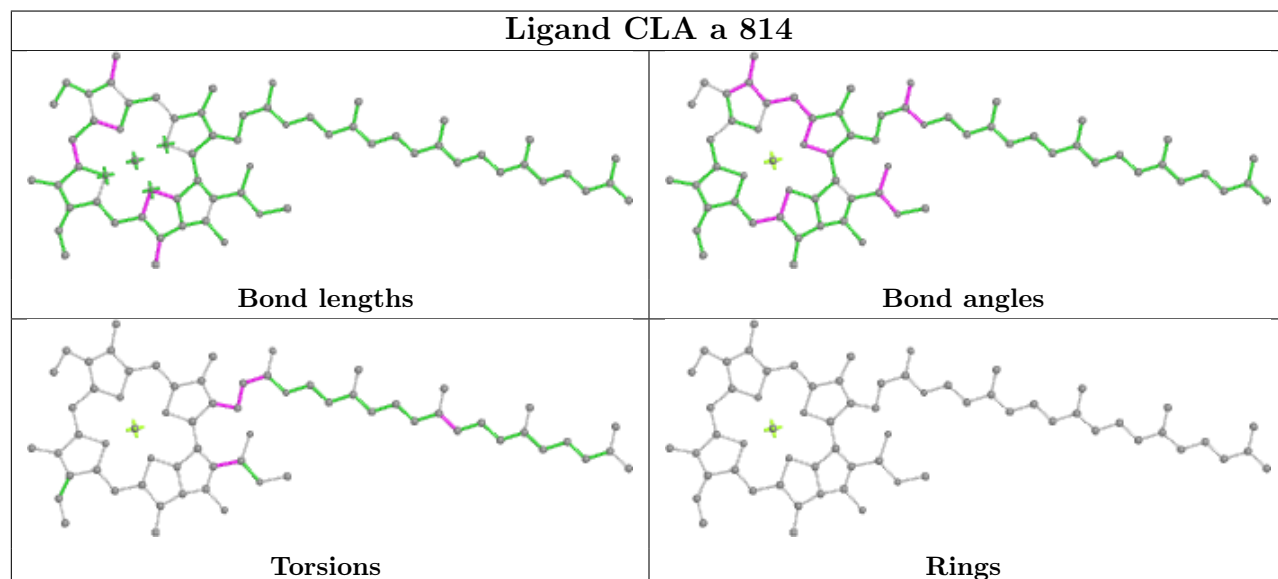
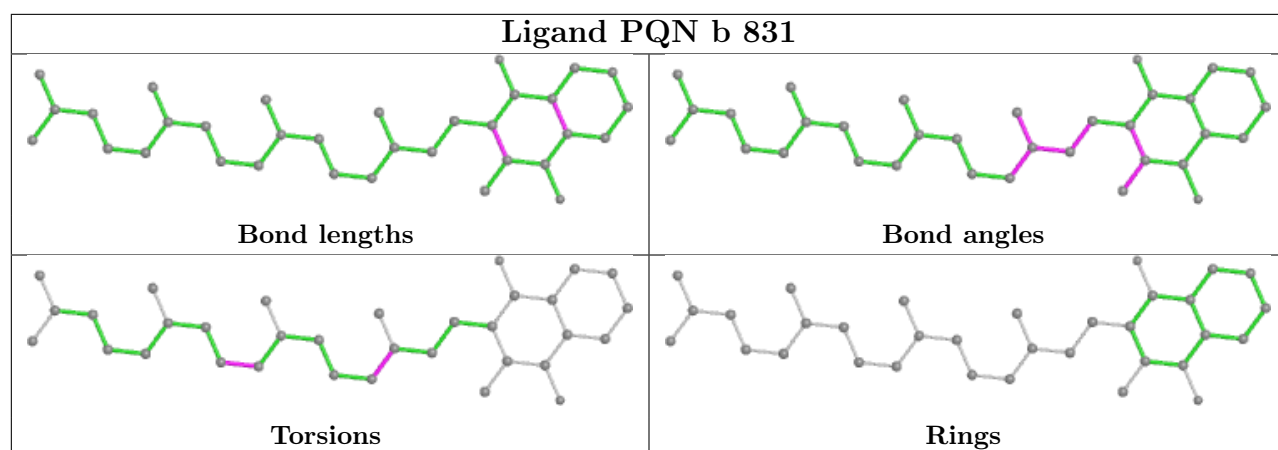


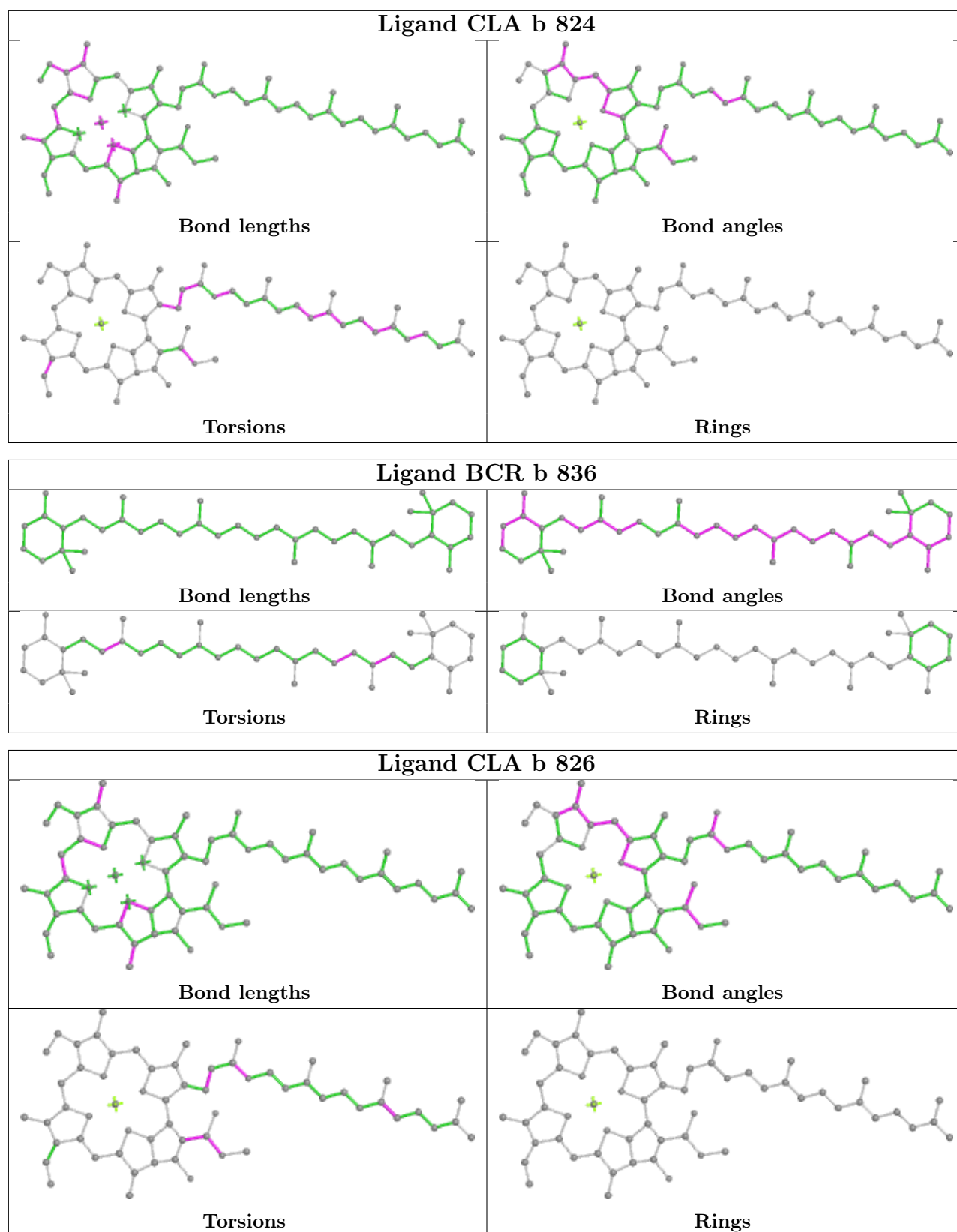


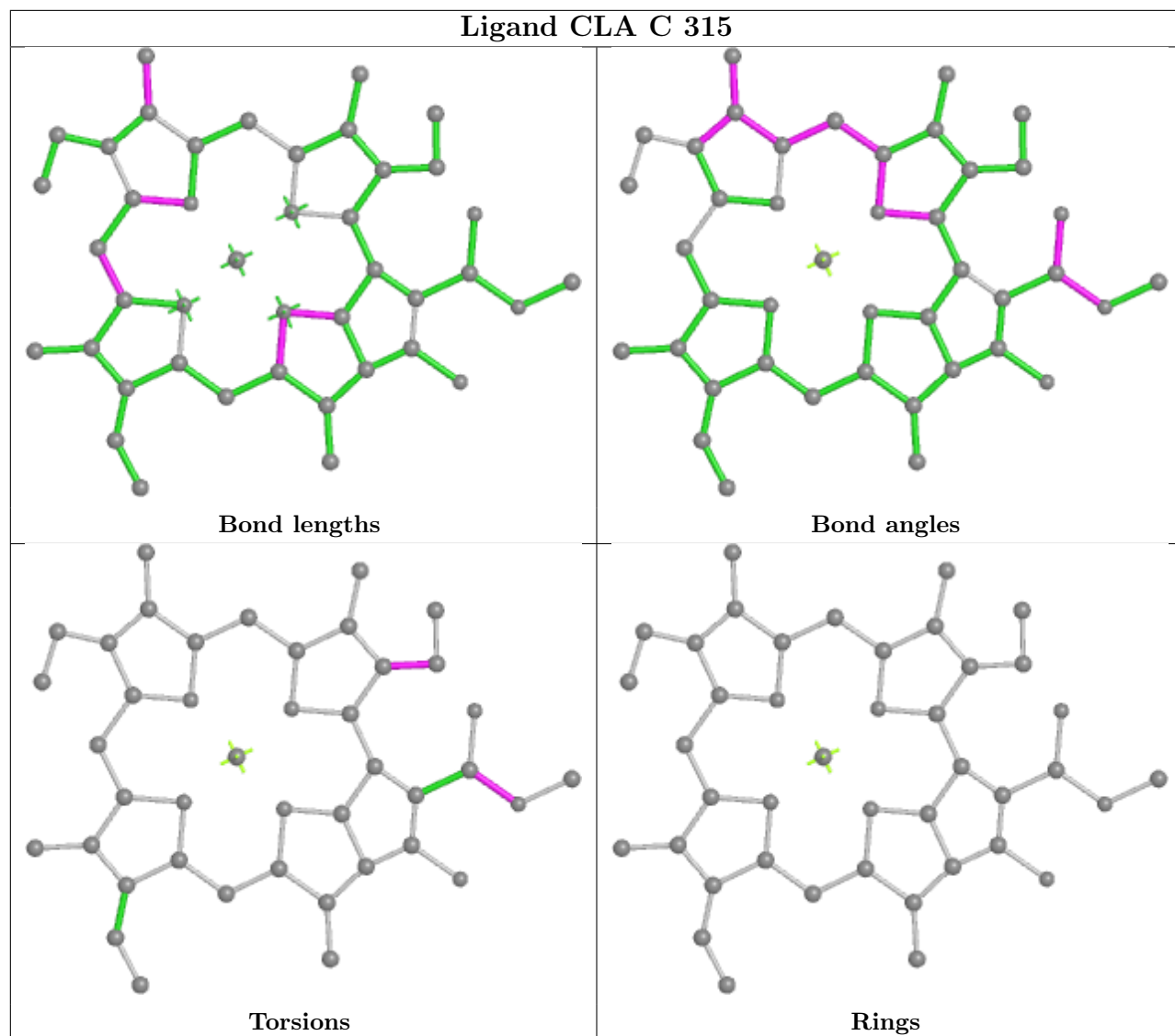


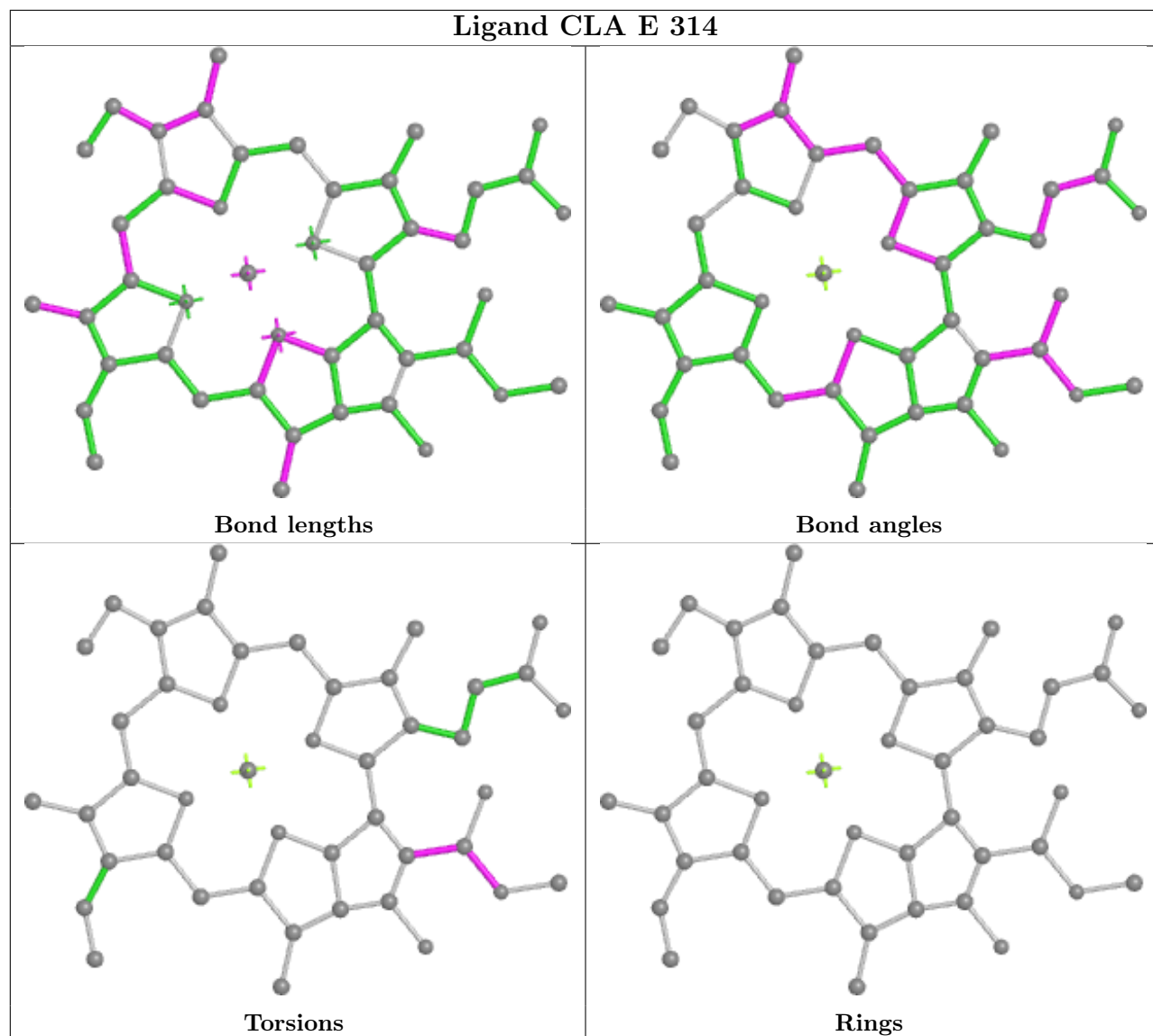


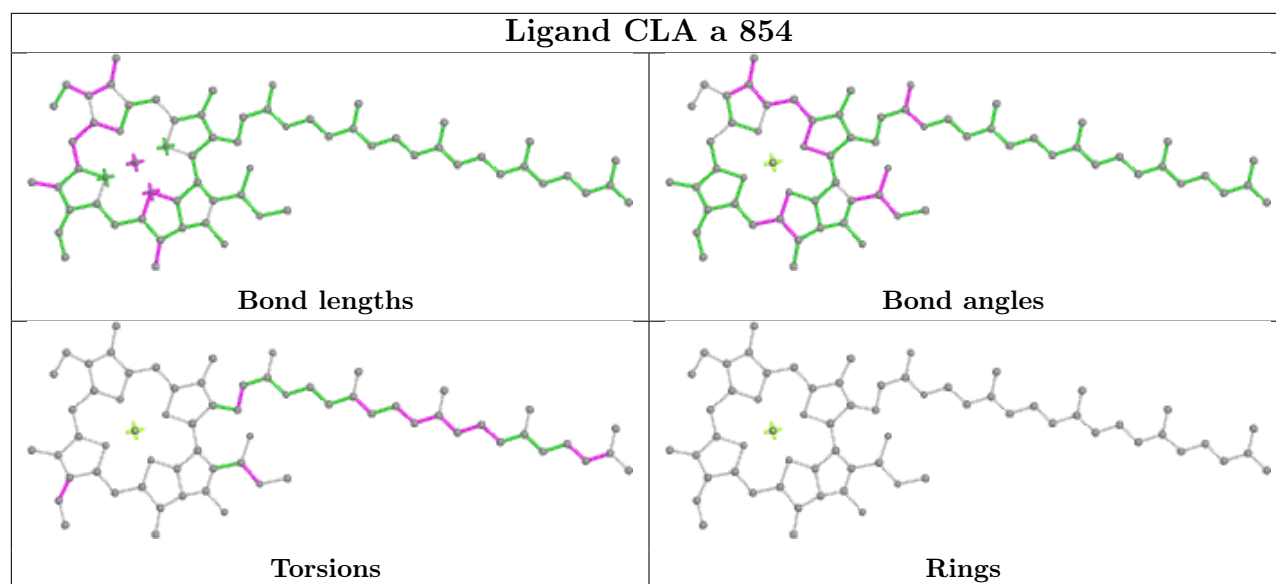
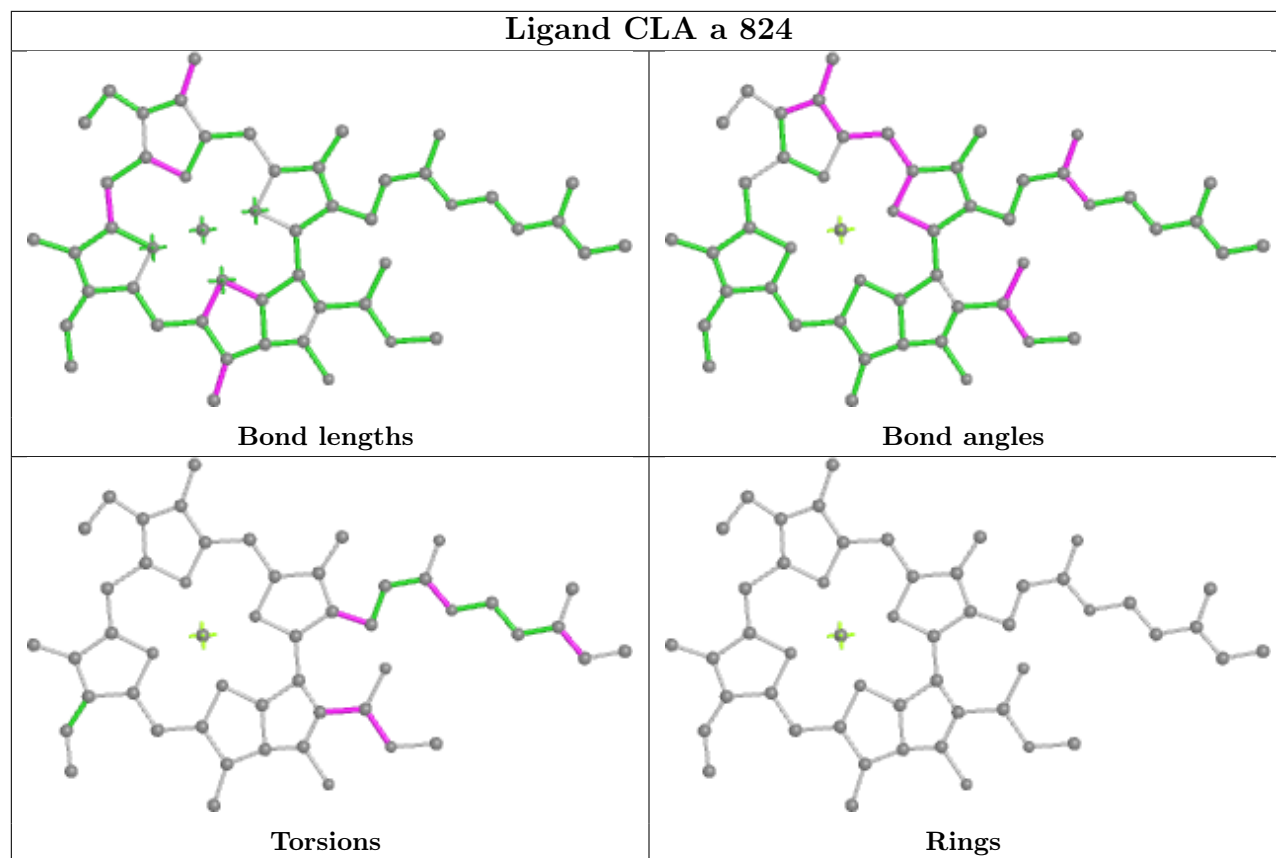


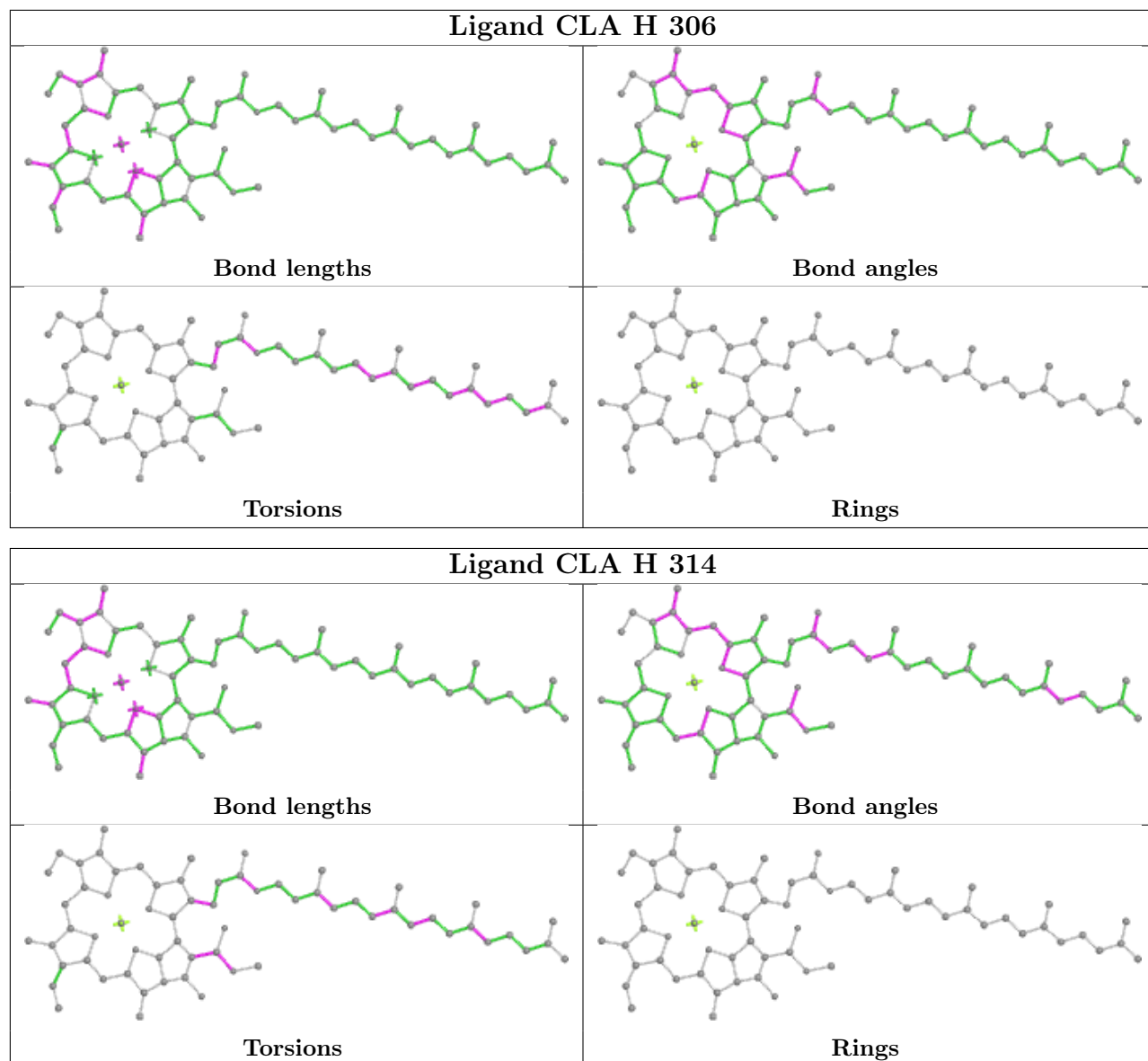


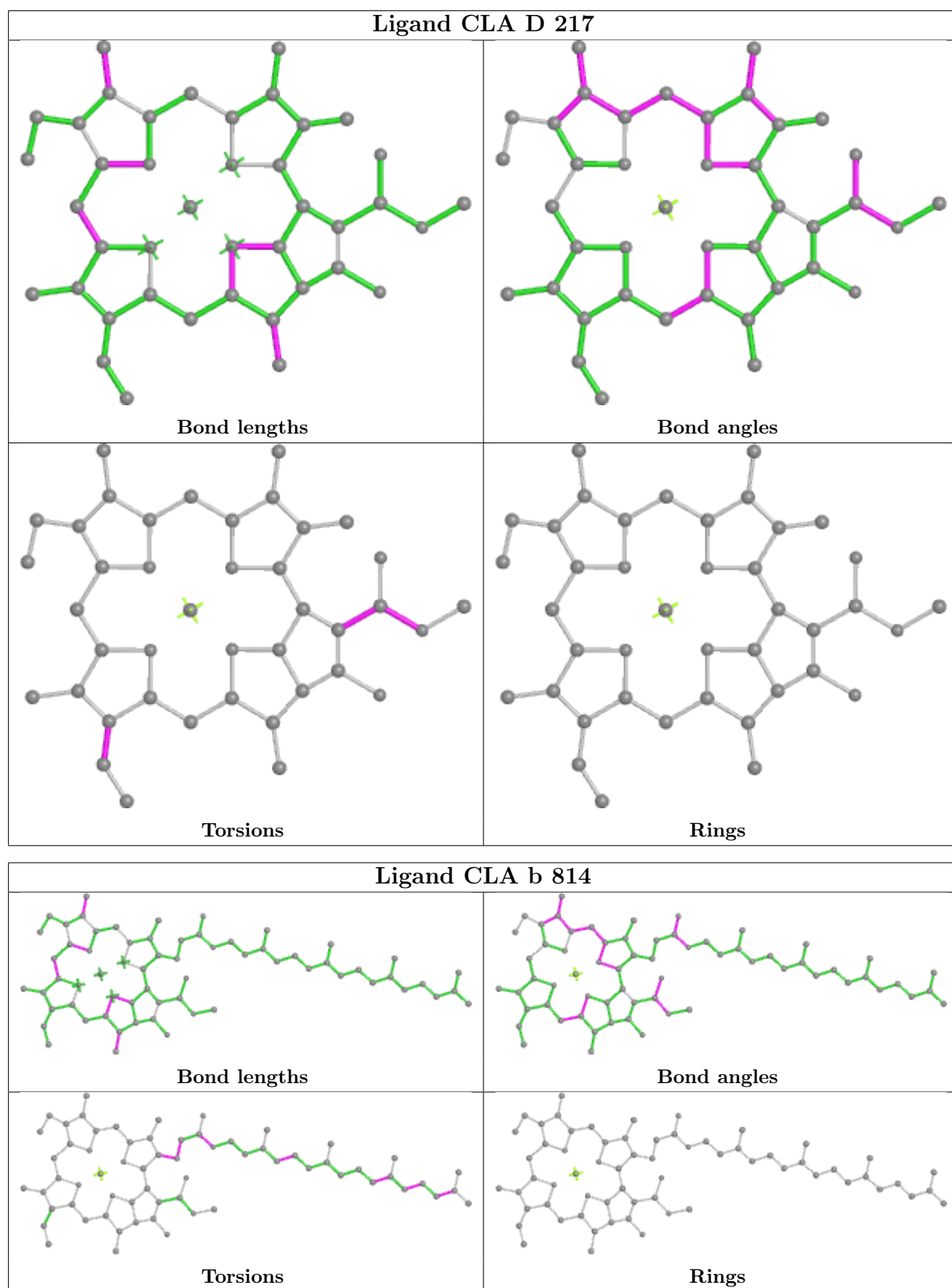


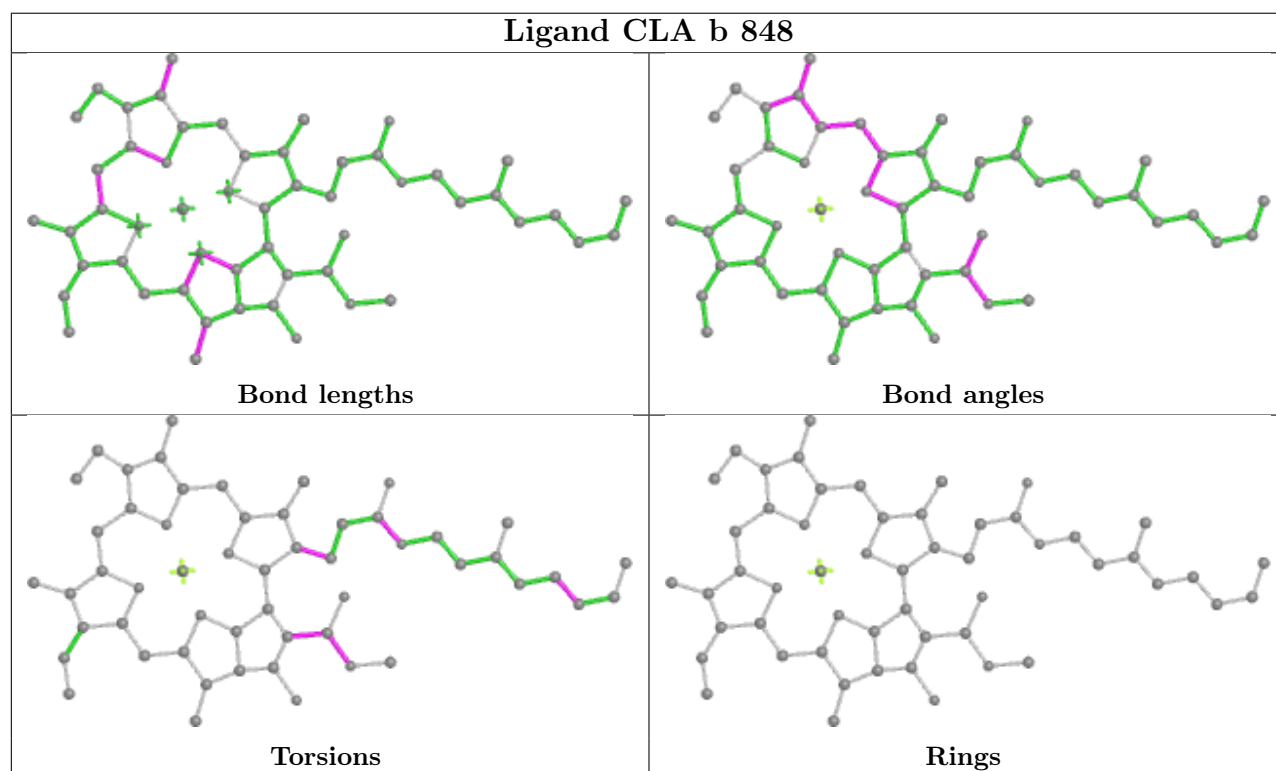
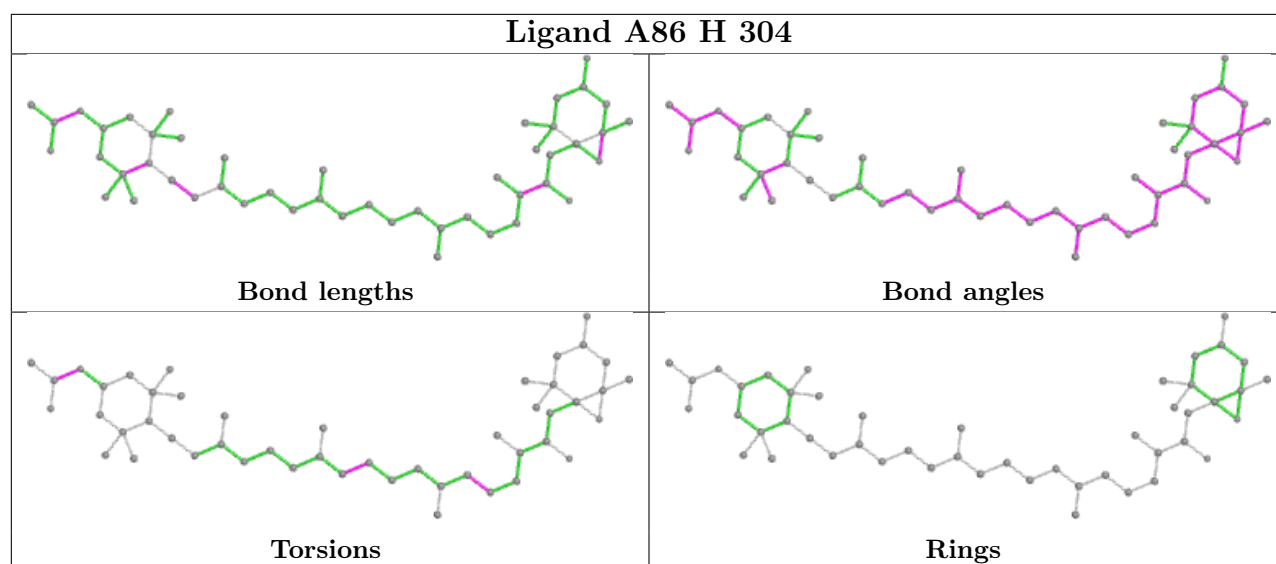


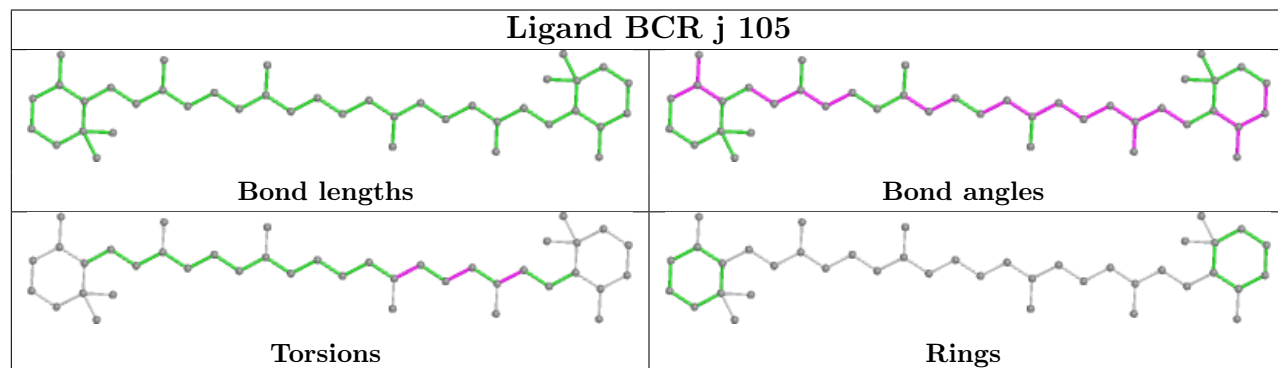
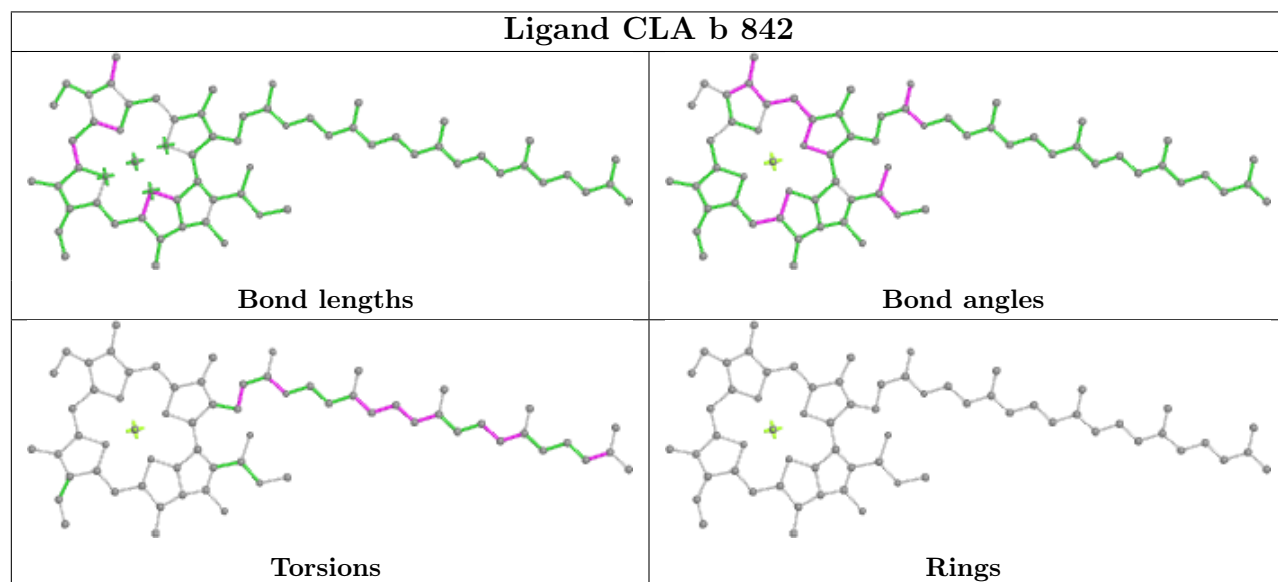
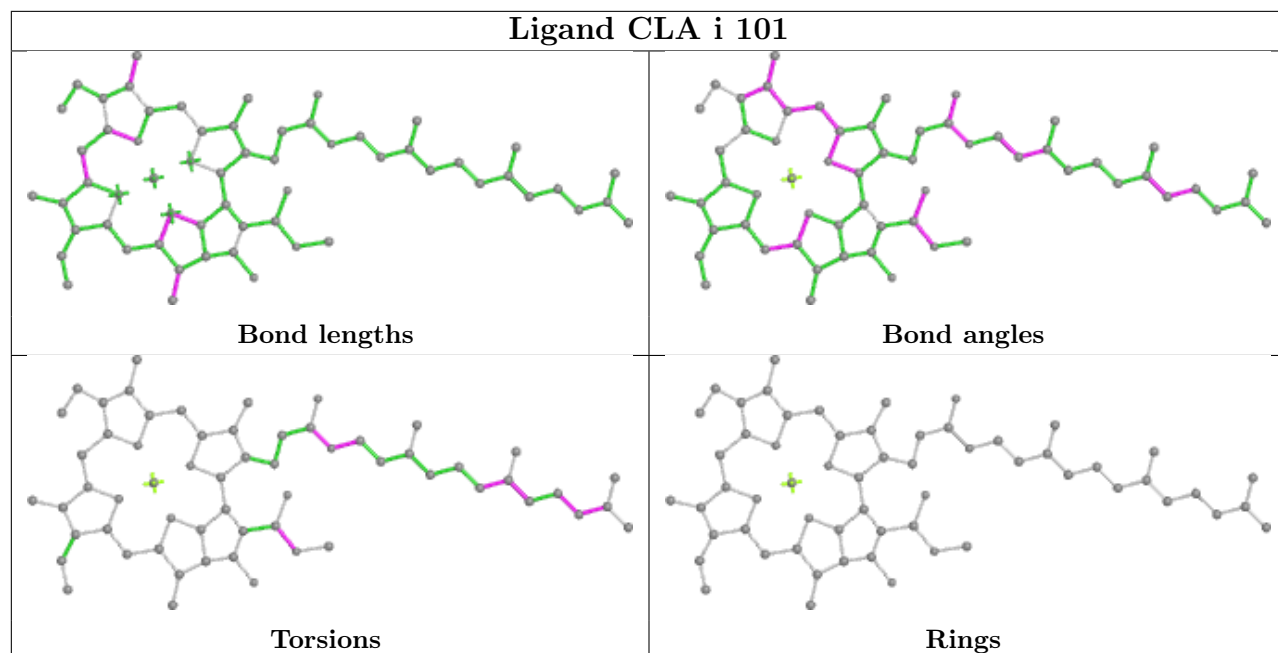


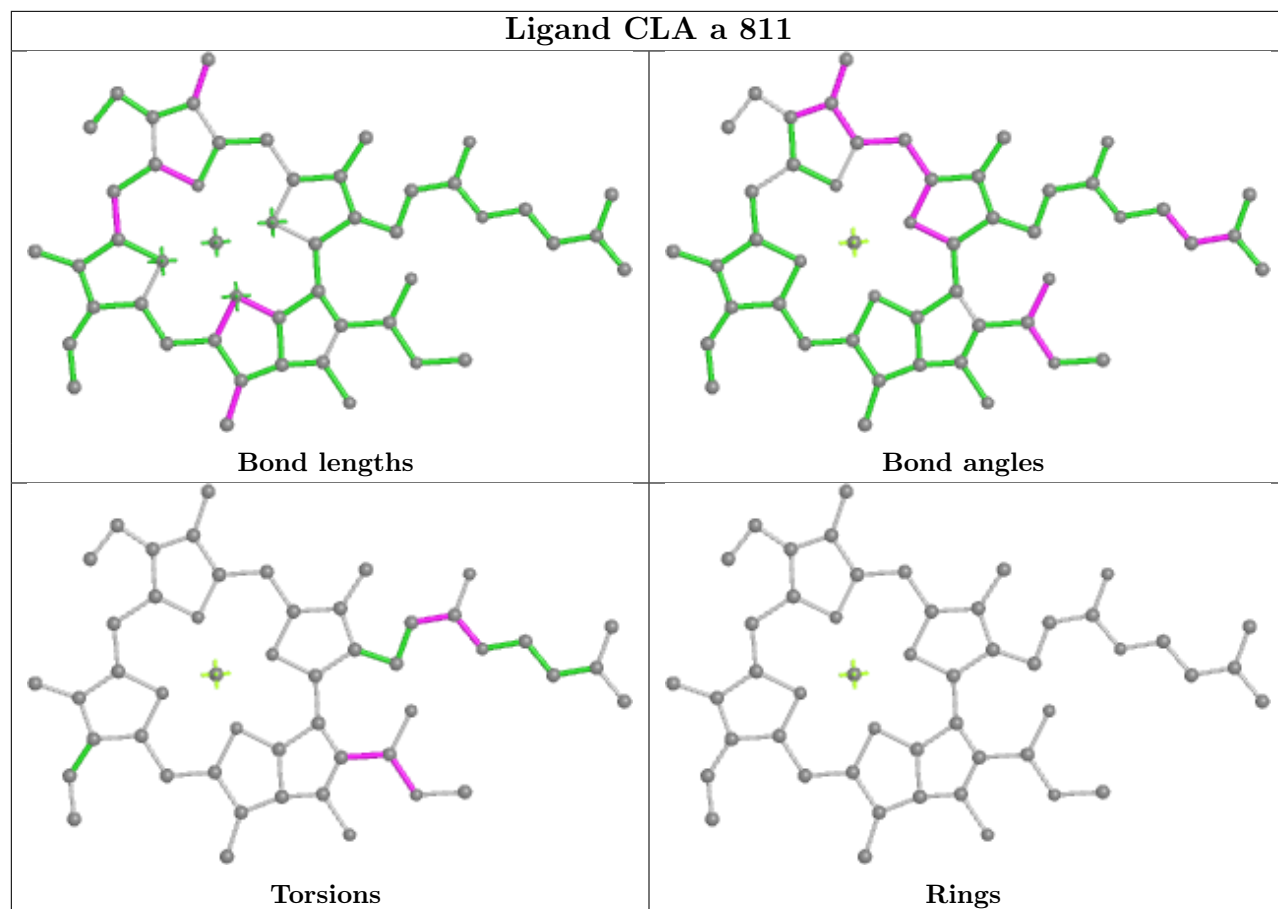


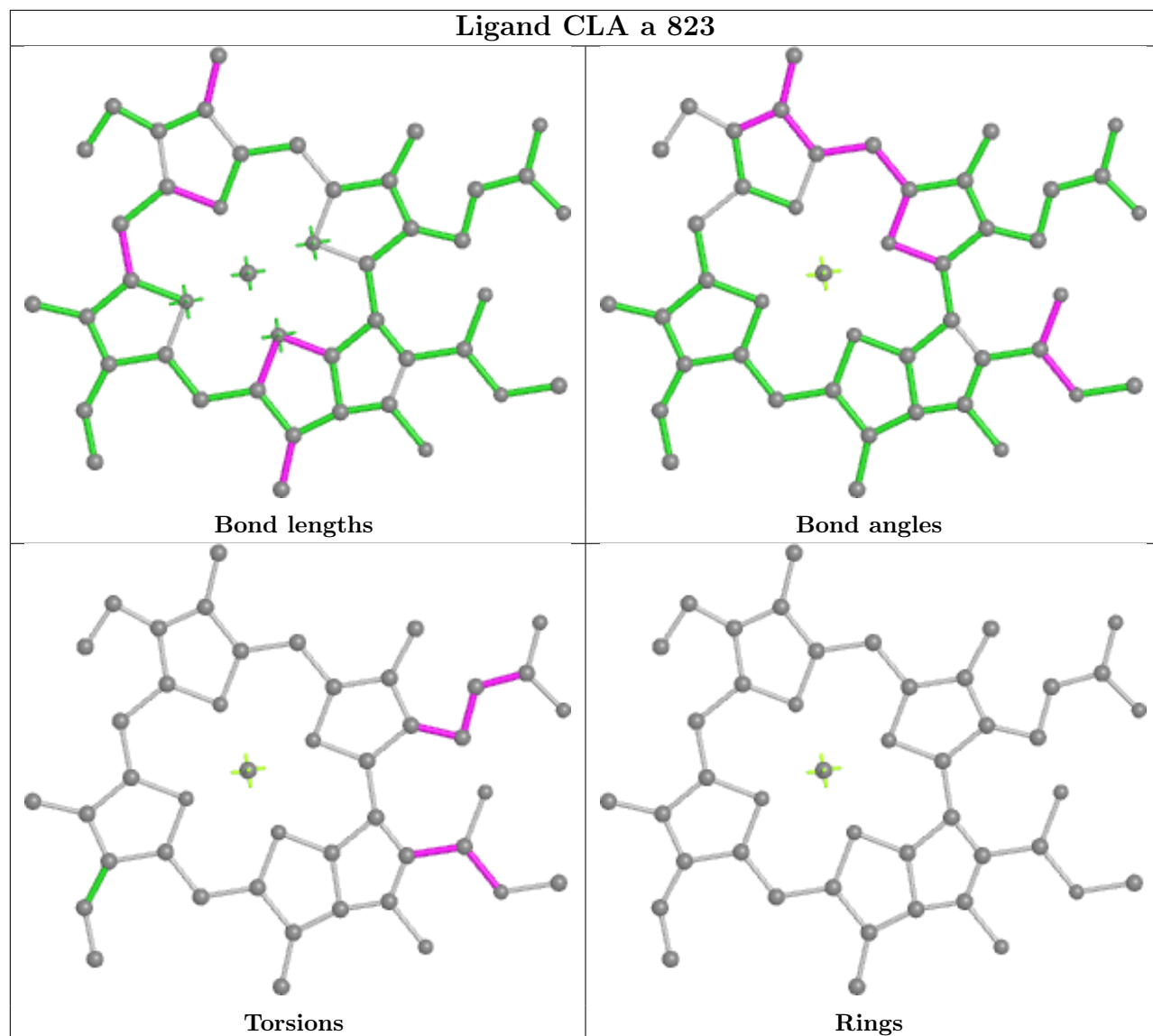


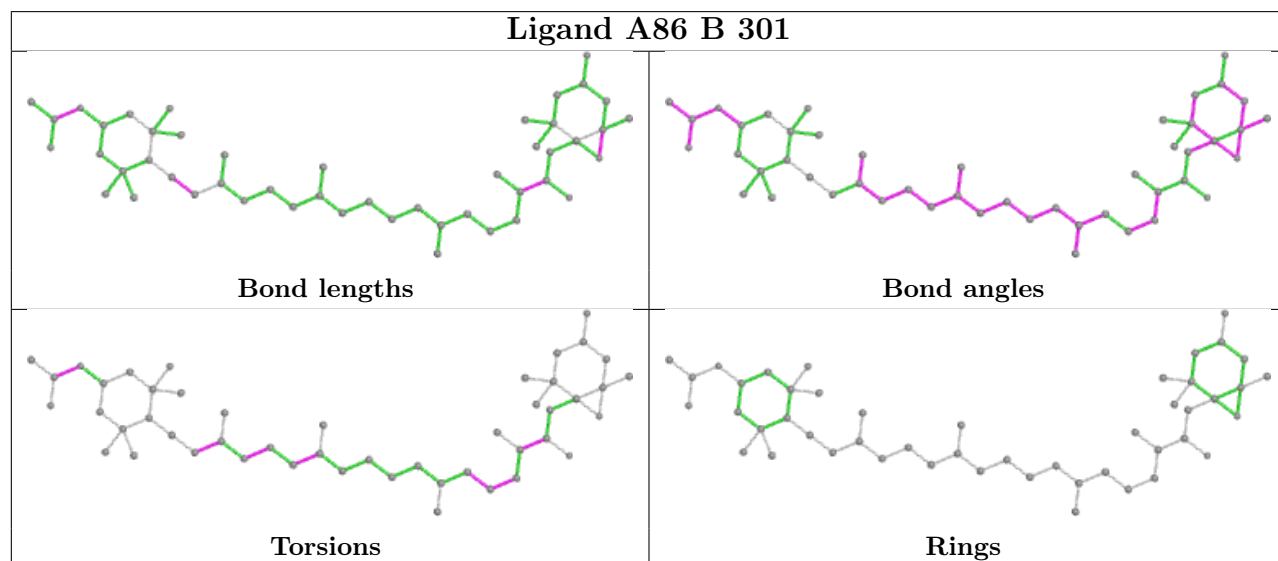
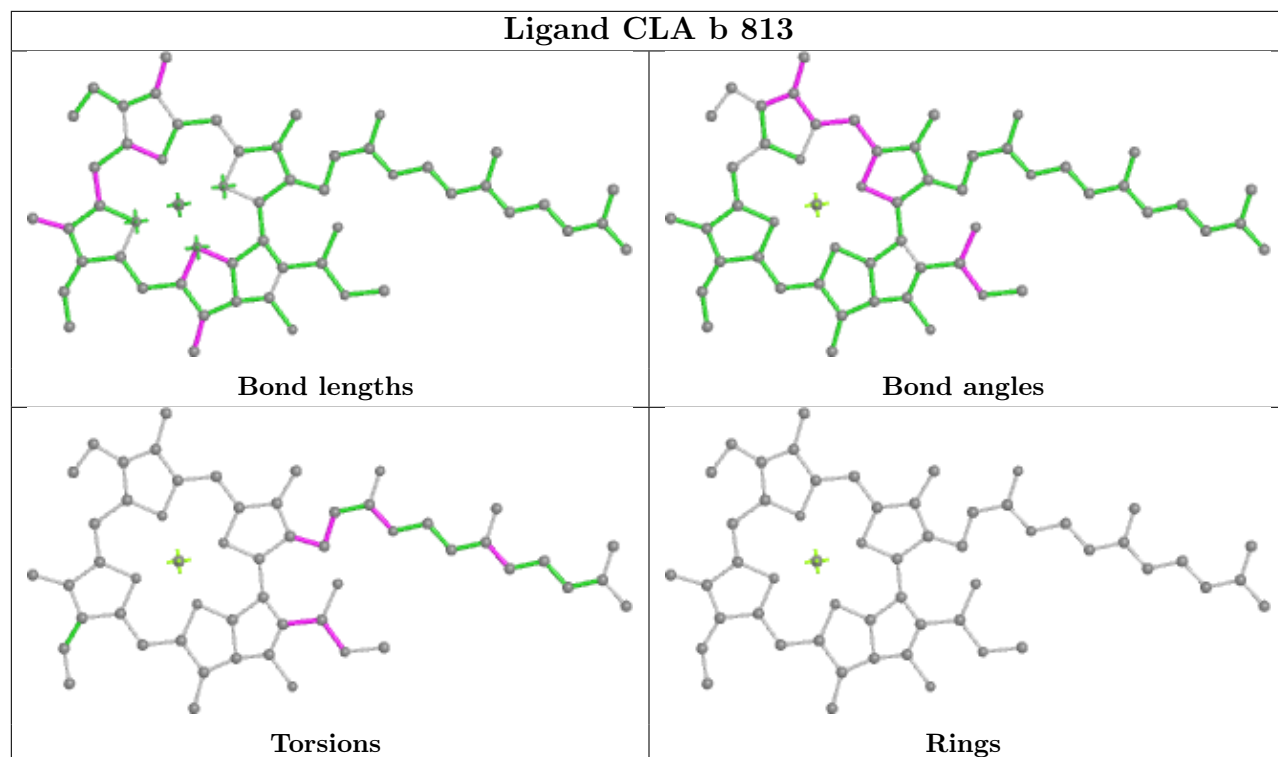


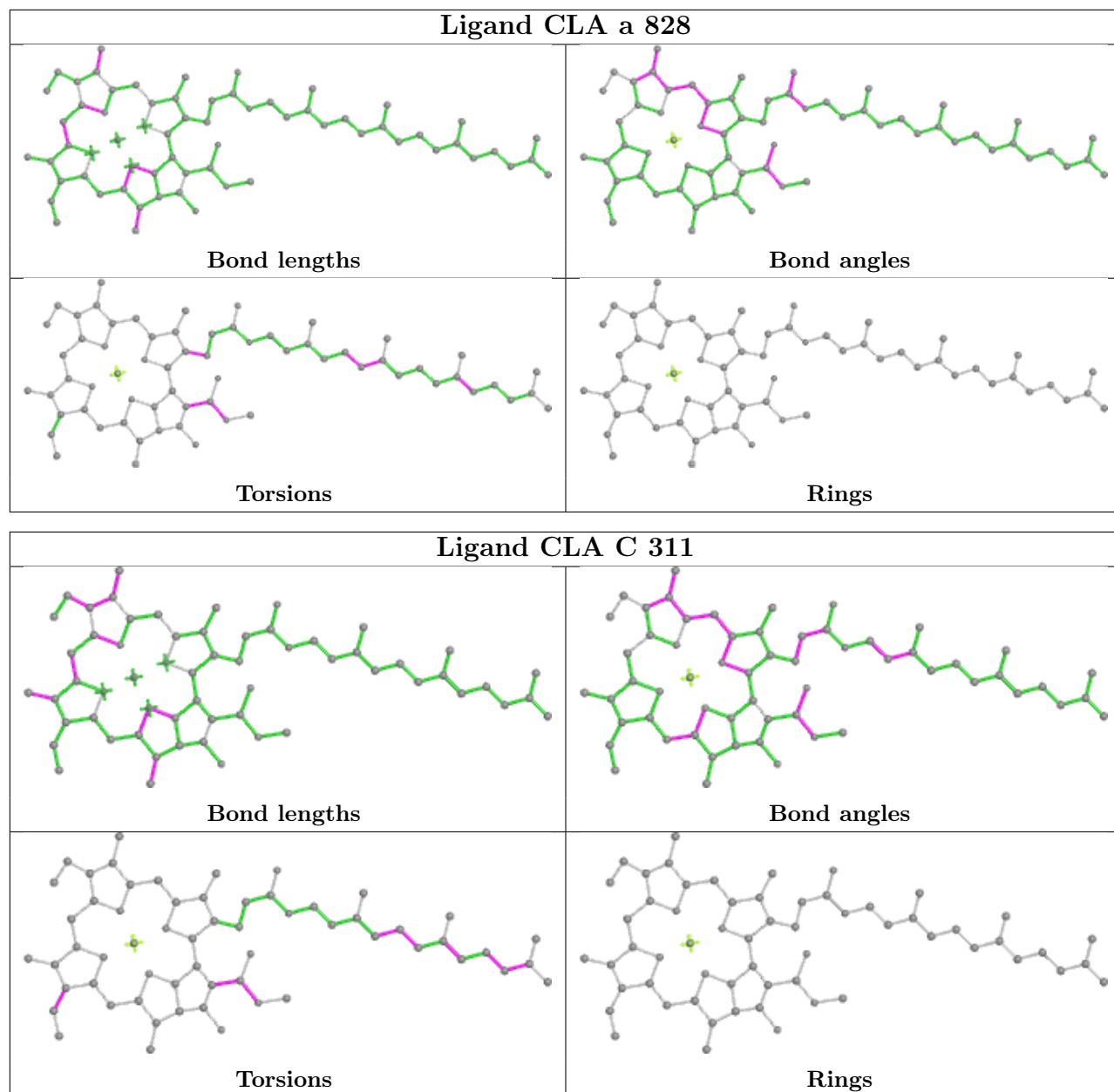


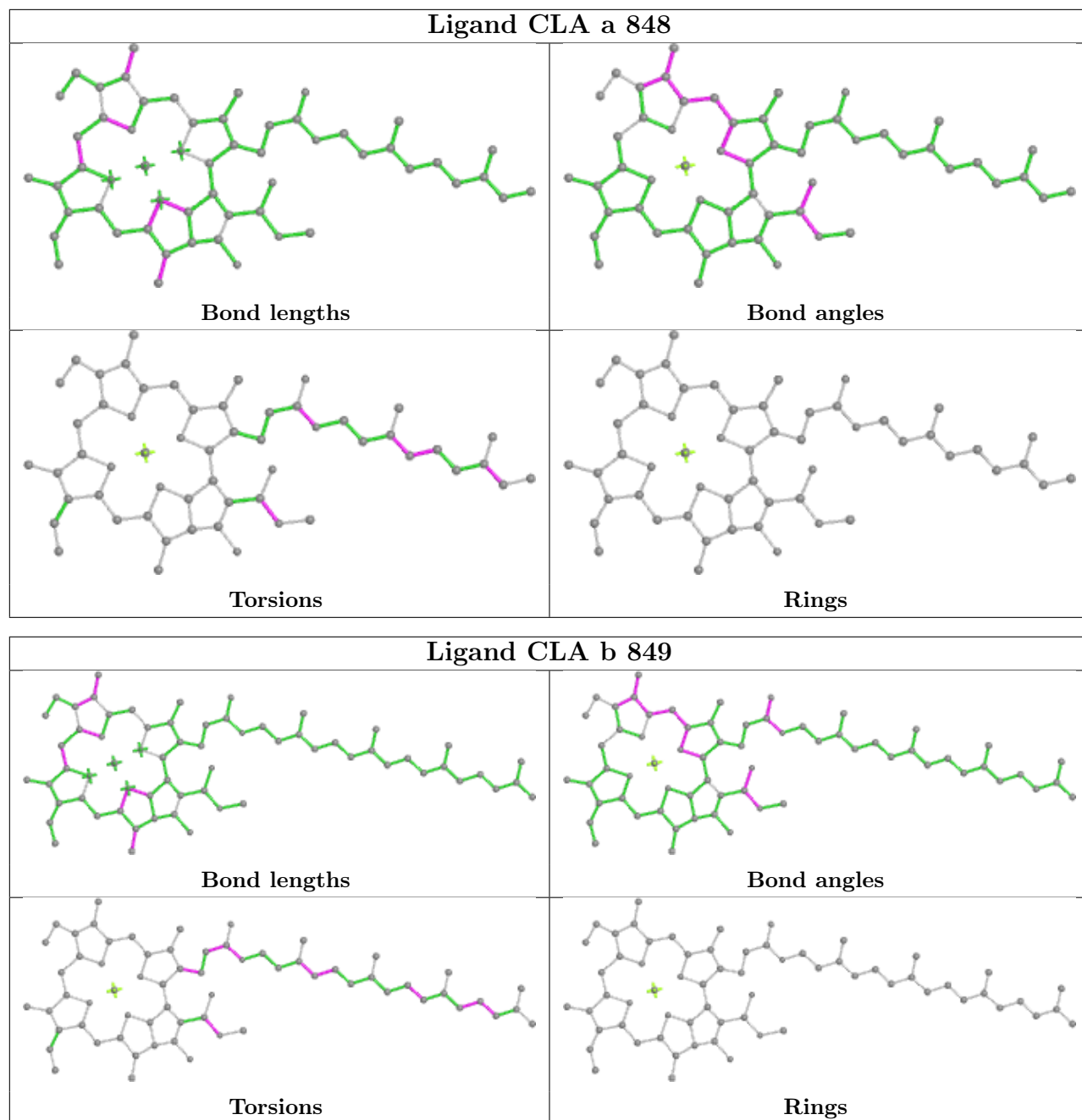


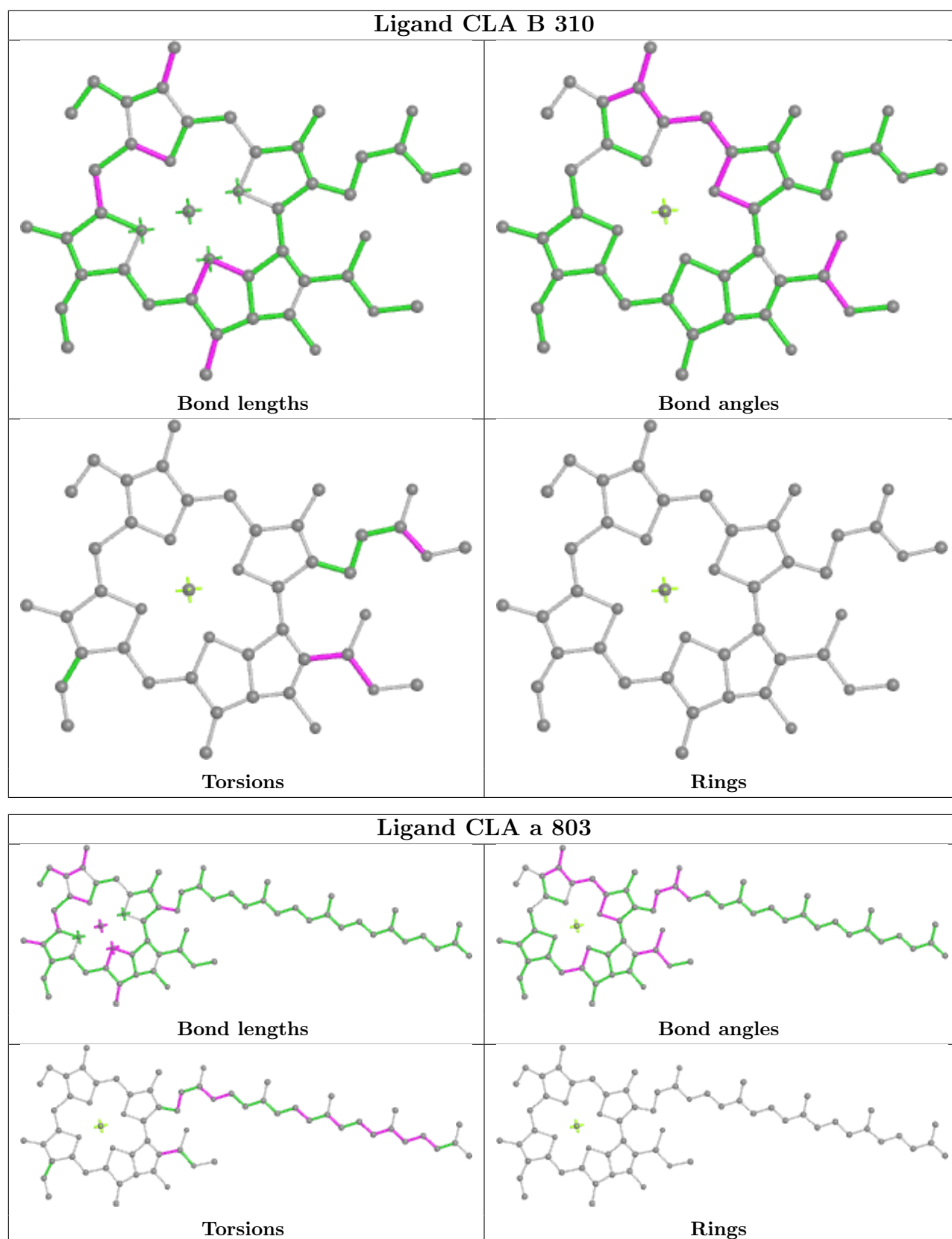


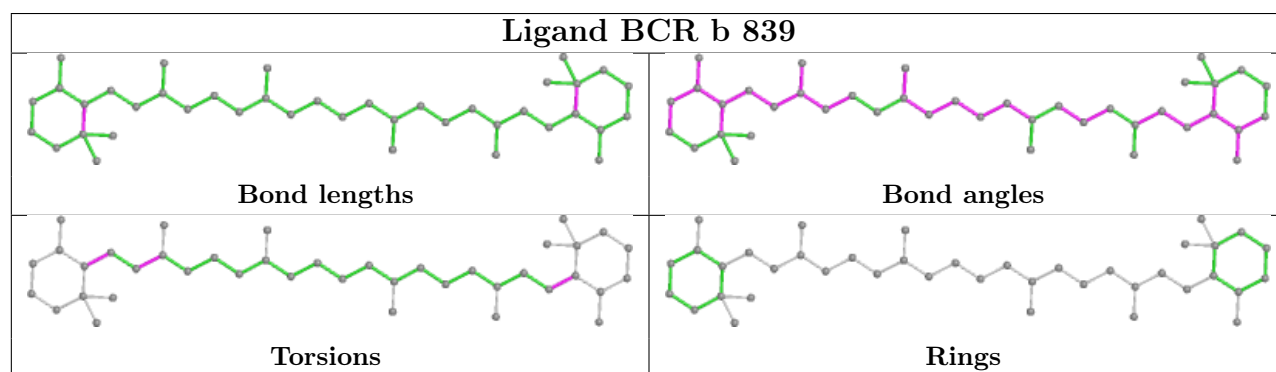
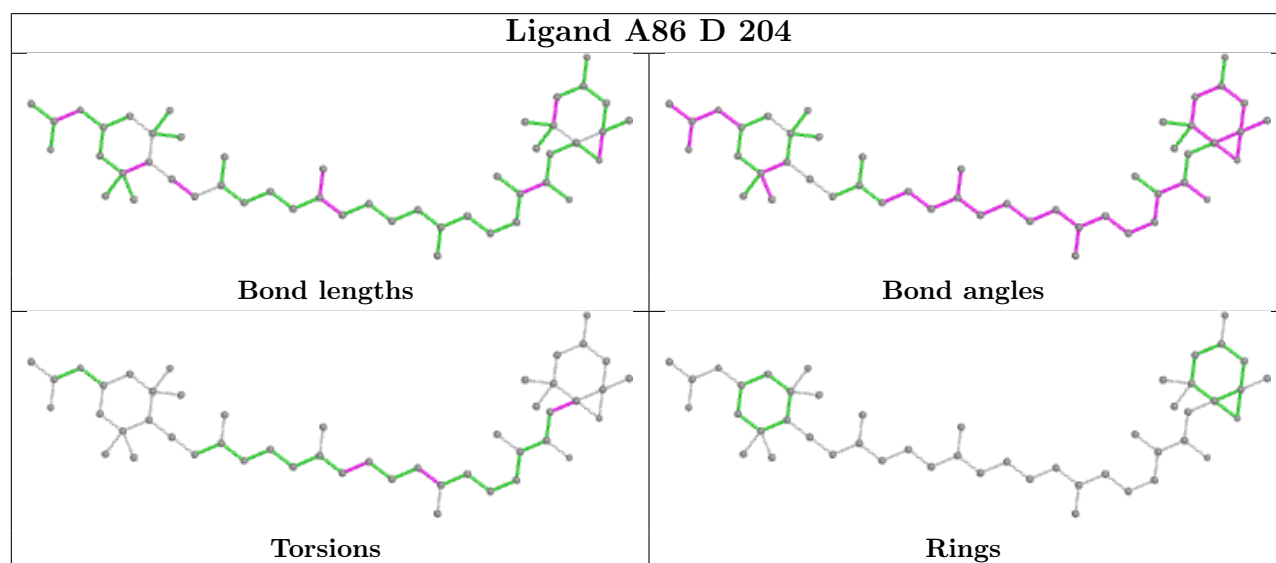
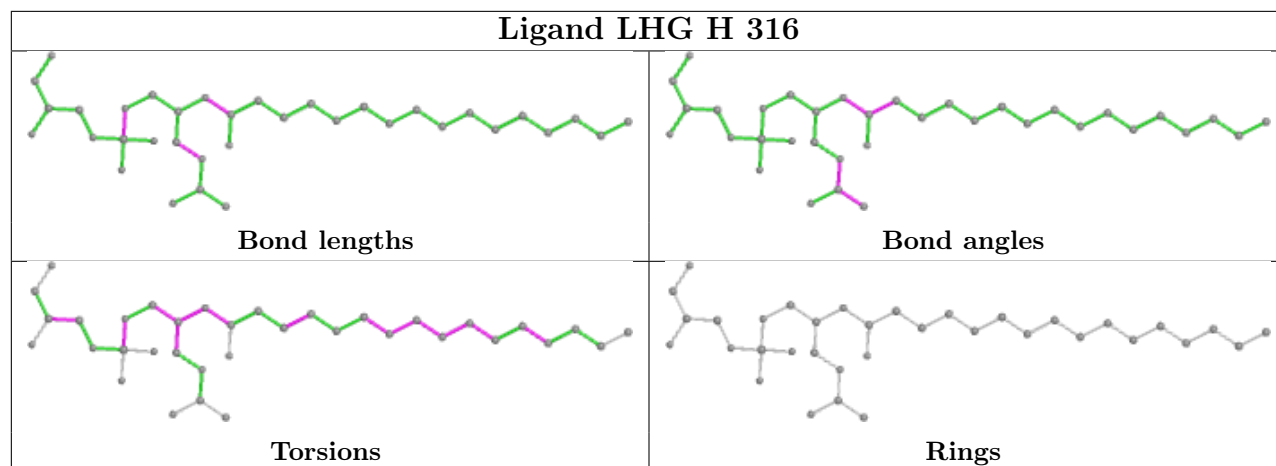


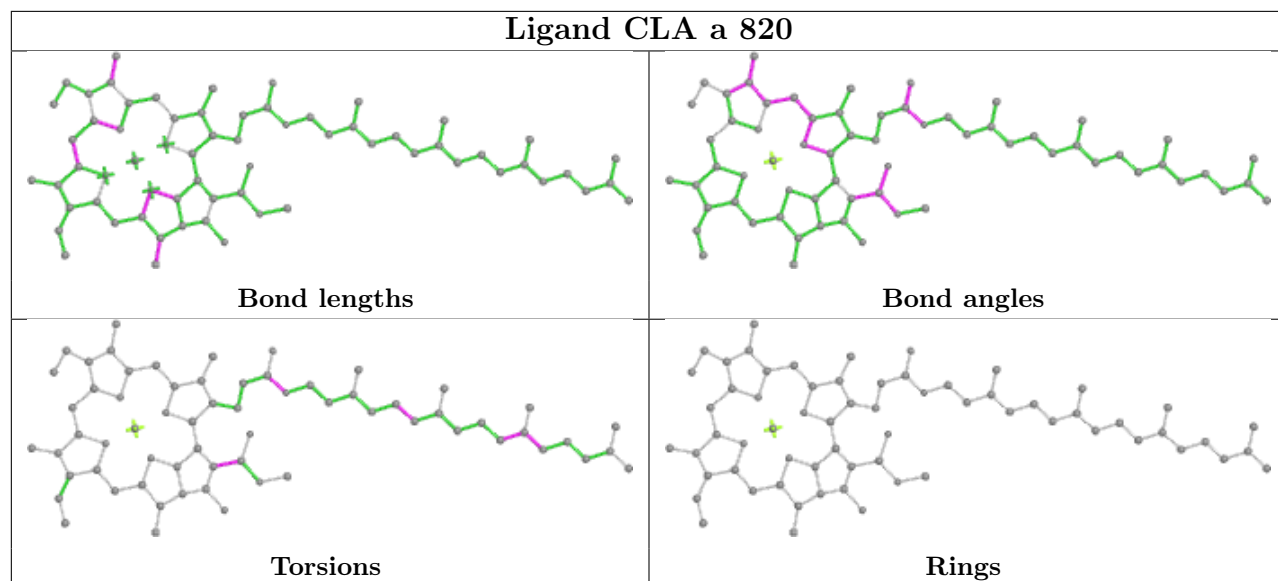
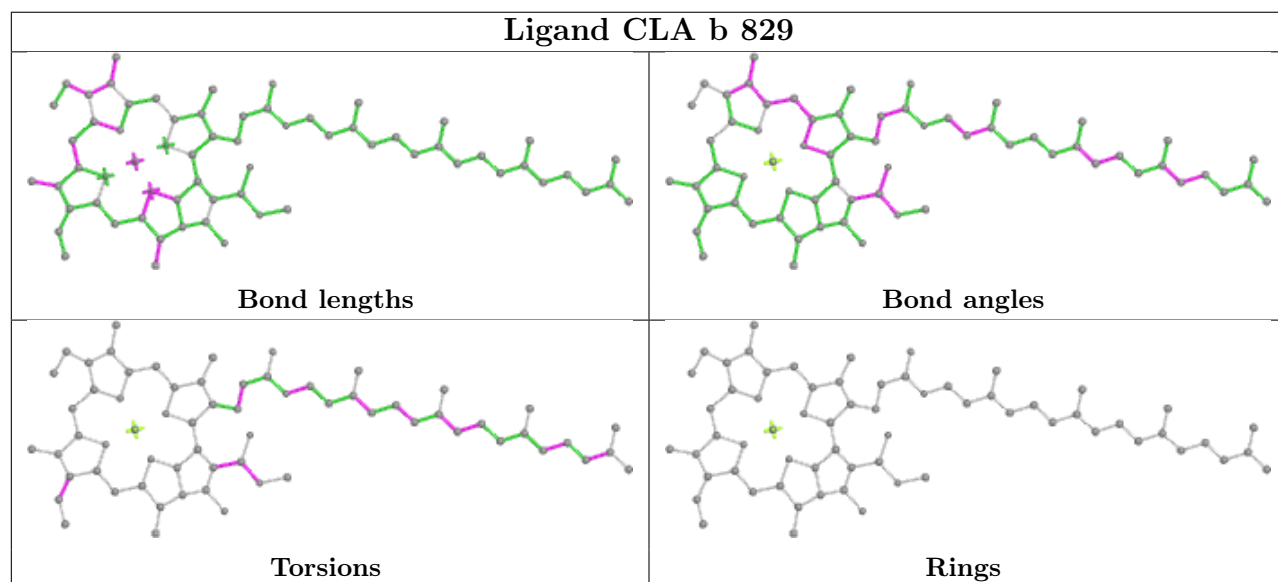
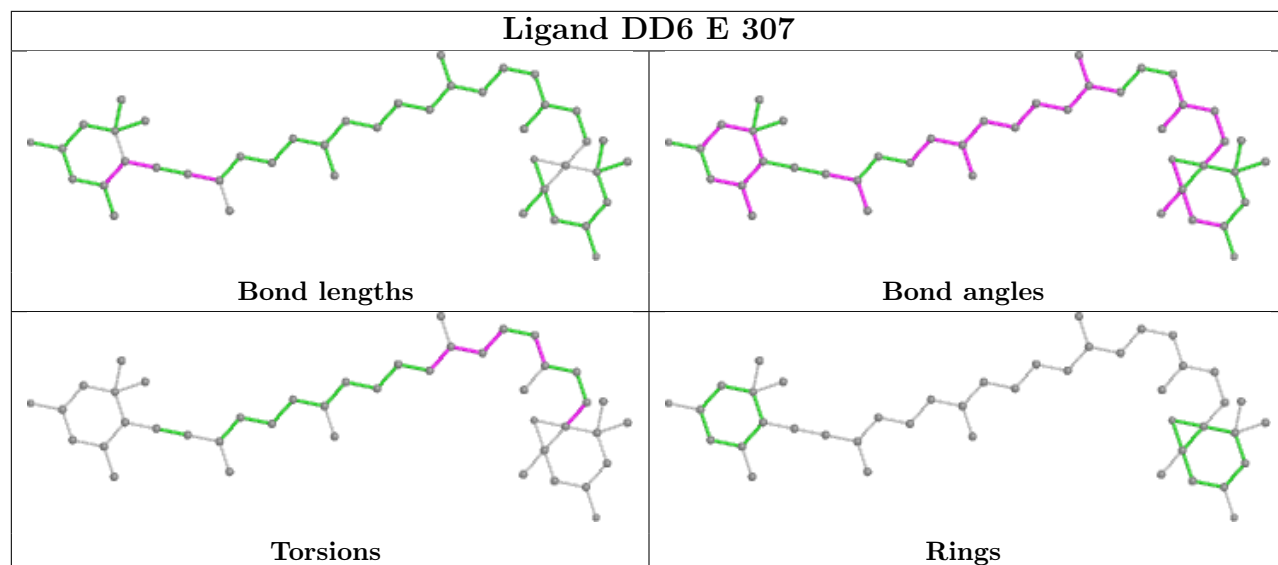


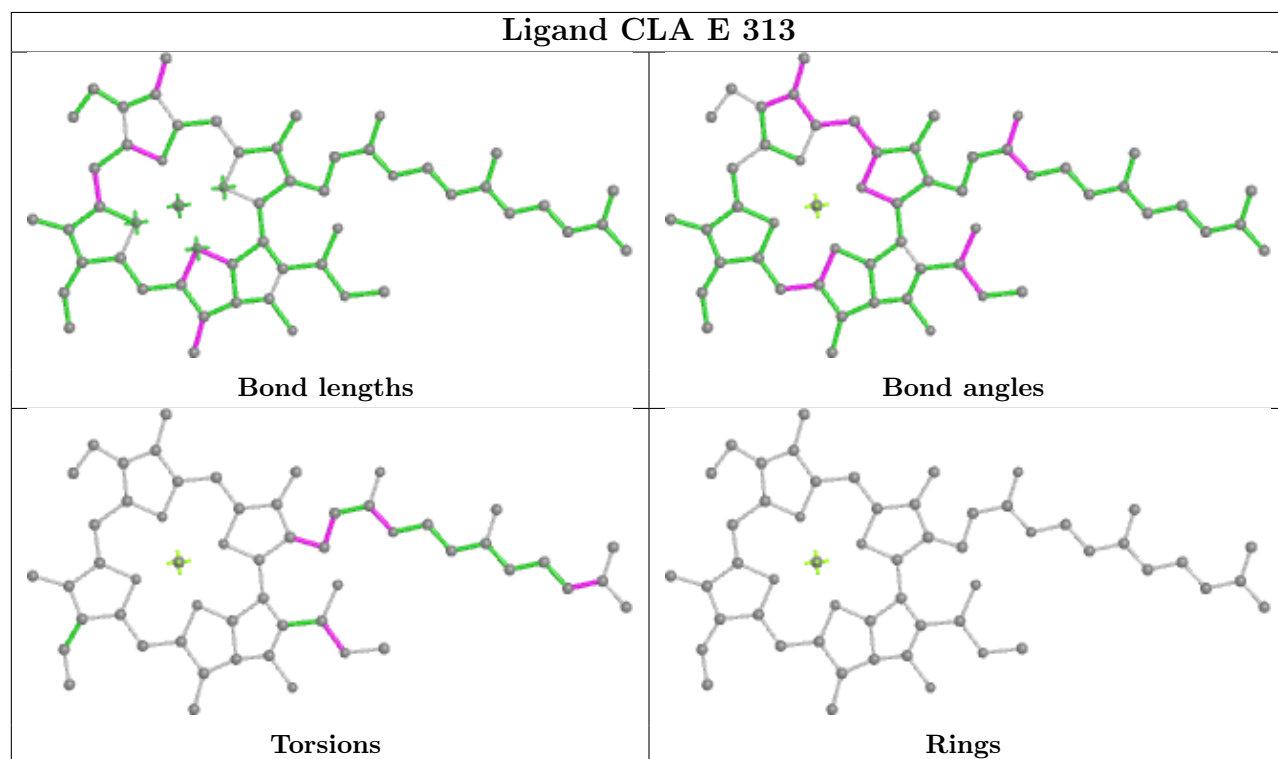
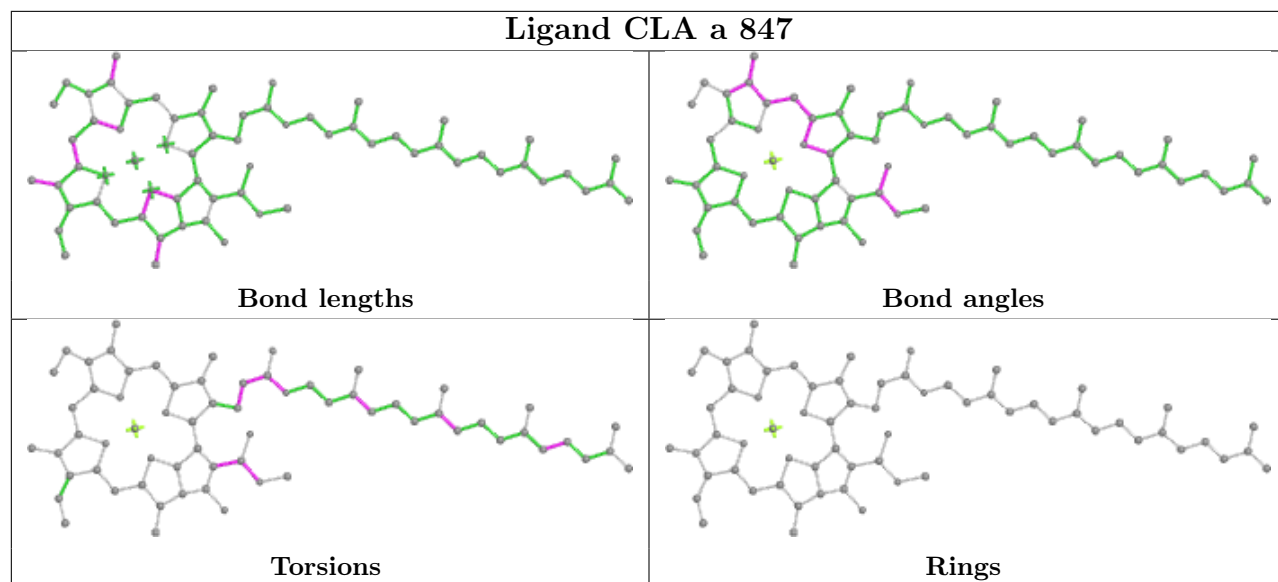


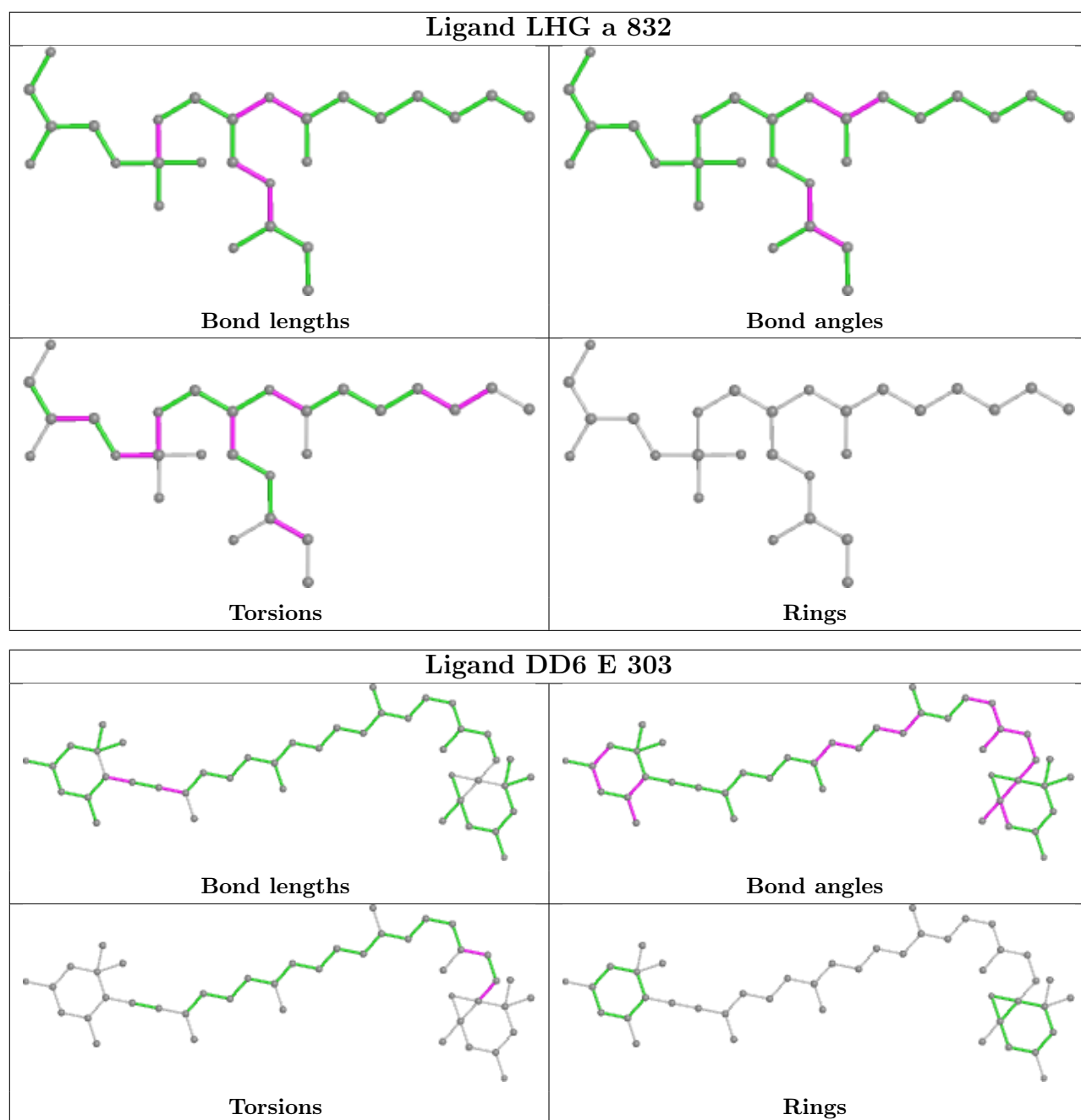


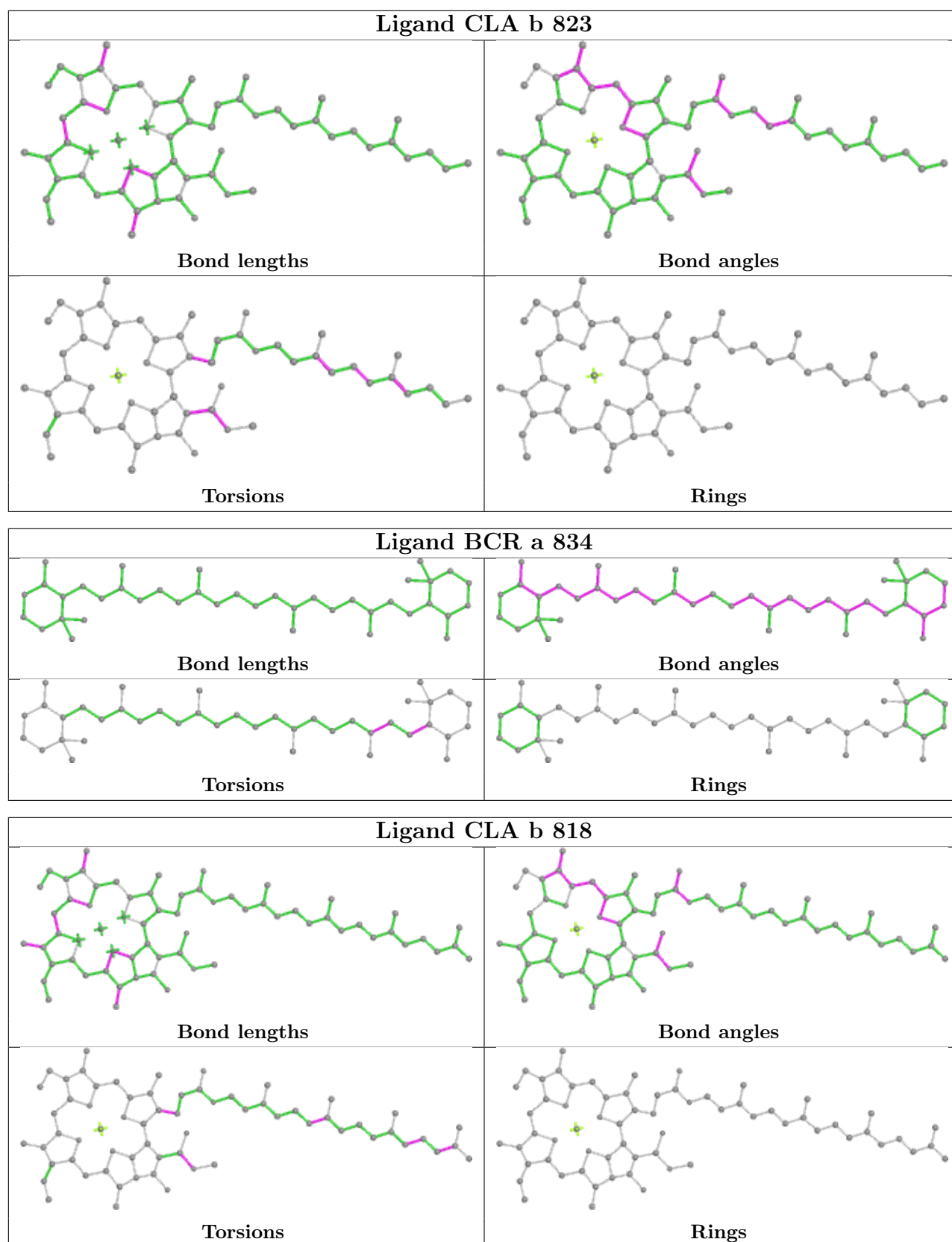


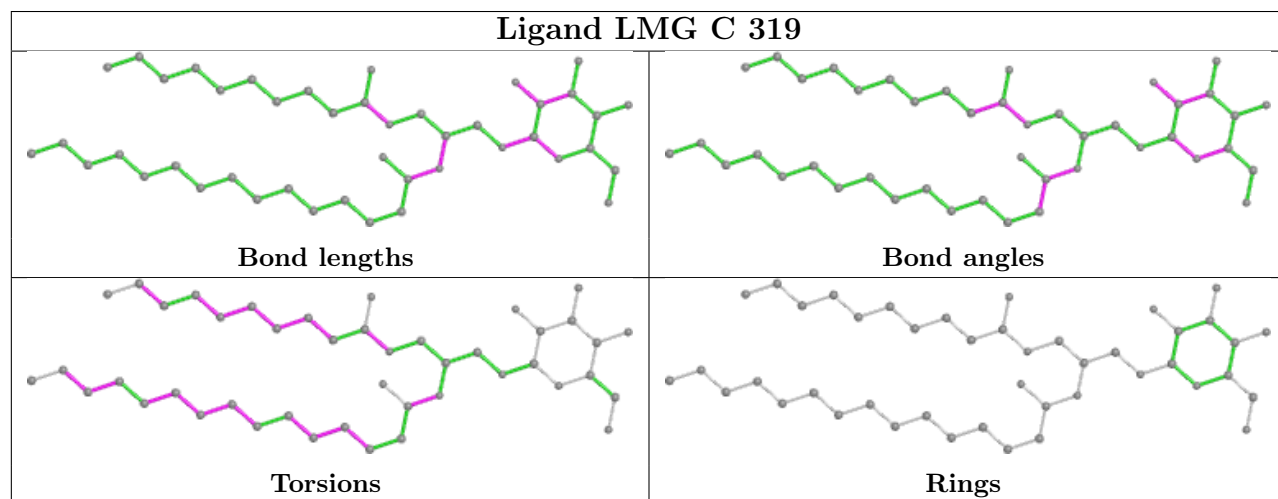
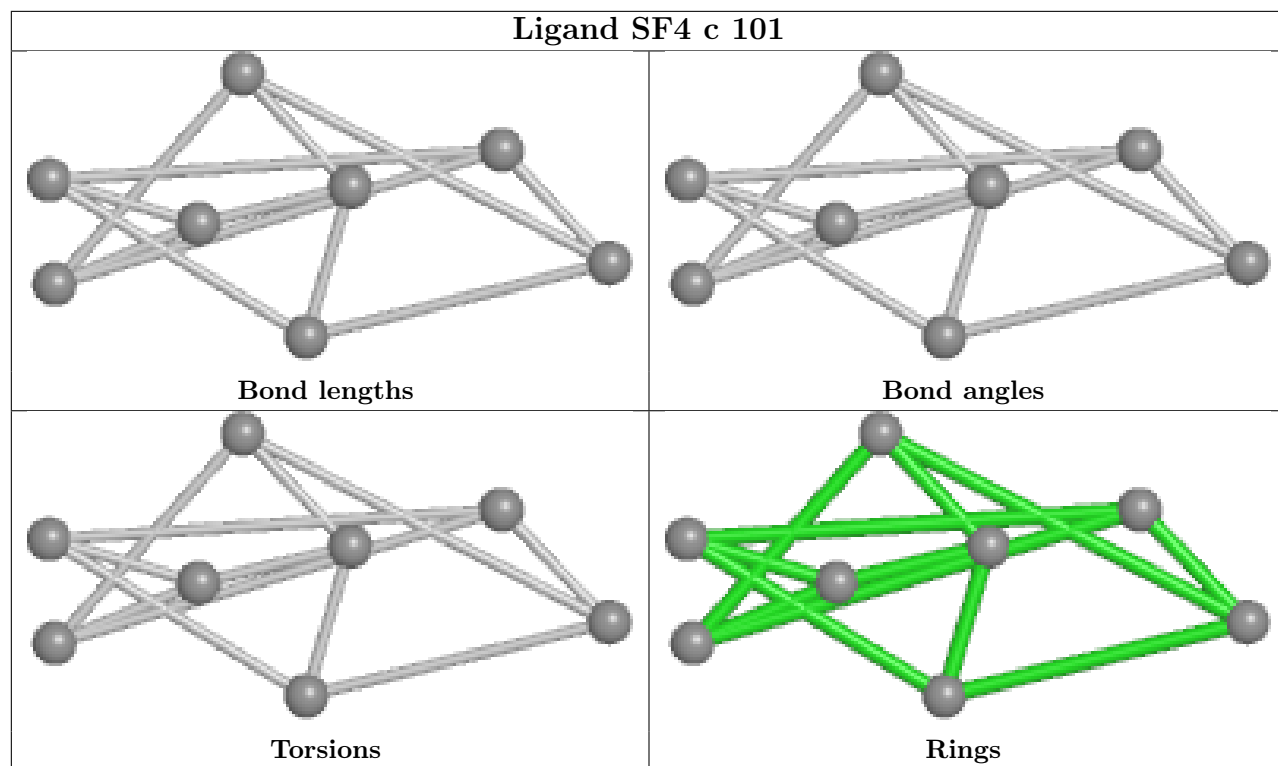


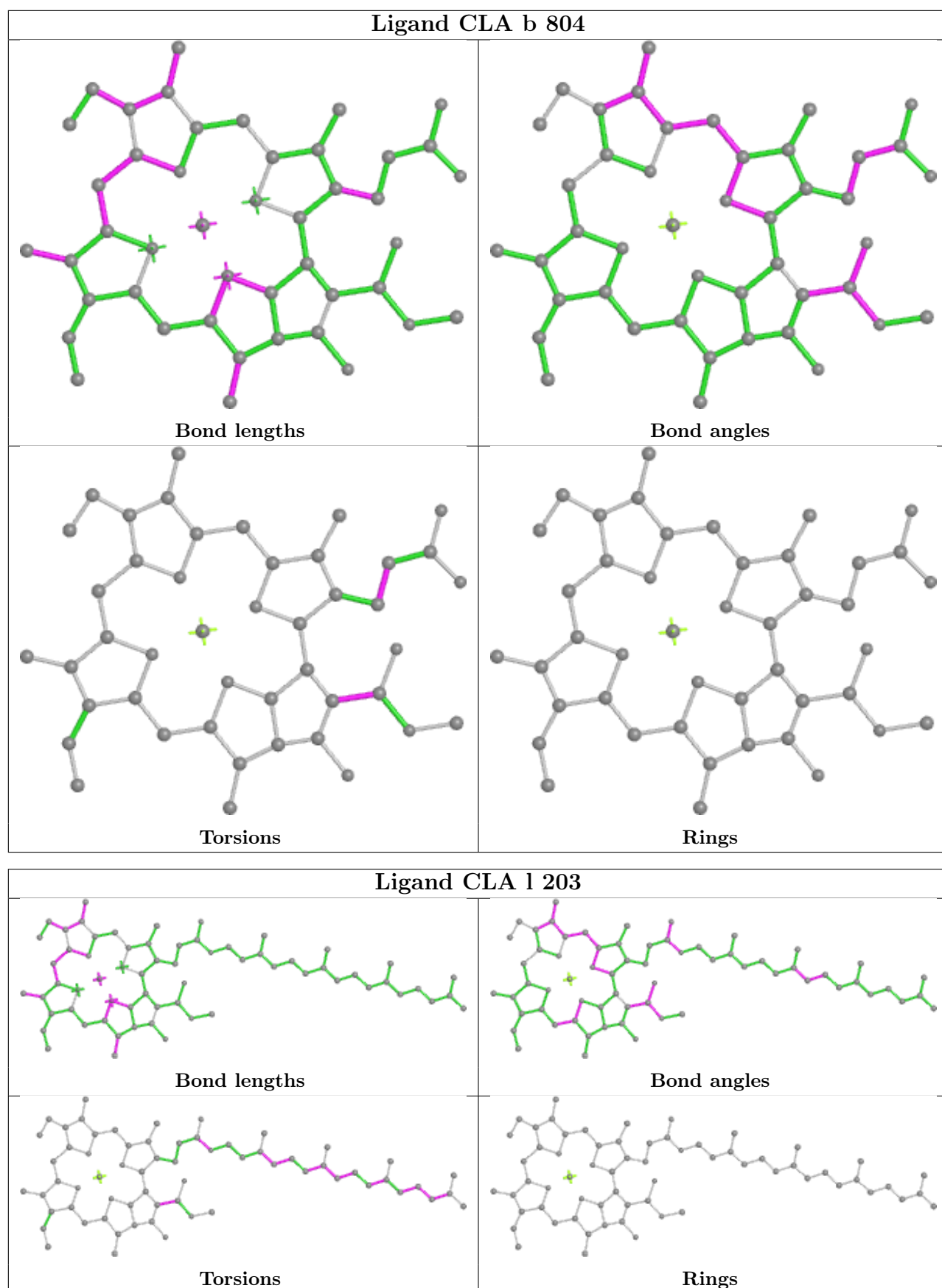


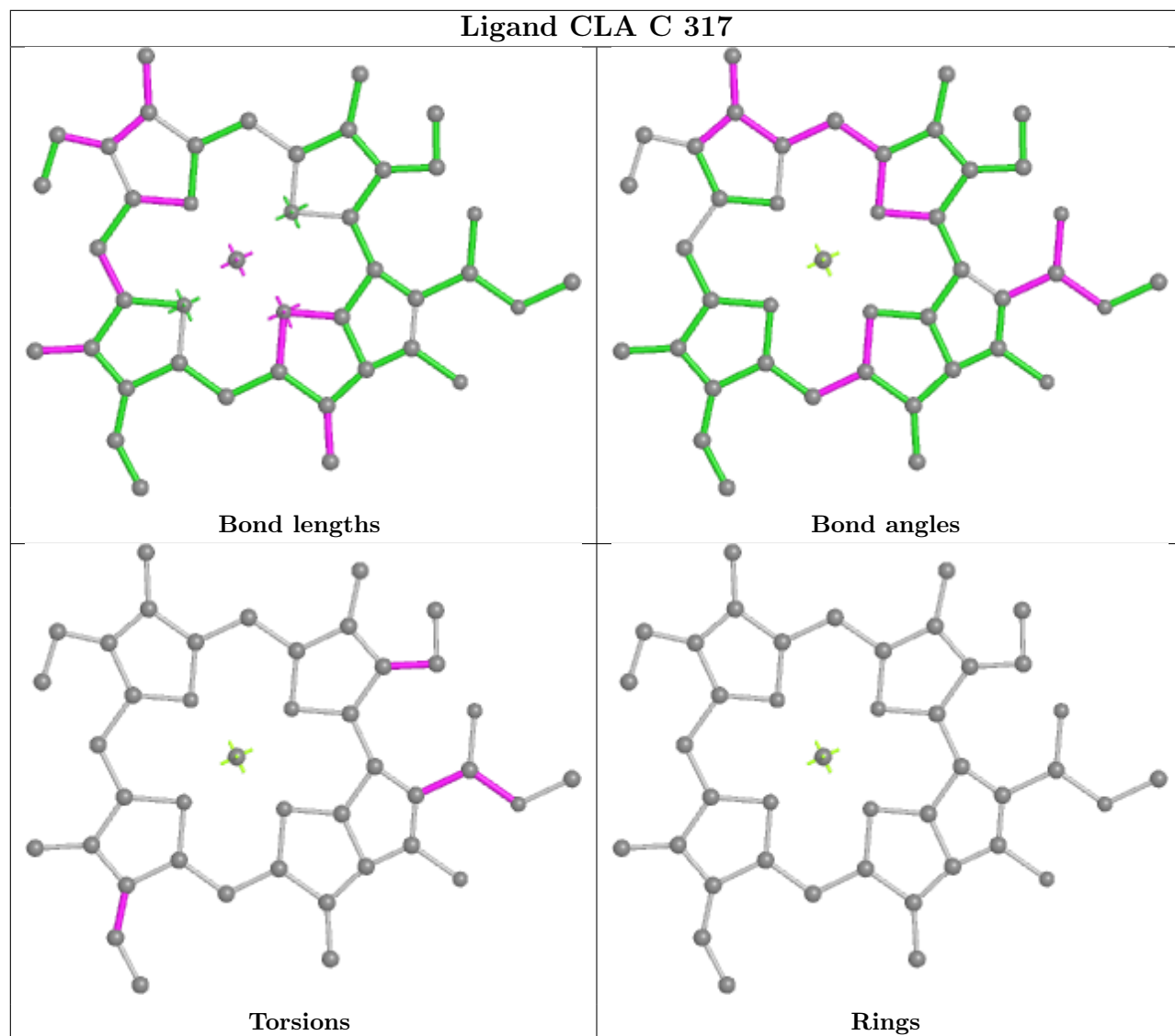


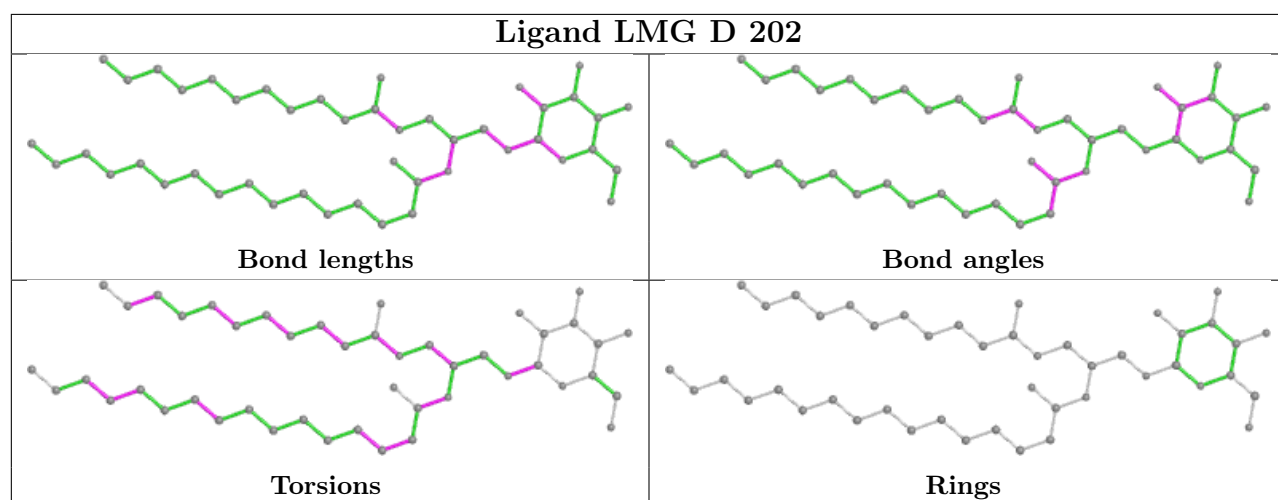
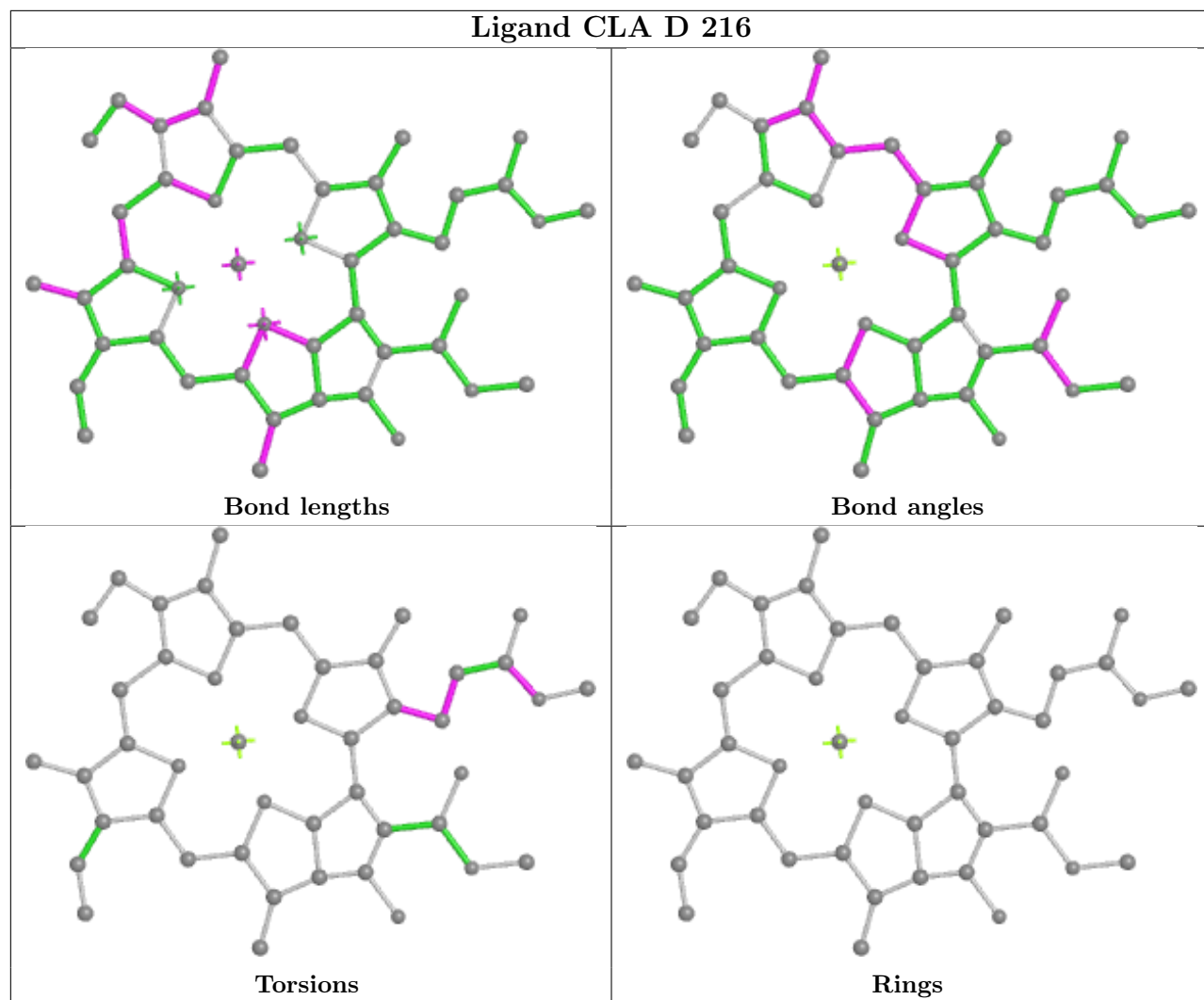


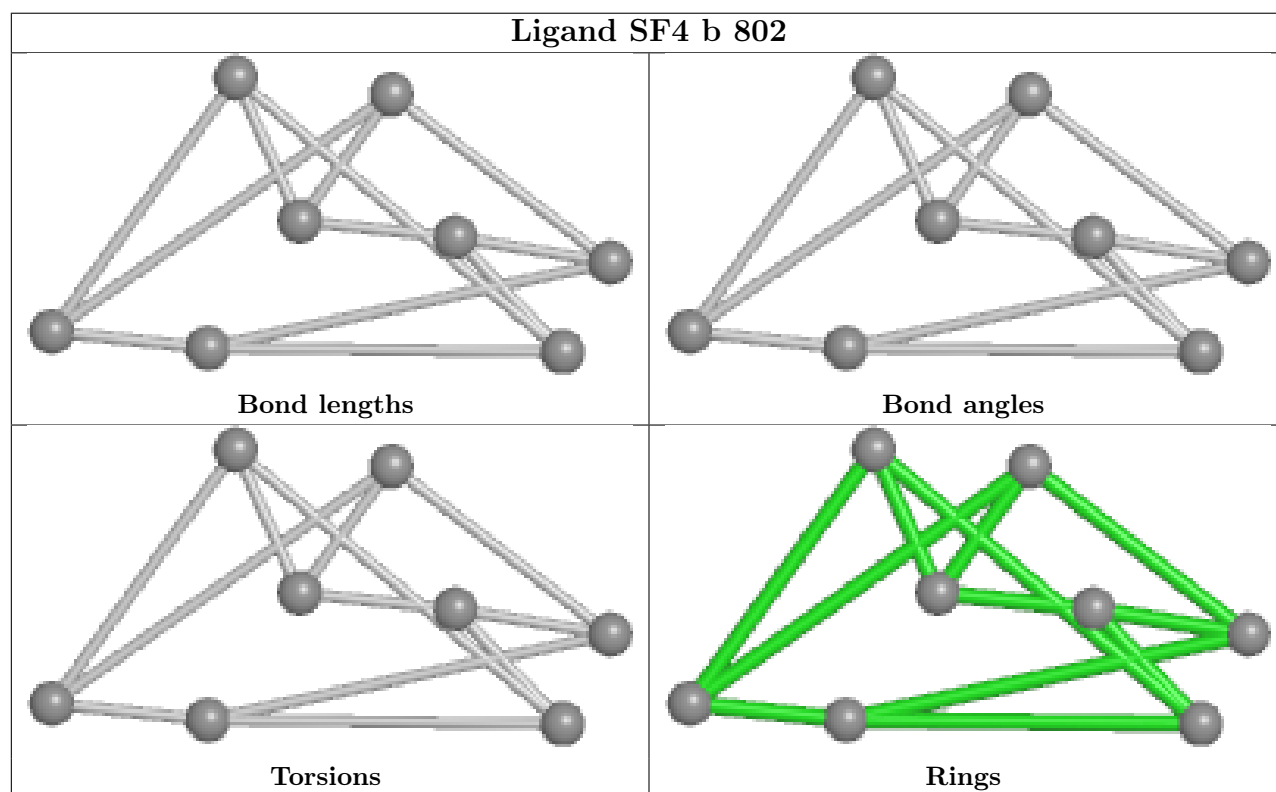
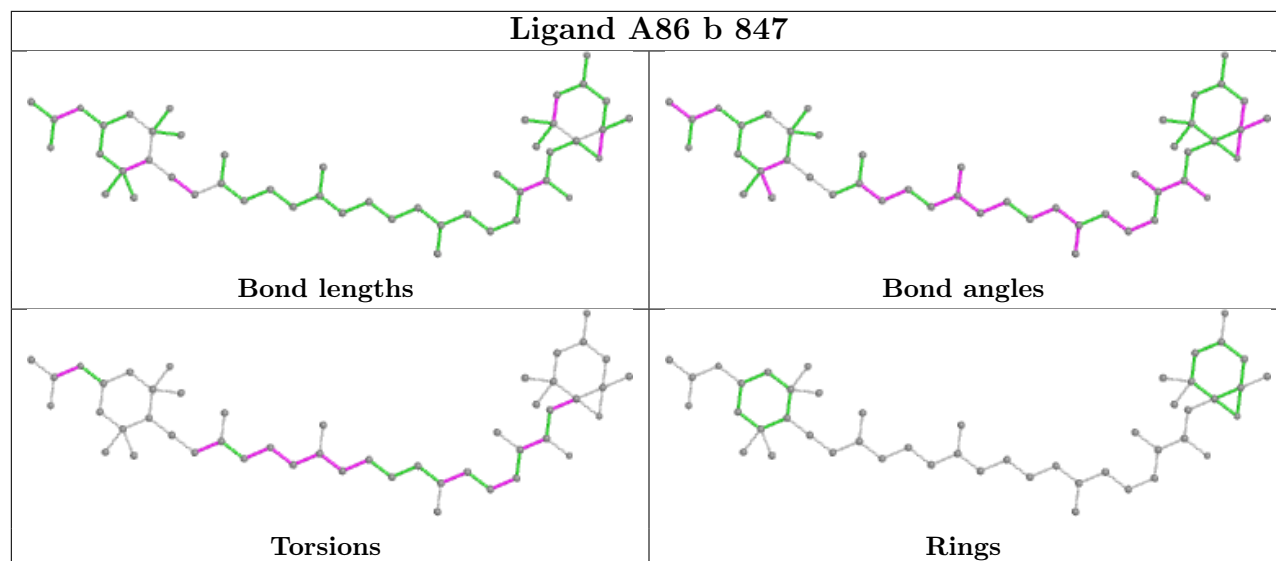


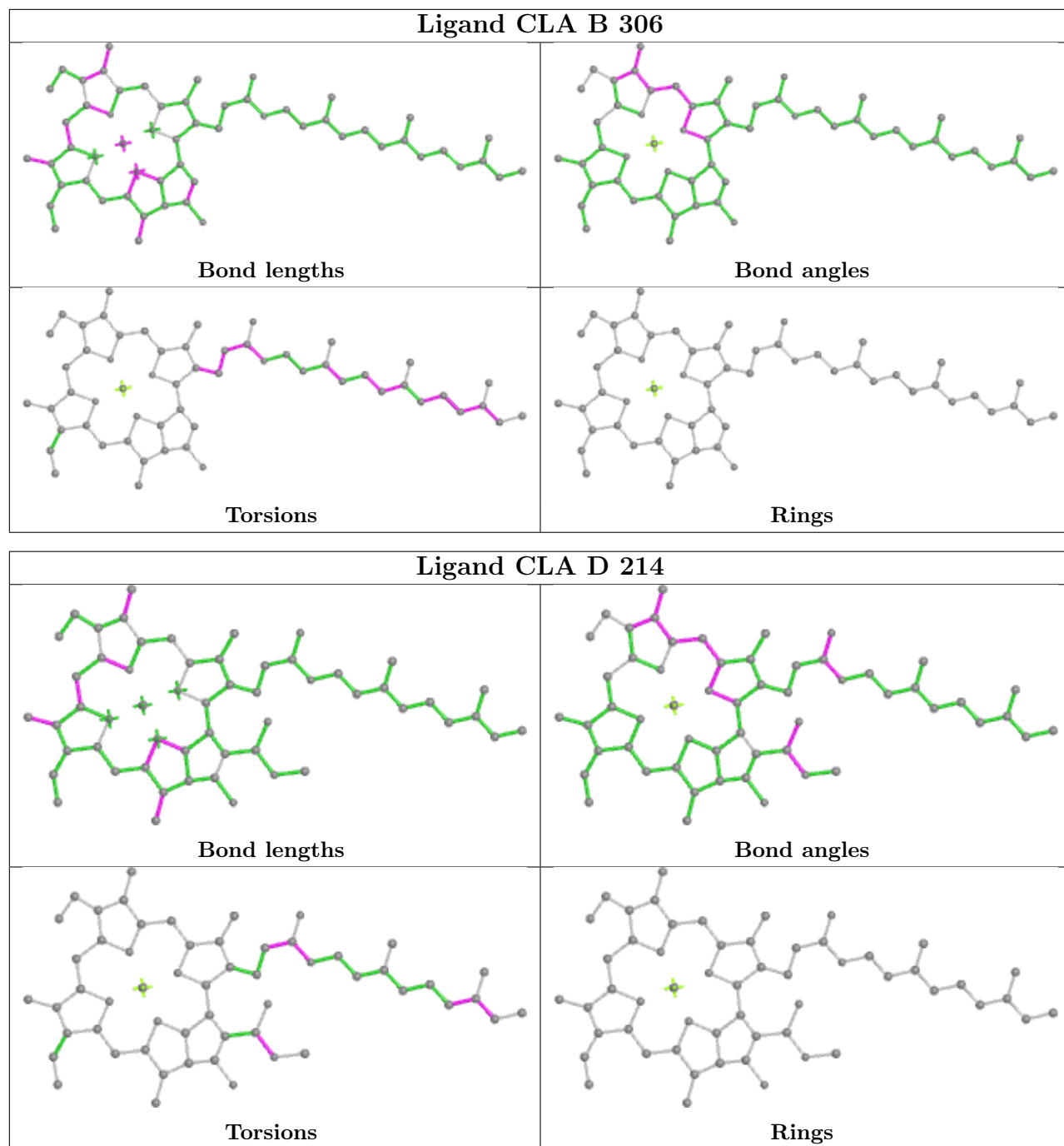


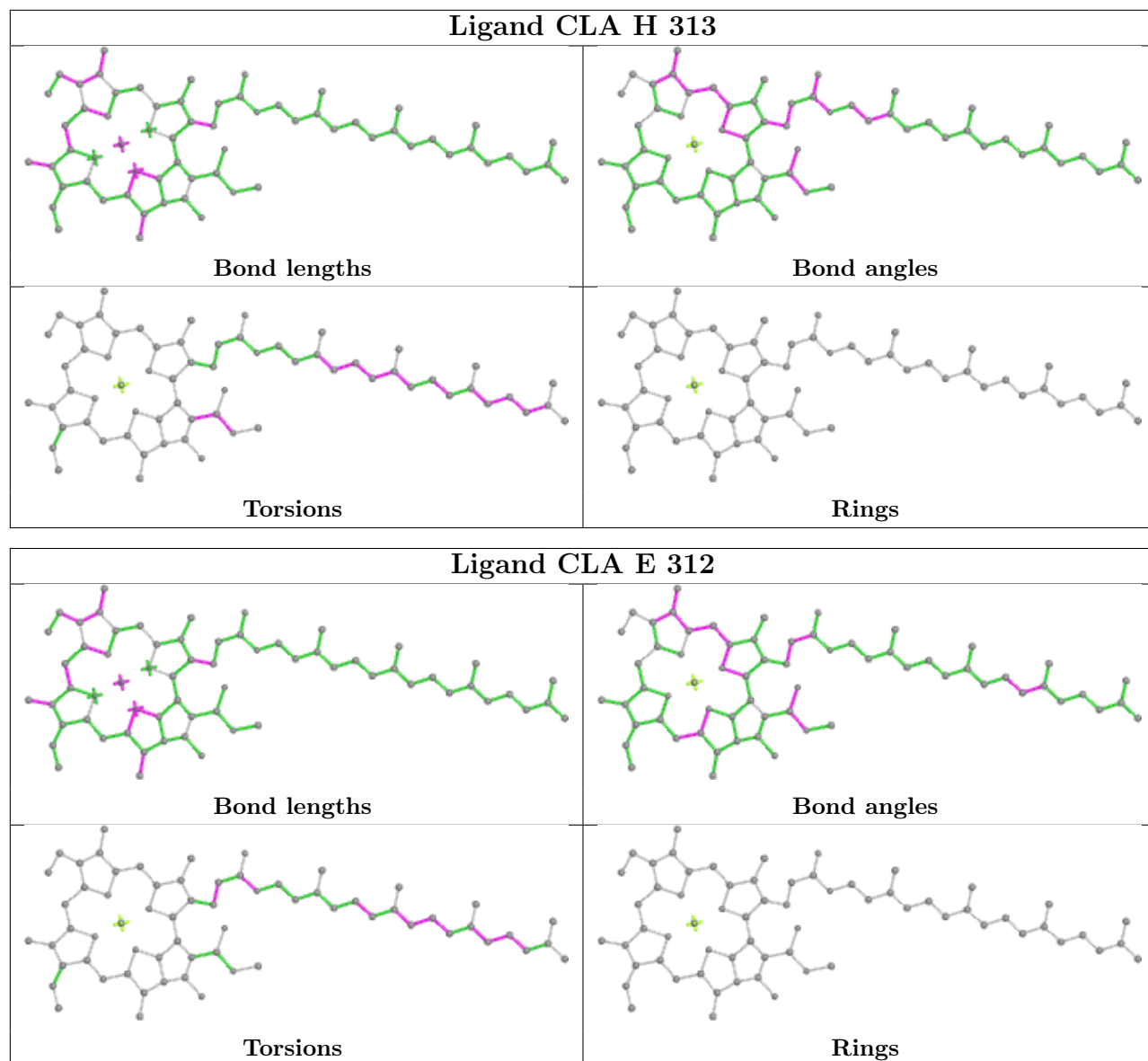


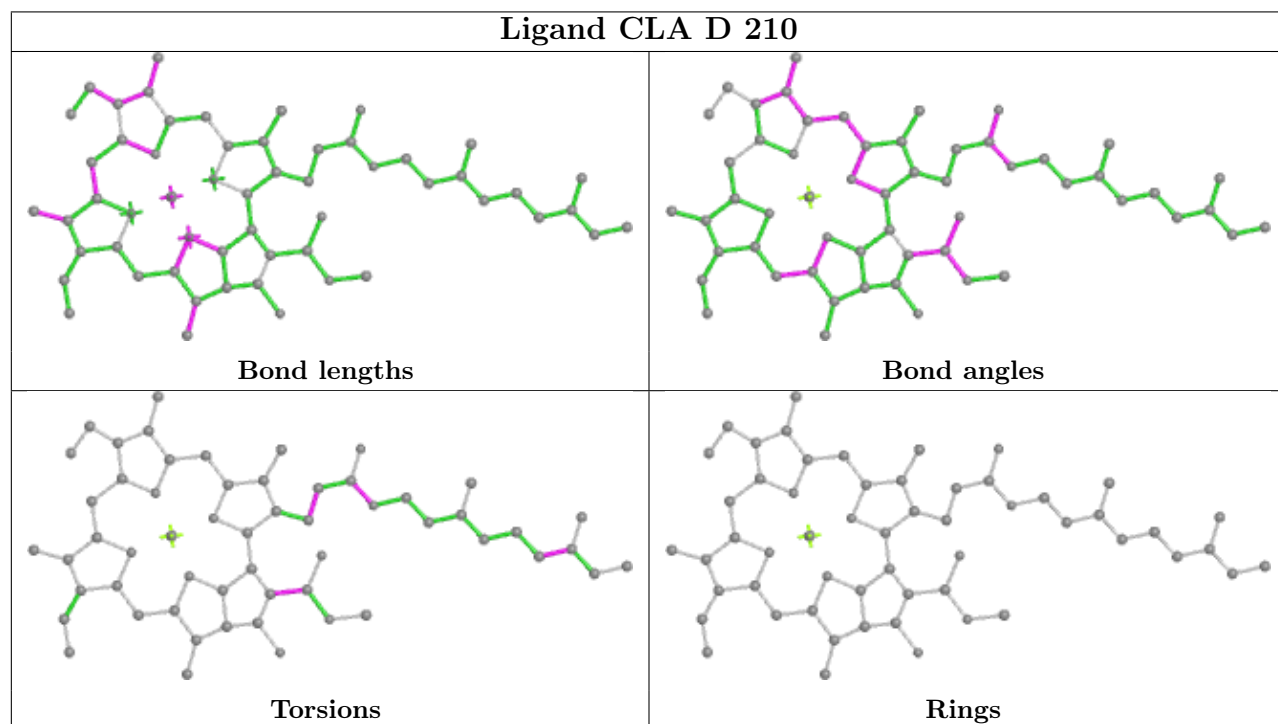
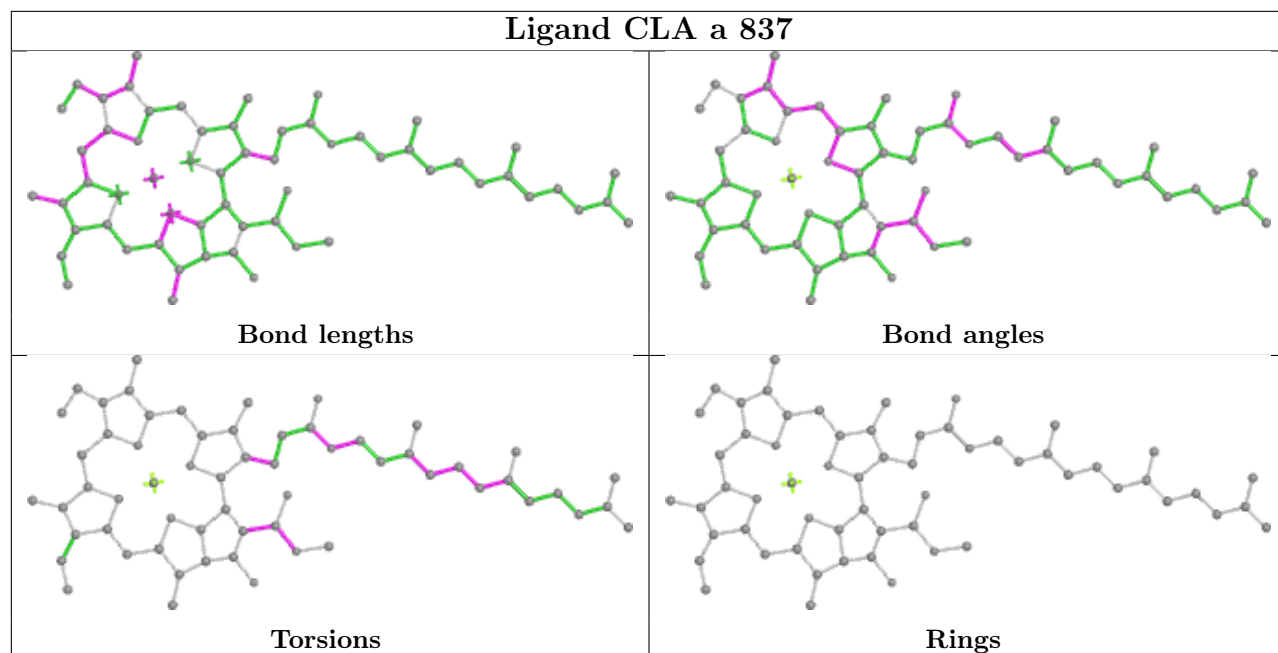


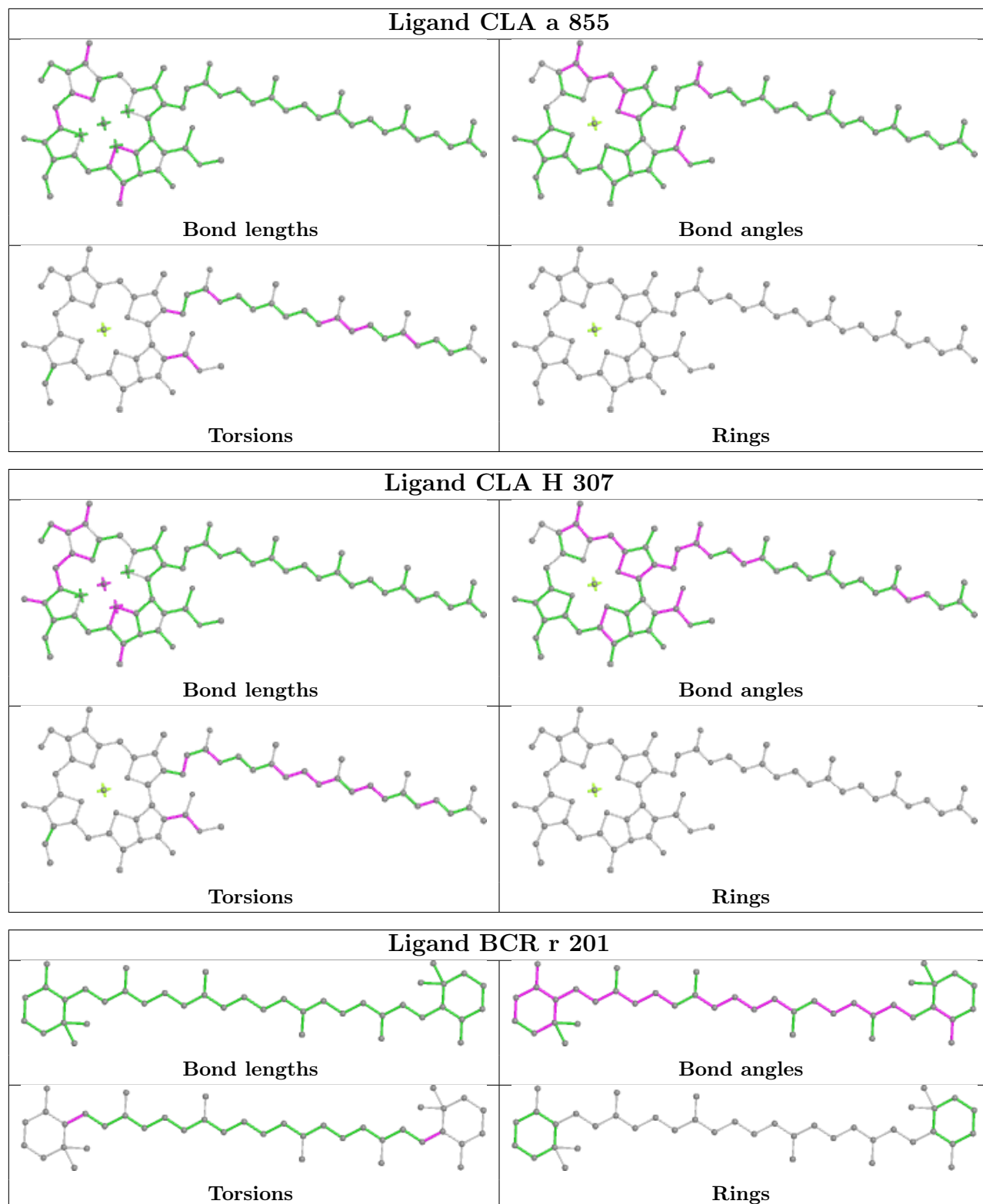


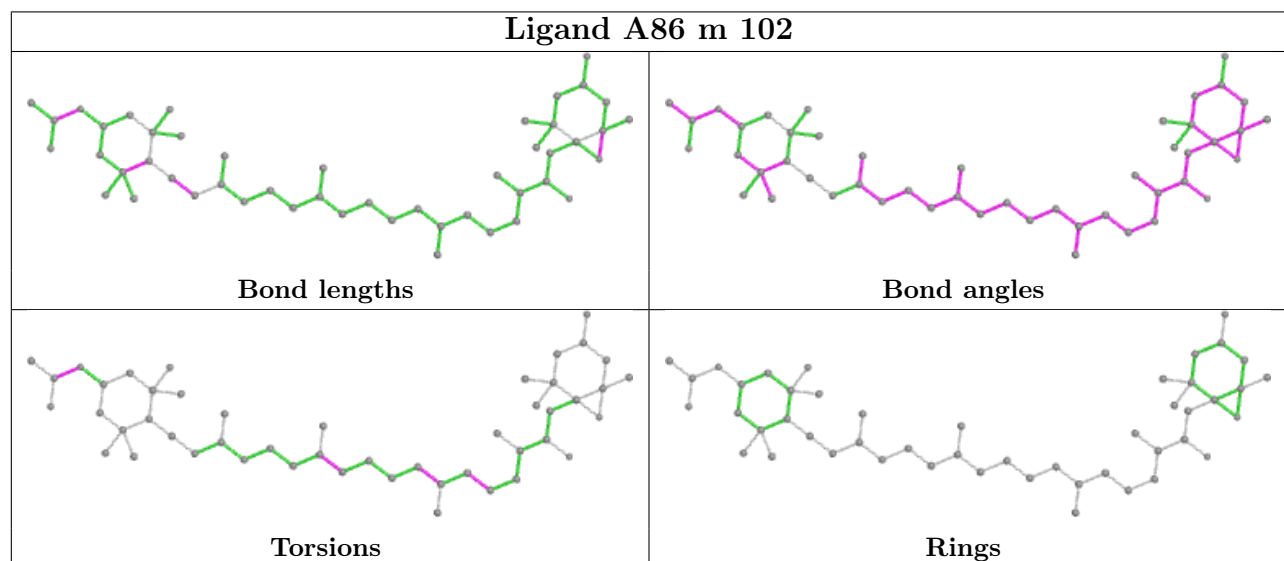
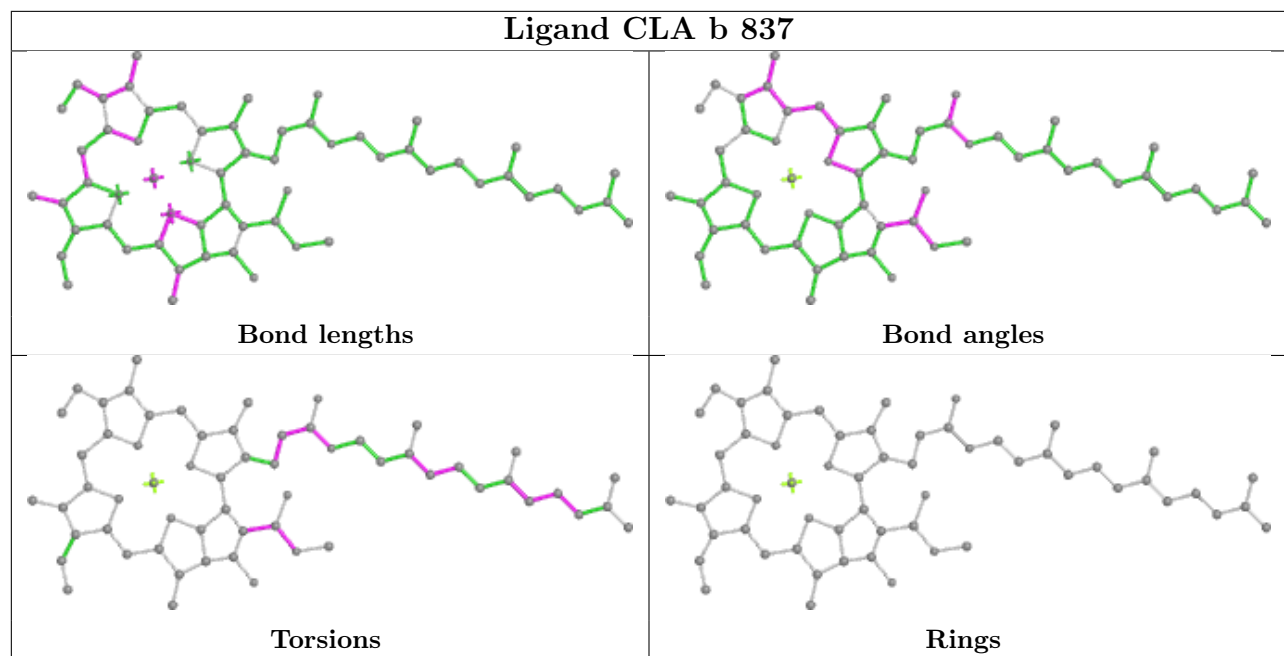


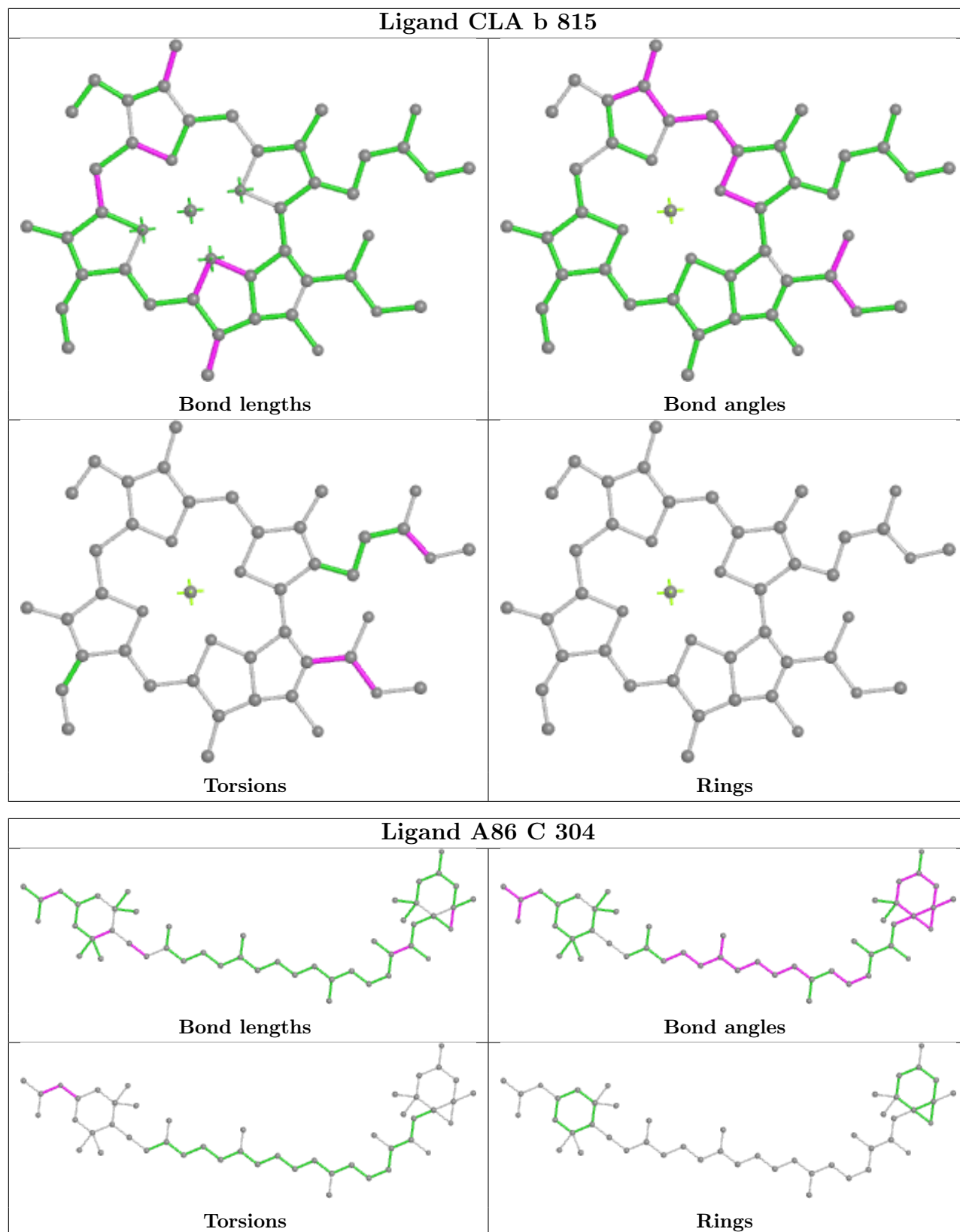


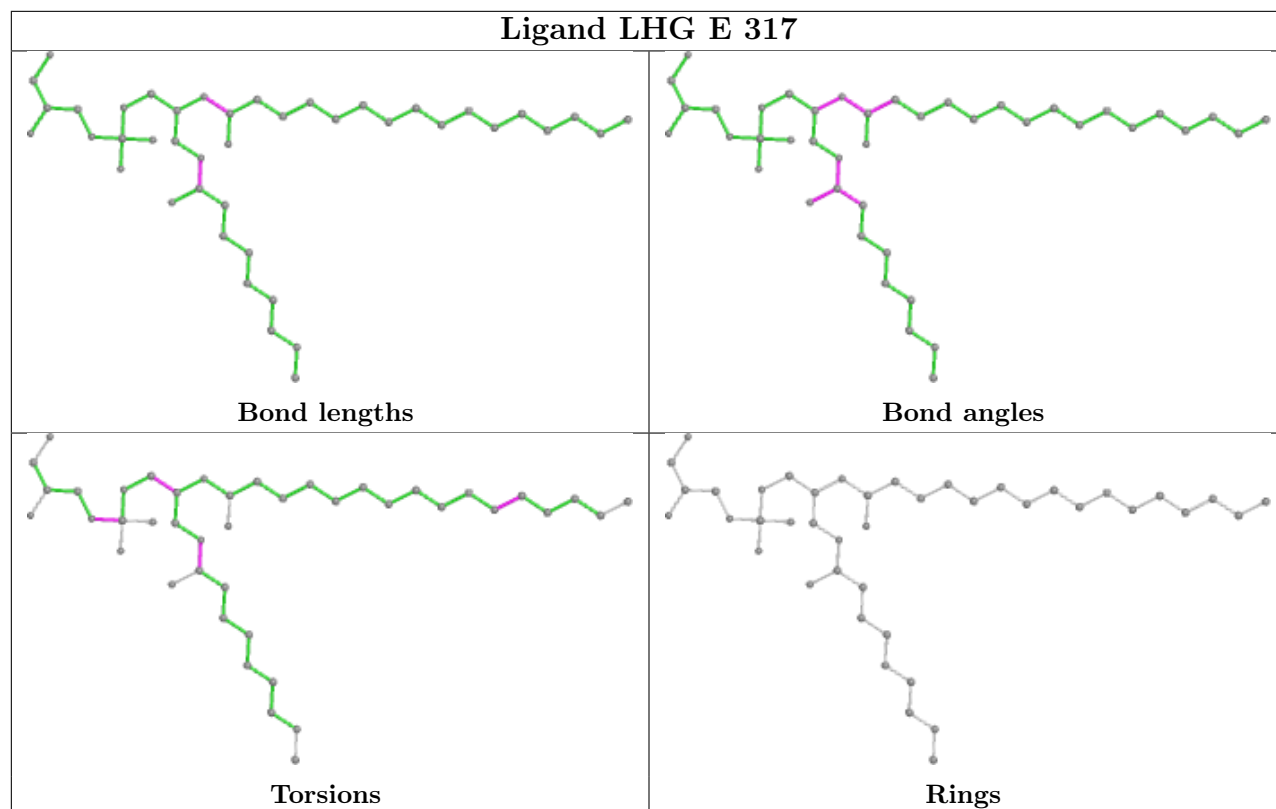
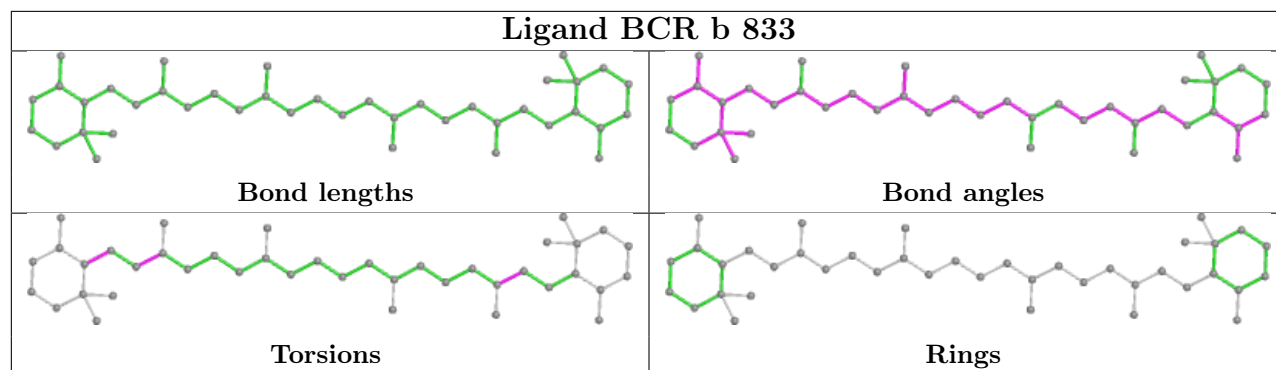


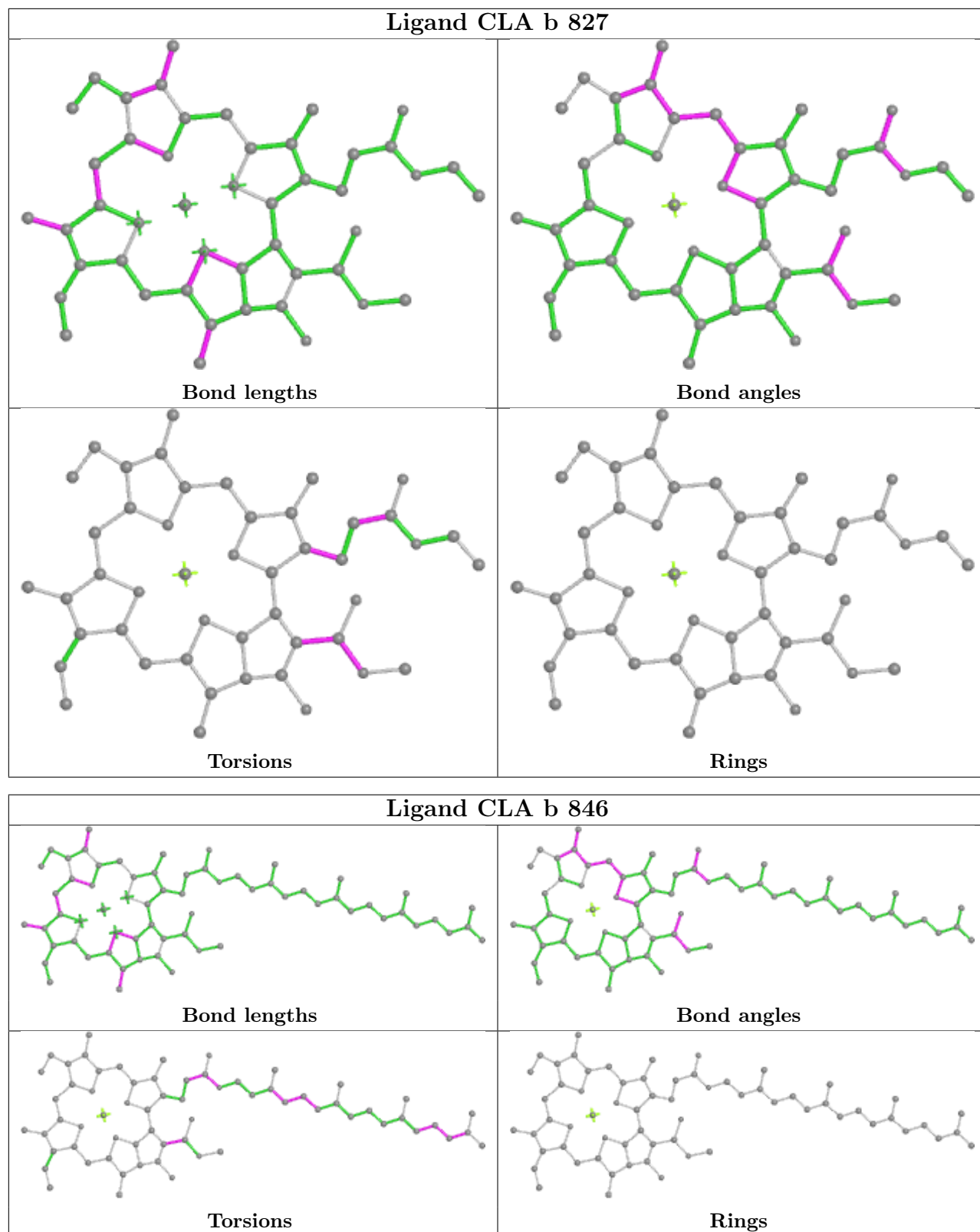


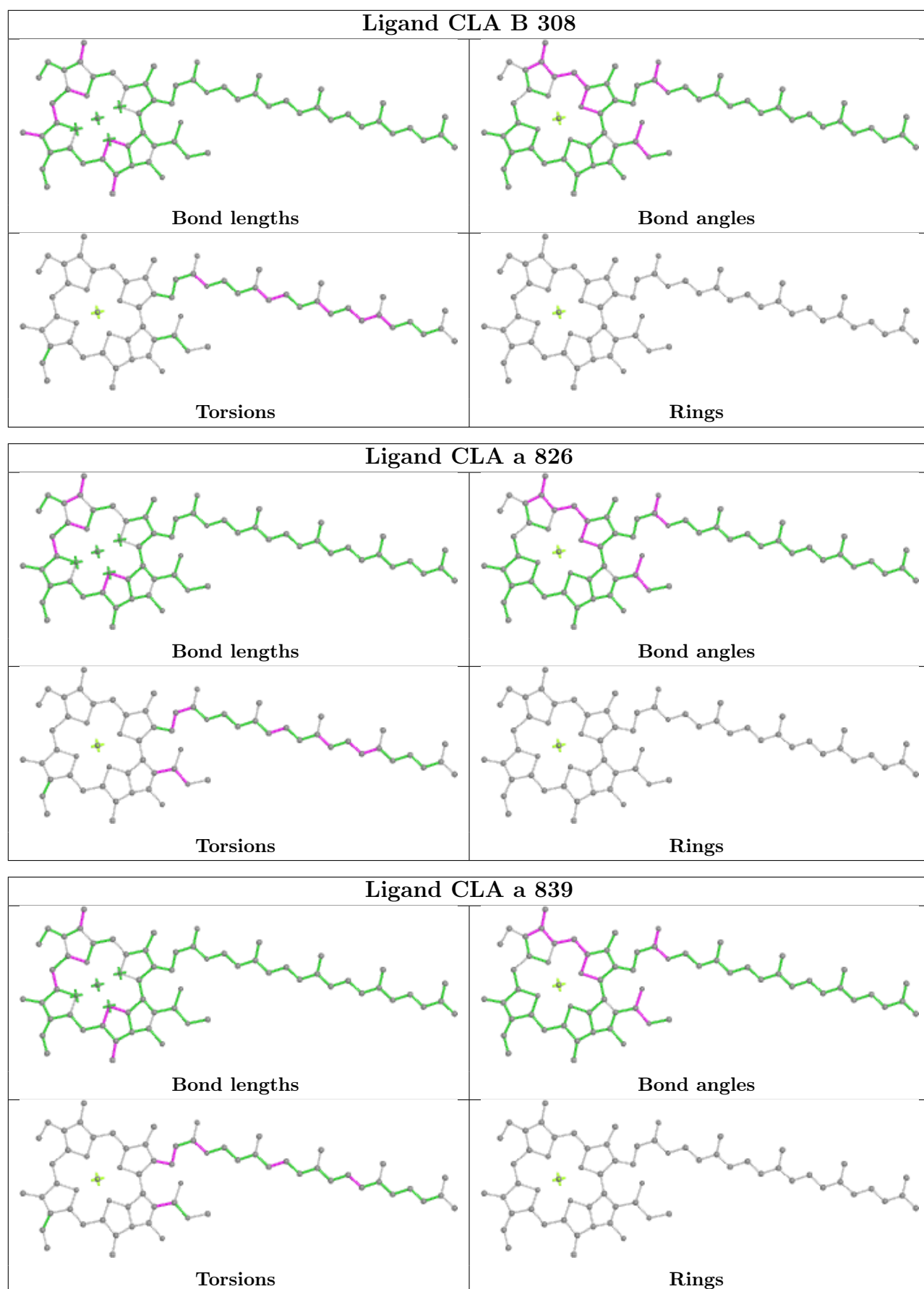


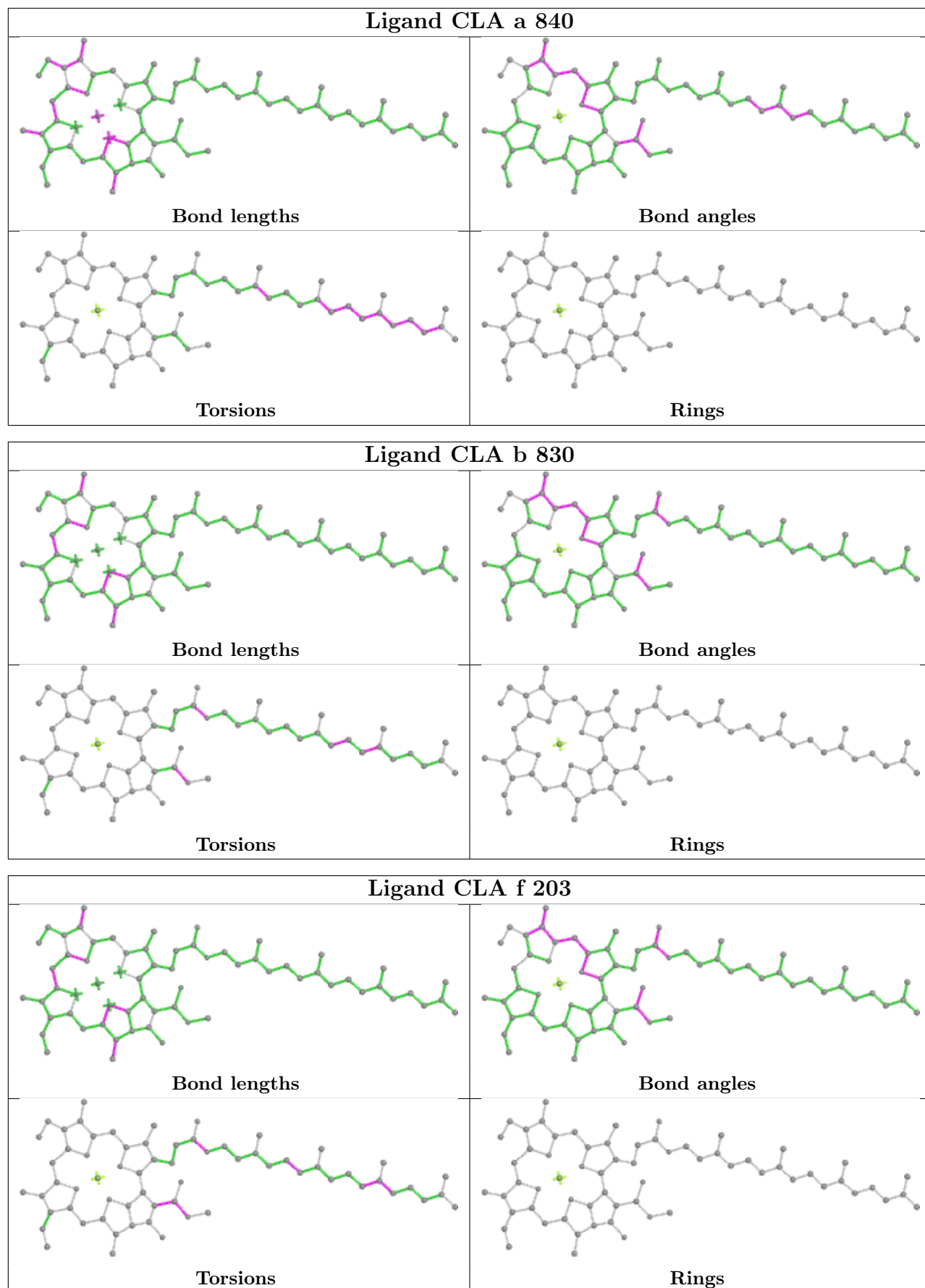


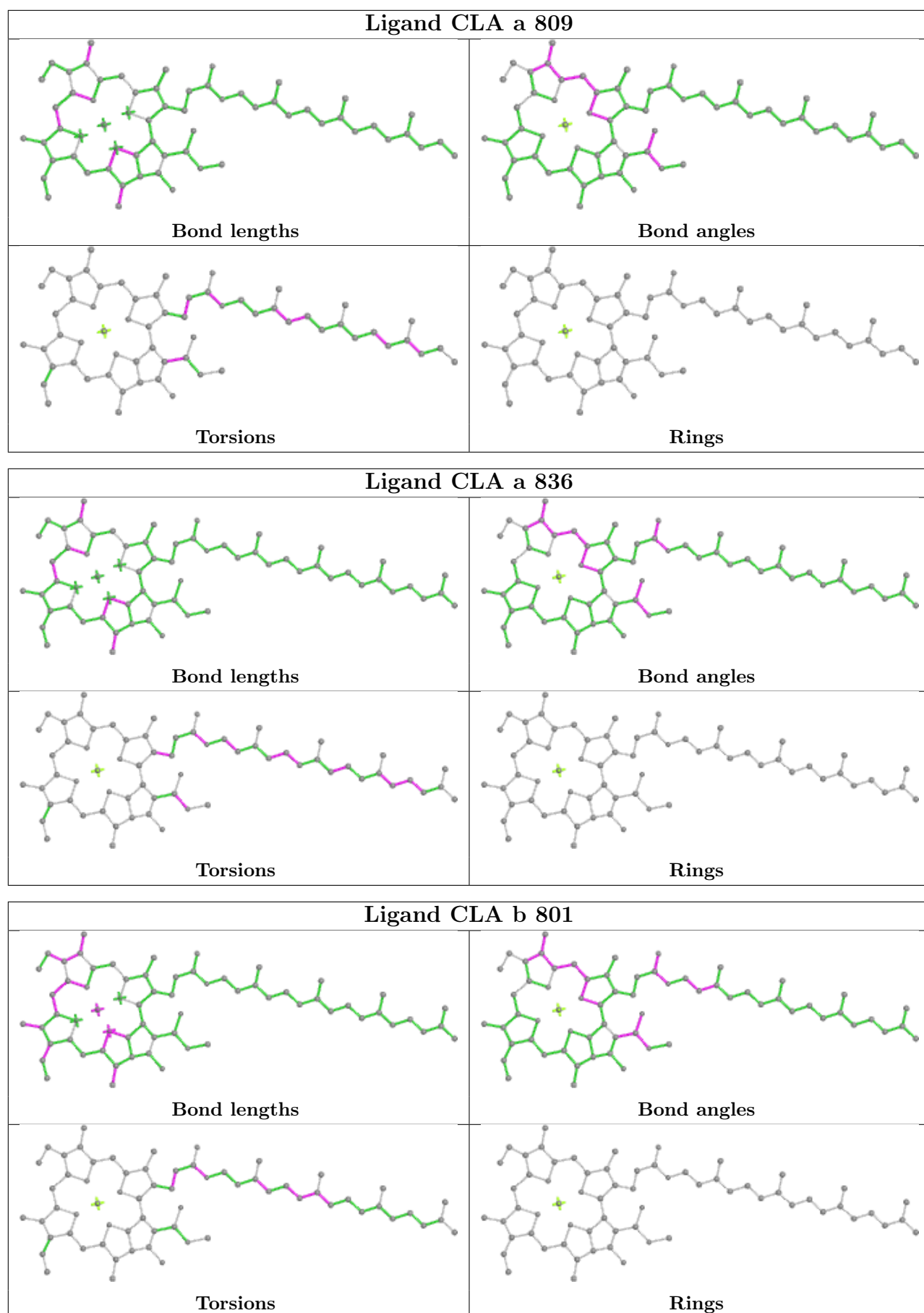


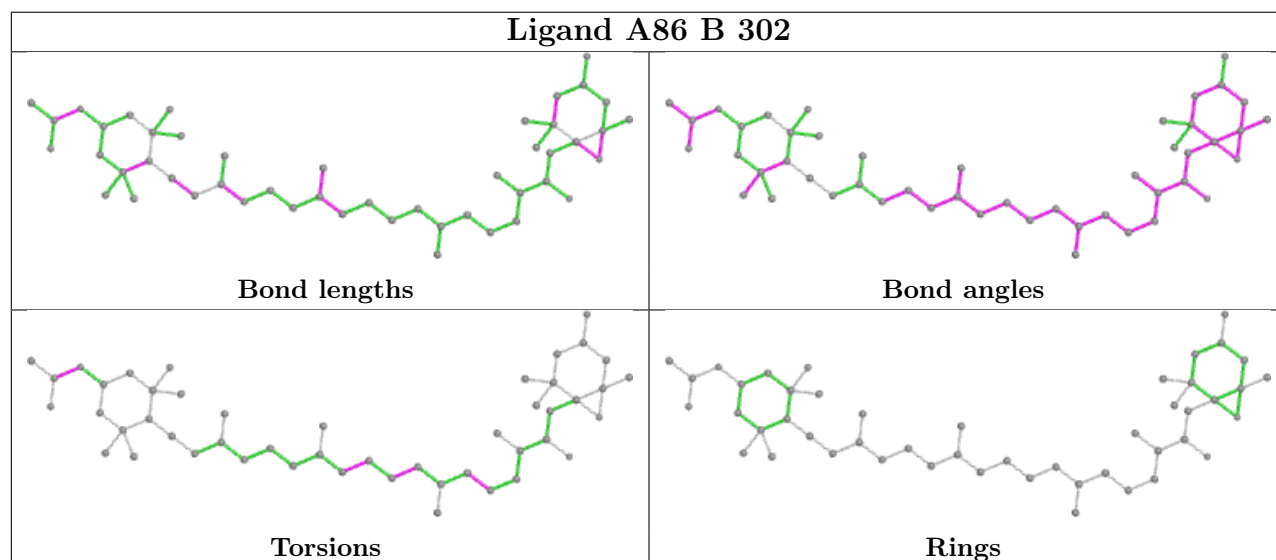
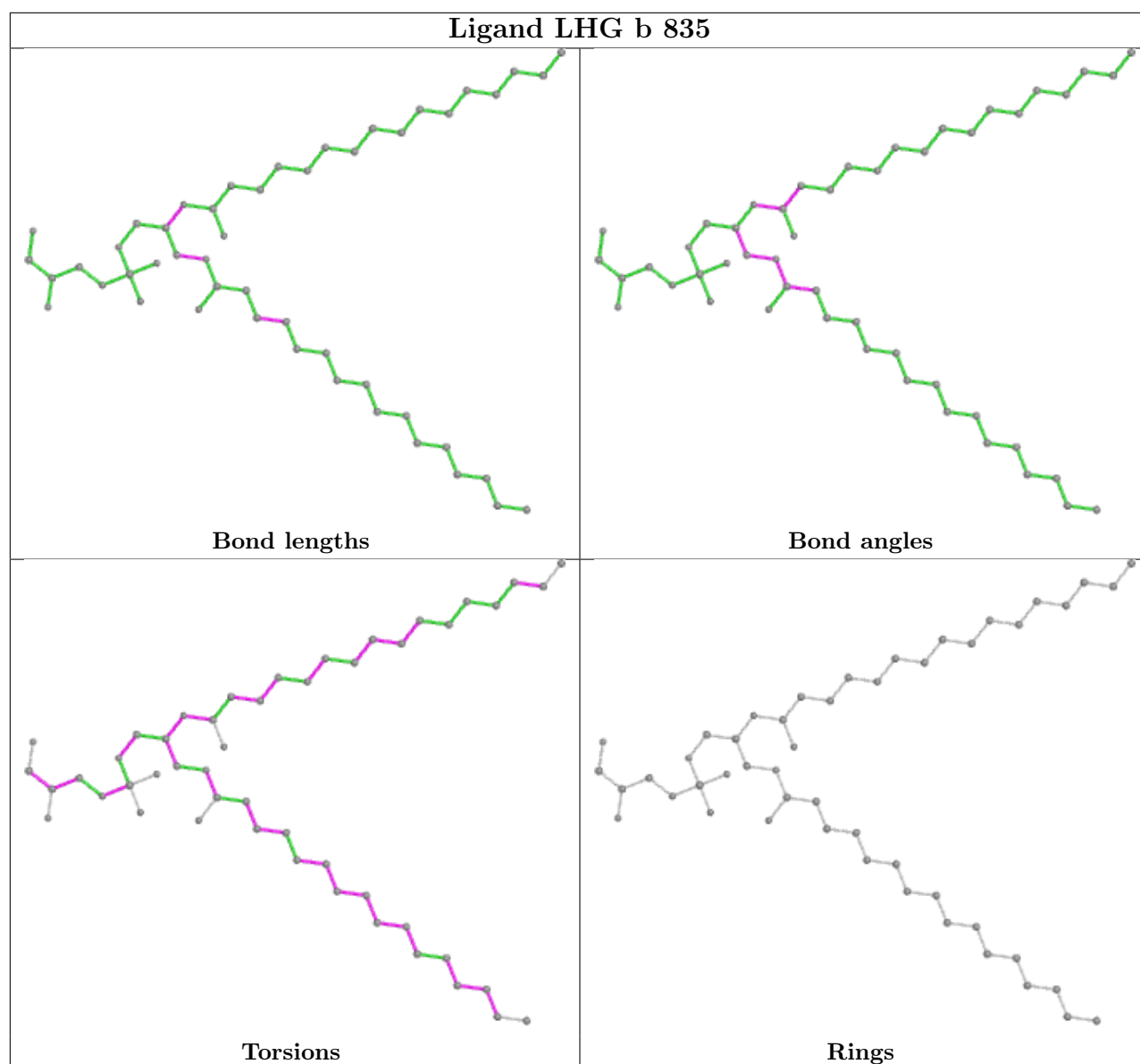


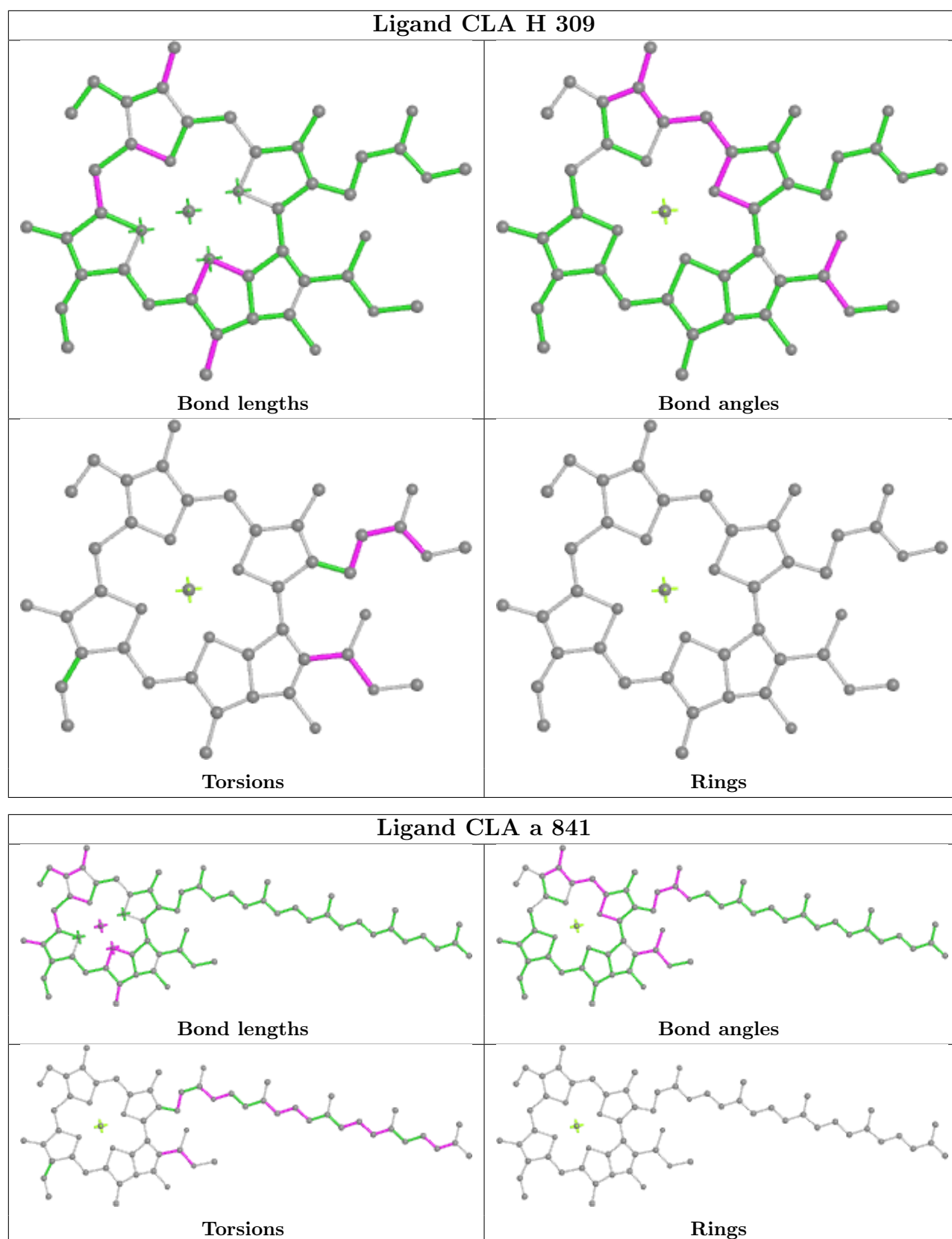


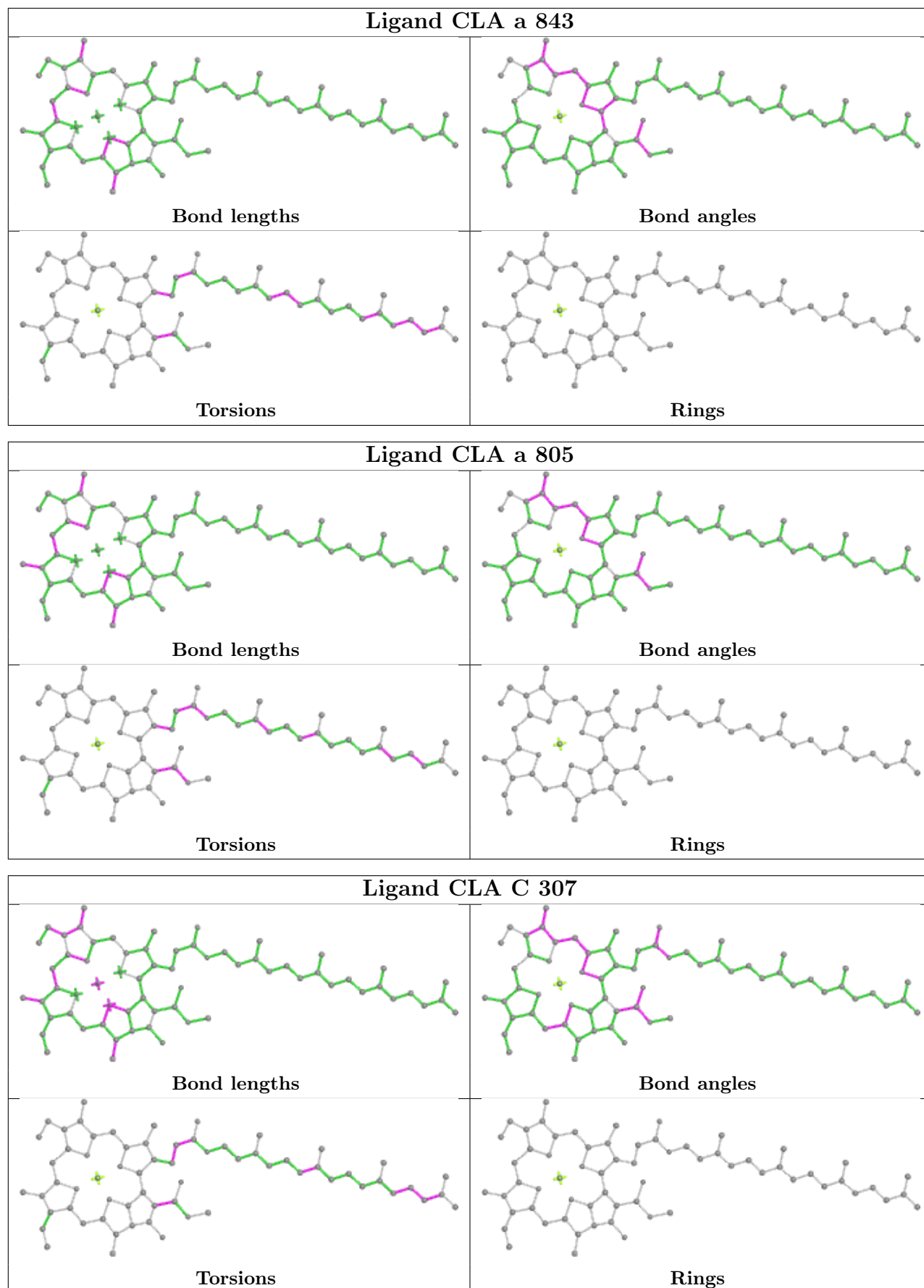


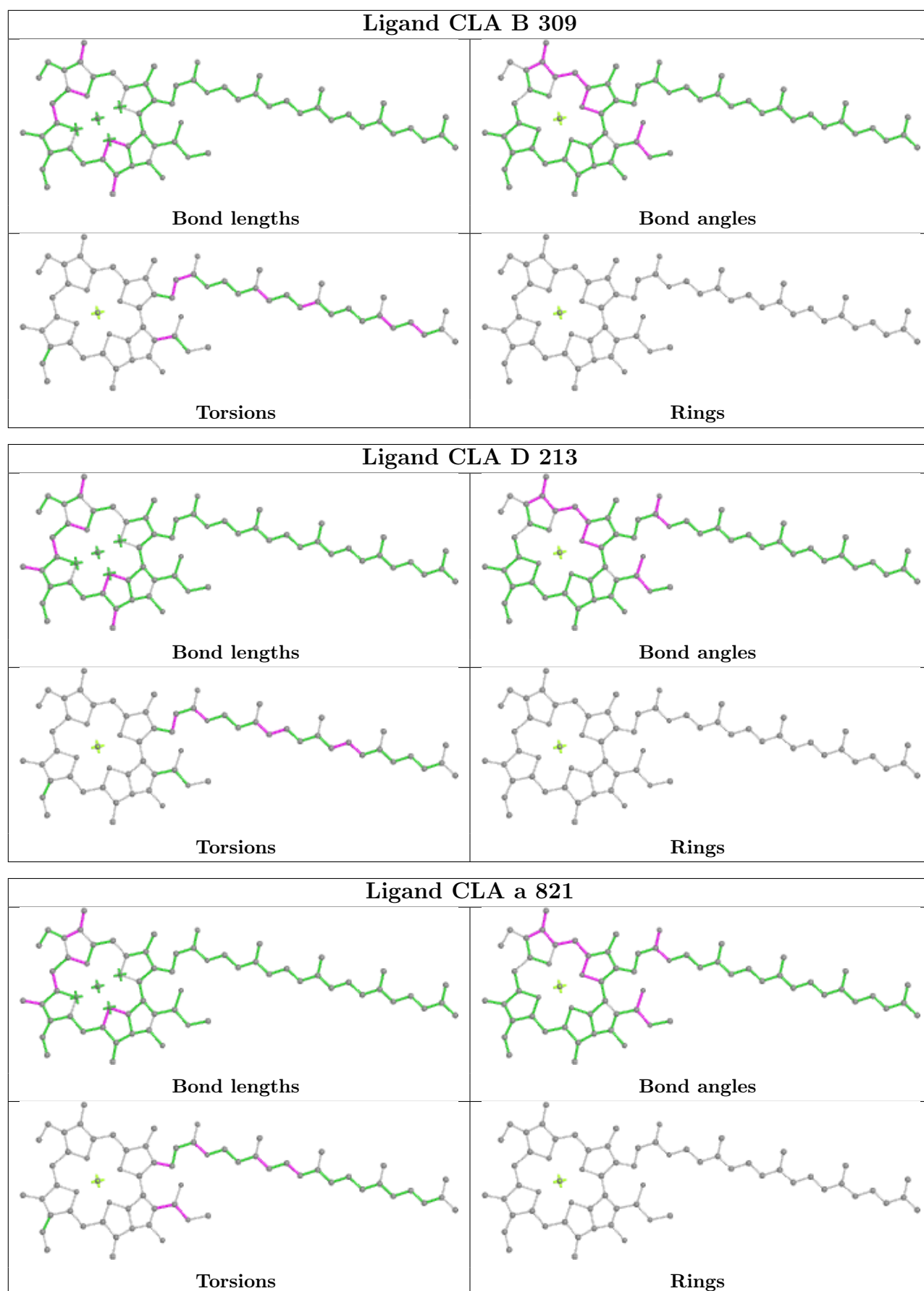


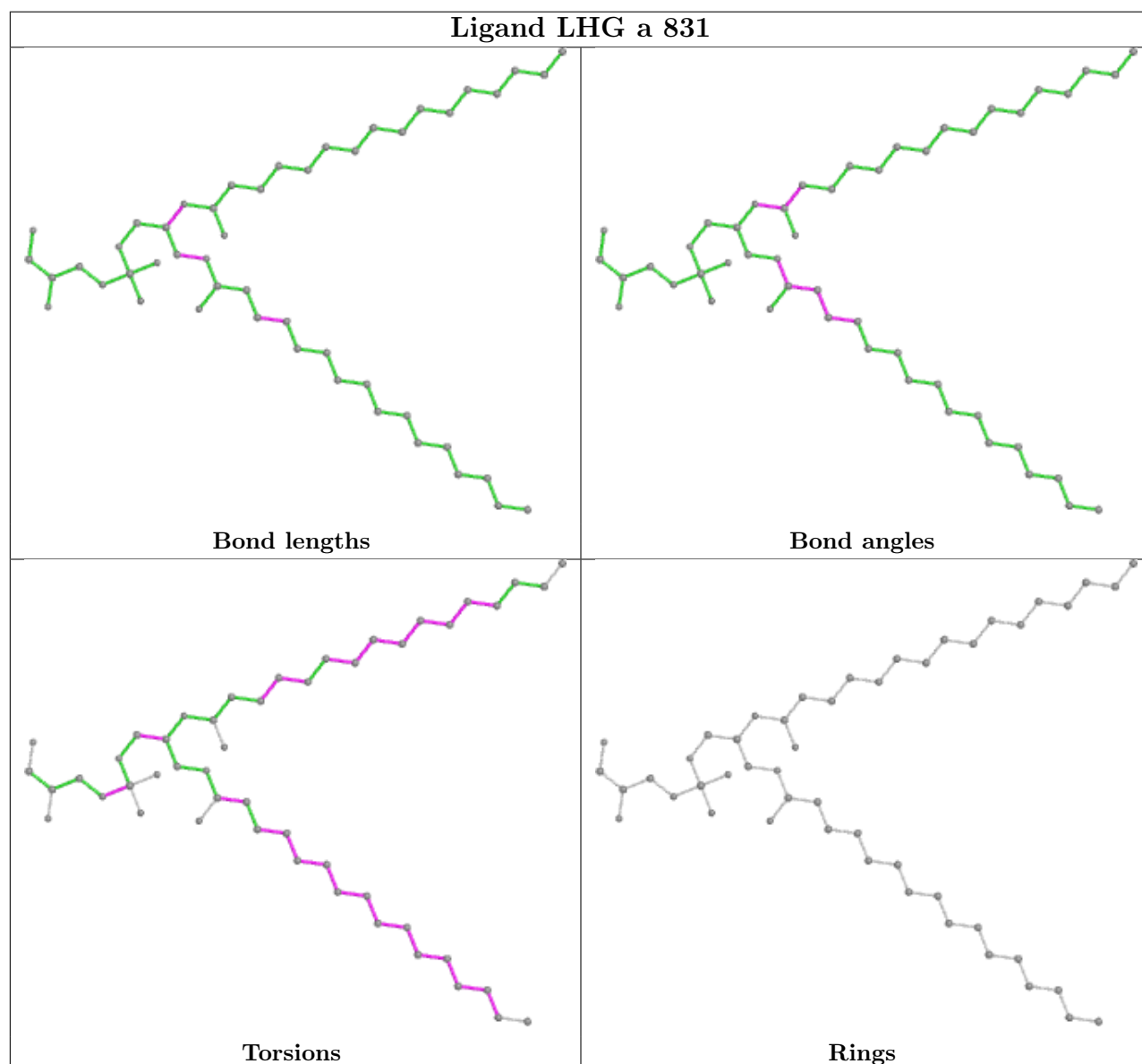
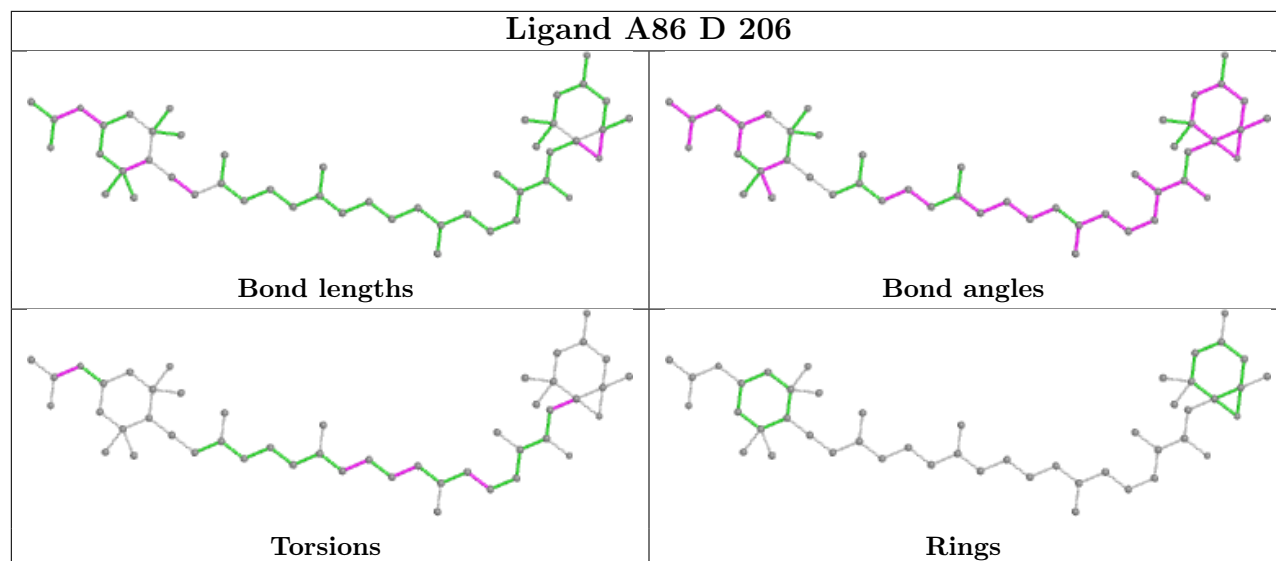


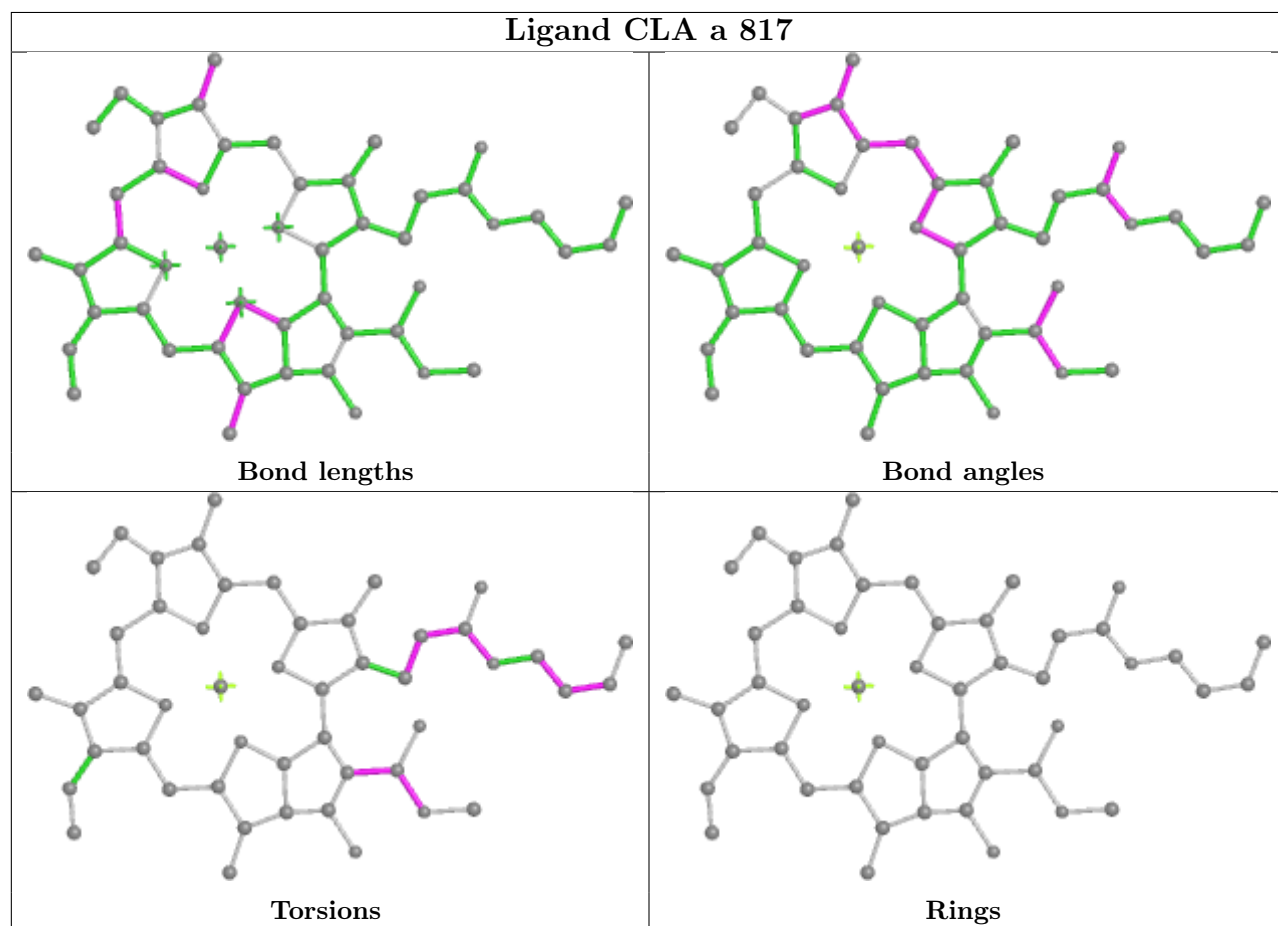
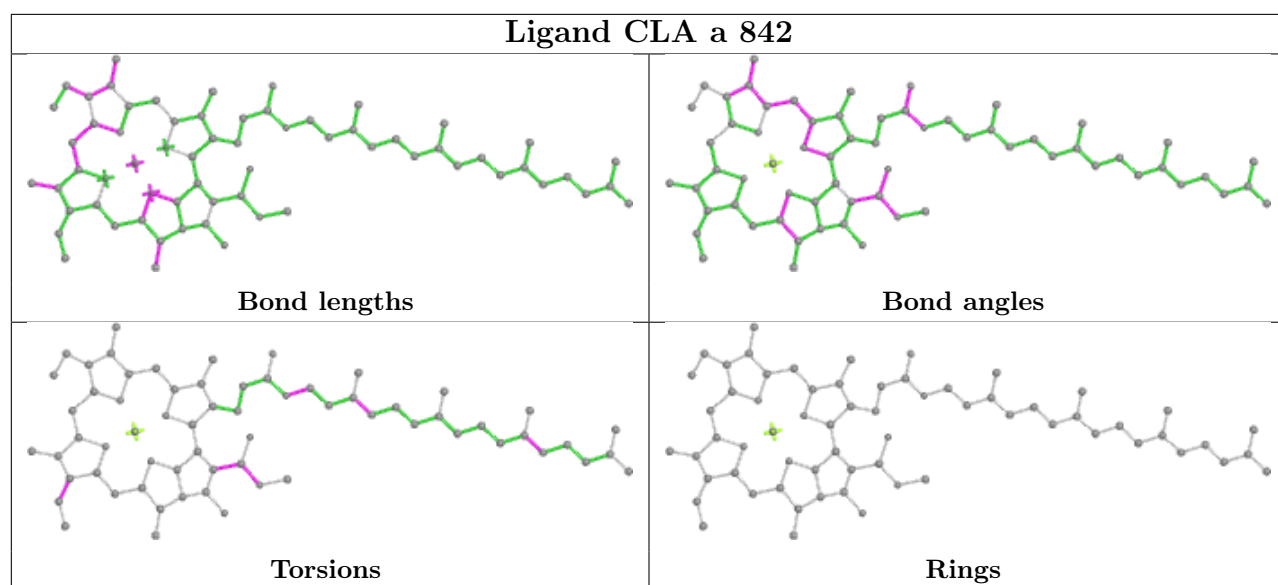


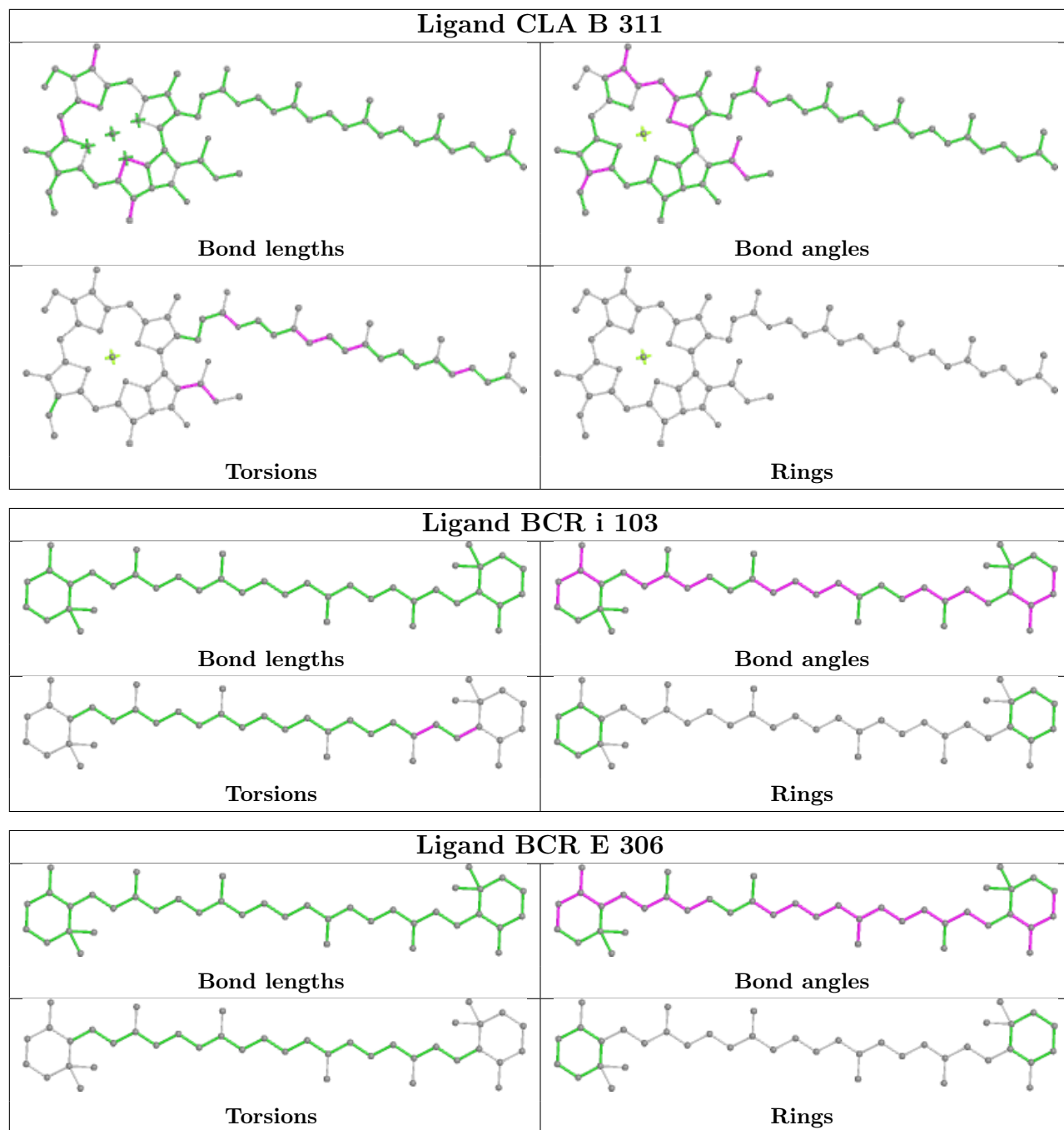


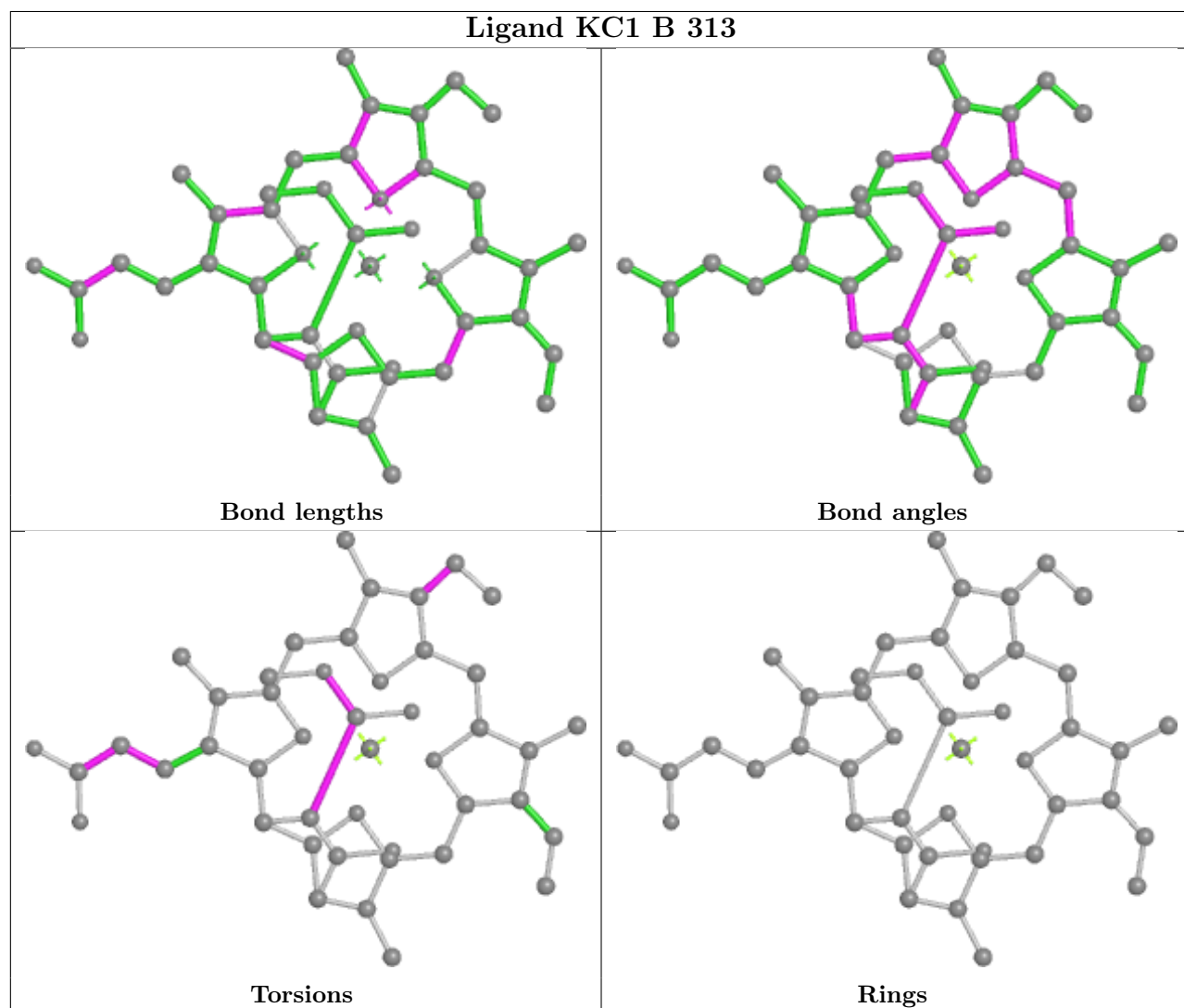
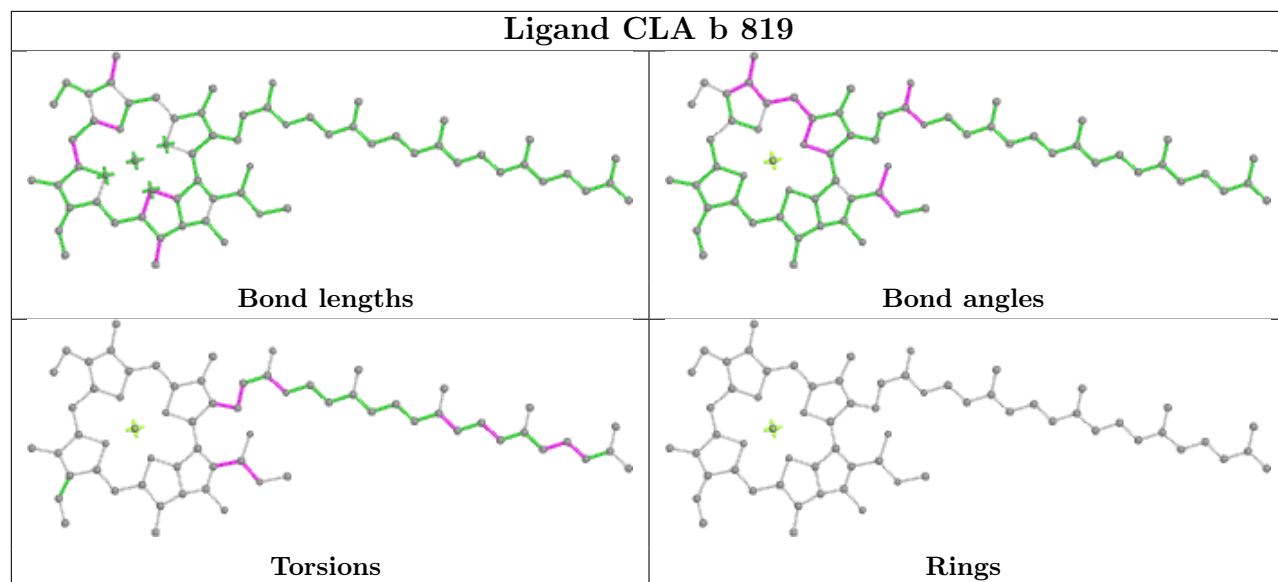


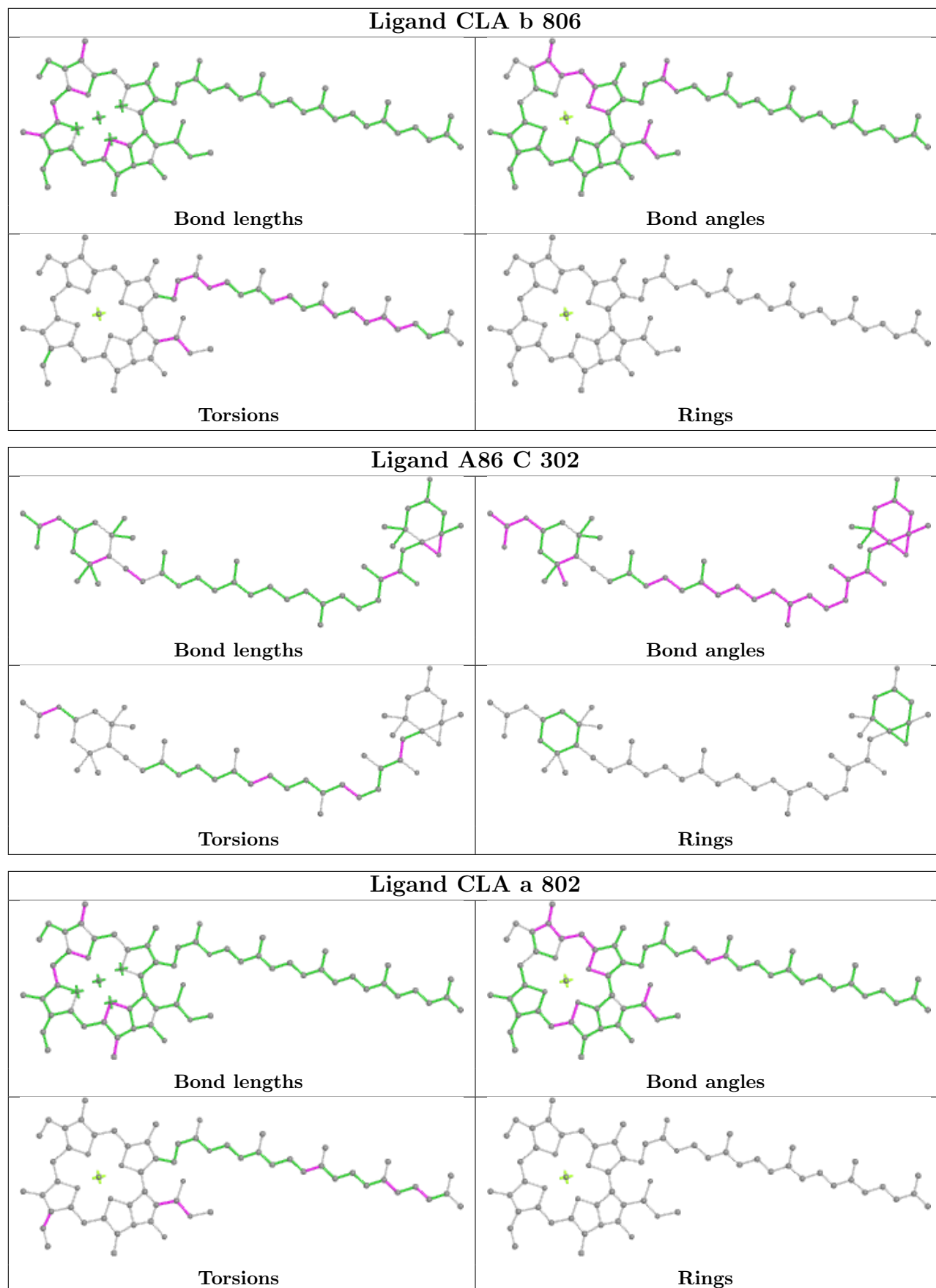


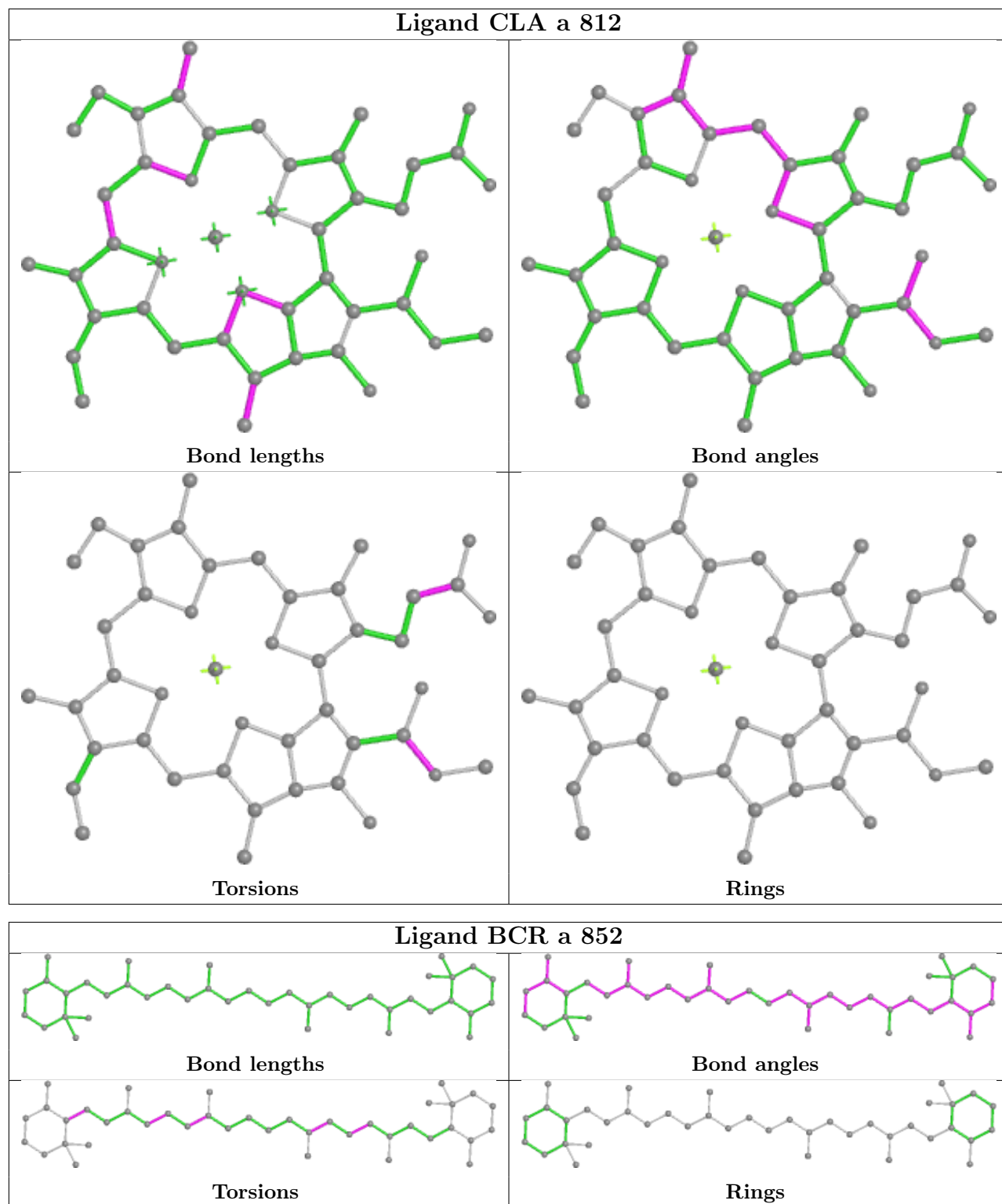


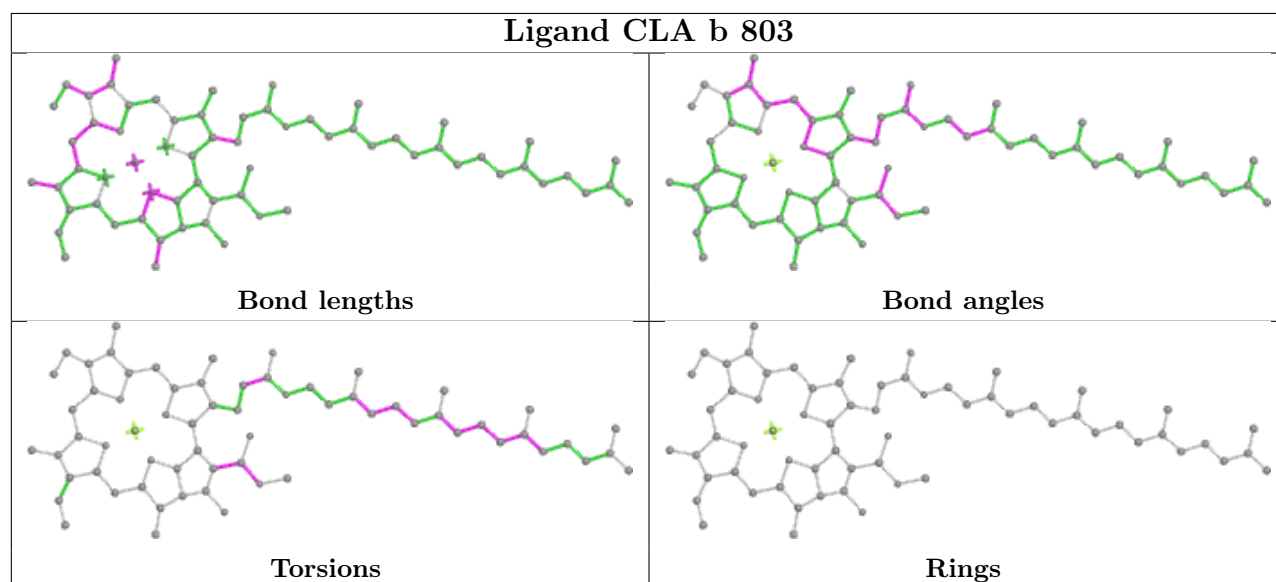
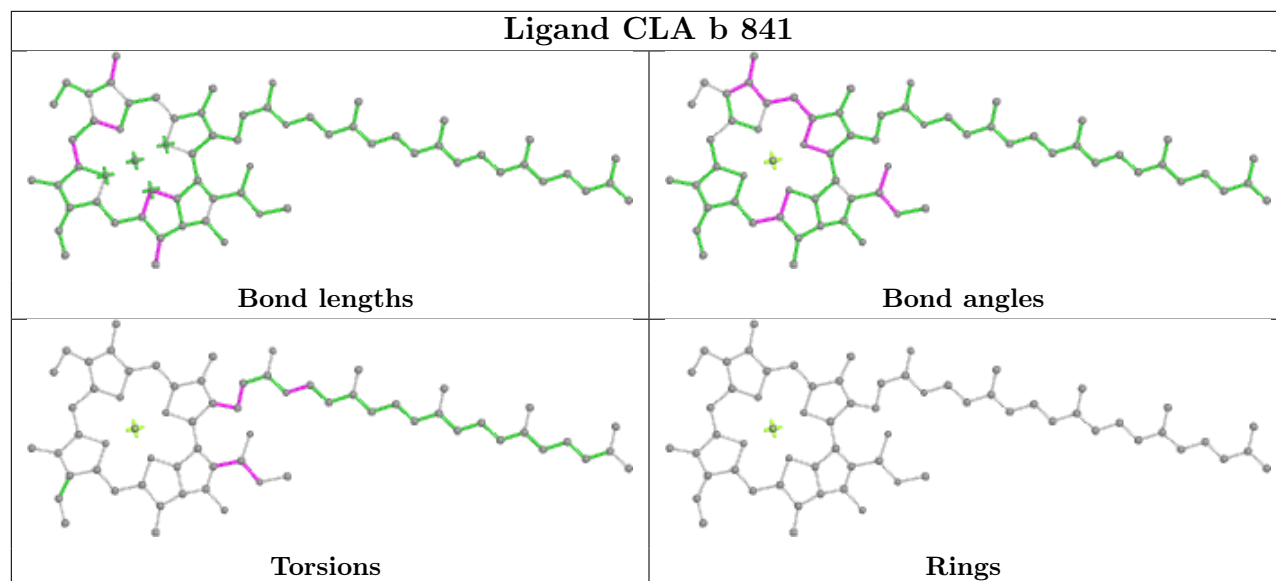
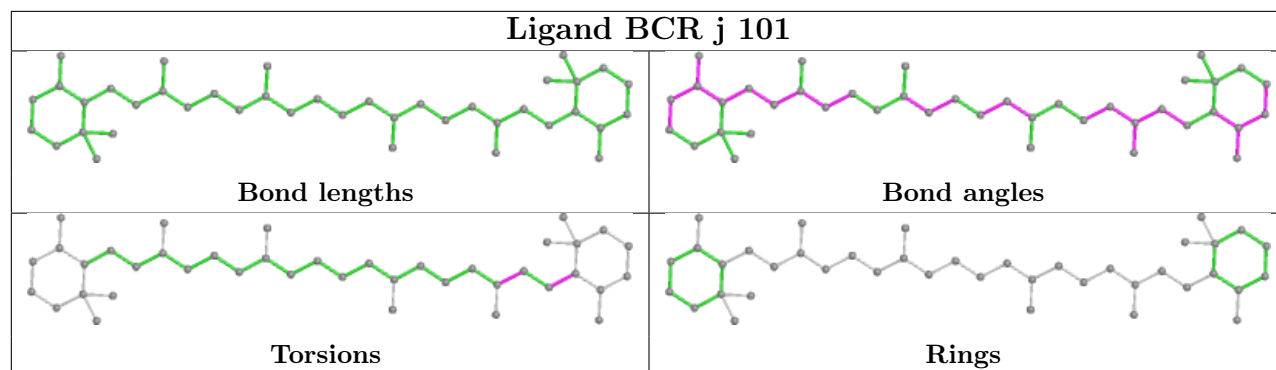


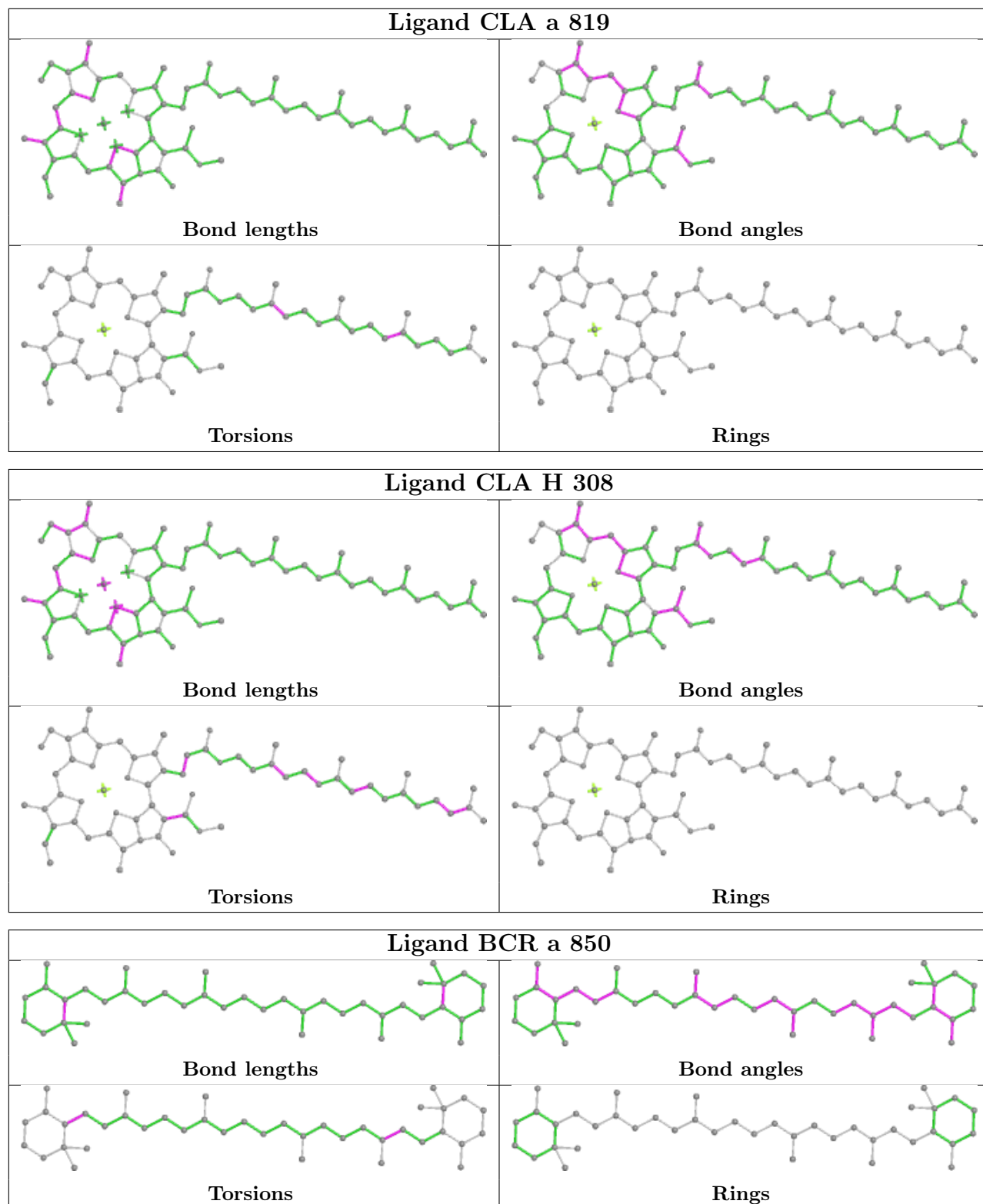


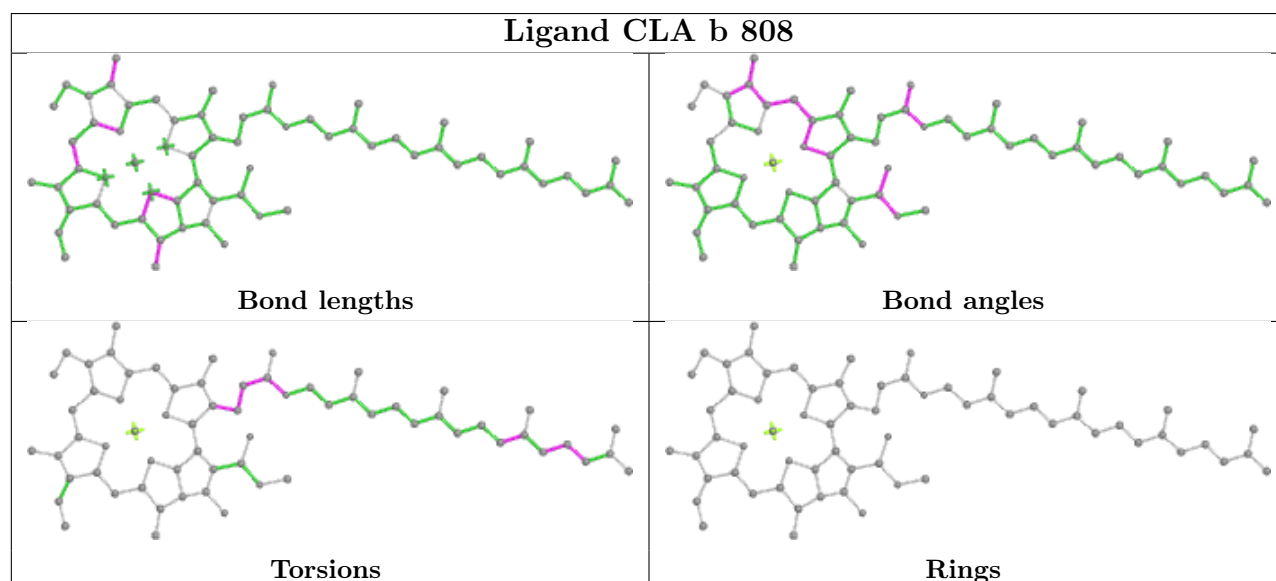
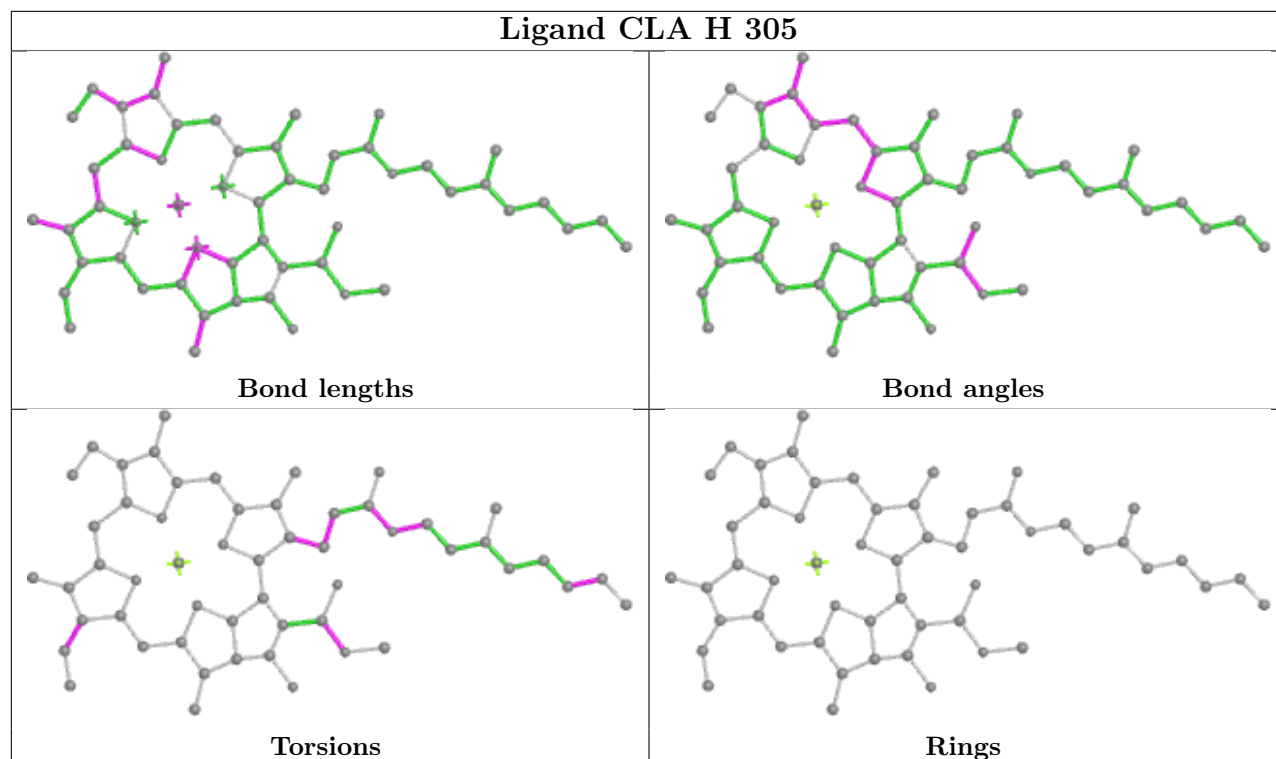
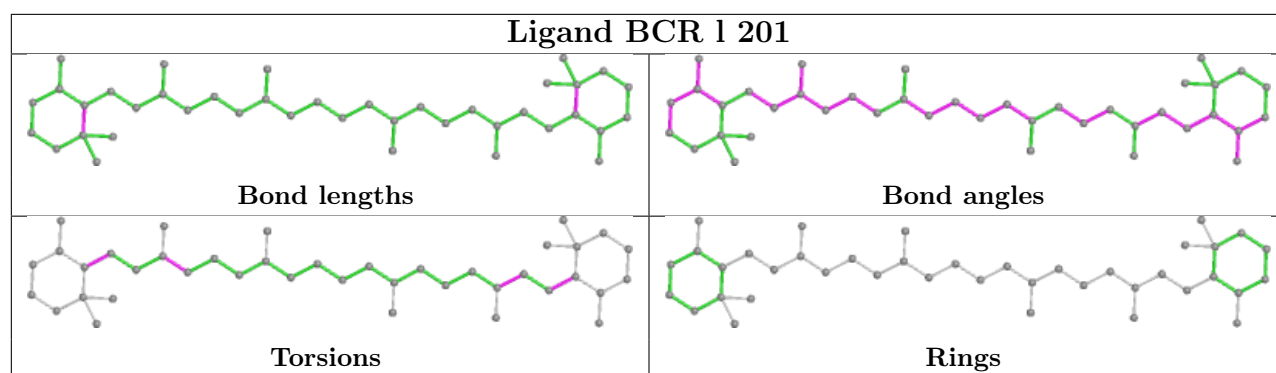


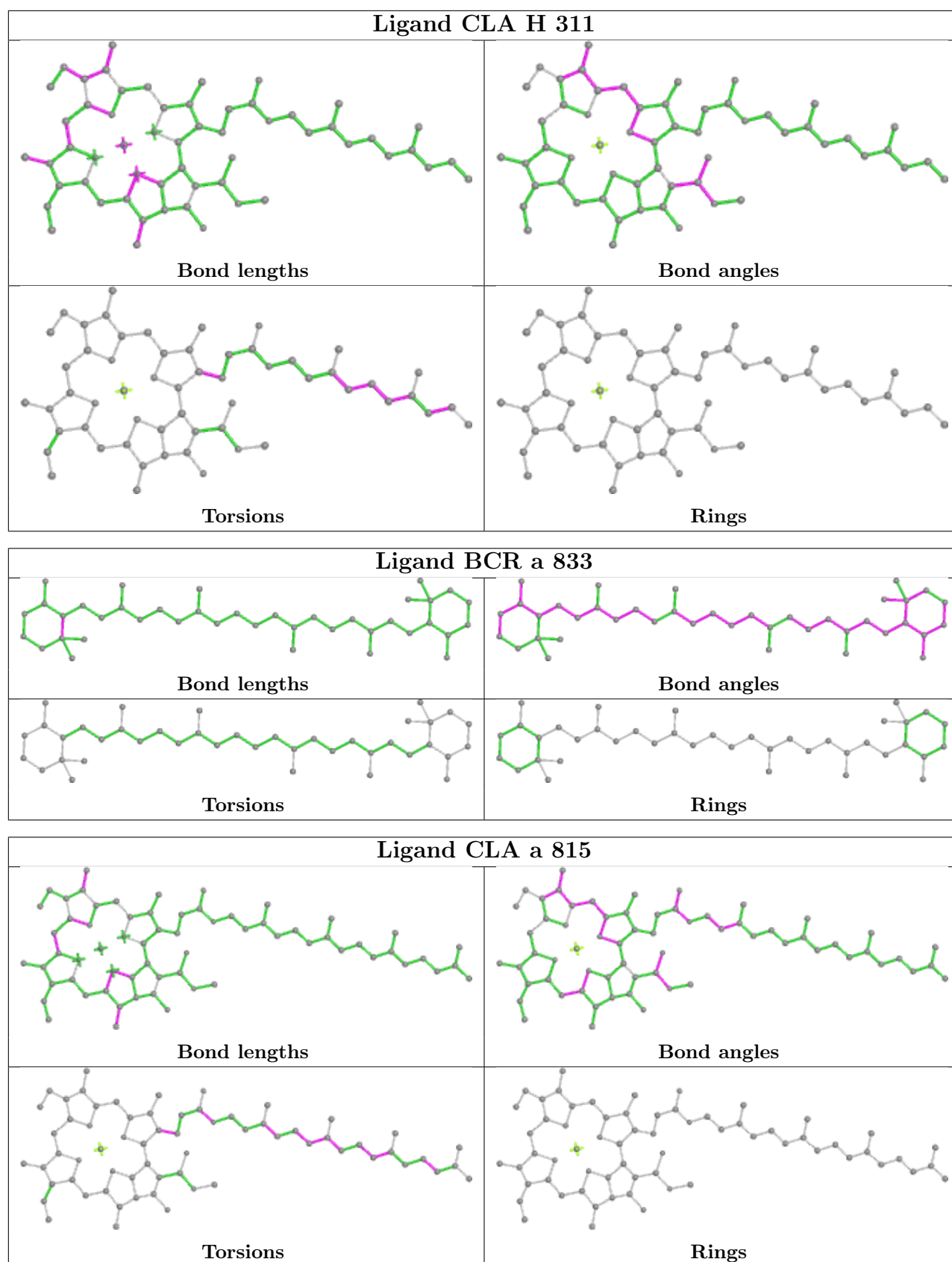


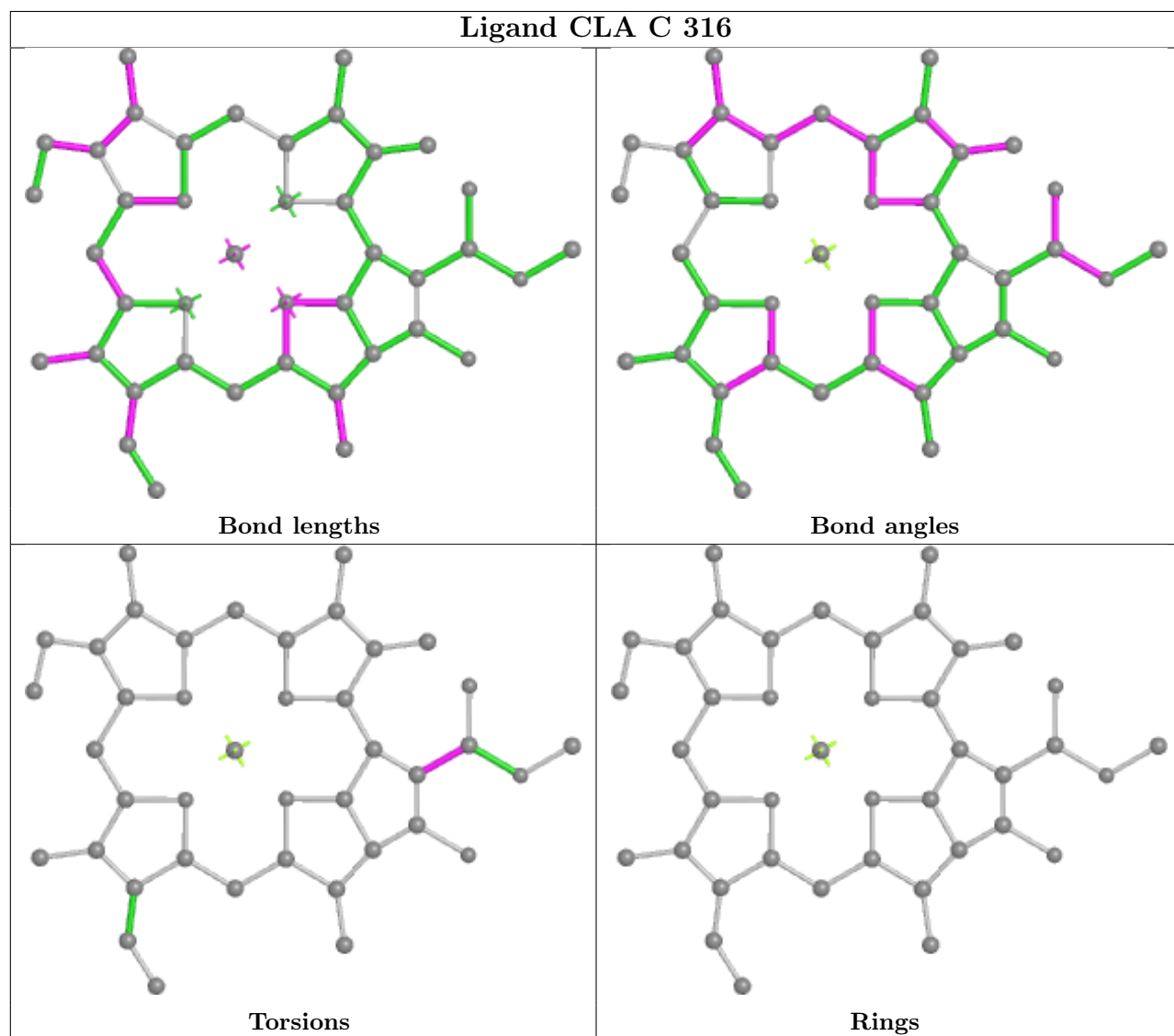
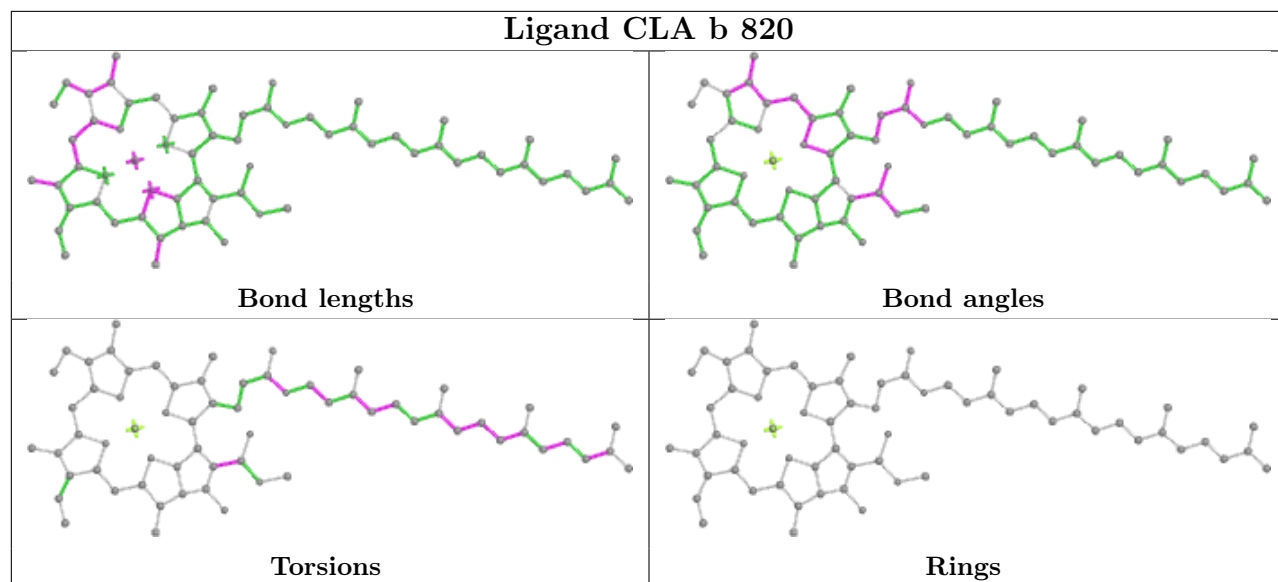


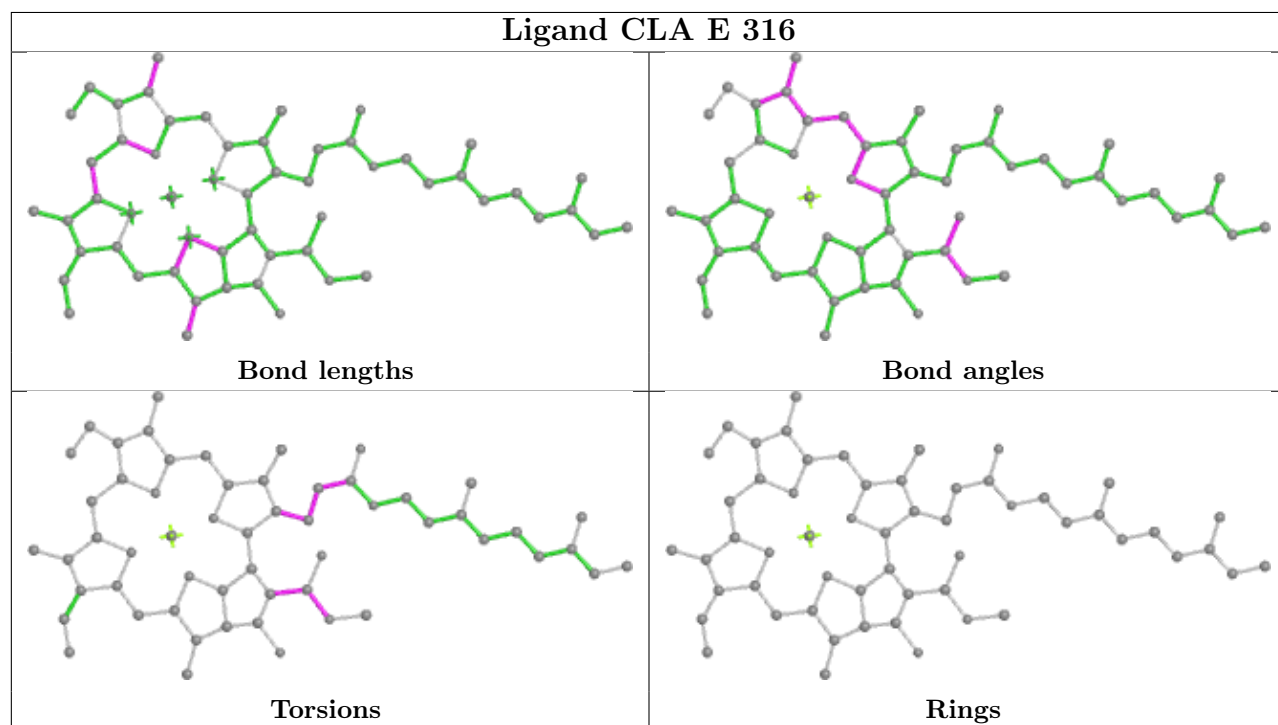
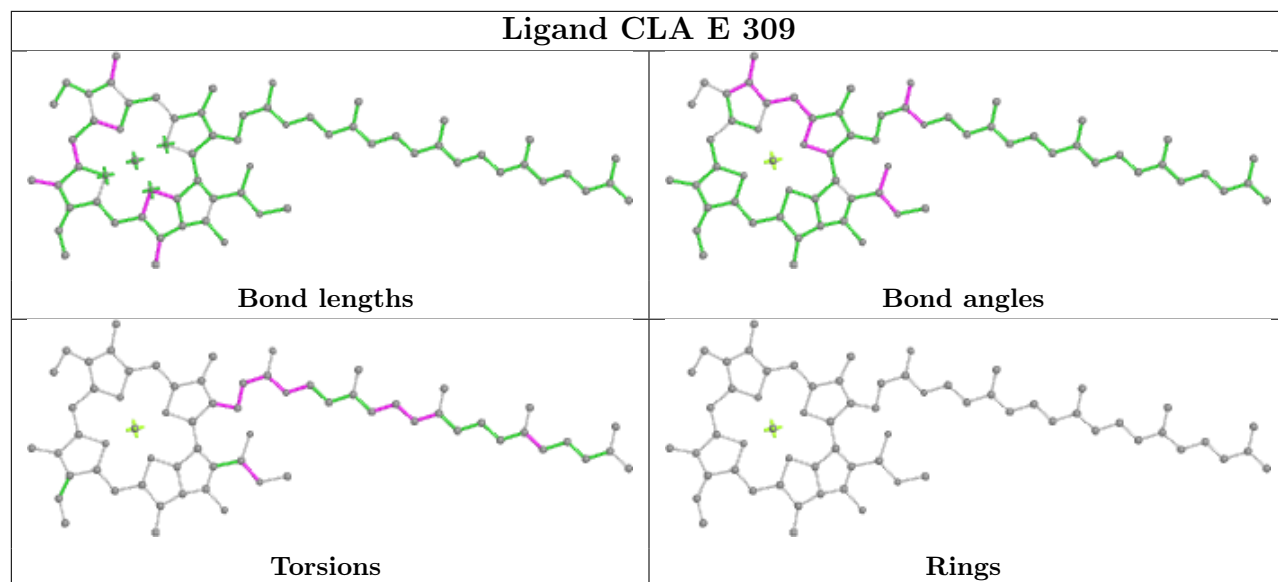


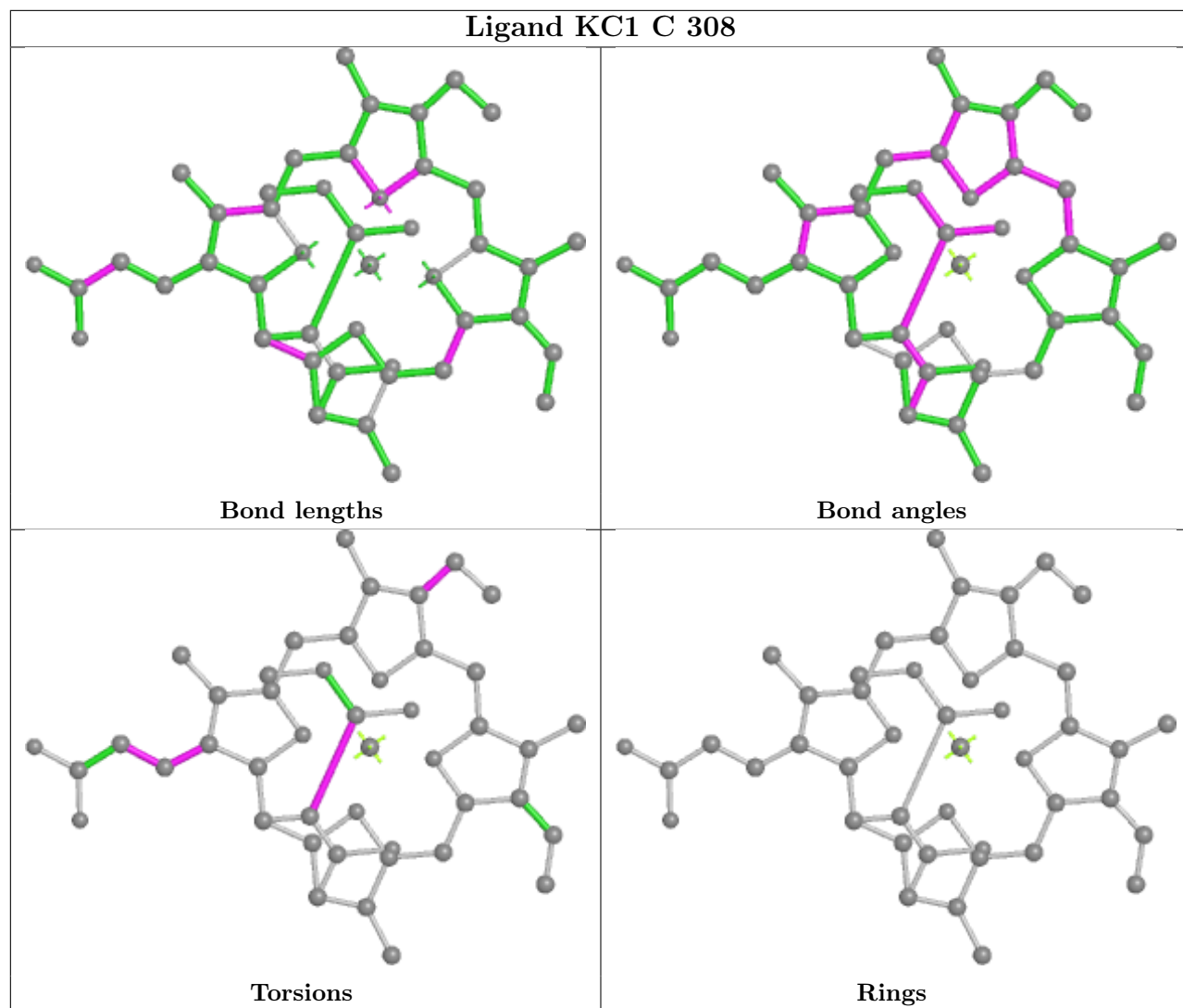


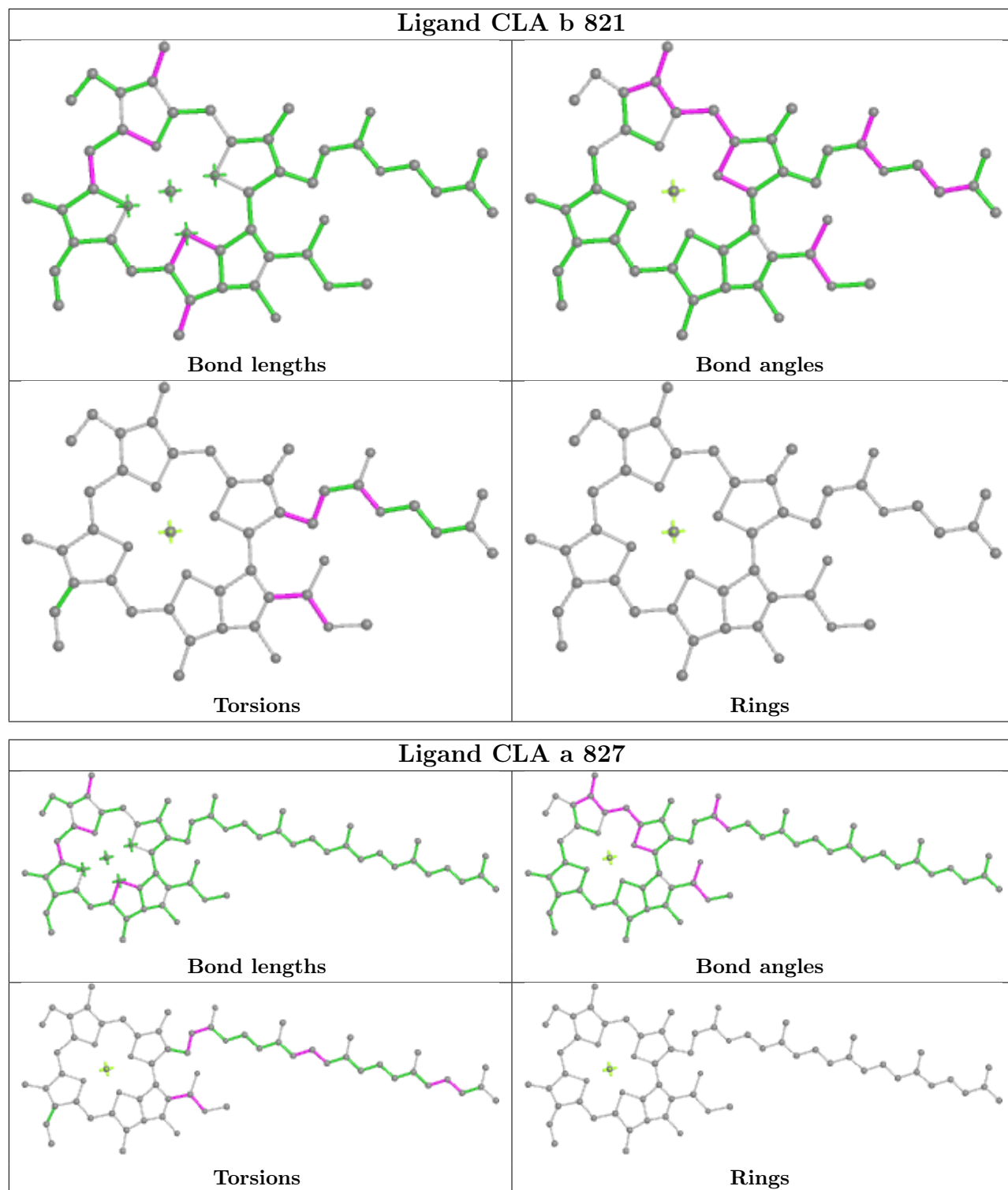


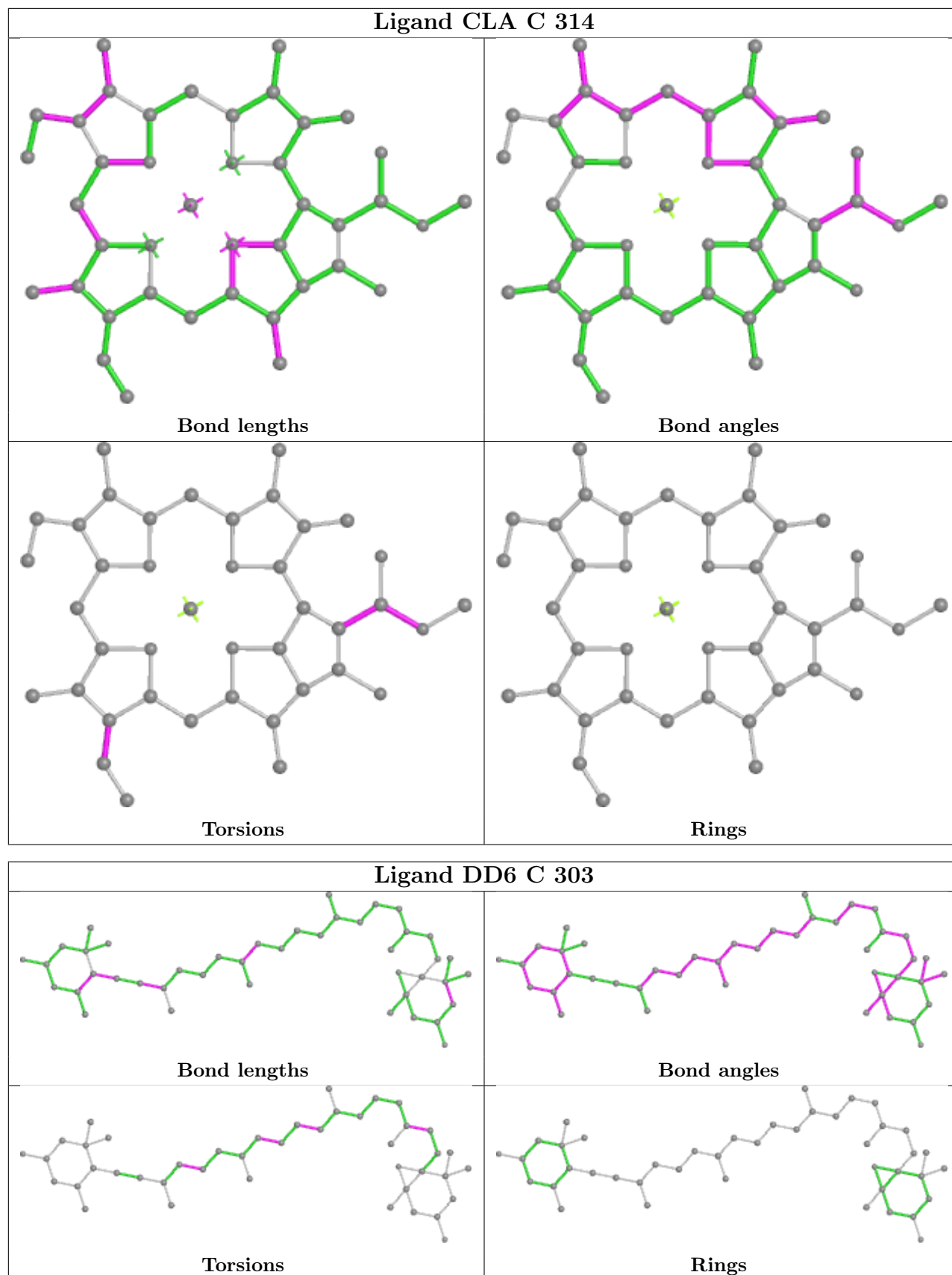


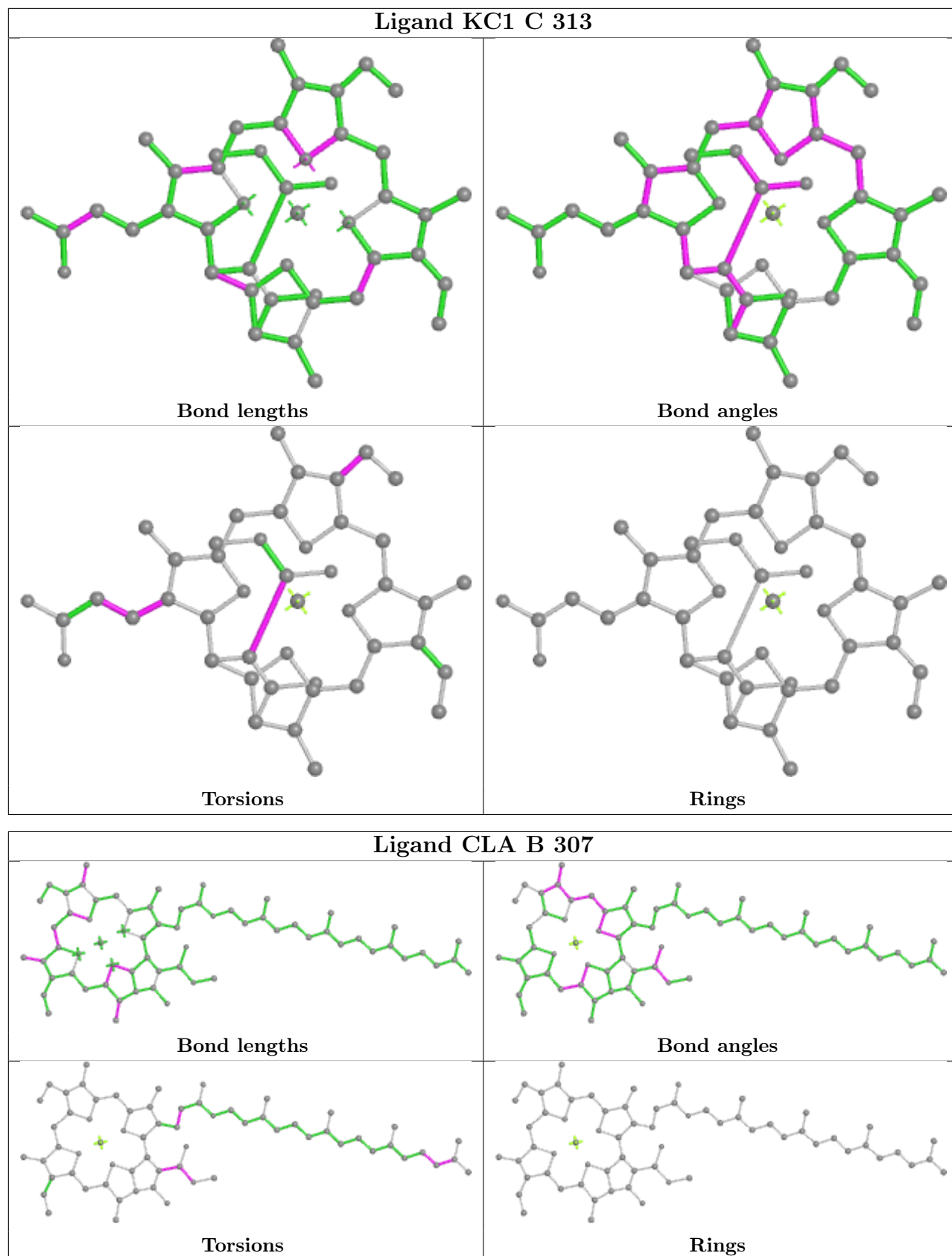


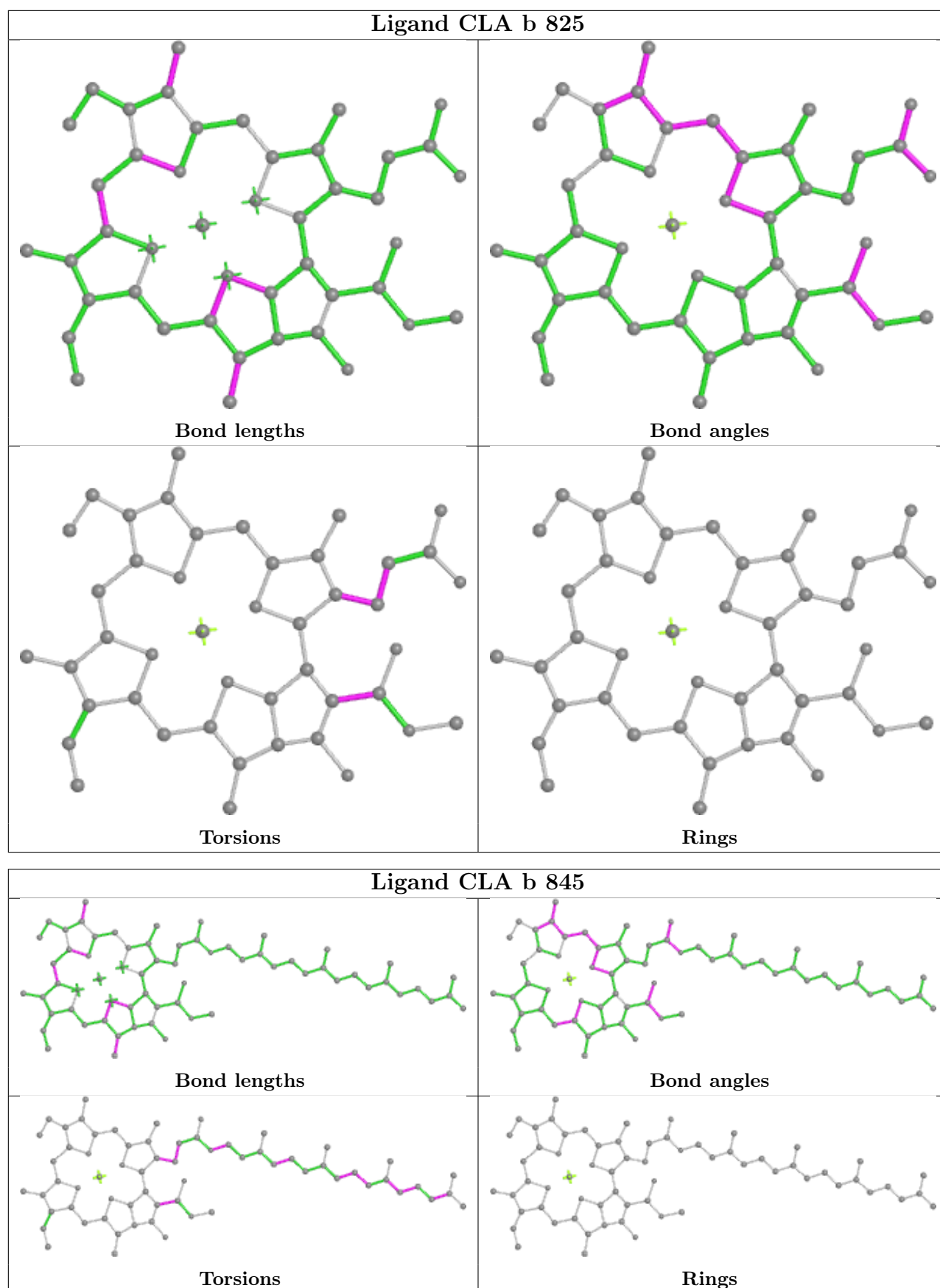


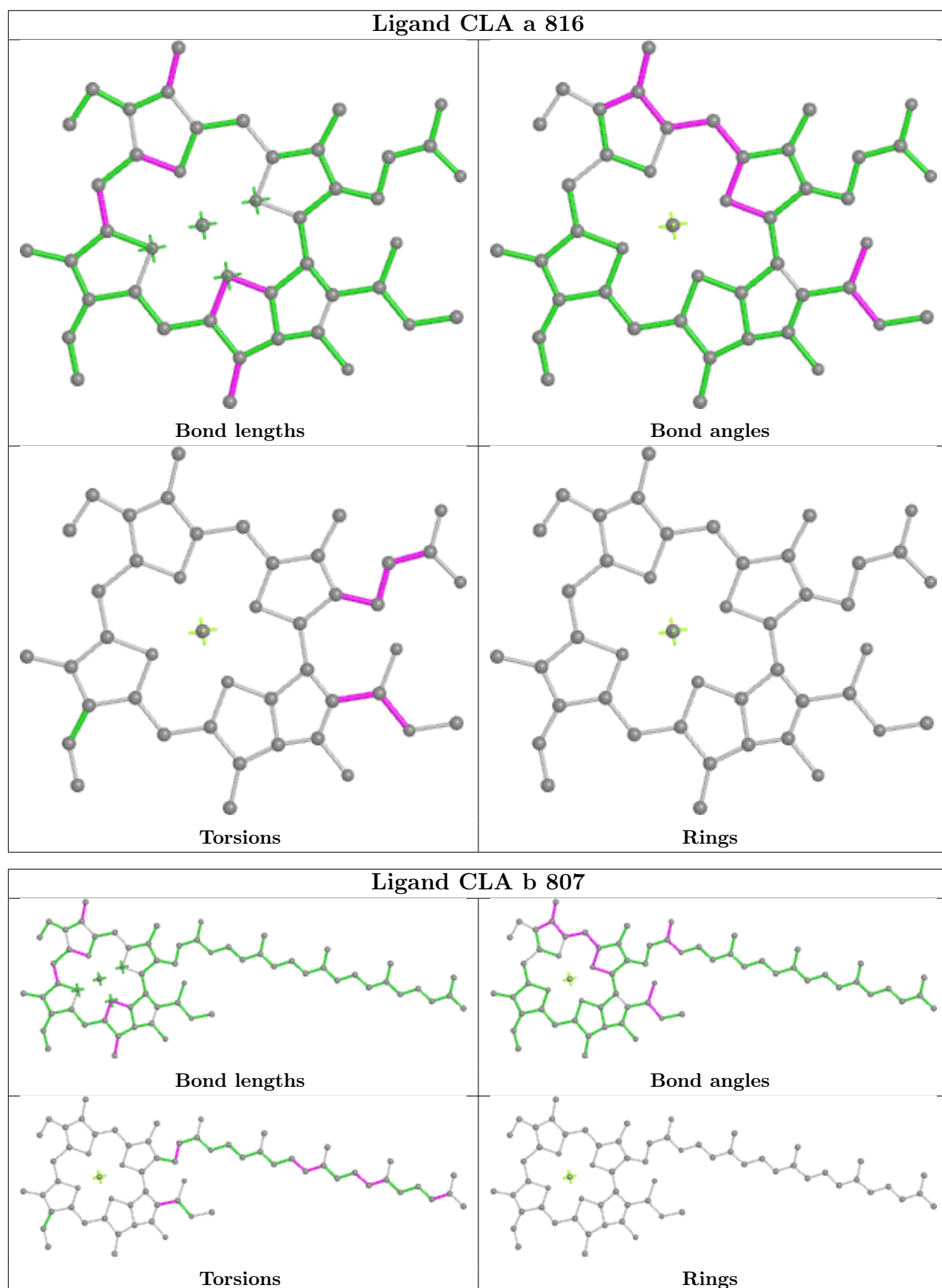


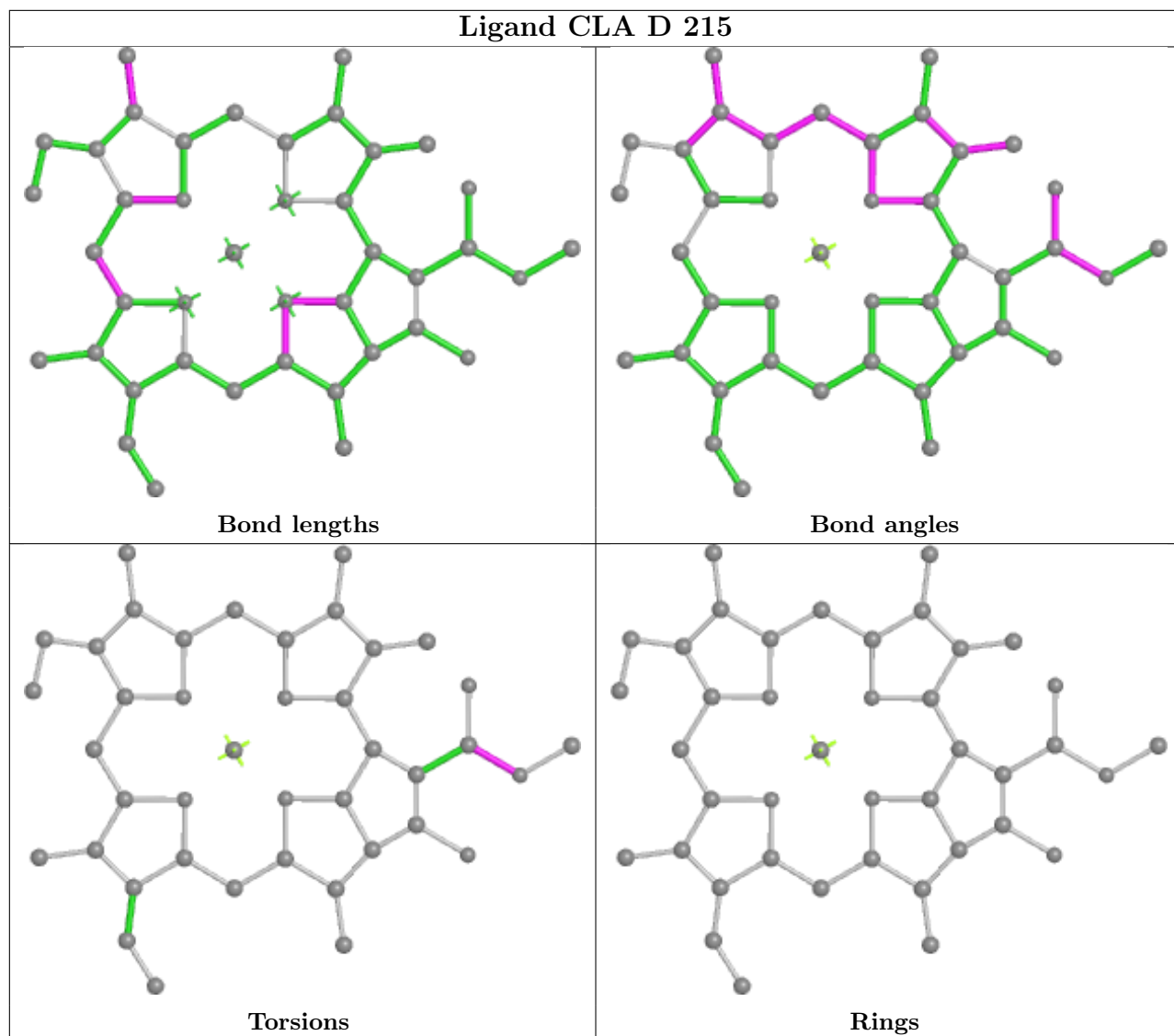


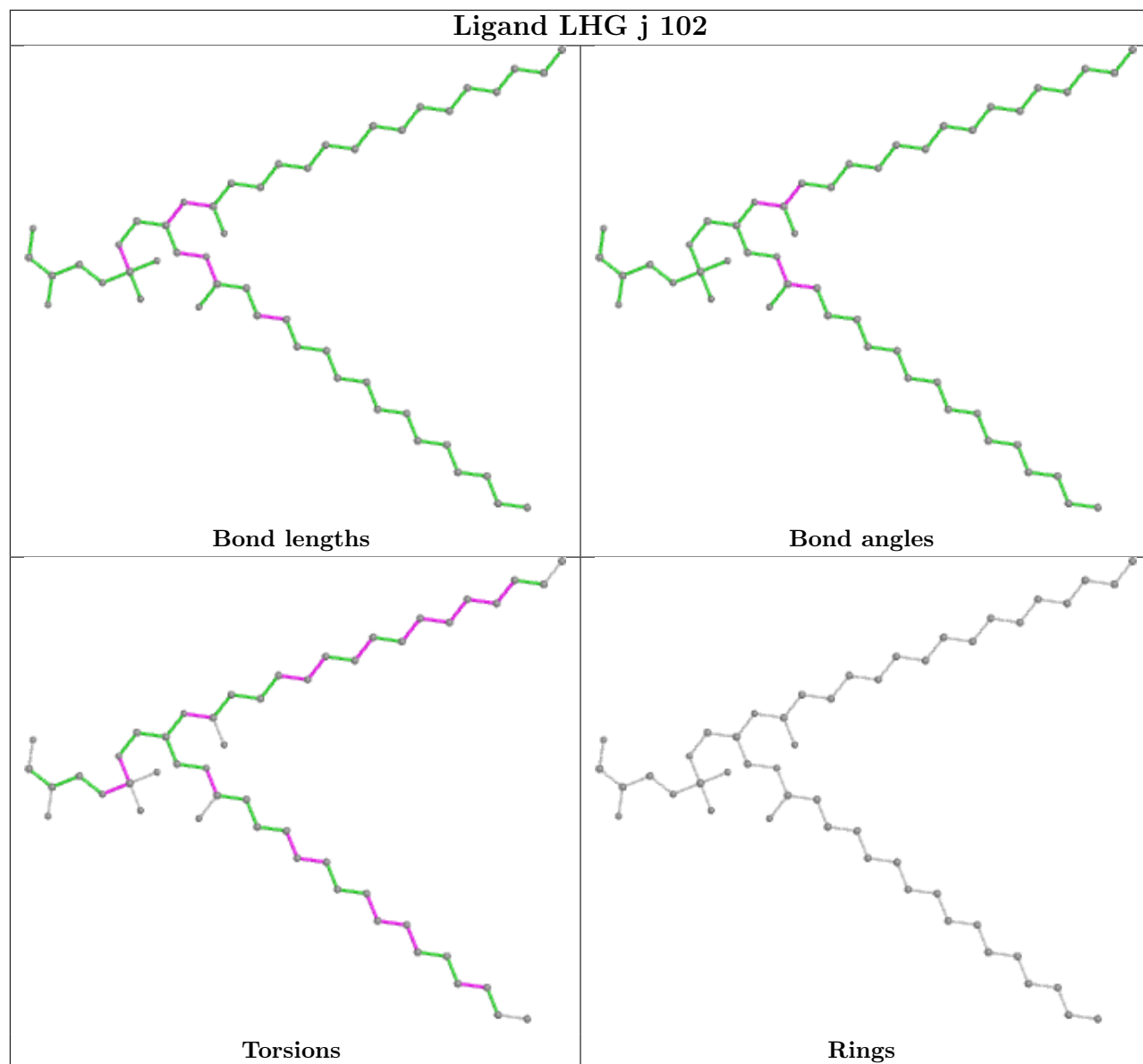


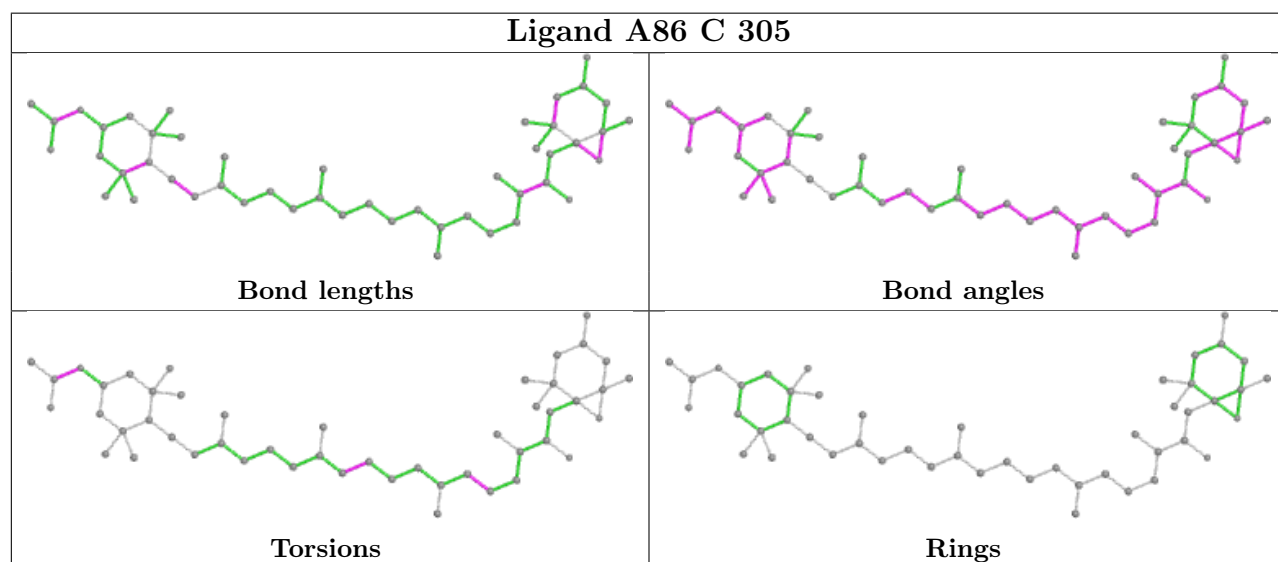
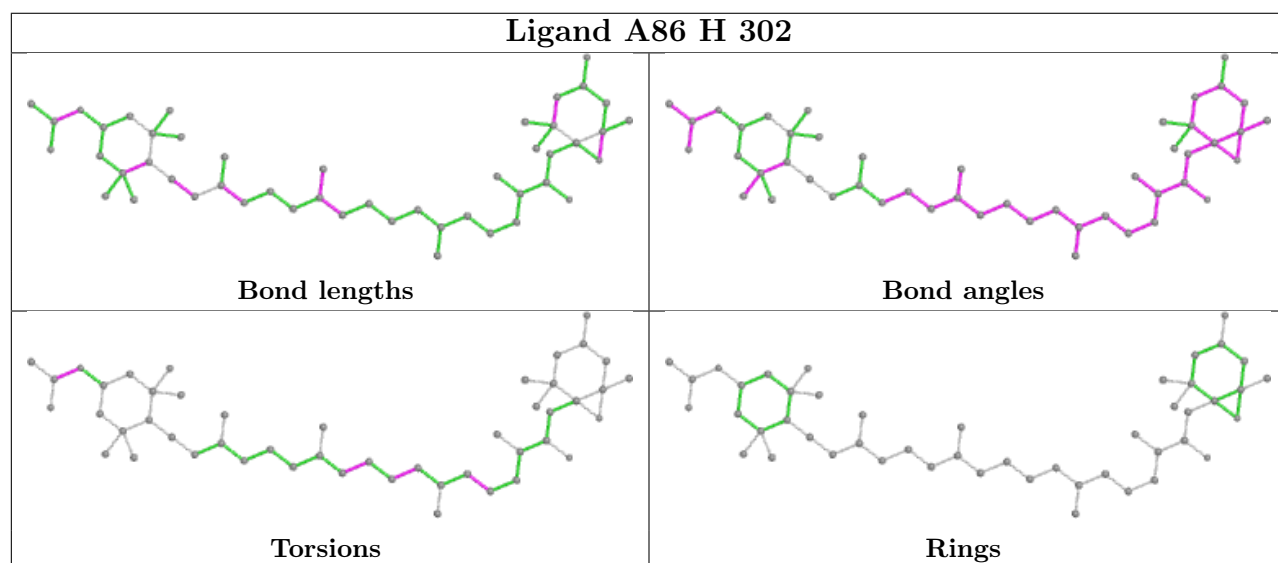
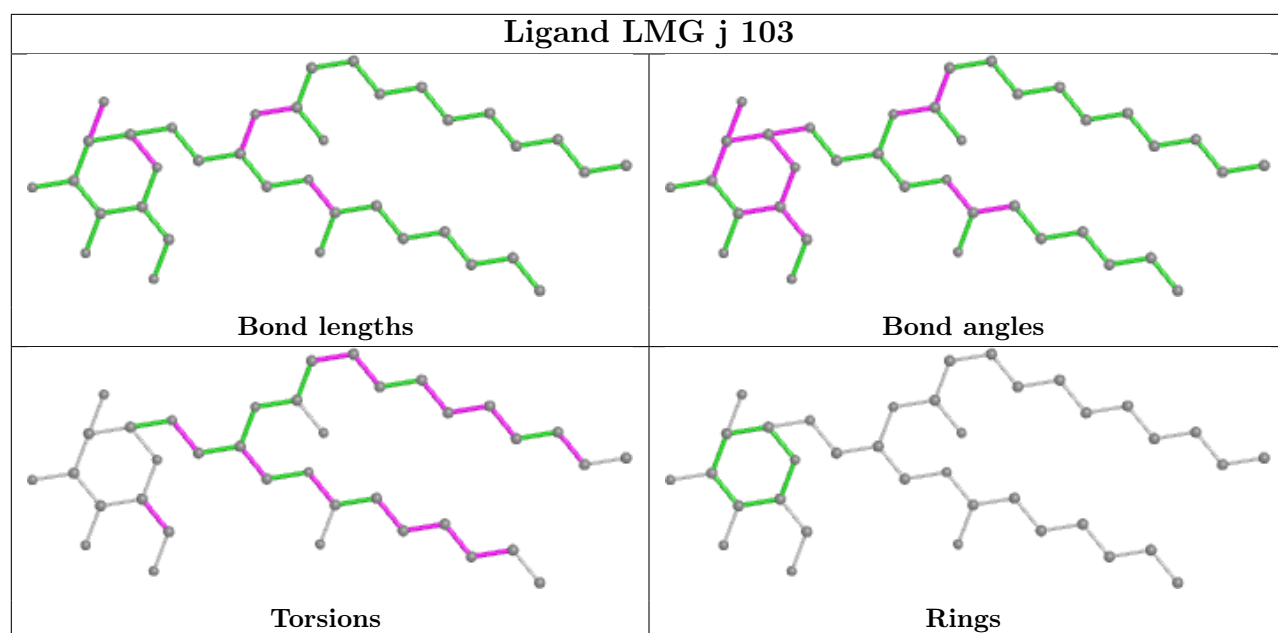


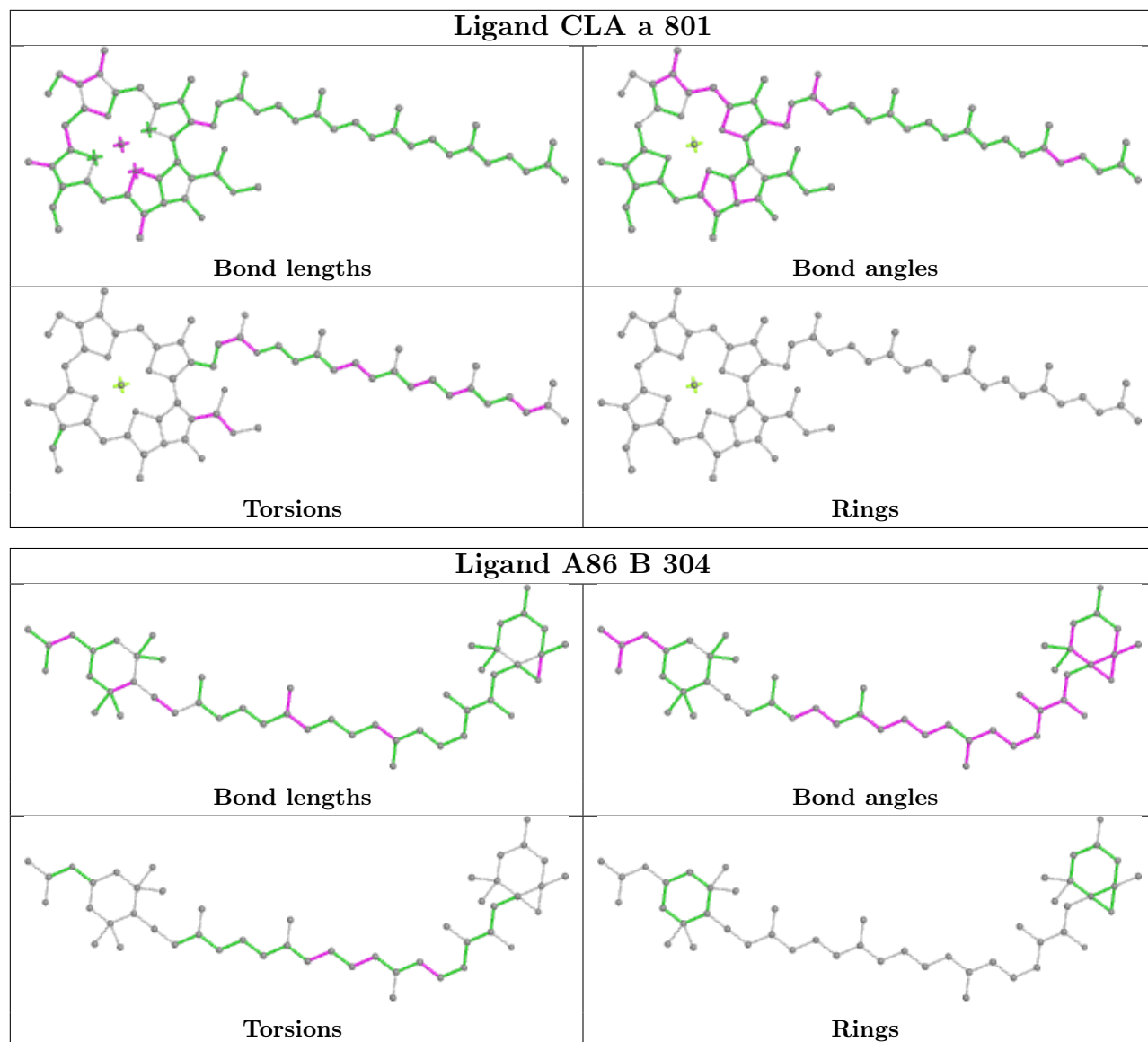


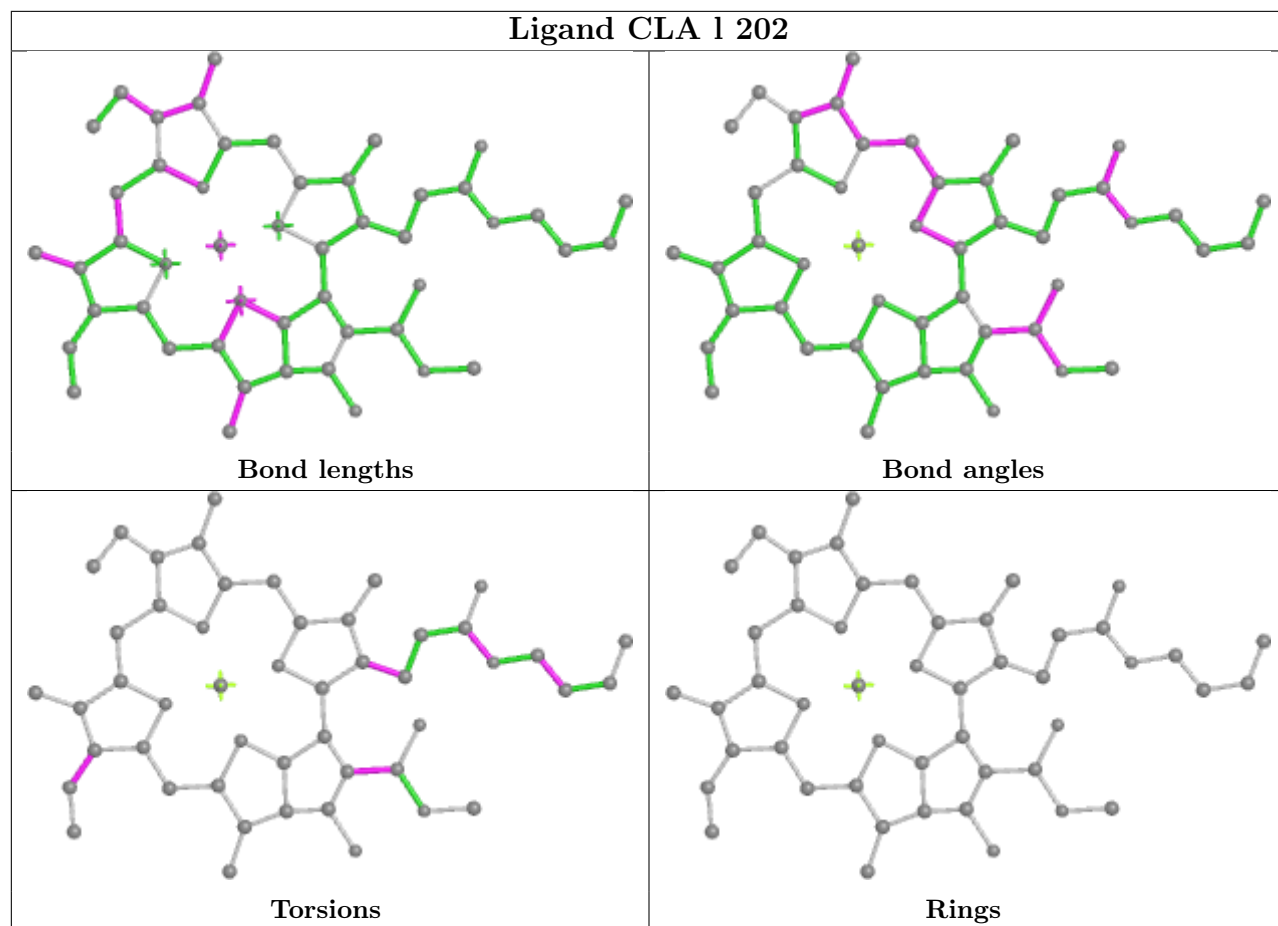


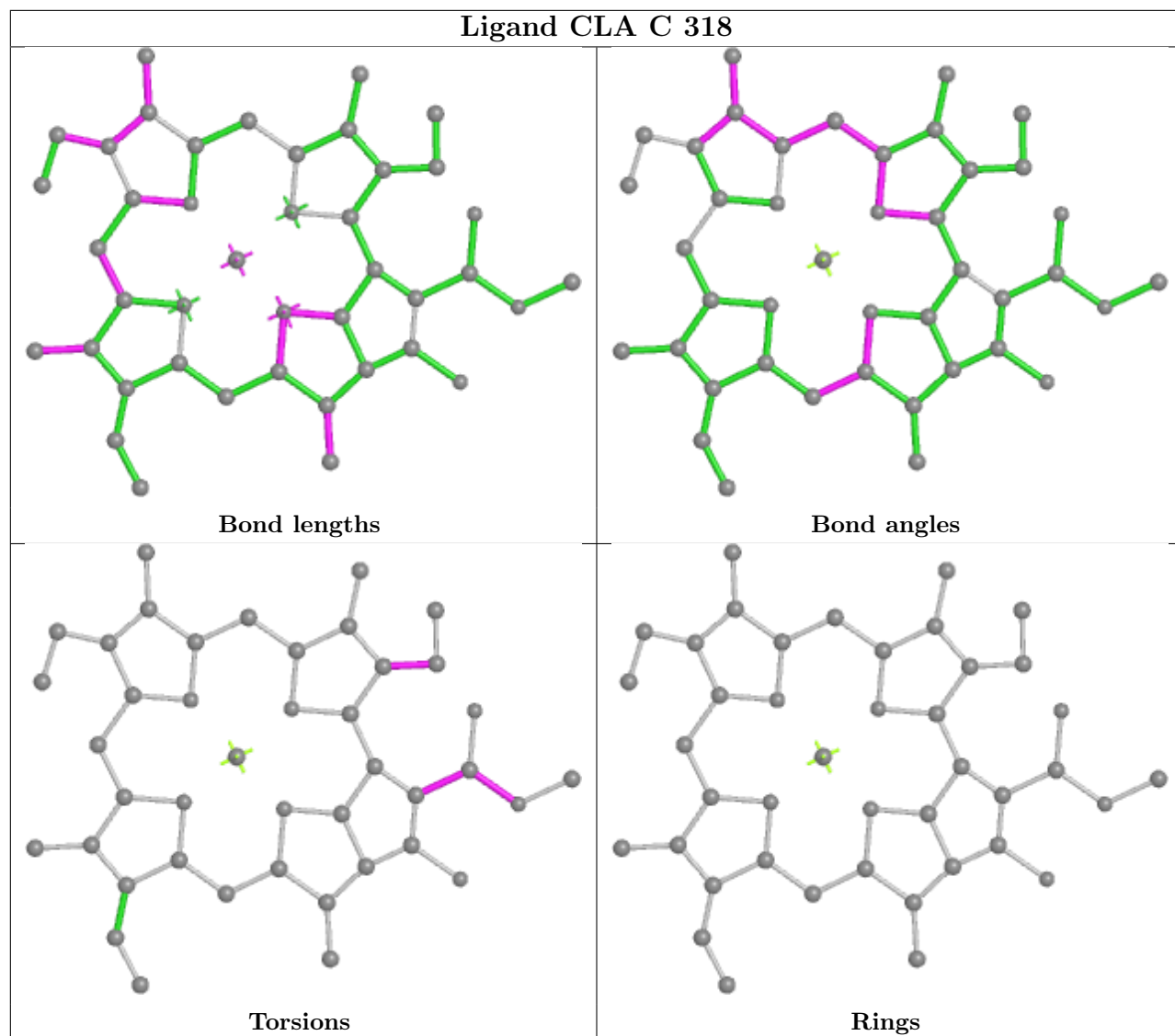


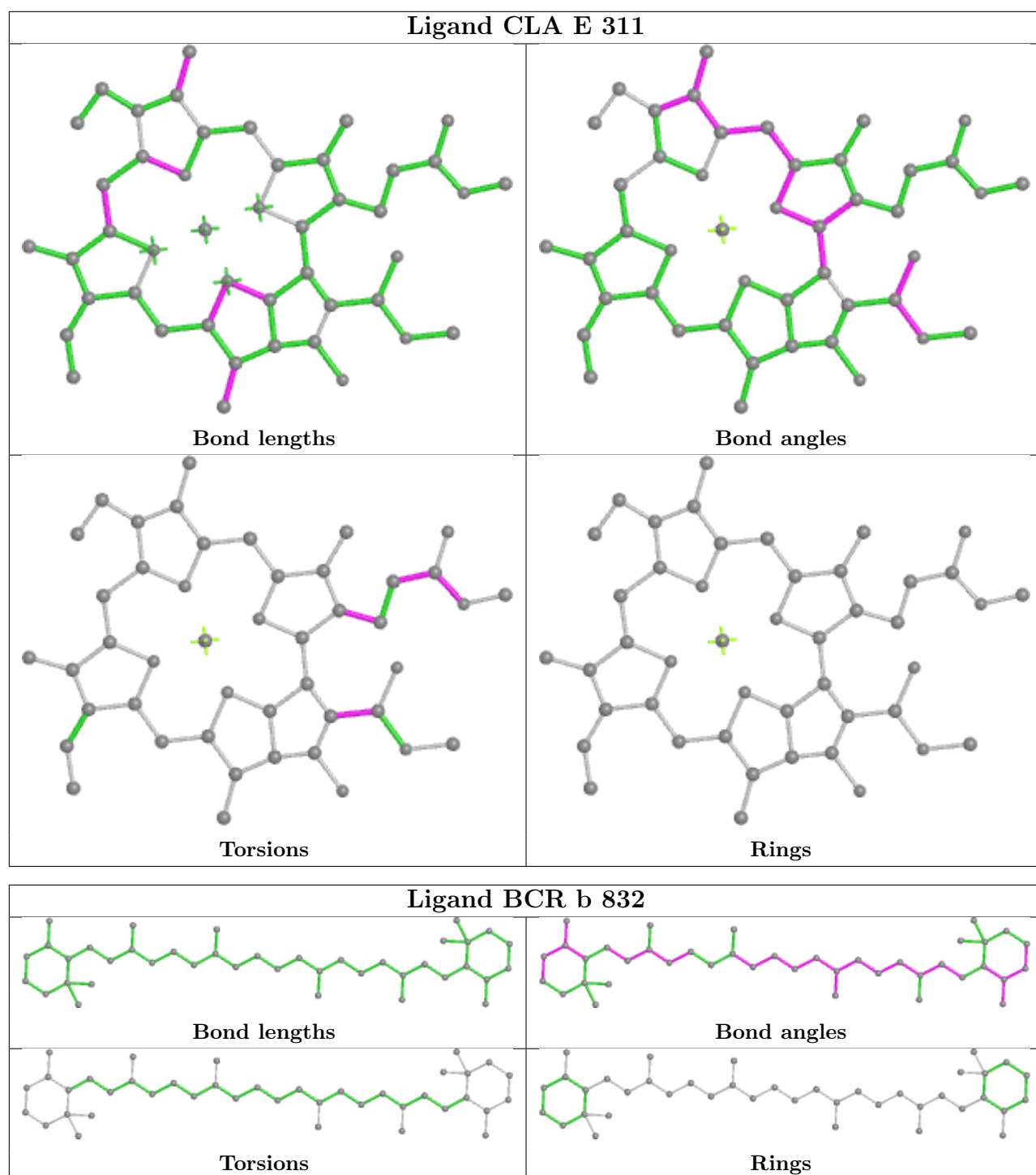


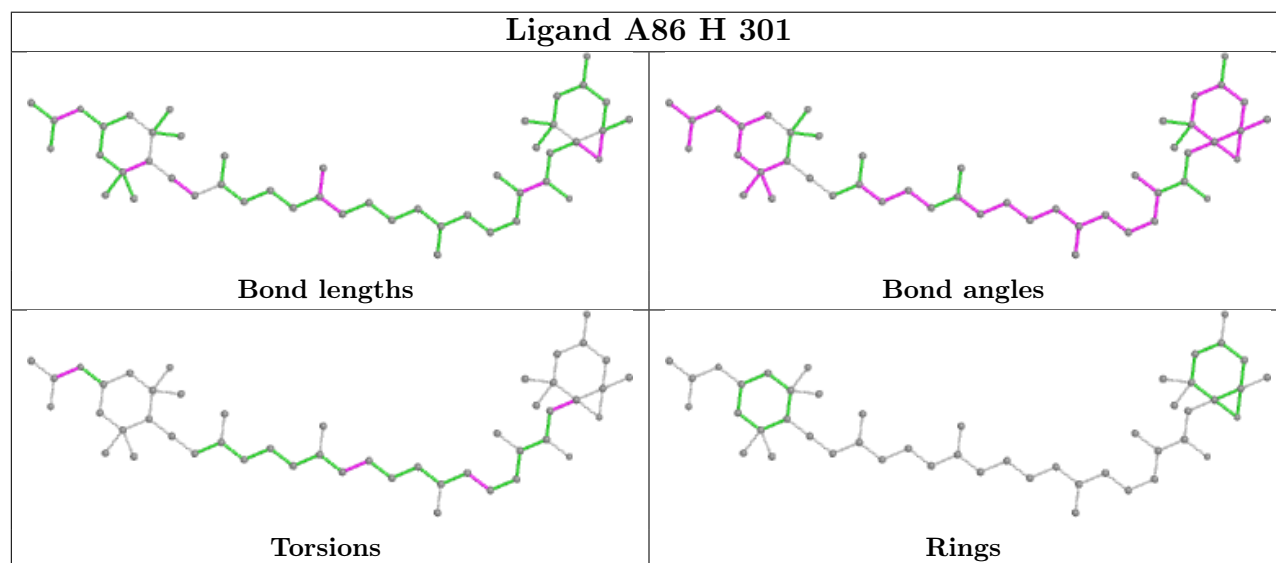
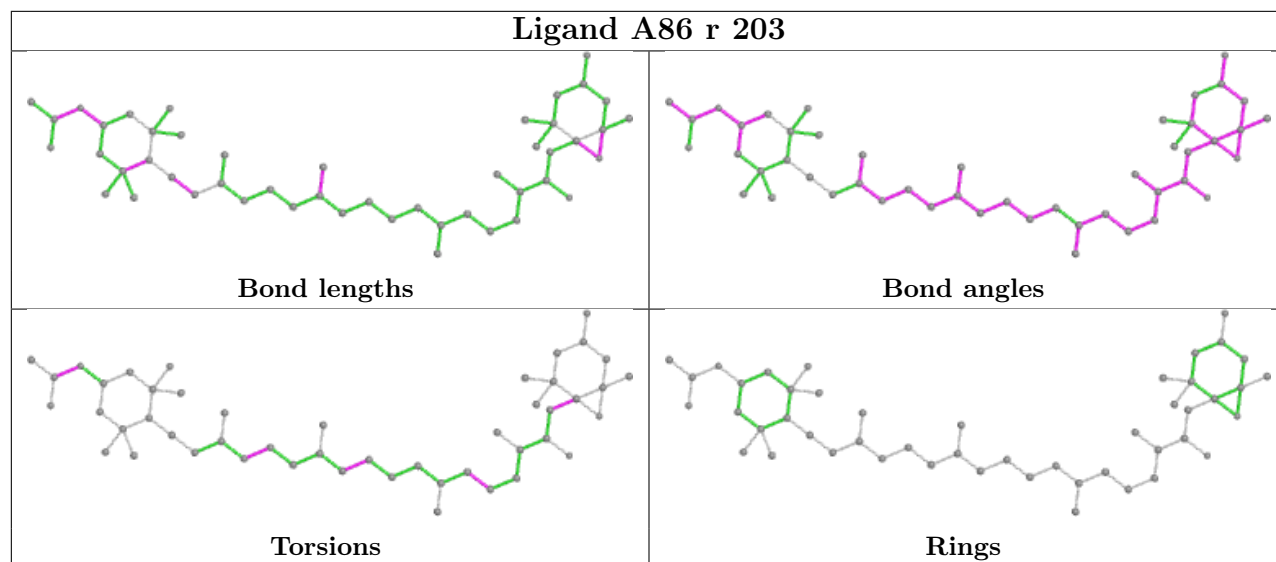
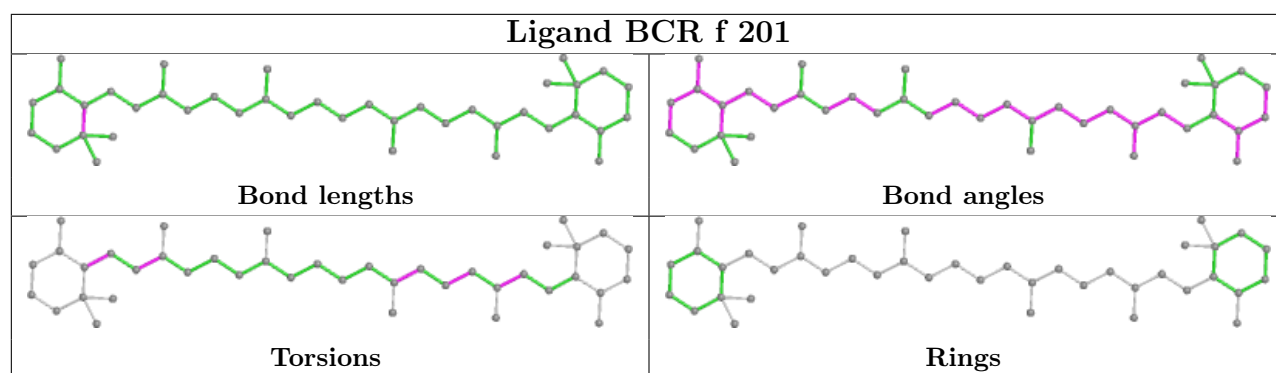


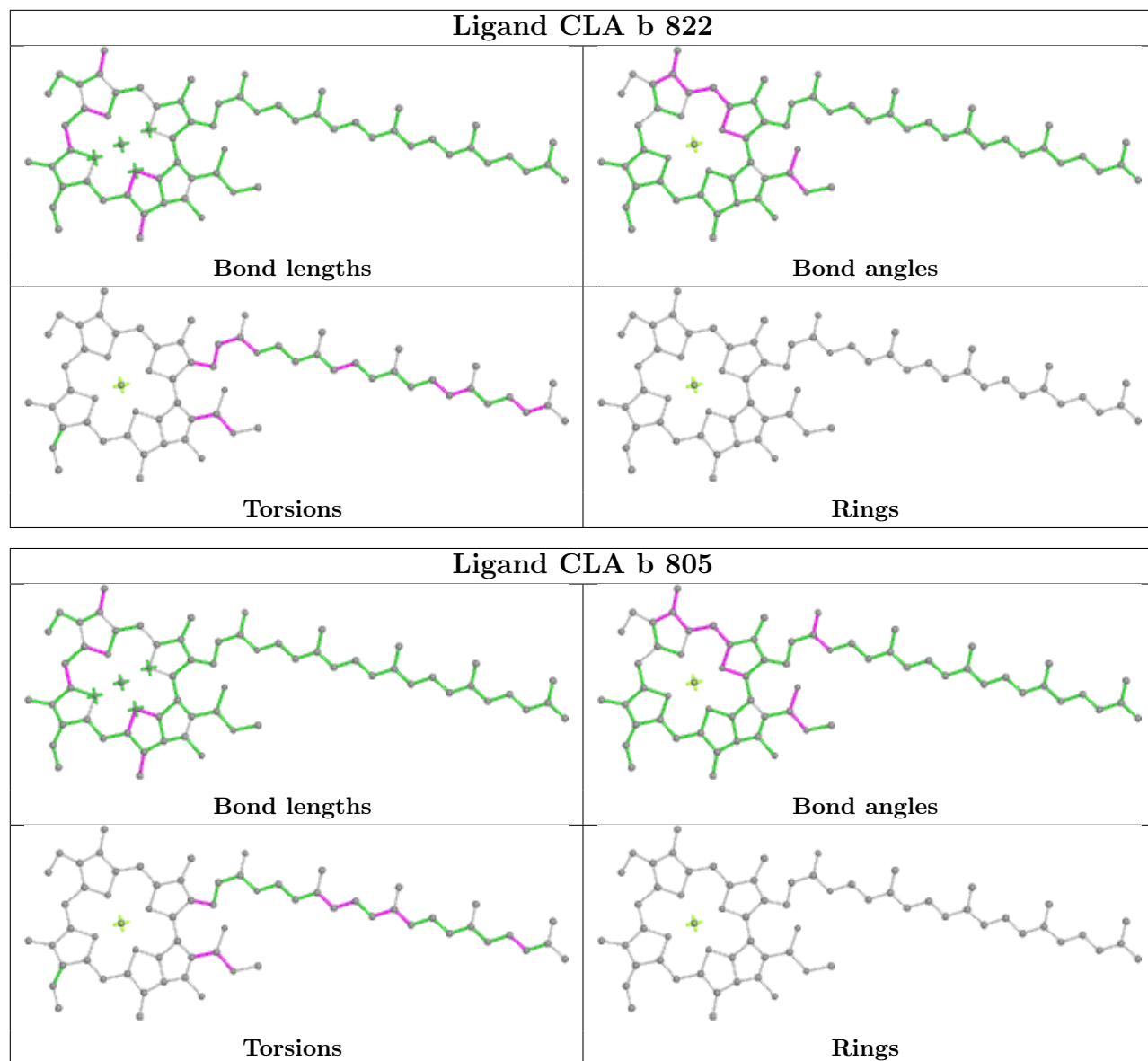


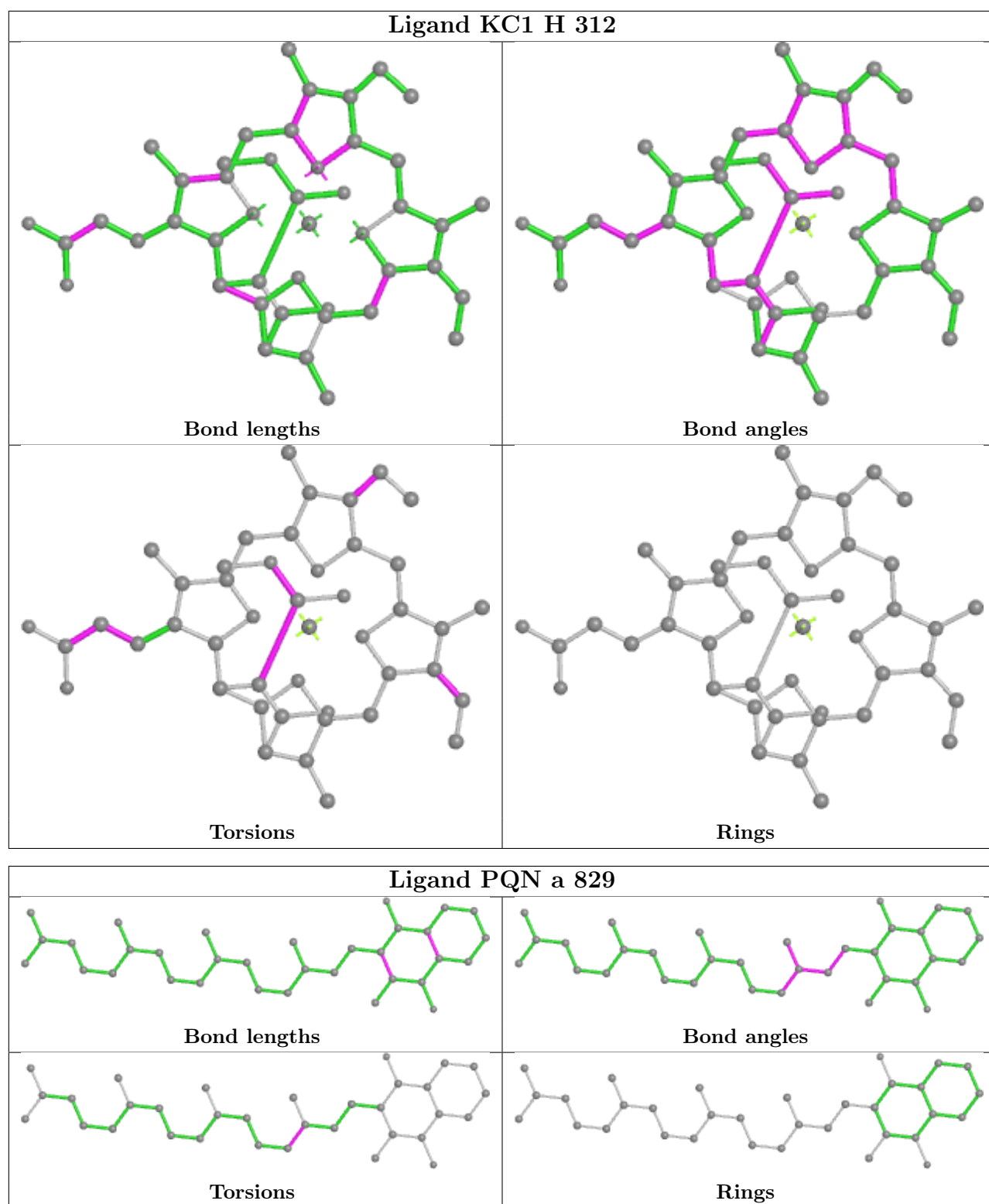


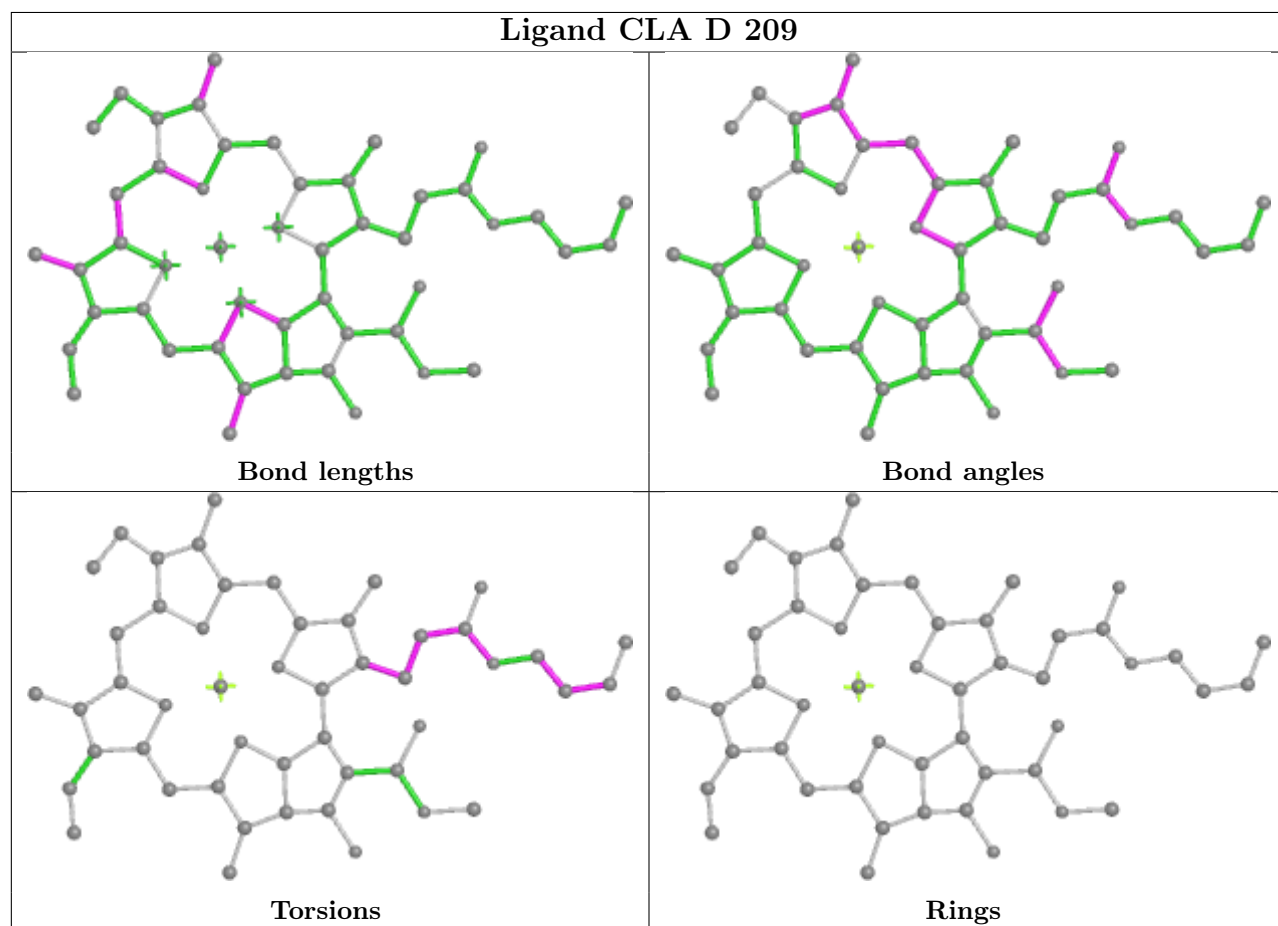
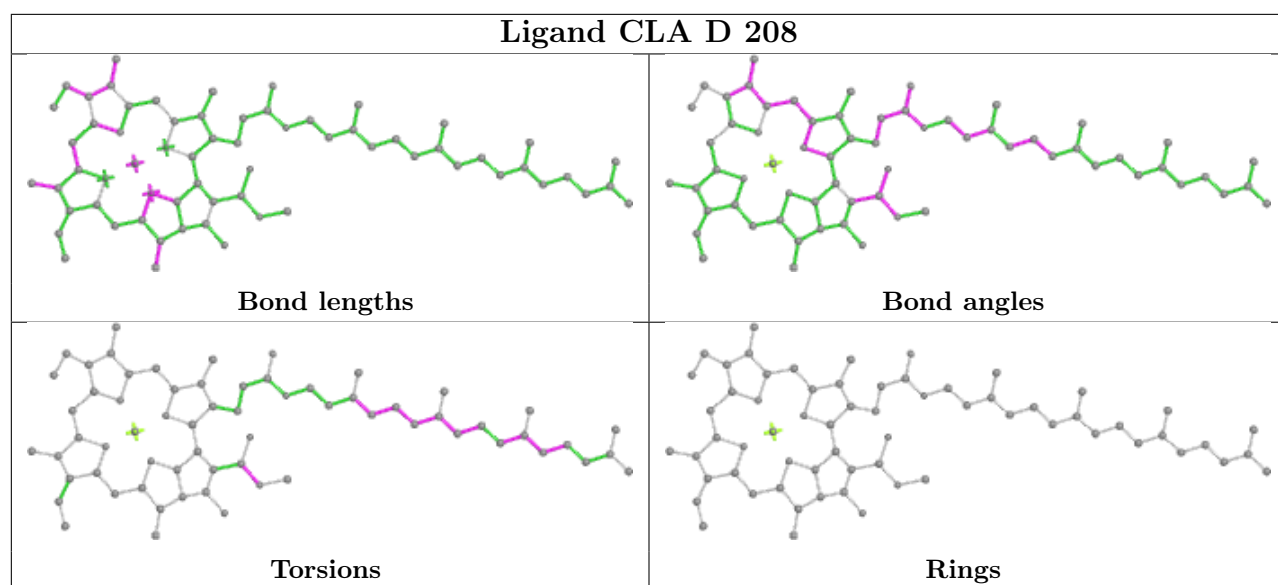


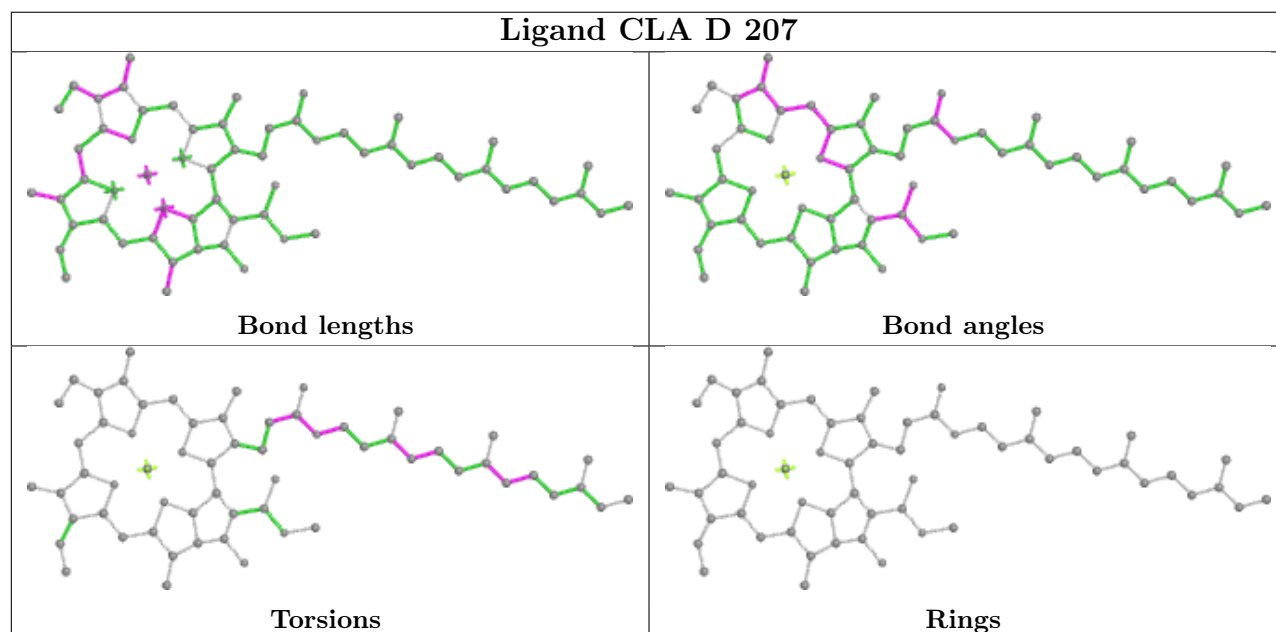
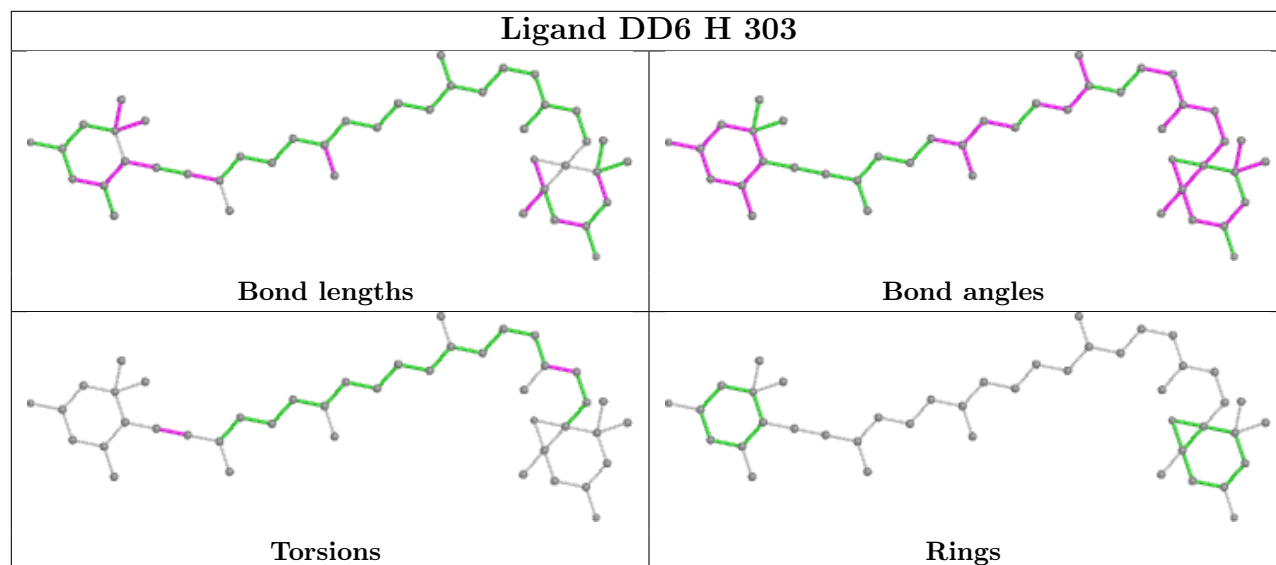


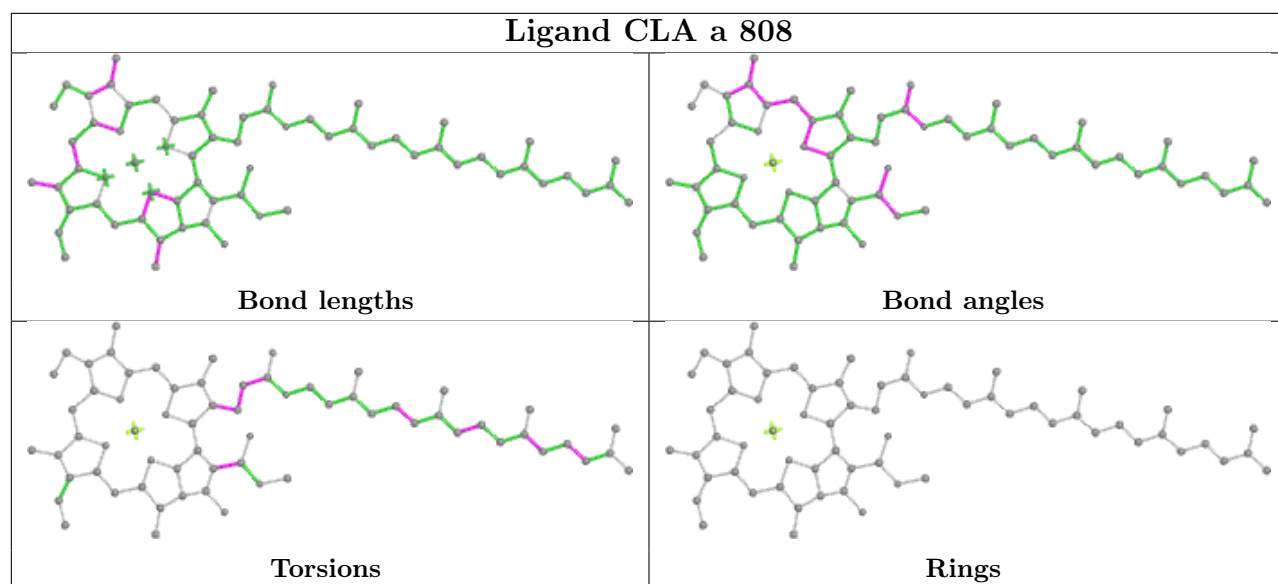
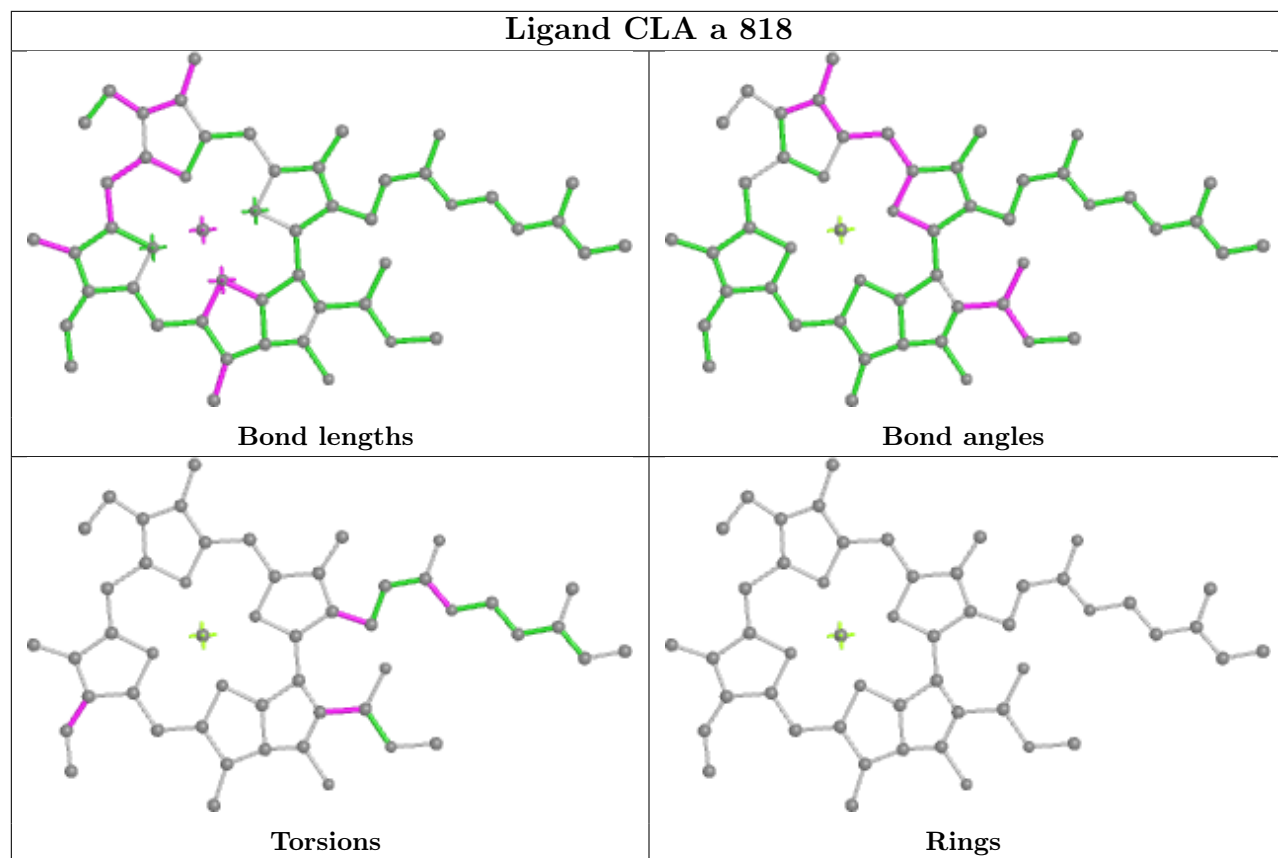


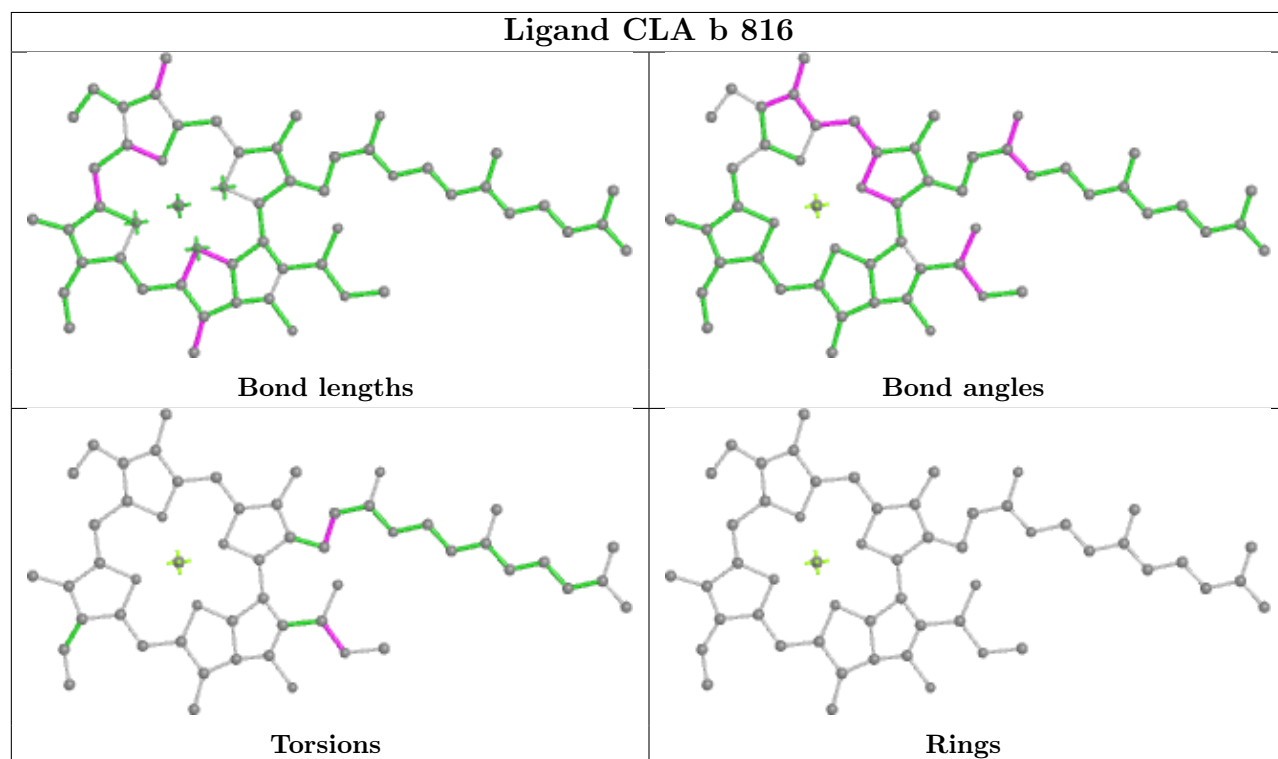
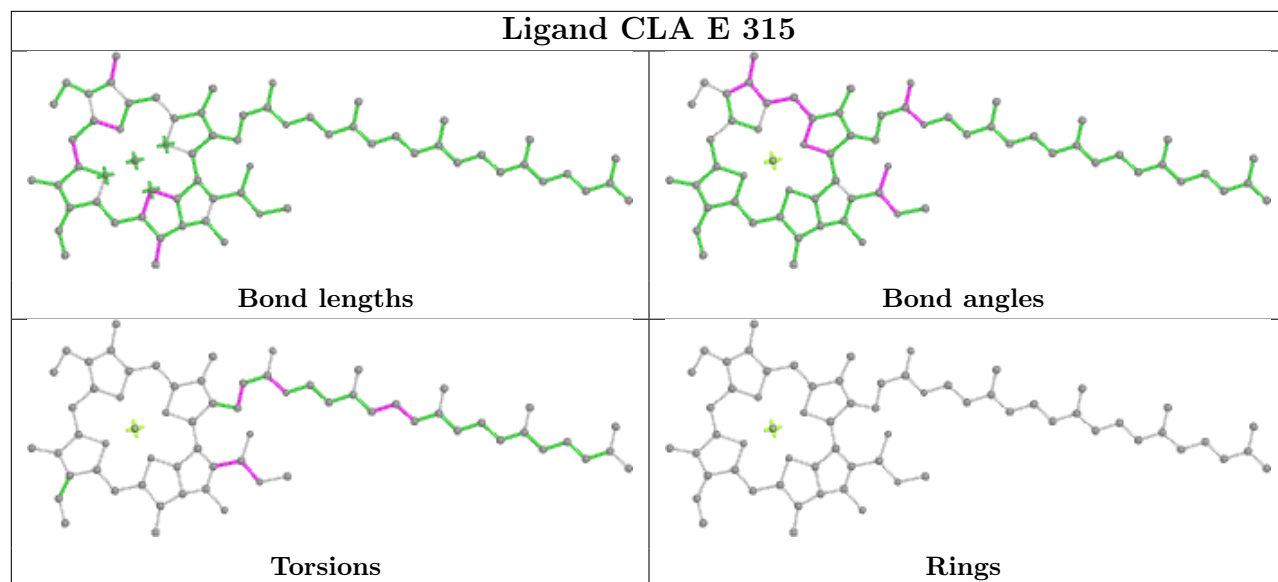


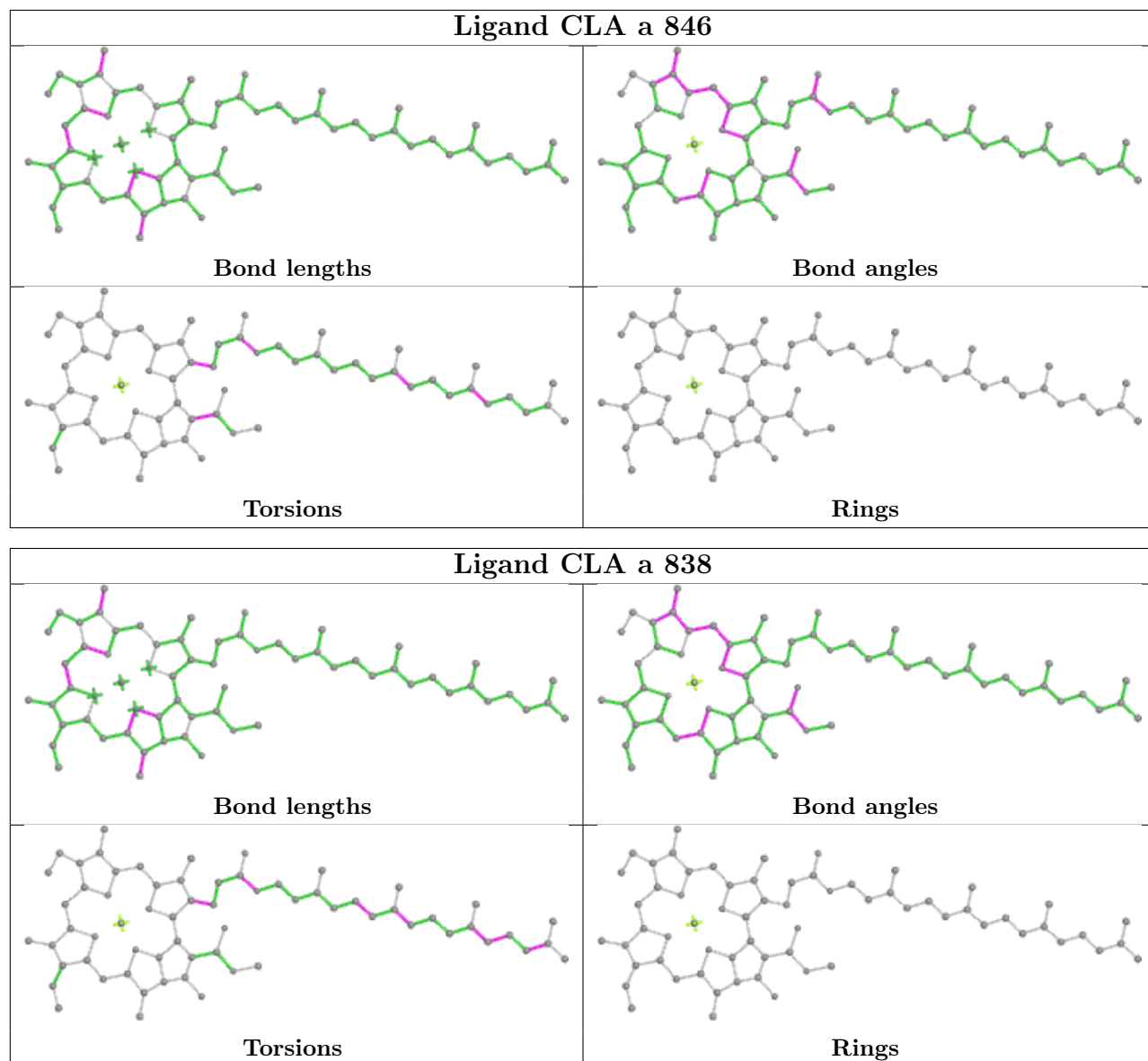


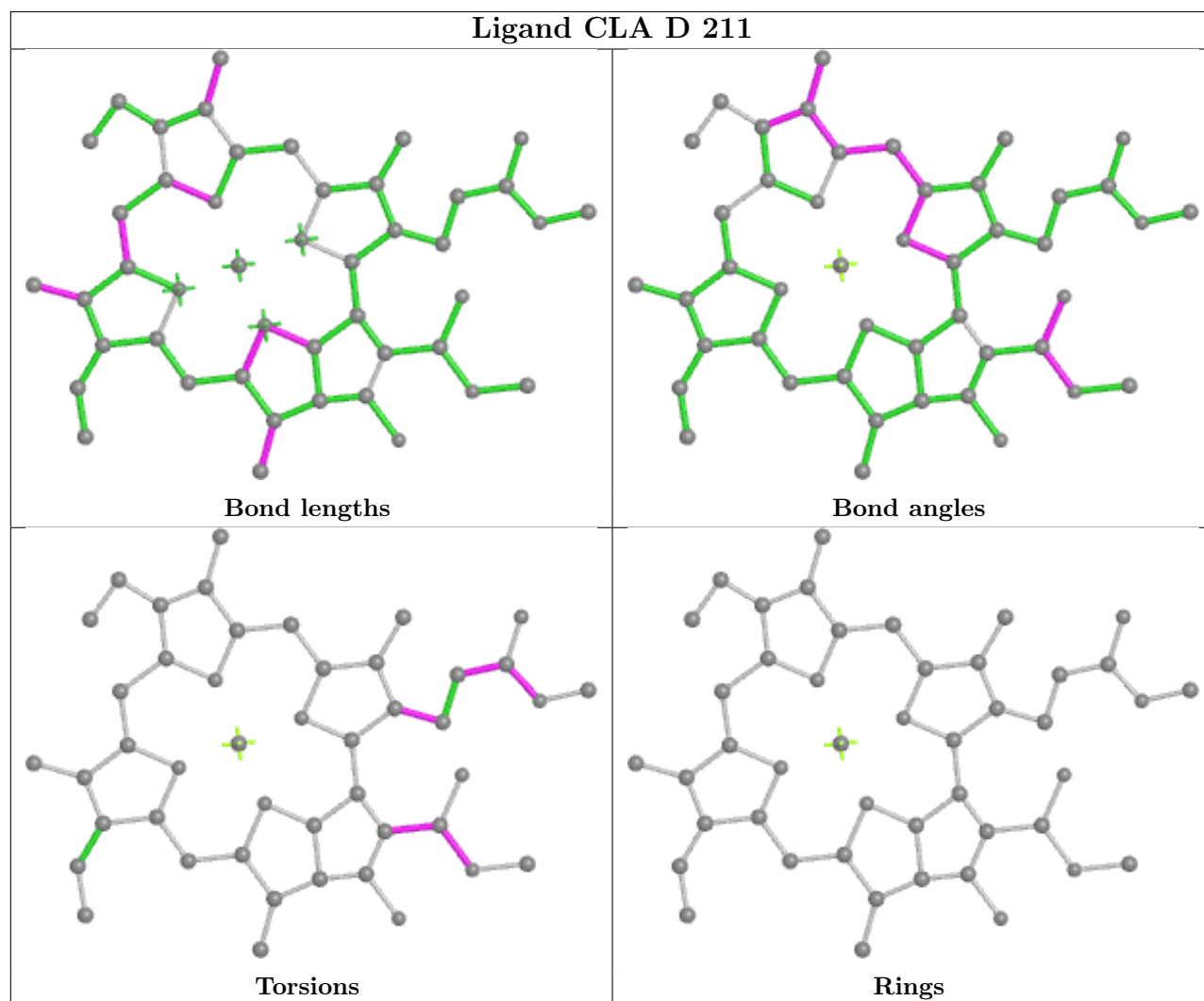
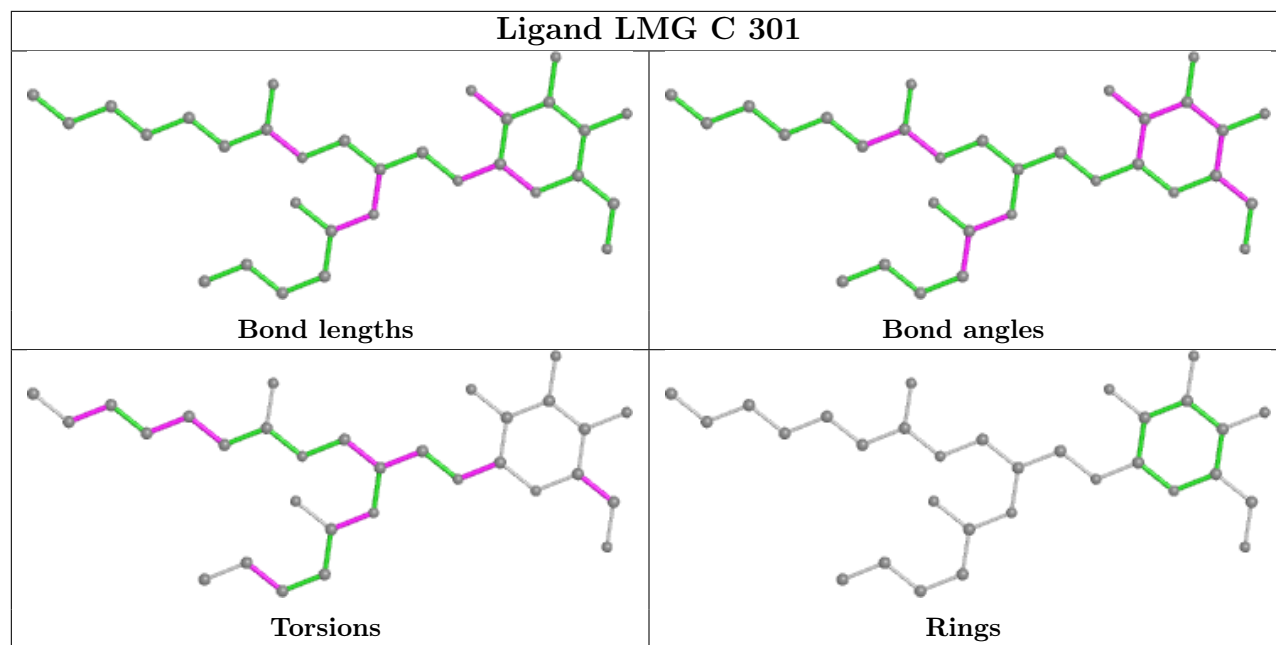


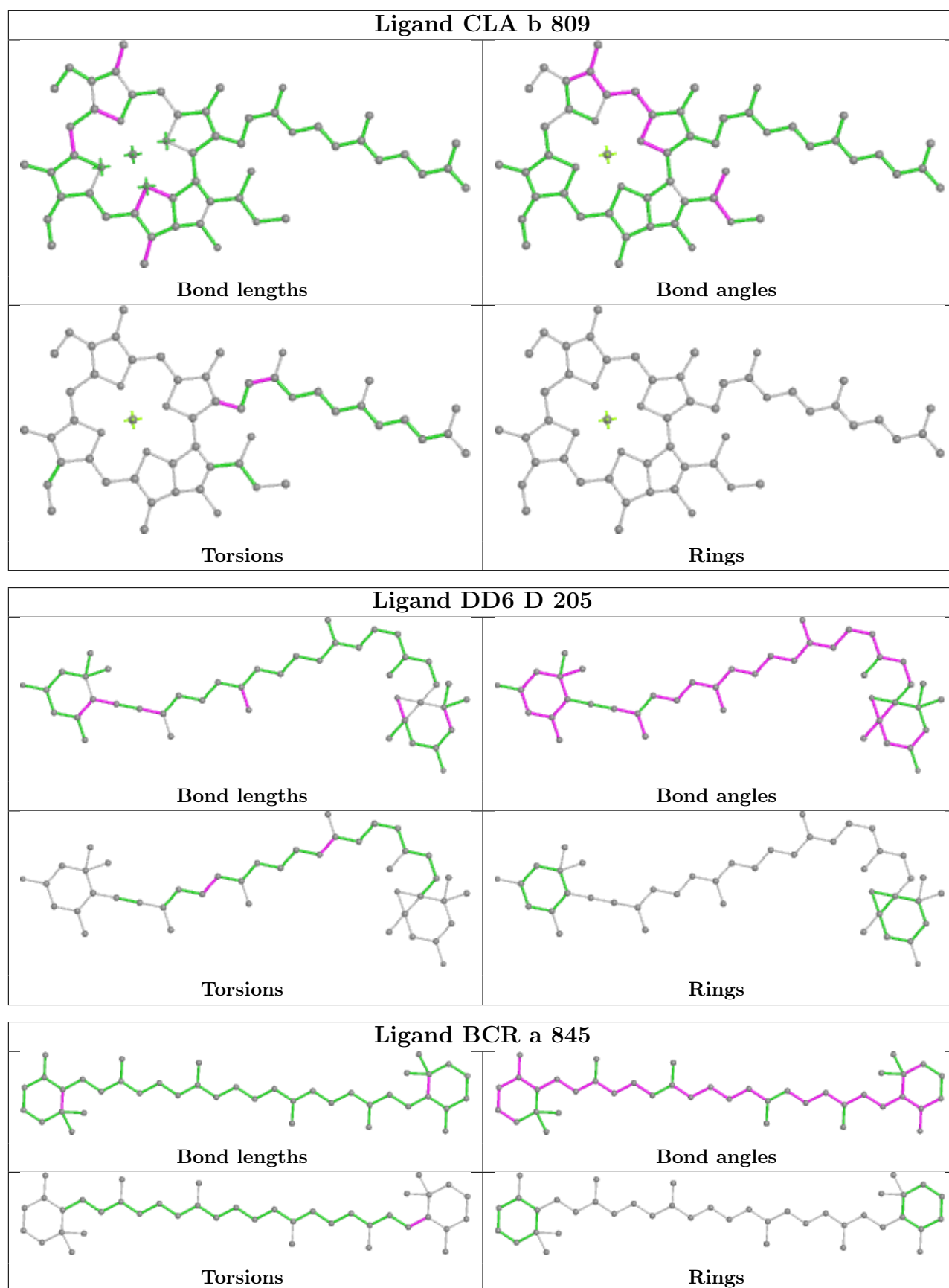


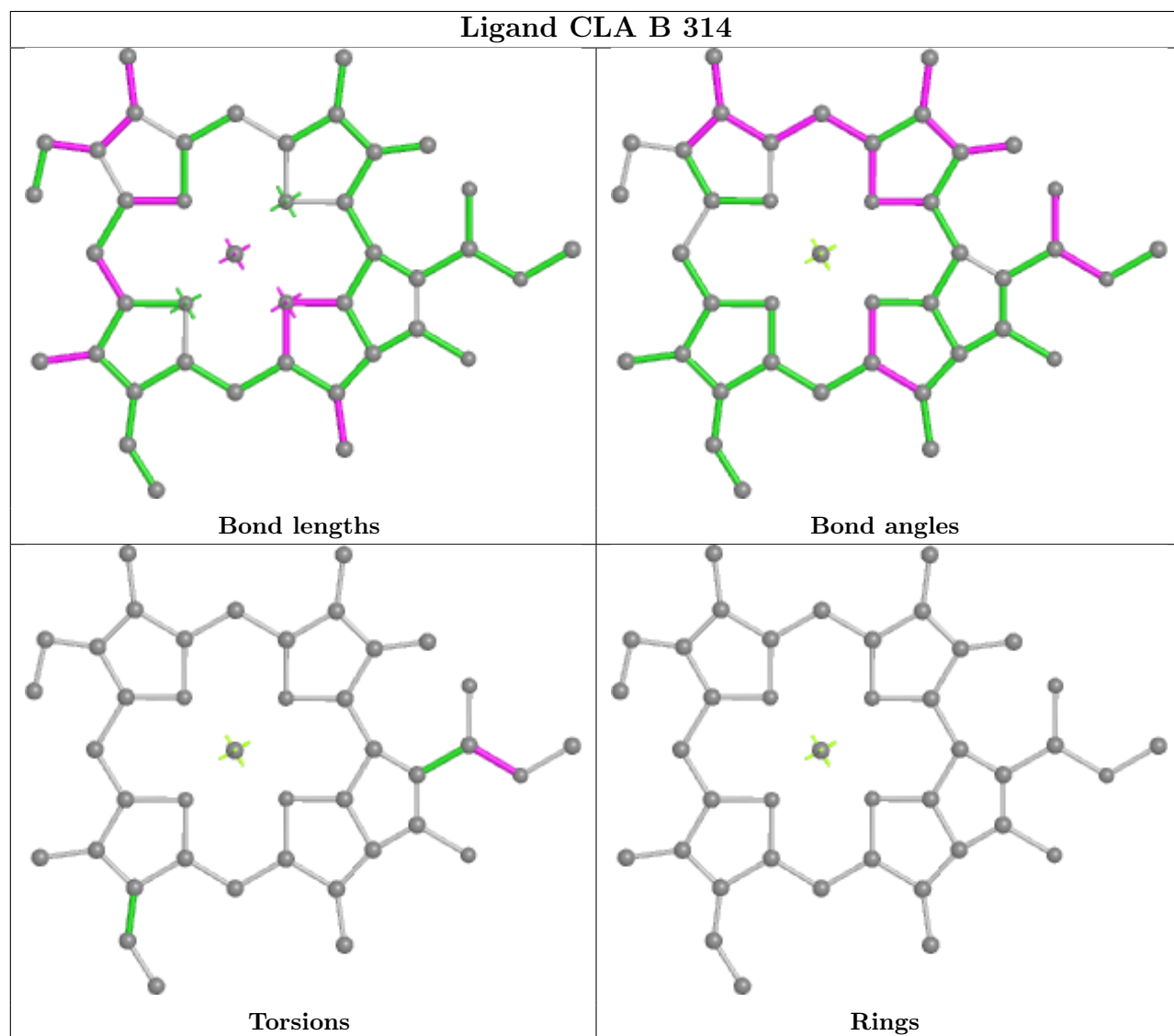
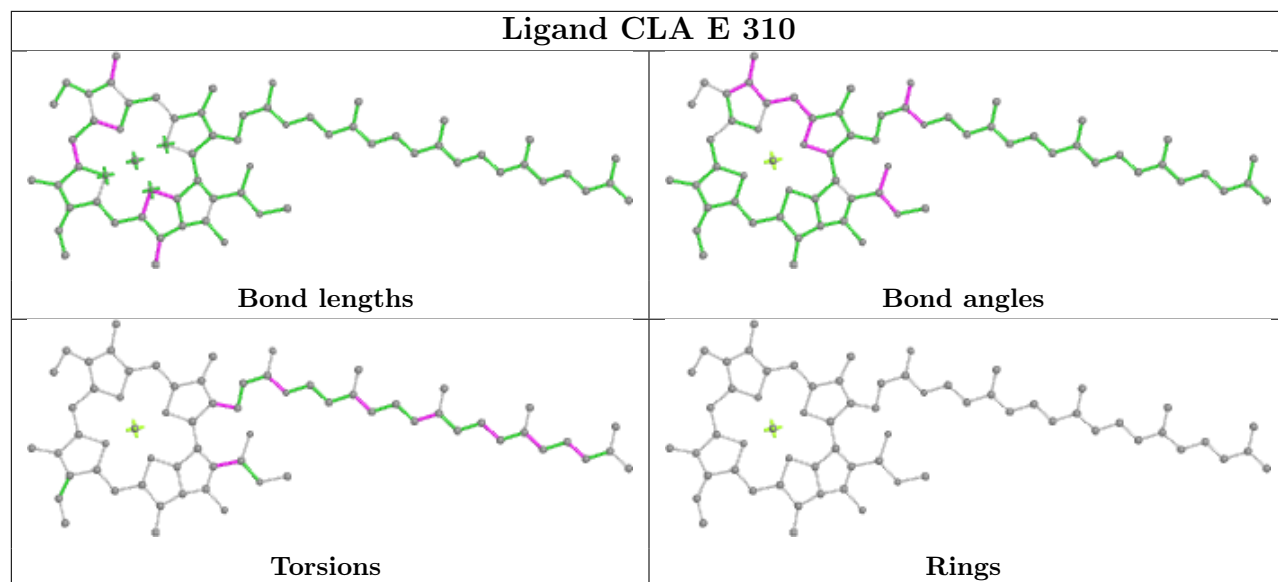


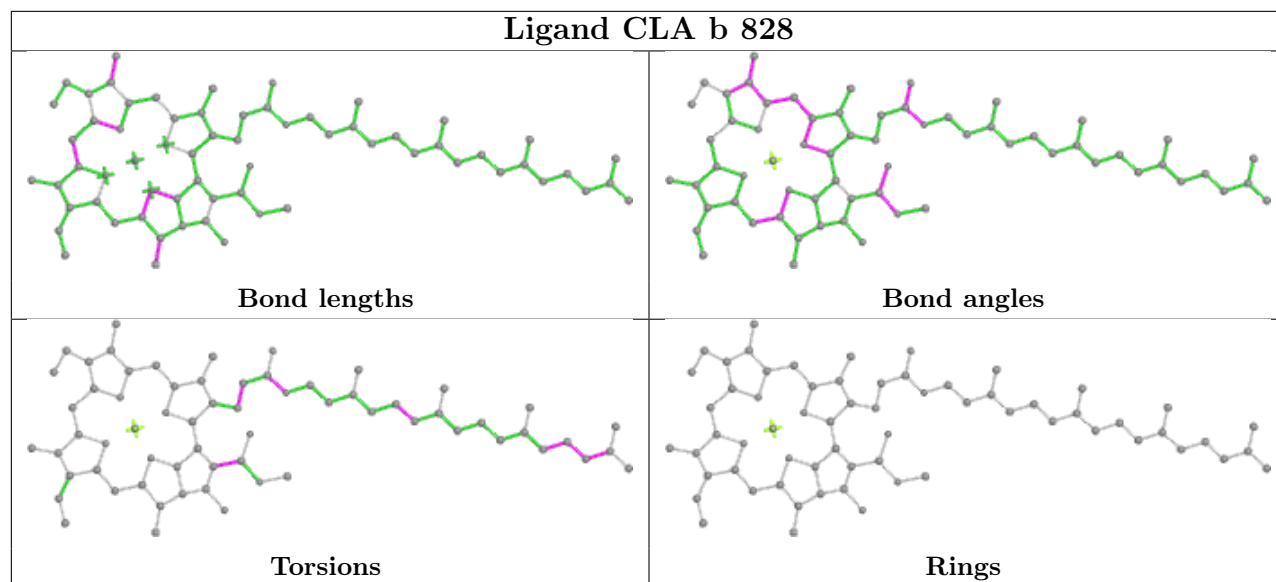












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

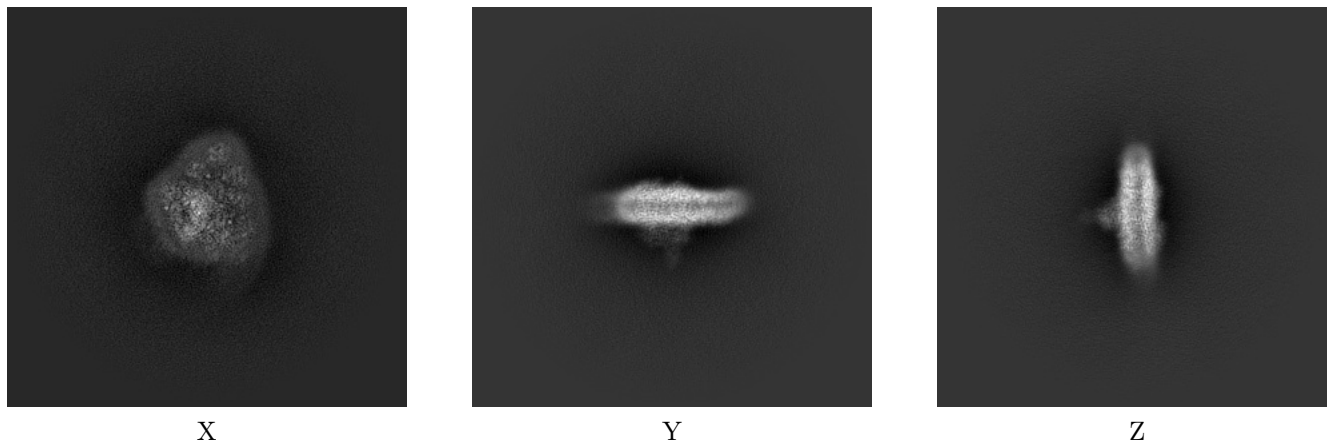
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60044. These allow visual inspection of the internal detail of the map and identification of artifacts.

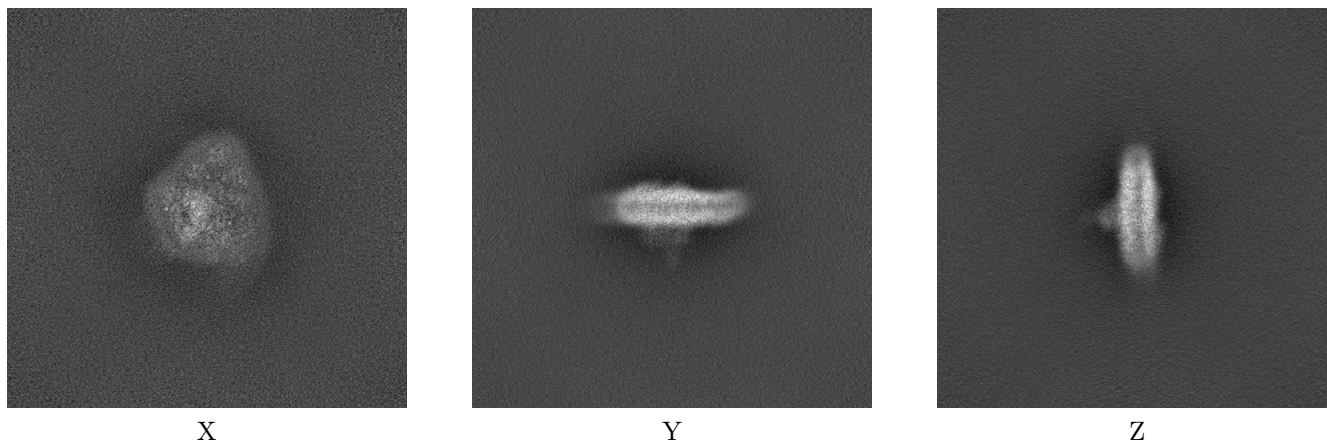
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



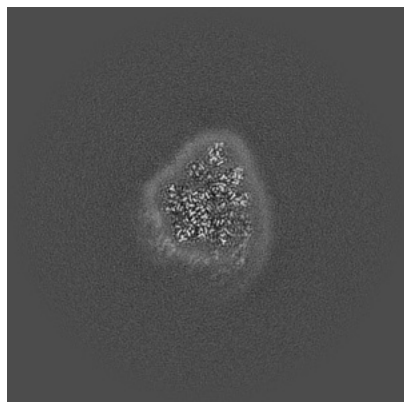
6.1.2 Raw map



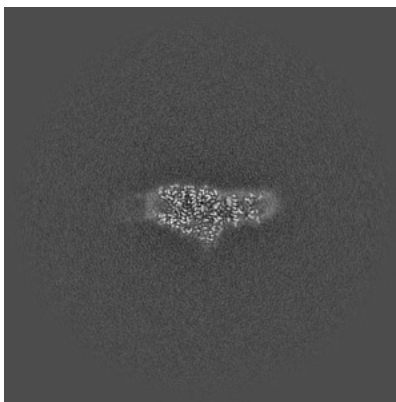
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

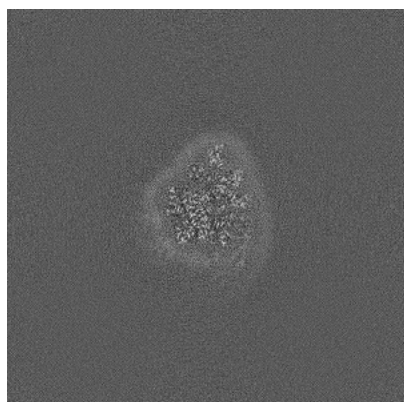


Y Index: 256

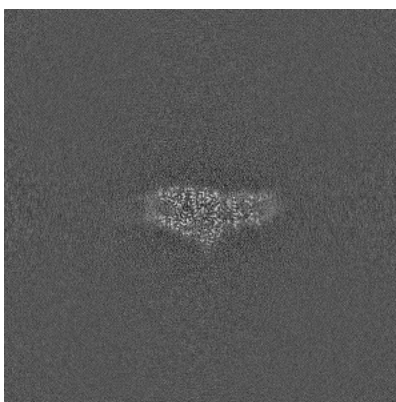


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

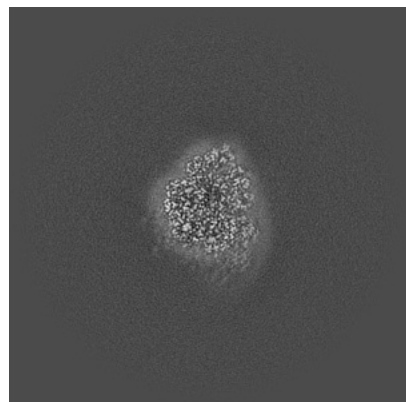


Z Index: 256

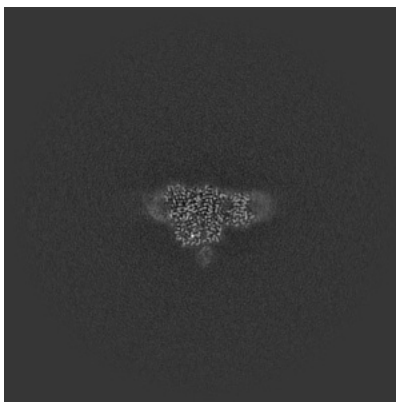
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

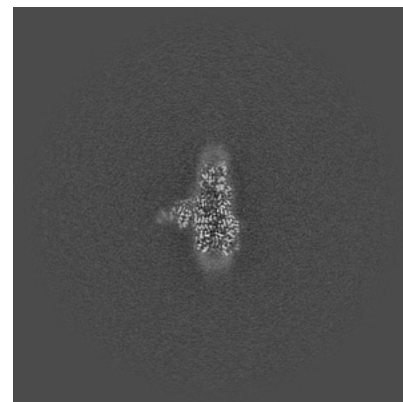
6.3.1 Primary map



X Index: 244

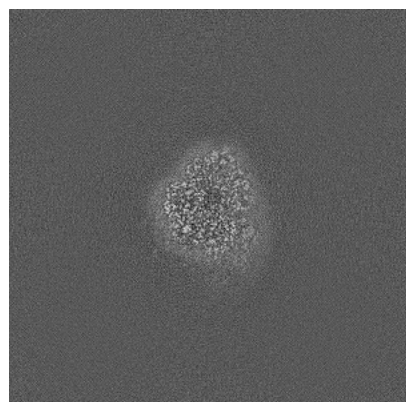


Y Index: 240

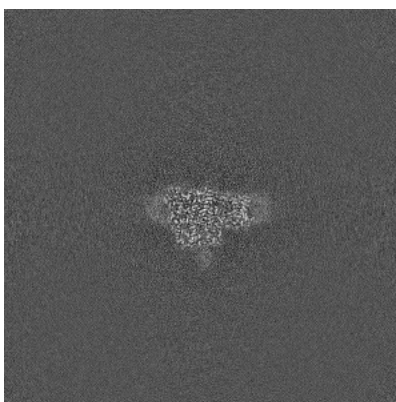


Z Index: 262

6.3.2 Raw map



X Index: 244



Y Index: 239

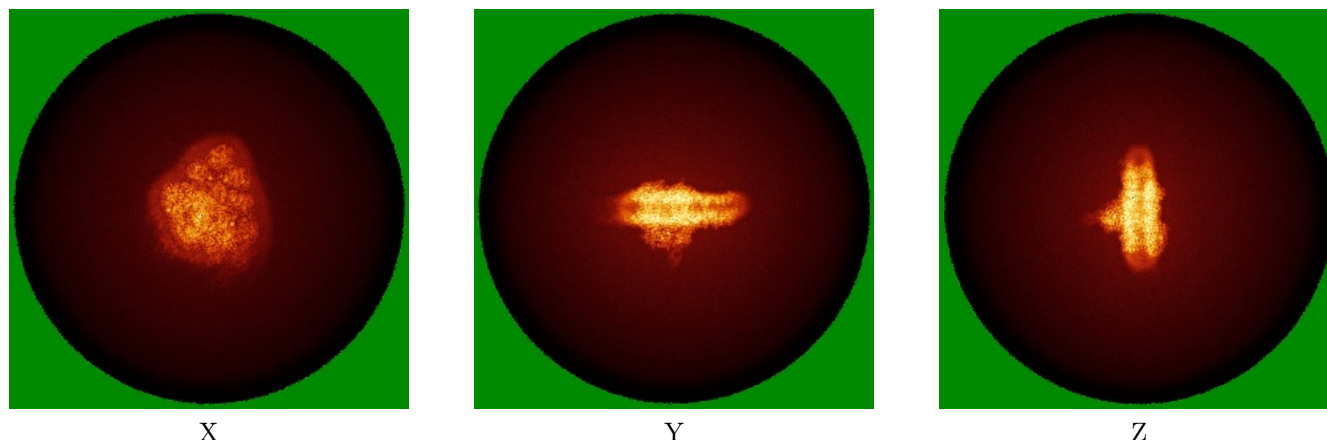


Z Index: 262

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

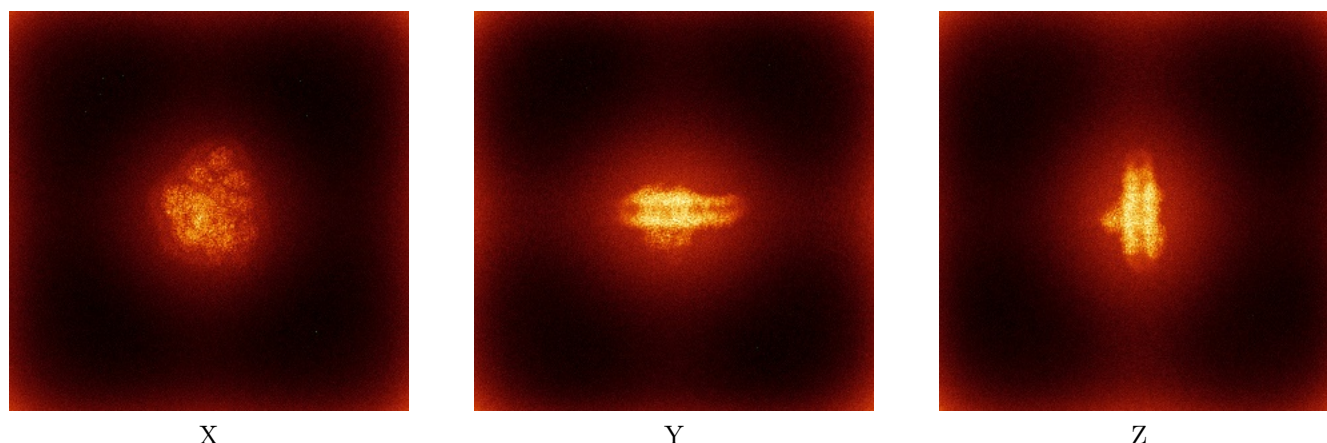


X

Y

Z

6.4.2 Raw map



X

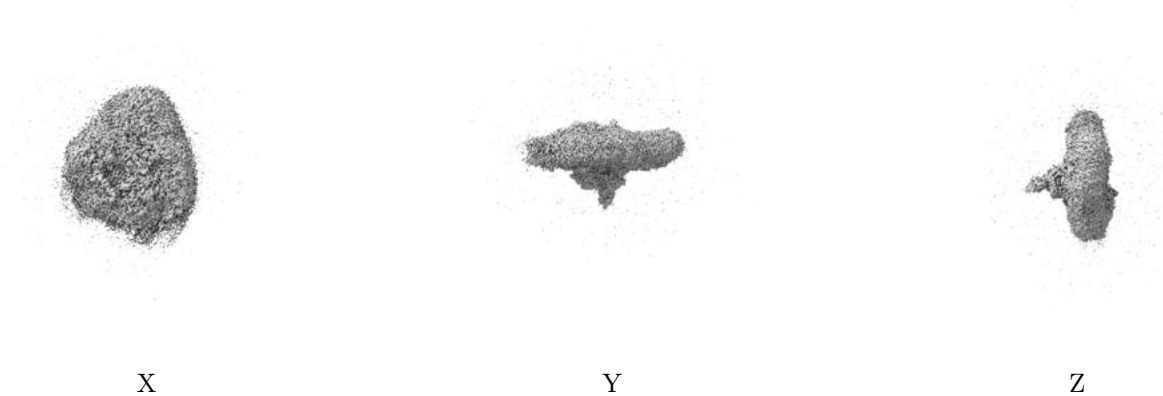
Y

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.

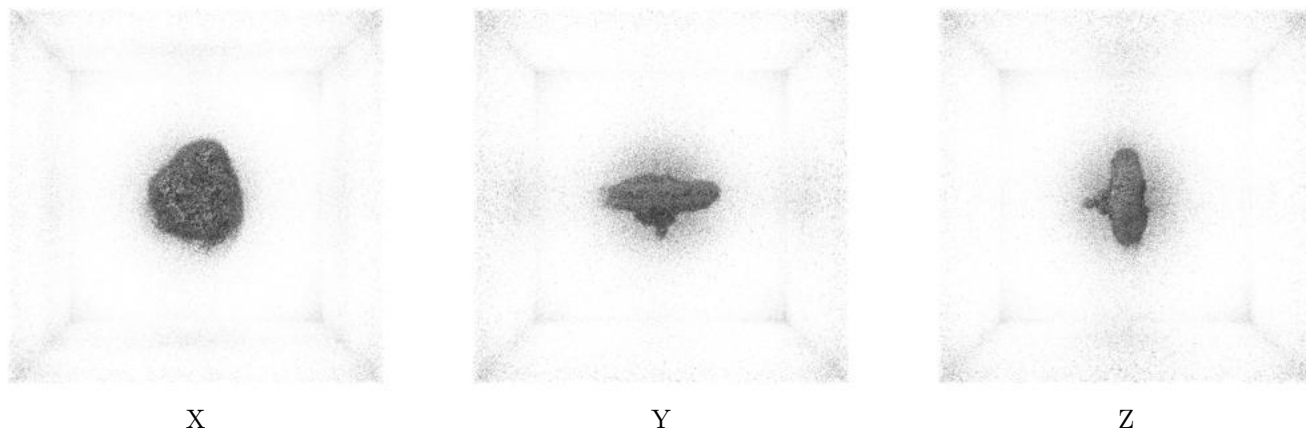
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

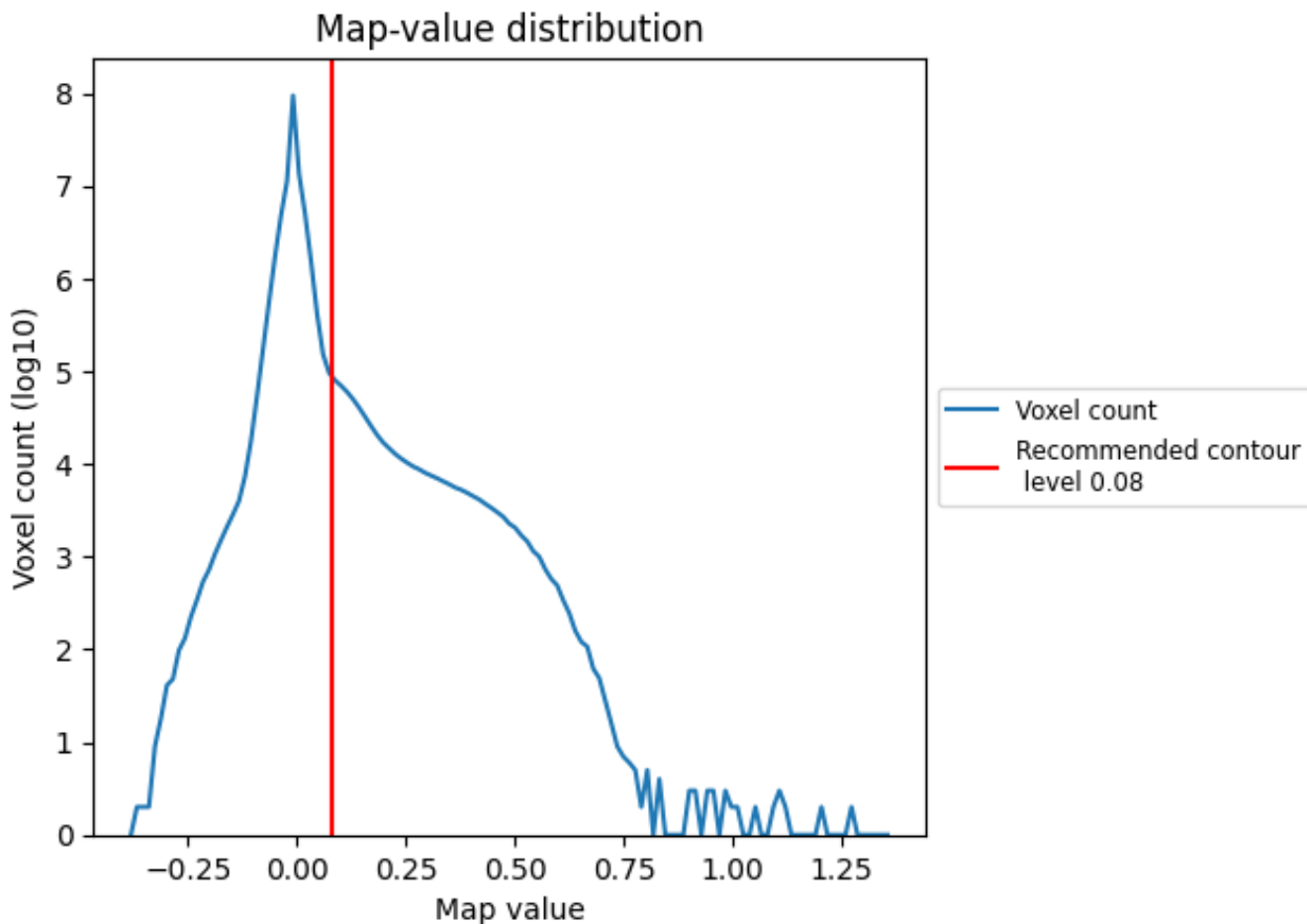
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

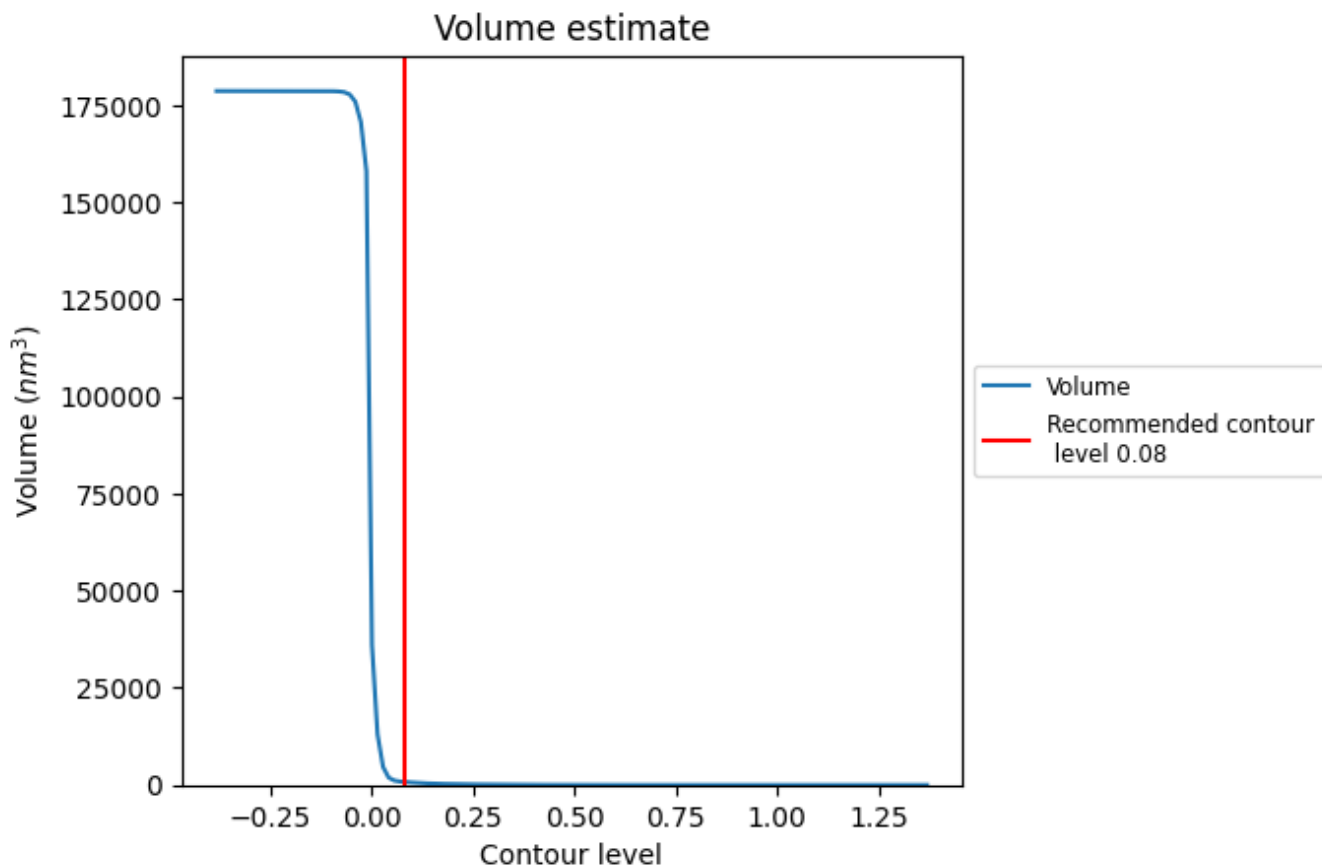
This section contains the results of statistical analysis of the map.

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.

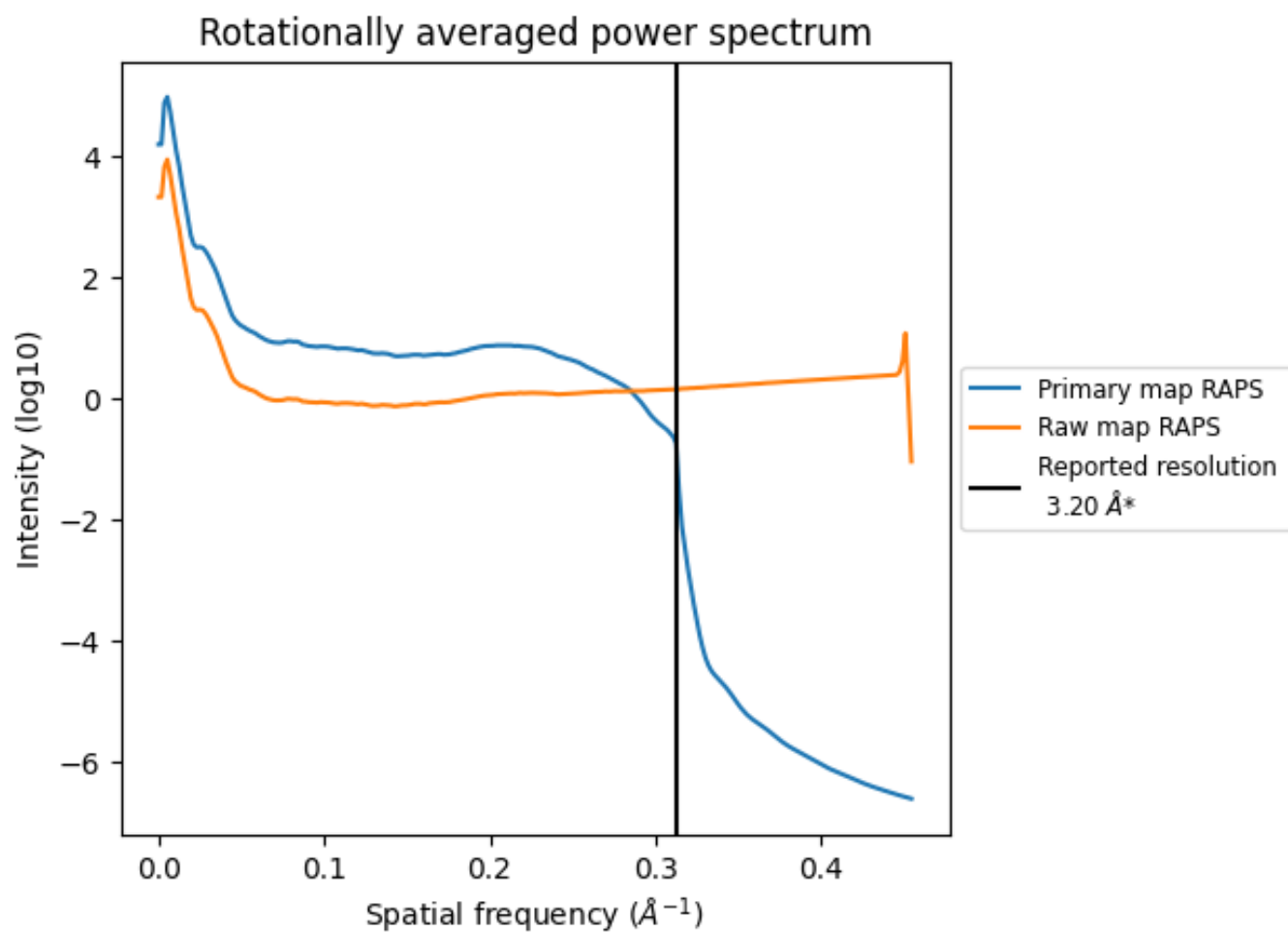
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 799 nm^3 ; this corresponds to an approximate mass of 722 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

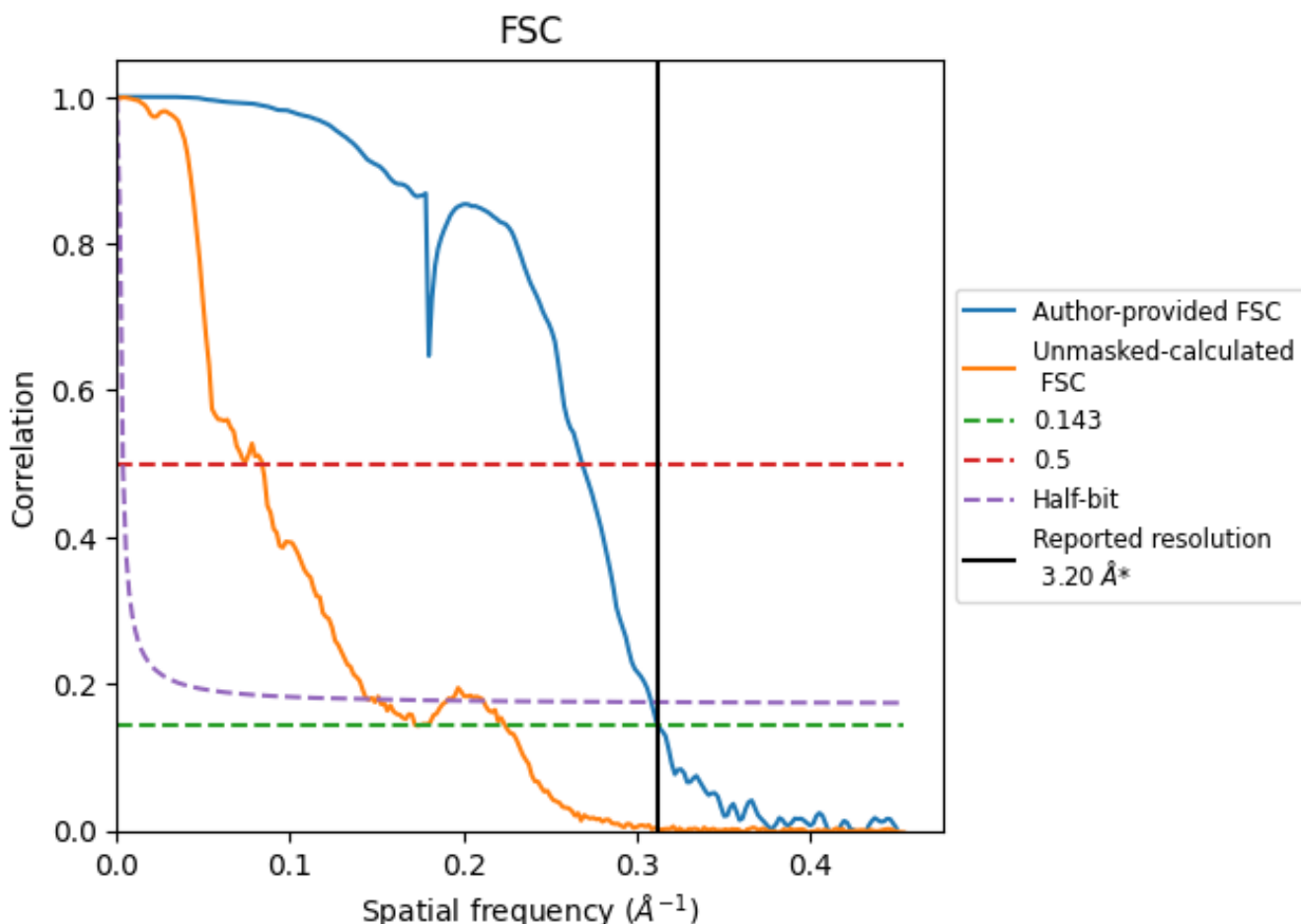


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

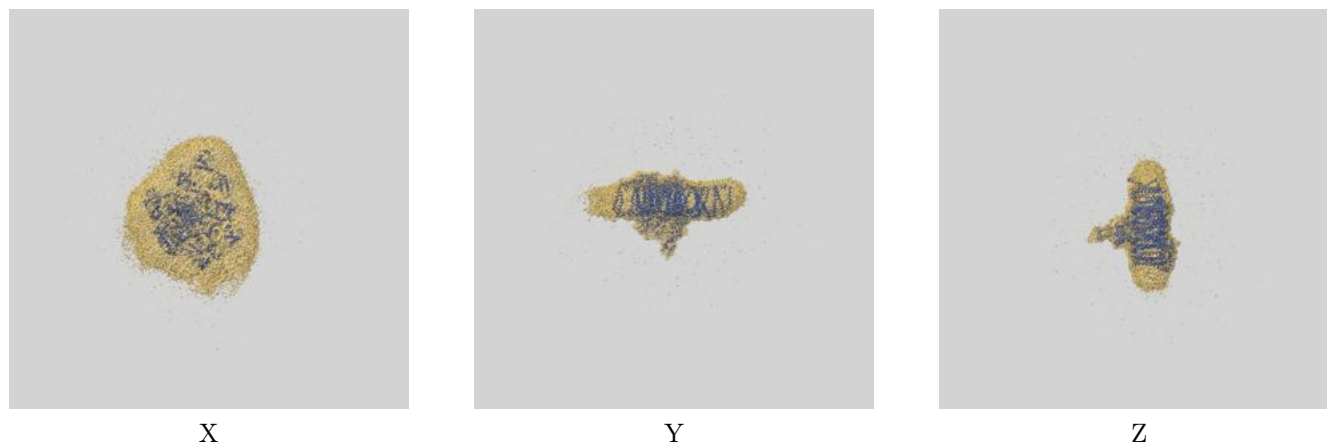
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.72	3.24
Unmasked-calculated*	5.75	11.93	6.88

*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 5.75 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60044 and PDB model 8ZET. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



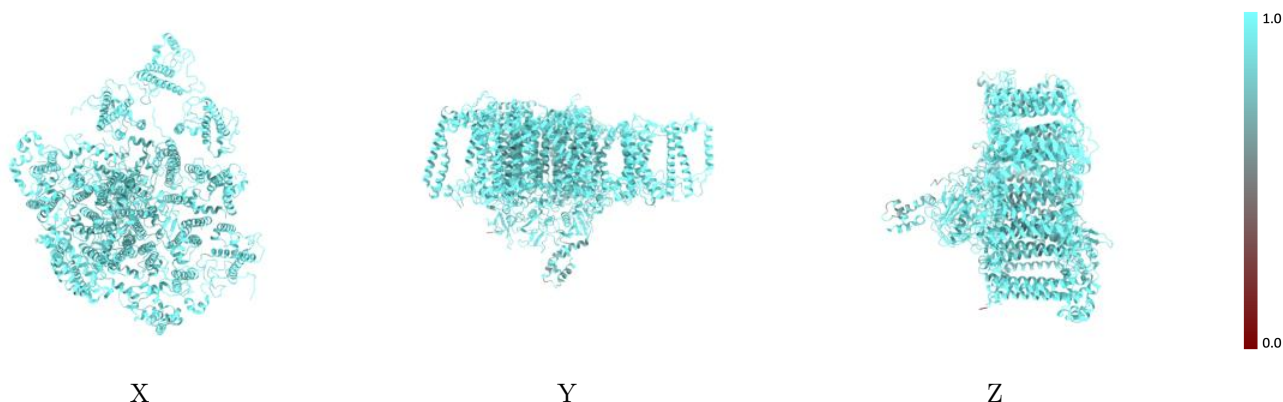
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



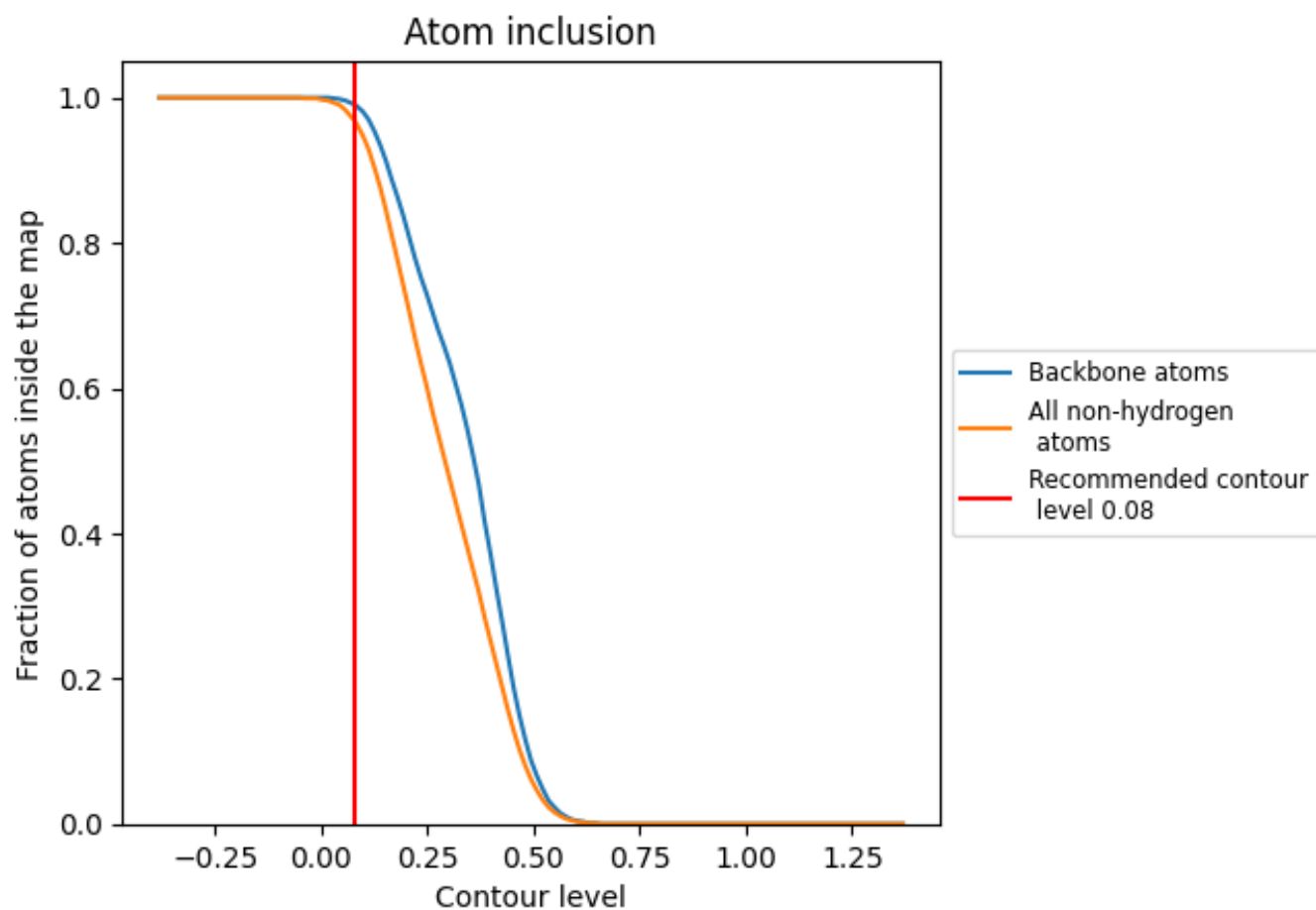
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9670	 0.4850
B	 0.9740	 0.4570
C	 0.9780	 0.4520
D	 0.9670	 0.4720
E	 0.9700	 0.4710
H	 0.9600	 0.4360
a	 0.9740	 0.5120
b	 0.9690	 0.5060
c	 0.9880	 0.5100
d	 0.9790	 0.5070
e	 0.9510	 0.4720
f	 0.9650	 0.4760
g	 0.8680	 0.4000
i	 0.9640	 0.5130
j	 0.9490	 0.4710
l	 0.9770	 0.5060
m	 0.9440	 0.4770
r	 0.9330	 0.3970

