



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:55 PM UTC

PDB ID : 8WMW / pdb_00008wmw
EMDB ID : EMD-37660
Title : The structure of PSI-11CAC at the stationary growth phase
Authors : Zhang, S.M.; Si, L.; Li, M.
Deposited on : 2023-10-04
Resolution : 3.30 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:

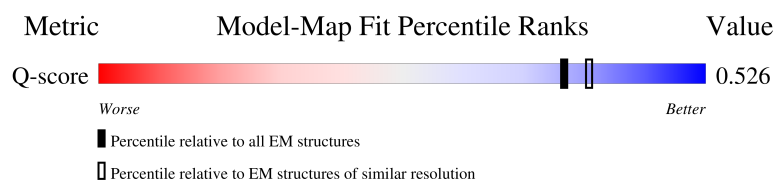
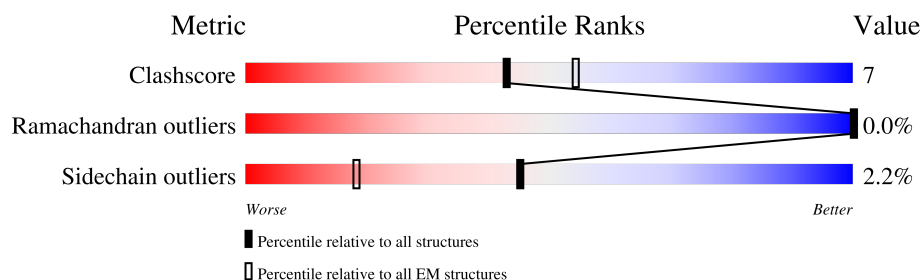
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



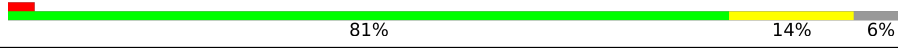
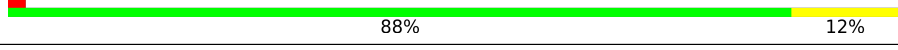
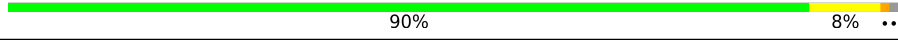
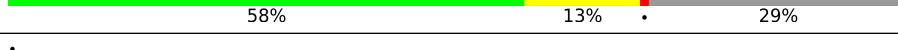
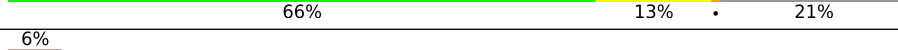
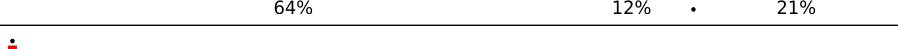
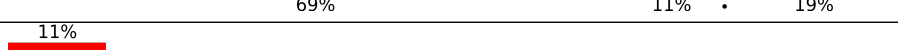
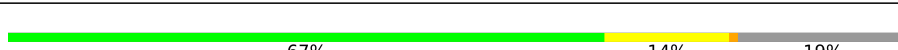
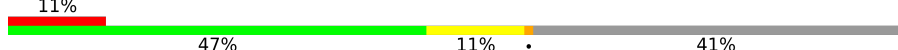
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	752	
2	B	734	
3	C	81	
4	D	141	

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	188	
7	I	36	
8	J	42	
9	L	153	
10	M	30	
11	O	146	
12	K	87	
13	c	216	
14	a	216	
15	b	223	
16	h	225	
17	e	203	
18	k	241	
19	f	212	
19	j	212	
20	i	218	
21	d	213	
22	g	255	
23	R	129	

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
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	807	X	-	-	-
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	830	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	839	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	841	X	-	-	-
24	CLA	A	842	X	-	-	-
24	CLA	A	852	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	A	855	X	-	-	-
24	CLA	A	856	X	-	-	-
24	CLA	B	801	X	-	-	-
24	CLA	B	803	X	-	-	-
24	CLA	B	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	807	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-
24	CLA	B	827	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	839	X	-	-	-
24	CLA	F	201	X	-	-	-
24	CLA	F	202	X	-	-	-
24	CLA	I	102	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	J	105	X	-	-	-
24	CLA	K	101	X	-	-	-
24	CLA	K	102	X	-	-	-
24	CLA	L	202	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	204	X	-	-	-
24	CLA	L	207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	O	201	X	-	-	-
24	CLA	O	205	X	-	-	-
24	CLA	R	203	X	-	-	-
24	CLA	a	302	X	-	-	-
24	CLA	a	303	X	-	-	-
24	CLA	a	304	X	-	-	-
24	CLA	a	305	X	-	-	-
24	CLA	a	306	X	-	-	-
24	CLA	a	307	X	-	-	-
24	CLA	a	308	X	-	-	-
24	CLA	a	309	X	-	-	-
24	CLA	a	310	X	-	-	-
24	CLA	a	311	X	-	-	-
24	CLA	a	312	X	-	-	-
24	CLA	b	303	X	-	-	-
24	CLA	b	304	X	-	-	-
24	CLA	b	305	X	-	-	-
24	CLA	b	307	X	-	-	-
24	CLA	b	308	X	-	-	-
24	CLA	b	309	X	-	-	-
24	CLA	b	310	X	-	-	-
24	CLA	b	311	X	-	-	-
24	CLA	b	312	X	-	-	-
24	CLA	b	313	X	-	-	-
24	CLA	c	601	X	-	-	-
24	CLA	c	602	X	-	-	-
24	CLA	c	603	X	-	-	-
24	CLA	c	604	X	-	-	-
24	CLA	c	605	X	-	-	-
24	CLA	c	607	X	-	-	-
24	CLA	c	608	X	-	-	-
24	CLA	c	609	X	-	-	-
24	CLA	c	611	X	-	-	-
24	CLA	c	612	X	-	-	-
24	CLA	d	301	X	-	-	-
24	CLA	d	302	X	-	-	-
24	CLA	d	303	X	-	-	-
24	CLA	d	304	X	-	-	-
24	CLA	d	306	X	-	-	-
24	CLA	d	307	X	-	-	-
24	CLA	d	308	X	-	-	-
24	CLA	d	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	e	601	X	-	-	-
24	CLA	e	602	X	-	-	-
24	CLA	e	603	X	-	-	-
24	CLA	e	604	X	-	-	-
24	CLA	e	605	X	-	-	-
24	CLA	e	606	X	-	-	-
24	CLA	e	607	X	-	-	-
24	CLA	e	608	X	-	-	-
24	CLA	e	611	X	-	-	-
24	CLA	f	601	X	-	-	-
24	CLA	f	602	X	-	-	-
24	CLA	f	603	X	-	-	-
24	CLA	f	607	X	-	-	-
24	CLA	f	608	X	-	-	-
24	CLA	f	609	X	-	-	-
24	CLA	f	610	X	-	-	-
24	CLA	f	612	X	-	-	-
24	CLA	f	613	X	-	-	-
24	CLA	g	302	X	-	-	-
24	CLA	g	303	X	-	-	-
24	CLA	g	304	X	-	-	-
24	CLA	g	305	X	-	-	-
24	CLA	g	306	X	-	-	-
24	CLA	g	307	X	-	-	-
24	CLA	g	308	X	-	-	-
24	CLA	g	309	X	-	-	-
24	CLA	g	310	X	-	-	-
24	CLA	g	311	X	-	-	-
24	CLA	g	315	X	-	-	-
24	CLA	g	322	X	-	-	-
24	CLA	h	301	X	-	-	-
24	CLA	h	302	X	-	-	-
24	CLA	h	303	X	-	-	-
24	CLA	h	304	X	-	-	-
24	CLA	h	305	X	-	-	-
24	CLA	h	306	X	-	-	-
24	CLA	h	307	X	-	-	-
24	CLA	h	312	X	-	-	-
24	CLA	i	601	X	-	-	-
24	CLA	i	602	X	-	-	-
24	CLA	i	603	X	-	-	-
24	CLA	i	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	i	605	X	-	-	-
24	CLA	i	606	X	-	-	-
24	CLA	i	607	X	-	-	-
24	CLA	i	608	X	-	-	-
24	CLA	i	610	X	-	-	-
24	CLA	i	611	X	-	-	-
24	CLA	j	302	X	-	-	-
24	CLA	j	303	X	-	-	-
24	CLA	j	304	X	-	-	-
24	CLA	j	306	X	-	-	-
24	CLA	j	307	X	-	-	-
24	CLA	j	308	X	-	-	-
24	CLA	j	309	X	-	-	-
24	CLA	j	310	X	-	-	-
24	CLA	j	311	X	-	-	-
24	CLA	j	313	X	-	-	-
24	CLA	j	314	X	-	-	-
24	CLA	k	601	X	-	-	-
24	CLA	k	602	X	-	-	-
24	CLA	k	603	X	-	-	-
24	CLA	k	604	X	-	-	-
24	CLA	k	605	X	-	-	-
24	CLA	k	607	X	-	-	-
24	CLA	k	608	X	-	-	-
24	CLA	k	609	X	-	-	-
24	CLA	k	610	X	-	-	-
29	SF4	A	854	-	-	X	-
29	SF4	C	101	-	-	X	-
29	SF4	C	102	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 51054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5825	3802	994	1001	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	1	0
			5826	3844	982	985	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			592	361	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1084	692	186	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	60	Total	C	N	O	0	0
			485	309	84	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1254	814	212	226	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			264	182	35	45	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	S	0	0
			351	240	49	59	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	151	Total	C	N	O	S	0	0
			1146	753	182	208	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			232	155	38	38	1		

- Molecule 11 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	104	Total	C	N	O	S	0	0
			773	515	117	138	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	69	Total	C	N	O	S	0	0
			488	319	80	87	2		

- Molecule 13 is a protein called CAC-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	170	Total	C	N	O	S	0	0
			1357	897	221	236	3		

- Molecule 14 is a protein called CAC-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	175	Total	C	N	O	S	0	0
			1361	889	217	245	10		

- Molecule 15 is a protein called CAC-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	194	Total	C	N	O	S	0	0
			1439	916	251	258	14		

- Molecule 16 is a protein called CAC-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	162	Total	C	N	O	S	0	0
			1200	778	202	214	6		

- Molecule 17 is a protein called CAC-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	169	Total	C	N	O	S	0	0
			1286	843	207	228	8		

- Molecule 18 is a protein called CAC-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	180	Total	C	N	O	S	0	0
			1346	872	223	239	12		

- Molecule 19 is a protein called CAC-f.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	174	Total	C	N	O	S	0	0
			1302	842	212	240	8		
19	j	172	Total	C	N	O	S	0	0
			1293	834	212	239	8		

- Molecule 20 is a protein called CAC-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	175	Total	C	N	O	S	0	0
			1324	849	227	237	11		

- Molecule 21 is a protein called CAC-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	126	Total	C	N	O	S	0	0
			950	609	165	167	9		

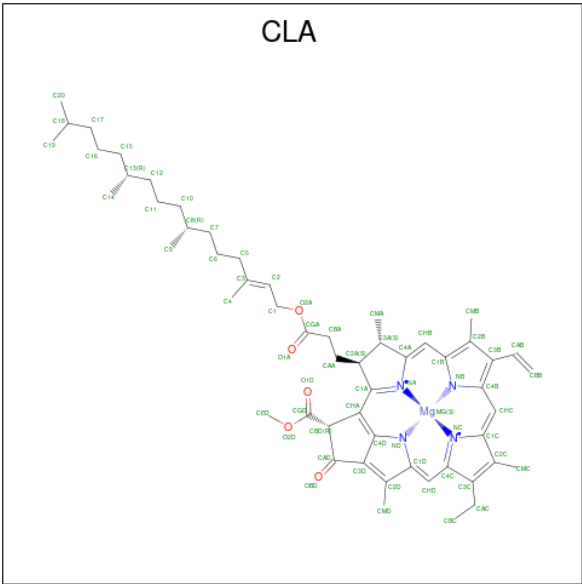
- Molecule 22 is a protein called CAC-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	219	Total	C	N	O	S	0	0
			1630	1060	267	292	11		

- Molecule 23 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	90	Total	C	N	O	S	0	0
			664	434	105	124	1		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	J	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	K	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	c	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	k	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 61	C 51	Mg 1	N 4	O 5	0

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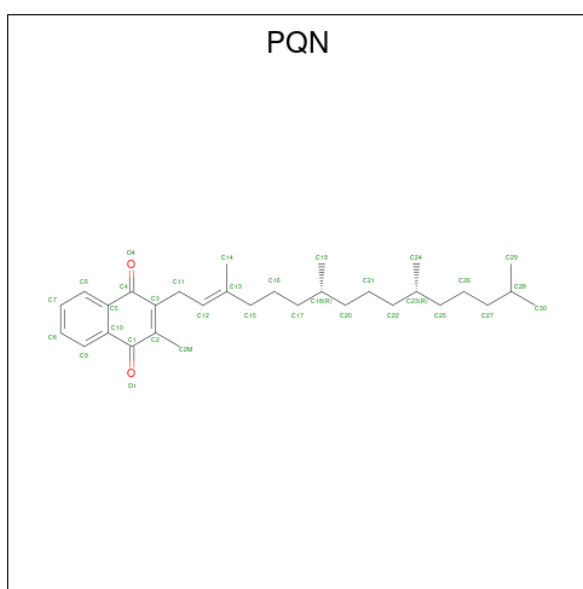
Mol	Chain	Residues	Atoms					AltConf
24	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
24	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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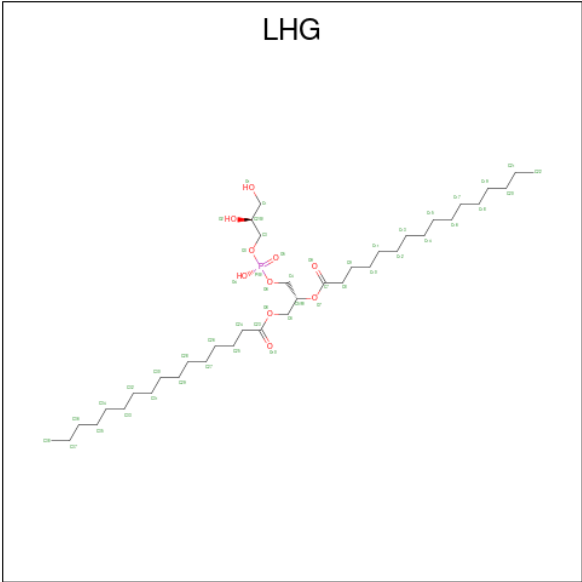
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



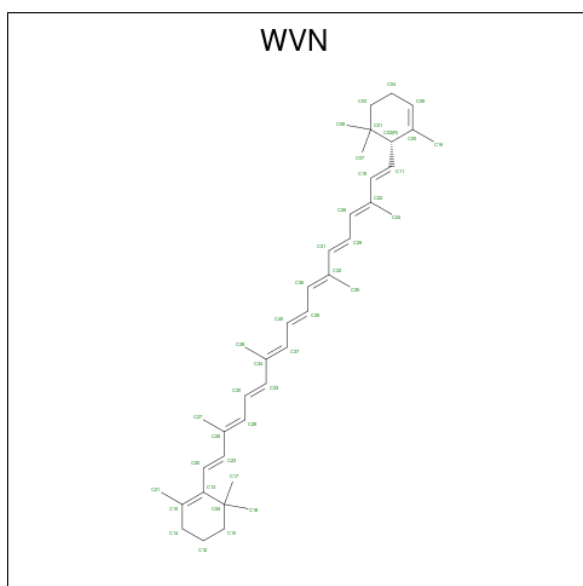
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			48	37	10	1	
26	A	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			38	27	10	1	
26	J	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	e	1	Total	C	O	P	0
			37	26	10	1	
26	k	1	Total	C	O	P	0
			37	26	10	1	
26	f	1	Total	C	O	P	0
			37	26	10	1	
26	f	1	Total	C	O	P	0
			49	38	10	1	
26	i	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	j	1	Total	C	O	P	0
			30	19	10	1	
26	d	1	Total	C	O	P	0
			37	26	10	1	
26	g	1	Total	C	O	P	0
			49	38	10	1	
26	g	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 27 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: C₄₀H₅₆).



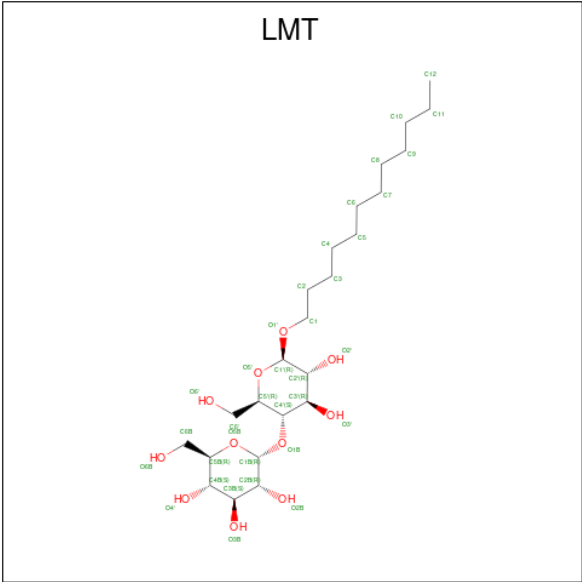
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	B	1	Total	C	0
			40	40	

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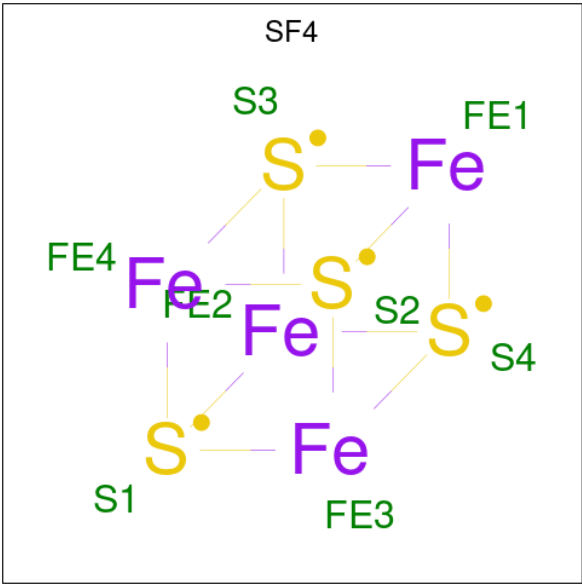
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	M	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	e	1	Total C 40 40	0
27	j	1	Total C 40 40	0
27	R	1	Total C 40 40	0
27	R	1	Total C 40 40	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



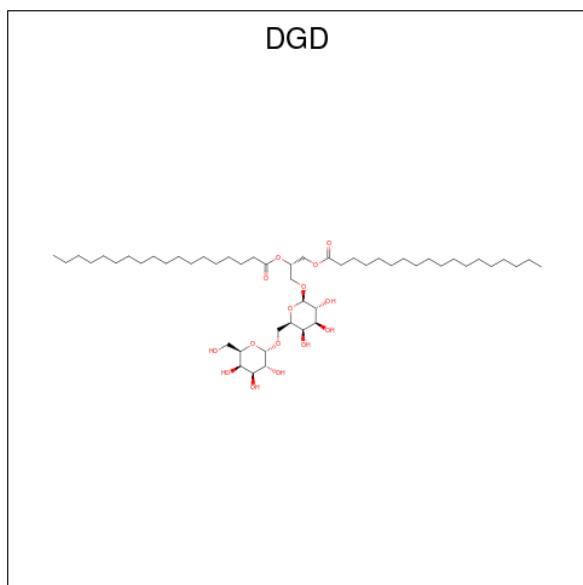
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	F	1	Total	C	O	0
			24	18	6	
28	a	1	Total	C	O	0
			35	24	11	
28	b	1	Total	C	O	0
			24	18	6	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



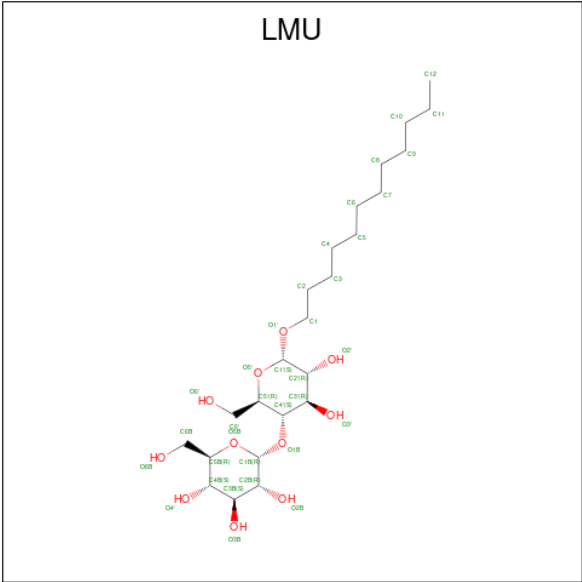
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



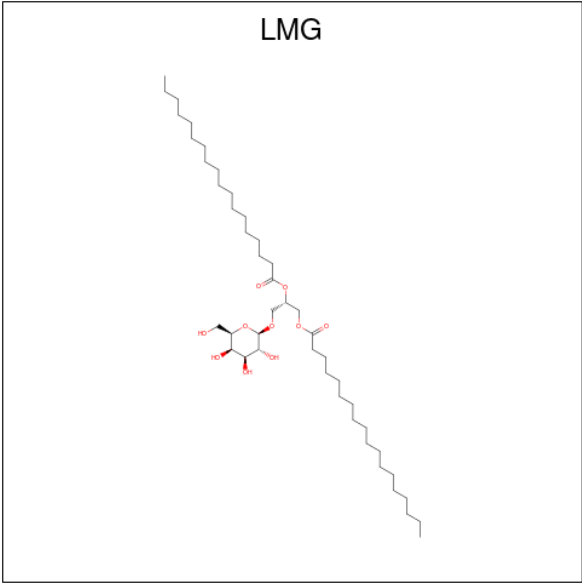
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			60	45	15	

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



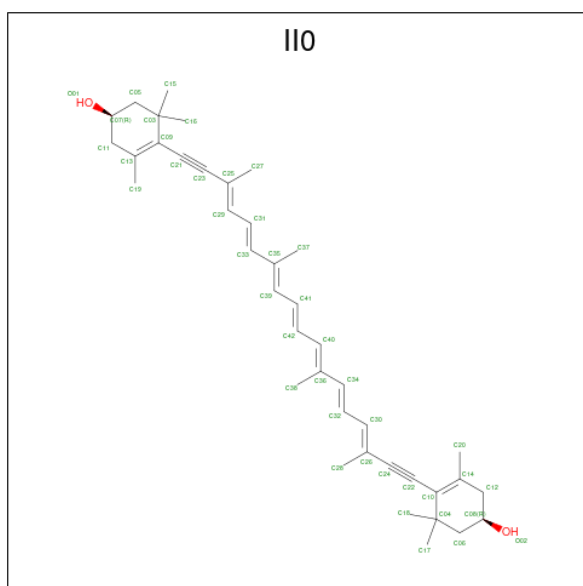
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			48	38	10	
32	J	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
32	L	1	Total	C	O	0
			55	45	10	
32	O	1	Total	C	O	0
			26	16	10	
32	b	1	Total	C	O	0
			55	45	10	

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(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-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	J	1	Total	C	O	0
			42	40	2	
33	O	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	a	1	Total	C	O	0
			42	40	2	
33	a	1	Total	C	O	0
			42	40	2	

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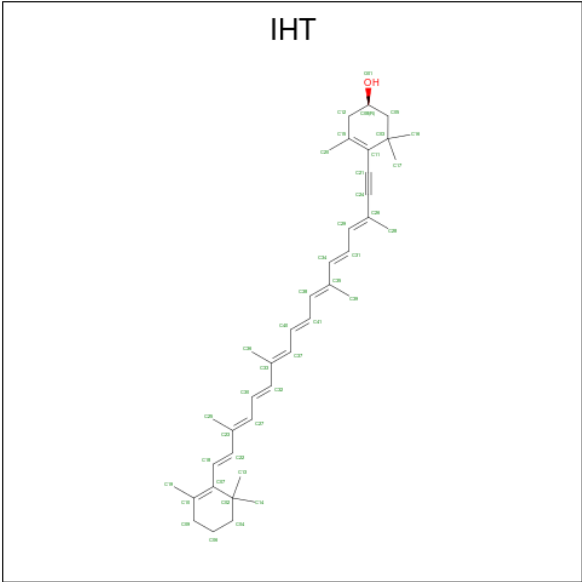
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total 42	C 40	O 2	0
33	a	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	h	1	Total 28	C 27	O 1	0
33	h	1	Total 42	C 40	O 2	0
33	h	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0

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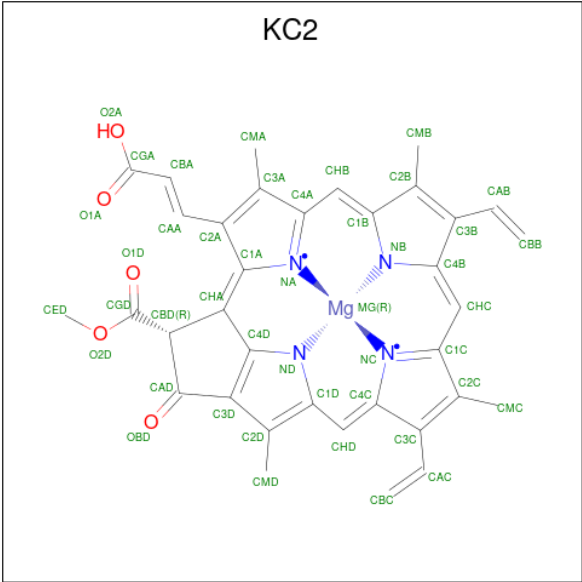
Mol	Chain	Residues	Atoms			AltConf
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	

- Molecule 34 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
34	O	1	Total	C	O	0
			41	40	1	
34	c	1	Total	C	O	0
			41	40	1	
34	a	1	Total	C	O	0
			41	40	1	
34	b	1	Total	C	O	0
			41	40	1	
34	b	1	Total	C	O	0
			41	40	1	
34	k	1	Total	C	O	0
			41	40	1	
34	f	1	Total	C	O	0
			41	40	1	
34	j	1	Total	C	O	0
			41	40	1	
34	g	1	Total	C	O	0
			41	40	1	
34	R	1	Total	C	O	0
			41	40	1	

- Molecule 35 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
35	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

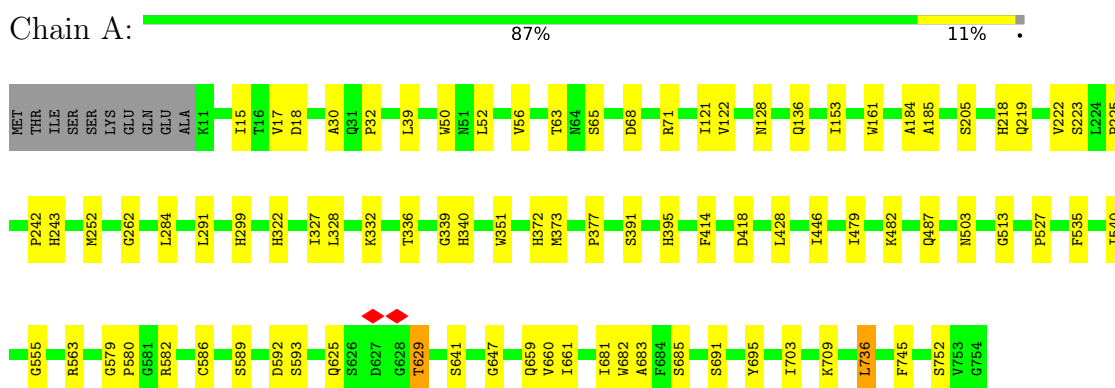
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	50	Total 50	O 50	0
36	B	59	Total 59	O 59	0
36	C	7	Total 7	O 7	0
36	D	1	Total 1	O 1	0
36	F	3	Total 3	O 3	0
36	I	1	Total 1	O 1	0
36	J	1	Total 1	O 1	0
36	L	1	Total 1	O 1	0
36	O	1	Total 1	O 1	0
36	K	1	Total 1	O 1	0
36	a	1	Total 1	O 1	0
36	b	1	Total 1	O 1	0
36	h	1	Total 1	O 1	0
36	e	4	Total 4	O 4	0

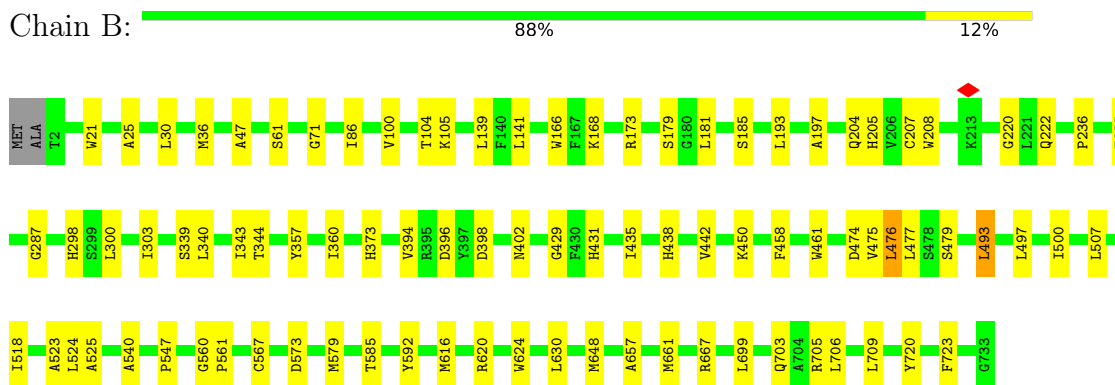
3 Residue-property plots

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

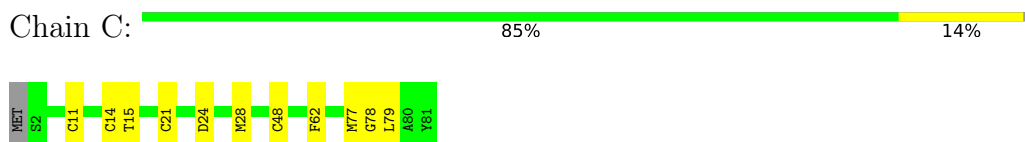
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

Chain D:  85% 13%



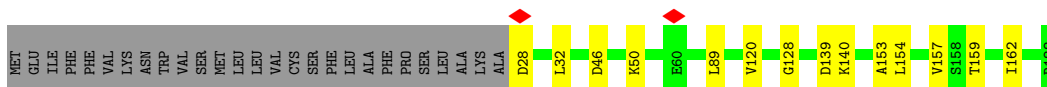
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  78% 14% 6%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  78% 7% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  81% 14% 6%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  88% 12%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L:  90% 8% ..

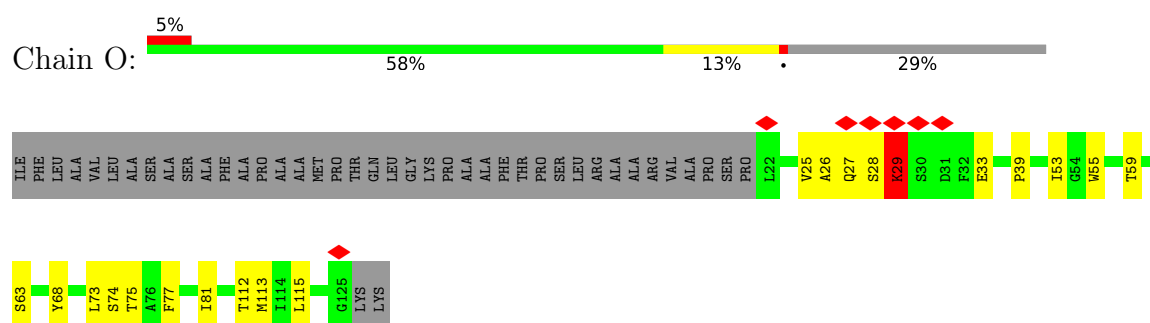


- Molecule 10: Photosystem I reaction center subunit XII

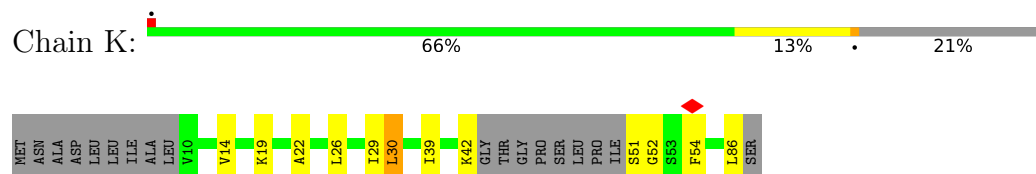
Chain M:  87% 13%



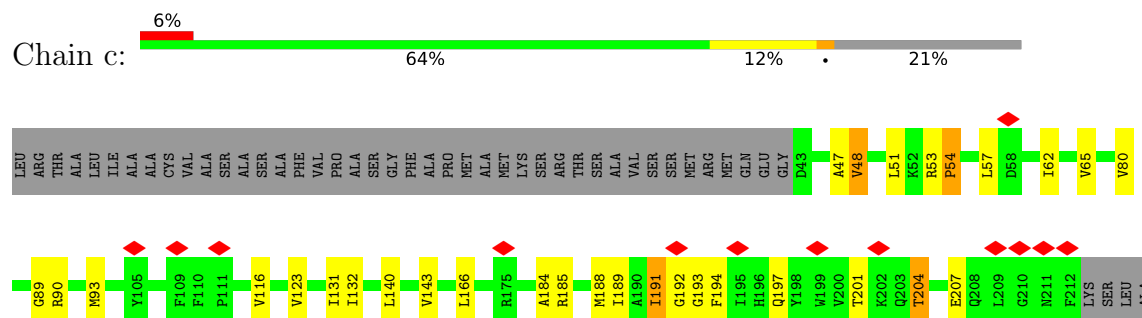
- Molecule 11: PsaO



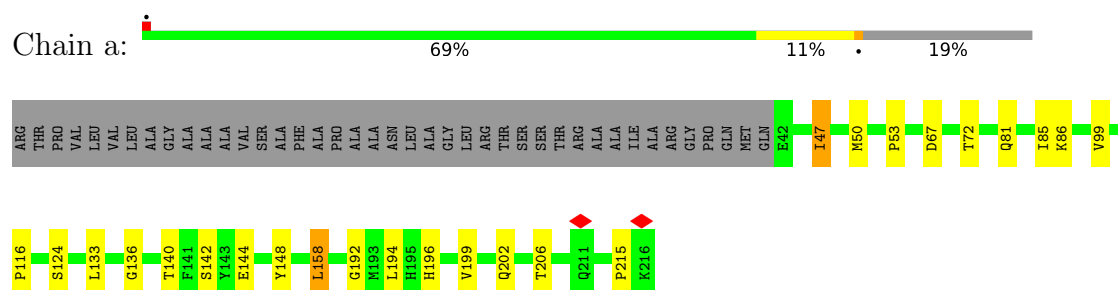
• Molecule 12: Photosystem I reaction center subunit PsaK



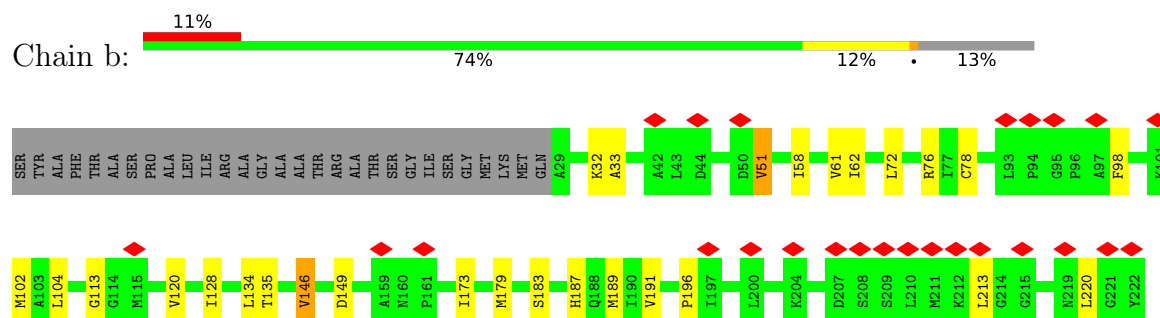
• Molecule 13: CAC-c



• Molecule 14: CAC-a

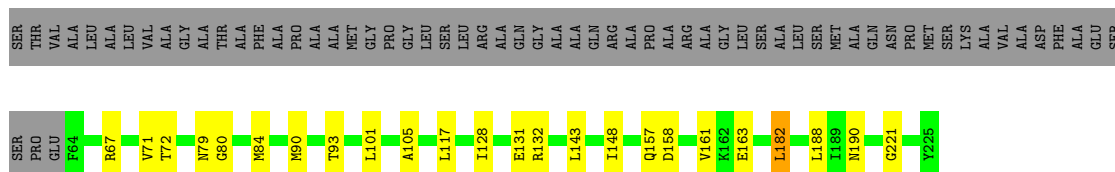


• Molecule 15: CAC-b



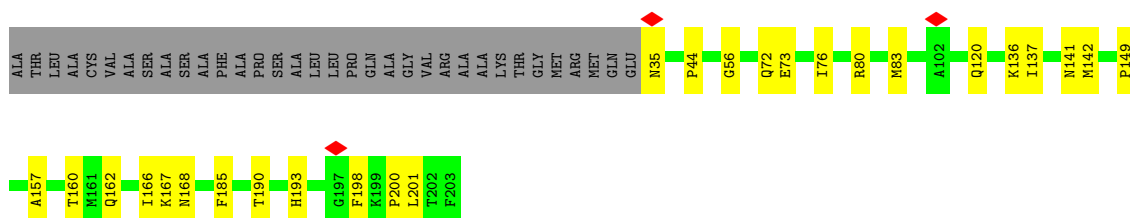
• Molecule 16: CAC-h

Chain h:  61% 10% 28%



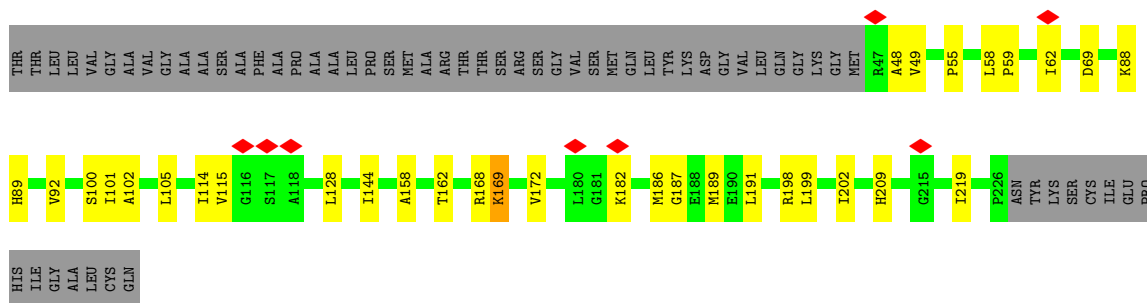
• Molecule 17: CAC-e

Chain e:  70% 13% 17%



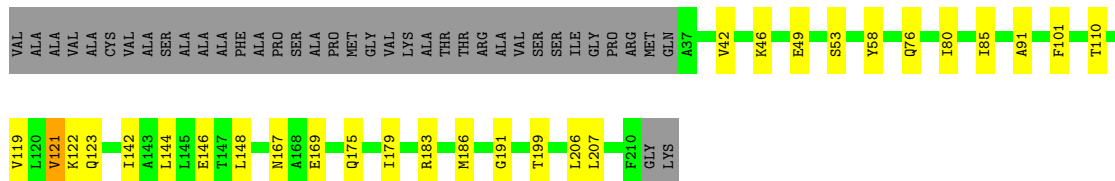
• Molecule 18: CAC-k

Chain k:  61% 13% 25%



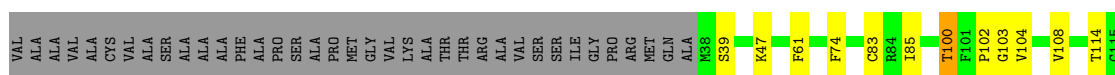
• Molecule 19: CAC-f

Chain f:  68% 13% 18%



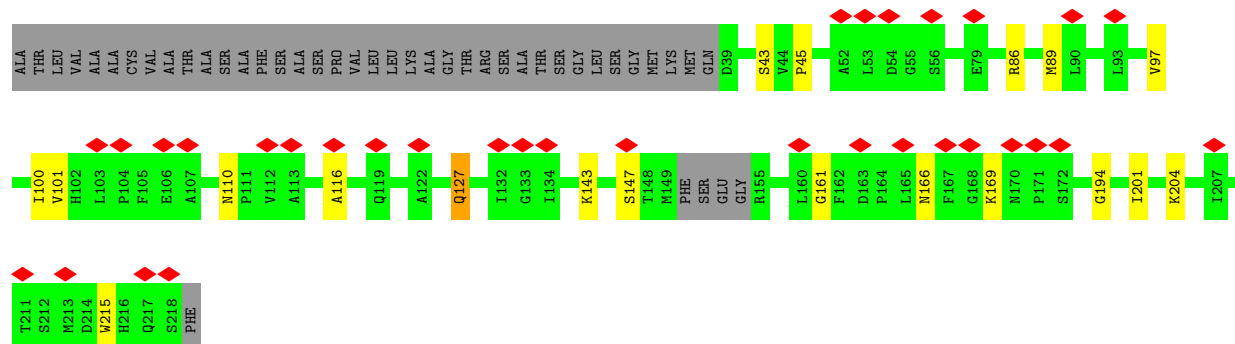
• Molecule 19: CAC-f

Chain j:  67% 14% 19%

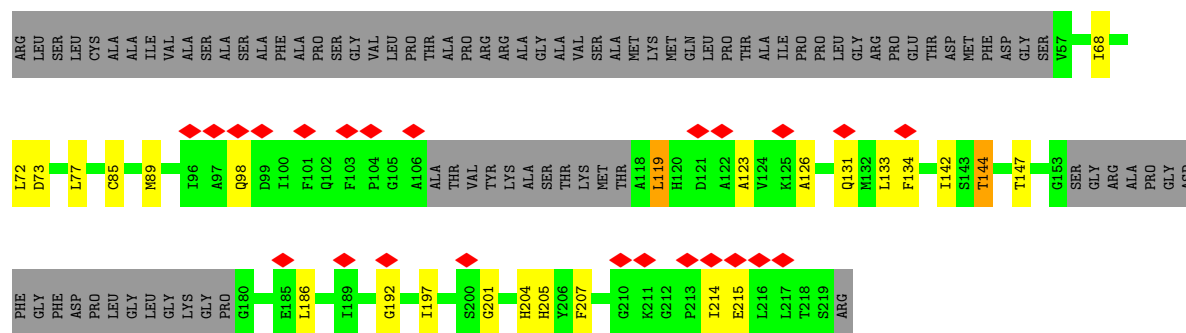




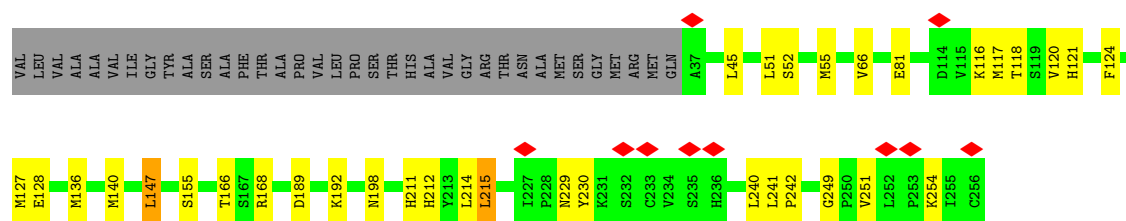
• Molecule 20: CAC-i



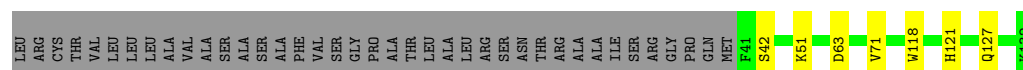
• Molecule 21: CAC-d



• Molecule 22: CAC-g



• Molecule 23: Psar



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31215	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	332.8131, 332.8131, 332.8131	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.040041, 1.040041, 1.040041	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, DGD, PQN, CLA, SF4, II0, IHT, LMU, LHG, KC2, WVN, LMT

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	0.48	0/6019	0.57	0/8204
2	B	0.48	0/6045	0.60	1/8254 (0.0%)
3	C	0.42	0/601	0.61	0/813
4	D	0.40	0/1109	0.57	0/1500
5	E	0.45	0/493	0.60	0/667
6	F	0.44	0/1287	0.57	0/1747
7	I	0.43	0/271	0.57	0/370
8	J	0.43	0/364	0.63	0/495
9	L	0.48	0/1175	0.69	0/1599
10	M	0.35	0/233	0.60	0/315
11	O	0.66	0/799	0.88	0/1094
12	K	0.36	0/495	0.59	0/672
13	c	0.39	0/1396	0.72	3/1889 (0.2%)
14	a	0.35	0/1406	0.59	0/1903
15	b	0.38	0/1469	0.66	0/1983
16	h	0.41	0/1226	0.65	2/1667 (0.1%)
17	e	0.38	0/1324	0.66	0/1795
18	k	0.48	0/1380	0.78	0/1869
19	f	0.55	0/1328	0.81	5/1790 (0.3%)
19	j	0.41	0/1318	0.71	0/1775
20	i	0.35	0/1359	0.74	2/1835 (0.1%)
21	d	0.60	0/969	0.87	0/1304
22	g	0.41	0/1673	0.73	4/2264 (0.2%)
23	R	0.36	0/686	0.50	0/940
All	All	0.45	0/34425	0.66	17/46744 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c	192	GLY	N-CA-C	-6.48	107.37	115.08
20	i	194	GLY	CA-C-N	5.92	128.50	120.44
20	i	194	GLY	C-N-CA	5.92	128.50	120.44
13	c	54	PRO	CA-C-N	5.58	132.20	121.54
13	c	54	PRO	C-N-CA	5.58	132.20	121.54
19	f	191	GLY	CA-C-N	5.43	127.83	120.44
19	f	191	GLY	C-N-CA	5.43	127.83	120.44
22	g	52	SER	CA-C-N	5.40	131.85	121.54
22	g	52	SER	C-N-CA	5.40	131.85	121.54
16	h	163	GLU	CA-C-N	5.22	131.51	121.54
16	h	163	GLU	C-N-CA	5.22	131.51	121.54
2	B	667	ARG	N-CA-C	5.21	116.95	111.28
19	f	121	VAL	N-CA-C	-5.20	105.46	110.72
22	g	229	ASN	CA-C-N	5.11	131.31	121.54
22	g	229	ASN	C-N-CA	5.11	131.31	121.54
19	f	167	ASN	CA-C-N	5.09	131.27	121.54
19	f	167	ASN	C-N-CA	5.09	131.27	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5678	67	0
2	B	5826	0	5642	68	0
3	C	592	0	574	10	0
4	D	1084	0	1080	11	0
5	E	485	0	489	6	0
6	F	1254	0	1264	11	0
7	I	264	0	276	4	0
8	J	351	0	344	4	0
9	L	1146	0	1160	12	0
10	M	232	0	265	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	O	773	0	763	19	0
12	K	488	0	516	8	0
13	c	1357	0	1337	21	0
14	a	1361	0	1305	16	0
15	b	1439	0	1456	23	0
16	h	1200	0	1228	13	0
17	e	1286	0	1262	18	0
18	k	1346	0	1349	22	0
19	f	1302	0	1320	11	0
19	j	1293	0	1321	20	0
20	i	1324	0	1298	9	0
21	d	950	0	949	18	0
22	g	1630	0	1644	21	0
23	R	664	0	647	4	0
24	A	2758	0	2820	94	0
24	B	2403	0	2442	70	0
24	F	117	0	115	9	0
24	I	65	0	72	2	0
24	J	93	0	72	3	0
24	K	93	0	72	1	0
24	L	215	0	191	7	0
24	O	130	0	144	9	0
24	R	51	0	41	0	0
24	a	601	0	551	11	0
24	b	673	0	696	33	0
24	c	586	0	520	17	0
24	d	498	0	407	6	0
24	e	582	0	578	20	0
24	f	700	0	695	23	0
24	g	661	0	611	15	0
24	h	440	0	398	3	0
24	i	528	0	451	7	0
24	j	637	0	556	9	0
24	k	596	0	534	18	0
25	A	33	0	46	2	0
25	B	33	0	46	5	0
26	A	75	0	93	1	0
26	B	38	0	49	3	0
26	J	49	0	74	8	0
26	a	49	0	74	0	0
26	b	98	0	148	7	0
26	c	74	0	88	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d	37	0	44	0	0
26	e	37	0	44	2	0
26	f	86	0	118	6	0
26	g	86	0	118	1	0
26	i	37	0	44	0	0
26	j	30	0	30	0	0
26	k	37	0	44	0	0
27	A	200	0	0	0	0
27	B	200	0	0	0	0
27	F	80	0	0	0	0
27	I	40	0	0	0	0
27	J	80	0	0	0	0
27	K	40	0	0	0	0
27	L	120	0	0	0	0
27	M	40	0	0	0	0
27	R	80	0	0	0	0
27	e	40	0	0	0	0
27	h	40	0	0	0	0
27	j	40	0	0	0	0
28	A	35	0	42	1	0
28	F	24	0	33	0	0
28	a	35	0	45	2	0
28	b	24	0	34	2	0
29	A	8	0	0	4	0
29	C	16	0	0	5	0
30	B	60	0	81	3	0
31	B	35	0	46	1	0
32	F	48	0	69	2	0
32	J	55	0	86	6	0
32	L	55	0	86	3	0
32	O	26	0	22	0	0
32	b	55	0	86	6	0
33	J	42	0	0	0	0
33	O	42	0	0	0	0
33	a	168	0	0	1	0
33	b	126	0	0	1	0
33	c	126	0	0	0	0
33	d	126	0	0	0	0
33	e	168	0	0	0	0
33	f	168	0	0	0	0
33	g	168	0	0	0	0
33	h	112	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	i	126	0	0	0	0
33	j	126	0	0	0	0
33	k	210	0	0	2	0
34	O	41	0	0	0	0
34	R	41	0	0	0	0
34	a	41	0	0	0	0
34	b	82	0	0	0	0
34	c	41	0	0	0	0
34	f	41	0	0	0	0
34	g	41	0	0	1	0
34	j	41	0	0	1	0
34	k	41	0	0	2	0
35	c	45	0	0	0	0
35	d	90	0	0	1	0
35	e	45	0	0	2	0
35	f	45	0	0	0	0
35	g	135	0	0	2	0
35	i	90	0	0	0	0
35	j	45	0	0	0	0
35	k	135	0	0	0	0
36	A	50	0	0	0	0
36	B	59	0	0	1	0
36	C	7	0	0	0	0
36	D	1	0	0	0	0
36	F	3	0	0	0	0
36	I	1	0	0	0	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	1	0
36	e	4	0	0	0	0
36	h	1	0	0	0	0
All	All	51054	0	46823	644	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 7.

All (644) 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)
1:A:586:CYS:HG	29:A:854:SF4:FE2	0.77	0.96
3:C:11:CYS:HG	29:C:102:SF4:FE4	0.66	0.95
3:C:48:CYS:HG	29:C:101:SF4:FE4	0.73	0.94
2:B:438:HIS:HE1	24:B:829:CLA:NA	1.62	0.92
29:A:854:SF4:FE1	2:B:567:CYS:HG	0.68	0.92
3:C:21:CYS:HG	29:C:101:SF4:FE2	0.66	0.90
24:A:822:CLA:HBB2	24:A:836:CLA:H18	1.58	0.86
2:B:339:SER:HB3	24:B:822:CLA:H42	1.57	0.86
24:c:612:CLA:H18	21:d:134:PHE:HA	1.58	0.85
2:B:438:HIS:CE1	24:B:829:CLA:NA	2.46	0.82
11:O:29:LYS:C	11:O:29:LYS:HE2	2.05	0.81
17:e:120:GLN:OE1	24:e:605:CLA:ND	2.18	0.77
24:A:814:CLA:H12	24:A:814:CLA:HBD	1.65	0.76
13:c:194:PHE:HA	13:c:197:GLN:HB2	1.68	0.75
20:i:143:LYS:HD2	20:i:147:SER:HB3	1.68	0.74
6:F:120:VAL:HG13	24:F:201:CLA:HAA1	1.69	0.73
13:c:54:PRO:HG2	13:c:57:LEU:HD22	1.70	0.73
3:C:14:CYS:SG	29:C:102:SF4:FE3	1.82	0.72
1:A:205:SER:HB3	24:A:819:CLA:HBC3	1.73	0.70
24:B:835:CLA:HAB	25:B:842:PQN:H162	1.71	0.70
26:b:302:LHG:H362	26:b:302:LHG:H191	1.74	0.69
1:A:586:CYS:SG	29:A:854:SF4:FE2	1.84	0.69
16:h:67:ARG:HB3	16:h:161:VAL:HG13	1.75	0.69
32:J:106:LMG:H332	15:b:62:ILE:HD11	1.74	0.69
21:d:73:ASP:O	21:d:77:LEU:HG	1.94	0.67
1:A:513:GLY:HA2	1:A:527:PRO:HB3	1.76	0.67
24:A:809:CLA:H2	24:A:811:CLA:HBC2	1.77	0.67
15:b:76:ARG:HB3	24:b:309:CLA:HBC3	1.77	0.67
11:O:55:TRP:HB2	11:O:112:THR:HG21	1.75	0.67
21:d:72:LEU:HD23	21:d:77:LEU:HD21	1.75	0.66
26:J:107:LHG:H331	15:b:120:VAL:HG21	1.76	0.66
11:O:75:THR:HG22	26:f:620:LHG:H241	1.76	0.66
32:J:106:LMG:H311	15:b:61:VAL:HG11	1.77	0.66
24:c:612:CLA:H203	21:d:133:LEU:HG	1.77	0.66
18:k:69:ASP:OD1	33:k:616:II0:O01	2.14	0.66
21:d:126:ALA:HB1	24:d:304:CLA:HBC1	1.78	0.66
18:k:199:LEU:HD12	18:k:202:ILE:HD11	1.78	0.65
21:d:204:HIS:HA	21:d:207:PHE:HD2	1.61	0.65
24:a:308:CLA:H101	24:a:310:CLA:HMA3	1.79	0.65
20:i:97:VAL:HA	20:i:100:ILE:HG12	1.79	0.64
4:D:42:VAL:HG22	4:D:52:ILE:HG12	1.80	0.64
18:k:198:ARG:HB3	24:k:602:CLA:HBC3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:852:CLA:H91	24:B:804:CLA:H101	1.80	0.63
4:D:135:THR:HG22	4:D:137:LYS:H	1.64	0.63
12:K:52:GLY:HA3	17:e:137:ILE:HG12	1.81	0.63
6:F:159:THR:HG22	15:b:135:THR:HB	1.81	0.62
24:F:201:CLA:H102	24:b:308:CLA:HBB1	1.80	0.62
15:b:189:MET:HE2	15:b:196:PRO:HD3	1.81	0.62
1:A:736:LEU:HD11	24:A:829:CLA:H18	1.82	0.62
18:k:58:LEU:HD21	24:k:602:CLA:HAA2	1.81	0.62
22:g:249:GLY:HA2	22:g:254:LYS:HB2	1.80	0.62
24:f:603:CLA:HAC2	26:f:620:LHG:H341	1.80	0.62
22:g:121:HIS:HD2	22:g:140:MET:HE2	1.65	0.61
17:e:120:GLN:OE1	24:e:605:CLA:C4D	2.48	0.61
24:A:839:CLA:HHC	24:A:839:CLA:HBB1	1.80	0.61
24:A:856:CLA:HMA1	32:b:301:LMG:HC92	1.82	0.61
26:b:302:LHG:H341	26:b:302:LHG:H212	1.83	0.61
22:g:211:HIS:HA	22:g:214:LEU:HD12	1.83	0.61
13:c:204:THR:HG22	13:c:207:GLU:H	1.65	0.60
23:R:51:LYS:HD2	23:R:63:ASP:HB3	1.83	0.60
4:D:64:ARG:NH2	4:D:66:GLU:OE1	2.34	0.60
4:D:25:ALA:HB1	4:D:30:LYS:HG3	1.82	0.60
13:c:89:GLY:HA3	13:c:184:ALA:HB1	1.84	0.60
8:J:41:PRO:HG2	24:J:105:CLA:HMD3	1.84	0.59
15:b:102:MET:HE2	15:b:104:LEU:HB2	1.84	0.59
2:B:398:ASP:O	2:B:402:ASN:ND2	2.31	0.59
24:B:807:CLA:H12	7:I:14:ILE:HG13	1.84	0.59
1:A:503:ASN:HB2	24:A:839:CLA:HED2	1.84	0.59
4:D:121:HIS:HB2	4:D:125:LYS:HD2	1.84	0.59
12:K:51:SER:HB3	12:K:54:PHE:HB3	1.83	0.59
21:d:201:GLY:O	21:d:205:HIS:ND1	2.35	0.59
15:b:33:ALA:HB2	15:b:51:VAL:HG13	1.84	0.59
6:F:32:LEU:HB2	6:F:89:LEU:HD23	1.85	0.58
12:K:26:LEU:HD11	24:e:606:CLA:H101	1.85	0.58
14:a:199:VAL:HG21	24:a:311:CLA:HAC1	1.84	0.58
17:e:35:ASN:HB3	17:e:56:GLY:HA3	1.85	0.58
17:e:35:ASN:HB2	17:e:44:PRO:HD2	1.85	0.58
2:B:204:GLN:NE2	2:B:205:HIS:O	2.37	0.58
2:B:461:TRP:HE1	2:B:475:VAL:HG21	1.69	0.58
24:b:313:CLA:H2	24:b:313:CLA:H102	1.86	0.58
20:i:110:ASN:HB3	20:i:116:ALA:HB2	1.86	0.58
2:B:475:VAL:HG12	2:B:476:LEU:HD22	1.86	0.58
24:A:831:CLA:HBA1	24:A:855:CLA:H42	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:189:ILE:HD11	24:c:602:CLA:HAC2	1.86	0.57
26:c:618:LHG:H252	24:b:312:CLA:H203	1.85	0.57
21:d:85:CYS:HB3	21:d:192:GLY:HA3	1.87	0.57
24:k:608:CLA:H2A	24:k:608:CLA:HED2	1.86	0.57
19:j:83:CYS:HB3	19:j:182:GLY:HA3	1.87	0.57
19:j:198:ILE:HG22	19:j:199:THR:HG23	1.87	0.57
1:A:284:LEU:HD21	1:A:377:PRO:HD2	1.87	0.56
11:O:59:THR:HG23	11:O:73:LEU:HB3	1.88	0.56
2:B:493:LEU:HD22	2:B:497:LEU:HG	1.88	0.56
24:B:810:CLA:HBA2	31:B:844:LMU:H41	1.88	0.56
24:A:853:CLA:HAA2	24:B:828:CLA:HMB1	1.87	0.56
26:J:107:LHG:H381	15:b:113:GLY:HA2	1.88	0.56
1:A:56:VAL:HG21	24:A:803:CLA:C2D	2.35	0.56
2:B:474:ASP:O	2:B:479:SER:HB2	2.05	0.56
20:i:86:ARG:HA	20:i:89:MET:HE3	1.87	0.56
24:b:307:CLA:C4D	36:b:401:HOH:O	2.49	0.55
18:k:186:MET:HG2	18:k:187:GLY:H	1.72	0.55
32:J:106:LMG:H312	28:b:319:LMT:H41	1.87	0.55
18:k:182:LYS:HA	18:k:186:MET:HG3	1.88	0.55
1:A:535:PHE:HA	24:A:835:CLA:HED1	1.86	0.55
1:A:372:HIS:ND1	24:A:817:CLA:OBD	2.37	0.55
16:h:221:GLY:HA3	24:h:307:CLA:HMA3	1.89	0.55
2:B:100:VAL:O	2:B:104:THR:OG1	2.24	0.55
12:K:22:ALA:HB1	24:e:611:CLA:H13	1.89	0.55
24:B:801:CLA:O1A	24:B:801:CLA:H3A	2.06	0.55
17:e:168:ASN:HD21	35:e:609:KC2:C1A	2.20	0.55
22:g:51:LEU:HD22	22:g:55:MET:HE1	1.89	0.55
2:B:236:PRO:HB3	2:B:255:THR:HG21	1.89	0.55
2:B:300:LEU:HD13	24:B:822:CLA:HAC2	1.89	0.54
19:j:120:LEU:HB3	19:j:125:ALA:HB3	1.90	0.54
1:A:15:ILE:HD13	24:A:809:CLA:HAA2	1.89	0.54
24:A:827:CLA:H92	26:B:802:LHG:H223	1.88	0.54
19:j:61:PHE:HE1	24:j:302:CLA:HBC3	1.72	0.54
24:c:606:CLA:HHC	24:c:606:CLA:HBB1	1.89	0.54
17:e:73:GLU:HB2	17:e:149:PRO:HB3	1.90	0.54
22:g:66:VAL:HG11	24:g:303:CLA:H2	1.90	0.54
24:O:201:CLA:H42	24:O:201:CLA:HBB	1.88	0.54
20:i:127:GLN:NE2	24:i:605:CLA:NB	2.56	0.54
1:A:153:ILE:HD13	24:A:813:CLA:HED3	1.90	0.54
16:h:128:ILE:HD11	16:h:132:ARG:HG2	1.91	0.53
24:A:856:CLA:NA	26:b:320:LHG:O4	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:839:CLA:HBB1	24:B:839:CLA:HHC	1.90	0.53
11:O:59:THR:CG2	11:O:73:LEU:HB3	2.39	0.53
24:B:811:CLA:HHC	24:B:811:CLA:HBB1	1.90	0.53
1:A:262:GLY:HA3	24:A:814:CLA:H42	1.89	0.53
24:A:802:CLA:H12	2:B:429:GLY:HA3	1.89	0.53
2:B:207:CYS:SG	2:B:208:TRP:N	2.80	0.53
15:b:102:MET:HE3	15:b:189:MET:HB3	1.91	0.53
19:j:175:GLN:O	19:j:179:ILE:HG12	2.09	0.53
3:C:21:CYS:SG	29:C:101:SF4:FE2	1.83	0.52
24:O:201:CLA:H202	24:O:201:CLA:HBB2	1.92	0.52
18:k:114:ILE:HG23	18:k:115:VAL:HG23	1.92	0.52
19:j:126:MET:HE3	24:j:308:CLA:HBC3	1.91	0.52
21:d:89:MET:HG3	21:d:192:GLY:HA2	1.92	0.52
1:A:32:PRO:HB3	24:A:842:CLA:HAC1	1.91	0.52
32:L:208:LMG:H291	24:g:308:CLA:H2	1.91	0.52
9:L:44:LEU:HD21	24:g:309:CLA:H202	1.92	0.52
13:c:193:GLY:HA2	24:c:611:CLA:C1C	2.39	0.52
22:g:127:MET:HE3	22:g:136:MET:HG3	1.90	0.52
1:A:161:TRP:CE2	24:A:815:CLA:HAA2	2.44	0.52
1:A:243:HIS:HB2	24:A:815:CLA:HBC3	1.91	0.52
1:A:482:LYS:HE3	1:A:487:GLN:HE22	1.74	0.52
24:A:840:CLA:H2	24:L:203:CLA:H43	1.92	0.52
24:B:823:CLA:H52	24:B:841:CLA:H201	1.91	0.52
14:a:192:GLY:O	14:a:196:HIS:ND1	2.43	0.52
24:A:814:CLA:HBA2	24:d:306:CLA:HMA2	1.91	0.52
13:c:166:LEU:HD13	24:c:608:CLA:H42	1.92	0.52
1:A:218:HIS:HB2	24:A:813:CLA:C1C	2.40	0.52
2:B:343:ILE:HG12	24:B:822:CLA:H43	1.91	0.52
24:f:608:CLA:H92	24:f:608:CLA:HAA1	1.92	0.51
2:B:298:HIS:HB3	2:B:303:ILE:HD11	1.93	0.51
17:e:200:PRO:HA	24:e:610:CLA:HED2	1.92	0.51
19:j:103:GLY:HA3	24:j:306:CLA:C1A	2.40	0.51
24:g:310:CLA:CGA	24:g:310:CLA:H3A	2.41	0.51
24:k:609:CLA:HAB	33:k:615:II0:C33	2.39	0.51
6:F:28:ASP:N	6:F:32:LEU:O	2.44	0.51
2:B:373:HIS:CE1	24:B:825:CLA:ND	2.79	0.51
17:e:185:PHE:HD2	17:e:201:LEU:HB3	1.76	0.51
24:A:818:CLA:H92	24:A:828:CLA:H91	1.93	0.51
2:B:193:LEU:HA	2:B:197:ALA:HB3	1.92	0.51
12:K:30:LEU:HD21	24:e:606:CLA:H152	1.93	0.51
28:A:851:LMT:O2B	28:A:851:LMT:O6'	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:201:CLA:H72	24:b:308:CLA:H11	1.91	0.50
24:O:205:CLA:HBA1	24:O:205:CLA:HBD	1.92	0.50
13:c:132:ILE:HG12	24:c:606:CLA:HAC1	1.92	0.50
21:d:205:HIS:NE2	35:d:311:KC2:NA	2.59	0.50
24:F:201:CLA:HBC2	8:J:20:LEU:HD11	1.93	0.50
19:j:74:PHE:HB2	19:j:148:LEU:HD21	1.93	0.50
2:B:525:ALA:HB1	2:B:585:THR:HB	1.93	0.50
15:b:32:LYS:HB3	24:b:303:CLA:HED1	1.93	0.50
18:k:88:LYS:O	18:k:92:VAL:HG23	2.12	0.50
5:E:34:TYR:HA	5:E:53:PHE:O	2.11	0.50
17:e:162:GLN:O	17:e:166:ILE:HG12	2.12	0.50
18:k:186:MET:HE2	18:k:189:MET:HB2	1.93	0.50
2:B:573:ASP:OD2	36:B:901:HOH:O	2.20	0.49
7:I:19:PRO:HA	7:I:22:VAL:HG22	1.94	0.49
19:j:102:PRO:HD2	24:j:306:CLA:HBC3	1.94	0.49
2:B:340:LEU:O	2:B:344:THR:HG22	2.12	0.49
11:O:28:SER:O	11:O:28:SER:OG	2.23	0.49
19:f:183:ARG:HA	19:f:186:MET:HE3	1.93	0.49
11:O:59:THR:HG22	11:O:74:SER:H	1.77	0.49
24:B:805:CLA:H93	24:B:812:CLA:H2	1.93	0.49
12:K:26:LEU:HB2	24:e:611:CLA:H141	1.95	0.49
18:k:144:ILE:HB	24:k:607:CLA:HBC1	1.93	0.49
24:k:603:CLA:HBC2	24:k:608:CLA:H171	1.95	0.49
24:A:811:CLA:HHC	24:A:811:CLA:HBB1	1.94	0.49
24:A:823:CLA:H2	24:A:836:CLA:H121	1.95	0.49
2:B:396:ASP:OD1	4:D:133:LYS:NZ	2.46	0.49
18:k:48:ALA:O	24:k:601:CLA:NA	2.46	0.49
24:B:816:CLA:H62	24:B:816:CLA:H102	1.61	0.49
15:b:187:HIS:NE2	24:b:313:CLA:NA	2.61	0.49
19:j:117:HIS:HD2	19:j:126:MET:HE2	1.78	0.49
21:d:98:GLN:HE22	21:d:119:LEU:HD22	1.76	0.49
24:B:815:CLA:C1D	24:B:816:CLA:HBB2	2.43	0.48
14:a:215:PRO:HD3	24:a:311:CLA:HMD3	1.94	0.48
18:k:102:ALA:HA	18:k:105:LEU:HG	1.94	0.48
5:E:11:LEU:HB2	5:E:57:GLU:HA	1.96	0.48
22:g:241:LEU:HD11	26:g:301:LHG:H141	1.94	0.48
2:B:168:LYS:NZ	23:R:42:SER:OG	2.40	0.48
2:B:394:VAL:HG23	2:B:540:ALA:HB1	1.96	0.48
24:e:611:CLA:HBA1	24:e:611:CLA:H12	1.53	0.48
1:A:625:GLN:HG2	1:A:629:THR:HG23	1.94	0.48
19:f:85:ILE:HD12	24:f:608:CLA:HMD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:OD2	1:A:71:ARG:NH2	2.35	0.48
1:A:579:GLY:HA2	2:B:561:PRO:HD3	1.95	0.48
24:A:836:CLA:C4D	24:O:205:CLA:H161	2.43	0.48
26:J:107:LHG:H383	28:a:318:LMT:H2'	1.96	0.48
26:f:619:LHG:H271	24:g:307:CLA:HBB2	1.96	0.48
1:A:589:SER:OG	1:A:592:ASP:OD2	2.31	0.48
24:B:835:CLA:H162	24:B:836:CLA:H111	1.95	0.48
23:R:118:TRP:CD1	23:R:121:HIS:HE1	2.31	0.48
29:A:854:SF4:FE1	2:B:567:CYS:SG	1.85	0.48
15:b:173:ILE:HG13	24:b:310:CLA:HED1	1.96	0.48
24:f:610:CLA:H112	24:f:610:CLA:H143	1.63	0.48
2:B:706:LEU:HD23	30:B:843:DGD:HA21	1.96	0.48
24:B:808:CLA:H62	24:B:808:CLA:H102	1.58	0.48
24:L:202:CLA:HHC	24:L:202:CLA:HBB1	1.96	0.48
16:h:80:GLY:O	16:h:84:MET:HG3	2.14	0.48
1:A:56:VAL:HG21	24:A:803:CLA:C3D	2.43	0.48
24:A:840:CLA:H61	24:A:840:CLA:H41	1.60	0.48
24:b:310:CLA:H162	24:b:310:CLA:H122	1.56	0.48
24:f:610:CLA:H41	24:f:610:CLA:H61	1.45	0.48
22:g:189:ASP:HA	22:g:192:LYS:HG2	1.96	0.48
1:A:63:THR:HG21	1:A:68:ASP:HB2	1.96	0.47
11:O:25:VAL:CG2	11:O:27:GLN:HG2	2.44	0.47
26:f:620:LHG:H281	26:f:620:LHG:H311	1.59	0.47
24:a:307:CLA:H151	24:a:307:CLA:H111	1.44	0.47
19:f:144:LEU:HD22	24:f:608:CLA:HMA2	1.96	0.47
22:g:118:THR:HB	34:g:319:IHT:C12	2.44	0.47
1:A:332:LYS:HB3	1:A:339:GLY:HA3	1.95	0.47
24:A:855:CLA:H101	24:A:855:CLA:H13	1.68	0.47
2:B:720:TYR:HB2	24:B:803:CLA:HED2	1.95	0.47
24:B:817:CLA:H3A	24:B:817:CLA:HBA2	1.72	0.47
3:C:15:THR:HG22	3:C:28:MET:HG3	1.96	0.47
8:J:23:THR:HA	8:J:26:PHE:CE2	2.49	0.47
32:b:301:LMG:H422	32:b:301:LMG:H391	1.63	0.47
24:g:304:CLA:HBA1	24:g:304:CLA:H3A	1.57	0.47
2:B:442:VAL:HG21	2:B:450:LYS:HB2	1.96	0.47
9:L:75:LEU:HA	9:L:75:LEU:HD23	1.70	0.47
13:c:47:ALA:HB2	13:c:65:VAL:HB	1.95	0.47
21:d:131:GLN:HG2	24:d:305:CLA:ND	2.30	0.47
2:B:620:ARG:HA	2:B:624:TRP:HB3	1.97	0.47
24:F:201:CLA:HED1	24:b:308:CLA:H43	1.96	0.47
24:a:303:CLA:H3A	24:a:303:CLA:HBA2	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TRP:HB3	24:A:804:CLA:HAC1	1.97	0.47
2:B:343:ILE:CG1	24:B:822:CLA:H43	2.44	0.47
24:B:801:CLA:H51	26:B:802:LHG:HC31	1.96	0.47
3:C:77:MET:HB3	3:C:79:LEU:HG	1.97	0.47
13:c:62:ILE:HD12	13:c:62:ILE:H	1.79	0.47
14:a:53:PRO:HG2	14:a:67:ASP:HB3	1.96	0.47
15:b:98:PHE:HD2	24:b:306:CLA:HBD	1.80	0.47
17:e:72:GLN:O	17:e:76:ILE:HG13	2.15	0.47
13:c:185:ARG:HB3	24:c:602:CLA:HBC2	1.97	0.47
1:A:225:PRO:HD3	1:A:252:MET:HE1	1.97	0.47
24:B:806:CLA:H151	24:B:826:CLA:HBB2	1.96	0.47
19:f:76:GLN:O	19:f:80:ILE:HG13	2.15	0.47
23:R:71:VAL:O	23:R:127:GLN:NE2	2.38	0.47
26:J:107:LHG:H141	26:J:107:LHG:H171	1.65	0.46
24:f:602:CLA:HBA2	24:f:602:CLA:H3A	1.46	0.46
24:j:311:CLA:H152	24:j:311:CLA:H112	1.55	0.46
1:A:322:HIS:CE1	24:A:821:CLA:NA	2.83	0.46
24:A:827:CLA:H111	24:A:829:CLA:H171	1.97	0.46
11:O:113:MET:SD	24:O:205:CLA:HAB	2.55	0.46
14:a:202:GLN:HB2	14:a:206:THR:HB	1.97	0.46
24:k:601:CLA:H3A	24:k:601:CLA:HBA2	1.71	0.46
1:A:563:ARG:NH2	4:D:18:THR:O	2.48	0.46
24:b:312:CLA:H152	24:b:312:CLA:H18	1.62	0.46
17:e:136:LYS:HD2	17:e:141:ASN:HB3	1.97	0.46
24:A:841:CLA:HAA1	24:A:842:CLA:H52	1.98	0.46
24:A:842:CLA:H141	24:A:842:CLA:H161	1.64	0.46
2:B:25:ALA:HB2	30:B:843:DGD:HA32	1.98	0.46
24:B:837:CLA:H52	24:B:837:CLA:H11	1.70	0.46
15:b:78:CYS:SG	15:b:179:MET:HG2	2.56	0.46
1:A:395:HIS:HE2	24:A:828:CLA:C1B	2.29	0.46
6:F:162:ILE:HD12	32:F:206:LMG:H111	1.97	0.46
24:L:203:CLA:H162	24:L:203:CLA:H121	1.73	0.46
15:b:58:ILE:HG21	24:b:304:CLA:H2	1.98	0.46
24:e:610:CLA:CAD	24:f:606:CLA:H3A	2.45	0.46
1:A:391:SER:HB3	24:A:827:CLA:HMA1	1.98	0.46
6:F:139:ASP:OD1	6:F:140:LYS:N	2.47	0.46
14:a:196:HIS:NE2	24:a:311:CLA:NC	2.63	0.46
24:A:837:CLA:HBA2	24:A:837:CLA:H3A	1.61	0.46
24:A:855:CLA:H192	9:L:58:LEU:HD21	1.97	0.46
6:F:46:ASP:O	6:F:50:LYS:HG2	2.16	0.46
19:j:100:THR:HG23	19:j:104:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ILE:HD13	24:A:853:CLA:HMD2	1.98	0.46
2:B:179:SER:HB3	2:B:287:GLY:HA3	1.97	0.46
24:B:836:CLA:H62	24:B:836:CLA:H41	1.51	0.46
24:c:603:CLA:H3A	24:c:603:CLA:HBA1	1.76	0.46
22:g:155:SER:HB2	24:g:309:CLA:HMA1	1.97	0.46
24:A:802:CLA:H111	24:A:802:CLA:H91	1.64	0.46
24:B:820:CLA:HBC2	24:B:821:CLA:HBA1	1.97	0.46
15:b:213:LEU:HB3	26:b:320:LHG:H241	1.97	0.46
24:b:307:CLA:H3A	24:b:307:CLA:HBA1	1.54	0.46
1:A:71:ARG:HG2	1:A:185:ALA:HB1	1.97	0.46
13:c:185:ARG:HA	13:c:188:MET:HE3	1.97	0.46
18:k:162:THR:HG22	18:k:168:ARG:HG3	1.98	0.46
18:k:209:HIS:HE1	34:k:618:IHT:C38	2.29	0.46
24:B:807:CLA:H93	24:B:807:CLA:H61	1.81	0.45
24:B:827:CLA:HAB	24:B:834:CLA:HBB2	1.98	0.45
11:O:26:ALA:O	19:f:148:LEU:HB3	2.16	0.45
24:e:601:CLA:H3A	24:e:601:CLA:HBA2	1.38	0.45
19:j:116:VAL:HG12	19:j:120:LEU:HD11	1.98	0.45
24:A:853:CLA:HBB2	6:F:128:GLY:HA3	1.98	0.45
11:O:29:LYS:HE2	11:O:29:LYS:CA	2.46	0.45
13:c:131:ILE:HD12	24:c:606:CLA:HBC1	1.97	0.45
22:g:240:LEU:O	22:g:242:PRO:HD3	2.16	0.45
24:A:840:CLA:H13	24:L:203:CLA:HAA2	1.99	0.45
24:b:305:CLA:H61	24:b:305:CLA:H41	1.58	0.45
17:e:168:ASN:HD21	35:e:609:KC2:C2A	2.28	0.45
24:f:602:CLA:H91	24:f:602:CLA:H111	1.78	0.45
1:A:709:LYS:HG2	24:B:828:CLA:HMA2	1.99	0.45
24:B:839:CLA:H141	24:B:839:CLA:H162	1.78	0.45
11:O:33:GLU:HA	11:O:39:PRO:HA	1.98	0.45
12:K:39:ILE:O	12:K:42:LYS:NZ	2.45	0.45
13:c:191:ILE:HD13	13:c:191:ILE:HA	1.72	0.45
2:B:181:LEU:O	2:B:185:SER:OG	2.32	0.45
24:B:817:CLA:H61	24:B:817:CLA:H102	1.84	0.45
24:J:105:CLA:NC	26:J:107:LHG:O4	2.50	0.45
26:b:320:LHG:H291	26:b:320:LHG:H262	1.86	0.45
19:j:114:THR:HB	34:j:317:IHT:C05	2.46	0.45
1:A:222:VAL:HG13	1:A:242:PRO:HB3	1.99	0.45
1:A:291:LEU:HD13	24:A:817:CLA:HMA2	1.97	0.45
1:A:328:LEU:O	1:A:340:HIS:HB2	2.17	0.45
24:A:839:CLA:H91	24:A:839:CLA:H111	1.74	0.45
2:B:431:HIS:O	2:B:435:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:202:CLA:HBA1	24:F:202:CLA:H3A	1.37	0.45
13:c:48:VAL:HG11	13:c:51:LEU:HD12	1.99	0.45
22:g:128:GLU:HG2	22:g:136:MET:C	2.42	0.45
1:A:660:VAL:HG11	1:A:745:PHE:HA	1.99	0.45
24:A:801:CLA:HED3	24:A:801:CLA:HBD	1.71	0.45
24:B:820:CLA:H92	24:B:820:CLA:H61	1.81	0.45
5:E:2:VAL:HG12	5:E:60:GLU:HG3	1.97	0.45
13:c:123:VAL:HG22	24:c:606:CLA:C2D	2.46	0.45
16:h:157:GLN:HG2	16:h:158:ASP:O	2.17	0.45
24:i:601:CLA:HBA2	24:i:601:CLA:H3A	1.46	0.45
1:A:446:ILE:HD13	1:A:446:ILE:HA	1.86	0.45
24:A:838:CLA:H62	24:A:838:CLA:H41	1.81	0.45
2:B:21:TRP:CG	2:B:703:GLN:HE22	2.35	0.45
32:b:301:LMG:H261	28:b:319:LMT:H102	1.98	0.45
24:f:607:CLA:H3A	24:f:607:CLA:HBA2	1.48	0.45
24:B:814:CLA:H91	24:B:814:CLA:H112	1.72	0.45
24:K:101:CLA:H12	24:K:101:CLA:H51	1.68	0.45
15:b:146:VAL:HG12	15:b:149:ASP:HB2	1.99	0.45
15:b:183:SER:HB3	24:b:312:CLA:HBC2	1.99	0.45
24:f:602:CLA:H41	24:f:602:CLA:H62	1.68	0.45
24:g:322:CLA:H142	24:g:322:CLA:H112	1.77	0.45
24:A:842:CLA:H143	24:A:842:CLA:H91	1.99	0.45
25:A:843:PQN:H302	25:A:843:PQN:H261	1.72	0.45
24:F:201:CLA:H192	33:b:315:II0:O01	2.17	0.45
24:b:304:CLA:HBA2	24:b:304:CLA:H3A	1.37	0.45
1:A:39:LEU:HD13	1:A:52:LEU:HA	1.99	0.44
2:B:30:LEU:HB3	2:B:36:MET:HE3	1.99	0.44
32:J:106:LMG:H452	32:J:106:LMG:H421	1.76	0.44
16:h:182:LEU:HG	24:h:305:CLA:HHB	1.98	0.44
1:A:482:LYS:HA	1:A:482:LYS:HD2	1.71	0.44
24:A:806:CLA:H18	32:J:106:LMG:H211	1.98	0.44
24:A:856:CLA:HHB	32:b:301:LMG:HC92	2.00	0.44
2:B:573:ASP:OD1	2:B:705:ARG:NH1	2.50	0.44
24:e:604:CLA:H161	24:e:604:CLA:H122	1.69	0.44
24:f:607:CLA:H143	24:f:607:CLA:H111	1.82	0.44
1:A:63:THR:HG22	1:A:65:SER:H	1.82	0.44
24:A:805:CLA:H112	24:A:805:CLA:H152	1.80	0.44
1:A:373:MET:HE3	24:A:818:CLA:HBA1	2.00	0.44
1:A:582:ARG:HG2	3:C:78:GLY:HA3	1.99	0.44
24:A:820:CLA:H152	24:A:820:CLA:H111	1.79	0.44
2:B:25:ALA:HB2	30:B:843:DGD:HA62	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:I:102:CLA:H51	16:h:117:LEU:HD13	1.99	0.44
24:k:610:CLA:HBA2	24:k:610:CLA:H12	1.61	0.44
1:A:50:TRP:HE1	24:A:841:CLA:HBB1	1.82	0.44
24:A:820:CLA:H2	24:A:820:CLA:H62	1.72	0.44
24:B:835:CLA:H162	24:B:835:CLA:H121	1.61	0.44
24:b:307:CLA:H93	24:b:307:CLA:H61	1.79	0.44
24:f:602:CLA:H62	24:f:602:CLA:H101	1.64	0.44
24:g:308:CLA:H3A	24:g:308:CLA:HBA1	1.80	0.44
24:A:818:CLA:H3A	24:A:818:CLA:HBA2	1.69	0.44
24:B:823:CLA:H112	24:B:841:CLA:H191	1.99	0.44
11:O:53:ILE:HG13	24:f:608:CLA:HMB2	1.99	0.44
24:i:606:CLA:H13	24:i:606:CLA:H102	1.79	0.44
24:A:806:CLA:HED1	15:b:220:LEU:HD22	1.99	0.44
2:B:373:HIS:HE1	24:B:825:CLA:ND	2.16	0.44
3:C:62:PHE:HD2	4:D:123:ILE:HG21	1.83	0.44
14:a:158:LEU:HD13	14:a:158:LEU:HA	1.87	0.44
26:e:617:LHG:H292	26:e:617:LHG:H261	1.75	0.44
19:f:142:ILE:O	19:f:146:GLU:HG2	2.18	0.44
19:j:191:GLY:HA2	24:j:313:CLA:NC	2.33	0.44
24:d:301:CLA:HBA2	24:d:301:CLA:H3A	1.34	0.44
24:g:303:CLA:HBA2	24:g:303:CLA:H3A	1.82	0.44
24:g:308:CLA:H151	24:g:322:CLA:HBC3	1.99	0.44
24:A:824:CLA:H13	24:A:824:CLA:H172	1.72	0.44
14:a:116:PRO:O	33:a:314:II0:O02	2.36	0.44
24:i:610:CLA:H3A	24:i:610:CLA:HBA2	1.59	0.44
24:B:801:CLA:H61	24:B:801:CLA:H41	1.58	0.44
5:E:34:TYR:CA	5:E:53:PHE:O	2.66	0.44
9:L:137:LEU:HD11	24:g:308:CLA:H42	2.00	0.44
24:e:607:CLA:H92	24:e:607:CLA:H61	1.84	0.44
24:A:835:CLA:H62	24:A:835:CLA:H41	1.90	0.43
24:B:832:CLA:H51	24:B:832:CLA:H11	1.72	0.43
18:k:115:VAL:HG11	24:k:604:CLA:HED2	2.00	0.43
24:k:610:CLA:O2D	24:k:610:CLA:H2A	2.18	0.43
19:j:144:LEU:HD22	24:j:309:CLA:HMA2	1.99	0.43
24:A:817:CLA:H3A	24:A:817:CLA:HBA2	1.59	0.43
2:B:47:ALA:HB3	10:M:28:LEU:HD21	2.00	0.43
24:B:801:CLA:H51	24:B:801:CLA:H12	1.84	0.43
24:b:308:CLA:H112	24:b:308:CLA:H91	1.78	0.43
24:b:308:CLA:H143	24:b:313:CLA:HAB	1.99	0.43
24:e:602:CLA:HBA2	24:e:602:CLA:H3A	1.56	0.43
24:e:607:CLA:H3A	24:e:607:CLA:HBA2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:91:ALA:HB1	24:f:609:CLA:H172	2.00	0.43
20:i:201:ILE:HD11	24:i:611:CLA:HED3	1.99	0.43
19:j:85:ILE:HD13	24:j:309:CLA:HBC3	2.00	0.43
3:C:24:ASP:OD1	4:D:106:PRO:HG3	2.19	0.43
13:c:143:VAL:HG22	24:c:607:CLA:HMA1	1.98	0.43
26:e:617:LHG:H271	24:f:606:CLA:HBB2	2.00	0.43
21:d:201:GLY:C	21:d:205:HIS:HD1	2.26	0.43
24:A:804:CLA:HBA1	24:A:804:CLA:H3A	1.64	0.43
2:B:616:MET:O	2:B:620:ARG:HG2	2.19	0.43
24:B:827:CLA:H3A	24:B:827:CLA:HBA2	1.58	0.43
9:L:124:LEU:HD21	16:h:148:ILE:HA	2.00	0.43
24:b:305:CLA:H202	24:b:305:CLA:H161	1.73	0.43
24:b:310:CLA:H62	24:b:310:CLA:H41	1.82	0.43
24:e:610:CLA:H161	24:e:610:CLA:H121	1.71	0.43
18:k:169:LYS:HG2	18:k:172:VAL:HG22	1.99	0.43
1:A:681:ILE:HD13	1:A:681:ILE:HA	1.87	0.43
24:F:201:CLA:H61	24:F:201:CLA:H101	1.58	0.43
24:c:605:CLA:O1A	24:b:312:CLA:HAA1	2.18	0.43
18:k:59:PRO:HB2	18:k:62:ILE:HG23	2.00	0.43
22:g:117:MET:HE2	22:g:117:MET:HB3	1.87	0.43
24:A:842:CLA:H112	24:A:842:CLA:H142	1.68	0.43
2:B:661:MET:HB2	24:B:804:CLA:C1C	2.49	0.43
24:B:819:CLA:HBA2	24:B:819:CLA:H3A	1.80	0.43
24:B:823:CLA:H93	24:B:823:CLA:H111	1.84	0.43
4:D:86:VAL:HB	4:D:99:HIS:HB3	2.01	0.43
26:J:107:LHG:H111	26:J:107:LHG:HC82	1.72	0.43
26:J:107:LHG:H121	26:J:107:LHG:H152	1.75	0.43
24:O:205:CLA:H193	24:O:205:CLA:H162	1.82	0.43
16:h:84:MET:HE3	16:h:190:ASN:HB3	2.00	0.43
19:j:47:LYS:HB3	19:j:47:LYS:HE3	1.67	0.43
24:B:836:CLA:H92	24:B:836:CLA:H61	1.74	0.43
24:L:207:CLA:H12	32:L:208:LMG:H273	2.00	0.43
1:A:661:ILE:HA	2:B:616:MET:HE3	2.00	0.43
2:B:220:GLY:C	2:B:222:GLN:H	2.27	0.43
24:B:803:CLA:H2	24:B:803:CLA:H62	1.61	0.43
9:L:7:PRO:HB3	9:L:12:PRO:HA	2.01	0.43
32:L:208:LMG:H141	32:L:208:LMG:H111	1.77	0.43
15:b:187:HIS:O	15:b:191:VAL:HG23	2.19	0.43
19:f:53:SER:HA	19:f:58:TYR:CD2	2.54	0.43
24:f:607:CLA:H193	24:f:613:CLA:HBB2	2.00	0.43
24:f:610:CLA:H202	24:f:610:CLA:H101	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:619:LHG:H272	26:f:619:LHG:H302	1.31	0.43
20:i:166:ASN:ND2	20:i:169:LYS:HD2	2.34	0.43
24:A:842:CLA:HBA1	24:A:842:CLA:H11	1.83	0.43
9:L:64:LYS:HA	9:L:64:LYS:HD2	1.81	0.43
11:O:77:PHE:CZ	11:O:81:ILE:HD11	2.54	0.43
14:a:81:GLN:O	14:a:85:ILE:HG13	2.18	0.43
1:A:121:ILE:HG13	1:A:122:VAL:HG13	2.00	0.43
1:A:219:GLN:HA	1:A:223:SER:HB2	2.00	0.43
24:B:820:CLA:CHC	24:B:841:CLA:HED1	2.49	0.43
24:B:837:CLA:H122	24:B:837:CLA:H51	2.01	0.43
12:K:14:VAL:HG21	12:K:86:LEU:HD22	2.01	0.43
24:b:305:CLA:H61	24:b:305:CLA:H92	1.72	0.43
24:f:610:CLA:H112	24:f:610:CLA:H91	1.57	0.43
25:B:842:PQN:H172	25:B:842:PQN:H211	1.75	0.42
6:F:154:LEU:HA	6:F:157:VAL:HG22	2.01	0.42
7:I:29:TYR:OH	10:M:29:TYR:OH	2.27	0.42
32:J:106:LMG:H211	32:J:106:LMG:H242	1.88	0.42
11:O:25:VAL:HG23	11:O:27:GLN:HG2	2.01	0.42
16:h:188:LEU:HD12	16:h:188:LEU:HA	1.79	0.42
24:i:602:CLA:HBA2	24:i:602:CLA:H3A	1.35	0.42
22:g:166:THR:HG22	22:g:168:ARG:H	1.84	0.42
22:g:215:LEU:HD22	22:g:230:TYR:OH	2.19	0.42
1:A:736:LEU:HD12	24:A:837:CLA:HMA1	2.01	0.42
24:A:830:CLA:HMA2	9:L:19:THR:HG21	2.01	0.42
24:b:309:CLA:H143	24:b:309:CLA:H162	1.85	0.42
16:h:90:MET:HA	16:h:93:THR:HG22	2.00	0.42
24:e:605:CLA:H92	24:e:605:CLA:H62	1.88	0.42
21:d:144:THR:HA	21:d:147:THR:HG22	2.00	0.42
1:A:299:HIS:HB2	24:A:817:CLA:C1B	2.49	0.42
24:A:802:CLA:HBA1	24:B:801:CLA:HBB2	1.99	0.42
24:A:823:CLA:H41	24:A:823:CLA:H61	1.76	0.42
2:B:139:LEU:HD22	10:M:13:LEU:HD12	2.02	0.42
24:B:820:CLA:H62	24:B:820:CLA:H2	1.85	0.42
24:O:205:CLA:H91	24:O:205:CLA:H112	1.86	0.42
24:k:603:CLA:HBB2	24:k:614:CLA:HHC	2.01	0.42
22:g:124:PHE:O	22:g:128:GLU:HG3	2.19	0.42
25:A:843:PQN:H242	25:A:843:PQN:H212	1.78	0.42
14:a:136:GLY:O	14:a:140:THR:HG23	2.19	0.42
26:b:320:LHG:H182	26:b:320:LHG:H152	1.79	0.42
17:e:167:LYS:HD3	24:e:608:CLA:O1D	2.19	0.42
19:f:175:GLN:O	19:f:179:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:630:LEU:HD22	2:B:723:PHE:HA	2.01	0.42
18:k:101:ILE:HG23	18:k:219:ILE:HD11	2.02	0.42
1:A:30:ALA:HB1	8:J:7:LYS:HG2	2.01	0.42
24:A:820:CLA:H162	24:A:820:CLA:H141	1.86	0.42
2:B:518:ILE:HG12	2:B:592:TYR:HB2	2.01	0.42
2:B:657:ALA:HB3	24:B:804:CLA:HBB2	2.02	0.42
24:B:836:CLA:H193	24:B:836:CLA:H162	1.88	0.42
26:J:107:LHG:H331	26:J:107:LHG:H302	1.91	0.42
9:L:125:VAL:HG21	24:g:309:CLA:H18	2.01	0.42
24:e:606:CLA:H143	24:e:606:CLA:H111	1.79	0.42
18:k:128:LEU:HA	18:k:128:LEU:HD23	1.80	0.42
24:k:608:CLA:H162	24:k:608:CLA:H122	1.63	0.42
21:d:123:ALA:HB2	24:d:303:CLA:HMA2	2.02	0.42
1:A:128:ASN:HB3	1:A:136:GLN:HB3	2.01	0.42
1:A:683:ALA:HB3	24:A:802:CLA:HBB2	2.02	0.42
24:A:806:CLA:OBD	24:A:856:CLA:HHD	2.20	0.42
24:A:806:CLA:H161	24:A:806:CLA:H141	1.79	0.42
19:j:117:HIS:CD2	19:j:126:MET:HE2	2.55	0.42
24:B:830:CLA:C4C	24:B:831:CLA:HAB	2.50	0.42
18:k:55:PRO:HD2	18:k:58:LEU:HD12	2.01	0.42
19:f:101:PHE:HE2	24:f:604:CLA:H11	1.84	0.42
22:g:81:GLU:HG3	24:g:309:CLA:HED1	2.01	0.42
22:g:147:LEU:HD13	22:g:147:LEU:HA	1.77	0.42
24:A:855:CLA:H61	24:A:855:CLA:H41	1.71	0.42
2:B:458:PHE:CE2	24:F:202:CLA:HBB1	2.55	0.42
2:B:476:LEU:HB3	2:B:477:LEU:H	1.65	0.42
4:D:12:PRO:HG3	4:D:58:ASN:HB3	2.02	0.42
32:b:301:LMG:H202	32:b:301:LMG:H232	1.93	0.42
16:h:79:ASN:HD21	24:h:302:CLA:C4D	2.32	0.42
18:k:158:ALA:O	18:k:162:THR:HG23	2.19	0.42
24:f:601:CLA:H3A	24:f:601:CLA:HBA2	1.66	0.42
2:B:141:LEU:HD23	2:B:141:LEU:HA	1.87	0.42
24:B:830:CLA:H61	24:B:830:CLA:H2	1.56	0.42
24:L:202:CLA:H3A	24:L:202:CLA:HBA2	1.51	0.42
14:a:144:GLU:HA	14:a:148:TYR:HD2	1.82	0.42
24:k:609:CLA:H122	24:k:609:CLA:H162	1.52	0.42
24:A:839:CLA:H111	24:A:839:CLA:H151	1.69	0.41
24:A:855:CLA:HBC1	25:B:842:PQN:H191	2.02	0.41
2:B:547:PRO:HB2	5:E:14:GLU:HG2	2.02	0.41
24:B:801:CLA:H71	26:B:802:LHG:HC12	2.02	0.41
22:g:116:LYS:HE2	22:g:116:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:THR:HB	1:A:428:LEU:HD21	2.03	0.41
1:A:555:GLY:HA3	1:A:593:SER:OG	2.20	0.41
1:A:695:TYR:OH	24:A:802:CLA:OBD	2.32	0.41
2:B:173:ARG:HB2	24:B:812:CLA:HBC2	2.01	0.41
24:B:824:CLA:H141	24:B:824:CLA:H162	1.90	0.41
24:B:837:CLA:H122	24:B:837:CLA:H8	1.84	0.41
11:O:27:GLN:HB3	19:f:148:LEU:HB3	2.01	0.41
13:c:80:VAL:HG13	24:c:607:CLA:HED1	2.01	0.41
16:h:105:ALA:HB1	16:h:131:GLU:HB2	2.01	0.41
24:j:311:CLA:H3A	24:j:311:CLA:HBA2	1.78	0.41
1:A:540:ILE:HG23	24:A:801:CLA:H193	2.02	0.41
24:A:806:CLA:H161	24:A:806:CLA:H202	1.87	0.41
24:A:840:CLA:H52	24:L:203:CLA:H12	2.02	0.41
24:A:841:CLA:H61	24:A:841:CLA:H2	1.80	0.41
26:A:844:LHG:H312	26:A:844:LHG:H282	1.86	0.41
24:B:827:CLA:HAA1	24:B:841:CLA:H41	2.02	0.41
24:B:832:CLA:H12	24:B:833:CLA:O1A	2.19	0.41
24:a:307:CLA:H92	24:a:307:CLA:H62	1.81	0.41
32:b:301:LMG:H202	32:b:301:LMG:H171	1.77	0.41
17:e:80:ARG:HA	17:e:83:MET:HE3	2.02	0.41
24:k:602:CLA:HBA2	24:k:602:CLA:H3A	1.57	0.41
2:B:648:MET:HE3	2:B:648:MET:HB2	1.81	0.41
5:E:30:SER:HB2	5:E:32:ILE:HG12	2.01	0.41
6:F:153:ALA:O	6:F:157:VAL:HG13	2.21	0.41
11:O:115:LEU:HD12	24:O:201:CLA:HBB1	2.02	0.41
24:c:601:CLA:HBC1	21:d:142:ILE:HG12	2.01	0.41
28:a:318:LMT:H51	28:a:318:LMT:H82	1.76	0.41
17:e:142:MET:HE1	24:e:606:CLA:HED2	2.02	0.41
26:f:619:LHG:H251	26:f:619:LHG:H281	1.83	0.41
1:A:659:GLN:HG2	1:A:752:SER:HB2	2.02	0.41
24:A:840:CLA:H151	24:A:840:CLA:H112	1.61	0.41
9:L:76:LEU:HD12	9:L:76:LEU:HA	1.86	0.41
9:L:140:ASN:HB3	24:g:308:CLA:HAA2	2.02	0.41
26:b:320:LHG:H282	26:b:320:LHG:H311	1.90	0.41
1:A:580:PRO:HD3	2:B:560:GLY:HA2	2.03	0.41
1:A:682:TRP:O	1:A:685:SER:OG	2.35	0.41
24:B:806:CLA:H112	24:B:806:CLA:H152	1.60	0.41
24:a:302:CLA:H3A	24:a:302:CLA:HBA2	1.68	0.41
20:i:45:PRO:HB2	19:j:158:LYS:HB2	2.02	0.41
11:O:59:THR:HG22	11:O:74:SER:N	2.35	0.41
24:O:205:CLA:H162	24:O:205:CLA:H122	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:72:LEU:HD23	15:b:72:LEU:HA	1.89	0.41
24:b:312:CLA:H112	24:b:312:CLA:H72	1.74	0.41
24:k:603:CLA:HBB2	34:k:618:IHT:C38	2.51	0.41
19:j:118:ASP:O	19:j:122:LYS:HG3	2.20	0.41
22:g:212:HIS:NE2	35:g:313:KC2:NA	2.69	0.41
1:A:327:ILE:HD13	24:A:822:CLA:HMD2	2.03	0.41
24:A:804:CLA:H51	24:A:812:CLA:H11	2.03	0.41
24:c:608:CLA:HBA2	24:c:608:CLA:H3A	1.31	0.41
14:a:47:ILE:HB	14:a:50:MET:HB2	2.01	0.41
24:a:308:CLA:H152	24:a:310:CLA:H101	2.02	0.41
24:k:607:CLA:H11	24:k:607:CLA:HBA1	1.72	0.41
24:A:853:CLA:H172	6:F:128:GLY:HA2	2.02	0.41
2:B:61:SER:HB3	2:B:141:LEU:HB2	2.03	0.41
2:B:105:LYS:H	2:B:105:LYS:HG2	1.73	0.41
2:B:579:MET:HB3	2:B:709:LEU:HD11	2.03	0.41
24:B:823:CLA:H101	24:B:823:CLA:H61	1.72	0.41
24:B:833:CLA:H142	24:B:833:CLA:H112	1.86	0.41
32:F:206:LMG:H222	32:F:206:LMG:H252	1.89	0.41
15:b:134:LEU:HD22	24:b:308:CLA:HMA1	2.03	0.41
24:b:306:CLA:H2	24:b:306:CLA:H61	1.58	0.41
24:b:312:CLA:H62	24:b:312:CLA:H41	1.79	0.41
24:b:313:CLA:H2	24:b:313:CLA:H62	1.75	0.41
24:b:313:CLA:H102	24:b:313:CLA:H62	1.72	0.41
17:e:157:ALA:HB2	24:e:607:CLA:HBA1	2.02	0.41
24:f:609:CLA:H162	24:f:609:CLA:H122	1.86	0.41
1:A:395:HIS:CE1	24:A:827:CLA:ND	2.88	0.41
1:A:414:PHE:CD1	1:A:418:ASP:HB2	2.56	0.41
24:A:856:CLA:HMA2	24:c:606:CLA:OBD	2.21	0.41
2:B:357:TYR:O	2:B:360:ILE:HG22	2.20	0.41
24:J:105:CLA:HBA2	24:J:105:CLA:H12	1.83	0.41
24:f:601:CLA:H12	24:f:601:CLA:HBA1	1.21	0.41
22:g:198:ASN:HD21	35:g:312:KC2:CHA	2.34	0.41
1:A:17:VAL:HG11	1:A:184:ALA:HB1	2.02	0.40
24:A:807:CLA:H161	24:A:807:CLA:H122	1.60	0.40
2:B:523:ALA:HB2	24:B:833:CLA:HMA1	2.03	0.40
2:B:699:LEU:HD21	25:B:842:PQN:H151	2.03	0.40
20:i:161:GLY:N	24:i:607:CLA:OBD	2.54	0.40
21:d:214:ILE:HG13	21:d:215:GLU:N	2.36	0.40
1:A:479:ILE:H	1:A:479:ILE:HG13	1.67	0.40
1:A:641:SER:O	1:A:647:GLY:HA3	2.20	0.40
24:A:802:CLA:HBA1	24:A:802:CLA:H11	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:GLY:HA2	2:B:86:ILE:CG2	2.52	0.40
2:B:166:TRP:CZ2	24:B:810:CLA:HBB	2.57	0.40
2:B:181:LEU:HD13	24:B:812:CLA:HBB	2.03	0.40
9:L:114:LYS:O	9:L:118:GLN:HG2	2.20	0.40
14:a:142:SER:HA	14:a:158:LEU:HD11	2.03	0.40
18:k:49:VAL:HG22	24:k:601:CLA:NC	2.36	0.40
21:d:119:LEU:HD23	24:d:303:CLA:HMA3	2.03	0.40
24:A:803:CLA:H52	24:A:803:CLA:H12	1.84	0.40
24:B:840:CLA:H62	24:B:840:CLA:H2	1.69	0.40
7:I:3:ALA:HB2	10:M:4:ASP:HB3	2.03	0.40
14:a:196:HIS:CE1	24:a:311:CLA:NA	2.89	0.40
24:a:307:CLA:H111	24:a:307:CLA:H91	1.68	0.40
24:A:829:CLA:H41	24:A:829:CLA:H61	1.65	0.40
24:B:837:CLA:H51	24:B:837:CLA:H8	1.82	0.40
25:B:842:PQN:H221	25:B:842:PQN:H261	1.75	0.40
14:a:50:MET:HE2	14:a:50:MET:HB3	1.77	0.40
14:a:86:LYS:HB2	14:a:86:LYS:HE3	1.93	0.40
24:b:313:CLA:H111	24:b:313:CLA:H142	1.72	0.40
24:A:855:CLA:H41	24:A:855:CLA:H112	2.02	0.40
2:B:340:LEU:HA	2:B:340:LEU:HD23	1.90	0.40
2:B:497:LEU:HA	2:B:500:ILE:HG22	2.04	0.40
24:B:823:CLA:H172	24:B:828:CLA:HBC1	2.03	0.40
24:I:102:CLA:H162	24:I:102:CLA:H141	1.91	0.40
11:O:63:SER:HB3	11:O:68:TYR:CD2	2.56	0.40
13:c:48:VAL:HG22	13:c:51:LEU:H	1.87	0.40
13:c:53:ARG:HA	13:c:54:PRO:HD3	1.96	0.40
13:c:90:ARG:HA	13:c:93:MET:HE3	2.03	0.40
17:e:193:HIS:CD2	17:e:198:PHE:HA	2.56	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	740/752 (98%)	723 (98%)	17 (2%)	0	100	100
2	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	58/64 (91%)	55 (95%)	3 (5%)	0	100	100
6	F	159/188 (85%)	155 (98%)	4 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	L	149/153 (97%)	147 (99%)	2 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	92 (90%)	9 (9%)	1 (1%)	12	40
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	c	168/216 (78%)	167 (99%)	1 (1%)	0	100	100
14	a	173/216 (80%)	171 (99%)	2 (1%)	0	100	100
15	b	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
16	h	160/225 (71%)	159 (99%)	1 (1%)	0	100	100
17	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
18	k	178/241 (74%)	174 (98%)	4 (2%)	0	100	100
19	f	172/212 (81%)	167 (97%)	5 (3%)	0	100	100
19	j	170/212 (80%)	167 (98%)	3 (2%)	0	100	100
20	i	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
21	d	120/213 (56%)	120 (100%)	0	0	100	100
22	g	217/255 (85%)	206 (95%)	11 (5%)	0	100	100
23	R	88/129 (68%)	87 (99%)	1 (1%)	0	100	100
All	All	4295/5017 (86%)	4194 (98%)	100 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	29	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	607/616 (98%)	604 (100%)	3 (0%)	81	83
2	B	593/593 (100%)	589 (99%)	4 (1%)	76	80
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	116/117 (99%)	115 (99%)	1 (1%)	70	78
5	E	55/58 (95%)	53 (96%)	2 (4%)	31	58
6	F	133/157 (85%)	133 (100%)	0	100	100
7	I	28/29 (97%)	28 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	123 (99%)	1 (1%)	73	79
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	81/110 (74%)	80 (99%)	1 (1%)	63	75
12	K	52/66 (79%)	49 (94%)	3 (6%)	18	47
13	c	138/171 (81%)	132 (96%)	6 (4%)	26	54
14	a	139/165 (84%)	132 (95%)	7 (5%)	22	50
15	b	149/168 (89%)	146 (98%)	3 (2%)	48	68
16	h	123/162 (76%)	118 (96%)	5 (4%)	27	55
17	e	130/155 (84%)	128 (98%)	2 (2%)	57	72
18	k	138/186 (74%)	134 (97%)	4 (3%)	37	62
19	f	135/161 (84%)	123 (91%)	12 (9%)	9	32
19	j	136/161 (84%)	129 (95%)	7 (5%)	21	50
20	i	138/168 (82%)	133 (96%)	5 (4%)	31	58
21	d	94/157 (60%)	89 (95%)	5 (5%)	20	49
22	g	171/199 (86%)	166 (97%)	5 (3%)	37	62
23	R	69/98 (70%)	69 (100%)	0	100	100
All	All	3480/3955 (88%)	3404 (98%)	76 (2%)	45	66

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	629	THR
1	A	691	SER
1	A	736	LEU
2	B	476	LEU
2	B	493	LEU
2	B	507	LEU
2	B	524	LEU
4	D	13	THR
5	E	54	SER
5	E	57	GLU
9	L	75	LEU
11	O	29	LYS
12	K	19	LYS
12	K	29	ILE
12	K	30	LEU
13	c	48	VAL
13	c	116	VAL
13	c	140	LEU
13	c	191	ILE
13	c	201	THR
13	c	204	THR
14	a	47	ILE
14	a	72	THR
14	a	99	VAL
14	a	124	SER
14	a	133	LEU
14	a	158	LEU
14	a	194	LEU
15	b	51	VAL
15	b	128	ILE
15	b	146	VAL
16	h	71	VAL
16	h	72	THR
16	h	101	LEU
16	h	143	LEU
16	h	182	LEU
17	e	160	THR
17	e	190	THR
18	k	89	HIS
18	k	100	SER
18	k	169	LYS
18	k	191	LEU
19	f	42	VAL

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Mol	Chain	Res	Type
19	f	46	LYS
19	f	49	GLU
19	f	110	THR
19	f	119	VAL
19	f	121	VAL
19	f	122	LYS
19	f	123	GLN
19	f	169	GLU
19	f	199	THR
19	f	206	LEU
19	f	207	LEU
20	i	43	SER
20	i	101	VAL
20	i	127	GLN
20	i	204	LYS
20	i	215	TRP
19	j	39	SER
19	j	100	THR
19	j	108	VAL
19	j	116	VAL
19	j	121	VAL
19	j	147	THR
19	j	204	LEU
21	d	68	ILE
21	d	119	LEU
21	d	144	THR
21	d	186	LEU
21	d	197	ILE
22	g	45	LEU
22	g	120	VAL
22	g	147	LEU
22	g	215	LEU
22	g	251	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	219	GLN
1	A	420	ASN
1	A	487	GLN
1	A	717	GLN

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Mol	Chain	Res	Type
2	B	9	GLN
2	B	13	GLN
2	B	75	GLN
2	B	97	GLN
2	B	438	HIS
4	D	96	GLN
4	D	128	ASN
4	D	131	GLN
4	D	140	ASN
11	O	84	ASN
13	c	125	GLN
15	b	92	HIS
15	b	100	GLN
16	h	139	HIS
17	e	72	GLN
17	e	78	ASN
18	k	89	HIS
18	k	210	HIS
20	i	137	HIS
20	i	166	ASN
20	i	216	HIS
19	j	76	GLN
22	g	80	GLN
22	g	222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

342 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	$\# Z > 2$
24	CLA	a	303	14	54,58,73	1.27	7 (12%)	64,95,113	1.33	8 (12%)
24	CLA	c	607	13	50,54,73	1.32	7 (14%)	59,90,113	1.20	5 (8%)
33	II0	f	614	-	39,43,43	6.63	21 (53%)	48,60,60	2.11	14 (29%)
24	CLA	B	837	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
33	II0	i	613	-	39,43,43	6.76	22 (56%)	48,60,60	1.69	10 (20%)
24	CLA	d	307	21	50,54,73	1.30	6 (12%)	59,90,113	1.35	5 (8%)
24	CLA	b	303	15	55,59,73	1.28	6 (10%)	64,96,113	1.45	6 (9%)
24	CLA	f	605	19	49,53,73	1.36	7 (14%)	58,89,113	1.29	4 (6%)
24	CLA	a	304	-	55,59,73	1.26	5 (9%)	64,96,113	1.36	4 (6%)
24	CLA	B	817	-	61,65,73	1.19	7 (11%)	72,103,113	1.42	10 (13%)
27	WVN	j	301	-	40,41,41	1.80	10 (25%)	51,56,56	2.25	16 (31%)
24	CLA	g	303	22	54,58,73	1.27	9 (16%)	64,95,113	1.33	8 (12%)
24	CLA	B	807	-	69,73,73	1.10	7 (10%)	82,113,113	1.45	7 (8%)
24	CLA	b	304	15	59,63,73	1.22	8 (13%)	70,101,113	1.41	7 (10%)
24	CLA	h	305	16	69,73,73	1.14	8 (11%)	82,113,113	1.22	8 (9%)
24	CLA	g	304	-	55,59,73	1.29	10 (18%)	64,96,113	1.45	13 (20%)
24	CLA	a	309	26	52,56,73	1.32	7 (13%)	61,92,113	1.22	5 (8%)
24	CLA	h	307	16	55,59,73	1.32	8 (14%)	64,96,113	1.47	9 (14%)
24	CLA	B	811	-	59,63,73	1.26	8 (13%)	70,101,113	1.26	5 (7%)
33	II0	g	320	-	39,43,43	6.71	21 (53%)	48,60,60	1.96	17 (35%)
32	LMG	J	106	-	55,55,55	0.86	3 (5%)	63,63,63	0.97	4 (6%)
33	II0	k	619	-	39,43,43	6.68	20 (51%)	48,60,60	1.94	14 (29%)
24	CLA	i	608	26	50,54,73	1.34	6 (12%)	59,90,113	1.21	3 (5%)
24	CLA	j	311	26	65,69,73	1.21	6 (9%)	77,108,113	1.10	4 (5%)
24	CLA	c	601	13	55,59,73	1.29	9 (16%)	64,96,113	1.36	7 (10%)
24	CLA	B	830	36	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
24	CLA	R	203	-	55,59,73	1.26	7 (12%)	64,96,113	1.46	9 (14%)
33	II0	d	315	-	39,43,43	6.83	23 (58%)	48,60,60	2.00	14 (29%)
29	SF4	A	854	1,2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMT	a	318	-	36,36,36	1.19	4 (11%)	47,47,47	1.16	3 (6%)
35	KC2	i	616	-	49,53,53	2.77	20 (40%)	60,89,89	3.73	32 (53%)
35	KC2	k	611	18	49,53,53	2.65	19 (38%)	60,89,89	3.84	33 (55%)
24	CLA	e	610	36	69,73,73	1.17	9 (13%)	82,113,113	1.33	10 (12%)
24	CLA	f	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.16	5 (6%)
26	LHG	A	844	-	47,47,48	0.91	2 (4%)	50,53,54	1.17	5 (10%)
24	CLA	B	809	2	69,73,73	1.16	9 (13%)	82,113,113	1.31	12 (14%)
27	WVN	I	101	-	40,41,41	1.71	10 (25%)	51,56,56	1.86	19 (37%)
24	CLA	j	308	-	55,59,73	1.28	6 (10%)	64,96,113	1.20	5 (7%)
24	CLA	k	603	-	55,59,73	1.33	7 (12%)	64,96,113	1.54	10 (15%)
33	II0	O	202	-	39,43,43	6.70	21 (53%)	48,60,60	1.84	10 (20%)
33	II0	k	621	-	39,43,43	6.86	22 (56%)	48,60,60	1.80	10 (20%)
24	CLA	A	853	-	69,73,73	1.13	8 (11%)	82,113,113	1.33	10 (12%)
24	CLA	c	606	-	56,60,73	1.33	7 (12%)	65,97,113	1.30	7 (10%)
33	II0	J	104	-	39,43,43	6.53	18 (46%)	48,60,60	1.94	13 (27%)
24	CLA	d	309	26	45,49,73	1.39	8 (17%)	54,84,113	1.25	4 (7%)
24	CLA	J	105	26	55,59,73	1.34	8 (14%)	64,96,113	1.51	7 (10%)
24	CLA	k	601	18	55,59,73	1.35	8 (14%)	64,96,113	1.48	6 (9%)
26	LHG	J	107	24	48,48,48	1.01	2 (4%)	51,54,54	1.09	3 (5%)
24	CLA	g	322	32	69,73,73	1.12	8 (11%)	82,113,113	1.25	6 (7%)
33	II0	j	316	-	39,43,43	6.62	21 (53%)	48,60,60	2.04	18 (37%)
24	CLA	B	827	-	54,58,73	1.25	7 (12%)	64,95,113	1.28	8 (12%)
26	LHG	e	617	24	36,36,48	1.12	2 (5%)	39,42,54	1.18	4 (10%)
24	CLA	B	804	-	69,73,73	1.12	11 (15%)	82,113,113	1.51	11 (13%)
24	CLA	A	814	-	54,58,73	1.28	5 (9%)	64,95,113	1.48	13 (20%)
24	CLA	h	302	16	54,58,73	1.27	8 (14%)	64,95,113	1.36	9 (14%)
34	IHT	c	615	-	40,42,42	6.30	26 (65%)	52,58,58	2.17	13 (25%)
24	CLA	A	856	26	45,49,73	1.44	9 (20%)	54,84,113	1.99	8 (14%)
24	CLA	A	813	-	49,53,73	1.37	6 (12%)	58,89,113	1.47	6 (10%)
24	CLA	b	306	-	69,73,73	1.20	9 (13%)	82,113,113	1.45	7 (8%)
24	CLA	A	833	-	54,58,73	1.31	8 (14%)	64,95,113	1.30	5 (7%)
24	CLA	j	303	19	54,58,73	1.30	8 (14%)	64,95,113	1.22	5 (7%)
33	II0	i	614	-	39,43,43	6.67	21 (53%)	48,60,60	1.97	15 (31%)
24	CLA	g	306	22	55,59,73	1.30	8 (14%)	64,96,113	1.22	5 (7%)
24	CLA	c	604	13	69,73,73	1.16	8 (11%)	82,113,113	1.16	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	J	101	-	40,41,41	1.74	10 (25%)	51,56,56	2.09	17 (33%)
24	CLA	e	604	36	69,73,73	1.15	7 (10%)	82,113,113	1.39	8 (9%)
24	CLA	B	803	-	69,73,73	1.14	7 (10%)	82,113,113	1.29	9 (10%)
24	CLA	A	810	-	66,70,73	1.15	7 (10%)	78,109,113	1.17	6 (7%)
24	CLA	c	602	13	54,58,73	1.29	8 (14%)	64,95,113	1.42	11 (17%)
24	CLA	A	825	36	69,73,73	1.11	7 (10%)	82,113,113	1.26	7 (8%)
24	CLA	d	308	21	45,49,73	1.38	7 (15%)	54,84,113	1.29	4 (7%)
24	CLA	B	829	-	54,58,73	1.30	8 (14%)	64,95,113	1.43	5 (7%)
33	II0	a	314	-	39,43,43	6.71	22 (56%)	48,60,60	1.98	16 (33%)
24	CLA	e	601	17	49,53,73	1.39	8 (16%)	58,89,113	1.48	5 (8%)
24	CLA	A	812	-	69,73,73	1.13	9 (13%)	82,113,113	1.46	10 (12%)
24	CLA	B	816	-	63,67,73	1.19	7 (11%)	74,105,113	1.35	9 (12%)
24	CLA	c	612	-	69,73,73	1.12	6 (8%)	82,113,113	1.20	9 (10%)
24	CLA	O	205	-	69,73,73	1.25	10 (14%)	82,113,113	1.58	21 (25%)
33	II0	i	612	-	39,43,43	6.59	22 (56%)	48,60,60	2.09	12 (25%)
24	CLA	A	819	-	49,53,73	1.38	9 (18%)	58,89,113	1.63	10 (17%)
24	CLA	f	609	19	69,73,73	1.13	7 (10%)	82,113,113	1.19	7 (8%)
34	IHT	f	617	-	40,42,42	6.23	26 (65%)	52,58,58	4.02	21 (40%)
24	CLA	A	855	36	69,73,73	1.21	8 (11%)	82,113,113	1.41	10 (12%)
25	PQN	B	842	-	34,34,34	1.87	5 (14%)	43,45,45	1.30	6 (13%)
24	CLA	d	304	21	55,59,73	1.33	4 (7%)	64,96,113	1.38	7 (10%)
24	CLA	A	820	36	69,73,73	1.17	8 (11%)	82,113,113	1.37	10 (12%)
26	LHG	a	301	24	48,48,48	0.94	2 (4%)	51,54,54	1.19	5 (9%)
24	CLA	i	610	-	55,59,73	1.34	9 (16%)	64,96,113	1.41	8 (12%)
24	CLA	L	207	36	55,59,73	1.26	7 (12%)	64,96,113	1.34	7 (10%)
24	CLA	A	828	-	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
24	CLA	B	813	-	64,68,73	1.18	7 (10%)	76,107,113	1.29	10 (13%)
24	CLA	j	313	-	55,59,73	1.34	7 (12%)	64,96,113	1.27	7 (10%)
33	II0	f	615	-	39,43,43	6.65	23 (58%)	48,60,60	1.86	13 (27%)
24	CLA	B	808	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	8 (9%)
24	CLA	B	801	36	69,73,73	1.14	9 (13%)	82,113,113	1.37	9 (10%)
24	CLA	A	822	-	55,59,73	1.30	8 (14%)	64,96,113	1.38	6 (9%)
24	CLA	k	604	18	69,73,73	1.15	6 (8%)	82,113,113	1.28	8 (9%)
24	CLA	e	606	17	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
24	CLA	A	806	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	KC2	e	609	17	49,53,53	2.64	19 (38%)	60,89,89	3.78	33 (55%)
24	CLA	L	204	36	54,58,73	1.27	7 (12%)	64,95,113	1.42	6 (9%)
24	CLA	f	610	26	69,73,73	1.15	7 (10%)	82,113,113	1.23	5 (6%)
28	LMT	A	851	-	36,36,36	1.19	6 (16%)	47,47,47	1.38	5 (10%)
27	WVN	A	846	-	40,41,41	1.75	12 (30%)	51,56,56	2.28	17 (33%)
24	CLA	e	607	17	69,73,73	1.10	6 (8%)	82,113,113	1.23	7 (8%)
24	CLA	A	832	-	69,73,73	1.14	6 (8%)	82,113,113	1.59	18 (21%)
27	WVN	M	101	-	40,41,41	1.70	10 (25%)	51,56,56	2.21	16 (31%)
24	CLA	B	823	36	68,72,73	1.17	11 (16%)	80,111,113	1.34	8 (10%)
24	CLA	g	307	22	55,59,73	1.27	8 (14%)	64,96,113	1.33	7 (10%)
33	II0	f	616	-	39,43,43	6.56	22 (56%)	48,60,60	1.95	14 (29%)
34	IHT	k	618	-	40,42,42	6.28	26 (65%)	52,58,58	1.78	15 (28%)
24	CLA	c	611	-	49,53,73	1.36	6 (12%)	58,89,113	1.68	9 (15%)
24	CLA	g	305	22	69,73,73	1.10	7 (10%)	82,113,113	1.27	7 (8%)
24	CLA	i	606	20	65,69,73	1.19	5 (7%)	77,108,113	1.12	6 (7%)
35	KC2	i	609	20	49,53,53	2.70	19 (38%)	60,89,89	3.87	35 (58%)
24	CLA	A	852	36	69,73,73	1.16	8 (11%)	82,113,113	1.37	11 (13%)
24	CLA	c	603	-	55,59,73	1.26	9 (16%)	64,96,113	1.33	6 (9%)
24	CLA	A	811	-	58,62,73	1.28	7 (12%)	68,99,113	1.39	8 (11%)
24	CLA	f	602	19	69,73,73	1.15	7 (10%)	82,113,113	1.23	6 (7%)
24	CLA	f	601	19	51,55,73	1.34	6 (11%)	60,91,113	1.32	4 (6%)
24	CLA	A	826	-	69,73,73	1.16	8 (11%)	82,113,113	1.45	13 (15%)
24	CLA	B	838	-	61,65,73	1.26	8 (13%)	72,103,113	1.24	6 (8%)
24	CLA	d	306	-	55,59,73	1.31	7 (12%)	64,96,113	1.07	3 (4%)
24	CLA	g	308	-	69,73,73	1.13	7 (10%)	82,113,113	1.23	7 (8%)
33	II0	g	317	-	39,43,43	6.63	24 (61%)	48,60,60	1.97	16 (33%)
24	CLA	k	605	18	49,53,73	1.35	7 (14%)	58,89,113	1.37	5 (8%)
24	CLA	k	608	18	69,73,73	1.14	6 (8%)	82,113,113	1.12	6 (7%)
27	WVN	R	202	-	40,41,41	1.68	10 (25%)	51,56,56	2.65	19 (37%)
24	CLA	a	305	36	69,73,73	1.11	9 (13%)	82,113,113	1.25	10 (12%)
24	CLA	A	815	36	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
24	CLA	g	302	22	46,50,73	1.35	10 (21%)	53,85,113	1.61	8 (15%)
35	KC2	k	612	35	49,53,53	2.77	18 (36%)	60,89,89	3.86	37 (61%)
32	LMG	L	208	24	55,55,55	0.91	2 (3%)	63,63,63	1.44	10 (15%)
24	CLA	A	809	-	60,64,73	1.24	7 (11%)	71,102,113	1.27	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	B	847	-	40,41,41	1.69	9 (22%)	51,56,56	2.63	18 (35%)
27	WVN	J	102	-	40,41,41	1.71	11 (27%)	51,56,56	2.25	17 (33%)
33	II0	c	616	-	39,43,43	6.82	22 (56%)	48,60,60	1.92	18 (37%)
35	KC2	k	613	35	49,53,53	2.76	21 (42%)	60,89,89	3.76	31 (51%)
33	II0	e	612	-	39,43,43	6.67	20 (51%)	48,60,60	1.69	9 (18%)
24	CLA	a	308	14	69,73,73	1.14	9 (13%)	82,113,113	1.36	6 (7%)
24	CLA	K	102	-	46,50,73	1.38	9 (19%)	53,85,113	1.51	7 (13%)
34	IHT	j	317	-	40,42,42	6.25	26 (65%)	52,58,58	2.34	16 (30%)
24	CLA	j	307	19	55,59,73	1.34	9 (16%)	64,96,113	1.58	8 (12%)
24	CLA	i	611	-	55,59,73	1.30	5 (9%)	64,96,113	1.31	9 (14%)
24	CLA	b	311	-	55,59,73	1.30	8 (14%)	64,96,113	1.45	9 (14%)
33	II0	j	315	-	39,43,43	6.55	22 (56%)	48,60,60	2.27	15 (31%)
24	CLA	j	305	19	69,73,73	1.14	7 (10%)	82,113,113	1.27	7 (8%)
24	CLA	d	312	-	55,59,73	1.30	6 (10%)	64,96,113	1.51	10 (15%)
24	CLA	a	307	14	69,73,73	1.16	7 (10%)	82,113,113	1.27	10 (12%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
24	CLA	g	315	-	55,59,73	1.26	7 (12%)	64,96,113	1.25	10 (15%)
24	CLA	c	605	13	55,59,73	1.30	7 (12%)	64,96,113	1.44	9 (14%)
24	CLA	e	602	17	54,58,73	1.27	8 (14%)	64,95,113	1.35	5 (7%)
33	II0	b	318	-	39,43,43	6.75	23 (58%)	48,60,60	2.05	15 (31%)
29	SF4	C	102	3	0,12,12	-	-	-	-	-
33	II0	k	615	-	39,43,43	6.62	21 (53%)	48,60,60	1.89	17 (35%)
24	CLA	K	101	36	55,59,73	1.27	9 (16%)	64,96,113	1.54	11 (17%)
24	CLA	j	306	19	49,53,73	1.40	7 (14%)	58,89,113	1.60	8 (13%)
33	II0	k	617	-	39,43,43	6.80	21 (53%)	48,60,60	2.25	14 (29%)
24	CLA	A	841	36	69,73,73	1.15	6 (8%)	82,113,113	1.27	6 (7%)
27	WVN	A	849	-	40,41,41	1.73	11 (27%)	51,56,56	2.45	21 (41%)
33	II0	a	317	-	39,43,43	6.93	21 (53%)	48,60,60	2.38	15 (31%)
24	CLA	j	314	-	69,73,73	1.13	6 (8%)	82,113,113	1.23	6 (7%)
24	CLA	L	202	9	53,57,73	1.35	7 (13%)	61,93,113	1.39	8 (13%)
27	WVN	K	103	-	40,41,41	1.70	11 (27%)	51,56,56	2.24	19 (37%)
27	WVN	A	848	-	40,41,41	1.66	9 (22%)	51,56,56	1.93	13 (25%)
24	CLA	a	302	14	56,60,73	1.28	9 (16%)	65,97,113	1.35	7 (10%)
35	KC2	j	312	19	49,53,53	2.64	19 (38%)	60,89,89	3.86	33 (55%)
24	CLA	f	612	-	55,59,73	1.29	9 (16%)	64,96,113	1.38	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	e	608	26	50,54,73	1.34	9 (18%)	59,90,113	1.61	6 (10%)
26	LHG	j	319	24	29,29,48	1.26	2 (6%)	32,35,54	1.36	4 (12%)
24	CLA	f	603	-	55,59,73	1.28	6 (10%)	64,96,113	1.43	8 (12%)
24	CLA	A	816	-	69,73,73	1.11	8 (11%)	82,113,113	1.45	10 (12%)
24	CLA	A	824	36	69,73,73	1.15	8 (11%)	82,113,113	1.26	10 (12%)
35	KC2	g	313	35	49,53,53	2.72	19 (38%)	60,89,89	3.73	33 (55%)
24	CLA	d	301	21	54,58,73	1.33	6 (11%)	64,95,113	1.36	5 (7%)
24	CLA	A	804	-	69,73,73	1.15	7 (10%)	82,113,113	1.36	8 (9%)
33	II0	g	316	-	39,43,43	6.82	21 (53%)	48,60,60	1.83	16 (33%)
24	CLA	B	831	36	49,53,73	1.39	8 (16%)	58,89,113	1.37	7 (12%)
24	CLA	A	817	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	12 (14%)
24	CLA	j	302	19	55,59,73	1.32	7 (12%)	64,96,113	1.26	5 (7%)
33	II0	h	311	-	39,43,43	6.69	21 (53%)	48,60,60	2.03	18 (37%)
33	II0	d	313	-	39,43,43	6.78	22 (56%)	48,60,60	2.04	13 (27%)
24	CLA	B	834	-	51,55,73	1.27	8 (15%)	60,91,113	1.55	7 (11%)
26	LHG	b	320	24	48,48,48	0.94	2 (4%)	51,54,54	1.12	5 (9%)
33	II0	e	616	-	39,43,43	6.73	20 (51%)	48,60,60	1.73	13 (27%)
24	CLA	A	842	-	69,73,73	1.15	9 (13%)	82,113,113	1.41	11 (13%)
33	II0	b	315	-	39,43,43	6.64	20 (51%)	48,60,60	2.73	19 (39%)
27	WVN	B	845	-	40,41,41	1.69	11 (27%)	51,56,56	2.60	20 (39%)
33	II0	a	313	-	39,43,43	6.60	22 (56%)	48,60,60	1.88	14 (29%)
24	CLA	I	102	36	69,73,73	1.18	8 (11%)	82,113,113	1.29	8 (9%)
26	LHG	f	620	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
24	CLA	h	306	16	61,65,73	1.26	7 (11%)	72,103,113	1.12	5 (6%)
24	CLA	B	819	-	50,54,73	1.27	7 (14%)	59,90,113	1.40	7 (11%)
24	CLA	f	608	19	69,73,73	1.11	8 (11%)	82,113,113	1.25	8 (9%)
24	CLA	b	310	26	69,73,73	1.20	6 (8%)	82,113,113	1.19	10 (12%)
26	LHG	c	618	24	36,36,48	1.11	2 (5%)	39,42,54	1.22	6 (15%)
26	LHG	c	617	24	36,36,48	1.08	2 (5%)	39,42,54	1.26	5 (12%)
24	CLA	c	608	13	69,73,73	1.15	7 (10%)	82,113,113	1.30	10 (12%)
24	CLA	g	310	22	55,59,73	1.28	8 (14%)	64,96,113	1.32	8 (12%)
26	LHG	g	321	24	36,36,48	1.08	2 (5%)	39,42,54	1.56	9 (23%)
34	IHT	b	316	-	40,42,42	6.27	26 (65%)	52,58,58	2.17	15 (28%)
24	CLA	b	309	15	69,73,73	1.18	8 (11%)	82,113,113	1.27	10 (12%)
24	CLA	B	839	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	KC2	d	310	21	49,53,53	2.70	21 (42%)	60,89,89	3.83	35 (58%)
24	CLA	i	601	20	55,59,73	1.29	6 (10%)	64,96,113	1.38	3 (4%)
24	CLA	f	606	19	55,59,73	1.28	6 (10%)	64,96,113	1.45	6 (9%)
27	WVN	F	204	-	40,41,41	1.69	11 (27%)	51,56,56	2.39	17 (33%)
24	CLA	B	805	-	69,73,73	1.12	7 (10%)	82,113,113	1.34	7 (8%)
24	CLA	B	812	-	69,73,73	1.16	10 (14%)	82,113,113	1.33	10 (12%)
24	CLA	B	832	-	62,66,73	1.20	9 (14%)	73,104,113	1.40	9 (12%)
24	CLA	k	602	18	54,58,73	1.32	8 (14%)	64,95,113	1.40	7 (10%)
28	LMT	F	203	-	24,24,36	1.05	2 (8%)	29,29,47	0.99	2 (6%)
24	CLA	A	838	26	56,60,73	1.27	8 (14%)	65,97,113	1.34	8 (12%)
24	CLA	B	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	10 (12%)
26	LHG	d	316	24	36,36,48	1.10	2 (5%)	39,42,54	1.25	5 (12%)
24	CLA	i	603	-	55,59,73	1.30	8 (14%)	64,96,113	1.39	6 (9%)
24	CLA	J	103	8	46,50,73	1.37	7 (15%)	53,85,113	1.43	6 (11%)
26	LHG	g	301	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	2 (3%)
33	II0	f	618	-	39,43,43	6.64	20 (51%)	48,60,60	2.11	11 (22%)
24	CLA	k	610	26	55,59,73	1.29	6 (10%)	64,96,113	1.32	6 (9%)
24	CLA	a	310	14	69,73,73	1.14	6 (8%)	82,113,113	1.27	4 (4%)
24	CLA	a	311	-	51,55,73	1.33	7 (13%)	60,91,113	1.77	12 (20%)
24	CLA	f	607	-	69,73,73	1.14	8 (11%)	82,113,113	1.16	6 (7%)
24	CLA	j	304	-	55,59,73	1.27	5 (9%)	64,96,113	1.39	7 (10%)
25	PQN	A	843	-	34,34,34	1.90	5 (14%)	43,45,45	1.24	6 (13%)
24	CLA	d	302	-	55,59,73	1.34	8 (14%)	64,96,113	1.34	11 (17%)
24	CLA	B	836	-	69,73,73	1.17	10 (14%)	82,113,113	1.43	11 (13%)
33	II0	k	616	-	39,43,43	6.78	22 (56%)	48,60,60	1.98	15 (31%)
24	CLA	B	828	-	53,57,73	1.25	9 (16%)	61,93,113	1.41	9 (14%)
27	WVN	e	615	-	40,41,41	1.79	10 (25%)	51,56,56	2.22	17 (33%)
24	CLA	F	202	6	56,60,73	1.26	7 (12%)	65,97,113	1.49	8 (12%)
27	WVN	L	206	-	40,41,41	1.67	10 (25%)	51,56,56	2.56	22 (43%)
24	CLA	h	312	36	69,73,73	1.15	6 (8%)	82,113,113	1.27	7 (8%)
35	KC2	g	312	22	49,53,53	2.72	18 (36%)	60,89,89	4.07	37 (61%)
24	CLA	B	818	36	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
24	CLA	B	835	36	69,73,73	1.14	7 (10%)	82,113,113	1.12	6 (7%)
35	KC2	d	311	-	49,53,53	2.73	20 (40%)	60,89,89	3.69	34 (56%)
24	CLA	F	201	36	69,73,73	1.18	8 (11%)	82,113,113	1.20	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	F	205	-	40,41,41	1.79	10 (25%)	51,56,56	3.10	20 (39%)
24	CLA	j	310	19	55,59,73	1.27	8 (14%)	64,96,113	1.27	7 (10%)
33	II0	h	310	-	39,43,43	6.50	19 (48%)	48,60,60	2.08	17 (35%)
26	LHG	i	615	24	36,36,48	1.12	2 (5%)	39,42,54	1.21	3 (7%)
27	WVN	h	308	-	40,41,41	1.74	9 (22%)	51,56,56	2.43	19 (37%)
24	CLA	B	815	-	59,63,73	1.24	7 (11%)	70,101,113	1.26	6 (8%)
33	II0	d	314	-	39,43,43	6.65	23 (58%)	48,60,60	1.88	10 (20%)
24	CLA	A	830	-	54,58,73	1.31	10 (18%)	64,95,113	1.42	9 (14%)
24	CLA	e	605	17	69,73,73	1.12	7 (10%)	82,113,113	1.21	7 (8%)
24	CLA	e	603	17	55,59,73	1.33	6 (10%)	64,96,113	1.36	10 (15%)
24	CLA	B	810	-	58,62,73	1.34	9 (15%)	71,100,113	1.17	5 (7%)
24	CLA	A	821	-	53,57,73	1.27	9 (16%)	61,93,113	1.47	7 (11%)
24	CLA	i	602	20	54,58,73	1.29	7 (12%)	64,95,113	1.37	6 (9%)
24	CLA	h	301	16	54,58,73	1.29	7 (12%)	64,95,113	1.31	5 (7%)
27	WVN	L	205	-	40,41,41	1.76	9 (22%)	51,56,56	2.16	16 (31%)
24	CLA	A	808	1	69,73,73	1.15	7 (10%)	82,113,113	1.42	10 (12%)
33	II0	j	318	-	39,43,43	6.63	24 (61%)	48,60,60	1.88	12 (25%)
24	CLA	L	203	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	11 (13%)
26	LHG	B	802	-	37,37,48	1.04	3 (8%)	40,43,54	1.16	4 (10%)
24	CLA	A	801	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	9 (10%)
32	LMG	F	206	-	48,48,55	0.97	2 (4%)	56,56,63	1.26	5 (8%)
24	CLA	d	303	21	69,73,73	1.16	7 (10%)	82,113,113	1.29	12 (14%)
24	CLA	g	311	26	58,62,73	1.23	8 (13%)	68,99,113	1.18	5 (7%)
35	KC2	f	611	19	49,53,53	2.64	19 (38%)	60,89,89	3.97	34 (56%)
27	WVN	B	849	-	40,41,41	1.75	10 (25%)	51,56,56	1.87	11 (21%)
24	CLA	a	306	14	49,53,73	1.40	7 (14%)	58,89,113	1.53	4 (6%)
24	CLA	B	821	-	57,61,73	1.22	8 (14%)	67,98,113	1.26	7 (10%)
24	CLA	h	304	-	55,59,73	1.26	7 (12%)	64,96,113	1.25	7 (10%)
24	CLA	A	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	7 (8%)
26	LHG	f	619	24	36,36,48	1.07	2 (5%)	39,42,54	1.23	3 (7%)
24	CLA	A	818	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	11 (13%)
24	CLA	i	604	20	69,73,73	1.20	6 (8%)	82,113,113	1.57	9 (10%)
24	CLA	B	841	26	69,73,73	1.16	8 (11%)	82,113,113	1.30	9 (10%)
33	II0	g	318	-	39,43,43	6.73	23 (58%)	48,60,60	1.92	14 (29%)
24	CLA	A	834	-	55,59,73	1.32	7 (12%)	64,96,113	1.61	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	308	15	65,69,73	1.19	7 (10%)	77,108,113	1.52	12 (15%)
24	CLA	b	313	-	69,73,73	1.18	7 (10%)	82,113,113	1.12	6 (7%)
35	KC2	g	314	35	49,53,53	2.73	20 (40%)	60,89,89	3.77	31 (51%)
24	CLA	i	605	20	55,59,73	1.33	8 (14%)	64,96,113	1.21	5 (7%)
24	CLA	B	825	-	69,73,73	1.17	11 (15%)	82,113,113	1.40	10 (12%)
26	LHG	A	845	24	26,26,48	1.26	2 (7%)	29,32,54	1.51	5 (17%)
24	CLA	B	824	-	69,73,73	1.12	8 (11%)	82,113,113	1.29	9 (10%)
26	LHG	k	620	24	36,36,48	1.15	2 (5%)	39,42,54	1.17	5 (12%)
35	KC2	c	610	-	49,53,53	2.73	21 (42%)	60,89,89	3.78	32 (53%)
24	CLA	e	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	9 (10%)
24	CLA	A	827	-	66,70,73	1.14	8 (12%)	78,109,113	1.32	11 (14%)
24	CLA	h	303	-	55,59,73	1.29	8 (14%)	64,96,113	1.42	10 (15%)
24	CLA	A	829	-	69,73,73	1.14	7 (10%)	82,113,113	1.24	7 (8%)
24	CLA	f	604	19	69,73,73	1.11	7 (10%)	82,113,113	1.25	7 (8%)
24	CLA	B	833	-	69,73,73	1.11	8 (11%)	82,113,113	1.35	9 (10%)
33	II0	c	613	-	39,43,43	6.71	22 (56%)	48,60,60	1.99	14 (29%)
27	WVN	B	848	-	40,41,41	1.75	11 (27%)	51,56,56	2.59	16 (31%)
24	CLA	O	201	-	69,73,73	1.18	10 (14%)	82,113,113	1.29	8 (9%)
30	DGD	B	843	-	61,61,67	0.88	2 (3%)	75,75,81	1.19	8 (10%)
31	LMU	B	844	-	36,36,36	1.13	2 (5%)	47,47,47	1.11	4 (8%)
24	CLA	A	839	1	69,73,73	1.20	8 (11%)	82,113,113	1.35	9 (10%)
33	II0	e	613	-	39,43,43	6.63	23 (58%)	48,60,60	1.80	14 (29%)
24	CLA	A	807	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	8 (9%)
34	IHT	O	203	-	40,42,42	6.25	26 (65%)	52,58,58	2.25	16 (30%)
27	WVN	A	850	-	40,41,41	1.69	12 (30%)	51,56,56	2.19	14 (27%)
33	II0	c	614	-	39,43,43	6.84	20 (51%)	48,60,60	2.14	17 (35%)
24	CLA	A	840	-	69,73,73	1.12	9 (13%)	82,113,113	1.22	7 (8%)
24	CLA	c	609	26	49,53,73	1.39	7 (14%)	58,89,113	1.28	8 (13%)
28	LMT	b	319	-	24,24,36	1.05	2 (8%)	29,29,47	1.03	1 (3%)
24	CLA	A	836	-	69,73,73	1.15	6 (8%)	82,113,113	1.46	11 (13%)
24	CLA	j	309	19	49,53,73	1.36	8 (16%)	58,89,113	1.40	7 (12%)
33	II0	h	309	-	26,28,43	6.09	12 (46%)	30,37,60	2.03	10 (33%)
32	LMG	O	204	-	26,26,55	1.27	2 (7%)	34,34,63	1.26	4 (11%)
24	CLA	A	823	-	59,63,73	1.25	7 (11%)	70,101,113	1.22	6 (8%)
34	IHT	g	319	-	40,42,42	6.16	26 (65%)	52,58,58	2.25	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	R	201	-	40,41,41	1.72	10 (25%)	51,56,56	2.07	13 (25%)
32	LMG	b	301	-	55,55,55	0.90	2 (3%)	63,63,63	1.13	5 (7%)
24	CLA	k	606	18	55,59,73	1.29	8 (14%)	64,96,113	1.33	5 (7%)
24	CLA	k	614	-	55,59,73	1.31	5 (9%)	64,96,113	1.27	7 (10%)
33	II0	a	315	-	39,43,43	6.89	22 (56%)	48,60,60	1.68	12 (25%)
24	CLA	g	309	22	69,73,73	1.16	7 (10%)	82,113,113	1.25	9 (10%)
33	II0	e	614	-	39,43,43	6.85	19 (48%)	48,60,60	1.91	15 (31%)
24	CLA	A	805	1	69,73,73	1.15	7 (10%)	82,113,113	1.40	11 (13%)
27	WVN	B	846	-	40,41,41	1.65	11 (27%)	51,56,56	2.29	19 (37%)
24	CLA	A	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	13 (15%)
24	CLA	k	607	-	55,59,73	1.34	7 (12%)	64,96,113	1.36	6 (9%)
24	CLA	A	837	-	69,73,73	1.15	7 (10%)	82,113,113	1.46	12 (14%)
24	CLA	b	307	36	69,73,73	1.19	6 (8%)	82,113,113	1.33	10 (12%)
34	IHT	b	317	-	40,42,42	6.34	26 (65%)	52,58,58	2.85	15 (28%)
24	CLA	b	312	15	69,73,73	1.17	7 (10%)	82,113,113	1.23	7 (8%)
24	CLA	A	803	-	59,63,73	1.23	7 (11%)	70,101,113	1.49	10 (14%)
24	CLA	b	305	-	69,73,73	1.14	7 (10%)	82,113,113	1.28	7 (8%)
27	WVN	L	201	-	40,41,41	1.70	11 (27%)	51,56,56	2.40	16 (31%)
33	II0	b	314	-	39,43,43	6.84	23 (58%)	48,60,60	2.02	11 (22%)
24	CLA	d	305	-	55,59,73	1.29	7 (12%)	64,96,113	1.19	8 (12%)
26	LHG	b	302	24	48,48,48	0.93	2 (4%)	51,54,54	1.21	5 (9%)
24	CLA	B	820	-	59,63,73	1.23	7 (11%)	70,101,113	1.31	9 (12%)
34	IHT	R	204	-	40,42,42	6.30	25 (62%)	52,58,58	2.18	17 (32%)
24	CLA	k	609	18	69,73,73	1.19	7 (10%)	82,113,113	1.30	10 (12%)
34	IHT	a	316	-	40,42,42	6.23	26 (65%)	52,58,58	2.07	16 (30%)
24	CLA	B	826	-	69,73,73	1.13	8 (11%)	82,113,113	1.22	7 (8%)
24	CLA	i	607	20	55,59,73	1.30	7 (12%)	64,96,113	1.30	9 (14%)
24	CLA	B	814	-	63,67,73	1.18	7 (11%)	74,105,113	1.34	8 (10%)
24	CLA	A	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.31	7 (8%)
24	CLA	B	822	36	69,73,73	1.19	7 (10%)	82,113,113	1.57	15 (18%)
24	CLA	B	806	-	69,73,73	1.16	10 (14%)	82,113,113	1.31	8 (9%)
27	WVN	A	847	-	40,41,41	1.72	11 (27%)	51,56,56	3.12	23 (45%)
24	CLA	a	312	-	52,56,73	1.36	9 (17%)	61,92,113	1.36	10 (16%)

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
24	CLA	a	303	14	1/1/12/20	7/21/97/115	-
24	CLA	c	607	13	1/1/11/20	3/17/93/115	-
33	II0	f	614	-	-	3/21/67/67	0/2/2/2
24	CLA	B	837	-	1/1/15/20	13/39/115/115	-
33	II0	i	613	-	-	3/21/67/67	0/2/2/2
24	CLA	d	307	21	1/1/11/20	6/17/93/115	-
24	CLA	b	303	15	1/1/12/20	10/23/99/115	-
24	CLA	f	605	19	-	8/15/91/115	-
24	CLA	a	304	-	1/1/12/20	3/23/99/115	-
24	CLA	B	817	-	-	7/30/106/115	-
27	WVN	j	301	-	-	9/29/63/63	0/2/2/2
24	CLA	g	303	22	1/1/12/20	7/21/97/115	-
24	CLA	B	807	-	1/1/15/20	10/39/115/115	-
24	CLA	b	304	15	1/1/13/20	8/27/103/115	-
24	CLA	h	305	16	1/1/15/20	10/39/115/115	-
24	CLA	g	304	-	1/1/12/20	4/23/99/115	-
24	CLA	a	309	26	1/1/11/20	6/19/95/115	-
24	CLA	h	307	16	1/1/12/20	9/23/99/115	-
24	CLA	B	811	-	1/1/13/20	6/27/103/115	-
33	II0	g	320	-	-	4/21/67/67	0/2/2/2
32	LMG	J	106	-	-	13/50/70/70	0/1/1/1
33	II0	k	619	-	-	5/21/67/67	0/2/2/2
24	CLA	i	608	26	1/1/11/20	6/17/93/115	-
24	CLA	j	311	26	1/1/14/20	15/35/111/115	-
24	CLA	c	601	13	1/1/12/20	13/23/99/115	-
24	CLA	B	830	36	1/1/15/20	11/39/115/115	-
24	CLA	R	203	-	1/1/12/20	8/23/99/115	-
33	II0	d	315	-	-	8/21/67/67	0/2/2/2
29	SF4	A	854	1,2	-	-	0/6/5/5
28	LMT	a	318	-	-	3/21/61/61	0/2/2/2
35	KC2	i	616	-	-	10/15/71/71	-
35	KC2	k	611	18	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	e	610	36	-	9/39/115/115	-
24	CLA	f	613	-	1/1/15/20	21/39/115/115	-
26	LHG	A	844	-	-	4/52/52/53	-
24	CLA	B	809	2	1/1/15/20	11/39/115/115	-
27	WVN	I	101	-	-	9/29/63/63	0/2/2/2
24	CLA	j	308	-	1/1/12/20	9/23/99/115	-
24	CLA	k	603	-	1/1/12/20	2/23/99/115	-
33	II0	O	202	-	-	3/21/67/67	0/2/2/2
33	II0	k	621	-	-	4/21/67/67	0/2/2/2
24	CLA	A	853	-	1/1/15/20	11/39/115/115	-
24	CLA	c	606	-	-	7/24/100/115	-
33	II0	J	104	-	-	7/21/67/67	0/2/2/2
24	CLA	d	309	26	1/1/10/20	2/10/86/115	-
24	CLA	J	105	26	1/1/12/20	6/23/99/115	-
24	CLA	k	601	18	1/1/12/20	9/23/99/115	-
26	LHG	J	107	24	-	19/53/53/53	-
24	CLA	g	322	32	1/1/15/20	14/39/115/115	-
33	II0	j	316	-	-	3/21/67/67	0/2/2/2
24	CLA	B	827	-	1/1/12/20	11/21/97/115	-
26	LHG	e	617	24	-	11/41/41/53	-
24	CLA	B	804	-	1/1/15/20	9/39/115/115	-
24	CLA	A	814	-	-	8/21/97/115	-
24	CLA	h	302	16	1/1/12/20	10/21/97/115	-
34	IHT	c	615	-	-	10/25/65/65	0/2/2/2
24	CLA	A	856	26	1/1/10/20	4/10/86/115	-
24	CLA	A	813	-	1/1/11/20	6/15/91/115	-
24	CLA	b	306	-	-	17/39/115/115	-
24	CLA	A	833	-	1/1/12/20	5/21/97/115	-
24	CLA	j	303	19	1/1/12/20	2/21/97/115	-
33	II0	i	614	-	-	4/21/67/67	0/2/2/2
24	CLA	g	306	22	1/1/12/20	9/23/99/115	-
24	CLA	c	604	13	1/1/15/20	4/39/115/115	-
27	WVN	J	101	-	-	8/29/63/63	0/2/2/2
24	CLA	e	604	36	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	803	-	1/1/15/20	19/39/115/115	-
24	CLA	A	810	-	1/1/14/20	9/36/112/115	-
24	CLA	c	602	13	1/1/12/20	12/21/97/115	-
24	CLA	A	825	36	1/1/15/20	8/39/115/115	-
24	CLA	d	308	21	1/1/10/20	2/10/86/115	-
24	CLA	B	829	-	1/1/12/20	4/21/97/115	-
33	II0	a	314	-	-	7/21/67/67	0/2/2/2
24	CLA	e	601	17	1/1/11/20	9/15/91/115	-
24	CLA	A	812	-	1/1/15/20	20/39/115/115	-
24	CLA	B	816	-	1/1/13/20	9/32/108/115	-
24	CLA	c	612	-	1/1/15/20	12/39/115/115	-
24	CLA	O	205	-	1/1/15/20	17/39/115/115	-
33	II0	i	612	-	-	7/21/67/67	0/2/2/2
24	CLA	A	819	-	1/1/11/20	6/15/91/115	-
24	CLA	f	609	19	1/1/15/20	4/39/115/115	-
34	IHT	f	617	-	-	4/25/65/65	0/2/2/2
24	CLA	A	855	36	1/1/15/20	15/39/115/115	-
25	PQN	B	842	-	-	13/23/43/43	0/2/2/2
24	CLA	d	304	21	1/1/12/20	8/23/99/115	-
24	CLA	A	820	36	1/1/15/20	5/39/115/115	-
26	LHG	a	301	24	-	15/53/53/53	-
24	CLA	i	610	-	1/1/12/20	7/23/99/115	-
24	CLA	L	207	36	1/1/12/20	5/23/99/115	-
24	CLA	A	828	-	1/1/15/20	8/39/115/115	-
24	CLA	B	813	-	1/1/14/20	13/33/109/115	-
24	CLA	j	313	-	1/1/12/20	5/23/99/115	-
33	II0	f	615	-	-	4/21/67/67	0/2/2/2
24	CLA	B	808	-	1/1/15/20	13/39/115/115	-
24	CLA	B	801	36	1/1/15/20	12/39/115/115	-
24	CLA	A	822	-	1/1/12/20	8/23/99/115	-
24	CLA	k	604	18	1/1/15/20	8/39/115/115	-
24	CLA	e	606	17	1/1/15/20	11/39/115/115	-
24	CLA	A	806	-	-	9/39/115/115	-
35	KC2	e	609	17	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	L	204	36	1/1/12/20	7/21/97/115	-
24	CLA	f	610	26	1/1/15/20	15/39/115/115	-
28	LMT	A	851	-	-	10/21/61/61	0/2/2/2
27	WVN	A	846	-	-	8/29/63/63	0/2/2/2
24	CLA	e	607	17	1/1/15/20	10/39/115/115	-
24	CLA	A	832	-	-	14/39/115/115	-
27	WVN	M	101	-	-	9/29/63/63	0/2/2/2
24	CLA	B	823	36	1/1/14/20	9/38/114/115	-
24	CLA	g	307	22	1/1/12/20	8/23/99/115	-
33	II0	f	616	-	-	3/21/67/67	0/2/2/2
34	IHT	k	618	-	-	7/25/65/65	0/2/2/2
24	CLA	c	611	-	1/1/11/20	8/15/91/115	-
24	CLA	g	305	22	1/1/15/20	14/39/115/115	-
24	CLA	i	606	20	1/1/14/20	9/35/111/115	-
35	KC2	i	609	20	-	8/15/71/71	-
24	CLA	A	852	36	1/1/15/20	2/39/115/115	-
24	CLA	c	603	-	1/1/12/20	2/23/99/115	-
24	CLA	A	811	-	1/1/12/20	7/26/102/115	-
24	CLA	f	602	19	1/1/15/20	19/39/115/115	-
24	CLA	f	601	19	1/1/11/20	12/18/94/115	-
24	CLA	A	826	-	1/1/15/20	7/39/115/115	-
24	CLA	B	838	-	1/1/13/20	9/30/106/115	-
24	CLA	d	306	-	1/1/12/20	11/23/99/115	-
24	CLA	g	308	-	1/1/15/20	19/39/115/115	-
33	II0	g	317	-	-	5/21/67/67	0/2/2/2
24	CLA	k	605	18	1/1/11/20	5/15/91/115	-
24	CLA	k	608	18	1/1/15/20	11/39/115/115	-
27	WVN	R	202	-	-	10/29/63/63	0/2/2/2
24	CLA	a	305	36	1/1/15/20	6/39/115/115	-
24	CLA	A	815	36	1/1/11/20	5/15/91/115	-
24	CLA	g	302	22	1/1/10/20	0/12/88/115	-
35	KC2	k	612	35	-	8/15/71/71	-
32	LMG	L	208	24	-	19/50/70/70	0/1/1/1
24	CLA	A	809	-	1/1/13/20	7/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	WVN	B	847	-	-	12/29/63/63	0/2/2/2
27	WVN	J	102	-	-	8/29/63/63	0/2/2/2
33	II0	c	616	-	-	3/21/67/67	0/2/2/2
35	KC2	k	613	35	-	7/15/71/71	-
33	II0	e	612	-	-	4/21/67/67	0/2/2/2
24	CLA	a	308	14	1/1/15/20	13/39/115/115	-
24	CLA	K	102	-	1/1/10/20	5/12/88/115	-
34	IHT	j	317	-	-	7/25/65/65	0/2/2/2
24	CLA	j	307	19	1/1/12/20	10/23/99/115	-
24	CLA	i	611	-	1/1/12/20	13/23/99/115	-
24	CLA	b	311	-	1/1/12/20	5/23/99/115	-
33	II0	j	315	-	-	4/21/67/67	0/2/2/2
24	CLA	j	305	19	-	9/39/115/115	-
24	CLA	d	312	-	-	6/23/99/115	-
24	CLA	a	307	14	1/1/15/20	16/39/115/115	-
29	SF4	C	101	3	-	-	0/6/5/5
24	CLA	g	315	-	1/1/12/20	7/23/99/115	-
24	CLA	c	605	13	1/1/12/20	9/23/99/115	-
24	CLA	e	602	17	1/1/12/20	7/21/97/115	-
33	II0	b	318	-	-	5/21/67/67	0/2/2/2
29	SF4	C	102	3	-	-	0/6/5/5
33	II0	k	615	-	-	6/21/67/67	0/2/2/2
24	CLA	K	101	36	1/1/12/20	2/23/99/115	-
24	CLA	j	306	19	1/1/11/20	7/15/91/115	-
33	II0	k	617	-	-	2/21/67/67	0/2/2/2
24	CLA	A	841	36	1/1/15/20	18/39/115/115	-
27	WVN	A	849	-	-	8/29/63/63	0/2/2/2
33	II0	a	317	-	-	7/21/67/67	0/2/2/2
24	CLA	j	314	-	1/1/15/20	14/39/115/115	-
24	CLA	L	202	9	1/1/11/20	8/20/96/115	-
27	WVN	K	103	-	-	5/29/63/63	0/2/2/2
27	WVN	A	848	-	-	9/29/63/63	0/2/2/2
24	CLA	a	302	14	1/1/12/20	11/24/100/115	-
35	KC2	j	312	19	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	f	612	-	1/1/12/20	6/23/99/115	-
24	CLA	e	608	26	1/1/11/20	9/17/93/115	-
26	LHG	j	319	24	-	5/34/34/53	-
24	CLA	f	603	-	1/1/12/20	6/23/99/115	-
24	CLA	A	816	-	1/1/15/20	14/39/115/115	-
24	CLA	A	824	36	1/1/15/20	9/39/115/115	-
35	KC2	g	313	35	-	2/15/71/71	-
24	CLA	d	301	21	1/1/12/20	7/21/97/115	-
24	CLA	A	804	-	1/1/15/20	5/39/115/115	-
33	II0	g	316	-	-	7/21/67/67	0/2/2/2
24	CLA	B	831	36	1/1/11/20	6/15/91/115	-
24	CLA	A	817	-	1/1/15/20	15/39/115/115	-
24	CLA	j	302	19	1/1/12/20	2/23/99/115	-
33	II0	h	311	-	-	6/21/67/67	0/2/2/2
33	II0	d	313	-	-	6/21/67/67	0/2/2/2
24	CLA	B	834	-	1/1/11/20	4/18/94/115	-
26	LHG	b	320	24	-	16/53/53/53	-
33	II0	e	616	-	-	5/21/67/67	0/2/2/2
24	CLA	A	842	-	1/1/15/20	21/39/115/115	-
33	II0	b	315	-	-	5/21/67/67	0/2/2/2
27	WVN	B	845	-	-	7/29/63/63	0/2/2/2
33	II0	a	313	-	-	1/21/67/67	0/2/2/2
24	CLA	I	102	36	1/1/15/20	17/39/115/115	-
26	LHG	f	620	-	-	17/53/53/53	-
24	CLA	h	306	16	1/1/13/20	9/30/106/115	-
24	CLA	f	608	19	1/1/15/20	8/39/115/115	-
24	CLA	B	819	-	-	2/17/93/115	-
24	CLA	b	310	26	1/1/15/20	10/39/115/115	-
26	LHG	c	618	24	-	11/41/41/53	-
26	LHG	c	617	24	-	13/41/41/53	-
24	CLA	c	608	13	1/1/15/20	16/39/115/115	-
24	CLA	g	310	22	1/1/12/20	6/23/99/115	-
26	LHG	g	321	24	-	12/41/41/53	-
34	IHT	b	316	-	-	3/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	309	15	1/1/15/20	18/39/115/115	-
24	CLA	B	839	-	1/1/15/20	10/39/115/115	-
35	KC2	d	310	21	-	6/15/71/71	-
24	CLA	i	601	20	1/1/12/20	7/23/99/115	-
24	CLA	f	606	19	-	6/23/99/115	-
27	WVN	F	204	-	-	8/29/63/63	0/2/2/2
24	CLA	B	805	-	1/1/15/20	14/39/115/115	-
24	CLA	B	812	-	1/1/15/20	12/39/115/115	-
24	CLA	B	832	-	1/1/13/20	6/31/107/115	-
24	CLA	k	602	18	1/1/12/20	6/21/97/115	-
28	LMT	F	203	-	-	4/15/35/61	0/1/1/2
24	CLA	A	838	26	1/1/12/20	5/24/100/115	-
24	CLA	B	840	-	-	10/39/115/115	-
26	LHG	d	316	24	-	10/41/41/53	-
24	CLA	i	603	-	1/1/12/20	3/23/99/115	-
24	CLA	J	103	8	1/1/10/20	3/12/88/115	-
26	LHG	g	301	-	-	14/53/53/53	-
33	II0	f	618	-	-	7/21/67/67	0/2/2/2
24	CLA	k	610	26	1/1/12/20	11/23/99/115	-
24	CLA	a	310	14	1/1/15/20	12/39/115/115	-
24	CLA	a	311	-	1/1/11/20	10/18/94/115	-
24	CLA	f	607	-	1/1/15/20	17/39/115/115	-
24	CLA	j	304	-	1/1/12/20	0/23/99/115	-
25	PQN	A	843	-	-	5/23/43/43	0/2/2/2
24	CLA	d	302	-	1/1/12/20	4/23/99/115	-
24	CLA	B	836	-	1/1/15/20	25/39/115/115	-
33	II0	k	616	-	-	6/21/67/67	0/2/2/2
24	CLA	B	828	-	-	5/20/96/115	-
27	WVN	e	615	-	-	11/29/63/63	0/2/2/2
24	CLA	F	202	6	1/1/12/20	10/24/100/115	-
27	WVN	L	206	-	-	3/29/63/63	0/2/2/2
24	CLA	h	312	36	1/1/15/20	9/39/115/115	-
35	KC2	g	312	22	-	8/15/71/71	-
24	CLA	B	818	36	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	835	36	1/1/15/20	11/39/115/115	-
35	KC2	d	311	-	-	6/15/71/71	-
24	CLA	F	201	36	1/1/15/20	15/39/115/115	-
27	WVN	F	205	-	-	12/29/63/63	0/2/2/2
24	CLA	j	310	19	1/1/12/20	3/23/99/115	-
33	II0	h	310	-	-	7/21/67/67	0/2/2/2
26	LHG	i	615	24	-	11/41/41/53	-
27	WVN	h	308	-	-	5/29/63/63	0/2/2/2
24	CLA	B	815	-	1/1/13/20	7/27/103/115	-
33	II0	d	314	-	-	5/21/67/67	0/2/2/2
24	CLA	A	830	-	1/1/12/20	4/21/97/115	-
24	CLA	e	605	17	1/1/15/20	13/39/115/115	-
24	CLA	e	603	17	1/1/12/20	4/23/99/115	-
24	CLA	B	810	-	1/1/13/20	4/25/101/115	-
24	CLA	A	821	-	1/1/11/20	7/20/96/115	-
24	CLA	i	602	20	1/1/12/20	9/21/97/115	-
24	CLA	h	301	16	1/1/12/20	6/21/97/115	-
27	WVN	L	205	-	-	6/29/63/63	0/2/2/2
24	CLA	A	808	1	1/1/15/20	10/39/115/115	-
33	II0	j	318	-	-	5/21/67/67	0/2/2/2
24	CLA	L	203	-	1/1/15/20	12/39/115/115	-
26	LHG	B	802	-	-	16/42/42/53	-
24	CLA	A	801	-	1/1/15/20	10/39/115/115	-
32	LMG	F	206	-	-	11/43/63/70	0/1/1/1
24	CLA	d	303	21	1/1/15/20	13/39/115/115	-
24	CLA	g	311	26	1/1/12/20	10/26/102/115	-
35	KC2	f	611	19	-	7/15/71/71	-
27	WVN	B	849	-	-	12/29/63/63	0/2/2/2
24	CLA	a	306	14	1/1/11/20	8/15/91/115	-
24	CLA	B	821	-	1/1/12/20	6/25/101/115	-
24	CLA	h	304	-	1/1/12/20	6/23/99/115	-
24	CLA	A	831	-	1/1/15/20	11/39/115/115	-
26	LHG	f	619	24	-	22/41/41/53	-
24	CLA	A	818	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	i	604	20	1/1/15/20	12/39/115/115	-
24	CLA	B	841	26	-	3/39/115/115	-
33	II0	g	318	-	-	2/21/67/67	0/2/2/2
24	CLA	A	834	-	1/1/12/20	2/23/99/115	-
24	CLA	b	308	15	1/1/14/20	14/35/111/115	-
24	CLA	b	313	-	1/1/15/20	23/39/115/115	-
35	KC2	g	314	35	-	9/15/71/71	-
24	CLA	i	605	20	1/1/12/20	8/23/99/115	-
24	CLA	B	825	-	1/1/15/20	9/39/115/115	-
26	LHG	A	845	24	-	5/31/31/53	-
24	CLA	B	824	-	1/1/15/20	3/39/115/115	-
26	LHG	k	620	24	-	12/41/41/53	-
35	KC2	c	610	-	-	10/15/71/71	-
24	CLA	e	611	-	1/1/15/20	14/39/115/115	-
24	CLA	A	827	-	1/1/14/20	8/36/112/115	-
24	CLA	h	303	-	1/1/12/20	6/23/99/115	-
24	CLA	A	829	-	1/1/15/20	14/39/115/115	-
24	CLA	f	604	19	-	5/39/115/115	-
24	CLA	B	833	-	1/1/15/20	8/39/115/115	-
33	II0	c	613	-	-	3/21/67/67	0/2/2/2
27	WVN	B	848	-	-	7/29/63/63	0/2/2/2
24	CLA	O	201	-	1/1/15/20	14/39/115/115	-
30	DGD	B	843	-	-	5/49/89/95	0/2/2/2
31	LMU	B	844	-	-	8/21/61/61	0/2/2/2
24	CLA	A	839	1	1/1/15/20	12/39/115/115	-
33	II0	e	613	-	-	5/21/67/67	0/2/2/2
24	CLA	A	807	1	1/1/15/20	9/39/115/115	-
34	IHT	O	203	-	-	5/25/65/65	0/2/2/2
27	WVN	A	850	-	-	13/29/63/63	0/2/2/2
33	II0	c	614	-	-	1/21/67/67	0/2/2/2
24	CLA	A	840	-	1/1/15/20	16/39/115/115	-
24	CLA	c	609	26	1/1/11/20	4/15/91/115	-
28	LMT	b	319	-	-	9/15/35/61	0/1/1/2
24	CLA	A	836	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	j	309	19	1/1/11/20	5/15/91/115	-
33	II0	h	309	-	-	3/17/40/67	0/1/1/2
32	LMG	O	204	-	-	7/21/41/70	0/1/1/1
24	CLA	A	823	-	1/1/13/20	6/27/103/115	-
34	IHT	g	319	-	-	11/25/65/65	0/2/2/2
27	WVN	R	201	-	-	6/29/63/63	0/2/2/2
32	LMG	b	301	-	-	18/50/70/70	0/1/1/1
24	CLA	k	606	18	-	8/23/99/115	-
24	CLA	k	614	-	-	8/23/99/115	-
33	II0	a	315	-	-	3/21/67/67	0/2/2/2
24	CLA	g	309	22	1/1/15/20	6/39/115/115	-
33	II0	e	614	-	-	3/21/67/67	0/2/2/2
24	CLA	A	805	1	1/1/15/20	7/39/115/115	-
27	WVN	B	846	-	-	0/29/63/63	0/2/2/2
24	CLA	A	802	-	1/1/15/20	16/39/115/115	-
24	CLA	k	607	-	1/1/12/20	9/23/99/115	-
24	CLA	A	837	-	1/1/15/20	9/39/115/115	-
24	CLA	b	307	36	1/1/15/20	10/39/115/115	-
34	IHT	b	317	-	-	7/25/65/65	0/2/2/2
24	CLA	b	312	15	1/1/15/20	21/39/115/115	-
24	CLA	A	803	-	1/1/13/20	6/27/103/115	-
24	CLA	b	305	-	1/1/15/20	13/39/115/115	-
27	WVN	L	201	-	-	10/29/63/63	0/2/2/2
33	II0	b	314	-	-	7/21/67/67	0/2/2/2
24	CLA	d	305	-	-	6/23/99/115	-
26	LHG	b	302	24	-	12/53/53/53	-
24	CLA	B	820	-	-	9/27/103/115	-
34	IHT	R	204	-	-	3/25/65/65	0/2/2/2
24	CLA	k	609	18	1/1/15/20	12/39/115/115	-
34	IHT	a	316	-	-	9/25/65/65	0/2/2/2
24	CLA	B	826	-	1/1/15/20	7/39/115/115	-
24	CLA	i	607	20	1/1/12/20	1/23/99/115	-
24	CLA	B	814	-	1/1/13/20	12/32/108/115	-
24	CLA	A	835	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	822	36	1/1/15/20	10/39/115/115	-
24	CLA	B	806	-	1/1/15/20	14/39/115/115	-
27	WVN	A	847	-	-	11/29/63/63	0/2/2/2
24	CLA	a	312	-	1/1/11/20	5/19/95/115	-

All (3377) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	317	IHT	C15-C11	25.56	1.63	1.35
34	R	204	IHT	C15-C11	25.44	1.63	1.35
34	c	615	IHT	C15-C11	25.28	1.63	1.35
34	k	618	IHT	C15-C11	25.23	1.63	1.35
34	j	317	IHT	C15-C11	25.14	1.62	1.35
34	b	316	IHT	C15-C11	25.09	1.62	1.35
34	f	617	IHT	C15-C11	24.92	1.62	1.35
34	O	203	IHT	C15-C11	24.81	1.62	1.35
34	a	316	IHT	C15-C11	24.76	1.62	1.35
33	b	318	II0	C13-C09	24.61	1.62	1.35
34	g	319	IHT	C15-C11	24.50	1.62	1.35
33	c	616	II0	C14-C10	23.84	1.61	1.35
33	d	315	II0	C14-C10	23.79	1.61	1.35
33	c	614	II0	C13-C09	23.76	1.61	1.35
33	a	315	II0	C13-C09	23.70	1.61	1.35
33	b	314	II0	C14-C10	23.69	1.61	1.35
33	e	614	II0	C13-C09	23.65	1.61	1.35
33	a	317	II0	C14-C10	23.63	1.61	1.35
33	a	317	II0	C13-C09	23.56	1.61	1.35
33	c	614	II0	C14-C10	23.56	1.61	1.35
33	a	315	II0	C14-C10	23.55	1.61	1.35
33	k	621	II0	C14-C10	23.50	1.61	1.35
33	k	621	II0	C13-C09	23.42	1.60	1.35
33	k	616	II0	C13-C09	23.40	1.60	1.35
33	e	614	II0	C14-C10	23.30	1.60	1.35
33	c	613	II0	C14-C10	23.24	1.60	1.35
33	i	613	II0	C13-C09	23.21	1.60	1.35
33	h	311	II0	C13-C09	23.20	1.60	1.35
33	k	617	II0	C14-C10	23.17	1.60	1.35
33	d	313	II0	C13-C09	23.14	1.60	1.35
33	g	316	II0	C14-C10	23.14	1.60	1.35
33	e	616	II0	C14-C10	23.10	1.60	1.35
33	j	318	II0	C13-C09	23.05	1.60	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	O	202	II0	C14-C10	23.04	1.60	1.35
33	b	314	II0	C13-C09	23.03	1.60	1.35
33	e	612	II0	C14-C10	22.99	1.60	1.35
33	h	309	II0	C13-C09	22.98	1.60	1.35
33	d	313	II0	C14-C10	22.96	1.60	1.35
33	g	320	II0	C14-C10	22.93	1.60	1.35
33	d	314	II0	C13-C09	22.91	1.60	1.35
33	g	318	II0	C14-C10	22.88	1.60	1.35
33	d	315	II0	C13-C09	22.86	1.60	1.35
33	j	316	II0	C14-C10	22.81	1.60	1.35
33	e	616	II0	C13-C09	22.77	1.60	1.35
33	c	616	II0	C13-C09	22.77	1.60	1.35
33	i	613	II0	C14-C10	22.75	1.60	1.35
33	b	315	II0	C14-C10	22.75	1.60	1.35
33	i	614	II0	C14-C10	22.74	1.60	1.35
33	f	615	II0	C13-C09	22.72	1.60	1.35
33	a	314	II0	C14-C10	22.71	1.60	1.35
33	g	318	II0	C13-C09	22.67	1.60	1.35
33	i	614	II0	C13-C09	22.56	1.60	1.35
33	j	315	II0	C14-C10	22.56	1.60	1.35
33	k	619	II0	C13-C09	22.56	1.60	1.35
33	f	615	II0	C14-C10	22.51	1.59	1.35
33	g	316	II0	C13-C09	22.51	1.59	1.35
33	h	311	II0	C14-C10	22.49	1.59	1.35
33	f	618	II0	C13-C09	22.49	1.59	1.35
33	a	313	II0	C14-C10	22.48	1.59	1.35
33	c	613	II0	C13-C09	22.47	1.59	1.35
33	k	619	II0	C14-C10	22.46	1.59	1.35
33	k	615	II0	C14-C10	22.38	1.59	1.35
33	g	317	II0	C13-C09	22.38	1.59	1.35
33	k	617	II0	C13-C09	22.38	1.59	1.35
33	k	616	II0	C14-C10	22.38	1.59	1.35
33	i	612	II0	C13-C09	22.33	1.59	1.35
33	e	613	II0	C14-C10	22.33	1.59	1.35
33	a	314	II0	C13-C09	22.31	1.59	1.35
33	O	202	II0	C13-C09	22.29	1.59	1.35
33	a	313	II0	C13-C09	22.28	1.59	1.35
33	j	316	II0	C13-C09	22.26	1.59	1.35
33	g	320	II0	C13-C09	22.24	1.59	1.35
33	J	104	II0	C14-C10	22.23	1.59	1.35
33	e	613	II0	C13-C09	22.23	1.59	1.35
33	f	618	II0	C14-C10	22.22	1.59	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	317	II0	C14-C10	22.18	1.59	1.35
33	b	315	II0	C13-C09	22.17	1.59	1.35
33	f	614	II0	C13-C09	22.17	1.59	1.35
33	f	614	II0	C14-C10	22.07	1.59	1.35
33	d	314	II0	C14-C10	22.02	1.59	1.35
33	f	616	II0	C14-C10	22.01	1.59	1.35
33	k	615	II0	C13-C09	22.00	1.59	1.35
33	i	612	II0	C14-C10	22.00	1.59	1.35
33	J	104	II0	C13-C09	21.97	1.59	1.35
33	f	616	II0	C13-C09	21.88	1.59	1.35
33	j	318	II0	C14-C10	21.79	1.59	1.35
33	j	315	II0	C13-C09	21.77	1.59	1.35
33	e	612	II0	C13-C09	21.72	1.59	1.35
33	h	310	II0	C13-C09	21.65	1.59	1.35
33	h	310	II0	C14-C10	21.36	1.58	1.35
33	b	318	II0	C14-C10	21.16	1.58	1.35
34	b	317	IHT	C10-C07	15.50	1.60	1.34
34	b	316	IHT	C10-C07	15.43	1.60	1.34
34	R	204	IHT	C10-C07	15.43	1.60	1.34
34	c	615	IHT	C10-C07	15.35	1.60	1.34
34	O	203	IHT	C10-C07	15.27	1.60	1.34
34	a	316	IHT	C10-C07	15.26	1.60	1.34
34	k	618	IHT	C10-C07	15.25	1.60	1.34
34	g	319	IHT	C10-C07	15.09	1.59	1.34
34	f	617	IHT	C10-C07	15.00	1.59	1.34
34	j	317	IHT	C10-C07	14.90	1.59	1.34
33	J	104	II0	C05-C07	-12.01	1.35	1.52
33	k	616	II0	C05-C07	-11.97	1.35	1.52
33	h	310	II0	C05-C07	-11.96	1.35	1.52
33	k	617	II0	C05-C07	-11.88	1.35	1.52
33	f	614	II0	C05-C07	-11.78	1.35	1.52
34	R	204	IHT	C05-C08	-11.75	1.35	1.52
34	f	617	IHT	C05-C08	-11.72	1.35	1.52
33	g	316	II0	C05-C07	-11.69	1.35	1.52
33	a	317	II0	C05-C07	-11.65	1.35	1.52
33	f	615	II0	C05-C07	-11.65	1.35	1.52
33	b	318	II0	C05-C07	-11.64	1.35	1.52
33	g	318	II0	C05-C07	-11.63	1.35	1.52
33	g	320	II0	C05-C07	-11.60	1.35	1.52
33	f	616	II0	C05-C07	-11.60	1.35	1.52
33	c	616	II0	C05-C07	-11.59	1.35	1.52
33	h	311	II0	C05-C07	-11.58	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	315	II0	C05-C07	-11.57	1.35	1.52
33	g	317	II0	C06-C08	-11.56	1.35	1.52
33	d	313	II0	C05-C07	-11.55	1.35	1.52
33	c	613	II0	C05-C07	-11.54	1.36	1.52
33	e	613	II0	C05-C07	-11.54	1.36	1.52
34	g	319	IHT	C05-C08	-11.52	1.36	1.52
34	b	316	IHT	C05-C08	-11.51	1.36	1.52
33	i	613	II0	C05-C07	-11.48	1.36	1.52
33	b	315	II0	C11-C07	11.46	1.72	1.52
34	O	203	IHT	C05-C08	-11.45	1.36	1.52
34	c	615	IHT	C05-C08	-11.45	1.36	1.52
34	k	618	IHT	C05-C08	-11.44	1.36	1.52
34	b	317	IHT	C05-C08	-11.41	1.36	1.52
33	e	614	II0	C05-C07	-11.40	1.36	1.52
33	O	202	II0	C05-C07	-11.39	1.36	1.52
33	j	315	II0	C05-C07	-11.38	1.36	1.52
33	e	616	II0	C11-C07	11.35	1.72	1.52
33	h	309	II0	C05-C07	-11.35	1.36	1.52
33	k	621	II0	C05-C07	-11.32	1.36	1.52
33	a	314	II0	C05-C07	-11.29	1.36	1.52
33	c	614	II0	C05-C07	-11.28	1.36	1.52
34	j	317	IHT	C05-C08	-11.28	1.36	1.52
33	a	313	II0	C05-C07	-11.26	1.36	1.52
33	k	615	II0	C05-C07	-11.23	1.36	1.52
33	b	315	II0	C06-C08	-11.17	1.36	1.52
33	j	316	II0	C05-C07	-11.15	1.36	1.52
33	b	315	II0	C05-C07	-11.13	1.36	1.52
33	b	314	II0	C05-C07	-11.12	1.36	1.52
33	d	314	II0	C05-C07	-11.09	1.36	1.52
33	g	317	II0	C11-C07	11.08	1.71	1.52
34	a	316	IHT	C05-C08	-11.06	1.36	1.52
33	j	318	II0	C05-C07	-11.05	1.36	1.52
34	j	317	IHT	C12-C08	11.04	1.71	1.52
33	e	612	II0	C11-C07	11.04	1.71	1.52
33	j	316	II0	C06-C08	-11.03	1.36	1.52
33	i	612	II0	C05-C07	-11.02	1.36	1.52
34	O	203	IHT	C12-C08	11.02	1.71	1.52
34	c	615	IHT	C12-C08	11.01	1.71	1.52
33	h	311	II0	C06-C08	-11.00	1.36	1.52
34	a	316	IHT	C12-C08	10.98	1.71	1.52
33	g	320	II0	C06-C08	-10.95	1.36	1.52
33	k	619	II0	C11-C07	10.91	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	e	612	II0	C05-C07	-10.91	1.36	1.52
33	c	614	II0	C06-C08	-10.86	1.36	1.52
33	f	618	II0	C11-C07	10.86	1.71	1.52
34	g	319	IHT	C12-C08	10.85	1.71	1.52
34	f	617	IHT	C12-C08	10.84	1.71	1.52
33	k	616	II0	C06-C08	-10.84	1.36	1.52
34	b	317	IHT	C12-C08	10.84	1.71	1.52
34	R	204	IHT	C12-C08	10.84	1.71	1.52
33	h	310	II0	C06-C08	-10.83	1.37	1.52
33	c	616	II0	C11-C07	10.82	1.71	1.52
33	g	317	II0	C05-C07	-10.82	1.37	1.52
34	b	316	IHT	C12-C08	10.81	1.71	1.52
33	O	202	II0	C06-C08	-10.80	1.37	1.52
33	k	619	II0	C05-C07	-10.80	1.37	1.52
33	i	612	II0	C06-C08	-10.77	1.37	1.52
33	k	617	II0	C11-C07	10.74	1.71	1.52
33	f	615	II0	C06-C08	-10.73	1.37	1.52
34	k	618	IHT	C12-C08	10.71	1.71	1.52
33	k	621	II0	C11-C07	10.70	1.71	1.52
33	d	315	II0	C05-C07	-10.68	1.37	1.52
33	e	616	II0	C05-C07	-10.67	1.37	1.52
33	d	315	II0	C11-C07	10.67	1.71	1.52
33	f	614	II0	C06-C08	-10.66	1.37	1.52
33	g	316	II0	C06-C08	-10.65	1.37	1.52
33	g	320	II0	C11-C07	10.65	1.70	1.52
33	b	314	II0	C11-C07	10.64	1.70	1.52
33	b	318	II0	C11-C07	10.61	1.70	1.52
33	J	104	II0	C06-C08	-10.60	1.37	1.52
33	i	614	II0	C05-C07	-10.60	1.37	1.52
33	g	318	II0	C11-C07	10.59	1.70	1.52
33	d	314	II0	C11-C07	10.58	1.70	1.52
33	e	612	II0	C06-C08	-10.58	1.37	1.52
33	f	618	II0	C06-C08	-10.57	1.37	1.52
33	b	314	II0	C06-C08	-10.57	1.37	1.52
33	j	315	II0	C11-C07	10.57	1.70	1.52
33	j	318	II0	C11-C07	10.56	1.70	1.52
33	k	615	II0	C06-C08	-10.55	1.37	1.52
33	f	616	II0	C11-C07	10.54	1.70	1.52
33	d	313	II0	C06-C08	-10.54	1.37	1.52
33	a	314	II0	C06-C08	-10.52	1.37	1.52
33	g	316	II0	C11-C07	10.49	1.70	1.52
33	d	313	II0	C11-C07	10.48	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	i	614	II0	C11-C07	10.47	1.70	1.52
33	f	618	II0	C05-C07	-10.47	1.37	1.52
33	e	614	II0	C11-C07	10.44	1.70	1.52
33	k	615	II0	C11-C07	10.42	1.70	1.52
33	d	315	II0	C06-C08	-10.40	1.37	1.52
33	k	621	II0	C06-C08	-10.40	1.37	1.52
33	h	310	II0	C11-C07	10.39	1.70	1.52
33	i	613	II0	C06-C08	-10.39	1.37	1.52
33	h	311	II0	C11-C07	10.37	1.70	1.52
33	a	317	II0	C11-C07	10.32	1.70	1.52
33	h	309	II0	C11-C07	10.30	1.70	1.52
33	j	315	II0	C06-C08	-10.30	1.37	1.52
33	c	613	II0	C06-C08	-10.26	1.37	1.52
33	e	613	II0	C06-C08	-10.24	1.37	1.52
33	i	613	II0	C11-C07	10.24	1.70	1.52
33	i	612	II0	C11-C07	10.23	1.70	1.52
33	b	318	II0	C06-C08	-10.23	1.37	1.52
33	a	313	II0	C11-C07	10.21	1.70	1.52
33	O	202	II0	C11-C07	10.21	1.70	1.52
33	f	614	II0	C11-C07	10.20	1.70	1.52
33	c	614	II0	C11-C07	10.20	1.70	1.52
33	a	315	II0	C11-C07	10.17	1.70	1.52
33	k	617	II0	C06-C08	-10.15	1.37	1.52
33	e	614	II0	C06-C08	-10.12	1.38	1.52
33	c	613	II0	C11-C07	10.11	1.70	1.52
33	k	616	II0	C11-C07	10.10	1.70	1.52
33	a	315	II0	C06-C08	-10.09	1.38	1.52
33	a	313	II0	C06-C08	-10.07	1.38	1.52
33	J	104	II0	C11-C07	10.01	1.69	1.52
33	c	616	II0	C06-C08	-10.00	1.38	1.52
33	e	613	II0	C11-C07	9.98	1.69	1.52
33	a	317	II0	C06-C08	-9.98	1.38	1.52
33	a	314	II0	C11-C07	9.98	1.69	1.52
33	j	316	II0	C11-C07	9.94	1.69	1.52
33	g	318	II0	C06-C08	-9.94	1.38	1.52
33	k	619	II0	C06-C08	-9.94	1.38	1.52
33	e	616	II0	C06-C08	-9.80	1.38	1.52
33	d	314	II0	C06-C08	-9.72	1.38	1.52
33	i	614	II0	C06-C08	-9.72	1.38	1.52
33	j	318	II0	C06-C08	-9.66	1.38	1.52
33	f	615	II0	C11-C07	9.63	1.69	1.52
33	f	616	II0	C06-C08	-9.49	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	f	616	II0	C12-C08	8.98	1.68	1.52
33	d	314	II0	C12-C08	8.83	1.67	1.52
33	c	613	II0	C12-C08	8.80	1.67	1.52
33	i	614	II0	C12-C08	8.71	1.67	1.52
33	j	318	II0	C12-C08	8.69	1.67	1.52
33	k	617	II0	C12-C08	8.67	1.67	1.52
33	b	318	II0	C12-C08	8.58	1.67	1.52
33	e	614	II0	C12-C08	8.56	1.67	1.52
33	f	614	II0	C12-C08	8.54	1.67	1.52
33	k	621	II0	C12-C08	8.50	1.67	1.52
33	a	315	II0	C12-C08	8.50	1.67	1.52
33	c	614	II0	C12-C08	8.48	1.67	1.52
33	c	616	II0	C12-C08	8.46	1.67	1.52
33	a	317	II0	C12-C08	8.45	1.67	1.52
33	k	615	II0	C12-C08	8.35	1.66	1.52
33	d	315	II0	C12-C08	8.34	1.66	1.52
33	g	316	II0	C12-C08	8.34	1.66	1.52
33	g	318	II0	C12-C08	8.34	1.66	1.52
33	i	613	II0	C12-C08	8.33	1.66	1.52
33	k	616	II0	C12-C08	8.29	1.66	1.52
33	f	615	II0	C12-C08	8.29	1.66	1.52
33	e	613	II0	C12-C08	8.29	1.66	1.52
33	e	616	II0	C12-C08	8.23	1.66	1.52
33	J	104	II0	C12-C08	8.22	1.66	1.52
33	j	316	II0	C12-C08	8.21	1.66	1.52
33	k	617	II0	C21-C09	8.21	1.58	1.42
33	f	618	II0	C12-C08	8.20	1.66	1.52
33	b	314	II0	C12-C08	8.19	1.66	1.52
33	k	619	II0	C12-C08	8.18	1.66	1.52
33	j	315	II0	C12-C08	8.17	1.66	1.52
33	i	612	II0	C12-C08	8.16	1.66	1.52
33	a	314	II0	C12-C08	8.11	1.66	1.52
33	g	320	II0	C12-C08	8.10	1.66	1.52
33	d	313	II0	C12-C08	8.08	1.66	1.52
33	e	612	II0	C12-C08	8.07	1.66	1.52
33	a	313	II0	C12-C08	8.07	1.66	1.52
33	O	202	II0	C12-C08	7.99	1.66	1.52
33	i	614	II0	C21-C09	7.98	1.57	1.42
33	a	315	II0	C21-C09	7.92	1.57	1.42
33	a	317	II0	C22-C10	7.89	1.57	1.42
33	e	616	II0	C22-C10	7.83	1.57	1.42
33	h	311	II0	C12-C08	7.82	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	318	II0	C21-C09	7.81	1.57	1.42
33	g	317	II0	C12-C08	7.77	1.65	1.52
33	d	315	II0	C22-C10	7.75	1.57	1.42
33	a	317	II0	C21-C09	7.68	1.57	1.42
33	c	616	II0	C22-C10	7.68	1.57	1.42
33	k	617	II0	C22-C10	7.68	1.57	1.42
25	A	843	PQN	C3-C2	7.67	1.49	1.35
33	h	310	II0	C12-C08	7.66	1.65	1.52
33	e	614	II0	C21-C09	7.63	1.56	1.42
33	a	315	II0	C22-C10	7.63	1.56	1.42
33	e	613	II0	C22-C10	7.62	1.56	1.42
33	g	318	II0	C21-C09	7.60	1.56	1.42
33	k	615	II0	C22-C10	7.60	1.56	1.42
33	b	315	II0	C12-C08	7.57	1.65	1.52
33	a	314	II0	C27-C25	7.56	1.55	1.50
33	k	616	II0	C22-C10	7.56	1.56	1.42
33	k	619	II0	C22-C10	7.56	1.56	1.42
33	k	621	II0	C21-C09	7.54	1.56	1.42
33	g	316	II0	C21-C09	7.51	1.56	1.42
35	d	311	KC2	C4C-NC	7.51	1.49	1.37
33	b	314	II0	C22-C10	7.50	1.56	1.42
33	g	316	II0	C27-C25	7.47	1.55	1.50
33	f	618	II0	C22-C10	7.46	1.56	1.42
33	c	614	II0	C21-C09	7.45	1.56	1.42
33	h	309	II0	C21-C09	7.45	1.56	1.42
25	B	842	PQN	C3-C2	7.43	1.48	1.35
33	e	614	II0	C22-C10	7.43	1.56	1.42
33	k	621	II0	C22-C10	7.42	1.56	1.42
33	d	314	II0	C21-C09	7.42	1.56	1.42
33	d	313	II0	C21-C09	7.42	1.56	1.42
33	a	313	II0	C21-C09	7.42	1.56	1.42
33	d	315	II0	C21-C09	7.38	1.56	1.42
33	c	616	II0	C21-C09	7.38	1.56	1.42
33	c	613	II0	C22-C10	7.37	1.56	1.42
33	k	619	II0	C21-C09	7.36	1.56	1.42
33	i	613	II0	C22-C10	7.36	1.56	1.42
35	k	612	KC2	C4C-NC	7.34	1.49	1.37
33	c	614	II0	C22-C10	7.31	1.56	1.42
33	f	616	II0	C22-C10	7.31	1.56	1.42
35	i	609	KC2	C4C-NC	7.31	1.49	1.37
33	g	316	II0	C22-C10	7.31	1.56	1.42
33	f	614	II0	C21-C09	7.30	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	e	612	II0	C22-C10	7.30	1.56	1.42
33	e	612	II0	C21-C09	7.26	1.56	1.42
33	d	313	II0	C22-C10	7.26	1.56	1.42
34	b	316	IHT	C04-C06	-7.24	1.35	1.52
33	i	612	II0	C22-C10	7.24	1.56	1.42
33	j	318	II0	C21-C09	7.24	1.56	1.42
33	g	320	II0	C21-C09	7.23	1.56	1.42
33	O	202	II0	C22-C10	7.22	1.56	1.42
33	f	616	II0	C21-C09	7.22	1.56	1.42
33	i	612	II0	C21-C09	7.21	1.56	1.42
34	a	316	IHT	C04-C06	-7.20	1.35	1.52
33	f	614	II0	C22-C10	7.20	1.56	1.42
35	i	616	KC2	C4C-NC	7.19	1.49	1.37
33	a	313	II0	C22-C10	7.18	1.56	1.42
34	f	617	IHT	C04-C06	-7.18	1.35	1.52
34	k	618	IHT	C04-C06	-7.17	1.35	1.52
34	R	204	IHT	C04-C06	-7.16	1.35	1.52
33	j	318	II0	C22-C10	7.15	1.56	1.42
33	g	320	II0	C22-C10	7.15	1.56	1.42
34	b	317	IHT	C04-C06	-7.15	1.35	1.52
34	b	317	IHT	C21-C11	7.14	1.56	1.42
33	a	314	II0	C22-C10	7.13	1.55	1.42
34	g	319	IHT	C04-C06	-7.12	1.35	1.52
34	O	203	IHT	C04-C06	-7.08	1.35	1.52
34	c	615	IHT	C04-C06	-7.07	1.35	1.52
33	b	315	II0	C21-C09	7.07	1.55	1.42
33	e	613	II0	C21-C09	7.07	1.55	1.42
35	d	310	KC2	C4C-NC	7.07	1.49	1.37
35	e	609	KC2	C4C-NC	7.06	1.49	1.37
33	f	618	II0	C21-C09	7.05	1.55	1.42
33	g	318	II0	C22-C10	7.05	1.55	1.42
33	f	615	II0	C21-C09	7.05	1.55	1.42
33	i	614	II0	C22-C10	7.04	1.55	1.42
33	O	202	II0	C21-C09	7.03	1.55	1.42
33	g	317	II0	C22-C10	7.03	1.55	1.42
34	j	317	IHT	C04-C06	-7.03	1.35	1.52
33	j	316	II0	C22-C10	7.02	1.55	1.42
33	b	314	II0	C21-C09	7.01	1.55	1.42
33	h	311	II0	C22-C10	6.97	1.55	1.42
35	f	611	KC2	C4C-NC	6.97	1.49	1.37
34	j	317	IHT	C02-C07	-6.97	1.44	1.53
35	c	610	KC2	C4C-NC	6.96	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	j	315	II0	C21-C09	6.96	1.55	1.42
34	k	618	IHT	C21-C11	6.94	1.55	1.42
34	j	317	IHT	C21-C11	6.94	1.55	1.42
33	h	310	II0	C21-C09	6.92	1.55	1.42
34	a	316	IHT	C21-C11	6.91	1.55	1.42
34	c	615	IHT	C21-C11	6.91	1.55	1.42
33	i	613	II0	C21-C09	6.90	1.55	1.42
33	h	310	II0	C22-C10	6.89	1.55	1.42
35	g	312	KC2	C4C-NC	6.88	1.48	1.37
33	k	616	II0	C21-C09	6.88	1.55	1.42
33	f	615	II0	C22-C10	6.88	1.55	1.42
34	O	203	IHT	C21-C11	6.87	1.55	1.42
35	k	611	KC2	C4C-NC	6.86	1.48	1.37
33	d	314	II0	C22-C10	6.85	1.55	1.42
35	g	314	KC2	C4C-NC	6.84	1.48	1.37
33	b	318	II0	C22-C10	6.83	1.55	1.42
34	b	316	IHT	C21-C11	6.81	1.55	1.42
35	j	312	KC2	C4C-NC	6.80	1.48	1.37
33	J	104	II0	C21-C09	6.79	1.55	1.42
34	g	319	IHT	C02-C07	-6.78	1.45	1.53
33	a	314	II0	C21-C09	6.78	1.55	1.42
34	O	203	IHT	C02-C07	-6.78	1.45	1.53
33	h	311	II0	C21-C09	6.77	1.55	1.42
33	c	613	II0	C21-C09	6.77	1.55	1.42
33	J	104	II0	C22-C10	6.76	1.55	1.42
33	j	316	II0	C21-C09	6.76	1.55	1.42
33	e	616	II0	C21-C09	6.74	1.55	1.42
34	a	316	IHT	C02-C07	-6.73	1.45	1.53
34	R	204	IHT	C21-C11	6.73	1.55	1.42
35	g	313	KC2	C4C-NC	6.71	1.48	1.37
34	f	617	IHT	C21-C11	6.70	1.55	1.42
33	g	317	II0	C21-C09	6.69	1.55	1.42
33	j	315	II0	C22-C10	6.64	1.55	1.42
35	k	613	KC2	C4C-NC	6.62	1.48	1.37
34	f	617	IHT	C02-C07	-6.61	1.45	1.53
33	k	615	II0	C21-C09	6.61	1.54	1.42
34	b	317	IHT	C02-C07	-6.52	1.45	1.53
34	g	319	IHT	C21-C11	6.50	1.54	1.42
34	b	316	IHT	C02-C07	-6.46	1.45	1.53
34	R	204	IHT	C02-C07	-6.46	1.45	1.53
34	c	615	IHT	C02-C07	-6.44	1.45	1.53
33	b	315	II0	C22-C10	6.27	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	k	618	IHT	C02-C07	-6.19	1.45	1.53
34	c	615	IHT	C22-C23	6.08	1.59	1.46
34	O	203	IHT	C22-C23	6.08	1.59	1.46
34	b	317	IHT	C22-C23	6.07	1.58	1.46
33	a	314	II0	C11-C13	-6.05	1.41	1.51
33	f	615	II0	C11-C13	-6.02	1.41	1.51
34	a	316	IHT	C22-C23	6.00	1.58	1.46
34	k	618	IHT	C22-C23	6.00	1.58	1.46
34	R	204	IHT	C22-C23	5.99	1.58	1.46
34	b	316	IHT	C22-C23	5.97	1.58	1.46
33	h	310	II0	C11-C13	-5.92	1.41	1.51
34	a	316	IHT	C12-C15	-5.91	1.41	1.51
34	j	317	IHT	C22-C23	5.90	1.58	1.46
34	g	319	IHT	C12-C15	-5.90	1.41	1.51
33	k	616	II0	C11-C13	-5.90	1.41	1.51
33	f	614	II0	C11-C13	-5.86	1.41	1.51
34	f	617	IHT	C22-C23	5.84	1.58	1.46
33	J	104	II0	C11-C13	-5.84	1.42	1.51
34	k	618	IHT	C12-C15	-5.83	1.42	1.51
35	g	313	KC2	C2A-C3A	5.79	1.48	1.37
33	i	612	II0	C11-C13	-5.78	1.42	1.51
34	O	203	IHT	C12-C15	-5.77	1.42	1.51
34	f	617	IHT	C12-C15	-5.77	1.42	1.51
35	i	609	KC2	C2A-C3A	5.76	1.48	1.37
33	e	613	II0	C11-C13	-5.74	1.42	1.51
34	j	317	IHT	C12-C15	-5.72	1.42	1.51
34	g	319	IHT	C22-C23	5.71	1.58	1.46
35	d	311	KC2	C2A-C3A	5.70	1.48	1.37
33	j	316	II0	C11-C13	-5.70	1.42	1.51
33	f	616	II0	C11-C13	-5.70	1.42	1.51
35	g	314	KC2	C2A-C3A	5.70	1.48	1.37
33	f	618	II0	C11-C13	-5.68	1.42	1.51
34	b	316	IHT	C12-C15	-5.68	1.42	1.51
34	b	317	IHT	C34-C35	5.66	1.58	1.46
35	i	616	KC2	C2A-C3A	5.66	1.48	1.37
33	k	615	II0	C11-C13	-5.65	1.42	1.51
33	a	317	II0	C11-C13	-5.64	1.42	1.51
33	i	613	II0	C11-C13	-5.64	1.42	1.51
33	b	314	II0	C11-C13	-5.64	1.42	1.51
35	d	310	KC2	C2A-C3A	5.60	1.48	1.37
35	g	312	KC2	C2A-C3A	5.60	1.48	1.37
35	e	609	KC2	C2A-C3A	5.60	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	613	KC2	C2A-C3A	5.60	1.48	1.37
34	b	317	IHT	C12-C15	-5.59	1.42	1.51
34	c	615	IHT	C12-C15	-5.58	1.42	1.51
35	k	611	KC2	C2A-C3A	5.57	1.48	1.37
33	g	318	II0	C11-C13	-5.57	1.42	1.51
34	k	618	IHT	C34-C35	5.57	1.57	1.46
33	O	202	II0	C11-C13	-5.56	1.42	1.51
35	g	314	KC2	C3C-C2C	5.55	1.48	1.37
33	c	614	II0	C11-C13	-5.54	1.42	1.51
35	g	313	KC2	CHD-C4C	5.54	1.49	1.38
33	h	309	II0	C11-C13	-5.53	1.42	1.51
33	h	311	II0	C11-C13	-5.53	1.42	1.51
33	c	613	II0	C11-C13	-5.52	1.42	1.51
35	c	610	KC2	C2A-C3A	5.51	1.48	1.37
33	d	313	II0	C11-C13	-5.50	1.42	1.51
33	e	614	II0	C11-C13	-5.49	1.42	1.51
34	c	615	IHT	C34-C35	5.48	1.57	1.46
35	k	612	KC2	C2A-C3A	5.47	1.48	1.37
34	O	203	IHT	C34-C35	5.47	1.57	1.46
34	R	204	IHT	C12-C15	-5.47	1.42	1.51
35	k	613	KC2	C3C-C2C	5.44	1.48	1.37
33	a	315	II0	C11-C13	-5.40	1.42	1.51
34	a	316	IHT	C34-C35	5.39	1.57	1.46
33	e	612	II0	C11-C13	-5.39	1.42	1.51
34	b	316	IHT	C34-C35	5.38	1.57	1.46
33	a	313	II0	C11-C13	-5.37	1.42	1.51
34	j	317	IHT	C34-C35	5.36	1.57	1.46
33	g	317	II0	C11-C13	-5.33	1.42	1.51
35	i	616	KC2	CHD-C4C	5.33	1.49	1.38
33	g	316	II0	C11-C13	-5.33	1.42	1.51
35	k	613	KC2	CHD-C4C	5.32	1.49	1.38
33	j	318	II0	C11-C13	-5.31	1.42	1.51
35	k	612	KC2	CHD-C4C	5.31	1.49	1.38
35	f	611	KC2	C2A-C3A	5.28	1.47	1.37
35	j	312	KC2	CHD-C4C	5.28	1.49	1.38
35	c	610	KC2	C3C-C2C	5.27	1.47	1.37
33	i	614	II0	C11-C13	-5.26	1.42	1.51
34	f	617	IHT	C34-C35	5.24	1.57	1.46
34	f	617	IHT	C04-C02	5.22	1.66	1.54
35	g	312	KC2	C1A-NA	5.22	1.48	1.38
33	d	314	II0	C11-C13	-5.22	1.42	1.51
33	e	616	II0	C11-C13	-5.21	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	610	KC2	CHD-C4C	5.21	1.48	1.38
33	k	619	II0	C11-C13	-5.20	1.42	1.51
34	k	618	IHT	C04-C02	5.20	1.66	1.54
34	R	204	IHT	C34-C35	5.19	1.57	1.46
35	g	314	KC2	CHD-C4C	5.19	1.48	1.38
35	i	616	KC2	C3C-C2C	5.17	1.47	1.37
34	a	316	IHT	C04-C02	5.16	1.65	1.54
34	R	204	IHT	C04-C02	5.15	1.65	1.54
34	g	319	IHT	C04-C02	5.14	1.65	1.54
33	b	314	II0	C31-C29	5.13	1.59	1.43
34	g	319	IHT	C34-C35	5.13	1.56	1.46
35	j	312	KC2	C3C-C2C	5.12	1.47	1.37
34	c	615	IHT	C04-C02	5.11	1.65	1.54
35	d	310	KC2	CHD-C4C	5.09	1.48	1.38
34	b	316	IHT	C04-C02	5.08	1.65	1.54
34	j	317	IHT	C04-C02	5.08	1.65	1.54
35	g	312	KC2	CHD-C4C	5.06	1.48	1.38
34	b	317	IHT	C04-C02	5.06	1.65	1.54
35	i	609	KC2	CHD-C4C	5.06	1.48	1.38
33	j	315	II0	C11-C13	-5.05	1.43	1.51
33	b	315	II0	C11-C13	-5.05	1.43	1.51
33	i	613	II0	C27-C25	5.05	1.54	1.50
35	d	311	KC2	CHD-C4C	5.05	1.48	1.38
33	k	621	II0	C11-C13	-5.04	1.43	1.51
35	d	310	KC2	C3B-C2B	5.03	1.47	1.37
33	e	612	II0	C27-C25	5.02	1.54	1.50
33	g	320	II0	C11-C13	-5.01	1.43	1.51
35	k	611	KC2	CHD-C4C	4.98	1.48	1.38
34	O	203	IHT	C04-C02	4.98	1.65	1.54
35	f	611	KC2	CHD-C4C	4.97	1.48	1.38
33	d	315	II0	C11-C13	-4.96	1.43	1.51
35	i	616	KC2	C3B-C2B	4.95	1.47	1.37
35	d	310	KC2	C3C-C2C	4.94	1.47	1.37
35	k	612	KC2	C3C-C2C	4.94	1.47	1.37
33	i	614	II0	C31-C29	4.94	1.58	1.43
35	k	612	KC2	C3B-C2B	4.93	1.47	1.37
35	c	610	KC2	C3B-C2B	4.91	1.47	1.37
35	g	314	KC2	C3B-C2B	4.90	1.47	1.37
35	e	609	KC2	C3C-C2C	4.89	1.47	1.37
35	d	311	KC2	C3C-C2C	4.88	1.47	1.37
35	j	312	KC2	C2A-C3A	4.88	1.47	1.37
35	k	613	KC2	O2D-CGD	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	311	KC2	C3B-C2B	4.86	1.47	1.37
35	g	312	KC2	C3C-C2C	4.86	1.47	1.37
35	e	609	KC2	C3B-C2B	4.84	1.47	1.37
35	f	611	KC2	C1A-NA	4.83	1.48	1.38
35	g	312	KC2	C3B-C2B	4.83	1.47	1.37
35	f	611	KC2	C3B-C2B	4.83	1.47	1.37
33	c	616	II0	C11-C13	-4.82	1.43	1.51
35	g	313	KC2	C3B-C2B	4.82	1.46	1.37
34	b	317	IHT	C06-C09	4.79	1.67	1.52
35	k	613	KC2	C1A-NA	4.79	1.48	1.38
35	k	611	KC2	C3C-C2C	4.78	1.46	1.37
35	k	612	KC2	C1A-NA	4.77	1.47	1.38
34	j	317	IHT	C06-C09	4.77	1.67	1.52
35	k	613	KC2	C3B-C2B	4.77	1.46	1.37
34	O	203	IHT	C06-C09	4.76	1.67	1.52
35	j	312	KC2	C3B-C2B	4.76	1.46	1.37
35	g	314	KC2	C1A-NA	4.75	1.47	1.38
35	k	611	KC2	C3B-C2B	4.74	1.46	1.37
34	c	615	IHT	C06-C09	4.73	1.67	1.52
35	k	611	KC2	O2D-CGD	4.73	1.44	1.33
33	b	315	II0	C31-C29	4.72	1.57	1.43
33	a	317	II0	C42-C40	4.72	1.57	1.43
35	f	611	KC2	C3C-C2C	4.71	1.46	1.37
35	d	311	KC2	C1A-NA	4.70	1.47	1.38
33	k	617	II0	C11-C13	-4.70	1.43	1.51
35	i	609	KC2	C3C-C2C	4.70	1.46	1.37
35	i	609	KC2	C1A-NA	4.70	1.47	1.38
33	k	616	II0	C32-C30	4.70	1.57	1.43
34	b	317	IHT	C30-C27	4.69	1.57	1.43
33	b	318	II0	C11-C13	-4.68	1.43	1.51
35	j	312	KC2	C1A-NA	4.68	1.47	1.38
34	a	316	IHT	C06-C09	4.68	1.67	1.52
33	k	617	II0	C27-C25	4.67	1.54	1.50
35	g	313	KC2	C3C-C2C	4.66	1.46	1.37
33	e	616	II0	C42-C40	4.66	1.57	1.43
34	k	618	IHT	C30-C27	4.66	1.57	1.43
34	f	617	IHT	C06-C09	4.65	1.67	1.52
35	c	610	KC2	C1A-NA	4.65	1.47	1.38
35	i	616	KC2	C1A-NA	4.65	1.47	1.38
34	c	615	IHT	C30-C27	4.64	1.57	1.43
34	b	316	IHT	C06-C09	4.64	1.67	1.52
34	f	617	IHT	C30-C27	4.64	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	k	618	IHT	C06-C09	4.63	1.67	1.52
35	c	610	KC2	O2D-CGD	4.63	1.44	1.33
35	i	616	KC2	O2D-CGD	4.63	1.44	1.33
34	R	204	IHT	C06-C09	4.62	1.67	1.52
33	g	320	II0	C32-C30	4.62	1.57	1.43
33	a	315	II0	C31-C29	4.60	1.57	1.43
35	k	611	KC2	C1A-NA	4.60	1.47	1.38
25	B	842	PQN	C10-C1	4.60	1.57	1.48
26	J	107	LHG	O8-C23	4.59	1.46	1.33
35	d	310	KC2	O2D-CGD	4.59	1.44	1.33
33	f	618	II0	C42-C40	4.58	1.57	1.43
35	e	609	KC2	CHD-C4C	4.57	1.47	1.38
25	A	843	PQN	C10-C1	4.57	1.57	1.48
35	d	310	KC2	C1A-NA	4.56	1.47	1.38
34	g	319	IHT	C06-C09	4.56	1.66	1.52
34	b	316	IHT	C30-C27	4.55	1.57	1.43
35	g	312	KC2	O2D-CGD	4.55	1.44	1.33
34	R	204	IHT	C30-C27	4.55	1.57	1.43
35	k	612	KC2	O2D-CGD	4.55	1.44	1.33
35	g	313	KC2	C1A-NA	4.53	1.47	1.38
33	d	315	II0	C31-C29	4.52	1.57	1.43
35	i	609	KC2	O2D-CGD	4.52	1.44	1.33
34	O	203	IHT	C30-C27	4.52	1.57	1.43
34	j	317	IHT	C30-C27	4.51	1.57	1.43
25	B	842	PQN	C5-C4	4.51	1.56	1.48
33	f	618	II0	C27-C25	4.50	1.53	1.50
34	a	316	IHT	C30-C27	4.50	1.57	1.43
26	j	319	LHG	O7-C7	4.49	1.47	1.34
33	e	612	II0	C42-C40	4.49	1.57	1.43
33	i	612	II0	C27-C25	4.49	1.53	1.50
25	A	843	PQN	C5-C4	4.49	1.56	1.48
33	i	612	II0	C31-C29	4.49	1.57	1.43
26	k	620	LHG	O7-C7	4.49	1.47	1.34
26	d	316	LHG	O8-C23	4.46	1.46	1.33
26	J	107	LHG	O7-C7	4.46	1.46	1.34
35	e	609	KC2	C1A-NA	4.46	1.47	1.38
35	i	609	KC2	C3B-C2B	4.45	1.46	1.37
33	k	619	II0	C31-C29	4.45	1.57	1.43
33	f	618	II0	C32-C30	4.44	1.57	1.43
34	g	319	IHT	C30-C27	4.44	1.56	1.43
33	a	317	II0	C32-C30	4.43	1.56	1.43
33	k	619	II0	C42-C40	4.43	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	k	616	II0	C42-C40	4.43	1.56	1.43
33	h	309	II0	C42-C40	4.42	1.56	1.43
33	k	615	II0	C32-C30	4.42	1.56	1.43
33	k	615	II0	C42-C40	4.41	1.56	1.43
33	c	613	II0	C27-C25	4.41	1.53	1.50
32	F	206	LMG	O8-C28	4.40	1.46	1.33
33	g	318	II0	C31-C29	4.40	1.56	1.43
33	e	613	II0	C32-C30	4.40	1.56	1.43
33	a	313	II0	C31-C29	4.39	1.56	1.43
33	k	621	II0	C27-C25	4.39	1.53	1.50
33	k	619	II0	C27-C25	4.38	1.53	1.50
35	g	313	KC2	O2D-CGD	4.37	1.44	1.33
33	a	317	II0	C27-C25	4.37	1.53	1.50
26	i	615	LHG	O8-C23	4.37	1.46	1.33
33	e	613	II0	C31-C29	4.37	1.56	1.43
33	k	616	II0	C31-C29	4.37	1.56	1.43
33	d	314	II0	C27-C25	4.37	1.53	1.50
32	O	204	LMG	O8-C28	4.36	1.46	1.33
35	k	612	KC2	CBC-CAC	4.36	1.51	1.30
33	b	318	II0	C31-C29	4.36	1.56	1.43
33	c	616	II0	C32-C30	4.36	1.56	1.43
33	g	320	II0	C42-C40	4.36	1.56	1.43
33	a	317	II0	C31-C29	4.35	1.56	1.43
33	f	614	II0	C42-C40	4.35	1.56	1.43
35	d	311	KC2	CBC-CAC	4.35	1.51	1.30
26	e	617	LHG	O7-C7	4.35	1.46	1.34
35	g	312	KC2	CBC-CAC	4.35	1.51	1.30
26	b	302	LHG	O8-C23	4.34	1.46	1.33
35	g	313	KC2	CBC-CAC	4.34	1.51	1.30
33	c	616	II0	C31-C29	4.34	1.56	1.43
33	k	621	II0	C31-C29	4.34	1.56	1.43
33	f	616	II0	C31-C29	4.34	1.56	1.43
33	O	202	II0	C42-C40	4.33	1.56	1.43
33	k	621	II0	C42-C40	4.32	1.56	1.43
33	b	314	II0	C42-C40	4.32	1.56	1.43
26	j	319	LHG	O8-C23	4.32	1.45	1.33
26	g	321	LHG	O7-C7	4.32	1.46	1.34
33	O	202	II0	C31-C29	4.32	1.56	1.43
33	a	313	II0	C06-C04	4.32	1.67	1.54
33	i	614	II0	C42-C40	4.31	1.56	1.43
33	i	613	II0	C42-C40	4.31	1.56	1.43
33	J	104	II0	C31-C29	4.31	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	609	KC2	O2D-CGD	4.31	1.43	1.33
33	e	614	II0	C31-C29	4.30	1.56	1.43
26	b	320	LHG	O8-C23	4.30	1.45	1.33
33	b	318	II0	C27-C25	4.30	1.53	1.50
33	a	317	II0	C06-C04	4.30	1.67	1.54
33	k	617	II0	C42-C40	4.30	1.56	1.43
33	d	314	II0	C42-C40	4.30	1.56	1.43
34	g	319	IHT	C09-C10	-4.29	1.43	1.51
33	f	614	II0	C31-C29	4.28	1.56	1.43
35	g	314	KC2	O2D-CGD	4.28	1.43	1.33
26	i	615	LHG	O7-C7	4.27	1.46	1.34
33	k	617	II0	C06-C04	4.27	1.67	1.54
35	k	612	KC2	CHD-C1D	4.27	1.49	1.39
33	f	614	II0	C06-C04	4.27	1.67	1.54
33	g	316	II0	C42-C40	4.27	1.56	1.43
33	k	617	II0	C32-C30	4.26	1.56	1.43
33	d	313	II0	C31-C29	4.26	1.56	1.43
35	j	312	KC2	O2D-CGD	4.26	1.43	1.33
35	k	613	KC2	OBD-CAD	4.25	1.29	1.22
35	i	616	KC2	CBC-CAC	4.25	1.50	1.30
35	i	616	KC2	CHB-C1B	4.24	1.46	1.38
33	g	320	II0	C31-C29	4.24	1.56	1.43
33	f	616	II0	C06-C04	4.24	1.67	1.54
35	d	311	KC2	O2D-CGD	4.24	1.43	1.33
33	e	616	II0	C32-C30	4.24	1.56	1.43
35	k	612	KC2	OBD-CAD	4.24	1.29	1.22
35	j	312	KC2	CBC-CAC	4.24	1.50	1.30
26	f	619	LHG	O8-C23	4.23	1.45	1.33
33	e	614	II0	C42-C40	4.23	1.56	1.43
33	c	614	II0	C31-C29	4.23	1.56	1.43
35	g	314	KC2	CBC-CAC	4.23	1.50	1.30
33	c	616	II0	C42-C40	4.23	1.56	1.43
33	g	318	II0	C06-C04	4.23	1.67	1.54
33	g	316	II0	C31-C29	4.23	1.56	1.43
33	d	314	II0	C31-C29	4.23	1.56	1.43
33	k	617	II0	C31-C29	4.22	1.56	1.43
35	g	314	KC2	OBD-CAD	4.22	1.29	1.22
24	O	205	CLA	C1D-ND	4.22	1.43	1.37
30	B	843	DGD	O2G-C1B	4.21	1.46	1.34
33	a	315	II0	C32-C30	4.21	1.56	1.43
33	d	315	II0	C42-C40	4.21	1.56	1.43
34	f	617	IHT	C09-C10	-4.21	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	h	311	II0	C31-C29	4.21	1.56	1.43
33	e	616	II0	C06-C04	4.21	1.67	1.54
35	f	611	KC2	O2D-CGD	4.20	1.43	1.33
26	e	617	LHG	O8-C23	4.20	1.45	1.33
26	c	617	LHG	O8-C23	4.20	1.45	1.33
26	A	844	LHG	O8-C23	4.20	1.45	1.33
26	A	845	LHG	O8-C23	4.20	1.45	1.33
26	k	620	LHG	O8-C23	4.20	1.45	1.33
35	k	613	KC2	CBC-CAC	4.20	1.50	1.30
35	g	312	KC2	CHD-C1D	4.20	1.48	1.39
33	h	310	II0	C42-C40	4.20	1.56	1.43
35	e	609	KC2	CBC-CAC	4.19	1.50	1.30
35	i	616	KC2	OBD-CAD	4.19	1.29	1.22
26	c	618	LHG	O7-C7	4.19	1.46	1.34
33	e	613	II0	C42-C40	4.19	1.56	1.43
33	i	614	II0	C32-C30	4.19	1.56	1.43
33	k	615	II0	C06-C04	4.19	1.67	1.54
33	i	613	II0	C31-C29	4.19	1.56	1.43
33	f	614	II0	C32-C30	4.18	1.56	1.43
35	k	611	KC2	CBC-CAC	4.18	1.50	1.30
33	j	318	II0	C06-C04	4.17	1.67	1.54
35	i	609	KC2	CBC-CAC	4.16	1.50	1.30
33	k	621	II0	C32-C30	4.16	1.56	1.43
33	c	616	II0	C06-C04	4.16	1.67	1.54
26	g	301	LHG	O7-C7	4.16	1.46	1.34
33	i	613	II0	C32-C30	4.16	1.56	1.43
35	d	310	KC2	CBC-CAC	4.16	1.50	1.30
33	i	614	II0	C06-C04	4.16	1.67	1.54
35	f	611	KC2	CBC-CAC	4.16	1.50	1.30
35	d	310	KC2	OBD-CAD	4.16	1.29	1.22
26	g	301	LHG	O8-C23	4.16	1.45	1.33
26	c	618	LHG	O8-C23	4.15	1.45	1.33
33	k	619	II0	C32-C30	4.15	1.56	1.43
33	d	315	II0	C06-C04	4.15	1.67	1.54
33	a	313	II0	C42-C40	4.15	1.56	1.43
33	d	315	II0	C32-C30	4.15	1.56	1.43
33	e	614	II0	C27-C25	4.15	1.53	1.50
33	b	315	II0	C42-C40	4.15	1.56	1.43
26	a	301	LHG	O8-C23	4.15	1.45	1.33
33	b	318	II0	C32-C30	4.14	1.56	1.43
33	e	612	II0	C32-C30	4.14	1.56	1.43
34	R	204	IHT	C09-C10	-4.13	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	e	614	II0	C06-C04	4.13	1.67	1.54
34	b	317	IHT	C41-C38	4.13	1.56	1.43
33	e	616	II0	C31-C29	4.13	1.56	1.43
35	g	313	KC2	CHC-C4B	4.12	1.46	1.38
33	j	315	II0	C42-C40	4.12	1.56	1.43
33	k	616	II0	C34-C36	4.12	1.54	1.46
33	c	614	II0	C32-C30	4.12	1.56	1.43
33	a	315	II0	C42-C40	4.12	1.56	1.43
33	j	318	II0	C42-C40	4.12	1.56	1.43
34	j	317	IHT	C09-C10	-4.12	1.43	1.51
33	a	315	II0	C06-C04	4.11	1.67	1.54
33	O	202	II0	C32-C30	4.11	1.55	1.43
33	e	612	II0	C41-C39	4.11	1.55	1.43
33	b	314	II0	C32-C30	4.11	1.55	1.43
35	k	613	KC2	CHC-C4B	4.10	1.46	1.38
32	L	208	LMG	O7-C10	4.10	1.45	1.34
26	c	617	LHG	O7-C7	4.10	1.45	1.34
33	e	613	II0	C06-C04	4.10	1.67	1.54
33	g	317	II0	C31-C29	4.10	1.55	1.43
33	h	310	II0	C31-C29	4.10	1.55	1.43
32	b	301	LMG	O8-C28	4.10	1.45	1.33
32	b	301	LMG	O7-C10	4.10	1.45	1.34
33	j	318	II0	C31-C29	4.09	1.55	1.43
33	k	619	II0	C06-C04	4.09	1.67	1.54
35	c	610	KC2	CHC-C4B	4.09	1.46	1.38
33	c	613	II0	C32-C30	4.09	1.55	1.43
26	B	802	LHG	O8-C23	4.09	1.45	1.33
35	g	314	KC2	CHB-C1B	4.09	1.46	1.38
33	d	314	II0	C06-C04	4.09	1.67	1.54
33	e	612	II0	C31-C29	4.08	1.55	1.43
33	e	614	II0	C32-C30	4.08	1.55	1.43
33	f	618	II0	C06-C04	4.08	1.67	1.54
26	d	316	LHG	O7-C7	4.07	1.45	1.34
33	c	613	II0	C31-C29	4.07	1.55	1.43
33	g	316	II0	C32-C30	4.07	1.55	1.43
35	g	313	KC2	OBD-CAD	4.07	1.29	1.22
33	j	315	II0	C31-C29	4.07	1.55	1.43
33	c	613	II0	C42-C40	4.06	1.55	1.43
33	f	616	II0	C42-C40	4.06	1.55	1.43
33	b	318	II0	C42-C40	4.06	1.55	1.43
34	k	618	IHT	C05-C03	4.06	1.67	1.54
34	a	316	IHT	C05-C03	4.06	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	610	KC2	CBC-CAC	4.05	1.49	1.30
33	d	313	II0	C42-C40	4.05	1.55	1.43
30	B	843	DGD	O1G-C1A	4.05	1.45	1.33
34	k	618	IHT	C09-C10	-4.05	1.43	1.51
33	g	316	II0	C06-C04	4.05	1.66	1.54
35	d	311	KC2	OBD-CAD	4.04	1.29	1.22
32	J	106	LMG	O8-C28	4.04	1.45	1.33
33	d	315	II0	C41-C39	4.04	1.55	1.43
33	k	615	II0	C41-C39	4.04	1.55	1.43
35	c	610	KC2	CHB-C1B	4.04	1.46	1.38
33	d	313	II0	C32-C30	4.04	1.55	1.43
33	a	317	II0	C41-C39	4.03	1.55	1.43
33	h	309	II0	C31-C29	4.03	1.55	1.43
26	f	619	LHG	O7-C7	4.03	1.45	1.34
33	k	621	II0	C06-C04	4.03	1.66	1.54
33	f	616	II0	C32-C30	4.03	1.55	1.43
33	O	202	II0	C06-C04	4.03	1.66	1.54
33	c	613	II0	C06-C04	4.03	1.66	1.54
33	b	318	II0	C06-C04	4.02	1.66	1.54
33	a	314	II0	C32-C30	4.02	1.55	1.43
26	f	620	LHG	O8-C23	4.02	1.45	1.33
33	a	314	II0	C31-C29	4.01	1.55	1.43
33	j	315	II0	C06-C04	4.01	1.66	1.54
26	b	320	LHG	O7-C7	4.01	1.45	1.34
26	a	301	LHG	O7-C7	4.00	1.45	1.34
32	L	208	LMG	O8-C28	4.00	1.45	1.33
35	g	312	KC2	OBD-CAD	4.00	1.29	1.22
33	i	612	II0	C42-C40	3.99	1.55	1.43
33	j	318	II0	C32-C30	3.99	1.55	1.43
33	h	310	II0	C27-C25	3.99	1.53	1.50
34	O	203	IHT	C41-C38	3.99	1.55	1.43
33	f	614	II0	C27-C25	3.99	1.53	1.50
34	k	618	IHT	C41-C38	3.99	1.55	1.43
33	g	317	II0	C32-C30	3.99	1.55	1.43
33	d	314	II0	C32-C30	3.98	1.55	1.43
33	a	313	II0	C32-C30	3.98	1.55	1.43
33	k	615	II0	C27-C25	3.98	1.53	1.50
33	g	320	II0	C27-C25	3.98	1.53	1.50
33	i	612	II0	C32-C30	3.98	1.55	1.43
26	b	302	LHG	O7-C7	3.98	1.45	1.34
33	a	315	II0	C41-C39	3.98	1.55	1.43
33	f	615	II0	C31-C29	3.98	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	h	310	II0	C12-C14	-3.98	1.44	1.51
33	i	613	II0	C06-C04	3.98	1.66	1.54
26	A	845	LHG	O7-C7	3.97	1.45	1.34
35	d	310	KC2	CHB-C1B	3.97	1.46	1.38
35	c	610	KC2	OBD-CAD	3.97	1.29	1.22
34	c	615	IHT	C09-C10	-3.97	1.43	1.51
34	O	203	IHT	C05-C03	3.97	1.66	1.54
34	b	316	IHT	C05-C03	3.97	1.66	1.54
35	i	609	KC2	OBD-CAD	3.97	1.29	1.22
33	j	316	II0	C31-C29	3.97	1.55	1.43
33	O	202	II0	C27-C25	3.97	1.53	1.50
34	c	615	IHT	C41-C38	3.96	1.55	1.43
34	b	316	IHT	C09-C10	-3.96	1.43	1.51
35	i	616	KC2	CHC-C4B	3.95	1.46	1.38
33	a	317	II0	C34-C36	3.95	1.54	1.46
35	c	610	KC2	CHD-C1D	3.95	1.48	1.39
33	d	313	II0	C06-C04	3.95	1.66	1.54
33	g	318	II0	C42-C40	3.95	1.55	1.43
33	i	614	II0	C41-C39	3.95	1.55	1.43
33	a	313	II0	C41-C39	3.95	1.55	1.43
33	i	612	II0	C06-C04	3.95	1.66	1.54
34	c	615	IHT	C05-C03	3.95	1.66	1.54
26	g	321	LHG	O8-C23	3.95	1.44	1.33
33	e	613	II0	C27-C25	3.95	1.53	1.50
33	d	313	II0	C27-C25	3.95	1.53	1.50
33	a	314	II0	C42-C40	3.94	1.55	1.43
33	f	615	II0	C42-C40	3.94	1.55	1.43
32	O	204	LMG	O7-C10	3.94	1.45	1.34
33	e	612	II0	C06-C04	3.94	1.66	1.54
35	k	611	KC2	CHB-C1B	3.94	1.46	1.38
34	j	317	IHT	C41-C38	3.94	1.55	1.43
33	f	618	II0	C31-C29	3.93	1.55	1.43
35	g	314	KC2	CHC-C4B	3.93	1.46	1.38
33	J	104	II0	C32-C30	3.93	1.55	1.43
35	g	313	KC2	CHD-C1D	3.93	1.48	1.39
33	b	314	II0	C06-C04	3.93	1.66	1.54
33	h	310	II0	C32-C30	3.93	1.55	1.43
35	k	613	KC2	CHD-C1D	3.92	1.48	1.39
33	j	316	II0	C32-C30	3.92	1.55	1.43
34	b	317	IHT	C05-C03	3.92	1.66	1.54
32	F	206	LMG	O7-C10	3.92	1.45	1.34
33	h	311	II0	C06-C04	3.91	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	k	618	IHT	C40-C37	3.91	1.55	1.43
34	b	316	IHT	C41-C38	3.91	1.55	1.43
33	f	615	II0	C27-C25	3.90	1.53	1.50
33	f	618	II0	C41-C39	3.90	1.55	1.43
35	i	616	KC2	CHD-C1D	3.90	1.48	1.39
34	g	319	IHT	C05-C03	3.90	1.66	1.54
33	j	316	II0	C42-C40	3.90	1.55	1.43
34	a	316	IHT	C09-C10	-3.90	1.43	1.51
33	g	318	II0	C32-C30	3.90	1.55	1.43
27	B	847	WVN	C31-C32	3.89	1.54	1.46
33	g	318	II0	C27-C25	3.88	1.53	1.50
33	h	309	II0	C34-C36	3.88	1.54	1.46
34	j	317	IHT	C05-C03	3.88	1.66	1.54
35	i	609	KC2	CHD-C1D	3.88	1.48	1.39
33	h	311	II0	C12-C14	-3.88	1.45	1.51
33	e	616	II0	C41-C39	3.88	1.55	1.43
33	d	315	II0	C27-C25	3.88	1.53	1.50
33	g	317	II0	C42-C40	3.88	1.55	1.43
34	f	617	IHT	C05-C03	3.87	1.66	1.54
33	c	614	II0	C06-C04	3.87	1.66	1.54
33	k	615	II0	C34-C36	3.87	1.54	1.46
34	O	203	IHT	C09-C10	-3.86	1.43	1.51
33	h	311	II0	C32-C30	3.86	1.55	1.43
33	b	315	II0	C06-C04	3.86	1.66	1.54
33	J	104	II0	C42-C40	3.86	1.55	1.43
34	c	615	IHT	C40-C37	3.86	1.55	1.43
35	j	312	KC2	CHD-C1D	3.86	1.48	1.39
33	k	619	II0	C41-C39	3.86	1.55	1.43
33	O	202	II0	C41-C39	3.86	1.55	1.43
35	j	312	KC2	OBD-CAD	3.86	1.29	1.22
33	k	616	II0	C06-C04	3.86	1.66	1.54
26	B	802	LHG	O7-C7	3.85	1.45	1.34
33	k	617	II0	C41-C39	3.85	1.55	1.43
34	a	316	IHT	C41-C38	3.85	1.55	1.43
33	c	614	II0	C42-C40	3.85	1.55	1.43
33	h	311	II0	C42-C40	3.85	1.55	1.43
34	f	617	IHT	C40-C37	3.84	1.55	1.43
34	R	204	IHT	C41-C38	3.84	1.55	1.43
33	b	315	II0	C12-C14	-3.84	1.45	1.51
33	g	320	II0	C06-C04	3.84	1.66	1.54
35	e	609	KC2	OBD-CAD	3.84	1.29	1.22
35	i	609	KC2	CHC-C4B	3.84	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	611	KC2	OBD-CAD	3.84	1.29	1.22
33	h	310	II0	C06-C04	3.83	1.66	1.54
33	f	615	II0	C32-C30	3.83	1.55	1.43
35	d	311	KC2	CHB-C1B	3.83	1.45	1.38
33	d	313	II0	C12-C14	-3.83	1.45	1.51
35	k	611	KC2	OBD-CAD	3.83	1.29	1.22
35	d	310	KC2	CHD-C1D	3.83	1.48	1.39
33	g	317	II0	C12-C14	-3.82	1.45	1.51
33	f	615	II0	C06-C04	3.82	1.66	1.54
34	b	317	IHT	C40-C37	3.82	1.55	1.43
33	h	310	II0	C41-C39	3.81	1.55	1.43
33	g	320	II0	C34-C36	3.81	1.54	1.46
24	b	307	CLA	C1D-ND	3.81	1.42	1.37
33	f	614	II0	C41-C39	3.81	1.55	1.43
33	k	619	II0	C05-C03	3.80	1.66	1.54
27	B	848	WVN	C30-C28	3.80	1.55	1.43
35	g	312	KC2	CHB-C1B	3.80	1.45	1.38
33	c	616	II0	C41-C39	3.80	1.55	1.43
33	h	309	II0	C41-C39	3.80	1.55	1.43
35	f	611	KC2	CHB-C1B	3.79	1.45	1.38
33	k	621	II0	C41-C39	3.79	1.54	1.43
26	f	620	LHG	O7-C7	3.79	1.45	1.34
33	b	314	II0	C41-C39	3.78	1.54	1.43
33	e	614	II0	C41-C39	3.78	1.54	1.43
34	b	317	IHT	C09-C10	-3.78	1.44	1.51
33	d	314	II0	C41-C39	3.78	1.54	1.43
33	e	616	II0	C27-C25	3.78	1.53	1.50
33	k	619	II0	C33-C35	3.78	1.54	1.46
35	k	613	KC2	CHB-C1B	3.78	1.45	1.38
33	f	616	II0	C41-C39	3.78	1.54	1.43
33	O	202	II0	C34-C36	3.77	1.54	1.46
33	f	618	II0	C34-C36	3.77	1.54	1.46
35	g	313	KC2	CHB-C1B	3.77	1.45	1.38
33	h	309	II0	C27-C25	3.77	1.53	1.50
34	a	316	IHT	C14-C02	3.76	1.60	1.53
24	c	606	CLA	C4B-NB	3.76	1.42	1.37
33	j	315	II0	C32-C30	3.76	1.54	1.43
34	g	319	IHT	C41-C38	3.75	1.54	1.43
27	L	205	WVN	C23-C25	3.75	1.54	1.46
24	e	603	CLA	C1D-ND	3.75	1.42	1.37
34	b	316	IHT	C40-C37	3.75	1.54	1.43
34	f	617	IHT	C41-C38	3.75	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	k	618	IHT	C14-C02	3.75	1.60	1.53
33	e	612	II0	C34-C36	3.75	1.54	1.46
35	f	611	KC2	CHC-C4B	3.75	1.45	1.38
33	k	619	II0	C12-C14	-3.74	1.45	1.51
33	i	613	II0	C41-C39	3.74	1.54	1.43
33	g	318	II0	C41-C39	3.74	1.54	1.43
33	a	314	II0	C05-C03	3.74	1.66	1.54
34	O	203	IHT	C40-C37	3.73	1.54	1.43
34	b	317	IHT	C14-C02	3.73	1.60	1.53
35	g	314	KC2	CHD-C1D	3.73	1.47	1.39
34	c	615	IHT	C14-C02	3.73	1.60	1.53
33	k	615	II0	C12-C14	-3.73	1.45	1.51
24	k	607	CLA	C4B-NB	3.73	1.42	1.37
34	b	317	IHT	C31-C29	3.73	1.54	1.43
34	R	204	IHT	C05-C03	3.73	1.66	1.54
33	a	314	II0	C06-C04	3.73	1.66	1.54
33	f	618	II0	C12-C14	-3.73	1.45	1.51
33	j	316	II0	C06-C04	3.72	1.66	1.54
33	g	316	II0	C41-C39	3.72	1.54	1.43
33	a	315	II0	C27-C25	3.72	1.53	1.50
35	e	609	KC2	CHB-C1B	3.72	1.45	1.38
33	b	315	II0	C41-C39	3.71	1.54	1.43
33	J	104	II0	C06-C04	3.71	1.65	1.54
33	b	314	II0	C27-C25	3.71	1.53	1.50
33	d	313	II0	C41-C39	3.71	1.54	1.43
24	b	306	CLA	C1D-ND	3.70	1.42	1.37
24	i	604	CLA	C1D-ND	3.70	1.42	1.37
35	i	609	KC2	CHB-C1B	3.70	1.45	1.38
24	d	304	CLA	C1D-ND	3.70	1.42	1.37
33	g	317	II0	C06-C04	3.70	1.65	1.54
33	a	314	II0	C41-C39	3.70	1.54	1.43
24	b	310	CLA	C1D-ND	3.70	1.42	1.37
35	j	312	KC2	CHB-C1B	3.69	1.45	1.38
24	j	307	CLA	C1D-ND	3.69	1.42	1.37
33	e	613	II0	C41-C39	3.69	1.54	1.43
34	b	316	IHT	C14-C02	3.69	1.60	1.53
34	a	316	IHT	C40-C37	3.69	1.54	1.43
24	j	313	CLA	C4B-NB	3.69	1.42	1.37
33	k	616	II0	C41-C39	3.69	1.54	1.43
33	j	315	II0	C27-C25	3.69	1.53	1.50
33	j	315	II0	C12-C14	-3.68	1.45	1.51
34	j	317	IHT	C40-C37	3.68	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	315	II0	C34-C36	3.68	1.53	1.46
35	k	611	KC2	CHC-C4B	3.68	1.45	1.38
33	b	315	II0	C33-C35	3.68	1.53	1.46
33	i	614	II0	C34-C36	3.67	1.53	1.46
33	j	318	II0	C41-C39	3.67	1.54	1.43
35	k	612	KC2	CHC-C4B	3.67	1.45	1.38
24	j	306	CLA	C1D-ND	3.67	1.42	1.37
34	O	203	IHT	C14-C02	3.67	1.60	1.53
33	a	313	II0	C34-C36	3.66	1.53	1.46
34	g	319	IHT	C14-C02	3.66	1.60	1.53
35	k	611	KC2	CHD-C1D	3.66	1.47	1.39
33	b	314	II0	C05-C03	3.66	1.65	1.54
33	j	318	II0	C27-C25	3.65	1.53	1.50
24	i	606	CLA	C1D-ND	3.65	1.42	1.37
33	d	313	II0	C05-C03	3.65	1.65	1.54
33	i	614	II0	C05-C03	3.65	1.65	1.54
35	g	312	KC2	C1B-NB	-3.65	1.33	1.37
33	f	615	II0	C12-C14	-3.64	1.45	1.51
33	c	614	II0	C41-C39	3.64	1.54	1.43
35	k	612	KC2	C3C-C4C	3.64	1.52	1.44
32	J	106	LMG	O7-C10	3.63	1.44	1.34
35	f	611	KC2	CHD-C1D	3.63	1.47	1.39
33	e	613	II0	C05-C03	3.63	1.65	1.54
27	B	845	WVN	C19-C22	3.63	1.53	1.46
33	f	614	II0	C34-C36	3.63	1.53	1.46
34	b	316	IHT	C28-C26	3.63	1.53	1.50
24	b	313	CLA	C1D-ND	3.63	1.42	1.37
34	a	316	IHT	C31-C29	3.63	1.54	1.43
34	R	204	IHT	C14-C02	3.62	1.60	1.53
34	c	615	IHT	C31-C29	3.62	1.54	1.43
34	k	618	IHT	C31-C29	3.62	1.54	1.43
33	b	315	II0	C32-C30	3.61	1.54	1.43
33	g	320	II0	C41-C39	3.61	1.54	1.43
33	i	612	II0	C41-C39	3.61	1.54	1.43
34	f	617	IHT	C14-C02	3.61	1.60	1.53
33	h	309	II0	C05-C03	3.61	1.65	1.54
24	k	603	CLA	C1D-ND	3.61	1.42	1.37
33	e	616	II0	C34-C36	3.61	1.53	1.46
35	g	312	KC2	CHC-C4B	3.61	1.45	1.38
33	b	318	II0	C41-C39	3.60	1.54	1.43
34	j	317	IHT	C14-C02	3.60	1.60	1.53
33	e	612	II0	C05-C03	3.60	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	j	315	II0	C05-C03	3.60	1.65	1.54
34	R	204	IHT	C40-C37	3.60	1.54	1.43
24	b	310	CLA	C4B-NB	3.60	1.42	1.37
34	O	203	IHT	C31-C29	3.59	1.54	1.43
33	f	616	II0	C34-C36	3.59	1.53	1.46
26	A	844	LHG	O7-C7	3.59	1.44	1.34
33	O	202	II0	C12-C14	-3.59	1.45	1.51
33	j	318	II0	C12-C14	-3.58	1.45	1.51
24	d	308	CLA	C1D-ND	3.58	1.42	1.37
33	c	616	II0	C34-C36	3.57	1.53	1.46
33	k	617	II0	C34-C36	3.57	1.53	1.46
33	k	616	II0	C27-C25	3.56	1.53	1.50
33	e	614	II0	C05-C03	3.56	1.65	1.54
33	e	616	II0	C12-C14	-3.56	1.45	1.51
33	j	316	II0	C12-C14	-3.56	1.45	1.51
33	c	613	II0	C41-C39	3.56	1.54	1.43
33	h	310	II0	C05-C03	3.56	1.65	1.54
24	i	608	CLA	C1D-ND	3.56	1.42	1.37
24	f	601	CLA	C1D-ND	3.55	1.42	1.37
34	R	204	IHT	C31-C29	3.55	1.54	1.43
33	k	621	II0	C34-C36	3.55	1.53	1.46
33	f	615	II0	C41-C39	3.55	1.54	1.43
24	j	310	CLA	C1D-ND	3.55	1.42	1.37
33	j	315	II0	C41-C39	3.55	1.54	1.43
24	g	309	CLA	C1D-ND	3.55	1.42	1.37
35	e	609	KC2	CHC-C4B	3.54	1.45	1.38
34	j	317	IHT	C28-C26	3.54	1.53	1.50
24	h	306	CLA	C1D-ND	3.54	1.42	1.37
34	g	319	IHT	C40-C37	3.54	1.54	1.43
35	j	312	KC2	CHC-C4B	3.54	1.45	1.38
33	k	615	II0	C05-C03	3.54	1.65	1.54
33	d	315	II0	C05-C03	3.54	1.65	1.54
24	k	614	CLA	C1D-ND	3.53	1.42	1.37
33	a	314	II0	C12-C14	-3.53	1.45	1.51
33	g	318	II0	C12-C14	-3.53	1.45	1.51
24	f	613	CLA	C1D-ND	3.53	1.42	1.37
24	a	306	CLA	C1D-ND	3.52	1.42	1.37
33	g	320	II0	C12-C14	-3.52	1.45	1.51
33	f	618	II0	C05-C03	3.52	1.65	1.54
24	b	309	CLA	C4B-NB	3.52	1.42	1.37
33	k	617	II0	C05-C03	3.52	1.65	1.54
34	b	316	IHT	C31-C29	3.52	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	312	CLA	C1D-ND	3.51	1.42	1.37
24	b	312	CLA	C1D-ND	3.51	1.42	1.37
33	k	617	II0	C33-C35	3.51	1.53	1.46
34	j	317	IHT	C31-C29	3.51	1.54	1.43
33	b	314	II0	C34-C36	3.51	1.53	1.46
24	A	801	CLA	C1D-ND	3.51	1.42	1.37
33	k	615	II0	C31-C29	3.51	1.54	1.43
27	L	206	WVN	C33-C34	3.51	1.53	1.46
35	d	311	KC2	CHB-C4A	3.50	1.47	1.39
35	e	609	KC2	CHD-C1D	3.49	1.47	1.39
35	d	310	KC2	CHC-C4B	3.49	1.45	1.38
33	c	616	II0	C05-C03	3.49	1.65	1.54
24	J	105	CLA	C1D-ND	3.49	1.42	1.37
33	f	616	II0	C05-C03	3.49	1.65	1.54
33	d	315	II0	C33-C35	3.49	1.53	1.46
33	a	313	II0	C05-C03	3.49	1.65	1.54
34	b	317	IHT	C32-C33	3.48	1.53	1.46
24	A	838	CLA	C1D-ND	3.48	1.42	1.37
33	e	614	II0	C34-C36	3.48	1.53	1.46
24	B	829	CLA	C4B-NB	3.48	1.42	1.37
33	g	317	II0	C41-C39	3.48	1.54	1.43
24	i	601	CLA	C1D-ND	3.48	1.42	1.37
27	L	205	WVN	C30-C28	3.48	1.54	1.43
33	f	614	II0	C05-C03	3.48	1.65	1.54
24	L	202	CLA	C1D-ND	3.47	1.42	1.37
24	A	855	CLA	C4B-NB	3.47	1.42	1.37
33	d	315	II0	C34-C36	3.47	1.53	1.46
34	b	317	IHT	C28-C26	3.47	1.53	1.50
33	i	613	II0	C34-C36	3.47	1.53	1.46
24	c	606	CLA	C1D-ND	3.47	1.42	1.37
34	f	617	IHT	C31-C29	3.47	1.53	1.43
24	b	305	CLA	C1D-ND	3.47	1.42	1.37
35	k	612	KC2	CHB-C1B	3.46	1.45	1.38
34	a	316	IHT	C28-C26	3.46	1.53	1.50
33	j	318	II0	C05-C03	3.46	1.65	1.54
33	h	311	II0	C41-C39	3.46	1.53	1.43
33	d	314	II0	C05-C03	3.46	1.65	1.54
24	c	605	CLA	C1D-ND	3.46	1.42	1.37
33	g	317	II0	C27-C25	3.46	1.53	1.50
24	b	303	CLA	C1D-ND	3.46	1.42	1.37
33	i	612	II0	C05-C03	3.46	1.65	1.54
34	c	615	IHT	C32-C33	3.46	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	205	WVN	C30-C28	3.45	1.53	1.43
24	h	307	CLA	C1D-ND	3.45	1.42	1.37
24	i	605	CLA	C4B-NB	3.45	1.42	1.37
24	i	610	CLA	C4B-NB	3.45	1.42	1.37
24	d	303	CLA	C1D-ND	3.45	1.42	1.37
33	j	316	II0	C05-C03	3.45	1.65	1.54
24	j	307	CLA	C4B-NB	3.45	1.42	1.37
34	k	618	IHT	C32-C33	3.45	1.53	1.46
33	j	316	II0	C41-C39	3.45	1.53	1.43
33	i	614	II0	C33-C35	3.44	1.53	1.46
34	c	615	IHT	C28-C26	3.44	1.53	1.50
33	g	316	II0	C34-C36	3.43	1.53	1.46
33	g	320	II0	C05-C03	3.43	1.65	1.54
35	d	311	KC2	CHD-C1D	3.43	1.47	1.39
24	e	601	CLA	C1D-ND	3.43	1.42	1.37
33	e	613	II0	C34-C36	3.43	1.53	1.46
33	i	614	II0	C12-C14	-3.43	1.45	1.51
24	B	839	CLA	C1D-ND	3.43	1.42	1.37
24	i	611	CLA	C1D-ND	3.43	1.42	1.37
34	O	203	IHT	C28-C26	3.43	1.53	1.50
33	a	317	II0	C12-C14	-3.43	1.45	1.51
24	c	601	CLA	C1D-ND	3.42	1.42	1.37
24	k	601	CLA	C1D-ND	3.42	1.42	1.37
33	f	615	II0	C05-C03	3.42	1.65	1.54
33	g	316	II0	C05-C03	3.42	1.65	1.54
33	a	313	II0	C12-C14	-3.41	1.45	1.51
35	i	616	KC2	CHB-C4A	3.41	1.47	1.39
24	e	608	CLA	C1D-ND	3.41	1.42	1.37
33	a	315	II0	C05-C03	3.41	1.65	1.54
33	k	621	II0	C05-C03	3.41	1.65	1.54
27	h	308	WVN	C23-C25	3.41	1.53	1.46
24	A	811	CLA	C4B-NB	3.41	1.42	1.37
33	d	313	II0	C34-C36	3.41	1.53	1.46
35	k	612	KC2	CHB-C4A	3.41	1.47	1.39
34	R	204	IHT	C32-C33	3.41	1.53	1.46
24	g	304	CLA	C1D-ND	3.41	1.42	1.37
33	e	612	II0	C12-C14	-3.40	1.45	1.51
33	a	317	II0	C05-C03	3.40	1.65	1.54
33	g	318	II0	C05-C03	3.40	1.65	1.54
24	d	302	CLA	C1D-ND	3.40	1.42	1.37
34	f	617	IHT	C32-C33	3.40	1.53	1.46
24	k	607	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	613	II0	C34-C36	3.39	1.53	1.46
24	A	856	CLA	C1D-ND	3.39	1.42	1.37
24	c	602	CLA	C1D-ND	3.39	1.42	1.37
34	b	316	IHT	C32-C33	3.39	1.53	1.46
33	e	616	II0	C05-C03	3.39	1.64	1.54
27	F	205	WVN	C23-C25	3.39	1.53	1.46
24	a	312	CLA	C4B-NB	3.39	1.42	1.37
24	h	301	CLA	C1D-ND	3.39	1.42	1.37
33	J	104	II0	C41-C39	3.39	1.53	1.43
35	k	611	KC2	CHB-C4A	3.38	1.46	1.39
33	c	614	II0	C05-C03	3.38	1.64	1.54
33	b	318	II0	C05-C03	3.38	1.64	1.54
33	g	317	II0	C05-C03	3.38	1.64	1.54
33	O	202	II0	C05-C03	3.37	1.64	1.54
24	c	604	CLA	C1D-ND	3.37	1.42	1.37
34	O	203	IHT	C32-C33	3.36	1.53	1.46
24	e	610	CLA	C1D-ND	3.36	1.42	1.37
34	g	319	IHT	C31-C29	3.36	1.53	1.43
33	e	613	II0	C12-C14	-3.36	1.45	1.51
24	d	301	CLA	C1D-ND	3.36	1.42	1.37
35	g	313	KC2	C1B-NB	-3.36	1.33	1.37
33	i	613	II0	C05-C03	3.35	1.64	1.54
27	j	301	WVN	C23-C25	3.35	1.53	1.46
33	j	316	II0	C34-C36	3.35	1.53	1.46
33	c	613	II0	C05-C03	3.35	1.64	1.54
24	j	308	CLA	C1D-ND	3.35	1.42	1.37
33	c	614	II0	C34-C36	3.35	1.53	1.46
24	c	612	CLA	C1D-ND	3.35	1.42	1.37
31	B	844	LMU	O5B-C1B	3.34	1.50	1.41
35	k	613	KC2	CHC-C1C	3.34	1.46	1.39
35	d	311	KC2	CHC-C4B	3.34	1.44	1.38
33	j	316	II0	C27-C25	3.34	1.53	1.50
27	j	301	WVN	C33-C34	3.34	1.53	1.46
35	k	612	KC2	C1B-NB	-3.34	1.33	1.37
33	J	104	II0	C12-C14	-3.33	1.45	1.51
24	k	610	CLA	C1D-ND	3.33	1.42	1.37
27	J	102	WVN	C39-C36	3.33	1.53	1.43
27	e	615	WVN	C19-C22	3.33	1.53	1.46
35	d	310	KC2	CHB-C4A	3.33	1.46	1.39
24	k	602	CLA	C1D-ND	3.33	1.42	1.37
24	O	201	CLA	C1D-ND	3.33	1.42	1.37
35	e	609	KC2	CHB-C4A	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	849	WVN	C30-C28	3.32	1.53	1.43
33	h	311	II0	C05-C03	3.32	1.64	1.54
27	A	847	WVN	C39-C36	3.32	1.53	1.43
27	j	301	WVN	C30-C28	3.32	1.53	1.43
24	f	602	CLA	C1D-ND	3.32	1.42	1.37
33	k	616	II0	C05-C03	3.32	1.64	1.54
24	k	605	CLA	C1D-ND	3.31	1.42	1.37
34	j	317	IHT	C32-C33	3.31	1.53	1.46
24	j	302	CLA	C1D-ND	3.31	1.42	1.37
24	f	610	CLA	C1D-ND	3.31	1.42	1.37
27	e	615	WVN	C29-C26	3.31	1.53	1.43
33	a	315	II0	C33-C35	3.31	1.53	1.46
33	i	613	II0	C33-C35	3.31	1.53	1.46
24	a	303	CLA	C1D-ND	3.31	1.42	1.37
24	f	612	CLA	C4B-NB	3.30	1.42	1.37
27	A	849	WVN	C33-C34	3.30	1.53	1.46
27	J	101	WVN	C33-C34	3.30	1.53	1.46
24	b	311	CLA	C1D-ND	3.30	1.42	1.37
33	f	614	II0	C12-C14	-3.30	1.45	1.51
24	c	609	CLA	C4B-NB	3.30	1.42	1.37
24	e	604	CLA	C1D-ND	3.30	1.42	1.37
27	L	201	WVN	C23-C25	3.30	1.53	1.46
24	R	203	CLA	C1D-ND	3.30	1.42	1.37
33	i	613	II0	C12-C14	-3.30	1.45	1.51
33	a	317	II0	C33-C35	3.29	1.53	1.46
24	h	305	CLA	C1D-ND	3.29	1.42	1.37
33	k	616	II0	C12-C14	-3.29	1.45	1.51
24	b	312	CLA	C4B-NB	3.29	1.42	1.37
24	A	839	CLA	C1D-ND	3.29	1.42	1.37
24	f	605	CLA	C1D-ND	3.28	1.42	1.37
35	g	313	KC2	CHC-C1C	3.28	1.46	1.39
24	d	309	CLA	C4B-NB	3.28	1.42	1.37
35	g	314	KC2	CHB-C4A	3.28	1.46	1.39
27	I	101	WVN	C31-C32	3.28	1.53	1.46
24	A	832	CLA	C1D-ND	3.28	1.42	1.37
27	h	308	WVN	C31-C32	3.28	1.53	1.46
34	R	204	IHT	C28-C26	3.28	1.53	1.50
33	k	619	II0	C34-C36	3.27	1.53	1.46
27	J	101	WVN	C30-C28	3.27	1.53	1.43
33	k	621	II0	C33-C35	3.27	1.53	1.46
24	f	607	CLA	C1D-ND	3.27	1.42	1.37
33	h	311	II0	C27-C25	3.27	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	609	CLA	C1D-ND	3.27	1.42	1.37
34	a	316	IHT	C32-C33	3.27	1.53	1.46
24	e	605	CLA	C4B-NB	3.27	1.42	1.37
33	b	314	II0	C12-C14	-3.27	1.45	1.51
33	c	616	II0	C27-C25	3.27	1.53	1.50
27	B	848	WVN	C33-C34	3.27	1.52	1.46
24	k	603	CLA	C4B-NB	3.27	1.42	1.37
34	g	319	IHT	C28-C26	3.27	1.53	1.50
27	A	846	WVN	C19-C22	3.27	1.52	1.46
27	A	846	WVN	C33-C34	3.27	1.52	1.46
33	f	615	II0	C34-C36	3.27	1.52	1.46
33	h	310	II0	C34-C36	3.27	1.52	1.46
27	e	615	WVN	C31-C32	3.26	1.52	1.46
24	a	304	CLA	C1D-ND	3.26	1.42	1.37
24	k	608	CLA	C4B-NB	3.26	1.42	1.37
24	d	301	CLA	C4B-NB	3.26	1.42	1.37
24	j	305	CLA	C1D-ND	3.26	1.42	1.37
24	j	304	CLA	C1D-ND	3.26	1.42	1.37
33	j	318	II0	C34-C36	3.26	1.52	1.46
24	A	837	CLA	C1D-ND	3.26	1.42	1.37
35	f	611	KC2	CHB-C4A	3.26	1.46	1.39
33	d	315	II0	C12-C14	-3.26	1.46	1.51
24	A	805	CLA	C1D-ND	3.26	1.42	1.37
24	f	604	CLA	C1D-ND	3.25	1.42	1.37
27	h	308	WVN	C29-C26	3.25	1.53	1.43
27	F	205	WVN	C33-C34	3.25	1.52	1.46
24	i	610	CLA	MG-NA	3.25	2.14	2.06
27	I	101	WVN	C29-C26	3.25	1.53	1.43
24	b	306	CLA	C4B-NB	3.25	1.42	1.37
33	b	318	II0	C12-C14	-3.25	1.46	1.51
24	A	826	CLA	C1D-ND	3.25	1.42	1.37
24	j	311	CLA	C1D-ND	3.25	1.42	1.37
24	d	309	CLA	C1D-ND	3.25	1.42	1.37
27	J	102	WVN	C33-C34	3.25	1.52	1.46
24	k	608	CLA	C1D-ND	3.24	1.42	1.37
24	k	614	CLA	C4B-NB	3.24	1.42	1.37
24	a	312	CLA	C1D-ND	3.24	1.42	1.37
24	b	313	CLA	C4B-NB	3.24	1.42	1.37
27	B	849	WVN	C33-C34	3.24	1.52	1.46
24	k	601	CLA	C4B-NB	3.24	1.42	1.37
33	f	616	II0	C27-C25	3.24	1.53	1.50
33	a	314	II0	C34-C36	3.24	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	e	615	WVN	C23-C25	3.24	1.52	1.46
33	b	315	II0	C34-C36	3.24	1.52	1.46
27	F	205	WVN	C29-C26	3.24	1.53	1.43
34	f	617	IHT	C28-C26	3.23	1.53	1.50
35	f	611	KC2	CHC-C1C	3.23	1.46	1.39
27	F	205	WVN	C40-C37	3.23	1.53	1.43
33	c	616	II0	C33-C35	3.23	1.52	1.46
24	k	609	CLA	CMA-C3A	-3.23	1.46	1.53
24	B	822	CLA	C1D-ND	3.23	1.42	1.37
33	c	614	II0	C12-C14	-3.23	1.46	1.51
24	B	819	CLA	C1D-ND	3.23	1.42	1.37
24	d	302	CLA	C4B-NB	3.23	1.42	1.37
24	a	307	CLA	C1D-ND	3.22	1.42	1.37
24	g	307	CLA	C1D-ND	3.22	1.42	1.37
27	B	849	WVN	C29-C26	3.22	1.53	1.43
24	A	806	CLA	C1D-ND	3.22	1.42	1.37
27	A	846	WVN	C30-C28	3.22	1.53	1.43
24	d	305	CLA	C1D-ND	3.22	1.42	1.37
24	f	603	CLA	C1D-ND	3.22	1.42	1.37
24	A	814	CLA	C1D-ND	3.22	1.42	1.37
27	J	101	WVN	C19-C22	3.22	1.52	1.46
24	B	808	CLA	C4B-NB	3.22	1.42	1.37
27	B	846	WVN	C33-C34	3.22	1.52	1.46
24	k	606	CLA	C4B-NB	3.22	1.42	1.37
24	B	810	CLA	CAB-C3B	-3.21	1.44	1.50
35	c	610	KC2	CHB-C4A	3.21	1.46	1.39
24	A	829	CLA	C4B-NB	3.21	1.42	1.37
33	g	316	II0	C12-C14	-3.21	1.46	1.51
27	A	847	WVN	C29-C26	3.21	1.53	1.43
24	A	835	CLA	C1D-ND	3.21	1.42	1.37
24	B	818	CLA	C1D-ND	3.21	1.42	1.37
27	F	205	WVN	C31-C32	3.21	1.52	1.46
27	j	301	WVN	C31-C32	3.21	1.52	1.46
27	j	301	WVN	C39-C36	3.21	1.53	1.43
27	e	615	WVN	C33-C34	3.20	1.52	1.46
24	f	613	CLA	C4B-NB	3.20	1.42	1.37
24	g	306	CLA	C1D-ND	3.20	1.42	1.37
33	J	104	II0	C05-C03	3.20	1.64	1.54
24	I	102	CLA	C1D-ND	3.20	1.42	1.37
24	B	838	CLA	C1D-ND	3.20	1.42	1.37
33	f	616	II0	C12-C14	-3.19	1.46	1.51
24	j	303	CLA	C1D-ND	3.19	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	849	WVN	C39-C36	3.19	1.53	1.43
24	A	828	CLA	C1D-ND	3.19	1.42	1.37
27	B	849	WVN	C30-C28	3.19	1.53	1.43
33	c	616	II0	C12-C14	-3.19	1.46	1.51
33	d	314	II0	C12-C14	-3.19	1.46	1.51
24	c	604	CLA	C4B-NB	3.19	1.42	1.37
33	a	314	II0	C33-C35	3.18	1.52	1.46
27	I	101	WVN	C39-C36	3.18	1.53	1.43
24	i	607	CLA	C1D-ND	3.18	1.42	1.37
24	i	608	CLA	C4B-NB	3.18	1.42	1.37
27	L	205	WVN	C29-C26	3.18	1.53	1.43
27	A	848	WVN	C23-C25	3.18	1.52	1.46
33	e	614	II0	C12-C14	-3.18	1.46	1.51
27	K	103	WVN	C23-C25	3.18	1.52	1.46
33	k	617	II0	C12-C14	-3.17	1.46	1.51
24	c	611	CLA	C1D-ND	3.17	1.42	1.37
35	d	311	KC2	C1B-NB	-3.17	1.33	1.37
33	J	104	II0	C34-C36	3.17	1.52	1.46
35	i	616	KC2	CHC-C1C	3.17	1.46	1.39
33	J	104	II0	C33-C35	3.17	1.52	1.46
24	F	201	CLA	C1D-ND	3.17	1.42	1.37
24	c	608	CLA	C1D-ND	3.17	1.42	1.37
24	A	823	CLA	C1D-ND	3.16	1.42	1.37
24	L	202	CLA	C4B-NB	3.16	1.42	1.37
24	e	602	CLA	C1D-ND	3.16	1.42	1.37
27	A	848	WVN	C30-C28	3.16	1.53	1.43
27	h	308	WVN	C39-C36	3.16	1.53	1.43
27	h	308	WVN	C33-C34	3.16	1.52	1.46
33	j	318	II0	C33-C35	3.16	1.52	1.46
24	i	605	CLA	C1D-ND	3.16	1.42	1.37
24	k	604	CLA	C4B-NB	3.16	1.42	1.37
24	e	603	CLA	C4B-NB	3.16	1.42	1.37
24	e	606	CLA	C1D-ND	3.16	1.42	1.37
24	e	611	CLA	C1D-ND	3.16	1.42	1.37
27	B	848	WVN	C31-C32	3.16	1.52	1.46
24	f	606	CLA	C1D-ND	3.16	1.42	1.37
27	R	201	WVN	C29-C26	3.16	1.53	1.43
33	d	314	II0	C34-C36	3.16	1.52	1.46
24	i	611	CLA	C4B-NB	3.15	1.42	1.37
27	h	308	WVN	C30-C28	3.15	1.53	1.43
27	e	615	WVN	C39-C36	3.15	1.53	1.43
24	j	302	CLA	C4B-NB	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	i	612	II0	C34-C36	3.15	1.52	1.46
27	J	101	WVN	C31-C32	3.15	1.52	1.46
24	F	202	CLA	C1D-ND	3.15	1.42	1.37
27	R	201	WVN	C31-C32	3.15	1.52	1.46
33	g	318	II0	C34-C36	3.14	1.52	1.46
27	A	846	WVN	C29-C26	3.14	1.52	1.43
24	F	201	CLA	C4B-NB	3.14	1.42	1.37
27	j	301	WVN	C29-C26	3.13	1.52	1.43
27	A	850	WVN	C39-C36	3.13	1.52	1.43
24	A	806	CLA	C4B-NB	3.13	1.42	1.37
33	g	317	II0	C34-C36	3.13	1.52	1.46
33	b	318	II0	C34-C36	3.13	1.52	1.46
35	i	609	KC2	CHB-C4A	3.13	1.46	1.39
24	B	825	CLA	C1D-ND	3.13	1.42	1.37
24	i	603	CLA	C4B-NB	3.13	1.42	1.37
24	a	309	CLA	C1D-ND	3.13	1.42	1.37
24	A	819	CLA	C1D-ND	3.13	1.42	1.37
24	c	607	CLA	C4B-NB	3.12	1.42	1.37
24	c	607	CLA	C1D-ND	3.12	1.42	1.37
24	d	307	CLA	C1D-ND	3.12	1.42	1.37
27	B	849	WVN	C19-C22	3.12	1.52	1.46
24	g	322	CLA	C1D-ND	3.12	1.42	1.37
27	I	101	WVN	C33-C34	3.12	1.52	1.46
33	g	316	II0	C33-C35	3.12	1.52	1.46
24	a	311	CLA	CMD-C2D	-3.12	1.44	1.50
27	I	101	WVN	C19-C22	3.11	1.52	1.46
24	k	604	CLA	C1D-ND	3.11	1.42	1.37
33	b	315	II0	C05-C03	3.11	1.64	1.54
33	d	314	II0	C33-C35	3.11	1.52	1.46
27	J	102	WVN	C23-C25	3.11	1.52	1.46
24	i	606	CLA	C4B-NB	3.11	1.41	1.37
27	R	201	WVN	C33-C34	3.11	1.52	1.46
24	a	309	CLA	C4B-NB	3.11	1.41	1.37
24	b	309	CLA	C1D-ND	3.11	1.41	1.37
33	g	320	II0	C33-C35	3.11	1.52	1.46
24	B	806	CLA	C1D-ND	3.11	1.41	1.37
24	A	815	CLA	C1D-ND	3.11	1.41	1.37
24	A	824	CLA	C1D-ND	3.11	1.41	1.37
24	i	602	CLA	C1D-ND	3.11	1.41	1.37
27	J	101	WVN	C39-C36	3.11	1.52	1.43
24	i	603	CLA	C1D-ND	3.10	1.41	1.37
27	B	846	WVN	C30-C28	3.10	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	308	CLA	C4B-NB	3.10	1.41	1.37
24	c	601	CLA	C4B-NB	3.10	1.41	1.37
24	A	813	CLA	C4B-NB	3.10	1.41	1.37
27	B	849	WVN	C40-C37	3.10	1.52	1.43
27	R	202	WVN	C23-C25	3.10	1.52	1.46
24	h	312	CLA	C1D-ND	3.10	1.41	1.37
27	J	101	WVN	C29-C26	3.10	1.52	1.43
24	B	812	CLA	C1D-ND	3.10	1.41	1.37
24	e	611	CLA	C4B-NB	3.10	1.41	1.37
33	O	202	II0	C33-C35	3.10	1.52	1.46
35	c	610	KC2	CHC-C1C	3.10	1.46	1.39
27	h	308	WVN	C40-C37	3.10	1.52	1.43
35	e	609	KC2	CHC-C1C	3.10	1.46	1.39
35	d	311	KC2	C3C-C4C	3.09	1.50	1.44
27	R	201	WVN	C30-C28	3.09	1.52	1.43
24	B	831	CLA	C1D-ND	3.09	1.41	1.37
27	F	205	WVN	C39-C36	3.09	1.52	1.43
24	a	310	CLA	C1D-ND	3.09	1.41	1.37
35	g	312	KC2	CHB-C4A	3.09	1.46	1.39
24	j	309	CLA	C1D-ND	3.09	1.41	1.37
27	I	101	WVN	C40-C37	3.08	1.52	1.43
24	f	612	CLA	C1D-ND	3.08	1.41	1.37
24	j	313	CLA	MG-NA	3.08	2.13	2.06
35	g	313	KC2	CHB-C4A	3.08	1.46	1.39
27	A	846	WVN	C40-C37	3.08	1.52	1.43
27	B	847	WVN	C40-C37	3.08	1.52	1.43
24	B	815	CLA	C1D-ND	3.08	1.41	1.37
24	i	601	CLA	C4B-NB	3.08	1.41	1.37
31	B	844	LMU	O5'-C1'	3.08	1.49	1.41
27	B	847	WVN	C30-C28	3.08	1.52	1.43
24	f	606	CLA	C4B-NB	3.08	1.41	1.37
27	L	205	WVN	C31-C32	3.08	1.52	1.46
34	k	618	IHT	C28-C26	3.08	1.52	1.50
24	d	312	CLA	C4B-NB	3.07	1.41	1.37
24	g	310	CLA	C1D-ND	3.07	1.41	1.37
24	A	856	CLA	C4B-NB	3.07	1.41	1.37
24	A	803	CLA	C1D-ND	3.07	1.41	1.37
24	f	608	CLA	C1D-ND	3.07	1.41	1.37
24	A	809	CLA	C1D-ND	3.07	1.41	1.37
24	g	311	CLA	C1D-ND	3.07	1.41	1.37
27	L	205	WVN	C40-C37	3.07	1.52	1.43
24	A	818	CLA	C1D-ND	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	601	CLA	C1B-C2B	3.07	1.50	1.43
27	F	204	WVN	C29-C26	3.07	1.52	1.43
27	J	101	WVN	C40-C37	3.07	1.52	1.43
27	J	102	WVN	C19-C22	3.07	1.52	1.46
33	i	612	II0	C12-C14	-3.07	1.46	1.51
24	J	103	CLA	C1D-ND	3.07	1.41	1.37
24	d	303	CLA	C4B-NB	3.06	1.41	1.37
33	b	318	II0	C33-C35	3.06	1.52	1.46
27	B	848	WVN	C19-C22	3.06	1.52	1.46
24	B	830	CLA	C1D-ND	3.06	1.41	1.37
33	a	315	II0	C12-C14	-3.06	1.46	1.51
24	d	306	CLA	C1D-ND	3.06	1.41	1.37
33	g	318	II0	C33-C35	3.06	1.52	1.46
27	F	205	WVN	C19-C22	3.06	1.52	1.46
24	c	611	CLA	C1B-C2B	3.06	1.50	1.43
27	B	846	WVN	C23-C25	3.06	1.52	1.46
24	A	813	CLA	C1D-ND	3.05	1.41	1.37
24	b	308	CLA	C4B-NB	3.05	1.41	1.37
24	B	824	CLA	C1D-ND	3.05	1.41	1.37
35	j	312	KC2	C1B-NB	-3.05	1.33	1.37
24	B	810	CLA	C1D-ND	3.05	1.41	1.37
24	B	814	CLA	C1D-ND	3.05	1.41	1.37
33	e	612	II0	C33-C35	3.05	1.52	1.46
34	g	319	IHT	C32-C33	3.05	1.52	1.46
35	k	611	KC2	CHC-C1C	3.05	1.46	1.39
24	a	310	CLA	C4B-NB	3.04	1.41	1.37
24	A	811	CLA	C1D-ND	3.04	1.41	1.37
24	A	842	CLA	C1D-ND	3.04	1.41	1.37
24	k	602	CLA	C4B-NB	3.04	1.41	1.37
24	A	816	CLA	C1D-ND	3.04	1.41	1.37
24	A	831	CLA	C1D-ND	3.04	1.41	1.37
27	A	850	WVN	C19-C22	3.03	1.52	1.46
27	R	202	WVN	C31-C32	3.03	1.52	1.46
33	j	315	II0	C33-C35	3.03	1.52	1.46
24	c	605	CLA	C4B-NB	3.03	1.41	1.37
27	A	846	WVN	C39-C36	3.03	1.52	1.43
24	A	808	CLA	C1D-ND	3.03	1.41	1.37
27	A	846	WVN	C23-C25	3.03	1.52	1.46
27	L	206	WVN	C39-C36	3.03	1.52	1.43
27	e	615	WVN	C30-C28	3.02	1.52	1.43
24	i	610	CLA	C1D-ND	3.02	1.41	1.37
35	g	312	KC2	C1A-CHA	3.02	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	j	301	WVN	C19-C22	3.02	1.52	1.46
24	i	606	CLA	C1B-C2B	3.02	1.50	1.43
24	B	835	CLA	C1D-ND	3.02	1.41	1.37
35	c	610	KC2	C1B-NB	-3.02	1.33	1.37
27	F	204	WVN	C40-C37	3.02	1.52	1.43
27	e	615	WVN	C40-C37	3.02	1.52	1.43
27	j	301	WVN	C40-C37	3.02	1.52	1.43
33	g	317	II0	C33-C35	3.02	1.52	1.46
27	J	102	WVN	C30-C28	3.02	1.52	1.43
27	B	848	WVN	C23-C25	3.02	1.52	1.46
27	F	204	WVN	C39-C36	3.02	1.52	1.43
24	A	818	CLA	CMB-C2B	-3.02	1.44	1.50
24	d	305	CLA	CMB-C2B	-3.01	1.44	1.50
27	I	101	WVN	C30-C28	3.01	1.52	1.43
24	L	207	CLA	C1D-ND	3.01	1.41	1.37
27	L	205	WVN	C39-C36	3.01	1.52	1.43
35	k	613	KC2	CHB-C4A	3.01	1.46	1.39
24	g	315	CLA	C1D-ND	3.01	1.41	1.37
33	h	310	II0	C33-C35	3.01	1.52	1.46
24	k	609	CLA	C4B-NB	3.01	1.41	1.37
27	B	848	WVN	C29-C26	3.01	1.52	1.43
24	c	603	CLA	C1D-ND	3.01	1.41	1.37
27	M	101	WVN	C29-C26	3.00	1.52	1.43
24	j	313	CLA	C1D-ND	3.00	1.41	1.37
24	L	207	CLA	C4B-NB	3.00	1.41	1.37
24	A	810	CLA	C4B-NB	3.00	1.41	1.37
35	e	609	KC2	C1B-NB	-3.00	1.33	1.37
27	B	848	WVN	C40-C37	3.00	1.52	1.43
27	A	848	WVN	C33-C34	3.00	1.52	1.46
24	B	811	CLA	C4B-NB	3.00	1.41	1.37
24	h	301	CLA	C4B-NB	3.00	1.41	1.37
24	e	601	CLA	C4B-NB	3.00	1.41	1.37
35	g	314	KC2	CHC-C1C	3.00	1.46	1.39
24	A	812	CLA	C1D-ND	3.00	1.41	1.37
24	A	820	CLA	CMB-C2B	-2.99	1.44	1.50
27	J	102	WVN	C40-C37	2.99	1.52	1.43
27	A	848	WVN	C40-C37	2.99	1.52	1.43
24	A	804	CLA	C1D-ND	2.99	1.41	1.37
24	O	205	CLA	C4B-NB	2.99	1.41	1.37
27	A	849	WVN	C40-C37	2.99	1.52	1.43
27	A	847	WVN	C40-C37	2.99	1.52	1.43
24	j	306	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	303	CLA	C1D-ND	2.98	1.41	1.37
27	M	101	WVN	C39-C36	2.98	1.52	1.43
24	B	831	CLA	CMB-C2B	-2.98	1.44	1.50
24	B	816	CLA	C1D-ND	2.98	1.41	1.37
24	A	801	CLA	C4B-NB	2.98	1.41	1.37
24	i	602	CLA	C4B-NB	2.98	1.41	1.37
33	h	311	II0	C34-C36	2.98	1.52	1.46
33	d	313	II0	C33-C35	2.98	1.52	1.46
27	M	101	WVN	C30-C28	2.98	1.52	1.43
35	j	312	KC2	CHB-C4A	2.97	1.46	1.39
24	b	307	CLA	C4B-NB	2.97	1.41	1.37
24	k	610	CLA	C4B-NB	2.97	1.41	1.37
27	A	850	WVN	C40-C37	2.97	1.52	1.43
24	h	302	CLA	C1D-ND	2.97	1.41	1.37
24	j	311	CLA	C4B-NB	2.97	1.41	1.37
33	d	315	II0	C28-C26	2.97	1.52	1.50
27	A	849	WVN	C39-C36	2.97	1.52	1.43
35	k	613	KC2	C1B-NB	-2.97	1.34	1.37
27	R	202	WVN	C30-C28	2.97	1.52	1.43
24	A	852	CLA	C1D-ND	2.97	1.41	1.37
33	k	621	II0	C12-C14	-2.97	1.46	1.51
24	J	105	CLA	CMD-C2D	-2.97	1.44	1.50
27	B	848	WVN	C39-C36	2.97	1.52	1.43
24	h	312	CLA	C4B-NB	2.96	1.41	1.37
24	K	102	CLA	C1D-ND	2.96	1.41	1.37
24	c	611	CLA	C4B-NB	2.96	1.41	1.37
35	f	611	KC2	C1B-NB	-2.96	1.34	1.37
35	g	312	KC2	C3C-C4C	2.96	1.50	1.44
24	a	307	CLA	C4B-NB	2.96	1.41	1.37
35	d	310	KC2	CHC-C1C	2.96	1.45	1.39
24	h	304	CLA	C1D-ND	2.96	1.41	1.37
24	f	610	CLA	C4B-NB	2.96	1.41	1.37
24	B	839	CLA	C4B-NB	2.96	1.41	1.37
24	c	602	CLA	C4B-NB	2.96	1.41	1.37
27	L	201	WVN	C33-C34	2.95	1.52	1.46
24	B	821	CLA	C1D-ND	2.95	1.41	1.37
27	K	103	WVN	C33-C34	2.95	1.52	1.46
24	A	833	CLA	C1D-ND	2.95	1.41	1.37
24	j	314	CLA	C1D-ND	2.95	1.41	1.37
24	d	307	CLA	C4B-NB	2.95	1.41	1.37
27	A	848	WVN	C39-C36	2.95	1.52	1.43
24	a	308	CLA	C1D-ND	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	845	WVN	C30-C28	2.95	1.52	1.43
33	f	618	II0	C33-C35	2.95	1.52	1.46
27	R	201	WVN	C23-C25	2.95	1.52	1.46
27	I	101	WVN	C23-C25	2.95	1.52	1.46
35	d	311	KC2	CHC-C1C	2.94	1.45	1.39
27	L	205	WVN	C33-C34	2.94	1.52	1.46
24	f	609	CLA	C1D-ND	2.94	1.41	1.37
27	A	850	WVN	C30-C28	2.94	1.52	1.43
27	L	201	WVN	C39-C36	2.94	1.52	1.43
24	b	304	CLA	C4B-NB	2.94	1.41	1.37
27	L	201	WVN	C30-C28	2.94	1.52	1.43
33	i	612	II0	C33-C35	2.94	1.52	1.46
27	J	102	WVN	C29-C26	2.94	1.52	1.43
27	R	201	WVN	C19-C22	2.94	1.52	1.46
24	j	314	CLA	C4B-NB	2.94	1.41	1.37
27	M	101	WVN	C40-C37	2.93	1.52	1.43
24	k	609	CLA	C1D-ND	2.93	1.41	1.37
24	g	302	CLA	C1D-ND	2.93	1.41	1.37
27	K	103	WVN	C30-C28	2.93	1.52	1.43
28	A	851	LMT	O3'-C3'	-2.93	1.35	1.43
27	L	206	WVN	C30-C28	2.93	1.52	1.43
24	j	311	CLA	C1B-C2B	2.93	1.50	1.43
24	B	811	CLA	C1D-ND	2.93	1.41	1.37
24	A	835	CLA	C4B-NB	2.93	1.41	1.37
27	B	849	WVN	C31-C32	2.93	1.52	1.46
24	a	302	CLA	C1D-ND	2.93	1.41	1.37
24	a	305	CLA	C1D-ND	2.92	1.41	1.37
24	j	304	CLA	C4B-NB	2.92	1.41	1.37
27	A	850	WVN	C29-C26	2.92	1.52	1.43
24	L	203	CLA	C1D-ND	2.92	1.41	1.37
24	A	817	CLA	C4B-NB	2.92	1.41	1.37
24	I	102	CLA	C4B-NB	2.92	1.41	1.37
27	A	848	WVN	C29-C26	2.92	1.52	1.43
24	j	310	CLA	C4B-NB	2.92	1.41	1.37
27	K	103	WVN	C20-C13	2.92	1.55	1.45
24	h	306	CLA	C4B-NB	2.92	1.41	1.37
24	a	311	CLA	MG-ND	-2.92	2.00	2.05
27	A	848	WVN	C31-C32	2.92	1.52	1.46
27	A	849	WVN	C23-C25	2.91	1.52	1.46
24	d	306	CLA	C4B-NB	2.91	1.41	1.37
24	A	807	CLA	C1D-ND	2.91	1.41	1.37
24	B	836	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	841	CLA	C1D-ND	2.91	1.41	1.37
24	A	836	CLA	C1D-ND	2.91	1.41	1.37
27	R	201	WVN	C39-C36	2.91	1.52	1.43
27	R	202	WVN	C29-C26	2.91	1.52	1.43
33	h	311	II0	C33-C35	2.91	1.52	1.46
24	e	608	CLA	C4B-NB	2.91	1.41	1.37
24	i	607	CLA	C4B-NB	2.91	1.41	1.37
24	a	310	CLA	C1B-C2B	2.91	1.49	1.43
24	j	313	CLA	C1B-C2B	2.90	1.49	1.43
33	j	315	II0	C34-C36	2.90	1.52	1.46
24	g	306	CLA	C4B-NB	2.90	1.41	1.37
24	B	814	CLA	C4B-NB	2.90	1.41	1.37
24	f	603	CLA	C4B-NB	2.90	1.41	1.37
33	c	613	II0	C33-C35	2.90	1.52	1.46
24	f	609	CLA	C4B-NB	2.90	1.41	1.37
27	K	103	WVN	C31-C32	2.89	1.52	1.46
24	B	820	CLA	C1D-ND	2.89	1.41	1.37
24	B	834	CLA	C1D-ND	2.89	1.41	1.37
24	g	303	CLA	C1D-ND	2.89	1.41	1.37
24	B	828	CLA	C1D-ND	2.89	1.41	1.37
27	B	847	WVN	C39-C36	2.89	1.52	1.43
24	b	304	CLA	C1D-ND	2.89	1.41	1.37
27	R	201	WVN	C40-C37	2.88	1.52	1.43
24	b	308	CLA	C1B-C2B	2.88	1.49	1.43
27	F	204	WVN	C30-C28	2.88	1.52	1.43
24	F	202	CLA	C4B-NB	2.88	1.41	1.37
24	B	837	CLA	C1D-ND	2.88	1.41	1.37
24	B	841	CLA	C1D-ND	2.88	1.41	1.37
27	F	204	WVN	C31-C32	2.87	1.52	1.46
24	A	834	CLA	C1D-ND	2.87	1.41	1.37
27	F	204	WVN	C19-C22	2.87	1.52	1.46
24	B	803	CLA	C1B-C2B	2.87	1.49	1.43
24	B	820	CLA	C4B-NB	2.87	1.41	1.37
27	B	847	WVN	C23-C25	2.87	1.52	1.46
24	A	817	CLA	C1D-ND	2.87	1.41	1.37
33	f	616	II0	C33-C35	2.87	1.52	1.46
27	K	103	WVN	C40-C37	2.86	1.52	1.43
24	A	856	CLA	C1B-C2B	2.86	1.49	1.43
24	B	817	CLA	C1D-ND	2.86	1.41	1.37
33	h	309	II0	C33-C35	2.86	1.52	1.46
33	f	614	II0	C33-C35	2.86	1.52	1.46
27	M	101	WVN	C31-C32	2.86	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	206	WVN	C40-C37	2.86	1.52	1.43
24	B	807	CLA	C1D-ND	2.85	1.41	1.37
24	A	815	CLA	CMB-C2B	-2.85	1.44	1.50
24	B	810	CLA	C4B-C3B	2.85	1.49	1.43
35	g	312	KC2	CHC-C1C	2.85	1.45	1.39
27	R	202	WVN	C40-C37	2.85	1.52	1.43
27	A	849	WVN	C31-C32	2.85	1.52	1.46
24	A	801	CLA	C1B-C2B	2.85	1.49	1.43
24	B	826	CLA	C1D-ND	2.85	1.41	1.37
24	a	306	CLA	C4B-NB	2.85	1.41	1.37
24	A	840	CLA	C1D-ND	2.85	1.41	1.37
27	A	850	WVN	C31-C32	2.85	1.52	1.46
24	i	604	CLA	C1B-C2B	2.84	1.49	1.43
24	a	312	CLA	MG-NA	2.84	2.13	2.06
27	A	847	WVN	C33-C34	2.84	1.52	1.46
33	e	616	II0	C33-C35	2.84	1.52	1.46
24	e	607	CLA	C1D-ND	2.84	1.41	1.37
27	B	849	WVN	C23-C25	2.84	1.52	1.46
24	A	829	CLA	C1D-ND	2.84	1.41	1.37
35	j	312	KC2	CHC-C1C	2.84	1.45	1.39
27	L	201	WVN	C40-C37	2.84	1.52	1.43
27	M	101	WVN	C19-C22	2.84	1.52	1.46
24	B	815	CLA	C4B-NB	2.83	1.41	1.37
24	A	831	CLA	C1B-C2B	2.83	1.49	1.43
24	A	833	CLA	CMB-C2B	-2.83	1.45	1.50
24	d	301	CLA	C1B-C2B	2.83	1.49	1.43
27	B	847	WVN	C33-C34	2.83	1.52	1.46
35	i	609	KC2	C1A-CHA	2.83	1.47	1.40
24	A	822	CLA	CMD-C2D	-2.83	1.45	1.50
27	L	205	WVN	C19-C22	2.83	1.52	1.46
24	B	808	CLA	C1D-ND	2.83	1.41	1.37
24	B	833	CLA	C1D-ND	2.83	1.41	1.37
27	A	847	WVN	C31-C32	2.82	1.52	1.46
24	A	855	CLA	C1D-ND	2.82	1.41	1.37
24	O	205	CLA	C1B-NB	-2.82	1.34	1.37
27	R	202	WVN	C39-C36	2.82	1.51	1.43
33	e	614	II0	C33-C35	2.82	1.52	1.46
24	c	612	CLA	C4B-NB	2.82	1.41	1.37
27	R	202	WVN	C33-C34	2.82	1.52	1.46
24	B	823	CLA	CMD-C2D	-2.82	1.45	1.50
24	h	307	CLA	C4B-NB	2.82	1.41	1.37
24	j	305	CLA	C4B-NB	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	311	CLA	C4B-NB	2.81	1.41	1.37
27	A	849	WVN	C19-C22	2.81	1.52	1.46
35	i	609	KC2	CHC-C1C	2.81	1.45	1.39
27	J	101	WVN	C02-C11	2.81	1.54	1.50
33	e	613	II0	C33-C35	2.81	1.52	1.46
33	c	613	II0	C12-C14	-2.81	1.46	1.51
33	a	313	II0	C33-C35	2.81	1.52	1.46
24	B	840	CLA	C4B-NB	2.81	1.41	1.37
27	A	850	WVN	C23-C25	2.81	1.52	1.46
27	B	846	WVN	C40-C37	2.81	1.51	1.43
24	j	303	CLA	C4B-NB	2.81	1.41	1.37
24	f	601	CLA	C4B-NB	2.80	1.41	1.37
24	j	308	CLA	C4B-NB	2.80	1.41	1.37
24	e	604	CLA	C4B-NB	2.80	1.41	1.37
24	f	612	CLA	MG-NA	2.80	2.12	2.06
24	B	803	CLA	CMD-C2D	-2.80	1.45	1.50
24	A	830	CLA	C4B-NB	2.79	1.41	1.37
24	g	310	CLA	C4B-NB	2.79	1.41	1.37
33	e	612	II0	C16-C03	2.79	1.59	1.53
28	F	203	LMT	O3'-C3'	-2.79	1.36	1.43
24	f	608	CLA	C4B-NB	2.78	1.41	1.37
27	K	103	WVN	C39-C36	2.78	1.51	1.43
24	A	802	CLA	C4B-NB	2.78	1.41	1.37
24	K	101	CLA	C4B-NB	2.78	1.41	1.37
24	A	814	CLA	C4B-NB	2.78	1.41	1.37
24	b	308	CLA	C1D-ND	2.78	1.41	1.37
33	k	616	II0	C33-C35	2.78	1.51	1.46
27	e	615	WVN	C20-C13	2.78	1.54	1.45
27	B	845	WVN	C31-C32	2.78	1.51	1.46
27	B	847	WVN	C29-C26	2.77	1.51	1.43
27	B	845	WVN	C40-C37	2.77	1.51	1.43
24	A	827	CLA	C4B-NB	2.77	1.41	1.37
27	K	103	WVN	C29-C26	2.77	1.51	1.43
27	A	847	WVN	C19-C22	2.77	1.51	1.46
24	B	837	CLA	C4B-NB	2.77	1.41	1.37
27	M	101	WVN	C23-C25	2.77	1.51	1.46
27	A	850	WVN	C33-C34	2.77	1.51	1.46
24	B	813	CLA	C1D-ND	2.77	1.41	1.37
27	B	846	WVN	C39-C36	2.76	1.51	1.43
24	i	602	CLA	CMD-C2D	-2.76	1.45	1.50
34	c	615	IHT	C25-C23	2.76	1.56	1.50
27	M	101	WVN	C02-C11	2.76	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	849	WVN	C29-C26	2.76	1.51	1.43
24	j	309	CLA	C4B-NB	2.76	1.41	1.37
34	b	317	IHT	C25-C23	2.75	1.56	1.50
24	k	605	CLA	C1B-C2B	2.75	1.49	1.43
24	d	304	CLA	C4B-NB	2.75	1.41	1.37
24	g	305	CLA	C1D-ND	2.75	1.41	1.37
24	e	606	CLA	C1B-C2B	2.75	1.49	1.43
24	A	834	CLA	CMD-C2D	-2.74	1.45	1.50
33	f	615	II0	C33-C35	2.74	1.51	1.46
24	i	602	CLA	C1B-C2B	2.74	1.49	1.43
24	b	311	CLA	C4B-NB	2.74	1.41	1.37
33	c	614	II0	C33-C35	2.74	1.51	1.46
27	L	201	WVN	C29-C26	2.74	1.51	1.43
27	A	846	WVN	C31-C32	2.74	1.51	1.46
27	B	845	WVN	C29-C26	2.74	1.51	1.43
35	i	609	KC2	C1B-NB	-2.74	1.34	1.37
24	B	810	CLA	C4B-NB	2.73	1.41	1.37
24	g	315	CLA	C4B-NB	2.73	1.41	1.37
24	B	809	CLA	CMB-C2B	-2.73	1.45	1.50
24	B	805	CLA	C1D-ND	2.72	1.41	1.37
24	e	610	CLA	CMC-C2C	-2.72	1.45	1.50
24	B	804	CLA	CMC-C2C	-2.72	1.45	1.50
35	e	609	KC2	C1A-CHA	2.72	1.47	1.40
27	B	846	WVN	C29-C26	2.72	1.51	1.43
24	B	817	CLA	C4B-NB	2.72	1.41	1.37
27	L	206	WVN	C23-C25	2.72	1.51	1.46
24	c	604	CLA	C1B-C2B	2.72	1.49	1.43
24	d	308	CLA	C1B-C2B	2.72	1.49	1.43
35	g	313	KC2	C1A-CHA	2.71	1.47	1.40
24	A	825	CLA	CMD-C2D	-2.71	1.45	1.50
24	A	823	CLA	C4B-NB	2.71	1.41	1.37
27	h	308	WVN	C19-C22	2.71	1.51	1.46
35	d	310	KC2	C1B-NB	-2.71	1.34	1.37
24	i	605	CLA	C1B-C2B	2.71	1.49	1.43
24	g	308	CLA	C1D-ND	2.71	1.41	1.37
33	i	614	II0	C27-C25	2.71	1.52	1.50
27	B	846	WVN	C31-C32	2.71	1.51	1.46
24	h	303	CLA	CMD-C2D	-2.71	1.45	1.50
34	g	319	IHT	C25-C23	2.70	1.56	1.50
24	k	602	CLA	CMC-C2C	-2.70	1.45	1.50
35	i	616	KC2	C4A-C3A	2.70	1.50	1.44
24	A	855	CLA	CMB-C2B	-2.70	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	304	CLA	C1B-C2B	2.70	1.49	1.43
24	J	103	CLA	C1B-NB	-2.70	1.34	1.37
34	k	618	IHT	C25-C23	2.70	1.56	1.50
24	O	201	CLA	C4B-NB	2.70	1.41	1.37
27	j	301	WVN	C20-C13	2.70	1.54	1.45
27	B	845	WVN	C33-C34	2.70	1.51	1.46
24	A	805	CLA	CMD-C2D	-2.70	1.45	1.50
24	A	813	CLA	C1B-C2B	2.70	1.49	1.43
24	B	840	CLA	C1D-ND	2.70	1.41	1.37
24	A	810	CLA	C1D-ND	2.70	1.41	1.37
24	e	604	CLA	C1B-C2B	2.70	1.49	1.43
27	B	845	WVN	C39-C36	2.69	1.51	1.43
35	i	609	KC2	C3C-C4C	2.69	1.50	1.44
24	A	820	CLA	C1B-NB	-2.69	1.34	1.37
35	k	612	KC2	CHC-C1C	2.69	1.45	1.39
27	j	301	WVN	C02-C11	2.69	1.54	1.50
24	B	835	CLA	CMD-C2D	-2.69	1.45	1.50
24	A	826	CLA	CMC-C2C	-2.69	1.45	1.50
24	B	815	CLA	CMC-C2C	-2.69	1.45	1.50
24	A	809	CLA	CMC-C2C	-2.69	1.45	1.50
24	B	801	CLA	C4B-NB	2.69	1.41	1.37
24	e	608	CLA	C1B-C2B	2.68	1.49	1.43
24	A	839	CLA	C3B-C4B	2.68	1.50	1.42
24	A	818	CLA	C4B-NB	2.68	1.41	1.37
24	L	204	CLA	CMD-C2D	-2.68	1.45	1.50
24	k	610	CLA	C1B-C2B	2.68	1.49	1.43
24	g	303	CLA	C4B-NB	2.68	1.41	1.37
24	a	302	CLA	C1B-C2B	2.68	1.49	1.43
24	B	826	CLA	CMD-C2D	-2.67	1.45	1.50
24	A	822	CLA	C4B-NB	2.67	1.41	1.37
24	B	818	CLA	C4B-NB	2.67	1.41	1.37
24	h	305	CLA	C4B-NB	2.67	1.41	1.37
24	k	607	CLA	C1B-C2B	2.67	1.49	1.43
24	a	305	CLA	C4B-NB	2.67	1.41	1.37
24	g	322	CLA	C4B-NB	2.67	1.41	1.37
28	b	319	LMT	O3'-C3'	-2.67	1.36	1.43
24	B	817	CLA	CMB-C2B	-2.67	1.45	1.50
24	b	305	CLA	C1B-C2B	2.67	1.49	1.43
24	B	818	CLA	CMB-C2B	-2.67	1.45	1.50
24	b	305	CLA	C4B-NB	2.67	1.41	1.37
24	e	610	CLA	C4B-NB	2.67	1.41	1.37
24	A	821	CLA	C4B-NB	2.67	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	205	WVN	C20-C13	2.67	1.54	1.45
27	B	847	WVN	C19-C22	2.67	1.51	1.46
34	c	615	IHT	C18-C07	2.67	1.54	1.45
24	c	607	CLA	C1B-C2B	2.66	1.49	1.43
24	B	834	CLA	C4B-NB	2.66	1.41	1.37
24	B	811	CLA	C3B-C4B	2.66	1.50	1.42
34	O	203	IHT	C18-C07	2.66	1.54	1.45
24	b	311	CLA	C1B-C2B	2.66	1.49	1.43
24	B	832	CLA	C1D-ND	2.66	1.41	1.37
24	A	806	CLA	C1B-C2B	2.66	1.49	1.43
34	a	316	IHT	C25-C23	2.66	1.56	1.50
24	d	303	CLA	C1B-C2B	2.66	1.49	1.43
24	A	841	CLA	C4B-NB	2.66	1.41	1.37
35	g	314	KC2	C1B-NB	-2.66	1.34	1.37
24	g	308	CLA	C4B-NB	2.65	1.41	1.37
34	k	618	IHT	C18-C07	2.65	1.54	1.45
24	b	306	CLA	C1B-C2B	2.65	1.49	1.43
24	a	306	CLA	C1B-C2B	2.65	1.49	1.43
24	A	830	CLA	C1D-ND	2.65	1.41	1.37
34	b	316	IHT	C18-C07	2.65	1.54	1.45
24	A	809	CLA	C4B-NB	2.65	1.41	1.37
34	b	316	IHT	C25-C23	2.64	1.56	1.50
24	B	822	CLA	C4B-NB	2.64	1.41	1.37
24	B	838	CLA	C4B-NB	2.64	1.41	1.37
24	c	608	CLA	C1B-C2B	2.64	1.49	1.43
24	J	105	CLA	C4B-NB	2.64	1.41	1.37
24	B	818	CLA	C3B-C4B	2.64	1.50	1.42
34	j	317	IHT	C25-C23	2.64	1.56	1.50
24	B	813	CLA	C4B-NB	2.64	1.41	1.37
27	L	206	WVN	C29-C26	2.64	1.51	1.43
27	J	102	WVN	C31-C32	2.64	1.51	1.46
24	d	302	CLA	C3B-C4B	2.64	1.50	1.42
24	d	306	CLA	C1B-C2B	2.64	1.49	1.43
34	b	317	IHT	C18-C07	2.63	1.54	1.45
24	a	304	CLA	C4B-NB	2.63	1.41	1.37
27	A	847	WVN	C30-C28	2.63	1.51	1.43
24	B	808	CLA	CMD-C2D	-2.63	1.45	1.50
24	f	601	CLA	C1B-C2B	2.63	1.49	1.43
27	M	101	WVN	C33-C34	2.63	1.51	1.46
24	k	603	CLA	C3B-C4B	2.63	1.50	1.42
27	R	201	WVN	C20-C13	2.63	1.54	1.45
24	B	827	CLA	C4B-NB	2.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	f	607	CLA	C4B-NB	2.63	1.41	1.37
24	A	802	CLA	C1D-ND	2.63	1.41	1.37
35	k	611	KC2	C1B-NB	-2.63	1.34	1.37
24	B	808	CLA	CMB-C2B	-2.63	1.45	1.50
24	j	307	CLA	C1B-C2B	2.62	1.49	1.43
24	B	836	CLA	C4B-NB	2.62	1.41	1.37
24	e	607	CLA	C4B-NB	2.62	1.41	1.37
34	R	204	IHT	C18-C07	2.62	1.54	1.45
24	B	815	CLA	C1B-C2B	2.62	1.49	1.43
27	B	849	WVN	C02-C11	2.62	1.54	1.50
27	J	101	WVN	C23-C25	2.62	1.51	1.46
24	A	830	CLA	CMB-C2B	-2.62	1.45	1.50
24	i	607	CLA	C1B-C2B	2.62	1.49	1.43
24	I	102	CLA	CMB-C2B	-2.62	1.45	1.50
24	B	816	CLA	C4B-NB	2.62	1.41	1.37
27	B	849	WVN	C20-C13	2.62	1.54	1.45
24	c	601	CLA	C1B-C2B	2.62	1.49	1.43
24	B	809	CLA	C1D-ND	2.62	1.41	1.37
24	k	609	CLA	C3B-C4B	2.61	1.50	1.42
24	B	839	CLA	C3B-C4B	2.61	1.50	1.42
24	B	830	CLA	C1B-C2B	2.61	1.49	1.43
27	A	848	WVN	C20-C13	2.61	1.54	1.45
24	B	831	CLA	C4B-NB	2.61	1.41	1.37
24	g	306	CLA	C1B-C2B	2.61	1.49	1.43
24	g	309	CLA	C4B-NB	2.61	1.41	1.37
24	g	309	CLA	C1B-C2B	2.61	1.49	1.43
24	f	606	CLA	C1B-C2B	2.60	1.49	1.43
24	a	309	CLA	C1B-C2B	2.60	1.49	1.43
24	g	305	CLA	C4B-NB	2.60	1.41	1.37
24	O	205	CLA	CMB-C2B	-2.60	1.45	1.50
24	g	307	CLA	C4B-NB	2.60	1.41	1.37
34	b	317	IHT	C20-C15	2.60	1.55	1.50
24	i	601	CLA	C1B-C2B	2.60	1.49	1.43
24	a	312	CLA	C1B-C2B	2.60	1.49	1.43
24	A	813	CLA	MG-NC	2.60	2.12	2.06
34	f	617	IHT	C18-C07	2.60	1.53	1.45
24	k	604	CLA	CMC-C2C	-2.59	1.45	1.50
34	a	316	IHT	C18-C07	2.59	1.53	1.45
24	B	801	CLA	MG-NB	-2.59	2.00	2.05
24	c	608	CLA	C4B-NB	2.59	1.41	1.37
24	k	606	CLA	C1B-C2B	2.59	1.49	1.43
27	R	202	WVN	C19-C22	2.59	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	313	CLA	C1B-C2B	2.59	1.49	1.43
24	A	811	CLA	C3B-C4B	2.59	1.50	1.42
24	i	608	CLA	C1B-C2B	2.59	1.49	1.43
24	a	309	CLA	CMD-C2D	-2.59	1.45	1.50
24	B	833	CLA	C4B-NB	2.59	1.41	1.37
24	A	838	CLA	C1B-C2B	2.58	1.49	1.43
24	a	303	CLA	C1B-C2B	2.58	1.49	1.43
24	f	605	CLA	C4B-NB	2.58	1.41	1.37
24	A	852	CLA	CMB-C2B	-2.58	1.45	1.50
24	c	606	CLA	C3B-C4B	2.58	1.50	1.42
24	a	302	CLA	C4B-NB	2.58	1.41	1.37
24	A	820	CLA	C1D-ND	2.58	1.41	1.37
24	B	827	CLA	CMB-C2B	-2.58	1.45	1.50
24	a	303	CLA	C4B-NB	2.58	1.41	1.37
24	g	311	CLA	C1B-C2B	2.58	1.49	1.43
33	j	316	II0	C33-C35	2.58	1.51	1.46
24	g	302	CLA	MG-NB	-2.58	2.00	2.05
24	O	201	CLA	CMD-C2D	-2.58	1.45	1.50
27	I	101	WVN	C20-C13	2.58	1.53	1.45
27	L	201	WVN	C31-C32	2.58	1.51	1.46
34	O	203	IHT	C25-C23	2.57	1.56	1.50
34	O	203	IHT	C20-C15	2.57	1.55	1.50
24	A	835	CLA	CMB-C2B	-2.57	1.45	1.50
24	L	202	CLA	C3B-C4B	2.57	1.50	1.42
24	B	838	CLA	CMD-C2D	-2.57	1.45	1.50
24	A	830	CLA	CMD-C2D	-2.57	1.45	1.50
24	A	824	CLA	C4B-NB	2.57	1.41	1.37
24	B	823	CLA	C1D-ND	2.57	1.41	1.37
24	k	606	CLA	CMD-C2D	-2.57	1.45	1.50
24	B	805	CLA	C1B-C2B	2.57	1.49	1.43
24	A	856	CLA	CMD-C2D	-2.56	1.45	1.50
24	A	828	CLA	C4B-NB	2.56	1.41	1.37
24	i	603	CLA	C1B-C2B	2.56	1.49	1.43
24	A	838	CLA	CMD-C2D	-2.56	1.45	1.50
24	f	602	CLA	C4B-NB	2.56	1.41	1.37
27	L	206	WVN	C19-C22	2.56	1.51	1.46
33	k	615	II0	C33-C35	2.56	1.51	1.46
24	B	837	CLA	C1B-C2B	2.56	1.49	1.43
35	e	609	KC2	CBD-CAD	-2.56	1.45	1.56
24	g	302	CLA	C4B-NB	2.56	1.41	1.37
24	c	602	CLA	CHC-C1C	2.56	1.43	1.38
24	c	603	CLA	C4B-NB	2.56	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	851	LMT	O4'-C4B	-2.56	1.36	1.43
24	d	305	CLA	CMC-C2C	-2.56	1.45	1.50
24	B	822	CLA	CMB-C2B	-2.55	1.45	1.50
24	c	606	CLA	C1B-C2B	2.55	1.49	1.43
24	B	813	CLA	C1B-C2B	2.55	1.49	1.43
24	A	806	CLA	CMD-C2D	-2.55	1.45	1.50
24	A	802	CLA	C1B-NB	-2.55	1.34	1.37
27	M	101	WVN	C20-C13	2.55	1.53	1.45
27	L	206	WVN	C31-C32	2.55	1.51	1.46
24	B	803	CLA	C4B-NB	2.55	1.41	1.37
24	e	602	CLA	C4B-NB	2.55	1.41	1.37
24	L	204	CLA	C1B-C2B	2.55	1.49	1.43
24	k	606	CLA	C1D-ND	2.55	1.41	1.37
24	B	813	CLA	CMD-C2D	-2.54	1.45	1.50
24	B	807	CLA	C1B-C2B	2.54	1.49	1.43
24	J	105	CLA	C1B-C2B	2.54	1.49	1.43
24	h	301	CLA	CMC-C2C	-2.54	1.45	1.50
27	h	308	WVN	C20-C13	2.54	1.53	1.45
24	A	822	CLA	MG-NB	-2.54	2.00	2.05
24	A	853	CLA	CMD-C2D	-2.54	1.45	1.50
24	b	306	CLA	CMB-C2B	-2.54	1.45	1.50
24	L	203	CLA	C4B-NB	2.54	1.41	1.37
24	h	303	CLA	C4B-NB	2.54	1.41	1.37
24	B	810	CLA	CMB-C2B	-2.54	1.45	1.50
24	B	825	CLA	MG-NB	-2.54	2.00	2.05
24	B	830	CLA	CMD-C2D	-2.54	1.45	1.50
24	j	306	CLA	C1B-C2B	2.54	1.49	1.43
24	j	302	CLA	C3B-C4B	2.54	1.50	1.42
24	e	611	CLA	CMD-C2D	-2.54	1.45	1.50
24	K	101	CLA	C1D-ND	2.54	1.41	1.37
24	A	821	CLA	C1D-ND	2.53	1.41	1.37
27	A	847	WVN	C23-C25	2.53	1.51	1.46
24	b	312	CLA	C1B-C2B	2.53	1.49	1.43
24	g	303	CLA	CMD-C2D	-2.53	1.45	1.50
24	i	610	CLA	C1B-C2B	2.53	1.49	1.43
34	j	317	IHT	C18-C07	2.53	1.53	1.45
24	B	820	CLA	CMD-C2D	-2.53	1.45	1.50
24	A	840	CLA	C4B-NB	2.53	1.41	1.37
24	B	809	CLA	MG-NB	-2.53	2.00	2.05
24	a	307	CLA	C3B-C4B	2.53	1.50	1.42
24	i	604	CLA	C4B-NB	2.52	1.41	1.37
24	A	839	CLA	C4B-NB	2.52	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	804	CLA	CMC-C2C	-2.52	1.45	1.50
24	j	302	CLA	CMB-C2B	-2.52	1.45	1.50
24	d	303	CLA	CMD-C2D	-2.52	1.45	1.50
24	A	831	CLA	CMD-C2D	-2.52	1.45	1.50
24	B	803	CLA	C1D-ND	2.52	1.41	1.37
24	h	312	CLA	CMB-C2B	-2.52	1.45	1.50
35	g	314	KC2	C3C-C4C	2.52	1.49	1.44
24	B	826	CLA	C4B-NB	2.51	1.41	1.37
24	g	304	CLA	C4B-NB	2.51	1.41	1.37
35	k	612	KC2	C1A-CHA	2.51	1.46	1.40
24	A	824	CLA	C1B-C2B	2.51	1.49	1.43
24	j	304	CLA	C1B-C2B	2.51	1.49	1.43
24	A	807	CLA	C4B-NB	2.51	1.41	1.37
24	A	812	CLA	CMC-C2C	-2.51	1.45	1.50
24	d	305	CLA	CHC-C4B	-2.51	1.33	1.39
24	e	605	CLA	MG-ND	-2.51	2.00	2.05
24	L	202	CLA	CMB-C2B	-2.51	1.45	1.50
24	B	841	CLA	C1B-C2B	2.51	1.49	1.43
24	A	855	CLA	CMC-C2C	-2.51	1.45	1.50
35	j	312	KC2	CBD-CAD	-2.51	1.45	1.56
24	k	604	CLA	C1B-C2B	2.51	1.49	1.43
24	e	601	CLA	C3B-C4B	2.50	1.50	1.42
27	F	204	WVN	C33-C34	2.50	1.51	1.46
24	A	809	CLA	CMB-C2B	-2.50	1.45	1.50
27	B	845	WVN	C23-C25	2.50	1.51	1.46
27	B	847	WVN	C20-C13	2.50	1.53	1.45
24	k	614	CLA	C1B-C2B	2.50	1.49	1.43
24	B	841	CLA	C4B-NB	2.50	1.41	1.37
24	a	311	CLA	C4B-NB	2.50	1.41	1.37
24	A	817	CLA	CMD-C2D	-2.50	1.45	1.50
24	A	837	CLA	C1B-C2B	2.50	1.49	1.43
35	j	312	KC2	C3C-C4C	2.50	1.49	1.44
24	d	304	CLA	C1B-C2B	2.50	1.49	1.43
27	J	102	WVN	C02-C11	2.50	1.54	1.50
24	b	313	CLA	C3B-C4B	2.50	1.50	1.42
24	A	819	CLA	CMB-C2B	-2.49	1.45	1.50
28	A	851	LMT	O2B-C2B	-2.49	1.36	1.43
24	c	603	CLA	C1B-C2B	2.49	1.49	1.43
24	h	306	CLA	C3B-C4B	2.49	1.50	1.42
24	A	807	CLA	CMB-C2B	-2.49	1.45	1.50
24	f	604	CLA	C1B-C2B	2.49	1.49	1.43
24	e	607	CLA	C1B-C2B	2.49	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	822	CLA	CMD-C2D	-2.49	1.45	1.50
24	d	312	CLA	C1B-C2B	2.49	1.49	1.43
24	A	815	CLA	C1B-NB	-2.49	1.34	1.37
33	k	615	II0	C16-C03	2.49	1.58	1.53
24	B	801	CLA	CHC-C1C	2.49	1.43	1.38
27	A	850	WVN	C20-C13	2.49	1.53	1.45
34	a	316	IHT	C20-C15	2.49	1.54	1.50
24	B	816	CLA	CMB-C2B	-2.49	1.45	1.50
24	f	609	CLA	C1B-C2B	2.49	1.49	1.43
24	b	309	CLA	C3B-C4B	2.49	1.50	1.42
24	B	821	CLA	C4B-NB	2.49	1.41	1.37
34	k	618	IHT	C39-C35	2.49	1.55	1.50
24	h	301	CLA	C1B-C2B	2.48	1.49	1.43
24	A	822	CLA	CMB-C2B	-2.48	1.45	1.50
24	B	801	CLA	CMD-C2D	-2.48	1.45	1.50
24	d	307	CLA	C1B-C2B	2.48	1.49	1.43
34	R	204	IHT	C25-C23	2.48	1.55	1.50
24	c	605	CLA	C1B-C2B	2.48	1.49	1.43
24	i	607	CLA	CMC-C2C	-2.48	1.45	1.50
24	b	310	CLA	C1B-C2B	2.48	1.48	1.43
24	k	608	CLA	C1B-C2B	2.48	1.48	1.43
24	f	605	CLA	C1B-C2B	2.48	1.48	1.43
33	b	318	II0	C16-C03	2.48	1.58	1.53
24	e	606	CLA	C4B-NB	2.48	1.41	1.37
33	g	318	II0	C18-C04	2.48	1.58	1.53
24	f	613	CLA	C3B-C4B	2.48	1.49	1.42
24	B	834	CLA	CMD-C2D	-2.48	1.45	1.50
24	e	603	CLA	C3B-C4B	2.48	1.49	1.42
24	B	809	CLA	C4B-NB	2.48	1.41	1.37
24	B	831	CLA	MG-NB	-2.48	2.00	2.05
24	A	855	CLA	C3B-C4B	2.47	1.49	1.42
24	A	856	CLA	CMB-C2B	-2.47	1.45	1.50
24	B	829	CLA	MG-ND	-2.47	2.00	2.05
24	A	853	CLA	C1D-ND	2.47	1.41	1.37
24	B	829	CLA	CMB-C2B	-2.47	1.45	1.50
24	B	818	CLA	CMD-C2D	-2.47	1.45	1.50
24	A	820	CLA	C4B-NB	2.47	1.41	1.37
24	B	832	CLA	CMC-C2C	-2.47	1.45	1.50
24	f	604	CLA	C4B-NB	2.47	1.41	1.37
24	B	823	CLA	MG-NB	-2.47	2.00	2.05
24	A	802	CLA	CMD-C2D	-2.47	1.45	1.50
34	c	615	IHT	C20-C15	2.47	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	e	611	CLA	C1B-C2B	2.47	1.48	1.43
24	j	305	CLA	CMD-C2D	-2.47	1.45	1.50
24	A	819	CLA	C4B-NB	2.47	1.41	1.37
24	k	602	CLA	C3B-C4B	2.47	1.49	1.42
24	B	814	CLA	CMB-C2B	-2.46	1.45	1.50
35	d	310	KC2	C3C-C4C	2.46	1.49	1.44
24	A	817	CLA	CMB-C2B	-2.46	1.45	1.50
24	A	816	CLA	C4B-NB	2.46	1.41	1.37
24	B	829	CLA	C1D-ND	2.46	1.41	1.37
24	B	801	CLA	C1D-ND	2.46	1.41	1.37
24	R	203	CLA	C4B-NB	2.46	1.41	1.37
34	O	203	IHT	C39-C35	2.46	1.55	1.50
24	e	605	CLA	C1B-C2B	2.46	1.48	1.43
33	g	317	II0	C28-C26	2.46	1.52	1.50
24	f	606	CLA	CMB-C2B	-2.46	1.45	1.50
24	B	830	CLA	C4B-NB	2.46	1.41	1.37
24	A	827	CLA	CMD-C2D	-2.46	1.45	1.50
35	i	616	KC2	C1B-NB	-2.46	1.34	1.37
24	f	606	CLA	CMC-C2C	-2.46	1.45	1.50
24	B	822	CLA	CMC-C2C	-2.46	1.45	1.50
24	j	314	CLA	C1B-C2B	2.46	1.48	1.43
24	A	815	CLA	MG-NB	-2.45	2.00	2.05
24	g	315	CLA	CMD-C2D	-2.45	1.45	1.50
24	k	603	CLA	C1B-C2B	2.45	1.48	1.43
24	a	304	CLA	C1B-C2B	2.45	1.48	1.43
34	f	617	IHT	C39-C35	2.45	1.55	1.50
24	f	610	CLA	C1B-C2B	2.45	1.48	1.43
24	B	837	CLA	CMD-C2D	-2.45	1.45	1.50
27	A	848	WVN	C19-C22	2.45	1.51	1.46
34	j	317	IHT	C20-C15	2.45	1.54	1.50
34	g	319	IHT	C18-C07	2.45	1.53	1.45
24	O	201	CLA	MG-NB	-2.45	2.00	2.05
24	b	312	CLA	C3B-C4B	2.45	1.49	1.42
24	L	204	CLA	CMC-C2C	-2.45	1.45	1.50
24	f	602	CLA	CMD-C2D	-2.45	1.45	1.50
27	B	845	WVN	C20-C13	2.45	1.53	1.45
24	B	814	CLA	C1B-C2B	2.45	1.48	1.43
24	e	603	CLA	C1B-C2B	2.45	1.48	1.43
27	J	102	WVN	C20-C13	2.45	1.53	1.45
24	B	809	CLA	CMC-C2C	-2.45	1.45	1.50
24	B	824	CLA	C1B-C2B	2.45	1.48	1.43
33	k	619	II0	C15-C03	2.44	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	313	II0	C16-C03	2.44	1.58	1.53
24	j	303	CLA	C1B-C2B	2.44	1.48	1.43
24	g	322	CLA	C1B-C2B	2.44	1.48	1.43
24	g	306	CLA	CMB-C2B	-2.44	1.45	1.50
33	d	314	II0	C16-C03	2.44	1.58	1.53
24	A	853	CLA	C4B-NB	2.44	1.41	1.37
24	c	602	CLA	C3B-C4B	2.44	1.49	1.42
24	A	828	CLA	C1B-C2B	2.44	1.48	1.43
24	B	823	CLA	C4B-NB	2.44	1.41	1.37
24	A	855	CLA	CMD-C2D	-2.44	1.45	1.50
35	i	609	KC2	CBD-CAD	-2.44	1.45	1.56
33	i	614	II0	C18-C04	2.44	1.58	1.53
35	d	311	KC2	C1A-CHA	2.44	1.46	1.40
24	A	817	CLA	CMC-C2C	-2.44	1.45	1.50
24	i	605	CLA	CMD-C2D	-2.44	1.45	1.50
35	g	313	KC2	CBD-CAD	-2.44	1.45	1.56
33	i	613	II0	C16-C03	2.44	1.58	1.53
24	A	853	CLA	C3B-C4B	2.44	1.49	1.42
24	A	824	CLA	CMD-C2D	-2.44	1.45	1.50
24	A	839	CLA	CMB-C2B	-2.44	1.45	1.50
24	J	103	CLA	CMD-C2D	-2.44	1.45	1.50
24	k	605	CLA	C4B-NB	2.44	1.41	1.37
24	K	102	CLA	CMD-C2D	-2.44	1.45	1.50
24	A	836	CLA	C1B-C2B	2.44	1.48	1.43
35	i	616	KC2	C3C-C4C	2.43	1.49	1.44
24	B	825	CLA	CMC-C2C	-2.43	1.45	1.50
24	g	303	CLA	C1B-C2B	2.43	1.48	1.43
24	L	202	CLA	CMD-C2D	-2.43	1.45	1.50
24	i	611	CLA	C1B-C2B	2.43	1.48	1.43
24	b	310	CLA	C3B-C4B	2.43	1.49	1.42
24	c	612	CLA	C1B-C2B	2.43	1.48	1.43
24	B	803	CLA	MG-NB	-2.43	2.01	2.05
24	F	201	CLA	CMD-C2D	-2.43	1.45	1.50
27	L	201	WVN	C19-C22	2.43	1.51	1.46
33	b	314	II0	C33-C35	2.43	1.51	1.46
24	A	852	CLA	C4B-NB	2.43	1.41	1.37
24	A	853	CLA	MG-NB	-2.43	2.01	2.05
33	a	317	II0	C18-C04	2.43	1.58	1.53
24	e	608	CLA	C3B-C4B	2.43	1.49	1.42
34	b	316	IHT	C39-C35	2.43	1.55	1.50
35	d	310	KC2	C1A-CHA	2.43	1.46	1.40
33	c	613	II0	C16-C03	2.43	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	826	CLA	CMD-C2D	-2.43	1.45	1.50
24	i	605	CLA	C3B-C4B	2.43	1.49	1.42
24	c	609	CLA	C3B-C4B	2.42	1.49	1.42
24	B	836	CLA	C1B-C2B	2.42	1.48	1.43
24	A	820	CLA	CMD-C2D	-2.42	1.45	1.50
24	A	821	CLA	CMD-C2D	-2.42	1.45	1.50
24	B	825	CLA	C4B-NB	2.42	1.41	1.37
24	B	804	CLA	C4B-NB	2.42	1.41	1.37
24	b	305	CLA	CMD-C2D	-2.42	1.45	1.50
24	K	101	CLA	CMC-C2C	-2.42	1.45	1.50
35	f	611	KC2	CBD-CAD	-2.42	1.45	1.56
34	c	615	IHT	C39-C35	2.42	1.55	1.50
34	f	617	IHT	C20-C15	2.42	1.54	1.50
24	h	304	CLA	C4B-NB	2.42	1.41	1.37
24	e	604	CLA	CMD-C2D	-2.42	1.45	1.50
27	L	201	WVN	C20-C13	2.42	1.53	1.45
24	a	308	CLA	MG-NB	-2.42	2.01	2.05
24	k	604	CLA	CMD-C2D	-2.42	1.45	1.50
34	j	317	IHT	C39-C35	2.42	1.55	1.50
34	R	204	IHT	C20-C15	2.42	1.54	1.50
28	a	318	LMT	O2B-C2B	-2.42	1.37	1.43
24	A	852	CLA	CMD-C2D	-2.41	1.45	1.50
35	j	312	KC2	C1A-CHA	2.41	1.46	1.40
24	j	307	CLA	CMB-C2B	-2.41	1.45	1.50
24	g	303	CLA	MG-NB	-2.41	2.01	2.05
24	A	833	CLA	CMD-C2D	-2.41	1.45	1.50
24	b	303	CLA	C4B-NB	2.41	1.41	1.37
24	A	806	CLA	C3B-C4B	2.41	1.49	1.42
24	f	603	CLA	C1B-C2B	2.41	1.48	1.43
24	A	841	CLA	CMB-C2B	-2.41	1.45	1.50
27	K	103	WVN	C19-C22	2.41	1.51	1.46
24	B	806	CLA	CMC-C2C	-2.41	1.45	1.50
27	F	204	WVN	C23-C25	2.41	1.51	1.46
24	B	812	CLA	CMC-C2C	-2.41	1.45	1.50
24	B	824	CLA	CMC-C2C	-2.41	1.45	1.50
24	k	601	CLA	CMB-C2B	-2.41	1.45	1.50
35	e	609	KC2	C3C-C4C	2.41	1.49	1.44
24	F	202	CLA	C3B-C4B	2.41	1.49	1.42
24	A	812	CLA	C1B-C2B	2.41	1.48	1.43
24	h	306	CLA	C1B-C2B	2.41	1.48	1.43
24	A	824	CLA	CMB-C2B	-2.40	1.45	1.50
24	g	322	CLA	CMD-C2D	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	105	CLA	C3B-C4B	2.40	1.49	1.42
24	f	602	CLA	C1B-C2B	2.40	1.48	1.43
33	a	313	II0	C28-C26	2.40	1.52	1.50
24	a	307	CLA	CMB-C2B	-2.40	1.45	1.50
24	d	303	CLA	CHC-C4B	-2.40	1.34	1.39
33	k	617	II0	C18-C04	2.40	1.58	1.53
35	c	610	KC2	CBD-CAD	-2.40	1.45	1.56
28	A	851	LMT	O2'-C2'	-2.40	1.37	1.43
24	b	304	CLA	CMC-C2C	-2.40	1.45	1.50
24	A	803	CLA	CMB-C2B	-2.40	1.45	1.50
24	A	808	CLA	CMD-C2D	-2.40	1.45	1.50
24	B	812	CLA	C4B-NB	2.40	1.41	1.37
24	B	808	CLA	C1B-C2B	2.40	1.48	1.43
24	d	306	CLA	MG-NA	2.39	2.12	2.06
24	e	605	CLA	C1D-ND	2.39	1.41	1.37
27	B	846	WVN	C19-C22	2.39	1.51	1.46
35	k	613	KC2	C3C-C4C	2.39	1.49	1.44
24	A	803	CLA	C4B-NB	2.39	1.41	1.37
24	k	601	CLA	CMD-C2D	-2.39	1.45	1.50
24	h	307	CLA	C3B-C4B	2.39	1.49	1.42
24	d	302	CLA	C1B-C2B	2.39	1.48	1.43
24	a	305	CLA	C3B-C4B	2.39	1.49	1.42
33	c	616	II0	C16-C03	2.39	1.58	1.53
24	b	303	CLA	C1B-C2B	2.39	1.48	1.43
24	d	306	CLA	CMD-C2D	-2.39	1.45	1.50
24	d	305	CLA	C1B-NB	-2.39	1.34	1.37
24	A	834	CLA	MG-NB	-2.39	2.01	2.05
24	h	302	CLA	C4B-NB	2.39	1.41	1.37
34	f	617	IHT	C25-C23	2.39	1.55	1.50
24	h	312	CLA	CMD-C2D	-2.39	1.45	1.50
24	B	835	CLA	CMB-C2B	-2.38	1.45	1.50
24	i	606	CLA	CMD-C2D	-2.38	1.45	1.50
35	k	613	KC2	C1A-CHA	2.38	1.46	1.40
24	A	812	CLA	C4B-NB	2.38	1.41	1.37
24	B	831	CLA	CMD-C2D	-2.38	1.45	1.50
24	A	810	CLA	C1B-C2B	2.38	1.48	1.43
33	i	612	II0	C16-C03	2.38	1.58	1.53
35	i	616	KC2	C1A-CHA	2.38	1.46	1.40
27	A	849	WVN	C02-C11	2.38	1.54	1.50
24	B	838	CLA	CMB-C2B	-2.38	1.45	1.50
34	a	316	IHT	C39-C35	2.38	1.55	1.50
24	A	825	CLA	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	204	CLA	C4B-NB	2.38	1.41	1.37
24	B	841	CLA	CMD-C2D	-2.38	1.45	1.50
33	j	318	II0	C16-C03	2.38	1.58	1.53
24	K	102	CLA	MG-NB	-2.37	2.01	2.05
24	b	303	CLA	CMD-C2D	-2.37	1.45	1.50
24	B	835	CLA	C4B-NB	2.37	1.41	1.37
24	A	833	CLA	MG-NB	-2.37	2.01	2.05
24	A	811	CLA	CMD-C2D	-2.37	1.45	1.50
24	a	306	CLA	CMB-C2B	-2.37	1.45	1.50
24	L	204	CLA	C1D-ND	2.37	1.41	1.37
24	g	310	CLA	C1B-C2B	2.37	1.48	1.43
24	A	822	CLA	C1D-ND	2.37	1.41	1.37
27	F	204	WVN	C20-C13	2.37	1.53	1.45
24	B	838	CLA	MG-NB	-2.37	2.01	2.05
27	J	101	WVN	C20-C13	2.37	1.53	1.45
35	k	613	KC2	C4B-NB	-2.37	1.34	1.37
24	j	304	CLA	C3B-C4B	2.37	1.49	1.42
33	f	614	II0	C16-C03	2.37	1.58	1.53
24	A	827	CLA	C1D-ND	2.37	1.41	1.37
24	h	302	CLA	MG-NB	-2.37	2.01	2.05
24	A	827	CLA	CMC-C2C	-2.37	1.45	1.50
24	f	610	CLA	C3B-C4B	2.36	1.49	1.42
24	b	307	CLA	C3B-C4B	2.36	1.49	1.42
24	B	832	CLA	C1B-NB	-2.36	1.34	1.37
27	A	849	WVN	C20-C13	2.36	1.53	1.45
24	g	315	CLA	C3B-C4B	2.36	1.49	1.42
24	b	308	CLA	CMD-C2D	-2.36	1.45	1.50
24	A	815	CLA	CMD-C2D	-2.36	1.45	1.50
24	b	312	CLA	CMB-C2B	-2.36	1.45	1.50
24	A	823	CLA	CMB-C2B	-2.36	1.45	1.50
35	c	610	KC2	C1A-CHA	2.36	1.46	1.40
24	b	308	CLA	CMC-C2C	-2.36	1.45	1.50
27	R	202	WVN	C20-C13	2.35	1.53	1.45
27	F	205	WVN	C02-C11	2.35	1.53	1.50
24	a	308	CLA	C4B-NB	2.35	1.41	1.37
24	B	810	CLA	C1B-C2B	2.35	1.48	1.43
24	A	827	CLA	CHC-C1C	2.35	1.43	1.38
24	a	311	CLA	C1B-C2B	2.35	1.48	1.43
24	B	836	CLA	CMD-C2D	-2.35	1.45	1.50
24	j	309	CLA	CMD-C2D	-2.35	1.46	1.50
24	A	824	CLA	MG-NB	-2.35	2.01	2.05
35	d	311	KC2	CBD-CAD	-2.35	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	105	CLA	CHC-C1C	2.35	1.43	1.38
24	j	308	CLA	CMD-C2D	-2.35	1.46	1.50
27	F	205	WVN	C20-C13	2.35	1.53	1.45
24	A	836	CLA	MG-NB	-2.35	2.01	2.05
24	f	603	CLA	CMD-C2D	-2.35	1.46	1.50
35	d	310	KC2	CBD-CAD	-2.35	1.46	1.56
24	g	309	CLA	CMD-C2D	-2.35	1.46	1.50
24	A	804	CLA	C4B-NB	2.35	1.40	1.37
35	g	313	KC2	C3C-C4C	2.35	1.49	1.44
24	A	804	CLA	CMD-C2D	-2.35	1.46	1.50
24	A	810	CLA	CMB-C2B	-2.35	1.46	1.50
24	A	825	CLA	C1D-ND	2.34	1.40	1.37
24	h	304	CLA	CMD-C2D	-2.34	1.46	1.50
24	A	810	CLA	CMC-C2C	-2.34	1.46	1.50
24	B	807	CLA	CMC-C2C	-2.34	1.46	1.50
24	L	203	CLA	CMB-C2B	-2.34	1.46	1.50
24	d	305	CLA	CMD-C2D	-2.34	1.46	1.50
24	A	815	CLA	C4B-NB	2.34	1.40	1.37
33	d	313	II0	C18-C04	2.34	1.58	1.53
24	B	804	CLA	MG-NB	-2.34	2.01	2.05
24	j	303	CLA	CMD-C2D	-2.34	1.46	1.50
24	B	812	CLA	C1B-NB	-2.34	1.34	1.37
24	i	610	CLA	C3B-C4B	2.34	1.49	1.42
24	B	834	CLA	C1B-C2B	2.34	1.48	1.43
27	B	846	WVN	C20-C13	2.34	1.53	1.45
34	R	204	IHT	C39-C35	2.34	1.55	1.50
27	A	846	WVN	C20-C13	2.34	1.53	1.45
24	b	309	CLA	CMB-C2B	-2.33	1.46	1.50
24	f	609	CLA	CMC-C2C	-2.33	1.46	1.50
24	A	833	CLA	C1B-C2B	2.33	1.48	1.43
24	A	812	CLA	CMD-C2D	-2.33	1.46	1.50
24	A	814	CLA	CMC-C2C	-2.33	1.46	1.50
24	A	828	CLA	CMB-C2B	-2.33	1.46	1.50
24	B	808	CLA	CMC-C2C	-2.33	1.46	1.50
24	A	824	CLA	CMC-C2C	-2.33	1.46	1.50
24	b	303	CLA	CMB-C2B	-2.33	1.46	1.50
24	B	807	CLA	MG-NB	-2.33	2.01	2.05
24	c	609	CLA	C1B-C2B	2.33	1.48	1.43
28	a	318	LMT	O3'-C3'	-2.33	1.37	1.43
24	L	207	CLA	C1B-C2B	2.33	1.48	1.43
24	c	611	CLA	CMC-C2C	-2.33	1.46	1.50
24	j	309	CLA	CMC-C2C	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	821	CLA	CMC-C2C	-2.33	1.46	1.50
24	B	814	CLA	CMD-C2D	-2.33	1.46	1.50
24	B	828	CLA	C4B-NB	2.33	1.40	1.37
24	L	203	CLA	C3B-C4B	2.33	1.49	1.42
24	A	805	CLA	CMB-C2B	-2.33	1.46	1.50
24	A	817	CLA	MG-NB	-2.33	2.01	2.05
24	d	309	CLA	C1B-C2B	2.33	1.48	1.43
33	k	621	II0	C18-C04	2.33	1.58	1.53
24	A	823	CLA	C1B-C2B	2.33	1.48	1.43
24	j	313	CLA	CMD-C2D	-2.33	1.46	1.50
24	A	830	CLA	C1B-NB	-2.33	1.34	1.37
24	A	834	CLA	C1B-NB	-2.33	1.34	1.37
24	A	819	CLA	CMD-C2D	-2.33	1.46	1.50
24	g	310	CLA	C3B-C4B	2.32	1.49	1.42
35	k	611	KC2	CBD-CAD	-2.32	1.46	1.56
24	d	309	CLA	C3B-C4B	2.32	1.49	1.42
24	B	829	CLA	C1B-C2B	2.32	1.48	1.43
24	A	814	CLA	C3B-C4B	2.32	1.49	1.42
24	R	203	CLA	CMB-C2B	-2.32	1.46	1.50
24	i	608	CLA	C3B-C4B	2.32	1.49	1.42
24	f	613	CLA	CMD-C2D	-2.32	1.46	1.50
24	e	602	CLA	CMD-C2D	-2.32	1.46	1.50
27	B	846	WVN	C26-C22	-2.32	1.30	1.35
24	g	304	CLA	CMD-C2D	-2.32	1.46	1.50
24	e	610	CLA	C1B-C2B	2.32	1.48	1.43
24	j	310	CLA	C3B-C4B	2.32	1.49	1.42
24	B	804	CLA	C1D-ND	2.32	1.40	1.37
24	h	304	CLA	CMB-C2B	-2.32	1.46	1.50
24	j	308	CLA	CMB-C2B	-2.32	1.46	1.50
24	g	307	CLA	CMB-C2B	-2.32	1.46	1.50
27	L	206	WVN	C26-C22	-2.32	1.30	1.35
24	h	303	CLA	C1B-C2B	2.32	1.48	1.43
24	B	836	CLA	CMB-C2B	-2.32	1.46	1.50
24	A	829	CLA	CMB-C2B	-2.32	1.46	1.50
24	A	840	CLA	CMD-C2D	-2.32	1.46	1.50
24	B	839	CLA	CMB-C2B	-2.32	1.46	1.50
24	k	602	CLA	C1B-C2B	2.32	1.48	1.43
24	h	301	CLA	CMD-C2D	-2.32	1.46	1.50
24	A	856	CLA	CAC-C3C	-2.32	1.45	1.51
24	A	813	CLA	CMD-C2D	-2.32	1.46	1.50
27	R	201	WVN	C02-C11	2.32	1.53	1.50
35	k	611	KC2	C3C-C4C	2.32	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	j	305	CLA	C1B-C2B	2.32	1.48	1.43
35	k	613	KC2	C1D-C2D	2.32	1.48	1.43
24	j	308	CLA	C1B-C2B	2.32	1.48	1.43
24	A	831	CLA	MG-NB	-2.31	2.01	2.05
24	B	806	CLA	MG-NB	-2.31	2.01	2.05
24	B	817	CLA	MG-NB	-2.31	2.01	2.05
24	A	810	CLA	C3B-C4B	2.31	1.49	1.42
24	L	207	CLA	CMD-C2D	-2.31	1.46	1.50
28	A	851	LMT	O3B-C3B	-2.31	1.37	1.43
34	b	316	IHT	C20-C15	2.31	1.54	1.50
24	d	302	CLA	MG-NB	-2.31	2.01	2.05
24	A	803	CLA	C3B-C4B	2.31	1.49	1.42
24	A	804	CLA	C1B-C2B	2.31	1.48	1.43
24	h	307	CLA	C1B-C2B	2.31	1.48	1.43
24	B	832	CLA	MG-NB	-2.31	2.01	2.05
24	k	609	CLA	C1B-C2B	2.31	1.48	1.43
24	c	603	CLA	C3B-C4B	2.31	1.49	1.42
24	b	311	CLA	CMD-C2D	-2.31	1.46	1.50
24	g	308	CLA	CMD-C2D	-2.31	1.46	1.50
24	f	613	CLA	C1B-C2B	2.31	1.48	1.43
24	d	303	CLA	MG-ND	-2.31	2.01	2.05
24	B	830	CLA	CMC-C2C	-2.31	1.46	1.50
24	e	603	CLA	CMD-C2D	-2.31	1.46	1.50
24	h	302	CLA	CMB-C2B	-2.30	1.46	1.50
24	j	310	CLA	CMC-C2C	-2.30	1.46	1.50
24	h	302	CLA	CMD-C2D	-2.30	1.46	1.50
24	B	811	CLA	CMD-C2D	-2.30	1.46	1.50
24	A	837	CLA	CMD-C2D	-2.30	1.46	1.50
27	A	850	WVN	C02-C11	2.30	1.53	1.50
24	a	307	CLA	C1B-C2B	2.30	1.48	1.43
24	A	836	CLA	CMD-C2D	-2.30	1.46	1.50
28	a	318	LMT	O4'-C4B	-2.30	1.37	1.43
24	A	806	CLA	CMB-C2B	-2.30	1.46	1.50
24	c	602	CLA	CMD-C2D	-2.30	1.46	1.50
24	c	606	CLA	CMB-C2B	-2.30	1.46	1.50
24	O	205	CLA	CHC-C4B	-2.30	1.34	1.39
24	R	203	CLA	C1B-C2B	2.30	1.48	1.43
34	g	319	IHT	C39-C35	2.30	1.55	1.50
24	b	306	CLA	CMC-C2C	-2.30	1.46	1.50
24	i	601	CLA	C3B-C4B	2.30	1.49	1.42
24	A	831	CLA	CMB-C2B	-2.30	1.46	1.50
35	f	611	KC2	C1A-CHA	2.30	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	842	PQN	O4-C4	-2.30	1.18	1.23
24	A	841	CLA	CMD-C2D	-2.30	1.46	1.50
24	k	608	CLA	CMB-C2B	-2.30	1.46	1.50
24	A	831	CLA	MG-ND	-2.30	2.01	2.05
24	i	604	CLA	CMD-C2D	-2.30	1.46	1.50
24	i	611	CLA	C3B-C4B	2.30	1.49	1.42
24	A	810	CLA	CMD-C2D	-2.30	1.46	1.50
33	k	616	II0	C16-C03	2.30	1.58	1.53
24	B	819	CLA	C4B-NB	2.30	1.40	1.37
24	A	826	CLA	C1B-C2B	2.30	1.48	1.43
24	f	608	CLA	CMC-C2C	-2.30	1.46	1.50
33	c	616	II0	C20-C14	2.30	1.54	1.50
24	A	830	CLA	CMC-C2C	-2.30	1.46	1.50
24	A	808	CLA	C1B-C2B	2.30	1.48	1.43
25	A	843	PQN	O4-C4	-2.29	1.18	1.23
24	I	102	CLA	CMC-C2C	-2.29	1.46	1.50
24	e	601	CLA	C1B-C2B	2.29	1.48	1.43
24	g	302	CLA	C1B-C2B	2.29	1.48	1.43
24	A	819	CLA	MG-NB	-2.29	2.01	2.05
24	F	201	CLA	C3B-C4B	2.29	1.49	1.42
24	B	803	CLA	CMB-C2B	-2.29	1.46	1.50
24	B	809	CLA	CMD-C2D	-2.29	1.46	1.50
33	O	202	II0	C16-C03	2.29	1.58	1.53
24	b	306	CLA	MG-NC	2.29	2.11	2.06
24	B	814	CLA	CMC-C2C	-2.29	1.46	1.50
24	a	308	CLA	CMD-C2D	-2.29	1.46	1.50
33	k	617	II0	C20-C14	2.29	1.54	1.50
24	B	806	CLA	CMD-C2D	-2.29	1.46	1.50
24	A	811	CLA	CMC-C2C	-2.29	1.46	1.50
24	b	309	CLA	CHC-C1C	2.29	1.43	1.38
24	A	828	CLA	CMD-C2D	-2.28	1.46	1.50
24	B	811	CLA	CMC-C2C	-2.28	1.46	1.50
24	I	102	CLA	C1B-C2B	2.28	1.48	1.43
24	A	820	CLA	MG-NB	-2.28	2.01	2.05
24	d	302	CLA	CHC-C1C	2.28	1.43	1.38
24	c	611	CLA	CMD-C2D	-2.28	1.46	1.50
24	e	611	CLA	CMB-C2B	-2.28	1.46	1.50
24	k	605	CLA	CMC-C2C	-2.28	1.46	1.50
24	B	823	CLA	CMC-C2C	-2.28	1.46	1.50
24	f	612	CLA	CMB-C2B	-2.28	1.46	1.50
24	B	829	CLA	MG-NC	2.28	2.11	2.06
24	B	805	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	304	CLA	CMD-C2D	-2.28	1.46	1.50
24	a	311	CLA	C1D-ND	2.28	1.40	1.37
24	A	836	CLA	MG-ND	-2.28	2.01	2.05
24	e	602	CLA	CMB-C2B	-2.28	1.46	1.50
24	c	607	CLA	CMD-C2D	-2.28	1.46	1.50
24	k	610	CLA	CMD-C2D	-2.28	1.46	1.50
24	j	313	CLA	C3B-C4B	2.28	1.49	1.42
24	B	801	CLA	C3B-C4B	2.28	1.49	1.42
24	f	605	CLA	CMB-C2B	-2.28	1.46	1.50
24	K	101	CLA	C1B-C2B	2.28	1.48	1.43
24	A	852	CLA	C1B-C2B	2.28	1.48	1.43
24	K	102	CLA	C4B-NB	2.28	1.40	1.37
24	B	826	CLA	CMB-C2B	-2.28	1.46	1.50
24	g	309	CLA	CMC-C2C	-2.28	1.46	1.50
24	c	601	CLA	C3B-C4B	2.27	1.49	1.42
34	b	317	IHT	C39-C35	2.27	1.55	1.50
27	B	848	WVN	C20-C13	2.27	1.52	1.45
24	g	302	CLA	C3B-C4B	2.27	1.49	1.42
27	A	849	WVN	C26-C22	-2.27	1.30	1.35
24	h	307	CLA	CHC-C1C	2.27	1.43	1.38
24	i	605	CLA	CMB-C2B	-2.27	1.46	1.50
27	A	847	WVN	C37-C34	-2.27	1.30	1.35
24	B	840	CLA	CMC-C2C	-2.27	1.46	1.50
24	e	601	CLA	CHC-C1C	2.27	1.43	1.38
24	O	205	CLA	C1B-C2B	2.27	1.48	1.43
24	B	835	CLA	C3B-C4B	2.27	1.49	1.42
24	c	605	CLA	CMB-C2B	-2.27	1.46	1.50
24	B	823	CLA	MG-ND	-2.27	2.01	2.05
33	d	315	II0	C18-C04	2.27	1.58	1.53
24	h	305	CLA	C3B-C4B	2.27	1.49	1.42
24	d	307	CLA	CMD-C2D	-2.27	1.46	1.50
24	B	820	CLA	C3B-C4B	2.27	1.49	1.42
24	a	308	CLA	CMC-C2C	-2.27	1.46	1.50
24	J	103	CLA	MG-NB	-2.27	2.01	2.05
24	B	827	CLA	C1D-ND	2.27	1.40	1.37
24	h	306	CLA	CMD-C2D	-2.27	1.46	1.50
24	B	840	CLA	CMD-C2D	-2.27	1.46	1.50
24	c	608	CLA	CMD-C2D	-2.27	1.46	1.50
24	R	203	CLA	CMC-C2C	-2.27	1.46	1.50
24	F	201	CLA	C1B-C2B	2.27	1.48	1.43
27	K	103	WVN	C36-C32	-2.27	1.30	1.35
24	a	302	CLA	CMD-C2D	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	k	621	II0	C16-C03	2.27	1.58	1.53
24	K	102	CLA	C1B-C2B	2.26	1.48	1.43
24	e	602	CLA	C1B-C2B	2.26	1.48	1.43
24	f	608	CLA	CMD-C2D	-2.26	1.46	1.50
32	J	106	LMG	O7-C8	-2.26	1.41	1.46
24	A	830	CLA	MG-NB	-2.26	2.01	2.05
24	B	801	CLA	CMC-C2C	-2.26	1.46	1.50
24	h	306	CLA	CMB-C2B	-2.26	1.46	1.50
24	k	606	CLA	C3B-C4B	2.26	1.49	1.42
24	f	607	CLA	C1B-C2B	2.26	1.48	1.43
24	g	310	CLA	CMC-C2C	-2.26	1.46	1.50
24	A	823	CLA	CMD-C2D	-2.26	1.46	1.50
24	F	202	CLA	CMC-C2C	-2.26	1.46	1.50
24	A	840	CLA	CMC-C2C	-2.26	1.46	1.50
24	A	842	CLA	CMD-C2D	-2.26	1.46	1.50
24	B	837	CLA	CMC-C2C	-2.26	1.46	1.50
24	f	601	CLA	CMD-C2D	-2.26	1.46	1.50
24	A	811	CLA	CMB-C2B	-2.26	1.46	1.50
24	B	833	CLA	CMD-C2D	-2.26	1.46	1.50
24	j	303	CLA	CMB-C2B	-2.26	1.46	1.50
24	B	815	CLA	CMD-C2D	-2.26	1.46	1.50
24	L	207	CLA	CMC-C2C	-2.26	1.46	1.50
24	c	608	CLA	C3B-C4B	2.26	1.49	1.42
24	B	808	CLA	C3B-C4B	2.26	1.49	1.42
24	B	831	CLA	C1B-NB	-2.26	1.34	1.37
24	j	304	CLA	CMD-C2D	-2.26	1.46	1.50
27	L	206	WVN	C20-C13	2.26	1.52	1.45
24	h	303	CLA	MG-NB	-2.26	2.01	2.05
24	A	837	CLA	CMB-C2B	-2.26	1.46	1.50
24	j	311	CLA	C3B-C4B	2.26	1.49	1.42
24	A	802	CLA	CMC-C2C	-2.26	1.46	1.50
24	B	807	CLA	CMB-C2B	-2.26	1.46	1.50
33	d	314	II0	C18-C04	2.26	1.58	1.53
24	B	816	CLA	CMC-C2C	-2.26	1.46	1.50
24	B	829	CLA	CMD-C2D	-2.26	1.46	1.50
24	f	607	CLA	CMD-C2D	-2.25	1.46	1.50
24	A	842	CLA	C1B-C2B	2.25	1.48	1.43
35	k	612	KC2	CBD-CAD	-2.25	1.46	1.56
24	j	311	CLA	CMD-C2D	-2.25	1.46	1.50
24	B	825	CLA	MG-ND	-2.25	2.01	2.05
24	a	308	CLA	CMB-C2B	-2.25	1.46	1.50
24	R	203	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	834	CLA	CMB-C2B	-2.25	1.46	1.50
24	B	839	CLA	CMD-C2D	-2.25	1.46	1.50
33	a	315	II0	C18-C04	2.25	1.58	1.53
24	A	831	CLA	C4B-NB	2.25	1.40	1.37
33	j	318	II0	C28-C26	2.25	1.52	1.50
24	A	820	CLA	CMC-C2C	-2.25	1.46	1.50
24	c	602	CLA	C1B-C2B	2.25	1.48	1.43
24	B	827	CLA	CMC-C2C	-2.25	1.46	1.50
24	c	609	CLA	CMD-C2D	-2.25	1.46	1.50
33	b	315	II0	C18-C04	2.25	1.58	1.53
24	B	818	CLA	CMC-C2C	-2.25	1.46	1.50
24	e	601	CLA	CMB-C2B	-2.25	1.46	1.50
24	a	310	CLA	C3B-C4B	2.25	1.49	1.42
24	O	201	CLA	CMC-C2C	-2.25	1.46	1.50
24	A	841	CLA	C1B-C2B	2.25	1.48	1.43
24	b	307	CLA	C1B-C2B	2.25	1.48	1.43
35	i	609	KC2	C4A-C3A	2.25	1.49	1.44
24	b	311	CLA	C3B-C4B	2.25	1.49	1.42
27	F	204	WVN	C28-C25	-2.25	1.30	1.35
24	B	810	CLA	CMD-C2D	-2.25	1.46	1.50
24	h	301	CLA	CMB-C2B	-2.25	1.46	1.50
24	A	821	CLA	CMB-C2B	-2.25	1.46	1.50
33	e	613	II0	C16-C03	2.25	1.58	1.53
24	O	201	CLA	C1B-C2B	2.25	1.48	1.43
24	B	825	CLA	CMD-C2D	-2.24	1.46	1.50
24	a	303	CLA	CMD-C2D	-2.24	1.46	1.50
24	A	817	CLA	C3B-C4B	2.24	1.49	1.42
24	A	835	CLA	C3B-C4B	2.24	1.49	1.42
24	B	823	CLA	CMB-C2B	-2.24	1.46	1.50
24	f	602	CLA	CMB-C2B	-2.24	1.46	1.50
24	B	828	CLA	CMC-C2C	-2.24	1.46	1.50
24	B	805	CLA	MG-NB	-2.24	2.01	2.05
24	B	827	CLA	CMD-C2D	-2.24	1.46	1.50
24	A	803	CLA	MG-NB	-2.24	2.01	2.05
24	A	835	CLA	C1B-C2B	2.24	1.48	1.43
24	A	832	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	832	CLA	CMB-C2B	-2.24	1.46	1.50
24	d	312	CLA	C3B-C4B	2.24	1.49	1.42
24	A	817	CLA	MG-ND	-2.24	2.01	2.05
24	B	815	CLA	C3B-C4B	2.24	1.49	1.42
24	A	837	CLA	CMC-C2C	-2.24	1.46	1.50
27	e	615	WVN	C02-C11	2.24	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	311	CLA	MG-NB	-2.24	2.01	2.05
27	K	103	WVN	C26-C22	-2.24	1.30	1.35
24	A	819	CLA	CAC-C3C	-2.24	1.45	1.51
24	B	804	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	812	CLA	CMD-C2D	-2.23	1.46	1.50
24	A	808	CLA	MG-NB	-2.23	2.01	2.05
24	O	205	CLA	MG-NC	2.23	2.11	2.06
24	A	832	CLA	CMB-C2B	-2.23	1.46	1.50
24	b	304	CLA	CMB-C2B	-2.23	1.46	1.50
24	f	612	CLA	C3B-C4B	2.23	1.49	1.42
24	B	841	CLA	MG-ND	-2.23	2.01	2.05
24	a	310	CLA	CMD-C2D	-2.23	1.46	1.50
24	A	841	CLA	MG-NB	-2.23	2.01	2.05
24	h	304	CLA	C1B-C2B	2.23	1.48	1.43
24	g	306	CLA	CMD-C2D	-2.23	1.46	1.50
24	j	305	CLA	C3B-C4B	2.23	1.49	1.42
24	e	604	CLA	CMC-C2C	-2.23	1.46	1.50
33	i	613	II0	C15-C03	2.23	1.58	1.53
24	j	302	CLA	C1B-C2B	2.23	1.48	1.43
24	A	839	CLA	CMC-C2C	-2.23	1.46	1.50
24	O	201	CLA	CHC-C1C	2.23	1.42	1.38
24	b	306	CLA	CMD-C2D	-2.23	1.46	1.50
24	c	608	CLA	CHC-C1C	2.23	1.42	1.38
24	e	610	CLA	CMD-C2D	-2.23	1.46	1.50
35	g	314	KC2	C4A-C3A	2.23	1.49	1.44
24	i	610	CLA	CMC-C2C	-2.23	1.46	1.50
24	f	604	CLA	CMD-C2D	-2.23	1.46	1.50
24	B	809	CLA	MG-ND	-2.23	2.01	2.05
33	d	315	II0	C16-C03	2.22	1.58	1.53
24	B	824	CLA	CMB-C2B	-2.22	1.46	1.50
24	h	305	CLA	CMC-C2C	-2.22	1.46	1.50
35	g	314	KC2	CBD-CAD	-2.22	1.46	1.56
24	f	613	CLA	CHC-C1C	2.22	1.42	1.38
24	A	818	CLA	C1B-NB	-2.22	1.34	1.37
24	B	804	CLA	MG-ND	-2.22	2.01	2.05
24	c	606	CLA	CMD-C2D	-2.22	1.46	1.50
24	B	828	CLA	CMD-C2D	-2.22	1.46	1.50
24	B	812	CLA	C1B-C2B	2.22	1.48	1.43
24	B	820	CLA	CMC-C2C	-2.22	1.46	1.50
24	B	833	CLA	MG-NB	-2.22	2.01	2.05
24	A	853	CLA	CMB-C2B	-2.22	1.46	1.50
24	B	837	CLA	C1B-NB	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	f	604	CLA	CMC-C2C	-2.22	1.46	1.50
24	B	823	CLA	C1B-NB	-2.22	1.34	1.37
24	g	305	CLA	C1B-C2B	2.22	1.48	1.43
24	A	842	CLA	CMC-C2C	-2.22	1.46	1.50
24	i	603	CLA	C3B-C4B	2.22	1.49	1.42
24	i	601	CLA	CMB-C2B	-2.22	1.46	1.50
24	f	604	CLA	C3B-C4B	2.22	1.49	1.42
24	B	832	CLA	C4B-NB	2.22	1.40	1.37
33	e	616	II0	C18-C04	2.22	1.57	1.53
24	f	607	CLA	CMB-C2B	-2.22	1.46	1.50
24	f	612	CLA	CMD-C2D	-2.22	1.46	1.50
24	B	822	CLA	C1B-C2B	2.22	1.48	1.43
24	A	853	CLA	CMC-C2C	-2.22	1.46	1.50
24	a	305	CLA	CMC-C2C	-2.22	1.46	1.50
35	i	616	KC2	C1D-C2D	2.22	1.48	1.43
24	a	308	CLA	C1B-C2B	2.21	1.48	1.43
24	h	303	CLA	C1B-NB	-2.21	1.35	1.37
35	f	611	KC2	C4B-NB	-2.21	1.35	1.37
35	k	613	KC2	CBD-CAD	-2.21	1.46	1.56
24	j	302	CLA	CMD-C2D	-2.21	1.46	1.50
24	e	607	CLA	C3B-C4B	2.21	1.49	1.42
24	c	602	CLA	CMC-C2C	-2.21	1.46	1.50
24	B	835	CLA	CMC-C2C	-2.21	1.46	1.50
24	f	613	CLA	CMC-C2C	-2.21	1.46	1.50
24	j	306	CLA	MG-ND	-2.21	2.01	2.05
24	a	304	CLA	CMD-C2D	-2.21	1.46	1.50
24	e	601	CLA	CMD-C2D	-2.21	1.46	1.50
24	A	839	CLA	C1B-NB	-2.21	1.35	1.37
27	J	102	WVN	C28-C25	-2.21	1.30	1.35
24	j	310	CLA	CMD-C2D	-2.21	1.46	1.50
24	j	314	CLA	CMD-C2D	-2.21	1.46	1.50
24	A	842	CLA	CMB-C2B	-2.21	1.46	1.50
24	B	819	CLA	CMC-C2C	-2.21	1.46	1.50
24	c	604	CLA	CMB-C2B	-2.21	1.46	1.50
24	B	813	CLA	CMC-C2C	-2.21	1.46	1.50
24	b	305	CLA	C3B-C4B	2.21	1.49	1.42
24	d	308	CLA	C3B-C4B	2.21	1.49	1.42
27	B	845	WVN	C28-C25	-2.21	1.30	1.35
24	A	852	CLA	MG-NB	-2.21	2.01	2.05
24	j	309	CLA	CMB-C2B	-2.21	1.46	1.50
33	a	315	II0	C16-C03	2.21	1.57	1.53
24	A	837	CLA	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	817	CLA	C1B-C2B	2.21	1.48	1.43
24	f	609	CLA	CMB-C2B	-2.21	1.46	1.50
24	f	601	CLA	C3B-C4B	2.21	1.49	1.42
24	e	602	CLA	MG-NB	-2.21	2.01	2.05
33	d	314	II0	C15-C03	2.21	1.57	1.53
24	B	816	CLA	CMD-C2D	-2.20	1.46	1.50
24	B	824	CLA	CMD-C2D	-2.20	1.46	1.50
24	B	834	CLA	C3B-C4B	2.20	1.49	1.42
24	B	838	CLA	CMC-C2C	-2.20	1.46	1.50
24	f	602	CLA	CMC-C2C	-2.20	1.46	1.50
24	A	804	CLA	CMB-C2B	-2.20	1.46	1.50
33	k	616	II0	C18-C04	2.20	1.57	1.53
35	f	611	KC2	C3C-C4C	2.20	1.49	1.44
24	L	204	CLA	MG-NB	-2.20	2.01	2.05
24	a	305	CLA	CHC-C1C	2.20	1.42	1.38
24	A	838	CLA	CMC-C2C	-2.20	1.46	1.50
24	B	806	CLA	CMB-C2B	-2.20	1.46	1.50
24	c	603	CLA	MG-NB	-2.20	2.01	2.05
24	O	205	CLA	CMC-C2C	-2.20	1.46	1.50
24	c	603	CLA	CMD-C2D	-2.20	1.46	1.50
24	A	835	CLA	CMD-C2D	-2.20	1.46	1.50
24	h	305	CLA	CMD-C2D	-2.20	1.46	1.50
24	k	604	CLA	C3B-C4B	2.20	1.49	1.42
24	i	603	CLA	MG-NB	-2.20	2.01	2.05
24	g	305	CLA	CMB-C2B	-2.20	1.46	1.50
24	O	205	CLA	MG-NA	2.20	2.11	2.06
24	A	829	CLA	C3B-C4B	2.20	1.49	1.42
27	A	846	WVN	C02-C11	2.20	1.53	1.50
24	i	608	CLA	CMD-C2D	-2.20	1.46	1.50
24	a	309	CLA	C3B-C4B	2.20	1.49	1.42
24	B	806	CLA	C4B-NB	2.20	1.40	1.37
24	e	610	CLA	C3B-C4B	2.20	1.49	1.42
24	d	301	CLA	CMD-C2D	-2.20	1.46	1.50
24	B	807	CLA	CHC-C4B	-2.20	1.34	1.39
24	A	816	CLA	CMC-C2C	-2.20	1.46	1.50
33	b	318	II0	C15-C03	2.20	1.57	1.53
24	B	817	CLA	CMC-C2C	-2.19	1.46	1.50
25	A	843	PQN	O1-C1	-2.19	1.18	1.23
24	A	821	CLA	C3B-C4B	2.19	1.49	1.42
24	B	834	CLA	MG-NB	-2.19	2.01	2.05
33	a	317	II0	C16-C03	2.19	1.57	1.53
27	A	847	WVN	C20-C13	2.19	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	612	CLA	C3B-C4B	2.19	1.49	1.42
24	A	803	CLA	CMD-C2D	-2.19	1.46	1.50
33	a	314	II0	C15-C03	2.19	1.57	1.53
24	B	835	CLA	MG-NB	-2.19	2.01	2.05
24	A	826	CLA	C3B-C4B	2.19	1.49	1.42
24	g	304	CLA	C3B-C4B	2.19	1.49	1.42
24	A	825	CLA	MG-NB	-2.19	2.01	2.05
24	K	101	CLA	MG-NB	-2.19	2.01	2.05
24	a	306	CLA	CMD-C2D	-2.19	1.46	1.50
24	a	309	CLA	CMB-C2B	-2.19	1.46	1.50
24	h	302	CLA	C1B-C2B	2.19	1.48	1.43
24	A	808	CLA	C4B-NB	2.19	1.40	1.37
24	k	607	CLA	CMB-C2B	-2.19	1.46	1.50
24	j	311	CLA	CMB-C2B	-2.19	1.46	1.50
24	B	804	CLA	C1B-C2B	2.19	1.48	1.43
35	c	610	KC2	C4B-NB	-2.19	1.35	1.37
24	B	807	CLA	CMD-C2D	-2.19	1.46	1.50
28	a	318	LMT	O2'-C2'	-2.19	1.37	1.43
24	g	311	CLA	C3B-C4B	2.19	1.49	1.42
24	f	612	CLA	C1B-C2B	2.19	1.48	1.43
24	B	825	CLA	C1B-NB	-2.19	1.35	1.37
24	g	305	CLA	CMD-C2D	-2.19	1.46	1.50
33	f	616	II0	C18-C04	2.19	1.57	1.53
24	A	839	CLA	MG-NB	-2.19	2.01	2.05
24	A	840	CLA	CMB-C2B	-2.19	1.46	1.50
24	L	203	CLA	CMC-C2C	-2.19	1.46	1.50
24	A	811	CLA	C1B-C2B	2.18	1.48	1.43
24	B	805	CLA	CMB-C2B	-2.18	1.46	1.50
24	I	102	CLA	C3B-C4B	2.18	1.49	1.42
24	A	830	CLA	C3B-C4B	2.18	1.49	1.42
24	d	307	CLA	C3B-C4B	2.18	1.49	1.42
24	B	819	CLA	CHC-C1C	2.18	1.42	1.38
24	g	311	CLA	CMC-C2C	-2.18	1.46	1.50
33	f	615	II0	C15-C03	2.18	1.57	1.53
35	c	610	KC2	C1D-C2D	2.18	1.48	1.43
24	A	826	CLA	CMB-C2B	-2.18	1.46	1.50
24	b	309	CLA	C1B-C2B	2.18	1.48	1.43
24	A	807	CLA	CMD-C2D	-2.18	1.46	1.50
33	d	315	II0	C20-C14	2.18	1.54	1.50
24	B	821	CLA	CMB-C2B	-2.18	1.46	1.50
35	k	611	KC2	C1A-CHA	2.18	1.45	1.40
24	c	607	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	202	CLA	MG-NB	-2.18	2.01	2.05
24	B	833	CLA	CMC-C2C	-2.18	1.46	1.50
24	i	610	CLA	CMD-C2D	-2.18	1.46	1.50
24	g	304	CLA	MG-NB	-2.18	2.01	2.05
33	g	316	II0	C20-C14	2.18	1.54	1.50
24	J	103	CLA	C3B-C4B	2.18	1.49	1.42
33	f	616	II0	C16-C03	2.18	1.57	1.53
35	d	311	KC2	C4A-C3A	2.18	1.48	1.44
24	A	802	CLA	CMB-C2B	-2.18	1.46	1.50
24	B	830	CLA	CMB-C2B	-2.18	1.46	1.50
24	d	302	CLA	CMD-C2D	-2.18	1.46	1.50
24	c	604	CLA	C3B-C4B	2.18	1.49	1.42
24	F	202	CLA	CMB-C2B	-2.18	1.46	1.50
24	e	610	CLA	CMB-C2B	-2.18	1.46	1.50
24	f	603	CLA	CMC-C2C	-2.18	1.46	1.50
24	B	812	CLA	CMB-C2B	-2.18	1.46	1.50
24	c	602	CLA	CMB-C2B	-2.18	1.46	1.50
24	g	303	CLA	CMB-C2B	-2.18	1.46	1.50
24	a	302	CLA	MG-ND	-2.18	2.01	2.05
24	F	202	CLA	CMD-C2D	-2.17	1.46	1.50
24	A	834	CLA	CMC-C2C	-2.17	1.46	1.50
24	e	608	CLA	CMD-C2D	-2.17	1.46	1.50
24	g	311	CLA	CMD-C2D	-2.17	1.46	1.50
24	g	308	CLA	C1B-C2B	2.17	1.48	1.43
24	A	834	CLA	C3B-C4B	2.17	1.49	1.42
24	L	207	CLA	C3B-C4B	2.17	1.49	1.42
24	A	833	CLA	CMC-C2C	-2.17	1.46	1.50
24	b	311	CLA	CMC-C2C	-2.17	1.46	1.50
24	A	821	CLA	C1B-C2B	2.17	1.48	1.43
24	A	829	CLA	CMC-C2C	-2.17	1.46	1.50
28	b	319	LMT	O2'-C2'	-2.17	1.37	1.43
24	B	814	CLA	C3B-C4B	2.17	1.49	1.42
33	j	316	II0	C20-C14	2.17	1.54	1.50
24	j	306	CLA	CMD-C2D	-2.17	1.46	1.50
24	A	832	CLA	MG-NB	-2.17	2.01	2.05
24	f	608	CLA	CHC-C1C	2.17	1.42	1.38
24	h	303	CLA	CMB-C2B	-2.17	1.46	1.50
24	B	804	CLA	CMB-C2B	-2.17	1.46	1.50
24	a	302	CLA	CMB-C2B	-2.17	1.46	1.50
24	f	610	CLA	CMB-C2B	-2.17	1.46	1.50
24	B	836	CLA	CMC-C2C	-2.17	1.46	1.50
24	k	602	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	306	CLA	MG-NB	-2.17	2.01	2.05
24	K	102	CLA	CMC-C2C	-2.17	1.46	1.50
24	e	602	CLA	CMC-C2C	-2.17	1.46	1.50
27	L	201	WVN	C28-C25	-2.17	1.30	1.35
24	B	841	CLA	CMC-C2C	-2.17	1.46	1.50
33	e	613	II0	C15-C03	2.17	1.57	1.53
33	j	318	II0	C15-C03	2.17	1.57	1.53
24	A	830	CLA	CHC-C1C	2.16	1.42	1.38
24	F	201	CLA	CMC-C2C	-2.16	1.46	1.50
24	B	827	CLA	MG-NB	-2.16	2.01	2.05
35	i	616	KC2	CBD-CAD	-2.16	1.46	1.56
24	F	201	CLA	CMB-C2B	-2.16	1.46	1.50
24	c	607	CLA	CMB-C2B	-2.16	1.46	1.50
24	h	302	CLA	CMC-C2C	-2.16	1.46	1.50
33	j	318	II0	C30-C26	-2.16	1.32	1.37
24	A	805	CLA	MG-ND	-2.16	2.01	2.05
24	k	608	CLA	C3B-C4B	2.16	1.49	1.42
24	g	304	CLA	CMC-C2C	-2.16	1.46	1.50
24	A	842	CLA	C4B-NB	2.16	1.40	1.37
24	d	309	CLA	CMC-C2C	-2.16	1.46	1.50
24	e	605	CLA	CMD-C2D	-2.16	1.46	1.50
24	A	815	CLA	MG-ND	-2.16	2.01	2.05
24	B	801	CLA	MG-ND	-2.16	2.01	2.05
24	A	807	CLA	CMC-C2C	-2.16	1.46	1.50
35	g	313	KC2	C1D-C2D	2.16	1.48	1.43
24	O	201	CLA	MG-ND	-2.16	2.01	2.05
33	i	612	II0	C18-C04	2.16	1.57	1.53
24	j	307	CLA	CAA-C2A	-2.16	1.50	1.54
24	i	605	CLA	MG-NB	-2.16	2.01	2.05
24	b	309	CLA	CMC-C2C	-2.16	1.46	1.50
24	f	605	CLA	CMC-C2C	-2.16	1.46	1.50
24	J	103	CLA	MG-ND	-2.16	2.01	2.05
24	B	801	CLA	CMB-C2B	-2.16	1.46	1.50
24	I	102	CLA	CMD-C2D	-2.16	1.46	1.50
24	k	606	CLA	CHC-C1C	2.16	1.42	1.38
24	j	309	CLA	C1B-C2B	2.16	1.48	1.43
24	d	301	CLA	MG-NA	2.16	2.11	2.06
35	g	314	KC2	C1A-CHA	2.16	1.45	1.40
24	a	312	CLA	C3B-C4B	2.16	1.49	1.42
24	B	823	CLA	C1B-C2B	2.16	1.48	1.43
24	A	801	CLA	CMD-C2D	-2.15	1.46	1.50
24	e	605	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	306	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	836	CLA	C3B-C4B	2.15	1.49	1.42
24	i	602	CLA	C3B-C4B	2.15	1.49	1.42
24	B	840	CLA	MG-NB	-2.15	2.01	2.05
24	b	303	CLA	MG-NB	-2.15	2.01	2.05
24	k	606	CLA	CMC-C2C	-2.15	1.46	1.50
24	d	309	CLA	CMB-C2B	-2.15	1.46	1.50
24	d	304	CLA	C3B-C4B	2.15	1.49	1.42
24	A	808	CLA	CMC-C2C	-2.15	1.46	1.50
24	a	307	CLA	CMC-C2C	-2.15	1.46	1.50
24	k	605	CLA	CMD-C2D	-2.15	1.46	1.50
24	g	310	CLA	CMB-C2B	-2.15	1.46	1.50
24	b	313	CLA	CMD-C2D	-2.15	1.46	1.50
33	b	314	II0	C18-C04	2.15	1.57	1.53
27	A	850	WVN	C37-C34	-2.15	1.30	1.35
24	L	203	CLA	CMD-C2D	-2.15	1.46	1.50
24	f	610	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	816	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	839	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	832	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	839	CLA	C1B-C2B	2.15	1.48	1.43
24	A	840	CLA	C3B-C4B	2.15	1.49	1.42
24	f	605	CLA	CMD-C2D	-2.15	1.46	1.50
24	i	611	CLA	CMD-C2D	-2.15	1.46	1.50
33	g	317	II0	C30-C26	-2.15	1.32	1.37
33	j	316	II0	C16-C03	2.15	1.57	1.53
25	B	842	PQN	O1-C1	-2.15	1.18	1.23
24	B	819	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	805	CLA	MG-ND	-2.15	2.01	2.05
28	A	851	LMT	O1'-C1'	-2.15	1.36	1.40
24	i	603	CLA	CMD-C2D	-2.15	1.46	1.50
24	g	307	CLA	C1B-C2B	2.14	1.48	1.43
24	A	827	CLA	C3B-C4B	2.14	1.49	1.42
34	b	317	IHT	C13-C02	2.14	1.57	1.53
24	A	828	CLA	CHC-C1C	2.14	1.42	1.38
24	A	833	CLA	C4B-NB	2.14	1.40	1.37
24	A	822	CLA	MG-ND	-2.14	2.01	2.05
24	a	302	CLA	MG-NB	-2.14	2.01	2.05
24	g	308	CLA	CMC-C2C	-2.14	1.46	1.50
34	O	203	IHT	C13-C02	2.14	1.57	1.53
24	f	605	CLA	MG-NB	-2.14	2.01	2.05
24	B	824	CLA	C4B-NB	2.14	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	825	CLA	CHC-C1C	2.14	1.42	1.38
24	b	313	CLA	MG-NC	2.14	2.11	2.06
34	g	319	IHT	C20-C15	2.14	1.54	1.50
24	A	838	CLA	CMB-C2B	-2.14	1.46	1.50
24	c	603	CLA	CHC-C1C	2.14	1.42	1.38
24	A	831	CLA	CMC-C2C	-2.14	1.46	1.50
24	j	307	CLA	CMC-C2C	-2.14	1.46	1.50
24	j	305	CLA	C1B-NB	-2.14	1.35	1.37
24	A	812	CLA	CMB-C2B	-2.14	1.46	1.50
24	c	607	CLA	CMC-C2C	-2.14	1.46	1.50
24	k	614	CLA	CMD-C2D	-2.14	1.46	1.50
27	A	846	WVN	C28-C25	-2.14	1.30	1.35
24	A	836	CLA	CMB-C2B	-2.14	1.46	1.50
24	k	608	CLA	CMD-C2D	-2.14	1.46	1.50
24	d	312	CLA	CMB-C2B	-2.14	1.46	1.50
24	B	840	CLA	C3B-C4B	2.14	1.49	1.42
24	g	302	CLA	CMD-C2D	-2.14	1.46	1.50
24	g	310	CLA	MG-NB	-2.14	2.01	2.05
24	h	312	CLA	CMC-C2C	-2.13	1.46	1.50
24	j	314	CLA	C3B-C4B	2.13	1.49	1.42
24	A	834	CLA	MG-ND	-2.13	2.01	2.05
24	A	823	CLA	CMC-C2C	-2.13	1.46	1.50
24	L	202	CLA	CMC-C2C	-2.13	1.46	1.50
24	c	604	CLA	CHC-C1C	2.13	1.42	1.38
24	f	601	CLA	CMB-C2B	-2.13	1.46	1.50
24	B	821	CLA	CHC-C1C	2.13	1.42	1.38
24	f	608	CLA	C3B-C4B	2.13	1.49	1.42
24	B	841	CLA	MG-NB	-2.13	2.01	2.05
24	g	307	CLA	C3B-C4B	2.13	1.49	1.42
24	h	305	CLA	C1B-C2B	2.13	1.48	1.43
24	B	813	CLA	CMB-C2B	-2.13	1.46	1.50
24	A	835	CLA	CMC-C2C	-2.13	1.46	1.50
27	F	204	WVN	C02-C11	2.13	1.53	1.50
24	g	306	CLA	CMC-C2C	-2.13	1.46	1.50
24	B	838	CLA	C1B-C2B	2.13	1.48	1.43
24	a	312	CLA	CMB-C2B	-2.13	1.46	1.50
24	i	608	CLA	CMB-C2B	-2.13	1.46	1.50
24	g	304	CLA	MG-ND	-2.13	2.01	2.05
33	a	313	II0	C15-C03	2.13	1.57	1.53
24	a	303	CLA	CMC-C2C	-2.13	1.46	1.50
24	k	606	CLA	CMB-C2B	-2.13	1.46	1.50
24	B	822	CLA	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	815	CLA	CMC-C2C	-2.13	1.46	1.50
24	a	302	CLA	CMC-C2C	-2.13	1.46	1.50
33	b	314	II0	C15-C03	2.13	1.57	1.53
33	g	317	II0	C16-C03	2.13	1.57	1.53
24	A	817	CLA	CHC-C1C	2.13	1.42	1.38
24	B	832	CLA	C1B-C2B	2.13	1.48	1.43
24	g	304	CLA	C1B-C2B	2.13	1.48	1.43
24	A	824	CLA	MG-ND	-2.13	2.01	2.05
24	K	102	CLA	CMB-C2B	-2.13	1.46	1.50
24	b	312	CLA	CMC-C2C	-2.13	1.46	1.50
24	A	826	CLA	MG-NB	-2.13	2.01	2.05
24	j	310	CLA	CMB-C2B	-2.13	1.46	1.50
24	A	840	CLA	CHC-C1C	2.13	1.42	1.38
24	e	606	CLA	CMC-C2C	-2.13	1.46	1.50
24	b	310	CLA	CHC-C1C	2.13	1.42	1.38
24	A	805	CLA	MG-NB	-2.13	2.01	2.05
24	A	818	CLA	CMD-C2D	-2.12	1.46	1.50
33	g	317	II0	C18-C04	2.12	1.57	1.53
24	A	813	CLA	CMC-C2C	-2.12	1.46	1.50
24	B	826	CLA	MG-ND	-2.12	2.01	2.05
35	g	314	KC2	C1D-C2D	2.12	1.48	1.43
24	B	811	CLA	CHC-C1C	2.12	1.42	1.38
24	c	603	CLA	CMC-C2C	-2.12	1.46	1.50
24	A	814	CLA	CMD-C2D	-2.12	1.46	1.50
24	c	601	CLA	CMC-C2C	-2.12	1.46	1.50
24	k	603	CLA	CMD-C2D	-2.12	1.46	1.50
24	R	203	CLA	CMD-C2D	-2.12	1.46	1.50
33	i	612	II0	C15-C03	2.12	1.57	1.53
24	L	203	CLA	MG-NB	-2.12	2.01	2.05
24	B	839	CLA	CMC-C2C	-2.12	1.46	1.50
24	h	307	CLA	CMC-C2C	-2.12	1.46	1.50
24	B	825	CLA	C3B-C4B	2.12	1.48	1.42
24	k	610	CLA	CMB-C2B	-2.12	1.46	1.50
24	d	308	CLA	CMC-C2C	-2.12	1.46	1.50
24	A	806	CLA	CMC-C2C	-2.12	1.46	1.50
24	A	809	CLA	CMD-C2D	-2.12	1.46	1.50
24	a	309	CLA	CMC-C2C	-2.12	1.46	1.50
24	b	312	CLA	CMD-C2D	-2.12	1.46	1.50
24	f	603	CLA	CMB-C2B	-2.12	1.46	1.50
24	e	606	CLA	C3B-C4B	2.12	1.48	1.42
33	h	311	II0	C30-C26	-2.12	1.32	1.37
24	I	102	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	j	307	CLA	CMD-C2D	-2.12	1.46	1.50
24	j	303	CLA	C3B-C4B	2.12	1.48	1.42
24	j	310	CLA	CHC-C1C	2.12	1.42	1.38
24	e	608	CLA	CMB-C2B	-2.12	1.46	1.50
24	A	805	CLA	C1B-C2B	2.12	1.48	1.43
24	A	819	CLA	C1B-C2B	2.12	1.48	1.43
24	g	309	CLA	C3B-C4B	2.12	1.48	1.42
24	B	806	CLA	MG-ND	-2.12	2.01	2.05
24	J	103	CLA	CHC-C1C	2.12	1.42	1.38
24	L	203	CLA	C1B-C2B	2.12	1.48	1.43
24	g	307	CLA	CMC-C2C	-2.12	1.46	1.50
24	B	825	CLA	C1B-C2B	2.12	1.48	1.43
33	c	614	II0	C20-C14	2.12	1.54	1.50
33	g	320	II0	C18-C04	2.12	1.57	1.53
24	F	202	CLA	C1B-C2B	2.12	1.48	1.43
24	A	852	CLA	MG-ND	-2.12	2.01	2.05
24	B	820	CLA	C1B-C2B	2.11	1.48	1.43
24	e	601	CLA	MG-NB	-2.11	2.01	2.05
24	A	825	CLA	CMC-C2C	-2.11	1.46	1.50
33	O	202	II0	C15-C03	2.11	1.57	1.53
24	h	307	CLA	CMD-C2D	-2.11	1.46	1.50
24	f	612	CLA	CMC-C2C	-2.11	1.46	1.50
24	B	810	CLA	C3B-C2B	-2.11	1.36	1.44
24	g	305	CLA	CHC-C4B	-2.11	1.34	1.39
24	b	304	CLA	C3B-C4B	2.11	1.48	1.42
24	B	825	CLA	CMB-C2B	-2.11	1.46	1.50
24	e	611	CLA	C3B-C4B	2.11	1.48	1.42
35	g	312	KC2	CBD-CAD	-2.11	1.47	1.56
24	B	804	CLA	C3B-C4B	2.11	1.48	1.42
35	d	311	KC2	C4B-NB	-2.11	1.35	1.37
24	b	304	CLA	CHC-C1C	2.11	1.42	1.38
24	g	315	CLA	MG-ND	-2.11	2.01	2.05
24	b	313	CLA	CMB-C2B	-2.11	1.46	1.50
24	f	607	CLA	C3B-C4B	2.11	1.48	1.42
24	A	801	CLA	CMB-C2B	-2.11	1.46	1.50
27	B	848	WVN	C02-C11	2.11	1.53	1.50
33	a	314	II0	C18-C04	2.11	1.57	1.53
24	A	856	CLA	CMC-C2C	-2.11	1.46	1.50
24	c	603	CLA	CMB-C2B	-2.11	1.46	1.50
24	A	812	CLA	C3B-C4B	2.11	1.48	1.42
33	i	614	II0	C20-C14	2.11	1.54	1.50
24	k	601	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	609	CLA	CMD-C2D	-2.11	1.46	1.50
24	A	807	CLA	C3B-C4B	2.11	1.48	1.42
24	j	310	CLA	C1B-C2B	2.11	1.48	1.43
24	B	817	CLA	CMD-C2D	-2.11	1.46	1.50
24	a	304	CLA	CMB-C2B	-2.11	1.46	1.50
24	B	834	CLA	CMC-C2C	-2.11	1.46	1.50
24	A	804	CLA	MG-NB	-2.11	2.01	2.05
24	k	602	CLA	CHC-C1C	2.11	1.42	1.38
24	B	828	CLA	C3B-C4B	2.11	1.48	1.42
24	B	813	CLA	C3B-C4B	2.11	1.48	1.42
24	B	832	CLA	MG-ND	-2.11	2.01	2.05
34	k	618	IHT	C20-C15	2.11	1.54	1.50
24	A	821	CLA	CMC-C2C	-2.11	1.46	1.50
24	d	308	CLA	CMD-C2D	-2.11	1.46	1.50
24	A	820	CLA	MG-ND	-2.11	2.01	2.05
24	a	312	CLA	MG-NC	2.10	2.11	2.06
24	d	301	CLA	C3B-C4B	2.10	1.48	1.42
35	k	611	KC2	C4A-C3A	2.10	1.48	1.44
24	A	805	CLA	C4B-NB	2.10	1.40	1.37
24	B	831	CLA	CMC-C2C	-2.10	1.46	1.50
24	b	309	CLA	CMD-C2D	-2.10	1.46	1.50
24	g	308	CLA	CMB-C2B	-2.10	1.46	1.50
24	B	833	CLA	CMB-C2B	-2.10	1.46	1.50
33	d	313	II0	C15-C03	2.10	1.57	1.53
24	A	829	CLA	C1B-C2B	2.10	1.48	1.43
24	h	305	CLA	CMB-C2B	-2.10	1.46	1.50
33	h	311	II0	C16-C03	2.10	1.57	1.53
24	a	305	CLA	C1B-C2B	2.10	1.48	1.43
24	B	811	CLA	C1B-NB	-2.10	1.35	1.37
24	k	601	CLA	MG-NB	-2.10	2.01	2.05
24	B	833	CLA	CHC-C1C	2.10	1.42	1.38
24	K	101	CLA	CMD-C2D	-2.10	1.46	1.50
27	B	846	WVN	C36-C32	-2.10	1.30	1.35
33	i	613	II0	C18-C04	2.10	1.57	1.53
24	B	828	CLA	CMB-C2B	-2.10	1.46	1.50
24	h	307	CLA	MG-NB	-2.10	2.01	2.05
24	h	301	CLA	C3B-C4B	2.10	1.48	1.42
24	c	601	CLA	CHC-C1C	2.09	1.42	1.38
24	A	808	CLA	MG-ND	-2.09	2.01	2.05
24	g	302	CLA	MG-ND	-2.09	2.01	2.05
24	e	604	CLA	C3B-C4B	2.09	1.48	1.42
24	A	837	CLA	C4B-NB	2.09	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	e	605	CLA	C3B-C4B	2.09	1.48	1.42
24	g	304	CLA	CHC-C1C	2.09	1.42	1.38
24	A	816	CLA	CMB-C2B	-2.09	1.46	1.50
24	B	838	CLA	MG-ND	-2.09	2.01	2.05
24	B	826	CLA	C3B-C4B	2.09	1.48	1.42
24	B	829	CLA	CMC-C2C	-2.09	1.46	1.50
24	a	305	CLA	CMB-C2B	-2.09	1.46	1.50
24	A	853	CLA	CHC-C1C	2.09	1.42	1.38
33	b	314	II0	C29-C25	2.09	1.41	1.37
24	B	837	CLA	C3B-C4B	2.09	1.48	1.42
24	A	842	CLA	C1B-NB	-2.09	1.35	1.37
24	O	201	CLA	CMB-C2B	-2.09	1.46	1.50
33	d	313	II0	C16-C03	2.09	1.57	1.53
24	c	609	CLA	MG-NB	-2.09	2.01	2.05
24	a	308	CLA	MG-ND	-2.09	2.01	2.05
24	g	315	CLA	CMB-C2B	-2.09	1.46	1.50
24	b	306	CLA	MG-ND	-2.09	2.01	2.05
24	A	802	CLA	C3B-C4B	2.09	1.48	1.42
24	A	828	CLA	C3B-C4B	2.09	1.48	1.42
24	j	309	CLA	C3B-C4B	2.09	1.48	1.42
24	e	607	CLA	CMC-C2C	-2.09	1.46	1.50
24	j	308	CLA	C3B-C4B	2.09	1.48	1.42
35	d	310	KC2	C4B-NB	-2.09	1.35	1.37
24	a	312	CLA	CMD-C2D	-2.09	1.46	1.50
24	i	602	CLA	CMC-C2C	-2.09	1.46	1.50
24	k	610	CLA	C3B-C4B	2.09	1.48	1.42
24	i	607	CLA	MG-NB	-2.09	2.01	2.05
24	b	306	CLA	CHC-C4B	-2.09	1.34	1.39
24	i	604	CLA	C3B-C4B	2.09	1.48	1.42
33	g	316	II0	C16-C03	2.09	1.57	1.53
24	B	823	CLA	CHC-C4B	-2.08	1.34	1.39
24	j	302	CLA	CMC-C2C	-2.08	1.46	1.50
24	j	306	CLA	CMB-C2B	-2.08	1.46	1.50
24	k	607	CLA	C3B-C4B	2.08	1.48	1.42
24	b	307	CLA	CHC-C1C	2.08	1.42	1.38
24	A	819	CLA	CHC-C4B	-2.08	1.34	1.39
24	b	308	CLA	C3B-C4B	2.08	1.48	1.42
24	e	611	CLA	CHC-C1C	2.08	1.42	1.38
24	k	602	CLA	CMB-C2B	-2.08	1.46	1.50
34	c	615	IHT	C13-C02	2.08	1.57	1.53
24	g	310	CLA	CMD-C2D	-2.08	1.46	1.50
24	B	836	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	614	CLA	C3B-C4B	2.08	1.48	1.42
35	k	613	KC2	C4A-C3A	2.08	1.48	1.44
24	A	802	CLA	MG-NB	-2.08	2.01	2.05
24	i	605	CLA	CHC-C1C	2.08	1.42	1.38
24	K	101	CLA	CMB-C2B	-2.08	1.46	1.50
24	f	607	CLA	CMC-C2C	-2.08	1.46	1.50
24	c	601	CLA	CMB-C2B	-2.08	1.46	1.50
24	i	603	CLA	CMB-C2B	-2.08	1.46	1.50
24	A	819	CLA	C3B-C4B	2.08	1.48	1.42
24	A	822	CLA	C3B-C4B	2.08	1.48	1.42
34	a	316	IHT	C13-C02	2.08	1.57	1.53
24	c	604	CLA	CMC-C2C	-2.08	1.46	1.50
24	c	601	CLA	MG-NB	-2.08	2.01	2.05
24	j	313	CLA	CMC-C2C	-2.08	1.46	1.50
24	L	207	CLA	CMB-C2B	-2.08	1.46	1.50
24	A	830	CLA	MG-ND	-2.08	2.01	2.05
27	A	847	WVN	C28-C25	-2.08	1.31	1.35
24	B	836	CLA	C1B-NB	-2.08	1.35	1.37
24	i	607	CLA	CMD-C2D	-2.07	1.46	1.50
34	k	618	IHT	C13-C02	2.07	1.57	1.53
24	a	305	CLA	CMD-C2D	-2.07	1.46	1.50
24	A	809	CLA	C3B-C4B	2.07	1.48	1.42
24	k	607	CLA	CMD-C2D	-2.07	1.46	1.50
24	e	608	CLA	MG-NB	-2.07	2.01	2.05
33	j	315	II0	C18-C04	2.07	1.57	1.53
24	A	842	CLA	MG-NB	-2.07	2.01	2.05
24	L	204	CLA	CMB-C2B	-2.07	1.46	1.50
24	c	609	CLA	CHC-C1C	2.07	1.42	1.38
24	O	205	CLA	C3B-C4B	2.07	1.48	1.42
24	g	303	CLA	C3B-C4B	2.07	1.48	1.42
24	h	302	CLA	MG-ND	-2.07	2.01	2.05
24	a	311	CLA	CMB-C2B	-2.07	1.46	1.50
24	B	812	CLA	CHC-C1C	2.07	1.42	1.38
24	B	819	CLA	C3B-C4B	2.07	1.48	1.42
24	j	306	CLA	C3B-C4B	2.07	1.48	1.42
33	e	613	II0	C20-C14	2.07	1.54	1.50
24	e	610	CLA	MG-NB	-2.07	2.01	2.05
24	A	852	CLA	CMC-C2C	-2.07	1.46	1.50
33	g	318	II0	C30-C26	-2.07	1.32	1.37
24	A	812	CLA	MG-NB	-2.07	2.01	2.05
24	g	322	CLA	CMC-C2C	-2.07	1.46	1.50
35	d	310	KC2	C4A-C3A	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	i	606	CLA	CMC-C2C	-2.07	1.46	1.50
24	A	827	CLA	C1B-C2B	2.07	1.48	1.43
24	h	305	CLA	CHC-C1C	2.07	1.42	1.38
33	b	318	II0	C20-C14	2.07	1.54	1.50
24	h	304	CLA	MG-NB	-2.07	2.01	2.05
24	O	201	CLA	C3B-C4B	2.07	1.48	1.42
33	g	320	II0	C16-C03	2.07	1.57	1.53
24	h	303	CLA	CMC-C2C	-2.07	1.46	1.50
24	B	836	CLA	MG-ND	-2.07	2.01	2.05
24	i	602	CLA	CHC-C1C	2.07	1.42	1.38
24	d	306	CLA	CMC-C2C	-2.07	1.46	1.50
33	a	315	II0	C20-C14	2.07	1.54	1.50
24	a	312	CLA	CMC-C2C	-2.07	1.46	1.50
24	d	308	CLA	CMB-C2B	-2.07	1.46	1.50
33	g	317	II0	C15-C03	2.07	1.57	1.53
24	A	856	CLA	MG-NB	-2.06	2.01	2.05
33	b	314	II0	C16-C03	2.06	1.57	1.53
24	i	601	CLA	CMD-C2D	-2.06	1.46	1.50
33	f	615	II0	C30-C26	-2.06	1.32	1.37
24	B	821	CLA	CMD-C2D	-2.06	1.46	1.50
24	g	302	CLA	CMC-C2C	-2.06	1.46	1.50
35	d	310	KC2	C1D-C2D	2.06	1.48	1.43
24	B	805	CLA	C4B-NB	2.06	1.40	1.37
24	g	303	CLA	MG-ND	-2.06	2.01	2.05
24	K	102	CLA	C3B-C4B	2.06	1.48	1.42
24	B	809	CLA	C1B-NB	-2.06	1.35	1.37
24	c	605	CLA	CMC-C2C	-2.06	1.46	1.50
24	B	826	CLA	MG-NB	-2.06	2.01	2.05
24	K	101	CLA	MG-ND	-2.06	2.01	2.05
24	B	840	CLA	C1B-C2B	2.06	1.48	1.43
24	c	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	B	804	CLA	C1B-NB	-2.06	1.35	1.37
24	B	810	CLA	CHC-C1C	2.06	1.42	1.38
33	f	614	II0	C18-C04	2.06	1.57	1.53
27	B	845	WVN	C36-C32	-2.06	1.31	1.35
34	b	316	IHT	C13-C02	2.06	1.57	1.53
24	A	818	CLA	C1B-C2B	2.06	1.48	1.43
24	g	304	CLA	CMB-C2B	-2.06	1.46	1.50
24	B	816	CLA	CAA-C2A	-2.06	1.50	1.54
24	k	607	CLA	CMC-C2C	-2.06	1.46	1.50
24	i	603	CLA	CMC-C2C	-2.06	1.46	1.50
24	e	604	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	806	CLA	C1B-NB	-2.06	1.35	1.37
34	j	317	IHT	C13-C02	2.06	1.57	1.53
24	K	102	CLA	MG-ND	-2.06	2.01	2.05
24	B	837	CLA	CMB-C2B	-2.06	1.46	1.50
35	c	610	KC2	C4A-C3A	2.06	1.48	1.44
24	g	308	CLA	C1B-NB	-2.06	1.35	1.37
24	B	837	CLA	MG-NB	-2.06	2.01	2.05
24	e	608	CLA	CHC-C1C	2.06	1.42	1.38
24	A	816	CLA	C1B-C2B	2.05	1.48	1.43
24	A	840	CLA	C1B-C2B	2.05	1.48	1.43
33	c	613	II0	C15-C03	2.05	1.57	1.53
24	A	816	CLA	MG-NB	-2.05	2.01	2.05
24	B	841	CLA	C3B-C4B	2.05	1.48	1.42
33	f	615	II0	C18-C04	2.05	1.57	1.53
24	B	830	CLA	MG-NB	-2.05	2.01	2.05
24	h	306	CLA	CMC-C2C	-2.05	1.46	1.50
24	A	826	CLA	C4B-NB	2.05	1.40	1.37
24	A	818	CLA	MG-NB	-2.05	2.01	2.05
33	k	621	II0	C20-C14	2.05	1.54	1.50
24	A	822	CLA	CMC-C2C	-2.05	1.46	1.50
24	b	310	CLA	CMB-C2B	-2.05	1.46	1.50
24	e	611	CLA	CMC-C2C	-2.05	1.46	1.50
24	b	311	CLA	CHC-C1C	2.05	1.42	1.38
24	A	833	CLA	MG-ND	-2.05	2.01	2.05
24	B	821	CLA	C1B-C2B	2.05	1.47	1.43
28	F	203	LMT	O1'-C1'	-2.05	1.36	1.40
24	g	303	CLA	CMC-C2C	-2.05	1.46	1.50
24	A	801	CLA	C3B-C4B	2.05	1.48	1.42
24	j	307	CLA	C3B-C4B	2.05	1.48	1.42
24	c	606	CLA	CMC-C2C	-2.05	1.46	1.50
24	B	818	CLA	C1B-C2B	2.05	1.47	1.43
24	A	828	CLA	CMC-C2C	-2.05	1.46	1.50
24	A	823	CLA	C3B-C4B	2.05	1.48	1.42
24	f	612	CLA	MG-NC	2.05	2.11	2.06
24	A	832	CLA	C3B-C4B	2.05	1.48	1.42
24	B	826	CLA	CMC-C2C	-2.05	1.46	1.50
24	e	606	CLA	CMD-C2D	-2.05	1.46	1.50
24	B	823	CLA	CAC-C3C	-2.05	1.45	1.51
27	B	848	WVN	C26-C22	-2.05	1.31	1.35
24	B	831	CLA	MG-ND	-2.05	2.01	2.05
24	k	603	CLA	MG-NA	2.05	2.11	2.06
24	g	305	CLA	C1B-NB	-2.05	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	j	303	CLA	CMC-C2C	-2.05	1.46	1.50
24	B	819	CLA	MG-NB	-2.05	2.01	2.05
24	f	606	CLA	C3B-C4B	2.05	1.48	1.42
24	d	309	CLA	CHC-C1C	2.04	1.42	1.38
24	g	309	CLA	CMB-C2B	-2.04	1.46	1.50
24	A	842	CLA	C3B-C4B	2.04	1.48	1.42
33	a	313	II0	C18-C04	2.04	1.57	1.53
24	f	609	CLA	C3B-C4B	2.04	1.48	1.42
33	f	615	II0	C16-C03	2.04	1.57	1.53
24	j	305	CLA	CMC-C2C	-2.04	1.46	1.50
24	c	605	CLA	CMD-C2D	-2.04	1.46	1.50
24	e	606	CLA	CMB-C2B	-2.04	1.46	1.50
24	d	307	CLA	CMB-C2B	-2.04	1.46	1.50
26	B	802	LHG	O7-C5	-2.04	1.41	1.46
24	B	804	CLA	CHC-C1C	2.04	1.42	1.38
24	K	101	CLA	CHC-C1C	2.04	1.42	1.38
24	B	833	CLA	C1B-C2B	2.04	1.47	1.43
24	f	602	CLA	CHC-C1C	2.04	1.42	1.38
24	A	829	CLA	CMD-C2D	-2.04	1.46	1.50
24	g	307	CLA	CMD-C2D	-2.04	1.46	1.50
33	d	314	II0	C20-C14	2.04	1.54	1.50
24	B	816	CLA	C1B-C2B	2.04	1.47	1.43
24	A	827	CLA	MG-NB	-2.04	2.01	2.05
24	a	307	CLA	CMD-C2D	-2.04	1.46	1.50
24	f	610	CLA	CMC-C2C	-2.04	1.46	1.50
34	f	617	IHT	C13-C02	2.04	1.57	1.53
24	c	612	CLA	CMD-C2D	-2.04	1.46	1.50
24	b	308	CLA	CMB-C2B	-2.04	1.46	1.50
33	j	318	II0	C20-C14	2.04	1.54	1.50
24	A	856	CLA	C3B-C4B	2.04	1.48	1.42
24	k	605	CLA	CMB-C2B	-2.04	1.46	1.50
24	g	315	CLA	C1B-C2B	2.04	1.47	1.43
33	j	315	II0	C16-C03	2.04	1.57	1.53
24	j	307	CLA	MG-NC	2.04	2.11	2.06
24	e	603	CLA	CHC-C1C	2.04	1.42	1.38
24	e	608	CLA	CMC-C2C	-2.03	1.46	1.50
24	d	309	CLA	CMD-C2D	-2.03	1.46	1.50
24	d	303	CLA	MG-NC	2.03	2.11	2.06
35	j	312	KC2	C4B-NB	-2.03	1.35	1.37
24	g	311	CLA	CMB-C2B	-2.03	1.46	1.50
24	k	601	CLA	MG-NC	2.03	2.11	2.06
24	f	608	CLA	C1B-C2B	2.03	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	302	CLA	CHC-C1C	2.03	1.42	1.38
24	B	803	CLA	CMC-C2C	-2.03	1.46	1.50
24	A	809	CLA	C1B-C2B	2.03	1.47	1.43
24	a	303	CLA	C3B-C4B	2.03	1.48	1.42
24	g	306	CLA	CHC-C1C	2.03	1.42	1.38
24	B	828	CLA	C1B-C2B	2.03	1.47	1.43
33	k	615	II0	C20-C14	2.03	1.54	1.50
24	a	303	CLA	CMB-C2B	-2.03	1.46	1.50
24	g	311	CLA	CHC-C1C	2.03	1.42	1.38
24	h	304	CLA	CMC-C2C	-2.03	1.46	1.50
24	B	815	CLA	CHC-C1C	2.03	1.42	1.38
33	k	616	II0	C15-C03	2.03	1.57	1.53
24	A	838	CLA	MG-NB	-2.03	2.01	2.05
24	A	821	CLA	C1B-NB	-2.03	1.35	1.37
24	a	305	CLA	MG-NB	-2.03	2.01	2.05
24	A	803	CLA	CMC-C2C	-2.03	1.46	1.50
24	h	312	CLA	C1B-C2B	2.03	1.47	1.43
24	k	605	CLA	MG-NB	-2.03	2.01	2.05
24	j	303	CLA	MG-NB	-2.03	2.01	2.05
24	A	838	CLA	C4B-NB	2.03	1.40	1.37
33	c	614	II0	C16-C03	2.03	1.57	1.53
24	B	812	CLA	MG-NB	-2.02	2.01	2.05
24	f	607	CLA	CHC-C4B	-2.02	1.34	1.39
24	c	608	CLA	CMC-C2C	-2.02	1.46	1.50
24	i	607	CLA	C3B-C4B	2.02	1.48	1.42
24	B	821	CLA	C3B-C4B	2.02	1.48	1.42
24	g	306	CLA	C3B-C4B	2.02	1.48	1.42
24	j	309	CLA	O2A-CGA	2.02	1.37	1.30
24	b	305	CLA	CMC-C2C	-2.02	1.46	1.50
35	c	610	KC2	C3C-C4C	2.02	1.48	1.44
24	g	302	CLA	C1B-NB	-2.02	1.35	1.37
24	A	825	CLA	C4B-NB	2.02	1.40	1.37
24	e	607	CLA	CMB-C2B	-2.02	1.46	1.50
24	B	840	CLA	MG-ND	-2.02	2.01	2.05
24	e	602	CLA	C3B-C4B	2.02	1.48	1.42
24	f	609	CLA	CMD-C2D	-2.02	1.46	1.50
24	j	314	CLA	CMB-C2B	-2.02	1.46	1.50
24	B	809	CLA	C1B-C2B	2.02	1.47	1.43
24	c	605	CLA	C3B-C4B	2.02	1.48	1.42
24	g	307	CLA	MG-NB	-2.02	2.01	2.05
24	g	322	CLA	C1B-NB	-2.02	1.35	1.37
33	b	315	II0	C16-C03	2.02	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	318	II0	C16-C03	2.02	1.57	1.53
24	i	610	CLA	MG-NC	2.02	2.11	2.06
24	g	322	CLA	MG-NB	-2.02	2.01	2.05
27	L	201	WVN	C36-C32	-2.02	1.31	1.35
24	A	825	CLA	MG-ND	-2.02	2.01	2.05
24	d	302	CLA	CMB-C2B	-2.02	1.46	1.50
24	f	608	CLA	CMB-C2B	-2.01	1.46	1.50
33	e	613	II0	C18-C04	2.01	1.57	1.53
24	A	802	CLA	C1B-C2B	2.01	1.47	1.43
24	c	611	CLA	O2A-CGA	2.01	1.37	1.30
24	a	310	CLA	CHC-C4B	-2.01	1.34	1.39
27	I	101	WVN	C02-C11	2.01	1.53	1.50
24	i	604	CLA	CMB-C2B	-2.01	1.46	1.50
24	J	105	CLA	MG-NB	-2.01	2.01	2.05
24	a	311	CLA	MG-NB	-2.01	2.01	2.05
33	c	613	II0	C18-C04	2.01	1.57	1.53
24	A	840	CLA	MG-NB	-2.01	2.01	2.05
24	f	613	CLA	CMB-C2B	-2.01	1.46	1.50
24	B	840	CLA	CMB-C2B	-2.01	1.46	1.50
24	A	812	CLA	CHC-C1C	2.01	1.42	1.38
24	B	806	CLA	C1B-C2B	2.01	1.47	1.43
33	g	318	II0	C15-C03	2.01	1.57	1.53
24	B	811	CLA	CMB-C2B	-2.01	1.46	1.50
24	A	855	CLA	CAC-C3C	-2.01	1.46	1.51
24	A	838	CLA	MG-ND	-2.01	2.01	2.05
24	b	307	CLA	CMD-C2D	-2.01	1.46	1.50
24	k	603	CLA	MG-NC	2.01	2.11	2.06
24	A	818	CLA	CHC-C4B	-2.01	1.34	1.39
24	B	828	CLA	MG-NB	-2.01	2.01	2.05
24	F	201	CLA	MG-NB	-2.01	2.01	2.05
24	k	609	CLA	CMC-C2C	-2.01	1.46	1.50
24	A	807	CLA	CHC-C1C	2.01	1.42	1.38
24	B	812	CLA	C3B-C4B	2.01	1.48	1.42
33	j	315	II0	C15-C03	2.01	1.57	1.53
24	a	308	CLA	C3B-C4B	2.01	1.48	1.42
24	B	824	CLA	MG-NB	-2.01	2.01	2.05
33	b	318	II0	C30-C26	-2.01	1.32	1.37
34	g	319	IHT	C13-C02	2.01	1.57	1.53
24	b	305	CLA	CMB-C2B	-2.01	1.46	1.50
33	f	618	II0	C15-C03	2.01	1.57	1.53
27	A	846	WVN	C37-C34	-2.00	1.31	1.35
24	e	610	CLA	MG-ND	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	832	CLA	C4B-NB	2.00	1.40	1.37
24	B	824	CLA	C1B-NB	-2.00	1.35	1.37
24	d	312	CLA	CMD-C2D	-2.00	1.46	1.50
24	B	827	CLA	C3B-C4B	2.00	1.48	1.42
24	A	821	CLA	CHC-C1C	2.00	1.42	1.38
33	c	616	II0	C18-C04	2.00	1.57	1.53
24	a	306	CLA	C3B-C4B	2.00	1.48	1.42
24	c	601	CLA	CMD-C2D	-2.00	1.46	1.50
35	e	609	KC2	C4B-NB	-2.00	1.35	1.37
24	d	305	CLA	MG-NB	-2.00	2.01	2.05
27	R	202	WVN	C28-C25	-2.00	1.31	1.35
24	a	302	CLA	C3B-C4B	2.00	1.48	1.42
24	A	828	CLA	MG-NB	-2.00	2.01	2.05
33	a	314	II0	C16-C03	2.00	1.57	1.53
24	g	322	CLA	C3B-C4B	2.00	1.48	1.42
24	i	610	CLA	CHC-C1C	2.00	1.42	1.38
24	A	816	CLA	C1B-NB	-2.00	1.35	1.37
24	c	612	CLA	CMB-C2B	-2.00	1.46	1.50
24	f	604	CLA	CMB-C2B	-2.00	1.46	1.50
24	B	820	CLA	MG-NB	-2.00	2.01	2.05
24	B	828	CLA	MG-ND	-2.00	2.01	2.05
24	B	806	CLA	C3B-C4B	2.00	1.48	1.42
24	J	105	CLA	CMB-C2B	-2.00	1.46	1.50
24	A	855	CLA	MG-NB	-2.00	2.01	2.05
33	f	616	II0	C20-C14	2.00	1.54	1.50
27	A	850	WVN	C28-C25	-2.00	1.31	1.35

All (3510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	617	IHT	C40-C37-C33	-13.79	107.93	127.28
34	b	317	IHT	C40-C37-C33	-12.64	109.55	127.28
35	f	611	KC2	C1A-NA-C4A	-12.27	101.08	106.68
34	f	617	IHT	C30-C27-C23	-11.91	110.57	127.28
35	k	613	KC2	C1A-NA-C4A	-11.62	101.38	106.68
35	c	610	KC2	C1A-NA-C4A	-11.08	101.63	106.68
35	g	314	KC2	C1A-NA-C4A	-11.06	101.64	106.68
35	j	312	KC2	C1A-NA-C4A	-11.01	101.66	106.68
35	d	310	KC2	C1A-NA-C4A	-10.83	101.74	106.68
35	i	609	KC2	C1A-NA-C4A	-10.82	101.74	106.68
35	i	616	KC2	C1A-NA-C4A	-10.44	101.92	106.68
35	g	312	KC2	C1A-NA-C4A	-10.35	101.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	g	313	KC2	C1A-NA-C4A	-10.21	102.02	106.68
35	k	611	KC2	C1A-NA-C4A	-10.02	102.11	106.68
34	f	617	IHT	C18-C22-C23	-9.83	111.69	126.23
27	F	205	WVN	C30-C28-C25	-9.78	113.56	127.28
24	A	856	CLA	C4A-NA-C1A	9.71	111.11	106.68
35	k	612	KC2	C1A-NA-C4A	-9.38	102.40	106.68
34	f	617	IHT	C41-C38-C35	-9.33	114.20	127.28
35	d	311	KC2	C1A-NA-C4A	-9.28	102.44	106.68
35	e	609	KC2	CHD-C4C-NC	9.22	138.20	124.31
35	i	616	KC2	CHD-C4C-NC	9.19	138.15	124.31
35	c	610	KC2	CHD-C4C-NC	9.17	138.13	124.31
35	k	611	KC2	CHD-C4C-NC	9.16	138.11	124.31
33	b	315	II0	C42-C40-C36	-9.04	114.60	127.28
24	b	306	CLA	C4A-NA-C1A	8.96	110.77	106.68
35	d	310	KC2	CHD-C4C-NC	8.86	137.66	124.31
27	F	205	WVN	C20-C23-C25	-8.82	113.18	126.23
35	g	313	KC2	CHD-C4C-NC	8.80	137.56	124.31
35	f	611	KC2	CHD-C4C-NC	8.77	137.51	124.31
27	A	847	WVN	C39-C36-C32	-8.76	115.00	127.28
24	B	807	CLA	C4A-NA-C1A	8.74	110.67	106.68
27	B	847	WVN	C02-C11-C19	-8.70	111.04	124.58
35	g	314	KC2	CHD-C4C-NC	8.69	137.40	124.31
35	j	312	KC2	CHD-C4C-NC	8.61	137.28	124.31
35	k	613	KC2	CHD-C4C-NC	8.43	137.00	124.31
27	R	202	WVN	C29-C26-C22	-8.39	115.51	127.28
35	i	609	KC2	CHD-C4C-NC	8.32	136.85	124.31
35	e	609	KC2	C1A-NA-C4A	-8.30	102.89	106.68
27	F	205	WVN	C40-C37-C34	-8.17	115.82	127.28
33	a	317	II0	C42-C40-C36	-8.15	115.85	127.28
24	c	611	CLA	C4A-NA-C1A	8.13	110.39	106.68
24	B	834	CLA	C4A-NA-C1A	8.12	110.38	106.68
24	i	604	CLA	C4A-NA-C1A	8.05	110.35	106.68
35	k	612	KC2	C4C-C3C-C2C	-7.97	99.95	107.28
27	B	848	WVN	C20-C23-C25	-7.92	114.52	126.23
24	e	608	CLA	C4A-NA-C1A	7.88	110.27	106.68
35	k	612	KC2	CHC-C4B-C3B	-7.87	111.94	125.21
35	g	312	KC2	O2D-CGD-O1D	-7.87	108.53	123.85
35	g	312	KC2	CHD-C4C-NC	7.84	136.12	124.31
24	j	307	CLA	C4A-NA-C1A	7.82	110.25	106.68
33	b	315	II0	C41-C39-C35	-7.82	116.31	127.28
34	R	204	IHT	C40-C37-C33	-7.69	116.49	127.28
24	k	601	CLA	C4A-NA-C1A	7.67	110.18	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	f	618	II0	C41-C39-C35	-7.59	116.63	127.28
35	d	310	KC2	CHC-C4B-C3B	-7.55	112.47	125.21
35	g	312	KC2	CHC-C4B-C3B	-7.54	112.49	125.21
35	k	612	KC2	OBD-CAD-C3D	-7.53	110.82	128.42
35	d	311	KC2	CHD-C4C-NC	7.49	135.59	124.31
27	A	847	WVN	C30-C28-C25	-7.48	116.78	127.28
35	k	611	KC2	CHC-C4B-C3B	-7.44	112.67	125.21
35	j	312	KC2	CHC-C4B-C3B	-7.44	112.67	125.21
35	e	609	KC2	CHC-C4B-C3B	-7.43	112.68	125.21
34	f	617	IHT	C30-C32-C33	-7.39	106.09	126.36
35	g	312	KC2	C2C-C1C-NC	7.39	119.60	110.45
35	i	609	KC2	C2C-C1C-NC	7.35	119.55	110.45
35	i	609	KC2	CHC-C4B-C3B	-7.31	112.89	125.21
27	A	846	WVN	C30-C28-C25	-7.30	117.04	127.28
35	g	312	KC2	CHB-C4A-C3A	-7.29	113.52	125.03
35	f	611	KC2	CHC-C4B-C3B	-7.26	112.97	125.21
35	k	612	KC2	CHC-C4B-NB	7.21	134.95	124.80
24	e	601	CLA	C4A-NA-C1A	7.20	109.97	106.68
35	j	312	KC2	C2C-C1C-NC	7.18	119.34	110.45
34	b	317	IHT	C18-C22-C23	-7.18	115.62	126.23
27	L	206	WVN	C02-C11-C19	-7.16	113.43	124.58
24	B	829	CLA	C4A-NA-C1A	7.14	109.94	106.68
33	a	314	II0	C41-C39-C35	-7.13	117.28	127.28
35	f	611	KC2	C1A-C2A-C3A	-7.12	100.73	107.28
35	f	611	KC2	CHB-C4A-C3A	-7.11	113.80	125.03
35	k	612	KC2	CHD-C4C-NC	7.10	135.01	124.31
35	e	609	KC2	CHB-C4A-C3A	-7.09	113.84	125.03
27	B	848	WVN	C40-C37-C34	-7.08	117.35	127.28
35	e	609	KC2	C2C-C1C-NC	7.07	119.20	110.45
35	i	609	KC2	CHB-C4A-C3A	-7.06	113.88	125.03
35	d	311	KC2	CHC-C4B-C3B	-7.03	113.35	125.21
35	d	311	KC2	C4C-C3C-C2C	-7.03	100.82	107.28
35	c	610	KC2	CHC-C4B-C3B	-7.01	113.38	125.21
24	B	825	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	R	201	WVN	C02-C11-C19	-6.97	113.72	124.58
33	i	612	II0	C42-C40-C36	-6.97	117.50	127.28
35	g	312	KC2	OBD-CAD-C3D	-6.92	112.24	128.42
35	j	312	KC2	CHB-C4A-C3A	-6.91	114.12	125.03
34	O	203	IHT	C40-C37-C33	-6.89	117.62	127.28
35	k	612	KC2	C2C-C1C-NC	6.86	118.95	110.45
24	a	308	CLA	C4A-NA-C1A	6.85	109.80	106.68
35	g	313	KC2	CHB-C4A-C3A	-6.84	114.23	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	e	604	CLA	C4A-NA-C1A	6.81	109.78	106.68
35	i	616	KC2	CHC-C4B-C3B	-6.80	113.74	125.21
34	f	617	IHT	C32-C33-C37	6.76	129.65	119.01
35	d	310	KC2	CHB-C4A-C3A	-6.76	114.36	125.03
27	h	308	WVN	C04-C09-C05	-6.75	118.38	124.83
33	b	314	II0	C41-C39-C35	-6.75	117.81	127.28
35	g	314	KC2	CHC-C4B-C3B	-6.74	113.85	125.21
24	f	606	CLA	C4A-NA-C1A	6.72	109.75	106.68
35	d	311	KC2	C2C-C1C-NC	6.72	118.77	110.45
33	c	613	II0	C41-C39-C35	-6.72	117.86	127.28
33	d	313	II0	C42-C40-C36	-6.70	117.88	127.28
35	k	611	KC2	C2C-C1C-NC	6.68	118.71	110.45
27	e	615	WVN	C30-C28-C25	-6.68	117.92	127.28
24	e	606	CLA	C4A-NA-C1A	6.67	109.72	106.68
35	g	313	KC2	CHC-C4B-C3B	-6.67	113.97	125.21
34	a	316	IHT	C41-C38-C35	-6.65	117.95	127.28
24	h	307	CLA	C4A-NA-C1A	6.65	109.71	106.68
24	b	308	CLA	C4A-NA-C1A	6.64	109.71	106.68
35	d	310	KC2	C2C-C1C-NC	6.64	118.67	110.45
35	k	612	KC2	C1D-ND-C4D	6.64	110.97	106.31
35	g	312	KC2	CHC-C4B-NB	6.60	134.09	124.80
27	L	201	WVN	C04-C09-C05	-6.59	118.54	124.83
27	A	847	WVN	C11-C19-C22	-6.59	112.16	126.32
35	d	310	KC2	CHC-C4B-NB	6.58	134.06	124.80
35	f	611	KC2	C4C-C3C-C2C	-6.58	101.23	107.28
35	j	312	KC2	C4C-C3C-C2C	-6.58	101.23	107.28
24	A	836	CLA	C4A-NA-C1A	6.57	109.68	106.68
27	B	847	WVN	C30-C28-C25	-6.57	118.07	127.28
35	k	612	KC2	CHB-C4A-C3A	-6.57	114.66	125.03
35	g	314	KC2	C2C-C1C-NC	6.55	118.56	110.45
35	k	611	KC2	CHC-C4B-NB	6.55	134.02	124.80
35	f	611	KC2	CHC-C4B-NB	6.54	134.01	124.80
35	g	314	KC2	CHC-C4B-NB	6.53	134.00	124.80
35	d	311	KC2	CHC-C4B-NB	6.53	133.99	124.80
33	c	614	II0	C41-C39-C35	-6.51	118.15	127.28
35	c	610	KC2	CHC-C4B-NB	6.51	133.96	124.80
35	i	616	KC2	CHC-C4B-NB	6.51	133.96	124.80
24	B	817	CLA	C4A-NA-C1A	6.50	109.64	106.68
24	g	302	CLA	C4A-NA-C1A	6.50	109.64	106.68
33	k	617	II0	C42-C40-C36	-6.48	118.19	127.28
24	J	105	CLA	C4A-NA-C1A	6.47	109.63	106.68
24	A	835	CLA	C4A-NA-C1A	6.46	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	609	KC2	C4C-C3C-C2C	-6.44	101.36	107.28
35	i	609	KC2	C4C-C3C-C2C	-6.44	101.36	107.28
35	k	613	KC2	CHB-C4A-C3A	-6.44	114.86	125.03
24	L	204	CLA	C4A-NA-C1A	6.44	109.62	106.68
27	B	848	WVN	C02-C11-C19	-6.44	114.56	124.58
35	g	313	KC2	CHC-C4B-NB	6.43	133.85	124.80
24	A	831	CLA	C4A-NA-C1A	6.42	109.61	106.68
35	i	609	KC2	CHC-C4B-NB	6.39	133.80	124.80
35	i	609	KC2	OBD-CAD-C3D	-6.39	113.48	128.42
27	A	847	WVN	C26-C29-C31	-6.39	104.69	123.20
35	i	616	KC2	C2C-C1C-NC	6.39	118.35	110.45
24	A	808	CLA	C4A-NA-C1A	6.38	109.59	106.68
24	A	826	CLA	C4A-NA-C1A	6.37	109.59	106.68
35	e	609	KC2	CHC-C4B-NB	6.37	133.77	124.80
35	j	312	KC2	CHC-C4B-NB	6.37	133.76	124.80
35	c	610	KC2	CHB-C4A-C3A	-6.36	114.98	125.03
35	k	611	KC2	CHB-C4A-C3A	-6.36	114.99	125.03
27	R	202	WVN	C02-C11-C19	-6.36	114.68	124.58
35	g	314	KC2	CHB-C4A-C3A	-6.34	115.02	125.03
27	B	845	WVN	C04-C09-C05	-6.32	118.80	124.83
33	h	309	II0	C42-C40-C36	-6.30	118.44	127.28
24	A	839	CLA	C4A-NA-C1A	6.30	109.55	106.68
35	k	613	KC2	CHC-C4B-C3B	-6.30	114.59	125.21
33	h	311	II0	C41-C39-C35	-6.29	118.45	127.28
33	b	318	II0	C42-C40-C36	-6.29	118.46	127.28
24	j	306	CLA	C4A-NA-C1A	6.28	109.55	106.68
35	f	611	KC2	OBD-CAD-C3D	-6.27	113.75	128.42
33	b	314	II0	C42-C40-C36	-6.27	118.48	127.28
27	J	102	WVN	C04-C09-C05	-6.27	118.84	124.83
27	F	205	WVN	C40-C39-C36	-6.26	110.72	123.52
27	A	850	WVN	C30-C28-C25	-6.25	118.52	127.28
27	R	201	WVN	C30-C28-C25	-6.24	118.52	127.28
24	A	812	CLA	C4A-NA-C1A	6.24	109.52	106.68
27	B	848	WVN	C21-C15-C13	-6.23	117.68	124.48
35	g	313	KC2	OBD-CAD-C3D	-6.23	113.85	128.42
33	c	614	II0	C42-C40-C36	-6.22	118.55	127.28
24	a	311	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	A	813	CLA	C4A-NA-C1A	6.20	109.51	106.68
35	k	613	KC2	CHC-C4B-NB	6.18	133.51	124.80
35	k	613	KC2	OBD-CAD-C3D	-6.17	113.99	128.42
27	F	204	WVN	C02-C11-C19	-6.16	114.99	124.58
34	g	319	IHT	C19-C10-C07	-6.15	117.77	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	i	601	CLA	C4A-NA-C1A	6.13	109.47	106.68
35	f	611	KC2	C2C-C1C-NC	6.13	118.03	110.45
35	i	609	KC2	C1D-ND-C4D	6.11	110.60	106.31
35	g	314	KC2	OBD-CAD-C3D	-6.10	114.15	128.42
35	g	312	KC2	C1D-ND-C4D	6.10	110.59	106.31
35	g	314	KC2	C4C-C3C-C2C	-6.10	101.67	107.28
27	B	846	WVN	C04-C09-C05	-6.10	119.01	124.83
35	k	613	KC2	C2C-C1C-NC	6.07	117.97	110.45
35	d	311	KC2	OBD-CAD-C3D	-6.06	114.24	128.42
33	j	315	II0	C19-C13-C09	-6.06	112.82	124.16
27	F	204	WVN	C39-C40-C37	-6.06	111.12	123.52
35	i	616	KC2	OBD-CAD-C3D	-6.04	114.30	128.42
24	c	605	CLA	C4A-NA-C1A	6.03	109.43	106.68
27	B	845	WVN	C24-C22-C19	6.03	127.29	118.09
24	b	303	CLA	C4A-NA-C1A	6.02	109.43	106.68
33	j	318	II0	C41-C39-C35	-6.02	118.84	127.28
27	A	847	WVN	C29-C26-C22	6.02	135.72	127.28
27	A	849	WVN	C20-C23-C25	-6.02	117.33	126.23
35	g	312	KC2	C4C-C3C-C2C	-6.02	101.75	107.28
27	L	206	WVN	C30-C28-C25	-6.01	118.85	127.28
27	B	846	WVN	C02-C11-C19	-6.01	115.23	124.58
27	B	849	WVN	C02-C11-C19	-6.00	115.25	124.58
24	c	603	CLA	C4A-NA-C1A	5.99	109.41	106.68
24	A	821	CLA	C4A-NA-C1A	5.99	109.41	106.68
24	B	814	CLA	C4A-NA-C1A	5.98	109.41	106.68
24	F	202	CLA	C4A-NA-C1A	5.98	109.41	106.68
35	c	610	KC2	C1A-C2A-C3A	-5.98	101.78	107.28
24	g	309	CLA	C4A-NA-C1A	5.98	109.41	106.68
27	h	308	WVN	C02-C11-C19	-5.96	115.30	124.58
33	f	616	II0	C42-C40-C36	-5.96	118.92	127.28
35	g	313	KC2	C2C-C1C-NC	5.96	117.82	110.45
33	d	314	II0	C41-C39-C35	-5.95	118.93	127.28
34	b	316	IHT	C30-C27-C23	-5.95	118.93	127.28
34	j	317	IHT	C09-C10-C07	-5.95	114.66	122.70
35	i	616	KC2	C1A-C2A-C3A	-5.95	101.81	107.28
24	A	806	CLA	C4A-NA-C1A	5.94	109.39	106.68
24	B	804	CLA	C4A-NA-C1A	5.93	109.39	106.68
33	k	621	II0	C42-C40-C36	-5.93	118.97	127.28
24	A	819	CLA	C4A-NA-C1A	5.93	109.38	106.68
35	k	613	KC2	C1A-C2A-C3A	-5.92	101.84	107.28
24	f	603	CLA	C4A-NA-C1A	5.92	109.38	106.68
35	g	314	KC2	C1A-C2A-C3A	-5.91	101.85	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	311	KC2	C1A-C2A-C3A	-5.90	101.86	107.28
24	B	803	CLA	C4A-NA-C1A	5.89	109.36	106.68
34	f	617	IHT	C19-C10-C07	-5.89	118.06	124.48
24	f	601	CLA	C4A-NA-C1A	5.87	109.36	106.68
35	d	310	KC2	OBD-CAD-C3D	-5.87	114.69	128.42
35	c	610	KC2	C2C-C1C-NC	5.87	117.72	110.45
33	g	317	II0	C41-C39-C35	-5.87	119.05	127.28
35	g	313	KC2	C4C-C3C-C2C	-5.86	101.89	107.28
35	d	311	KC2	CHB-C4A-C3A	-5.86	115.78	125.03
24	B	822	CLA	C4A-NA-C1A	5.85	109.35	106.68
33	k	616	II0	C29-C31-C33	-5.85	106.25	123.20
35	k	611	KC2	OBD-CAD-C3D	-5.85	114.75	128.42
35	c	610	KC2	OBD-CAD-C3D	-5.84	114.76	128.42
35	j	312	KC2	OBD-CAD-C3D	-5.80	114.86	128.42
35	d	310	KC2	C1A-C2A-C3A	-5.80	101.95	107.28
33	d	315	II0	C41-C39-C35	-5.80	119.15	127.28
24	K	101	CLA	C4A-NA-C1A	5.80	109.32	106.68
33	i	612	II0	C20-C14-C10	-5.80	113.32	124.16
27	A	849	WVN	C30-C28-C25	-5.79	119.15	127.28
27	J	101	WVN	C30-C28-C25	-5.79	119.16	127.28
35	d	310	KC2	C4C-C3C-C2C	-5.78	101.97	107.28
24	b	311	CLA	C4A-NA-C1A	5.77	109.31	106.68
34	c	615	IHT	C41-C38-C35	-5.76	119.20	127.28
33	e	612	II0	C19-C13-C09	-5.76	113.40	124.16
35	k	613	KC2	C4C-C3C-C2C	-5.76	101.99	107.28
24	A	832	CLA	C4A-NA-C1A	5.74	109.30	106.68
33	e	614	II0	C41-C39-C35	-5.74	119.22	127.28
35	k	611	KC2	C4C-C3C-C2C	-5.74	102.00	107.28
33	j	315	II0	C41-C39-C35	-5.73	119.24	127.28
35	i	609	KC2	C1A-C2A-C3A	-5.72	102.02	107.28
35	i	616	KC2	CHB-C4A-C3A	-5.72	116.00	125.03
24	A	803	CLA	C4A-NA-C1A	5.72	109.29	106.68
27	j	301	WVN	C02-C11-C19	-5.71	115.69	124.58
24	g	305	CLA	C4A-NA-C1A	5.71	109.28	106.68
35	e	609	KC2	CHD-C4C-C3C	-5.71	106.70	125.91
24	B	805	CLA	C4A-NA-C1A	5.70	109.28	106.68
35	k	612	KC2	CMD-C2D-C1D	-5.69	116.75	125.42
27	A	848	WVN	C02-C11-C19	-5.69	115.73	124.58
35	i	616	KC2	C4C-C3C-C2C	-5.69	102.05	107.28
33	k	617	II0	C19-C13-C09	-5.68	113.54	124.16
27	K	103	WVN	C30-C28-C25	-5.66	119.33	127.28
24	B	833	CLA	C4A-NA-C1A	5.66	109.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	308	WVN	C29-C26-C22	-5.66	119.35	127.28
33	j	316	II0	C42-C40-C36	-5.64	119.37	127.28
24	g	322	CLA	C4A-NA-C1A	5.64	109.25	106.68
35	e	609	KC2	OBD-CAD-C3D	-5.63	115.25	128.42
33	f	614	II0	C41-C39-C35	-5.63	119.39	127.28
24	B	836	CLA	CAC-C3C-C4C	5.62	132.10	124.79
35	k	611	KC2	CMD-C2D-C1D	-5.61	116.88	125.42
35	c	610	KC2	C4C-C3C-C2C	-5.61	102.13	107.28
27	R	202	WVN	C04-C09-C05	-5.60	119.48	124.83
27	B	847	WVN	C04-C09-C05	-5.60	119.48	124.83
35	k	611	KC2	C1A-C2A-C3A	-5.60	102.14	107.28
24	B	840	CLA	C4A-NA-C1A	5.59	109.23	106.68
35	g	313	KC2	C1A-C2A-C3A	-5.58	102.15	107.28
24	F	201	CLA	C4A-NA-C1A	5.58	109.22	106.68
34	b	316	IHT	C41-C38-C35	-5.56	119.47	127.28
24	B	841	CLA	C4A-NA-C1A	5.56	109.22	106.68
27	A	846	WVN	C04-C09-C05	-5.56	119.53	124.83
27	K	103	WVN	C02-C11-C19	-5.55	115.94	124.58
24	d	301	CLA	C4A-NA-C1A	5.55	109.21	106.68
33	d	313	II0	C41-C39-C35	-5.54	119.50	127.28
24	A	804	CLA	C4A-NA-C1A	5.54	109.21	106.68
24	A	828	CLA	C4A-NA-C1A	5.54	109.21	106.68
35	d	311	KC2	CMD-C2D-C1D	-5.54	116.99	125.42
33	j	316	II0	C41-C39-C35	-5.53	119.52	127.28
35	j	312	KC2	C4B-CHC-C1C	-5.53	114.27	126.02
24	A	824	CLA	C4A-NA-C1A	5.53	109.20	106.68
27	A	850	WVN	C39-C36-C32	-5.50	119.56	127.28
24	B	824	CLA	C4A-NA-C1A	5.50	109.19	106.68
27	M	101	WVN	C01-C02-C11	-5.49	106.51	112.83
35	g	312	KC2	C1A-C2A-C3A	-5.49	102.23	107.28
35	e	609	KC2	C4B-CHC-C1C	-5.48	114.36	126.02
27	j	301	WVN	C29-C26-C22	-5.48	119.60	127.28
24	B	812	CLA	C4A-NA-C1A	5.48	109.18	106.68
34	c	615	IHT	C30-C27-C23	-5.47	119.60	127.28
27	A	849	WVN	C21-C15-C13	-5.47	118.51	124.48
33	e	614	II0	C42-C40-C36	-5.46	119.62	127.28
24	B	815	CLA	C4A-NA-C1A	5.46	109.17	106.68
33	a	317	II0	C30-C32-C34	-5.45	107.39	123.20
24	h	301	CLA	C4A-NA-C1A	5.45	109.17	106.68
33	O	202	II0	C42-C40-C36	-5.45	119.64	127.28
24	a	310	CLA	C4A-NA-C1A	5.45	109.16	106.68
24	a	304	CLA	C4A-NA-C1A	5.44	109.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	601	CLA	C4A-NA-C1A	5.44	109.16	106.68
35	k	611	KC2	CHD-C4C-C3C	-5.44	107.62	125.91
35	g	312	KC2	O1D-CGD-CBD	-5.43	113.81	124.52
35	g	312	KC2	C4B-CHC-C1C	-5.43	114.48	126.02
34	b	316	IHT	C40-C37-C33	-5.42	119.67	127.28
27	B	847	WVN	C40-C39-C36	-5.42	112.44	123.52
34	j	317	IHT	C41-C38-C35	-5.42	119.68	127.28
35	g	313	KC2	CHC-C1C-NC	-5.41	115.84	124.23
24	e	611	CLA	C4A-NA-C1A	5.41	109.15	106.68
33	j	315	II0	C42-C40-C36	-5.40	119.70	127.28
24	e	610	CLA	C4A-NA-C1A	5.40	109.14	106.68
24	f	610	CLA	C4A-NA-C1A	5.40	109.14	106.68
24	d	304	CLA	C4A-NA-C1A	5.40	109.14	106.68
33	h	310	II0	C41-C39-C35	-5.40	119.71	127.28
27	L	201	WVN	C40-C37-C34	-5.39	119.71	127.28
27	L	205	WVN	C29-C26-C22	-5.39	119.72	127.28
33	f	615	II0	C41-C39-C35	-5.39	119.72	127.28
33	d	315	II0	C42-C40-C36	-5.38	119.74	127.28
24	I	102	CLA	C4A-NA-C1A	5.37	109.13	106.68
24	e	602	CLA	C4A-NA-C1A	5.37	109.13	106.68
35	k	613	KC2	CHB-C1B-NB	5.36	132.35	124.80
24	B	801	CLA	C4A-NA-C1A	5.36	109.12	106.68
24	i	603	CLA	C4A-NA-C1A	5.35	109.12	106.68
27	R	202	WVN	C39-C36-C32	-5.35	119.78	127.28
34	f	617	IHT	C09-C10-C07	-5.35	115.48	122.70
27	L	205	WVN	C02-C11-C19	-5.35	116.26	124.58
24	B	806	CLA	C4A-NA-C1A	5.35	109.12	106.68
24	A	815	CLA	C4A-NA-C1A	5.33	109.11	106.68
24	g	306	CLA	C4A-NA-C1A	5.33	109.11	106.68
24	b	305	CLA	C4A-NA-C1A	5.33	109.11	106.68
35	f	611	KC2	CHD-C4C-C3C	-5.32	108.00	125.91
27	L	206	WVN	C04-C09-C05	-5.32	119.75	124.83
24	A	833	CLA	C4A-NA-C1A	5.32	109.11	106.68
35	i	616	KC2	CHB-C1B-NB	5.31	132.28	124.80
27	B	848	WVN	C04-C09-C05	-5.31	119.76	124.83
24	a	306	CLA	C4A-NA-C1A	5.30	109.09	106.68
35	j	312	KC2	CHD-C4C-C3C	-5.29	108.10	125.91
24	B	818	CLA	C4A-NA-C1A	5.29	109.09	106.68
27	J	102	WVN	C29-C26-C22	-5.29	119.86	127.28
35	i	616	KC2	CHD-C4C-C3C	-5.29	108.11	125.91
35	k	613	KC2	CHC-C1C-NC	-5.29	116.04	124.23
35	c	610	KC2	CHB-C1B-NB	5.28	132.24	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	f	614	II0	C20-C14-C10	-5.28	114.29	124.16
35	d	310	KC2	C4B-CHC-C1C	-5.28	114.80	126.02
27	h	308	WVN	C30-C28-C25	-5.27	119.88	127.28
35	k	613	KC2	CHD-C1D-ND	-5.27	116.14	124.05
24	O	201	CLA	C4A-NA-C1A	5.27	109.08	106.68
30	B	843	DGD	O2G-C1B-C2B	5.27	122.88	111.48
34	j	317	IHT	C30-C27-C23	-5.27	119.89	127.28
35	k	611	KC2	C4B-CHC-C1C	-5.27	114.82	126.02
35	d	311	KC2	C4B-CHC-C1C	-5.26	114.85	126.02
24	A	825	CLA	C4A-NA-C1A	5.25	109.08	106.68
33	d	314	II0	C41-C42-C40	-5.25	112.78	123.52
24	B	809	CLA	C4A-NA-C1A	5.25	109.07	106.68
35	c	610	KC2	CHD-C4C-C3C	-5.24	108.26	125.91
35	j	312	KC2	CHB-C1B-NB	5.24	132.18	124.80
35	g	313	KC2	C1D-ND-C4D	5.24	109.99	106.31
27	J	102	WVN	C39-C36-C32	-5.24	119.93	127.28
27	M	101	WVN	C20-C23-C25	-5.24	118.48	126.23
27	F	204	WVN	C29-C26-C22	-5.24	119.93	127.28
35	g	313	KC2	CHB-C1B-NB	5.23	132.17	124.80
24	d	307	CLA	C4A-NA-C1A	5.23	109.06	106.68
35	g	312	KC2	O2D-CGD-CBD	5.21	120.34	111.23
34	k	618	IHT	C18-C22-C23	-5.21	118.53	126.23
35	i	616	KC2	CHC-C1C-NC	-5.21	116.16	124.23
35	g	314	KC2	CHB-C1B-NB	5.20	132.13	124.80
35	d	311	KC2	C1B-CHB-C4A	-5.20	114.96	126.02
35	i	609	KC2	CHD-C4C-C3C	-5.19	108.46	125.91
35	g	314	KC2	CHD-C4C-C3C	-5.18	108.46	125.91
34	c	615	IHT	C40-C37-C33	-5.18	120.01	127.28
33	a	317	II0	C31-C33-C35	-5.18	112.15	126.36
35	f	611	KC2	CHC-C1C-NC	-5.18	116.20	124.23
35	d	310	KC2	CHD-C4C-C3C	-5.17	108.50	125.91
27	L	206	WVN	C20-C23-C25	-5.17	118.59	126.23
24	k	605	CLA	C4A-NA-C1A	5.17	109.04	106.68
27	B	847	WVN	C35-C32-C31	5.17	125.98	118.09
24	b	304	CLA	C4A-NA-C1A	5.16	109.03	106.68
27	A	846	WVN	C39-C36-C32	-5.16	120.05	127.28
33	k	621	II0	C41-C39-C35	-5.16	120.05	127.28
34	O	203	IHT	C30-C27-C23	-5.16	120.05	127.28
35	d	311	KC2	CHB-C1B-NB	5.15	132.05	124.80
35	f	611	KC2	C4B-CHC-C1C	-5.15	115.08	126.02
27	L	206	WVN	C38-C34-C33	5.14	125.94	118.09
24	A	805	CLA	C4A-NA-C1A	5.13	109.02	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	304	CLA	C4A-NA-C1A	5.13	109.02	106.68
34	j	317	IHT	C40-C37-C33	-5.13	120.08	127.28
34	j	317	IHT	C02-C07-C10	-5.13	115.63	122.64
24	A	842	CLA	C4A-NA-C1A	5.13	109.02	106.68
35	k	611	KC2	O2D-CGD-CBD	5.13	120.19	111.23
24	B	804	CLA	CAC-C3C-C4C	5.12	131.45	124.79
35	k	612	KC2	C1A-C2A-C3A	-5.11	102.58	107.28
34	g	319	IHT	C09-C10-C07	-5.11	115.80	122.70
24	j	309	CLA	C4A-NA-C1A	5.10	109.01	106.68
35	d	310	KC2	CHB-C1B-NB	5.10	131.99	124.80
27	B	846	WVN	C40-C37-C34	-5.10	120.12	127.28
24	A	809	CLA	C4A-NA-C1A	5.10	109.01	106.68
27	A	849	WVN	C08-C01-C02	5.10	117.27	109.55
24	k	602	CLA	C4A-NA-C1A	5.10	109.00	106.68
33	k	617	II0	C16-C03-C09	-5.10	101.39	110.52
33	a	315	II0	C42-C40-C36	-5.09	120.13	127.28
34	b	317	IHT	C32-C33-C37	5.09	127.02	119.01
27	R	202	WVN	C30-C28-C25	-5.09	120.14	127.28
34	g	319	IHT	C40-C37-C33	-5.09	120.15	127.28
35	g	314	KC2	CMD-C2D-C1D	-5.09	117.68	125.42
34	O	203	IHT	C41-C38-C35	-5.08	120.15	127.28
35	e	609	KC2	CHB-C1B-NB	5.08	131.95	124.80
35	i	609	KC2	C4B-CHC-C1C	-5.07	115.25	126.02
24	f	604	CLA	C4A-NA-C1A	5.06	108.99	106.68
24	A	811	CLA	C4A-NA-C1A	5.06	108.99	106.68
24	L	202	CLA	C4A-NA-C1A	5.06	108.99	106.68
24	a	302	CLA	C4A-NA-C1A	5.05	108.98	106.68
26	g	321	LHG	O7-C7-C8	5.05	122.40	111.48
27	A	847	WVN	C19-C22-C26	5.04	126.94	119.01
24	B	820	CLA	C4A-NA-C1A	5.04	108.98	106.68
34	j	317	IHT	C18-C22-C23	-5.04	118.78	126.23
35	f	611	KC2	CHB-C1B-NB	5.04	131.89	124.80
35	i	616	KC2	C4B-CHC-C1C	-5.03	115.32	126.02
33	b	318	II0	C41-C39-C35	-5.03	120.22	127.28
35	j	312	KC2	C1A-C2A-C3A	-5.02	102.67	107.28
35	g	313	KC2	CHD-C4C-C3C	-5.01	109.04	125.91
35	e	609	KC2	CHB-C1B-C2B	-5.01	115.07	125.49
24	A	830	CLA	C4A-NA-C1A	5.01	108.96	106.68
35	i	609	KC2	CHB-C1B-NB	5.00	131.84	124.80
27	M	101	WVN	C39-C36-C32	-5.00	120.27	127.28
24	c	604	CLA	C4A-NA-C1A	5.00	108.96	106.68
24	f	609	CLA	C4A-NA-C1A	4.99	108.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	837	CLA	C4A-NA-C1A	4.99	108.95	106.68
34	c	615	IHT	C02-C07-C10	-4.98	115.83	122.64
24	A	841	CLA	C4A-NA-C1A	4.97	108.95	106.68
35	k	613	KC2	C3A-C4A-NA	4.97	116.60	110.45
35	g	314	KC2	CHC-C1C-NC	-4.97	116.53	124.23
35	e	609	KC2	CMD-C2D-C1D	-4.97	117.86	125.42
35	k	613	KC2	CHD-C4C-C3C	-4.97	109.19	125.91
34	R	204	IHT	C30-C27-C23	-4.96	120.31	127.28
24	i	602	CLA	C4A-NA-C1A	4.96	108.94	106.68
35	i	616	KC2	CMD-C2D-C1D	-4.96	117.86	125.42
24	j	305	CLA	C4A-NA-C1A	4.96	108.94	106.68
35	j	312	KC2	CMD-C2D-C1D	-4.96	117.87	125.42
35	j	312	KC2	CHB-C1B-C2B	-4.95	115.18	125.49
27	B	849	WVN	C30-C28-C25	-4.95	120.34	127.28
27	j	301	WVN	C39-C36-C32	-4.95	120.34	127.28
24	L	203	CLA	C4A-NA-C1A	4.94	108.94	106.68
24	A	820	CLA	C4A-NA-C1A	4.94	108.93	106.68
35	g	314	KC2	C4B-CHC-C1C	-4.94	115.53	126.02
27	B	845	WVN	C40-C37-C34	-4.93	120.36	127.28
33	b	315	II0	C32-C34-C36	-4.93	112.84	126.36
34	g	319	IHT	C18-C22-C23	-4.91	118.97	126.23
24	B	831	CLA	C4A-NA-C1A	4.91	108.92	106.68
35	c	610	KC2	C4B-CHC-C1C	-4.91	115.58	126.02
27	L	201	WVN	C39-C36-C32	-4.91	120.40	127.28
27	F	205	WVN	C30-C33-C34	-4.90	112.92	126.36
27	B	845	WVN	C02-C11-C19	4.90	132.21	124.58
33	k	615	II0	C19-C13-C09	-4.90	115.01	124.16
35	e	609	KC2	C1A-C2A-C3A	-4.89	102.78	107.28
24	b	307	CLA	C4A-NA-C1A	4.89	108.91	106.68
24	A	807	CLA	C4A-NA-C1A	4.88	108.91	106.68
35	c	610	KC2	CHC-C1C-NC	-4.88	116.67	124.23
27	L	205	WVN	C30-C28-C25	-4.88	120.44	127.28
24	k	608	CLA	C4A-NA-C1A	4.87	108.90	106.68
27	h	308	WVN	C39-C36-C32	-4.87	120.44	127.28
24	A	832	CLA	O2D-CGD-O1D	-4.87	114.36	123.85
35	g	313	KC2	CHB-C1B-C2B	-4.87	115.35	125.49
27	L	201	WVN	C02-C11-C19	-4.87	117.00	124.58
33	k	616	II0	C41-C42-C40	-4.87	113.56	123.52
34	b	317	IHT	C02-C07-C10	-4.87	115.98	122.64
35	k	611	KC2	CHB-C1B-NB	4.87	131.65	124.80
27	L	201	WVN	C29-C26-C22	-4.87	120.45	127.28
33	a	317	II0	C28-C26-C30	-4.87	114.73	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	846	WVN	C21-C15-C13	-4.86	119.18	124.48
35	d	311	KC2	CHD-C4C-C3C	-4.86	109.57	125.91
27	j	301	WVN	C40-C37-C34	-4.85	120.47	127.28
35	c	610	KC2	CHD-C1D-ND	-4.85	116.77	124.05
35	k	611	KC2	C1B-CHB-C4A	-4.85	115.71	126.02
27	F	204	WVN	C06-C13-C15	-4.85	116.01	122.64
35	j	312	KC2	C4B-C3B-C2B	-4.85	102.61	106.81
33	g	318	II0	C41-C39-C35	-4.84	120.48	127.28
34	b	317	IHT	C40-C41-C38	-4.84	113.61	123.52
35	c	610	KC2	CMD-C2D-C1D	-4.84	118.06	125.42
33	f	618	II0	C31-C33-C35	-4.84	113.10	126.36
35	g	314	KC2	CHD-C1D-ND	-4.83	116.80	124.05
35	g	313	KC2	CHD-C1D-ND	-4.83	116.80	124.05
27	M	101	WVN	C40-C37-C34	-4.83	120.50	127.28
33	i	614	II0	C41-C39-C35	-4.83	120.50	127.28
35	k	613	KC2	CHB-C1B-C2B	-4.83	115.44	125.49
24	A	801	CLA	C4A-NA-C1A	4.83	108.88	106.68
24	f	602	CLA	C4A-NA-C1A	4.83	108.88	106.68
24	B	839	CLA	C4A-NA-C1A	4.82	108.88	106.68
24	h	303	CLA	C4A-NA-C1A	4.82	108.88	106.68
27	A	850	WVN	C02-C11-C19	-4.82	117.08	124.58
24	A	834	CLA	C4A-NA-C1A	4.82	108.88	106.68
24	k	604	CLA	C4A-NA-C1A	4.81	108.88	106.68
35	g	312	KC2	CHD-C4C-C3C	-4.81	109.73	125.91
24	A	852	CLA	C4A-NA-C1A	4.80	108.87	106.68
33	k	617	II0	C41-C39-C35	-4.79	120.55	127.28
35	i	609	KC2	C3A-C4A-NA	4.79	116.38	110.45
24	A	822	CLA	C4A-NA-C1A	4.79	108.86	106.68
35	i	609	KC2	CHB-C1B-C2B	-4.79	115.53	125.49
24	B	813	CLA	C4A-NA-C1A	4.78	108.86	106.68
24	B	819	CLA	C4A-NA-C1A	4.78	108.86	106.68
35	d	310	KC2	CHC-C1C-NC	-4.78	116.82	124.23
27	B	846	WVN	C20-C23-C25	-4.78	119.16	126.23
24	K	102	CLA	C4A-NA-C1A	4.78	108.86	106.68
35	d	311	KC2	CHB-C1B-C2B	-4.78	115.54	125.49
24	h	302	CLA	C4A-NA-C1A	4.78	108.86	106.68
27	A	846	WVN	C40-C37-C34	-4.78	120.58	127.28
27	A	847	WVN	C31-C32-C36	4.77	126.52	119.01
24	A	856	CLA	CAA-C2A-C3A	-4.76	105.31	116.23
35	g	312	KC2	CHB-C1B-NB	4.76	131.50	124.80
24	A	840	CLA	C4A-NA-C1A	4.76	108.85	106.68
35	g	312	KC2	C3A-C4A-NA	4.76	116.34	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	617	IHT	C22-C23-C27	4.75	126.49	119.01
35	i	609	KC2	C1B-CHB-C4A	-4.75	115.92	126.02
35	f	611	KC2	C1B-CHB-C4A	-4.75	115.92	126.02
35	g	312	KC2	C4B-C3B-C2B	-4.75	102.70	106.81
35	k	612	KC2	C1B-CHB-C4A	-4.74	115.94	126.02
35	d	310	KC2	C1D-ND-C4D	4.74	109.64	106.31
33	i	614	II0	C42-C40-C36	-4.73	120.64	127.28
35	j	312	KC2	C1B-CHB-C4A	-4.73	115.97	126.02
33	h	310	II0	C42-C40-C36	-4.73	120.65	127.28
34	O	203	IHT	C02-C07-C10	-4.72	116.18	122.64
35	g	313	KC2	C1B-CHB-C4A	-4.72	115.98	126.02
35	e	609	KC2	CHC-C1C-NC	-4.72	116.92	124.23
33	a	313	II0	C20-C14-C10	-4.72	115.34	124.16
33	b	315	II0	C19-C13-C11	4.72	123.09	114.42
35	g	312	KC2	CMD-C2D-C1D	-4.71	118.24	125.42
35	e	609	KC2	C1B-CHB-C4A	-4.71	116.01	126.02
24	B	830	CLA	C4A-NA-C1A	4.71	108.83	106.68
35	g	313	KC2	C4B-CHC-C1C	-4.71	116.02	126.02
35	k	612	KC2	C4B-CHC-C1C	-4.70	116.02	126.02
34	k	618	IHT	C19-C10-C07	-4.69	119.36	124.48
33	J	104	II0	C42-C40-C36	-4.69	120.70	127.28
27	e	615	WVN	C04-C09-C05	-4.69	120.35	124.83
35	e	609	KC2	C1D-ND-C4D	4.69	109.60	106.31
24	f	605	CLA	C4A-NA-C1A	4.68	108.82	106.68
26	i	615	LHG	O7-C7-C8	4.68	121.61	111.48
35	f	611	KC2	CMD-C2D-C1D	-4.68	118.29	125.42
27	A	848	WVN	C21-C15-C13	-4.68	119.38	124.48
35	f	611	KC2	CHB-C1B-C2B	-4.68	115.76	125.49
24	A	837	CLA	C4A-NA-C1A	4.68	108.81	106.68
35	d	310	KC2	C4B-C3B-C2B	-4.68	102.76	106.81
33	g	320	II0	C41-C39-C35	-4.67	120.72	127.28
35	k	613	KC2	C4B-CHC-C1C	-4.67	116.08	126.02
24	A	815	CLA	CMB-C2B-C1B	-4.67	118.31	125.42
35	g	314	KC2	CHB-C1B-C2B	-4.67	115.77	125.49
24	B	835	CLA	C4A-NA-C1A	4.67	108.81	106.68
34	b	316	IHT	C19-C10-C07	-4.67	119.39	124.48
35	d	310	KC2	CHB-C1B-C2B	-4.66	115.79	125.49
26	f	619	LHG	O7-C7-C8	4.66	121.56	111.48
24	b	312	CLA	C4A-NA-C1A	4.65	108.80	106.68
24	B	811	CLA	C4A-NA-C1A	4.65	108.80	106.68
24	i	610	CLA	C4A-NA-C1A	-4.65	104.56	106.68
35	i	616	KC2	CHD-C1D-ND	-4.65	117.08	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	610	KC2	CHB-C1B-C2B	-4.64	115.84	125.49
26	b	302	LHG	O7-C7-C8	4.64	121.51	111.48
35	i	609	KC2	CHC-C1C-NC	-4.64	117.04	124.23
33	j	315	II0	C32-C34-C36	-4.63	113.66	126.36
27	J	102	WVN	C40-C37-C34	-4.62	120.80	127.28
33	J	104	II0	C32-C34-C36	-4.62	113.69	126.36
27	J	101	WVN	C21-C15-C13	-4.62	119.44	124.48
34	a	316	IHT	C19-C10-C07	-4.62	119.44	124.48
24	j	304	CLA	C4A-NA-C1A	4.62	108.79	106.68
35	j	312	KC2	C3A-C4A-NA	4.62	116.17	110.45
35	g	314	KC2	C1B-CHB-C4A	-4.62	116.21	126.02
35	k	611	KC2	C4B-C3B-C2B	-4.62	102.81	106.81
35	g	313	KC2	C3A-C4A-NA	4.60	116.14	110.45
35	f	611	KC2	C1D-ND-C4D	4.60	109.54	106.31
26	c	617	LHG	O7-C7-C8	4.60	121.43	111.48
33	g	320	II0	C42-C40-C36	-4.60	120.83	127.28
27	F	204	WVN	C26-C29-C31	-4.59	109.90	123.20
35	k	613	KC2	C1D-ND-C4D	4.59	109.53	106.31
35	g	312	KC2	CHB-C1B-C2B	-4.58	115.95	125.49
33	c	616	II0	C42-C40-C36	-4.58	120.85	127.28
35	k	611	KC2	CHC-C1C-NC	-4.58	117.13	124.23
27	A	847	WVN	C04-C09-C05	-4.57	120.47	124.83
35	d	310	KC2	CMD-C2D-C1D	-4.57	118.46	125.42
35	d	311	KC2	CHD-C1D-ND	-4.57	117.19	124.05
35	g	312	KC2	CHC-C1C-NC	-4.56	117.16	124.23
26	A	845	LHG	O7-C7-C8	4.56	121.35	111.48
24	A	828	CLA	C1-C2-C3	-4.56	118.73	126.20
24	A	827	CLA	C4A-NA-C1A	4.56	108.76	106.68
24	A	836	CLA	CAA-CBA-CGA	-4.55	100.28	113.21
33	k	617	II0	C05-C03-C09	4.55	118.46	109.49
24	B	836	CLA	C4A-NA-C1A	4.55	108.75	106.68
24	B	808	CLA	C4A-NA-C1A	4.55	108.75	106.68
27	B	845	WVN	C39-C40-C37	-4.55	114.21	123.52
27	F	205	WVN	C23-C25-C28	4.55	126.16	119.01
33	f	618	II0	C06-C04-C10	4.55	118.45	109.49
33	i	613	II0	C41-C39-C35	-4.55	120.90	127.28
35	k	611	KC2	C1D-ND-C4D	4.55	109.50	106.31
35	d	310	KC2	C1B-CHB-C4A	-4.54	116.37	126.02
24	c	606	CLA	C4A-NA-C1A	4.54	108.75	106.68
24	B	816	CLA	C4A-NA-C1A	4.54	108.75	106.68
27	K	103	WVN	C04-C09-C05	-4.53	120.50	124.83
27	e	615	WVN	C21-C15-C13	-4.53	119.54	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	609	KC2	C4B-C3B-C2B	-4.52	102.89	106.81
24	B	818	CLA	CMB-C2B-C1B	-4.51	118.55	125.42
28	A	851	LMT	C3'-C4'-C5'	-4.51	100.94	110.93
35	d	310	KC2	C3A-C4A-NA	4.50	116.02	110.45
35	k	613	KC2	C1B-CHB-C4A	-4.49	116.47	126.02
33	a	317	II0	C34-C36-C40	4.49	126.07	119.01
27	A	848	WVN	C40-C37-C34	-4.49	120.98	127.28
35	c	610	KC2	C1B-CHB-C4A	-4.49	116.48	126.02
35	c	610	KC2	C3A-C4A-NA	4.48	116.00	110.45
35	g	314	KC2	C3A-C4A-NA	4.47	115.99	110.45
24	k	603	CLA	O2D-CGD-CBD	4.47	119.05	111.23
34	f	617	IHT	C36-C33-C37	-4.47	115.58	122.82
33	i	614	II0	C05-C03-C09	4.47	118.29	109.49
32	b	301	LMG	O7-C10-C11	4.47	121.14	111.48
24	A	838	CLA	C4A-NA-C1A	4.46	108.72	106.68
24	k	606	CLA	C4A-NA-C1A	4.46	108.71	106.68
35	k	611	KC2	CHB-C1B-C2B	-4.46	116.22	125.49
35	d	311	KC2	CHC-C1C-NC	-4.45	117.33	124.23
35	i	616	KC2	CHB-C1B-C2B	-4.45	116.24	125.49
27	R	201	WVN	C39-C36-C32	-4.45	121.04	127.28
35	j	312	KC2	C1D-ND-C4D	4.44	109.43	106.31
24	i	604	CLA	CAA-CBA-CGA	-4.44	100.60	113.21
35	f	611	KC2	C3A-C4A-NA	4.44	115.94	110.45
24	i	605	CLA	C4A-NA-C1A	4.44	108.70	106.68
24	k	603	CLA	CAA-C2A-C3A	-4.43	101.02	113.00
27	J	101	WVN	C40-C37-C34	-4.43	121.06	127.28
35	j	312	KC2	CHC-C1C-NC	-4.43	117.37	124.23
24	B	832	CLA	C4A-NA-C1A	4.43	108.70	106.68
35	i	609	KC2	CMD-C2D-C1D	-4.42	118.69	125.42
27	K	103	WVN	C06-C13-C15	-4.42	116.60	122.64
24	B	828	CLA	C4A-NA-C1A	4.41	108.69	106.68
34	j	317	IHT	C19-C10-C07	-4.41	119.67	124.48
24	L	207	CLA	C4A-NA-C1A	4.40	108.69	106.68
35	f	611	KC2	O2D-CGD-CBD	4.39	118.91	111.23
33	O	202	II0	C20-C14-C10	-4.39	115.95	124.16
33	f	616	II0	C41-C39-C35	-4.39	121.12	127.28
35	i	616	KC2	C1D-ND-C4D	4.39	109.39	106.31
24	e	605	CLA	C4A-NA-C1A	4.38	108.68	106.68
27	B	845	WVN	C19-C22-C26	-4.38	112.12	119.01
33	f	614	II0	C19-C13-C09	-4.38	115.98	124.16
26	j	319	LHG	O7-C7-C8	4.38	120.95	111.48
33	g	317	II0	C42-C40-C36	-4.37	121.15	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	305	CLA	C4A-NA-C1A	4.37	108.67	106.68
34	b	317	IHT	C27-C30-C32	-4.37	110.55	123.20
33	O	202	II0	C31-C33-C35	-4.35	114.43	126.36
27	K	103	WVN	C40-C37-C34	-4.34	121.19	127.28
27	B	845	WVN	C39-C36-C32	-4.34	121.20	127.28
33	f	614	II0	C42-C40-C36	-4.33	121.20	127.28
24	A	802	CLA	C4A-NA-C1A	4.32	108.65	106.68
33	d	315	II0	C32-C34-C36	-4.31	114.53	126.36
35	c	610	KC2	C1D-ND-C4D	4.31	109.34	106.31
24	e	607	CLA	C4A-NA-C1A	4.31	108.65	106.68
27	A	847	WVN	C20-C23-C25	-4.31	119.86	126.23
24	c	608	CLA	C4A-NA-C1A	4.31	108.64	106.68
24	k	607	CLA	C1-C2-C3	-4.31	119.14	126.20
24	a	307	CLA	C4A-NA-C1A	4.30	108.64	106.68
27	A	847	WVN	C21-C15-C13	-4.30	119.79	124.48
24	c	602	CLA	O2D-CGD-O1D	-4.29	115.50	123.85
24	B	837	CLA	O2D-CGD-O1D	-4.29	115.50	123.85
35	k	612	KC2	CHB-C1B-NB	4.29	130.84	124.80
34	k	618	IHT	C09-C10-C07	-4.29	116.91	122.70
26	a	301	LHG	O7-C7-C8	4.28	120.75	111.48
27	j	301	WVN	C30-C28-C25	-4.28	121.28	127.28
24	j	303	CLA	C4A-NA-C1A	4.27	108.63	106.68
35	d	311	KC2	C4B-C3B-C2B	-4.27	103.11	106.81
27	B	845	WVN	C11-C19-C22	4.27	135.51	126.32
35	k	612	KC2	CHD-C4C-C3C	-4.27	111.54	125.91
35	i	609	KC2	C4B-C3B-C2B	-4.27	103.11	106.81
34	R	204	IHT	C18-C22-C23	-4.27	119.92	126.23
35	k	613	KC2	CMD-C2D-C1D	-4.26	118.93	125.42
34	g	319	IHT	C41-C38-C35	-4.26	121.31	127.28
33	i	613	II0	C20-C14-C10	-4.25	116.21	124.16
27	e	615	WVN	C29-C26-C22	-4.25	121.32	127.28
33	g	320	II0	C32-C34-C36	-4.25	114.71	126.36
24	A	853	CLA	C4A-NA-C1A	4.25	108.62	106.68
33	k	619	II0	C31-C33-C35	-4.25	114.72	126.36
34	R	204	IHT	C09-C10-C07	-4.24	116.97	122.70
35	i	616	KC2	C1B-CHB-C4A	-4.23	117.02	126.02
33	h	310	II0	C19-C13-C11	4.23	122.20	114.42
34	c	615	IHT	C09-C10-C07	-4.23	116.99	122.70
27	A	850	WVN	C30-C33-C34	-4.22	114.78	126.36
24	k	609	CLA	C4A-NA-C1A	4.22	108.61	106.68
35	c	610	KC2	C4B-C3B-C2B	-4.22	103.15	106.81
27	A	850	WVN	C04-C09-C05	-4.21	120.81	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	810	CLA	C4A-NA-C1A	4.20	108.60	106.68
24	d	312	CLA	C4A-NA-C1A	4.20	108.59	106.68
32	F	206	LMG	O7-C10-C11	4.19	120.55	111.48
27	J	102	WVN	C02-C11-C19	-4.19	118.05	124.58
27	J	101	WVN	C02-C11-C19	-4.18	118.07	124.58
24	g	303	CLA	C4A-NA-C1A	4.18	108.59	106.68
35	e	609	KC2	C3A-C4A-NA	4.18	115.62	110.45
26	d	316	LHG	O7-C7-C8	4.17	120.51	111.48
27	L	201	WVN	C08-C01-C02	-4.17	103.23	109.55
24	i	608	CLA	C4A-NA-C1A	4.17	108.58	106.68
24	A	823	CLA	C4A-NA-C1A	4.17	108.58	106.68
35	j	312	KC2	CHD-C1D-ND	-4.16	117.80	124.05
27	M	101	WVN	C30-C28-C25	-4.16	121.44	127.28
32	L	208	LMG	O7-C10-C11	4.16	120.47	111.48
35	j	312	KC2	O2D-CGD-O1D	-4.15	115.76	123.85
35	f	611	KC2	C4B-C3B-C2B	-4.15	103.21	106.81
33	c	613	II0	C42-C40-C36	-4.15	121.46	127.28
33	k	616	II0	C41-C39-C35	-4.15	121.46	127.28
35	k	612	KC2	C4B-C3B-C2B	-4.15	103.22	106.81
35	d	310	KC2	CHD-C1D-ND	-4.14	117.84	124.05
24	A	820	CLA	CMB-C2B-C1B	-4.14	119.12	125.42
33	e	613	II0	C41-C39-C35	-4.13	121.48	127.28
35	k	612	KC2	CHB-C1B-C2B	-4.13	116.90	125.49
35	g	314	KC2	C1D-ND-C4D	4.13	109.21	106.31
33	f	616	II0	C20-C14-C12	4.12	122.00	114.42
24	i	606	CLA	C4A-NA-C1A	4.11	108.56	106.68
33	c	616	II0	C32-C34-C36	-4.11	115.09	126.36
27	A	850	WVN	C40-C37-C34	-4.11	121.52	127.28
26	e	617	LHG	O7-C7-C8	4.11	120.36	111.48
27	I	101	WVN	C29-C26-C22	-4.11	121.52	127.28
24	g	307	CLA	C4A-NA-C1A	4.10	108.55	106.68
27	B	846	WVN	C40-C39-C36	-4.10	115.13	123.52
24	A	853	CLA	C1-C2-C3	-4.10	119.48	126.20
24	b	304	CLA	O2D-CGD-CBD	4.10	118.39	111.23
27	B	847	WVN	C40-C37-C34	-4.10	121.53	127.28
24	A	855	CLA	O2D-CGD-CBD	4.10	118.39	111.23
24	f	613	CLA	C4A-NA-C1A	4.09	108.55	106.68
33	b	318	II0	C20-C14-C10	-4.09	116.51	124.16
35	k	611	KC2	O2D-CGD-O1D	-4.08	115.90	123.85
24	A	817	CLA	C4A-NA-C1A	4.07	108.54	106.68
24	A	832	CLA	O2D-CGD-CBD	4.07	118.34	111.23
33	a	313	II0	C42-C40-C36	-4.07	121.57	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	609	KC2	CHB-C4A-NA	4.07	130.53	124.23
33	j	316	II0	C41-C42-C40	-4.06	115.21	123.52
27	A	847	WVN	C24-C22-C26	-4.06	116.24	122.82
27	j	301	WVN	C21-C15-C13	-4.06	120.06	124.48
24	j	314	CLA	C4A-NA-C1A	4.06	108.53	106.68
33	g	316	II0	C42-C40-C36	-4.05	121.60	127.28
35	k	611	KC2	C3A-C4A-NA	4.05	115.46	110.45
35	d	311	KC2	C3A-C4A-NA	4.04	115.45	110.45
33	k	619	II0	C20-C14-C12	4.04	121.85	114.42
27	L	205	WVN	C01-C02-C11	-4.04	108.18	112.83
27	F	205	WVN	C21-C15-C13	-4.03	120.08	124.48
24	g	310	CLA	C4A-NA-C1A	4.03	108.52	106.68
24	j	311	CLA	C4A-NA-C1A	4.03	108.52	106.68
24	A	816	CLA	C4A-NA-C1A	4.02	108.52	106.68
33	h	310	II0	C20-C14-C12	4.02	121.82	114.42
33	b	315	II0	C21-C23-C25	-4.02	162.56	176.23
33	k	615	II0	C31-C33-C35	-4.02	115.34	126.36
33	j	318	II0	C31-C33-C35	-4.02	115.34	126.36
33	e	616	II0	C42-C40-C36	-4.02	121.65	127.28
33	k	619	II0	C42-C40-C36	-4.01	121.65	127.28
35	k	611	KC2	CHD-C1D-ND	-4.01	118.03	124.05
27	L	201	WVN	C21-C15-C13	-4.01	120.11	124.48
26	A	844	LHG	O7-C7-C8	4.01	120.16	111.48
24	d	308	CLA	C4A-NA-C1A	4.01	108.51	106.68
27	e	615	WVN	C20-C23-C25	-4.01	120.30	126.23
27	J	101	WVN	C04-C09-C05	-4.01	121.00	124.83
33	e	613	II0	C22-C24-C26	-4.01	162.61	176.23
24	h	312	CLA	CMB-C2B-C1B	-4.00	119.32	125.42
35	i	616	KC2	C3A-C4A-NA	4.00	115.40	110.45
24	k	603	CLA	O2D-CGD-O1D	-4.00	116.06	123.85
27	I	101	WVN	C06-C13-C15	-4.00	117.17	122.64
33	c	613	II0	C19-C13-C09	-4.00	116.69	124.16
33	g	318	II0	C42-C40-C36	-3.99	121.68	127.28
24	J	103	CLA	C4A-NA-C1A	3.99	108.50	106.68
24	B	821	CLA	C4A-NA-C1A	3.98	108.50	106.68
35	g	312	KC2	C1B-CHB-C4A	-3.98	117.56	126.02
24	g	308	CLA	C4A-NA-C1A	3.97	108.49	106.68
24	A	805	CLA	CAA-C2A-C3A	-3.97	102.27	113.00
26	k	620	LHG	O7-C7-C8	3.97	120.07	111.48
24	A	830	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
24	k	610	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
27	L	201	WVN	C30-C28-C25	-3.95	121.73	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	612	KC2	CHC-C1C-NC	-3.95	118.11	124.23
33	f	618	II0	C41-C42-C40	-3.95	115.44	123.52
33	a	314	II0	C19-C13-C11	3.94	121.67	114.42
27	R	202	WVN	C20-C23-C25	-3.93	120.42	126.23
33	e	616	II0	C41-C39-C35	-3.93	121.76	127.28
26	b	320	LHG	O7-C7-C8	3.93	119.98	111.48
35	i	616	KC2	O2D-CGD-CBD	3.93	118.09	111.23
24	f	608	CLA	C4A-NA-C1A	3.93	108.47	106.68
35	f	611	KC2	CHD-C1D-ND	-3.92	118.17	124.05
24	A	855	CLA	C4A-NA-C1A	3.91	108.47	106.68
35	k	612	KC2	C3A-C4A-NA	3.91	115.29	110.45
24	i	611	CLA	C4A-NA-C1A	3.91	108.46	106.68
24	A	855	CLA	O2D-CGD-O1D	-3.91	116.24	123.85
27	B	845	WVN	C30-C28-C25	-3.90	121.80	127.28
26	f	620	LHG	O7-C7-C8	3.90	119.92	111.48
33	b	315	II0	C20-C14-C12	3.90	121.59	114.42
33	g	318	II0	C20-C14-C10	-3.90	116.88	124.16
24	A	842	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
24	B	838	CLA	C4A-NA-C1A	3.89	108.45	106.68
35	g	313	KC2	C4B-C3B-C2B	-3.89	103.44	106.81
35	f	611	KC2	CHB-C4A-NA	3.88	130.25	124.23
34	a	316	IHT	C29-C31-C34	-3.88	111.95	123.20
26	g	301	LHG	O7-C7-C8	3.87	119.85	111.48
26	J	107	LHG	O7-C7-C8	3.87	119.85	111.48
24	A	837	CLA	CAA-CBA-CGA	-3.87	102.22	113.21
24	b	304	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
24	A	814	CLA	C4A-NA-C1A	3.86	108.44	106.68
27	L	205	WVN	C06-C13-C15	-3.86	117.36	122.64
27	A	849	WVN	C39-C36-C32	-3.85	121.87	127.28
34	b	317	IHT	C36-C33-C37	-3.85	116.58	122.82
24	A	837	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
27	F	204	WVN	C21-C15-C13	-3.84	120.29	124.48
35	g	313	KC2	CMD-C2D-C1D	-3.84	119.58	125.42
33	k	615	II0	C37-C35-C33	-3.84	112.23	118.09
33	j	318	II0	C41-C42-C40	-3.83	115.67	123.52
24	i	607	CLA	C4A-NA-C1A	3.83	108.43	106.68
33	e	613	II0	C19-C13-C11	3.83	121.46	114.42
24	e	608	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
27	M	101	WVN	C11-C19-C22	-3.82	118.10	126.32
33	g	317	II0	C19-C13-C11	3.82	121.45	114.42
24	O	205	CLA	C1D-ND-C4D	-3.82	103.63	106.31
34	O	203	IHT	C09-C10-C07	-3.82	117.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	618	LHG	O7-C7-C8	3.82	119.74	111.48
33	k	617	II0	C19-C13-C11	3.81	121.43	114.42
27	A	849	WVN	C06-C13-C20	3.81	125.99	115.65
24	A	829	CLA	C4A-NA-C1A	3.81	108.42	106.68
24	A	817	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
33	c	613	II0	C41-C42-C40	-3.81	115.72	123.52
24	A	834	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
35	f	611	KC2	C2A-C1A-NA	3.81	115.44	109.34
24	b	309	CLA	C4A-NA-C1A	3.81	108.42	106.68
33	i	612	II0	C41-C39-C35	-3.81	121.94	127.28
35	g	312	KC2	CHB-C4A-NA	3.81	130.13	124.23
33	j	318	II0	C20-C14-C10	-3.81	117.05	124.16
24	j	302	CLA	C4A-NA-C1A	3.80	108.41	106.68
24	A	835	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
24	B	805	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
24	a	303	CLA	C4A-NA-C1A	3.80	108.41	106.68
27	B	849	WVN	C26-C29-C31	-3.80	112.20	123.20
33	f	615	II0	C42-C40-C36	-3.79	121.96	127.28
24	i	602	CLA	O2D-CGD-CBD	3.79	117.86	111.23
33	h	309	II0	C41-C39-C35	-3.79	121.96	127.28
27	B	846	WVN	C30-C28-C25	-3.79	121.96	127.28
24	A	816	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
24	F	202	CLA	O2D-CGD-O1D	-3.79	116.48	123.85
33	i	613	II0	C42-C40-C36	-3.79	121.97	127.28
35	k	611	KC2	CMD-C2D-C3D	3.78	137.60	125.67
35	k	613	KC2	O2D-CGD-CBD	3.78	117.84	111.23
24	a	311	CLA	CBC-CAC-C3C	3.78	122.67	112.42
35	i	609	KC2	CHD-C1D-ND	-3.78	118.38	124.05
24	A	802	CLA	C1-C2-C3	-3.78	120.01	126.20
35	k	612	KC2	CMD-C2D-C3D	3.77	137.57	125.67
24	A	811	CLA	C1-C2-C3	-3.77	120.02	126.20
24	A	807	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
24	B	801	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
24	B	837	CLA	O2D-CGD-CBD	3.76	117.81	111.23
24	A	814	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
33	k	619	II0	C16-C03-C09	-3.76	103.78	110.52
24	h	306	CLA	C4A-NA-C1A	3.76	108.39	106.68
27	K	103	WVN	C39-C36-C32	-3.75	122.01	127.28
35	c	610	KC2	O2D-CGD-CBD	3.75	117.79	111.23
24	a	311	CLA	C2A-C1A-CHA	3.75	130.38	123.87
24	j	313	CLA	C4A-NA-C1A	-3.75	104.97	106.68
33	e	616	II0	C19-C13-C11	3.74	121.30	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	849	WVN	C29-C26-C22	-3.74	122.03	127.28
32	F	206	LMG	C8-O7-C10	-3.74	108.86	117.80
24	B	828	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
35	k	612	KC2	CHB-C4A-NA	3.73	130.02	124.23
24	A	822	CLA	C3B-C4B-NB	-3.73	107.20	110.53
33	j	315	II0	C29-C31-C33	-3.73	112.40	123.20
24	h	312	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
24	A	803	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
33	g	316	II0	C19-C13-C09	-3.72	117.20	124.16
27	L	206	WVN	C01-C02-C11	-3.72	108.55	112.83
24	A	834	CLA	CMB-C2B-C1B	-3.71	119.77	125.42
27	A	850	WVN	C40-C39-C36	-3.71	115.93	123.52
35	i	616	KC2	C4B-C3B-C2B	-3.71	103.60	106.81
27	I	101	WVN	C04-C09-C05	-3.71	121.29	124.83
34	a	316	IHT	C09-C10-C07	-3.70	117.70	122.70
24	B	807	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
33	g	320	II0	C20-C14-C10	-3.70	117.24	124.16
24	B	827	CLA	C4A-NA-C1A	3.70	108.37	106.68
24	j	310	CLA	C4A-NA-C1A	3.70	108.36	106.68
27	B	847	WVN	C21-C15-C13	-3.69	120.45	124.48
24	B	803	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
33	h	311	II0	C42-C40-C36	-3.69	122.10	127.28
33	b	315	II0	C31-C29-C25	-3.69	116.28	126.61
35	d	311	KC2	C1D-ND-C4D	3.69	108.90	106.31
24	a	305	CLA	C4A-NA-C1A	3.69	108.36	106.68
24	A	821	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
24	L	202	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
24	K	101	CLA	C1-C2-C3	-3.68	120.16	126.20
24	g	311	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
24	B	839	CLA	CAA-C2A-C3A	-3.68	103.05	113.00
33	g	316	II0	C41-C42-C40	-3.68	115.99	123.52
27	J	102	WVN	C21-C15-C13	-3.67	120.48	124.48
32	L	208	LMG	C4-C3-C2	3.67	117.27	110.83
27	F	205	WVN	C33-C34-C37	3.67	124.78	119.01
33	J	104	II0	C20-C14-C12	3.67	121.16	114.42
24	a	303	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
27	F	205	WVN	C29-C26-C22	-3.66	122.15	127.28
33	j	315	II0	C20-C14-C10	-3.66	117.32	124.16
35	d	311	KC2	CMD-C2D-C3D	3.66	137.20	125.67
34	b	316	IHT	C09-C10-C07	-3.65	117.77	122.70
33	b	314	II0	C19-C13-C09	-3.65	117.33	124.16
24	A	814	CLA	CMB-C2B-C1B	-3.64	119.87	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	615	IHT	C19-C10-C07	-3.64	120.51	124.48
24	A	827	CLA	CMB-C2B-C1B	-3.64	119.88	125.42
27	L	206	WVN	C24-C22-C19	3.63	123.64	118.09
35	d	311	KC2	O2D-CGD-O1D	-3.63	116.78	123.85
24	h	312	CLA	C4A-NA-C1A	3.63	108.33	106.68
35	e	609	KC2	CHD-C1D-ND	-3.63	118.61	124.05
33	a	317	II0	C05-C03-C09	3.63	116.64	109.49
24	j	304	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
24	k	607	CLA	C4A-NA-C1A	3.63	108.33	106.68
24	A	818	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
25	B	842	PQN	C11-C12-C13	-3.62	120.59	126.83
24	e	607	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
24	A	818	CLA	C1-C2-C3	-3.62	120.27	126.20
24	B	836	CLA	CAC-C3C-C2C	-3.61	120.92	127.56
34	b	317	IHT	C19-C10-C07	-3.61	120.54	124.48
24	I	102	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
27	e	615	WVN	C39-C36-C32	-3.61	122.22	127.28
24	B	823	CLA	C4A-NA-C1A	3.61	108.32	106.68
27	B	849	WVN	C40-C37-C34	-3.61	122.22	127.28
26	B	802	LHG	O7-C7-C8	3.61	119.28	111.48
27	A	846	WVN	C23-C25-C28	3.60	124.68	119.01
34	b	317	IHT	C09-C10-C07	-3.60	117.84	122.70
27	R	202	WVN	C06-C13-C15	-3.60	117.72	122.64
35	g	314	KC2	C4B-C3B-C2B	-3.59	103.70	106.81
35	k	613	KC2	C4B-C3B-C2B	-3.59	103.70	106.81
24	J	105	CLA	C3B-C4B-NB	-3.59	107.33	110.53
33	J	104	II0	C31-C33-C35	-3.59	116.53	126.36
24	A	804	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
33	i	612	II0	C19-C13-C11	3.58	121.01	114.42
24	O	205	CLA	O2A-CGA-O1A	-3.58	114.66	123.63
27	F	205	WVN	C35-C32-C31	3.58	123.56	118.09
35	e	609	KC2	CMD-C2D-C3D	3.58	136.97	125.67
26	A	844	LHG	O8-C23-C24	3.58	122.75	111.83
24	A	811	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
33	d	313	II0	C19-C13-C11	3.57	120.99	114.42
35	i	616	KC2	C2A-C1A-NA	3.57	115.07	109.34
24	d	312	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
34	R	204	IHT	C02-C07-C10	-3.57	117.76	122.64
33	i	612	II0	C30-C32-C34	-3.57	112.86	123.20
27	R	201	WVN	C40-C37-C34	-3.57	122.27	127.28
24	A	853	CLA	C3B-C4B-NB	-3.57	107.34	110.53
33	b	315	II0	C37-C35-C33	3.57	123.54	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	606	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
27	B	847	WVN	C29-C26-C22	-3.56	122.28	127.28
24	B	840	CLA	CMB-C2B-C1B	-3.56	119.99	125.42
24	B	826	CLA	C4A-NA-C1A	3.56	108.30	106.68
33	g	318	II0	C30-C32-C34	-3.56	112.89	123.20
24	b	307	CLA	CMB-C2B-C1B	-3.55	120.01	125.42
35	i	609	KC2	CHB-C4A-NA	3.55	129.74	124.23
35	i	616	KC2	CBC-CAC-C3C	-3.55	109.80	127.53
24	g	302	CLA	CMB-C2B-C1B	-3.55	120.02	125.42
27	F	204	WVN	C23-C20-C13	-3.55	117.53	127.00
27	J	101	WVN	C23-C20-C13	-3.55	117.53	127.00
24	i	602	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
24	L	203	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
34	c	615	IHT	C18-C22-C23	-3.53	121.01	126.23
27	R	202	WVN	C40-C37-C34	-3.53	122.32	127.28
24	j	306	CLA	C2A-C1A-CHA	3.53	130.00	123.87
35	j	312	KC2	CHB-C4A-NA	3.53	129.71	124.23
24	B	822	CLA	C4-C3-C5	3.53	121.36	115.23
24	j	306	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
35	c	610	KC2	CBC-CAC-C3C	-3.53	109.89	127.53
24	A	840	CLA	CMB-C2B-C1B	-3.53	120.05	125.42
27	A	847	WVN	C29-C31-C32	3.53	136.03	126.36
24	B	819	CLA	CMB-C2B-C1B	-3.52	120.05	125.42
33	h	310	II0	C42-C41-C39	-3.52	116.31	123.52
27	h	308	WVN	C40-C37-C34	-3.52	122.34	127.28
33	d	314	II0	C19-C13-C11	3.52	120.90	114.42
33	h	311	II0	C18-C04-C17	-3.52	98.55	108.63
24	A	818	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
35	g	314	KC2	O2D-CGD-O1D	-3.52	116.99	123.85
33	c	614	II0	C29-C31-C33	-3.52	113.01	123.20
24	k	609	CLA	CHB-C4A-NA	3.52	129.47	124.40
33	d	315	II0	C19-C13-C09	-3.52	117.59	124.16
27	A	849	WVN	C23-C25-C28	3.52	124.54	119.01
24	A	827	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
33	b	315	II0	C32-C30-C26	-3.51	116.78	126.61
33	f	618	II0	C20-C14-C12	3.51	120.88	114.42
35	d	310	KC2	O2D-CGD-CBD	3.51	117.37	111.23
24	A	816	CLA	CMB-C2B-C1B	-3.51	120.07	125.42
35	d	311	KC2	C1D-CHD-C4C	-3.51	118.00	126.25
24	A	856	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
27	B	846	WVN	C26-C29-C31	-3.50	113.06	123.20
24	e	604	CLA	O2D-CGD-O1D	-3.50	117.04	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	822	CLA	C4-C3-C2	-3.50	114.65	123.63
34	O	203	IHT	C19-C10-C07	-3.49	120.67	124.48
24	B	823	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
24	R	203	CLA	C1-C2-C3	-3.49	120.47	126.20
27	L	205	WVN	C27-C25-C28	-3.49	117.16	122.82
33	k	619	II0	C32-C34-C36	-3.49	116.79	126.36
27	R	202	WVN	C21-C15-C13	-3.49	120.68	124.48
27	R	202	WVN	C03-C04-C09	-3.49	106.22	112.07
24	B	808	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
33	d	314	II0	C20-C14-C12	3.48	120.83	114.42
24	f	612	CLA	C4A-NA-C1A	-3.48	105.09	106.68
24	g	304	CLA	CMB-C2B-C1B	-3.48	120.12	125.42
27	B	848	WVN	C40-C39-C36	-3.48	116.39	123.52
35	c	610	KC2	CMD-C2D-C3D	3.48	136.65	125.67
35	d	310	KC2	CHB-C4A-NA	3.48	129.63	124.23
24	A	838	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
24	k	610	CLA	O2D-CGD-CBD	3.48	117.31	111.23
24	J	103	CLA	CMB-C2B-C1B	-3.48	120.13	125.42
35	g	313	KC2	CHB-C4A-NA	3.48	129.62	124.23
35	k	612	KC2	CAC-C3C-C4C	3.47	139.75	124.39
24	A	829	CLA	O2D-CGD-O1D	-3.47	117.08	123.85
27	A	848	WVN	C39-C40-C37	-3.47	116.41	123.52
35	j	312	KC2	CMD-C2D-C3D	3.47	136.61	125.67
27	F	205	WVN	C04-C09-C05	-3.47	121.52	124.83
24	B	820	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
24	e	604	CLA	C1-C2-C3	-3.47	120.52	126.20
35	k	611	KC2	CBC-CAC-C3C	-3.46	110.22	127.53
35	g	314	KC2	C2A-C1A-NA	3.46	114.89	109.34
24	B	814	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
26	A	845	LHG	O8-C23-C24	3.45	121.64	111.15
27	L	205	WVN	C14-C15-C13	-3.45	118.04	122.70
27	e	615	WVN	C40-C37-C34	-3.45	122.44	127.28
24	a	309	CLA	C4A-NA-C1A	3.45	108.25	106.68
35	g	314	KC2	CMD-C2D-C3D	3.45	136.55	125.67
34	g	319	IHT	C30-C27-C23	-3.45	122.44	127.28
33	c	616	II0	C41-C39-C35	-3.45	122.44	127.28
35	i	616	KC2	CMD-C2D-C3D	3.44	136.53	125.67
34	b	316	IHT	C18-C22-C23	-3.44	121.14	126.23
24	A	838	CLA	C1-C2-C3	-3.44	120.56	126.20
34	a	316	IHT	C02-C07-C10	-3.44	117.94	122.64
24	c	611	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
34	g	319	IHT	C41-C40-C37	-3.44	116.48	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	322	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
24	c	602	CLA	C4A-NA-C1A	3.43	108.25	106.68
24	g	308	CLA	CMB-C2B-C1B	-3.43	120.19	125.42
24	f	602	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
35	k	611	KC2	CHB-C4A-NA	3.43	129.55	124.23
24	b	303	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
27	A	847	WVN	C30-C33-C34	-3.43	116.96	126.36
27	M	101	WVN	C14-C15-C13	-3.43	118.07	122.70
33	i	614	II0	C15-C03-C09	-3.43	104.38	110.52
33	d	314	II0	C20-C14-C10	-3.43	117.75	124.16
35	d	310	KC2	CBC-CAC-C3C	-3.43	110.41	127.53
35	f	611	KC2	CMD-C2D-C3D	3.43	136.47	125.67
27	K	103	WVN	C26-C29-C31	-3.42	113.28	123.20
24	A	825	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
24	B	801	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
33	f	615	II0	C41-C42-C40	-3.42	116.52	123.52
27	F	204	WVN	C01-C02-C11	-3.42	108.89	112.83
35	c	610	KC2	C2A-C1A-NA	3.42	114.82	109.34
33	d	314	II0	C42-C40-C36	-3.42	122.48	127.28
34	R	204	IHT	C40-C41-C38	-3.42	116.53	123.52
33	O	202	II0	C41-C39-C35	-3.41	122.49	127.28
24	A	856	CLA	CHB-C4A-NA	3.41	129.32	124.40
24	B	834	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
33	k	619	II0	C06-C04-C10	3.41	116.21	109.49
24	e	611	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
24	e	611	CLA	C1-C2-C3	-3.41	120.61	126.20
35	e	609	KC2	C1D-CHD-C4C	-3.40	118.25	126.25
24	A	803	CLA	CMB-C2B-C1B	-3.39	120.25	125.42
24	B	804	CLA	CBC-CAC-C3C	3.39	121.62	112.42
27	B	845	WVN	C07-C01-C02	3.39	114.69	109.55
24	b	313	CLA	C4A-NA-C1A	3.39	108.23	106.68
24	c	602	CLA	O2D-CGD-CBD	3.39	117.16	111.23
24	B	816	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
24	A	818	CLA	C4A-NA-C1A	3.39	108.23	106.68
33	a	315	II0	C41-C39-C35	-3.39	122.53	127.28
33	k	619	II0	C19-C13-C11	3.39	120.65	114.42
24	B	832	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
33	k	621	II0	C32-C34-C36	-3.39	117.08	126.36
27	L	206	WVN	C30-C33-C34	3.39	135.65	126.36
24	c	605	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
24	B	823	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
32	L	208	LMG	C8-O7-C10	-3.38	109.70	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	845	WVN	C26-C29-C31	-3.38	113.40	123.20
24	i	603	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
24	B	826	CLA	CMB-C2B-C1B	-3.38	120.28	125.42
24	B	804	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
33	f	614	II0	C05-C03-C09	3.38	116.14	109.49
33	a	313	II0	C19-C13-C09	-3.37	117.85	124.16
27	A	849	WVN	C21-C15-C14	3.37	120.79	113.60
33	f	614	II0	C20-C14-C12	3.37	120.63	114.42
24	O	205	CLA	CAC-C3C-C4C	3.37	129.18	124.79
33	h	310	II0	C05-C03-C09	3.37	116.13	109.49
24	A	834	CLA	CMB-C2B-C3B	3.37	134.48	126.55
34	g	319	IHT	C31-C34-C35	-3.37	117.12	126.36
34	g	319	IHT	C04-C02-C07	3.37	115.33	110.44
24	a	306	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
26	b	302	LHG	C5-O7-C7	-3.37	109.73	117.80
35	k	611	KC2	C1D-CHD-C4C	-3.37	118.33	126.25
33	h	311	II0	C41-C42-C40	-3.37	116.63	123.52
33	a	313	II0	C20-C14-C12	3.37	120.61	114.42
33	e	616	II0	C06-C04-C10	3.37	116.12	109.49
33	J	104	II0	C41-C39-C35	-3.36	122.56	127.28
33	f	616	II0	C19-C13-C11	3.36	120.61	114.42
24	j	308	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
33	c	614	II0	C30-C32-C34	-3.36	113.45	123.20
35	k	613	KC2	C2A-C1A-NA	3.36	114.73	109.34
33	d	313	II0	C20-C14-C12	3.36	120.60	114.42
27	K	103	WVN	C14-C15-C13	-3.36	118.17	122.70
24	L	204	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
27	B	845	WVN	C23-C20-C13	-3.36	118.03	127.00
34	a	316	IHT	C22-C18-C07	-3.36	118.03	127.00
34	b	316	IHT	C02-C07-C10	-3.36	118.05	122.64
24	c	608	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
27	F	204	WVN	C14-C15-C13	-3.36	118.17	122.70
33	c	616	II0	C19-C13-C09	-3.35	117.89	124.16
24	d	302	CLA	CMB-C2B-C1B	-3.35	120.31	125.42
33	j	318	II0	C19-C13-C09	-3.35	117.90	124.16
27	B	845	WVN	C01-C02-C11	-3.35	108.97	112.83
33	a	313	II0	C31-C33-C35	-3.35	117.19	126.36
24	B	822	CLA	O2A-C1-C2	-3.35	95.23	108.11
24	a	311	CLA	CHB-C4A-NA	3.35	129.23	124.40
33	a	313	II0	C41-C39-C35	-3.34	122.59	127.28
24	A	832	CLA	CAA-CBA-CGA	-3.34	103.72	113.21
24	b	304	CLA	C1-C2-C3	-3.34	120.72	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	206	WVN	C26-C29-C31	-3.34	113.52	123.20
33	g	316	II0	C06-C04-C10	3.34	116.07	109.49
24	R	203	CLA	C4A-NA-C1A	3.34	108.20	106.68
35	d	310	KC2	C2A-C1A-NA	3.33	114.69	109.34
33	k	617	II0	C27-C25-C29	-3.33	117.71	124.18
33	J	104	II0	C42-C41-C39	-3.33	116.70	123.52
24	A	829	CLA	CMB-C2B-C1B	-3.33	120.34	125.42
24	B	813	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
33	f	615	II0	C20-C14-C12	3.33	120.55	114.42
33	g	317	II0	C41-C42-C40	-3.33	116.71	123.52
24	c	609	CLA	CMB-C2B-C1B	-3.33	120.35	125.42
24	a	305	CLA	CMB-C2B-C1B	-3.33	120.35	125.42
24	J	103	CLA	CMB-C2B-C3B	3.33	134.38	126.55
24	j	310	CLA	CMB-C2B-C1B	-3.33	120.35	125.42
24	K	102	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	B	829	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
33	g	320	II0	C19-C13-C09	-3.33	117.94	124.16
24	f	607	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
24	F	202	CLA	C1-O2A-CGA	3.31	124.67	116.65
35	k	612	KC2	O2D-CGD-O1D	-3.31	117.40	123.85
24	A	802	CLA	CMB-C2B-C1B	-3.31	120.38	125.42
27	J	102	WVN	C28-C30-C33	-3.31	113.62	123.20
33	i	612	II0	C19-C13-C09	-3.31	117.98	124.16
33	h	309	II0	C42-C41-C39	-3.31	116.75	123.52
27	F	204	WVN	C20-C23-C25	-3.31	121.34	126.23
33	e	616	II0	C41-C42-C40	-3.30	116.76	123.52
24	O	205	CLA	CAA-C2A-C3A	-3.30	104.07	113.00
34	j	317	IHT	C19-C10-C09	3.30	120.64	113.60
24	B	837	CLA	C1-C2-C3	-3.30	120.79	126.20
35	g	312	KC2	CHD-C1D-ND	-3.30	119.09	124.05
33	k	616	II0	C20-C14-C12	3.30	120.49	114.42
24	f	603	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
33	J	104	II0	C19-C13-C11	3.30	120.48	114.42
24	A	837	CLA	O2D-CGD-CBD	3.29	116.99	111.23
34	f	617	IHT	C31-C34-C35	-3.29	117.33	126.36
33	e	612	II0	C42-C40-C36	-3.29	122.66	127.28
24	A	815	CLA	CMB-C2B-C3B	3.29	134.29	126.55
27	A	850	WVN	C29-C26-C22	-3.29	122.67	127.28
33	b	315	II0	C29-C31-C33	3.29	132.72	123.20
33	a	317	II0	C06-C04-C10	3.28	115.96	109.49
33	d	315	II0	C41-C42-C40	-3.28	116.80	123.52
24	B	838	CLA	O2D-CGD-O1D	-3.28	117.46	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	104	II0	C37-C35-C33	3.28	123.10	118.09
24	B	817	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
24	g	308	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
24	i	603	CLA	CMB-C2B-C1B	-3.27	120.44	125.42
27	B	849	WVN	C40-C39-C36	-3.27	116.83	123.52
24	L	202	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	A	852	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
33	c	616	II0	C32-C30-C26	-3.27	117.47	126.61
35	d	310	KC2	CMD-C2D-C3D	3.27	135.97	125.67
27	B	847	WVN	C02-C05-C09	-3.27	117.45	121.47
32	F	206	LMG	O1-C1-C2	3.26	113.22	108.27
33	a	313	II0	C19-C13-C11	3.26	120.42	114.42
24	B	828	CLA	CMB-C2B-C1B	-3.26	120.46	125.42
24	O	201	CLA	C1-C2-C3	-3.26	120.86	126.20
35	k	613	KC2	C3B-C2B-C1B	-3.26	103.96	107.05
33	b	314	II0	C05-C03-C09	3.26	115.91	109.49
24	B	806	CLA	CMB-C2B-C1B	-3.26	120.46	125.42
24	A	822	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
26	i	615	LHG	O8-C23-C24	3.25	121.75	111.83
24	d	307	CLA	CHB-C4A-NA	3.25	129.09	124.40
24	f	608	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
24	R	203	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
25	A	843	PQN	C14-C13-C15	3.25	120.87	115.23
24	B	809	CLA	CMB-C2B-C1B	-3.24	120.48	125.42
24	B	839	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
24	b	311	CLA	C1-C2-C3	-3.24	120.89	126.20
24	g	322	CLA	O2D-CGD-CBD	3.24	116.89	111.23
35	k	611	KC2	C2A-C1A-NA	3.24	114.53	109.34
24	B	821	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
24	d	312	CLA	CHB-C4A-NA	3.24	129.07	124.40
33	g	316	II0	C41-C39-C35	-3.24	122.74	127.28
27	L	206	WVN	C19-C22-C26	-3.23	113.92	119.01
24	a	310	CLA	CHB-C4A-NA	3.23	129.07	124.40
33	f	614	II0	C41-C42-C40	-3.23	116.91	123.52
24	B	805	CLA	O2D-CGD-CBD	3.23	116.88	111.23
35	e	609	KC2	CBC-CAC-C3C	-3.23	111.40	127.53
33	e	613	II0	C41-C42-C40	-3.23	116.92	123.52
35	k	612	KC2	CHD-C1D-ND	-3.23	119.21	124.05
27	A	846	WVN	C02-C11-C19	-3.23	119.56	124.58
35	g	312	KC2	CMD-C2D-C3D	3.23	135.84	125.67
33	j	315	II0	C06-C04-C10	3.23	115.84	109.49
35	k	612	KC2	C3B-C2B-C1B	-3.22	103.99	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	g	319	IHT	C30-C32-C33	-3.22	117.52	126.36
24	K	101	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
34	O	203	IHT	C18-C22-C23	-3.22	121.47	126.23
24	a	312	CLA	C4A-NA-C1A	-3.22	105.21	106.68
34	O	203	IHT	C30-C32-C33	-3.22	117.54	126.36
24	g	303	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
24	f	609	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
34	f	617	IHT	C27-C30-C32	3.21	132.51	123.20
24	A	819	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
24	b	311	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
34	g	319	IHT	C02-C07-C10	-3.21	118.25	122.64
24	A	826	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
33	k	615	II0	C31-C29-C25	-3.21	117.63	126.61
24	A	817	CLA	C3B-C4B-NB	-3.21	107.66	110.53
24	g	311	CLA	C4A-NA-C1A	3.21	108.14	106.68
24	b	308	CLA	CAC-C3C-C4C	-3.21	120.61	124.79
24	B	822	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
24	A	836	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
24	a	307	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
24	d	312	CLA	CAA-C2A-C3A	-3.21	104.34	113.00
33	f	614	II0	C17-C04-C10	-3.20	104.78	110.52
24	B	804	CLA	CMB-C2B-C1B	-3.20	120.54	125.42
34	f	617	IHT	C02-C07-C10	-3.20	118.26	122.64
27	B	848	WVN	C26-C29-C31	-3.20	113.92	123.20
33	g	316	II0	C12-C14-C10	-3.20	113.84	120.50
24	i	604	CLA	C1-C2-C3	-3.20	120.95	126.20
35	i	609	KC2	CMD-C2D-C3D	3.20	135.76	125.67
34	b	317	IHT	C22-C23-C27	3.20	124.04	119.01
33	f	614	II0	C31-C33-C35	-3.20	117.59	126.36
24	B	805	CLA	CHB-C4A-NA	3.20	129.02	124.40
24	A	831	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
33	d	314	II0	C32-C34-C36	-3.20	117.60	126.36
33	h	310	II0	C16-C03-C09	-3.20	104.79	110.52
24	A	822	CLA	O2A-CGA-O1A	-3.20	115.64	123.63
24	g	307	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
35	e	609	KC2	C3B-C2B-C1B	-3.19	104.03	107.05
35	k	613	KC2	CMD-C2D-C3D	3.19	135.73	125.67
24	A	816	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
33	f	615	II0	C19-C13-C11	3.19	120.28	114.42
24	a	304	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
35	g	314	KC2	C3B-C2B-C1B	-3.19	104.03	107.05
27	h	308	WVN	C30-C33-C34	-3.19	117.63	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	849	WVN	C06-C13-C15	-3.18	118.28	122.64
24	A	805	CLA	C7-C6-C5	-3.18	104.78	113.26
27	J	102	WVN	C29-C31-C32	-3.18	117.64	126.36
24	B	819	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
33	f	615	II0	C31-C33-C35	-3.18	117.64	126.36
24	a	309	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	f	608	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
33	j	316	II0	C19-C13-C11	3.18	120.27	114.42
24	A	841	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
35	f	611	KC2	C3B-C2B-C1B	-3.18	104.04	107.05
27	I	101	WVN	C23-C20-C13	-3.17	118.52	127.00
33	k	615	II0	C41-C42-C40	-3.17	117.03	123.52
24	i	610	CLA	C1D-ND-C4D	-3.17	104.09	106.31
27	j	301	WVN	C40-C39-C36	-3.17	117.03	123.52
24	c	612	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
24	B	810	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
24	c	608	CLA	CAA-CBA-CGA	-3.17	104.22	113.21
33	b	315	II0	C03-C05-C07	-3.17	106.65	113.59
27	j	301	WVN	C06-C13-C15	-3.16	118.31	122.64
24	R	203	CLA	CMB-C2B-C1B	-3.16	120.60	125.42
24	A	855	CLA	C3B-C4B-NB	-3.16	107.71	110.53
35	i	609	KC2	C1D-CHD-C4C	-3.16	118.81	126.25
35	g	312	KC2	CBC-CAC-C3C	-3.16	111.72	127.53
33	d	313	II0	C42-C41-C39	-3.16	117.05	123.52
27	L	206	WVN	C39-C40-C37	-3.16	117.05	123.52
35	f	611	KC2	O2D-CGD-O1D	-3.16	117.70	123.85
33	h	311	II0	C19-C13-C09	-3.16	118.26	124.16
35	i	609	KC2	C2A-C1A-NA	3.15	114.40	109.34
27	h	308	WVN	C29-C31-C32	-3.15	117.72	126.36
33	i	612	II0	C31-C33-C35	-3.15	117.72	126.36
33	a	314	II0	C41-C42-C40	-3.15	117.07	123.52
24	A	805	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
33	k	616	II0	C11-C13-C09	-3.15	113.94	120.50
24	B	826	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
33	a	314	II0	C42-C40-C36	-3.15	122.86	127.28
24	A	802	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
34	R	204	IHT	C19-C10-C09	3.15	120.31	113.60
24	d	303	CLA	CHB-C4A-NA	3.15	128.94	124.40
35	g	314	KC2	O2D-CGD-CBD	3.15	116.73	111.23
33	c	614	II0	C06-C04-C10	3.14	115.69	109.49
34	j	317	IHT	C30-C32-C33	-3.14	117.74	126.36
33	i	612	II0	C41-C42-C40	-3.14	117.09	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	101	WVN	C07-C01-C02	3.14	114.30	109.55
24	i	606	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
35	k	613	KC2	CBC-CAC-C3C	-3.14	111.83	127.53
27	A	846	WVN	C39-C40-C37	-3.14	117.09	123.52
24	c	612	CLA	C4A-NA-C1A	3.14	108.11	106.68
33	k	616	II0	C20-C14-C10	-3.14	118.29	124.16
33	J	104	II0	C41-C42-C40	-3.14	117.09	123.52
33	b	318	II0	C20-C14-C12	3.14	120.19	114.42
24	h	303	CLA	C2A-C1A-CHA	3.14	129.31	123.87
33	c	616	II0	C22-C24-C26	-3.13	165.58	176.23
33	f	618	II0	C11-C13-C09	-3.13	113.98	120.50
24	a	302	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
27	A	847	WVN	C39-C40-C37	-3.13	117.11	123.52
33	k	619	II0	C31-C29-C25	-3.13	117.85	126.61
33	i	614	II0	C20-C14-C12	3.13	120.17	114.42
24	A	806	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
24	i	604	CLA	CHB-C4A-NA	3.12	128.91	124.40
24	O	205	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	g	310	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
34	f	617	IHT	C41-C40-C37	3.12	129.91	123.52
26	f	620	LHG	C5-O7-C7	-3.12	110.32	117.80
24	d	303	CLA	C4A-NA-C1A	3.12	108.10	106.68
35	g	313	KC2	C3B-C2B-C1B	-3.12	104.09	107.05
24	A	807	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
34	R	204	IHT	C41-C38-C35	-3.12	122.90	127.28
35	e	609	KC2	CAA-CBA-CGA	-3.12	111.19	127.05
34	a	316	IHT	C20-C15-C12	3.12	120.15	114.42
24	h	302	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
27	F	205	WVN	C31-C32-C36	-3.12	114.11	119.01
35	g	313	KC2	CBC-CAC-C3C	-3.11	111.96	127.53
24	g	315	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
26	g	321	LHG	O8-C23-C24	3.11	121.33	111.83
33	a	317	II0	C32-C34-C36	3.11	134.90	126.36
27	B	848	WVN	C27-C25-C23	-3.11	113.34	118.09
24	L	204	CLA	CAA-CBA-CGA	-3.11	104.39	113.21
27	e	615	WVN	C18-C06-C13	3.10	115.11	110.24
24	R	203	CLA	CAA-C2A-C3A	-3.10	104.61	113.00
24	J	105	CLA	C2A-C1A-CHA	3.10	129.25	123.87
27	R	202	WVN	C29-C31-C32	-3.10	117.87	126.36
33	g	317	II0	C20-C14-C10	-3.10	118.37	124.16
24	a	312	CLA	CMB-C2B-C1B	-3.10	120.70	125.42
33	d	313	II0	C32-C34-C36	-3.10	117.87	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	g	313	KC2	C2A-C1A-NA	3.10	114.31	109.34
27	e	615	WVN	C11-C19-C22	-3.10	119.66	126.32
33	e	614	II0	C41-C42-C40	-3.09	117.19	123.52
24	A	816	CLA	CMB-C2B-C3B	3.09	133.82	126.55
24	B	811	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
27	J	101	WVN	C23-C25-C28	3.09	123.87	119.01
24	A	803	CLA	CAA-CBA-CGA	-3.09	104.44	113.21
26	J	107	LHG	O8-C23-C24	3.09	121.25	111.83
35	c	610	KC2	CHB-C4A-NA	3.09	129.02	124.23
27	M	101	WVN	C21-C15-C13	-3.09	121.12	124.48
24	i	604	CLA	C3A-C2A-C1A	3.09	105.96	101.34
24	B	840	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
27	A	850	WVN	C21-C15-C13	-3.08	121.12	124.48
33	b	318	II0	C06-C04-C10	3.08	115.56	109.49
24	a	305	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
24	k	604	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
24	A	819	CLA	CBC-CAC-C3C	-3.08	104.07	112.42
27	L	205	WVN	C21-C15-C13	-3.08	121.12	124.48
33	f	615	II0	C42-C41-C39	-3.08	117.22	123.52
24	A	820	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
34	g	319	IHT	C22-C18-C07	-3.08	118.77	127.00
24	f	612	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
24	B	825	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
24	a	308	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
33	g	317	II0	O02-C08-C06	-3.08	103.45	109.75
24	h	303	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
35	g	314	KC2	CHB-C4A-NA	3.07	129.00	124.23
33	i	614	II0	C41-C42-C40	-3.07	117.23	123.52
35	d	311	KC2	C2A-C1A-NA	3.07	114.26	109.34
33	g	318	II0	C06-C04-C10	3.07	115.54	109.49
34	a	316	IHT	C19-C10-C09	3.07	120.14	113.60
24	h	301	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
24	d	309	CLA	CAA-C2A-C3A	-3.07	109.20	116.23
33	j	316	II0	C19-C13-C09	-3.07	118.43	124.16
24	B	804	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	e	610	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
32	F	206	LMG	C7-O1-C1	-3.06	107.23	113.80
24	L	207	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
27	F	204	WVN	C28-C30-C33	-3.06	114.33	123.20
25	B	842	PQN	C14-C13-C15	3.06	120.54	115.23
24	A	824	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	B	833	CLA	O2D-CGD-O1D	-3.06	117.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	842	CLA	CMB-C2B-C1B	-3.05	120.77	125.42
24	J	105	CLA	CHB-C4A-NA	3.05	128.81	124.40
34	f	617	IHT	C25-C23-C27	-3.05	117.87	122.82
34	O	203	IHT	C19-C10-C09	3.05	120.10	113.60
33	g	318	II0	C41-C42-C40	-3.05	117.28	123.52
24	B	817	CLA	O2D-CGD-CBD	3.05	116.56	111.23
27	R	201	WVN	C04-C09-C05	-3.05	121.92	124.83
33	e	612	II0	C31-C33-C35	-3.05	118.00	126.36
33	h	310	II0	C20-C14-C10	-3.05	118.46	124.16
24	e	607	CLA	C1-C2-C3	-3.05	121.20	126.20
33	g	318	II0	C19-C13-C11	3.05	120.03	114.42
24	e	602	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
24	A	834	CLA	CHB-C4A-NA	3.05	128.80	124.40
33	e	614	II0	C06-C04-C10	3.05	115.49	109.49
24	B	801	CLA	CMB-C2B-C3B	3.05	133.71	126.55
24	A	826	CLA	CHB-C4A-NA	3.05	128.79	124.40
24	B	822	CLA	CMB-C2B-C1B	-3.04	120.78	125.42
24	A	813	CLA	O2D-CGD-CBD	3.04	116.55	111.23
27	J	101	WVN	C26-C29-C31	-3.04	114.38	123.20
24	B	801	CLA	O2A-CGA-O1A	-3.04	116.02	123.63
33	k	617	II0	C30-C32-C34	-3.04	114.39	123.20
24	j	305	CLA	CMB-C2B-C1B	-3.04	120.79	125.42
24	b	305	CLA	CHB-C4A-NA	3.04	128.79	124.40
24	A	855	CLA	C1-O2A-CGA	3.04	124.01	116.65
27	A	847	WVN	C01-C02-C11	-3.04	109.33	112.83
35	d	311	KC2	CAC-C3C-C4C	3.04	137.81	124.39
24	J	103	CLA	CHB-C4A-NA	3.04	128.78	124.40
24	e	605	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
24	A	821	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
24	f	606	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
24	B	829	CLA	O2D-CGD-CBD	3.03	116.53	111.23
28	a	318	LMT	C2'-C3'-C4'	3.03	116.56	109.68
28	A	851	LMT	C3B-C4B-C5B	-3.03	104.73	110.23
24	e	610	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
24	b	310	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	A	841	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
24	h	303	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
27	A	846	WVN	C27-C25-C28	-3.03	117.91	122.82
33	f	618	II0	C20-C14-C10	-3.02	118.51	124.16
26	j	319	LHG	O8-C23-C24	3.02	121.05	111.83
24	A	808	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	A	812	CLA	CHB-C4A-NA	3.02	128.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	612	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
24	A	830	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
27	L	205	WVN	C04-C09-C05	-3.02	121.95	124.83
24	A	855	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
33	a	315	II0	C05-C03-C09	3.02	115.44	109.49
27	I	101	WVN	C01-C02-C11	-3.02	109.36	112.83
33	g	320	II0	C19-C13-C11	3.02	119.97	114.42
27	R	202	WVN	C02-C05-C09	-3.02	117.76	121.47
35	g	312	KC2	C3B-C2B-C1B	-3.02	104.19	107.05
33	a	314	II0	C31-C29-C25	-3.01	118.18	126.61
24	B	832	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
24	k	604	CLA	CHB-C4A-NA	3.01	128.75	124.40
24	h	301	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
32	O	204	LMG	O8-C28-C29	3.01	121.02	111.83
24	K	101	CLA	CHB-C4A-NA	3.01	128.75	124.40
24	B	811	CLA	C3B-C4B-NB	-3.01	107.84	110.53
24	B	824	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
27	B	847	WVN	C23-C20-C13	-3.01	118.95	127.00
35	k	612	KC2	CAA-CBA-CGA	-3.01	111.74	127.05
24	A	840	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
27	h	308	WVN	C06-C13-C15	-3.01	118.52	122.64
24	k	604	CLA	O2A-CGA-O1A	-3.01	116.10	123.63
33	a	317	II0	C38-C36-C40	-3.01	117.94	122.82
27	A	848	WVN	C06-C13-C20	3.01	123.81	115.65
24	e	608	CLA	CHB-C4A-NA	3.01	128.74	124.40
24	e	602	CLA	CMB-C2B-C1B	-3.00	120.84	125.42
24	g	305	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
24	B	833	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
33	d	315	II0	C06-C04-C10	3.00	115.40	109.49
27	L	206	WVN	C28-C30-C33	3.00	131.89	123.20
34	c	615	IHT	C31-C34-C35	-3.00	118.14	126.36
26	a	301	LHG	C5-O7-C7	-3.00	110.62	117.80
33	d	315	II0	C31-C33-C35	-3.00	118.14	126.36
24	h	307	CLA	CHB-C4A-NA	3.00	128.72	124.40
33	c	614	II0	C21-C23-C25	-3.00	166.05	176.23
26	g	321	LHG	C6-C5-C4	-3.00	104.80	111.78
27	F	204	WVN	C21-C15-C14	2.99	119.98	113.60
24	g	315	CLA	C3B-C4B-NB	-2.99	107.86	110.53
24	B	827	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	A	842	CLA	CHB-C4A-NA	2.99	128.71	124.40
24	j	313	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
33	J	104	II0	C20-C14-C10	-2.99	118.57	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	310	CLA	C4A-NA-C1A	2.99	108.04	106.68
24	g	309	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
34	a	316	IHT	C30-C32-C33	-2.99	118.18	126.36
35	i	609	KC2	CMB-C2B-C1B	2.99	129.99	124.73
34	b	317	IHT	C25-C23-C27	-2.99	117.98	122.82
35	j	312	KC2	C1D-CHD-C4C	-2.98	119.23	126.25
27	L	201	WVN	C10-C06-C13	2.98	114.77	110.44
24	j	307	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	A	810	CLA	C4A-NA-C1A	2.98	108.04	106.68
24	B	828	CLA	CMB-C2B-C3B	2.98	133.57	126.55
32	L	208	LMG	O8-C28-C29	2.98	120.93	111.83
28	a	318	LMT	O5'-C1'-C2'	-2.98	104.24	110.37
33	b	314	II0	C11-C13-C09	-2.98	114.30	120.50
24	g	302	CLA	CMB-C2B-C3B	2.98	133.56	126.55
24	R	203	CLA	O2A-CGA-O1A	-2.98	116.17	123.63
27	B	849	WVN	C01-C02-C11	-2.98	109.40	112.83
34	c	615	IHT	C19-C10-C09	2.98	119.95	113.60
24	A	827	CLA	CMB-C2B-C3B	2.98	133.55	126.55
24	d	307	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
33	e	612	II0	C20-C14-C12	2.98	119.89	114.42
33	i	612	II0	C20-C14-C12	2.98	119.89	114.42
24	j	309	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	B	836	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	j	314	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
33	k	616	II0	C05-C03-C09	2.97	115.35	109.49
24	F	202	CLA	CHB-C4A-NA	2.97	128.69	124.40
27	h	308	WVN	C21-C15-C13	-2.97	121.24	124.48
27	A	846	WVN	C20-C23-C25	-2.97	121.84	126.23
24	A	828	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	h	304	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
33	k	619	II0	C27-C25-C29	-2.96	118.42	124.18
33	i	614	II0	C19-C13-C09	-2.96	118.62	124.16
24	A	813	CLA	CAA-CBA-CGA	-2.96	104.59	112.49
27	J	101	WVN	C39-C40-C37	-2.96	117.46	123.52
24	A	808	CLA	CHB-C4A-NA	2.96	128.67	124.40
27	A	850	WVN	C26-C29-C31	-2.96	114.62	123.20
33	d	314	II0	C29-C31-C33	-2.96	114.62	123.20
24	j	311	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
27	B	845	WVN	C28-C30-C33	-2.96	114.63	123.20
33	i	614	II0	C20-C14-C10	-2.96	118.63	124.16
24	B	832	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
27	M	101	WVN	C29-C26-C22	-2.96	123.13	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	815	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
33	c	616	II0	C20-C14-C12	2.96	119.86	114.42
35	i	609	KC2	CBC-CAC-C3C	-2.96	112.76	127.53
27	B	846	WVN	C21-C15-C13	-2.95	121.26	124.48
33	j	316	II0	C31-C33-C35	-2.95	118.27	126.36
35	g	313	KC2	CMD-C2D-C3D	2.95	134.98	125.67
24	j	314	CLA	CMB-C2B-C1B	-2.95	120.92	125.42
33	a	314	II0	C30-C32-C34	-2.95	114.65	123.20
35	e	609	KC2	O2D-CGD-O1D	-2.95	118.11	123.85
24	a	311	CLA	CAA-C2A-C3A	-2.95	105.03	113.00
24	B	806	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	L	207	CLA	CHB-C4A-NA	2.95	128.65	124.40
33	a	314	II0	C20-C14-C10	-2.95	118.65	124.16
32	L	208	LMG	C3-C4-C5	2.95	115.57	110.23
24	A	814	CLA	CMB-C2B-C3B	2.94	133.47	126.55
24	B	819	CLA	CMB-C2B-C3B	2.94	133.47	126.55
24	g	304	CLA	CMB-C2B-C3B	2.94	133.47	126.55
33	k	621	II0	C20-C14-C12	2.94	119.83	114.42
35	d	311	KC2	C3B-C2B-C1B	-2.94	104.27	107.05
35	d	310	KC2	O2D-CGD-O1D	-2.94	118.13	123.85
24	A	834	CLA	CAA-C2A-C3A	-2.94	105.06	113.00
24	b	304	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	d	302	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
35	k	612	KC2	CAB-C3B-C2B	2.93	137.97	128.43
33	b	318	II0	C37-C35-C33	2.93	122.57	118.09
24	A	801	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	g	308	CLA	CMB-C2B-C3B	2.93	133.45	126.55
24	f	602	CLA	C3B-C4B-NB	-2.93	107.91	110.53
33	a	315	II0	C42-C41-C39	-2.93	117.52	123.52
24	B	831	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	K	101	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
24	h	305	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
27	F	205	WVN	C20-C13-C15	-2.93	114.81	121.56
33	h	309	II0	C31-C33-C35	-2.93	118.33	126.36
25	A	843	PQN	C11-C12-C13	-2.93	121.78	126.83
33	g	320	II0	C06-C04-C10	2.93	115.26	109.49
24	c	606	CLA	C1-C2-C3	-2.93	121.40	126.20
24	c	602	CLA	CAC-C3C-C4C	2.93	128.60	124.79
24	k	608	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	d	305	CLA	C3B-C4B-NB	-2.93	107.92	110.53
33	e	612	II0	C42-C41-C39	-2.93	117.53	123.52
27	B	847	WVN	C29-C31-C32	2.92	134.38	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	311	KC2	O2D-CGD-CBD	2.92	116.34	111.23
30	B	843	DGD	O1G-C1A-C2A	2.92	120.75	111.83
24	K	101	CLA	CAA-C2A-C1A	2.92	121.55	111.97
24	A	803	CLA	CMB-C2B-C3B	2.92	133.43	126.55
24	B	812	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
27	L	201	WVN	C40-C39-C36	-2.92	117.54	123.52
24	d	303	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
35	d	311	KC2	CHB-C4A-NA	2.92	128.76	124.23
33	a	314	II0	C05-C03-C09	2.92	115.24	109.49
24	j	302	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	c	607	CLA	C4A-NA-C1A	2.92	108.01	106.68
24	K	102	CLA	CHB-C4A-NA	2.92	128.61	124.40
24	f	605	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
33	k	617	II0	C20-C14-C12	2.91	119.78	114.42
24	A	817	CLA	C1-C2-C3	-2.91	121.43	126.20
24	e	601	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	A	812	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	A	806	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
27	R	202	WVN	C39-C40-C37	-2.91	117.57	123.52
33	j	316	II0	C20-C14-C10	-2.91	118.73	124.16
24	B	840	CLA	CMB-C2B-C3B	2.90	133.38	126.55
35	j	312	KC2	C2A-C1A-NA	2.90	114.00	109.34
27	J	101	WVN	C39-C36-C32	-2.90	123.21	127.28
33	a	315	II0	C19-C13-C11	2.90	119.76	114.42
33	c	613	II0	C20-C14-C10	-2.90	118.74	124.16
33	c	614	II0	C19-C13-C11	2.90	119.75	114.42
24	A	833	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	g	302	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
27	J	102	WVN	C30-C28-C25	-2.90	123.21	127.28
33	j	315	II0	C16-C03-C09	-2.90	105.32	110.52
33	j	315	II0	C42-C41-C39	-2.90	117.59	123.52
24	A	814	CLA	C1-C2-C3	-2.90	122.07	126.76
24	A	804	CLA	CMB-C2B-C1B	-2.90	121.01	125.42
24	A	830	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	j	305	CLA	C1-C2-C3	-2.90	121.45	126.20
33	e	613	II0	C20-C14-C12	2.90	119.75	114.42
24	A	802	CLA	CMB-C2B-C3B	2.90	133.36	126.55
35	i	609	KC2	C3B-C2B-C1B	-2.90	104.31	107.05
26	g	301	LHG	O8-C23-C24	2.89	120.66	111.83
27	A	849	WVN	C11-C19-C22	-2.89	120.10	126.32
33	a	315	II0	C20-C14-C12	2.89	119.74	114.42
33	e	613	II0	C20-C14-C10	-2.89	118.76	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	305	CLA	CMB-C2B-C3B	2.89	133.35	126.55
24	B	801	CLA	O2D-CGD-CBD	2.89	116.28	111.23
33	h	311	II0	C20-C14-C12	2.89	119.73	114.42
34	O	203	IHT	C22-C18-C07	-2.89	119.28	127.00
27	I	101	WVN	C39-C40-C37	-2.89	117.61	123.52
24	B	811	CLA	CHB-C4A-NA	2.89	128.57	124.40
24	c	612	CLA	CAA-C2A-C3A	-2.89	105.20	113.00
34	O	203	IHT	C20-C15-C12	2.89	119.73	114.42
24	A	819	CLA	CAA-CBA-CGA	-2.88	104.80	112.49
24	h	307	CLA	C3B-C4B-NB	-2.88	107.95	110.53
27	A	848	WVN	C20-C13-C15	-2.88	114.91	121.56
35	c	610	KC2	C3B-C2B-C1B	-2.88	104.32	107.05
35	i	616	KC2	C3B-C2B-C1B	-2.88	104.32	107.05
24	A	811	CLA	C3B-C4B-NB	-2.88	107.96	110.53
27	A	848	WVN	C12-C14-C15	-2.88	108.92	114.06
34	b	316	IHT	C22-C18-C07	-2.88	119.30	127.00
24	B	832	CLA	CMB-C2B-C3B	2.88	133.33	126.55
24	A	842	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
24	B	830	CLA	CAA-CBA-CGA	-2.88	105.03	113.21
24	A	855	CLA	C4-C3-C5	2.88	120.23	115.23
33	c	614	II0	C31-C33-C35	-2.88	118.47	126.36
24	h	304	CLA	C4A-NA-C1A	2.88	107.99	106.68
24	i	607	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	F	205	WVN	C27-C25-C28	-2.88	118.15	122.82
24	b	307	CLA	CMB-C2B-C3B	2.88	133.32	126.55
24	f	613	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
35	j	312	KC2	CAB-C3B-C2B	2.87	137.78	128.43
24	f	608	CLA	CMB-C2B-C3B	2.87	133.31	126.55
24	B	815	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
33	g	316	II0	C38-C36-C34	2.87	122.47	118.09
24	B	821	CLA	C3B-C4B-NB	-2.87	107.97	110.53
27	L	201	WVN	C07-C01-C02	2.87	113.89	109.55
24	b	308	CLA	CAA-CBA-CGA	-2.86	105.07	113.21
27	A	848	WVN	C20-C23-C25	-2.86	122.00	126.23
24	e	604	CLA	CHB-C4A-NA	2.86	128.53	124.40
24	A	812	CLA	C6-C5-C3	-2.86	106.50	113.47
27	L	205	WVN	C40-C37-C34	-2.86	123.27	127.28
24	A	806	CLA	C11-C10-C8	-2.86	106.46	115.97
24	g	315	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
34	c	615	IHT	C22-C18-C07	-2.86	119.36	127.00
24	B	825	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
33	J	104	II0	C19-C13-C09	-2.86	118.82	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	310	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
24	A	836	CLA	C7-C6-C5	-2.85	105.65	113.26
24	A	804	CLA	CHB-C4A-NA	2.85	128.51	124.40
24	i	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
33	e	614	II0	C32-C34-C36	-2.85	118.55	126.36
33	i	614	II0	C12-C14-C10	-2.85	114.57	120.50
33	d	313	II0	C05-C03-C09	2.85	115.10	109.49
33	c	614	II0	C41-C42-C40	-2.85	117.69	123.52
33	i	613	II0	C19-C13-C09	-2.84	118.85	124.16
24	A	840	CLA	CMB-C2B-C3B	2.84	133.23	126.55
33	a	317	II0	C41-C42-C40	-2.84	117.71	123.52
24	e	603	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
24	i	601	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
27	L	206	WVN	C33-C34-C37	-2.84	114.54	119.01
24	d	309	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
33	g	316	II0	C05-C03-C09	2.84	115.08	109.49
24	a	304	CLA	CHB-C4A-NA	2.83	128.49	124.40
24	h	312	CLA	CMB-C2B-C3B	2.83	133.22	126.55
24	d	301	CLA	CAA-CBA-CGA	-2.83	105.16	113.21
33	g	316	II0	C20-C14-C12	2.83	119.63	114.42
24	c	607	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
34	a	316	IHT	C18-C22-C23	-2.83	122.05	126.23
34	k	618	IHT	C19-C10-C09	2.83	119.63	113.60
35	d	310	KC2	C3B-C2B-C1B	-2.83	104.37	107.05
24	h	305	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
28	a	318	LMT	O5'-C5'-C4'	2.83	115.58	109.72
24	B	817	CLA	CHB-C4A-NA	2.83	128.49	124.40
24	B	808	CLA	O2D-CGD-CBD	2.83	116.17	111.23
24	d	312	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
27	I	101	WVN	C11-C19-C22	-2.83	120.24	126.32
24	j	308	CLA	CHB-C4A-NA	2.83	128.48	124.40
24	c	608	CLA	O2D-CGD-CBD	2.83	116.17	111.23
33	h	311	II0	C17-C04-C10	2.82	115.58	110.52
27	L	201	WVN	C20-C23-C25	-2.82	122.06	126.23
24	B	818	CLA	C1-C2-C3	-2.82	121.57	126.20
35	j	312	KC2	C3B-C2B-C1B	-2.82	104.37	107.05
24	B	838	CLA	C3B-C4B-NB	-2.82	108.01	110.53
33	b	318	II0	C17-C04-C10	-2.82	105.46	110.52
33	e	613	II0	C42-C40-C36	-2.82	123.32	127.28
24	B	806	CLA	CMB-C2B-C3B	2.82	133.18	126.55
24	d	302	CLA	CMB-C2B-C3B	2.82	133.18	126.55
35	g	313	KC2	O2D-CGD-CBD	2.82	116.16	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	612	KC2	C2A-C1A-NA	2.82	113.86	109.34
24	f	604	CLA	CHB-C4A-NA	2.82	128.47	124.40
35	d	310	KC2	CAB-C3B-C2B	2.82	137.59	128.43
33	b	314	II0	C27-C25-C29	2.82	129.66	124.18
24	a	308	CLA	C3B-C4B-NB	-2.82	108.02	110.53
33	a	313	II0	C30-C32-C34	-2.82	115.04	123.20
24	c	608	CLA	C1-C2-C3	-2.82	121.58	126.20
24	B	826	CLA	CMB-C2B-C3B	2.82	133.17	126.55
35	i	616	KC2	CHB-C4A-NA	2.81	128.59	124.23
33	f	616	II0	C20-C14-C10	-2.81	118.90	124.16
26	c	617	LHG	O8-C23-C24	2.81	120.41	111.83
24	A	835	CLA	O2D-CGD-CBD	2.81	116.15	111.23
34	j	317	IHT	C22-C18-C07	-2.81	119.49	127.00
24	i	602	CLA	C1-C2-C3	-2.81	122.21	126.76
24	g	304	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	A	839	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
34	O	203	IHT	C40-C41-C38	-2.81	117.77	123.52
24	d	305	CLA	C4A-NA-C1A	2.81	107.96	106.68
24	I	102	CLA	C3B-C4B-NB	-2.81	108.02	110.53
27	L	205	WVN	C20-C23-C25	-2.81	122.08	126.23
33	e	613	II0	C05-C03-C09	2.81	115.02	109.49
35	e	609	KC2	C2B-C1B-NB	2.81	112.91	110.13
24	e	603	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	d	301	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	A	829	CLA	O2D-CGD-CBD	2.81	116.14	111.23
24	A	803	CLA	O2D-CGD-CBD	2.81	116.14	111.23
24	A	810	CLA	C1-C2-C3	-2.81	121.60	126.20
27	B	848	WVN	C24-C22-C19	2.81	122.37	118.09
33	h	309	II0	C31-C29-C25	-2.80	118.77	126.61
24	f	613	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	e	603	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
24	J	103	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	d	302	CLA	CAA-C2A-C3A	-2.80	105.42	113.00
24	B	841	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
33	k	621	II0	C19-C13-C09	-2.80	118.92	124.16
35	f	611	KC2	CAB-C3B-C2B	2.80	137.53	128.43
24	B	827	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	a	301	LHG	O8-C23-C24	2.80	120.37	111.83
33	f	618	II0	C16-C03-C09	-2.80	105.50	110.52
32	b	301	LMG	C8-O7-C10	-2.80	111.11	117.80
24	d	309	CLA	C4A-NA-C1A	2.79	107.95	106.68
24	j	310	CLA	CMB-C2B-C3B	2.79	133.12	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	e	608	CLA	O2D-CGD-CBD	2.79	116.11	111.23
24	j	305	CLA	CHB-C4A-NA	2.79	128.43	124.40
24	c	609	CLA	CMB-C2B-C3B	2.79	133.12	126.55
24	a	307	CLA	CHB-C4A-NA	2.79	128.43	124.40
24	A	826	CLA	CMC-C2C-C1C	-2.79	120.67	125.03
33	e	612	II0	C32-C34-C36	-2.79	118.71	126.36
24	g	305	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	k	603	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
24	A	820	CLA	CMB-C2B-C3B	2.79	133.11	126.55
26	c	618	LHG	O8-C23-C24	2.79	120.33	111.83
24	a	307	CLA	C1-C2-C3	-2.79	121.63	126.20
24	g	310	CLA	C1-C2-C3	-2.79	121.63	126.20
33	j	316	II0	C30-C32-C34	-2.78	115.13	123.20
24	A	842	CLA	O2D-CGD-CBD	2.78	116.10	111.23
24	b	309	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
24	c	605	CLA	O2D-CGD-CBD	2.78	116.09	111.23
24	b	306	CLA	CHB-C4A-NA	2.78	128.42	124.40
27	A	849	WVN	C39-C40-C37	-2.78	117.83	123.52
24	A	808	CLA	CAA-CBA-CGA	-2.78	105.31	113.21
24	B	807	CLA	O2D-CGD-CBD	2.78	116.09	111.23
24	f	601	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
24	A	853	CLA	CHB-C4A-NA	2.78	128.41	124.40
24	A	835	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	b	307	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
35	k	613	KC2	CHB-C4A-NA	2.78	128.54	124.23
34	O	203	IHT	C31-C29-C26	-2.78	118.84	126.61
24	K	102	CLA	O1D-CGD-CBD	2.78	130.00	124.52
33	j	316	II0	C29-C31-C33	-2.78	115.16	123.20
26	g	321	LHG	O3-P-O5	-2.78	97.93	108.94
24	A	817	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	A	827	CLA	C3B-C4B-NB	-2.77	108.05	110.53
24	d	308	CLA	CAA-C2A-C3A	-2.77	109.87	116.23
24	A	817	CLA	O2D-CGD-CBD	2.77	116.08	111.23
24	A	807	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	e	603	CLA	CHB-C1B-C2B	-2.77	119.38	127.43
24	A	805	CLA	C1-C2-C3	-2.77	121.66	126.20
24	a	310	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
24	a	312	CLA	C1D-ND-C4D	-2.77	104.37	106.31
24	c	609	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	g	310	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
27	B	847	WVN	C31-C32-C36	-2.77	114.65	119.01
33	k	616	II0	C37-C35-C33	2.77	122.32	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	311	CLA	C2D-C1D-ND	-2.77	107.39	110.13
24	d	303	CLA	C1-C2-C3	-2.77	121.66	126.20
27	B	848	WVN	C02-C05-C09	-2.77	118.06	121.47
24	L	202	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
24	i	610	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
33	i	613	II0	C30-C32-C34	-2.77	115.19	123.20
33	b	318	II0	C30-C32-C34	-2.77	115.19	123.20
27	h	308	WVN	C07-C01-C02	2.76	113.73	109.55
27	K	103	WVN	C35-C32-C31	2.76	122.31	118.09
24	B	832	CLA	C1-C2-C3	-2.76	121.68	126.20
24	f	604	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
24	b	308	CLA	CAC-C3C-C2C	2.76	132.62	127.56
24	B	836	CLA	CAA-CBA-CGA	-2.76	105.38	113.21
27	R	201	WVN	C20-C23-C25	-2.76	122.16	126.23
34	k	618	IHT	C04-C02-C07	2.76	114.44	110.44
24	j	303	CLA	C3B-C4B-NB	-2.75	108.07	110.53
33	k	616	II0	C03-C05-C07	-2.75	107.55	113.59
34	R	204	IHT	C29-C31-C34	-2.75	115.22	123.20
24	A	820	CLA	C7-C6-C5	-2.75	105.92	113.26
24	A	823	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	c	609	CLA	C3B-C4B-NB	-2.75	108.07	110.53
26	e	617	LHG	O8-C23-C24	2.75	120.22	111.83
24	j	304	CLA	CHB-C4A-NA	2.75	128.37	124.40
24	h	304	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
24	A	825	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
33	j	315	II0	C41-C42-C40	-2.75	117.90	123.52
33	c	616	II0	C42-C41-C39	-2.75	117.90	123.52
24	A	812	CLA	C1-C2-C3	-2.75	121.70	126.20
24	e	605	CLA	CMD-C2D-C1D	-2.75	119.89	124.73
24	K	101	CLA	C2A-C1A-CHA	2.74	128.63	123.87
26	c	617	LHG	C5-O7-C7	-2.74	111.23	117.80
33	e	614	II0	C31-C33-C35	-2.74	118.84	126.36
24	A	809	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	R	203	CLA	CMB-C2B-C3B	2.74	133.00	126.55
32	J	106	LMG	O8-C28-C29	2.74	120.20	111.83
24	B	825	CLA	CMB-C2B-C3B	2.74	133.00	126.55
33	d	313	II0	C38-C36-C34	2.74	122.28	118.09
24	c	602	CLA	CHB-C4A-NA	2.74	128.36	124.40
33	k	616	II0	C32-C30-C26	-2.74	118.94	126.61
24	i	605	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
27	I	101	WVN	C40-C37-C34	-2.74	123.44	127.28
27	A	849	WVN	C26-C29-C31	-2.74	115.26	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	f	611	KC2	C1D-CHD-C4C	-2.74	119.81	126.25
24	f	606	CLA	CHB-C4A-NA	2.74	128.35	124.40
24	b	312	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
24	h	306	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	A	818	CLA	O2D-CGD-CBD	2.73	116.01	111.23
24	A	834	CLA	O2D-CGD-CBD	2.73	116.01	111.23
33	a	317	II0	C32-C30-C26	2.73	134.26	126.61
24	B	825	CLA	C2A-C1A-CHA	2.73	128.61	123.87
24	a	303	CLA	C1-C2-C3	-2.73	122.34	126.76
24	B	822	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	j	306	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	B	828	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	A	855	CLA	C4-C3-C2	-2.73	116.61	123.63
24	B	823	CLA	CMB-C2B-C3B	2.73	132.97	126.55
27	h	308	WVN	C23-C20-C13	-2.73	119.70	127.00
27	L	205	WVN	C39-C36-C32	-2.73	123.45	127.28
24	g	310	CLA	CMB-C2B-C3B	2.73	132.97	126.55
32	J	106	LMG	O7-C10-C11	2.73	117.39	111.48
24	d	304	CLA	CHB-C4A-NA	2.73	128.34	124.40
27	I	101	WVN	C28-C30-C33	-2.73	115.29	123.20
34	O	203	IHT	C31-C34-C35	-2.73	118.88	126.36
27	A	850	WVN	C20-C23-C25	-2.73	122.20	126.23
33	b	318	II0	C12-C14-C10	-2.73	114.82	120.50
27	B	847	WVN	C12-C14-C15	-2.73	109.19	114.06
33	f	618	II0	C19-C13-C11	2.73	119.44	114.42
24	A	817	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
24	A	802	CLA	CAA-CBA-CGA	-2.73	105.47	113.21
34	b	316	IHT	C30-C32-C33	-2.73	118.89	126.36
24	A	808	CLA	CMB-C2B-C1B	-2.73	121.27	125.42
24	e	605	CLA	CMD-C2D-C3D	2.73	133.94	127.69
24	g	302	CLA	CHB-C4A-NA	2.72	128.33	124.40
33	h	311	II0	C42-C41-C39	-2.72	117.95	123.52
34	c	615	IHT	C20-C15-C12	2.72	119.42	114.42
33	j	318	II0	C20-C14-C12	2.72	119.42	114.42
24	A	832	CLA	CHB-C4A-NA	2.72	128.32	124.40
35	d	310	KC2	C1D-CHD-C4C	-2.72	119.85	126.25
24	A	811	CLA	O2D-CGD-CBD	2.72	115.98	111.23
34	j	317	IHT	C20-C15-C12	2.72	119.42	114.42
24	A	802	CLA	C11-C12-C13	-2.71	106.94	115.97
27	B	847	WVN	C19-C22-C26	-2.71	114.74	119.01
24	B	822	CLA	O2D-CGD-CBD	2.71	115.97	111.23
24	O	205	CLA	C4A-NA-C1A	2.71	107.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	312	KC2	CBC-CAC-C3C	-2.71	113.98	127.53
24	k	605	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
24	A	836	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
27	I	101	WVN	C39-C36-C32	-2.71	123.48	127.28
24	b	309	CLA	CAA-CBA-CGA	-2.71	105.52	113.21
24	B	804	CLA	CMB-C2B-C3B	2.71	132.92	126.55
24	O	201	CLA	C3B-C4B-NB	-2.71	108.11	110.53
33	i	612	II0	C42-C41-C39	-2.71	117.98	123.52
27	J	102	WVN	C18-C06-C13	-2.71	106.00	110.24
24	g	303	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	h	303	CLA	CMB-C2B-C3B	2.70	132.91	126.55
24	A	820	CLA	CHB-C4A-NA	2.70	128.30	124.40
27	I	101	WVN	C21-C15-C13	-2.70	121.53	124.48
26	b	302	LHG	O8-C23-C24	2.70	120.08	111.83
24	A	826	CLA	CAA-CBA-CGA	-2.70	105.53	113.21
24	c	607	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
33	c	616	II0	C19-C13-C11	2.70	119.39	114.42
24	k	606	CLA	C3B-C4B-NB	-2.70	108.12	110.53
33	d	314	II0	C32-C30-C26	-2.70	119.05	126.61
27	e	615	WVN	C06-C13-C20	2.70	122.98	115.65
24	B	827	CLA	C1-C2-C3	-2.70	122.39	126.76
33	e	616	II0	C31-C33-C35	-2.70	118.96	126.36
24	i	611	CLA	CHB-C4A-NA	2.70	128.29	124.40
27	j	301	WVN	C20-C23-C25	-2.70	122.25	126.23
33	h	311	II0	C06-C04-C10	2.70	114.80	109.49
33	b	315	II0	C23-C21-C09	-2.70	169.20	175.48
35	g	312	KC2	C2A-C1A-NA	2.70	113.66	109.34
33	b	315	II0	C19-C13-C09	-2.69	119.12	124.16
24	g	305	CLA	CHB-C4A-NA	2.69	128.29	124.40
24	e	601	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
34	O	203	IHT	C12-C15-C11	-2.69	114.89	120.50
24	e	605	CLA	CHB-C4A-NA	2.69	128.29	124.40
27	J	102	WVN	C31-C32-C36	2.69	123.25	119.01
24	A	806	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	B	817	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
24	B	809	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
33	k	617	II0	C42-C41-C39	-2.69	118.02	123.52
24	a	310	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
24	k	602	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
34	f	617	IHT	C04-C02-C07	2.69	114.34	110.44
24	B	812	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
34	b	316	IHT	C19-C10-C09	2.68	119.32	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	822	CLA	C7-C6-C5	2.68	120.41	113.26
24	A	837	CLA	C1-C2-C3	-2.68	121.80	126.20
33	g	318	II0	C31-C29-C25	-2.68	119.11	126.61
24	B	831	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
24	B	813	CLA	CBA-CAA-C2A	2.68	121.77	113.79
24	k	610	CLA	CHB-C4A-NA	2.68	128.27	124.40
24	K	101	CLA	CMB-C2B-C3B	2.68	132.85	126.55
33	h	311	II0	C19-C13-C11	2.68	119.35	114.42
27	L	205	WVN	C39-C40-C37	-2.68	118.04	123.52
33	k	615	II0	C20-C14-C12	2.68	119.34	114.42
24	i	607	CLA	CAA-C2A-C1A	2.68	120.75	111.97
35	c	610	KC2	CAB-C3B-C2B	2.67	137.13	128.43
24	A	837	CLA	CAC-C3C-C4C	2.67	128.27	124.79
24	j	307	CLA	CHB-C4A-NA	2.67	128.26	124.40
24	g	306	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
24	A	818	CLA	C7-C6-C5	-2.67	106.14	113.26
27	M	101	WVN	C06-C13-C15	-2.67	118.98	122.64
27	I	101	WVN	C02-C11-C19	-2.67	120.42	124.58
24	h	301	CLA	CHB-C4A-NA	2.67	128.25	124.40
24	e	606	CLA	CHB-C4A-NA	2.67	128.25	124.40
33	g	316	II0	C20-C14-C10	-2.67	119.17	124.16
24	j	304	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
24	c	605	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
24	A	830	CLA	O2D-CGD-CBD	2.67	115.89	111.23
24	i	602	CLA	CHB-C4A-NA	2.67	128.25	124.40
33	g	318	II0	C42-C41-C39	-2.67	118.06	123.52
24	b	307	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
24	a	305	CLA	C1-C2-C3	-2.67	121.83	126.20
34	a	316	IHT	C12-C15-C11	-2.66	114.95	120.50
33	e	612	II0	C19-C13-C11	2.66	119.32	114.42
24	b	313	CLA	C1-C2-C3	-2.66	121.83	126.20
27	R	202	WVN	C23-C20-C13	-2.66	119.88	127.00
33	e	612	II0	C20-C14-C10	-2.66	119.18	124.16
24	k	610	CLA	C4A-NA-C1A	2.66	107.89	106.68
24	k	603	CLA	CHB-C4A-NA	2.66	128.24	124.40
24	j	304	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
28	A	851	LMT	O5B-C5B-C4B	2.66	114.49	109.70
24	c	612	CLA	CMB-C2B-C3B	2.66	132.81	126.55
33	O	202	II0	C11-C13-C09	-2.66	114.96	120.50
34	f	617	IHT	C20-C15-C12	2.66	119.31	114.42
35	g	312	KC2	CAB-C3B-C2B	2.66	137.07	128.43
27	e	615	WVN	C30-C33-C34	-2.66	119.08	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	601	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
33	h	309	II0	C19-C13-C11	2.66	119.31	114.42
24	O	201	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
24	A	842	CLA	CMB-C2B-C3B	2.66	132.80	126.55
24	a	311	CLA	CAC-C3C-C2C	2.66	132.44	127.56
24	i	610	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
33	k	616	II0	C19-C13-C09	-2.66	119.19	124.16
24	a	311	CLA	CHA-C1A-NA	-2.65	120.38	126.39
27	F	205	WVN	C26-C29-C31	-2.65	115.51	123.20
24	L	203	CLA	C1-C2-C3	-2.65	121.85	126.20
24	A	810	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	A	812	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
24	k	603	CLA	C3A-C2A-C1A	2.65	105.31	101.34
24	L	203	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	h	303	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	b	308	CLA	CMC-C2C-C1C	-2.65	120.89	125.03
24	c	601	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	f	610	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	h	303	CLA	CAA-CBA-CGA	-2.65	105.69	113.21
32	b	301	LMG	O8-C28-C29	2.65	119.90	111.83
24	A	826	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
34	R	204	IHT	C20-C15-C12	2.65	119.29	114.42
24	A	821	CLA	CHB-C4A-NA	2.65	128.22	124.40
33	h	311	II0	C30-C32-C34	-2.65	115.54	123.20
24	f	604	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
24	k	603	CLA	CAA-C2A-C1A	-2.64	103.31	111.97
24	A	804	CLA	CMB-C2B-C3B	2.64	132.77	126.55
35	g	313	KC2	CAB-C3B-C2B	2.64	137.02	128.43
24	d	302	CLA	C1-C2-C3	-2.64	121.87	126.20
24	j	306	CLA	CHA-C1A-NA	-2.64	120.41	126.39
24	B	816	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
35	k	612	KC2	CMB-C2B-C1B	2.64	129.38	124.73
33	k	621	II0	C29-C31-C33	-2.64	115.56	123.20
27	A	847	WVN	C40-C37-C34	-2.64	123.58	127.28
24	e	607	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
34	k	618	IHT	C30-C32-C33	-2.64	119.13	126.36
24	k	607	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
24	B	818	CLA	CMB-C2B-C3B	2.64	132.75	126.55
32	L	208	LMG	C1-C2-C3	2.63	115.55	110.01
35	i	616	KC2	O2D-CGD-O1D	-2.63	118.72	123.85
24	k	603	CLA	CMB-C2B-C3B	2.63	132.75	126.55
32	O	204	LMG	O7-C10-C11	2.63	120.60	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	848	WVN	C28-C30-C33	-2.63	115.58	123.20
24	B	833	CLA	C4-C3-C5	2.63	119.80	115.23
24	J	105	CLA	CBA-CAA-C2A	-2.63	105.97	113.79
27	B	848	WVN	C30-C28-C25	2.63	130.97	127.28
33	b	315	II0	C06-C04-C10	2.63	114.67	109.49
24	O	201	CLA	CBC-CAC-C3C	2.63	119.55	112.42
24	g	303	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
24	A	826	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
24	d	306	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
33	g	320	II0	C38-C36-C34	2.63	122.10	118.09
24	A	825	CLA	CHB-C4A-NA	2.63	128.19	124.40
24	B	837	CLA	CMB-C2B-C1B	-2.63	121.42	125.42
24	A	805	CLA	CHB-C4A-NA	2.62	128.19	124.40
24	L	207	CLA	CMB-C2B-C3B	2.62	132.72	126.55
24	B	824	CLA	CHB-C4A-NA	2.62	128.19	124.40
33	O	202	II0	C42-C41-C39	-2.62	118.15	123.52
34	b	317	IHT	C19-C10-C09	2.62	119.19	113.60
24	d	308	CLA	CHB-C4A-NA	2.62	128.19	124.40
24	J	105	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
27	B	845	WVN	C35-C32-C31	2.62	122.09	118.09
24	a	302	CLA	CHB-C4A-NA	2.62	128.19	124.40
24	b	311	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
33	e	614	II0	C05-C03-C09	2.62	114.66	109.49
33	g	317	II0	C19-C13-C09	-2.62	119.26	124.16
24	f	608	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	A	807	CLA	O2D-CGD-CBD	2.62	115.81	111.23
24	B	830	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
34	c	615	IHT	C30-C32-C33	-2.62	119.18	126.36
24	k	614	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
27	R	201	WVN	C30-C33-C34	-2.62	119.18	126.36
24	g	308	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	g	322	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	g	321	LHG	C5-O7-C7	-2.62	111.53	117.80
33	k	616	II0	C06-C04-C10	2.62	114.64	109.49
33	k	617	II0	C31-C33-C35	-2.62	119.19	126.36
24	h	312	CLA	O2D-CGD-CBD	2.62	115.80	111.23
27	A	847	WVN	C35-C32-C31	-2.62	114.09	118.09
30	B	843	DGD	C2G-O2G-C1B	-2.62	111.54	117.80
33	d	314	II0	C31-C29-C25	-2.61	119.30	126.61
33	b	314	II0	C06-C04-C10	2.61	114.64	109.49
33	b	314	II0	C21-C23-C25	-2.61	167.35	176.23
24	j	314	CLA	CMB-C2B-C3B	2.61	132.69	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	e	612	II0	C06-C04-C10	2.61	114.64	109.49
24	A	819	CLA	CMC-C2C-C3C	2.61	133.21	126.15
24	j	303	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
24	B	834	CLA	CHB-C4A-NA	2.61	128.16	124.40
24	B	839	CLA	C3B-C4B-NB	-2.61	108.20	110.53
33	a	314	II0	C20-C14-C12	2.61	119.22	114.42
33	d	313	II0	C31-C33-C35	-2.61	119.22	126.36
24	c	605	CLA	C1-C2-C3	-2.61	121.93	126.20
33	f	616	II0	C31-C33-C35	-2.61	119.22	126.36
25	B	842	PQN	C2M-C2-C3	-2.61	120.17	124.45
24	h	305	CLA	CMB-C2B-C3B	2.61	132.68	126.55
27	A	849	WVN	C16-C05-C09	-2.61	113.61	122.37
34	j	317	IHT	C31-C34-C35	-2.61	119.22	126.36
26	d	316	LHG	O8-C23-C24	2.61	119.78	111.83
24	B	818	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
24	B	833	CLA	CMB-C2B-C3B	2.60	132.67	126.55
33	i	613	II0	C41-C42-C40	-2.60	118.19	123.52
24	b	304	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
35	k	612	KC2	C2D-C1D-ND	-2.60	107.63	110.33
35	e	609	KC2	CAB-C3B-C2B	2.60	136.89	128.43
27	A	849	WVN	C20-C13-C15	-2.60	115.56	121.56
27	F	204	WVN	C16-C05-C09	-2.60	113.62	122.37
24	i	604	CLA	C2A-C1A-CHA	2.60	128.38	123.87
24	e	608	CLA	C3B-C4B-NB	-2.60	108.21	110.53
35	g	313	KC2	CAA-CBA-CGA	-2.60	113.82	127.05
24	B	822	CLA	C11-C12-C13	-2.60	107.32	115.97
24	h	307	CLA	C2A-C1A-CHA	2.60	128.38	123.87
35	d	310	KC2	CAA-CBA-CGA	-2.60	113.83	127.05
24	A	803	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	A	816	CLA	CHB-C4A-NA	2.60	128.15	124.40
33	c	613	II0	C29-C31-C33	-2.60	115.67	123.20
24	c	602	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
24	f	601	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	i	604	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
24	A	806	CLA	CAA-CBA-CGA	-2.60	105.84	113.21
24	A	809	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
24	A	810	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
24	g	304	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	e	603	CLA	CHB-C4A-NA	2.59	128.14	124.40
27	L	201	WVN	C26-C29-C31	-2.59	115.69	123.20
26	f	619	LHG	O8-C23-C24	2.59	119.74	111.83
24	e	611	CLA	O2A-CGA-O1A	-2.59	117.14	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	309	CLA	CHB-C4A-NA	2.59	128.14	124.40
33	k	617	II0	C31-C29-C25	-2.59	119.36	126.61
24	O	205	CLA	CBA-CAA-C2A	2.59	121.50	113.79
24	B	836	CLA	CBC-CAC-C3C	2.59	119.44	112.42
24	f	603	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	j	309	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
24	c	604	CLA	C1-C2-C3	-2.59	121.96	126.20
24	e	610	CLA	CMB-C2B-C3B	2.59	132.64	126.55
27	B	849	WVN	C39-C36-C32	-2.59	123.65	127.28
24	B	835	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
27	A	847	WVN	C12-C14-C15	-2.59	109.44	114.06
24	a	307	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
24	e	601	CLA	CHB-C4A-NA	2.58	128.13	124.40
30	B	843	DGD	C3G-O3G-C1D	-2.58	108.26	113.80
33	f	615	II0	C30-C32-C34	-2.58	115.72	123.20
24	B	803	CLA	CHC-C4B-NB	2.58	127.92	124.05
27	K	103	WVN	C01-C02-C11	-2.58	109.86	112.83
24	A	810	CLA	CHB-C4A-NA	2.58	128.12	124.40
35	k	613	KC2	O2D-CGD-O1D	-2.58	118.83	123.85
35	k	613	KC2	CHD-C1D-C2D	2.58	134.91	127.43
33	e	616	II0	C32-C34-C36	-2.58	119.29	126.36
32	L	208	LMG	C1-O6-C5	-2.58	108.68	113.72
24	j	314	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	B	826	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	B	804	CLA	CAC-C3C-C2C	-2.58	122.82	127.56
24	A	828	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
24	B	820	CLA	C3B-C4B-NB	-2.58	108.23	110.53
24	B	820	CLA	CHB-C4A-NA	2.57	128.12	124.40
24	A	829	CLA	CMB-C2B-C3B	2.57	132.60	126.55
33	e	614	II0	C20-C14-C12	2.57	119.15	114.42
24	f	610	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
33	k	621	II0	C20-C14-C10	-2.57	119.35	124.16
33	j	318	II0	C12-C14-C10	-2.57	115.15	120.50
24	d	308	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
24	A	802	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
35	k	611	KC2	CAB-C3B-C2B	2.57	136.78	128.43
35	c	610	KC2	C1D-CHD-C4C	-2.57	120.21	126.25
33	e	616	II0	C31-C29-C25	-2.57	119.43	126.61
24	f	606	CLA	C1-C2-C3	-2.57	121.99	126.20
24	k	604	CLA	CMB-C2B-C3B	2.57	132.59	126.55
24	j	313	CLA	C1D-ND-C4D	-2.57	104.51	106.31
31	B	844	LMU	O1B-C4'-C3'	2.57	113.75	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	g	317	II0	C20-C14-C12	2.57	119.14	114.42
33	d	315	II0	C32-C30-C26	-2.57	119.43	126.61
24	A	805	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
27	K	103	WVN	C39-C40-C37	-2.57	118.27	123.52
24	a	308	CLA	CHB-C4A-NA	2.57	128.10	124.40
35	c	610	KC2	O2D-CGD-O1D	-2.56	118.86	123.85
24	B	813	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
24	c	608	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
27	A	848	WVN	C07-C01-C02	2.56	113.43	109.55
24	j	309	CLA	C3B-C4B-NB	-2.56	108.24	110.53
24	B	801	CLA	C1-C2-C3	-2.56	122.00	126.20
24	A	807	CLA	CMB-C2B-C3B	2.56	132.57	126.55
24	b	308	CLA	CMC-C2C-C3C	2.56	133.07	126.15
24	i	607	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
24	j	305	CLA	CMB-C2B-C3B	2.56	132.57	126.55
27	F	204	WVN	C12-C14-C15	-2.56	109.49	114.06
24	B	814	CLA	CHB-C4A-NA	2.56	128.09	124.40
27	L	206	WVN	C29-C26-C22	-2.56	123.69	127.28
33	j	315	II0	C19-C13-C11	2.56	119.12	114.42
24	A	812	CLA	CAC-C3C-C4C	2.56	128.12	124.79
24	g	307	CLA	C3B-C4B-NB	-2.56	108.25	110.53
24	h	302	CLA	O2D-CGD-CBD	2.56	115.70	111.23
24	A	824	CLA	C2A-C1A-CHA	2.56	128.30	123.87
35	g	313	KC2	CHD-C1D-C2D	2.56	134.84	127.43
24	h	304	CLA	CMB-C2B-C3B	2.56	132.56	126.55
24	B	834	CLA	O2D-CGD-CBD	2.55	115.69	111.23
33	g	317	II0	C06-C04-C10	2.55	114.52	109.49
24	A	813	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	k	608	CLA	CHB-C4A-NA	2.55	128.08	124.40
33	k	615	II0	C41-C39-C35	-2.55	123.70	127.28
34	f	617	IHT	C31-C29-C26	-2.55	119.47	126.61
24	f	613	CLA	CHB-C4A-NA	2.55	128.08	124.40
24	A	838	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
24	f	602	CLA	C1-O2A-CGA	2.55	122.83	116.65
24	A	826	CLA	O2D-CGD-CBD	2.55	115.69	111.23
24	i	603	CLA	CMB-C2B-C3B	2.55	132.55	126.55
33	b	318	II0	C41-C42-C40	-2.55	118.30	123.52
24	A	808	CLA	CMB-C2B-C3B	2.55	132.55	126.55
24	e	603	CLA	CMB-C2B-C3B	2.55	132.55	126.55
33	c	613	II0	C31-C33-C35	-2.55	119.37	126.36
24	A	828	CLA	CHB-C4A-NA	2.55	128.08	124.40
24	a	306	CLA	O2A-CGA-O1A	-2.55	116.78	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I	102	CLA	C6-C7-C8	-2.55	107.50	115.97
24	j	307	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
24	B	806	CLA	O1D-CGD-CBD	2.55	129.54	124.52
24	B	806	CLA	C3B-C4B-NB	-2.55	108.26	110.53
33	c	614	II0	C20-C14-C12	2.54	119.10	114.42
33	k	615	II0	C12-C14-C10	-2.54	115.20	120.50
33	f	614	II0	C30-C32-C34	-2.54	115.83	123.20
27	B	846	WVN	C39-C36-C32	-2.54	123.71	127.28
24	A	812	CLA	CAA-CBA-CGA	-2.54	105.99	113.21
24	A	855	CLA	CHB-C1B-NB	2.54	127.86	124.05
24	B	827	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	f	604	CLA	CMB-C2B-C3B	2.54	132.53	126.55
24	d	303	CLA	CAC-C3C-C4C	2.54	128.10	124.79
24	a	303	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
24	B	820	CLA	O2D-CGD-CBD	2.54	115.67	111.23
27	A	846	WVN	C38-C34-C37	-2.54	118.70	122.82
24	e	604	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
33	c	613	II0	C31-C29-C25	-2.54	119.51	126.61
24	k	609	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
24	j	309	CLA	CHB-C4A-NA	2.54	128.06	124.40
26	B	802	LHG	O8-C23-C24	2.54	119.57	111.83
24	k	614	CLA	CHB-C4A-NA	2.54	128.06	124.40
33	a	315	II0	C06-C04-C10	2.54	114.49	109.49
24	c	601	CLA	C3B-C4B-NB	-2.54	108.27	110.53
24	B	816	CLA	CHB-C4A-NA	2.54	128.06	124.40
33	f	616	II0	C41-C42-C40	-2.54	118.33	123.52
33	c	614	II0	C18-C04-C10	-2.53	105.98	110.52
24	h	306	CLA	CHB-C4A-NA	2.53	128.06	124.40
24	A	852	CLA	C4D-C3D-CAD	-2.53	105.35	108.11
24	A	836	CLA	CMB-C2B-C3B	2.53	132.51	126.55
27	e	615	WVN	C02-C11-C19	-2.53	120.64	124.58
33	c	614	II0	C42-C41-C39	-2.53	118.33	123.52
33	c	614	II0	C38-C36-C34	2.53	121.96	118.09
24	i	608	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
24	B	807	CLA	CHB-C4A-NA	2.53	128.06	124.40
24	a	303	CLA	CHB-C4A-NA	2.53	128.06	124.40
27	h	308	WVN	C20-C23-C25	-2.53	122.49	126.23
35	g	314	KC2	CBC-CAC-C3C	-2.53	114.88	127.53
33	g	318	II0	C31-C33-C35	-2.53	119.42	126.36
34	b	316	IHT	C20-C15-C12	2.53	119.08	114.42
27	L	205	WVN	C23-C25-C28	2.53	122.99	119.01
27	B	845	WVN	C12-C14-C15	-2.53	109.54	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	306	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
24	A	817	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
24	d	303	CLA	C2C-C1C-NC	2.53	112.64	109.98
27	B	846	WVN	C19-C22-C26	-2.53	115.03	119.01
33	a	315	II0	C16-C03-C09	-2.53	105.99	110.52
24	g	310	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
33	c	616	II0	C27-C25-C29	-2.53	119.28	124.18
24	h	302	CLA	C3B-C4B-NB	-2.53	108.28	110.53
35	j	312	KC2	CAA-CBA-CGA	-2.53	114.21	127.05
33	k	621	II0	C19-C13-C11	2.52	119.06	114.42
24	f	602	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	A	821	CLA	CMB-C2B-C3B	2.52	132.49	126.55
33	g	316	II0	C31-C29-C25	-2.52	119.55	126.61
24	A	836	CLA	O2D-CGD-CBD	2.52	115.64	111.23
24	B	812	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	B	835	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	B	808	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
24	A	805	CLA	O2D-CGD-CBD	2.52	115.64	111.23
33	b	315	II0	C11-C13-C09	-2.52	115.25	120.50
24	A	852	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
24	k	602	CLA	CMC-C2C-C1C	-2.52	121.09	125.03
24	e	603	CLA	O2D-CGD-CBD	2.52	115.64	111.23
27	F	205	WVN	C39-C40-C37	2.52	128.68	123.52
24	h	302	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
24	g	304	CLA	C1-C2-C3	-2.52	122.07	126.20
35	i	616	KC2	C1D-CHD-C4C	-2.52	120.32	126.25
24	g	305	CLA	CMB-C2B-C3B	2.52	132.47	126.55
27	B	846	WVN	C23-C20-C13	-2.52	120.27	127.00
31	B	844	LMU	C3'-C4'-C5'	-2.52	105.35	110.93
35	k	612	KC2	CAB-C3B-C4B	-2.52	118.81	124.82
33	j	315	II0	C20-C14-C12	2.52	119.05	114.42
35	j	312	KC2	C2B-C1B-NB	2.52	112.62	110.13
32	O	204	LMG	C8-O7-C10	-2.52	111.78	117.80
33	j	315	II0	C17-C04-C10	-2.52	106.01	110.52
33	j	318	II0	C37-C35-C33	2.51	121.93	118.09
35	k	611	KC2	C3B-C2B-C1B	-2.51	104.67	107.05
27	B	845	WVN	C21-C15-C13	-2.51	121.74	124.48
27	K	103	WVN	C30-C33-C34	-2.51	119.48	126.36
35	c	610	KC2	CAA-CBA-CGA	-2.51	114.28	127.05
24	B	801	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	B	828	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	k	607	CLA	CHB-C4A-NA	2.51	128.02	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	310	CLA	C1-C2-C3	-2.51	122.09	126.20
35	k	612	KC2	CAC-C3C-C2C	-2.51	120.29	128.43
32	F	206	LMG	O8-C28-C29	2.51	119.47	111.83
24	h	307	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
24	k	601	CLA	CAA-CBA-CGA	-2.50	106.10	113.21
24	O	201	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	e	606	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
24	k	606	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	F	202	CLA	O2D-CGD-CBD	2.50	115.60	111.23
33	e	616	II0	C20-C14-C12	2.50	119.02	114.42
24	f	603	CLA	O2D-CGD-CBD	2.50	115.60	111.23
24	B	803	CLA	O1D-CGD-CBD	2.50	129.44	124.52
24	B	822	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
24	d	302	CLA	CHB-C1B-NB	2.50	127.79	124.05
33	g	317	II0	C29-C31-C33	-2.50	115.97	123.20
24	A	814	CLA	O2D-CGD-CBD	2.50	115.59	111.23
26	A	845	LHG	C9-C8-C7	-2.50	104.55	113.69
24	c	608	CLA	CED-O2D-CGD	2.50	121.58	115.92
24	a	309	CLA	O2A-CGA-O1A	-2.50	117.39	123.63
25	B	842	PQN	C12-C11-C3	-2.50	105.94	112.08
33	j	315	II0	C37-C35-C33	2.49	121.90	118.09
24	c	608	CLA	CMB-C2B-C3B	2.49	132.41	126.55
24	A	825	CLA	CMB-C2B-C3B	2.49	132.41	126.55
24	h	312	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	B	809	CLA	CHB-C1B-NB	2.49	127.79	124.05
24	B	824	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
24	c	604	CLA	O1D-CGD-CBD	2.49	129.43	124.52
24	b	309	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	B	807	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
24	B	821	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
24	g	309	CLA	O2D-CGD-CBD	2.49	115.58	111.23
35	g	312	KC2	CAC-C3C-C4C	2.49	135.39	124.39
24	O	205	CLA	CAA-CBA-CGA	2.49	120.27	113.21
27	A	847	WVN	C07-C01-C02	2.49	113.31	109.55
24	i	601	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	A	830	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	f	609	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	A	826	CLA	C3A-C2A-C1A	2.49	105.06	101.34
33	a	313	II0	C41-C42-C40	-2.49	118.43	123.52
24	B	822	CLA	C2A-C1A-CHA	2.49	128.18	123.87
33	j	316	II0	C12-C14-C10	-2.49	115.33	120.50
24	e	602	CLA	CMB-C2B-C3B	2.49	132.40	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	319	LMT	C3'-C4'-C5'	-2.48	105.73	110.23
24	j	305	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
24	a	305	CLA	O2A-CGA-O1A	-2.48	117.41	123.63
24	B	833	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	c	618	LHG	C5-O7-C7	-2.48	111.85	117.80
33	k	615	II0	C20-C14-C10	-2.48	119.52	124.16
24	c	612	CLA	O1D-CGD-CBD	2.48	129.41	124.52
34	b	316	IHT	C31-C29-C26	-2.48	119.67	126.61
24	I	102	CLA	CHB-C4A-NA	2.48	127.98	124.40
24	c	612	CLA	CHB-C4A-NA	2.48	127.98	124.40
31	B	844	LMU	O5'-C5'-C4'	2.48	114.85	109.72
24	A	814	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
27	J	101	WVN	C30-C33-C34	-2.48	119.56	126.36
35	i	609	KC2	CGD-CBD-CAD	-2.48	102.82	110.85
24	B	831	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	A	812	CLA	CMB-C2B-C3B	2.48	132.37	126.55
24	f	612	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
33	d	315	II0	C05-C03-C09	2.48	114.37	109.49
24	b	305	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
24	f	603	CLA	CAA-C2A-C3A	-2.47	106.31	113.00
24	B	840	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	f	603	CLA	C3B-C4B-NB	-2.47	108.32	110.53
33	j	318	II0	C32-C34-C36	-2.47	119.58	126.36
24	d	312	CLA	C2A-C1A-CHA	2.47	128.16	123.87
24	B	822	CLA	CMB-C2B-C3B	2.47	132.37	126.55
24	K	102	CLA	C2A-C1A-CHA	2.47	128.16	123.87
33	a	315	II0	C30-C32-C34	-2.47	116.04	123.20
24	k	605	CLA	CHB-C4A-NA	2.47	127.97	124.40
27	F	205	WVN	C38-C34-C37	-2.47	118.81	122.82
24	A	835	CLA	CHB-C4A-NA	2.47	127.97	124.40
33	O	202	II0	C19-C13-C09	-2.47	119.54	124.16
24	g	302	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	B	830	CLA	CHB-C4A-NA	2.47	127.96	124.40
35	g	314	KC2	C1D-CHD-C4C	-2.47	120.44	126.25
24	L	207	CLA	CAC-C3C-C4C	2.47	128.00	124.79
33	c	616	II0	C31-C29-C25	-2.47	119.71	126.61
24	i	610	CLA	CMB-C2B-C3B	2.47	132.35	126.55
34	b	316	IHT	C04-C02-C07	2.47	114.02	110.44
24	B	824	CLA	C1-C2-C3	-2.47	122.16	126.20
35	e	609	KC2	C2A-C1A-NA	2.47	113.29	109.34
24	b	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
24	A	839	CLA	C1-O2A-CGA	-2.47	110.68	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	302	CLA	CHB-C4A-NA	2.46	127.96	124.40
31	B	844	LMU	O1'-C1'-C2'	2.46	112.02	108.27
28	A	851	LMT	C1B-O5B-C5B	2.46	118.53	113.72
24	A	837	CLA	CHC-C4B-NB	2.46	127.75	124.05
24	c	609	CLA	CHB-C1B-NB	2.46	127.75	124.05
24	f	607	CLA	CAA-CBA-CGA	-2.46	106.22	113.21
35	i	609	KC2	C2B-C1B-NB	2.46	112.56	110.13
24	h	305	CLA	C1-C2-C3	-2.46	122.16	126.20
24	A	825	CLA	O2D-CGD-CBD	2.46	115.53	111.23
24	k	614	CLA	O2D-CGD-CBD	2.46	115.53	111.23
34	k	618	IHT	C02-C07-C10	-2.46	119.27	122.64
24	b	307	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	A	816	CLA	CBA-CAA-C2A	2.46	121.12	113.79
24	A	806	CLA	C11-C12-C13	-2.46	107.79	115.97
33	b	318	II0	C31-C29-C25	-2.46	119.73	126.61
24	B	838	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
33	h	310	II0	C11-C13-C09	-2.46	115.38	120.50
27	B	845	WVN	C06-C13-C15	-2.46	119.28	122.64
24	B	806	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	e	602	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	B	807	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
24	e	610	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	e	603	CLA	CHB-C1B-NB	2.46	127.73	124.05
33	c	613	II0	C32-C34-C36	-2.46	119.63	126.36
28	A	851	LMT	O1B-C4'-C3'	2.46	113.47	107.23
35	g	312	KC2	C1D-CHD-C4C	-2.45	120.47	126.25
34	b	317	IHT	C20-C15-C12	2.45	118.94	114.42
33	e	613	II0	C31-C33-C35	-2.45	119.63	126.36
27	e	615	WVN	C40-C39-C36	-2.45	118.50	123.52
24	e	604	CLA	C11-C10-C8	-2.45	107.81	115.97
24	A	840	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	i	610	CLA	C2B-C1B-NB	2.45	112.87	110.33
24	f	612	CLA	CHB-C1B-C2B	-2.45	120.31	127.43
24	e	608	CLA	C2A-C1A-CHA	2.45	128.12	123.87
24	A	818	CLA	CHB-C1B-NB	2.45	127.73	124.05
33	j	316	II0	C06-C04-C10	2.45	114.32	109.49
24	e	611	CLA	CHB-C4A-NA	2.45	127.94	124.40
33	k	615	II0	C06-C04-C10	2.45	114.32	109.49
34	k	618	IHT	C40-C41-C38	-2.45	118.51	123.52
24	d	302	CLA	C3B-C4B-NB	-2.45	108.34	110.53
24	B	823	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
24	A	802	CLA	CHB-C4A-NA	2.45	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	f	608	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	c	603	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
27	B	849	WVN	C21-C15-C13	-2.45	121.81	124.48
34	R	204	IHT	C22-C18-C07	-2.45	120.46	127.00
24	A	838	CLA	O2D-CGD-CBD	2.45	115.51	111.23
27	L	206	WVN	C39-C36-C32	-2.45	123.85	127.28
24	A	835	CLA	C1-C2-C3	-2.45	122.19	126.20
24	B	841	CLA	CMB-C2B-C1B	-2.45	121.70	125.42
24	A	817	CLA	CHB-C1B-NB	2.44	127.72	124.05
33	b	318	II0	C42-C41-C39	-2.44	118.52	123.52
24	B	818	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
24	a	311	CLA	C2C-C1C-NC	2.44	112.55	109.98
33	f	614	II0	C16-C03-C09	-2.44	106.14	110.52
24	a	303	CLA	O2D-CGD-CBD	2.44	115.50	111.23
27	B	847	WVN	C28-C30-C33	-2.44	116.13	123.20
24	B	808	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	j	311	CLA	CHB-C4A-NA	2.44	127.92	124.40
33	g	318	II0	C27-C25-C29	-2.44	119.44	124.18
24	A	826	CLA	CMB-C2B-C3B	2.44	132.29	126.55
24	c	611	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	g	307	CLA	CHB-C4A-NA	2.44	127.92	124.40
33	g	317	II0	C32-C34-C36	-2.44	119.67	126.36
24	A	831	CLA	C1-C2-C3	-2.44	122.20	126.20
24	b	303	CLA	O2D-CGD-CBD	2.44	115.49	111.23
24	b	313	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	A	807	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	g	322	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
26	B	802	LHG	C5-O7-C7	-2.44	111.96	117.80
33	c	613	II0	C20-C14-C12	2.44	118.90	114.42
24	L	202	CLA	O2D-CGD-CBD	2.44	115.49	111.23
24	A	801	CLA	C1-C2-C3	-2.44	122.21	126.20
33	j	316	II0	C38-C36-C34	2.44	121.81	118.09
24	e	607	CLA	CMB-C2B-C3B	2.44	132.28	126.55
34	R	204	IHT	C36-C33-C37	-2.44	118.87	122.82
26	j	319	LHG	C6-C5-C4	-2.44	106.11	111.78
33	g	320	II0	C38-C36-C40	-2.44	118.87	122.82
24	A	834	CLA	C1-C2-C3	-2.43	122.21	126.20
24	j	314	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
24	d	309	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	k	609	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	d	302	CLA	O2D-CGD-CBD	2.43	115.48	111.23
35	i	616	KC2	CMB-C2B-C1B	2.43	129.01	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	315	CLA	C1-C2-C3	-2.43	122.21	126.20
24	a	302	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
35	f	611	KC2	CBC-CAC-C3C	-2.43	115.38	127.53
33	k	615	II0	C28-C26-C30	-2.43	119.46	124.18
24	A	838	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	R	203	CLA	CHB-C4A-NA	2.43	127.91	124.40
27	M	101	WVN	C04-C09-C05	-2.43	122.51	124.83
24	j	304	CLA	CMB-C2B-C3B	2.43	132.27	126.55
26	g	321	LHG	O8-C23-O10	-2.43	117.55	123.63
24	c	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
24	A	824	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
24	O	205	CLA	C4-C3-C5	2.43	119.44	115.23
27	I	101	WVN	C07-C01-C02	2.43	113.22	109.55
24	A	819	CLA	O2D-CGD-CBD	2.43	115.47	111.23
27	B	846	WVN	C02-C05-C09	-2.43	118.48	121.47
24	a	312	CLA	CMB-C2B-C3B	2.43	132.26	126.55
27	e	615	WVN	C20-C13-C15	-2.43	115.97	121.56
24	A	832	CLA	C6-C7-C8	-2.43	107.90	115.97
35	k	612	KC2	O1D-CGD-CBD	-2.43	119.73	124.52
35	g	312	KC2	C2B-C1B-NB	2.43	112.53	110.13
24	b	312	CLA	CHB-C4A-NA	2.43	127.90	124.40
24	j	310	CLA	CHB-C4A-NA	2.42	127.90	124.40
24	A	816	CLA	C4-C3-C2	-2.42	117.40	123.63
24	j	309	CLA	O2D-CGD-CBD	2.42	115.46	111.23
24	B	809	CLA	C3B-C4B-NB	-2.42	108.37	110.53
33	a	313	II0	C31-C29-C25	-2.42	119.85	126.61
24	K	101	CLA	O2D-CGD-CBD	2.42	115.46	111.23
24	d	312	CLA	CBA-CAA-C2A	2.42	120.99	113.79
24	B	815	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
33	h	311	II0	C31-C29-C25	-2.42	119.85	126.61
24	A	838	CLA	CMB-C2B-C3B	2.42	132.24	126.55
24	d	306	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	A	831	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	k	601	CLA	CHB-C4A-NA	2.41	127.89	124.40
34	c	615	IHT	C31-C29-C26	-2.41	119.86	126.61
35	i	616	KC2	CAB-C3B-C2B	2.41	136.28	128.43
33	h	310	II0	C32-C30-C26	-2.41	119.86	126.61
24	B	812	CLA	CMB-C2B-C1B	-2.41	121.74	125.42
33	g	318	II0	C05-C03-C09	2.41	114.24	109.49
24	A	803	CLA	C3B-C4B-NB	-2.41	108.38	110.53
34	b	316	IHT	C31-C34-C35	-2.41	119.75	126.36
27	B	846	WVN	C24-C22-C19	2.41	121.77	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	303	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	k	609	CLA	CAA-C2A-C1A	2.41	119.87	111.97
24	i	605	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	g	315	CLA	CMB-C2B-C3B	2.41	132.22	126.55
35	g	312	KC2	C4D-CHA-C1A	-2.41	115.11	122.45
24	e	611	CLA	CAA-C2A-C3A	-2.41	106.49	113.00
24	O	205	CLA	O2D-CGD-CBD	2.41	115.44	111.23
24	B	833	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	A	842	CLA	C1-C2-C3	-2.41	122.25	126.20
24	O	205	CLA	C1-C2-C3	-2.41	122.25	126.20
26	k	620	LHG	C6-C5-C4	-2.41	106.17	111.78
24	A	806	CLA	CHB-C4A-NA	2.41	127.87	124.40
24	k	603	CLA	CHB-C1B-C2B	-2.41	120.44	127.43
24	g	311	CLA	CHB-C4A-NA	2.41	127.87	124.40
24	B	835	CLA	CMB-C2B-C1B	-2.41	121.76	125.42
35	g	312	KC2	CAA-CBA-CGA	-2.41	114.82	127.05
34	a	316	IHT	C40-C41-C38	-2.40	118.60	123.52
24	A	834	CLA	C3B-C4B-NB	-2.40	108.38	110.53
24	A	815	CLA	CHB-C1B-NB	2.40	127.65	124.05
24	b	308	CLA	C1-C2-C3	-2.40	122.26	126.20
24	A	839	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	f	612	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
33	a	314	II0	C38-C36-C34	2.40	121.75	118.09
24	a	303	CLA	CMB-C2B-C3B	2.40	132.19	126.55
27	K	103	WVN	C40-C39-C36	-2.40	118.61	123.52
24	g	307	CLA	O2D-CGD-CBD	2.40	115.42	111.23
24	A	802	CLA	C3B-C4B-NB	-2.40	108.39	110.53
33	b	314	II0	C20-C14-C12	2.40	118.83	114.42
35	i	609	KC2	CAA-CBA-CGA	-2.40	114.86	127.05
27	j	301	WVN	C23-C20-C13	-2.40	120.59	127.00
24	A	814	CLA	C3B-C4B-NB	-2.40	108.39	110.53
24	e	611	CLA	C3B-C4B-NB	-2.40	108.39	110.53
33	f	615	II0	C31-C29-C25	-2.40	119.91	126.61
24	A	841	CLA	CMB-C2B-C3B	2.40	132.19	126.55
24	d	312	CLA	CMB-C2B-C3B	2.40	132.19	126.55
24	e	606	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	h	301	CLA	CMB-C2B-C3B	2.40	132.19	126.55
24	a	312	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
33	c	613	II0	C38-C36-C34	2.39	121.75	118.09
26	d	316	LHG	O3-P-O5	-2.39	99.45	108.94
24	B	826	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
24	B	818	CLA	O2A-CGA-O1A	-2.39	117.64	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	315	II0	C20-C14-C12	2.39	118.82	114.42
33	f	616	II0	C32-C34-C36	-2.39	119.80	126.36
33	i	614	II0	C32-C34-C36	-2.39	119.80	126.36
24	B	821	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	B	812	CLA	C7-C6-C5	-2.39	106.89	113.26
24	A	810	CLA	C3B-C4B-NB	-2.39	108.39	110.53
24	B	813	CLA	O2D-CGD-CBD	2.39	115.41	111.23
24	A	807	CLA	C11-C10-C8	-2.39	108.02	115.97
24	A	824	CLA	CHA-C1A-NA	-2.39	120.98	126.39
33	g	318	II0	C16-C03-C09	-2.39	106.24	110.52
24	g	308	CLA	O2D-CGD-CBD	2.39	115.41	111.23
24	B	808	CLA	C1-C2-C3	-2.39	122.28	126.20
33	h	311	II0	C31-C33-C35	-2.39	119.82	126.36
24	e	611	CLA	O2D-CGD-CBD	2.39	115.40	111.23
34	j	317	IHT	C40-C41-C38	-2.39	118.64	123.52
27	L	201	WVN	C28-C30-C33	-2.38	116.29	123.20
24	k	609	CLA	CMB-C2B-C3B	2.38	132.16	126.55
34	g	319	IHT	C06-C09-C10	-2.38	109.81	114.06
24	A	830	CLA	CMB-C2B-C3B	2.38	132.16	126.55
26	A	845	LHG	O8-C23-O10	-2.38	117.67	123.63
24	B	832	CLA	CHB-C4A-NA	2.38	127.84	124.40
24	e	606	CLA	O1D-CGD-CBD	2.38	129.22	124.52
24	j	305	CLA	C11-C12-C13	-2.38	108.05	115.97
24	c	601	CLA	C1-C2-C3	-2.38	122.30	126.20
24	e	605	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
24	i	611	CLA	C2A-C1A-CHA	2.38	128.00	123.87
35	d	311	KC2	CBC-CAC-C3C	-2.38	115.64	127.53
24	b	310	CLA	C3B-C4B-NB	-2.38	108.41	110.53
24	c	601	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
27	h	308	WVN	C08-C01-C02	-2.38	105.94	109.55
24	i	607	CLA	CMB-C2B-C3B	2.38	132.14	126.55
24	h	305	CLA	C11-C12-C13	-2.38	108.06	115.97
24	i	607	CLA	CHB-C4A-NA	2.38	127.83	124.40
27	B	849	WVN	C23-C20-C13	-2.38	120.65	127.00
24	c	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
35	i	609	KC2	CAC-C3C-C4C	2.38	134.89	124.39
24	B	839	CLA	C16-C15-C13	-2.38	108.07	115.97
34	R	204	IHT	C30-C32-C33	-2.38	119.85	126.36
24	j	302	CLA	CMB-C2B-C1B	-2.37	121.80	125.42
35	k	612	KC2	CMC-C2C-C1C	-2.37	121.32	125.03
24	B	841	CLA	CHB-C4A-NA	2.37	127.83	124.40
27	M	101	WVN	C28-C30-C33	-2.37	116.32	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	846	WVN	C06-C13-C15	-2.37	119.39	122.64
24	j	307	CLA	O2D-CGD-CBD	2.37	115.38	111.23
35	g	314	KC2	CHD-C1D-C2D	2.37	134.31	127.43
27	j	301	WVN	C08-C01-C03	-2.37	104.08	109.01
24	f	607	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	d	303	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
34	k	618	IHT	C29-C31-C34	-2.37	116.33	123.20
26	a	301	LHG	O7-C7-O9	-2.37	118.16	123.70
24	B	833	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
24	k	606	CLA	O2D-CGD-CBD	2.37	115.37	111.23
24	B	815	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	d	301	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	A	808	CLA	CAA-C2A-C1A	2.37	119.74	111.97
24	F	201	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
24	O	205	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	k	604	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
24	I	102	CLA	CBA-CAA-C2A	-2.37	106.75	113.79
24	B	803	CLA	CBA-CAA-C2A	-2.37	106.75	113.79
27	h	308	WVN	C21-C15-C14	2.37	118.64	113.60
26	f	620	LHG	O8-C23-C24	2.37	119.05	111.83
24	B	824	CLA	C16-C15-C13	-2.37	108.10	115.97
33	f	616	II0	C32-C30-C26	-2.37	119.99	126.61
24	A	814	CLA	CHB-C4A-NA	2.37	127.81	124.40
33	i	614	II0	C07-C11-C13	2.37	118.07	112.18
24	d	307	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	O	205	CLA	C6-C7-C8	-2.36	108.11	115.97
24	f	608	CLA	O2D-CGD-CBD	2.36	115.36	111.23
24	L	203	CLA	O2D-CGD-CBD	2.36	115.36	111.23
24	B	808	CLA	CBA-CAA-C2A	2.36	120.82	113.79
24	L	207	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	c	603	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
24	B	824	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
27	A	846	WVN	C23-C20-C13	-2.36	120.69	127.00
24	A	832	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	L	203	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	A	837	CLA	C6-C7-C8	-2.36	108.12	115.97
24	a	309	CLA	CHB-C4A-NA	2.36	127.81	124.40
33	b	318	II0	C31-C33-C35	-2.36	119.90	126.36
32	J	106	LMG	O8-C28-O10	-2.36	117.73	123.63
33	e	616	II0	C29-C31-C33	-2.36	116.37	123.20
27	F	205	WVN	C02-C11-C19	-2.36	120.91	124.58
24	b	308	CLA	O2D-CGD-O1D	-2.36	119.26	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	814	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
24	A	815	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	A	819	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	c	605	CLA	C3B-C4B-NB	-2.35	108.43	110.53
24	B	812	CLA	C1-C2-C3	-2.35	122.34	126.20
26	f	619	LHG	O7-C7-O9	-2.35	118.20	123.70
24	h	306	CLA	C3B-C4B-NB	-2.35	108.43	110.53
26	c	618	LHG	C6-C5-C4	-2.35	106.30	111.78
24	b	303	CLA	CHB-C4A-NA	2.35	127.80	124.40
33	g	316	II0	C19-C13-C11	2.35	118.75	114.42
24	A	837	CLA	CHB-C4A-NA	2.35	127.80	124.40
24	A	832	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
24	B	819	CLA	C3B-C4B-NB	-2.35	108.43	110.53
35	f	611	KC2	CAB-C3B-C4B	-2.35	119.21	124.82
33	h	310	II0	C12-C14-C10	-2.35	115.61	120.50
24	a	305	CLA	CHB-C4A-NA	2.35	127.79	124.40
33	f	616	II0	C29-C31-C33	-2.35	116.40	123.20
24	c	608	CLA	C3B-C4B-NB	-2.35	108.44	110.53
24	f	612	CLA	C1-C2-C3	-2.35	122.35	126.20
24	e	611	CLA	C7-C6-C5	-2.35	107.01	113.26
24	h	302	CLA	C1-C2-C3	-2.34	122.97	126.76
24	B	820	CLA	C1-C2-C3	-2.34	122.36	126.20
24	c	607	CLA	CMB-C2B-C3B	2.34	132.06	126.55
35	i	616	KC2	CHD-C1D-C2D	2.34	134.23	127.43
27	F	205	WVN	C28-C30-C33	2.34	129.99	123.20
24	A	839	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	f	607	CLA	C1-O2A-CGA	2.34	122.32	116.65
33	f	615	II0	C38-C36-C34	2.34	121.67	118.09
27	L	206	WVN	C02-C05-C09	-2.34	118.59	121.47
33	g	320	II0	C20-C14-C12	2.34	118.72	114.42
24	B	805	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
27	L	206	WVN	C23-C20-C13	-2.34	120.75	127.00
24	b	310	CLA	O2D-CGD-CBD	2.34	115.32	111.23
24	A	822	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	e	615	WVN	C07-C01-C02	2.34	113.09	109.55
24	B	836	CLA	O1D-CGD-CBD	2.34	129.13	124.52
35	k	612	KC2	O2D-CGD-CBD	2.34	115.32	111.23
24	k	602	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
24	a	305	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	A	831	CLA	C7-C6-C5	-2.34	107.04	113.26
24	g	310	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	c	602	CLA	C1-C2-C3	-2.34	122.98	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	837	CLA	C6-C5-C3	-2.34	107.78	113.47
24	d	304	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
32	b	301	LMG	O1-C1-C2	2.33	111.82	108.27
24	B	817	CLA	CMB-C2B-C3B	2.33	132.04	126.55
24	i	603	CLA	O2D-CGD-CBD	2.33	115.31	111.23
26	e	617	LHG	O7-C7-O9	-2.33	118.25	123.70
33	b	314	II0	C20-C14-C10	-2.33	119.80	124.16
33	h	311	II0	C32-C34-C36	-2.33	119.97	126.36
24	a	306	CLA	CHB-C4A-NA	2.33	127.77	124.40
33	e	613	II0	C29-C31-C33	-2.33	116.44	123.20
24	k	607	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
24	j	310	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
24	g	315	CLA	C4A-NA-C1A	2.33	107.74	106.68
35	g	312	KC2	C2D-C1D-ND	-2.33	107.91	110.33
24	A	841	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
24	B	817	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	d	305	CLA	CHB-C1B-NB	2.33	127.55	124.05
24	h	304	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	c	604	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
24	c	611	CLA	CAC-C3C-C4C	2.33	127.82	124.79
24	d	302	CLA	CHB-C1B-C2B	-2.33	120.66	127.43
35	i	609	KC2	O2D-CGD-O1D	-2.33	119.31	123.85
33	g	320	II0	C31-C29-C25	-2.33	120.09	126.61
24	k	614	CLA	CBC-CAC-C3C	2.33	118.73	112.42
24	i	605	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
27	A	849	WVN	C30-C33-C34	-2.33	119.98	126.36
27	J	102	WVN	C27-C25-C23	2.33	121.64	118.09
24	c	601	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
32	J	106	LMG	C8-O7-C10	-2.33	112.23	117.80
24	A	852	CLA	CAC-C3C-C4C	2.33	127.82	124.79
24	i	610	CLA	CHB-C1B-C2B	-2.33	120.67	127.43
24	A	824	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	e	607	CLA	CHB-C4A-NA	2.32	127.75	124.40
33	b	315	II0	C27-C25-C29	-2.32	119.67	124.18
34	a	316	IHT	C25-C23-C22	2.32	121.64	118.09
24	A	842	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
24	f	607	CLA	O2D-CGD-CBD	2.32	115.29	111.23
26	g	321	LHG	O4-P-O5	2.32	123.25	112.44
24	c	606	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	f	604	CLA	CHD-C1D-ND	-2.32	121.53	124.80
24	A	805	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
26	c	617	LHG	O7-C7-O9	-2.32	118.28	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	313	II0	C31-C29-C25	-2.32	120.12	126.61
33	i	613	II0	C19-C13-C11	2.32	118.69	114.42
24	B	816	CLA	C3B-C4B-NB	-2.32	108.46	110.53
35	c	610	KC2	CHD-C1D-C2D	2.32	134.16	127.43
33	h	310	II0	C29-C31-C33	-2.32	116.48	123.20
24	g	311	CLA	O2D-CGD-CBD	2.32	115.28	111.23
33	g	317	II0	C38-C36-C34	2.32	121.63	118.09
24	h	305	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	k	610	CLA	C1-C2-C3	-2.32	122.40	126.20
24	B	841	CLA	CAC-C3C-C4C	2.32	127.81	124.79
33	h	311	II0	C38-C36-C34	2.32	121.63	118.09
24	A	803	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
24	F	201	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
24	B	814	CLA	O2D-CGD-CBD	2.32	115.28	111.23
24	a	308	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
24	k	604	CLA	C1-C2-C3	-2.32	122.40	126.20
33	k	617	II0	C20-C14-C10	-2.32	119.83	124.16
32	b	301	LMG	O7-C10-O9	-2.32	118.29	123.70
33	e	614	II0	C38-C36-C34	2.32	121.62	118.09
24	e	603	CLA	C2B-C1B-NB	2.32	112.73	110.33
33	c	614	II0	C31-C29-C25	-2.31	120.14	126.61
24	A	856	CLA	CMA-C3A-C2A	-2.31	110.92	116.23
27	R	201	WVN	C07-C01-C02	2.31	113.05	109.55
24	B	834	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
35	g	312	KC2	CMB-C2B-C1B	2.31	128.80	124.73
24	A	831	CLA	CHC-C4B-NB	2.31	127.52	124.05
27	A	847	WVN	C10-C06-C13	2.31	113.80	110.44
24	f	613	CLA	C1-O2A-CGA	2.31	122.24	116.65
27	B	848	WVN	C33-C34-C37	2.31	122.64	119.01
27	A	849	WVN	C14-C15-C13	-2.31	119.58	122.70
34	R	204	IHT	C04-C02-C07	2.31	113.79	110.44
24	i	606	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
33	e	613	II0	C31-C29-C25	-2.31	120.16	126.61
24	B	824	CLA	CMB-C2B-C3B	2.31	131.98	126.55
33	k	615	II0	C30-C32-C34	-2.31	116.52	123.20
24	k	602	CLA	CAA-CBA-CGA	-2.31	106.66	113.21
24	B	816	CLA	CHD-C1D-ND	-2.31	121.56	124.80
24	b	305	CLA	O1D-CGD-CBD	2.31	129.06	124.52
24	B	819	CLA	O2D-CGD-CBD	2.31	115.26	111.23
27	R	202	WVN	C30-C33-C34	-2.30	120.05	126.36
24	c	605	CLA	CHB-C4A-NA	2.30	127.72	124.40
34	a	316	IHT	C31-C29-C26	-2.30	120.17	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	202	CLA	CHB-C1B-NB	2.30	127.50	124.05
33	k	621	II0	C41-C42-C40	-2.30	118.81	123.52
24	g	305	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
24	B	807	CLA	CMB-C2B-C3B	2.30	131.96	126.55
24	A	818	CLA	CMB-C2B-C3B	2.30	131.96	126.55
24	B	840	CLA	C3B-C4B-NB	-2.30	108.48	110.53
24	B	830	CLA	CAC-C3C-C4C	2.30	127.78	124.79
24	B	820	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
24	c	612	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	b	309	CLA	CHB-C1B-NB	2.30	127.50	124.05
24	h	303	CLA	CHA-C1A-NA	-2.30	121.19	126.39
24	c	606	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
24	B	803	CLA	C3B-C4B-NB	-2.30	108.48	110.53
24	A	811	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
27	L	206	WVN	C21-C15-C13	-2.29	121.98	124.48
33	e	614	II0	C32-C30-C26	-2.29	120.19	126.61
24	O	205	CLA	C2C-C1C-NC	2.29	112.39	109.98
26	B	802	LHG	C6-C5-C4	-2.29	106.44	111.78
33	e	613	II0	C16-C03-C09	-2.29	106.41	110.52
35	d	311	KC2	CAB-C3B-C2B	2.29	135.89	128.43
34	j	317	IHT	C31-C29-C26	-2.29	120.19	126.61
24	f	602	CLA	O2D-CGD-CBD	2.29	115.24	111.23
24	j	309	CLA	CMB-C2B-C3B	2.29	131.94	126.55
27	J	102	WVN	C10-C06-C13	2.29	113.77	110.44
26	k	620	LHG	O8-C23-C24	2.29	118.82	111.83
24	B	837	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
24	f	608	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
24	b	311	CLA	CHB-C4A-NA	2.29	127.71	124.40
24	A	804	CLA	O2D-CGD-CBD	2.29	115.23	111.23
24	B	841	CLA	CMB-C2B-C3B	2.29	131.94	126.55
24	B	827	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	B	841	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
24	B	836	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
24	d	303	CLA	C2B-C1B-NB	2.29	112.70	110.33
24	B	826	CLA	C3B-C4B-NB	-2.29	108.49	110.53
24	f	606	CLA	CAC-C3C-C4C	2.29	127.77	124.79
24	b	313	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
35	k	612	KC2	C1D-CHD-C4C	-2.29	120.87	126.25
24	A	814	CLA	CAA-C2A-C1A	-2.29	104.48	111.97
24	d	305	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
26	A	844	LHG	O8-C23-O10	-2.29	117.91	123.63
24	A	829	CLA	C11-C12-C13	-2.29	108.36	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	312	CLA	CHB-C1B-NB	2.29	127.48	124.05
33	f	616	II0	C11-C13-C09	-2.29	115.74	120.50
24	g	315	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	a	309	CLA	C3B-C4B-NB	-2.29	108.49	110.53
24	B	816	CLA	CMB-C2B-C3B	2.28	131.92	126.55
24	i	605	CLA	CHB-C4A-NA	2.28	127.70	124.40
24	g	303	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
33	a	313	II0	C28-C26-C30	-2.28	119.75	124.18
24	A	822	CLA	O2D-CGD-CBD	2.28	115.22	111.23
33	f	614	II0	C06-C04-C10	2.28	113.99	109.49
24	A	852	CLA	CMB-C2B-C3B	2.28	131.92	126.55
33	h	309	II0	C30-C32-C34	-2.28	120.69	125.28
24	g	304	CLA	O1D-CGD-CBD	2.28	129.02	124.52
35	j	312	KC2	CAA-C2A-C1A	2.28	134.64	124.64
33	c	614	II0	C20-C14-C10	-2.28	119.89	124.16
34	a	316	IHT	C36-C33-C32	2.28	121.57	118.09
27	A	846	WVN	C29-C31-C32	-2.28	120.11	126.36
33	e	613	II0	C19-C13-C09	-2.28	119.90	124.16
33	k	619	II0	C41-C42-C40	-2.28	118.86	123.52
33	a	313	II0	C06-C04-C10	2.28	113.98	109.49
24	e	601	CLA	C2A-C1A-CHA	2.28	127.82	123.87
33	b	314	II0	C30-C32-C34	-2.28	116.60	123.20
24	g	306	CLA	CHB-C4A-NA	2.28	127.69	124.40
33	d	315	II0	C28-C26-C30	-2.28	119.76	124.18
24	A	832	CLA	C11-C10-C8	-2.28	108.40	115.97
34	k	618	IHT	C22-C18-C07	-2.28	120.92	127.00
24	A	823	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
24	j	310	CLA	C3B-C4B-NB	-2.28	108.50	110.53
33	J	104	II0	C33-C35-C39	-2.27	115.43	119.01
24	b	310	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
24	i	603	CLA	CHB-C4A-NA	2.27	127.68	124.40
35	g	314	KC2	CMB-C2B-C1B	2.27	128.73	124.73
24	k	601	CLA	C1-C2-C3	-2.27	122.47	126.20
33	k	619	II0	C05-C03-C09	2.27	113.97	109.49
24	A	813	CLA	CHB-C4A-NA	2.27	127.68	124.40
24	g	302	CLA	C2A-C1A-CHA	2.27	127.81	123.87
24	d	302	CLA	C4A-NA-C1A	2.27	107.72	106.68
32	L	208	LMG	O7-C10-O9	-2.27	118.39	123.70
24	A	801	CLA	CHB-C4A-NA	2.27	127.68	124.40
35	k	611	KC2	CMB-C2B-C1B	2.27	128.73	124.73
27	B	847	WVN	C10-C06-C13	2.27	113.74	110.44
24	k	614	CLA	CHC-C4B-NB	2.27	127.46	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	836	CLA	CHB-C4A-NA	2.27	127.68	124.40
24	f	612	CLA	CHB-C4A-NA	2.27	127.68	124.40
24	f	610	CLA	C3B-C4B-NB	-2.27	108.50	110.53
24	b	306	CLA	CHC-C4B-NB	2.27	127.45	124.05
24	k	601	CLA	CHC-C4B-NB	2.27	127.45	124.05
33	a	313	II0	C42-C41-C39	-2.27	118.88	123.52
24	a	307	CLA	C3B-C4B-NB	-2.27	108.50	110.53
34	g	319	IHT	C20-C15-C12	2.27	118.59	114.42
26	d	316	LHG	O4-P-O5	2.27	122.99	112.44
24	b	306	CLA	CAC-C3C-C4C	2.27	127.74	124.79
24	c	604	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
24	c	609	CLA	C4A-NA-C1A	2.27	107.71	106.68
35	g	313	KC2	C2B-C1B-NB	2.27	112.37	110.13
24	A	809	CLA	O1D-CGD-CBD	2.27	128.99	124.52
24	b	311	CLA	CMB-C2B-C3B	2.26	131.88	126.55
24	c	606	CLA	CHB-C4A-NA	2.26	127.67	124.40
24	B	825	CLA	C3B-C4B-NB	-2.26	108.51	110.53
32	O	204	LMG	O7-C10-O9	-2.26	118.41	123.70
24	A	820	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
33	f	616	II0	C12-C14-C10	-2.26	115.79	120.50
27	J	102	WVN	C23-C20-C13	-2.26	120.95	127.00
34	g	319	IHT	C19-C10-C09	2.26	118.42	113.60
24	B	809	CLA	C1-C2-C3	-2.26	122.49	126.20
24	b	305	CLA	C4-C3-C5	2.26	119.15	115.23
27	M	101	WVN	C40-C39-C36	-2.26	118.89	123.52
27	M	101	WVN	C26-C29-C31	-2.26	116.65	123.20
33	k	619	II0	C41-C39-C35	-2.26	124.11	127.28
35	e	609	KC2	O2D-CGD-CBD	2.26	115.18	111.23
35	k	611	KC2	CAA-CBA-CGA	-2.26	115.56	127.05
33	g	320	II0	C29-C31-C33	-2.26	116.66	123.20
26	d	316	LHG	C5-O7-C7	-2.26	112.39	117.80
27	A	847	WVN	C17-C06-C13	2.26	113.78	110.24
33	e	614	II0	C28-C26-C30	-2.26	119.80	124.18
24	g	304	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
24	B	815	CLA	CMB-C2B-C3B	2.26	131.86	126.55
24	i	611	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
24	c	608	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	B	832	CLA	O2D-CGD-CBD	2.25	115.17	111.23
27	R	201	WVN	C06-C13-C15	-2.25	119.56	122.64
27	j	301	WVN	C04-C09-C05	-2.25	122.68	124.83
30	B	843	DGD	O3G-C1D-C2D	2.25	111.69	108.27
24	A	804	CLA	C6-C7-C8	-2.25	108.48	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	836	CLA	C2A-C1A-CHA	2.25	127.78	123.87
27	R	201	WVN	C40-C39-C36	-2.25	118.91	123.52
24	a	307	CLA	C6-C7-C8	-2.25	108.48	115.97
24	B	834	CLA	C3B-C4B-NB	-2.25	108.52	110.53
24	j	303	CLA	CHB-C4A-NA	2.25	127.65	124.40
33	k	616	II0	C28-C26-C30	-2.25	119.81	124.18
35	g	314	KC2	CAB-C3B-C2B	2.25	135.75	128.43
24	A	816	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	L	201	WVN	C29-C31-C32	-2.25	120.19	126.36
33	j	316	II0	C32-C30-C26	-2.25	120.32	126.61
33	g	318	II0	C38-C36-C34	2.25	121.53	118.09
26	b	320	LHG	O8-C23-C24	2.25	118.69	111.83
24	B	813	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	B	805	CLA	CMB-C2B-C3B	2.25	131.84	126.55
33	a	313	II0	C38-C36-C34	2.25	121.52	118.09
24	A	820	CLA	CHB-C1B-NB	2.25	127.42	124.05
33	e	614	II0	C19-C13-C11	2.25	118.56	114.42
24	A	827	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	A	808	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
24	i	604	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
24	e	610	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
24	f	612	CLA	CMB-C2B-C3B	2.25	131.83	126.55
24	L	203	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
27	B	846	WVN	C28-C30-C33	-2.24	116.70	123.20
24	B	825	CLA	CHA-C1A-NA	-2.24	121.31	126.39
33	J	104	II0	C15-C03-C09	-2.24	106.50	110.52
35	e	609	KC2	CGD-CBD-CAD	-2.24	103.58	110.85
35	f	611	KC2	C2B-C1B-NB	2.24	112.35	110.13
24	A	821	CLA	CHD-C1D-ND	-2.24	121.65	124.80
24	g	304	CLA	C3B-C4B-NB	-2.24	108.53	110.53
35	i	609	KC2	O2D-CGD-CBD	2.24	115.15	111.23
26	c	618	LHG	O7-C7-O9	-2.24	118.46	123.70
24	B	803	CLA	C1-C2-C3	-2.24	122.53	126.20
24	a	302	CLA	CBC-CAC-C3C	2.24	118.50	112.42
24	B	840	CLA	CHB-C1B-NB	2.24	127.41	124.05
34	O	203	IHT	C28-C26-C29	-2.24	119.83	124.18
24	f	607	CLA	C4A-NA-C1A	2.24	107.70	106.68
24	B	838	CLA	O2D-CGD-CBD	2.24	115.14	111.23
24	A	853	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
24	c	611	CLA	O2A-CGA-O1A	-2.24	117.57	123.33
27	R	201	WVN	C16-C05-C09	-2.24	114.84	122.37
33	f	618	II0	C28-C26-C30	-2.24	119.83	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	844	LHG	C5-O7-C7	-2.24	112.44	117.80
27	A	850	WVN	C01-C02-C11	-2.24	110.25	112.83
24	i	608	CLA	CHB-C4A-NA	2.24	127.63	124.40
33	c	613	II0	C42-C41-C39	-2.24	118.94	123.52
33	i	614	II0	C27-C25-C29	-2.24	119.84	124.18
24	j	308	CLA	CHB-C1B-NB	2.24	127.40	124.05
33	f	618	II0	C05-C03-C09	2.24	113.89	109.49
34	R	204	IHT	C03-C05-C08	-2.24	108.69	113.59
24	d	312	CLA	CHA-C1A-NA	-2.24	121.33	126.39
24	g	309	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
27	R	202	WVN	C14-C15-C13	-2.23	119.69	122.70
24	g	303	CLA	C1-C2-C3	-2.23	123.15	126.76
24	B	823	CLA	O1D-CGD-CBD	2.23	128.92	124.52
24	f	609	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
24	g	307	CLA	C1-C2-C3	-2.23	122.54	126.20
35	f	611	KC2	CAA-CBA-CGA	-2.23	115.70	127.05
24	B	837	CLA	CMB-C2B-C3B	2.23	131.80	126.55
26	i	615	LHG	O7-C7-O9	-2.23	118.49	123.70
33	c	614	II0	C05-C03-C09	2.23	113.89	109.49
24	g	315	CLA	CHB-C1B-NB	2.23	127.39	124.05
33	j	316	II0	C20-C14-C12	2.23	118.52	114.42
24	j	313	CLA	CHB-C4A-NA	2.23	127.62	124.40
24	L	203	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
24	A	828	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
24	B	829	CLA	CHB-C4A-NA	2.23	127.61	124.40
24	j	307	CLA	CHC-C4B-NB	2.23	127.39	124.05
24	B	817	CLA	C1-C2-C3	-2.23	122.55	126.20
27	B	848	WVN	C20-C13-C15	-2.23	116.43	121.56
27	A	848	WVN	C29-C31-C32	-2.23	120.26	126.36
27	h	308	WVN	C06-C13-C20	2.23	121.69	115.65
24	A	818	CLA	CHB-C4A-NA	2.23	127.61	124.40
24	d	304	CLA	CMB-C2B-C3B	2.22	131.78	126.55
24	B	841	CLA	C1-C2-C3	-2.22	122.56	126.20
33	f	616	II0	C42-C41-C39	-2.22	118.97	123.52
33	i	613	II0	C42-C41-C39	-2.22	118.97	123.52
24	h	302	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
24	i	611	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
24	L	202	CLA	CHB-C4A-NA	2.22	127.61	124.40
35	k	613	KC2	C1D-CHD-C4C	-2.22	121.02	126.25
26	c	617	LHG	O8-C23-O10	-2.22	118.07	123.63
24	A	816	CLA	O2D-CGD-CBD	2.22	115.11	111.23
27	j	301	WVN	C29-C31-C32	-2.22	120.28	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	WVN	C19-C22-C26	-2.22	115.52	119.01
26	k	620	LHG	C5-O7-C7	-2.22	112.48	117.80
24	h	304	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
35	i	609	KC2	C2D-C1D-ND	-2.22	108.03	110.33
32	L	208	LMG	C30-C29-C28	-2.22	105.56	113.69
27	A	847	WVN	C35-C32-C36	-2.22	119.22	122.82
24	B	840	CLA	CBC-CAC-C3C	2.22	118.43	112.42
27	L	201	WVN	C11-C19-C22	-2.22	121.55	126.32
24	A	852	CLA	C1-C2-C3	-2.22	122.56	126.20
27	j	301	WVN	C14-C15-C13	-2.22	119.71	122.70
33	k	617	II0	C12-C14-C10	-2.22	115.89	120.50
24	a	302	CLA	C1-C2-C3	-2.22	122.56	126.20
24	B	834	CLA	CAC-C3C-C4C	2.22	127.67	124.79
24	b	306	CLA	O1D-CGD-CBD	2.22	128.89	124.52
24	c	603	CLA	CMB-C2B-C3B	2.22	131.76	126.55
24	b	310	CLA	CAA-CBA-CGA	-2.21	106.92	113.21
24	A	801	CLA	CBA-CAA-C2A	-2.21	107.20	113.79
35	g	313	KC2	CAB-C3B-C4B	-2.21	119.53	124.82
26	b	320	LHG	C5-O7-C7	-2.21	112.50	117.80
33	e	613	II0	C30-C32-C34	-2.21	116.79	123.20
33	b	315	II0	C18-C04-C10	-2.21	106.56	110.52
24	B	813	CLA	C1-C2-C3	-2.21	122.57	126.20
24	A	852	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	i	606	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	k	620	LHG	O7-C7-O9	-2.21	118.54	123.70
24	A	840	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	B	815	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	g	309	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
24	A	827	CLA	CHB-C1B-NB	2.21	127.36	124.05
33	g	317	II0	C42-C41-C39	-2.21	119.00	123.52
24	k	609	CLA	C1-C2-C3	-2.21	122.58	126.20
34	j	317	IHT	C02-C07-C18	2.21	121.64	115.65
33	c	616	II0	C06-C04-C10	2.21	113.84	109.49
33	h	311	II0	C34-C36-C40	-2.21	115.53	119.01
24	a	311	CLA	CMA-C3A-C4A	2.21	117.71	111.77
24	A	823	CLA	CHB-C4A-NA	2.21	127.59	124.40
33	i	612	II0	C18-C04-C10	-2.21	106.56	110.52
27	B	849	WVN	C38-C34-C33	2.21	121.46	118.09
24	A	835	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
24	B	819	CLA	CHB-C4A-NA	2.21	127.58	124.40
24	b	309	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
24	g	303	CLA	CMB-C2B-C3B	2.21	131.74	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	k	618	IHT	C41-C38-C35	-2.21	124.19	127.28
33	c	616	II0	C05-C03-C09	2.21	113.83	109.49
24	A	852	CLA	O2D-CGD-CBD	2.20	115.08	111.23
24	F	201	CLA	C3B-C4B-NB	-2.20	108.56	110.53
24	e	607	CLA	O1D-CGD-CBD	2.20	128.87	124.52
27	L	205	WVN	C40-C39-C36	-2.20	119.01	123.52
27	B	845	WVN	C02-C05-C09	-2.20	118.76	121.47
33	g	316	II0	C30-C32-C34	-2.20	116.82	123.20
24	A	811	CLA	CHB-C4A-NA	2.20	127.58	124.40
33	g	320	II0	C15-C03-C09	-2.20	106.58	110.52
24	c	611	CLA	C2A-C1A-CHA	2.20	127.69	123.87
24	B	810	CLA	C3B-C4B-NB	-2.20	108.04	110.33
24	b	306	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
24	A	814	CLA	CHB-C1B-NB	2.20	127.35	124.05
24	e	610	CLA	C1-C2-C3	-2.20	122.59	126.20
24	B	805	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
24	A	852	CLA	C6-C7-C8	-2.20	108.66	115.97
30	B	843	DGD	O6D-C5D-C6D	2.20	111.05	106.69
27	A	848	WVN	C26-C29-C31	-2.20	116.83	123.20
24	B	836	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	B	842	PQN	C11-C3-C2	-2.20	121.12	124.89
27	A	850	WVN	C08-C01-C07	-2.20	104.68	107.87
24	c	604	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	c	606	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
33	h	309	II0	C27-C25-C29	-2.20	119.92	124.18
24	B	835	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
26	b	320	LHG	O7-C7-O9	-2.19	118.57	123.70
24	i	604	CLA	CMB-C2B-C3B	2.19	131.71	126.55
35	g	313	KC2	CAC-C3C-C4C	2.19	134.09	124.39
24	B	813	CLA	CMB-C2B-C3B	2.19	131.71	126.55
24	A	839	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
33	e	614	II0	C29-C31-C33	-2.19	116.84	123.20
24	i	610	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	c	602	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
24	A	853	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
35	j	312	KC2	CAB-C3B-C4B	-2.19	119.59	124.82
24	B	813	CLA	CHB-C4A-NA	2.19	127.56	124.40
35	i	616	KC2	CAA-CBA-CGA	-2.19	115.91	127.05
33	h	310	II0	C31-C33-C35	-2.19	120.36	126.36
33	k	615	II0	C08-C12-C14	2.19	117.63	112.18
24	B	822	CLA	C3B-C4B-NB	-2.19	108.58	110.53
24	c	611	CLA	O1A-CGA-CBA	2.19	130.04	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	311	CLA	CMC-C2C-C3C	2.19	132.07	126.15
24	b	309	CLA	CHB-C4A-NA	2.19	127.56	124.40
33	i	614	II0	C19-C13-C11	2.19	118.45	114.42
24	A	805	CLA	C3B-C4B-NB	-2.19	108.58	110.53
24	A	809	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
27	F	204	WVN	C40-C39-C36	2.19	128.00	123.52
33	e	616	II0	C20-C14-C10	-2.19	120.07	124.16
27	B	848	WVN	C35-C32-C31	2.19	121.43	118.09
33	h	311	II0	C20-C14-C10	-2.19	120.07	124.16
24	g	309	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
33	g	317	II0	C31-C33-C35	-2.19	120.37	126.36
33	e	616	II0	C19-C13-C09	-2.19	120.07	124.16
24	A	801	CLA	C3B-C4B-NB	-2.18	108.58	110.53
24	d	312	CLA	O1D-CGD-CBD	2.18	128.83	124.52
27	J	102	WVN	C40-C39-C36	-2.18	119.05	123.52
34	R	204	IHT	C19-C10-C07	-2.18	122.10	124.48
26	A	844	LHG	O7-C7-O9	-2.18	118.60	123.70
24	i	602	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
24	d	305	CLA	O1D-CGD-CBD	2.18	128.82	124.52
24	A	832	CLA	C7-C6-C5	-2.18	107.44	113.26
27	A	850	WVN	C23-C20-C13	-2.18	121.17	127.00
24	K	101	CLA	CHA-C1A-NA	-2.18	121.45	126.39
24	A	853	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
24	g	306	CLA	C3B-C4B-NB	-2.18	108.58	110.53
27	j	301	WVN	C06-C13-C20	2.18	121.56	115.65
24	B	825	CLA	CHB-C4A-NA	2.18	127.55	124.40
33	g	320	II0	C31-C33-C35	-2.18	120.39	126.36
24	c	607	CLA	CHB-C4A-NA	2.18	127.54	124.40
35	d	311	KC2	CAC-C3C-C2C	-2.18	121.35	128.43
24	B	841	CLA	CHA-C1A-NA	-2.18	121.46	126.39
24	b	307	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
24	A	812	CLA	C3B-C4B-NB	-2.18	108.59	110.53
27	K	103	WVN	C24-C22-C19	2.18	121.41	118.09
33	f	615	II0	C05-C03-C09	2.18	113.78	109.49
26	J	107	LHG	O4-P-O6	2.17	117.42	107.57
25	A	843	PQN	C16-C17-C18	-2.17	108.74	115.97
24	A	808	CLA	C2A-C1A-CHA	2.17	127.64	123.87
24	b	310	CLA	CED-O2D-CGD	2.17	120.85	115.92
24	B	804	CLA	O1D-CGD-CBD	2.17	128.81	124.52
24	c	601	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
24	e	610	CLA	C3B-C4B-NB	-2.17	108.59	110.53
34	b	317	IHT	C41-C38-C35	-2.17	124.23	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	e	606	CLA	CMB-C2B-C3B	2.17	131.66	126.55
24	j	302	CLA	CHB-C1B-NB	2.17	127.31	124.05
34	f	617	IHT	C34-C35-C38	2.17	122.42	119.01
24	j	313	CLA	C2B-C1B-NB	2.17	112.58	110.33
24	A	833	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	f	601	CLA	C3B-C4B-NB	-2.17	108.59	110.53
34	f	617	IHT	C36-C33-C32	-2.17	114.77	118.09
24	g	309	CLA	C2A-C1A-CHA	2.17	127.63	123.87
33	a	314	II0	C27-C25-C29	-2.17	119.97	124.18
35	d	310	KC2	CAB-C3B-C4B	-2.17	119.64	124.82
24	A	832	CLA	CMC-C2C-C3C	2.17	132.02	126.15
24	f	612	CLA	C1D-ND-C4D	-2.17	104.79	106.31
33	e	614	II0	C20-C14-C10	-2.17	120.10	124.16
24	B	808	CLA	C3B-C4B-NB	-2.17	108.59	110.53
27	I	101	WVN	C20-C23-C25	-2.17	123.03	126.23
24	A	856	CLA	O1D-CGD-CBD	2.17	128.79	124.52
24	k	610	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
24	A	855	CLA	O2A-CGA-CBA	2.17	118.45	111.83
35	g	312	KC2	CGD-CBD-CAD	-2.17	103.83	110.85
34	g	319	IHT	C20-C15-C11	-2.17	120.11	124.16
24	c	604	CLA	C3B-C4B-NB	-2.17	108.59	110.53
33	g	320	II0	C11-C13-C09	-2.17	115.99	120.50
24	A	827	CLA	O1D-CGD-CBD	2.17	128.79	124.52
24	B	810	CLA	CAA-CBA-CGA	-2.17	107.06	113.21
27	J	101	WVN	C03-C04-C09	-2.17	108.43	112.07
24	d	307	CLA	O2D-CGD-CBD	2.17	115.02	111.23
24	A	834	CLA	CHB-C1B-C2B	-2.17	121.14	127.43
24	a	304	CLA	O2D-CGD-CBD	2.17	115.02	111.23
26	e	617	LHG	O4-P-O5	2.16	122.51	112.44
24	b	309	CLA	CBC-CAC-C3C	2.16	118.29	112.42
27	I	101	WVN	C30-C28-C25	-2.16	124.24	127.28
33	k	615	II0	C32-C30-C26	-2.16	120.56	126.61
27	F	204	WVN	C07-C01-C02	2.16	112.82	109.55
33	j	316	II0	C42-C41-C39	-2.16	119.09	123.52
24	B	809	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	k	602	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	B	828	CLA	CHB-C1B-NB	2.16	127.29	124.05
24	f	612	CLA	CHB-C1B-NB	2.16	127.29	124.05
24	e	604	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	b	305	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
33	h	310	II0	C06-C04-C10	2.16	113.75	109.49
24	h	302	CLA	CHB-C4A-NA	2.16	127.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	849	WVN	C40-C37-C34	-2.16	124.25	127.28
24	e	610	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	L	203	CLA	CMB-C2B-C3B	2.16	131.63	126.55
24	e	604	CLA	O2D-CGD-CBD	2.16	115.00	111.23
33	k	616	II0	C07-C11-C13	-2.16	106.80	112.18
24	b	312	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	a	307	CLA	C2A-C1A-CHA	2.16	127.61	123.87
33	j	316	II0	C32-C34-C36	-2.16	120.45	126.36
24	A	823	CLA	C3B-C4B-NB	-2.16	108.61	110.53
24	b	308	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
24	k	607	CLA	O2D-CGD-CBD	2.16	115.00	111.23
24	A	805	CLA	CMB-C2B-C3B	2.16	131.62	126.55
24	a	312	CLA	O1D-CGD-CBD	2.16	128.77	124.52
33	k	619	II0	C20-C14-C10	-2.16	120.13	124.16
24	B	825	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
24	k	608	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
27	J	101	WVN	C08-C01-C02	-2.15	106.28	109.55
33	i	613	II0	C31-C29-C25	-2.15	120.59	126.61
33	c	613	II0	C30-C32-C34	-2.15	116.96	123.20
24	a	307	CLA	O2D-CGD-CBD	2.15	114.99	111.23
24	g	304	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	F	205	WVN	C11-C19-C22	-2.15	121.70	126.32
24	f	612	CLA	CAA-C2A-C1A	2.15	119.02	111.97
24	A	813	CLA	O2A-CGA-O1A	-2.15	117.80	123.33
27	e	615	WVN	C06-C13-C15	-2.15	119.70	122.64
27	A	849	WVN	C17-C06-C13	2.15	113.61	110.24
33	h	309	II0	C05-C03-C09	2.15	113.73	109.49
24	a	303	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	A	839	CLA	O2D-CGD-CBD	2.15	114.99	111.23
34	a	316	IHT	C41-C40-C37	-2.15	119.12	123.52
33	e	614	II0	C16-C03-C09	-2.15	106.67	110.52
24	F	202	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
24	A	809	CLA	CHB-C4A-NA	2.15	127.50	124.40
33	h	310	II0	C31-C29-C25	-2.15	120.60	126.61
24	e	603	CLA	C4A-NA-C1A	2.15	107.66	106.68
24	b	312	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
27	L	206	WVN	C16-C05-C09	-2.15	115.15	122.37
24	B	816	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
24	A	826	CLA	CMC-C2C-C3C	2.15	131.95	126.15
24	A	830	CLA	CHB-C1B-NB	2.15	127.27	124.05
24	f	605	CLA	C3B-C4B-NB	-2.15	108.61	110.53
24	B	824	CLA	O2D-CGD-CBD	2.15	114.98	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	604	CLA	CMB-C2B-C3B	2.14	131.59	126.55
24	A	833	CLA	CHB-C4A-NA	2.14	127.49	124.40
34	f	617	IHT	C39-C35-C38	-2.14	119.34	122.82
24	d	305	CLA	C2B-C1B-NB	-2.14	108.10	110.33
33	a	314	II0	C31-C33-C35	-2.14	120.49	126.36
24	A	801	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
24	j	304	CLA	O2D-CGD-CBD	2.14	114.97	111.23
24	O	201	CLA	C11-C12-C13	-2.14	108.85	115.97
27	h	308	WVN	C39-C40-C37	-2.14	119.14	123.52
27	B	846	WVN	C08-C01-C02	-2.14	106.30	109.55
35	d	311	KC2	CHD-C1D-C2D	2.14	133.64	127.43
35	d	311	KC2	C2B-C1B-NB	2.14	112.24	110.13
35	c	610	KC2	CAB-C3B-C4B	-2.14	119.71	124.82
24	c	611	CLA	O2D-CGD-CBD	2.14	114.97	111.23
24	A	838	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	B	803	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	J	101	WVN	C08-C01-C03	-2.14	104.56	109.01
27	A	846	WVN	C01-C02-C11	-2.14	110.37	112.83
24	O	205	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	B	809	CLA	CHB-C4A-NA	2.14	127.48	124.40
26	c	618	LHG	O4-P-O5	2.14	122.38	112.44
24	A	856	CLA	C2A-C1A-CHA	2.14	127.56	123.86
24	L	204	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
24	B	803	CLA	CHB-C4A-NA	2.14	127.48	124.40
27	J	101	WVN	C07-C01-C02	2.13	112.78	109.55
24	a	307	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	d	301	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	J	105	CLA	CHA-C1A-NA	-2.13	121.56	126.39
33	a	314	II0	C32-C34-C36	-2.13	120.51	126.36
35	k	611	KC2	O1D-CGD-CBD	-2.13	120.31	124.52
24	B	825	CLA	O2D-CGD-CBD	2.13	114.96	111.23
27	B	847	WVN	C35-C32-C36	-2.13	119.36	122.82
33	d	315	II0	C27-C25-C29	-2.13	120.04	124.18
33	i	612	II0	C38-C36-C34	2.13	121.35	118.09
24	A	832	CLA	C1-C2-C3	-2.13	122.70	126.20
33	h	311	II0	C15-C03-C09	-2.13	106.70	110.52
24	B	828	CLA	O2D-CGD-CBD	2.13	114.96	111.23
24	B	832	CLA	C1-O2A-CGA	2.13	121.81	116.65
24	A	825	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
33	f	615	II0	C20-C14-C10	-2.13	120.18	124.16
24	L	204	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
24	A	811	CLA	CAC-C3C-C4C	2.13	127.56	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	311	KC2	CAA-CBA-CGA	-2.13	116.22	127.05
24	B	829	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
24	A	831	CLA	O1D-CGD-CBD	2.13	128.72	124.52
24	B	835	CLA	C3B-C4B-NB	-2.13	108.63	110.53
33	h	310	II0	C30-C32-C34	-2.13	117.03	123.20
33	c	613	II0	C19-C13-C11	2.13	118.33	114.42
24	A	842	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
24	A	821	CLA	O2D-CGD-CBD	2.13	114.95	111.23
24	f	612	CLA	O1D-CGD-CBD	2.13	128.71	124.52
24	i	607	CLA	CBA-CAA-C2A	2.13	120.12	113.79
27	h	308	WVN	C19-C22-C26	2.13	122.35	119.01
24	A	842	CLA	C3A-C2A-C1A	2.13	104.52	101.34
33	d	313	II0	C41-C42-C40	-2.13	119.17	123.52
24	d	304	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
24	B	806	CLA	C7-C6-C5	-2.13	107.60	113.26
33	g	320	II0	C05-C03-C09	2.12	113.68	109.49
24	A	819	CLA	C1C-C2C-C3C	-2.12	104.75	106.98
24	d	304	CLA	C3B-C4B-NB	-2.12	108.63	110.53
24	O	205	CLA	CHC-C1C-C2C	-2.12	120.91	126.95
24	B	814	CLA	C1-C2-C3	-2.12	122.72	126.20
24	g	306	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
26	b	302	LHG	C9-C8-C7	-2.12	105.92	113.69
24	A	836	CLA	C3A-C2A-C1A	2.12	104.52	101.34
24	B	812	CLA	CMB-C2B-C3B	2.12	131.54	126.55
27	e	615	WVN	C27-C25-C28	-2.12	119.38	122.82
35	f	611	KC2	CAC-C3C-C4C	2.12	133.76	124.39
24	K	101	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
24	a	312	CLA	CED-O2D-CGD	2.12	120.73	115.92
24	A	820	CLA	C16-C15-C13	-2.12	108.92	115.97
24	A	853	CLA	CMB-C2B-C3B	2.12	131.54	126.55
24	i	611	CLA	CMB-C2B-C3B	2.12	131.54	126.55
24	A	824	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	b	308	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	R	201	WVN	C26-C29-C31	-2.12	117.06	123.20
24	O	205	CLA	C2A-C1A-CHA	2.12	127.55	123.87
24	h	312	CLA	CHB-C1B-NB	2.12	127.23	124.05
33	a	317	II0	C15-C03-C09	-2.12	106.72	110.52
27	L	206	WVN	C14-C15-C13	-2.12	119.84	122.70
27	B	845	WVN	C27-C25-C23	2.12	121.32	118.09
24	B	839	CLA	O1D-CGD-CBD	2.12	128.69	124.52
24	B	814	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
27	A	846	WVN	C38-C34-C33	2.11	121.32	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	313	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
35	i	609	KC2	CHD-C1D-C2D	2.11	133.56	127.43
24	c	605	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
24	B	810	CLA	CHB-C4A-NA	2.11	127.45	124.40
27	R	202	WVN	C17-C06-C13	-2.11	106.93	110.24
24	A	834	CLA	C3A-C2A-C1A	2.11	104.50	101.34
26	b	302	LHG	O7-C7-O9	-2.11	118.77	123.70
33	k	615	II0	C16-C03-C09	-2.11	106.74	110.52
24	L	204	CLA	C1-C2-C3	-2.11	123.35	126.76
24	h	304	CLA	C1-C2-C3	-2.11	122.74	126.20
32	L	208	LMG	O8-C28-O10	-2.11	118.35	123.63
28	F	203	LMT	C1'-O5'-C5'	-2.11	109.60	113.72
24	B	801	CLA	CHB-C4A-NA	2.11	127.44	124.40
24	A	837	CLA	C1-O2A-CGA	2.11	121.75	116.65
33	f	616	II0	C19-C13-C09	-2.11	120.22	124.16
24	B	809	CLA	CMB-C2B-C3B	2.11	131.51	126.55
24	b	312	CLA	C4-C3-C5	2.11	118.89	115.23
24	B	838	CLA	CHB-C1B-NB	2.11	127.21	124.05
24	b	311	CLA	O1D-CGD-CBD	2.11	128.67	124.52
33	c	616	II0	C31-C33-C35	-2.11	120.59	126.36
33	k	616	II0	C33-C35-C39	-2.11	115.69	119.01
24	A	826	CLA	C2A-C1A-CHA	2.11	127.52	123.87
24	A	834	CLA	CAA-CBA-CGA	-2.11	107.23	113.21
24	F	202	CLA	C3B-C4B-NB	-2.11	108.65	110.53
24	b	303	CLA	C1-C2-C3	-2.11	122.75	126.20
24	j	306	CLA	O1D-CGD-CBD	2.11	128.67	124.52
27	j	301	WVN	C12-C14-C15	-2.10	110.30	114.06
35	d	310	KC2	C2B-C1B-NB	2.10	112.21	110.13
24	a	312	CLA	CGD-CBD-CAD	-2.10	104.03	110.85
24	I	102	CLA	O2D-CGD-CBD	2.10	114.91	111.23
24	b	309	CLA	CHB-C1B-C2B	-2.10	121.32	127.43
33	c	614	II0	C19-C13-C09	-2.10	120.23	124.16
24	i	607	CLA	CAC-C3C-C4C	2.10	127.53	124.79
24	B	823	CLA	C3B-C4B-NB	-2.10	108.65	110.53
24	A	832	CLA	CHB-C1B-NB	2.10	127.20	124.05
24	A	818	CLA	CMC-C2C-C3C	2.10	131.84	126.15
27	J	101	WVN	C38-C34-C37	-2.10	119.41	122.82
24	j	308	CLA	O2D-CGD-CBD	2.10	114.90	111.23
24	c	605	CLA	CHC-C4B-NB	2.10	127.20	124.05
24	B	837	CLA	CHB-C4A-NA	2.10	127.43	124.40
27	K	103	WVN	C11-C19-C22	-2.10	121.81	126.32
24	j	313	CLA	O2A-CGA-O1A	-2.10	118.37	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	312	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
24	i	611	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
24	B	831	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	B	839	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	A	819	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
24	A	832	CLA	CMC-C2C-C1C	-2.10	121.75	125.03
24	c	612	CLA	C2A-C1A-CHA	2.10	127.51	123.87
24	b	306	CLA	C2A-C1A-CHA	2.10	127.51	123.87
27	I	101	WVN	C12-C14-C15	-2.10	110.32	114.06
24	B	833	CLA	O2D-CGD-CBD	2.10	114.90	111.23
24	J	103	CLA	C3B-C4B-NB	-2.10	108.66	110.53
24	d	305	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
33	a	317	II0	C20-C14-C12	2.10	118.28	114.42
27	h	308	WVN	C27-C25-C28	-2.10	119.42	122.82
33	b	315	II0	C37-C35-C39	-2.10	119.42	122.82
24	b	311	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	B	814	CLA	C4-C3-C5	2.09	118.86	115.23
27	L	206	WVN	C21-C15-C14	2.09	118.06	113.60
35	k	613	KC2	C2B-C1B-NB	2.09	112.20	110.13
24	h	307	CLA	CHA-C1A-NA	-2.09	121.65	126.39
26	j	319	LHG	O7-C7-O9	-2.09	118.81	123.70
24	h	305	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	k	605	CLA	C2A-C1A-CHA	2.09	127.50	123.87
24	g	304	CLA	CHA-C1A-NA	-2.09	121.66	126.39
27	L	205	WVN	C12-C14-C15	-2.09	110.33	114.06
24	B	822	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	B	842	PQN	C26-C25-C23	-2.09	109.02	115.97
35	d	310	KC2	CAC-C3C-C4C	2.09	133.62	124.39
24	b	310	CLA	C1D-ND-C4D	-2.09	104.85	106.31
24	e	610	CLA	CHC-C1C-NC	2.09	127.45	124.31
24	k	602	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
26	g	321	LHG	O7-C7-O9	-2.09	118.83	123.70
24	j	306	CLA	O2A-CGA-O1A	-2.09	117.97	123.33
24	b	305	CLA	C1-C2-C3	-2.09	122.78	126.20
33	h	310	II0	C32-C34-C36	-2.09	120.64	126.36
24	b	313	CLA	C3B-C4B-NB	-2.09	108.67	110.53
33	b	318	II0	C38-C36-C34	2.08	121.27	118.09
24	c	609	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	g	310	CLA	C3B-C4B-NB	-2.08	108.67	110.53
34	k	618	IHT	C30-C27-C23	-2.08	124.36	127.28
33	O	202	II0	C30-C32-C34	-2.08	117.16	123.20
24	A	836	CLA	CHC-C4B-NB	2.08	127.17	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	824	CLA	CMB-C2B-C3B	2.08	131.45	126.55
33	c	616	II0	C20-C14-C10	-2.08	120.27	124.16
24	a	302	CLA	C3B-C4B-NB	-2.08	108.67	110.53
24	f	606	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	I	102	CLA	CHD-C1D-ND	-2.08	121.87	124.80
33	g	316	II0	C27-C25-C29	-2.08	120.14	124.18
33	j	318	II0	C38-C36-C34	2.08	121.27	118.09
24	k	608	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
24	A	853	CLA	CHB-C1B-NB	2.08	127.17	124.05
33	c	616	II0	C15-C03-C09	-2.08	106.79	110.52
24	g	304	CLA	C2A-C1A-CHA	2.08	127.48	123.87
35	e	609	KC2	CAC-C3C-C4C	2.08	133.58	124.39
24	A	829	CLA	CHB-C4A-NA	2.08	127.40	124.40
24	j	307	CLA	CBA-CAA-C2A	-2.08	107.61	113.79
24	O	201	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
24	b	312	CLA	O1D-CGD-CBD	2.08	128.62	124.52
24	A	808	CLA	CHA-C1A-NA	-2.08	121.68	126.39
34	b	317	IHT	C41-C40-C37	2.08	127.77	123.52
24	B	836	CLA	C1-C2-C3	-2.08	122.79	126.20
24	k	609	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
24	h	303	CLA	O2D-CGD-CBD	2.08	114.86	111.23
24	O	205	CLA	CAA-C2A-C1A	2.08	118.78	111.97
33	k	615	II0	C19-C13-C11	2.08	118.24	114.42
27	J	102	WVN	C03-C04-C09	-2.08	108.58	112.07
24	A	817	CLA	C6-C7-C8	-2.08	109.06	115.97
27	R	202	WVN	C28-C30-C33	-2.08	117.18	123.20
27	A	846	WVN	C11-C19-C22	-2.08	121.86	126.32
24	b	309	CLA	C1-C2-C3	-2.08	122.79	126.20
24	g	322	CLA	C11-C10-C8	-2.08	109.06	115.97
24	A	839	CLA	CHB-C1B-NB	2.08	127.16	124.05
24	k	614	CLA	CHB-C1B-NB	2.08	127.16	124.05
35	d	310	KC2	CHD-C1D-C2D	2.08	133.45	127.43
26	A	845	LHG	C6-C5-C4	-2.08	106.95	111.78
24	B	821	CLA	CHD-C1D-ND	-2.08	121.88	124.80
34	j	317	IHT	C28-C26-C29	-2.07	120.15	124.18
24	K	102	CLA	CHA-C1A-NA	-2.07	121.69	126.39
24	g	308	CLA	C1-C2-C3	-2.07	122.80	126.20
24	c	611	CLA	CMD-C2D-C3D	2.07	132.45	127.69
24	f	609	CLA	O1D-CGD-CBD	2.07	128.61	124.52
33	j	316	II0	C05-C03-C09	2.07	113.58	109.49
24	d	303	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
33	j	318	II0	C34-C36-C40	-2.07	115.75	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	303	CLA	CMB-C2B-C3B	2.07	131.43	126.55
24	j	311	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
27	B	848	WVN	C39-C36-C32	-2.07	124.37	127.28
24	B	804	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	B	811	CLA	CHB-C1B-NB	2.07	127.16	124.05
33	a	315	II0	C27-C25-C29	-2.07	120.16	124.18
33	j	315	II0	C34-C36-C40	2.07	122.27	119.01
28	F	203	LMT	O5'-C5'-C6'	2.07	111.57	106.44
24	A	802	CLA	CHB-C1B-NB	2.07	127.16	124.05
24	A	814	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
24	k	604	CLA	C7-C6-C5	-2.07	107.75	113.26
33	f	615	II0	C32-C34-C36	-2.07	120.69	126.36
34	k	618	IHT	C39-C35-C34	2.07	121.25	118.09
24	B	809	CLA	CHC-C4B-NB	2.07	127.15	124.05
24	A	832	CLA	CMB-C2B-C3B	2.07	131.41	126.55
24	F	201	CLA	C1-C2-C3	-2.07	122.81	126.20
24	A	841	CLA	CHB-C4A-NA	2.07	127.38	124.40
24	B	818	CLA	CHB-C4A-NA	2.07	127.38	124.40
24	A	834	CLA	CHB-C1B-NB	2.07	127.15	124.05
24	A	853	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
24	A	837	CLA	C16-C15-C13	-2.07	109.10	115.97
24	c	609	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
27	B	847	WVN	C24-C22-C19	2.07	121.24	118.09
24	F	201	CLA	CHA-C1A-NA	-2.07	121.71	126.39
24	B	820	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
27	R	201	WVN	C03-C04-C09	-2.07	108.60	112.07
33	j	316	II0	C31-C29-C25	-2.06	120.84	126.61
24	j	308	CLA	C4A-NA-C1A	2.06	107.62	106.68
24	k	614	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
24	O	205	CLA	C7-C6-C5	-2.06	107.76	113.26
27	A	849	WVN	C07-C01-C02	-2.06	106.42	109.55
24	A	802	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
24	F	201	CLA	CHB-C4A-NA	2.06	127.38	124.40
24	A	856	CLA	CHC-C1C-NC	2.06	127.42	124.31
24	f	605	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
33	a	317	II0	C19-C13-C09	-2.06	120.30	124.16
24	A	817	CLA	CMB-C2B-C3B	2.06	131.40	126.55
24	k	603	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
24	A	839	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
24	A	827	CLA	CHB-C4A-NA	2.06	127.38	124.40
27	B	849	WVN	C07-C01-C02	2.06	112.67	109.55
24	g	302	CLA	CHA-C1A-NA	-2.06	121.72	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	CLA	C3B-C4B-NB	-2.06	108.69	110.53
24	d	304	CLA	C2A-C1A-CHA	2.06	127.44	123.87
24	a	305	CLA	CHB-C1B-NB	2.06	127.14	124.05
24	b	307	CLA	CHB-C1B-NB	2.06	127.14	124.05
33	O	202	II0	C19-C13-C11	2.06	118.21	114.42
24	a	311	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	B	848	WVN	C14-C15-C13	-2.06	119.92	122.70
27	R	202	WVN	C21-C15-C14	2.06	117.98	113.60
24	i	607	CLA	C3B-C4B-NB	-2.06	108.69	110.53
24	A	827	CLA	C1-C2-C3	-2.06	122.83	126.20
33	c	616	II0	C28-C26-C30	-2.06	120.19	124.18
24	h	307	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
27	A	849	WVN	C12-C14-C15	-2.05	110.39	114.06
35	f	611	KC2	C4D-CHA-C1A	-2.05	116.19	122.45
24	A	830	CLA	CHD-C1D-ND	-2.05	121.91	124.80
33	h	309	II0	C19-C13-C09	-2.05	120.32	124.16
33	a	317	II0	C19-C13-C11	2.05	118.20	114.42
33	d	313	II0	C19-C13-C09	-2.05	120.32	124.16
33	d	315	II0	C20-C14-C10	-2.05	120.32	124.16
27	I	101	WVN	C14-C15-C13	-2.05	119.93	122.70
24	b	311	CLA	C3B-C4B-NB	-2.05	108.70	110.53
33	i	613	II0	C31-C33-C35	-2.05	120.74	126.36
24	c	603	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	b	303	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
24	A	809	CLA	CMB-C2B-C3B	2.05	131.37	126.55
24	L	203	CLA	C11-C10-C8	-2.05	109.15	115.97
35	k	611	KC2	CAC-C3C-C4C	2.05	133.45	124.39
24	a	308	CLA	CMB-C2B-C3B	2.05	131.37	126.55
24	f	609	CLA	CMB-C2B-C3B	2.05	131.37	126.55
34	b	316	IHT	C20-C15-C11	-2.05	120.33	124.16
24	B	827	CLA	CHB-C1B-NB	2.05	127.12	124.05
24	b	310	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	A	826	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	b	320	LHG	C26-C25-C24	-2.05	105.60	113.13
24	A	828	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	d	302	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
24	f	604	CLA	C11-C12-C13	-2.05	109.16	115.97
33	g	317	II0	C03-C05-C07	2.05	118.08	113.59
33	a	314	II0	C37-C35-C39	-2.05	119.50	122.82
24	b	307	CLA	C2A-C1A-CHA	2.05	127.42	123.87
24	A	827	CLA	CAC-C3C-C4C	2.05	127.45	124.79
24	A	823	CLA	O2D-CGD-CBD	2.04	114.81	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	PQN	C11-C3-C2	-2.04	121.39	124.89
27	M	101	WVN	C12-C14-C15	-2.04	110.41	114.06
24	g	307	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
24	d	305	CLA	CHD-C1D-ND	-2.04	121.93	124.80
33	d	315	II0	C31-C29-C25	-2.04	120.90	126.61
26	a	301	LHG	O4-P-O5	2.04	121.95	112.44
33	j	318	II0	C42-C40-C36	-2.04	124.41	127.28
24	f	610	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
27	A	848	WVN	C27-C25-C23	2.04	121.21	118.09
33	a	315	II0	C19-C13-C09	-2.04	120.34	124.16
24	g	305	CLA	CMC-C2C-C3C	2.04	131.67	126.15
30	B	843	DGD	C6E-C5E-C4E	-2.04	108.01	113.02
24	A	818	CLA	CMC-C2C-C1C	-2.04	121.85	125.03
24	B	816	CLA	CBA-CAA-C2A	-2.04	107.72	113.79
24	h	303	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
34	k	618	IHT	C12-C15-C11	-2.04	116.26	120.50
24	c	602	CLA	CMB-C2B-C3B	2.04	131.34	126.55
24	c	602	CLA	CHB-C1B-NB	2.04	127.11	124.05
33	g	316	II0	C31-C33-C35	-2.04	120.77	126.36
24	g	315	CLA	O2D-CGD-CBD	2.04	114.79	111.23
24	j	306	CLA	O1A-CGA-CBA	2.04	129.55	123.09
33	b	315	II0	C31-C33-C35	2.04	131.94	126.36
27	J	102	WVN	C20-C23-C25	-2.04	123.22	126.23
27	I	101	WVN	C27-C25-C23	2.04	121.20	118.09
27	L	206	WVN	C38-C34-C37	-2.03	119.52	122.82
24	k	605	CLA	O2A-CGA-O1A	-2.03	118.10	123.33
25	A	843	PQN	C26-C25-C23	-2.03	109.20	115.97
24	i	606	CLA	O2D-CGD-CBD	2.03	114.78	111.23
24	a	305	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
33	a	314	II0	C34-C36-C40	-2.03	115.81	119.01
27	A	847	WVN	C18-C06-C17	-2.03	102.82	108.63
26	g	321	LHG	C25-C24-C23	-2.03	106.25	113.69
27	K	103	WVN	C29-C26-C22	-2.03	124.43	127.28
24	b	304	CLA	C1-O2A-CGA	-2.03	111.73	116.65
24	F	202	CLA	C3A-C2A-C1A	2.03	104.38	101.34
24	B	812	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	B	823	CLA	CHC-C4B-NB	2.03	127.09	124.05
35	g	313	KC2	CGD-CBD-CAD	-2.03	104.28	110.85
24	g	315	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
24	A	820	CLA	O2D-CGD-CBD	2.03	114.78	111.23
24	A	832	CLA	CHD-C1D-ND	-2.03	121.95	124.80
24	B	831	CLA	O1A-CGA-CBA	2.03	129.52	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	303	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
30	B	843	DGD	C3B-C2B-C1B	-2.03	106.27	113.69
24	g	304	CLA	CHB-C1B-NB	2.03	127.09	124.05
33	i	614	II0	C16-C03-C15	-2.03	102.83	108.63
24	i	606	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
24	L	207	CLA	C1-C2-C3	-2.03	122.88	126.20
35	k	612	KC2	CBC-CAC-C3C	-2.03	117.41	127.53
24	A	802	CLA	O1D-CGD-CBD	2.03	128.51	124.52
35	j	312	KC2	CHD-C1D-C2D	2.03	133.31	127.43
24	B	812	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
26	f	620	LHG	O7-C7-O9	-2.02	118.97	123.70
33	f	614	II0	C12-C14-C10	-2.02	116.29	120.50
24	B	836	CLA	C3B-C4B-NB	-2.02	108.72	110.53
24	B	840	CLA	C6-C7-C8	-2.02	109.24	115.97
24	h	307	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
33	b	318	II0	C37-C35-C39	-2.02	119.54	122.82
35	k	613	KC2	CAA-CBA-CGA	-2.02	116.76	127.05
24	A	801	CLA	CHC-C4B-NB	2.02	127.08	124.05
24	A	801	CLA	O1D-CGD-CBD	2.02	128.51	124.52
24	A	803	CLA	CHD-C1D-ND	-2.02	121.96	124.80
24	A	840	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
33	d	313	II0	C16-C03-C09	-2.02	106.90	110.52
24	O	205	CLA	C11-C12-C13	-2.02	109.25	115.97
27	J	101	WVN	C16-C05-C09	-2.02	115.57	122.37
27	A	846	WVN	C26-C29-C31	-2.02	117.34	123.20
24	B	813	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
24	f	603	CLA	C3A-C2A-C1A	2.02	104.36	101.34
24	A	824	CLA	CBA-CAA-C2A	2.02	119.80	113.79
24	B	817	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
24	k	609	CLA	C3B-C4B-NB	-2.02	108.73	110.53
24	k	608	CLA	CMB-C2B-C3B	2.02	131.30	126.55
24	e	605	CLA	C4D-C3D-CAD	-2.02	105.91	108.11
24	h	302	CLA	CHC-C4B-NB	2.02	127.08	124.05
33	a	314	II0	C42-C41-C39	-2.02	119.39	123.52
34	k	618	IHT	C20-C15-C11	-2.02	120.39	124.16
24	g	309	CLA	CMB-C2B-C3B	2.02	131.30	126.55
24	B	831	CLA	CHB-C1B-NB	2.02	127.08	124.05
27	B	846	WVN	C21-C15-C14	2.02	117.90	113.60
24	B	809	CLA	O2D-CGD-CBD	2.02	114.76	111.23
25	A	843	PQN	C2M-C2-C3	-2.02	121.14	124.45
27	K	103	WVN	C27-C25-C28	-2.02	119.55	122.82
24	A	833	CLA	CHC-C4B-NB	2.02	127.07	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	i	611	CLA	CHA-C1A-NA	-2.02	121.83	126.39
24	k	609	CLA	CHD-C1D-ND	-2.02	121.97	124.80
24	B	820	CLA	CHB-C1B-NB	2.02	127.07	124.05
24	A	819	CLA	CMC-C2C-C1C	-2.02	121.89	125.03
24	A	832	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
24	A	804	CLA	CAC-C3C-C4C	2.01	127.41	124.79
24	f	603	CLA	CMB-C2B-C3B	2.01	131.29	126.55
24	j	313	CLA	C1-C2-C3	-2.01	122.90	126.20
24	L	203	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	A	817	CLA	C16-C15-C13	-2.01	109.28	115.97
24	b	307	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
33	e	616	II0	C27-C25-C29	-2.01	120.28	124.18
24	j	303	CLA	O2D-CGD-CBD	2.01	114.75	111.23
24	L	202	CLA	CMB-C2B-C3B	2.01	131.28	126.55
27	B	846	WVN	C11-C19-C22	-2.01	122.00	126.32
24	c	606	CLA	CHB-C1B-NB	2.01	127.06	124.05
24	g	311	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
34	R	204	IHT	C20-C15-C11	-2.01	120.40	124.16
33	c	616	II0	C29-C31-C33	-2.01	117.38	123.20
24	O	205	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
24	f	609	CLA	C3B-C4B-NB	-2.01	108.74	110.53
24	B	828	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
24	B	840	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
24	B	804	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	A	852	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	h	307	CLA	CMB-C2B-C3B	2.01	131.28	126.55
24	A	824	CLA	CHC-C4B-NB	2.01	127.06	124.05
24	B	817	CLA	CHC-C4B-NB	2.01	127.06	124.05
33	f	614	II0	C28-C26-C30	-2.01	120.28	124.18
33	k	621	II0	C06-C04-C10	2.01	113.45	109.49
24	b	308	CLA	CHD-C4C-NC	2.01	127.34	124.23
33	i	614	II0	C03-C05-C07	2.01	118.00	113.59
24	B	827	CLA	O1D-CGD-CBD	2.01	128.48	124.52
33	g	316	II0	C15-C03-C09	-2.01	106.92	110.52
27	F	204	WVN	C30-C33-C34	-2.01	120.86	126.36
33	k	615	II0	C33-C35-C39	2.01	122.17	119.01
33	a	315	II0	C20-C14-C10	-2.01	120.41	124.16
24	R	203	CLA	O2A-CGA-CBA	2.01	117.95	111.83
24	d	303	CLA	CHA-C1A-NA	-2.01	121.85	126.39
24	j	307	CLA	C1-C2-C3	-2.01	122.91	126.20
27	I	101	WVN	C21-C15-C14	2.01	117.87	113.60
27	B	846	WVN	C14-C15-C13	-2.01	119.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	g	320	II0	C42-C41-C39	-2.01	119.42	123.52
24	A	814	CLA	CHD-C1D-ND	-2.00	121.98	124.80
27	K	103	WVN	C07-C01-C02	2.00	112.58	109.55
24	h	306	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
24	B	809	CLA	CHA-C1A-NA	-2.00	121.85	126.39
24	A	832	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
24	B	821	CLA	O2D-CGD-CBD	2.00	114.73	111.23
33	k	619	II0	C12-C14-C10	-2.00	116.33	120.50
35	d	310	KC2	C4D-CHA-C1A	-2.00	116.35	122.45
24	B	830	CLA	C16-C15-C13	-2.00	109.31	115.97
33	g	317	II0	C30-C32-C34	-2.00	117.40	123.20
33	O	202	II0	C05-C03-C09	2.00	113.43	109.49

All (197) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	801	CLA	ND
24	A	802	CLA	ND
24	A	803	CLA	ND
24	A	804	CLA	ND
24	A	805	CLA	ND
24	A	807	CLA	ND
24	A	808	CLA	ND
24	A	809	CLA	ND
24	A	810	CLA	ND
24	A	811	CLA	ND
24	A	812	CLA	ND
24	A	813	CLA	ND
24	A	815	CLA	ND
24	A	816	CLA	ND
24	A	817	CLA	ND
24	A	819	CLA	ND
24	A	820	CLA	ND
24	A	821	CLA	ND
24	A	822	CLA	ND
24	A	823	CLA	ND
24	A	824	CLA	ND
24	A	825	CLA	ND
24	A	826	CLA	ND
24	A	827	CLA	ND
24	A	828	CLA	ND
24	A	829	CLA	ND

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Mol	Chain	Res	Type	Atom
24	A	830	CLA	ND
24	A	831	CLA	ND
24	A	833	CLA	ND
24	A	834	CLA	ND
24	A	835	CLA	ND
24	A	836	CLA	ND
24	A	837	CLA	ND
24	A	838	CLA	ND
24	A	839	CLA	ND
24	A	840	CLA	ND
24	A	841	CLA	ND
24	A	842	CLA	ND
24	A	852	CLA	ND
24	A	853	CLA	ND
24	A	855	CLA	ND
24	A	856	CLA	ND
24	B	801	CLA	ND
24	B	803	CLA	ND
24	B	804	CLA	ND
24	B	805	CLA	ND
24	B	806	CLA	ND
24	B	807	CLA	ND
24	B	808	CLA	ND
24	B	809	CLA	ND
24	B	810	CLA	ND
24	B	811	CLA	ND
24	B	812	CLA	ND
24	B	813	CLA	ND
24	B	814	CLA	ND
24	B	815	CLA	ND
24	B	816	CLA	ND
24	B	818	CLA	ND
24	B	821	CLA	ND
24	B	822	CLA	ND
24	B	823	CLA	ND
24	B	824	CLA	ND
24	B	825	CLA	ND
24	B	826	CLA	ND
24	B	827	CLA	ND
24	B	829	CLA	ND
24	B	830	CLA	ND
24	B	831	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	832	CLA	ND
24	B	833	CLA	ND
24	B	834	CLA	ND
24	B	835	CLA	ND
24	B	836	CLA	ND
24	B	837	CLA	ND
24	B	838	CLA	ND
24	B	839	CLA	ND
24	F	201	CLA	ND
24	F	202	CLA	ND
24	I	102	CLA	ND
24	J	103	CLA	ND
24	J	105	CLA	ND
24	L	202	CLA	ND
24	L	203	CLA	ND
24	L	204	CLA	ND
24	L	207	CLA	ND
24	O	201	CLA	ND
24	O	205	CLA	ND
24	K	101	CLA	ND
24	K	102	CLA	ND
24	c	601	CLA	ND
24	c	602	CLA	ND
24	c	603	CLA	ND
24	c	604	CLA	ND
24	c	605	CLA	ND
24	c	607	CLA	ND
24	c	608	CLA	ND
24	c	609	CLA	ND
24	c	611	CLA	ND
24	c	612	CLA	ND
24	a	302	CLA	ND
24	a	303	CLA	ND
24	a	304	CLA	ND
24	a	305	CLA	ND
24	a	306	CLA	ND
24	a	307	CLA	ND
24	a	308	CLA	ND
24	a	309	CLA	ND
24	a	310	CLA	ND
24	a	311	CLA	ND
24	a	312	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	303	CLA	ND
24	b	304	CLA	ND
24	b	305	CLA	ND
24	b	307	CLA	ND
24	b	308	CLA	ND
24	b	309	CLA	ND
24	b	310	CLA	ND
24	b	311	CLA	ND
24	b	312	CLA	ND
24	b	313	CLA	ND
24	h	301	CLA	ND
24	h	302	CLA	ND
24	h	303	CLA	ND
24	h	304	CLA	ND
24	h	305	CLA	ND
24	h	306	CLA	ND
24	h	307	CLA	ND
24	h	312	CLA	ND
24	e	601	CLA	ND
24	e	602	CLA	ND
24	e	603	CLA	ND
24	e	604	CLA	ND
24	e	605	CLA	ND
24	e	606	CLA	ND
24	e	607	CLA	ND
24	e	608	CLA	ND
24	e	611	CLA	ND
24	k	601	CLA	ND
24	k	602	CLA	ND
24	k	603	CLA	ND
24	k	604	CLA	ND
24	k	605	CLA	ND
24	k	607	CLA	ND
24	k	608	CLA	ND
24	k	609	CLA	ND
24	k	610	CLA	ND
24	f	601	CLA	ND
24	f	602	CLA	ND
24	f	603	CLA	ND
24	f	607	CLA	ND
24	f	608	CLA	ND
24	f	609	CLA	ND

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Mol	Chain	Res	Type	Atom
24	f	610	CLA	ND
24	f	612	CLA	ND
24	f	613	CLA	ND
24	i	601	CLA	ND
24	i	602	CLA	ND
24	i	603	CLA	ND
24	i	604	CLA	ND
24	i	605	CLA	ND
24	i	606	CLA	ND
24	i	607	CLA	ND
24	i	608	CLA	ND
24	i	610	CLA	ND
24	i	611	CLA	ND
24	j	302	CLA	ND
24	j	303	CLA	ND
24	j	304	CLA	ND
24	j	306	CLA	ND
24	j	307	CLA	ND
24	j	308	CLA	ND
24	j	309	CLA	ND
24	j	310	CLA	ND
24	j	311	CLA	ND
24	j	313	CLA	ND
24	j	314	CLA	ND
24	d	301	CLA	ND
24	d	302	CLA	ND
24	d	303	CLA	ND
24	d	304	CLA	ND
24	d	306	CLA	ND
24	d	307	CLA	ND
24	d	308	CLA	ND
24	d	309	CLA	ND
24	g	302	CLA	ND
24	g	303	CLA	ND
24	g	304	CLA	ND
24	g	305	CLA	ND
24	g	306	CLA	ND
24	g	307	CLA	ND
24	g	308	CLA	ND
24	g	309	CLA	ND
24	g	310	CLA	ND
24	g	311	CLA	ND

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Mol	Chain	Res	Type	Atom
24	g	315	CLA	ND
24	g	322	CLA	ND
24	R	203	CLA	ND

All (2874) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	801	CLA	CBD-CGD-O2D-CED
24	A	802	CLA	C1A-C2A-CAA-CBA
24	A	802	CLA	CBA-CGA-O2A-C1
24	A	802	CLA	O1A-CGA-O2A-C1
24	A	802	CLA	C11-C10-C8-C9
24	A	803	CLA	C1A-C2A-CAA-CBA
24	A	803	CLA	C3A-C2A-CAA-CBA
24	A	804	CLA	C3A-C2A-CAA-CBA
24	A	804	CLA	CAD-CBD-CGD-O2D
24	A	805	CLA	C1A-C2A-CAA-CBA
24	A	807	CLA	CHA-CBD-CGD-O1D
24	A	807	CLA	CHA-CBD-CGD-O2D
24	A	810	CLA	C1A-C2A-CAA-CBA
24	A	810	CLA	C3A-C2A-CAA-CBA
24	A	810	CLA	C11-C10-C8-C7
24	A	813	CLA	C1A-C2A-CAA-CBA
24	A	813	CLA	C3A-C2A-CAA-CBA
24	A	815	CLA	CBD-CGD-O2D-CED
24	A	816	CLA	C1A-C2A-CAA-CBA
24	A	816	CLA	CHA-CBD-CGD-O1D
24	A	816	CLA	CHA-CBD-CGD-O2D
24	A	817	CLA	C1A-C2A-CAA-CBA
24	A	817	CLA	C3A-C2A-CAA-CBA
24	A	818	CLA	C3A-C2A-CAA-CBA
24	A	822	CLA	C4B-C3B-CAB-CBB
24	A	827	CLA	C11-C12-C13-C14
24	A	829	CLA	CHA-CBD-CGD-O1D
24	A	829	CLA	CHA-CBD-CGD-O2D
24	A	831	CLA	C2B-C3B-CAB-CBB
24	A	831	CLA	C4B-C3B-CAB-CBB
24	A	832	CLA	CHA-CBD-CGD-O1D
24	A	832	CLA	CHA-CBD-CGD-O2D
24	A	837	CLA	C3A-C2A-CAA-CBA
24	A	838	CLA	C1A-C2A-CAA-CBA
24	A	838	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	A	838	CLA	C4-C3-C5-C6
24	A	842	CLA	C1A-C2A-CAA-CBA
24	A	855	CLA	CBA-CGA-O2A-C1
24	A	855	CLA	O1A-CGA-O2A-C1
24	A	856	CLA	C2B-C3B-CAB-CBB
24	A	856	CLA	C4B-C3B-CAB-CBB
24	B	805	CLA	C3A-C2A-CAA-CBA
24	B	808	CLA	CHA-CBD-CGD-O1D
24	B	808	CLA	CHA-CBD-CGD-O2D
24	B	808	CLA	C14-C13-C15-C16
24	B	815	CLA	C1A-C2A-CAA-CBA
24	B	817	CLA	C3A-C2A-CAA-CBA
24	B	819	CLA	C1A-C2A-CAA-CBA
24	B	819	CLA	C3A-C2A-CAA-CBA
24	B	821	CLA	C2B-C3B-CAB-CBB
24	B	821	CLA	C4B-C3B-CAB-CBB
24	B	822	CLA	CHA-CBD-CGD-O1D
24	B	822	CLA	CHA-CBD-CGD-O2D
24	B	826	CLA	C1A-C2A-CAA-CBA
24	B	826	CLA	C3A-C2A-CAA-CBA
24	B	827	CLA	C1A-C2A-CAA-CBA
24	B	827	CLA	C3A-C2A-CAA-CBA
24	B	831	CLA	C1A-C2A-CAA-CBA
24	B	831	CLA	C2B-C3B-CAB-CBB
24	B	831	CLA	C4B-C3B-CAB-CBB
24	B	832	CLA	C1A-C2A-CAA-CBA
24	B	839	CLA	C1A-C2A-CAA-CBA
24	B	840	CLA	C1A-C2A-CAA-CBA
24	F	202	CLA	C1A-C2A-CAA-CBA
24	F	202	CLA	C3A-C2A-CAA-CBA
24	J	103	CLA	C1A-C2A-CAA-CBA
24	L	202	CLA	C1A-C2A-CAA-CBA
24	L	202	CLA	C3A-C2A-CAA-CBA
24	L	204	CLA	C1A-C2A-CAA-CBA
24	L	204	CLA	C3A-C2A-CAA-CBA
24	L	207	CLA	C2-C3-C5-C6
24	L	207	CLA	C4-C3-C5-C6
24	O	201	CLA	C1A-C2A-CAA-CBA
24	O	201	CLA	CAD-CBD-CGD-O1D
24	O	201	CLA	CAD-CBD-CGD-O2D
24	O	201	CLA	C11-C10-C8-C9
24	O	205	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	K	102	CLA	C3A-C2A-CAA-CBA
24	K	102	CLA	CBD-CGD-O2D-CED
24	c	601	CLA	C1A-C2A-CAA-CBA
24	c	601	CLA	C2B-C3B-CAB-CBB
24	c	601	CLA	C4B-C3B-CAB-CBB
24	c	601	CLA	C2-C3-C5-C6
24	c	602	CLA	C3A-C2A-CAA-CBA
24	c	602	CLA	CHA-CBD-CGD-O1D
24	c	602	CLA	CHA-CBD-CGD-O2D
24	c	605	CLA	C2B-C3B-CAB-CBB
24	c	605	CLA	C4B-C3B-CAB-CBB
24	c	605	CLA	C2-C3-C5-C6
24	c	605	CLA	C4-C3-C5-C6
24	c	606	CLA	C3A-C2A-CAA-CBA
24	c	606	CLA	CBD-CGD-O2D-CED
24	c	608	CLA	C3A-C2A-CAA-CBA
24	c	608	CLA	CBD-CGD-O2D-CED
24	c	612	CLA	C3A-C2A-CAA-CBA
24	c	612	CLA	CBD-CGD-O2D-CED
24	a	302	CLA	C1A-C2A-CAA-CBA
24	a	302	CLA	C3A-C2A-CAA-CBA
24	a	302	CLA	C2B-C3B-CAB-CBB
24	a	302	CLA	C4B-C3B-CAB-CBB
24	a	303	CLA	C1A-C2A-CAA-CBA
24	a	303	CLA	C3A-C2A-CAA-CBA
24	a	307	CLA	CHA-CBD-CGD-O2D
24	a	307	CLA	C14-C13-C15-C16
24	a	310	CLA	C6-C7-C8-C9
24	a	311	CLA	C3A-C2A-CAA-CBA
24	b	303	CLA	CHA-CBD-CGD-O2D
24	b	304	CLA	C3A-C2A-CAA-CBA
24	b	304	CLA	CHA-CBD-CGD-O1D
24	b	304	CLA	CHA-CBD-CGD-O2D
24	b	306	CLA	CAD-CBD-CGD-O2D
24	b	308	CLA	C2B-C3B-CAB-CBB
24	b	308	CLA	C4B-C3B-CAB-CBB
24	b	308	CLA	CBD-CGD-O2D-CED
24	b	309	CLA	C2B-C3B-CAB-CBB
24	b	309	CLA	C4B-C3B-CAB-CBB
24	b	312	CLA	C2B-C3B-CAB-CBB
24	b	312	CLA	C4B-C3B-CAB-CBB
24	b	312	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	h	301	CLA	CBD-CGD-O2D-CED
24	h	303	CLA	C1A-C2A-CAA-CBA
24	h	303	CLA	C3A-C2A-CAA-CBA
24	h	304	CLA	C1A-C2A-CAA-CBA
24	h	304	CLA	C3A-C2A-CAA-CBA
24	h	307	CLA	CAD-CBD-CGD-O1D
24	h	307	CLA	CAD-CBD-CGD-O2D
24	e	601	CLA	C1A-C2A-CAA-CBA
24	e	601	CLA	C3A-C2A-CAA-CBA
24	e	601	CLA	CHA-CBD-CGD-O2D
24	e	602	CLA	C1A-C2A-CAA-CBA
24	e	602	CLA	C3A-C2A-CAA-CBA
24	e	603	CLA	CBD-CGD-O2D-CED
24	e	605	CLA	CBD-CGD-O2D-CED
24	e	606	CLA	CHA-CBD-CGD-O1D
24	e	606	CLA	CHA-CBD-CGD-O2D
24	e	607	CLA	CHA-CBD-CGD-O1D
24	e	607	CLA	CHA-CBD-CGD-O2D
24	e	608	CLA	C1A-C2A-CAA-CBA
24	e	611	CLA	C2B-C3B-CAB-CBB
24	e	611	CLA	C4B-C3B-CAB-CBB
24	e	611	CLA	CBD-CGD-O2D-CED
24	k	601	CLA	C1A-C2A-CAA-CBA
24	k	601	CLA	C3A-C2A-CAA-CBA
24	k	601	CLA	C2B-C3B-CAB-CBB
24	k	601	CLA	C4B-C3B-CAB-CBB
24	k	602	CLA	C1A-C2A-CAA-CBA
24	k	602	CLA	C3A-C2A-CAA-CBA
24	k	606	CLA	CBD-CGD-O2D-CED
24	k	607	CLA	CBA-CGA-O2A-C1
24	k	607	CLA	CBD-CGD-O2D-CED
24	k	608	CLA	C1A-C2A-CAA-CBA
24	k	608	CLA	C3A-C2A-CAA-CBA
24	k	609	CLA	CBD-CGD-O2D-CED
24	k	609	CLA	O1D-CGD-O2D-CED
24	k	610	CLA	C1A-C2A-CAA-CBA
24	k	610	CLA	C3A-C2A-CAA-CBA
24	k	610	CLA	C4B-C3B-CAB-CBB
24	k	614	CLA	C1A-C2A-CAA-CBA
24	k	614	CLA	C2B-C3B-CAB-CBB
24	k	614	CLA	C4B-C3B-CAB-CBB
24	k	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	f	601	CLA	CBA-CGA-O2A-C1
24	f	601	CLA	O1A-CGA-O2A-C1
24	f	602	CLA	C3A-C2A-CAA-CBA
24	f	604	CLA	CAD-CBD-CGD-O1D
24	f	604	CLA	CAD-CBD-CGD-O2D
24	f	605	CLA	C3A-C2A-CAA-CBA
24	f	605	CLA	CBD-CGD-O2D-CED
24	f	607	CLA	C1A-C2A-CAA-CBA
24	f	607	CLA	C3A-C2A-CAA-CBA
24	f	609	CLA	C11-C10-C8-C9
24	f	610	CLA	CBD-CGD-O2D-CED
24	i	601	CLA	C3A-C2A-CAA-CBA
24	i	602	CLA	C3A-C2A-CAA-CBA
24	i	602	CLA	CHA-CBD-CGD-O1D
24	i	602	CLA	CHA-CBD-CGD-O2D
24	i	604	CLA	C6-C7-C8-C9
24	i	604	CLA	C11-C12-C13-C14
24	i	606	CLA	C11-C10-C8-C9
24	i	608	CLA	C1A-C2A-CAA-CBA
24	i	608	CLA	CBD-CGD-O2D-CED
24	i	608	CLA	O1D-CGD-O2D-CED
24	i	610	CLA	C3A-C2A-CAA-CBA
24	i	611	CLA	C1A-C2A-CAA-CBA
24	i	611	CLA	C2-C3-C5-C6
24	i	611	CLA	C4-C3-C5-C6
24	j	303	CLA	CHA-CBD-CGD-O1D
24	j	303	CLA	CHA-CBD-CGD-O2D
24	j	305	CLA	C11-C10-C8-C9
24	j	306	CLA	C2B-C3B-CAB-CBB
24	j	306	CLA	C4B-C3B-CAB-CBB
24	j	307	CLA	C2B-C3B-CAB-CBB
24	j	307	CLA	C4B-C3B-CAB-CBB
24	j	307	CLA	CHA-CBD-CGD-O1D
24	j	307	CLA	CHA-CBD-CGD-O2D
24	j	308	CLA	CHA-CBD-CGD-O1D
24	j	308	CLA	CHA-CBD-CGD-O2D
24	j	311	CLA	C1A-C2A-CAA-CBA
24	j	311	CLA	C3A-C2A-CAA-CBA
24	d	301	CLA	C3A-C2A-CAA-CBA
24	d	301	CLA	CHA-CBD-CGD-O1D
24	d	301	CLA	CHA-CBD-CGD-O2D
24	d	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	d	304	CLA	C1A-C2A-CAA-CBA
24	d	304	CLA	C3A-C2A-CAA-CBA
24	d	305	CLA	C4B-C3B-CAB-CBB
24	d	306	CLA	C1A-C2A-CAA-CBA
24	d	306	CLA	C3A-C2A-CAA-CBA
24	d	307	CLA	CBA-CGA-O2A-C1
24	g	303	CLA	C3A-C2A-CAA-CBA
24	g	304	CLA	CBD-CGD-O2D-CED
24	g	305	CLA	CAD-CBD-CGD-O1D
24	g	305	CLA	CAD-CBD-CGD-O2D
24	g	306	CLA	C4B-C3B-CAB-CBB
24	g	308	CLA	C1A-C2A-CAA-CBA
24	g	308	CLA	C6-C7-C8-C9
24	g	310	CLA	C1A-C2A-CAA-CBA
24	g	310	CLA	C3A-C2A-CAA-CBA
24	g	310	CLA	CBA-CGA-O2A-C1
24	g	310	CLA	O1A-CGA-O2A-C1
24	g	310	CLA	CHA-CBD-CGD-O1D
24	g	310	CLA	CHA-CBD-CGD-O2D
24	g	311	CLA	C1A-C2A-CAA-CBA
24	g	311	CLA	C3A-C2A-CAA-CBA
24	g	311	CLA	C2B-C3B-CAB-CBB
24	g	311	CLA	C4B-C3B-CAB-CBB
24	g	315	CLA	C1A-C2A-CAA-CBA
24	g	315	CLA	C3A-C2A-CAA-CBA
24	g	315	CLA	C4B-C3B-CAB-CBB
24	g	315	CLA	CBD-CGD-O2D-CED
24	g	322	CLA	CHA-CBD-CGD-O1D
24	g	322	CLA	CHA-CBD-CGD-O2D
26	A	844	LHG	C4-O6-P-O3
26	A	845	LHG	O1-C1-C2-C3
26	A	845	LHG	C3-O3-P-O5
26	B	802	LHG	C3-O3-P-O5
26	B	802	LHG	C3-O3-P-O6
26	B	802	LHG	C4-O6-P-O3
26	B	802	LHG	C4-O6-P-O4
26	B	802	LHG	C4-O6-P-O5
26	B	802	LHG	C8-C7-O7-C5
26	J	107	LHG	C3-O3-P-O4
26	J	107	LHG	C3-O3-P-O6
26	c	617	LHG	C4-O6-P-O3
26	c	617	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
26	c	617	LHG	C4-O6-P-O5
26	c	617	LHG	O9-C7-O7-C5
26	c	617	LHG	C8-C7-O7-C5
26	c	618	LHG	C3-O3-P-O6
26	c	618	LHG	C4-O6-P-O3
26	a	301	LHG	C3-O3-P-O6
26	a	301	LHG	O9-C7-O7-C5
26	b	302	LHG	C4-O6-P-O3
26	b	302	LHG	C4-O6-P-O4
26	b	302	LHG	C4-O6-P-O5
26	b	320	LHG	C3-O3-P-O4
26	b	320	LHG	C3-O3-P-O5
26	b	320	LHG	C3-O3-P-O6
26	b	320	LHG	C8-C7-O7-C5
26	e	617	LHG	C3-O3-P-O4
26	e	617	LHG	C4-O6-P-O3
26	e	617	LHG	C4-O6-P-O5
26	e	617	LHG	O9-C7-O7-C5
26	e	617	LHG	C8-C7-O7-C5
26	e	617	LHG	O10-C23-O8-C6
26	e	617	LHG	C24-C23-O8-C6
26	k	620	LHG	C3-O3-P-O5
26	k	620	LHG	C3-O3-P-O6
26	k	620	LHG	O9-C7-O7-C5
26	f	619	LHG	O1-C1-C2-C3
26	f	619	LHG	C3-O3-P-O4
26	f	619	LHG	C3-O3-P-O5
26	f	619	LHG	C3-O3-P-O6
26	f	619	LHG	C4-O6-P-O4
26	f	619	LHG	O9-C7-O7-C5
26	f	619	LHG	C8-C7-O7-C5
26	f	620	LHG	C3-O3-P-O4
26	f	620	LHG	C3-O3-P-O5
26	f	620	LHG	C3-O3-P-O6
26	f	620	LHG	C4-O6-P-O3
26	f	620	LHG	C4-O6-P-O4
26	f	620	LHG	C4-O6-P-O5
26	f	620	LHG	O9-C7-O7-C5
26	i	615	LHG	C3-O3-P-O5
26	i	615	LHG	C3-O3-P-O6
26	i	615	LHG	C4-O6-P-O3
26	i	615	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
26	j	319	LHG	C4-O6-P-O3
26	j	319	LHG	C4-O6-P-O4
26	d	316	LHG	C3-O3-P-O4
26	d	316	LHG	C3-O3-P-O5
26	d	316	LHG	C3-O3-P-O6
26	g	301	LHG	C3-O3-P-O6
26	g	301	LHG	C4-O6-P-O3
26	g	321	LHG	C3-O3-P-O4
26	g	321	LHG	C3-O3-P-O6
26	g	321	LHG	C4-O6-P-O3
26	g	321	LHG	C4-O6-P-O4
26	g	321	LHG	O9-C7-O7-C5
26	g	321	LHG	C8-C7-O7-C5
27	A	846	WVN	C01-C02-C11-C19
27	A	847	WVN	C20-C23-C25-C27
27	A	847	WVN	C20-C23-C25-C28
27	A	848	WVN	C06-C13-C20-C23
27	A	848	WVN	C15-C13-C20-C23
27	A	848	WVN	C20-C23-C25-C27
27	A	848	WVN	C20-C23-C25-C28
27	A	849	WVN	C05-C02-C11-C19
27	A	849	WVN	C06-C13-C20-C23
27	A	849	WVN	C15-C13-C20-C23
27	A	849	WVN	C30-C33-C34-C37
27	A	850	WVN	C11-C19-C22-C24
27	A	850	WVN	C11-C19-C22-C26
27	A	850	WVN	C29-C31-C32-C35
27	A	850	WVN	C29-C31-C32-C36
27	A	850	WVN	C30-C33-C34-C38
27	B	845	WVN	C30-C33-C34-C37
27	B	847	WVN	C15-C13-C20-C23
27	B	847	WVN	C20-C23-C25-C27
27	B	847	WVN	C20-C23-C25-C28
27	B	848	WVN	C15-C13-C20-C23
27	B	848	WVN	C20-C23-C25-C27
27	B	848	WVN	C20-C23-C25-C28
27	B	849	WVN	C11-C19-C22-C24
27	B	849	WVN	C11-C19-C22-C26
27	B	849	WVN	C20-C23-C25-C27
27	B	849	WVN	C20-C23-C25-C28
27	B	849	WVN	C30-C33-C34-C37
27	B	849	WVN	C30-C33-C34-C38

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Mol	Chain	Res	Type	Atoms
27	F	204	WVN	C11-C19-C22-C24
27	F	204	WVN	C11-C19-C22-C26
27	F	204	WVN	C22-C26-C29-C31
27	F	205	WVN	C05-C02-C11-C19
27	F	205	WVN	C15-C13-C20-C23
27	F	205	WVN	C11-C19-C22-C26
27	I	101	WVN	C01-C02-C11-C19
27	I	101	WVN	C05-C02-C11-C19
27	I	101	WVN	C11-C19-C22-C24
27	I	101	WVN	C11-C19-C22-C26
27	J	101	WVN	C15-C13-C20-C23
27	J	101	WVN	C29-C31-C32-C36
27	J	102	WVN	C11-C19-C22-C24
27	J	102	WVN	C11-C19-C22-C26
27	J	102	WVN	C20-C23-C25-C27
27	J	102	WVN	C20-C23-C25-C28
27	J	102	WVN	C30-C33-C34-C37
27	J	102	WVN	C30-C33-C34-C38
27	L	201	WVN	C05-C02-C11-C19
27	L	201	WVN	C15-C13-C20-C23
27	L	201	WVN	C11-C19-C22-C26
27	L	205	WVN	C06-C13-C20-C23
27	L	205	WVN	C11-C19-C22-C24
27	L	205	WVN	C11-C19-C22-C26
27	M	101	WVN	C05-C02-C11-C19
27	M	101	WVN	C20-C23-C25-C27
27	M	101	WVN	C20-C23-C25-C28
27	M	101	WVN	C30-C33-C34-C37
27	M	101	WVN	C30-C33-C34-C38
27	h	308	WVN	C30-C33-C34-C38
27	e	615	WVN	C05-C02-C11-C19
27	e	615	WVN	C15-C13-C20-C23
27	e	615	WVN	C11-C19-C22-C26
27	e	615	WVN	C30-C33-C34-C37
27	j	301	WVN	C29-C31-C32-C36
27	R	202	WVN	C15-C13-C20-C23
27	R	202	WVN	C29-C31-C32-C35
28	A	851	LMT	C2'-C1'-O1'-C1
28	A	851	LMT	O5'-C1'-O1'-C1
28	F	203	LMT	O5'-C1'-O1'-C1
28	b	319	LMT	O5'-C1'-O1'-C1
32	L	208	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	L	208	LMG	O6-C1-O1-C7
33	J	104	II0	C25-C29-C31-C33
33	J	104	II0	C32-C34-C36-C38
33	J	104	II0	C32-C34-C36-C40
33	c	613	II0	C26-C30-C32-C34
33	c	616	II0	C32-C34-C36-C38
33	c	616	II0	C32-C34-C36-C40
33	a	317	II0	C31-C33-C35-C37
33	a	317	II0	C31-C33-C35-C39
33	b	314	II0	C32-C34-C36-C40
33	b	318	II0	C31-C33-C35-C39
33	h	310	II0	C32-C34-C36-C40
33	h	311	II0	C25-C29-C31-C33
33	e	612	II0	C26-C30-C32-C34
33	e	612	II0	C32-C34-C36-C38
33	e	612	II0	C32-C34-C36-C40
33	e	613	II0	C25-C29-C31-C33
33	e	614	II0	C26-C30-C32-C34
33	e	614	II0	C32-C34-C36-C38
33	e	614	II0	C32-C34-C36-C40
33	k	616	II0	C31-C33-C35-C37
33	k	616	II0	C31-C33-C35-C39
33	k	619	II0	C31-C33-C35-C39
33	k	619	II0	C32-C34-C36-C40
33	k	621	II0	C31-C33-C35-C37
33	k	621	II0	C31-C33-C35-C39
33	f	614	II0	C26-C30-C32-C34
33	f	615	II0	C32-C34-C36-C40
33	f	616	II0	C31-C33-C35-C37
33	f	616	II0	C31-C33-C35-C39
33	f	618	II0	C25-C29-C31-C33
33	f	618	II0	C32-C34-C36-C40
33	i	613	II0	C32-C34-C36-C40
33	i	614	II0	C25-C29-C31-C33
33	i	614	II0	C32-C34-C36-C38
33	i	614	II0	C32-C34-C36-C40
33	j	315	II0	C31-C33-C35-C37
33	j	315	II0	C31-C33-C35-C39
33	j	318	II0	C31-C33-C35-C37
33	j	318	II0	C31-C33-C35-C39
33	d	313	II0	C32-C34-C36-C38
33	d	313	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
33	d	314	II0	C31-C33-C35-C37
33	d	314	II0	C31-C33-C35-C39
33	d	315	II0	C25-C29-C31-C33
33	d	315	II0	C32-C34-C36-C38
33	d	315	II0	C32-C34-C36-C40
33	g	316	II0	C32-C34-C36-C40
33	g	317	II0	C32-C34-C36-C38
33	g	317	II0	C32-C34-C36-C40
33	g	320	II0	C32-C34-C36-C38
33	g	320	II0	C32-C34-C36-C40
34	c	615	IHT	C30-C32-C33-C36
34	c	615	IHT	C30-C32-C33-C37
34	a	316	IHT	C31-C34-C35-C39
34	k	618	IHT	C23-C27-C30-C32
34	k	618	IHT	C33-C37-C40-C41
34	k	618	IHT	C35-C38-C41-C40
34	f	617	IHT	C10-C07-C18-C22
34	f	617	IHT	C18-C22-C23-C27
34	g	319	IHT	C18-C22-C23-C27
34	g	319	IHT	C23-C27-C30-C32
35	c	610	KC2	C1A-C2A-CAA-CBA
35	c	610	KC2	C3A-C2A-CAA-CBA
35	c	610	KC2	C2C-C3C-CAC-CBC
35	c	610	KC2	C4C-C3C-CAC-CBC
35	c	610	KC2	C2A-CAA-CBA-CGA
35	c	610	KC2	CHA-CBD-CGD-O1D
35	c	610	KC2	CHA-CBD-CGD-O2D
35	e	609	KC2	C2C-C3C-CAC-CBC
35	e	609	KC2	C4C-C3C-CAC-CBC
35	k	611	KC2	C2C-C3C-CAC-CBC
35	k	611	KC2	C4C-C3C-CAC-CBC
35	k	611	KC2	CHA-CBD-CGD-O1D
35	k	611	KC2	CHA-CBD-CGD-O2D
35	k	612	KC2	C2B-C3B-CAB-CBB
35	k	613	KC2	C3A-C2A-CAA-CBA
35	k	613	KC2	C2C-C3C-CAC-CBC
35	k	613	KC2	C4C-C3C-CAC-CBC
35	k	613	KC2	C2A-CAA-CBA-CGA
35	f	611	KC2	C2C-C3C-CAC-CBC
35	f	611	KC2	C2A-CAA-CBA-CGA
35	f	611	KC2	CHA-CBD-CGD-O2D
35	i	609	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
35	i	609	KC2	C4B-C3B-CAB-CBB
35	i	609	KC2	C2C-C3C-CAC-CBC
35	i	609	KC2	C4C-C3C-CAC-CBC
35	i	616	KC2	C3A-C2A-CAA-CBA
35	i	616	KC2	C2C-C3C-CAC-CBC
35	i	616	KC2	C4C-C3C-CAC-CBC
35	i	616	KC2	C2A-CAA-CBA-CGA
35	i	616	KC2	CBD-CGD-O2D-CED
35	i	616	KC2	O1D-CGD-O2D-CED
35	d	310	KC2	C2C-C3C-CAC-CBC
35	d	310	KC2	C4C-C3C-CAC-CBC
35	d	310	KC2	C2A-CAA-CBA-CGA
35	d	310	KC2	CHA-CBD-CGD-O2D
35	d	311	KC2	C3A-C2A-CAA-CBA
35	d	311	KC2	C2A-CAA-CBA-CGA
35	g	312	KC2	C1A-C2A-CAA-CBA
35	g	312	KC2	C2C-C3C-CAC-CBC
35	g	312	KC2	C4C-C3C-CAC-CBC
35	g	312	KC2	C2A-CAA-CBA-CGA
35	g	312	KC2	CHA-CBD-CGD-O1D
35	g	313	KC2	C2C-C3C-CAC-CBC
35	g	314	KC2	C3A-C2A-CAA-CBA
35	g	314	KC2	C2A-CAA-CBA-CGA
24	A	801	CLA	O1D-CGD-O2D-CED
24	A	815	CLA	O1D-CGD-O2D-CED
24	A	856	CLA	O1D-CGD-O2D-CED
24	c	603	CLA	O1D-CGD-O2D-CED
24	c	608	CLA	O1D-CGD-O2D-CED
24	c	611	CLA	O1D-CGD-O2D-CED
24	b	311	CLA	O1D-CGD-O2D-CED
24	k	607	CLA	O1D-CGD-O2D-CED
24	k	610	CLA	O1D-CGD-O2D-CED
24	f	613	CLA	O1D-CGD-O2D-CED
24	d	306	CLA	O1D-CGD-O2D-CED
35	g	312	KC2	O1D-CGD-O2D-CED
31	B	844	LMU	O5B-C1B-O1B-C4'
24	a	311	CLA	C4C-C3C-CAC-CBC
24	K	102	CLA	O1D-CGD-O2D-CED
24	b	310	CLA	O1D-CGD-O2D-CED
24	k	614	CLA	O1D-CGD-O2D-CED
24	f	610	CLA	O1D-CGD-O2D-CED
24	A	813	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	816	CLA	CBD-CGD-O2D-CED
24	A	856	CLA	CBD-CGD-O2D-CED
24	B	804	CLA	CBD-CGD-O2D-CED
24	B	806	CLA	CBD-CGD-O2D-CED
24	B	830	CLA	CBD-CGD-O2D-CED
24	L	202	CLA	CBD-CGD-O2D-CED
24	O	201	CLA	CBD-CGD-O2D-CED
24	c	603	CLA	CBD-CGD-O2D-CED
24	c	609	CLA	CBD-CGD-O2D-CED
24	c	611	CLA	CBD-CGD-O2D-CED
24	a	312	CLA	CBD-CGD-O2D-CED
24	b	310	CLA	CBD-CGD-O2D-CED
24	b	311	CLA	CBD-CGD-O2D-CED
24	b	313	CLA	CBD-CGD-O2D-CED
24	e	604	CLA	CBD-CGD-O2D-CED
24	e	610	CLA	CBD-CGD-O2D-CED
24	k	601	CLA	CBD-CGD-O2D-CED
24	k	610	CLA	CBD-CGD-O2D-CED
24	f	612	CLA	CBD-CGD-O2D-CED
24	f	613	CLA	CBD-CGD-O2D-CED
24	i	605	CLA	CBD-CGD-O2D-CED
24	i	610	CLA	CBD-CGD-O2D-CED
24	i	611	CLA	CBD-CGD-O2D-CED
24	j	306	CLA	CBD-CGD-O2D-CED
24	j	311	CLA	CBD-CGD-O2D-CED
24	j	313	CLA	CBD-CGD-O2D-CED
24	j	314	CLA	CBD-CGD-O2D-CED
24	d	302	CLA	CBD-CGD-O2D-CED
24	d	306	CLA	CBD-CGD-O2D-CED
24	d	312	CLA	CBD-CGD-O2D-CED
35	k	611	KC2	CBD-CGD-O2D-CED
35	g	312	KC2	CBD-CGD-O2D-CED
28	A	851	LMT	O5B-C1B-O1B-C4'
24	A	811	CLA	O1A-CGA-O2A-C1
24	A	821	CLA	O1A-CGA-O2A-C1
24	A	842	CLA	O1A-CGA-O2A-C1
24	B	813	CLA	O1A-CGA-O2A-C1
24	F	201	CLA	O1A-CGA-O2A-C1
24	J	105	CLA	O1A-CGA-O2A-C1
24	b	308	CLA	O1A-CGA-O2A-C1
24	h	301	CLA	O1A-CGA-O2A-C1
24	e	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	k	607	CLA	O1A-CGA-O2A-C1
24	k	610	CLA	O1A-CGA-O2A-C1
26	B	802	LHG	O10-C23-O8-C6
26	c	617	LHG	O10-C23-O8-C6
24	d	307	CLA	O1A-CGA-O2A-C1
24	B	804	CLA	C2C-C3C-CAC-CBC
24	a	311	CLA	C2C-C3C-CAC-CBC
35	k	611	KC2	O1D-CGD-O2D-CED
24	c	609	CLA	O1D-CGD-O2D-CED
24	f	612	CLA	O1D-CGD-O2D-CED
24	i	610	CLA	O1D-CGD-O2D-CED
24	A	811	CLA	CBA-CGA-O2A-C1
24	A	842	CLA	CBA-CGA-O2A-C1
24	J	105	CLA	CBA-CGA-O2A-C1
24	h	301	CLA	CBA-CGA-O2A-C1
24	e	611	CLA	CBA-CGA-O2A-C1
24	k	610	CLA	CBA-CGA-O2A-C1
26	B	802	LHG	C24-C23-O8-C6
26	c	617	LHG	C24-C23-O8-C6
24	h	302	CLA	CBD-CGD-O2D-CED
24	A	803	CLA	O1A-CGA-O2A-C1
24	A	814	CLA	O1A-CGA-O2A-C1
24	A	835	CLA	O1A-CGA-O2A-C1
24	B	830	CLA	O1A-CGA-O2A-C1
24	a	310	CLA	O1A-CGA-O2A-C1
24	h	302	CLA	O1A-CGA-O2A-C1
24	e	606	CLA	O1A-CGA-O2A-C1
24	f	610	CLA	O1A-CGA-O2A-C1
24	i	605	CLA	O1A-CGA-O2A-C1
24	j	307	CLA	O1A-CGA-O2A-C1
24	j	308	CLA	O1A-CGA-O2A-C1
24	g	322	CLA	O1A-CGA-O2A-C1
26	k	620	LHG	O10-C23-O8-C6
26	i	615	LHG	O10-C23-O8-C6
24	A	813	CLA	O1D-CGD-O2D-CED
24	B	804	CLA	O1D-CGD-O2D-CED
24	c	612	CLA	O1D-CGD-O2D-CED
24	a	312	CLA	O1D-CGD-O2D-CED
24	b	308	CLA	O1D-CGD-O2D-CED
24	e	604	CLA	O1D-CGD-O2D-CED
24	e	605	CLA	O1D-CGD-O2D-CED
24	f	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	j	311	CLA	O1D-CGD-O2D-CED
24	g	304	CLA	O1D-CGD-O2D-CED
35	k	613	KC2	CAA-CBA-CGA-O1A
35	i	609	KC2	CAA-CBA-CGA-O2A
24	b	312	CLA	O1D-CGD-O2D-CED
24	e	603	CLA	O1D-CGD-O2D-CED
24	B	813	CLA	CBD-CGD-O2D-CED
24	i	602	CLA	CBD-CGD-O2D-CED
35	j	312	KC2	CBD-CGD-O2D-CED
26	B	802	LHG	O9-C7-O7-C5
24	c	606	CLA	O1D-CGD-O2D-CED
24	A	802	CLA	C3-C5-C6-C7
24	A	820	CLA	C3-C5-C6-C7
24	A	840	CLA	C3-C5-C6-C7
24	B	808	CLA	C3-C5-C6-C7
24	B	830	CLA	C3-C5-C6-C7
24	B	836	CLA	C3-C5-C6-C7
24	O	201	CLA	C3-C5-C6-C7
24	b	309	CLA	C3-C5-C6-C7
24	f	610	CLA	C3-C5-C6-C7
24	e	611	CLA	O1D-CGD-O2D-CED
24	k	606	CLA	O1D-CGD-O2D-CED
24	A	803	CLA	CBA-CGA-O2A-C1
24	A	840	CLA	CBA-CGA-O2A-C1
24	B	813	CLA	CBA-CGA-O2A-C1
24	F	201	CLA	CBA-CGA-O2A-C1
24	c	608	CLA	CBA-CGA-O2A-C1
24	a	310	CLA	CBA-CGA-O2A-C1
24	b	308	CLA	CBA-CGA-O2A-C1
24	h	302	CLA	CBA-CGA-O2A-C1
24	h	306	CLA	CBA-CGA-O2A-C1
24	f	602	CLA	CBA-CGA-O2A-C1
24	f	610	CLA	CBA-CGA-O2A-C1
24	j	307	CLA	CBA-CGA-O2A-C1
24	j	308	CLA	CBA-CGA-O2A-C1
26	k	620	LHG	C24-C23-O8-C6
24	A	808	CLA	CBD-CGD-O2D-CED
24	B	814	CLA	CBD-CGD-O2D-CED
24	B	837	CLA	CBD-CGD-O2D-CED
24	F	202	CLA	CBD-CGD-O2D-CED
24	a	305	CLA	CBD-CGD-O2D-CED
24	a	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	h	304	CLA	CBD-CGD-O2D-CED
24	k	608	CLA	CBD-CGD-O2D-CED
24	i	603	CLA	CBD-CGD-O2D-CED
24	j	307	CLA	CBD-CGD-O2D-CED
24	d	308	CLA	CBD-CGD-O2D-CED
24	g	306	CLA	CBD-CGD-O2D-CED
35	k	612	KC2	CBD-CGD-O2D-CED
26	a	301	LHG	C8-C7-O7-C5
26	k	620	LHG	C8-C7-O7-C5
26	f	620	LHG	C8-C7-O7-C5
24	O	201	CLA	O1D-CGD-O2D-CED
24	h	301	CLA	O1D-CGD-O2D-CED
24	g	315	CLA	O1D-CGD-O2D-CED
24	d	303	CLA	O1D-CGD-O2D-CED
35	k	612	KC2	CAA-CBA-CGA-O1A
35	i	609	KC2	CAA-CBA-CGA-O1A
24	A	811	CLA	C4-C3-C5-C6
24	A	829	CLA	C4-C3-C5-C6
24	A	840	CLA	C4-C3-C5-C6
24	B	801	CLA	C4-C3-C5-C6
24	b	305	CLA	C4-C3-C5-C6
24	b	310	CLA	C4-C3-C5-C6
24	f	610	CLA	C4-C3-C5-C6
24	A	829	CLA	C2-C3-C5-C6
24	A	838	CLA	C2-C3-C5-C6
24	A	840	CLA	C2-C3-C5-C6
24	B	801	CLA	C2-C3-C5-C6
24	b	305	CLA	C2-C3-C5-C6
24	b	310	CLA	C2-C3-C5-C6
24	c	607	CLA	CBA-CGA-O2A-C1
24	e	608	CLA	CBA-CGA-O2A-C1
24	d	305	CLA	CBD-CGD-O2D-CED
24	A	842	CLA	C2A-CAA-CBA-CGA
24	B	809	CLA	C2A-CAA-CBA-CGA
24	f	607	CLA	C2A-CAA-CBA-CGA
24	B	811	CLA	O1A-CGA-O2A-C1
24	c	605	CLA	O1A-CGA-O2A-C1
24	b	306	CLA	C3-C5-C6-C7
24	B	836	CLA	C2C-C3C-CAC-CBC
24	A	814	CLA	CBA-CGA-O2A-C1
24	A	821	CLA	CBA-CGA-O2A-C1
24	A	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	A	835	CLA	CBA-CGA-O2A-C1
24	B	828	CLA	CBA-CGA-O2A-C1
24	B	830	CLA	CBA-CGA-O2A-C1
24	B	837	CLA	CBA-CGA-O2A-C1
24	O	205	CLA	CBA-CGA-O2A-C1
24	a	302	CLA	CBA-CGA-O2A-C1
24	e	606	CLA	CBA-CGA-O2A-C1
24	i	605	CLA	CBA-CGA-O2A-C1
24	g	322	CLA	CBA-CGA-O2A-C1
26	i	615	LHG	C24-C23-O8-C6
24	c	607	CLA	O1A-CGA-O2A-C1
27	I	101	WVN	C22-C26-C29-C31
33	J	104	II0	C26-C30-C32-C34
33	O	202	II0	C25-C29-C31-C33
33	c	616	II0	C26-C30-C32-C34
33	a	317	II0	C35-C39-C41-C42
33	b	314	II0	C25-C29-C31-C33
33	b	314	II0	C26-C30-C32-C34
33	h	310	II0	C26-C30-C32-C34
33	h	310	II0	C36-C40-C42-C41
33	k	617	II0	C25-C29-C31-C33
33	k	621	II0	C25-C29-C31-C33
33	i	612	II0	C26-C30-C32-C34
33	i	612	II0	C36-C40-C42-C41
33	d	314	II0	C35-C39-C41-C42
34	c	615	IHT	C33-C37-C40-C41
34	c	615	IHT	C35-C38-C41-C40
34	a	316	IHT	C26-C29-C31-C34
24	A	823	CLA	O1A-CGA-O2A-C1
24	A	830	CLA	O1A-CGA-O2A-C1
24	B	837	CLA	O1A-CGA-O2A-C1
24	c	601	CLA	O1A-CGA-O2A-C1
24	c	608	CLA	O1A-CGA-O2A-C1
24	b	303	CLA	O1A-CGA-O2A-C1
24	h	304	CLA	O1A-CGA-O2A-C1
24	k	601	CLA	O1A-CGA-O2A-C1
24	f	602	CLA	O1A-CGA-O2A-C1
24	i	606	CLA	O1A-CGA-O2A-C1
24	j	311	CLA	O1A-CGA-O2A-C1
26	b	320	LHG	O9-C7-O7-C5
26	i	615	LHG	O9-C7-O7-C5
24	e	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	j	313	CLA	O1D-CGD-O2D-CED
24	B	830	CLA	O1D-CGD-O2D-CED
24	k	601	CLA	O1D-CGD-O2D-CED
24	i	611	CLA	O1D-CGD-O2D-CED
24	d	302	CLA	O1D-CGD-O2D-CED
35	k	612	KC2	CAA-CBA-CGA-O2A
24	A	829	CLA	C3-C5-C6-C7
24	B	803	CLA	C3-C5-C6-C7
24	B	823	CLA	C3-C5-C6-C7
24	O	205	CLA	C3-C5-C6-C7
24	A	837	CLA	CBD-CGD-O2D-CED
24	B	810	CLA	CBD-CGD-O2D-CED
24	B	831	CLA	CBD-CGD-O2D-CED
24	a	306	CLA	CBD-CGD-O2D-CED
24	h	312	CLA	CBD-CGD-O2D-CED
24	f	607	CLA	CBD-CGD-O2D-CED
24	g	305	CLA	CBD-CGD-O2D-CED
26	f	619	LHG	O2-C2-C3-O3
26	g	301	LHG	O2-C2-C3-O3
24	L	202	CLA	O1D-CGD-O2D-CED
24	b	313	CLA	O1D-CGD-O2D-CED
24	d	312	CLA	O1D-CGD-O2D-CED
24	A	818	CLA	CBA-CGA-O2A-C1
24	B	817	CLA	CBA-CGA-O2A-C1
24	c	601	CLA	CBA-CGA-O2A-C1
24	b	303	CLA	CBA-CGA-O2A-C1
24	b	313	CLA	CBA-CGA-O2A-C1
24	h	304	CLA	CBA-CGA-O2A-C1
24	j	311	CLA	CBA-CGA-O2A-C1
24	j	313	CLA	CBA-CGA-O2A-C1
24	g	308	CLA	CBA-CGA-O2A-C1
26	b	302	LHG	C24-C23-O8-C6
26	d	316	LHG	C24-C23-O8-C6
28	b	319	LMT	O5'-C5'-C6'-O6'
31	B	844	LMU	O5'-C5'-C6'-O6'
24	A	840	CLA	O1A-CGA-O2A-C1
24	h	306	CLA	O1A-CGA-O2A-C1
24	i	605	CLA	O1D-CGD-O2D-CED
24	A	831	CLA	CBD-CGD-O2D-CED
24	A	841	CLA	CBD-CGD-O2D-CED
24	B	805	CLA	CBD-CGD-O2D-CED
24	k	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	f	602	CLA	CBD-CGD-O2D-CED
35	d	310	KC2	CBD-CGD-O2D-CED
24	b	309	CLA	C2C-C3C-CAC-CBC
24	A	818	CLA	O1A-CGA-O2A-C1
24	B	828	CLA	O1A-CGA-O2A-C1
24	g	308	CLA	O1A-CGA-O2A-C1
24	A	816	CLA	O1D-CGD-O2D-CED
24	j	306	CLA	O1D-CGD-O2D-CED
24	j	314	CLA	O1D-CGD-O2D-CED
24	B	812	CLA	C3-C5-C6-C7
24	B	814	CLA	C3-C5-C6-C7
24	B	803	CLA	CBD-CGD-O2D-CED
24	f	601	CLA	CBD-CGD-O2D-CED
24	k	614	CLA	C2C-C3C-CAC-CBC
24	B	806	CLA	O1D-CGD-O2D-CED
24	B	813	CLA	O1D-CGD-O2D-CED
24	A	823	CLA	CBA-CGA-O2A-C1
24	B	811	CLA	CBA-CGA-O2A-C1
24	c	605	CLA	CBA-CGA-O2A-C1
24	k	601	CLA	CBA-CGA-O2A-C1
24	i	606	CLA	CBA-CGA-O2A-C1
35	c	610	KC2	CAA-CBA-CGA-O2A
24	A	812	CLA	C4-C3-C5-C6
24	A	835	CLA	C4-C3-C5-C6
24	B	836	CLA	C4-C3-C5-C6
24	b	312	CLA	C4-C3-C5-C6
24	A	816	CLA	C2-C3-C5-C6
24	A	855	CLA	C2-C3-C5-C6
24	B	836	CLA	C2-C3-C5-C6
24	b	312	CLA	C2-C3-C5-C6
24	f	610	CLA	C2-C3-C5-C6
24	j	313	CLA	O1A-CGA-O2A-C1
24	B	821	CLA	CBD-CGD-O2D-CED
35	e	609	KC2	CBD-CGD-O2D-CED
31	B	844	LMU	C4'-C5'-C6'-O6'
24	A	819	CLA	C2A-CAA-CBA-CGA
24	k	605	CLA	C2A-CAA-CBA-CGA
24	h	302	CLA	O1D-CGD-O2D-CED
24	B	817	CLA	O1A-CGA-O2A-C1
24	a	302	CLA	O1A-CGA-O2A-C1
26	d	316	LHG	O10-C23-O8-C6
24	B	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	b	307	CLA	CBA-CGA-O2A-C1
24	A	802	CLA	CBD-CGD-O2D-CED
24	A	814	CLA	CBD-CGD-O2D-CED
24	A	817	CLA	CBD-CGD-O2D-CED
24	A	818	CLA	CBD-CGD-O2D-CED
24	A	832	CLA	CBD-CGD-O2D-CED
24	A	853	CLA	CBD-CGD-O2D-CED
24	B	822	CLA	CBD-CGD-O2D-CED
24	I	102	CLA	CBD-CGD-O2D-CED
24	c	601	CLA	CBD-CGD-O2D-CED
24	b	303	CLA	CBD-CGD-O2D-CED
24	e	608	CLA	CBD-CGD-O2D-CED
35	d	311	KC2	CBD-CGD-O2D-CED
24	e	608	CLA	O1A-CGA-O2A-C1
24	b	313	CLA	O1A-CGA-O2A-C1
26	b	302	LHG	O10-C23-O8-C6
24	h	303	CLA	CBD-CGD-O2D-CED
24	h	305	CLA	CBD-CGD-O2D-CED
24	j	308	CLA	CBD-CGD-O2D-CED
32	J	106	LMG	C28-C29-C30-C31
33	h	310	II0	C35-C39-C41-C42
33	k	616	II0	C25-C29-C31-C33
33	k	619	II0	C25-C29-C31-C33
33	k	621	II0	C26-C30-C32-C34
33	f	616	II0	C25-C29-C31-C33
34	j	317	IHT	C23-C27-C30-C32
24	O	205	CLA	O1A-CGA-O2A-C1
24	A	822	CLA	CBA-CGA-O2A-C1
24	A	837	CLA	CBA-CGA-O2A-C1
24	B	803	CLA	CBA-CGA-O2A-C1
24	B	805	CLA	CBA-CGA-O2A-C1
24	B	809	CLA	CBA-CGA-O2A-C1
24	B	815	CLA	CBA-CGA-O2A-C1
24	B	827	CLA	CBA-CGA-O2A-C1
24	B	838	CLA	CBA-CGA-O2A-C1
24	F	202	CLA	CBA-CGA-O2A-C1
24	c	612	CLA	CBA-CGA-O2A-C1
24	h	307	CLA	CBA-CGA-O2A-C1
24	e	607	CLA	CBA-CGA-O2A-C1
24	i	602	CLA	CBA-CGA-O2A-C1
26	c	618	LHG	C24-C23-O8-C6
26	g	321	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	A	811	CLA	CBD-CGD-O2D-CED
26	f	619	LHG	C25-C26-C27-C28
26	f	619	LHG	C27-C28-C29-C30
26	f	620	LHG	C28-C29-C30-C31
24	B	814	CLA	O1D-CGD-O2D-CED
24	i	602	CLA	O1D-CGD-O2D-CED
35	k	613	KC2	CAA-CBA-CGA-O2A
35	g	314	KC2	CAA-CBA-CGA-O2A
24	A	816	CLA	C4-C3-C5-C6
24	A	855	CLA	C4-C3-C5-C6
24	b	308	CLA	C4-C3-C5-C6
24	A	811	CLA	C2-C3-C5-C6
24	A	835	CLA	C2-C3-C5-C6
24	b	308	CLA	C2-C3-C5-C6
24	B	801	CLA	CBD-CGD-O2D-CED
24	L	204	CLA	CBD-CGD-O2D-CED
24	A	809	CLA	C6-C7-C8-C9
24	A	812	CLA	C11-C12-C13-C14
24	A	817	CLA	C11-C10-C8-C9
24	A	824	CLA	C11-C12-C13-C14
24	A	825	CLA	C6-C7-C8-C9
24	A	827	CLA	C14-C13-C15-C16
24	A	839	CLA	C11-C10-C8-C9
24	A	839	CLA	C14-C13-C15-C16
24	A	840	CLA	C14-C13-C15-C16
24	A	853	CLA	C14-C13-C15-C16
24	B	801	CLA	C11-C10-C8-C9
24	B	803	CLA	C11-C12-C13-C14
24	B	807	CLA	C6-C7-C8-C9
24	B	812	CLA	C14-C13-C15-C16
24	B	814	CLA	C11-C10-C8-C9
24	B	822	CLA	C14-C13-C15-C16
24	B	823	CLA	C11-C12-C13-C14
24	B	836	CLA	C6-C7-C8-C9
24	B	837	CLA	C11-C12-C13-C14
24	B	839	CLA	C6-C7-C8-C9
24	B	839	CLA	C11-C12-C13-C14
24	F	201	CLA	C11-C10-C8-C9
24	F	201	CLA	C11-C12-C13-C14
24	L	203	CLA	C6-C7-C8-C9
24	L	203	CLA	C11-C12-C13-C14
24	c	608	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	608	CLA	C11-C12-C13-C14
24	c	608	CLA	C14-C13-C15-C16
24	c	612	CLA	C14-C13-C15-C16
24	a	307	CLA	C11-C10-C8-C9
24	a	308	CLA	C6-C7-C8-C9
24	b	306	CLA	C11-C10-C8-C9
24	b	307	CLA	C14-C13-C15-C16
24	b	309	CLA	C14-C13-C15-C16
24	b	313	CLA	C11-C12-C13-C14
24	b	313	CLA	C14-C13-C15-C16
24	h	305	CLA	C11-C10-C8-C9
24	e	605	CLA	C6-C7-C8-C9
24	e	605	CLA	C11-C10-C8-C9
24	e	606	CLA	C6-C7-C8-C9
24	e	606	CLA	C11-C10-C8-C9
24	e	607	CLA	C14-C13-C15-C16
24	k	608	CLA	C6-C7-C8-C9
24	k	608	CLA	C11-C10-C8-C9
24	k	609	CLA	C6-C7-C8-C9
24	f	602	CLA	C14-C13-C15-C16
24	f	607	CLA	C11-C12-C13-C14
24	f	607	CLA	C14-C13-C15-C16
24	f	610	CLA	C11-C12-C13-C14
24	f	613	CLA	C11-C12-C13-C14
24	j	311	CLA	C11-C10-C8-C9
24	j	314	CLA	C11-C12-C13-C14
24	j	314	CLA	C14-C13-C15-C16
24	g	305	CLA	C11-C12-C13-C14
24	g	308	CLA	C11-C12-C13-C14
24	g	308	CLA	C14-C13-C15-C16
25	B	842	PQN	C21-C22-C23-C24
24	A	808	CLA	O1D-CGD-O2D-CED
24	F	202	CLA	O1D-CGD-O2D-CED
28	b	319	LMT	C2'-C1'-O1'-C1
24	A	837	CLA	O1A-CGA-O2A-C1
24	B	803	CLA	O1A-CGA-O2A-C1
24	B	809	CLA	O1A-CGA-O2A-C1
24	h	307	CLA	O1A-CGA-O2A-C1
27	A	847	WVN	C30-C33-C34-C38
27	A	849	WVN	C30-C33-C34-C38
27	B	845	WVN	C20-C23-C25-C27
27	B	845	WVN	C30-C33-C34-C38

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Mol	Chain	Res	Type	Atoms
27	B	847	WVN	C30-C33-C34-C38
27	B	848	WVN	C30-C33-C34-C38
27	B	849	WVN	C29-C31-C32-C35
27	F	204	WVN	C29-C31-C32-C35
27	F	205	WVN	C11-C19-C22-C24
27	F	205	WVN	C29-C31-C32-C35
27	J	101	WVN	C29-C31-C32-C35
27	L	201	WVN	C11-C19-C22-C24
27	L	205	WVN	C20-C23-C25-C27
27	e	615	WVN	C11-C19-C22-C24
27	e	615	WVN	C30-C33-C34-C38
27	j	301	WVN	C29-C31-C32-C35
27	R	201	WVN	C11-C19-C22-C24
33	J	104	II0	C31-C33-C35-C37
33	c	613	II0	C32-C34-C36-C38
33	b	314	II0	C32-C34-C36-C38
33	h	310	II0	C32-C34-C36-C38
33	h	311	II0	C31-C33-C35-C37
33	k	616	II0	C32-C34-C36-C38
33	k	619	II0	C31-C33-C35-C37
33	k	619	II0	C32-C34-C36-C38
33	f	614	II0	C32-C34-C36-C38
33	f	615	II0	C32-C34-C36-C38
33	f	618	II0	C32-C34-C36-C38
33	i	612	II0	C32-C34-C36-C38
33	i	613	II0	C32-C34-C36-C38
33	d	315	II0	C31-C33-C35-C37
33	g	316	II0	C32-C34-C36-C38
34	O	203	IHT	C18-C22-C23-C25
34	c	615	IHT	C18-C22-C23-C25
34	c	615	IHT	C31-C34-C35-C39
34	b	316	IHT	C18-C22-C23-C25
34	f	617	IHT	C18-C22-C23-C25
34	j	317	IHT	C18-C22-C23-C25
34	j	317	IHT	C30-C32-C33-C36
34	g	319	IHT	C18-C22-C23-C25
34	g	319	IHT	C31-C34-C35-C39
34	R	204	IHT	C18-C22-C23-C25
27	A	847	WVN	C30-C33-C34-C37
27	A	850	WVN	C30-C33-C34-C37
27	B	845	WVN	C20-C23-C25-C28
27	B	849	WVN	C29-C31-C32-C36

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Mol	Chain	Res	Type	Atoms
27	F	205	WVN	C29-C31-C32-C36
27	L	201	WVN	C20-C23-C25-C28
27	L	205	WVN	C20-C23-C25-C28
27	h	308	WVN	C30-C33-C34-C37
27	R	201	WVN	C11-C19-C22-C26
27	R	202	WVN	C29-C31-C32-C36
33	J	104	II0	C31-C33-C35-C39
33	O	202	II0	C31-C33-C35-C39
33	c	613	II0	C32-C34-C36-C40
33	k	616	II0	C32-C34-C36-C40
33	f	614	II0	C32-C34-C36-C40
33	i	612	II0	C32-C34-C36-C40
33	d	315	II0	C31-C33-C35-C39
34	O	203	IHT	C18-C22-C23-C27
34	c	615	IHT	C18-C22-C23-C27
34	a	316	IHT	C31-C34-C35-C38
34	b	316	IHT	C18-C22-C23-C27
34	j	317	IHT	C18-C22-C23-C27
34	j	317	IHT	C30-C32-C33-C37
34	g	319	IHT	C31-C34-C35-C38
34	R	204	IHT	C18-C22-C23-C27
24	A	821	CLA	C2A-CAA-CBA-CGA
24	k	610	CLA	C2A-CAA-CBA-CGA
24	B	805	CLA	O1A-CGA-O2A-C1
24	B	815	CLA	O1A-CGA-O2A-C1
24	B	827	CLA	O1A-CGA-O2A-C1
24	A	832	CLA	C15-C16-C17-C18
28	b	319	LMT	C4'-C5'-C6'-O6'
24	a	308	CLA	O1D-CGD-O2D-CED
35	i	609	KC2	CBD-CGD-O2D-CED
32	b	301	LMG	C11-C10-O7-C8
24	B	804	CLA	C4C-C3C-CAC-CBC
24	A	839	CLA	CBA-CGA-O2A-C1
24	A	841	CLA	CBA-CGA-O2A-C1
24	a	311	CLA	CBA-CGA-O2A-C1
24	f	603	CLA	CBA-CGA-O2A-C1
24	B	830	CLA	C2-C1-O2A-CGA
24	I	102	CLA	C2-C1-O2A-CGA
24	j	307	CLA	O1D-CGD-O2D-CED
24	d	308	CLA	O1D-CGD-O2D-CED
24	a	310	CLA	CBD-CGD-O2D-CED
24	O	205	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	b	304	CLA	C5-C6-C7-C8
24	b	305	CLA	C15-C16-C17-C18
24	A	812	CLA	C6-C7-C8-C10
24	A	818	CLA	C12-C13-C15-C16
24	A	825	CLA	C11-C12-C13-C15
24	A	836	CLA	C6-C7-C8-C10
24	A	839	CLA	C11-C12-C13-C15
24	A	840	CLA	C11-C12-C13-C15
24	B	806	CLA	C11-C12-C13-C15
24	B	812	CLA	C11-C10-C8-C7
24	F	201	CLA	C6-C7-C8-C10
24	I	102	CLA	C11-C12-C13-C15
24	a	307	CLA	C11-C12-C13-C15
24	b	305	CLA	C12-C13-C15-C16
24	b	312	CLA	C11-C10-C8-C7
24	b	313	CLA	C6-C7-C8-C10
24	h	305	CLA	C6-C7-C8-C10
24	e	611	CLA	C12-C13-C15-C16
24	k	604	CLA	C11-C12-C13-C15
25	A	843	PQN	C22-C23-C25-C26
24	A	801	CLA	CBA-CGA-O2A-C1
24	a	308	CLA	C4-C3-C5-C6
24	B	837	CLA	O1D-CGD-O2D-CED
24	i	603	CLA	O1D-CGD-O2D-CED
27	K	103	WVN	C32-C36-C39-C40
27	R	202	WVN	C22-C26-C29-C31
33	a	314	II0	C35-C39-C41-C42
33	k	616	II0	C26-C30-C32-C34
33	i	613	II0	C26-C30-C32-C34
33	d	314	II0	C25-C29-C31-C33
33	g	316	II0	C26-C30-C32-C34
33	g	317	II0	C25-C29-C31-C33
33	g	320	II0	C26-C30-C32-C34
34	O	203	IHT	C23-C27-C30-C32
34	c	615	IHT	C23-C27-C30-C32
34	c	615	IHT	C26-C29-C31-C34
24	g	306	CLA	O1D-CGD-O2D-CED
24	B	838	CLA	C5-C6-C7-C8
25	A	843	PQN	C18-C20-C21-C22
32	L	208	LMG	C38-C39-C40-C41
24	B	838	CLA	O1A-CGA-O2A-C1
24	a	311	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	b	307	CLA	O1A-CGA-O2A-C1
24	A	827	CLA	CBD-CGD-O2D-CED
24	B	820	CLA	CBD-CGD-O2D-CED
24	B	836	CLA	C13-C15-C16-C17
24	b	306	CLA	C5-C6-C7-C8
24	A	811	CLA	C2A-CAA-CBA-CGA
24	A	822	CLA	C2A-CAA-CBA-CGA
24	B	813	CLA	C2A-CAA-CBA-CGA
24	B	835	CLA	C2A-CAA-CBA-CGA
24	L	204	CLA	C2A-CAA-CBA-CGA
24	c	602	CLA	C2A-CAA-CBA-CGA
24	c	608	CLA	C2A-CAA-CBA-CGA
24	b	313	CLA	C2A-CAA-CBA-CGA
24	h	301	CLA	C2A-CAA-CBA-CGA
24	h	302	CLA	C2A-CAA-CBA-CGA
24	f	601	CLA	C2A-CAA-CBA-CGA
24	f	612	CLA	C2A-CAA-CBA-CGA
24	i	602	CLA	C2A-CAA-CBA-CGA
24	i	610	CLA	C2A-CAA-CBA-CGA
24	g	315	CLA	C2A-CAA-CBA-CGA
24	A	802	CLA	C5-C6-C7-C8
24	B	814	CLA	C8-C10-C11-C12
24	F	201	CLA	C5-C6-C7-C8
24	b	305	CLA	C5-C6-C7-C8
24	b	306	CLA	C13-C15-C16-C17
24	b	308	CLA	C10-C11-C12-C13
24	b	313	CLA	C5-C6-C7-C8
24	e	604	CLA	C13-C15-C16-C17
24	e	605	CLA	C5-C6-C7-C8
24	g	322	CLA	C13-C15-C16-C17
26	a	301	LHG	C7-C8-C9-C10
32	F	206	LMG	C10-C11-C12-C13
24	c	612	CLA	O1A-CGA-O2A-C1
24	i	602	CLA	O1A-CGA-O2A-C1
26	c	618	LHG	O10-C23-O8-C6
26	g	321	LHG	O10-C23-O8-C6
24	A	839	CLA	C3-C5-C6-C7
24	A	840	CLA	CBD-CGD-O2D-CED
24	A	842	CLA	C15-C16-C17-C18
24	B	836	CLA	C10-C11-C12-C13
24	c	604	CLA	C13-C15-C16-C17
24	b	313	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	f	607	CLA	C10-C11-C12-C13
24	f	610	CLA	C13-C15-C16-C17
25	B	842	PQN	C18-C20-C21-C22
24	A	832	CLA	CBA-CGA-O2A-C1
24	j	309	CLA	CBD-CGD-O2D-CED
24	g	303	CLA	CBD-CGD-O2D-CED
24	B	823	CLA	O1A-CGA-O2A-C1
24	F	202	CLA	O1A-CGA-O2A-C1
24	e	607	CLA	O1A-CGA-O2A-C1
24	B	817	CLA	C8-C10-C11-C12
24	B	820	CLA	C5-C6-C7-C8
24	B	841	CLA	C13-C15-C16-C17
24	b	309	CLA	C13-C15-C16-C17
24	b	312	CLA	C5-C6-C7-C8
24	h	304	CLA	O1D-CGD-O2D-CED
24	f	607	CLA	O1D-CGD-O2D-CED
24	B	810	CLA	O1D-CGD-O2D-CED
24	a	305	CLA	O1D-CGD-O2D-CED
24	a	306	CLA	O1D-CGD-O2D-CED
24	k	608	CLA	O1D-CGD-O2D-CED
24	A	802	CLA	C8-C10-C11-C12
24	A	807	CLA	C8-C10-C11-C12
24	A	826	CLA	C5-C6-C7-C8
24	c	612	CLA	C8-C10-C11-C12
24	b	305	CLA	C8-C10-C11-C12
24	b	309	CLA	C15-C16-C17-C18
35	f	611	KC2	CAA-CBA-CGA-O1A
24	A	818	CLA	C2C-C3C-CAC-CBC
24	a	307	CLA	CBD-CGD-O2D-CED
24	d	301	CLA	CBD-CGD-O2D-CED
26	i	615	LHG	C7-C8-C9-C10
28	b	319	LMT	C7-C8-C9-C10
24	B	831	CLA	O1D-CGD-O2D-CED
24	h	312	CLA	O1D-CGD-O2D-CED
24	d	305	CLA	O1D-CGD-O2D-CED
24	g	305	CLA	O1D-CGD-O2D-CED
24	B	833	CLA	C13-C15-C16-C17
24	O	201	CLA	C5-C6-C7-C8
24	f	607	CLA	CBA-CGA-O2A-C1
32	O	204	LMG	C29-C28-O8-C9
24	a	309	CLA	O2A-C1-C2-C3
24	e	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	e	609	KC2	C2A-CAA-CBA-CGA
35	k	612	KC2	C2A-CAA-CBA-CGA
24	A	822	CLA	O1A-CGA-O2A-C1
24	A	841	CLA	O1A-CGA-O2A-C1
24	A	837	CLA	O1D-CGD-O2D-CED
24	A	805	CLA	C3-C5-C6-C7
24	b	309	CLA	C4C-C3C-CAC-CBC
27	B	849	WVN	C32-C36-C39-C40
27	F	204	WVN	C32-C36-C39-C40
27	F	205	WVN	C22-C26-C29-C31
33	a	314	II0	C26-C30-C32-C34
33	a	317	II0	C25-C29-C31-C33
33	e	616	II0	C36-C40-C42-C41
33	j	315	II0	C25-C29-C31-C33
33	j	318	II0	C25-C29-C31-C33
33	g	318	II0	C25-C29-C31-C33
34	a	316	IHT	C23-C27-C30-C32
24	b	306	CLA	C10-C11-C12-C13
30	B	843	DGD	C1B-C2B-C3B-C4B
32	b	301	LMG	O9-C10-O7-C8
24	B	827	CLA	C2A-CAA-CBA-CGA
24	F	202	CLA	C2A-CAA-CBA-CGA
24	b	304	CLA	C2A-CAA-CBA-CGA
24	A	826	CLA	CBA-CGA-O2A-C1
24	L	203	CLA	CBA-CGA-O2A-C1
24	c	602	CLA	CBA-CGA-O2A-C1
24	i	611	CLA	CBA-CGA-O2A-C1
32	b	301	LMG	C29-C28-O8-C9
26	g	321	LHG	C25-C26-C27-C28
24	A	829	CLA	C8-C10-C11-C12
24	b	310	CLA	C13-C15-C16-C17
24	F	201	CLA	C15-C16-C17-C18
24	O	205	CLA	C10-C11-C12-C13
24	e	611	CLA	C13-C15-C16-C17
24	A	829	CLA	C15-C16-C17-C18
24	A	835	CLA	C15-C16-C17-C18
24	A	842	CLA	C8-C10-C11-C12
24	a	307	CLA	C15-C16-C17-C18
24	b	312	CLA	C10-C11-C12-C13
24	f	602	CLA	C8-C10-C11-C12
24	k	602	CLA	O1D-CGD-O2D-CED
24	g	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	g	311	CLA	CBA-CGA-O2A-C1
24	f	602	CLA	C4-C3-C5-C6
24	f	602	CLA	O1D-CGD-O2D-CED
24	A	812	CLA	CBD-CGD-O2D-CED
26	g	301	LHG	C8-C7-O7-C5
24	B	803	CLA	O1D-CGD-O2D-CED
26	g	301	LHG	O9-C7-O7-C5
32	L	208	LMG	O9-C10-O7-C8
28	F	203	LMT	C2'-C1'-O1'-C1
31	B	844	LMU	C2'-C1'-O1'-C1
32	b	301	LMG	C2-C1-O1-C7
24	O	205	CLA	C13-C15-C16-C17
24	A	801	CLA	O1A-CGA-O2A-C1
24	f	607	CLA	O1A-CGA-O2A-C1
24	B	832	CLA	CBD-CGD-O2D-CED
24	B	807	CLA	C5-C6-C7-C8
27	A	846	WVN	C11-C19-C22-C24
27	A	846	WVN	C20-C23-C25-C27
27	A	847	WVN	C29-C31-C32-C35
27	I	101	WVN	C29-C31-C32-C35
27	J	101	WVN	C20-C23-C25-C27
27	L	201	WVN	C20-C23-C25-C27
27	h	308	WVN	C11-C19-C22-C24
27	j	301	WVN	C20-C23-C25-C27
27	R	201	WVN	C30-C33-C34-C38
27	R	202	WVN	C30-C33-C34-C38
33	O	202	II0	C31-C33-C35-C37
33	a	314	II0	C32-C34-C36-C38
33	h	309	II0	C32-C34-C36-C38
33	j	318	II0	C32-C34-C36-C38
33	d	313	II0	C31-C33-C35-C37
34	a	316	IHT	C30-C32-C33-C36
27	A	846	WVN	C20-C23-C25-C28
27	A	847	WVN	C29-C31-C32-C36
27	F	204	WVN	C29-C31-C32-C36
27	I	101	WVN	C29-C31-C32-C36
27	J	101	WVN	C20-C23-C25-C28
27	h	308	WVN	C11-C19-C22-C26
27	j	301	WVN	C20-C23-C25-C28
33	a	314	II0	C32-C34-C36-C40
33	h	309	II0	C32-C34-C36-C40
33	h	311	II0	C31-C33-C35-C39

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Mol	Chain	Res	Type	Atoms
33	j	318	II0	C32-C34-C36-C40
34	c	615	IHT	C31-C34-C35-C38
34	a	316	IHT	C30-C32-C33-C37
24	f	603	CLA	O1A-CGA-O2A-C1
24	A	808	CLA	C2A-CAA-CBA-CGA
24	A	817	CLA	C2A-CAA-CBA-CGA
24	A	828	CLA	C2A-CAA-CBA-CGA
24	B	815	CLA	C2A-CAA-CBA-CGA
24	B	816	CLA	C2A-CAA-CBA-CGA
24	B	840	CLA	C2A-CAA-CBA-CGA
24	i	611	CLA	C2A-CAA-CBA-CGA
24	d	301	CLA	C2A-CAA-CBA-CGA
24	O	205	CLA	C2C-C3C-CAC-CBC
24	B	833	CLA	C16-C17-C18-C19
24	b	313	CLA	C16-C17-C18-C19
24	A	831	CLA	O1D-CGD-O2D-CED
24	B	805	CLA	O1D-CGD-O2D-CED
24	f	601	CLA	O1D-CGD-O2D-CED
24	A	826	CLA	O1A-CGA-O2A-C1
32	O	204	LMG	O10-C28-O8-C9
32	b	301	LMG	O10-C28-O8-C9
31	B	844	LMU	O5'-C1'-O1'-C1
32	b	301	LMG	O6-C1-O1-C7
32	L	208	LMG	C11-C10-O7-C8
35	c	610	KC2	CAA-CBA-CGA-O1A
24	B	814	CLA	C5-C6-C7-C8
24	A	812	CLA	C2-C3-C5-C6
24	A	841	CLA	O1D-CGD-O2D-CED
24	A	828	CLA	CBA-CGA-O2A-C1
24	B	836	CLA	C5-C6-C7-C8
24	A	818	CLA	C4C-C3C-CAC-CBC
24	h	302	CLA	C2-C1-O2A-CGA
24	f	602	CLA	C2-C1-O2A-CGA
24	B	813	CLA	C11-C12-C13-C15
24	k	609	CLA	C16-C17-C18-C19
24	A	832	CLA	O1A-CGA-O2A-C1
26	c	617	LHG	C5-C6-O8-C23
24	B	821	CLA	O1D-CGD-O2D-CED
24	B	840	CLA	C2C-C3C-CAC-CBC
26	A	844	LHG	C11-C12-C13-C14
26	f	619	LHG	C30-C31-C32-C33
32	L	208	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
24	B	822	CLA	O1D-CGD-O2D-CED
24	A	805	CLA	CBA-CGA-O2A-C1
24	L	207	CLA	CBA-CGA-O2A-C1
26	B	802	LHG	C11-C10-C9-C8
26	i	615	LHG	C27-C28-C29-C30
26	A	845	LHG	O1-C1-C2-O2
26	f	619	LHG	O1-C1-C2-O2
28	A	851	LMT	C2-C1-O1'-C1'
31	B	844	LMU	C2-C1-O1'-C1'
33	a	314	II0	C10-C22-C24-C26
33	b	314	II0	C10-C22-C24-C26
33	k	617	II0	C10-C22-C24-C26
33	g	318	II0	C10-C22-C24-C26
26	a	301	LHG	C9-C10-C11-C12
24	A	810	CLA	C4B-C3B-CAB-CBB
24	A	823	CLA	C4B-C3B-CAB-CBB
24	B	827	CLA	C4B-C3B-CAB-CBB
24	B	829	CLA	C4B-C3B-CAB-CBB
24	B	838	CLA	C4B-C3B-CAB-CBB
24	J	105	CLA	C4B-C3B-CAB-CBB
24	K	102	CLA	C4B-C3B-CAB-CBB
24	a	304	CLA	C4B-C3B-CAB-CBB
24	a	309	CLA	C4B-C3B-CAB-CBB
24	b	303	CLA	C4B-C3B-CAB-CBB
24	h	302	CLA	C4B-C3B-CAB-CBB
24	h	306	CLA	C4B-C3B-CAB-CBB
24	e	605	CLA	C4B-C3B-CAB-CBB
24	k	606	CLA	C4B-C3B-CAB-CBB
24	f	602	CLA	C4B-C3B-CAB-CBB
24	f	606	CLA	C4B-C3B-CAB-CBB
24	j	308	CLA	C4B-C3B-CAB-CBB
24	j	311	CLA	C4B-C3B-CAB-CBB
24	d	306	CLA	C4B-C3B-CAB-CBB
24	d	309	CLA	C4B-C3B-CAB-CBB
24	g	307	CLA	C4B-C3B-CAB-CBB
26	J	107	LHG	C15-C16-C17-C18
24	B	824	CLA	C16-C17-C18-C19
24	B	833	CLA	C16-C17-C18-C20
24	b	313	CLA	C16-C17-C18-C20
24	k	609	CLA	C16-C17-C18-C20
25	A	843	PQN	C26-C27-C28-C29
24	B	826	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	L	202	CLA	C2A-CAA-CBA-CGA
24	i	604	CLA	C2A-CAA-CBA-CGA
24	j	302	CLA	C2A-CAA-CBA-CGA
24	A	840	CLA	C10-C11-C12-C13
24	b	310	CLA	C15-C16-C17-C18
24	A	826	CLA	C12-C13-C15-C16
24	A	831	CLA	C11-C12-C13-C15
24	A	841	CLA	C6-C7-C8-C10
24	L	203	CLA	C12-C13-C15-C16
24	b	310	CLA	C11-C10-C8-C7
24	b	310	CLA	C12-C13-C15-C16
24	e	607	CLA	C12-C13-C15-C16
24	k	609	CLA	C12-C13-C15-C16
24	f	610	CLA	C12-C13-C15-C16
24	j	311	CLA	C11-C12-C13-C15
24	d	303	CLA	C6-C7-C8-C10
24	e	602	CLA	CBA-CGA-O2A-C1
24	A	809	CLA	C5-C6-C7-C8
24	B	807	CLA	C15-C16-C17-C18
28	A	851	LMT	C7-C8-C9-C10
32	J	106	LMG	C13-C14-C15-C16
24	c	602	CLA	O1A-CGA-O2A-C1
24	i	611	CLA	O1A-CGA-O2A-C1
24	A	814	CLA	C3A-C2A-CAA-CBA
24	A	816	CLA	C3A-C2A-CAA-CBA
24	A	831	CLA	C3A-C2A-CAA-CBA
24	A	834	CLA	C3A-C2A-CAA-CBA
24	A	841	CLA	C3A-C2A-CAA-CBA
24	A	842	CLA	C3A-C2A-CAA-CBA
24	B	812	CLA	C3A-C2A-CAA-CBA
24	B	813	CLA	C3A-C2A-CAA-CBA
24	B	832	CLA	C3A-C2A-CAA-CBA
24	B	839	CLA	C3A-C2A-CAA-CBA
24	J	105	CLA	C3A-C2A-CAA-CBA
24	O	201	CLA	C3A-C2A-CAA-CBA
24	O	205	CLA	C3A-C2A-CAA-CBA
24	a	306	CLA	C3A-C2A-CAA-CBA
24	a	307	CLA	C3A-C2A-CAA-CBA
24	h	306	CLA	C3A-C2A-CAA-CBA
24	e	608	CLA	C3A-C2A-CAA-CBA
24	k	614	CLA	C3A-C2A-CAA-CBA
24	i	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	j	307	CLA	C3A-C2A-CAA-CBA
24	d	312	CLA	C3A-C2A-CAA-CBA
24	g	306	CLA	C3A-C2A-CAA-CBA
24	e	608	CLA	O1D-CGD-O2D-CED
24	B	816	CLA	CBD-CGD-O2D-CED
24	A	829	CLA	C5-C6-C7-C8
24	B	825	CLA	C13-C15-C16-C17
24	b	309	CLA	C5-C6-C7-C8
24	f	613	CLA	C8-C10-C11-C12
24	f	613	CLA	C10-C11-C12-C13
24	A	832	CLA	O1D-CGD-O2D-CED
27	I	101	WVN	C32-C36-C39-C40
33	a	317	II0	C36-C40-C42-C41
24	A	835	CLA	C16-C17-C18-C19
25	A	843	PQN	C26-C27-C28-C30
28	A	851	LMT	C1-C2-C3-C4
24	L	203	CLA	O1A-CGA-O2A-C1
24	g	306	CLA	O1A-CGA-O2A-C1
24	k	602	CLA	C2C-C3C-CAC-CBC
24	c	602	CLA	CBD-CGD-O2D-CED
24	a	303	CLA	CBD-CGD-O2D-CED
26	f	619	LHG	C10-C11-C12-C13
24	c	606	CLA	CBA-CGA-O2A-C1
24	a	309	CLA	CBA-CGA-O2A-C1
24	f	612	CLA	CBA-CGA-O2A-C1
24	i	601	CLA	CBA-CGA-O2A-C1
24	L	203	CLA	C3-C5-C6-C7
24	b	313	CLA	C3-C5-C6-C7
24	A	802	CLA	O1D-CGD-O2D-CED
28	b	319	LMT	C4-C5-C6-C7
24	A	839	CLA	O1A-CGA-O2A-C1
24	e	602	CLA	O1A-CGA-O2A-C1
24	A	817	CLA	O1D-CGD-O2D-CED
24	c	601	CLA	O1D-CGD-O2D-CED
26	d	316	LHG	C25-C26-C27-C28
24	A	814	CLA	O1D-CGD-O2D-CED
24	A	853	CLA	O1D-CGD-O2D-CED
24	h	305	CLA	O1D-CGD-O2D-CED
24	j	308	CLA	O1D-CGD-O2D-CED
24	A	822	CLA	C2B-C3B-CAB-CBB
24	A	823	CLA	C2B-C3B-CAB-CBB
24	B	838	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	a	309	CLA	C2B-C3B-CAB-CBB
24	a	311	CLA	C2B-C3B-CAB-CBB
24	b	303	CLA	C2B-C3B-CAB-CBB
24	h	306	CLA	C2B-C3B-CAB-CBB
24	e	605	CLA	C2B-C3B-CAB-CBB
24	k	610	CLA	C2B-C3B-CAB-CBB
24	j	311	CLA	C2B-C3B-CAB-CBB
24	d	306	CLA	C2B-C3B-CAB-CBB
24	g	306	CLA	C2B-C3B-CAB-CBB
24	g	315	CLA	C2B-C3B-CAB-CBB
27	A	846	WVN	C06-C13-C20-C23
27	A	847	WVN	C06-C13-C20-C23
27	A	847	WVN	C15-C13-C20-C23
27	A	850	WVN	C15-C13-C20-C23
27	B	847	WVN	C06-C13-C20-C23
27	B	848	WVN	C06-C13-C20-C23
27	B	849	WVN	C15-C13-C20-C23
27	J	101	WVN	C06-C13-C20-C23
27	J	102	WVN	C15-C13-C20-C23
27	L	205	WVN	C15-C13-C20-C23
27	M	101	WVN	C06-C13-C20-C23
27	M	101	WVN	C15-C13-C20-C23
27	K	103	WVN	C06-C13-C20-C23
27	e	615	WVN	C06-C13-C20-C23
34	O	203	IHT	C02-C07-C18-C22
34	f	617	IHT	C02-C07-C18-C22
24	A	812	CLA	CBA-CGA-O2A-C1
24	A	840	CLA	C5-C6-C7-C8
24	e	605	CLA	C3-C5-C6-C7
24	a	302	CLA	C2C-C3C-CAC-CBC
32	L	208	LMG	C19-C20-C21-C22
31	B	844	LMU	C1-C2-C3-C4
24	A	815	CLA	C2A-CAA-CBA-CGA
24	A	818	CLA	C13-C15-C16-C17
24	A	828	CLA	O1A-CGA-O2A-C1
24	L	207	CLA	O1A-CGA-O2A-C1
24	g	311	CLA	O1A-CGA-O2A-C1
24	a	308	CLA	C2-C3-C5-C6
26	f	620	LHG	C7-C8-C9-C10
24	A	818	CLA	O1D-CGD-O2D-CED
24	A	809	CLA	CBA-CGA-O2A-C1
24	B	826	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	O	201	CLA	CBA-CGA-O2A-C1
24	d	306	CLA	CBA-CGA-O2A-C1
24	B	801	CLA	C11-C12-C13-C14
32	L	208	LMG	C32-C33-C34-C35
24	A	812	CLA	O1A-CGA-O2A-C1
26	f	619	LHG	C26-C27-C28-C29
31	B	844	LMU	C4-C5-C6-C7
24	B	836	CLA	C8-C10-C11-C12
24	B	809	CLA	C3-C5-C6-C7
24	B	829	CLA	CBA-CGA-O2A-C1
27	A	850	WVN	C34-C37-C40-C39
27	B	849	WVN	C22-C26-C29-C31
33	a	314	II0	C36-C40-C42-C41
33	f	618	II0	C35-C39-C41-C42
33	i	612	II0	C25-C29-C31-C33
34	g	319	IHT	C35-C38-C41-C40
32	F	206	LMG	O6-C5-C6-O5
24	A	840	CLA	C16-C17-C18-C20
26	c	618	LHG	C8-C7-O7-C5
32	F	206	LMG	C11-C12-C13-C14
24	f	602	CLA	C10-C11-C12-C13
27	A	849	WVN	C20-C23-C25-C27
27	j	301	WVN	C11-C19-C22-C24
33	b	318	II0	C31-C33-C35-C37
27	B	847	WVN	C30-C33-C34-C37
27	B	848	WVN	C30-C33-C34-C37
27	j	301	WVN	C11-C19-C22-C26
26	f	619	LHG	C28-C29-C30-C31
24	B	837	CLA	C2A-CAA-CBA-CGA
24	B	807	CLA	C16-C17-C18-C19
24	B	807	CLA	C16-C17-C18-C20
35	i	616	KC2	C2B-C3B-CAB-CBB
28	b	319	LMT	C3-C4-C5-C6
26	B	802	LHG	C9-C10-C11-C12
24	f	612	CLA	O1A-CGA-O2A-C1
24	i	601	CLA	O1A-CGA-O2A-C1
25	A	843	PQN	C13-C15-C16-C17
32	L	208	LMG	C34-C35-C36-C37
32	O	204	LMG	O6-C5-C6-O5
24	B	836	CLA	C15-C16-C17-C18
35	k	612	KC2	C4B-C3B-CAB-CBB
35	f	611	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
35	g	313	KC2	C4C-C3C-CAC-CBC
24	B	837	CLA	C16-C17-C18-C19
24	B	837	CLA	C16-C17-C18-C20
24	g	305	CLA	C2C-C3C-CAC-CBC
24	A	805	CLA	O1A-CGA-O2A-C1
24	O	201	CLA	O1A-CGA-O2A-C1
24	a	309	CLA	O1A-CGA-O2A-C1
24	I	102	CLA	O1D-CGD-O2D-CED
26	f	619	LHG	C9-C10-C11-C12
32	F	206	LMG	O7-C8-C9-O8
24	b	303	CLA	O1D-CGD-O2D-CED
24	h	303	CLA	O1D-CGD-O2D-CED
28	A	851	LMT	C3-C4-C5-C6
24	A	840	CLA	C8-C10-C11-C12
24	A	841	CLA	C10-C11-C12-C13
32	b	301	LMG	C34-C35-C36-C37
24	A	811	CLA	O1D-CGD-O2D-CED
24	b	313	CLA	C4-C3-C5-C6
25	B	842	PQN	C14-C13-C15-C16
24	b	313	CLA	C2-C3-C5-C6
26	g	301	LHG	C1-C2-C3-O3
24	A	838	CLA	C2A-CAA-CBA-CGA
24	A	852	CLA	C2A-CAA-CBA-CGA
24	B	801	CLA	C2A-CAA-CBA-CGA
24	d	306	CLA	C2A-CAA-CBA-CGA
24	d	306	CLA	O1A-CGA-O2A-C1
24	b	305	CLA	C10-C11-C12-C13
24	c	606	CLA	O1A-CGA-O2A-C1
24	A	804	CLA	C1A-C2A-CAA-CBA
24	A	808	CLA	C1A-C2A-CAA-CBA
24	A	809	CLA	C1A-C2A-CAA-CBA
24	A	814	CLA	C1A-C2A-CAA-CBA
24	A	818	CLA	C1A-C2A-CAA-CBA
24	A	819	CLA	C1A-C2A-CAA-CBA
24	A	831	CLA	C1A-C2A-CAA-CBA
24	A	833	CLA	C1A-C2A-CAA-CBA
24	A	834	CLA	C1A-C2A-CAA-CBA
24	A	837	CLA	C1A-C2A-CAA-CBA
24	A	841	CLA	C1A-C2A-CAA-CBA
24	A	855	CLA	C1A-C2A-CAA-CBA
24	B	805	CLA	C1A-C2A-CAA-CBA
24	B	812	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	813	CLA	C1A-C2A-CAA-CBA
24	B	817	CLA	C1A-C2A-CAA-CBA
24	B	825	CLA	C1A-C2A-CAA-CBA
24	J	105	CLA	C1A-C2A-CAA-CBA
24	L	207	CLA	C1A-C2A-CAA-CBA
24	c	602	CLA	C1A-C2A-CAA-CBA
24	c	606	CLA	C1A-C2A-CAA-CBA
24	c	608	CLA	C1A-C2A-CAA-CBA
24	c	612	CLA	C1A-C2A-CAA-CBA
24	a	306	CLA	C1A-C2A-CAA-CBA
24	a	307	CLA	C1A-C2A-CAA-CBA
24	a	309	CLA	C1A-C2A-CAA-CBA
24	a	311	CLA	C1A-C2A-CAA-CBA
24	b	304	CLA	C1A-C2A-CAA-CBA
24	b	308	CLA	C1A-C2A-CAA-CBA
24	b	312	CLA	C1A-C2A-CAA-CBA
24	h	301	CLA	C1A-C2A-CAA-CBA
24	h	306	CLA	C1A-C2A-CAA-CBA
24	h	307	CLA	C1A-C2A-CAA-CBA
24	e	610	CLA	C1A-C2A-CAA-CBA
24	k	607	CLA	C1A-C2A-CAA-CBA
24	f	601	CLA	C1A-C2A-CAA-CBA
24	f	602	CLA	C1A-C2A-CAA-CBA
24	f	605	CLA	C1A-C2A-CAA-CBA
24	i	601	CLA	C1A-C2A-CAA-CBA
24	i	602	CLA	C1A-C2A-CAA-CBA
24	i	610	CLA	C1A-C2A-CAA-CBA
24	j	302	CLA	C1A-C2A-CAA-CBA
24	j	307	CLA	C1A-C2A-CAA-CBA
24	d	301	CLA	C1A-C2A-CAA-CBA
24	d	312	CLA	C1A-C2A-CAA-CBA
24	g	303	CLA	C1A-C2A-CAA-CBA
24	g	306	CLA	C1A-C2A-CAA-CBA
24	A	818	CLA	C8-C10-C11-C12
24	B	805	CLA	C10-C11-C12-C13
24	B	835	CLA	C10-C11-C12-C13
24	k	614	CLA	C4C-C3C-CAC-CBC
26	c	618	LHG	O9-C7-O7-C5
24	A	802	CLA	C11-C12-C13-C15
24	A	806	CLA	C6-C7-C8-C10
24	A	810	CLA	C11-C12-C13-C15
24	A	812	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	A	825	CLA	C11-C10-C8-C7
24	A	829	CLA	C11-C10-C8-C7
24	A	853	CLA	C11-C10-C8-C7
24	A	855	CLA	C6-C7-C8-C10
24	A	855	CLA	C11-C10-C8-C7
24	B	803	CLA	C6-C7-C8-C10
24	B	807	CLA	C11-C10-C8-C7
24	B	814	CLA	C6-C7-C8-C10
24	B	818	CLA	C11-C12-C13-C15
24	B	832	CLA	C11-C10-C8-C7
24	B	833	CLA	C12-C13-C15-C16
24	B	839	CLA	C11-C10-C8-C7
24	F	201	CLA	C11-C12-C13-C15
24	O	205	CLA	C6-C7-C8-C10
24	c	608	CLA	C11-C10-C8-C7
24	c	612	CLA	C12-C13-C15-C16
24	a	308	CLA	C6-C7-C8-C10
24	a	310	CLA	C6-C7-C8-C10
24	b	309	CLA	C12-C13-C15-C16
24	b	312	CLA	C11-C12-C13-C15
24	h	306	CLA	C6-C7-C8-C10
24	h	312	CLA	C12-C13-C15-C16
24	e	606	CLA	C11-C10-C8-C7
24	f	607	CLA	C11-C12-C13-C15
24	f	608	CLA	C12-C13-C15-C16
24	f	613	CLA	C6-C7-C8-C10
24	i	604	CLA	C11-C10-C8-C7
24	g	305	CLA	C11-C10-C8-C7
24	g	322	CLA	C12-C13-C15-C16
24	A	840	CLA	C16-C17-C18-C19
24	B	801	CLA	C16-C17-C18-C20
24	B	830	CLA	C16-C17-C18-C19
24	b	306	CLA	C16-C17-C18-C20
24	B	806	CLA	O1A-CGA-O2A-C1
24	B	829	CLA	O1A-CGA-O2A-C1
24	J	103	CLA	C3A-C2A-CAA-CBA
24	d	301	CLA	O1D-CGD-O2D-CED
26	B	802	LHG	C16-C17-C18-C19
24	g	307	CLA	CBD-CGD-O2D-CED
35	g	314	KC2	CAA-CBA-CGA-O1A
24	f	613	CLA	C15-C16-C17-C18
24	A	806	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	B	823	CLA	C5-C6-C7-C8
26	b	302	LHG	C8-C7-O7-C5
24	f	602	CLA	C2A-CAA-CBA-CGA
24	i	601	CLA	C2A-CAA-CBA-CGA
24	R	203	CLA	C2A-CAA-CBA-CGA
24	A	802	CLA	C11-C12-C13-C14
24	A	806	CLA	C6-C7-C8-C9
24	A	808	CLA	C6-C7-C8-C9
24	A	810	CLA	C11-C12-C13-C14
24	A	824	CLA	C11-C10-C8-C9
24	A	839	CLA	C11-C12-C13-C14
24	A	840	CLA	C11-C12-C13-C14
24	A	841	CLA	C14-C13-C15-C16
24	A	855	CLA	C6-C7-C8-C9
24	B	803	CLA	C6-C7-C8-C9
24	B	812	CLA	C11-C10-C8-C9
24	B	813	CLA	C6-C7-C8-C9
24	B	823	CLA	C11-C10-C8-C9
24	B	832	CLA	C11-C10-C8-C9
24	B	833	CLA	C14-C13-C15-C16
24	B	836	CLA	C11-C12-C13-C14
24	a	305	CLA	C11-C12-C13-C14
24	a	308	CLA	C11-C10-C8-C9
24	b	312	CLA	C11-C12-C13-C14
24	h	305	CLA	C11-C12-C13-C14
24	e	604	CLA	C6-C7-C8-C9
24	f	613	CLA	C6-C7-C8-C9
24	j	314	CLA	C6-C7-C8-C9
32	J	106	LMG	C20-C21-C22-C23
27	I	101	WVN	C34-C37-C40-C39
27	h	308	WVN	C25-C28-C30-C33
24	A	806	CLA	CBA-CGA-O2A-C1
24	B	806	CLA	CBA-CGA-O2A-C1
24	h	312	CLA	CBA-CGA-O2A-C1
24	g	307	CLA	CBA-CGA-O2A-C1
24	b	308	CLA	C14-C13-C15-C16
26	J	107	LHG	C4-C5-C6-O8
32	O	204	LMG	C7-C8-C9-O8
32	F	206	LMG	C19-C20-C21-C22
24	b	313	CLA	C10-C11-C12-C13
24	g	322	CLA	C15-C16-C17-C18
26	b	320	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	e	607	CLA	O1D-CGD-O2D-CED
24	A	817	CLA	CBA-CGA-O2A-C1
26	g	301	LHG	C24-C23-O8-C6
28	a	318	LMT	O5'-C5'-C6'-O6'
24	A	812	CLA	C16-C17-C18-C20
24	k	608	CLA	C16-C17-C18-C20
24	L	204	CLA	O1D-CGD-O2D-CED
24	b	308	CLA	C5-C6-C7-C8
24	A	809	CLA	O1A-CGA-O2A-C1
26	g	301	LHG	O10-C23-O8-C6
24	A	841	CLA	C4-C3-C5-C6
24	B	820	CLA	C4-C3-C5-C6
24	B	823	CLA	C8-C10-C11-C12
27	A	850	WVN	C20-C23-C25-C27
27	L	206	WVN	C20-C23-C25-C27
27	R	202	WVN	C11-C19-C22-C24
34	k	618	IHT	C18-C22-C23-C25
34	g	319	IHT	C30-C32-C33-C36
24	B	801	CLA	C16-C17-C18-C19
27	A	849	WVN	C20-C23-C25-C28
27	A	850	WVN	C20-C23-C25-C28
27	K	103	WVN	C20-C23-C25-C28
27	R	202	WVN	C11-C19-C22-C26
34	b	317	IHT	C30-C32-C33-C37
34	k	618	IHT	C18-C22-C23-C27
24	g	307	CLA	O1A-CGA-O2A-C1
32	L	208	LMG	C36-C37-C38-C39
26	f	620	LHG	C23-C24-C25-C26
28	b	319	LMT	C2-C3-C4-C5
33	h	311	II0	C26-C30-C32-C34
33	i	612	II0	C35-C39-C41-C42
24	g	303	CLA	O1D-CGD-O2D-CED
24	B	826	CLA	O1A-CGA-O2A-C1
24	a	310	CLA	O1D-CGD-O2D-CED
24	g	311	CLA	C6-C7-C8-C9
24	A	828	CLA	C2-C3-C5-C6
24	A	841	CLA	C2-C3-C5-C6
26	f	619	LHG	C31-C32-C33-C34
24	b	310	CLA	C16-C17-C18-C20
32	F	206	LMG	C15-C16-C17-C18
24	B	821	CLA	CBA-CGA-O2A-C1
24	B	805	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	R	203	CLA	CAA-CBA-CGA-O2A
32	J	106	LMG	C18-C19-C20-C21
24	c	605	CLA	C2A-CAA-CBA-CGA
24	B	814	CLA	C11-C12-C13-C14
24	I	102	CLA	CBA-CGA-O2A-C1
24	b	309	CLA	CBD-CGD-O2D-CED
24	R	203	CLA	CBD-CGD-O2D-CED
32	L	208	LMG	C22-C23-C24-C25
24	A	835	CLA	C13-C15-C16-C17
26	B	802	LHG	C10-C11-C12-C13
24	j	309	CLA	O1D-CGD-O2D-CED
24	B	835	CLA	C8-C10-C11-C12
24	c	602	CLA	O1D-CGD-O2D-CED
27	B	848	WVN	C25-C28-C30-C33
24	i	606	CLA	C14-C13-C15-C16
24	j	311	CLA	C14-C13-C15-C16
24	b	310	CLA	C16-C17-C18-C19
24	B	820	CLA	C2-C3-C5-C6
26	J	107	LHG	C14-C15-C16-C17
26	b	320	LHG	C12-C13-C14-C15
24	A	829	CLA	CBA-CGA-O2A-C1
24	a	312	CLA	CBA-CGA-O2A-C1
24	b	304	CLA	CBA-CGA-O2A-C1
24	b	311	CLA	CBA-CGA-O2A-C1
24	A	840	CLA	O1D-CGD-O2D-CED
33	b	315	II0	C10-C22-C24-C26
33	f	615	II0	C09-C21-C23-C25
33	i	612	II0	C10-C22-C24-C26
33	d	315	II0	C09-C21-C23-C25
33	d	315	II0	C10-C22-C24-C26
33	g	316	II0	C10-C22-C24-C26
24	A	818	CLA	C14-C13-C15-C16
24	A	825	CLA	C11-C10-C8-C9
24	A	829	CLA	C11-C10-C8-C9
24	A	831	CLA	C14-C13-C15-C16
24	A	835	CLA	C6-C7-C8-C9
24	A	853	CLA	C11-C10-C8-C9
24	B	805	CLA	C14-C13-C15-C16
24	B	806	CLA	C11-C10-C8-C9
24	B	806	CLA	C14-C13-C15-C16
24	B	807	CLA	C11-C10-C8-C9
24	B	813	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	814	CLA	C6-C7-C8-C9
24	B	818	CLA	C14-C13-C15-C16
24	B	822	CLA	C6-C7-C8-C9
24	B	835	CLA	C11-C10-C8-C9
24	B	838	CLA	C11-C10-C8-C9
24	B	839	CLA	C11-C10-C8-C9
24	O	205	CLA	C6-C7-C8-C9
24	a	308	CLA	C14-C13-C15-C16
24	e	611	CLA	C14-C13-C15-C16
24	f	613	CLA	C14-C13-C15-C16
24	i	604	CLA	C11-C10-C8-C9
24	j	305	CLA	C14-C13-C15-C16
24	g	305	CLA	C11-C10-C8-C9
24	g	322	CLA	C14-C13-C15-C16
24	A	806	CLA	C15-C16-C17-C18
24	A	829	CLA	C10-C11-C12-C13
24	A	842	CLA	C10-C11-C12-C13
24	a	307	CLA	C13-C15-C16-C17
24	A	801	CLA	C4B-C3B-CAB-CBB
24	A	832	CLA	C4B-C3B-CAB-CBB
24	A	853	CLA	C4B-C3B-CAB-CBB
24	B	803	CLA	C4B-C3B-CAB-CBB
24	I	102	CLA	C4B-C3B-CAB-CBB
24	c	602	CLA	C4B-C3B-CAB-CBB
24	a	306	CLA	C4B-C3B-CAB-CBB
24	a	311	CLA	C4B-C3B-CAB-CBB
24	h	307	CLA	C4B-C3B-CAB-CBB
24	e	601	CLA	C4B-C3B-CAB-CBB
24	i	605	CLA	C4B-C3B-CAB-CBB
24	i	611	CLA	C4B-C3B-CAB-CBB
24	g	322	CLA	C4B-C3B-CAB-CBB
24	B	801	CLA	O1D-CGD-O2D-CED
24	a	307	CLA	O1D-CGD-O2D-CED
24	B	838	CLA	CAA-CBA-CGA-O2A
32	J	106	LMG	C41-C42-C43-C44
26	f	620	LHG	C34-C35-C36-C37
24	g	307	CLA	CAA-CBA-CGA-O2A
24	A	812	CLA	C12-C13-C15-C16
24	A	817	CLA	C11-C10-C8-C7
24	A	824	CLA	C11-C10-C8-C7
24	A	827	CLA	C11-C12-C13-C15
24	A	835	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	A	837	CLA	C12-C13-C15-C16
24	A	853	CLA	C11-C12-C13-C15
24	B	805	CLA	C11-C12-C13-C15
24	B	806	CLA	C12-C13-C15-C16
24	B	813	CLA	C6-C7-C8-C10
24	B	818	CLA	C12-C13-C15-C16
24	B	822	CLA	C6-C7-C8-C10
24	B	835	CLA	C11-C10-C8-C7
24	B	836	CLA	C11-C12-C13-C15
24	B	836	CLA	C12-C13-C15-C16
24	B	837	CLA	C11-C10-C8-C7
24	F	201	CLA	C12-C13-C15-C16
24	L	203	CLA	C6-C7-C8-C10
24	O	201	CLA	C11-C10-C8-C7
24	c	608	CLA	C12-C13-C15-C16
24	a	308	CLA	C11-C10-C8-C7
24	a	308	CLA	C12-C13-C15-C16
24	b	307	CLA	C11-C10-C8-C7
24	b	309	CLA	C11-C12-C13-C15
24	b	312	CLA	C6-C7-C8-C10
24	h	305	CLA	C11-C10-C8-C7
24	h	305	CLA	C11-C12-C13-C15
24	e	604	CLA	C6-C7-C8-C10
24	k	609	CLA	C6-C7-C8-C10
24	f	609	CLA	C11-C10-C8-C7
24	f	613	CLA	C12-C13-C15-C16
24	i	604	CLA	C6-C7-C8-C10
24	i	604	CLA	C11-C12-C13-C15
24	i	606	CLA	C11-C10-C8-C7
24	j	305	CLA	C11-C10-C8-C7
24	j	305	CLA	C12-C13-C15-C16
24	j	311	CLA	C11-C10-C8-C7
24	j	314	CLA	C6-C7-C8-C10
24	d	303	CLA	C12-C13-C15-C16
24	g	309	CLA	C6-C7-C8-C10
24	A	802	CLA	C3A-C2A-CAA-CBA
24	B	831	CLA	C3A-C2A-CAA-CBA
24	B	836	CLA	C3A-C2A-CAA-CBA
24	B	840	CLA	C3A-C2A-CAA-CBA
24	c	601	CLA	C3A-C2A-CAA-CBA
24	f	601	CLA	C3A-C2A-CAA-CBA
24	g	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	k	605	CLA	C4C-C3C-CAC-CBC
24	A	817	CLA	O1A-CGA-O2A-C1
24	B	820	CLA	O1D-CGD-O2D-CED
27	A	848	WVN	C32-C36-C39-C40
27	A	848	WVN	C34-C37-C40-C39
27	A	850	WVN	C32-C36-C39-C40
33	c	614	II0	C25-C29-C31-C33
33	a	314	II0	C25-C29-C31-C33
33	a	315	II0	C25-C29-C31-C33
33	b	315	II0	C25-C29-C31-C33
33	e	612	II0	C25-C29-C31-C33
33	e	616	II0	C35-C39-C41-C42
33	d	313	II0	C25-C29-C31-C33
33	g	316	II0	C36-C40-C42-C41
34	a	316	IHT	C35-C38-C41-C40
34	b	317	IHT	C33-C37-C40-C41
34	g	319	IHT	C26-C29-C31-C34
24	A	812	CLA	C16-C17-C18-C19
24	h	305	CLA	C16-C17-C18-C20
27	J	101	WVN	C11-C19-C22-C24
34	b	317	IHT	C18-C22-C23-C25
34	b	317	IHT	C30-C32-C33-C36
24	c	601	CLA	C4-C3-C5-C6
24	A	806	CLA	O1A-CGA-O2A-C1
24	h	312	CLA	O1A-CGA-O2A-C1
35	f	611	KC2	CBD-CGD-O2D-CED
27	L	206	WVN	C20-C23-C25-C28
27	R	201	WVN	C20-C23-C25-C28
26	f	619	LHG	C11-C12-C13-C14
26	b	320	LHG	C1-C2-C3-O3
26	f	619	LHG	C1-C2-C3-O3
24	a	312	CLA	O2A-C1-C2-C3
24	B	811	CLA	C2A-CAA-CBA-CGA
26	f	620	LHG	C31-C32-C33-C34
26	g	301	LHG	C4-C5-C6-O8
26	g	321	LHG	C4-C5-C6-O8
32	F	206	LMG	C7-C8-C9-O8
24	j	305	CLA	C3-C5-C6-C7
26	b	320	LHG	C9-C10-C11-C12
26	b	320	LHG	C7-C8-C9-C10
24	B	830	CLA	C16-C17-C18-C20
24	e	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	A	842	CLA	C13-C15-C16-C17
24	A	853	CLA	C8-C10-C11-C12
24	B	803	CLA	C5-C6-C7-C8
26	a	301	LHG	C27-C28-C29-C30
24	A	828	CLA	C4-C3-C5-C6
24	b	309	CLA	C4-C3-C5-C6
24	k	606	CLA	CAA-CBA-CGA-O2A
24	b	312	CLA	C15-C16-C17-C18
24	a	303	CLA	O1D-CGD-O2D-CED
24	A	827	CLA	O1D-CGD-O2D-CED
26	b	302	LHG	O9-C7-O7-C5
24	A	810	CLA	C2B-C3B-CAB-CBB
24	a	306	CLA	C2B-C3B-CAB-CBB
24	j	308	CLA	C2B-C3B-CAB-CBB
27	A	846	WVN	C15-C13-C20-C23
27	F	205	WVN	C06-C13-C20-C23
27	j	301	WVN	C06-C13-C20-C23
27	R	202	WVN	C06-C13-C20-C23
34	k	618	IHT	C02-C07-C18-C22
34	g	319	IHT	C10-C07-C18-C22
24	A	801	CLA	CAA-CBA-CGA-O2A
26	J	107	LHG	C29-C30-C31-C32
35	c	610	KC2	CBD-CGD-O2D-CED
33	d	313	II0	C26-C30-C32-C34
24	A	806	CLA	C16-C17-C18-C20
24	B	824	CLA	C16-C17-C18-C20
24	O	205	CLA	C16-C17-C18-C19
26	g	321	LHG	O7-C5-C6-O8
24	B	832	CLA	O1D-CGD-O2D-CED
24	B	838	CLA	C8-C10-C11-C12
24	I	102	CLA	O1A-CGA-O2A-C1
24	A	832	CLA	C4C-C3C-CAC-CBC
24	i	604	CLA	C2C-C3C-CAC-CBC
24	B	812	CLA	C4-C3-C5-C6
25	B	842	PQN	C12-C13-C15-C16
24	A	835	CLA	C16-C17-C18-C20
24	B	813	CLA	C11-C12-C13-C14
24	b	306	CLA	C16-C17-C18-C19
24	k	608	CLA	C16-C17-C18-C19
26	J	107	LHG	C7-C8-C9-C10
24	A	826	CLA	C3-C5-C6-C7
24	A	837	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	804	CLA	C6-C7-C8-C9
24	B	825	CLA	C6-C7-C8-C9
24	B	835	CLA	C11-C12-C13-C14
24	F	201	CLA	C14-C13-C15-C16
24	I	102	CLA	C11-C12-C13-C14
24	b	309	CLA	C11-C12-C13-C14
24	f	604	CLA	C14-C13-C15-C16
24	f	610	CLA	C11-C10-C8-C9
24	d	303	CLA	C11-C10-C8-C9
24	g	309	CLA	C6-C7-C8-C9
35	j	312	KC2	CAA-CBA-CGA-O2A
26	J	107	LHG	C12-C13-C14-C15
24	B	812	CLA	C16-C17-C18-C20
24	d	303	CLA	C16-C17-C18-C20
24	L	202	CLA	O2A-C1-C2-C3
32	J	106	LMG	C42-C43-C44-C45
26	b	320	LHG	C29-C30-C31-C32
24	a	312	CLA	O1A-CGA-O2A-C1
27	B	847	WVN	C25-C28-C30-C33
27	B	849	WVN	C34-C37-C40-C39
33	b	314	II0	C36-C40-C42-C41
33	f	615	II0	C25-C29-C31-C33
33	i	614	II0	C26-C30-C32-C34
33	j	316	II0	C35-C39-C41-C42
24	O	205	CLA	C16-C17-C18-C20
24	e	607	CLA	C5-C6-C7-C8
26	k	620	LHG	C26-C27-C28-C29
24	g	305	CLA	C4C-C3C-CAC-CBC
24	B	836	CLA	C4C-C3C-CAC-CBC
24	j	314	CLA	CBA-CGA-O2A-C1
24	b	307	CLA	C8-C10-C11-C12
28	a	318	LMT	C5-C6-C7-C8
24	B	839	CLA	C16-C17-C18-C19
24	g	322	CLA	C16-C17-C18-C20
25	B	842	PQN	C26-C27-C28-C29
26	J	107	LHG	C34-C35-C36-C37
27	F	204	WVN	C30-C33-C34-C38
27	K	103	WVN	C20-C23-C25-C27
27	e	615	WVN	C20-C23-C25-C27
27	R	201	WVN	C20-C23-C25-C27
33	a	317	II0	C32-C34-C36-C38
33	b	318	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
33	f	618	II0	C31-C33-C35-C37
24	A	816	CLA	C11-C10-C8-C7
24	A	817	CLA	C11-C12-C13-C15
24	A	829	CLA	C6-C7-C8-C10
24	A	831	CLA	C12-C13-C15-C16
24	A	839	CLA	C6-C7-C8-C10
24	A	839	CLA	C11-C10-C8-C7
24	A	839	CLA	C12-C13-C15-C16
24	A	841	CLA	C12-C13-C15-C16
24	A	853	CLA	C12-C13-C15-C16
24	B	803	CLA	C11-C12-C13-C15
24	B	804	CLA	C6-C7-C8-C10
24	B	808	CLA	C12-C13-C15-C16
24	B	812	CLA	C12-C13-C15-C16
24	B	813	CLA	C11-C10-C8-C7
24	B	817	CLA	C11-C10-C8-C7
24	B	825	CLA	C6-C7-C8-C10
24	B	830	CLA	C6-C7-C8-C10
24	B	836	CLA	C6-C7-C8-C10
24	B	837	CLA	C11-C12-C13-C15
24	c	608	CLA	C6-C7-C8-C10
24	a	307	CLA	C12-C13-C15-C16
24	b	305	CLA	C11-C12-C13-C15
24	e	605	CLA	C6-C7-C8-C10
24	f	604	CLA	C12-C13-C15-C16
24	f	613	CLA	C11-C12-C13-C15
24	i	606	CLA	C6-C7-C8-C10
24	g	308	CLA	C11-C10-C8-C7
24	g	308	CLA	C12-C13-C15-C16
25	B	842	PQN	C21-C22-C23-C25
24	B	806	CLA	C15-C16-C17-C18
27	A	846	WVN	C11-C19-C22-C26
27	A	848	WVN	C29-C31-C32-C36
27	e	615	WVN	C20-C23-C25-C28
27	R	201	WVN	C30-C33-C34-C37
33	a	317	II0	C32-C34-C36-C40
33	f	618	II0	C31-C33-C35-C39
34	g	319	IHT	C30-C32-C33-C37
24	f	608	CLA	CBA-CGA-O2A-C1
24	B	804	CLA	C2A-CAA-CBA-CGA
24	A	807	CLA	C16-C17-C18-C20
24	B	803	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	B	815	CLA	C6-C7-C8-C9
24	B	816	CLA	O1D-CGD-O2D-CED
24	B	808	CLA	C4-C3-C5-C6
35	j	312	KC2	C2C-C3C-CAC-CBC
35	d	311	KC2	C2C-C3C-CAC-CBC
35	g	314	KC2	C2C-C3C-CAC-CBC
24	I	102	CLA	O2A-C1-C2-C3
26	b	320	LHG	C28-C29-C30-C31
27	F	204	WVN	C34-C37-C40-C39
24	B	812	CLA	C16-C17-C18-C19
24	h	305	CLA	C16-C17-C18-C19
24	A	829	CLA	O1A-CGA-O2A-C1
24	B	821	CLA	O1A-CGA-O2A-C1
24	b	304	CLA	O1A-CGA-O2A-C1
32	F	206	LMG	C32-C33-C34-C35
24	A	821	CLA	O2A-C1-C2-C3
25	B	842	PQN	C15-C16-C17-C18
35	i	616	KC2	C4B-C3B-CAB-CBB
35	d	311	KC2	C4C-C3C-CAC-CBC
24	A	855	CLA	C16-C17-C18-C20
24	e	610	CLA	C16-C17-C18-C19
24	B	801	CLA	C3-C5-C6-C7
24	f	608	CLA	O1A-CGA-O2A-C1
24	B	808	CLA	C2-C3-C5-C6
24	B	812	CLA	C2-C3-C5-C6
24	f	602	CLA	C2-C3-C5-C6
26	b	320	LHG	C26-C27-C28-C29
26	J	107	LHG	O7-C5-C6-O8
24	A	808	CLA	C11-C12-C13-C14
24	A	817	CLA	C11-C12-C13-C14
24	A	825	CLA	C14-C13-C15-C16
24	A	842	CLA	C6-C7-C8-C9
24	B	817	CLA	C11-C10-C8-C9
24	B	818	CLA	C11-C12-C13-C14
24	c	612	CLA	C6-C7-C8-C9
24	b	305	CLA	C11-C12-C13-C14
24	k	604	CLA	C11-C12-C13-C14
24	b	311	CLA	O1A-CGA-O2A-C1
24	f	613	CLA	O1A-CGA-O2A-C1
27	B	845	WVN	C02-C11-C19-C22
24	k	605	CLA	C2C-C3C-CAC-CBC
32	b	301	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	i	601	CLA	CAA-CBA-CGA-O2A
24	F	202	CLA	C2-C1-O2A-CGA
27	A	846	WVN	C32-C36-C39-C40
33	h	309	II0	C36-C40-C42-C41
34	a	316	IHT	C33-C37-C40-C41
24	B	809	CLA	C16-C17-C18-C19
24	k	604	CLA	C16-C17-C18-C20
24	f	613	CLA	C16-C17-C18-C20
24	c	604	CLA	C5-C6-C7-C8
32	L	208	LMG	C17-C18-C19-C20
24	a	302	CLA	C4C-C3C-CAC-CBC
26	c	618	LHG	C23-C24-C25-C26
24	b	309	CLA	C2-C3-C5-C6
24	B	811	CLA	C6-C7-C8-C10
24	B	836	CLA	C16-C17-C18-C19
24	A	855	CLA	C3-C5-C6-C7
24	b	305	CLA	C3-C5-C6-C7
24	A	812	CLA	O1D-CGD-O2D-CED
26	J	107	LHG	C30-C31-C32-C33
24	A	807	CLA	C16-C17-C18-C19
24	B	836	CLA	C16-C17-C18-C20
25	B	842	PQN	C26-C27-C28-C30
33	J	104	II0	C09-C21-C23-C25
33	a	313	II0	C09-C21-C23-C25
33	e	613	II0	C10-C22-C24-C26
27	A	848	WVN	C29-C31-C32-C35
27	F	205	WVN	C30-C33-C34-C38
33	h	310	II0	C31-C33-C35-C37
24	A	817	CLA	C4B-C3B-CAB-CBB
24	B	828	CLA	C1A-C2A-CAA-CBA
24	B	834	CLA	C4B-C3B-CAB-CBB
24	B	835	CLA	C4B-C3B-CAB-CBB
24	F	202	CLA	C4B-C3B-CAB-CBB
24	b	309	CLA	C1A-C2A-CAA-CBA
24	b	313	CLA	C4B-C3B-CAB-CBB
24	e	608	CLA	C4B-C3B-CAB-CBB
24	k	607	CLA	C4B-C3B-CAB-CBB
24	f	601	CLA	C4B-C3B-CAB-CBB
24	f	607	CLA	C4B-C3B-CAB-CBB
24	f	613	CLA	C4B-C3B-CAB-CBB
24	i	608	CLA	C4B-C3B-CAB-CBB
24	d	307	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	d	307	CLA	C4B-C3B-CAB-CBB
24	B	836	CLA	CBA-CGA-O2A-C1
27	J	101	WVN	C11-C19-C22-C26
27	M	101	WVN	C11-C19-C22-C26
33	d	313	II0	C31-C33-C35-C39
34	b	317	IHT	C18-C22-C23-C27
34	j	317	IHT	C26-C29-C31-C34
26	f	620	LHG	C27-C28-C29-C30
24	e	605	CLA	C16-C17-C18-C19
24	A	823	CLA	CBD-CGD-O2D-CED
24	j	314	CLA	O1A-CGA-O2A-C1
24	R	203	CLA	C2-C3-C5-C6
24	A	808	CLA	C12-C13-C15-C16
24	A	816	CLA	C12-C13-C15-C16
24	A	832	CLA	C11-C12-C13-C15
24	B	816	CLA	C11-C10-C8-C7
24	B	822	CLA	C12-C13-C15-C16
24	B	839	CLA	C11-C12-C13-C15
24	O	205	CLA	C11-C12-C13-C15
24	a	310	CLA	C12-C13-C15-C16
24	b	306	CLA	C6-C7-C8-C10
24	b	306	CLA	C11-C12-C13-C15
24	e	605	CLA	C11-C10-C8-C7
24	k	608	CLA	C6-C7-C8-C10
24	f	608	CLA	C11-C12-C13-C15
24	f	610	CLA	C11-C12-C13-C15
24	f	613	CLA	C11-C10-C8-C7
24	I	102	CLA	C16-C17-C18-C20
24	f	602	CLA	C16-C17-C18-C19
26	J	107	LHG	O2-C2-C3-O3
26	a	301	LHG	C14-C15-C16-C17
24	f	613	CLA	CBA-CGA-O2A-C1
24	A	832	CLA	C2C-C3C-CAC-CBC
24	f	609	CLA	CBD-CGD-O2D-CED
32	L	208	LMG	C41-C42-C43-C44
24	A	805	CLA	C3A-C2A-CAA-CBA
24	A	806	CLA	C16-C17-C18-C19
24	B	811	CLA	C6-C7-C8-C9
24	a	308	CLA	C16-C17-C18-C20
24	d	303	CLA	C16-C17-C18-C19
32	F	206	LMG	C23-C24-C25-C26
24	A	816	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	L	203	CLA	C14-C13-C15-C16
24	c	608	CLA	C6-C7-C8-C9
24	b	305	CLA	C14-C13-C15-C16
24	b	306	CLA	C11-C12-C13-C14
24	b	312	CLA	C6-C7-C8-C9
24	i	606	CLA	C6-C7-C8-C9
24	g	308	CLA	C11-C10-C8-C9
24	e	604	CLA	C5-C6-C7-C8
27	j	301	WVN	C32-C36-C39-C40
33	h	311	II0	C35-C39-C41-C42
33	e	613	II0	C36-C40-C42-C41
33	f	618	II0	C36-C40-C42-C41
33	d	314	II0	C36-C40-C42-C41
34	R	204	IHT	C23-C27-C30-C32
24	g	307	CLA	O1D-CGD-O2D-CED
24	A	821	CLA	C1-C2-C3-C4
24	B	828	CLA	C1-C2-C3-C4
27	e	615	WVN	C01-C02-C11-C19
35	k	612	KC2	C1A-C2A-CAA-CBA
35	k	613	KC2	C1A-C2A-CAA-CBA
35	f	611	KC2	C3A-C2A-CAA-CBA
35	i	609	KC2	C3A-C2A-CAA-CBA
35	i	616	KC2	C1A-C2A-CAA-CBA
35	g	312	KC2	C3A-C2A-CAA-CBA
26	g	301	LHG	O7-C5-C6-O8
26	J	107	LHG	C1-C2-C3-O3
24	e	605	CLA	C16-C17-C18-C20
24	B	825	CLA	C4-C3-C5-C6
24	B	816	CLA	CAA-CBA-CGA-O2A
24	k	604	CLA	CBD-CGD-O2D-CED
24	A	813	CLA	CAD-CBD-CGD-O2D
24	A	814	CLA	CAD-CBD-CGD-O2D
24	A	855	CLA	CAD-CBD-CGD-O2D
24	B	833	CLA	CAD-CBD-CGD-O2D
24	c	611	CLA	CAD-CBD-CGD-O2D
24	i	604	CLA	CAD-CBD-CGD-O2D
24	j	305	CLA	CAD-CBD-CGD-O2D
24	d	303	CLA	CAD-CBD-CGD-O2D
24	d	304	CLA	CAD-CBD-CGD-O2D
24	d	306	CLA	CAD-CBD-CGD-O2D
35	i	616	KC2	CAD-CBD-CGD-O2D
24	f	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	g	311	CLA	CBD-CGD-O2D-CED
24	B	820	CLA	C6-C7-C8-C9
24	b	305	CLA	C16-C17-C18-C20
24	A	807	CLA	C2A-CAA-CBA-CGA
25	B	842	PQN	C25-C26-C27-C28
24	A	804	CLA	CAD-CBD-CGD-O1D
24	A	813	CLA	CAD-CBD-CGD-O1D
24	A	814	CLA	CAD-CBD-CGD-O1D
24	A	821	CLA	CHA-CBD-CGD-O1D
24	A	821	CLA	CHA-CBD-CGD-O2D
24	A	842	CLA	CHA-CBD-CGD-O1D
24	A	842	CLA	CHA-CBD-CGD-O2D
24	A	855	CLA	CAD-CBD-CGD-O1D
24	B	812	CLA	CAD-CBD-CGD-O1D
24	B	827	CLA	CAD-CBD-CGD-O1D
24	B	833	CLA	CAD-CBD-CGD-O1D
24	c	601	CLA	CHA-CBD-CGD-O1D
24	c	601	CLA	CHA-CBD-CGD-O2D
24	c	611	CLA	CAD-CBD-CGD-O1D
24	a	303	CLA	CHA-CBD-CGD-O1D
24	a	303	CLA	CHA-CBD-CGD-O2D
24	a	307	CLA	CHA-CBD-CGD-O1D
24	b	303	CLA	CHA-CBD-CGD-O1D
24	b	306	CLA	CAD-CBD-CGD-O1D
24	h	303	CLA	CHA-CBD-CGD-O1D
24	h	303	CLA	CHA-CBD-CGD-O2D
24	e	601	CLA	CHA-CBD-CGD-O1D
24	e	602	CLA	CHA-CBD-CGD-O1D
24	f	603	CLA	CHA-CBD-CGD-O1D
24	f	603	CLA	CHA-CBD-CGD-O2D
24	f	606	CLA	CHA-CBD-CGD-O1D
24	f	606	CLA	CHA-CBD-CGD-O2D
24	i	604	CLA	CAD-CBD-CGD-O1D
24	j	305	CLA	CAD-CBD-CGD-O1D
24	d	302	CLA	CHA-CBD-CGD-O1D
24	d	302	CLA	CHA-CBD-CGD-O2D
24	d	303	CLA	CAD-CBD-CGD-O1D
24	d	304	CLA	CAD-CBD-CGD-O1D
24	d	306	CLA	CAD-CBD-CGD-O1D
24	d	312	CLA	CHA-CBD-CGD-O1D
24	d	312	CLA	CHA-CBD-CGD-O2D
24	g	308	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	g	308	CLA	CHA-CBD-CGD-O2D
26	A	844	LHG	C4-O6-P-O5
26	B	802	LHG	C3-O3-P-O4
26	c	617	LHG	C3-O3-P-O5
26	c	618	LHG	C3-O3-P-O5
26	c	618	LHG	C4-O6-P-O5
26	a	301	LHG	C3-O3-P-O5
26	b	320	LHG	C4-O6-P-O5
26	e	617	LHG	C3-O3-P-O5
26	e	617	LHG	C3-O3-P-O6
26	k	620	LHG	C3-O3-P-O4
26	f	619	LHG	C4-O6-P-O3
26	f	619	LHG	C4-O6-P-O5
26	i	615	LHG	C4-O6-P-O5
26	j	319	LHG	C4-O6-P-O5
26	d	316	LHG	C4-O6-P-O5
26	g	301	LHG	C3-O3-P-O5
26	g	301	LHG	C4-O6-P-O5
26	g	321	LHG	C3-O3-P-O5
27	A	849	WVN	C25-C28-C30-C33
27	A	850	WVN	C25-C28-C30-C33
27	R	202	WVN	C25-C28-C30-C33
33	b	314	II0	C35-C39-C41-C42
33	e	616	II0	C25-C29-C31-C33
33	k	615	II0	C35-C39-C41-C42
33	j	315	II0	C36-C40-C42-C41
34	g	319	IHT	C33-C37-C40-C41
35	d	310	KC2	CHA-CBD-CGD-O1D
35	g	314	KC2	CAD-CBD-CGD-O1D
24	g	309	CLA	C3-C5-C6-C7
26	A	844	LHG	C10-C11-C12-C13
32	J	106	LMG	C37-C38-C39-C40
24	A	817	CLA	C2B-C3B-CAB-CBB
24	A	853	CLA	C2B-C3B-CAB-CBB
24	B	827	CLA	C2B-C3B-CAB-CBB
24	B	829	CLA	C2B-C3B-CAB-CBB
24	I	102	CLA	C2B-C3B-CAB-CBB
24	K	102	CLA	C2B-C3B-CAB-CBB
24	c	602	CLA	C2B-C3B-CAB-CBB
24	e	601	CLA	C2B-C3B-CAB-CBB
24	k	606	CLA	C2B-C3B-CAB-CBB
24	f	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	f	606	CLA	C2B-C3B-CAB-CBB
24	f	613	CLA	C2B-C3B-CAB-CBB
24	i	611	CLA	C2B-C3B-CAB-CBB
24	d	305	CLA	C2B-C3B-CAB-CBB
24	g	307	CLA	C2B-C3B-CAB-CBB
24	B	834	CLA	CBD-CGD-O2D-CED
24	B	841	CLA	CAA-CBA-CGA-O2A
24	I	102	CLA	CAA-CBA-CGA-O2A
24	c	608	CLA	C13-C15-C16-C17
26	B	802	LHG	C5-C4-O6-P
27	L	201	WVN	C29-C31-C32-C35
33	e	613	II0	C31-C33-C35-C37
33	k	615	II0	C32-C34-C36-C38
24	d	304	CLA	C4C-C3C-CAC-CBC
24	e	610	CLA	C3-C5-C6-C7
32	b	301	LMG	C15-C16-C17-C18
24	b	312	CLA	C16-C17-C18-C19
26	f	619	LHG	C23-C24-C25-C26
24	A	839	CLA	C5-C6-C7-C8
24	j	311	CLA	C12-C13-C15-C16
26	e	617	LHG	C6-C5-O7-C7
27	B	847	WVN	C26-C29-C31-C32
27	L	206	WVN	C28-C30-C33-C34
33	b	315	II0	C29-C31-C33-C35
24	f	610	CLA	C10-C11-C12-C13
24	L	203	CLA	C16-C17-C18-C19
24	A	818	CLA	C11-C12-C13-C14
24	A	826	CLA	C11-C12-C13-C14
24	A	836	CLA	C6-C7-C8-C9
24	B	805	CLA	C11-C12-C13-C14
24	B	816	CLA	C11-C10-C8-C9
24	B	836	CLA	C14-C13-C15-C16
24	B	837	CLA	C11-C10-C8-C9
24	I	102	CLA	C11-C10-C8-C9
24	O	205	CLA	C11-C12-C13-C14
24	b	307	CLA	C11-C10-C8-C9
24	b	308	CLA	C6-C7-C8-C9
24	b	312	CLA	C11-C10-C8-C9
24	e	610	CLA	C11-C10-C8-C9
24	e	610	CLA	C11-C12-C13-C14
24	e	611	CLA	C6-C7-C8-C9
24	e	611	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	f	608	CLA	C11-C12-C13-C14
24	A	823	CLA	O1D-CGD-O2D-CED
24	A	824	CLA	C12-C13-C15-C16
24	A	840	CLA	C12-C13-C15-C16
24	B	818	CLA	C6-C7-C8-C10
24	B	835	CLA	C6-C7-C8-C10
24	e	610	CLA	C11-C10-C8-C7
24	f	602	CLA	C12-C13-C15-C16
25	B	842	PQN	C17-C18-C20-C21
32	J	106	LMG	C31-C32-C33-C34
24	B	814	CLA	O1A-CGA-O2A-C1
26	b	302	LHG	C14-C15-C16-C17
26	b	320	LHG	C11-C10-C9-C8
24	L	203	CLA	C16-C17-C18-C20
24	k	604	CLA	C16-C17-C18-C19
26	f	620	LHG	C12-C13-C14-C15
26	c	617	LHG	O7-C5-C6-O8
32	O	204	LMG	O7-C8-C9-O8
24	h	306	CLA	CAA-CBA-CGA-O2A
27	L	201	WVN	C22-C26-C29-C31
24	f	610	CLA	C8-C10-C11-C12
26	J	107	LHG	C25-C26-C27-C28
26	J	107	LHG	C24-C23-O8-C6
24	A	842	CLA	C4-C3-C5-C6
24	A	817	CLA	CAA-CBA-CGA-O2A
24	g	311	CLA	C3-C5-C6-C7
24	A	804	CLA	CAA-CBA-CGA-O2A
24	g	306	CLA	CAA-CBA-CGA-O2A
27	M	101	WVN	C11-C19-C22-C24
32	b	301	LMG	C12-C13-C14-C15
24	A	817	CLA	C16-C17-C18-C19
27	R	202	WVN	C30-C33-C34-C37
24	B	810	CLA	CBA-CGA-O2A-C1
30	B	843	DGD	C5D-C6D-O5D-C1E
24	A	855	CLA	C2A-CAA-CBA-CGA
24	b	306	CLA	C2A-CAA-CBA-CGA
24	f	604	CLA	C2A-CAA-CBA-CGA
24	j	305	CLA	C2A-CAA-CBA-CGA
24	g	305	CLA	C2A-CAA-CBA-CGA
27	B	847	WVN	C34-C37-C40-C39
27	F	205	WVN	C25-C28-C30-C33
27	F	205	WVN	C34-C37-C40-C39

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Mol	Chain	Res	Type	Atoms
27	j	301	WVN	C34-C37-C40-C39
33	h	311	II0	C36-C40-C42-C41
33	d	315	II0	C26-C30-C32-C34
33	g	316	II0	C35-C39-C41-C42
32	b	301	LMG	C24-C25-C26-C27
24	B	803	CLA	C16-C17-C18-C19
24	B	815	CLA	C6-C7-C8-C10
24	g	322	CLA	C16-C17-C18-C19
24	A	802	CLA	C4-C3-C5-C6
33	h	310	II0	C09-C21-C23-C25
24	A	801	CLA	C16-C17-C18-C20
24	f	613	CLA	C16-C17-C18-C19
35	e	609	KC2	CAA-CBA-CGA-O1A
24	A	812	CLA	C14-C13-C15-C16
24	A	816	CLA	C14-C13-C15-C16
24	B	835	CLA	C6-C7-C8-C9
24	b	306	CLA	C6-C7-C8-C9
24	k	609	CLA	C14-C13-C15-C16
24	f	613	CLA	C11-C10-C8-C9
24	d	303	CLA	C14-C13-C15-C16
24	A	820	CLA	O1D-CGD-O2D-CED
24	B	816	CLA	C4B-C3B-CAB-CBB
24	b	306	CLA	C4B-C3B-CAB-CBB
24	f	605	CLA	C4B-C3B-CAB-CBB
26	b	302	LHG	C31-C32-C33-C34
24	a	310	CLA	C16-C17-C18-C19
24	K	101	CLA	CBA-CGA-O2A-C1
24	k	606	CLA	CBA-CGA-O2A-C1
24	d	303	CLA	CBA-CGA-O2A-C1
24	g	303	CLA	CBA-CGA-O2A-C1
30	B	843	DGD	C2A-C1A-O1G-C1G
32	L	208	LMG	C29-C28-O8-C9
24	A	824	CLA	C8-C10-C11-C12
24	b	307	CLA	C5-C6-C7-C8
30	B	843	DGD	C8B-C9B-CAB-CBB
24	A	842	CLA	C2-C3-C5-C6
24	B	825	CLA	C2-C3-C5-C6
24	k	602	CLA	C4C-C3C-CAC-CBC
28	A	851	LMT	C6-C7-C8-C9
24	k	603	CLA	O1A-CGA-O2A-C1
27	A	850	WVN	C22-C26-C29-C31
33	e	613	II0	C26-C30-C32-C34

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Mol	Chain	Res	Type	Atoms
35	k	611	KC2	C2A-CAA-CBA-CGA
24	A	807	CLA	C12-C13-C15-C16
24	B	803	CLA	C11-C10-C8-C7
24	B	804	CLA	C11-C10-C8-C7
24	B	808	CLA	C6-C7-C8-C10
24	e	606	CLA	C6-C7-C8-C10
24	f	608	CLA	C6-C7-C8-C10
24	j	314	CLA	C11-C12-C13-C15
26	B	802	LHG	C24-C25-C26-C27
24	A	816	CLA	C8-C10-C11-C12
24	k	603	CLA	CBA-CGA-O2A-C1
24	A	801	CLA	C16-C17-C18-C19
24	A	841	CLA	C16-C17-C18-C19
24	f	602	CLA	C16-C17-C18-C20
24	A	824	CLA	C13-C15-C16-C17
24	B	836	CLA	O1A-CGA-O2A-C1
24	K	101	CLA	O1A-CGA-O2A-C1
24	k	606	CLA	O1A-CGA-O2A-C1
24	d	303	CLA	O1A-CGA-O2A-C1
32	J	106	LMG	O1-C7-C8-O7
24	A	809	CLA	C3A-C2A-CAA-CBA
24	A	819	CLA	C3A-C2A-CAA-CBA
24	A	830	CLA	C3A-C2A-CAA-CBA
24	B	809	CLA	C3A-C2A-CAA-CBA
24	B	815	CLA	C3A-C2A-CAA-CBA
24	i	611	CLA	C3A-C2A-CAA-CBA
24	g	304	CLA	C3A-C2A-CAA-CBA
24	f	601	CLA	C4C-C3C-CAC-CBC
24	a	307	CLA	C8-C10-C11-C12
27	A	847	WVN	C24-C22-C26-C29
33	b	315	II0	C37-C35-C39-C41
34	b	317	IHT	C25-C23-C27-C30
28	b	319	LMT	O1'-C1-C2-C3
24	B	825	CLA	C15-C16-C17-C18
24	B	805	CLA	C2-C1-O2A-CGA
24	i	605	CLA	C2-C1-O2A-CGA
33	k	615	II0	C26-C30-C32-C34
24	R	203	CLA	O1D-CGD-O2D-CED
24	B	801	CLA	C13-C15-C16-C17
24	B	806	CLA	C10-C11-C12-C13
27	B	847	WVN	C29-C31-C32-C35
32	J	106	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	A	820	CLA	C2C-C3C-CAC-CBC
24	a	307	CLA	CAA-CBA-CGA-O2A
24	A	855	CLA	C16-C17-C18-C19
24	B	808	CLA	C16-C17-C18-C20
24	g	305	CLA	C15-C16-C17-C18
24	B	814	CLA	CBA-CGA-O2A-C1
24	B	803	CLA	C15-C16-C17-C18
28	A	851	LMT	C2-C3-C4-C5
24	B	840	CLA	C3-C5-C6-C7
24	k	604	CLA	O1D-CGD-O2D-CED
24	A	806	CLA	C11-C12-C13-C14
24	A	810	CLA	C11-C10-C8-C9
24	A	812	CLA	C6-C7-C8-C9
24	A	820	CLA	C11-C10-C8-C9
24	A	831	CLA	C11-C12-C13-C14
24	A	842	CLA	C14-C13-C15-C16
24	B	804	CLA	C11-C12-C13-C14
24	B	806	CLA	C11-C12-C13-C14
24	B	808	CLA	C11-C12-C13-C14
24	B	809	CLA	C11-C12-C13-C14
24	a	305	CLA	C14-C13-C15-C16
24	a	307	CLA	C11-C12-C13-C14
24	b	312	CLA	C14-C13-C15-C16
24	h	312	CLA	C11-C10-C8-C9
24	e	607	CLA	C6-C7-C8-C9
24	k	609	CLA	C11-C12-C13-C14
24	f	607	CLA	C6-C7-C8-C9
24	g	309	CLA	C11-C10-C8-C9
24	g	322	CLA	C11-C12-C13-C14
24	B	839	CLA	C16-C17-C18-C20
24	B	807	CLA	C3-C5-C6-C7
33	k	615	II0	C36-C40-C42-C41
28	a	318	LMT	C7-C8-C9-C10
24	F	201	CLA	C4-C3-C5-C6
24	A	822	CLA	CBD-CGD-O2D-CED
24	f	613	CLA	CAA-CBA-CGA-O2A
32	F	206	LMG	C14-C15-C16-C17
26	a	301	LHG	O10-C23-O8-C6
24	k	607	CLA	C2A-CAA-CBA-CGA
24	B	822	CLA	O1A-CGA-O2A-C1
24	A	815	CLA	C1A-C2A-CAA-CBA
24	A	830	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	820	CLA	C1A-C2A-CAA-CBA
24	B	836	CLA	C1A-C2A-CAA-CBA
24	I	102	CLA	C1A-C2A-CAA-CBA
24	f	612	CLA	C1A-C2A-CAA-CBA
24	j	310	CLA	C1A-C2A-CAA-CBA
24	g	304	CLA	C1A-C2A-CAA-CBA
27	A	847	WVN	C19-C22-C26-C29
33	b	315	II0	C33-C35-C39-C41
34	b	317	IHT	C22-C23-C27-C30
24	A	841	CLA	C16-C17-C18-C20
24	B	809	CLA	C16-C17-C18-C20
24	A	832	CLA	C2B-C3B-CAB-CBB
24	A	833	CLA	C2B-C3B-CAB-CBB
24	B	803	CLA	C2B-C3B-CAB-CBB
24	B	816	CLA	C2B-C3B-CAB-CBB
24	B	834	CLA	C2B-C3B-CAB-CBB
24	B	835	CLA	C2B-C3B-CAB-CBB
24	F	202	CLA	C2B-C3B-CAB-CBB
24	J	105	CLA	C2B-C3B-CAB-CBB
24	c	611	CLA	C2B-C3B-CAB-CBB
24	a	304	CLA	C2B-C3B-CAB-CBB
24	b	306	CLA	C2B-C3B-CAB-CBB
24	b	313	CLA	C2B-C3B-CAB-CBB
24	h	302	CLA	C2B-C3B-CAB-CBB
24	e	608	CLA	C2B-C3B-CAB-CBB
24	k	607	CLA	C2B-C3B-CAB-CBB
24	f	601	CLA	C2B-C3B-CAB-CBB
24	f	607	CLA	C2B-C3B-CAB-CBB
24	i	605	CLA	C2B-C3B-CAB-CBB
24	i	608	CLA	C2B-C3B-CAB-CBB
24	d	307	CLA	C2B-C3B-CAB-CBB
24	d	309	CLA	C2B-C3B-CAB-CBB
27	B	845	WVN	C15-C13-C20-C23
34	a	316	IHT	C10-C07-C18-C22
34	b	316	IHT	C10-C07-C18-C22
34	k	618	IHT	C10-C07-C18-C22
24	e	601	CLA	CAA-CBA-CGA-O2A
24	A	807	CLA	O1D-CGD-O2D-CED
24	k	608	CLA	C8-C10-C11-C12
24	O	201	CLA	C4-C3-C5-C6
32	L	208	LMG	C39-C40-C41-C42
24	e	601	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	A	818	CLA	C11-C12-C13-C15
24	A	824	CLA	C11-C12-C13-C15
24	A	825	CLA	C6-C7-C8-C10
24	A	826	CLA	C6-C7-C8-C10
24	A	827	CLA	C12-C13-C15-C16
24	B	807	CLA	C6-C7-C8-C10
24	B	814	CLA	C11-C10-C8-C7
24	F	201	CLA	C11-C10-C8-C7
24	L	203	CLA	C11-C12-C13-C15
24	a	307	CLA	C11-C10-C8-C7
24	b	307	CLA	C11-C12-C13-C15
24	b	312	CLA	C12-C13-C15-C16
24	e	611	CLA	C6-C7-C8-C10
24	k	604	CLA	C12-C13-C15-C16
24	k	608	CLA	C12-C13-C15-C16
24	i	606	CLA	C11-C12-C13-C15
24	j	314	CLA	C12-C13-C15-C16
25	B	842	PQN	C22-C23-C25-C26
24	B	808	CLA	C16-C17-C18-C19
24	b	312	CLA	C16-C17-C18-C20
24	A	835	CLA	C2A-CAA-CBA-CGA
24	a	302	CLA	C2A-CAA-CBA-CGA
24	j	314	CLA	C2A-CAA-CBA-CGA
26	k	620	LHG	O7-C5-C6-O8
24	A	825	CLA	CBA-CGA-O2A-C1
28	F	203	LMT	C4-C5-C6-C7
32	b	301	LMG	C39-C40-C41-C42
24	b	308	CLA	C12-C13-C15-C16
24	i	606	CLA	C12-C13-C15-C16
24	B	834	CLA	O1D-CGD-O2D-CED
33	g	320	II0	C31-C33-C35-C39
24	f	608	CLA	C16-C17-C18-C20
24	B	837	CLA	C15-C16-C17-C18
32	O	204	LMG	C28-C29-C30-C31
24	g	303	CLA	O1A-CGA-O2A-C1
24	c	604	CLA	C2A-CAA-CBA-CGA
24	c	611	CLA	CAA-CBA-CGA-O2A
24	B	809	CLA	C14-C13-C15-C16
24	f	608	CLA	C11-C10-C8-C9
26	J	107	LHG	C33-C34-C35-C36
32	O	204	LMG	O6-C1-O1-C7
30	B	843	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
24	A	827	CLA	C4-C3-C5-C6
24	a	308	CLA	C8-C10-C11-C12
24	c	611	CLA	CAA-CBA-CGA-O1A
26	a	301	LHG	C5-C4-O6-P
26	d	316	LHG	C2-C3-O3-P
26	g	301	LHG	C2-C3-O3-P
24	B	826	CLA	C2-C3-C5-C6
24	A	820	CLA	CBD-CGD-O2D-CED
32	b	301	LMG	C31-C32-C33-C34
24	c	608	CLA	C10-C11-C12-C13
24	B	810	CLA	O1A-CGA-O2A-C1
24	k	605	CLA	CAA-CBA-CGA-O2A
26	J	107	LHG	O10-C23-O8-C6
24	B	822	CLA	CBA-CGA-O2A-C1
24	B	807	CLA	C2A-CAA-CBA-CGA
24	e	601	CLA	C2A-CAA-CBA-CGA
24	g	322	CLA	C2A-CAA-CBA-CGA
24	B	825	CLA	C16-C17-C18-C20
32	b	301	LMG	C38-C39-C40-C41
28	F	203	LMT	C1-C2-C3-C4
24	a	306	CLA	CAA-CBA-CGA-O2A
24	A	841	CLA	C15-C16-C17-C18
26	a	301	LHG	O1-C1-C2-O2
33	a	315	II0	C10-C22-C24-C26
33	b	318	II0	C09-C21-C23-C25
33	e	616	II0	C10-C22-C24-C26
33	g	316	II0	C09-C21-C23-C25
33	g	317	II0	C09-C21-C23-C25
33	g	317	II0	C10-C22-C24-C26
24	f	607	CLA	C4-C3-C5-C6
24	A	801	CLA	CAA-CBA-CGA-O1A
24	R	203	CLA	CAA-CBA-CGA-O1A
24	A	842	CLA	C16-C17-C18-C20
24	A	833	CLA	C4B-C3B-CAB-CBB
24	B	820	CLA	C4B-C3B-CAB-CBB
24	f	603	CLA	C4B-C3B-CAB-CBB
24	g	303	CLA	C4B-C3B-CAB-CBB
32	L	208	LMG	O10-C28-O8-C9
32	L	208	LMG	C37-C38-C39-C40
24	A	819	CLA	CAA-CBA-CGA-O2A
24	e	606	CLA	C16-C17-C18-C20
26	c	617	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	B	838	CLA	CAA-CBA-CGA-O1A
24	A	827	CLA	C2-C3-C5-C6
26	b	302	LHG	C18-C19-C20-C21
26	k	620	LHG	C28-C29-C30-C31
26	J	107	LHG	C2-C3-O3-P
24	B	809	CLA	C11-C12-C13-C15
24	B	823	CLA	C11-C12-C13-C15
24	g	305	CLA	C11-C12-C13-C15
33	a	315	II0	C36-C40-C42-C41
33	j	316	II0	C36-C40-C42-C41
24	A	805	CLA	C11-C10-C8-C9
24	A	841	CLA	C6-C7-C8-C9
24	A	853	CLA	C11-C12-C13-C14
24	B	803	CLA	C11-C10-C8-C9
24	B	805	CLA	C6-C7-C8-C9
24	B	808	CLA	C11-C10-C8-C9
24	F	201	CLA	C6-C7-C8-C9
24	a	310	CLA	C14-C13-C15-C16
24	b	305	CLA	C6-C7-C8-C9
24	b	313	CLA	C6-C7-C8-C9
24	j	311	CLA	C11-C12-C13-C14
24	g	307	CLA	CAA-CBA-CGA-O1A
24	e	602	CLA	C2A-CAA-CBA-CGA
24	A	832	CLA	C2-C1-O2A-CGA
24	A	833	CLA	C2-C1-O2A-CGA
24	f	610	CLA	C2-C1-O2A-CGA
24	B	825	CLA	C16-C17-C18-C19
24	A	812	CLA	C3A-C2A-CAA-CBA
24	A	815	CLA	C3A-C2A-CAA-CBA
24	A	818	CLA	C4-C3-C5-C6
24	b	313	CLA	C3A-C2A-CAA-CBA
32	b	301	LMG	O6-C5-C6-O5
24	j	310	CLA	O1A-CGA-O2A-C1
26	b	302	LHG	C10-C11-C12-C13
26	a	301	LHG	O1-C1-C2-C3
24	f	601	CLA	C2-C1-O2A-CGA
24	c	609	CLA	CAA-CBA-CGA-O2A
24	b	309	CLA	O1D-CGD-O2D-CED
24	B	818	CLA	CBA-CGA-O2A-C1
24	d	304	CLA	CBA-CGA-O2A-C1
26	a	301	LHG	C24-C23-O8-C6
24	k	605	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	f	605	CLA	CAA-CBA-CGA-O1A
24	j	309	CLA	CAA-CBA-CGA-O2A
26	c	618	LHG	C29-C30-C31-C32
24	B	823	CLA	C10-C11-C12-C13
24	c	604	CLA	CBD-CGD-O2D-CED
24	A	842	CLA	C16-C17-C18-C19
24	a	306	CLA	CAA-CBA-CGA-O1A
25	B	842	PQN	C13-C15-C16-C17
24	A	818	CLA	C2-C3-C5-C6
32	b	301	LMG	C13-C14-C15-C16
24	k	606	CLA	CAA-CBA-CGA-O1A
24	A	819	CLA	CAA-CBA-CGA-O1A
24	A	812	CLA	C3-C5-C6-C7
24	k	609	CLA	C15-C16-C17-C18
24	g	309	CLA	CBA-CGA-O2A-C1
24	j	306	CLA	CAA-CBA-CGA-O2A
26	c	617	LHG	C4-C5-C6-O8
26	k	620	LHG	C4-C5-C6-O8
32	J	106	LMG	C34-C35-C36-C37
24	B	833	CLA	C5-C6-C7-C8
35	j	312	KC2	C4C-C3C-CAC-CBC
35	g	314	KC2	C4C-C3C-CAC-CBC
26	e	617	LHG	C28-C29-C30-C31
24	A	822	CLA	O1D-CGD-O2D-CED
24	j	309	CLA	CAA-CBA-CGA-O1A
27	B	845	WVN	C34-C37-C40-C39
27	K	103	WVN	C22-C26-C29-C31
27	e	615	WVN	C32-C36-C39-C40
24	c	609	CLA	CAA-CBA-CGA-O1A
24	j	306	CLA	CAA-CBA-CGA-O1A
24	A	828	CLA	CAA-CBA-CGA-O2A
26	a	301	LHG	O7-C5-C6-O8
24	A	832	CLA	C11-C12-C13-C14
24	f	602	CLA	C11-C10-C8-C9
24	a	310	CLA	C16-C17-C18-C20
24	f	607	CLA	C16-C17-C18-C20
24	B	803	CLA	CAA-CBA-CGA-O2A
24	g	308	CLA	CAA-CBA-CGA-O2A
32	L	208	LMG	C23-C24-C25-C26
24	B	826	CLA	C4-C3-C5-C6
24	A	802	CLA	C2-C3-C5-C6
24	e	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	A	809	CLA	C6-C7-C8-C10
24	A	841	CLA	C11-C12-C13-C15
24	A	852	CLA	C11-C10-C8-C7
24	B	801	CLA	C11-C10-C8-C7
24	B	808	CLA	C11-C10-C8-C7
24	B	816	CLA	C6-C7-C8-C10
24	B	824	CLA	C11-C10-C8-C7
24	B	839	CLA	C6-C7-C8-C10
24	O	205	CLA	C12-C13-C15-C16
24	a	305	CLA	C11-C12-C13-C15
24	b	313	CLA	C11-C12-C13-C15
24	h	312	CLA	C11-C10-C8-C7
24	e	606	CLA	C12-C13-C15-C16
24	k	609	CLA	C11-C12-C13-C15
24	g	305	CLA	C12-C13-C15-C16
24	g	308	CLA	C6-C7-C8-C10
24	A	841	CLA	C8-C10-C11-C12
24	j	305	CLA	C5-C6-C7-C8
24	j	314	CLA	C3-C5-C6-C7
24	g	308	CLA	C3-C5-C6-C7
24	B	805	CLA	CAA-CBA-CGA-O1A
24	A	801	CLA	C2B-C3B-CAB-CBB
24	A	842	CLA	C2B-C3B-CAB-CBB
24	B	820	CLA	C2B-C3B-CAB-CBB
24	L	203	CLA	C2B-C3B-CAB-CBB
24	c	607	CLA	C2B-C3B-CAB-CBB
24	h	307	CLA	C2B-C3B-CAB-CBB
24	h	312	CLA	C2B-C3B-CAB-CBB
24	e	604	CLA	C2B-C3B-CAB-CBB
24	f	605	CLA	C2B-C3B-CAB-CBB
24	g	322	CLA	C2B-C3B-CAB-CBB
27	J	102	WVN	C06-C13-C20-C23
34	O	203	IHT	C10-C07-C18-C22
34	j	317	IHT	C10-C07-C18-C22
24	A	802	CLA	C2-C1-O2A-CGA
24	A	805	CLA	C2-C1-O2A-CGA
24	B	836	CLA	C2-C1-O2A-CGA
24	c	602	CLA	C2-C1-O2A-CGA
24	c	612	CLA	C2-C1-O2A-CGA
24	b	303	CLA	C2-C1-O2A-CGA
24	b	311	CLA	C2-C1-O2A-CGA
24	k	601	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	B	840	CLA	O1A-CGA-O2A-C1
24	f	613	CLA	C13-C15-C16-C17
24	h	302	CLA	CAA-CBA-CGA-O2A
24	e	603	CLA	CAA-CBA-CGA-O2A
26	d	316	LHG	O7-C7-C8-C9
24	A	842	CLA	CBD-CGD-O2D-CED
24	g	305	CLA	C8-C10-C11-C12
32	F	206	LMG	C24-C25-C26-C27
26	J	107	LHG	C16-C17-C18-C19
24	f	601	CLA	C2C-C3C-CAC-CBC
24	j	310	CLA	CBA-CGA-O2A-C1
24	a	308	CLA	C16-C17-C18-C19
24	e	606	CLA	C16-C17-C18-C19
24	L	204	CLA	O1A-CGA-O2A-C1
24	R	203	CLA	O1A-CGA-O2A-C1
24	A	812	CLA	CAA-CBA-CGA-O2A
24	B	806	CLA	CAA-CBA-CGA-O2A
26	A	845	LHG	O7-C7-C8-C9
24	k	609	CLA	C4-C3-C5-C6
26	a	301	LHG	C25-C26-C27-C28
24	A	836	CLA	CAA-CBA-CGA-O2A
24	B	840	CLA	CAA-CBA-CGA-O2A
24	c	605	CLA	CAA-CBA-CGA-O2A
24	a	311	CLA	CAA-CBA-CGA-O2A
24	A	812	CLA	C8-C10-C11-C12
24	g	308	CLA	C8-C10-C11-C12
24	L	202	CLA	CAA-CBA-CGA-O2A
24	h	307	CLA	CAA-CBA-CGA-O2A
33	j	316	II0	C10-C22-C24-C26
24	h	312	CLA	C6-C7-C8-C9
24	A	842	CLA	O1D-CGD-O2D-CED
24	e	605	CLA	C15-C16-C17-C18
24	B	836	CLA	CAA-CBA-CGA-O2A
24	A	812	CLA	C1A-C2A-CAA-CBA
24	A	819	CLA	C4B-C3B-CAB-CBB
24	A	822	CLA	C1A-C2A-CAA-CBA
24	A	835	CLA	C4B-C3B-CAB-CBB
24	B	809	CLA	C1A-C2A-CAA-CBA
24	c	611	CLA	C4B-C3B-CAB-CBB
24	b	313	CLA	C1A-C2A-CAA-CBA
24	f	606	CLA	C1A-C2A-CAA-CBA
26	k	620	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	a	302	CLA	CAA-CBA-CGA-O2A
24	a	310	CLA	CAA-CBA-CGA-O2A
26	j	319	LHG	O8-C23-C24-C25
27	F	205	WVN	C30-C33-C34-C37
27	L	201	WVN	C29-C31-C32-C36
33	b	318	II0	C32-C34-C36-C40
33	e	616	II0	C32-C34-C36-C40
33	k	615	II0	C32-C34-C36-C40
27	A	848	WVN	C22-C26-C29-C31
27	B	847	WVN	C32-C36-C39-C40
24	A	837	CLA	C16-C17-C18-C20
24	i	604	CLA	C16-C17-C18-C20
24	g	308	CLA	C16-C17-C18-C20
24	f	605	CLA	CAA-CBA-CGA-O2A
24	B	827	CLA	CAA-CBA-CGA-O2A
24	k	610	CLA	CAA-CBA-CGA-O2A
24	i	610	CLA	CAA-CBA-CGA-O2A
24	a	303	CLA	C2A-CAA-CBA-CGA
24	d	303	CLA	C2A-CAA-CBA-CGA
24	g	311	CLA	O1D-CGD-O2D-CED
24	e	611	CLA	C16-C17-C18-C20
24	b	303	CLA	C2-C3-C5-C6
24	j	313	CLA	C2-C3-C5-C6
24	d	305	CLA	C2-C3-C5-C6
24	A	824	CLA	C4-C3-C5-C6
24	A	816	CLA	C2-C1-O2A-CGA
24	L	204	CLA	C2-C1-O2A-CGA
24	c	601	CLA	C2-C1-O2A-CGA
24	h	306	CLA	C2-C1-O2A-CGA
26	i	615	LHG	O7-C7-C8-C9
24	A	802	CLA	C11-C10-C8-C7
24	A	828	CLA	C12-C13-C15-C16
24	B	830	CLA	C11-C10-C8-C7
24	I	102	CLA	C6-C7-C8-C10
24	O	201	CLA	C12-C13-C15-C16
24	b	307	CLA	C12-C13-C15-C16
24	f	607	CLA	C12-C13-C15-C16
24	g	308	CLA	C11-C12-C13-C15
24	F	201	CLA	C2-C3-C5-C6
24	A	836	CLA	C8-C10-C11-C12
24	A	842	CLA	C5-C6-C7-C8
24	B	803	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	j	314	CLA	C5-C6-C7-C8
24	A	825	CLA	C8-C10-C11-C12
24	O	205	CLA	C5-C6-C7-C8
32	L	208	LMG	C11-C12-C13-C14
24	A	818	CLA	C2A-CAA-CBA-CGA
24	b	309	CLA	C2A-CAA-CBA-CGA
24	k	604	CLA	C2A-CAA-CBA-CGA
24	B	828	CLA	O2A-C1-C2-C3
24	A	855	CLA	C10-C11-C12-C13
24	B	806	CLA	CAA-CBA-CGA-O1A
24	d	304	CLA	O1A-CGA-O2A-C1
24	A	808	CLA	C3A-C2A-CAA-CBA
24	I	102	CLA	C3A-C2A-CAA-CBA
24	b	312	CLA	C3A-C2A-CAA-CBA
24	k	607	CLA	C3A-C2A-CAA-CBA
24	R	203	CLA	C3A-C2A-CAA-CBA
24	A	831	CLA	C16-C17-C18-C20
24	A	812	CLA	CAA-CBA-CGA-O1A
24	a	311	CLA	CAA-CBA-CGA-O1A
24	h	302	CLA	CAA-CBA-CGA-O1A
24	e	603	CLA	CAA-CBA-CGA-O1A
24	i	601	CLA	CAA-CBA-CGA-O1A
24	g	309	CLA	O1A-CGA-O2A-C1
26	b	320	LHG	C15-C16-C17-C18
32	b	301	LMG	C21-C22-C23-C24
26	d	316	LHG	O9-C7-C8-C9
26	f	620	LHG	C35-C36-C37-C38
26	b	302	LHG	C29-C30-C31-C32
24	b	306	CLA	C8-C10-C11-C12
24	A	808	CLA	C14-C13-C15-C16
24	A	839	CLA	C6-C7-C8-C9
24	b	307	CLA	C11-C12-C13-C14
24	c	606	CLA	CAA-CBA-CGA-O2A
24	j	311	CLA	CAA-CBA-CGA-O2A
24	c	605	CLA	CAA-CBA-CGA-O1A
24	B	840	CLA	CBD-CGD-O2D-CED
26	f	620	LHG	C33-C34-C35-C36
33	k	615	II0	C25-C29-C31-C33
24	B	840	CLA	CAA-CBA-CGA-O1A
24	a	302	CLA	CAA-CBA-CGA-O1A
24	f	606	CLA	CAA-CBA-CGA-O2A
27	L	201	WVN	C01-C02-C11-C19

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Mol	Chain	Res	Type	Atoms
35	k	612	KC2	C3A-C2A-CAA-CBA
35	j	312	KC2	C1A-C2A-CAA-CBA
35	d	311	KC2	C1A-C2A-CAA-CBA
35	g	314	KC2	C1A-C2A-CAA-CBA
24	L	202	CLA	CAA-CBA-CGA-O1A
26	j	319	LHG	O10-C23-C24-C25
24	A	810	CLA	C10-C11-C12-C13
24	B	806	CLA	C16-C17-C18-C19
24	A	807	CLA	CBD-CGD-O2D-CED
27	B	847	WVN	C29-C31-C32-C36
24	A	828	CLA	CAA-CBA-CGA-O1A
24	g	308	CLA	CAA-CBA-CGA-O1A
24	b	313	CLA	C15-C16-C17-C18
25	B	842	PQN	C20-C21-C22-C23
32	J	106	LMG	C8-C7-O1-C1
24	h	305	CLA	O1A-CGA-O2A-C1
24	i	610	CLA	CAA-CBA-CGA-O1A
26	A	845	LHG	O9-C7-C8-C9
24	B	835	CLA	C15-C16-C17-C18
24	d	305	CLA	CAA-CBA-CGA-O2A
24	A	824	CLA	C2-C3-C5-C6
35	g	314	KC2	C2B-C3B-CAB-CBB
32	b	301	LMG	C17-C18-C19-C20
27	A	847	WVN	C34-C37-C40-C39
24	A	836	CLA	CAA-CBA-CGA-O1A
26	c	617	LHG	C23-C24-C25-C26
24	I	102	CLA	C16-C17-C18-C19
24	i	604	CLA	C16-C17-C18-C19
24	A	803	CLA	CAD-CBD-CGD-O2D
24	B	827	CLA	CAD-CBD-CGD-O2D
24	B	837	CLA	CAD-CBD-CGD-O2D
24	B	840	CLA	CAD-CBD-CGD-O2D
24	B	841	CLA	CAD-CBD-CGD-O2D
24	F	201	CLA	CAD-CBD-CGD-O2D
24	a	304	CLA	CAD-CBD-CGD-O2D
24	i	605	CLA	CAD-CBD-CGD-O2D
24	i	607	CLA	CAD-CBD-CGD-O2D
24	j	306	CLA	CAD-CBD-CGD-O2D
24	j	309	CLA	CAD-CBD-CGD-O2D
24	j	314	CLA	CAD-CBD-CGD-O2D
24	e	602	CLA	O1D-CGD-O2D-CED
24	d	304	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	A	851	LMT	O5'-C5'-C6'-O6'
24	B	811	CLA	C2C-C3C-CAC-CBC
24	J	103	CLA	CBD-CGD-O2D-CED
32	J	106	LMG	C16-C17-C18-C19
24	A	803	CLA	C2-C1-O2A-CGA
24	i	611	CLA	C2-C1-O2A-CGA
26	g	301	LHG	C11-C10-C9-C8
24	B	827	CLA	CAA-CBA-CGA-O1A
24	a	310	CLA	CAA-CBA-CGA-O1A
24	c	612	CLA	C16-C17-C18-C19
24	a	305	CLA	CAA-CBA-CGA-O2A
24	e	608	CLA	CAA-CBA-CGA-O2A
24	f	603	CLA	CAA-CBA-CGA-O2A
24	i	611	CLA	CAA-CBA-CGA-O2A
24	j	308	CLA	CAA-CBA-CGA-O2A
24	d	307	CLA	CAA-CBA-CGA-O2A
24	A	808	CLA	CAA-CBA-CGA-O2A
24	A	833	CLA	CAA-CBA-CGA-O2A
24	B	830	CLA	CAA-CBA-CGA-O2A
24	e	611	CLA	CAA-CBA-CGA-O2A
24	i	603	CLA	CAA-CBA-CGA-O2A
26	c	618	LHG	C31-C32-C33-C34
24	B	836	CLA	CAA-CBA-CGA-O1A
24	h	307	CLA	CAA-CBA-CGA-O1A
24	k	610	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

200 monomers are involved in 404 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	303	CLA	1	0
24	c	607	CLA	2	0
24	B	837	CLA	4	0
24	b	303	CLA	1	0
24	B	817	CLA	2	0
24	g	303	CLA	2	0
24	B	807	CLA	2	0
24	b	304	CLA	2	0
24	h	305	CLA	1	0
24	g	304	CLA	1	0
24	h	307	CLA	1	0
24	B	811	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	J	106	LMG	6	0
24	j	311	CLA	2	0
24	c	601	CLA	1	0
24	B	830	CLA	2	0
29	A	854	SF4	4	0
28	a	318	LMT	2	0
24	e	610	CLA	3	0
24	f	613	CLA	1	0
26	A	844	LHG	1	0
24	j	308	CLA	1	0
24	k	603	CLA	3	0
24	A	853	CLA	4	0
24	c	606	CLA	5	0
24	J	105	CLA	3	0
24	k	601	CLA	3	0
26	J	107	LHG	8	0
24	g	322	CLA	2	0
24	B	827	CLA	3	0
26	e	617	LHG	2	0
24	B	804	CLA	3	0
24	A	814	CLA	3	0
24	h	302	CLA	1	0
24	A	856	CLA	5	0
24	A	813	CLA	2	0
24	b	306	CLA	2	0
24	e	604	CLA	1	0
24	B	803	CLA	2	0
24	c	602	CLA	2	0
24	B	829	CLA	2	0
33	a	314	II0	1	0
24	e	601	CLA	1	0
24	A	812	CLA	1	0
24	B	816	CLA	2	0
24	c	612	CLA	2	0
24	O	205	CLA	6	0
24	A	819	CLA	1	0
24	f	609	CLA	2	0
24	A	855	CLA	6	0
25	B	842	PQN	5	0
24	d	304	CLA	1	0
24	A	820	CLA	3	0
24	i	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	L	207	CLA	1	0
24	A	828	CLA	2	0
24	j	313	CLA	1	0
24	B	808	CLA	1	0
24	B	801	CLA	6	0
24	A	822	CLA	2	0
24	k	604	CLA	1	0
24	e	606	CLA	4	0
24	A	806	CLA	5	0
35	e	609	KC2	2	0
24	f	610	CLA	4	0
28	A	851	LMT	1	0
24	e	607	CLA	3	0
24	B	823	CLA	5	0
24	g	307	CLA	1	0
34	k	618	IHT	2	0
24	c	611	CLA	1	0
24	i	606	CLA	1	0
24	A	852	CLA	1	0
24	c	603	CLA	1	0
24	A	811	CLA	2	0
24	f	602	CLA	4	0
24	f	601	CLA	2	0
24	d	306	CLA	1	0
24	g	308	CLA	5	0
24	k	608	CLA	3	0
24	A	815	CLA	2	0
32	L	208	LMG	3	0
24	A	809	CLA	2	0
24	a	308	CLA	2	0
34	j	317	IHT	1	0
24	i	611	CLA	1	0
24	a	307	CLA	3	0
29	C	101	SF4	3	0
24	c	605	CLA	1	0
24	e	602	CLA	1	0
29	C	102	SF4	2	0
33	k	615	II0	1	0
24	K	101	CLA	1	0
24	j	306	CLA	2	0
24	A	841	CLA	3	0
24	L	202	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	302	CLA	1	0
24	e	608	CLA	1	0
24	f	603	CLA	1	0
24	A	824	CLA	1	0
35	g	313	KC2	1	0
24	d	301	CLA	1	0
24	A	804	CLA	3	0
24	B	831	CLA	1	0
24	A	817	CLA	4	0
24	j	302	CLA	1	0
24	B	834	CLA	1	0
26	b	320	LHG	5	0
24	A	842	CLA	6	0
33	b	315	II0	1	0
24	I	102	CLA	2	0
26	f	620	LHG	3	0
24	B	819	CLA	1	0
24	f	608	CLA	4	0
24	b	310	CLA	3	0
26	c	618	LHG	1	0
24	c	608	CLA	2	0
24	g	310	CLA	1	0
24	b	309	CLA	2	0
24	B	839	CLA	2	0
24	i	601	CLA	1	0
24	f	606	CLA	2	0
24	B	805	CLA	1	0
24	B	812	CLA	3	0
24	B	832	CLA	2	0
24	k	602	CLA	3	0
24	A	838	CLA	1	0
24	B	840	CLA	1	0
26	g	301	LHG	1	0
24	k	610	CLA	2	0
24	a	310	CLA	2	0
24	a	311	CLA	4	0
24	f	607	CLA	3	0
25	A	843	PQN	2	0
24	B	836	CLA	4	0
33	k	616	II0	1	0
24	B	828	CLA	3	0
24	F	202	CLA	2	0

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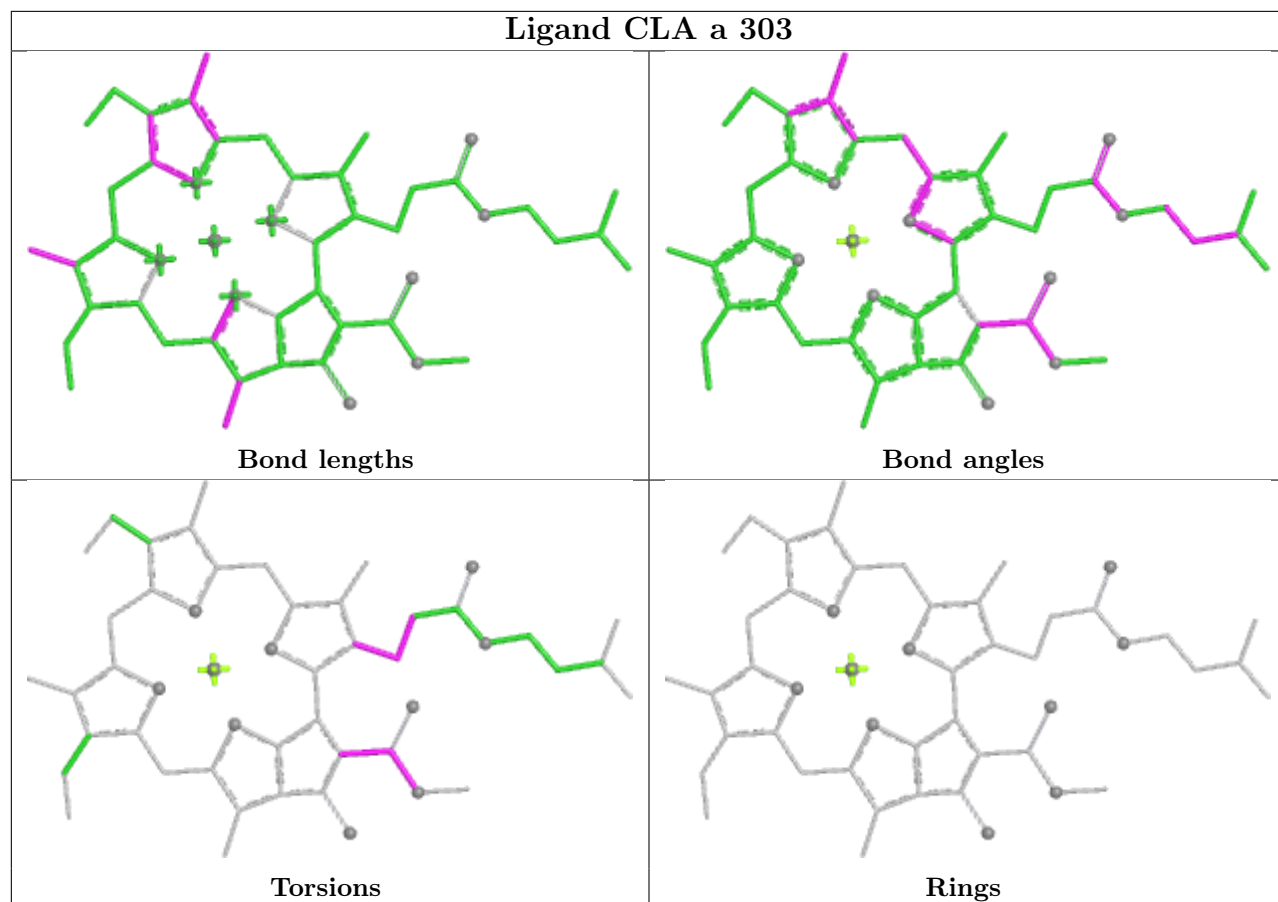
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	g	312	KC2	1	0
24	B	835	CLA	3	0
35	d	311	KC2	1	0
24	F	201	CLA	7	0
24	B	815	CLA	1	0
24	A	830	CLA	1	0
24	e	605	CLA	3	0
24	B	810	CLA	2	0
24	A	821	CLA	1	0
24	i	602	CLA	1	0
24	L	203	CLA	4	0
26	B	802	LHG	3	0
24	A	801	CLA	2	0
32	F	206	LMG	2	0
24	d	303	CLA	2	0
24	B	821	CLA	1	0
24	A	831	CLA	1	0
26	f	619	LHG	3	0
24	A	818	CLA	3	0
24	B	841	CLA	4	0
24	b	308	CLA	6	0
24	b	313	CLA	6	0
24	i	605	CLA	1	0
24	B	825	CLA	2	0
24	B	824	CLA	1	0
24	e	611	CLA	3	0
24	A	827	CLA	4	0
24	A	829	CLA	3	0
24	f	604	CLA	1	0
24	B	833	CLA	3	0
24	O	201	CLA	3	0
30	B	843	DGD	3	0
31	B	844	LMU	1	0
24	A	839	CLA	4	0
24	A	807	CLA	1	0
24	A	840	CLA	5	0
28	b	319	LMT	2	0
24	A	836	CLA	3	0
24	j	309	CLA	2	0
24	A	823	CLA	2	0
34	g	319	IHT	1	0
32	b	301	LMG	6	0

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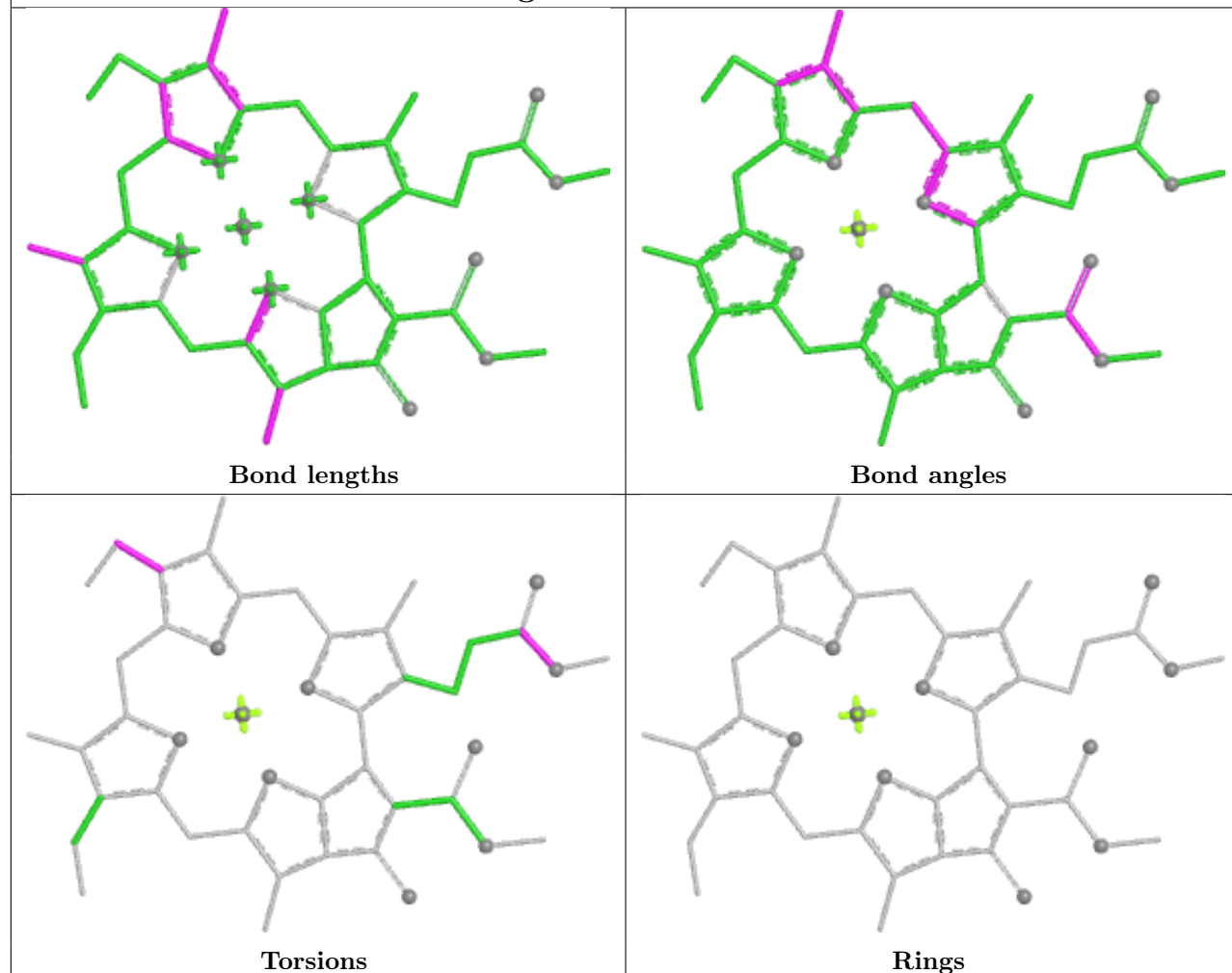
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	k	614	CLA	1	0
24	g	309	CLA	4	0
24	A	805	CLA	1	0
24	A	802	CLA	6	0
24	k	607	CLA	2	0
24	A	837	CLA	2	0
24	b	307	CLA	3	0
24	b	312	CLA	6	0
24	A	803	CLA	3	0
24	b	305	CLA	3	0
24	d	305	CLA	1	0
26	b	302	LHG	2	0
24	B	820	CLA	4	0
24	k	609	CLA	2	0
24	B	826	CLA	1	0
24	i	607	CLA	1	0
24	B	814	CLA	1	0
24	A	835	CLA	2	0
24	B	822	CLA	4	0
24	B	806	CLA	2	0

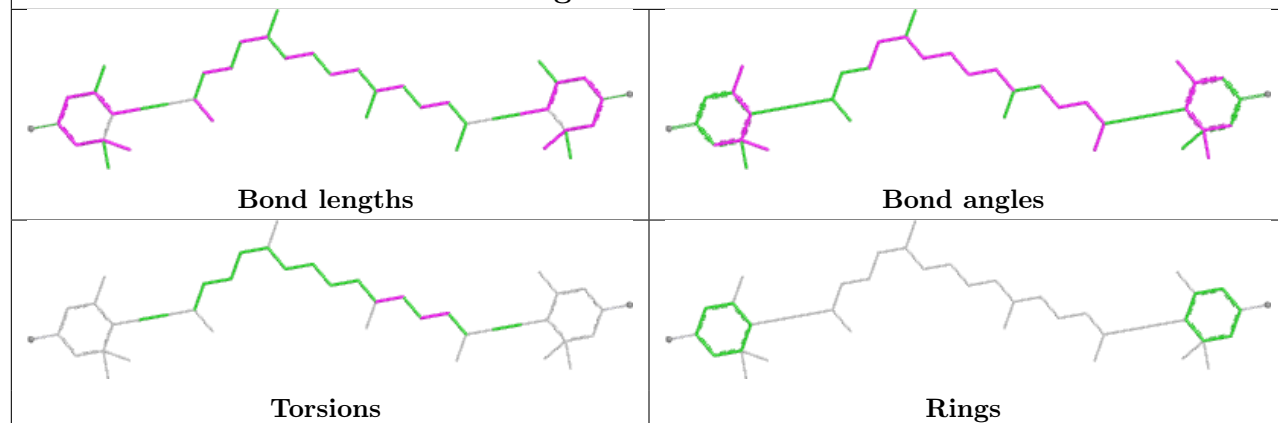
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

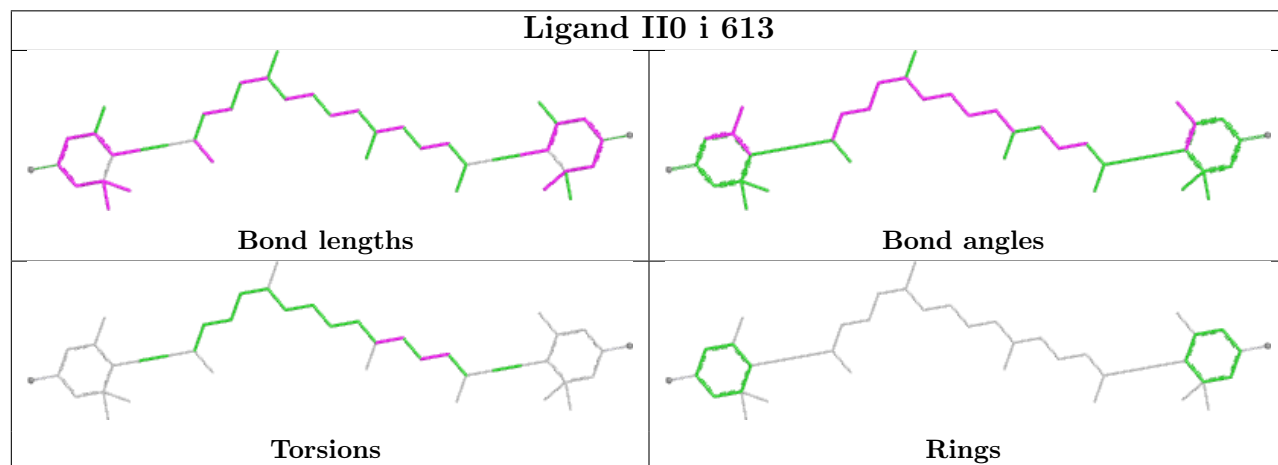
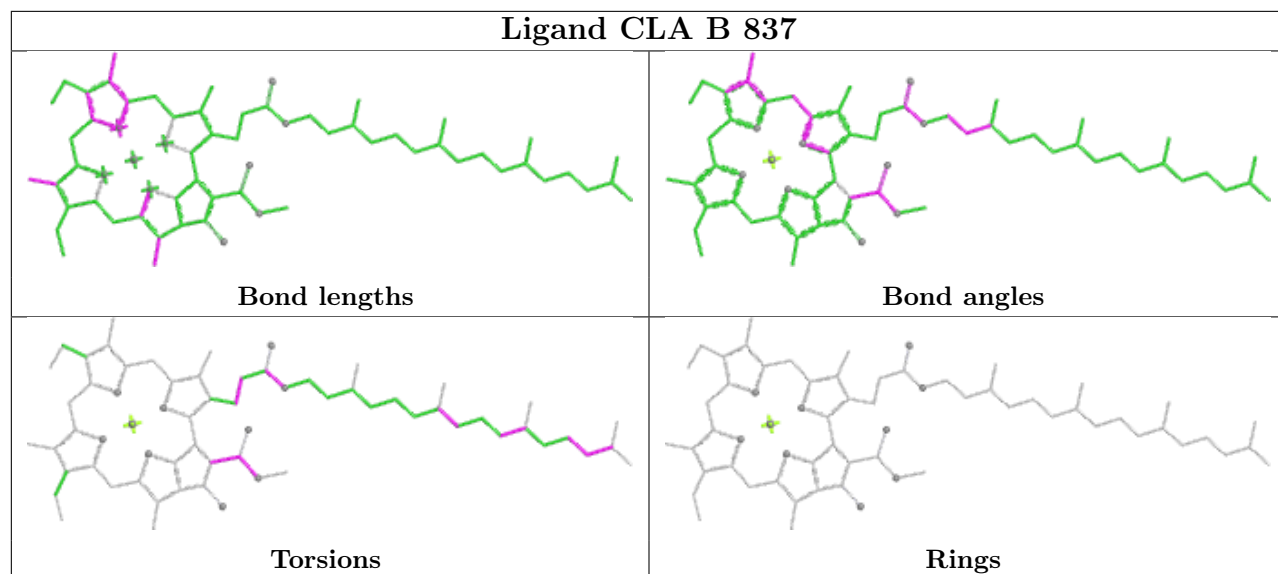


Ligand CLA c 607

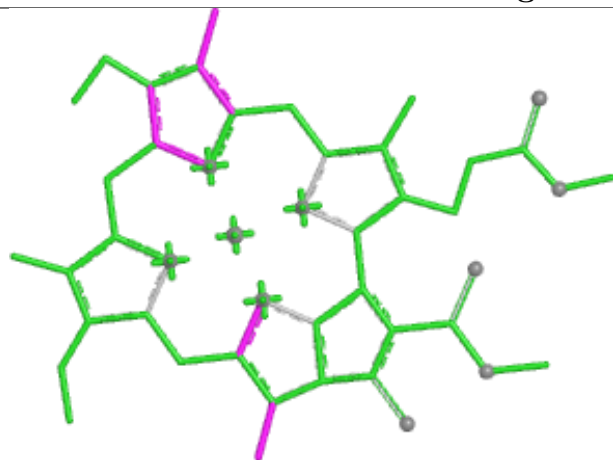


Ligand II0 f 614

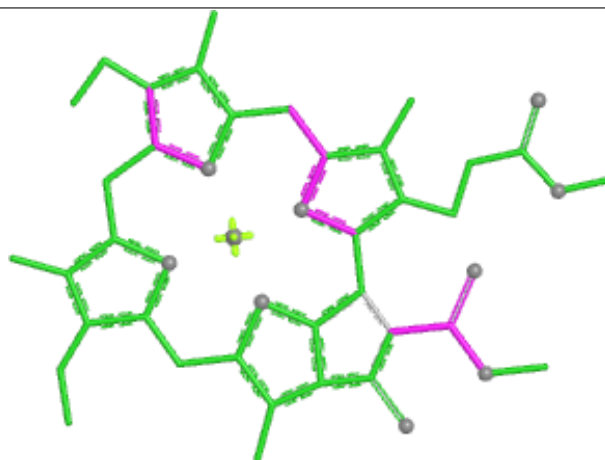




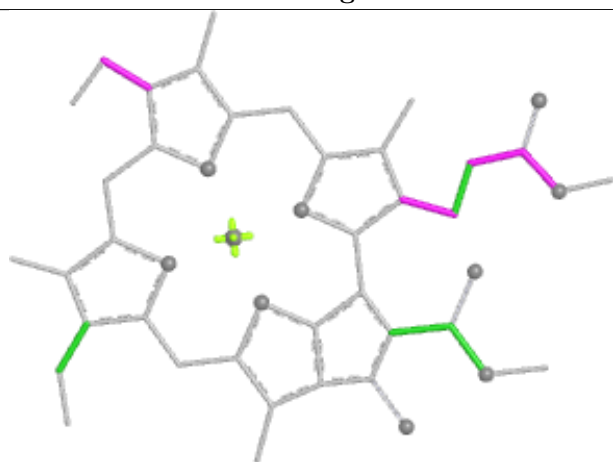
Ligand CLA d 307



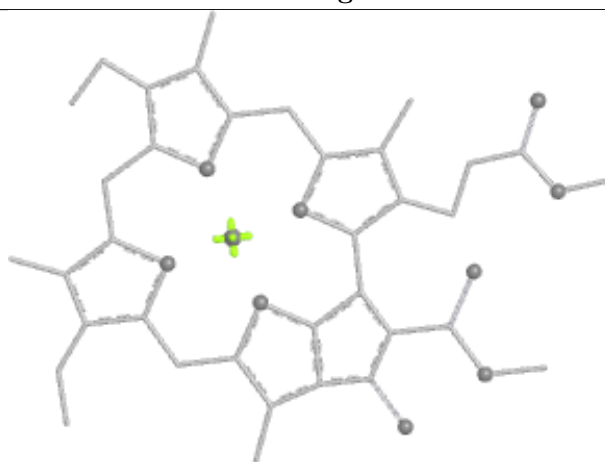
Bond lengths



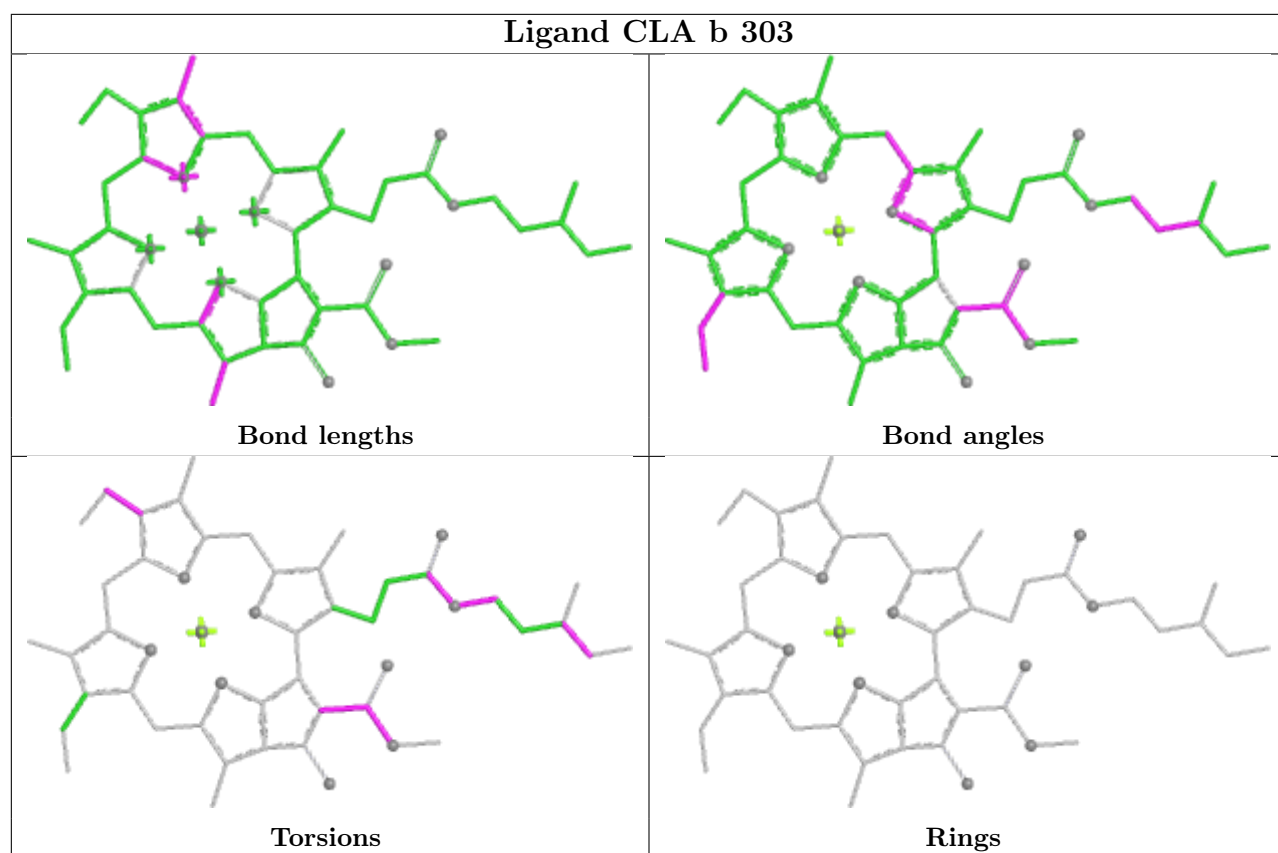
Bond angles



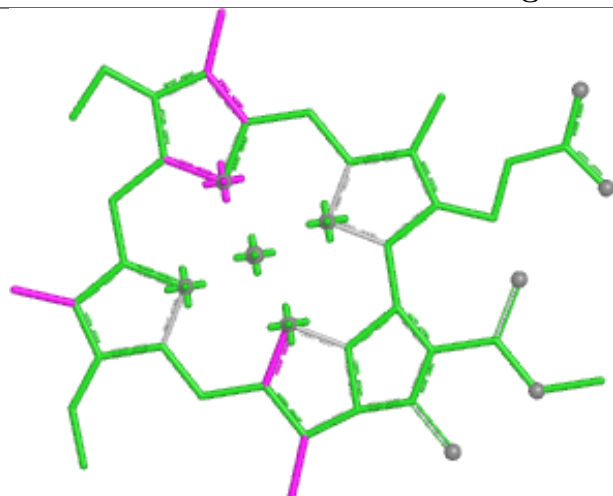
Torsions



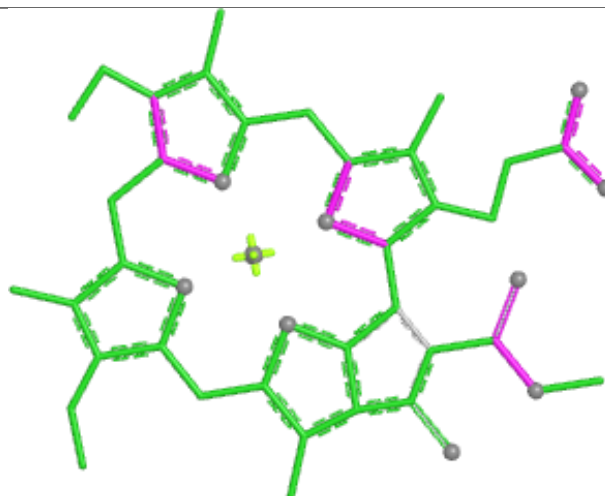
Rings



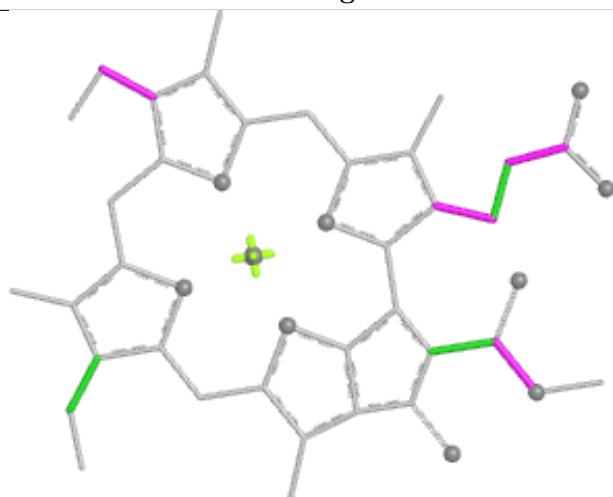
Ligand CLA f 605



Bond lengths



Bond angles

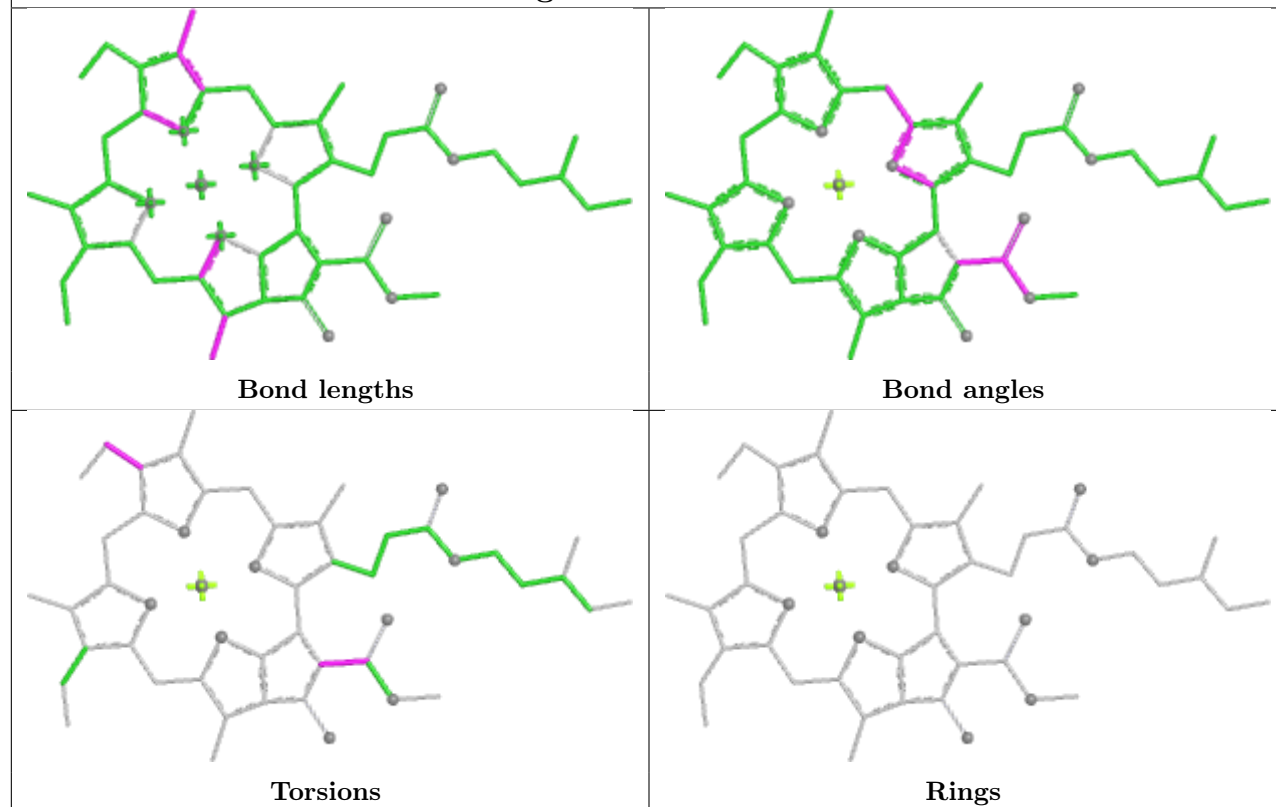


Torsions

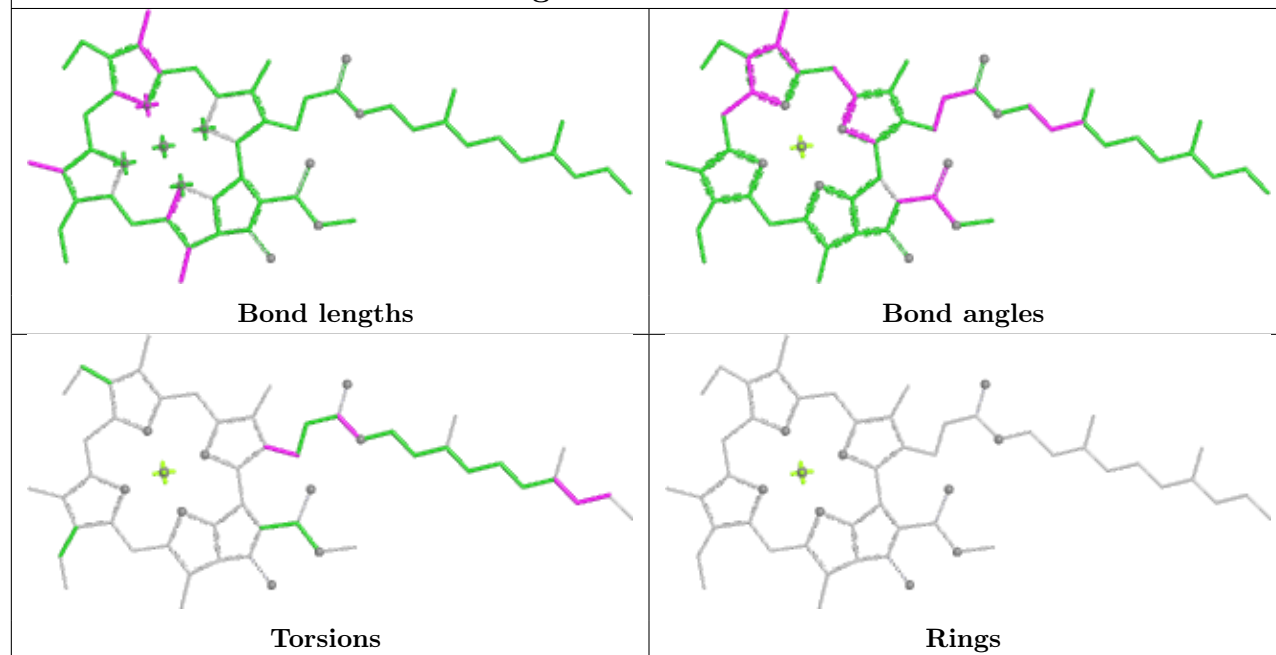


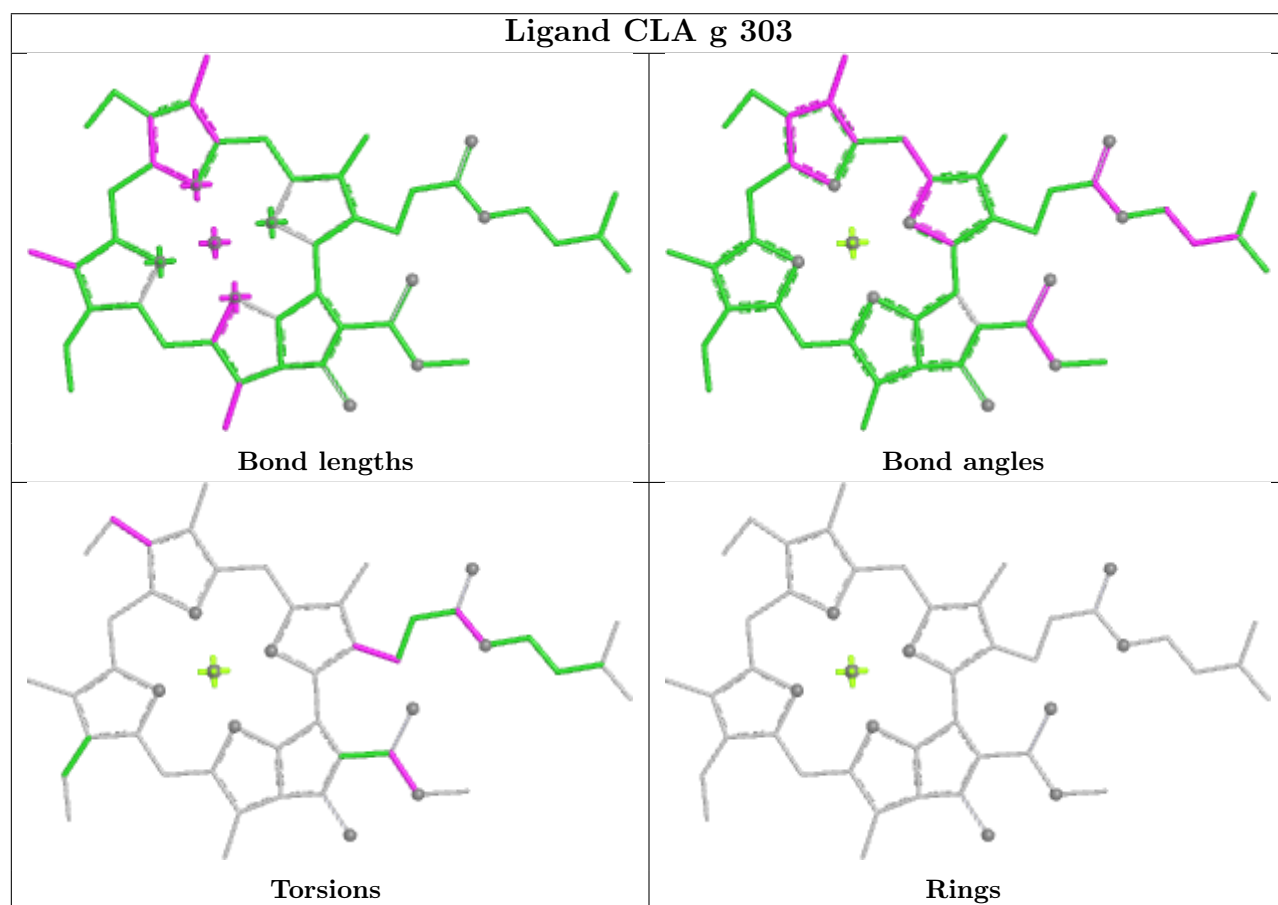
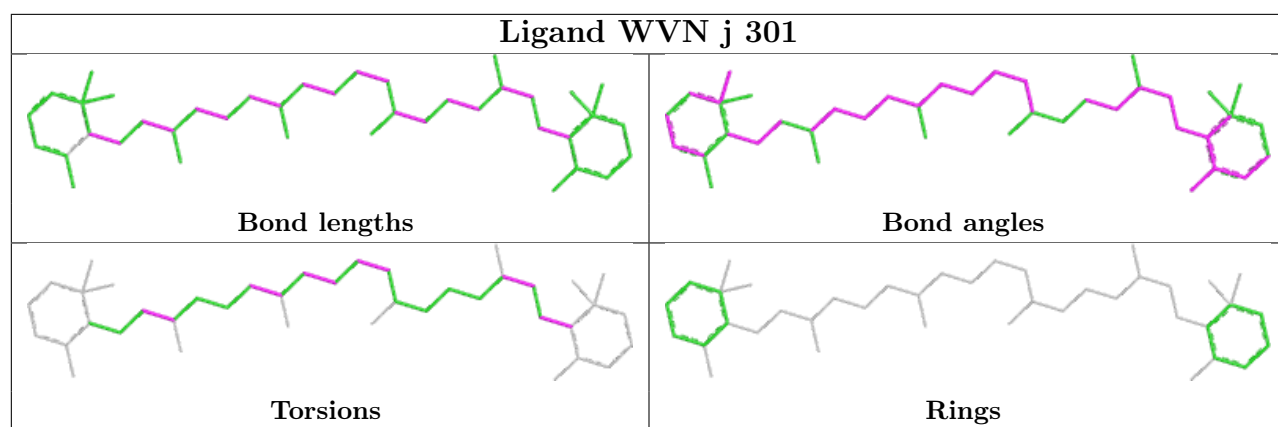
Rings

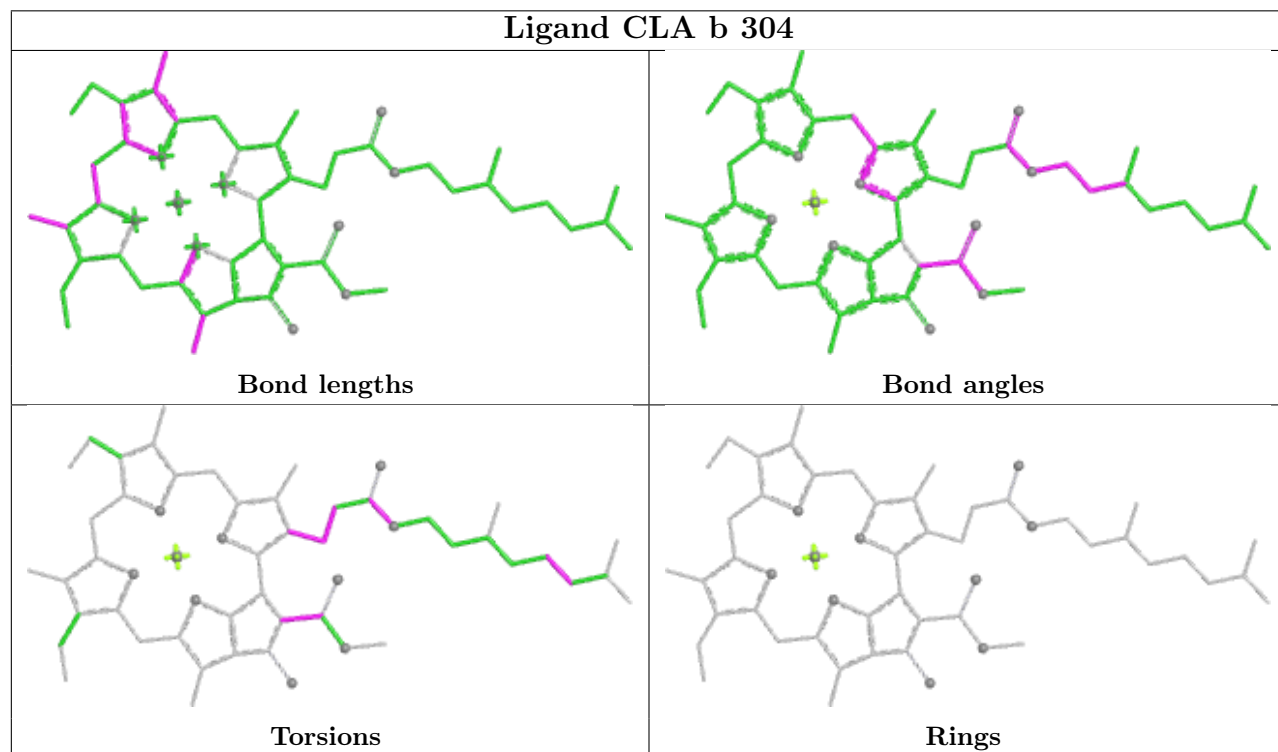
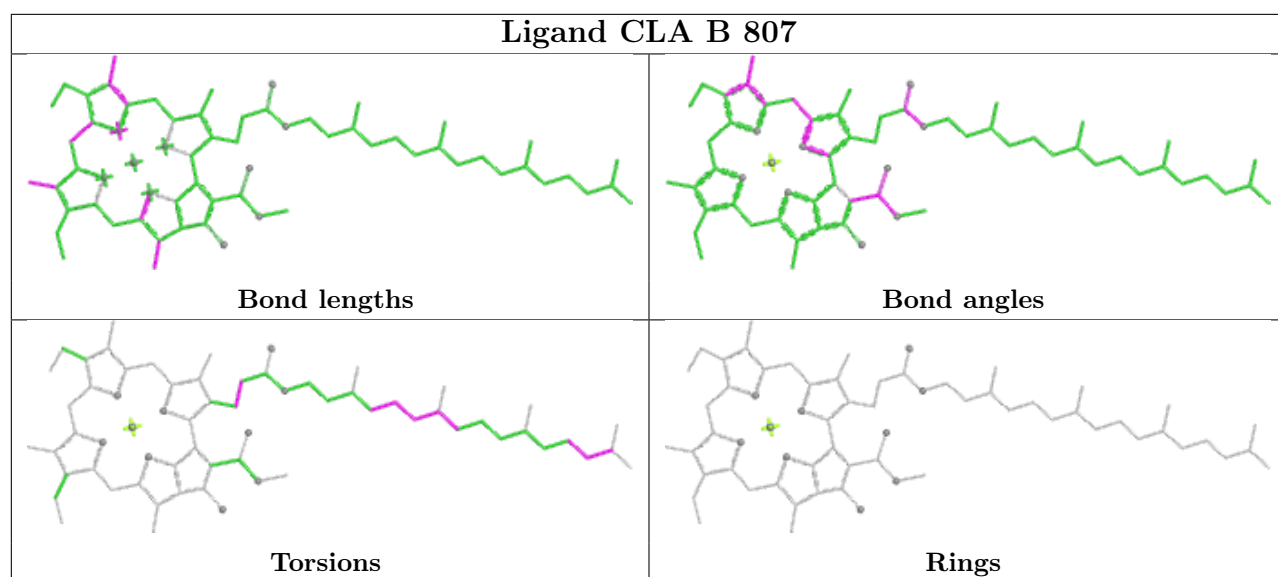
Ligand CLA a 304

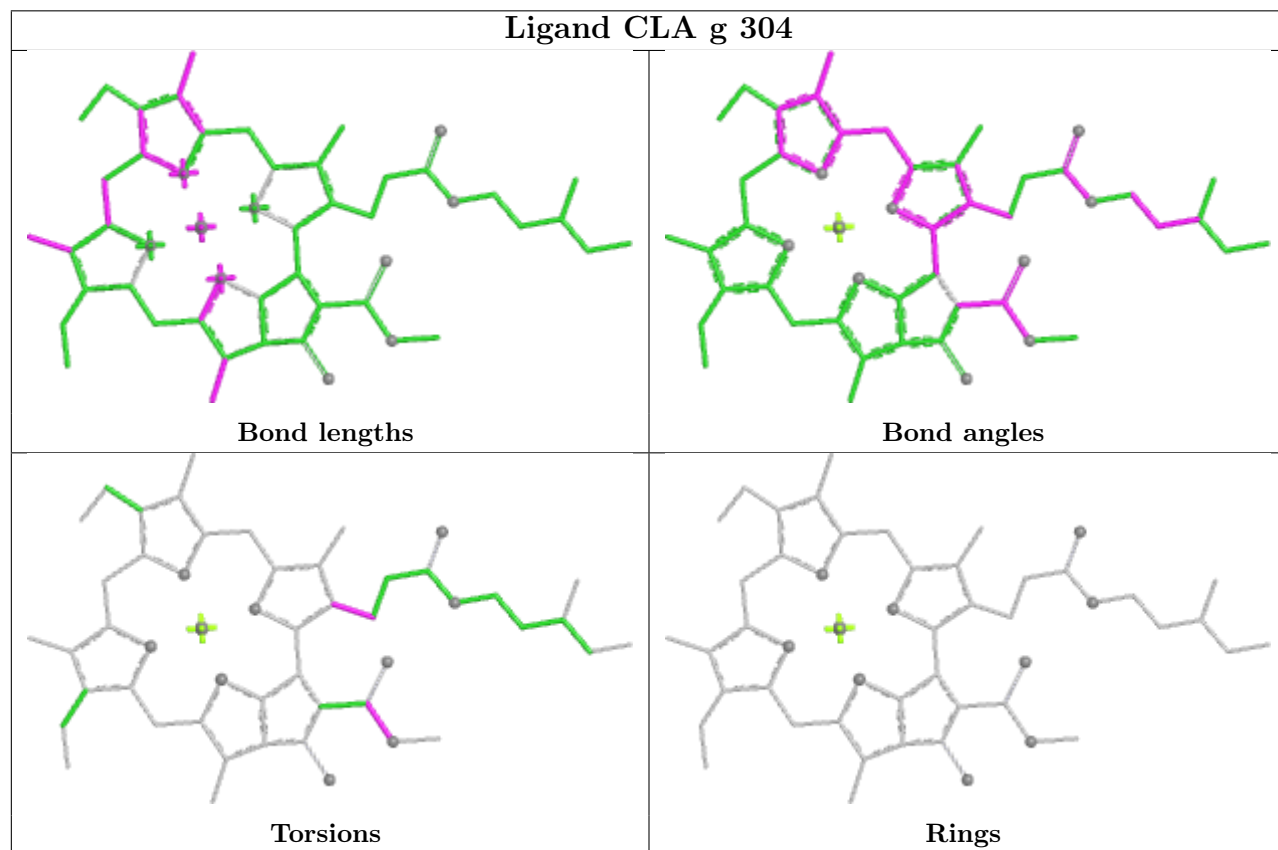
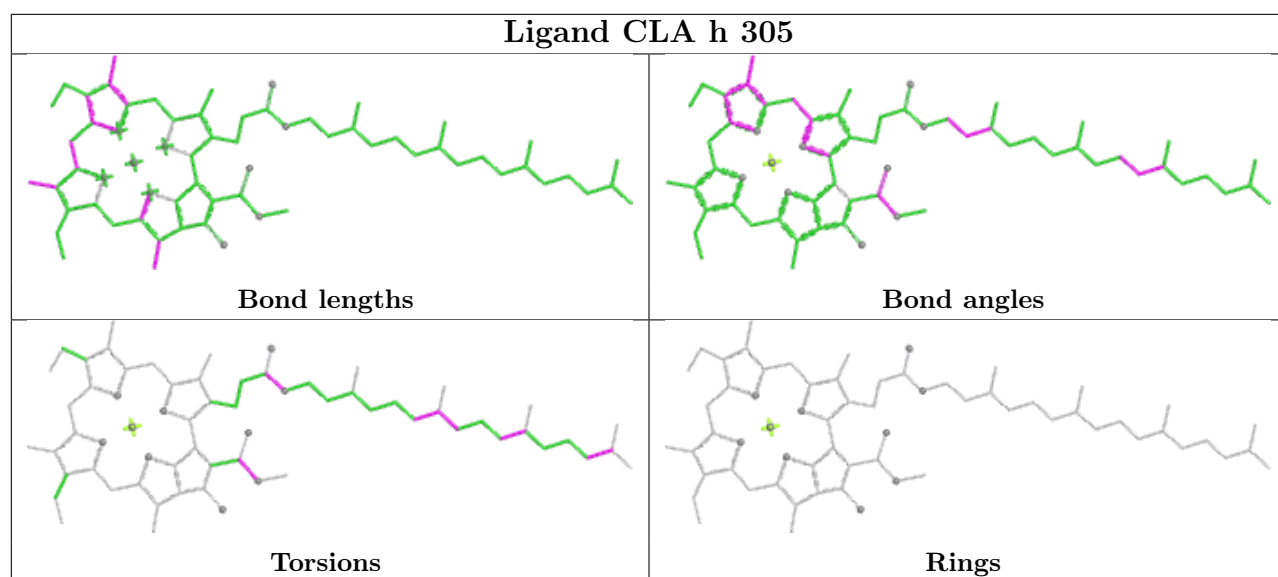


Ligand CLA B 817

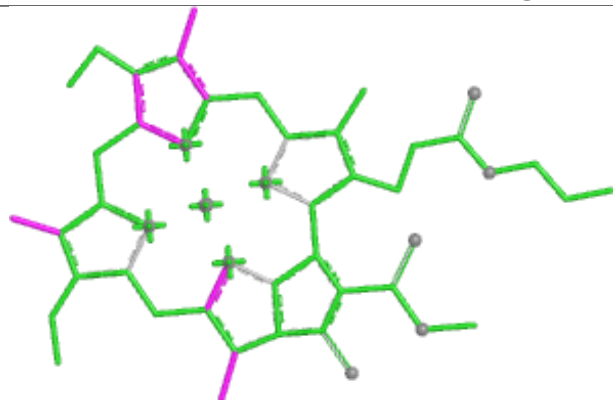




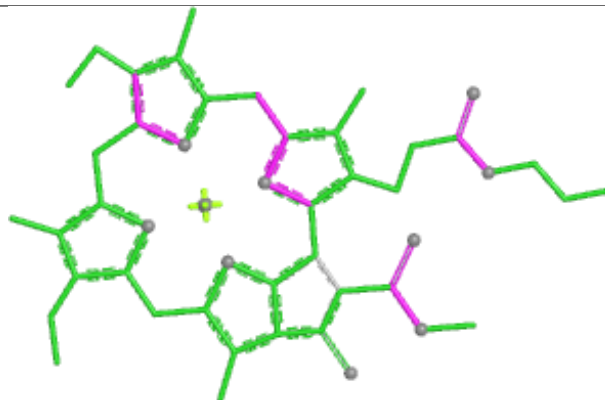




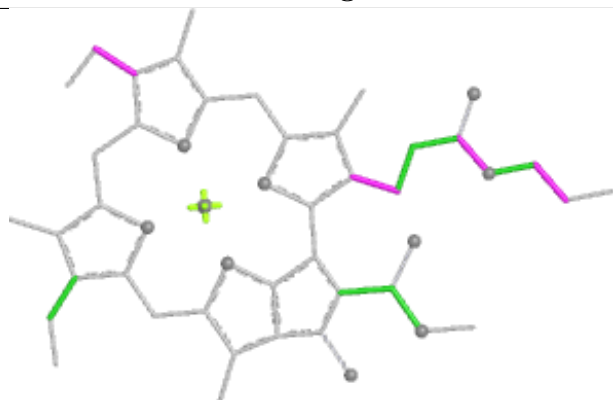
Ligand CLA a 309



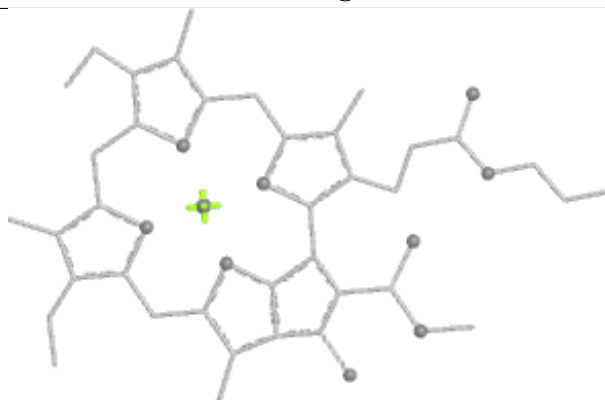
Bond lengths



Bond angles

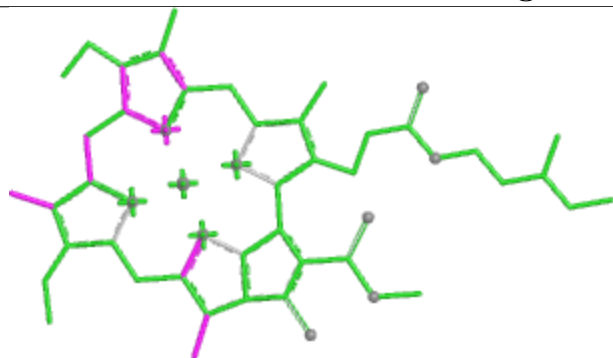


Torsions

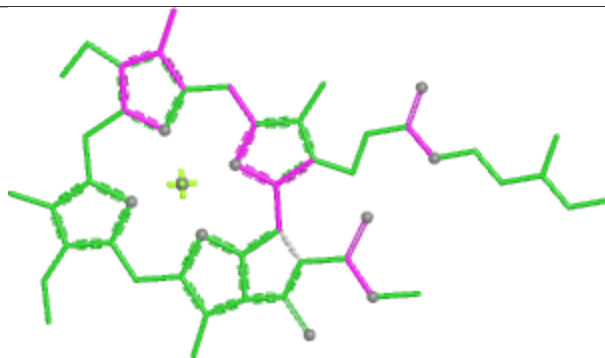


Rings

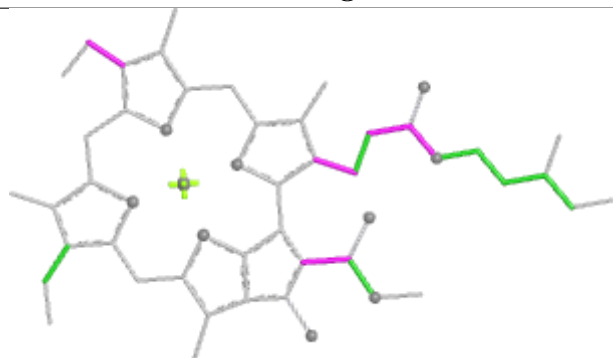
Ligand CLA h 307



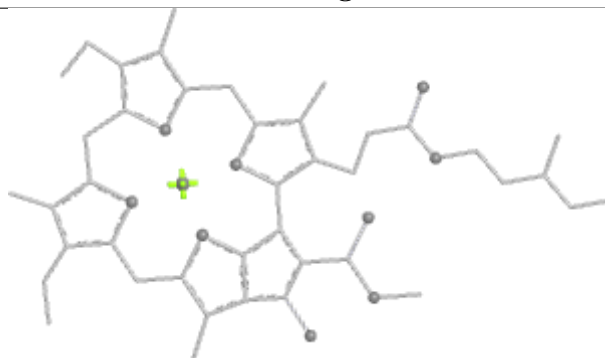
Bond lengths



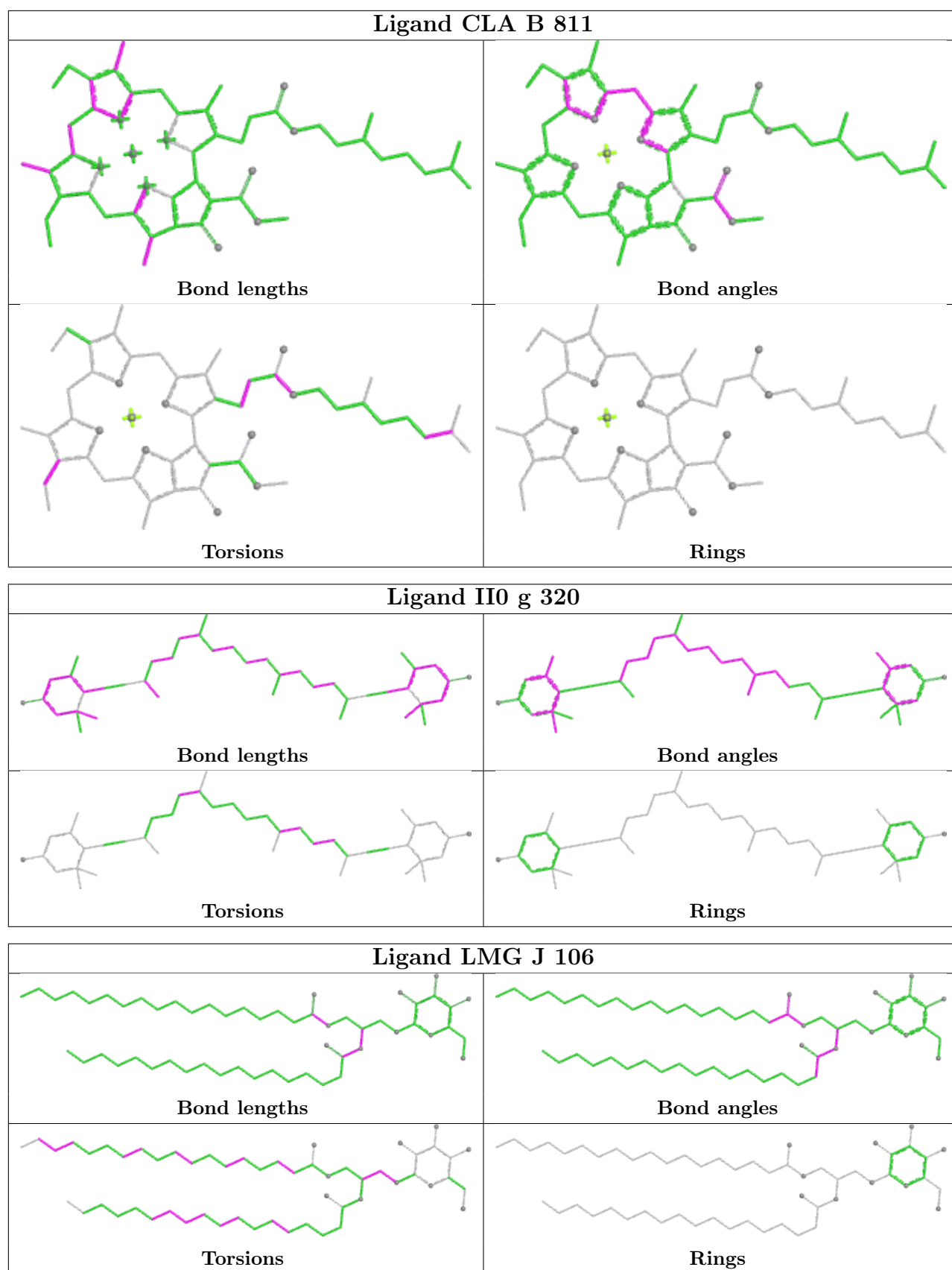
Bond angles

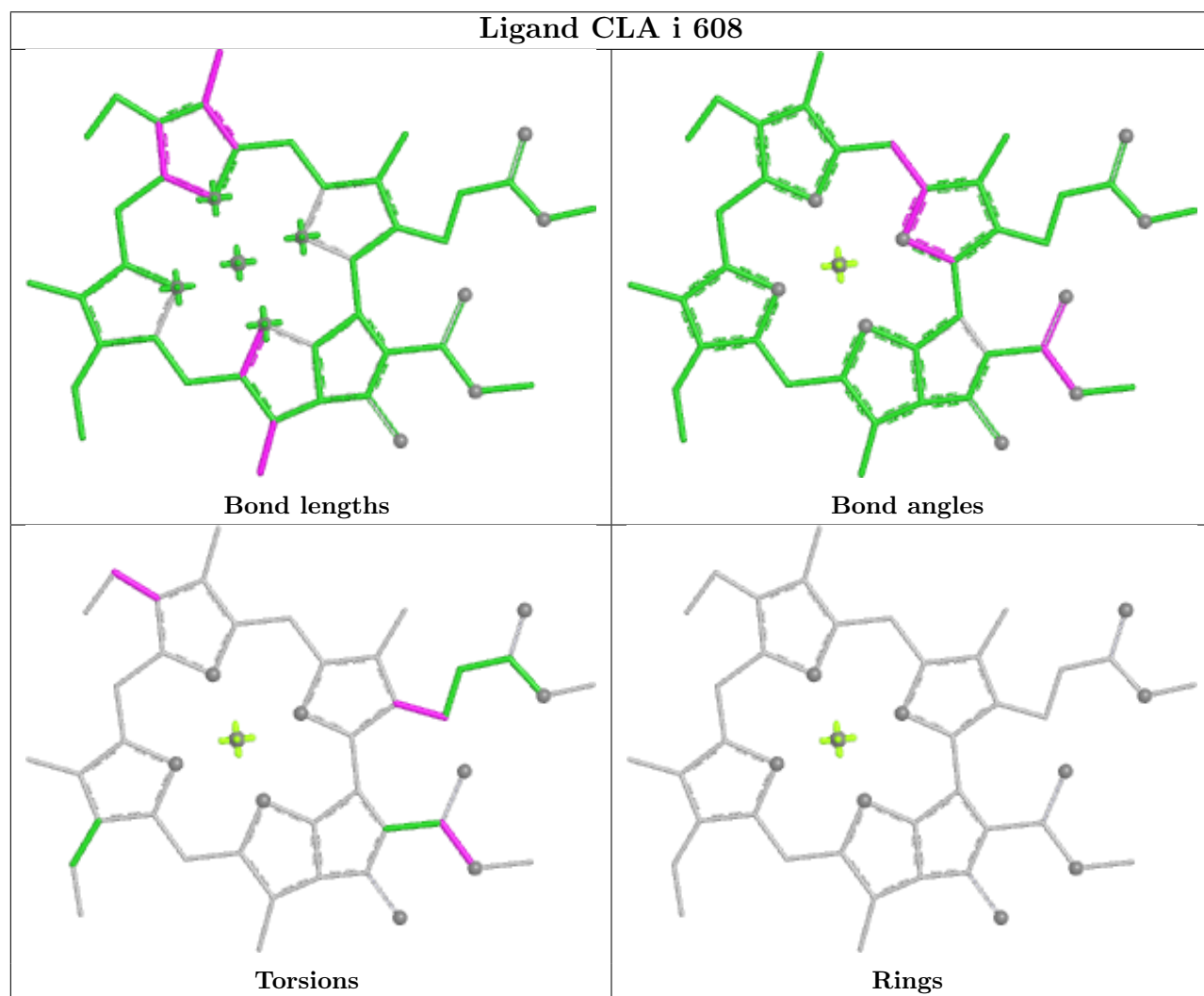
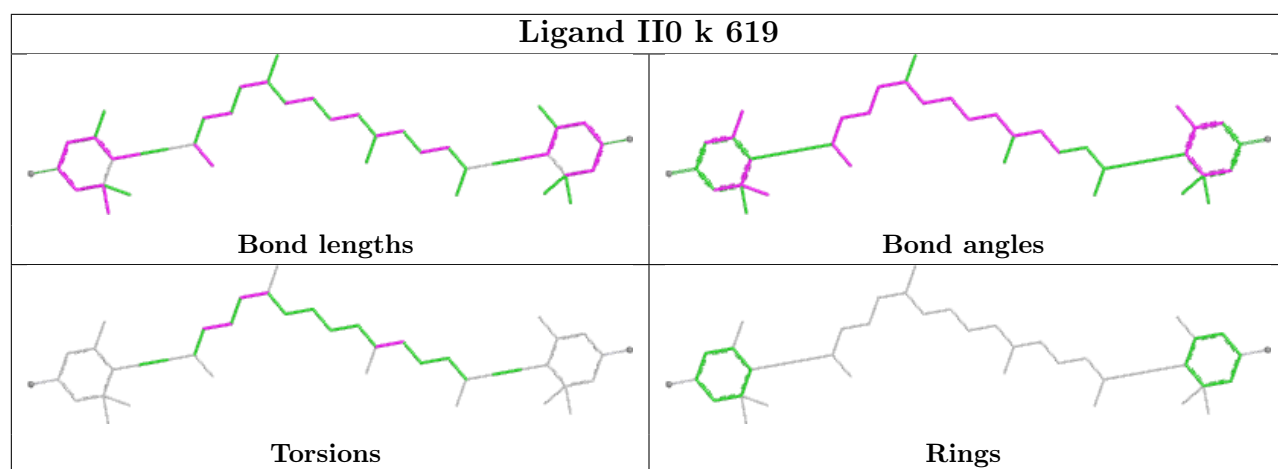


Torsions

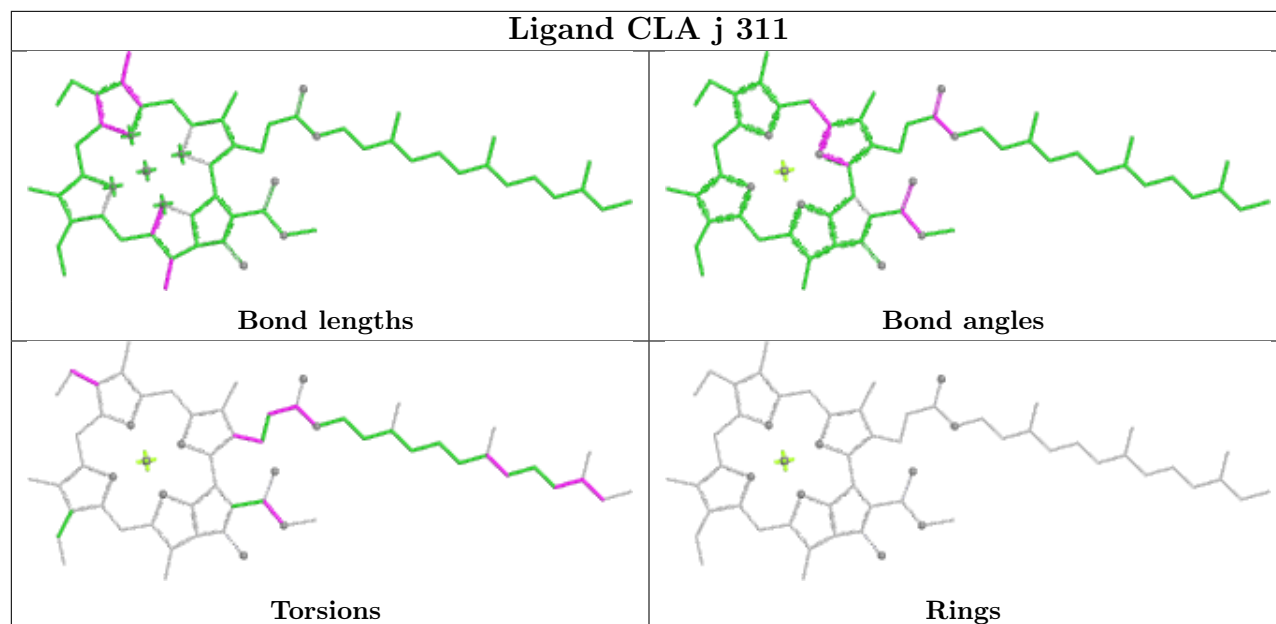


Rings

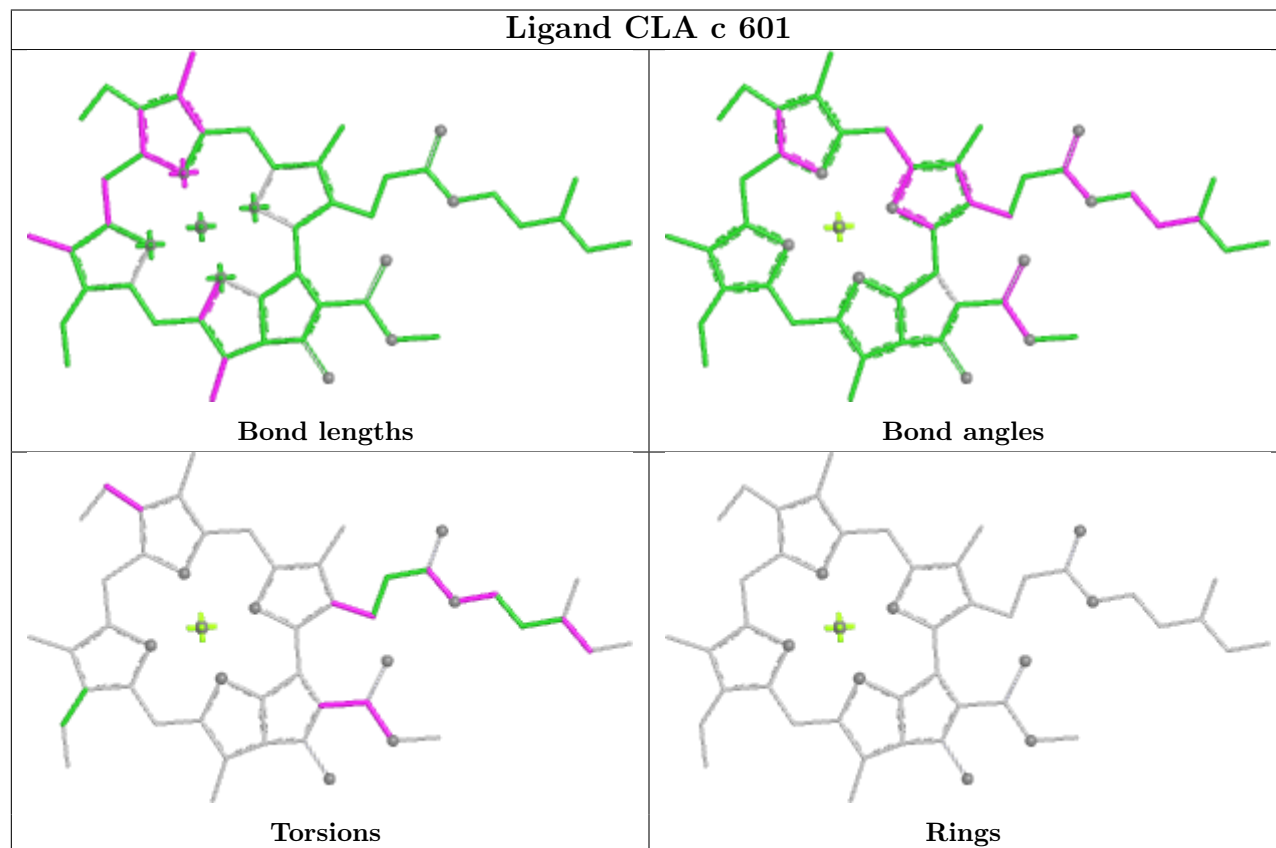




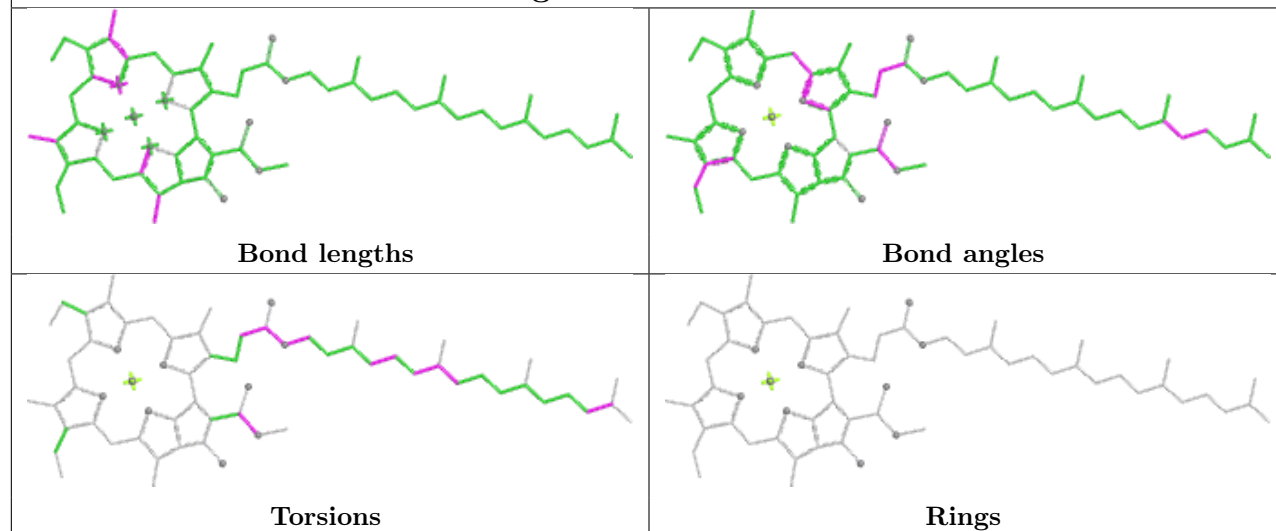
Ligand CLA j 311



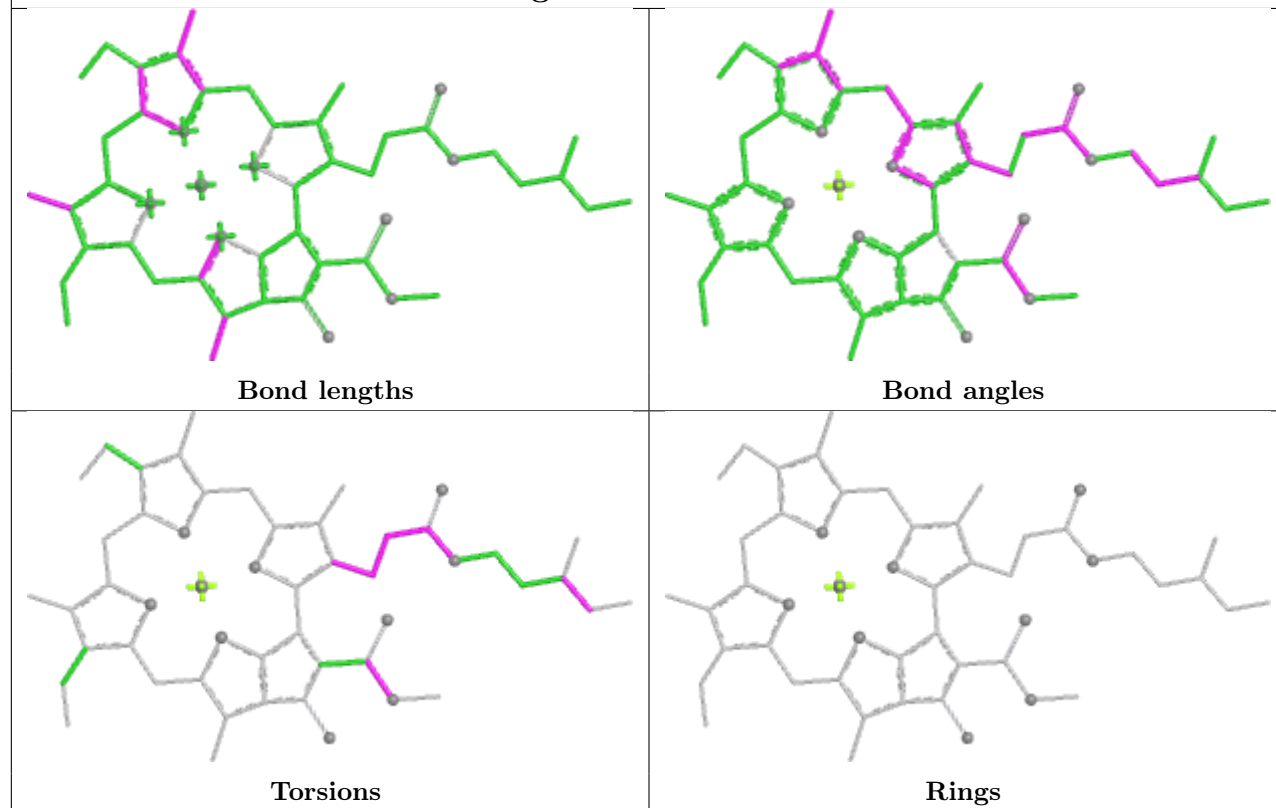
Ligand CLA c 601

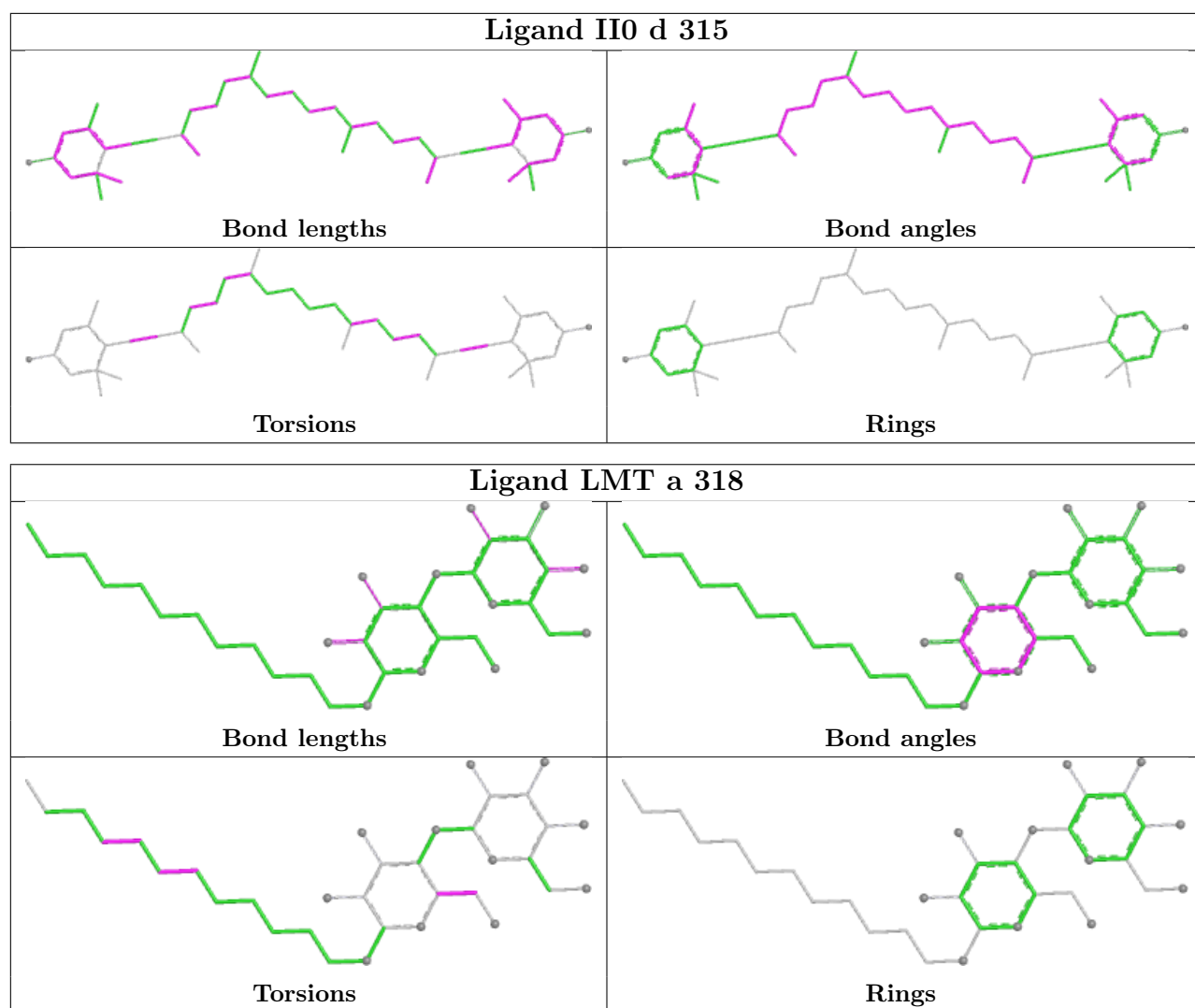


Ligand CLA B 830

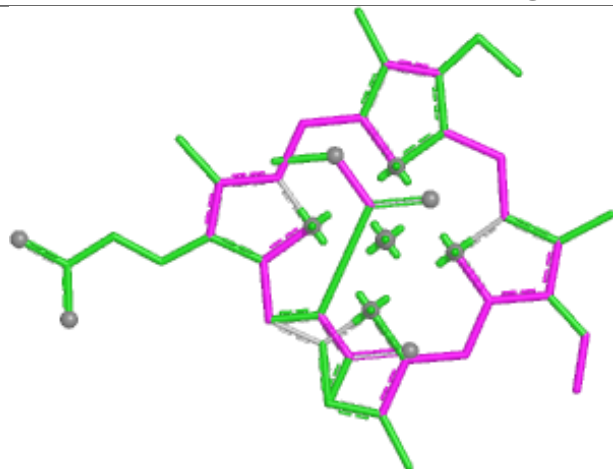


Ligand CLA R 203

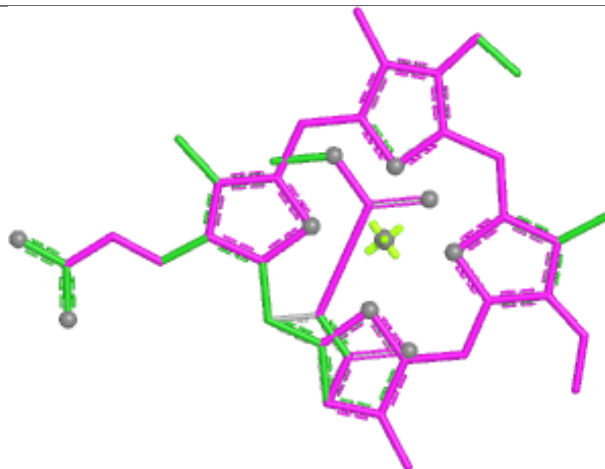




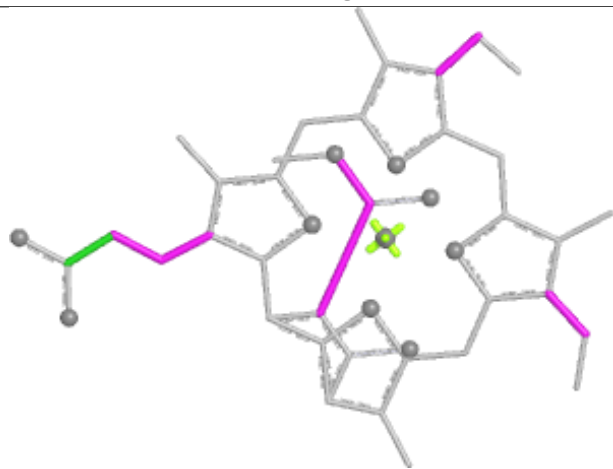
Ligand KC2 i 616



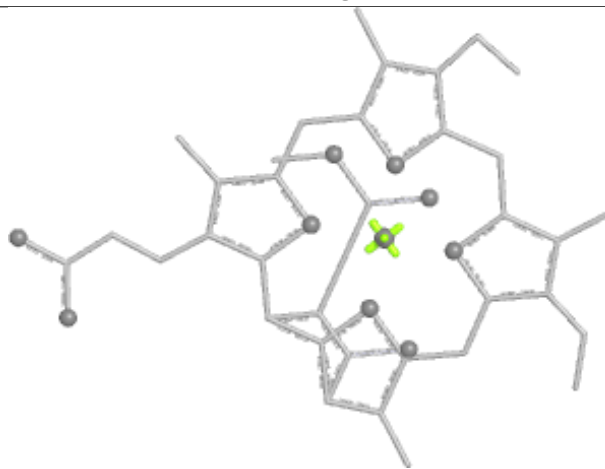
Bond lengths



Bond angles

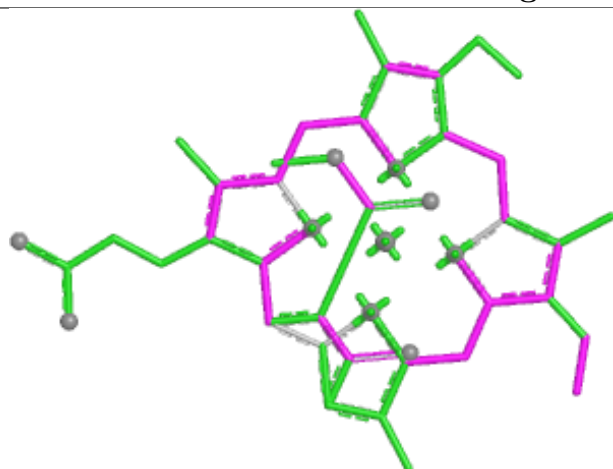


Torsions

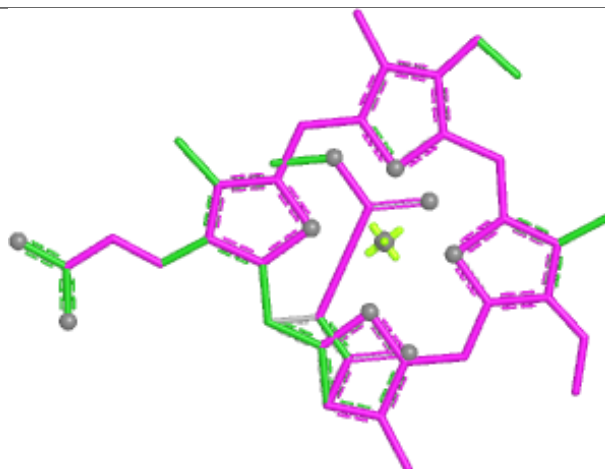


Rings

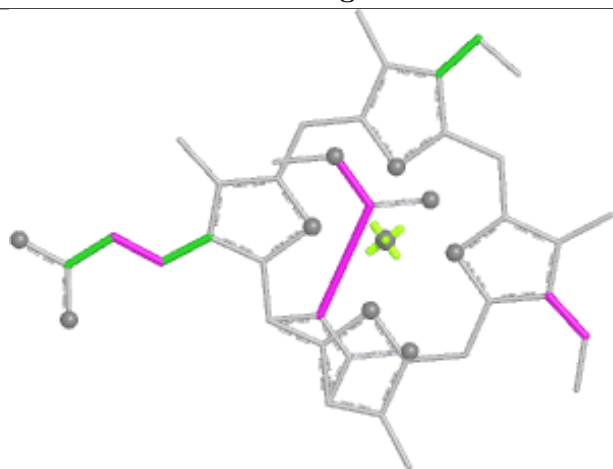
Ligand KC2 k 611



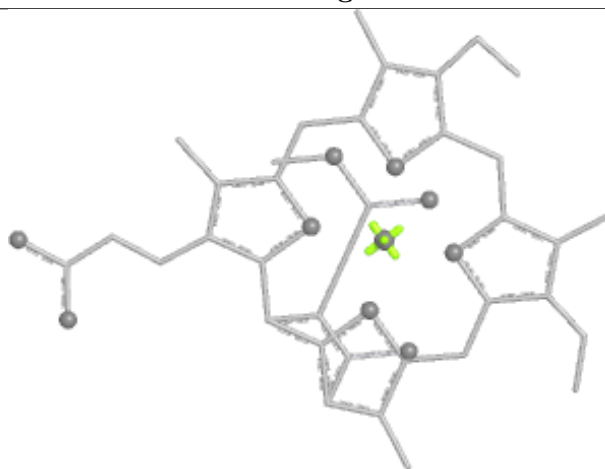
Bond lengths



Bond angles

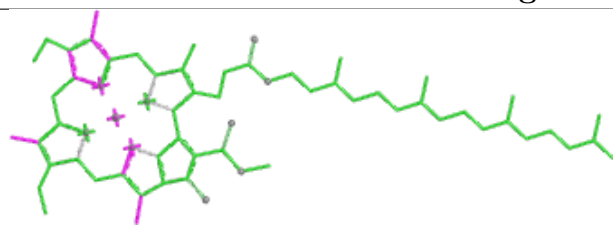


Torsions

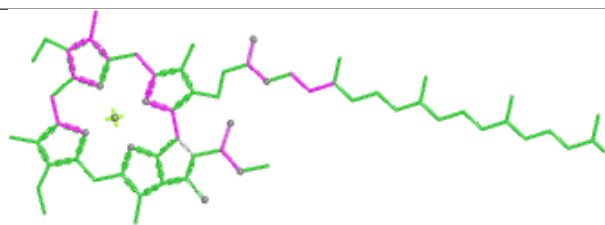


Rings

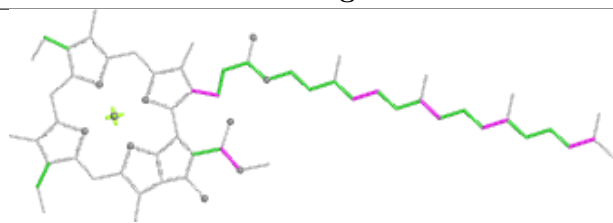
Ligand CLA e 610



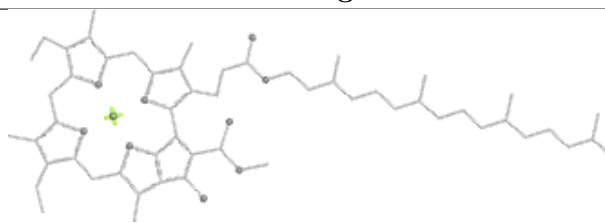
Bond lengths



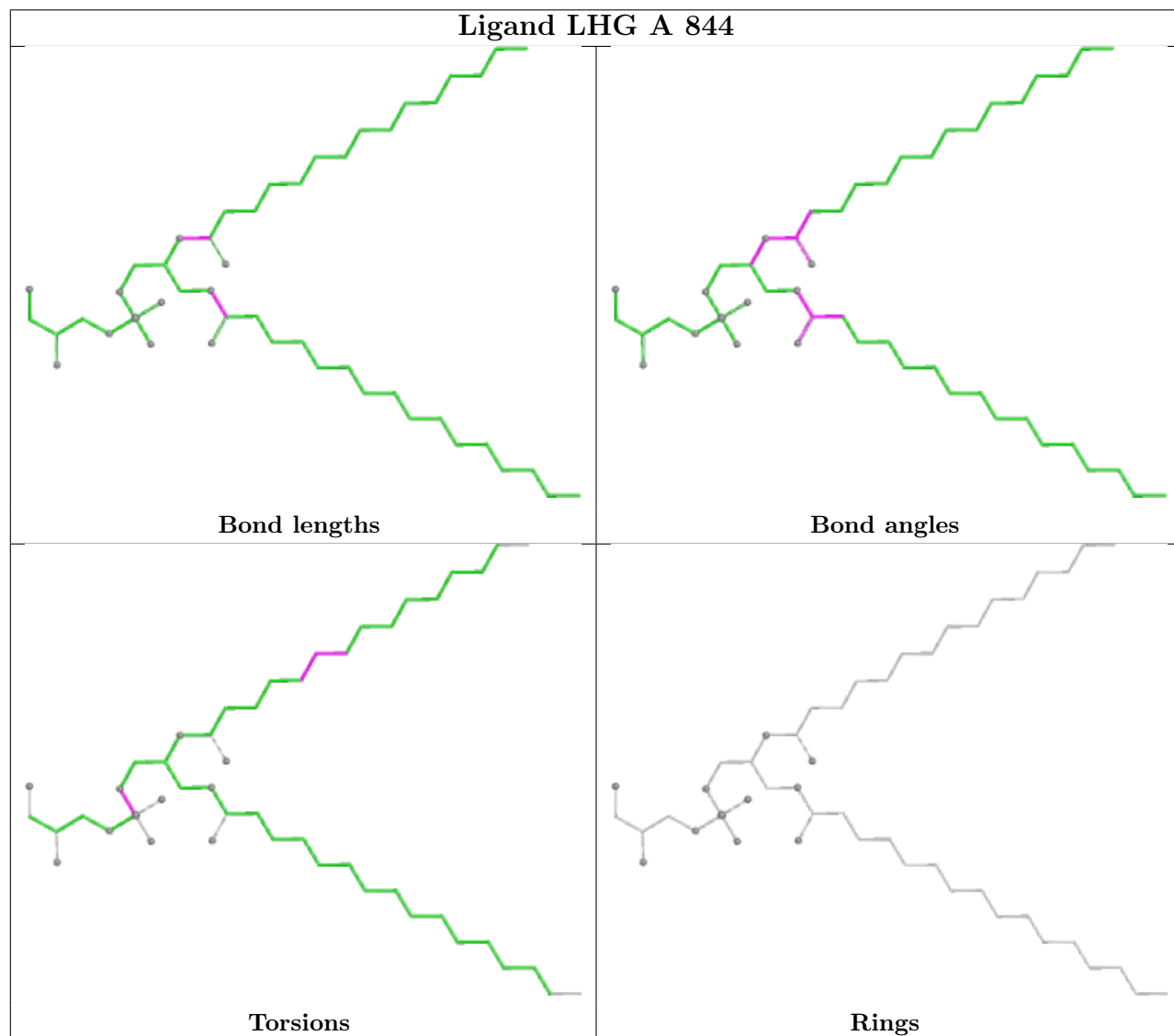
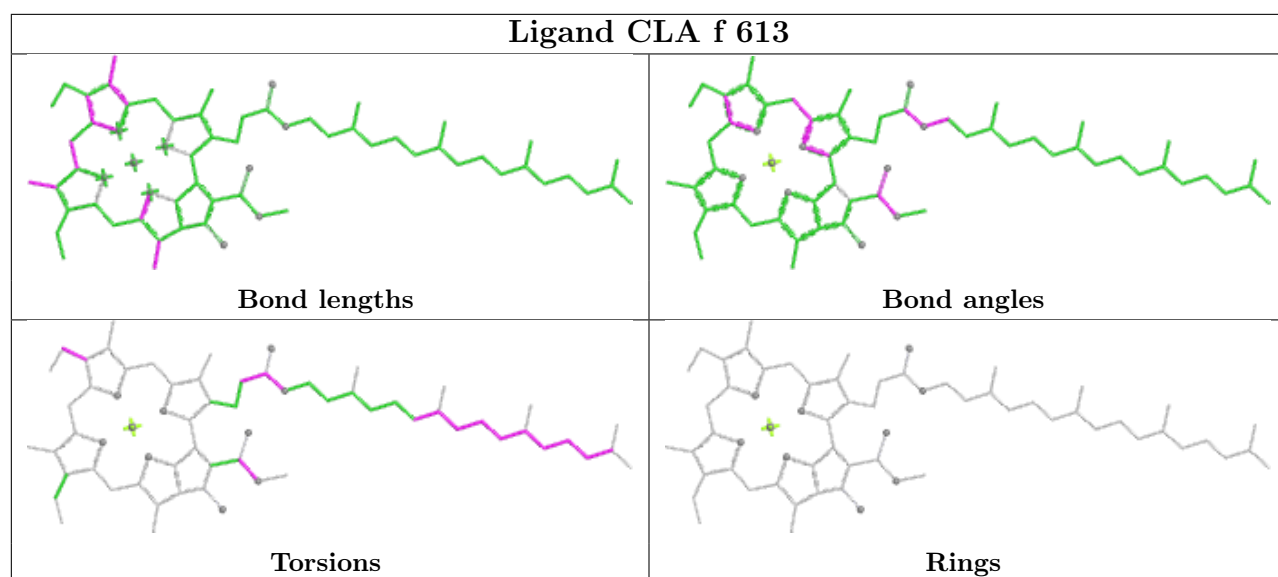
Bond angles

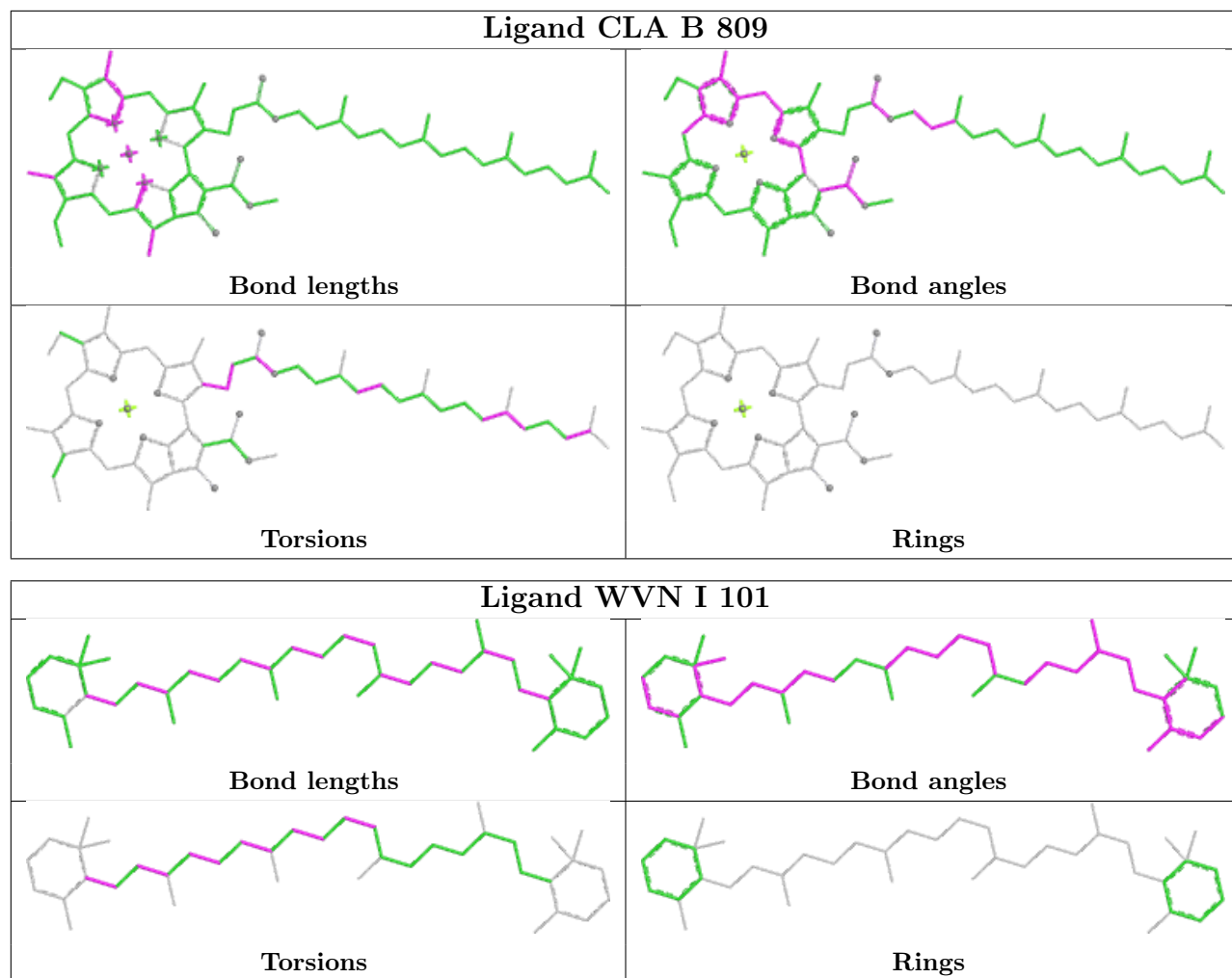


Torsions

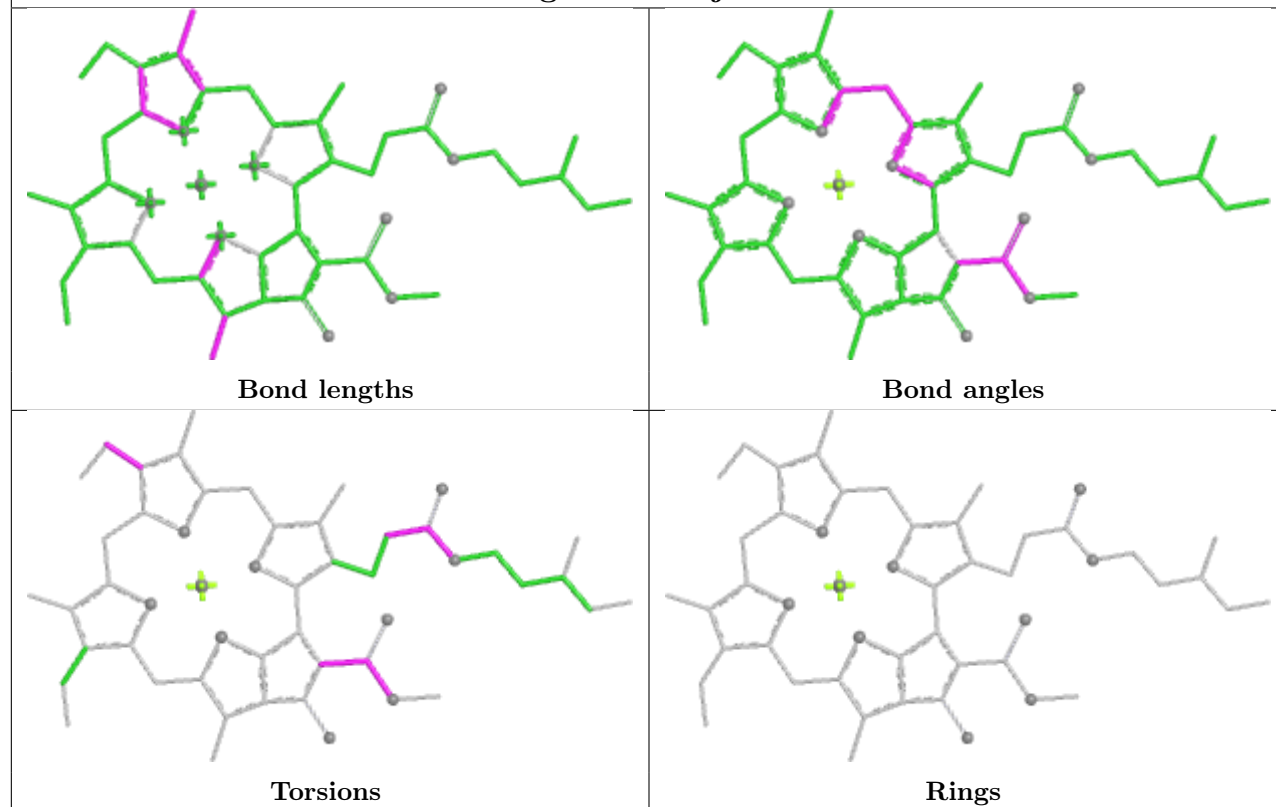


Rings

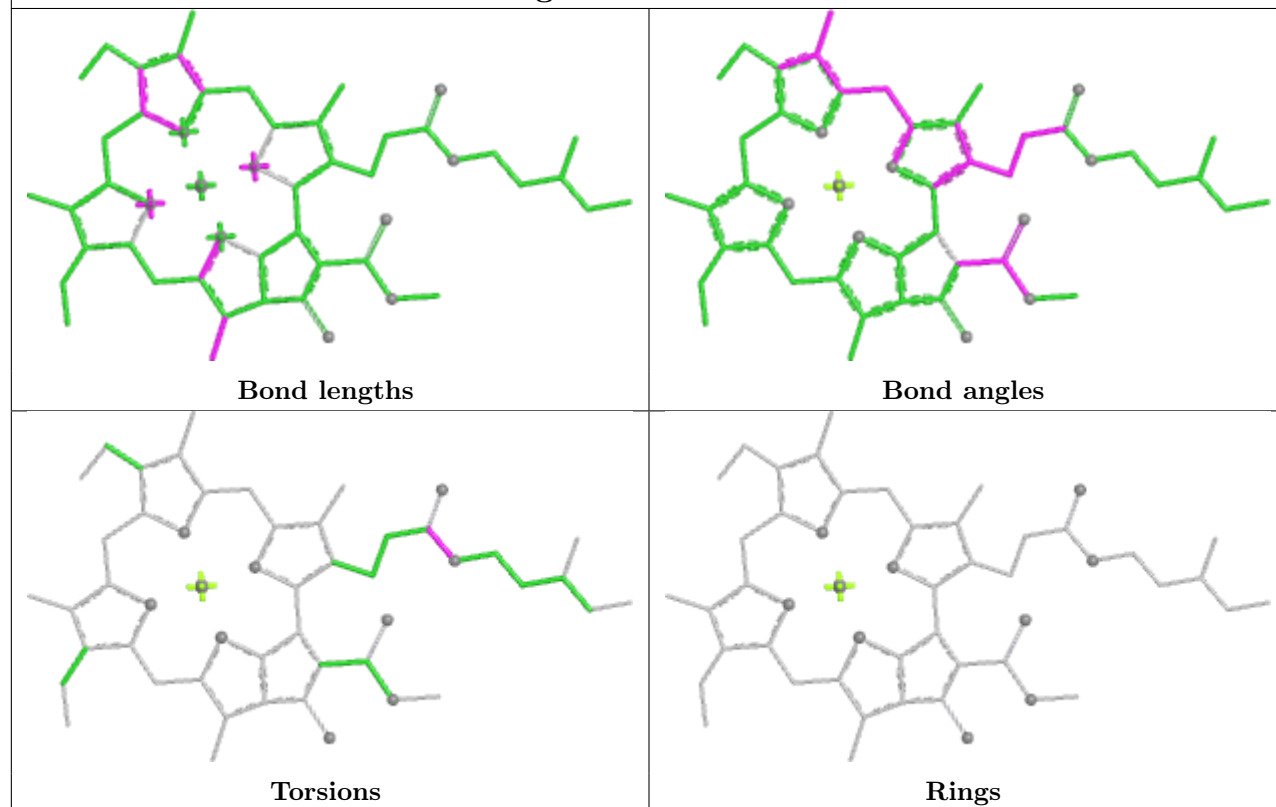




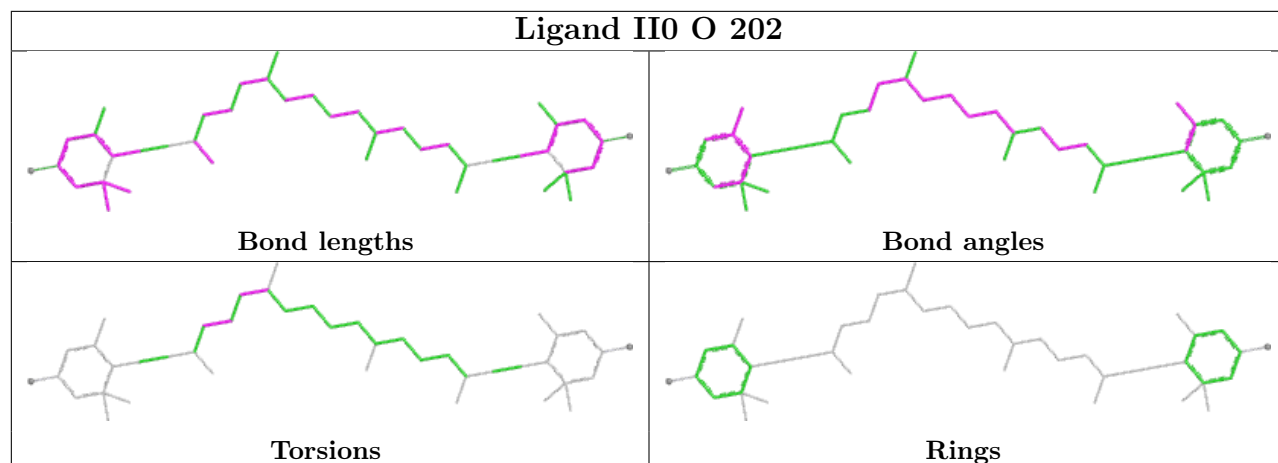
Ligand CLA j 308



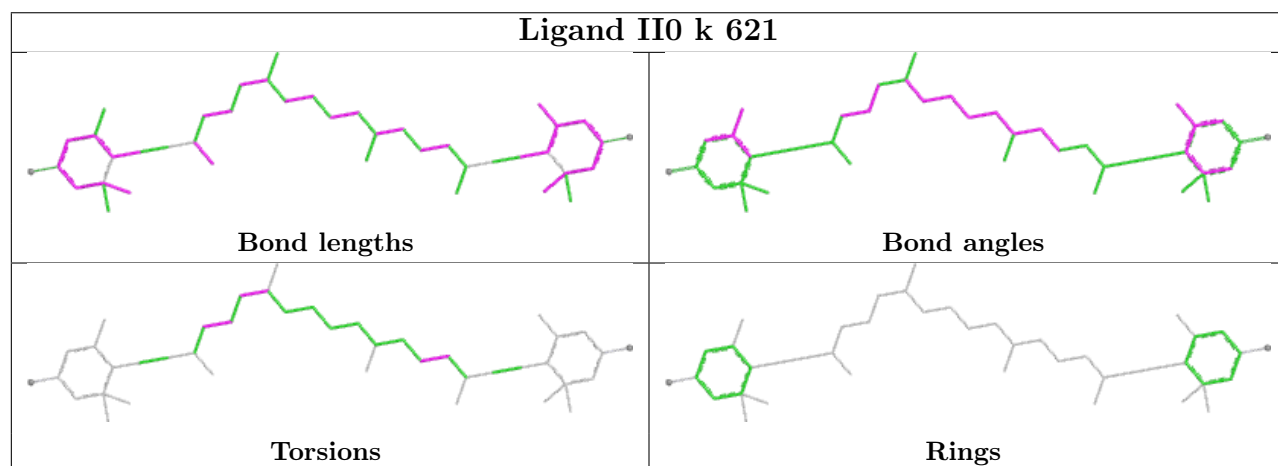
Ligand CLA k 603



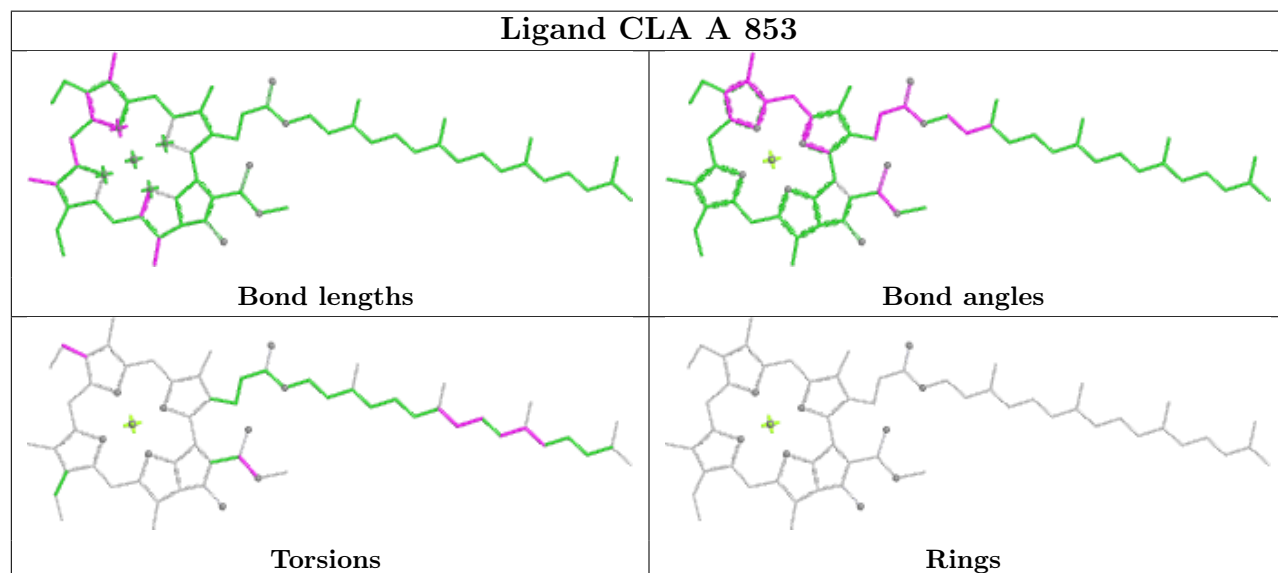
Ligand II0 O 202

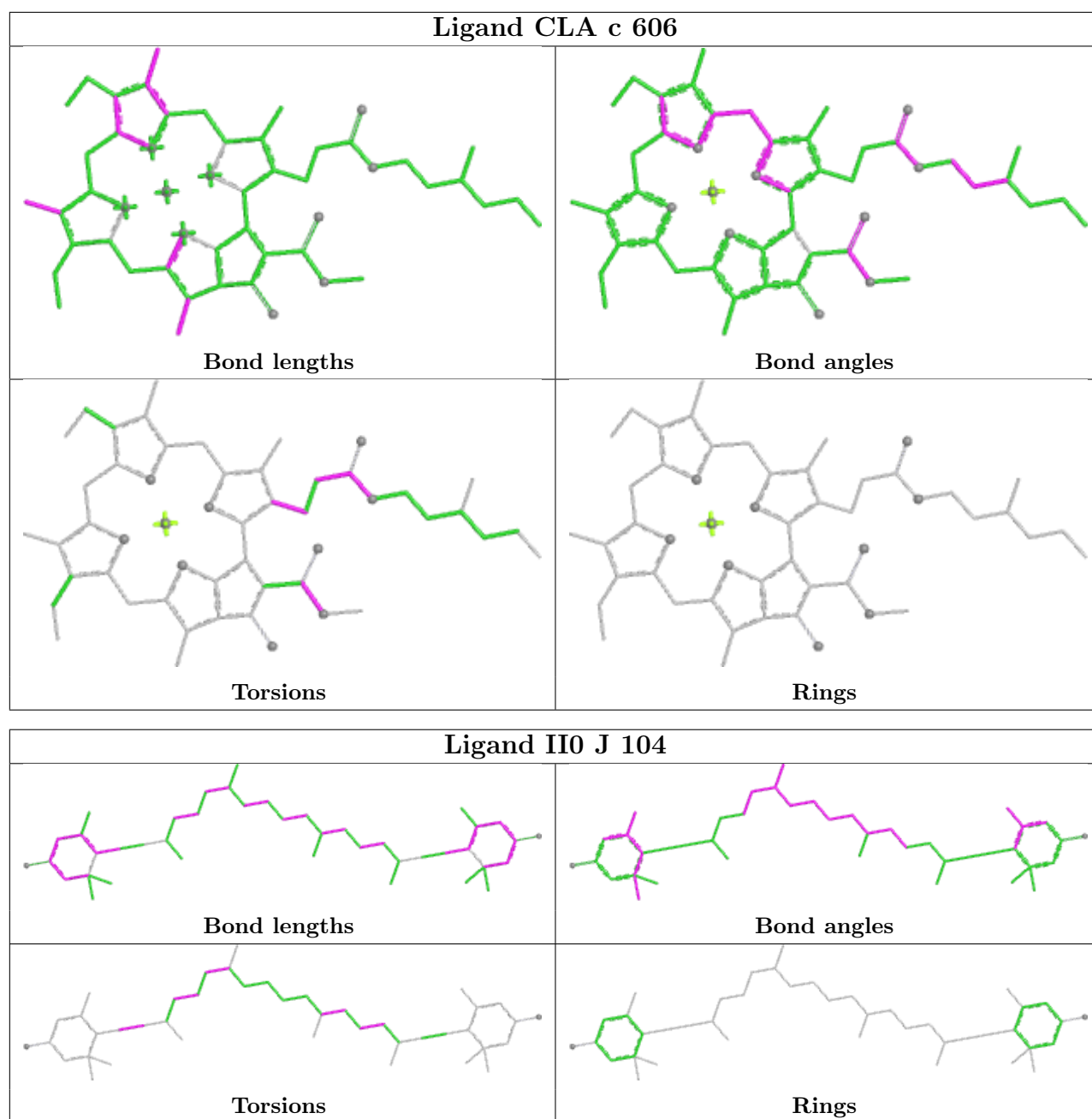


Ligand II0 k 621

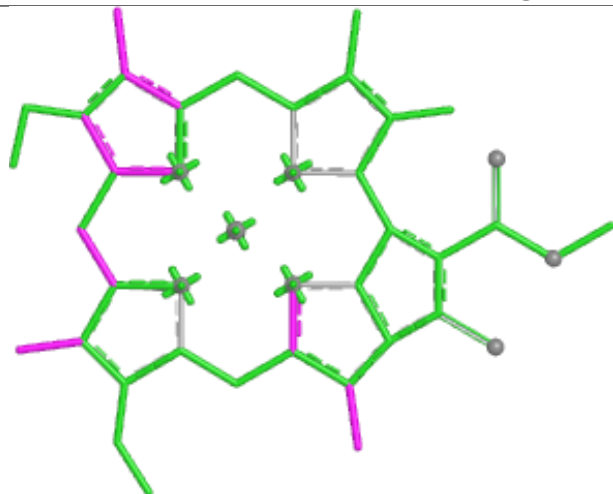


Ligand CLA A 853

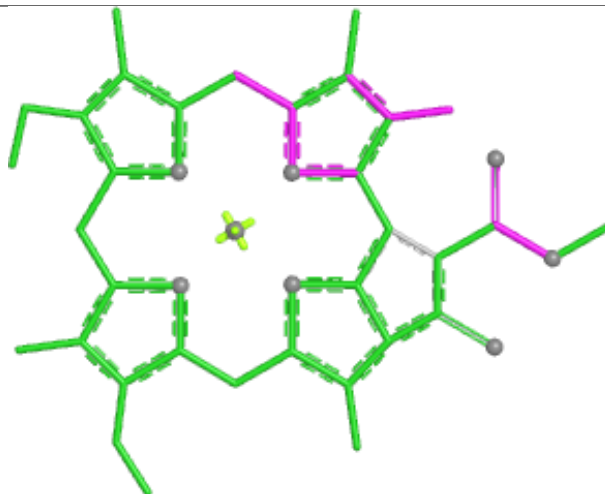




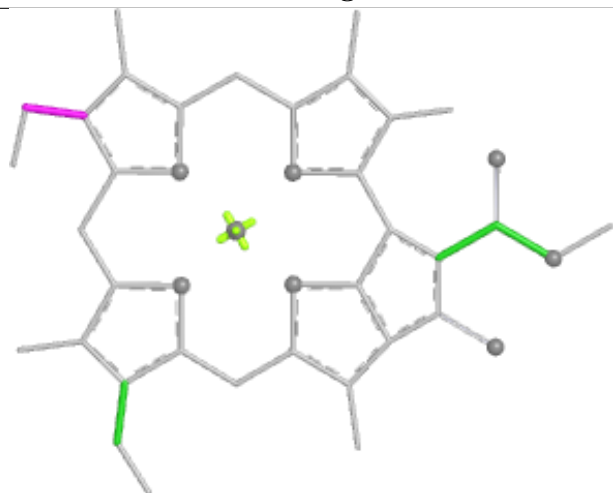
Ligand CLA d 309



Bond lengths



Bond angles

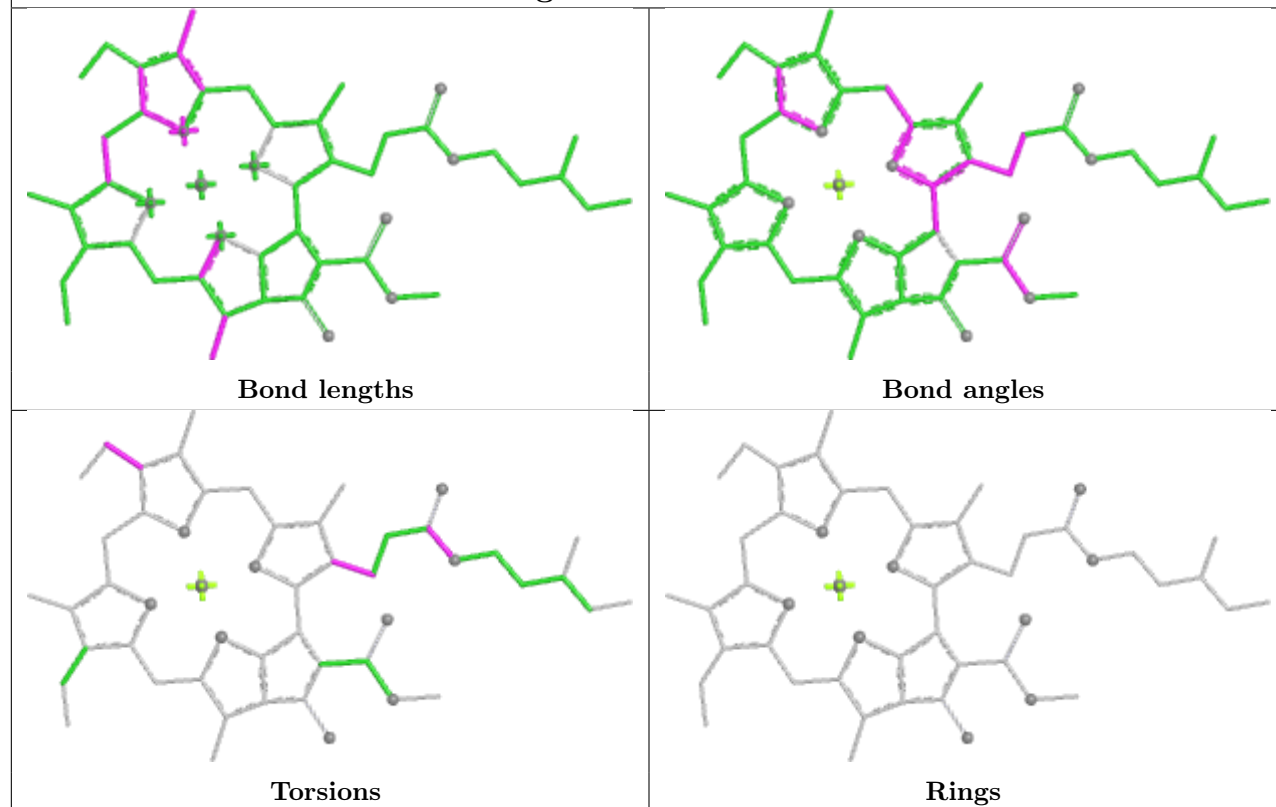


Torsions

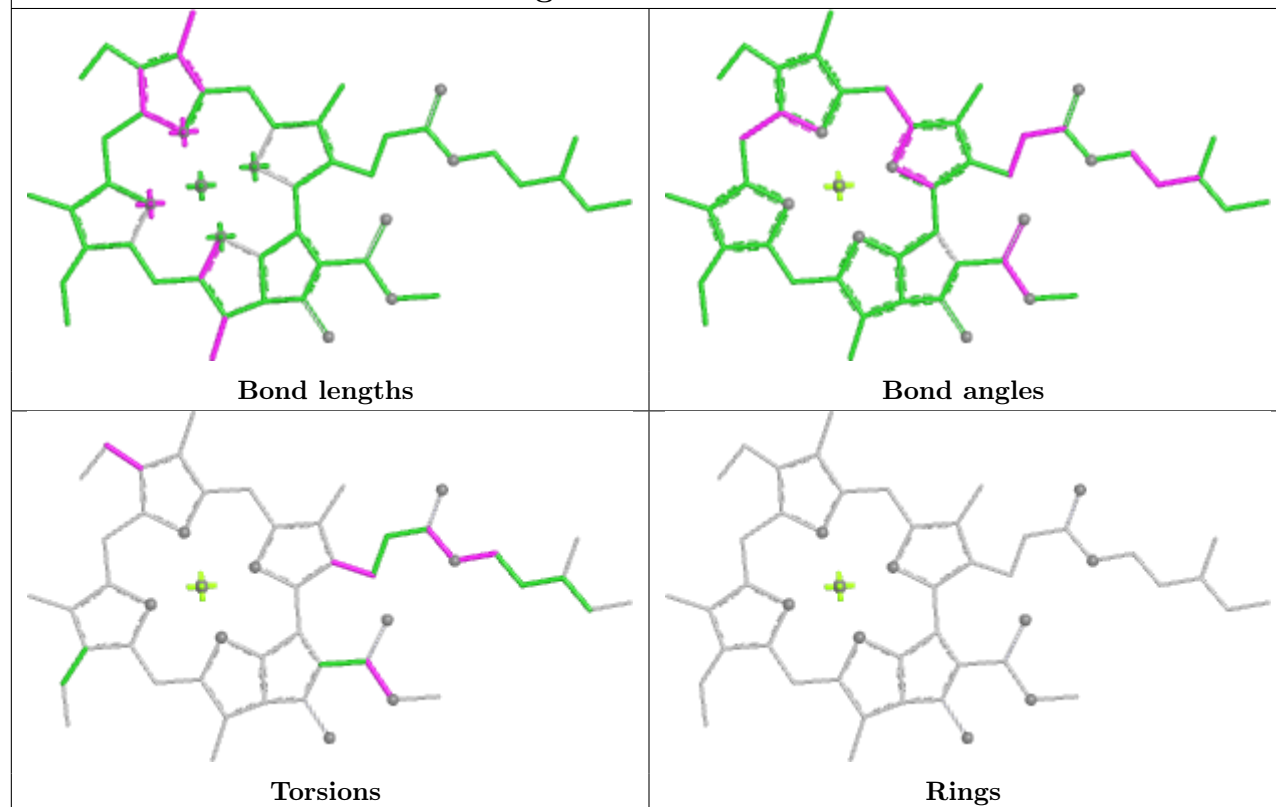


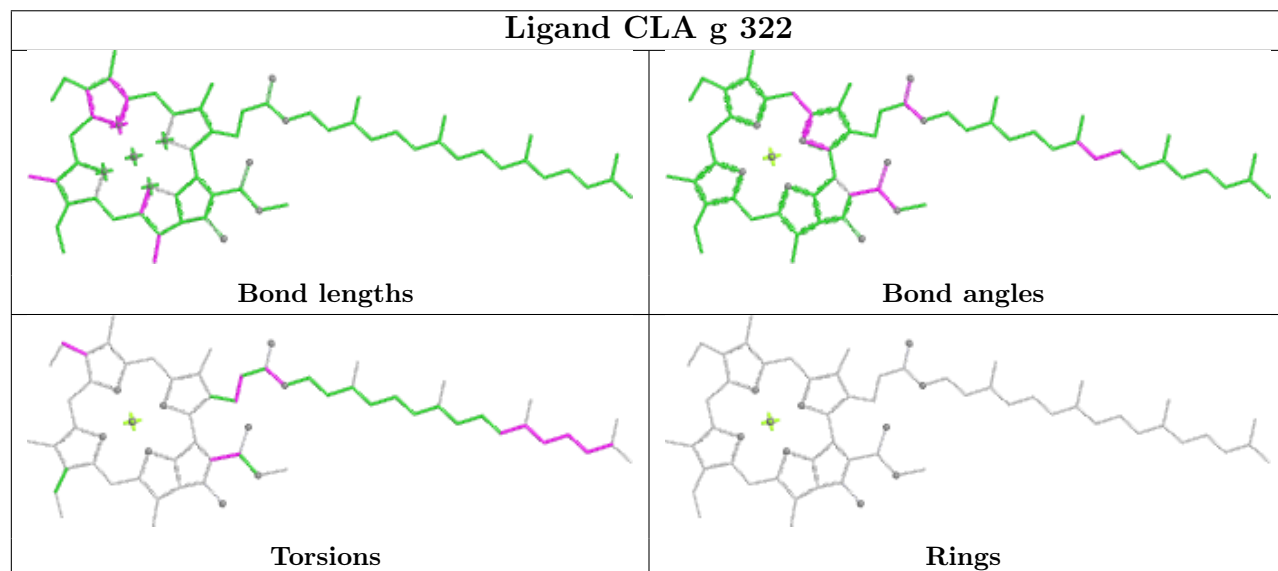
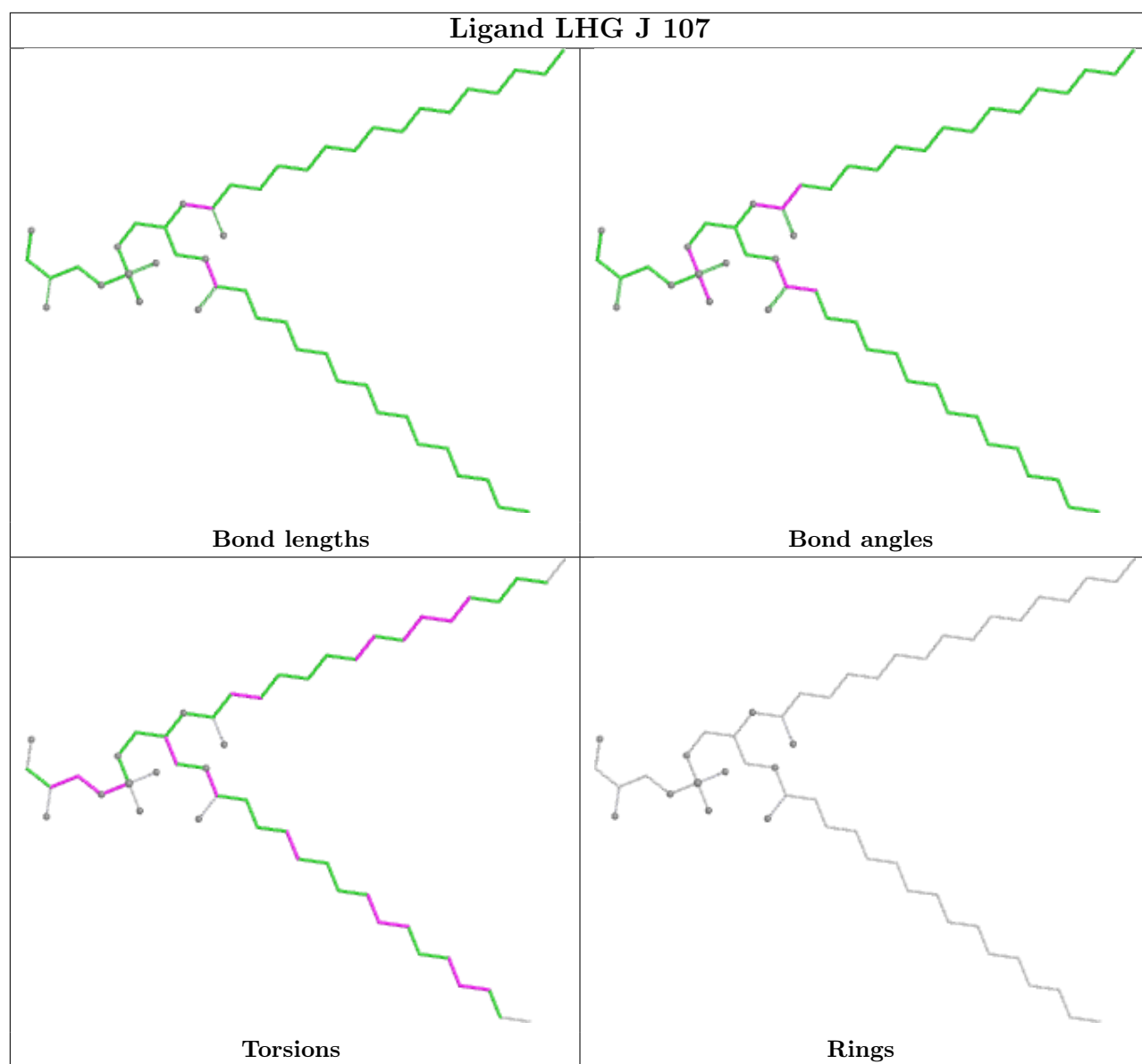
Rings

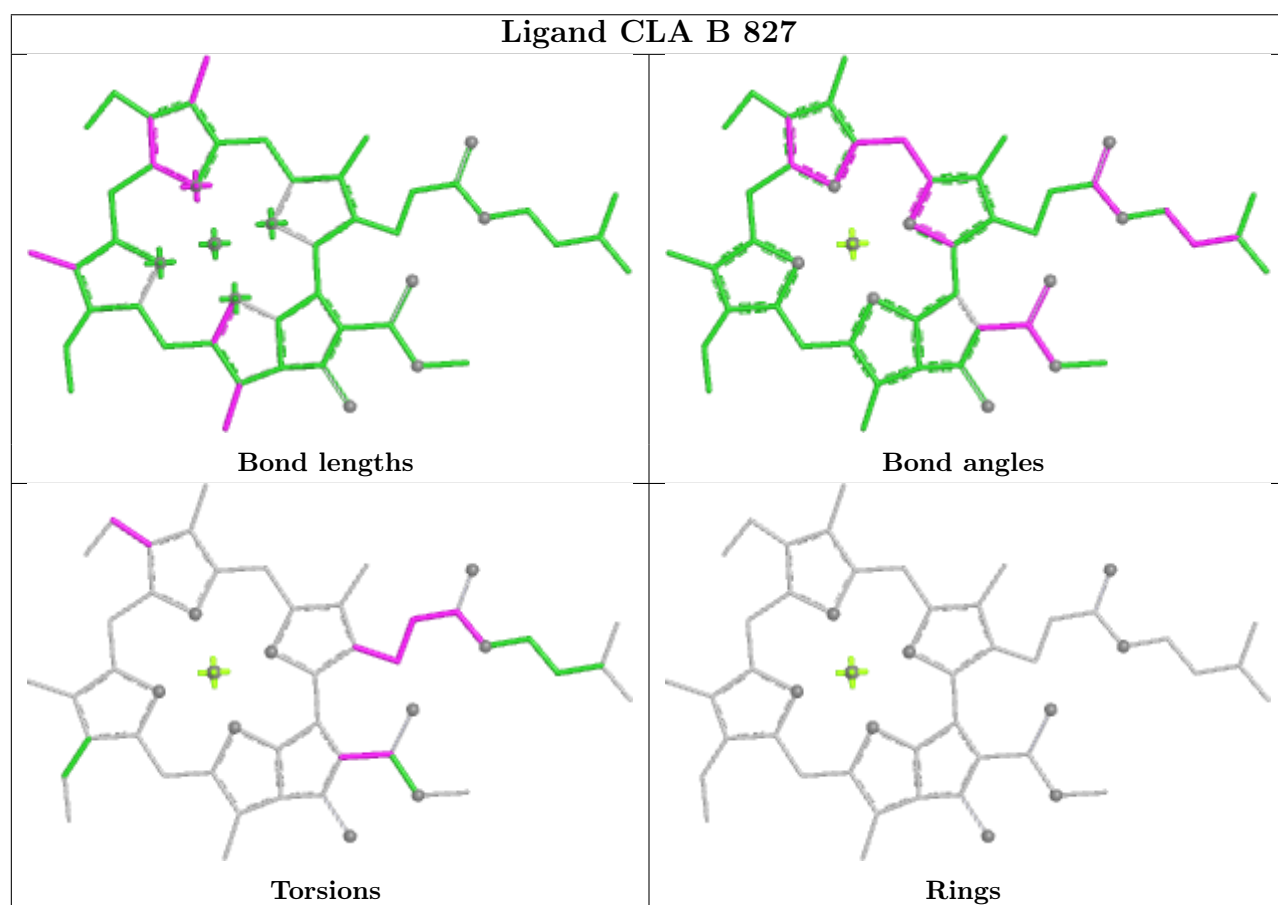
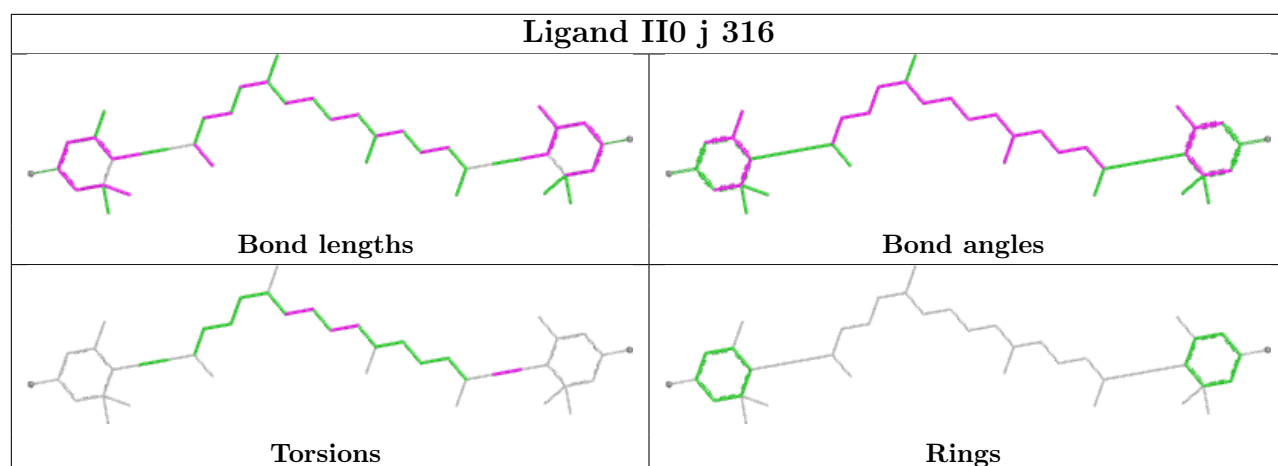
Ligand CLA J 105

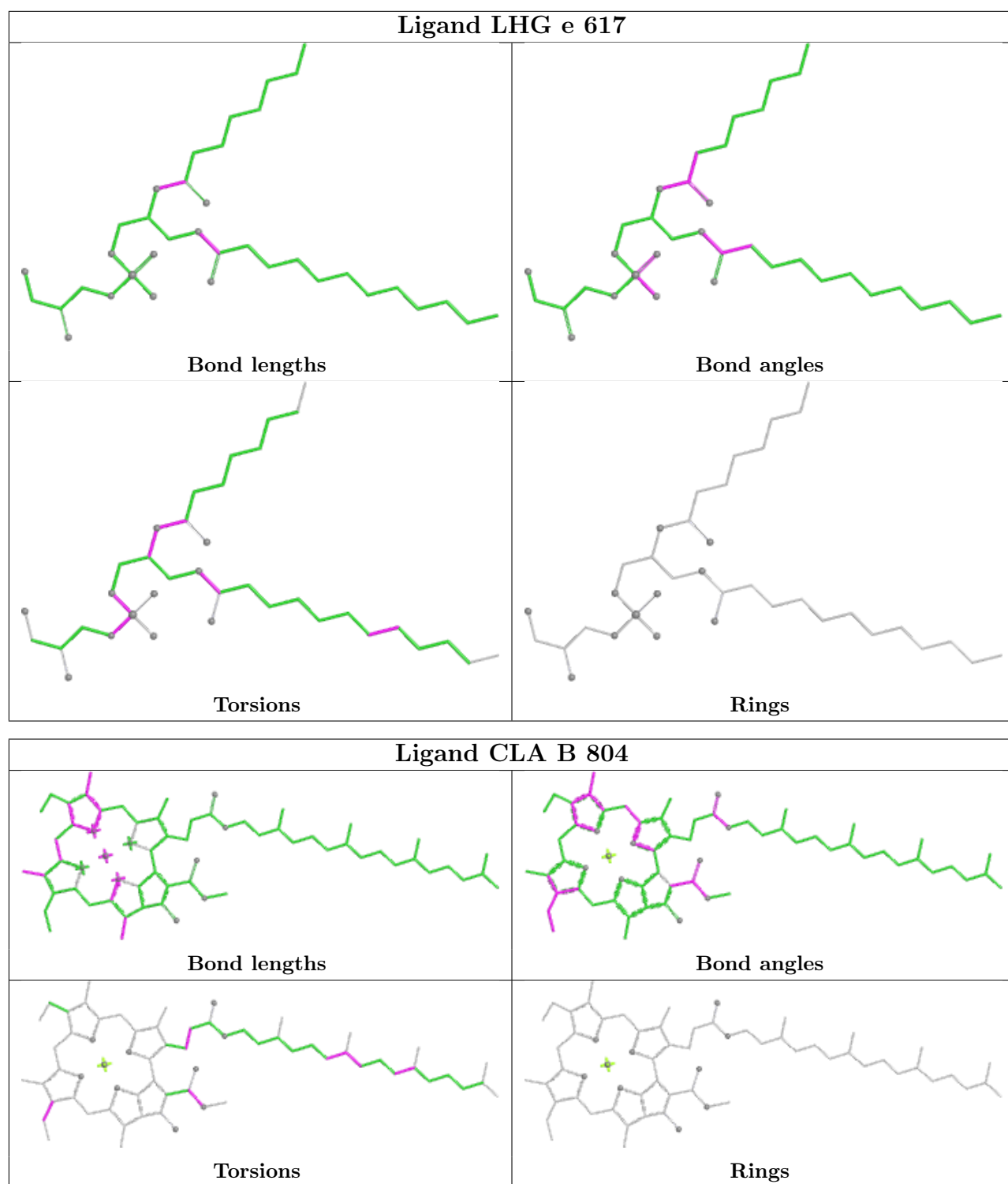


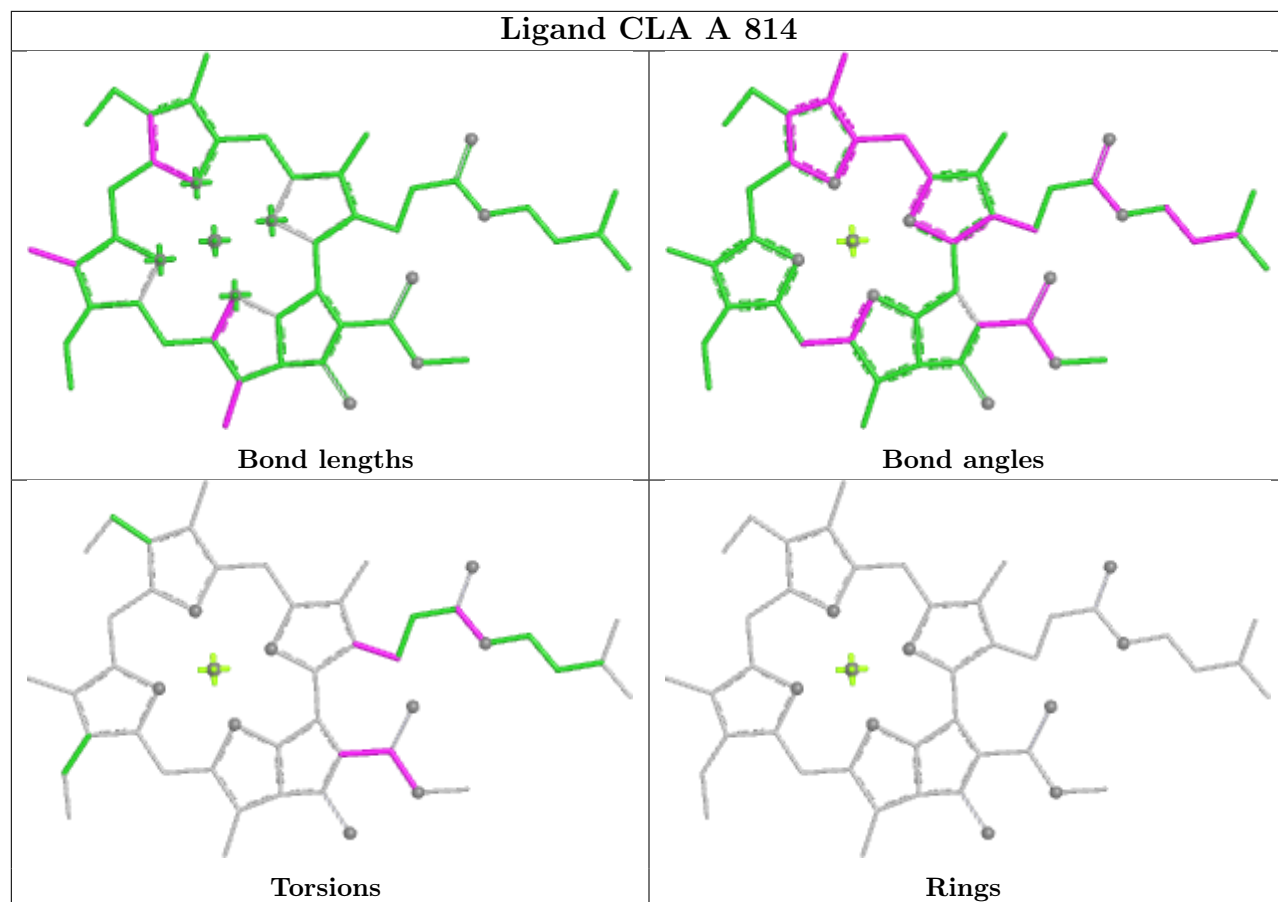
Ligand CLA k 601



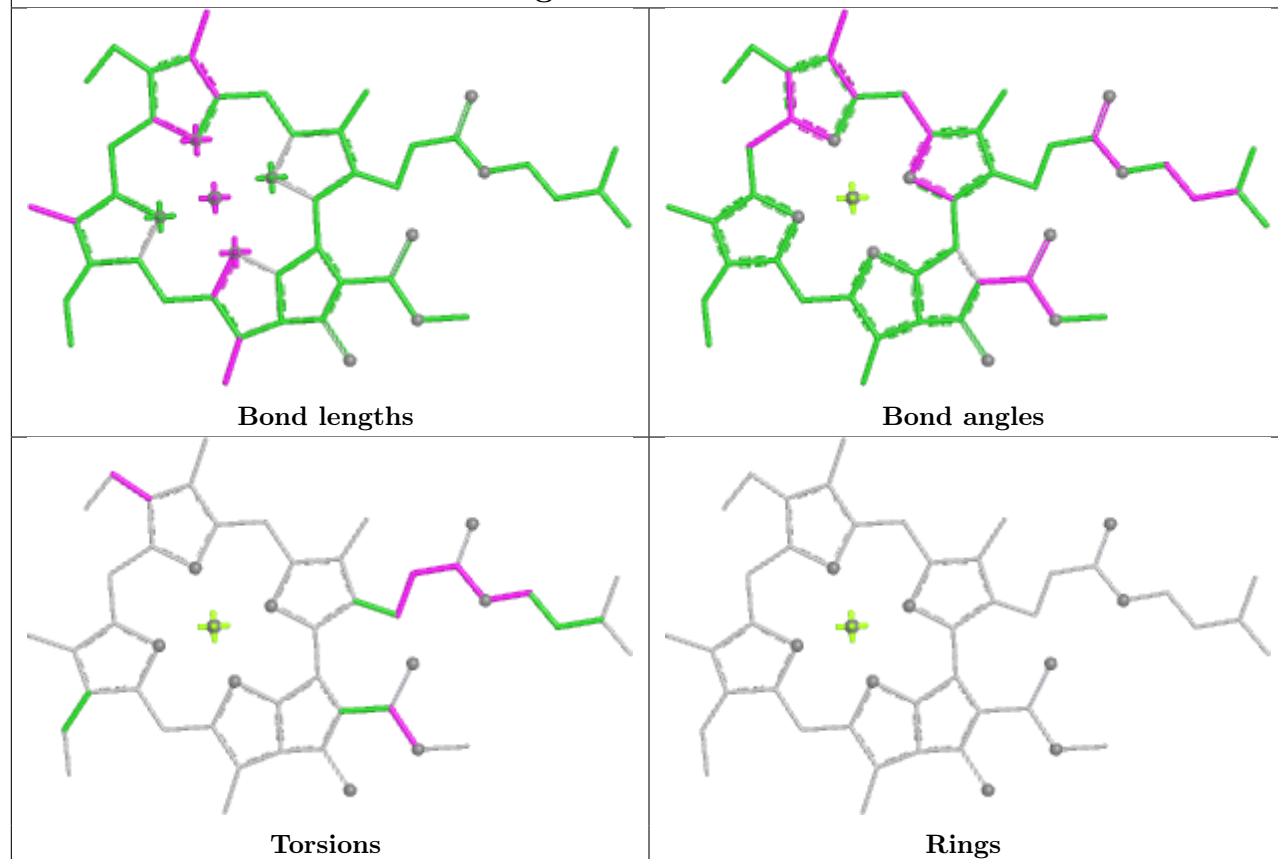




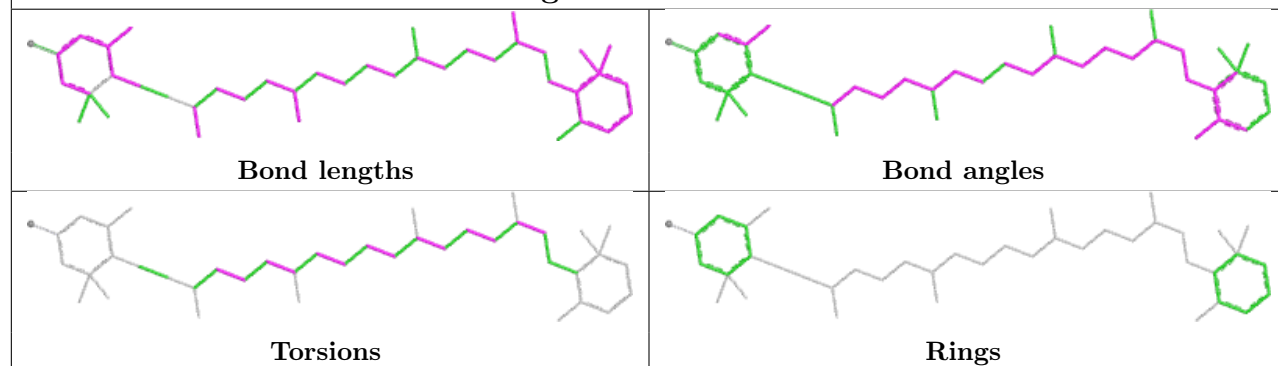




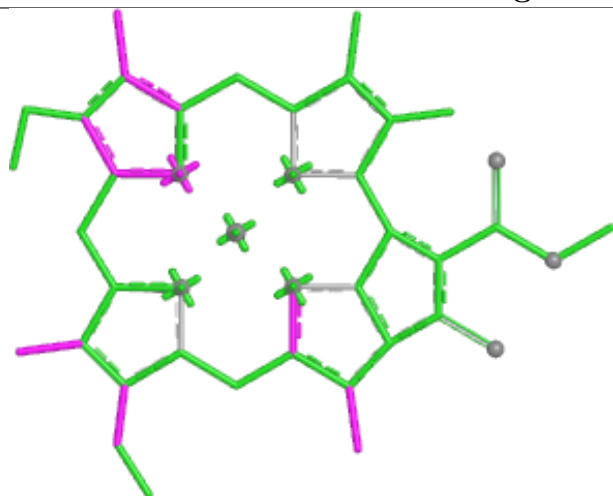
Ligand CLA h 302



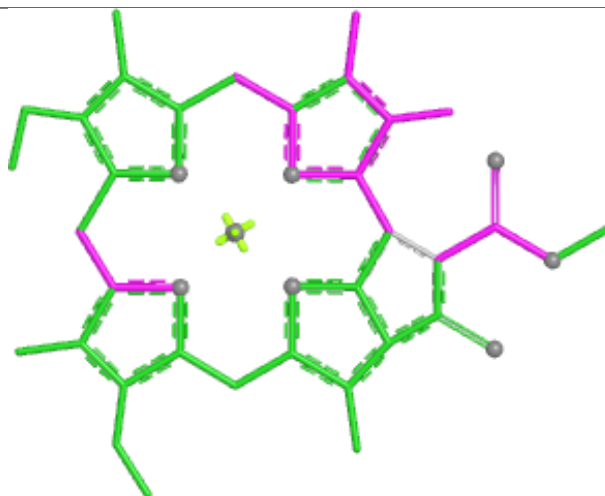
Ligand IHT c 615



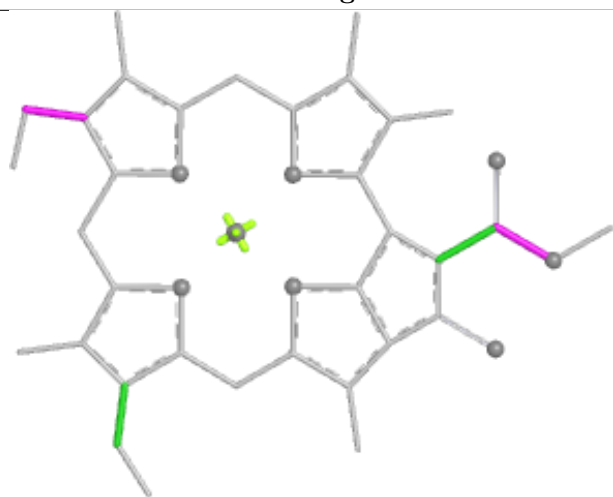
Ligand CLA A 856



Bond lengths



Bond angles

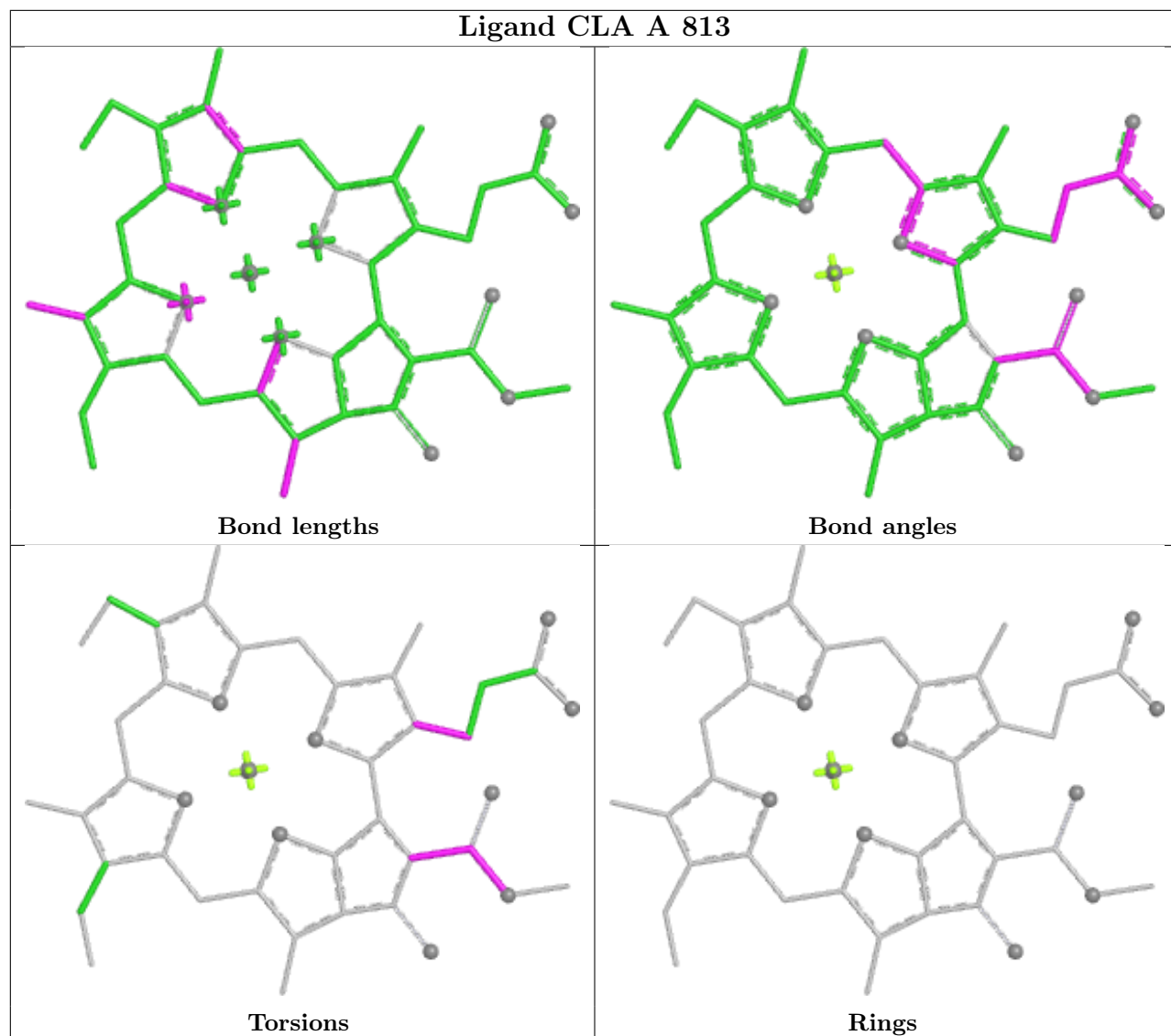


Torsions

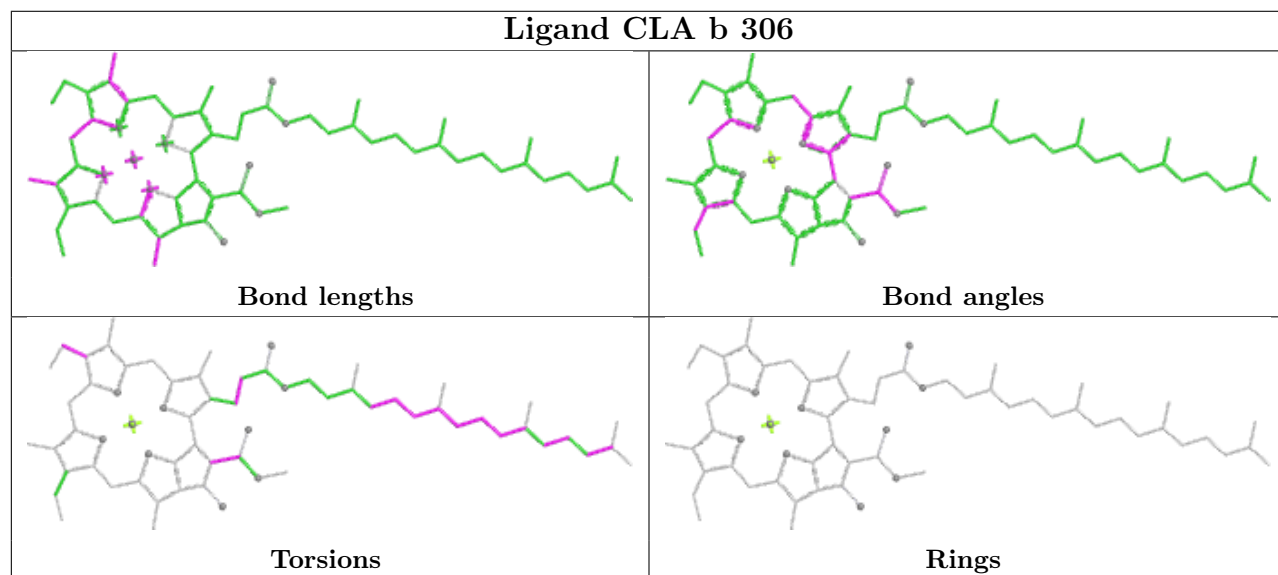


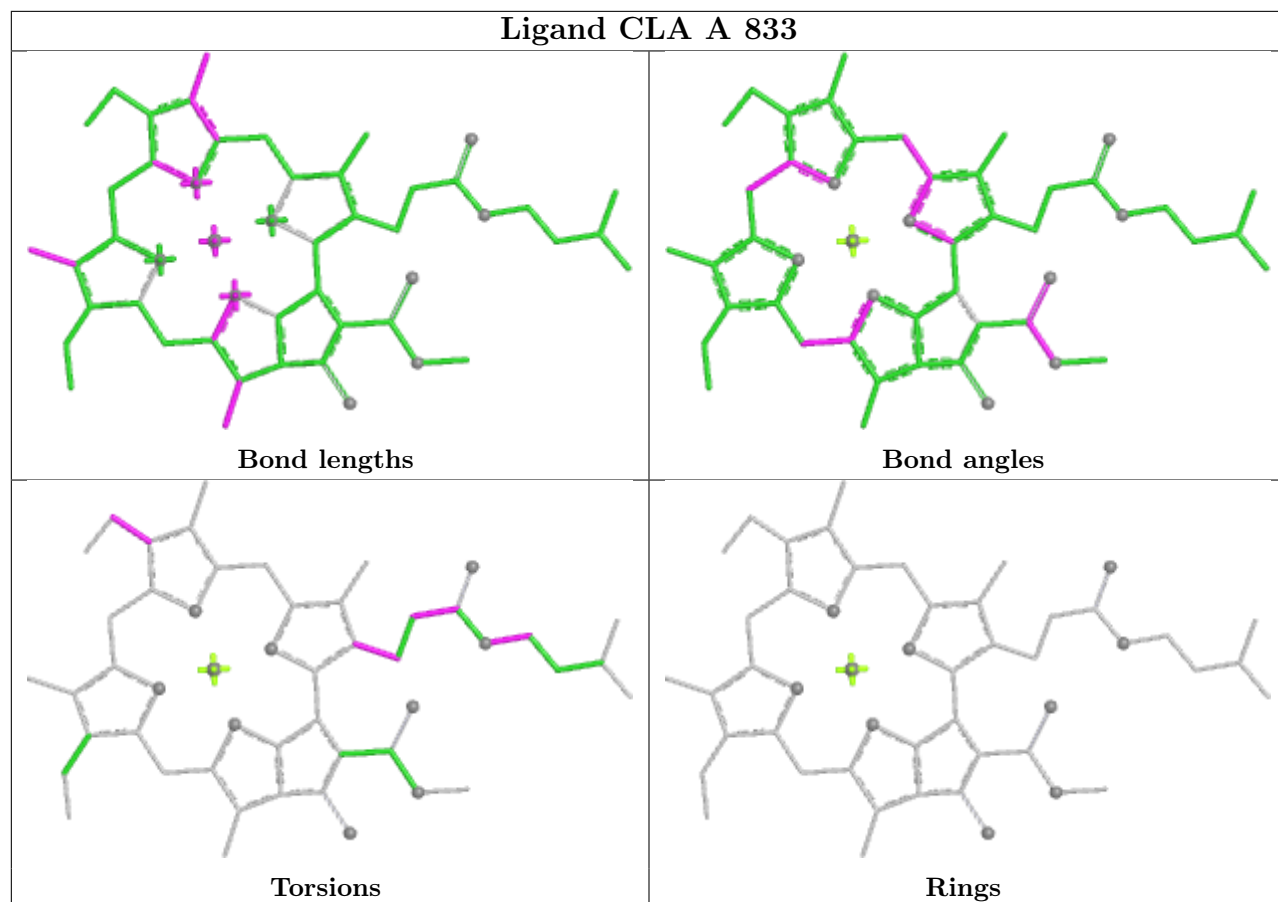
Rings

Ligand CLA A 813

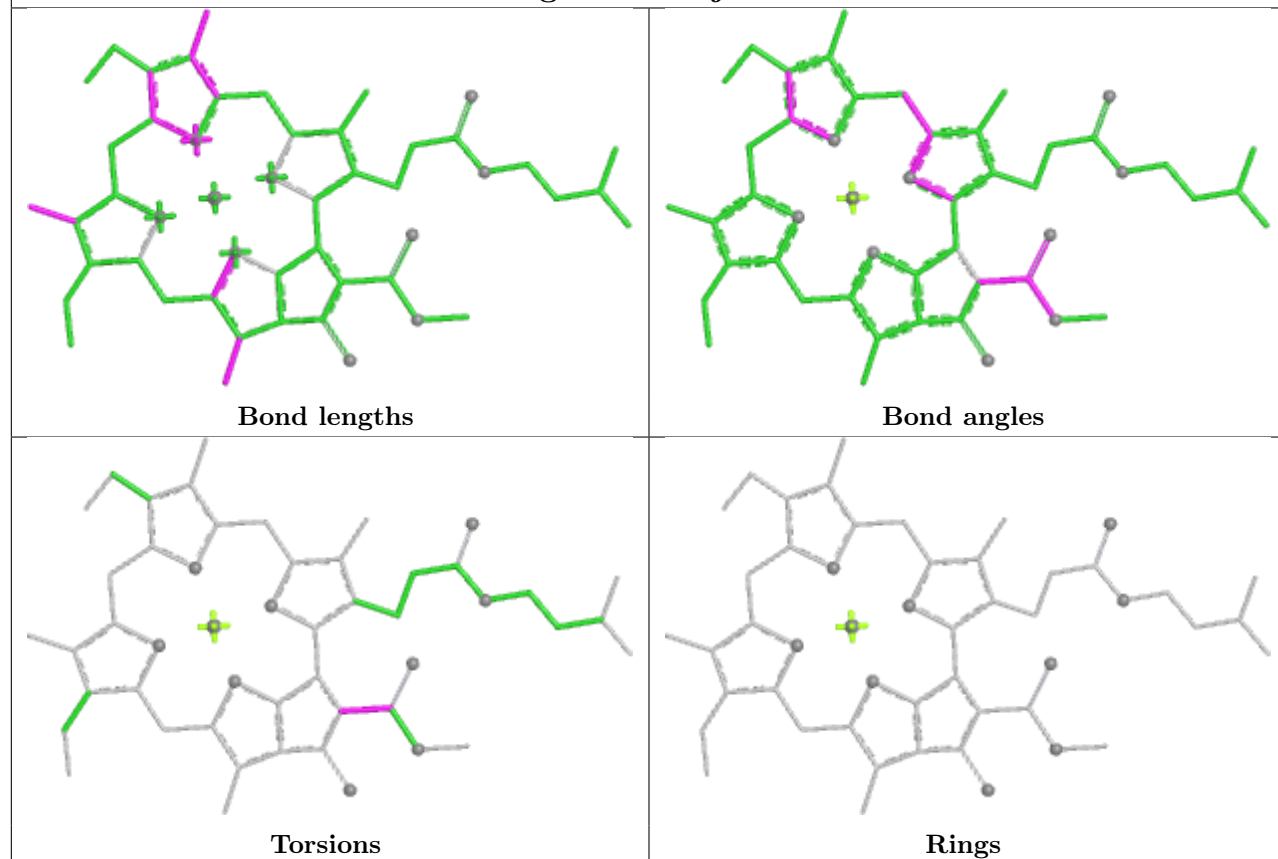


Ligand CLA b 306

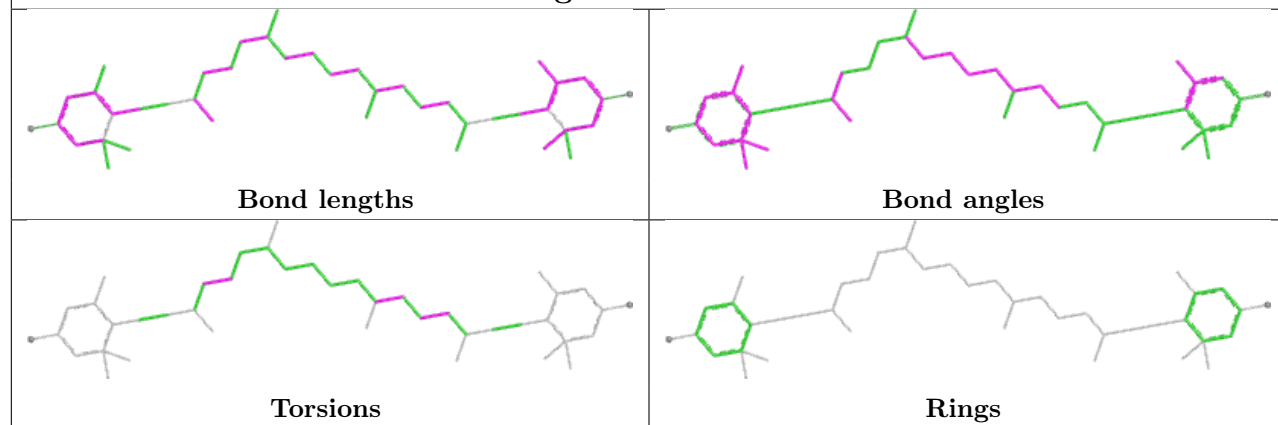




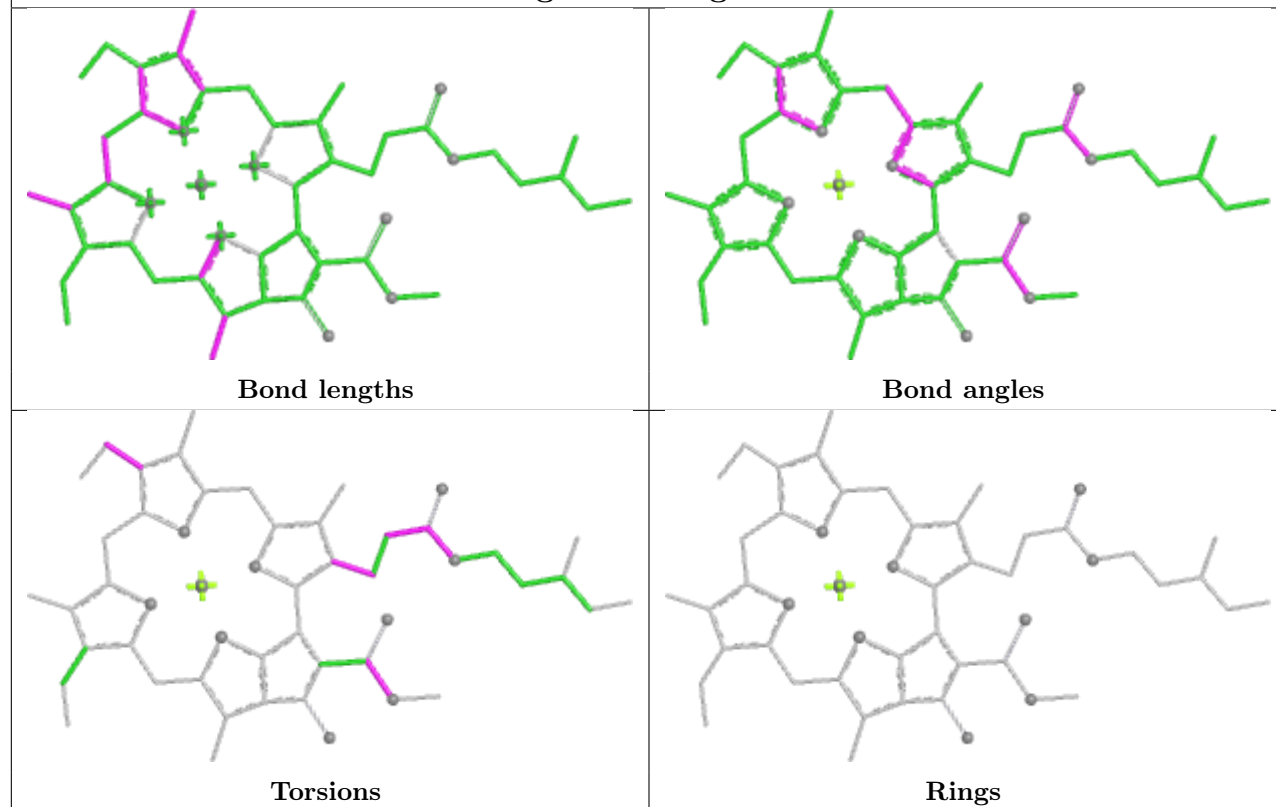
Ligand CLA j 303



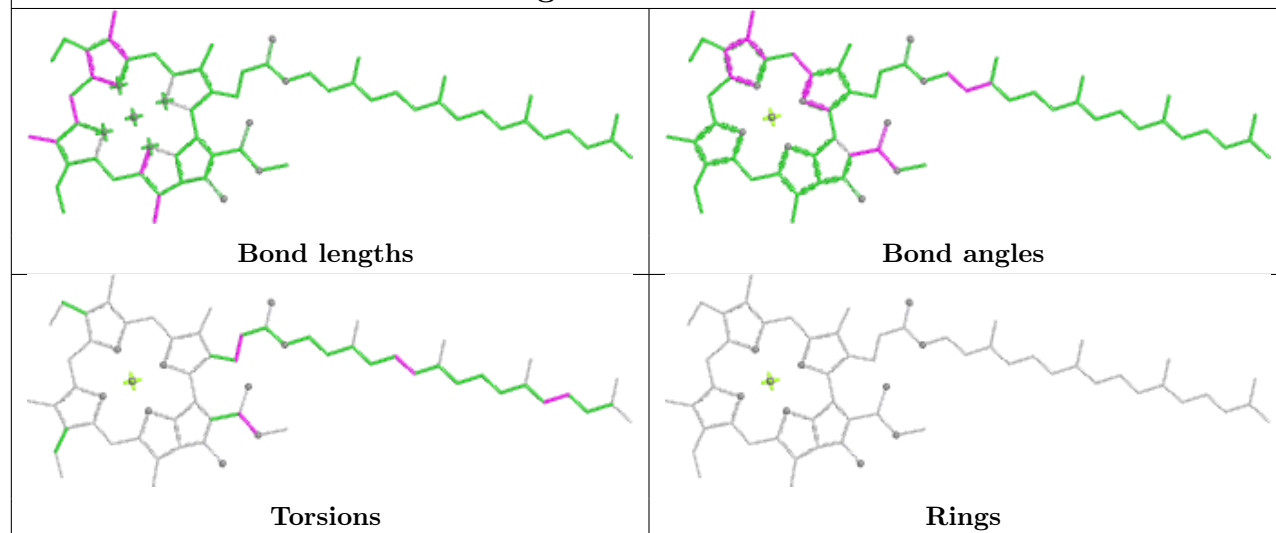
Ligand II0 i 614

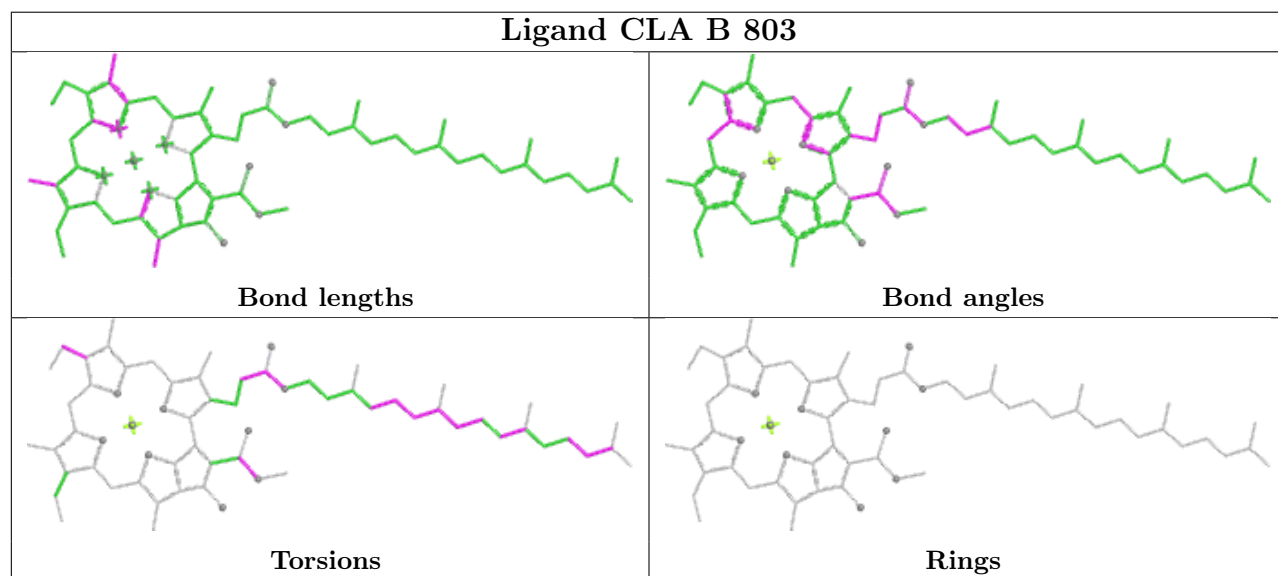
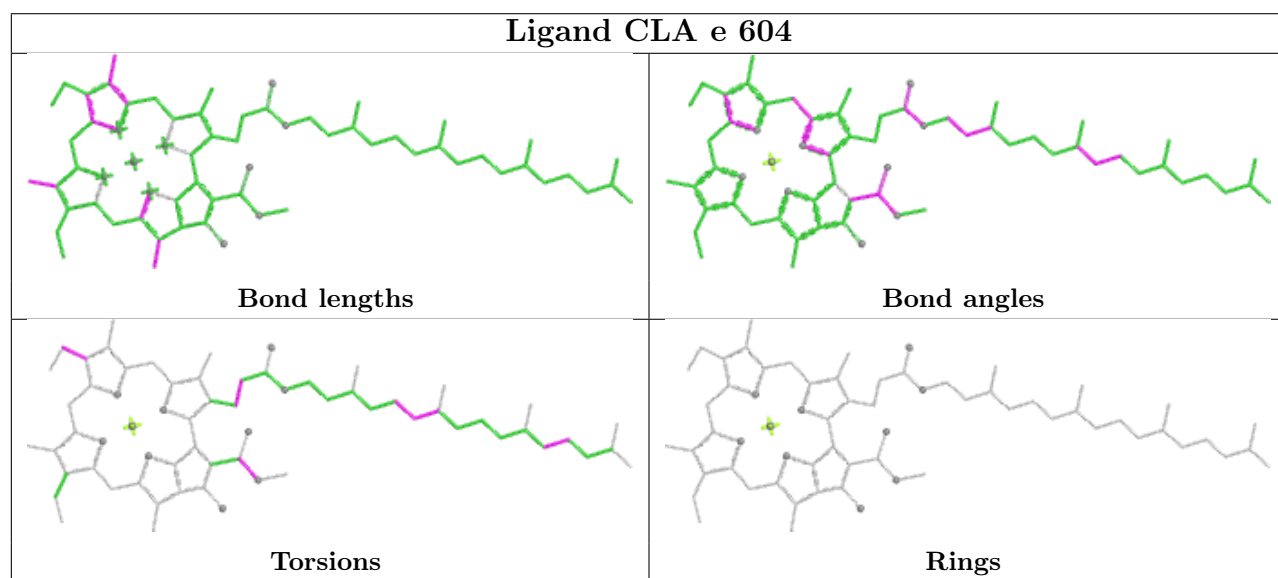
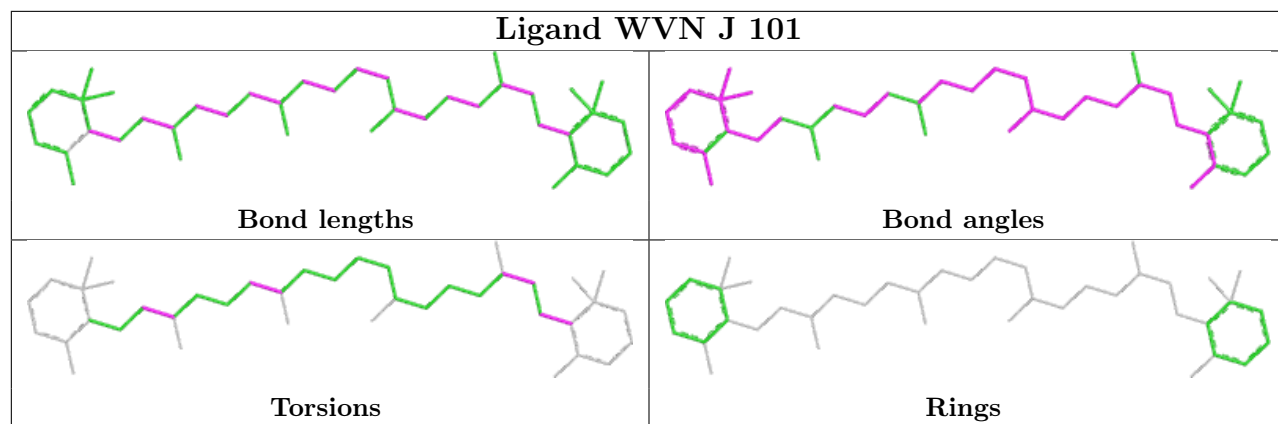


Ligand CLA g 306

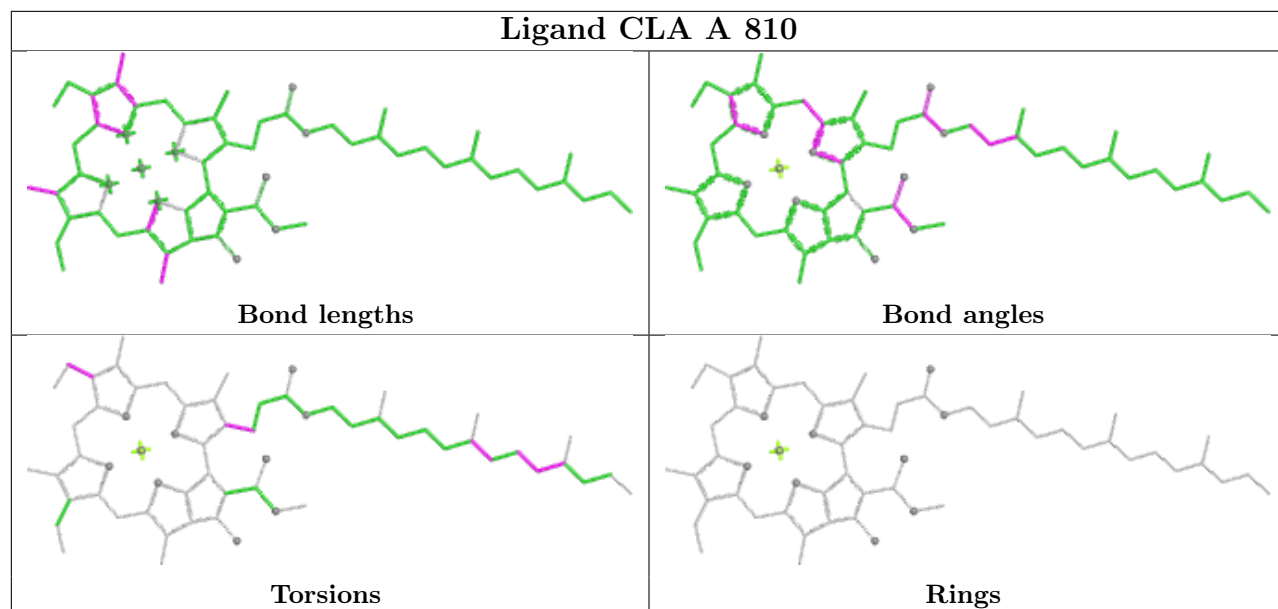


Ligand CLA c 604

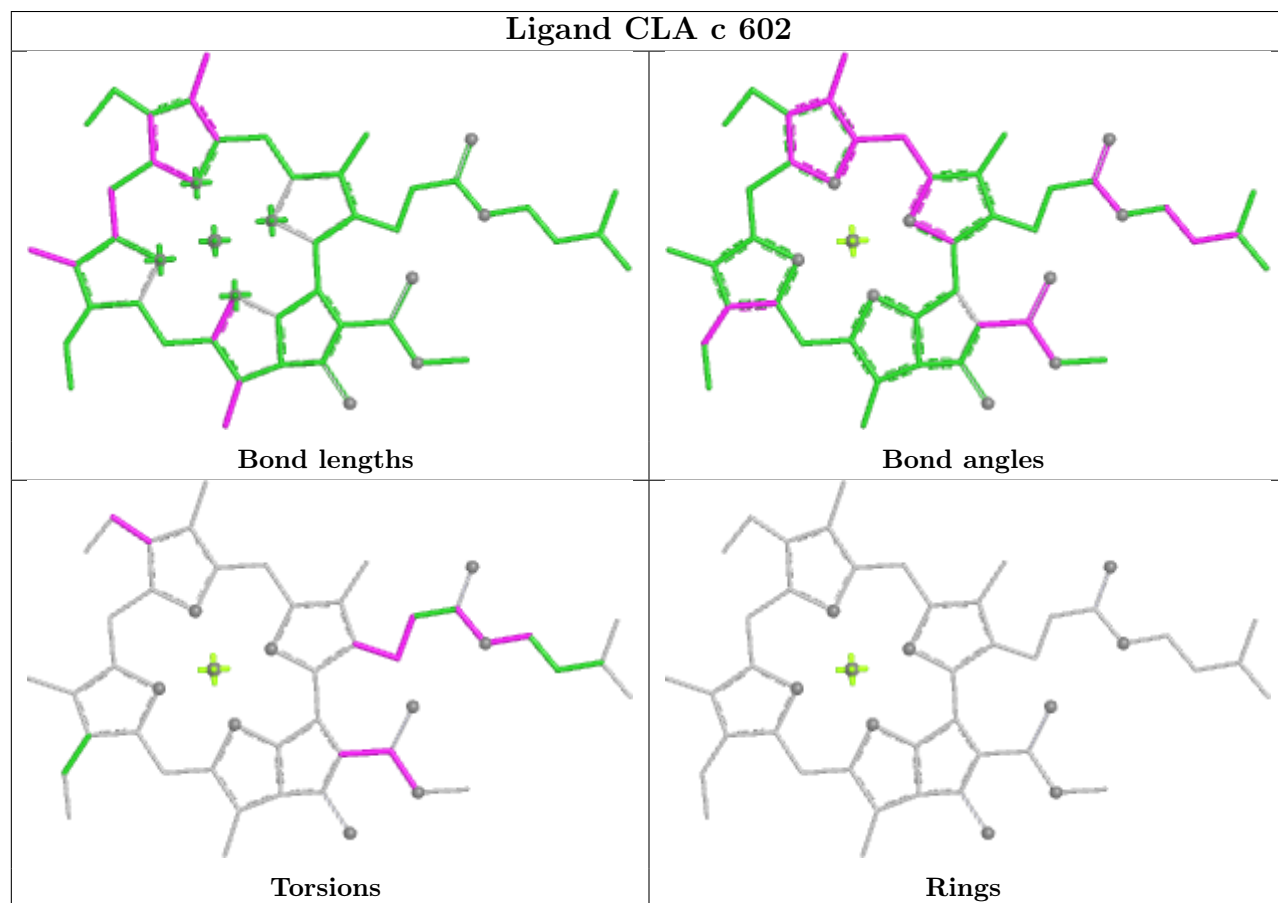




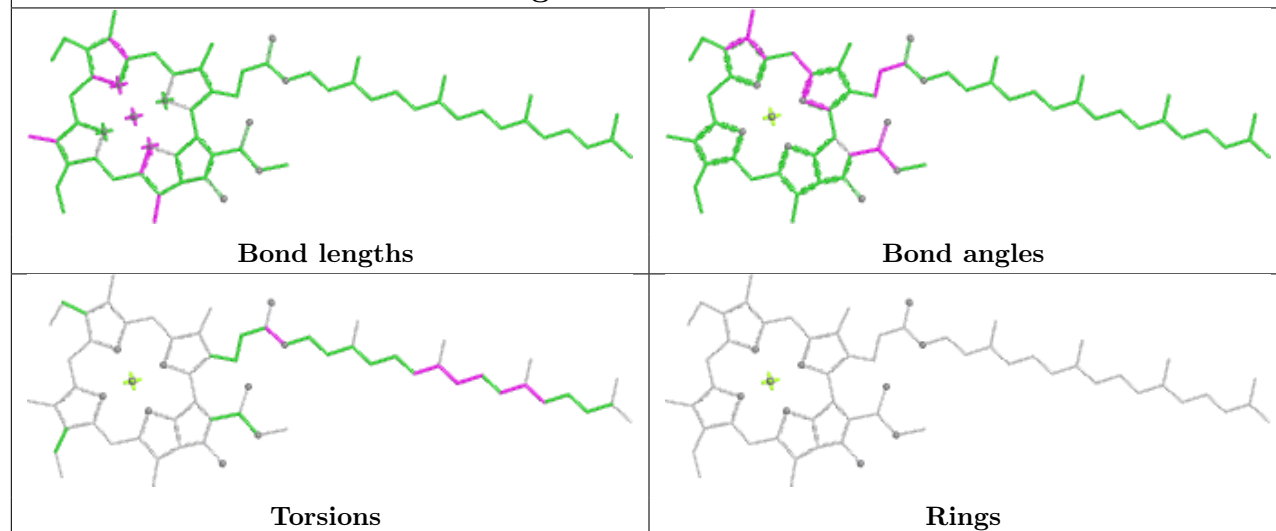
Ligand CLA A 810



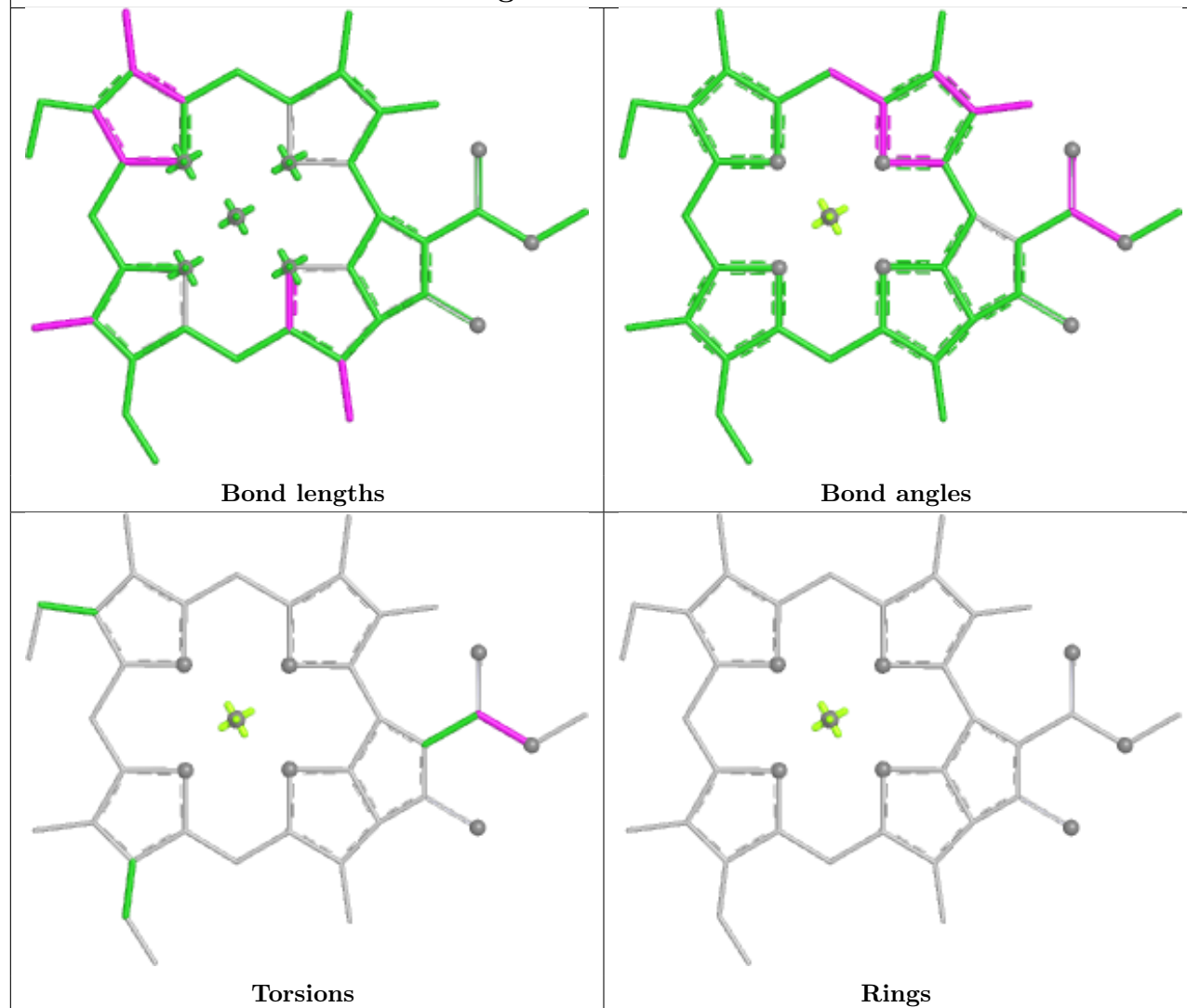
Ligand CLA c 602



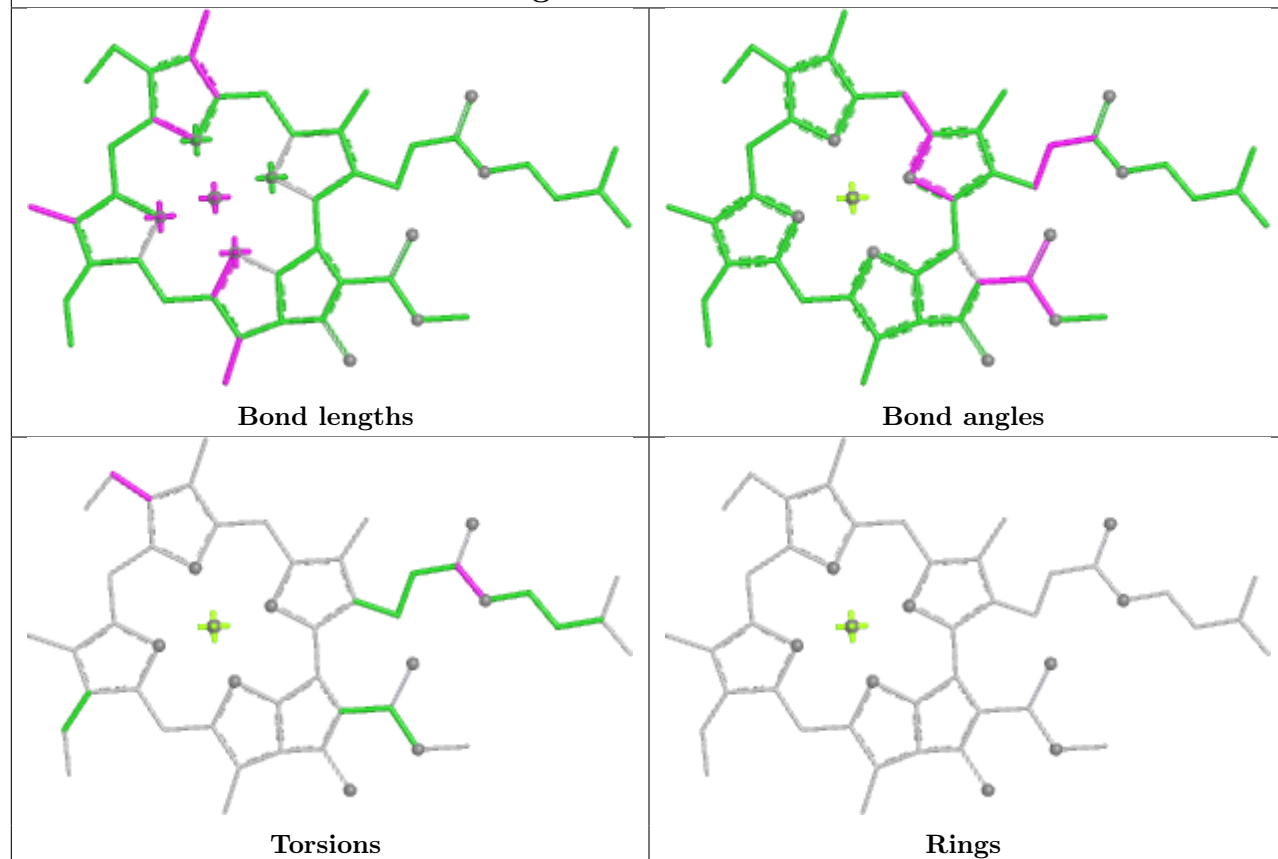
Ligand CLA A 825



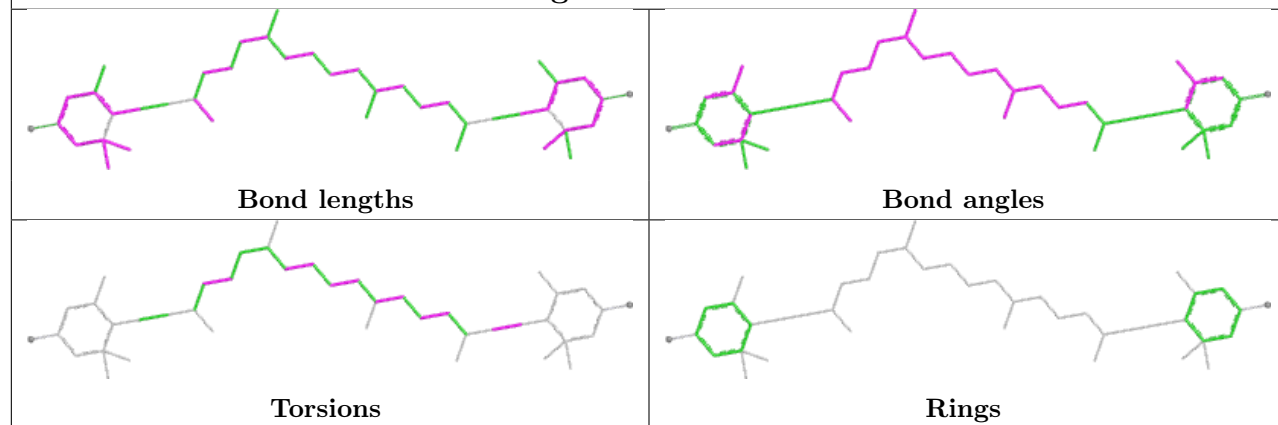
Ligand CLA d 308



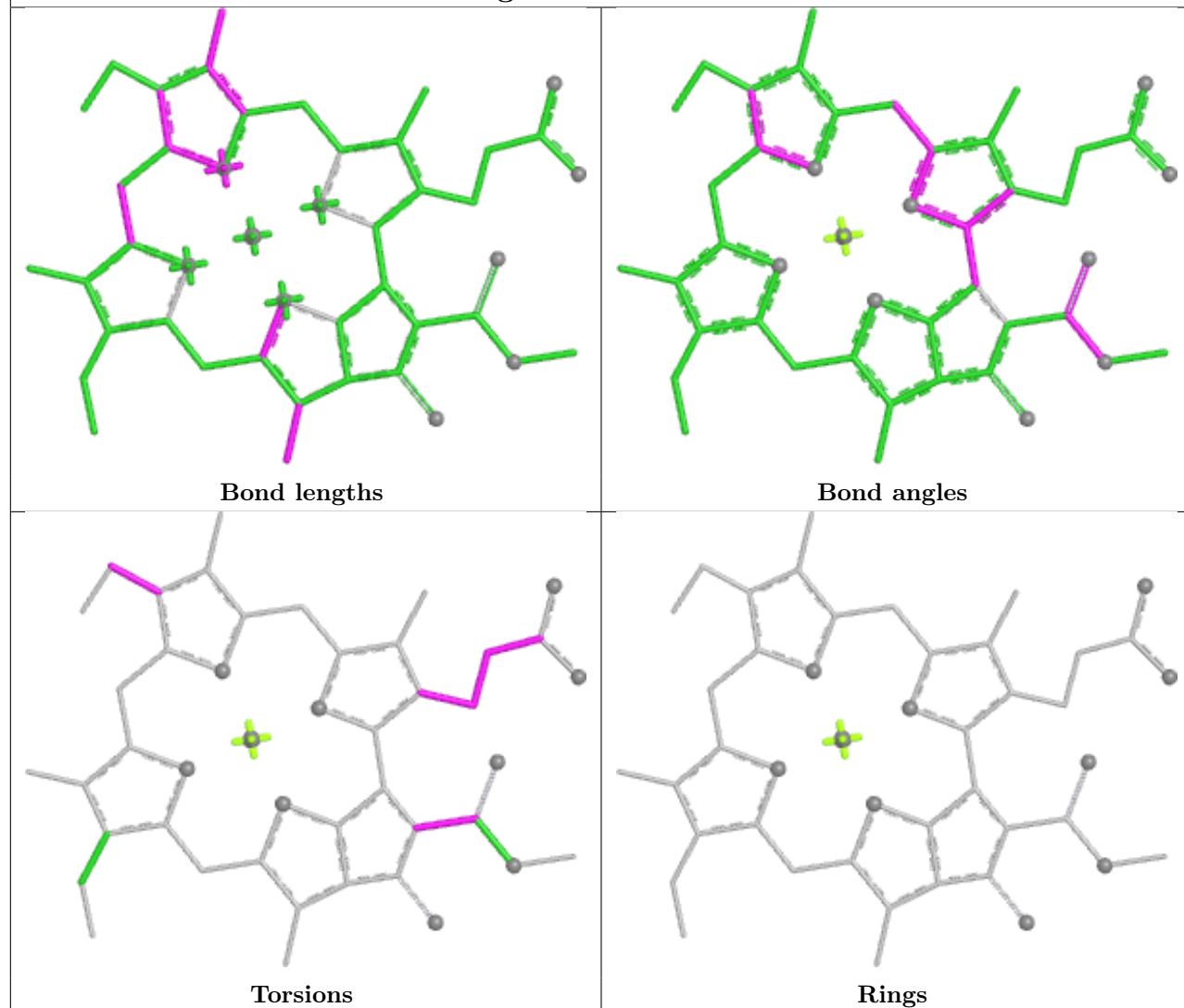
Ligand CLA B 829



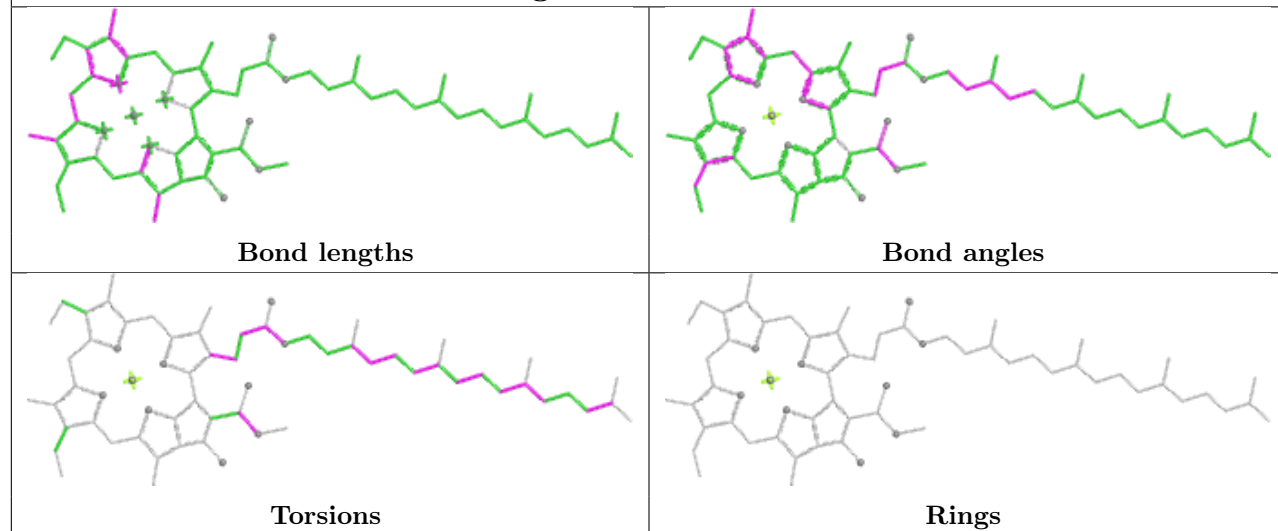
Ligand II0 a 314



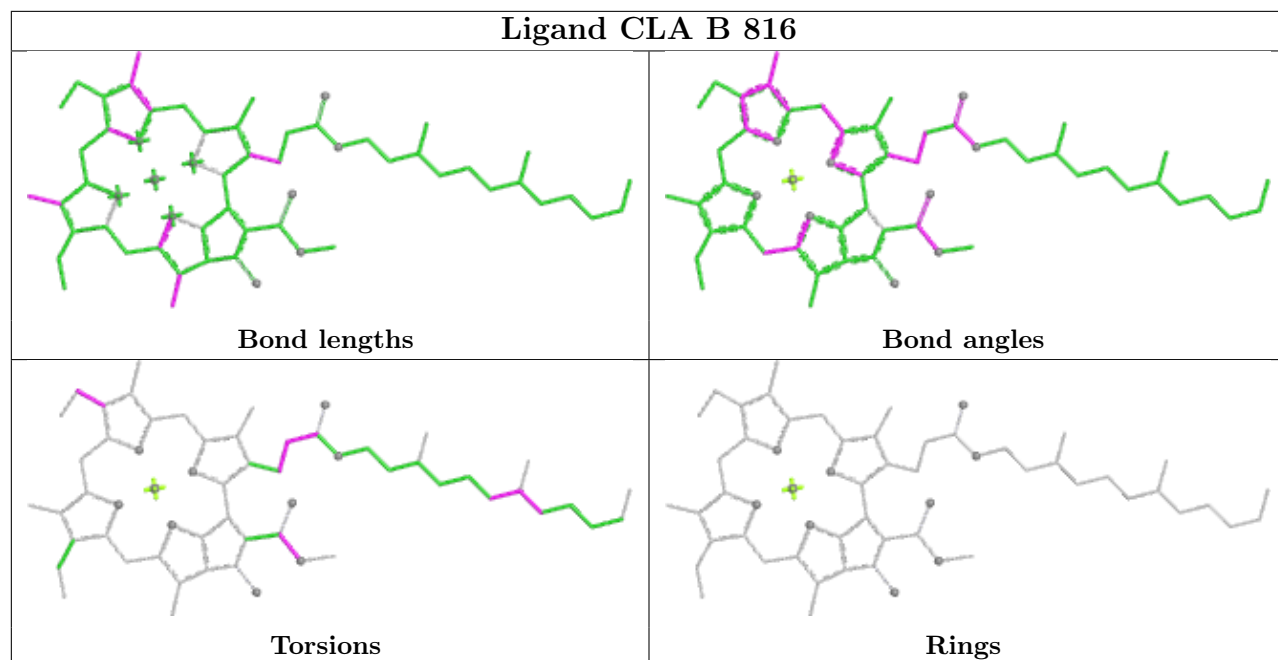
Ligand CLA e 601



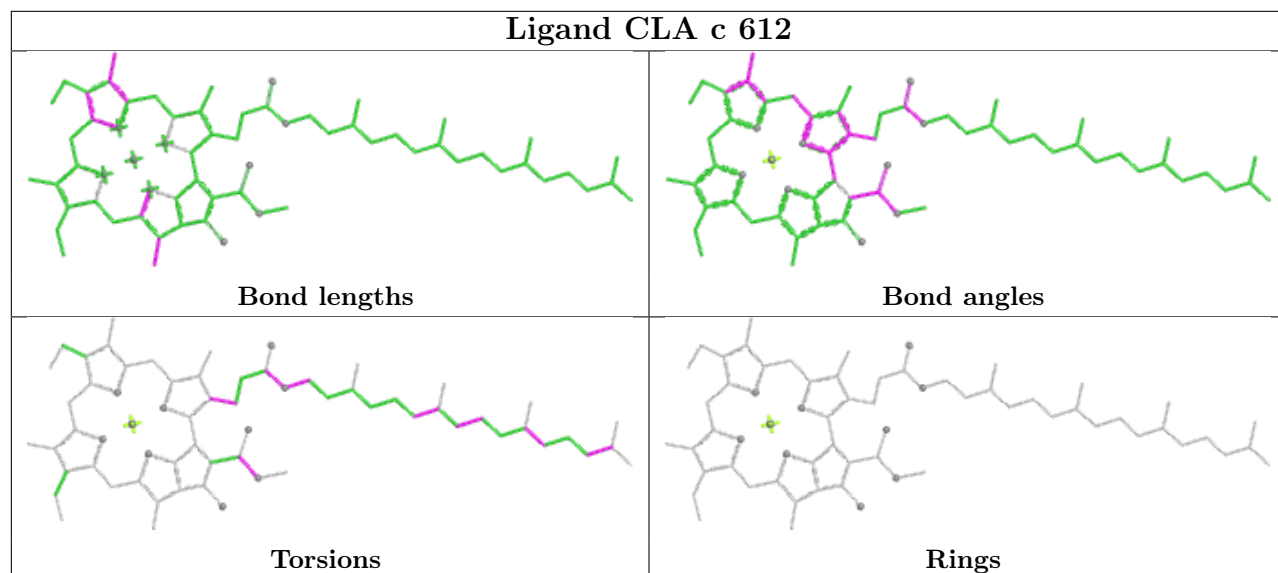
Ligand CLA A 812

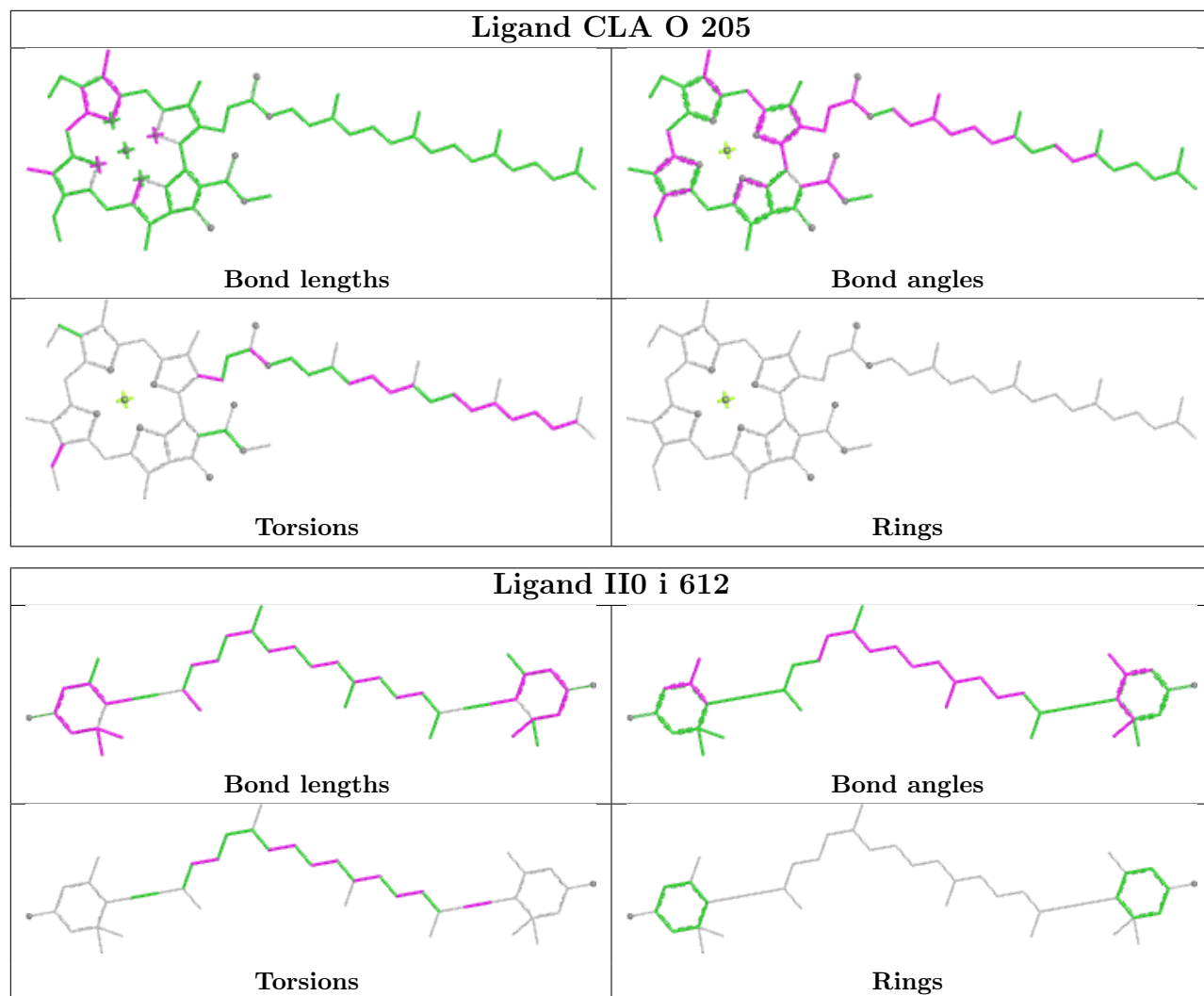


Ligand CLA B 816

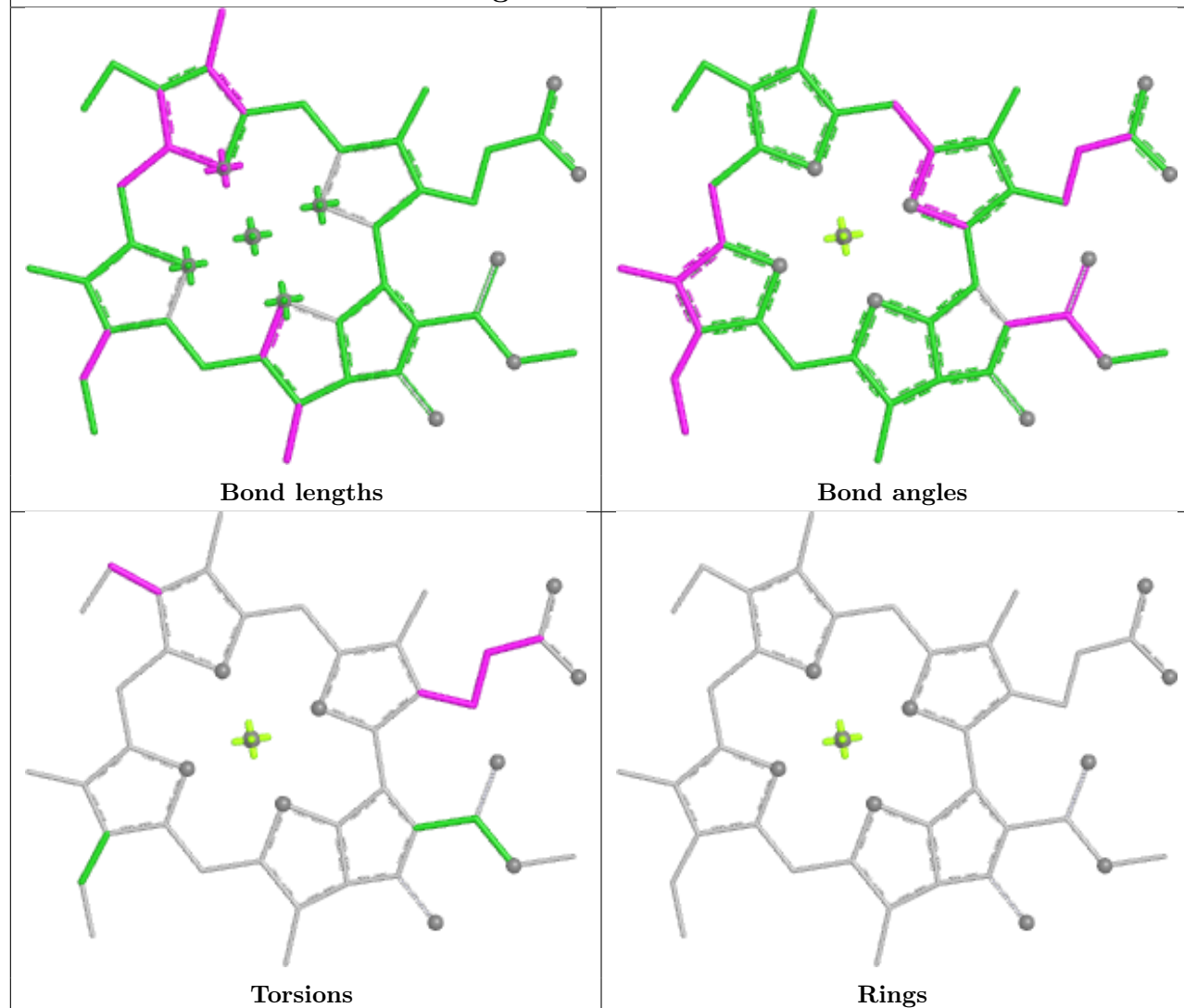


Ligand CLA c 612

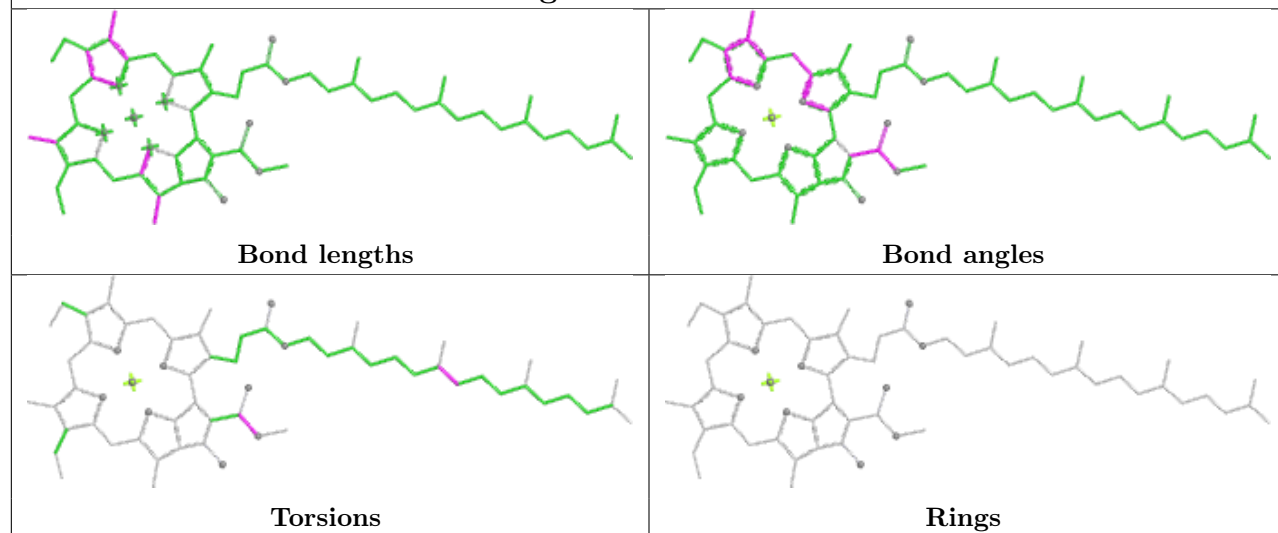


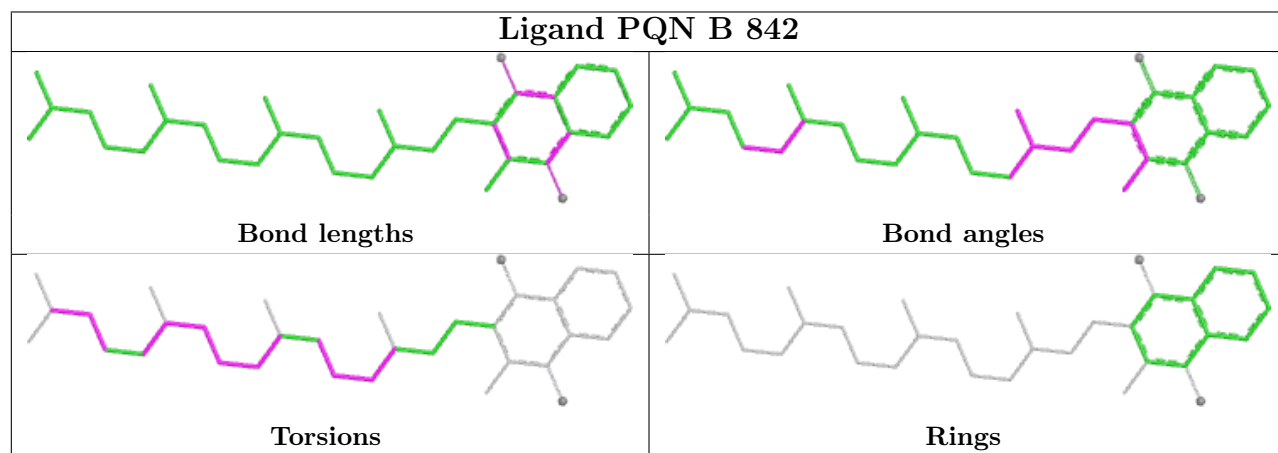
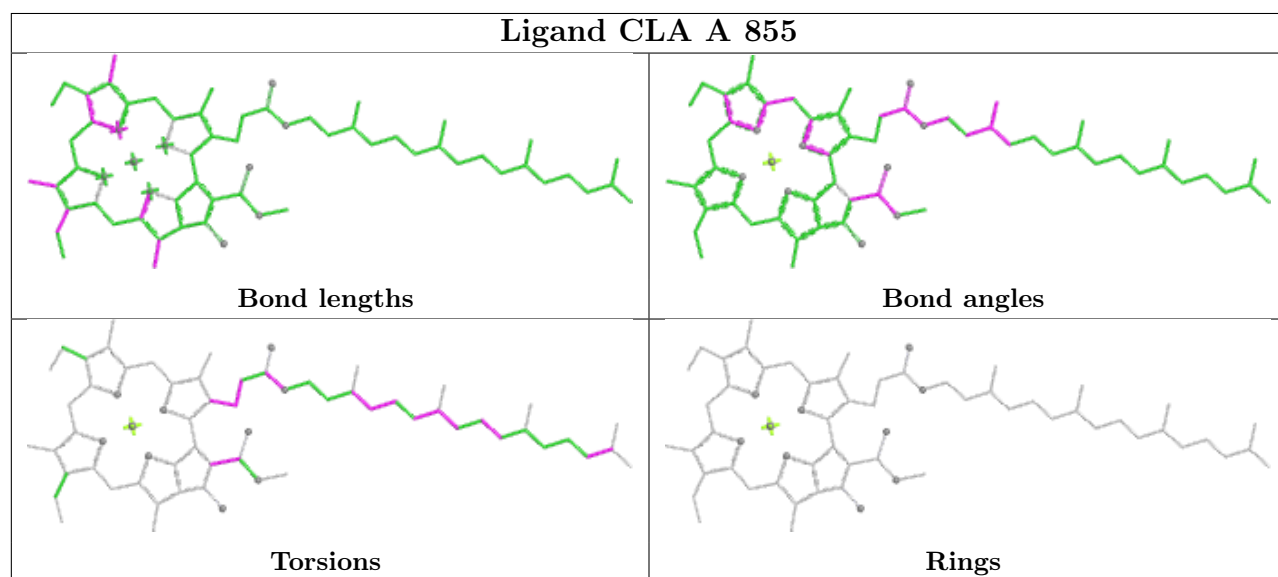
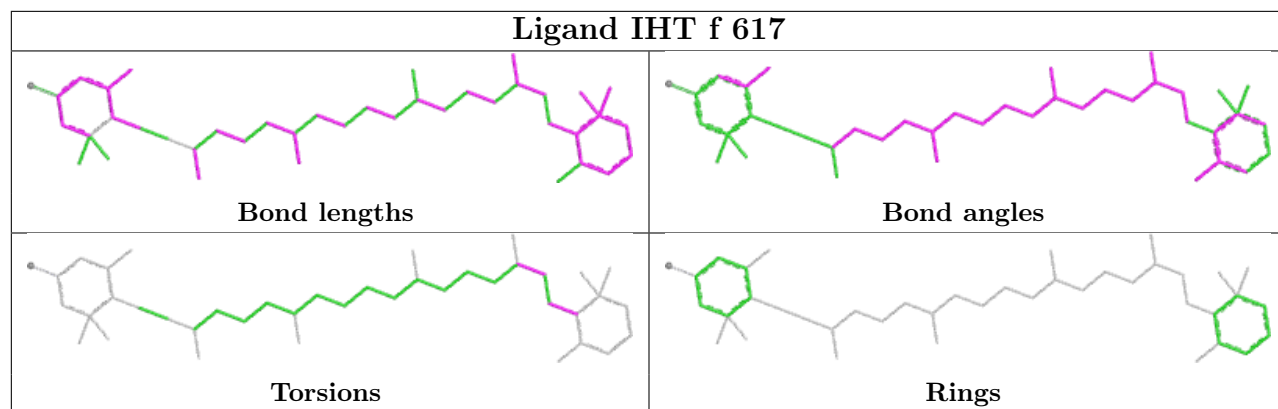


Ligand CLA A 819

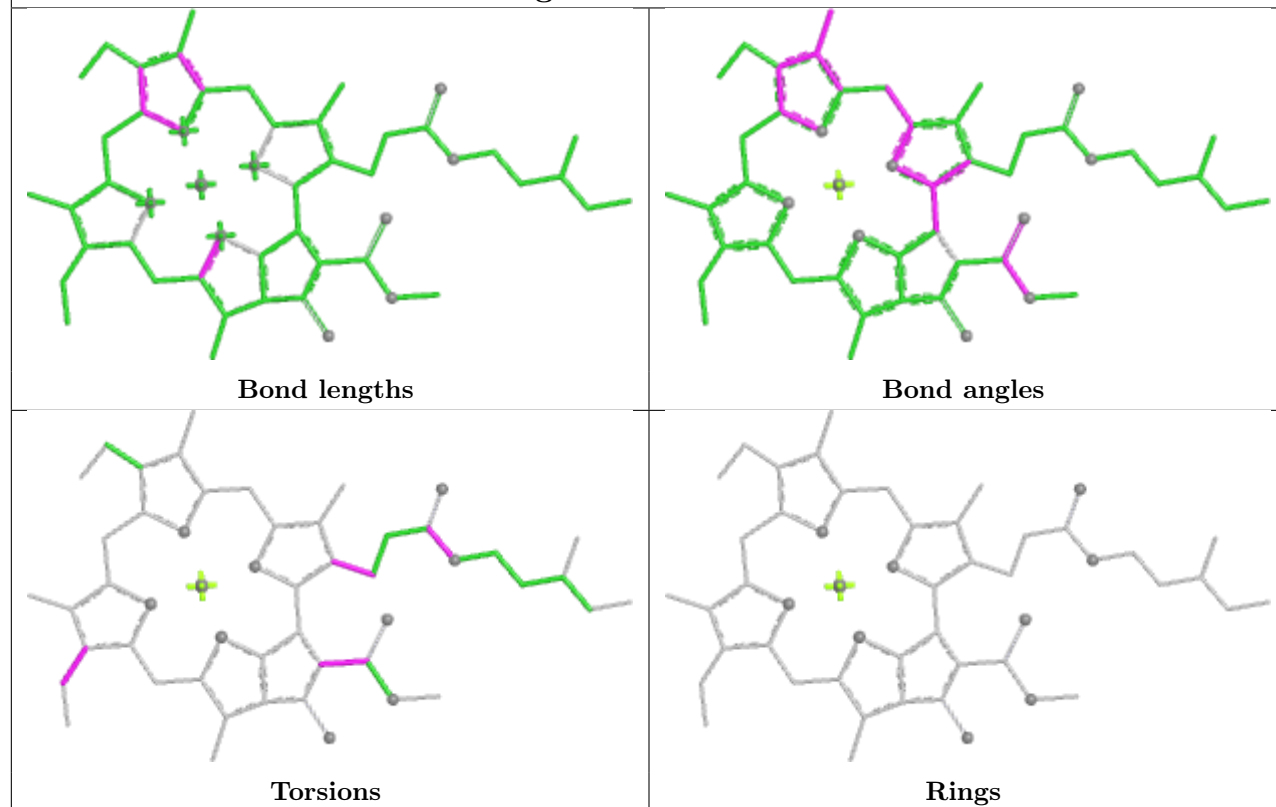


Ligand CLA f 609

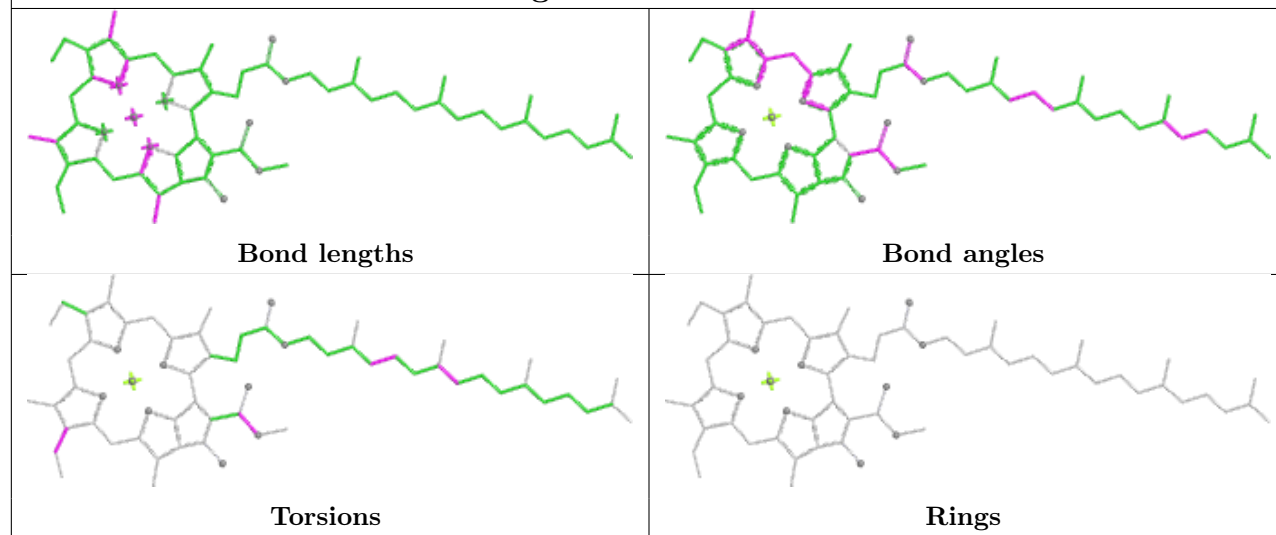


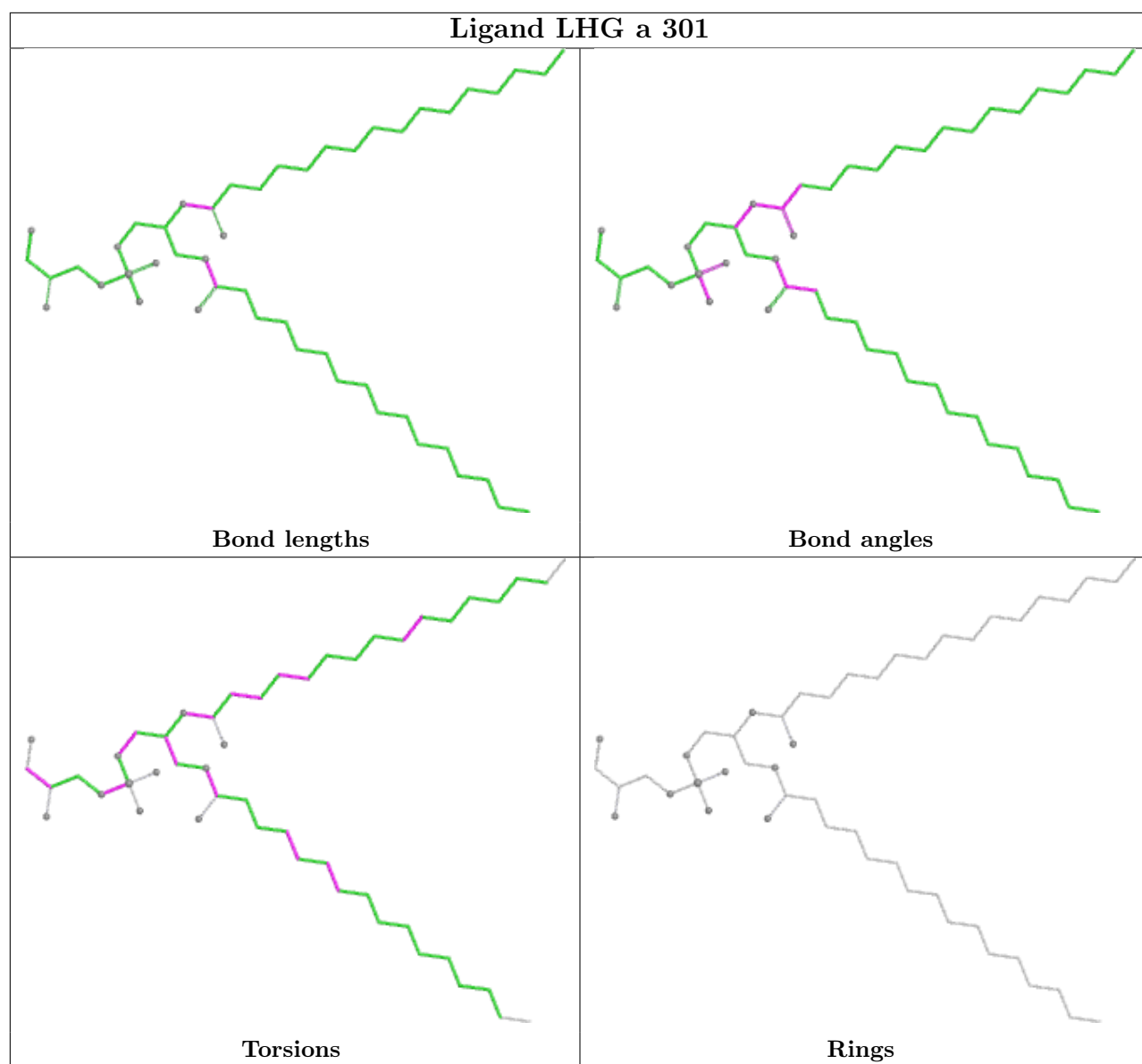


Ligand CLA d 304

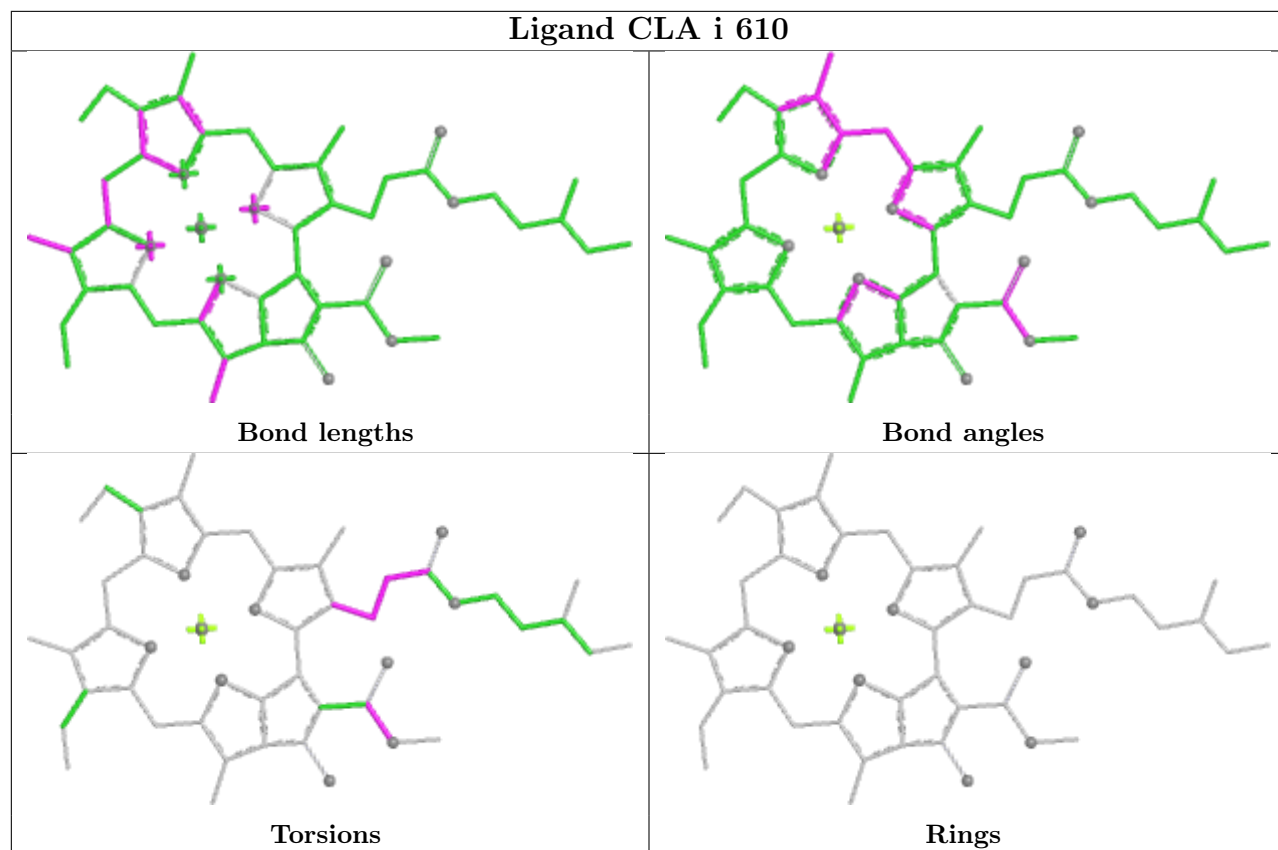


Ligand CLA A 820

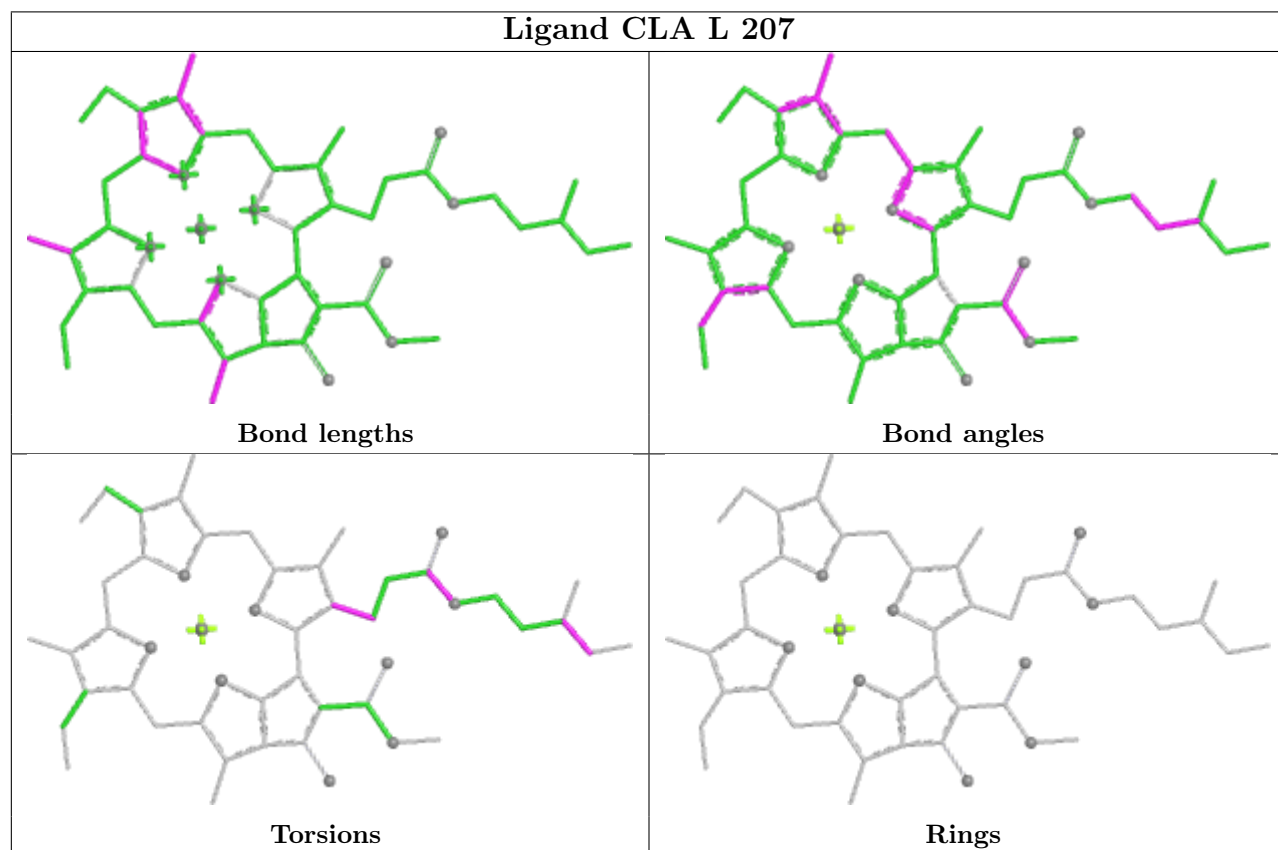


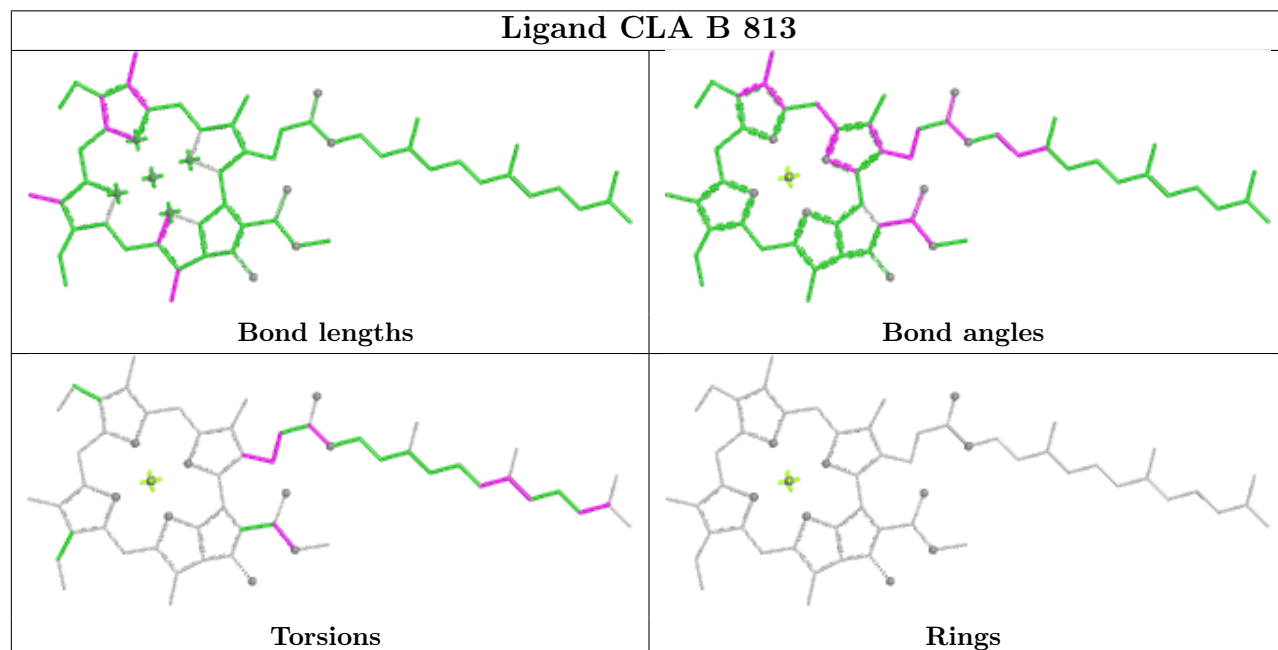
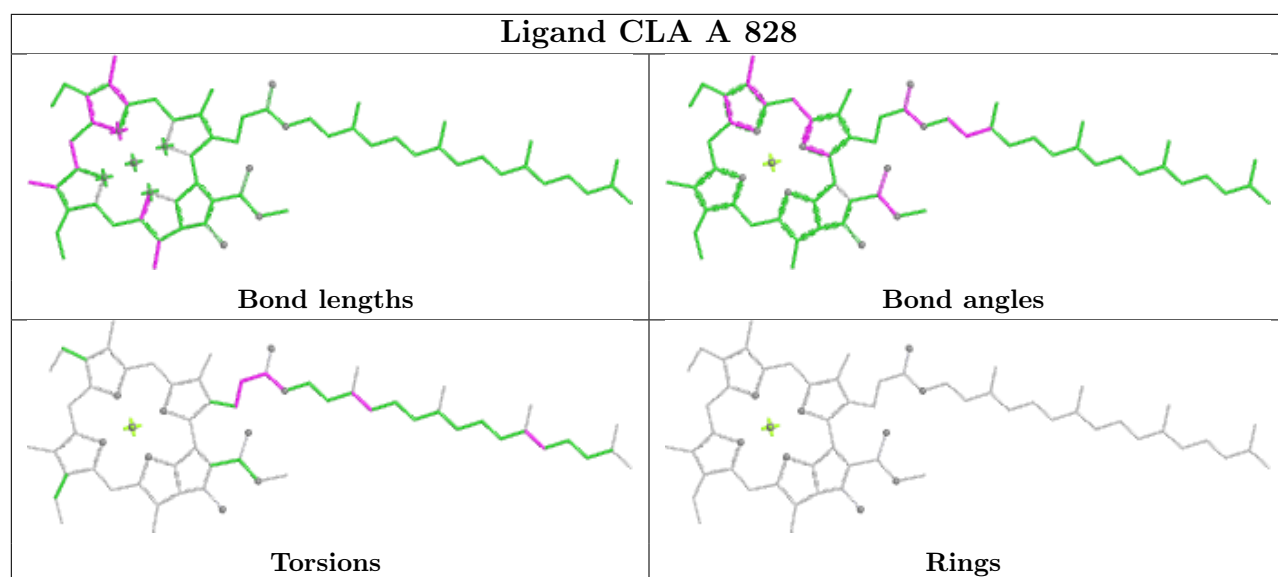


Ligand CLA i 610

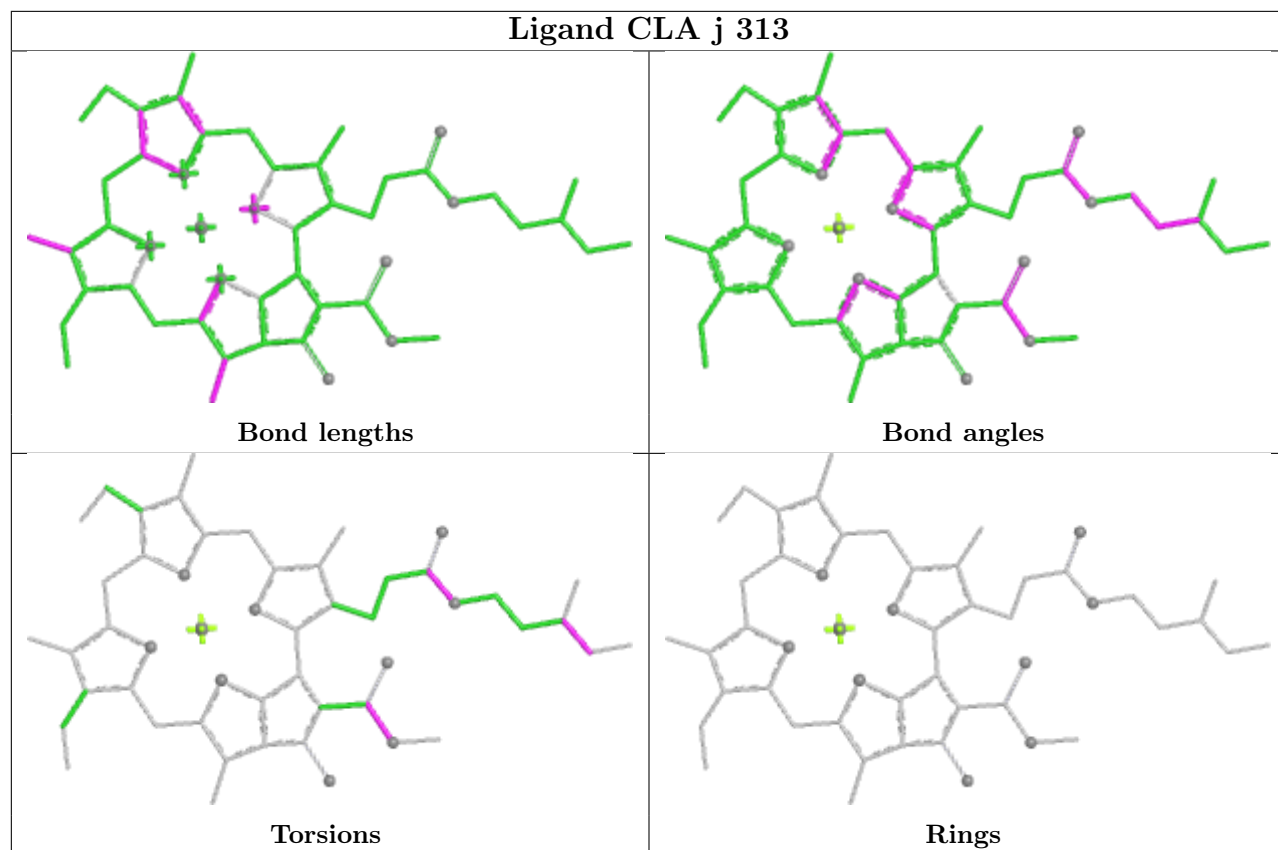


Ligand CLA L 207

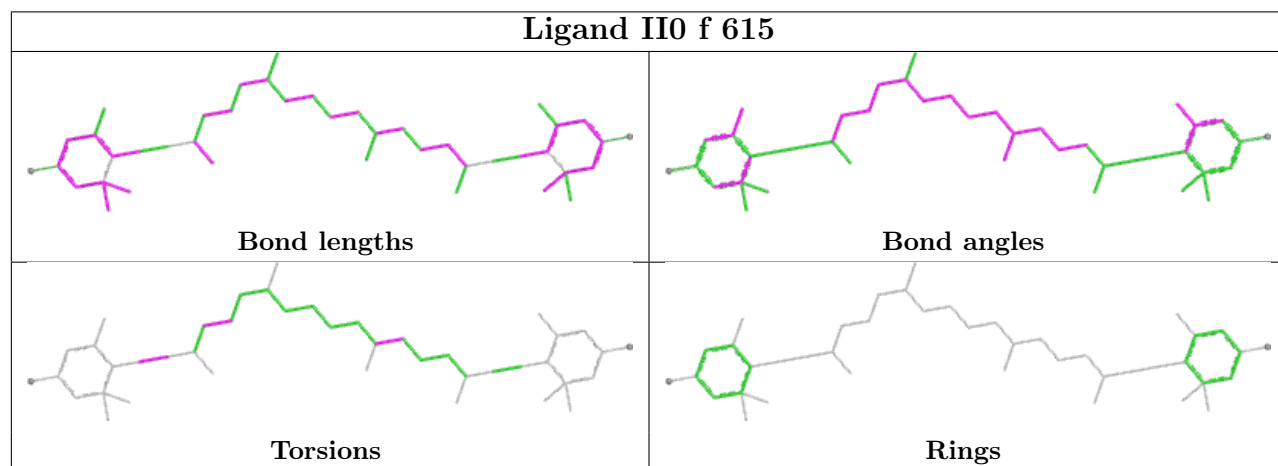


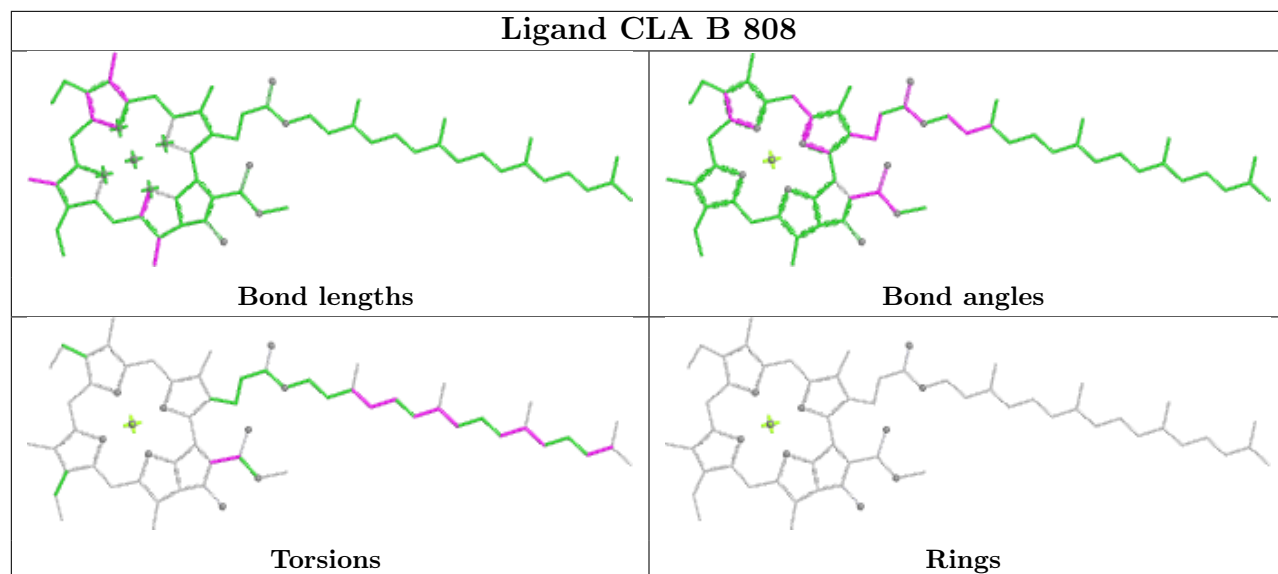
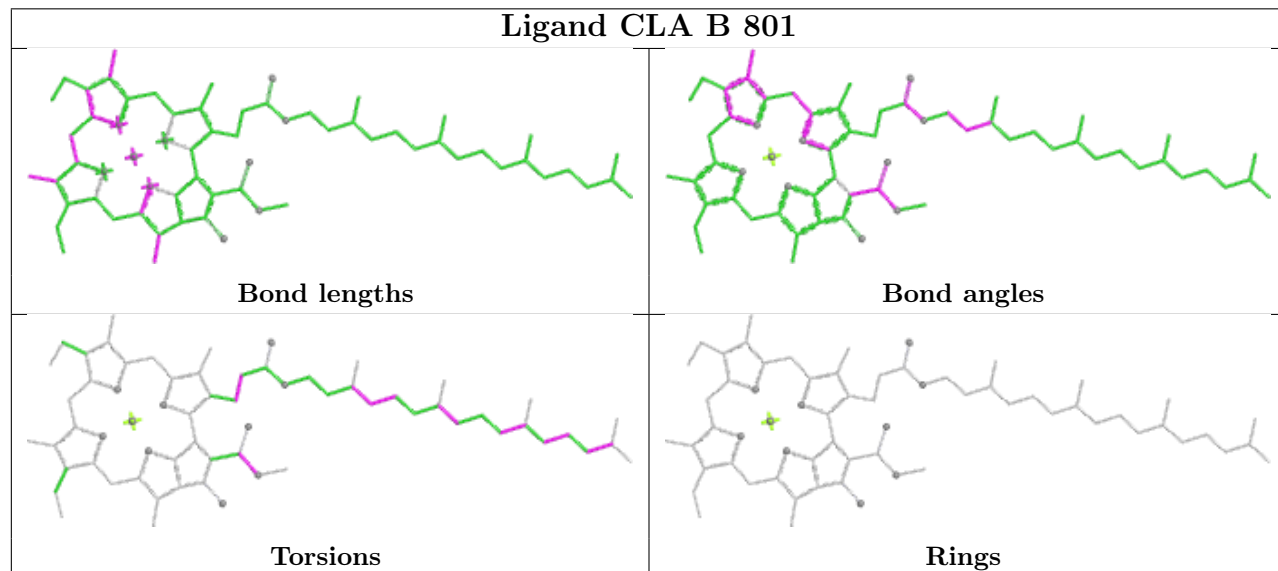


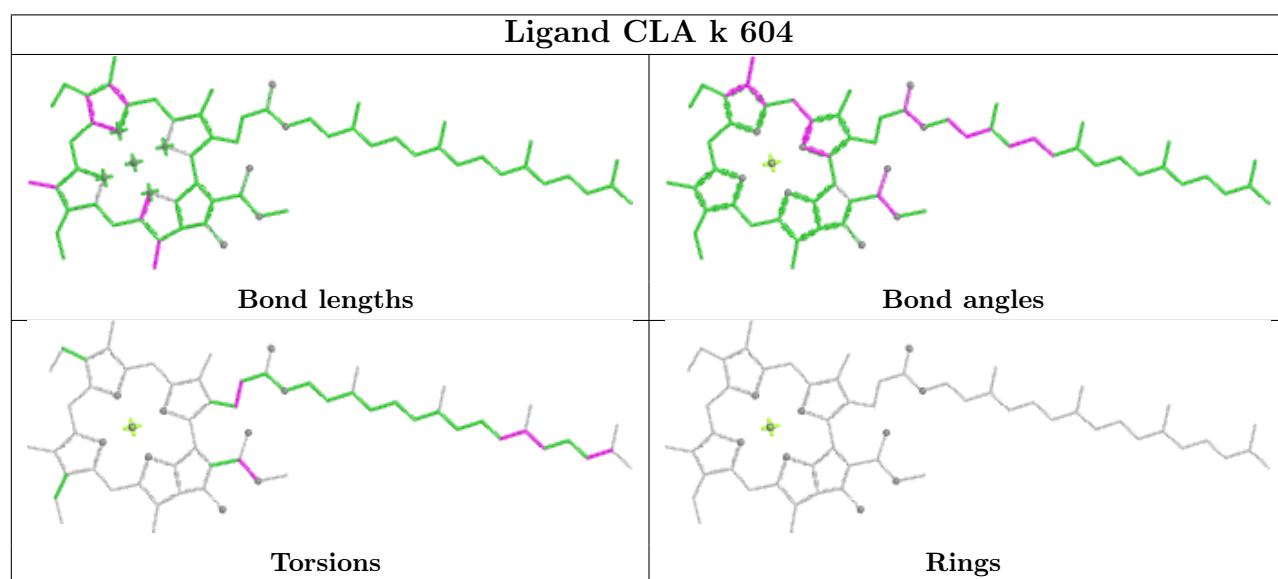
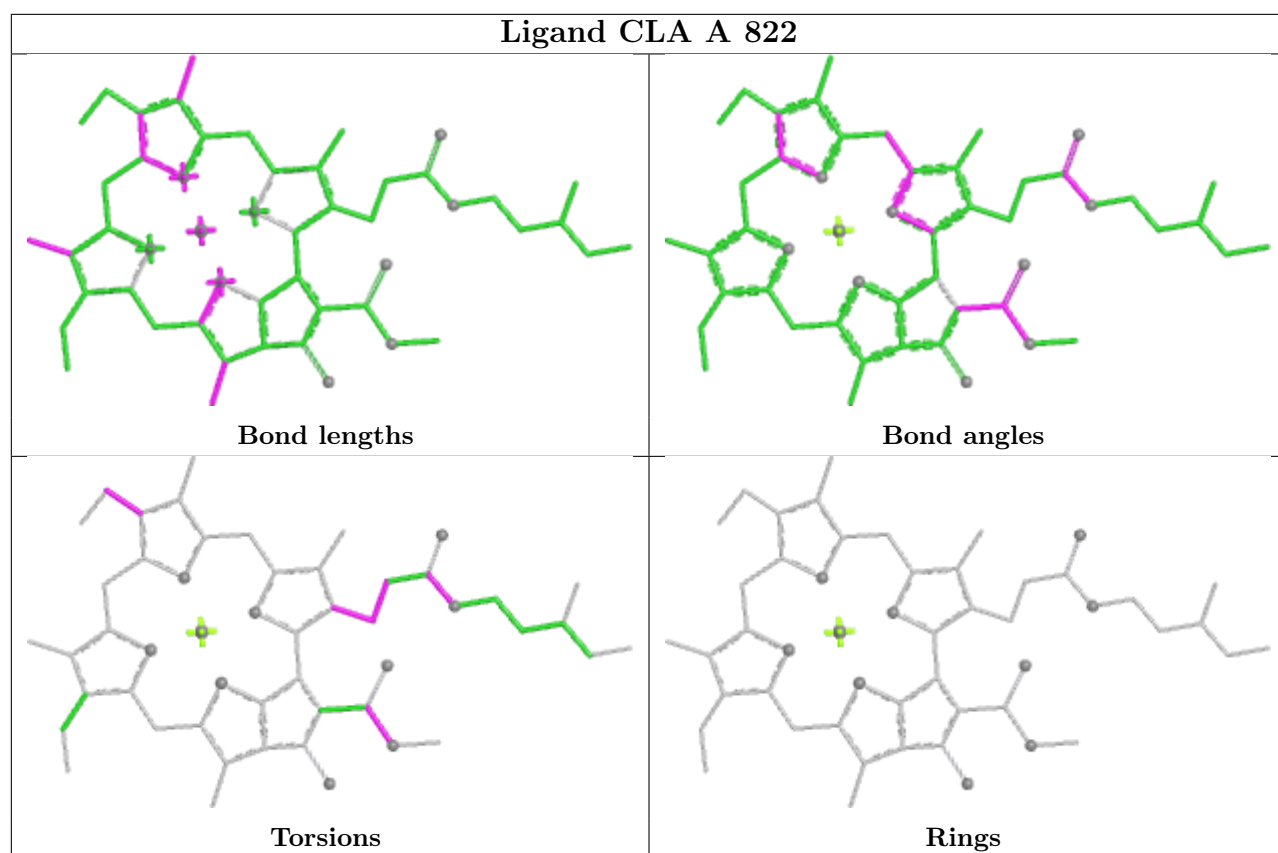
Ligand CLA j 313

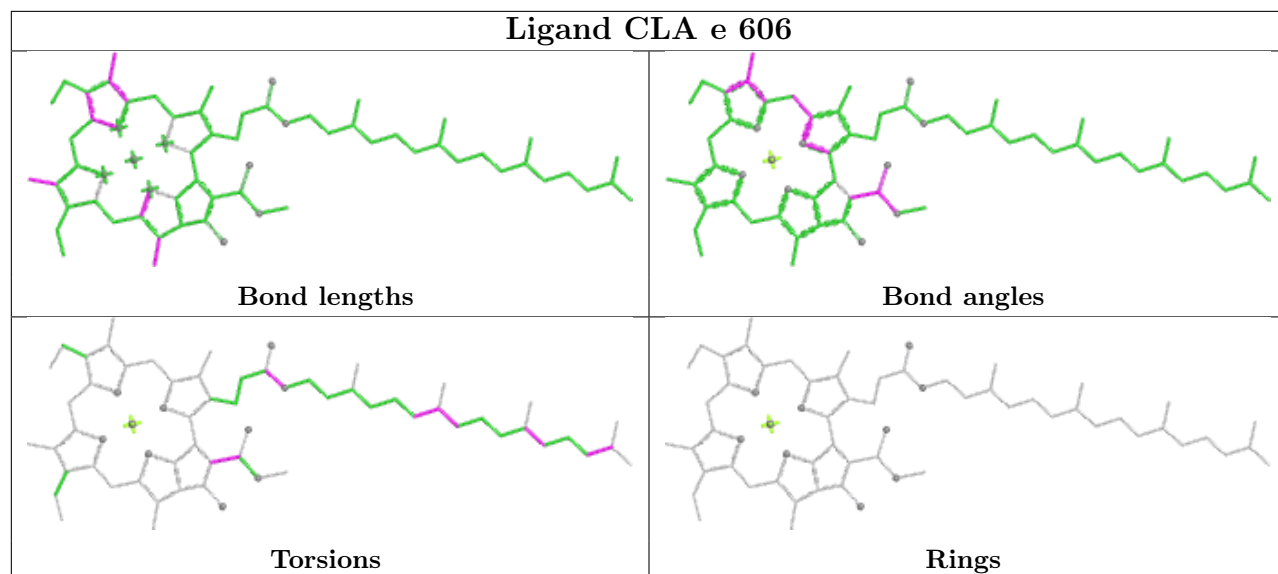
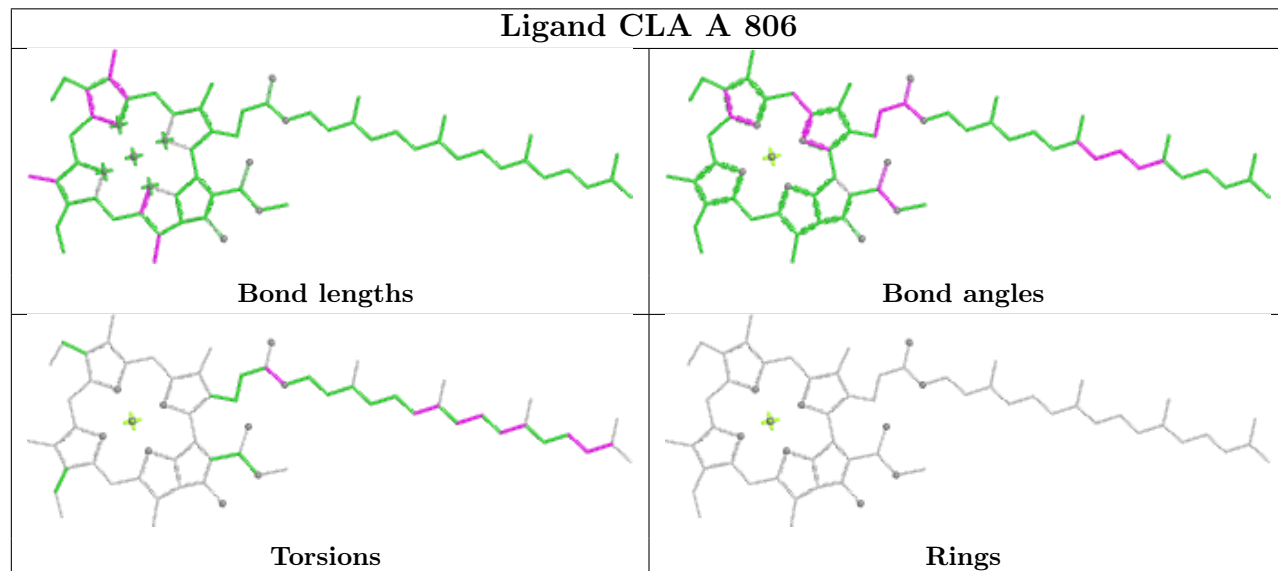


Ligand II0 f 615

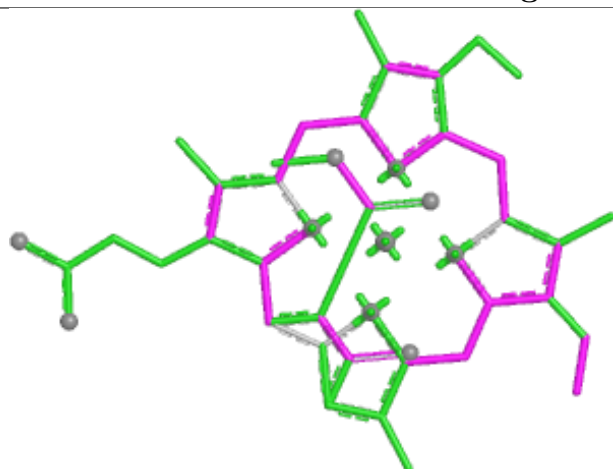


Ligand CLA B 808**Ligand CLA B 801**

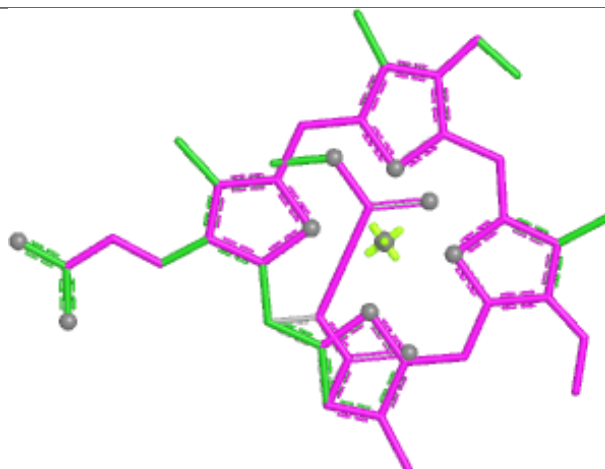


Ligand CLA e 606**Ligand CLA A 806**

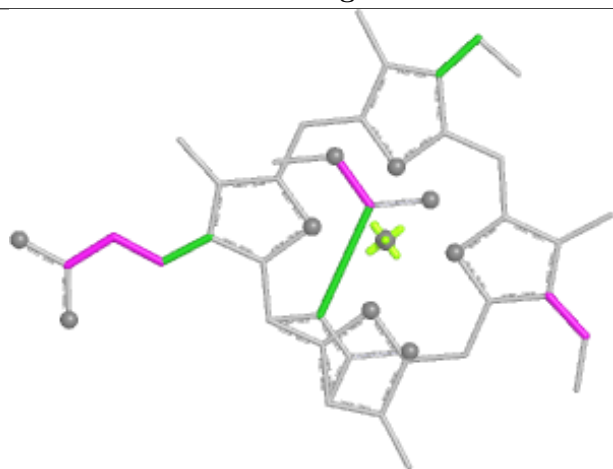
Ligand KC2 e 609



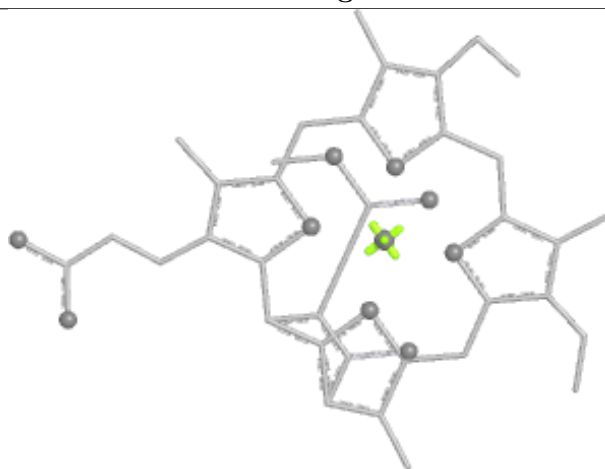
Bond lengths



Bond angles

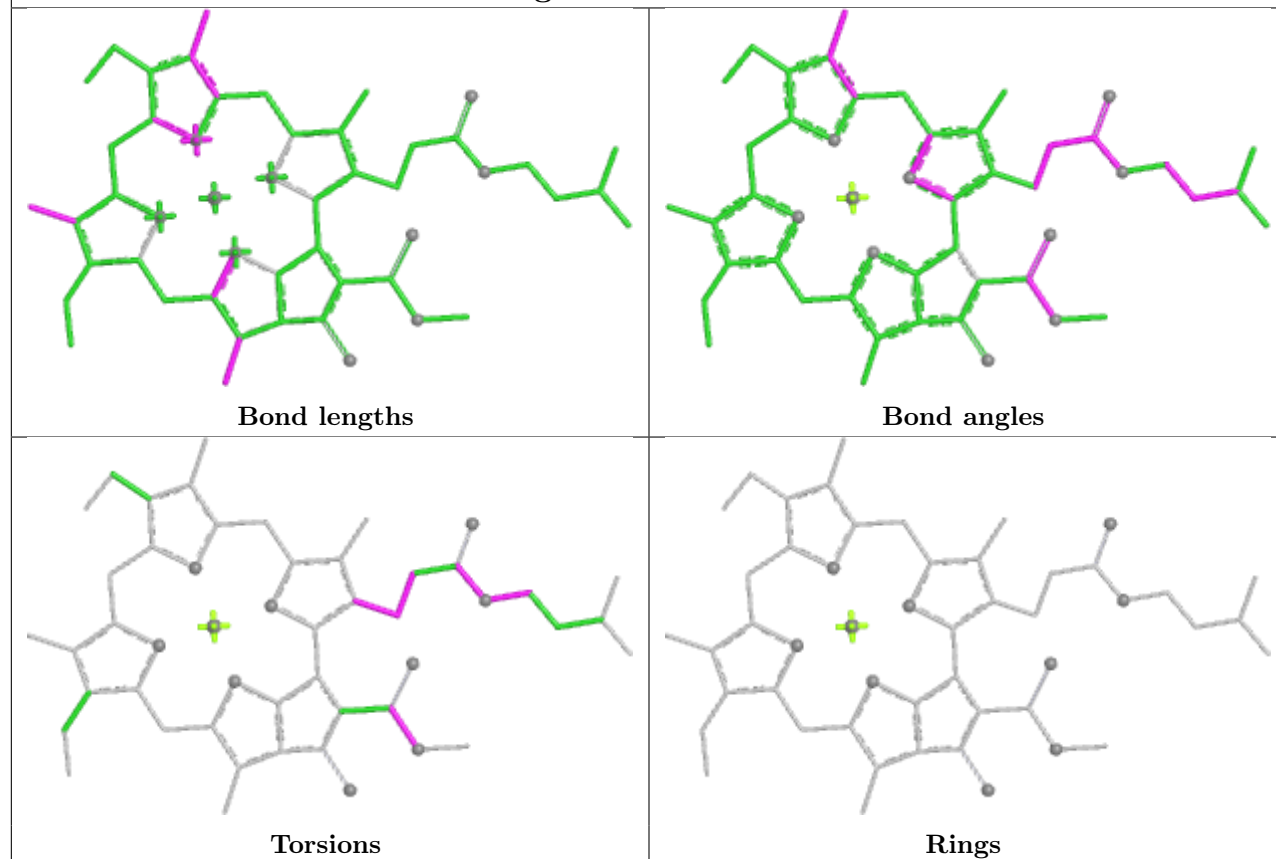


Torsions

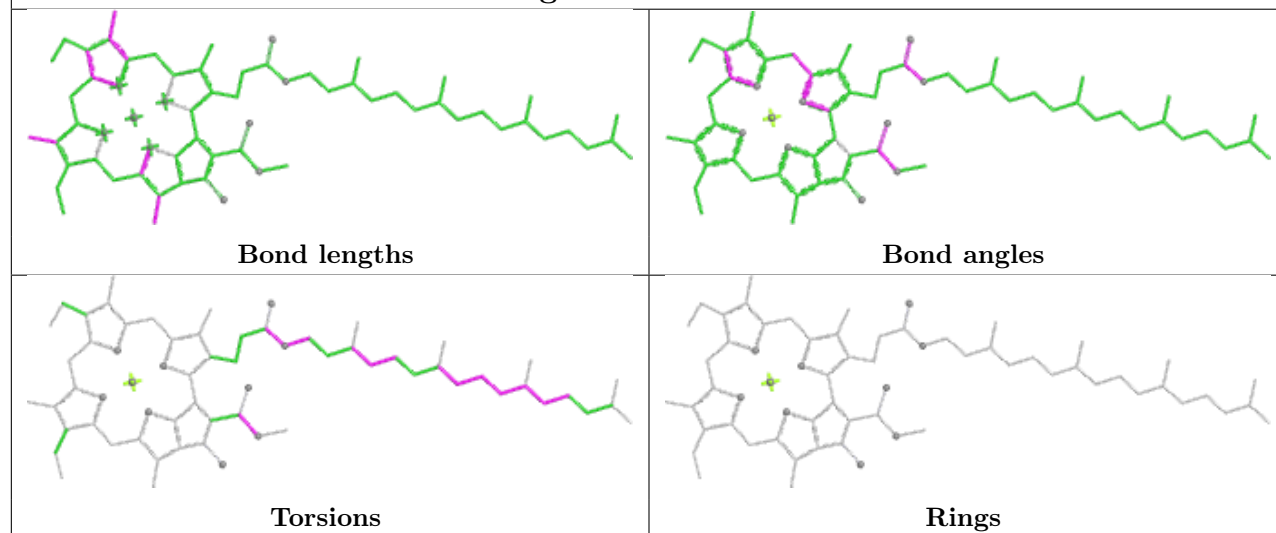


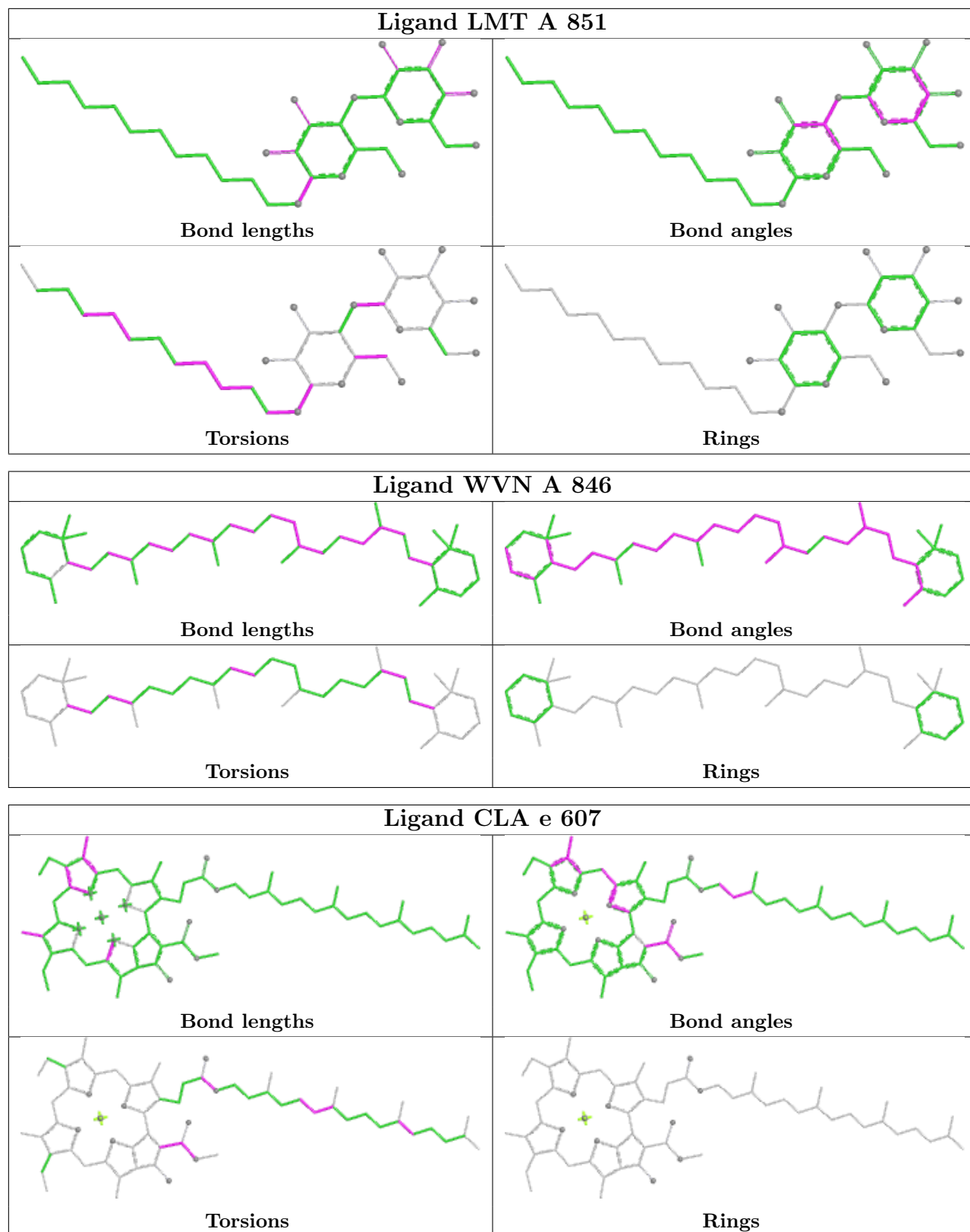
Rings

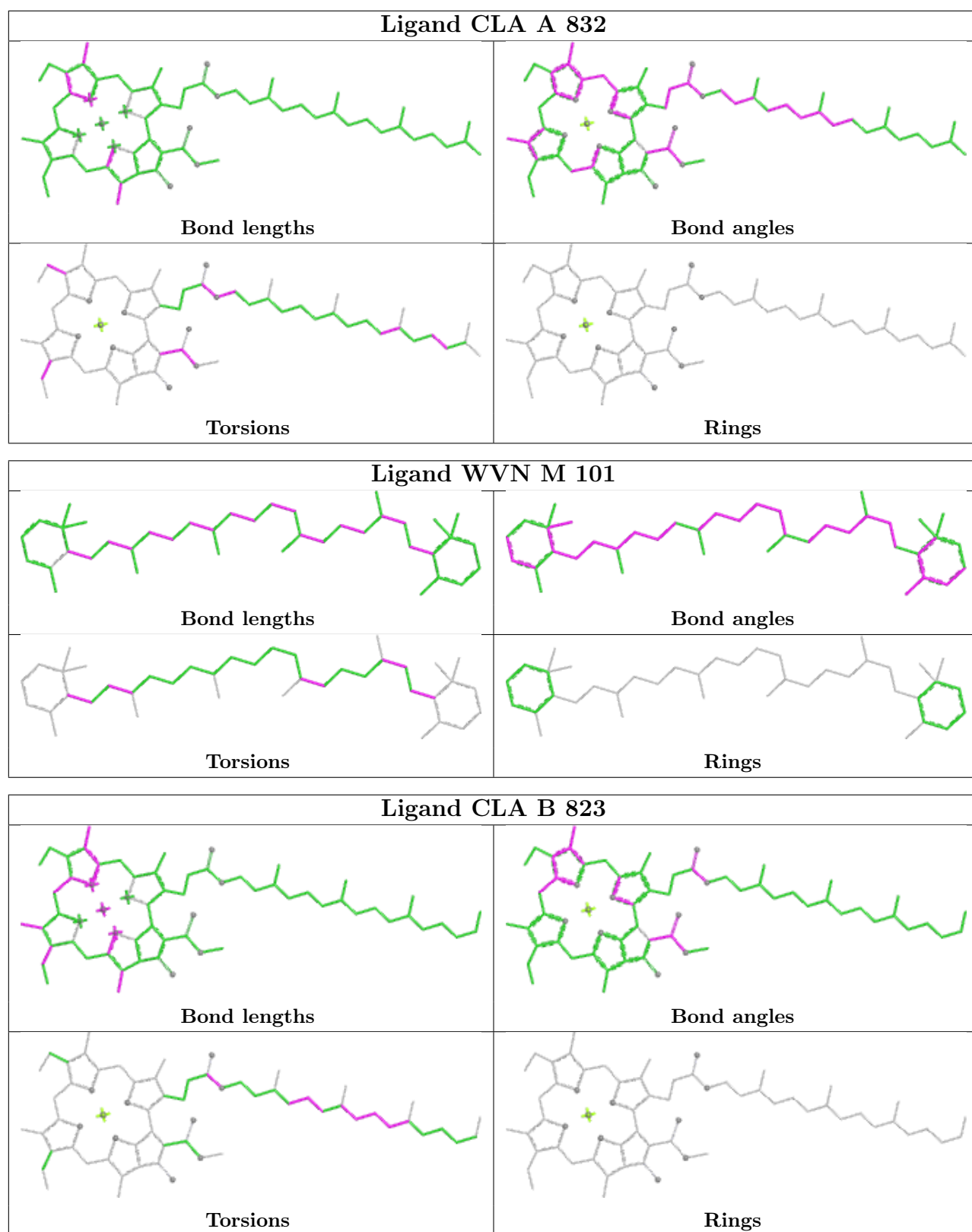
Ligand CLA L 204



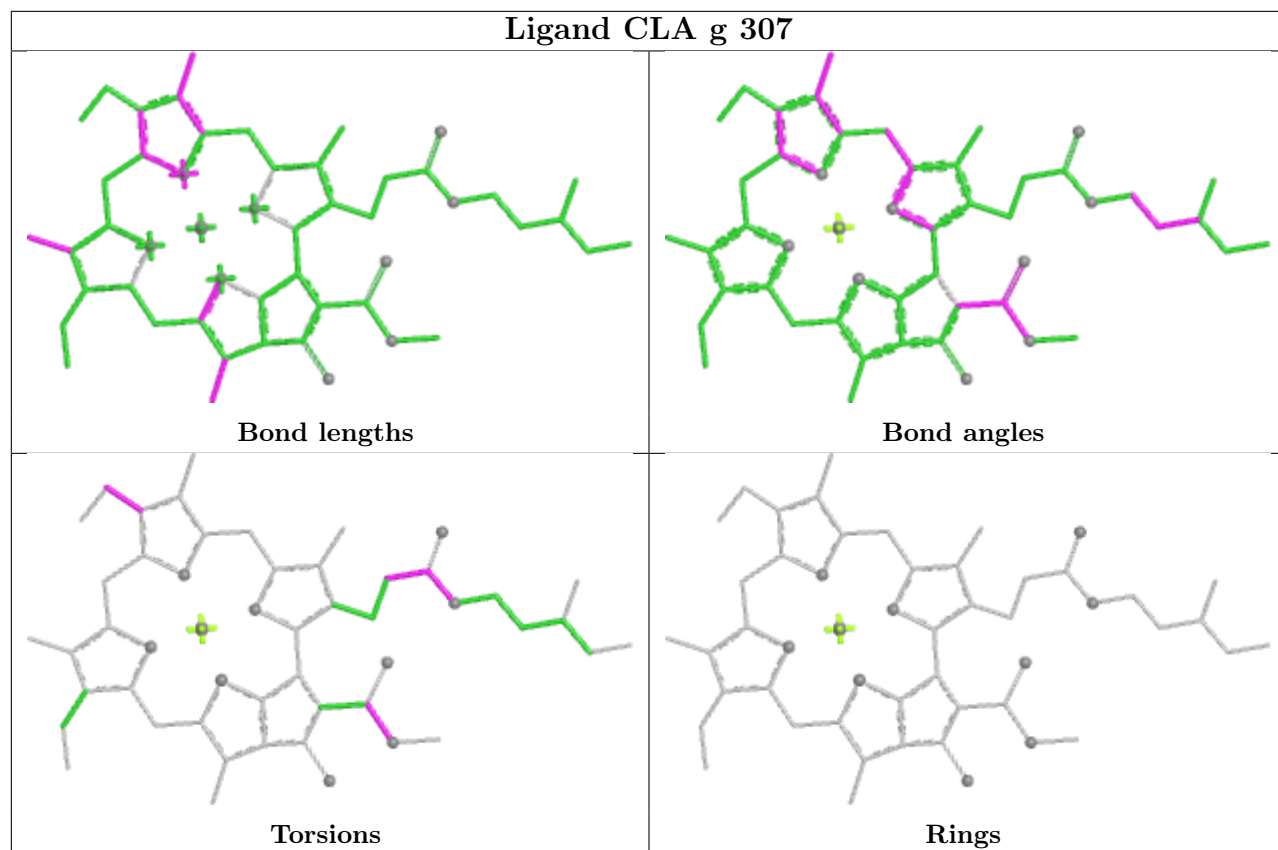
Ligand CLA f 610



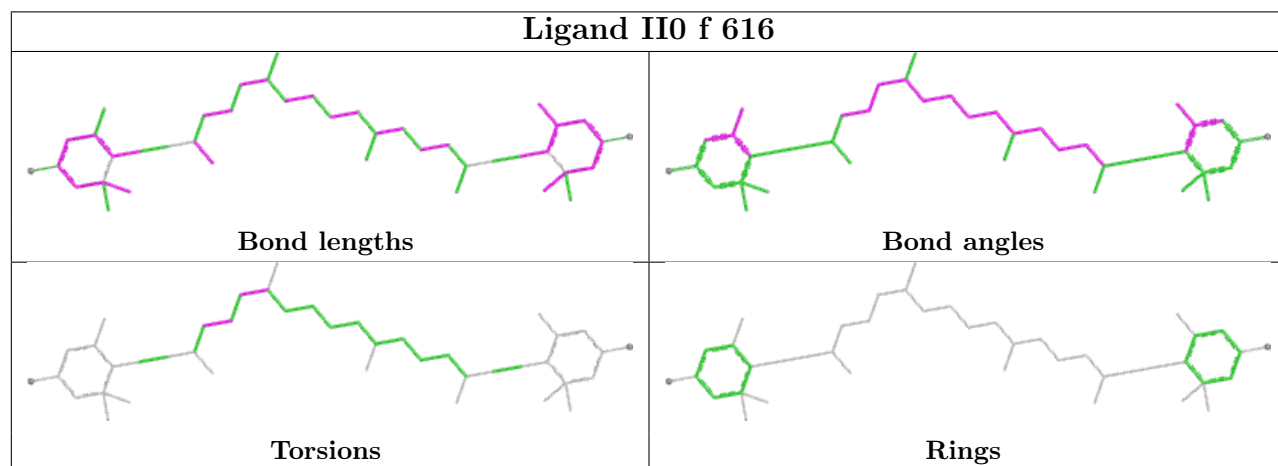




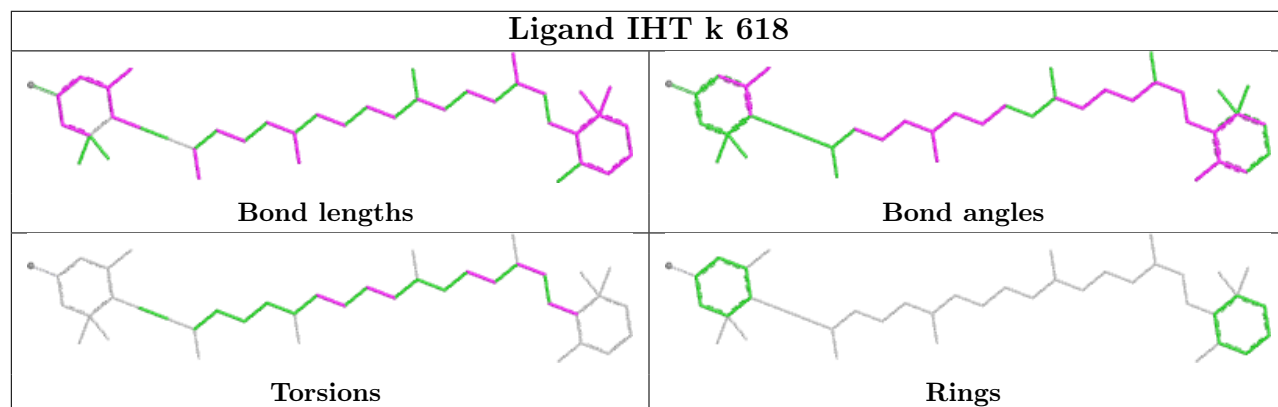
Ligand CLA g 307



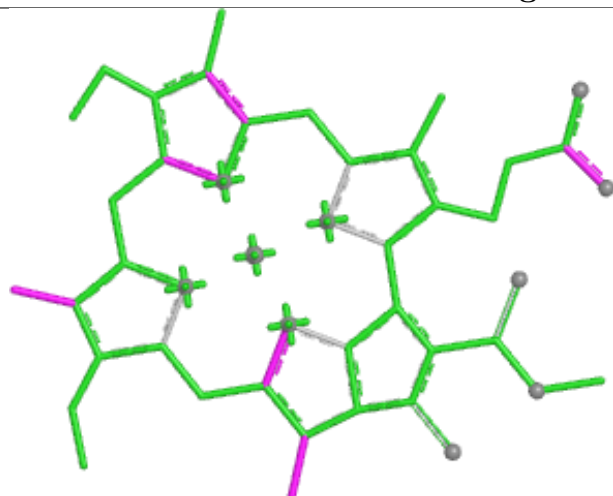
Ligand II0 f 616



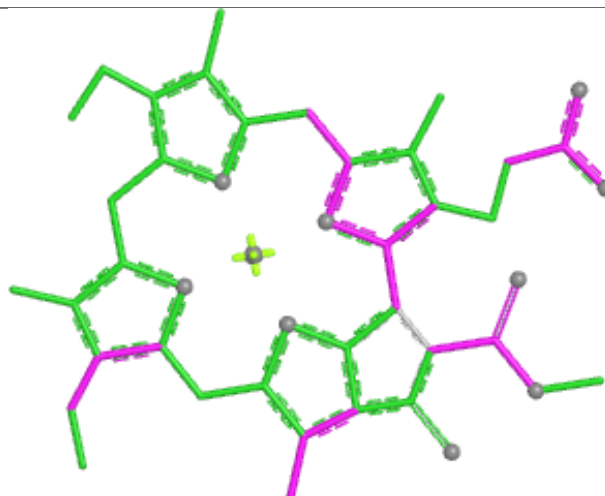
Ligand IHT k 618



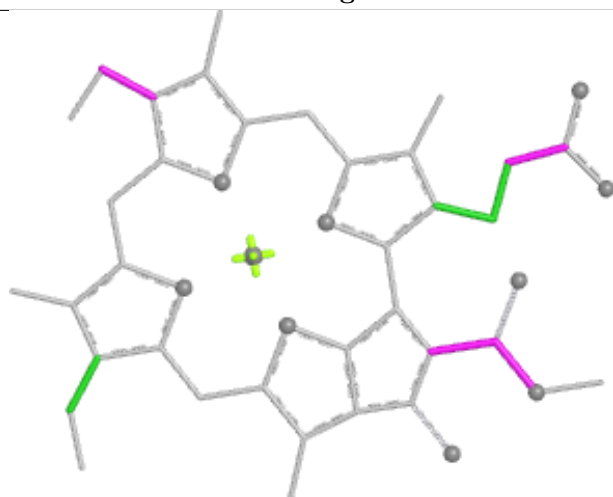
Ligand CLA c 611



Bond lengths



Bond angles

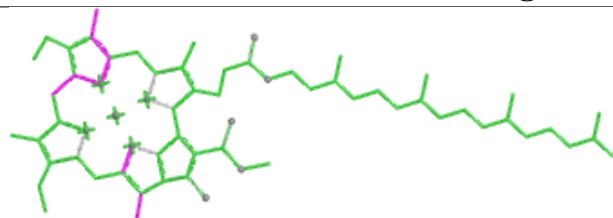


Torsions

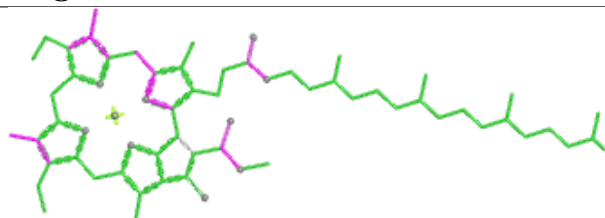


Rings

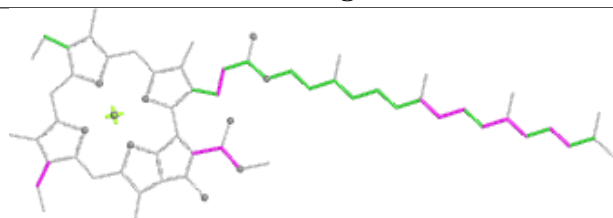
Ligand CLA g 305



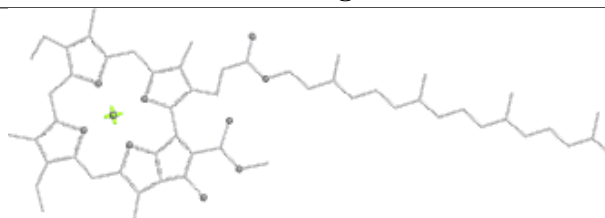
Bond lengths



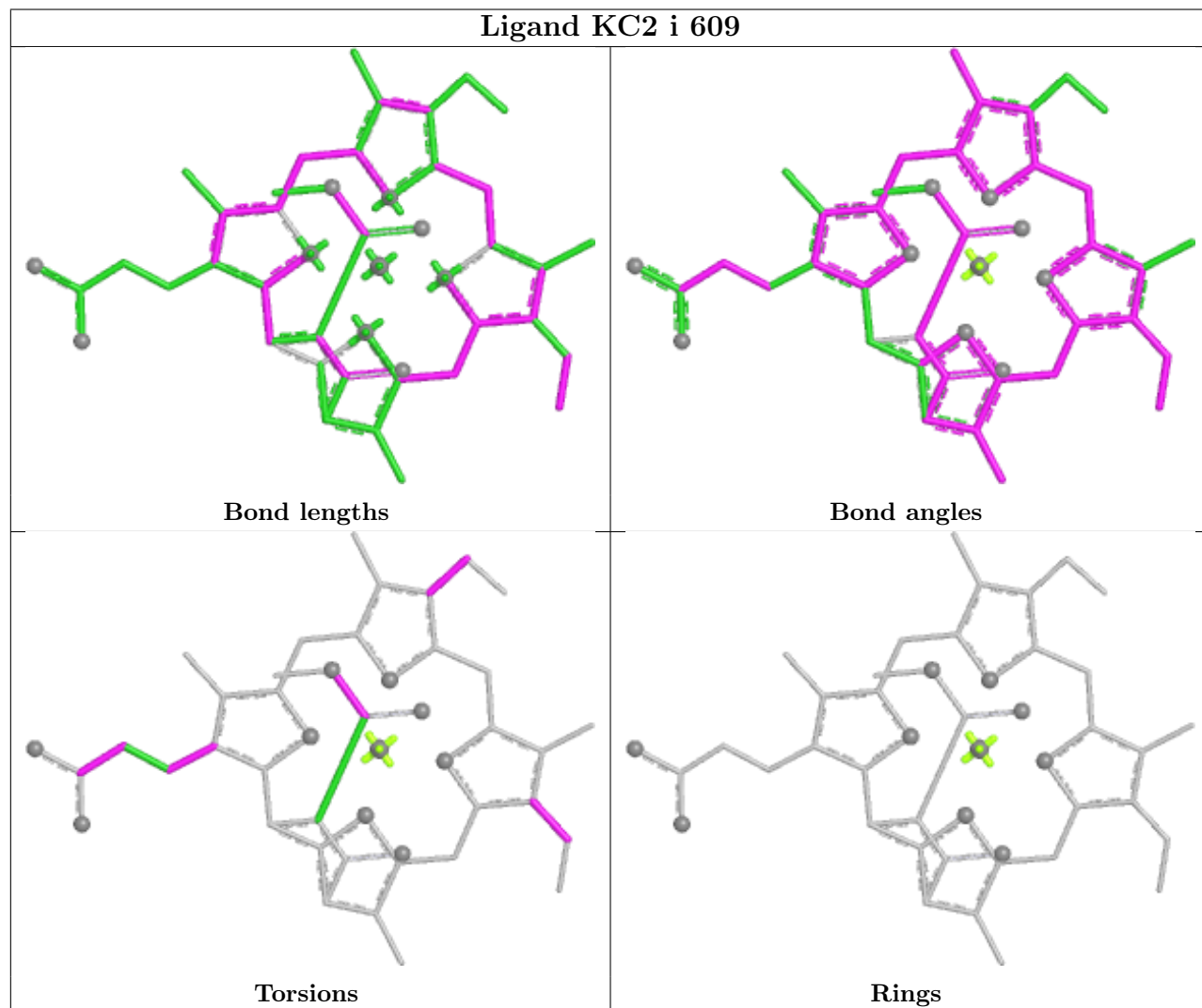
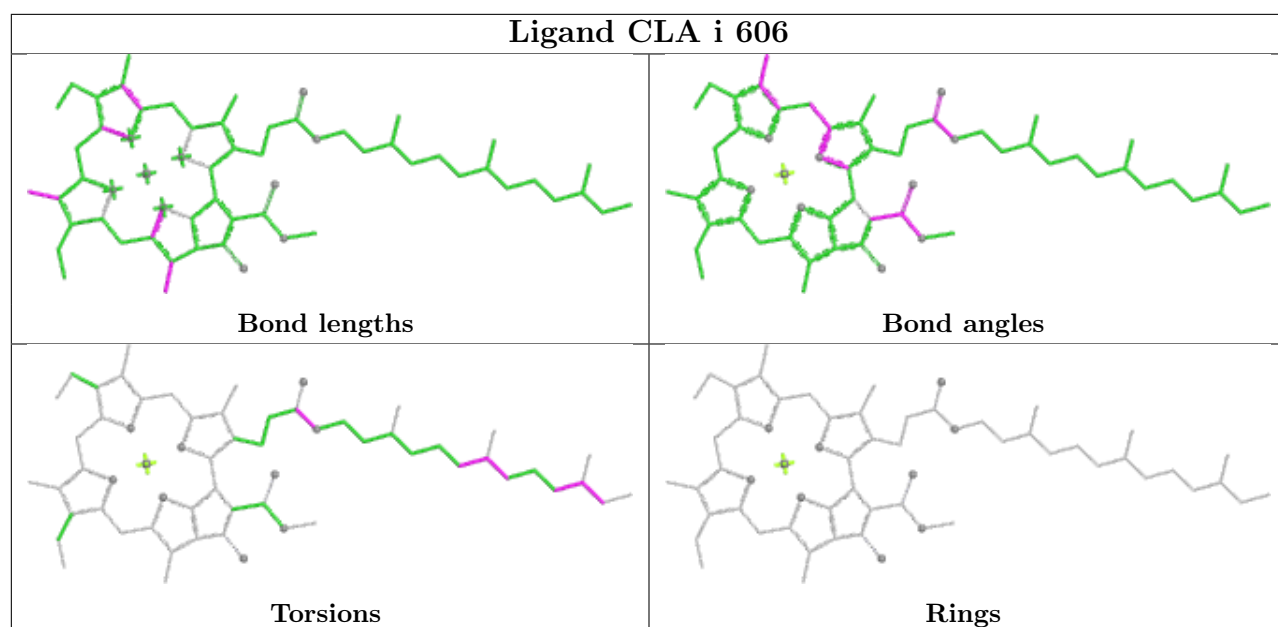
Bond angles

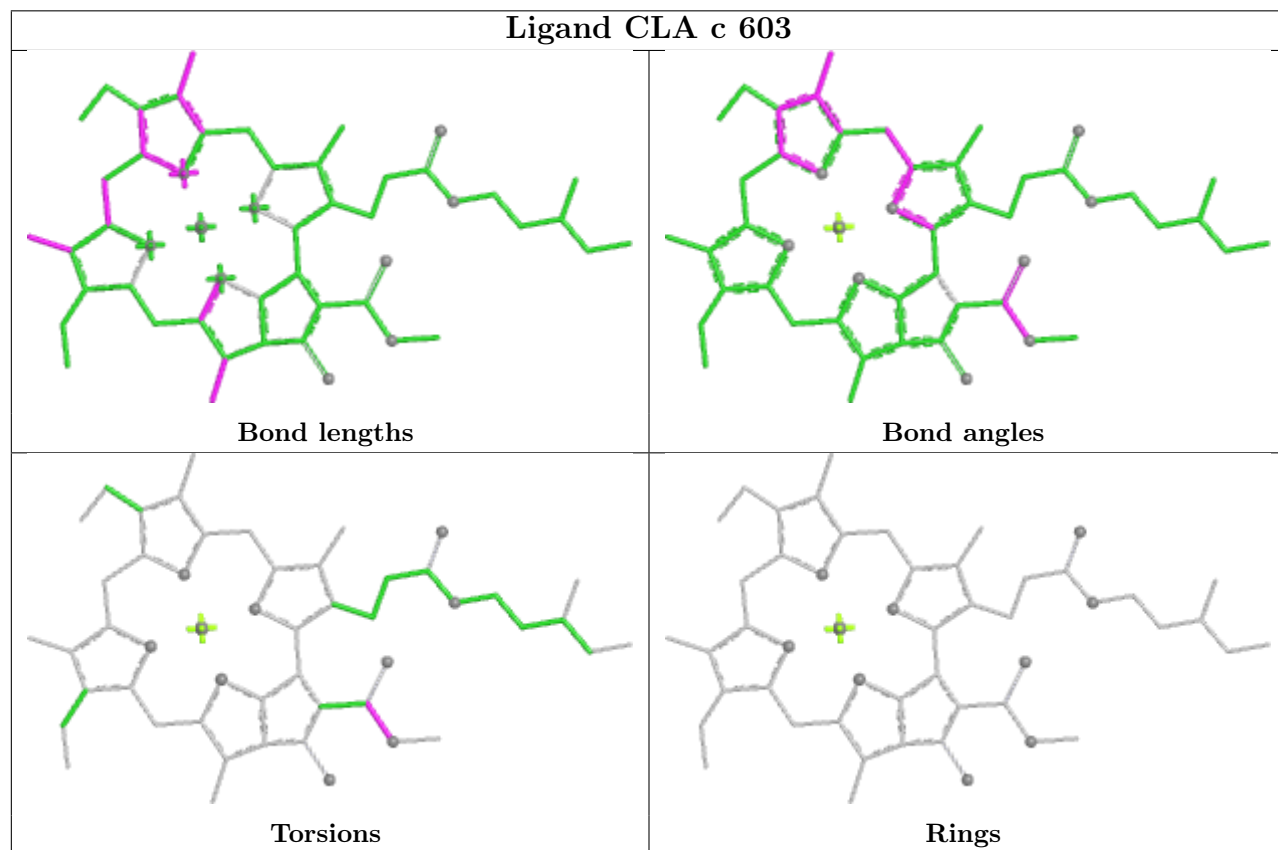
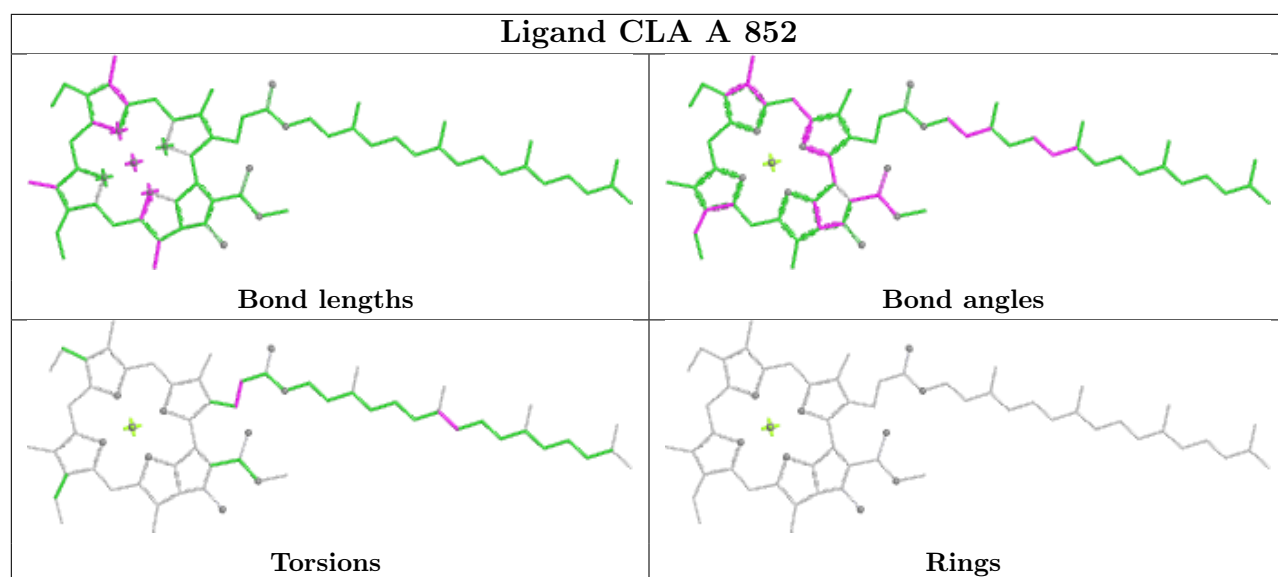


Torsions

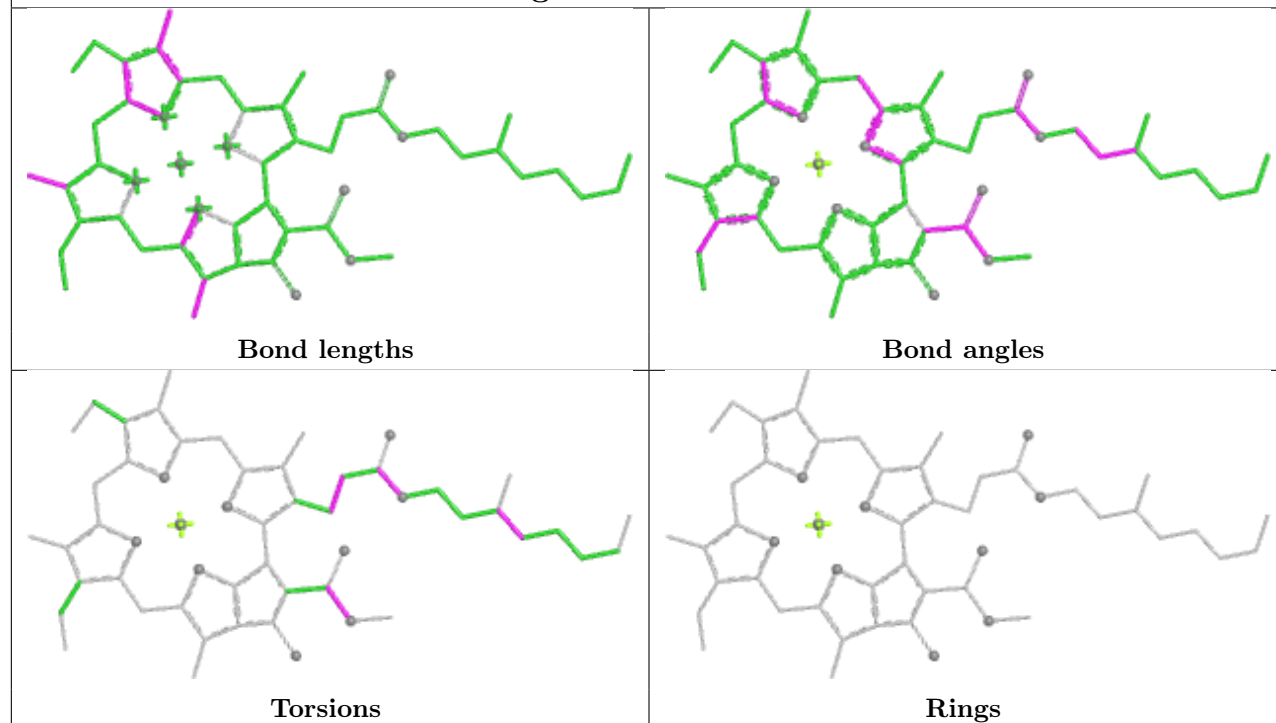


Rings

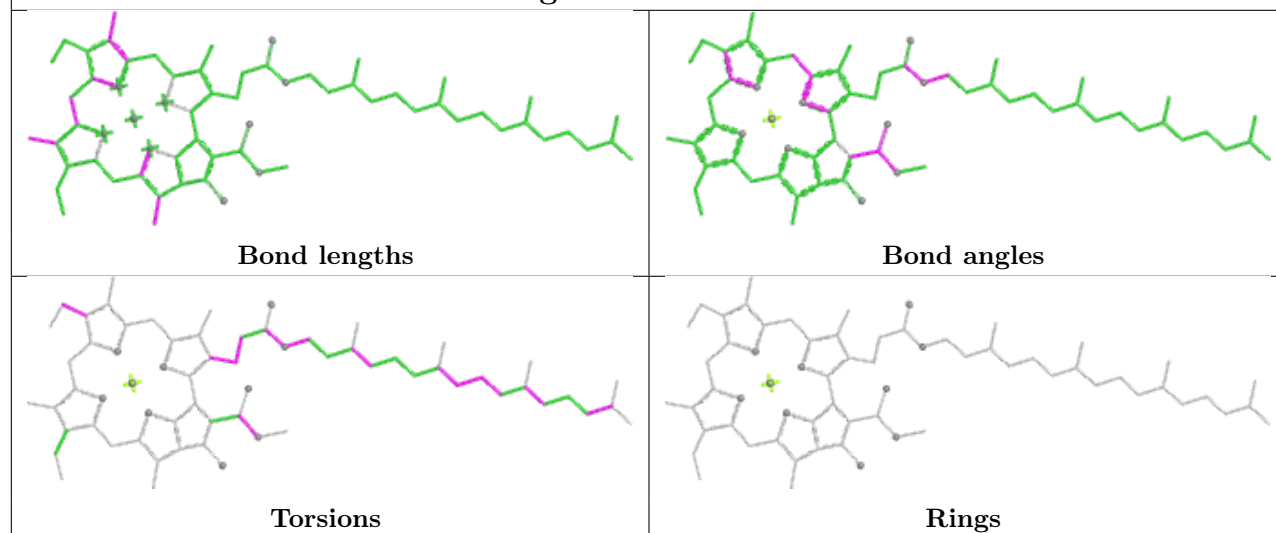




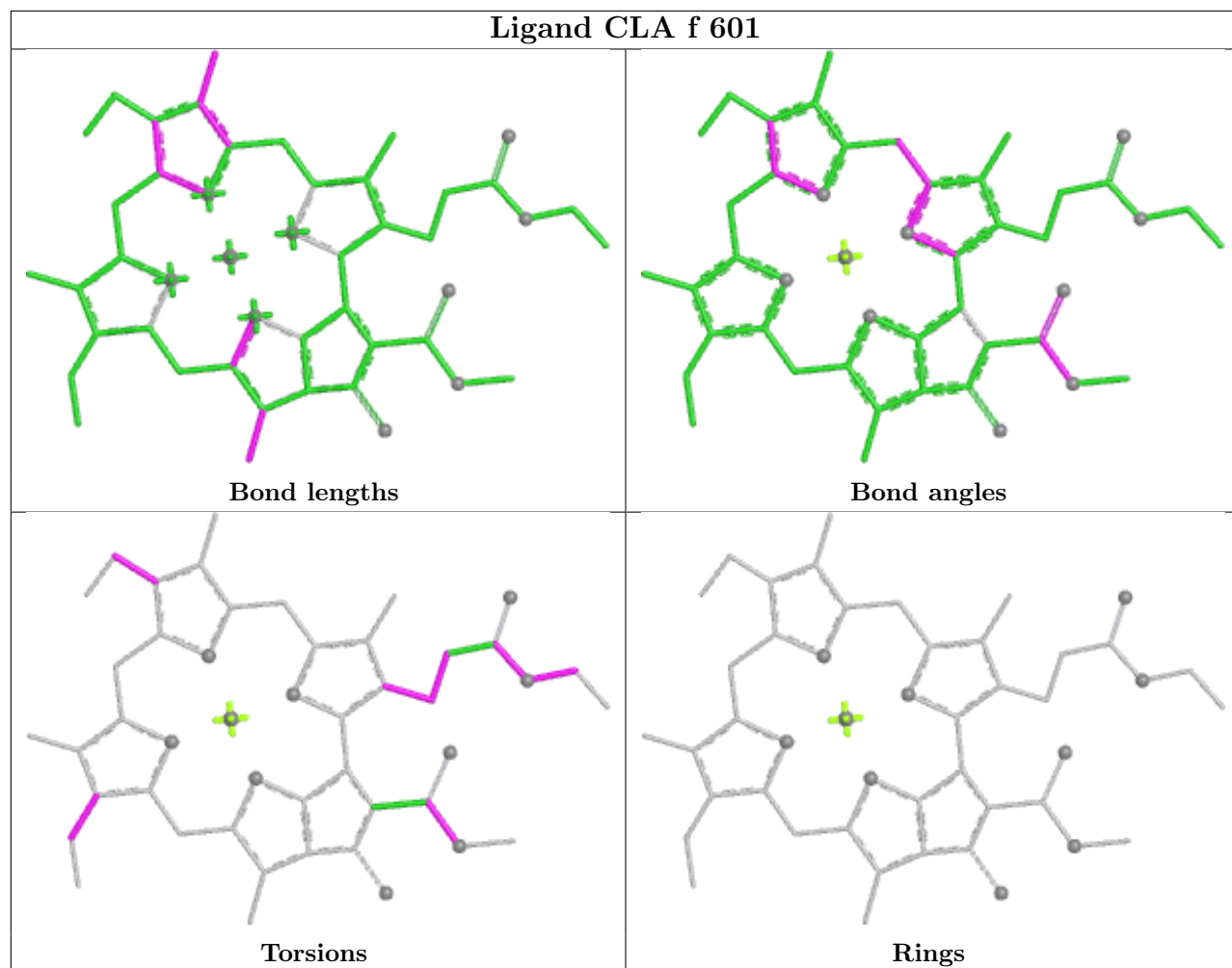
Ligand CLA A 811



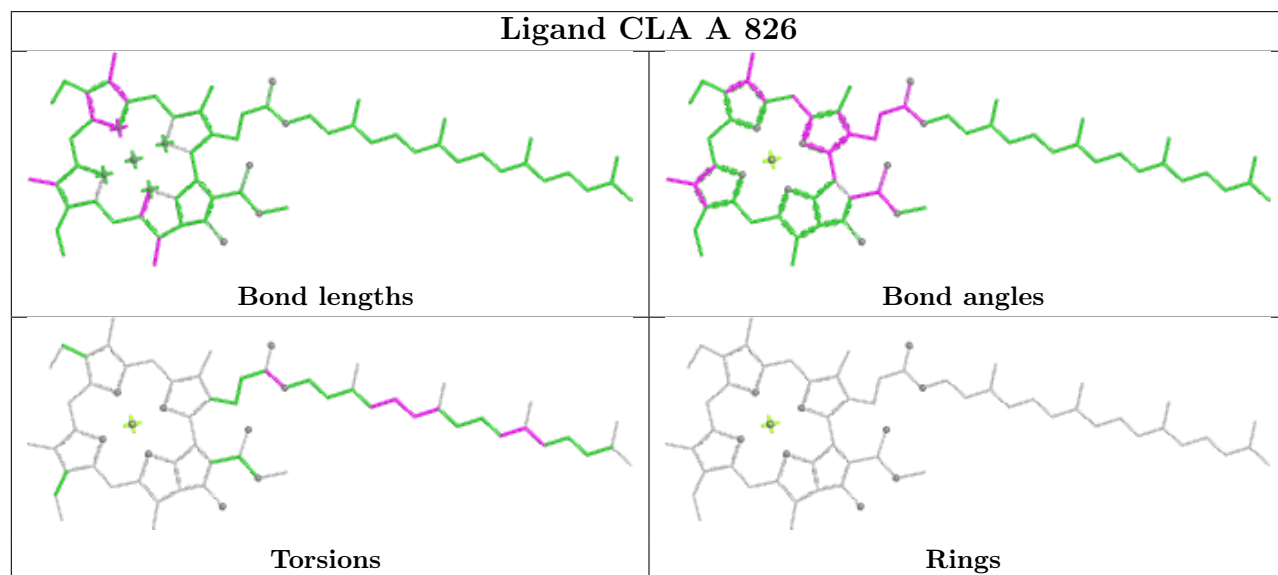
Ligand CLA f 602



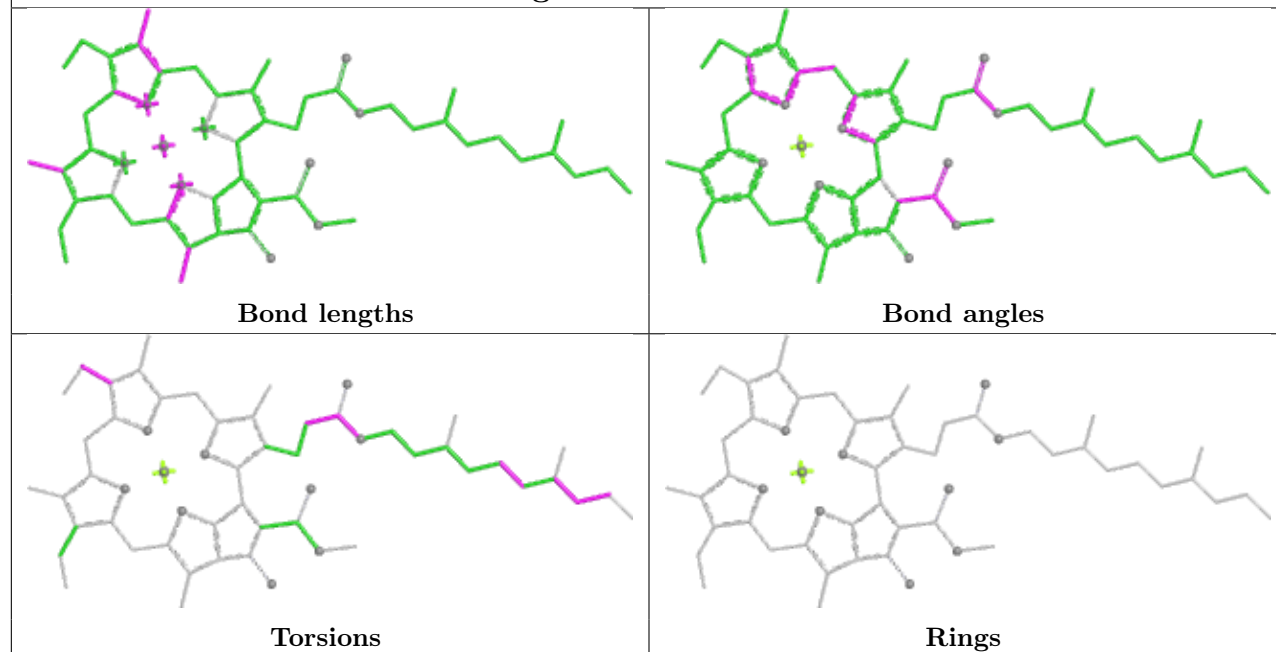
Ligand CLA f 601



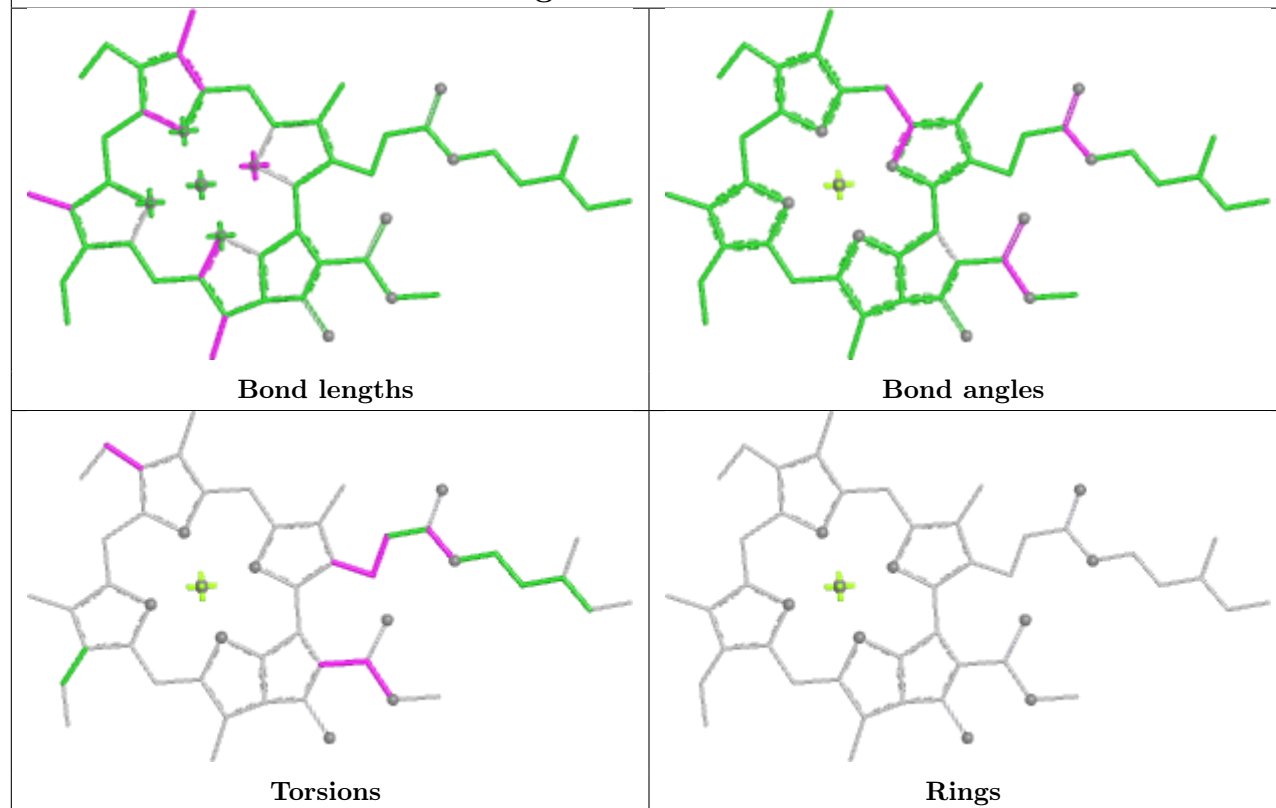
Ligand CLA A 826

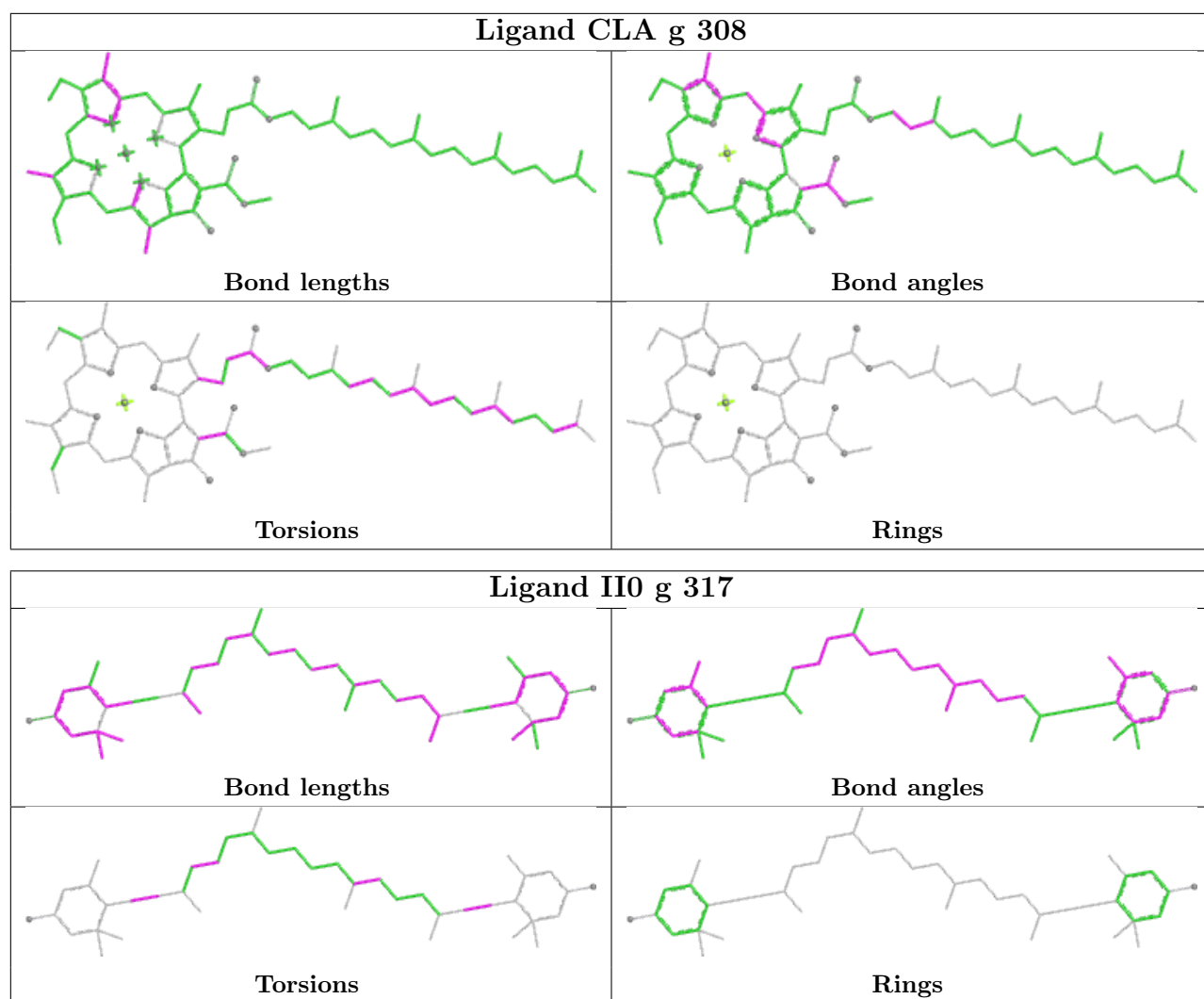


Ligand CLA B 838

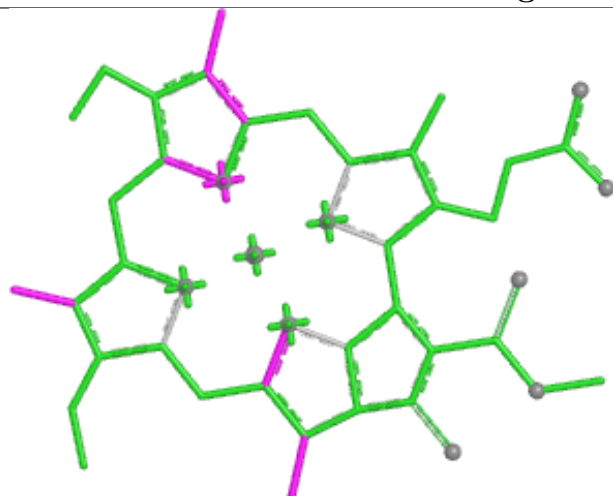


Ligand CLA d 306

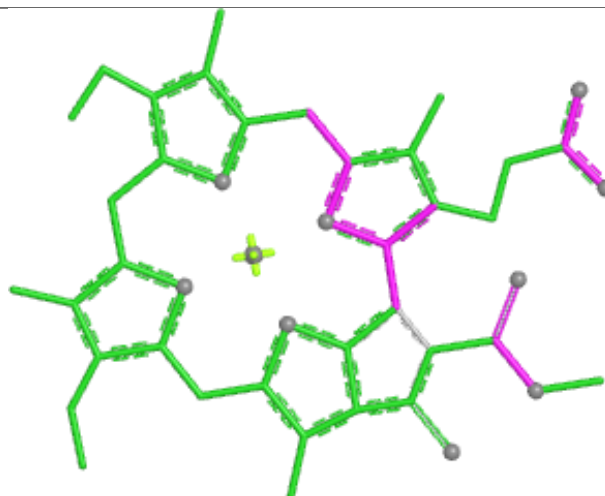




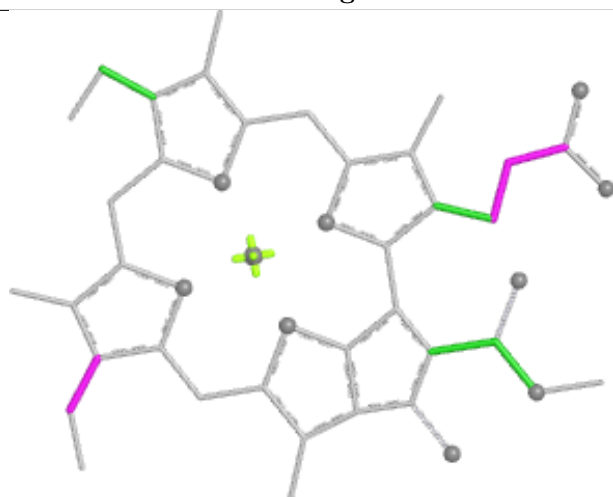
Ligand CLA k 605



Bond lengths



Bond angles

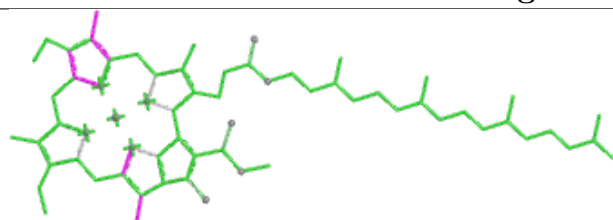


Torsions

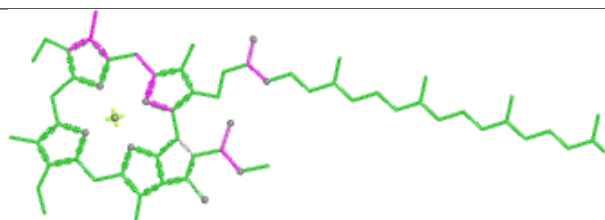


Rings

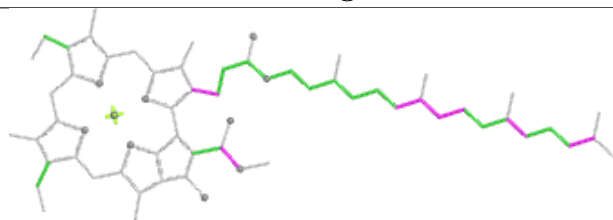
Ligand CLA k 608



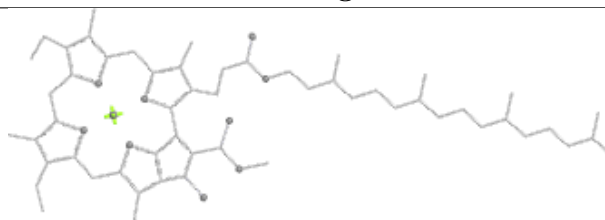
Bond lengths



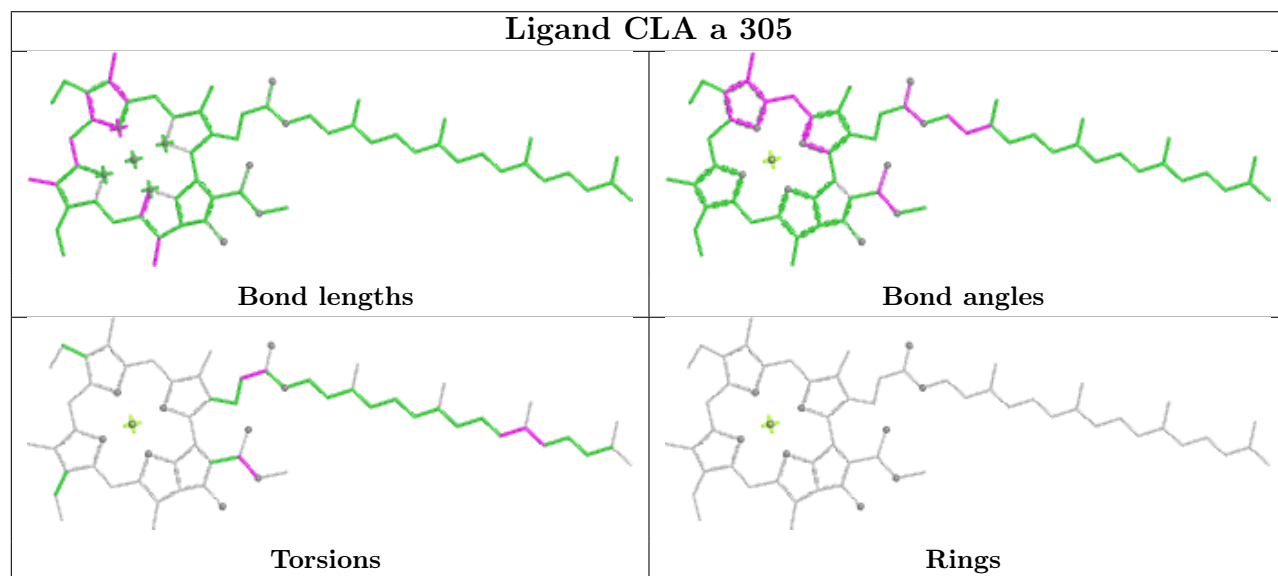
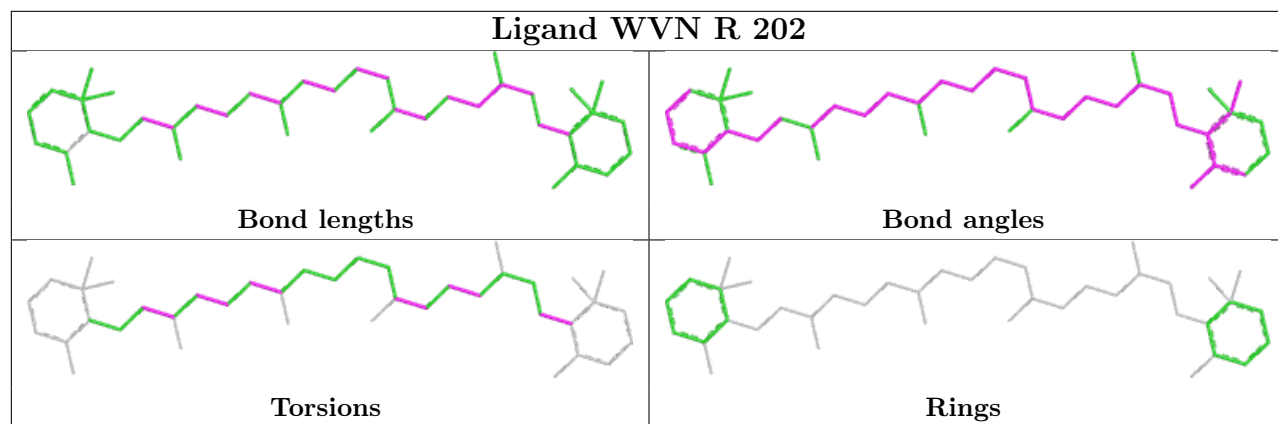
Bond angles



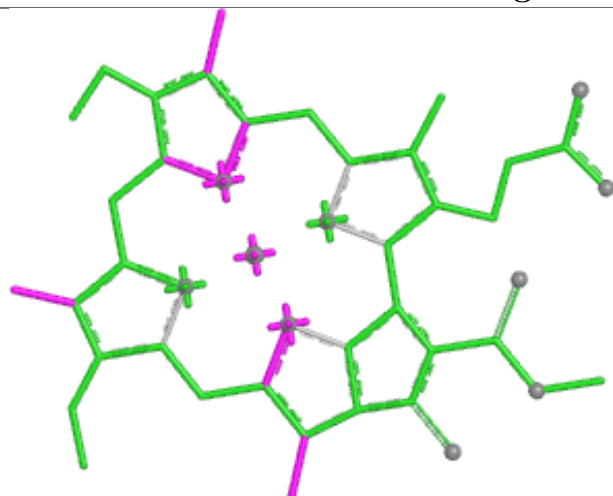
Torsions



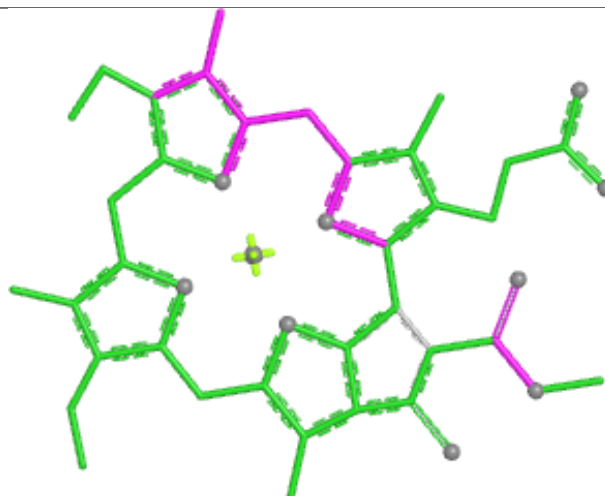
Rings



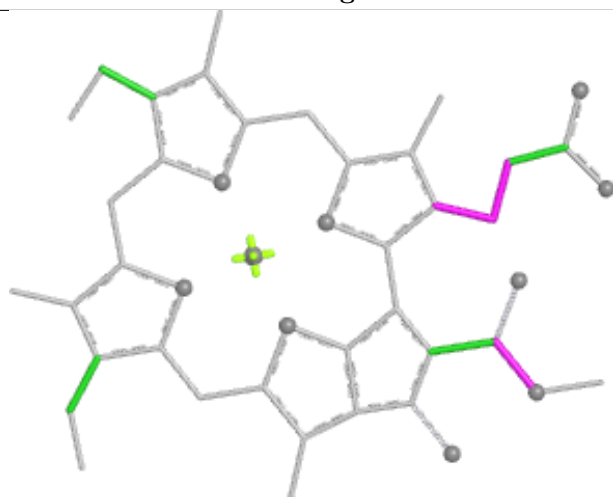
Ligand CLA A 815



Bond lengths



Bond angles

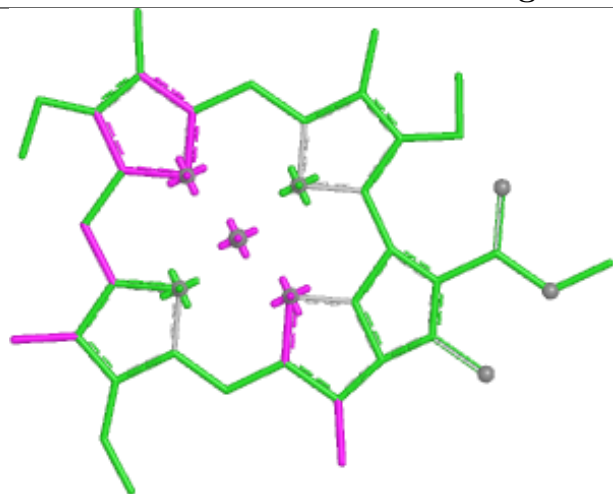


Torsions



Rings

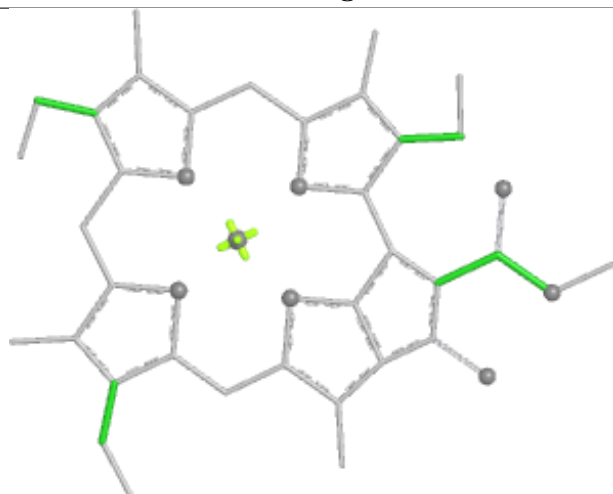
Ligand CLA g 302



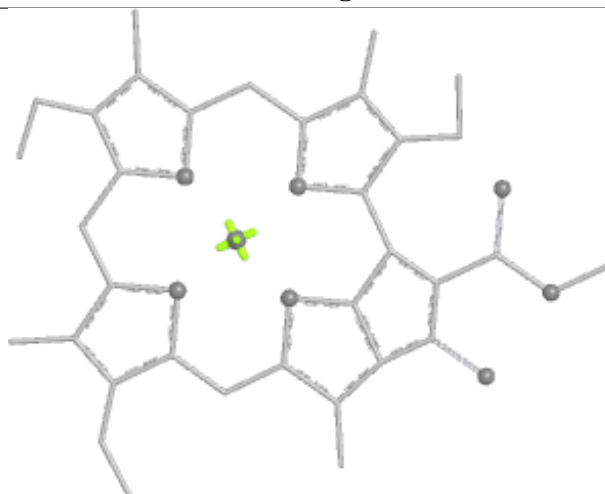
Bond lengths



Bond angles

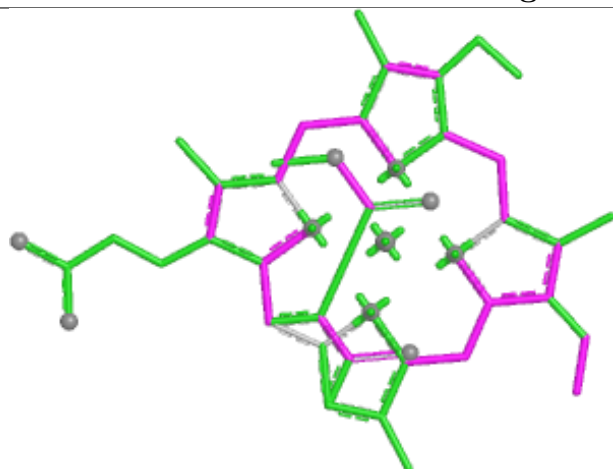


Torsions

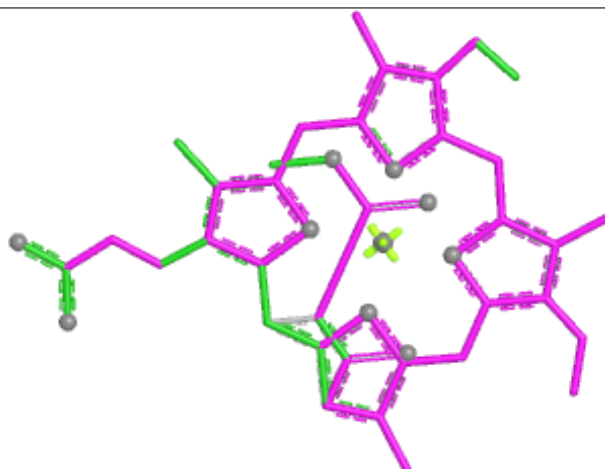


Rings

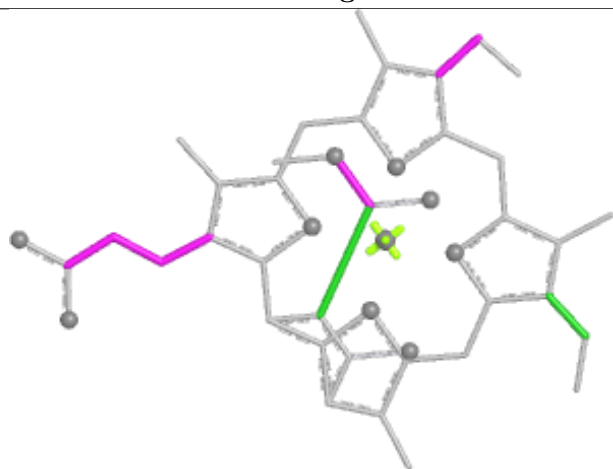
Ligand KC2 k 612



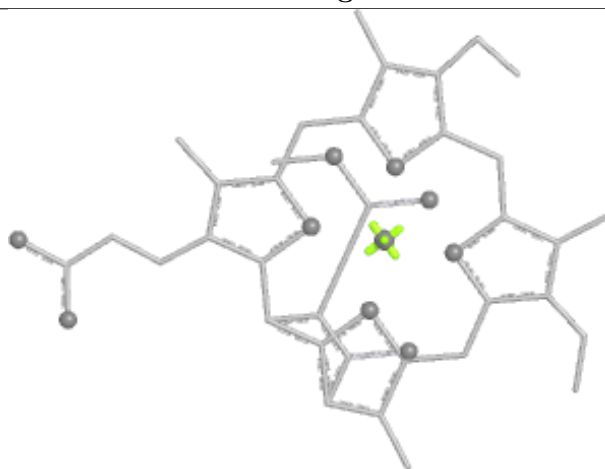
Bond lengths



Bond angles

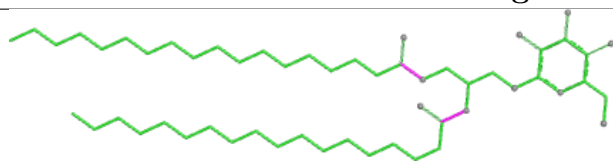


Torsions

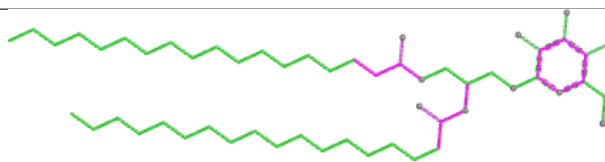


Rings

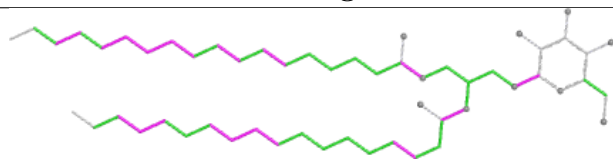
Ligand LMG L 208



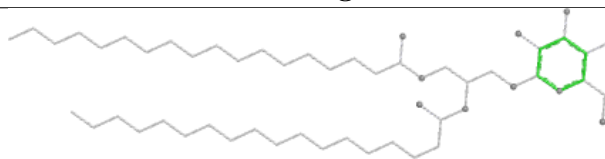
Bond lengths



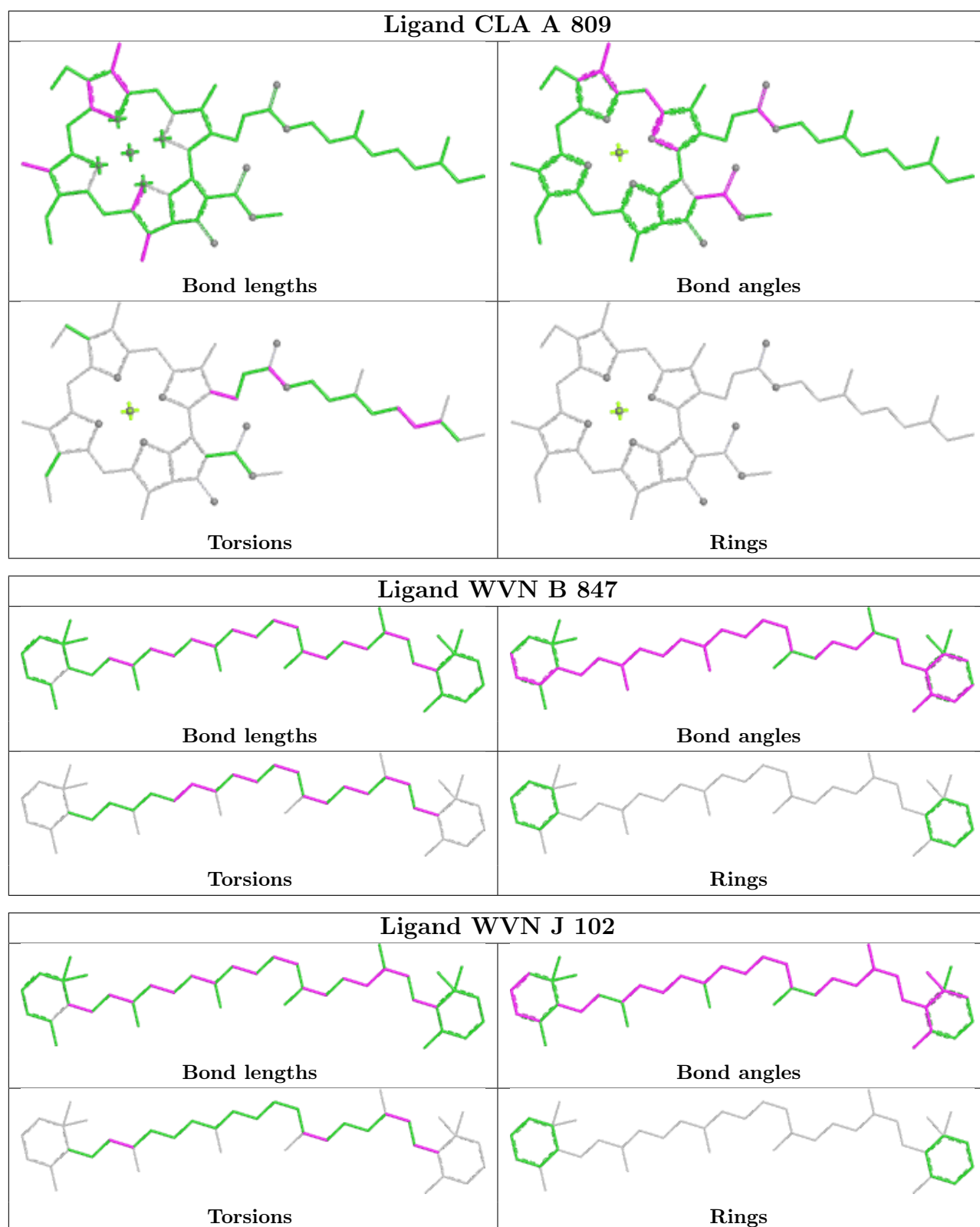
Bond angles



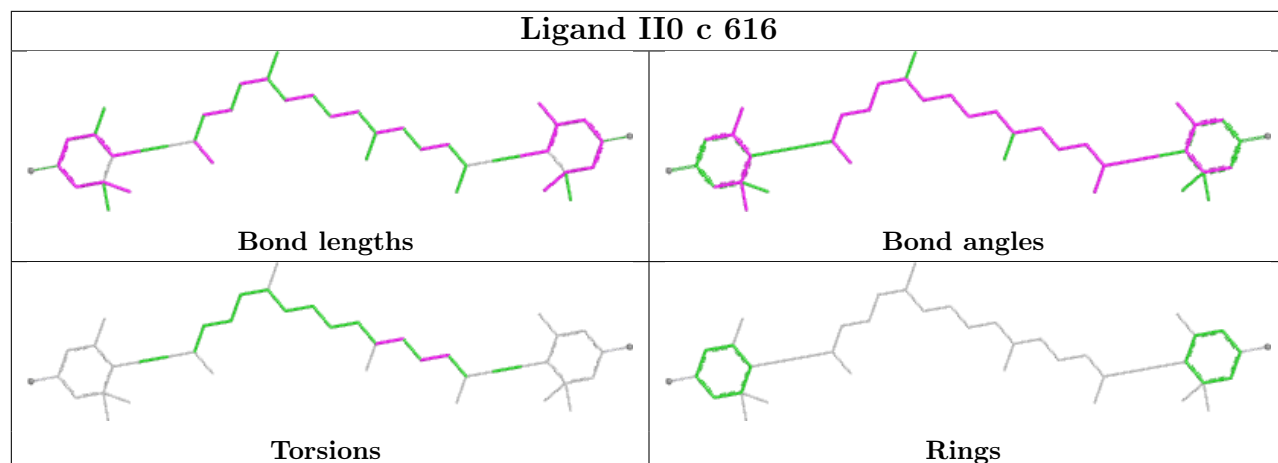
Torsions



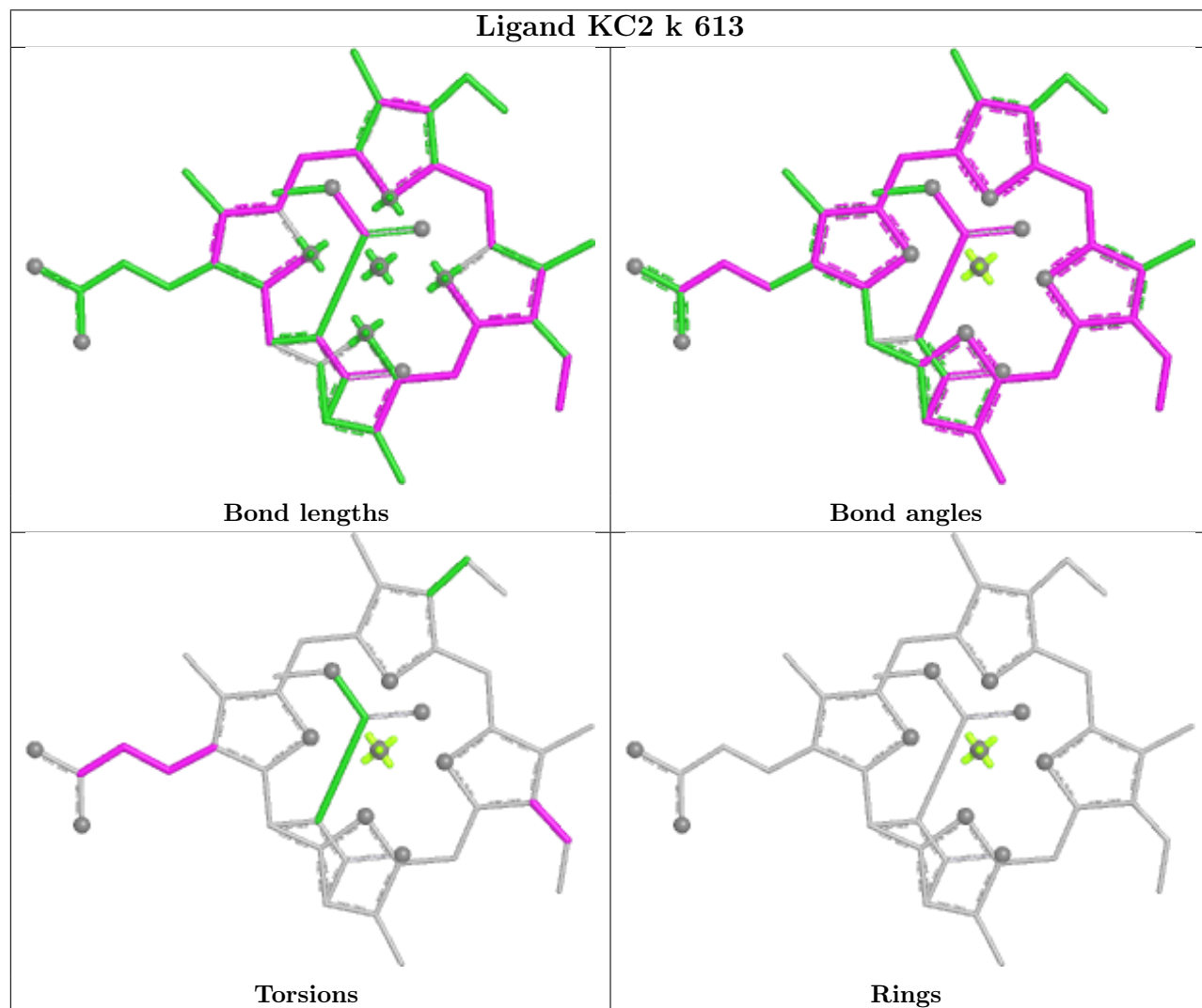
Rings

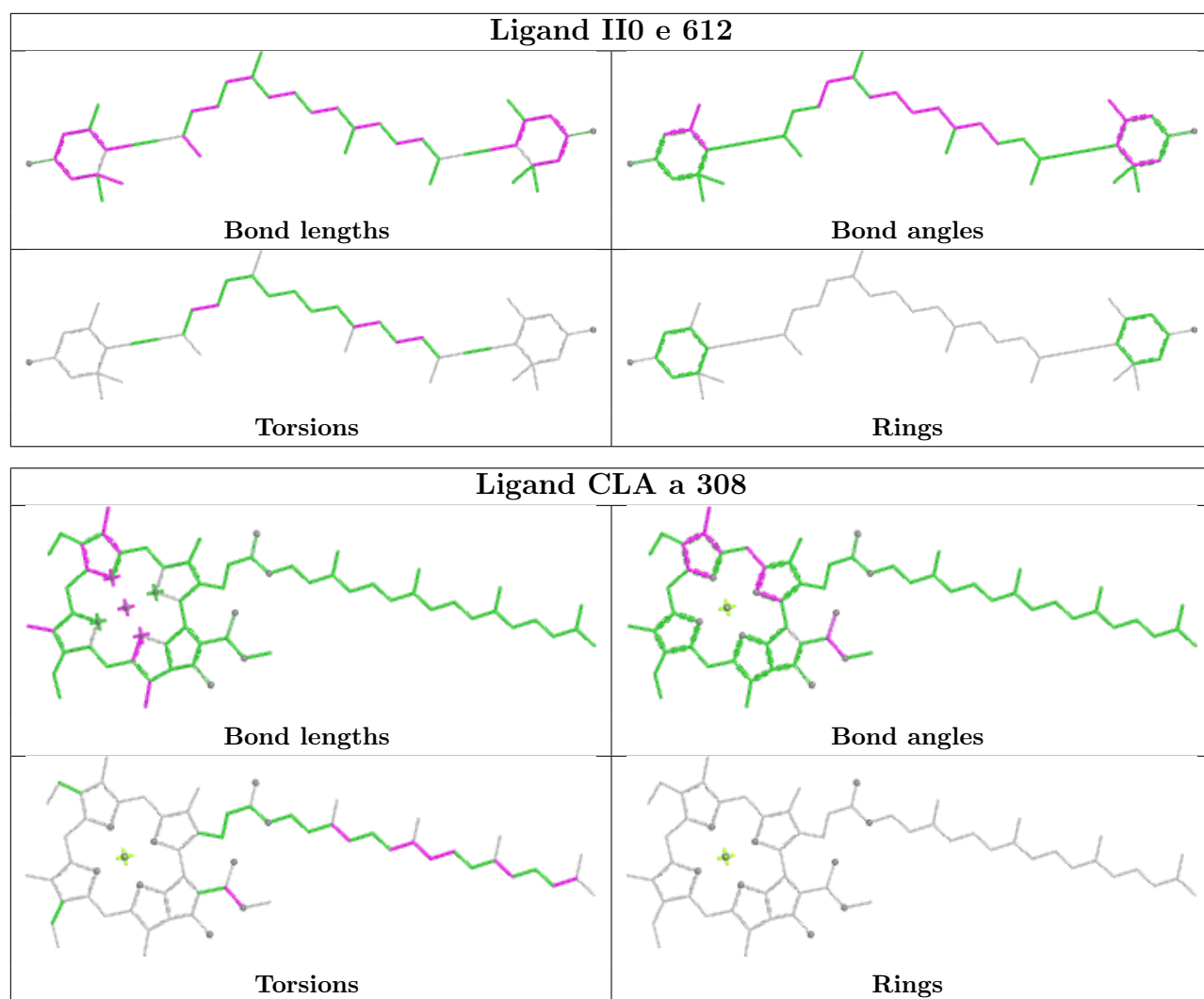


Ligand II0 c 616

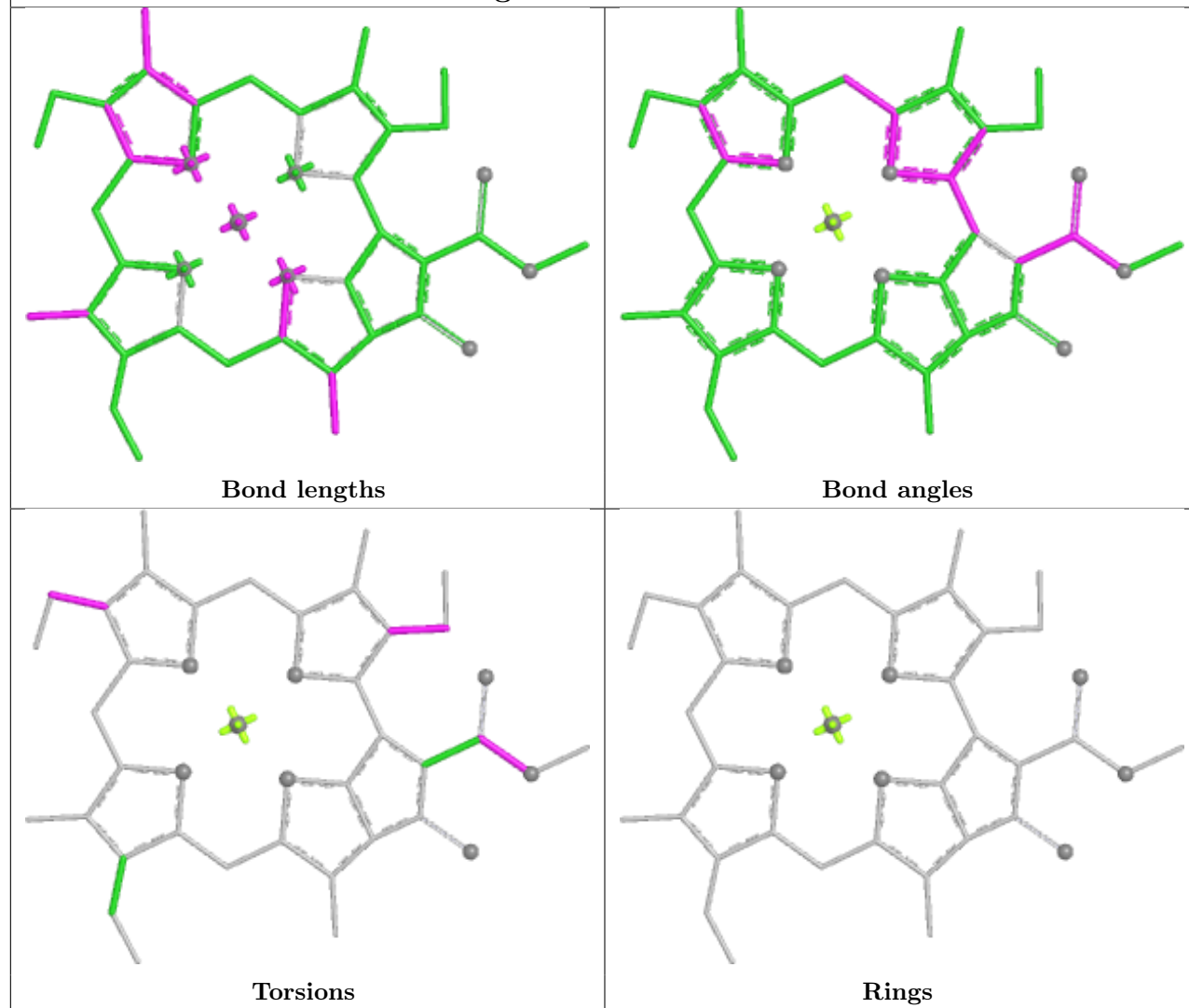


Ligand KC2 k 613

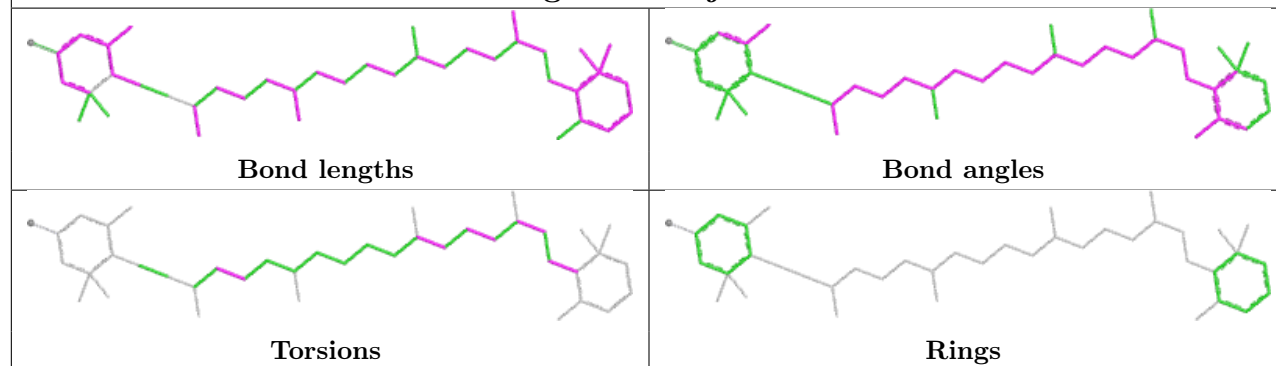




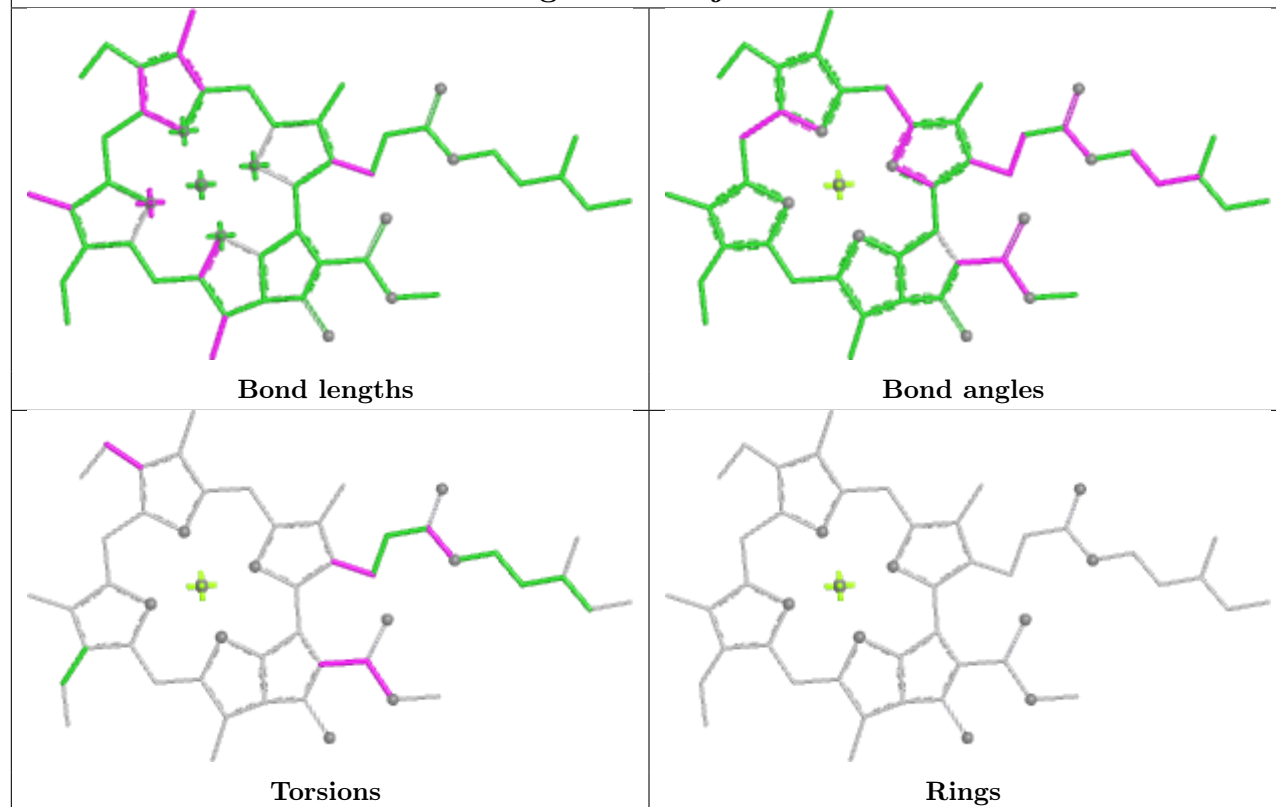
Ligand CLA K 102



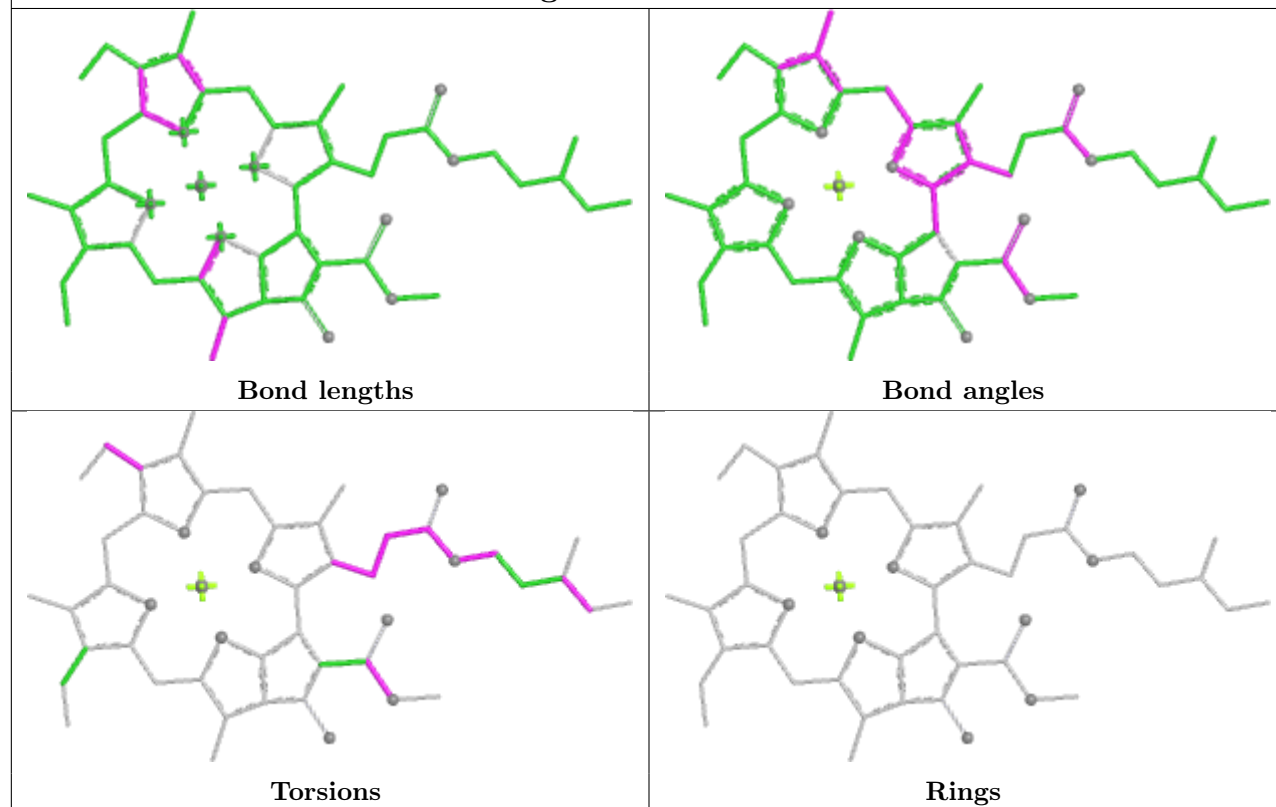
Ligand IHT j 317



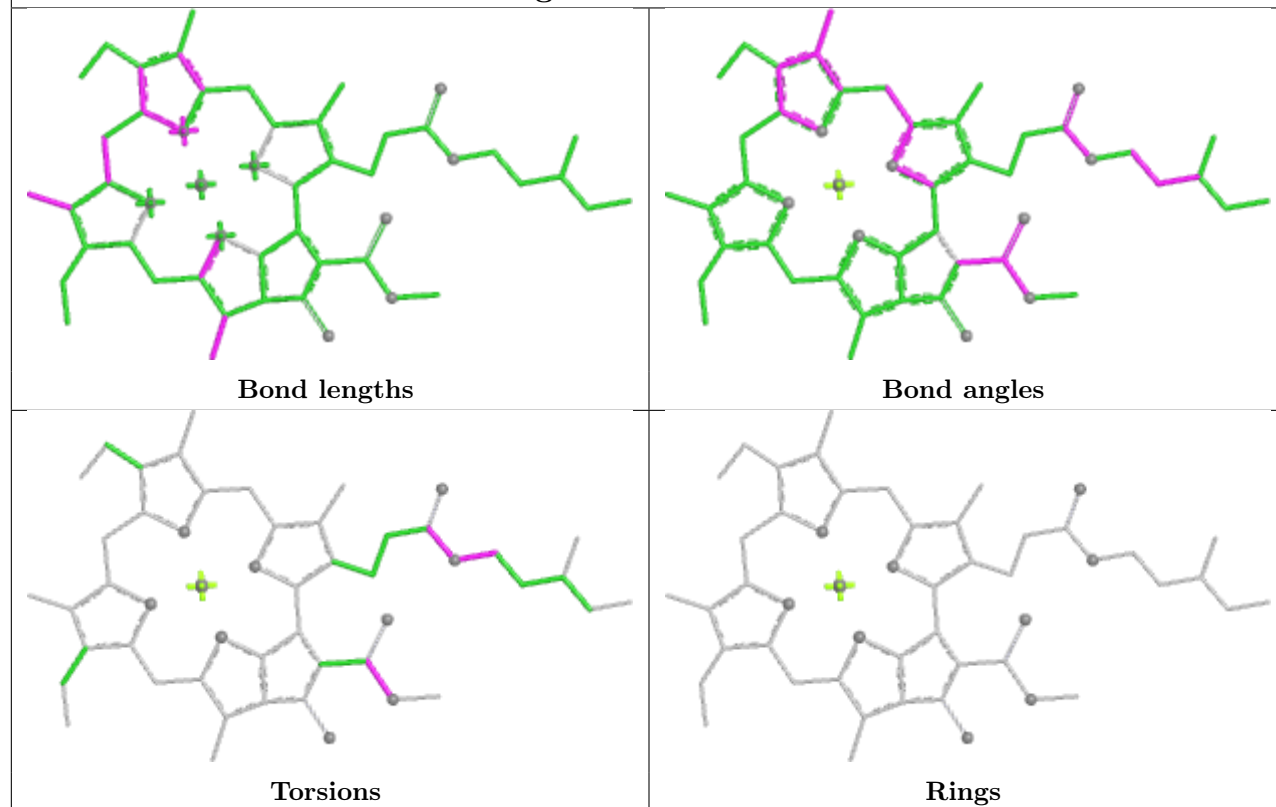
Ligand CLA j 307



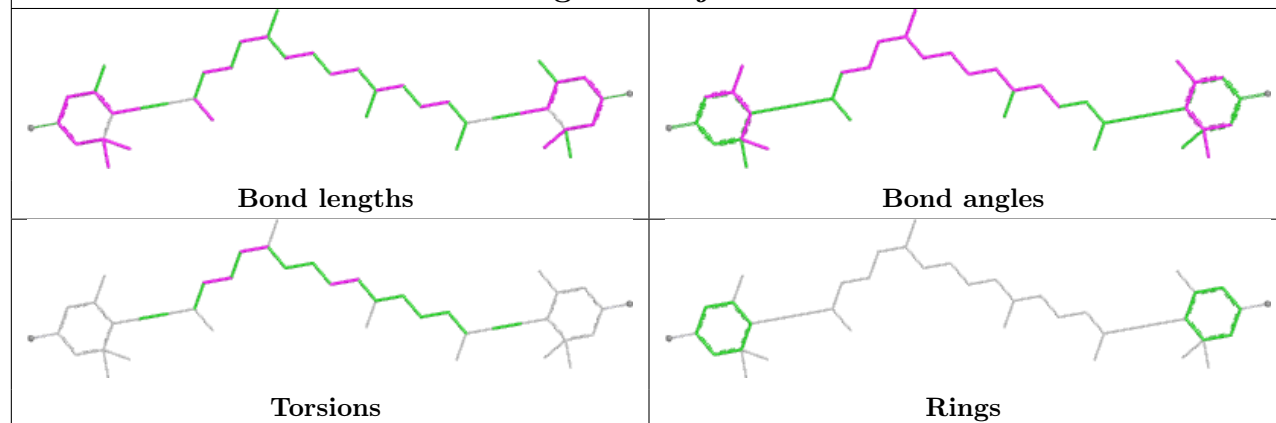
Ligand CLA i 611

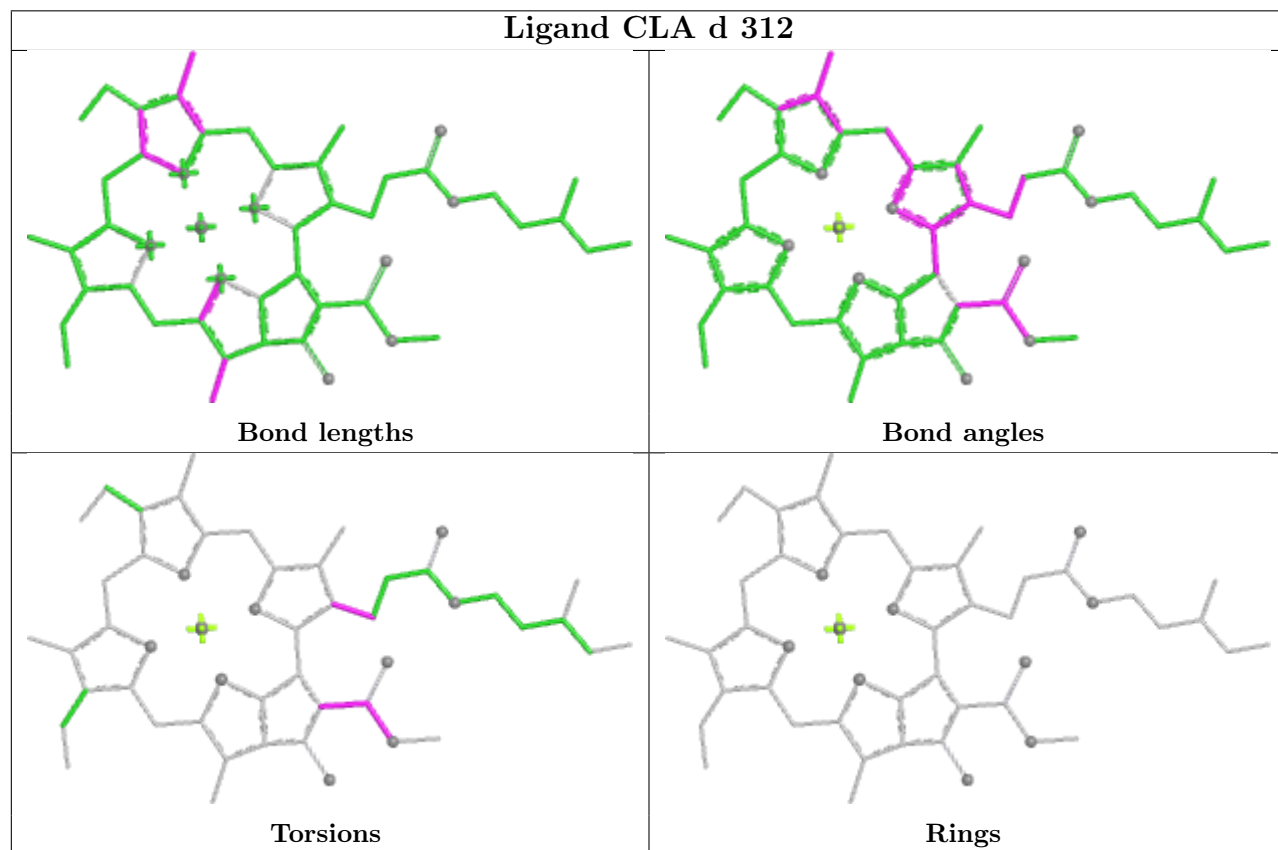
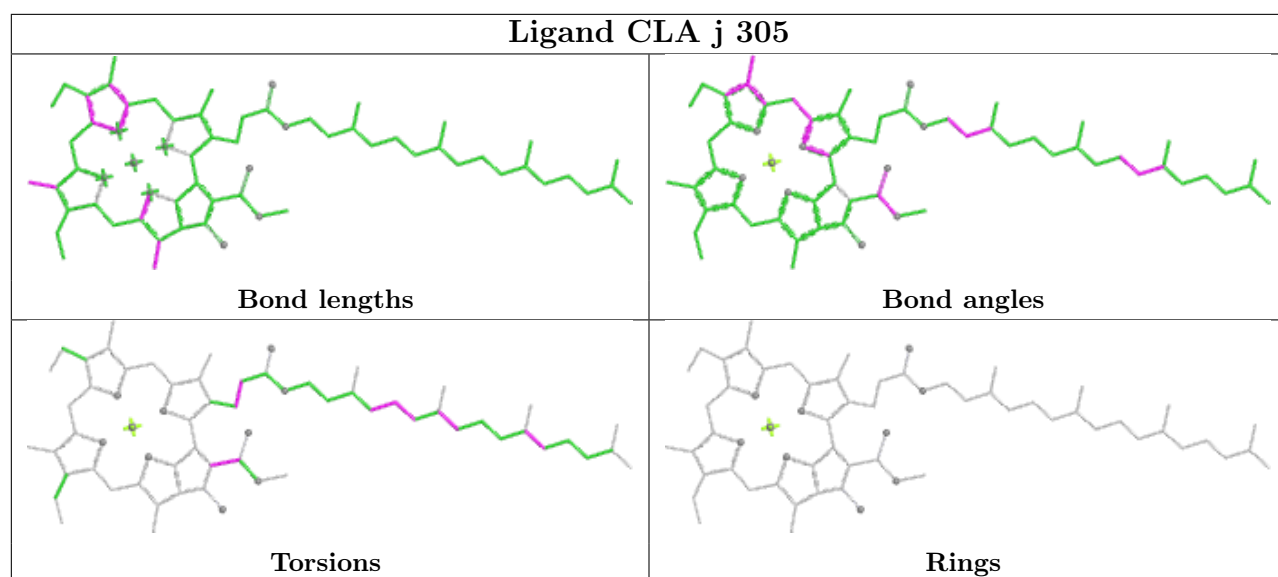


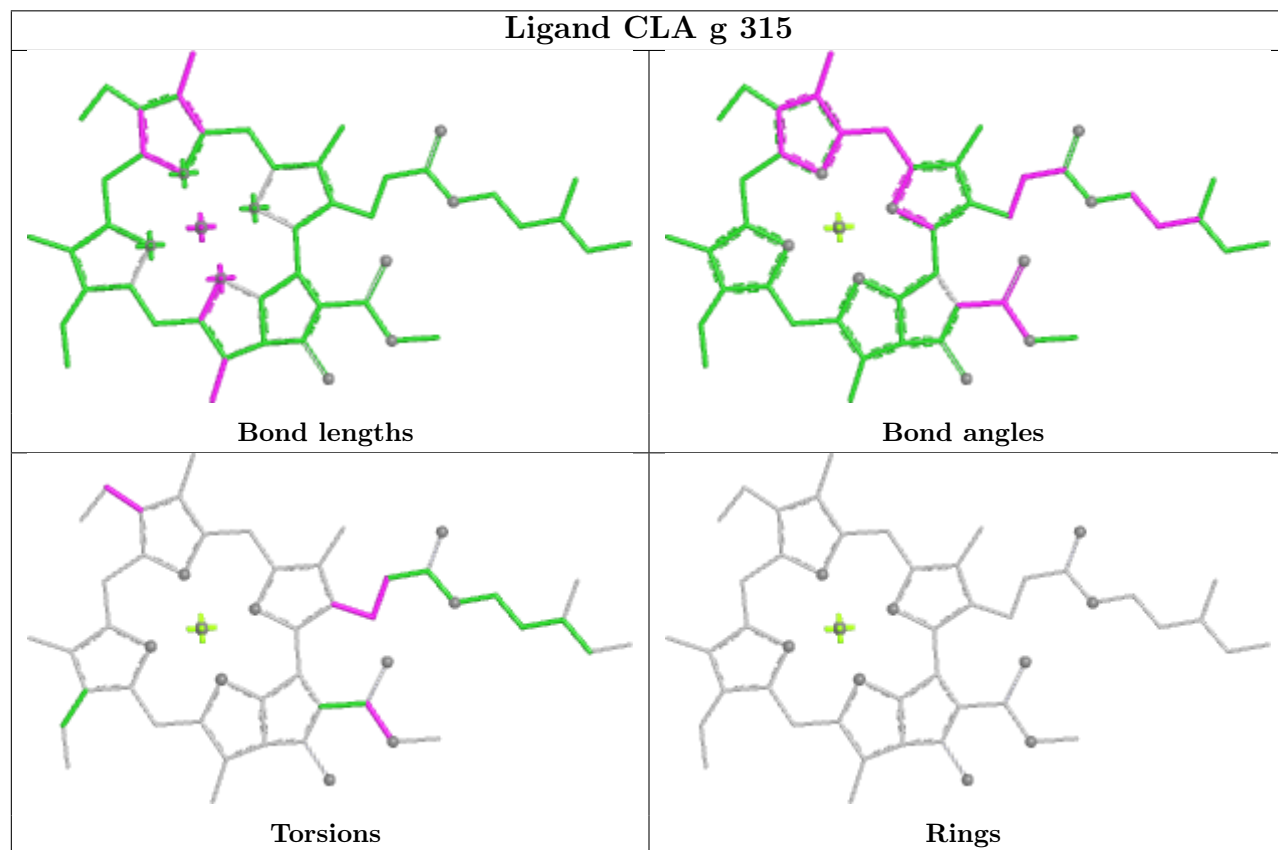
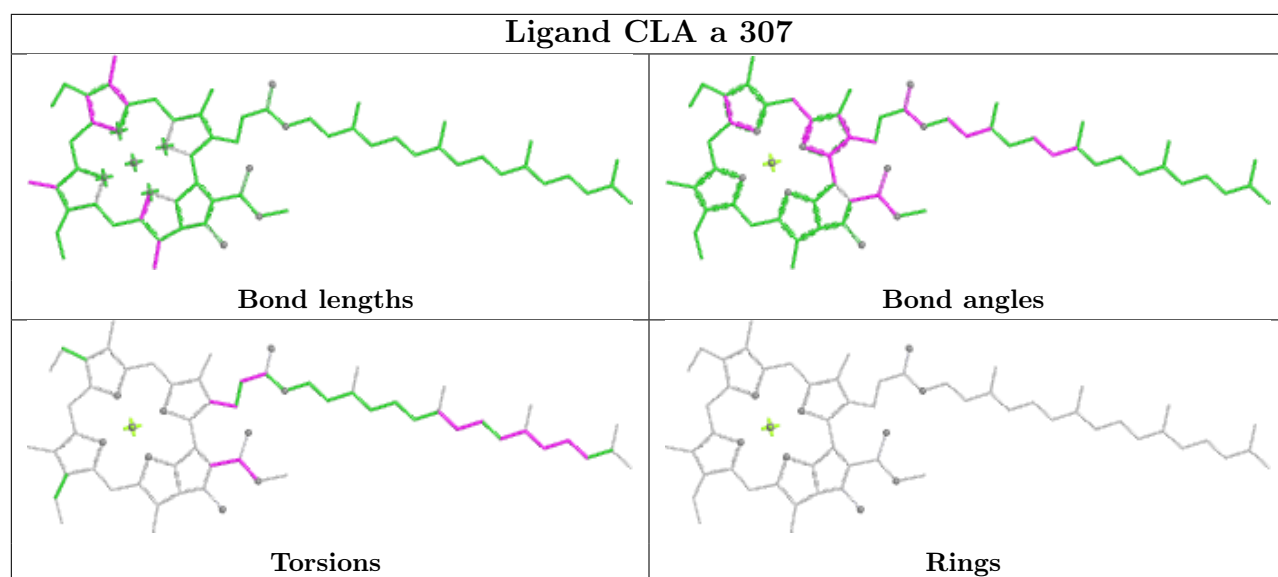
Ligand CLA b 311



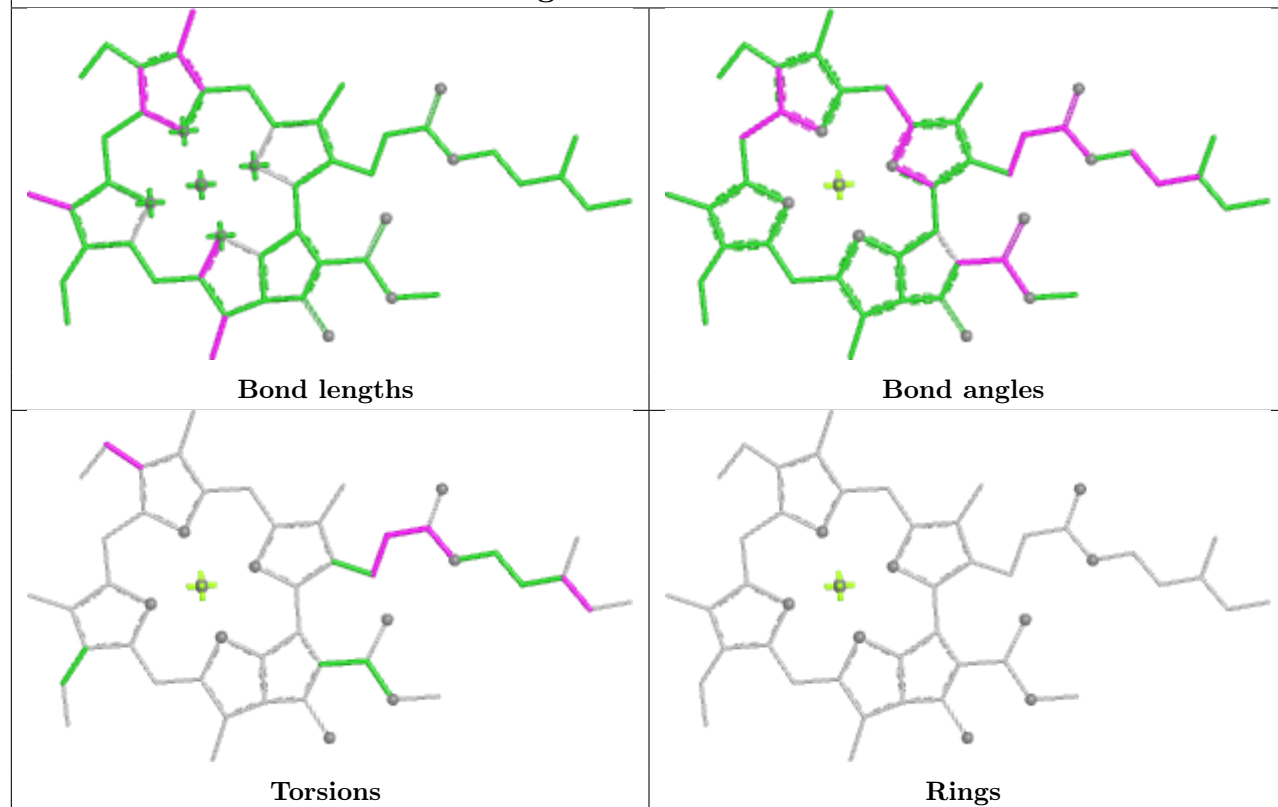
Ligand II0 j 315



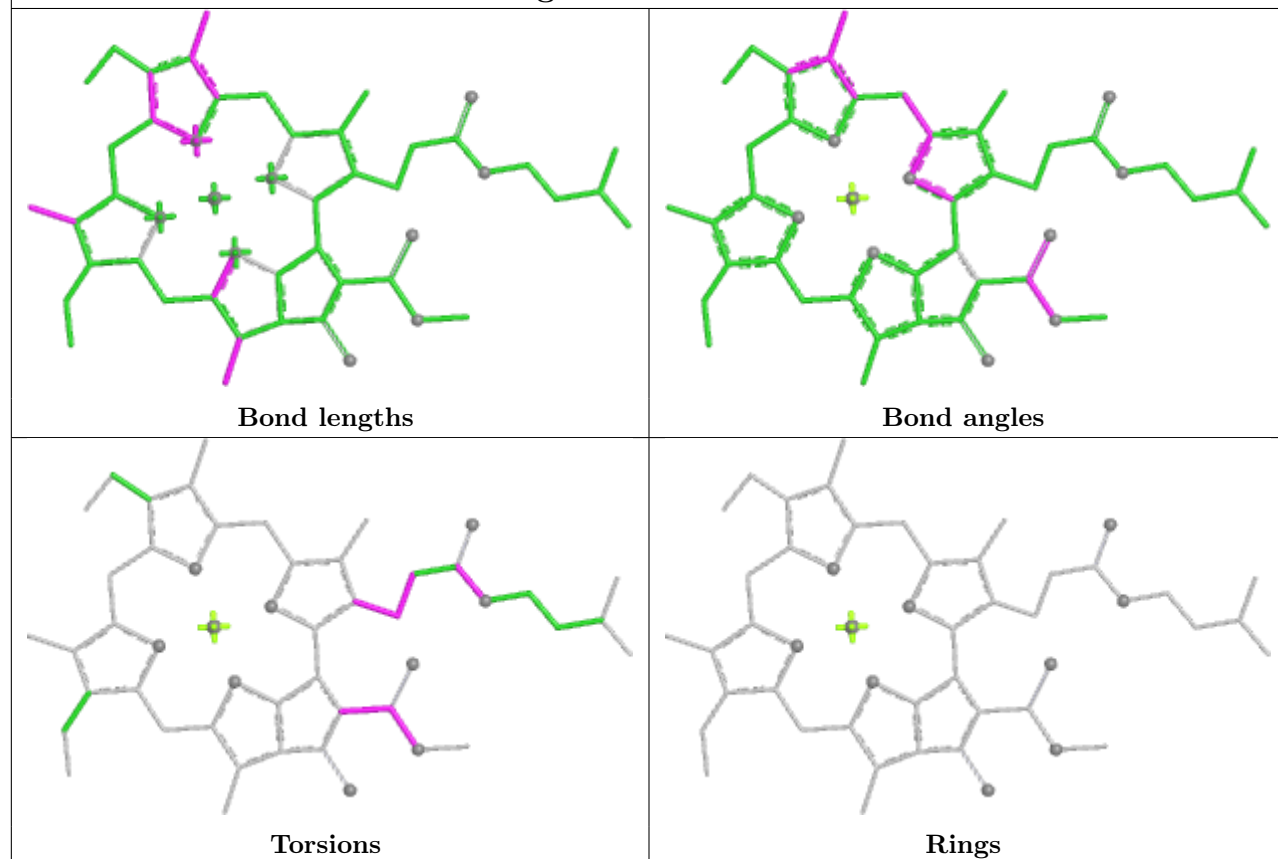




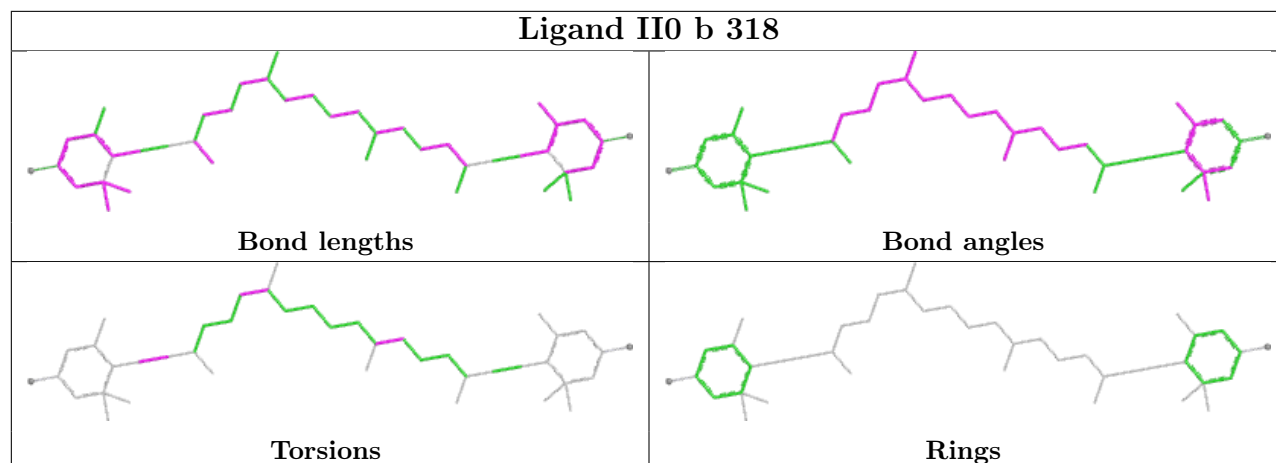
Ligand CLA c 605



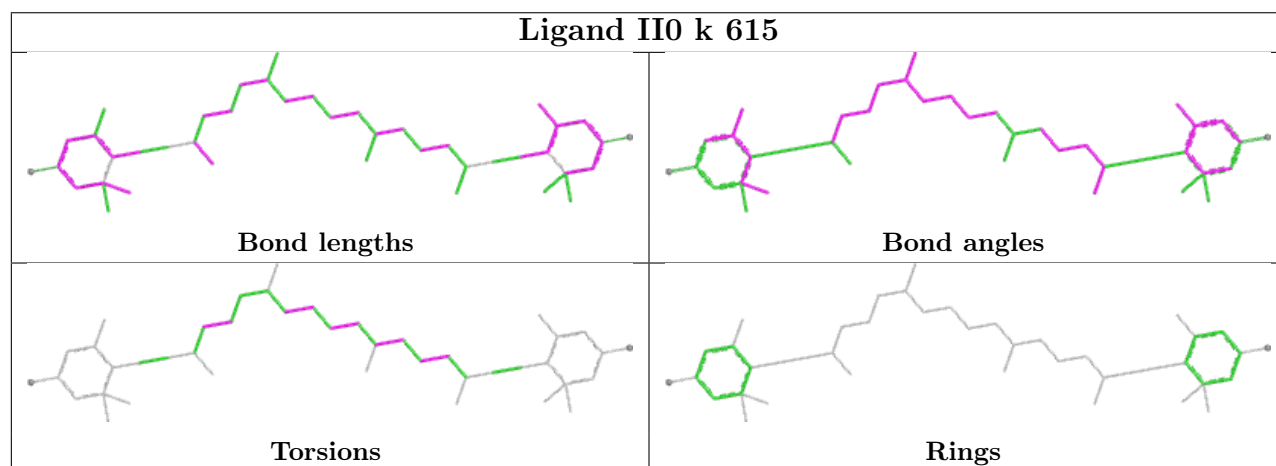
Ligand CLA e 602



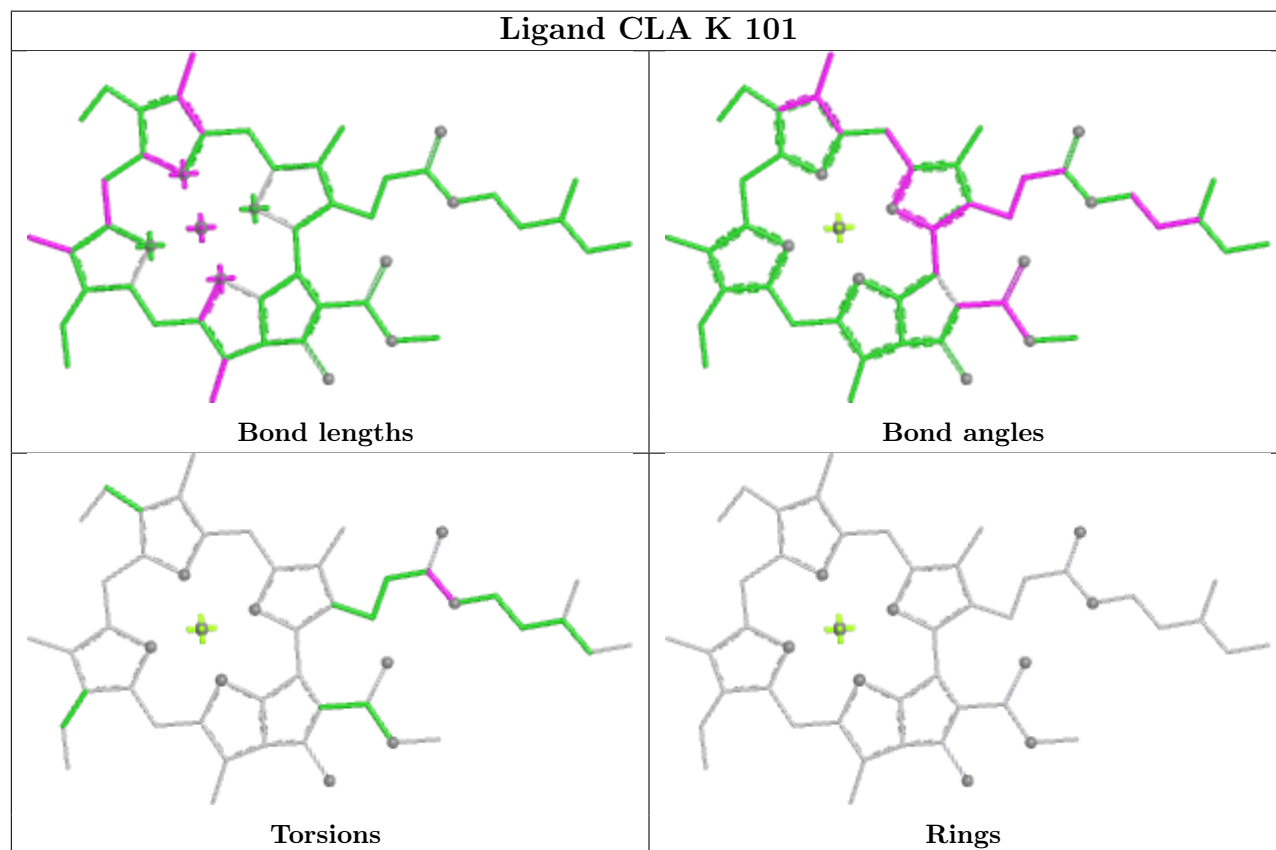
Ligand II0 b 318



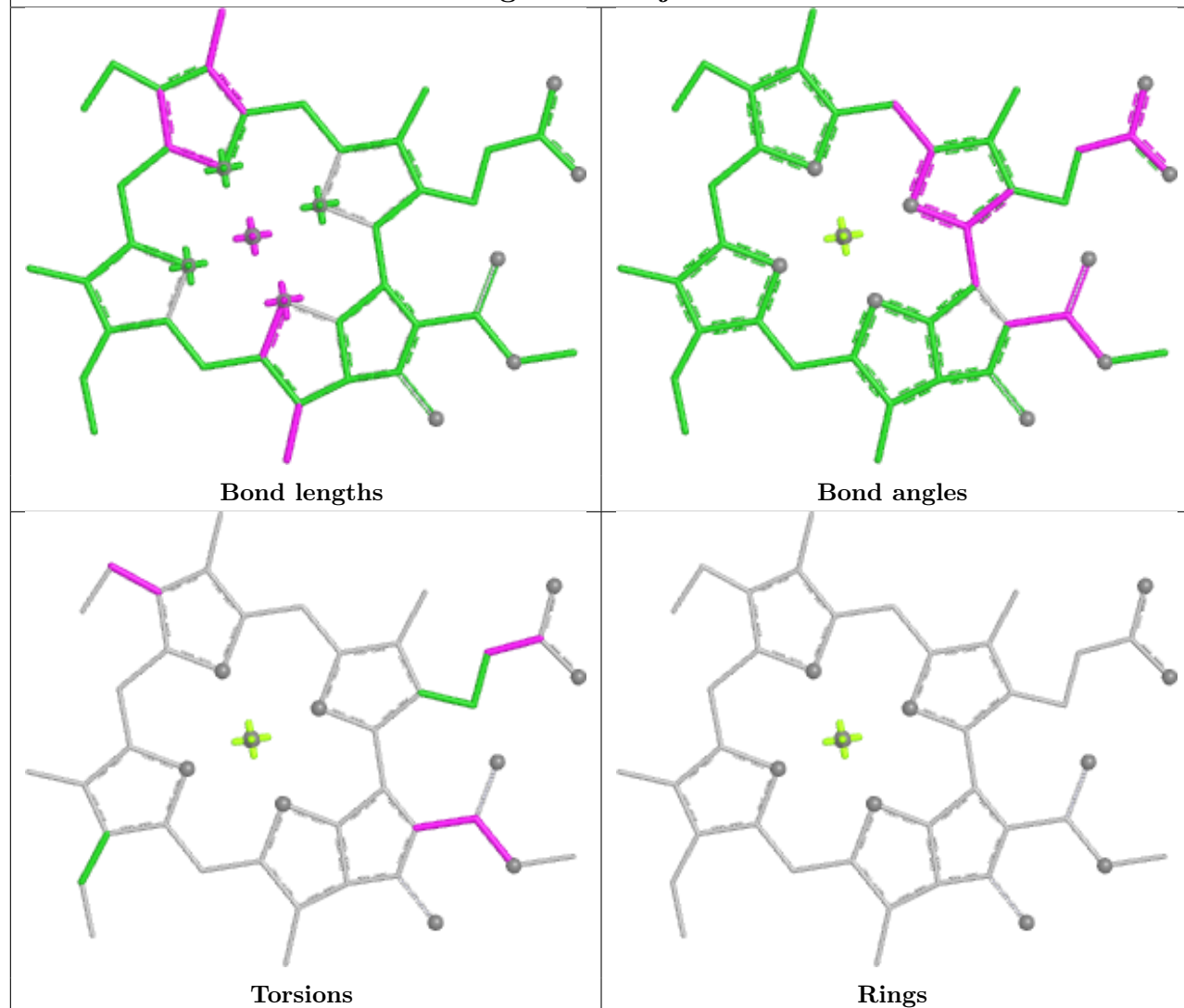
Ligand II0 k 615



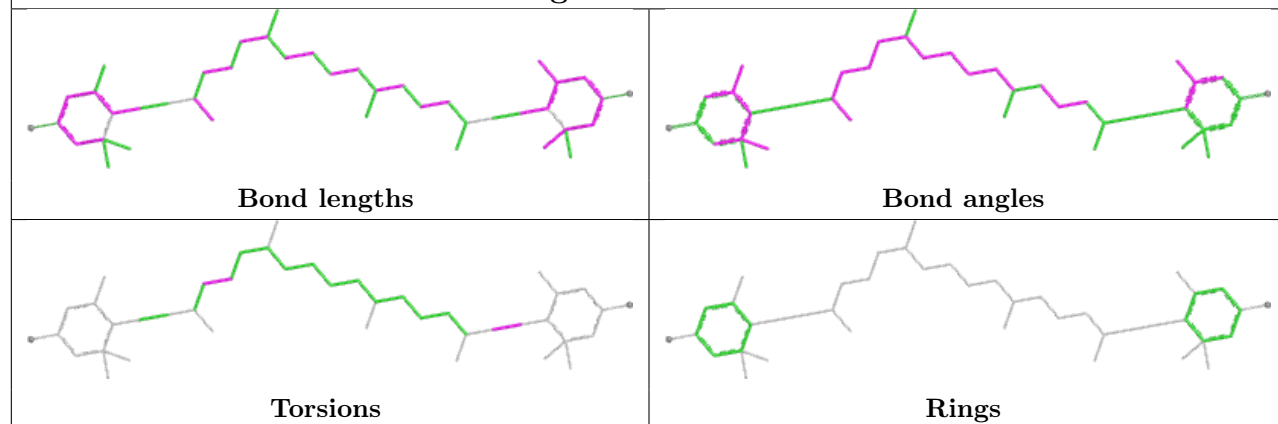
Ligand CLA K 101

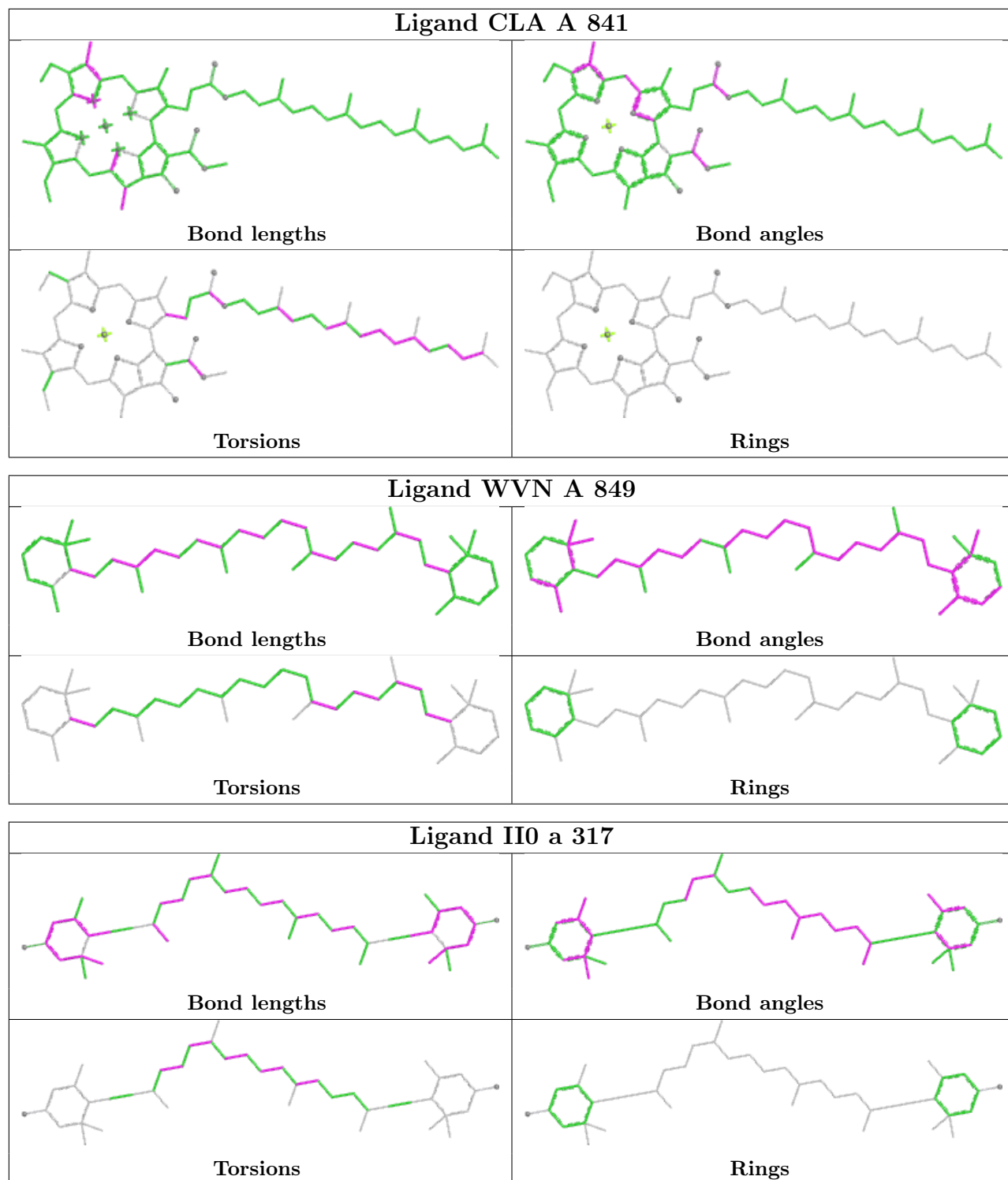


Ligand CLA j 306

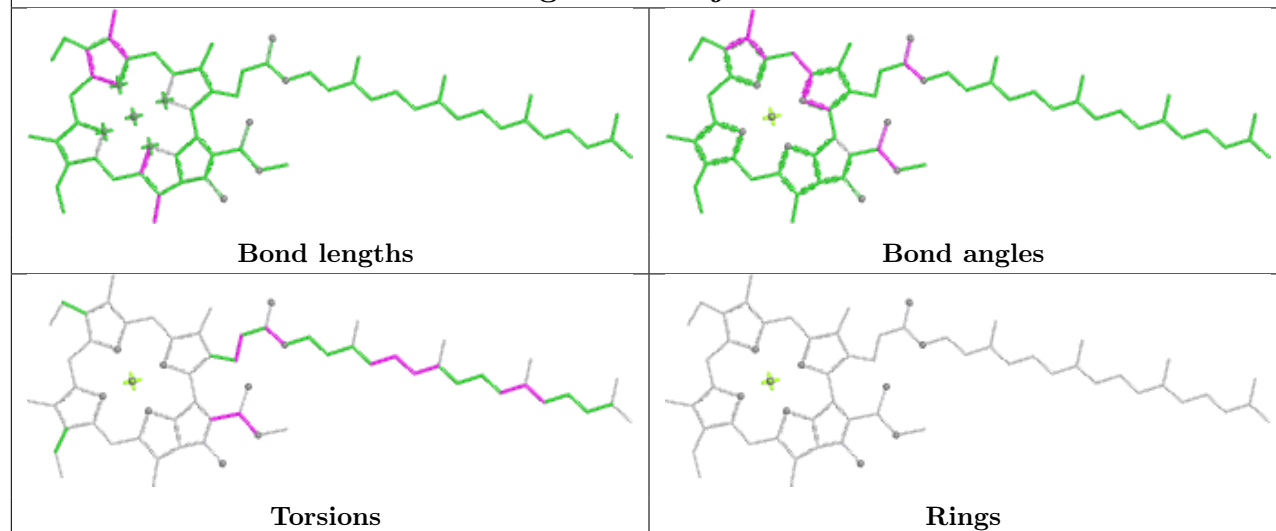


Ligand II0 k 617

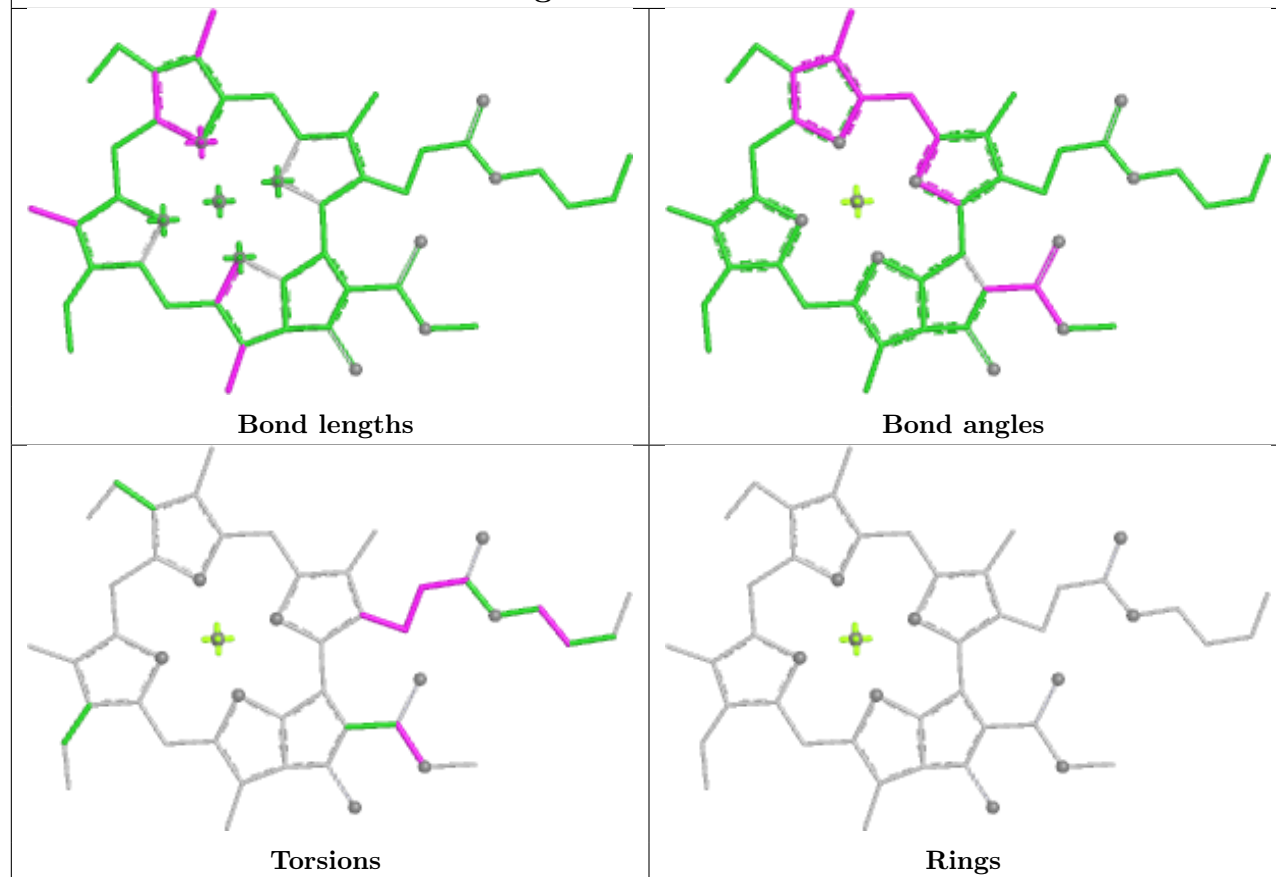


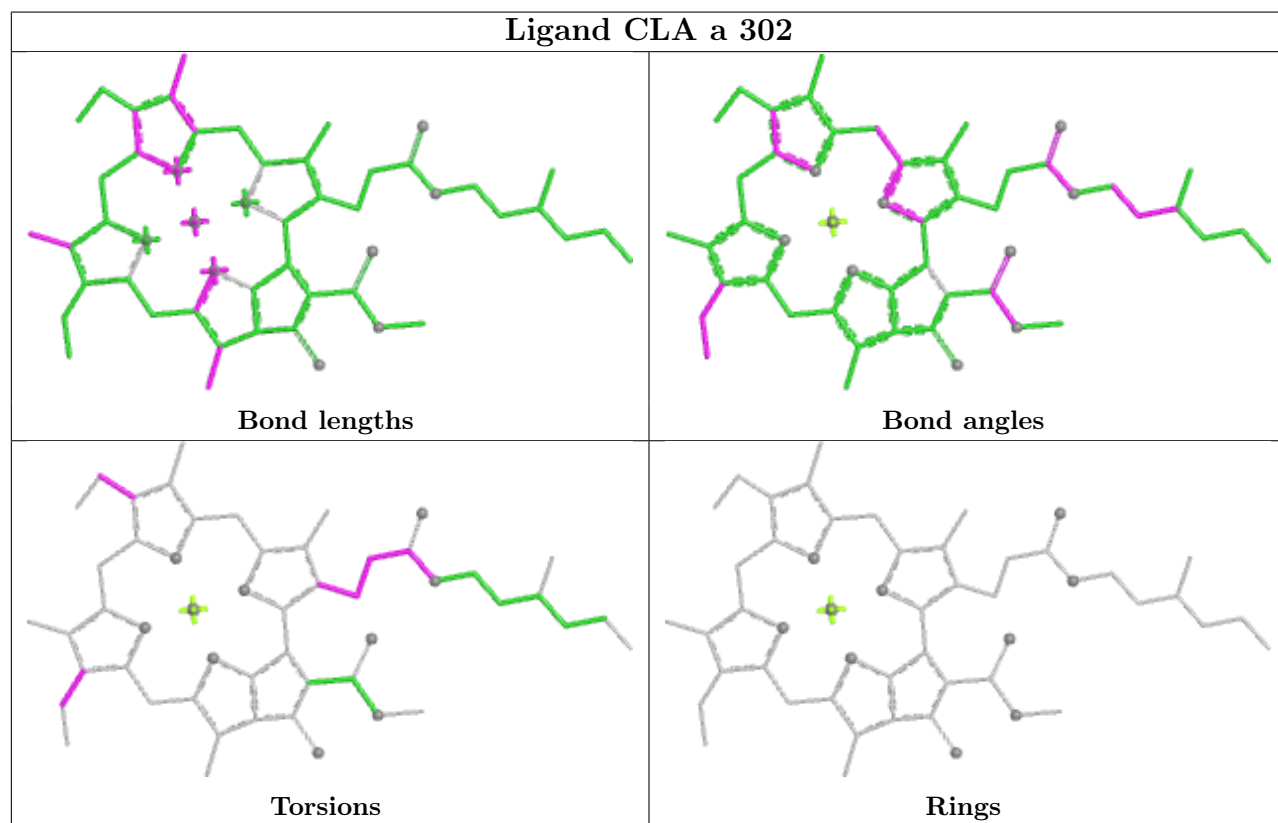
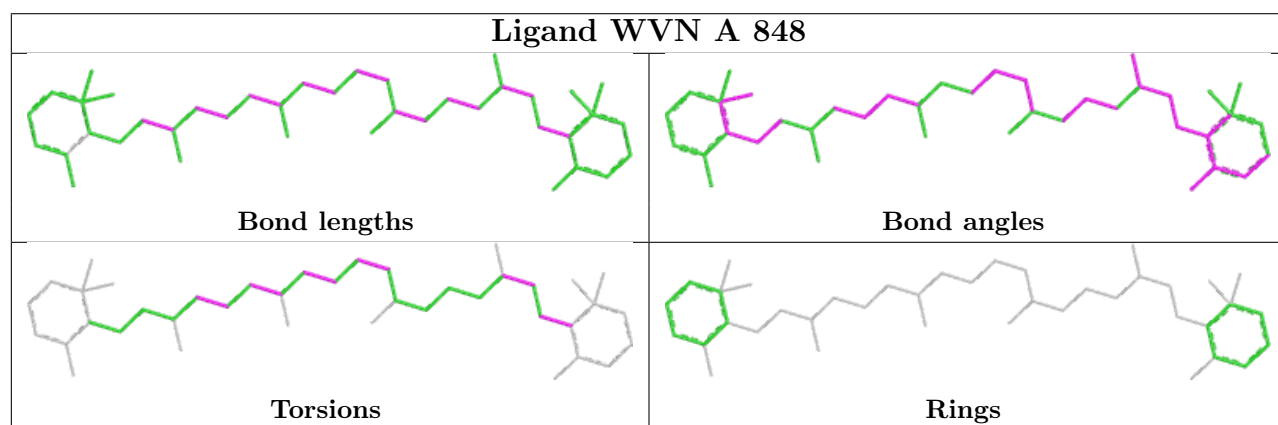
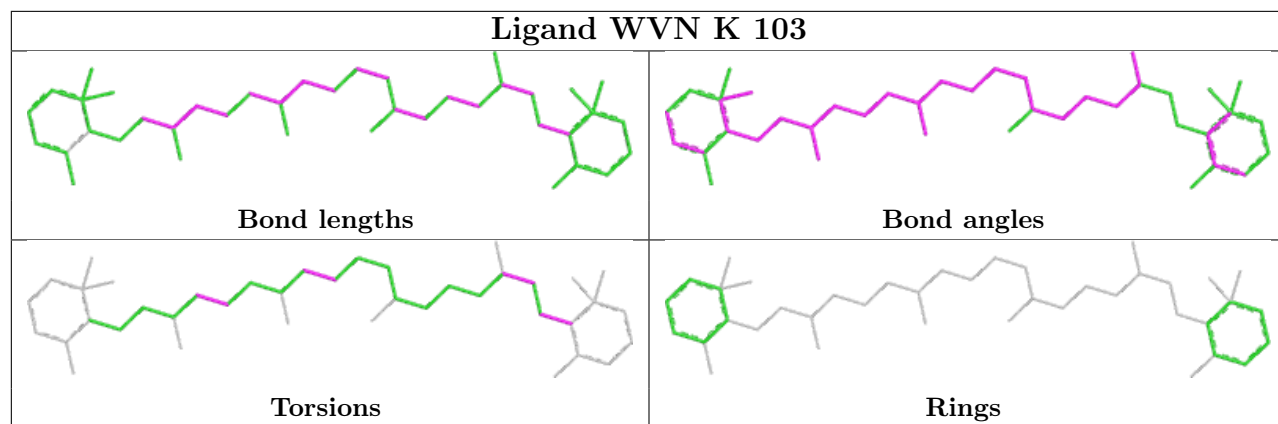


Ligand CLA j 314

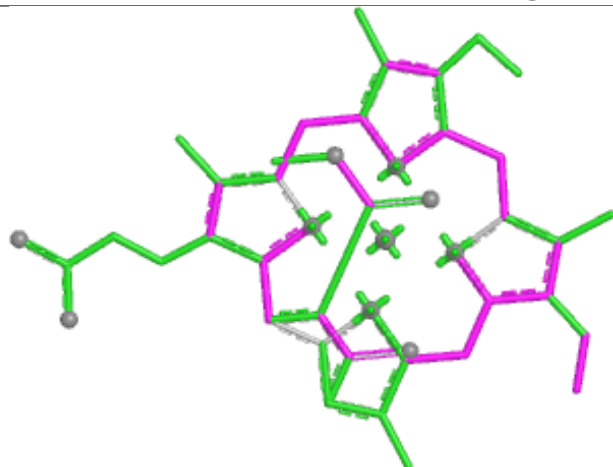


Ligand CLA L 202

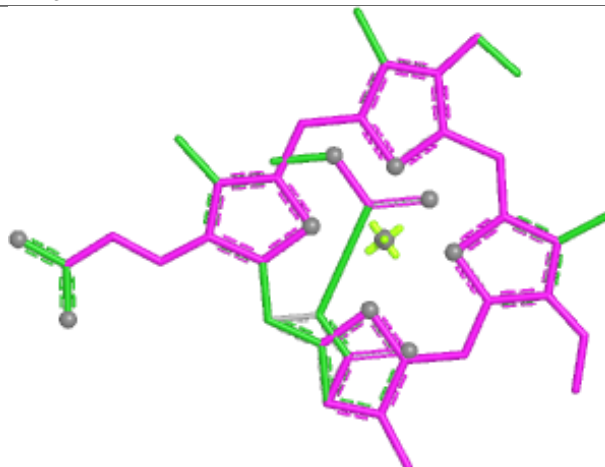




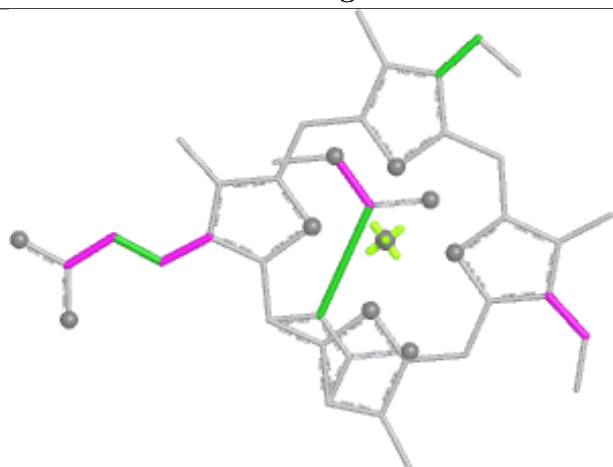
Ligand KC2 j 312



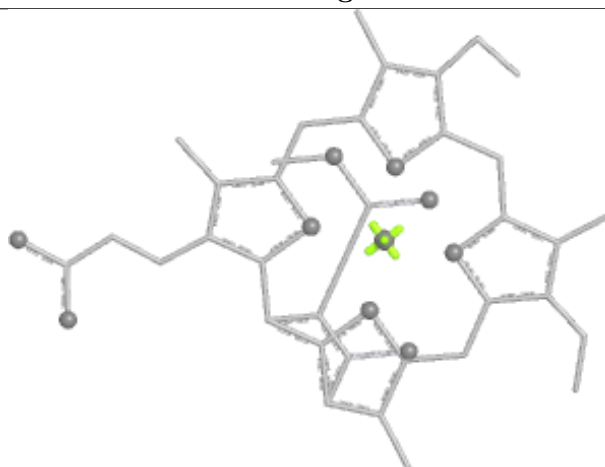
Bond lengths



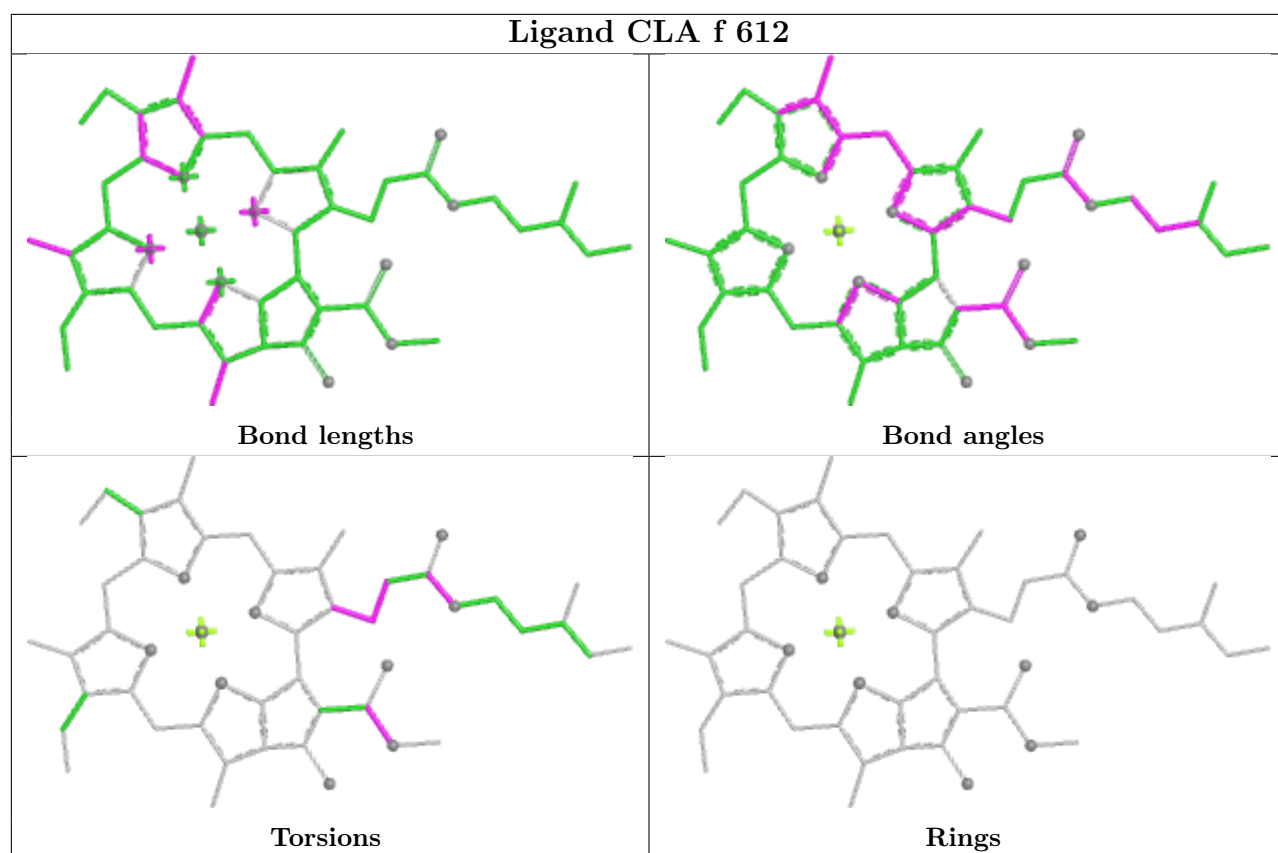
Bond angles



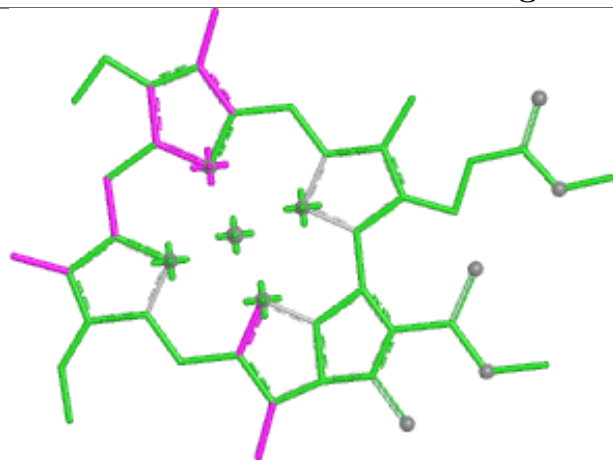
Torsions



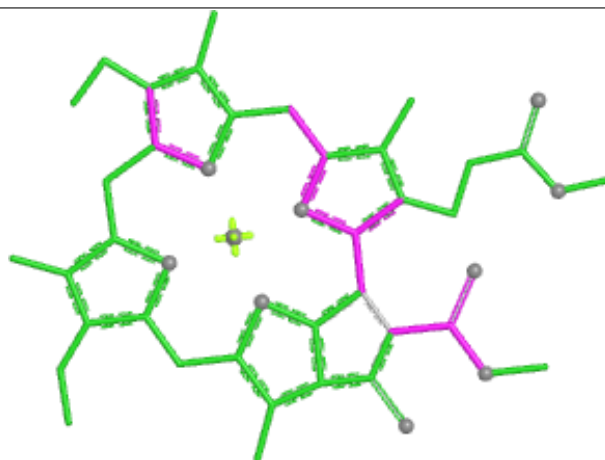
Rings



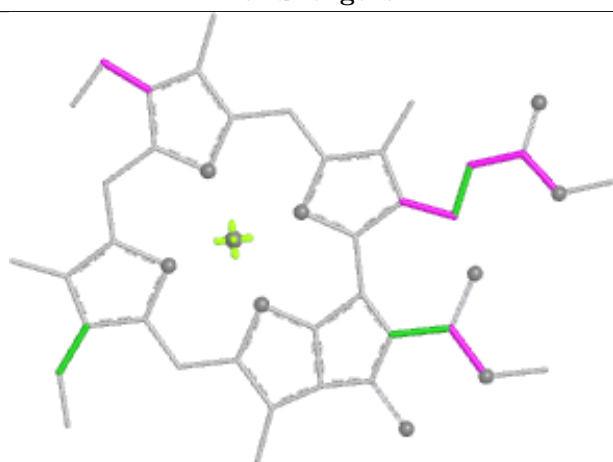
Ligand CLA e 608



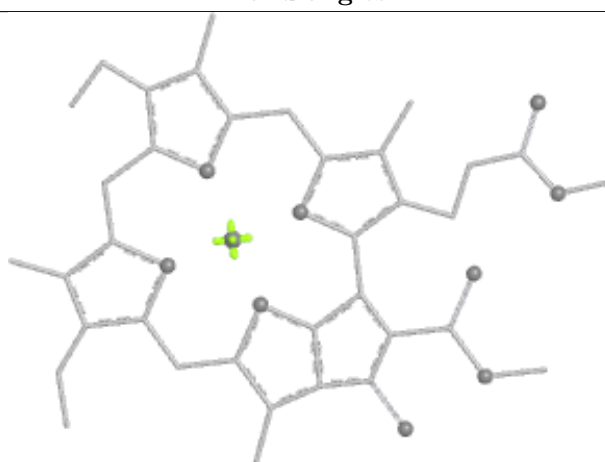
Bond lengths



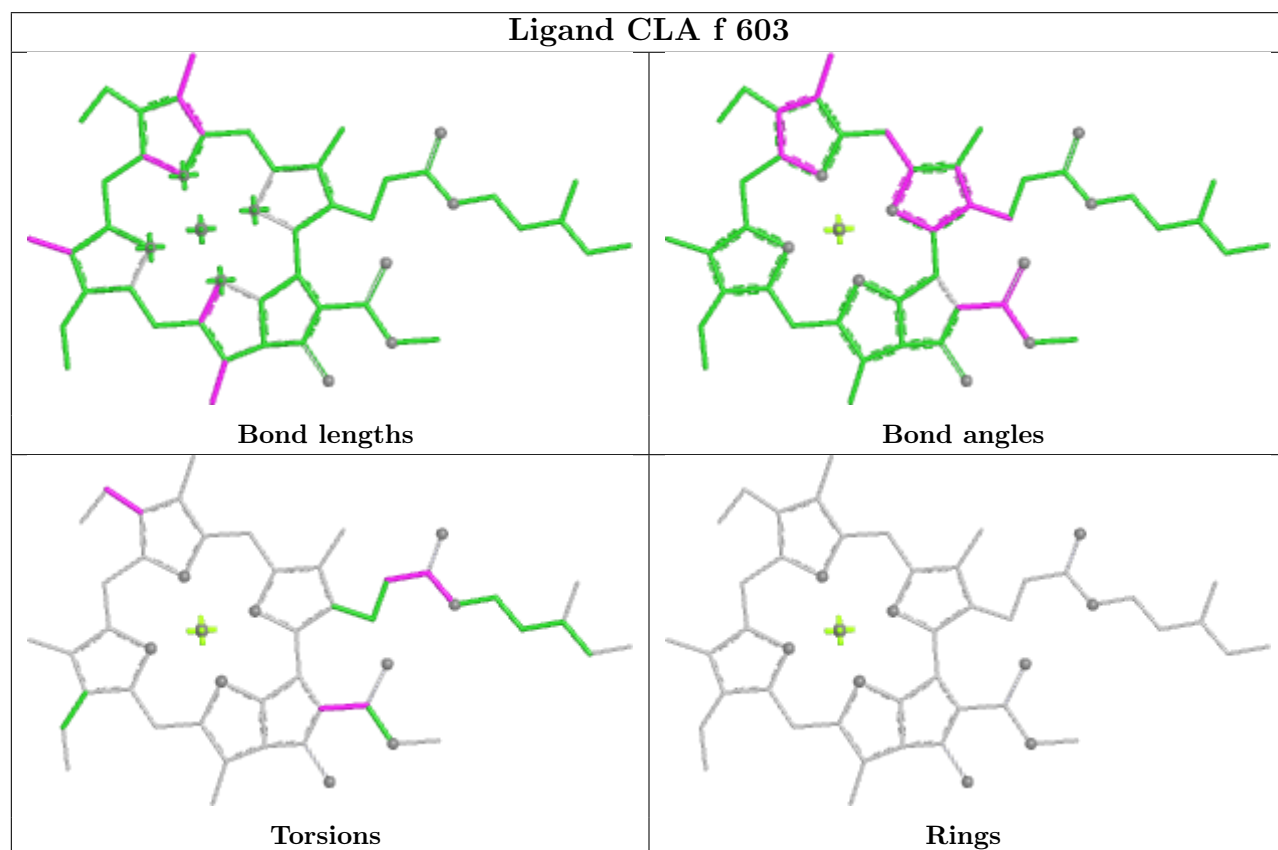
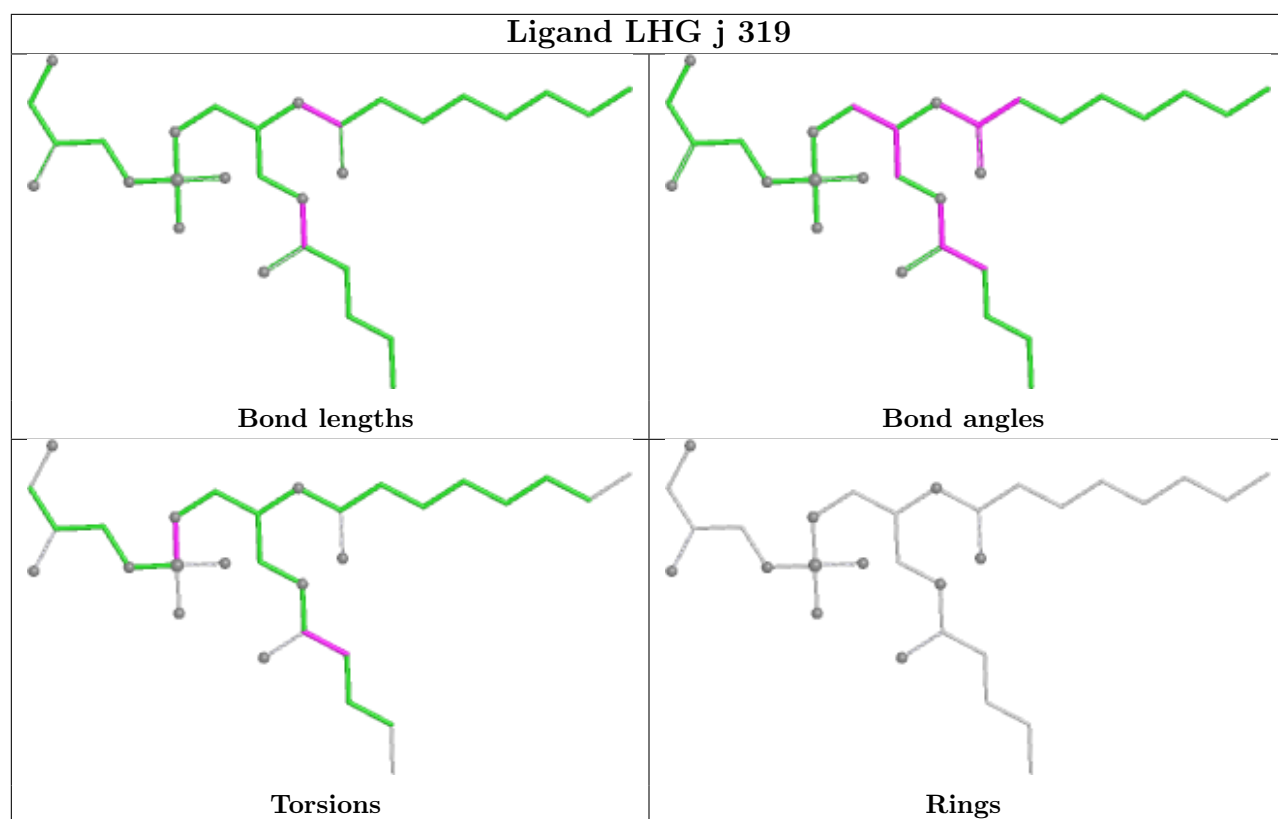
Bond angles

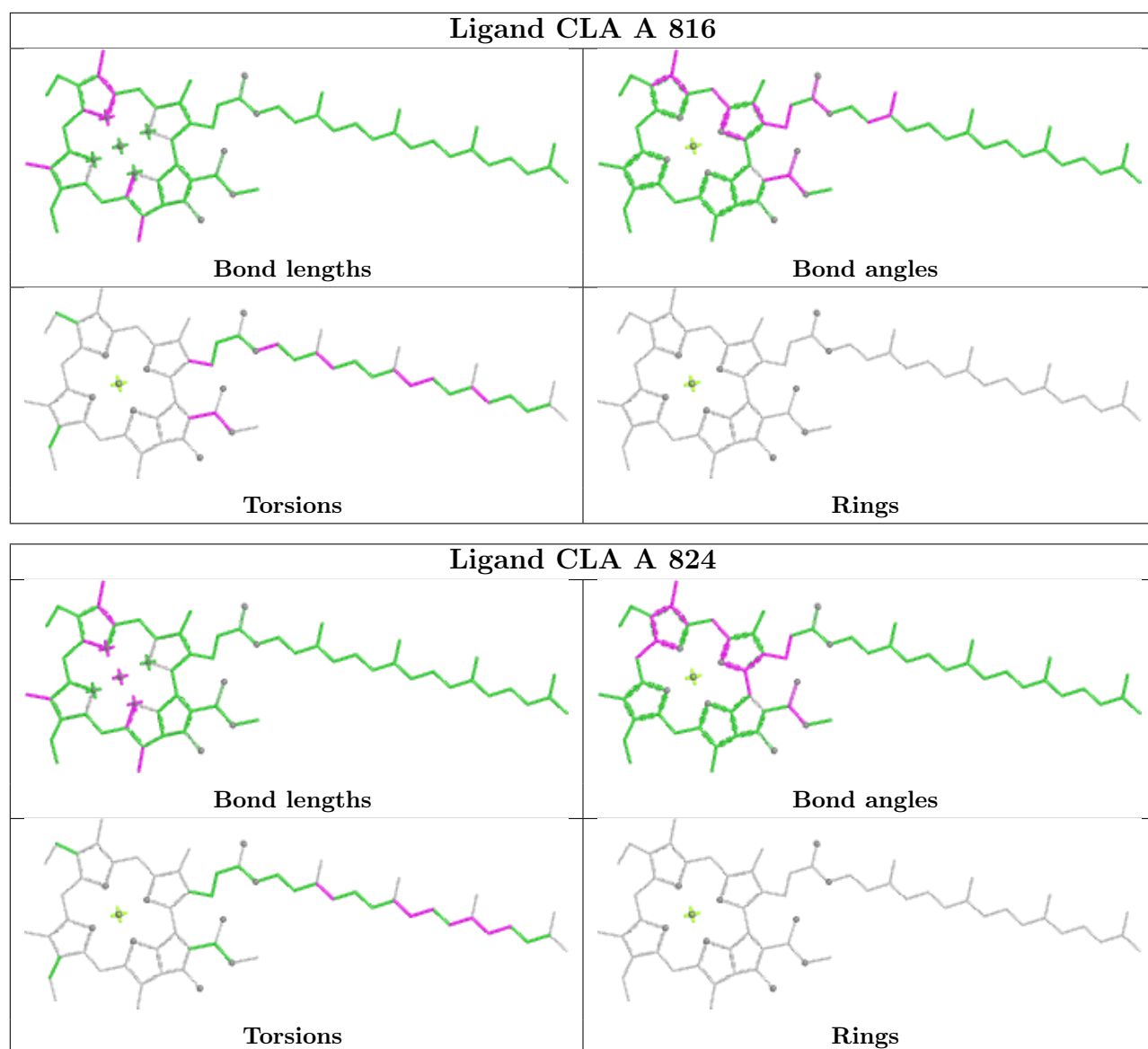


Torsions

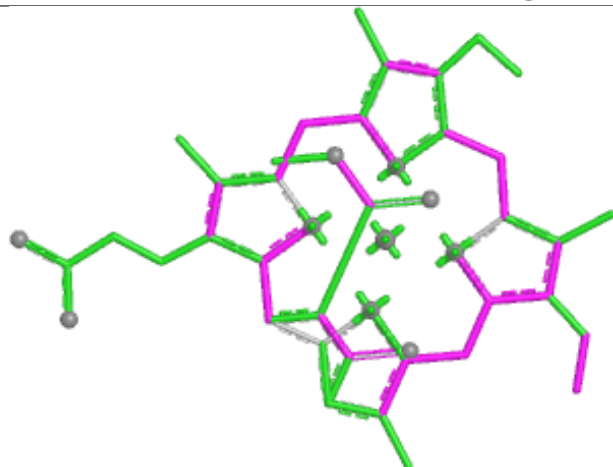


Rings

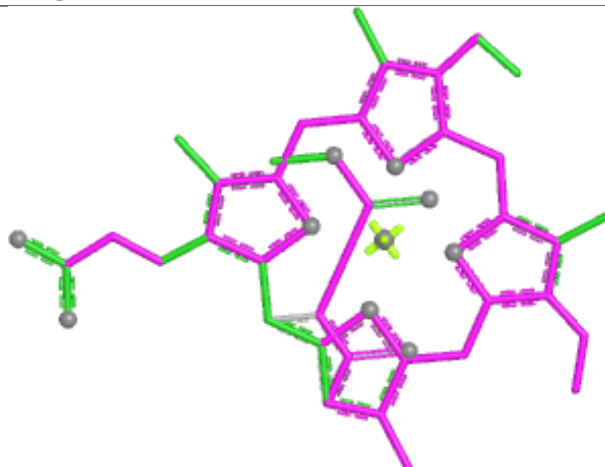




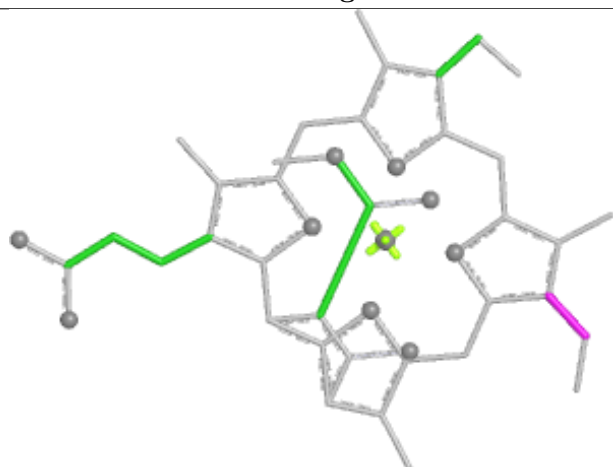
Ligand KC2 g 313



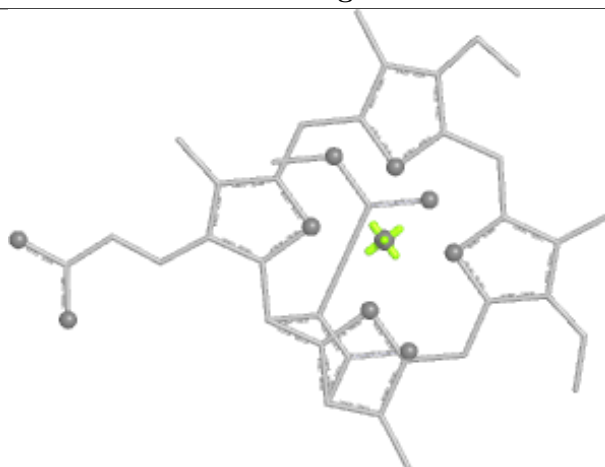
Bond lengths



Bond angles

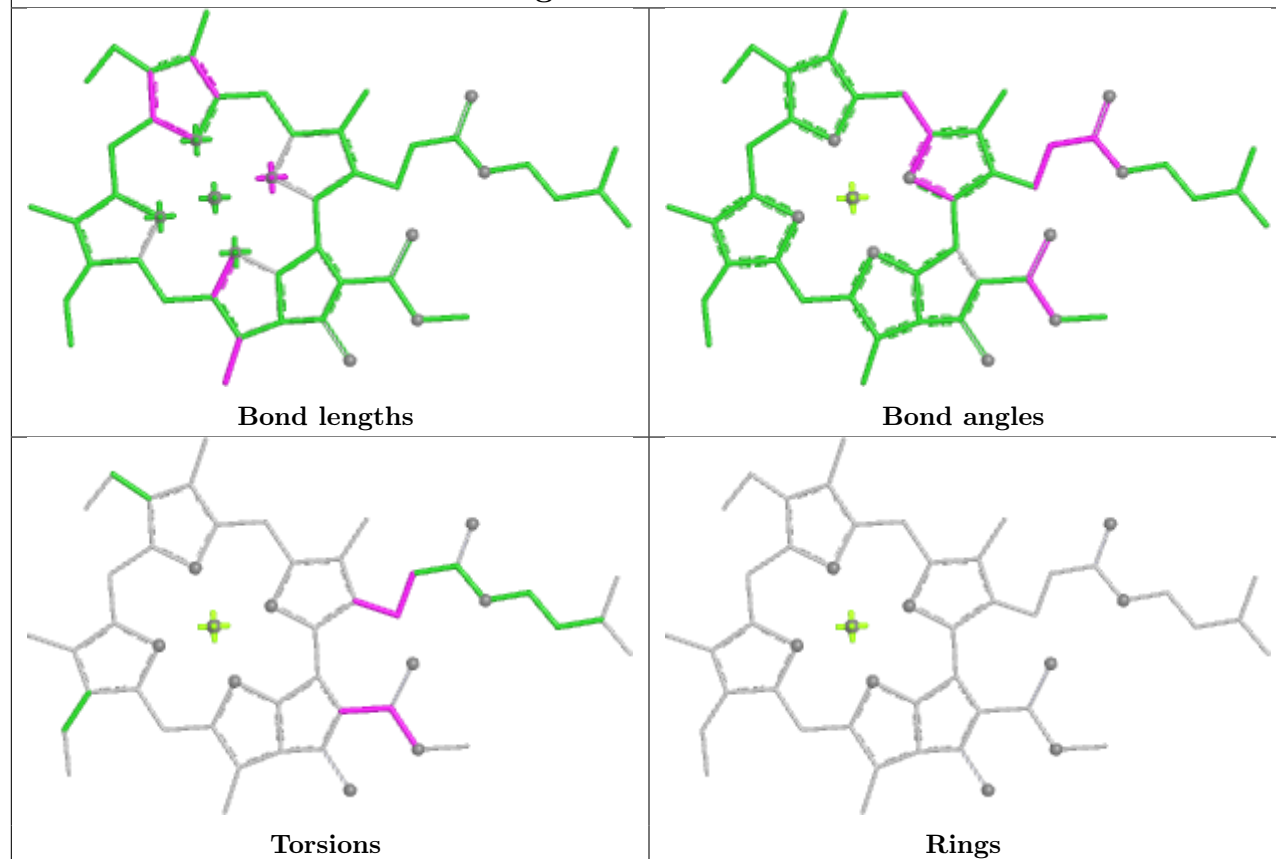


Torsions

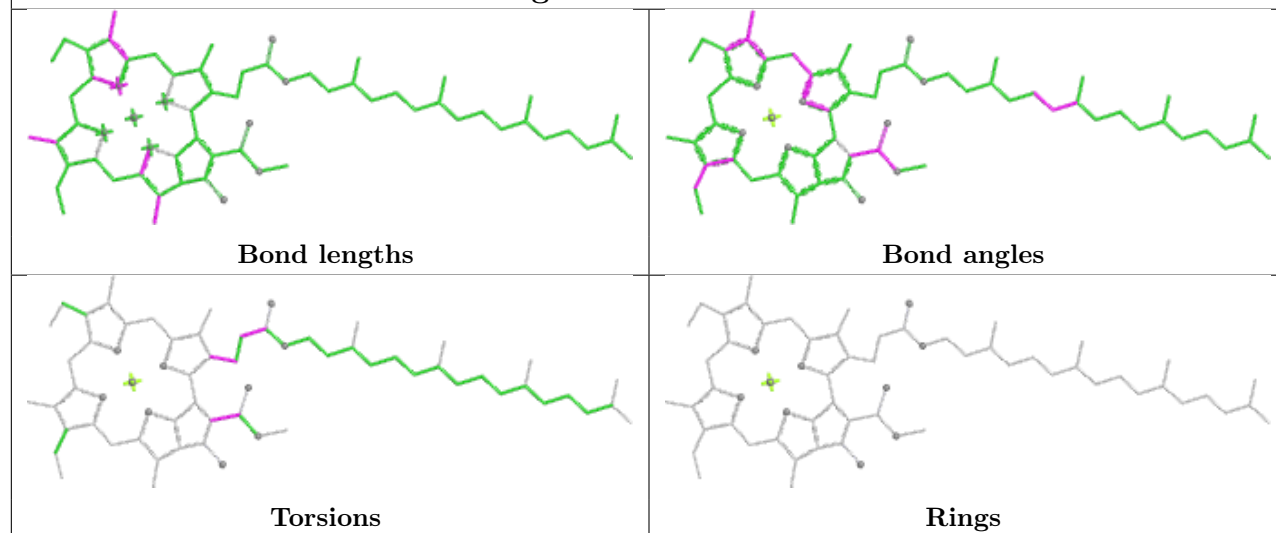


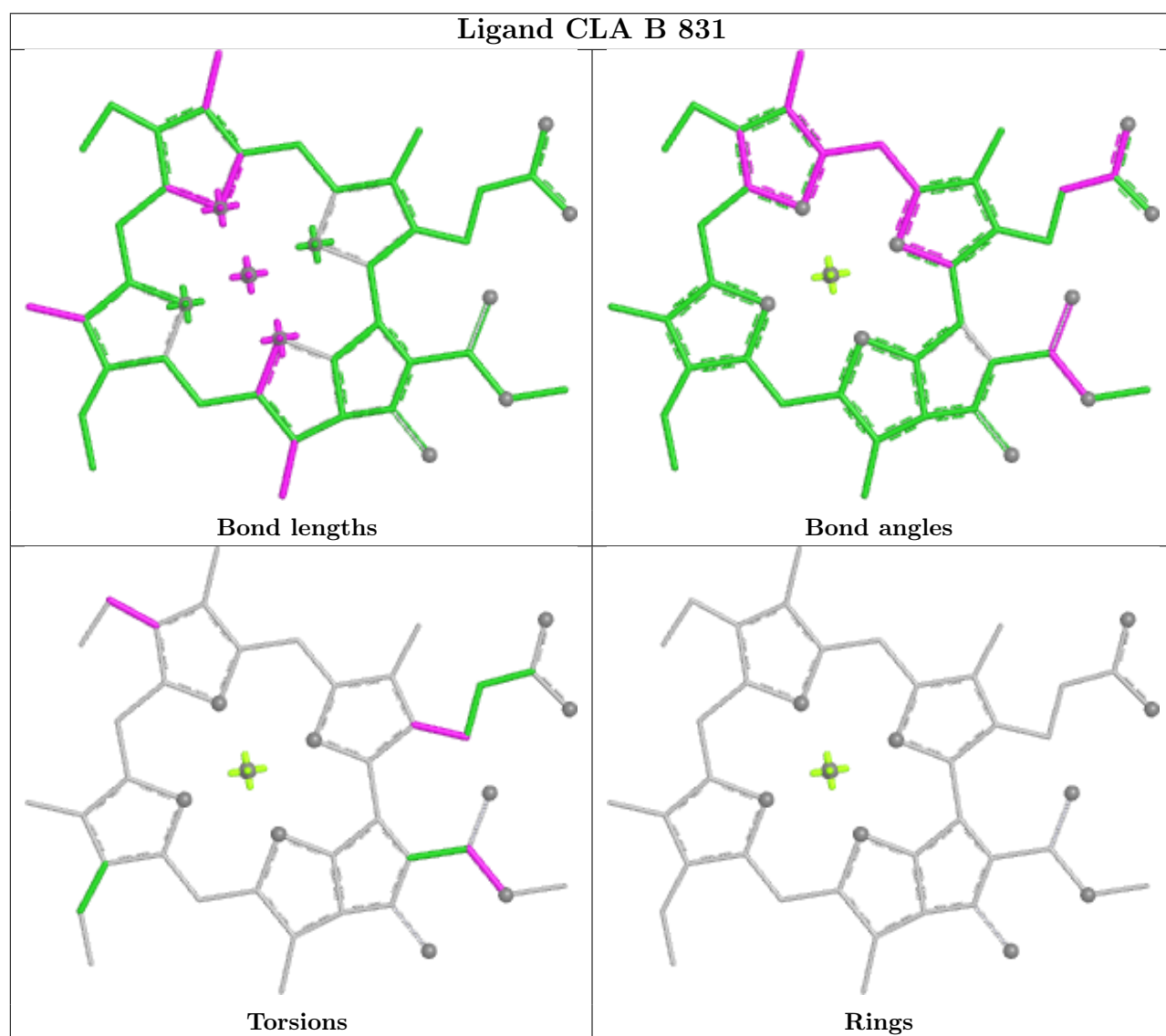
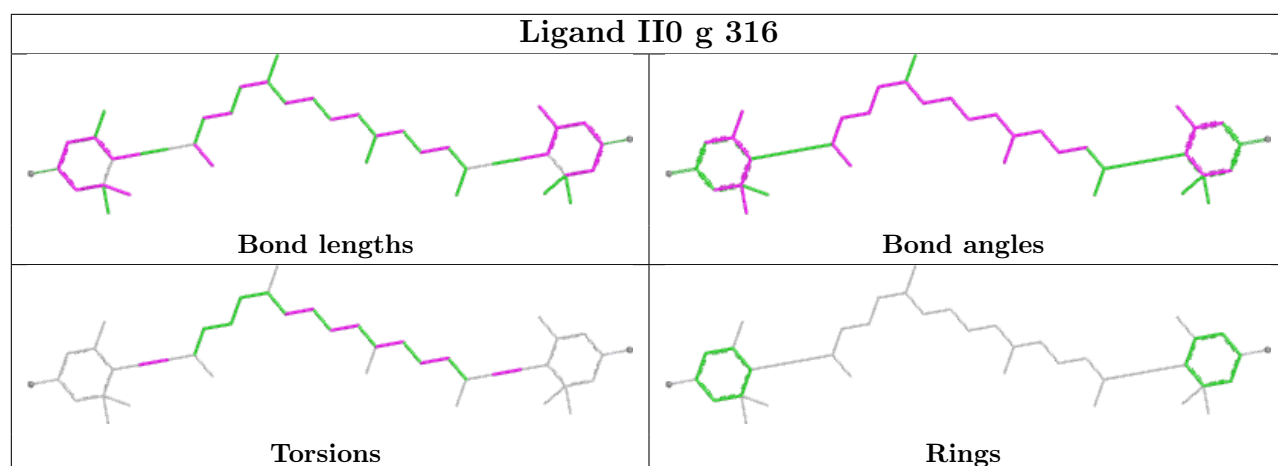
Rings

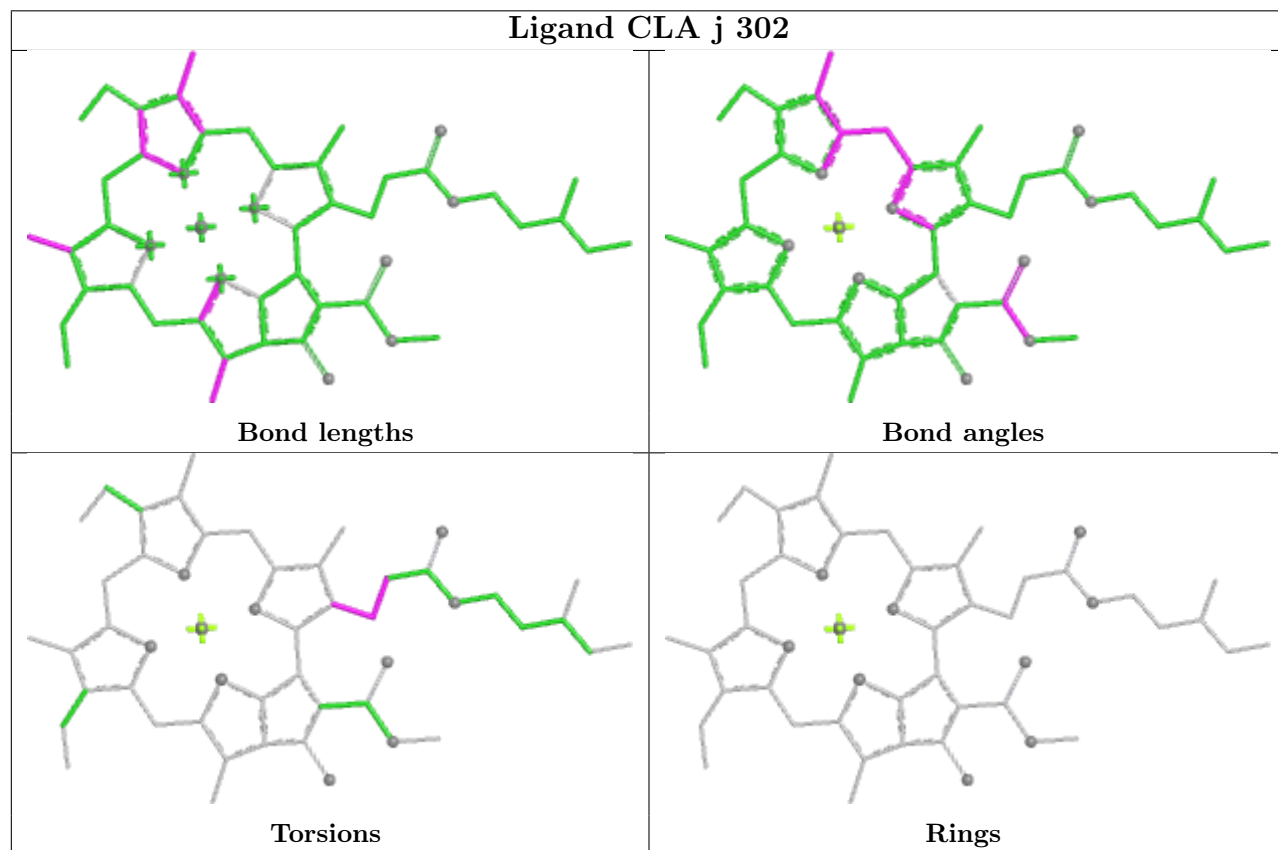
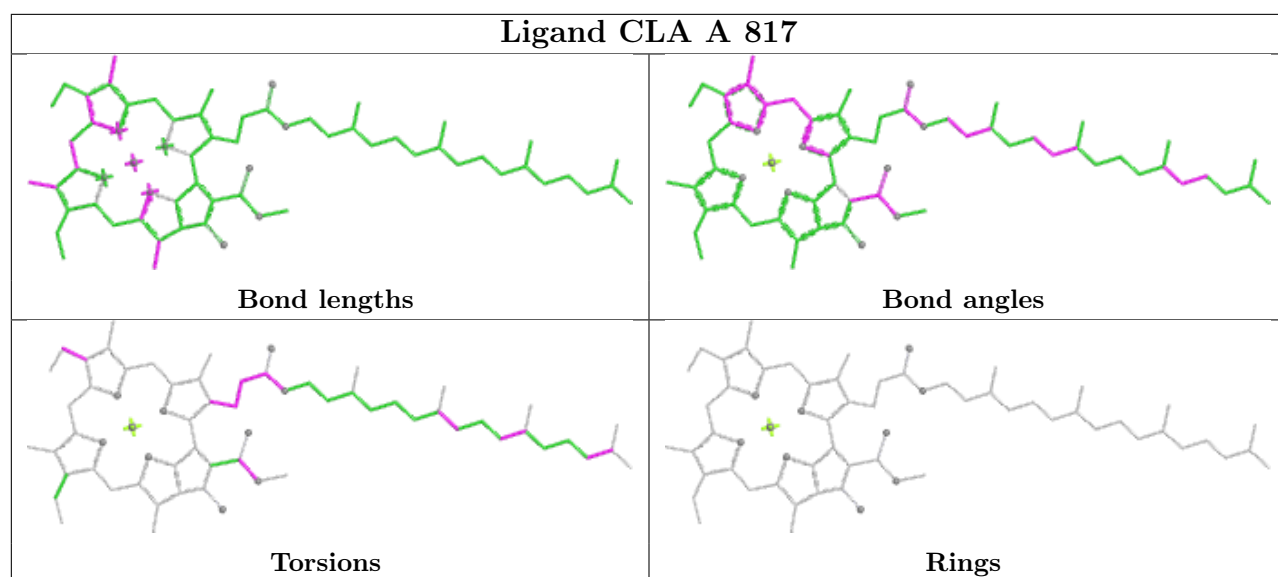
Ligand CLA d 301

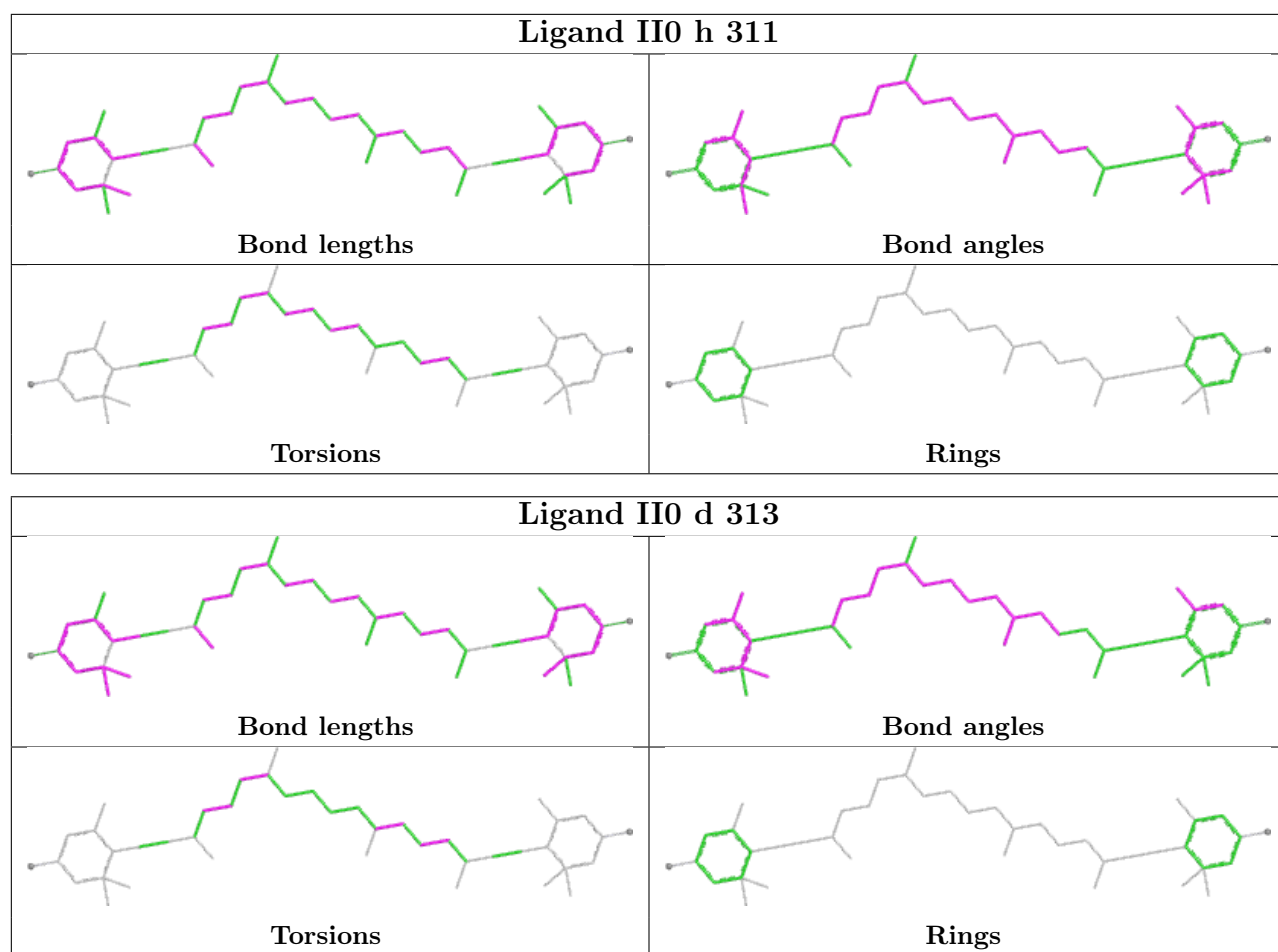


Ligand CLA A 804

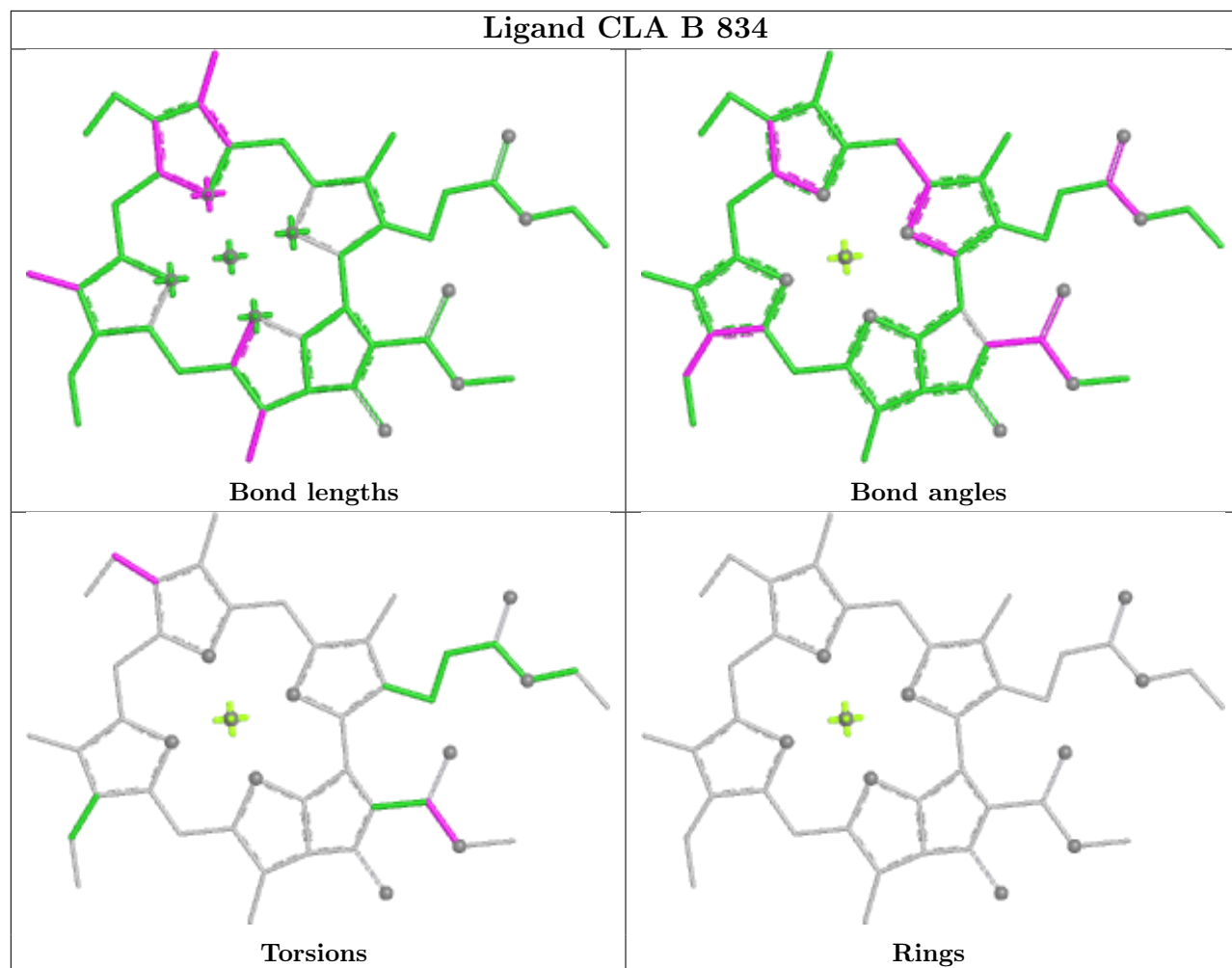


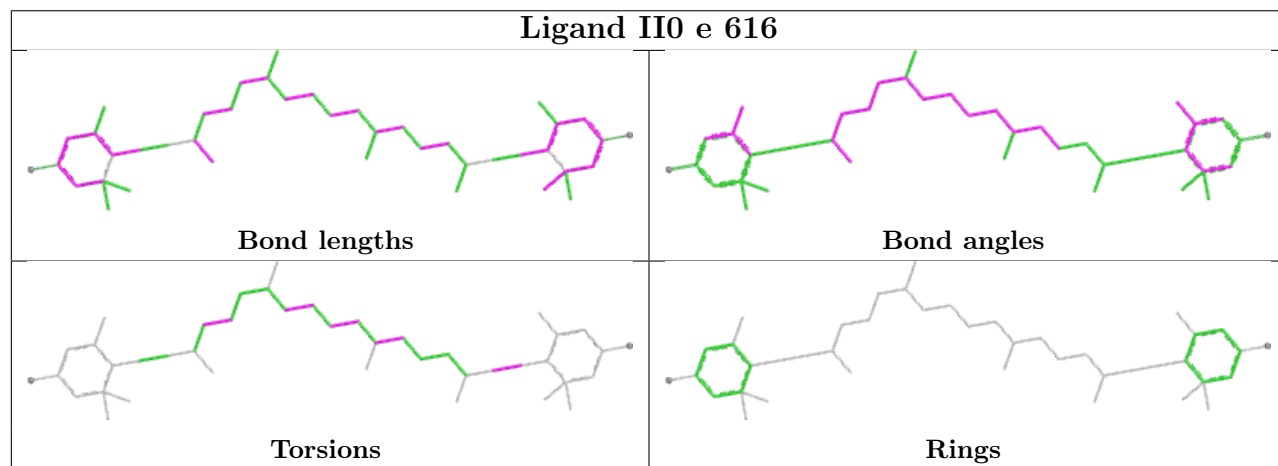
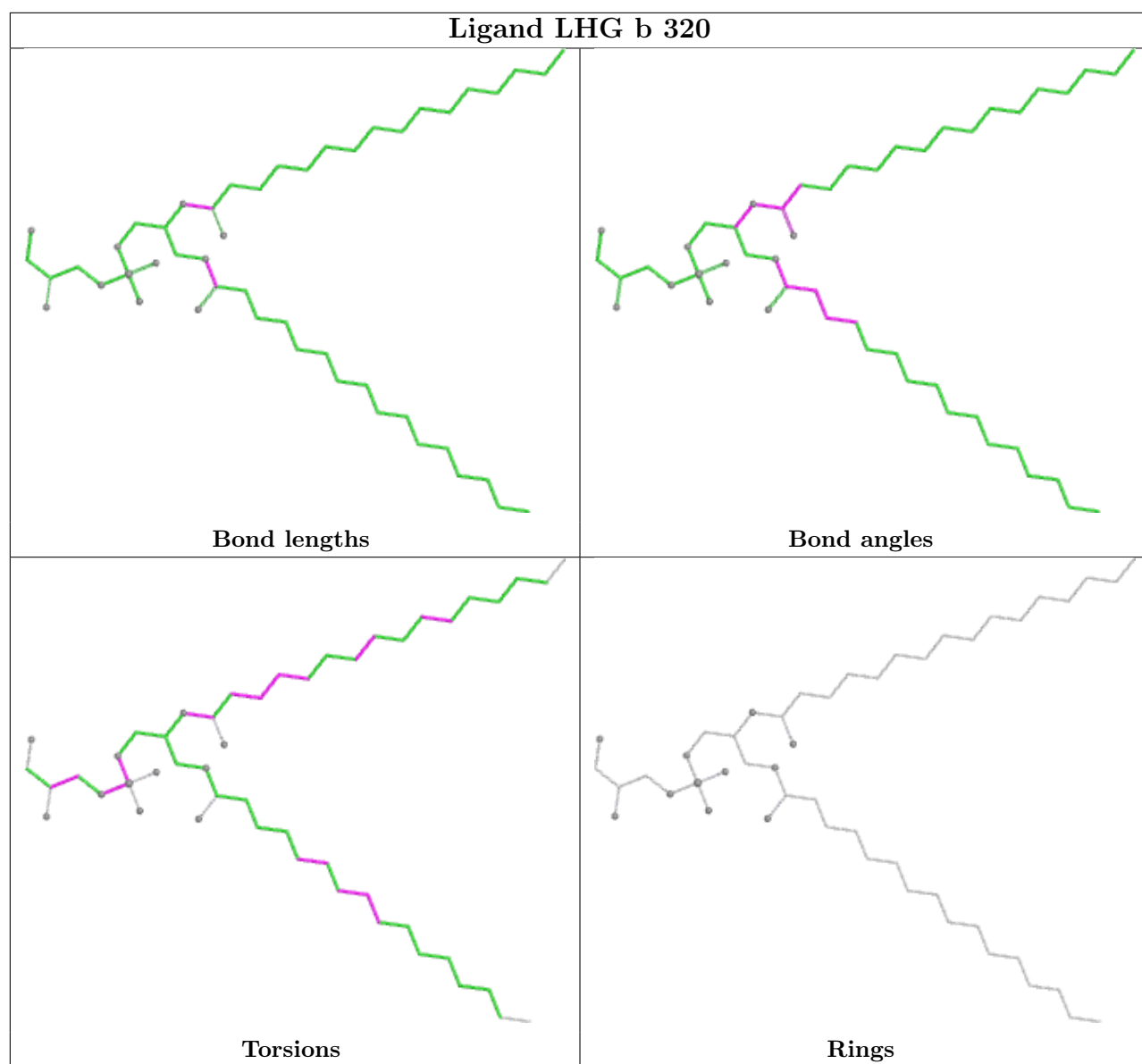


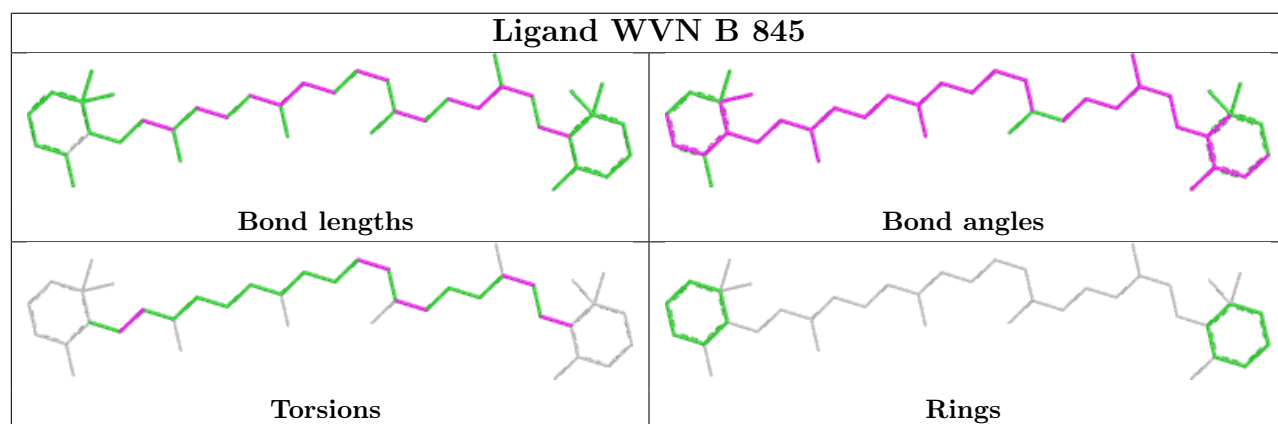
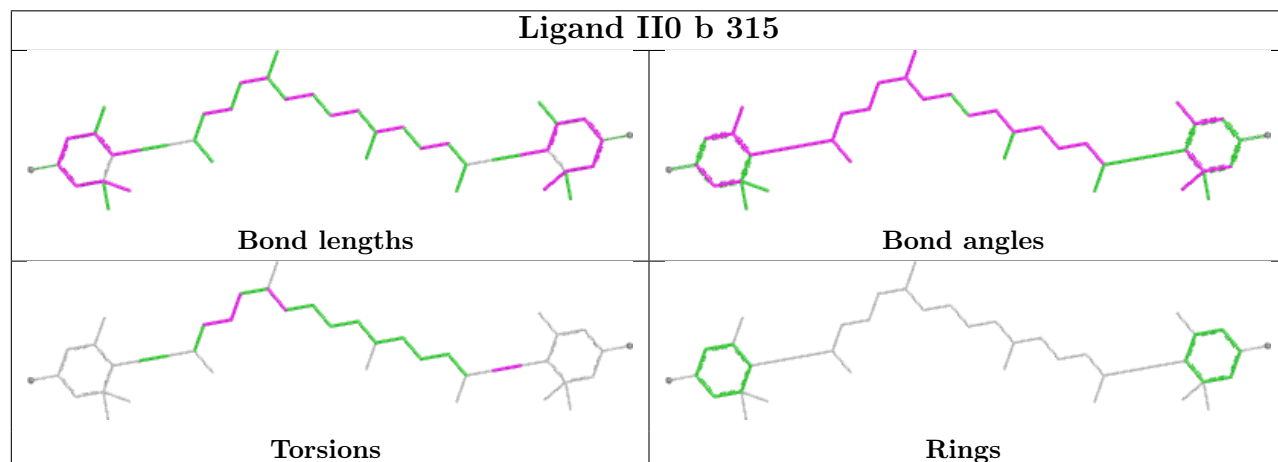
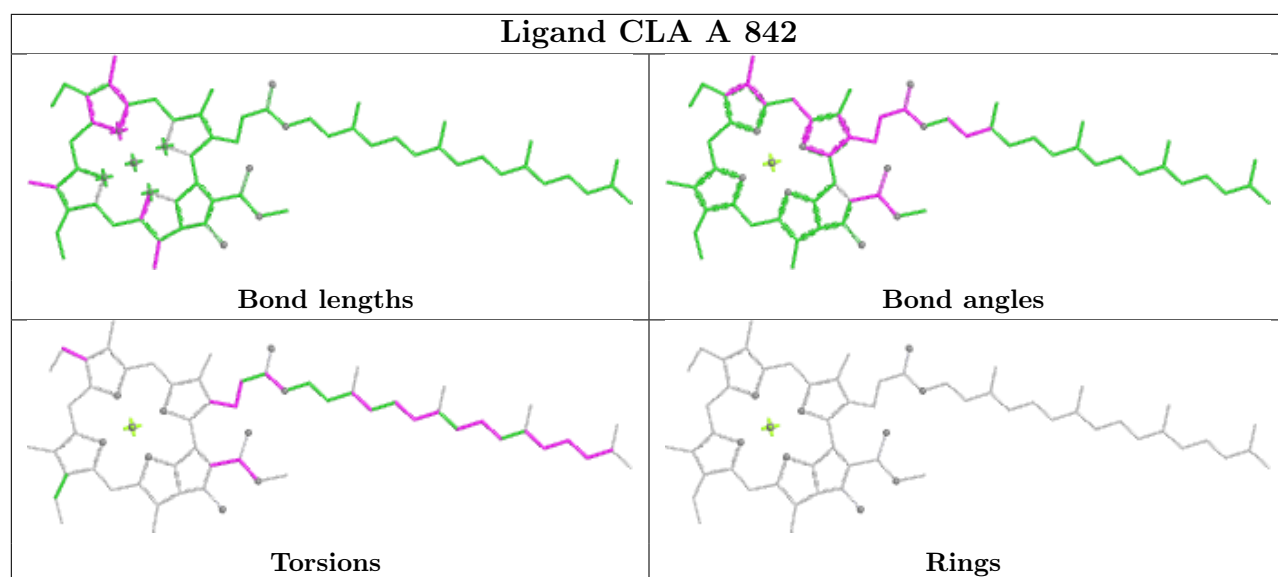


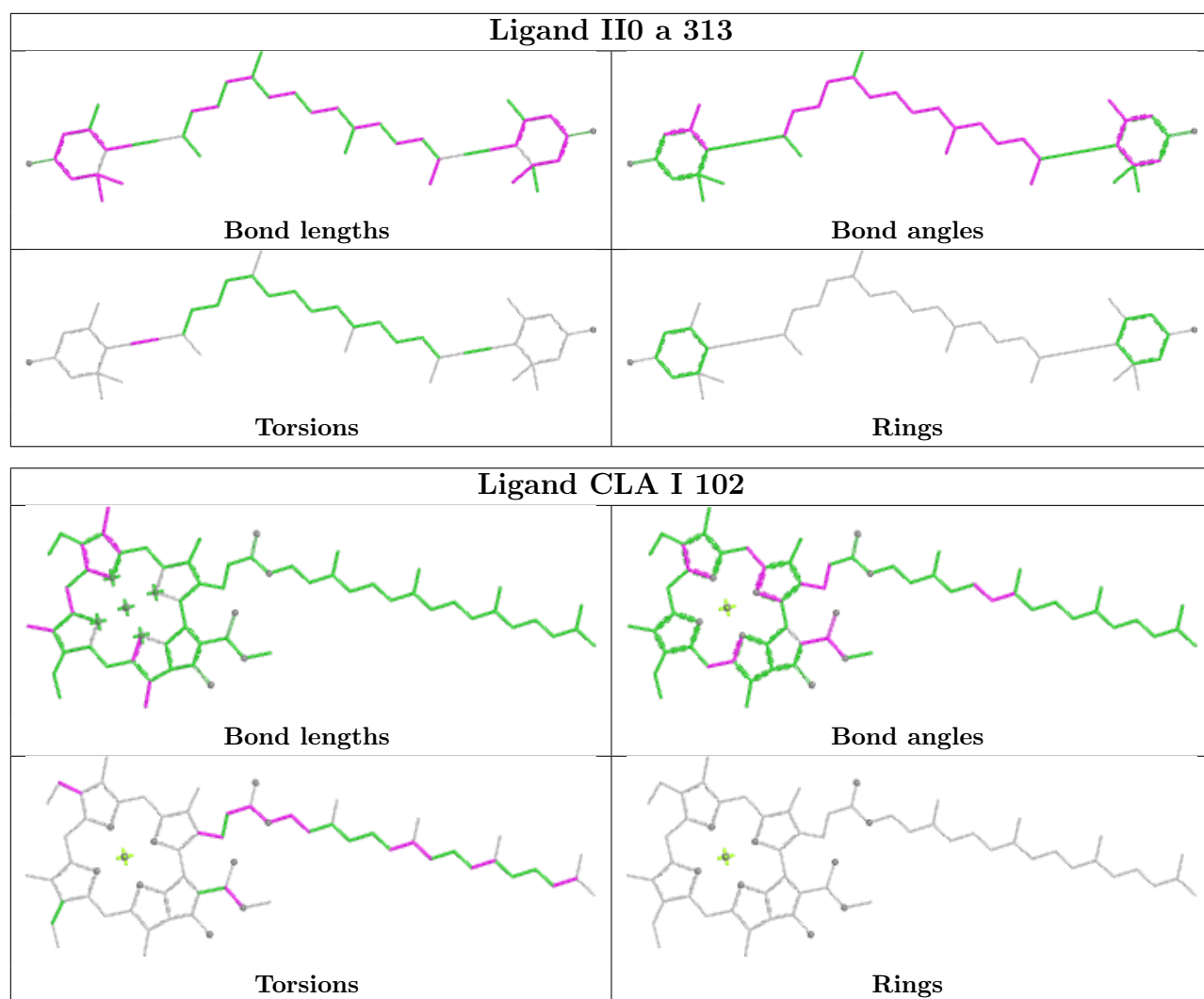


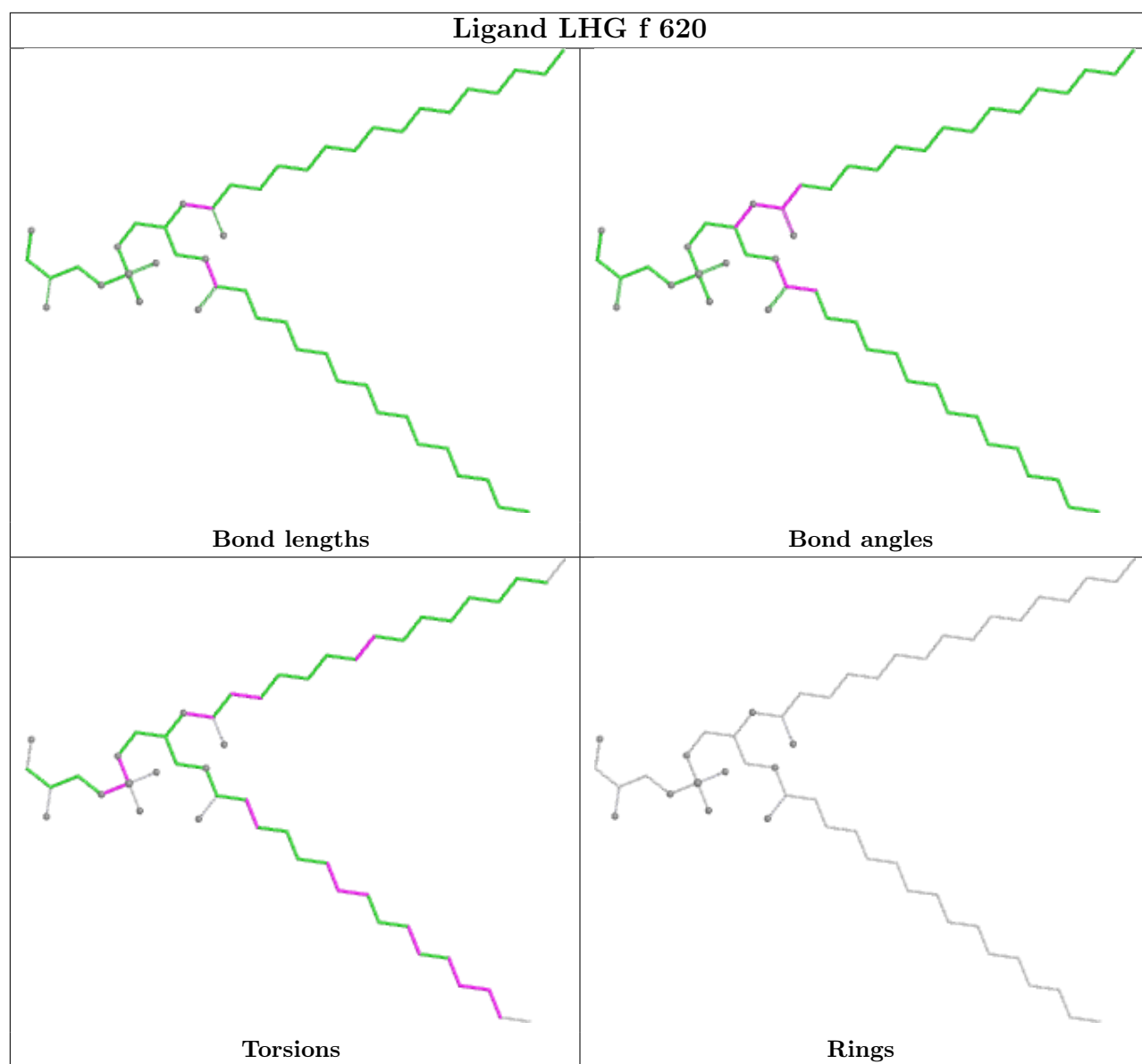
Ligand CLA B 834



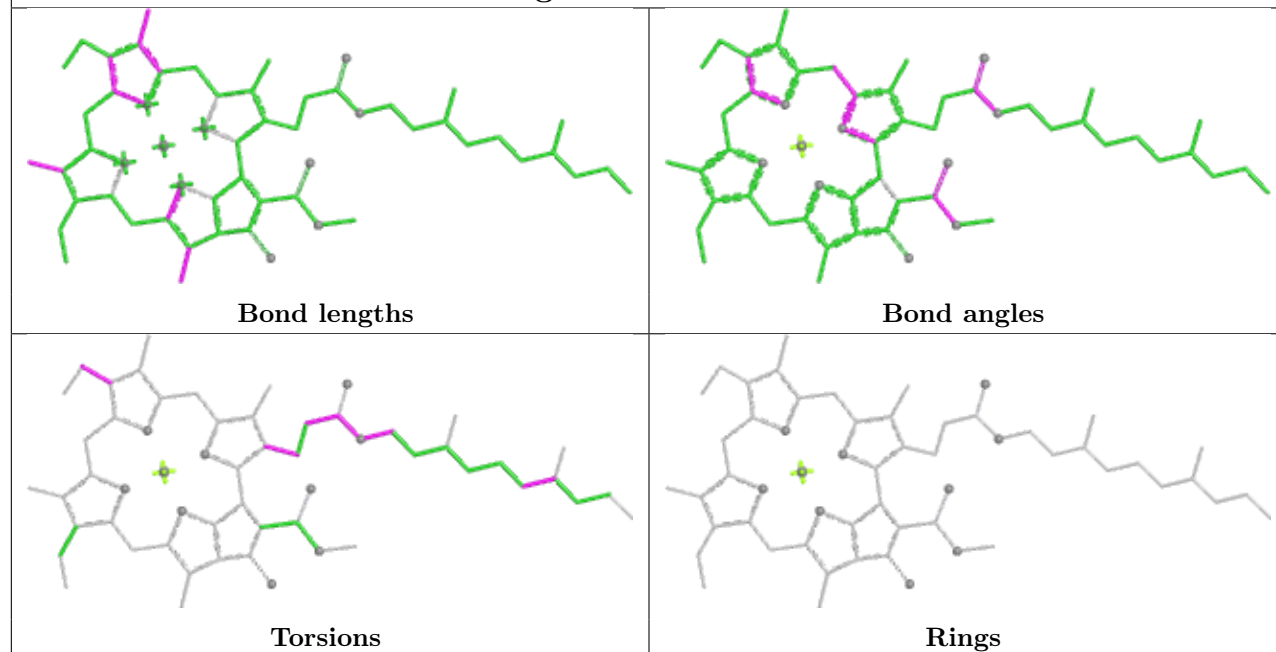




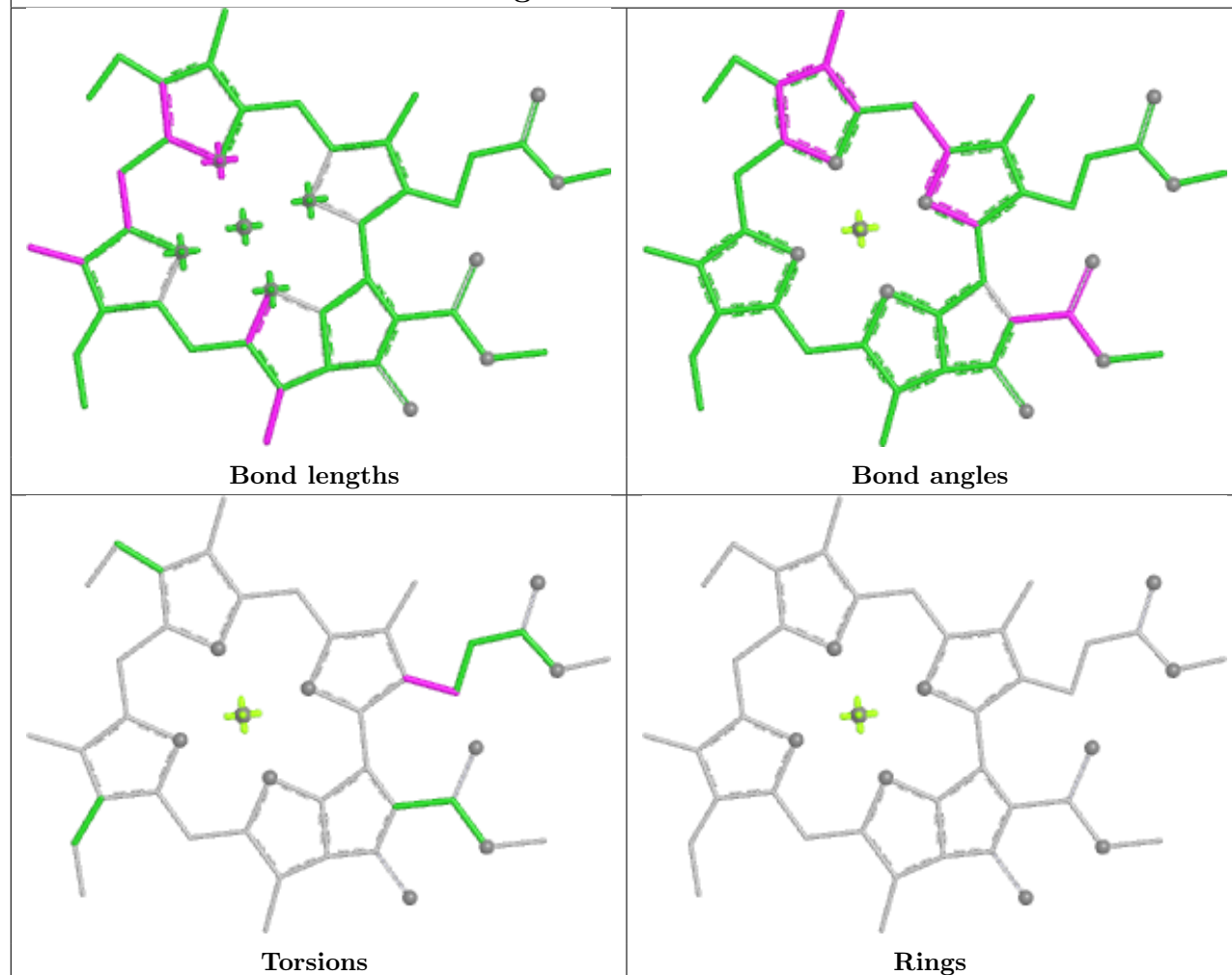


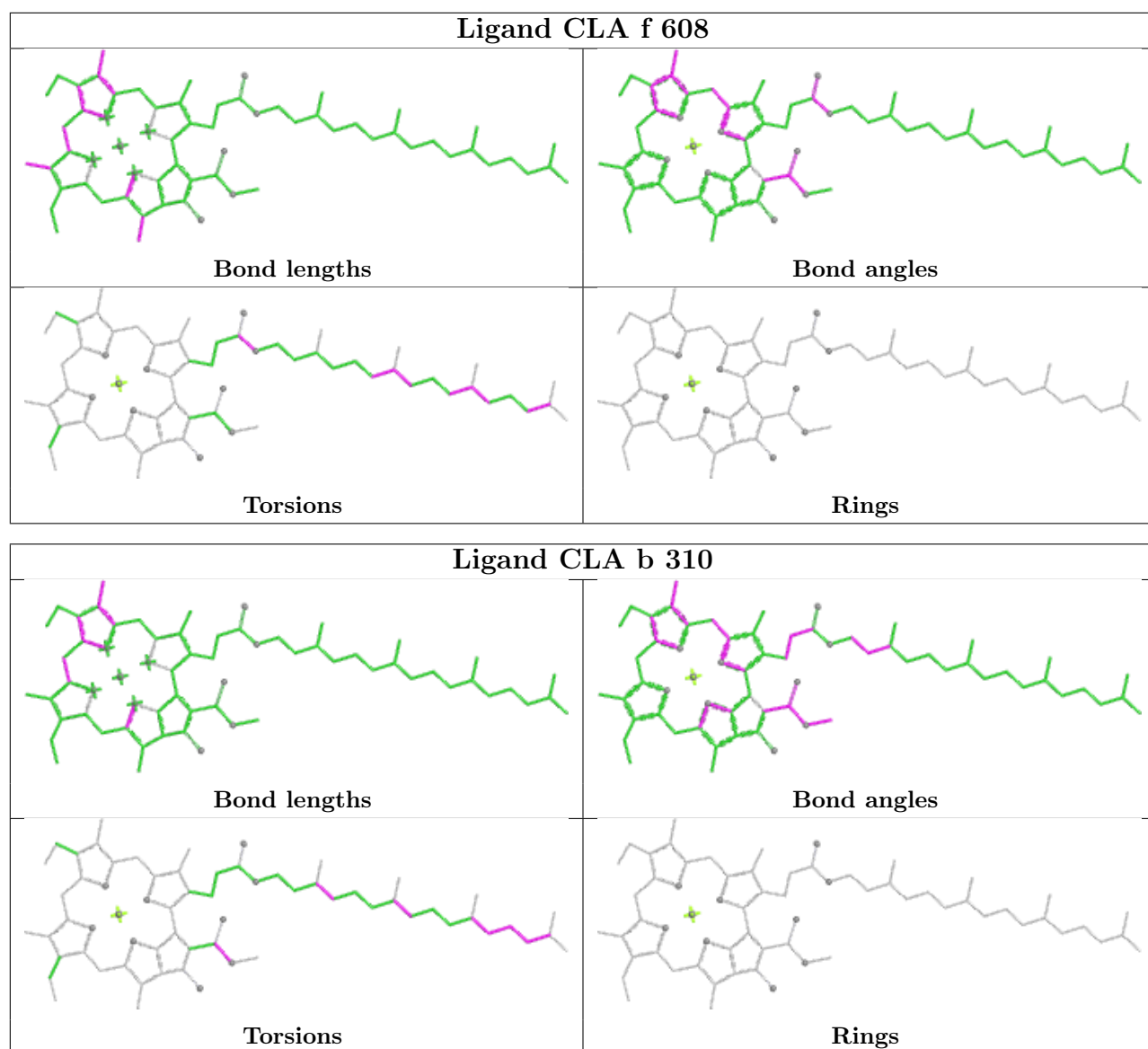


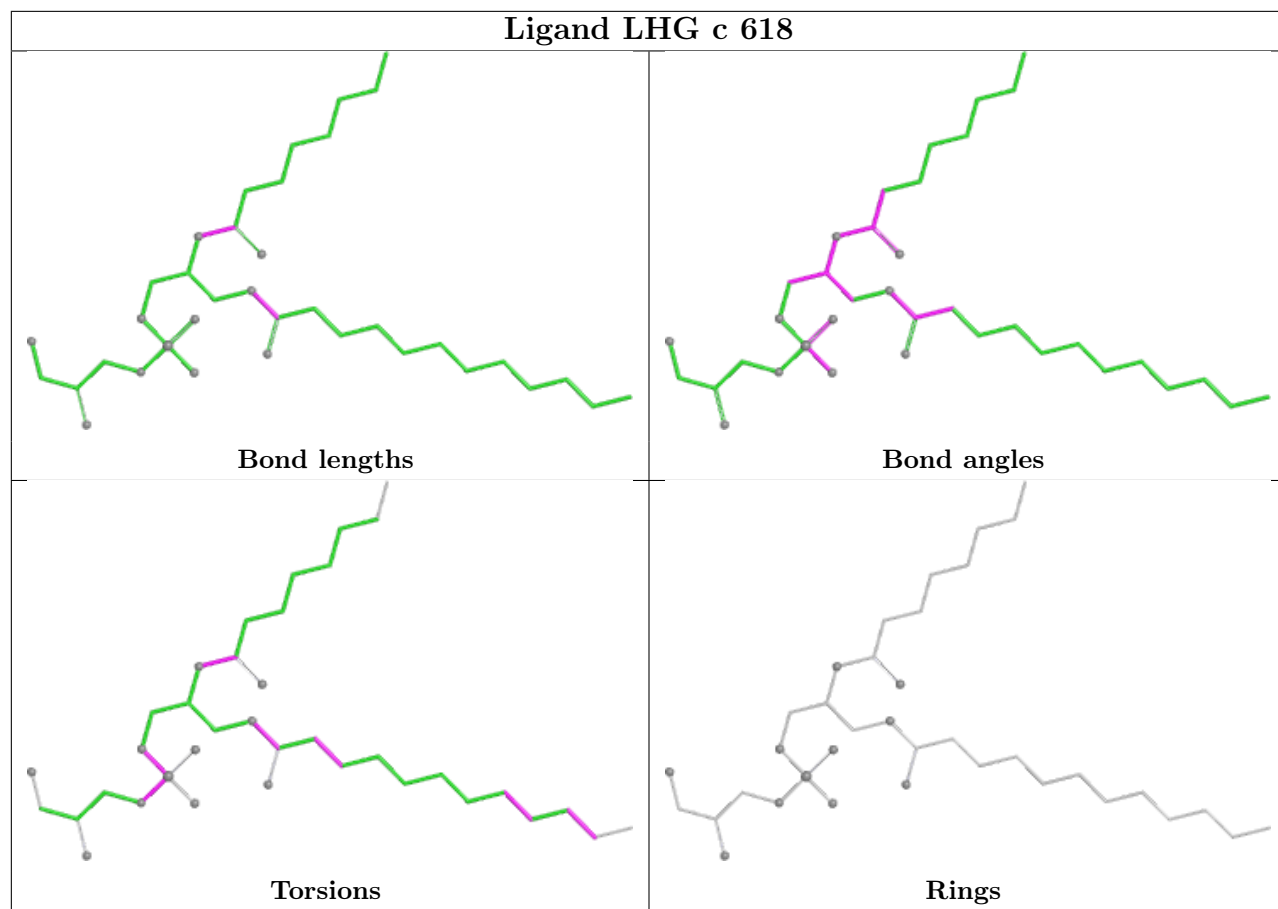
Ligand CLA h 306

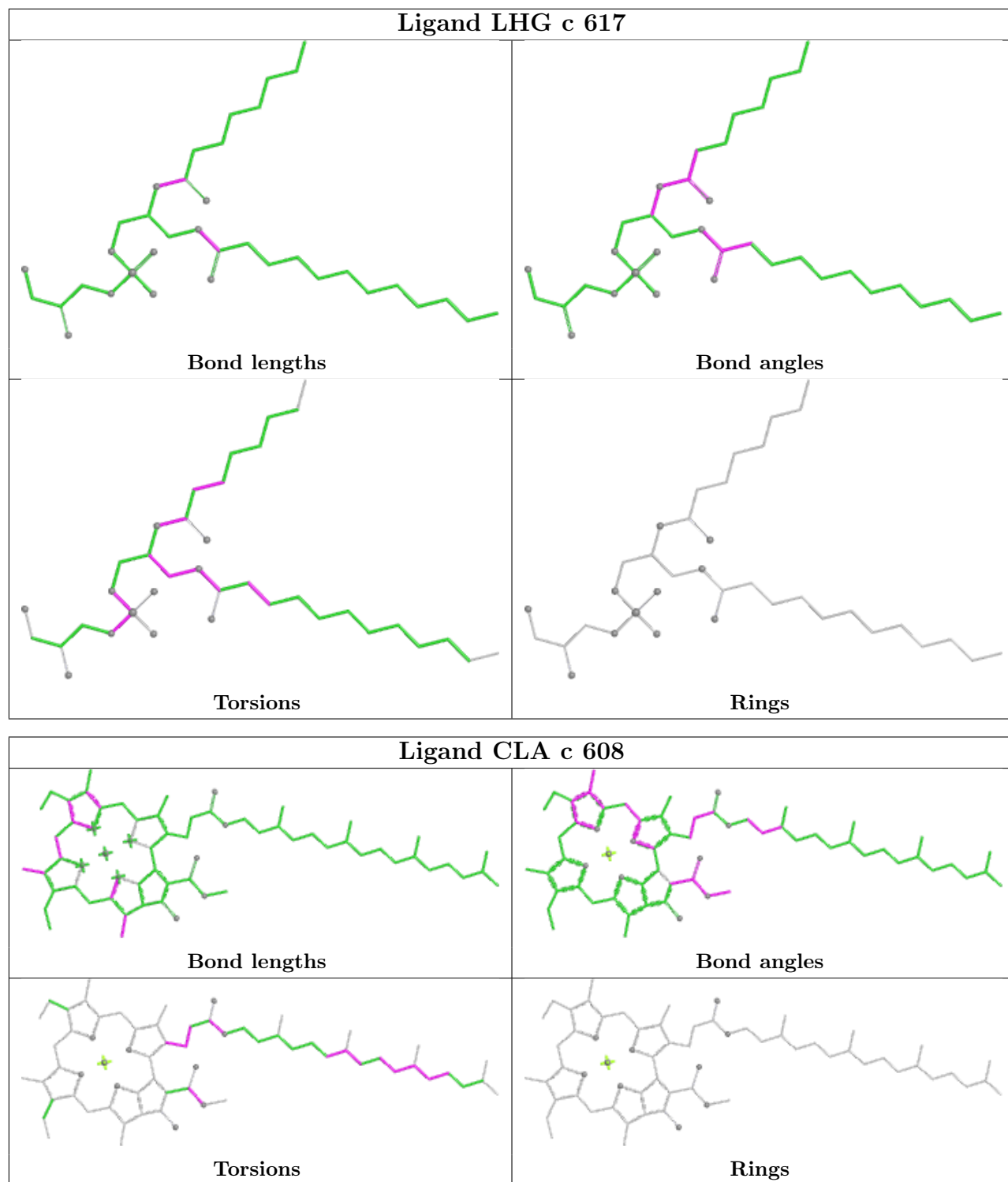


Ligand CLA B 819

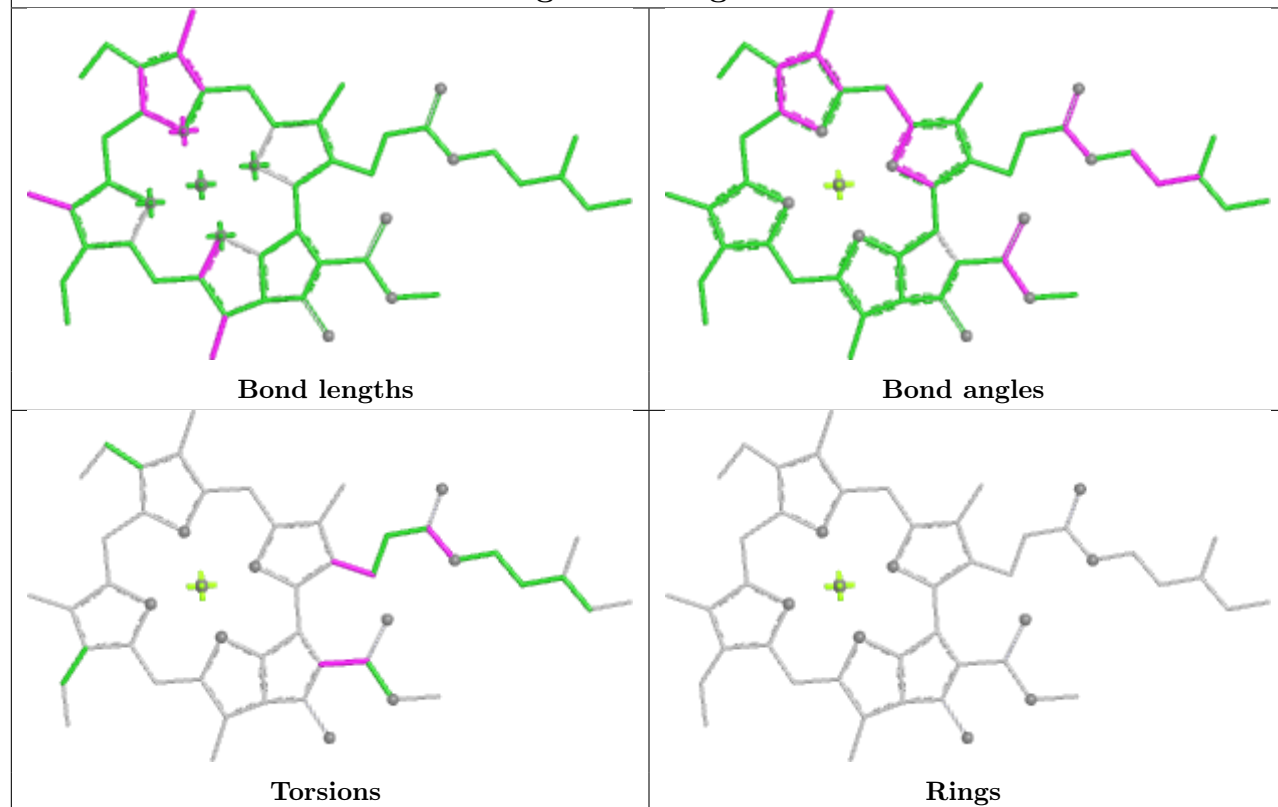




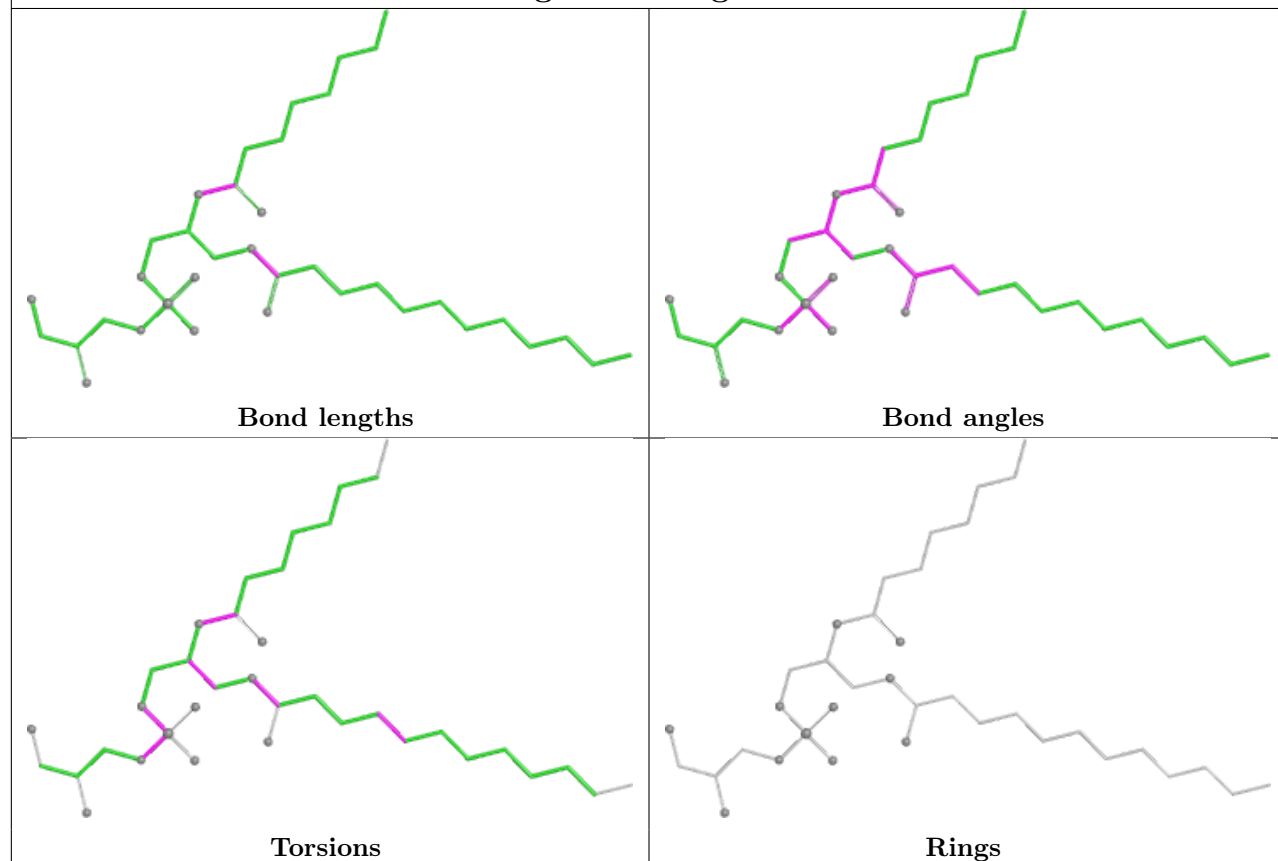


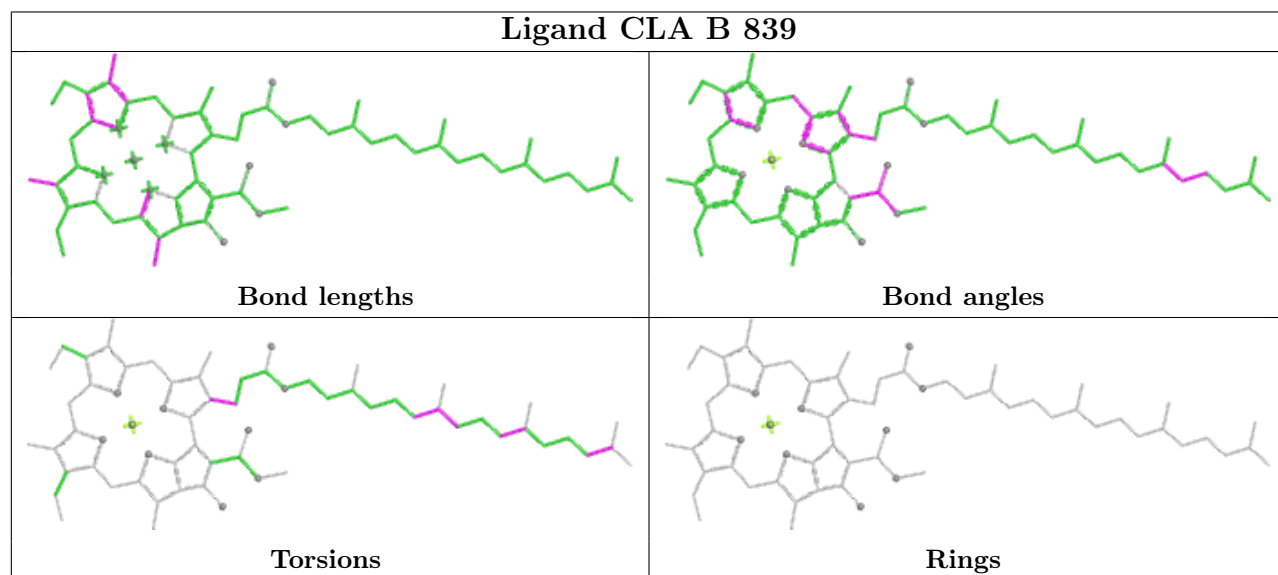
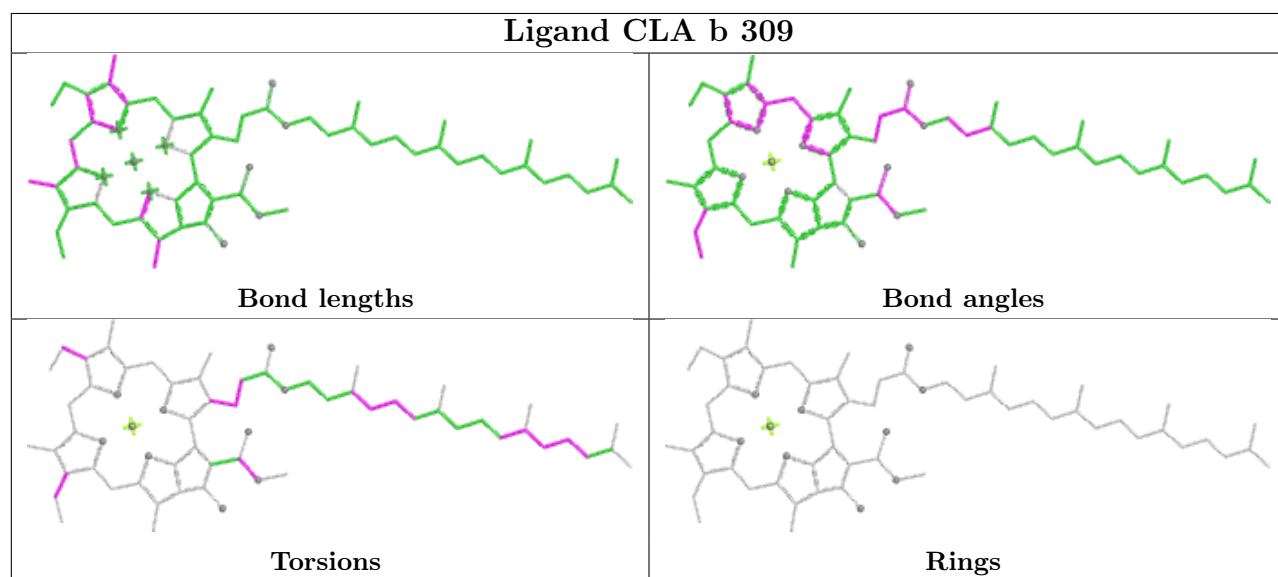
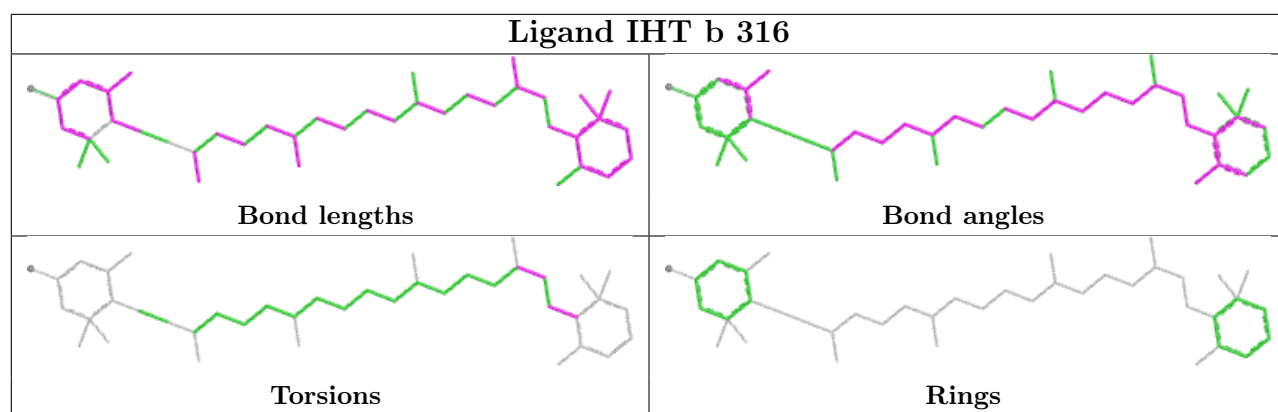


Ligand CLA g 310

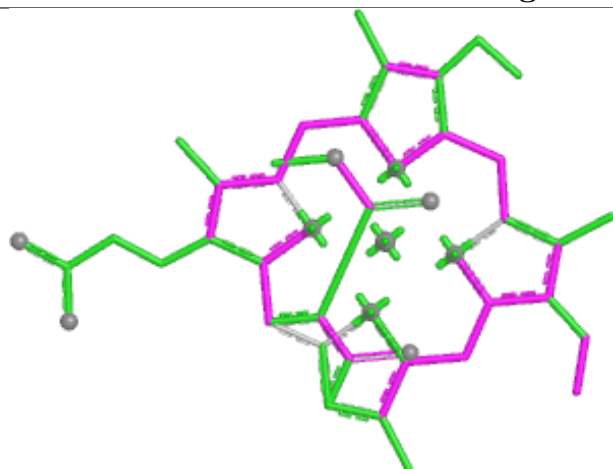


Ligand LHG g 321

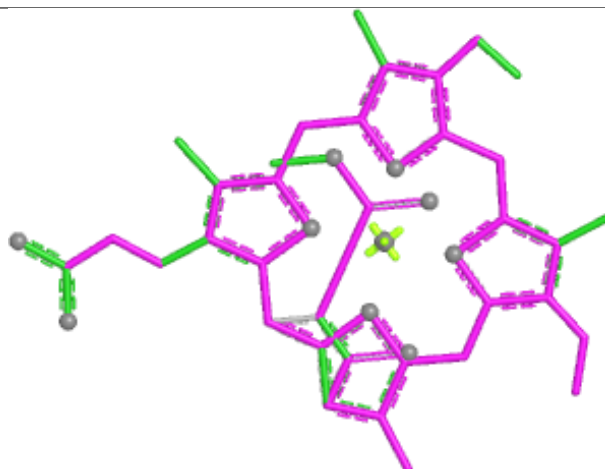




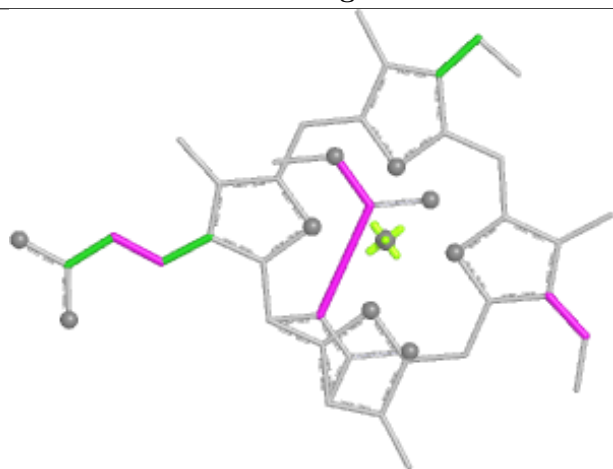
Ligand KC2 d 310



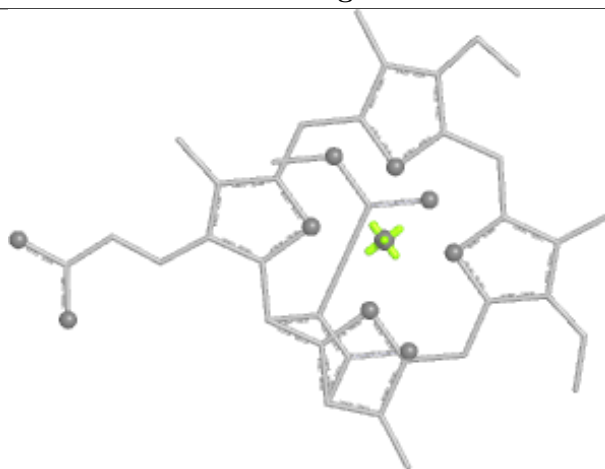
Bond lengths



Bond angles

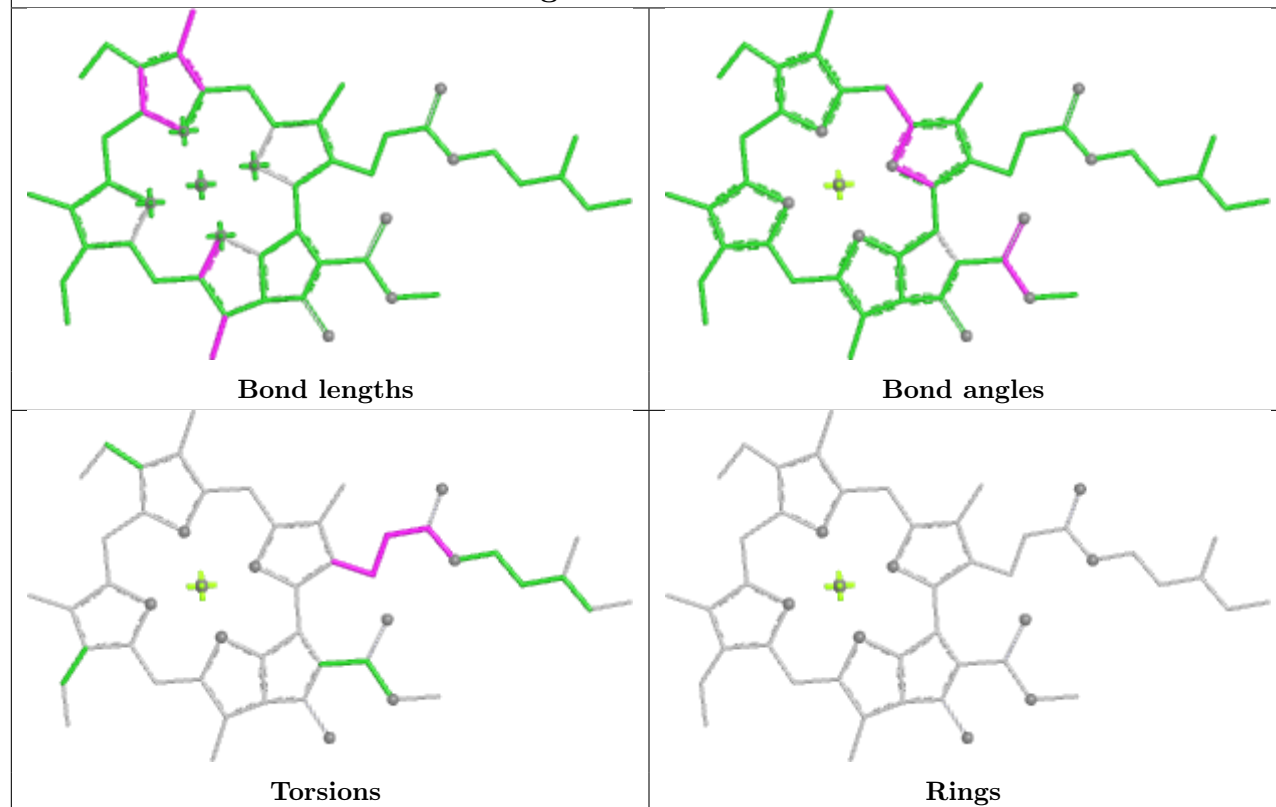


Torsions

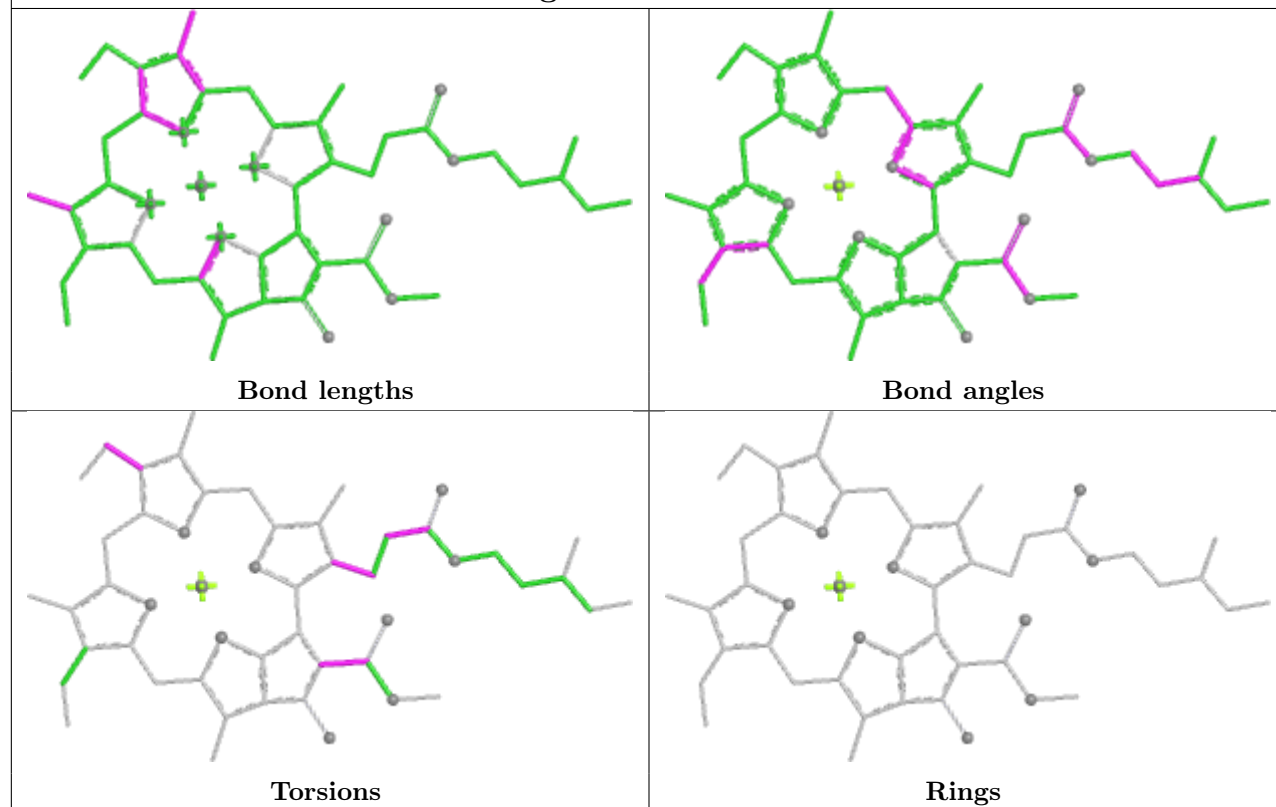


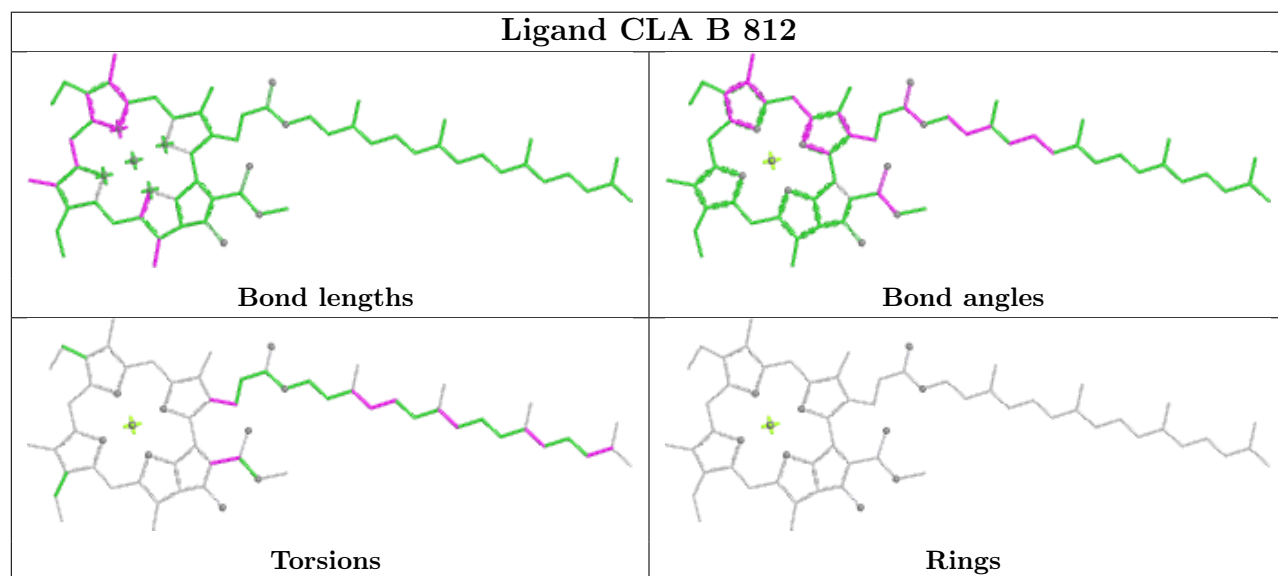
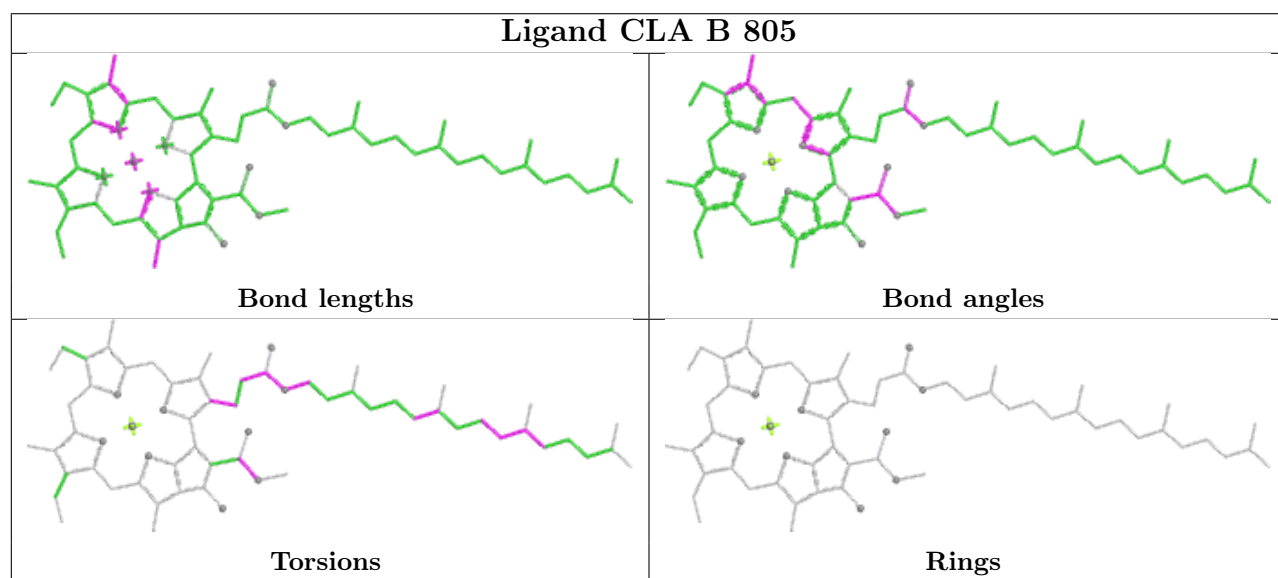
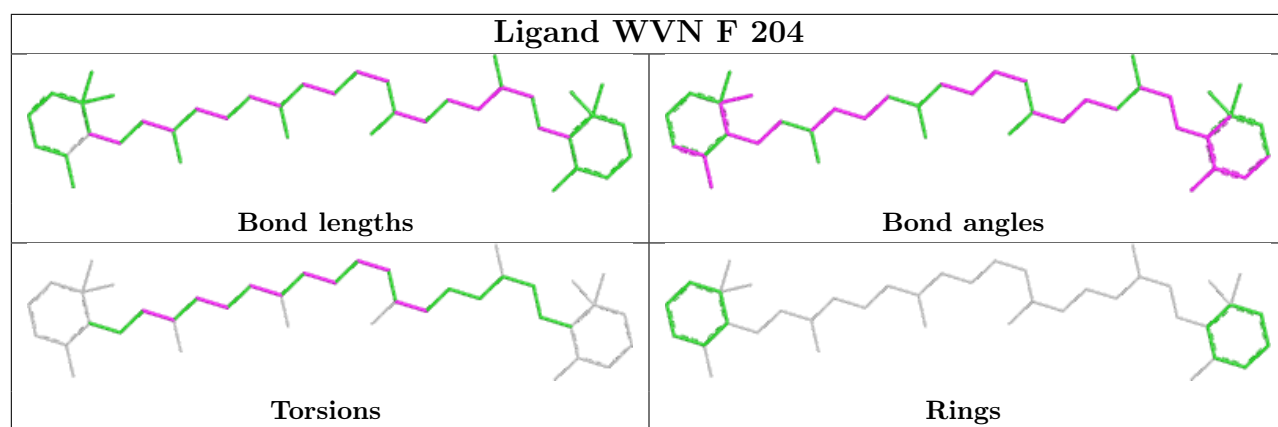
Rings

Ligand CLA i 601

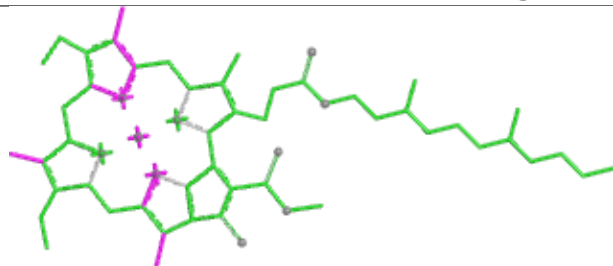


Ligand CLA f 606

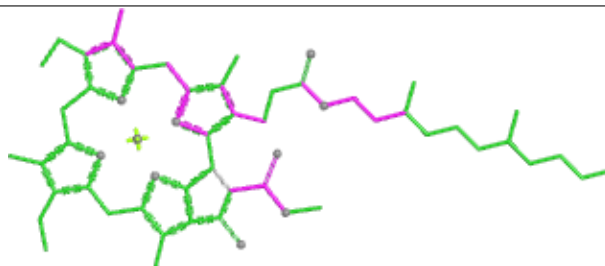




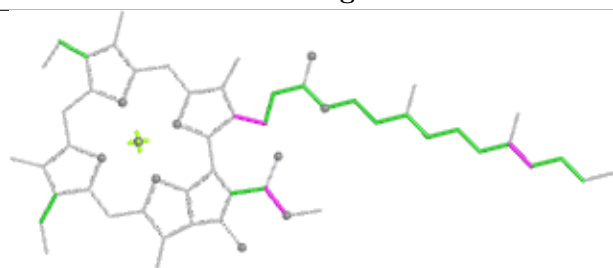
Ligand CLA B 832



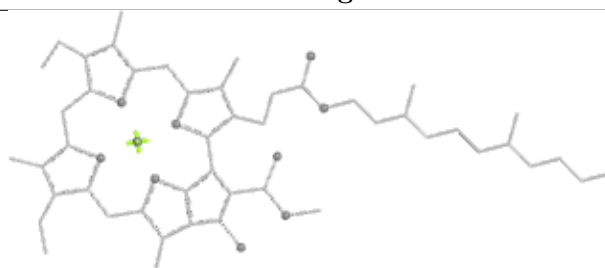
Bond lengths



Bond angles

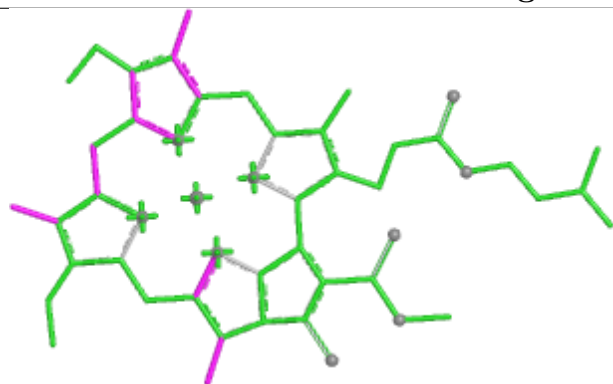


Torsions

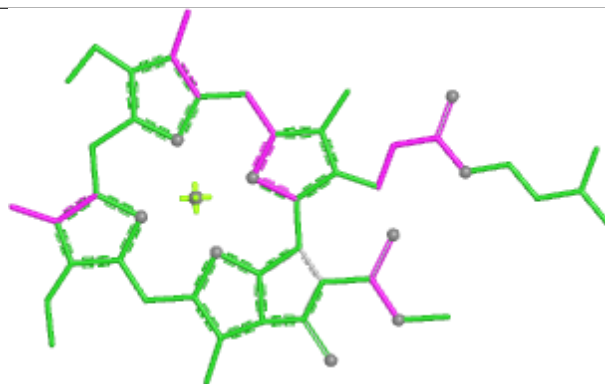


Rings

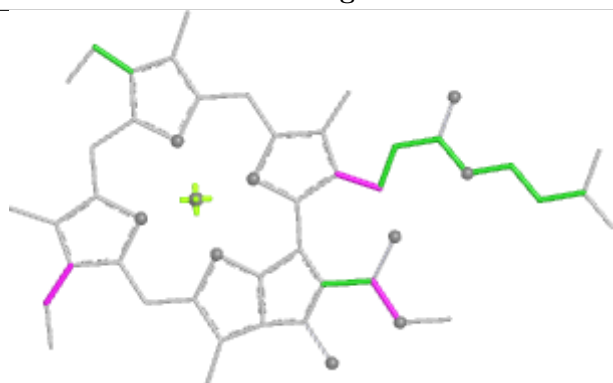
Ligand CLA k 602



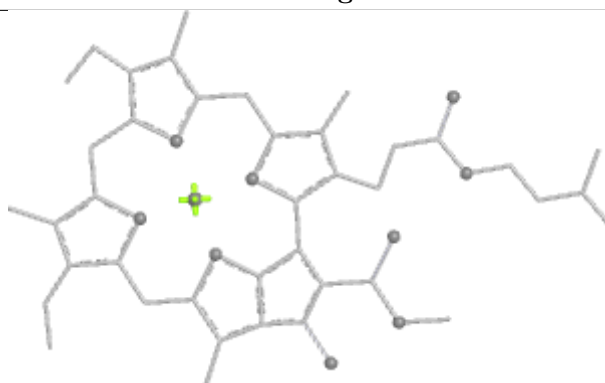
Bond lengths



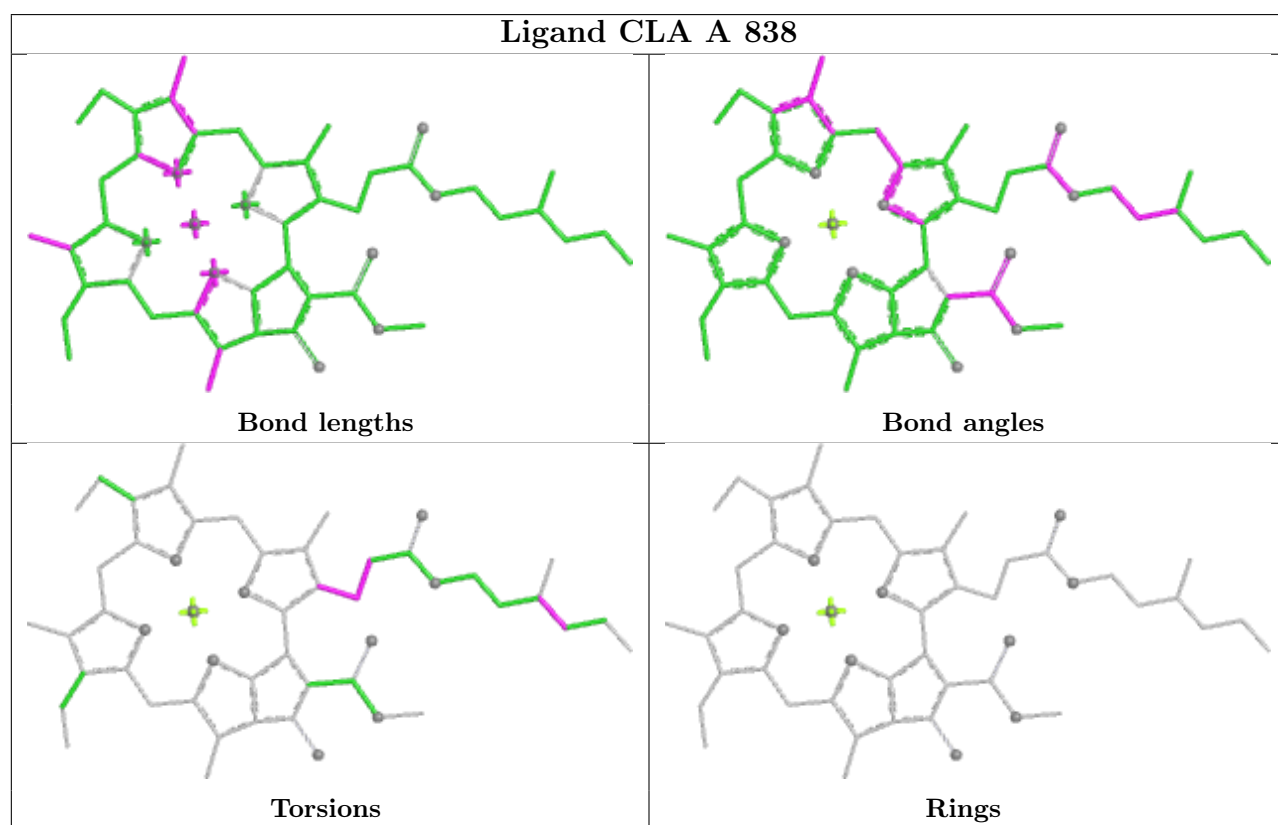
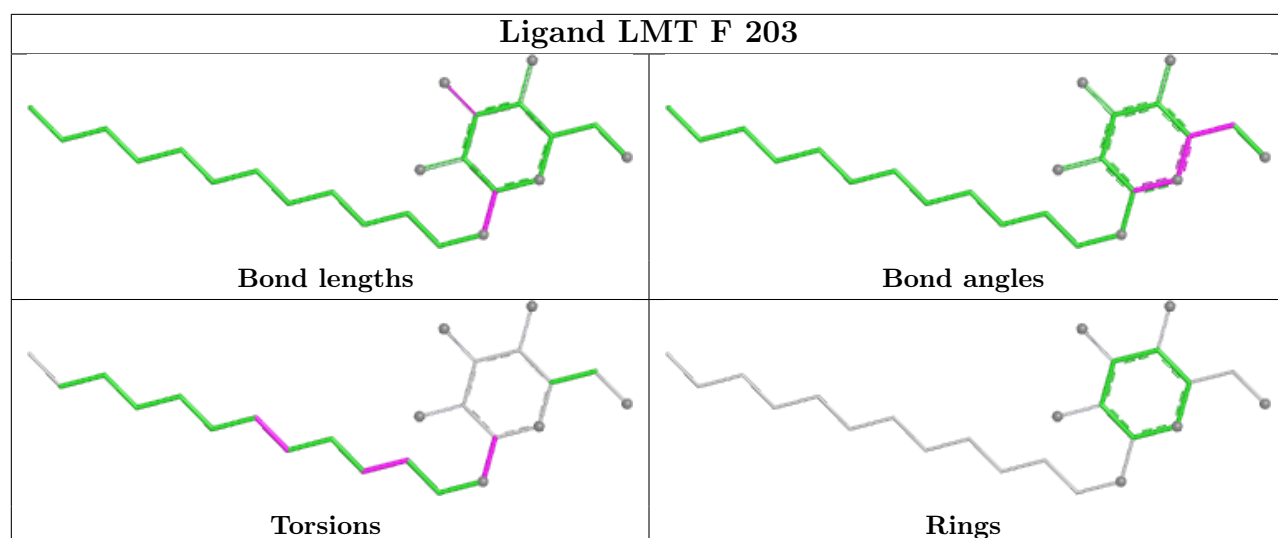
Bond angles

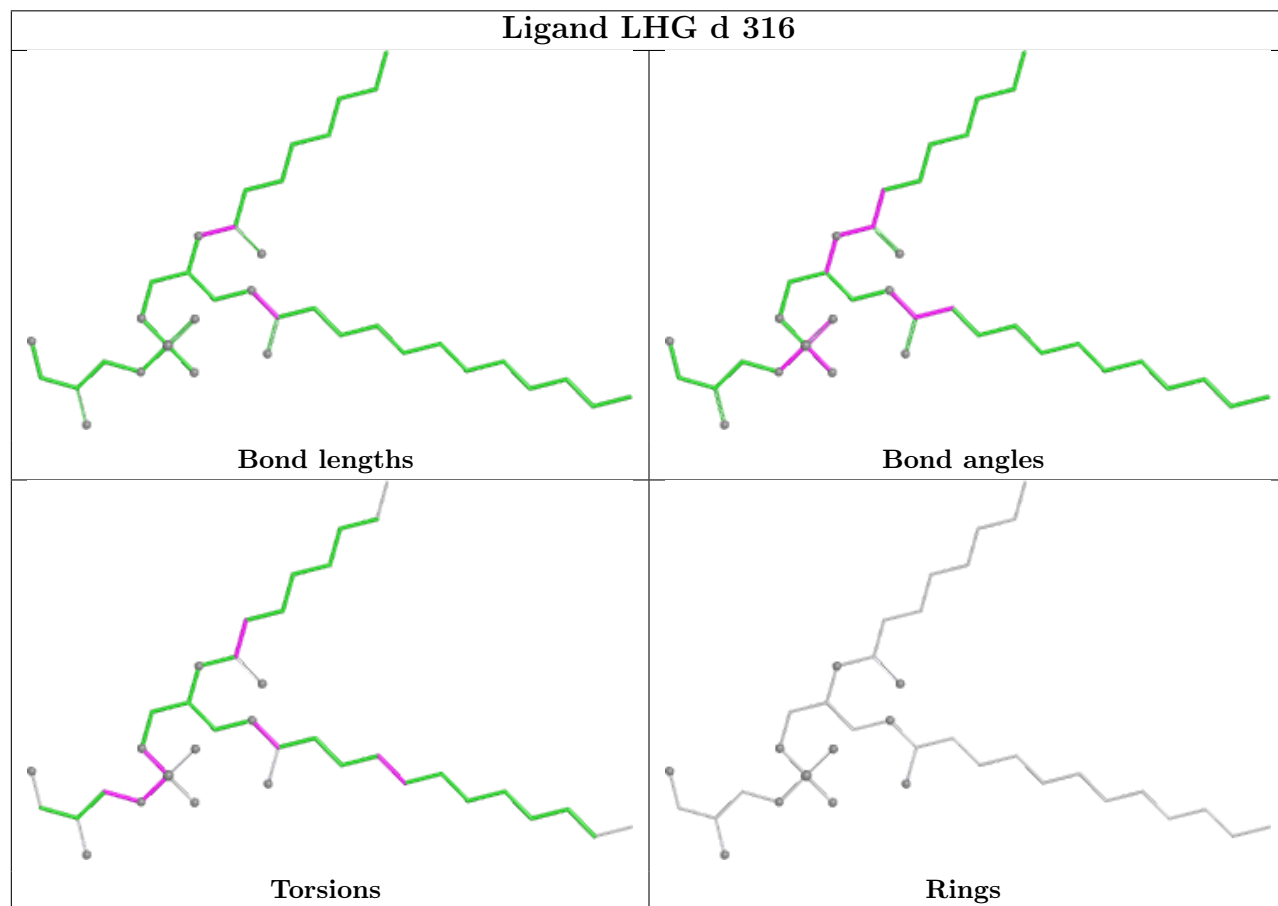
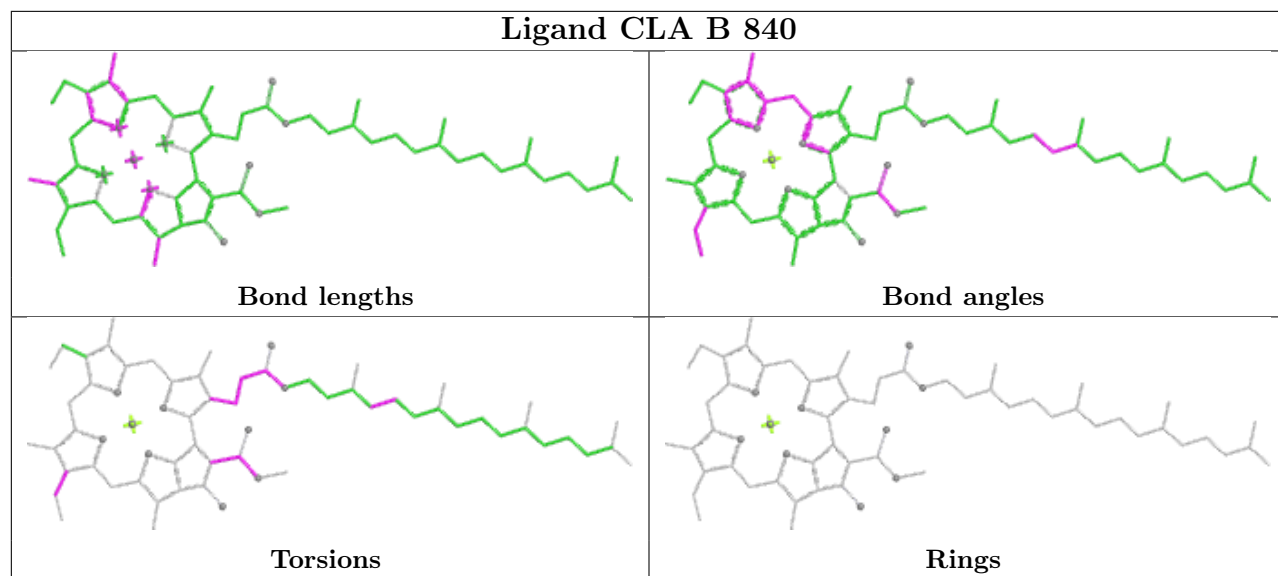


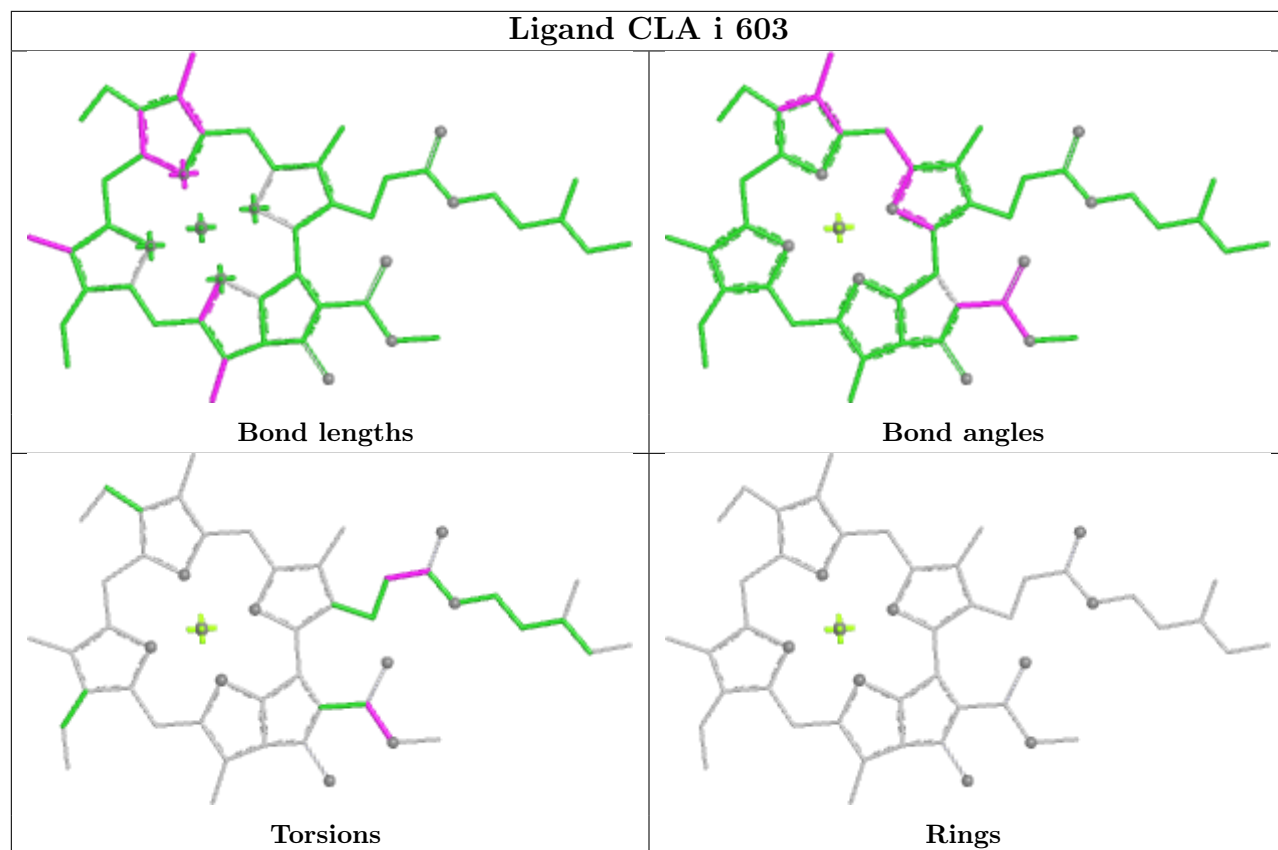
Torsions



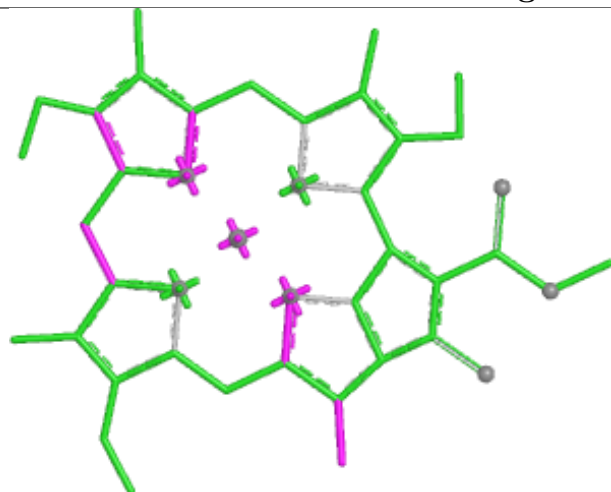
Rings







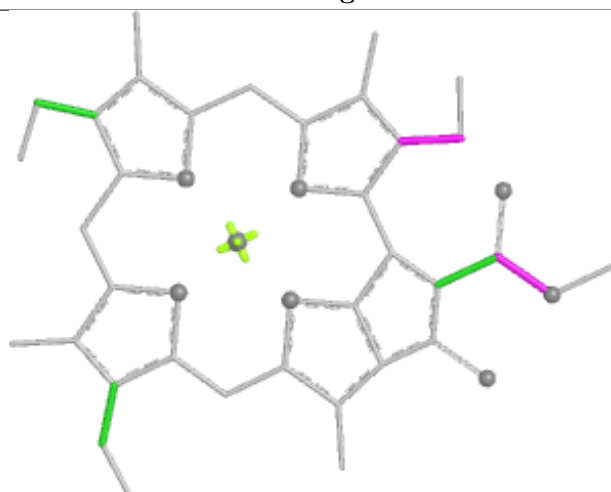
Ligand CLA J 103



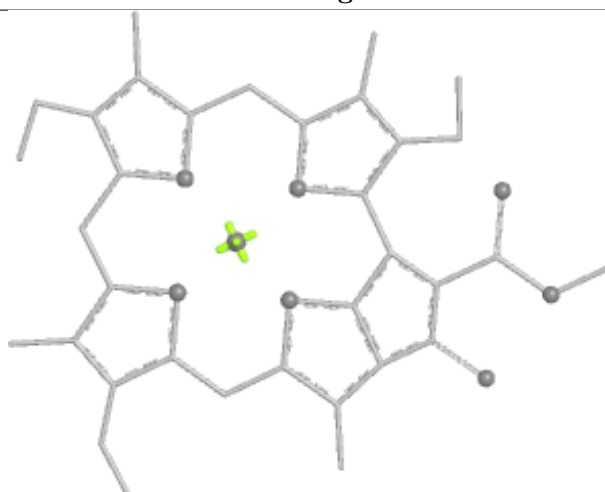
Bond lengths



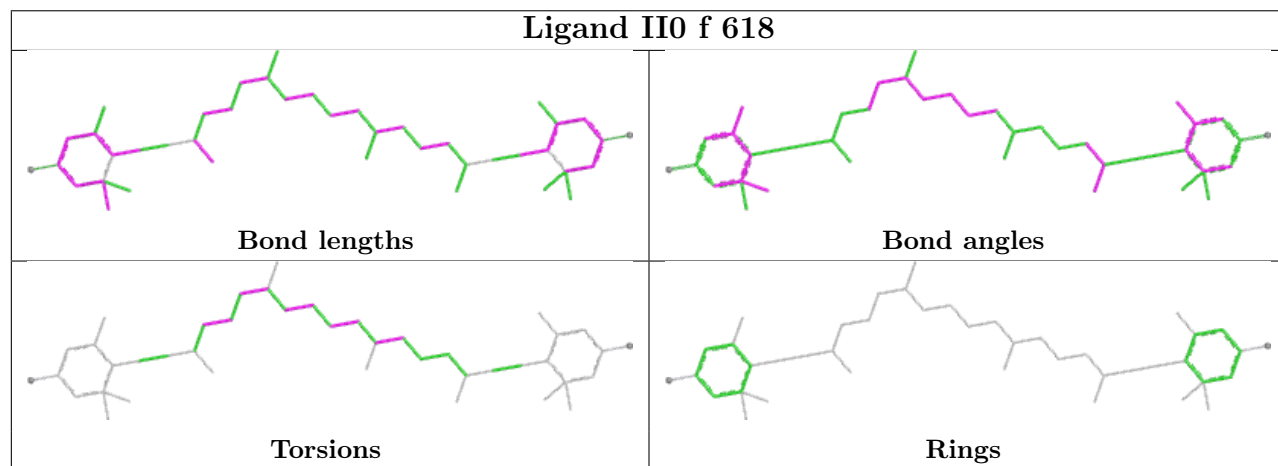
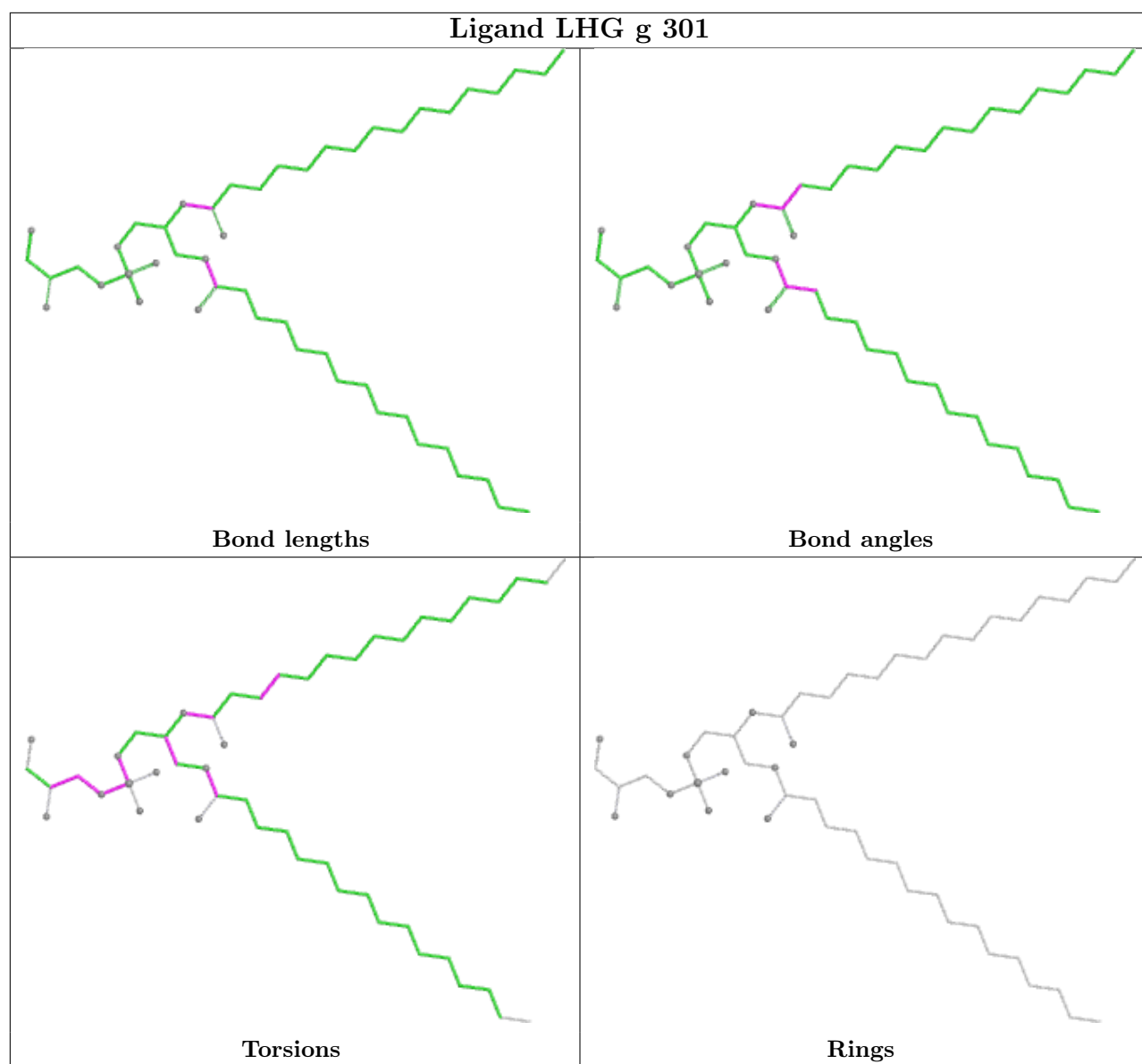
Bond angles



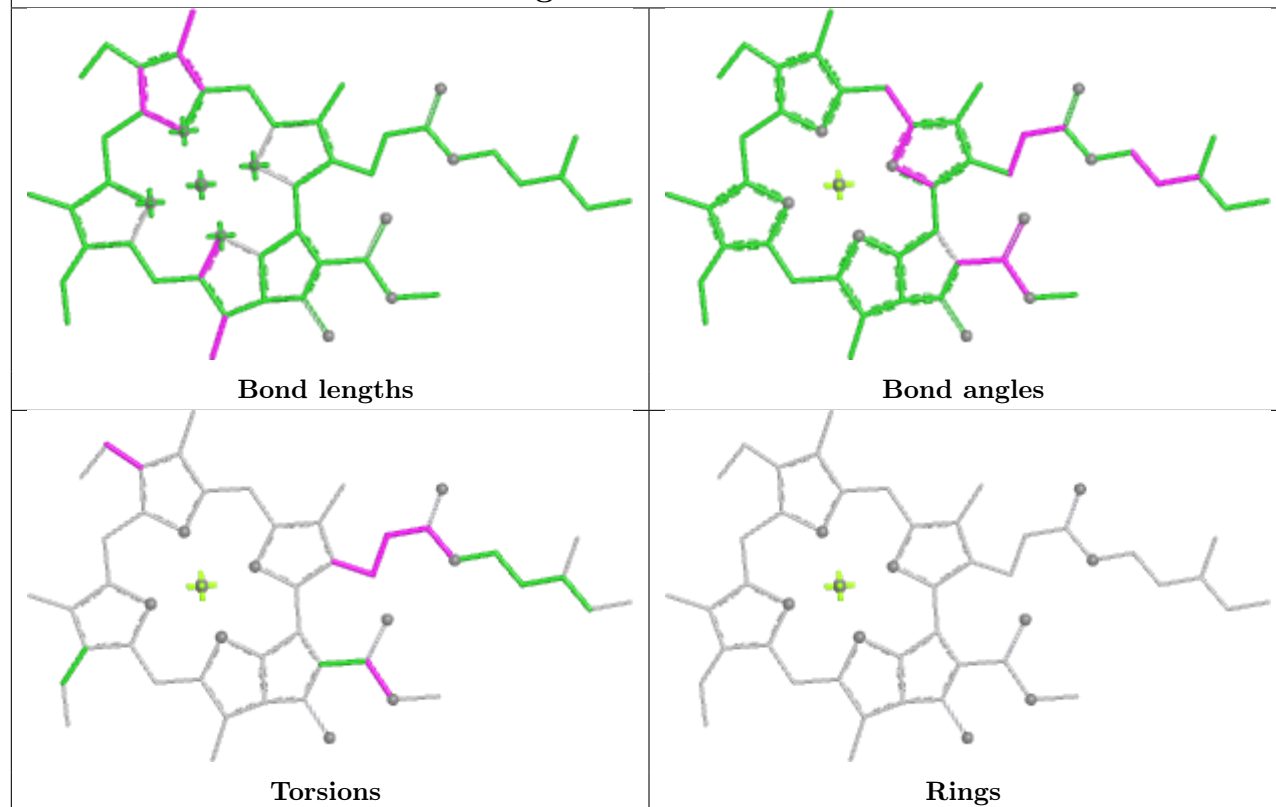
Torsions



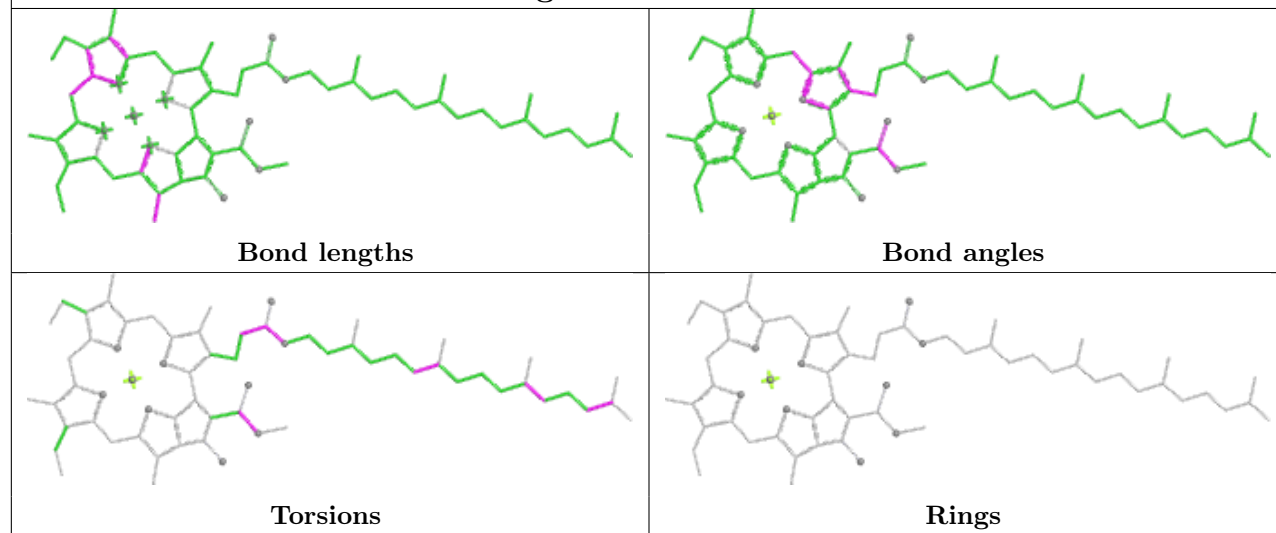
Rings



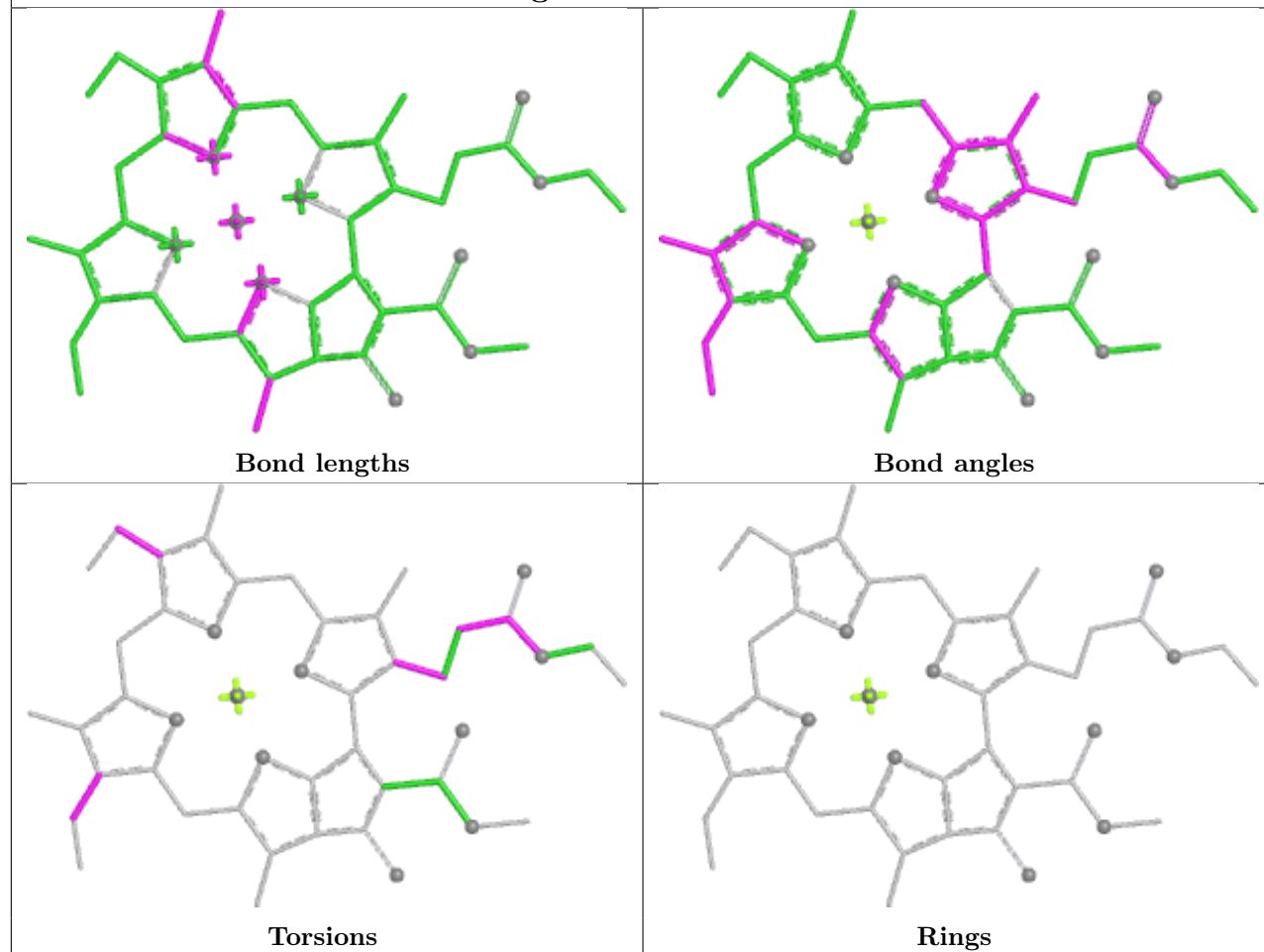
Ligand CLA k 610



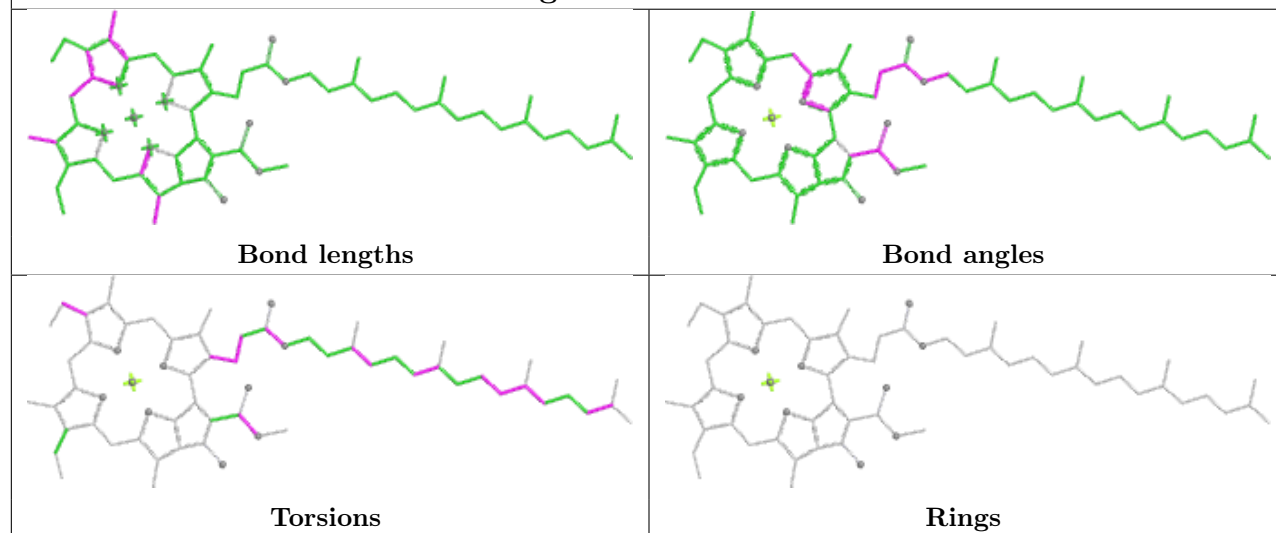
Ligand CLA a 310



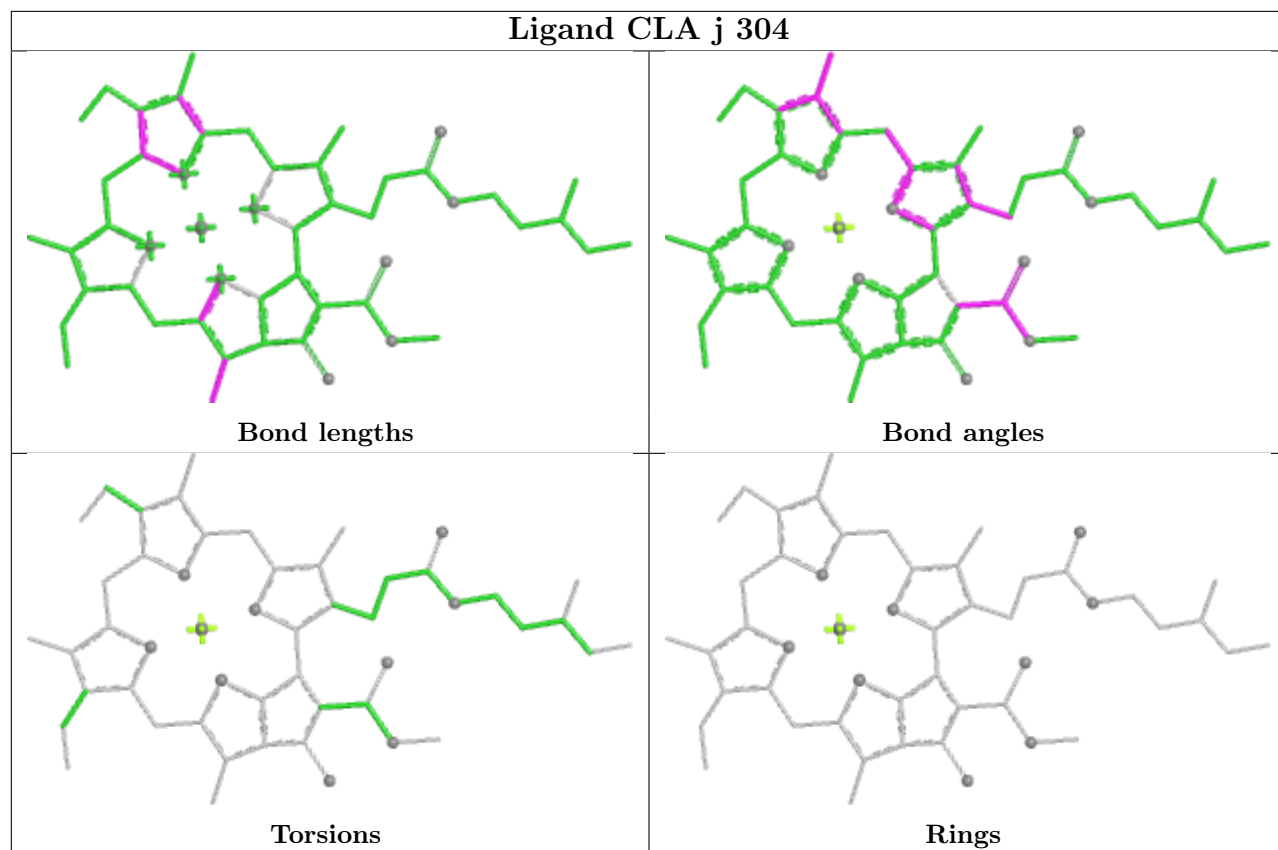
Ligand CLA a 311



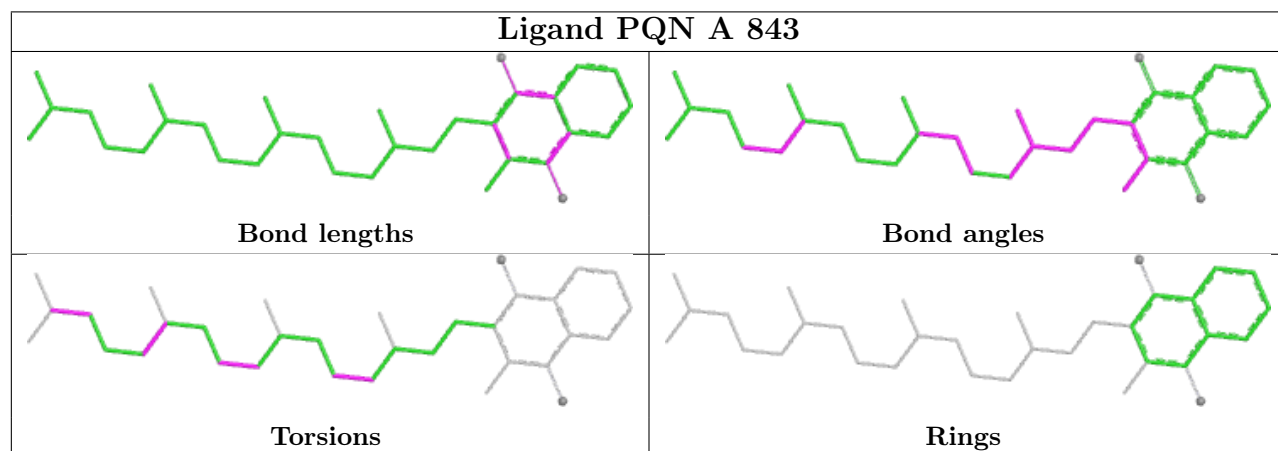
Ligand CLA f 607



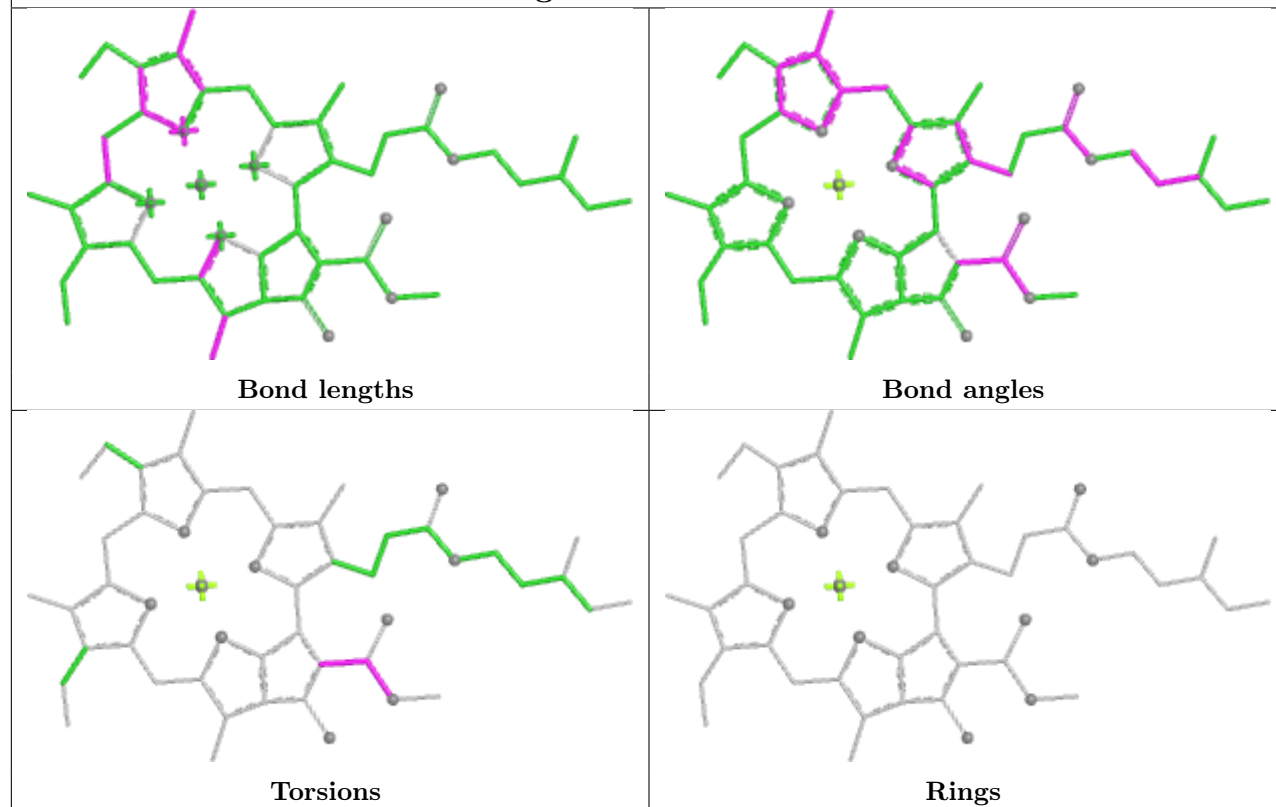
Ligand CLA j 304



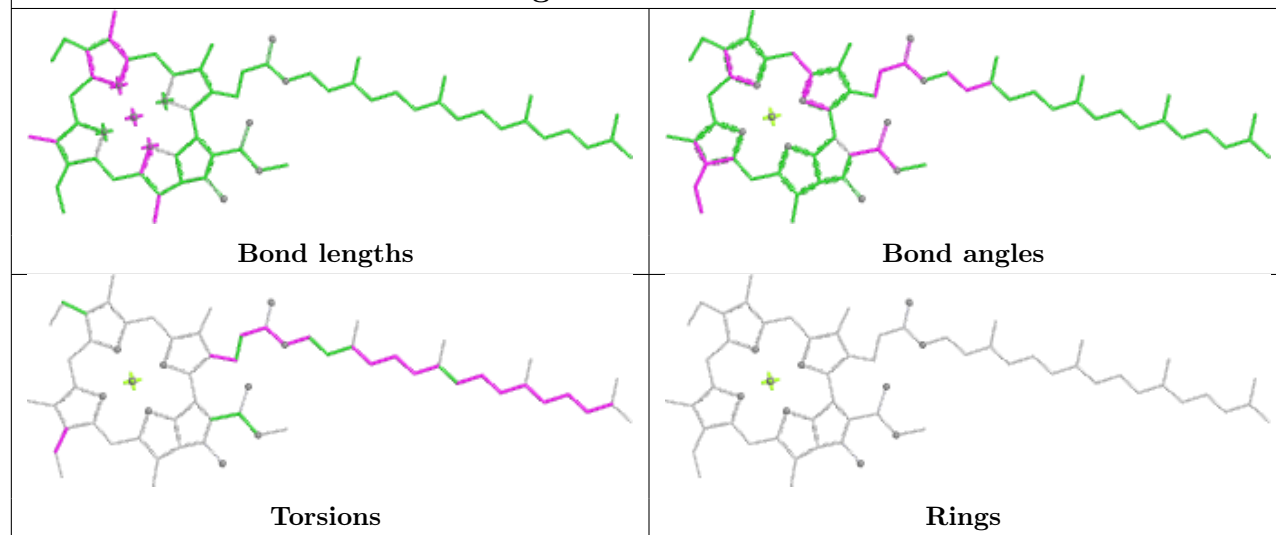
Ligand PQN A 843

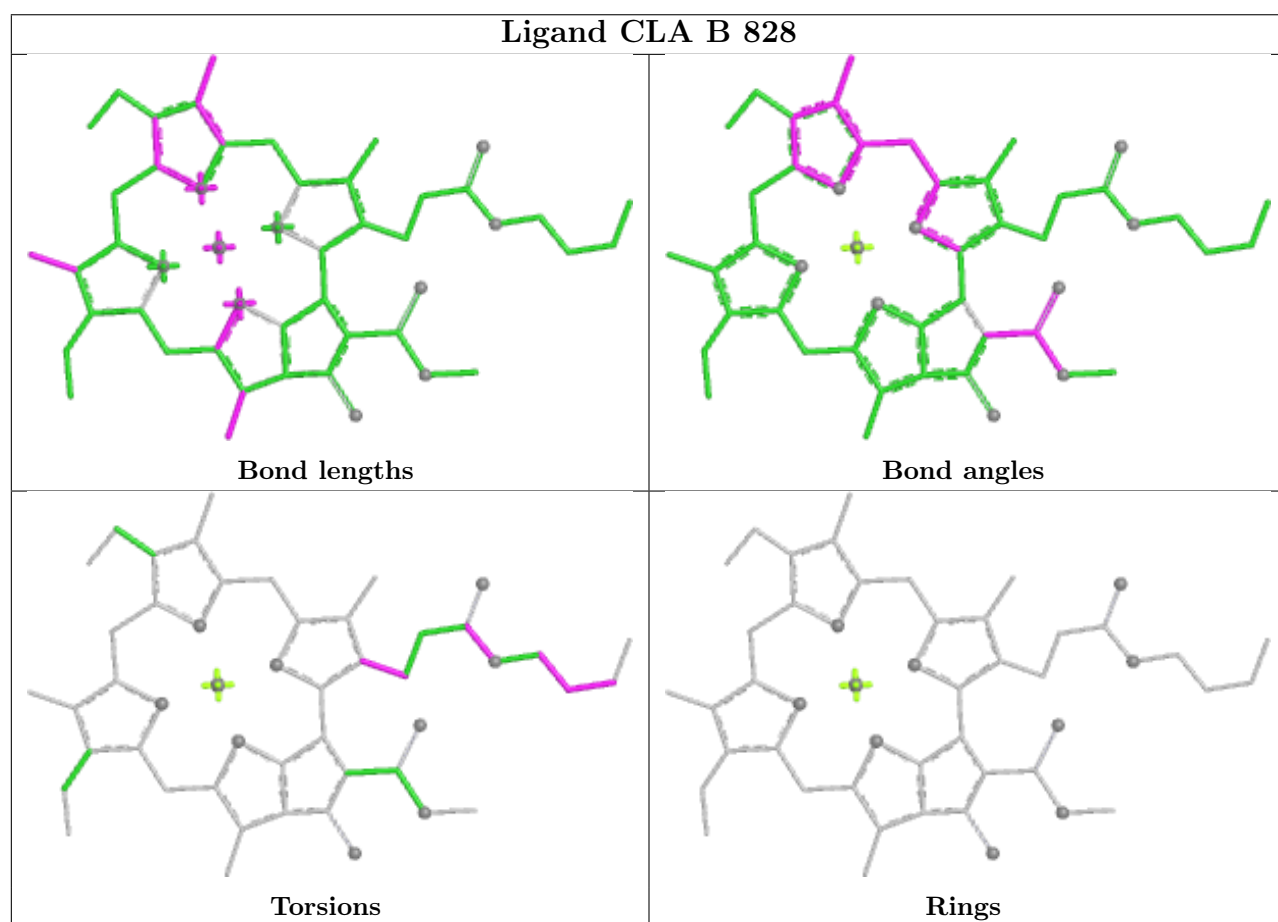
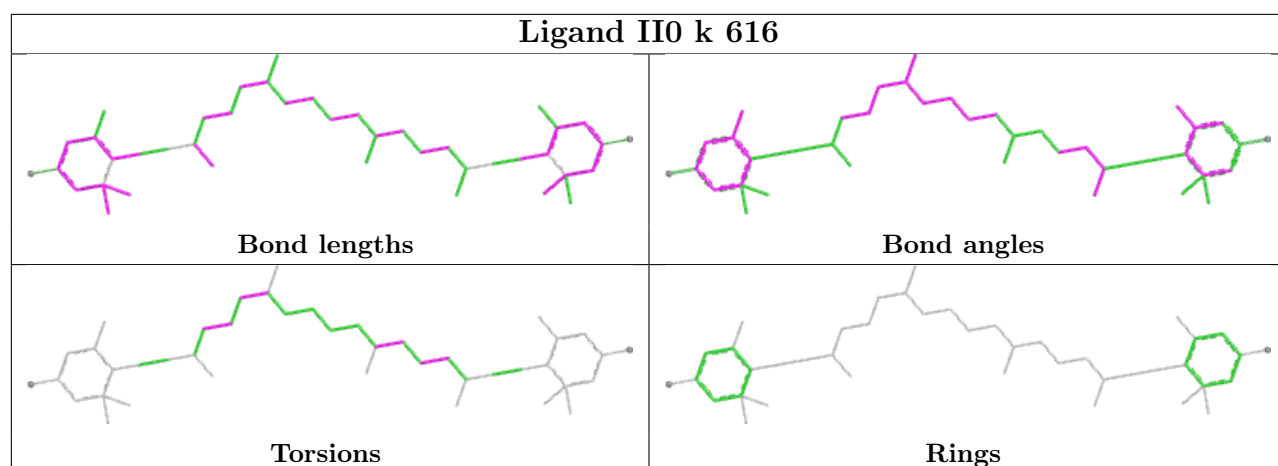


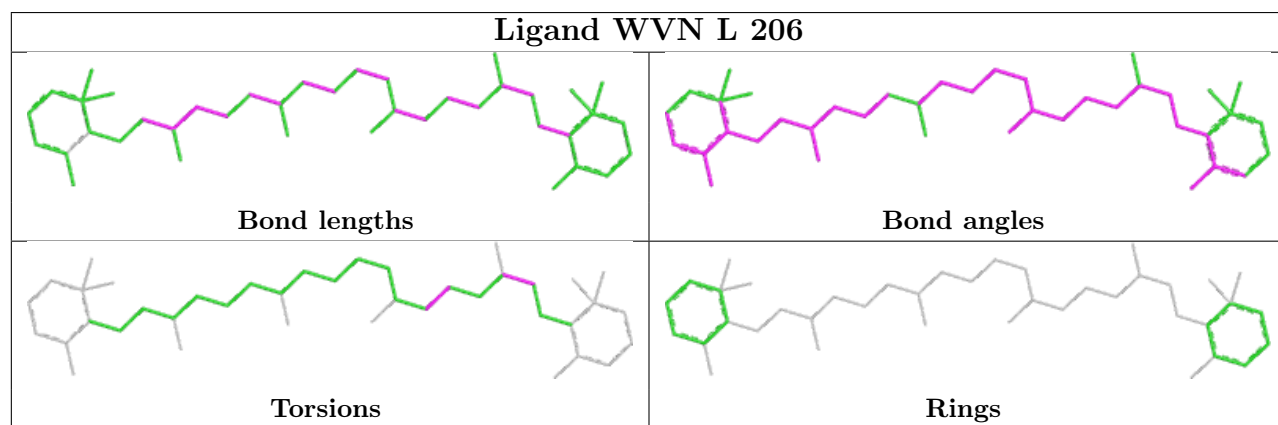
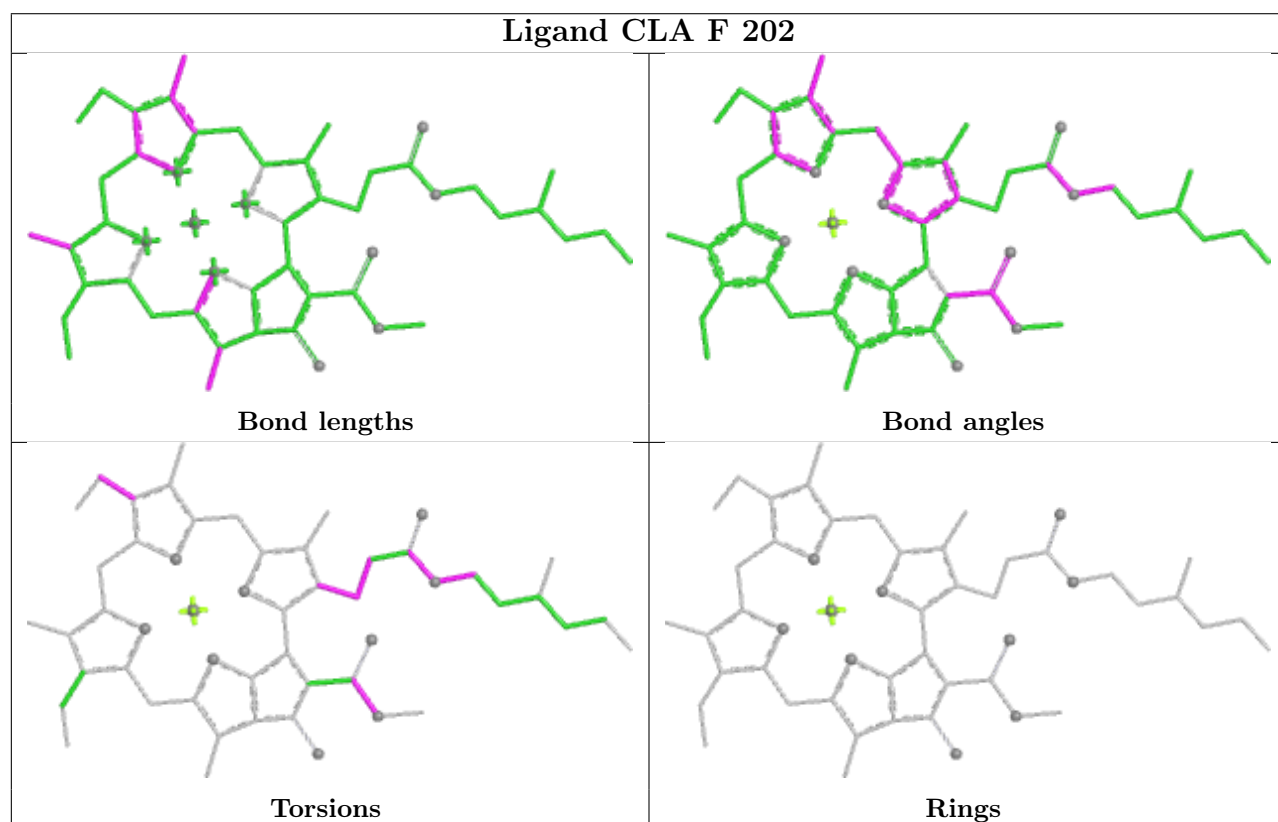
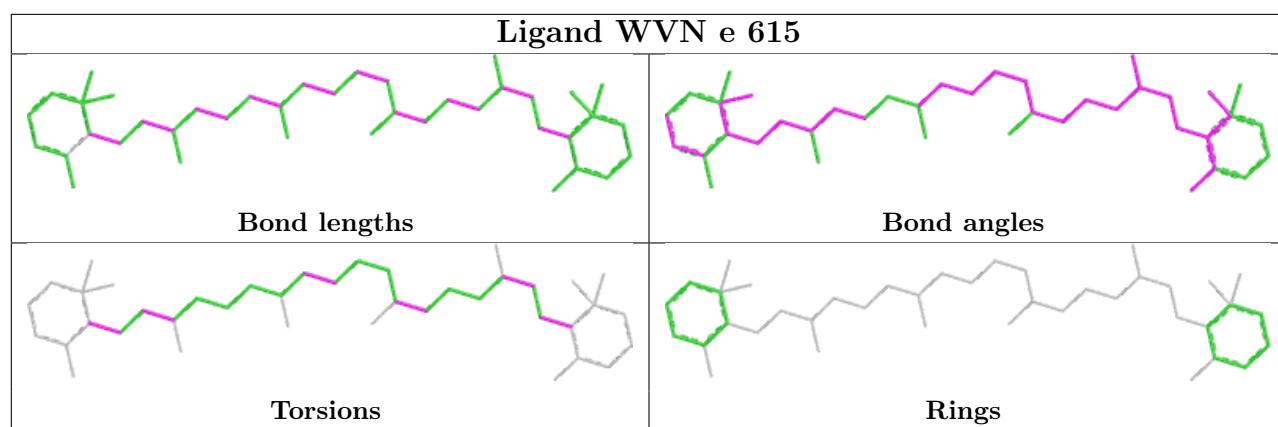
Ligand CLA d 302



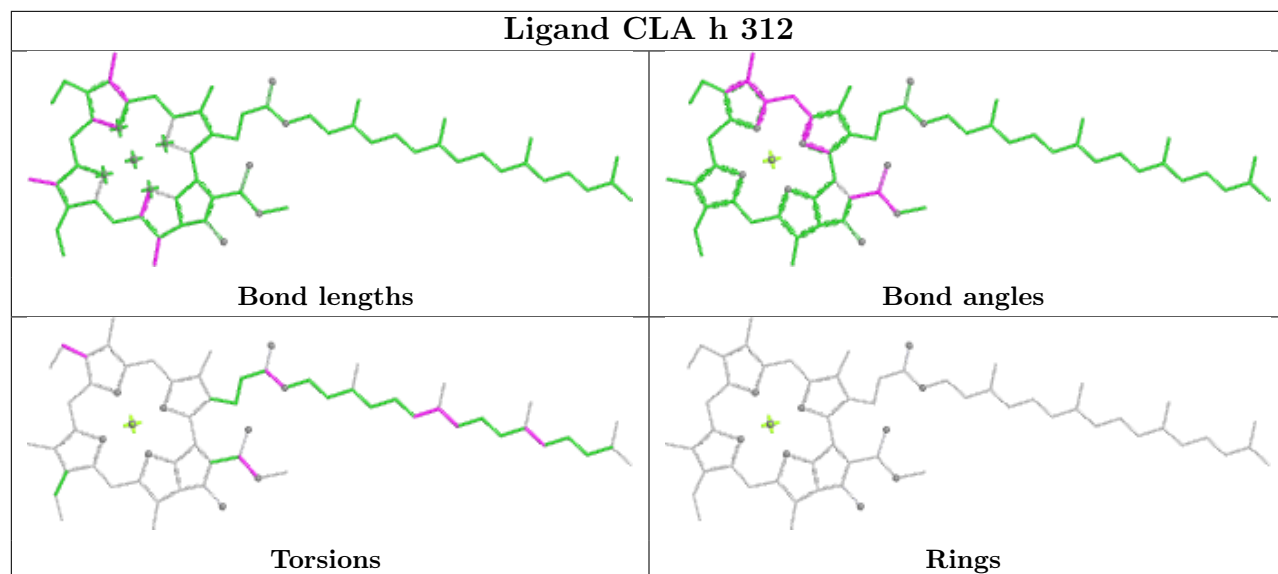
Ligand CLA B 836



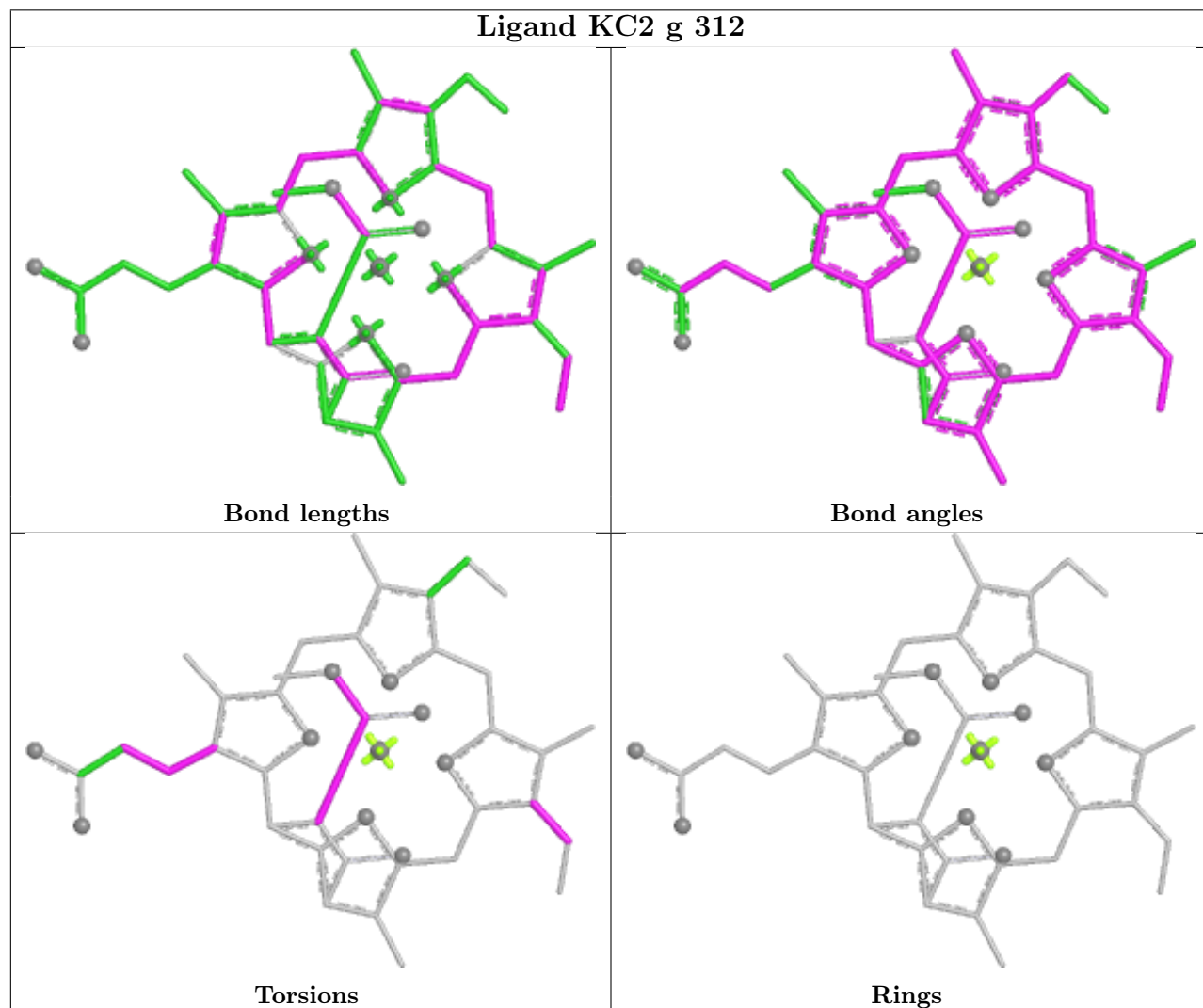


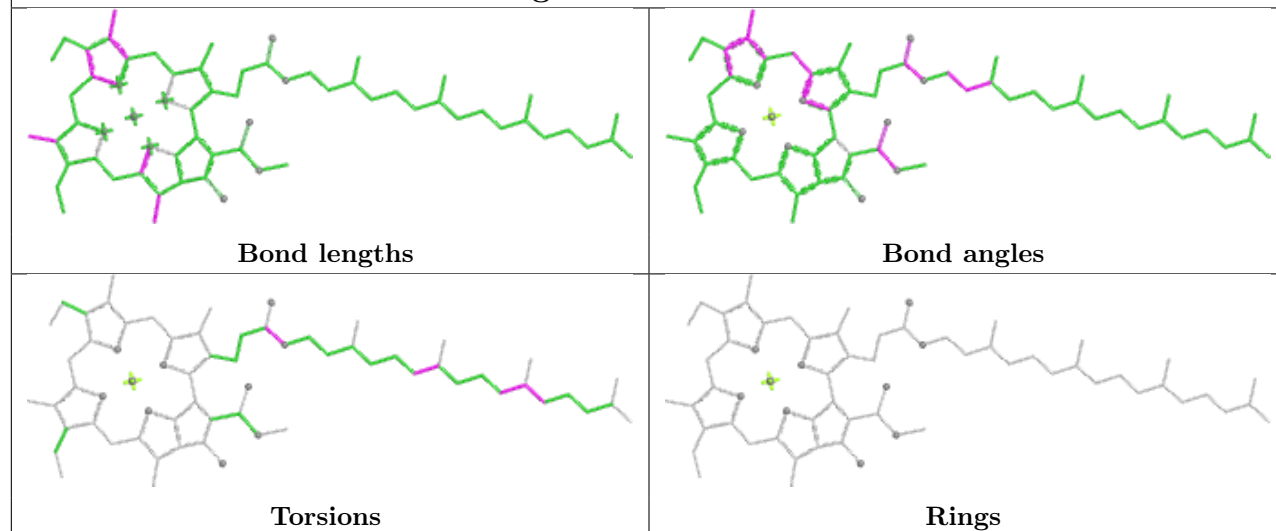
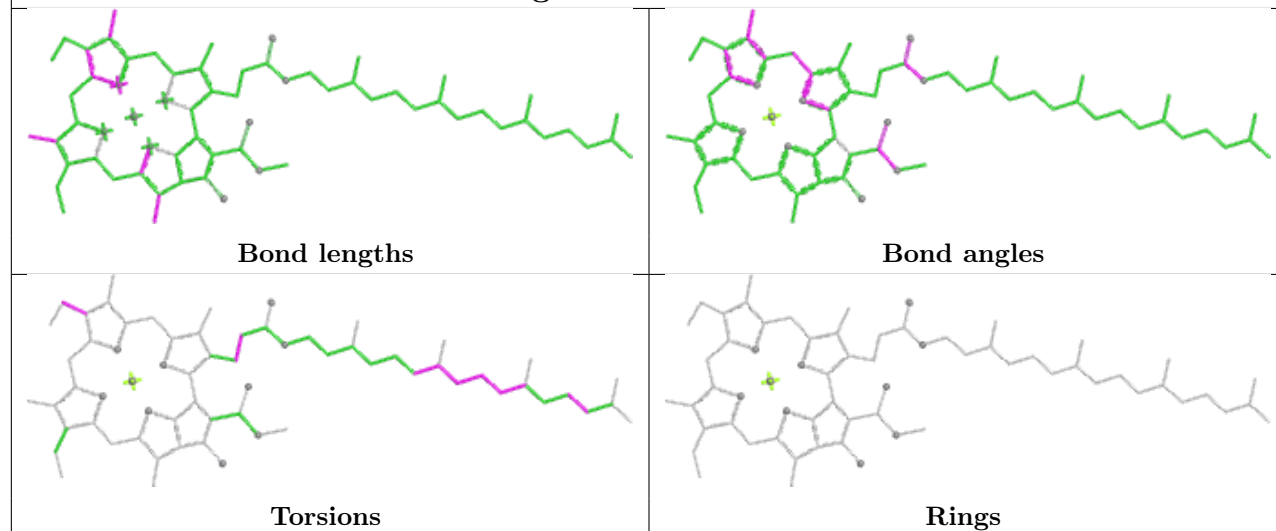


Ligand CLA h 312

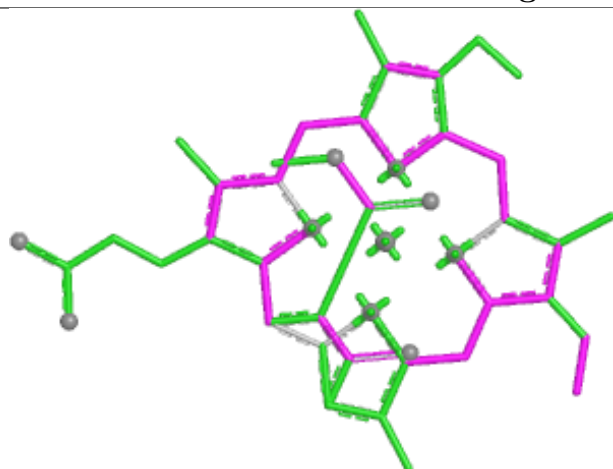


Ligand KC2 g 312

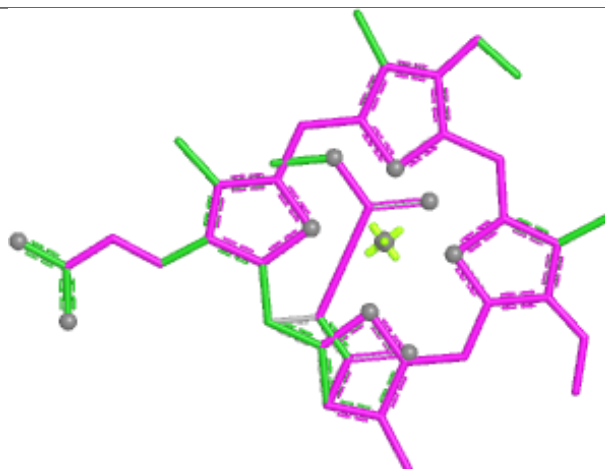


Ligand CLA B 818**Ligand CLA B 835**

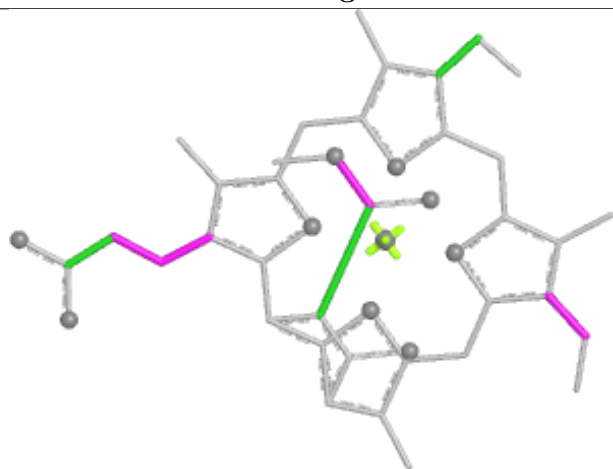
Ligand KC2 d 311



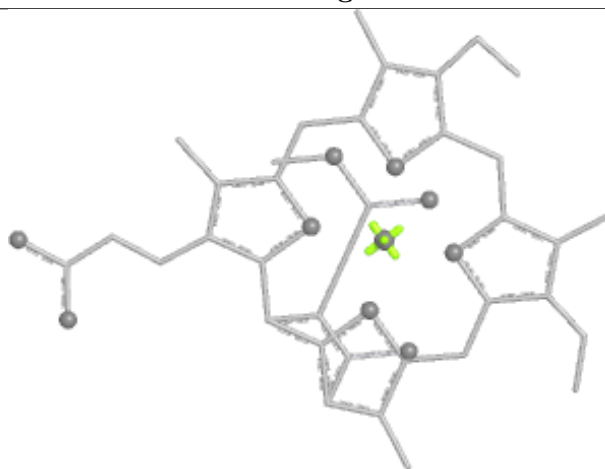
Bond lengths



Bond angles

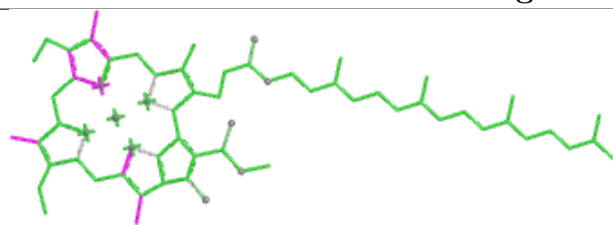


Torsions

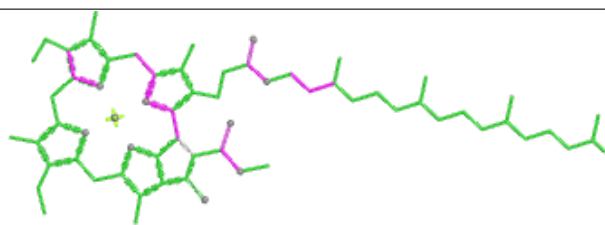


Rings

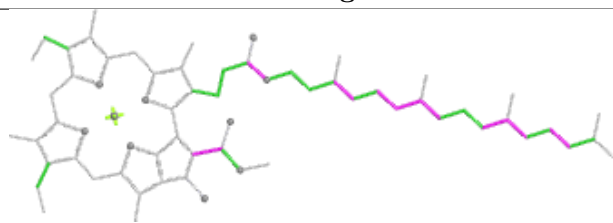
Ligand CLA F 201



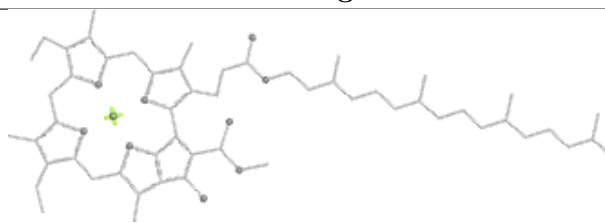
Bond lengths



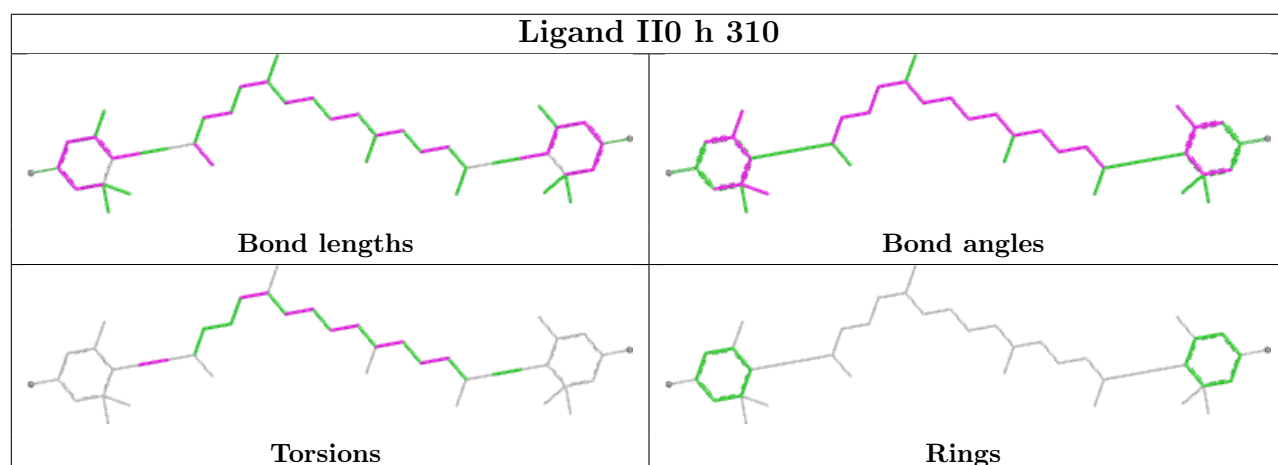
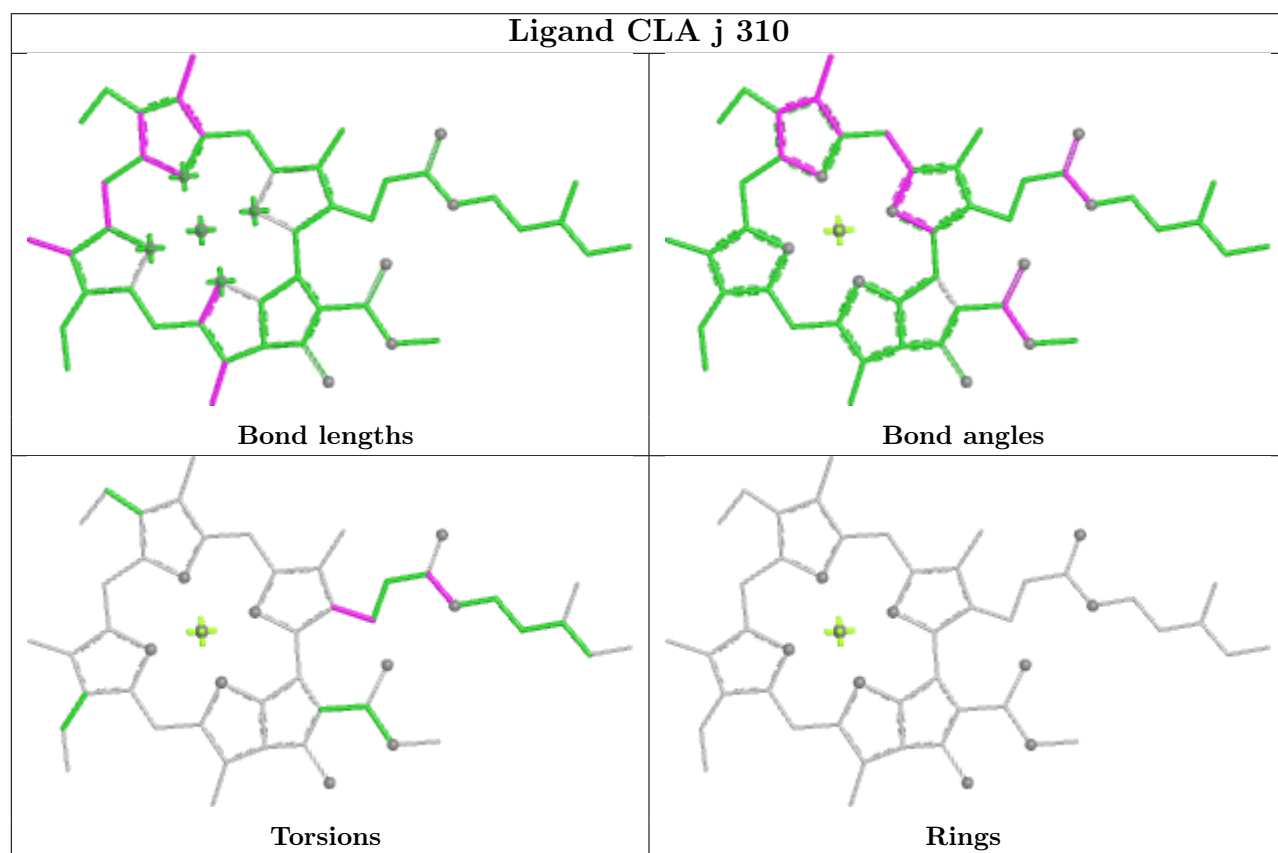
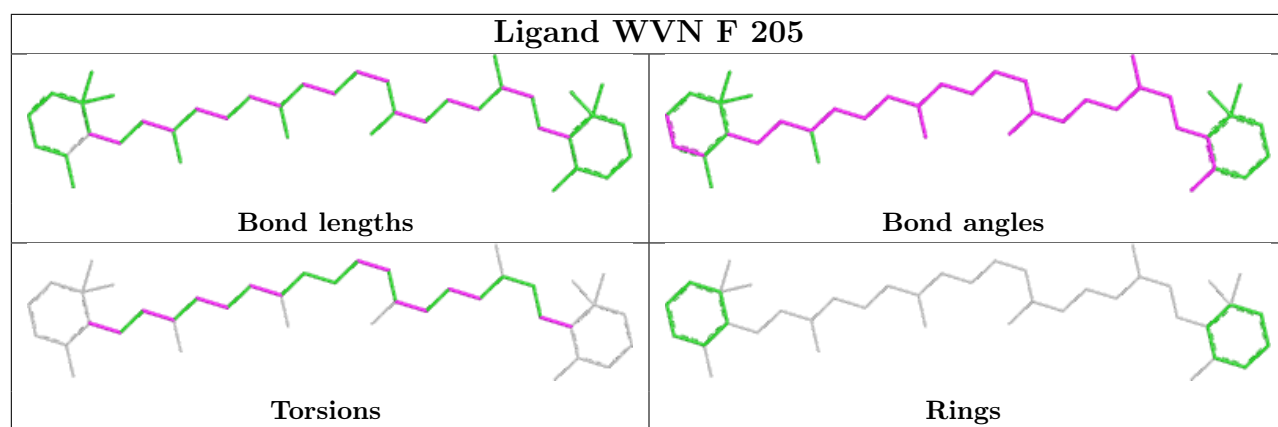
Bond angles

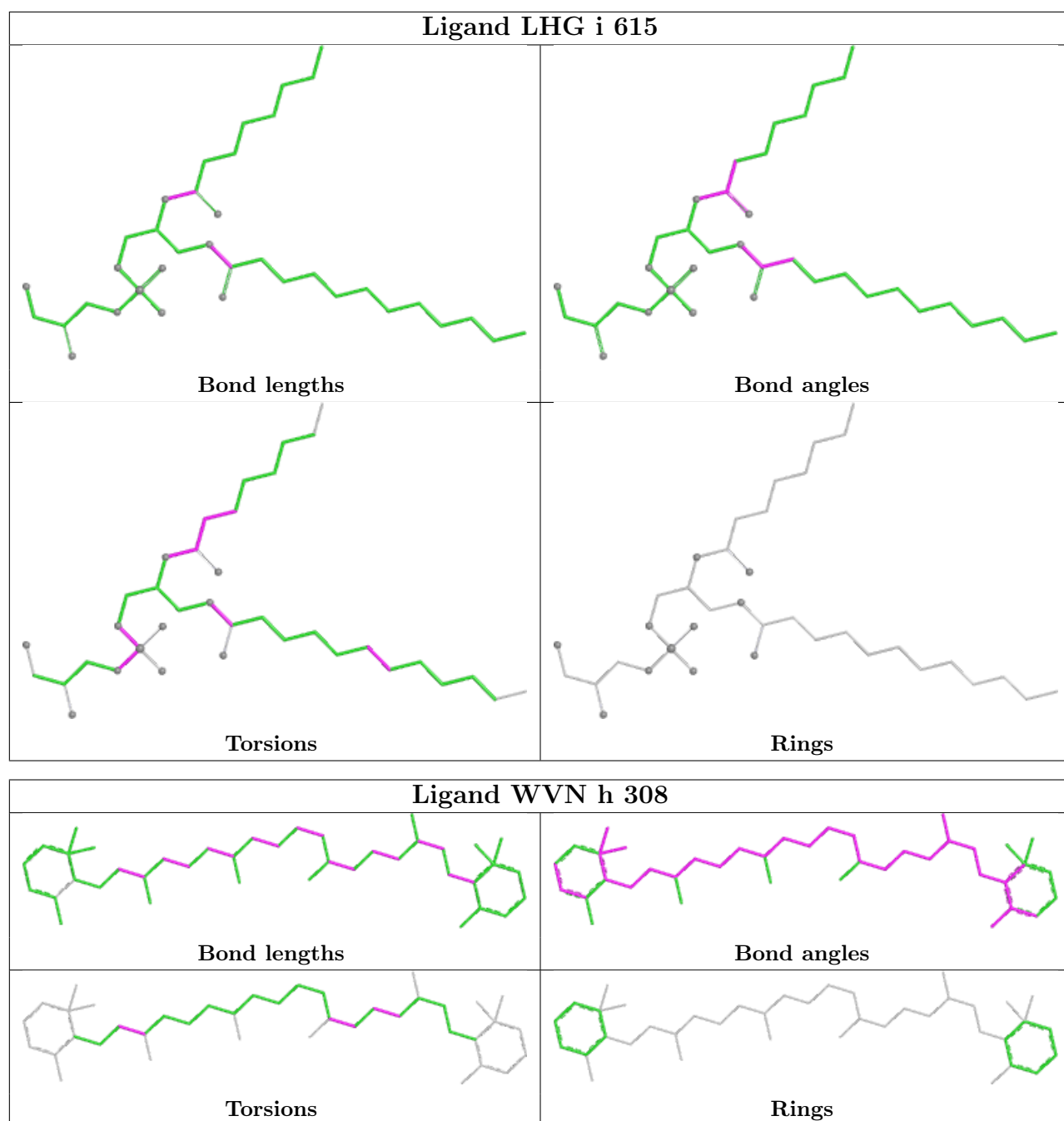


Torsions

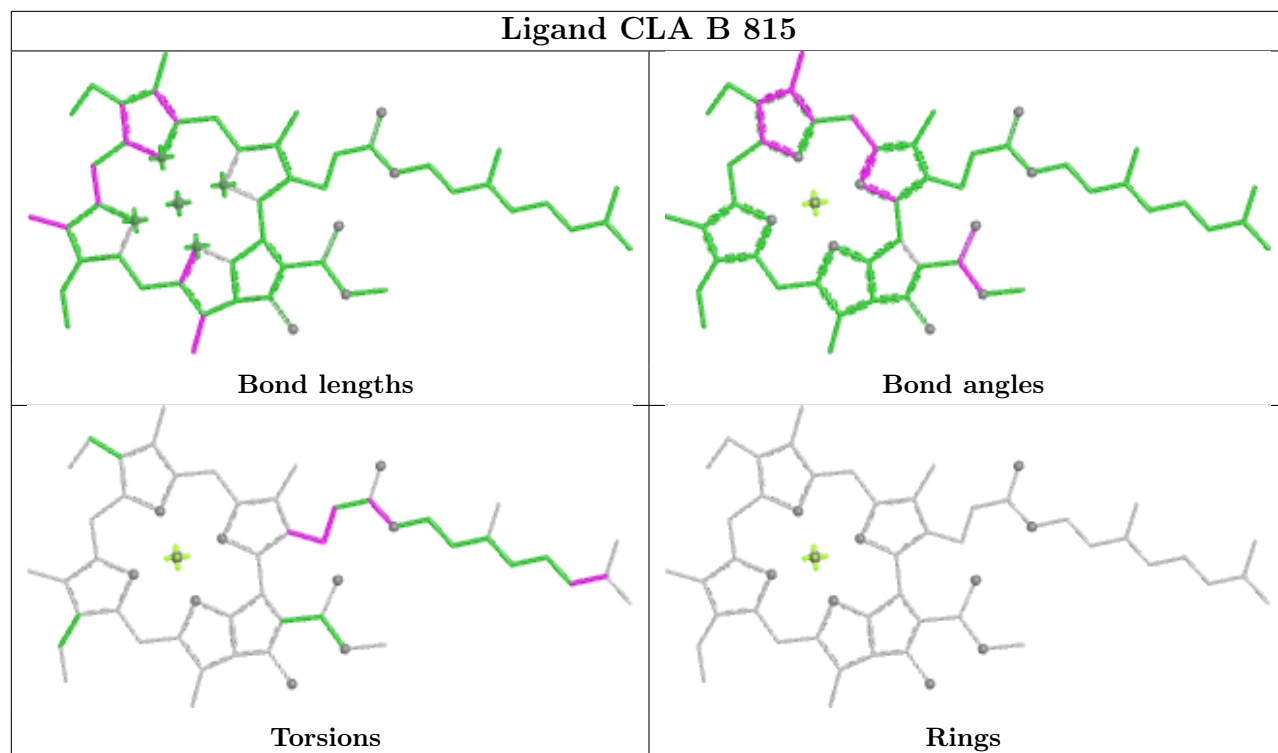


Rings

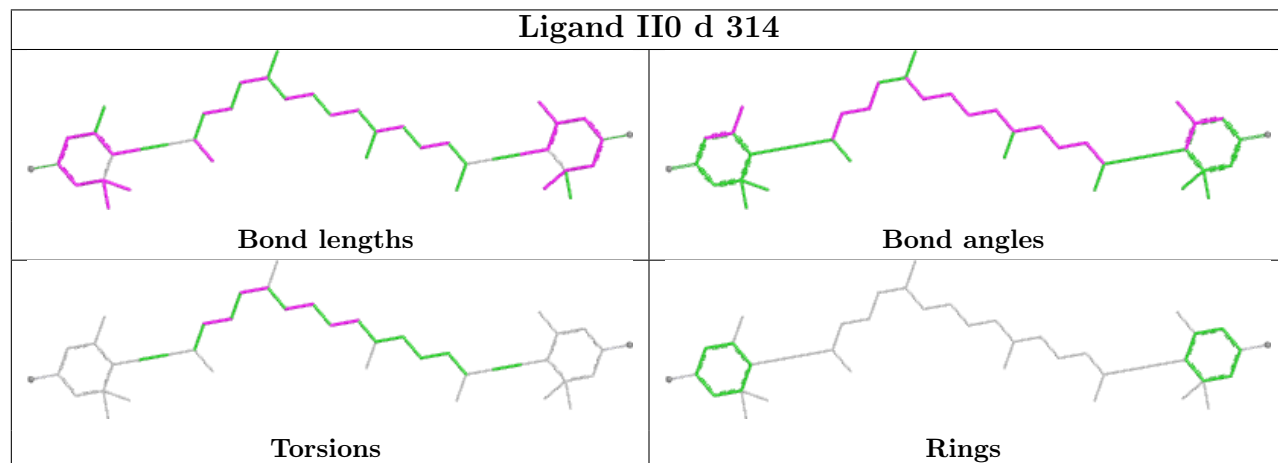




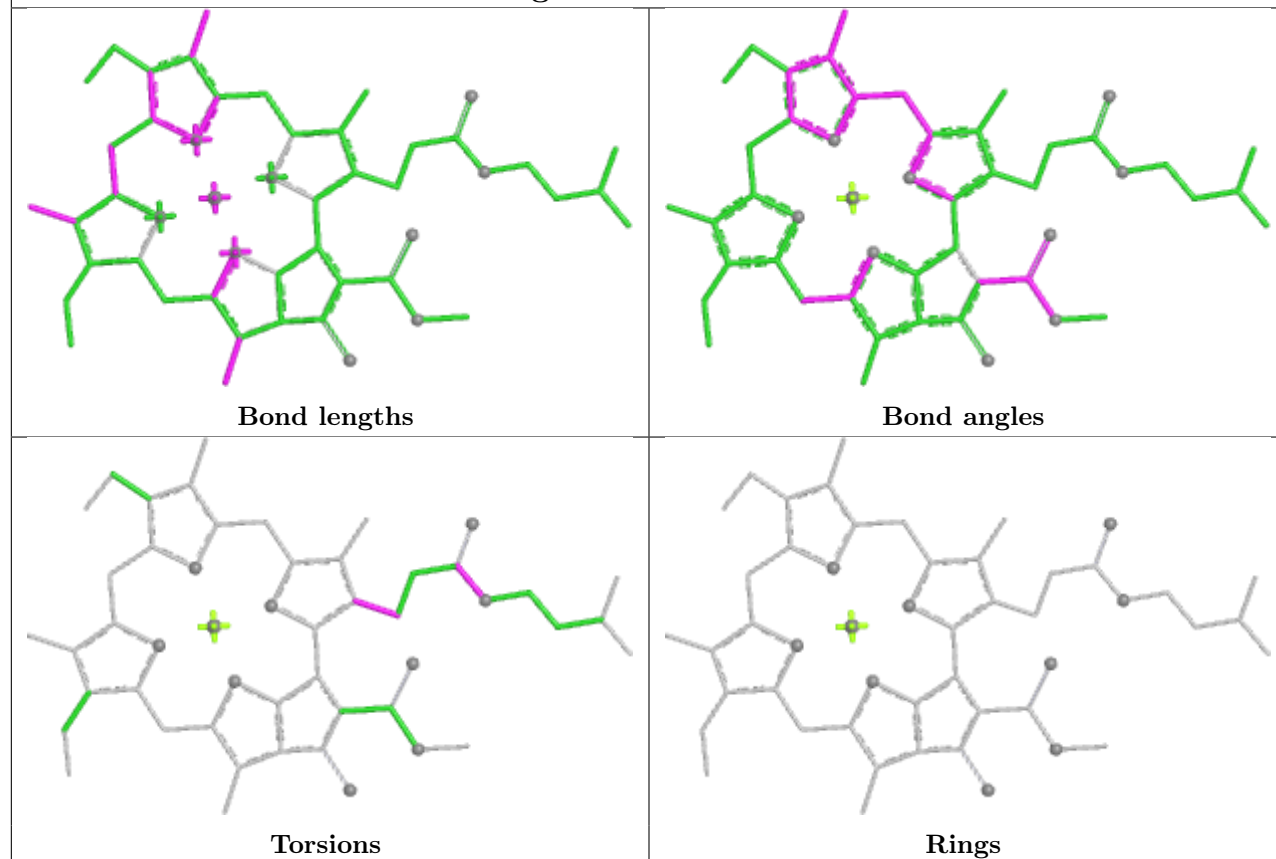
Ligand CLA B 815



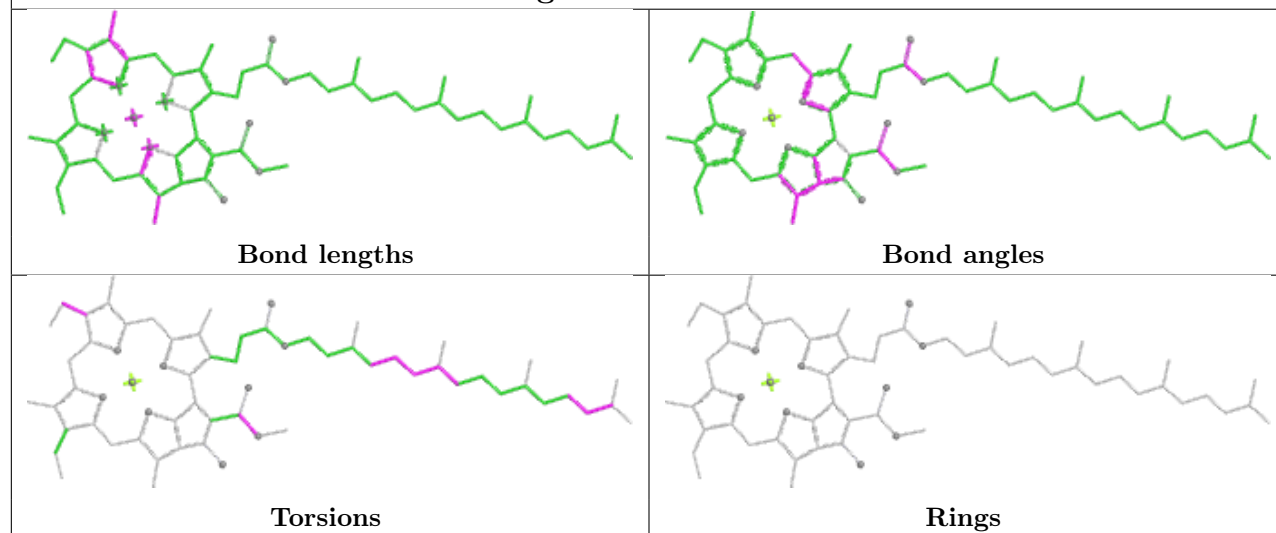
Ligand II0 d 314



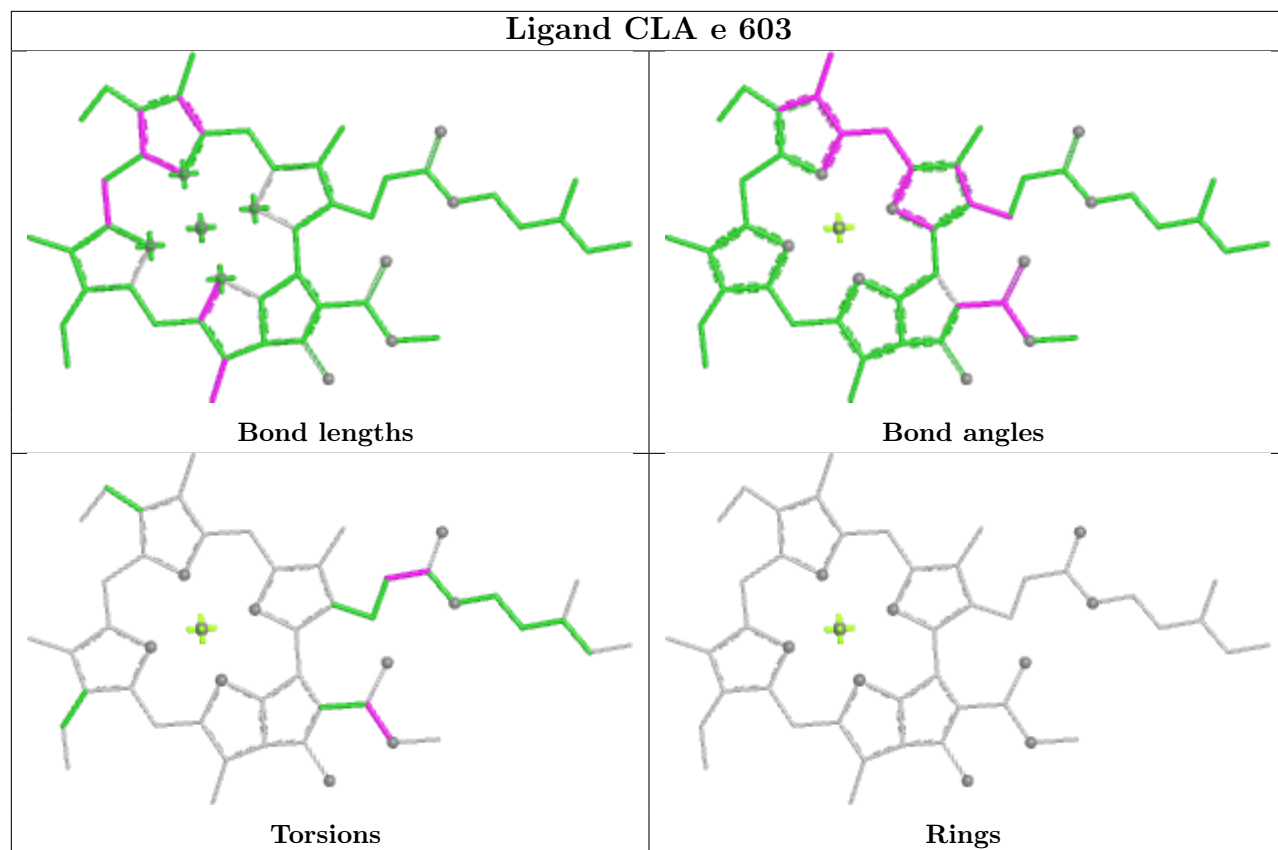
Ligand CLA A 830



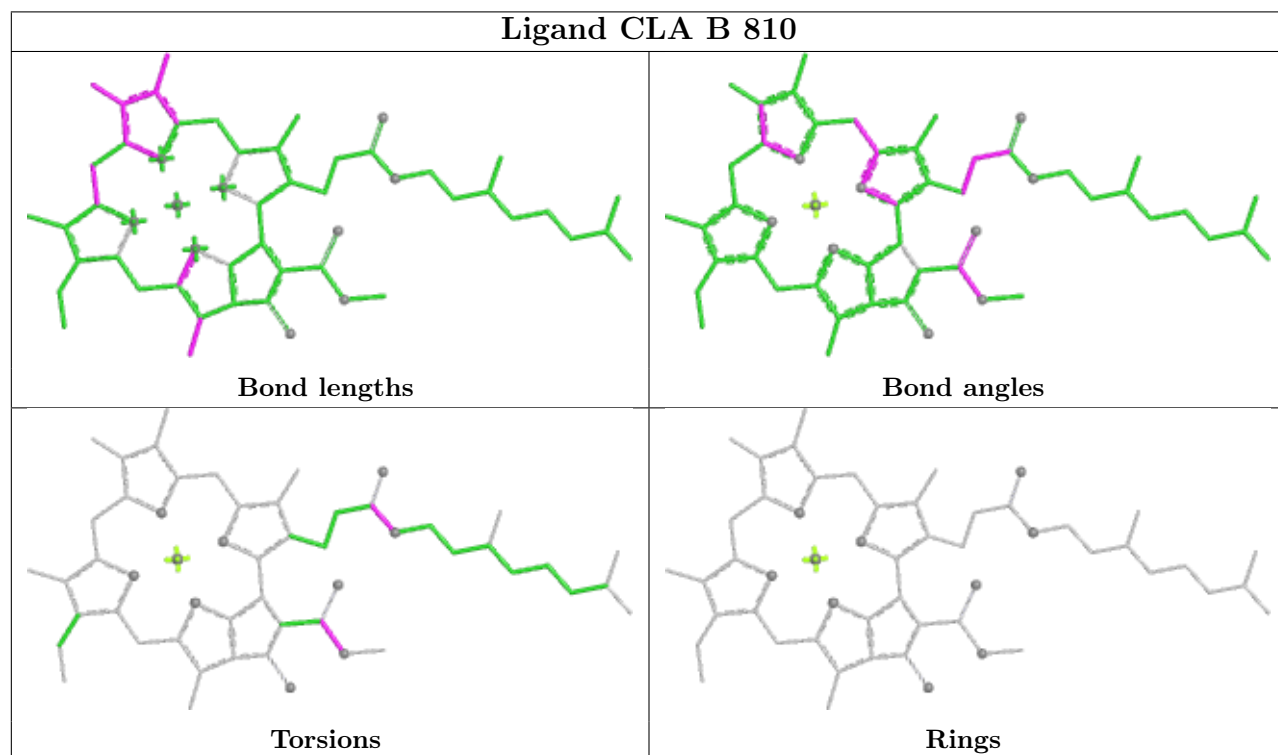
Ligand CLA e 605

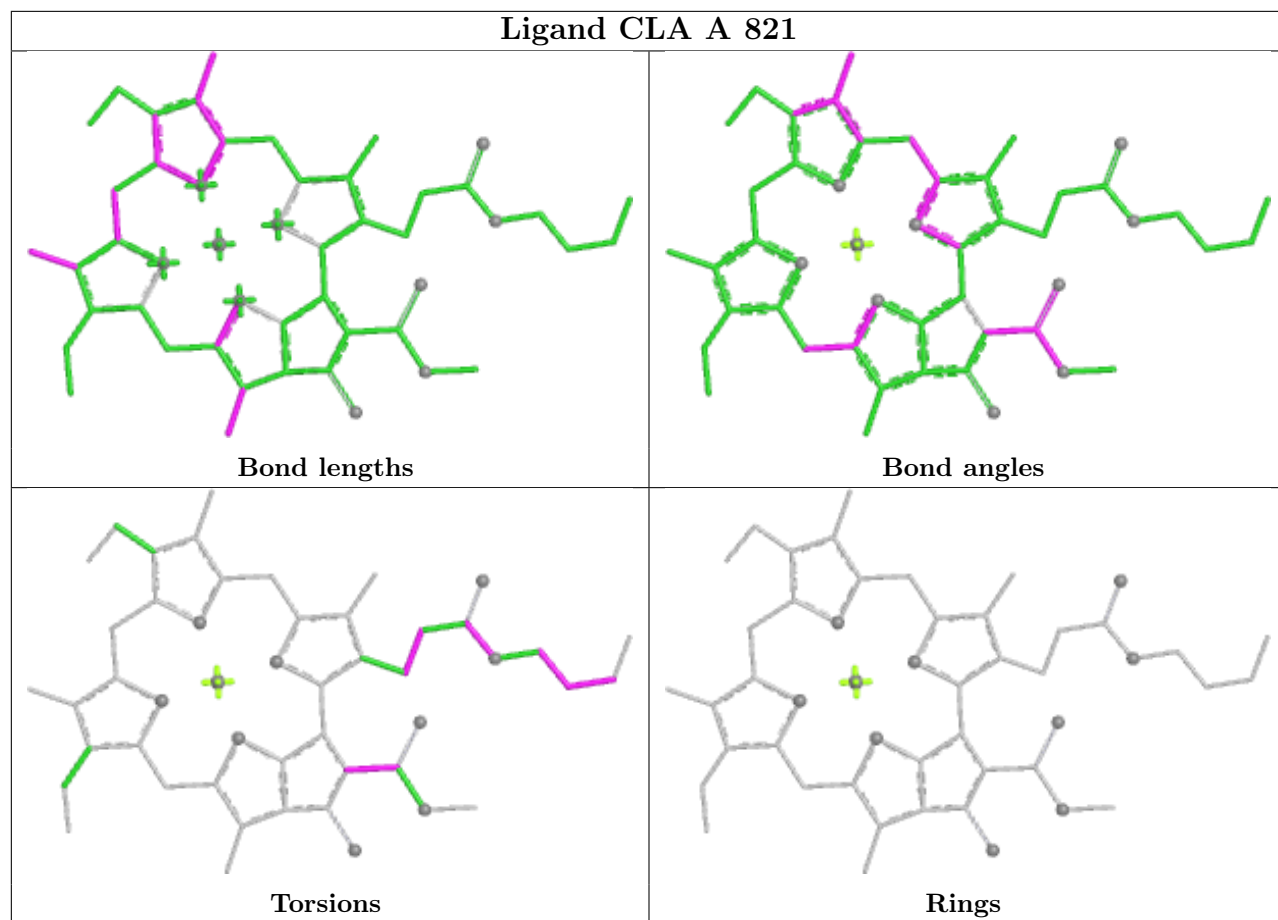


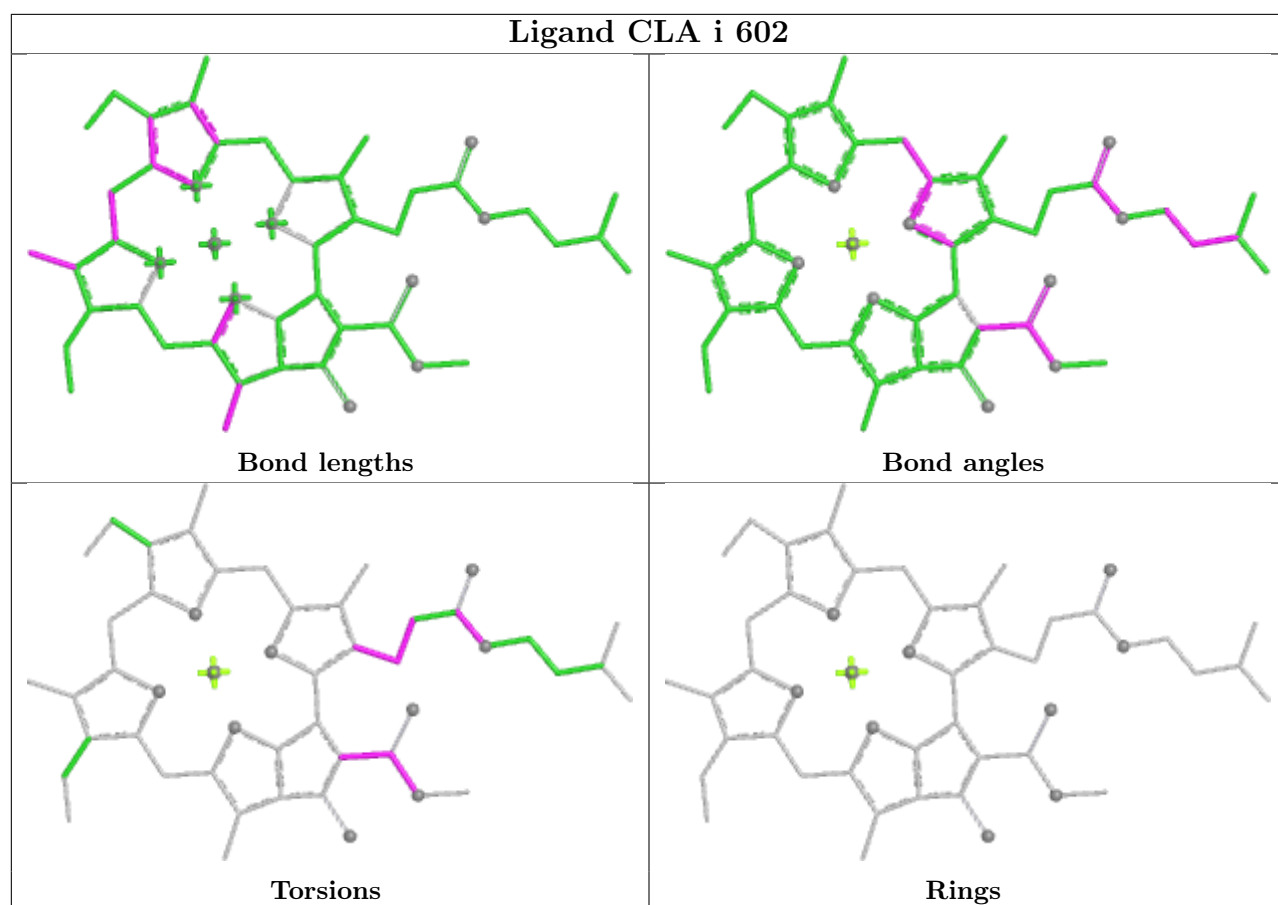
Ligand CLA e 603



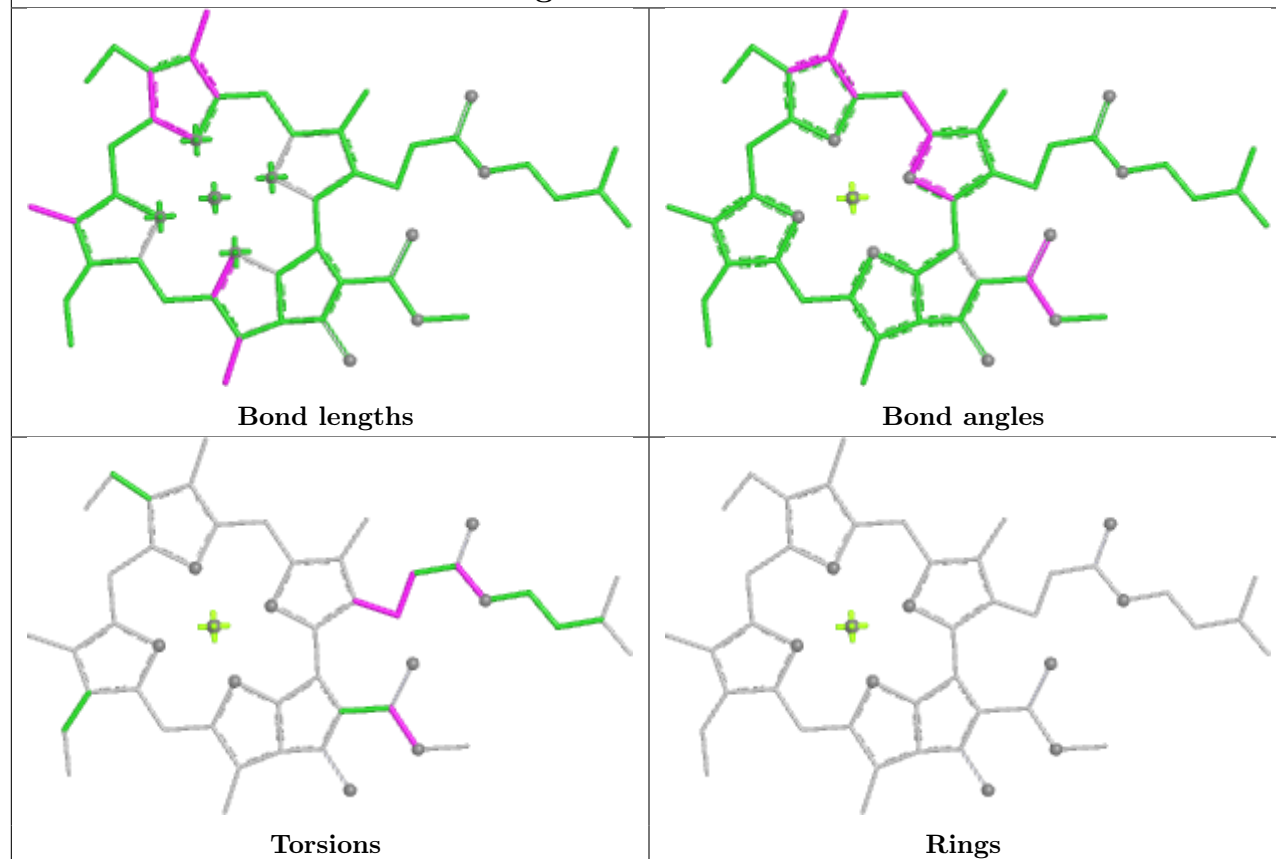
Ligand CLA B 810



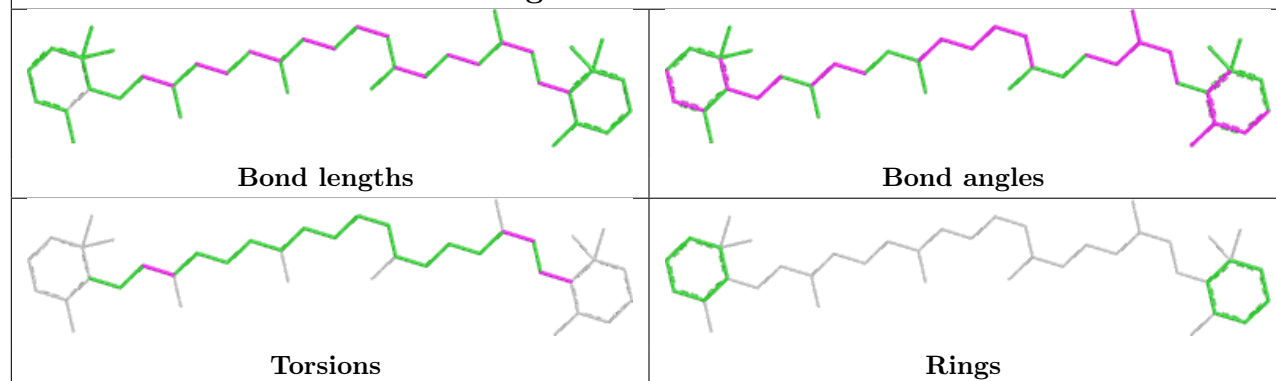


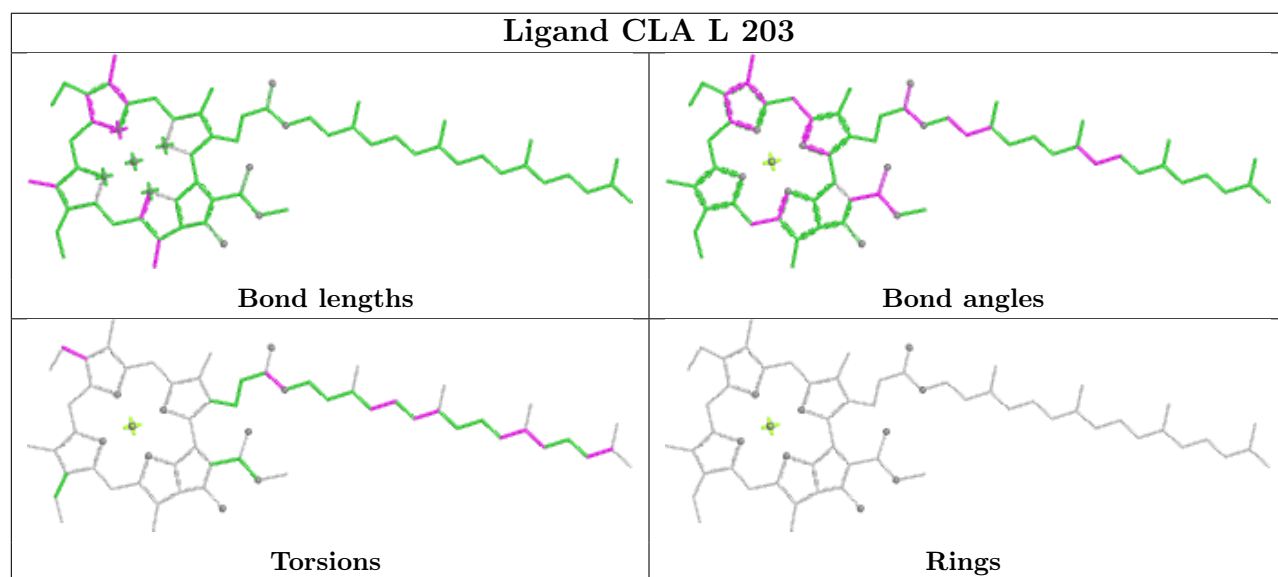
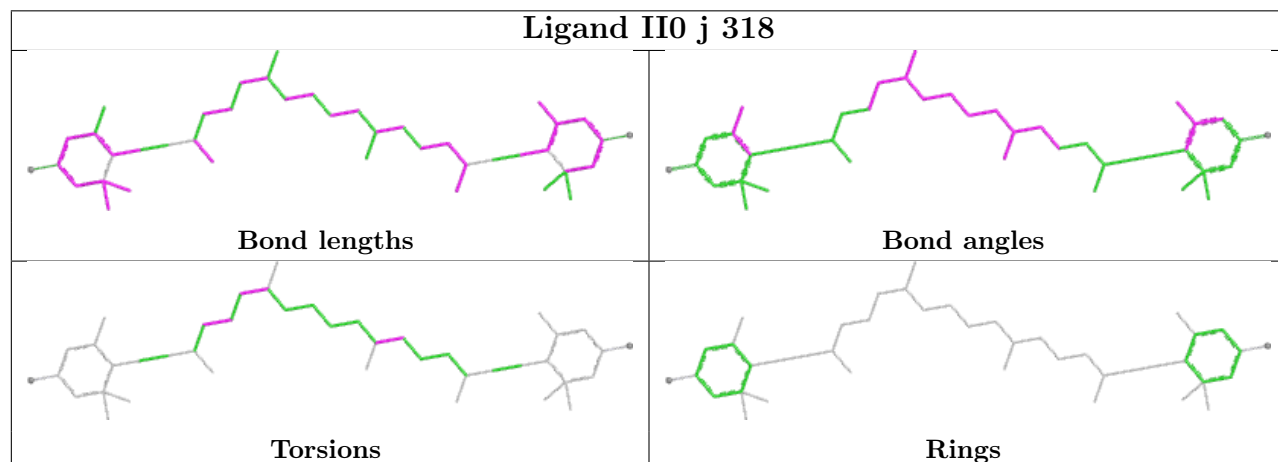
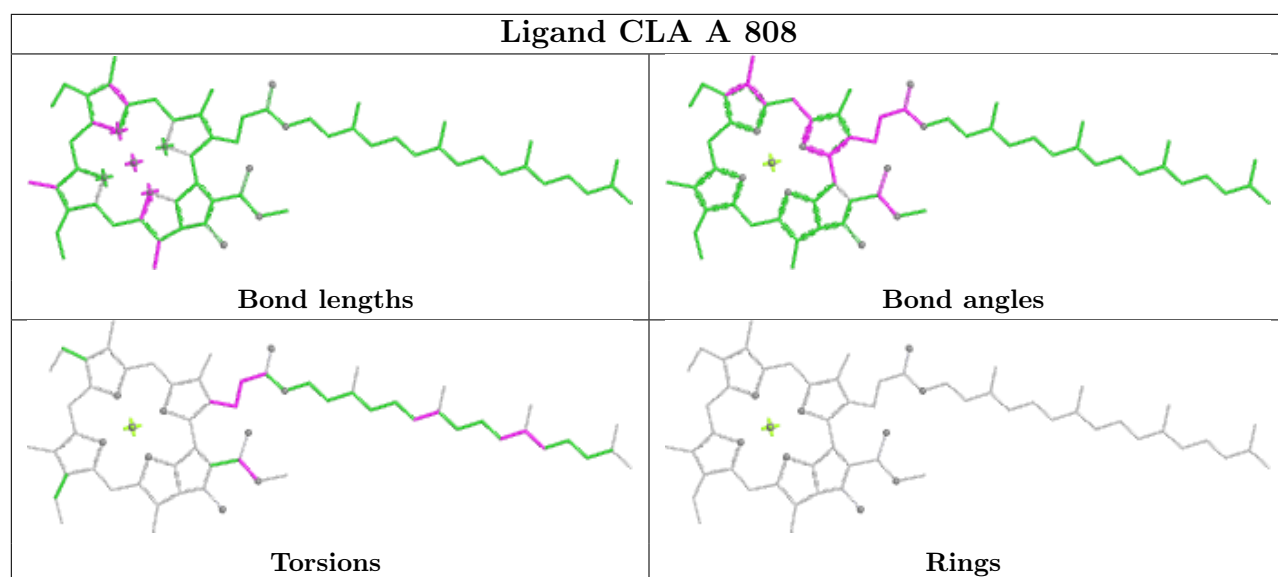


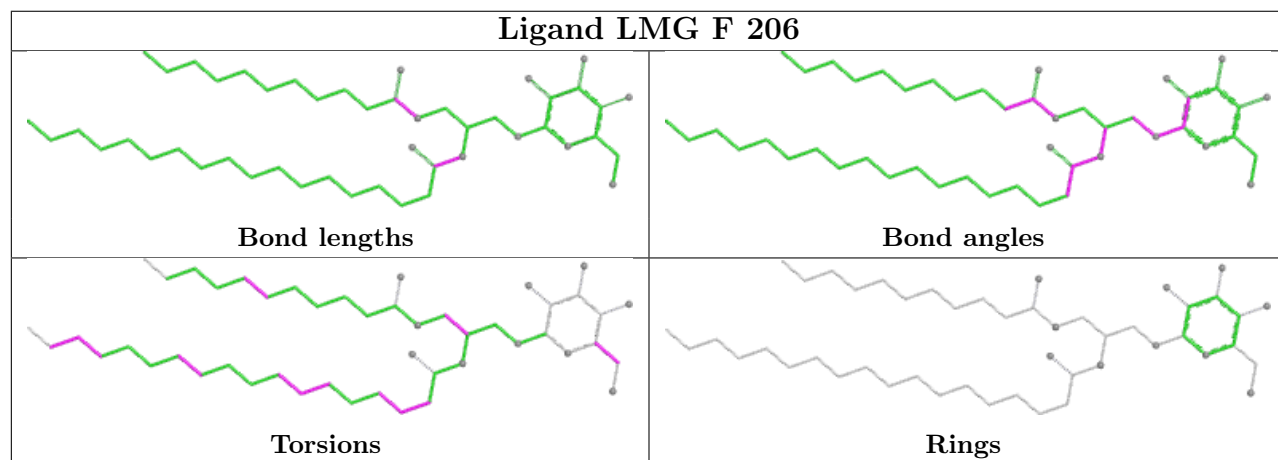
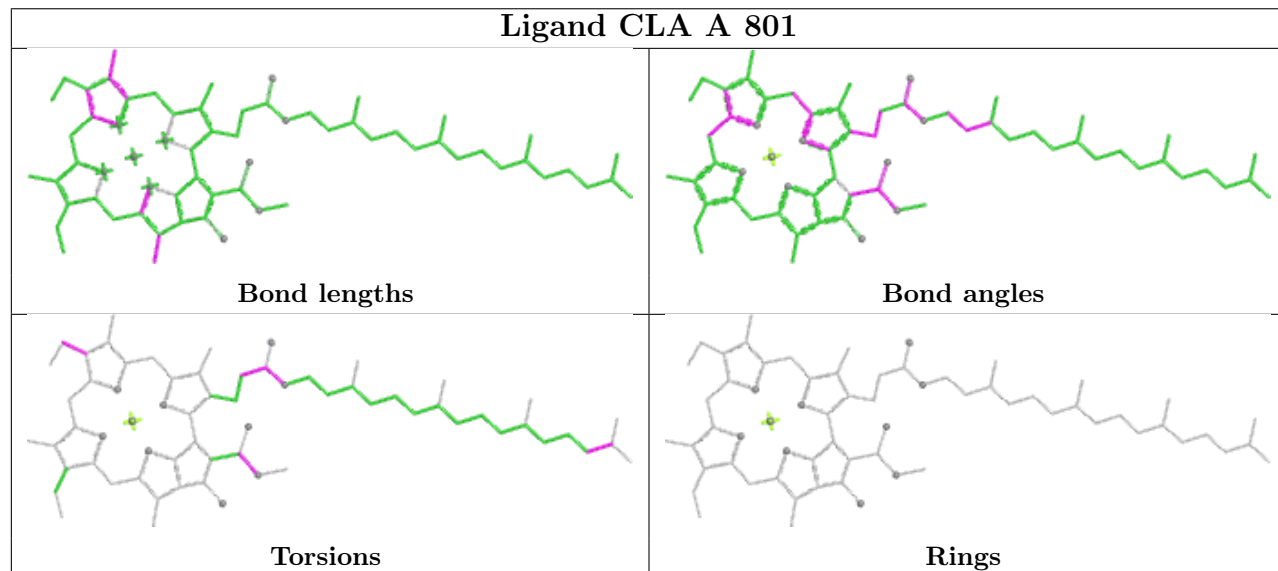
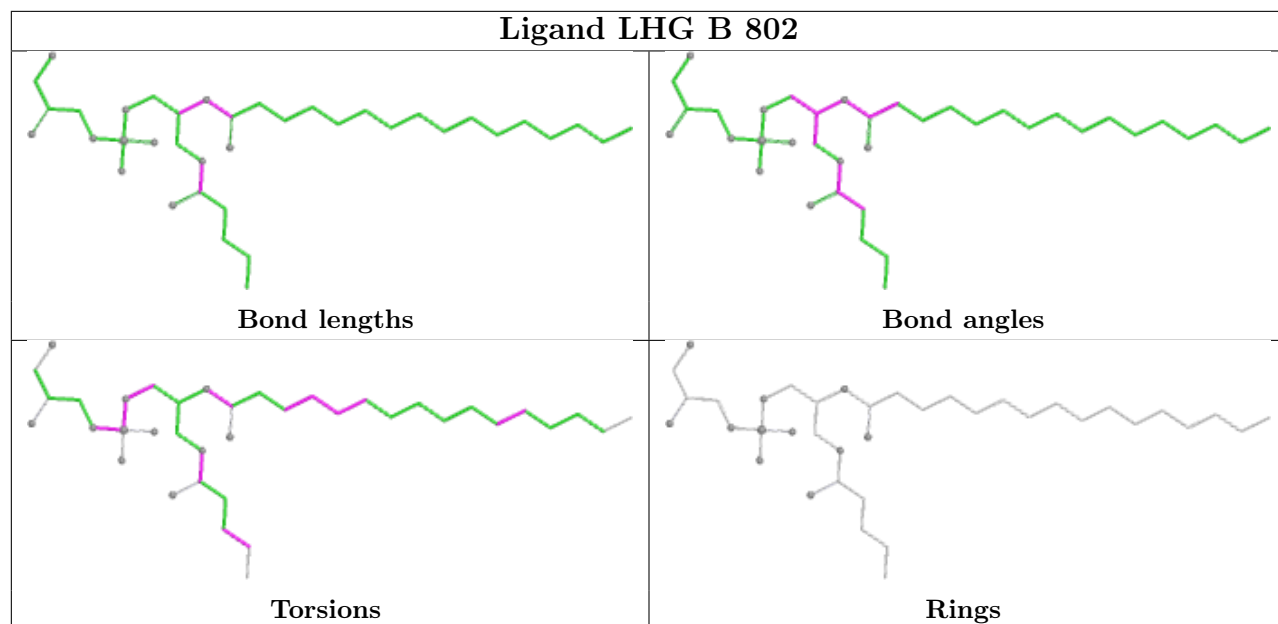
Ligand CLA h 301

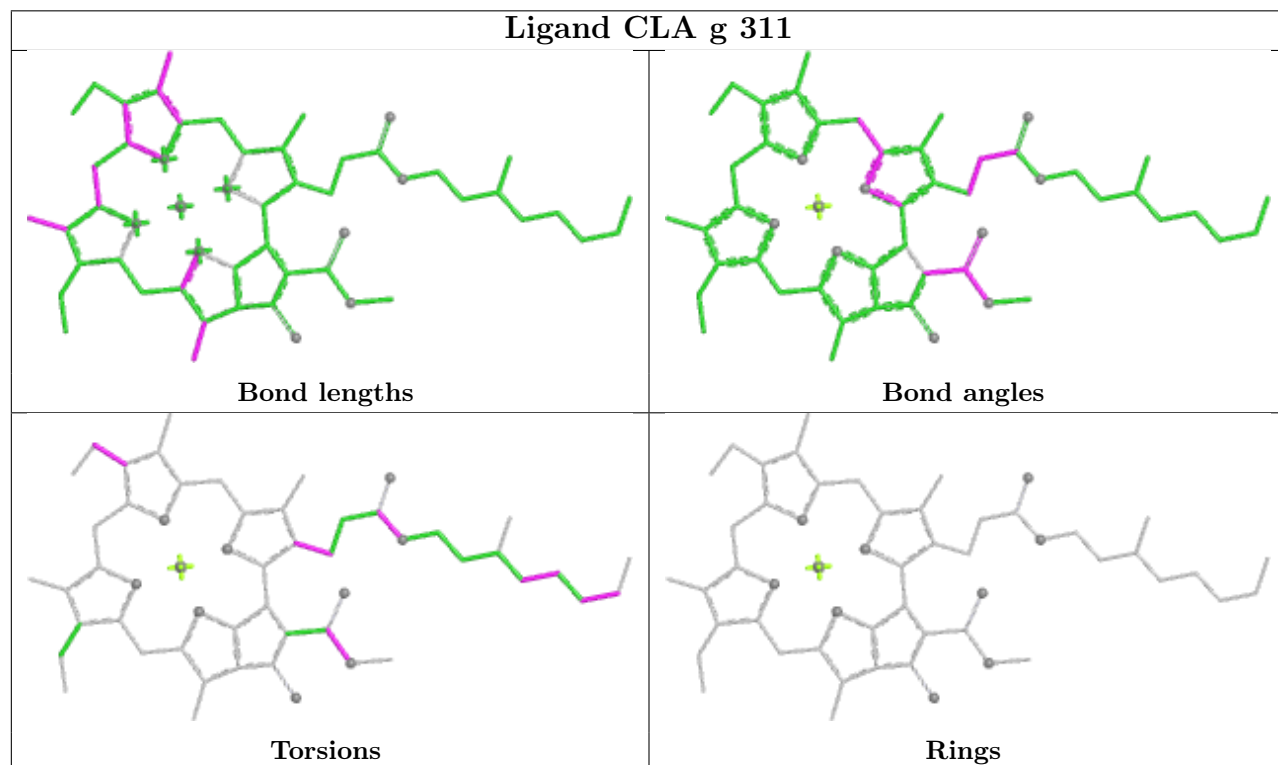
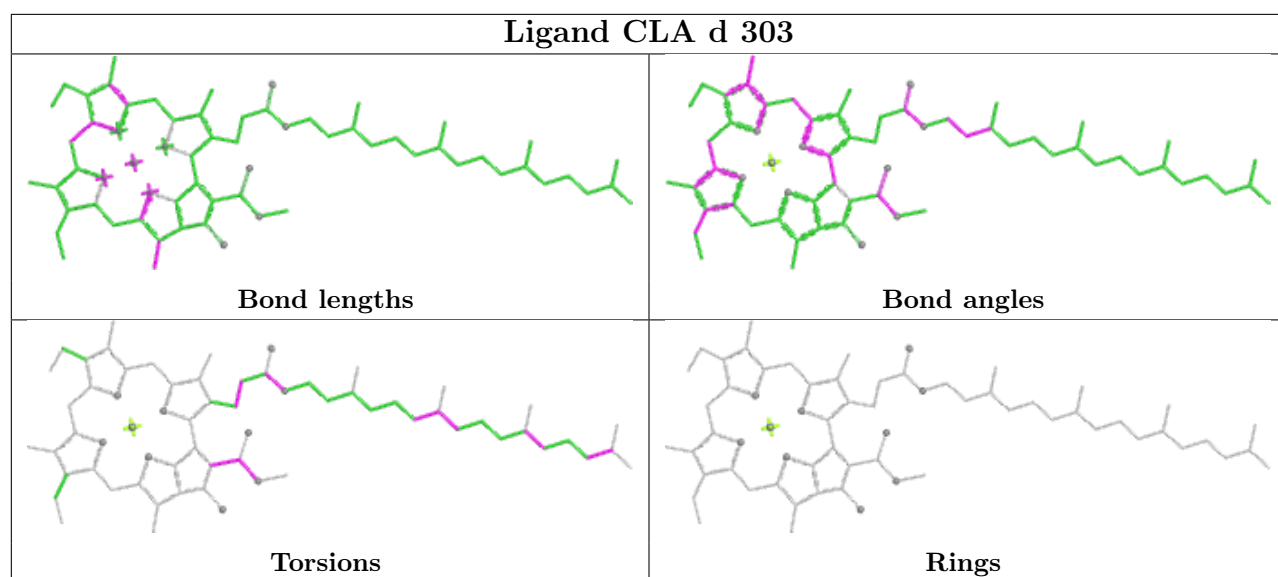


Ligand WVN L 205

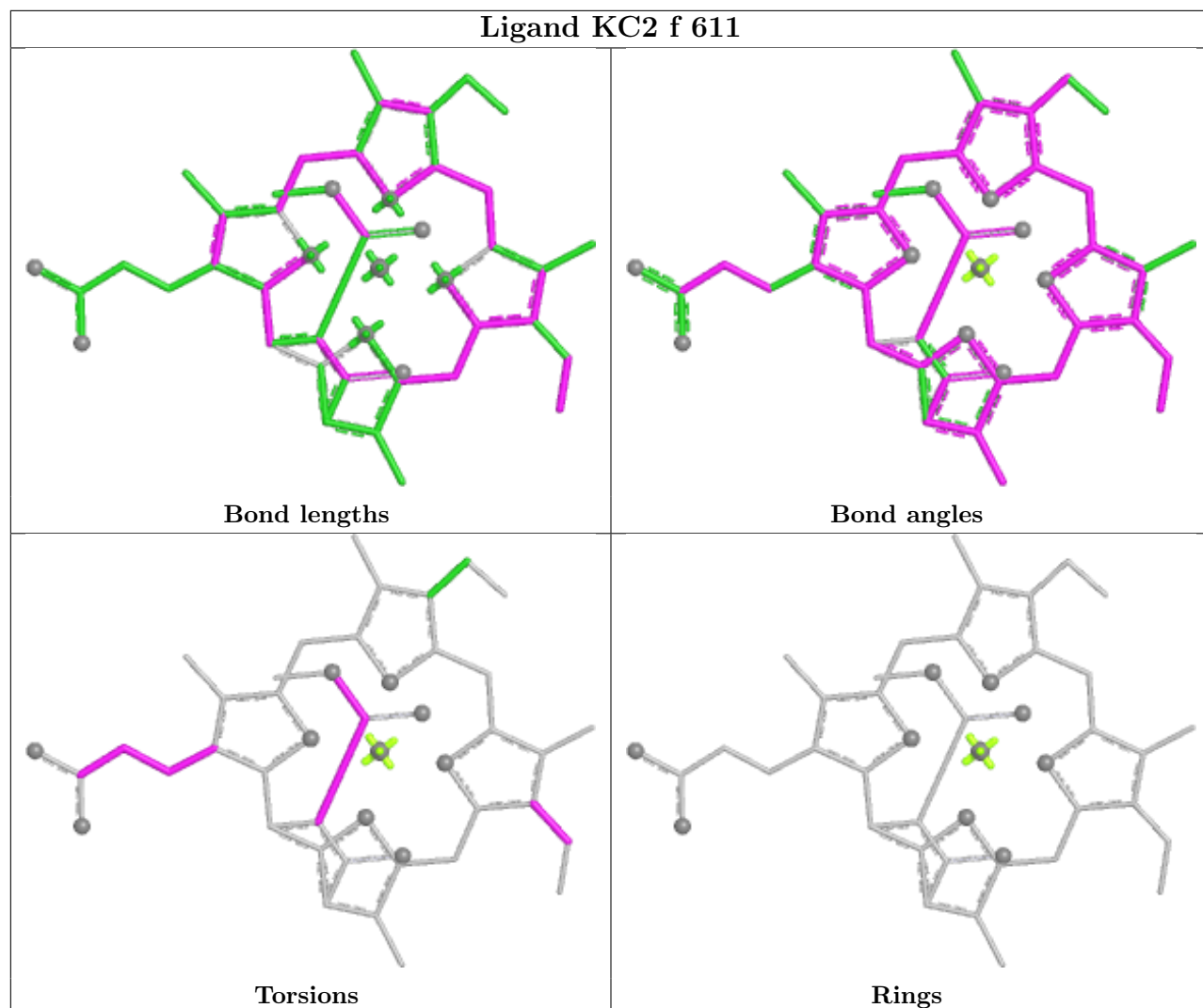




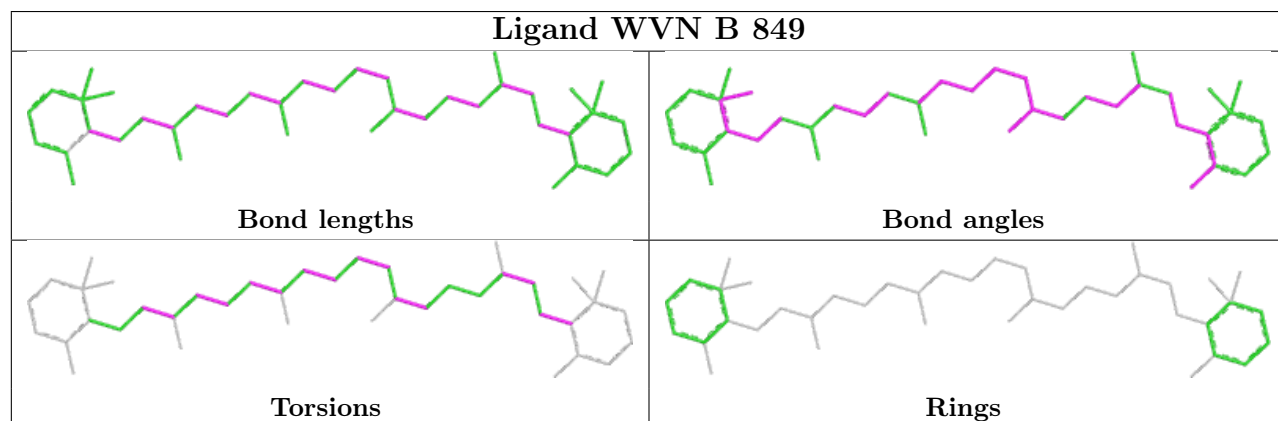




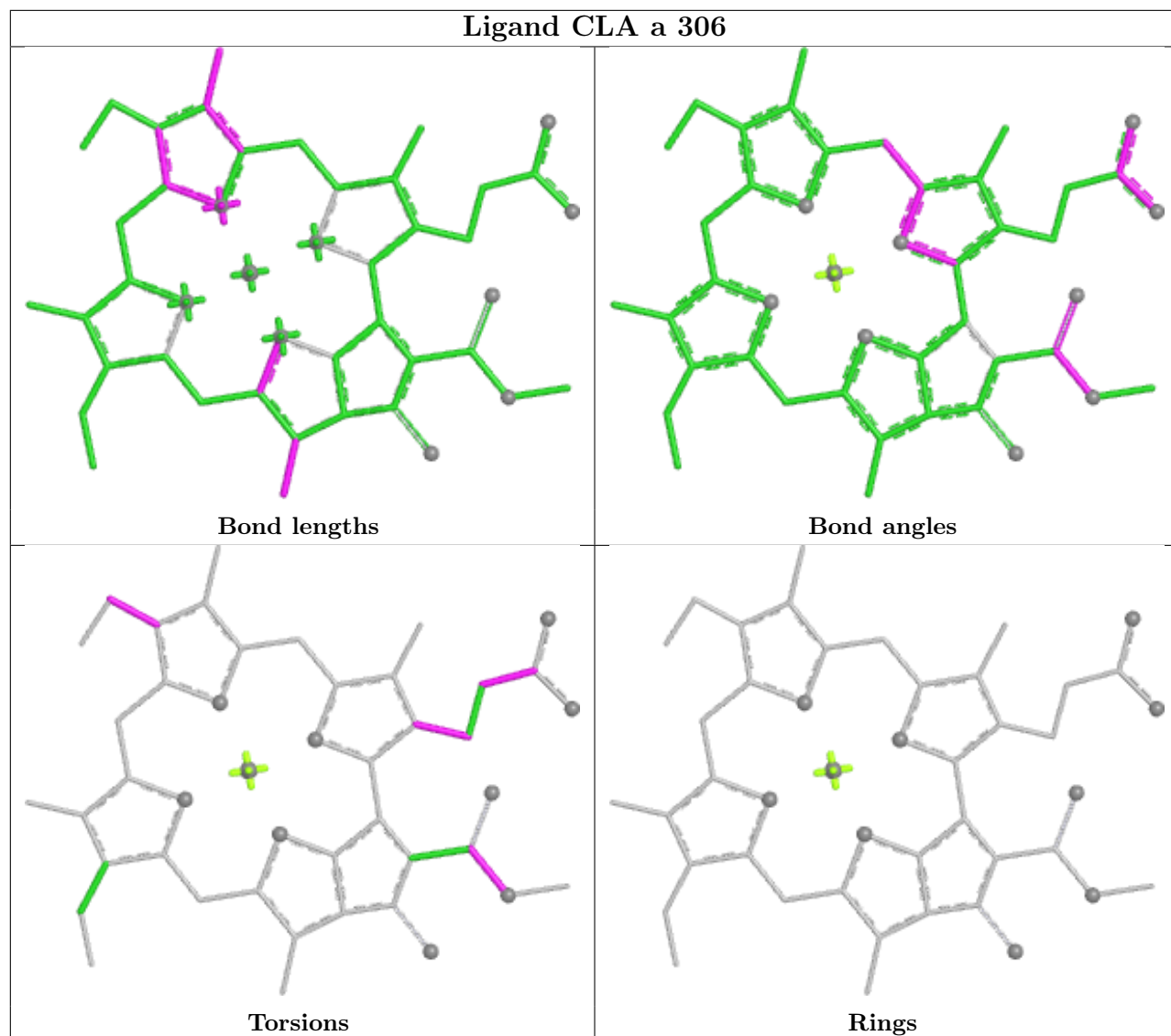
Ligand KC2 f 611



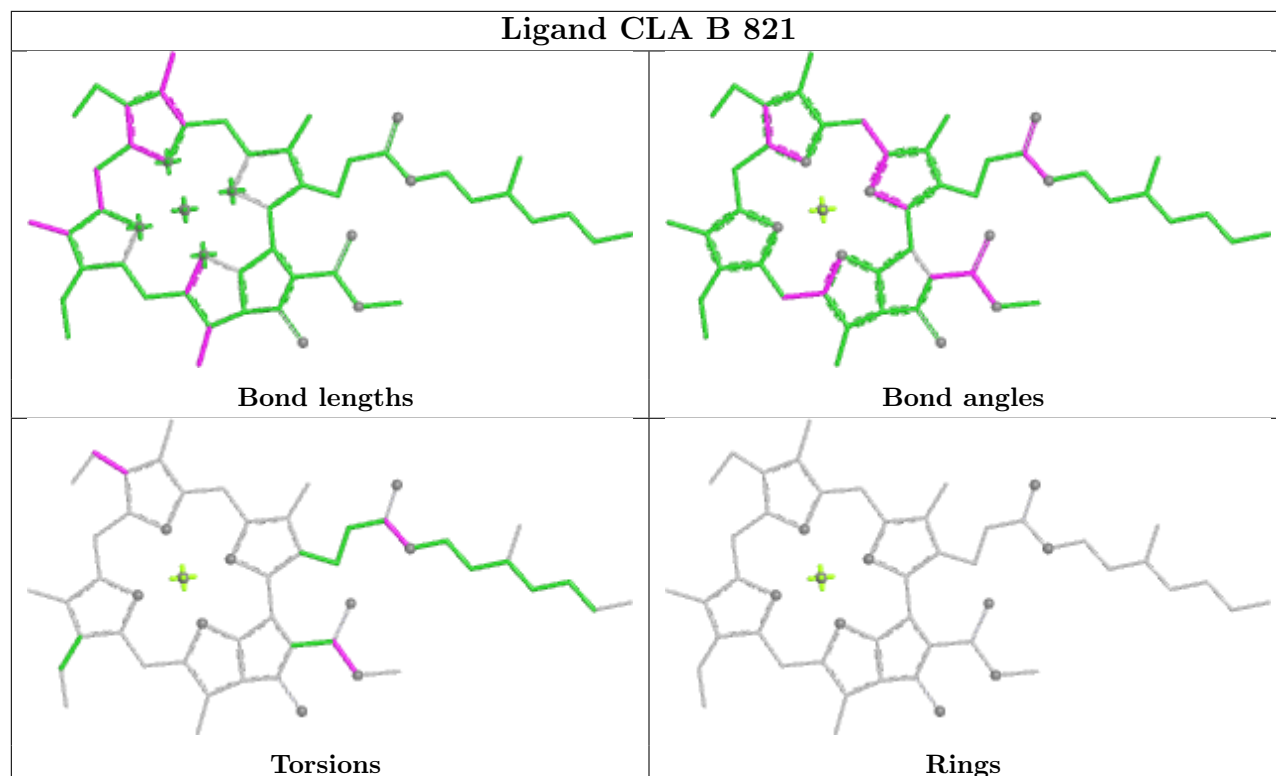
Ligand WVN B 849



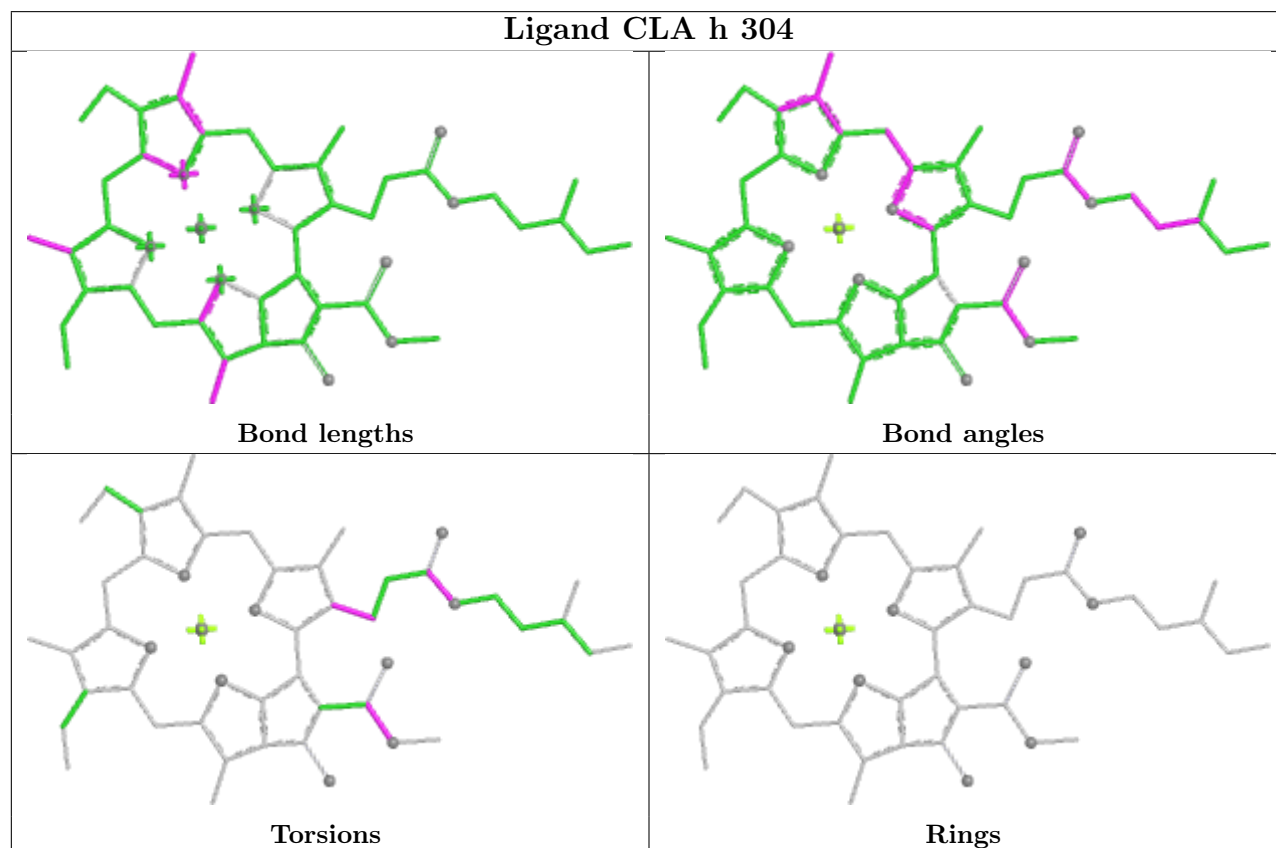
Ligand CLA a 306



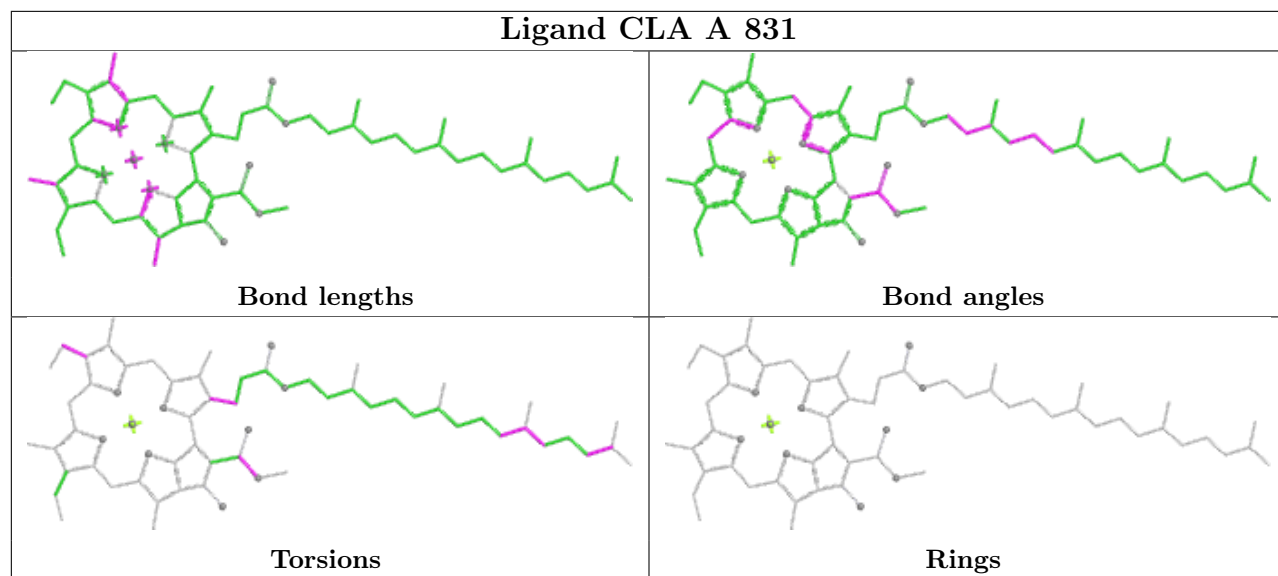
Ligand CLA B 821



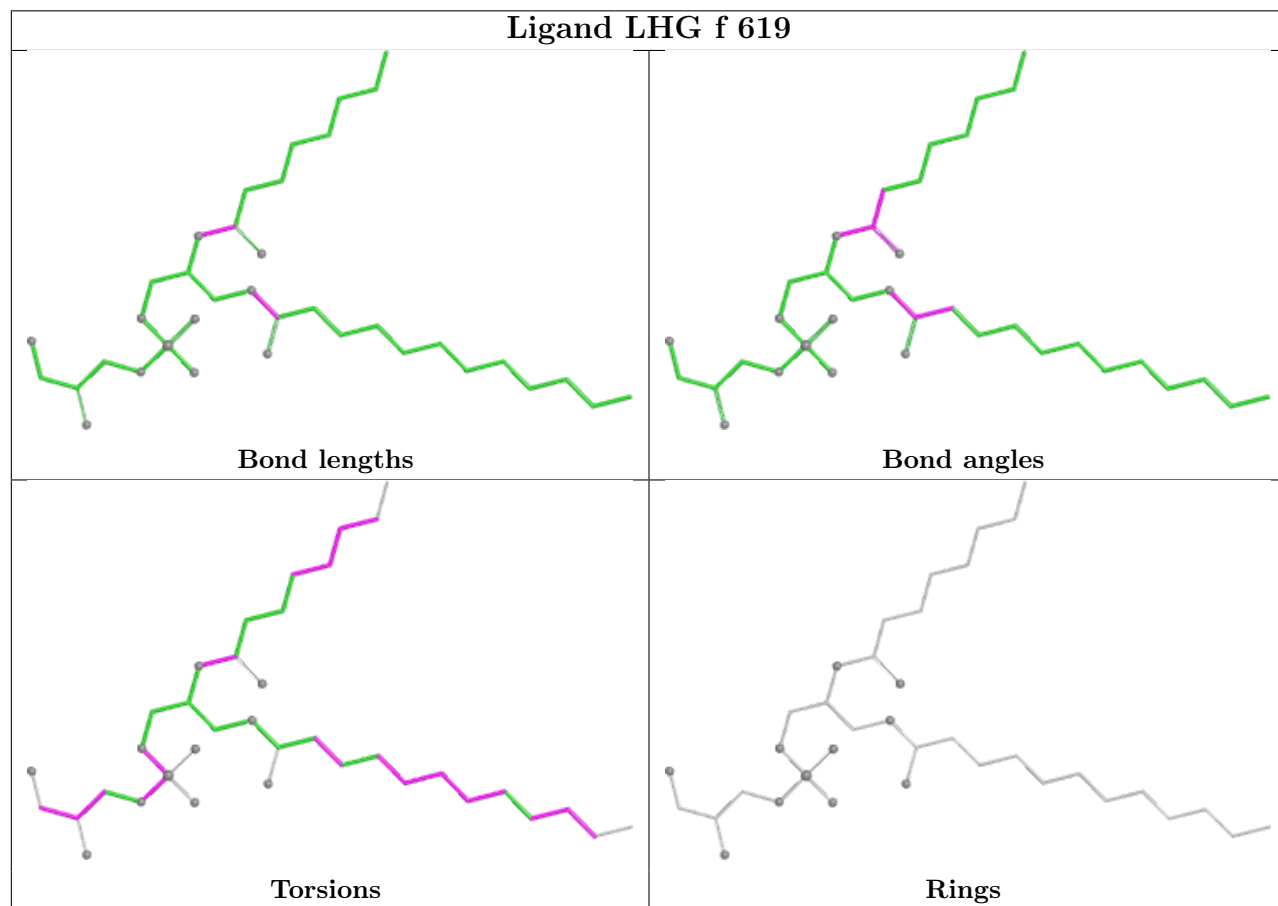
Ligand CLA h 304

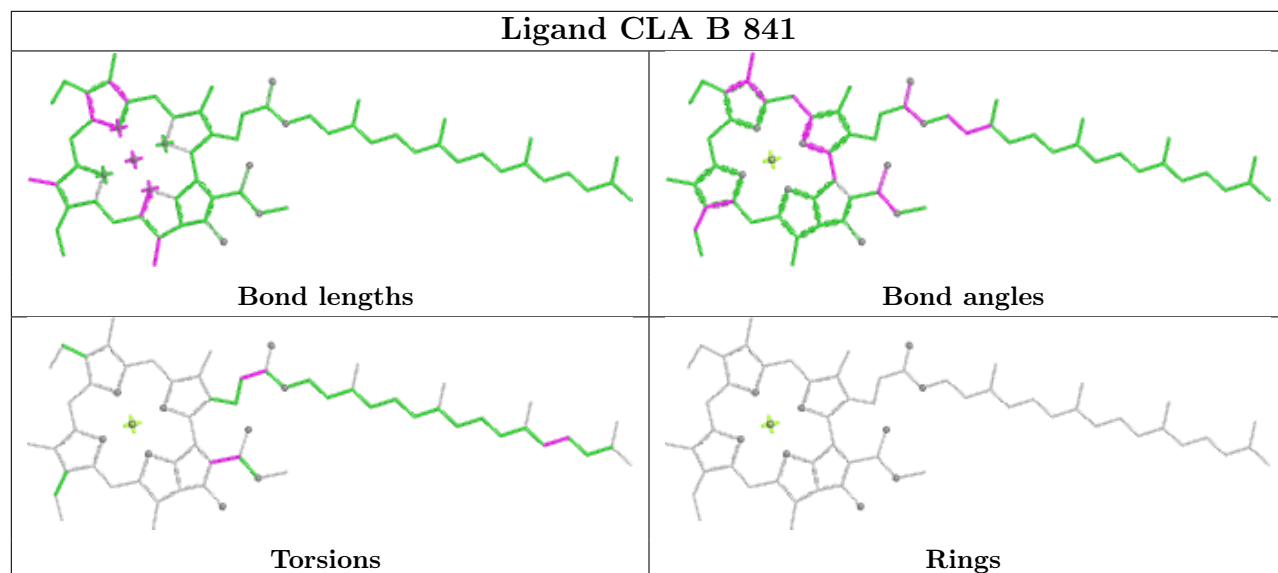
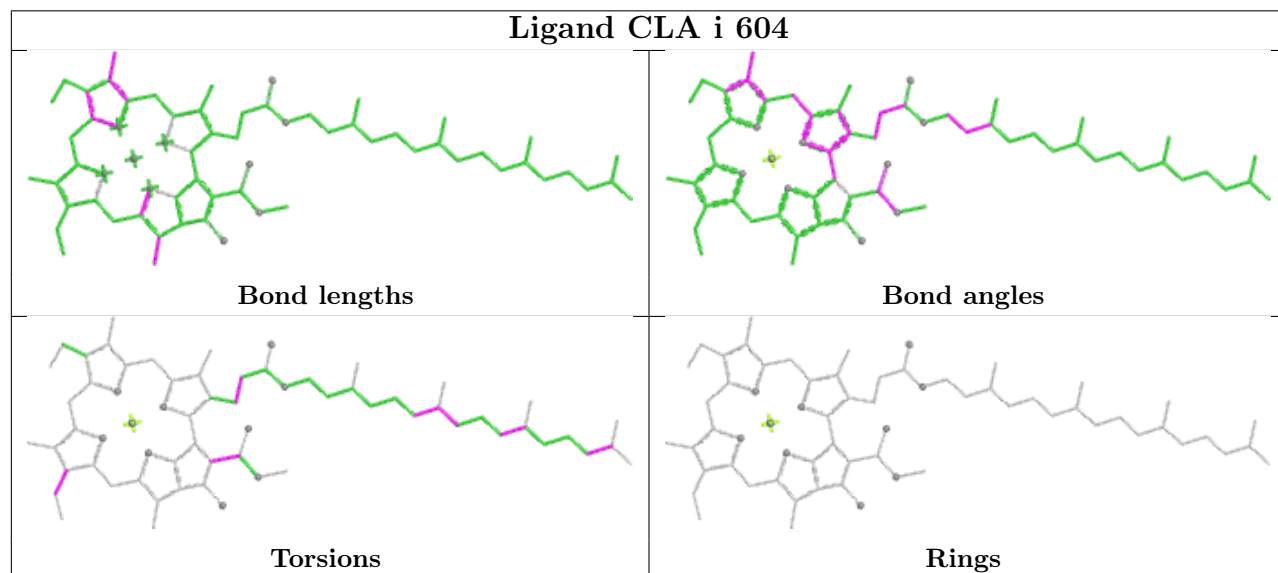
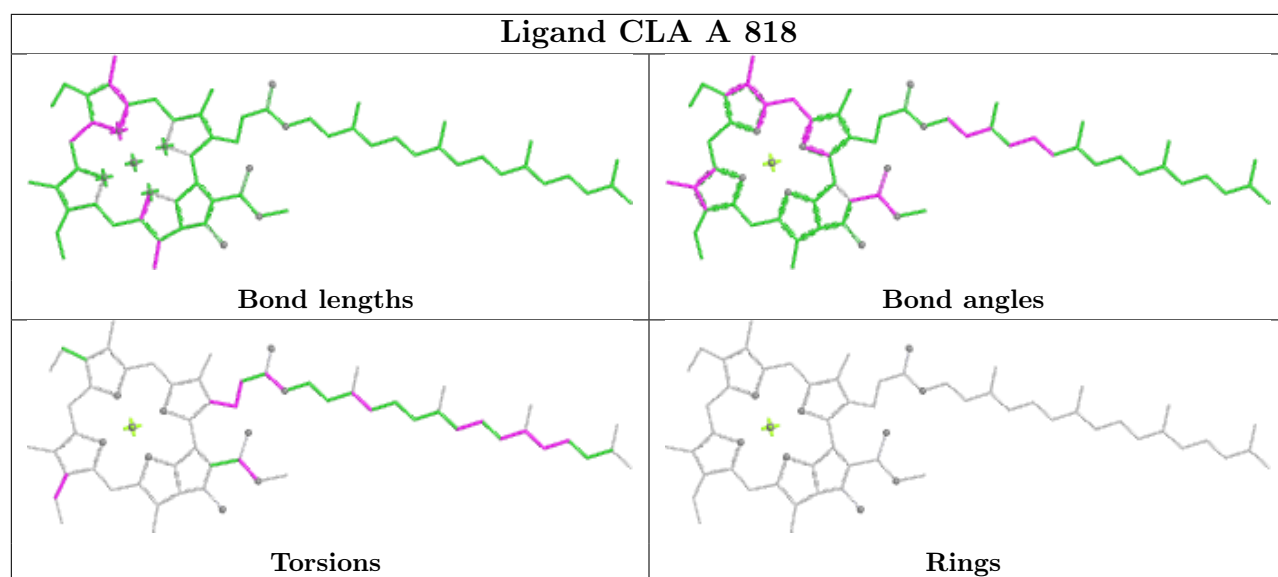


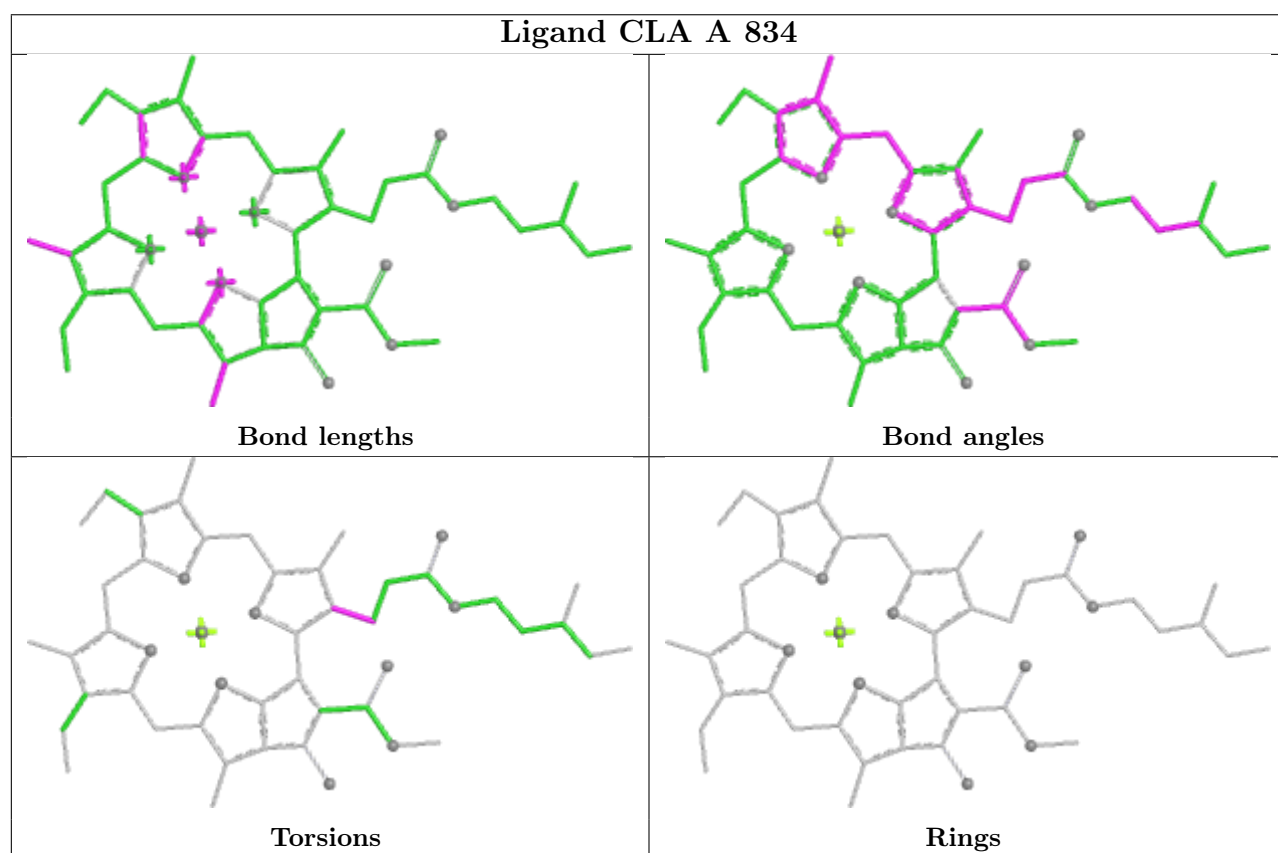
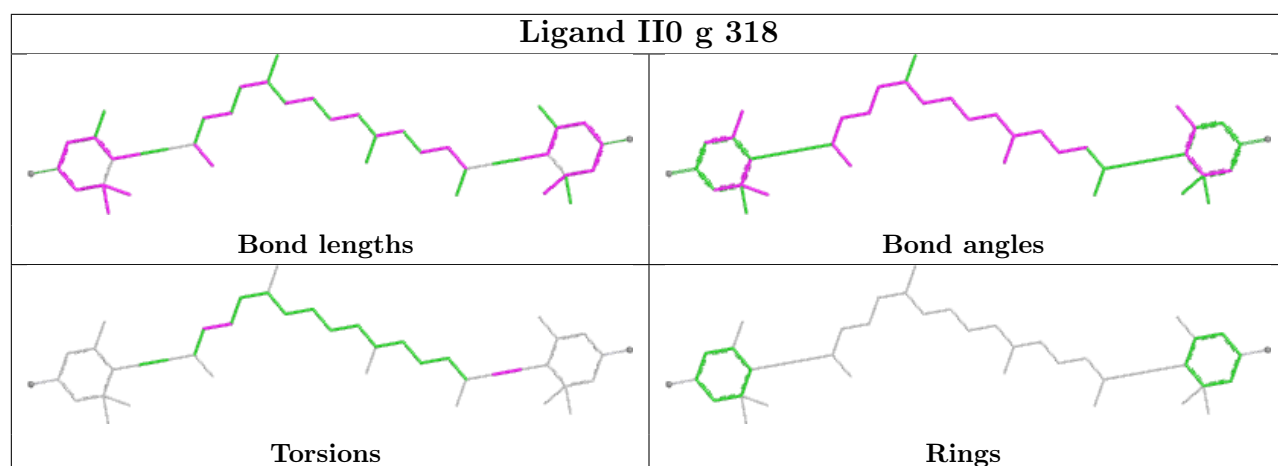
Ligand CLA A 831



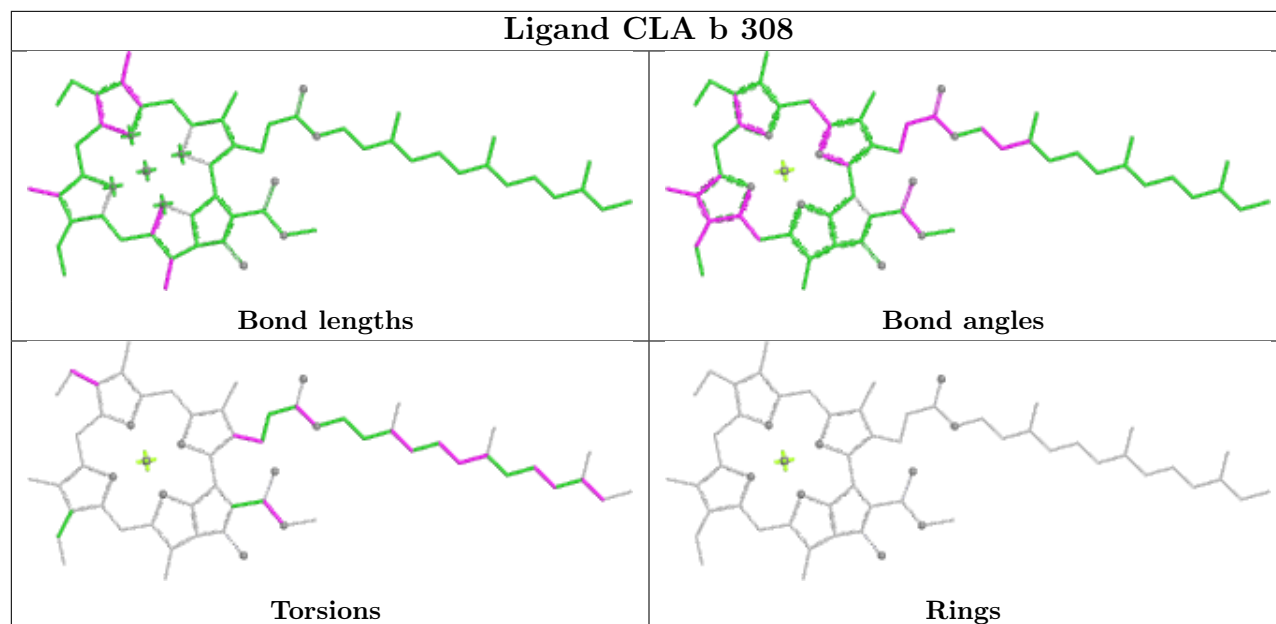
Ligand LHG f 619



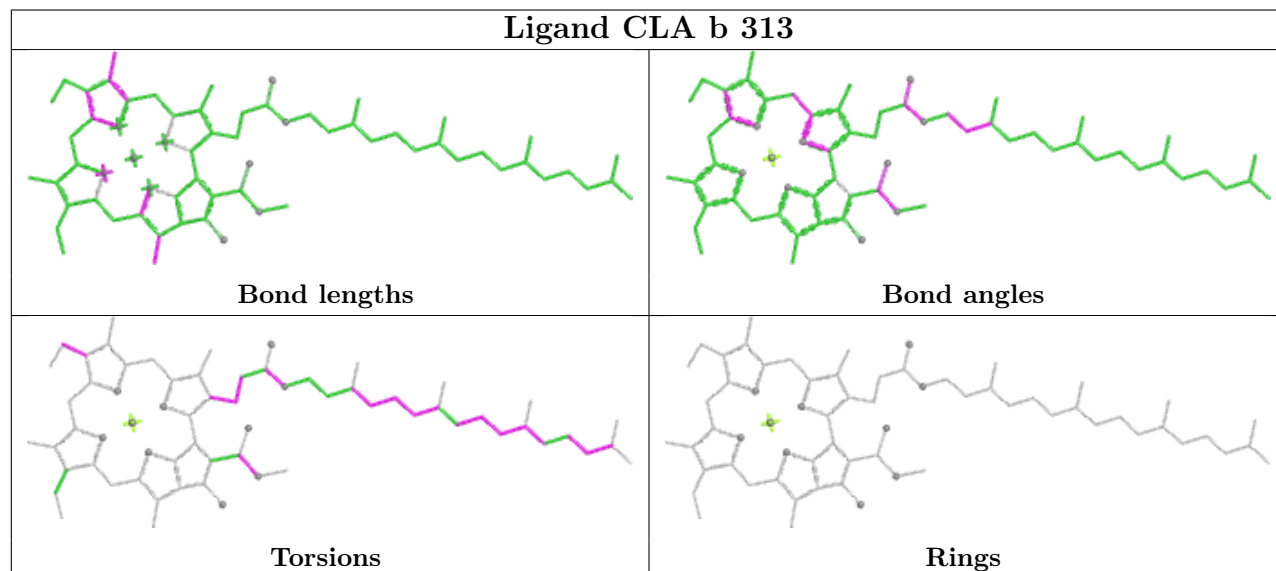




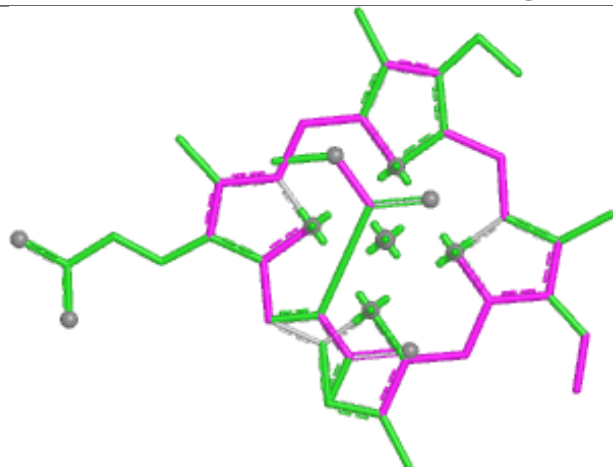
Ligand CLA b 308



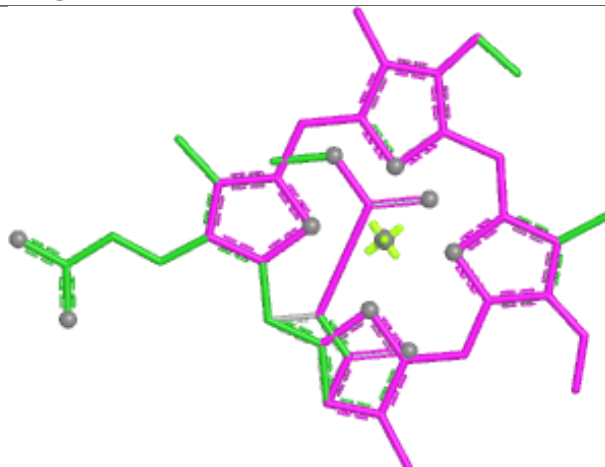
Ligand CLA b 313



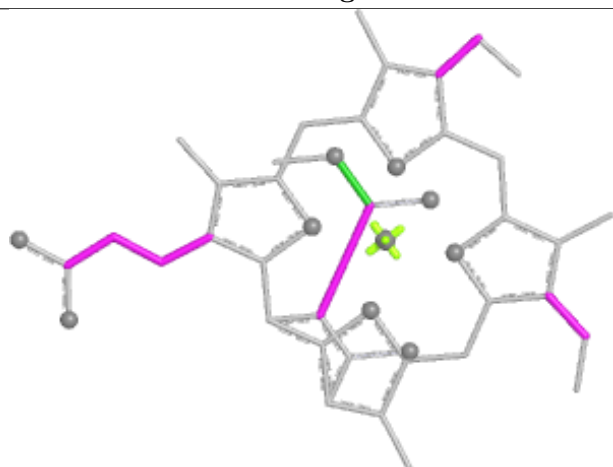
Ligand KC2 g 314



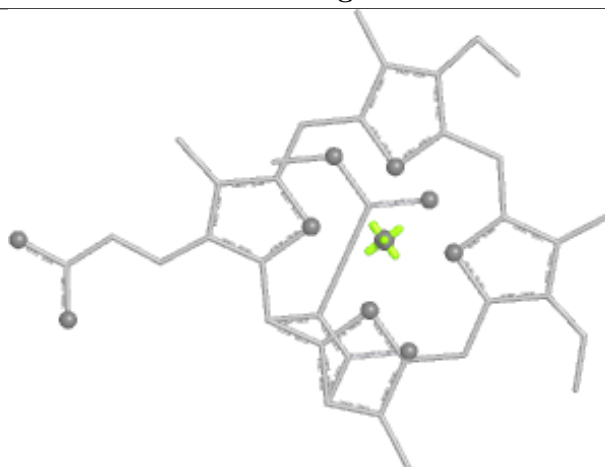
Bond lengths



Bond angles

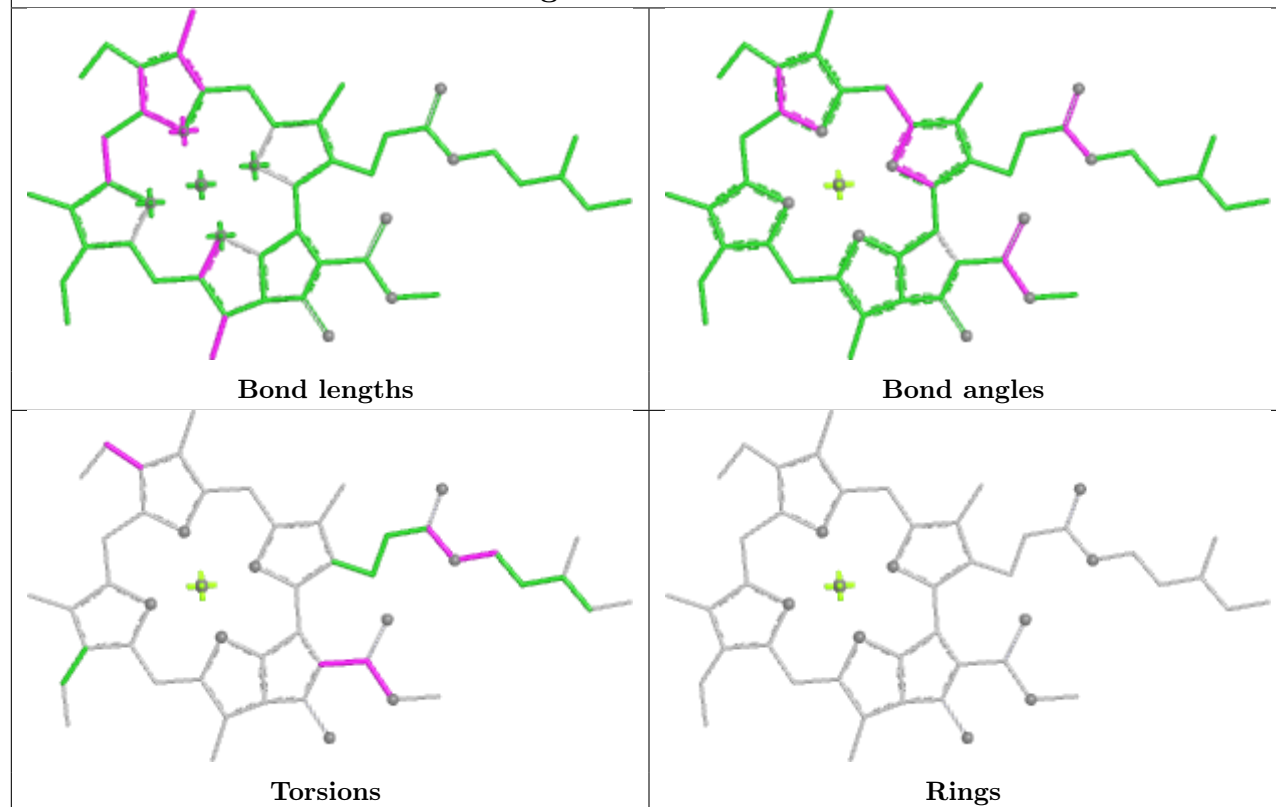


Torsions

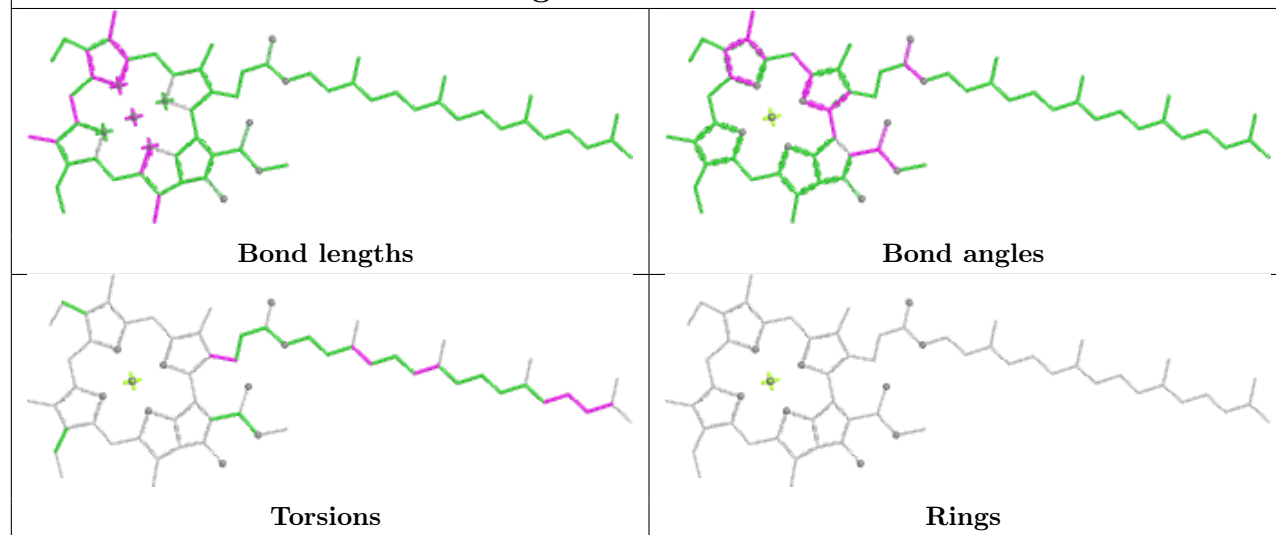


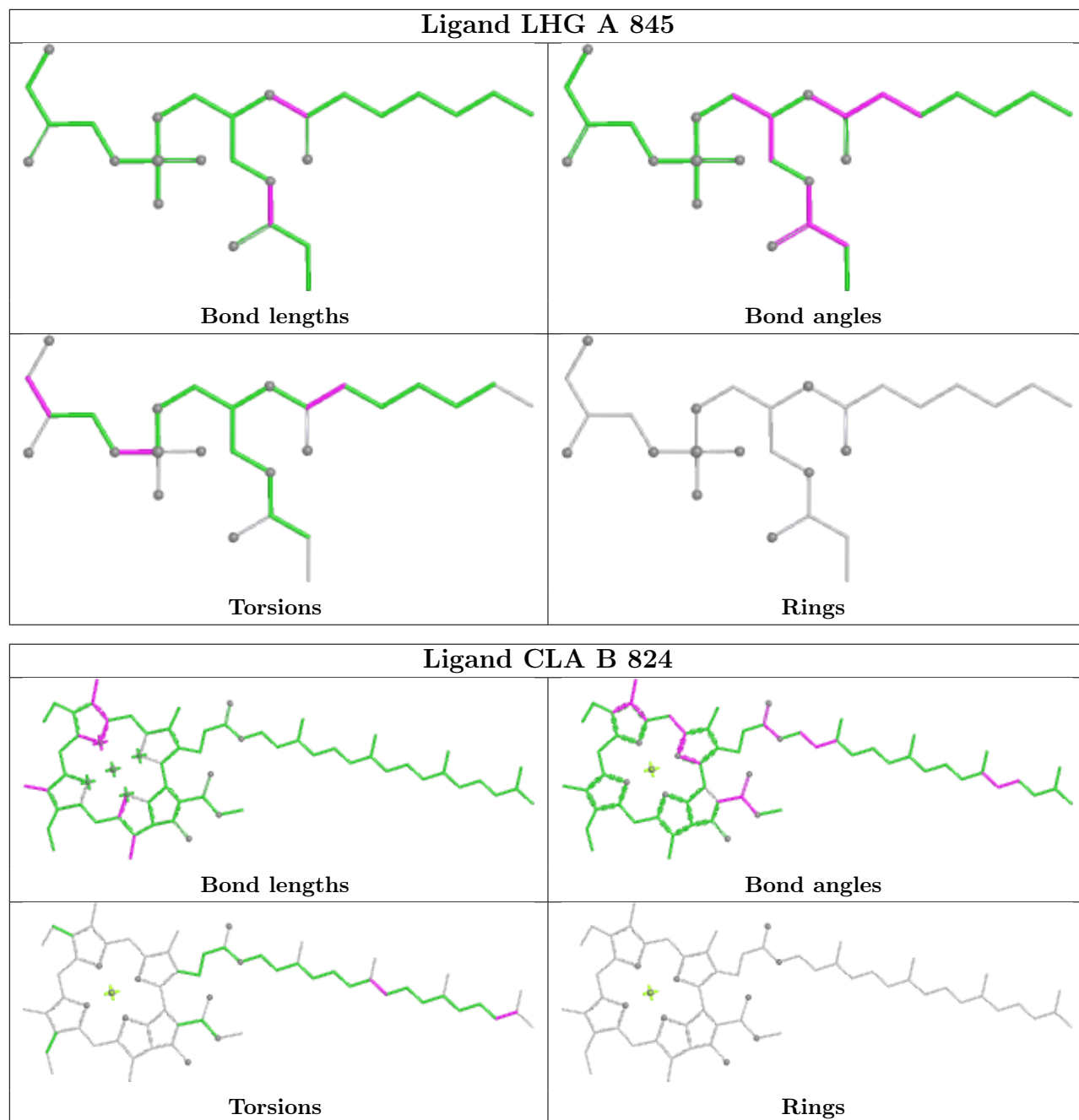
Rings

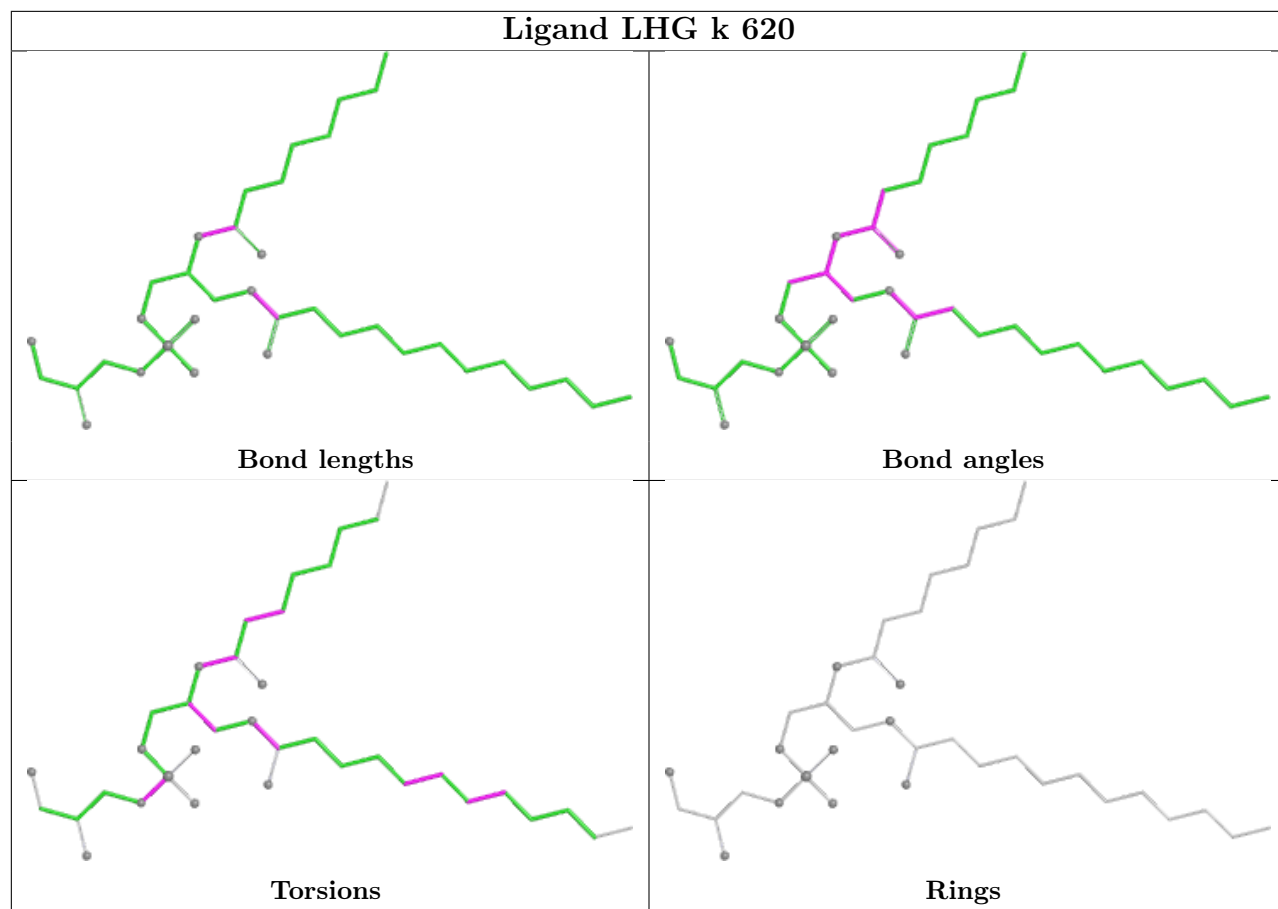
Ligand CLA i 605



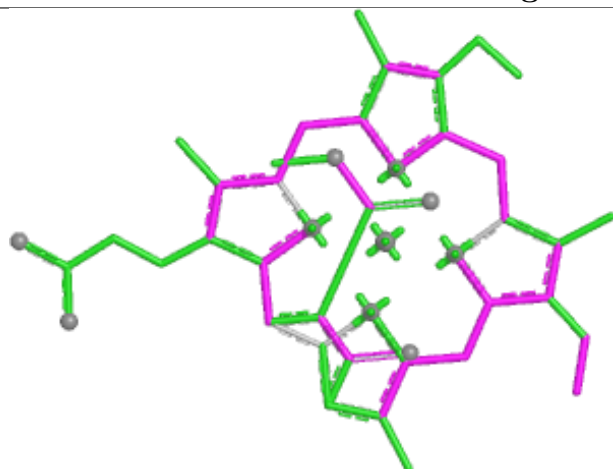
Ligand CLA B 825



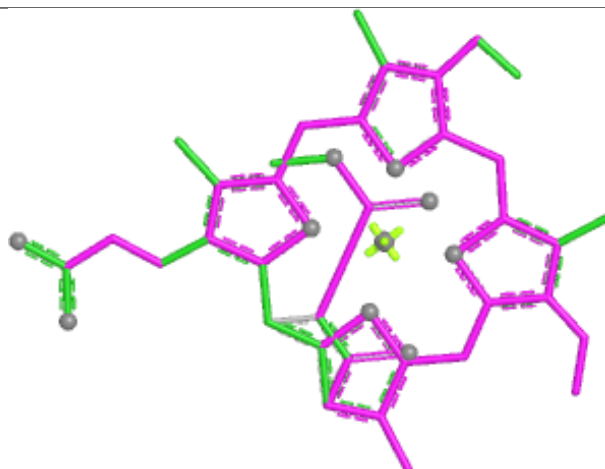




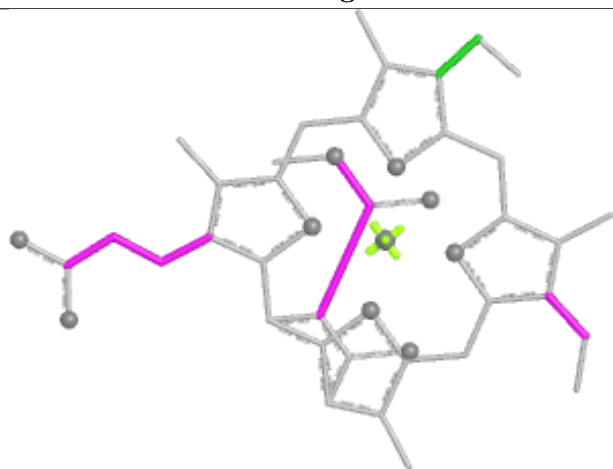
Ligand KC2 c 610



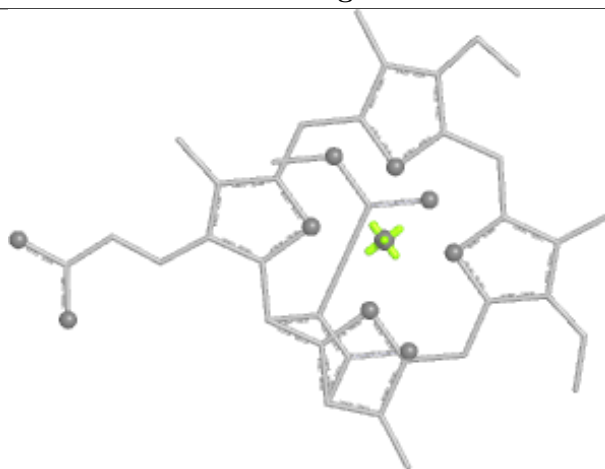
Bond lengths



Bond angles

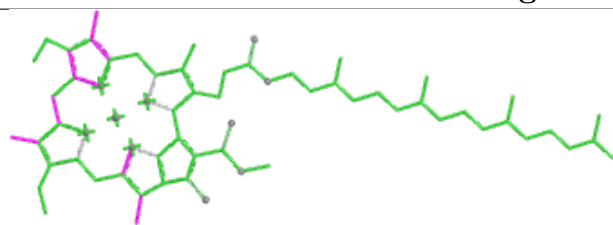


Torsions

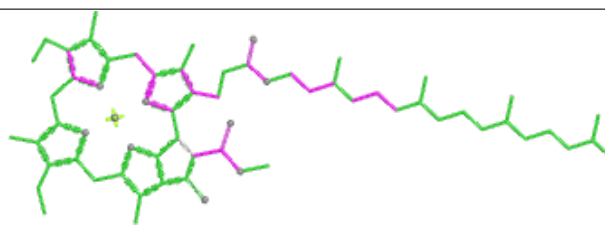


Rings

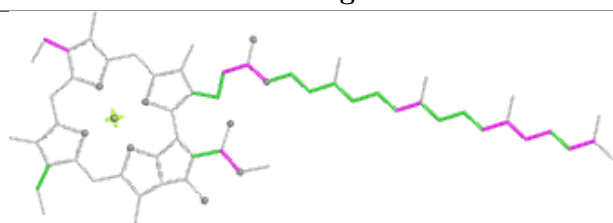
Ligand CLA e 611



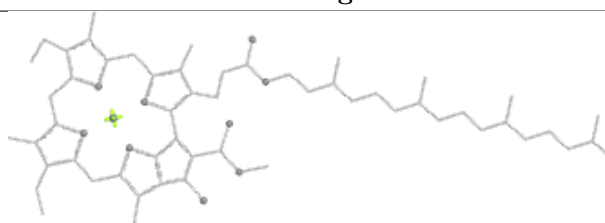
Bond lengths



Bond angles

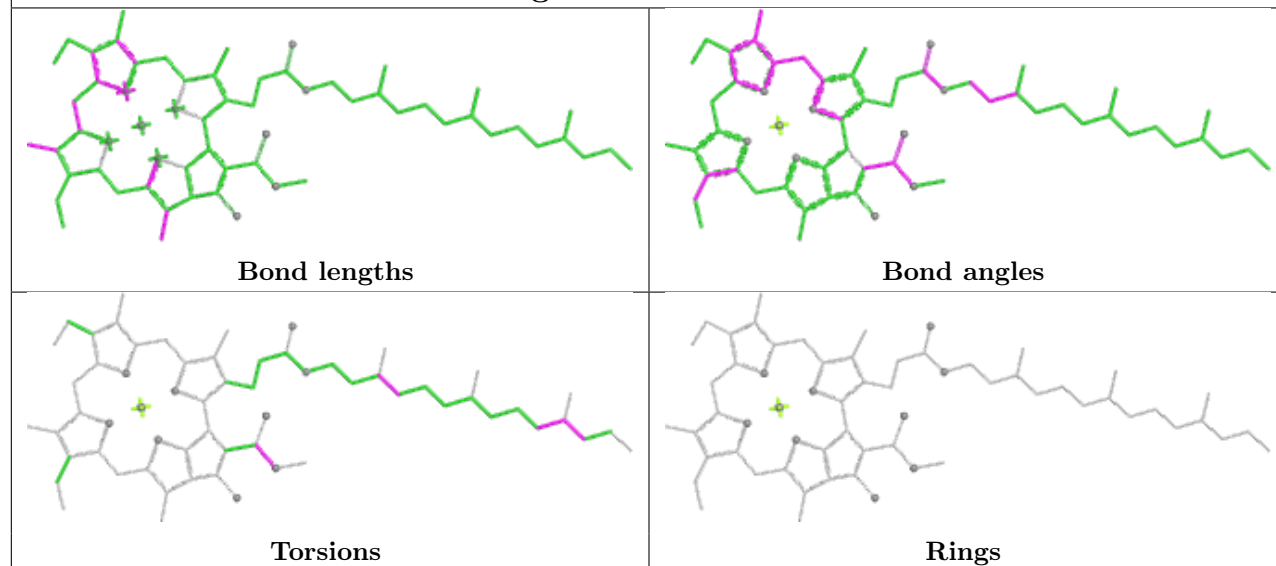


Torsions

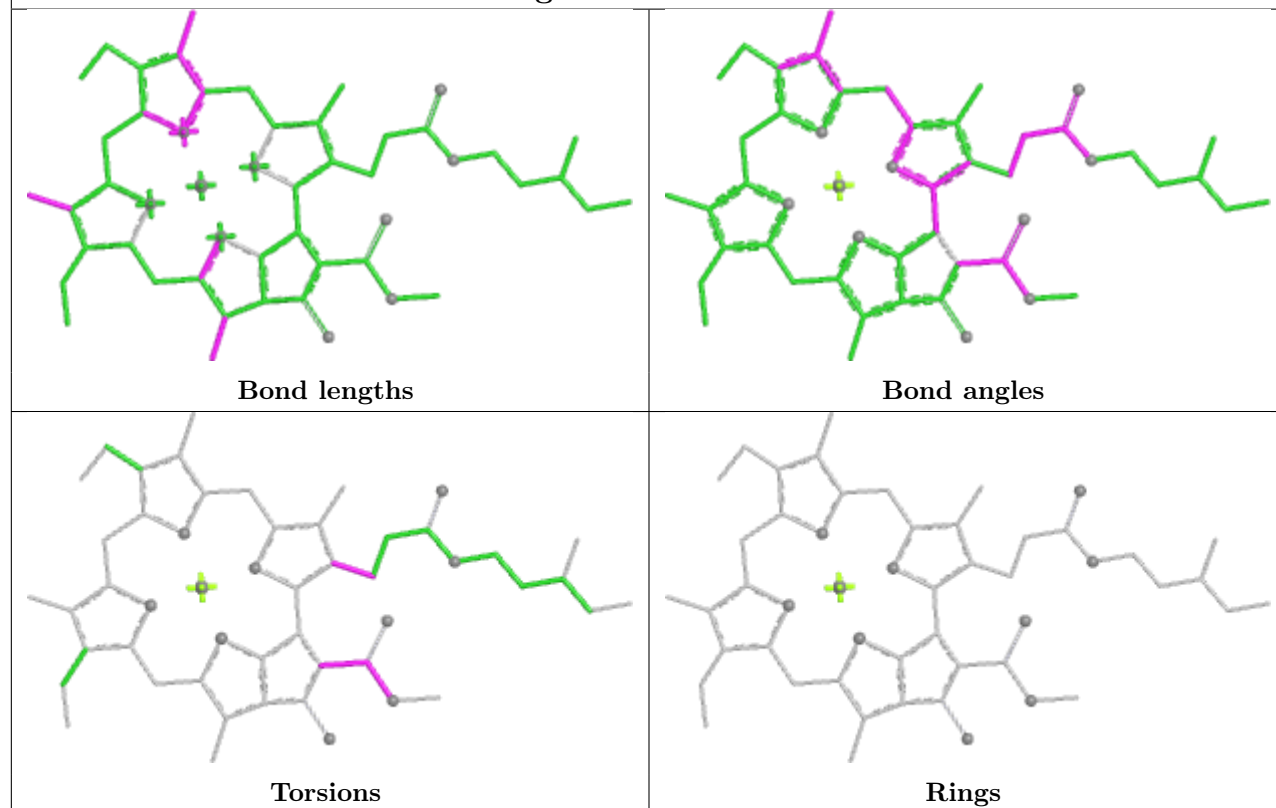


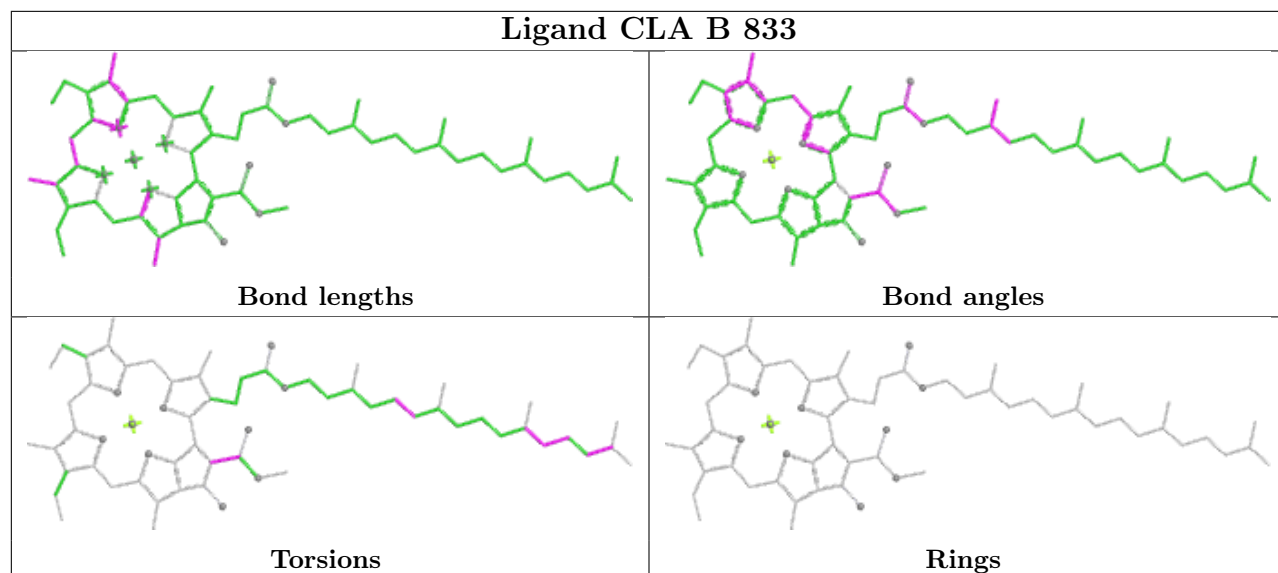
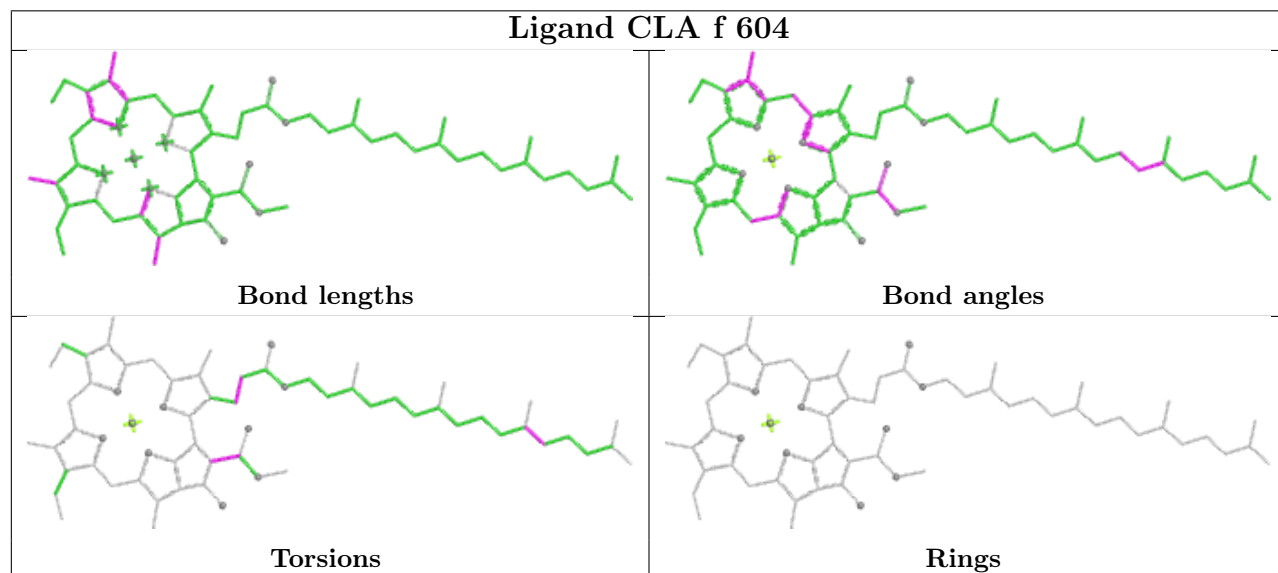
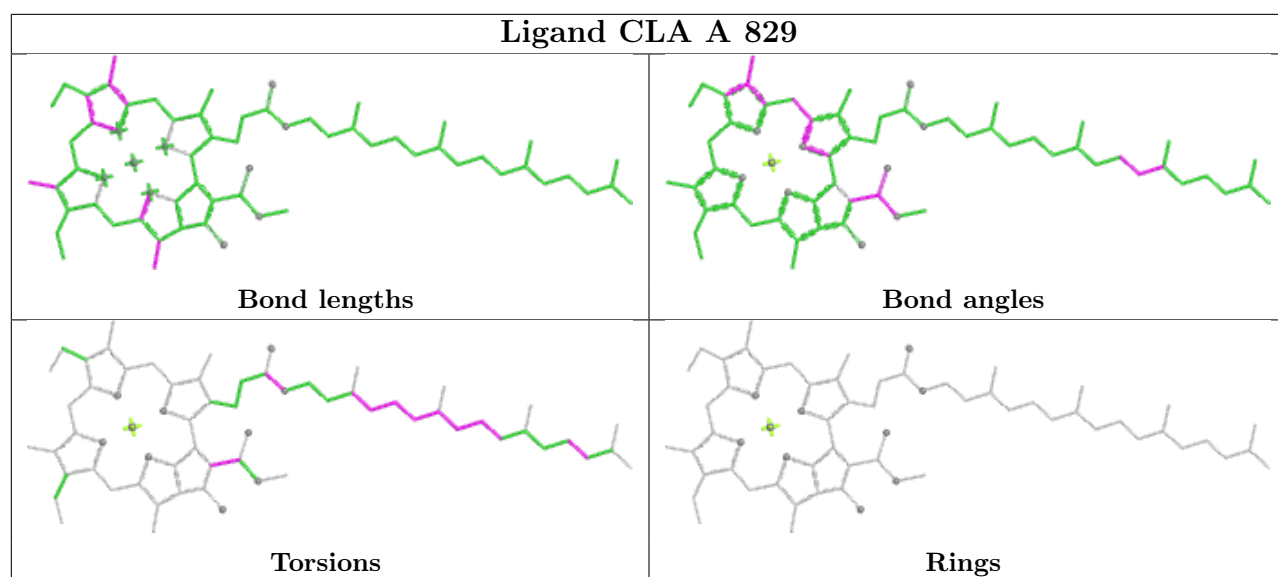
Rings

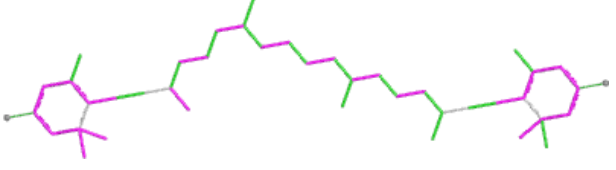
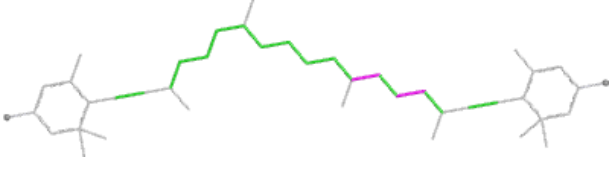
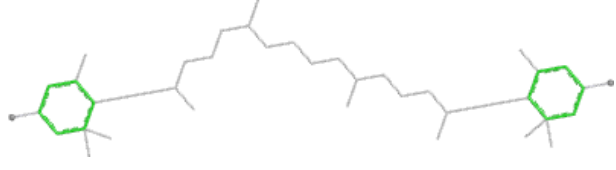
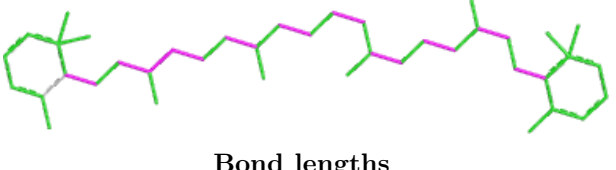
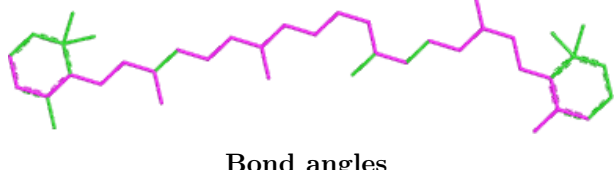
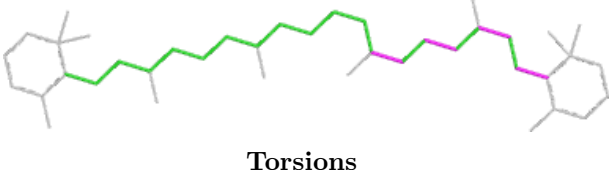
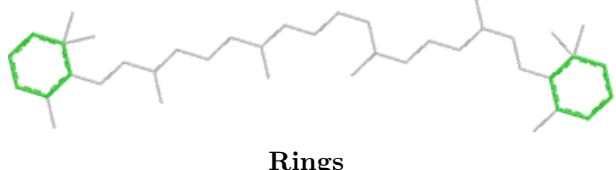
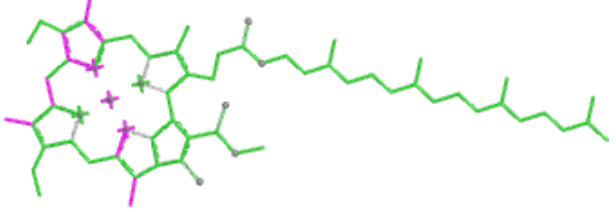
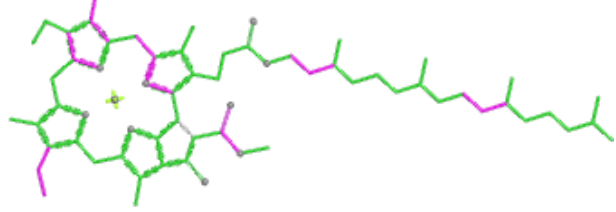
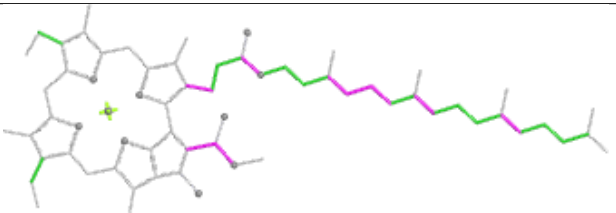
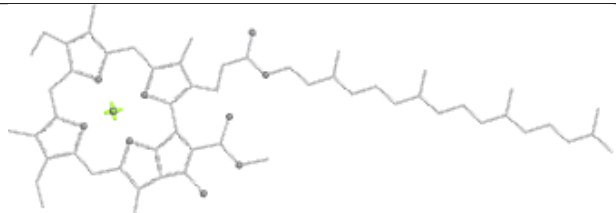
Ligand CLA A 827

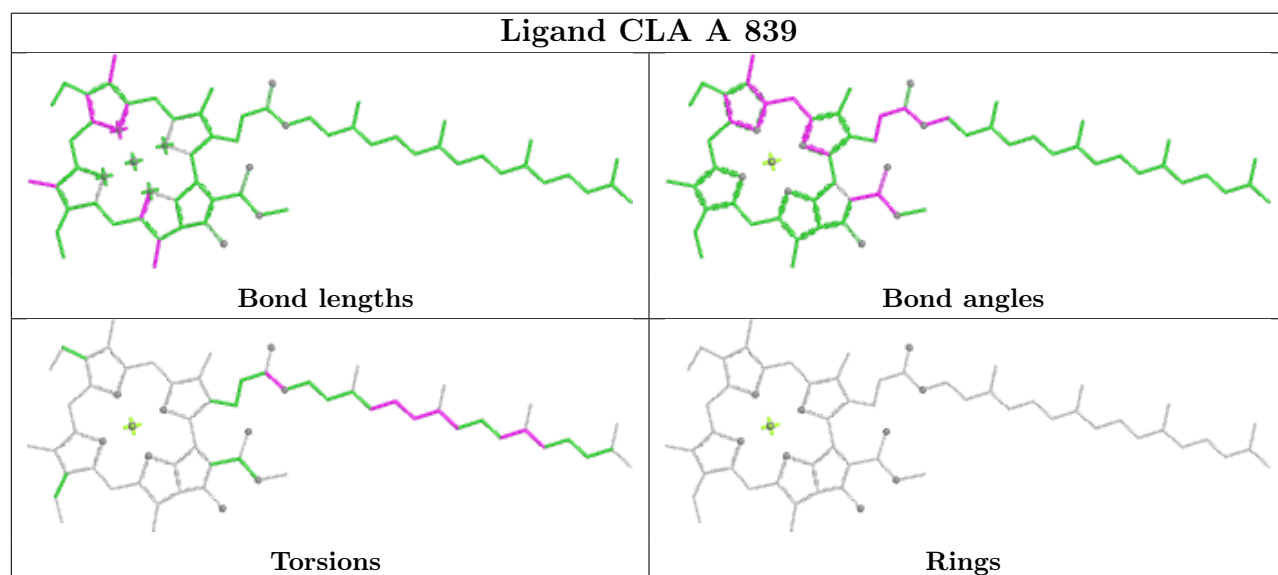
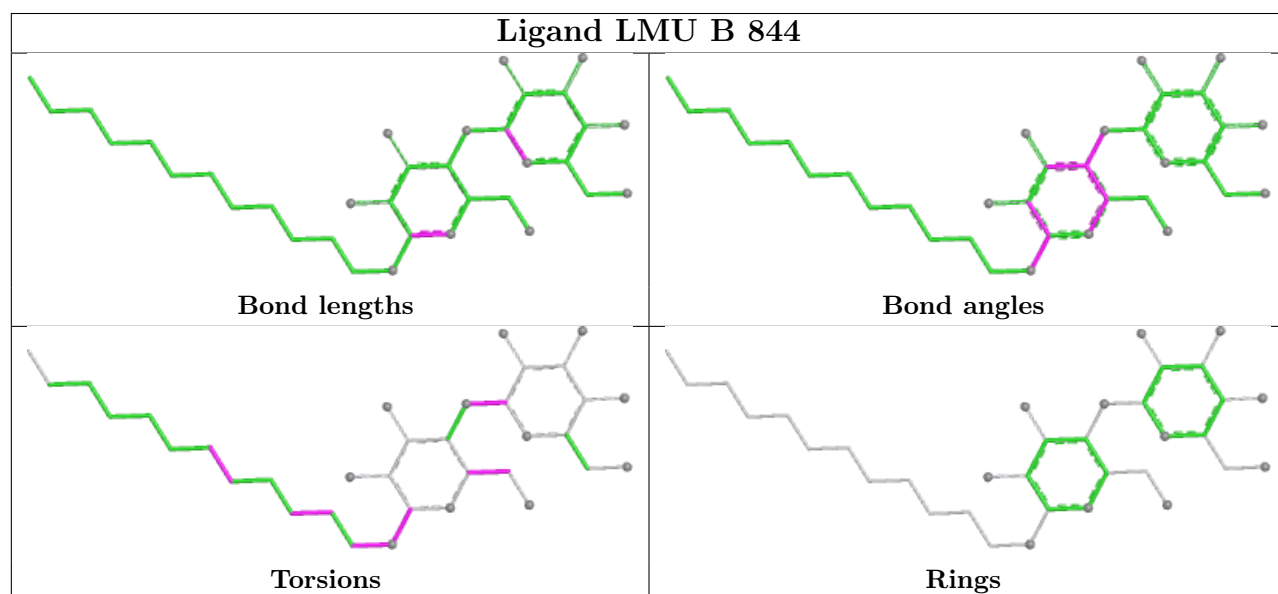
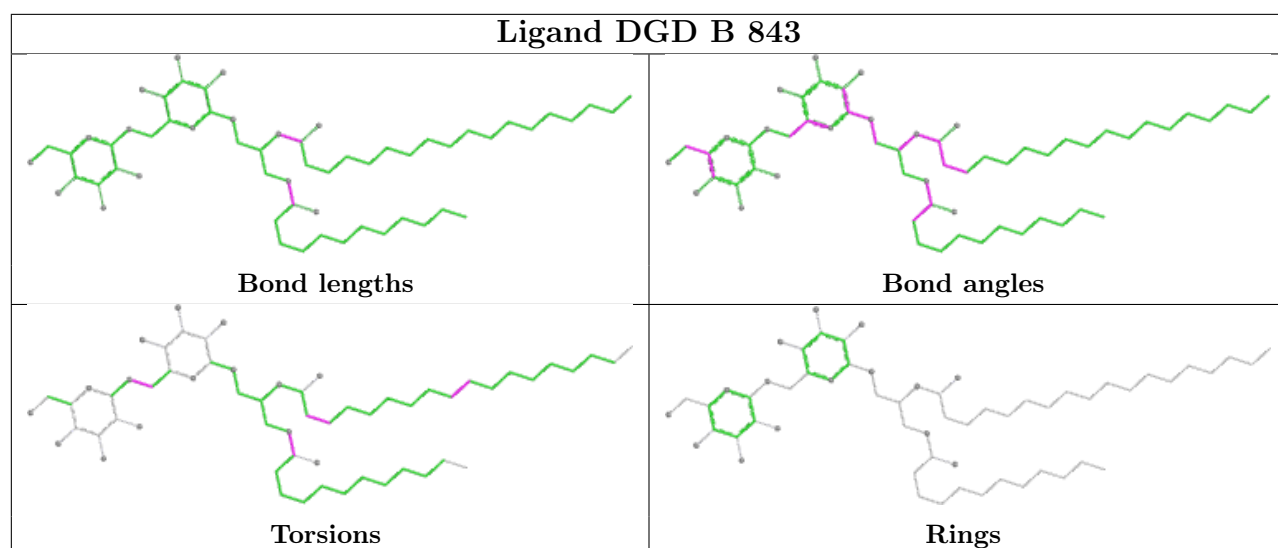


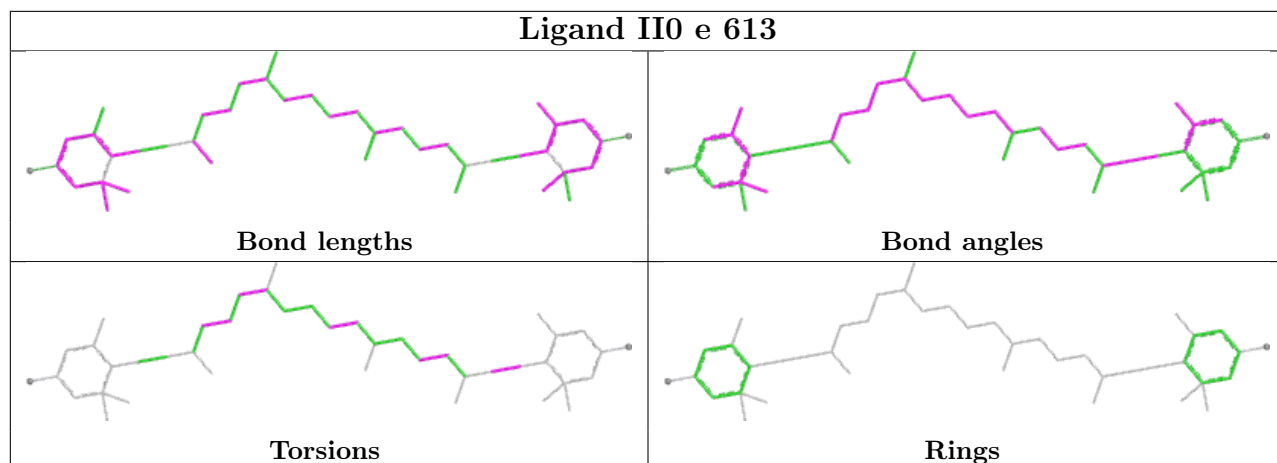
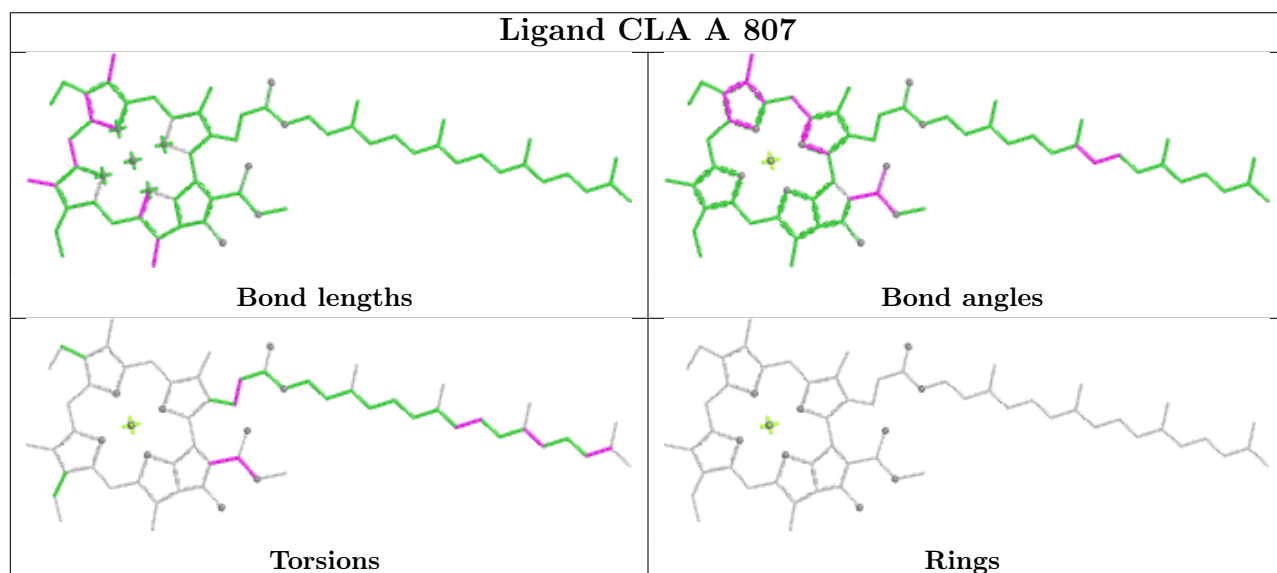
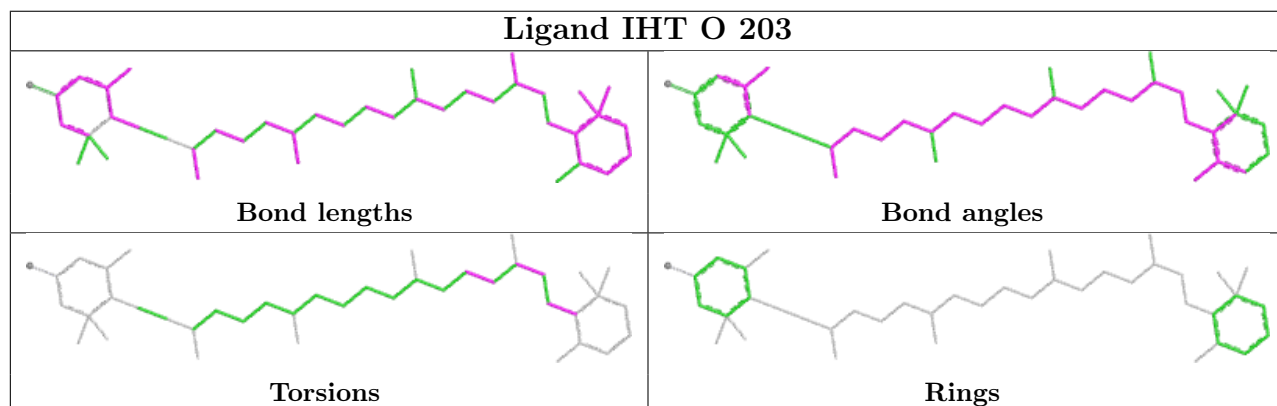
Ligand CLA h 303

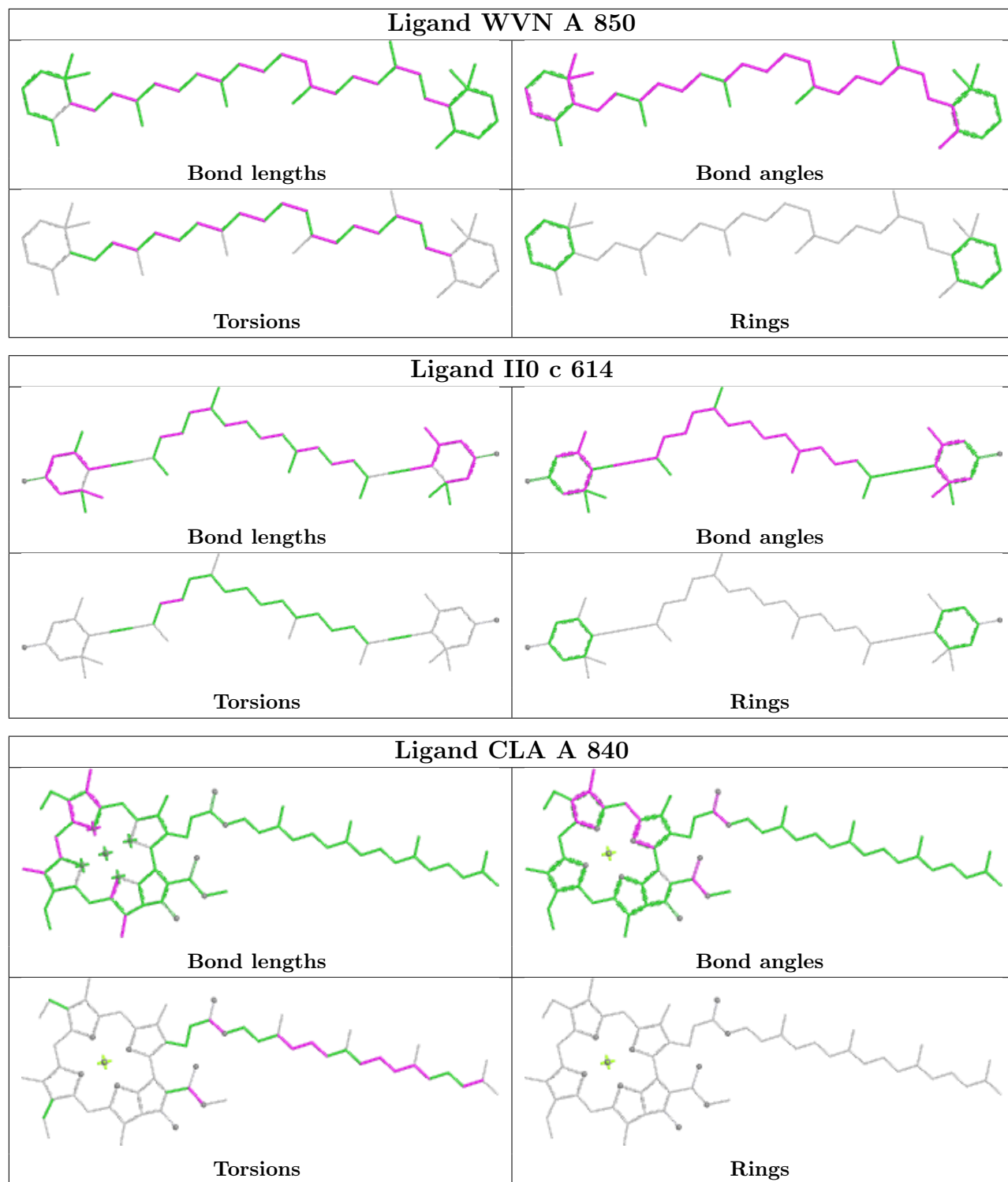




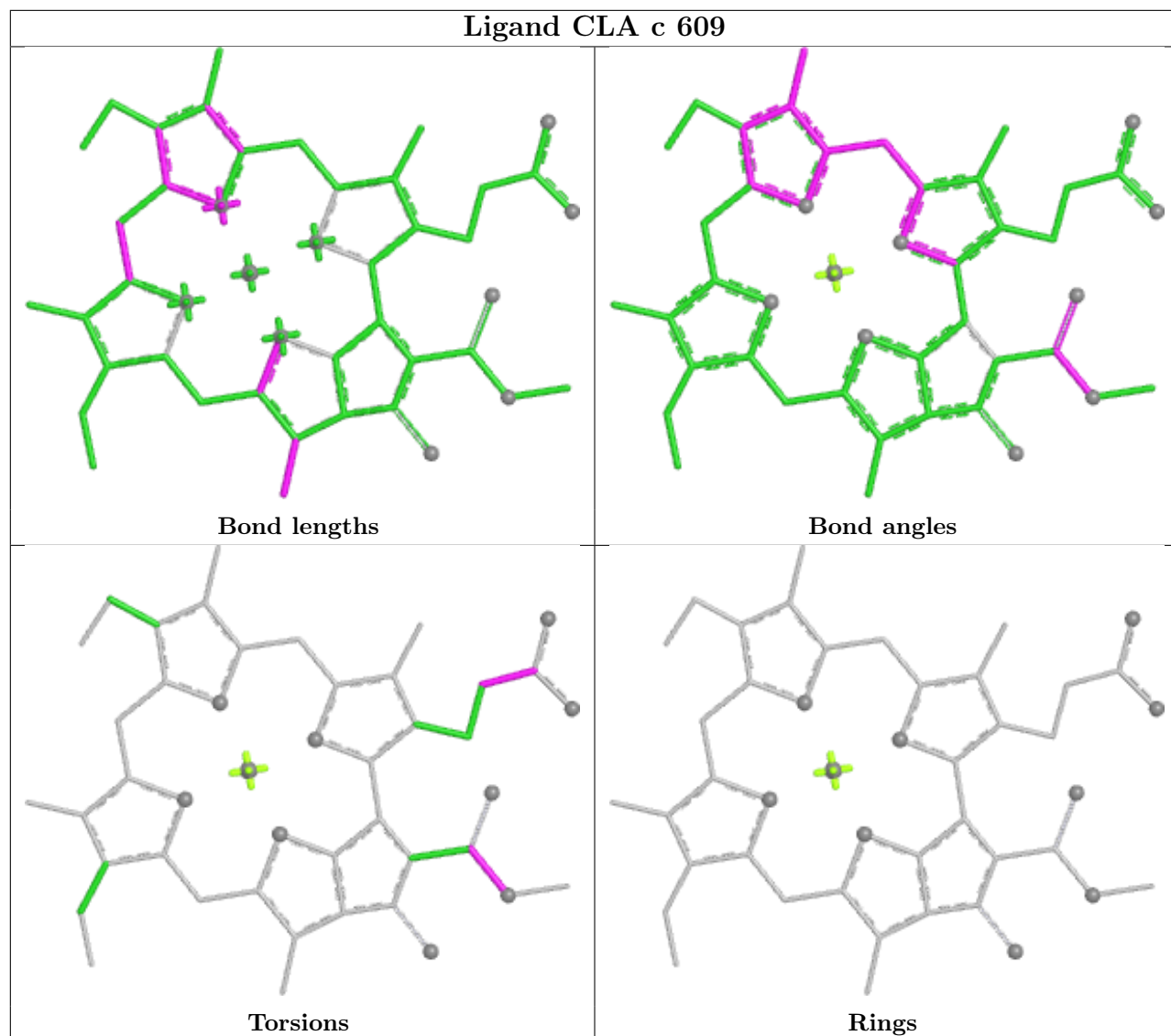
Ligand II0 c 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA O 201	
 Bond lengths	 Bond angles
 Torsions	 Rings



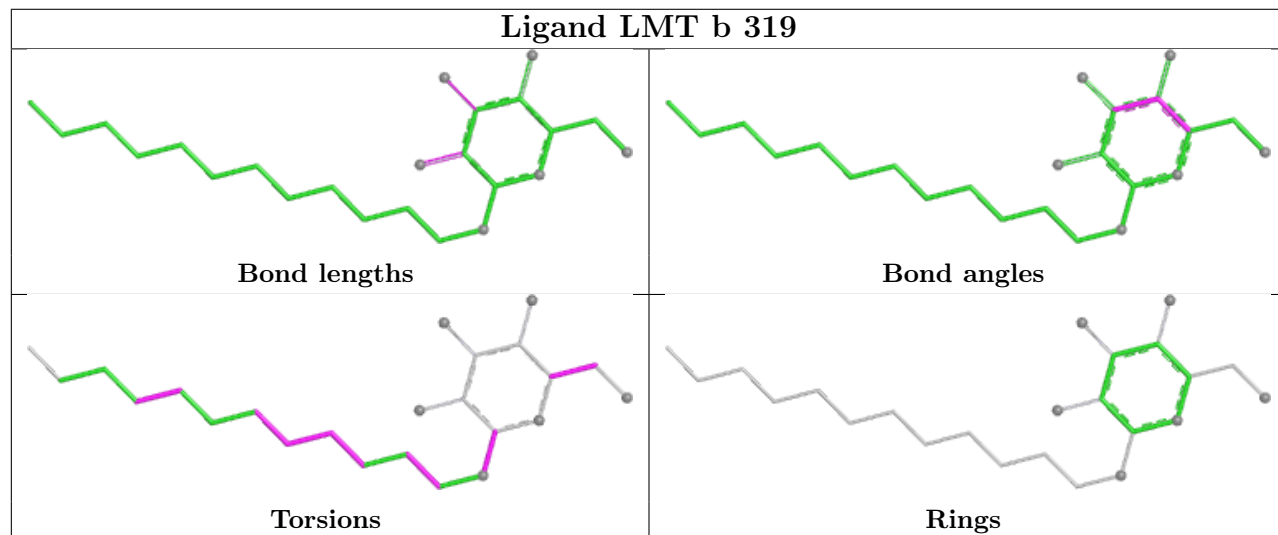
Ligand IIO e 613**Ligand CLA A 807****Ligand IHT O 203**



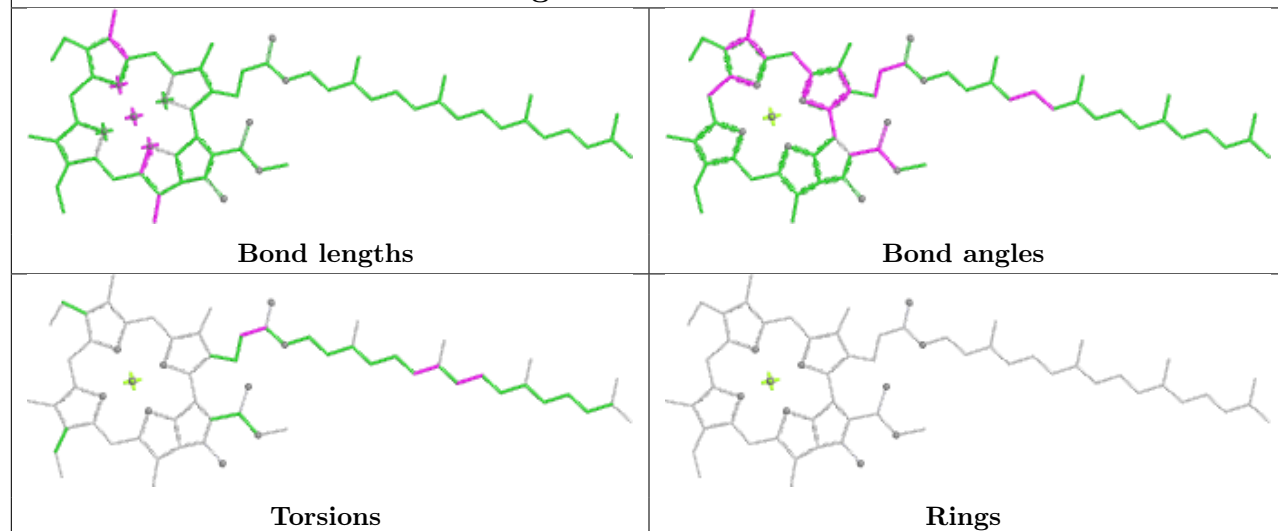
Ligand CLA c 609



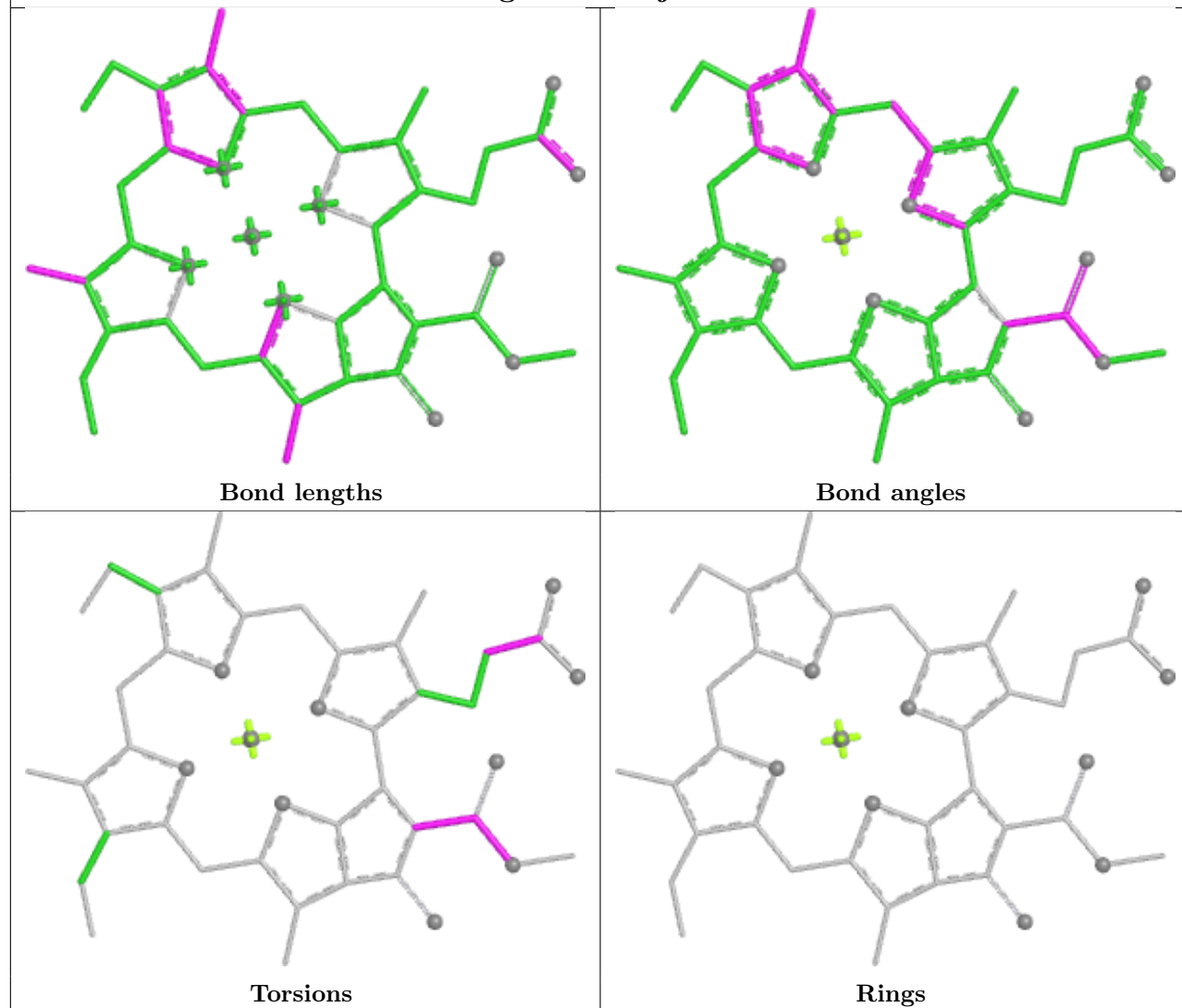
Ligand LMT b 319

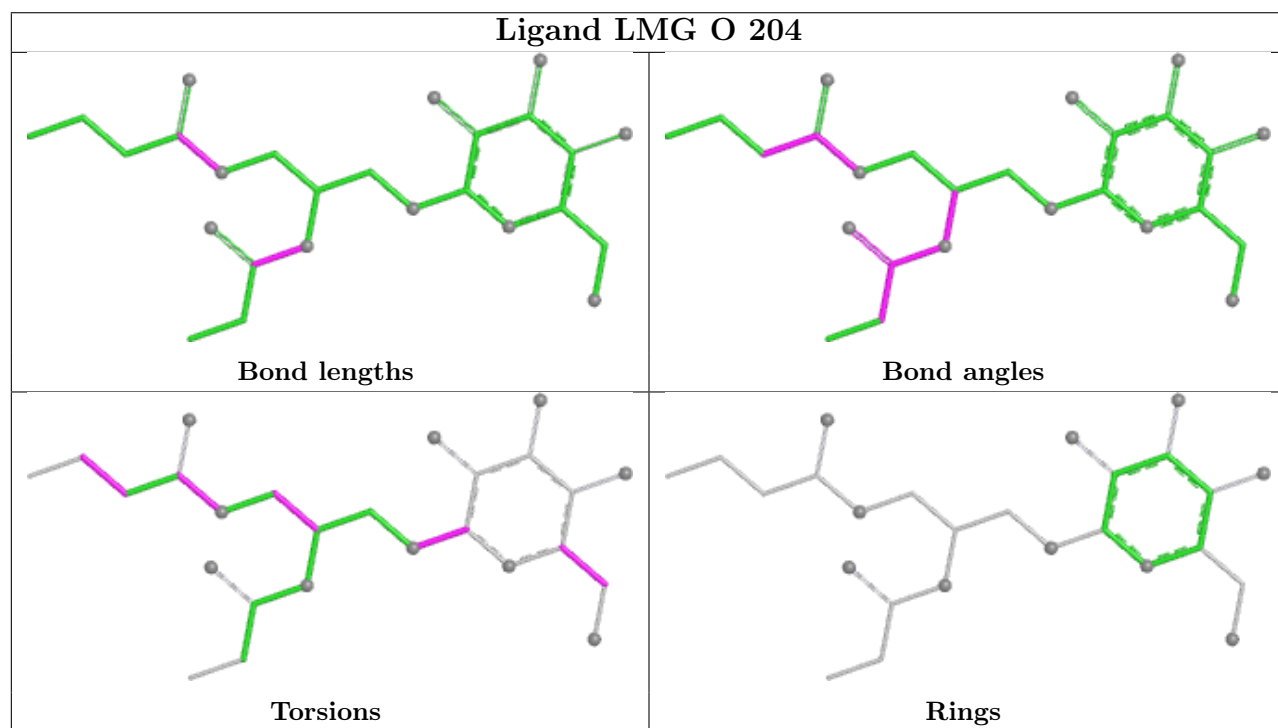
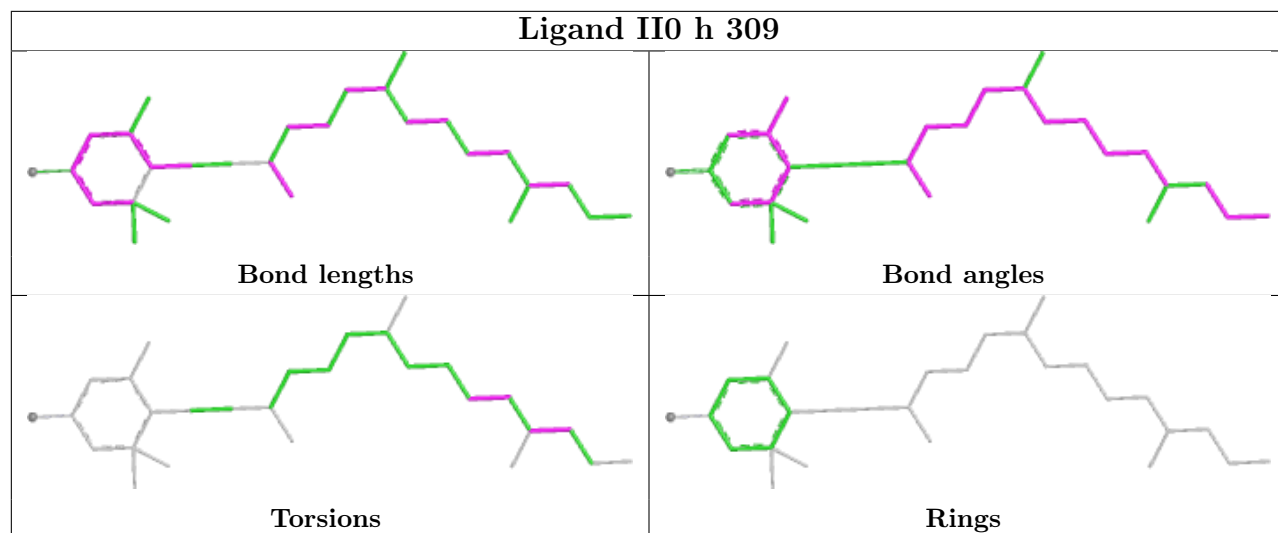


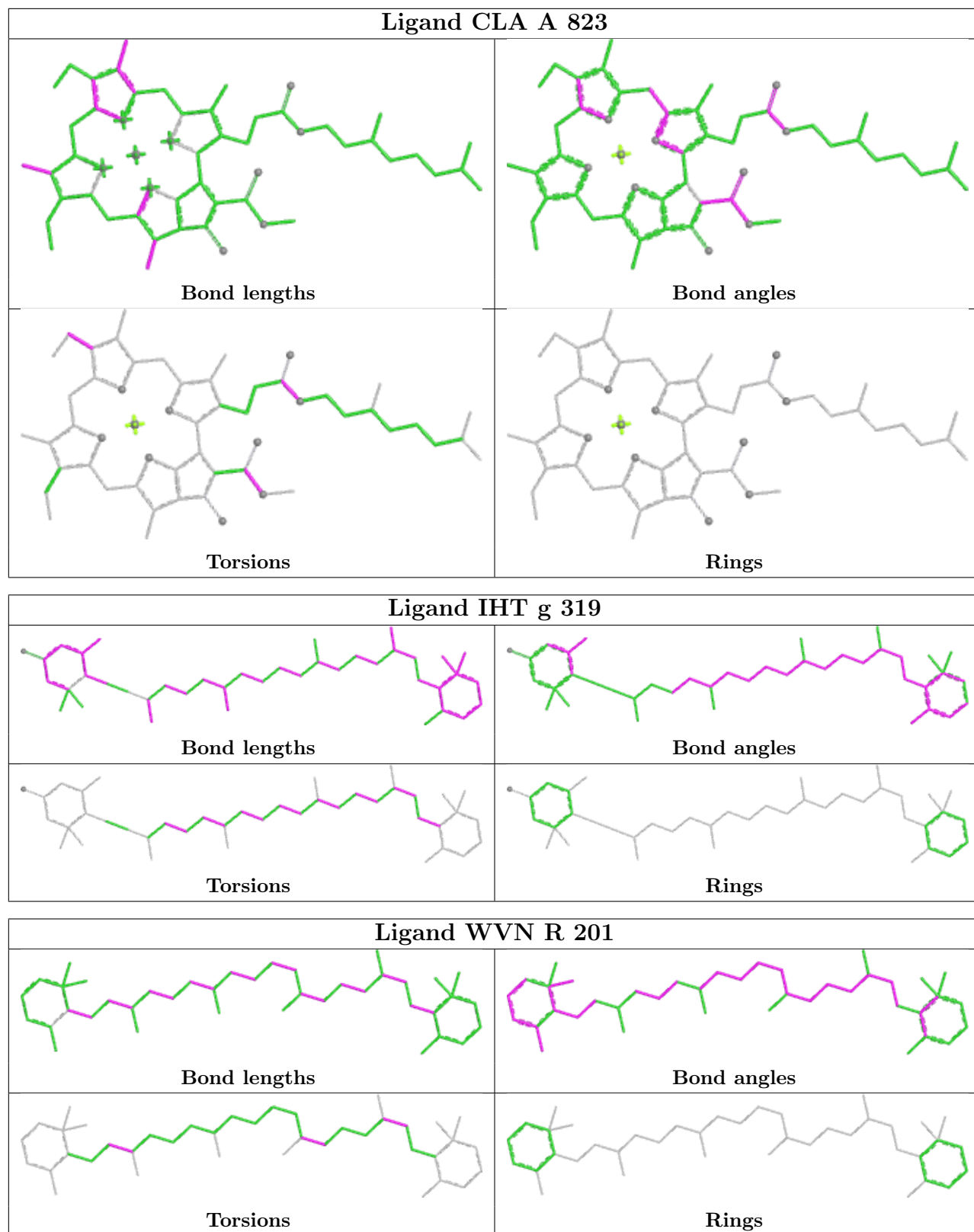
Ligand CLA A 836

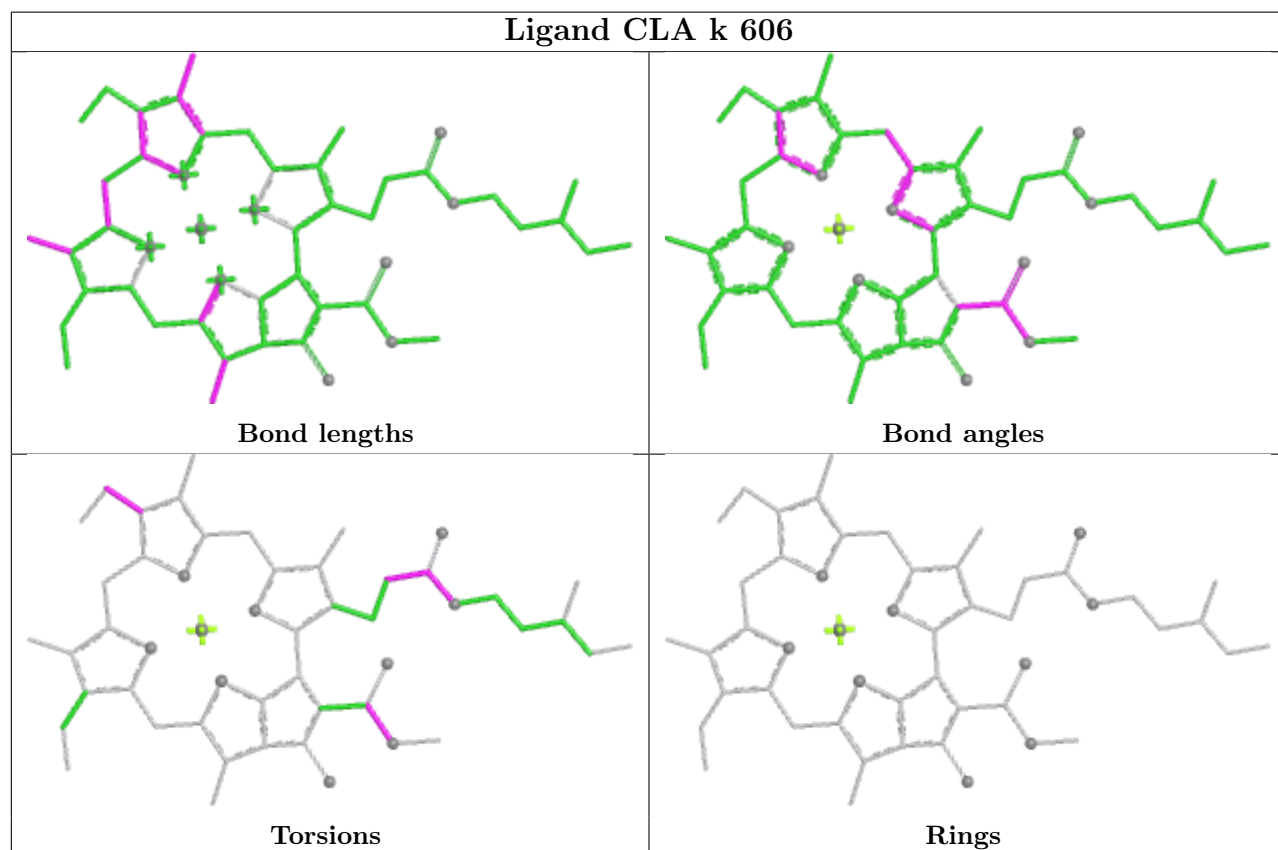
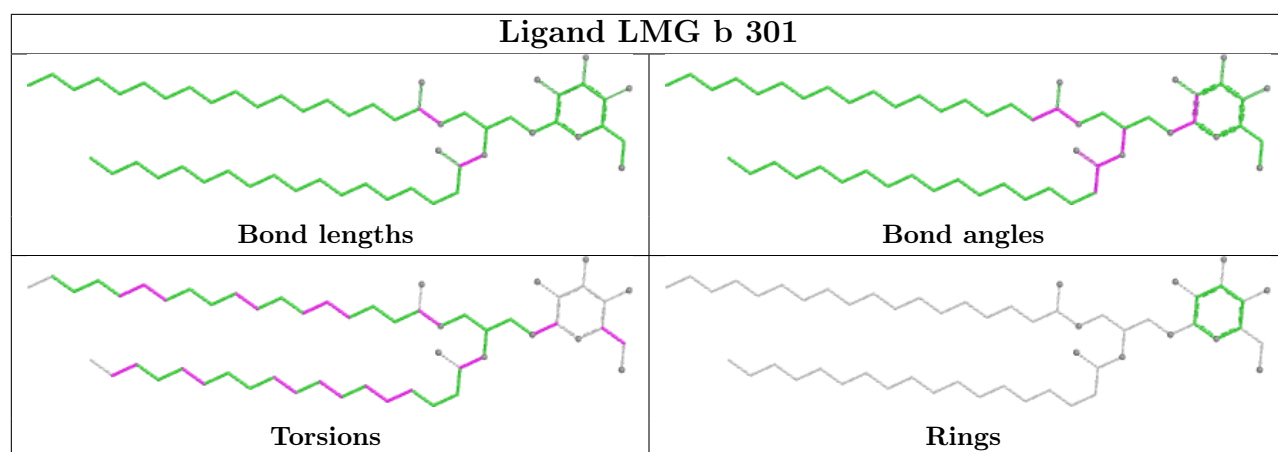


Ligand CLA j 309

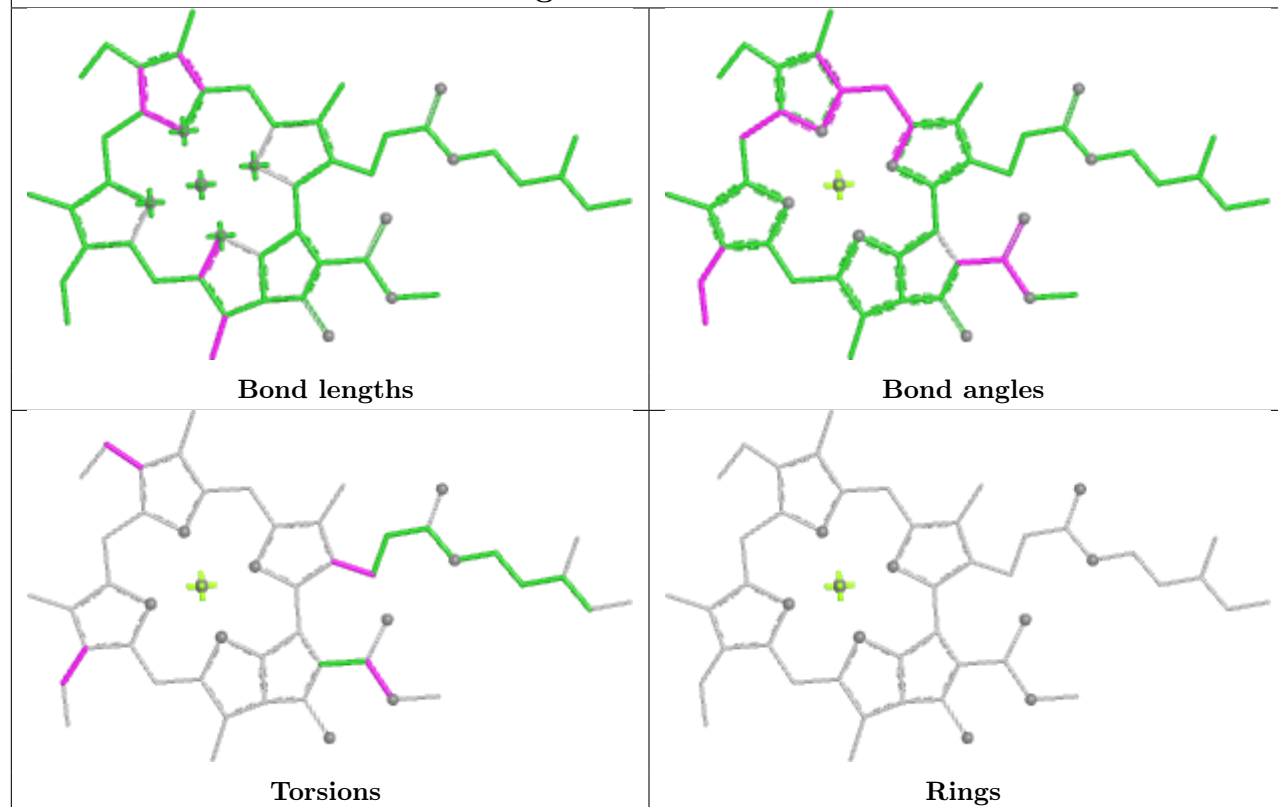




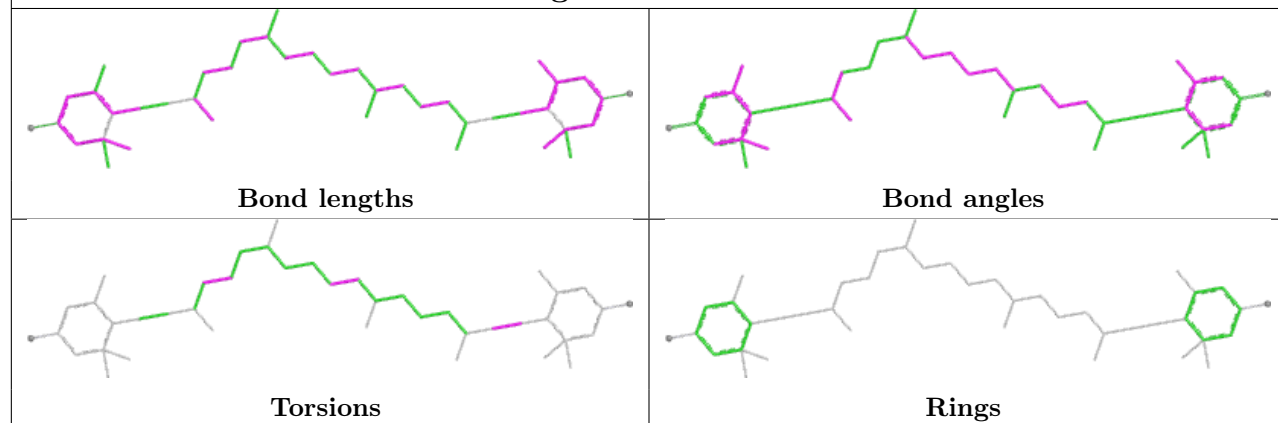




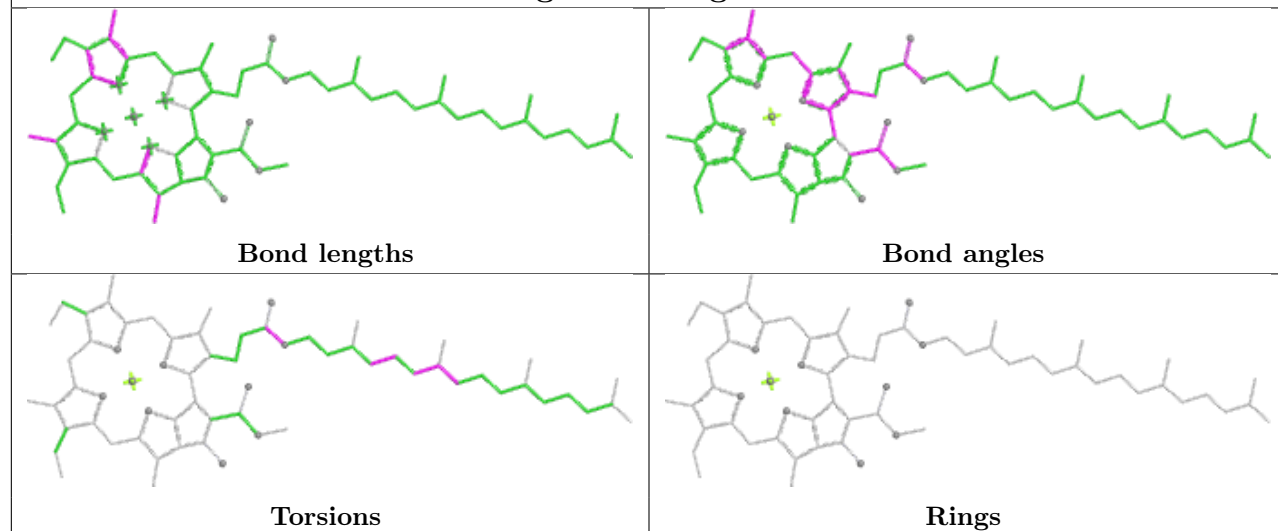
Ligand CLA k 614



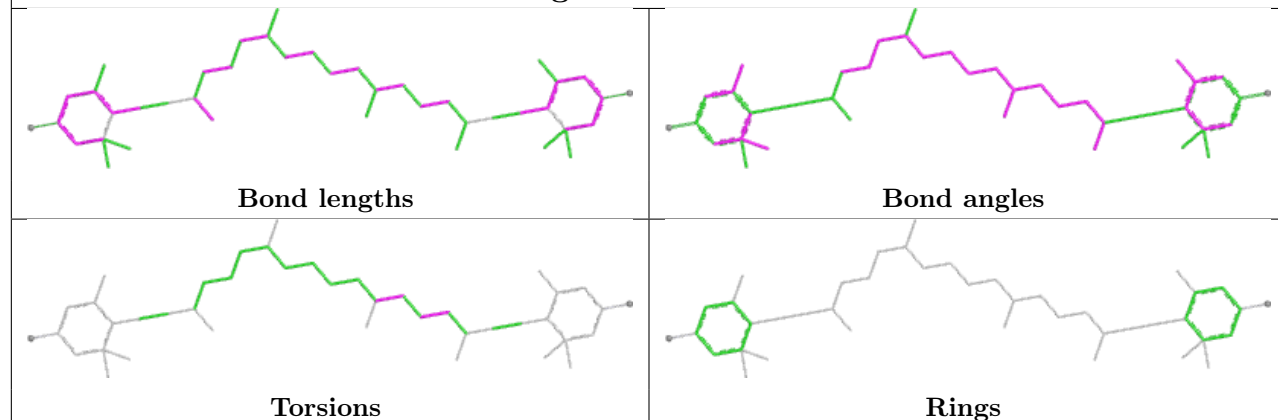
Ligand II0 a 315



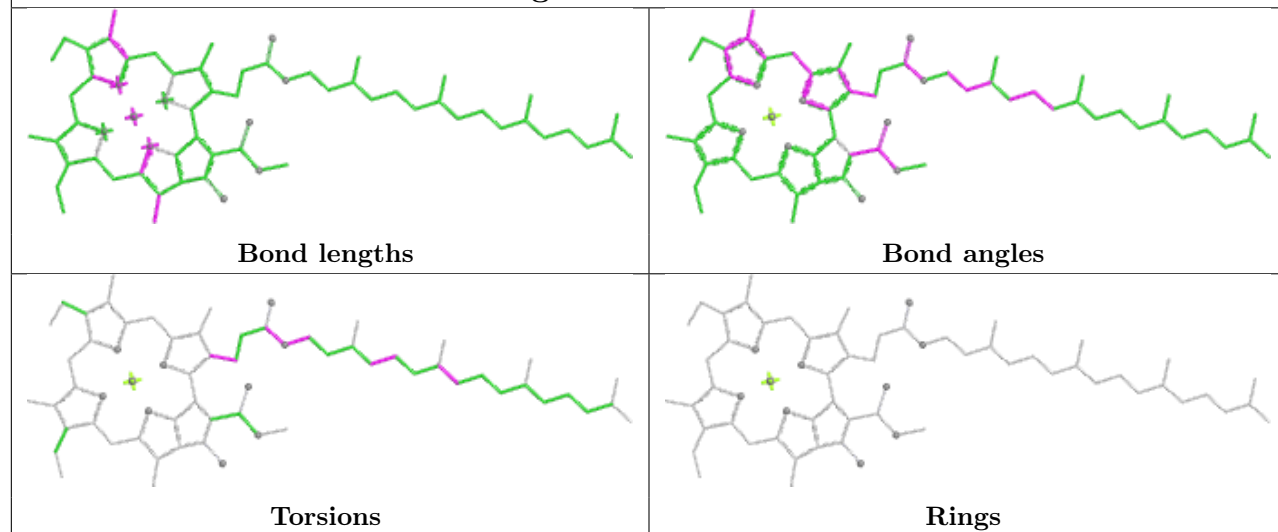
Ligand CLA g 309

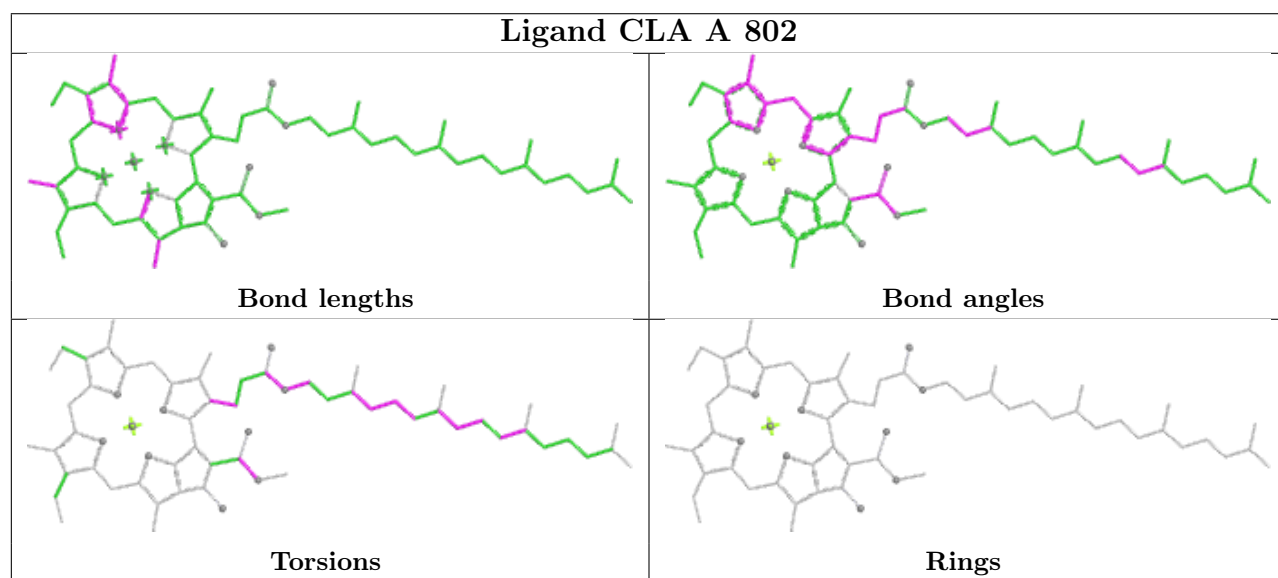
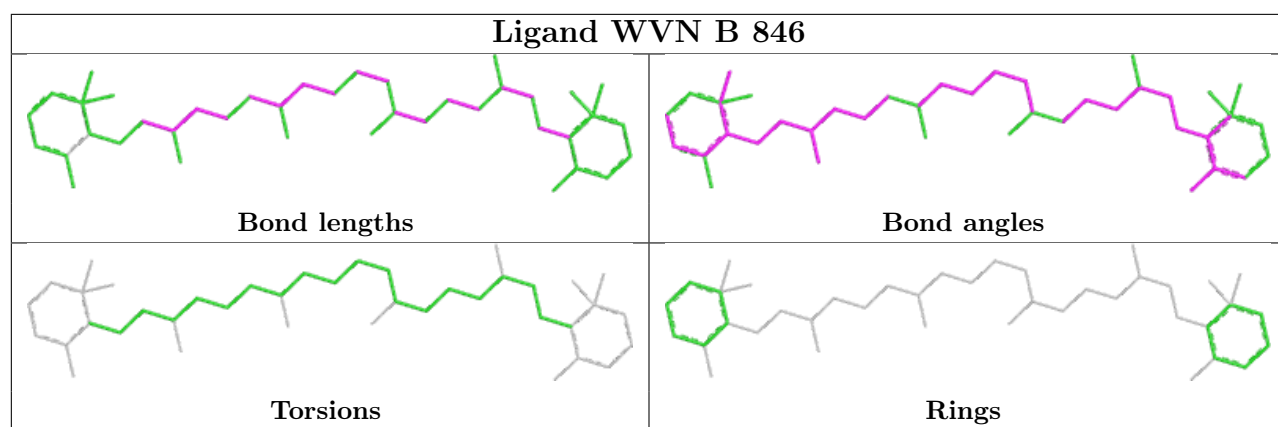


Ligand II0 e 614

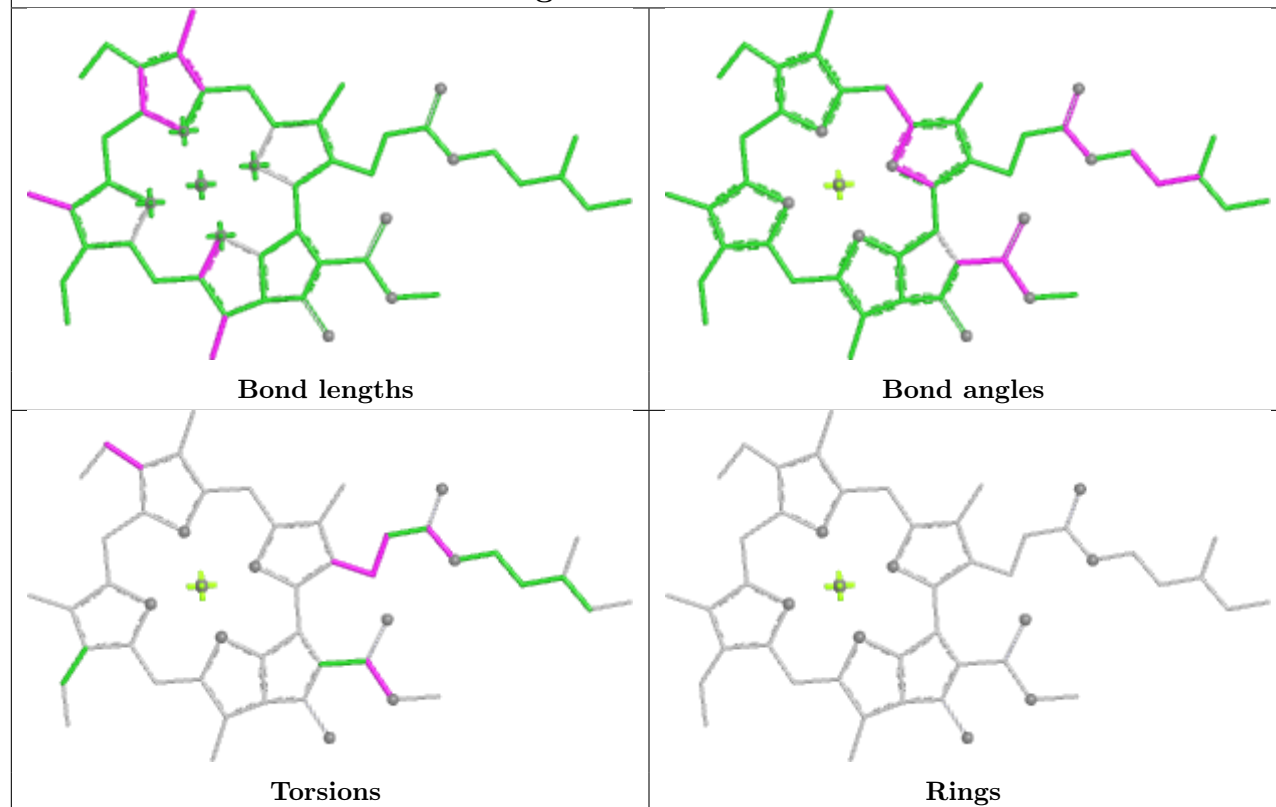


Ligand CLA A 805

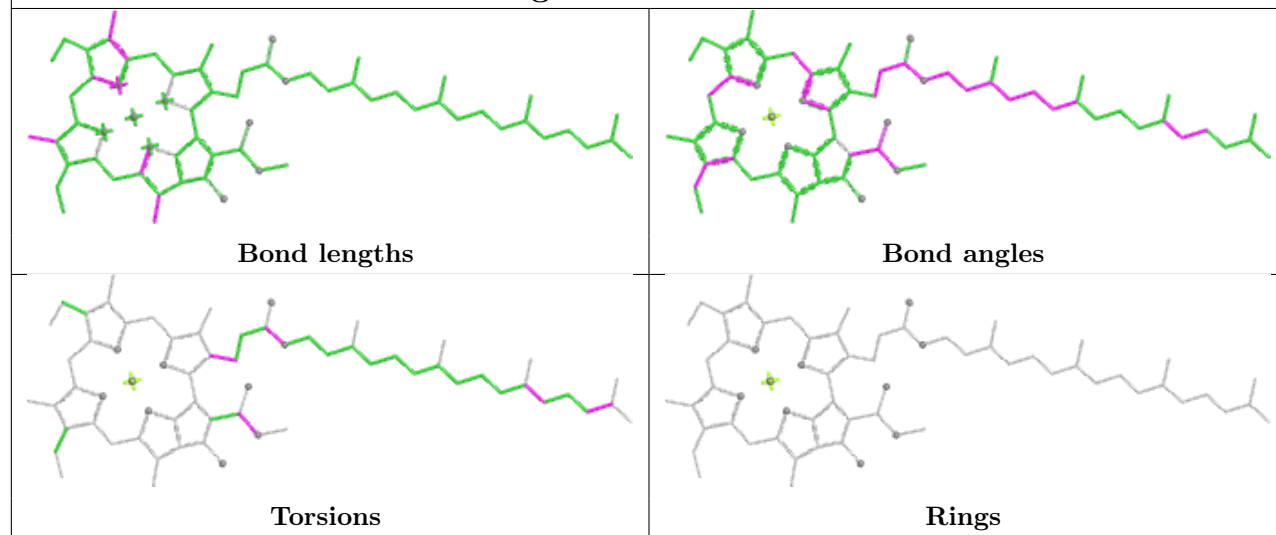


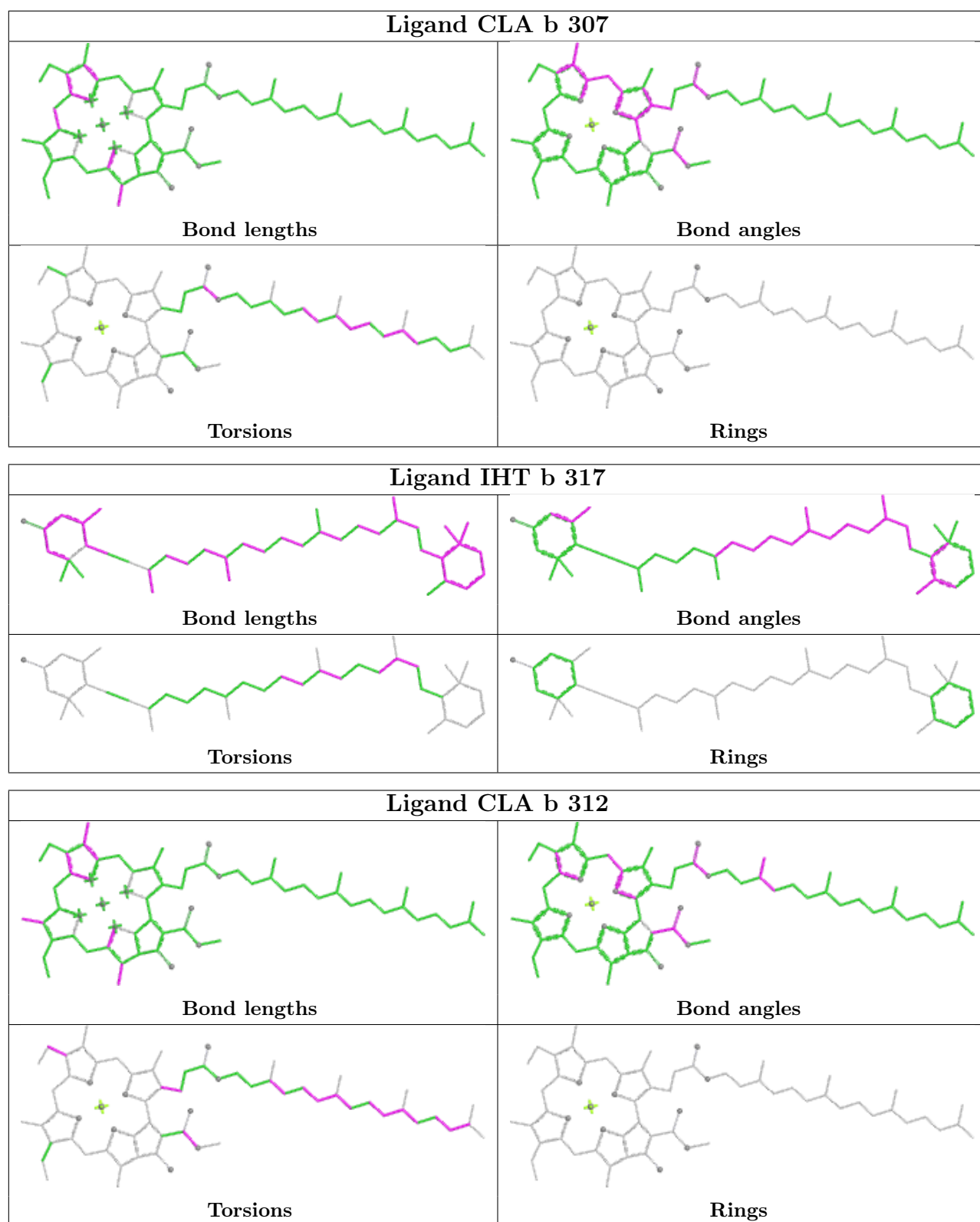


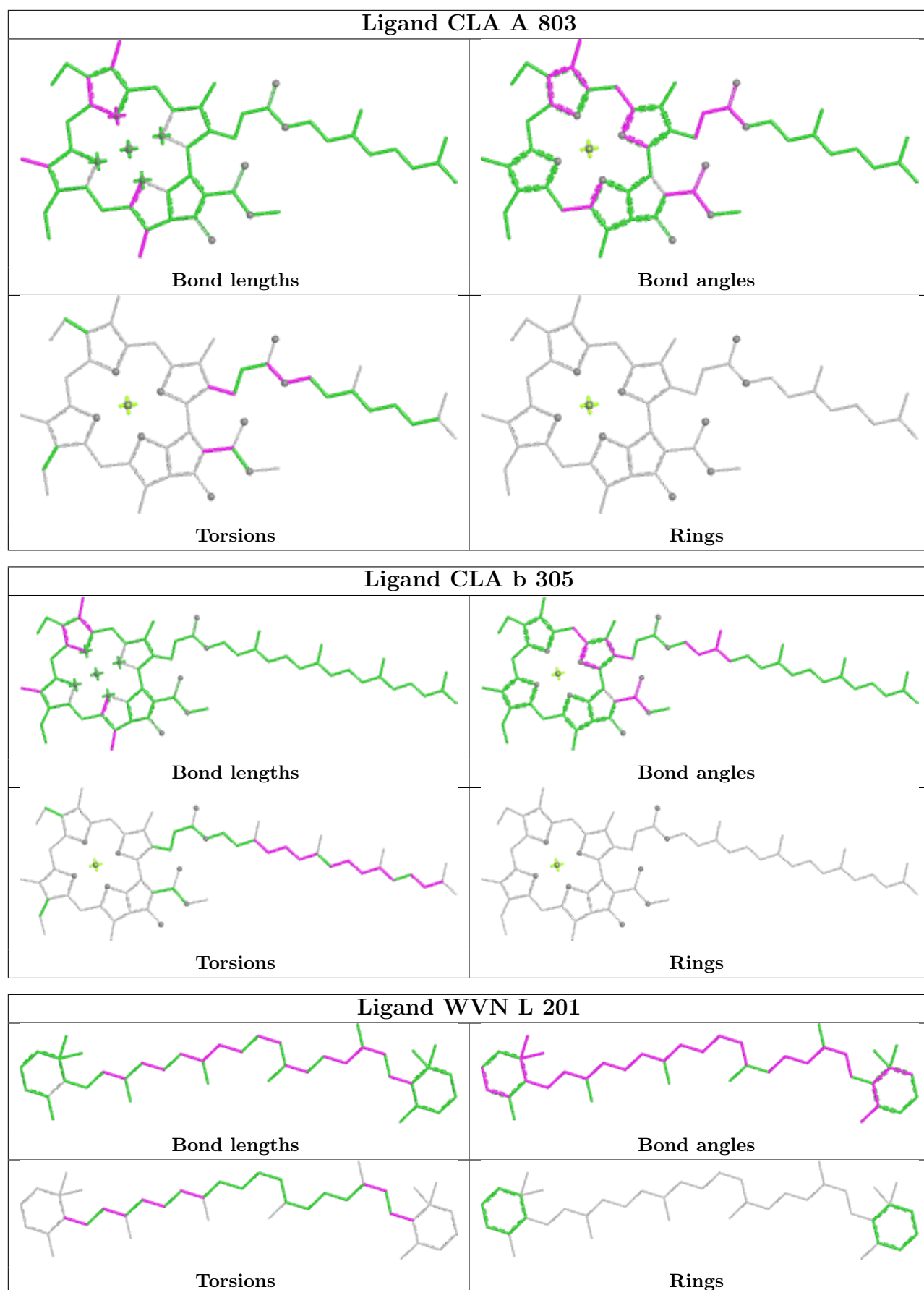
Ligand CLA k 607

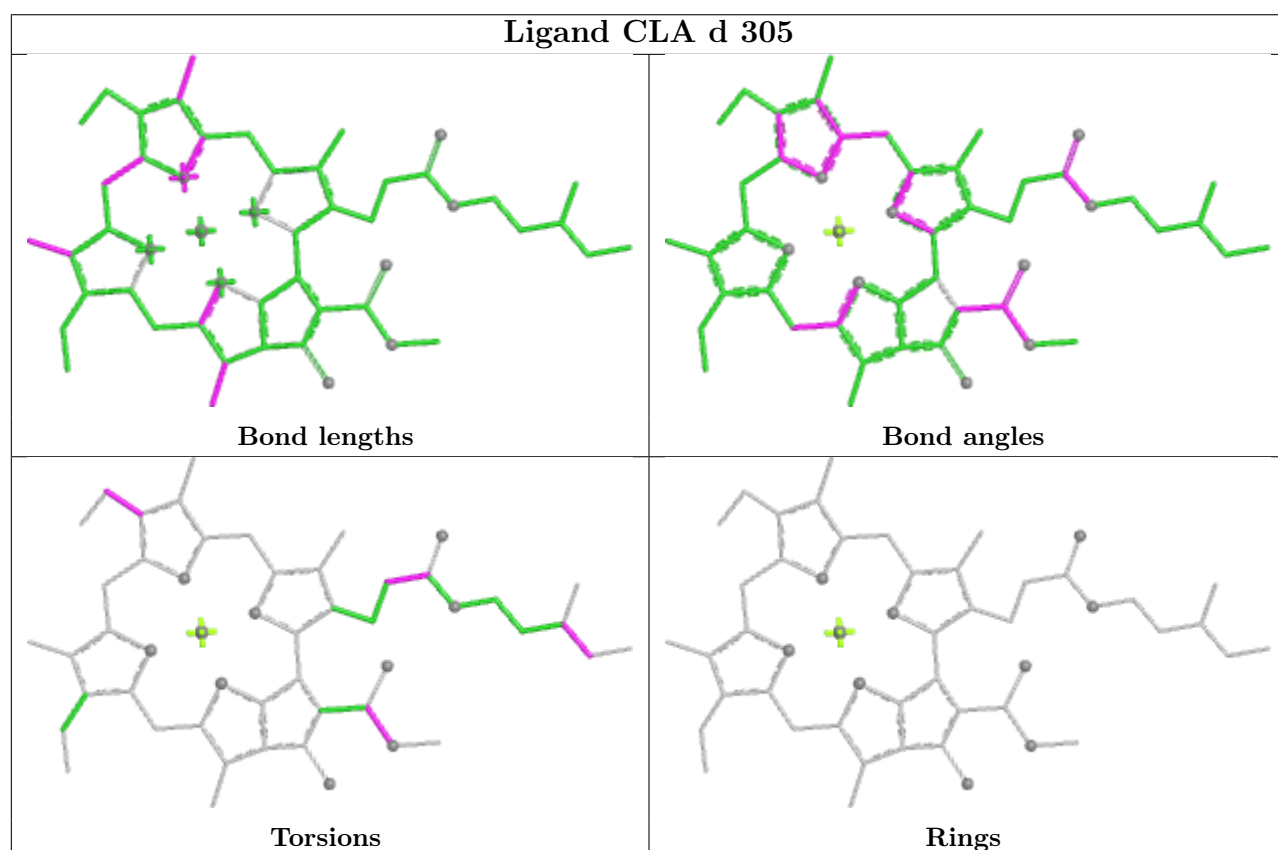
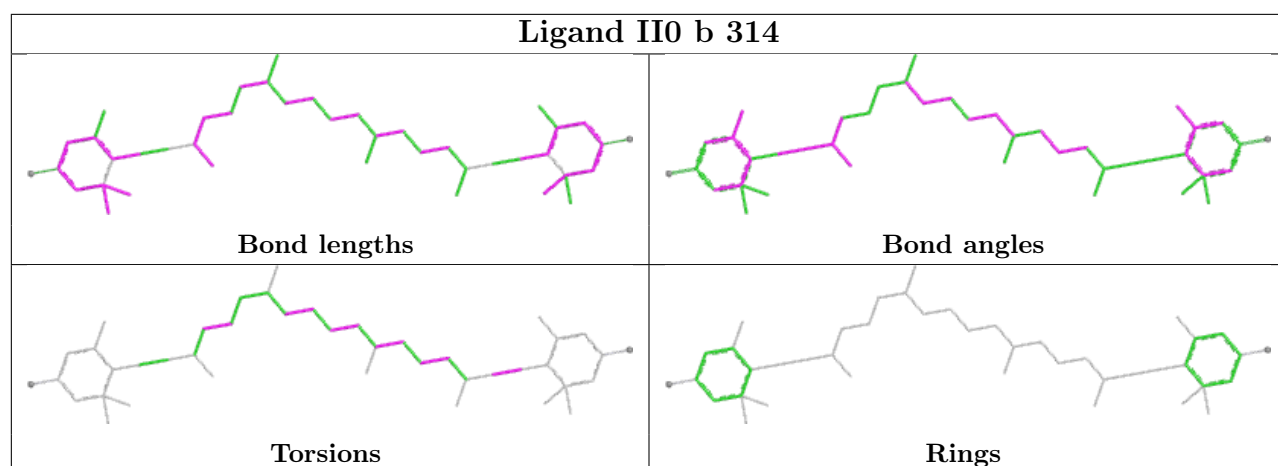


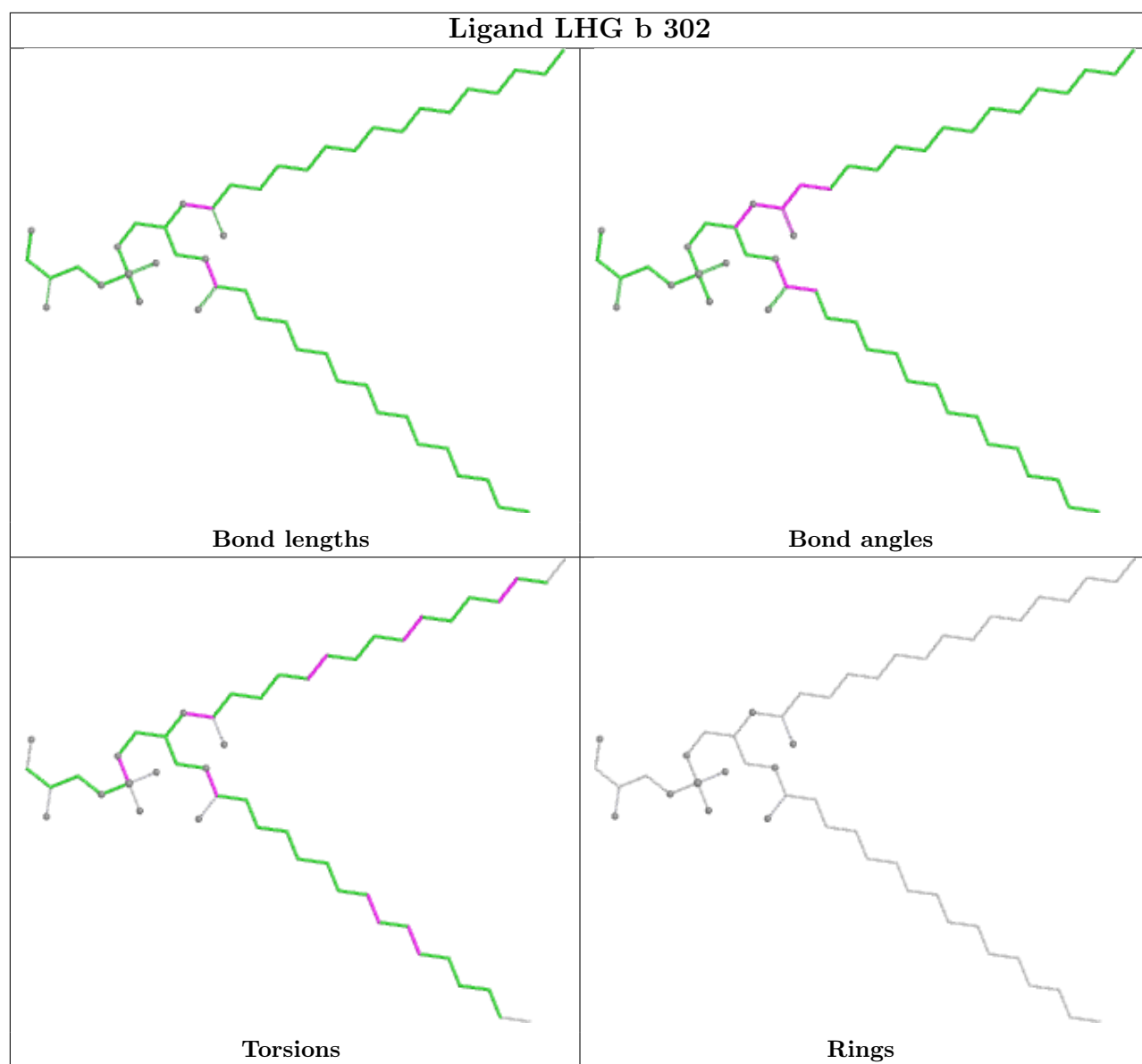
Ligand CLA A 837



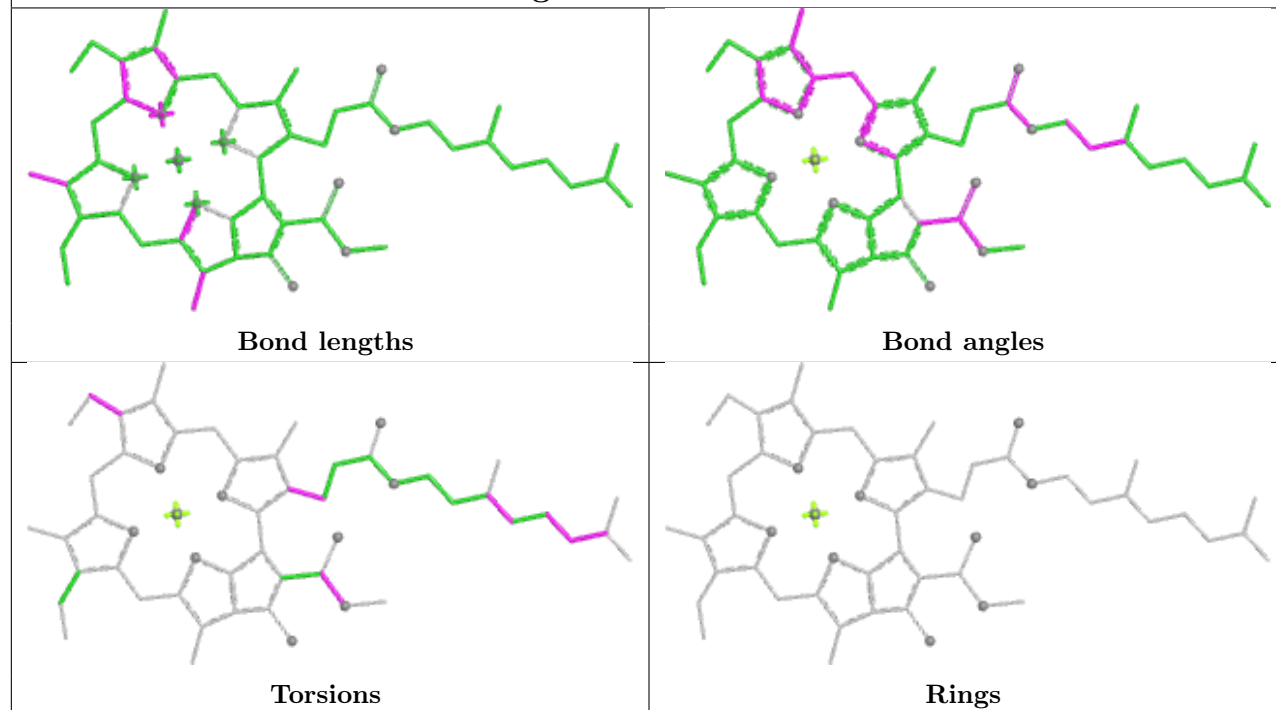




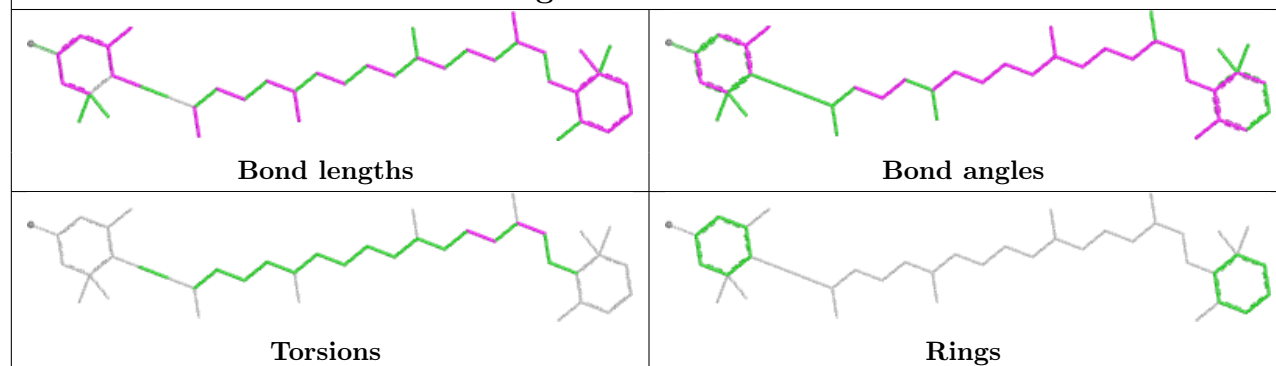




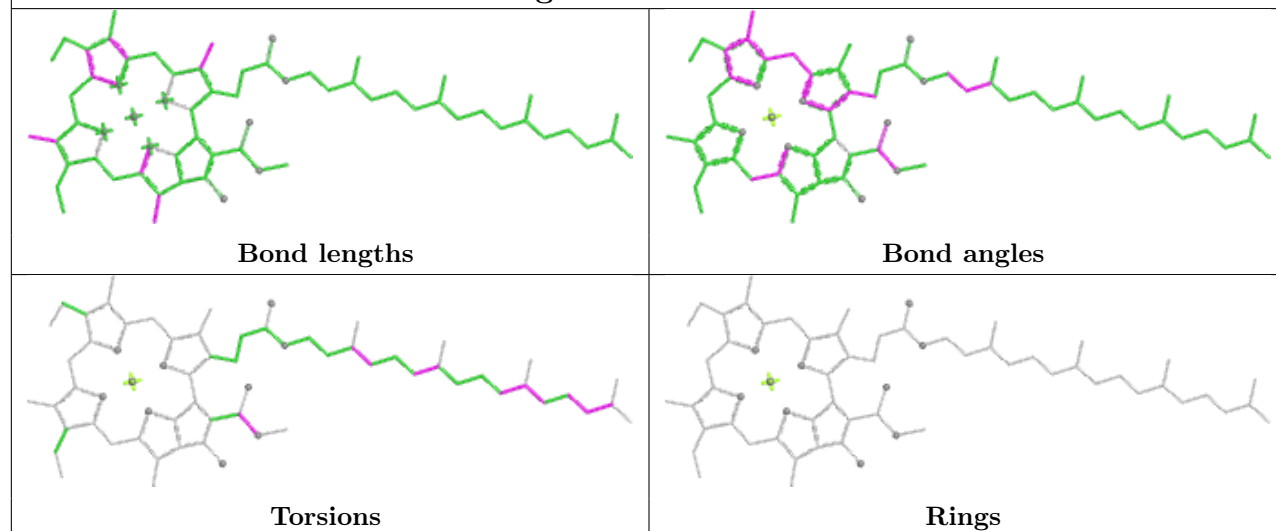
Ligand CLA B 820

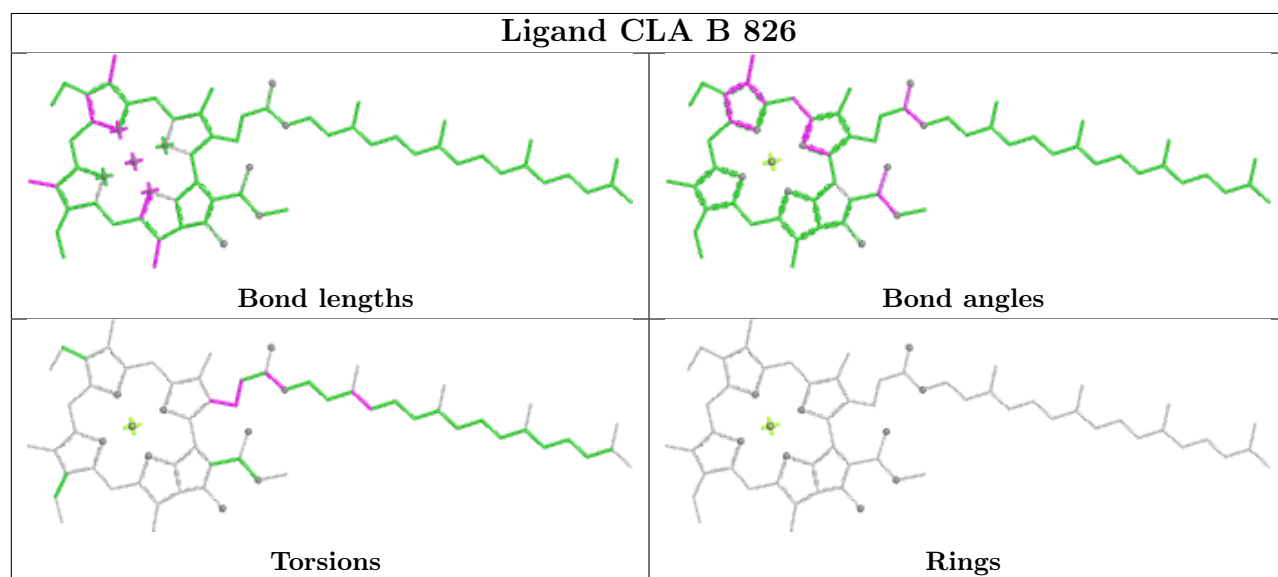
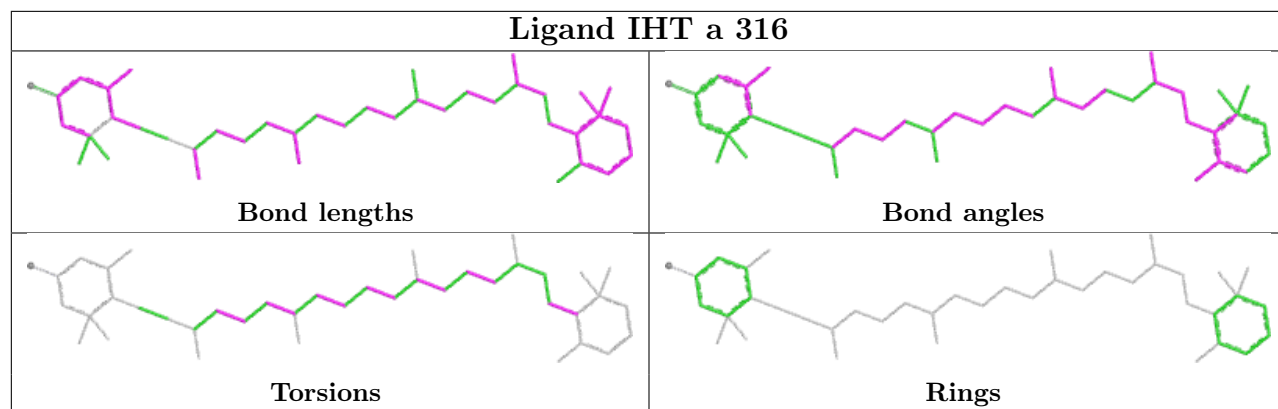


Ligand IHT R 204

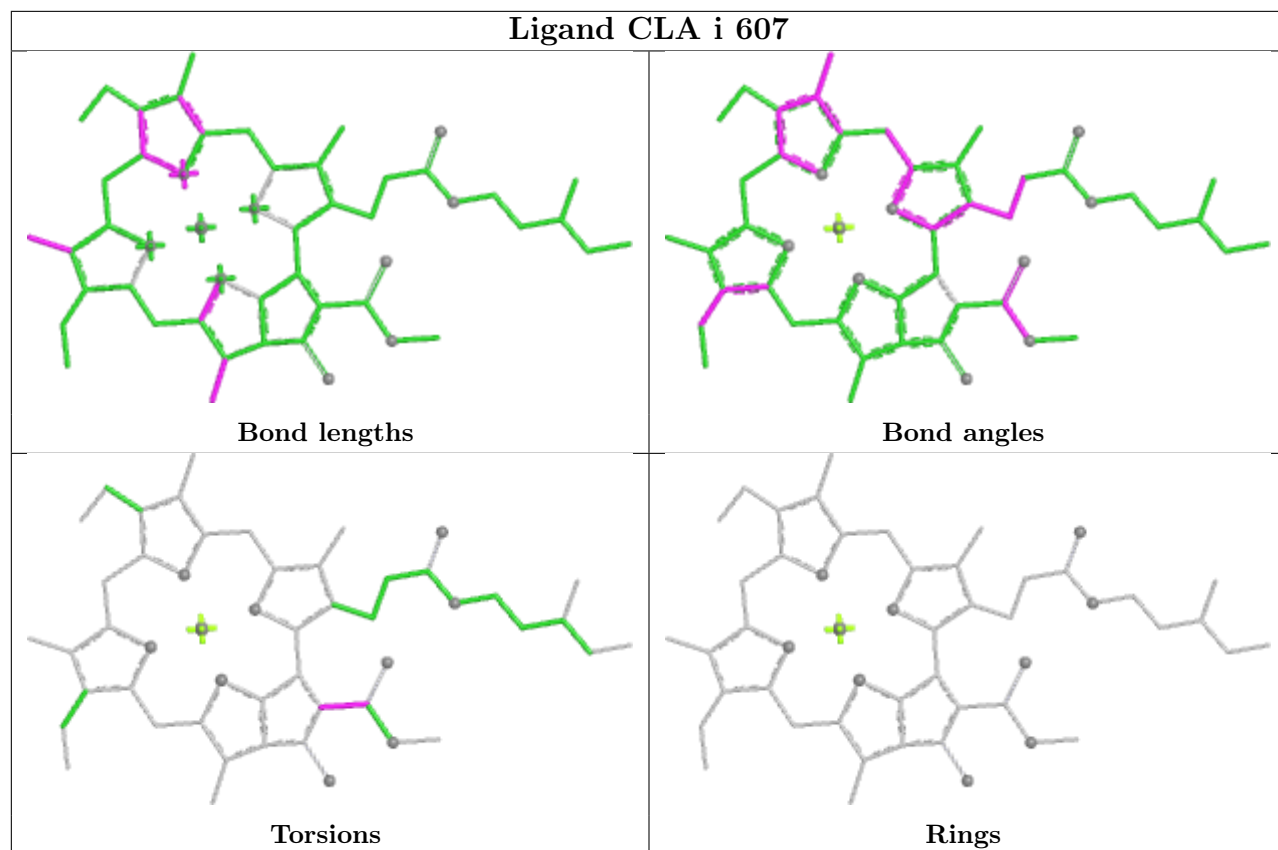


Ligand CLA k 609

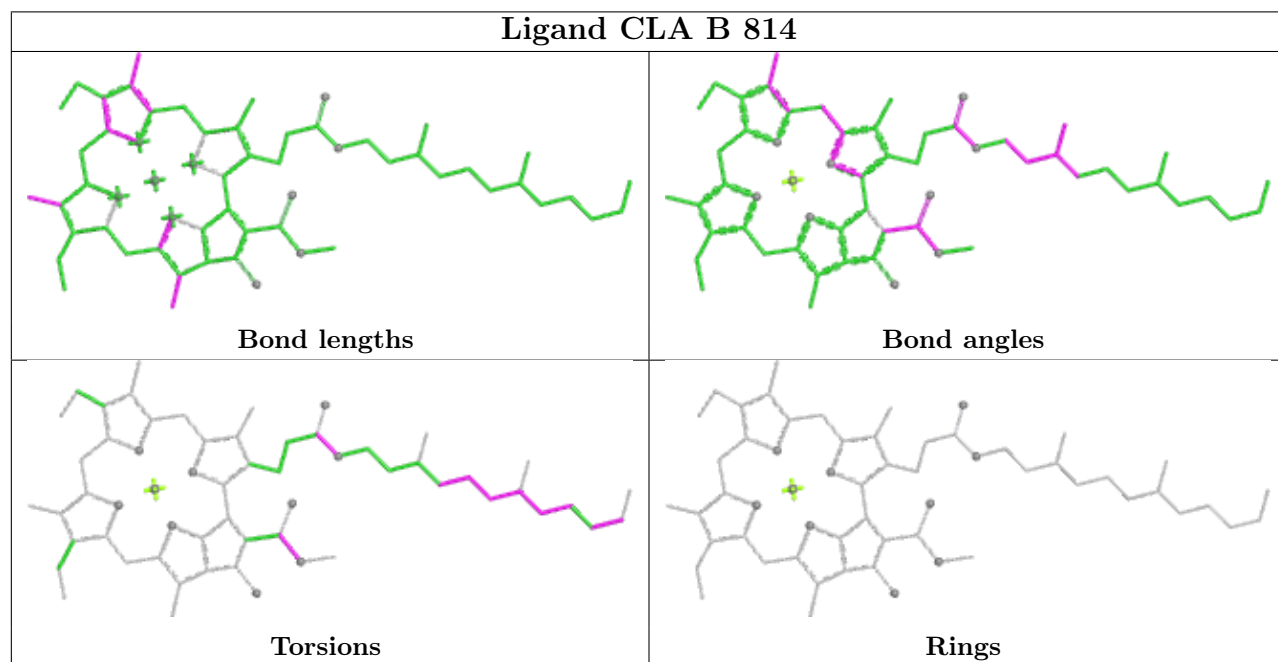


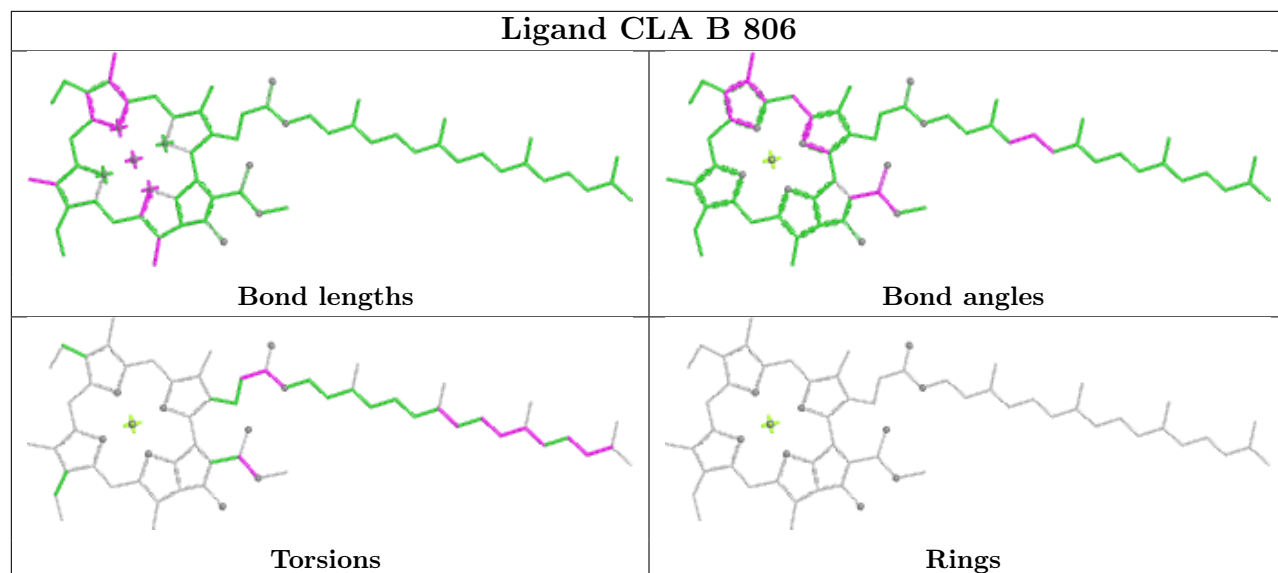
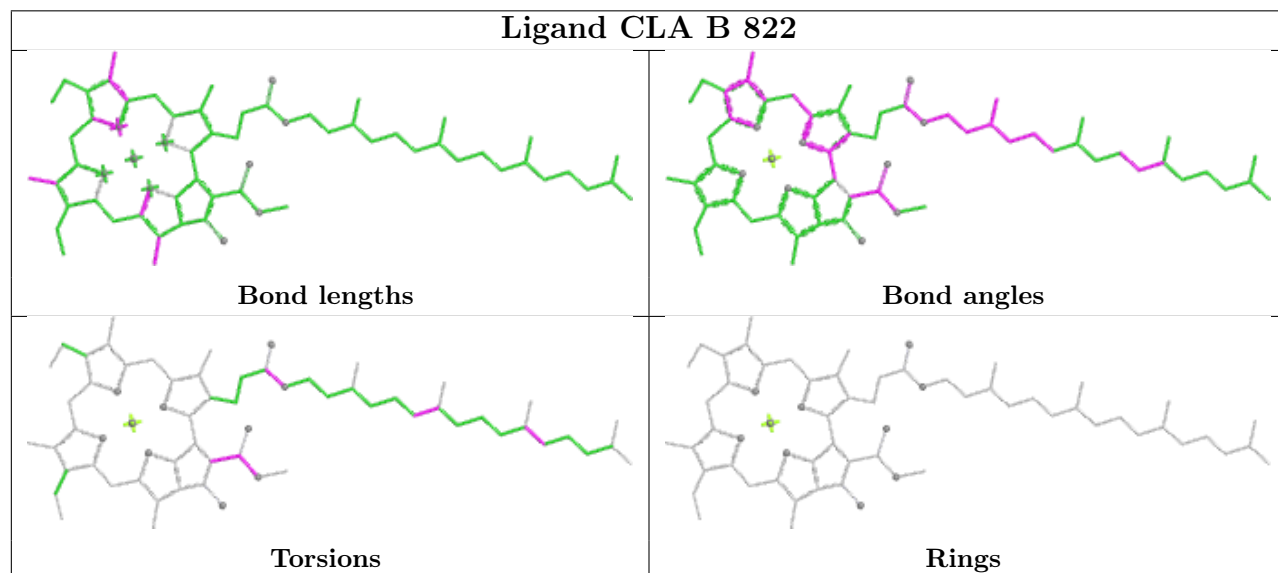
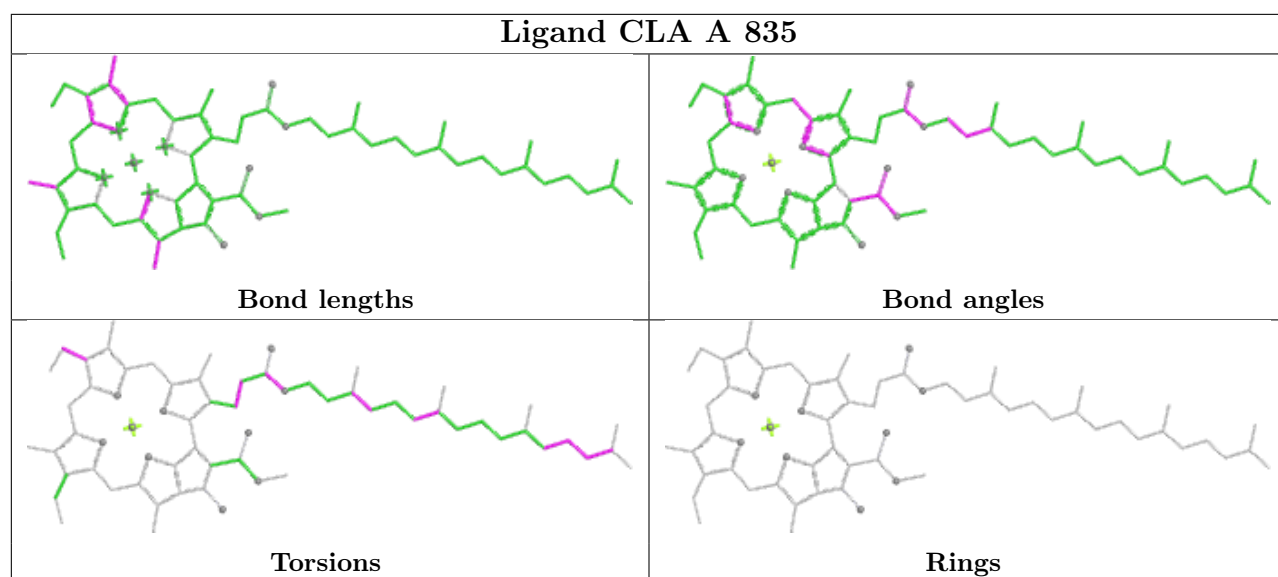


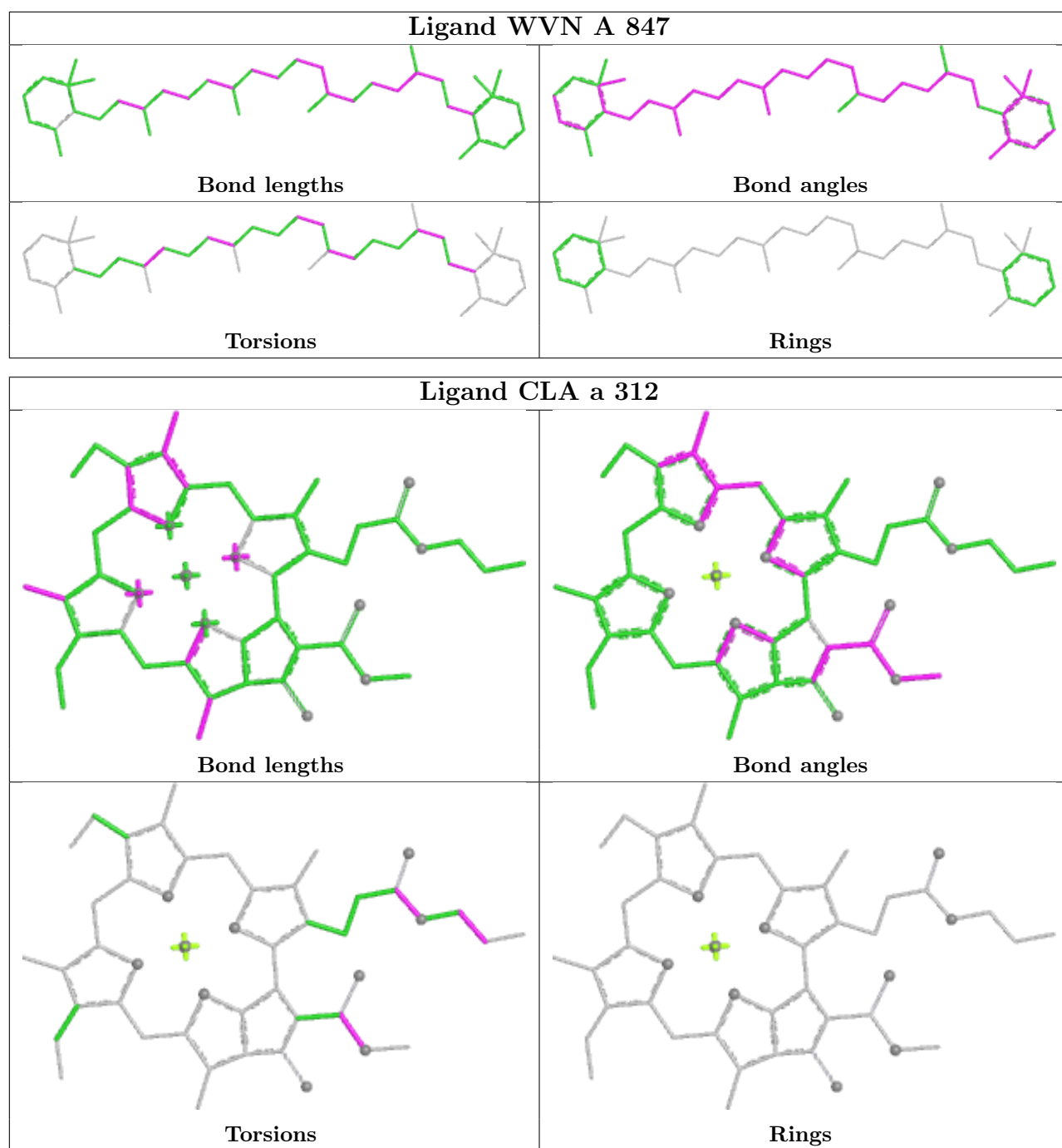
Ligand CLA i 607



Ligand CLA B 814







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.

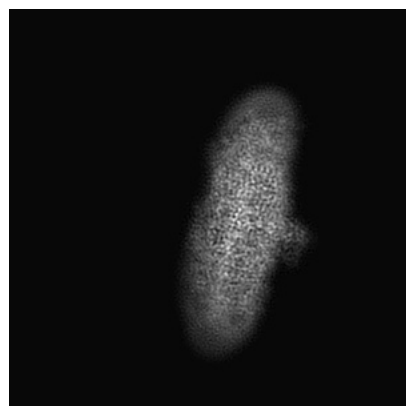
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37660. These allow visual inspection of the internal detail of the map and identification of artifacts.

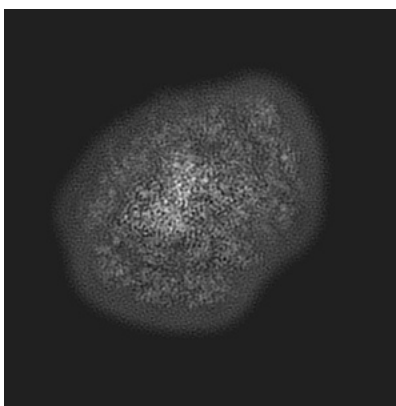
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

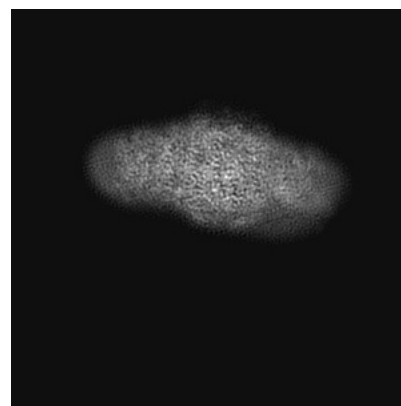
6.1.1 Primary map



X

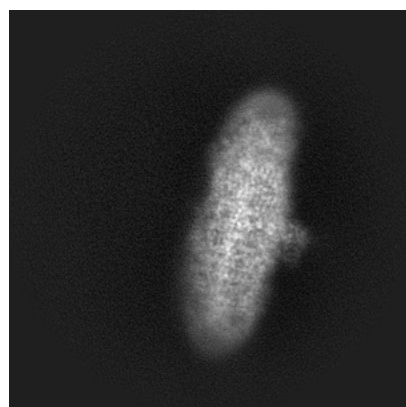


Y

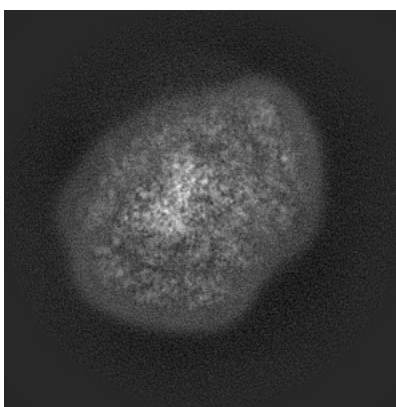


Z

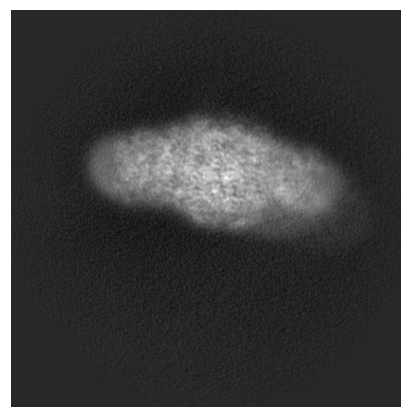
6.1.2 Raw map



X



Y

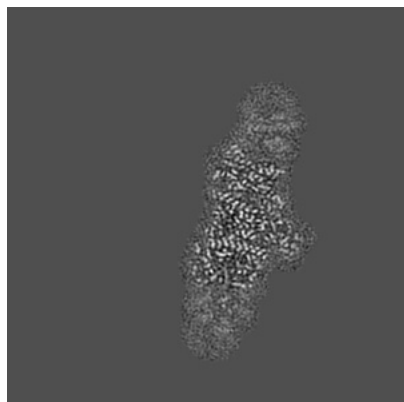


Z

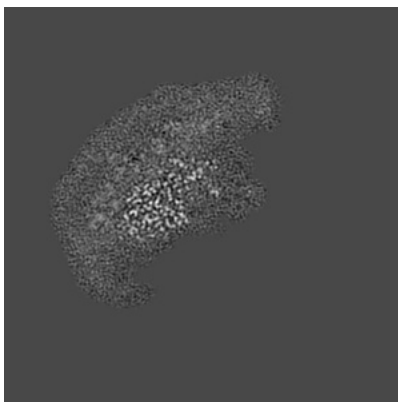
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

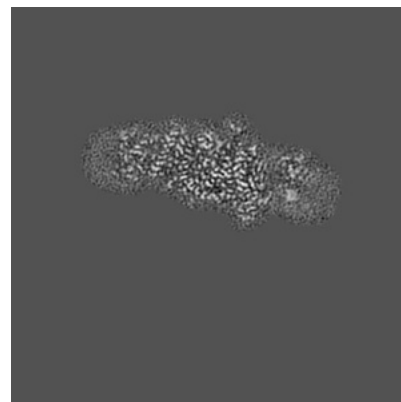
6.2.1 Primary map



X Index: 160

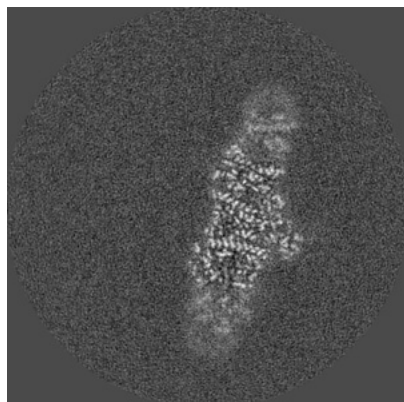


Y Index: 160

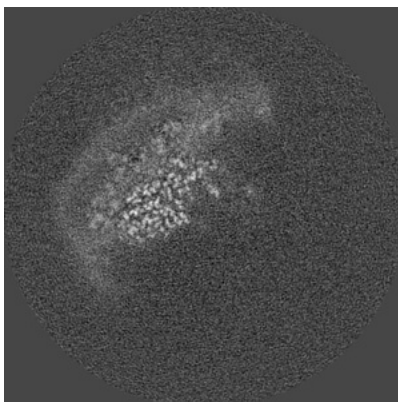


Z Index: 160

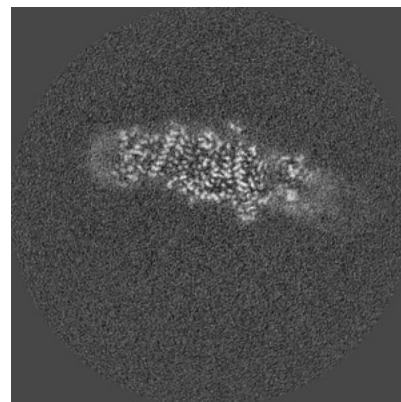
6.2.2 Raw map



X Index: 160



Y Index: 160

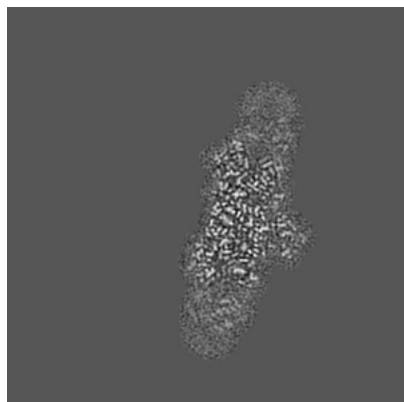


Z Index: 160

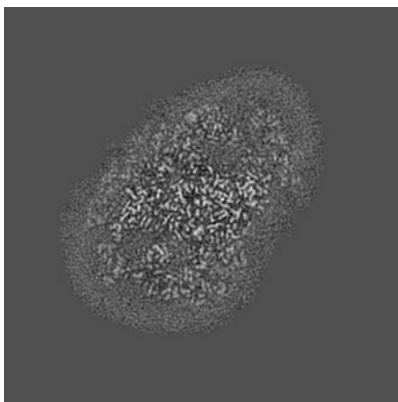
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

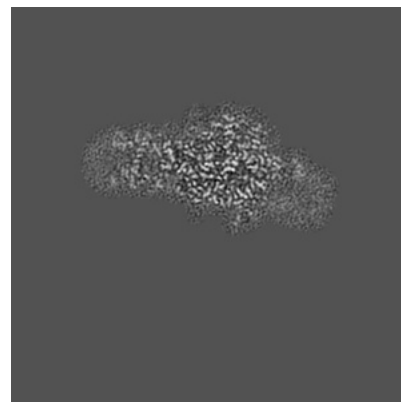
6.3.1 Primary map



X Index: 164

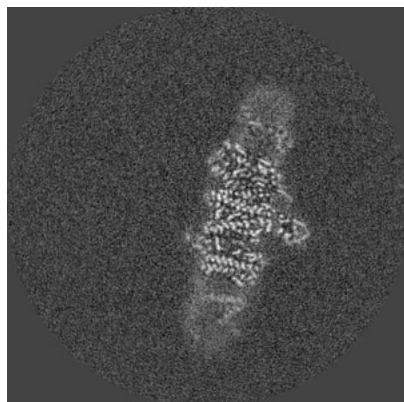


Y Index: 185

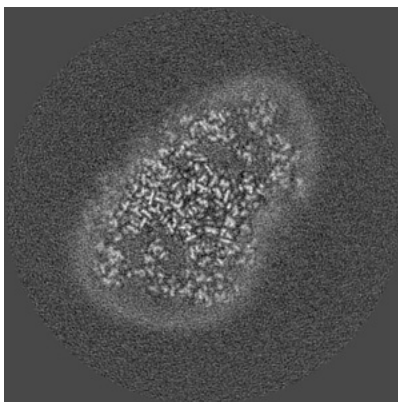


Z Index: 148

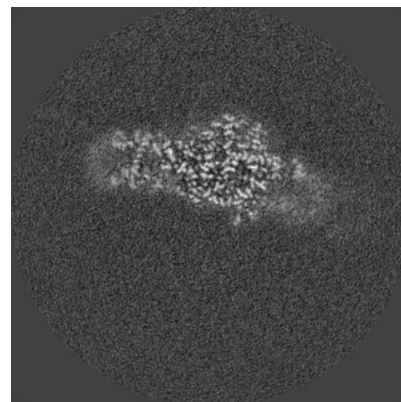
6.3.2 Raw map



X Index: 173



Y Index: 189

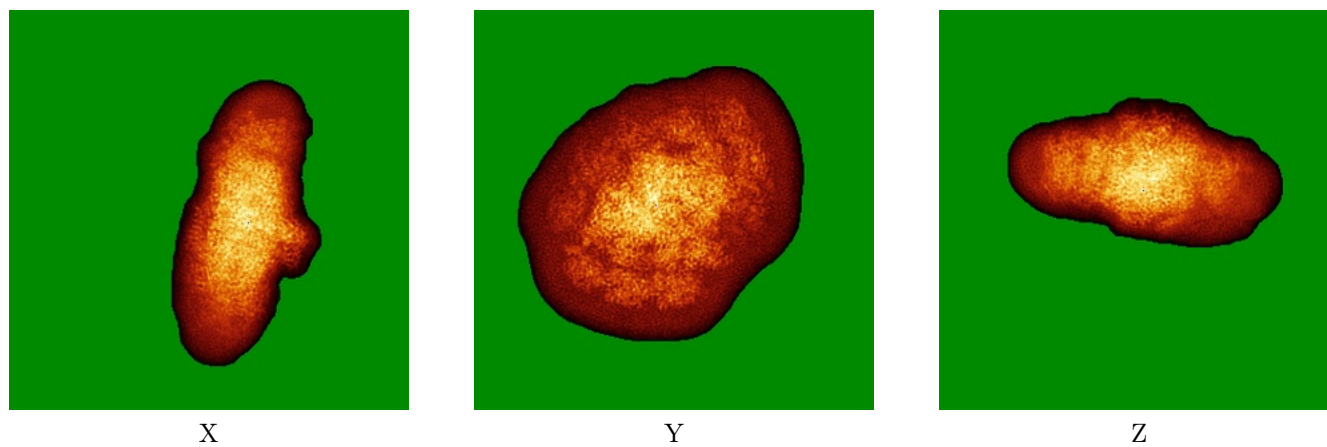


Z Index: 148

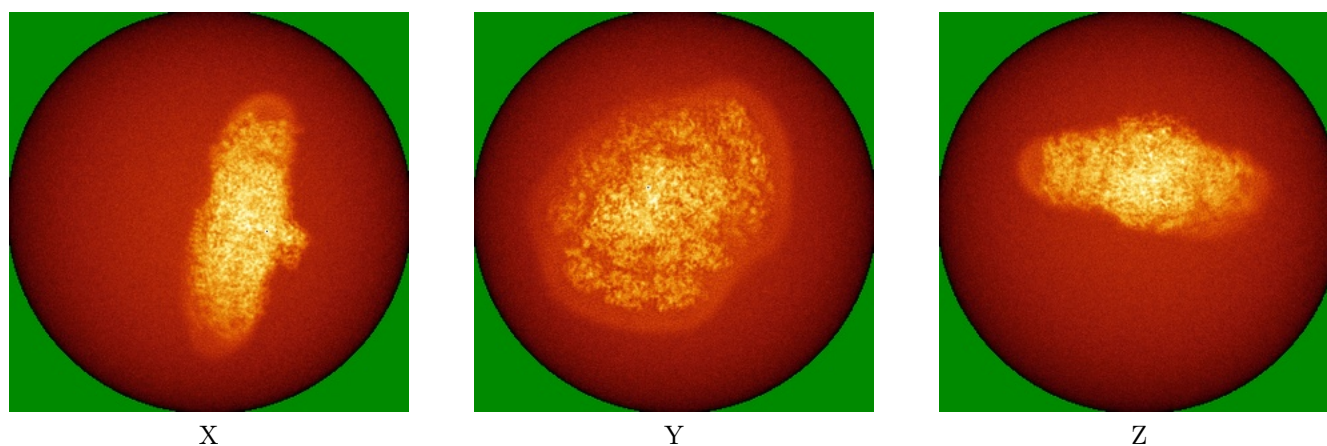
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

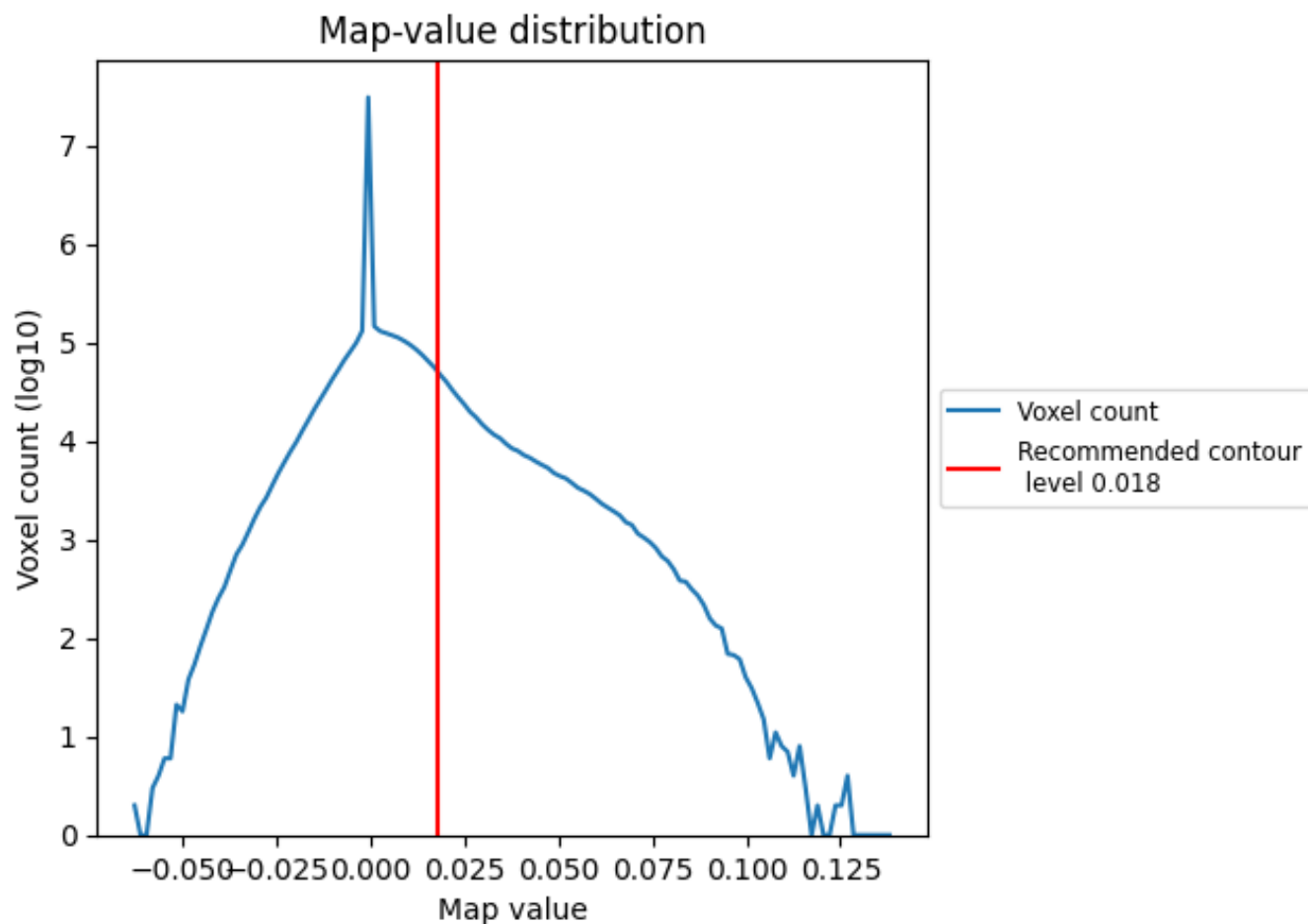
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

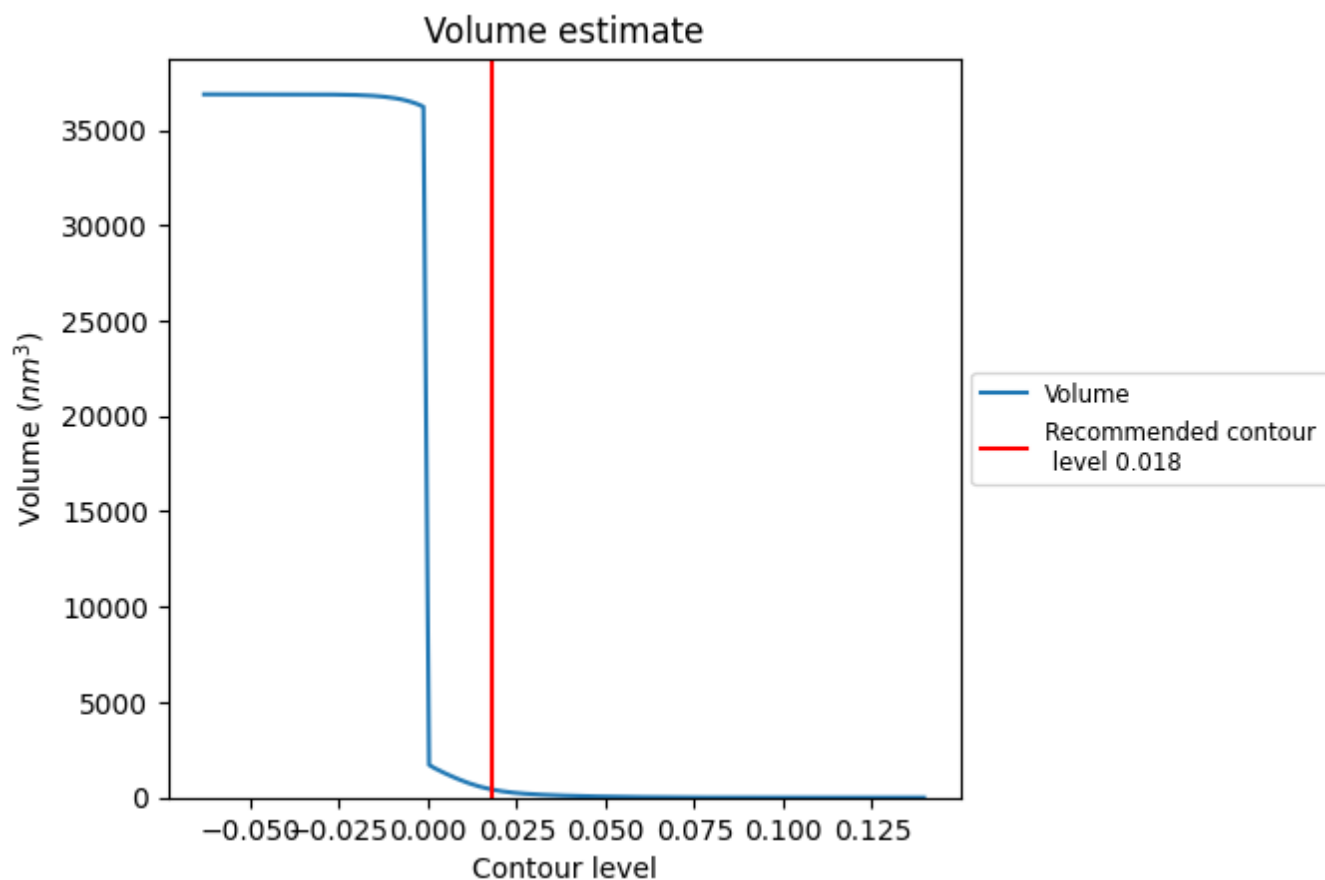
This section contains the results of statistical analysis of the map.

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.

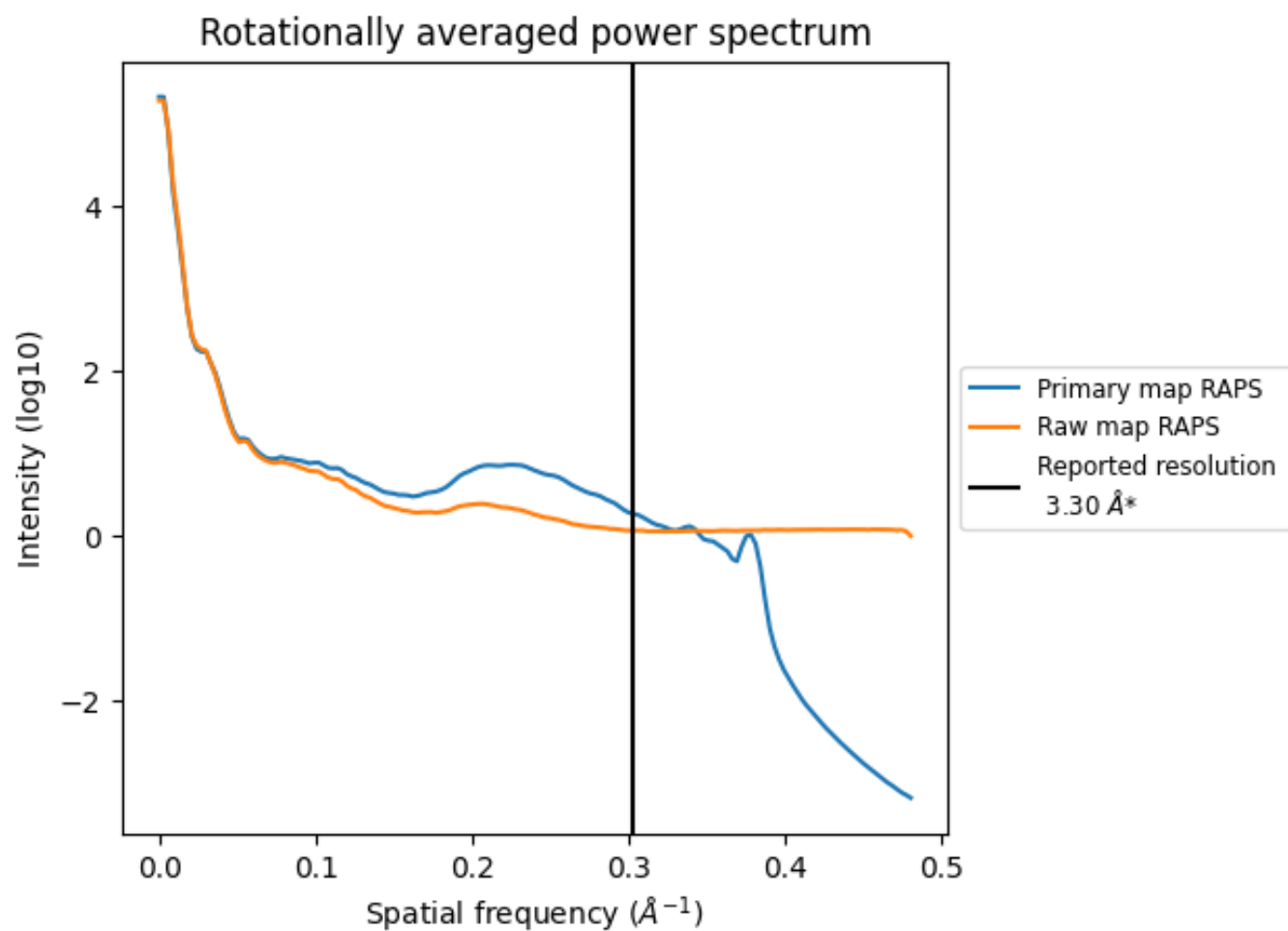
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm^3 ; this corresponds to an approximate mass of 384 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

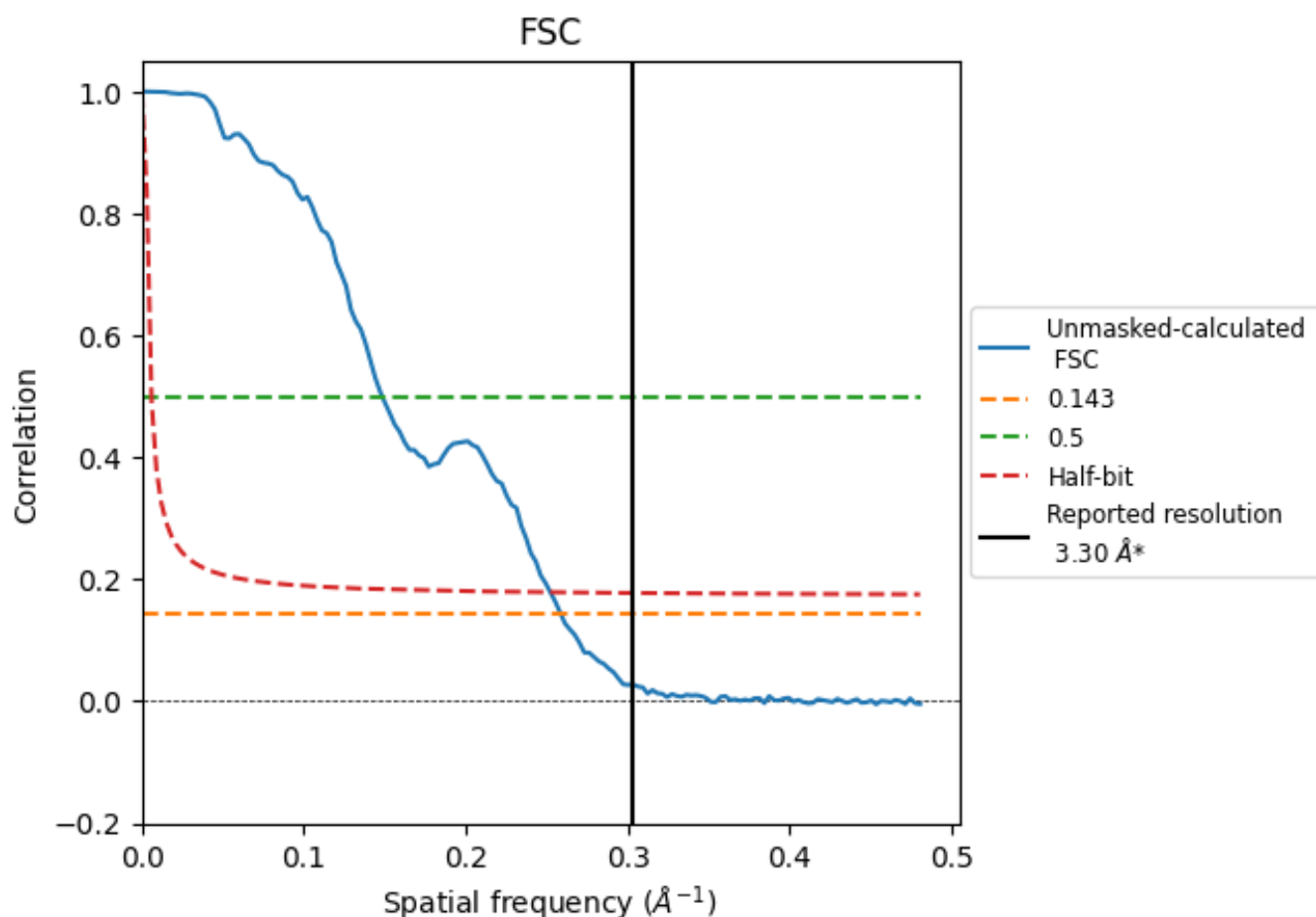


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

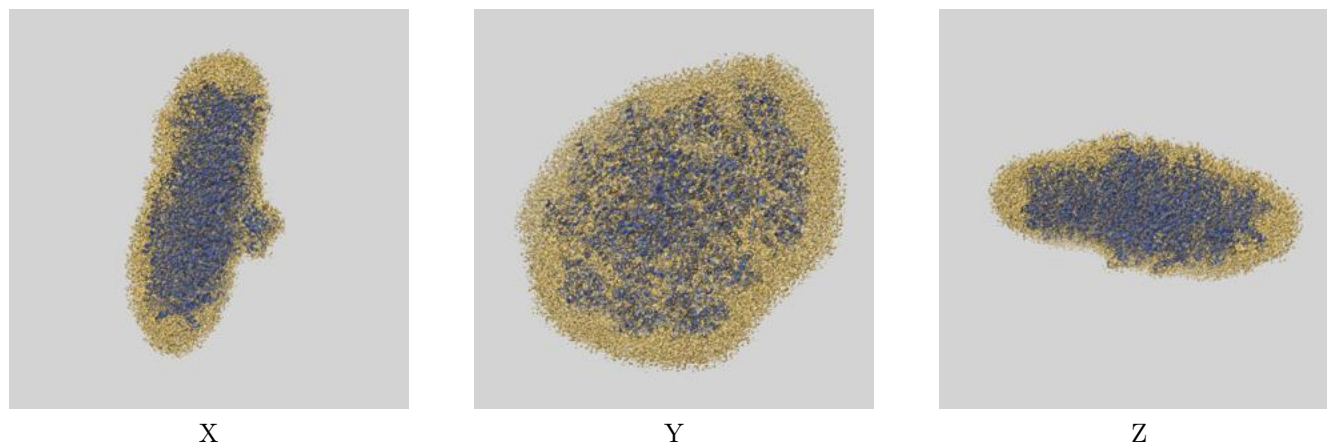
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.73	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

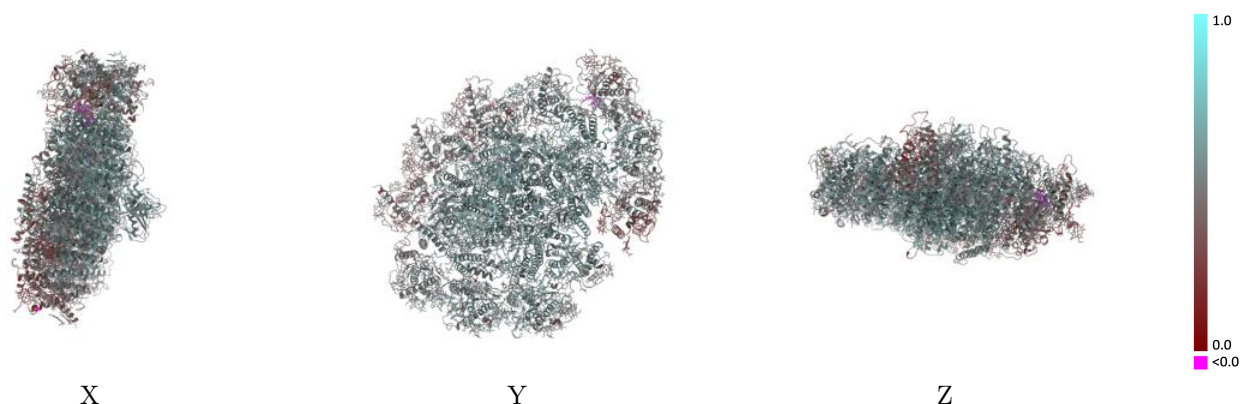
This section contains information regarding the fit between EMDB map EMD-37660 and PDB model 8WMW. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



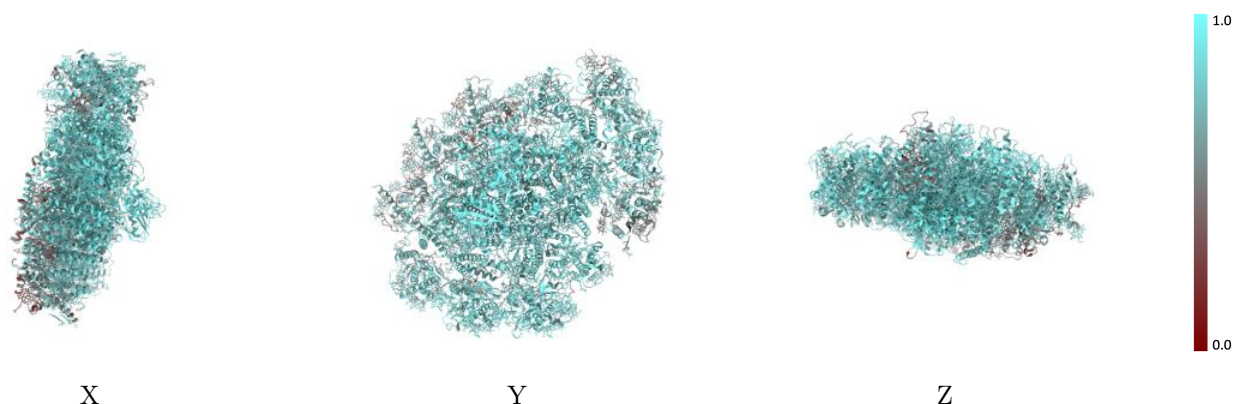
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



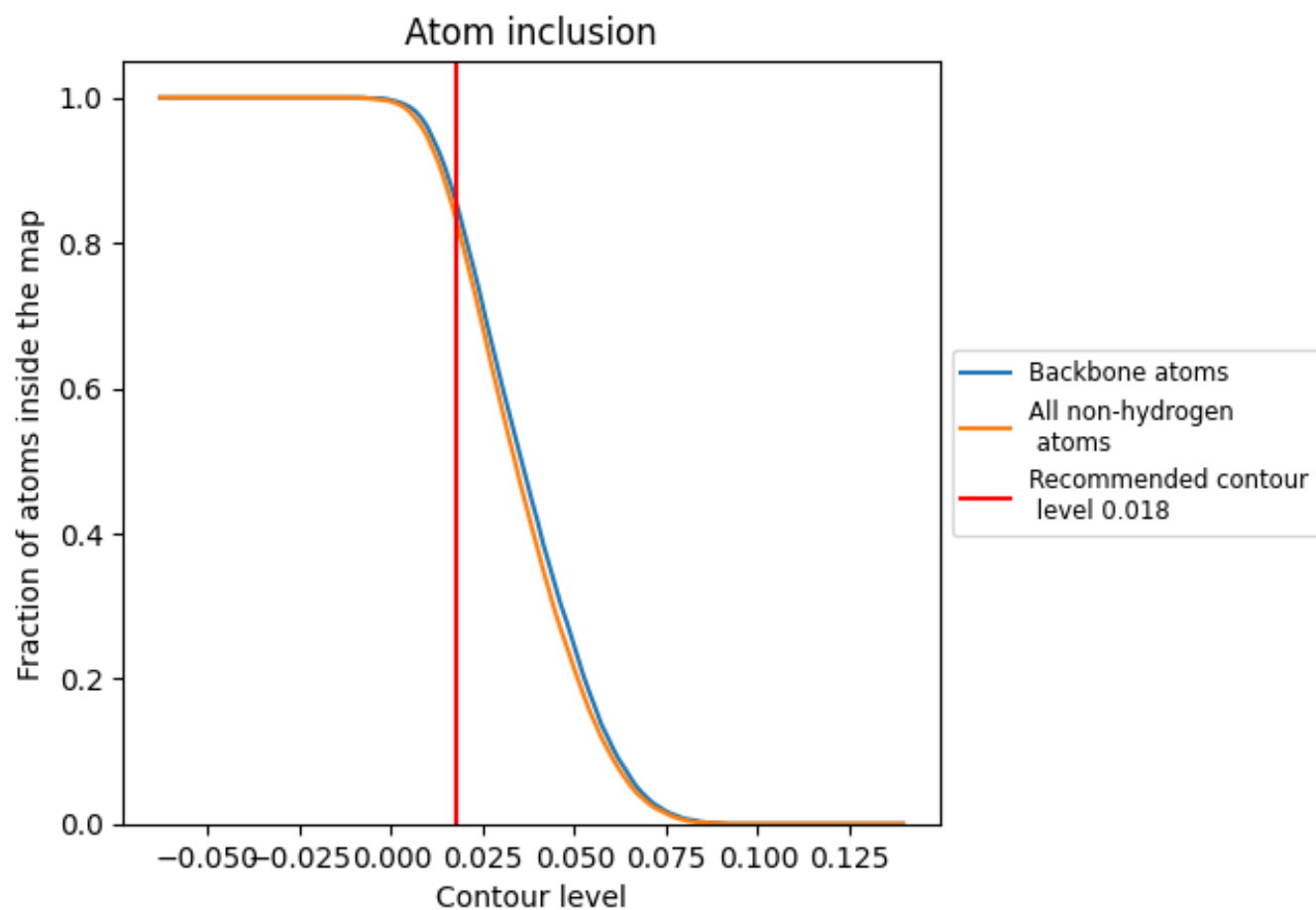
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5260
A	 0.9240	 0.5940
B	 0.9400	 0.6010
C	 0.9580	 0.5970
D	 0.8850	 0.5460
E	 0.8530	 0.5280
F	 0.8620	 0.5410
I	 0.9090	 0.5670
J	 0.7980	 0.5290
K	 0.8520	 0.5270
L	 0.8780	 0.5610
M	 0.8990	 0.5650
O	 0.8330	 0.5300
R	 0.8860	 0.5630
a	 0.7950	 0.4970
b	 0.6090	 0.4170
c	 0.6560	 0.4220
d	 0.6030	 0.3760
e	 0.7660	 0.4850
f	 0.8260	 0.5290
g	 0.8100	 0.5240
h	 0.8530	 0.5400
i	 0.6260	 0.3890
j	 0.8120	 0.5130
k	 0.7100	 0.4220

