



Full wwPDB EM Validation Report ⓘ

Nov 20, 2025 – 04:58 PM JST

PDB ID : 9L0K / pdb_00009l0k
EMDB ID : EMD-62717
Title : Cryo-EM structure of PSI-11ACPIs from Rhodomonas sp. NIES-2332 at 2.14 angstrom resolution
Authors : Zhang, W.Y.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-12
Resolution : 2.14 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:

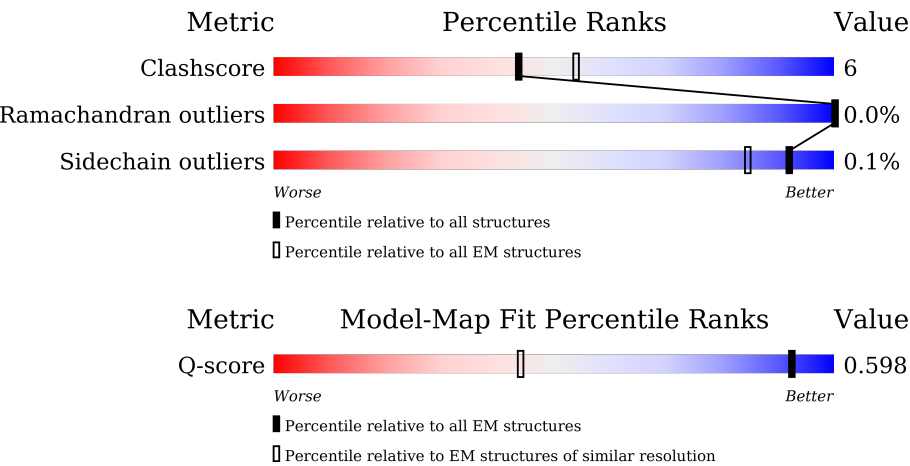
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.14 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.











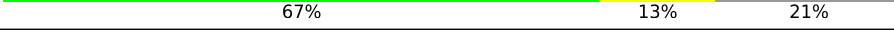
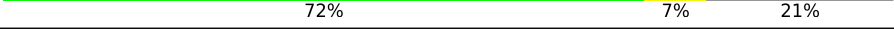
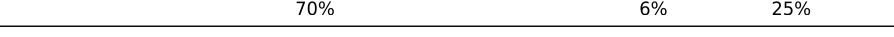

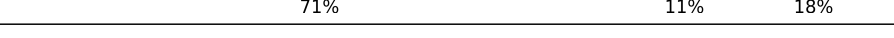
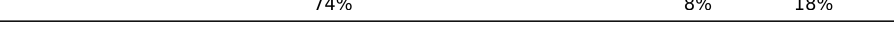
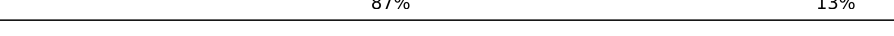


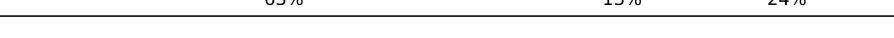
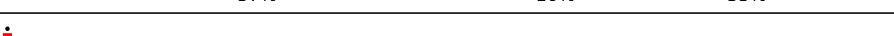


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2493 (1.66 - 2.64)

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	<div><div></div><div>84%</div><div>15%</div><div>.</div></div>
2	B	734	<div><div></div><div>85%</div><div>15%</div><div></div></div>
3	C	81	<div><div></div><div>85%</div><div>14%</div><div>.</div></div>
4	D	141	<div><div></div><div>91%</div><div>7%</div><div>.</div></div>

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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	K	87	
12	s	302	
13	c	215	
14	a	217	
15	b	236	
16	h	229	
17	j	212	
17	m	212	
18	l	175	
19	k	232	
20	i	200	
21	d	219	
22	R	135	
23	n	220	
24	Q	233	

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
25	CL0	A	801	X	-	-	-
26	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	A	803	X	-	-	-
26	CLA	A	804	X	-	-	-
26	CLA	A	805	X	-	-	-
26	CLA	A	806	X	-	-	-
26	CLA	A	807	X	-	-	-
26	CLA	A	808	X	-	-	-
26	CLA	A	809	X	-	-	-
26	CLA	A	810	X	-	-	-
26	CLA	A	811	X	-	-	-
26	CLA	A	812	X	-	-	-
26	CLA	A	813	X	-	-	-
26	CLA	A	814	X	-	-	-
26	CLA	A	815	X	-	-	-
26	CLA	A	816	X	-	-	-
26	CLA	A	817	X	-	-	-
26	CLA	A	818	X	-	-	-
26	CLA	A	819	X	-	-	-
26	CLA	A	820	X	-	-	-
26	CLA	A	821	X	-	-	-
26	CLA	A	822	X	-	-	-
26	CLA	A	823	X	-	-	-
26	CLA	A	824	X	-	-	-
26	CLA	A	825	X	-	-	-
26	CLA	A	826	X	-	-	-
26	CLA	A	827	X	-	-	-
26	CLA	A	828	X	-	-	-
26	CLA	A	829	X	-	-	-
26	CLA	A	830	X	-	-	-
26	CLA	A	831	X	-	-	-
26	CLA	A	832	X	-	-	-
26	CLA	A	833	X	-	-	-
26	CLA	A	834	X	-	-	-
26	CLA	A	835	X	-	-	-
26	CLA	A	836	X	-	-	-
26	CLA	A	837	X	-	-	-
26	CLA	A	838	X	-	-	-
26	CLA	A	839	X	-	-	-
26	CLA	A	840	X	-	-	-
26	CLA	A	841	X	-	-	-
26	CLA	A	851	X	-	-	-
26	CLA	A	852	X	-	-	-
26	CLA	A	856	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	801	X	-	-	-
26	CLA	B	802	X	-	-	-
26	CLA	B	803	X	-	-	-
26	CLA	B	804	X	-	-	-
26	CLA	B	805	X	-	-	-
26	CLA	B	806	X	-	-	-
26	CLA	B	807	X	-	-	-
26	CLA	B	808	X	-	-	-
26	CLA	B	809	X	-	-	-
26	CLA	B	810	X	-	-	-
26	CLA	B	811	X	-	-	-
26	CLA	B	812	X	-	-	-
26	CLA	B	813	X	-	-	-
26	CLA	B	814	X	-	-	-
26	CLA	B	815	X	-	-	-
26	CLA	B	816	X	-	-	-
26	CLA	B	817	X	-	-	-
26	CLA	B	818	X	-	-	-
26	CLA	B	819	X	-	-	-
26	CLA	B	820	X	-	-	-
26	CLA	B	821	X	-	-	-
26	CLA	B	822	X	-	-	-
26	CLA	B	823	X	-	-	-
26	CLA	B	824	X	-	-	-
26	CLA	B	825	X	-	-	-
26	CLA	B	826	X	-	-	-
26	CLA	B	827	X	-	-	-
26	CLA	B	828	X	-	-	-
26	CLA	B	829	X	-	-	-
26	CLA	B	830	X	-	-	-
26	CLA	B	831	X	-	-	-
26	CLA	B	832	X	-	-	-
26	CLA	B	833	X	-	-	-
26	CLA	B	834	X	-	-	-
26	CLA	B	836	X	-	-	-
26	CLA	B	837	X	-	-	-
26	CLA	B	838	X	-	-	-
26	CLA	B	839	X	-	-	-
26	CLA	B	840	X	-	-	-
26	CLA	B	841	X	-	-	-
26	CLA	B	842	X	-	-	-
26	CLA	F	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	F	202	X	-	-	-
26	CLA	J	103	X	-	-	-
26	CLA	K	101	X	-	-	-
26	CLA	L	202	X	-	-	-
26	CLA	L	203	X	-	-	-
26	CLA	L	204	X	-	-	-
26	CLA	L	206	X	-	-	-
26	CLA	Q	302	X	-	-	-
26	CLA	R	201	X	-	-	-
26	CLA	a	301	X	-	-	-
26	CLA	a	302	X	-	-	-
26	CLA	a	303	X	-	-	-
26	CLA	a	304	X	-	-	-
26	CLA	a	305	X	-	-	-
26	CLA	a	306	X	-	-	-
26	CLA	a	307	X	-	-	-
26	CLA	a	308	X	-	-	-
26	CLA	a	309	X	-	-	-
26	CLA	a	311	X	-	-	-
26	CLA	b	303	X	-	-	-
26	CLA	b	304	X	-	-	-
26	CLA	b	305	X	-	-	-
26	CLA	b	306	X	-	-	-
26	CLA	b	307	X	-	-	-
26	CLA	b	308	X	-	-	-
26	CLA	b	309	X	-	-	-
26	CLA	b	310	X	-	-	-
26	CLA	b	311	X	-	-	-
26	CLA	b	312	X	-	-	-
26	CLA	b	313	X	-	-	-
26	CLA	c	301	X	-	-	-
26	CLA	c	303	X	-	-	-
26	CLA	c	304	X	-	-	-
26	CLA	c	305	X	-	-	-
26	CLA	c	306	X	-	-	-
26	CLA	c	307	X	-	-	-
26	CLA	c	308	X	-	-	-
26	CLA	c	311	X	-	-	-
26	CLA	c	312	X	-	-	-
26	CLA	d	302	X	-	-	-
26	CLA	d	303	X	-	-	-
26	CLA	d	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	d	305	X	-	-	-
26	CLA	d	306	X	-	-	-
26	CLA	d	307	X	-	-	-
26	CLA	d	308	X	-	-	-
26	CLA	d	309	X	-	-	-
26	CLA	d	310	X	-	-	-
26	CLA	d	313	X	-	-	-
26	CLA	d	318	X	-	-	-
26	CLA	h	301	X	-	-	-
26	CLA	h	302	X	-	-	-
26	CLA	h	303	X	-	-	-
26	CLA	h	304	X	-	-	-
26	CLA	h	305	X	-	-	-
26	CLA	h	306	X	-	-	-
26	CLA	h	307	X	-	-	-
26	CLA	h	308	X	-	-	-
26	CLA	h	313	X	-	-	-
26	CLA	i	301	X	-	-	-
26	CLA	i	302	X	-	-	-
26	CLA	i	303	X	-	-	-
26	CLA	i	304	X	-	-	-
26	CLA	i	305	X	-	-	-
26	CLA	i	306	X	-	-	-
26	CLA	i	307	X	-	-	-
26	CLA	i	308	X	-	-	-
26	CLA	i	310	X	-	-	-
26	CLA	i	311	X	-	-	-
26	CLA	j	601	X	-	-	-
26	CLA	j	602	X	-	-	-
26	CLA	j	603	X	-	-	-
26	CLA	j	604	X	-	-	-
26	CLA	j	605	X	-	-	-
26	CLA	j	606	X	-	-	-
26	CLA	j	607	X	-	-	-
26	CLA	j	608	X	-	-	-
26	CLA	j	609	X	-	-	-
26	CLA	j	610	X	-	-	-
26	CLA	j	612	X	-	-	-
26	CLA	j	613	X	-	-	-
26	CLA	k	601	X	-	-	-
26	CLA	k	602	X	-	-	-
26	CLA	k	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	k	605	X	-	-	-
26	CLA	k	606	X	-	-	-
26	CLA	k	607	X	-	-	-
26	CLA	k	608	X	-	-	-
26	CLA	k	609	X	-	-	-
26	CLA	k	610	X	-	-	-
26	CLA	k	614	X	-	-	-
26	CLA	l	301	X	-	-	-
26	CLA	l	304	X	-	-	-
26	CLA	l	305	X	-	-	-
26	CLA	l	306	X	-	-	-
26	CLA	l	307	X	-	-	-
26	CLA	l	308	X	-	-	-
26	CLA	l	309	X	-	-	-
26	CLA	l	310	X	-	-	-
26	CLA	l	311	X	-	-	-
26	CLA	l	313	X	-	-	-
26	CLA	m	601	X	-	-	-
26	CLA	m	602	X	-	-	-
26	CLA	m	603	X	-	-	-
26	CLA	m	604	X	-	-	-
26	CLA	m	605	X	-	-	-
26	CLA	m	606	X	-	-	-
26	CLA	m	607	X	-	-	-
26	CLA	m	608	X	-	-	-
26	CLA	m	609	X	-	-	-
26	CLA	m	610	X	-	-	-
26	CLA	m	612	X	-	-	-
26	CLA	m	613	X	-	-	-
26	CLA	n	601	X	-	-	-
26	CLA	n	602	X	-	-	-
26	CLA	n	603	X	-	-	-
26	CLA	n	604	X	-	-	-
26	CLA	n	605	X	-	-	-
26	CLA	n	607	X	-	-	-
26	CLA	n	608	X	-	-	-
26	CLA	n	609	X	-	-	-
26	CLA	n	610	X	-	-	-
26	CLA	n	613	X	-	-	-
26	CLA	s	402	X	-	-	-
26	CLA	s	403	X	-	-	-
26	CLA	s	406	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	s	408	X	-	-	-
29	WVN	A	845	-	X	-	-
29	WVN	A	846	-	X	-	-
29	WVN	A	847	-	X	-	-
29	WVN	A	848	-	X	-	-
29	WVN	A	857	-	X	-	-
29	WVN	B	846	-	X	-	-
29	WVN	B	847	-	X	-	-
29	WVN	B	848	-	X	-	-
29	WVN	B	849	-	X	-	-
29	WVN	B	850	-	X	-	-
29	WVN	B	853	-	X	-	-
29	WVN	F	203	-	X	-	-
29	WVN	I	101	-	X	-	-
29	WVN	J	101	-	X	-	-
29	WVN	J	102	-	X	-	-
29	WVN	K	102	-	X	-	-
29	WVN	L	201	-	X	-	-
29	WVN	L	205	-	X	-	-
29	WVN	M	101	-	X	-	-
29	WVN	R	200	-	X	-	-
29	WVN	h	309	-	X	-	-
29	WVN	i	315	-	X	-	-
29	WVN	l	303	-	X	-	-
29	WVN	l	316	-	X	-	-
29	WVN	s	407	-	X	-	-
35	II0	h	310	-	X	-	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 53701 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
			5826	3805	994	999	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	2	0
			5832	3849	982	987	14		

- 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	138	Total	C	N	O	S	0	0
			1075	687	185	200	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
			484	309	84	91		

- 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
			1257	818	213	224	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	33	Total	C	N	O	S	0	0
			255	177	34	42	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	1	0
			1158	763	183	209	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 Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	68	Total	C	N	O	S	0	0
			482	316	79	85	2		

- Molecule 12 is a protein called ACPI-s.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	s	154	Total	C	N	O	S	0	0
			1146	725	195	219	7		

- Molecule 13 is a protein called ACPI-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	170	Total	C	N	O	S	0	0
			1362	899	222	238	3		

- Molecule 14 is a protein called ACPI-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	172	Total	C	N	O	S	0	0
			1331	865	213	242	11		

- Molecule 15 is a protein called ACPI-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	178	Total	C	N	O	S	0	0
			1332	847	234	238	13		

- Molecule 16 is a protein called ACPI-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	162	Total	C	N	O	S	0	0
			1201	779	202	214	6		

- Molecule 17 is a protein called ACPI-m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	m	174	Total	C	N	O	S	0	0
			1313	850	217	238	8		
17	j	173	Total	C	N	O	S	0	0
			1302	841	216	237	8		

- Molecule 18 is a protein called ACPI-l.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	175	Total	C	N	O	S	0	0
			1333	859	227	239	8		

- Molecule 19 is a protein called ACPI-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	189	Total	C	N	O	S	0	0
			1412	916	241	246	9		

- Molecule 20 is a protein called ACPI-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	180	Total	C	N	O	S	0	0
			1363	874	231	247	11		

- Molecule 21 is a protein called ACPI-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	166	Total	C	N	O	S	0	0
			1231	788	210	220	13		

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	90	Total	C	N	O	S	0	0
			666	434	105	125	2		

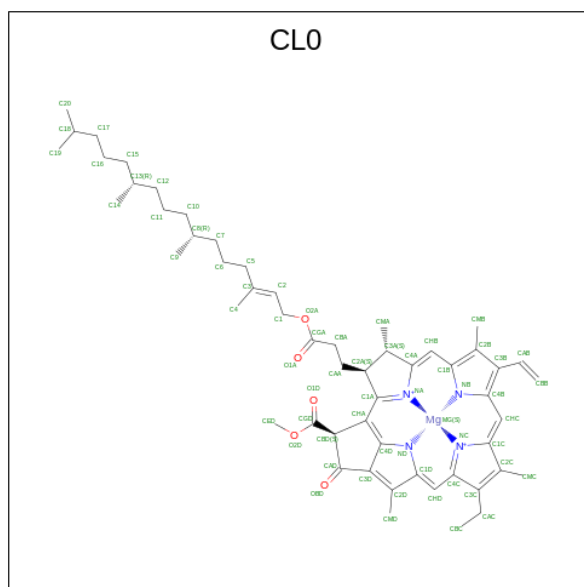
- Molecule 23 is a protein called ACPI-n.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	n	181	Total	C	N	O	S	0	0
			1343	862	226	245	10		

- Molecule 24 is a protein called PsaQ.

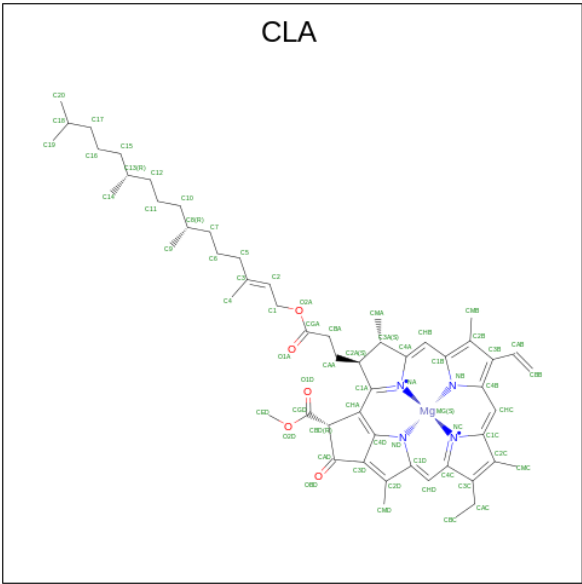
Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	143	Total	C	N	O	S	0	0
			1041	654	179	203	5		

- Molecule 25 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	c	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	h	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	m	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	l	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	l	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	k	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	i	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 46	C 36	Mg 1	N 4	O 5	0

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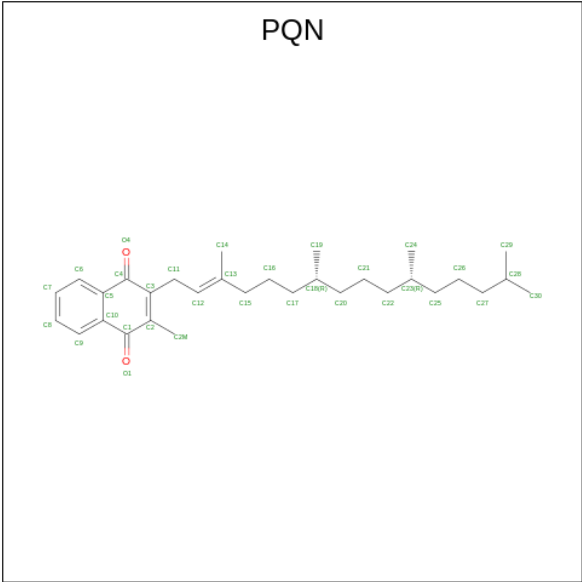
Mol	Chain	Residues	Atoms					AltConf
26	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	d	1	Total 46	C 36	Mg 1	N 4	O 5	0

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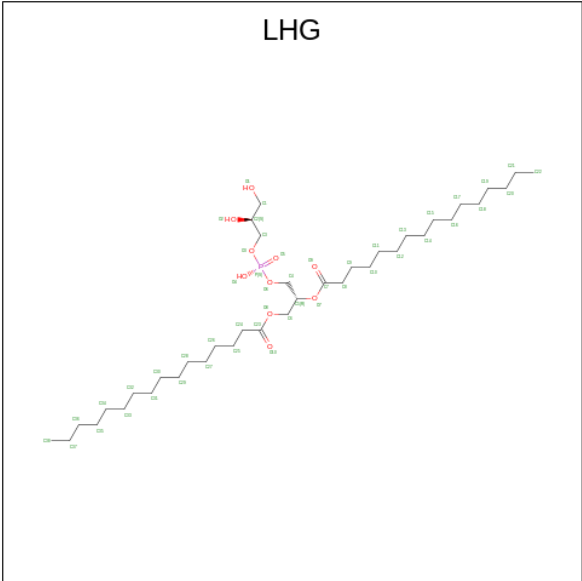
Mol	Chain	Residues	Atoms					AltConf
26	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



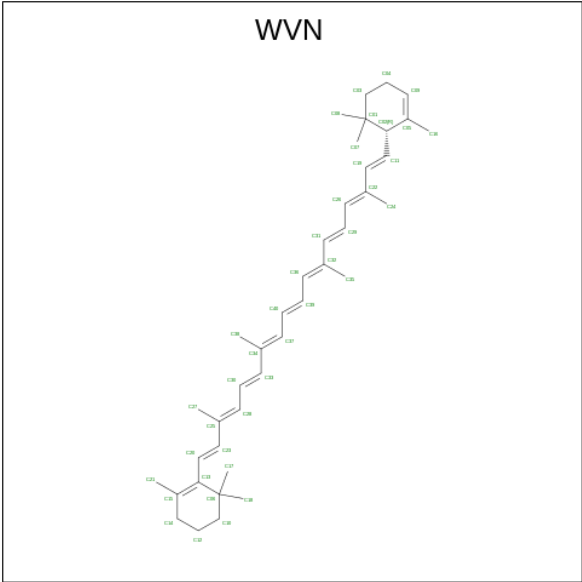
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	37	10	1	

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Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			27	16	10	1	
28	A	1	Total	C	O	P	0
			27	20	6	1	
28	A	1	Total	C	O	P	0
			36	25	10	1	
28	B	1	Total	C	O	P	0
			49	38	10	1	
28	J	1	Total	C	O	P	0
			33	22	10	1	
28	L	1	Total	C	O	P	0
			47	36	10	1	
28	L	1	Total	C	O	P	0
			45	34	10	1	
28	s	1	Total	C	O	P	0
			33	24	8	1	
28	c	1	Total	C	O	P	0
			37	26	10	1	
28	c	1	Total	C	O	P	0
			49	38	10	1	
28	b	1	Total	C	O	P	0
			49	38	10	1	
28	b	1	Total	C	O	P	0
			49	38	10	1	
28	m	1	Total	C	O	P	0
			37	26	10	1	
28	l	1	Total	C	O	P	0
			32	21	10	1	
28	i	1	Total	C	O	P	0
			37	26	10	1	
28	j	1	Total	C	O	P	0
			30	19	10	1	
28	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 29 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) (labeled as "Ligand of Interest" by depositor).



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

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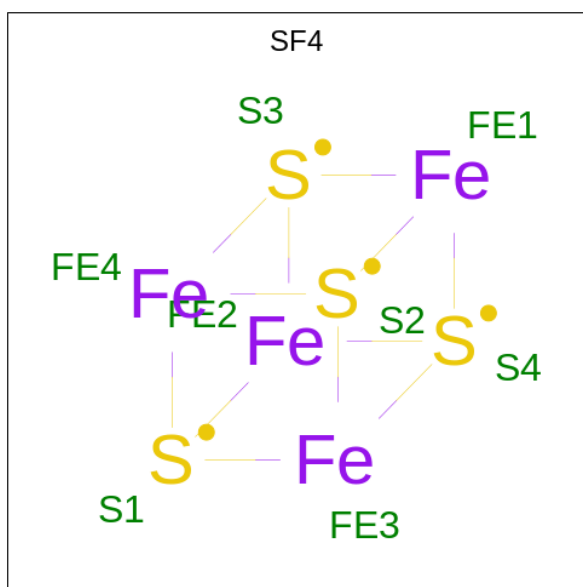
Mol	Chain	Residues	Atoms	AltConf
29	I	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	M	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	s	1	Total C 40 40	0
29	s	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	i	1	Total C 40 40	0
29	R	1	Total C 40 40	0

- Molecule 30 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



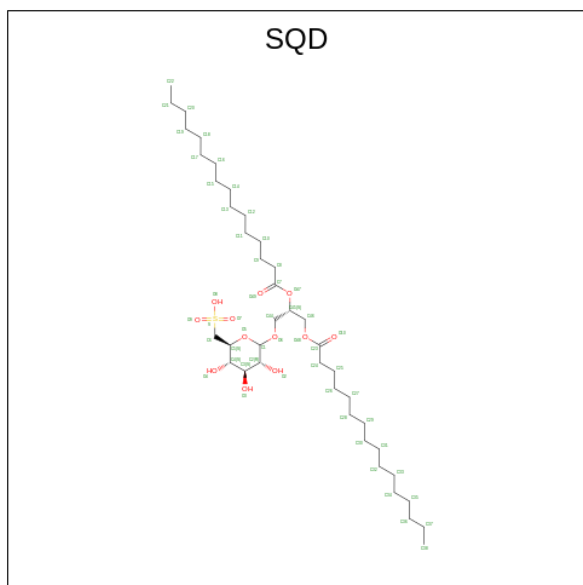
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total 35	C 24	O 11	0
30	A	1	Total 34	C 23	O 11	0
30	B	1	Total 35	C 24	O 11	0
30	a	1	Total 35	C 24	O 11	0
30	i	1	Total 35	C 24	O 11	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



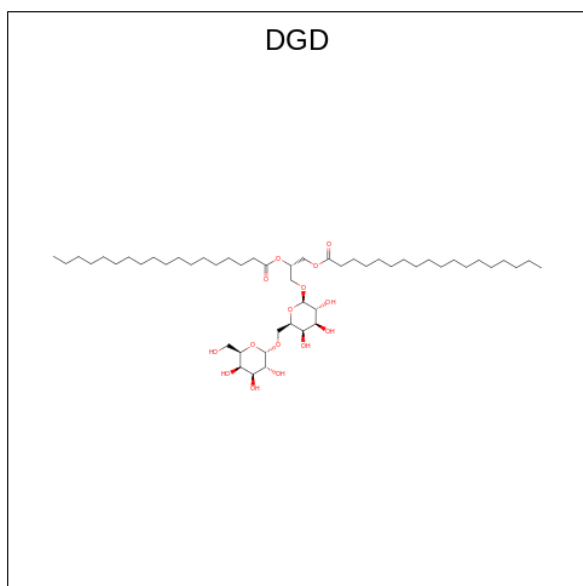
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



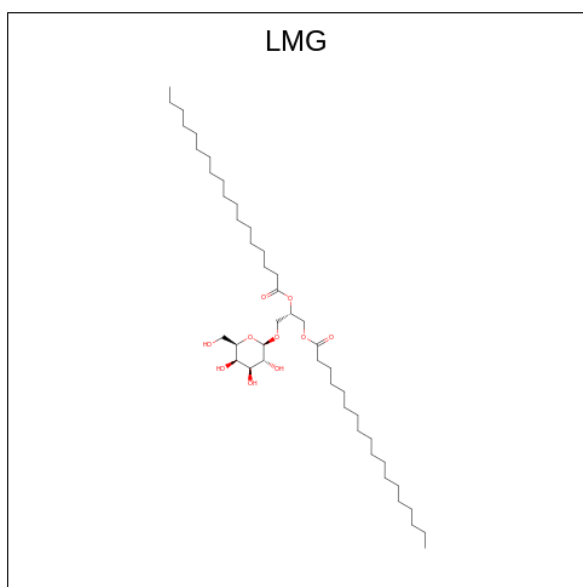
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



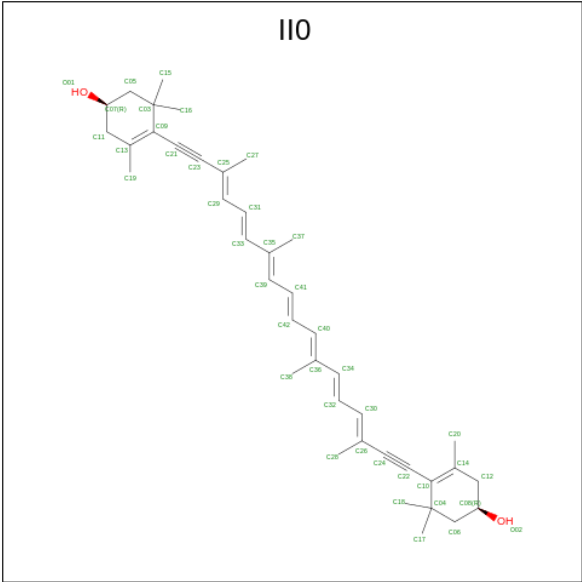
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O		0
			66	51	15		
33	j	1	Total	C	O		0
			62	47	15		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total	C	O	0
			53	43	10	
34	F	1	Total	C	O	0
			41	31	10	
34	L	1	Total	C	O	0
			45	35	10	
34	c	1	Total	C	O	0
			55	45	10	
34	c	1	Total	C	O	0
			43	33	10	
34	b	1	Total	C	O	0
			42	32	10	
34	n	1	Total	C	O	0
			51	41	10	
34	Q	1	Total	C	O	0
			38	28	10	

- Molecule 35 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
35	J	1	Total	C	O	0
			42	40	2	
35	c	1	Total	C	O	0
			42	40	2	
35	c	1	Total	C	O	0
			42	40	2	
35	c	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	
35	h	1	Total	C	O	0
			28	27	1	
35	h	1	Total	C	O	0
			42	40	2	
35	h	1	Total	C	O	0
			42	40	2	

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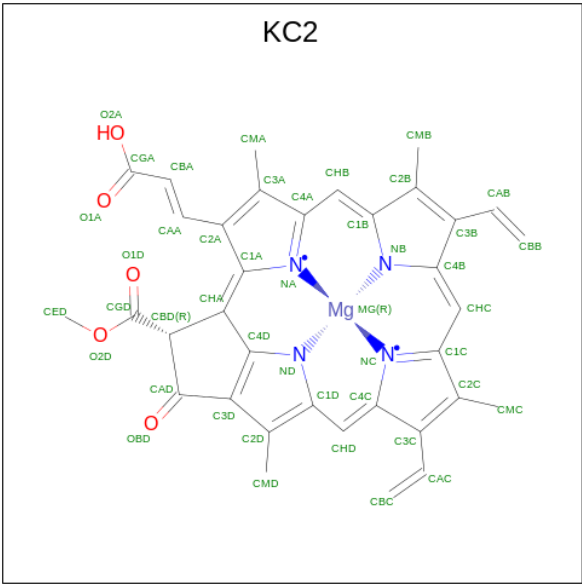
Mol	Chain	Residues	Atoms			AltConf
35	m	1	Total 42	C 40	O 2	0
35	m	1	Total 42	C 40	O 2	0
35	m	1	Total 42	C 40	O 2	0
35	m	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	j	1	Total 42	C 40	O 2	0
35	j	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
35	d	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
35	d	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
35	d	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
35	n	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
35	n	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
35	n	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	

- Molecule 36 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



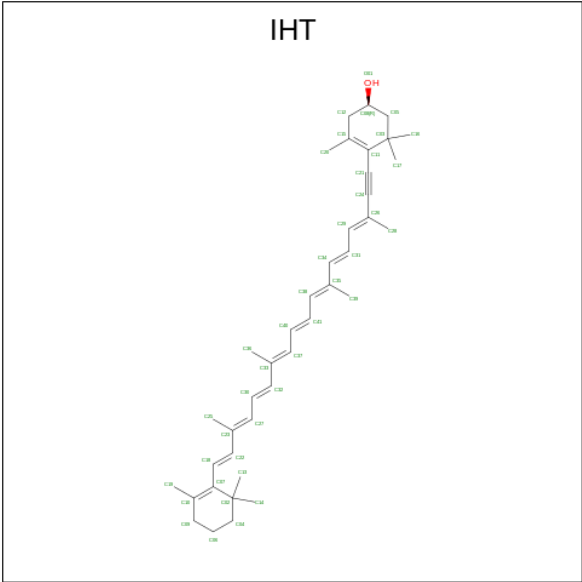
Mol	Chain	Residues	Atoms					AltConf
36	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 37 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) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	c	1	Total	C	O	0
			41	40	1	
37	a	1	Total	C	O	0
			41	40	1	
37	b	1	Total	C	O	0
			41	40	1	
37	b	1	Total	C	O	0
			41	40	1	
37	m	1	Total	C	O	0
			41	40	1	
37	j	1	Total	C	O	0
			41	40	1	
37	R	1	Total	C	O	0
			41	40	1	
37	n	1	Total	C	O	0
			41	40	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	130	Total	O	0
			130	130	
38	B	147	Total	O	0
			147	147	
38	C	25	Total	O	0
			25	25	
38	D	15	Total	O	0
			15	15	

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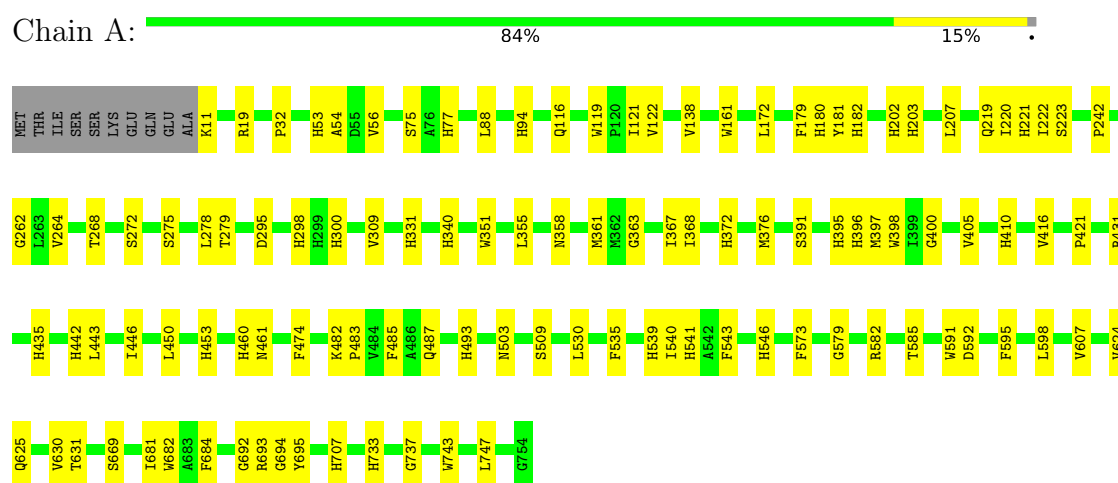
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Mol	Chain	Residues	Atoms		AltConf
38	E	6	Total 6	O 6	0
38	F	15	Total 15	O 15	0
38	J	2	Total 2	O 2	0
38	L	12	Total 12	O 12	0
38	M	2	Total 2	O 2	0
38	s	10	Total 10	O 10	0
38	c	2	Total 2	O 2	0
38	a	16	Total 16	O 16	0
38	b	18	Total 18	O 18	0
38	h	9	Total 9	O 9	0
38	m	1	Total 1	O 1	0
38	R	1	Total 1	O 1	0

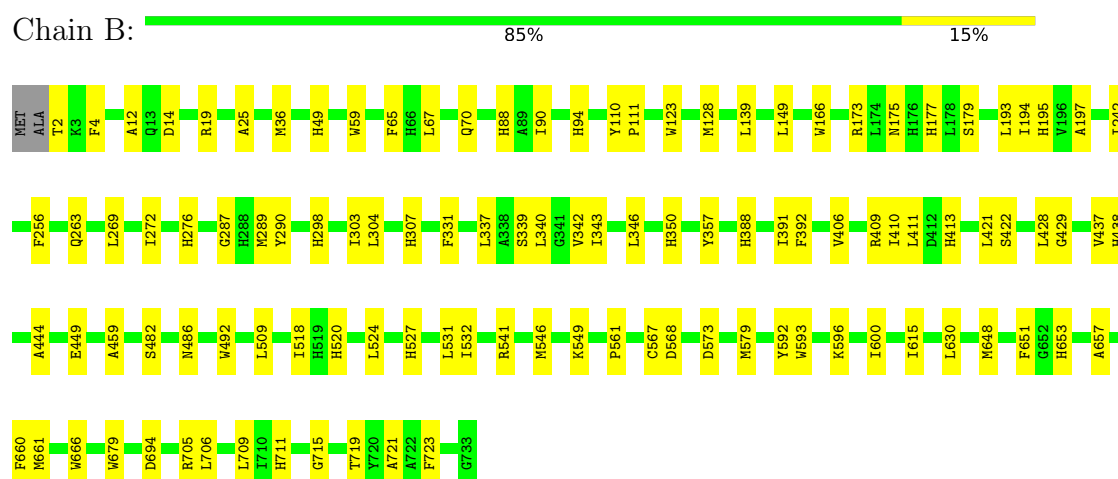
3 Residue-property plots

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.

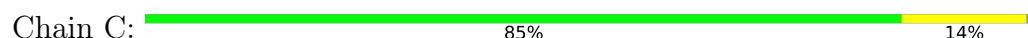
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- 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: 91% 7% •



- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 92% • 6%



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 75% 11% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 81% 11% 8%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 88% 12%




- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 6% 90% 8% ••



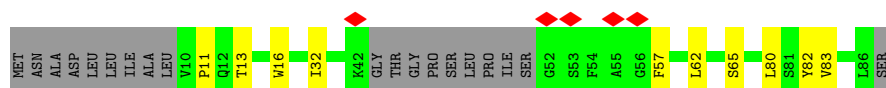
- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  87% 13%



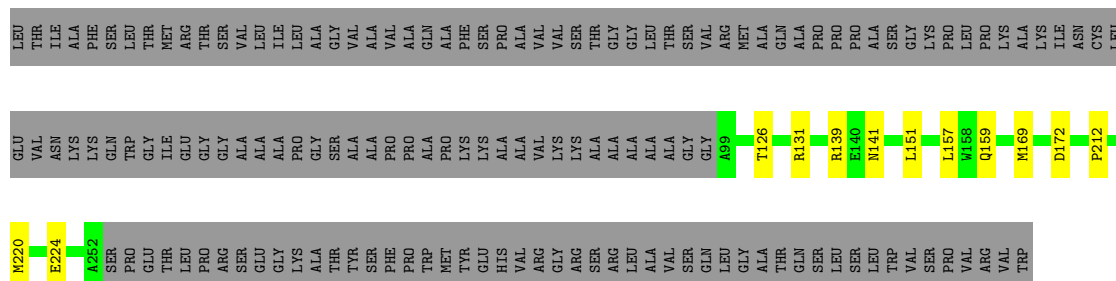
- Molecule 11: Photosystem I reaction center subunit PsaK

Chain K:  6% 67% 11% 22%



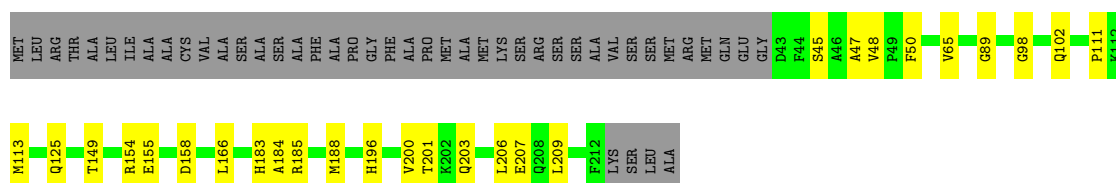
- Molecule 12: ACPI-s

Chain s:  47% 49%



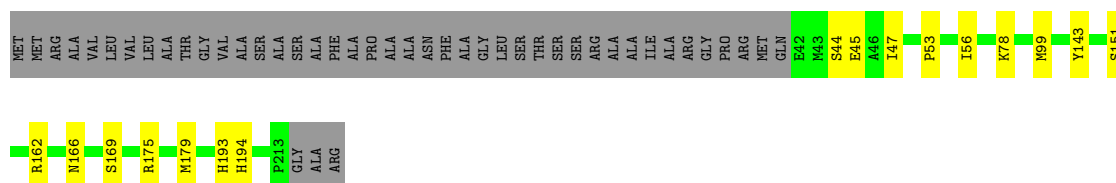
- Molecule 13: ACPI-c

Chain c:  67% 13% 21%



- Molecule 14: ACPI-a

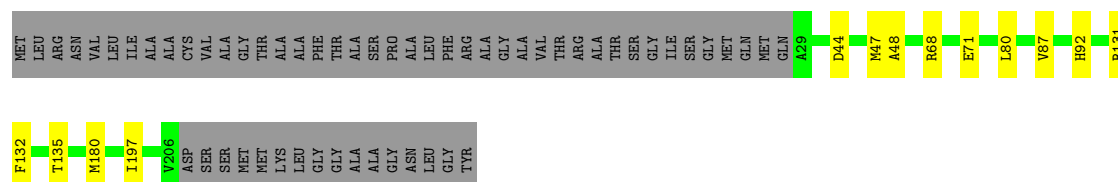
Chain a:  72% 7% 21%



- Molecule 15: ACPI-b

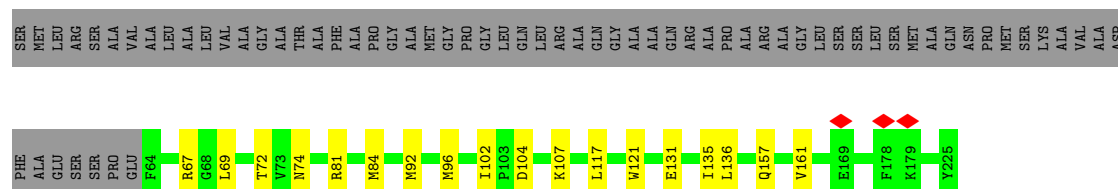
Chain b:  70% 6% 25%

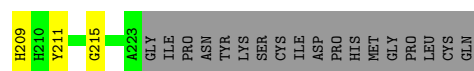




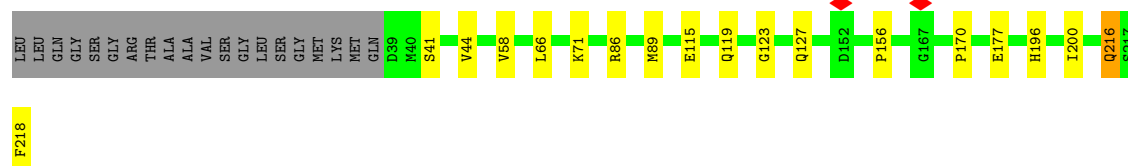
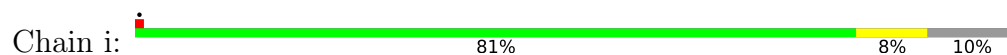
• Molecule 16: ACPI-h

Chain h: 63% 8% 29%

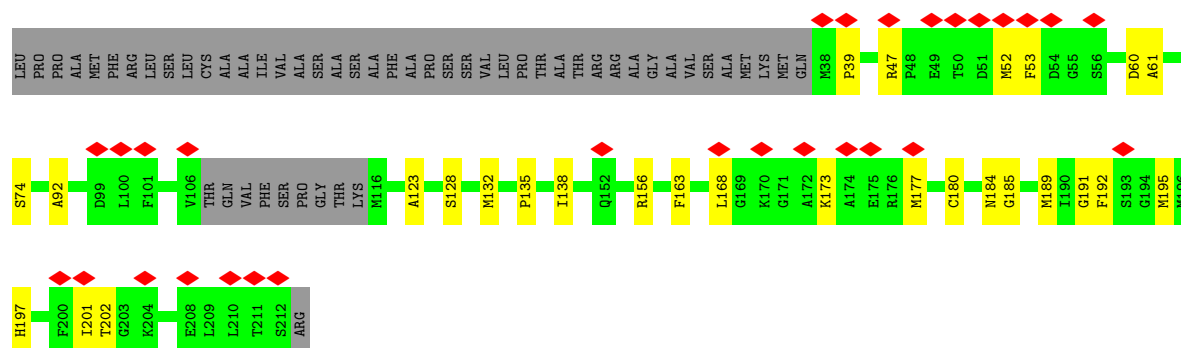




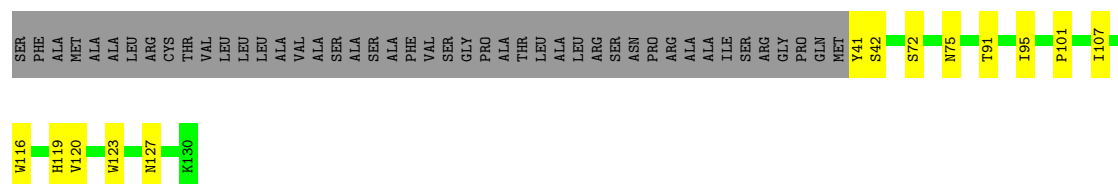
- Molecule 20: ACPI-i



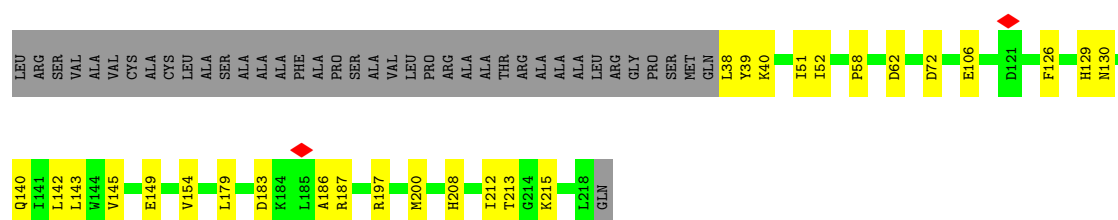
- Molecule 21: ACPI-d



- Molecule 22: PsaR



- Molecule 23: ACPI-n



- Molecule 24: PsaQ



TYR	VAL	ALA	LEU	ALA	ALA	ALA	SER	ALA	GLU	ALA	PHE	SER	SER	PRO	ALA	LEU	SER	GLY	LEU	LYS	MET	SER	THR	ALA	GLU	PRO	THR	GLN	ILE	SER	ARG	LYS	ASP	LEU	LEU	SER	THR	ALA	ALA	ALA	GLY	ILE	ILE	ALA	VAL	PRO	ALA	ALA	ILE	ALA	GLY	ALA	SER	LEU	ASP	PRO	LYS	THR	GLY	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	VAL	GLN	SER	GLY	GLY	ARG	ASP	THR	LEU	CYS	GLY	GLY	SER	SER	ALA	ALA	GLY	CYS	GLN	PRO	LYS	MET	THR	GLN	K189	K107	V118	K125	K126	L142	L145	K160	K161	G165	I168	P169	G172	K175	S176	T177	I193	K194	M197	V212	K231	PRO
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PRO	ILE	VAL	PHE	ASN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.363	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, LMG, DGD, KC2, CLA, LMU, IHT, SF4, SQD, PQN, WVN, LHG, IIO

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	0.20	0/6020	0.44	0/8205
2	B	0.21	0/6055	0.48	0/8266
3	C	0.15	0/601	0.50	0/813
4	D	0.16	0/1100	0.44	0/1488
5	E	0.14	0/492	0.41	0/666
6	F	0.23	0/1291	0.49	0/1750
7	I	0.25	0/262	0.54	0/358
8	J	0.20	0/364	0.51	0/495
9	L	0.20	0/1188	0.47	0/1616
10	M	0.18	0/233	0.40	0/315
11	K	0.22	0/489	0.52	0/664
12	s	0.18	0/1177	0.50	0/1591
13	c	0.21	0/1401	0.50	0/1896
14	a	0.20	0/1372	0.45	0/1858
15	b	0.21	0/1360	0.51	0/1834
16	h	0.21	0/1228	0.50	0/1671
17	j	0.22	0/1329	0.50	0/1789
17	m	0.23	0/1341	0.51	0/1805
18	l	0.21	0/1365	0.45	0/1845
19	k	0.33	0/1445	0.69	0/1954
20	i	0.35	1/1400 (0.1%)	0.66	3/1891 (0.2%)
21	d	0.25	0/1259	0.58	0/1700
22	R	0.20	0/687	0.46	0/940
23	n	0.22	0/1371	0.60	2/1847 (0.1%)
24	Q	0.22	0/1053	0.51	0/1418
All	All	0.22	1/35883 (0.0%)	0.51	5/48675 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	i	156	PRO	CG-CD	-6.83	1.27	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	i	156	PRO	N-CD-CG	-9.02	89.67	103.20
20	i	156	PRO	CA-N-CD	-7.29	101.79	112.00
23	n	140	GLN	CA-CB-CG	7.03	128.16	114.10
20	i	170	PRO	CA-N-CD	-5.17	104.76	112.00
23	n	140	GLN	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	666	TRP	Peptide
3	C	61	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5826	0	5682	99	0
2	B	5832	0	5643	94	0
3	C	592	0	567	6	0
4	D	1075	0	1074	7	0
5	E	484	0	486	1	0
6	F	1257	0	1266	15	0
7	I	255	0	270	4	0
8	J	351	0	344	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	1158	0	1170	10	0
10	M	232	0	265	4	0
11	K	482	0	511	7	0
12	s	1146	0	1095	10	0
13	c	1362	0	1338	17	0
14	a	1331	0	1284	11	0
15	b	1332	0	1336	12	0
16	h	1201	0	1228	13	0
17	j	1302	0	1316	17	0
17	m	1313	0	1326	15	0
18	l	1333	0	1311	16	0
19	k	1412	0	1429	17	0
20	i	1363	0	1322	13	0
21	d	1231	0	1237	23	0
22	R	666	0	655	9	0
23	n	1343	0	1356	22	0
24	Q	1041	0	1071	11	0
25	A	65	0	72	4	0
26	A	2663	0	2789	112	0
26	B	2592	0	2717	108	0
26	F	117	0	115	4	0
26	J	42	0	31	1	0
26	K	42	0	31	0	0
26	L	225	0	209	8	0
26	Q	65	0	72	0	0
26	R	55	0	49	4	0
26	a	638	0	629	13	0
26	b	659	0	663	22	0
26	c	607	0	560	14	0
26	d	529	0	417	9	0
26	h	519	0	501	15	0
26	i	608	0	621	7	0
26	j	669	0	622	14	0
26	k	603	0	548	13	0
26	l	597	0	601	17	0
26	m	680	0	655	21	0
26	n	614	0	570	16	0
26	s	260	0	288	5	0
27	A	33	0	46	4	0
27	B	33	0	46	2	0
28	A	138	0	170	7	0
28	B	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	33	0	36	0	0
28	L	92	0	126	0	0
28	b	98	0	147	3	0
28	c	86	0	118	4	0
28	i	37	0	44	0	0
28	j	30	0	29	0	0
28	l	32	0	34	0	0
28	m	37	0	44	0	0
28	n	43	0	59	1	0
28	s	33	0	40	3	0
29	A	200	0	0	0	0
29	B	280	0	0	0	0
29	F	80	0	0	0	0
29	I	40	0	0	0	0
29	J	80	0	0	0	0
29	K	40	0	0	0	0
29	L	80	0	0	0	0
29	M	40	0	0	0	0
29	R	40	0	0	0	0
29	h	40	0	0	0	0
29	i	40	0	0	0	0
29	l	80	0	0	0	0
29	s	80	0	0	0	0
30	A	69	0	87	2	0
30	B	35	0	46	1	0
30	a	35	0	46	0	0
30	i	35	0	46	2	0
31	A	8	0	0	0	0
31	C	16	0	0	1	0
32	A	54	0	78	0	0
33	B	66	0	96	6	0
33	j	62	0	84	3	0
34	F	94	0	134	2	0
34	L	45	0	61	2	0
34	Q	38	0	46	3	0
34	b	42	0	54	1	0
34	c	98	0	141	1	0
34	n	51	0	75	3	0
35	J	42	0	0	0	0
35	a	168	0	0	0	0
35	b	126	0	0	1	0
35	c	126	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	252	0	0	1	0
35	h	112	0	0	0	0
35	i	210	0	0	1	0
35	j	84	0	0	0	0
35	k	252	0	0	0	0
35	l	168	0	0	0	0
35	m	168	0	0	0	0
35	n	168	0	0	1	0
36	c	45	0	0	0	0
36	d	90	0	0	3	0
36	i	90	0	0	0	0
36	j	45	0	0	0	0
36	k	135	0	0	0	0
36	l	45	0	0	0	0
36	m	45	0	0	0	0
36	n	90	0	0	1	0
36	s	90	0	0	2	0
37	R	41	0	0	0	0
37	a	41	0	0	0	0
37	b	82	0	0	1	0
37	c	41	0	0	0	0
37	j	41	0	0	0	0
37	m	41	0	0	0	0
37	n	41	0	0	0	0
38	A	130	0	0	0	0
38	B	147	0	0	2	0
38	C	25	0	0	0	0
38	D	15	0	0	0	0
38	E	6	0	0	0	0
38	F	15	0	0	0	0
38	J	2	0	0	0	0
38	L	12	0	0	0	0
38	M	2	0	0	0	0
38	R	1	0	0	0	0
38	a	16	0	0	0	0
38	b	18	0	0	0	0
38	c	2	0	0	0	0
38	h	9	0	0	0	0
38	m	1	0	0	0	0
38	s	10	0	0	0	0
All	All	53701	0	49349	641	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 6.

All (641) 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)
20:i:218:PHE:CE1	20:i:218:PHE:CE2	2.35	1.02
21:d:201:ILE:CD1	36:d:312:KC2:CED	2.38	0.99
1:A:410:HIS:HE1	26:A:829:CLA:NA	1.74	0.86
2:B:388:HIS:HE1	26:B:827:CLA:NA	1.80	0.80
21:d:201:ILE:HD13	36:d:312:KC2:CED	2.12	0.79
2:B:438:HIS:HE1	26:B:830:CLA:NA	1.80	0.78
1:A:395:HIS:HE1	26:A:827:CLA:ND	1.81	0.77
18:l:53:LEU:HB3	18:l:74:ARG:HH21	1.52	0.74
1:A:94:HIS:HE1	26:A:806:CLA:NA	1.86	0.73
19:k:100:SER:HA	19:k:120:MET:HE1	1.69	0.73
1:A:53:HIS:HE1	26:A:841:CLA:ND	1.85	0.72
21:d:201:ILE:HD11	36:d:312:KC2:CED	2.21	0.71
16:h:92:MET:HG3	16:h:96:MET:HE2	1.73	0.71
14:a:194:HIS:HE1	26:a:310:CLA:NB	1.89	0.70
6:F:63:THR:HG22	6:F:65:PRO:HD2	1.73	0.69
19:k:103:GLN:HE22	26:k:604:CLA:HMA3	1.58	0.69
26:c:303:CLA:HAC1	26:c:306:CLA:HAB	1.74	0.69
1:A:460:HIS:HE1	26:A:832:CLA:NA	1.91	0.68
23:n:51:ILE:HG13	23:n:52:ILE:HD12	1.75	0.68
1:A:376:MET:HG2	1:A:509:SER:HB2	1.76	0.67
1:A:693:ARG:H	2:B:567:CYS:HB2	1.59	0.66
2:B:195:HIS:HE1	26:B:814:CLA:NA	1.94	0.66
26:A:822:CLA:HBB2	26:A:836:CLA:H18	1.77	0.65
26:A:831:CLA:H102	26:B:836:CLA:H51	1.80	0.64
24:Q:142:LEU:HB3	24:Q:197:MET:HE1	1.78	0.64
26:A:840:CLA:H52	26:A:852:CLA:H162	1.79	0.64
21:d:201:ILE:HG13	21:d:202:THR:HG23	1.81	0.63
15:b:47:MET:HB3	15:b:68:ARG:HH21	1.64	0.62
2:B:337:LEU:HD21	26:B:827:CLA:HAB	1.81	0.62
19:k:74:SER:HB3	26:k:602:CLA:HBA1	1.81	0.62
13:c:155:GLU:HB2	13:c:158:ASP:HB2	1.81	0.62
23:n:142:LEU:HD23	34:n:620:LMG:H291	1.82	0.62
23:n:38:LEU:HD23	23:n:40:LYS:H	1.64	0.61
23:n:154:VAL:HG22	26:n:608:CLA:HMA1	1.82	0.61
1:A:355:LEU:HD11	26:A:829:CLA:HBB1	1.82	0.61
6:F:120:VAL:O	6:F:123:TRP:HB3	2.00	0.61
26:A:837:CLA:H101	8:J:17:THR:HG23	1.82	0.61
1:A:443:LEU:HD22	26:A:836:CLA:HBB1	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:HIS:HE1	26:B:840:CLA:NB	1.98	0.60
26:B:821:CLA:HAB	26:B:828:CLA:HMD2	1.83	0.60
26:l:301:CLA:H2A	26:l:301:CLA:HED2	1.82	0.60
20:i:58:VAL:HG11	20:i:177:GLU:HB3	1.83	0.60
19:k:100:SER:CA	19:k:120:MET:HE1	2.32	0.60
3:C:17:CYS:HB3	31:C:102:SF4:S4	2.42	0.59
8:J:12:ALA:O	8:J:16:PHE:HB2	2.03	0.59
17:j:147:THR:OG1	17:j:152:ARG:NH1	2.34	0.59
28:A:855:LHG:H132	26:L:204:CLA:HAB	1.83	0.59
21:d:47:ARG:HE	21:d:53:PHE:HB3	1.66	0.59
1:A:182:HIS:HE1	26:A:810:CLA:NA	2.00	0.59
2:B:128:MET:HE3	26:B:813:CLA:HMA2	1.84	0.59
2:B:661:MET:HB2	26:B:804:CLA:C1C	2.31	0.59
26:B:801:CLA:H72	26:B:836:CLA:H43	1.83	0.59
26:B:821:CLA:H2A	26:B:821:CLA:HED3	1.84	0.59
6:F:104:TRP:HA	6:F:107:SER:HB3	1.85	0.59
12:s:151:LEU:HD23	34:b:319:LMG:H342	1.83	0.59
26:b:313:CLA:HAA1	28:b:318:LHG:HC62	1.83	0.59
2:B:482:SER:O	2:B:486:ASN:ND2	2.35	0.59
26:B:842:CLA:HMC2	26:R:201:CLA:H3A	1.83	0.59
1:A:300:HIS:HE1	26:A:818:CLA:NA	1.98	0.59
26:A:839:CLA:H142	26:L:203:CLA:HAA2	1.85	0.59
26:B:842:CLA:HBB2	26:R:201:CLA:H11	1.84	0.58
26:d:313:CLA:H2A	26:d:313:CLA:HED2	1.85	0.58
23:n:179:LEU:HD12	26:n:609:CLA:H2	1.84	0.58
1:A:222:ILE:HD12	1:A:242:PRO:HB3	1.85	0.58
1:A:503:ASN:HB2	26:A:838:CLA:HED2	1.86	0.58
12:s:169:MET:HE1	26:l:313:CLA:HED2	1.85	0.58
26:n:610:CLA:H72	26:n:610:CLA:HAA1	1.86	0.58
14:a:162:ARG:NH2	19:k:53:LEU:O	2.36	0.57
14:a:78:LYS:NZ	14:a:151:SER:O	2.36	0.57
1:A:19:ARG:NH1	30:A:858:LMU:H6E	2.19	0.57
2:B:653:HIS:CD2	26:B:803:CLA:NB	2.72	0.57
16:h:157:GLN:NE2	26:h:305:CLA:OBD	2.37	0.57
19:k:124:HIS:HE1	26:k:607:CLA:NA	2.02	0.57
2:B:298:HIS:HB3	2:B:303:ILE:HD11	1.87	0.57
9:L:61:PRO:HB3	26:L:204:CLA:HBB1	1.86	0.57
2:B:413:HIS:CE1	26:B:828:CLA:ND	2.72	0.57
26:b:309:CLA:H193	26:m:613:CLA:H121	1.86	0.57
26:l:306:CLA:HAC2	26:l:309:CLA:H91	1.87	0.56
1:A:398:TRP:CD1	26:A:827:CLA:HAB	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:HIS:HE1	26:A:852:CLA:ND	2.03	0.56
30:B:852:LMU:H122	26:j:603:CLA:HBC1	1.87	0.56
26:A:803:CLA:HBD	26:A:810:CLA:H2	1.87	0.56
1:A:446:ILE:HD11	26:A:835:CLA:HBB2	1.86	0.56
2:B:14:ASP:HB3	2:B:19:ARG:HB2	1.87	0.56
1:A:358:ASN:ND2	26:A:804:CLA:OBD	2.36	0.56
2:B:721:ALA:HB2	26:B:825:CLA:HBB1	1.87	0.56
17:m:194:HIS:CD2	26:m:613:CLA:NA	2.74	0.56
13:c:98:GLY:O	13:c:102:GLN:HB3	2.05	0.56
1:A:693:ARG:NH2	38:B:903:HOH:O	2.37	0.56
2:B:339:SER:HB3	26:B:822:CLA:H42	1.87	0.56
2:B:437:VAL:HG12	26:B:830:CLA:HAC1	1.87	0.55
26:B:818:CLA:HMB3	26:B:822:CLA:H52	1.86	0.55
6:F:28:ASP:N	6:F:32:LEU:O	2.38	0.55
18:l:203:GLN:NE2	26:l:313:CLA:O1D	2.39	0.55
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.89	0.55
1:A:681:ILE:HD13	26:A:837:CLA:HBB1	1.87	0.55
1:A:743:TRP:NE1	26:A:827:CLA:O1A	2.37	0.55
2:B:307:HIS:HE1	26:B:820:CLA:ND	2.05	0.55
19:k:121:ILE:HD11	19:k:208:VAL:HG22	1.87	0.55
15:b:48:ALA:O	15:b:68:ARG:NH2	2.40	0.55
23:n:126:PHE:O	23:n:130:ASN:ND2	2.40	0.55
26:A:851:CLA:H143	26:B:840:CLA:HBC3	1.89	0.55
2:B:421:LEU:HD13	2:B:531:LEU:HA	1.89	0.55
17:m:147:THR:OG1	17:m:152:ARG:NH1	2.39	0.55
1:A:262:GLY:HA3	26:A:814:CLA:H42	1.88	0.55
26:B:831:CLA:H2	26:B:832:CLA:HMB1	1.87	0.55
1:A:435:HIS:CE1	26:A:830:CLA:ND	2.75	0.55
12:s:126:THR:OG1	12:s:139:ARG:NH1	2.40	0.55
17:j:71:ASP:HB2	33:j:618:DGD:HD3	1.88	0.55
26:A:816:CLA:HBA1	11:K:11:PRO:HG2	1.89	0.54
28:B:851:LHG:H02	14:a:143:TYR:HH	1.54	0.54
18:l:193:GLN:NE2	18:l:200:THR:OG1	2.37	0.54
19:k:209:HIS:CD2	26:k:614:CLA:NA	2.75	0.54
20:i:196:HIS:CD2	26:i:311:CLA:NA	2.76	0.54
2:B:527:HIS:CD2	26:B:835:CLA:NB	2.76	0.54
26:B:825:CLA:H141	33:B:844:DGD:HAV1	1.89	0.54
16:h:81:ARG:HA	16:h:84:MET:HE3	1.89	0.54
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.89	0.54
7:I:8:SER:OG	26:h:301:CLA:O1D	2.23	0.54
18:l:104:ASN:ND2	18:l:105:GLY:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:HIS:CE1	26:B:805:CLA:ND	2.76	0.54
3:C:29:VAL:HG12	4:D:113:ARG:HB3	1.90	0.54
18:l:40:MET:HG3	18:l:43:LEU:HD12	1.90	0.54
17:j:194:HIS:CD2	26:j:613:CLA:NA	2.75	0.54
34:F:205:LMG:H411	26:b:307:CLA:HBB2	1.90	0.54
18:l:191:HIS:CD2	26:l:301:CLA:NA	2.76	0.54
1:A:453:HIS:HE1	26:A:831:CLA:NA	2.02	0.54
17:j:96:GLN:OE1	26:j:604:CLA:ND	2.41	0.54
1:A:546:HIS:CD2	26:A:836:CLA:NB	2.76	0.53
2:B:648:MET:O	2:B:651:PHE:HB3	2.08	0.53
26:B:836:CLA:H62	26:B:837:CLA:H121	1.89	0.53
13:c:196:HIS:CD2	26:c:312:CLA:NA	2.76	0.53
17:j:117:HIS:HE1	26:j:607:CLA:NA	2.02	0.53
1:A:340:HIS:CD2	26:A:823:CLA:ND	2.75	0.53
17:j:39:SER:OG	17:j:42:VAL:O	2.27	0.53
2:B:272:ILE:HG23	26:B:817:CLA:HMA3	1.91	0.53
20:i:200:ILE:HG13	26:i:311:CLA:HED3	1.89	0.53
9:L:46:ARG:HD2	9:L:110:LEU:HD21	1.90	0.53
13:c:125:GLN:NE2	26:c:305:CLA:O2D	2.42	0.53
13:c:200:VAL:HG23	13:c:201:THR:HG23	1.90	0.53
1:A:485:PHE:HB3	26:A:834:CLA:H2	1.90	0.53
26:A:802:CLA:H3A	26:A:802:CLA:C2	2.39	0.53
13:c:45:SER:OG	13:c:48:VAL:O	2.26	0.53
26:A:818:CLA:HAB	26:A:818:CLA:H8	1.90	0.53
13:c:206:LEU:HD13	13:c:209:LEU:HD12	1.91	0.53
17:j:94:ILE:HG23	17:j:204:LEU:HD11	1.91	0.53
26:B:810:CLA:HAB	30:i:300:LMU:H102	1.91	0.53
1:A:54:ALA:HB2	28:A:843:LHG:HC82	1.91	0.53
1:A:220:ILE:HD11	1:A:278:LEU:HD21	1.91	0.53
6:F:159:THR:HG22	15:b:135:THR:HB	1.91	0.53
17:m:198:ILE:HG12	26:m:613:CLA:HED3	1.91	0.52
2:B:193:LEU:HA	2:B:197:ALA:HB3	1.92	0.52
24:Q:169:PRO:HD3	34:Q:301:LMG:HC92	1.92	0.52
2:B:579:MET:HG3	2:B:709:LEU:HD21	1.92	0.52
16:h:96:MET:HE1	26:h:304:CLA:H8	1.92	0.52
18:l:40:MET:HE1	18:l:59:PHE:HA	1.92	0.52
13:c:50:PHE:HB2	21:d:156:ARG:HD2	1.92	0.52
2:B:449:GLU:OE2	6:F:79:ARG:NH1	2.43	0.52
28:c:320:LHG:H272	26:b:312:CLA:HBA1	1.91	0.52
21:d:39:PRO:O	21:d:47:ARG:NH1	2.43	0.52
26:A:823:CLA:H2	26:A:836:CLA:H121	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:841:CLA:H2	26:A:841:CLA:HMA1	1.91	0.51
2:B:388:HIS:HA	2:B:391:ILE:HD12	1.93	0.51
18:l:192:GLN:OE1	26:l:313:CLA:NA	2.43	0.51
23:n:145:VAL:HG11	26:n:608:CLA:HBC2	1.92	0.51
19:k:128:ILE:O	19:k:132:HIS:N	2.44	0.51
19:k:159:LEU:HD22	26:k:608:CLA:HED2	1.93	0.51
1:A:482:LYS:HD3	1:A:483:PRO:HD2	1.93	0.51
1:A:607:VAL:HG21	25:A:801:CL0:H69	1.92	0.51
23:n:149:GLU:HG2	26:n:608:CLA:NB	2.26	0.51
19:k:211:TYR:O	19:k:215:GLY:N	2.41	0.51
17:j:80:LEU:HD13	17:j:155:GLY:HA3	1.93	0.51
1:A:669:SER:HB2	2:B:444:ALA:HB1	1.94	0.50
26:B:811:CLA:H2	20:i:71:LYS:HE2	1.93	0.50
5:E:19:GLN:NE2	6:F:183:ILE:O	2.41	0.50
26:n:609:CLA:HAB	35:n:614:II0:C34	2.41	0.50
26:A:805:CLA:HBB	26:A:829:CLA:HAB	1.92	0.50
17:m:192:MET:HG2	17:m:203:PRO:HB3	1.93	0.50
2:B:173:ARG:HB2	26:B:812:CLA:HBC2	1.92	0.50
12:s:159:GLN:HG2	12:s:212:PRO:HB3	1.93	0.50
6:F:150:VAL:HG21	34:F:206:LMG:H112	1.94	0.50
21:d:92:ALA:HA	21:d:195:MET:HE1	1.92	0.50
23:n:197:ARG:HA	23:n:200:MET:HE3	1.94	0.50
17:m:198:ILE:HG22	17:m:199:THR:HG23	1.93	0.50
1:A:579:GLY:HA2	2:B:561:PRO:HD3	1.93	0.49
26:A:837:CLA:H201	26:F:201:CLA:HBB1	1.93	0.49
26:A:851:CLA:H91	26:B:804:CLA:H101	1.94	0.49
2:B:70:GLN:NE2	26:B:807:CLA:O1D	2.45	0.49
26:j:603:CLA:H51	33:j:618:DGD:HA62	1.94	0.49
24:Q:194:LYS:O	24:Q:197:MET:HB2	2.11	0.49
26:A:852:CLA:OBD	2:B:422:SER:OG	2.24	0.49
20:i:119:GLN:HG3	24:Q:160:ALA:HB2	1.94	0.49
26:h:301:CLA:HBC2	26:h:313:CLA:HAC2	1.94	0.49
26:j:603:CLA:H12	33:j:618:DGD:HG12	1.93	0.49
2:B:428:LEU:HB3	2:B:524:LEU:HB2	1.93	0.49
23:n:39:TYR:HA	23:n:186:ALA:HB3	1.94	0.49
26:B:834:CLA:H191	6:F:111:VAL:HG13	1.94	0.49
1:A:32:PRO:HB3	26:A:841:CLA:HAC1	1.94	0.49
1:A:77:HIS:CE1	26:A:804:CLA:ND	2.80	0.49
28:A:855:LHG:H262	28:A:855:LHG:H111	1.95	0.49
26:B:840:CLA:H162	34:L:209:LMG:H192	1.94	0.49
23:n:129:HIS:HE1	26:n:607:CLA:NA	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:n:213:THR:HG22	23:n:215:LYS:HE2	1.95	0.49
24:Q:161:LYS:NZ	24:Q:177:THR:O	2.41	0.49
26:A:838:CLA:H43	26:A:856:CLA:H71	1.95	0.49
15:b:68:ARG:NH1	15:b:71:GLU:OE1	2.46	0.49
2:B:421:LEU:HG	26:B:835:CLA:HBB1	1.94	0.49
9:L:98:VAL:HG13	16:h:67:ARG:HH22	1.78	0.48
26:b:309:CLA:H2	26:n:608:CLA:H12	1.95	0.48
26:b:310:CLA:HBB2	26:m:613:CLA:H192	1.95	0.48
26:l:306:CLA:H2	26:l:306:CLA:HED2	1.95	0.48
2:B:242:ILE:HG23	2:B:263[A]:GLN:HE22	1.78	0.48
26:B:815:CLA:H11	22:R:101:PRO:HG2	1.95	0.48
1:A:351:TRP:HB3	26:A:804:CLA:HAC1	1.95	0.48
2:B:520:HIS:HE1	26:B:834:CLA:ND	2.10	0.48
2:B:679:TRP:NE1	9:L:15:GLY:O	2.41	0.48
1:A:395:HIS:HE1	26:A:827:CLA:C1D	2.26	0.48
1:A:582:ARG:HH11	1:A:585:THR:HG21	1.77	0.48
26:A:829:CLA:H102	26:A:837:CLA:HAA2	1.96	0.48
2:B:350:HIS:CD2	26:B:824:CLA:NC	2.79	0.48
2:B:615:ILE:HG21	26:B:802:CLA:HBA2	1.95	0.48
16:h:72:THR:HG22	16:h:74:ASN:H	1.78	0.48
23:n:106:GLU:OE2	26:n:604:CLA:ND	2.46	0.48
20:i:41:SER:OG	20:i:44:VAL:O	2.31	0.48
2:B:4:PHE:HB2	7:I:30:ILE:HA	1.95	0.48
6:F:120:VAL:HG13	26:F:201:CLA:HAA1	1.95	0.48
9:L:57[B]:PHE:HZ	26:L:203:CLA:HBB1	1.78	0.48
13:c:149:THR:OG1	13:c:154:ARG:NH1	2.45	0.48
1:A:405:VAL:HG11	1:A:598:LEU:HG	1.95	0.48
9:L:90:VAL:HG21	9:L:124:LEU:HD13	1.96	0.48
26:B:829:CLA:H142	26:B:841:CLA:H143	1.95	0.47
26:F:202:CLA:HBA1	26:F:202:CLA:H3A	1.58	0.47
12:s:224:GLU:OE2	15:b:92:HIS:NE2	2.47	0.47
26:k:610:CLA:HBA2	26:k:610:CLA:H3A	1.42	0.47
26:A:823:CLA:H2A	26:A:823:CLA:HED3	1.95	0.47
2:B:546:MET:HE2	2:B:549:LYS:HA	1.95	0.47
12:s:131:ARG:O	15:b:131:ARG:NH2	2.47	0.47
26:d:302:CLA:H151	26:d:313:CLA:HBB2	1.96	0.47
24:Q:169:PRO:HG3	34:Q:301:LMG:HC2	1.96	0.47
1:A:298:HIS:HE1	26:A:816:CLA:C4D	2.27	0.47
26:A:835:CLA:H141	26:A:835:CLA:H161	1.77	0.47
26:c:301:CLA:HAB	21:d:163:PHE:HD1	1.79	0.47
26:b:304:CLA:HBA2	26:b:304:CLA:H3A	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:m:88:LEU:HB3	26:m:604:CLA:HAB	1.96	0.47
21:d:52:MET:HE3	21:d:74:SER:HA	1.96	0.47
26:d:308:CLA:H3A	26:d:308:CLA:HBA2	1.50	0.47
1:A:179:PHE:CE1	30:A:858:LMU:H6D	2.49	0.47
17:m:183:ARG:HB3	26:m:602:CLA:HBC3	1.96	0.47
21:d:168:LEU:HB3	21:d:177:MET:HE1	1.97	0.47
24:Q:193:ILE:HG22	24:Q:197:MET:HE2	1.96	0.47
1:A:219:GLN:HA	1:A:223:SER:HB2	1.95	0.47
26:A:818:CLA:H3A	26:A:818:CLA:HBA2	1.70	0.47
2:B:67:LEU:HG	2:B:123:TRP:HZ3	1.80	0.47
26:L:202:CLA:H3A	26:L:202:CLA:HBA2	1.51	0.47
1:A:372:HIS:CD2	26:A:826:CLA:NC	2.81	0.47
1:A:421:PRO:HG3	4:D:44:GLU:HB2	1.96	0.47
2:B:459:ALA:HB1	26:B:833:CLA:HBD	1.96	0.47
11:K:11:PRO:HB3	11:K:82:TYR:HD1	1.79	0.47
26:m:601:CLA:HED2	26:m:601:CLA:H2A	1.97	0.47
15:b:180:MET:HE2	37:b:301:IHT:C34	2.44	0.47
16:h:102:ILE:HG21	16:h:131:GLU:HG3	1.97	0.47
26:m:608:CLA:H3A	26:m:608:CLA:HBA2	1.57	0.47
20:i:216:GLN:NE2	35:i:319:II0:C06	2.78	0.47
2:B:596:LYS:NZ	38:B:940:HOH:O	2.48	0.47
6:F:115:LEU:HD23	6:F:118:LEU:HD12	1.96	0.47
14:a:99:MET:HE3	14:a:99:MET:HB2	1.88	0.47
26:B:807:CLA:HHB	26:B:808:CLA:HHB	1.96	0.47
14:a:166:ASN:HB3	14:a:169:SER:HB2	1.97	0.47
1:A:363:GLY:HA2	1:A:400:GLY:HA2	1.98	0.46
26:A:802:CLA:H11	2:B:429:GLY:HA3	1.96	0.46
26:B:831:CLA:H2	26:B:831:CLA:H61	1.62	0.46
4:D:121:HIS:NE2	4:D:140:ASN:O	2.44	0.46
26:c:302:CLA:H3A	26:c:302:CLA:HBA2	1.53	0.46
17:j:201:LYS:HE3	17:j:205:GLU:HG2	1.97	0.46
26:A:841:CLA:H11	27:A:842:PQN:H211	1.97	0.46
26:b:309:CLA:H43	23:n:154:VAL:HG11	1.97	0.46
2:B:166:TRP:CZ2	26:B:810:CLA:HHB	2.50	0.46
26:l:305:CLA:H2A	26:l:305:CLA:HED2	1.96	0.46
26:l:305:CLA:H3A	26:l:305:CLA:HBA2	1.57	0.46
26:n:607:CLA:H61	26:n:607:CLA:H41	1.61	0.46
1:A:684:PHE:HZ	26:A:837:CLA:HBC2	1.80	0.46
25:A:801:CL0:H7	26:B:803:CLA:HMB3	1.97	0.46
26:n:608:CLA:HBA2	26:n:608:CLA:H3A	1.61	0.46
26:A:840:CLA:HAB	27:A:842:PQN:H151	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:TYR:HB3	16:h:121:TRP:HB3	1.97	0.46
13:c:203:GLN:HB3	13:c:207:GLU:HG3	1.98	0.46
17:m:186:MET:SD	26:m:602:CLA:HAB	2.56	0.46
26:A:817:CLA:H3A	26:A:817:CLA:HBA2	1.55	0.46
12:s:220:MET:HG2	28:s:409:LHG:H371	1.97	0.46
13:c:111:PRO:HG2	13:c:113:MET:HE1	1.97	0.46
26:a:301:CLA:H3A	26:a:301:CLA:HBA2	1.61	0.46
15:b:44:ASP:OD1	15:b:44:ASP:N	2.47	0.46
17:m:61:PHE:HE1	26:m:601:CLA:HBC3	1.81	0.46
26:A:812:CLA:H102	26:A:812:CLA:H61	1.79	0.46
2:B:177:HIS:CD2	26:B:812:CLA:NB	2.83	0.46
26:B:808:CLA:HAB	26:B:809:CLA:HAA2	1.97	0.46
26:B:841:CLA:H62	26:B:841:CLA:H2	1.71	0.46
26:a:301:CLA:HBC2	15:b:132:PHE:HZ	1.81	0.46
1:A:56:VAL:HG21	26:A:803:CLA:C2D	2.46	0.46
26:A:830:CLA:H62	28:A:844:LHG:H121	1.97	0.46
20:i:86:ARG:HA	20:i:89:MET:HE3	1.98	0.46
21:d:123:ALA:HB1	21:d:128:SER:HB3	1.96	0.46
1:A:460:HIS:HE1	26:A:832:CLA:C1A	2.28	0.45
26:A:816:CLA:H62	26:A:816:CLA:H41	1.66	0.45
26:B:810:CLA:H42	26:B:811:CLA:H12	1.97	0.45
6:F:154:LEU:HA	6:F:157:VAL:HG22	1.98	0.45
15:b:87:VAL:HG11	26:b:306:CLA:HAC2	1.97	0.45
26:h:301:CLA:H61	26:h:301:CLA:H93	1.83	0.45
26:h:306:CLA:H3A	26:h:306:CLA:HBA2	1.77	0.45
26:A:819:CLA:H142	26:A:819:CLA:H112	1.77	0.45
28:s:409:LHG:H242	26:m:607:CLA:HMB3	1.97	0.45
17:m:77:GLU:OE1	17:m:155:GLY:N	2.48	0.45
21:d:192:PHE:HA	21:d:195:MET:HE2	1.98	0.45
2:B:342:VAL:HG13	26:B:823:CLA:HED1	1.99	0.45
17:m:74:PHE:HB2	17:m:148:LEU:HD21	1.99	0.45
26:k:603:CLA:H3A	26:k:603:CLA:HBA1	1.71	0.45
26:i:301:CLA:H3A	26:i:301:CLA:HBA2	1.43	0.45
21:d:135:PRO:HA	21:d:138:ILE:HG22	1.98	0.45
1:A:535:PHE:HA	26:A:835:CLA:HED1	1.99	0.45
13:c:47:ALA:HB2	13:c:65:VAL:HB	1.99	0.45
17:m:176:LEU:HD23	26:m:610:CLA:HED2	1.97	0.45
26:j:613:CLA:H2	26:j:613:CLA:H61	1.66	0.45
2:B:194:ILE:HD13	26:B:814:CLA:HAC1	1.99	0.45
26:s:402:CLA:H161	26:s:402:CLA:H141	1.73	0.45
18:l:59:PHE:HE1	26:l:304:CLA:HAC2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:d:185:GLY:O	21:d:189:MET:HG3	2.16	0.45
21:d:197:HIS:CD2	26:d:313:CLA:NA	2.84	0.45
26:m:602:CLA:H91	26:m:602:CLA:H111	1.74	0.45
19:k:208:VAL:O	19:k:211:TYR:HB3	2.16	0.45
26:k:602:CLA:HBA2	26:k:602:CLA:H3A	1.51	0.45
26:B:816:CLA:H62	26:B:816:CLA:H41	1.83	0.45
17:m:183:ARG:HA	17:m:186:MET:HE3	1.98	0.45
26:m:603:CLA:H3A	26:m:603:CLA:HBA1	1.62	0.45
26:k:609:CLA:H3A	26:k:609:CLA:HBA2	1.61	0.45
17:j:176:LEU:HD23	26:j:610:CLA:HED2	1.99	0.45
26:A:805:CLA:H2	26:A:829:CLA:H61	1.99	0.45
4:D:34:THR:HA	4:D:58:ASN:O	2.17	0.45
26:b:310:CLA:HBC3	26:n:608:CLA:H142	1.99	0.45
24:Q:107:ALA:HB3	24:Q:145:LEU:HD13	1.99	0.45
1:A:539:HIS:CD2	26:A:835:CLA:NB	2.84	0.45
26:A:836:CLA:H122	26:A:836:CLA:H8	1.85	0.45
26:B:817:CLA:HBA2	26:B:817:CLA:H3A	1.51	0.45
26:a:301:CLA:H62	26:a:301:CLA:H41	1.56	0.45
26:h:307:CLA:HBB2	26:h:308:CLA:HBB2	1.98	0.45
26:l:309:CLA:H3A	26:l:309:CLA:HBA2	1.71	0.45
1:A:180:HIS:HE1	26:A:809:CLA:NA	2.09	0.44
26:A:817:CLA:HAC1	26:A:833:CLA:H42	1.99	0.44
2:B:139:LEU:HD22	10:M:13:LEU:HD12	1.99	0.44
2:B:715:GLY:O	2:B:719:THR:OG1	2.31	0.44
26:h:305:CLA:HBA2	26:h:305:CLA:HED3	1.98	0.44
26:m:610:CLA:H3A	26:m:610:CLA:HBA2	1.68	0.44
26:B:817:CLA:H142	26:B:817:CLA:H112	1.85	0.44
34:L:209:LMG:H261	26:h:313:CLA:H152	1.98	0.44
19:k:162:THR:OG1	19:k:168:ARG:NH1	2.45	0.44
20:i:115:GLU:HG2	24:Q:165:GLY:HA3	1.98	0.44
1:A:119:TRP:CD2	26:A:808:CLA:HED3	2.52	0.44
1:A:624:VAL:HG22	1:A:630:VAL:HG22	1.99	0.44
2:B:706:LEU:HD21	33:B:844:DGD:HA81	1.99	0.44
26:B:801:CLA:H61	26:B:801:CLA:H41	1.74	0.44
23:n:208:HIS:CD2	26:n:613:CLA:NA	2.85	0.44
1:A:331:HIS:HE1	26:A:822:CLA:ND	2.15	0.44
26:B:827:CLA:H51	33:B:844:DGD:HA91	1.99	0.44
26:a:306:CLA:H171	26:a:306:CLA:H91	1.99	0.44
26:m:602:CLA:H3A	26:m:602:CLA:HBA2	1.57	0.44
26:i:307:CLA:H3A	26:i:307:CLA:HBA2	1.61	0.44
23:n:143:LEU:HD12	34:n:620:LMG:H362	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:HIS:CD2	26:A:812:CLA:NB	2.85	0.44
26:A:802:CLA:HMD3	2:B:532:ILE:HG12	1.99	0.44
2:B:630:LEU:HD22	2:B:723:PHE:HA	2.00	0.44
26:m:609:CLA:H3A	26:m:609:CLA:HBA2	1.54	0.44
18:l:139:LEU:HG	26:l:309:CLA:HMA1	1.99	0.44
26:B:818:CLA:HBB1	26:B:822:CLA:H72	1.99	0.44
26:B:828:CLA:HBA2	26:B:828:CLA:H3A	1.56	0.44
28:s:409:LHG:H272	26:m:607:CLA:HMB1	2.00	0.44
14:a:53:PRO:HB2	14:a:56:ILE:HG12	2.00	0.44
28:b:302:LHG:H322	28:b:302:LHG:H161	1.98	0.44
26:i:306:CLA:H3A	26:i:306:CLA:HBA2	1.48	0.44
1:A:116:GLN:HB3	1:A:138:VAL:HB	1.98	0.44
19:k:204:VAL:O	19:k:208:VAL:N	2.50	0.44
2:B:346:LEU:HD12	2:B:346:LEU:HA	1.84	0.44
26:B:823:CLA:H3A	26:B:823:CLA:HBA2	1.73	0.44
26:i:311:CLA:HBB1	26:i:311:CLA:H112	2.00	0.44
2:B:438:HIS:HE1	26:B:830:CLA:C1A	2.30	0.44
2:B:518:ILE:HG12	2:B:592:TYR:HB2	1.99	0.44
13:c:185:ARG:HA	13:c:188:MET:HE3	2.00	0.44
26:c:307:CLA:HBA2	26:c:307:CLA:H3A	1.47	0.44
21:d:173:LYS:HB3	21:d:177:MET:HE3	2.00	0.44
22:R:116:TRP:HA	22:R:119:HIS:HD1	1.83	0.44
22:R:116:TRP:HE1	26:R:201:CLA:C3B	2.31	0.44
26:B:814:CLA:H102	26:B:814:CLA:H13	1.87	0.43
26:B:819:CLA:H3A	26:B:819:CLA:HBA2	1.44	0.43
26:B:838:CLA:HAA2	10:M:28:LEU:HB3	2.00	0.43
21:d:132:MET:HG3	26:d:306:CLA:HBC3	2.00	0.43
26:A:827:CLA:H142	26:A:829:CLA:H162	2.00	0.43
6:F:156:PHE:O	6:F:159:THR:OG1	2.28	0.43
26:a:301:CLA:H161	26:l:301:CLA:H121	2.01	0.43
15:b:80:LEU:HD13	26:b:306:CLA:H91	1.99	0.43
17:j:188:GLY:O	17:j:192:MET:HG3	2.18	0.43
22:R:72:SER:OG	22:R:75:ASN:OD1	2.35	0.43
1:A:692:GLY:HA3	2:B:568:ASP:HB2	2.00	0.43
1:A:733:HIS:CD2	26:A:837:CLA:NB	2.85	0.43
2:B:573:ASP:OD2	2:B:705:ARG:NH1	2.51	0.43
1:A:202:HIS:HE1	26:A:811:CLA:NA	2.14	0.43
25:A:801:CL0:O1D	26:B:803:CLA:HBB2	2.18	0.43
26:s:406:CLA:HBA2	15:b:197:ILE:HG23	2.00	0.43
26:B:817:CLA:H192	26:B:831:CLA:H11	2.00	0.43
20:i:71:LYS:HD2	30:i:300:LMU:H3'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:n:58:PRO:HG3	23:n:72:ASP:HB3	1.99	0.43
1:A:461:ASN:HD21	1:A:474:PHE:HB2	1.83	0.43
2:B:88:HIS:CD2	26:B:808:CLA:NA	2.87	0.43
2:B:406:VAL:O	2:B:410:ILE:HG12	2.18	0.43
14:a:193:HIS:CD2	26:a:311:CLA:NA	2.87	0.43
26:b:312:CLA:H3A	26:b:312:CLA:HBA2	1.64	0.43
17:m:77:GLU:HG2	17:m:144:LEU:HD13	2.01	0.43
19:k:103:GLN:NE2	26:k:604:CLA:HMA3	2.31	0.43
23:n:40:LYS:NZ	26:n:610:CLA:O1A	2.51	0.43
26:A:831:CLA:HBB1	26:A:832:CLA:H2	2.00	0.43
26:A:841:CLA:H93	26:A:841:CLA:H61	1.86	0.43
2:B:90:ILE:HB	2:B:111:PRO:HB2	2.01	0.43
33:B:844:DGD:HB51	33:B:844:DGD:HB22	1.80	0.43
26:c:301:CLA:HAB	21:d:163:PHE:CD1	2.54	0.43
34:c:319:LMG:H131	26:b:311:CLA:H172	2.00	0.43
14:a:44:SER:OG	14:a:47:ILE:O	2.35	0.43
26:b:306:CLA:H93	26:b:306:CLA:H111	1.88	0.43
16:h:69:LEU:HD21	16:h:161:VAL:HG12	2.01	0.43
1:A:361:MET:HG3	26:A:824:CLA:HHB	2.01	0.43
1:A:391:SER:HB3	26:A:827:CLA:HMA1	2.00	0.43
1:A:591:TRP:CD1	26:A:829:CLA:HMD1	2.54	0.43
26:A:825:CLA:HBB1	26:A:836:CLA:HHB	2.01	0.43
28:A:849:LHG:H141	26:B:802:CLA:H111	2.00	0.43
2:B:357:TYR:OH	26:B:826:CLA:OBD	2.30	0.43
26:B:807:CLA:HAA1	7:I:11:VAL:HG22	2.00	0.43
28:c:320:LHG:H282	28:c:320:LHG:H311	1.90	0.43
1:A:450:LEU:HB3	1:A:543:PHE:HB2	2.00	0.43
27:A:842:PQN:H111	27:A:842:PQN:H2M1	1.83	0.43
2:B:304:LEU:HD11	26:B:822:CLA:HMC3	2.00	0.43
26:B:825:CLA:H192	26:B:825:CLA:H162	1.91	0.43
11:K:80:LEU:HA	11:K:83:VAL:HG22	2.01	0.43
26:h:304:CLA:H92	26:h:304:CLA:H61	1.86	0.43
26:j:608:CLA:H3A	26:j:608:CLA:HBA2	1.59	0.43
26:j:610:CLA:HBA2	26:j:610:CLA:H3A	1.48	0.43
26:A:826:CLA:H101	26:A:826:CLA:H61	1.91	0.43
2:B:541:ARG:NH2	4:D:128:ASN:OD1	2.43	0.43
2:B:711:HIS:HE1	26:B:837:CLA:C4D	2.32	0.43
12:s:141:ASN:HB3	18:l:67:TYR:HE1	1.84	0.43
16:h:135:ILE:HG13	26:h:313:CLA:HED2	2.00	0.43
26:j:609:CLA:H3A	26:j:609:CLA:HBA2	1.55	0.43
1:A:367:ILE:HG23	1:A:397:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:824:CLA:HBA1	26:A:828:CLA:H193	2.01	0.42
26:L:204:CLA:H93	26:L:206:CLA:HAB	2.00	0.42
26:s:406:CLA:H92	26:s:406:CLA:H61	1.91	0.42
18:l:74:ARG:HH12	18:l:176:VAL:HG21	1.83	0.42
26:B:814:CLA:H122	26:B:814:CLA:H161	1.85	0.42
26:B:838:CLA:H52	26:B:838:CLA:H11	1.76	0.42
28:B:851:LHG:H222	26:a:303:CLA:HAC2	2.00	0.42
26:c:304:CLA:H112	26:c:304:CLA:H152	1.82	0.42
26:b:309:CLA:H142	26:b:309:CLA:H111	1.88	0.42
24:Q:118:VAL:HG21	24:Q:212:VAL:HG11	2.01	0.42
2:B:289:MET:HB2	26:B:819:CLA:HAC1	2.01	0.42
26:B:824:CLA:H191	26:B:842:CLA:H152	2.00	0.42
11:K:57:PHE:HE2	11:K:62:LEU:HD12	1.83	0.42
16:h:117:LEU:HD13	26:h:301:CLA:H92	2.00	0.42
17:j:88:LEU:HB3	26:j:604:CLA:HAB	2.01	0.42
22:R:123:TRP:O	22:R:127:ASN:ND2	2.45	0.42
24:Q:168:ILE:HG22	34:Q:301:LMG:H292	2.01	0.42
1:A:221:HIS:HE1	26:A:814:CLA:ND	2.17	0.42
26:B:812:CLA:H193	26:B:826:CLA:H2	2.01	0.42
13:c:89:GLY:HA3	13:c:184:ALA:HB1	2.01	0.42
26:c:308:CLA:H192	26:c:308:CLA:H162	1.89	0.42
26:a:307:CLA:H102	26:a:307:CLA:H62	1.63	0.42
26:B:815:CLA:H93	22:R:107:ILE:HG13	2.02	0.42
26:B:836:CLA:H121	26:B:837:CLA:H13	2.02	0.42
26:b:312:CLA:H102	26:b:312:CLA:H62	1.76	0.42
23:n:212:ILE:HG22	26:n:613:CLA:HED3	2.00	0.42
1:A:161:TRP:CD1	26:A:815:CLA:HAA2	2.55	0.42
26:A:805:CLA:H2	26:A:805:CLA:HED2	2.01	0.42
26:A:832:CLA:H2A	26:A:832:CLA:HED2	2.01	0.42
2:B:59:TRP:NE1	26:B:825:CLA:OBD	2.52	0.42
2:B:340:LEU:HD12	2:B:343:ILE:HD11	2.01	0.42
26:B:807:CLA:H12	7:I:14:ILE:HG13	2.00	0.42
26:B:825:CLA:H121	26:B:825:CLA:H161	1.82	0.42
3:C:26:LEU:HA	3:C:41:SER:O	2.19	0.42
26:b:309:CLA:H152	26:m:613:CLA:H202	2.01	0.42
1:A:279:THR:OG1	1:A:295:ASP:OD1	2.35	0.42
1:A:396:HIS:CD2	26:A:828:CLA:NC	2.87	0.42
1:A:540:ILE:HD12	25:A:801:CL0:H63	2.01	0.42
26:A:805:CLA:H151	26:A:828:CLA:HBB2	2.01	0.42
26:A:841:CLA:H62	26:A:841:CLA:H41	1.81	0.42
2:B:411:LEU:HD23	2:B:411:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:839:CLA:HBA2	26:B:839:CLA:H3A	1.79	0.42
13:c:183:HIS:CE1	26:c:309:CLA:OBD	2.72	0.42
26:b:310:CLA:H203	26:b:310:CLA:H162	1.88	0.42
26:h:307:CLA:H61	26:h:307:CLA:H102	1.88	0.42
26:A:812:CLA:H61	26:A:812:CLA:H41	1.66	0.42
2:B:175:ASN:ND2	2:B:290:TYR:O	2.52	0.42
27:B:843:PQN:H111	27:B:843:PQN:H2M1	1.89	0.42
26:F:202:CLA:H61	26:F:202:CLA:H2	1.73	0.42
26:J:103:CLA:HBB1	28:c:320:LHG:H151	2.02	0.42
9:L:34:LEU:HD22	26:L:203:CLA:HBD	2.01	0.42
9:L:54:HIS:HE1	26:L:203:CLA:C4D	2.32	0.42
11:K:32:ILE:HA	11:K:65:SER:HB2	2.01	0.42
26:a:301:CLA:H51	26:a:308:CLA:HBB2	2.02	0.42
16:h:104:ASP:HB3	16:h:107:LYS:HB2	2.02	0.42
1:A:592:ASP:HA	1:A:595:PHE:HB3	2.01	0.42
1:A:747:LEU:HD23	1:A:747:LEU:HA	1.90	0.42
26:A:837:CLA:H171	8:J:24:ALA:HB2	2.02	0.42
2:B:67:LEU:HD13	2:B:67:LEU:HA	1.89	0.42
2:B:195:HIS:HE1	26:B:814:CLA:C1A	2.31	0.42
2:B:256:PHE:HE2	2:B:492:TRP:CE3	2.37	0.42
26:i:304:CLA:H93	26:i:304:CLA:H61	1.86	0.42
23:n:62:ASP:OD1	23:n:62:ASP:N	2.53	0.42
26:A:822:CLA:H41	26:A:822:CLA:H62	1.78	0.42
2:B:65:PHE:HZ	10:M:7:ILE:HG23	1.85	0.42
26:B:823:CLA:C2B	26:B:835:CLA:H3A	2.50	0.42
26:B:837:CLA:HAA1	27:B:843:PQN:H251	2.02	0.42
28:c:320:LHG:H152	28:c:320:LHG:H182	1.89	0.42
14:a:45:GLU:OE1	14:a:45:GLU:N	2.52	0.42
21:d:180:CYS:O	21:d:184:ASN:ND2	2.39	0.42
1:A:268:THR:HB	11:K:16:TRP:HB2	2.01	0.41
1:A:487:GLN:NE2	1:A:530:LEU:O	2.53	0.41
1:A:625:GLN:NE2	1:A:631:THR:OG1	2.42	0.41
1:A:695:TYR:OH	26:A:802:CLA:OBD	2.37	0.41
2:B:409:ARG:NE	26:B:828:CLA:OBD	2.38	0.41
26:s:406:CLA:H141	26:s:406:CLA:H161	1.84	0.41
26:b:309:CLA:HHB	28:n:619:LHG:HC82	2.02	0.41
26:b:310:CLA:H162	34:n:620:LMG:H392	2.02	0.41
17:j:113:MET:HE3	17:j:113:MET:HB3	1.93	0.41
1:A:682:TRP:HB2	1:A:737:GLY:HA3	2.02	0.41
2:B:179:SER:HB3	2:B:287:GLY:HA3	2.01	0.41
26:B:815:CLA:HBC1	26:B:816:CLA:H202	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:THR:HG22	3:C:28:MET:HE2	2.01	0.41
6:F:82:ARG:HH12	8:J:36:ASP:HB2	1.85	0.41
26:A:803:CLA:H52	26:A:803:CLA:H12	1.78	0.41
26:A:831:CLA:H11	26:A:831:CLA:H52	1.77	0.41
2:B:2:THR:OG1	2:B:12:ALA:O	2.37	0.41
2:B:25:ALA:HB2	33:B:844:DGD:HA52	2.01	0.41
2:B:343:ILE:HD13	26:B:822:CLA:H43	2.03	0.41
2:B:593:TRP:CD1	26:B:833:CLA:HAC1	2.55	0.41
26:B:802:CLA:H41	26:B:802:CLA:H61	1.65	0.41
26:B:808:CLA:H2A	26:B:808:CLA:CED	2.51	0.41
23:n:187:ARG:HH22	36:n:611:KC2:CAD	2.33	0.41
1:A:431:ARG:NH2	26:A:830:CLA:O1D	2.53	0.41
26:A:807:CLA:H61	26:A:807:CLA:H2	1.78	0.41
26:A:841:CLA:H92	27:A:842:PQN:H251	2.03	0.41
2:B:711:HIS:HE1	26:B:837:CLA:ND	2.17	0.41
18:l:82:ARG:HA	18:l:85:MET:HE3	2.03	0.41
18:l:122:GLN:HE22	26:l:308:CLA:C1A	2.33	0.41
21:d:60:ASP:OD1	21:d:60:ASP:N	2.50	0.41
26:d:304:CLA:H3A	26:d:304:CLA:HBA2	1.66	0.41
1:A:272:SER:O	1:A:275:SER:HB3	2.20	0.41
1:A:368:ILE:HG21	26:A:818:CLA:H191	2.03	0.41
26:A:805:CLA:H192	26:A:805:CLA:H161	1.86	0.41
2:B:331:PHE:HB2	2:B:392:PHE:CD1	2.55	0.41
26:m:602:CLA:H41	26:m:602:CLA:H61	1.60	0.41
17:j:144:LEU:HD22	26:j:608:CLA:HED2	2.03	0.41
23:n:183:ASP:OD1	23:n:183:ASP:N	2.47	0.41
26:A:833:CLA:H41	26:A:833:CLA:H62	1.76	0.41
28:A:849:LHG:H142	28:A:849:LHG:H111	1.78	0.41
26:B:806:CLA:H151	26:B:826:CLA:HBB2	2.02	0.41
26:B:817:CLA:H162	26:B:817:CLA:H141	1.83	0.41
26:B:833:CLA:H11	26:B:833:CLA:H51	1.87	0.41
13:c:166:LEU:HD13	26:c:308:CLA:H42	2.02	0.41
16:h:136:LEU:HD21	26:h:301:CLA:H121	2.03	0.41
20:i:123:GLY:O	20:i:127:GLN:HG3	2.20	0.41
1:A:367:ILE:HG22	26:A:825:CLA:HED2	2.03	0.41
1:A:416:VAL:HG11	1:A:573:PHE:N	2.35	0.41
26:A:827:CLA:H3A	26:A:827:CLA:HBA2	1.77	0.41
2:B:276:HIS:CD2	26:B:817:CLA:NC	2.88	0.41
2:B:520:HIS:CD2	26:B:834:CLA:NB	2.86	0.41
26:B:801:CLA:HAB	26:B:801:CLA:H71	2.02	0.41
26:B:806:CLA:H41	33:B:844:DGD:HB61	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:819:CLA:H62	26:B:819:CLA:H41	1.66	0.41
26:B:820:CLA:H122	26:B:820:CLA:H162	1.79	0.41
4:D:88:ARG:HB2	4:D:98:LEU:HD11	2.03	0.41
26:j:610:CLA:H142	26:j:610:CLA:H112	1.94	0.41
1:A:442:HIS:CD2	26:A:839:CLA:NC	2.89	0.41
26:A:804:CLA:H141	26:A:804:CLA:H162	1.85	0.41
12:s:172:ASP:OD1	12:s:172:ASP:N	2.51	0.41
36:s:401:KC2:CAB	26:m:608:CLA:H193	2.51	0.41
13:c:102:GLN:OE1	26:c:304:CLA:NA	2.54	0.41
26:a:304:CLA:H141	26:a:304:CLA:H161	1.89	0.41
26:b:312:CLA:H141	26:b:312:CLA:H162	1.90	0.41
17:m:52:ASP:OD1	17:m:52:ASP:N	2.54	0.41
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.96	0.41
1:A:450:LEU:HD13	1:A:543:PHE:HA	2.02	0.41
1:A:694:GLY:N	2:B:567:CYS:O	2.45	0.41
26:A:823:CLA:HBB2	28:A:844:LHG:HC82	2.02	0.41
2:B:149:LEU:HD22	10:M:21:ALA:HA	2.03	0.41
2:B:269:LEU:HD23	2:B:272:ILE:HD12	2.02	0.41
2:B:518:ILE:HD13	26:B:803:CLA:H141	2.03	0.41
2:B:657:ALA:O	2:B:660:PHE:HB2	2.21	0.41
36:s:404:KC2:O1D	26:a:301:CLA:HMB2	2.21	0.41
14:a:175:ARG:O	14:a:179:MET:HG2	2.21	0.41
26:l:308:CLA:H92	26:l:308:CLA:H61	1.85	0.41
19:k:173:PHE:HB2	26:k:609:CLA:HMD1	2.02	0.41
20:i:66:LEU:HD23	17:j:142:ILE:HD11	2.02	0.41
17:j:201:LYS:HD3	17:j:206:LEU:HD23	2.02	0.41
1:A:11:LYS:HD2	1:A:11:LYS:HA	1.94	0.41
1:A:264:VAL:HG11	26:d:313:CLA:H43	2.03	0.41
1:A:300:HIS:HE1	26:A:818:CLA:C1A	2.34	0.41
2:B:509:LEU:HD22	2:B:600:ILE:HD13	2.02	0.41
12:s:157:LEU:HD21	26:l:305:CLA:H112	2.04	0.41
21:d:191:GLY:HA3	35:d:319:II0:C28	2.51	0.41
26:n:607:CLA:H111	26:n:607:CLA:H151	1.86	0.41
9:L:16:ASN:OD1	9:L:17:LEU:N	2.54	0.40
18:l:99:LEU:HD13	18:l:101:GLN:HE21	1.85	0.40
26:l:306:CLA:HBC1	26:l:309:CLA:H102	2.02	0.40
26:k:609:CLA:H93	26:k:609:CLA:H61	1.91	0.40
21:d:61:ALA:HB3	26:d:302:CLA:HMD1	2.02	0.40
1:A:75:SER:OG	1:A:181:TYR:HB2	2.22	0.40
1:A:541:HIS:HE1	1:A:607:VAL:HG12	1.86	0.40
2:B:438:HIS:HB2	26:B:830:CLA:C1C	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:840:CLA:H102	9:L:84:GLY:HA3	2.03	0.40
3:C:24:ASP:OD1	4:D:99:HIS:ND1	2.43	0.40
26:c:308:CLA:HBA2	26:c:308:CLA:H3A	1.42	0.40
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.93	0.40
1:A:493:HIS:HE1	26:A:833:CLA:NB	2.15	0.40
26:B:804:CLA:H52	26:B:804:CLA:HMB1	2.02	0.40
17:j:204:LEU:HD23	17:j:207:LEU:HD12	2.03	0.40
22:R:91:THR:O	22:R:95:ILE:HG12	2.21	0.40
1:A:56:VAL:HG21	26:A:803:CLA:C3D	2.51	0.40
1:A:207:LEU:HD11	26:A:812:CLA:H2	2.02	0.40
1:A:272:SER:HB3	11:K:13:THR:HG23	2.03	0.40
2:B:36:MET:HE2	2:B:36:MET:HB2	1.93	0.40
26:B:821:CLA:HBB	26:B:842:CLA:O1D	2.22	0.40
26:c:312:CLA:H62	26:c:312:CLA:H2	1.67	0.40
26:b:310:CLA:HBB1	35:b:314:II0:C42	2.52	0.40
26:h:301:CLA:H3A	26:h:301:CLA:HBA2	1.79	0.40
19:k:108:PHE:CE1	26:k:605:CLA:HAB	2.56	0.40
1:A:309:VAL:HG11	26:A:816:CLA:H161	2.04	0.40
1:A:331:HIS:CD2	26:A:822:CLA:NB	2.89	0.40
26:A:805:CLA:H13	26:A:805:CLA:H101	1.84	0.40
2:B:19:ARG:NH2	2:B:694:ASP:OD2	2.48	0.40
26:B:823:CLA:H141	26:B:823:CLA:H161	1.89	0.40
6:F:155:SER:O	6:F:159:THR:HG23	2.22	0.40
26:s:402:CLA:H112	26:s:402:CLA:H72	1.68	0.40
26:a:301:CLA:HBD	28:b:302:LHG:HC41	2.02	0.40
18:l:110:ASP:HA	18:l:113:PHE:HD2	1.86	0.40
26:d:302:CLA:H3A	26:d:302:CLA:HBA2	1.44	0.40
22:R:41:TYR:HB2	22:R:42:SER:H	1.65	0.40
22:R:120:VAL:HA	26:R:201:CLA:HMA3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	740 (100%)	0	0	100	100
2	B	732/734 (100%)	730 (100%)	2 (0%)	0	100	100
3	C	78/81 (96%)	77 (99%)	0	1 (1%)	10	4
4	D	136/141 (96%)	136 (100%)	0	0	100	100
5	E	58/64 (91%)	58 (100%)	0	0	100	100
6	F	159/188 (85%)	159 (100%)	0	0	100	100
7	I	31/36 (86%)	31 (100%)	0	0	100	100
8	J	40/42 (95%)	40 (100%)	0	0	100	100
9	L	150/153 (98%)	150 (100%)	0	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	K	64/87 (74%)	64 (100%)	0	0	100	100
12	s	152/302 (50%)	151 (99%)	1 (1%)	0	100	100
13	c	168/215 (78%)	168 (100%)	0	0	100	100
14	a	170/217 (78%)	170 (100%)	0	0	100	100
15	b	176/236 (75%)	176 (100%)	0	0	100	100
16	h	160/229 (70%)	160 (100%)	0	0	100	100
17	j	171/212 (81%)	170 (99%)	1 (1%)	0	100	100
17	m	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
18	l	173/175 (99%)	173 (100%)	0	0	100	100
19	k	187/232 (81%)	185 (99%)	2 (1%)	0	100	100
20	i	178/200 (89%)	178 (100%)	0	0	100	100
21	d	162/219 (74%)	161 (99%)	1 (1%)	0	100	100
22	R	88/135 (65%)	88 (100%)	0	0	100	100
23	n	179/220 (81%)	179 (100%)	0	0	100	100
24	Q	141/233 (60%)	140 (99%)	1 (1%)	0	100	100
All	All	4493/5345 (84%)	4483 (100%)	9 (0%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE

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	605/614 (98%)	605 (100%)	0	100	100
2	B	595/594 (100%)	595 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/117 (98%)	115 (100%)	0	100	100
5	E	54/58 (93%)	54 (100%)	0	100	100
6	F	132/156 (85%)	132 (100%)	0	100	100
7	I	27/29 (93%)	27 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	125/126 (99%)	123 (98%)	2 (2%)	58	63
10	M	25/25 (100%)	25 (100%)	0	100	100
11	K	51/66 (77%)	51 (100%)	0	100	100
12	s	119/228 (52%)	119 (100%)	0	100	100
13	c	139/171 (81%)	139 (100%)	0	100	100
14	a	139/167 (83%)	139 (100%)	0	100	100
15	b	136/174 (78%)	136 (100%)	0	100	100
16	h	124/167 (74%)	124 (100%)	0	100	100
17	j	135/161 (84%)	135 (100%)	0	100	100
17	m	136/161 (84%)	136 (100%)	0	100	100
18	l	136/137 (99%)	136 (100%)	0	100	100
19	k	143/178 (80%)	142 (99%)	1 (1%)	81	85
20	i	142/156 (91%)	141 (99%)	1 (1%)	81	85
21	d	125/165 (76%)	125 (100%)	0	100	100
22	R	72/104 (69%)	72 (100%)	0	100	100
23	n	141/167 (84%)	141 (100%)	0	100	100
24	Q	106/169 (63%)	106 (100%)	0	100	100
All	All	3628/4197 (86%)	3624 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	57[A]	PHE
9	L	57[B]	PHE
19	k	101	LEU
20	i	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	444	ASN
1	A	640	GLN
1	A	725	GLN
2	B	367	GLN
2	B	402	ASN
2	B	405	ASN
2	B	703	GLN
3	C	38	GLN
4	D	77	ASN
6	F	70	GLN
6	F	106	HIS
12	s	170	GLN
13	c	56	ASN
13	c	125	GLN
14	a	81	GLN
15	b	130	ASN
15	b	144	ASN
18	l	101	GLN
18	l	104	ASN
18	l	193	GLN
18	l	198	GLN
18	l	203	GLN
19	k	103	GLN
19	k	142	HIS
19	k	196	ASN
20	i	216	GLN
22	R	93	GLN
23	n	50	ASN
23	n	195	ASN
24	Q	229	GLN
24	Q	231	ASN

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 ⓘ

354 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	$\# Z > 2$
35	II0	h	310	-	26,28,43	6.56	14 (53%)	31,37,60	7.02	20 (64%)
35	II0	n	614	-	39,43,43	0.21	0	50,60,60	0.45	0
29	WVN	A	848	-	40,41,41	5.60	20 (50%)	50,56,56	6.48	33 (66%)
35	II0	m	615	-	39,43,43	6.59	22 (56%)	50,60,60	6.80	30 (60%)
34	LMG	Q	301	-	38,38,55	0.87	0	46,46,63	1.23	3 (6%)
29	WVN	B	846	-	40,41,41	5.55	20 (50%)	50,56,56	6.45	33 (66%)
29	WVN	s	405	-	40,41,41	5.69	19 (47%)	50,56,56	6.21	29 (58%)
26	CLA	m	613	17	65,73,73	1.51	6 (9%)	76,113,113	1.39	6 (7%)
35	II0	j	614	-	39,43,43	6.52	22 (56%)	50,60,60	6.99	29 (58%)
26	CLA	d	304	-	45,53,73	1.79	5 (11%)	52,89,113	1.62	6 (11%)
29	WVN	K	102	-	40,41,41	5.62	18 (45%)	50,56,56	6.49	32 (64%)
36	KC2	m	611	17	48,53,53	1.73	9 (18%)	54,89,89	0.97	3 (5%)
26	CLA	A	824	38	65,73,73	1.47	6 (9%)	76,113,113	1.50	7 (9%)
26	CLA	c	307	13	46,54,73	1.74	6 (13%)	53,90,113	1.58	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	829	2	65,73,73	1.49	5 (7%)	76,113,113	1.45	9 (11%)
26	CLA	A	813	1	56,64,73	1.64	6 (10%)	65,102,113	1.52	10 (15%)
26	CLA	d	307	21	45,53,73	1.81	6 (13%)	52,89,113	1.55	7 (13%)
26	CLA	j	609	17	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
26	CLA	A	817	1	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
29	WVN	B	848	-	40,41,41	5.69	18 (45%)	50,56,56	6.31	32 (64%)
26	CLA	c	308	13	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
29	WVN	l	316	-	40,41,41	5.72	19 (47%)	50,56,56	6.40	32 (64%)
26	CLA	j	608	17	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
26	CLA	B	809	2	65,73,73	1.51	7 (10%)	76,113,113	1.41	6 (7%)
35	II0	h	312	-	39,43,43	6.55	22 (56%)	50,60,60	6.85	28 (56%)
29	WVN	A	845	-	40,41,41	5.80	20 (50%)	50,56,56	6.07	32 (64%)
35	II0	l	315	-	39,43,43	6.57	22 (56%)	50,60,60	6.72	26 (52%)
26	CLA	i	303	20	65,73,73	1.51	5 (7%)	76,113,113	1.39	8 (10%)
26	CLA	A	804	1	65,73,73	1.47	6 (9%)	76,113,113	1.48	6 (7%)
27	PQN	B	843	-	34,34,34	3.07	12 (35%)	42,45,45	2.01	5 (11%)
34	LMG	n	620	-	51,51,55	0.83	2 (3%)	59,59,63	1.24	5 (8%)
26	CLA	n	603	23	51,59,73	1.76	7 (13%)	59,96,113	1.51	10 (16%)
26	CLA	h	307	16	57,65,73	1.64	5 (8%)	66,103,113	1.51	8 (12%)
26	CLA	k	601	19	51,59,73	1.68	5 (9%)	59,96,113	1.56	7 (11%)
29	WVN	L	201	-	40,41,41	5.59	20 (50%)	50,56,56	6.45	34 (68%)
28	LHG	L	207	-	46,46,48	0.65	1 (2%)	49,52,54	1.28	6 (12%)
35	II0	c	316	-	39,43,43	6.63	22 (56%)	50,60,60	7.02	28 (56%)
36	KC2	k	612	19	48,53,53	1.71	10 (20%)	54,89,89	0.81	0
26	CLA	d	306	21	51,59,73	1.72	7 (13%)	59,96,113	1.53	8 (13%)
26	CLA	F	201	38	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
26	CLA	a	309	14	65,73,73	1.51	5 (7%)	76,113,113	1.42	7 (9%)
25	CL0	A	801	-	65,73,73	1.49	8 (12%)	76,113,113	0.87	4 (5%)
26	CLA	A	812	1	65,73,73	1.48	5 (7%)	76,113,113	1.41	6 (7%)
26	CLA	n	607	23	65,73,73	1.50	6 (9%)	76,113,113	1.35	6 (7%)
26	CLA	a	305	14	45,53,73	1.80	5 (11%)	52,89,113	1.60	7 (13%)
35	II0	k	620	-	39,43,43	6.39	22 (56%)	50,60,60	6.93	27 (54%)
26	CLA	j	612	-	51,59,73	1.69	6 (11%)	59,96,113	1.53	6 (10%)
26	CLA	B	802	38	65,73,73	1.50	5 (7%)	76,113,113	1.45	8 (10%)
27	PQN	A	842	-	34,34,34	3.06	13 (38%)	42,45,45	2.08	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	A	849	-	26,26,48	0.68	0	28,29,54	1.42	4 (14%)
35	II0	a	314	-	39,43,43	6.41	21 (53%)	50,60,60	6.95	29 (58%)
35	II0	k	618	-	39,43,43	0.22	0	50,60,60	0.51	1 (2%)
26	CLA	A	803	1	55,63,73	1.70	6 (10%)	64,101,113	1.48	7 (10%)
35	II0	d	315	-	39,43,43	6.54	22 (56%)	50,60,60	6.83	28 (56%)
26	CLA	s	408	38	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
26	CLA	B	842	28	65,73,73	1.48	7 (10%)	76,113,113	1.42	7 (9%)
35	II0	n	615	-	39,43,43	6.48	21 (53%)	50,60,60	6.90	27 (54%)
34	LMG	F	206	-	41,41,55	0.86	0	49,49,63	1.25	3 (6%)
28	LHG	s	409	-	32,32,48	0.80	1 (3%)	36,37,54	1.61	4 (11%)
32	SQD	A	854	-	53,54,54	0.93	3 (5%)	62,65,65	1.70	12 (19%)
36	KC2	s	404	-	48,53,53	1.82	11 (22%)	54,89,89	0.86	1 (1%)
26	CLA	i	307	20	65,73,73	1.49	6 (9%)	76,113,113	1.37	6 (7%)
36	KC2	i	318	20	48,53,53	1.67	10 (20%)	54,89,89	0.93	1 (1%)
26	CLA	A	834	1	60,68,73	1.50	5 (8%)	70,107,113	1.51	7 (10%)
26	CLA	d	303	21	51,59,73	1.69	5 (9%)	59,96,113	1.60	7 (11%)
26	CLA	A	852	1	65,73,73	1.50	6 (9%)	76,113,113	1.41	6 (7%)
26	CLA	b	307	15	61,69,73	1.54	6 (9%)	71,108,113	1.40	8 (11%)
26	CLA	d	313	21	51,59,73	1.70	6 (11%)	59,96,113	1.63	9 (15%)
26	CLA	h	302	16	50,58,73	1.69	7 (14%)	58,95,113	1.59	8 (13%)
26	CLA	k	610	-	51,59,73	1.71	5 (9%)	59,96,113	1.55	8 (13%)
26	CLA	h	308	16	51,59,73	1.70	5 (9%)	59,96,113	1.54	8 (13%)
26	CLA	A	808	1	65,73,73	1.51	6 (9%)	76,113,113	1.43	8 (10%)
29	WVN	B	853	-	40,41,41	5.63	21 (52%)	50,56,56	6.38	33 (66%)
29	WVN	J	102	-	40,41,41	5.71	19 (47%)	50,56,56	6.32	29 (58%)
28	LHG	n	619	-	42,42,48	0.65	1 (2%)	45,48,54	1.20	4 (8%)
30	LMU	A	850	-	36,36,36	1.78	11 (30%)	47,47,47	1.03	2 (4%)
26	CLA	B	841	2	65,73,73	1.52	5 (7%)	76,113,113	1.40	7 (9%)
26	CLA	B	831	38	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
28	LHG	A	844	-	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
26	CLA	A	831	1	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
26	CLA	A	856	38	65,73,73	1.48	5 (7%)	76,113,113	1.44	9 (11%)
26	CLA	A	826	1	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
26	CLA	B	820	2	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
35	II0	i	312	-	39,43,43	6.60	22 (56%)	50,60,60	6.93	30 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	a	303	14	51,59,73	1.71	6 (11%)	59,96,113	1.58	9 (15%)
35	II0	a	316	-	39,43,43	6.63	22 (56%)	50,60,60	6.88	30 (60%)
36	KC2	i	309	20	48,53,53	1.68	10 (20%)	54,89,89	1.11	5 (9%)
26	CLA	j	606	17	51,59,73	1.70	5 (9%)	59,96,113	1.57	7 (11%)
26	CLA	A	841	1	65,73,73	1.49	5 (7%)	76,113,113	1.50	10 (13%)
26	CLA	B	807	2	65,73,73	1.45	5 (7%)	76,113,113	1.40	6 (7%)
29	WVN	A	846	-	40,41,41	5.66	20 (50%)	50,56,56	6.50	32 (64%)
26	CLA	l	305	18	65,73,73	1.41	5 (7%)	76,113,113	1.50	8 (10%)
29	WVN	B	847	-	40,41,41	5.69	20 (50%)	50,56,56	6.18	31 (62%)
26	CLA	b	310	15	65,73,73	1.50	7 (10%)	76,113,113	1.36	8 (10%)
26	CLA	B	818	38	65,73,73	1.50	8 (12%)	76,113,113	1.40	7 (9%)
26	CLA	B	810	2	65,73,73	1.52	5 (7%)	76,113,113	1.33	8 (10%)
26	CLA	h	313	38	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
26	CLA	A	830	1	60,68,73	1.58	6 (10%)	70,107,113	1.40	6 (8%)
26	CLA	i	302	20	65,73,73	1.47	7 (10%)	76,113,113	1.42	8 (10%)
26	CLA	B	825	2	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
26	CLA	A	806	1	60,68,73	1.56	5 (8%)	70,107,113	1.41	7 (10%)
26	CLA	s	402	12	65,73,73	1.53	6 (9%)	76,113,113	1.42	11 (14%)
26	CLA	A	816	1	65,73,73	1.46	6 (9%)	76,113,113	1.58	9 (11%)
26	CLA	l	309	18	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
34	LMG	c	319	26	43,43,55	0.83	0	51,51,63	1.24	4 (7%)
26	CLA	n	605	23	51,59,73	1.69	5 (9%)	59,96,113	1.54	8 (13%)
26	CLA	A	809	1	56,64,73	1.62	6 (10%)	65,102,113	1.45	7 (10%)
35	II0	a	312	-	39,43,43	6.44	22 (56%)	50,60,60	6.74	28 (56%)
26	CLA	A	805	1	65,73,73	1.48	6 (9%)	76,113,113	1.43	7 (9%)
26	CLA	m	602	17	60,68,73	1.53	7 (11%)	70,107,113	1.53	10 (14%)
26	CLA	a	307	14	65,73,73	1.49	5 (7%)	76,113,113	1.35	6 (7%)
26	CLA	k	602	19	65,73,73	1.44	6 (9%)	76,113,113	1.46	6 (7%)
35	II0	d	317	-	39,43,43	6.52	22 (56%)	50,60,60	6.98	27 (54%)
26	CLA	h	301	38	65,73,73	1.50	6 (9%)	76,113,113	3.33	9 (11%)
29	WVN	F	204	-	40,41,41	0.17	0	50,56,56	0.51	0
26	CLA	n	604	23	60,68,73	1.54	5 (8%)	70,107,113	1.58	10 (14%)
26	CLA	d	309	21	41,49,73	1.86	5 (12%)	47,84,113	1.69	9 (19%)
26	CLA	d	308	21	46,54,73	1.78	5 (10%)	53,90,113	1.46	6 (11%)
28	LHG	c	317	-	36,36,48	0.71	1 (2%)	39,42,54	1.26	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	j	605	17	45,53,73	1.82	5 (11%)	52,89,113	1.70	7 (13%)
26	CLA	B	836	38	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
26	CLA	m	605	17	42,50,73	1.84	5 (11%)	48,85,113	1.66	7 (14%)
26	CLA	A	811	1	54,62,73	1.67	5 (9%)	62,99,113	1.46	7 (11%)
26	CLA	m	603	17	59,67,73	1.58	6 (10%)	68,105,113	1.39	6 (8%)
36	KC2	d	311	-	48,53,53	1.70	9 (18%)	54,89,89	1.01	1 (1%)
26	CLA	a	302	14	56,64,73	1.54	6 (10%)	65,102,113	1.54	7 (10%)
36	KC2	d	312	-	48,53,53	1.72	11 (22%)	54,89,89	1.13	6 (11%)
26	CLA	a	304	38	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
36	KC2	k	611	19	48,53,53	1.71	10 (20%)	54,89,89	1.01	3 (5%)
30	LMU	B	852	-	36,36,36	0.23	0	47,47,47	0.37	0
29	WVN	M	101	-	40,41,41	5.64	19 (47%)	50,56,56	6.43	34 (68%)
26	CLA	c	302	13	60,68,73	1.59	6 (10%)	70,107,113	1.41	9 (12%)
26	CLA	A	833	1	65,73,73	1.52	5 (7%)	76,113,113	1.33	6 (7%)
35	II0	m	616	-	39,43,43	6.75	22 (56%)	50,60,60	6.61	26 (52%)
26	CLA	A	838	1	65,73,73	1.53	5 (7%)	76,113,113	1.37	7 (9%)
29	WVN	R	200	-	40,41,41	5.70	20 (50%)	50,56,56	6.42	29 (58%)
26	CLA	l	307	18	65,73,73	1.47	5 (7%)	76,113,113	1.48	7 (9%)
35	II0	k	619	-	39,43,43	6.38	21 (53%)	50,60,60	6.92	28 (56%)
26	CLA	A	819	1	65,73,73	1.50	6 (9%)	76,113,113	1.43	8 (10%)
26	CLA	c	304	13	62,70,73	1.52	5 (8%)	72,109,113	1.51	6 (8%)
26	CLA	L	204	38	60,68,73	1.57	6 (10%)	70,107,113	1.45	7 (10%)
35	II0	b	314	-	39,43,43	6.39	21 (53%)	50,60,60	6.91	29 (58%)
28	LHG	m	618	26	36,36,48	0.70	0	39,42,54	1.23	4 (10%)
26	CLA	A	827	1	62,70,73	1.55	6 (9%)	72,109,113	1.50	8 (11%)
26	CLA	A	832	1	65,73,73	1.52	5 (7%)	76,113,113	1.37	7 (9%)
26	CLA	Q	302	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	7 (9%)
36	KC2	n	612	-	48,53,53	1.69	10 (20%)	54,89,89	1.03	4 (7%)
26	CLA	a	310	14	65,73,73	1.53	6 (9%)	76,113,113	1.38	7 (9%)
26	CLA	i	304	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	6 (7%)
26	CLA	k	607	19	51,59,73	1.69	7 (13%)	59,96,113	1.60	10 (16%)
28	LHG	c	320	-	48,48,48	0.60	0	51,54,54	1.25	6 (11%)
26	CLA	b	308	15	65,73,73	1.48	5 (7%)	76,113,113	1.39	6 (7%)
26	CLA	B	808	2	65,73,73	1.49	7 (10%)	76,113,113	1.52	9 (11%)
26	CLA	A	829	1	65,73,73	1.53	7 (10%)	76,113,113	1.37	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	a	306	14	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
26	CLA	j	603	17	51,59,73	1.66	6 (11%)	59,96,113	1.60	6 (10%)
26	CLA	i	311	20	65,73,73	1.52	6 (9%)	76,113,113	1.41	8 (10%)
35	II0	j	615	-	39,43,43	6.53	22 (56%)	50,60,60	6.88	29 (58%)
26	CLA	B	826	2	65,73,73	1.51	6 (9%)	76,113,113	1.34	7 (9%)
26	CLA	A	818	1	65,73,73	1.50	6 (9%)	76,113,113	1.48	9 (11%)
26	CLA	m	601	17	42,50,73	1.85	5 (11%)	48,85,113	1.62	7 (14%)
35	II0	d	301	-	39,43,43	6.42	21 (53%)	50,60,60	6.82	29 (58%)
26	CLA	s	406	38	65,73,73	1.49	6 (9%)	76,113,113	1.47	10 (13%)
26	CLA	A	820	38	65,73,73	1.50	6 (9%)	76,113,113	1.42	7 (9%)
26	CLA	l	310	18	57,65,73	1.58	6 (10%)	66,103,113	1.48	7 (10%)
34	LMG	b	319	-	42,42,55	0.88	2 (4%)	50,50,63	1.19	4 (8%)
35	II0	k	615	-	39,43,43	6.70	22 (56%)	50,60,60	6.57	30 (60%)
26	CLA	m	604	17	65,73,73	1.47	6 (9%)	76,113,113	1.52	7 (9%)
35	II0	d	316	-	39,43,43	6.59	22 (56%)	50,60,60	6.69	28 (56%)
26	CLA	K	101	11	42,50,73	1.86	6 (14%)	48,85,113	1.67	8 (16%)
35	II0	m	619	-	39,43,43	6.64	22 (56%)	50,60,60	6.80	29 (58%)
26	CLA	j	607	17	51,59,73	1.68	8 (15%)	59,96,113	1.67	12 (20%)
28	LHG	i	317	26	36,36,48	0.70	1 (2%)	39,42,54	1.24	4 (10%)
26	CLA	j	610	28	61,69,73	1.55	5 (8%)	71,108,113	1.42	6 (8%)
29	WVN	B	849	-	40,41,41	5.75	19 (47%)	50,56,56	6.16	30 (60%)
29	WVN	h	309	-	40,41,41	5.65	20 (50%)	50,56,56	6.21	33 (66%)
30	LMU	i	300	-	36,36,36	1.79	10 (27%)	47,47,47	0.88	0
26	CLA	B	840	2	65,73,73	1.51	6 (9%)	76,113,113	1.43	8 (10%)
26	CLA	c	309	-	45,53,73	2.42	12 (26%)	52,89,113	4.77	25 (48%)
26	CLA	A	802	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	8 (10%)
26	CLA	B	830	2	50,58,73	1.70	6 (12%)	58,95,113	1.51	9 (15%)
26	CLA	h	303	16	50,58,73	1.71	5 (10%)	58,95,113	1.55	8 (13%)
35	II0	l	317	-	39,43,43	0.21	0	50,60,60	0.27	0
26	CLA	m	608	17	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
26	CLA	F	202	6	52,60,73	1.69	5 (9%)	60,97,113	1.46	6 (10%)
28	LHG	b	302	26	48,48,48	0.60	0	51,54,54	1.23	5 (9%)
28	LHG	j	617	26	29,29,48	0.78	1 (3%)	32,35,54	1.28	3 (9%)
26	CLA	i	306	20	61,69,73	1.57	5 (8%)	71,108,113	1.38	7 (9%)
26	CLA	m	610	28	55,63,73	1.63	5 (9%)	64,101,113	1.49	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	II0	k	617	-	39,43,43	0.23	0	50,60,60	0.52	1 (2%)
26	CLA	A	825	38	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
26	CLA	B	812	2	65,73,73	1.48	5 (7%)	76,113,113	1.46	7 (9%)
26	CLA	k	605	19	45,53,73	1.81	5 (11%)	52,89,113	1.62	7 (13%)
35	II0	h	311	-	39,43,43	6.30	21 (53%)	50,60,60	7.04	28 (56%)
35	II0	n	616	-	39,43,43	6.59	22 (56%)	50,60,60	6.93	27 (54%)
26	CLA	B	814	2	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
35	II0	m	614	-	39,43,43	6.57	21 (53%)	50,60,60	6.89	30 (60%)
26	CLA	b	304	15	55,63,73	1.56	5 (9%)	64,101,113	1.60	8 (12%)
26	CLA	l	311	28	61,69,73	1.55	5 (8%)	71,108,113	1.43	7 (9%)
26	CLA	B	839	2	57,65,73	1.60	6 (10%)	66,103,113	1.42	7 (10%)
26	CLA	B	828	2	50,58,73	1.74	6 (12%)	58,95,113	1.48	9 (15%)
35	II0	a	313	-	39,43,43	6.53	22 (56%)	50,60,60	6.68	29 (58%)
29	WVN	A	847	-	40,41,41	5.59	19 (47%)	50,56,56	6.69	33 (66%)
26	CLA	B	823	38	64,72,73	1.49	7 (10%)	74,111,113	1.38	8 (10%)
33	DGD	j	618	-	63,63,67	0.97	2 (3%)	77,77,81	1.53	12 (15%)
26	CLA	B	805	2	65,73,73	1.46	5 (7%)	76,113,113	1.56	7 (9%)
26	CLA	B	813	2	60,68,73	1.56	6 (10%)	70,107,113	1.51	10 (14%)
26	CLA	b	306	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
29	WVN	B	850	-	40,41,41	5.68	19 (47%)	50,56,56	6.14	32 (64%)
31	SF4	A	853	2,1	0,12,12	-	-	-	-	-
30	LMU	a	317	-	36,36,36	0.17	0	47,47,47	0.46	0
26	CLA	A	815	38	45,53,73	1.80	6 (13%)	52,89,113	1.68	6 (11%)
35	II0	c	314	-	39,43,43	0.30	0	50,60,60	0.53	1 (2%)
26	CLA	k	603	19	51,59,73	1.74	6 (11%)	59,96,113	1.44	6 (10%)
35	II0	i	314	-	39,43,43	6.59	22 (56%)	50,60,60	6.89	29 (58%)
26	CLA	l	306	18	51,59,73	1.66	5 (9%)	59,96,113	1.65	7 (11%)
26	CLA	s	403	12	65,73,73	1.49	6 (9%)	76,113,113	1.44	8 (10%)
28	LHG	B	851	26	48,48,48	0.60	0	51,54,54	1.23	6 (11%)
26	CLA	c	312	13	65,73,73	1.52	5 (7%)	76,113,113	1.35	6 (7%)
34	LMG	F	205	-	53,53,55	0.75	0	61,61,63	1.33	8 (13%)
26	CLA	L	206	-	51,59,73	1.71	5 (9%)	59,96,113	1.48	6 (10%)
26	CLA	B	804	-	65,73,73	1.49	8 (12%)	76,113,113	1.73	13 (17%)
35	II0	i	313	-	39,43,43	6.60	22 (56%)	50,60,60	6.71	28 (56%)
26	CLA	A	807	1	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.66	7 (13%)
26	CLA	k	609	19	57,65,73	1.63	5 (8%)	66,103,113	1.48	7 (10%)
36	KC2	k	613	-	48,53,53	1.69	10 (20%)	54,89,89	0.89	1 (1%)
26	CLA	n	608	-	65,73,73	1.54	6 (9%)	76,113,113	1.30	9 (11%)
26	CLA	B	801	38	65,73,73	1.50	6 (9%)	76,113,113	1.34	6 (7%)
26	CLA	a	311	14	48,56,73	1.75	5 (10%)	55,92,113	1.54	6 (10%)
26	CLA	n	609	23	65,73,73	1.48	5 (7%)	76,113,113	1.33	7 (9%)
26	CLA	n	610	-	60,68,73	1.57	5 (8%)	70,107,113	1.45	8 (11%)
35	II0	J	104	-	39,43,43	6.41	22 (56%)	50,60,60	7.04	29 (58%)
26	CLA	A	810	1	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
26	CLA	j	604	17	65,73,73	1.47	6 (9%)	76,113,113	1.51	8 (10%)
26	CLA	i	301	20	65,73,73	1.51	5 (7%)	76,113,113	1.40	7 (9%)
26	CLA	b	313	28	51,59,73	1.69	6 (11%)	59,96,113	1.57	10 (16%)
37	IHT	m	617	-	40,42,42	0.25	0	53,58,58	0.58	1 (1%)
26	CLA	m	606	17	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
30	LMU	A	858	-	35,35,36	0.20	0	46,46,47	0.50	0
26	CLA	b	312	15	65,73,73	1.51	5 (7%)	76,113,113	1.38	6 (7%)
37	IHT	b	316	-	40,42,42	0.27	0	53,58,58	0.88	3 (5%)
28	LHG	A	843	-	47,47,48	0.62	1 (2%)	50,53,54	1.23	5 (10%)
35	II0	k	616	-	39,43,43	6.65	22 (56%)	50,60,60	6.66	26 (52%)
26	CLA	l	313	18	56,64,73	1.64	5 (8%)	65,102,113	1.55	7 (10%)
29	WVN	J	101	-	40,41,41	5.63	18 (45%)	50,56,56	6.31	32 (64%)
26	CLA	B	816	2	65,73,73	1.52	5 (7%)	76,113,113	1.33	7 (9%)
29	WVN	B	845	-	40,41,41	0.15	0	50,56,56	0.41	0
26	CLA	A	840	38	65,73,73	1.52	6 (9%)	76,113,113	1.45	8 (10%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
26	CLA	B	803	2	65,73,73	1.48	8 (12%)	76,113,113	1.28	7 (9%)
28	LHG	A	855	-	35,35,48	0.69	0	38,41,54	1.25	4 (10%)
26	CLA	d	302	21	62,70,73	1.54	6 (9%)	72,109,113	1.40	7 (9%)
26	CLA	A	836	1	65,73,73	1.53	6 (9%)	76,113,113	1.43	7 (9%)
26	CLA	B	834	2	65,73,73	1.49	5 (7%)	76,113,113	1.46	8 (10%)
26	CLA	d	310	21	41,49,73	1.89	6 (14%)	47,84,113	1.65	8 (17%)
31	SF4	C	101	3	0,12,12	-	-	-	-	-
26	CLA	l	301	18	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
26	CLA	j	602	17	54,62,73	1.60	6 (11%)	62,99,113	1.56	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	822	38	65,73,73	1.50	7 (10%)	76,113,113	1.51	8 (10%)
26	CLA	h	306	16	65,73,73	1.51	6 (9%)	76,113,113	1.40	9 (11%)
28	LHG	J	105	26	32,32,48	0.75	1 (3%)	35,38,54	1.26	3 (8%)
26	CLA	n	602	23	50,58,73	1.63	6 (12%)	58,95,113	1.65	7 (12%)
28	LHG	b	318	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
29	WVN	A	857	-	40,41,41	5.69	20 (50%)	50,56,56	6.42	31 (62%)
26	CLA	c	306	13	52,60,73	1.70	7 (13%)	60,97,113	1.45	8 (13%)
26	CLA	c	303	13	51,59,73	1.70	5 (9%)	59,96,113	1.55	6 (10%)
35	II0	d	319	-	39,43,43	0.29	0	50,60,60	0.80	2 (4%)
26	CLA	b	303	15	51,59,73	1.68	5 (9%)	59,96,113	1.55	7 (11%)
37	IHT	R	202	-	40,42,42	0.23	0	53,58,58	0.36	0
34	LMG	c	318	-	55,55,55	0.71	0	63,63,63	1.38	9 (14%)
26	CLA	n	606	23	51,59,73	1.75	7 (13%)	59,96,113	1.48	7 (11%)
26	CLA	j	613	17	65,73,73	1.52	6 (9%)	76,113,113	1.39	8 (10%)
26	CLA	d	305	-	51,59,73	1.69	5 (9%)	59,96,113	1.56	7 (11%)
26	CLA	B	824	2	65,73,73	1.49	6 (9%)	76,113,113	1.39	6 (7%)
26	CLA	A	839	1	60,68,73	1.55	5 (8%)	70,107,113	1.45	6 (8%)
35	II0	l	314	-	39,43,43	6.42	22 (56%)	50,60,60	7.01	30 (60%)
29	WVN	I	101	-	40,41,41	5.50	19 (47%)	50,56,56	6.42	33 (66%)
26	CLA	h	304	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
37	IHT	j	616	-	40,42,42	0.23	0	53,58,58	0.84	3 (5%)
26	CLA	L	202	9	49,57,73	1.72	5 (10%)	55,93,113	1.56	7 (12%)
26	CLA	L	203	9	65,73,73	1.48	5 (7%)	76,113,113	1.46	8 (10%)
28	LHG	l	318	26	31,31,48	0.77	1 (3%)	34,37,54	1.28	4 (11%)
26	CLA	i	308	28	46,54,73	1.77	5 (10%)	53,90,113	1.58	6 (11%)
26	CLA	A	823	1	55,63,73	1.64	5 (9%)	64,101,113	1.52	8 (12%)
26	CLA	k	608	19	65,73,73	1.49	7 (10%)	76,113,113	1.32	7 (9%)
37	IHT	n	617	-	40,42,42	0.22	0	53,58,58	0.60	0
36	KC2	s	401	12	48,53,53	3.26	22 (45%)	54,89,89	3.94	30 (55%)
37	IHT	c	315	-	40,42,42	0.54	0	53,58,58	0.41	0
26	CLA	B	817	2	65,73,73	1.52	5 (7%)	76,113,113	1.38	6 (7%)
26	CLA	k	604	-	65,73,73	1.61	7 (10%)	76,113,113	1.35	8 (10%)
35	II0	b	315	-	39,43,43	6.51	21 (53%)	50,60,60	6.77	24 (48%)
26	CLA	A	822	1	56,64,73	1.61	6 (10%)	65,102,113	1.48	7 (10%)
26	CLA	k	606	19	51,59,73	1.67	6 (11%)	59,96,113	1.54	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	KC2	n	611	23	48,53,53	1.70	10 (20%)	54,89,89	1.11	4 (7%)
33	DGD	B	844	-	67,67,67	0.87	1 (1%)	81,81,81	1.44	9 (11%)
35	II0	b	317	-	39,43,43	0.41	0	50,60,60	0.51	0
26	CLA	h	305	16	51,59,73	1.69	6 (11%)	59,96,113	1.55	8 (13%)
29	WVN	i	315	-	40,41,41	5.71	21 (52%)	50,56,56	6.49	30 (60%)
26	CLA	B	819	2	65,73,73	1.53	7 (10%)	76,113,113	1.54	11 (14%)
36	KC2	l	312	18	48,53,53	1.71	11 (22%)	54,89,89	1.01	2 (3%)
26	CLA	B	806	2	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
26	CLA	m	609	17	60,68,73	1.56	5 (8%)	70,107,113	1.42	7 (10%)
26	CLA	b	309	34	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)
26	CLA	c	305	13	65,73,73	1.52	6 (9%)	76,113,113	1.36	6 (7%)
35	II0	i	319	-	39,43,43	6.56	21 (53%)	50,60,60	6.72	29 (58%)
26	CLA	A	814	1	50,58,73	1.68	6 (12%)	58,95,113	1.59	8 (13%)
26	CLA	b	305	15	52,60,73	1.67	6 (11%)	60,97,113	1.60	7 (11%)
26	CLA	l	304	18	47,55,73	1.76	5 (10%)	54,91,113	1.56	7 (12%)
26	CLA	B	827	2	51,59,73	1.69	6 (11%)	59,96,113	1.69	9 (15%)
26	CLA	b	311	15	64,72,73	1.52	6 (9%)	74,111,113	1.42	7 (9%)
26	CLA	B	832	38	45,53,73	1.83	5 (11%)	52,89,113	1.64	6 (11%)
36	KC2	j	611	17	48,53,53	1.69	9 (18%)	54,89,89	0.92	2 (3%)
26	CLA	R	201	22	55,63,73	1.70	5 (9%)	64,101,113	1.62	10 (15%)
26	CLA	B	835	2	47,55,73	1.83	7 (14%)	54,91,113	1.53	9 (16%)
29	WVN	s	407	-	40,41,41	5.65	19 (47%)	50,56,56	6.62	32 (64%)
35	II0	d	314	-	39,43,43	0.19	0	50,60,60	0.62	2 (4%)
35	II0	n	618	-	39,43,43	6.58	22 (56%)	50,60,60	6.87	29 (58%)
26	CLA	B	821	2	53,61,73	1.66	6 (11%)	61,98,113	1.46	9 (14%)
29	WVN	L	205	-	40,41,41	5.69	19 (47%)	50,56,56	6.21	30 (60%)
26	CLA	n	601	23	45,53,73	1.80	5 (11%)	52,89,113	1.61	7 (13%)
26	CLA	A	821	1	49,57,73	1.72	5 (10%)	55,93,113	1.65	8 (14%)
34	LMG	L	209	-	45,45,55	0.83	1 (2%)	53,53,63	1.23	3 (5%)
26	CLA	B	811	2	55,63,73	1.65	6 (10%)	64,101,113	1.44	7 (10%)
26	CLA	l	308	18	65,73,73	1.49	5 (7%)	76,113,113	1.37	6 (7%)
26	CLA	d	318	-	45,53,73	1.79	5 (11%)	52,89,113	1.63	6 (11%)
26	CLA	B	837	2	65,73,73	1.51	6 (9%)	76,113,113	1.32	5 (6%)
37	IHT	a	315	-	40,42,42	0.24	0	53,58,58	0.59	1 (1%)
26	CLA	i	310	-	60,68,73	1.55	6 (10%)	70,107,113	1.48	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	301	13	51,59,73	1.68	5 (9%)	59,96,113	1.54	6 (10%)
26	CLA	a	308	28	48,56,73	1.74	5 (10%)	55,92,113	1.57	7 (12%)
26	CLA	J	103	8	42,50,73	1.86	5 (11%)	48,85,113	1.66	7 (14%)
35	II0	l	302	-	39,43,43	6.71	21 (53%)	50,60,60	6.91	28 (56%)
26	CLA	A	835	1	65,73,73	1.50	5 (7%)	76,113,113	1.38	7 (9%)
26	CLA	k	614	19	51,59,73	1.72	6 (11%)	59,96,113	1.57	7 (11%)
26	CLA	A	851	38	65,73,73	1.53	6 (9%)	76,113,113	1.43	6 (7%)
26	CLA	j	601	17	65,73,73	1.51	6 (9%)	76,113,113	1.41	7 (9%)
35	II0	c	313	-	39,43,43	6.50	22 (56%)	50,60,60	6.90	29 (58%)
26	CLA	B	833	2	55,63,73	1.64	5 (9%)	64,101,113	1.57	8 (12%)
26	CLA	m	607	17	51,59,73	1.71	5 (9%)	59,96,113	1.46	7 (11%)
37	IHT	b	301	-	40,42,42	0.30	0	53,58,58	0.54	0
26	CLA	B	838	2	65,73,73	1.48	6 (9%)	76,113,113	1.43	8 (10%)
26	CLA	n	613	23	51,59,73	1.72	5 (9%)	59,96,113	1.51	9 (15%)
35	II0	i	316	-	39,43,43	6.50	21 (53%)	50,60,60	6.98	33 (66%)
29	WVN	F	203	-	40,41,41	5.66	18 (45%)	50,56,56	6.17	32 (64%)
26	CLA	m	612	38	51,59,73	1.68	6 (11%)	59,96,113	1.57	9 (15%)
26	CLA	a	301	14	65,73,73	1.50	7 (10%)	76,113,113	1.46	8 (10%)
26	CLA	B	815	2	55,63,73	1.62	5 (9%)	64,101,113	1.47	6 (9%)
36	KC2	c	310	13	48,53,53	3.32	20 (41%)	54,89,89	3.83	29 (53%)
26	CLA	A	837	1	65,73,73	1.52	6 (9%)	76,113,113	1.36	6 (7%)
26	CLA	i	305	20	51,59,73	1.70	8 (15%)	59,96,113	1.67	8 (13%)
28	LHG	L	208	-	44,44,48	0.64	0	47,50,54	1.25	5 (10%)
26	CLA	A	828	1	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
29	WVN	l	303	-	40,41,41	5.63	19 (47%)	50,56,56	6.28	32 (64%)

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
35	II0	h	310	-	-	11/17/40/67	0/1/1/2
35	II0	n	614	-	-	1/21/67/67	0/2/2/2
29	WVN	A	848	-	-	18/29/63/63	0/2/2/2
35	II0	m	615	-	-	11/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	Q	301	-	-	15/33/53/70	0/1/1/1
29	WVN	B	846	-	-	15/29/63/63	0/2/2/2
29	WVN	s	405	-	-	16/29/63/63	0/2/2/2
26	CLA	m	613	17	1/1/15/20	12/37/115/115	-
35	II0	j	614	-	-	13/21/67/67	0/2/2/2
26	CLA	d	304	-	1/1/11/20	8/13/91/115	-
29	WVN	K	102	-	-	17/29/63/63	0/2/2/2
36	KC2	m	611	17	-	10/15/71/71	-
26	CLA	A	824	38	1/1/15/20	10/37/115/115	-
26	CLA	c	307	13	1/1/11/20	7/15/93/115	-
26	CLA	B	829	2	1/1/15/20	11/37/115/115	-
26	CLA	A	813	1	1/1/13/20	10/27/105/115	-
26	CLA	d	307	21	1/1/11/20	7/13/91/115	-
26	CLA	j	609	17	1/1/15/20	15/37/115/115	-
26	CLA	A	817	1	1/1/15/20	11/37/115/115	-
29	WVN	B	848	-	-	17/29/63/63	0/2/2/2
26	CLA	c	308	13	1/1/15/20	17/37/115/115	-
29	WVN	l	316	-	-	17/29/63/63	0/2/2/2
26	CLA	j	608	17	1/1/11/20	5/13/91/115	-
26	CLA	B	809	2	1/1/15/20	7/37/115/115	-
35	II0	h	312	-	-	11/21/67/67	0/2/2/2
29	WVN	A	845	-	-	16/29/63/63	0/2/2/2
35	II0	l	315	-	-	11/21/67/67	0/2/2/2
26	CLA	i	303	20	1/1/15/20	6/37/115/115	-
26	CLA	A	804	1	1/1/15/20	9/37/115/115	-
27	PQN	B	843	-	-	7/23/43/43	0/2/2/2
34	LMG	n	620	-	-	17/46/66/70	0/1/1/1
26	CLA	n	603	23	1/1/12/20	6/21/99/115	-
26	CLA	h	307	16	1/1/13/20	7/28/106/115	-
26	CLA	k	601	19	1/1/12/20	5/21/99/115	-
29	WVN	L	201	-	-	16/29/63/63	0/2/2/2
28	LHG	L	207	-	-	19/51/51/53	-
35	II0	c	316	-	-	13/21/67/67	0/2/2/2
36	KC2	k	612	19	-	9/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	d	306	21	1/1/12/20	5/21/99/115	-
26	CLA	F	201	38	1/1/15/20	15/37/115/115	-
26	CLA	a	309	14	1/1/15/20	10/37/115/115	-
25	CL0	A	801	-	2/2/20/25	16/37/135/135	-
26	CLA	A	812	1	1/1/15/20	12/37/115/115	-
26	CLA	n	607	23	1/1/15/20	11/37/115/115	-
26	CLA	a	305	14	1/1/11/20	5/13/91/115	-
35	II0	k	620	-	-	13/21/67/67	0/2/2/2
26	CLA	j	612	-	1/1/12/20	9/21/99/115	-
26	CLA	B	802	38	1/1/15/20	13/37/115/115	-
27	PQN	A	842	-	-	10/23/43/43	0/2/2/2
28	LHG	A	849	-	-	14/27/27/53	-
35	II0	a	314	-	-	14/21/67/67	0/2/2/2
35	II0	k	618	-	-	1/21/67/67	0/2/2/2
26	CLA	A	803	1	1/1/13/20	4/25/103/115	-
35	II0	d	315	-	-	12/21/67/67	0/2/2/2
26	CLA	s	408	38	1/1/15/20	9/37/115/115	-
26	CLA	B	842	28	1/1/15/20	11/37/115/115	-
35	II0	n	615	-	-	11/21/67/67	0/2/2/2
34	LMG	F	206	-	-	12/36/56/70	0/1/1/1
28	LHG	s	409	-	-	15/34/34/53	-
32	SQD	A	854	-	-	19/49/69/69	0/1/1/1
36	KC2	s	404	-	-	1/15/71/71	-
26	CLA	i	307	20	1/1/15/20	10/37/115/115	-
36	KC2	i	318	20	-	11/15/71/71	-
26	CLA	A	834	1	1/1/14/20	7/31/109/115	-
26	CLA	d	303	21	1/1/12/20	7/21/99/115	-
26	CLA	A	852	1	1/1/15/20	12/37/115/115	-
26	CLA	b	307	15	1/1/14/20	9/33/111/115	-
26	CLA	d	313	21	1/1/12/20	7/21/99/115	-
26	CLA	h	302	16	1/1/12/20	6/19/97/115	-
26	CLA	k	610	-	1/1/12/20	10/21/99/115	-
26	CLA	h	308	16	1/1/12/20	6/21/99/115	-
26	CLA	A	808	1	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	WVN	B	853	-	-	20/29/63/63	0/2/2/2
29	WVN	J	102	-	-	19/29/63/63	0/2/2/2
28	LHG	n	619	-	-	23/47/47/53	-
30	LMU	A	850	-	-	13/21/61/61	0/2/2/2
26	CLA	B	841	2	1/1/15/20	15/37/115/115	-
26	CLA	B	831	38	1/1/15/20	12/37/115/115	-
28	LHG	A	844	-	-	8/31/31/53	-
26	CLA	A	831	1	1/1/15/20	13/37/115/115	-
26	CLA	A	856	38	1/1/15/20	11/37/115/115	-
26	CLA	A	826	1	1/1/15/20	11/37/115/115	-
26	CLA	B	820	2	1/1/15/20	9/37/115/115	-
35	II0	i	312	-	-	12/21/67/67	0/2/2/2
26	CLA	a	303	14	1/1/12/20	0/21/99/115	-
35	II0	a	316	-	-	10/21/67/67	0/2/2/2
36	KC2	i	309	20	-	11/15/71/71	-
26	CLA	j	606	17	1/1/12/20	6/21/99/115	-
26	CLA	A	841	1	1/1/15/20	13/37/115/115	-
26	CLA	B	807	2	1/1/15/20	11/37/115/115	-
29	WVN	A	846	-	-	16/29/63/63	0/2/2/2
26	CLA	l	305	18	1/1/15/20	14/37/115/115	-
29	WVN	B	847	-	-	16/29/63/63	0/2/2/2
26	CLA	b	310	15	1/1/15/20	13/37/115/115	-
26	CLA	B	818	38	1/1/15/20	10/37/115/115	-
26	CLA	B	810	2	1/1/15/20	13/37/115/115	-
26	CLA	h	313	38	1/1/15/20	4/37/115/115	-
26	CLA	A	830	1	1/1/14/20	8/31/109/115	-
26	CLA	i	302	20	1/1/15/20	16/37/115/115	-
26	CLA	B	825	2	1/1/15/20	19/37/115/115	-
26	CLA	A	806	1	1/1/14/20	5/31/109/115	-
26	CLA	s	402	12	1/1/15/20	21/37/115/115	-
26	CLA	A	816	1	1/1/15/20	20/37/115/115	-
26	CLA	l	309	18	1/1/15/20	6/37/115/115	-
34	LMG	c	319	26	-	21/38/58/70	0/1/1/1
26	CLA	n	605	23	1/1/12/20	7/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	809	1	1/1/13/20	11/27/105/115	-
35	II0	a	312	-	-	11/21/67/67	0/2/2/2
26	CLA	A	805	1	1/1/15/20	14/37/115/115	-
26	CLA	m	602	17	1/1/14/20	15/31/109/115	-
26	CLA	a	307	14	1/1/15/20	13/37/115/115	-
26	CLA	k	602	19	1/1/15/20	15/37/115/115	-
35	II0	d	317	-	-	13/21/67/67	0/2/2/2
26	CLA	h	301	38	1/1/15/20	10/37/115/115	-
29	WVN	F	204	-	-	6/29/63/63	0/2/2/2
26	CLA	n	604	23	1/1/14/20	11/31/109/115	-
26	CLA	d	309	21	1/1/10/20	2/8/86/115	-
26	CLA	d	308	21	1/1/11/20	9/15/93/115	-
28	LHG	c	317	-	-	19/41/41/53	-
26	CLA	j	605	17	1/1/11/20	8/13/91/115	-
26	CLA	B	836	38	1/1/15/20	15/37/115/115	-
26	CLA	m	605	17	1/1/10/20	5/10/88/115	-
26	CLA	A	811	1	1/1/12/20	8/24/102/115	-
26	CLA	m	603	17	1/1/13/20	7/30/108/115	-
36	KC2	d	311	-	-	13/15/71/71	-
26	CLA	a	302	14	1/1/13/20	5/27/105/115	-
36	KC2	d	312	-	-	11/15/71/71	-
26	CLA	a	304	38	1/1/15/20	8/37/115/115	-
36	KC2	k	611	19	-	13/15/71/71	-
30	LMU	B	852	-	-	2/21/61/61	0/2/2/2
29	WVN	M	101	-	-	18/29/63/63	0/2/2/2
26	CLA	c	302	13	-	15/31/109/115	-
26	CLA	A	833	1	1/1/15/20	16/37/115/115	-
35	II0	m	616	-	-	12/21/67/67	0/2/2/2
26	CLA	A	838	1	1/1/15/20	10/37/115/115	-
29	WVN	R	200	-	-	17/29/63/63	0/2/2/2
26	CLA	l	307	18	1/1/15/20	14/37/115/115	-
35	II0	k	619	-	-	10/21/67/67	0/2/2/2
26	CLA	A	819	1	1/1/15/20	19/37/115/115	-
26	CLA	c	304	13	1/1/14/20	13/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	L	204	38	1/1/14/20	6/31/109/115	-
35	II0	b	314	-	-	11/21/67/67	0/2/2/2
28	LHG	m	618	26	-	11/41/41/53	-
26	CLA	A	827	1	1/1/14/20	8/34/112/115	-
26	CLA	A	832	1	1/1/15/20	6/37/115/115	-
26	CLA	Q	302	-	1/1/15/20	13/37/115/115	-
36	KC2	n	612	-	-	11/15/71/71	-
26	CLA	a	310	14	-	12/37/115/115	-
26	CLA	i	304	-	1/1/15/20	15/37/115/115	-
26	CLA	k	607	19	1/1/12/20	11/21/99/115	-
28	LHG	c	320	-	-	21/53/53/53	-
26	CLA	b	308	15	1/1/15/20	13/37/115/115	-
26	CLA	B	808	2	1/1/15/20	8/37/115/115	-
26	CLA	A	829	1	1/1/15/20	5/37/115/115	-
26	CLA	a	306	14	1/1/15/20	12/37/115/115	-
26	CLA	j	603	17	1/1/12/20	5/21/99/115	-
26	CLA	i	311	20	1/1/15/20	12/37/115/115	-
35	II0	j	615	-	-	10/21/67/67	0/2/2/2
26	CLA	B	826	2	1/1/15/20	16/37/115/115	-
26	CLA	A	818	1	1/1/15/20	16/37/115/115	-
26	CLA	m	601	17	1/1/10/20	4/10/88/115	-
35	II0	d	301	-	-	10/21/67/67	0/2/2/2
26	CLA	s	406	38	1/1/15/20	10/37/115/115	-
26	CLA	A	820	38	1/1/15/20	8/37/115/115	-
26	CLA	l	310	18	1/1/13/20	9/28/106/115	-
34	LMG	b	319	-	-	15/37/57/70	0/1/1/1
35	II0	k	615	-	-	13/21/67/67	0/2/2/2
26	CLA	m	604	17	1/1/15/20	12/37/115/115	-
35	II0	d	316	-	-	13/21/67/67	0/2/2/2
26	CLA	K	101	11	1/1/10/20	4/10/88/115	-
35	II0	m	619	-	-	11/21/67/67	0/2/2/2
26	CLA	j	607	17	1/1/12/20	11/21/99/115	-
28	LHG	i	317	26	-	17/41/41/53	-
26	CLA	j	610	28	1/1/14/20	8/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	WVN	B	849	-	-	17/29/63/63	0/2/2/2
29	WVN	h	309	-	-	19/29/63/63	0/2/2/2
30	LMU	i	300	-	-	13/21/61/61	0/2/2/2
26	CLA	B	840	2	1/1/15/20	8/37/115/115	-
26	CLA	h	303	16	1/1/12/20	7/19/97/115	-
26	CLA	A	802	-	1/1/15/20	7/37/115/115	-
26	CLA	B	830	2	1/1/12/20	9/19/97/115	-
26	CLA	c	309	-	-	4/13/91/115	-
35	II0	l	317	-	-	3/21/67/67	0/2/2/2
26	CLA	m	608	17	1/1/15/20	12/37/115/115	-
26	CLA	F	202	6	1/1/12/20	11/22/100/115	-
28	LHG	b	302	26	-	22/53/53/53	-
28	LHG	j	617	26	-	16/34/34/53	-
26	CLA	i	306	20	1/1/14/20	15/33/111/115	-
26	CLA	m	610	28	1/1/13/20	12/25/103/115	-
35	II0	k	617	-	-	2/21/67/67	0/2/2/2
26	CLA	A	825	38	1/1/15/20	5/37/115/115	-
26	CLA	B	812	2	1/1/15/20	14/37/115/115	-
26	CLA	k	605	19	1/1/11/20	5/13/91/115	-
35	II0	h	311	-	-	14/21/67/67	0/2/2/2
35	II0	n	616	-	-	13/21/67/67	0/2/2/2
26	CLA	B	814	2	1/1/15/20	12/37/115/115	-
35	II0	m	614	-	-	13/21/67/67	0/2/2/2
26	CLA	b	304	15	1/1/13/20	11/25/103/115	-
26	CLA	l	311	28	1/1/14/20	11/33/111/115	-
26	CLA	B	839	2	1/1/13/20	9/28/106/115	-
26	CLA	B	828	2	1/1/12/20	10/19/97/115	-
35	II0	a	313	-	-	11/21/67/67	0/2/2/2
29	WVN	A	847	-	-	17/29/63/63	0/2/2/2
26	CLA	B	823	38	1/1/14/20	10/36/114/115	-
33	DGD	j	618	-	-	23/51/91/95	0/2/2/2
26	CLA	B	805	2	1/1/15/20	13/37/115/115	-
26	CLA	B	813	2	1/1/14/20	13/31/109/115	-
26	CLA	b	306	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	WVN	B	850	-	-	17/29/63/63	0/2/2/2
31	SF4	A	853	2,1	-	-	0/6/5/5
30	LMU	a	317	-	-	15/21/61/61	0/2/2/2
26	CLA	A	815	38	1/1/11/20	5/13/91/115	-
35	II0	c	314	-	-	1/21/67/67	0/2/2/2
26	CLA	k	603	19	1/1/12/20	5/21/99/115	-
35	II0	i	314	-	-	13/21/67/67	0/2/2/2
26	CLA	l	306	18	1/1/12/20	1/21/99/115	-
26	CLA	s	403	12	1/1/15/20	10/37/115/115	-
28	LHG	B	851	26	-	32/53/53/53	-
26	CLA	c	312	13	1/1/15/20	14/37/115/115	-
34	LMG	F	205	-	-	29/48/68/70	0/1/1/1
26	CLA	L	206	-	1/1/12/20	4/21/99/115	-
26	CLA	B	804	-	1/1/15/20	10/37/115/115	-
35	II0	i	313	-	-	13/21/67/67	0/2/2/2
26	CLA	A	807	1	1/1/15/20	11/37/115/115	-
26	CLA	c	311	-	1/1/11/20	6/13/91/115	-
26	CLA	k	609	19	1/1/13/20	9/28/106/115	-
36	KC2	k	613	-	-	12/15/71/71	-
26	CLA	n	608	-	1/1/15/20	16/37/115/115	-
26	CLA	B	801	38	1/1/15/20	17/37/115/115	-
26	CLA	a	311	14	1/1/11/20	8/17/95/115	-
26	CLA	n	609	23	1/1/15/20	11/37/115/115	-
26	CLA	n	610	-	1/1/14/20	11/31/109/115	-
35	II0	J	104	-	-	12/21/67/67	0/2/2/2
26	CLA	A	810	1	1/1/15/20	12/37/115/115	-
26	CLA	j	604	17	1/1/15/20	11/37/115/115	-
26	CLA	i	301	20	1/1/15/20	20/37/115/115	-
26	CLA	b	313	28	1/1/12/20	6/21/99/115	-
37	IHT	m	617	-	-	4/25/65/65	0/2/2/2
26	CLA	m	606	17	1/1/15/20	17/37/115/115	-
30	LMU	A	858	-	-	6/20/60/61	0/2/2/2
26	CLA	b	312	15	1/1/15/20	13/37/115/115	-
37	IHT	b	316	-	-	5/25/65/65	0/2/2/2
28	LHG	A	843	-	-	19/52/52/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	II0	k	616	-	-	10/21/67/67	0/2/2/2
26	CLA	l	313	18	1/1/13/20	9/27/105/115	-
29	WVN	J	101	-	-	19/29/63/63	0/2/2/2
26	CLA	B	816	2	1/1/15/20	16/37/115/115	-
29	WVN	B	845	-	-	2/29/63/63	0/2/2/2
26	CLA	A	840	38	1/1/15/20	10/37/115/115	-
31	SF4	C	102	3	-	-	0/6/5/5
26	CLA	B	803	2	1/1/15/20	16/37/115/115	-
28	LHG	A	855	-	-	23/40/40/53	-
26	CLA	d	302	21	1/1/14/20	17/34/112/115	-
26	CLA	A	836	1	1/1/15/20	10/37/115/115	-
26	CLA	B	834	2	1/1/15/20	11/37/115/115	-
26	CLA	d	310	21	1/1/10/20	4/8/86/115	-
31	SF4	C	101	3	-	-	0/6/5/5
26	CLA	l	301	18	1/1/15/20	12/37/115/115	-
26	CLA	j	602	17	1/1/12/20	9/24/102/115	-
26	CLA	B	822	38	1/1/15/20	19/37/115/115	-
26	CLA	h	306	16	1/1/15/20	9/37/115/115	-
28	LHG	J	105	26	-	14/37/37/53	-
26	CLA	n	602	23	1/1/12/20	5/19/97/115	-
28	LHG	b	318	-	-	32/53/53/53	-
29	WVN	A	857	-	-	18/29/63/63	0/2/2/2
26	CLA	c	306	13	1/1/12/20	6/22/100/115	-
26	CLA	c	303	13	1/1/12/20	6/21/99/115	-
35	II0	d	319	-	-	11/21/67/67	0/2/2/2
26	CLA	b	303	15	1/1/12/20	5/21/99/115	-
37	IHT	R	202	-	-	2/25/65/65	0/2/2/2
34	LMG	c	318	-	-	24/50/70/70	0/1/1/1
26	CLA	n	606	23	-	4/21/99/115	-
26	CLA	j	613	17	1/1/15/20	13/37/115/115	-
26	CLA	d	305	-	1/1/12/20	6/21/99/115	-
26	CLA	B	824	2	1/1/15/20	8/37/115/115	-
26	CLA	A	839	1	1/1/14/20	2/31/109/115	-
35	II0	l	314	-	-	12/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	WVN	I	101	-	-	17/29/63/63	0/2/2/2
26	CLA	h	304	-	1/1/15/20	16/37/115/115	-
37	IHT	j	616	-	-	3/25/65/65	0/2/2/2
26	CLA	L	202	9	1/1/11/20	8/18/96/115	-
26	CLA	L	203	9	1/1/15/20	4/37/115/115	-
28	LHG	l	318	26	-	9/36/36/53	-
26	CLA	i	308	28	1/1/11/20	7/15/93/115	-
26	CLA	A	823	1	1/1/13/20	9/25/103/115	-
26	CLA	k	608	19	1/1/15/20	14/37/115/115	-
37	IHT	n	617	-	-	3/25/65/65	0/2/2/2
36	KC2	s	401	12	-	5/15/71/71	-
37	IHT	c	315	-	-	0/25/65/65	0/2/2/2
26	CLA	B	817	2	1/1/15/20	10/37/115/115	-
26	CLA	k	604	-	-	9/37/115/115	-
35	II0	b	315	-	-	13/21/67/67	0/2/2/2
26	CLA	A	822	1	1/1/13/20	16/27/105/115	-
26	CLA	k	606	19	1/1/12/20	5/21/99/115	-
36	KC2	n	611	23	-	12/15/71/71	-
33	DGD	B	844	-	-	27/55/95/95	0/2/2/2
35	II0	b	317	-	-	0/21/67/67	0/2/2/2
26	CLA	h	305	16	1/1/12/20	6/21/99/115	-
29	WVN	i	315	-	-	15/29/63/63	0/2/2/2
26	CLA	B	819	2	1/1/15/20	19/37/115/115	-
36	KC2	l	312	18	-	5/15/71/71	-
26	CLA	B	806	2	1/1/15/20	12/37/115/115	-
26	CLA	m	609	17	1/1/14/20	12/31/109/115	-
26	CLA	b	309	34	1/1/15/20	6/37/115/115	-
26	CLA	c	305	13	1/1/15/20	4/37/115/115	-
35	II0	i	319	-	-	12/21/67/67	0/2/2/2
26	CLA	A	814	1	1/1/12/20	9/19/97/115	-
26	CLA	b	305	15	1/1/12/20	4/22/100/115	-
26	CLA	l	304	18	1/1/11/20	5/16/94/115	-
26	CLA	B	827	2	1/1/12/20	4/21/99/115	-
26	CLA	b	311	15	1/1/14/20	12/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	832	38	1/1/11/20	2/13/91/115	-
36	KC2	j	611	17	-	11/15/71/71	-
26	CLA	R	201	22	1/1/13/20	5/25/103/115	-
26	CLA	B	835	2	-	2/16/94/115	-
29	WVN	s	407	-	-	18/29/63/63	0/2/2/2
35	II0	d	314	-	-	0/21/67/67	0/2/2/2
35	II0	n	618	-	-	11/21/67/67	0/2/2/2
26	CLA	B	821	2	1/1/12/20	7/23/101/115	-
29	WVN	L	205	-	-	16/29/63/63	0/2/2/2
26	CLA	n	601	23	1/1/11/20	5/13/91/115	-
26	CLA	A	821	1	1/1/11/20	7/18/96/115	-
34	LMG	L	209	-	-	18/40/60/70	0/1/1/1
26	CLA	B	811	2	1/1/13/20	3/25/103/115	-
26	CLA	l	308	18	1/1/15/20	5/37/115/115	-
26	CLA	d	318	-	1/1/11/20	5/13/91/115	-
26	CLA	B	837	2	1/1/15/20	15/37/115/115	-
37	IHT	a	315	-	-	5/25/65/65	0/2/2/2
26	CLA	i	310	-	1/1/14/20	10/31/109/115	-
26	CLA	c	301	13	1/1/12/20	9/21/99/115	-
26	CLA	a	308	28	1/1/11/20	3/17/95/115	-
26	CLA	J	103	8	1/1/10/20	3/10/88/115	-
35	II0	l	302	-	-	12/21/67/67	0/2/2/2
26	CLA	A	835	1	1/1/15/20	11/37/115/115	-
26	CLA	k	614	19	1/1/12/20	10/21/99/115	-
26	CLA	A	851	38	1/1/15/20	3/37/115/115	-
26	CLA	j	601	17	1/1/15/20	14/37/115/115	-
35	II0	c	313	-	-	12/21/67/67	0/2/2/2
26	CLA	B	833	2	1/1/13/20	5/25/103/115	-
26	CLA	m	607	17	1/1/12/20	5/21/99/115	-
37	IHT	b	301	-	-	4/25/65/65	0/2/2/2
26	CLA	B	838	2	1/1/15/20	11/37/115/115	-
26	CLA	n	613	23	1/1/12/20	8/21/99/115	-
35	II0	i	316	-	-	13/21/67/67	0/2/2/2
29	WVN	F	203	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	m	612	38	1/1/12/20	7/21/99/115	-
26	CLA	a	301	14	1/1/15/20	16/37/115/115	-
26	CLA	B	815	2	1/1/13/20	8/25/103/115	-
36	KC2	c	310	13	-	7/15/71/71	-
26	CLA	A	837	1	1/1/15/20	14/37/115/115	-
26	CLA	i	305	20	1/1/12/20	7/21/99/115	-
28	LHG	L	208	-	-	23/49/49/53	-
26	CLA	A	828	1	1/1/15/20	11/37/115/115	-
29	WVN	l	303	-	-	16/29/63/63	0/2/2/2

All (2797) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	615	II0	C14-C10	20.87	1.58	1.34
35	m	616	II0	C13-C09	19.92	1.57	1.34
35	h	310	II0	C13-C09	19.86	1.57	1.34
35	h	312	II0	C13-C09	19.71	1.56	1.34
35	c	316	II0	C14-C10	19.66	1.56	1.34
35	m	615	II0	C14-C10	19.57	1.56	1.34
35	k	616	II0	C14-C10	19.55	1.56	1.34
35	n	616	II0	C14-C10	19.55	1.56	1.34
35	a	316	II0	C13-C09	19.53	1.56	1.34
35	i	314	II0	C13-C09	19.46	1.56	1.34
35	l	302	II0	C14-C10	19.45	1.56	1.34
35	i	312	II0	C14-C10	19.44	1.56	1.34
35	j	614	II0	C13-C09	19.40	1.56	1.34
35	j	615	II0	C14-C10	19.38	1.56	1.34
35	d	317	II0	C14-C10	19.34	1.56	1.34
35	m	619	II0	C14-C10	19.31	1.56	1.34
35	a	313	II0	C13-C09	19.22	1.56	1.34
35	i	319	II0	C13-C09	19.15	1.56	1.34
35	i	313	II0	C14-C10	19.11	1.56	1.34
35	l	302	II0	C13-C09	19.08	1.56	1.34
35	d	315	II0	C13-C09	19.01	1.56	1.34
35	a	316	II0	C14-C10	19.00	1.56	1.34
35	c	316	II0	C13-C09	18.95	1.56	1.34
35	m	615	II0	C13-C09	18.94	1.56	1.34
35	c	313	II0	C14-C10	18.90	1.56	1.34
35	d	316	II0	C13-C09	18.86	1.55	1.34
35	a	312	II0	C13-C09	18.85	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	619	II0	C13-C09	18.83	1.55	1.34
35	l	315	II0	C14-C10	18.79	1.55	1.34
35	n	618	II0	C13-C09	18.79	1.55	1.34
35	m	616	II0	C14-C10	18.79	1.55	1.34
35	k	616	II0	C13-C09	18.76	1.55	1.34
35	n	618	II0	C14-C10	18.73	1.55	1.34
35	i	316	II0	C14-C10	18.73	1.55	1.34
35	m	614	II0	C13-C09	18.72	1.55	1.34
35	i	314	II0	C14-C10	18.69	1.55	1.34
35	d	316	II0	C14-C10	18.69	1.55	1.34
35	d	315	II0	C14-C10	18.62	1.55	1.34
35	m	614	II0	C14-C10	18.46	1.55	1.34
35	d	301	II0	C14-C10	18.45	1.55	1.34
35	n	615	II0	C13-C09	18.45	1.55	1.34
35	a	314	II0	C14-C10	18.44	1.55	1.34
35	i	312	II0	C13-C09	18.38	1.55	1.34
35	l	314	II0	C14-C10	18.14	1.55	1.34
35	i	316	II0	C13-C09	18.12	1.55	1.34
35	J	104	II0	C13-C09	18.08	1.55	1.34
35	n	616	II0	C13-C09	18.01	1.55	1.34
35	k	620	II0	C14-C10	17.98	1.55	1.34
35	l	315	II0	C13-C09	17.95	1.54	1.34
35	i	319	II0	C14-C10	17.93	1.54	1.34
35	k	615	II0	C13-C09	17.86	1.54	1.34
35	j	615	II0	C13-C09	17.82	1.54	1.34
35	l	314	II0	C13-C09	17.82	1.54	1.34
35	n	615	II0	C14-C10	17.81	1.54	1.34
35	b	315	II0	C14-C10	17.78	1.54	1.34
35	c	313	II0	C13-C09	17.76	1.54	1.34
35	k	619	II0	C14-C10	17.70	1.54	1.34
35	j	614	II0	C14-C10	17.70	1.54	1.34
35	a	312	II0	C14-C10	17.69	1.54	1.34
35	h	312	II0	C14-C10	17.68	1.54	1.34
35	i	313	II0	C13-C09	17.68	1.54	1.34
35	J	104	II0	C14-C10	17.63	1.54	1.34
35	k	620	II0	C13-C09	17.62	1.54	1.34
35	b	314	II0	C14-C10	17.62	1.54	1.34
35	a	313	II0	C14-C10	17.49	1.54	1.34
35	k	619	II0	C13-C09	17.49	1.54	1.34
35	b	314	II0	C13-C09	17.42	1.54	1.34
35	d	317	II0	C13-C09	17.39	1.54	1.34
35	b	315	II0	C13-C09	17.38	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	311	II0	C13-C09	17.36	1.54	1.34
35	d	301	II0	C13-C09	17.35	1.54	1.34
35	h	311	II0	C14-C10	17.26	1.54	1.34
35	a	314	II0	C13-C09	17.19	1.54	1.34
35	i	313	II0	C39-C35	14.94	1.55	1.35
35	l	315	II0	C39-C35	14.92	1.55	1.35
35	b	315	II0	C40-C36	14.91	1.55	1.35
35	b	314	II0	C39-C35	14.89	1.55	1.35
35	m	616	II0	C39-C35	14.89	1.55	1.35
35	a	313	II0	C40-C36	14.85	1.55	1.35
35	i	313	II0	C40-C36	14.74	1.55	1.35
35	d	315	II0	C39-C35	14.73	1.55	1.35
35	l	315	II0	C40-C36	14.72	1.55	1.35
35	b	315	II0	C39-C35	14.69	1.55	1.35
35	i	312	II0	C39-C35	14.68	1.55	1.35
35	l	302	II0	C40-C36	14.65	1.55	1.35
35	k	616	II0	C39-C35	14.63	1.55	1.35
35	m	614	II0	C39-C35	14.63	1.55	1.35
35	a	313	II0	C39-C35	14.63	1.55	1.35
35	i	312	II0	C40-C36	14.63	1.55	1.35
35	d	316	II0	C39-C35	14.57	1.55	1.35
35	k	616	II0	C40-C36	14.56	1.55	1.35
35	n	615	II0	C39-C35	14.56	1.55	1.35
35	d	317	II0	C39-C35	14.55	1.55	1.35
35	l	302	II0	C39-C35	14.55	1.55	1.35
35	b	314	II0	C40-C36	14.55	1.55	1.35
35	k	615	II0	C39-C35	14.54	1.55	1.35
35	h	310	II0	C40-C36	14.51	1.55	1.35
35	c	313	II0	C40-C36	14.49	1.55	1.35
35	l	314	II0	C39-C35	14.49	1.55	1.35
35	i	314	II0	C39-C35	14.47	1.55	1.35
35	a	316	II0	C39-C35	14.46	1.55	1.35
35	J	104	II0	C39-C35	14.45	1.54	1.35
35	m	619	II0	C40-C36	14.45	1.54	1.35
35	c	313	II0	C39-C35	14.45	1.54	1.35
35	j	614	II0	C40-C36	14.45	1.54	1.35
35	k	619	II0	C40-C36	14.44	1.54	1.35
35	n	615	II0	C40-C36	14.43	1.54	1.35
35	n	616	II0	C39-C35	14.42	1.54	1.35
35	m	619	II0	C39-C35	14.41	1.54	1.35
35	d	317	II0	C40-C36	14.41	1.54	1.35
29	A	845	WVN	C28-C25	14.41	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	312	II0	C39-C35	14.40	1.54	1.35
35	i	316	II0	C39-C35	14.40	1.54	1.35
35	k	619	II0	C39-C35	14.40	1.54	1.35
35	j	615	II0	C39-C35	14.40	1.54	1.35
29	L	205	WVN	C26-C22	14.38	1.54	1.35
35	k	620	II0	C40-C36	14.38	1.54	1.35
35	i	319	II0	C39-C35	14.38	1.54	1.35
35	h	310	II0	C39-C35	14.37	1.54	1.35
29	s	407	WVN	C26-C22	14.36	1.54	1.35
35	n	618	II0	C39-C35	14.35	1.54	1.35
29	F	203	WVN	C26-C22	14.35	1.54	1.35
29	s	405	WVN	C37-C34	14.33	1.54	1.35
29	l	316	WVN	C37-C34	14.33	1.54	1.35
29	A	845	WVN	C26-C22	14.32	1.54	1.35
35	m	614	II0	C40-C36	14.31	1.54	1.35
35	h	312	II0	C40-C36	14.31	1.54	1.35
35	d	316	II0	C40-C36	14.30	1.54	1.35
35	a	314	II0	C40-C36	14.29	1.54	1.35
35	m	615	II0	C39-C35	14.29	1.54	1.35
35	a	312	II0	C39-C35	14.29	1.54	1.35
29	B	849	WVN	C28-C25	14.29	1.54	1.35
35	h	311	II0	C39-C35	14.28	1.54	1.35
35	J	104	II0	C40-C36	14.28	1.54	1.35
35	m	616	II0	C40-C36	14.28	1.54	1.35
35	j	615	II0	C40-C36	14.27	1.54	1.35
35	l	314	II0	C40-C36	14.27	1.54	1.35
35	k	615	II0	C40-C36	14.27	1.54	1.35
35	i	319	II0	C40-C36	14.26	1.54	1.35
35	a	312	II0	C40-C36	14.25	1.54	1.35
35	k	620	II0	C39-C35	14.25	1.54	1.35
29	J	102	WVN	C37-C34	14.25	1.54	1.35
35	n	618	II0	C40-C36	14.24	1.54	1.35
35	i	316	II0	C40-C36	14.24	1.54	1.35
29	J	101	WVN	C26-C22	14.23	1.54	1.35
35	a	316	II0	C40-C36	14.23	1.54	1.35
29	l	316	WVN	C26-C22	14.22	1.54	1.35
35	d	315	II0	C40-C36	14.22	1.54	1.35
35	d	301	II0	C40-C36	14.21	1.54	1.35
35	n	616	II0	C40-C36	14.21	1.54	1.35
29	A	857	WVN	C28-C25	14.18	1.54	1.35
35	c	316	II0	C39-C35	14.17	1.54	1.35
35	a	314	II0	C39-C35	14.17	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	301	II0	C39-C35	14.17	1.54	1.35
35	i	314	II0	C40-C36	14.16	1.54	1.35
29	B	849	WVN	C26-C22	14.15	1.54	1.35
29	K	102	WVN	C37-C34	14.14	1.54	1.35
35	j	614	II0	C39-C35	14.13	1.54	1.35
29	i	315	WVN	C37-C34	14.12	1.54	1.35
29	B	849	WVN	C37-C34	14.11	1.54	1.35
29	A	847	WVN	C26-C22	14.11	1.54	1.35
29	h	309	WVN	C26-C22	14.10	1.54	1.35
29	B	850	WVN	C37-C34	14.07	1.54	1.35
29	l	303	WVN	C26-C22	14.06	1.54	1.35
29	B	848	WVN	C28-C25	14.05	1.54	1.35
29	B	850	WVN	C26-C22	14.05	1.54	1.35
29	A	857	WVN	C37-C34	14.04	1.54	1.35
35	m	615	II0	C40-C36	14.03	1.54	1.35
29	B	848	WVN	C37-C34	14.03	1.54	1.35
35	h	311	II0	C40-C36	14.02	1.54	1.35
29	M	101	WVN	C37-C34	14.01	1.54	1.35
29	s	405	WVN	C26-C22	14.00	1.54	1.35
29	B	847	WVN	C26-C22	14.00	1.54	1.35
29	K	102	WVN	C26-C22	13.99	1.54	1.35
29	A	846	WVN	C37-C34	13.98	1.54	1.35
29	A	845	WVN	C37-C34	13.98	1.54	1.35
29	R	200	WVN	C26-C22	13.96	1.54	1.35
29	A	847	WVN	C37-C34	13.96	1.54	1.35
29	B	847	WVN	C37-C34	13.96	1.54	1.35
29	B	848	WVN	C26-C22	13.95	1.54	1.35
29	L	205	WVN	C37-C34	13.95	1.54	1.35
29	A	846	WVN	C26-C22	13.94	1.54	1.35
35	c	316	II0	C40-C36	13.94	1.54	1.35
29	s	407	WVN	C37-C34	13.94	1.54	1.35
29	R	200	WVN	C37-C34	13.93	1.54	1.35
29	R	200	WVN	C28-C25	13.92	1.54	1.35
29	B	846	WVN	C28-C25	13.92	1.54	1.35
29	A	857	WVN	C26-C22	13.91	1.54	1.35
29	B	850	WVN	C28-C25	13.90	1.54	1.35
29	J	101	WVN	C37-C34	13.89	1.54	1.35
29	F	203	WVN	C28-C25	13.88	1.54	1.35
29	A	848	WVN	C37-C34	13.87	1.54	1.35
29	B	853	WVN	C26-C22	13.86	1.54	1.35
29	J	102	WVN	C28-C25	13.85	1.54	1.35
29	i	315	WVN	C28-C25	13.85	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	853	WVN	C37-C34	13.85	1.54	1.35
29	A	846	WVN	C28-C25	13.84	1.54	1.35
29	B	847	WVN	C28-C25	13.83	1.54	1.35
29	L	205	WVN	C28-C25	13.83	1.54	1.35
29	F	203	WVN	C36-C32	13.82	1.54	1.35
29	l	316	WVN	C36-C32	13.81	1.54	1.35
29	M	101	WVN	C26-C22	13.81	1.54	1.35
29	l	303	WVN	C37-C34	13.81	1.54	1.35
29	i	315	WVN	C26-C22	13.79	1.54	1.35
29	K	102	WVN	C28-C25	13.79	1.54	1.35
29	h	309	WVN	C37-C34	13.79	1.54	1.35
29	A	847	WVN	C28-C25	13.77	1.54	1.35
29	L	201	WVN	C37-C34	13.77	1.54	1.35
29	J	102	WVN	C36-C32	13.76	1.54	1.35
29	B	853	WVN	C28-C25	13.75	1.54	1.35
29	l	303	WVN	C28-C25	13.75	1.54	1.35
29	B	846	WVN	C37-C34	13.75	1.54	1.35
29	L	201	WVN	C26-C22	13.73	1.54	1.35
29	M	101	WVN	C28-C25	13.72	1.54	1.35
29	s	407	WVN	C28-C25	13.71	1.54	1.35
29	I	101	WVN	C37-C34	13.71	1.54	1.35
29	h	309	WVN	C28-C25	13.70	1.53	1.35
29	J	102	WVN	C26-C22	13.70	1.53	1.35
29	F	203	WVN	C37-C34	13.69	1.53	1.35
29	s	405	WVN	C28-C25	13.68	1.53	1.35
29	B	846	WVN	C26-C22	13.67	1.53	1.35
29	J	101	WVN	C28-C25	13.63	1.53	1.35
29	I	101	WVN	C26-C22	13.62	1.53	1.35
29	M	101	WVN	C36-C32	13.59	1.53	1.35
29	B	848	WVN	C36-C32	13.56	1.53	1.35
29	A	848	WVN	C26-C22	13.55	1.53	1.35
29	B	847	WVN	C36-C32	13.54	1.53	1.35
29	R	200	WVN	C36-C32	13.54	1.53	1.35
29	L	201	WVN	C28-C25	13.53	1.53	1.35
29	l	316	WVN	C28-C25	13.51	1.53	1.35
29	A	848	WVN	C28-C25	13.49	1.53	1.35
29	I	101	WVN	C28-C25	13.49	1.53	1.35
29	A	845	WVN	C36-C32	13.49	1.53	1.35
29	B	849	WVN	C36-C32	13.48	1.53	1.35
29	A	857	WVN	C36-C32	13.46	1.53	1.35
29	s	405	WVN	C36-C32	13.45	1.53	1.35
29	A	847	WVN	C36-C32	13.44	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	101	WVN	C36-C32	13.42	1.53	1.35
29	L	205	WVN	C36-C32	13.40	1.53	1.35
29	i	315	WVN	C36-C32	13.40	1.53	1.35
29	A	848	WVN	C36-C32	13.39	1.53	1.35
29	A	846	WVN	C36-C32	13.38	1.53	1.35
29	h	309	WVN	C36-C32	13.33	1.53	1.35
29	s	407	WVN	C36-C32	13.32	1.53	1.35
29	l	303	WVN	C36-C32	13.30	1.53	1.35
29	B	853	WVN	C36-C32	13.26	1.53	1.35
29	B	850	WVN	C36-C32	13.26	1.53	1.35
29	L	201	WVN	C36-C32	13.24	1.53	1.35
29	K	102	WVN	C36-C32	13.12	1.53	1.35
29	I	101	WVN	C36-C32	13.07	1.53	1.35
29	A	845	WVN	C15-C13	12.96	1.56	1.34
29	B	846	WVN	C36-C32	12.93	1.52	1.35
29	L	201	WVN	C15-C13	12.84	1.56	1.34
29	i	315	WVN	C15-C13	12.71	1.56	1.34
29	B	846	WVN	C15-C13	12.55	1.56	1.34
29	A	848	WVN	C15-C13	12.52	1.56	1.34
29	B	849	WVN	C15-C13	12.51	1.56	1.34
29	R	200	WVN	C15-C13	12.49	1.56	1.34
29	J	102	WVN	C15-C13	12.46	1.56	1.34
29	A	857	WVN	C15-C13	12.43	1.56	1.34
29	B	847	WVN	C15-C13	12.42	1.56	1.34
29	M	101	WVN	C15-C13	12.42	1.56	1.34
29	h	309	WVN	C15-C13	12.37	1.55	1.34
29	s	405	WVN	C15-C13	12.22	1.55	1.34
29	B	850	WVN	C15-C13	12.20	1.55	1.34
29	L	205	WVN	C15-C13	12.20	1.55	1.34
29	A	846	WVN	C15-C13	12.17	1.55	1.34
29	l	303	WVN	C15-C13	12.17	1.55	1.34
29	s	407	WVN	C15-C13	12.13	1.55	1.34
29	B	853	WVN	C15-C13	12.06	1.55	1.34
29	B	848	WVN	C15-C13	12.01	1.55	1.34
29	l	316	WVN	C15-C13	11.92	1.55	1.34
29	l	316	WVN	C09-C05	11.89	1.56	1.32
29	B	850	WVN	C09-C05	11.85	1.56	1.32
29	A	845	WVN	C09-C05	11.85	1.56	1.32
29	J	101	WVN	C15-C13	11.84	1.55	1.34
29	J	101	WVN	C09-C05	11.76	1.55	1.32
29	F	203	WVN	C09-C05	11.73	1.55	1.32
29	L	205	WVN	C09-C05	11.73	1.55	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	848	WVN	C09-C05	11.73	1.55	1.32
29	B	853	WVN	C09-C05	11.73	1.55	1.32
29	h	309	WVN	C09-C05	11.71	1.55	1.32
29	K	102	WVN	C15-C13	11.71	1.54	1.34
29	J	102	WVN	C09-C05	11.71	1.55	1.32
29	s	405	WVN	C09-C05	11.70	1.55	1.32
29	A	847	WVN	C15-C13	11.67	1.54	1.34
29	l	303	WVN	C09-C05	11.66	1.55	1.32
29	B	849	WVN	C09-C05	11.65	1.55	1.32
29	I	101	WVN	C09-C05	11.62	1.55	1.32
29	K	102	WVN	C09-C05	11.61	1.55	1.32
29	F	203	WVN	C15-C13	11.56	1.54	1.34
29	M	101	WVN	C09-C05	11.53	1.55	1.32
29	s	407	WVN	C09-C05	11.53	1.55	1.32
29	L	201	WVN	C09-C05	11.49	1.55	1.32
29	B	847	WVN	C09-C05	11.49	1.55	1.32
29	I	101	WVN	C15-C13	11.47	1.54	1.34
29	A	848	WVN	C09-C05	11.47	1.55	1.32
29	A	846	WVN	C09-C05	11.45	1.55	1.32
29	R	200	WVN	C09-C05	11.44	1.55	1.32
29	i	315	WVN	C09-C05	11.42	1.55	1.32
29	A	857	WVN	C09-C05	11.35	1.55	1.32
29	B	846	WVN	C09-C05	11.21	1.54	1.32
29	A	847	WVN	C09-C05	11.00	1.54	1.32
26	c	309	CLA	C1D-ND	9.34	1.49	1.37
35	i	316	II0	C29-C25	9.25	1.56	1.37
35	i	319	II0	C29-C25	9.23	1.56	1.37
35	i	313	II0	C29-C25	9.14	1.56	1.37
35	c	316	II0	C29-C25	9.10	1.56	1.37
35	m	616	II0	C29-C25	9.09	1.56	1.37
35	l	302	II0	C29-C25	9.06	1.56	1.37
35	d	301	II0	C29-C25	9.06	1.56	1.37
36	c	310	KC2	C1D-ND	9.06	1.43	1.35
35	a	314	II0	C29-C25	9.03	1.56	1.37
35	n	616	II0	C29-C25	9.02	1.55	1.37
35	l	315	II0	C29-C25	9.01	1.55	1.37
35	n	615	II0	C29-C25	8.99	1.55	1.37
35	b	315	II0	C29-C25	8.99	1.55	1.37
35	n	618	II0	C29-C25	8.99	1.55	1.37
35	h	311	II0	C29-C25	8.99	1.55	1.37
35	m	614	II0	C29-C25	8.98	1.55	1.37
35	k	620	II0	C29-C25	8.97	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	317	II0	C29-C25	8.97	1.55	1.37
35	k	619	II0	C29-C25	8.96	1.55	1.37
35	J	104	II0	C29-C25	8.95	1.55	1.37
35	j	614	II0	C29-C25	8.92	1.55	1.37
35	i	314	II0	C29-C25	8.91	1.55	1.37
27	A	842	PQN	C12-C13	8.91	1.54	1.33
35	j	615	II0	C29-C25	8.91	1.55	1.37
35	h	312	II0	C29-C25	8.91	1.55	1.37
35	a	312	II0	C29-C25	8.87	1.55	1.37
27	B	843	PQN	C12-C13	8.85	1.54	1.33
35	b	314	II0	C29-C25	8.85	1.55	1.37
35	m	619	II0	C29-C25	8.85	1.55	1.37
35	m	615	II0	C29-C25	8.84	1.55	1.37
35	d	315	II0	C29-C25	8.83	1.55	1.37
35	l	302	II0	C30-C26	8.83	1.55	1.37
35	l	314	II0	C29-C25	8.81	1.55	1.37
35	d	316	II0	C29-C25	8.77	1.55	1.37
35	a	313	II0	C29-C25	8.77	1.55	1.37
35	l	315	II0	C30-C26	8.77	1.55	1.37
35	c	313	II0	C29-C25	8.76	1.55	1.37
35	h	310	II0	C29-C25	8.74	1.55	1.37
35	a	316	II0	C29-C25	8.70	1.55	1.37
35	h	311	II0	C30-C26	8.68	1.55	1.37
35	i	312	II0	C29-C25	8.68	1.55	1.37
35	b	315	II0	C30-C26	8.67	1.55	1.37
35	m	614	II0	C30-C26	8.66	1.55	1.37
35	k	615	II0	C29-C25	8.64	1.55	1.37
35	m	619	II0	C30-C26	8.62	1.55	1.37
35	m	616	II0	C30-C26	8.59	1.55	1.37
35	n	615	II0	C30-C26	8.59	1.55	1.37
35	k	616	II0	C29-C25	8.58	1.55	1.37
35	c	313	II0	C30-C26	8.57	1.55	1.37
35	b	314	II0	C30-C26	8.56	1.55	1.37
26	k	604	CLA	C4B-NB	8.56	1.42	1.35
35	j	614	II0	C30-C26	8.54	1.54	1.37
35	a	316	II0	C30-C26	8.54	1.54	1.37
35	d	301	II0	C30-C26	8.53	1.54	1.37
35	a	313	II0	C30-C26	8.52	1.54	1.37
35	k	619	II0	C30-C26	8.51	1.54	1.37
35	h	312	II0	C30-C26	8.50	1.54	1.37
35	j	615	II0	C30-C26	8.50	1.54	1.37
35	a	314	II0	C30-C26	8.49	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	618	II0	C30-C26	8.47	1.54	1.37
35	n	616	II0	C30-C26	8.44	1.54	1.37
35	m	615	II0	C30-C26	8.43	1.54	1.37
35	k	616	II0	C30-C26	8.43	1.54	1.37
27	B	843	PQN	O1-C1	8.34	1.40	1.23
26	A	803	CLA	C4B-NB	8.33	1.42	1.35
35	i	319	II0	C30-C26	8.33	1.54	1.37
27	A	842	PQN	O1-C1	8.30	1.40	1.23
27	B	843	PQN	O4-C4	8.29	1.40	1.23
26	B	835	CLA	C4B-NB	8.29	1.42	1.35
35	d	317	II0	C30-C26	8.28	1.54	1.37
35	k	620	II0	C30-C26	8.27	1.54	1.37
35	d	316	II0	C30-C26	8.26	1.54	1.37
35	i	314	II0	C30-C26	8.23	1.54	1.37
35	l	314	II0	C30-C26	8.23	1.54	1.37
35	i	313	II0	C30-C26	8.22	1.54	1.37
35	J	104	II0	C30-C26	8.22	1.54	1.37
27	A	842	PQN	O4-C4	8.22	1.40	1.23
35	k	615	II0	C22-C10	8.22	1.59	1.42
35	k	615	II0	C30-C26	8.20	1.54	1.37
35	a	312	II0	C30-C26	8.20	1.54	1.37
35	i	316	II0	C30-C26	8.19	1.54	1.37
35	d	315	II0	C30-C26	8.19	1.54	1.37
36	s	401	KC2	C1D-ND	8.18	1.42	1.35
35	i	312	II0	C30-C26	8.16	1.54	1.37
35	c	316	II0	C30-C26	8.16	1.54	1.37
26	R	201	CLA	C4B-NB	8.11	1.42	1.35
26	n	603	CLA	C4B-NB	8.06	1.42	1.35
26	k	603	CLA	C4B-NB	8.00	1.42	1.35
26	n	606	CLA	C4B-NB	7.94	1.42	1.35
26	n	608	CLA	C4B-NB	7.93	1.42	1.35
26	A	836	CLA	C4B-NB	7.87	1.42	1.35
26	a	310	CLA	C4B-NB	7.86	1.42	1.35
26	B	817	CLA	C4B-NB	7.85	1.42	1.35
26	h	307	CLA	C4B-NB	7.84	1.42	1.35
26	i	306	CLA	C4B-NB	7.84	1.42	1.35
26	A	838	CLA	C4B-NB	7.82	1.42	1.35
26	B	832	CLA	C4B-NB	7.81	1.42	1.35
26	A	837	CLA	C4B-NB	7.81	1.42	1.35
26	B	810	CLA	C4B-NB	7.79	1.42	1.35
26	l	313	CLA	C4B-NB	7.78	1.42	1.35
26	c	312	CLA	C4B-NB	7.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	306	CLA	C4B-NB	7.77	1.42	1.35
35	m	616	II0	C23-C25	7.76	1.57	1.42
26	A	832	CLA	C4B-NB	7.76	1.42	1.35
26	A	828	CLA	C4B-NB	7.76	1.42	1.35
26	A	829	CLA	C4B-NB	7.75	1.42	1.35
26	j	601	CLA	C4B-NB	7.75	1.42	1.35
26	b	310	CLA	C4B-NB	7.75	1.42	1.35
26	J	103	CLA	C4B-NB	7.75	1.42	1.35
26	n	613	CLA	C4B-NB	7.74	1.42	1.35
26	F	202	CLA	C4B-NB	7.74	1.42	1.35
26	A	813	CLA	C4B-NB	7.73	1.42	1.35
26	l	301	CLA	C4B-NB	7.73	1.42	1.35
26	A	852	CLA	C4B-NB	7.73	1.42	1.35
26	c	302	CLA	C4B-NB	7.73	1.42	1.35
26	B	813	CLA	C4B-NB	7.72	1.42	1.35
26	d	310	CLA	C4B-NB	7.72	1.42	1.35
26	i	301	CLA	C4B-NB	7.72	1.42	1.35
26	A	811	CLA	C4B-NB	7.72	1.42	1.35
26	K	101	CLA	C4B-NB	7.72	1.42	1.35
26	n	610	CLA	C4B-NB	7.72	1.42	1.35
26	F	201	CLA	C4B-NB	7.71	1.42	1.35
26	h	304	CLA	C4B-NB	7.71	1.42	1.35
26	B	840	CLA	C4B-NB	7.70	1.42	1.35
26	s	402	CLA	C4B-NB	7.69	1.42	1.35
26	B	811	CLA	C4B-NB	7.69	1.42	1.35
26	b	312	CLA	C4B-NB	7.69	1.42	1.35
26	j	613	CLA	C4B-NB	7.69	1.42	1.35
26	d	306	CLA	C4B-NB	7.69	1.42	1.35
26	L	206	CLA	C4B-NB	7.68	1.42	1.35
26	i	303	CLA	C4B-NB	7.68	1.42	1.35
26	a	311	CLA	C4B-NB	7.68	1.42	1.35
26	m	601	CLA	C4B-NB	7.68	1.42	1.35
26	A	851	CLA	C4B-NB	7.68	1.42	1.35
26	B	841	CLA	C4B-NB	7.68	1.42	1.35
26	A	840	CLA	C4B-NB	7.67	1.42	1.35
26	B	820	CLA	C4B-NB	7.67	1.42	1.35
26	b	311	CLA	C4B-NB	7.67	1.42	1.35
26	L	202	CLA	C4B-NB	7.67	1.42	1.35
26	A	833	CLA	C4B-NB	7.66	1.42	1.35
26	A	806	CLA	C4B-NB	7.66	1.42	1.35
26	l	304	CLA	C4B-NB	7.66	1.42	1.35
26	d	313	CLA	C4B-NB	7.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	826	CLA	C4B-NB	7.66	1.42	1.35
26	h	301	CLA	C4B-NB	7.66	1.42	1.35
26	A	830	CLA	C4B-NB	7.65	1.42	1.35
26	B	828	CLA	C4B-NB	7.65	1.42	1.35
26	L	204	CLA	C4B-NB	7.65	1.42	1.35
26	k	614	CLA	C4B-NB	7.65	1.42	1.35
26	m	609	CLA	C4B-NB	7.65	1.42	1.35
26	a	309	CLA	C4B-NB	7.64	1.42	1.35
26	b	306	CLA	C4B-NB	7.64	1.42	1.35
26	A	809	CLA	C4B-NB	7.64	1.42	1.35
26	m	606	CLA	C4B-NB	7.64	1.42	1.35
26	k	610	CLA	C4B-NB	7.64	1.42	1.35
26	b	305	CLA	C4B-NB	7.64	1.42	1.35
26	i	311	CLA	C4B-NB	7.64	1.42	1.35
26	B	838	CLA	C4B-NB	7.63	1.42	1.35
26	c	305	CLA	C4B-NB	7.63	1.42	1.35
26	j	612	CLA	C4B-NB	7.63	1.42	1.35
26	d	309	CLA	C4B-NB	7.63	1.42	1.35
26	b	303	CLA	C4B-NB	7.63	1.42	1.35
26	A	815	CLA	C4B-NB	7.62	1.42	1.35
26	A	820	CLA	C4B-NB	7.62	1.42	1.35
26	B	834	CLA	C4B-NB	7.62	1.42	1.35
26	h	308	CLA	C4B-NB	7.62	1.42	1.35
26	j	605	CLA	C4B-NB	7.62	1.42	1.35
26	s	408	CLA	C4B-NB	7.61	1.42	1.35
26	c	303	CLA	C4B-NB	7.61	1.42	1.35
26	l	311	CLA	C4B-NB	7.61	1.42	1.35
26	B	833	CLA	C4B-NB	7.60	1.42	1.35
26	B	819	CLA	C4B-NB	7.60	1.42	1.35
26	B	802	CLA	C4B-NB	7.60	1.42	1.35
26	l	306	CLA	C4B-NB	7.60	1.42	1.35
26	i	308	CLA	C4B-NB	7.60	1.42	1.35
26	B	839	CLA	C4B-NB	7.59	1.42	1.35
26	h	303	CLA	C4B-NB	7.59	1.42	1.35
26	k	609	CLA	C4B-NB	7.59	1.42	1.35
26	B	837	CLA	C4B-NB	7.58	1.42	1.35
35	i	313	II0	C23-C25	7.58	1.57	1.42
26	B	830	CLA	C4B-NB	7.58	1.42	1.35
26	d	303	CLA	C4B-NB	7.57	1.42	1.35
26	a	305	CLA	C4B-NB	7.56	1.42	1.35
26	A	816	CLA	C4B-NB	7.56	1.42	1.35
26	d	308	CLA	C4B-NB	7.56	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	816	CLA	C4B-NB	7.56	1.42	1.35
26	m	605	CLA	C4B-NB	7.56	1.42	1.35
26	d	302	CLA	C4B-NB	7.56	1.42	1.35
26	a	308	CLA	C4B-NB	7.56	1.42	1.35
26	d	307	CLA	C4B-NB	7.56	1.41	1.35
26	B	814	CLA	C4B-NB	7.55	1.41	1.35
26	c	306	CLA	C4B-NB	7.55	1.41	1.35
26	A	823	CLA	C4B-NB	7.55	1.41	1.35
26	A	819	CLA	C4B-NB	7.55	1.41	1.35
26	j	610	CLA	C4B-NB	7.55	1.41	1.35
26	B	808	CLA	C4B-NB	7.55	1.41	1.35
26	B	827	CLA	C4B-NB	7.55	1.41	1.35
26	B	806	CLA	C4B-NB	7.55	1.41	1.35
26	h	313	CLA	C4B-NB	7.55	1.41	1.35
26	m	613	CLA	C4B-NB	7.55	1.41	1.35
26	s	406	CLA	C4B-NB	7.54	1.41	1.35
26	m	607	CLA	C4B-NB	7.54	1.41	1.35
26	h	302	CLA	C4B-NB	7.54	1.41	1.35
26	d	304	CLA	C4B-NB	7.54	1.41	1.35
26	B	815	CLA	C4B-NB	7.54	1.41	1.35
26	n	601	CLA	C4B-NB	7.54	1.41	1.35
26	A	821	CLA	C4B-NB	7.53	1.41	1.35
26	A	831	CLA	C4B-NB	7.53	1.41	1.35
26	d	305	CLA	C4B-NB	7.52	1.41	1.35
26	B	809	CLA	C4B-NB	7.52	1.41	1.35
35	i	319	II0	C22-C10	7.52	1.58	1.42
26	a	303	CLA	C4B-NB	7.52	1.41	1.35
26	a	304	CLA	C4B-NB	7.52	1.41	1.35
26	B	822	CLA	C4B-NB	7.51	1.41	1.35
26	L	203	CLA	C4B-NB	7.51	1.41	1.35
26	s	403	CLA	C4B-NB	7.51	1.41	1.35
26	b	307	CLA	C4B-NB	7.51	1.41	1.35
26	d	318	CLA	C4B-NB	7.51	1.41	1.35
35	k	616	II0	C21-C09	7.51	1.58	1.42
26	j	608	CLA	C4B-NB	7.51	1.41	1.35
26	B	829	CLA	C4B-NB	7.50	1.41	1.35
26	c	304	CLA	C4B-NB	7.50	1.41	1.35
26	m	610	CLA	C4B-NB	7.50	1.41	1.35
26	m	603	CLA	C4B-NB	7.50	1.41	1.35
26	h	306	CLA	C4B-NB	7.50	1.41	1.35
26	k	605	CLA	C4B-NB	7.50	1.41	1.35
26	A	841	CLA	C4B-NB	7.50	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	856	CLA	C4B-NB	7.50	1.41	1.35
26	A	804	CLA	C4B-NB	7.50	1.41	1.35
26	A	822	CLA	C4B-NB	7.50	1.41	1.35
26	a	307	CLA	C4B-NB	7.50	1.41	1.35
26	n	607	CLA	C4B-NB	7.50	1.41	1.35
35	b	315	II0	C22-C10	7.50	1.58	1.42
26	A	805	CLA	C4B-NB	7.49	1.41	1.35
26	n	605	CLA	C4B-NB	7.49	1.41	1.35
26	l	309	CLA	C4B-NB	7.49	1.41	1.35
26	B	801	CLA	C4B-NB	7.49	1.41	1.35
26	b	313	CLA	C4B-NB	7.49	1.41	1.35
26	j	603	CLA	C4B-NB	7.49	1.41	1.35
26	m	608	CLA	C4B-NB	7.49	1.41	1.35
26	Q	302	CLA	C4B-NB	7.48	1.41	1.35
26	B	821	CLA	C4B-NB	7.47	1.41	1.35
26	l	310	CLA	C4B-NB	7.47	1.41	1.35
26	j	606	CLA	C4B-NB	7.47	1.41	1.35
26	i	307	CLA	C4B-NB	7.46	1.41	1.35
26	A	808	CLA	C4B-NB	7.46	1.41	1.35
26	a	301	CLA	C4B-NB	7.46	1.41	1.35
26	A	839	CLA	C4B-NB	7.46	1.41	1.35
26	c	311	CLA	C4B-NB	7.45	1.41	1.35
26	B	842	CLA	C4B-NB	7.45	1.41	1.35
26	j	609	CLA	C4B-NB	7.45	1.41	1.35
26	B	836	CLA	C4B-NB	7.45	1.41	1.35
26	m	612	CLA	C4B-NB	7.45	1.41	1.35
26	i	310	CLA	C4B-NB	7.44	1.41	1.35
26	B	831	CLA	C4B-NB	7.44	1.41	1.35
26	n	604	CLA	C4B-NB	7.44	1.41	1.35
26	k	608	CLA	C4B-NB	7.43	1.41	1.35
26	A	817	CLA	C4B-NB	7.43	1.41	1.35
26	A	810	CLA	C4B-NB	7.42	1.41	1.35
26	A	827	CLA	C4B-NB	7.42	1.41	1.35
26	A	818	CLA	C4B-NB	7.42	1.41	1.35
26	k	607	CLA	C4B-NB	7.42	1.41	1.35
26	c	301	CLA	C4B-NB	7.42	1.41	1.35
26	b	309	CLA	C4B-NB	7.42	1.41	1.35
26	k	606	CLA	C4B-NB	7.41	1.41	1.35
26	k	601	CLA	C4B-NB	7.41	1.41	1.35
26	i	304	CLA	C4B-NB	7.41	1.41	1.35
26	h	305	CLA	C4B-NB	7.41	1.41	1.35
26	c	308	CLA	C4B-NB	7.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	616	II0	C23-C25	7.40	1.56	1.42
26	A	814	CLA	C4B-NB	7.40	1.41	1.35
26	B	818	CLA	C4B-NB	7.40	1.41	1.35
26	B	805	CLA	C4B-NB	7.39	1.41	1.35
26	A	835	CLA	C4B-NB	7.39	1.41	1.35
26	B	823	CLA	C4B-NB	7.39	1.41	1.35
26	A	802	CLA	C4B-NB	7.38	1.41	1.35
26	l	308	CLA	C4B-NB	7.38	1.41	1.35
35	l	302	II0	C24-C26	7.36	1.56	1.42
26	B	824	CLA	C4B-NB	7.36	1.41	1.35
26	c	307	CLA	C4B-NB	7.35	1.41	1.35
26	b	308	CLA	C4B-NB	7.35	1.41	1.35
35	n	618	II0	C24-C26	7.35	1.56	1.42
26	A	807	CLA	C4B-NB	7.35	1.41	1.35
35	b	315	II0	C24-C26	7.35	1.56	1.42
26	i	302	CLA	C4B-NB	7.34	1.41	1.35
26	n	609	CLA	C4B-NB	7.33	1.41	1.35
35	h	312	II0	C24-C26	7.32	1.56	1.42
26	A	824	CLA	C4B-NB	7.32	1.41	1.35
26	m	604	CLA	C4B-NB	7.31	1.41	1.35
35	l	302	II0	C21-C09	7.30	1.57	1.42
26	j	602	CLA	C4B-NB	7.30	1.41	1.35
26	B	804	CLA	C4B-NB	7.29	1.41	1.35
26	A	812	CLA	C4B-NB	7.28	1.41	1.35
35	d	316	II0	C21-C09	7.27	1.57	1.42
26	B	803	CLA	C4B-NB	7.27	1.41	1.35
26	B	825	CLA	C4B-NB	7.27	1.41	1.35
35	a	316	II0	C21-C09	7.26	1.57	1.42
26	l	307	CLA	C4B-NB	7.25	1.41	1.35
35	l	315	II0	C24-C26	7.25	1.56	1.42
26	j	604	CLA	C4B-NB	7.24	1.41	1.35
26	m	602	CLA	C4B-NB	7.23	1.41	1.35
35	m	619	II0	C22-C10	7.23	1.57	1.42
35	c	316	II0	C22-C10	7.22	1.57	1.42
35	n	615	II0	C21-C09	7.22	1.57	1.42
35	l	302	II0	C22-C10	7.21	1.57	1.42
35	m	619	II0	C24-C26	7.20	1.56	1.42
26	A	825	CLA	C4B-NB	7.20	1.41	1.35
35	k	620	II0	C24-C26	7.20	1.56	1.42
26	A	826	CLA	C4B-NB	7.20	1.41	1.35
35	b	315	II0	C23-C25	7.20	1.56	1.42
35	d	316	II0	C23-C25	7.19	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	614	II0	C24-C26	7.19	1.56	1.42
35	c	316	II0	C23-C25	7.18	1.56	1.42
35	a	314	II0	C24-C26	7.18	1.56	1.42
35	d	301	II0	C24-C26	7.18	1.56	1.42
35	i	313	II0	C24-C26	7.18	1.56	1.42
35	d	317	II0	C22-C10	7.17	1.57	1.42
35	i	314	II0	C24-C26	7.16	1.56	1.42
35	d	316	II0	C24-C26	7.16	1.56	1.42
35	n	616	II0	C22-C10	7.16	1.57	1.42
35	a	313	II0	C24-C26	7.16	1.56	1.42
26	B	807	CLA	C4B-NB	7.16	1.41	1.35
35	i	313	II0	C22-C10	7.15	1.57	1.42
35	j	615	II0	C22-C10	7.15	1.57	1.42
26	B	812	CLA	C4B-NB	7.15	1.41	1.35
35	d	317	II0	C24-C26	7.14	1.56	1.42
35	j	615	II0	C24-C26	7.14	1.56	1.42
35	c	313	II0	C24-C26	7.13	1.56	1.42
35	c	316	II0	C24-C26	7.13	1.56	1.42
35	i	312	II0	C22-C10	7.13	1.57	1.42
35	i	319	II0	C21-C09	7.12	1.57	1.42
35	m	615	II0	C22-C10	7.12	1.57	1.42
35	i	314	II0	C21-C09	7.12	1.57	1.42
35	a	316	II0	C24-C26	7.10	1.56	1.42
35	h	310	II0	C21-C09	7.10	1.57	1.42
35	n	615	II0	C24-C26	7.10	1.56	1.42
35	i	319	II0	C24-C26	7.10	1.56	1.42
35	m	616	II0	C24-C26	7.10	1.56	1.42
35	m	614	II0	C21-C09	7.09	1.57	1.42
35	k	619	II0	C24-C26	7.08	1.56	1.42
35	j	614	II0	C24-C26	7.08	1.56	1.42
35	n	616	II0	C24-C26	7.07	1.56	1.42
35	i	314	II0	C22-C10	7.07	1.57	1.42
35	m	616	II0	C21-C09	7.07	1.57	1.42
35	k	616	II0	C22-C10	7.06	1.57	1.42
35	n	618	II0	C22-C10	7.05	1.57	1.42
35	d	315	II0	C24-C26	7.05	1.56	1.42
35	h	312	II0	C21-C09	7.05	1.57	1.42
35	m	616	II0	C22-C10	7.04	1.57	1.42
35	a	316	II0	C22-C10	7.04	1.57	1.42
35	J	104	II0	C24-C26	7.03	1.56	1.42
35	a	312	II0	C24-C26	7.03	1.56	1.42
35	k	615	II0	C24-C26	7.03	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	619	II0	C21-C09	7.02	1.57	1.42
35	l	314	II0	C24-C26	7.01	1.56	1.42
26	a	302	CLA	C4B-NB	7.01	1.41	1.35
26	n	602	CLA	C4B-NB	7.01	1.41	1.35
35	i	316	II0	C24-C26	7.00	1.56	1.42
35	c	313	II0	C22-C10	7.00	1.57	1.42
35	k	616	II0	C24-C26	7.00	1.56	1.42
35	d	316	II0	C22-C10	7.00	1.57	1.42
35	i	316	II0	C21-C09	6.99	1.57	1.42
35	i	312	II0	C24-C26	6.98	1.56	1.42
35	j	614	II0	C21-C09	6.98	1.57	1.42
35	m	615	II0	C24-C26	6.98	1.56	1.42
26	i	305	CLA	C4B-NB	6.96	1.41	1.35
35	a	314	II0	C22-C10	6.96	1.57	1.42
26	b	304	CLA	C4B-NB	6.95	1.41	1.35
35	J	104	II0	C21-C09	6.94	1.57	1.42
35	m	614	II0	C22-C10	6.94	1.57	1.42
35	h	311	II0	C24-C26	6.93	1.55	1.42
26	k	602	CLA	C4B-NB	6.93	1.41	1.35
35	l	315	II0	C21-C09	6.92	1.57	1.42
35	l	314	II0	C22-C10	6.92	1.57	1.42
35	d	301	II0	C22-C10	6.90	1.56	1.42
35	d	315	II0	C22-C10	6.90	1.56	1.42
35	a	313	II0	C21-C09	6.89	1.56	1.42
35	i	316	II0	C23-C25	6.88	1.55	1.42
35	b	314	II0	C24-C26	6.88	1.55	1.42
35	b	314	II0	C21-C09	6.87	1.56	1.42
35	h	312	II0	C22-C10	6.87	1.56	1.42
35	k	620	II0	C21-C09	6.87	1.56	1.42
35	a	312	II0	C21-C09	6.86	1.56	1.42
35	k	619	II0	C21-C09	6.85	1.56	1.42
35	d	317	II0	C21-C09	6.84	1.56	1.42
26	A	834	CLA	C4B-NB	6.84	1.41	1.35
35	n	616	II0	C21-C09	6.84	1.56	1.42
35	c	316	II0	C21-C09	6.84	1.56	1.42
35	b	315	II0	C21-C09	6.83	1.56	1.42
36	s	401	KC2	C2A-C3A	6.83	1.51	1.37
35	i	312	II0	C21-C09	6.82	1.56	1.42
35	n	615	II0	C22-C10	6.82	1.56	1.42
35	n	618	II0	C21-C09	6.81	1.56	1.42
35	l	315	II0	C22-C10	6.80	1.56	1.42
35	J	104	II0	C23-C25	6.80	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	i	316	II0	C22-C10	6.78	1.56	1.42
35	i	313	II0	C21-C09	6.77	1.56	1.42
35	k	620	II0	C22-C10	6.77	1.56	1.42
35	l	314	II0	C21-C09	6.77	1.56	1.42
26	j	607	CLA	C4B-NB	6.76	1.41	1.35
35	c	313	II0	C21-C09	6.74	1.56	1.42
35	k	619	II0	C22-C10	6.74	1.56	1.42
35	m	615	II0	C21-C09	6.74	1.56	1.42
35	k	615	II0	C21-C09	6.73	1.56	1.42
35	i	312	II0	C23-C25	6.73	1.55	1.42
35	h	311	II0	C22-C10	6.72	1.56	1.42
35	j	615	II0	C21-C09	6.72	1.56	1.42
35	k	616	II0	C23-C25	6.71	1.55	1.42
35	i	319	II0	C23-C25	6.70	1.55	1.42
35	j	614	II0	C22-C10	6.69	1.56	1.42
35	a	313	II0	C22-C10	6.68	1.56	1.42
35	a	314	II0	C21-C09	6.68	1.56	1.42
35	d	315	II0	C21-C09	6.67	1.56	1.42
35	d	301	II0	C21-C09	6.67	1.56	1.42
35	k	615	II0	C23-C25	6.66	1.55	1.42
35	J	104	II0	C22-C10	6.66	1.56	1.42
36	c	310	KC2	C2A-C3A	6.64	1.50	1.37
35	h	311	II0	C21-C09	6.63	1.56	1.42
35	l	302	II0	C23-C25	6.60	1.55	1.42
35	m	614	II0	C23-C25	6.59	1.55	1.42
35	a	312	II0	C22-C10	6.59	1.56	1.42
35	k	619	II0	C23-C25	6.58	1.55	1.42
35	m	619	II0	C23-C25	6.53	1.55	1.42
35	b	314	II0	C22-C10	6.53	1.56	1.42
35	h	311	II0	C23-C25	6.53	1.55	1.42
35	b	314	II0	C23-C25	6.51	1.55	1.42
35	n	615	II0	C23-C25	6.49	1.55	1.42
35	l	315	II0	C23-C25	6.48	1.55	1.42
35	d	301	II0	C23-C25	6.46	1.55	1.42
35	n	618	II0	C23-C25	6.45	1.55	1.42
35	h	312	II0	C23-C25	6.43	1.54	1.42
35	a	316	II0	C23-C25	6.40	1.54	1.42
26	l	305	CLA	C4B-NB	6.39	1.40	1.35
35	d	317	II0	C23-C25	6.39	1.54	1.42
35	a	314	II0	C23-C25	6.38	1.54	1.42
35	d	315	II0	C23-C25	6.35	1.54	1.42
35	a	312	II0	C23-C25	6.35	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	310	KC2	CBA-CAA	6.34	1.52	1.33
35	k	620	II0	C23-C25	6.34	1.54	1.42
35	m	615	II0	C23-C25	6.33	1.54	1.42
35	j	614	II0	C23-C25	6.32	1.54	1.42
35	c	313	II0	C23-C25	6.32	1.54	1.42
35	i	314	II0	C23-C25	6.31	1.54	1.42
35	j	615	II0	C23-C25	6.30	1.54	1.42
36	s	401	KC2	CBA-CAA	6.26	1.52	1.33
35	l	314	II0	C23-C25	6.26	1.54	1.42
35	a	313	II0	C23-C25	6.20	1.54	1.42
35	i	313	II0	C24-C22	6.18	1.38	1.20
35	i	314	II0	C24-C22	6.17	1.38	1.20
35	m	619	II0	C24-C22	6.14	1.38	1.20
35	d	317	II0	C24-C22	6.13	1.38	1.20
35	l	302	II0	C24-C22	6.12	1.38	1.20
35	j	615	II0	C24-C22	6.11	1.38	1.20
35	b	315	II0	C24-C22	6.11	1.38	1.20
35	k	615	II0	C24-C22	6.10	1.38	1.20
35	h	310	II0	C23-C25	6.07	1.54	1.42
35	m	616	II0	C24-C22	6.05	1.38	1.20
35	c	316	II0	C24-C22	6.05	1.37	1.20
35	k	616	II0	C24-C22	6.04	1.37	1.20
35	n	618	II0	C24-C22	6.03	1.37	1.20
35	m	615	II0	C24-C22	6.03	1.37	1.20
35	i	319	II0	C24-C22	6.02	1.37	1.20
35	n	616	II0	C23-C21	6.01	1.37	1.20
35	h	312	II0	C24-C22	5.97	1.37	1.20
35	a	314	II0	C24-C22	5.92	1.37	1.20
35	i	312	II0	C24-C22	5.92	1.37	1.20
35	a	316	II0	C23-C21	5.90	1.37	1.20
35	d	316	II0	C23-C21	5.89	1.37	1.20
35	n	616	II0	C24-C22	5.89	1.37	1.20
35	i	314	II0	C23-C21	5.88	1.37	1.20
35	k	616	II0	C23-C21	5.88	1.37	1.20
35	m	614	II0	C24-C22	5.86	1.37	1.20
35	a	313	II0	C24-C22	5.85	1.37	1.20
35	m	616	II0	C23-C21	5.85	1.37	1.20
35	i	313	II0	C23-C21	5.85	1.37	1.20
35	d	316	II0	C24-C22	5.85	1.37	1.20
35	l	314	II0	C24-C22	5.83	1.37	1.20
35	j	614	II0	C24-C22	5.81	1.37	1.20
36	s	401	KC2	C3B-C2B	5.80	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	620	II0	C24-C22	5.80	1.37	1.20
35	c	313	II0	C24-C22	5.80	1.37	1.20
35	b	315	II0	C23-C21	5.79	1.37	1.20
35	d	301	II0	C24-C22	5.79	1.37	1.20
35	d	315	II0	C24-C22	5.77	1.37	1.20
35	a	316	II0	C24-C22	5.77	1.37	1.20
35	d	317	II0	C23-C21	5.77	1.37	1.20
35	J	104	II0	C24-C22	5.77	1.37	1.20
35	n	615	II0	C24-C22	5.75	1.37	1.20
35	i	316	II0	C24-C22	5.75	1.37	1.20
35	n	615	II0	C23-C21	5.74	1.37	1.20
35	i	312	II0	C23-C21	5.74	1.37	1.20
35	i	316	II0	C23-C21	5.73	1.37	1.20
35	k	619	II0	C24-C22	5.73	1.37	1.20
36	c	310	KC2	O2A-CGA	5.72	1.45	1.30
35	h	311	II0	C23-C21	5.72	1.37	1.20
35	h	311	II0	C24-C22	5.72	1.37	1.20
35	a	312	II0	C24-C22	5.70	1.36	1.20
35	l	315	II0	C24-C22	5.69	1.36	1.20
35	k	615	II0	C23-C21	5.68	1.36	1.20
35	a	314	II0	C23-C21	5.67	1.36	1.20
35	l	315	II0	C23-C21	5.67	1.36	1.20
35	d	301	II0	C23-C21	5.67	1.36	1.20
35	b	314	II0	C24-C22	5.66	1.36	1.20
35	b	314	II0	C23-C21	5.66	1.36	1.20
35	k	620	II0	C23-C21	5.66	1.36	1.20
35	m	614	II0	C23-C21	5.64	1.36	1.20
35	k	619	II0	C23-C21	5.64	1.36	1.20
36	s	401	KC2	O2A-CGA	5.64	1.45	1.30
35	J	104	II0	C23-C21	5.63	1.36	1.20
35	c	316	II0	C23-C21	5.62	1.36	1.20
35	l	314	II0	C23-C21	5.61	1.36	1.20
35	a	312	II0	C23-C21	5.60	1.36	1.20
35	j	615	II0	C23-C21	5.60	1.36	1.20
35	i	319	II0	C23-C21	5.57	1.36	1.20
35	c	313	II0	C23-C21	5.57	1.36	1.20
35	m	615	II0	C23-C21	5.57	1.36	1.20
35	j	614	II0	C23-C21	5.57	1.36	1.20
35	h	310	II0	C23-C21	5.56	1.36	1.20
35	m	619	II0	C23-C21	5.56	1.36	1.20
35	l	302	II0	C23-C21	5.55	1.36	1.20
36	s	404	KC2	C4D-ND	-5.55	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	313	II0	C23-C21	5.54	1.36	1.20
35	d	315	II0	C23-C21	5.54	1.36	1.20
35	h	312	II0	C23-C21	5.53	1.36	1.20
35	n	618	II0	C23-C21	5.51	1.36	1.20
36	c	310	KC2	C3B-C2B	5.38	1.48	1.37
36	c	310	KC2	C1A-NA	-5.38	1.27	1.38
36	s	401	KC2	C1A-NA	-5.37	1.27	1.38
29	l	316	WVN	C19-C22	5.27	1.57	1.45
35	m	616	II0	C33-C35	5.26	1.57	1.45
29	B	850	WVN	C19-C22	5.20	1.57	1.45
36	c	310	KC2	C3D-C2D	5.20	1.48	1.39
36	d	312	KC2	C4D-ND	-5.19	1.30	1.35
29	l	316	WVN	C31-C32	5.18	1.57	1.45
29	B	849	WVN	C19-C22	5.18	1.57	1.45
29	B	848	WVN	C19-C22	5.16	1.57	1.45
36	c	310	KC2	CHD-C4C	5.16	1.48	1.35
36	s	401	KC2	C3D-C2D	5.15	1.48	1.39
29	A	845	WVN	C02-C11	5.12	1.57	1.50
29	A	846	WVN	C19-C22	5.12	1.56	1.45
29	i	315	WVN	C19-C22	5.12	1.56	1.45
29	s	407	WVN	C19-C22	5.10	1.56	1.45
29	R	200	WVN	C19-C22	5.10	1.56	1.45
29	B	853	WVN	C19-C22	5.09	1.56	1.45
36	c	310	KC2	C3C-C2C	5.08	1.47	1.37
29	B	847	WVN	C19-C22	5.08	1.56	1.45
29	A	845	WVN	C19-C22	5.06	1.56	1.45
29	l	303	WVN	C19-C22	5.05	1.56	1.45
29	B	847	WVN	C31-C32	5.04	1.56	1.45
29	L	205	WVN	C19-C22	5.04	1.56	1.45
29	F	203	WVN	C19-C22	5.03	1.56	1.45
29	K	102	WVN	C19-C22	5.03	1.56	1.45
36	s	401	KC2	CHD-C4C	5.02	1.47	1.35
36	n	611	KC2	C4D-ND	-5.02	1.30	1.35
29	A	857	WVN	C19-C22	5.02	1.56	1.45
29	K	102	WVN	C31-C32	5.02	1.56	1.45
29	B	850	WVN	C31-C32	5.01	1.56	1.45
29	J	102	WVN	C19-C22	5.00	1.56	1.45
29	B	849	WVN	C31-C32	5.00	1.56	1.45
29	R	200	WVN	C31-C32	4.99	1.56	1.45
36	m	611	KC2	C4D-ND	-4.99	1.30	1.35
29	B	848	WVN	C31-C32	4.98	1.56	1.45
29	i	315	WVN	C31-C32	4.97	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	848	WVN	C19-C22	4.97	1.56	1.45
29	J	101	WVN	C19-C22	4.96	1.56	1.45
29	s	405	WVN	C19-C22	4.96	1.56	1.45
29	h	309	WVN	C19-C22	4.96	1.56	1.45
36	d	311	KC2	C4D-ND	-4.94	1.30	1.35
29	h	309	WVN	C31-C32	4.93	1.56	1.45
29	A	845	WVN	C31-C32	4.93	1.56	1.45
29	A	846	WVN	C31-C32	4.93	1.56	1.45
29	M	101	WVN	C31-C32	4.92	1.56	1.45
29	F	203	WVN	C31-C32	4.91	1.56	1.45
29	L	205	WVN	C31-C32	4.90	1.56	1.45
29	s	405	WVN	C31-C32	4.90	1.56	1.45
29	A	857	WVN	C31-C32	4.90	1.56	1.45
29	l	303	WVN	C31-C32	4.89	1.56	1.45
29	l	316	WVN	C39-C36	4.89	1.58	1.43
29	B	853	WVN	C31-C32	4.89	1.56	1.45
29	l	316	WVN	C02-C11	4.88	1.57	1.50
36	l	312	KC2	C4D-ND	-4.88	1.30	1.35
29	A	847	WVN	C31-C32	4.86	1.56	1.45
29	s	407	WVN	C31-C32	4.86	1.56	1.45
29	A	847	WVN	C19-C22	4.85	1.56	1.45
25	A	801	CL0	C4B-NB	4.84	1.39	1.35
29	I	101	WVN	C19-C22	4.83	1.56	1.45
29	A	848	WVN	C02-C11	4.83	1.57	1.50
29	J	102	WVN	C39-C36	4.82	1.58	1.43
36	k	611	KC2	C4D-ND	-4.82	1.30	1.35
25	A	801	CL0	MG-NA	4.81	2.17	2.06
36	j	611	KC2	C4D-ND	-4.81	1.30	1.35
26	c	309	CLA	O2D-CGD	4.81	1.44	1.33
29	J	101	WVN	C31-C32	4.80	1.56	1.45
29	i	315	WVN	C02-C11	4.79	1.57	1.50
36	c	310	KC2	O2D-CGD	4.78	1.44	1.33
29	l	316	WVN	C40-C37	4.76	1.58	1.43
35	i	313	II0	C41-C39	4.76	1.58	1.43
29	J	102	WVN	C31-C32	4.75	1.56	1.45
29	B	853	WVN	C02-C11	4.75	1.57	1.50
35	b	315	II0	C42-C40	4.75	1.58	1.43
29	B	847	WVN	C02-C11	4.74	1.57	1.50
35	b	315	II0	C41-C39	4.74	1.58	1.43
29	R	200	WVN	C02-C11	4.74	1.57	1.50
36	s	401	KC2	C3C-C2C	4.74	1.46	1.37
35	b	314	II0	C31-C29	4.73	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	302	II0	C31-C29	4.73	1.58	1.43
35	b	314	II0	C41-C39	4.73	1.58	1.43
29	i	315	WVN	C39-C36	4.72	1.58	1.43
35	n	615	II0	C31-C29	4.72	1.58	1.43
29	I	101	WVN	C02-C11	4.72	1.57	1.50
29	A	847	WVN	C39-C36	4.72	1.58	1.43
29	J	102	WVN	C02-C11	4.71	1.57	1.50
29	B	850	WVN	C39-C36	4.71	1.58	1.43
29	B	849	WVN	C39-C36	4.71	1.58	1.43
29	I	101	WVN	C31-C32	4.71	1.56	1.45
35	b	315	II0	C31-C29	4.70	1.58	1.43
29	A	857	WVN	C39-C36	4.70	1.58	1.43
35	k	619	II0	C31-C29	4.70	1.58	1.43
35	b	314	II0	C33-C35	4.70	1.56	1.45
29	A	846	WVN	C39-C36	4.70	1.58	1.43
35	m	619	II0	C31-C29	4.70	1.58	1.43
26	i	305	CLA	C1D-ND	4.69	1.43	1.37
29	B	848	WVN	C39-C36	4.69	1.58	1.43
35	k	620	II0	C31-C29	4.69	1.58	1.43
29	A	845	WVN	C39-C36	4.69	1.58	1.43
29	R	200	WVN	C39-C36	4.69	1.58	1.43
29	K	102	WVN	C39-C36	4.69	1.58	1.43
29	B	847	WVN	C39-C36	4.69	1.58	1.43
29	M	101	WVN	C39-C36	4.68	1.58	1.43
29	J	102	WVN	C40-C37	4.68	1.57	1.43
35	m	614	II0	C31-C29	4.68	1.57	1.43
35	i	313	II0	C31-C29	4.68	1.57	1.43
35	m	616	II0	C31-C29	4.67	1.57	1.43
35	J	104	II0	C31-C29	4.67	1.57	1.43
29	L	201	WVN	C31-C32	4.67	1.56	1.45
35	a	314	II0	C33-C35	4.67	1.56	1.45
35	m	616	II0	C41-C39	4.67	1.57	1.43
29	L	205	WVN	C39-C36	4.67	1.57	1.43
36	i	309	KC2	C4D-ND	-4.67	1.31	1.35
29	F	203	WVN	C39-C36	4.66	1.57	1.43
35	a	313	II0	C31-C29	4.66	1.57	1.43
35	l	315	II0	C41-C39	4.66	1.57	1.43
29	A	857	WVN	C02-C11	4.66	1.57	1.50
35	k	619	II0	C33-C35	4.65	1.55	1.45
35	n	618	II0	C31-C29	4.65	1.57	1.43
26	c	309	CLA	C3D-C4D	-4.65	1.33	1.44
29	s	405	WVN	C39-C36	4.65	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	201	WVN	C19-C22	4.64	1.55	1.45
35	l	315	II0	C31-C29	4.64	1.57	1.43
35	n	615	II0	C41-C39	4.64	1.57	1.43
35	m	614	II0	C41-C39	4.64	1.57	1.43
29	F	203	WVN	C02-C11	4.63	1.57	1.50
35	j	614	II0	C31-C29	4.63	1.57	1.43
35	k	619	II0	C41-C39	4.63	1.57	1.43
35	d	301	II0	C33-C35	4.62	1.55	1.45
29	s	407	WVN	C39-C36	4.62	1.57	1.43
29	A	846	WVN	C02-C11	4.62	1.57	1.50
35	i	316	II0	C31-C29	4.62	1.57	1.43
35	i	319	II0	C31-C29	4.62	1.57	1.43
35	k	615	II0	C41-C39	4.62	1.57	1.43
29	B	850	WVN	C40-C37	4.62	1.57	1.43
35	d	317	II0	C41-C39	4.61	1.57	1.43
35	h	312	II0	C31-C29	4.61	1.57	1.43
29	B	848	WVN	C02-C11	4.61	1.57	1.50
35	a	314	II0	C31-C29	4.61	1.57	1.43
35	d	301	II0	C31-C29	4.61	1.57	1.43
35	i	313	II0	C42-C40	4.61	1.57	1.43
35	m	619	II0	C41-C39	4.61	1.57	1.43
35	a	313	II0	C41-C39	4.61	1.57	1.43
35	d	317	II0	C31-C29	4.61	1.57	1.43
29	J	101	WVN	C39-C36	4.61	1.57	1.43
35	i	312	II0	C41-C39	4.61	1.57	1.43
29	M	101	WVN	C19-C22	4.61	1.55	1.45
29	B	853	WVN	C39-C36	4.60	1.57	1.43
29	B	849	WVN	C40-C37	4.60	1.57	1.43
29	l	303	WVN	C39-C36	4.60	1.57	1.43
35	a	312	II0	C31-C29	4.60	1.57	1.43
29	i	315	WVN	C40-C37	4.60	1.57	1.43
36	s	401	KC2	O2D-CGD	4.60	1.44	1.33
35	d	315	II0	C41-C39	4.60	1.57	1.43
35	d	316	II0	C41-C39	4.60	1.57	1.43
35	i	319	II0	C41-C39	4.59	1.57	1.43
35	j	615	II0	C31-C29	4.59	1.57	1.43
35	m	615	II0	C31-C29	4.59	1.57	1.43
29	J	101	WVN	C02-C11	4.59	1.57	1.50
29	h	309	WVN	C02-C11	4.59	1.57	1.50
29	h	309	WVN	C39-C36	4.59	1.57	1.43
35	l	302	II0	C32-C30	4.59	1.57	1.43
35	h	311	II0	C31-C29	4.59	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	J	104	II0	C41-C39	4.58	1.57	1.43
35	i	314	II0	C31-C29	4.58	1.57	1.43
29	A	857	WVN	C40-C37	4.58	1.57	1.43
35	l	302	II0	C42-C40	4.58	1.57	1.43
35	i	313	II0	C33-C35	4.58	1.55	1.45
35	a	316	II0	C31-C29	4.57	1.57	1.43
35	i	314	II0	C41-C39	4.57	1.57	1.43
35	l	314	II0	C31-C29	4.57	1.57	1.43
35	n	616	II0	C41-C39	4.57	1.57	1.43
35	l	314	II0	C41-C39	4.56	1.57	1.43
29	l	303	WVN	C02-C11	4.56	1.57	1.50
35	c	313	II0	C41-C39	4.56	1.57	1.43
29	B	849	WVN	C02-C11	4.56	1.57	1.50
35	j	615	II0	C41-C39	4.56	1.57	1.43
35	n	618	II0	C41-C39	4.56	1.57	1.43
35	i	316	II0	C41-C39	4.56	1.57	1.43
29	L	205	WVN	C02-C11	4.56	1.57	1.50
29	A	847	WVN	C40-C37	4.56	1.57	1.43
29	R	200	WVN	C40-C37	4.55	1.57	1.43
35	c	316	II0	C31-C29	4.55	1.57	1.43
35	a	312	II0	C41-C39	4.55	1.57	1.43
35	n	618	II0	C32-C30	4.55	1.57	1.43
35	h	312	II0	C41-C39	4.55	1.57	1.43
35	l	302	II0	C33-C35	4.55	1.55	1.45
35	a	316	II0	C41-C39	4.55	1.57	1.43
35	h	311	II0	C32-C30	4.55	1.57	1.43
29	B	846	WVN	C39-C36	4.55	1.57	1.43
35	c	313	II0	C31-C29	4.55	1.57	1.43
26	A	827	CLA	C1D-ND	4.54	1.43	1.37
35	j	614	II0	C41-C39	4.54	1.57	1.43
29	A	846	WVN	C40-C37	4.54	1.57	1.43
29	B	847	WVN	C40-C37	4.54	1.57	1.43
35	d	316	II0	C31-C29	4.54	1.57	1.43
35	h	311	II0	C41-C39	4.54	1.57	1.43
35	m	619	II0	C33-C35	4.53	1.55	1.45
35	m	614	II0	C33-C35	4.53	1.55	1.45
35	n	616	II0	C31-C29	4.53	1.57	1.43
29	A	848	WVN	C39-C36	4.53	1.57	1.43
35	b	315	II0	C32-C30	4.53	1.57	1.43
29	B	849	WVN	C23-C25	4.53	1.55	1.45
29	A	845	WVN	C40-C37	4.53	1.57	1.43
29	s	405	WVN	C40-C37	4.53	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	615	II0	C42-C40	4.53	1.57	1.43
35	k	620	II0	C41-C39	4.53	1.57	1.43
35	k	616	II0	C41-C39	4.53	1.57	1.43
35	d	315	II0	C31-C29	4.52	1.57	1.43
35	j	614	II0	C33-C35	4.52	1.55	1.45
29	M	101	WVN	C40-C37	4.52	1.57	1.43
29	L	201	WVN	C39-C36	4.52	1.57	1.43
35	a	313	II0	C42-C40	4.52	1.57	1.43
35	m	614	II0	C42-C40	4.52	1.57	1.43
35	m	614	II0	C32-C30	4.52	1.57	1.43
29	A	848	WVN	C31-C32	4.52	1.55	1.45
35	l	315	II0	C33-C35	4.52	1.55	1.45
35	a	314	II0	C41-C39	4.51	1.57	1.43
35	m	619	II0	C32-C30	4.51	1.57	1.43
36	k	612	KC2	C4D-ND	-4.51	1.31	1.35
35	m	616	II0	C42-C40	4.51	1.57	1.43
29	F	203	WVN	C23-C25	4.50	1.55	1.45
29	s	405	WVN	C02-C11	4.50	1.56	1.50
29	s	407	WVN	C02-C11	4.50	1.56	1.50
35	b	314	II0	C42-C40	4.50	1.57	1.43
35	l	315	II0	C32-C30	4.50	1.57	1.43
29	l	316	WVN	C29-C26	4.50	1.57	1.43
29	K	102	WVN	C40-C37	4.50	1.57	1.43
35	a	313	II0	C32-C30	4.50	1.57	1.43
29	I	101	WVN	C39-C36	4.49	1.57	1.43
29	B	848	WVN	C40-C37	4.49	1.57	1.43
35	d	301	II0	C41-C39	4.49	1.57	1.43
36	c	310	KC2	CHC-C4B	4.49	1.47	1.38
29	L	205	WVN	C40-C37	4.48	1.57	1.43
35	d	317	II0	C42-C40	4.48	1.57	1.43
35	c	316	II0	C41-C39	4.48	1.57	1.43
29	J	101	WVN	C40-C37	4.48	1.57	1.43
35	m	619	II0	C42-C40	4.48	1.57	1.43
29	F	203	WVN	C40-C37	4.48	1.57	1.43
35	i	312	II0	C31-C29	4.48	1.57	1.43
35	a	314	II0	C32-C30	4.48	1.57	1.43
35	n	615	II0	C32-C30	4.47	1.57	1.43
35	a	316	II0	C32-C30	4.47	1.57	1.43
25	A	801	CL0	MG-NC	4.47	2.16	2.06
29	A	845	WVN	C23-C25	4.47	1.55	1.45
35	i	319	II0	C42-C40	4.47	1.57	1.43
35	b	315	II0	C33-C35	4.47	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	309	CLA	O2A-CGA	4.47	1.45	1.30
35	l	302	II0	C41-C39	4.47	1.57	1.43
35	h	310	II0	C31-C29	4.47	1.57	1.43
35	h	310	II0	C41-C39	4.46	1.57	1.43
29	A	846	WVN	C23-C25	4.46	1.55	1.45
35	h	311	II0	C33-C35	4.46	1.55	1.45
35	m	615	II0	C41-C39	4.46	1.57	1.43
35	i	312	II0	C42-C40	4.46	1.57	1.43
35	m	616	II0	C32-C30	4.46	1.57	1.43
35	J	104	II0	C42-C40	4.46	1.57	1.43
35	a	316	II0	C42-C40	4.45	1.57	1.43
29	B	853	WVN	C40-C37	4.45	1.57	1.43
35	c	313	II0	C32-C30	4.45	1.57	1.43
35	n	616	II0	C32-C30	4.45	1.57	1.43
35	h	312	II0	C32-C30	4.45	1.57	1.43
35	j	614	II0	C42-C40	4.45	1.57	1.43
35	d	301	II0	C32-C30	4.45	1.57	1.43
35	c	313	II0	C42-C40	4.45	1.57	1.43
35	k	616	II0	C31-C29	4.44	1.57	1.43
29	s	407	WVN	C40-C37	4.44	1.57	1.43
35	d	316	II0	C32-C30	4.44	1.57	1.43
35	k	615	II0	C42-C40	4.44	1.57	1.43
29	L	205	WVN	C23-C25	4.44	1.55	1.45
29	h	309	WVN	C40-C37	4.44	1.57	1.43
35	k	619	II0	C32-C30	4.44	1.57	1.43
35	k	619	II0	C42-C40	4.44	1.57	1.43
35	d	316	II0	C42-C40	4.44	1.57	1.43
35	i	313	II0	C32-C30	4.43	1.57	1.43
35	j	615	II0	C32-C30	4.43	1.57	1.43
29	B	850	WVN	C02-C11	4.43	1.56	1.50
35	d	317	II0	C32-C30	4.43	1.57	1.43
29	l	303	WVN	C40-C37	4.43	1.57	1.43
29	B	846	WVN	C31-C32	4.43	1.55	1.45
35	k	615	II0	C31-C29	4.42	1.57	1.43
29	A	847	WVN	C02-C11	4.42	1.56	1.50
26	k	604	CLA	C1D-ND	4.42	1.43	1.37
35	l	314	II0	C42-C40	4.42	1.57	1.43
35	d	301	II0	C42-C40	4.41	1.57	1.43
35	d	315	II0	C42-C40	4.41	1.57	1.43
35	i	319	II0	C32-C30	4.41	1.57	1.43
35	i	316	II0	C42-C40	4.41	1.57	1.43
35	k	616	II0	C32-C30	4.41	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	846	WVN	C40-C37	4.41	1.57	1.43
35	n	618	II0	C42-C40	4.41	1.57	1.43
29	B	848	WVN	C23-C25	4.41	1.55	1.45
29	B	853	WVN	C23-C25	4.41	1.55	1.45
29	A	845	WVN	C30-C28	4.40	1.57	1.43
29	s	407	WVN	C29-C26	4.40	1.57	1.43
35	j	614	II0	C32-C30	4.40	1.57	1.43
29	A	847	WVN	C23-C25	4.40	1.55	1.45
29	B	850	WVN	C29-C26	4.40	1.57	1.43
35	k	616	II0	C42-C40	4.40	1.57	1.43
35	a	312	II0	C42-C40	4.40	1.57	1.43
35	h	310	II0	C42-C40	4.40	1.57	1.43
35	m	615	II0	C32-C30	4.40	1.57	1.43
29	B	850	WVN	C23-C25	4.39	1.55	1.45
35	j	615	II0	C42-C40	4.39	1.57	1.43
35	n	616	II0	C42-C40	4.39	1.57	1.43
29	L	201	WVN	C40-C37	4.39	1.57	1.43
29	J	102	WVN	C30-C28	4.39	1.57	1.43
35	h	312	II0	C42-C40	4.39	1.57	1.43
35	k	615	II0	C32-C30	4.39	1.57	1.43
29	B	847	WVN	C23-C25	4.39	1.55	1.45
29	K	102	WVN	C29-C26	4.38	1.57	1.43
35	a	314	II0	C42-C40	4.38	1.57	1.43
29	B	849	WVN	C30-C28	4.38	1.57	1.43
29	M	101	WVN	C23-C25	4.38	1.55	1.45
35	k	620	II0	C32-C30	4.38	1.57	1.43
35	i	314	II0	C32-C30	4.38	1.57	1.43
29	A	845	WVN	C29-C26	4.38	1.57	1.43
29	K	102	WVN	C02-C11	4.38	1.56	1.50
29	I	101	WVN	C40-C37	4.38	1.57	1.43
29	i	315	WVN	C23-C25	4.38	1.55	1.45
35	i	314	II0	C42-C40	4.38	1.57	1.43
26	B	825	CLA	C1D-ND	4.37	1.43	1.37
35	l	314	II0	C32-C30	4.37	1.57	1.43
29	L	205	WVN	C29-C26	4.37	1.57	1.43
29	B	846	WVN	C30-C28	4.36	1.57	1.43
35	i	312	II0	C32-C30	4.36	1.57	1.43
29	R	200	WVN	C30-C28	4.36	1.57	1.43
35	i	316	II0	C32-C30	4.36	1.57	1.43
29	A	857	WVN	C23-C25	4.36	1.55	1.45
29	B	848	WVN	C29-C26	4.36	1.57	1.43
29	B	847	WVN	C30-C28	4.36	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	620	II0	C42-C40	4.36	1.57	1.43
35	c	316	II0	C32-C30	4.36	1.56	1.43
29	A	848	WVN	C40-C37	4.36	1.56	1.43
35	d	315	II0	C32-C30	4.36	1.56	1.43
30	i	300	LMU	O5'-C5'	4.36	1.54	1.44
29	J	101	WVN	C23-C25	4.36	1.55	1.45
35	n	615	II0	C33-C35	4.36	1.55	1.45
35	J	104	II0	C32-C30	4.35	1.56	1.43
26	k	609	CLA	C1D-ND	4.35	1.43	1.37
35	b	314	II0	C32-C30	4.35	1.56	1.43
29	K	102	WVN	C23-C25	4.35	1.55	1.45
29	A	847	WVN	C29-C26	4.35	1.56	1.43
29	J	102	WVN	C23-C25	4.35	1.55	1.45
29	s	405	WVN	C30-C28	4.35	1.56	1.43
35	k	620	II0	C33-C35	4.34	1.55	1.45
35	l	314	II0	C33-C35	4.34	1.55	1.45
29	F	203	WVN	C29-C26	4.34	1.56	1.43
29	l	303	WVN	C29-C26	4.34	1.56	1.43
29	s	405	WVN	C23-C25	4.34	1.55	1.45
29	i	315	WVN	C30-C28	4.34	1.56	1.43
35	a	312	II0	C32-C30	4.33	1.56	1.43
35	h	311	II0	C42-C40	4.33	1.56	1.43
35	h	312	II0	C33-C35	4.33	1.55	1.45
29	B	853	WVN	C29-C26	4.33	1.56	1.43
29	L	201	WVN	C02-C11	4.33	1.56	1.50
29	A	846	WVN	C29-C26	4.33	1.56	1.43
36	s	401	KC2	CHB-C1B	4.33	1.46	1.38
35	c	316	II0	C42-C40	4.33	1.56	1.43
29	L	205	WVN	C30-C28	4.33	1.56	1.43
29	l	316	WVN	C30-C28	4.33	1.56	1.43
35	J	104	II0	C33-C35	4.33	1.55	1.45
29	i	315	WVN	C29-C26	4.33	1.56	1.43
36	c	310	KC2	CHB-C1B	4.33	1.46	1.38
29	R	200	WVN	C29-C26	4.32	1.56	1.43
29	B	847	WVN	C29-C26	4.32	1.56	1.43
25	A	801	CL0	C1C-C2C	-4.32	1.36	1.44
35	i	316	II0	C33-C35	4.32	1.55	1.45
30	A	850	LMU	O5'-C5'	4.32	1.54	1.44
29	A	857	WVN	C30-C28	4.32	1.56	1.43
29	R	200	WVN	C23-C25	4.32	1.55	1.45
36	n	612	KC2	C4D-ND	-4.32	1.31	1.35
29	B	849	WVN	C29-C26	4.32	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	848	WVN	C30-C28	4.32	1.56	1.43
29	F	203	WVN	C30-C28	4.32	1.56	1.43
29	s	405	WVN	C29-C26	4.32	1.56	1.43
29	h	309	WVN	C29-C26	4.32	1.56	1.43
35	m	615	II0	C42-C40	4.31	1.56	1.43
35	a	316	II0	C33-C35	4.31	1.55	1.45
35	d	315	II0	C33-C35	4.31	1.55	1.45
35	i	319	II0	C33-C35	4.31	1.55	1.45
25	A	801	CL0	C4C-C3C	-4.31	1.37	1.45
29	A	846	WVN	C30-C28	4.31	1.56	1.43
29	A	857	WVN	C29-C26	4.30	1.56	1.43
36	k	613	KC2	C4D-ND	-4.30	1.31	1.35
29	J	101	WVN	C29-C26	4.30	1.56	1.43
35	c	316	II0	C33-C35	4.30	1.55	1.45
35	l	315	II0	C42-C40	4.30	1.56	1.43
35	d	317	II0	C33-C35	4.30	1.55	1.45
36	k	613	KC2	C1D-ND	4.29	1.39	1.35
35	n	618	II0	C33-C35	4.29	1.55	1.45
35	k	615	II0	C33-C35	4.29	1.55	1.45
36	k	612	KC2	C1D-ND	4.29	1.39	1.35
26	B	816	CLA	C1D-ND	4.28	1.43	1.37
35	i	314	II0	C33-C35	4.28	1.55	1.45
29	l	303	WVN	C30-C28	4.28	1.56	1.43
29	M	101	WVN	C30-C28	4.28	1.56	1.43
29	K	102	WVN	C30-C28	4.28	1.56	1.43
35	a	313	II0	C33-C35	4.28	1.55	1.45
29	A	847	WVN	C30-C28	4.28	1.56	1.43
29	h	309	WVN	C30-C28	4.27	1.56	1.43
29	l	303	WVN	C23-C25	4.27	1.55	1.45
35	a	312	II0	C33-C35	4.27	1.55	1.45
35	d	316	II0	C33-C35	4.27	1.55	1.45
29	B	846	WVN	C19-C22	4.26	1.55	1.45
29	B	853	WVN	C30-C28	4.25	1.56	1.43
35	n	616	II0	C33-C35	4.25	1.55	1.45
29	s	407	WVN	C30-C28	4.25	1.56	1.43
29	B	850	WVN	C30-C28	4.25	1.56	1.43
29	J	101	WVN	C30-C28	4.25	1.56	1.43
29	h	309	WVN	C23-C25	4.25	1.55	1.45
35	l	302	II0	C34-C36	4.25	1.55	1.45
35	b	315	II0	C34-C36	4.24	1.55	1.45
35	c	313	II0	C33-C35	4.24	1.55	1.45
29	J	102	WVN	C29-C26	4.24	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	101	WVN	C02-C11	4.24	1.56	1.50
26	A	817	CLA	C1D-ND	4.23	1.43	1.37
36	s	401	KC2	C4B-NB	-4.23	1.32	1.37
35	l	315	II0	C34-C36	4.23	1.55	1.45
26	A	841	CLA	C1D-ND	4.22	1.43	1.37
35	j	615	II0	C33-C35	4.21	1.55	1.45
29	s	407	WVN	C23-C25	4.20	1.55	1.45
29	B	846	WVN	C23-C25	4.20	1.55	1.45
36	i	318	KC2	C4D-ND	-4.20	1.31	1.35
29	L	201	WVN	C30-C28	4.20	1.56	1.43
36	k	611	KC2	C1D-ND	4.19	1.38	1.35
29	L	201	WVN	C29-C26	4.19	1.56	1.43
29	A	848	WVN	C23-C25	4.19	1.55	1.45
29	I	101	WVN	C23-C25	4.19	1.54	1.45
29	L	201	WVN	C23-C25	4.19	1.54	1.45
26	n	606	CLA	C1D-ND	4.18	1.42	1.37
29	J	102	WVN	C33-C34	4.18	1.54	1.45
30	i	300	LMU	O5B-C5B	4.18	1.54	1.44
35	i	312	II0	C33-C35	4.18	1.54	1.45
29	M	101	WVN	C29-C26	4.18	1.56	1.43
26	n	608	CLA	C1D-ND	4.17	1.42	1.37
29	A	848	WVN	C30-C28	4.17	1.56	1.43
35	a	313	II0	C34-C36	4.17	1.54	1.45
29	B	850	WVN	C33-C34	4.17	1.54	1.45
30	A	850	LMU	O5B-C5B	4.16	1.54	1.44
29	R	200	WVN	C33-C34	4.16	1.54	1.45
29	B	849	WVN	C33-C34	4.16	1.54	1.45
29	l	316	WVN	C23-C25	4.15	1.54	1.45
26	A	823	CLA	C1D-ND	4.15	1.42	1.37
29	I	101	WVN	C30-C28	4.14	1.56	1.43
35	h	310	II0	C33-C35	4.14	1.54	1.45
29	I	101	WVN	C29-C26	4.13	1.56	1.43
35	m	619	II0	C34-C36	4.13	1.54	1.45
26	c	309	CLA	C3C-C2C	4.13	1.45	1.36
29	A	848	WVN	C29-C26	4.12	1.56	1.43
35	m	614	II0	C34-C36	4.12	1.54	1.45
26	A	821	CLA	C1D-ND	4.12	1.42	1.37
35	n	618	II0	C34-C36	4.11	1.54	1.45
29	i	315	WVN	C33-C34	4.11	1.54	1.45
35	n	615	II0	C34-C36	4.11	1.54	1.45
36	n	612	KC2	C1D-ND	4.11	1.38	1.35
35	d	317	II0	C34-C36	4.10	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	845	WVN	C33-C34	4.09	1.54	1.45
29	B	846	WVN	C29-C26	4.09	1.56	1.43
26	l	313	CLA	C1D-ND	4.08	1.42	1.37
36	l	312	KC2	C3B-C4B	-4.08	1.38	1.46
35	i	313	II0	C34-C36	4.08	1.54	1.45
35	a	312	II0	C34-C36	4.08	1.54	1.45
26	h	306	CLA	C1D-ND	4.07	1.42	1.37
29	s	405	WVN	C33-C34	4.07	1.54	1.45
35	k	616	II0	C33-C35	4.07	1.54	1.45
29	A	846	WVN	C33-C34	4.06	1.54	1.45
29	B	853	WVN	C33-C34	4.06	1.54	1.45
36	s	401	KC2	CHC-C4B	4.06	1.46	1.38
26	a	303	CLA	C1D-ND	4.06	1.42	1.37
26	A	812	CLA	C1D-ND	4.05	1.42	1.37
36	m	611	KC2	C3B-C4B	-4.05	1.38	1.46
36	s	401	KC2	C1B-NB	-4.05	1.32	1.37
29	l	303	WVN	C33-C34	4.05	1.54	1.45
36	j	611	KC2	C1D-ND	4.05	1.38	1.35
26	B	837	CLA	C1D-ND	4.04	1.42	1.37
29	B	847	WVN	C33-C34	4.04	1.54	1.45
35	m	615	II0	C33-C35	4.04	1.54	1.45
26	m	610	CLA	C1D-ND	4.04	1.42	1.37
29	K	102	WVN	C33-C34	4.03	1.54	1.45
35	j	615	II0	C34-C36	4.03	1.54	1.45
26	K	101	CLA	C1D-ND	4.03	1.42	1.37
29	L	205	WVN	C33-C34	4.03	1.54	1.45
29	l	316	WVN	C33-C34	4.03	1.54	1.45
26	j	606	CLA	C1D-ND	4.03	1.42	1.37
26	R	201	CLA	C1D-ND	4.03	1.42	1.37
36	s	404	KC2	C3B-C4B	-4.03	1.38	1.46
26	B	832	CLA	C1D-ND	4.03	1.42	1.37
26	m	601	CLA	C1D-ND	4.03	1.42	1.37
26	n	603	CLA	C1D-ND	4.03	1.42	1.37
36	c	310	KC2	C1B-NB	-4.03	1.32	1.37
26	j	605	CLA	C1D-ND	4.02	1.42	1.37
26	d	306	CLA	C1D-ND	4.02	1.42	1.37
26	j	610	CLA	C1D-ND	4.02	1.42	1.37
29	B	848	WVN	C33-C34	4.02	1.54	1.45
26	c	302	CLA	C1D-ND	4.02	1.42	1.37
26	B	833	CLA	C1D-ND	4.02	1.42	1.37
26	c	303	CLA	C1D-ND	4.02	1.42	1.37
26	B	815	CLA	C1D-ND	4.01	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	311	KC2	C1D-ND	4.01	1.38	1.35
26	b	304	CLA	C1D-ND	4.01	1.42	1.37
26	A	840	CLA	C1D-ND	4.00	1.42	1.37
26	j	607	CLA	C1D-ND	4.00	1.42	1.37
26	d	303	CLA	C1D-ND	4.00	1.42	1.37
26	a	309	CLA	C1D-ND	4.00	1.42	1.37
26	A	834	CLA	C1D-ND	4.00	1.42	1.37
29	A	847	WVN	C33-C34	3.99	1.54	1.45
26	B	812	CLA	C1D-ND	3.99	1.42	1.37
36	i	318	KC2	C1D-ND	3.99	1.38	1.35
36	k	613	KC2	C3B-C4B	-3.99	1.39	1.46
35	m	616	II0	C34-C36	3.99	1.54	1.45
26	B	824	CLA	C1D-ND	3.99	1.42	1.37
26	j	608	CLA	C1D-ND	3.99	1.42	1.37
35	k	615	II0	C34-C36	3.99	1.54	1.45
29	A	857	WVN	C33-C34	3.99	1.54	1.45
26	A	838	CLA	C1D-ND	3.98	1.42	1.37
26	d	305	CLA	C1D-ND	3.98	1.42	1.37
26	A	836	CLA	C1D-ND	3.98	1.42	1.37
36	c	310	KC2	OBD-CAD	3.98	1.27	1.22
35	a	316	II0	C34-C36	3.98	1.54	1.45
26	k	610	CLA	C1D-ND	3.98	1.42	1.37
26	A	835	CLA	C1D-ND	3.98	1.42	1.37
26	n	609	CLA	C1D-ND	3.98	1.42	1.37
26	B	805	CLA	C1D-ND	3.98	1.42	1.37
26	A	826	CLA	C1D-ND	3.98	1.42	1.37
26	b	312	CLA	C1D-ND	3.98	1.42	1.37
26	i	301	CLA	C1D-ND	3.98	1.42	1.37
27	A	842	PQN	C11-C3	3.98	1.57	1.51
36	k	612	KC2	C3B-C4B	-3.98	1.39	1.46
26	n	613	CLA	C1D-ND	3.98	1.42	1.37
26	B	811	CLA	C1D-ND	3.97	1.42	1.37
35	k	620	II0	C34-C36	3.97	1.54	1.45
36	k	611	KC2	C3B-C4B	-3.97	1.39	1.46
26	F	202	CLA	C1D-ND	3.97	1.42	1.37
35	d	301	II0	C34-C36	3.97	1.54	1.45
26	a	308	CLA	C1D-ND	3.96	1.42	1.37
29	M	101	WVN	C33-C34	3.96	1.54	1.45
26	c	307	CLA	C1D-ND	3.96	1.42	1.37
35	c	313	II0	C34-C36	3.96	1.54	1.45
35	k	616	II0	C34-C36	3.96	1.54	1.45
26	B	803	CLA	C1D-ND	3.96	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l	308	CLA	C1D-ND	3.96	1.42	1.37
35	h	312	II0	C34-C36	3.96	1.54	1.45
36	i	318	KC2	C3B-C4B	-3.96	1.39	1.46
26	h	307	CLA	C1D-ND	3.95	1.42	1.37
29	h	309	WVN	C33-C34	3.95	1.54	1.45
35	i	319	II0	C34-C36	3.95	1.54	1.45
26	c	309	CLA	C3B-C2B	3.95	1.45	1.40
26	d	318	CLA	C1D-ND	3.95	1.42	1.37
29	B	846	WVN	C02-C11	3.95	1.56	1.50
26	a	306	CLA	C1D-ND	3.95	1.42	1.37
26	k	601	CLA	C1D-ND	3.95	1.42	1.37
26	d	310	CLA	C1D-ND	3.95	1.42	1.37
29	F	203	WVN	C33-C34	3.95	1.54	1.45
26	i	307	CLA	C1D-ND	3.95	1.42	1.37
26	A	811	CLA	C1D-ND	3.95	1.42	1.37
26	A	837	CLA	C1D-ND	3.95	1.42	1.37
26	B	831	CLA	C1D-ND	3.95	1.42	1.37
26	A	808	CLA	C1D-ND	3.95	1.42	1.37
26	m	603	CLA	C1D-ND	3.95	1.42	1.37
26	m	613	CLA	C1D-ND	3.95	1.42	1.37
26	k	605	CLA	C1D-ND	3.94	1.42	1.37
26	j	613	CLA	C1D-ND	3.94	1.42	1.37
26	A	818	CLA	C1D-ND	3.94	1.42	1.37
26	i	310	CLA	C1D-ND	3.94	1.42	1.37
26	B	841	CLA	C1D-ND	3.94	1.42	1.37
26	A	822	CLA	C1D-ND	3.94	1.42	1.37
26	A	824	CLA	C1D-ND	3.94	1.42	1.37
26	B	806	CLA	C1D-ND	3.94	1.42	1.37
26	c	301	CLA	C1D-ND	3.94	1.42	1.37
35	k	619	II0	C34-C36	3.94	1.54	1.45
26	b	311	CLA	C1D-ND	3.94	1.42	1.37
26	A	832	CLA	C1D-ND	3.94	1.42	1.37
35	J	104	II0	C34-C36	3.93	1.54	1.45
26	F	201	CLA	C1D-ND	3.93	1.42	1.37
26	h	308	CLA	C1D-ND	3.93	1.42	1.37
35	i	316	II0	C34-C36	3.93	1.54	1.45
36	j	611	KC2	C3B-C4B	-3.93	1.39	1.46
26	B	838	CLA	C1D-ND	3.93	1.42	1.37
26	b	303	CLA	C1D-ND	3.92	1.42	1.37
26	A	806	CLA	C1D-ND	3.92	1.42	1.37
26	a	310	CLA	C1D-ND	3.92	1.42	1.37
26	i	306	CLA	C1D-ND	3.92	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	820	CLA	C1D-ND	3.92	1.42	1.37
26	i	303	CLA	C1D-ND	3.92	1.42	1.37
26	m	607	CLA	C1D-ND	3.92	1.42	1.37
26	B	821	CLA	C1D-ND	3.92	1.42	1.37
26	J	103	CLA	C1D-ND	3.92	1.42	1.37
26	b	307	CLA	C1D-ND	3.92	1.42	1.37
29	J	101	WVN	C33-C34	3.92	1.54	1.45
36	s	401	KC2	OBD-CAD	3.92	1.27	1.22
35	i	312	II0	C34-C36	3.92	1.54	1.45
26	B	828	CLA	C1D-ND	3.92	1.42	1.37
26	b	309	CLA	C1D-ND	3.92	1.42	1.37
26	l	307	CLA	C1D-ND	3.91	1.42	1.37
35	i	314	II0	C34-C36	3.91	1.54	1.45
36	l	312	KC2	C1B-C2B	-3.91	1.37	1.45
26	B	810	CLA	C1D-ND	3.91	1.42	1.37
26	c	312	CLA	C1D-ND	3.91	1.42	1.37
26	B	819	CLA	C1D-ND	3.91	1.42	1.37
35	a	314	II0	C34-C36	3.91	1.54	1.45
26	i	308	CLA	C1D-ND	3.91	1.42	1.37
26	a	304	CLA	C1D-ND	3.91	1.42	1.37
26	A	814	CLA	C1D-ND	3.90	1.42	1.37
26	n	601	CLA	C1D-ND	3.90	1.42	1.37
36	s	404	KC2	C1B-C2B	-3.90	1.37	1.45
26	B	840	CLA	C1D-ND	3.90	1.42	1.37
26	h	305	CLA	C1D-ND	3.90	1.42	1.37
26	m	608	CLA	C1D-ND	3.90	1.42	1.37
26	k	614	CLA	C1D-ND	3.90	1.42	1.37
26	d	309	CLA	C1D-ND	3.90	1.42	1.37
26	A	815	CLA	C1D-ND	3.90	1.42	1.37
26	B	817	CLA	C1D-ND	3.90	1.42	1.37
26	s	402	CLA	C1D-ND	3.90	1.42	1.37
36	m	611	KC2	C1D-ND	3.90	1.38	1.35
35	d	315	II0	C34-C36	3.90	1.54	1.45
35	n	616	II0	C34-C36	3.90	1.54	1.45
26	m	604	CLA	C1D-ND	3.90	1.42	1.37
26	a	311	CLA	C1D-ND	3.89	1.42	1.37
26	L	204	CLA	C1D-ND	3.89	1.42	1.37
26	d	307	CLA	C1D-ND	3.89	1.42	1.37
26	d	313	CLA	C1D-ND	3.89	1.42	1.37
26	n	605	CLA	C1D-ND	3.89	1.42	1.37
26	L	206	CLA	C1D-ND	3.89	1.42	1.37
26	l	304	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	304	CLA	C1D-ND	3.89	1.42	1.37
26	A	852	CLA	C1D-ND	3.89	1.42	1.37
26	B	835	CLA	C1D-ND	3.89	1.42	1.37
26	c	306	CLA	C1D-ND	3.89	1.42	1.37
26	i	304	CLA	C1D-ND	3.89	1.42	1.37
26	A	830	CLA	C1D-ND	3.89	1.42	1.37
35	h	310	II0	C34-C36	3.88	1.54	1.45
26	s	408	CLA	C1D-ND	3.88	1.42	1.37
26	n	610	CLA	C1D-ND	3.88	1.42	1.37
26	A	820	CLA	C1D-ND	3.88	1.42	1.37
26	L	202	CLA	C1D-ND	3.88	1.42	1.37
26	l	301	CLA	C1D-ND	3.88	1.42	1.37
36	n	611	KC2	C1D-ND	3.88	1.38	1.35
35	d	316	II0	C34-C36	3.87	1.54	1.45
36	m	611	KC2	C4A-C3A	-3.87	1.37	1.44
36	d	312	KC2	C3B-C4B	-3.87	1.39	1.46
26	B	808	CLA	C1D-ND	3.87	1.42	1.37
26	L	203	CLA	C1D-ND	3.87	1.42	1.37
35	c	316	II0	C34-C36	3.87	1.54	1.45
29	B	846	WVN	C33-C34	3.87	1.54	1.45
26	c	304	CLA	C1D-ND	3.87	1.42	1.37
36	n	611	KC2	C3B-C4B	-3.87	1.39	1.46
26	A	813	CLA	C1D-ND	3.87	1.42	1.37
26	l	306	CLA	C1D-ND	3.87	1.42	1.37
26	j	601	CLA	C1D-ND	3.87	1.42	1.37
26	A	851	CLA	C1D-ND	3.87	1.42	1.37
26	m	612	CLA	C1D-ND	3.87	1.42	1.37
26	b	313	CLA	C1D-ND	3.86	1.42	1.37
26	d	308	CLA	C1D-ND	3.86	1.42	1.37
26	A	809	CLA	C1D-ND	3.86	1.42	1.37
26	A	829	CLA	C1D-ND	3.86	1.42	1.37
26	B	834	CLA	C1D-ND	3.86	1.42	1.37
26	s	406	CLA	C1D-ND	3.86	1.42	1.37
35	h	311	II0	C34-C36	3.86	1.54	1.45
26	h	303	CLA	C1D-ND	3.86	1.42	1.37
26	h	304	CLA	C1D-ND	3.86	1.42	1.37
26	B	829	CLA	C1D-ND	3.86	1.42	1.37
26	Q	302	CLA	C1D-ND	3.86	1.42	1.37
29	L	201	WVN	C33-C34	3.86	1.54	1.45
26	A	807	CLA	C1D-ND	3.86	1.42	1.37
26	A	831	CLA	C1D-ND	3.86	1.42	1.37
26	d	302	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	843	PQN	C11-C3	3.86	1.57	1.51
26	A	833	CLA	C1D-ND	3.85	1.42	1.37
26	B	802	CLA	C1D-ND	3.85	1.42	1.37
26	l	311	CLA	C1D-ND	3.85	1.42	1.37
26	j	603	CLA	C1D-ND	3.85	1.42	1.37
26	j	609	CLA	C1D-ND	3.85	1.42	1.37
35	l	314	II0	C34-C36	3.85	1.54	1.45
26	B	827	CLA	C1D-ND	3.85	1.42	1.37
26	b	306	CLA	C1D-ND	3.85	1.42	1.37
26	h	302	CLA	C1D-ND	3.85	1.42	1.37
26	i	311	CLA	C1D-ND	3.85	1.42	1.37
26	m	605	CLA	C1D-ND	3.84	1.42	1.37
26	m	606	CLA	C1D-ND	3.84	1.42	1.37
26	A	805	CLA	C1D-ND	3.84	1.42	1.37
26	h	301	CLA	C1D-ND	3.84	1.42	1.37
36	l	312	KC2	C1D-ND	3.84	1.38	1.35
26	B	839	CLA	C1D-ND	3.84	1.42	1.37
36	d	312	KC2	C1B-C2B	-3.84	1.37	1.45
36	s	404	KC2	C4A-C3A	-3.84	1.37	1.44
26	c	305	CLA	C1D-ND	3.84	1.42	1.37
26	h	313	CLA	C1D-ND	3.84	1.42	1.37
36	i	309	KC2	C3B-C4B	-3.84	1.39	1.46
26	B	807	CLA	C1D-ND	3.84	1.42	1.37
35	m	615	II0	C34-C36	3.84	1.54	1.45
26	A	828	CLA	C1D-ND	3.83	1.42	1.37
36	n	612	KC2	C3B-C4B	-3.83	1.39	1.46
26	k	608	CLA	C1D-ND	3.83	1.42	1.37
36	l	312	KC2	C4A-C3A	-3.83	1.37	1.44
26	a	305	CLA	C1D-ND	3.83	1.42	1.37
26	B	813	CLA	C1D-ND	3.83	1.42	1.37
26	b	305	CLA	C1D-ND	3.83	1.42	1.37
26	k	607	CLA	C1D-ND	3.82	1.42	1.37
29	A	848	WVN	C33-C34	3.82	1.54	1.45
35	j	614	II0	C34-C36	3.82	1.54	1.45
26	l	305	CLA	C1D-ND	3.82	1.42	1.37
36	d	311	KC2	C3B-C4B	-3.82	1.39	1.46
29	s	407	WVN	C33-C34	3.82	1.54	1.45
26	l	310	CLA	C1D-ND	3.82	1.42	1.37
26	A	810	CLA	C1D-ND	3.82	1.42	1.37
26	A	816	CLA	C1D-ND	3.82	1.42	1.37
26	b	308	CLA	C1D-ND	3.81	1.42	1.37
26	A	839	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	804	CLA	C1D-ND	3.81	1.42	1.37
26	c	311	CLA	C1D-ND	3.81	1.42	1.37
26	B	809	CLA	C1D-ND	3.81	1.42	1.37
26	a	301	CLA	C1D-ND	3.80	1.42	1.37
26	A	819	CLA	C1D-ND	3.80	1.42	1.37
26	B	836	CLA	C1D-ND	3.80	1.42	1.37
26	n	607	CLA	C1D-ND	3.79	1.42	1.37
35	b	314	II0	C34-C36	3.79	1.54	1.45
29	I	101	WVN	C33-C34	3.79	1.54	1.45
36	i	309	KC2	C1D-ND	3.78	1.38	1.35
26	A	825	CLA	C1D-ND	3.78	1.42	1.37
26	j	604	CLA	C1D-ND	3.77	1.42	1.37
26	b	310	CLA	C1D-ND	3.77	1.42	1.37
26	j	612	CLA	C1D-ND	3.77	1.42	1.37
36	i	309	KC2	C4A-C3A	-3.77	1.37	1.44
26	n	604	CLA	C1D-ND	3.77	1.42	1.37
36	m	611	KC2	C1C-C2C	-3.77	1.37	1.44
26	c	309	CLA	CHC-C1C	3.77	1.44	1.35
26	m	609	CLA	C1D-ND	3.76	1.42	1.37
27	A	842	PQN	C11-C12	3.76	1.56	1.50
26	k	606	CLA	C1D-ND	3.76	1.42	1.37
26	B	801	CLA	C1D-ND	3.75	1.42	1.37
29	i	315	WVN	C20-C13	3.75	1.58	1.45
26	s	403	CLA	C1D-ND	3.75	1.42	1.37
26	B	826	CLA	C1D-ND	3.75	1.42	1.37
26	l	309	CLA	C1D-ND	3.75	1.42	1.37
26	n	602	CLA	C1D-ND	3.75	1.42	1.37
27	B	843	PQN	C2-C1	-3.73	1.40	1.48
26	B	822	CLA	C1D-ND	3.73	1.42	1.37
36	c	310	KC2	CHC-C1C	3.73	1.47	1.39
26	j	602	CLA	C1D-ND	3.72	1.42	1.37
36	k	612	KC2	C1B-C2B	-3.71	1.38	1.45
36	n	612	KC2	C1B-C2B	-3.71	1.38	1.45
26	a	307	CLA	C1D-ND	3.71	1.42	1.37
26	A	856	CLA	C1D-ND	3.71	1.42	1.37
36	i	318	KC2	C4A-C3A	-3.70	1.37	1.44
36	n	611	KC2	C1B-C2B	-3.70	1.38	1.45
26	A	803	CLA	C1D-ND	3.70	1.42	1.37
26	k	603	CLA	C1D-ND	3.69	1.42	1.37
36	i	318	KC2	C1B-C2B	-3.67	1.38	1.45
26	B	842	CLA	C1D-ND	3.66	1.42	1.37
36	d	311	KC2	C1B-C2B	-3.66	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	i	309	KC2	C1B-C2B	-3.66	1.38	1.45
36	j	611	KC2	C4A-C3A	-3.66	1.37	1.44
36	k	612	KC2	C4A-C3A	-3.65	1.37	1.44
26	m	602	CLA	C1D-ND	3.65	1.42	1.37
36	k	613	KC2	C1B-C2B	-3.65	1.38	1.45
36	n	612	KC2	C4A-C3A	-3.64	1.37	1.44
36	m	611	KC2	C1B-C2B	-3.64	1.38	1.45
26	B	814	CLA	C1D-ND	3.64	1.42	1.37
26	a	302	CLA	C1D-ND	3.64	1.42	1.37
27	B	843	PQN	C11-C12	3.64	1.55	1.50
29	s	405	WVN	C20-C13	3.63	1.58	1.45
36	s	404	KC2	C1D-ND	3.62	1.38	1.35
26	c	308	CLA	C1D-ND	3.62	1.42	1.37
35	k	615	II0	C20-C14	3.61	1.56	1.50
36	k	611	KC2	C4A-C3A	-3.61	1.37	1.44
36	j	611	KC2	C1B-C2B	-3.61	1.38	1.45
26	B	830	CLA	C1D-ND	3.61	1.42	1.37
26	k	602	CLA	C1D-ND	3.61	1.42	1.37
26	i	302	CLA	C1D-ND	3.61	1.42	1.37
29	R	200	WVN	C20-C13	3.61	1.57	1.45
36	k	611	KC2	C1B-C2B	-3.60	1.38	1.45
29	A	848	WVN	C20-C13	3.59	1.57	1.45
27	A	842	PQN	C2-C1	-3.58	1.40	1.48
36	k	613	KC2	C4A-C3A	-3.58	1.37	1.44
26	B	818	CLA	C1D-ND	3.57	1.42	1.37
26	B	823	CLA	C1D-ND	3.57	1.42	1.37
36	l	312	KC2	C1C-C2C	-3.56	1.37	1.44
36	s	404	KC2	C1C-C2C	-3.55	1.37	1.44
36	c	310	KC2	C4D-ND	3.50	1.38	1.35
36	k	613	KC2	C1C-C2C	-3.50	1.37	1.44
36	d	311	KC2	C4A-C3A	-3.49	1.37	1.44
36	n	611	KC2	C4A-C3A	-3.49	1.37	1.44
36	d	312	KC2	C4A-C3A	-3.49	1.37	1.44
26	A	802	CLA	C1D-ND	3.45	1.42	1.37
26	B	804	CLA	C1D-ND	3.45	1.42	1.37
26	A	803	CLA	CHC-C1C	3.44	1.43	1.35
36	n	612	KC2	C1C-C2C	-3.38	1.38	1.44
26	B	818	CLA	CHC-C1C	3.37	1.43	1.35
29	B	846	WVN	C20-C13	3.34	1.57	1.45
36	k	612	KC2	C1C-C2C	-3.34	1.38	1.44
26	B	819	CLA	CHC-C1C	3.33	1.43	1.35
36	i	318	KC2	C1C-C2C	-3.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	611	KC2	C1C-C2C	-3.31	1.38	1.44
26	B	823	CLA	CHC-C1C	3.31	1.43	1.35
36	k	611	KC2	C1C-C2C	-3.30	1.38	1.44
26	j	602	CLA	CHC-C1C	3.30	1.43	1.35
36	c	310	KC2	C4B-NB	-3.29	1.33	1.37
26	A	813	CLA	CHC-C1C	3.29	1.43	1.35
36	d	312	KC2	C1D-ND	3.28	1.38	1.35
26	B	842	CLA	CHC-C1C	3.28	1.43	1.35
26	m	602	CLA	CHC-C1C	3.28	1.43	1.35
26	m	609	CLA	CHC-C1C	3.28	1.43	1.35
36	i	309	KC2	C1C-C2C	-3.28	1.38	1.44
26	A	825	CLA	CHC-C1C	3.27	1.43	1.35
26	l	309	CLA	CHC-C1C	3.27	1.43	1.35
36	s	401	KC2	CHC-C1C	3.26	1.46	1.39
29	A	845	WVN	C20-C13	3.26	1.56	1.45
26	k	603	CLA	CHC-C1C	3.26	1.43	1.35
26	B	841	CLA	CHC-C1C	3.26	1.43	1.35
26	A	817	CLA	CHC-C1C	3.25	1.43	1.35
26	h	302	CLA	CHC-C1C	3.25	1.43	1.35
26	B	834	CLA	CHC-C1C	3.24	1.43	1.35
26	l	310	CLA	CHC-C1C	3.24	1.43	1.35
26	s	406	CLA	CHC-C1C	3.24	1.43	1.35
26	B	802	CLA	CHC-C1C	3.24	1.43	1.35
36	c	310	KC2	C1A-CHA	3.24	1.49	1.40
26	h	305	CLA	CHC-C1C	3.23	1.43	1.35
26	B	833	CLA	CHC-C1C	3.23	1.43	1.35
26	j	608	CLA	CHC-C1C	3.23	1.43	1.35
26	d	309	CLA	CHC-C1C	3.23	1.43	1.35
26	A	839	CLA	CHC-C1C	3.22	1.43	1.35
26	B	815	CLA	CHC-C1C	3.22	1.43	1.35
26	A	802	CLA	CHC-C1C	3.22	1.43	1.35
26	B	821	CLA	CHC-C1C	3.21	1.43	1.35
26	d	302	CLA	CHC-C1C	3.21	1.43	1.35
26	a	307	CLA	CHC-C1C	3.21	1.43	1.35
26	A	827	CLA	CHC-C1C	3.21	1.43	1.35
26	c	307	CLA	CHC-C1C	3.21	1.43	1.35
26	a	304	CLA	CHC-C1C	3.21	1.43	1.35
26	b	305	CLA	CHC-C1C	3.21	1.43	1.35
26	n	609	CLA	CHC-C1C	3.20	1.43	1.35
26	J	103	CLA	CHC-C1C	3.20	1.43	1.35
26	B	829	CLA	CHC-C1C	3.20	1.43	1.35
26	B	830	CLA	CHC-C1C	3.20	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	822	CLA	CHC-C1C	3.20	1.43	1.35
26	A	805	CLA	CHC-C1C	3.20	1.43	1.35
26	b	306	CLA	CHC-C1C	3.20	1.43	1.35
36	n	611	KC2	C1C-C2C	-3.20	1.38	1.44
26	c	303	CLA	CHC-C1C	3.20	1.43	1.35
26	c	308	CLA	CHC-C1C	3.19	1.43	1.35
26	h	304	CLA	CHC-C1C	3.19	1.43	1.35
26	L	204	CLA	CHC-C1C	3.19	1.43	1.35
36	d	311	KC2	C1C-C2C	-3.19	1.38	1.44
26	m	605	CLA	CHC-C1C	3.19	1.43	1.35
26	d	305	CLA	CHC-C1C	3.19	1.43	1.35
26	B	838	CLA	CHC-C1C	3.19	1.43	1.35
26	k	608	CLA	CHC-C1C	3.18	1.43	1.35
26	L	206	CLA	CHC-C1C	3.18	1.43	1.35
29	B	848	WVN	C20-C13	3.18	1.56	1.45
26	A	841	CLA	CHC-C1C	3.18	1.43	1.35
26	A	840	CLA	CHC-C1C	3.18	1.43	1.35
26	i	302	CLA	CHC-C1C	3.18	1.43	1.35
26	s	403	CLA	CHC-C1C	3.18	1.43	1.35
26	A	856	CLA	CHC-C1C	3.18	1.43	1.35
26	j	612	CLA	CHC-C1C	3.17	1.43	1.35
26	B	831	CLA	CHC-C1C	3.17	1.43	1.35
26	l	311	CLA	CHC-C1C	3.17	1.43	1.35
32	A	854	SQD	O48-C23	3.17	1.42	1.33
26	m	608	CLA	CHC-C1C	3.17	1.43	1.35
26	h	313	CLA	CHC-C1C	3.17	1.43	1.35
29	R	200	WVN	C19-C11	3.17	1.39	1.32
26	d	304	CLA	CHC-C1C	3.17	1.43	1.35
26	i	305	CLA	CHC-C1C	3.16	1.43	1.35
26	B	807	CLA	CHC-C1C	3.16	1.43	1.35
26	i	310	CLA	CHC-C1C	3.16	1.43	1.35
26	B	810	CLA	CHC-C1C	3.16	1.43	1.35
26	m	604	CLA	CHC-C1C	3.16	1.43	1.35
26	i	304	CLA	CHC-C1C	3.16	1.43	1.35
29	B	847	WVN	C20-C13	3.16	1.56	1.45
26	B	816	CLA	CHC-C1C	3.16	1.43	1.35
26	d	308	CLA	CHC-C1C	3.16	1.43	1.35
26	h	308	CLA	CHC-C1C	3.16	1.43	1.35
26	j	605	CLA	CHC-C1C	3.16	1.43	1.35
26	i	303	CLA	CHC-C1C	3.15	1.43	1.35
35	n	618	II0	C20-C14	3.15	1.56	1.50
26	k	609	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	813	CLA	CHC-C1C	3.15	1.43	1.35
26	A	816	CLA	CHC-C1C	3.15	1.43	1.35
26	n	604	CLA	CHC-C1C	3.15	1.43	1.35
26	n	607	CLA	CHC-C1C	3.15	1.43	1.35
26	L	203	CLA	CHC-C1C	3.15	1.43	1.35
26	k	606	CLA	CHC-C1C	3.15	1.43	1.35
26	B	826	CLA	CHC-C1C	3.15	1.43	1.35
26	B	836	CLA	CHC-C1C	3.15	1.43	1.35
26	A	810	CLA	CHC-C1C	3.15	1.43	1.35
26	B	811	CLA	CHC-C1C	3.15	1.43	1.35
29	A	846	WVN	C20-C13	3.14	1.56	1.45
26	A	807	CLA	CHC-C1C	3.14	1.43	1.35
26	i	307	CLA	CHC-C1C	3.14	1.43	1.35
26	b	307	CLA	CHC-C1C	3.14	1.43	1.35
26	A	828	CLA	CHC-C1C	3.14	1.43	1.35
29	i	315	WVN	C19-C11	3.14	1.39	1.32
26	B	806	CLA	CHC-C1C	3.14	1.43	1.35
26	a	311	CLA	CHC-C1C	3.14	1.43	1.35
26	m	613	CLA	CHC-C1C	3.14	1.43	1.35
26	j	609	CLA	CHC-C1C	3.14	1.43	1.35
26	i	308	CLA	CHC-C1C	3.14	1.43	1.35
26	n	610	CLA	CHC-C1C	3.14	1.43	1.35
26	i	306	CLA	CHC-C1C	3.14	1.43	1.35
26	Q	302	CLA	CHC-C1C	3.14	1.43	1.35
26	a	302	CLA	CHC-C1C	3.14	1.43	1.35
29	B	853	WVN	C20-C13	3.14	1.56	1.45
26	A	820	CLA	CHC-C1C	3.13	1.43	1.35
26	a	309	CLA	CHC-C1C	3.13	1.43	1.35
26	n	608	CLA	CHC-C1C	3.13	1.43	1.35
26	d	313	CLA	CHC-C1C	3.13	1.43	1.35
26	A	814	CLA	CHC-C1C	3.13	1.43	1.35
26	A	829	CLA	CMB-C2B	-3.13	1.45	1.51
26	l	304	CLA	CHC-C1C	3.13	1.43	1.35
26	A	821	CLA	CHC-C1C	3.13	1.43	1.35
26	A	838	CLA	CHC-C1C	3.13	1.43	1.35
26	j	613	CLA	CHC-C1C	3.13	1.43	1.35
29	J	102	WVN	C20-C13	3.13	1.56	1.45
26	A	819	CLA	CHC-C1C	3.13	1.43	1.35
26	B	825	CLA	CHC-C1C	3.12	1.43	1.35
26	A	833	CLA	CHC-C1C	3.12	1.43	1.35
26	A	852	CLA	CHC-C1C	3.12	1.43	1.35
26	B	817	CLA	CHC-C1C	3.12	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	310	CLA	CHC-C1C	3.12	1.43	1.35
26	b	313	CLA	CHC-C1C	3.12	1.43	1.35
26	k	605	CLA	CHC-C1C	3.12	1.43	1.35
26	l	306	CLA	CHC-C1C	3.12	1.43	1.35
26	d	303	CLA	CHC-C1C	3.12	1.43	1.35
26	a	308	CLA	CHC-C1C	3.12	1.43	1.35
26	b	309	CLA	CHC-C1C	3.12	1.43	1.35
26	j	604	CLA	CHC-C1C	3.12	1.43	1.35
26	c	302	CLA	CHC-C1C	3.12	1.43	1.35
26	l	308	CLA	CHC-C1C	3.12	1.43	1.35
26	A	806	CLA	CHC-C1C	3.11	1.42	1.35
26	h	303	CLA	CHC-C1C	3.11	1.42	1.35
26	a	310	CLA	CHC-C1C	3.11	1.42	1.35
26	k	607	CLA	CHC-C1C	3.11	1.42	1.35
29	A	857	WVN	C19-C11	3.11	1.39	1.32
26	h	306	CLA	CHC-C1C	3.11	1.42	1.35
26	F	202	CLA	CHC-C1C	3.11	1.42	1.35
26	A	811	CLA	CHC-C1C	3.11	1.42	1.35
26	j	603	CLA	CHC-C1C	3.11	1.42	1.35
29	B	849	WVN	C20-C13	3.11	1.56	1.45
26	c	312	CLA	CHC-C1C	3.11	1.42	1.35
26	c	306	CLA	CHC-C1C	3.10	1.42	1.35
29	s	407	WVN	C19-C11	3.10	1.39	1.32
26	B	828	CLA	CHC-C1C	3.10	1.42	1.35
26	n	601	CLA	CHC-C1C	3.10	1.42	1.35
26	l	313	CLA	CHC-C1C	3.10	1.42	1.35
26	n	603	CLA	CHC-C1C	3.10	1.42	1.35
36	s	404	KC2	MG-NA	3.10	2.13	2.06
29	A	857	WVN	C20-C13	3.10	1.56	1.45
29	M	101	WVN	C20-C13	3.10	1.56	1.45
26	A	835	CLA	CHC-C1C	3.10	1.42	1.35
26	A	831	CLA	CHC-C1C	3.10	1.42	1.35
26	B	824	CLA	CHC-C1C	3.10	1.42	1.35
26	c	311	CLA	CHC-C1C	3.10	1.42	1.35
26	n	605	CLA	CHC-C1C	3.10	1.42	1.35
26	l	305	CLA	CHC-C1C	3.09	1.42	1.35
26	j	601	CLA	CHC-C1C	3.09	1.42	1.35
26	s	408	CLA	CHC-C1C	3.09	1.42	1.35
26	m	606	CLA	CHC-C1C	3.09	1.42	1.35
26	A	812	CLA	CHC-C1C	3.09	1.42	1.35
26	k	601	CLA	CHC-C1C	3.09	1.42	1.35
26	j	610	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	311	CLA	CHC-C1C	3.09	1.42	1.35
26	k	610	CLA	CHC-C1C	3.09	1.42	1.35
26	d	318	CLA	CHC-C1C	3.09	1.42	1.35
26	A	832	CLA	CHC-C1C	3.09	1.42	1.35
26	m	607	CLA	CHC-C1C	3.08	1.42	1.35
26	B	840	CLA	CHC-C1C	3.08	1.42	1.35
26	k	614	CLA	CHC-C1C	3.08	1.42	1.35
26	B	839	CLA	CHC-C1C	3.08	1.42	1.35
26	a	305	CLA	CHC-C1C	3.08	1.42	1.35
36	s	401	KC2	C1A-CHA	3.08	1.48	1.40
26	m	612	CLA	CHC-C1C	3.08	1.42	1.35
36	d	312	KC2	C1C-C2C	-3.08	1.38	1.44
26	i	311	CLA	CHC-C1C	3.08	1.42	1.35
26	R	201	CLA	CHC-C1C	3.08	1.42	1.35
26	b	310	CLA	CHC-C1C	3.08	1.42	1.35
26	l	307	CLA	CHC-C1C	3.08	1.42	1.35
26	L	202	CLA	CHC-C1C	3.07	1.42	1.35
26	F	201	CLA	CHC-C1C	3.07	1.42	1.35
26	a	306	CLA	CHC-C1C	3.07	1.42	1.35
26	m	610	CLA	CHC-C1C	3.07	1.42	1.35
26	A	822	CLA	CHC-C1C	3.07	1.42	1.35
26	A	851	CLA	CHC-C1C	3.07	1.42	1.35
29	h	309	WVN	C20-C13	3.07	1.56	1.45
27	B	843	PQN	C3-C4	-3.07	1.39	1.47
26	m	601	CLA	CHC-C1C	3.06	1.42	1.35
26	c	304	CLA	CHC-C1C	3.06	1.42	1.35
26	j	606	CLA	CHC-C1C	3.06	1.42	1.35
26	s	402	CLA	CHC-C1C	3.06	1.42	1.35
26	b	308	CLA	CHC-C1C	3.06	1.42	1.35
26	k	602	CLA	CHC-C1C	3.06	1.42	1.35
29	A	846	WVN	C19-C11	3.06	1.39	1.32
26	b	304	CLA	CHC-C1C	3.06	1.42	1.35
26	B	801	CLA	CHC-C1C	3.06	1.42	1.35
26	B	804	CLA	CHC-C1C	3.06	1.42	1.35
26	A	809	CLA	CHC-C1C	3.06	1.42	1.35
26	n	602	CLA	CHC-C1C	3.06	1.42	1.35
26	a	301	CLA	CHC-C1C	3.05	1.42	1.35
26	A	836	CLA	CHC-C1C	3.05	1.42	1.35
26	B	808	CLA	CHC-C1C	3.05	1.42	1.35
26	A	837	CLA	CHC-C1C	3.05	1.42	1.35
29	A	847	WVN	C20-C13	3.05	1.55	1.45
26	A	815	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	301	CLA	CHC-C1C	3.05	1.42	1.35
26	A	834	CLA	CHC-C1C	3.05	1.42	1.35
29	A	847	WVN	C19-C11	3.05	1.39	1.32
26	A	830	CLA	CHC-C1C	3.05	1.42	1.35
26	A	823	CLA	CHC-C1C	3.04	1.42	1.35
36	s	404	KC2	C3C-C4C	-3.04	1.38	1.44
26	h	307	CLA	C4D-ND	-3.04	1.33	1.37
26	l	305	CLA	C4D-ND	-3.04	1.33	1.37
26	m	603	CLA	CHC-C1C	3.04	1.42	1.35
35	d	315	II0	C19-C13	3.04	1.55	1.50
26	c	305	CLA	CHC-C1C	3.04	1.42	1.35
26	B	812	CLA	CHC-C1C	3.04	1.42	1.35
26	A	818	CLA	CHC-C1C	3.04	1.42	1.35
26	B	814	CLA	CHC-C1C	3.03	1.42	1.35
29	J	101	WVN	C20-C13	3.03	1.55	1.45
26	A	817	CLA	C4D-ND	-3.03	1.33	1.37
26	B	835	CLA	CHC-C1C	3.02	1.42	1.35
26	i	301	CLA	CHC-C1C	3.02	1.42	1.35
29	K	102	WVN	C20-C13	3.02	1.55	1.45
36	m	611	KC2	C3C-C4C	-3.02	1.38	1.44
26	B	805	CLA	CHC-C1C	3.02	1.42	1.35
29	L	201	WVN	C20-C13	3.02	1.55	1.45
35	d	316	II0	C20-C14	3.02	1.55	1.50
26	h	307	CLA	CHC-C1C	3.02	1.42	1.35
26	d	307	CLA	CHC-C1C	3.02	1.42	1.35
29	L	205	WVN	C20-C13	3.01	1.55	1.45
27	A	842	PQN	C3-C4	-3.01	1.39	1.47
26	A	804	CLA	CHC-C1C	3.01	1.42	1.35
29	F	203	WVN	C20-C13	3.01	1.55	1.45
26	B	828	CLA	C4D-ND	-3.01	1.33	1.37
29	l	316	WVN	C20-C13	3.00	1.55	1.45
26	l	313	CLA	C4D-ND	-3.00	1.33	1.37
35	a	312	II0	C19-C13	3.00	1.55	1.50
26	m	609	CLA	C4D-ND	-3.00	1.33	1.37
26	A	826	CLA	CHC-C1C	3.00	1.42	1.35
26	B	842	CLA	C4D-ND	-3.00	1.33	1.37
29	l	316	WVN	C19-C11	3.00	1.39	1.32
26	K	101	CLA	CHC-C1C	2.99	1.42	1.35
29	s	407	WVN	C20-C13	2.99	1.55	1.45
26	B	803	CLA	CHC-C1C	2.99	1.42	1.35
29	B	847	WVN	C19-C11	2.99	1.39	1.32
26	n	613	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	851	CLA	C4D-ND	-2.99	1.33	1.37
36	j	611	KC2	C3C-C4C	-2.99	1.38	1.44
29	B	848	WVN	C19-C11	2.99	1.39	1.32
26	B	807	CLA	C4D-ND	-2.98	1.33	1.37
29	B	850	WVN	C19-C11	2.98	1.39	1.32
26	A	826	CLA	C4D-ND	-2.98	1.33	1.37
26	l	301	CLA	CHC-C1C	2.98	1.42	1.35
26	m	602	CLA	C4D-ND	-2.98	1.33	1.37
26	B	832	CLA	CHC-C1C	2.97	1.42	1.35
27	B	843	PQN	C3-C2	2.97	1.40	1.35
26	A	824	CLA	CHC-C1C	2.97	1.42	1.35
35	l	302	II0	C20-C14	2.97	1.55	1.50
26	B	821	CLA	C4D-ND	-2.96	1.33	1.37
26	a	303	CLA	CHC-C1C	2.96	1.42	1.35
26	k	604	CLA	CHC-C1C	2.96	1.42	1.35
36	l	312	KC2	C3C-C4C	-2.95	1.39	1.44
26	B	820	CLA	CHC-C1C	2.95	1.42	1.35
26	A	825	CLA	C4D-ND	-2.95	1.33	1.37
36	d	312	KC2	C3C-C4C	-2.95	1.39	1.44
29	B	850	WVN	C20-C13	2.95	1.55	1.45
29	s	405	WVN	C19-C11	2.95	1.39	1.32
35	n	616	II0	C20-C14	2.95	1.55	1.50
36	n	611	KC2	C3C-C4C	-2.95	1.39	1.44
29	F	203	WVN	C19-C11	2.95	1.39	1.32
26	F	201	CLA	C4D-ND	-2.95	1.33	1.37
26	d	306	CLA	CHC-C1C	2.95	1.42	1.35
26	i	311	CLA	C4D-ND	-2.94	1.33	1.37
29	I	101	WVN	C20-C13	2.94	1.55	1.45
35	n	618	II0	C19-C13	2.94	1.55	1.50
26	b	312	CLA	CHC-C1C	2.94	1.42	1.35
29	A	845	WVN	C19-C11	2.94	1.39	1.32
26	b	303	CLA	CHC-C1C	2.94	1.42	1.35
26	B	841	CLA	C4D-ND	-2.94	1.33	1.37
36	i	318	KC2	C3C-C4C	-2.93	1.39	1.44
25	A	801	CL0	MG-ND	-2.93	2.00	2.05
36	n	612	KC2	C3C-C4C	-2.93	1.39	1.44
29	l	303	WVN	C20-C13	2.93	1.55	1.45
26	h	304	CLA	C4D-ND	-2.93	1.33	1.37
27	B	843	PQN	C10-C1	-2.93	1.42	1.48
26	A	830	CLA	C4D-ND	-2.92	1.33	1.37
26	k	602	CLA	C4D-ND	-2.92	1.33	1.37
26	c	302	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	616	II0	C20-C14	2.92	1.55	1.50
26	c	301	CLA	CHC-C1C	2.92	1.42	1.35
26	c	308	CLA	C4D-ND	-2.92	1.33	1.37
26	a	302	CLA	C4D-ND	-2.92	1.33	1.37
26	B	829	CLA	C4D-ND	-2.92	1.33	1.37
35	c	316	II0	C19-C13	2.92	1.55	1.50
35	h	312	II0	C19-C13	2.92	1.55	1.50
35	i	312	II0	C20-C14	2.91	1.55	1.50
26	h	302	CLA	C4D-ND	-2.91	1.33	1.37
35	m	615	II0	C19-C13	2.91	1.55	1.50
26	j	602	CLA	C4D-ND	-2.91	1.33	1.37
26	A	829	CLA	C4D-ND	-2.91	1.33	1.37
26	B	809	CLA	CHC-C1C	2.91	1.42	1.35
26	c	312	CLA	C4D-ND	-2.91	1.33	1.37
36	i	309	KC2	C3C-C4C	-2.91	1.39	1.44
35	a	316	II0	C20-C14	2.90	1.55	1.50
26	n	606	CLA	CHC-C1C	2.90	1.42	1.35
36	k	611	KC2	C3C-C4C	-2.90	1.39	1.44
36	d	311	KC2	C3C-C4C	-2.90	1.39	1.44
26	B	831	CLA	C4D-ND	-2.90	1.33	1.37
35	m	616	II0	C19-C13	2.90	1.55	1.50
26	A	819	CLA	C4D-ND	-2.90	1.33	1.37
26	B	818	CLA	C4D-ND	-2.90	1.33	1.37
26	j	609	CLA	C4D-ND	-2.90	1.33	1.37
26	n	604	CLA	C4D-ND	-2.90	1.33	1.37
35	d	317	II0	C20-C14	2.90	1.55	1.50
35	j	615	II0	C20-C14	2.89	1.55	1.50
35	i	316	II0	C20-C14	2.89	1.55	1.50
35	d	301	II0	C20-C14	2.89	1.55	1.50
26	B	827	CLA	CHC-C1C	2.89	1.42	1.35
35	a	313	II0	C19-C13	2.89	1.55	1.50
26	h	303	CLA	C4D-ND	-2.88	1.33	1.37
27	A	842	PQN	C3-C2	2.88	1.40	1.35
26	i	302	CLA	C4D-ND	-2.88	1.33	1.37
36	k	613	KC2	C3C-C4C	-2.88	1.39	1.44
26	A	808	CLA	CHC-C1C	2.88	1.42	1.35
26	l	301	CLA	C4D-ND	-2.88	1.33	1.37
35	c	316	II0	C20-C14	2.88	1.55	1.50
26	j	604	CLA	C4D-ND	-2.88	1.33	1.37
26	B	824	CLA	C4D-ND	-2.87	1.33	1.37
29	J	102	WVN	C19-C11	2.87	1.39	1.32
36	s	401	KC2	C4D-ND	2.87	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	313	CLA	C4D-ND	-2.87	1.33	1.37
26	n	602	CLA	C4D-ND	-2.87	1.33	1.37
35	j	614	II0	C19-C13	2.87	1.55	1.50
29	B	849	WVN	C19-C11	2.87	1.39	1.32
35	m	615	II0	C20-C14	2.87	1.55	1.50
26	A	808	CLA	C4D-ND	-2.87	1.33	1.37
26	A	835	CLA	C4D-ND	-2.87	1.33	1.37
26	A	856	CLA	C4D-ND	-2.87	1.33	1.37
29	L	205	WVN	C19-C11	2.87	1.39	1.32
26	a	304	CLA	C4D-ND	-2.87	1.33	1.37
26	j	607	CLA	CHC-C1C	2.86	1.42	1.35
26	B	809	CLA	CMB-C2B	-2.86	1.45	1.51
26	B	835	CLA	C4D-ND	-2.86	1.33	1.37
26	l	310	CLA	C4D-ND	-2.86	1.33	1.37
29	A	848	WVN	C19-C11	2.86	1.39	1.32
29	B	853	WVN	C19-C11	2.86	1.39	1.32
26	L	206	CLA	C4D-ND	-2.86	1.33	1.37
26	n	613	CLA	C4D-ND	-2.86	1.33	1.37
26	A	806	CLA	C4D-ND	-2.86	1.33	1.37
26	A	839	CLA	C4D-ND	-2.86	1.33	1.37
26	a	311	CLA	C4D-ND	-2.85	1.33	1.37
26	B	837	CLA	CHC-C1C	2.85	1.42	1.35
35	m	614	II0	C19-C13	2.85	1.55	1.50
26	B	811	CLA	C4D-ND	-2.85	1.33	1.37
26	k	614	CLA	C4D-ND	-2.85	1.33	1.37
35	i	319	II0	C19-C13	2.85	1.55	1.50
26	B	801	CLA	C4D-ND	-2.84	1.33	1.37
26	n	609	CLA	C4D-ND	-2.84	1.33	1.37
26	A	809	CLA	C4D-ND	-2.84	1.33	1.37
26	d	310	CLA	C4D-ND	-2.84	1.33	1.37
32	A	854	SQD	O47-C7	2.84	1.42	1.34
26	i	304	CLA	C4D-ND	-2.84	1.33	1.37
29	l	303	WVN	C19-C11	2.84	1.39	1.32
26	s	408	CLA	C4D-ND	-2.84	1.33	1.37
26	l	307	CLA	C4D-ND	-2.84	1.33	1.37
33	j	618	DGD	C3D-C2D	2.84	1.59	1.52
26	k	608	CLA	C4D-ND	-2.84	1.33	1.37
26	h	308	CLA	C4D-ND	-2.84	1.33	1.37
36	k	612	KC2	C3C-C4C	-2.84	1.39	1.44
26	b	306	CLA	C4D-ND	-2.83	1.33	1.37
26	B	827	CLA	CMB-C2B	-2.83	1.45	1.51
26	s	406	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	821	CLA	C4D-ND	-2.83	1.33	1.37
26	B	833	CLA	C4D-ND	-2.83	1.33	1.37
26	L	204	CLA	C4D-ND	-2.83	1.33	1.37
26	b	308	CLA	C4D-ND	-2.83	1.33	1.37
26	d	309	CLA	C4D-ND	-2.83	1.33	1.37
26	h	301	CLA	C4D-ND	-2.83	1.33	1.37
29	K	102	WVN	C19-C11	2.83	1.39	1.32
29	h	309	WVN	C19-C11	2.83	1.39	1.32
29	J	101	WVN	C19-C11	2.82	1.39	1.32
26	B	808	CLA	C4D-ND	-2.82	1.33	1.37
26	d	302	CLA	C4D-ND	-2.82	1.33	1.37
26	a	307	CLA	C4D-ND	-2.82	1.33	1.37
26	a	308	CLA	C4D-ND	-2.82	1.33	1.37
26	a	301	CLA	C4D-ND	-2.82	1.33	1.37
26	j	613	CLA	C4D-ND	-2.82	1.33	1.37
26	i	307	CLA	C4D-ND	-2.82	1.33	1.37
26	A	805	CLA	C4D-ND	-2.82	1.33	1.37
26	B	836	CLA	C4D-ND	-2.82	1.33	1.37
26	A	810	CLA	C4D-ND	-2.82	1.33	1.37
26	h	313	CLA	C4D-ND	-2.81	1.33	1.37
26	A	838	CLA	C4D-ND	-2.81	1.33	1.37
26	b	307	CLA	C4D-ND	-2.81	1.33	1.37
26	b	311	CLA	C4D-ND	-2.81	1.33	1.37
26	d	305	CLA	C4D-ND	-2.81	1.33	1.37
26	m	613	CLA	C4D-ND	-2.81	1.33	1.37
26	B	806	CLA	C4D-ND	-2.81	1.33	1.37
26	B	802	CLA	C4D-ND	-2.81	1.33	1.37
36	s	401	KC2	CHB-C4A	-2.81	1.32	1.39
26	A	815	CLA	C4D-ND	-2.80	1.33	1.37
26	B	826	CLA	C4D-ND	-2.80	1.33	1.37
26	b	312	CLA	C4D-ND	-2.80	1.33	1.37
35	d	316	II0	C12-C14	2.80	1.55	1.51
26	B	809	CLA	C4D-ND	-2.80	1.33	1.37
35	c	313	II0	C20-C14	2.80	1.55	1.50
26	m	605	CLA	C4D-ND	-2.80	1.33	1.37
26	B	840	CLA	C4D-ND	-2.80	1.33	1.37
26	A	807	CLA	C4D-ND	-2.80	1.33	1.37
26	B	822	CLA	C4D-ND	-2.80	1.33	1.37
26	c	305	CLA	C4D-ND	-2.79	1.33	1.37
26	A	811	CLA	C4D-ND	-2.79	1.33	1.37
26	Q	302	CLA	C4D-ND	-2.79	1.33	1.37
26	J	103	CLA	C4D-ND	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	202	CLA	C4D-ND	-2.79	1.33	1.37
26	c	311	CLA	C4D-ND	-2.79	1.33	1.37
26	B	804	CLA	C4D-ND	-2.79	1.33	1.37
26	m	604	CLA	C4D-ND	-2.79	1.33	1.37
26	s	403	CLA	C4D-ND	-2.79	1.33	1.37
26	A	818	CLA	C4D-ND	-2.78	1.33	1.37
26	a	305	CLA	C4D-ND	-2.78	1.33	1.37
30	i	300	LMU	C6B-C5B	-2.78	1.42	1.51
26	k	607	CLA	C4D-ND	-2.78	1.33	1.37
26	A	834	CLA	C4D-ND	-2.78	1.33	1.37
26	a	309	CLA	C4D-ND	-2.78	1.33	1.37
26	l	309	CLA	C4D-ND	-2.78	1.33	1.37
35	d	315	II0	C20-C14	2.78	1.55	1.50
26	c	306	CLA	C4D-ND	-2.78	1.33	1.37
26	k	606	CLA	C4D-ND	-2.78	1.33	1.37
26	c	304	CLA	C4D-ND	-2.78	1.33	1.37
26	d	304	CLA	C4D-ND	-2.78	1.33	1.37
26	d	308	CLA	C4D-ND	-2.78	1.33	1.37
26	h	305	CLA	C4D-ND	-2.78	1.33	1.37
35	m	616	II0	C11-C13	2.78	1.55	1.51
26	A	841	CLA	C4D-ND	-2.77	1.33	1.37
26	B	827	CLA	C4D-ND	-2.77	1.33	1.37
26	A	802	CLA	C4D-ND	-2.77	1.33	1.37
26	c	307	CLA	C4D-ND	-2.77	1.33	1.37
26	B	817	CLA	C4D-ND	-2.77	1.33	1.37
30	A	850	LMU	C6B-C5B	-2.77	1.42	1.51
26	n	610	CLA	C4D-ND	-2.77	1.33	1.37
26	h	306	CLA	C4D-ND	-2.77	1.33	1.37
26	m	610	CLA	C4D-ND	-2.77	1.33	1.37
26	l	311	CLA	C4D-ND	-2.77	1.33	1.37
26	n	603	CLA	C4D-ND	-2.77	1.33	1.37
26	A	823	CLA	C4D-ND	-2.76	1.33	1.37
26	c	301	CLA	C4D-ND	-2.76	1.33	1.37
26	k	605	CLA	C4D-ND	-2.76	1.33	1.37
26	s	402	CLA	C4D-ND	-2.76	1.33	1.37
26	j	610	CLA	C4D-ND	-2.76	1.33	1.37
26	K	101	CLA	C4D-ND	-2.76	1.33	1.37
26	k	601	CLA	C4D-ND	-2.76	1.33	1.37
35	m	619	II0	C20-C14	2.76	1.55	1.50
26	m	601	CLA	C4D-ND	-2.76	1.33	1.37
26	m	608	CLA	C4D-ND	-2.75	1.33	1.37
26	A	829	CLA	CHC-C1C	2.75	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	820	CLA	C4D-ND	-2.75	1.33	1.37
26	B	812	CLA	C4D-ND	-2.75	1.33	1.37
35	m	616	II0	C20-C14	2.75	1.55	1.50
26	m	606	CLA	C4D-ND	-2.75	1.33	1.37
26	A	813	CLA	C4D-ND	-2.75	1.33	1.37
26	n	607	CLA	C4D-ND	-2.75	1.33	1.37
26	c	309	CLA	CHD-C1D	2.75	1.43	1.38
26	A	833	CLA	C4D-ND	-2.75	1.33	1.37
26	A	812	CLA	C4D-ND	-2.74	1.33	1.37
26	B	834	CLA	C4D-ND	-2.74	1.33	1.37
35	h	310	II0	C19-C13	2.74	1.55	1.50
35	l	302	II0	C19-C13	2.74	1.55	1.50
26	b	309	CLA	C4D-ND	-2.74	1.33	1.37
26	d	318	CLA	C4D-ND	-2.74	1.33	1.37
26	B	819	CLA	C4D-ND	-2.74	1.33	1.37
26	A	803	CLA	C4D-ND	-2.73	1.33	1.37
26	n	605	CLA	C4D-ND	-2.73	1.33	1.37
26	A	852	CLA	C4D-ND	-2.73	1.33	1.37
35	m	619	II0	C19-C13	2.73	1.55	1.50
26	A	814	CLA	C4D-ND	-2.73	1.33	1.37
26	k	610	CLA	C4D-ND	-2.73	1.33	1.37
26	i	308	CLA	C4D-ND	-2.73	1.33	1.37
26	L	202	CLA	C4D-ND	-2.73	1.33	1.37
26	B	823	CLA	C4D-ND	-2.73	1.33	1.37
26	j	603	CLA	C4D-ND	-2.73	1.33	1.37
26	c	309	CLA	CHD-C4C	2.72	1.45	1.39
26	b	304	CLA	C4D-ND	-2.72	1.33	1.37
26	B	830	CLA	C4D-ND	-2.72	1.33	1.37
26	B	839	CLA	C4D-ND	-2.72	1.33	1.37
26	j	608	CLA	C4D-ND	-2.72	1.33	1.37
35	n	618	II0	C12-C14	2.72	1.55	1.51
26	A	832	CLA	C4D-ND	-2.72	1.34	1.37
26	B	832	CLA	C4D-ND	-2.72	1.34	1.37
35	i	314	II0	C20-C14	2.71	1.55	1.50
26	j	612	CLA	C4D-ND	-2.71	1.34	1.37
26	R	201	CLA	C4D-ND	-2.71	1.34	1.37
35	d	301	II0	C12-C14	2.71	1.55	1.51
35	a	313	II0	C11-C13	2.71	1.55	1.51
35	i	314	II0	C19-C13	2.71	1.55	1.50
26	A	824	CLA	C4D-ND	-2.71	1.34	1.37
26	B	825	CLA	C4D-ND	-2.71	1.34	1.37
26	n	601	CLA	C4D-ND	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l	304	CLA	C4D-ND	-2.70	1.34	1.37
26	i	310	CLA	C4D-ND	-2.70	1.34	1.37
26	m	612	CLA	C4D-ND	-2.70	1.34	1.37
26	m	607	CLA	C4D-ND	-2.70	1.34	1.37
26	j	601	CLA	C4D-ND	-2.69	1.34	1.37
35	k	616	II0	C19-C13	2.69	1.55	1.50
35	i	319	II0	C20-C14	2.69	1.55	1.50
26	B	838	CLA	C4D-ND	-2.69	1.34	1.37
26	d	303	CLA	C4D-ND	-2.69	1.34	1.37
26	d	307	CLA	C4D-ND	-2.69	1.34	1.37
29	M	101	WVN	C19-C11	2.69	1.38	1.32
35	c	316	II0	C11-C13	2.69	1.55	1.51
26	A	831	CLA	C4D-ND	-2.69	1.34	1.37
26	j	607	CLA	C4D-ND	-2.69	1.34	1.37
26	B	815	CLA	C4D-ND	-2.69	1.34	1.37
35	a	314	II0	C20-C14	2.69	1.55	1.50
35	i	312	II0	C19-C13	2.68	1.55	1.50
26	a	306	CLA	C4D-ND	-2.68	1.34	1.37
26	A	804	CLA	C4D-ND	-2.68	1.34	1.37
26	b	303	CLA	C4D-ND	-2.68	1.34	1.37
26	b	313	CLA	C4D-ND	-2.68	1.34	1.37
26	B	810	CLA	C4D-ND	-2.68	1.34	1.37
35	k	615	II0	C12-C14	2.68	1.55	1.51
26	j	605	CLA	C4D-ND	-2.68	1.34	1.37
29	I	101	WVN	C19-C11	2.68	1.38	1.32
26	L	203	CLA	C4D-ND	-2.68	1.34	1.37
26	B	820	CLA	C4D-ND	-2.68	1.34	1.37
36	k	611	KC2	MG-NA	2.68	2.12	2.06
35	d	316	II0	C19-C13	2.68	1.55	1.50
26	k	609	CLA	C4D-ND	-2.67	1.34	1.37
26	B	816	CLA	CMB-C2B	-2.67	1.46	1.51
35	a	316	II0	C19-C13	2.67	1.55	1.50
26	B	814	CLA	C4D-ND	-2.67	1.34	1.37
26	A	828	CLA	C4D-ND	-2.67	1.34	1.37
35	m	614	II0	C20-C14	2.67	1.55	1.50
35	i	312	II0	C11-C13	2.67	1.55	1.51
26	B	801	CLA	CMB-C2B	-2.66	1.46	1.51
26	i	306	CLA	C4D-ND	-2.66	1.34	1.37
26	b	305	CLA	C4D-ND	-2.66	1.34	1.37
35	l	315	II0	C20-C14	2.66	1.55	1.50
26	A	837	CLA	C4D-ND	-2.66	1.34	1.37
30	i	300	LMU	C6'-C5'	-2.65	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	310	KC2	CHB-C4A	-2.65	1.33	1.39
35	n	618	II0	C11-C13	2.65	1.55	1.51
26	B	813	CLA	C4D-ND	-2.64	1.34	1.37
26	A	822	CLA	C4D-ND	-2.64	1.34	1.37
26	j	606	CLA	C4D-ND	-2.64	1.34	1.37
36	n	612	KC2	CHD-C4C	2.64	1.41	1.35
26	A	827	CLA	C4D-ND	-2.64	1.34	1.37
26	c	309	CLA	OBD-CAD	2.64	1.27	1.22
26	a	310	CLA	C4D-ND	-2.64	1.34	1.37
26	i	301	CLA	C4D-ND	-2.64	1.34	1.37
29	A	848	WVN	C21-C15	2.63	1.55	1.50
26	k	603	CLA	C4D-ND	-2.63	1.34	1.37
26	c	303	CLA	C4D-ND	-2.63	1.34	1.37
26	A	816	CLA	C4D-ND	-2.63	1.34	1.37
29	A	845	WVN	C21-C15	2.63	1.55	1.50
26	d	306	CLA	C4D-ND	-2.63	1.34	1.37
26	d	306	CLA	CMB-C2B	-2.62	1.46	1.51
27	A	842	PQN	C10-C1	-2.62	1.43	1.48
35	c	313	II0	C12-C14	2.62	1.55	1.51
26	l	308	CLA	C4D-ND	-2.62	1.34	1.37
35	k	620	II0	C20-C14	2.62	1.55	1.50
35	l	314	II0	C20-C14	2.61	1.55	1.50
26	B	828	CLA	CMB-C2B	-2.61	1.46	1.51
30	A	850	LMU	C6'-C5'	-2.61	1.43	1.51
26	A	836	CLA	C4D-ND	-2.61	1.34	1.37
35	i	316	II0	C19-C13	2.60	1.55	1.50
35	n	616	II0	C19-C13	2.60	1.55	1.50
26	c	305	CLA	CMB-C2B	-2.60	1.46	1.51
26	B	805	CLA	C4D-ND	-2.60	1.34	1.37
29	i	315	WVN	C21-C15	2.60	1.55	1.50
35	h	311	II0	C20-C14	2.60	1.55	1.50
35	b	315	II0	C20-C14	2.59	1.55	1.50
26	a	303	CLA	C4D-ND	-2.58	1.34	1.37
26	s	402	CLA	CMB-C2B	-2.58	1.46	1.51
26	m	603	CLA	C4D-ND	-2.57	1.34	1.37
26	B	818	CLA	CMB-C2B	-2.57	1.46	1.51
35	a	312	II0	C11-C13	2.57	1.55	1.51
26	B	832	CLA	CMB-C2B	-2.57	1.46	1.51
36	d	311	KC2	CHD-C4C	2.57	1.41	1.35
35	m	619	II0	C11-C13	2.57	1.55	1.51
35	k	615	II0	C11-C13	2.57	1.55	1.51
26	B	816	CLA	C4D-ND	-2.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	101	WVN	C21-C15	2.57	1.55	1.50
26	B	840	CLA	CMB-C2B	-2.57	1.46	1.51
35	k	619	II0	C19-C13	2.56	1.55	1.50
27	A	842	PQN	C9-C10	2.56	1.44	1.39
35	k	615	II0	C19-C13	2.56	1.55	1.50
35	h	311	II0	C19-C13	2.56	1.55	1.50
29	h	309	WVN	C21-C15	2.55	1.55	1.50
35	j	614	II0	C20-C14	2.55	1.55	1.50
29	L	201	WVN	C21-C15	2.55	1.55	1.50
26	i	305	CLA	MG-ND	-2.55	2.00	2.05
26	i	303	CLA	C4D-ND	-2.55	1.34	1.37
29	B	849	WVN	C21-C15	2.55	1.55	1.50
29	R	200	WVN	C21-C15	2.55	1.55	1.50
26	B	836	CLA	CMB-C2B	-2.55	1.46	1.51
26	B	837	CLA	CMB-C2B	-2.55	1.46	1.51
35	h	312	II0	C20-C14	2.55	1.55	1.50
35	J	104	II0	C20-C14	2.54	1.55	1.50
29	J	102	WVN	C21-C15	2.54	1.55	1.50
35	b	314	II0	C20-C14	2.54	1.55	1.50
35	j	614	II0	C11-C13	2.54	1.55	1.51
35	n	615	II0	C19-C13	2.54	1.55	1.50
26	B	837	CLA	C4D-ND	-2.54	1.34	1.37
26	B	822	CLA	CMB-C2B	-2.54	1.46	1.51
26	A	833	CLA	CMB-C2B	-2.53	1.46	1.51
26	A	840	CLA	CMB-C2B	-2.53	1.46	1.51
29	L	201	WVN	C19-C11	2.53	1.38	1.32
26	a	303	CLA	CMB-C2B	-2.53	1.46	1.51
26	A	840	CLA	C4D-ND	-2.53	1.34	1.37
35	j	615	II0	C19-C13	2.53	1.55	1.50
26	b	310	CLA	C4D-ND	-2.53	1.34	1.37
36	k	612	KC2	CHD-C4C	2.53	1.41	1.35
26	A	820	CLA	CMB-C2B	-2.52	1.46	1.51
29	l	303	WVN	C21-C15	2.52	1.55	1.50
35	d	301	II0	C19-C13	2.52	1.55	1.50
35	h	312	II0	C11-C13	2.52	1.55	1.51
26	k	604	CLA	C4D-ND	-2.52	1.34	1.37
35	a	312	II0	C20-C14	2.52	1.55	1.50
35	l	314	II0	C19-C13	2.52	1.55	1.50
27	B	843	PQN	C5-C4	-2.52	1.43	1.48
26	m	606	CLA	CMB-C2B	-2.52	1.46	1.51
35	i	313	II0	C20-C14	2.51	1.55	1.50
26	A	818	CLA	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	616	II0	C12-C14	2.51	1.55	1.51
26	a	310	CLA	CMB-C2B	-2.50	1.46	1.51
26	A	837	CLA	CMB-C2B	-2.50	1.46	1.51
26	a	307	CLA	CMB-C2B	-2.50	1.46	1.51
26	A	830	CLA	CMB-C2B	-2.50	1.46	1.51
26	k	604	CLA	C3B-C2B	-2.50	1.36	1.40
36	k	613	KC2	CHD-C4C	2.50	1.41	1.35
26	A	852	CLA	CMB-C2B	-2.50	1.46	1.51
26	J	103	CLA	CMB-C2B	-2.49	1.46	1.51
26	l	306	CLA	C4D-ND	-2.49	1.34	1.37
35	i	319	II0	C12-C14	2.49	1.54	1.51
26	A	839	CLA	CMB-C2B	-2.48	1.46	1.51
26	B	827	CLA	CMD-C2D	-2.48	1.45	1.50
29	B	846	WVN	C21-C15	2.48	1.55	1.50
26	d	308	CLA	CMB-C2B	-2.48	1.46	1.51
26	c	304	CLA	CMB-C2B	-2.48	1.46	1.51
26	B	820	CLA	CMB-C2B	-2.48	1.46	1.51
35	m	615	II0	C11-C13	2.48	1.54	1.51
36	j	611	KC2	CHD-C4C	2.48	1.41	1.35
26	B	804	CLA	CMB-C2B	-2.48	1.46	1.51
29	B	847	WVN	C21-C15	2.47	1.55	1.50
35	c	313	II0	C19-C13	2.47	1.55	1.50
26	b	310	CLA	CMB-C2B	-2.47	1.46	1.51
35	a	313	II0	C20-C14	2.47	1.55	1.50
35	k	619	II0	C20-C14	2.47	1.55	1.50
36	i	309	KC2	CHD-C4C	2.47	1.41	1.35
26	b	311	CLA	CMB-C2B	-2.47	1.46	1.51
36	s	401	KC2	C3D-C4D	-2.47	1.37	1.40
26	A	826	CLA	CMB-C2B	-2.47	1.46	1.51
26	A	815	CLA	CMB-C2B	-2.47	1.46	1.51
26	d	307	CLA	CMB-C2B	-2.47	1.46	1.51
26	A	808	CLA	CMB-C2B	-2.47	1.46	1.51
26	m	613	CLA	CMB-C2B	-2.47	1.46	1.51
26	k	609	CLA	CMB-C2B	-2.47	1.46	1.51
26	i	305	CLA	C4D-ND	-2.47	1.34	1.37
26	h	313	CLA	CMB-C2B	-2.47	1.46	1.51
29	B	850	WVN	C21-C15	2.46	1.55	1.50
29	L	205	WVN	C21-C15	2.46	1.55	1.50
35	j	614	II0	C12-C14	2.46	1.54	1.51
26	A	802	CLA	CMB-C2B	-2.46	1.46	1.51
26	n	606	CLA	C4D-ND	-2.46	1.34	1.37
26	L	202	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	307	CLA	CMB-C2B	-2.46	1.46	1.51
35	j	615	II0	C11-C13	2.46	1.54	1.51
35	l	314	II0	C11-C13	2.46	1.54	1.51
26	B	824	CLA	CMB-C2B	-2.45	1.46	1.51
26	h	305	CLA	CMB-C2B	-2.45	1.46	1.51
26	F	201	CLA	CMB-C2B	-2.45	1.46	1.51
26	j	606	CLA	CMB-C2B	-2.45	1.46	1.51
26	B	835	CLA	CMB-C2B	-2.45	1.46	1.51
26	B	830	CLA	CMB-C2B	-2.45	1.46	1.51
26	k	605	CLA	CMB-C2B	-2.45	1.46	1.51
26	s	408	CLA	CMB-C2B	-2.45	1.46	1.51
35	m	614	II0	C12-C14	2.45	1.54	1.51
26	j	601	CLA	CMB-C2B	-2.45	1.46	1.51
26	h	303	CLA	CMB-C2B	-2.44	1.46	1.51
26	i	307	CLA	CMB-C2B	-2.44	1.46	1.51
29	s	405	WVN	C21-C15	2.44	1.54	1.50
26	A	813	CLA	CMB-C2B	-2.44	1.46	1.51
30	A	850	LMU	O3'-C3'	2.44	1.48	1.43
26	B	817	CLA	CMB-C2B	-2.44	1.46	1.51
26	n	601	CLA	CMB-C2B	-2.44	1.46	1.51
26	m	603	CLA	CMB-C2B	-2.44	1.46	1.51
29	B	846	WVN	C19-C11	2.44	1.38	1.32
26	m	607	CLA	CMB-C2B	-2.43	1.46	1.51
35	a	314	II0	C19-C13	2.43	1.54	1.50
36	k	612	KC2	MG-NA	2.43	2.12	2.06
26	l	304	CLA	CMB-C2B	-2.43	1.46	1.51
26	A	824	CLA	CMB-C2B	-2.43	1.46	1.51
26	A	807	CLA	CMB-C2B	-2.43	1.46	1.51
26	b	312	CLA	CMB-C2B	-2.43	1.46	1.51
26	A	809	CLA	CMB-C2B	-2.43	1.46	1.51
26	a	306	CLA	CMB-C2B	-2.43	1.46	1.51
35	l	315	II0	C11-C13	2.43	1.54	1.51
29	A	846	WVN	C21-C15	2.43	1.54	1.50
26	i	301	CLA	CMB-C2B	-2.43	1.46	1.51
26	K	101	CLA	CMB-C2B	-2.43	1.46	1.51
26	l	305	CLA	CMB-C2B	-2.43	1.46	1.51
26	a	308	CLA	CMB-C2B	-2.43	1.46	1.51
26	B	812	CLA	CMB-C2B	-2.42	1.46	1.51
26	A	819	CLA	CMB-C2B	-2.42	1.46	1.51
35	d	317	II0	C19-C13	2.42	1.54	1.50
30	A	850	LMU	O5'-C1'	2.42	1.48	1.41
26	A	835	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	301	CLA	CMB-C2B	-2.42	1.46	1.51
26	i	306	CLA	CMB-C2B	-2.42	1.46	1.51
35	b	314	II0	C19-C13	2.42	1.54	1.50
26	l	301	CLA	CMB-C2B	-2.42	1.46	1.51
26	R	201	CLA	CMB-C2B	-2.42	1.46	1.51
26	m	601	CLA	CMB-C2B	-2.42	1.46	1.51
35	i	316	II0	C12-C14	2.42	1.54	1.51
26	k	603	CLA	CMB-C2B	-2.42	1.46	1.51
26	k	604	CLA	CMB-C2B	-2.42	1.46	1.51
26	B	841	CLA	CMB-C2B	-2.42	1.46	1.51
26	L	206	CLA	CMB-C2B	-2.41	1.46	1.51
36	d	312	KC2	CHD-C4C	2.41	1.41	1.35
26	l	308	CLA	CMB-C2B	-2.41	1.46	1.51
26	n	610	CLA	CMB-C2B	-2.41	1.46	1.51
26	l	311	CLA	CMB-C2B	-2.41	1.46	1.51
26	A	831	CLA	CMB-C2B	-2.41	1.46	1.51
26	h	306	CLA	CMB-C2B	-2.41	1.46	1.51
26	c	306	CLA	CMB-C2B	-2.41	1.46	1.51
26	i	302	CLA	CMB-C2B	-2.41	1.46	1.51
26	n	606	CLA	CMB-C2B	-2.41	1.46	1.51
26	j	609	CLA	CMB-C2B	-2.41	1.46	1.51
35	d	315	II0	C11-C13	2.41	1.54	1.51
26	k	608	CLA	CMB-C2B	-2.41	1.46	1.51
26	a	305	CLA	CMB-C2B	-2.41	1.46	1.51
26	j	607	CLA	C3C-C2C	2.41	1.41	1.36
26	A	817	CLA	CMB-C2B	-2.41	1.46	1.51
26	m	612	CLA	CMB-C2B	-2.41	1.46	1.51
35	J	104	II0	C19-C13	2.41	1.54	1.50
35	c	316	II0	C12-C14	2.40	1.54	1.51
26	l	310	CLA	CMB-C2B	-2.40	1.46	1.51
26	k	610	CLA	CMB-C2B	-2.40	1.46	1.51
26	b	303	CLA	CMB-C2B	-2.40	1.46	1.51
26	h	308	CLA	CMB-C2B	-2.40	1.46	1.51
26	A	822	CLA	CMB-C2B	-2.40	1.46	1.51
26	A	851	CLA	CMB-C2B	-2.40	1.46	1.51
26	m	608	CLA	CMB-C2B	-2.40	1.46	1.51
26	B	813	CLA	CMB-C2B	-2.40	1.46	1.51
26	A	832	CLA	CMB-C2B	-2.40	1.46	1.51
26	A	806	CLA	CMB-C2B	-2.40	1.46	1.51
26	d	304	CLA	CMB-C2B	-2.40	1.46	1.51
26	i	303	CLA	CMB-C2B	-2.40	1.46	1.51
26	A	811	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	403	CLA	CMB-C2B	-2.40	1.46	1.51
26	m	610	CLA	CMB-C2B	-2.39	1.46	1.51
29	A	857	WVN	C21-C15	2.39	1.54	1.50
26	j	610	CLA	CMB-C2B	-2.39	1.46	1.51
26	c	312	CLA	CMB-C2B	-2.39	1.46	1.51
26	h	304	CLA	CMB-C2B	-2.39	1.46	1.51
26	n	608	CLA	CMB-C2B	-2.39	1.46	1.51
26	n	607	CLA	CMB-C2B	-2.39	1.46	1.51
34	n	620	LMG	C4-C5	2.39	1.58	1.53
26	n	603	CLA	CMB-C2B	-2.39	1.46	1.51
29	s	407	WVN	C21-C15	2.39	1.54	1.50
26	b	307	CLA	CMB-C2B	-2.39	1.46	1.51
26	j	605	CLA	CMB-C2B	-2.39	1.46	1.51
26	B	811	CLA	CMB-C2B	-2.39	1.46	1.51
26	B	803	CLA	C4D-ND	-2.39	1.34	1.37
26	n	605	CLA	CMB-C2B	-2.39	1.46	1.51
26	B	839	CLA	CMB-C2B	-2.39	1.46	1.51
26	B	829	CLA	CMB-C2B	-2.39	1.46	1.51
26	d	310	CLA	CMB-C2B	-2.38	1.46	1.51
26	b	308	CLA	CMB-C2B	-2.38	1.46	1.51
26	i	310	CLA	CMB-C2B	-2.38	1.46	1.51
26	Q	302	CLA	CMB-C2B	-2.38	1.46	1.51
26	B	831	CLA	CMB-C2B	-2.38	1.46	1.51
26	b	313	CLA	CMB-C2B	-2.38	1.46	1.51
26	j	613	CLA	CMB-C2B	-2.38	1.46	1.51
26	b	305	CLA	CMB-C2B	-2.38	1.46	1.51
35	n	615	II0	C20-C14	2.38	1.54	1.50
26	j	612	CLA	CMB-C2B	-2.38	1.46	1.51
26	l	309	CLA	CMD-C2D	-2.38	1.45	1.50
29	I	101	WVN	C21-C15	2.38	1.54	1.50
26	c	303	CLA	CMB-C2B	-2.38	1.46	1.51
35	c	313	II0	C11-C13	2.38	1.54	1.51
26	a	301	CLA	CMB-C2B	-2.38	1.46	1.51
26	j	608	CLA	CMB-C2B	-2.38	1.46	1.51
26	d	309	CLA	CMB-C2B	-2.38	1.46	1.51
26	l	309	CLA	CMB-C2B	-2.38	1.46	1.51
26	A	823	CLA	CMB-C2B	-2.38	1.46	1.51
26	L	203	CLA	CMB-C2B	-2.38	1.46	1.51
26	m	605	CLA	CMB-C2B	-2.38	1.46	1.51
26	A	812	CLA	CMB-C2B	-2.38	1.46	1.51
26	n	613	CLA	CMB-C2B	-2.37	1.46	1.51
26	B	826	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m	604	CLA	CMB-C2B	-2.37	1.46	1.51
26	F	202	CLA	CMB-C2B	-2.37	1.46	1.51
26	b	309	CLA	CMB-C2B	-2.37	1.46	1.51
35	k	620	II0	C12-C14	2.37	1.54	1.51
26	c	301	CLA	CMB-C2B	-2.37	1.46	1.51
26	A	838	CLA	CMB-C2B	-2.37	1.46	1.51
35	i	313	II0	C19-C13	2.37	1.54	1.50
26	i	308	CLA	CMB-C2B	-2.37	1.46	1.51
26	l	313	CLA	CMB-C2B	-2.37	1.46	1.51
26	A	836	CLA	CMB-C2B	-2.36	1.46	1.51
26	B	803	CLA	CMB-C2B	-2.36	1.46	1.51
26	L	204	CLA	CMB-C2B	-2.36	1.46	1.51
26	k	606	CLA	CMB-C2B	-2.36	1.46	1.51
26	k	614	CLA	CMB-C2B	-2.36	1.46	1.51
26	A	804	CLA	CMB-C2B	-2.36	1.46	1.51
26	k	601	CLA	CMB-C2B	-2.36	1.46	1.51
30	i	300	LMU	O3'-C3'	2.36	1.48	1.43
26	a	311	CLA	CMB-C2B	-2.36	1.46	1.51
26	b	306	CLA	CMB-C2B	-2.36	1.46	1.51
26	c	311	CLA	CMB-C2B	-2.36	1.46	1.51
35	l	315	II0	C19-C13	2.36	1.54	1.50
26	B	810	CLA	CMB-C2B	-2.35	1.46	1.51
26	c	302	CLA	CMB-C2B	-2.35	1.46	1.51
35	J	104	II0	C11-C13	2.35	1.54	1.51
26	d	318	CLA	CMB-C2B	-2.35	1.46	1.51
35	l	315	II0	C12-C14	2.35	1.54	1.51
26	B	808	CLA	CMB-C2B	-2.35	1.46	1.51
26	i	305	CLA	CMB-C2B	-2.35	1.46	1.51
26	B	806	CLA	CMB-C2B	-2.35	1.46	1.51
35	a	314	II0	C12-C14	2.35	1.54	1.51
26	c	309	CLA	C1D-C2D	2.35	1.50	1.45
26	a	309	CLA	CMB-C2B	-2.35	1.46	1.51
25	A	801	CL0	C3D-C4D	-2.34	1.38	1.44
26	B	821	CLA	CMB-C2B	-2.34	1.46	1.51
26	d	302	CLA	CMB-C2B	-2.34	1.46	1.51
29	i	315	WVN	C14-C15	2.34	1.55	1.51
26	B	814	CLA	CMB-C2B	-2.34	1.46	1.51
25	A	801	CL0	C1D-C2D	-2.34	1.40	1.45
26	c	308	CLA	CMB-C2B	-2.34	1.46	1.51
26	A	821	CLA	CMB-C2B	-2.34	1.46	1.51
35	b	315	II0	C19-C13	2.34	1.54	1.50
26	n	604	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	843	PQN	C10-C5	-2.34	1.36	1.40
36	i	318	KC2	CHD-C4C	2.34	1.41	1.35
26	m	609	CLA	CMB-C2B	-2.34	1.46	1.51
29	B	848	WVN	C21-C15	2.34	1.54	1.50
33	B	844	DGD	C1D-C2D	2.33	1.59	1.52
26	i	311	CLA	CMB-C2B	-2.33	1.46	1.51
26	j	604	CLA	CMB-C2B	-2.33	1.46	1.51
26	A	810	CLA	CMB-C2B	-2.33	1.46	1.51
26	a	304	CLA	CMB-C2B	-2.33	1.46	1.51
26	A	828	CLA	CMB-C2B	-2.33	1.46	1.51
36	k	611	KC2	CHD-C4C	2.33	1.40	1.35
26	s	406	CLA	CMB-C2B	-2.33	1.46	1.51
29	K	102	WVN	C21-C15	2.32	1.54	1.50
26	d	303	CLA	CMB-C2B	-2.32	1.46	1.51
26	B	842	CLA	CMB-C2B	-2.32	1.46	1.51
26	B	815	CLA	CMB-C2B	-2.32	1.46	1.51
29	A	845	WVN	C14-C15	2.32	1.55	1.51
26	d	313	CLA	CMB-C2B	-2.31	1.46	1.51
26	A	856	CLA	CMB-C2B	-2.31	1.46	1.51
26	l	307	CLA	CMB-C2B	-2.31	1.46	1.51
26	h	302	CLA	CMB-C2B	-2.31	1.46	1.51
26	d	305	CLA	CMB-C2B	-2.31	1.46	1.51
26	A	803	CLA	CMB-C2B	-2.31	1.46	1.51
36	d	312	KC2	MG-NB	-2.31	2.01	2.05
26	n	609	CLA	CMB-C2B	-2.31	1.46	1.51
26	A	816	CLA	CMB-C2B	-2.31	1.46	1.51
26	A	814	CLA	CMB-C2B	-2.30	1.46	1.51
26	k	607	CLA	CMB-C2B	-2.30	1.46	1.51
36	i	318	KC2	MG-NA	2.30	2.11	2.06
26	i	304	CLA	CMB-C2B	-2.30	1.46	1.51
35	l	314	II0	C12-C14	2.30	1.54	1.51
26	n	607	CLA	CMD-C2D	-2.30	1.45	1.50
26	n	608	CLA	C4D-ND	-2.30	1.34	1.37
26	B	823	CLA	CMD-C2D	-2.29	1.45	1.50
26	B	825	CLA	CMB-C2B	-2.29	1.46	1.51
26	A	825	CLA	CMB-C2B	-2.29	1.46	1.51
26	B	819	CLA	C3C-C2C	2.29	1.41	1.36
26	B	807	CLA	CMB-C2B	-2.29	1.46	1.51
26	B	823	CLA	CMB-C2B	-2.29	1.46	1.51
26	A	805	CLA	CMB-C2B	-2.29	1.46	1.51
26	B	833	CLA	CMB-C2B	-2.28	1.46	1.51
26	k	602	CLA	CMB-C2B	-2.28	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	841	CLA	CMB-C2B	-2.28	1.46	1.51
26	j	607	CLA	CMB-C2B	-2.28	1.46	1.51
35	k	620	II0	C19-C13	2.28	1.54	1.50
33	j	618	DGD	O2G-C2G	-2.28	1.40	1.46
30	i	300	LMU	O5'-C1'	2.28	1.47	1.41
29	B	853	WVN	C21-C15	2.28	1.54	1.50
26	B	834	CLA	CMB-C2B	-2.28	1.46	1.51
26	B	838	CLA	CMB-C2B	-2.28	1.46	1.51
29	A	847	WVN	C21-C15	2.27	1.54	1.50
26	B	819	CLA	CMB-C2B	-2.27	1.46	1.51
27	A	842	PQN	C6-C5	2.27	1.43	1.39
26	B	802	CLA	CMB-C2B	-2.27	1.46	1.51
30	A	850	LMU	O5B-C1B	2.26	1.47	1.41
36	c	310	KC2	C4A-C3A	2.26	1.48	1.44
26	n	602	CLA	CMB-C2B	-2.26	1.46	1.51
35	h	312	II0	C12-C14	2.26	1.54	1.51
26	k	604	CLA	C1B-NB	2.26	1.37	1.35
26	c	307	CLA	CMB-C2B	-2.26	1.46	1.51
35	k	616	II0	C11-C13	2.26	1.54	1.51
34	n	620	LMG	C7-C8	2.26	1.57	1.50
35	m	615	II0	C12-C14	2.26	1.54	1.51
27	A	842	PQN	C5-C4	-2.26	1.43	1.48
35	k	619	II0	C12-C14	2.25	1.54	1.51
27	B	843	PQN	C9-C10	2.25	1.43	1.39
35	m	619	II0	C12-C14	2.25	1.54	1.51
26	l	306	CLA	CMB-C2B	-2.25	1.47	1.51
30	i	300	LMU	O5B-C1B	2.25	1.47	1.41
26	c	309	CLA	C3D-C2D	2.25	1.45	1.39
35	d	317	II0	C12-C14	2.25	1.54	1.51
26	B	822	CLA	CMD-C2D	-2.25	1.46	1.50
35	J	104	II0	C12-C14	2.25	1.54	1.51
26	a	302	CLA	CMB-C2B	-2.25	1.47	1.51
26	B	826	CLA	CMD-C2D	-2.25	1.46	1.50
26	s	403	CLA	CMD-C2D	-2.25	1.46	1.50
35	j	615	II0	C12-C14	2.25	1.54	1.51
26	a	302	CLA	CMD-C2D	-2.24	1.46	1.50
36	n	611	KC2	CHD-C4C	2.24	1.40	1.35
26	a	310	CLA	CMD-C2D	-2.24	1.46	1.50
35	a	313	II0	C12-C14	2.24	1.54	1.51
26	B	803	CLA	CMD-C2D	-2.24	1.46	1.50
35	k	616	II0	C12-C14	2.24	1.54	1.51
35	b	315	II0	C12-C14	2.24	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	101	WVN	C21-C15	2.24	1.54	1.50
26	B	836	CLA	CMD-C2D	-2.23	1.46	1.50
30	i	300	LMU	C2-C1	2.23	1.60	1.51
29	A	848	WVN	C16-C05	2.23	1.54	1.50
35	i	314	II0	C12-C14	2.23	1.54	1.51
26	j	603	CLA	CMB-C2B	-2.22	1.47	1.51
35	h	310	II0	C11-C13	2.22	1.54	1.51
36	s	404	KC2	CHD-C4C	2.22	1.40	1.35
36	k	613	KC2	MG-NA	2.22	2.11	2.06
26	B	805	CLA	CMB-C2B	-2.22	1.47	1.51
26	A	827	CLA	CMB-C2B	-2.22	1.47	1.51
30	i	300	LMU	O3B-C3B	2.22	1.48	1.43
26	b	304	CLA	CMB-C2B	-2.21	1.47	1.51
27	A	842	PQN	C10-C5	-2.21	1.37	1.40
26	A	802	CLA	CMD-C2D	-2.21	1.46	1.50
29	F	203	WVN	C21-C15	2.21	1.54	1.50
29	B	847	WVN	C14-C15	2.21	1.55	1.51
35	l	302	II0	C12-C14	2.20	1.54	1.51
29	l	316	WVN	C21-C15	2.20	1.54	1.50
26	A	840	CLA	CMD-C2D	-2.20	1.46	1.50
26	A	834	CLA	CMB-C2B	-2.20	1.47	1.51
30	A	850	LMU	O3B-C3B	2.20	1.48	1.43
35	d	315	II0	C12-C14	2.20	1.54	1.51
35	n	615	II0	C12-C14	2.20	1.54	1.51
29	J	102	WVN	C14-C15	2.19	1.55	1.51
26	B	818	CLA	CMD-C2D	-2.19	1.46	1.50
34	b	319	LMG	C7-C8	2.19	1.57	1.50
35	a	312	II0	C12-C14	2.19	1.54	1.51
35	i	312	II0	C12-C14	2.19	1.54	1.51
35	m	616	II0	C12-C14	2.19	1.54	1.51
26	A	813	CLA	CMD-C2D	-2.19	1.46	1.50
36	s	401	KC2	C4A-C3A	2.19	1.48	1.44
30	A	850	LMU	C2-C1	2.18	1.60	1.51
26	j	602	CLA	CMB-C2B	-2.18	1.47	1.51
26	i	302	CLA	CMC-C2C	-2.18	1.46	1.50
26	m	602	CLA	CMB-C2B	-2.18	1.47	1.51
35	i	313	II0	C12-C14	2.18	1.54	1.51
26	k	603	CLA	C3B-C2B	-2.18	1.37	1.40
29	A	846	WVN	C06-C13	2.18	1.56	1.53
26	j	607	CLA	CMD-C2D	-2.18	1.46	1.50
28	s	409	LHG	P-O6	2.18	1.67	1.60
26	B	803	CLA	C1B-NB	2.17	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	305	CLA	CMD-C2D	-2.17	1.46	1.50
36	s	401	KC2	CAA-C2A	2.17	1.53	1.46
29	B	850	WVN	C14-C15	2.17	1.55	1.51
26	i	310	CLA	CMD-C2D	-2.17	1.46	1.50
26	A	830	CLA	CMD-C2D	-2.17	1.46	1.50
29	B	853	WVN	C16-C05	2.16	1.54	1.50
26	k	607	CLA	CMD-C2D	-2.16	1.46	1.50
36	m	611	KC2	CHD-C4C	2.16	1.40	1.35
36	n	612	KC2	C1A-CHA	2.16	1.46	1.40
26	c	305	CLA	CMD-C2D	-2.15	1.46	1.50
26	k	602	CLA	CMD-C2D	-2.15	1.46	1.50
36	s	404	KC2	C1B-NB	-2.15	1.35	1.37
26	B	824	CLA	CMC-C2C	-2.15	1.46	1.50
35	b	314	II0	C12-C14	2.15	1.54	1.51
29	h	309	WVN	C14-C15	2.15	1.55	1.51
26	B	842	CLA	CMD-C2D	-2.14	1.46	1.50
26	i	305	CLA	C3B-C2B	-2.14	1.37	1.40
26	B	820	CLA	CMD-C2D	-2.14	1.46	1.50
26	h	301	CLA	CMD-C2D	-2.14	1.46	1.50
29	A	857	WVN	C14-C15	2.14	1.55	1.51
26	m	603	CLA	CMD-C2D	-2.14	1.46	1.50
29	I	101	WVN	C16-C05	2.14	1.54	1.50
26	A	804	CLA	CMD-C2D	-2.13	1.46	1.50
32	A	854	SQD	O2-C2	-2.13	1.38	1.43
36	i	309	KC2	C1B-NB	-2.13	1.35	1.37
26	i	302	CLA	CMD-C2D	-2.13	1.46	1.50
28	A	843	LHG	O7-C5	-2.13	1.41	1.46
36	l	312	KC2	CHD-C4C	2.12	1.40	1.35
26	A	826	CLA	CMC-C2C	-2.12	1.46	1.50
26	B	830	CLA	CMD-C2D	-2.12	1.46	1.50
34	L	209	LMG	C7-C8	2.12	1.57	1.50
26	A	805	CLA	CMD-C2D	-2.12	1.46	1.50
26	A	822	CLA	CMD-C2D	-2.12	1.46	1.50
26	n	603	CLA	C3B-C2B	-2.12	1.37	1.40
26	s	406	CLA	CMD-C2D	-2.12	1.46	1.50
29	B	849	WVN	C14-C15	2.12	1.55	1.51
26	B	804	CLA	C4C-C3C	2.12	1.48	1.45
36	d	312	KC2	C1B-NB	-2.12	1.35	1.37
26	d	307	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	809	CLA	CMC-C2C	-2.12	1.46	1.50
26	n	602	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	835	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	846	WVN	C14-C15	2.11	1.55	1.51
26	b	311	CLA	CMD-C2D	-2.11	1.46	1.50
36	i	318	KC2	C1A-CHA	2.11	1.46	1.40
26	a	303	CLA	C3B-C2B	-2.11	1.37	1.40
29	s	405	WVN	C14-C15	2.11	1.55	1.51
26	B	814	CLA	CMD-C2D	-2.11	1.46	1.50
29	A	857	WVN	C16-C05	2.10	1.54	1.50
26	B	835	CLA	C3B-C2B	-2.10	1.37	1.40
28	l	318	LHG	O7-C5	-2.10	1.41	1.46
26	B	842	CLA	CMC-C2C	-2.10	1.46	1.50
26	k	608	CLA	CMC-C2C	-2.10	1.46	1.50
26	h	306	CLA	CMD-C2D	-2.10	1.46	1.50
26	b	310	CLA	CMD-C2D	-2.10	1.46	1.50
35	a	316	II0	C11-C13	2.10	1.54	1.51
26	B	825	CLA	CMD-C2D	-2.10	1.46	1.50
26	a	306	CLA	CMD-C2D	-2.10	1.46	1.50
26	k	608	CLA	CMD-C2D	-2.10	1.46	1.50
36	l	312	KC2	C1B-NB	-2.09	1.35	1.37
29	A	845	WVN	C16-C05	2.09	1.54	1.50
29	L	205	WVN	C14-C15	2.09	1.55	1.51
26	B	821	CLA	CMC-C2C	-2.09	1.46	1.50
29	A	847	WVN	C14-C15	2.09	1.55	1.51
29	l	303	WVN	C14-C15	2.09	1.55	1.51
26	k	606	CLA	CMD-C2D	-2.09	1.46	1.50
26	c	311	CLA	CMD-C2D	-2.09	1.46	1.50
26	A	817	CLA	CMC-C2C	-2.09	1.46	1.50
26	h	313	CLA	CMD-C2D	-2.09	1.46	1.50
26	h	302	CLA	CMC-C2C	-2.09	1.46	1.50
26	n	606	CLA	CMD-C2D	-2.09	1.46	1.50
28	n	619	LHG	O7-C5	-2.09	1.41	1.46
26	d	306	CLA	CMD-C2D	-2.09	1.46	1.50
29	A	848	WVN	C14-C15	2.09	1.55	1.51
36	l	312	KC2	C1A-CHA	2.08	1.46	1.40
26	A	824	CLA	CMD-C2D	-2.08	1.46	1.50
28	L	207	LHG	O7-C5	-2.08	1.41	1.46
28	b	318	LHG	O7-C5	-2.08	1.41	1.46
26	b	313	CLA	CMD-C2D	-2.08	1.46	1.50
26	B	804	CLA	CMC-C2C	-2.08	1.46	1.50
26	k	614	CLA	C3C-C2C	2.08	1.41	1.36
26	B	818	CLA	C3B-CAB	-2.08	1.43	1.47
36	j	611	KC2	C1A-CHA	2.08	1.46	1.40
26	A	808	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	n	612	KC2	C1B-NB	-2.08	1.35	1.37
36	i	309	KC2	C1A-CHA	2.08	1.46	1.40
26	a	301	CLA	CMC-C2C	-2.08	1.46	1.50
29	i	315	WVN	C06-C13	2.08	1.56	1.53
26	B	822	CLA	CMC-C2C	-2.08	1.46	1.50
36	d	312	KC2	C1A-CHA	2.08	1.46	1.40
29	A	846	WVN	C14-C15	2.08	1.55	1.51
26	B	801	CLA	CMD-C2D	-2.08	1.46	1.50
26	A	828	CLA	CMD-C2D	-2.07	1.46	1.50
35	d	317	II0	C11-C13	2.07	1.54	1.51
29	R	200	WVN	C14-C15	2.07	1.55	1.51
29	B	853	WVN	C14-C15	2.07	1.55	1.51
26	c	306	CLA	CMD-C2D	-2.07	1.46	1.50
26	d	313	CLA	CMD-C2D	-2.07	1.46	1.50
28	c	317	LHG	O7-C5	-2.07	1.41	1.46
26	a	301	CLA	CMD-C2D	-2.06	1.46	1.50
26	m	604	CLA	CMD-C2D	-2.06	1.46	1.50
36	m	611	KC2	C1B-NB	-2.06	1.35	1.37
26	d	310	CLA	CMD-C2D	-2.06	1.46	1.50
36	k	611	KC2	C1A-CHA	2.06	1.46	1.40
26	j	607	CLA	C3B-CAB	-2.06	1.43	1.47
26	m	612	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	813	CLA	CMD-C2D	-2.06	1.46	1.50
26	A	829	CLA	CMD-C2D	-2.06	1.46	1.50
26	A	825	CLA	CMD-C2D	-2.06	1.46	1.50
36	k	613	KC2	C1A-CHA	2.06	1.46	1.40
29	R	200	WVN	C16-C05	2.06	1.54	1.50
35	i	313	II0	C11-C13	2.05	1.54	1.51
29	i	315	WVN	C16-C05	2.05	1.54	1.50
36	n	611	KC2	C1A-CHA	2.05	1.46	1.40
26	c	302	CLA	CMC-C2C	-2.05	1.46	1.50
35	h	311	II0	C12-C14	2.05	1.54	1.51
26	A	837	CLA	CMD-C2D	-2.05	1.46	1.50
26	A	836	CLA	CMD-C2D	-2.05	1.46	1.50
26	B	808	CLA	CMD-C2D	-2.05	1.46	1.50
36	d	311	KC2	C1A-CHA	2.05	1.46	1.40
26	B	804	CLA	C3D-C4D	2.04	1.48	1.44
26	A	815	CLA	CMD-C2D	-2.04	1.46	1.50
26	n	606	CLA	C3B-C2B	-2.04	1.37	1.40
35	d	316	II0	C11-C13	2.04	1.54	1.51
26	B	839	CLA	CMD-C2D	-2.04	1.46	1.50
26	h	302	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	850	LMU	O2'-C2'	2.04	1.47	1.43
26	i	305	CLA	CMD-C2D	-2.04	1.46	1.50
26	j	613	CLA	CMD-C2D	-2.04	1.46	1.50
35	n	616	II0	C11-C13	2.04	1.54	1.51
36	s	404	KC2	C1A-CHA	2.04	1.46	1.40
28	j	617	LHG	O7-C5	-2.04	1.41	1.46
26	B	809	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	829	CLA	C3B-C2B	-2.04	1.37	1.40
36	n	611	KC2	C1B-NB	-2.04	1.35	1.37
26	a	304	CLA	CMD-C2D	-2.03	1.46	1.50
29	L	201	WVN	C14-C15	2.03	1.55	1.51
34	b	319	LMG	O7-C8	-2.03	1.41	1.46
26	j	604	CLA	CMD-C2D	-2.03	1.46	1.50
26	K	101	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	808	CLA	CMC-C2C	-2.03	1.46	1.50
26	n	603	CLA	CMC-C2C	-2.03	1.46	1.50
26	i	304	CLA	CMD-C2D	-2.03	1.46	1.50
26	B	811	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	828	CLA	CMD-C2D	-2.03	1.46	1.50
26	j	601	CLA	CMD-C2D	-2.03	1.46	1.50
26	n	608	CLA	C1B-NB	2.03	1.37	1.35
35	k	620	II0	C11-C13	2.03	1.54	1.51
29	l	316	WVN	C16-C05	2.03	1.54	1.50
26	b	310	CLA	CMC-C2C	-2.03	1.46	1.50
26	d	302	CLA	CMD-C2D	-2.03	1.46	1.50
29	B	846	WVN	C06-C13	2.03	1.56	1.53
26	c	308	CLA	CMD-C2D	-2.03	1.46	1.50
26	l	310	CLA	CMD-C2D	-2.03	1.46	1.50
26	A	810	CLA	CMC-C2C	-2.03	1.46	1.50
28	i	317	LHG	O7-C5	-2.03	1.41	1.46
26	B	819	CLA	CMD-C2D	-2.03	1.46	1.50
26	b	307	CLA	CMD-C2D	-2.03	1.46	1.50
26	m	602	CLA	CMC-C2C	-2.03	1.46	1.50
29	M	101	WVN	C16-C05	2.02	1.54	1.50
26	B	837	CLA	CMD-C2D	-2.02	1.46	1.50
28	J	105	LHG	P-O6	2.02	1.67	1.59
26	A	810	CLA	CMD-C2D	-2.02	1.46	1.50
26	B	823	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	840	CLA	CMD-C2D	-2.02	1.46	1.50
26	i	311	CLA	C3C-C2C	2.02	1.41	1.36
26	L	204	CLA	CMD-C2D	-2.02	1.46	1.50
26	A	831	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l	301	CLA	CMD-C2D	-2.02	1.46	1.50
26	c	306	CLA	C3B-C2B	-2.02	1.37	1.40
29	h	309	WVN	C16-C05	2.02	1.54	1.50
26	A	816	CLA	CMD-C2D	-2.02	1.46	1.50
26	m	606	CLA	CMD-C2D	-2.02	1.46	1.50
26	m	602	CLA	C3C-C2C	2.02	1.41	1.36
35	a	316	II0	C12-C14	2.02	1.54	1.51
26	j	612	CLA	CMD-C2D	-2.02	1.46	1.50
26	b	306	CLA	CMD-C2D	-2.02	1.46	1.50
26	j	602	CLA	CMD-C2D	-2.02	1.46	1.50
26	c	307	CLA	CMD-C2D	-2.02	1.46	1.50
26	B	818	CLA	C3B-C2B	-2.02	1.37	1.40
26	A	819	CLA	CMD-C2D	-2.02	1.46	1.50
26	s	402	CLA	CMD-C2D	-2.02	1.46	1.50
26	A	814	CLA	CMD-C2D	-2.01	1.46	1.50
26	A	803	CLA	CMD-C2D	-2.01	1.46	1.50
26	F	201	CLA	CMD-C2D	-2.01	1.46	1.50
29	B	847	WVN	C16-C05	2.01	1.54	1.50
36	k	612	KC2	C1A-CHA	2.01	1.45	1.40
26	i	307	CLA	CMC-C2C	-2.01	1.46	1.50
26	j	603	CLA	CMC-C2C	-2.01	1.46	1.50
29	L	201	WVN	C16-C05	2.01	1.54	1.50
26	A	818	CLA	C3B-C2B	-2.01	1.37	1.40
26	B	803	CLA	CMC-C2C	-2.01	1.46	1.50
26	b	305	CLA	CMD-C2D	-2.01	1.46	1.50
26	B	838	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	850	LMU	O2B-C2B	2.00	1.47	1.43
29	s	407	WVN	C16-C05	2.00	1.54	1.50
30	i	300	LMU	O2B-C2B	2.00	1.47	1.43
26	A	827	CLA	CMD-C2D	-2.00	1.46	1.50
29	B	853	WVN	C06-C13	2.00	1.56	1.53
35	i	314	II0	C11-C13	2.00	1.54	1.51
26	m	613	CLA	CMD-C2D	-2.00	1.46	1.50
36	l	312	KC2	MG-NA	2.00	2.11	2.06
26	d	306	CLA	C3B-C2B	-2.00	1.37	1.40
26	A	809	CLA	CMD-C2D	-2.00	1.46	1.50
26	A	851	CLA	CMD-C2D	-2.00	1.46	1.50
26	A	852	CLA	CMD-C2D	-2.00	1.46	1.50
26	A	820	CLA	CMC-C2C	-2.00	1.46	1.50
26	k	607	CLA	C3C-C2C	2.00	1.41	1.36

All (3776) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	312	II0	C23-C21-C09	-26.03	109.52	175.43
35	c	316	II0	C23-C21-C09	-26.02	109.55	175.43
35	n	618	II0	C23-C21-C09	-25.82	110.04	175.43
35	h	310	II0	C23-C21-C09	-25.69	110.38	175.43
35	j	614	II0	C23-C21-C09	-25.41	111.10	175.43
35	b	315	II0	C23-C21-C09	-25.31	111.33	175.43
35	k	615	II0	C23-C21-C09	-25.31	111.33	175.43
35	J	104	II0	C23-C21-C09	-25.26	111.46	175.43
35	d	315	II0	C23-C21-C09	-25.24	111.52	175.43
35	l	314	II0	C23-C21-C09	-25.18	111.68	175.43
35	l	302	II0	C23-C21-C09	-25.13	111.81	175.43
35	i	312	II0	C24-C22-C10	-25.10	111.86	175.43
35	c	313	II0	C24-C22-C10	-25.06	111.98	175.43
35	a	316	II0	C23-C21-C09	-25.03	112.05	175.43
35	m	615	II0	C24-C22-C10	-25.02	112.08	175.43
35	l	314	II0	C24-C22-C10	-24.94	112.28	175.43
35	i	314	II0	C23-C21-C09	-24.90	112.38	175.43
35	m	615	II0	C23-C21-C09	-24.89	112.41	175.43
35	k	620	II0	C23-C21-C09	-24.85	112.50	175.43
35	d	317	II0	C23-C21-C09	-24.83	112.56	175.43
35	d	315	II0	C24-C22-C10	-24.81	112.62	175.43
35	n	615	II0	C23-C21-C09	-24.81	112.62	175.43
35	j	615	II0	C23-C21-C09	-24.77	112.72	175.43
35	i	319	II0	C23-C21-C09	-24.74	112.78	175.43
35	i	316	II0	C24-C22-C10	-24.74	112.79	175.43
35	k	616	II0	C24-C22-C10	-24.74	112.79	175.43
35	h	312	II0	C23-C21-C09	-24.72	112.85	175.43
35	m	619	II0	C23-C21-C09	-24.72	112.85	175.43
35	l	315	II0	C23-C21-C09	-24.67	112.96	175.43
35	a	314	II0	C24-C22-C10	-24.62	113.08	175.43
35	j	615	II0	C24-C22-C10	-24.60	113.15	175.43
35	n	616	II0	C23-C21-C09	-24.60	113.15	175.43
35	b	314	II0	C23-C21-C09	-24.57	113.22	175.43
35	c	316	II0	C24-C22-C10	-24.56	113.25	175.43
35	m	614	II0	C23-C21-C09	-24.53	113.33	175.43
35	m	616	II0	C23-C21-C09	-24.52	113.34	175.43
35	m	614	II0	C24-C22-C10	-24.50	113.39	175.43
35	c	313	II0	C23-C21-C09	-24.50	113.40	175.43
35	h	311	II0	C23-C21-C09	-24.48	113.44	175.43
35	a	313	II0	C23-C21-C09	-24.47	113.48	175.43
35	n	616	II0	C24-C22-C10	-24.44	113.56	175.43
35	i	316	II0	C23-C21-C09	-24.41	113.63	175.43
35	h	312	II0	C24-C22-C10	-24.37	113.73	175.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	301	II0	C24-C22-C10	-24.35	113.78	175.43
35	a	312	II0	C23-C21-C09	-24.34	113.80	175.43
35	n	615	II0	C24-C22-C10	-24.33	113.81	175.43
35	i	313	II0	C23-C21-C09	-24.29	113.93	175.43
35	d	317	II0	C24-C22-C10	-24.26	113.99	175.43
35	k	619	II0	C24-C22-C10	-24.25	114.02	175.43
35	n	618	II0	C24-C22-C10	-24.24	114.05	175.43
35	a	314	II0	C23-C21-C09	-24.19	114.17	175.43
35	h	311	II0	C24-C22-C10	-24.18	114.22	175.43
35	j	614	II0	C24-C22-C10	-24.15	114.28	175.43
35	k	619	II0	C23-C21-C09	-24.15	114.29	175.43
35	m	619	II0	C24-C22-C10	-24.09	114.44	175.43
35	i	314	II0	C24-C22-C10	-24.06	114.51	175.43
35	l	315	II0	C24-C22-C10	-24.05	114.53	175.43
35	d	301	II0	C23-C21-C09	-24.02	114.61	175.43
35	a	316	II0	C24-C22-C10	-23.95	114.78	175.43
35	d	316	II0	C24-C22-C10	-23.92	114.87	175.43
35	J	104	II0	C24-C22-C10	-23.86	115.03	175.43
35	i	313	II0	C24-C22-C10	-23.82	115.11	175.43
35	b	314	II0	C24-C22-C10	-23.80	115.17	175.43
35	a	313	II0	C24-C22-C10	-23.72	115.38	175.43
35	l	302	II0	C24-C22-C10	-23.61	115.65	175.43
35	k	616	II0	C23-C21-C09	-23.57	115.74	175.43
35	m	616	II0	C24-C22-C10	-23.57	115.76	175.43
35	a	312	II0	C24-C22-C10	-23.45	116.06	175.43
35	d	316	II0	C23-C21-C09	-23.31	116.40	175.43
35	k	620	II0	C24-C22-C10	-23.09	116.97	175.43
35	i	319	II0	C24-C22-C10	-20.57	123.34	175.43
35	b	315	II0	C24-C22-C10	-20.31	124.01	175.43
26	h	301	CLA	O2A-CGA-O1A	-19.80	73.62	123.59
35	k	615	II0	C24-C22-C10	-19.54	125.94	175.43
29	s	407	WVN	C20-C23-C25	18.35	153.96	126.23
29	B	848	WVN	C20-C23-C25	18.25	153.82	126.23
29	l	316	WVN	C20-C23-C25	18.13	153.62	126.23
26	c	309	CLA	C1D-ND-C4D	-18.03	93.53	106.33
29	A	845	WVN	C20-C23-C25	17.94	153.34	126.23
29	J	102	WVN	C20-C23-C25	17.88	153.25	126.23
29	A	848	WVN	C20-C23-C25	17.78	153.10	126.23
29	L	201	WVN	C20-C23-C25	17.66	152.91	126.23
29	B	853	WVN	C20-C23-C25	17.58	152.80	126.23
29	R	200	WVN	C20-C23-C25	17.57	152.78	126.23
29	K	102	WVN	C20-C23-C25	17.51	152.70	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	205	WVN	C20-C23-C25	17.50	152.68	126.23
29	B	846	WVN	C20-C23-C25	17.49	152.66	126.23
29	i	315	WVN	C20-C23-C25	17.35	152.46	126.23
29	A	857	WVN	C20-C23-C25	17.34	152.43	126.23
29	B	849	WVN	C20-C23-C25	17.26	152.31	126.23
29	M	101	WVN	C20-C23-C25	17.26	152.31	126.23
29	h	309	WVN	C20-C23-C25	17.13	152.11	126.23
29	A	847	WVN	C20-C23-C25	17.08	152.04	126.23
29	J	101	WVN	C20-C23-C25	17.00	151.93	126.23
29	A	846	WVN	C20-C23-C25	16.82	151.65	126.23
29	A	847	WVN	C04-C09-C05	-16.79	108.75	124.85
29	s	405	WVN	C20-C23-C25	16.60	151.32	126.23
29	l	303	WVN	C20-C23-C25	16.58	151.29	126.23
29	B	850	WVN	C20-C23-C25	16.27	150.83	126.23
29	F	203	WVN	C20-C23-C25	16.22	150.75	126.23
29	B	847	WVN	C20-C23-C25	16.17	150.68	126.23
29	I	101	WVN	C20-C23-C25	15.98	150.38	126.23
29	i	315	WVN	C04-C09-C05	-15.15	110.32	124.85
29	A	857	WVN	C04-C09-C05	-15.07	110.40	124.85
29	A	846	WVN	C04-C09-C05	-14.81	110.65	124.85
26	h	301	CLA	O2A-CGA-CBA	14.63	157.84	111.91
29	s	407	WVN	C04-C09-C05	-14.61	110.84	124.85
35	h	310	II0	C31-C33-C35	-14.28	86.29	126.42
35	i	316	II0	C31-C33-C35	-14.17	86.61	126.42
29	M	101	WVN	C04-C09-C05	-14.10	111.33	124.85
35	n	616	II0	C31-C33-C35	-14.00	87.10	126.42
35	a	316	II0	C31-C33-C35	-13.99	87.13	126.42
35	d	315	II0	C31-C33-C35	-13.98	87.15	126.42
35	d	316	II0	C31-C33-C35	-13.95	87.22	126.42
29	B	846	WVN	C21-C15-C13	-13.91	108.91	124.53
29	s	407	WVN	C21-C15-C13	-13.90	108.92	124.53
35	n	615	II0	C31-C33-C35	-13.89	87.40	126.42
35	i	319	II0	C31-C33-C35	-13.77	87.73	126.42
35	i	314	II0	C31-C33-C35	-13.69	87.95	126.42
29	R	200	WVN	C04-C09-C05	-13.69	111.73	124.85
29	L	201	WVN	C04-C09-C05	-13.65	111.76	124.85
29	A	847	WVN	C21-C15-C13	-13.62	109.23	124.53
35	h	311	II0	C31-C33-C35	-13.57	88.29	126.42
35	n	618	II0	C31-C33-C35	-13.54	88.39	126.42
35	h	312	II0	C31-C33-C35	-13.53	88.39	126.42
35	i	312	II0	C31-C33-C35	-13.53	88.40	126.42
35	d	317	II0	C31-C33-C35	-13.52	88.42	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	316	II0	C31-C33-C35	-13.49	88.53	126.42
35	J	104	II0	C31-C33-C35	-13.47	88.58	126.42
29	A	848	WVN	C04-C09-C05	-13.29	112.11	124.85
35	m	614	II0	C31-C33-C35	-13.24	89.23	126.42
35	k	615	II0	C31-C33-C35	-13.18	89.39	126.42
29	l	316	WVN	C21-C15-C13	-13.17	109.74	124.53
35	m	619	II0	C31-C33-C35	-13.13	89.53	126.42
35	k	616	II0	C31-C33-C35	-13.11	89.58	126.42
35	l	302	II0	C42-C40-C36	-13.06	108.67	127.31
35	l	302	II0	C31-C33-C35	-13.01	89.86	126.42
35	i	313	II0	C31-C33-C35	-12.95	90.02	126.42
35	k	620	II0	C31-C33-C35	-12.95	90.04	126.42
35	j	615	II0	C31-C33-C35	-12.89	90.22	126.42
35	c	313	II0	C31-C33-C35	-12.81	90.43	126.42
29	K	102	WVN	C21-C15-C13	-12.78	110.17	124.53
35	j	614	II0	C31-C33-C35	-12.71	90.72	126.42
35	b	314	II0	C31-C33-C35	-12.70	90.74	126.42
29	B	853	WVN	C21-C15-C13	-12.69	110.28	124.53
29	L	205	WVN	C21-C15-C13	-12.66	110.31	124.53
35	b	315	II0	C31-C33-C35	-12.66	90.86	126.42
35	a	314	II0	C31-C33-C35	-12.64	90.91	126.42
35	l	314	II0	C31-C33-C35	-12.64	90.92	126.42
35	k	619	II0	C31-C33-C35	-12.58	91.06	126.42
35	m	615	II0	C31-C33-C35	-12.58	91.07	126.42
29	B	850	WVN	C21-C15-C13	-12.58	110.40	124.53
29	l	303	WVN	C21-C15-C13	-12.29	110.73	124.53
29	h	309	WVN	C21-C15-C13	-12.28	110.74	124.53
35	d	301	II0	C31-C33-C35	-12.24	92.04	126.42
29	B	846	WVN	C40-C37-C34	-12.22	109.88	127.31
35	k	619	II0	C20-C14-C10	-12.17	107.81	124.35
29	s	405	WVN	C21-C15-C13	-12.16	110.88	124.53
29	A	848	WVN	C29-C26-C22	-12.12	110.01	127.31
35	a	312	II0	C31-C33-C35	-12.09	92.46	126.42
35	h	311	II0	C42-C40-C36	-12.02	110.16	127.31
35	k	620	II0	C20-C14-C10	-11.99	108.06	124.35
29	B	847	WVN	C21-C15-C13	-11.95	111.11	124.53
35	m	619	II0	C42-C40-C36	-11.93	110.29	127.31
35	a	313	II0	C31-C33-C35	-11.89	93.00	126.42
35	k	616	II0	C19-C13-C09	-11.86	108.23	124.35
29	A	846	WVN	C21-C15-C13	-11.73	111.35	124.53
29	F	203	WVN	C21-C15-C13	-11.72	111.36	124.53
29	K	102	WVN	C04-C09-C05	-11.72	113.61	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	620	II0	C42-C40-C36	-11.71	110.59	127.31
35	n	615	II0	C20-C14-C10	-11.67	108.49	124.35
29	J	102	WVN	C21-C15-C13	-11.65	111.45	124.53
35	j	614	II0	C20-C14-C10	-11.64	108.53	124.35
29	A	845	WVN	C39-C36-C32	-11.63	110.72	127.31
29	A	857	WVN	C21-C15-C13	-11.61	111.49	124.53
35	l	315	II0	C31-C33-C35	-11.60	93.82	126.42
35	i	313	II0	C19-C13-C09	-11.59	108.61	124.35
36	c	310	KC2	CMA-C3A-C4A	-11.57	107.42	125.04
36	s	401	KC2	CMA-C3A-C4A	-11.57	107.42	125.04
35	a	314	II0	C42-C40-C36	-11.56	110.81	127.31
29	B	848	WVN	C21-C15-C13	-11.53	111.58	124.53
35	m	616	II0	C41-C39-C35	-11.46	110.95	127.31
35	J	104	II0	C20-C14-C10	-11.45	108.79	124.35
29	A	847	WVN	C39-C36-C32	-11.44	110.98	127.31
29	R	200	WVN	C21-C15-C13	-11.44	111.69	124.53
35	b	314	II0	C42-C40-C36	-11.43	110.99	127.31
29	I	101	WVN	C21-C15-C13	-11.41	111.72	124.53
29	J	101	WVN	C21-C15-C13	-11.40	111.72	124.53
29	i	315	WVN	C40-C37-C34	-11.40	111.05	127.31
29	B	850	WVN	C40-C37-C34	-11.40	111.05	127.31
29	B	849	WVN	C21-C15-C13	-11.38	111.75	124.53
29	l	316	WVN	C40-C37-C34	-11.37	111.08	127.31
29	A	848	WVN	C21-C15-C13	-11.31	111.83	124.53
29	B	849	WVN	C40-C37-C34	-11.28	111.21	127.31
35	k	619	II0	C19-C13-C09	-11.27	109.03	124.35
29	s	407	WVN	C39-C36-C32	-11.26	111.24	127.31
29	M	101	WVN	C39-C36-C32	-11.25	111.25	127.31
29	s	407	WVN	C29-C26-C22	-11.25	111.26	127.31
29	B	848	WVN	C40-C37-C34	-11.24	111.27	127.31
35	b	314	II0	C20-C14-C10	-11.24	109.08	124.35
29	l	303	WVN	C39-C36-C32	-11.18	111.36	127.31
35	j	614	II0	C42-C40-C36	-11.17	111.37	127.31
29	B	847	WVN	C39-C36-C32	-11.17	111.37	127.31
35	l	302	II0	C37-C35-C39	-11.16	107.30	122.92
29	s	405	WVN	C04-C09-C05	-11.15	114.16	124.85
29	i	315	WVN	C21-C15-C13	-11.15	112.01	124.53
35	a	313	II0	C20-C14-C10	-11.14	109.21	124.35
35	a	312	II0	C20-C14-C10	-11.13	109.22	124.35
35	i	316	II0	C42-C40-C36	-11.09	111.48	127.31
29	K	102	WVN	C40-C37-C34	-11.07	111.51	127.31
29	A	857	WVN	C29-C26-C22	-11.07	111.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	853	WVN	C04-C09-C05	-11.05	114.25	124.85
29	J	101	WVN	C39-C36-C32	-11.05	111.54	127.31
29	A	857	WVN	C40-C37-C34	-11.02	111.59	127.31
29	h	309	WVN	C40-C37-C34	-11.01	111.60	127.31
35	c	313	II0	C19-C13-C09	-10.99	109.41	124.35
35	l	314	II0	C19-C13-C09	-10.96	109.46	124.35
29	A	848	WVN	C30-C28-C25	-10.95	111.68	127.31
29	J	101	WVN	C30-C28-C25	-10.93	111.71	127.31
35	h	312	II0	C42-C40-C36	-10.93	111.71	127.31
29	J	101	WVN	C04-C09-C05	-10.92	114.38	124.85
35	a	316	II0	C42-C40-C36	-10.91	111.74	127.31
29	A	847	WVN	C29-C26-C22	-10.91	111.74	127.31
29	s	405	WVN	C39-C36-C32	-10.90	111.75	127.31
29	L	201	WVN	C40-C37-C34	-10.90	111.76	127.31
35	l	315	II0	C38-C36-C40	-10.89	107.67	122.92
29	B	849	WVN	C39-C36-C32	-10.88	111.78	127.31
35	k	615	II0	C19-C13-C09	-10.87	109.57	124.35
35	b	314	II0	C19-C13-C09	-10.87	109.58	124.35
29	A	845	WVN	C21-C15-C13	-10.86	112.33	124.53
35	J	104	II0	C42-C40-C36	-10.86	111.82	127.31
29	i	315	WVN	C39-C36-C32	-10.84	111.84	127.31
35	k	619	II0	C42-C40-C36	-10.84	111.84	127.31
35	j	615	II0	C19-C13-C09	-10.83	109.63	124.35
29	L	205	WVN	C39-C36-C32	-10.79	111.91	127.31
35	a	312	II0	C42-C40-C36	-10.79	111.92	127.31
29	F	203	WVN	C04-C09-C05	-10.78	114.51	124.85
29	B	853	WVN	C30-C28-C25	-10.78	111.92	127.31
35	d	317	II0	C42-C40-C36	-10.77	111.94	127.31
35	k	619	II0	C37-C35-C39	-10.76	107.86	122.92
35	h	312	II0	C20-C14-C10	-10.73	109.77	124.35
29	M	101	WVN	C21-C15-C13	-10.72	112.49	124.53
35	a	314	II0	C19-C13-C09	-10.71	109.80	124.35
29	K	102	WVN	C29-C26-C22	-10.68	112.06	127.31
35	a	314	II0	C37-C35-C39	-10.68	107.97	122.92
35	h	311	II0	C20-C14-C10	-10.67	109.85	124.35
35	m	616	II0	C31-C33-C35	-10.67	96.44	126.42
35	m	614	II0	C42-C40-C36	-10.66	112.10	127.31
29	F	203	WVN	C30-C28-C25	-10.65	112.11	127.31
29	R	200	WVN	C40-C37-C34	-10.64	112.12	127.31
29	L	205	WVN	C40-C37-C34	-10.64	112.13	127.31
29	L	205	WVN	C04-C09-C05	-10.63	114.66	124.85
29	L	201	WVN	C30-C28-C25	-10.60	112.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	314	II0	C42-C40-C36	-10.60	112.18	127.31
29	I	101	WVN	C39-C36-C32	-10.60	112.19	127.31
35	n	616	II0	C42-C40-C36	-10.58	112.21	127.31
29	R	200	WVN	C39-C36-C32	-10.56	112.24	127.31
35	d	316	II0	C42-C40-C36	-10.55	112.25	127.31
29	L	201	WVN	C39-C36-C32	-10.55	112.25	127.31
29	B	848	WVN	C04-C09-C05	-10.55	114.73	124.85
29	M	101	WVN	C30-C28-C25	-10.55	112.25	127.31
29	I	101	WVN	C40-C37-C34	-10.53	112.28	127.31
35	n	615	II0	C42-C40-C36	-10.52	112.30	127.31
29	J	102	WVN	C30-C28-C25	-10.50	112.32	127.31
29	J	102	WVN	C04-C09-C05	-10.50	114.79	124.85
29	l	303	WVN	C04-C09-C05	-10.47	114.81	124.85
29	A	847	WVN	C30-C28-C25	-10.47	112.36	127.31
29	B	849	WVN	C04-C09-C05	-10.47	114.81	124.85
35	k	620	II0	C19-C13-C09	-10.47	110.13	124.35
29	J	102	WVN	C29-C26-C22	-10.46	112.38	127.31
35	d	315	II0	C42-C40-C36	-10.45	112.40	127.31
29	B	848	WVN	C29-C26-C22	-10.44	112.42	127.31
35	d	301	II0	C19-C13-C09	-10.43	110.18	124.35
29	L	201	WVN	C21-C15-C13	-10.42	112.82	124.53
29	K	102	WVN	C30-C28-C25	-10.41	112.45	127.31
29	B	846	WVN	C30-C33-C34	10.41	155.66	126.42
29	A	846	WVN	C40-C37-C34	-10.40	112.46	127.31
35	j	614	II0	C37-C35-C39	-10.40	108.36	122.92
29	i	315	WVN	C29-C26-C22	-10.38	112.50	127.31
29	L	201	WVN	C29-C26-C22	-10.37	112.50	127.31
29	l	303	WVN	C40-C37-C34	-10.37	112.51	127.31
29	B	853	WVN	C39-C36-C32	-10.37	112.51	127.31
35	d	301	II0	C42-C40-C36	-10.36	112.52	127.31
29	R	200	WVN	C30-C28-C25	-10.35	112.54	127.31
35	c	316	II0	C41-C39-C35	-10.34	112.55	127.31
29	B	849	WVN	C29-C26-C22	-10.34	112.56	127.31
29	B	853	WVN	C29-C26-C22	-10.33	112.56	127.31
35	c	316	II0	C37-C35-C39	-10.33	108.45	122.92
29	A	846	WVN	C30-C28-C25	-10.33	112.57	127.31
29	B	847	WVN	C30-C28-C25	-10.32	112.58	127.31
29	B	850	WVN	C29-C26-C22	-10.32	112.59	127.31
35	b	315	II0	C42-C40-C36	-10.31	112.59	127.31
29	B	853	WVN	C40-C37-C34	-10.30	112.61	127.31
29	B	847	WVN	C40-C37-C34	-10.29	112.62	127.31
29	A	848	WVN	C24-C22-C26	-10.28	108.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	302	II0	C38-C36-C40	-10.28	108.53	122.92
29	A	845	WVN	C40-C37-C34	-10.27	112.65	127.31
35	i	319	II0	C42-C40-C36	-10.27	112.65	127.31
35	b	315	II0	C19-C13-C09	-10.26	110.41	124.35
35	k	620	II0	C37-C35-C39	-10.23	108.59	122.92
29	l	316	WVN	C29-C26-C22	-10.23	112.71	127.31
29	B	849	WVN	C38-C34-C37	-10.20	108.63	122.92
29	B	850	WVN	C04-C09-C05	-10.20	115.07	124.85
35	l	315	II0	C03-C09-C13	-10.19	108.24	122.63
29	K	102	WVN	C35-C32-C36	-10.18	108.66	122.92
29	l	316	WVN	C38-C34-C37	-10.18	108.66	122.92
29	J	102	WVN	C27-C25-C28	-10.18	108.66	122.92
35	h	311	II0	C19-C13-C09	-10.18	110.52	124.35
29	l	303	WVN	C30-C28-C25	-10.16	112.81	127.31
29	h	309	WVN	C30-C28-C25	-10.13	112.85	127.31
26	h	301	CLA	O1A-CGA-CBA	-10.13	84.22	123.73
29	A	845	WVN	C04-C09-C05	-10.12	115.15	124.85
35	d	301	II0	C37-C35-C39	-10.11	108.76	122.92
35	m	616	II0	C42-C40-C36	-10.09	112.92	127.31
29	i	315	WVN	C38-C34-C37	-10.08	108.80	122.92
29	A	846	WVN	C39-C36-C32	-10.07	112.93	127.31
29	A	857	WVN	C24-C22-C26	-10.06	108.83	122.92
29	l	316	WVN	C30-C33-C34	10.06	154.67	126.42
29	A	846	WVN	C29-C26-C22	-10.04	112.98	127.31
29	I	101	WVN	C29-C26-C22	-10.04	112.98	127.31
29	h	309	WVN	C29-C26-C22	-10.04	112.99	127.31
29	s	405	WVN	C30-C28-C25	-10.03	112.99	127.31
29	J	102	WVN	C29-C31-C32	10.02	154.56	126.42
29	B	847	WVN	C29-C26-C22	-10.00	113.04	127.31
29	A	845	WVN	C35-C32-C36	-9.99	108.92	122.92
29	R	200	WVN	C29-C26-C22	-9.98	113.06	127.31
29	B	846	WVN	C38-C34-C37	-9.97	108.95	122.92
35	c	316	II0	C42-C40-C36	-9.96	113.09	127.31
29	s	407	WVN	C30-C28-C25	-9.96	113.10	127.31
29	B	846	WVN	C30-C28-C25	-9.96	113.10	127.31
29	J	102	WVN	C39-C36-C32	-9.95	113.11	127.31
29	s	407	WVN	C40-C37-C34	-9.93	113.14	127.31
29	B	850	WVN	C27-C25-C28	-9.93	109.02	122.92
29	R	200	WVN	C38-C34-C37	-9.91	109.04	122.92
35	k	615	II0	C38-C36-C40	-9.91	109.04	122.92
26	c	309	CLA	C4A-NA-C1A	-9.91	102.25	106.71
29	B	847	WVN	C04-C09-C05	-9.91	115.35	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	846	WVN	C29-C26-C22	-9.84	113.26	127.31
29	A	857	WVN	C39-C36-C32	-9.84	113.27	127.31
29	l	316	WVN	C24-C22-C26	-9.84	109.14	122.92
29	I	101	WVN	C04-C09-C05	-9.83	115.43	124.85
29	B	850	WVN	C24-C22-C26	-9.82	109.16	122.92
29	M	101	WVN	C29-C26-C22	-9.82	113.29	127.31
29	i	315	WVN	C30-C28-C25	-9.82	113.29	127.31
35	d	317	II0	C03-C09-C13	-9.82	108.77	122.63
29	A	848	WVN	C27-C25-C28	-9.80	109.19	122.92
35	d	316	II0	C32-C34-C36	9.79	153.92	126.42
29	B	849	WVN	C35-C32-C36	-9.79	109.21	122.92
29	i	315	WVN	C35-C32-C36	-9.78	109.22	122.92
29	J	102	WVN	C40-C37-C34	-9.78	113.36	127.31
35	m	614	II0	C38-C36-C40	-9.77	109.23	122.92
35	d	317	II0	C38-C36-C40	-9.77	109.23	122.92
35	a	316	II0	C38-C36-C40	-9.77	109.23	122.92
35	d	317	II0	C32-C34-C36	9.77	153.85	126.42
35	i	319	II0	C38-C36-C40	-9.76	109.25	122.92
29	s	405	WVN	C35-C32-C36	-9.76	109.25	122.92
29	A	847	WVN	C40-C37-C34	-9.76	113.39	127.31
29	F	203	WVN	C40-C37-C34	-9.75	113.39	127.31
29	B	850	WVN	C30-C28-C25	-9.75	113.39	127.31
35	i	316	II0	C32-C34-C36	9.75	153.81	126.42
35	m	619	II0	C19-C13-C09	-9.75	111.10	124.35
29	K	102	WVN	C24-C22-C26	-9.75	109.27	122.92
35	J	104	II0	C19-C13-C09	-9.74	111.11	124.35
29	A	846	WVN	C27-C25-C28	-9.74	109.28	122.92
35	m	614	II0	C20-C14-C10	-9.74	111.11	124.35
35	j	615	II0	C42-C40-C36	-9.74	113.41	127.31
29	J	101	WVN	C35-C32-C36	-9.72	109.30	122.92
35	i	316	II0	C38-C36-C40	-9.72	109.31	122.92
35	h	311	II0	C37-C35-C39	-9.72	109.31	122.92
29	M	101	WVN	C27-C25-C28	-9.71	109.32	122.92
35	h	311	II0	C38-C36-C40	-9.69	109.35	122.92
35	i	312	II0	C32-C34-C36	9.69	153.63	126.42
29	i	315	WVN	C24-C22-C26	-9.69	109.36	122.92
29	B	853	WVN	C35-C32-C36	-9.67	109.38	122.92
35	l	314	II0	C42-C40-C36	-9.67	113.51	127.31
29	L	205	WVN	C38-C34-C37	-9.67	109.38	122.92
29	B	853	WVN	C27-C25-C28	-9.66	109.39	122.92
35	m	614	II0	C37-C35-C39	-9.66	109.39	122.92
29	F	203	WVN	C29-C26-C22	-9.66	113.52	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	201	WVN	C38-C34-C37	-9.66	109.39	122.92
29	B	850	WVN	C35-C32-C36	-9.66	109.40	122.92
29	A	845	WVN	C29-C26-C22	-9.65	113.53	127.31
35	a	312	II0	C37-C35-C39	-9.65	109.40	122.92
29	A	846	WVN	C35-C32-C36	-9.65	109.41	122.92
29	B	850	WVN	C38-C34-C37	-9.65	109.41	122.92
29	A	847	WVN	C27-C25-C28	-9.65	109.41	122.92
29	J	102	WVN	C24-C22-C26	-9.64	109.41	122.92
29	l	303	WVN	C35-C32-C36	-9.64	109.41	122.92
35	b	315	II0	C20-C14-C10	-9.64	111.25	124.35
35	n	616	II0	C38-C36-C40	-9.64	109.42	122.92
29	l	303	WVN	C38-C34-C37	-9.63	109.43	122.92
29	h	309	WVN	C27-C25-C28	-9.63	109.44	122.92
29	h	309	WVN	C04-C09-C05	-9.63	115.62	124.85
35	d	301	II0	C20-C14-C10	-9.63	111.27	124.35
29	l	316	WVN	C30-C28-C25	-9.62	113.58	127.31
29	B	847	WVN	C38-C34-C37	-9.61	109.46	122.92
29	I	101	WVN	C27-C25-C28	-9.61	109.46	122.92
29	B	853	WVN	C29-C31-C32	9.61	153.40	126.42
29	l	303	WVN	C29-C26-C22	-9.61	113.60	127.31
35	b	315	II0	C37-C35-C39	-9.60	109.47	122.92
29	B	848	WVN	C24-C22-C26	-9.60	109.48	122.92
35	c	316	II0	C38-C36-C40	-9.60	109.48	122.92
29	A	846	WVN	C38-C34-C37	-9.59	109.48	122.92
29	B	848	WVN	C30-C28-C25	-9.59	113.62	127.31
35	n	618	II0	C38-C36-C40	-9.59	109.49	122.92
35	n	618	II0	C19-C13-C09	-9.59	111.32	124.35
29	A	845	WVN	C38-C34-C37	-9.59	109.49	122.92
35	a	314	II0	C38-C36-C40	-9.59	109.49	122.92
35	m	619	II0	C37-C35-C39	-9.59	109.49	122.92
29	L	205	WVN	C30-C28-C25	-9.58	113.64	127.31
29	R	200	WVN	C24-C22-C26	-9.57	109.51	122.92
29	i	315	WVN	C29-C31-C32	9.57	153.31	126.42
29	A	847	WVN	C35-C32-C36	-9.57	109.51	122.92
29	A	857	WVN	C38-C34-C37	-9.57	109.52	122.92
29	I	101	WVN	C06-C13-C15	-9.57	109.14	122.61
29	A	846	WVN	C24-C22-C26	-9.56	109.53	122.92
29	s	405	WVN	C27-C25-C28	-9.56	109.53	122.92
35	m	615	II0	C42-C40-C36	-9.56	113.67	127.31
35	J	104	II0	C38-C36-C40	-9.56	109.53	122.92
29	A	848	WVN	C40-C37-C34	-9.55	113.67	127.31
29	h	309	WVN	C38-C34-C37	-9.55	109.54	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	203	WVN	C38-C34-C37	-9.55	109.54	122.92
29	l	303	WVN	C30-C33-C34	9.55	153.24	126.42
35	n	618	II0	C37-C35-C39	-9.55	109.55	122.92
29	R	200	WVN	C27-C25-C28	-9.54	109.56	122.92
35	l	315	II0	C37-C35-C39	-9.54	109.56	122.92
29	l	316	WVN	C29-C31-C32	9.54	153.22	126.42
29	l	316	WVN	C27-C25-C28	-9.53	109.57	122.92
35	i	312	II0	C42-C40-C36	-9.53	113.71	127.31
35	i	314	II0	C38-C36-C40	-9.53	109.57	122.92
29	K	102	WVN	C27-C25-C28	-9.53	109.58	122.92
35	k	615	II0	C42-C40-C36	-9.53	113.72	127.31
26	c	309	CLA	C2C-C1C-NC	9.52	118.89	109.97
29	K	102	WVN	C30-C33-C34	9.52	153.16	126.42
29	B	847	WVN	C30-C33-C34	9.52	153.16	126.42
35	d	317	II0	C19-C13-C09	-9.51	111.43	124.35
29	s	407	WVN	C35-C32-C36	-9.50	109.62	122.92
29	s	405	WVN	C29-C26-C22	-9.50	113.76	127.31
29	I	101	WVN	C35-C32-C36	-9.49	109.62	122.92
35	l	314	II0	C20-C14-C10	-9.49	111.45	124.35
29	B	848	WVN	C38-C34-C37	-9.49	109.63	122.92
29	h	309	WVN	C30-C33-C34	9.49	153.07	126.42
29	M	101	WVN	C29-C31-C32	9.49	153.06	126.42
35	h	311	II0	C41-C39-C35	-9.48	113.78	127.31
35	i	313	II0	C32-C34-C36	9.48	153.05	126.42
35	b	315	II0	C38-C36-C40	-9.47	109.65	122.92
35	i	316	II0	C19-C13-C09	-9.47	111.48	124.35
29	l	316	WVN	C35-C32-C36	-9.46	109.67	122.92
29	l	303	WVN	C27-C25-C28	-9.45	109.68	122.92
35	c	313	II0	C20-C14-C10	-9.44	111.52	124.35
35	a	314	II0	C20-C14-C10	-9.44	111.52	124.35
29	J	101	WVN	C27-C25-C28	-9.44	109.70	122.92
35	i	319	II0	C37-C35-C39	-9.44	109.70	122.92
29	B	853	WVN	C24-C22-C26	-9.44	109.70	122.92
29	L	201	WVN	C27-C25-C28	-9.44	109.71	122.92
29	R	200	WVN	C35-C32-C36	-9.43	109.71	122.92
29	B	847	WVN	C35-C32-C36	-9.43	109.71	122.92
35	d	316	II0	C20-C14-C10	-9.43	111.53	124.35
29	l	316	WVN	C39-C36-C32	-9.40	113.89	127.31
29	L	201	WVN	C35-C32-C36	-9.40	109.75	122.92
29	F	203	WVN	C06-C13-C15	-9.40	109.38	122.61
35	l	302	II0	C41-C39-C35	-9.39	113.91	127.31
29	A	846	WVN	C30-C33-C34	9.39	152.79	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	205	WVN	C35-C32-C36	-9.38	109.78	122.92
29	I	101	WVN	C24-C22-C26	-9.38	109.78	122.92
29	s	405	WVN	C30-C33-C34	9.38	152.76	126.42
29	R	200	WVN	C29-C31-C32	9.38	152.76	126.42
35	a	313	II0	C42-C40-C36	-9.38	113.93	127.31
35	n	616	II0	C32-C34-C36	9.37	152.75	126.42
29	l	303	WVN	C29-C31-C32	9.37	152.75	126.42
29	K	102	WVN	C38-C34-C37	-9.36	109.81	122.92
29	I	101	WVN	C30-C28-C25	-9.35	113.96	127.31
35	c	313	II0	C42-C40-C36	-9.35	113.96	127.31
29	h	309	WVN	C39-C36-C32	-9.35	113.97	127.31
29	L	201	WVN	C30-C33-C34	9.35	152.67	126.42
35	c	316	II0	C32-C34-C36	9.34	152.67	126.42
29	A	857	WVN	C35-C32-C36	-9.34	109.83	122.92
29	A	847	WVN	C30-C33-C34	9.33	152.63	126.42
29	s	405	WVN	C29-C31-C32	9.33	152.63	126.42
35	k	619	II0	C38-C36-C40	-9.33	109.85	122.92
35	d	316	II0	C19-C13-C09	-9.33	111.67	124.35
35	n	616	II0	C19-C13-C09	-9.32	111.68	124.35
35	m	616	II0	C32-C34-C36	9.31	152.57	126.42
29	A	848	WVN	C30-C33-C34	9.31	152.57	126.42
35	d	315	II0	C38-C36-C40	-9.30	109.89	122.92
35	J	104	II0	C37-C35-C39	-9.30	109.90	122.92
29	F	203	WVN	C39-C36-C32	-9.30	114.04	127.31
29	I	101	WVN	C30-C33-C34	9.28	152.49	126.42
35	a	312	II0	C19-C13-C09	-9.26	111.76	124.35
29	B	850	WVN	C29-C31-C32	9.26	152.43	126.42
35	i	319	II0	C20-C14-C10	-9.25	111.77	124.35
35	i	314	II0	C32-C34-C36	9.25	152.41	126.42
35	l	314	II0	C32-C34-C36	9.25	152.41	126.42
29	A	845	WVN	C30-C33-C34	9.25	152.40	126.42
29	I	101	WVN	C29-C31-C32	9.25	152.40	126.42
35	d	315	II0	C32-C34-C36	9.25	152.39	126.42
29	B	846	WVN	C04-C09-C05	-9.25	115.99	124.85
29	L	205	WVN	C30-C33-C34	9.24	152.38	126.42
35	l	315	II0	C19-C13-C09	-9.24	111.79	124.35
35	n	615	II0	C19-C13-C09	-9.24	111.80	124.35
35	c	313	II0	C32-C34-C36	9.24	152.37	126.42
29	M	101	WVN	C30-C33-C34	9.24	152.37	126.42
29	B	853	WVN	C38-C34-C37	-9.24	109.98	122.92
35	d	317	II0	C37-C35-C39	-9.24	109.98	122.92
29	B	848	WVN	C39-C36-C32	-9.24	114.13	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	847	WVN	C38-C34-C37	-9.23	109.99	122.92
29	B	847	WVN	C27-C25-C28	-9.23	109.99	122.92
29	h	309	WVN	C35-C32-C36	-9.23	109.99	122.92
29	A	846	WVN	C29-C31-C32	9.23	152.35	126.42
35	j	615	II0	C37-C35-C39	-9.22	110.01	122.92
35	l	314	II0	C37-C35-C39	-9.21	110.02	122.92
29	L	205	WVN	C29-C31-C32	9.21	152.29	126.42
35	m	614	II0	C19-C13-C09	-9.21	111.83	124.35
35	a	313	II0	C32-C34-C36	9.21	152.29	126.42
29	B	848	WVN	C29-C31-C32	9.21	152.28	126.42
35	k	616	II0	C32-C34-C36	9.20	152.27	126.42
35	a	313	II0	C37-C35-C39	-9.20	110.03	122.92
29	i	315	WVN	C27-C25-C28	-9.20	110.04	122.92
35	j	614	II0	C19-C13-C09	-9.20	111.85	124.35
35	d	301	II0	C38-C36-C40	-9.18	110.06	122.92
35	a	316	II0	C37-C35-C39	-9.18	110.06	122.92
35	k	615	II0	C32-C34-C36	9.18	152.21	126.42
35	a	316	II0	C41-C39-C35	-9.18	114.21	127.31
35	m	619	II0	C38-C36-C40	-9.17	110.07	122.92
35	i	319	II0	C32-C34-C36	9.17	152.17	126.42
35	a	313	II0	C19-C13-C09	-9.17	111.89	124.35
29	J	101	WVN	C29-C26-C22	-9.17	114.23	127.31
35	n	615	II0	C38-C36-C40	-9.17	110.08	122.92
35	m	614	II0	C32-C34-C36	9.16	152.16	126.42
29	R	200	WVN	C30-C33-C34	9.16	152.14	126.42
29	A	857	WVN	C29-C31-C32	9.15	152.13	126.42
29	s	407	WVN	C30-C33-C34	9.15	152.13	126.42
29	A	848	WVN	C39-C36-C32	-9.15	114.26	127.31
29	I	101	WVN	C38-C34-C37	-9.14	110.12	122.92
35	n	618	II0	C41-C39-C35	-9.14	114.27	127.31
29	B	847	WVN	C24-C22-C26	-9.14	110.12	122.92
29	L	205	WVN	C27-C25-C28	-9.12	110.15	122.92
29	B	849	WVN	C30-C28-C25	-9.11	114.31	127.31
35	m	616	II0	C38-C36-C40	-9.09	110.18	122.92
35	m	615	II0	C19-C13-C09	-9.09	111.99	124.35
35	h	312	II0	C37-C35-C39	-9.07	110.22	122.92
29	J	101	WVN	C40-C37-C34	-9.07	114.37	127.31
35	j	614	II0	C38-C36-C40	-9.07	110.22	122.92
29	h	309	WVN	C29-C31-C32	9.07	151.89	126.42
35	i	313	II0	C37-C35-C39	-9.07	110.22	122.92
29	J	102	WVN	C38-C34-C37	-9.06	110.24	122.92
35	J	104	II0	C32-C34-C36	9.05	151.85	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	315	II0	C38-C36-C34	-9.05	103.81	118.08
35	n	615	II0	C41-C39-C35	-9.05	114.39	127.31
29	B	853	WVN	C30-C33-C34	9.04	151.80	126.42
29	s	407	WVN	C27-C25-C28	-9.02	110.28	122.92
35	h	310	II0	C41-C39-C35	-9.02	114.43	127.31
29	J	101	WVN	C30-C33-C34	9.02	151.76	126.42
35	b	314	II0	C37-C35-C39	-9.02	110.29	122.92
35	l	314	II0	C38-C36-C40	-9.02	110.29	122.92
35	d	316	II0	C38-C36-C40	-9.02	110.29	122.92
29	B	848	WVN	C35-C32-C36	-9.01	110.30	122.92
35	b	314	II0	C38-C36-C40	-9.01	110.31	122.92
35	k	615	II0	C37-C35-C39	-9.00	110.31	122.92
29	M	101	WVN	C40-C37-C34	-9.00	114.46	127.31
35	h	311	II0	C32-C34-C36	9.00	151.70	126.42
35	k	620	II0	C38-C36-C40	-9.00	110.32	122.92
29	s	407	WVN	C38-C34-C37	-9.00	110.32	122.92
29	K	102	WVN	C29-C31-C32	9.00	151.69	126.42
35	k	620	II0	C32-C34-C36	8.99	151.68	126.42
29	M	101	WVN	C24-C22-C26	-8.98	110.34	122.92
29	s	407	WVN	C24-C22-C26	-8.98	110.35	122.92
35	j	615	II0	C38-C36-C40	-8.98	110.35	122.92
35	m	614	II0	C41-C39-C35	-8.97	114.51	127.31
35	d	301	II0	C32-C34-C36	8.96	151.60	126.42
35	b	314	II0	C32-C34-C36	8.96	151.59	126.42
29	J	101	WVN	C38-C34-C37	-8.96	110.38	122.92
35	n	616	II0	C41-C39-C35	-8.95	114.53	127.31
35	i	314	II0	C37-C35-C39	-8.95	110.39	122.92
29	J	101	WVN	C29-C31-C32	8.95	151.55	126.42
35	d	315	II0	C20-C14-C10	-8.94	112.20	124.35
35	j	615	II0	C32-C34-C36	8.94	151.52	126.42
35	n	615	II0	C37-C35-C39	-8.93	110.41	122.92
29	J	102	WVN	C30-C33-C34	8.92	151.49	126.42
29	B	846	WVN	C35-C32-C36	-8.92	110.42	122.92
35	a	314	II0	C32-C34-C36	8.92	151.48	126.42
29	A	845	WVN	C29-C31-C32	8.91	151.46	126.42
35	n	618	II0	C32-C34-C36	8.91	151.44	126.42
35	c	313	II0	C37-C35-C39	-8.91	110.45	122.92
35	c	316	II0	C19-C13-C09	-8.91	112.25	124.35
29	L	201	WVN	C24-C22-C26	-8.90	110.45	122.92
35	m	615	II0	C32-C34-C36	8.89	151.40	126.42
29	L	201	WVN	C29-C31-C32	8.89	151.40	126.42
29	h	309	WVN	C24-C22-C26	-8.89	110.47	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	846	WVN	C39-C36-C32	-8.88	114.64	127.31
35	i	314	II0	C20-C14-C10	-8.87	112.29	124.35
35	i	316	II0	C37-C35-C39	-8.87	110.50	122.92
35	i	313	II0	C20-C14-C10	-8.86	112.31	124.35
29	B	848	WVN	C30-C33-C34	8.85	151.27	126.42
36	c	310	KC2	C2A-C3A-C4A	-8.84	99.93	106.49
35	n	616	II0	C37-C35-C39	-8.83	110.55	122.92
29	B	847	WVN	C29-C31-C32	8.83	151.23	126.42
29	l	303	WVN	C24-C22-C26	-8.83	110.55	122.92
29	F	203	WVN	C30-C33-C34	8.83	151.22	126.42
29	K	102	WVN	C39-C36-C32	-8.83	114.71	127.31
35	h	312	II0	C38-C36-C40	-8.83	110.56	122.92
29	A	857	WVN	C30-C33-C34	8.82	151.20	126.42
35	b	315	II0	C03-C09-C13	-8.82	110.17	122.63
35	i	314	II0	C41-C39-C35	-8.82	114.72	127.31
29	F	203	WVN	C27-C25-C28	-8.81	110.58	122.92
35	n	618	II0	C42-C40-C36	-8.80	114.74	127.31
35	i	319	II0	C41-C39-C35	-8.80	114.75	127.31
35	l	314	II0	C41-C39-C35	-8.80	114.76	127.31
29	M	101	WVN	C38-C34-C37	-8.80	110.60	122.92
29	s	405	WVN	C24-C22-C26	-8.79	110.61	122.92
35	i	316	II0	C41-C39-C35	-8.79	114.77	127.31
29	J	102	WVN	C35-C32-C36	-8.79	110.61	122.92
35	a	316	II0	C32-C34-C36	8.78	151.09	126.42
35	a	314	II0	C41-C39-C35	-8.78	114.78	127.31
35	h	312	II0	C19-C13-C09	-8.76	112.44	124.35
29	B	846	WVN	C27-C25-C28	-8.76	110.65	122.92
29	A	848	WVN	C29-C31-C32	8.76	151.03	126.42
26	c	309	CLA	C2D-C1D-ND	8.75	116.55	110.10
35	i	316	II0	C20-C14-C10	-8.75	112.46	124.35
35	d	317	II0	C41-C39-C35	-8.75	114.82	127.31
35	a	312	II0	C32-C34-C36	8.75	150.99	126.42
35	j	614	II0	C32-C34-C36	8.73	150.95	126.42
35	h	310	II0	C42-C40-C36	-8.73	114.85	127.31
35	i	312	II0	C03-C09-C13	-8.73	110.31	122.63
35	l	315	II0	C20-C14-C10	-8.72	112.50	124.35
35	l	315	II0	C41-C39-C35	-8.71	114.88	127.31
35	h	312	II0	C32-C34-C36	8.71	150.89	126.42
29	M	101	WVN	C35-C32-C36	-8.71	110.72	122.92
29	B	846	WVN	C29-C31-C32	8.69	150.82	126.42
35	m	615	II0	C37-C35-C39	-8.69	110.75	122.92
35	m	616	II0	C37-C35-C39	-8.68	110.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	h	310	II0	C19-C13-C09	-8.68	112.55	124.35
29	M	101	WVN	C02-C05-C09	-8.68	110.79	121.47
35	n	616	II0	C20-C14-C10	-8.65	112.59	124.35
35	h	310	II0	C37-C35-C39	-8.63	110.84	122.92
35	i	312	II0	C19-C13-C09	-8.62	112.64	124.35
35	a	316	II0	C19-C13-C09	-8.62	112.64	124.35
35	m	616	II0	C20-C14-C10	-8.61	112.65	124.35
35	k	619	II0	C32-C34-C36	8.60	150.56	126.42
29	F	203	WVN	C29-C31-C32	8.59	150.56	126.42
35	n	618	II0	C20-C14-C10	-8.59	112.68	124.35
27	A	842	PQN	C11-C12-C13	-8.58	112.51	126.79
29	B	849	WVN	C29-C31-C32	8.58	150.51	126.42
29	A	848	WVN	C38-C34-C37	-8.57	110.91	122.92
35	J	104	II0	C41-C39-C35	-8.56	115.09	127.31
27	B	843	PQN	C11-C12-C13	-8.55	112.56	126.79
35	m	615	II0	C33-C35-C39	-8.55	105.83	118.94
29	i	315	WVN	C30-C33-C34	8.55	150.43	126.42
29	B	850	WVN	C39-C36-C32	-8.53	115.14	127.31
36	s	401	KC2	CMA-C3A-C2A	-8.52	107.44	128.30
35	i	319	II0	C19-C13-C09	-8.52	112.77	124.35
29	B	849	WVN	C24-C22-C26	-8.52	111.00	122.92
29	B	849	WVN	C30-C33-C34	8.49	150.27	126.42
29	A	847	WVN	C24-C22-C26	-8.49	111.03	122.92
35	m	619	II0	C32-C34-C36	8.49	150.25	126.42
35	d	315	II0	C19-C13-C09	-8.48	112.82	124.35
29	L	205	WVN	C29-C26-C22	-8.48	115.21	127.31
36	s	401	KC2	C2A-C3A-C4A	-8.48	100.19	106.49
35	n	615	II0	C32-C34-C36	8.46	150.17	126.42
35	a	312	II0	C38-C36-C40	-8.45	111.08	122.92
35	m	619	II0	C20-C14-C10	-8.45	112.86	124.35
35	i	313	II0	C42-C40-C36	-8.45	115.26	127.31
35	m	615	II0	C38-C36-C40	-8.43	111.12	122.92
29	A	846	WVN	C02-C05-C09	-8.43	111.10	121.47
29	B	848	WVN	C27-C25-C28	-8.43	111.12	122.92
35	c	313	II0	C38-C36-C40	-8.42	111.13	122.92
29	J	101	WVN	C06-C13-C15	-8.41	110.76	122.61
29	A	857	WVN	C30-C28-C25	-8.41	115.30	127.31
35	j	615	II0	C41-C39-C35	-8.40	115.31	127.31
35	i	314	II0	C19-C13-C09	-8.40	112.93	124.35
35	j	615	II0	C20-C14-C10	-8.39	112.95	124.35
35	m	619	II0	C41-C39-C35	-8.38	115.35	127.31
35	d	301	II0	C33-C35-C39	-8.38	106.09	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	316	WVN	C04-C09-C05	-8.36	116.83	124.85
35	n	616	II0	C03-C09-C13	-8.36	110.83	122.63
35	c	316	II0	C20-C14-C10	-8.35	113.00	124.35
35	d	316	II0	C37-C35-C39	-8.35	111.22	122.92
35	a	312	II0	C41-C39-C35	-8.35	115.39	127.31
35	j	614	II0	C41-C39-C35	-8.35	115.39	127.31
29	s	407	WVN	C02-C05-C09	-8.35	111.20	121.47
29	B	850	WVN	C30-C33-C34	8.35	149.86	126.42
35	i	312	II0	C38-C36-C40	-8.34	111.24	122.92
29	A	845	WVN	C24-C22-C26	-8.34	111.24	122.92
35	d	317	II0	C20-C14-C10	-8.33	113.04	124.35
35	l	302	II0	C19-C13-C09	-8.32	113.04	124.35
29	I	101	WVN	C14-C15-C13	-8.32	110.65	122.73
35	d	301	II0	C03-C09-C13	-8.30	110.91	122.63
35	m	616	II0	C19-C13-C09	-8.26	113.13	124.35
29	B	846	WVN	C24-C22-C19	-8.25	105.08	118.08
35	h	312	II0	C41-C39-C35	-8.23	115.56	127.31
35	d	316	II0	C41-C39-C35	-8.23	115.57	127.31
35	k	615	II0	C41-C39-C35	-8.22	115.58	127.31
35	a	316	II0	C20-C14-C10	-8.22	113.18	124.35
29	B	849	WVN	C27-C25-C28	-8.17	111.48	122.92
35	a	313	II0	C33-C35-C39	-8.16	106.41	118.94
35	a	312	II0	C33-C35-C39	-8.13	106.47	118.94
35	k	616	II0	C20-C14-C10	-8.12	113.31	124.35
35	l	302	II0	C20-C14-C10	-8.12	113.31	124.35
29	s	405	WVN	C40-C37-C34	-8.12	115.72	127.31
35	m	615	II0	C20-C14-C10	-8.11	113.33	124.35
29	s	405	WVN	C02-C05-C09	-8.10	111.50	121.47
29	A	847	WVN	C29-C31-C32	8.10	149.16	126.42
35	c	313	II0	C41-C39-C35	-8.07	115.79	127.31
29	A	845	WVN	C30-C28-C25	-8.06	115.80	127.31
35	i	312	II0	C20-C14-C10	-8.06	113.40	124.35
29	l	316	WVN	C38-C34-C33	-8.05	105.40	118.08
26	c	309	CLA	C1B-CHB-C4A	-8.05	114.19	130.12
35	k	616	II0	C33-C35-C39	-8.03	106.63	118.94
35	l	302	II0	C32-C34-C36	8.02	148.93	126.42
35	d	315	II0	C41-C39-C35	-8.01	115.88	127.31
29	F	203	WVN	C24-C22-C26	-8.00	111.71	122.92
29	s	405	WVN	C06-C13-C15	-8.00	111.34	122.61
29	J	102	WVN	C35-C32-C31	-8.00	105.47	118.08
35	h	311	II0	C03-C09-C13	-8.00	111.34	122.63
29	s	407	WVN	C29-C31-C32	7.99	148.86	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	315	II0	C37-C35-C39	-7.98	111.74	122.92
36	s	401	KC2	C1A-C2A-C3A	-7.96	100.79	107.11
26	c	309	CLA	CMD-C2D-C1D	7.96	138.75	124.71
36	c	310	KC2	CMA-C3A-C2A	-7.94	108.86	128.30
35	k	620	II0	C03-C09-C13	-7.94	111.42	122.63
29	B	846	WVN	C02-C05-C09	-7.94	111.70	121.47
29	J	101	WVN	C24-C22-C26	-7.88	111.88	122.92
29	A	848	WVN	C35-C32-C36	-7.88	111.89	122.92
35	a	314	II0	C03-C09-C13	-7.88	111.51	122.63
35	b	315	II0	C38-C36-C34	-7.88	105.67	118.08
29	s	405	WVN	C38-C34-C37	-7.87	111.90	122.92
35	h	310	II0	C38-C36-C40	-7.83	111.95	122.92
26	B	832	CLA	C4A-NA-C1A	7.82	110.22	106.71
26	l	313	CLA	C4A-NA-C1A	7.82	110.22	106.71
35	k	616	II0	C41-C39-C35	-7.82	116.16	127.31
29	M	101	WVN	C19-C22-C26	-7.81	106.95	118.94
26	B	805	CLA	C4A-NA-C1A	7.81	110.22	106.71
29	i	315	WVN	C06-C13-C15	-7.80	111.63	122.61
35	b	314	II0	C03-C09-C13	-7.79	111.63	122.63
35	b	314	II0	C38-C36-C34	-7.78	105.82	118.08
35	a	313	II0	C38-C36-C40	-7.76	112.05	122.92
35	k	620	II0	C41-C39-C35	-7.76	116.24	127.31
29	F	203	WVN	C14-C15-C13	-7.73	111.51	122.73
29	A	845	WVN	C27-C25-C28	-7.71	112.12	122.92
35	b	315	II0	C32-C34-C36	7.71	148.06	126.42
35	k	615	II0	C03-C09-C13	-7.70	111.76	122.63
29	A	857	WVN	C27-C25-C28	-7.70	112.14	122.92
35	i	312	II0	C37-C35-C39	-7.70	112.14	122.92
29	B	846	WVN	C24-C22-C26	-7.69	112.15	122.92
35	i	313	II0	C38-C36-C40	-7.68	112.16	122.92
35	j	615	II0	C03-C09-C13	-7.67	111.80	122.63
29	L	205	WVN	C24-C22-C26	-7.67	112.18	122.92
29	A	848	WVN	C06-C13-C15	-7.67	111.81	122.61
29	I	101	WVN	C23-C25-C28	-7.67	107.18	118.94
35	i	319	II0	C04-C10-C14	-7.66	111.82	122.63
35	m	615	II0	C41-C39-C35	-7.66	116.38	127.31
29	I	101	WVN	C19-C22-C26	-7.65	107.20	118.94
29	F	203	WVN	C35-C32-C36	-7.65	112.20	122.92
35	d	301	II0	C41-C39-C35	-7.65	116.40	127.31
26	k	602	CLA	C4A-NA-C1A	7.64	110.14	106.71
35	k	616	II0	C38-C36-C40	-7.64	112.22	122.92
35	j	614	II0	C33-C35-C39	-7.63	107.24	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	313	II0	C41-C39-C35	-7.60	116.46	127.31
29	K	102	WVN	C02-C05-C09	-7.59	112.14	121.47
29	R	200	WVN	C06-C13-C15	-7.58	111.93	122.61
35	k	616	II0	C42-C40-C36	-7.56	116.52	127.31
26	B	834	CLA	C4A-NA-C1A	7.55	110.10	106.71
26	i	305	CLA	C4A-NA-C1A	7.55	110.10	106.71
26	c	304	CLA	C4A-NA-C1A	7.54	110.10	106.71
29	A	848	WVN	C31-C32-C36	-7.54	107.37	118.94
35	c	313	II0	C03-C09-C13	-7.53	112.00	122.63
26	B	808	CLA	C4A-NA-C1A	7.52	110.09	106.71
29	A	847	WVN	C02-C05-C09	-7.52	112.22	121.47
35	l	314	II0	C03-C09-C13	-7.50	112.05	122.63
35	k	620	II0	C33-C35-C39	-7.50	107.44	118.94
35	a	314	II0	C33-C35-C39	-7.48	107.47	118.94
35	k	616	II0	C37-C35-C39	-7.47	112.45	122.92
29	i	315	WVN	C02-C05-C09	-7.46	112.28	121.47
35	l	314	II0	C33-C35-C39	-7.42	107.56	118.94
26	j	605	CLA	C4A-NA-C1A	7.42	110.04	106.71
26	c	309	CLA	C3D-C4D-ND	7.41	122.22	110.24
26	A	852	CLA	C4A-NA-C1A	7.38	110.03	106.71
26	l	307	CLA	C4A-NA-C1A	7.35	110.01	106.71
26	L	203	CLA	C4A-NA-C1A	7.34	110.00	106.71
29	R	200	WVN	C02-C05-C09	-7.33	112.44	121.47
26	c	309	CLA	C3C-C4C-NC	7.33	118.79	110.57
26	a	310	CLA	C4A-NA-C1A	7.32	110.00	106.71
36	c	310	KC2	C1A-C2A-C3A	-7.31	101.31	107.11
29	A	848	WVN	C33-C34-C37	-7.28	107.77	118.94
35	c	313	II0	C33-C35-C39	-7.28	107.77	118.94
26	c	309	CLA	CHD-C1D-ND	-7.26	117.78	124.45
35	i	312	II0	C33-C35-C39	-7.25	107.82	118.94
26	A	835	CLA	C4A-NA-C1A	7.24	109.96	106.71
26	A	816	CLA	C4A-NA-C1A	7.23	109.96	106.71
29	A	847	WVN	C06-C13-C15	-7.23	112.44	122.61
26	A	824	CLA	C4A-NA-C1A	7.22	109.95	106.71
35	J	104	II0	C03-C09-C13	-7.20	112.46	122.63
35	k	619	II0	C33-C35-C39	-7.20	107.90	118.94
26	b	311	CLA	C4A-NA-C1A	7.19	109.94	106.71
26	A	804	CLA	C4A-NA-C1A	7.18	109.94	106.71
29	B	846	WVN	C19-C22-C26	-7.18	107.93	118.94
35	b	315	II0	C41-C39-C35	-7.18	117.07	127.31
26	A	815	CLA	C4A-NA-C1A	7.16	109.92	106.71
35	m	619	II0	C33-C35-C39	-7.16	107.96	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	840	CLA	C4A-NA-C1A	7.13	109.91	106.71
26	j	601	CLA	C4A-NA-C1A	7.12	109.91	106.71
35	l	315	II0	C33-C35-C39	-7.12	108.02	118.94
35	i	314	II0	C04-C10-C14	-7.11	112.59	122.63
29	L	201	WVN	C19-C22-C26	-7.11	108.03	118.94
35	j	614	II0	C38-C36-C34	-7.11	106.87	118.08
29	K	102	WVN	C06-C13-C15	-7.10	112.61	122.61
29	J	102	WVN	C27-C25-C23	-7.09	106.91	118.08
26	B	807	CLA	C4A-NA-C1A	7.09	109.89	106.71
29	I	101	WVN	C31-C32-C36	-7.09	108.07	118.94
26	s	403	CLA	C4A-NA-C1A	7.08	109.89	106.71
26	b	303	CLA	C4A-NA-C1A	7.06	109.88	106.71
26	n	610	CLA	C4A-NA-C1A	7.06	109.88	106.71
26	b	312	CLA	C4A-NA-C1A	7.05	109.88	106.71
26	B	838	CLA	C4A-NA-C1A	7.05	109.87	106.71
26	a	304	CLA	C4A-NA-C1A	7.04	109.87	106.71
35	i	312	II0	C41-C39-C35	-7.04	117.27	127.31
26	B	822	CLA	C4A-NA-C1A	7.04	109.87	106.71
26	A	836	CLA	C4A-NA-C1A	7.03	109.87	106.71
26	i	310	CLA	C4A-NA-C1A	7.03	109.87	106.71
26	B	804	CLA	CAC-C3C-C4C	7.01	133.91	124.81
26	A	856	CLA	C4A-NA-C1A	7.01	109.86	106.71
26	K	101	CLA	C4A-NA-C1A	7.01	109.86	106.71
26	m	613	CLA	C4A-NA-C1A	7.00	109.85	106.71
35	k	619	II0	C41-C39-C35	-6.99	117.33	127.31
26	a	301	CLA	C4A-NA-C1A	6.99	109.85	106.71
26	Q	302	CLA	C4A-NA-C1A	6.99	109.85	106.71
26	i	301	CLA	C4A-NA-C1A	6.99	109.85	106.71
26	A	837	CLA	C4A-NA-C1A	6.97	109.84	106.71
35	b	315	II0	C04-C10-C14	-6.97	112.79	122.63
36	c	310	KC2	C2B-C1B-NB	6.97	115.24	110.10
26	B	809	CLA	C4A-NA-C1A	6.97	109.84	106.71
26	k	610	CLA	C4A-NA-C1A	6.97	109.84	106.71
35	h	310	II0	C33-C35-C39	-6.96	108.25	118.94
29	J	101	WVN	C02-C05-C09	-6.96	112.90	121.47
26	A	820	CLA	C4A-NA-C1A	6.96	109.84	106.71
26	a	309	CLA	C4A-NA-C1A	6.96	109.84	106.71
26	h	303	CLA	C4A-NA-C1A	6.96	109.83	106.71
26	h	308	CLA	C4A-NA-C1A	6.95	109.83	106.71
26	A	808	CLA	C4A-NA-C1A	6.94	109.83	106.71
26	A	822	CLA	C4A-NA-C1A	6.94	109.83	106.71
26	d	318	CLA	C4A-NA-C1A	6.93	109.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m	604	CLA	C4A-NA-C1A	6.92	109.82	106.71
35	a	313	II0	C41-C39-C35	-6.92	117.43	127.31
26	a	308	CLA	C4A-NA-C1A	6.91	109.81	106.71
26	c	311	CLA	C4A-NA-C1A	6.91	109.81	106.71
26	h	302	CLA	C4A-NA-C1A	6.91	109.81	106.71
29	B	846	WVN	C27-C25-C23	-6.90	107.21	118.08
26	l	301	CLA	C4A-NA-C1A	6.90	109.81	106.71
29	B	848	WVN	C14-C15-C13	-6.89	112.72	122.73
26	B	835	CLA	C4A-NA-C1A	6.89	109.80	106.71
29	J	101	WVN	C33-C34-C37	-6.89	108.37	118.94
26	A	823	CLA	C4A-NA-C1A	6.88	109.80	106.71
26	j	612	CLA	C4A-NA-C1A	6.88	109.80	106.71
29	J	101	WVN	C14-C15-C13	-6.88	112.74	122.73
29	A	857	WVN	C02-C05-C09	-6.88	113.00	121.47
26	b	313	CLA	C4A-NA-C1A	6.86	109.79	106.71
26	B	841	CLA	C4A-NA-C1A	6.86	109.79	106.71
26	b	308	CLA	C4A-NA-C1A	6.86	109.79	106.71
35	m	616	II0	C04-C10-C14	-6.86	112.95	122.63
26	h	304	CLA	C4A-NA-C1A	6.86	109.79	106.71
29	B	847	WVN	C02-C05-C09	-6.85	113.05	121.47
26	j	606	CLA	C4A-NA-C1A	6.84	109.78	106.71
26	A	806	CLA	C4A-NA-C1A	6.83	109.78	106.71
26	i	302	CLA	C4A-NA-C1A	6.83	109.78	106.71
26	A	802	CLA	C4A-NA-C1A	6.82	109.77	106.71
26	A	821	CLA	C4A-NA-C1A	6.82	109.77	106.71
35	h	312	II0	C04-C10-C14	-6.82	113.00	122.63
35	b	314	II0	C41-C39-C35	-6.82	117.58	127.31
36	s	401	KC2	C2B-C1B-NB	6.81	115.12	110.10
26	h	307	CLA	C4A-NA-C1A	6.81	109.77	106.71
35	j	615	II0	C33-C35-C39	-6.80	108.50	118.94
29	B	846	WVN	C35-C32-C31	-6.80	107.37	118.08
26	i	307	CLA	C4A-NA-C1A	6.79	109.76	106.71
29	F	203	WVN	C02-C05-C09	-6.79	113.12	121.47
26	A	810	CLA	C4A-NA-C1A	6.78	109.76	106.71
26	B	814	CLA	C4A-NA-C1A	6.78	109.75	106.71
26	L	202	CLA	C4A-NA-C1A	6.78	109.75	106.71
26	i	304	CLA	C4A-NA-C1A	6.78	109.75	106.71
26	d	304	CLA	C4A-NA-C1A	6.77	109.75	106.71
29	A	847	WVN	C24-C22-C19	-6.76	107.42	118.08
35	h	311	II0	C33-C35-C39	-6.76	108.57	118.94
26	m	605	CLA	C4A-NA-C1A	6.76	109.74	106.71
26	A	812	CLA	C4A-NA-C1A	6.76	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	826	CLA	C4A-NA-C1A	6.76	109.74	106.71
26	c	301	CLA	C4A-NA-C1A	6.76	109.74	106.71
29	s	407	WVN	C24-C22-C19	-6.74	107.45	118.08
26	l	311	CLA	C4A-NA-C1A	6.74	109.74	106.71
26	s	408	CLA	C4A-NA-C1A	6.74	109.73	106.71
26	A	829	CLA	C4A-NA-C1A	6.74	109.73	106.71
29	A	847	WVN	C35-C32-C31	-6.72	107.48	118.08
26	k	609	CLA	C4A-NA-C1A	6.72	109.73	106.71
26	c	309	CLA	C4D-CHA-C1A	-6.72	113.07	121.25
26	b	306	CLA	C4A-NA-C1A	6.72	109.72	106.71
26	d	305	CLA	C4A-NA-C1A	6.72	109.72	106.71
26	b	309	CLA	C4A-NA-C1A	6.70	109.72	106.71
29	L	201	WVN	C31-C32-C36	-6.70	108.66	118.94
26	A	811	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	B	811	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	n	605	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	B	820	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	m	609	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	k	601	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	A	809	CLA	C4A-NA-C1A	6.70	109.72	106.71
29	L	201	WVN	C23-C25-C28	-6.69	108.67	118.94
26	j	610	CLA	C4A-NA-C1A	6.69	109.71	106.71
26	j	613	CLA	C4A-NA-C1A	6.69	109.71	106.71
26	d	306	CLA	C4A-NA-C1A	6.69	109.71	106.71
26	A	838	CLA	C4A-NA-C1A	6.69	109.71	106.71
26	l	304	CLA	C4A-NA-C1A	6.68	109.71	106.71
26	B	801	CLA	C4A-NA-C1A	6.68	109.71	106.71
26	A	830	CLA	C4A-NA-C1A	6.68	109.71	106.71
35	k	619	II0	C03-C09-C13	-6.67	113.21	122.63
29	K	102	WVN	C24-C22-C19	-6.67	107.56	118.08
26	n	604	CLA	C4A-NA-C1A	6.67	109.70	106.71
26	i	308	CLA	C4A-NA-C1A	6.67	109.70	106.71
26	k	604	CLA	C4A-NA-C1A	6.66	109.70	106.71
26	n	602	CLA	C4A-NA-C1A	6.66	109.70	106.71
35	a	313	II0	C04-C10-C14	-6.66	113.23	122.63
26	l	308	CLA	C4A-NA-C1A	6.66	109.70	106.71
26	A	833	CLA	C4A-NA-C1A	6.66	109.70	106.71
26	j	604	CLA	C4A-NA-C1A	6.65	109.70	106.71
26	B	813	CLA	C4A-NA-C1A	6.65	109.69	106.71
26	h	301	CLA	C4A-NA-C1A	6.64	109.69	106.71
26	m	601	CLA	C4A-NA-C1A	6.64	109.69	106.71
26	A	818	CLA	C4A-NA-C1A	6.64	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m	602	CLA	C4A-NA-C1A	6.64	109.69	106.71
26	B	812	CLA	C4A-NA-C1A	6.64	109.69	106.71
26	m	610	CLA	C4A-NA-C1A	6.64	109.69	106.71
26	L	204	CLA	C4A-NA-C1A	6.64	109.69	106.71
35	b	315	II0	C27-C25-C23	-6.64	103.70	116.84
29	K	102	WVN	C14-C15-C13	-6.63	113.10	122.73
29	A	857	WVN	C23-C25-C28	-6.63	108.76	118.94
29	K	102	WVN	C31-C32-C36	-6.63	108.77	118.94
26	J	103	CLA	C4A-NA-C1A	6.61	109.68	106.71
26	c	308	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	M	101	WVN	C33-C34-C37	-6.60	108.82	118.94
26	a	305	CLA	C4A-NA-C1A	6.58	109.67	106.71
26	B	831	CLA	C4A-NA-C1A	6.58	109.67	106.71
26	n	601	CLA	C4A-NA-C1A	6.58	109.66	106.71
35	n	618	II0	C33-C35-C39	-6.58	108.85	118.94
35	h	310	II0	C30-C32-C34	-6.58	112.37	125.34
26	k	605	CLA	C4A-NA-C1A	6.57	109.66	106.71
26	A	819	CLA	C4A-NA-C1A	6.57	109.66	106.71
26	j	609	CLA	C4A-NA-C1A	6.57	109.66	106.71
35	l	315	II0	C32-C34-C36	6.56	144.86	126.42
26	b	310	CLA	C4A-NA-C1A	6.56	109.66	106.71
29	s	407	WVN	C33-C34-C37	-6.56	108.87	118.94
35	c	316	II0	C33-C35-C39	-6.56	108.88	118.94
26	h	306	CLA	C4A-NA-C1A	6.56	109.66	106.71
26	L	206	CLA	C4A-NA-C1A	6.56	109.65	106.71
35	h	312	II0	C33-C35-C39	-6.56	108.88	118.94
29	A	848	WVN	C19-C22-C26	-6.55	108.89	118.94
26	d	313	CLA	C4A-NA-C1A	6.55	109.65	106.71
26	B	839	CLA	C4A-NA-C1A	6.53	109.64	106.71
26	A	827	CLA	C4A-NA-C1A	6.53	109.64	106.71
26	A	831	CLA	C4A-NA-C1A	6.52	109.64	106.71
29	l	303	WVN	C02-C05-C09	-6.51	113.46	121.47
35	i	319	II0	C33-C35-C39	-6.51	108.96	118.94
35	i	314	II0	C33-C35-C39	-6.50	108.97	118.94
29	h	309	WVN	C23-C25-C28	-6.50	108.97	118.94
26	A	841	CLA	C4A-NA-C1A	6.50	109.63	106.71
26	l	310	CLA	C4A-NA-C1A	6.49	109.63	106.71
29	s	407	WVN	C23-C25-C28	-6.49	108.98	118.94
29	s	405	WVN	C27-C25-C23	-6.49	107.85	118.08
29	I	101	WVN	C33-C34-C37	-6.49	108.98	118.94
26	F	202	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	B	850	WVN	C38-C34-C33	-6.49	107.86	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	603	CLA	C4A-NA-C1A	6.49	109.62	106.71
35	k	615	II0	C33-C35-C39	-6.49	108.99	118.94
26	A	828	CLA	C4A-NA-C1A	6.48	109.62	106.71
26	A	807	CLA	C4A-NA-C1A	6.47	109.62	106.71
26	a	303	CLA	C4A-NA-C1A	6.47	109.61	106.71
29	A	848	WVN	C35-C32-C31	-6.47	107.89	118.08
26	b	304	CLA	C4A-NA-C1A	6.46	109.61	106.71
35	J	104	II0	C33-C35-C39	-6.46	109.03	118.94
29	B	850	WVN	C31-C32-C36	-6.46	109.03	118.94
35	b	314	II0	C33-C35-C39	-6.45	109.04	118.94
26	b	307	CLA	C4A-NA-C1A	6.45	109.61	106.71
26	B	836	CLA	C4A-NA-C1A	6.44	109.60	106.71
29	J	101	WVN	C19-C22-C26	-6.44	109.05	118.94
35	i	316	II0	C33-C35-C39	-6.44	109.06	118.94
35	h	311	II0	C04-C10-C14	-6.44	113.55	122.63
29	A	846	WVN	C14-C15-C13	-6.43	113.40	122.73
35	i	313	II0	C04-C10-C14	-6.43	113.56	122.63
35	d	316	II0	C38-C36-C34	-6.43	107.95	118.08
29	s	407	WVN	C35-C32-C31	-6.42	107.96	118.08
29	F	203	WVN	C35-C32-C31	-6.42	107.96	118.08
35	d	317	II0	C33-C35-C39	-6.42	109.09	118.94
26	i	311	CLA	C4A-NA-C1A	6.42	109.59	106.71
26	d	302	CLA	C4A-NA-C1A	6.41	109.59	106.71
29	s	405	WVN	C33-C34-C37	-6.41	109.10	118.94
26	k	606	CLA	C4A-NA-C1A	6.41	109.59	106.71
29	s	405	WVN	C19-C22-C26	-6.40	109.11	118.94
29	A	846	WVN	C06-C13-C15	-6.39	113.61	122.61
29	l	303	WVN	C20-C13-C15	-6.39	105.98	121.46
29	L	201	WVN	C33-C34-C37	-6.39	109.14	118.94
26	A	839	CLA	C4A-NA-C1A	6.39	109.58	106.71
26	F	201	CLA	C4A-NA-C1A	6.39	109.58	106.71
35	l	302	II0	C38-C36-C34	-6.38	108.03	118.08
35	m	615	II0	C34-C36-C40	-6.37	109.16	118.94
26	B	827	CLA	C4A-NA-C1A	6.37	109.57	106.71
26	k	608	CLA	C4A-NA-C1A	6.37	109.57	106.71
26	A	805	CLA	C4A-NA-C1A	6.36	109.57	106.71
26	B	815	CLA	C4A-NA-C1A	6.36	109.57	106.71
26	c	312	CLA	C4A-NA-C1A	6.36	109.56	106.71
29	B	850	WVN	C27-C25-C23	-6.36	108.06	118.08
29	M	101	WVN	C24-C22-C19	-6.35	108.07	118.08
26	B	825	CLA	C4A-NA-C1A	6.35	109.56	106.71
26	B	824	CLA	C4A-NA-C1A	6.35	109.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	315	II0	C33-C35-C39	-6.34	109.21	118.94
26	a	311	CLA	C4A-NA-C1A	6.34	109.56	106.71
29	B	849	WVN	C02-C05-C09	-6.34	113.67	121.47
29	A	848	WVN	C23-C25-C28	-6.34	109.22	118.94
26	B	816	CLA	C4A-NA-C1A	6.34	109.56	106.71
29	B	850	WVN	C20-C13-C15	-6.33	106.12	121.46
26	c	305	CLA	C4A-NA-C1A	6.33	109.55	106.71
29	l	303	WVN	C19-C22-C26	-6.33	109.23	118.94
35	k	619	II0	C38-C36-C34	-6.33	108.11	118.08
29	L	205	WVN	C02-C05-C09	-6.32	113.69	121.47
36	s	401	KC2	C3B-C2B-C1B	-6.31	101.05	107.08
26	a	302	CLA	C4A-NA-C1A	6.31	109.54	106.71
26	B	842	CLA	C4A-NA-C1A	6.30	109.54	106.71
29	l	316	WVN	C27-C25-C23	-6.30	108.15	118.08
29	L	205	WVN	C19-C22-C26	-6.30	109.28	118.94
26	h	313	CLA	C4A-NA-C1A	6.29	109.53	106.71
35	m	614	II0	C33-C35-C39	-6.29	109.29	118.94
35	k	615	II0	C38-C36-C34	-6.28	108.17	118.08
35	j	614	II0	C04-C10-C14	-6.28	113.76	122.63
26	c	302	CLA	C4A-NA-C1A	6.28	109.53	106.71
35	i	313	II0	C33-C35-C39	-6.28	109.31	118.94
29	i	315	WVN	C38-C34-C33	-6.26	108.22	118.08
35	J	104	II0	C04-C10-C14	-6.25	113.81	122.63
26	R	201	CLA	C4A-NA-C1A	6.24	109.51	106.71
29	B	846	WVN	C38-C34-C33	-6.24	108.24	118.08
29	l	303	WVN	C33-C34-C37	-6.23	109.38	118.94
35	l	315	II0	C42-C40-C36	-6.23	118.42	127.31
29	B	846	WVN	C31-C32-C36	-6.23	109.39	118.94
26	B	803	CLA	C4A-NA-C1A	6.22	109.50	106.71
29	B	849	WVN	C35-C32-C31	-6.22	108.28	118.08
29	l	303	WVN	C27-C25-C23	-6.22	108.28	118.08
29	A	845	WVN	C27-C25-C23	-6.21	108.30	118.08
26	A	834	CLA	C4A-NA-C1A	6.20	109.50	106.71
29	F	203	WVN	C24-C22-C19	-6.20	108.30	118.08
26	d	309	CLA	C4A-NA-C1A	6.20	109.49	106.71
29	L	205	WVN	C20-C13-C15	-6.20	106.45	121.46
29	h	309	WVN	C31-C32-C36	-6.19	109.44	118.94
35	n	616	II0	C33-C35-C39	-6.19	109.44	118.94
29	R	200	WVN	C27-C25-C23	-6.19	108.33	118.08
26	n	603	CLA	C4A-NA-C1A	6.19	109.49	106.71
35	d	316	II0	C37-C35-C33	-6.18	108.33	118.08
36	s	401	KC2	CHB-C4A-C3A	-6.18	115.32	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	828	CLA	C4A-NA-C1A	6.18	109.48	106.71
35	a	316	II0	C33-C35-C39	-6.18	109.46	118.94
26	A	840	CLA	C4A-NA-C1A	6.18	109.48	106.71
35	k	615	II0	C37-C35-C33	-6.17	108.35	118.08
29	B	848	WVN	C02-C05-C09	-6.17	113.87	121.47
26	B	826	CLA	C4A-NA-C1A	6.17	109.48	106.71
26	A	814	CLA	C4A-NA-C1A	6.17	109.48	106.71
35	i	319	II0	C38-C36-C34	-6.17	108.36	118.08
26	B	806	CLA	C4A-NA-C1A	6.17	109.48	106.71
35	c	316	II0	C34-C36-C40	-6.17	109.48	118.94
26	i	306	CLA	C4A-NA-C1A	6.16	109.47	106.71
29	s	407	WVN	C27-C25-C23	-6.15	108.38	118.08
35	k	616	II0	C34-C36-C40	-6.15	109.50	118.94
26	c	303	CLA	C4A-NA-C1A	6.14	109.47	106.71
29	i	315	WVN	C23-C25-C28	-6.14	109.52	118.94
26	B	804	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	m	608	CLA	C4A-NA-C1A	6.14	109.47	106.71
29	A	857	WVN	C24-C22-C19	-6.13	108.41	118.08
29	B	848	WVN	C27-C25-C23	-6.13	108.42	118.08
29	l	316	WVN	C35-C32-C31	-6.13	108.42	118.08
26	B	817	CLA	C4A-NA-C1A	6.12	109.46	106.71
35	i	316	II0	C03-C09-C13	-6.12	113.99	122.63
29	L	205	WVN	C23-C25-C28	-6.12	109.55	118.94
26	k	614	CLA	C4A-NA-C1A	6.11	109.45	106.71
35	d	315	II0	C33-C35-C39	-6.11	109.56	118.94
29	l	316	WVN	C20-C13-C15	-6.11	106.67	121.46
26	l	306	CLA	C4A-NA-C1A	6.10	109.45	106.71
35	a	314	II0	C04-C10-C14	-6.10	114.02	122.63
26	d	303	CLA	C4A-NA-C1A	6.10	109.45	106.71
26	a	307	CLA	C4A-NA-C1A	6.10	109.45	106.71
35	l	314	II0	C38-C36-C34	-6.09	108.48	118.08
26	a	306	CLA	C4A-NA-C1A	6.09	109.44	106.71
29	l	316	WVN	C23-C25-C28	-6.09	109.60	118.94
26	j	608	CLA	C4A-NA-C1A	6.08	109.44	106.71
26	d	310	CLA	C4A-NA-C1A	6.08	109.44	106.71
29	B	850	WVN	C24-C22-C19	-6.08	108.50	118.08
26	l	309	CLA	C4A-NA-C1A	6.07	109.44	106.71
29	J	102	WVN	C19-C22-C26	-6.07	109.63	118.94
29	A	845	WVN	C24-C22-C19	-6.07	108.52	118.08
35	l	314	II0	C04-C10-C14	-6.07	114.07	122.63
36	s	401	KC2	O2D-CGD-CBD	6.07	122.05	111.27
35	i	312	II0	C38-C36-C34	-6.06	108.53	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	n	616	II0	C37-C35-C33	-6.06	108.53	118.08
26	j	602	CLA	C4A-NA-C1A	6.05	109.43	106.71
26	B	837	CLA	C4A-NA-C1A	6.05	109.43	106.71
36	c	310	KC2	CHB-C4A-C3A	-6.05	115.53	124.98
35	c	313	II0	C38-C36-C34	-6.04	108.56	118.08
35	i	314	II0	C03-C09-C13	-6.03	114.12	122.63
29	K	102	WVN	C23-C25-C28	-6.03	109.69	118.94
35	i	313	II0	C03-C09-C13	-6.02	114.14	122.63
29	J	102	WVN	C02-C05-C09	-6.02	114.07	121.47
29	A	845	WVN	C35-C32-C31	-6.01	108.60	118.08
26	m	612	CLA	C4A-NA-C1A	6.01	109.41	106.71
26	A	803	CLA	C4A-NA-C1A	6.01	109.41	106.71
35	h	310	II0	C34-C36-C40	-6.00	109.73	118.94
26	d	307	CLA	C4A-NA-C1A	6.00	109.40	106.71
29	B	853	WVN	C19-C22-C26	-5.99	109.74	118.94
29	J	102	WVN	C38-C34-C33	-5.99	108.64	118.08
36	s	401	KC2	C3A-C4A-NA	5.98	117.11	110.57
29	s	407	WVN	C23-C20-C13	-5.98	110.39	127.20
35	J	104	II0	C38-C36-C34	-5.98	108.65	118.08
26	m	606	CLA	C4A-NA-C1A	5.97	109.39	106.71
26	n	609	CLA	C4A-NA-C1A	5.97	109.39	106.71
29	B	847	WVN	C24-C22-C19	-5.97	108.68	118.08
26	A	832	CLA	C4A-NA-C1A	5.97	109.39	106.71
26	A	817	CLA	C4A-NA-C1A	5.96	109.39	106.71
26	m	607	CLA	C4A-NA-C1A	5.96	109.39	106.71
26	d	308	CLA	C4A-NA-C1A	5.96	109.38	106.71
27	B	843	PQN	C15-C13-C12	-5.96	109.06	121.12
29	A	847	WVN	C33-C34-C37	-5.96	109.80	118.94
29	A	857	WVN	C35-C32-C31	-5.95	108.70	118.08
29	J	101	WVN	C24-C22-C19	-5.95	108.71	118.08
29	i	315	WVN	C35-C32-C31	-5.95	108.71	118.08
29	l	316	WVN	C14-C15-C13	-5.94	114.11	122.73
35	n	615	II0	C38-C36-C34	-5.94	108.72	118.08
35	a	312	II0	C04-C10-C14	-5.94	114.25	122.63
26	n	606	CLA	C4A-NA-C1A	5.93	109.37	106.71
35	m	614	II0	C04-C10-C14	-5.93	114.26	122.63
29	L	205	WVN	C24-C22-C19	-5.93	108.74	118.08
29	L	201	WVN	C35-C32-C31	-5.92	108.75	118.08
29	F	203	WVN	C33-C34-C37	-5.91	109.86	118.94
29	B	847	WVN	C27-C25-C23	-5.91	108.77	118.08
29	B	846	WVN	C23-C25-C28	-5.90	109.88	118.94
29	l	316	WVN	C23-C20-C13	-5.90	110.62	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	316	II0	C38-C36-C34	-5.90	108.78	118.08
29	A	847	WVN	C14-C15-C13	-5.89	114.17	122.73
29	h	309	WVN	C20-C13-C15	-5.89	107.20	121.46
29	J	101	WVN	C35-C32-C31	-5.88	108.81	118.08
35	d	315	II0	C38-C36-C34	-5.88	108.82	118.08
29	l	316	WVN	C24-C22-C19	-5.87	108.83	118.08
29	h	309	WVN	C19-C22-C26	-5.87	109.93	118.94
26	B	833	CLA	C4A-NA-C1A	5.86	109.34	106.71
26	s	406	CLA	C4A-NA-C1A	5.86	109.34	106.71
29	B	853	WVN	C31-C32-C36	-5.86	109.95	118.94
29	s	407	WVN	C20-C13-C15	-5.86	107.27	121.46
29	M	101	WVN	C23-C25-C28	-5.86	109.96	118.94
26	B	810	CLA	C4A-NA-C1A	5.85	109.34	106.71
27	A	842	PQN	C15-C13-C12	-5.85	109.28	121.12
29	A	857	WVN	C27-C25-C23	-5.85	108.86	118.08
35	i	314	II0	C37-C35-C33	-5.84	108.88	118.08
29	A	846	WVN	C31-C32-C36	-5.84	109.99	118.94
29	B	849	WVN	C23-C25-C28	-5.83	109.99	118.94
29	s	405	WVN	C24-C22-C19	-5.83	108.89	118.08
29	h	309	WVN	C33-C34-C37	-5.83	110.00	118.94
29	B	848	WVN	C35-C32-C31	-5.82	108.91	118.08
26	m	603	CLA	C4A-NA-C1A	5.81	109.32	106.71
29	A	857	WVN	C38-C34-C33	-5.81	108.92	118.08
29	l	303	WVN	C23-C25-C28	-5.80	110.04	118.94
29	B	847	WVN	C33-C34-C37	-5.80	110.05	118.94
29	A	847	WVN	C23-C25-C28	-5.79	110.05	118.94
29	B	853	WVN	C14-C15-C13	-5.79	114.32	122.73
26	B	802	CLA	C4A-NA-C1A	5.79	109.31	106.71
35	d	317	II0	C38-C36-C34	-5.78	108.96	118.08
29	B	848	WVN	C31-C32-C36	-5.78	110.07	118.94
36	c	310	KC2	C3A-C4A-NA	5.78	116.88	110.57
29	B	849	WVN	C38-C34-C33	-5.77	108.98	118.08
35	h	311	II0	C28-C26-C24	-5.77	105.42	116.84
29	K	102	WVN	C38-C34-C33	-5.76	108.99	118.08
29	A	857	WVN	C31-C32-C36	-5.76	110.09	118.94
29	F	203	WVN	C27-C25-C23	-5.76	109.00	118.08
29	F	203	WVN	C38-C34-C33	-5.76	109.01	118.08
29	s	407	WVN	C38-C34-C33	-5.75	109.01	118.08
29	B	853	WVN	C33-C34-C37	-5.75	110.11	118.94
35	m	614	II0	C38-C36-C34	-5.75	109.02	118.08
29	B	847	WVN	C35-C32-C31	-5.75	109.02	118.08
29	B	849	WVN	C27-C25-C23	-5.75	109.02	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	101	WVN	C38-C34-C33	-5.74	109.03	118.08
29	L	201	WVN	C27-C25-C23	-5.74	109.03	118.08
26	B	830	CLA	C4A-NA-C1A	5.74	109.29	106.71
29	L	205	WVN	C33-C34-C37	-5.74	110.14	118.94
35	d	316	II0	C33-C35-C39	-5.74	110.14	118.94
29	B	848	WVN	C23-C25-C28	-5.73	110.14	118.94
29	R	200	WVN	C14-C15-C13	-5.73	114.41	122.73
29	B	848	WVN	C06-C13-C15	-5.73	114.55	122.61
26	i	303	CLA	C4A-NA-C1A	5.72	109.28	106.71
29	A	847	WVN	C38-C34-C33	-5.72	109.06	118.08
26	s	402	CLA	C4A-NA-C1A	5.71	109.28	106.71
29	J	101	WVN	C38-C34-C33	-5.71	109.07	118.08
29	J	101	WVN	C31-C32-C36	-5.71	110.18	118.94
26	n	613	CLA	C4A-NA-C1A	5.71	109.27	106.71
29	A	846	WVN	C33-C34-C37	-5.71	110.18	118.94
35	j	615	II0	C37-C35-C33	-5.71	109.09	118.08
29	J	101	WVN	C23-C25-C28	-5.70	110.20	118.94
29	R	200	WVN	C19-C22-C26	-5.70	110.20	118.94
35	a	316	II0	C38-C36-C34	-5.70	109.10	118.08
29	B	853	WVN	C06-C13-C15	-5.70	114.59	122.61
35	d	317	II0	C37-C35-C33	-5.69	109.10	118.08
29	l	303	WVN	C31-C32-C36	-5.69	110.21	118.94
28	s	409	LHG	O4-P-O5	5.69	132.96	110.68
35	h	311	II0	C38-C36-C34	-5.68	109.13	118.08
29	A	845	WVN	C19-C22-C26	-5.66	110.25	118.94
29	B	849	WVN	C24-C22-C19	-5.66	109.16	118.08
29	h	309	WVN	C35-C32-C31	-5.65	109.17	118.08
26	c	309	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
35	j	615	II0	C04-C10-C14	-5.65	114.65	122.63
29	s	405	WVN	C31-C32-C36	-5.64	110.28	118.94
35	m	616	II0	C38-C36-C34	-5.64	109.19	118.08
29	s	405	WVN	C38-C34-C33	-5.64	109.20	118.08
29	h	309	WVN	C27-C25-C23	-5.63	109.20	118.08
29	l	303	WVN	C24-C22-C19	-5.63	109.21	118.08
29	A	848	WVN	C27-C25-C23	-5.63	109.21	118.08
29	F	203	WVN	C31-C32-C36	-5.63	110.31	118.94
36	c	310	KC2	C3B-C2B-C1B	-5.63	101.70	107.08
26	l	305	CLA	C4A-NA-C1A	5.63	109.23	106.71
29	A	846	WVN	C19-C22-C26	-5.63	110.31	118.94
35	h	310	II0	C38-C36-C34	-5.62	109.22	118.08
29	L	205	WVN	C27-C25-C23	-5.62	109.22	118.08
29	A	848	WVN	C38-C34-C33	-5.62	109.22	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	405	WVN	C35-C32-C31	-5.62	109.23	118.08
35	a	316	II0	C37-C35-C33	-5.61	109.23	118.08
29	B	853	WVN	C35-C32-C31	-5.61	109.24	118.08
26	c	307	CLA	C4A-NA-C1A	5.60	109.22	106.71
35	a	316	II0	C03-C09-C13	-5.60	114.73	122.63
29	B	853	WVN	C20-C13-C15	-5.60	107.91	121.46
35	n	615	II0	C33-C35-C39	-5.59	110.36	118.94
29	s	405	WVN	C14-C15-C13	-5.59	114.62	122.73
35	m	619	II0	C04-C10-C14	-5.59	114.75	122.63
26	B	823	CLA	C4A-NA-C1A	5.59	109.22	106.71
35	m	616	II0	C31-C29-C25	-5.58	110.37	126.58
29	A	847	WVN	C27-C25-C23	-5.58	109.29	118.08
29	i	315	WVN	C19-C22-C26	-5.57	110.40	118.94
35	n	616	II0	C38-C36-C34	-5.57	109.31	118.08
29	i	315	WVN	C27-C25-C23	-5.56	109.31	118.08
29	A	857	WVN	C06-C13-C15	-5.56	114.78	122.61
29	A	846	WVN	C35-C32-C31	-5.56	109.31	118.08
35	a	314	II0	C38-C36-C34	-5.56	109.32	118.08
29	M	101	WVN	C35-C32-C31	-5.56	109.32	118.08
35	c	316	II0	C38-C36-C34	-5.56	109.32	118.08
26	B	827	CLA	CMB-C2B-C1B	-5.55	119.93	128.46
29	A	846	WVN	C23-C25-C28	-5.55	110.42	118.94
29	J	102	WVN	C23-C20-C13	-5.55	111.62	127.20
35	n	616	II0	C34-C36-C40	-5.55	110.43	118.94
35	i	316	II0	C37-C35-C33	-5.55	109.34	118.08
35	d	315	II0	C37-C35-C33	-5.54	109.34	118.08
35	c	313	II0	C34-C36-C40	-5.54	110.44	118.94
35	a	313	II0	C38-C36-C34	-5.54	109.35	118.08
29	i	315	WVN	C24-C22-C19	-5.54	109.35	118.08
35	b	315	II0	C37-C35-C33	-5.54	109.35	118.08
35	i	313	II0	C38-C36-C34	-5.53	109.36	118.08
35	i	312	II0	C37-C35-C33	-5.53	109.36	118.08
29	J	102	WVN	C06-C13-C15	-5.53	114.82	122.61
29	A	845	WVN	C33-C34-C37	-5.53	110.46	118.94
29	R	200	WVN	C24-C22-C19	-5.53	109.37	118.08
29	K	102	WVN	C27-C25-C23	-5.53	109.37	118.08
35	J	104	II0	C37-C35-C33	-5.53	109.37	118.08
35	i	314	II0	C34-C36-C40	-5.52	110.47	118.94
29	M	101	WVN	C14-C15-C13	-5.52	114.72	122.73
29	R	200	WVN	C31-C32-C36	-5.52	110.47	118.94
29	A	848	WVN	C14-C15-C13	-5.51	114.73	122.73
29	M	101	WVN	C38-C34-C33	-5.50	109.41	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	825	CLA	C4A-NA-C1A	5.50	109.18	106.71
29	B	848	WVN	C23-C20-C13	-5.48	111.81	127.20
29	B	850	WVN	C35-C32-C31	-5.48	109.44	118.08
36	s	401	KC2	C1A-NA-C4A	-5.48	104.24	106.71
35	l	302	II0	C33-C35-C39	-5.48	110.53	118.94
29	B	849	WVN	C19-C22-C26	-5.47	110.54	118.94
29	L	201	WVN	C24-C22-C19	-5.47	109.46	118.08
26	c	306	CLA	C4A-NA-C1A	5.47	109.17	106.71
29	B	848	WVN	C24-C22-C19	-5.47	109.46	118.08
29	A	845	WVN	C38-C34-C33	-5.47	109.46	118.08
35	c	316	II0	C31-C29-C25	-5.46	110.71	126.58
29	B	849	WVN	C06-C13-C15	-5.45	114.93	122.61
35	d	301	II0	C38-C36-C34	-5.45	109.48	118.08
29	s	405	WVN	C23-C25-C28	-5.45	110.58	118.94
35	n	618	II0	C34-C36-C40	-5.45	110.58	118.94
29	R	200	WVN	C23-C25-C28	-5.44	110.59	118.94
29	A	845	WVN	C23-C25-C28	-5.44	110.59	118.94
29	B	853	WVN	C23-C25-C28	-5.44	110.59	118.94
26	A	813	CLA	C4A-NA-C1A	5.44	109.15	106.71
29	h	309	WVN	C38-C34-C33	-5.44	109.51	118.08
26	B	818	CLA	C4A-NA-C1A	5.43	109.15	106.71
29	F	203	WVN	C19-C22-C26	-5.43	110.60	118.94
29	A	846	WVN	C24-C22-C19	-5.43	109.52	118.08
35	h	312	II0	C38-C36-C34	-5.43	109.52	118.08
29	h	309	WVN	C24-C22-C19	-5.43	109.52	118.08
29	A	846	WVN	C38-C34-C33	-5.43	109.52	118.08
35	i	314	II0	C38-C36-C34	-5.43	109.53	118.08
35	d	315	II0	C34-C36-C40	-5.42	110.62	118.94
29	M	101	WVN	C27-C25-C23	-5.42	109.54	118.08
35	n	618	II0	C38-C36-C34	-5.42	109.54	118.08
29	I	101	WVN	C35-C32-C31	-5.41	109.55	118.08
29	l	303	WVN	C35-C32-C31	-5.41	109.55	118.08
36	s	401	KC2	C4C-C3C-C2C	-5.41	102.82	107.11
35	c	313	II0	C37-C35-C33	-5.41	109.56	118.08
35	j	615	II0	C34-C36-C40	-5.39	110.67	118.94
35	l	314	II0	C34-C36-C40	-5.39	110.67	118.94
29	R	200	WVN	C35-C32-C31	-5.39	109.58	118.08
26	B	819	CLA	C4A-NA-C1A	5.39	109.13	106.71
29	B	847	WVN	C38-C34-C33	-5.39	109.59	118.08
36	c	310	KC2	CMD-C2D-C1D	5.39	136.74	128.46
26	b	305	CLA	C4A-NA-C1A	5.39	109.13	106.71
35	d	317	II0	C04-C10-C14	-5.38	115.04	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	306	CLA	CMB-C2B-C1B	-5.38	120.20	128.46
29	B	847	WVN	C23-C25-C28	-5.38	110.69	118.94
36	c	310	KC2	C4C-C3C-C2C	-5.37	102.85	107.11
29	B	848	WVN	C38-C34-C33	-5.37	109.61	118.08
35	i	312	II0	C34-C36-C40	-5.37	110.71	118.94
35	i	319	II0	C37-C35-C33	-5.36	109.62	118.08
35	l	302	II0	C27-C25-C23	-5.34	106.26	116.84
29	K	102	WVN	C33-C34-C37	-5.34	110.75	118.94
29	A	857	WVN	C14-C15-C13	-5.34	114.98	122.73
26	B	821	CLA	C4A-NA-C1A	5.34	109.11	106.71
29	R	200	WVN	C38-C34-C33	-5.34	109.67	118.08
27	A	842	PQN	C14-C13-C12	-5.34	109.99	123.68
35	m	614	II0	C27-C25-C23	-5.33	106.28	116.84
29	B	853	WVN	C24-C22-C19	-5.33	109.69	118.08
29	L	205	WVN	C35-C32-C31	-5.32	109.69	118.08
35	b	314	II0	C04-C10-C14	-5.32	115.12	122.63
29	B	848	WVN	C19-C22-C26	-5.32	110.78	118.94
35	n	618	II0	C37-C35-C33	-5.32	109.70	118.08
29	J	102	WVN	C24-C22-C19	-5.31	109.70	118.08
29	A	847	WVN	C20-C13-C15	-5.31	108.60	121.46
35	i	316	II0	C27-C25-C23	-5.31	106.32	116.84
35	n	615	II0	C04-C10-C14	-5.30	115.14	122.63
35	c	313	II0	C04-C10-C14	-5.29	115.16	122.63
35	b	314	II0	C27-C25-C23	-5.29	106.37	116.84
29	L	205	WVN	C38-C34-C33	-5.28	109.75	118.08
35	a	313	II0	C37-C35-C33	-5.27	109.77	118.08
35	J	104	II0	C31-C29-C25	-5.27	111.27	126.58
29	B	853	WVN	C27-C25-C23	-5.26	109.80	118.08
35	i	319	II0	C27-C25-C23	-5.25	106.44	116.84
26	c	309	CLA	C1D-CHD-C4C	-5.25	114.73	126.06
29	L	201	WVN	C23-C20-C13	-5.22	112.53	127.20
29	J	101	WVN	C27-C25-C23	-5.22	109.86	118.08
27	B	843	PQN	C14-C13-C12	-5.21	110.30	123.68
26	B	829	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
29	L	205	WVN	C23-C20-C13	-5.21	112.57	127.20
35	i	313	II0	C34-C36-C40	-5.21	110.95	118.94
26	c	309	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
35	b	315	II0	C32-C30-C26	-5.20	111.47	126.58
26	l	305	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
29	R	200	WVN	C33-C34-C37	-5.20	110.96	118.94
35	k	620	II0	C38-C36-C34	-5.20	109.89	118.08
35	j	615	II0	C38-C36-C34	-5.20	109.89	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	802	CLA	CMB-C2B-C1B	-5.19	120.48	128.46
29	A	848	WVN	C02-C05-C09	-5.19	115.08	121.47
35	a	313	II0	C03-C09-C13	-5.19	115.30	122.63
29	B	853	WVN	C38-C34-C33	-5.18	109.91	118.08
29	L	205	WVN	C31-C32-C36	-5.18	110.99	118.94
29	K	102	WVN	C20-C13-C15	-5.17	108.94	121.46
35	m	619	II0	C38-C36-C34	-5.16	109.94	118.08
26	c	309	CLA	C3B-C4B-NB	5.16	115.89	109.21
29	I	101	WVN	C24-C22-C19	-5.16	109.95	118.08
29	B	848	WVN	C33-C34-C37	-5.16	111.02	118.94
35	n	615	II0	C37-C35-C33	-5.16	109.95	118.08
29	A	845	WVN	C23-C20-C13	-5.15	112.73	127.20
35	m	615	II0	C03-C09-C13	-5.14	115.37	122.63
35	h	310	II0	C37-C35-C33	-5.14	109.98	118.08
35	n	618	II0	C04-C10-C14	-5.14	115.38	122.63
29	L	201	WVN	C38-C34-C33	-5.13	109.99	118.08
35	c	316	II0	C04-C10-C14	-5.13	115.39	122.63
35	d	301	II0	C34-C36-C40	-5.13	111.07	118.94
29	A	857	WVN	C19-C22-C26	-5.12	111.08	118.94
26	j	602	CLA	CMB-C2B-C1B	-5.12	120.59	128.46
35	h	312	II0	C37-C35-C33	-5.12	110.01	118.08
35	m	615	II0	C38-C36-C34	-5.12	110.01	118.08
26	h	305	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
36	s	401	KC2	C2A-C1A-NA	5.11	117.60	109.40
29	A	846	WVN	C27-C25-C23	-5.11	110.02	118.08
26	B	829	CLA	C4A-NA-C1A	5.10	109.00	106.71
26	b	305	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
35	n	615	II0	C27-C25-C23	-5.09	106.75	116.84
29	M	101	WVN	C23-C20-C13	-5.08	112.92	127.20
29	B	847	WVN	C20-C13-C15	-5.08	109.17	121.46
35	k	616	II0	C38-C36-C34	-5.07	110.08	118.08
35	h	312	II0	C34-C36-C40	-5.07	111.16	118.94
29	J	102	WVN	C33-C34-C37	-5.07	111.17	118.94
29	A	857	WVN	C23-C20-C13	-5.05	113.02	127.20
35	i	313	II0	C37-C35-C33	-5.05	110.12	118.08
26	n	608	CLA	C4A-NA-C1A	5.04	108.97	106.71
29	I	101	WVN	C27-C25-C23	-5.04	110.13	118.08
35	n	616	II0	C31-C29-C25	-5.04	111.95	126.58
35	a	314	II0	C34-C36-C40	-5.03	111.23	118.94
29	l	303	WVN	C38-C34-C33	-5.02	110.17	118.08
36	s	401	KC2	C3C-C2C-C1C	-5.01	102.77	106.49
26	m	604	CLA	CMB-C2B-C1B	-5.01	120.76	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	851	CLA	C4A-NA-C1A	5.01	108.96	106.71
29	J	102	WVN	C14-C15-C13	-4.99	115.49	122.73
35	b	314	II0	C31-C29-C25	-4.99	112.09	126.58
35	l	314	II0	C32-C30-C26	-4.98	112.11	126.58
35	k	616	II0	C04-C10-C14	-4.98	115.60	122.63
26	B	833	CLA	CMB-C2B-C1B	-4.98	120.81	128.46
35	i	319	II0	C34-C36-C40	-4.98	111.30	118.94
29	h	309	WVN	C02-C05-C09	-4.97	115.36	121.47
35	m	615	II0	C04-C10-C14	-4.97	115.62	122.63
29	A	846	WVN	C20-C13-C15	-4.96	109.44	121.46
26	a	302	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
35	a	312	II0	C03-C09-C13	-4.95	115.65	122.63
29	i	315	WVN	C31-C32-C36	-4.94	111.37	118.94
35	d	315	II0	C32-C30-C26	-4.94	112.25	126.58
35	d	316	II0	C34-C36-C40	-4.94	111.37	118.94
35	a	313	II0	C29-C31-C33	-4.93	107.82	123.22
35	l	314	II0	C37-C35-C33	-4.93	110.31	118.08
26	b	304	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
29	I	101	WVN	C20-C13-C15	-4.92	109.54	121.46
35	k	620	II0	C37-C35-C33	-4.92	110.32	118.08
35	k	615	II0	C32-C30-C26	-4.92	112.31	126.58
35	J	104	II0	C32-C30-C26	-4.91	112.31	126.58
26	h	305	CLA	C4A-NA-C1A	4.91	108.91	106.71
29	B	849	WVN	C14-C15-C13	-4.91	115.61	122.73
29	l	303	WVN	C23-C20-C13	-4.91	113.42	127.20
35	a	312	II0	C32-C30-C26	-4.90	112.35	126.58
26	k	603	CLA	C4A-NA-C1A	4.89	108.91	106.71
35	a	312	II0	C38-C36-C34	-4.89	110.37	118.08
35	a	316	II0	C34-C36-C40	-4.89	111.44	118.94
35	J	104	II0	C34-C36-C40	-4.88	111.45	118.94
36	c	310	KC2	C2A-C1A-NA	4.88	117.23	109.40
35	c	316	II0	C32-C30-C26	-4.88	112.40	126.58
26	B	805	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
29	B	847	WVN	C19-C22-C26	-4.87	111.46	118.94
35	b	315	II0	C20-C14-C12	-4.87	105.33	114.36
29	L	201	WVN	C06-C13-C15	-4.87	115.75	122.61
36	c	310	KC2	O2D-CGD-CBD	4.87	119.92	111.27
35	c	316	II0	C37-C35-C33	-4.87	110.41	118.08
26	j	603	CLA	CMB-C2B-C1B	-4.87	120.99	128.46
26	A	851	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
26	j	604	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
35	d	316	II0	C03-C09-C13	-4.86	115.78	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	802	CLA	CMB-C2B-C1B	-4.85	121.00	128.46
35	k	620	II0	C32-C30-C26	-4.85	112.49	126.58
35	n	615	II0	C03-C09-C13	-4.85	115.79	122.63
35	i	319	II0	C20-C14-C12	-4.84	105.38	114.36
35	k	616	II0	C19-C13-C11	-4.84	105.39	114.36
35	J	104	II0	C27-C25-C23	-4.83	107.28	116.84
29	K	102	WVN	C35-C32-C31	-4.83	110.47	118.08
35	m	615	II0	C37-C35-C33	-4.82	110.48	118.08
35	d	316	II0	C32-C30-C26	-4.82	112.59	126.58
29	B	846	WVN	C33-C34-C37	-4.82	111.55	118.94
29	B	850	WVN	C23-C20-C13	-4.81	113.69	127.20
35	a	313	II0	C34-C36-C40	-4.81	111.56	118.94
36	c	310	KC2	C1A-NA-C4A	-4.81	104.54	106.71
35	l	302	II0	C37-C35-C33	-4.80	110.51	118.08
29	i	315	WVN	C14-C15-C13	-4.79	115.77	122.73
29	K	102	WVN	C19-C22-C26	-4.79	111.59	118.94
35	i	316	II0	C32-C30-C26	-4.78	112.71	126.58
35	i	316	II0	C34-C36-C40	-4.77	111.62	118.94
29	A	847	WVN	C19-C22-C26	-4.77	111.62	118.94
35	l	315	II0	C29-C31-C33	-4.77	108.34	123.22
35	k	620	II0	C34-C36-C40	-4.76	111.63	118.94
35	m	614	II0	C37-C35-C33	-4.76	110.58	118.08
35	d	317	II0	C32-C30-C26	-4.76	112.77	126.58
29	F	203	WVN	C23-C25-C28	-4.75	111.66	118.94
29	B	853	WVN	C23-C20-C13	-4.74	113.88	127.20
35	a	312	II0	C37-C35-C33	-4.74	110.61	118.08
35	d	301	II0	C04-C10-C14	-4.73	115.95	122.63
35	a	316	II0	C31-C29-C25	-4.72	112.86	126.58
35	d	317	II0	C34-C36-C40	-4.72	111.70	118.94
26	A	824	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
35	a	312	II0	C34-C36-C40	-4.71	111.72	118.94
26	A	805	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
29	B	847	WVN	C31-C32-C36	-4.71	111.72	118.94
29	B	849	WVN	C23-C20-C13	-4.70	113.99	127.20
26	c	309	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
29	K	102	WVN	C23-C20-C13	-4.70	114.00	127.20
26	A	834	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
26	n	602	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
29	B	850	WVN	C19-C22-C26	-4.70	111.73	118.94
35	k	619	II0	C04-C10-C14	-4.69	116.01	122.63
26	A	816	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
29	F	203	WVN	C20-C13-C15	-4.68	110.12	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	316	WVN	C19-C22-C26	-4.68	111.76	118.94
26	k	607	CLA	C4A-NA-C1A	4.67	108.81	106.71
35	c	316	II0	C03-C09-C13	-4.67	116.04	122.63
29	B	850	WVN	C23-C25-C28	-4.67	111.77	118.94
29	J	101	WVN	C20-C13-C15	-4.67	110.16	121.46
29	M	101	WVN	C20-C13-C15	-4.67	110.16	121.46
35	i	313	II0	C32-C30-C26	-4.66	113.04	126.58
26	B	819	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
26	c	307	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
29	A	847	WVN	C16-C05-C09	-4.66	105.76	122.33
35	i	319	II0	C28-C26-C24	-4.66	107.61	116.84
35	j	614	II0	C27-C25-C23	-4.66	107.61	116.84
35	k	616	II0	C29-C31-C33	-4.66	108.69	123.22
35	h	311	II0	C27-C25-C23	-4.65	107.62	116.84
35	i	312	II0	C32-C30-C26	-4.65	113.07	126.58
36	s	401	KC2	CBC-CAC-C3C	-4.65	104.49	127.62
35	i	313	II0	C20-C14-C12	-4.64	105.75	114.36
35	k	615	II0	C20-C14-C12	-4.64	105.76	114.36
35	m	615	II0	C29-C31-C33	-4.64	108.74	123.22
35	m	619	II0	C03-C09-C13	-4.64	116.08	122.63
35	j	614	II0	C03-C09-C13	-4.63	116.09	122.63
35	l	302	II0	C04-C10-C14	-4.63	116.10	122.63
35	k	615	II0	C34-C36-C40	-4.62	111.85	118.94
29	h	309	WVN	C23-C20-C13	-4.62	114.22	127.20
35	l	302	II0	C03-C09-C13	-4.62	116.11	122.63
29	A	847	WVN	C23-C20-C13	-4.61	114.24	127.20
26	n	607	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
29	l	316	WVN	C31-C32-C36	-4.61	111.87	118.94
35	n	618	II0	C03-C09-C13	-4.61	116.13	122.63
35	a	312	II0	C29-C31-C33	-4.60	108.85	123.22
35	k	616	II0	C03-C09-C13	-4.60	116.13	122.63
26	B	819	CLA	CBC-CAC-C3C	4.58	125.07	112.43
35	b	315	II0	C31-C29-C25	-4.58	113.28	126.58
29	A	857	WVN	C33-C34-C37	-4.58	111.91	118.94
26	B	842	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
29	B	846	WVN	C20-C13-C15	-4.57	110.40	121.46
35	k	616	II0	C37-C35-C33	-4.57	110.88	118.08
35	b	315	II0	C28-C26-C24	-4.56	107.80	116.84
29	A	847	WVN	C31-C32-C36	-4.55	111.96	118.94
36	s	401	KC2	CMD-C2D-C1D	4.54	135.44	128.46
29	L	201	WVN	C14-C15-C13	-4.53	116.15	122.73
26	l	306	CLA	CMB-C2B-C3B	4.52	133.14	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	822	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
29	J	102	WVN	C31-C32-C36	-4.51	112.01	118.94
36	c	310	KC2	CHC-C1C-C2C	-4.51	117.93	124.98
26	l	309	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
35	i	312	II0	C29-C31-C33	-4.51	109.15	123.22
35	m	614	II0	C03-C09-C13	-4.51	116.27	122.63
35	l	302	II0	C28-C26-C24	-4.51	107.92	116.84
35	d	316	II0	C04-C10-C14	-4.50	116.27	122.63
26	A	841	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
36	s	401	KC2	C2C-C1C-NC	4.50	115.48	110.57
35	m	619	II0	C20-C14-C12	-4.49	106.03	114.36
29	B	849	WVN	C31-C32-C36	-4.49	112.05	118.94
35	k	619	II0	C34-C36-C40	-4.48	112.07	118.94
26	d	303	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
35	c	316	II0	C20-C14-C12	-4.47	106.08	114.36
35	m	614	II0	C34-C36-C40	-4.47	112.08	118.94
35	h	311	II0	C34-C36-C40	-4.47	112.09	118.94
35	i	319	II0	C03-C09-C13	-4.47	116.33	122.63
35	m	615	II0	C28-C26-C24	-4.47	107.99	116.84
26	A	803	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
35	n	618	II0	C27-C25-C23	-4.45	108.03	116.84
35	l	315	II0	C37-C35-C33	-4.44	111.08	118.08
29	l	303	WVN	C14-C15-C13	-4.44	116.28	122.73
26	R	201	CLA	CAA-C2A-C3A	-4.44	100.62	112.78
35	i	314	II0	C32-C30-C26	-4.43	113.73	126.58
33	j	618	DGD	O3G-C3G-C2G	-4.42	100.23	110.90
29	B	847	WVN	C06-C13-C15	-4.42	116.39	122.61
26	B	836	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
26	A	814	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
35	h	312	II0	C32-C30-C26	-4.41	113.76	126.58
35	k	620	II0	C04-C10-C14	-4.41	116.40	122.63
26	B	829	CLA	CMB-C2B-C3B	4.41	132.93	124.68
29	I	101	WVN	C02-C05-C09	-4.40	116.05	121.47
26	A	839	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
35	m	616	II0	C34-C36-C40	-4.40	112.19	118.94
29	s	407	WVN	C31-C32-C36	-4.40	112.19	118.94
26	A	825	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
36	s	401	KC2	CHC-C1C-C2C	-4.40	118.11	124.98
35	l	302	II0	C05-C03-C09	4.39	118.52	109.62
35	a	316	II0	C27-C25-C23	-4.39	108.15	116.84
28	s	409	LHG	O3-P-O6	-4.38	95.07	106.73
35	n	618	II0	C28-C26-C24	-4.38	108.16	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	315	II0	C12-C14-C10	-4.38	110.63	120.57
35	d	317	II0	C20-C14-C12	-4.38	106.24	114.36
35	k	619	II0	C37-C35-C33	-4.38	111.18	118.08
26	k	607	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
29	A	845	WVN	C20-C13-C15	-4.37	110.88	121.46
26	j	602	CLA	CMB-C2B-C3B	4.36	132.84	124.68
36	c	310	KC2	C3C-C2C-C1C	-4.36	103.25	106.49
29	A	845	WVN	C31-C32-C36	-4.36	112.25	118.94
35	h	311	II0	C37-C35-C33	-4.35	111.22	118.08
35	n	615	II0	C20-C14-C12	-4.34	106.31	114.36
26	h	313	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
35	i	319	II0	C12-C14-C10	-4.34	110.72	120.57
26	l	305	CLA	CMB-C2B-C3B	4.34	132.79	124.68
35	d	317	II0	C11-C13-C09	-4.33	110.74	120.57
35	n	615	II0	C28-C26-C24	-4.33	108.27	116.84
35	k	615	II0	C12-C14-C10	-4.33	110.75	120.57
26	s	406	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
29	A	848	WVN	C16-C05-C09	-4.32	106.97	122.33
35	c	313	II0	C29-C31-C33	-4.31	109.76	123.22
35	n	616	II0	C20-C14-C12	-4.30	106.39	114.36
26	A	851	CLA	CMB-C2B-C3B	4.30	132.72	124.68
29	B	847	WVN	C14-C15-C13	-4.30	116.49	122.73
29	l	316	WVN	C16-C05-C09	-4.30	107.05	122.33
29	B	850	WVN	C14-C15-C13	-4.29	116.50	122.73
35	k	619	II0	C27-C25-C23	-4.29	108.34	116.84
26	c	303	CLA	CMB-C2B-C1B	-4.29	121.88	128.46
35	j	614	II0	C28-C26-C24	-4.29	108.35	116.84
29	B	849	WVN	C20-C13-C15	-4.28	111.08	121.46
35	d	315	II0	C31-C29-C25	-4.28	114.14	126.58
26	B	802	CLA	CMB-C2B-C3B	4.28	132.69	124.68
29	B	847	WVN	C23-C20-C13	-4.28	115.18	127.20
26	i	303	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
26	B	827	CLA	CMB-C2B-C3B	4.28	132.68	124.68
26	A	802	CLA	CMB-C2B-C3B	4.28	132.68	124.68
29	B	849	WVN	C33-C34-C37	-4.27	112.39	118.94
26	b	305	CLA	CMB-C2B-C3B	4.27	132.67	124.68
35	a	316	II0	C04-C10-C14	-4.27	116.61	122.63
26	B	825	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
26	b	304	CLA	CMB-C2B-C3B	4.27	132.66	124.68
29	M	101	WVN	C31-C32-C36	-4.26	112.40	118.94
26	A	834	CLA	CMB-C2B-C3B	4.26	132.65	124.68
26	B	833	CLA	CMB-C2B-C3B	4.26	132.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	n	618	II0	C32-C30-C26	-4.25	114.24	126.58
29	A	857	WVN	C20-C13-C15	-4.25	111.17	121.46
35	l	302	II0	C31-C29-C25	-4.25	114.25	126.58
29	B	847	WVN	C16-C05-C09	-4.25	107.23	122.33
26	A	815	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
29	s	407	WVN	C14-C15-C13	-4.24	116.57	122.73
29	A	846	WVN	C23-C20-C13	-4.24	115.29	127.20
29	s	407	WVN	C19-C22-C26	-4.24	112.44	118.94
26	A	804	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
29	I	101	WVN	C16-C05-C09	-4.23	107.27	122.33
35	l	315	II0	C11-C13-C09	-4.23	110.96	120.57
26	m	604	CLA	CMB-C2B-C3B	4.23	132.60	124.68
26	B	817	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
26	B	815	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
26	l	310	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
35	m	614	II0	C31-C29-C25	-4.23	114.31	126.58
35	c	313	II0	C28-C26-C24	-4.22	108.48	116.84
35	m	616	II0	C20-C14-C12	-4.22	106.54	114.36
28	m	618	LHG	O4-P-O5	4.22	133.09	112.24
26	n	607	CLA	C4A-NA-C1A	4.21	108.60	106.71
28	A	849	LHG	O4-P-O5	4.21	133.06	112.24
26	A	813	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
28	J	105	LHG	O4-P-O5	4.21	133.05	112.24
36	c	310	KC2	CBC-CAC-C3C	-4.21	106.69	127.62
35	h	310	II0	C19-C13-C11	-4.21	106.56	114.36
29	h	309	WVN	C14-C15-C13	-4.21	116.62	122.73
26	i	305	CLA	C1D-ND-C4D	-4.20	103.35	106.33
26	a	302	CLA	CMB-C2B-C3B	4.20	132.53	124.68
28	n	619	LHG	O4-P-O5	4.20	133.00	112.24
28	i	317	LHG	O4-P-O5	4.20	132.99	112.24
28	c	317	LHG	O4-P-O5	4.20	132.99	112.24
35	i	319	II0	C32-C30-C26	-4.20	114.39	126.58
28	b	302	LHG	O4-P-O5	4.20	132.98	112.24
28	B	851	LHG	O4-P-O5	4.20	132.98	112.24
35	j	614	II0	C19-C13-C11	-4.19	106.58	114.36
28	A	844	LHG	O4-P-O5	4.19	132.97	112.24
28	b	318	LHG	O4-P-O5	4.19	132.96	112.24
28	L	208	LHG	O4-P-O5	4.19	132.95	112.24
26	B	812	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
26	h	302	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
29	L	205	WVN	C14-C15-C13	-4.18	116.66	122.73
28	c	320	LHG	O4-P-O5	4.18	132.92	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	805	CLA	CMB-C2B-C3B	4.18	132.50	124.68
28	A	843	LHG	O4-P-O5	4.18	132.90	112.24
28	L	207	LHG	O4-P-O5	4.18	132.90	112.24
28	A	855	LHG	O4-P-O5	4.18	132.89	112.24
26	m	609	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
32	A	854	SQD	C4-C3-C2	4.17	118.11	110.82
29	l	316	WVN	C10-C06-C13	4.17	116.91	110.48
35	m	619	II0	C28-C26-C24	-4.17	108.57	116.84
28	j	617	LHG	O4-P-O5	4.17	132.87	112.24
28	l	318	LHG	O4-P-O5	4.17	132.86	112.24
26	j	604	CLA	CMB-C2B-C3B	4.17	132.48	124.68
35	l	302	II0	C20-C14-C12	-4.17	106.63	114.36
26	B	807	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
29	h	309	WVN	C16-C05-C09	-4.16	107.52	122.33
26	B	818	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
35	b	314	II0	C28-C26-C24	-4.16	108.60	116.84
26	A	817	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
35	k	615	II0	C29-C31-C33	-4.16	110.24	123.22
35	l	315	II0	C32-C30-C26	-4.16	114.51	126.58
35	a	316	II0	C19-C13-C11	-4.15	106.66	114.36
35	k	619	II0	C28-C26-C24	-4.15	108.62	116.84
26	j	603	CLA	CMB-C2B-C3B	4.15	132.45	124.68
35	a	312	II0	C20-C14-C12	-4.15	106.67	114.36
26	h	305	CLA	CMB-C2B-C3B	4.15	132.44	124.68
26	A	840	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
35	m	614	II0	C28-C26-C24	-4.15	108.62	116.84
35	l	314	II0	C29-C31-C33	-4.15	110.28	123.22
35	J	104	II0	C19-C13-C11	-4.15	106.67	114.36
29	B	846	WVN	C06-C13-C15	-4.14	116.78	122.61
35	m	616	II0	C19-C13-C11	-4.14	106.68	114.36
35	b	315	II0	C11-C13-C09	-4.14	111.17	120.57
29	F	203	WVN	C23-C20-C13	-4.14	115.59	127.20
29	J	102	WVN	C23-C25-C28	-4.13	112.60	118.94
26	c	309	CLA	O2D-CGD-CBD	4.13	118.61	111.27
35	m	615	II0	C20-C14-C12	-4.13	106.71	114.36
26	n	602	CLA	CMB-C2B-C3B	4.12	132.39	124.68
35	k	615	II0	C06-C08-C12	4.12	115.94	110.30
26	B	804	CLA	CAC-C3C-C2C	-4.12	120.49	127.53
35	i	314	II0	C27-C25-C23	-4.12	108.69	116.84
35	d	301	II0	C28-C26-C24	-4.11	108.69	116.84
35	m	616	II0	C03-C09-C13	-4.11	116.82	122.63
32	A	854	SQD	O5-C5-C4	4.11	117.16	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	313	II0	C28-C26-C24	-4.11	108.70	116.84
26	n	608	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
35	l	315	II0	C04-C10-C14	-4.11	116.84	122.63
35	d	315	II0	C04-C10-C14	-4.10	116.84	122.63
26	d	305	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
26	A	827	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
35	k	615	II0	C04-C10-C14	-4.09	116.86	122.63
26	n	607	CLA	CMB-C2B-C3B	4.09	132.33	124.68
26	A	819	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
26	B	838	CLA	CMB-C2B-C1B	-4.09	122.19	128.46
29	I	101	WVN	C23-C20-C13	-4.08	115.74	127.20
33	B	844	DGD	O6D-C1D-O3G	-4.08	100.31	109.97
29	B	848	WVN	C20-C13-C15	-4.08	111.59	121.46
35	m	615	II0	C32-C30-C26	-4.07	114.75	126.58
35	i	313	II0	C31-C29-C25	-4.07	114.75	126.58
35	l	315	II0	C28-C26-C24	-4.07	108.78	116.84
26	A	829	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
35	j	615	II0	C29-C31-C33	-4.06	110.56	123.22
26	A	807	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
35	i	313	II0	C19-C13-C11	-4.05	106.84	114.36
29	J	101	WVN	C23-C20-C13	-4.05	115.82	127.20
26	B	814	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
35	n	616	II0	C28-C26-C24	-4.05	108.82	116.84
35	d	315	II0	C03-C09-C13	-4.05	116.92	122.63
35	m	619	II0	C37-C35-C33	-4.04	111.71	118.08
35	j	615	II0	C28-C26-C24	-4.04	108.83	116.84
35	k	619	II0	C32-C30-C26	-4.04	114.84	126.58
35	j	614	II0	C34-C36-C40	-4.04	112.74	118.94
29	J	102	WVN	C20-C13-C15	-4.04	111.68	121.46
35	j	614	II0	C32-C30-C26	-4.03	114.87	126.58
26	c	311	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
35	m	619	II0	C32-C30-C26	-4.03	114.89	126.58
26	l	307	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
29	B	853	WVN	C02-C05-C09	-4.02	116.52	121.47
29	i	315	WVN	C33-C34-C37	-4.02	112.77	118.94
26	d	313	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
35	k	619	II0	C20-C14-C12	-4.02	106.91	114.36
35	a	316	II0	C28-C26-C24	-4.02	108.88	116.84
26	a	304	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
29	L	201	WVN	C01-C02-C05	4.02	118.62	111.42
35	i	312	II0	C04-C10-C14	-4.02	116.96	122.63
29	h	309	WVN	C06-C13-C15	-4.01	116.97	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	826	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
35	k	615	II0	C28-C26-C24	-4.01	108.90	116.84
29	J	102	WVN	C16-C05-C09	-4.01	108.08	122.33
35	m	619	II0	C27-C25-C23	-4.01	108.91	116.84
29	B	846	WVN	C16-C05-C09	-4.00	108.08	122.33
29	A	845	WVN	C06-C13-C15	-4.00	116.97	122.61
26	n	609	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
29	L	205	WVN	C16-C05-C09	-4.00	108.10	122.33
35	n	615	II0	C34-C36-C40	-4.00	112.80	118.94
35	a	316	II0	C06-C04-C10	4.00	117.72	109.62
26	F	201	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
35	h	312	II0	C27-C25-C23	-3.99	108.93	116.84
26	k	603	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
35	i	316	II0	C04-C10-C14	-3.99	117.00	122.63
26	L	203	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
26	i	304	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
35	d	301	II0	C32-C30-C26	-3.98	115.02	126.58
35	n	615	II0	C32-C30-C26	-3.98	115.02	126.58
35	l	302	II0	C06-C04-C10	3.98	117.69	109.62
26	c	307	CLA	CMB-C2B-C3B	3.98	132.12	124.68
29	L	201	WVN	C16-C05-C09	-3.97	108.19	122.33
26	L	204	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
29	B	848	WVN	C16-C05-C09	-3.97	108.20	122.33
35	m	619	II0	C34-C36-C40	-3.97	112.85	118.94
26	i	305	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
35	a	314	II0	C28-C26-C24	-3.97	108.98	116.84
29	M	101	WVN	C06-C13-C15	-3.96	117.03	122.61
35	d	316	II0	C19-C13-C11	-3.96	107.01	114.36
26	j	607	CLA	C4A-NA-C1A	3.96	108.49	106.71
29	A	845	WVN	C16-C05-C09	-3.96	108.24	122.33
35	h	312	II0	C19-C13-C11	-3.96	107.02	114.36
35	n	616	II0	C32-C30-C26	-3.96	115.09	126.58
35	h	311	II0	C11-C13-C09	-3.95	111.59	120.57
26	B	842	CLA	CMB-C2B-C3B	3.95	132.06	124.68
26	A	821	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
26	A	805	CLA	CMB-C2B-C3B	3.95	132.06	124.68
35	a	314	II0	C32-C30-C26	-3.95	115.12	126.58
26	A	816	CLA	CMB-C2B-C3B	3.94	132.05	124.68
26	J	103	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
29	B	849	WVN	C16-C05-C09	-3.94	108.33	122.33
35	j	615	II0	C20-C14-C12	-3.94	107.06	114.36
29	I	101	WVN	C26-C29-C31	-3.94	110.94	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	616	II0	C20-C14-C12	-3.93	107.07	114.36
35	h	311	II0	C31-C29-C25	-3.93	115.17	126.58
26	a	307	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
35	a	313	II0	C28-C26-C24	-3.93	109.06	116.84
29	B	850	WVN	C16-C05-C09	-3.93	108.37	122.33
35	n	616	II0	C04-C10-C14	-3.92	117.10	122.63
35	i	319	II0	C05-C03-C09	3.92	117.56	109.62
36	c	310	KC2	C4B-C3B-C2B	-3.92	103.53	106.75
35	j	614	II0	C37-C35-C33	-3.91	111.91	118.08
35	i	314	II0	C28-C26-C24	-3.91	109.10	116.84
29	l	303	WVN	C16-C05-C09	-3.91	108.44	122.33
26	l	305	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
27	A	842	PQN	C14-C13-C15	-3.90	108.71	115.27
35	h	312	II0	C20-C14-C12	-3.90	107.13	114.36
26	B	813	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
26	B	804	CLA	CBC-CAC-C3C	3.89	123.17	112.43
26	B	819	CLA	CMB-C2B-C3B	3.89	131.96	124.68
35	c	313	II0	C32-C30-C26	-3.89	115.28	126.58
29	A	857	WVN	C16-C05-C09	-3.89	108.49	122.33
26	n	604	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
26	j	608	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
29	i	315	WVN	C16-C05-C09	-3.88	108.54	122.33
29	B	850	WVN	C33-C34-C37	-3.88	112.99	118.94
26	A	856	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
29	B	846	WVN	C28-C30-C33	-3.87	111.13	123.22
29	A	845	WVN	C21-C15-C14	-3.87	106.18	113.62
35	n	615	II0	C31-C29-C25	-3.87	115.35	126.58
26	A	812	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
29	R	200	WVN	C16-C05-C09	-3.87	108.58	122.33
26	B	806	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
35	a	312	II0	C28-C26-C24	-3.87	109.18	116.84
26	B	824	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
26	A	803	CLA	CMB-C2B-C3B	3.86	131.91	124.68
26	d	303	CLA	CMB-C2B-C3B	3.86	131.91	124.68
35	i	316	II0	C31-C29-C25	-3.86	115.37	126.58
35	k	615	II0	C31-C29-C25	-3.86	115.38	126.58
35	a	314	II0	C11-C13-C09	-3.85	111.84	120.57
29	B	848	WVN	C10-C06-C13	3.84	116.40	110.48
35	k	620	II0	C19-C13-C11	-3.84	107.23	114.36
35	d	317	II0	C29-C31-C33	-3.84	111.22	123.22
35	k	616	II0	C32-C30-C26	-3.84	115.42	126.58
35	b	314	II0	C32-C30-C26	-3.84	115.42	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	312	II0	C06-C04-C10	3.84	117.41	109.62
29	l	303	WVN	C06-C13-C15	-3.84	117.20	122.61
29	F	203	WVN	C16-C05-C09	-3.84	108.68	122.33
26	d	309	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
26	c	309	CLA	C2A-C1A-CHA	-3.84	117.15	123.86
26	k	607	CLA	CMB-C2B-C3B	3.83	131.85	124.68
26	m	612	CLA	CAA-C2A-C3A	-3.83	102.28	112.78
35	m	616	II0	C28-C26-C24	-3.83	109.25	116.84
26	A	810	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
29	B	850	WVN	C06-C13-C15	-3.83	117.22	122.61
26	A	824	CLA	CMB-C2B-C3B	3.83	131.84	124.68
32	A	854	SQD	C1-O5-C5	3.83	121.20	113.69
35	d	317	II0	C28-C26-C24	-3.82	109.27	116.84
35	d	316	II0	C28-C26-C24	-3.82	109.28	116.84
26	a	306	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
35	m	614	II0	C32-C30-C26	-3.82	115.50	126.58
26	A	825	CLA	CMB-C2B-C3B	3.81	131.81	124.68
35	k	620	II0	C28-C26-C24	-3.81	109.29	116.84
26	A	841	CLA	CMB-C2B-C3B	3.81	131.81	124.68
35	h	311	II0	C32-C30-C26	-3.81	115.52	126.58
35	a	316	II0	C32-C30-C26	-3.81	115.52	126.58
29	L	205	WVN	C06-C13-C15	-3.81	117.25	122.61
35	J	104	II0	C28-C26-C24	-3.81	109.30	116.84
35	i	312	II0	C19-C13-C11	-3.80	107.31	114.36
26	l	309	CLA	CMB-C2B-C3B	3.80	131.79	124.68
26	i	306	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
29	I	101	WVN	C28-C30-C33	-3.79	111.38	123.22
26	s	402	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
26	c	304	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
26	k	602	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
35	k	616	II0	C28-C26-C24	-3.79	109.33	116.84
32	A	854	SQD	O47-C7-C8	3.79	119.67	111.50
35	h	310	II0	C29-C31-C33	-3.79	111.39	123.22
35	l	302	II0	C32-C30-C26	-3.79	115.58	126.58
26	A	820	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
26	B	834	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
26	d	304	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
35	i	319	II0	C31-C29-C25	-3.77	115.62	126.58
29	B	853	WVN	C16-C05-C09	-3.77	108.92	122.33
35	b	315	II0	C29-C31-C33	-3.77	111.46	123.22
35	d	301	II0	C11-C13-C09	-3.77	112.02	120.57
26	A	827	CLA	CMB-C2B-C3B	3.77	131.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	314	II0	C29-C31-C33	-3.77	111.46	123.22
32	A	854	SQD	O7-S-C6	3.77	111.42	106.94
35	j	615	II0	C32-C30-C26	-3.77	115.65	126.58
26	B	821	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
35	i	316	II0	C28-C26-C24	-3.76	109.39	116.84
26	A	840	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
35	h	310	II0	C15-C03-C09	-3.76	104.50	110.47
29	A	848	WVN	C28-C30-C33	-3.76	111.49	123.22
33	B	844	DGD	O3G-C3G-C2G	-3.76	101.84	110.90
35	m	616	II0	C32-C30-C26	-3.75	115.68	126.58
35	l	302	II0	C19-C13-C11	-3.75	107.41	114.36
26	A	828	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
29	B	846	WVN	C21-C15-C14	-3.75	106.42	113.62
26	l	313	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
35	m	616	II0	C29-C31-C33	-3.74	111.54	123.22
26	B	825	CLA	CMB-C2B-C3B	3.74	131.68	124.68
26	m	602	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
35	n	618	II0	C29-C31-C33	-3.74	111.55	123.22
35	b	314	II0	C37-C35-C33	-3.74	112.19	118.08
35	l	314	II0	C28-C26-C24	-3.73	109.45	116.84
26	A	818	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
29	l	316	WVN	C06-C13-C15	-3.73	117.36	122.61
35	n	616	II0	C11-C13-C09	-3.73	112.11	120.57
35	i	312	II0	C11-C13-C09	-3.72	112.11	120.57
35	n	615	II0	C19-C13-C11	-3.72	107.46	114.36
35	d	315	II0	C28-C26-C24	-3.72	109.47	116.84
35	i	319	II0	C19-C13-C11	-3.72	107.46	114.36
29	J	102	WVN	C26-C29-C31	-3.72	111.61	123.22
29	B	846	WVN	C26-C29-C31	-3.72	111.61	123.22
35	h	312	II0	C31-C29-C25	-3.72	115.79	126.58
29	J	101	WVN	C16-C05-C09	-3.72	109.11	122.33
36	c	310	KC2	C2C-C1C-NC	3.71	114.63	110.57
35	i	314	II0	C19-C13-C11	-3.71	107.48	114.36
35	h	312	II0	C28-C26-C24	-3.70	109.51	116.84
26	i	311	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
35	i	316	II0	C11-C13-C09	-3.70	112.17	120.57
26	a	309	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
26	k	609	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
35	d	317	II0	C27-C25-C23	-3.70	109.52	116.84
35	j	614	II0	C20-C14-C12	-3.70	107.51	114.36
35	i	316	II0	C05-C03-C09	3.69	117.11	109.62
26	A	814	CLA	CMB-C2B-C3B	3.69	131.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	313	II0	C20-C14-C12	-3.69	107.52	114.36
26	s	403	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	b	306	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	h	304	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
29	L	201	WVN	C28-C30-C33	-3.69	111.72	123.22
35	i	312	II0	C28-C26-C24	-3.68	109.54	116.84
29	l	316	WVN	C28-C30-C33	-3.68	111.73	123.22
29	B	846	WVN	C23-C20-C13	-3.68	116.86	127.20
36	s	401	KC2	C4B-C3B-C2B	-3.68	103.73	106.75
35	J	104	II0	C20-C14-C12	-3.67	107.55	114.36
35	b	314	II0	C20-C14-C12	-3.67	107.56	114.36
26	A	826	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
35	k	620	II0	C31-C29-C25	-3.67	115.94	126.58
29	s	407	WVN	C16-C05-C09	-3.67	109.29	122.33
26	k	606	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
29	M	101	WVN	C16-C05-C09	-3.66	109.31	122.33
35	i	314	II0	C31-C29-C25	-3.66	115.95	126.58
26	i	307	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	A	836	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	A	851	CLA	C1B-CHB-C4A	-3.66	122.88	130.12
35	d	316	II0	C29-C31-C33	-3.66	111.81	123.22
26	B	820	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
33	j	618	DGD	C1E-O6E-C5E	3.65	120.86	113.69
32	A	854	SQD	O9-S-O7	-3.65	101.32	113.95
26	j	607	CLA	CMB-C2B-C3B	3.65	131.50	124.68
29	s	405	WVN	C16-C05-C09	-3.65	109.36	122.33
35	d	317	II0	C31-C29-C25	-3.64	116.00	126.58
35	a	313	II0	C20-C14-C12	-3.64	107.61	114.36
35	d	315	II0	C29-C31-C33	-3.64	111.86	123.22
26	c	303	CLA	CMB-C2B-C3B	3.64	131.48	124.68
26	h	313	CLA	CMB-C2B-C3B	3.64	131.48	124.68
26	s	406	CLA	CMB-C2B-C3B	3.63	131.48	124.68
29	h	309	WVN	C28-C30-C33	-3.63	111.88	123.22
26	A	852	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	B	817	CLA	CMB-C2B-C3B	3.63	131.47	124.68
26	j	607	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
35	i	314	II0	C20-C14-C12	-3.63	107.63	114.36
33	j	618	DGD	O6D-C1D-O3G	-3.63	101.38	109.97
26	k	614	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
26	B	809	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
26	i	308	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
29	A	848	WVN	C26-C29-C31	-3.62	111.91	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	315	II0	C27-C25-C23	-3.62	109.67	116.84
26	A	839	CLA	CMB-C2B-C3B	3.61	131.44	124.68
35	b	314	II0	C34-C36-C40	-3.61	113.40	118.94
32	A	854	SQD	O9-S-C6	3.61	111.23	106.94
29	A	846	WVN	C16-C05-C09	-3.61	109.49	122.33
26	c	308	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
26	B	818	CLA	CMB-C2B-C3B	3.61	131.42	124.68
26	n	613	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
29	L	201	WVN	C20-C13-C15	-3.60	112.73	121.46
26	c	302	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
35	j	615	II0	C31-C29-C25	-3.59	116.14	126.58
35	l	315	II0	C20-C14-C12	-3.59	107.70	114.36
26	B	831	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
26	B	822	CLA	CMB-C2B-C3B	3.59	131.39	124.68
26	a	311	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
35	l	314	II0	C27-C25-C23	-3.58	109.74	116.84
26	h	301	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
26	B	836	CLA	CMB-C2B-C3B	3.58	131.38	124.68
26	B	823	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
35	i	312	II0	C30-C32-C34	-3.57	112.07	123.22
29	K	102	WVN	C16-C05-C09	-3.57	109.62	122.33
35	k	620	II0	C27-C25-C23	-3.57	109.77	116.84
35	d	315	II0	C20-C14-C12	-3.57	107.74	114.36
35	a	316	II0	C05-C03-C09	3.57	116.86	109.62
26	R	201	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
26	a	303	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
35	a	313	II0	C32-C30-C26	-3.57	116.23	126.58
26	i	302	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
26	B	808	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
26	s	406	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
35	n	615	II0	C05-C03-C09	3.56	116.83	109.62
26	B	807	CLA	CMB-C2B-C3B	3.56	131.33	124.68
35	c	316	II0	C28-C26-C24	-3.55	109.80	116.84
26	L	202	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
35	h	312	II0	C29-C31-C33	-3.55	112.14	123.22
26	A	832	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
35	h	310	II0	C03-C09-C13	-3.55	117.62	122.63
35	b	314	II0	C11-C13-C09	-3.55	112.52	120.57
26	d	307	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	A	809	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	B	840	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
35	d	301	II0	C29-C31-C33	-3.54	112.16	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	308	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	j	613	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
26	k	608	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
26	k	604	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
26	i	310	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
35	h	310	II0	C27-C25-C23	-3.52	109.86	116.84
26	h	306	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	i	303	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	h	302	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	B	810	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	n	601	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	A	831	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
35	j	614	II0	C31-C29-C25	-3.52	116.36	126.58
26	d	313	CLA	CMB-C2B-C3B	3.52	131.26	124.68
26	d	302	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
29	B	853	WVN	C26-C29-C31	-3.51	112.26	123.22
26	b	313	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
26	B	815	CLA	CMB-C2B-C3B	3.51	131.24	124.68
29	K	102	WVN	C28-C30-C33	-3.51	112.27	123.22
26	b	307	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
26	k	601	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
26	c	312	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
35	j	615	II0	C27-C25-C23	-3.50	109.90	116.84
35	n	616	II0	C29-C31-C33	-3.50	112.29	123.22
26	n	606	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
26	l	307	CLA	CMB-C2B-C3B	3.50	131.23	124.68
26	k	603	CLA	CMB-C2B-C3B	3.50	131.23	124.68
26	A	804	CLA	CMB-C2B-C3B	3.50	131.22	124.68
35	k	620	II0	C20-C14-C12	-3.50	107.87	114.36
26	l	310	CLA	CMB-C2B-C3B	3.49	131.22	124.68
26	n	605	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
26	B	812	CLA	CMB-C2B-C3B	3.49	131.21	124.68
29	s	407	WVN	C06-C13-C15	-3.49	117.70	122.61
29	M	101	WVN	C26-C29-C31	-3.49	112.33	123.22
26	c	309	CLA	C4C-C3C-C2C	-3.48	101.82	106.90
26	Q	302	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
35	i	319	II0	C29-C31-C33	-3.48	112.35	123.22
26	j	605	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
26	j	609	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
26	l	308	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
26	s	406	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
26	A	813	CLA	CMB-C2B-C3B	3.48	131.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	605	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
27	B	843	PQN	C14-C13-C15	-3.48	109.42	115.27
35	i	316	II0	C15-C03-C09	-3.48	104.94	110.47
26	B	830	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
26	h	303	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
26	b	312	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
26	a	301	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
26	b	311	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
35	a	316	II0	C20-C14-C12	-3.47	107.93	114.36
26	m	605	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
26	A	817	CLA	CMB-C2B-C3B	3.47	131.16	124.68
26	B	838	CLA	CMB-C2B-C3B	3.46	131.16	124.68
26	m	602	CLA	CMB-C2B-C3B	3.46	131.16	124.68
35	k	620	II0	C29-C31-C33	-3.46	112.41	123.22
26	A	823	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
26	F	202	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
35	d	316	II0	C31-C29-C25	-3.45	116.56	126.58
26	s	403	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
35	n	616	II0	C06-C04-C10	3.45	116.61	109.62
26	B	839	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
29	M	101	WVN	C01-C02-C11	-3.45	108.34	112.70
26	c	309	CLA	CHC-C1C-C2C	-3.45	117.19	126.72
29	l	303	WVN	C26-C29-C31	-3.45	112.46	123.22
35	k	616	II0	C30-C32-C34	-3.45	112.46	123.22
26	m	609	CLA	CMB-C2B-C3B	3.45	131.12	124.68
26	i	302	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
35	k	620	II0	C11-C13-C09	-3.44	112.76	120.57
29	B	846	WVN	C14-C15-C13	-3.44	117.74	122.73
26	b	303	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
26	B	828	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
26	l	311	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
35	c	316	II0	C30-C32-C34	-3.44	112.49	123.22
26	d	305	CLA	CMB-C2B-C3B	3.44	131.11	124.68
26	d	318	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	A	815	CLA	CMB-C2B-C3B	3.42	131.09	124.68
26	B	841	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
26	j	601	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
29	L	201	WVN	C02-C05-C09	-3.42	117.26	121.47
35	a	316	II0	C29-C31-C33	-3.42	112.55	123.22
26	m	606	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
26	c	311	CLA	CMB-C2B-C3B	3.41	131.07	124.68
26	A	819	CLA	CMB-C2B-C3B	3.41	131.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	615	II0	C11-C13-C09	-3.41	112.83	120.57
26	a	304	CLA	CMB-C2B-C3B	3.41	131.06	124.68
29	L	201	WVN	C26-C29-C31	-3.41	112.58	123.22
26	j	607	CLA	C2D-C1D-ND	-3.41	107.59	110.10
29	s	407	WVN	C28-C30-C33	-3.41	112.58	123.22
26	n	613	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
26	B	826	CLA	CMB-C2B-C3B	3.40	131.04	124.68
26	m	603	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
35	J	104	II0	C11-C13-C09	-3.40	112.85	120.57
35	k	619	II0	C31-C29-C25	-3.40	116.71	126.58
26	A	830	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
35	a	313	II0	C27-C25-C23	-3.40	110.11	116.84
35	i	316	II0	C29-C31-C33	-3.40	112.62	123.22
26	A	807	CLA	CMB-C2B-C3B	3.40	131.03	124.68
36	s	401	KC2	O2D-CGD-O1D	-3.39	117.20	123.84
26	A	806	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	i	304	CLA	CMB-C2B-C3B	3.39	131.03	124.68
26	n	604	CLA	CMB-C2B-C3B	3.39	131.03	124.68
26	L	206	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	j	612	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
35	h	312	II0	C03-C09-C13	-3.39	117.85	122.63
35	j	614	II0	C29-C31-C33	-3.39	112.64	123.22
35	m	619	II0	C31-C29-C25	-3.39	116.75	126.58
35	n	618	II0	C31-C29-C25	-3.39	116.75	126.58
26	B	808	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
26	n	607	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
26	b	309	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
29	i	315	WVN	C26-C29-C31	-3.38	112.67	123.22
29	L	205	WVN	C26-C29-C31	-3.38	112.67	123.22
26	i	301	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
26	l	304	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
26	j	610	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
35	l	314	II0	C30-C32-C34	-3.37	112.70	123.22
26	m	610	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
26	n	609	CLA	CMB-C2B-C3B	3.37	130.98	124.68
26	h	308	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
35	c	313	II0	C11-C13-C09	-3.37	112.92	120.57
26	m	601	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
29	J	101	WVN	C28-C30-C33	-3.36	112.72	123.22
35	m	614	II0	C19-C13-C11	-3.36	108.12	114.36
29	A	846	WVN	C28-C30-C33	-3.36	112.72	123.22
26	a	305	CLA	CMB-C2B-C1B	-3.36	123.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	811	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
26	m	612	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
26	a	308	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
26	k	610	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
26	k	602	CLA	CMB-C2B-C3B	3.36	130.96	124.68
26	L	203	CLA	CMB-C2B-C3B	3.35	130.95	124.68
35	d	315	II0	C30-C32-C34	-3.35	112.75	123.22
26	c	301	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
26	A	838	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
35	n	616	II0	C30-C32-C34	-3.35	112.77	123.22
26	A	837	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
26	n	610	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
35	d	316	II0	C30-C32-C34	-3.35	112.77	123.22
29	l	303	WVN	C28-C30-C33	-3.35	112.77	123.22
26	A	840	CLA	CMB-C2B-C3B	3.34	130.94	124.68
35	k	619	II0	C29-C31-C33	-3.34	112.78	123.22
35	l	314	II0	C11-C13-C09	-3.34	112.98	120.57
35	m	619	II0	C19-C13-C11	-3.34	108.17	114.36
26	A	822	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
26	c	305	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
26	j	606	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
26	B	816	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
26	B	840	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
26	A	821	CLA	CMB-C2B-C3B	3.33	130.90	124.68
26	d	310	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
29	A	847	WVN	C28-C30-C33	-3.32	112.85	123.22
26	i	302	CLA	O2D-CGD-CBD	3.32	117.17	111.27
35	h	310	II0	C05-C03-C09	3.32	116.35	109.62
35	m	616	II0	C30-C32-C34	-3.32	112.85	123.22
26	b	310	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
29	B	847	WVN	C28-C30-C33	-3.32	112.87	123.22
26	A	811	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
29	M	101	WVN	C28-C30-C33	-3.31	112.87	123.22
35	l	314	II0	C12-C14-C10	-3.31	113.05	120.57
35	l	314	II0	C31-C29-C25	-3.31	116.97	126.58
26	B	804	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
35	i	312	II0	C20-C14-C12	-3.31	108.23	114.36
26	B	814	CLA	CMB-C2B-C3B	3.31	130.86	124.68
35	d	317	II0	C06-C04-C10	3.31	116.32	109.62
35	J	104	II0	C29-C31-C33	-3.30	112.91	123.22
35	a	312	II0	C27-C25-C23	-3.30	110.31	116.84
26	K	101	CLA	CMB-C2B-C1B	-3.30	123.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	856	CLA	CMB-C2B-C3B	3.30	130.85	124.68
26	B	823	CLA	CMB-C2B-C3B	3.30	130.85	124.68
35	m	619	II0	C06-C04-C10	3.30	116.30	109.62
26	d	313	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
35	b	315	II0	C19-C13-C11	-3.30	108.25	114.36
29	I	101	WVN	C01-C02-C05	3.29	117.32	111.42
26	j	612	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
26	s	402	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
28	A	844	LHG	O8-C23-C24	3.29	120.01	111.38
35	m	615	II0	C19-C13-C11	-3.29	108.26	114.36
35	c	316	II0	C29-C31-C33	-3.29	112.96	123.22
26	j	607	CLA	CMC-C2C-C1C	-3.28	120.04	125.04
35	i	316	II0	C19-C13-C11	-3.28	108.28	114.36
26	A	836	CLA	CMB-C2B-C3B	3.28	130.82	124.68
26	n	603	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
35	h	311	II0	C12-C14-C10	-3.27	113.14	120.57
26	A	816	CLA	CBA-CAA-C2A	3.27	123.52	113.86
35	h	311	II0	C20-C14-C12	-3.27	108.29	114.36
26	L	204	CLA	CMB-C2B-C3B	3.27	130.79	124.68
35	b	314	II0	C30-C32-C34	-3.27	113.02	123.22
26	m	608	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
26	a	307	CLA	CMB-C2B-C3B	3.27	130.79	124.68
29	B	847	WVN	C10-C06-C13	3.26	115.50	110.48
29	L	205	WVN	C28-C30-C33	-3.26	113.05	123.22
35	k	615	II0	C11-C13-C09	-3.26	113.17	120.57
35	h	310	II0	C31-C29-C25	-3.26	117.12	126.58
26	A	812	CLA	CMB-C2B-C3B	3.26	130.77	124.68
26	B	838	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
26	B	813	CLA	CMB-C2B-C3B	3.25	130.76	124.68
26	c	306	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
35	i	313	II0	C29-C31-C33	-3.25	113.08	123.22
26	h	307	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
26	n	608	CLA	CMB-C2B-C3B	3.25	130.75	124.68
26	A	810	CLA	CMB-C2B-C3B	3.25	130.75	124.68
26	A	828	CLA	CMB-C2B-C3B	3.25	130.75	124.68
35	i	316	II0	C20-C14-C12	-3.24	108.34	114.36
26	d	309	CLA	CAA-C2A-C3A	-3.24	108.54	116.10
26	B	806	CLA	CMB-C2B-C3B	3.24	130.74	124.68
26	j	608	CLA	CMB-C2B-C3B	3.24	130.74	124.68
35	m	614	II0	C20-C14-C12	-3.24	108.36	114.36
29	B	848	WVN	C26-C29-C31	-3.23	113.13	123.22
29	A	857	WVN	C28-C30-C33	-3.23	113.15	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	853	WVN	C21-C15-C14	-3.23	107.42	113.62
26	k	607	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
35	d	301	II0	C27-C25-C23	-3.22	110.46	116.84
29	s	405	WVN	C26-C29-C31	-3.22	113.18	123.22
35	i	316	II0	C30-C32-C34	-3.21	113.18	123.22
26	m	613	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
26	B	821	CLA	CMB-C2B-C3B	3.21	130.68	124.68
26	A	832	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
26	m	607	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
26	n	613	CLA	CMB-C2B-C3B	3.20	130.67	124.68
36	c	310	KC2	CAA-CBA-CGA	-3.20	110.81	127.26
26	B	824	CLA	CMB-C2B-C3B	3.20	130.67	124.68
26	i	310	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
35	m	614	II0	C05-C03-C09	3.20	116.10	109.62
26	B	801	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
26	J	103	CLA	CMB-C2B-C3B	3.20	130.66	124.68
26	d	309	CLA	CMB-C2B-C3B	3.19	130.65	124.68
29	s	405	WVN	C28-C30-C33	-3.19	113.26	123.22
35	d	317	II0	C30-C32-C34	-3.19	113.26	123.22
35	i	319	II0	C06-C08-C12	3.19	114.67	110.30
29	A	846	WVN	C26-C29-C31	-3.19	113.27	123.22
26	i	311	CLA	CMB-C2B-C3B	3.19	130.64	124.68
35	c	316	II0	C27-C25-C23	-3.19	110.53	116.84
26	a	309	CLA	CMB-C2B-C3B	3.19	130.64	124.68
26	A	818	CLA	CMB-C2B-C3B	3.18	130.64	124.68
26	m	610	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
35	c	313	II0	C31-C29-C25	-3.18	117.34	126.58
26	B	805	CLA	CHB-C4A-NA	3.18	128.91	124.51
26	B	802	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
29	B	847	WVN	C26-C29-C31	-3.18	113.29	123.22
35	J	104	II0	C30-C32-C34	-3.18	113.30	123.22
26	B	803	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
35	h	312	II0	C05-C03-C09	3.17	116.05	109.62
35	j	614	II0	C05-C07-C11	3.17	114.65	110.30
35	b	314	II0	C29-C31-C33	-3.17	113.33	123.22
29	A	848	WVN	C01-C02-C11	-3.17	108.70	112.70
26	d	306	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
26	c	304	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
35	n	618	II0	C20-C14-C12	-3.16	108.50	114.36
26	a	310	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
26	l	301	CLA	CMB-C2B-C1B	-3.15	123.61	128.46
35	m	615	II0	C30-C32-C34	-3.15	113.39	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	619	II0	C19-C13-C11	-3.15	108.52	114.36
26	B	834	CLA	CMB-C2B-C3B	3.15	130.56	124.68
26	B	808	CLA	CMB-C2B-C3B	3.14	130.56	124.68
35	m	615	II0	C27-C25-C23	-3.14	110.61	116.84
35	b	314	II0	C19-C13-C11	-3.14	108.53	114.36
29	R	200	WVN	C26-C29-C31	-3.14	113.41	123.22
35	i	314	II0	C30-C32-C34	-3.14	113.42	123.22
35	a	314	II0	C20-C14-C12	-3.14	108.54	114.36
35	m	619	II0	C29-C31-C33	-3.14	113.42	123.22
26	c	304	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	j	610	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
26	c	302	CLA	CMB-C2B-C3B	3.13	130.54	124.68
35	l	314	II0	C06-C08-C12	3.13	114.59	110.30
36	c	310	KC2	CAA-C2A-C1A	-3.13	110.35	124.75
26	b	304	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
35	j	615	II0	C06-C04-C10	3.13	115.96	109.62
26	l	313	CLA	CMB-C2B-C3B	3.13	130.53	124.68
35	a	312	II0	C31-C29-C25	-3.13	117.50	126.58
26	k	609	CLA	CMB-C2B-C3B	3.13	130.53	124.68
35	k	619	II0	C11-C13-C09	-3.13	113.47	120.57
29	A	848	WVN	C24-C22-C19	-3.13	113.15	118.08
26	n	610	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
26	B	841	CLA	CHB-C4A-NA	3.12	128.83	124.51
26	k	614	CLA	CMB-C2B-C3B	3.12	130.52	124.68
29	B	850	WVN	C01-C02-C05	3.12	117.01	111.42
35	i	313	II0	C30-C32-C34	-3.12	113.48	123.22
35	d	301	II0	C20-C14-C12	-3.12	108.58	114.36
29	B	853	WVN	C28-C30-C33	-3.12	113.48	123.22
26	h	304	CLA	CMB-C2B-C3B	3.12	130.51	124.68
26	A	825	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
26	k	604	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
35	d	316	II0	C05-C03-C09	3.11	115.93	109.62
35	l	314	II0	C20-C14-C12	-3.11	108.59	114.36
29	A	857	WVN	C26-C29-C31	-3.11	113.51	123.22
35	i	316	II0	C05-C07-C11	3.11	114.56	110.30
35	a	314	II0	C29-C31-C33	-3.11	113.51	123.22
26	j	607	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
26	d	304	CLA	CMB-C2B-C3B	3.11	130.50	124.68
29	R	200	WVN	C28-C30-C33	-3.11	113.52	123.22
30	A	850	LMU	C2'-C3'-C4'	3.11	116.78	109.68
32	A	854	SQD	C44-O6-C1	3.11	119.81	113.74
35	l	314	II0	C19-C13-C11	-3.11	108.60	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	606	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	B	820	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	c	308	CLA	CMB-C2B-C3B	3.10	130.47	124.68
35	l	302	II0	C29-C31-C33	-3.10	113.55	123.22
26	m	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
29	B	847	WVN	C21-C15-C14	-3.10	107.67	113.62
26	d	306	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
26	i	306	CLA	CMB-C2B-C3B	3.09	130.47	124.68
35	k	616	II0	C06-C04-C10	3.09	115.89	109.62
29	l	316	WVN	C01-C02-C05	3.09	116.96	111.42
26	j	613	CLA	CMB-C2B-C3B	3.09	130.46	124.68
26	j	607	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
26	F	201	CLA	CMB-C2B-C3B	3.09	130.46	124.68
26	B	835	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
35	m	614	II0	C29-C31-C33	-3.09	113.57	123.22
35	i	314	II0	C05-C03-C09	3.09	115.88	109.62
35	k	615	II0	C30-C32-C34	-3.09	113.57	123.22
29	K	102	WVN	C21-C15-C14	-3.09	107.68	113.62
35	n	615	II0	C11-C13-C09	-3.09	113.56	120.57
29	i	315	WVN	C10-C06-C13	3.09	115.24	110.48
26	b	306	CLA	CMB-C2B-C3B	3.09	130.46	124.68
35	d	301	II0	C37-C35-C33	-3.09	113.21	118.08
26	B	829	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
33	B	844	DGD	O5D-C6D-C5D	-3.08	103.34	109.05
26	b	308	CLA	CMB-C2B-C3B	3.08	130.45	124.68
29	L	201	WVN	C21-C15-C14	-3.08	107.69	113.62
29	B	846	WVN	C40-C39-C36	-3.08	117.16	123.47
26	s	403	CLA	CMB-C2B-C3B	3.08	130.44	124.68
35	m	616	II0	C33-C35-C39	-3.08	114.22	118.94
29	J	101	WVN	C21-C15-C14	-3.08	107.70	113.62
26	B	831	CLA	CMB-C2B-C3B	3.08	130.43	124.68
26	B	822	CLA	CHB-C4A-NA	3.08	128.77	124.51
26	c	306	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
26	j	601	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
26	R	201	CLA	CMB-C2B-C3B	3.07	130.42	124.68
26	n	606	CLA	CMB-C2B-C3B	3.07	130.42	124.68
35	m	615	II0	C06-C04-C10	3.07	115.84	109.62
26	A	808	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
26	m	607	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	A	833	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
35	a	314	II0	C12-C14-C10	-3.06	113.62	120.57
35	c	313	II0	C27-C25-C23	-3.06	110.78	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	845	WVN	C01-C02-C05	3.06	116.90	111.42
35	h	311	II0	C29-C31-C33	-3.06	113.67	123.22
26	B	823	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
26	n	604	CLA	CBA-CAA-C2A	3.06	122.89	113.86
26	a	311	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	i	308	CLA	CMB-C2B-C3B	3.05	130.39	124.68
29	A	845	WVN	C14-C15-C13	-3.05	118.30	122.73
25	A	801	CL0	CHA-C1A-NA	-3.05	119.41	126.40
26	d	302	CLA	CMB-C2B-C3B	3.05	130.39	124.68
26	i	307	CLA	CMB-C2B-C3B	3.05	130.38	124.68
26	k	607	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
26	s	402	CLA	CMB-C2B-C3B	3.05	130.38	124.68
26	R	201	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
26	A	820	CLA	CMB-C2B-C3B	3.04	130.37	124.68
29	R	200	WVN	C20-C13-C15	-3.04	114.09	121.46
26	B	827	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
35	a	313	II0	C30-C32-C34	-3.04	113.73	123.22
26	A	826	CLA	CMB-C2B-C3B	3.04	130.37	124.68
26	d	308	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
26	k	604	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
35	d	316	II0	C20-C14-C12	-3.04	108.73	114.36
26	n	604	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
26	i	304	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	h	309	WVN	C26-C29-C31	-3.03	113.75	123.22
26	A	835	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
26	A	831	CLA	CMB-C2B-C3B	3.03	130.35	124.68
26	B	802	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
26	j	609	CLA	CMB-C2B-C3B	3.03	130.34	124.68
26	i	305	CLA	CMB-C2B-C3B	3.03	130.34	124.68
26	B	810	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	b	313	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	k	608	CLA	CMB-C2B-C3B	3.02	130.32	124.68
26	A	852	CLA	CMB-C2B-C3B	3.02	130.32	124.68
35	k	620	II0	C42-C41-C39	-3.02	117.30	123.47
29	B	853	WVN	C01-C02-C05	3.02	116.82	111.42
26	s	402	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
26	A	807	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
26	d	313	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
26	A	832	CLA	CMB-C2B-C3B	3.01	130.31	124.68
35	m	614	II0	C30-C32-C34	-3.01	113.83	123.22
26	i	301	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
35	h	312	II0	C12-C14-C10	-3.00	113.75	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	301	II0	C30-C32-C34	-3.00	113.85	123.22
29	A	845	WVN	C28-C30-C33	-3.00	113.85	123.22
35	c	313	II0	C30-C32-C34	-3.00	113.85	123.22
26	n	606	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	k	609	CLA	CHB-C4A-NA	3.00	128.66	124.51
26	B	810	CLA	CMB-C2B-C3B	3.00	130.29	124.68
26	k	610	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
26	a	306	CLA	CMB-C2B-C3B	3.00	130.29	124.68
35	m	614	II0	C11-C13-C09	-3.00	113.77	120.57
35	a	314	II0	C06-C08-C12	3.00	114.41	110.30
26	A	813	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
29	B	850	WVN	C26-C29-C31	-2.99	113.87	123.22
26	s	408	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
26	i	308	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
26	d	302	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
29	K	102	WVN	C26-C29-C31	-2.99	113.88	123.22
29	A	848	WVN	C01-C02-C05	2.99	116.78	111.42
26	A	818	CLA	CHB-C4A-NA	2.99	128.65	124.51
26	j	602	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
26	d	307	CLA	CMB-C2B-C3B	2.99	130.27	124.68
26	n	601	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
29	J	101	WVN	C26-C29-C31	-2.99	113.90	123.22
35	n	616	II0	C19-C13-C11	-2.99	108.82	114.36
35	a	314	II0	C37-C35-C33	-2.98	113.38	118.08
26	A	810	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
26	m	606	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	k	605	CLA	CMB-C2B-C3B	2.98	130.26	124.68
26	B	832	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	l	311	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
27	A	842	PQN	C2M-C2-C3	-2.98	119.54	124.40
35	n	615	II0	C29-C31-C33	-2.97	113.94	123.22
35	k	615	II0	C08-C12-C14	2.97	117.78	111.85
35	m	616	II0	C37-C35-C33	-2.97	113.39	118.08
26	m	601	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	i	302	CLA	CMB-C2B-C3B	2.97	130.24	124.68
35	a	316	II0	C30-C32-C34	-2.97	113.94	123.22
26	h	306	CLA	CMB-C2B-C3B	2.97	130.24	124.68
35	j	614	II0	C42-C41-C39	-2.97	117.39	123.47
26	B	835	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
26	k	601	CLA	CMB-C2B-C3B	2.97	130.23	124.68
35	a	312	II0	C19-C13-C11	-2.97	108.86	114.36
35	c	316	II0	C19-C13-C11	-2.97	108.86	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	804	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
26	i	310	CLA	CMB-C2B-C3B	2.96	130.22	124.68
35	k	620	II0	C30-C32-C34	-2.96	113.97	123.22
26	A	818	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
26	n	604	CLA	CHB-C4A-NA	2.96	128.61	124.51
26	c	301	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
26	a	303	CLA	CHB-C4A-NA	2.96	128.60	124.51
26	a	306	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
26	k	603	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
29	B	848	WVN	C28-C30-C33	-2.96	113.99	123.22
29	s	407	WVN	C10-C06-C13	2.95	115.03	110.48
26	j	605	CLA	CHB-C4A-NA	2.95	128.60	124.51
26	B	841	CLA	CMB-C2B-C3B	2.95	130.21	124.68
35	n	618	II0	C19-C13-C11	-2.95	108.89	114.36
29	l	316	WVN	C26-C29-C31	-2.95	114.00	123.22
26	R	201	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	A	857	WVN	C21-C15-C14	-2.95	107.95	113.62
26	A	818	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
26	A	823	CLA	CMB-C2B-C3B	2.95	130.19	124.68
26	A	809	CLA	CMB-C2B-C3B	2.95	130.19	124.68
35	j	615	II0	C30-C32-C34	-2.95	114.03	123.22
35	a	313	II0	C12-C14-C10	-2.95	113.89	120.57
26	k	601	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
26	d	303	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
26	B	829	CLA	CAA-C2A-C3A	-2.94	104.71	112.78
35	h	311	II0	C19-C13-C11	-2.94	108.90	114.36
35	a	312	II0	C30-C32-C34	-2.94	114.03	123.22
26	a	303	CLA	CMB-C2B-C3B	2.94	130.19	124.68
35	c	313	II0	C19-C13-C11	-2.94	108.90	114.36
35	a	314	II0	C30-C32-C34	-2.94	114.03	123.22
34	b	319	LMG	O6-C1-O1	-2.94	103.01	109.97
26	b	307	CLA	CMB-C2B-C3B	2.94	130.17	124.68
35	d	316	II0	C06-C04-C10	2.94	115.57	109.62
26	j	605	CLA	CMB-C2B-C3B	2.94	130.17	124.68
26	n	605	CLA	CMB-C2B-C3B	2.94	130.17	124.68
26	m	603	CLA	CMB-C2B-C3B	2.93	130.17	124.68
26	k	606	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
26	A	856	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	l	308	CLA	CMB-C2B-C3B	2.93	130.16	124.68
26	Q	302	CLA	CMB-C2B-C3B	2.93	130.16	124.68
26	n	601	CLA	CMB-C2B-C3B	2.93	130.16	124.68
26	A	806	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	615	II0	C06-C04-C10	2.93	115.55	109.62
35	a	316	II0	C15-C03-C09	-2.93	105.82	110.47
26	L	203	CLA	CHB-C4A-NA	2.92	128.55	124.51
28	L	207	LHG	O8-C23-C24	2.92	121.08	111.91
26	a	308	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
26	c	306	CLA	CMB-C2B-C3B	2.92	130.15	124.68
26	A	824	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	c	309	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	b	306	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	j	608	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
36	c	310	KC2	CHD-C4C-NC	2.92	128.63	124.20
26	a	301	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
26	n	602	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
35	a	314	II0	C19-C13-C11	-2.92	108.95	114.36
26	A	852	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
26	n	603	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
29	A	845	WVN	C26-C29-C31	-2.91	114.12	123.22
26	A	830	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
26	k	614	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	L	202	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
35	m	615	II0	C31-C29-C25	-2.91	118.14	126.58
26	B	813	CLA	CHB-C4A-NA	2.91	128.53	124.51
26	b	309	CLA	CMB-C2B-C3B	2.90	130.10	124.68
26	A	802	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
26	c	307	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
26	h	303	CLA	CMB-C2B-C3B	2.90	130.10	124.68
26	n	603	CLA	CMB-C2B-C3B	2.90	130.10	124.68
26	l	309	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
36	l	312	KC2	C3C-C2C-C1C	2.89	108.63	106.49
26	j	613	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
26	m	605	CLA	CMB-C2B-C3B	2.89	130.09	124.68
35	h	312	II0	C30-C32-C34	-2.89	114.19	123.22
26	B	830	CLA	CMB-C2B-C3B	2.89	130.09	124.68
26	k	602	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	B	807	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	B	833	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	A	831	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	B	808	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	a	301	CLA	CMB-C2B-C3B	2.89	130.08	124.68
26	A	834	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	d	308	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	B	817	CLA	C1B-CHB-C4A	-2.89	124.40	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	836	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	B	819	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	l	307	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
29	A	845	WVN	C02-C05-C09	-2.88	117.92	121.47
26	A	822	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	A	816	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
26	A	827	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
26	l	304	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	k	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	L	206	CLA	CMB-C2B-C3B	2.88	130.07	124.68
26	A	819	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	l	316	WVN	C33-C34-C37	-2.88	114.53	118.94
26	L	202	CLA	CMB-C2B-C3B	2.88	130.06	124.68
26	B	820	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
26	R	201	CLA	CBA-CAA-C2A	2.88	122.35	113.86
26	l	308	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	l	307	CLA	CHB-C4A-NA	2.87	128.48	124.51
26	B	840	CLA	CMB-C2B-C3B	2.87	130.05	124.68
26	c	302	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	B	820	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	i	315	WVN	C28-C30-C33	-2.87	114.27	123.22
35	m	614	II0	C12-C14-C10	-2.87	114.06	120.57
35	m	619	II0	C05-C03-C09	2.87	115.43	109.62
26	m	613	CLA	CHB-C4A-NA	2.87	128.48	124.51
26	h	307	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
26	m	612	CLA	CMB-C2B-C3B	2.87	130.04	124.68
26	d	318	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	B	808	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
26	l	311	CLA	CMB-C2B-C3B	2.87	130.04	124.68
26	b	303	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
26	c	305	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
26	B	837	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
26	A	812	CLA	CHB-C4A-NA	2.86	128.47	124.51
26	c	304	CLA	CHB-C4A-NA	2.86	128.47	124.51
26	l	310	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
26	d	318	CLA	CMB-C2B-C3B	2.86	130.03	124.68
35	d	301	II0	C06-C04-C10	2.86	115.42	109.62
26	a	309	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	h	304	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	d	309	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	m	607	CLA	CMB-C2B-C3B	2.86	130.03	124.68
29	A	847	WVN	C21-C15-C14	-2.86	108.12	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	308	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	m	605	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	K	101	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	c	312	CLA	CMB-C2B-C3B	2.86	130.02	124.68
26	B	835	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	B	850	WVN	C28-C30-C33	-2.85	114.31	123.22
26	B	818	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	a	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	A	808	CLA	CHB-C4A-NA	2.85	128.46	124.51
35	j	615	II0	C19-C13-C11	-2.85	109.07	114.36
26	d	310	CLA	CMB-C2B-C3B	2.85	130.01	124.68
26	B	822	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	m	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	l	306	CLA	CHB-C4A-NA	2.85	128.46	124.51
26	k	607	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	B	812	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	B	808	CLA	O2A-CGA-O1A	-2.85	116.40	123.59
26	A	815	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	B	836	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	n	607	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
26	A	804	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	L	204	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	a	305	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	h	301	CLA	CMB-C2B-C3B	2.84	129.99	124.68
26	d	313	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	A	835	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	A	813	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	A	841	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	l	316	WVN	C21-C15-C14	-2.84	108.17	113.62
26	A	826	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	A	823	CLA	CHB-C4A-NA	2.84	128.43	124.51
26	m	608	CLA	CMB-C2B-C3B	2.84	129.98	124.68
26	A	816	CLA	CHB-C4A-NA	2.84	128.43	124.51
28	j	617	LHG	O8-C23-C24	2.84	120.81	111.91
35	c	316	II0	C06-C04-C10	2.83	115.36	109.62
26	b	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	m	612	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
35	k	619	II0	C30-C32-C34	-2.83	114.37	123.22
26	J	103	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	b	305	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	m	613	CLA	CMB-C2B-C3B	2.83	129.98	124.68
35	d	301	II0	C19-C13-C11	-2.83	109.11	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Q	301	LMG	O6-C1-O1	-2.83	103.27	109.97
26	A	825	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
26	n	606	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	k	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
35	m	616	II0	C06-C04-C10	2.83	115.36	109.62
26	m	610	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	A	827	CLA	CHD-C1D-ND	-2.83	121.85	124.45
35	k	615	II0	C19-C13-C11	-2.83	109.11	114.36
26	A	823	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
35	n	618	II0	C06-C04-C10	2.83	115.35	109.62
26	A	821	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	b	309	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	l	301	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	A	814	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	b	313	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	k	614	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	h	307	CLA	CHB-C4A-NA	2.83	128.42	124.51
35	j	614	II0	C30-C32-C34	-2.83	114.40	123.22
35	j	614	II0	C06-C04-C10	2.83	115.35	109.62
26	c	312	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
26	A	830	CLA	CMB-C2B-C3B	2.82	129.96	124.68
26	j	605	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	m	605	CLA	CAA-C2A-C3A	-2.82	107.21	114.26
26	a	311	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	B	818	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
26	b	313	CLA	CHB-C4A-NA	2.82	128.41	124.51
26	h	308	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	k	610	CLA	CMB-C2B-C3B	2.82	129.96	124.68
35	d	314	II0	C05-C07-C11	-2.82	106.44	110.30
26	j	609	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	j	607	CLA	CMC-C2C-C3C	2.82	133.77	126.12
26	A	838	CLA	CMB-C2B-C3B	2.82	129.95	124.68
26	A	828	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	A	837	CLA	CMB-C2B-C3B	2.81	129.94	124.68
26	c	303	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	m	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
33	B	844	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
26	B	824	CLA	CHB-C4A-NA	2.81	128.40	124.51
29	L	201	WVN	C08-C01-C02	-2.81	105.28	109.55
26	l	304	CLA	CMB-C2B-C3B	2.81	129.94	124.68
35	a	314	II0	C27-C25-C23	-2.81	111.27	116.84
26	A	827	CLA	CHB-C4A-NA	2.81	128.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	818	CLA	CHB-C4A-NA	2.81	128.40	124.51
26	A	836	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
26	B	839	CLA	CMB-C2B-C3B	2.81	129.93	124.68
26	j	613	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	A	837	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	d	304	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	B	834	CLA	CHB-C4A-NA	2.81	128.39	124.51
26	A	831	CLA	CHB-C4A-NA	2.80	128.39	124.51
26	i	310	CLA	CHB-C4A-NA	2.80	128.39	124.51
26	a	308	CLA	CMB-C2B-C3B	2.80	129.92	124.68
35	d	315	II0	C12-C14-C10	-2.80	114.21	120.57
26	b	311	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	c	306	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	j	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	A	822	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	A	824	CLA	CHB-C4A-NA	2.80	128.38	124.51
26	k	605	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
26	a	305	CLA	CMB-C2B-C3B	2.80	129.91	124.68
35	m	614	II0	C06-C08-C12	2.80	114.13	110.30
26	B	811	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	m	601	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	j	612	CLA	CMB-C2B-C3B	2.79	129.91	124.68
26	A	820	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	A	854	SQD	O8-S-C6	2.79	110.19	105.74
26	K	101	CLA	CMB-C2B-C3B	2.79	129.90	124.68
26	B	832	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
26	B	829	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	c	301	CLA	CMB-C2B-C3B	2.79	129.90	124.68
26	m	606	CLA	CMB-C2B-C3B	2.79	129.90	124.68
35	d	301	II0	C42-C41-C39	-2.79	117.76	123.47
35	i	312	II0	C31-C29-C25	-2.79	118.48	126.58
26	A	809	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	b	305	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	a	310	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	h	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	k	602	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	n	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	B	815	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	j	606	CLA	CHB-C4A-NA	2.79	128.36	124.51
26	n	605	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	B	828	CLA	CMB-C2B-C3B	2.79	129.89	124.68
26	F	202	CLA	CMB-C2B-C3B	2.78	129.89	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	848	WVN	C20-C13-C15	-2.78	114.72	121.46
26	A	803	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
26	j	610	CLA	CMB-C2B-C3B	2.78	129.88	124.68
26	B	828	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	a	307	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	M	101	WVN	C21-C15-C14	-2.78	108.27	113.62
26	s	403	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	j	604	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	B	809	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	L	203	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
34	c	318	LMG	O1-C7-C8	-2.78	104.19	110.90
26	A	827	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	B	817	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	l	313	CLA	CHB-C4A-NA	2.78	128.35	124.51
26	d	307	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	B	832	CLA	CHB-C4A-NA	2.78	128.35	124.51
26	h	308	CLA	CMB-C2B-C3B	2.78	129.87	124.68
26	c	311	CLA	CHB-C4A-NA	2.77	128.35	124.51
26	B	813	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
26	j	606	CLA	CMB-C2B-C3B	2.77	129.87	124.68
26	A	836	CLA	CHB-C4A-NA	2.77	128.35	124.51
26	B	801	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
35	a	316	II0	C12-C14-C10	-2.77	114.28	120.57
26	b	310	CLA	CMB-C2B-C3B	2.77	129.86	124.68
26	b	311	CLA	CMB-C2B-C3B	2.77	129.86	124.68
26	j	604	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	m	613	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
26	A	856	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	m	607	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
26	b	310	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	A	805	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
26	B	834	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
26	n	610	CLA	CMB-C2B-C3B	2.77	129.85	124.68
26	F	202	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
26	A	811	CLA	CMB-C2B-C3B	2.76	129.85	124.68
26	A	833	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
26	m	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	F	201	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	F	203	WVN	C28-C30-C33	-2.76	114.60	123.22
35	l	302	II0	C11-C13-C09	-2.76	114.30	120.57
29	B	849	WVN	C26-C29-C31	-2.76	114.60	123.22
26	a	302	CLA	O2D-CGD-O1D	-2.76	118.44	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	h	311	II0	C30-C32-C34	-2.76	114.60	123.22
26	B	826	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	k	609	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	j	601	CLA	CMB-C2B-C3B	2.76	129.84	124.68
26	n	605	CLA	CHB-C4A-NA	2.76	128.32	124.51
29	B	849	WVN	C21-C15-C14	-2.76	108.32	113.62
26	m	610	CLA	CHB-C4A-NA	2.76	128.32	124.51
26	i	306	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
26	l	313	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
35	d	319	II0	C04-C10-C14	-2.75	118.75	122.63
26	A	841	CLA	CHB-C4A-NA	2.75	128.31	124.51
35	m	615	II0	C05-C03-C09	2.75	115.19	109.62
26	d	305	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	B	848	WVN	C17-C06-C13	-2.75	105.84	110.30
29	F	203	WVN	C26-C29-C31	-2.75	114.64	123.22
35	i	313	II0	C06-C04-C10	2.75	115.19	109.62
29	s	407	WVN	C01-C02-C11	-2.75	109.23	112.70
26	n	609	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	d	318	CLA	CHB-C4A-NA	2.75	128.31	124.51
26	h	307	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
35	d	315	II0	C19-C13-C11	-2.75	109.27	114.36
26	A	811	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	b	312	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
26	A	803	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
26	A	817	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
26	c	311	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
26	n	610	CLA	CHB-C4A-NA	2.74	128.30	124.51
28	b	302	LHG	O8-C23-C24	2.74	120.51	111.91
26	B	824	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	A	839	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	B	825	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	h	306	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	B	812	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	i	307	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
26	n	602	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	B	830	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
26	b	307	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
26	i	303	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
26	B	826	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
26	b	303	CLA	CHB-C4A-NA	2.73	128.29	124.51
29	B	849	WVN	C28-C30-C33	-2.73	114.69	123.22
26	i	306	CLA	O2D-CGD-O1D	-2.73	118.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	302	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
26	A	834	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	s	408	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
37	b	316	IHT	C05-C08-C12	2.73	114.04	110.30
26	k	605	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	A	851	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
26	j	606	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
26	i	301	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	j	605	CLA	C2A-C1A-CHA	2.73	128.62	123.86
26	i	303	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	B	839	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
26	Q	302	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	B	827	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
37	j	616	IHT	C18-C22-C23	2.72	130.35	126.23
26	j	612	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	m	613	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	d	310	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
26	b	303	CLA	CMB-C2B-C3B	2.72	129.77	124.68
26	l	301	CLA	CMB-C2B-C3B	2.72	129.77	124.68
26	a	304	CLA	CHB-C4A-NA	2.72	128.27	124.51
36	s	401	KC2	CAA-CBA-CGA	-2.72	113.30	127.26
26	h	302	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
26	a	308	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	l	305	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
35	b	314	II0	C12-C14-C10	-2.71	114.41	120.57
26	i	307	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	i	311	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	n	604	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
35	i	319	II0	C11-C13-C09	-2.71	114.42	120.57
26	A	820	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	A	816	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	h	303	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
26	m	602	CLA	CBC-CAC-C3C	2.71	119.90	112.43
26	B	806	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	A	835	CLA	CHB-C4A-NA	2.71	128.25	124.51
26	B	842	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
26	J	103	CLA	CHB-C4A-NA	2.71	128.25	124.51
34	L	209	LMG	O6-C1-O1	-2.71	103.57	109.97
26	m	612	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	B	816	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
26	j	601	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	b	312	CLA	CMB-C2B-C3B	2.70	129.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	309	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	i	311	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
34	F	205	LMG	O6-C1-O1	-2.70	103.58	109.97
26	j	610	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	h	307	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	d	304	CLA	CHB-C4A-NA	2.70	128.25	124.51
28	J	105	LHG	O8-C23-C24	2.70	120.38	111.91
26	B	814	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
26	h	305	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	l	311	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	Q	302	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
26	s	402	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
35	n	618	II0	C05-C03-C09	2.70	115.08	109.62
26	h	304	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	i	301	CLA	CMB-C2B-C3B	2.69	129.72	124.68
26	A	838	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
26	F	202	CLA	CHB-C4A-NA	2.69	128.24	124.51
26	A	829	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	A	806	CLA	CMB-C2B-C3B	2.69	129.71	124.68
26	k	601	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	s	408	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	b	309	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	h	313	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
26	i	305	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	A	808	CLA	CMB-C2B-C3B	2.69	129.70	124.68
26	b	304	CLA	CHB-C4A-NA	2.69	128.22	124.51
26	l	301	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	h	308	CLA	CHB-C4A-NA	2.68	128.22	124.51
29	A	847	WVN	C10-C06-C13	2.68	114.61	110.48
26	A	819	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	m	602	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	k	610	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	B	811	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
26	h	305	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
35	i	313	II0	C11-C13-C09	-2.68	114.49	120.57
26	A	822	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	k	614	CLA	CBC-CAC-C3C	2.68	119.81	112.43
26	n	608	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
26	B	807	CLA	CHB-C4A-NA	2.67	128.21	124.51
28	m	618	LHG	O8-C23-C24	2.67	120.30	111.91
26	a	303	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
26	d	305	CLA	CHB-C4A-NA	2.67	128.21	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	302	CLA	CHB-C4A-NA	2.67	128.20	124.51
26	B	808	CLA	O2D-CGD-CBD	2.67	116.01	111.27
26	A	826	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	d	303	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
26	d	310	CLA	CAA-C2A-C3A	-2.67	109.87	116.10
26	j	609	CLA	CHB-C4A-NA	2.67	128.20	124.51
35	d	301	II0	C31-C29-C25	-2.67	118.84	126.58
26	c	312	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
26	B	809	CLA	CMB-C2B-C3B	2.66	129.66	124.68
26	A	809	CLA	CHB-C4A-NA	2.66	128.19	124.51
28	c	320	LHG	O8-C23-C24	2.66	120.25	111.91
26	b	308	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	h	306	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	a	311	CLA	CHB-C4A-NA	2.66	128.18	124.51
26	B	804	CLA	CMB-C2B-C3B	2.65	129.65	124.68
26	R	201	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	J	105	LHG	C11-C10-C9	-2.65	100.95	114.42
26	c	308	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	k	606	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	c	305	CLA	CMB-C2B-C3B	2.65	129.64	124.68
26	m	609	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
28	l	318	LHG	O8-C23-C24	2.65	120.23	111.91
26	s	403	CLA	O2D-CGD-CBD	2.65	115.98	111.27
26	B	839	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	A	852	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	B	821	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
35	c	313	II0	C06-C08-C12	2.65	113.93	110.30
33	B	844	DGD	C3D-C4D-C5D	-2.65	105.51	110.24
26	m	608	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	B	831	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	l	304	CLA	CHB-C4A-NA	2.65	128.17	124.51
26	l	306	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	B	838	CLA	CHB-C4A-NA	2.65	128.17	124.51
26	h	305	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
26	a	304	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
26	B	841	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	m	606	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
29	l	316	WVN	C12-C14-C15	-2.64	109.36	114.08
26	b	311	CLA	CHB-C4A-NA	2.64	128.17	124.51
26	B	816	CLA	CHB-C4A-NA	2.64	128.17	124.51
29	s	407	WVN	C21-C15-C14	-2.64	108.54	113.62
26	A	852	CLA	O2D-CGD-O1D	-2.64	118.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	838	CLA	O2D-CGD-CBD	2.64	115.96	111.27
26	A	807	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	b	308	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
26	B	806	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	l	310	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	L	206	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
26	d	303	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	h	301	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	h	313	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
26	i	308	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	m	608	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
35	i	314	II0	C12-C14-C10	-2.63	114.61	120.57
26	L	206	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	A	829	CLA	CMB-C2B-C3B	2.63	129.59	124.68
26	l	305	CLA	O2D-CGD-CBD	2.63	115.93	111.27
34	c	318	LMG	O1-C1-C2	-2.62	104.20	108.30
26	B	807	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
35	i	314	II0	C06-C04-C10	2.62	114.93	109.62
26	A	821	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	n	613	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
26	A	813	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
26	A	832	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
26	B	804	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
26	l	309	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
29	i	315	WVN	C17-C06-C13	-2.62	106.06	110.30
35	J	104	II0	C12-C14-C10	-2.61	114.64	120.57
26	k	607	CLA	C2D-C1D-ND	-2.61	108.18	110.10
35	m	616	II0	C12-C14-C10	-2.61	114.64	120.57
26	B	801	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
26	l	301	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
26	m	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
35	d	315	II0	C06-C04-C10	2.61	114.91	109.62
26	A	804	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	A	840	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	B	831	CLA	CHB-C4A-NA	2.61	128.12	124.51
35	n	615	II0	C30-C32-C34	-2.61	115.08	123.22
26	c	303	CLA	CHB-C4A-NA	2.61	128.12	124.51
34	n	620	LMG	O6-C1-O1	-2.61	103.80	109.97
36	s	401	KC2	CBA-CAA-C2A	-2.60	115.34	125.27
26	B	803	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
35	i	319	II0	C30-C32-C34	-2.60	115.09	123.22
35	a	312	II0	C05-C03-C09	2.60	114.89	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	805	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
26	j	613	CLA	CHB-C4A-NA	2.60	128.11	124.51
28	c	317	LHG	O8-C23-C24	2.60	120.07	111.91
29	A	846	WVN	C21-C15-C14	-2.60	108.62	113.62
26	m	608	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	A	837	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
35	a	312	II0	C12-C14-C10	-2.60	114.68	120.57
26	k	604	CLA	CMB-C2B-C3B	2.60	129.54	124.68
26	A	828	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
26	a	301	CLA	CHB-C4A-NA	2.60	128.10	124.51
26	B	840	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	a	310	CLA	CMB-C2B-C3B	2.59	129.53	124.68
26	n	603	CLA	CHB-C4A-NA	2.59	128.09	124.51
35	a	313	II0	C19-C13-C11	-2.59	109.56	114.36
26	k	609	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
26	i	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	A	802	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
26	c	305	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
35	J	104	II0	C05-C03-C09	2.59	114.86	109.62
35	k	615	II0	C17-C04-C10	-2.59	106.36	110.47
33	j	618	DGD	CDB-CCB-CBB	-2.59	101.30	114.42
26	j	603	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	A	832	CLA	CHB-C4A-NA	2.58	128.09	124.51
26	b	312	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	B	823	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
26	m	606	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	a	311	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
35	d	317	II0	C19-C13-C11	-2.58	109.57	114.36
26	B	825	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
26	B	827	CLA	C2D-C1D-ND	-2.58	108.20	110.10
26	A	809	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
26	A	812	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
35	c	316	II0	C05-C03-C09	2.58	114.84	109.62
26	L	202	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	A	838	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
26	B	837	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
26	i	304	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	n	601	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	A	838	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	s	406	CLA	O2D-CGD-CBD	2.57	115.84	111.27
28	c	320	LHG	C11-C10-C9	-2.57	101.37	114.42
26	d	302	CLA	C1B-CHB-C4A	-2.57	125.03	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	i	305	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	s	402	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
26	a	310	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	i	302	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	m	605	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	B	831	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
26	c	301	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	m	603	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	b	312	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
26	A	805	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	a	302	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	K	101	CLA	CHB-C4A-NA	2.56	128.05	124.51
35	k	620	II0	C06-C04-C10	2.56	114.80	109.62
26	d	313	CLA	C2A-C1A-CHA	2.56	128.33	123.86
26	A	810	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	d	310	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
26	b	306	CLA	CHB-C4A-NA	2.55	128.04	124.51
28	A	855	LHG	O8-C23-C24	2.55	119.92	111.91
26	L	206	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
26	A	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
35	k	619	II0	C42-C41-C39	-2.55	118.25	123.47
26	n	608	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
35	i	316	II0	C12-C14-C10	-2.55	114.78	120.57
28	L	208	LHG	C11-C10-C9	-2.55	101.47	114.42
26	n	609	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
35	c	316	II0	C11-C13-C09	-2.55	114.79	120.57
26	A	835	CLA	CMB-C2B-C3B	2.55	129.45	124.68
36	i	309	KC2	OBD-CAD-CBD	-2.55	122.25	125.89
26	B	833	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	A	808	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
28	b	302	LHG	C11-C10-C9	-2.54	101.52	114.42
26	s	406	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	h	302	CLA	CHB-C4A-NA	2.54	128.03	124.51
29	K	102	WVN	C40-C39-C36	-2.54	118.27	123.47
35	n	616	II0	C17-C04-C10	-2.54	106.43	110.47
26	A	841	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
35	b	314	II0	C42-C41-C39	-2.54	118.28	123.47
26	B	830	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
28	s	409	LHG	O8-C23-C24	2.54	119.86	111.91
26	B	816	CLA	CMB-C2B-C3B	2.54	129.42	124.68
26	A	833	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	B	814	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	m	615	II0	C42-C41-C39	-2.53	118.29	123.47
26	B	804	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	j	604	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
35	m	619	II0	C42-C41-C39	-2.53	118.30	123.47
26	K	101	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
26	B	814	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
26	B	841	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
26	A	815	CLA	CHB-C4A-NA	2.52	128.00	124.51
35	d	315	II0	C11-C13-C09	-2.52	114.84	120.57
26	B	835	CLA	CMB-C2B-C3B	2.52	129.39	124.68
28	A	844	LHG	C11-C10-C9	-2.52	101.63	114.42
26	k	602	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
26	B	836	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	A	814	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	A	839	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	b	305	CLA	C1B-CHB-C4A	-2.52	125.14	130.12
26	d	306	CLA	C1B-CHB-C4A	-2.52	125.14	130.12
26	A	829	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
26	j	608	CLA	CHB-C4A-NA	2.51	127.99	124.51
28	A	843	LHG	C11-C10-C9	-2.51	101.68	114.42
29	B	853	WVN	C01-C02-C11	-2.51	109.53	112.70
28	i	317	LHG	C11-C10-C9	-2.51	101.68	114.42
35	k	619	II0	C05-C03-C09	2.51	114.70	109.62
26	B	821	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
35	i	312	II0	C42-C41-C39	-2.51	118.34	123.47
26	a	305	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	l	305	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	n	607	CLA	C2D-C1D-ND	-2.51	108.26	110.10
29	s	405	WVN	C20-C13-C15	-2.51	115.39	121.46
26	l	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	s	408	CLA	CMB-C2B-C3B	2.50	129.36	124.68
26	B	842	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	k	610	CLA	C2A-C1A-CHA	2.50	128.23	123.86
26	A	807	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
35	n	618	II0	C12-C14-C10	-2.50	114.90	120.57
26	m	612	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
28	j	617	LHG	C11-C10-C9	-2.49	101.76	114.42
28	L	208	LHG	O8-C23-C24	2.49	119.73	111.91
29	B	850	WVN	C02-C05-C09	-2.49	118.40	121.47
26	A	833	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
26	a	309	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
26	m	601	CLA	CHB-C4A-NA	2.49	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	602	CLA	CHB-C4A-NA	2.49	127.95	124.51
35	j	614	II0	C07-C11-C13	2.49	116.81	111.85
28	c	317	LHG	C11-C10-C9	-2.49	101.79	114.42
28	l	318	LHG	C11-C10-C9	-2.49	101.79	114.42
26	A	841	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
35	m	619	II0	C30-C32-C34	-2.49	115.46	123.22
30	A	850	LMU	C1'-C2'-C3'	2.49	115.17	110.00
36	c	310	KC2	CHD-C4C-C3C	-2.49	117.10	126.11
26	B	801	CLA	CMB-C2B-C3B	2.49	129.33	124.68
26	a	307	CLA	CHB-C4A-NA	2.48	127.94	124.51
35	d	319	II0	C05-C07-C11	-2.48	106.91	110.30
35	n	618	II0	C30-C32-C34	-2.48	115.47	123.22
26	c	309	CLA	CAC-C3C-C4C	2.48	128.03	124.81
29	I	101	WVN	C06-C13-C20	-2.48	108.76	115.78
28	m	618	LHG	C11-C10-C9	-2.48	101.83	114.42
26	A	831	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
26	B	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	A	833	CLA	CMB-C2B-C3B	2.47	129.31	124.68
26	A	811	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
26	A	819	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
26	d	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	A	849	LHG	C20-C19-C18	-2.47	101.89	114.42
36	c	310	KC2	CMB-C2B-C1B	2.47	129.06	124.71
36	n	611	KC2	C3C-C2C-C1C	2.47	108.32	106.49
26	c	303	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
26	a	304	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
26	l	305	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
26	h	307	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	A	814	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
35	l	315	II0	C12-C14-C10	-2.46	114.98	120.57
29	F	203	WVN	C39-C40-C37	-2.46	118.43	123.47
29	J	102	WVN	C28-C30-C33	-2.46	115.54	123.22
26	F	201	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	d	309	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	k	606	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
36	c	310	KC2	CBA-CAA-C2A	-2.46	115.90	125.27
26	B	822	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
35	l	315	II0	C19-C13-C11	-2.45	109.81	114.36
29	L	205	WVN	C21-C15-C14	-2.45	108.90	113.62
26	m	604	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
26	d	306	CLA	CHB-C4A-NA	2.45	127.90	124.51
28	A	849	LHG	C11-C10-C9	-2.45	101.98	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	301	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
28	L	207	LHG	C11-C10-C9	-2.45	101.98	114.42
26	B	833	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
35	i	314	II0	C15-C03-C09	-2.45	106.58	110.47
26	B	804	CLA	CHD-C4C-C3C	2.45	128.44	124.84
26	B	813	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
26	A	808	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
26	A	811	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	A	847	WVN	C26-C29-C31	-2.45	115.58	123.22
26	B	815	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	n	609	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	a	306	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	n	604	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
26	J	103	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
35	a	313	II0	C05-C03-C09	2.44	114.56	109.62
26	A	817	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	s	402	CLA	CHB-C4A-NA	2.44	127.88	124.51
28	A	843	LHG	O8-C23-C24	2.44	119.56	111.91
35	a	313	II0	C42-C41-C39	-2.44	118.48	123.47
35	i	312	II0	C17-C04-C10	-2.43	106.60	110.47
36	d	312	KC2	CHC-C4B-C3B	2.43	129.42	125.26
28	n	619	LHG	O8-C23-C24	2.43	119.55	111.91
26	B	810	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	A	803	CLA	CHB-C4A-NA	2.43	127.88	124.51
26	A	828	CLA	CHB-C4A-NA	2.43	127.88	124.51
34	c	318	LMG	C40-C39-C38	-2.43	102.08	114.42
26	l	306	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	B	816	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	j	609	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	h	303	CLA	C1-C2-C3	-2.43	122.82	126.75
26	A	822	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
28	B	851	LHG	O8-C23-C24	2.43	119.52	111.91
29	M	101	WVN	C39-C40-C37	-2.43	118.50	123.47
26	B	811	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
35	a	314	II0	C31-C29-C25	-2.42	119.54	126.58
26	c	305	CLA	CHB-C4A-NA	2.42	127.86	124.51
35	c	314	II0	C05-C07-C11	-2.42	106.99	110.30
26	k	608	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
29	B	848	WVN	C21-C15-C14	-2.42	108.97	113.62
26	j	603	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
27	B	843	PQN	C2M-C2-C3	-2.42	120.45	124.40
26	A	837	CLA	CHB-C4A-NA	2.42	127.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	d	306	CLA	CMB-C2B-C3B	2.42	129.20	124.68
26	B	836	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
26	a	307	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
26	d	307	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
28	A	855	LHG	C11-C10-C9	-2.41	102.17	114.42
26	b	308	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
26	B	803	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
26	d	308	CLA	CMB-C2B-C3B	2.41	129.19	124.68
26	B	820	CLA	CHB-C4A-NA	2.41	127.85	124.51
28	b	318	LHG	C20-C19-C18	-2.41	102.18	114.42
26	h	303	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	L	202	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
26	h	313	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	B	825	CLA	CHB-C4A-NA	2.41	127.84	124.51
29	A	848	WVN	C10-C06-C13	2.41	114.19	110.48
34	F	206	LMG	O6-C1-O1	-2.41	104.27	109.97
26	a	302	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
26	A	840	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
34	F	205	LMG	O1-C7-C8	-2.41	105.09	110.90
26	d	308	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
26	K	101	CLA	C2A-C1A-CHA	2.40	128.06	123.86
26	A	840	CLA	O1D-CGD-CBD	2.40	129.40	124.48
34	F	205	LMG	C40-C39-C38	-2.40	102.22	114.42
26	A	823	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	b	318	LHG	C11-C10-C9	-2.40	102.24	114.42
26	k	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	m	608	CLA	CHD-C1D-ND	-2.40	122.25	124.45
28	L	207	LHG	C20-C19-C18	-2.40	102.25	114.42
35	l	315	II0	C31-C29-C25	-2.40	119.62	126.58
26	B	805	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
26	B	822	CLA	C2A-C1A-CHA	2.40	128.05	123.86
28	b	318	LHG	O8-C23-C24	2.40	119.43	111.91
26	a	305	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
26	b	304	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
26	L	204	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	c	302	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	c	304	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	A	830	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	A	825	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	B	830	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	B	815	CLA	C1B-CHB-C4A	-2.39	125.39	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	801	CLA	CHB-C4A-NA	2.39	127.81	124.51
26	d	308	CLA	CHB-C4A-NA	2.39	127.81	124.51
26	B	834	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
26	d	310	CLA	CHB-C4A-NA	2.39	127.81	124.51
35	k	616	II0	C31-C29-C25	-2.39	119.66	126.58
26	B	828	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
36	s	401	KC2	CAA-C2A-C1A	-2.39	113.78	124.75
27	A	842	PQN	C2M-C2-C1	2.38	120.22	116.27
26	k	610	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
26	B	838	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
28	i	317	LHG	O8-C23-C24	2.38	119.37	111.91
26	c	312	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	B	809	CLA	CHB-C4A-NA	2.38	127.80	124.51
28	B	851	LHG	C11-C10-C9	-2.38	102.36	114.42
26	m	609	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
26	B	826	CLA	CHB-C4A-NA	2.37	127.80	124.51
29	A	857	WVN	C07-C01-C02	2.37	113.14	109.55
36	s	401	KC2	CMC-C2C-C1C	2.37	128.65	125.04
35	a	314	II0	C42-C41-C39	-2.37	118.62	123.47
26	m	602	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	l	310	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	s	408	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
26	k	614	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	d	309	CLA	CMA-C3A-C2A	-2.37	110.57	116.10
28	c	320	LHG	C20-C19-C18	-2.37	102.41	114.42
26	L	203	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
26	A	802	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	A	817	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	B	823	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	A	801	CL0	C4D-CHA-C1A	2.36	124.12	121.25
36	s	404	KC2	OBD-CAD-CBD	-2.36	122.52	125.89
26	j	608	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
33	j	618	DGD	O5D-C6D-C5D	-2.36	104.68	109.05
26	i	305	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
26	A	834	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
34	n	620	LMG	C38-C37-C36	-2.36	102.45	114.42
26	b	313	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
26	B	832	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	A	821	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	s	406	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	i	306	CLA	CHB-C4A-NA	2.36	127.77	124.51
33	B	844	DGD	CFB-CEB-CDB	-2.36	102.47	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m	603	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	B	833	CLA	C2A-C1A-CHA	2.36	127.98	123.86
35	h	312	II0	C15-C03-C09	-2.35	106.72	110.47
35	h	311	II0	C06-C04-C10	2.35	114.39	109.62
26	l	313	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
26	j	606	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
26	n	603	CLA	C2A-C1A-CHA	2.35	127.97	123.86
28	n	619	LHG	C11-C10-C9	-2.35	102.49	114.42
28	B	851	LHG	C20-C19-C18	-2.35	102.50	114.42
26	B	817	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	B	810	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	i	302	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
35	l	315	II0	C18-C04-C10	-2.35	106.74	110.47
26	m	607	CLA	CHB-C4A-NA	2.34	127.75	124.51
26	K	101	CLA	CAA-C2A-C3A	-2.34	108.41	114.26
26	b	313	CLA	C2A-C1A-CHA	2.34	127.95	123.86
26	b	306	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
26	l	307	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
29	A	846	WVN	C10-C06-C13	2.34	114.08	110.48
36	s	401	KC2	CHD-C4C-C3C	-2.34	117.63	126.11
26	A	810	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
26	B	825	CLA	CHD-C1D-ND	-2.34	122.31	124.45
26	c	308	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
26	B	826	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
33	j	618	DGD	O2D-C2D-C1D	-2.34	104.37	110.05
35	k	619	II0	C06-C04-C10	2.33	114.35	109.62
26	B	808	CLA	C1-C2-C3	-2.33	122.01	126.04
26	m	601	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	m	610	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	i	307	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
37	a	315	IHT	C05-C08-C12	-2.33	107.12	110.30
35	d	316	II0	C11-C13-C09	-2.33	115.29	120.57
26	A	816	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
26	A	821	CLA	CHD-C1D-ND	-2.33	122.32	124.45
26	R	201	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
26	B	842	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	A	816	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
35	k	616	II0	C15-C03-C09	2.33	114.16	110.47
26	A	818	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
26	B	828	CLA	CHB-C4A-NA	2.32	127.73	124.51
26	A	830	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	b	302	LHG	C20-C19-C18	-2.32	102.63	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	i	310	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	d	306	CLA	O2D-CGD-CBD	2.32	115.39	111.27
26	a	306	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
34	c	318	LMG	C38-C37-C36	-2.32	102.66	114.42
26	A	820	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	n	602	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	h	301	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
33	j	618	DGD	O6E-C5E-C4E	2.32	113.90	109.69
26	A	839	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	a	308	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
26	A	806	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	k	607	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	c	307	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	j	602	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	c	308	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	F	201	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
34	Q	301	LMG	O7-C10-O9	-2.31	118.12	123.70
29	B	850	WVN	C21-C15-C14	-2.31	109.18	113.62
26	i	303	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
26	k	604	CLA	CHB-C4A-NA	2.31	127.70	124.51
26	A	813	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	A	835	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	n	608	CLA	C2A-C1A-CHA	2.30	127.89	123.86
26	B	837	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	b	311	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	B	841	CLA	C2A-C1A-CHA	2.30	127.88	123.86
36	m	611	KC2	C2A-C3A-C4A	2.30	108.19	106.49
26	B	805	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	b	310	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	c	309	CLA	CMC-C2C-C1C	2.30	128.54	125.04
29	h	309	WVN	C07-C01-C02	2.30	113.03	109.55
35	i	314	II0	C11-C13-C09	-2.30	115.35	120.57
26	A	815	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
26	c	302	CLA	C1-C2-C3	-2.30	122.07	126.04
26	l	304	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
26	n	601	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
26	k	608	CLA	CHB-C4A-NA	2.30	127.69	124.51
34	c	318	LMG	O6-C1-O1	-2.29	104.54	109.97
26	d	307	CLA	CHB-C4A-NA	2.29	127.68	124.51
32	A	854	SQD	O48-C23-C24	2.29	119.11	111.91
26	A	825	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
26	B	809	CLA	C1B-CHB-C4A	-2.29	125.58	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	601	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	d	309	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	i	308	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	B	834	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
32	A	854	SQD	C3-C4-C5	2.29	114.32	110.24
26	j	610	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
34	c	319	LMG	O1-C7-C8	-2.29	105.38	110.90
26	B	830	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
26	A	802	CLA	CHB-C4A-NA	2.29	127.67	124.51
26	J	103	CLA	CAA-C2A-C3A	-2.29	108.55	114.26
36	d	312	KC2	C1A-NA-C4A	2.28	107.73	106.71
32	A	854	SQD	O6-C1-C2	2.28	111.87	108.30
26	a	310	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
35	l	315	II0	C06-C04-C10	2.28	114.25	109.62
26	A	804	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
26	B	802	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	A	826	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
26	A	812	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
36	k	611	KC2	C2A-C3A-C4A	2.28	108.17	106.49
26	k	607	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
35	m	615	II0	C11-C13-C09	-2.28	115.41	120.57
36	n	612	KC2	C3C-C2C-C1C	2.28	108.17	106.49
26	A	808	CLA	C2A-C1A-CHA	2.27	127.84	123.86
26	b	313	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
26	Q	302	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
26	b	307	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	A	821	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
29	l	303	WVN	C21-C15-C14	-2.27	109.25	113.62
26	B	821	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	B	837	CLA	CMB-C2B-C3B	2.27	128.93	124.68
33	j	618	DGD	CFB-CEB-CDB	-2.27	102.91	114.42
26	B	829	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	b	304	CLA	O2D-CGD-CBD	2.26	115.29	111.27
28	A	843	LHG	C27-C26-C25	-2.26	102.93	114.42
26	A	825	CLA	CHD-C1D-ND	-2.26	122.38	124.45
26	B	820	CLA	O2D-CGD-CBD	2.26	115.29	111.27
35	b	314	II0	C06-C04-C10	2.26	114.20	109.62
26	B	812	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
35	m	616	II0	C05-C03-C09	2.26	114.20	109.62
28	b	318	LHG	C27-C26-C25	-2.26	102.96	114.42
29	h	309	WVN	C21-C15-C14	-2.26	109.28	113.62
26	i	304	CLA	C1B-CHB-C4A	-2.26	125.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	204	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
26	B	822	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
26	l	309	CLA	O1D-CGD-CBD	2.25	129.10	124.48
29	h	309	WVN	C06-C13-C20	-2.25	109.40	115.78
26	A	824	CLA	C2A-C1A-CHA	2.25	127.80	123.86
26	j	607	CLA	CBC-CAC-C3C	2.25	118.64	112.43
28	A	843	LHG	C18-C17-C16	-2.25	102.99	114.42
29	B	846	WVN	C07-C01-C02	2.25	112.96	109.55
36	c	310	KC2	O2D-CGD-O1D	-2.25	119.44	123.84
26	j	612	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	R	200	WVN	C10-C06-C13	2.25	113.95	110.48
26	m	612	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
26	B	818	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	i	301	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	i	305	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	l	311	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
26	B	827	CLA	CHB-C4A-NA	2.25	127.62	124.51
35	l	302	II0	C15-C03-C09	-2.25	106.90	110.47
29	K	102	WVN	C06-C13-C20	-2.25	109.42	115.78
34	c	319	LMG	O6-C1-O1	-2.25	104.66	109.97
26	A	856	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
34	F	205	LMG	C38-C37-C36	-2.24	103.03	114.42
34	c	318	LMG	C42-C41-C40	-2.24	103.03	114.42
26	k	606	CLA	CHD-C1D-ND	-2.24	122.39	124.45
35	d	314	II0	C06-C08-C12	-2.24	107.23	110.30
26	n	604	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
29	F	203	WVN	C21-C15-C14	-2.24	109.31	113.62
36	d	312	KC2	OBD-CAD-CBD	-2.24	122.69	125.89
28	b	302	LHG	C27-C26-C25	-2.24	103.06	114.42
36	i	309	KC2	CHB-C1B-NB	-2.24	122.40	124.45
26	h	306	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
35	a	312	II0	C11-C13-C09	-2.24	115.49	120.57
35	m	615	II0	C17-C04-C10	-2.24	106.91	110.47
29	h	309	WVN	C01-C02-C05	2.24	115.42	111.42
29	A	845	WVN	C10-C06-C13	2.24	113.92	110.48
36	s	401	KC2	CHD-C4C-NC	2.24	127.60	124.20
26	l	308	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
26	L	202	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
26	k	605	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
26	h	302	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
29	l	303	WVN	C06-C13-C20	-2.23	109.46	115.78
34	F	205	LMG	O3-C3-C2	-2.23	105.19	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	304	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
36	n	612	KC2	OBD-CAD-CBD	-2.23	122.71	125.89
35	h	312	II0	C42-C41-C39	-2.23	118.91	123.47
35	n	618	II0	C11-C13-C09	-2.23	115.51	120.57
36	l	312	KC2	OBD-CAD-CBD	-2.23	122.71	125.89
35	i	316	II0	C16-C03-C09	2.23	114.01	110.47
26	j	605	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
34	c	318	LMG	O3-C3-C2	-2.23	105.20	110.35
26	B	819	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
26	c	309	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
35	i	316	II0	C06-C04-C10	2.22	114.12	109.62
35	a	312	II0	C42-C41-C39	-2.22	118.92	123.47
26	l	306	CLA	C2A-C1A-CHA	2.22	127.74	123.86
26	n	613	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
26	B	810	CLA	CHD-C1D-ND	-2.22	122.41	124.45
33	B	844	DGD	CBB-CAB-C9B	-2.22	103.15	114.42
26	d	305	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
26	A	818	CLA	C1-C2-C3	-2.22	122.20	126.04
35	n	615	II0	C12-C14-C10	-2.22	115.53	120.57
35	a	316	II0	C18-C04-C10	-2.22	106.94	110.47
26	a	302	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
34	L	209	LMG	O3-C3-C2	-2.22	105.22	110.35
26	n	608	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
28	L	208	LHG	C18-C17-C16	-2.22	103.18	114.42
26	B	835	CLA	CHB-C4A-NA	2.22	127.58	124.51
35	l	315	II0	C27-C25-C23	-2.22	112.45	116.84
26	B	839	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
26	h	307	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
28	s	409	LHG	C27-C26-C25	-2.21	103.18	114.42
26	m	606	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
26	A	841	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
26	F	202	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
26	i	301	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
36	i	318	KC2	OBD-CAD-CBD	-2.21	122.74	125.89
29	A	848	WVN	C39-C40-C37	-2.21	118.94	123.47
28	B	851	LHG	C27-C26-C25	-2.21	103.20	114.42
26	B	803	CLA	CMB-C2B-C3B	2.21	128.81	124.68
26	A	806	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
34	F	205	LMG	C42-C41-C40	-2.21	103.21	114.42
26	d	318	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
26	m	612	CLA	C2A-C1A-CHA	2.21	127.72	123.86
26	n	613	CLA	C2A-C1A-CHA	2.21	127.72	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
28	c	320	LHG	C27-C26-C25	-2.21	103.21	114.42
36	s	401	KC2	C2A-C1A-CHA	-2.21	120.14	127.44
26	c	302	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
26	a	303	CLA	C2A-C1A-CHA	2.21	127.72	123.86
26	l	309	CLA	C2D-C1D-ND	-2.21	108.48	110.10
36	m	611	KC2	OBD-CAD-CBD	-2.21	122.74	125.89
34	b	319	LMG	O3-C3-C2	-2.21	105.25	110.35
36	s	401	KC2	CHB-C1B-NB	-2.21	122.43	124.45
26	B	819	CLA	C2D-C1D-ND	-2.21	108.48	110.10
26	B	810	CLA	O2D-CGD-CBD	2.20	115.19	111.27
35	c	313	II0	C08-C12-C14	2.20	116.25	111.85
26	h	304	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
35	j	615	II0	C12-C14-C10	-2.20	115.57	120.57
35	i	313	II0	C05-C03-C09	2.20	114.08	109.62
26	c	311	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
26	A	805	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
29	s	405	WVN	C10-C06-C13	2.20	113.87	110.48
26	h	303	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
34	Q	301	LMG	O3-C3-C2	-2.20	105.26	110.35
26	j	601	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
29	L	201	WVN	C03-C04-C09	-2.20	108.35	112.00
29	M	101	WVN	C10-C06-C13	2.20	113.86	110.48
34	n	620	LMG	O3-C3-C2	-2.20	105.27	110.35
26	a	303	CLA	C3A-C2A-C1A	2.20	104.63	101.34
26	c	307	CLA	CHB-C4A-NA	2.19	127.55	124.51
26	B	832	CLA	CMB-C2B-C3B	2.19	128.78	124.68
26	B	839	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
35	b	314	II0	C05-C03-C09	2.19	114.07	109.62
26	a	306	CLA	O2D-CGD-CBD	2.19	115.17	111.27
26	B	821	CLA	CAA-CBA-CGA	-2.19	106.84	113.25
26	B	828	CLA	C1-C2-C3	-2.19	123.20	126.75
26	B	821	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
28	L	207	LHG	C18-C17-C16	-2.19	103.29	114.42
26	B	838	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
36	c	310	KC2	CHB-C1B-NB	-2.19	122.44	124.45
28	L	208	LHG	C27-C26-C25	-2.19	103.31	114.42
26	c	309	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
26	l	310	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
34	F	206	LMG	O3-C3-C2	-2.19	105.29	110.35
26	n	608	CLA	C1D-ND-C4D	-2.19	104.78	106.33
26	B	803	CLA	CHB-C4A-NA	2.19	127.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	604	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	j	607	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
26	a	309	CLA	C2A-C1A-CHA	2.19	127.68	123.86
26	b	309	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
26	c	309	CLA	C3D-C4D-CHA	-2.19	107.72	112.72
26	A	814	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
26	B	806	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
28	A	855	LHG	C27-C26-C25	-2.18	103.33	114.42
33	j	618	DGD	CAB-C9B-C8B	-2.18	103.34	114.42
28	i	317	LHG	C27-C26-C25	-2.18	103.34	114.42
36	d	311	KC2	OBD-CAD-CBD	-2.18	122.78	125.89
26	B	824	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
28	n	619	LHG	C27-C26-C25	-2.18	103.35	114.42
26	B	819	CLA	CAC-C3C-C2C	2.18	131.26	127.53
26	B	834	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	A	813	CLA	C2D-C1D-ND	-2.18	108.50	110.10
26	h	308	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
26	B	812	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
36	c	310	KC2	C2A-C1A-CHA	-2.18	120.23	127.44
35	c	313	II0	C05-C03-C09	2.18	114.04	109.62
26	a	301	CLA	C2A-C1A-CHA	2.18	127.67	123.86
35	i	312	II0	C05-C03-C09	2.18	114.03	109.62
26	c	306	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	b	307	CLA	CHD-C1D-ND	-2.18	122.45	124.45
36	m	611	KC2	C3C-C2C-C1C	2.18	108.10	106.49
26	A	856	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
26	n	610	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
26	A	822	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
35	d	301	II0	C12-C14-C10	-2.17	115.64	120.57
26	B	836	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	b	303	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
26	h	301	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
36	n	612	KC2	CHC-C4B-C3B	2.17	128.97	125.26
26	B	816	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
26	a	304	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	n	605	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
26	A	825	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
26	a	303	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
34	b	319	LMG	O2-C2-C1	-2.16	104.79	110.05
35	j	615	II0	C05-C03-C09	2.16	114.01	109.62
36	d	312	KC2	CHB-C4A-C3A	2.16	128.36	124.98
36	n	611	KC2	OBD-CAD-CBD	-2.16	122.81	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	814	CLA	C1-C2-C3	-2.16	123.25	126.75
26	k	606	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	s	408	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	j	608	CLA	CHD-C1D-ND	-2.16	122.47	124.45
25	A	801	CL0	C2A-C1A-CHA	2.16	127.64	123.86
26	A	823	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	B	821	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	h	305	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	d	302	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
35	i	312	II0	C06-C08-C12	-2.16	107.35	110.30
35	n	618	II0	C15-C03-C09	-2.15	107.04	110.47
35	i	316	II0	C42-C41-C39	-2.15	119.06	123.47
35	a	313	II0	C11-C13-C09	-2.15	115.68	120.57
26	h	313	CLA	CHD-C1D-ND	-2.15	122.47	124.45
26	A	802	CLA	O1D-CGD-CBD	2.15	128.89	124.48
26	A	810	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
26	B	835	CLA	O2D-CGD-CBD	2.15	115.09	111.27
26	B	829	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
26	k	608	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
28	A	849	LHG	C18-C17-C16	-2.15	103.50	114.42
28	L	207	LHG	C27-C26-C25	-2.15	103.50	114.42
26	A	813	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	A	841	CLA	C2A-C1A-CHA	2.15	127.62	123.86
26	j	607	CLA	CHB-C4A-NA	2.15	127.48	124.51
26	s	403	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
26	c	306	CLA	CHD-C1D-ND	-2.15	122.48	124.45
36	i	309	KC2	CHC-C4B-NB	-2.15	122.48	124.45
26	i	303	CLA	C2A-C1A-CHA	2.15	127.61	123.86
34	c	318	LMG	O2-C2-C1	-2.15	104.83	110.05
35	l	302	II0	C34-C36-C40	-2.15	115.65	118.94
36	c	310	KC2	CHB-C4A-NA	2.15	127.58	124.20
29	B	853	WVN	C10-C06-C13	2.14	113.78	110.48
29	M	101	WVN	C06-C13-C20	-2.14	109.71	115.78
29	J	101	WVN	C39-C40-C37	-2.14	119.08	123.47
26	L	203	CLA	CHD-C1D-ND	-2.14	122.48	124.45
26	n	603	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
35	a	313	II0	C31-C29-C25	-2.14	120.36	126.58
34	c	319	LMG	O2-C2-C1	-2.14	104.85	110.05
35	j	615	II0	C17-C04-C10	-2.14	107.07	110.47
28	m	618	LHG	C27-C26-C25	-2.14	103.57	114.42
26	b	311	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
28	b	318	LHG	C18-C17-C16	-2.14	103.58	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	m	619	II0	C12-C14-C10	-2.13	115.72	120.57
26	B	829	CLA	CHD-C1D-ND	-2.13	122.49	124.45
26	B	819	CLA	CMC-C2C-C1C	-2.13	121.79	125.04
37	j	616	IHT	C22-C18-C07	-2.13	121.21	127.20
26	A	809	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	i	302	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	B	836	CLA	C2D-C1D-ND	-2.13	108.53	110.10
26	i	306	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
35	j	614	II0	C12-C14-C10	-2.13	115.73	120.57
26	B	802	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	B	813	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	j	613	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	m	609	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
26	B	823	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
26	n	613	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
34	F	205	LMG	O2-C2-C1	-2.13	104.88	110.05
36	j	611	KC2	C3C-C2C-C1C	2.13	108.06	106.49
26	m	605	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
26	B	804	CLA	CHC-C1C-NC	2.13	127.43	124.20
26	B	831	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	B	813	CLA	C2A-C1A-CHA	2.13	127.58	123.86
37	j	616	IHT	C27-C30-C32	2.12	129.85	123.22
26	h	302	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	A	818	CLA	CHD-C1D-ND	-2.12	122.50	124.45
36	s	401	KC2	CHB-C4A-NA	2.12	127.55	124.20
26	A	819	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	A	835	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
35	m	614	II0	C18-C04-C10	-2.12	107.09	110.47
26	A	851	CLA	C2D-C1D-ND	-2.12	108.54	110.10
36	n	611	KC2	CHB-C1B-NB	-2.12	122.50	124.45
29	A	848	WVN	C23-C20-C13	-2.12	121.25	127.20
26	l	313	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
26	i	311	CLA	CBC-CAC-C3C	2.12	118.27	112.43
34	b	319	LMG	O1-C1-C2	-2.12	105.00	108.30
34	c	319	LMG	O3-C3-C2	-2.12	105.45	110.35
34	F	206	LMG	O2-C2-C1	-2.12	104.90	110.05
26	m	602	CLA	O2D-CGD-CBD	2.12	115.03	111.27
26	k	610	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
35	a	313	II0	C05-C07-C11	-2.12	107.41	110.30
26	n	610	CLA	O2D-CGD-CBD	2.11	115.03	111.27
26	A	813	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
35	d	316	II0	C08-C12-C14	2.11	116.06	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	203	WVN	C06-C13-C20	-2.11	109.81	115.78
36	k	611	KC2	C3C-C2C-C1C	2.11	108.05	106.49
35	l	314	II0	C06-C04-C10	2.11	113.89	109.62
35	i	313	II0	C27-C25-C23	-2.11	112.67	116.84
26	n	602	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
26	B	819	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
26	n	606	CLA	CHB-C4A-NA	2.10	127.42	124.51
29	A	846	WVN	C01-C02-C11	-2.10	110.04	112.70
29	s	407	WVN	C26-C29-C31	-2.10	116.66	123.22
35	m	614	II0	C06-C04-C10	2.10	113.88	109.62
26	A	820	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
36	d	312	KC2	CHC-C4B-NB	-2.10	122.52	124.45
36	n	611	KC2	CHB-C4A-C3A	2.10	128.26	124.98
35	l	314	II0	C05-C03-C09	2.10	113.88	109.62
26	A	836	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
26	B	842	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	h	305	CLA	C2D-C1D-ND	-2.10	108.56	110.10
26	m	607	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	j	604	CLA	C2D-C1D-ND	-2.10	108.56	110.10
26	A	817	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	I	101	WVN	C40-C39-C36	-2.10	119.18	123.47
34	n	620	LMG	O2-C2-C1	-2.10	104.96	110.05
35	a	314	II0	C06-C04-C10	2.09	113.86	109.62
26	b	310	CLA	C2A-C1A-CHA	2.09	127.52	123.86
26	F	201	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
35	h	310	II0	C42-C41-C39	-2.09	119.19	123.47
35	h	311	II0	C42-C41-C39	-2.09	119.19	123.47
26	A	803	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
26	A	826	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
36	j	611	KC2	OBD-CAD-CBD	-2.09	122.91	125.89
35	i	313	II0	C12-C14-C10	-2.09	115.83	120.57
26	a	301	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
26	d	306	CLA	C2D-C1D-ND	-2.09	108.57	110.10
26	m	610	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	B	804	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
33	B	844	DGD	CAB-C9B-C8B	-2.09	103.83	114.42
26	s	402	CLA	CHD-C1D-ND	-2.09	122.54	124.45
29	l	303	WVN	C39-C40-C37	-2.08	119.20	123.47
35	c	313	II0	C42-C41-C39	-2.08	119.21	123.47
26	i	303	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	m	604	CLA	C2D-C1D-ND	-2.08	108.57	110.10
26	n	606	CLA	O2A-CGA-O1A	-2.08	118.34	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	615	II0	C18-C04-C10	2.08	113.77	110.47
26	B	825	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	B	827	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	s	402	CLA	C1-C2-C3	-2.08	122.45	126.04
33	j	618	DGD	C5B-C4B-C3B	-2.08	103.87	114.42
26	j	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
28	c	317	LHG	C27-C26-C25	-2.08	103.88	114.42
26	B	827	CLA	O2D-CGD-CBD	2.08	114.96	111.27
28	c	320	LHG	C18-C17-C16	-2.08	103.88	114.42
26	A	856	CLA	CHD-C1D-ND	-2.08	122.55	124.45
26	A	824	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
37	b	316	IHT	C30-C27-C23	2.08	130.27	127.31
35	J	104	II0	C42-C41-C39	-2.07	119.22	123.47
26	B	840	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
35	a	316	II0	C11-C13-C09	-2.07	115.87	120.57
26	A	856	CLA	C2A-C1A-CHA	2.07	127.48	123.86
26	B	802	CLA	CHB-C4A-NA	2.07	127.38	124.51
26	l	307	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
28	B	851	LHG	C18-C17-C16	-2.07	103.91	114.42
35	m	619	II0	C17-C04-C10	-2.07	107.18	110.47
26	A	819	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
26	n	603	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	s	402	CLA	C2A-C1A-CHA	2.07	127.48	123.86
26	d	303	CLA	C2A-C1A-CHA	2.07	127.48	123.86
34	n	620	LMG	O1-C1-C2	-2.07	105.07	108.30
35	d	317	II0	C12-C14-C10	-2.07	115.88	120.57
36	k	611	KC2	OBD-CAD-CBD	-2.07	122.94	125.89
26	j	606	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
35	i	312	II0	C12-C14-C10	-2.07	115.88	120.57
35	l	314	II0	C18-C04-C10	-2.07	107.18	110.47
37	b	316	IHT	C03-C11-C15	-2.07	119.72	122.63
26	A	832	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	B	828	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
36	k	613	KC2	OBD-CAD-CBD	-2.06	122.95	125.89
35	k	616	II0	C12-C14-C10	-2.06	115.89	120.57
26	n	613	CLA	CHB-C4A-NA	2.06	127.36	124.51
26	A	840	CLA	C2D-C1D-ND	-2.06	108.58	110.10
36	i	309	KC2	C3C-C2C-C1C	2.06	108.02	106.49
36	n	612	KC2	CHC-C4B-NB	-2.06	122.56	124.45
26	a	310	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
26	L	204	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	A	847	WVN	C01-C02-C11	-2.06	110.10	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	605	CLA	C2A-C1A-CHA	2.06	127.46	123.86
26	c	311	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
35	i	319	II0	C42-C41-C39	-2.06	119.26	123.47
26	A	808	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
36	c	310	KC2	CHC-C1C-NC	2.06	127.44	124.20
26	B	840	CLA	O2D-CGD-CBD	2.06	114.92	111.27
33	j	618	DGD	C3G-C2G-C1G	-2.05	106.93	111.79
26	n	601	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
26	k	604	CLA	O2D-CGD-CBD	2.05	114.92	111.27
26	s	406	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	h	306	CLA	C2D-C1D-ND	-2.05	108.59	110.10
26	B	819	CLA	CHB-C4A-NA	2.05	127.35	124.51
26	b	307	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	l	311	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	m	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	A	823	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	A	831	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	A	841	CLA	CHA-C1A-NA	-2.05	121.70	126.40
36	i	309	KC2	CHC-C4B-C3B	2.05	128.76	125.26
26	a	304	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	b	303	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
37	m	617	IHT	C05-C08-C12	-2.05	107.50	110.30
29	B	846	WVN	C10-C06-C13	2.05	113.63	110.48
26	m	602	CLA	CAC-C3C-C2C	2.05	131.03	127.53
35	m	615	II0	C12-C14-C10	-2.05	115.92	120.57
26	k	601	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	A	834	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
26	R	201	CLA	C1-C2-C3	-2.05	122.51	126.04
29	i	315	WVN	C20-C13-C15	-2.04	116.51	121.46
26	d	310	CLA	C2D-C1D-ND	-2.04	108.60	110.10
35	k	615	II0	C05-C03-C09	2.04	113.76	109.62
26	A	828	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	m	601	CLA	CAA-C2A-C3A	-2.04	109.16	114.26
29	B	850	WVN	C06-C13-C20	-2.04	110.00	115.78
26	n	605	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	h	304	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	c	316	II0	C15-C03-C09	-2.04	107.22	110.47
26	n	605	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	k	604	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	c	302	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	n	610	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	d	301	II0	C17-C04-C10	-2.04	107.23	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	j	618	DGD	C4E-C3E-C2E	-2.04	107.26	110.82
26	d	307	CLA	C2D-C1D-ND	-2.04	108.60	110.10
26	k	607	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	n	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	L	201	WVN	C07-C01-C02	2.04	112.63	109.55
26	a	301	CLA	C4-C3-C5	2.04	118.70	115.27
26	B	806	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	b	313	CLA	C1-C2-C3	-2.04	122.52	126.04
29	J	101	WVN	C06-C13-C20	-2.03	110.02	115.78
26	B	823	CLA	O2D-CGD-CBD	2.03	114.88	111.27
26	j	604	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	A	847	WVN	C39-C40-C37	-2.03	119.31	123.47
26	c	306	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
35	k	617	II0	C05-C07-C11	-2.03	107.52	110.30
26	B	833	CLA	CHA-C1A-NA	-2.03	121.74	126.40
33	B	844	DGD	C3G-C2G-C1G	-2.03	106.98	111.79
36	s	401	KC2	CHC-C4B-C3B	-2.03	121.78	125.26
26	b	306	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
34	F	205	LMG	O7-C10-O9	-2.03	118.80	123.70
26	B	835	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	B	828	CLA	CHD-C1D-ND	-2.03	122.59	124.45
35	l	302	II0	C06-C08-C12	-2.03	107.53	110.30
28	c	317	LHG	C5-O7-C7	-2.03	112.80	117.79
35	d	316	II0	C12-C14-C10	-2.03	115.97	120.57
26	A	807	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	s	406	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	j	613	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	B	803	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	b	305	CLA	C2A-C1A-CHA	2.03	127.40	123.86
34	L	209	LMG	O2-C2-C1	-2.03	105.13	110.05
26	B	840	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
26	b	310	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
35	k	618	II0	C04-C10-C14	2.02	125.49	122.63
26	h	302	CLA	C1-C2-C3	-2.02	123.48	126.75
36	s	401	KC2	O2A-CGA-O1A	-2.02	118.47	122.67
28	l	318	LHG	C27-C26-C25	-2.02	104.16	114.42
26	j	607	CLA	C1D-ND-C4D	2.02	107.77	106.33
26	b	307	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
26	B	830	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	B	811	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	Q	302	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	a	308	CLA	O2A-CGA-O1A	-2.02	118.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	313	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	I	101	WVN	C07-C01-C02	2.02	112.60	109.55
26	A	838	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
35	d	315	II0	C18-C04-C10	-2.02	107.26	110.47
26	B	806	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	i	311	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	h	308	CLA	C2A-C1A-CHA	2.02	127.38	123.86
26	B	804	CLA	C1-C2-C3	-2.02	122.56	126.04
26	n	608	CLA	CHA-C1A-NA	-2.01	121.78	126.40
26	A	811	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
34	c	318	LMG	O7-C10-O9	-2.01	118.84	123.70
26	B	813	CLA	CHA-C1A-NA	-2.01	121.79	126.40
26	a	305	CLA	CHD-C1D-ND	-2.01	122.60	124.45
26	A	805	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	b	304	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	B	830	CLA	C1-C2-C3	-2.01	123.50	126.75
26	j	601	CLA	O2D-CGD-CBD	2.01	114.84	111.27
26	j	609	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	d	305	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	h	306	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	B	813	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	A	827	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
26	l	301	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
26	b	313	CLA	CHA-C1A-NA	-2.01	121.80	126.40
26	d	309	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	s	403	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
25	A	801	CL0	CHD-C4C-C3C	2.00	127.79	124.84
26	h	306	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	L	203	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
35	n	616	II0	C05-C03-C09	2.00	113.68	109.62
26	l	304	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
35	i	316	II0	C18-C04-C10	-2.00	107.29	110.47
26	B	835	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	n	609	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	h	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
36	d	312	KC2	C3C-C2C-C1C	2.00	107.97	106.49
35	J	104	II0	C15-C03-C09	-2.00	107.29	110.47

All (214) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	801	CL0	NA

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Mol	Chain	Res	Type	Atom
25	A	801	CL0	ND
26	A	802	CLA	ND
26	A	803	CLA	ND
26	A	804	CLA	ND
26	A	805	CLA	ND
26	A	806	CLA	ND
26	A	807	CLA	ND
26	A	808	CLA	ND
26	A	809	CLA	ND
26	A	810	CLA	ND
26	A	811	CLA	ND
26	A	812	CLA	ND
26	A	813	CLA	ND
26	A	814	CLA	ND
26	A	815	CLA	ND
26	A	816	CLA	ND
26	A	817	CLA	ND
26	A	818	CLA	ND
26	A	819	CLA	ND
26	A	820	CLA	ND
26	A	821	CLA	ND
26	A	822	CLA	ND
26	A	823	CLA	ND
26	A	824	CLA	ND
26	A	825	CLA	ND
26	A	826	CLA	ND
26	A	827	CLA	ND
26	A	828	CLA	ND
26	A	829	CLA	ND
26	A	830	CLA	ND
26	A	831	CLA	ND
26	A	832	CLA	ND
26	A	833	CLA	ND
26	A	834	CLA	ND
26	A	835	CLA	ND
26	A	836	CLA	ND
26	A	837	CLA	ND
26	A	838	CLA	ND
26	A	839	CLA	ND
26	A	840	CLA	ND
26	A	841	CLA	ND
26	A	851	CLA	ND

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Mol	Chain	Res	Type	Atom
26	A	852	CLA	ND
26	A	856	CLA	ND
26	B	801	CLA	ND
26	B	802	CLA	ND
26	B	803	CLA	ND
26	B	804	CLA	ND
26	B	805	CLA	ND
26	B	806	CLA	ND
26	B	807	CLA	ND
26	B	808	CLA	ND
26	B	809	CLA	ND
26	B	810	CLA	ND
26	B	811	CLA	ND
26	B	812	CLA	ND
26	B	813	CLA	ND
26	B	814	CLA	ND
26	B	815	CLA	ND
26	B	816	CLA	ND
26	B	817	CLA	ND
26	B	818	CLA	ND
26	B	819	CLA	ND
26	B	820	CLA	ND
26	B	821	CLA	ND
26	B	822	CLA	ND
26	B	823	CLA	ND
26	B	824	CLA	ND
26	B	825	CLA	ND
26	B	826	CLA	ND
26	B	827	CLA	ND
26	B	828	CLA	ND
26	B	829	CLA	ND
26	B	830	CLA	ND
26	B	831	CLA	ND
26	B	832	CLA	ND
26	B	833	CLA	ND
26	B	834	CLA	ND
26	B	836	CLA	ND
26	B	837	CLA	ND
26	B	838	CLA	ND
26	B	839	CLA	ND
26	B	840	CLA	ND
26	B	841	CLA	ND

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Mol	Chain	Res	Type	Atom
26	B	842	CLA	ND
26	F	201	CLA	ND
26	F	202	CLA	ND
26	J	103	CLA	ND
26	L	202	CLA	ND
26	L	203	CLA	ND
26	L	204	CLA	ND
26	L	206	CLA	ND
26	K	101	CLA	ND
26	s	402	CLA	ND
26	s	403	CLA	ND
26	s	406	CLA	ND
26	s	408	CLA	ND
26	c	301	CLA	ND
26	c	303	CLA	ND
26	c	304	CLA	ND
26	c	305	CLA	ND
26	c	306	CLA	ND
26	c	307	CLA	ND
26	c	308	CLA	ND
26	c	311	CLA	ND
26	c	312	CLA	ND
26	a	301	CLA	ND
26	a	302	CLA	ND
26	a	303	CLA	ND
26	a	304	CLA	ND
26	a	305	CLA	ND
26	a	306	CLA	ND
26	a	307	CLA	ND
26	a	308	CLA	ND
26	a	309	CLA	ND
26	a	311	CLA	ND
26	b	303	CLA	ND
26	b	304	CLA	ND
26	b	305	CLA	ND
26	b	306	CLA	ND
26	b	307	CLA	ND
26	b	308	CLA	ND
26	b	309	CLA	ND
26	b	310	CLA	ND
26	b	311	CLA	ND
26	b	312	CLA	ND

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Mol	Chain	Res	Type	Atom
26	b	313	CLA	ND
26	h	301	CLA	ND
26	h	302	CLA	ND
26	h	303	CLA	ND
26	h	304	CLA	ND
26	h	305	CLA	ND
26	h	306	CLA	ND
26	h	307	CLA	ND
26	h	308	CLA	ND
26	h	313	CLA	ND
26	m	601	CLA	ND
26	m	602	CLA	ND
26	m	603	CLA	ND
26	m	604	CLA	ND
26	m	605	CLA	ND
26	m	606	CLA	ND
26	m	607	CLA	ND
26	m	608	CLA	ND
26	m	609	CLA	ND
26	m	610	CLA	ND
26	m	612	CLA	ND
26	m	613	CLA	ND
26	l	301	CLA	ND
26	l	304	CLA	ND
26	l	305	CLA	ND
26	l	306	CLA	ND
26	l	307	CLA	ND
26	l	308	CLA	ND
26	l	309	CLA	ND
26	l	310	CLA	ND
26	l	311	CLA	ND
26	l	313	CLA	ND
26	k	601	CLA	ND
26	k	602	CLA	ND
26	k	603	CLA	ND
26	k	605	CLA	ND
26	k	606	CLA	ND
26	k	607	CLA	ND
26	k	608	CLA	ND
26	k	609	CLA	ND
26	k	610	CLA	ND
26	k	614	CLA	ND

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Mol	Chain	Res	Type	Atom
26	i	301	CLA	ND
26	i	302	CLA	ND
26	i	303	CLA	ND
26	i	304	CLA	ND
26	i	305	CLA	ND
26	i	306	CLA	ND
26	i	307	CLA	ND
26	i	308	CLA	ND
26	i	310	CLA	ND
26	i	311	CLA	ND
26	j	601	CLA	ND
26	j	602	CLA	ND
26	j	603	CLA	ND
26	j	604	CLA	ND
26	j	605	CLA	ND
26	j	606	CLA	ND
26	j	607	CLA	ND
26	j	608	CLA	ND
26	j	609	CLA	ND
26	j	610	CLA	ND
26	j	612	CLA	ND
26	j	613	CLA	ND
26	d	302	CLA	ND
26	d	303	CLA	ND
26	d	304	CLA	ND
26	d	305	CLA	ND
26	d	306	CLA	ND
26	d	307	CLA	ND
26	d	308	CLA	ND
26	d	309	CLA	ND
26	d	310	CLA	ND
26	d	313	CLA	ND
26	d	318	CLA	ND
26	R	201	CLA	ND
26	n	601	CLA	ND
26	n	602	CLA	ND
26	n	603	CLA	ND
26	n	604	CLA	ND
26	n	605	CLA	ND
26	n	607	CLA	ND
26	n	608	CLA	ND
26	n	609	CLA	ND

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Mol	Chain	Res	Type	Atom
26	n	610	CLA	ND
26	n	613	CLA	ND
26	Q	302	CLA	ND

All (3811) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CL0	C1-C2-C3-C4
26	A	804	CLA	CHA-CBD-CGD-O1D
26	A	804	CLA	CHA-CBD-CGD-O2D
26	A	804	CLA	CAD-CBD-CGD-O1D
26	A	809	CLA	CBD-CGD-O2D-CED
26	A	810	CLA	CBD-CGD-O2D-CED
26	A	812	CLA	C2-C3-C5-C6
26	A	812	CLA	C4-C3-C5-C6
26	A	813	CLA	C1A-C2A-CAA-CBA
26	A	814	CLA	C1A-C2A-CAA-CBA
26	A	815	CLA	CHA-CBD-CGD-O1D
26	A	815	CLA	CHA-CBD-CGD-O2D
26	A	816	CLA	C1A-C2A-CAA-CBA
26	A	816	CLA	C3A-C2A-CAA-CBA
26	A	816	CLA	C2-C3-C5-C6
26	A	816	CLA	C4-C3-C5-C6
26	A	817	CLA	C3A-C2A-CAA-CBA
26	A	818	CLA	C1A-C2A-CAA-CBA
26	A	818	CLA	C3A-C2A-CAA-CBA
26	A	818	CLA	CHA-CBD-CGD-O1D
26	A	818	CLA	CHA-CBD-CGD-O2D
26	A	819	CLA	CHA-CBD-CGD-O1D
26	A	819	CLA	CHA-CBD-CGD-O2D
26	A	819	CLA	CBD-CGD-O2D-CED
26	A	822	CLA	CHA-CBD-CGD-O1D
26	A	822	CLA	CHA-CBD-CGD-O2D
26	A	823	CLA	C1A-C2A-CAA-CBA
26	A	823	CLA	C3A-C2A-CAA-CBA
26	A	823	CLA	CHA-CBD-CGD-O1D
26	A	823	CLA	CHA-CBD-CGD-O2D
26	A	827	CLA	C1A-C2A-CAA-CBA
26	A	827	CLA	C3A-C2A-CAA-CBA
26	A	836	CLA	CHA-CBD-CGD-O1D
26	A	836	CLA	CHA-CBD-CGD-O2D
26	A	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	A	837	CLA	C3A-C2A-CAA-CBA
26	A	837	CLA	C2A-CAA-CBA-CGA
26	A	838	CLA	CHA-CBD-CGD-O1D
26	A	838	CLA	CHA-CBD-CGD-O2D
26	A	841	CLA	C1A-C2A-CAA-CBA
26	A	852	CLA	CHA-CBD-CGD-O1D
26	A	852	CLA	CHA-CBD-CGD-O2D
26	B	802	CLA	CHA-CBD-CGD-O1D
26	B	802	CLA	CHA-CBD-CGD-O2D
26	B	802	CLA	CAD-CBD-CGD-O1D
26	B	802	CLA	C2-C3-C5-C6
26	B	802	CLA	C4-C3-C5-C6
26	B	803	CLA	CHA-CBD-CGD-O1D
26	B	803	CLA	CHA-CBD-CGD-O2D
26	B	803	CLA	CBD-CGD-O2D-CED
26	B	804	CLA	C2C-C3C-CAC-CBC
26	B	804	CLA	C4C-C3C-CAC-CBC
26	B	805	CLA	C1A-C2A-CAA-CBA
26	B	805	CLA	C3A-C2A-CAA-CBA
26	B	807	CLA	CHA-CBD-CGD-O1D
26	B	807	CLA	CHA-CBD-CGD-O2D
26	B	808	CLA	CHA-CBD-CGD-O1D
26	B	808	CLA	CHA-CBD-CGD-O2D
26	B	813	CLA	C1A-C2A-CAA-CBA
26	B	816	CLA	C1A-C2A-CAA-CBA
26	B	816	CLA	C3A-C2A-CAA-CBA
26	B	816	CLA	C2-C3-C5-C6
26	B	816	CLA	C4-C3-C5-C6
26	B	817	CLA	C3A-C2A-CAA-CBA
26	B	819	CLA	C1A-C2A-CAA-CBA
26	B	819	CLA	C3A-C2A-CAA-CBA
26	B	819	CLA	CBD-CGD-O2D-CED
26	B	819	CLA	C2-C3-C5-C6
26	B	819	CLA	C4-C3-C5-C6
26	B	821	CLA	C1A-C2A-CAA-CBA
26	B	821	CLA	C3A-C2A-CAA-CBA
26	B	824	CLA	C1A-C2A-CAA-CBA
26	B	824	CLA	C3A-C2A-CAA-CBA
26	B	828	CLA	C1A-C2A-CAA-CBA
26	B	828	CLA	C3A-C2A-CAA-CBA
26	B	829	CLA	C1A-C2A-CAA-CBA
26	B	830	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	B	832	CLA	CBD-CGD-O2D-CED
26	B	833	CLA	C1A-C2A-CAA-CBA
26	B	837	CLA	C3A-C2A-CAA-CBA
26	B	837	CLA	CHA-CBD-CGD-O1D
26	B	837	CLA	CHA-CBD-CGD-O2D
26	B	839	CLA	C6-C7-C8-C9
26	B	840	CLA	C3A-C2A-CAA-CBA
26	B	841	CLA	C2A-CAA-CBA-CGA
26	J	103	CLA	CBD-CGD-O2D-CED
26	L	202	CLA	C1A-C2A-CAA-CBA
26	L	202	CLA	C3A-C2A-CAA-CBA
26	L	204	CLA	CBD-CGD-O2D-CED
26	K	101	CLA	C3A-C2A-CAA-CBA
26	s	402	CLA	C1A-C2A-CAA-CBA
26	s	402	CLA	C2A-CAA-CBA-CGA
26	s	403	CLA	CBD-CGD-O2D-CED
26	s	406	CLA	C1A-C2A-CAA-CBA
26	c	301	CLA	C1A-C2A-CAA-CBA
26	c	302	CLA	C1A-C2A-CAA-CBA
26	c	302	CLA	C3A-C2A-CAA-CBA
26	c	302	CLA	CBD-CGD-O2D-CED
26	c	303	CLA	CHA-CBD-CGD-O1D
26	c	303	CLA	CHA-CBD-CGD-O2D
26	c	303	CLA	CAD-CBD-CGD-O1D
26	c	304	CLA	CHA-CBD-CGD-O1D
26	c	304	CLA	CHA-CBD-CGD-O2D
26	c	306	CLA	CBD-CGD-O2D-CED
26	c	307	CLA	C1A-C2A-CAA-CBA
26	c	307	CLA	C3A-C2A-CAA-CBA
26	c	308	CLA	C1A-C2A-CAA-CBA
26	c	308	CLA	C3A-C2A-CAA-CBA
26	c	311	CLA	C3A-C2A-CAA-CBA
26	c	312	CLA	CBD-CGD-O2D-CED
26	a	301	CLA	C1A-C2A-CAA-CBA
26	a	301	CLA	C3A-C2A-CAA-CBA
26	a	304	CLA	CHA-CBD-CGD-O1D
26	a	304	CLA	CHA-CBD-CGD-O2D
26	a	306	CLA	C1A-C2A-CAA-CBA
26	a	306	CLA	C3A-C2A-CAA-CBA
26	a	308	CLA	CBD-CGD-O2D-CED
26	a	311	CLA	C1A-C2A-CAA-CBA
26	a	311	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	a	311	CLA	CBD-CGD-O2D-CED
26	b	304	CLA	C1A-C2A-CAA-CBA
26	b	304	CLA	C3A-C2A-CAA-CBA
26	b	305	CLA	CBD-CGD-O2D-CED
26	b	306	CLA	CHA-CBD-CGD-O1D
26	b	306	CLA	CHA-CBD-CGD-O2D
26	b	306	CLA	CAD-CBD-CGD-O1D
26	b	306	CLA	CAD-CBD-CGD-O2D
26	b	311	CLA	CBD-CGD-O2D-CED
26	b	312	CLA	C1A-C2A-CAA-CBA
26	b	312	CLA	C3A-C2A-CAA-CBA
26	b	313	CLA	O1A-CGA-O2A-C1
26	h	302	CLA	O1A-CGA-O2A-C1
26	h	302	CLA	CBD-CGD-O2D-CED
26	h	304	CLA	CBD-CGD-O2D-CED
26	h	305	CLA	C1A-C2A-CAA-CBA
26	h	305	CLA	C3A-C2A-CAA-CBA
26	h	307	CLA	C1A-C2A-CAA-CBA
26	m	602	CLA	C1A-C2A-CAA-CBA
26	m	602	CLA	C3A-C2A-CAA-CBA
26	m	602	CLA	CHA-CBD-CGD-O1D
26	m	602	CLA	CHA-CBD-CGD-O2D
26	m	602	CLA	CBD-CGD-O2D-CED
26	m	603	CLA	C1A-C2A-CAA-CBA
26	m	603	CLA	C3A-C2A-CAA-CBA
26	m	604	CLA	CHA-CBD-CGD-O1D
26	m	604	CLA	CHA-CBD-CGD-O2D
26	m	604	CLA	CAD-CBD-CGD-O1D
26	m	605	CLA	C1A-C2A-CAA-CBA
26	m	605	CLA	C3A-C2A-CAA-CBA
26	m	608	CLA	C1A-C2A-CAA-CBA
26	m	608	CLA	C3A-C2A-CAA-CBA
26	m	609	CLA	C1A-C2A-CAA-CBA
26	m	609	CLA	C3A-C2A-CAA-CBA
26	m	609	CLA	CBD-CGD-O2D-CED
26	m	610	CLA	C1A-C2A-CAA-CBA
26	m	612	CLA	CBD-CGD-O2D-CED
26	m	613	CLA	CBD-CGD-O2D-CED
26	l	305	CLA	C1A-C2A-CAA-CBA
26	l	305	CLA	C3A-C2A-CAA-CBA
26	l	307	CLA	CBD-CGD-O2D-CED
26	l	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	l	309	CLA	C3A-C2A-CAA-CBA
26	k	601	CLA	CBD-CGD-O2D-CED
26	k	602	CLA	C1A-C2A-CAA-CBA
26	k	602	CLA	C3A-C2A-CAA-CBA
26	k	602	CLA	CBD-CGD-O2D-CED
26	k	604	CLA	CHA-CBD-CGD-O1D
26	k	604	CLA	CHA-CBD-CGD-O2D
26	k	605	CLA	CHA-CBD-CGD-O1D
26	k	605	CLA	CHA-CBD-CGD-O2D
26	k	609	CLA	C1A-C2A-CAA-CBA
26	k	609	CLA	C3A-C2A-CAA-CBA
26	k	609	CLA	CBD-CGD-O2D-CED
26	k	609	CLA	O1D-CGD-O2D-CED
26	k	610	CLA	C1A-C2A-CAA-CBA
26	k	610	CLA	C3A-C2A-CAA-CBA
26	k	610	CLA	CBD-CGD-O2D-CED
26	k	614	CLA	C1A-C2A-CAA-CBA
26	k	614	CLA	CBD-CGD-O2D-CED
26	i	301	CLA	C1A-C2A-CAA-CBA
26	i	301	CLA	C3A-C2A-CAA-CBA
26	i	301	CLA	CHA-CBD-CGD-O1D
26	i	301	CLA	CHA-CBD-CGD-O2D
26	i	304	CLA	CAD-CBD-CGD-O1D
26	i	304	CLA	CAD-CBD-CGD-O2D
26	i	305	CLA	C1A-C2A-CAA-CBA
26	i	306	CLA	C1A-C2A-CAA-CBA
26	i	306	CLA	C3A-C2A-CAA-CBA
26	i	307	CLA	C1A-C2A-CAA-CBA
26	i	307	CLA	C3A-C2A-CAA-CBA
26	i	308	CLA	CBA-CGA-O2A-C1
26	j	601	CLA	C1A-C2A-CAA-CBA
26	j	601	CLA	C3A-C2A-CAA-CBA
26	j	601	CLA	C2A-CAA-CBA-CGA
26	j	604	CLA	CHA-CBD-CGD-O1D
26	j	604	CLA	CHA-CBD-CGD-O2D
26	j	604	CLA	CAD-CBD-CGD-O1D
26	j	605	CLA	C1A-C2A-CAA-CBA
26	j	609	CLA	C1A-C2A-CAA-CBA
26	j	609	CLA	C3A-C2A-CAA-CBA
26	j	609	CLA	CBD-CGD-O2D-CED
26	j	610	CLA	C3A-C2A-CAA-CBA
26	j	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	j	612	CLA	CAD-CBD-CGD-O1D
26	j	612	CLA	CAD-CBD-CGD-O2D
26	j	612	CLA	CBD-CGD-O2D-CED
26	d	302	CLA	C1A-C2A-CAA-CBA
26	d	302	CLA	C3A-C2A-CAA-CBA
26	d	303	CLA	C2-C3-C5-C6
26	d	303	CLA	C4-C3-C5-C6
26	d	304	CLA	CHA-CBD-CGD-O1D
26	d	304	CLA	CHA-CBD-CGD-O2D
26	d	304	CLA	CBD-CGD-O2D-CED
26	d	306	CLA	CHA-CBD-CGD-O2D
26	d	307	CLA	C1A-C2A-CAA-CBA
26	d	308	CLA	C3A-C2A-CAA-CBA
26	d	308	CLA	C2A-CAA-CBA-CGA
26	d	309	CLA	CBD-CGD-O2D-CED
26	d	310	CLA	CHA-CBD-CGD-O1D
26	d	310	CLA	CHA-CBD-CGD-O2D
26	d	318	CLA	CBD-CGD-O2D-CED
26	n	603	CLA	C1A-C2A-CAA-CBA
26	n	604	CLA	C1A-C2A-CAA-CBA
26	n	604	CLA	C2-C3-C5-C6
26	n	604	CLA	C4-C3-C5-C6
26	n	607	CLA	C2-C3-C5-C6
26	n	607	CLA	C4-C3-C5-C6
26	n	608	CLA	C3A-C2A-CAA-CBA
26	n	609	CLA	C2-C3-C5-C6
26	n	609	CLA	C4-C3-C5-C6
26	n	610	CLA	C1A-C2A-CAA-CBA
26	n	610	CLA	C3A-C2A-CAA-CBA
26	n	613	CLA	C1A-C2A-CAA-CBA
26	n	613	CLA	C2A-CAA-CBA-CGA
26	Q	302	CLA	C1A-C2A-CAA-CBA
28	A	843	LHG	O1-C1-C2-C3
28	A	843	LHG	C3-O3-P-O5
28	A	844	LHG	O7-C5-C6-O8
28	A	849	LHG	C3-O3-P-O5
28	A	849	LHG	C4-O6-P-O5
28	A	855	LHG	O1-C1-C2-C3
28	B	851	LHG	C3-O3-P-O4
28	B	851	LHG	C4-O6-P-O4
28	B	851	LHG	O9-C7-O7-C5
28	B	851	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
28	L	207	LHG	C2-C3-O3-P
28	L	207	LHG	C3-O3-P-O4
28	L	207	LHG	C4-O6-P-O3
28	L	207	LHG	C4-O6-P-O4
28	L	208	LHG	C4-O6-P-O5
28	s	409	LHG	C4-O6-P-O3
28	s	409	LHG	C4-O6-P-O4
28	s	409	LHG	O9-C7-O7-C5
28	s	409	LHG	C8-C7-O7-C5
28	c	317	LHG	C8-C7-O7-C5
28	c	320	LHG	O1-C1-C2-C3
28	c	320	LHG	C3-O3-P-O5
28	c	320	LHG	C8-C7-O7-C5
28	b	302	LHG	O1-C1-C2-C3
28	b	302	LHG	C3-O3-P-O5
28	b	302	LHG	O7-C5-C6-O8
28	b	318	LHG	C3-O3-P-O5
28	b	318	LHG	C3-O3-P-O6
28	b	318	LHG	C8-C7-O7-C5
28	m	618	LHG	O7-C5-C6-O8
28	i	317	LHG	C8-C7-O7-C5
28	j	617	LHG	C4-O6-P-O5
28	n	619	LHG	O1-C1-C2-C3
28	n	619	LHG	O9-C7-O7-C5
28	n	619	LHG	C8-C7-O7-C5
29	A	845	WVN	C15-C13-C20-C23
29	A	845	WVN	C11-C19-C22-C26
29	A	845	WVN	C20-C23-C25-C27
29	A	845	WVN	C23-C25-C28-C30
29	A	845	WVN	C35-C32-C36-C39
29	A	845	WVN	C30-C33-C34-C37
29	A	845	WVN	C38-C34-C37-C40
29	A	846	WVN	C15-C13-C20-C23
29	A	846	WVN	C11-C19-C22-C26
29	A	846	WVN	C19-C22-C26-C29
29	A	846	WVN	C24-C22-C26-C29
29	A	846	WVN	C20-C23-C25-C27
29	A	846	WVN	C23-C25-C28-C30
29	A	846	WVN	C27-C25-C28-C30
29	A	846	WVN	C29-C31-C32-C35
29	A	846	WVN	C29-C31-C32-C36
29	A	846	WVN	C35-C32-C36-C39

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Mol	Chain	Res	Type	Atoms
29	A	846	WVN	C38-C34-C37-C40
29	A	847	WVN	C15-C13-C20-C23
29	A	847	WVN	C11-C19-C22-C24
29	A	847	WVN	C24-C22-C26-C29
29	A	847	WVN	C20-C23-C25-C28
29	A	847	WVN	C23-C25-C28-C30
29	A	847	WVN	C27-C25-C28-C30
29	A	847	WVN	C35-C32-C36-C39
29	A	847	WVN	C38-C34-C37-C40
29	A	848	WVN	C06-C13-C20-C23
29	A	848	WVN	C24-C22-C26-C29
29	A	848	WVN	C23-C25-C28-C30
29	A	848	WVN	C29-C31-C32-C35
29	A	848	WVN	C29-C31-C32-C36
29	A	848	WVN	C31-C32-C36-C39
29	A	848	WVN	C30-C33-C34-C38
29	A	848	WVN	C38-C34-C37-C40
29	A	857	WVN	C15-C13-C20-C23
29	A	857	WVN	C11-C19-C22-C24
29	A	857	WVN	C24-C22-C26-C29
29	A	857	WVN	C20-C23-C25-C27
29	A	857	WVN	C23-C25-C28-C30
29	A	857	WVN	C22-C26-C29-C31
29	A	857	WVN	C29-C31-C32-C36
29	A	857	WVN	C35-C32-C36-C39
29	A	857	WVN	C38-C34-C37-C40
29	B	845	WVN	C01-C02-C11-C19
29	B	845	WVN	C05-C02-C11-C19
29	B	846	WVN	C19-C22-C26-C29
29	B	846	WVN	C23-C25-C28-C30
29	B	846	WVN	C27-C25-C28-C30
29	B	846	WVN	C29-C31-C32-C35
29	B	846	WVN	C29-C31-C32-C36
29	B	846	WVN	C35-C32-C36-C39
29	B	846	WVN	C30-C33-C34-C38
29	B	846	WVN	C38-C34-C37-C40
29	B	847	WVN	C15-C13-C20-C23
29	B	847	WVN	C11-C19-C22-C24
29	B	847	WVN	C19-C22-C26-C29
29	B	847	WVN	C20-C23-C25-C27
29	B	847	WVN	C23-C25-C28-C30
29	B	847	WVN	C27-C25-C28-C30

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Mol	Chain	Res	Type	Atoms
29	B	847	WVN	C29-C31-C32-C35
29	B	847	WVN	C35-C32-C36-C39
29	B	847	WVN	C30-C33-C34-C38
29	B	847	WVN	C38-C34-C37-C40
29	B	848	WVN	C15-C13-C20-C23
29	B	848	WVN	C24-C22-C26-C29
29	B	848	WVN	C20-C23-C25-C27
29	B	848	WVN	C27-C25-C28-C30
29	B	848	WVN	C35-C32-C36-C39
29	B	848	WVN	C30-C33-C34-C38
29	B	848	WVN	C38-C34-C37-C40
29	B	849	WVN	C15-C13-C20-C23
29	B	849	WVN	C11-C19-C22-C24
29	B	849	WVN	C24-C22-C26-C29
29	B	849	WVN	C20-C23-C25-C27
29	B	849	WVN	C20-C23-C25-C28
29	B	849	WVN	C23-C25-C28-C30
29	B	849	WVN	C25-C28-C30-C33
29	B	849	WVN	C29-C31-C32-C35
29	B	849	WVN	C35-C32-C36-C39
29	B	849	WVN	C38-C34-C37-C40
29	B	850	WVN	C24-C22-C26-C29
29	B	850	WVN	C20-C23-C25-C28
29	B	850	WVN	C23-C25-C28-C30
29	B	850	WVN	C29-C31-C32-C35
29	B	850	WVN	C35-C32-C36-C39
29	B	850	WVN	C30-C33-C34-C37
29	B	850	WVN	C38-C34-C37-C40
29	B	850	WVN	C32-C36-C39-C40
29	B	850	WVN	C34-C37-C40-C39
29	B	853	WVN	C01-C02-C11-C19
29	B	853	WVN	C05-C02-C11-C19
29	B	853	WVN	C15-C13-C20-C23
29	B	853	WVN	C11-C19-C22-C24
29	B	853	WVN	C19-C22-C26-C29
29	B	853	WVN	C24-C22-C26-C29
29	B	853	WVN	C23-C25-C28-C30
29	B	853	WVN	C27-C25-C28-C30
29	B	853	WVN	C35-C32-C36-C39
29	B	853	WVN	C38-C34-C37-C40
29	F	203	WVN	C15-C13-C20-C23
29	F	203	WVN	C11-C19-C22-C24

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Mol	Chain	Res	Type	Atoms
29	F	203	WVN	C11-C19-C22-C26
29	F	203	WVN	C19-C22-C26-C29
29	F	203	WVN	C20-C23-C25-C27
29	F	203	WVN	C27-C25-C28-C30
29	F	203	WVN	C31-C32-C36-C39
29	F	203	WVN	C30-C33-C34-C37
29	F	203	WVN	C30-C33-C34-C38
29	F	203	WVN	C38-C34-C37-C40
29	F	204	WVN	C06-C13-C20-C23
29	F	204	WVN	C15-C13-C20-C23
29	I	101	WVN	C15-C13-C20-C23
29	I	101	WVN	C19-C22-C26-C29
29	I	101	WVN	C24-C22-C26-C29
29	I	101	WVN	C23-C25-C28-C30
29	I	101	WVN	C27-C25-C28-C30
29	I	101	WVN	C35-C32-C36-C39
29	I	101	WVN	C30-C33-C34-C38
29	I	101	WVN	C38-C34-C37-C40
29	J	101	WVN	C15-C13-C20-C23
29	J	101	WVN	C19-C22-C26-C29
29	J	101	WVN	C20-C23-C25-C27
29	J	101	WVN	C20-C23-C25-C28
29	J	101	WVN	C27-C25-C28-C30
29	J	101	WVN	C22-C26-C29-C31
29	J	101	WVN	C35-C32-C36-C39
29	J	101	WVN	C38-C34-C37-C40
29	J	101	WVN	C34-C37-C40-C39
29	J	102	WVN	C15-C13-C20-C23
29	J	102	WVN	C11-C19-C22-C26
29	J	102	WVN	C19-C22-C26-C29
29	J	102	WVN	C24-C22-C26-C29
29	J	102	WVN	C20-C23-C25-C27
29	J	102	WVN	C23-C25-C28-C30
29	J	102	WVN	C27-C25-C28-C30
29	J	102	WVN	C29-C31-C32-C36
29	J	102	WVN	C35-C32-C36-C39
29	J	102	WVN	C30-C33-C34-C37
29	J	102	WVN	C38-C34-C37-C40
29	L	201	WVN	C15-C13-C20-C23
29	L	201	WVN	C11-C19-C22-C26
29	L	201	WVN	C24-C22-C26-C29
29	L	201	WVN	C20-C23-C25-C27

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Mol	Chain	Res	Type	Atoms
29	L	201	WVN	C20-C23-C25-C28
29	L	201	WVN	C23-C25-C28-C30
29	L	201	WVN	C27-C25-C28-C30
29	L	201	WVN	C25-C28-C30-C33
29	L	201	WVN	C29-C31-C32-C36
29	L	201	WVN	C35-C32-C36-C39
29	L	201	WVN	C30-C33-C34-C37
29	L	201	WVN	C38-C34-C37-C40
29	L	205	WVN	C19-C22-C26-C29
29	L	205	WVN	C20-C23-C25-C27
29	L	205	WVN	C20-C23-C25-C28
29	L	205	WVN	C27-C25-C28-C30
29	L	205	WVN	C29-C31-C32-C36
29	L	205	WVN	C35-C32-C36-C39
29	L	205	WVN	C30-C33-C34-C37
29	L	205	WVN	C38-C34-C37-C40
29	M	101	WVN	C15-C13-C20-C23
29	M	101	WVN	C11-C19-C22-C24
29	M	101	WVN	C24-C22-C26-C29
29	M	101	WVN	C20-C23-C25-C27
29	M	101	WVN	C23-C25-C28-C30
29	M	101	WVN	C27-C25-C28-C30
29	M	101	WVN	C29-C31-C32-C35
29	M	101	WVN	C29-C31-C32-C36
29	M	101	WVN	C35-C32-C36-C39
29	M	101	WVN	C30-C33-C34-C37
29	M	101	WVN	C38-C34-C37-C40
29	K	102	WVN	C15-C13-C20-C23
29	K	102	WVN	C19-C22-C26-C29
29	K	102	WVN	C24-C22-C26-C29
29	K	102	WVN	C20-C23-C25-C28
29	K	102	WVN	C23-C25-C28-C30
29	K	102	WVN	C27-C25-C28-C30
29	K	102	WVN	C35-C32-C36-C39
29	K	102	WVN	C30-C33-C34-C37
29	K	102	WVN	C30-C33-C34-C38
29	K	102	WVN	C38-C34-C37-C40
29	s	405	WVN	C06-C13-C20-C23
29	s	405	WVN	C11-C19-C22-C24
29	s	405	WVN	C11-C19-C22-C26
29	s	405	WVN	C24-C22-C26-C29
29	s	405	WVN	C23-C25-C28-C30

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Mol	Chain	Res	Type	Atoms
29	s	405	WVN	C27-C25-C28-C30
29	s	405	WVN	C29-C31-C32-C35
29	s	405	WVN	C35-C32-C36-C39
29	s	405	WVN	C33-C34-C37-C40
29	s	407	WVN	C15-C13-C20-C23
29	s	407	WVN	C11-C19-C22-C24
29	s	407	WVN	C24-C22-C26-C29
29	s	407	WVN	C20-C23-C25-C27
29	s	407	WVN	C20-C23-C25-C28
29	s	407	WVN	C27-C25-C28-C30
29	s	407	WVN	C35-C32-C36-C39
29	s	407	WVN	C38-C34-C37-C40
29	h	309	WVN	C06-C13-C20-C23
29	h	309	WVN	C24-C22-C26-C29
29	h	309	WVN	C23-C25-C28-C30
29	h	309	WVN	C27-C25-C28-C30
29	h	309	WVN	C29-C31-C32-C36
29	h	309	WVN	C35-C32-C36-C39
29	h	309	WVN	C30-C33-C34-C37
29	h	309	WVN	C38-C34-C37-C40
29	l	303	WVN	C11-C19-C22-C24
29	l	303	WVN	C24-C22-C26-C29
29	l	303	WVN	C27-C25-C28-C30
29	l	303	WVN	C29-C31-C32-C35
29	l	303	WVN	C29-C31-C32-C36
29	l	303	WVN	C35-C32-C36-C39
29	l	303	WVN	C38-C34-C37-C40
29	l	316	WVN	C11-C19-C22-C24
29	l	316	WVN	C24-C22-C26-C29
29	l	316	WVN	C23-C25-C28-C30
29	l	316	WVN	C27-C25-C28-C30
29	l	316	WVN	C35-C32-C36-C39
29	l	316	WVN	C38-C34-C37-C40
29	i	315	WVN	C19-C22-C26-C29
29	i	315	WVN	C24-C22-C26-C29
29	i	315	WVN	C27-C25-C28-C30
29	i	315	WVN	C29-C31-C32-C35
29	i	315	WVN	C29-C31-C32-C36
29	i	315	WVN	C35-C32-C36-C39
29	i	315	WVN	C30-C33-C34-C37
29	i	315	WVN	C38-C34-C37-C40
29	R	200	WVN	C06-C13-C20-C23

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Mol	Chain	Res	Type	Atoms
29	R	200	WVN	C19-C22-C26-C29
29	R	200	WVN	C24-C22-C26-C29
29	R	200	WVN	C23-C25-C28-C30
29	R	200	WVN	C27-C25-C28-C30
29	R	200	WVN	C25-C28-C30-C33
29	R	200	WVN	C29-C31-C32-C35
29	R	200	WVN	C35-C32-C36-C39
29	R	200	WVN	C38-C34-C37-C40
30	A	850	LMU	O5B-C1B-O1B-C4'
30	A	850	LMU	C2-C1-O1'-C1'
30	i	300	LMU	C2'-C1'-O1'-C1
30	i	300	LMU	O5'-C1'-O1'-C1
30	i	300	LMU	C2-C1-O1'-C1'
32	A	854	SQD	C2-C1-O6-C44
32	A	854	SQD	O5-C1-O6-C44
32	A	854	SQD	O5-C5-C6-S
33	B	844	DGD	O6D-C1D-O3G-C3G
34	Q	301	LMG	C2-C1-O1-C7
34	Q	301	LMG	O6-C1-O1-C7
34	Q	301	LMG	C11-C10-O7-C8
35	J	104	II0	C27-C25-C29-C31
35	J	104	II0	C24-C26-C30-C32
35	J	104	II0	C28-C26-C30-C32
35	J	104	II0	C31-C33-C35-C37
35	J	104	II0	C31-C33-C35-C39
35	J	104	II0	C32-C34-C36-C38
35	J	104	II0	C37-C35-C39-C41
35	J	104	II0	C38-C36-C40-C42
35	c	313	II0	C23-C25-C29-C31
35	c	313	II0	C24-C26-C30-C32
35	c	313	II0	C31-C33-C35-C37
35	c	313	II0	C31-C33-C35-C39
35	c	313	II0	C32-C34-C36-C40
35	c	313	II0	C33-C35-C39-C41
35	c	316	II0	C23-C25-C29-C31
35	c	316	II0	C24-C26-C30-C32
35	c	316	II0	C28-C26-C30-C32
35	c	316	II0	C31-C33-C35-C37
35	c	316	II0	C32-C34-C36-C40
35	c	316	II0	C37-C35-C39-C41
35	c	316	II0	C38-C36-C40-C42
35	a	312	II0	C23-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
35	a	312	II0	C24-C26-C30-C32
35	a	312	II0	C28-C26-C30-C32
35	a	312	II0	C26-C30-C32-C34
35	a	312	II0	C37-C35-C39-C41
35	a	312	II0	C38-C36-C40-C42
35	a	313	II0	C23-C25-C29-C31
35	a	313	II0	C24-C26-C30-C32
35	a	313	II0	C31-C33-C35-C37
35	a	313	II0	C31-C33-C35-C39
35	a	313	II0	C32-C34-C36-C40
35	a	313	II0	C37-C35-C39-C41
35	a	313	II0	C38-C36-C40-C42
35	a	314	II0	C23-C25-C29-C31
35	a	314	II0	C24-C26-C30-C32
35	a	314	II0	C32-C34-C36-C38
35	a	314	II0	C37-C35-C39-C41
35	a	314	II0	C38-C36-C40-C42
35	a	316	II0	C27-C25-C29-C31
35	a	316	II0	C24-C26-C30-C32
35	a	316	II0	C25-C29-C31-C33
35	a	316	II0	C26-C30-C32-C34
35	a	316	II0	C31-C33-C35-C37
35	a	316	II0	C37-C35-C39-C41
35	a	316	II0	C38-C36-C40-C42
35	b	314	II0	C27-C25-C29-C31
35	b	314	II0	C24-C26-C30-C32
35	b	314	II0	C32-C34-C36-C38
35	b	314	II0	C33-C35-C39-C41
35	b	314	II0	C38-C36-C40-C42
35	b	315	II0	C27-C25-C29-C31
35	b	315	II0	C24-C26-C30-C32
35	b	315	II0	C28-C26-C30-C32
35	b	315	II0	C25-C29-C31-C33
35	b	315	II0	C31-C33-C35-C37
35	b	315	II0	C37-C35-C39-C41
35	b	315	II0	C38-C36-C40-C42
35	h	310	II0	C23-C25-C29-C31
35	h	310	II0	C32-C34-C36-C38
35	h	310	II0	C37-C35-C39-C41
35	h	310	II0	C34-C36-C40-C42
35	h	311	II0	C23-C25-C29-C31
35	h	311	II0	C27-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
35	h	311	II0	C24-C26-C30-C32
35	h	311	II0	C25-C29-C31-C33
35	h	311	II0	C31-C33-C35-C37
35	h	311	II0	C32-C34-C36-C40
35	h	311	II0	C37-C35-C39-C41
35	h	311	II0	C38-C36-C40-C42
35	h	312	II0	C23-C25-C29-C31
35	h	312	II0	C24-C26-C30-C32
35	h	312	II0	C31-C33-C35-C37
35	h	312	II0	C31-C33-C35-C39
35	h	312	II0	C33-C35-C39-C41
35	h	312	II0	C38-C36-C40-C42
35	m	614	II0	C23-C25-C29-C31
35	m	614	II0	C27-C25-C29-C31
35	m	614	II0	C24-C26-C30-C32
35	m	614	II0	C31-C33-C35-C37
35	m	614	II0	C37-C35-C39-C41
35	m	614	II0	C38-C36-C40-C42
35	m	615	II0	C23-C25-C29-C31
35	m	615	II0	C24-C26-C30-C32
35	m	615	II0	C26-C30-C32-C34
35	m	615	II0	C31-C33-C35-C37
35	m	615	II0	C31-C33-C35-C39
35	m	615	II0	C32-C34-C36-C38
35	m	615	II0	C37-C35-C39-C41
35	m	615	II0	C38-C36-C40-C42
35	m	616	II0	C23-C25-C29-C31
35	m	616	II0	C27-C25-C29-C31
35	m	616	II0	C24-C26-C30-C32
35	m	616	II0	C31-C33-C35-C39
35	m	616	II0	C32-C34-C36-C40
35	m	616	II0	C37-C35-C39-C41
35	m	616	II0	C38-C36-C40-C42
35	m	619	II0	C23-C25-C29-C31
35	m	619	II0	C27-C25-C29-C31
35	m	619	II0	C24-C26-C30-C32
35	m	619	II0	C25-C29-C31-C33
35	m	619	II0	C31-C33-C35-C37
35	m	619	II0	C32-C34-C36-C38
35	m	619	II0	C37-C35-C39-C41
35	m	619	II0	C38-C36-C40-C42
35	l	302	II0	C23-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
35	l	302	II0	C27-C25-C29-C31
35	l	302	II0	C24-C26-C30-C32
35	l	302	II0	C31-C33-C35-C37
35	l	302	II0	C32-C34-C36-C38
35	l	302	II0	C32-C34-C36-C40
35	l	302	II0	C33-C35-C39-C41
35	l	302	II0	C37-C35-C39-C41
35	l	302	II0	C38-C36-C40-C42
35	l	314	II0	C23-C25-C29-C31
35	l	314	II0	C28-C26-C30-C32
35	l	314	II0	C26-C30-C32-C34
35	l	314	II0	C31-C33-C35-C37
35	l	314	II0	C32-C34-C36-C40
35	l	314	II0	C38-C36-C40-C42
35	l	315	II0	C23-C25-C29-C31
35	l	315	II0	C24-C26-C30-C32
35	l	315	II0	C32-C34-C36-C38
35	l	315	II0	C37-C35-C39-C41
35	l	315	II0	C34-C36-C40-C42
35	l	317	II0	C23-C25-C29-C31
35	k	615	II0	C23-C25-C29-C31
35	k	615	II0	C27-C25-C29-C31
35	k	615	II0	C24-C26-C30-C32
35	k	615	II0	C28-C26-C30-C32
35	k	615	II0	C31-C33-C35-C37
35	k	615	II0	C37-C35-C39-C41
35	k	615	II0	C34-C36-C40-C42
35	k	615	II0	C38-C36-C40-C42
35	k	616	II0	C27-C25-C29-C31
35	k	616	II0	C24-C26-C30-C32
35	k	616	II0	C26-C30-C32-C34
35	k	616	II0	C31-C33-C35-C37
35	k	616	II0	C31-C33-C35-C39
35	k	616	II0	C32-C34-C36-C38
35	k	616	II0	C33-C35-C39-C41
35	k	616	II0	C34-C36-C40-C42
35	k	617	II0	C23-C25-C29-C31
35	k	619	II0	C23-C25-C29-C31
35	k	619	II0	C24-C26-C30-C32
35	k	619	II0	C33-C35-C39-C41
35	k	619	II0	C37-C35-C39-C41
35	k	619	II0	C38-C36-C40-C42

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Mol	Chain	Res	Type	Atoms
35	k	620	II0	C23-C25-C29-C31
35	k	620	II0	C27-C25-C29-C31
35	k	620	II0	C24-C26-C30-C32
35	k	620	II0	C31-C33-C35-C37
35	k	620	II0	C32-C34-C36-C40
35	k	620	II0	C37-C35-C39-C41
35	k	620	II0	C38-C36-C40-C42
35	i	312	II0	C27-C25-C29-C31
35	i	312	II0	C24-C26-C30-C32
35	i	312	II0	C28-C26-C30-C32
35	i	312	II0	C31-C33-C35-C37
35	i	312	II0	C31-C33-C35-C39
35	i	312	II0	C32-C34-C36-C40
35	i	312	II0	C33-C35-C39-C41
35	i	313	II0	C27-C25-C29-C31
35	i	313	II0	C24-C26-C30-C32
35	i	313	II0	C28-C26-C30-C32
35	i	313	II0	C31-C33-C35-C37
35	i	313	II0	C31-C33-C35-C39
35	i	313	II0	C32-C34-C36-C38
35	i	313	II0	C32-C34-C36-C40
35	i	313	II0	C37-C35-C39-C41
35	i	313	II0	C38-C36-C40-C42
35	i	314	II0	C23-C25-C29-C31
35	i	314	II0	C24-C26-C30-C32
35	i	314	II0	C28-C26-C30-C32
35	i	314	II0	C32-C34-C36-C38
35	i	314	II0	C32-C34-C36-C40
35	i	314	II0	C37-C35-C39-C41
35	i	314	II0	C38-C36-C40-C42
35	i	316	II0	C23-C25-C29-C31
35	i	316	II0	C24-C26-C30-C32
35	i	316	II0	C28-C26-C30-C32
35	i	316	II0	C31-C33-C35-C37
35	i	316	II0	C32-C34-C36-C40
35	i	316	II0	C37-C35-C39-C41
35	i	316	II0	C38-C36-C40-C42
35	i	319	II0	C23-C25-C29-C31
35	i	319	II0	C24-C26-C30-C32
35	i	319	II0	C31-C33-C35-C37
35	i	319	II0	C31-C33-C35-C39
35	i	319	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
35	i	319	II0	C37-C35-C39-C41
35	i	319	II0	C38-C36-C40-C42
35	j	614	II0	C23-C25-C29-C31
35	j	614	II0	C24-C26-C30-C32
35	j	614	II0	C32-C34-C36-C38
35	j	614	II0	C37-C35-C39-C41
35	j	614	II0	C38-C36-C40-C42
35	j	615	II0	C23-C25-C29-C31
35	j	615	II0	C24-C26-C30-C32
35	j	615	II0	C26-C30-C32-C34
35	j	615	II0	C31-C33-C35-C37
35	j	615	II0	C31-C33-C35-C39
35	j	615	II0	C33-C35-C39-C41
35	j	615	II0	C38-C36-C40-C42
35	d	301	II0	C23-C25-C29-C31
35	d	301	II0	C24-C26-C30-C32
35	d	301	II0	C37-C35-C39-C41
35	d	301	II0	C38-C36-C40-C42
35	d	315	II0	C23-C25-C29-C31
35	d	315	II0	C27-C25-C29-C31
35	d	315	II0	C28-C26-C30-C32
35	d	315	II0	C31-C33-C35-C37
35	d	315	II0	C31-C33-C35-C39
35	d	315	II0	C32-C34-C36-C38
35	d	315	II0	C32-C34-C36-C40
35	d	315	II0	C33-C35-C39-C41
35	d	315	II0	C38-C36-C40-C42
35	d	316	II0	C23-C25-C29-C31
35	d	316	II0	C27-C25-C29-C31
35	d	316	II0	C24-C26-C30-C32
35	d	316	II0	C28-C26-C30-C32
35	d	316	II0	C31-C33-C35-C37
35	d	316	II0	C33-C35-C39-C41
35	d	316	II0	C38-C36-C40-C42
35	d	317	II0	C23-C25-C29-C31
35	d	317	II0	C24-C26-C30-C32
35	d	317	II0	C28-C26-C30-C32
35	d	317	II0	C31-C33-C35-C37
35	d	317	II0	C31-C33-C35-C39
35	d	317	II0	C37-C35-C39-C41
35	d	317	II0	C38-C36-C40-C42
35	d	319	II0	C23-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
35	d	319	II0	C27-C25-C29-C31
35	d	319	II0	C24-C26-C30-C32
35	d	319	II0	C28-C26-C30-C32
35	d	319	II0	C25-C29-C31-C33
35	d	319	II0	C31-C33-C35-C37
35	d	319	II0	C31-C33-C35-C39
35	d	319	II0	C32-C34-C36-C38
35	n	615	II0	C23-C25-C29-C31
35	n	615	II0	C27-C25-C29-C31
35	n	615	II0	C24-C26-C30-C32
35	n	615	II0	C31-C33-C35-C37
35	n	615	II0	C32-C34-C36-C38
35	n	615	II0	C32-C34-C36-C40
35	n	615	II0	C37-C35-C39-C41
35	n	615	II0	C38-C36-C40-C42
35	n	616	II0	C23-C25-C29-C31
35	n	616	II0	C27-C25-C29-C31
35	n	616	II0	C24-C26-C30-C32
35	n	616	II0	C26-C30-C32-C34
35	n	616	II0	C31-C33-C35-C37
35	n	616	II0	C32-C34-C36-C40
35	n	616	II0	C37-C35-C39-C41
35	n	616	II0	C38-C36-C40-C42
35	n	618	II0	C23-C25-C29-C31
35	n	618	II0	C24-C26-C30-C32
35	n	618	II0	C28-C26-C30-C32
35	n	618	II0	C31-C33-C35-C37
35	n	618	II0	C31-C33-C35-C39
35	n	618	II0	C37-C35-C39-C41
35	n	618	II0	C38-C36-C40-C42
36	s	401	KC2	C3A-C2A-CAA-CBA
36	s	401	KC2	C2C-C3C-CAC-CBC
36	s	401	KC2	C4C-C3C-CAC-CBC
36	s	401	KC2	C2A-CAA-CBA-CGA
36	c	310	KC2	C1A-C2A-CAA-CBA
36	c	310	KC2	C2C-C3C-CAC-CBC
36	c	310	KC2	C4C-C3C-CAC-CBC
36	c	310	KC2	C2A-CAA-CBA-CGA
36	m	611	KC2	C1A-C2A-CAA-CBA
36	m	611	KC2	C3A-C2A-CAA-CBA
36	m	611	KC2	C2C-C3C-CAC-CBC
36	m	611	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
36	m	611	KC2	C2A-CAA-CBA-CGA
36	l	312	KC2	C2B-C3B-CAB-CBB
36	k	611	KC2	C1A-C2A-CAA-CBA
36	k	611	KC2	C3A-C2A-CAA-CBA
36	k	611	KC2	C2B-C3B-CAB-CBB
36	k	611	KC2	C4B-C3B-CAB-CBB
36	k	612	KC2	C2B-C3B-CAB-CBB
36	k	612	KC2	C4B-C3B-CAB-CBB
36	k	612	KC2	CBD-CGD-O2D-CED
36	k	613	KC2	C1A-C2A-CAA-CBA
36	k	613	KC2	C3A-C2A-CAA-CBA
36	k	613	KC2	C2B-C3B-CAB-CBB
36	k	613	KC2	C4B-C3B-CAB-CBB
36	k	613	KC2	C2C-C3C-CAC-CBC
36	k	613	KC2	C4C-C3C-CAC-CBC
36	k	613	KC2	CBD-CGD-O2D-CED
36	i	309	KC2	C1A-C2A-CAA-CBA
36	i	309	KC2	C3A-C2A-CAA-CBA
36	i	309	KC2	C2B-C3B-CAB-CBB
36	i	309	KC2	C4B-C3B-CAB-CBB
36	i	318	KC2	C1A-C2A-CAA-CBA
36	i	318	KC2	C3A-C2A-CAA-CBA
36	i	318	KC2	C2B-C3B-CAB-CBB
36	i	318	KC2	C4B-C3B-CAB-CBB
36	i	318	KC2	CBD-CGD-O2D-CED
36	i	318	KC2	O1D-CGD-O2D-CED
36	j	611	KC2	C1A-C2A-CAA-CBA
36	j	611	KC2	C3A-C2A-CAA-CBA
36	j	611	KC2	C2B-C3B-CAB-CBB
36	j	611	KC2	C4B-C3B-CAB-CBB
36	j	611	KC2	C2C-C3C-CAC-CBC
36	j	611	KC2	C4C-C3C-CAC-CBC
36	j	611	KC2	CBD-CGD-O2D-CED
36	d	311	KC2	C1A-C2A-CAA-CBA
36	d	311	KC2	C3A-C2A-CAA-CBA
36	d	311	KC2	C2C-C3C-CAC-CBC
36	d	311	KC2	C4C-C3C-CAC-CBC
36	d	311	KC2	C2A-CAA-CBA-CGA
36	d	312	KC2	C1A-C2A-CAA-CBA
36	d	312	KC2	C3A-C2A-CAA-CBA
36	n	611	KC2	C1A-C2A-CAA-CBA
36	n	611	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	n	611	KC2	C2B-C3B-CAB-CBB
36	n	611	KC2	C2C-C3C-CAC-CBC
36	n	611	KC2	C4C-C3C-CAC-CBC
36	n	611	KC2	C2A-CAA-CBA-CGA
36	n	611	KC2	CBD-CGD-O2D-CED
36	n	612	KC2	C1A-C2A-CAA-CBA
36	n	612	KC2	C3A-C2A-CAA-CBA
36	n	612	KC2	C2C-C3C-CAC-CBC
36	n	612	KC2	C4C-C3C-CAC-CBC
36	n	612	KC2	C2A-CAA-CBA-CGA
37	a	315	IHT	C02-C07-C18-C22
37	a	315	IHT	C24-C26-C29-C31
37	b	301	IHT	C18-C22-C23-C25
37	b	301	IHT	C18-C22-C23-C27
37	b	316	IHT	C18-C22-C23-C25
37	b	316	IHT	C18-C22-C23-C27
37	b	316	IHT	C30-C32-C33-C36
37	b	316	IHT	C30-C32-C33-C37
37	m	617	IHT	C18-C22-C23-C25
37	m	617	IHT	C18-C22-C23-C27
37	R	202	IHT	C02-C07-C18-C22
25	A	801	CL0	O1D-CGD-O2D-CED
26	A	809	CLA	O1D-CGD-O2D-CED
26	A	810	CLA	O1D-CGD-O2D-CED
26	A	840	CLA	O1D-CGD-O2D-CED
26	B	803	CLA	O1D-CGD-O2D-CED
26	L	204	CLA	O1D-CGD-O2D-CED
26	K	101	CLA	O1D-CGD-O2D-CED
26	c	302	CLA	O1D-CGD-O2D-CED
26	c	308	CLA	O1D-CGD-O2D-CED
26	m	603	CLA	O1D-CGD-O2D-CED
26	m	609	CLA	O1D-CGD-O2D-CED
26	k	601	CLA	O1D-CGD-O2D-CED
26	i	310	CLA	O1D-CGD-O2D-CED
26	j	609	CLA	O1D-CGD-O2D-CED
26	d	303	CLA	O1D-CGD-O2D-CED
36	k	612	KC2	O1D-CGD-O2D-CED
36	k	613	KC2	O1D-CGD-O2D-CED
36	n	611	KC2	O1D-CGD-O2D-CED
26	A	819	CLA	O1D-CGD-O2D-CED
26	c	305	CLA	O1D-CGD-O2D-CED
26	b	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	k	614	CLA	O1D-CGD-O2D-CED
26	d	304	CLA	O1D-CGD-O2D-CED
26	n	601	CLA	O1D-CGD-O2D-CED
36	k	611	KC2	O1D-CGD-O2D-CED
25	A	801	CL0	CBD-CGD-O2D-CED
26	A	814	CLA	CBD-CGD-O2D-CED
26	A	815	CLA	CBD-CGD-O2D-CED
26	A	821	CLA	CBD-CGD-O2D-CED
26	A	822	CLA	CBD-CGD-O2D-CED
26	A	827	CLA	CBD-CGD-O2D-CED
26	A	831	CLA	CBD-CGD-O2D-CED
26	A	832	CLA	CBD-CGD-O2D-CED
26	A	840	CLA	CBD-CGD-O2D-CED
26	B	804	CLA	CBD-CGD-O2D-CED
26	B	808	CLA	CBD-CGD-O2D-CED
26	B	825	CLA	CBD-CGD-O2D-CED
26	B	827	CLA	CBD-CGD-O2D-CED
26	B	828	CLA	CBD-CGD-O2D-CED
26	B	840	CLA	CBD-CGD-O2D-CED
26	B	842	CLA	CBD-CGD-O2D-CED
26	F	202	CLA	CBD-CGD-O2D-CED
26	K	101	CLA	CBD-CGD-O2D-CED
26	c	303	CLA	CBD-CGD-O2D-CED
26	c	305	CLA	CBD-CGD-O2D-CED
26	c	308	CLA	CBD-CGD-O2D-CED
26	a	305	CLA	CBD-CGD-O2D-CED
26	b	306	CLA	CBD-CGD-O2D-CED
26	b	312	CLA	CBD-CGD-O2D-CED
26	m	603	CLA	CBD-CGD-O2D-CED
26	l	301	CLA	CBD-CGD-O2D-CED
26	l	309	CLA	CBD-CGD-O2D-CED
26	k	607	CLA	CBD-CGD-O2D-CED
26	i	301	CLA	CBD-CGD-O2D-CED
26	i	307	CLA	CBD-CGD-O2D-CED
26	i	308	CLA	CBD-CGD-O2D-CED
26	i	310	CLA	CBD-CGD-O2D-CED
26	j	601	CLA	CBD-CGD-O2D-CED
26	j	610	CLA	CBD-CGD-O2D-CED
26	j	613	CLA	CBD-CGD-O2D-CED
26	d	302	CLA	CBD-CGD-O2D-CED
26	d	303	CLA	CBD-CGD-O2D-CED
26	d	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	R	201	CLA	CBD-CGD-O2D-CED
26	n	601	CLA	CBD-CGD-O2D-CED
26	n	613	CLA	CBD-CGD-O2D-CED
36	k	611	KC2	CBD-CGD-O2D-CED
36	d	311	KC2	CBD-CGD-O2D-CED
36	d	312	KC2	CBD-CGD-O2D-CED
26	a	310	CLA	O1A-CGA-O2A-C1
26	b	303	CLA	O1A-CGA-O2A-C1
26	i	308	CLA	O1A-CGA-O2A-C1
26	A	815	CLA	O1D-CGD-O2D-CED
26	A	827	CLA	O1D-CGD-O2D-CED
26	B	825	CLA	O1D-CGD-O2D-CED
26	J	103	CLA	O1D-CGD-O2D-CED
26	c	303	CLA	O1D-CGD-O2D-CED
26	b	312	CLA	O1D-CGD-O2D-CED
26	h	302	CLA	O1D-CGD-O2D-CED
26	m	602	CLA	O1D-CGD-O2D-CED
26	j	601	CLA	O1D-CGD-O2D-CED
26	n	613	CLA	O1D-CGD-O2D-CED
36	j	611	KC2	O1D-CGD-O2D-CED
36	d	311	KC2	O1D-CGD-O2D-CED
36	d	312	KC2	O1D-CGD-O2D-CED
26	B	819	CLA	C4C-C3C-CAC-CBC
30	a	317	LMU	O5B-C1B-O1B-C4'
30	i	300	LMU	O5B-C1B-O1B-C4'
26	B	804	CLA	O1D-CGD-O2D-CED
26	s	403	CLA	O1D-CGD-O2D-CED
26	c	306	CLA	O1D-CGD-O2D-CED
26	c	312	CLA	O1D-CGD-O2D-CED
26	a	311	CLA	O1D-CGD-O2D-CED
26	h	304	CLA	O1D-CGD-O2D-CED
26	m	612	CLA	O1D-CGD-O2D-CED
26	m	613	CLA	O1D-CGD-O2D-CED
26	k	610	CLA	O1D-CGD-O2D-CED
26	j	613	CLA	O1D-CGD-O2D-CED
26	d	309	CLA	O1D-CGD-O2D-CED
26	d	318	CLA	O1D-CGD-O2D-CED
26	a	310	CLA	CBA-CGA-O2A-C1
26	b	303	CLA	CBA-CGA-O2A-C1
28	A	849	LHG	C8-C7-O7-C5
26	A	804	CLA	CBD-CGD-O2D-CED
26	A	813	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	823	CLA	CBD-CGD-O2D-CED
26	A	836	CLA	CBD-CGD-O2D-CED
26	B	821	CLA	CBD-CGD-O2D-CED
26	B	830	CLA	CBD-CGD-O2D-CED
26	B	841	CLA	CBD-CGD-O2D-CED
26	s	402	CLA	CBD-CGD-O2D-CED
26	c	301	CLA	CBD-CGD-O2D-CED
26	c	304	CLA	CBD-CGD-O2D-CED
26	c	307	CLA	CBD-CGD-O2D-CED
26	b	307	CLA	CBD-CGD-O2D-CED
26	h	305	CLA	CBD-CGD-O2D-CED
26	h	308	CLA	CBD-CGD-O2D-CED
26	m	601	CLA	CBD-CGD-O2D-CED
26	m	605	CLA	CBD-CGD-O2D-CED
26	m	606	CLA	CBD-CGD-O2D-CED
26	m	610	CLA	CBD-CGD-O2D-CED
26	l	304	CLA	CBD-CGD-O2D-CED
26	l	310	CLA	CBD-CGD-O2D-CED
26	k	603	CLA	CBD-CGD-O2D-CED
26	i	304	CLA	CBD-CGD-O2D-CED
26	j	602	CLA	CBD-CGD-O2D-CED
26	j	603	CLA	CBD-CGD-O2D-CED
26	j	608	CLA	CBD-CGD-O2D-CED
26	d	306	CLA	CBD-CGD-O2D-CED
26	n	610	CLA	CBD-CGD-O2D-CED
26	A	818	CLA	O1A-CGA-O2A-C1
26	A	835	CLA	O1A-CGA-O2A-C1
26	A	839	CLA	O1A-CGA-O2A-C1
26	B	811	CLA	O1A-CGA-O2A-C1
26	B	813	CLA	O1A-CGA-O2A-C1
26	B	816	CLA	O1A-CGA-O2A-C1
26	B	831	CLA	O1A-CGA-O2A-C1
26	b	307	CLA	O1A-CGA-O2A-C1
26	h	301	CLA	O1A-CGA-O2A-C1
26	h	303	CLA	O1A-CGA-O2A-C1
26	m	610	CLA	O1A-CGA-O2A-C1
26	k	601	CLA	O1A-CGA-O2A-C1
26	k	610	CLA	O1A-CGA-O2A-C1
26	i	311	CLA	O1A-CGA-O2A-C1
26	n	606	CLA	O1A-CGA-O2A-C1
26	n	608	CLA	O1A-CGA-O2A-C1
28	A	849	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
28	L	208	LHG	O10-C23-O8-C6
28	c	317	LHG	O10-C23-O8-C6
28	i	317	LHG	O10-C23-O8-C6
34	c	319	LMG	O10-C28-O8-C9
34	Q	301	LMG	O10-C28-O8-C9
26	B	819	CLA	O1D-CGD-O2D-CED
26	k	602	CLA	O1D-CGD-O2D-CED
26	j	612	CLA	O1D-CGD-O2D-CED
36	k	612	KC2	CAA-CBA-CGA-O2A
36	d	312	KC2	CAA-CBA-CGA-O2A
26	B	832	CLA	O1D-CGD-O2D-CED
26	a	308	CLA	O1D-CGD-O2D-CED
26	l	307	CLA	O1D-CGD-O2D-CED
33	j	618	DGD	O6D-C5D-C6D-O5D
26	B	802	CLA	CBD-CGD-O2D-CED
26	B	813	CLA	CBD-CGD-O2D-CED
26	B	822	CLA	CBD-CGD-O2D-CED
26	B	833	CLA	CBD-CGD-O2D-CED
26	a	302	CLA	CBD-CGD-O2D-CED
26	b	310	CLA	CBD-CGD-O2D-CED
26	b	313	CLA	CBD-CGD-O2D-CED
26	A	814	CLA	O1D-CGD-O2D-CED
26	b	311	CLA	O1D-CGD-O2D-CED
28	c	317	LHG	O9-C7-O7-C5
28	c	320	LHG	O9-C7-O7-C5
28	b	318	LHG	O9-C7-O7-C5
28	i	317	LHG	O9-C7-O7-C5
33	B	844	DGD	O1B-C1B-O2G-C2G
34	F	205	LMG	O9-C10-O7-C8
34	c	318	LMG	O9-C10-O7-C8
34	Q	301	LMG	O9-C10-O7-C8
26	A	803	CLA	O1A-CGA-O2A-C1
26	n	610	CLA	O1A-CGA-O2A-C1
26	A	830	CLA	C3-C5-C6-C7
26	A	834	CLA	C3-C5-C6-C7
26	A	856	CLA	C3-C5-C6-C7
26	B	809	CLA	C3-C5-C6-C7
26	B	822	CLA	C3-C5-C6-C7
26	B	831	CLA	C3-C5-C6-C7
26	c	302	CLA	C3-C5-C6-C7
26	c	304	CLA	C3-C5-C6-C7
26	h	306	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	m	602	CLA	C3-C5-C6-C7
26	l	301	CLA	C3-C5-C6-C7
26	l	310	CLA	C3-C5-C6-C7
26	k	602	CLA	C3-C5-C6-C7
26	i	304	CLA	C3-C5-C6-C7
26	d	302	CLA	C3-C5-C6-C7
26	n	609	CLA	C3-C5-C6-C7
26	A	819	CLA	CBA-CGA-O2A-C1
26	A	835	CLA	CBA-CGA-O2A-C1
26	B	811	CLA	CBA-CGA-O2A-C1
26	B	813	CLA	CBA-CGA-O2A-C1
26	B	816	CLA	CBA-CGA-O2A-C1
26	L	206	CLA	CBA-CGA-O2A-C1
26	c	306	CLA	CBA-CGA-O2A-C1
26	b	307	CLA	CBA-CGA-O2A-C1
26	b	313	CLA	CBA-CGA-O2A-C1
26	h	302	CLA	CBA-CGA-O2A-C1
26	h	303	CLA	CBA-CGA-O2A-C1
26	h	305	CLA	CBA-CGA-O2A-C1
26	m	610	CLA	CBA-CGA-O2A-C1
26	k	610	CLA	CBA-CGA-O2A-C1
26	i	310	CLA	CBA-CGA-O2A-C1
26	n	606	CLA	CBA-CGA-O2A-C1
26	n	608	CLA	CBA-CGA-O2A-C1
28	L	208	LHG	C24-C23-O8-C6
34	c	319	LMG	C29-C28-O8-C9
34	Q	301	LMG	C29-C28-O8-C9
26	B	819	CLA	C2C-C3C-CAC-CBC
34	c	319	LMG	C11-C10-O7-C8
26	B	842	CLA	O1D-CGD-O2D-CED
26	l	301	CLA	O1D-CGD-O2D-CED
26	l	305	CLA	CBD-CGD-O2D-CED
26	l	313	CLA	CBD-CGD-O2D-CED
26	d	308	CLA	CBD-CGD-O2D-CED
26	A	809	CLA	O1A-CGA-O2A-C1
36	l	312	KC2	CAA-CBA-CGA-O1A
36	l	312	KC2	CAA-CBA-CGA-O2A
36	j	611	KC2	CAA-CBA-CGA-O1A
36	j	611	KC2	CAA-CBA-CGA-O2A
26	B	801	CLA	C4-C3-C5-C6
26	B	836	CLA	CBD-CGD-O2D-CED
26	k	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	i	302	CLA	CBD-CGD-O2D-CED
26	A	807	CLA	C2A-CAA-CBA-CGA
26	A	815	CLA	C2A-CAA-CBA-CGA
26	B	822	CLA	C2A-CAA-CBA-CGA
26	B	829	CLA	C2A-CAA-CBA-CGA
26	B	836	CLA	C2A-CAA-CBA-CGA
26	a	311	CLA	C2A-CAA-CBA-CGA
26	b	311	CLA	C2A-CAA-CBA-CGA
26	b	312	CLA	C2A-CAA-CBA-CGA
26	h	307	CLA	C2A-CAA-CBA-CGA
26	m	613	CLA	C2A-CAA-CBA-CGA
26	l	313	CLA	C2A-CAA-CBA-CGA
26	k	605	CLA	C2A-CAA-CBA-CGA
26	i	306	CLA	C2A-CAA-CBA-CGA
26	l	311	CLA	O1A-CGA-O2A-C1
26	B	828	CLA	O1D-CGD-O2D-CED
26	A	809	CLA	C3-C5-C6-C7
26	B	801	CLA	C3-C5-C6-C7
26	B	817	CLA	C3-C5-C6-C7
26	a	301	CLA	C3-C5-C6-C7
26	b	310	CLA	C3-C5-C6-C7
26	i	306	CLA	C3-C5-C6-C7
26	i	310	CLA	C3-C5-C6-C7
26	A	803	CLA	CBA-CGA-O2A-C1
26	A	809	CLA	CBA-CGA-O2A-C1
26	A	818	CLA	CBA-CGA-O2A-C1
26	A	837	CLA	CBA-CGA-O2A-C1
26	A	839	CLA	CBA-CGA-O2A-C1
26	B	831	CLA	CBA-CGA-O2A-C1
26	B	838	CLA	CBA-CGA-O2A-C1
26	l	308	CLA	CBA-CGA-O2A-C1
26	l	311	CLA	CBA-CGA-O2A-C1
26	k	601	CLA	CBA-CGA-O2A-C1
26	k	609	CLA	CBA-CGA-O2A-C1
26	i	302	CLA	CBA-CGA-O2A-C1
26	i	311	CLA	CBA-CGA-O2A-C1
26	d	305	CLA	CBA-CGA-O2A-C1
26	n	602	CLA	CBA-CGA-O2A-C1
26	n	610	CLA	CBA-CGA-O2A-C1
28	c	317	LHG	C24-C23-O8-C6
30	a	317	LMU	O5B-C5B-C6B-O6B
26	A	832	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	a	305	CLA	O1D-CGD-O2D-CED
27	A	842	PQN	C11-C12-C13-C14
27	B	843	PQN	C11-C12-C13-C14
26	A	807	CLA	CBD-CGD-O2D-CED
26	i	306	CLA	CBD-CGD-O2D-CED
26	n	602	CLA	CBD-CGD-O2D-CED
26	A	821	CLA	O1D-CGD-O2D-CED
26	i	301	CLA	O1D-CGD-O2D-CED
26	d	313	CLA	O1D-CGD-O2D-CED
26	B	828	CLA	O1A-CGA-O2A-C1
26	B	838	CLA	O1A-CGA-O2A-C1
26	c	306	CLA	O1A-CGA-O2A-C1
26	b	312	CLA	O1A-CGA-O2A-C1
26	k	609	CLA	O1A-CGA-O2A-C1
26	i	310	CLA	O1A-CGA-O2A-C1
26	d	305	CLA	O1A-CGA-O2A-C1
26	j	607	CLA	C2C-C3C-CAC-CBC
26	A	831	CLA	O1D-CGD-O2D-CED
26	i	308	CLA	O1D-CGD-O2D-CED
26	d	302	CLA	O1D-CGD-O2D-CED
29	A	845	WVN	C22-C26-C29-C31
29	A	847	WVN	C25-C28-C30-C33
29	A	848	WVN	C25-C28-C30-C33
29	B	846	WVN	C25-C28-C30-C33
29	B	848	WVN	C22-C26-C29-C31
29	B	849	WVN	C22-C26-C29-C31
29	B	853	WVN	C25-C28-C30-C33
29	I	101	WVN	C22-C26-C29-C31
29	J	101	WVN	C25-C28-C30-C33
29	J	101	WVN	C32-C36-C39-C40
29	L	205	WVN	C22-C26-C29-C31
29	K	102	WVN	C34-C37-C40-C39
29	s	405	WVN	C22-C26-C29-C31
29	s	405	WVN	C25-C28-C30-C33
29	s	407	WVN	C25-C28-C30-C33
29	h	309	WVN	C25-C28-C30-C33
29	i	315	WVN	C22-C26-C29-C31
35	c	313	II0	C26-C30-C32-C34
35	a	314	II0	C25-C29-C31-C33
35	a	314	II0	C26-C30-C32-C34
35	b	315	II0	C26-C30-C32-C34
35	h	310	II0	C25-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
35	h	312	II0	C25-C29-C31-C33
35	m	614	II0	C25-C29-C31-C33
35	m	614	II0	C26-C30-C32-C34
35	m	616	II0	C25-C29-C31-C33
35	m	616	II0	C26-C30-C32-C34
35	l	302	II0	C25-C29-C31-C33
35	k	616	II0	C25-C29-C31-C33
35	k	618	II0	C26-C30-C32-C34
35	k	619	II0	C26-C30-C32-C34
35	k	620	II0	C26-C30-C32-C34
35	i	312	II0	C26-C30-C32-C34
35	d	315	II0	C26-C30-C32-C34
35	d	317	II0	C26-C30-C32-C34
35	d	319	II0	C36-C40-C42-C41
35	n	615	II0	C26-C30-C32-C34
35	n	618	II0	C25-C29-C31-C33
35	n	618	II0	C26-C30-C32-C34
37	b	316	IHT	C23-C27-C30-C32
34	L	209	LMG	O6-C5-C6-O5
26	A	820	CLA	CBD-CGD-O2D-CED
26	A	824	CLA	CBD-CGD-O2D-CED
26	A	828	CLA	CBD-CGD-O2D-CED
26	A	837	CLA	CBD-CGD-O2D-CED
26	B	809	CLA	CBD-CGD-O2D-CED
26	B	838	CLA	CBD-CGD-O2D-CED
26	L	202	CLA	CBD-CGD-O2D-CED
26	a	307	CLA	CBD-CGD-O2D-CED
26	b	304	CLA	CBD-CGD-O2D-CED
26	d	307	CLA	CBD-CGD-O2D-CED
26	n	603	CLA	CBD-CGD-O2D-CED
26	n	606	CLA	CBD-CGD-O2D-CED
28	A	844	LHG	O2-C2-C3-O3
28	A	855	LHG	O2-C2-C3-O3
28	B	851	LHG	O2-C2-C3-O3
28	b	318	LHG	O2-C2-C3-O3
26	A	836	CLA	C3-C5-C6-C7
26	B	807	CLA	C3-C5-C6-C7
26	B	813	CLA	C3-C5-C6-C7
26	s	403	CLA	C3-C5-C6-C7
26	l	311	CLA	C3-C5-C6-C7
26	j	610	CLA	C3-C5-C6-C7
26	j	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	n	604	CLA	C3-C5-C6-C7
26	A	820	CLA	CBA-CGA-O2A-C1
26	B	815	CLA	CBA-CGA-O2A-C1
26	B	840	CLA	CBA-CGA-O2A-C1
26	s	403	CLA	CBA-CGA-O2A-C1
26	c	301	CLA	CBA-CGA-O2A-C1
26	b	312	CLA	CBA-CGA-O2A-C1
26	h	301	CLA	CBA-CGA-O2A-C1
26	h	308	CLA	CBA-CGA-O2A-C1
26	m	607	CLA	CBA-CGA-O2A-C1
26	j	612	CLA	CBA-CGA-O2A-C1
26	A	819	CLA	O1A-CGA-O2A-C1
26	L	206	CLA	O1A-CGA-O2A-C1
26	h	305	CLA	O1A-CGA-O2A-C1
34	F	206	LMG	O6-C5-C6-O5
34	L	209	LMG	C4-C5-C6-O5
26	B	808	CLA	O1D-CGD-O2D-CED
26	B	827	CLA	O1D-CGD-O2D-CED
26	B	840	CLA	O1D-CGD-O2D-CED
26	F	202	CLA	O1D-CGD-O2D-CED
26	B	812	CLA	CBD-CGD-O2D-CED
26	B	826	CLA	CBD-CGD-O2D-CED
26	a	301	CLA	CBD-CGD-O2D-CED
26	a	310	CLA	CBD-CGD-O2D-CED
26	b	309	CLA	CBD-CGD-O2D-CED
26	k	605	CLA	CBD-CGD-O2D-CED
30	a	317	LMU	C4B-C5B-C6B-O6B
26	s	403	CLA	O1A-CGA-O2A-C1
26	n	602	CLA	O1A-CGA-O2A-C1
33	B	844	DGD	O6E-C5E-C6E-O5E
26	l	309	CLA	O1D-CGD-O2D-CED
30	a	317	LMU	O1'-C1-C2-C3
26	B	823	CLA	CBD-CGD-O2D-CED
26	B	806	CLA	C3-C5-C6-C7
26	F	201	CLA	C3-C5-C6-C7
26	c	312	CLA	C3-C5-C6-C7
26	a	307	CLA	C3-C5-C6-C7
26	B	828	CLA	CBA-CGA-O2A-C1
26	R	201	CLA	CBA-CGA-O2A-C1
28	i	317	LHG	C24-C23-O8-C6
36	k	612	KC2	CAA-CBA-CGA-O1A
36	d	312	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
36	n	612	KC2	CAA-CBA-CGA-O1A
26	m	607	CLA	O1A-CGA-O2A-C1
26	l	308	CLA	O1A-CGA-O2A-C1
26	i	302	CLA	O1A-CGA-O2A-C1
33	j	618	DGD	O1A-C1A-O1G-C1G
25	A	801	CL0	C4-C3-C5-C6
26	a	301	CLA	C4-C3-C5-C6
26	m	602	CLA	C4-C3-C5-C6
25	A	801	CL0	C2-C3-C5-C6
26	B	801	CLA	C2-C3-C5-C6
26	a	301	CLA	C2-C3-C5-C6
26	m	602	CLA	C2-C3-C5-C6
26	A	806	CLA	CBD-CGD-O2D-CED
26	n	605	CLA	CBD-CGD-O2D-CED
26	A	851	CLA	C2A-CAA-CBA-CGA
26	s	406	CLA	C2A-CAA-CBA-CGA
26	h	302	CLA	C2A-CAA-CBA-CGA
26	h	303	CLA	C2A-CAA-CBA-CGA
26	i	307	CLA	C2A-CAA-CBA-CGA
26	d	305	CLA	C2A-CAA-CBA-CGA
26	b	306	CLA	O1D-CGD-O2D-CED
34	n	620	LMG	O6-C5-C6-O5
26	A	820	CLA	O1A-CGA-O2A-C1
26	A	837	CLA	O1A-CGA-O2A-C1
26	B	815	CLA	O1A-CGA-O2A-C1
26	B	840	CLA	O1A-CGA-O2A-C1
26	h	308	CLA	O1A-CGA-O2A-C1
26	j	612	CLA	O1A-CGA-O2A-C1
26	R	201	CLA	O1A-CGA-O2A-C1
26	A	810	CLA	CBA-CGA-O2A-C1
26	A	834	CLA	CBA-CGA-O2A-C1
26	B	825	CLA	CBA-CGA-O2A-C1
26	c	308	CLA	CBA-CGA-O2A-C1
26	a	301	CLA	CBA-CGA-O2A-C1
36	c	310	KC2	CBD-CGD-O2D-CED
26	A	822	CLA	O1D-CGD-O2D-CED
34	F	206	LMG	C4-C5-C6-O5
28	c	317	LHG	C28-C29-C30-C31
26	B	821	CLA	O1D-CGD-O2D-CED
26	b	307	CLA	O1D-CGD-O2D-CED
26	m	605	CLA	O1D-CGD-O2D-CED
26	k	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	i	307	CLA	O1D-CGD-O2D-CED
26	j	603	CLA	O1D-CGD-O2D-CED
26	j	610	CLA	O1D-CGD-O2D-CED
26	R	201	CLA	O1D-CGD-O2D-CED
26	c	301	CLA	O1A-CGA-O2A-C1
34	L	209	LMG	O10-C28-O8-C9
36	d	311	KC2	CAA-CBA-CGA-O1A
36	n	611	KC2	CAA-CBA-CGA-O2A
25	A	801	CL0	C1-C2-C3-C5
26	A	804	CLA	O1D-CGD-O2D-CED
26	i	304	CLA	O1D-CGD-O2D-CED
26	B	830	CLA	O1D-CGD-O2D-CED
26	h	305	CLA	O1D-CGD-O2D-CED
28	A	844	LHG	C1-C2-C3-O3
28	A	855	LHG	C1-C2-C3-O3
28	b	318	LHG	C1-C2-C3-O3
26	A	810	CLA	O1A-CGA-O2A-C1
26	A	834	CLA	O1A-CGA-O2A-C1
26	c	308	CLA	O1A-CGA-O2A-C1
26	a	301	CLA	O1A-CGA-O2A-C1
26	B	803	CLA	C3-C5-C6-C7
26	s	402	CLA	C3-C5-C6-C7
26	c	307	CLA	O1D-CGD-O2D-CED
26	A	805	CLA	CBA-CGA-O2A-C1
26	A	838	CLA	CBA-CGA-O2A-C1
26	A	856	CLA	CBA-CGA-O2A-C1
26	B	802	CLA	CBA-CGA-O2A-C1
26	B	805	CLA	CBA-CGA-O2A-C1
26	B	814	CLA	CBA-CGA-O2A-C1
26	B	826	CLA	CBA-CGA-O2A-C1
26	B	839	CLA	CBA-CGA-O2A-C1
26	B	841	CLA	CBA-CGA-O2A-C1
26	L	203	CLA	CBA-CGA-O2A-C1
26	s	408	CLA	CBA-CGA-O2A-C1
26	b	311	CLA	CBA-CGA-O2A-C1
26	i	301	CLA	CBA-CGA-O2A-C1
26	d	302	CLA	CBA-CGA-O2A-C1
26	n	605	CLA	CBA-CGA-O2A-C1
28	B	851	LHG	C24-C23-O8-C6
33	j	618	DGD	C2A-C1A-O1G-C1G
34	L	209	LMG	C29-C28-O8-C9
26	B	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	n	607	CLA	CBD-CGD-O2D-CED
34	n	620	LMG	C4-C5-C6-O5
26	m	610	CLA	O1D-CGD-O2D-CED
29	A	845	WVN	C25-C28-C30-C33
29	A	846	WVN	C22-C26-C29-C31
29	A	857	WVN	C25-C28-C30-C33
29	B	850	WVN	C25-C28-C30-C33
29	J	102	WVN	C25-C28-C30-C33
29	K	102	WVN	C25-C28-C30-C33
29	h	309	WVN	C22-C26-C29-C31
29	l	316	WVN	C22-C26-C29-C31
35	k	620	II0	C25-C29-C31-C33
35	i	314	II0	C26-C30-C32-C34
35	i	319	II0	C25-C29-C31-C33
35	d	301	II0	C36-C40-C42-C41
35	d	316	II0	C25-C29-C31-C33
26	A	834	CLA	C5-C6-C7-C8
26	s	408	CLA	C15-C16-C17-C18
36	k	613	KC2	CAA-CBA-CGA-O2A
36	n	611	KC2	CAA-CBA-CGA-O1A
36	n	612	KC2	CAA-CBA-CGA-O2A
33	B	844	DGD	C4E-C5E-C6E-O5E
26	s	403	CLA	C15-C16-C17-C18
26	a	306	CLA	C15-C16-C17-C18
26	b	310	CLA	C15-C16-C17-C18
26	l	310	CLA	C5-C6-C7-C8
28	L	208	LHG	O2-C2-C3-O3
26	F	202	CLA	C3-C5-C6-C7
33	B	844	DGD	C2D-C1D-O3G-C3G
34	c	319	LMG	C2-C1-O1-C7
33	B	844	DGD	O1G-C1G-C2G-O2G
26	l	305	CLA	CBA-CGA-O2A-C1
30	A	850	LMU	O5'-C5'-C6'-O6'
26	A	841	CLA	C6-C7-C8-C9
26	B	804	CLA	C11-C12-C13-C14
26	F	201	CLA	C14-C13-C15-C16
26	s	408	CLA	C6-C7-C8-C9
26	a	310	CLA	C11-C12-C13-C14
26	k	602	CLA	C11-C12-C13-C14
26	i	301	CLA	C11-C10-C8-C9
26	A	813	CLA	O1D-CGD-O2D-CED
26	B	841	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	h	308	CLA	O1D-CGD-O2D-CED
26	l	304	CLA	O1D-CGD-O2D-CED
26	n	610	CLA	O1D-CGD-O2D-CED
26	k	608	CLA	CBD-CGD-O2D-CED
26	j	610	CLA	C5-C6-C7-C8
26	F	202	CLA	C2A-CAA-CBA-CGA
26	c	307	CLA	C2A-CAA-CBA-CGA
29	A	845	WVN	C11-C19-C22-C24
29	A	846	WVN	C30-C33-C34-C38
29	A	847	WVN	C30-C33-C34-C38
29	A	848	WVN	C11-C19-C22-C24
29	A	848	WVN	C20-C23-C25-C27
29	A	857	WVN	C29-C31-C32-C35
29	A	857	WVN	C30-C33-C34-C38
29	B	846	WVN	C20-C23-C25-C27
29	B	848	WVN	C11-C19-C22-C24
29	B	850	WVN	C11-C19-C22-C24
29	B	853	WVN	C20-C23-C25-C27
29	B	853	WVN	C29-C31-C32-C35
29	F	203	WVN	C29-C31-C32-C35
29	F	204	WVN	C20-C23-C25-C27
29	I	101	WVN	C11-C19-C22-C24
29	I	101	WVN	C20-C23-C25-C27
29	I	101	WVN	C29-C31-C32-C35
29	J	101	WVN	C29-C31-C32-C35
29	J	101	WVN	C30-C33-C34-C38
29	J	102	WVN	C29-C31-C32-C35
29	L	205	WVN	C30-C33-C34-C38
29	K	102	WVN	C20-C23-C25-C27
29	s	405	WVN	C20-C23-C25-C27
29	s	405	WVN	C30-C33-C34-C38
29	h	309	WVN	C20-C23-C25-C27
29	h	309	WVN	C29-C31-C32-C35
29	h	309	WVN	C30-C33-C34-C38
29	l	316	WVN	C29-C31-C32-C35
29	l	316	WVN	C30-C33-C34-C38
29	R	200	WVN	C20-C23-C25-C27
35	a	312	II0	C31-C33-C35-C37
35	a	314	II0	C31-C33-C35-C37
35	b	314	II0	C31-C33-C35-C37
35	h	312	II0	C32-C34-C36-C38
35	l	314	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
35	l	315	II0	C31-C33-C35-C37
35	k	619	II0	C31-C33-C35-C37
35	k	620	II0	C32-C34-C36-C38
35	i	312	II0	C32-C34-C36-C38
35	j	614	II0	C31-C33-C35-C37
35	j	615	II0	C32-C34-C36-C38
35	d	301	II0	C31-C33-C35-C37
35	n	616	II0	C32-C34-C36-C38
37	j	616	IHT	C18-C22-C23-C25
37	n	617	IHT	C18-C22-C23-C25
29	A	847	WVN	C29-C31-C32-C36
29	A	857	WVN	C11-C19-C22-C26
29	B	846	WVN	C11-C19-C22-C26
29	B	846	WVN	C30-C33-C34-C37
29	B	848	WVN	C29-C31-C32-C36
29	B	848	WVN	C30-C33-C34-C37
29	B	849	WVN	C11-C19-C22-C26
29	B	853	WVN	C30-C33-C34-C37
29	F	204	WVN	C20-C23-C25-C28
29	I	101	WVN	C30-C33-C34-C37
29	J	101	WVN	C11-C19-C22-C26
29	J	102	WVN	C20-C23-C25-C28
29	M	101	WVN	C11-C19-C22-C26
29	K	102	WVN	C11-C19-C22-C26
29	K	102	WVN	C29-C31-C32-C36
29	s	405	WVN	C29-C31-C32-C36
29	s	407	WVN	C29-C31-C32-C36
29	s	407	WVN	C30-C33-C34-C37
29	h	309	WVN	C11-C19-C22-C26
29	l	303	WVN	C20-C23-C25-C28
29	l	316	WVN	C11-C19-C22-C26
29	l	316	WVN	C20-C23-C25-C28
29	i	315	WVN	C11-C19-C22-C26
29	i	315	WVN	C20-C23-C25-C28
29	R	200	WVN	C11-C19-C22-C26
29	R	200	WVN	C29-C31-C32-C36
29	R	200	WVN	C30-C33-C34-C37
35	J	104	II0	C32-C34-C36-C40
35	a	312	II0	C32-C34-C36-C40
35	a	314	II0	C32-C34-C36-C40
35	b	314	II0	C32-C34-C36-C40
35	b	315	II0	C31-C33-C35-C39

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Mol	Chain	Res	Type	Atoms
35	b	315	II0	C32-C34-C36-C40
35	h	310	II0	C32-C34-C36-C40
35	m	614	II0	C32-C34-C36-C40
35	k	615	II0	C32-C34-C36-C40
35	k	616	II0	C32-C34-C36-C40
35	i	316	II0	C31-C33-C35-C39
35	j	614	II0	C32-C34-C36-C40
35	d	301	II0	C32-C34-C36-C40
35	d	316	II0	C31-C33-C35-C39
35	d	316	II0	C32-C34-C36-C40
35	d	317	II0	C32-C34-C36-C40
35	n	615	II0	C31-C33-C35-C39
35	n	616	II0	C31-C33-C35-C39
37	j	616	IHT	C18-C22-C23-C27
37	n	617	IHT	C18-C22-C23-C27
33	B	844	DGD	C2B-C1B-O2G-C2G
28	i	317	LHG	C23-C24-C25-C26
26	A	805	CLA	O1A-CGA-O2A-C1
26	B	814	CLA	O1A-CGA-O2A-C1
26	B	826	CLA	O1A-CGA-O2A-C1
26	L	203	CLA	O1A-CGA-O2A-C1
28	A	855	LHG	O10-C23-O8-C6
26	A	817	CLA	C13-C15-C16-C17
26	a	307	CLA	C15-C16-C17-C18
26	A	823	CLA	O1D-CGD-O2D-CED
26	j	608	CLA	O1D-CGD-O2D-CED
34	c	319	LMG	C4-C5-C6-O5
36	i	309	KC2	CAA-CBA-CGA-O1A
36	i	318	KC2	CAA-CBA-CGA-O1A
36	i	318	KC2	CAA-CBA-CGA-O2A
36	d	311	KC2	CAA-CBA-CGA-O2A
26	A	836	CLA	O1D-CGD-O2D-CED
26	B	801	CLA	CBA-CGA-O2A-C1
26	B	806	CLA	CBA-CGA-O2A-C1
26	m	609	CLA	CBA-CGA-O2A-C1
26	l	310	CLA	CBA-CGA-O2A-C1
26	k	602	CLA	CBA-CGA-O2A-C1
26	i	306	CLA	CBA-CGA-O2A-C1
26	B	820	CLA	C15-C16-C17-C18
26	B	834	CLA	C8-C10-C11-C12
26	B	836	CLA	C10-C11-C12-C13
26	F	201	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	s	408	CLA	C8-C10-C11-C12
26	b	304	CLA	C5-C6-C7-C8
26	b	306	CLA	C8-C10-C11-C12
26	n	608	CLA	C5-C6-C7-C8
28	A	849	LHG	C7-C8-C9-C10
28	L	208	LHG	C23-C24-C25-C26
28	b	302	LHG	C23-C24-C25-C26
28	j	617	LHG	C23-C24-C25-C26
34	c	319	LMG	C28-C29-C30-C31
26	m	601	CLA	O1D-CGD-O2D-CED
26	A	807	CLA	C15-C16-C17-C18
26	A	818	CLA	C13-C15-C16-C17
26	A	819	CLA	C13-C15-C16-C17
26	A	826	CLA	C5-C6-C7-C8
26	A	841	CLA	C5-C6-C7-C8
26	B	808	CLA	C15-C16-C17-C18
26	B	822	CLA	C13-C15-C16-C17
26	s	402	CLA	C10-C11-C12-C13
26	m	603	CLA	C5-C6-C7-C8
26	m	608	CLA	C15-C16-C17-C18
26	l	305	CLA	C10-C11-C12-C13
26	l	307	CLA	C13-C15-C16-C17
26	k	602	CLA	C13-C15-C16-C17
26	i	301	CLA	C5-C6-C7-C8
26	n	608	CLA	C10-C11-C12-C13
27	A	842	PQN	C20-C21-C22-C23
26	k	614	CLA	C2C-C3C-CAC-CBC
28	B	851	LHG	C23-C24-C25-C26
28	J	105	LHG	C23-C24-C25-C26
28	b	302	LHG	C7-C8-C9-C10
28	b	318	LHG	C23-C24-C25-C26
28	l	318	LHG	C7-C8-C9-C10
28	j	617	LHG	C7-C8-C9-C10
28	n	619	LHG	C23-C24-C25-C26
26	B	816	CLA	CBD-CGD-O2D-CED
26	d	306	CLA	O1D-CGD-O2D-CED
26	A	812	CLA	C13-C15-C16-C17
26	A	831	CLA	C13-C15-C16-C17
26	A	852	CLA	C15-C16-C17-C18
26	B	836	CLA	C15-C16-C17-C18
26	F	201	CLA	C8-C10-C11-C12
26	s	406	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	b	306	CLA	C13-C15-C16-C17
26	h	304	CLA	C15-C16-C17-C18
26	k	608	CLA	C15-C16-C17-C18
27	B	843	PQN	C15-C16-C17-C18
26	n	604	CLA	CBA-CGA-O2A-C1
26	j	607	CLA	C4C-C3C-CAC-CBC
26	s	402	CLA	O1D-CGD-O2D-CED
26	c	301	CLA	O1D-CGD-O2D-CED
36	k	613	KC2	CAA-CBA-CGA-O1A
36	i	309	KC2	CAA-CBA-CGA-O2A
26	B	831	CLA	C2-C1-O2A-CGA
26	h	301	CLA	C2-C1-O2A-CGA
25	A	801	CL0	C5-C6-C7-C8
26	B	807	CLA	C5-C6-C7-C8
26	b	307	CLA	C10-C11-C12-C13
26	i	303	CLA	C8-C10-C11-C12
26	j	601	CLA	C13-C15-C16-C17
26	j	601	CLA	C15-C16-C17-C18
26	j	613	CLA	C15-C16-C17-C18
26	B	805	CLA	O1A-CGA-O2A-C1
26	c	309	CLA	CBD-CGD-O2D-CED
26	B	817	CLA	C10-C11-C12-C13
26	B	834	CLA	C13-C15-C16-C17
26	a	306	CLA	C5-C6-C7-C8
26	h	304	CLA	C13-C15-C16-C17
26	j	610	CLA	C8-C10-C11-C12
26	A	822	CLA	C6-C7-C8-C10
26	A	841	CLA	C6-C7-C8-C10
26	B	834	CLA	C12-C13-C15-C16
26	B	839	CLA	C6-C7-C8-C10
26	F	201	CLA	C6-C7-C8-C10
26	n	610	CLA	C6-C7-C8-C10
26	B	802	CLA	O1A-CGA-O2A-C1
26	b	311	CLA	O1A-CGA-O2A-C1
26	i	301	CLA	O1A-CGA-O2A-C1
26	d	302	CLA	O1A-CGA-O2A-C1
26	n	605	CLA	O1A-CGA-O2A-C1
29	A	846	WVN	C25-C28-C30-C33
29	B	846	WVN	C22-C26-C29-C31
29	B	848	WVN	C25-C28-C30-C33
29	B	853	WVN	C22-C26-C29-C31
29	B	853	WVN	C32-C36-C39-C40

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Mol	Chain	Res	Type	Atoms
29	F	203	WVN	C32-C36-C39-C40
29	I	101	WVN	C25-C28-C30-C33
29	J	102	WVN	C22-C26-C29-C31
29	M	101	WVN	C22-C26-C29-C31
29	K	102	WVN	C22-C26-C29-C31
29	s	407	WVN	C32-C36-C39-C40
29	l	316	WVN	C25-C28-C30-C33
29	R	200	WVN	C22-C26-C29-C31
35	c	316	II0	C25-C29-C31-C33
35	c	316	II0	C26-C30-C32-C34
35	h	311	II0	C26-C30-C32-C34
35	m	619	II0	C26-C30-C32-C34
35	l	302	II0	C26-C30-C32-C34
35	k	615	II0	C26-C30-C32-C34
35	i	313	II0	C25-C29-C31-C33
35	i	316	II0	C25-C29-C31-C33
35	i	316	II0	C26-C30-C32-C34
35	j	614	II0	C25-C29-C31-C33
35	d	301	II0	C26-C30-C32-C34
35	n	615	II0	C25-C29-C31-C33
30	A	858	LMU	O5B-C1B-O1B-C4'
26	A	802	CLA	C2A-CAA-CBA-CGA
26	A	821	CLA	C2A-CAA-CBA-CGA
26	m	607	CLA	C2A-CAA-CBA-CGA
26	m	608	CLA	C2A-CAA-CBA-CGA
26	k	614	CLA	C2A-CAA-CBA-CGA
26	B	813	CLA	O1D-CGD-O2D-CED
26	B	822	CLA	O1D-CGD-O2D-CED
26	B	833	CLA	O1D-CGD-O2D-CED
26	c	304	CLA	O1D-CGD-O2D-CED
26	a	302	CLA	O1D-CGD-O2D-CED
26	b	310	CLA	O1D-CGD-O2D-CED
26	b	313	CLA	O1D-CGD-O2D-CED
26	m	606	CLA	O1D-CGD-O2D-CED
26	l	310	CLA	O1D-CGD-O2D-CED
26	k	603	CLA	O1D-CGD-O2D-CED
26	j	602	CLA	O1D-CGD-O2D-CED
26	A	816	CLA	C5-C6-C7-C8
26	A	840	CLA	C15-C16-C17-C18
26	B	816	CLA	C5-C6-C7-C8
26	L	203	CLA	C8-C10-C11-C12
26	s	406	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	c	308	CLA	C15-C16-C17-C18
26	c	312	CLA	C8-C10-C11-C12
26	i	303	CLA	C10-C11-C12-C13
26	i	304	CLA	C5-C6-C7-C8
26	n	608	CLA	C8-C10-C11-C12
26	A	838	CLA	O1A-CGA-O2A-C1
26	A	856	CLA	O1A-CGA-O2A-C1
26	B	841	CLA	O1A-CGA-O2A-C1
26	s	408	CLA	O1A-CGA-O2A-C1
26	k	602	CLA	O1A-CGA-O2A-C1
34	c	318	LMG	O6-C1-O1-C7
26	A	838	CLA	C5-C6-C7-C8
26	B	802	CLA	O1D-CGD-O2D-CED
30	A	858	LMU	C5'-C4'-O1B-C1B
30	a	317	LMU	O5'-C5'-C6'-O6'
30	i	300	LMU	O5'-C5'-C6'-O6'
28	L	207	LHG	O2-C2-C3-O3
26	B	808	CLA	C3-C5-C6-C7
26	b	308	CLA	C3-C5-C6-C7
26	n	608	CLA	C3-C5-C6-C7
26	A	810	CLA	C8-C10-C11-C12
26	B	805	CLA	C10-C11-C12-C13
26	B	822	CLA	C10-C11-C12-C13
26	h	301	CLA	C13-C15-C16-C17
25	A	801	CL0	CBA-CGA-O2A-C1
26	d	313	CLA	CBA-CGA-O2A-C1
28	n	619	LHG	C24-C23-O8-C6
34	c	318	LMG	C29-C28-O8-C9
26	B	825	CLA	O1A-CGA-O2A-C1
26	B	839	CLA	O1A-CGA-O2A-C1
26	A	835	CLA	C13-C15-C16-C17
26	A	852	CLA	C8-C10-C11-C12
26	B	810	CLA	C13-C15-C16-C17
26	B	816	CLA	C10-C11-C12-C13
26	m	606	CLA	C15-C16-C17-C18
26	m	610	CLA	C5-C6-C7-C8
26	l	313	CLA	O1D-CGD-O2D-CED
26	B	806	CLA	O1A-CGA-O2A-C1
26	m	609	CLA	O1A-CGA-O2A-C1
26	l	305	CLA	O1A-CGA-O2A-C1
34	F	205	LMG	C11-C10-O7-C8
34	c	318	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	A	812	CLA	C15-C16-C17-C18
26	A	813	CLA	C5-C6-C7-C8
26	B	810	CLA	C15-C16-C17-C18
26	B	818	CLA	C8-C10-C11-C12
26	B	825	CLA	C13-C15-C16-C17
26	B	829	CLA	C5-C6-C7-C8
26	B	837	CLA	C13-C15-C16-C17
26	s	402	CLA	C15-C16-C17-C18
26	m	606	CLA	C5-C6-C7-C8
26	l	313	CLA	C5-C6-C7-C8
26	d	302	CLA	C10-C11-C12-C13
26	n	608	CLA	C13-C15-C16-C17
28	A	843	LHG	C4-O6-P-O3
28	A	855	LHG	C4-O6-P-O3
28	L	207	LHG	C3-O3-P-O6
28	c	317	LHG	C3-O3-P-O6
28	b	302	LHG	C3-O3-P-O6
28	b	318	LHG	C4-O6-P-O3
28	m	618	LHG	C3-O3-P-O6
28	l	318	LHG	C3-O3-P-O6
28	i	317	LHG	C3-O3-P-O6
28	j	617	LHG	C4-O6-P-O3
28	n	619	LHG	C3-O3-P-O6
26	B	802	CLA	C3-C5-C6-C7
26	A	821	CLA	CBA-CGA-O2A-C1
26	A	822	CLA	CBA-CGA-O2A-C1
26	A	823	CLA	CBA-CGA-O2A-C1
26	A	826	CLA	CBA-CGA-O2A-C1
26	i	303	CLA	CBA-CGA-O2A-C1
26	j	609	CLA	CBA-CGA-O2A-C1
26	n	607	CLA	CBA-CGA-O2A-C1
26	A	819	CLA	C15-C16-C17-C18
26	m	602	CLA	C8-C10-C11-C12
27	A	842	PQN	C23-C25-C26-C27
26	l	305	CLA	O1D-CGD-O2D-CED
26	k	606	CLA	O1D-CGD-O2D-CED
26	d	308	CLA	O1D-CGD-O2D-CED
28	L	207	LHG	C1-C2-C3-O3
28	b	302	LHG	C1-C2-C3-O3
34	c	319	LMG	O9-C10-O7-C8
26	A	809	CLA	C4-C3-C5-C6
26	h	304	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	i	302	CLA	C4-C3-C5-C6
26	A	819	CLA	C8-C10-C11-C12
26	b	308	CLA	C10-C11-C12-C13
26	A	818	CLA	CBD-CGD-O2D-CED
26	A	817	CLA	C2A-CAA-CBA-CGA
26	B	804	CLA	C2A-CAA-CBA-CGA
26	m	610	CLA	C2A-CAA-CBA-CGA
26	m	612	CLA	C2A-CAA-CBA-CGA
26	k	610	CLA	C2A-CAA-CBA-CGA
26	i	301	CLA	C2A-CAA-CBA-CGA
26	B	834	CLA	C16-C17-C18-C19
26	c	302	CLA	C11-C12-C13-C14
26	m	610	CLA	C6-C7-C8-C9
26	Q	302	CLA	C16-C17-C18-C20
26	B	823	CLA	CBA-CGA-O2A-C1
26	Q	302	CLA	CBA-CGA-O2A-C1
28	A	855	LHG	C24-C23-O8-C6
35	c	313	II0	C28-C26-C30-C32
35	c	316	II0	C27-C25-C29-C31
35	h	310	II0	C27-C25-C29-C31
35	h	312	II0	C28-C26-C30-C32
35	k	620	II0	C28-C26-C30-C32
35	i	314	II0	C27-C25-C29-C31
35	i	319	II0	C28-C26-C30-C32
35	j	614	II0	C27-C25-C29-C31
35	d	317	II0	C27-C25-C29-C31
37	a	315	IHT	C28-C26-C29-C31
26	B	801	CLA	O1A-CGA-O2A-C1
26	c	304	CLA	C10-C11-C12-C13
26	h	301	CLA	C5-C6-C7-C8
26	i	302	CLA	O1D-CGD-O2D-CED
29	A	848	WVN	C32-C36-C39-C40
29	B	847	WVN	C25-C28-C30-C33
29	B	848	WVN	C34-C37-C40-C39
29	B	850	WVN	C22-C26-C29-C31
29	F	203	WVN	C25-C28-C30-C33
29	L	201	WVN	C22-C26-C29-C31
29	L	205	WVN	C25-C28-C30-C33
29	M	101	WVN	C25-C28-C30-C33
29	M	101	WVN	C32-C36-C39-C40
29	l	303	WVN	C22-C26-C29-C31
29	l	303	WVN	C25-C28-C30-C33

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Mol	Chain	Res	Type	Atoms
35	a	313	II0	C26-C30-C32-C34
35	a	314	II0	C36-C40-C42-C41
35	b	314	II0	C26-C30-C32-C34
35	k	619	II0	C25-C29-C31-C33
35	i	319	II0	C26-C30-C32-C34
35	j	614	II0	C26-C30-C32-C34
35	d	301	II0	C25-C29-C31-C33
35	d	316	II0	C26-C30-C32-C34
28	L	207	LHG	C27-C28-C29-C30
28	s	409	LHG	C32-C33-C34-C35
26	F	201	CLA	CBD-CGD-O2D-CED
26	A	856	CLA	C15-C16-C17-C18
29	A	845	WVN	C24-C22-C26-C29
29	A	848	WVN	C27-C25-C28-C30
29	A	848	WVN	C35-C32-C36-C39
29	B	846	WVN	C24-C22-C26-C29
29	B	849	WVN	C27-C25-C28-C30
29	F	203	WVN	C24-C22-C26-C29
29	J	101	WVN	C24-C22-C26-C29
35	c	313	II0	C37-C35-C39-C41
35	c	313	II0	C38-C36-C40-C42
35	h	312	II0	C37-C35-C39-C41
35	l	314	II0	C37-C35-C39-C41
35	i	312	II0	C38-C36-C40-C42
35	j	615	II0	C37-C35-C39-C41
28	B	851	LHG	C24-C25-C26-C27
28	L	207	LHG	C25-C26-C27-C28
28	L	207	LHG	C30-C31-C32-C33
28	L	208	LHG	C13-C14-C15-C16
32	A	854	SQD	C11-C10-C9-C8
33	B	844	DGD	C7B-C8B-C9B-CAB
34	F	205	LMG	C16-C17-C18-C19
34	c	319	LMG	C29-C30-C31-C32
26	B	836	CLA	O1D-CGD-O2D-CED
36	k	611	KC2	C2A-CAA-CBA-CGA
36	i	309	KC2	C2A-CAA-CBA-CGA
36	i	318	KC2	C2A-CAA-CBA-CGA
36	j	611	KC2	C2A-CAA-CBA-CGA
36	d	312	KC2	C2A-CAA-CBA-CGA
26	A	856	CLA	C16-C17-C18-C19
28	c	317	LHG	C27-C28-C29-C30
28	c	320	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	m	618	LHG	C27-C28-C29-C30
28	n	619	LHG	C28-C29-C30-C31
34	Q	301	LMG	C30-C31-C32-C33
34	c	318	LMG	C7-C8-O7-C10
26	i	306	CLA	O1D-CGD-O2D-CED
26	m	604	CLA	C15-C16-C17-C18
28	b	302	LHG	C27-C28-C29-C30
33	j	618	DGD	C6A-C7A-C8A-C9A
34	L	209	LMG	C18-C19-C20-C21
26	n	603	CLA	O1D-CGD-O2D-CED
26	l	310	CLA	O1A-CGA-O2A-C1
26	i	306	CLA	O1A-CGA-O2A-C1
28	i	317	LHG	C24-C25-C26-C27
32	A	854	SQD	C11-C12-C13-C14
26	A	807	CLA	O1D-CGD-O2D-CED
26	L	202	CLA	O1D-CGD-O2D-CED
26	s	402	CLA	C13-C15-C16-C17
28	j	617	LHG	O2-C2-C3-O3
28	n	619	LHG	O2-C2-C3-O3
30	a	317	LMU	C11-C10-C9-C8
30	i	300	LMU	C2-C3-C4-C5
26	B	838	CLA	O1D-CGD-O2D-CED
29	A	845	WVN	C19-C22-C26-C29
29	A	847	WVN	C19-C22-C26-C29
29	A	848	WVN	C33-C34-C37-C40
29	B	848	WVN	C23-C25-C28-C30
29	B	849	WVN	C19-C22-C26-C29
29	B	850	WVN	C19-C22-C26-C29
29	J	101	WVN	C23-C25-C28-C30
29	J	101	WVN	C33-C34-C37-C40
29	J	102	WVN	C33-C34-C37-C40
29	M	101	WVN	C33-C34-C37-C40
29	s	407	WVN	C19-C22-C26-C29
29	s	407	WVN	C33-C34-C37-C40
29	h	309	WVN	C19-C22-C26-C29
29	h	309	WVN	C31-C32-C36-C39
29	l	303	WVN	C19-C22-C26-C29
29	l	303	WVN	C23-C25-C28-C30
29	l	316	WVN	C19-C22-C26-C29
30	A	850	LMU	C2'-C1'-O1'-C1
33	j	618	DGD	C2D-C1D-O3G-C3G
34	b	319	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
35	J	104	II0	C33-C35-C39-C41
35	c	313	II0	C34-C36-C40-C42
35	a	312	II0	C33-C35-C39-C41
35	a	313	II0	C34-C36-C40-C42
35	a	314	II0	C33-C35-C39-C41
35	a	314	II0	C34-C36-C40-C42
35	a	316	II0	C33-C35-C39-C41
35	b	315	II0	C33-C35-C39-C41
35	b	315	II0	C34-C36-C40-C42
35	h	310	II0	C33-C35-C39-C41
35	m	615	II0	C33-C35-C39-C41
35	m	616	II0	C33-C35-C39-C41
35	l	314	II0	C33-C35-C39-C41
35	l	314	II0	C34-C36-C40-C42
35	k	615	II0	C33-C35-C39-C41
35	i	312	II0	C34-C36-C40-C42
35	i	313	II0	C33-C35-C39-C41
35	i	313	II0	C34-C36-C40-C42
35	i	314	II0	C33-C35-C39-C41
35	i	316	II0	C33-C35-C39-C41
35	d	316	II0	C34-C36-C40-C42
35	d	317	II0	C33-C35-C39-C41
35	n	616	II0	C33-C35-C39-C41
28	A	855	LHG	O7-C5-C6-O8
26	L	204	CLA	CBA-CGA-O2A-C1
26	c	302	CLA	CBA-CGA-O2A-C1
28	n	619	LHG	C11-C10-C9-C8
30	A	850	LMU	C5-C6-C7-C8
34	F	205	LMG	C31-C32-C33-C34
26	A	808	CLA	C15-C16-C17-C18
26	a	310	CLA	C15-C16-C17-C18
26	i	303	CLA	O1A-CGA-O2A-C1
26	n	604	CLA	O1A-CGA-O2A-C1
26	n	607	CLA	O1A-CGA-O2A-C1
26	i	301	CLA	C16-C17-C18-C20
26	A	824	CLA	O1D-CGD-O2D-CED
26	A	828	CLA	O1D-CGD-O2D-CED
26	B	809	CLA	O1D-CGD-O2D-CED
26	d	307	CLA	O1D-CGD-O2D-CED
28	L	208	LHG	C14-C15-C16-C17
28	s	409	LHG	C29-C30-C31-C32
30	i	300	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	c	318	LMG	C18-C19-C20-C21
26	A	809	CLA	C2-C3-C5-C6
26	h	304	CLA	C2-C3-C5-C6
26	A	824	CLA	C14-C13-C15-C16
26	B	816	CLA	C14-C13-C15-C16
26	B	824	CLA	C6-C7-C8-C9
26	a	307	CLA	C11-C10-C8-C9
26	a	310	CLA	C11-C10-C8-C9
26	h	313	CLA	C11-C10-C8-C9
26	d	302	CLA	C14-C13-C15-C16
26	n	602	CLA	O1D-CGD-O2D-CED
28	A	849	LHG	C11-C10-C9-C8
28	L	208	LHG	C11-C10-C9-C8
28	s	409	LHG	C27-C28-C29-C30
28	b	302	LHG	C26-C27-C28-C29
32	A	854	SQD	C9-C10-C11-C12
33	B	844	DGD	CEB-CFB-CGB-CHB
26	B	820	CLA	C10-C11-C12-C13
26	B	836	CLA	C5-C6-C7-C8
26	B	840	CLA	C8-C10-C11-C12
26	c	304	CLA	C8-C10-C11-C12
26	b	310	CLA	C13-C15-C16-C17
26	l	307	CLA	C8-C10-C11-C12
26	A	828	CLA	C2A-CAA-CBA-CGA
26	c	311	CLA	C2A-CAA-CBA-CGA
26	h	304	CLA	C2A-CAA-CBA-CGA
25	A	801	CL0	O1A-CGA-O2A-C1
26	A	823	CLA	O1A-CGA-O2A-C1
26	j	609	CLA	O1A-CGA-O2A-C1
29	A	845	WVN	C30-C33-C34-C38
29	B	849	WVN	C30-C33-C34-C38
29	J	102	WVN	C30-C33-C34-C38
29	L	201	WVN	C11-C19-C22-C24
29	L	205	WVN	C11-C19-C22-C24
29	L	205	WVN	C29-C31-C32-C35
29	M	101	WVN	C30-C33-C34-C38
29	l	303	WVN	C30-C33-C34-C38
29	i	315	WVN	C20-C23-C25-C27
35	a	316	II0	C32-C34-C36-C38
35	h	311	II0	C32-C34-C36-C38
35	m	616	II0	C31-C33-C35-C37
35	k	619	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
34	F	205	LMG	C33-C34-C35-C36
34	c	319	LMG	C16-C17-C18-C19
28	J	105	LHG	O1-C1-C2-C3
28	L	207	LHG	O1-C1-C2-C3
28	L	208	LHG	O1-C1-C2-C3
28	l	318	LHG	O1-C1-C2-C3
28	i	317	LHG	O1-C1-C2-C3
28	j	617	LHG	O1-C1-C2-C3
29	A	845	WVN	C20-C23-C25-C28
29	A	845	WVN	C29-C31-C32-C36
29	A	848	WVN	C30-C33-C34-C37
29	B	847	WVN	C30-C33-C34-C37
29	B	850	WVN	C29-C31-C32-C36
29	I	101	WVN	C29-C31-C32-C36
29	J	101	WVN	C29-C31-C32-C36
29	R	200	WVN	C20-C23-C25-C28
35	a	316	II0	C31-C33-C35-C39
35	h	310	II0	C31-C33-C35-C39
35	m	619	II0	C32-C34-C36-C40
35	i	314	II0	C31-C33-C35-C39
35	n	618	II0	C32-C34-C36-C40
26	l	308	CLA	C3-C5-C6-C7
26	B	812	CLA	C8-C10-C11-C12
26	B	826	CLA	C10-C11-C12-C13
26	m	613	CLA	C13-C15-C16-C17
26	m	613	CLA	C15-C16-C17-C18
28	j	617	LHG	C8-C7-O7-C5
28	A	843	LHG	C11-C10-C9-C8
28	A	843	LHG	C24-C25-C26-C27
28	L	208	LHG	C32-C33-C34-C35
34	n	620	LMG	C29-C30-C31-C32
28	A	855	LHG	C23-C24-C25-C26
28	L	207	LHG	C23-C24-C25-C26
28	c	320	LHG	C23-C24-C25-C26
26	m	602	CLA	C2C-C3C-CAC-CBC
28	A	843	LHG	C30-C31-C32-C33
28	A	843	LHG	C31-C32-C33-C34
28	A	855	LHG	C27-C28-C29-C30
28	B	851	LHG	C32-C33-C34-C35
28	c	320	LHG	C24-C25-C26-C27
28	l	318	LHG	C11-C10-C9-C8
28	n	619	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	a	317	LMU	C6-C7-C8-C9
34	F	205	LMG	C32-C33-C34-C35
34	c	319	LMG	C18-C19-C20-C21
34	n	620	LMG	C31-C32-C33-C34
25	A	801	CL0	C16-C17-C18-C19
26	b	304	CLA	C6-C7-C8-C9
26	b	304	CLA	C6-C7-C8-C10
26	m	609	CLA	C11-C12-C13-C14
26	m	609	CLA	C11-C12-C13-C15
30	A	850	LMU	O5'-C1'-O1'-C1
33	j	618	DGD	O6D-C1D-O3G-C3G
34	b	319	LMG	O6-C1-O1-C7
26	b	310	CLA	C10-C11-C12-C13
28	B	851	LHG	C9-C10-C11-C12
28	B	851	LHG	C27-C28-C29-C30
26	A	820	CLA	O1D-CGD-O2D-CED
28	A	843	LHG	C28-C29-C30-C31
32	A	854	SQD	C16-C17-C18-C19
33	B	844	DGD	C4A-C5A-C6A-C7A
34	F	205	LMG	C17-C18-C19-C20
34	c	318	LMG	C23-C24-C25-C26
34	Q	301	LMG	C15-C16-C17-C18
34	Q	301	LMG	C31-C32-C33-C34
34	F	206	LMG	C17-C18-C19-C20
34	c	319	LMG	C32-C33-C34-C35
34	n	620	LMG	C37-C38-C39-C40
34	c	319	LMG	O6-C5-C6-O5
26	A	813	CLA	CBA-CGA-O2A-C1
26	l	309	CLA	CBA-CGA-O2A-C1
26	j	613	CLA	CBA-CGA-O2A-C1
28	A	855	LHG	C24-C25-C26-C27
34	F	206	LMG	C16-C17-C18-C19
26	b	304	CLA	O1D-CGD-O2D-CED
26	n	606	CLA	O1D-CGD-O2D-CED
26	A	805	CLA	C3A-C2A-CAA-CBA
26	A	814	CLA	C3A-C2A-CAA-CBA
26	A	831	CLA	C3A-C2A-CAA-CBA
26	A	834	CLA	C3A-C2A-CAA-CBA
26	A	840	CLA	C3A-C2A-CAA-CBA
26	A	841	CLA	C3A-C2A-CAA-CBA
26	A	851	CLA	C3A-C2A-CAA-CBA
26	B	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	B	830	CLA	C3A-C2A-CAA-CBA
26	B	833	CLA	C3A-C2A-CAA-CBA
26	c	306	CLA	C3A-C2A-CAA-CBA
26	a	305	CLA	C3A-C2A-CAA-CBA
26	h	307	CLA	C3A-C2A-CAA-CBA
26	k	614	CLA	C3A-C2A-CAA-CBA
26	j	605	CLA	C3A-C2A-CAA-CBA
26	j	606	CLA	C3A-C2A-CAA-CBA
26	d	307	CLA	C3A-C2A-CAA-CBA
26	n	601	CLA	C3A-C2A-CAA-CBA
26	n	603	CLA	C3A-C2A-CAA-CBA
26	n	604	CLA	C3A-C2A-CAA-CBA
29	A	847	WVN	C22-C26-C29-C31
35	i	312	II0	C25-C29-C31-C33
28	b	318	LHG	C26-C27-C28-C29
33	B	844	DGD	CBA-CCA-CDA-CEA
34	c	319	LMG	C30-C31-C32-C33
34	b	319	LMG	C14-C15-C16-C17
26	A	837	CLA	O1D-CGD-O2D-CED
26	a	307	CLA	O1D-CGD-O2D-CED
26	A	822	CLA	O1A-CGA-O2A-C1
26	d	313	CLA	O1A-CGA-O2A-C1
26	m	610	CLA	C6-C7-C8-C10
28	L	208	LHG	C27-C28-C29-C30
28	b	318	LHG	C12-C13-C14-C15
33	j	618	DGD	C4A-C5A-C6A-C7A
30	i	300	LMU	C1-C2-C3-C4
26	B	820	CLA	CBD-CGD-O2D-CED
26	j	607	CLA	CBD-CGD-O2D-CED
34	F	205	LMG	C18-C19-C20-C21
26	m	613	CLA	C3-C5-C6-C7
26	n	607	CLA	C3-C5-C6-C7
34	c	319	LMG	C10-C11-C12-C13
28	j	617	LHG	C9-C10-C11-C12
26	A	821	CLA	O1A-CGA-O2A-C1
26	A	826	CLA	C4-C3-C5-C6
26	B	803	CLA	C4-C3-C5-C6
26	B	815	CLA	C4-C3-C5-C6
26	B	834	CLA	C4-C3-C5-C6
26	m	603	CLA	C4-C3-C5-C6
27	A	842	PQN	C14-C13-C15-C16
26	A	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	F	201	CLA	CBA-CGA-O2A-C1
26	l	313	CLA	CBA-CGA-O2A-C1
26	A	826	CLA	C2-C3-C5-C6
26	A	838	CLA	C2-C3-C5-C6
26	B	803	CLA	C2-C3-C5-C6
26	B	813	CLA	C2-C3-C5-C6
26	B	834	CLA	C2-C3-C5-C6
26	m	603	CLA	C2-C3-C5-C6
28	b	318	LHG	C32-C33-C34-C35
34	c	319	LMG	C31-C32-C33-C34
28	c	320	LHG	O1-C1-C2-O2
28	b	302	LHG	O1-C1-C2-O2
28	i	317	LHG	O1-C1-C2-O2
28	n	619	LHG	O1-C1-C2-O2
26	A	826	CLA	O1A-CGA-O2A-C1
26	A	816	CLA	C16-C17-C18-C19
26	B	834	CLA	C16-C17-C18-C20
28	n	619	LHG	C32-C33-C34-C35
33	j	618	DGD	C4B-C5B-C6B-C7B
26	B	819	CLA	C3-C5-C6-C7
26	B	841	CLA	C3-C5-C6-C7
26	b	309	CLA	C3-C5-C6-C7
26	B	823	CLA	O1A-CGA-O2A-C1
26	Q	302	CLA	O1A-CGA-O2A-C1
28	B	851	LHG	O10-C23-O8-C6
28	l	318	LHG	C23-C24-C25-C26
26	B	824	CLA	C10-C11-C12-C13
26	b	310	CLA	C8-C10-C11-C12
26	h	304	CLA	C5-C6-C7-C8
26	A	833	CLA	CBD-CGD-O2D-CED
26	a	309	CLA	CBD-CGD-O2D-CED
30	A	850	LMU	C2-C3-C4-C5
26	B	801	CLA	C2-C1-O2A-CGA
26	m	602	CLA	C4C-C3C-CAC-CBC
28	A	843	LHG	C9-C10-C11-C12
28	s	409	LHG	C24-C25-C26-C27
30	A	850	LMU	C7-C8-C9-C10
34	L	209	LMG	C23-C24-C25-C26
26	B	814	CLA	C15-C16-C17-C18
26	k	609	CLA	C5-C6-C7-C8
26	i	307	CLA	C5-C6-C7-C8
33	j	618	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
26	c	302	CLA	O1A-CGA-O2A-C1
28	n	619	LHG	C27-C28-C29-C30
30	A	858	LMU	C3'-C4'-O1B-C1B
26	A	816	CLA	C3-C5-C6-C7
26	i	307	CLA	C3-C5-C6-C7
29	B	846	WVN	C15-C13-C20-C23
29	B	850	WVN	C15-C13-C20-C23
29	L	205	WVN	C06-C13-C20-C23
29	l	303	WVN	C15-C13-C20-C23
29	l	316	WVN	C15-C13-C20-C23
29	i	315	WVN	C06-C13-C20-C23
37	a	315	IHT	C10-C07-C18-C22
37	m	617	IHT	C02-C07-C18-C22
37	m	617	IHT	C10-C07-C18-C22
37	R	202	IHT	C10-C07-C18-C22
28	B	851	LHG	C31-C32-C33-C34
28	L	207	LHG	C32-C33-C34-C35
33	B	844	DGD	CAB-CBB-CCB-CDB
26	b	309	CLA	O1D-CGD-O2D-CED
26	B	822	CLA	CBA-CGA-O2A-C1
26	B	827	CLA	CBA-CGA-O2A-C1
26	F	202	CLA	CBA-CGA-O2A-C1
26	b	304	CLA	CBA-CGA-O2A-C1
26	m	612	CLA	CBA-CGA-O2A-C1
26	j	607	CLA	CBA-CGA-O2A-C1
26	A	809	CLA	C5-C6-C7-C8
26	A	856	CLA	C13-C15-C16-C17
26	b	310	CLA	C5-C6-C7-C8
26	i	310	CLA	C8-C10-C11-C12
26	i	310	CLA	C10-C11-C12-C13
28	c	317	LHG	C30-C31-C32-C33
28	b	302	LHG	C24-C25-C26-C27
32	A	854	SQD	C12-C13-C14-C15
34	c	318	LMG	C22-C23-C24-C25
26	L	204	CLA	O1A-CGA-O2A-C1
34	c	318	LMG	O6-C5-C6-O5
28	n	619	LHG	C7-C8-C9-C10
34	n	620	LMG	C17-C18-C19-C20
26	B	837	CLA	C15-C16-C17-C18
26	m	608	CLA	C13-C15-C16-C17
28	b	302	LHG	C29-C30-C31-C32
34	c	318	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	A	838	CLA	C4-C3-C5-C6
26	B	813	CLA	C4-C3-C5-C6
26	l	307	CLA	C4-C3-C5-C6
26	a	301	CLA	O1D-CGD-O2D-CED
26	A	828	CLA	C2-C3-C5-C6
26	A	833	CLA	C12-C13-C15-C16
26	B	807	CLA	C11-C10-C8-C7
26	B	816	CLA	C12-C13-C15-C16
26	B	824	CLA	C6-C7-C8-C10
26	B	829	CLA	C6-C7-C8-C10
26	B	836	CLA	C6-C7-C8-C10
26	F	201	CLA	C12-C13-C15-C16
26	s	403	CLA	C6-C7-C8-C10
26	a	307	CLA	C11-C10-C8-C7
26	a	310	CLA	C11-C10-C8-C7
26	h	313	CLA	C11-C10-C8-C7
26	m	608	CLA	C12-C13-C15-C16
26	l	307	CLA	C2-C3-C5-C6
26	l	311	CLA	C11-C10-C8-C7
26	j	601	CLA	C11-C10-C8-C7
26	d	302	CLA	C6-C7-C8-C10
27	A	842	PQN	C17-C18-C20-C21
26	A	813	CLA	O1A-CGA-O2A-C1
26	A	817	CLA	O1A-CGA-O2A-C1
26	F	201	CLA	O1A-CGA-O2A-C1
26	l	309	CLA	O1A-CGA-O2A-C1
26	l	313	CLA	O1A-CGA-O2A-C1
26	j	613	CLA	O1A-CGA-O2A-C1
26	l	301	CLA	C15-C16-C17-C18
29	F	203	WVN	C22-C26-C29-C31
35	i	313	II0	C26-C30-C32-C34
35	i	314	II0	C25-C29-C31-C33
26	A	856	CLA	C16-C17-C18-C20
26	a	301	CLA	C16-C17-C18-C19
26	B	823	CLA	O1D-CGD-O2D-CED
26	B	826	CLA	O1D-CGD-O2D-CED
26	k	605	CLA	O1D-CGD-O2D-CED
28	j	617	LHG	O9-C7-O7-C5
26	A	806	CLA	CBA-CGA-O2A-C1
26	A	831	CLA	CBA-CGA-O2A-C1
26	h	307	CLA	CBA-CGA-O2A-C1
26	m	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	l	301	CLA	CBA-CGA-O2A-C1
26	k	607	CLA	CBA-CGA-O2A-C1
26	i	305	CLA	CBA-CGA-O2A-C1
26	j	606	CLA	CBA-CGA-O2A-C1
26	n	603	CLA	CBA-CGA-O2A-C1
28	L	208	LHG	C28-C29-C30-C31
28	n	619	LHG	C30-C31-C32-C33
33	B	844	DGD	C2A-C3A-C4A-C5A
33	j	618	DGD	CDB-CEB-CFB-CGB
26	B	802	CLA	C2A-CAA-CBA-CGA
26	B	813	CLA	C2A-CAA-CBA-CGA
26	c	308	CLA	C2A-CAA-CBA-CGA
26	i	304	CLA	C2A-CAA-CBA-CGA
26	j	613	CLA	C2A-CAA-CBA-CGA
26	n	602	CLA	C2A-CAA-CBA-CGA
26	A	835	CLA	C5-C6-C7-C8
26	B	841	CLA	C15-C16-C17-C18
26	i	307	CLA	C13-C15-C16-C17
26	j	601	CLA	C8-C10-C11-C12
28	A	843	LHG	C13-C14-C15-C16
34	n	620	LMG	C33-C34-C35-C36
28	b	318	LHG	C7-C8-C9-C10
33	j	618	DGD	C1A-C2A-C3A-C4A
26	B	812	CLA	O1D-CGD-O2D-CED
26	h	304	CLA	C8-C10-C11-C12
36	m	611	KC2	C2B-C3B-CAB-CBB
36	k	611	KC2	C2C-C3C-CAC-CBC
36	i	309	KC2	C2C-C3C-CAC-CBC
36	d	311	KC2	C2B-C3B-CAB-CBB
36	n	612	KC2	C2B-C3B-CAB-CBB
30	A	850	LMU	C4'-C5'-C6'-O6'
26	B	836	CLA	C13-C15-C16-C17
26	l	311	CLA	C5-C6-C7-C8
26	a	310	CLA	O1D-CGD-O2D-CED
26	n	605	CLA	O1D-CGD-O2D-CED
26	k	614	CLA	C4C-C3C-CAC-CBC
34	F	205	LMG	C38-C39-C40-C41
28	A	843	LHG	C23-C24-C25-C26
28	c	317	LHG	C7-C8-C9-C10
36	l	312	KC2	C4B-C3B-CAB-CBB
36	l	312	KC2	C4C-C3C-CAC-CBC
36	k	611	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
36	i	309	KC2	C4C-C3C-CAC-CBC
36	d	311	KC2	C4B-C3B-CAB-CBB
36	n	611	KC2	C4B-C3B-CAB-CBB
26	A	807	CLA	C8-C10-C11-C12
26	A	838	CLA	C8-C10-C11-C12
27	A	842	PQN	C18-C20-C21-C22
36	n	612	KC2	CBD-CGD-O2D-CED
26	A	841	CLA	C3-C5-C6-C7
28	A	849	LHG	C9-C10-C11-C12
28	b	318	LHG	C25-C26-C27-C28
34	c	319	LMG	O1-C7-C8-O7
34	b	319	LMG	O6-C5-C6-O5
28	b	318	LHG	C30-C31-C32-C33
26	B	822	CLA	O1A-CGA-O2A-C1
26	i	301	CLA	C16-C17-C18-C19
26	Q	302	CLA	C16-C17-C18-C19
28	B	851	LHG	C28-C29-C30-C31
33	B	844	DGD	C8A-C9A-CAA-CBA
34	F	205	LMG	C30-C31-C32-C33
26	A	828	CLA	C4-C3-C5-C6
28	L	208	LHG	C7-C8-C9-C10
26	B	815	CLA	C2-C3-C5-C6
26	i	302	CLA	C2-C3-C5-C6
35	c	314	II0	C10-C22-C24-C26
37	n	617	IHT	C11-C21-C24-C26
26	A	822	CLA	C6-C7-C8-C9
26	A	833	CLA	C14-C13-C15-C16
26	A	837	CLA	C6-C7-C8-C9
26	A	841	CLA	C11-C12-C13-C14
26	B	801	CLA	C11-C10-C8-C9
26	B	829	CLA	C6-C7-C8-C9
26	B	829	CLA	C14-C13-C15-C16
26	B	834	CLA	C14-C13-C15-C16
26	B	836	CLA	C6-C7-C8-C9
26	B	841	CLA	C6-C7-C8-C9
26	b	308	CLA	C6-C7-C8-C9
26	b	311	CLA	C14-C13-C15-C16
26	h	304	CLA	C11-C12-C13-C14
26	m	608	CLA	C14-C13-C15-C16
26	l	311	CLA	C11-C10-C8-C9
26	i	301	CLA	C14-C13-C15-C16
26	j	601	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	n	610	CLA	C6-C7-C8-C9
27	A	842	PQN	C19-C18-C20-C21
32	A	854	SQD	C14-C15-C16-C17
26	A	840	CLA	C3-C5-C6-C7
26	A	806	CLA	O1D-CGD-O2D-CED
26	A	808	CLA	C2A-CAA-CBA-CGA
26	A	810	CLA	C2A-CAA-CBA-CGA
26	B	838	CLA	C2A-CAA-CBA-CGA
26	l	307	CLA	C2A-CAA-CBA-CGA
26	i	302	CLA	C2A-CAA-CBA-CGA
26	i	311	CLA	C2A-CAA-CBA-CGA
26	d	302	CLA	C2A-CAA-CBA-CGA
26	Q	302	CLA	C2A-CAA-CBA-CGA
26	k	614	CLA	CBA-CGA-O2A-C1
29	K	102	WVN	C29-C31-C32-C35
29	h	309	WVN	C11-C19-C22-C24
35	a	313	II0	C32-C34-C36-C38
35	h	310	II0	C31-C33-C35-C37
35	m	616	II0	C32-C34-C36-C38
35	i	314	II0	C31-C33-C35-C37
35	i	316	II0	C32-C34-C36-C38
35	d	316	II0	C32-C34-C36-C38
35	n	618	II0	C32-C34-C36-C38
26	d	305	CLA	CBD-CGD-O2D-CED
26	d	310	CLA	CBD-CGD-O2D-CED
28	n	619	LHG	C24-C25-C26-C27
29	A	846	WVN	C20-C23-C25-C28
29	A	846	WVN	C30-C33-C34-C37
29	A	857	WVN	C20-C23-C25-C28
29	B	848	WVN	C20-C23-C25-C28
29	B	853	WVN	C11-C19-C22-C26
29	B	853	WVN	C20-C23-C25-C28
29	I	101	WVN	C11-C19-C22-C26
29	L	205	WVN	C11-C19-C22-C26
29	h	309	WVN	C20-C23-C25-C28
35	l	315	II0	C32-C34-C36-C40
35	k	615	II0	C31-C33-C35-C39
35	k	620	II0	C31-C33-C35-C39
35	i	319	II0	C32-C34-C36-C40
26	B	827	CLA	O1A-CGA-O2A-C1
26	F	202	CLA	O1A-CGA-O2A-C1
26	b	304	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	j	607	CLA	O1A-CGA-O2A-C1
26	n	603	CLA	O1A-CGA-O2A-C1
26	A	805	CLA	C1A-C2A-CAA-CBA
26	A	808	CLA	C1A-C2A-CAA-CBA
26	A	810	CLA	C1A-C2A-CAA-CBA
26	A	817	CLA	C1A-C2A-CAA-CBA
26	A	831	CLA	C1A-C2A-CAA-CBA
26	A	832	CLA	C1A-C2A-CAA-CBA
26	A	833	CLA	C1A-C2A-CAA-CBA
26	A	834	CLA	C1A-C2A-CAA-CBA
26	A	840	CLA	C1A-C2A-CAA-CBA
26	B	815	CLA	C1A-C2A-CAA-CBA
26	B	817	CLA	C1A-C2A-CAA-CBA
26	B	818	CLA	C1A-C2A-CAA-CBA
26	B	820	CLA	C1A-C2A-CAA-CBA
26	B	835	CLA	C1A-C2A-CAA-CBA
26	B	837	CLA	C1A-C2A-CAA-CBA
26	B	840	CLA	C1A-C2A-CAA-CBA
26	c	306	CLA	C1A-C2A-CAA-CBA
26	c	311	CLA	C1A-C2A-CAA-CBA
26	a	302	CLA	C1A-C2A-CAA-CBA
26	a	305	CLA	C1A-C2A-CAA-CBA
26	h	302	CLA	C1A-C2A-CAA-CBA
26	h	308	CLA	C1A-C2A-CAA-CBA
26	m	607	CLA	C1A-C2A-CAA-CBA
26	j	606	CLA	C1A-C2A-CAA-CBA
26	j	610	CLA	C1A-C2A-CAA-CBA
26	d	304	CLA	C1A-C2A-CAA-CBA
26	d	306	CLA	C1A-C2A-CAA-CBA
26	d	308	CLA	C1A-C2A-CAA-CBA
26	n	601	CLA	C1A-C2A-CAA-CBA
26	n	607	CLA	C1A-C2A-CAA-CBA
26	n	608	CLA	C1A-C2A-CAA-CBA
26	n	609	CLA	C1A-C2A-CAA-CBA
26	A	816	CLA	C16-C17-C18-C20
30	a	317	LMU	C4-C5-C6-C7
34	F	205	LMG	C20-C21-C22-C23
35	J	104	II0	C26-C30-C32-C34
35	b	315	II0	C36-C40-C42-C41
35	h	310	II0	C35-C39-C41-C42
35	m	615	II0	C25-C29-C31-C33
26	A	802	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	c	308	CLA	C10-C11-C12-C13
26	k	604	CLA	C5-C6-C7-C8
28	B	851	LHG	C4-O6-P-O3
28	J	105	LHG	C4-O6-P-O3
28	j	617	LHG	C3-O3-P-O6
34	F	205	LMG	C15-C16-C17-C18
26	B	826	CLA	C3-C5-C6-C7
28	i	317	LHG	C25-C26-C27-C28
33	B	844	DGD	CEA-CFA-CGA-CHA
26	j	606	CLA	O1A-CGA-O2A-C1
26	A	819	CLA	C10-C11-C12-C13
28	B	851	LHG	O6-C4-C5-C6
28	c	317	LHG	O6-C4-C5-C6
34	b	319	LMG	C33-C34-C35-C36
34	L	209	LMG	C17-C18-C19-C20
34	F	205	LMG	O6-C5-C6-O5
26	s	403	CLA	C5-C6-C7-C8
26	c	302	CLA	C11-C12-C13-C15
36	m	611	KC2	CAA-CBA-CGA-O1A
26	n	607	CLA	O1D-CGD-O2D-CED
28	L	207	LHG	C11-C10-C9-C8
34	n	620	LMG	C19-C20-C21-C22
28	j	617	LHG	C1-C2-C3-O3
30	A	858	LMU	O5'-C5'-C6'-O6'
28	c	320	LHG	C25-C26-C27-C28
28	B	851	LHG	C11-C10-C9-C8
26	m	606	CLA	O1A-CGA-O2A-C1
26	m	612	CLA	O1A-CGA-O2A-C1
26	l	301	CLA	O1A-CGA-O2A-C1
26	A	814	CLA	C2A-CAA-CBA-CGA
26	d	318	CLA	C2A-CAA-CBA-CGA
26	B	810	CLA	C16-C17-C18-C20
26	a	301	CLA	C16-C17-C18-C20
28	A	844	LHG	C4-C5-C6-O8
28	A	855	LHG	C4-C5-C6-O8
28	j	617	LHG	C4-C5-C6-O8
33	j	618	DGD	O1G-C1G-C2G-C3G
33	j	618	DGD	C1G-C2G-C3G-O3G
34	F	206	LMG	C7-C8-C9-O8
34	c	319	LMG	O1-C7-C8-C9
34	Q	301	LMG	C7-C8-C9-O8
36	k	611	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	A	828	CLA	C15-C16-C17-C18
33	B	844	DGD	C5A-C6A-C7A-C8A
33	B	844	DGD	C6B-C7B-C8B-C9B
26	A	806	CLA	O1A-CGA-O2A-C1
26	k	607	CLA	O1A-CGA-O2A-C1
26	i	305	CLA	O1A-CGA-O2A-C1
26	B	815	CLA	O1D-CGD-O2D-CED
28	B	851	LHG	C25-C26-C27-C28
26	k	608	CLA	O1D-CGD-O2D-CED
26	A	852	CLA	C13-C15-C16-C17
26	A	856	CLA	CAA-CBA-CGA-O2A
26	A	831	CLA	O1A-CGA-O2A-C1
26	h	307	CLA	O1A-CGA-O2A-C1
28	L	207	LHG	C12-C13-C14-C15
28	L	208	LHG	C29-C30-C31-C32
34	b	319	LMG	C17-C18-C19-C20
34	Q	301	LMG	C17-C18-C19-C20
28	A	855	LHG	O1-C1-C2-O2
28	L	207	LHG	O1-C1-C2-O2
28	j	617	LHG	O1-C1-C2-O2
28	i	317	LHG	C27-C28-C29-C30
26	b	311	CLA	C13-C15-C16-C17
28	A	855	LHG	C7-C8-C9-C10
28	j	617	LHG	C24-C25-C26-C27
28	l	318	LHG	C8-C7-O7-C5
33	j	618	DGD	C6B-C7B-C8B-C9B
36	c	310	KC2	O1D-CGD-O2D-CED
26	B	812	CLA	C15-C16-C17-C18
26	B	806	CLA	C4-C3-C5-C6
28	L	208	LHG	C11-C12-C13-C14
30	a	317	LMU	C4'-C5'-C6'-O6'
36	k	613	KC2	C2A-CAA-CBA-CGA
26	A	811	CLA	CBA-CGA-O2A-C1
26	h	306	CLA	CBA-CGA-O2A-C1
28	J	105	LHG	C24-C23-O8-C6
34	F	206	LMG	C29-C28-O8-C9
28	A	855	LHG	C28-C29-C30-C31
26	A	816	CLA	CBD-CGD-O2D-CED
26	B	839	CLA	C5-C6-C7-C8
33	B	844	DGD	C3G-C2G-O2G-C1B
34	F	205	LMG	C9-C8-O7-C10
34	Q	301	LMG	C7-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
36	m	611	KC2	CAA-CBA-CGA-O2A
26	B	801	CLA	C5-C6-C7-C8
26	B	836	CLA	C8-C10-C11-C12
26	h	303	CLA	C2-C1-O2A-CGA
34	F	205	LMG	C22-C23-C24-C25
34	L	209	LMG	C16-C17-C18-C19
26	B	816	CLA	O1D-CGD-O2D-CED
28	B	851	LHG	C33-C34-C35-C36
28	L	208	LHG	O6-C4-C5-O7
26	B	810	CLA	C16-C17-C18-C19
26	i	311	CLA	C16-C17-C18-C20
26	A	837	CLA	C13-C15-C16-C17
34	F	205	LMG	C41-C42-C43-C44
28	b	302	LHG	O2-C2-C3-O3
26	k	614	CLA	O1A-CGA-O2A-C1
36	k	611	KC2	CAA-CBA-CGA-O2A
26	B	804	CLA	C15-C16-C17-C18
26	B	822	CLA	C5-C6-C7-C8
26	F	201	CLA	C5-C6-C7-C8
29	B	848	WVN	C31-C32-C36-C39
35	j	614	II0	C33-C35-C39-C41
35	j	614	II0	C34-C36-C40-C42
26	B	819	CLA	CBA-CGA-O2A-C1
26	A	852	CLA	C4-C3-C5-C6
27	B	843	PQN	C14-C13-C15-C16
26	A	805	CLA	C6-C7-C8-C10
26	A	816	CLA	C6-C7-C8-C10
26	A	819	CLA	C6-C7-C8-C10
26	A	825	CLA	C11-C10-C8-C7
26	A	830	CLA	C11-C10-C8-C7
26	A	833	CLA	C11-C10-C8-C7
26	A	837	CLA	C6-C7-C8-C10
26	A	840	CLA	C11-C10-C8-C7
26	A	841	CLA	C11-C10-C8-C7
26	A	841	CLA	C11-C12-C13-C15
26	A	852	CLA	C2-C3-C5-C6
26	A	852	CLA	C11-C10-C8-C7
26	B	801	CLA	C6-C7-C8-C10
26	B	801	CLA	C11-C10-C8-C7
26	B	803	CLA	C6-C7-C8-C10
26	B	803	CLA	C11-C10-C8-C7
26	B	809	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	B	818	CLA	C11-C10-C8-C7
26	B	822	CLA	C11-C12-C13-C15
26	B	825	CLA	C12-C13-C15-C16
26	B	826	CLA	C11-C10-C8-C7
26	B	829	CLA	C12-C13-C15-C16
26	B	831	CLA	C11-C10-C8-C7
26	B	838	CLA	C12-C13-C15-C16
26	B	841	CLA	C6-C7-C8-C10
26	s	402	CLA	C11-C10-C8-C7
26	s	408	CLA	C6-C7-C8-C10
26	a	301	CLA	C12-C13-C15-C16
26	a	309	CLA	C6-C7-C8-C10
26	a	310	CLA	C6-C7-C8-C10
26	b	306	CLA	C11-C12-C13-C15
26	b	308	CLA	C6-C7-C8-C10
26	b	309	CLA	C11-C10-C8-C7
26	b	310	CLA	C11-C10-C8-C7
26	b	311	CLA	C12-C13-C15-C16
26	h	304	CLA	C11-C12-C13-C15
26	m	606	CLA	C6-C7-C8-C10
26	l	311	CLA	C11-C12-C13-C15
26	l	313	CLA	C6-C7-C8-C10
26	k	608	CLA	C6-C7-C8-C10
26	i	301	CLA	C11-C10-C8-C7
26	i	301	CLA	C12-C13-C15-C16
26	d	302	CLA	C11-C12-C13-C15
27	A	842	PQN	C21-C22-C23-C25
26	A	805	CLA	C6-C7-C8-C9
26	A	816	CLA	C6-C7-C8-C9
26	A	816	CLA	C11-C10-C8-C9
26	A	819	CLA	C6-C7-C8-C9
26	A	825	CLA	C11-C10-C8-C9
26	A	830	CLA	C11-C10-C8-C9
26	A	852	CLA	C11-C10-C8-C9
26	B	801	CLA	C6-C7-C8-C9
26	B	803	CLA	C6-C7-C8-C9
26	B	803	CLA	C11-C10-C8-C9
26	B	804	CLA	C6-C7-C8-C9
26	B	807	CLA	C11-C10-C8-C9
26	B	809	CLA	C11-C12-C13-C14
26	B	818	CLA	C11-C12-C13-C14
26	B	819	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	B	822	CLA	C11-C12-C13-C14
26	B	825	CLA	C11-C10-C8-C9
26	B	826	CLA	C11-C10-C8-C9
26	B	831	CLA	C11-C10-C8-C9
26	B	838	CLA	C14-C13-C15-C16
26	s	403	CLA	C6-C7-C8-C9
26	c	304	CLA	C11-C10-C8-C9
26	a	301	CLA	C14-C13-C15-C16
26	a	304	CLA	C11-C10-C8-C9
26	a	306	CLA	C14-C13-C15-C16
26	a	309	CLA	C6-C7-C8-C9
26	a	310	CLA	C6-C7-C8-C9
26	b	306	CLA	C11-C10-C8-C9
26	b	306	CLA	C11-C12-C13-C14
26	b	309	CLA	C11-C10-C8-C9
26	b	310	CLA	C11-C10-C8-C9
26	m	606	CLA	C14-C13-C15-C16
26	m	613	CLA	C11-C10-C8-C9
26	k	602	CLA	C11-C10-C8-C9
26	k	608	CLA	C6-C7-C8-C9
26	j	609	CLA	C14-C13-C15-C16
26	j	613	CLA	C6-C7-C8-C9
26	d	302	CLA	C6-C7-C8-C9
26	d	302	CLA	C11-C12-C13-C14
26	Q	302	CLA	C11-C10-C8-C9
27	A	842	PQN	C21-C22-C23-C24
35	l	315	II0	C26-C30-C32-C34
26	l	304	CLA	CBA-CGA-O2A-C1
26	k	606	CLA	CBA-CGA-O2A-C1
26	b	306	CLA	C2A-CAA-CBA-CGA
28	J	105	LHG	C13-C14-C15-C16
26	c	309	CLA	O1D-CGD-O2D-CED
29	B	853	WVN	C30-C33-C34-C38
29	L	201	WVN	C30-C33-C34-C38
29	i	315	WVN	C11-C19-C22-C24
35	a	312	II0	C32-C34-C36-C38
35	m	614	II0	C32-C34-C36-C38
35	k	615	II0	C32-C34-C36-C38
35	d	301	II0	C32-C34-C36-C38
35	d	317	II0	C32-C34-C36-C38
26	B	837	CLA	C16-C17-C18-C20
29	A	848	WVN	C11-C19-C22-C26

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Mol	Chain	Res	Type	Atoms
29	B	850	WVN	C11-C19-C22-C26
29	B	853	WVN	C29-C31-C32-C36
29	I	101	WVN	C20-C23-C25-C28
29	s	405	WVN	C30-C33-C34-C37
29	l	303	WVN	C11-C19-C22-C26
29	l	303	WVN	C30-C33-C34-C37
35	c	316	II0	C31-C33-C35-C39
35	m	619	II0	C31-C33-C35-C39
35	d	319	II0	C32-C34-C36-C40
34	L	209	LMG	C19-C20-C21-C22
34	n	620	LMG	C14-C15-C16-C17
26	A	805	CLA	C3-C5-C6-C7
26	A	820	CLA	C3-C5-C6-C7
26	A	822	CLA	C3-C5-C6-C7
26	h	301	CLA	C3-C5-C6-C7
26	i	306	CLA	C5-C6-C7-C8
28	m	618	LHG	C8-C7-O7-C5
34	c	318	LMG	C42-C43-C44-C45
26	B	817	CLA	CBA-CGA-O2A-C1
28	c	317	LHG	C5-C6-O8-C23
28	A	844	LHG	O6-C4-C5-C6
28	i	317	LHG	O6-C4-C5-C6
28	b	302	LHG	C10-C11-C12-C13
34	F	205	LMG	C40-C41-C42-C43
34	L	209	LMG	C30-C31-C32-C33
26	B	818	CLA	CBA-CGA-O2A-C1
26	s	402	CLA	CBA-CGA-O2A-C1
26	h	304	CLA	C10-C11-C12-C13
28	l	318	LHG	C27-C28-C29-C30
26	A	820	CLA	C4-C3-C5-C6
26	A	856	CLA	C4-C3-C5-C6
26	b	305	CLA	C4-C3-C5-C6
26	n	608	CLA	C4-C3-C5-C6
26	i	311	CLA	C2C-C3C-CAC-CBC
26	j	607	CLA	O1D-CGD-O2D-CED
26	A	836	CLA	C15-C16-C17-C18
26	b	307	CLA	C14-C13-C15-C16
26	l	311	CLA	C14-C13-C15-C16
26	h	306	CLA	O1A-CGA-O2A-C1
28	A	855	LHG	C9-C10-C11-C12
26	B	814	CLA	C16-C17-C18-C20
26	s	402	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	l	301	CLA	C16-C17-C18-C20
26	A	818	CLA	O1D-CGD-O2D-CED
26	B	820	CLA	CBA-CGA-O2A-C1
26	k	608	CLA	CBA-CGA-O2A-C1
26	B	839	CLA	CAA-CBA-CGA-O2A
26	m	606	CLA	CAA-CBA-CGA-O2A
26	A	810	CLA	C3A-C2A-CAA-CBA
26	F	202	CLA	C3A-C2A-CAA-CBA
26	m	610	CLA	C3A-C2A-CAA-CBA
26	i	305	CLA	C3A-C2A-CAA-CBA
26	d	304	CLA	C3A-C2A-CAA-CBA
26	Q	302	CLA	C3A-C2A-CAA-CBA
30	A	858	LMU	C4-C5-C6-C7
34	b	319	LMG	C34-C35-C36-C37
29	A	847	WVN	C32-C36-C39-C40
35	d	315	II0	C36-C40-C42-C41
26	F	201	CLA	O1D-CGD-O2D-CED
33	j	618	DGD	C8B-C9B-CAB-CBB
26	B	808	CLA	CBA-CGA-O2A-C1
26	L	202	CLA	CBA-CGA-O2A-C1
26	b	306	CLA	CBA-CGA-O2A-C1
26	B	810	CLA	C10-C11-C12-C13
28	m	618	LHG	C4-C5-C6-O8
32	A	854	SQD	C44-C45-C46-O48
33	B	844	DGD	O1G-C1G-C2G-C3G
26	j	609	CLA	C3-C5-C6-C7
34	n	620	LMG	C34-C35-C36-C37
26	B	819	CLA	C5-C6-C7-C8
26	A	822	CLA	C4-C3-C5-C6
26	A	833	CLA	C4-C3-C5-C6
26	A	841	CLA	C4-C3-C5-C6
26	b	312	CLA	C4-C3-C5-C6
25	A	801	CL0	C16-C17-C18-C20
26	B	818	CLA	C16-C17-C18-C20
26	i	311	CLA	C16-C17-C18-C19
26	A	820	CLA	C2-C3-C5-C6
26	B	806	CLA	C2-C3-C5-C6
26	b	305	CLA	C2-C3-C5-C6
26	n	608	CLA	C2-C3-C5-C6
34	b	319	LMG	C11-C12-C13-C14
28	n	619	LHG	C33-C34-C35-C36
26	A	802	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	d	308	CLA	CBA-CGA-O2A-C1
28	L	208	LHG	C3-O3-P-O6
28	c	320	LHG	C3-O3-P-O6
26	B	801	CLA	C2A-CAA-CBA-CGA
26	i	308	CLA	C2A-CAA-CBA-CGA
28	A	843	LHG	O1-C1-C2-O2
28	l	318	LHG	O1-C1-C2-O2
34	F	205	LMG	C37-C38-C39-C40
28	B	851	LHG	O6-C4-C5-O7
26	A	811	CLA	O1A-CGA-O2A-C1
26	B	819	CLA	O1A-CGA-O2A-C1
26	s	402	CLA	O1A-CGA-O2A-C1
26	l	304	CLA	O1A-CGA-O2A-C1
34	c	318	LMG	C15-C16-C17-C18
33	j	618	DGD	O2G-C2G-C3G-O3G
34	F	206	LMG	O7-C8-C9-O8
26	B	810	CLA	CBA-CGA-O2A-C1
26	B	834	CLA	CBA-CGA-O2A-C1
26	B	805	CLA	C15-C16-C17-C18
26	l	308	CLA	C5-C6-C7-C8
28	B	851	LHG	C1-C2-C3-O3
34	L	209	LMG	C11-C12-C13-C14
34	c	318	LMG	C16-C17-C18-C19
26	B	814	CLA	C4-C3-C5-C6
26	B	811	CLA	C2-C1-O2A-CGA
26	m	613	CLA	C2-C1-O2A-CGA
26	l	313	CLA	C2-C1-O2A-CGA
26	i	302	CLA	C2-C1-O2A-CGA
26	j	609	CLA	C2-C1-O2A-CGA
26	n	604	CLA	C2-C1-O2A-CGA
26	n	609	CLA	C2-C1-O2A-CGA
26	k	606	CLA	O1A-CGA-O2A-C1
26	A	816	CLA	C14-C13-C15-C16
26	A	829	CLA	C11-C10-C8-C9
26	A	841	CLA	C11-C10-C8-C9
26	B	813	CLA	C6-C7-C8-C9
26	B	818	CLA	C11-C10-C8-C9
26	B	831	CLA	C11-C12-C13-C14
26	B	837	CLA	C14-C13-C15-C16
26	c	304	CLA	C6-C7-C8-C9
26	a	306	CLA	C11-C12-C13-C14
26	b	306	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	h	306	CLA	C11-C12-C13-C14
26	i	304	CLA	C11-C12-C13-C14
26	j	601	CLA	C6-C7-C8-C9
28	A	843	LHG	C27-C28-C29-C30
28	A	849	LHG	C14-C15-C16-C17
34	c	318	LMG	C31-C32-C33-C34
25	A	801	CL0	C8-C10-C11-C12
28	c	320	LHG	C2-C3-O3-P
36	k	612	KC2	C1A-C2A-CAA-CBA
26	B	817	CLA	O1A-CGA-O2A-C1
26	m	604	CLA	C2A-CAA-CBA-CGA
26	j	604	CLA	C2A-CAA-CBA-CGA
26	B	814	CLA	C16-C17-C18-C19
26	s	402	CLA	C16-C17-C18-C20
26	m	606	CLA	C16-C17-C18-C19
26	l	305	CLA	C16-C17-C18-C19
26	b	307	CLA	C3-C5-C6-C7
30	A	850	LMU	C6-C7-C8-C9
30	i	300	LMU	C4-C5-C6-C7
35	c	316	II0	C32-C34-C36-C38
34	c	318	LMG	O10-C28-O8-C9
26	A	833	CLA	O1D-CGD-O2D-CED
26	J	103	CLA	C1A-C2A-CAA-CBA
26	K	101	CLA	C1A-C2A-CAA-CBA
26	m	601	CLA	C1A-C2A-CAA-CBA
29	B	849	WVN	C29-C31-C32-C36
29	M	101	WVN	C20-C23-C25-C28
29	l	316	WVN	C30-C33-C34-C37
35	h	311	II0	C31-C33-C35-C39
35	m	614	II0	C31-C33-C35-C39
35	m	615	II0	C32-C34-C36-C40
26	B	804	CLA	C5-C6-C7-C8
34	F	205	LMG	C42-C43-C44-C45
28	b	318	LHG	C11-C12-C13-C14
30	A	850	LMU	C11-C10-C9-C8
30	B	852	LMU	C11-C10-C9-C8
26	a	308	CLA	O2A-C1-C2-C3
26	a	311	CLA	O2A-C1-C2-C3
28	b	302	LHG	C35-C36-C37-C38
35	a	314	II0	C27-C25-C29-C31
35	h	312	II0	C27-C25-C29-C31
35	k	617	II0	C27-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
35	i	316	II0	C27-C25-C29-C31
28	A	855	LHG	O6-C4-C5-C6
34	F	205	LMG	C34-C35-C36-C37
26	A	816	CLA	C11-C10-C8-C7
26	A	816	CLA	C12-C13-C15-C16
26	A	817	CLA	C11-C12-C13-C15
26	A	818	CLA	C11-C12-C13-C15
26	A	831	CLA	C11-C10-C8-C7
26	A	833	CLA	C11-C12-C13-C15
26	A	837	CLA	C12-C13-C15-C16
26	B	803	CLA	C12-C13-C15-C16
26	B	804	CLA	C6-C7-C8-C10
26	B	812	CLA	C6-C7-C8-C10
26	B	813	CLA	C6-C7-C8-C10
26	B	814	CLA	C2-C3-C5-C6
26	B	818	CLA	C11-C12-C13-C15
26	B	819	CLA	C12-C13-C15-C16
26	B	823	CLA	C6-C7-C8-C10
26	B	825	CLA	C11-C10-C8-C7
26	B	831	CLA	C11-C12-C13-C15
26	B	837	CLA	C12-C13-C15-C16
26	c	304	CLA	C11-C10-C8-C7
26	c	308	CLA	C6-C7-C8-C10
26	c	312	CLA	C11-C10-C8-C7
26	a	304	CLA	C11-C10-C8-C7
26	a	306	CLA	C11-C12-C13-C15
26	a	306	CLA	C12-C13-C15-C16
26	a	310	CLA	C11-C12-C13-C15
26	b	306	CLA	C6-C7-C8-C10
26	b	311	CLA	C11-C12-C13-C15
26	b	312	CLA	C2-C3-C5-C6
26	m	606	CLA	C12-C13-C15-C16
26	m	613	CLA	C11-C10-C8-C7
26	k	602	CLA	C11-C10-C8-C7
26	k	609	CLA	C11-C10-C8-C7
26	i	302	CLA	C12-C13-C15-C16
26	i	304	CLA	C11-C10-C8-C7
26	i	304	CLA	C11-C12-C13-C15
26	i	311	CLA	C11-C10-C8-C7
26	i	311	CLA	C11-C12-C13-C15
26	j	604	CLA	C6-C7-C8-C10
26	j	609	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	j	609	CLA	C12-C13-C15-C16
26	j	613	CLA	C6-C7-C8-C10
26	d	302	CLA	C12-C13-C15-C16
36	n	612	KC2	O1D-CGD-O2D-CED
28	c	317	LHG	C11-C10-C9-C8
33	B	844	DGD	C6A-C7A-C8A-C9A
26	A	810	CLA	C15-C16-C17-C18
26	j	609	CLA	C15-C16-C17-C18
35	J	104	II0	C25-C29-C31-C33
35	h	311	II0	C36-C40-C42-C41
35	m	614	II0	C36-C40-C42-C41
35	d	317	II0	C25-C29-C31-C33
26	B	818	CLA	C16-C17-C18-C19
26	B	837	CLA	C16-C17-C18-C19
26	l	301	CLA	C16-C17-C18-C19
26	m	602	CLA	CBA-CGA-O2A-C1
28	s	409	LHG	C34-C35-C36-C37
26	j	609	CLA	C10-C11-C12-C13
26	A	802	CLA	CAA-CBA-CGA-O2A
28	m	618	LHG	C30-C31-C32-C33
30	i	300	LMU	C4'-C5'-C6'-O6'
26	B	829	CLA	C15-C16-C17-C18
28	i	317	LHG	C28-C29-C30-C31
29	F	203	WVN	C35-C32-C36-C39
33	B	844	DGD	CDB-CEB-CFB-CGB
34	c	318	LMG	C38-C39-C40-C41
33	j	618	DGD	C5A-C6A-C7A-C8A
34	L	209	LMG	C32-C33-C34-C35
28	L	208	LHG	C24-C25-C26-C27
26	a	309	CLA	O1D-CGD-O2D-CED
26	A	804	CLA	CAD-CBD-CGD-O2D
26	A	805	CLA	CAD-CBD-CGD-O2D
26	A	806	CLA	CAD-CBD-CGD-O2D
26	A	811	CLA	CAD-CBD-CGD-O2D
26	A	816	CLA	CAD-CBD-CGD-O2D
26	A	821	CLA	CAD-CBD-CGD-O2D
26	A	824	CLA	CAD-CBD-CGD-O2D
26	B	802	CLA	CAD-CBD-CGD-O2D
26	B	814	CLA	CAD-CBD-CGD-O2D
26	B	819	CLA	CAD-CBD-CGD-O2D
26	B	830	CLA	CAD-CBD-CGD-O2D
26	B	835	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	B	836	CLA	CAD-CBD-CGD-O2D
26	B	841	CLA	CAD-CBD-CGD-O2D
26	a	305	CLA	CAD-CBD-CGD-O2D
26	b	307	CLA	CAD-CBD-CGD-O2D
26	h	304	CLA	CAD-CBD-CGD-O2D
26	h	313	CLA	CAD-CBD-CGD-O2D
26	m	604	CLA	CAD-CBD-CGD-O2D
26	l	304	CLA	CAD-CBD-CGD-O2D
26	l	308	CLA	CAD-CBD-CGD-O2D
26	k	607	CLA	CAD-CBD-CGD-O2D
26	k	614	CLA	CAD-CBD-CGD-O2D
26	i	306	CLA	CAD-CBD-CGD-O2D
26	j	613	CLA	CAD-CBD-CGD-O2D
26	n	604	CLA	CAD-CBD-CGD-O2D
26	n	608	CLA	CAD-CBD-CGD-O2D
26	n	609	CLA	CAD-CBD-CGD-O2D
36	s	404	KC2	CAD-CBD-CGD-O2D
36	c	310	KC2	CAD-CBD-CGD-O2D
36	i	318	KC2	C2C-C3C-CAC-CBC
36	d	312	KC2	C2B-C3B-CAB-CBB
34	Q	301	LMG	O6-C5-C6-O5
34	n	620	LMG	C38-C39-C40-C41
26	A	807	CLA	C13-C15-C16-C17
26	B	803	CLA	C8-C10-C11-C12
26	A	816	CLA	CBA-CGA-O2A-C1
26	B	842	CLA	CBA-CGA-O2A-C1
26	j	602	CLA	CBA-CGA-O2A-C1
26	l	305	CLA	C16-C17-C18-C20
30	A	858	LMU	O5'-C1'-O1'-C1
34	c	319	LMG	O6-C1-O1-C7
26	B	834	CLA	C15-C16-C17-C18
26	B	812	CLA	C2-C3-C5-C6
28	b	318	LHG	C27-C28-C29-C30
28	A	855	LHG	C2-C3-O3-P
28	b	302	LHG	C4-C5-C6-O8
28	b	318	LHG	C4-C5-C6-O8
34	L	209	LMG	O1-C7-C8-C9
34	n	620	LMG	O1-C7-C8-C9
28	A	855	LHG	O6-C4-C5-O7
28	i	317	LHG	O6-C4-C5-O7
26	A	813	CLA	C3-C5-C6-C7
26	B	805	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	L	202	CLA	O2A-C1-C2-C3
34	c	318	LMG	C39-C40-C41-C42
36	m	611	KC2	C4B-C3B-CAB-CBB
36	n	612	KC2	C4B-C3B-CAB-CBB
26	A	828	CLA	CBA-CGA-O2A-C1
26	A	823	CLA	C2A-CAA-CBA-CGA
26	j	610	CLA	C2A-CAA-CBA-CGA
26	m	602	CLA	O1A-CGA-O2A-C1
34	F	206	LMG	C13-C14-C15-C16
26	B	820	CLA	O1D-CGD-O2D-CED
28	n	619	LHG	C1-C2-C3-O3
26	A	814	CLA	CHA-CBD-CGD-O1D
26	A	814	CLA	CHA-CBD-CGD-O2D
26	A	826	CLA	CHA-CBD-CGD-O1D
26	A	826	CLA	CHA-CBD-CGD-O2D
26	A	835	CLA	CHA-CBD-CGD-O1D
26	A	835	CLA	CHA-CBD-CGD-O2D
26	B	805	CLA	CHA-CBD-CGD-O1D
26	B	805	CLA	CHA-CBD-CGD-O2D
26	B	821	CLA	CHA-CBD-CGD-O1D
26	B	823	CLA	CHA-CBD-CGD-O1D
26	B	823	CLA	CHA-CBD-CGD-O2D
26	B	838	CLA	CHA-CBD-CGD-O1D
26	B	838	CLA	CHA-CBD-CGD-O2D
26	s	402	CLA	CHA-CBD-CGD-O1D
26	s	402	CLA	CHA-CBD-CGD-O2D
26	c	302	CLA	CHA-CBD-CGD-O1D
26	c	302	CLA	CHA-CBD-CGD-O2D
26	a	311	CLA	CHA-CBD-CGD-O1D
26	m	613	CLA	CHA-CBD-CGD-O1D
26	l	307	CLA	CHA-CBD-CGD-O1D
26	l	307	CLA	CHA-CBD-CGD-O2D
26	i	302	CLA	CHA-CBD-CGD-O1D
26	i	302	CLA	CHA-CBD-CGD-O2D
26	j	605	CLA	CHA-CBD-CGD-O1D
26	j	605	CLA	CHA-CBD-CGD-O2D
26	d	306	CLA	CHA-CBD-CGD-O1D
26	n	610	CLA	CHA-CBD-CGD-O1D
26	n	610	CLA	CHA-CBD-CGD-O2D
36	k	611	KC2	CHA-CBD-CGD-O1D
36	k	611	KC2	CHA-CBD-CGD-O2D
26	R	201	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	d	305	CLA	O1D-CGD-O2D-CED
26	A	812	CLA	C3-C5-C6-C7
26	B	818	CLA	O1A-CGA-O2A-C1
26	b	306	CLA	O1A-CGA-O2A-C1
26	k	608	CLA	O1A-CGA-O2A-C1
35	h	311	II0	C33-C35-C39-C41
35	m	614	II0	C33-C35-C39-C41
35	n	616	II0	C34-C36-C40-C42
26	l	311	CLA	C8-C10-C11-C12
28	B	851	LHG	O7-C5-C6-O8
28	j	617	LHG	O7-C5-C6-O8
32	A	854	SQD	O47-C45-C46-O48
34	F	205	LMG	O7-C8-C9-O8
34	L	209	LMG	O1-C7-C8-O7
26	i	311	CLA	C4C-C3C-CAC-CBC
26	A	829	CLA	C15-C16-C17-C18
26	m	606	CLA	C13-C15-C16-C17
28	n	619	LHG	O10-C23-O8-C6
26	h	307	CLA	CAA-CBA-CGA-O2A
32	A	854	SQD	C25-C26-C27-C28
26	m	606	CLA	C16-C17-C18-C20
28	L	208	LHG	O1-C1-C2-O2
28	A	843	LHG	C12-C13-C14-C15
28	J	105	LHG	C9-C10-C11-C12
34	L	209	LMG	C31-C32-C33-C34
26	A	826	CLA	C3-C5-C6-C7
34	F	206	LMG	C28-C29-C30-C31
26	B	812	CLA	C4-C3-C5-C6
26	B	825	CLA	C4-C3-C5-C6
26	Q	302	CLA	C4-C3-C5-C6
34	c	318	LMG	C21-C22-C23-C24
34	c	319	LMG	C11-C12-C13-C14
26	B	820	CLA	O1A-CGA-O2A-C1
26	L	202	CLA	O1A-CGA-O2A-C1
26	A	816	CLA	O1D-CGD-O2D-CED
35	l	317	II0	C10-C22-C24-C26
37	a	315	IHT	C11-C21-C24-C26
26	A	807	CLA	CBA-CGA-O2A-C1
26	A	818	CLA	C11-C10-C8-C9
26	A	837	CLA	C14-C13-C15-C16
26	B	823	CLA	C6-C7-C8-C9
26	a	307	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	l	305	CLA	C6-C7-C8-C9
26	k	609	CLA	C11-C10-C8-C9
26	i	304	CLA	C11-C10-C8-C9
26	i	307	CLA	C6-C7-C8-C9
26	B	810	CLA	O1A-CGA-O2A-C1
26	A	805	CLA	C15-C16-C17-C18
26	B	807	CLA	C2A-CAA-CBA-CGA
29	J	102	WVN	C11-C19-C22-C24
29	l	316	WVN	C20-C23-C25-C27
29	R	200	WVN	C30-C33-C34-C38
35	c	313	II0	C32-C34-C36-C38
29	A	847	WVN	C30-C33-C34-C37
29	A	848	WVN	C20-C23-C25-C28
29	J	101	WVN	C30-C33-C34-C37
29	s	407	WVN	C11-C19-C22-C26
29	l	316	WVN	C29-C31-C32-C36
26	A	824	CLA	C1A-C2A-CAA-CBA
26	A	836	CLA	C1A-C2A-CAA-CBA
26	A	851	CLA	C1A-C2A-CAA-CBA
26	B	810	CLA	C1A-C2A-CAA-CBA
26	B	812	CLA	C1A-C2A-CAA-CBA
26	B	831	CLA	C1A-C2A-CAA-CBA
26	F	202	CLA	C1A-C2A-CAA-CBA
26	L	206	CLA	C1A-C2A-CAA-CBA
26	b	308	CLA	C1A-C2A-CAA-CBA
26	i	302	CLA	C1A-C2A-CAA-CBA
26	j	602	CLA	C1A-C2A-CAA-CBA
26	d	313	CLA	C1A-C2A-CAA-CBA
32	A	854	SQD	C7-C8-C9-C10
26	b	313	CLA	C2-C1-O2A-CGA
26	A	824	CLA	CBA-CGA-O2A-C1
34	b	319	LMG	C30-C31-C32-C33
27	A	842	PQN	C15-C16-C17-C18
28	A	843	LHG	C3-O3-P-O6
28	B	851	LHG	C3-O3-P-O6
28	L	208	LHG	C4-O6-P-O3
26	B	836	CLA	C4-C3-C5-C6
26	A	816	CLA	O1A-CGA-O2A-C1
28	A	843	LHG	C4-O6-P-O5
28	A	855	LHG	C4-O6-P-O5
28	J	105	LHG	C4-O6-P-O5
28	L	208	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
28	c	317	LHG	C3-O3-P-O5
28	b	318	LHG	C4-O6-P-O5
28	m	618	LHG	C3-O3-P-O5
28	m	618	LHG	C4-O6-P-O4
28	l	318	LHG	C3-O3-P-O5
28	i	317	LHG	C3-O3-P-O5
28	j	617	LHG	C3-O3-P-O5
28	n	619	LHG	C3-O3-P-O5
26	B	841	CLA	C16-C17-C18-C19
28	b	318	LHG	C19-C20-C21-C22
28	L	208	LHG	O6-C4-C5-C6
26	j	602	CLA	O1A-CGA-O2A-C1
30	i	300	LMU	C5-C6-C7-C8
26	i	302	CLA	C13-C15-C16-C17
26	A	811	CLA	C3-C5-C6-C7
28	L	207	LHG	C24-C25-C26-C27
26	A	814	CLA	CAD-CBD-CGD-O1D
26	A	822	CLA	CAD-CBD-CGD-O1D
26	A	826	CLA	CAD-CBD-CGD-O1D
26	A	835	CLA	CAD-CBD-CGD-O1D
26	B	805	CLA	CAD-CBD-CGD-O1D
26	c	302	CLA	CAD-CBD-CGD-O1D
26	a	304	CLA	CAD-CBD-CGD-O1D
26	m	607	CLA	C2-C3-C5-C6
26	l	307	CLA	CAD-CBD-CGD-O1D
26	k	604	CLA	CAD-CBD-CGD-O1D
26	k	610	CLA	C2-C3-C5-C6
26	i	301	CLA	CAD-CBD-CGD-O1D
26	n	613	CLA	C2-C3-C5-C6
33	j	618	DGD	C1B-C2B-C3B-C4B
34	c	318	LMG	C33-C34-C35-C36
26	c	308	CLA	C13-C15-C16-C17
28	m	618	LHG	C7-C8-C9-C10
28	i	317	LHG	C29-C30-C31-C32
26	A	808	CLA	C16-C17-C18-C20
26	A	809	CLA	C6-C7-C8-C10
26	A	831	CLA	C12-C13-C15-C16
26	A	835	CLA	C6-C7-C8-C10
26	B	805	CLA	C11-C12-C13-C15
26	B	806	CLA	C6-C7-C8-C10
26	B	810	CLA	C11-C10-C8-C7
26	B	814	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	B	816	CLA	C11-C12-C13-C15
26	B	825	CLA	C6-C7-C8-C10
26	B	839	CLA	C11-C10-C8-C7
26	B	841	CLA	C12-C13-C15-C16
26	B	842	CLA	C11-C10-C8-C7
26	F	201	CLA	C11-C12-C13-C15
26	c	312	CLA	C6-C7-C8-C10
26	a	307	CLA	C12-C13-C15-C16
26	b	308	CLA	C11-C12-C13-C15
26	m	604	CLA	C6-C7-C8-C10
26	m	608	CLA	C11-C10-C8-C7
26	m	609	CLA	C11-C10-C8-C7
26	l	301	CLA	C11-C12-C13-C15
26	l	305	CLA	C6-C7-C8-C10
26	i	306	CLA	C11-C12-C13-C15
26	i	307	CLA	C6-C7-C8-C10
26	i	310	CLA	C6-C7-C8-C10
26	Q	302	CLA	C11-C10-C8-C7
27	B	843	PQN	C21-C22-C23-C25
28	A	844	LHG	O6-C4-C5-O7
28	c	317	LHG	O6-C4-C5-O7
28	c	320	LHG	C28-C29-C30-C31
26	B	842	CLA	O1A-CGA-O2A-C1
34	c	319	LMG	C33-C34-C35-C36
26	n	613	CLA	CAA-CBA-CGA-O2A
26	B	813	CLA	C5-C6-C7-C8
26	B	834	CLA	O1A-CGA-O2A-C1
33	j	618	DGD	C5B-C6B-C7B-C8B
26	s	408	CLA	CBD-CGD-O2D-CED
36	i	309	KC2	CBD-CGD-O2D-CED
26	b	308	CLA	C2A-CAA-CBA-CGA
26	L	204	CLA	C11-C12-C13-C14
28	B	851	LHG	C4-C5-C6-O8
28	J	105	LHG	C11-C10-C9-C8
28	c	317	LHG	C4-C5-C6-O8
33	B	844	DGD	C3B-C4B-C5B-C6B
34	F	205	LMG	C7-C8-C9-O8
26	A	824	CLA	O1A-CGA-O2A-C1
26	A	828	CLA	O1A-CGA-O2A-C1
28	c	317	LHG	O7-C5-C6-O8
28	b	318	LHG	O7-C5-C6-O8
33	j	618	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
34	b	319	LMG	O1-C7-C8-O7
34	Q	301	LMG	O7-C8-C9-O8
26	A	807	CLA	O1A-CGA-O2A-C1
34	F	205	LMG	C39-C40-C41-C42
26	s	406	CLA	O1D-CGD-O2D-CED
26	b	308	CLA	C16-C17-C18-C19
34	b	319	LMG	C35-C36-C37-C38
28	c	320	LHG	C29-C30-C31-C32
26	B	808	CLA	O1A-CGA-O2A-C1
26	B	837	CLA	C2C-C3C-CAC-CBC
26	Q	302	CLA	C2-C3-C5-C6
35	l	315	II0	C28-C26-C30-C32
26	s	406	CLA	C5-C6-C7-C8
26	Q	302	CLA	C15-C16-C17-C18
26	A	817	CLA	C11-C12-C13-C14
26	A	818	CLA	C11-C12-C13-C14
26	A	828	CLA	C6-C7-C8-C9
26	A	831	CLA	C11-C10-C8-C9
26	A	833	CLA	C11-C12-C13-C14
26	B	803	CLA	C14-C13-C15-C16
26	B	812	CLA	C6-C7-C8-C9
26	F	201	CLA	C6-C7-C8-C9
26	c	308	CLA	C6-C7-C8-C9
26	c	312	CLA	C11-C10-C8-C9
26	b	311	CLA	C11-C12-C13-C14
26	l	311	CLA	C11-C12-C13-C14
26	l	313	CLA	C6-C7-C8-C9
26	i	311	CLA	C11-C10-C8-C9
26	i	311	CLA	C11-C12-C13-C14
26	j	604	CLA	C6-C7-C8-C9
26	j	609	CLA	C11-C10-C8-C9
26	Q	302	CLA	C6-C7-C8-C9
27	B	843	PQN	C21-C22-C23-C24
26	A	808	CLA	C16-C17-C18-C19
26	B	812	CLA	C5-C6-C7-C8
28	i	317	LHG	C11-C10-C9-C8
30	a	317	LMU	C2-C3-C4-C5
35	d	319	II0	C30-C32-C34-C36
35	j	614	II0	C36-C40-C42-C41
34	F	205	LMG	C21-C22-C23-C24
33	B	844	DGD	C5B-C6B-C7B-C8B
29	B	847	WVN	C20-C23-C25-C28

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Mol	Chain	Res	Type	Atoms
32	A	854	SQD	C19-C20-C21-C22
26	c	302	CLA	C8-C10-C11-C12
28	c	320	LHG	C9-C10-C11-C12
28	b	318	LHG	C29-C30-C31-C32
26	B	836	CLA	C2-C3-C5-C6
26	i	311	CLA	C15-C16-C17-C18
26	A	821	CLA	C1-C2-C3-C4
26	k	607	CLA	CAA-CBA-CGA-O2A
26	A	822	CLA	C2A-CAA-CBA-CGA
26	A	835	CLA	C2A-CAA-CBA-CGA
26	B	828	CLA	C2A-CAA-CBA-CGA
26	c	304	CLA	C2A-CAA-CBA-CGA
26	l	310	CLA	C2A-CAA-CBA-CGA
26	k	604	CLA	C2A-CAA-CBA-CGA
26	k	607	CLA	C2A-CAA-CBA-CGA
26	j	602	CLA	C2A-CAA-CBA-CGA
25	A	801	CL0	C2-C1-O2A-CGA
26	A	820	CLA	C2-C1-O2A-CGA
26	A	822	CLA	C2-C1-O2A-CGA
26	F	201	CLA	C2-C1-O2A-CGA
26	k	608	CLA	C2-C1-O2A-CGA
28	b	302	LHG	C11-C10-C9-C8
33	B	844	DGD	C9A-CAA-CBA-CCA
26	k	606	CLA	CAA-CBA-CGA-O2A
26	k	608	CLA	C5-C6-C7-C8
26	s	408	CLA	O1D-CGD-O2D-CED
28	s	409	LHG	C4-O6-P-O5
29	B	848	WVN	C06-C13-C20-C23
29	J	102	WVN	C06-C13-C20-C23
37	b	301	IHT	C02-C07-C18-C22
26	B	825	CLA	C2-C3-C5-C6
26	i	304	CLA	C10-C11-C12-C13
26	l	301	CLA	C5-C6-C7-C8
26	A	809	CLA	C2A-CAA-CBA-CGA
29	A	847	WVN	C33-C34-C37-C40
29	A	857	WVN	C31-C32-C36-C39
34	n	620	LMG	O1-C7-C8-O7
26	a	301	CLA	C2C-C3C-CAC-CBC
28	A	844	LHG	C3-O3-P-O6
28	A	849	LHG	C3-O3-P-O6
28	A	849	LHG	C4-O6-P-O3
28	J	105	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	c	320	LHG	C4-O6-P-O3
28	c	317	LHG	C11-C12-C13-C14
28	A	843	LHG	C32-C33-C34-C35
26	d	310	CLA	O1D-CGD-O2D-CED
34	b	319	LMG	O1-C7-C8-C9
26	m	609	CLA	C4-C3-C5-C6
26	A	829	CLA	C11-C10-C8-C7
26	A	832	CLA	C11-C12-C13-C15
26	A	841	CLA	C2-C3-C5-C6
26	b	306	CLA	C11-C10-C8-C7
26	i	302	CLA	C6-C7-C8-C10
26	j	601	CLA	C6-C7-C8-C10
34	n	620	LMG	C23-C24-C25-C26
26	A	809	CLA	C6-C7-C8-C9
26	A	831	CLA	C14-C13-C15-C16
26	A	833	CLA	C11-C10-C8-C9
26	A	840	CLA	C11-C10-C8-C9
26	B	810	CLA	C11-C10-C8-C9
26	B	814	CLA	C11-C12-C13-C14
26	B	825	CLA	C6-C7-C8-C9
26	B	842	CLA	C11-C10-C8-C9
26	c	312	CLA	C6-C7-C8-C9
26	m	604	CLA	C6-C7-C8-C9
26	m	606	CLA	C6-C7-C8-C9
26	m	608	CLA	C11-C10-C8-C9
26	i	302	CLA	C14-C13-C15-C16
26	B	810	CLA	C8-C10-C11-C12
29	B	847	WVN	C32-C36-C39-C40
29	s	407	WVN	C34-C37-C40-C39
35	l	315	II0	C25-C29-C31-C33
35	k	620	II0	C36-C40-C42-C41
26	A	803	CLA	C6-C7-C8-C10
26	k	602	CLA	C15-C16-C17-C18
36	i	309	KC2	O1D-CGD-O2D-CED
26	A	830	CLA	CBD-CGD-O2D-CED
26	B	825	CLA	C2A-CAA-CBA-CGA
28	A	849	LHG	C13-C14-C15-C16
26	j	606	CLA	CAA-CBA-CGA-O2A
26	j	607	CLA	CAA-CBA-CGA-O2A
26	B	802	CLA	C5-C6-C7-C8
26	B	819	CLA	C8-C10-C11-C12
26	b	307	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	L	208	LHG	C1-C2-C3-O3
26	B	829	CLA	C4-C3-C5-C6
26	A	856	CLA	C2-C3-C5-C6
33	j	618	DGD	C2B-C3B-C4B-C5B
26	B	841	CLA	C16-C17-C18-C20
26	A	856	CLA	CAA-CBA-CGA-O1A
36	k	612	KC2	C2C-C3C-CAC-CBC
26	s	406	CLA	CBD-CGD-O2D-CED
26	d	304	CLA	CAA-CBA-CGA-O2A
28	A	849	LHG	C12-C13-C14-C15
26	k	608	CLA	CAA-CBA-CGA-O2A
26	B	803	CLA	C5-C6-C7-C8
26	B	817	CLA	C5-C6-C7-C8
26	a	307	CLA	C8-C10-C11-C12
26	i	301	CLA	C13-C15-C16-C17
34	F	205	LMG	C10-C11-C12-C13
26	A	811	CLA	C2A-CAA-CBA-CGA
26	b	308	CLA	C16-C17-C18-C20
30	a	317	LMU	O5'-C1'-O1'-C1
29	L	201	WVN	C34-C37-C40-C39
29	h	309	WVN	C34-C37-C40-C39
35	c	316	II0	C35-C39-C41-C42
35	a	312	II0	C36-C40-C42-C41
35	h	311	II0	C35-C39-C41-C42
26	A	833	CLA	C3-C5-C6-C7
26	j	605	CLA	CAA-CBA-CGA-O2A
26	A	841	CLA	CAA-CBA-CGA-O2A
36	i	318	KC2	C4C-C3C-CAC-CBC
36	d	312	KC2	C4B-C3B-CAB-CBB
26	A	818	CLA	C2-C3-C5-C6
26	A	830	CLA	O1D-CGD-O2D-CED
26	A	824	CLA	C13-C15-C16-C17
26	a	309	CLA	C15-C16-C17-C18
34	L	209	LMG	C20-C21-C22-C23
26	A	817	CLA	CAA-CBA-CGA-O2A
26	A	833	CLA	C2-C1-O2A-CGA
26	A	852	CLA	C2-C1-O2A-CGA
26	B	830	CLA	C2-C1-O2A-CGA
26	c	308	CLA	C2-C1-O2A-CGA
26	i	301	CLA	C2-C1-O2A-CGA
26	i	303	CLA	O1D-CGD-O2D-CED
30	a	317	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
28	B	851	LHG	C30-C31-C32-C33
26	A	812	CLA	C2A-CAA-CBA-CGA
26	B	826	CLA	C2A-CAA-CBA-CGA
26	a	307	CLA	C2A-CAA-CBA-CGA
26	h	306	CLA	C2A-CAA-CBA-CGA
28	c	317	LHG	C9-C10-C11-C12
28	A	855	LHG	C5-C4-O6-P
26	B	812	CLA	C3A-C2A-CAA-CBA
26	s	402	CLA	C3A-C2A-CAA-CBA
26	s	406	CLA	C3A-C2A-CAA-CBA
26	d	313	CLA	C3A-C2A-CAA-CBA
26	n	613	CLA	C3A-C2A-CAA-CBA
26	B	819	CLA	C16-C17-C18-C20
28	A	843	LHG	C15-C16-C17-C18
26	c	311	CLA	CBD-CGD-O2D-CED
26	i	303	CLA	CBD-CGD-O2D-CED
29	i	315	WVN	C25-C28-C30-C33
28	b	318	LHG	C24-C23-O8-C6
26	a	310	CLA	C10-C11-C12-C13
26	c	309	CLA	CAA-CBA-CGA-O2A
26	A	818	CLA	C4-C3-C5-C6
26	c	312	CLA	C2-C3-C5-C6
35	n	614	II0	C09-C21-C23-C25
26	A	810	CLA	C11-C10-C8-C9
26	A	835	CLA	C6-C7-C8-C9
26	B	807	CLA	C14-C13-C15-C16
26	B	819	CLA	C11-C10-C8-C9
26	B	836	CLA	C11-C10-C8-C9
26	B	841	CLA	C14-C13-C15-C16
26	k	608	CLA	C11-C10-C8-C9
26	i	306	CLA	C6-C7-C8-C9
26	n	609	CLA	C14-C13-C15-C16
28	b	318	LHG	C28-C29-C30-C31
29	B	850	WVN	C27-C25-C28-C30
29	F	204	WVN	C35-C32-C36-C39
35	l	315	II0	C38-C36-C40-C42
26	d	308	CLA	O1A-CGA-O2A-C1
26	k	607	CLA	C2C-C3C-CAC-CBC
26	c	312	CLA	C2A-CAA-CBA-CGA
26	L	204	CLA	C11-C12-C13-C15
26	A	802	CLA	CBA-CGA-O2A-C1
26	c	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	b	302	LHG	C17-C18-C19-C20
28	b	318	LHG	C13-C14-C15-C16
26	B	801	CLA	C10-C11-C12-C13
28	B	851	LHG	C17-C18-C19-C20
26	c	312	CLA	C4-C3-C5-C6
26	A	807	CLA	C1A-C2A-CAA-CBA
26	A	812	CLA	C1A-C2A-CAA-CBA
26	A	829	CLA	C1A-C2A-CAA-CBA
26	B	814	CLA	C1A-C2A-CAA-CBA
26	B	825	CLA	C1A-C2A-CAA-CBA
26	B	826	CLA	C1A-C2A-CAA-CBA
26	a	307	CLA	C1A-C2A-CAA-CBA
26	m	612	CLA	C1A-C2A-CAA-CBA
26	l	310	CLA	C1A-C2A-CAA-CBA
26	k	607	CLA	C1A-C2A-CAA-CBA
26	j	607	CLA	C1A-C2A-CAA-CBA
26	A	818	CLA	C11-C10-C8-C7
26	A	822	CLA	C2-C3-C5-C6
26	A	825	CLA	C11-C12-C13-C15
26	A	828	CLA	C6-C7-C8-C10
26	A	833	CLA	C2-C3-C5-C6
26	A	836	CLA	C11-C10-C8-C7
26	B	810	CLA	C11-C12-C13-C15
26	B	837	CLA	C11-C10-C8-C7
26	c	304	CLA	C6-C7-C8-C10
26	h	306	CLA	C11-C12-C13-C15
26	m	606	CLA	C11-C10-C8-C7
26	l	307	CLA	C12-C13-C15-C16
26	k	602	CLA	C6-C7-C8-C10
28	A	855	LHG	C13-C14-C15-C16
29	R	200	WVN	C32-C36-C39-C40
35	l	314	II0	C35-C39-C41-C42
28	b	318	LHG	C34-C35-C36-C37
26	c	305	CLA	CAA-CBA-CGA-O2A
26	d	318	CLA	CAA-CBA-CGA-O2A
26	b	309	CLA	C10-C11-C12-C13
26	B	823	CLA	C16-C17-C18-C19
26	B	837	CLA	C4C-C3C-CAC-CBC
26	b	304	CLA	C3-C5-C6-C7
26	i	302	CLA	C3-C5-C6-C7
28	b	318	LHG	O1-C1-C2-O2
26	A	825	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	B	826	CLA	C8-C10-C11-C12
26	s	406	CLA	C13-C15-C16-C17
26	n	609	CLA	C13-C15-C16-C17
26	i	301	CLA	CAA-CBA-CGA-O2A
27	B	843	PQN	C20-C21-C22-C23
26	d	318	CLA	CAA-CBA-CGA-O1A
34	F	206	LMG	C19-C20-C21-C22
26	j	605	CLA	CBD-CGD-O2D-CED
28	m	618	LHG	C24-C23-O8-C6
29	F	204	WVN	C31-C32-C36-C39
29	L	205	WVN	C23-C25-C28-C30
29	s	405	WVN	C19-C22-C26-C29
29	s	407	WVN	C23-C25-C28-C30
28	c	320	LHG	C10-C11-C12-C13
28	m	618	LHG	C28-C29-C30-C31
34	F	206	LMG	O1-C7-C8-O7
26	A	832	CLA	C5-C6-C7-C8
26	A	819	CLA	C2A-CAA-CBA-CGA
29	A	857	WVN	C32-C36-C39-C40
26	c	309	CLA	CAA-CBA-CGA-O1A
26	c	305	CLA	C10-C11-C12-C13
26	B	822	CLA	C8-C10-C11-C12
28	J	105	LHG	C1-C2-C3-O3
34	F	205	LMG	C19-C20-C21-C22
26	A	817	CLA	O1D-CGD-O2D-CED
26	A	838	CLA	O1D-CGD-O2D-CED
26	A	830	CLA	C2-C1-O2A-CGA
26	B	825	CLA	C2-C1-O2A-CGA
26	B	837	CLA	C2-C1-O2A-CGA
26	b	303	CLA	C2-C1-O2A-CGA
26	A	802	CLA	O1A-CGA-O2A-C1
26	i	306	CLA	CAA-CBA-CGA-O2A
26	s	402	CLA	C6-C7-C8-C9
26	c	302	CLA	C11-C10-C8-C9
26	j	602	CLA	C6-C7-C8-C9
26	j	605	CLA	CAA-CBA-CGA-O1A
26	d	304	CLA	CAA-CBA-CGA-O1A
28	s	409	LHG	C25-C26-C27-C28
28	c	320	LHG	C31-C32-C33-C34
26	n	613	CLA	C4-C3-C5-C6
28	n	619	LHG	C34-C35-C36-C37
26	A	852	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	a	304	CLA	C2A-CAA-CBA-CGA
26	a	306	CLA	C2A-CAA-CBA-CGA
26	n	610	CLA	C2A-CAA-CBA-CGA
26	a	301	CLA	C4C-C3C-CAC-CBC
26	k	607	CLA	C4C-C3C-CAC-CBC
26	c	312	CLA	O1A-CGA-O2A-C1
37	b	301	IHT	C10-C07-C18-C22
37	j	616	IHT	C02-C07-C18-C22
26	j	605	CLA	O1D-CGD-O2D-CED
26	B	803	CLA	CAA-CBA-CGA-O2A
26	b	311	CLA	C15-C16-C17-C18
26	d	307	CLA	CAA-CBA-CGA-O2A
26	A	817	CLA	CBD-CGD-O2D-CED
26	A	804	CLA	O1A-CGA-O2A-C1
29	B	849	WVN	C32-C36-C39-C40
29	s	407	WVN	C22-C26-C29-C31
29	A	847	WVN	C11-C19-C22-C26
26	B	826	CLA	C2-C3-C5-C6
26	A	811	CLA	C6-C7-C8-C9
26	A	819	CLA	C16-C17-C18-C19
26	A	828	CLA	C3-C5-C6-C7
30	i	300	LMU	C9-C10-C11-C12
26	B	806	CLA	CBD-CGD-O2D-CED
28	b	318	LHG	O6-C4-C5-O7
35	k	619	II0	C28-C26-C30-C32
35	j	615	II0	C27-C25-C29-C31
35	n	616	II0	C28-C26-C30-C32
26	j	613	CLA	C5-C6-C7-C8
26	a	302	CLA	CBA-CGA-O2A-C1
26	B	830	CLA	O1A-CGA-O2A-C1
26	B	806	CLA	O1D-CGD-O2D-CED
26	B	817	CLA	C16-C17-C18-C20
34	F	205	LMG	C11-C12-C13-C14
25	A	801	CL0	CAA-CBA-CGA-O2A
26	A	826	CLA	C6-C7-C8-C10
26	B	836	CLA	C11-C10-C8-C7
26	c	302	CLA	C11-C10-C8-C7
26	B	830	CLA	CBA-CGA-O2A-C1
26	A	825	CLA	C8-C10-C11-C12
28	c	317	LHG	C23-C24-C25-C26
28	c	320	LHG	C27-C28-C29-C30
34	L	209	LMG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	B	839	CLA	CAA-CBA-CGA-O1A
29	A	857	WVN	C34-C37-C40-C39
35	a	313	II0	C25-C29-C31-C33
26	s	402	CLA	CAA-CBA-CGA-O2A
26	c	312	CLA	CBA-CGA-O2A-C1
28	b	318	LHG	C17-C18-C19-C20
30	a	317	LMU	C2B-C1B-O1B-C4'
26	A	819	CLA	C5-C6-C7-C8
26	F	202	CLA	CAA-CBA-CGA-O2A
29	B	847	WVN	C24-C22-C26-C29
26	A	819	CLA	CAA-CBA-CGA-O2A
26	d	308	CLA	CAA-CBA-CGA-O2A
34	n	620	LMG	O8-C28-C29-C30
26	B	807	CLA	C4-C3-C5-C6
26	B	822	CLA	C4-C3-C5-C6
26	s	406	CLA	C4-C3-C5-C6
26	j	601	CLA	C4-C3-C5-C6
26	A	803	CLA	C5-C6-C7-C8
26	m	604	CLA	C10-C11-C12-C13
26	m	604	CLA	C4C-C3C-CAC-CBC
26	h	306	CLA	C2-C3-C5-C6
26	j	613	CLA	C2-C3-C5-C6
28	b	302	LHG	C14-C15-C16-C17
26	B	819	CLA	C16-C17-C18-C19
30	B	852	LMU	C6-C7-C8-C9
26	l	311	CLA	C12-C13-C15-C16
26	A	805	CLA	C11-C10-C8-C9
26	B	801	CLA	C11-C12-C13-C14
26	B	805	CLA	C11-C12-C13-C14
26	B	807	CLA	C11-C12-C13-C14
26	B	810	CLA	C11-C12-C13-C14
26	B	816	CLA	C11-C12-C13-C14
26	B	839	CLA	C11-C10-C8-C9
26	s	402	CLA	C11-C10-C8-C9
26	b	308	CLA	C11-C12-C13-C14
26	m	609	CLA	C11-C10-C8-C9
26	l	301	CLA	C11-C12-C13-C14
26	l	307	CLA	C14-C13-C15-C16
26	i	310	CLA	C6-C7-C8-C9
26	j	609	CLA	C11-C12-C13-C14
26	n	607	CLA	C8-C10-C11-C12
26	A	812	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	A	824	CLA	C3A-C2A-CAA-CBA
26	B	826	CLA	C3A-C2A-CAA-CBA
26	c	301	CLA	C3A-C2A-CAA-CBA
26	k	603	CLA	C3A-C2A-CAA-CBA
26	j	607	CLA	C3A-C2A-CAA-CBA
26	j	608	CLA	C3A-C2A-CAA-CBA
26	A	822	CLA	CAA-CBA-CGA-O2A
26	h	304	CLA	CAA-CBA-CGA-O2A
26	n	604	CLA	CAA-CBA-CGA-O2A
34	F	205	LMG	C35-C36-C37-C38
26	A	812	CLA	CAD-CBD-CGD-O2D
26	A	834	CLA	CAD-CBD-CGD-O2D
26	A	840	CLA	CAD-CBD-CGD-O2D
26	B	815	CLA	CAD-CBD-CGD-O2D
26	B	824	CLA	CAD-CBD-CGD-O2D
26	F	202	CLA	CAD-CBD-CGD-O2D
26	L	206	CLA	CAD-CBD-CGD-O2D
26	s	403	CLA	CAD-CBD-CGD-O2D
26	c	312	CLA	CAD-CBD-CGD-O2D
26	a	311	CLA	CAD-CBD-CGD-O2D
26	b	310	CLA	CAD-CBD-CGD-O2D
26	b	312	CLA	CAD-CBD-CGD-O2D
26	h	303	CLA	CAD-CBD-CGD-O2D
26	h	307	CLA	CAD-CBD-CGD-O2D
26	m	612	CLA	CAD-CBD-CGD-O2D
26	m	613	CLA	CAD-CBD-CGD-O2D
26	k	603	CLA	CAD-CBD-CGD-O2D
26	j	603	CLA	CAD-CBD-CGD-O2D
26	j	604	CLA	CAD-CBD-CGD-O2D
26	d	302	CLA	CAD-CBD-CGD-O2D
26	d	305	CLA	CAD-CBD-CGD-O2D
26	n	601	CLA	CAD-CBD-CGD-O2D
36	s	401	KC2	CAD-CBD-CGD-O2D
36	m	611	KC2	CAD-CBD-CGD-O2D
30	A	850	LMU	C9-C10-C11-C12
32	A	854	SQD	O49-C7-O47-C45
28	c	320	LHG	C13-C14-C15-C16
26	c	301	CLA	C2-C1-O2A-CGA
26	j	606	CLA	C2-C1-O2A-CGA
26	m	606	CLA	CAA-CBA-CGA-O1A
26	A	827	CLA	C4-C3-C5-C6
26	B	826	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	d	307	CLA	CAA-CBA-CGA-O1A
34	n	620	LMG	O6-C1-O1-C7
26	m	608	CLA	C5-C6-C7-C8
26	B	806	CLA	CAA-CBA-CGA-O2A
26	B	842	CLA	CAA-CBA-CGA-O2A
26	h	303	CLA	CAA-CBA-CGA-O2A
26	n	605	CLA	CAA-CBA-CGA-O2A
30	i	300	LMU	C3-C4-C5-C6
26	A	838	CLA	CBD-CGD-O2D-CED
26	d	303	CLA	O1A-CGA-O2A-C1
35	b	314	II0	C31-C33-C35-C39
35	l	314	II0	C31-C33-C35-C39
35	l	317	II0	C32-C34-C36-C40
30	a	317	LMU	C7-C8-C9-C10
26	B	820	CLA	CAA-CBA-CGA-O2A
26	a	309	CLA	CAA-CBA-CGA-O2A
26	b	312	CLA	CAA-CBA-CGA-O2A
26	m	610	CLA	CAA-CBA-CGA-O2A
26	B	831	CLA	O2A-C1-C2-C3
26	h	301	CLA	O2A-C1-C2-C3
36	k	612	KC2	C4C-C3C-CAC-CBC
26	A	804	CLA	CBA-CGA-O2A-C1
34	c	318	LMG	O7-C10-C11-C12
34	c	318	LMG	C40-C41-C42-C43
26	B	824	CLA	CBD-CGD-O2D-CED
26	n	609	CLA	O1D-CGD-O2D-CED
25	A	801	CL0	CHA-CBD-CGD-O1D
25	A	801	CL0	CHA-CBD-CGD-O2D
26	A	807	CLA	CHA-CBD-CGD-O1D
26	A	807	CLA	CHA-CBD-CGD-O2D
26	A	810	CLA	CHA-CBD-CGD-O1D
26	A	810	CLA	CHA-CBD-CGD-O2D
26	A	813	CLA	CHA-CBD-CGD-O1D
26	A	827	CLA	CHA-CBD-CGD-O1D
26	A	827	CLA	CHA-CBD-CGD-O2D
26	A	829	CLA	CHA-CBD-CGD-O2D
26	B	801	CLA	CHA-CBD-CGD-O2D
26	B	812	CLA	CHA-CBD-CGD-O1D
26	B	814	CLA	CHA-CBD-CGD-O2D
26	B	821	CLA	CHA-CBD-CGD-O2D
26	B	822	CLA	CHA-CBD-CGD-O1D
26	B	822	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	B	825	CLA	CHA-CBD-CGD-O1D
26	B	825	CLA	CHA-CBD-CGD-O2D
26	B	830	CLA	CHA-CBD-CGD-O2D
26	B	842	CLA	CHA-CBD-CGD-O1D
26	c	301	CLA	CHA-CBD-CGD-O1D
26	c	301	CLA	CHA-CBD-CGD-O2D
26	a	301	CLA	CHA-CBD-CGD-O1D
26	a	309	CLA	CHA-CBD-CGD-O1D
26	a	309	CLA	CHA-CBD-CGD-O2D
26	b	303	CLA	CHA-CBD-CGD-O1D
26	b	303	CLA	CHA-CBD-CGD-O2D
26	b	304	CLA	CHA-CBD-CGD-O1D
26	b	308	CLA	CHA-CBD-CGD-O2D
26	b	312	CLA	CHA-CBD-CGD-O1D
26	h	304	CLA	CHA-CBD-CGD-O2D
26	m	601	CLA	CHA-CBD-CGD-O1D
26	m	605	CLA	CHA-CBD-CGD-O2D
26	l	305	CLA	CHA-CBD-CGD-O2D
26	l	306	CLA	CHA-CBD-CGD-O2D
26	l	310	CLA	CHA-CBD-CGD-O2D
26	k	608	CLA	CHA-CBD-CGD-O1D
26	k	608	CLA	CHA-CBD-CGD-O2D
26	i	304	CLA	CHA-CBD-CGD-O2D
26	j	602	CLA	CHA-CBD-CGD-O1D
26	j	602	CLA	CHA-CBD-CGD-O2D
26	j	607	CLA	CHA-CBD-CGD-O1D
26	j	607	CLA	CHA-CBD-CGD-O2D
26	j	612	CLA	CHA-CBD-CGD-O2D
26	d	303	CLA	CHA-CBD-CGD-O1D
26	d	307	CLA	CHA-CBD-CGD-O2D
26	n	605	CLA	CHA-CBD-CGD-O2D
26	n	607	CLA	CHA-CBD-CGD-O1D
26	n	607	CLA	CHA-CBD-CGD-O2D
36	k	613	KC2	CHA-CBD-CGD-O2D
36	d	311	KC2	CHA-CBD-CGD-O1D
36	d	311	KC2	CHA-CBD-CGD-O2D
36	d	312	KC2	CHA-CBD-CGD-O1D
36	d	312	KC2	CHA-CBD-CGD-O2D
36	n	611	KC2	CHA-CBD-CGD-O2D
26	A	840	CLA	C4-C3-C5-C6
32	A	854	SQD	O47-C7-C8-C9
26	A	827	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	j	601	CLA	C2-C3-C5-C6
26	A	837	CLA	CAA-CBA-CGA-O2A
28	A	849	LHG	O7-C7-C8-C9
26	j	604	CLA	C5-C6-C7-C8
26	h	306	CLA	C10-C11-C12-C13
26	B	801	CLA	CAA-CBA-CGA-O2A
26	B	816	CLA	CAA-CBA-CGA-O2A
26	c	307	CLA	CAA-CBA-CGA-O2A
26	h	301	CLA	CAA-CBA-CGA-O2A
26	m	608	CLA	CAA-CBA-CGA-O2A
26	i	305	CLA	CAA-CBA-CGA-O2A
28	c	320	LHG	O8-C23-C24-C25
28	b	302	LHG	O8-C23-C24-C25
28	L	207	LHG	C28-C29-C30-C31
26	B	817	CLA	C2A-CAA-CBA-CGA
28	J	105	LHG	O1-C1-C2-O2
26	d	303	CLA	CBA-CGA-O2A-C1
34	b	319	LMG	C29-C28-O8-C9
26	c	308	CLA	CAA-CBA-CGA-O2A
26	k	610	CLA	CAA-CBA-CGA-O2A
32	A	854	SQD	C17-C18-C19-C20
28	A	843	LHG	C29-C30-C31-C32
28	L	207	LHG	O10-C23-O8-C6
26	A	824	CLA	C11-C12-C13-C15
26	B	822	CLA	C11-C10-C8-C7
26	B	831	CLA	C2-C3-C5-C6
26	B	842	CLA	C11-C12-C13-C15
26	m	609	CLA	C2-C3-C5-C6
26	k	604	CLA	C6-C7-C8-C10
26	n	608	CLA	C11-C12-C13-C15
26	B	824	CLA	O1D-CGD-O2D-CED
34	b	319	LMG	O8-C28-C29-C30
26	A	831	CLA	C6-C7-C8-C9
26	A	832	CLA	C11-C12-C13-C14
26	A	833	CLA	C6-C7-C8-C9
26	A	836	CLA	C11-C10-C8-C9
26	B	822	CLA	C11-C10-C8-C9
26	B	825	CLA	C14-C13-C15-C16
26	B	837	CLA	C11-C10-C8-C9
26	B	840	CLA	C11-C12-C13-C14
26	B	842	CLA	C11-C12-C13-C14
26	F	201	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	m	606	CLA	C11-C10-C8-C9
26	k	602	CLA	C6-C7-C8-C9
26	k	604	CLA	C6-C7-C8-C9
26	i	306	CLA	C11-C12-C13-C14
26	n	608	CLA	C6-C7-C8-C9
26	n	608	CLA	C11-C12-C13-C14
29	B	847	WVN	C22-C26-C29-C31
29	F	203	WVN	C34-C37-C40-C39
35	i	319	II0	C35-C39-C41-C42
33	j	618	DGD	CCB-CDB-CEB-CFB
33	B	844	DGD	C8B-C9B-CAB-CBB
32	A	854	SQD	C4-C5-C6-S
26	A	819	CLA	C16-C17-C18-C20
34	F	206	LMG	O10-C28-O8-C9
26	L	202	CLA	C2A-CAA-CBA-CGA
28	s	409	LHG	O7-C7-C8-C9
26	B	823	CLA	C13-C15-C16-C17
26	l	305	CLA	C8-C10-C11-C12
35	b	314	II0	C28-C26-C30-C32
28	b	318	LHG	C10-C11-C12-C13
26	A	822	CLA	CAA-CBA-CGA-O1A
26	b	312	CLA	CAA-CBA-CGA-O1A
28	s	409	LHG	O10-C23-C24-C25
28	b	318	LHG	O9-C7-C8-C9
34	b	319	LMG	O10-C28-C29-C30
26	A	830	CLA	C8-C10-C11-C12
26	B	817	CLA	C16-C17-C18-C19
26	B	822	CLA	C16-C17-C18-C19
26	b	308	CLA	C4-C3-C5-C6
28	b	318	LHG	O1-C1-C2-C3
26	B	829	CLA	C2-C3-C5-C6
26	B	806	CLA	C5-C6-C7-C8
28	b	302	LHG	C19-C20-C21-C22
26	B	820	CLA	CAA-CBA-CGA-O1A
26	n	605	CLA	CAA-CBA-CGA-O1A
28	A	855	LHG	O10-C23-C24-C25
26	A	811	CLA	C1A-C2A-CAA-CBA
26	A	819	CLA	C1A-C2A-CAA-CBA
26	B	822	CLA	C1A-C2A-CAA-CBA
26	a	309	CLA	C1A-C2A-CAA-CBA
26	b	313	CLA	C1A-C2A-CAA-CBA
26	m	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	k	601	CLA	C1A-C2A-CAA-CBA
26	k	603	CLA	C1A-C2A-CAA-CBA
26	i	308	CLA	C1A-C2A-CAA-CBA
26	j	608	CLA	C1A-C2A-CAA-CBA
26	j	612	CLA	C1A-C2A-CAA-CBA
26	s	402	CLA	CAA-CBA-CGA-O1A
26	m	610	CLA	CAA-CBA-CGA-O1A
26	d	308	CLA	CAA-CBA-CGA-O1A
26	A	818	CLA	C8-C10-C11-C12
26	s	408	CLA	C5-C6-C7-C8
26	a	302	CLA	O1A-CGA-O2A-C1
26	B	805	CLA	C2-C1-O2A-CGA
26	m	602	CLA	C2-C1-O2A-CGA
26	B	806	CLA	CAA-CBA-CGA-O1A
26	h	303	CLA	CAA-CBA-CGA-O1A
28	s	409	LHG	O9-C7-C8-C9
28	b	302	LHG	O10-C23-C24-C25
26	A	812	CLA	CAA-CBA-CGA-O2A
26	j	604	CLA	CAA-CBA-CGA-O2A
26	i	305	CLA	C2A-CAA-CBA-CGA
26	n	609	CLA	C2A-CAA-CBA-CGA
26	j	604	CLA	C4C-C3C-CAC-CBC
26	F	202	CLA	CAA-CBA-CGA-O1A
26	B	806	CLA	C15-C16-C17-C18
26	a	306	CLA	C8-C10-C11-C12
26	l	305	CLA	C13-C15-C16-C17
26	A	811	CLA	C5-C6-C7-C8
26	B	826	CLA	CAA-CBA-CGA-O2A
28	b	318	LHG	O7-C7-C8-C9
26	A	837	CLA	CAA-CBA-CGA-O1A
26	h	301	CLA	CAA-CBA-CGA-O1A
26	i	305	CLA	CAA-CBA-CGA-O1A
28	A	849	LHG	O9-C7-C8-C9
34	L	209	LMG	C13-C14-C15-C16
28	B	851	LHG	C18-C19-C20-C21
28	A	844	LHG	C3-O3-P-O5
28	B	851	LHG	C3-O3-P-O5
28	B	851	LHG	C4-O6-P-O5
28	J	105	LHG	C3-O3-P-O5
26	A	805	CLA	C16-C17-C18-C19
26	A	819	CLA	CAA-CBA-CGA-O1A
26	A	833	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	J	105	LHG	O10-C23-O8-C6
34	c	318	LMG	C32-C33-C34-C35
26	h	304	CLA	CAA-CBA-CGA-O1A
32	A	854	SQD	O49-C7-C8-C9
33	B	844	DGD	O2G-C1B-C2B-C3B
34	c	318	LMG	C29-C30-C31-C32
26	c	307	CLA	CAA-CBA-CGA-O1A
26	a	309	CLA	CAA-CBA-CGA-O1A
26	n	604	CLA	CAA-CBA-CGA-O1A
26	l	301	CLA	CAA-CBA-CGA-O2A
26	h	306	CLA	C4-C3-C5-C6
26	j	613	CLA	C4-C3-C5-C6
26	A	813	CLA	CAD-CBD-CGD-O1D
26	B	812	CLA	CAD-CBD-CGD-O1D
26	B	821	CLA	CAD-CBD-CGD-O1D
26	B	825	CLA	CAD-CBD-CGD-O1D
26	B	828	CLA	CAD-CBD-CGD-O1D
26	B	833	CLA	CAD-CBD-CGD-O1D
26	B	842	CLA	CAD-CBD-CGD-O1D
26	L	203	CLA	CAD-CBD-CGD-O1D
26	i	310	CLA	CAD-CBD-CGD-O1D
28	B	851	LHG	C6-C5-O7-C7
35	b	314	II0	C23-C25-C29-C31
26	A	802	CLA	CAA-CBA-CGA-O1A
26	B	816	CLA	CAA-CBA-CGA-O1A
26	c	308	CLA	CAA-CBA-CGA-O1A
26	k	610	CLA	CAA-CBA-CGA-O1A
28	c	320	LHG	O10-C23-C24-C25
34	c	319	LMG	C20-C21-C22-C23
26	i	304	CLA	CAA-CBA-CGA-O2A
28	A	855	LHG	O8-C23-C24-C25
30	A	850	LMU	O5B-C5B-C6B-O6B
28	J	105	LHG	O2-C2-C3-O3
26	A	805	CLA	C14-C13-C15-C16
26	A	812	CLA	C14-C13-C15-C16
26	B	838	CLA	C11-C10-C8-C9
26	c	308	CLA	C14-C13-C15-C16
26	b	310	CLA	C11-C12-C13-C14
34	Q	301	LMG	C29-C30-C31-C32
26	A	805	CLA	C5-C6-C7-C8
26	A	836	CLA	CAA-CBA-CGA-O2A
26	B	812	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	B	828	CLA	CAA-CBA-CGA-O2A
26	c	304	CLA	CAA-CBA-CGA-O2A
26	m	604	CLA	CAA-CBA-CGA-O2A
26	j	603	CLA	CAA-CBA-CGA-O2A
28	B	851	LHG	O8-C23-C24-C25
28	s	409	LHG	O8-C23-C24-C25
26	A	830	CLA	C5-C6-C7-C8
26	m	608	CLA	CAA-CBA-CGA-O1A
26	d	313	CLA	C2A-CAA-CBA-CGA
33	B	844	DGD	CFA-CGA-CHA-CIA
26	A	808	CLA	CAA-CBA-CGA-O2A
26	A	814	CLA	CAA-CBA-CGA-O2A
26	B	809	CLA	CAA-CBA-CGA-O2A
26	c	303	CLA	CAA-CBA-CGA-O2A
26	a	304	CLA	CAA-CBA-CGA-O2A
26	a	306	CLA	CAA-CBA-CGA-O2A
26	b	308	CLA	CAA-CBA-CGA-O2A
26	h	313	CLA	CAA-CBA-CGA-O2A
26	k	604	CLA	CAA-CBA-CGA-O2A
26	A	835	CLA	C15-C16-C17-C18
26	c	311	CLA	CAA-CBA-CGA-O2A
26	B	826	CLA	CAA-CBA-CGA-O1A
26	B	831	CLA	C4-C3-C5-C6
26	i	306	CLA	C4-C3-C5-C6
33	j	618	DGD	CAB-CBB-CCB-CDB
26	A	805	CLA	C12-C13-C15-C16
26	A	813	CLA	C3A-C2A-CAA-CBA
26	A	831	CLA	C6-C7-C8-C10
26	A	833	CLA	C6-C7-C8-C10
26	B	807	CLA	C12-C13-C15-C16
26	B	829	CLA	C3A-C2A-CAA-CBA
26	B	838	CLA	C11-C10-C8-C7
26	s	402	CLA	C6-C7-C8-C10
26	c	308	CLA	C12-C13-C15-C16
26	a	307	CLA	C6-C7-C8-C10
26	a	307	CLA	C11-C12-C13-C15
26	b	310	CLA	C11-C12-C13-C15
26	b	311	CLA	C6-C7-C8-C10
26	h	301	CLA	C11-C10-C8-C7
26	k	602	CLA	C11-C12-C13-C15
26	k	607	CLA	C3A-C2A-CAA-CBA
26	k	608	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	d	302	CLA	C11-C10-C8-C7
26	n	608	CLA	C6-C7-C8-C10
29	A	845	WVN	C05-C02-C11-C19
26	A	812	CLA	CAA-CBA-CGA-O1A
28	B	851	LHG	C10-C11-C12-C13
26	h	308	CLA	CAA-CBA-CGA-O2A
26	l	307	CLA	CAA-CBA-CGA-O2A
29	A	857	WVN	C30-C33-C34-C37
35	l	302	II0	C31-C33-C35-C39
26	B	801	CLA	CAA-CBA-CGA-O1A
26	m	604	CLA	CAA-CBA-CGA-O1A
26	l	307	CLA	CAA-CBA-CGA-O1A
35	a	314	II0	C35-C39-C41-C42
35	d	315	II0	C35-C39-C41-C42
28	n	619	LHG	C31-C32-C33-C34
26	n	609	CLA	CBD-CGD-O2D-CED
30	a	317	LMU	C2-C1-O1'-C1'
26	i	308	CLA	CAA-CBA-CGA-O2A
28	n	619	LHG	O7-C7-C8-C9
26	A	808	CLA	CAA-CBA-CGA-O1A
26	j	603	CLA	CAA-CBA-CGA-O1A
26	A	852	CLA	O1D-CGD-O2D-CED
34	n	620	LMG	C32-C33-C34-C35
34	c	318	LMG	C36-C37-C38-C39
26	A	816	CLA	C13-C15-C16-C17
26	B	841	CLA	C5-C6-C7-C8
26	a	306	CLA	CAA-CBA-CGA-O1A
26	j	604	CLA	CAA-CBA-CGA-O1A
34	F	205	LMG	O9-C10-C11-C12
26	j	608	CLA	C2A-CAA-CBA-CGA
27	B	843	PQN	C25-C26-C27-C28
26	B	809	CLA	CAA-CBA-CGA-O1A
26	B	828	CLA	CAA-CBA-CGA-O1A
26	a	304	CLA	CAA-CBA-CGA-O1A
26	k	604	CLA	CAA-CBA-CGA-O1A
26	i	304	CLA	CAA-CBA-CGA-O1A
26	A	804	CLA	CAA-CBA-CGA-O2A
26	A	826	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

208 monomers are involved in 424 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	n	614	II0	1	0
34	Q	301	LMG	3	0
26	m	613	CLA	5	0
26	d	304	CLA	1	0
26	A	824	CLA	2	0
26	c	307	CLA	1	0
26	B	829	CLA	1	0
26	j	609	CLA	1	0
26	A	817	CLA	2	0
26	c	308	CLA	3	0
26	j	608	CLA	2	0
26	B	809	CLA	1	0
26	A	804	CLA	4	0
27	B	843	PQN	2	0
34	n	620	LMG	3	0
26	h	307	CLA	2	0
26	d	306	CLA	1	0
26	F	201	CLA	2	0
25	A	801	CL0	4	0
26	A	812	CLA	4	0
26	n	607	CLA	3	0
26	B	802	CLA	3	0
27	A	842	PQN	4	0
28	A	849	LHG	2	0
26	A	803	CLA	4	0
26	B	842	CLA	4	0
34	F	206	LMG	1	0
28	s	409	LHG	3	0
36	s	404	KC2	1	0
26	i	307	CLA	1	0
26	A	834	CLA	1	0
26	A	852	CLA	3	0
26	b	307	CLA	1	0
26	d	313	CLA	4	0
26	k	610	CLA	1	0
26	h	308	CLA	1	0
26	A	808	CLA	1	0
28	n	619	LHG	1	0
26	B	841	CLA	2	0
26	B	831	CLA	3	0
28	A	844	LHG	2	0
26	A	831	CLA	4	0
26	A	856	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	826	CLA	2	0
26	B	820	CLA	2	0
26	a	303	CLA	1	0
26	A	841	CLA	7	0
26	B	807	CLA	4	0
26	l	305	CLA	3	0
26	b	310	CLA	5	0
26	B	818	CLA	2	0
26	B	810	CLA	3	0
26	h	313	CLA	3	0
26	A	830	CLA	3	0
26	B	825	CLA	5	0
26	A	806	CLA	1	0
26	s	402	CLA	2	0
26	A	816	CLA	4	0
26	l	309	CLA	4	0
34	c	319	LMG	1	0
26	A	809	CLA	1	0
26	A	805	CLA	6	0
26	m	602	CLA	5	0
26	a	307	CLA	1	0
26	k	602	CLA	2	0
26	h	301	CLA	6	0
26	n	604	CLA	1	0
26	d	308	CLA	1	0
26	B	836	CLA	4	0
26	A	811	CLA	1	0
26	m	603	CLA	1	0
36	d	312	KC2	3	0
26	a	304	CLA	1	0
30	B	852	LMU	1	0
26	c	302	CLA	1	0
26	A	833	CLA	3	0
26	A	838	CLA	2	0
26	A	819	CLA	1	0
26	c	304	CLA	2	0
26	L	204	CLA	3	0
35	b	314	II0	1	0
26	A	827	CLA	7	0
26	A	832	CLA	4	0
26	a	310	CLA	1	0
26	i	304	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	k	607	CLA	1	0
28	c	320	LHG	4	0
26	B	808	CLA	4	0
26	A	829	CLA	7	0
26	a	306	CLA	1	0
26	j	603	CLA	3	0
26	i	311	CLA	3	0
26	B	826	CLA	3	0
26	A	818	CLA	5	0
26	m	601	CLA	2	0
26	s	406	CLA	3	0
34	b	319	LMG	1	0
26	m	604	CLA	1	0
26	j	607	CLA	1	0
26	j	610	CLA	3	0
30	i	300	LMU	2	0
26	B	840	CLA	4	0
26	c	309	CLA	1	0
26	A	802	CLA	4	0
26	B	830	CLA	4	0
26	m	608	CLA	2	0
26	F	202	CLA	2	0
28	b	302	LHG	2	0
26	i	306	CLA	1	0
26	m	610	CLA	2	0
26	A	825	CLA	2	0
26	B	812	CLA	3	0
26	k	605	CLA	1	0
26	B	814	CLA	5	0
26	b	304	CLA	1	0
26	B	839	CLA	1	0
26	B	828	CLA	4	0
26	B	823	CLA	4	0
33	j	618	DGD	3	0
26	B	805	CLA	1	0
26	B	813	CLA	1	0
26	b	306	CLA	3	0
26	A	815	CLA	1	0
26	k	603	CLA	1	0
26	l	306	CLA	3	0
28	B	851	LHG	2	0
26	c	312	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	F	205	LMG	1	0
26	L	206	CLA	1	0
26	B	804	CLA	3	0
26	A	807	CLA	1	0
26	k	609	CLA	3	0
26	n	608	CLA	6	0
26	B	801	CLA	3	0
26	a	311	CLA	1	0
26	n	609	CLA	2	0
26	n	610	CLA	2	0
26	A	810	CLA	2	0
26	j	604	CLA	2	0
26	i	301	CLA	1	0
26	b	313	CLA	1	0
30	A	858	LMU	2	0
26	b	312	CLA	4	0
28	A	843	LHG	1	0
26	l	313	CLA	3	0
26	B	816	CLA	2	0
26	A	840	CLA	2	0
31	C	102	SF4	1	0
26	B	803	CLA	4	0
28	A	855	LHG	2	0
26	d	302	CLA	3	0
26	A	836	CLA	6	0
26	B	834	CLA	3	0
26	l	301	CLA	3	0
26	B	822	CLA	5	0
26	h	306	CLA	1	0
28	b	318	LHG	1	0
26	c	306	CLA	1	0
26	c	303	CLA	1	0
35	d	319	II0	1	0
26	j	613	CLA	2	0
26	B	824	CLA	2	0
26	A	839	CLA	2	0
26	h	304	CLA	2	0
26	L	202	CLA	1	0
26	L	203	CLA	4	0
26	A	823	CLA	4	0
26	k	608	CLA	1	0
36	s	401	KC2	1	0

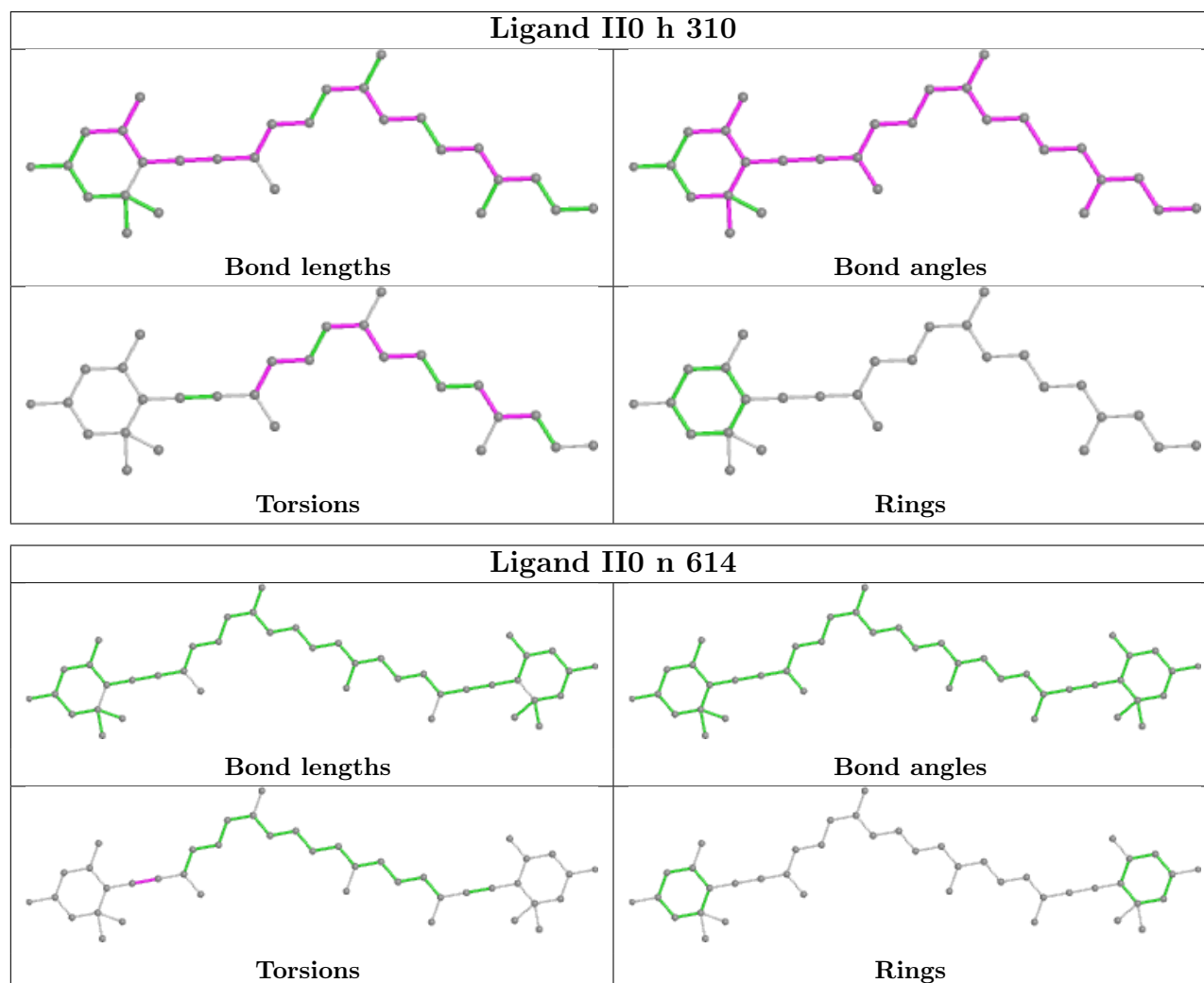
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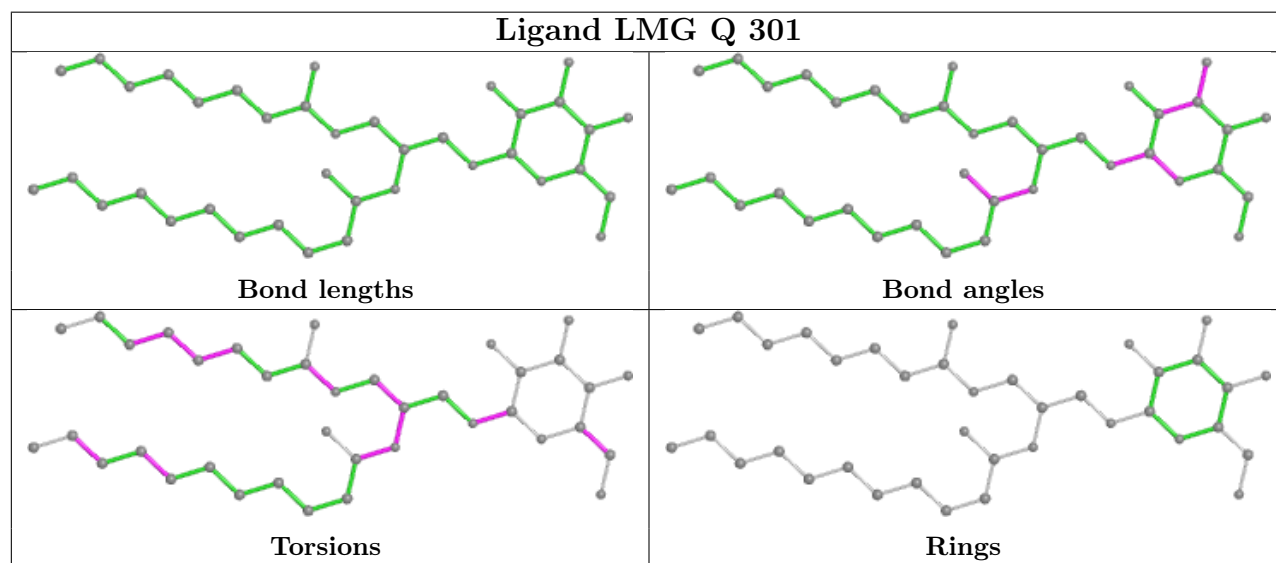
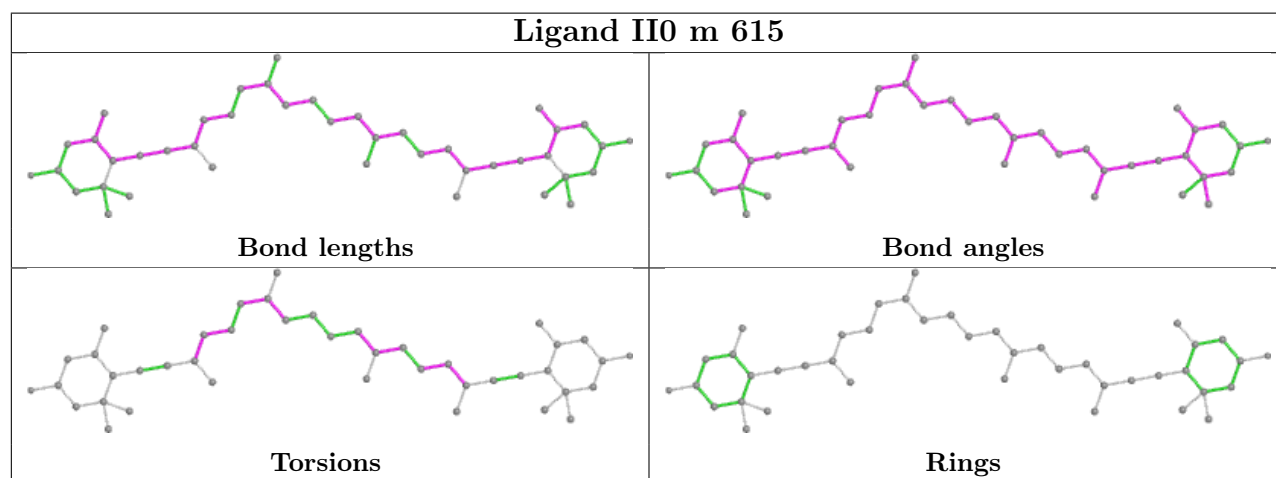
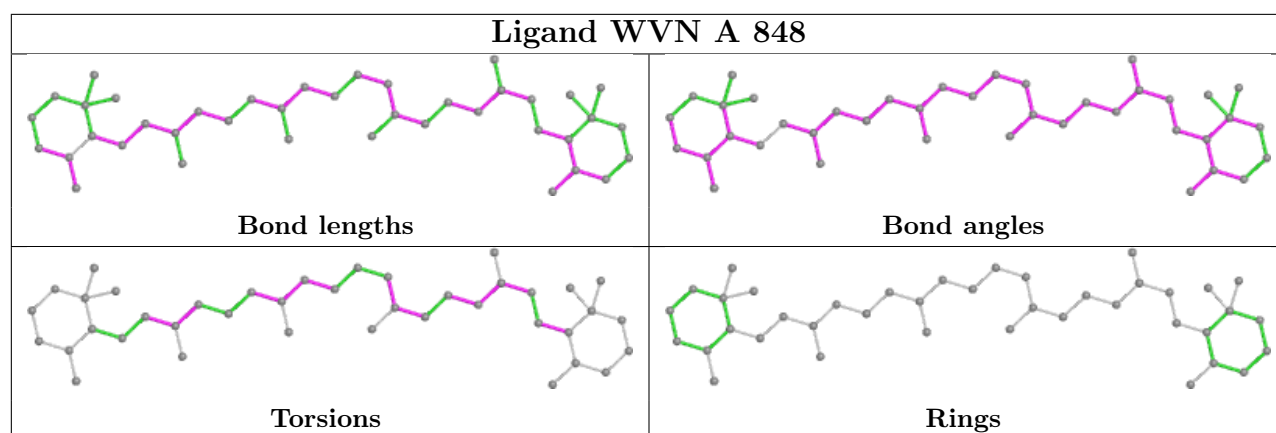
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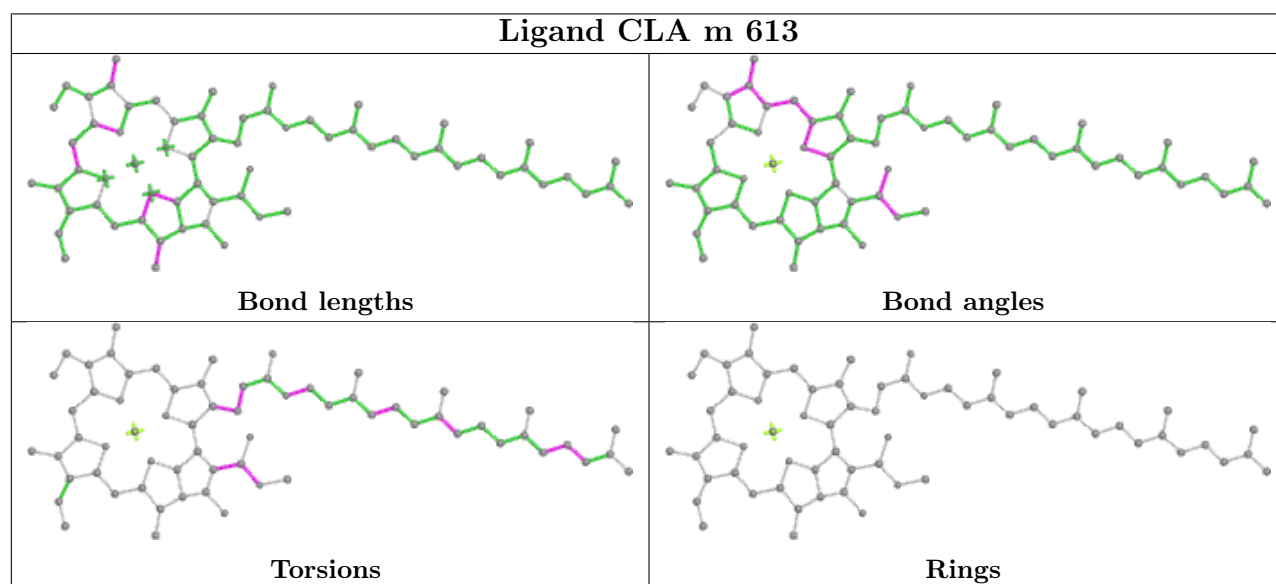
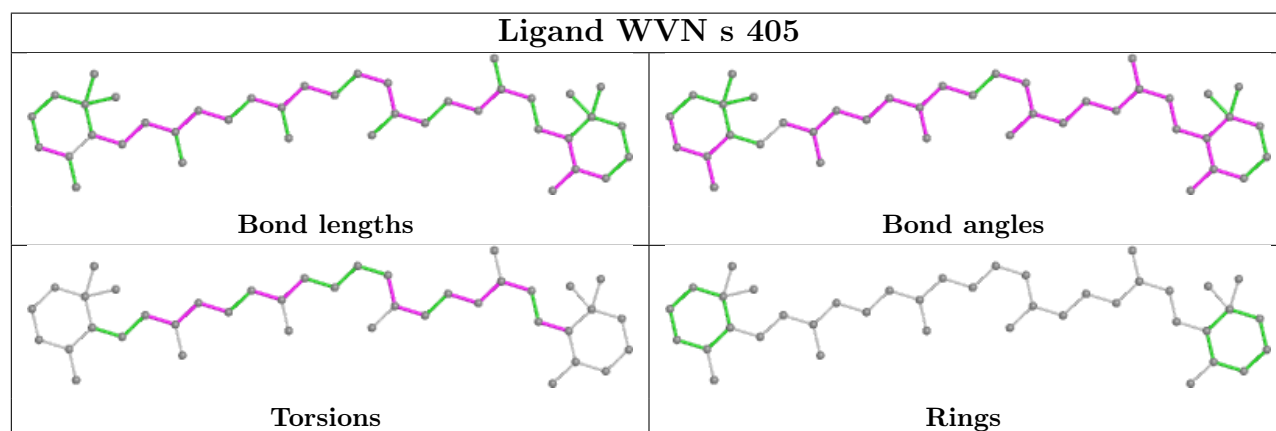
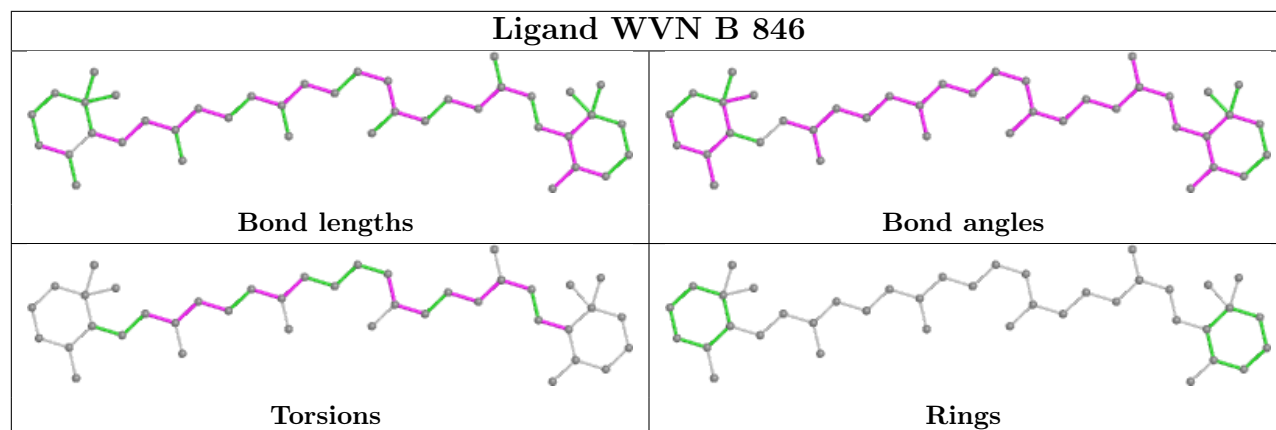
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	817	CLA	6	0
26	k	604	CLA	2	0
26	A	822	CLA	4	0
36	n	611	KC2	1	0
33	B	844	DGD	6	0
26	h	305	CLA	2	0
26	B	819	CLA	3	0
26	B	806	CLA	2	0
26	m	609	CLA	1	0
26	b	309	CLA	6	0
26	c	305	CLA	1	0
35	i	319	II0	1	0
26	A	814	CLA	2	0
26	l	304	CLA	1	0
26	B	827	CLA	3	0
26	b	311	CLA	1	0
26	B	832	CLA	1	0
26	R	201	CLA	4	0
26	B	835	CLA	3	0
26	B	821	CLA	3	0
34	L	209	LMG	2	0
26	B	811	CLA	2	0
26	l	308	CLA	2	0
26	B	837	CLA	5	0
26	c	301	CLA	2	0
26	a	308	CLA	1	0
26	J	103	CLA	1	0
26	A	835	CLA	4	0
26	k	614	CLA	1	0
26	A	851	CLA	2	0
26	B	833	CLA	3	0
26	m	607	CLA	2	0
37	b	301	IHT	1	0
26	B	838	CLA	2	0
26	n	613	CLA	2	0
26	a	301	CLA	7	0
26	B	815	CLA	3	0
26	A	837	CLA	7	0
26	A	828	CLA	3	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

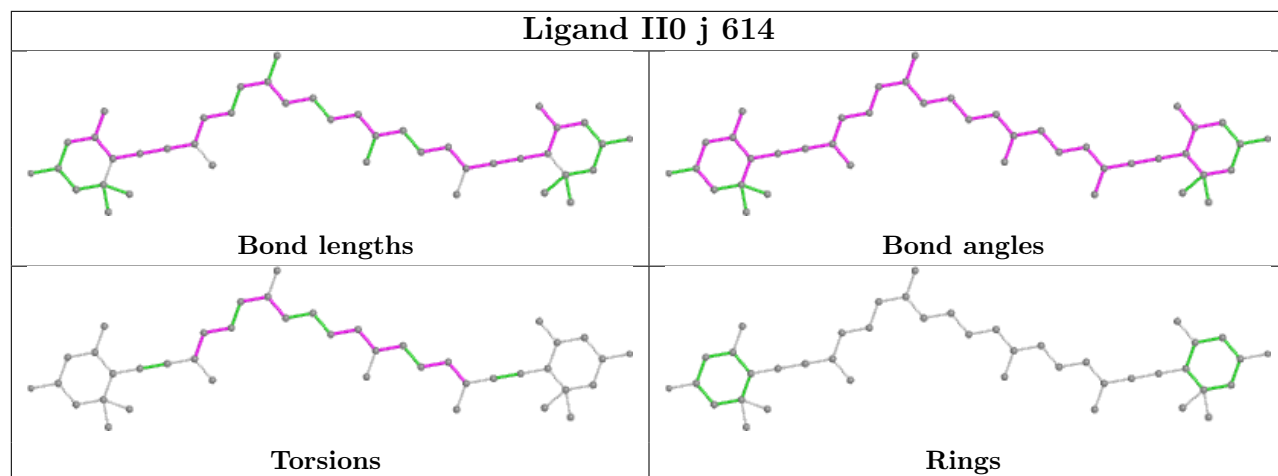
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



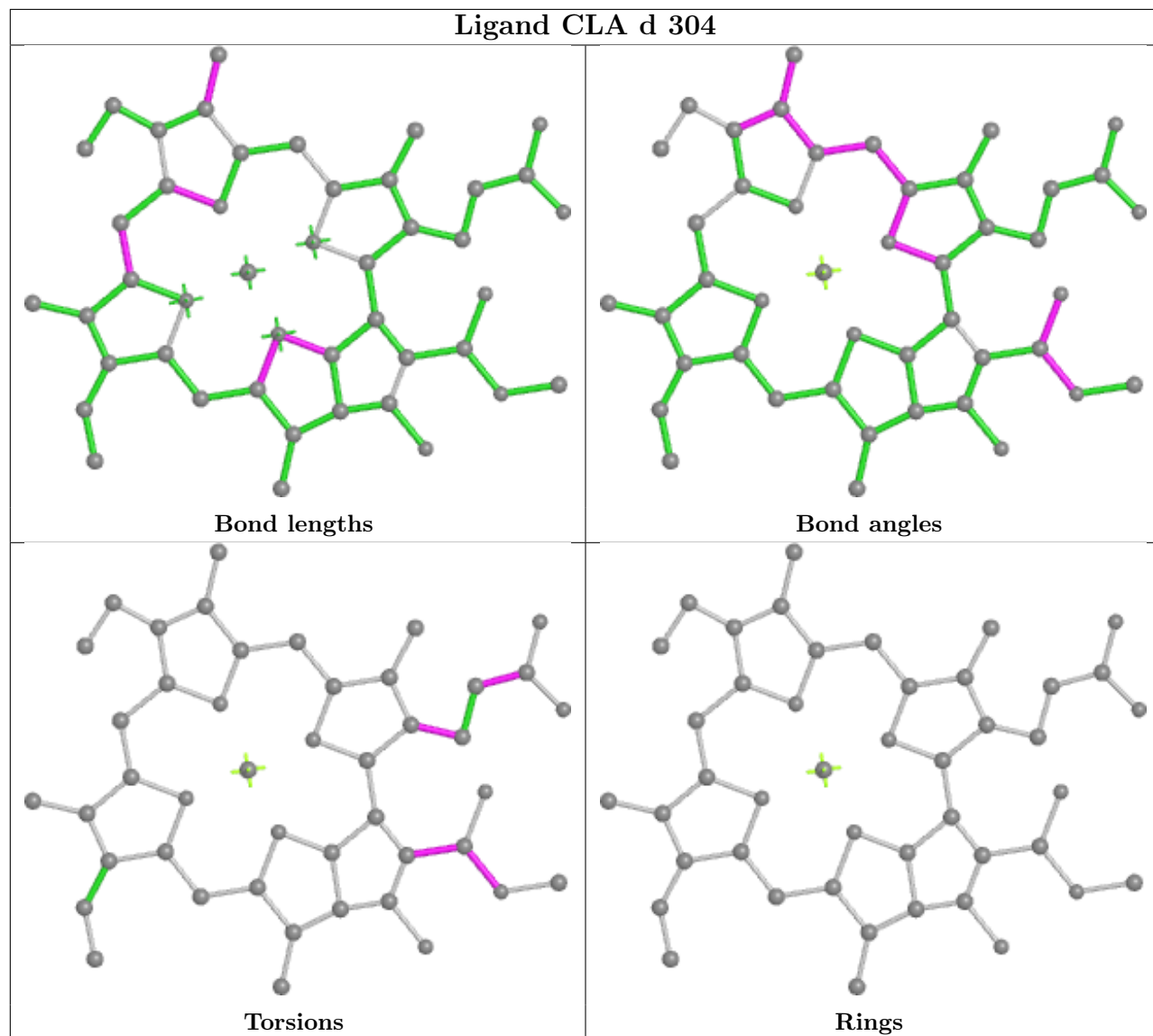


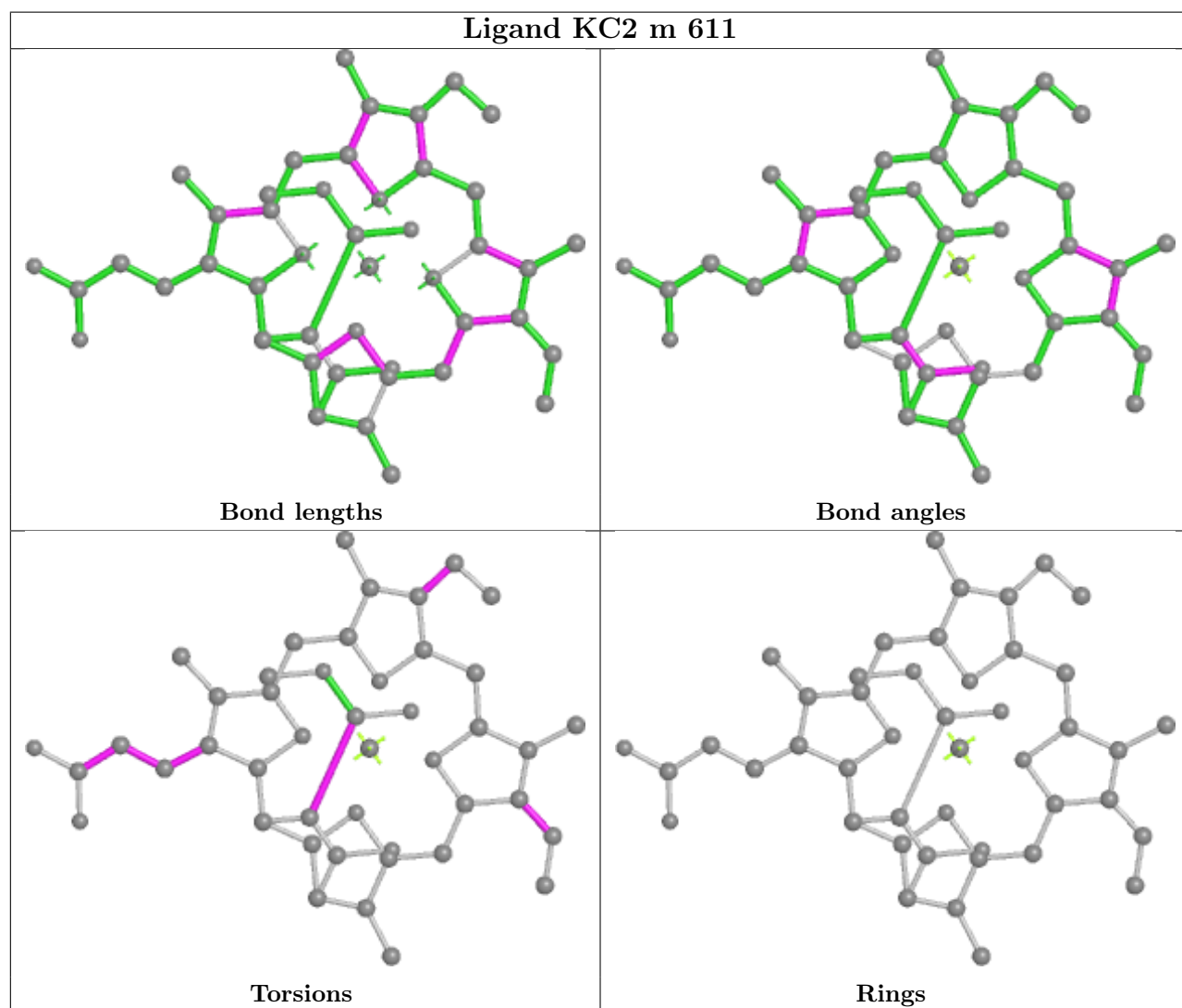
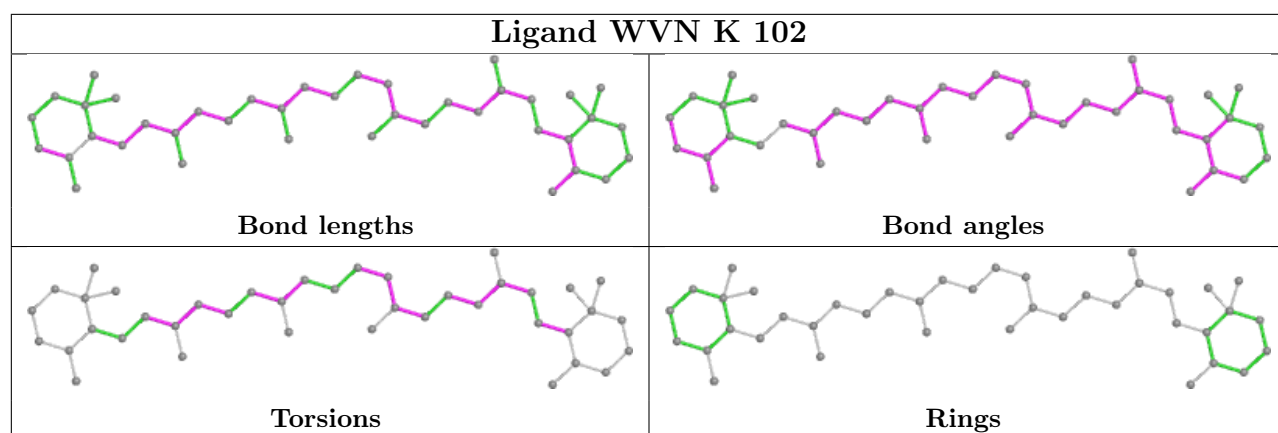


Ligand II0 j 614

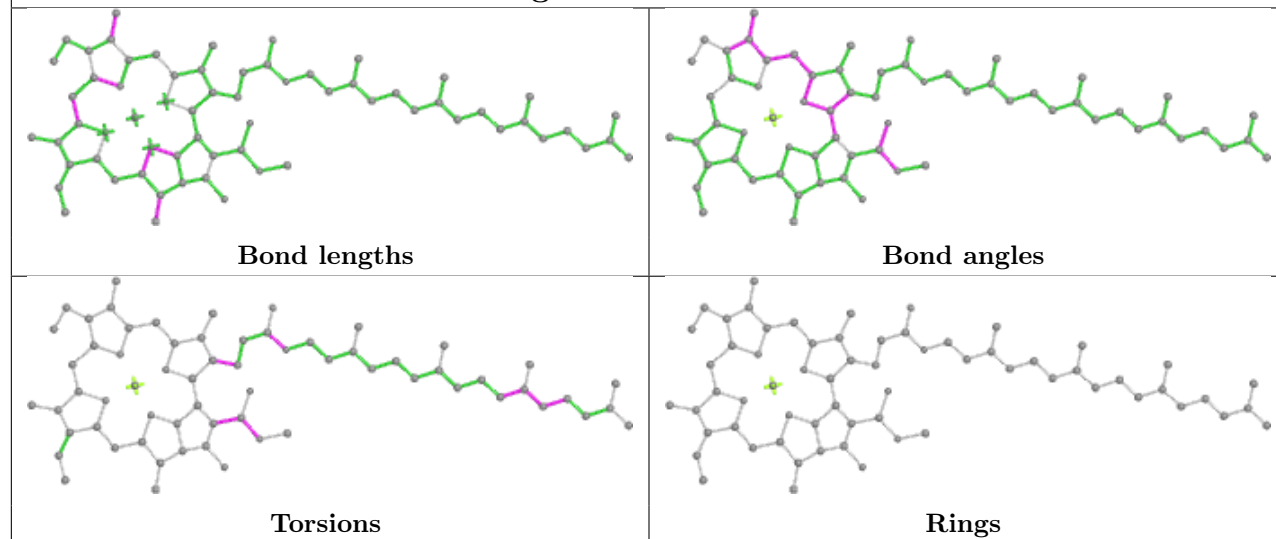


Ligand CLA d 304

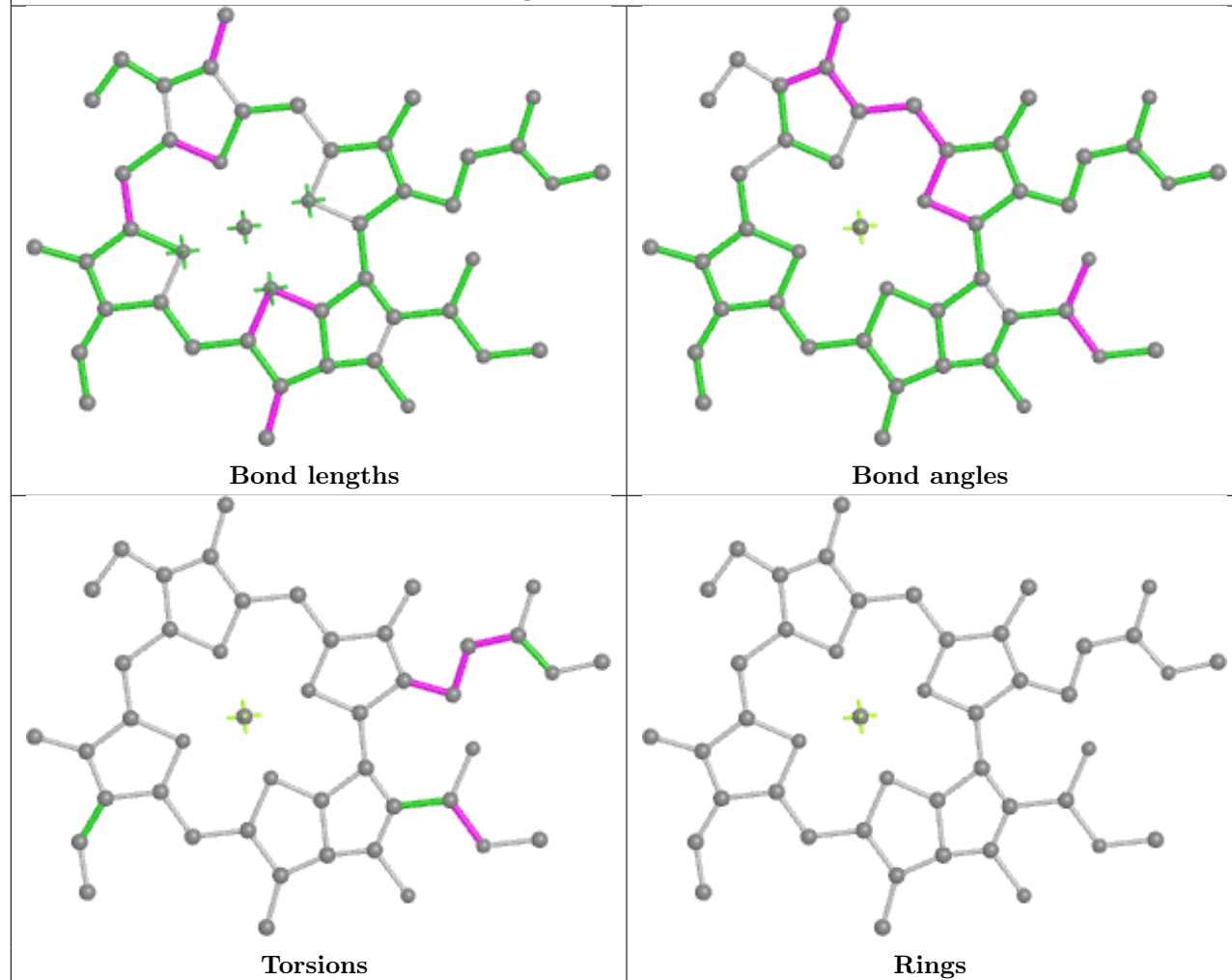




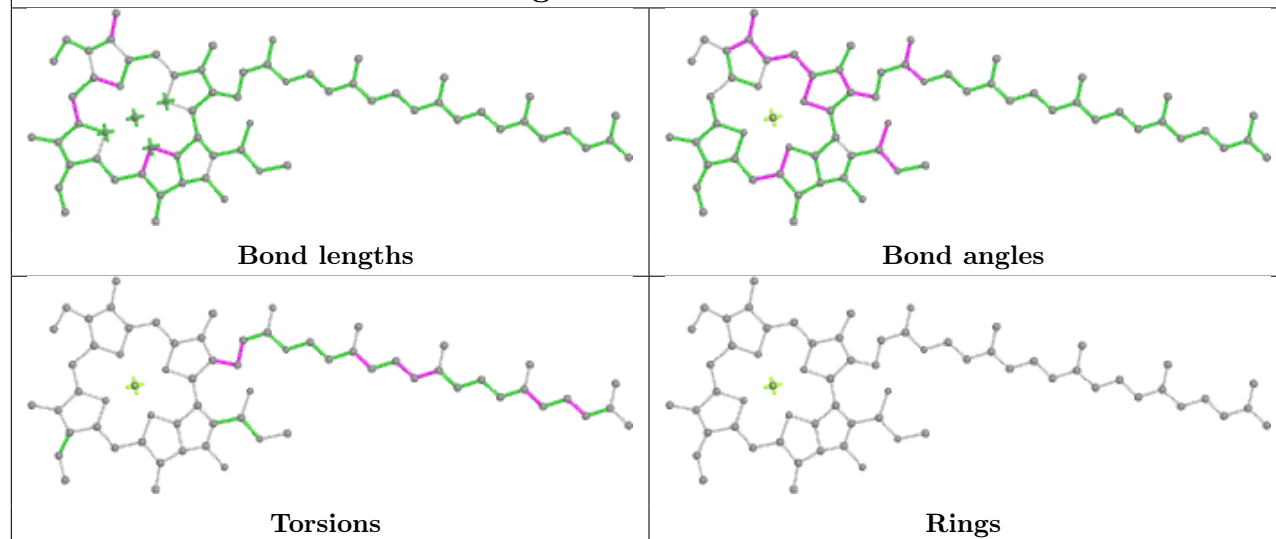
Ligand CLA A 824



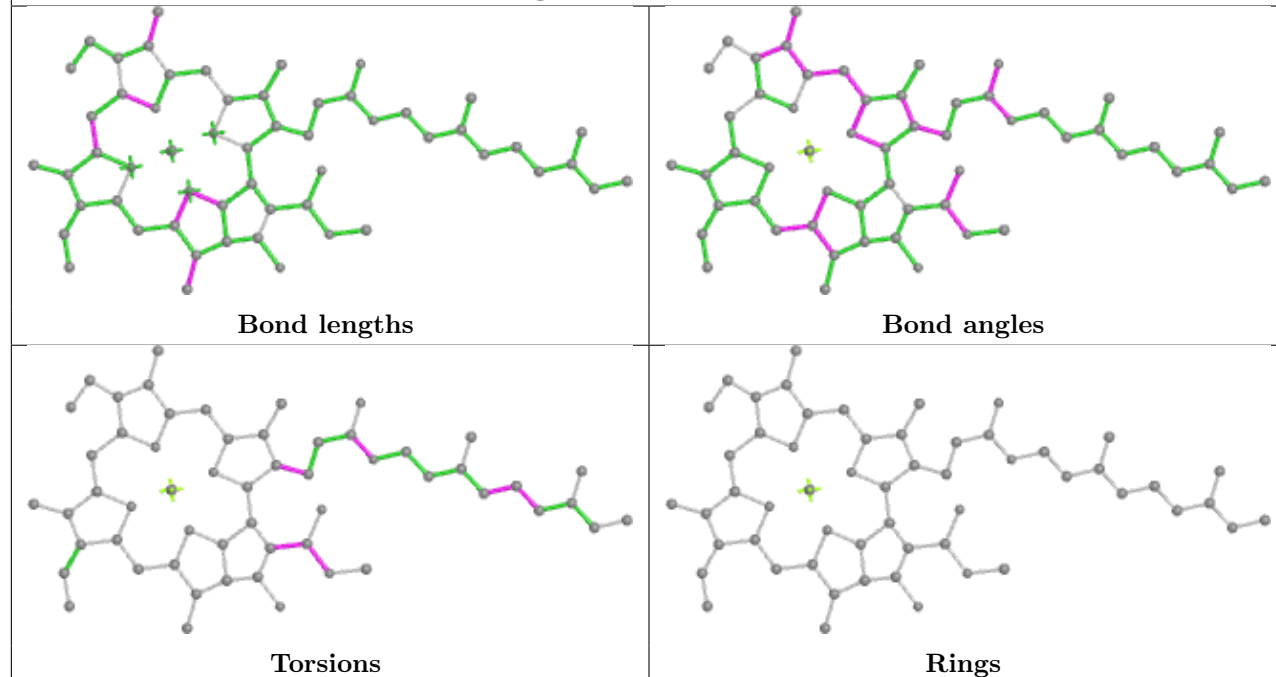
Ligand CLA c 307



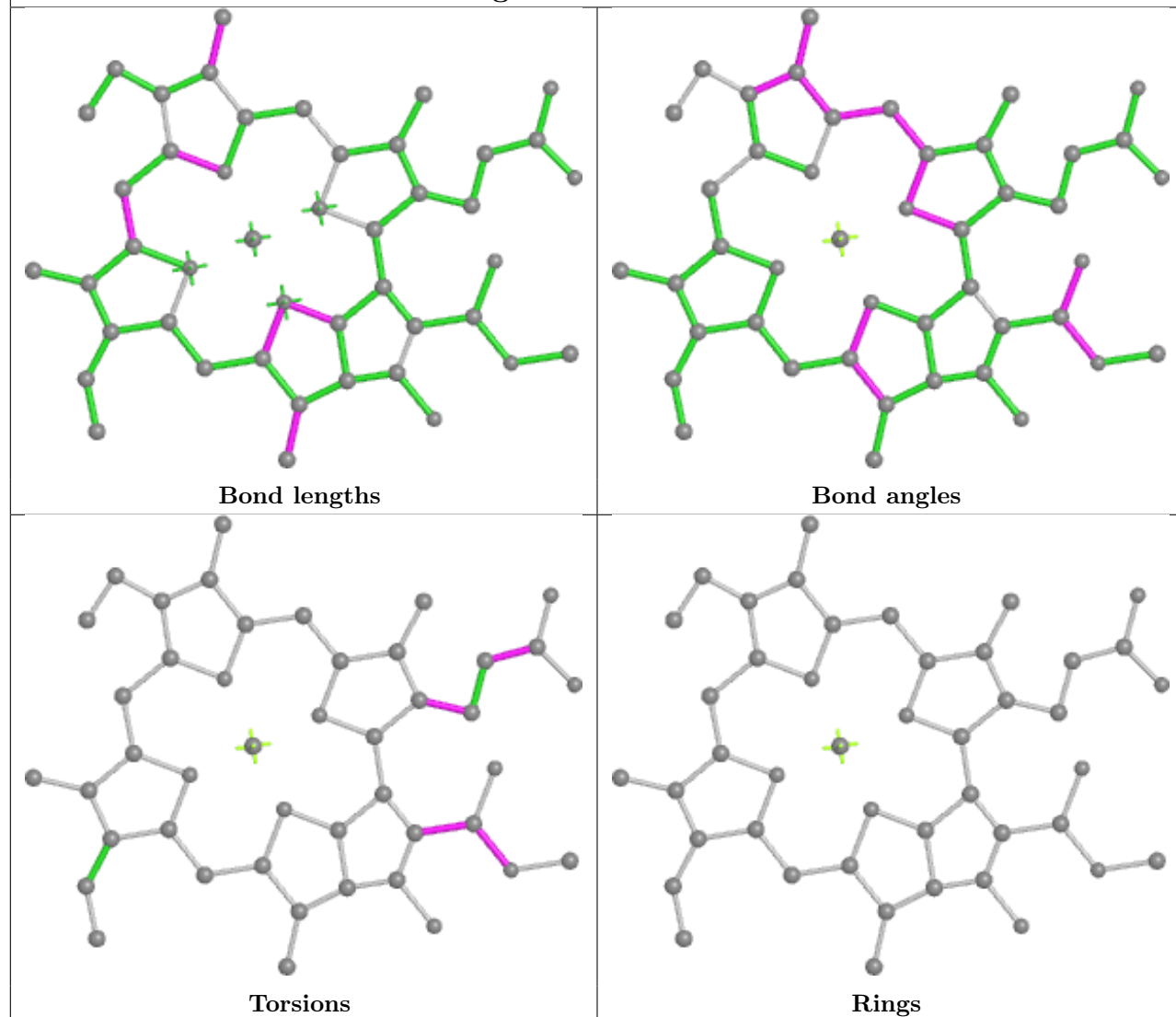
Ligand CLA B 829



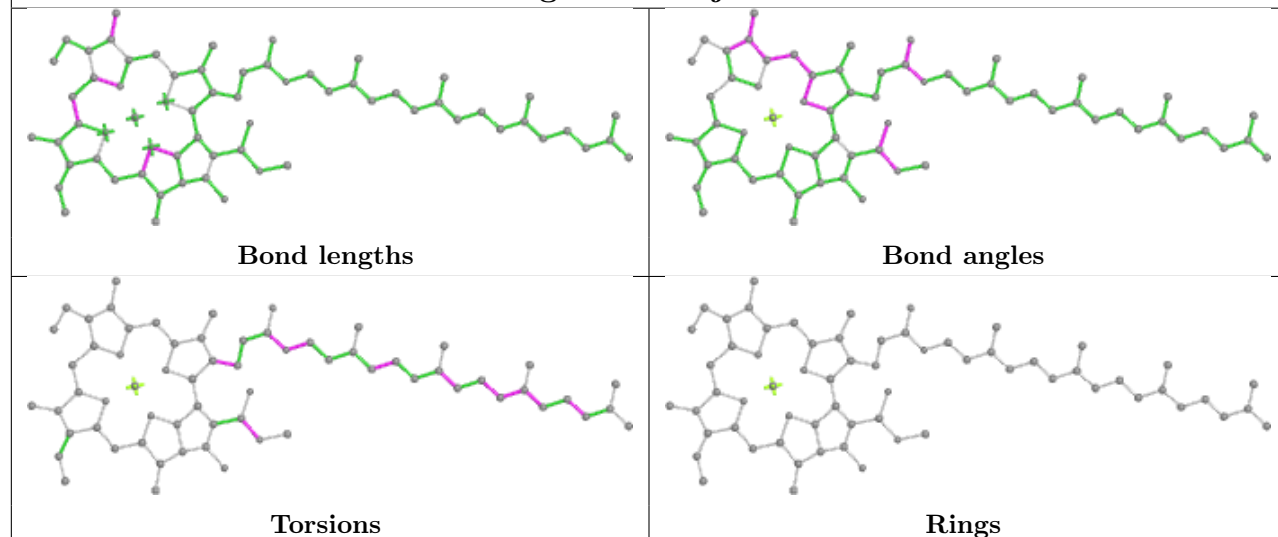
Ligand CLA A 813



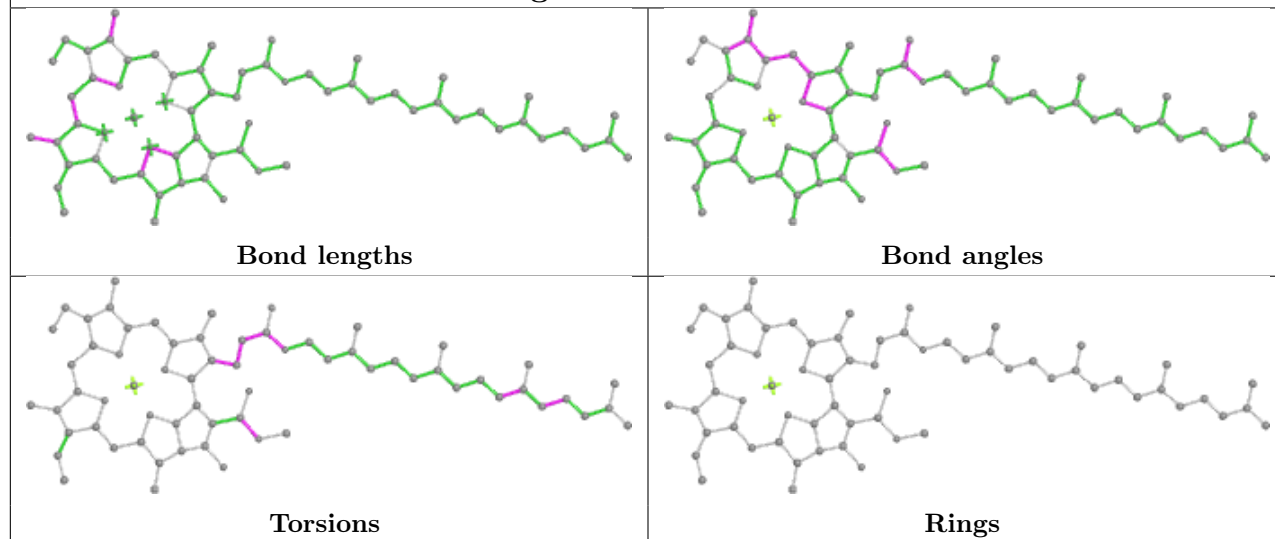
Ligand CLA d 307



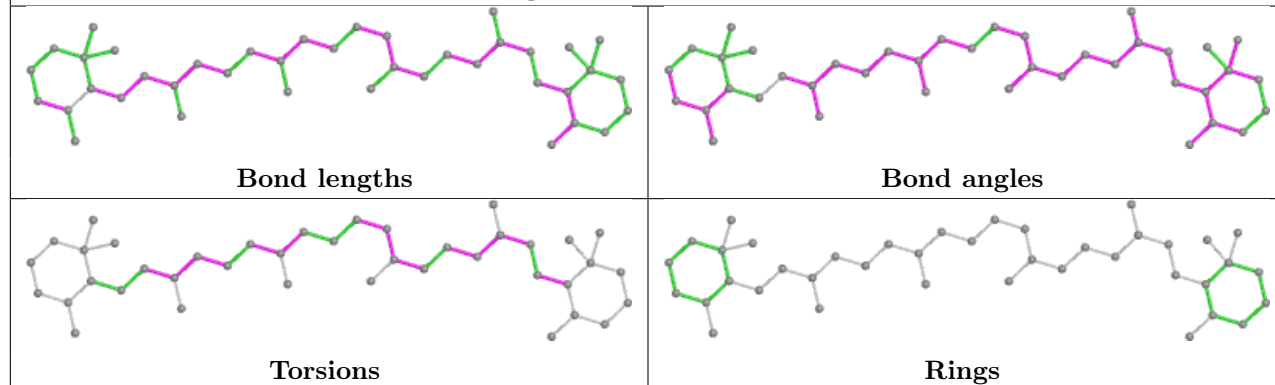
Ligand CLA j 609



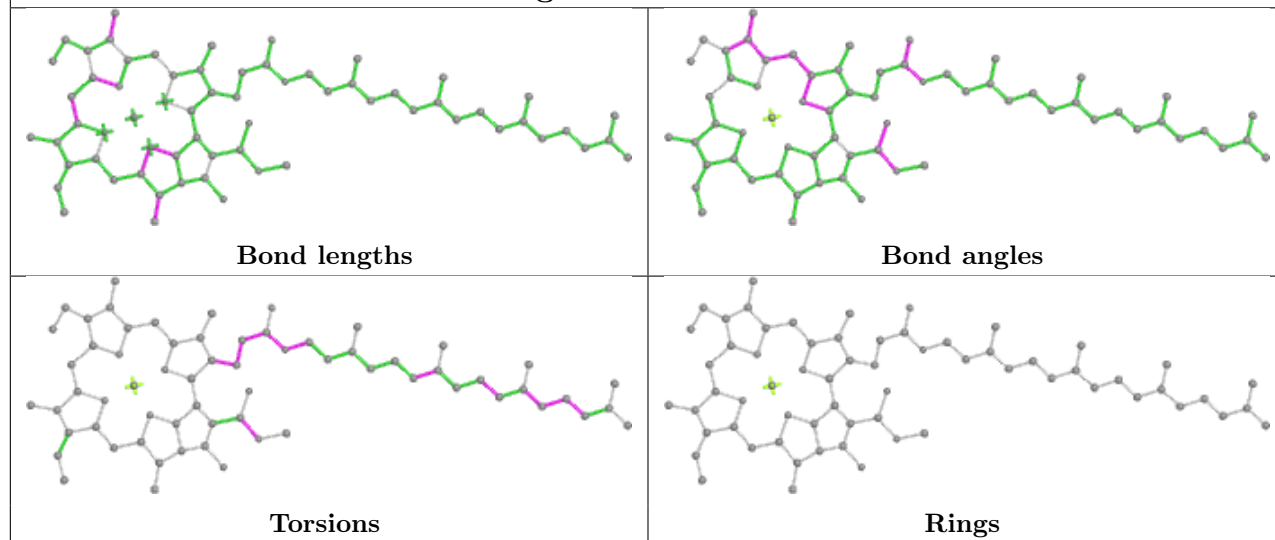
Ligand CLA A 817

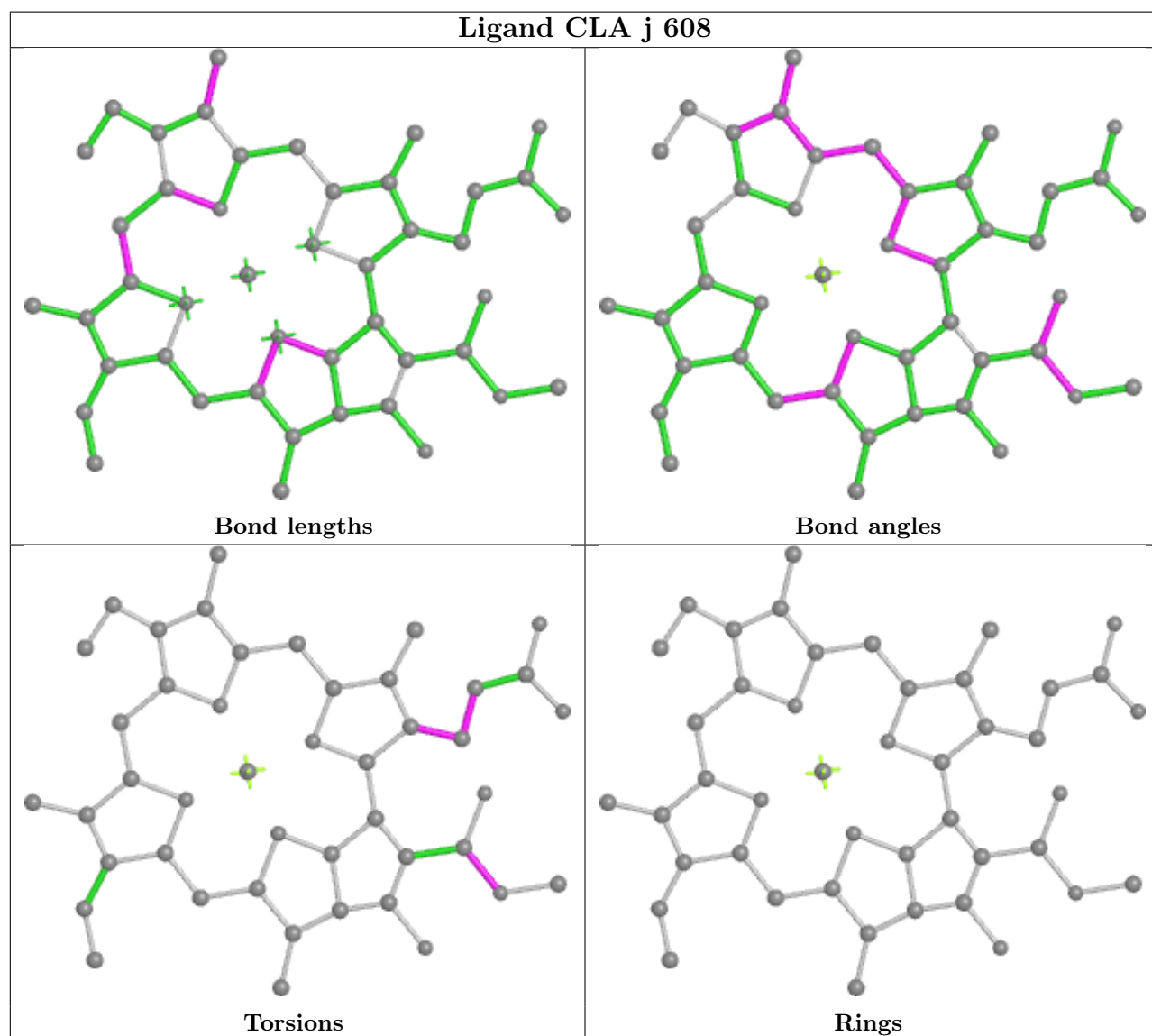
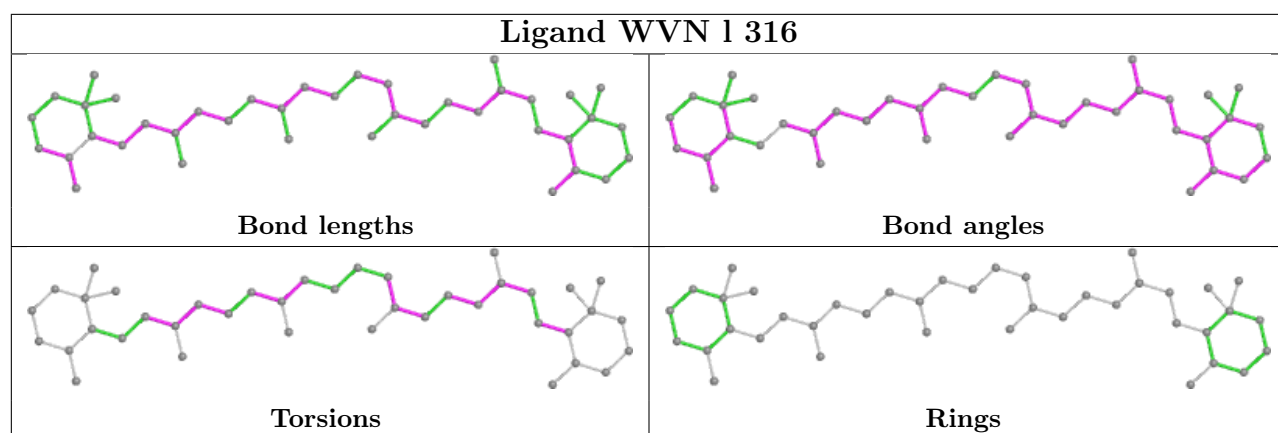


Ligand WVN B 848

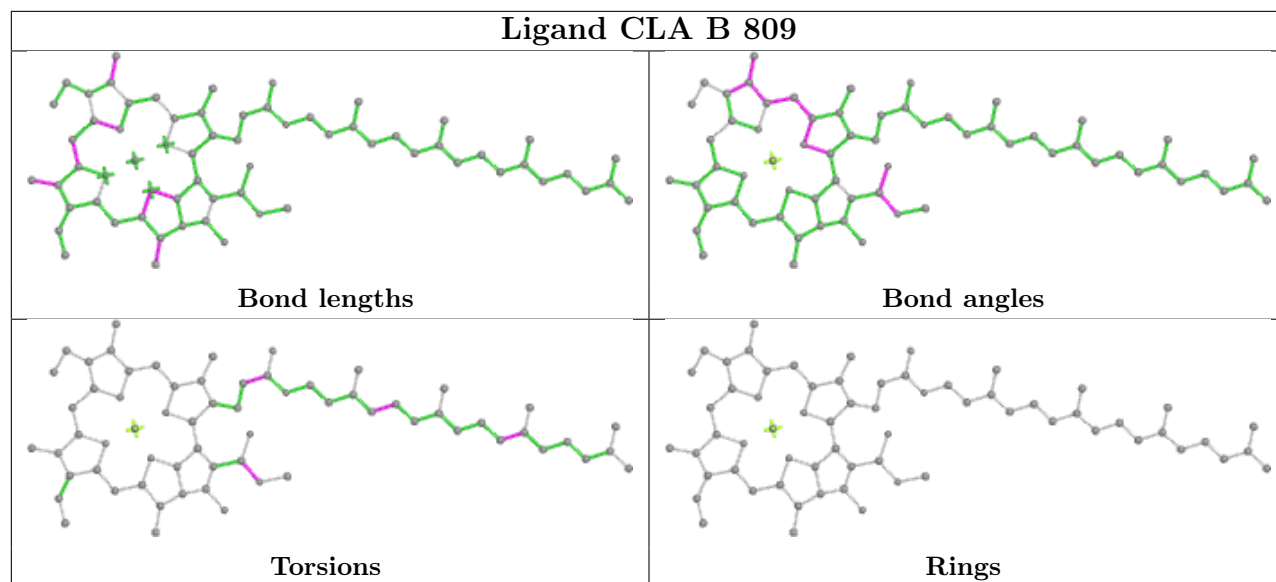


Ligand CLA c 308

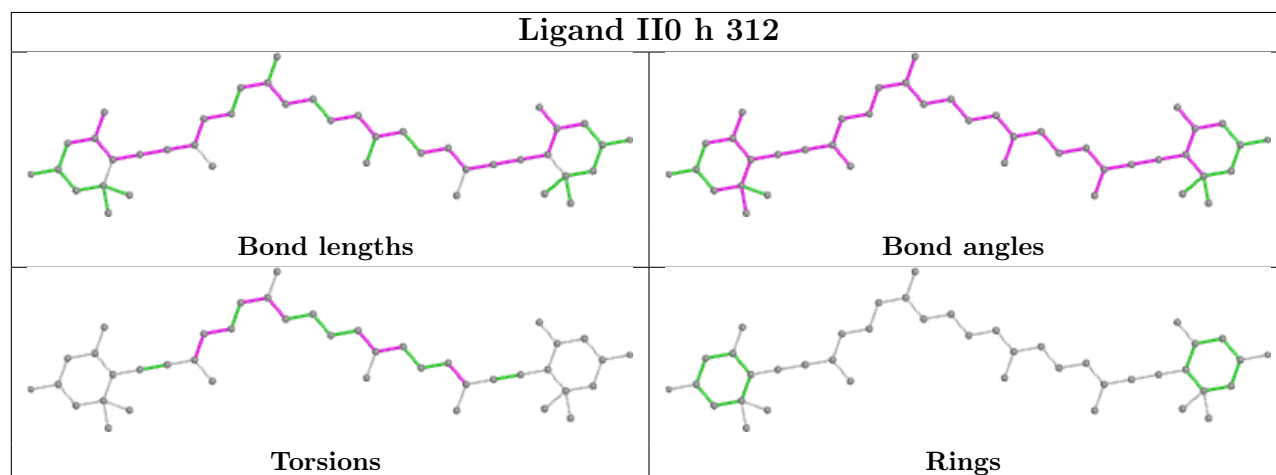




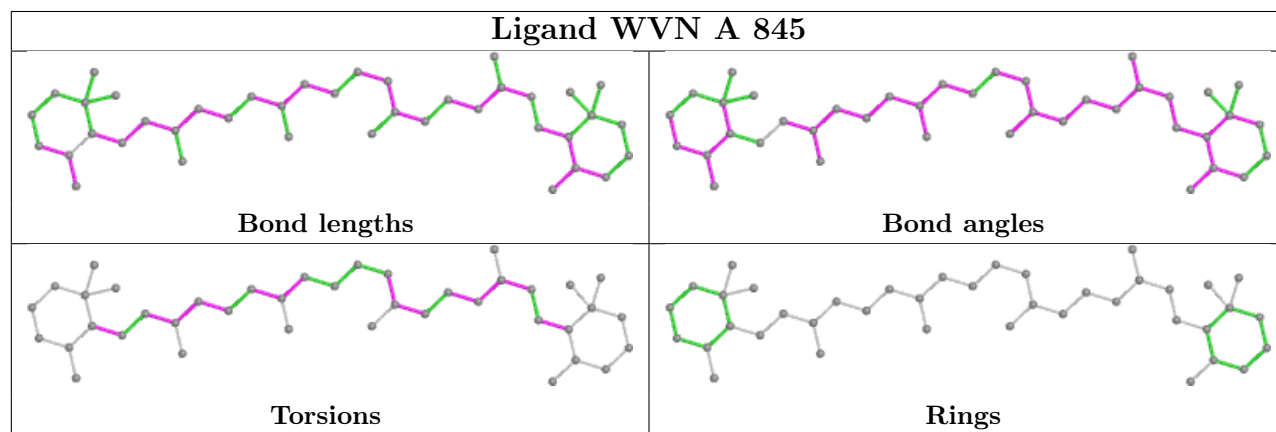
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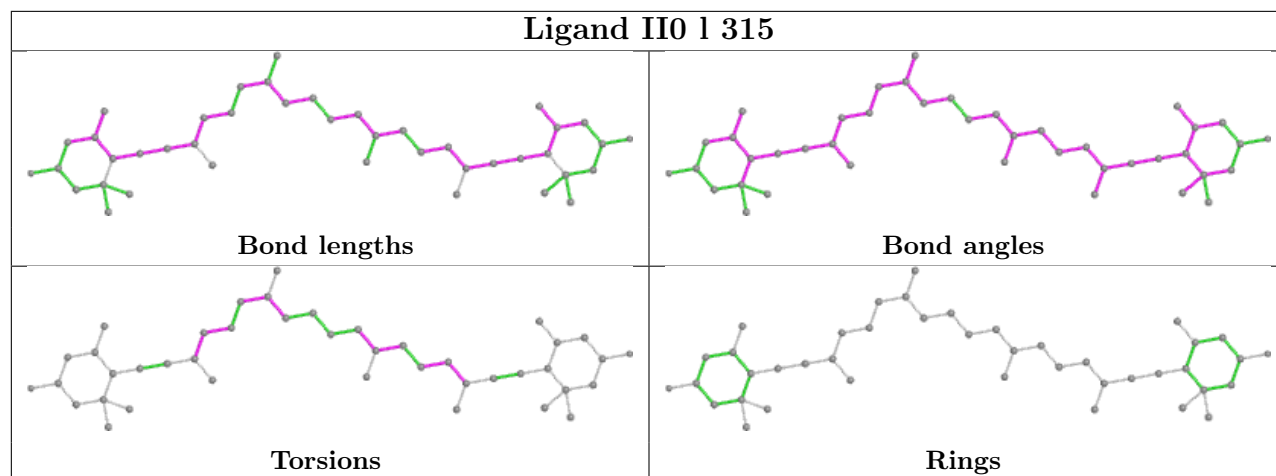
Ligand II0 h 312



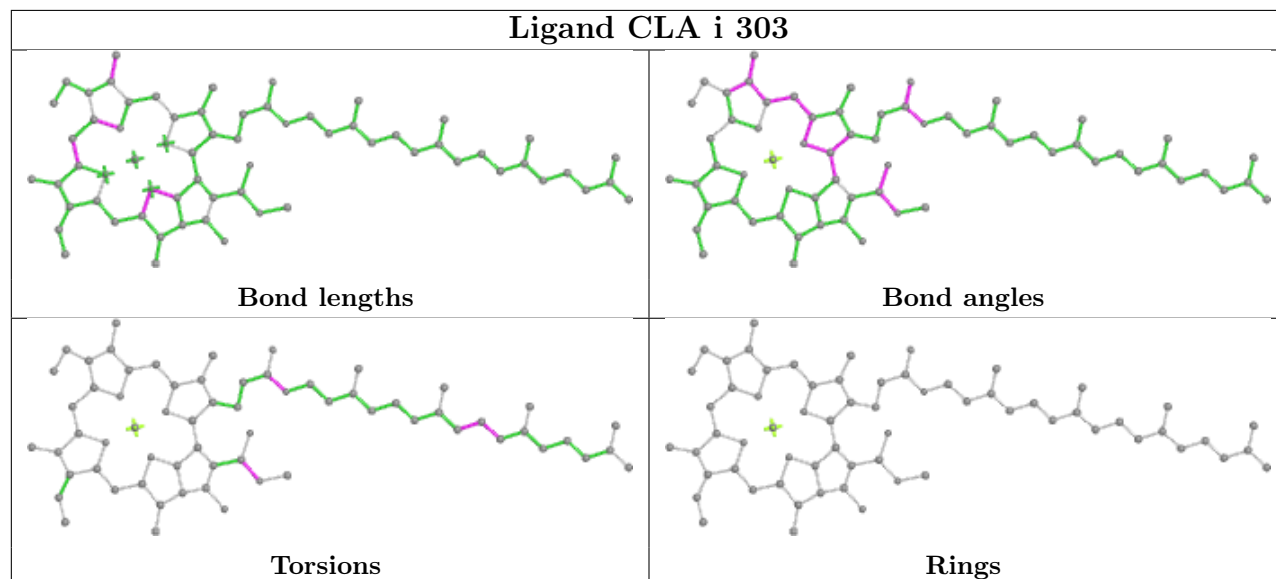
Ligand WVN A 845



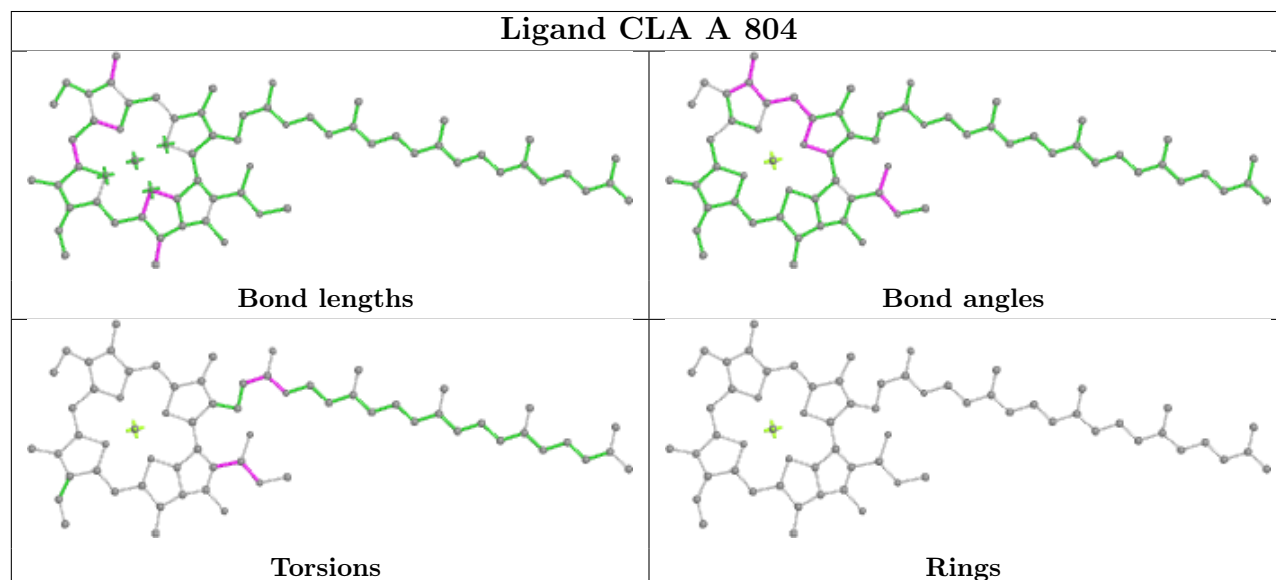
Ligand II0 I 315

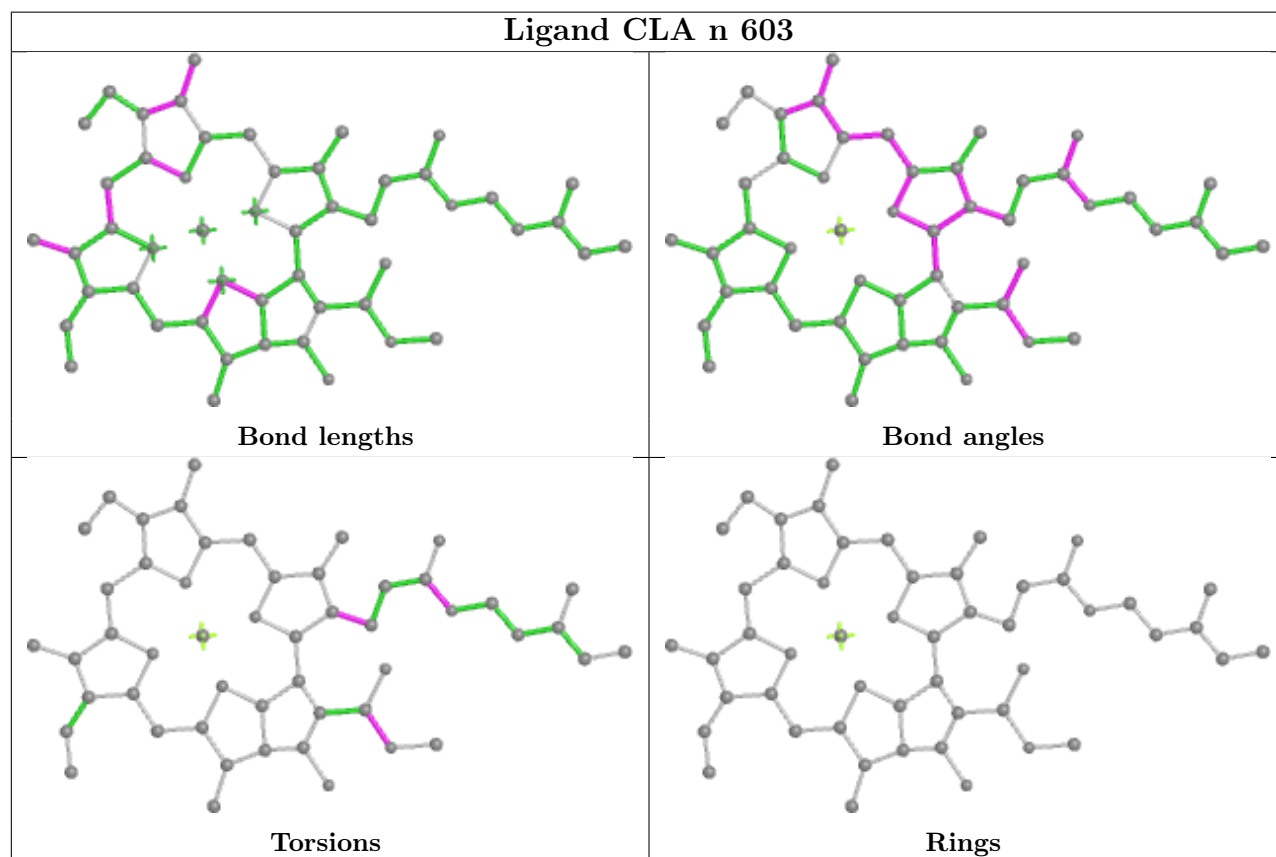
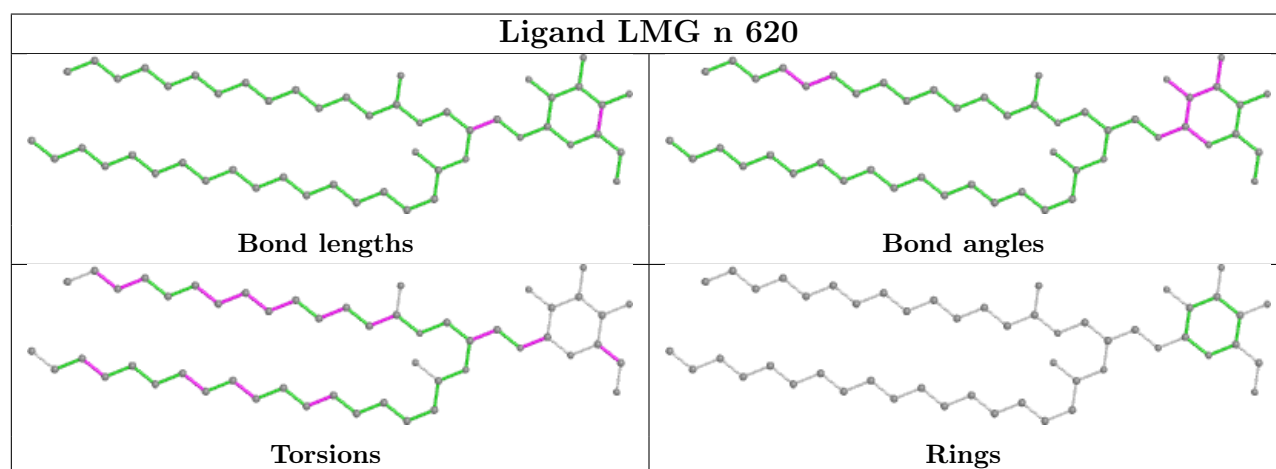
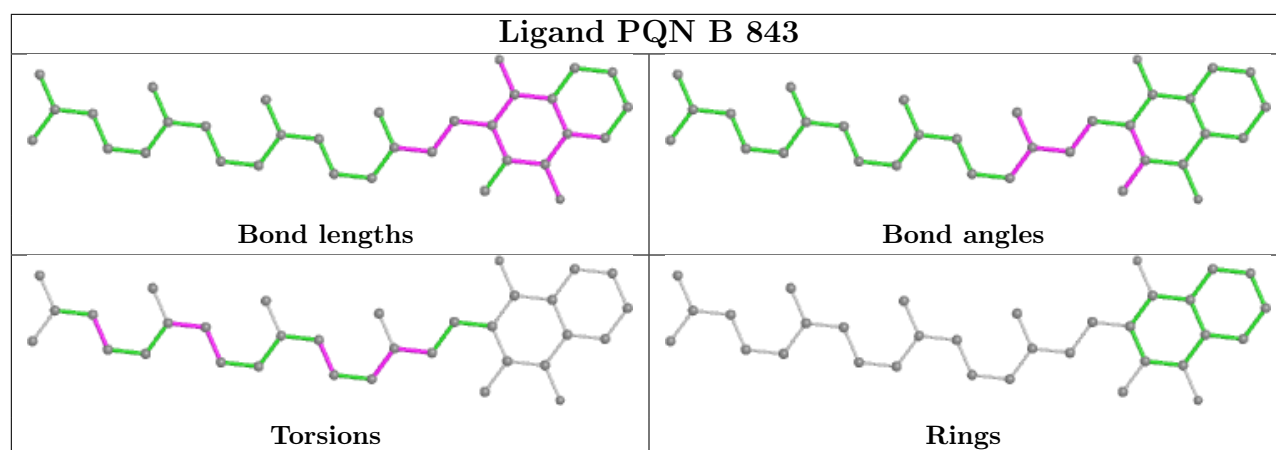


Ligand CLA i 303

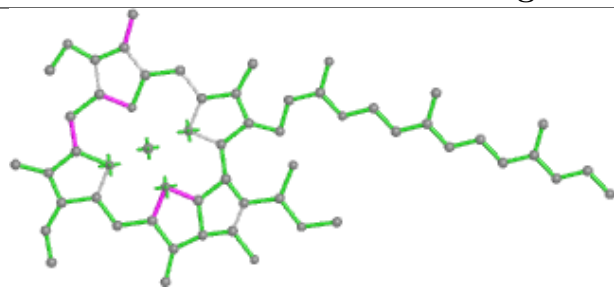


Ligand CLA A 804

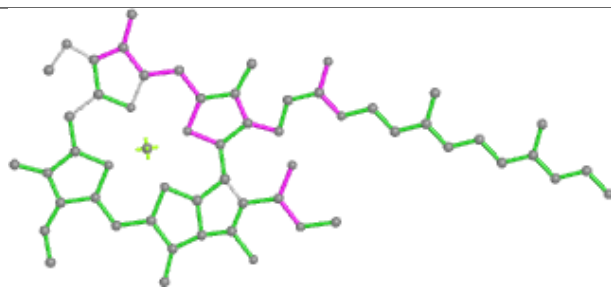




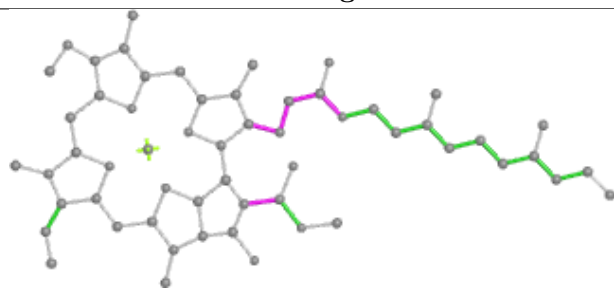
Ligand CLA h 307



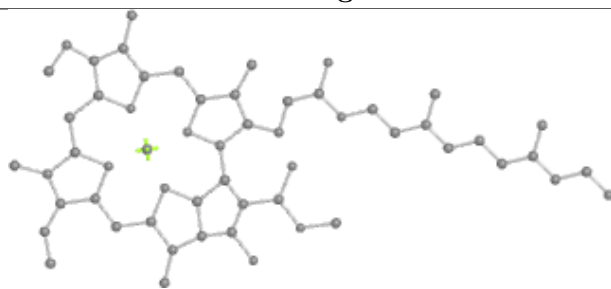
Bond lengths



Bond angles

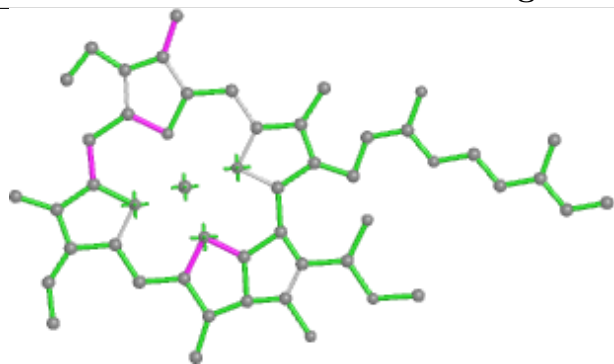


Torsions

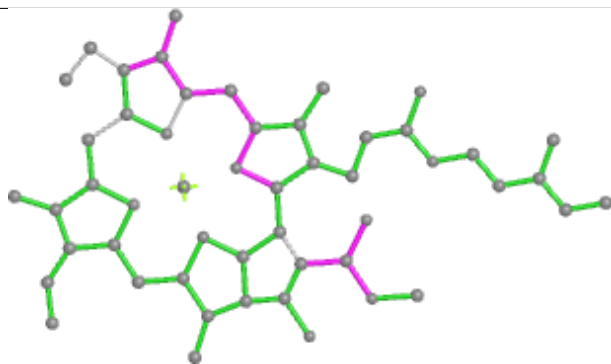


Rings

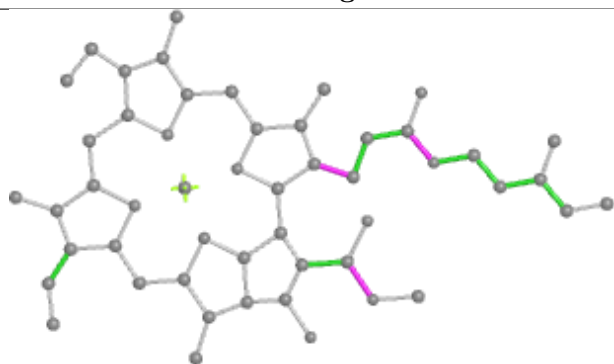
Ligand CLA k 601



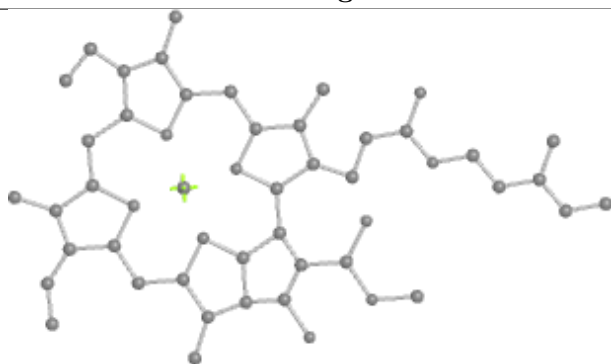
Bond lengths



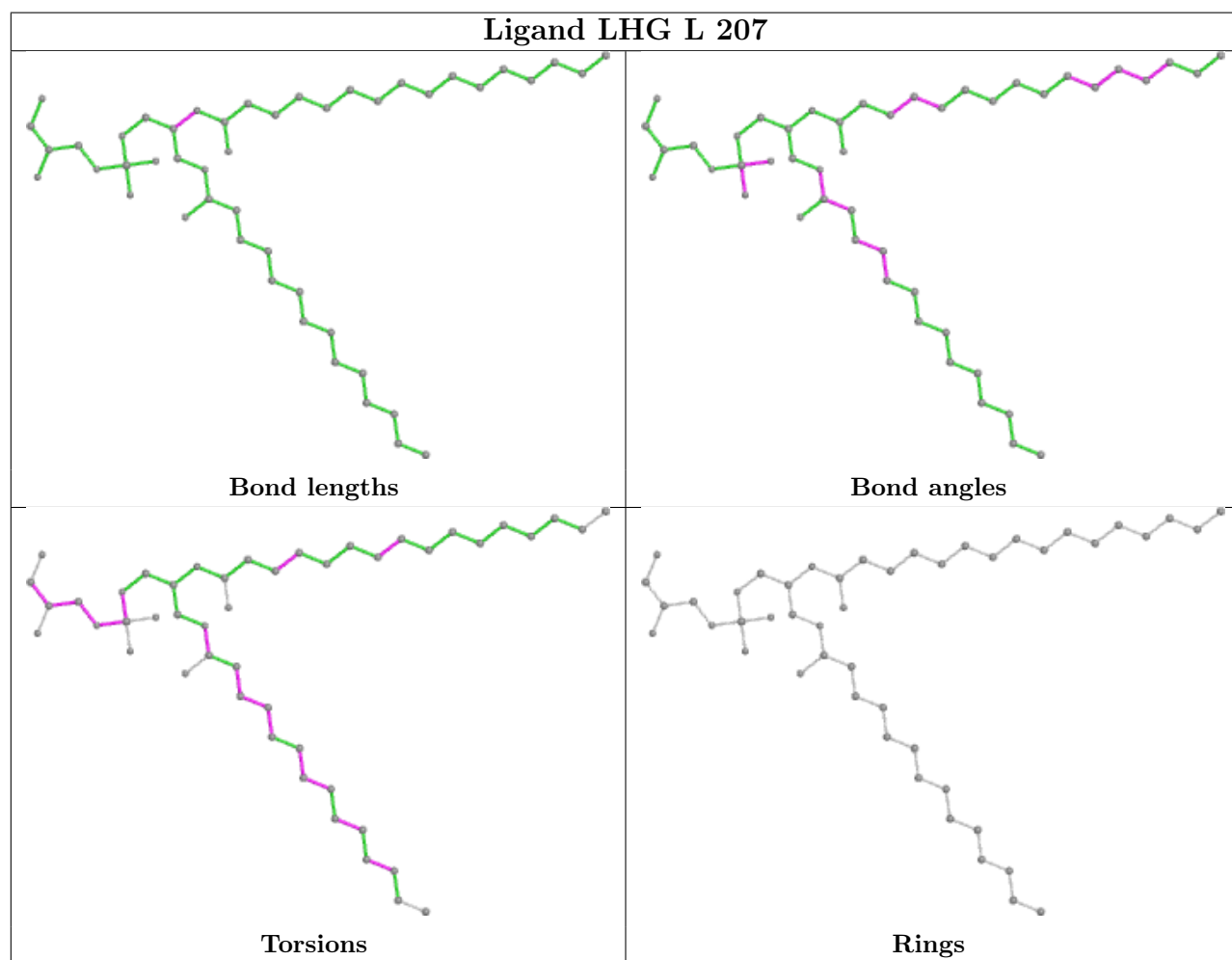
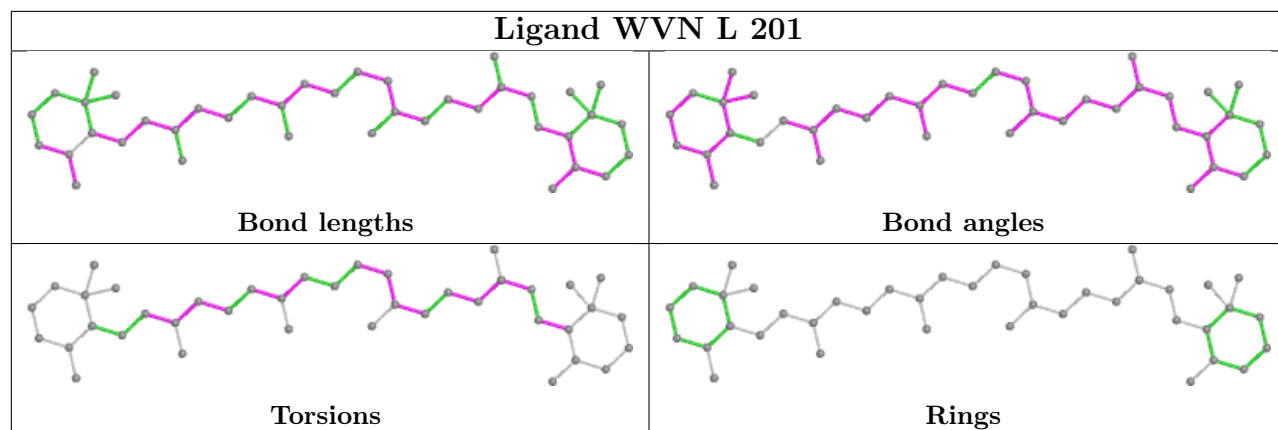
Bond angles



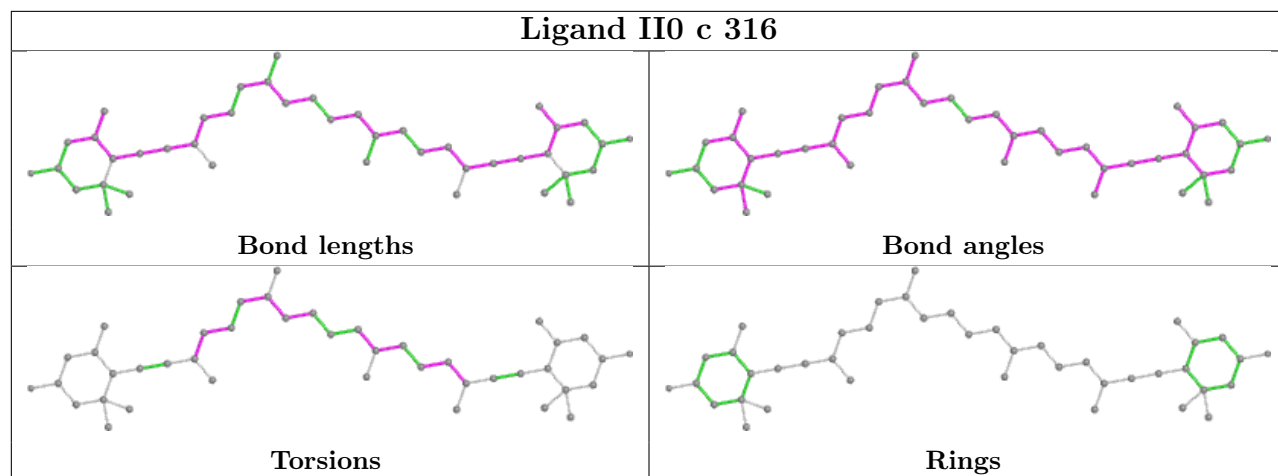
Torsions



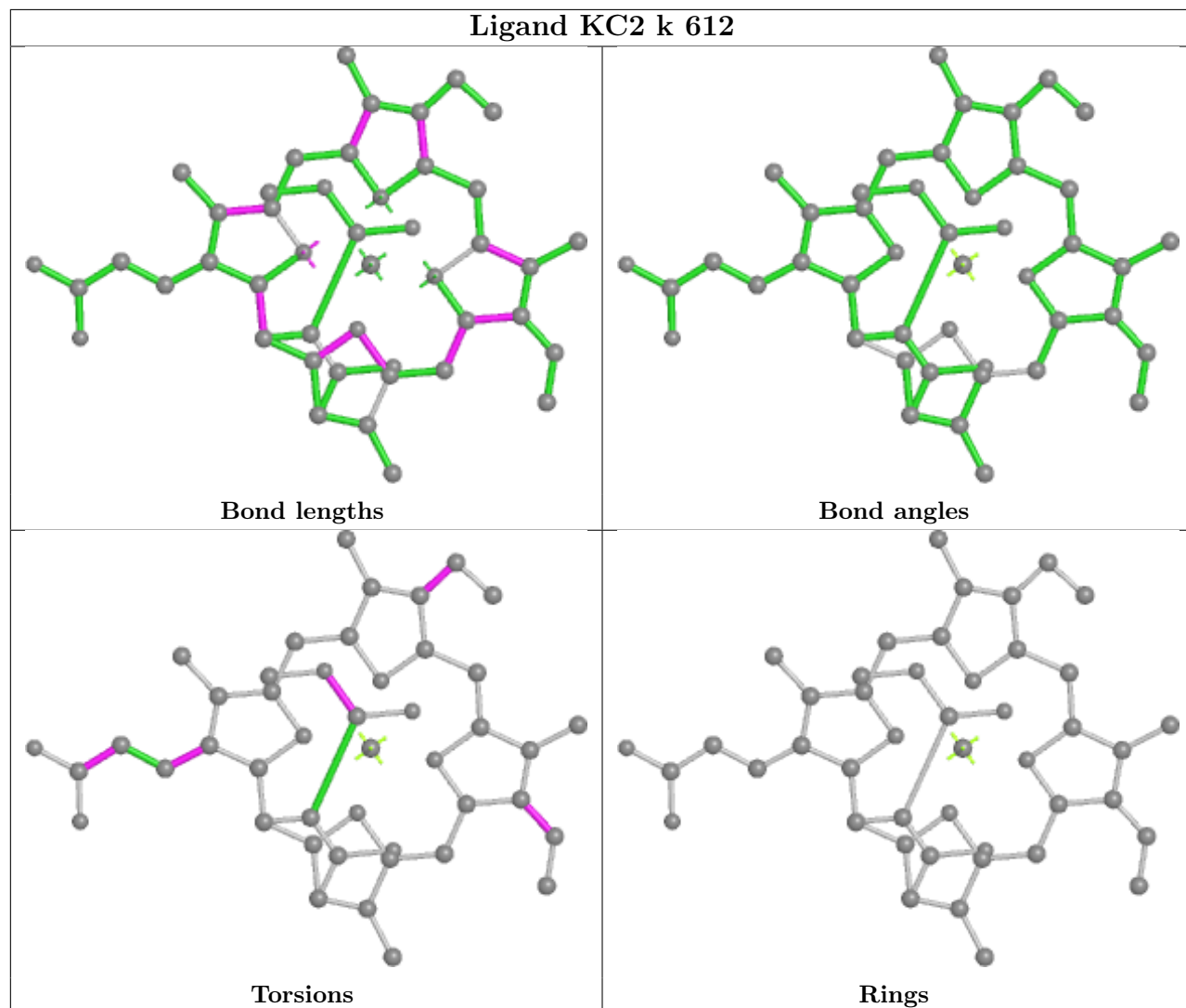
Rings



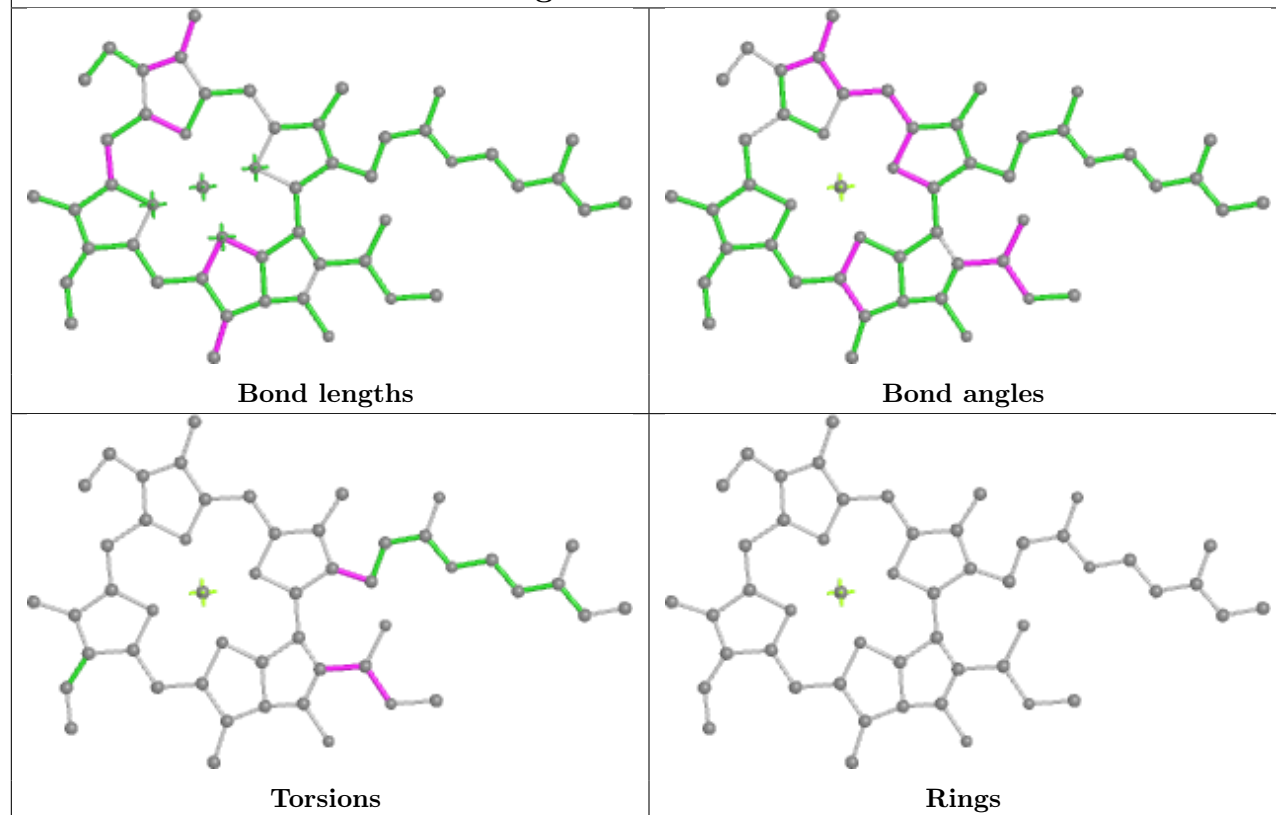
Ligand II0 c 316



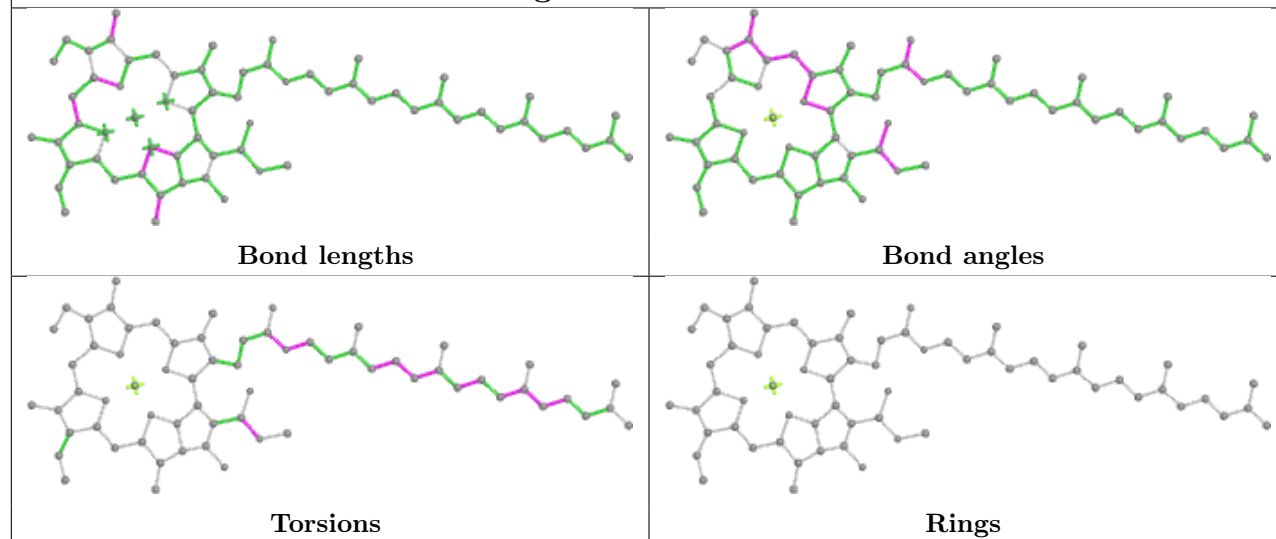
Ligand KC2 k 612



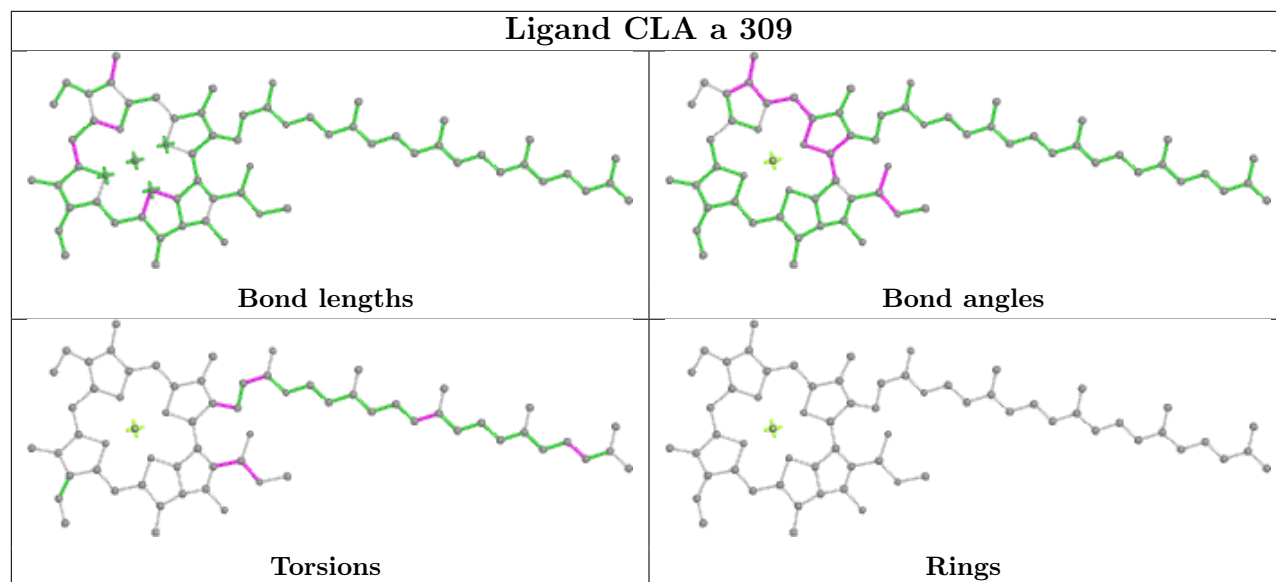
Ligand CLA d 306



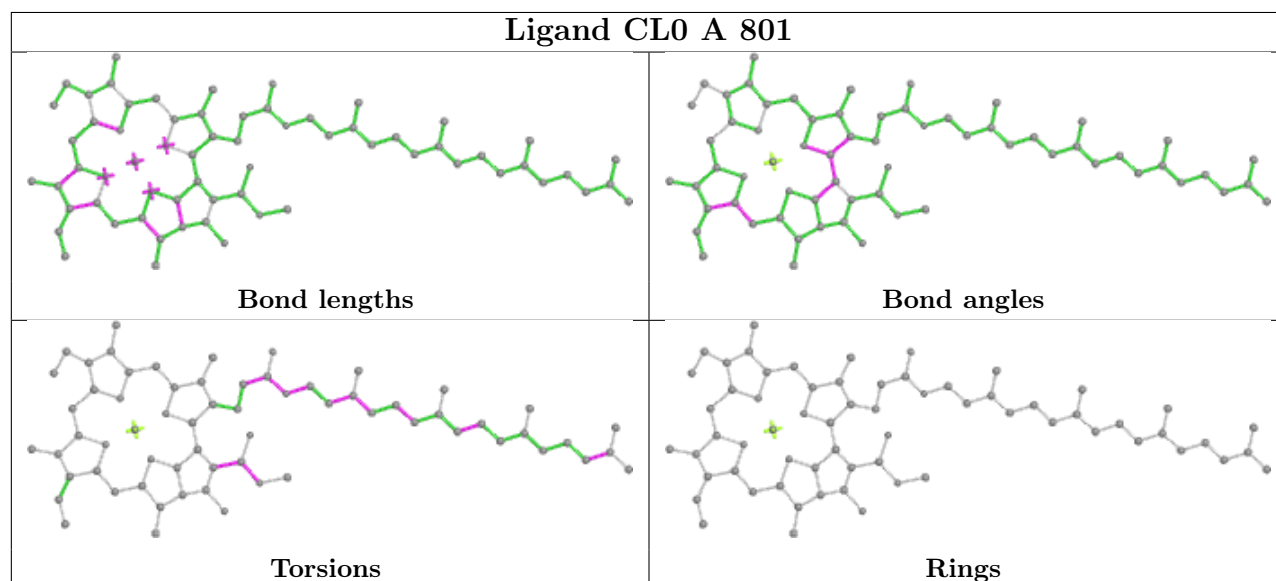
Ligand CLA F 201



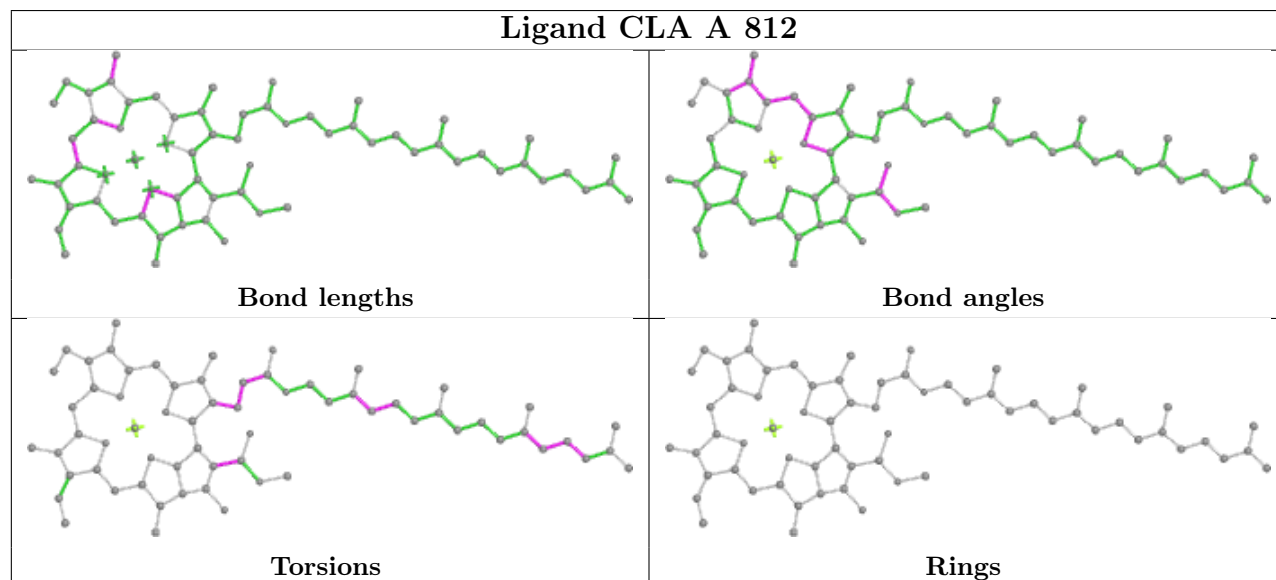
Ligand CLA a 309



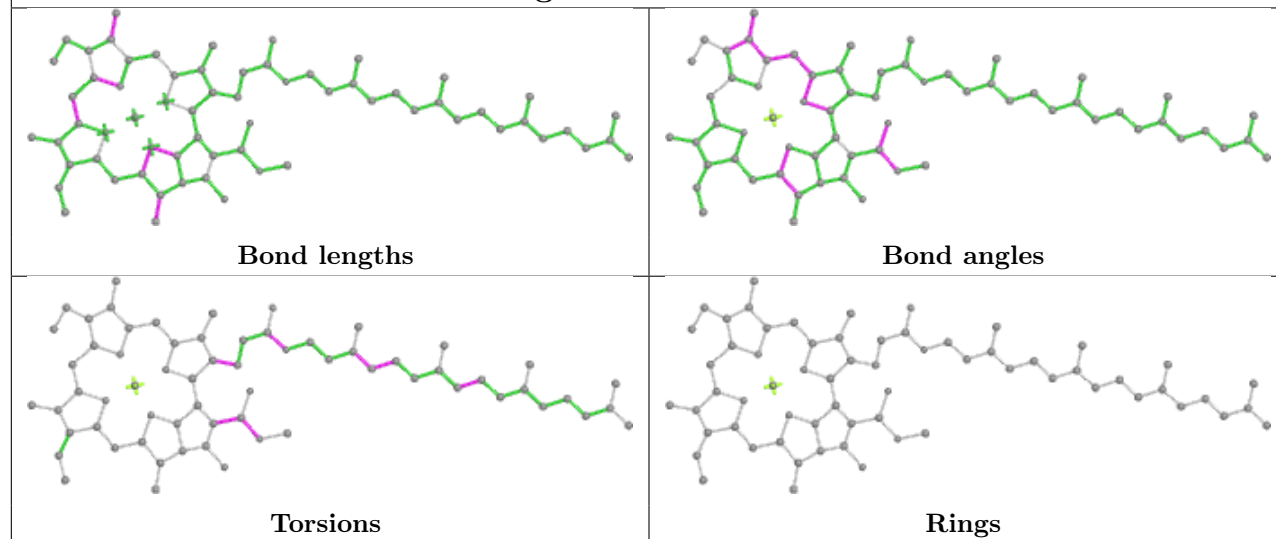
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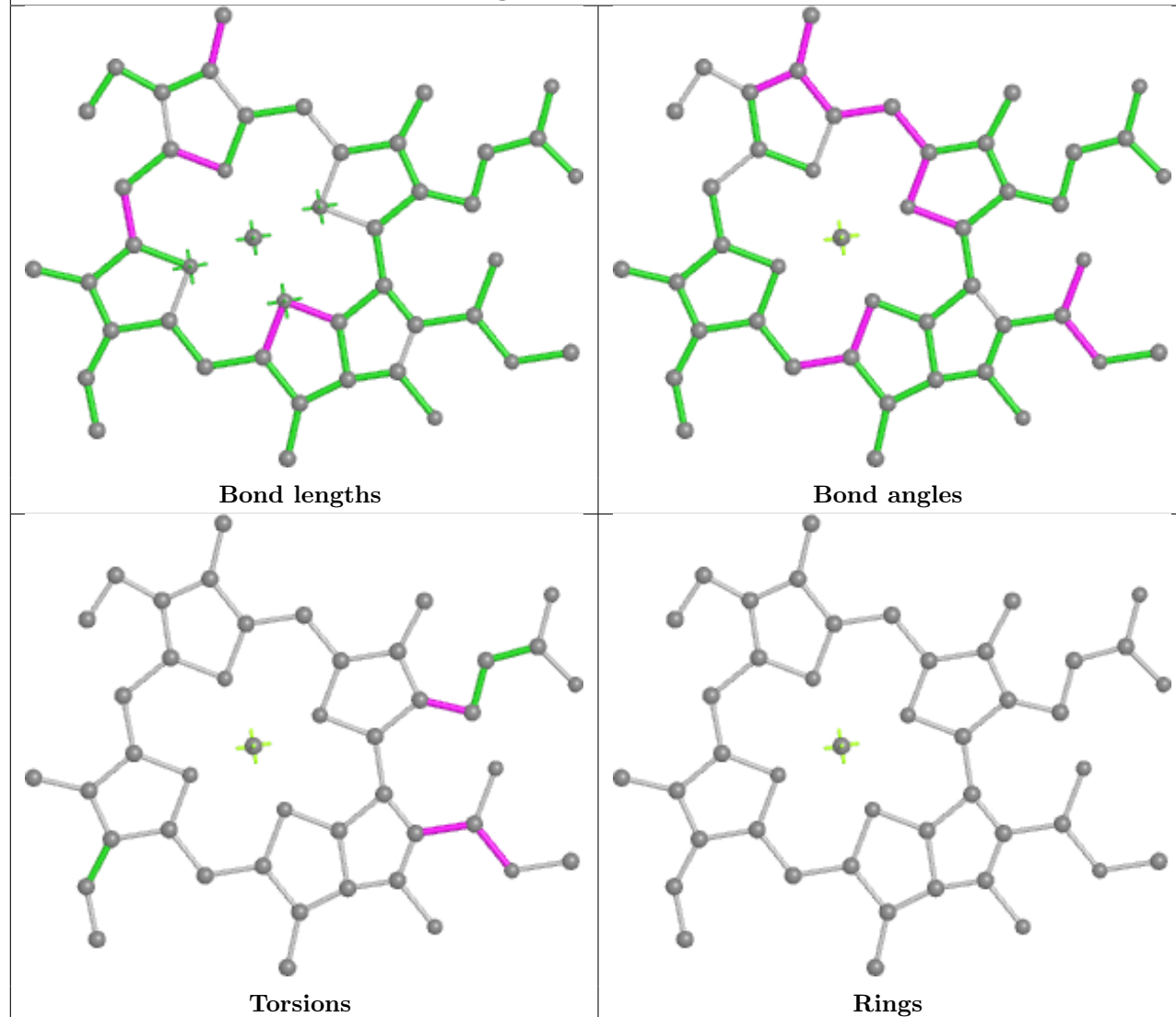
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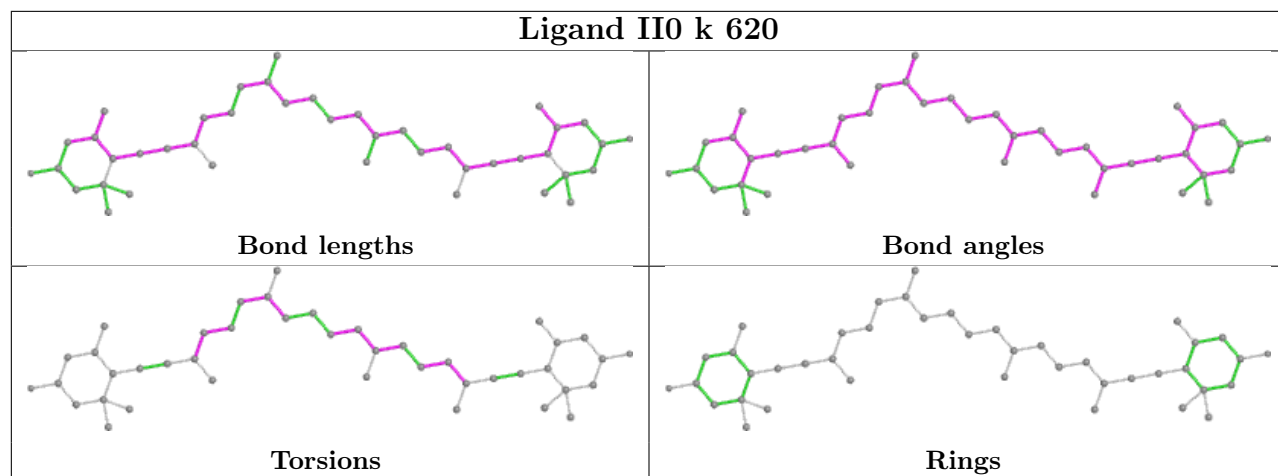
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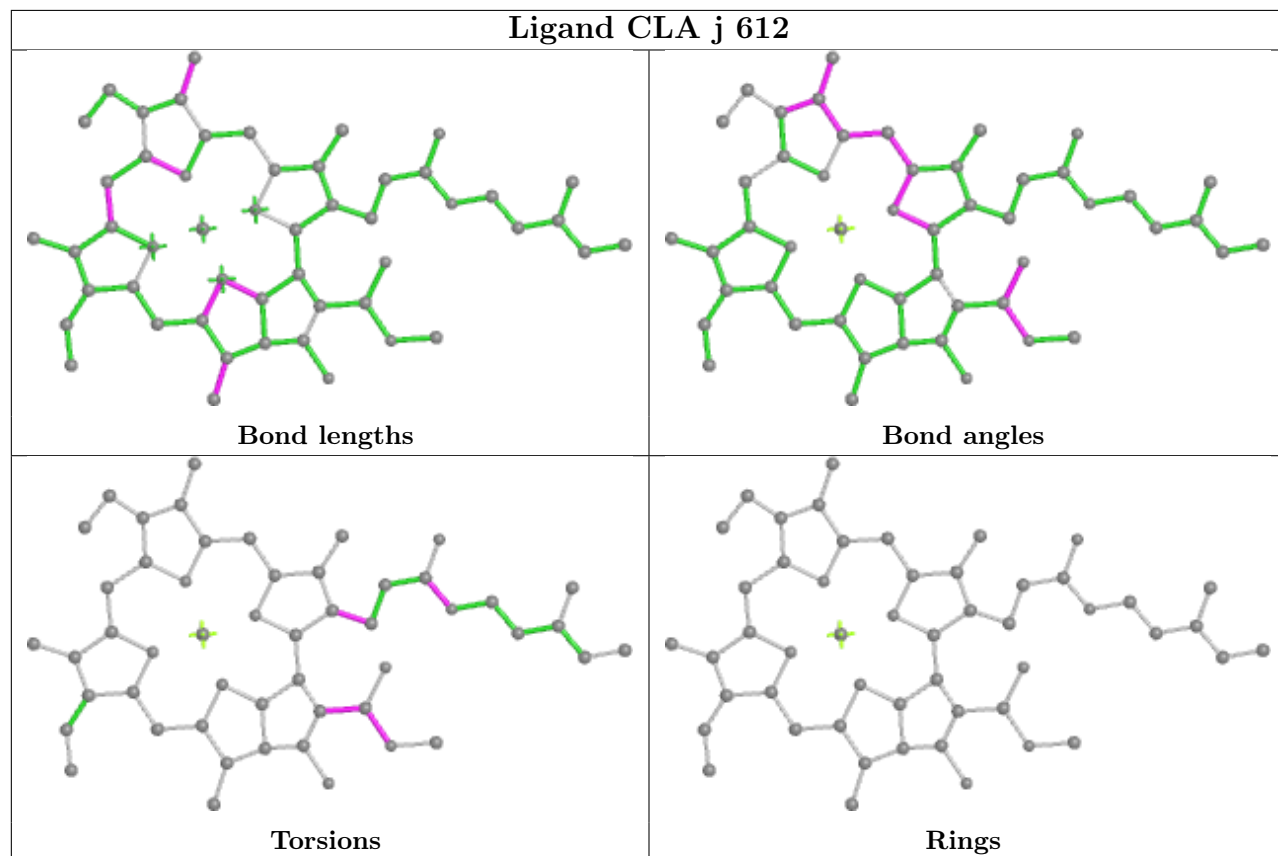
Ligand CLA a 305



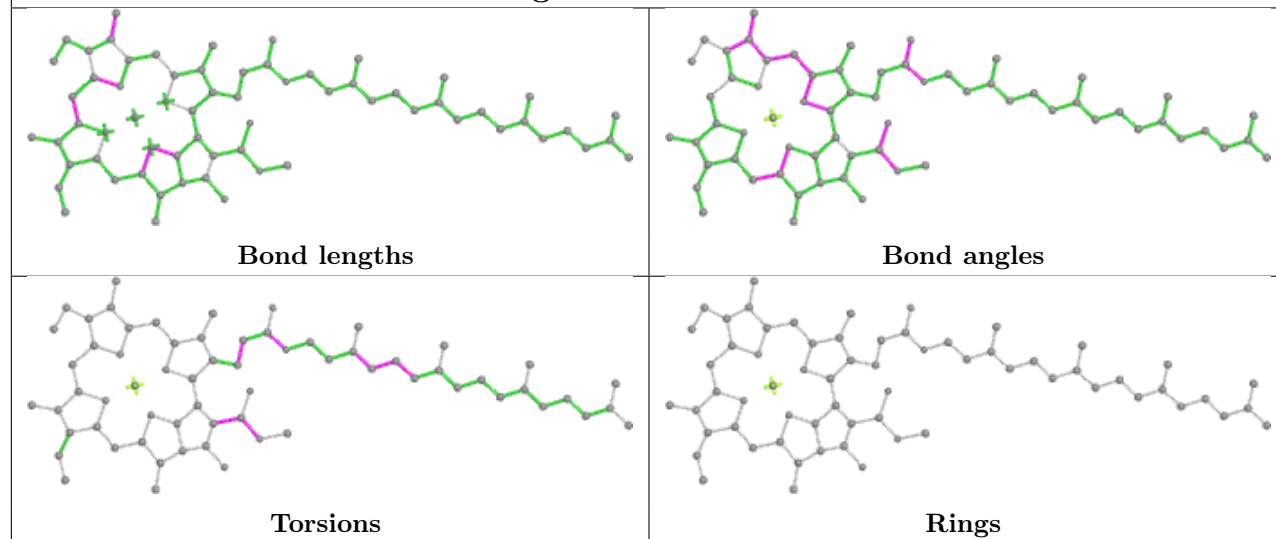
Ligand II0 k 620



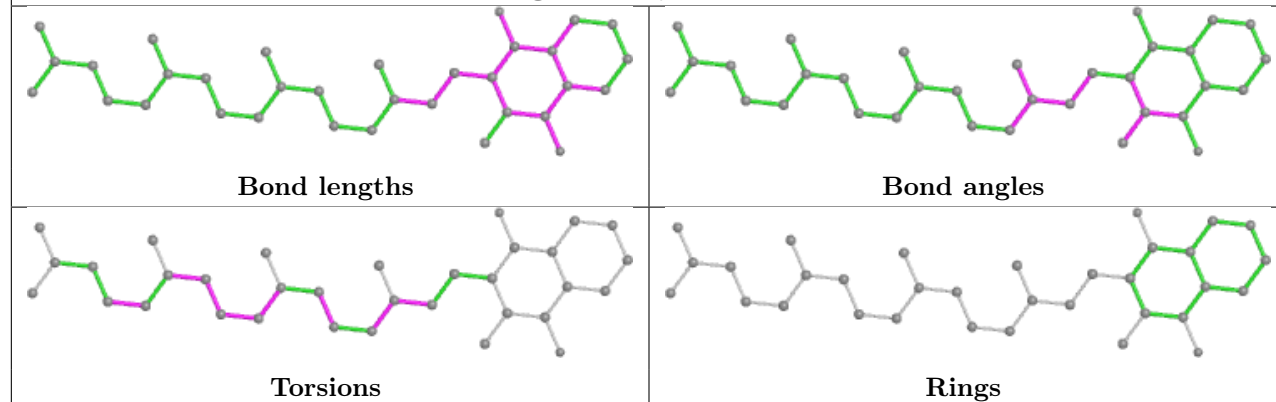
Ligand CLA j 612



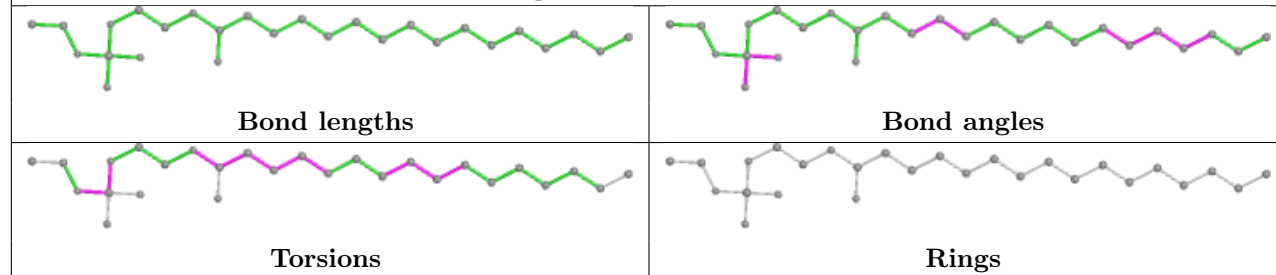
Ligand CLA B 802



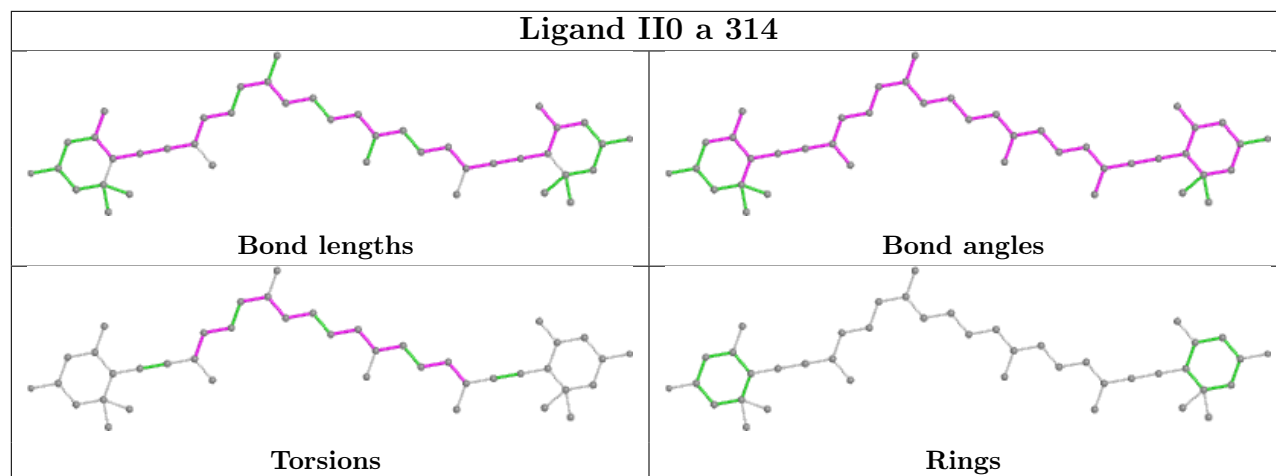
Ligand PQN A 842



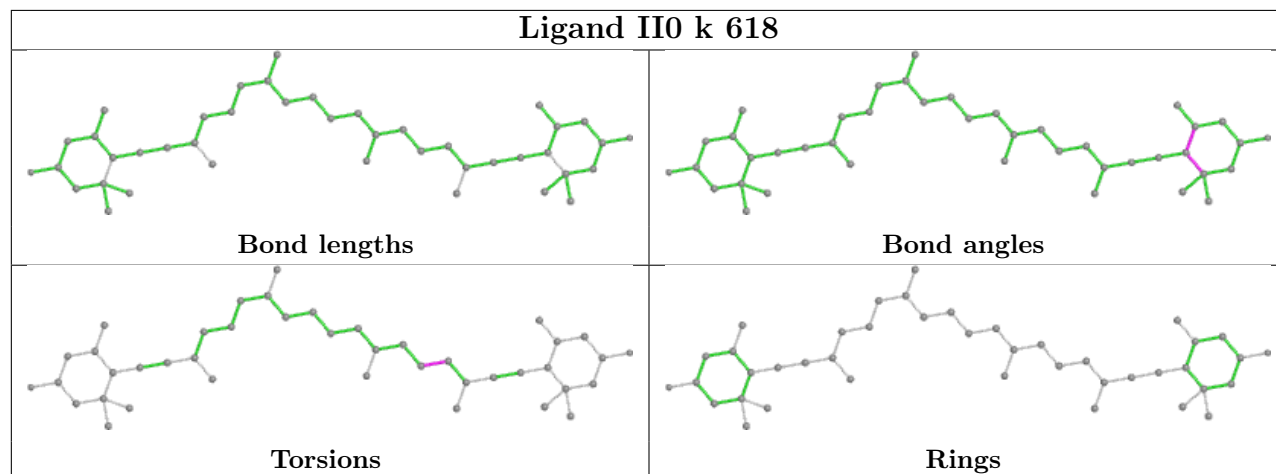
Ligand LHG A 849



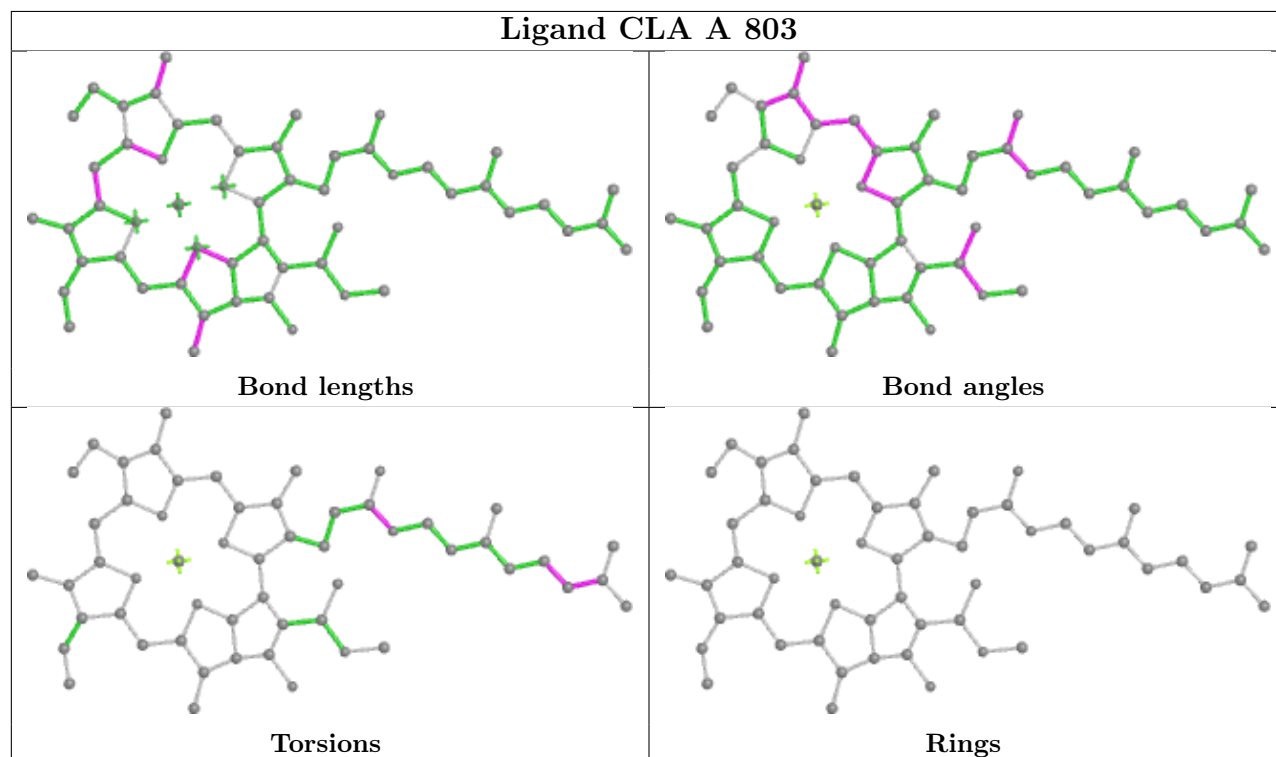
Ligand II0 a 314



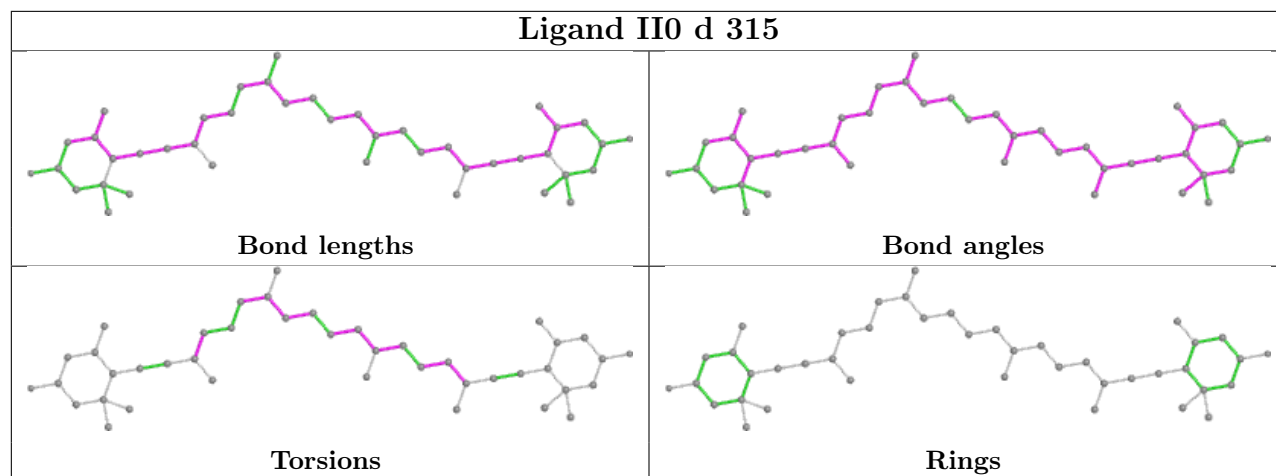
Ligand II0 k 618



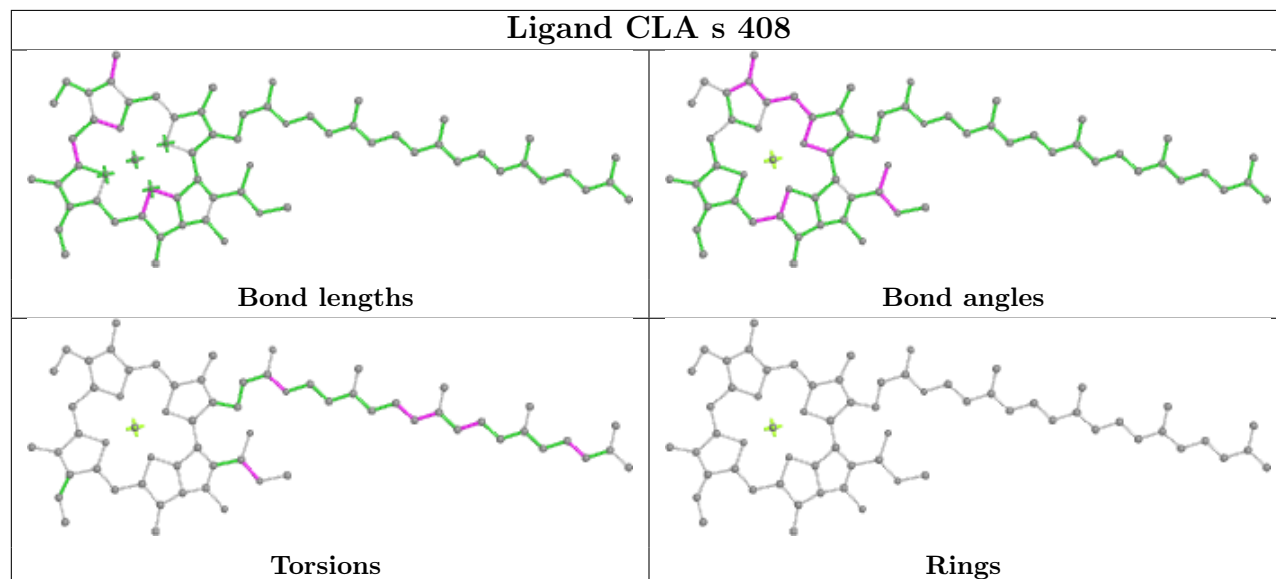
Ligand CLA A 803



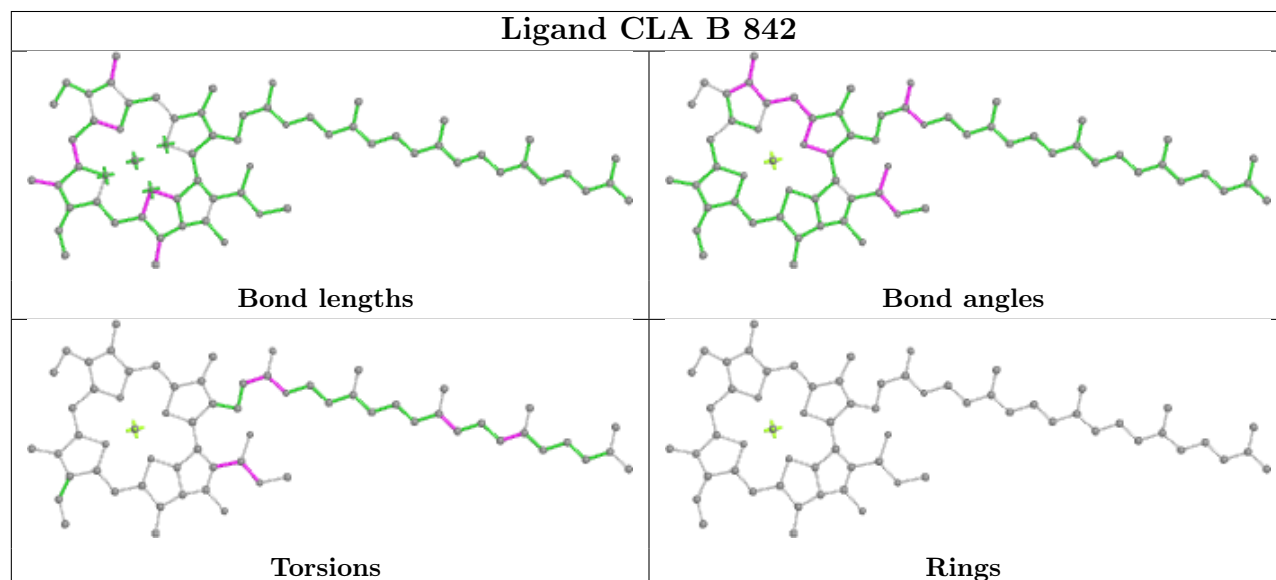
Ligand II0 d 315



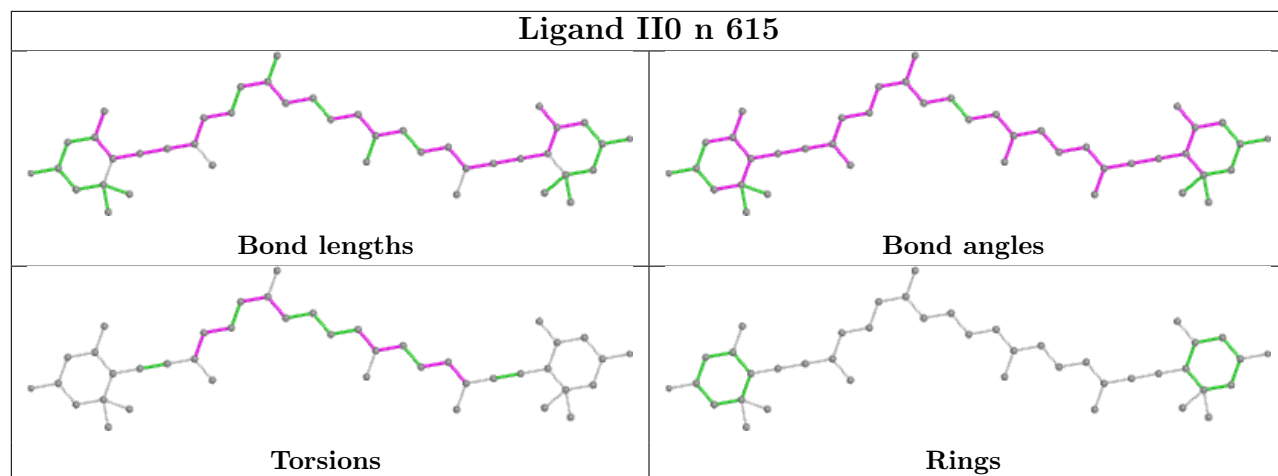
Ligand CLA s 408



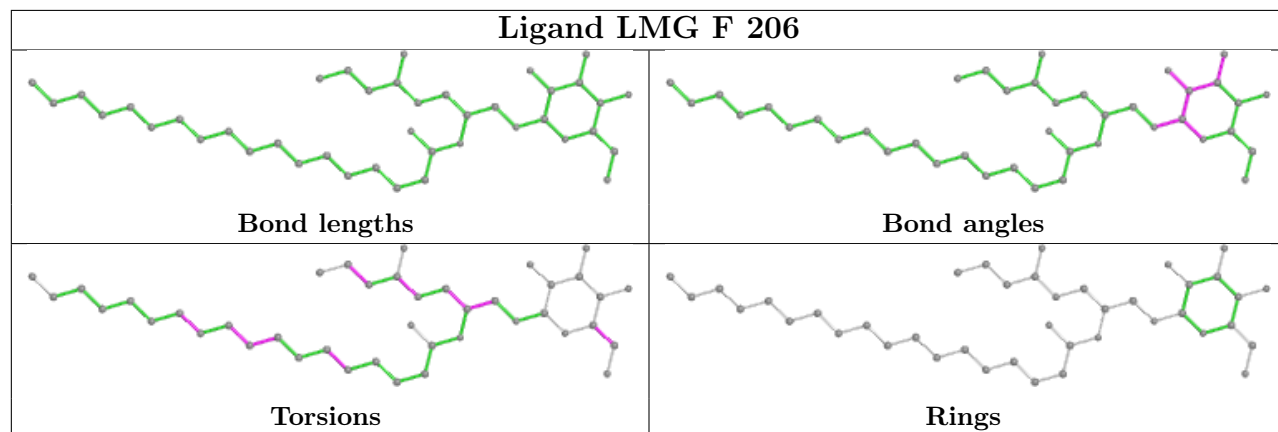
Ligand CLA B 842



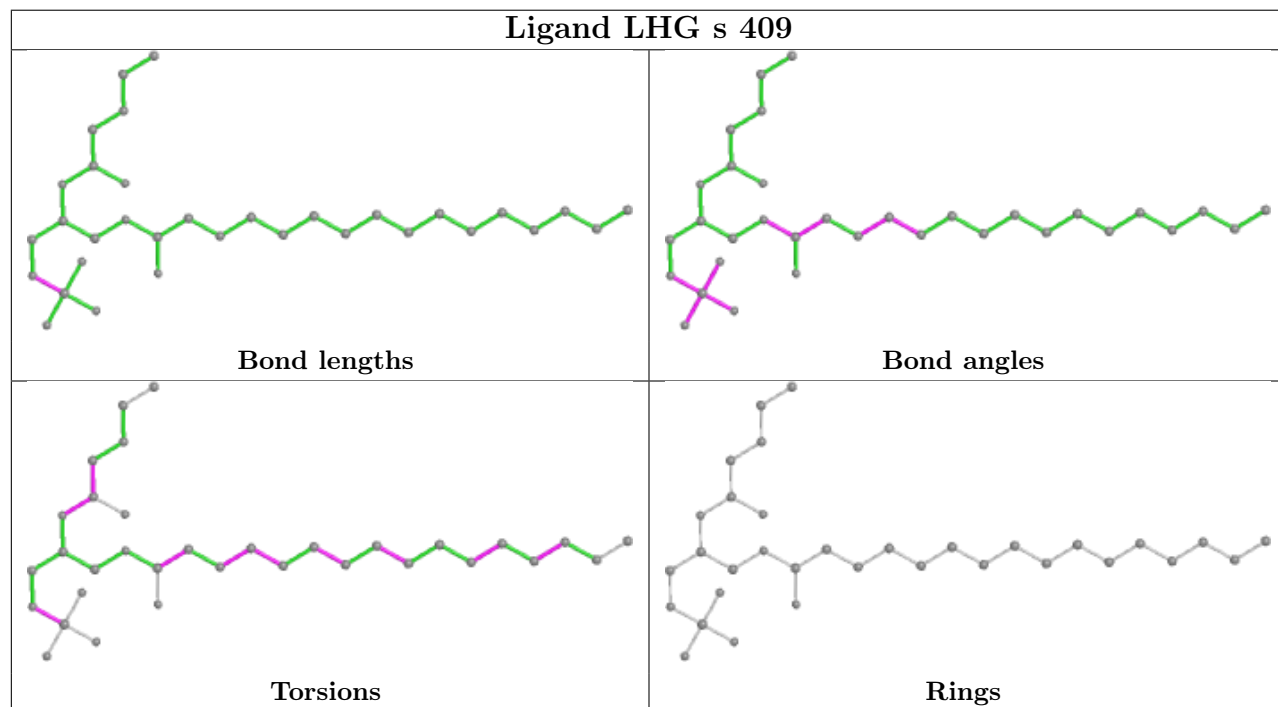
Ligand II0 n 615

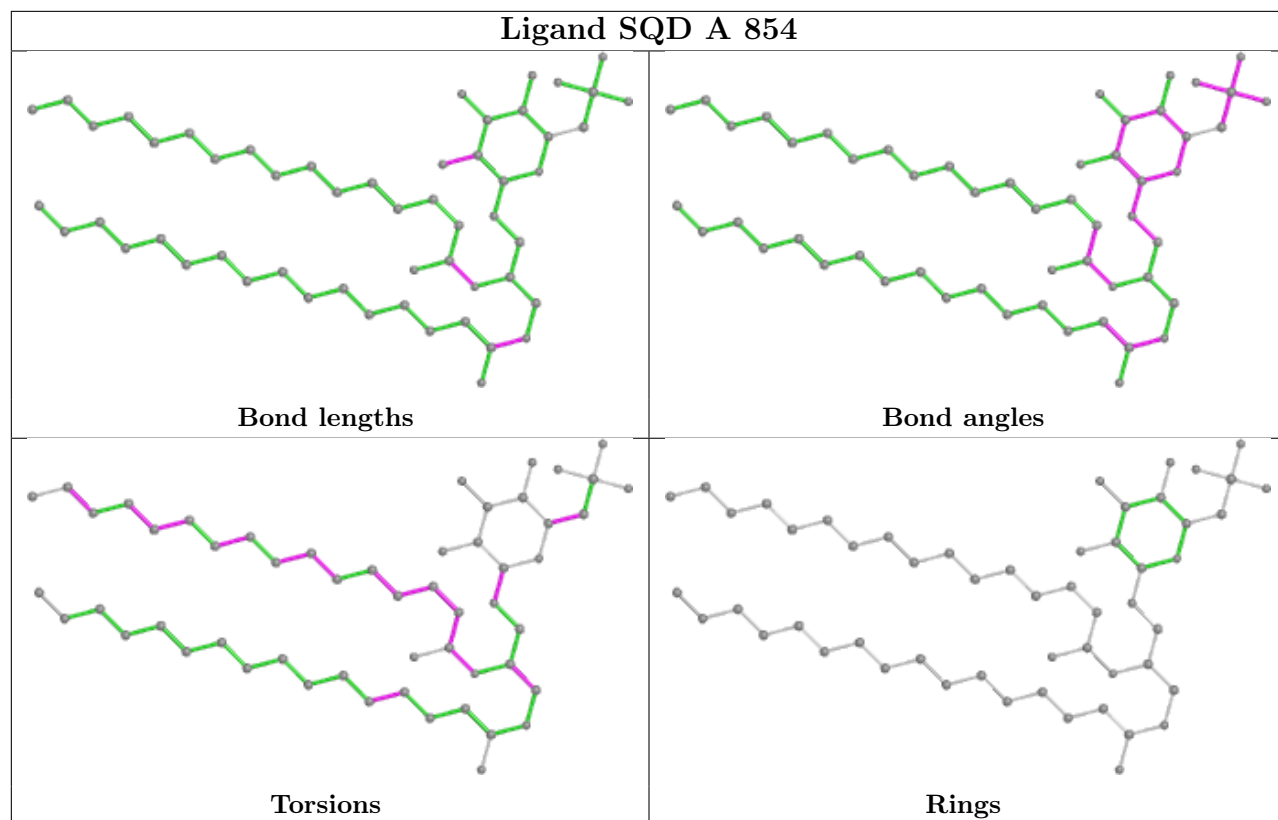


Ligand LMG F 206

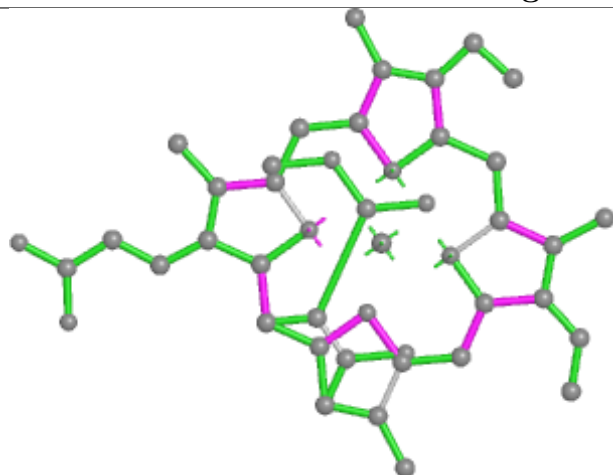


Ligand LHG s 409

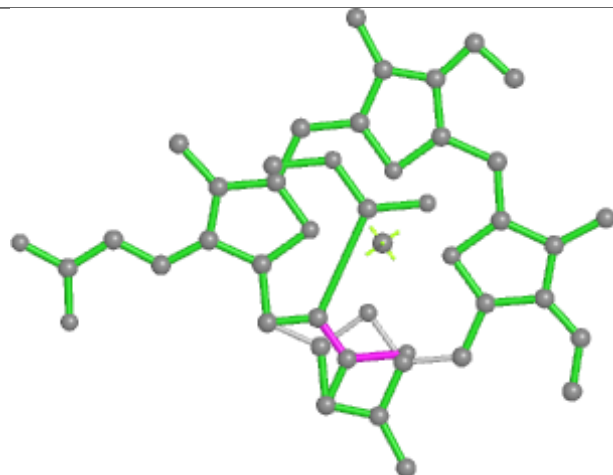




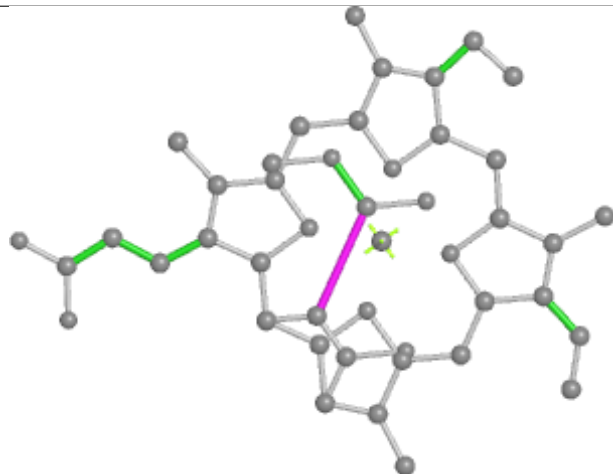
Ligand KC2 s 404



Bond lengths



Bond angles

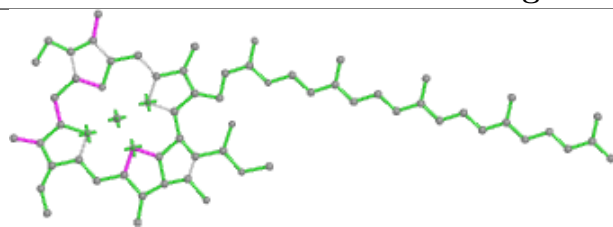


Torsions

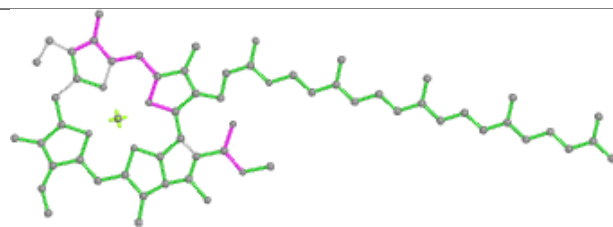


Rings

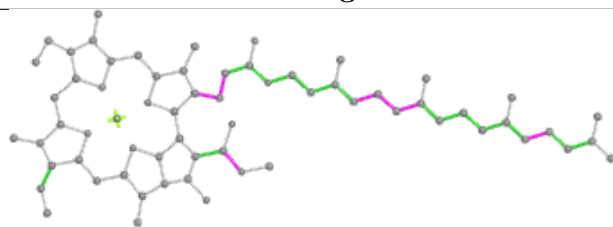
Ligand CLA i 307



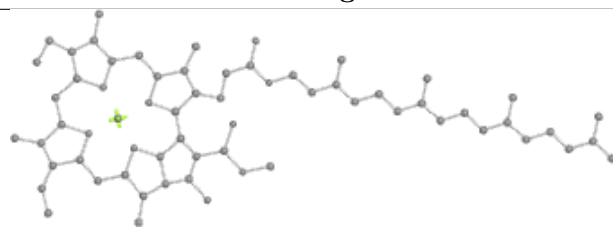
Bond lengths



Bond angles

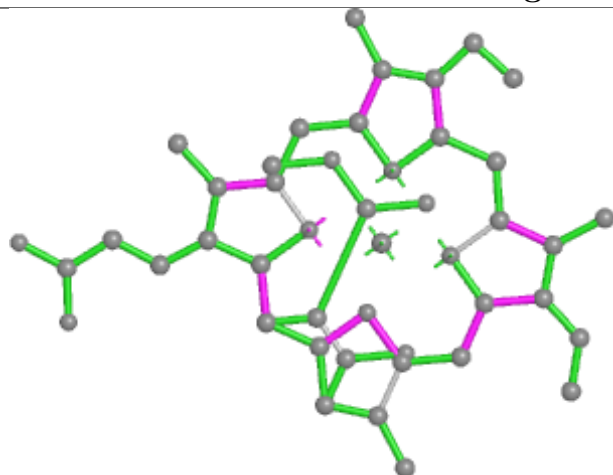


Torsions

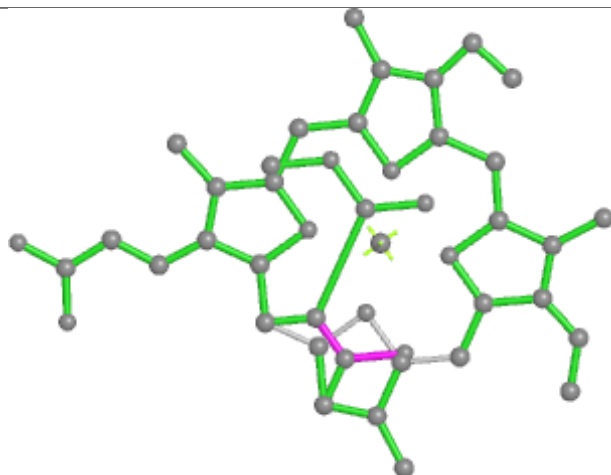


Rings

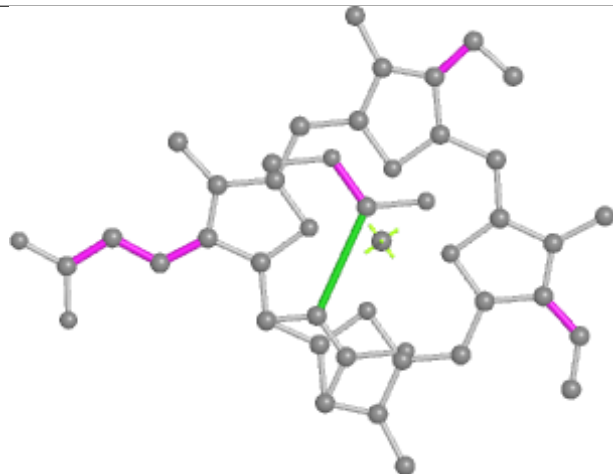
Ligand KC2 i 318



Bond lengths



Bond angles

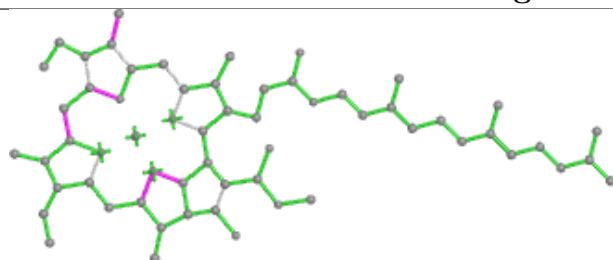


Torsions

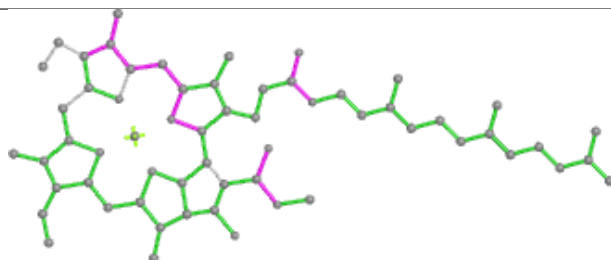


Rings

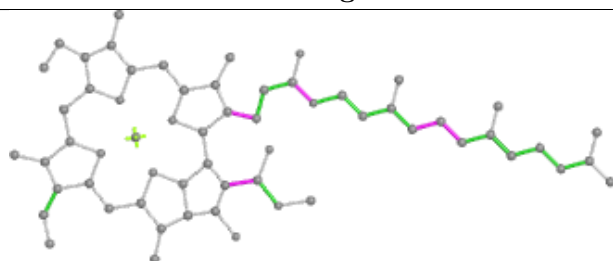
Ligand CLA A 834



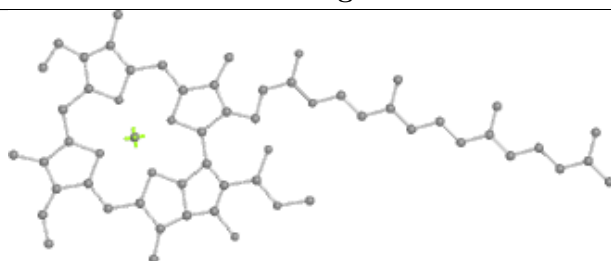
Bond lengths



Bond angles

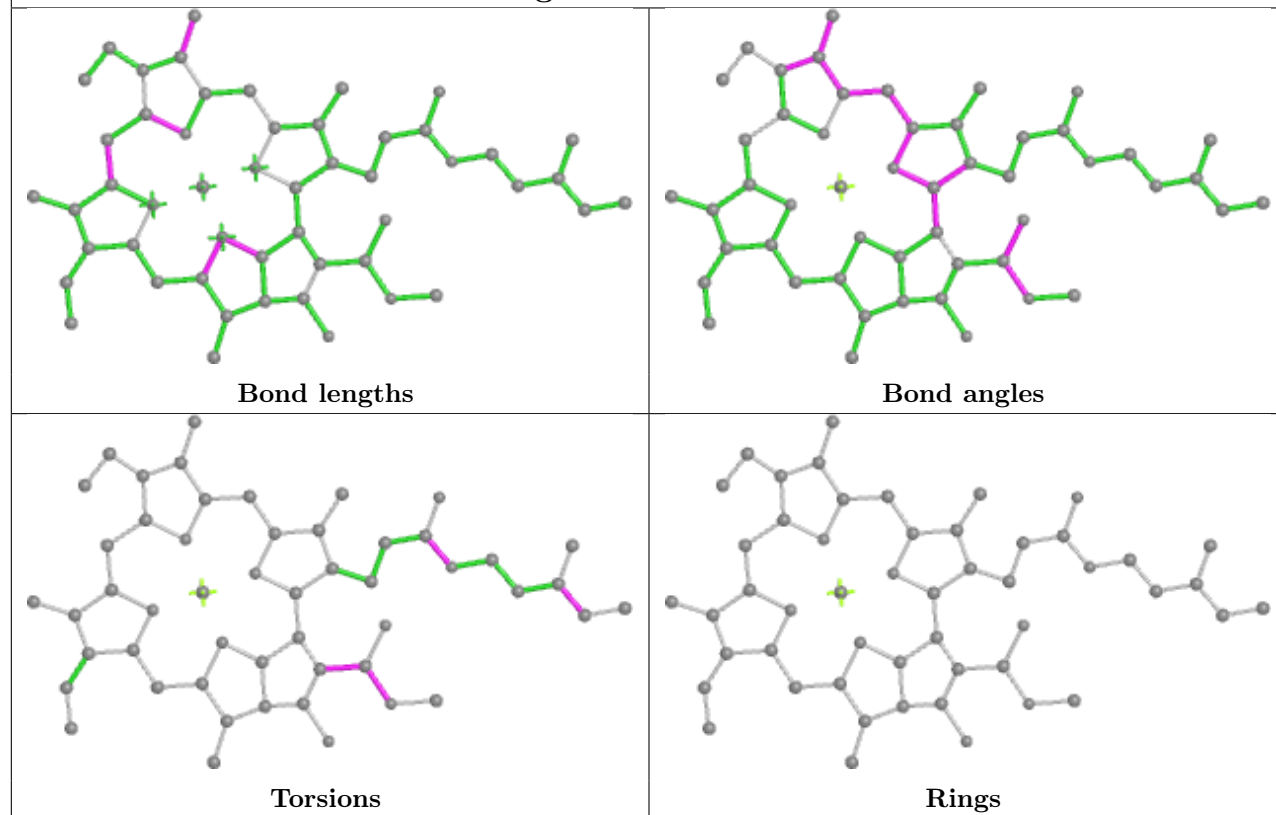


Torsions

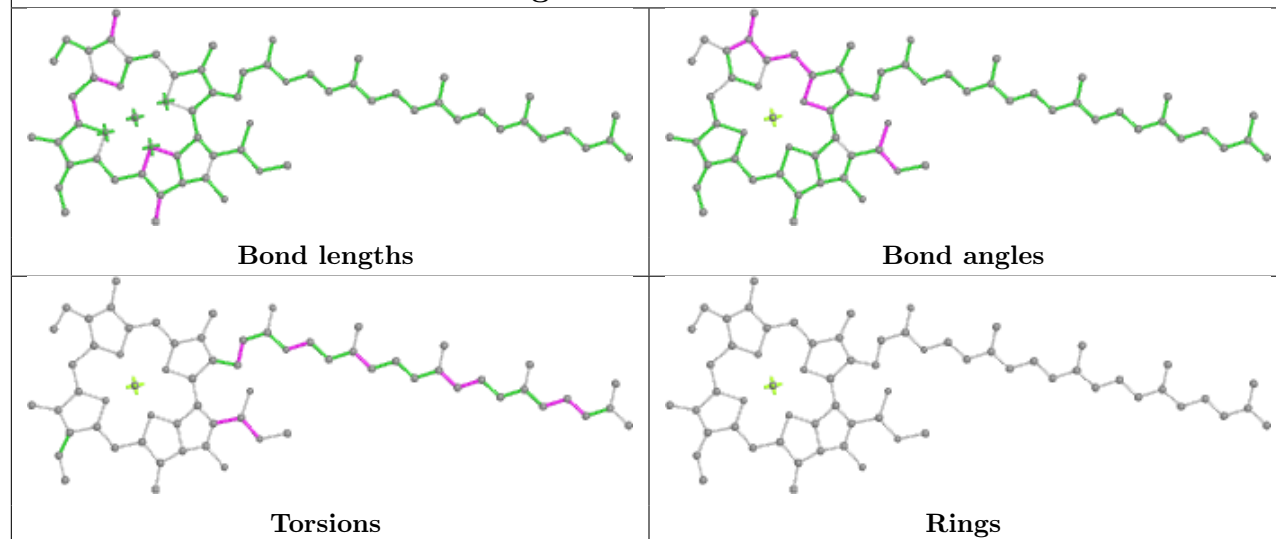


Rings

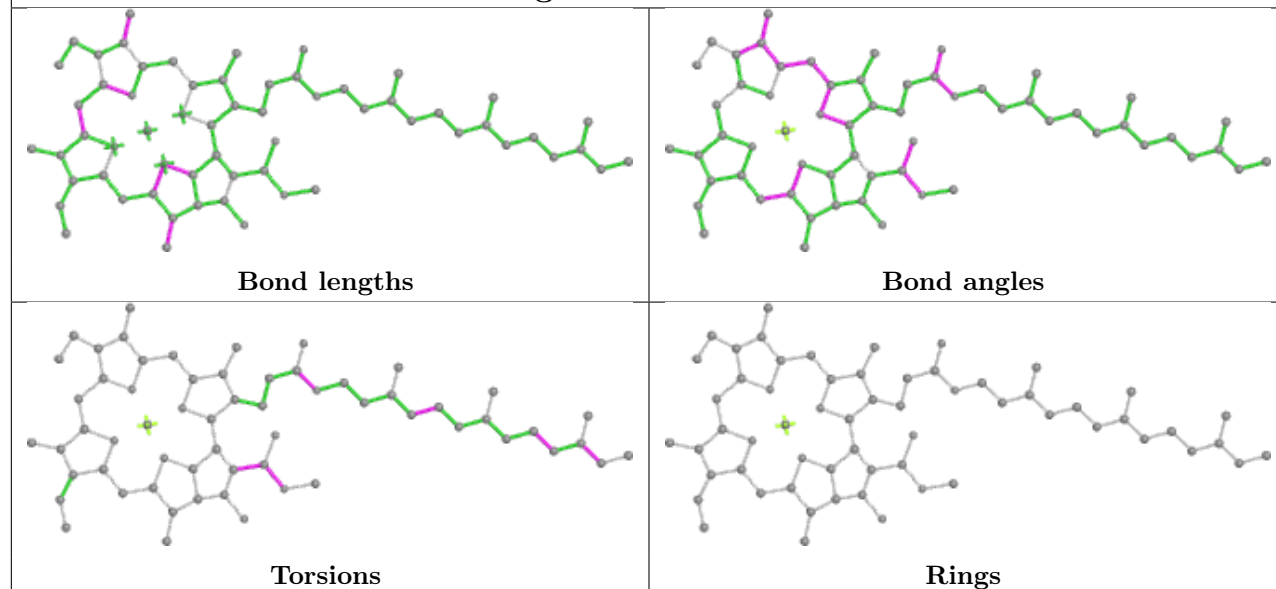
Ligand CLA d 303



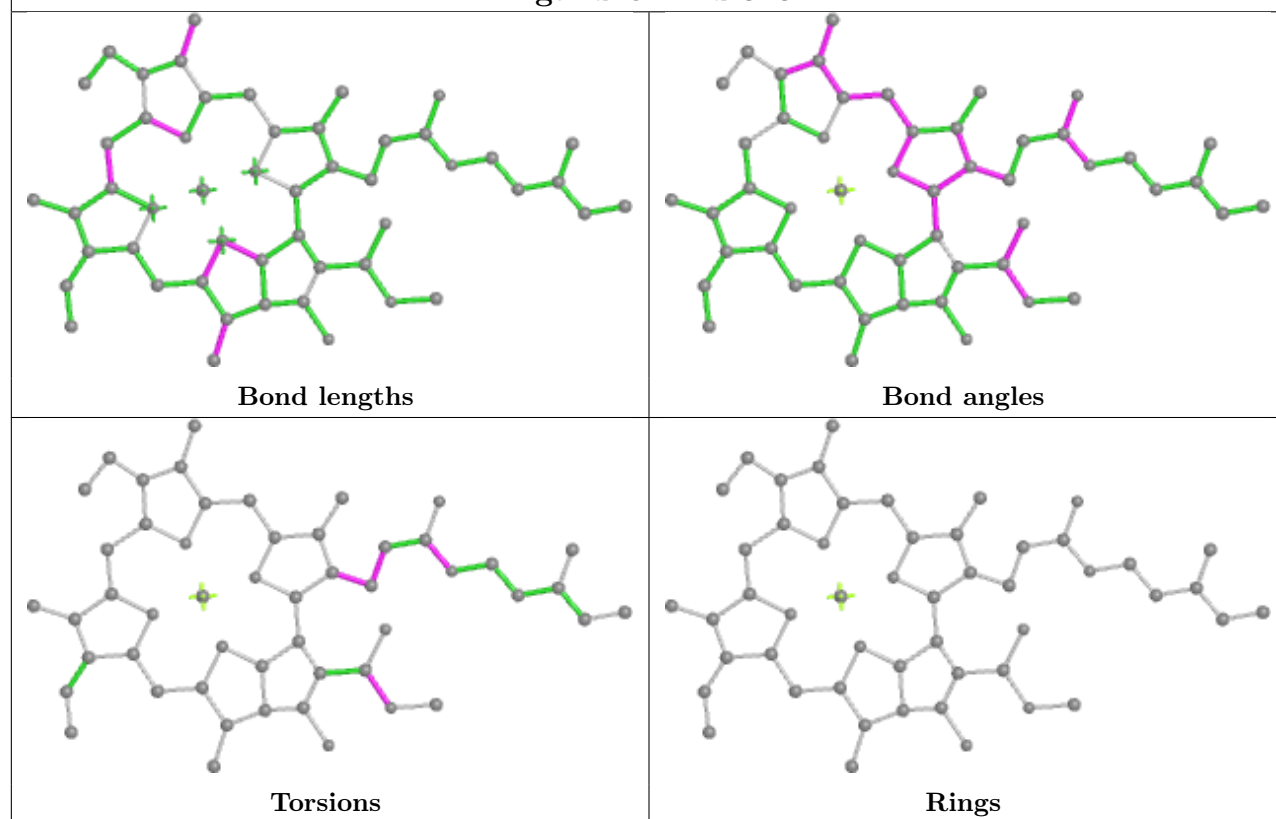
Ligand CLA A 852



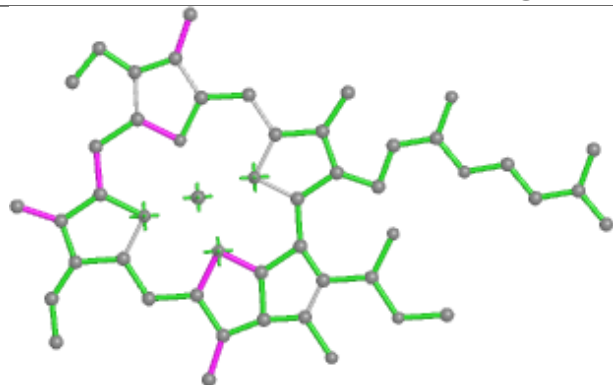
Ligand CLA b 307



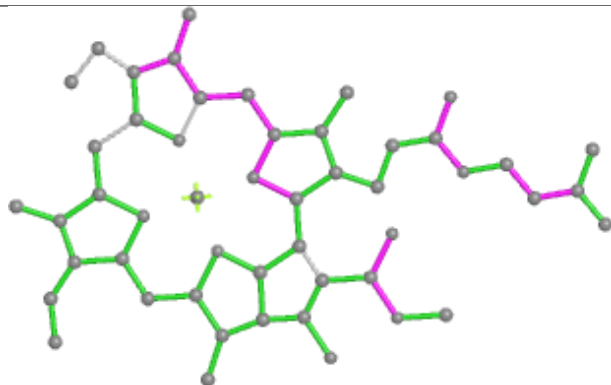
Ligand CLA d 313



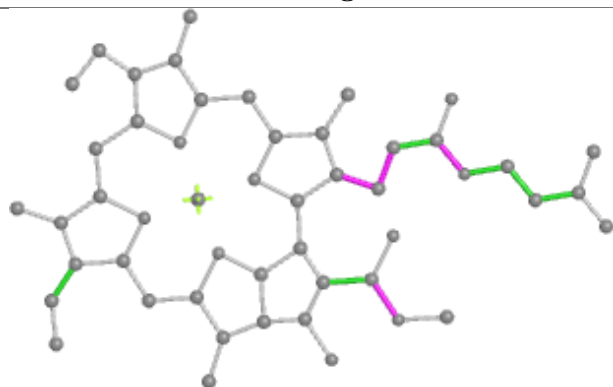
Ligand CLA h 302



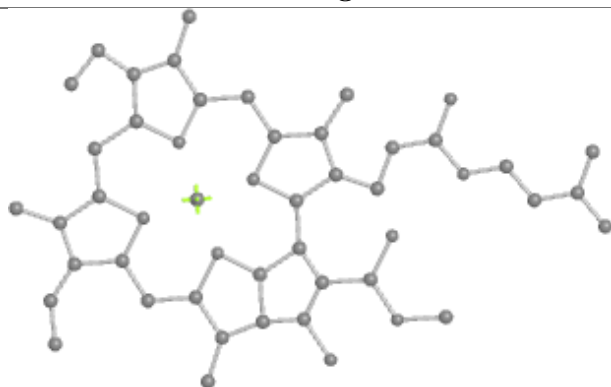
Bond lengths



Bond angles

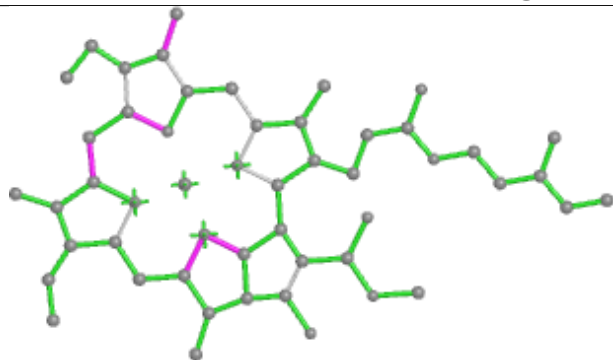


Torsions

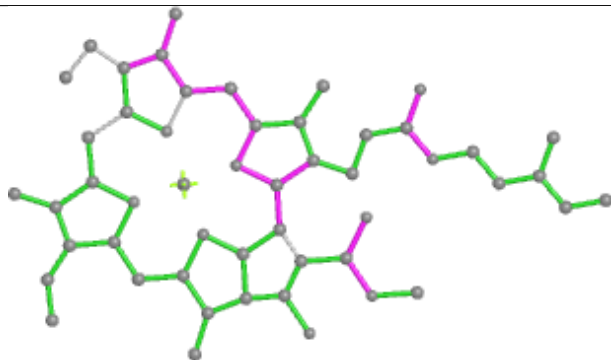


Rings

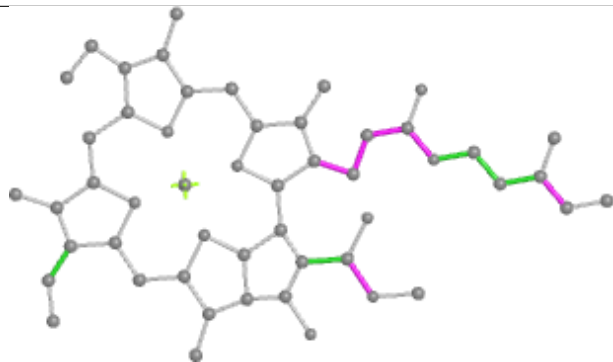
Ligand CLA k 610



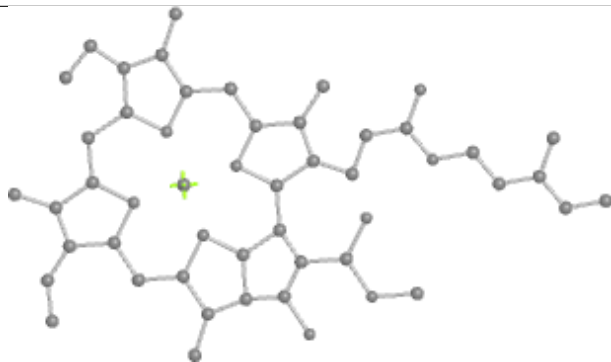
Bond lengths



Bond angles

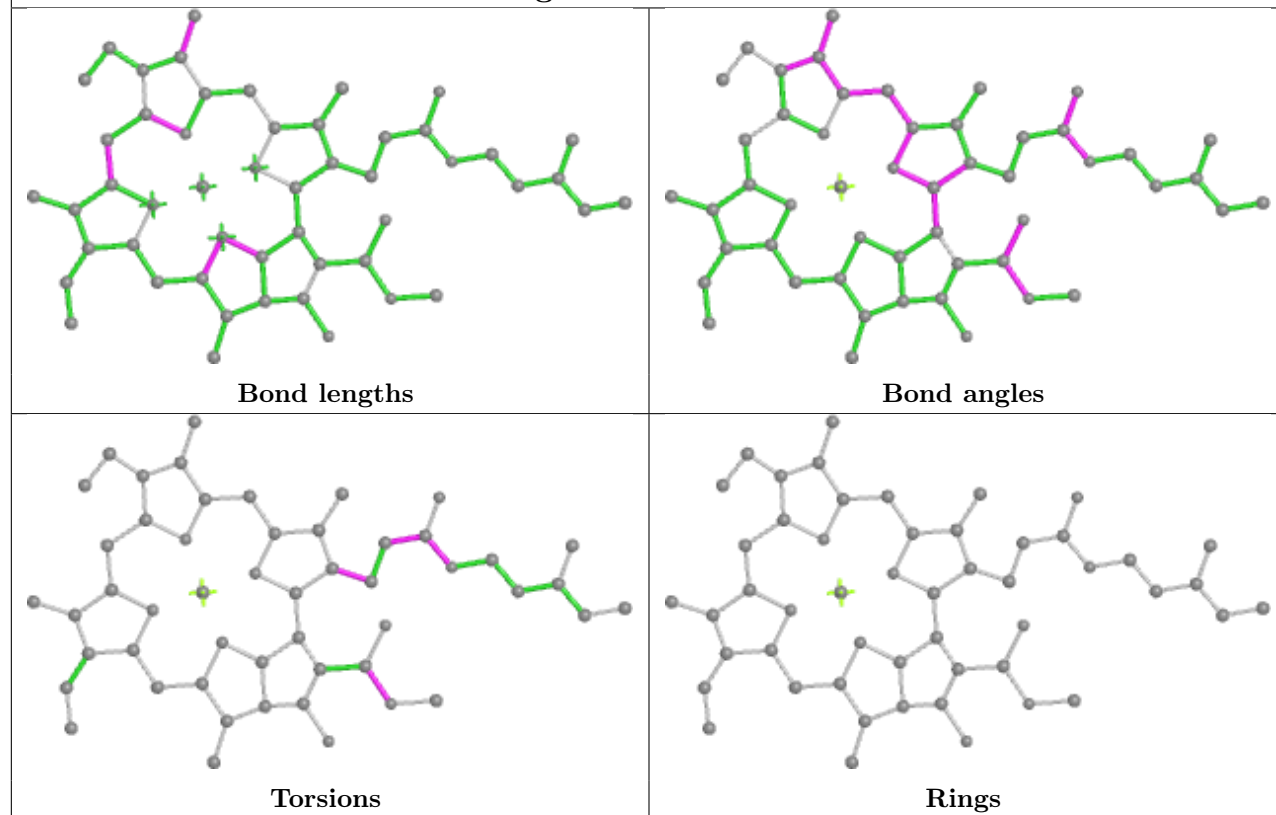


Torsions

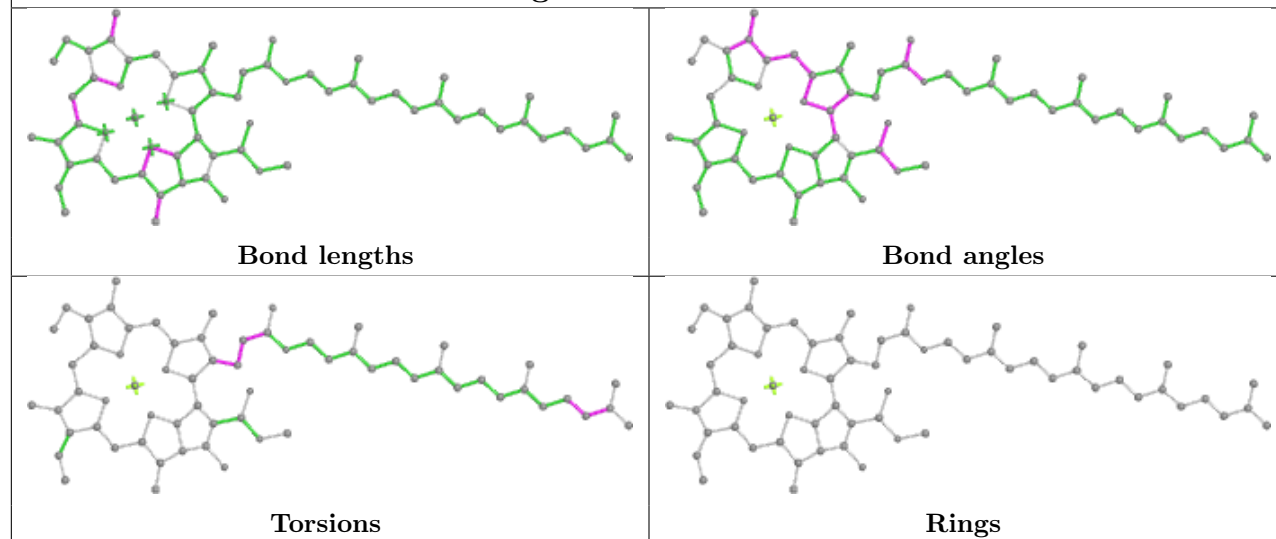


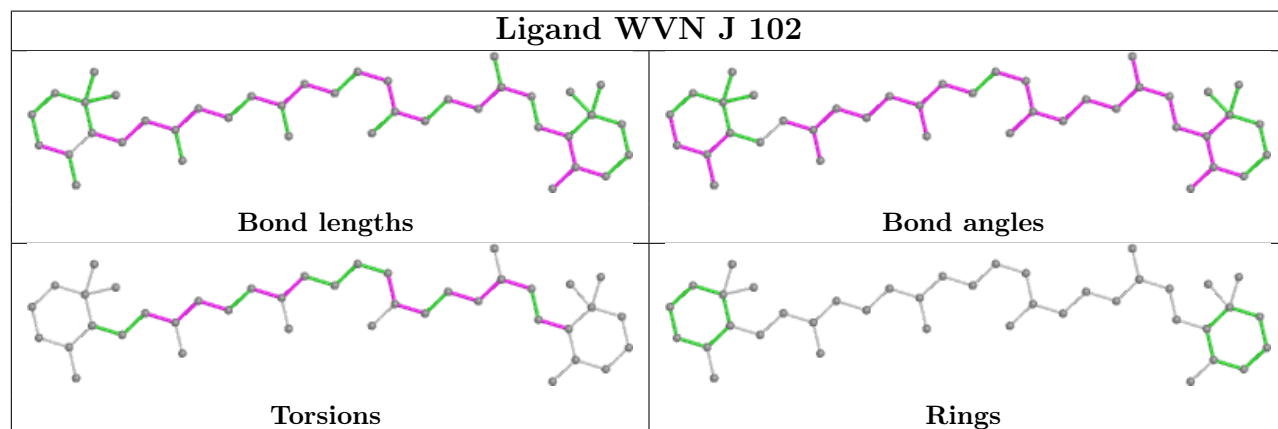
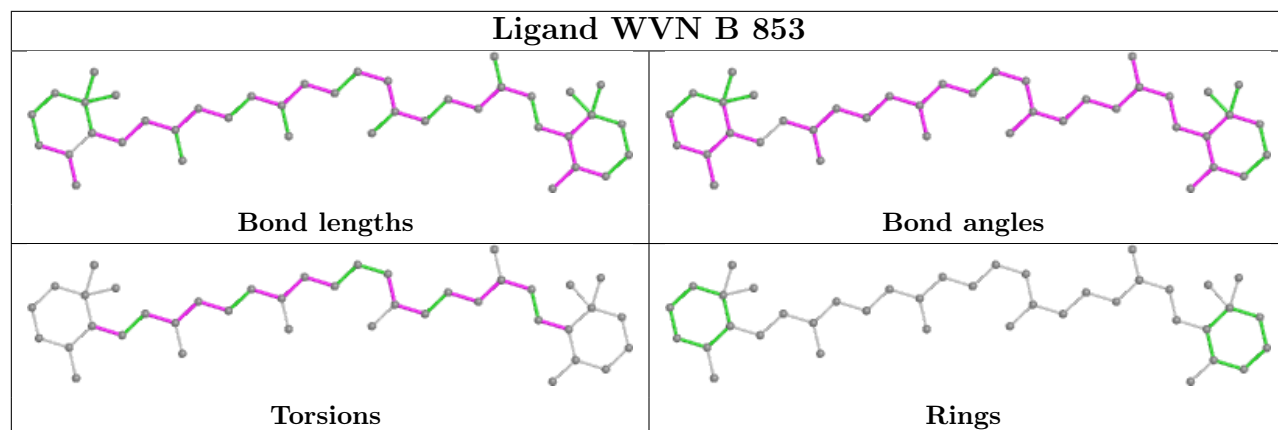
Rings

Ligand CLA h 308

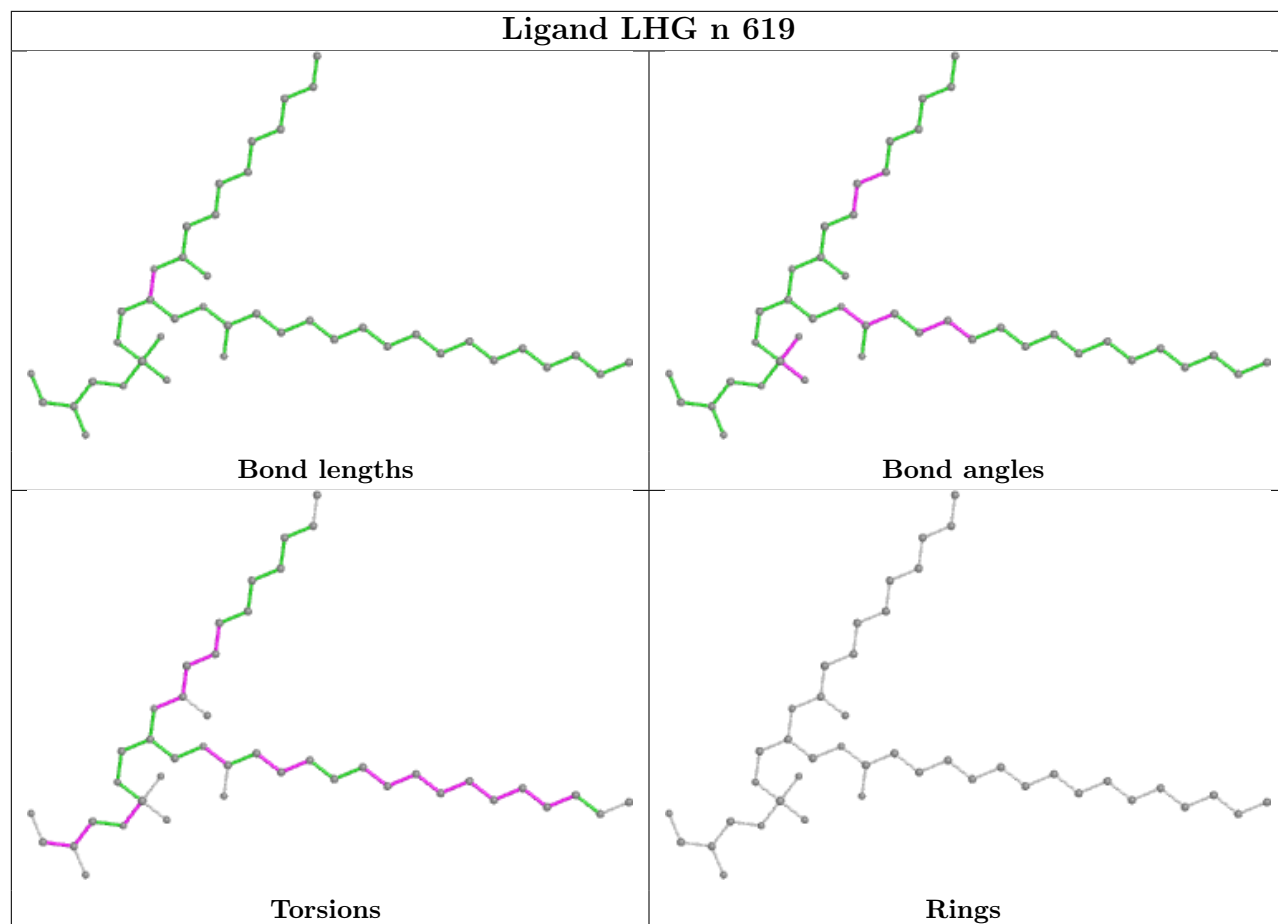


Ligand CLA A 808

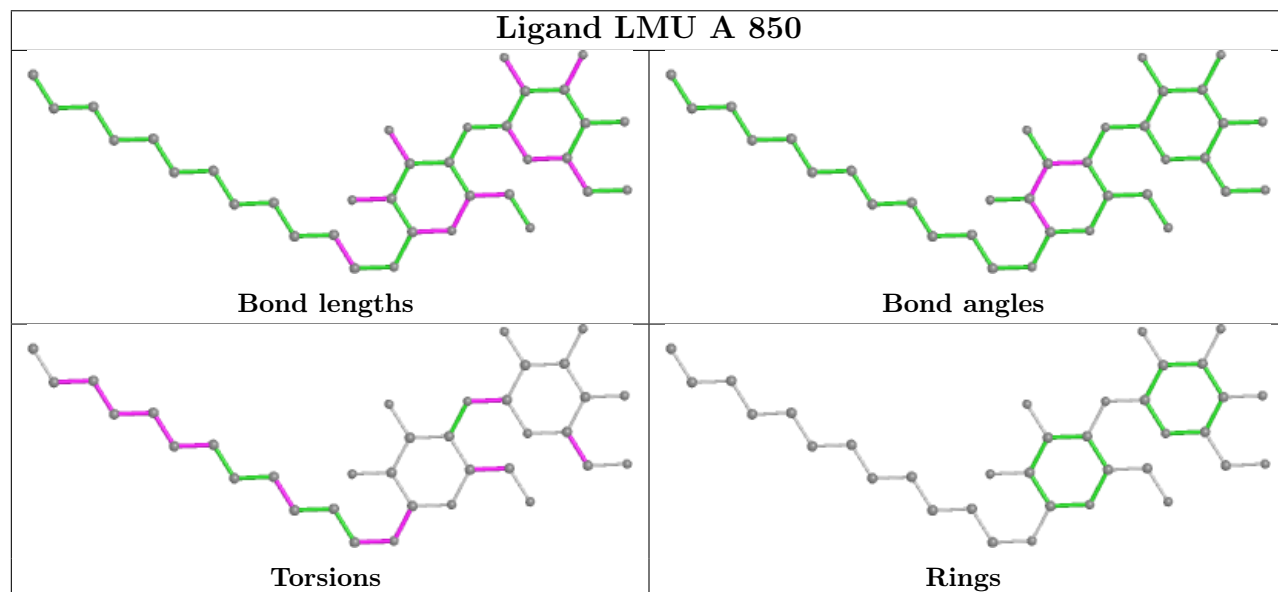




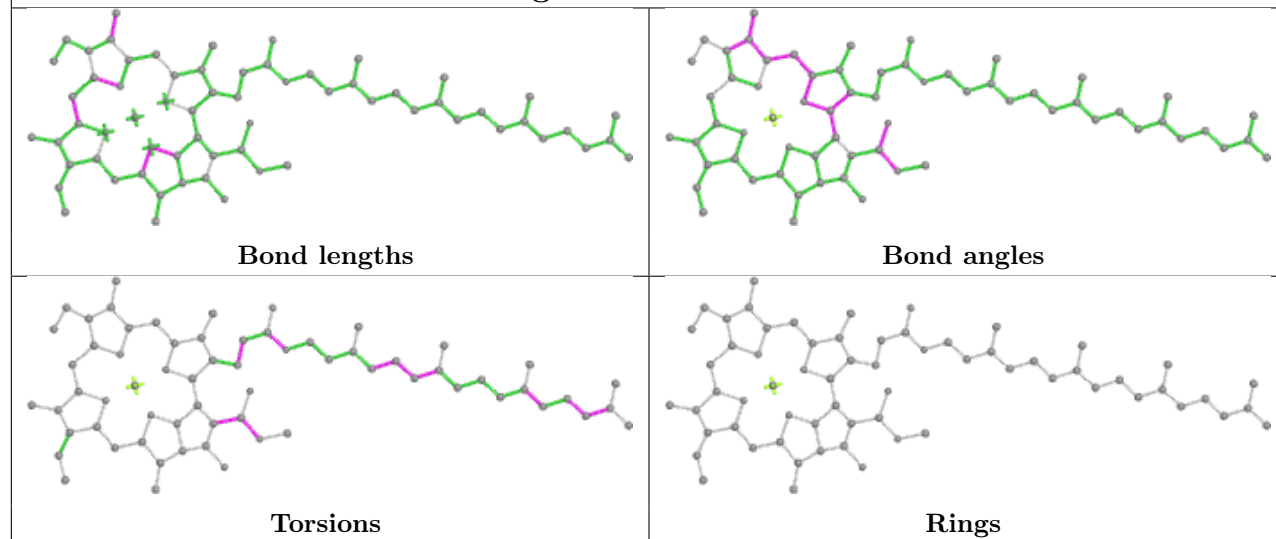
Ligand LHG n 619



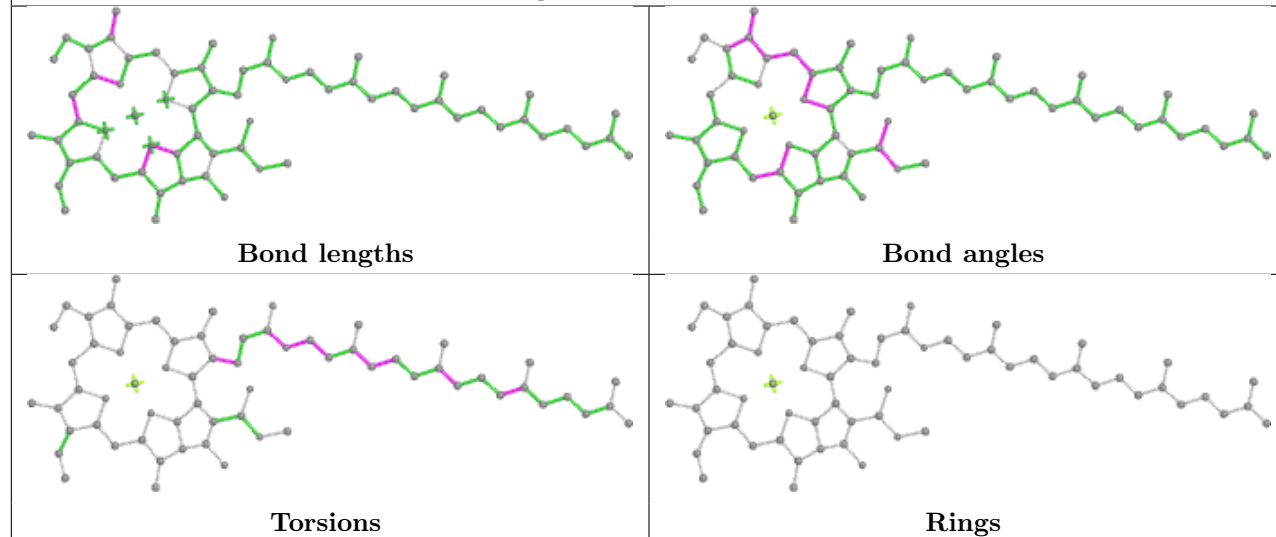
Ligand LMU A 850

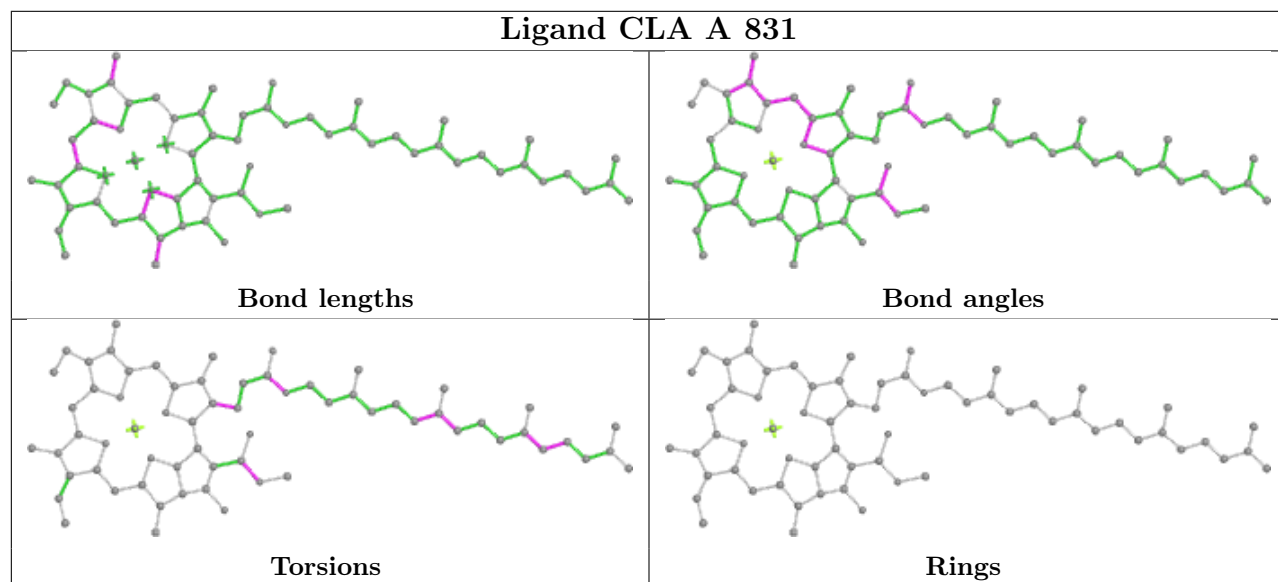
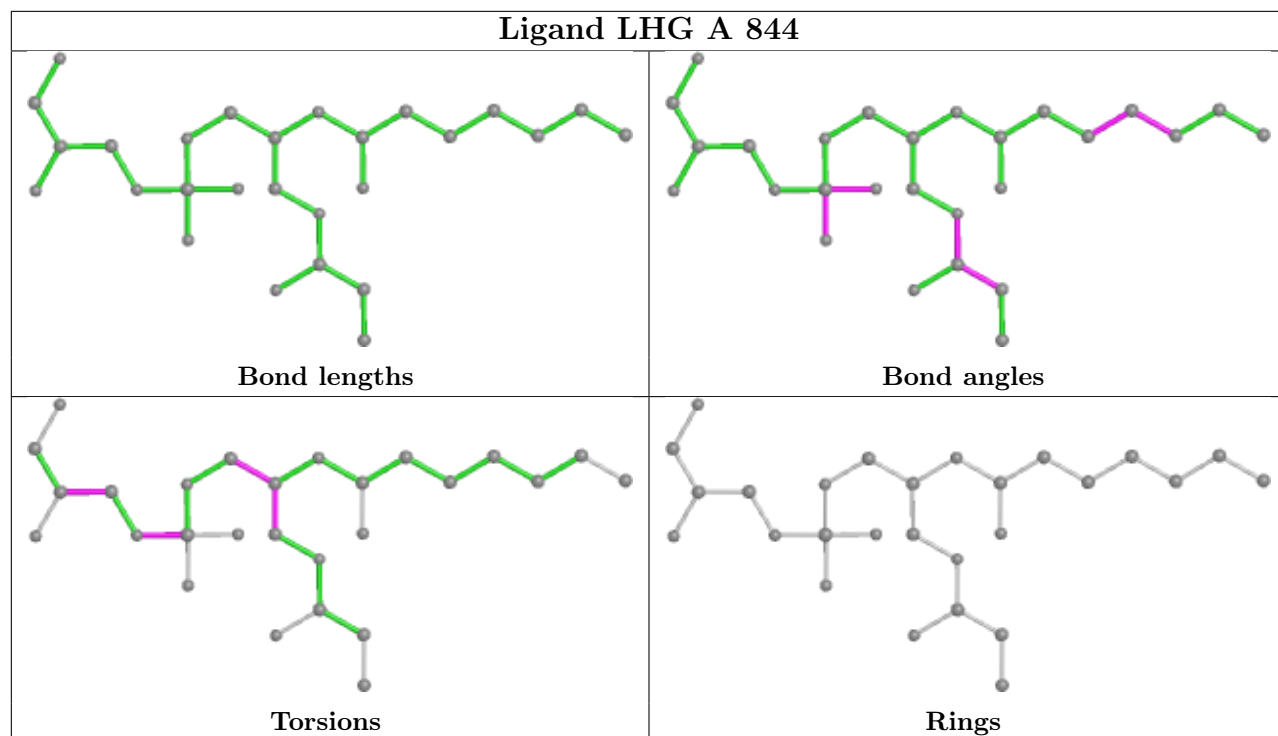


Ligand CLA B 841

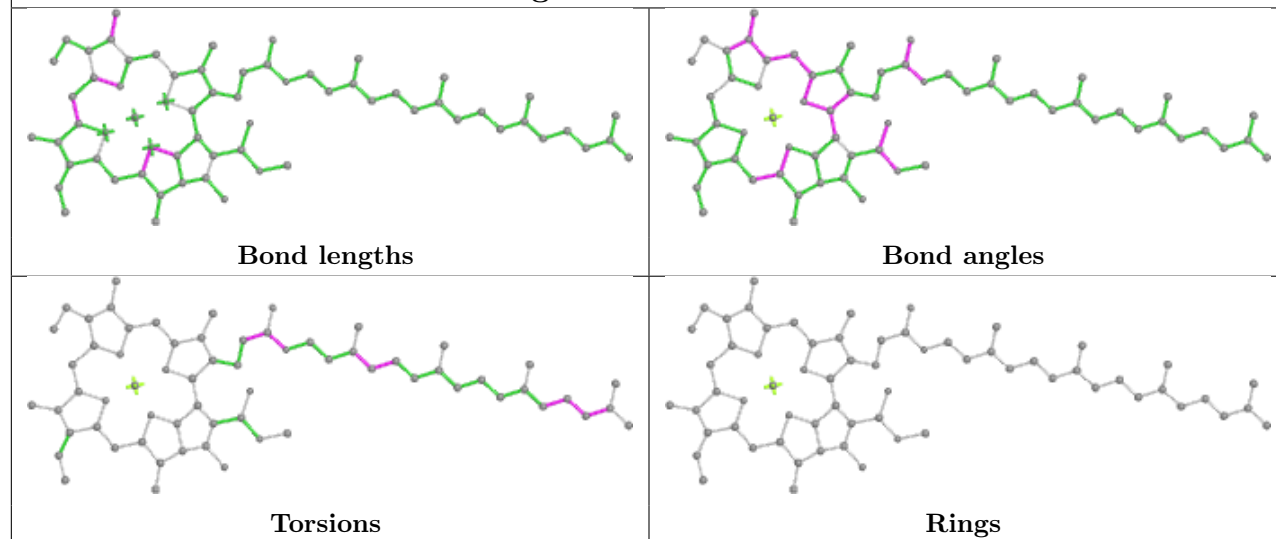


Ligand CLA B 831

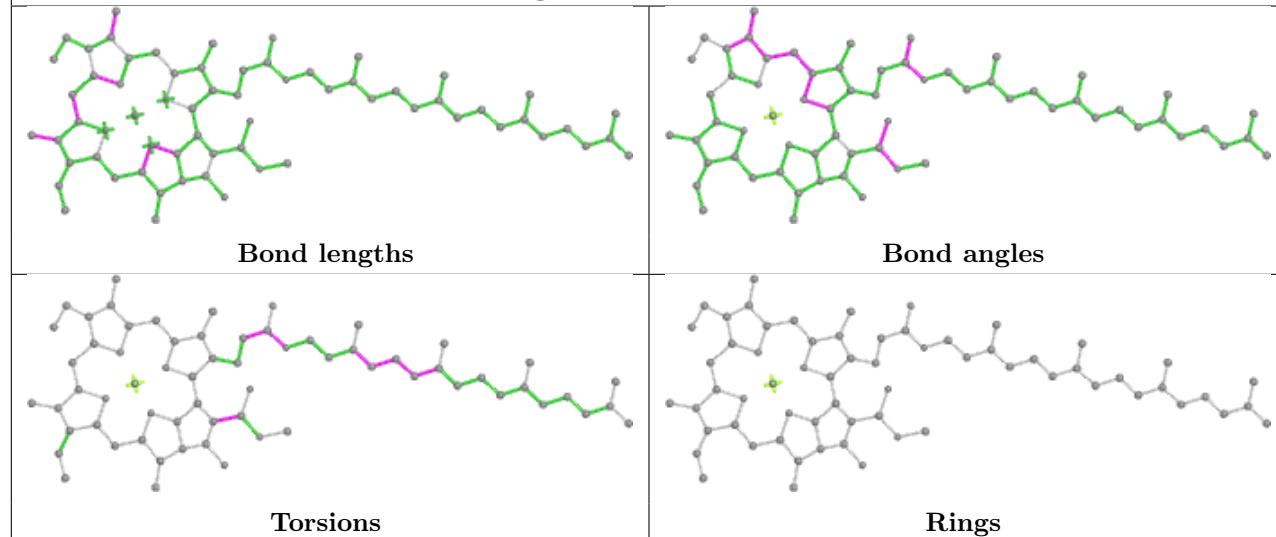




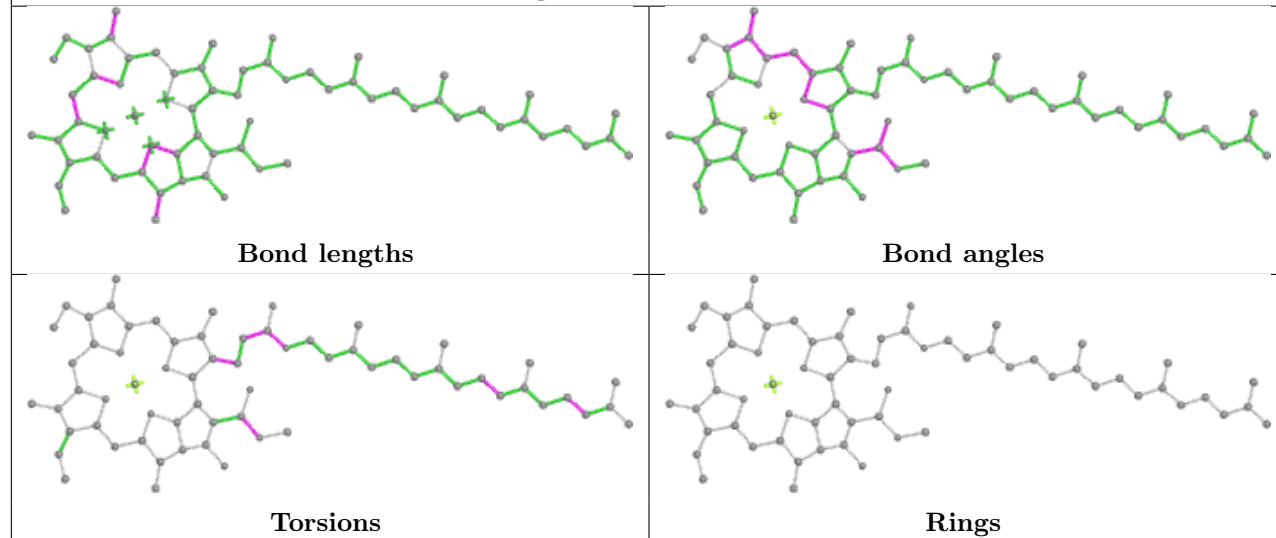
Ligand CLA A 856

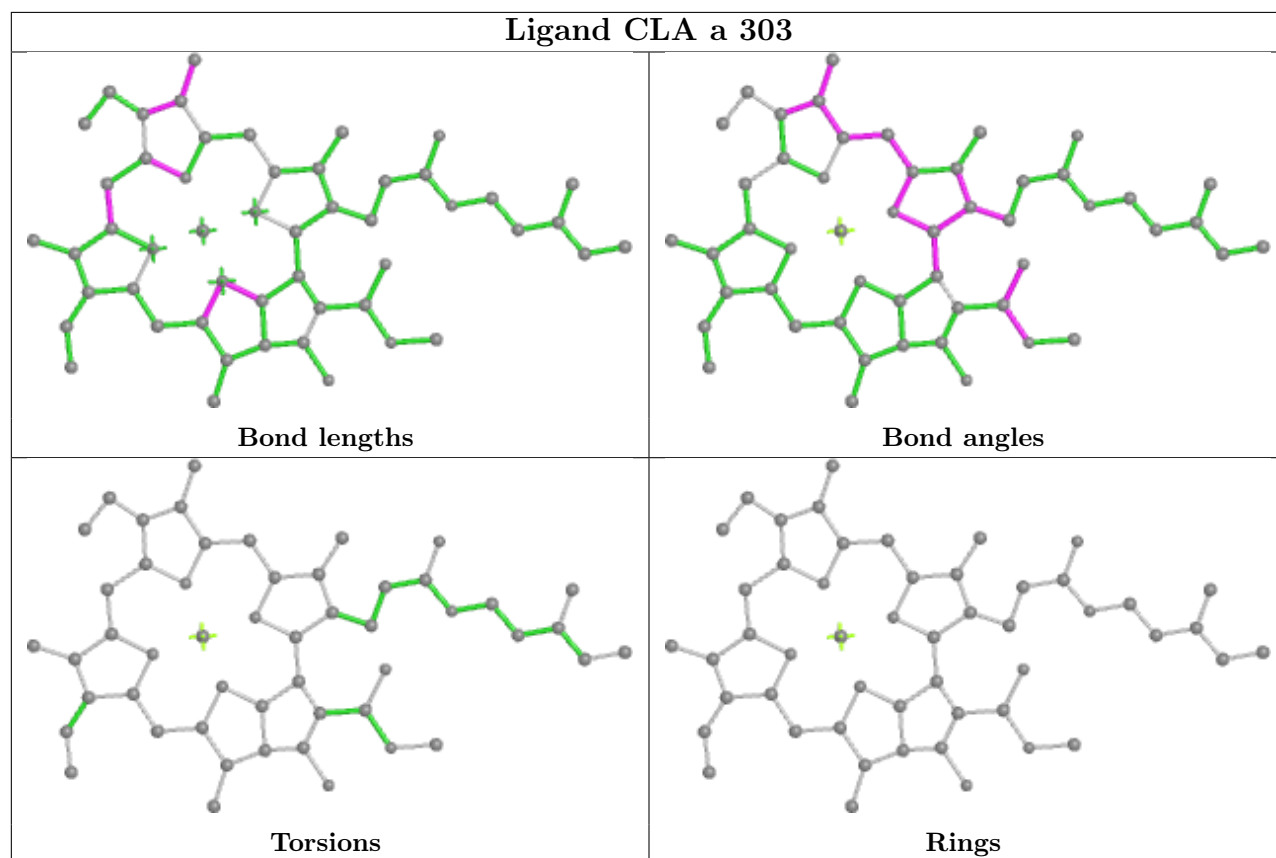
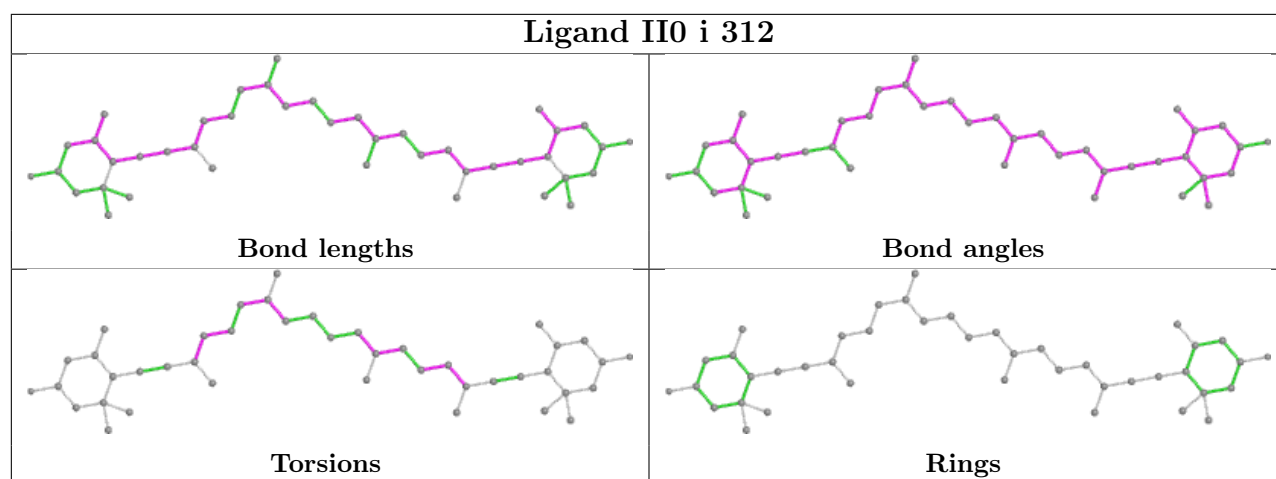


Ligand CLA A 826

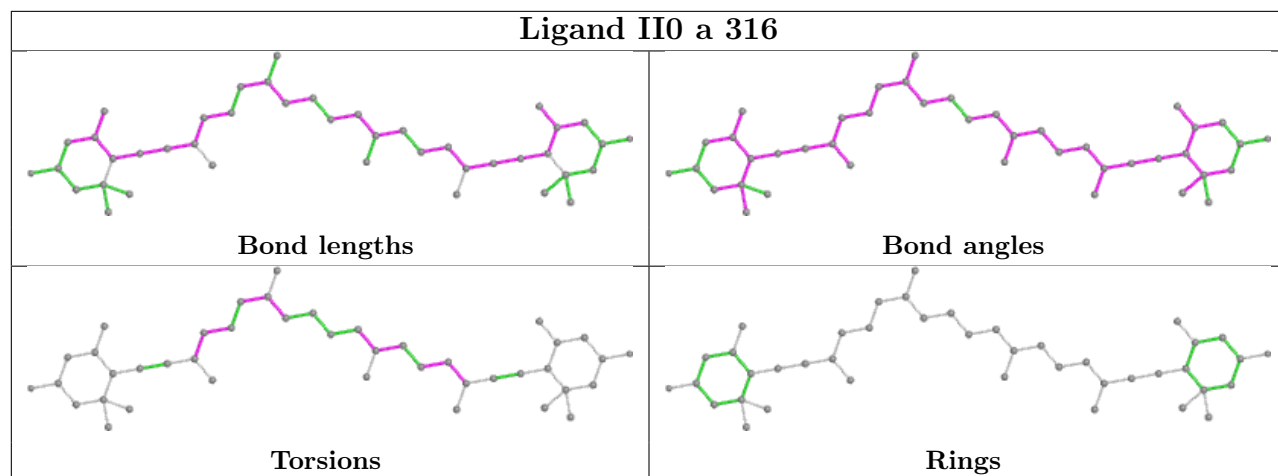


Ligand CLA B 820

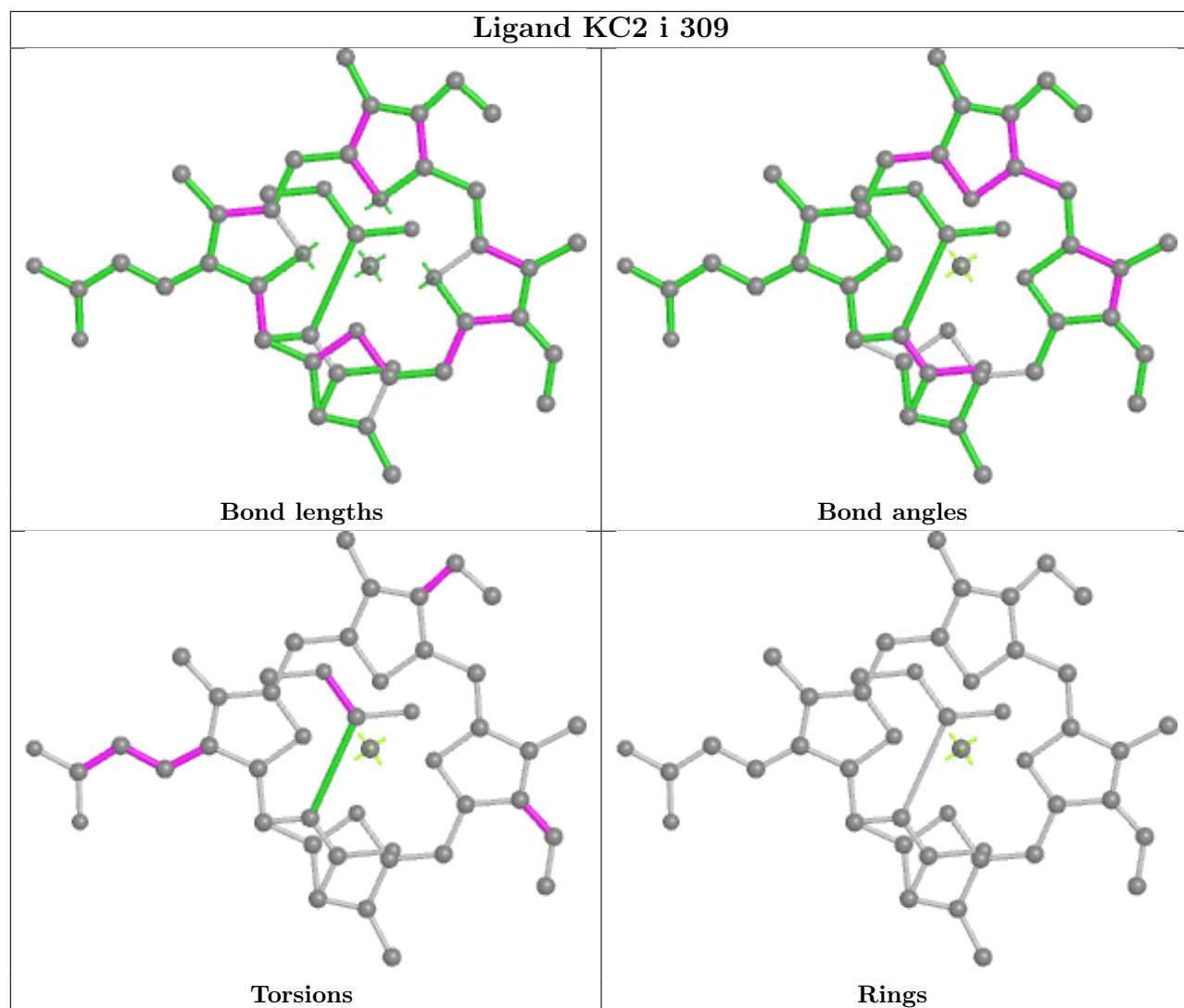




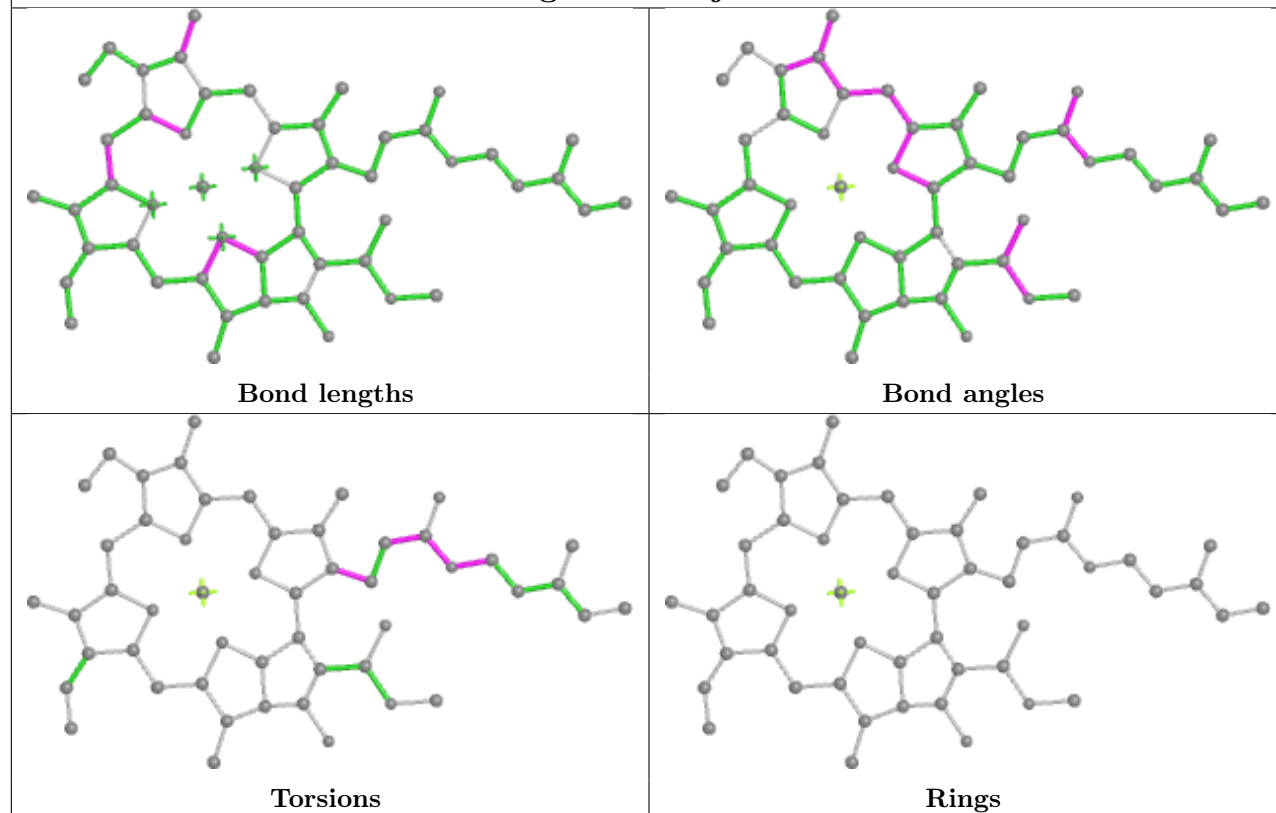
Ligand II0 a 316



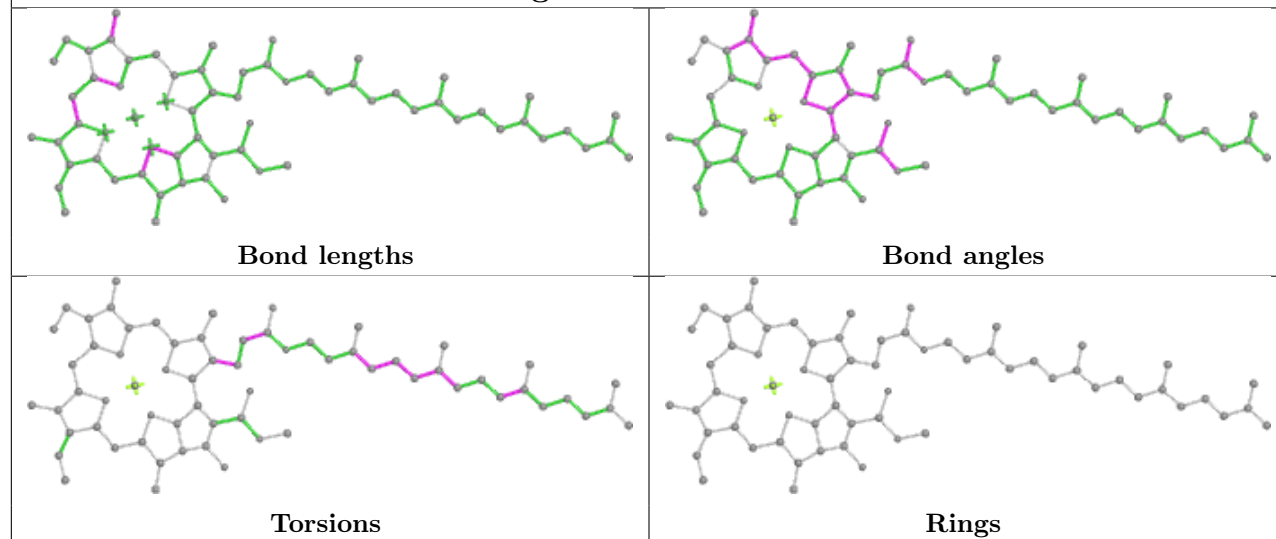
Ligand KC2 i 309



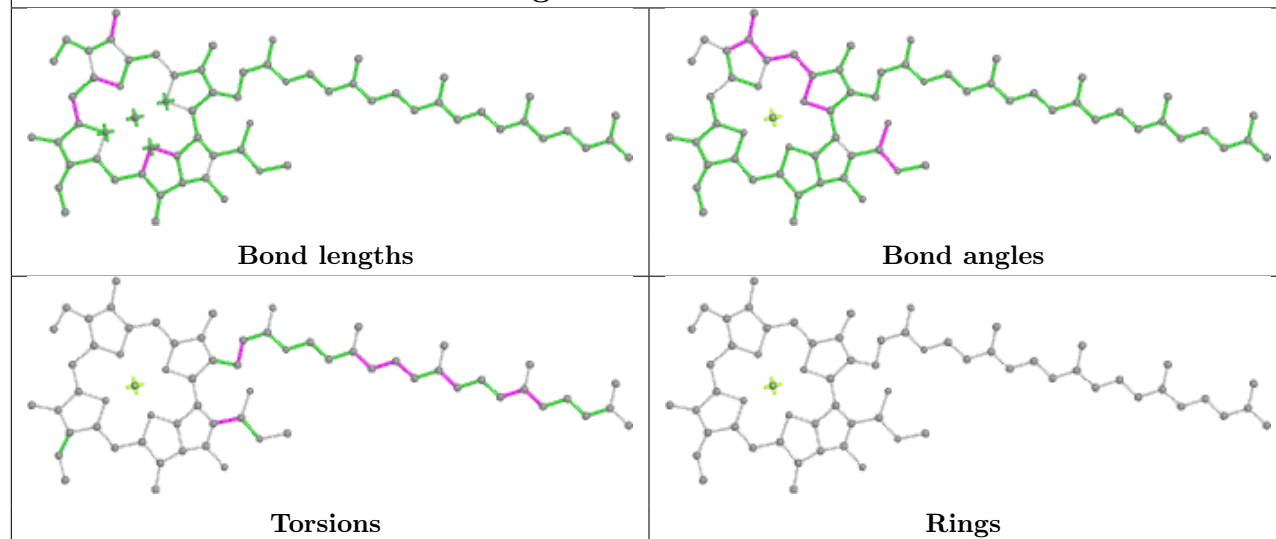
Ligand CLA j 606



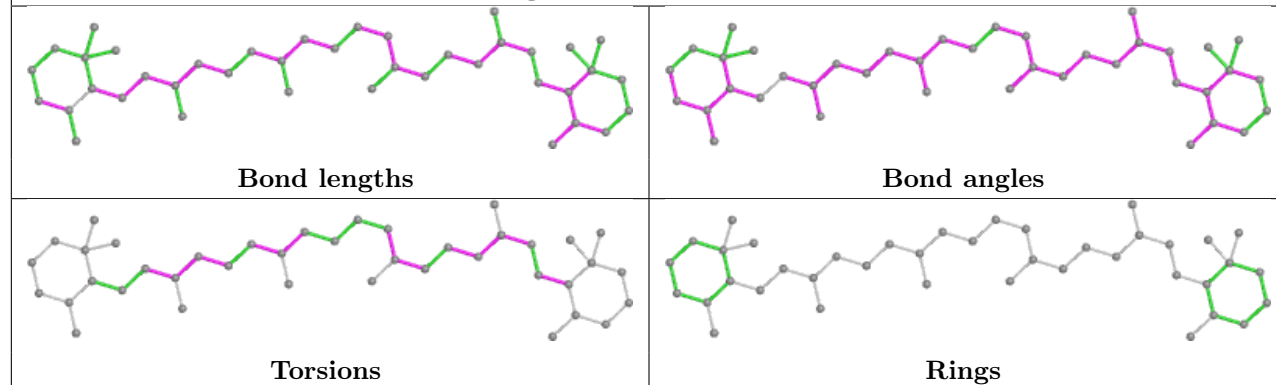
Ligand CLA A 841



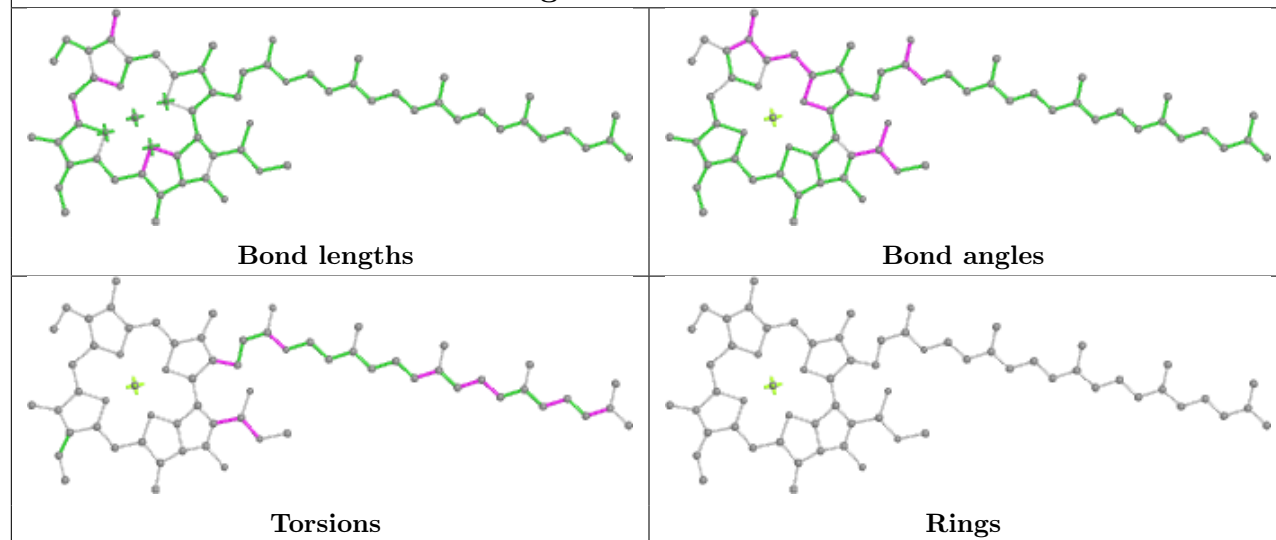
Ligand CLA B 807

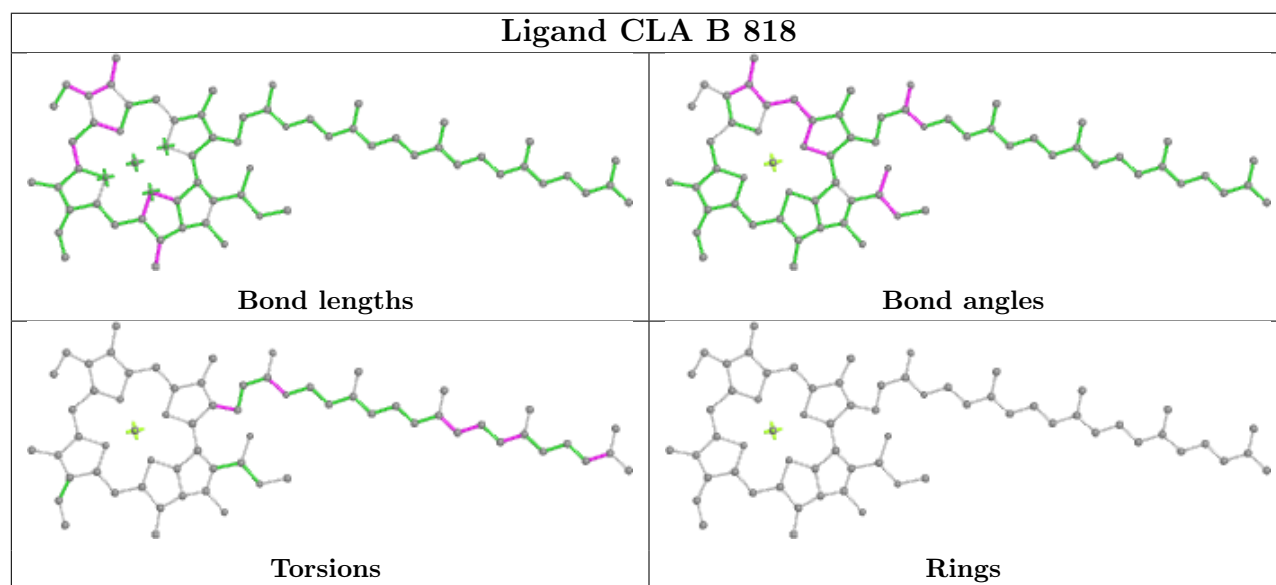
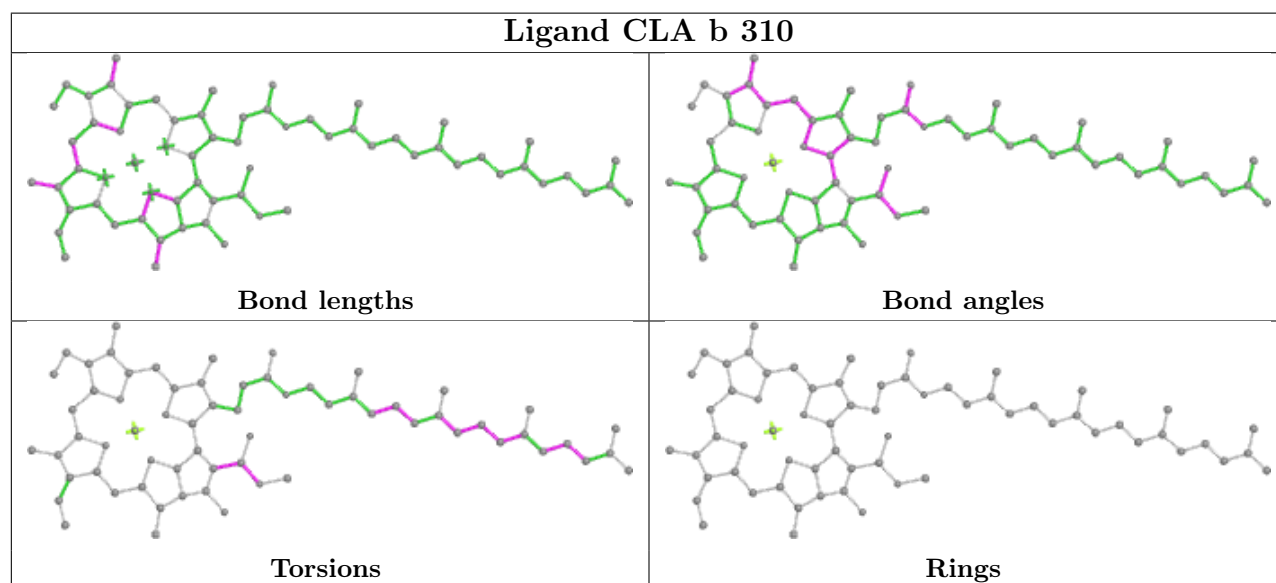
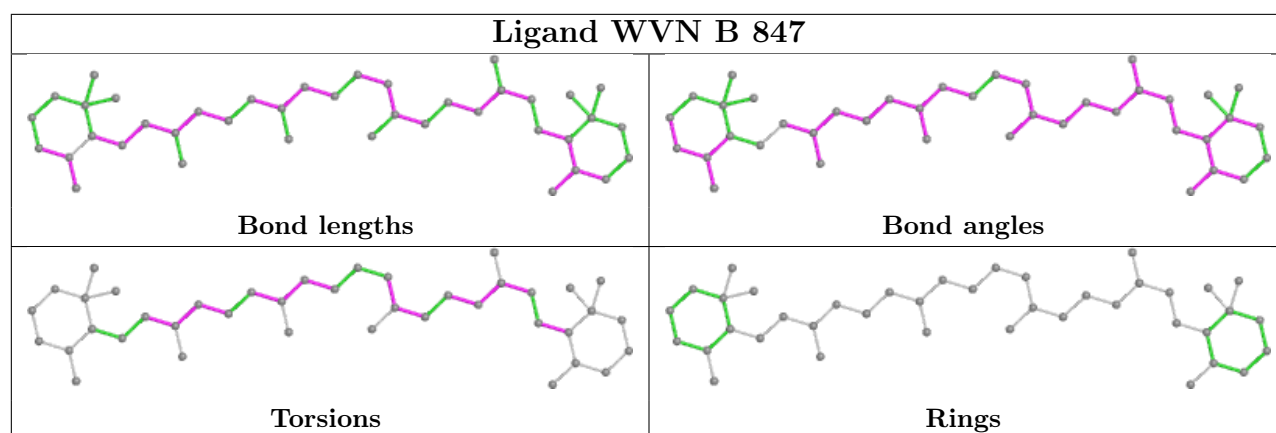


Ligand WVN A 846

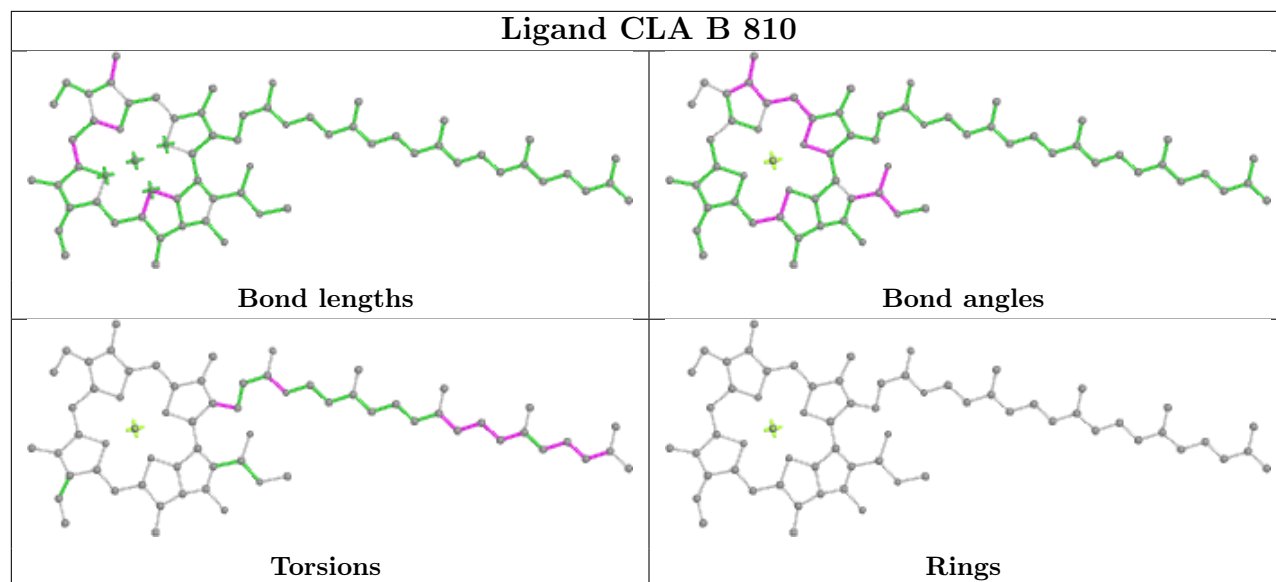


Ligand CLA I 305

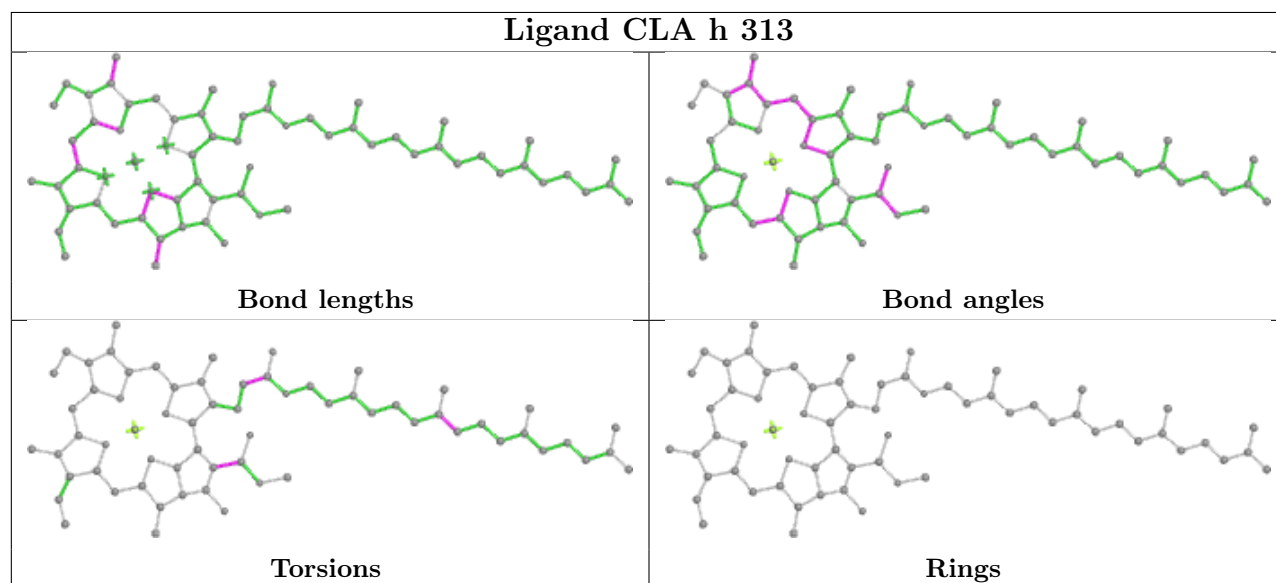


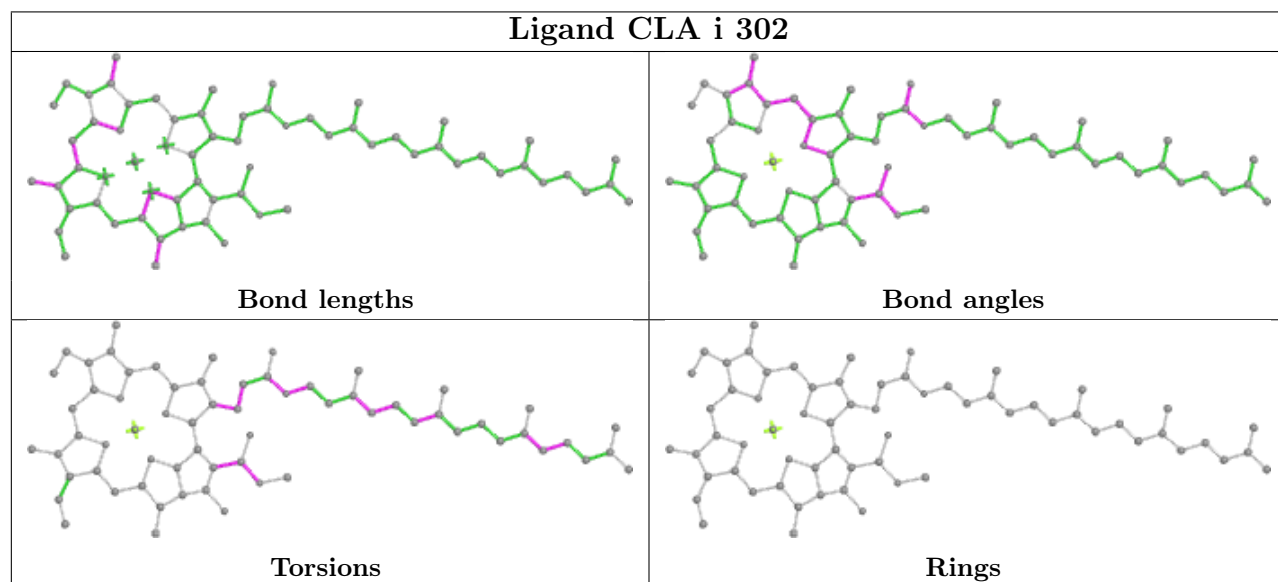
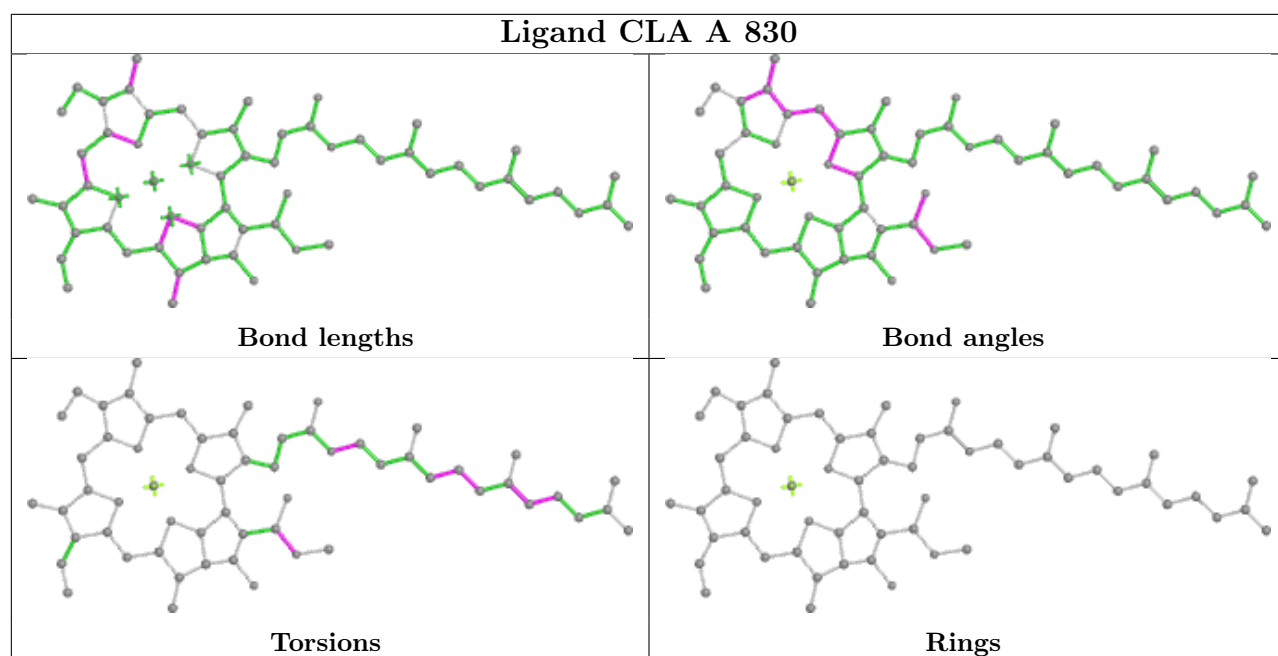


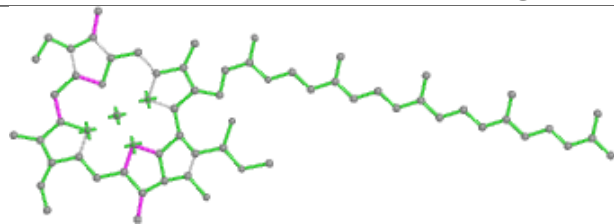
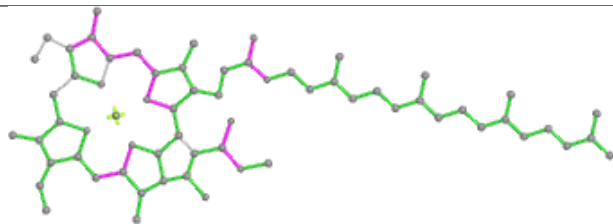
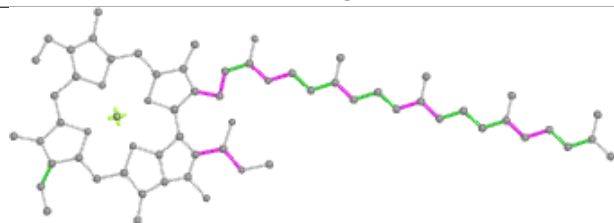
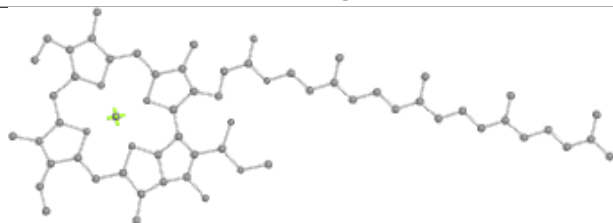
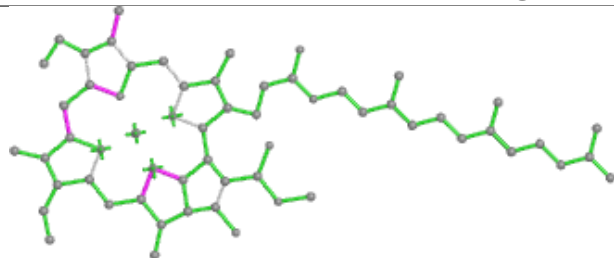
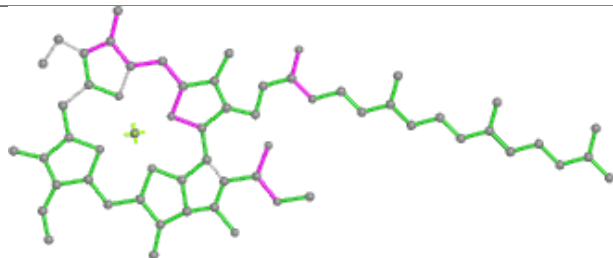
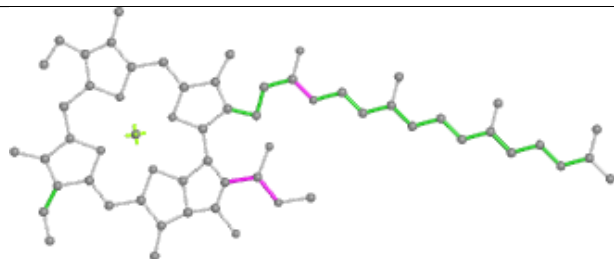
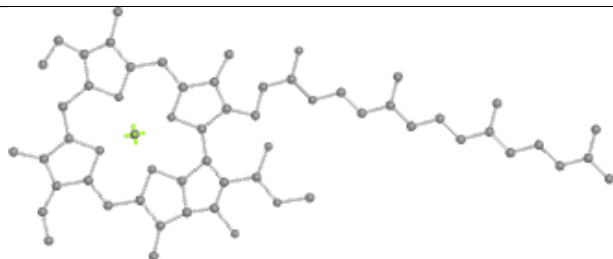
Ligand CLA B 810



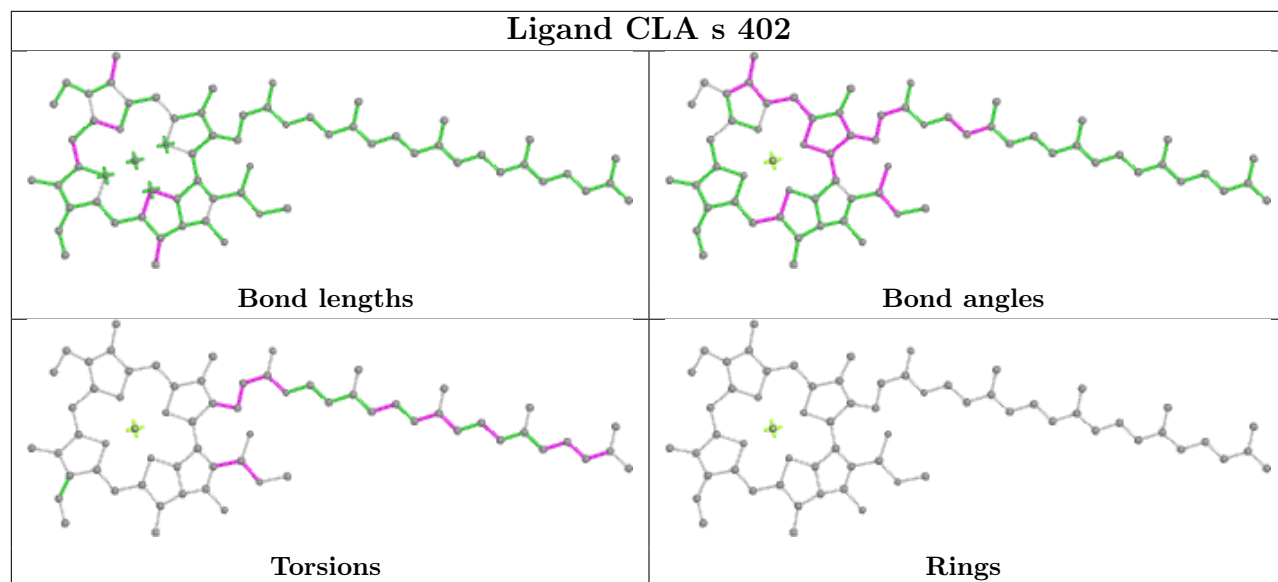
Ligand CLA h 313



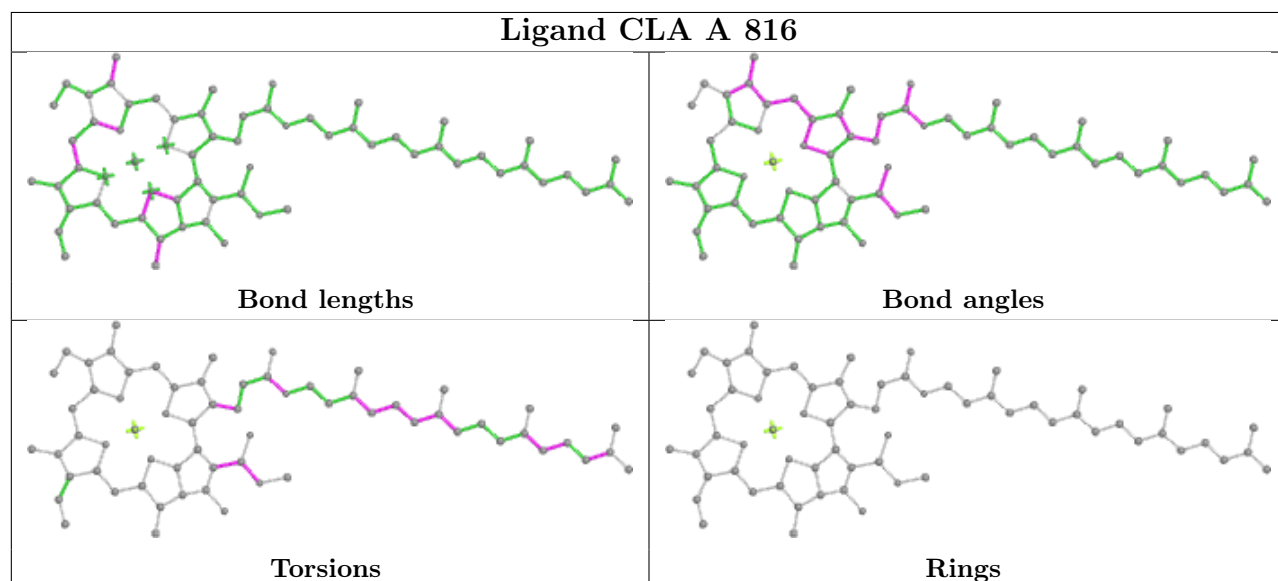


Ligand CLA B 825**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 806****Bond lengths****Bond angles****Torsions****Rings**

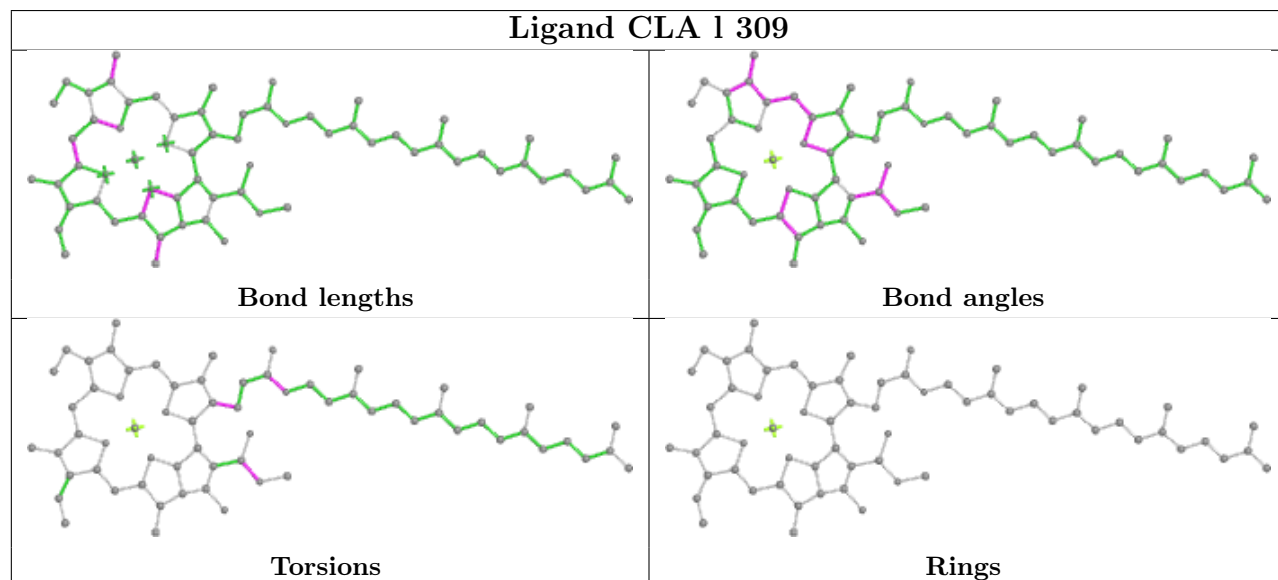
Ligand CLA s 402

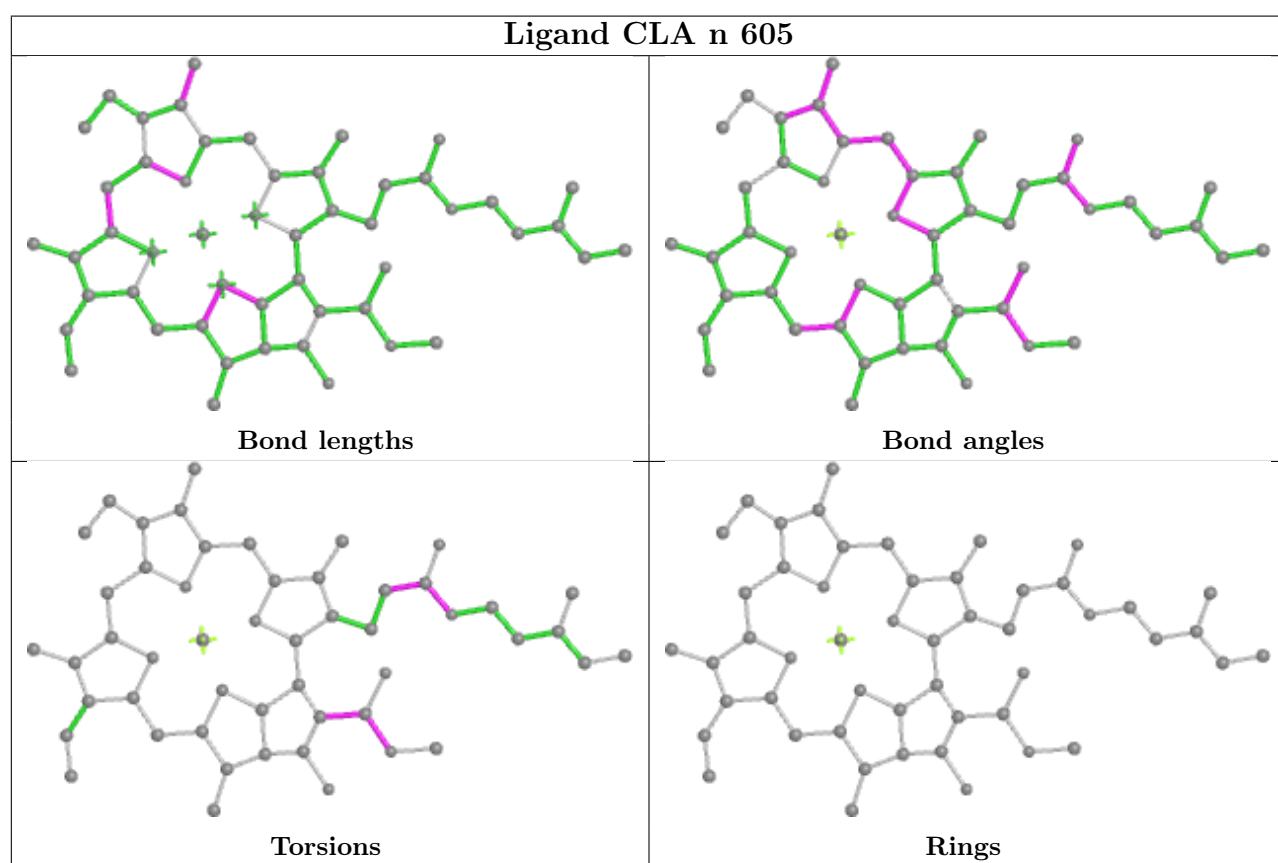
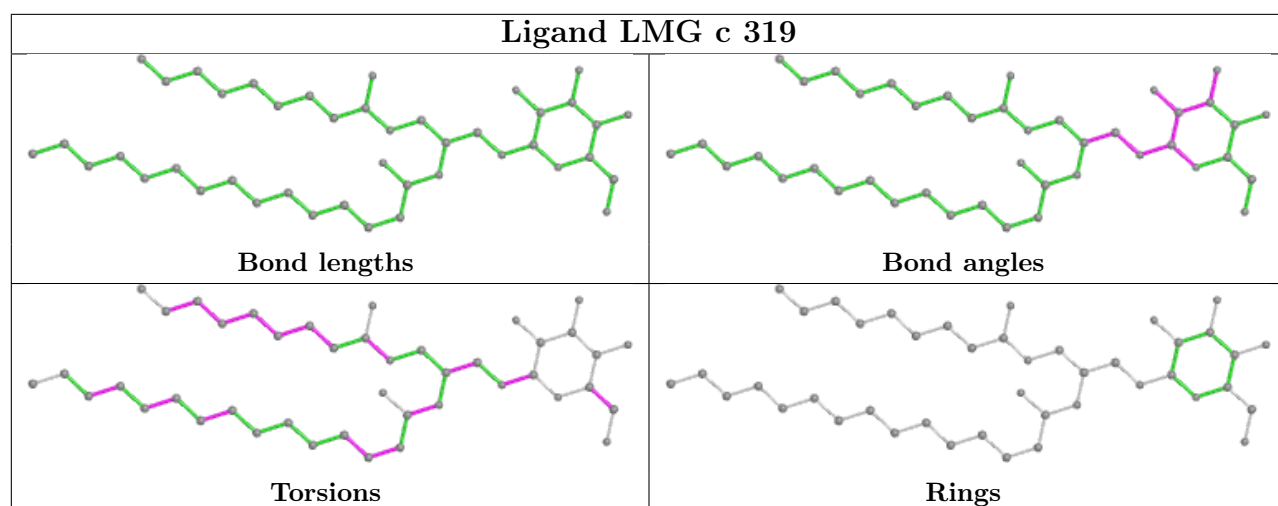


Ligand CLA A 816

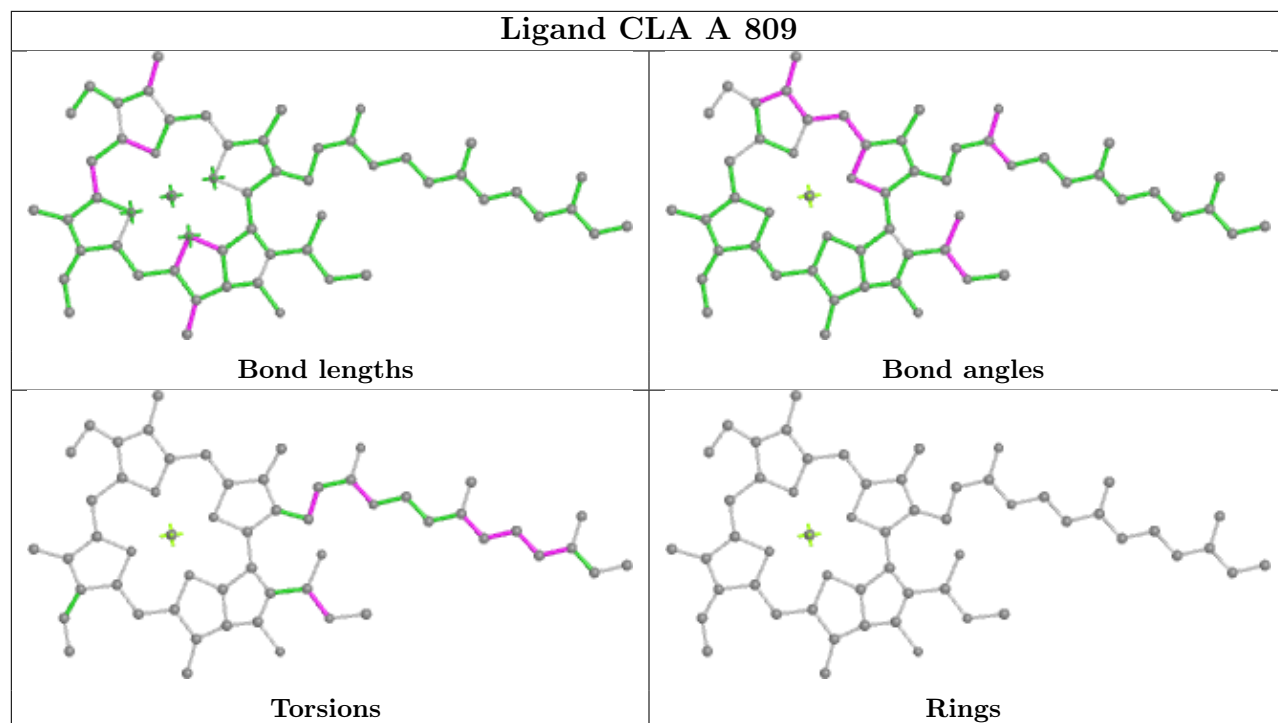


Ligand CLA l 309

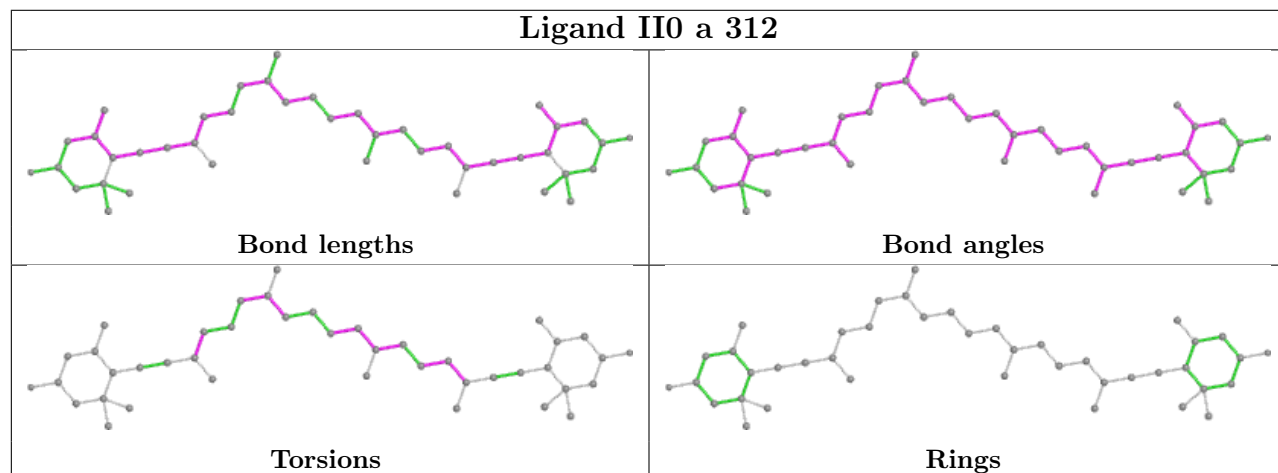




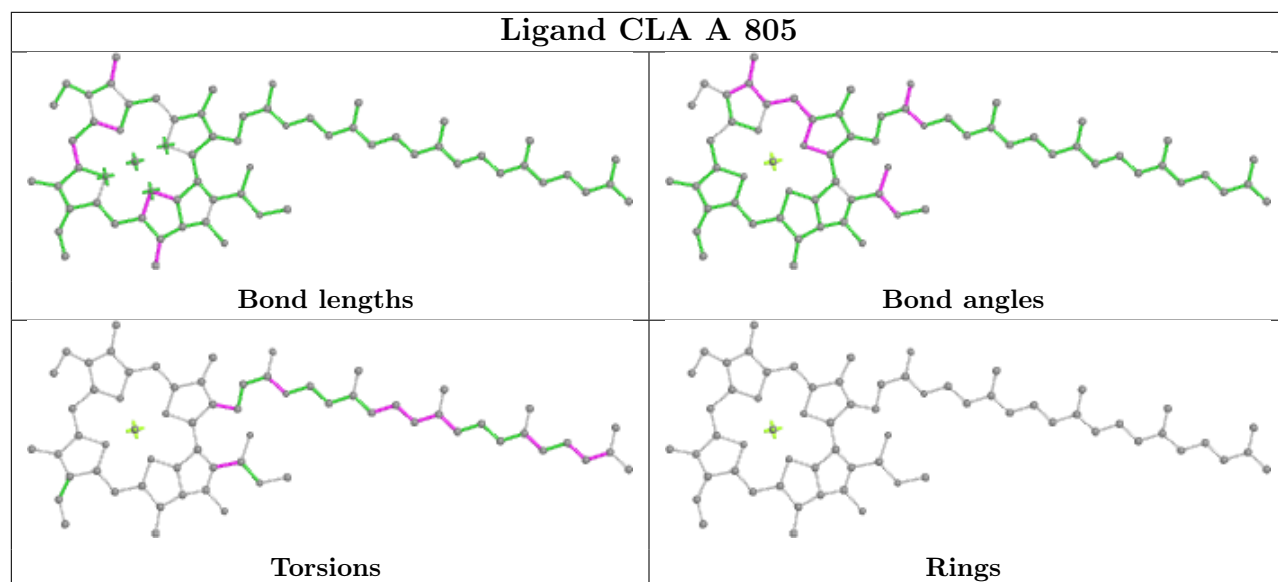
Ligand CLA A 809

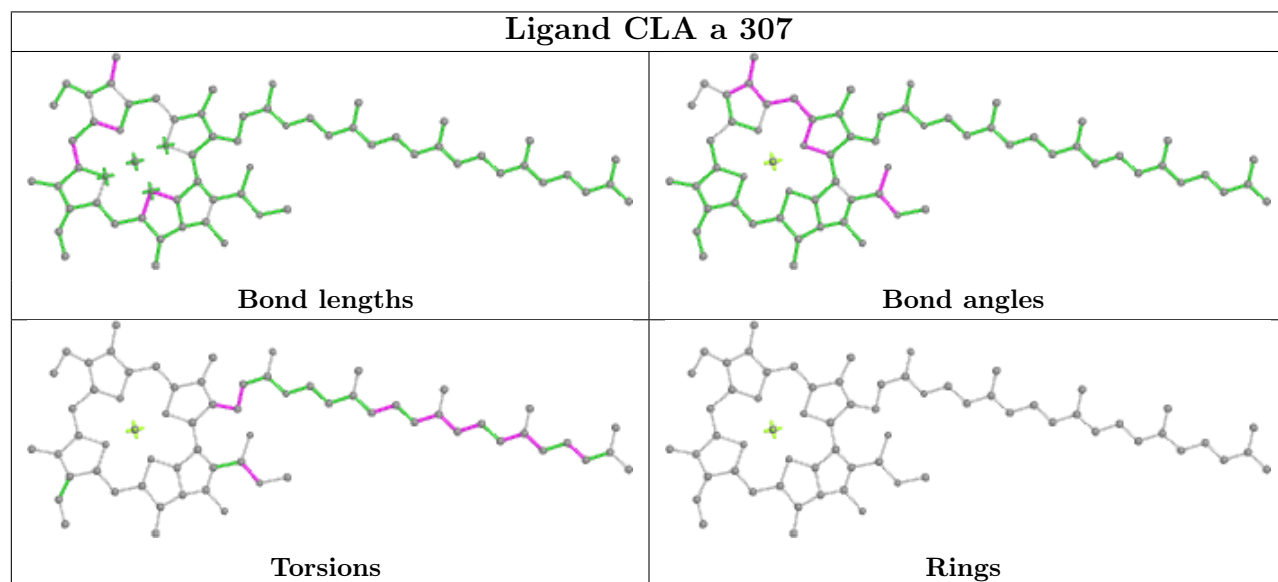
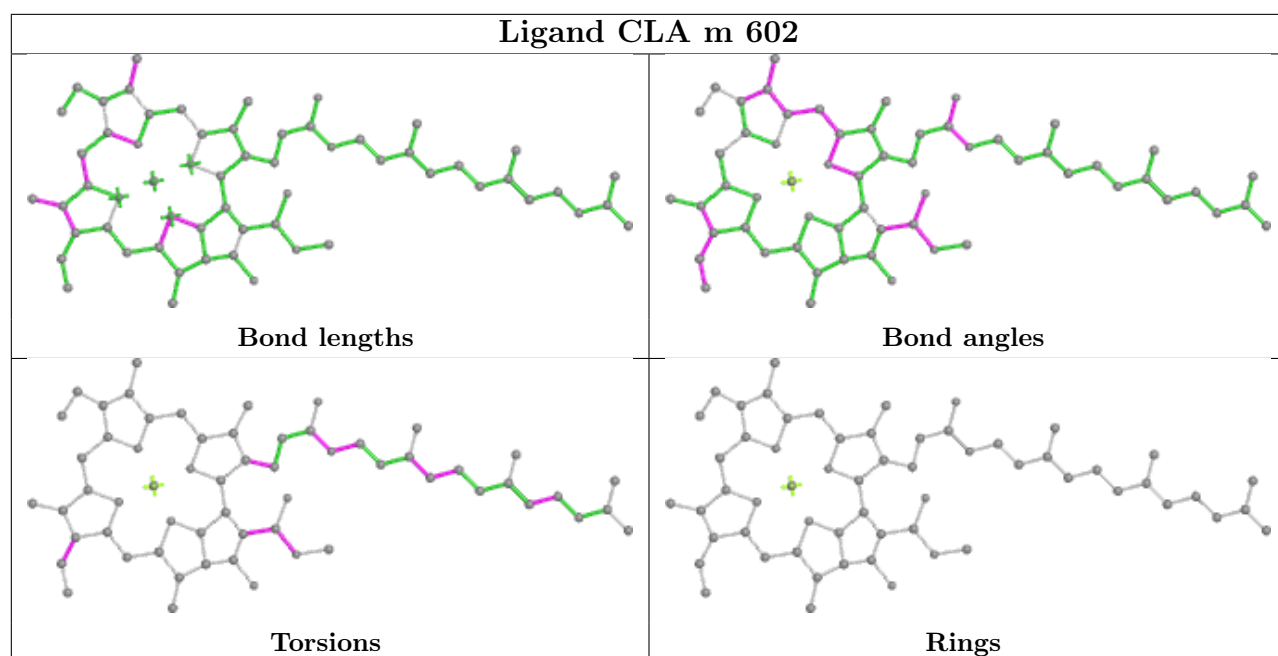


Ligand II0 a 312

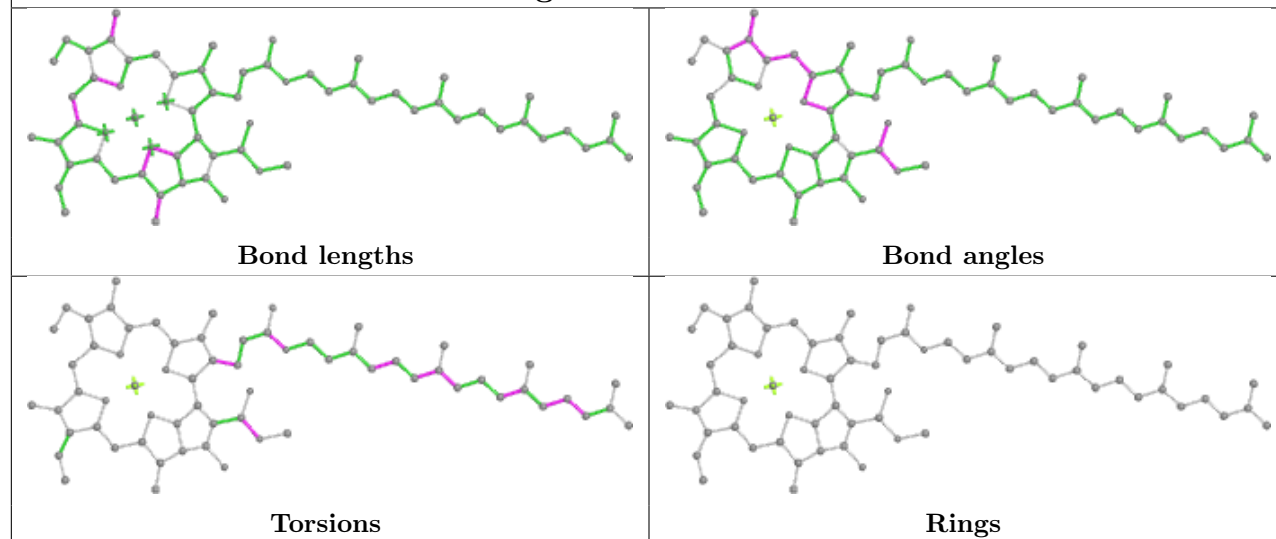


Ligand CLA A 805

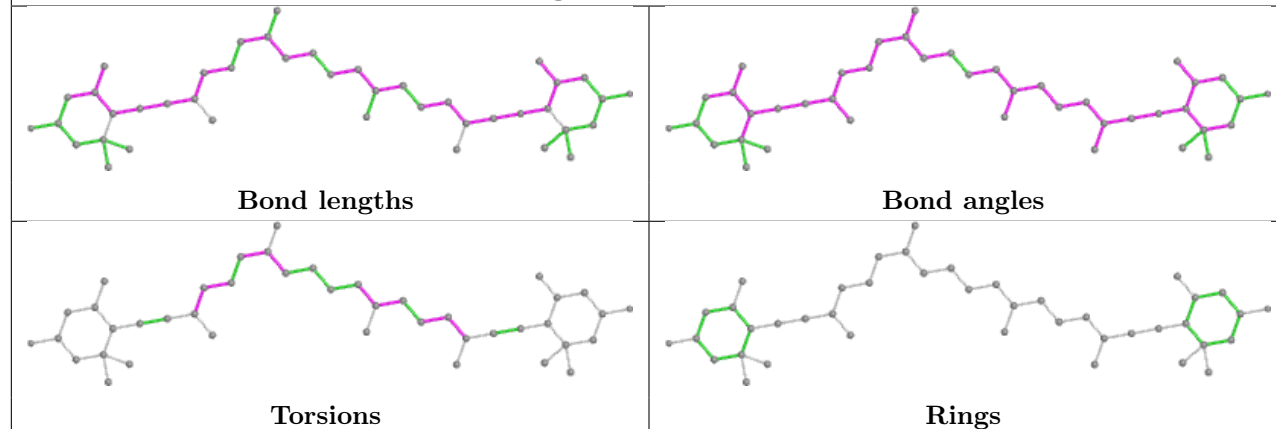




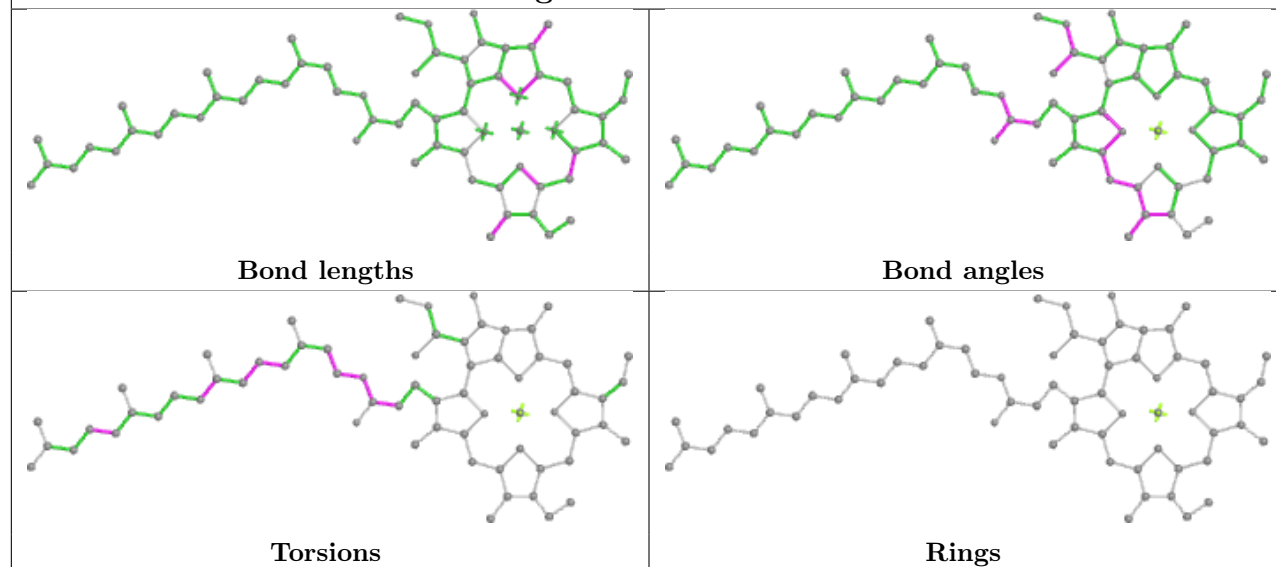
Ligand CLA k 602

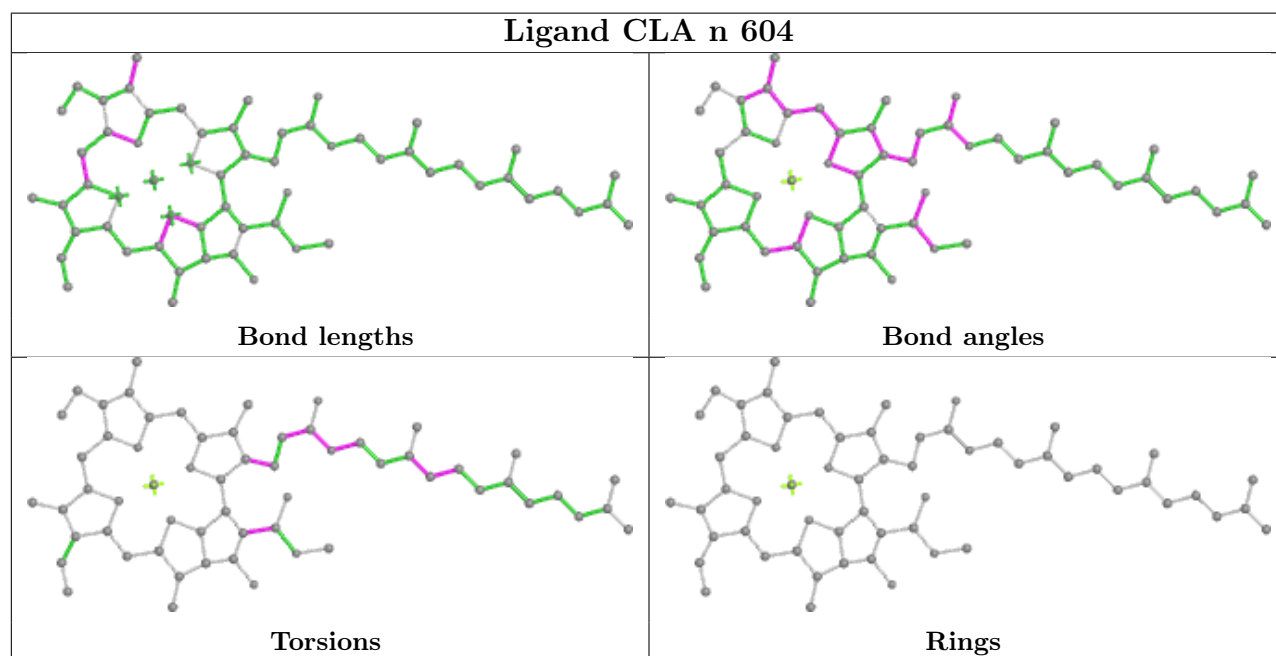
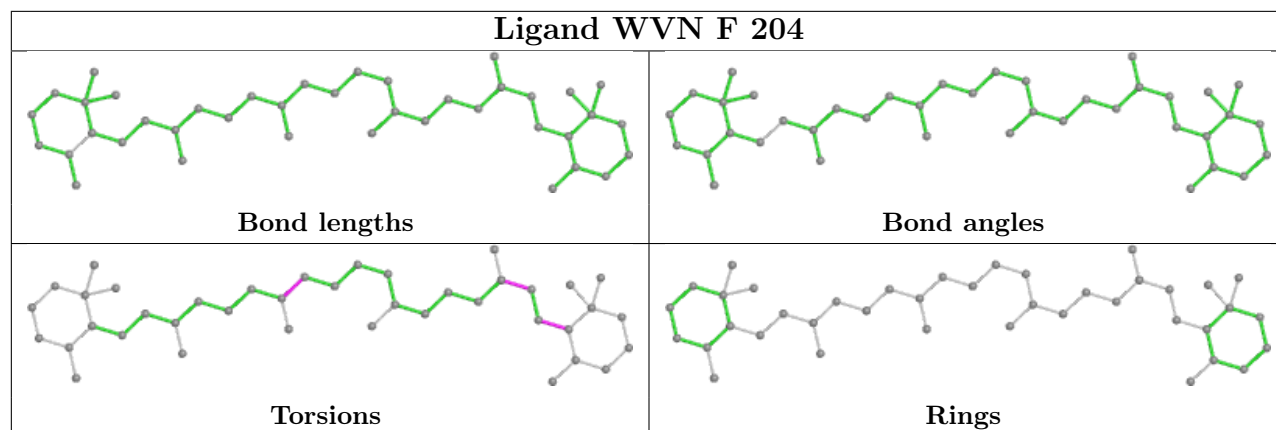


Ligand II0 d 317

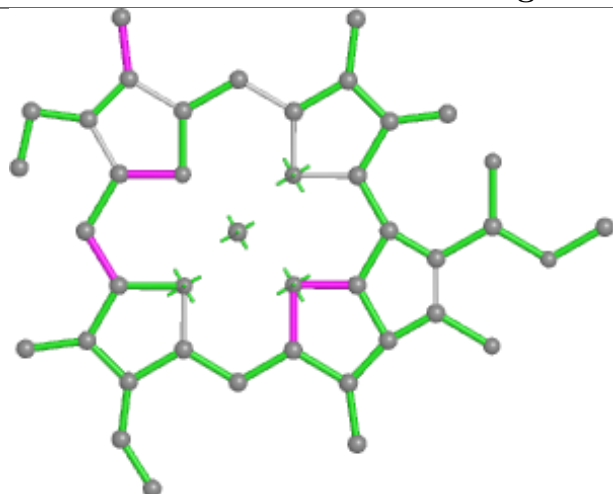


Ligand CLA h 301

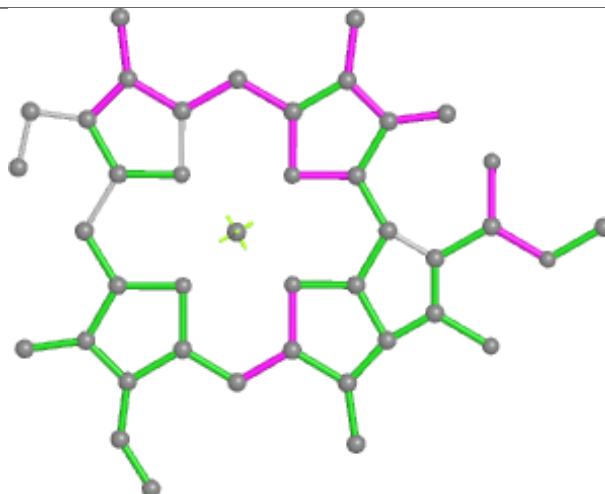




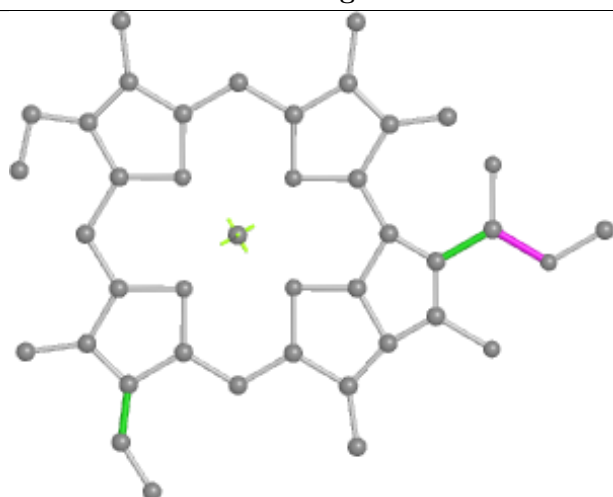
Ligand CLA d 309



Bond lengths



Bond angles

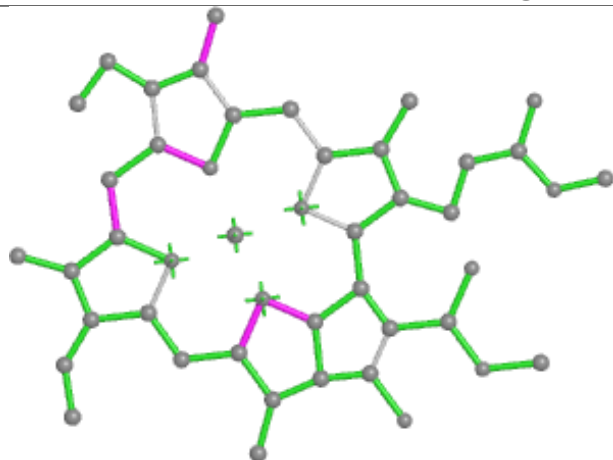


Torsions

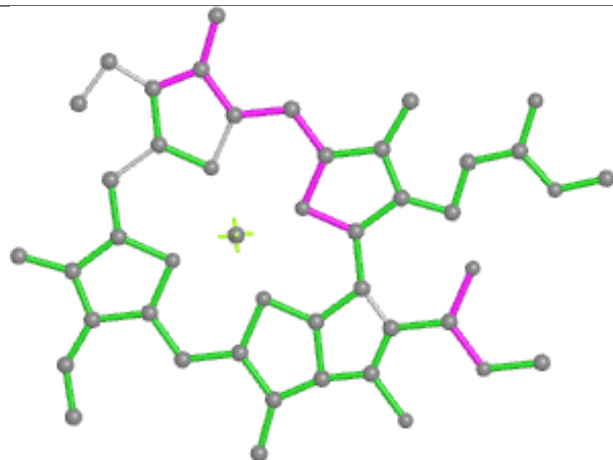


Rings

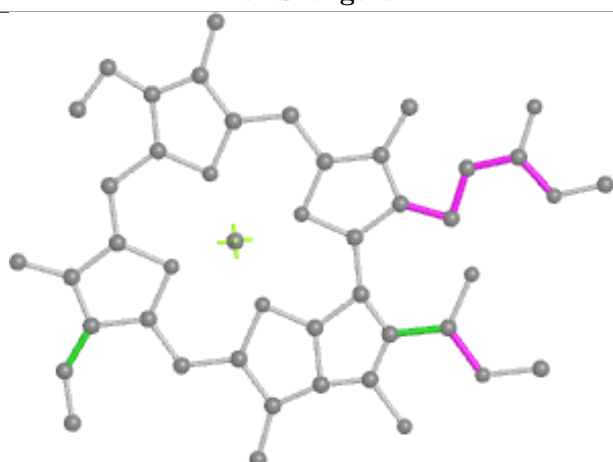
Ligand CLA d 308



Bond lengths



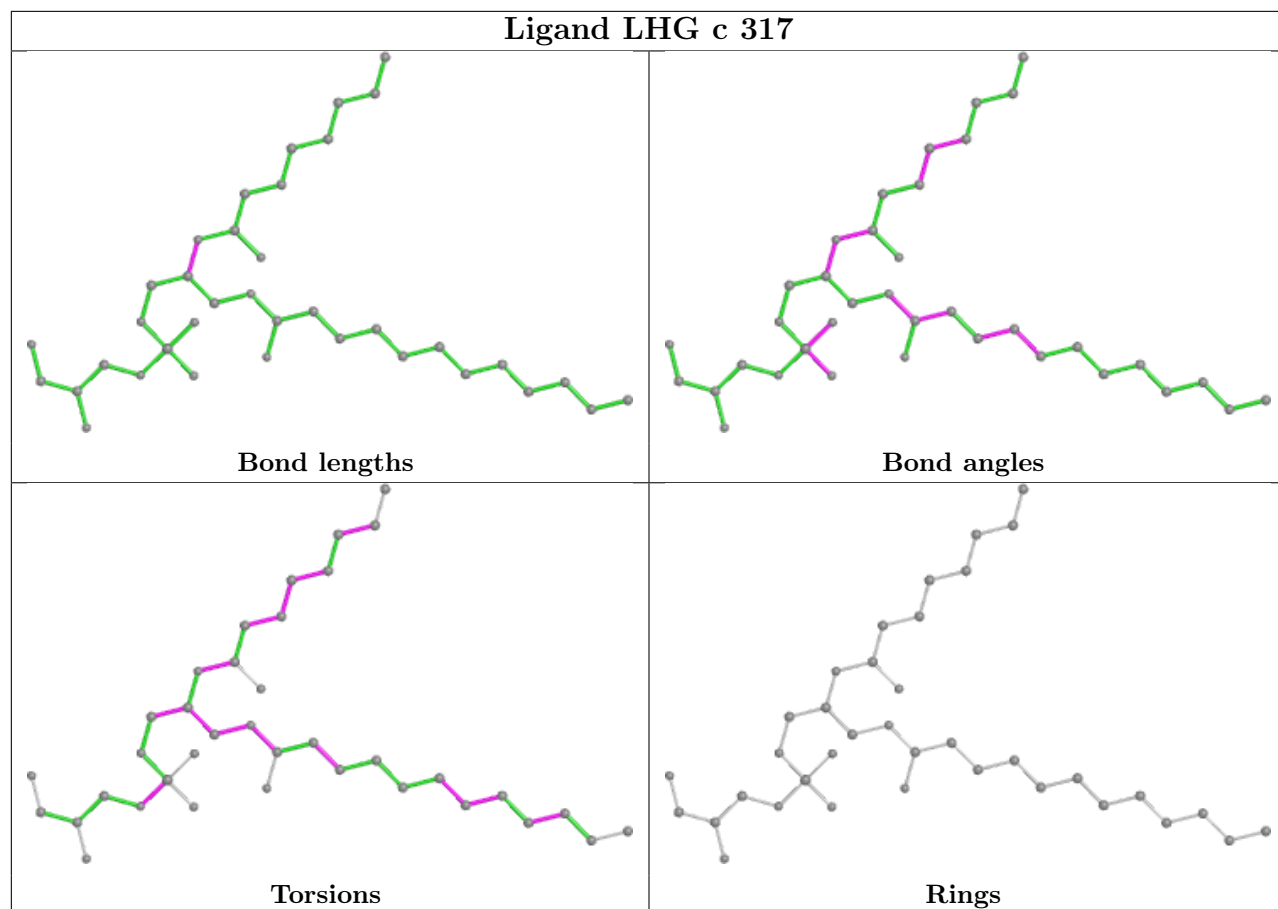
Bond angles



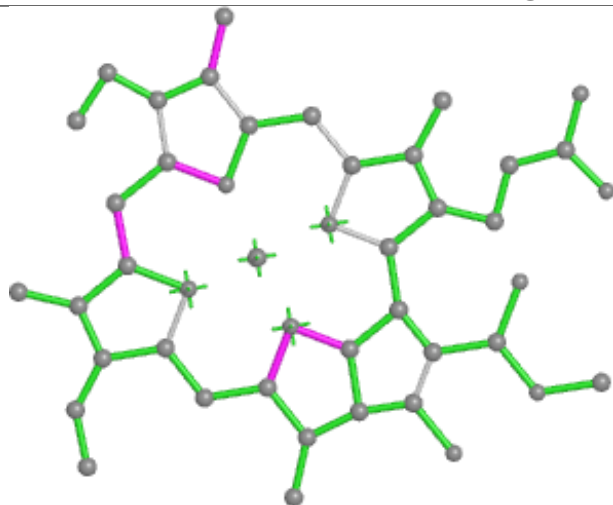
Torsions



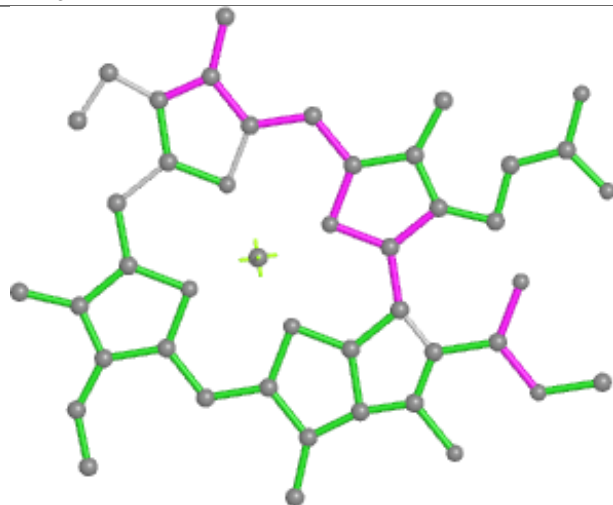
Rings



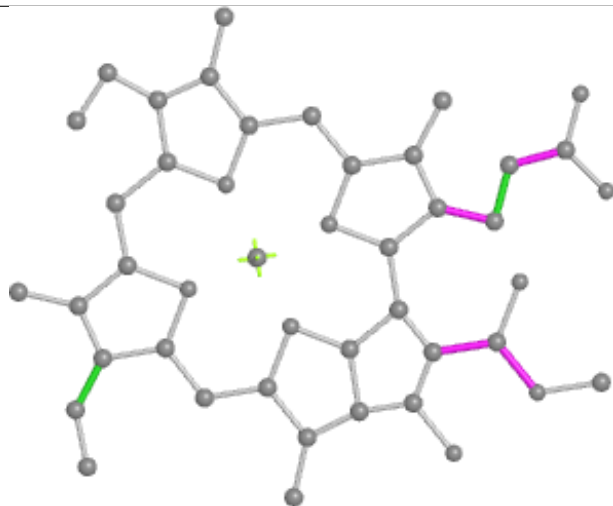
Ligand CLA j 605



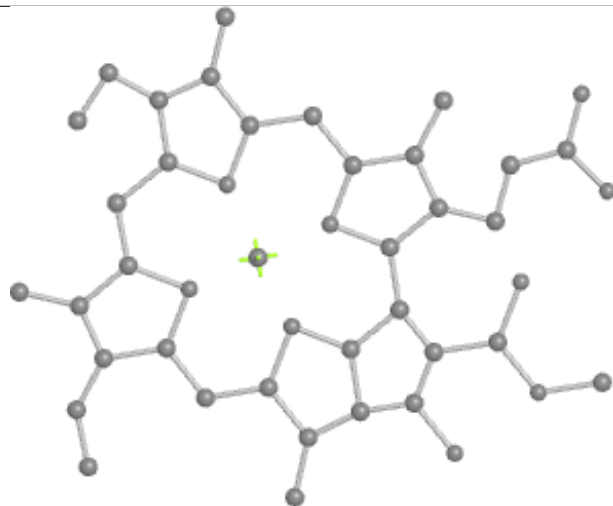
Bond lengths



Bond angles

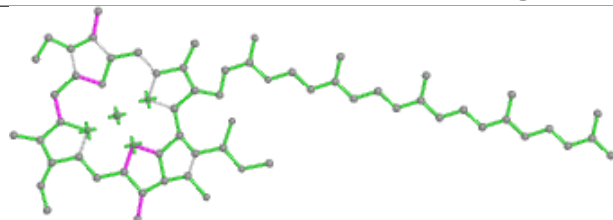


Torsions

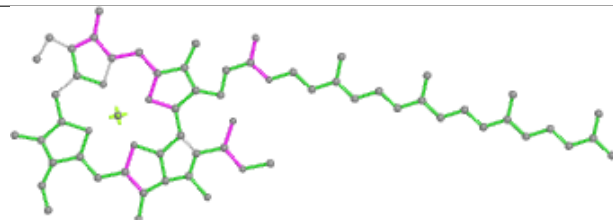


Rings

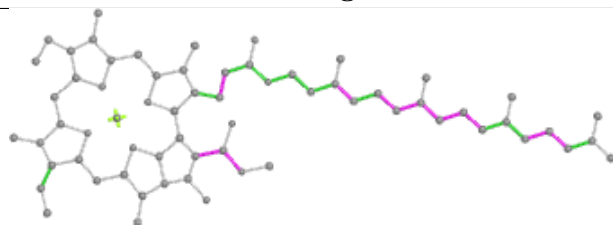
Ligand CLA B 836



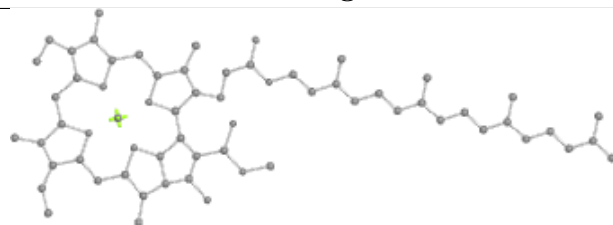
Bond lengths



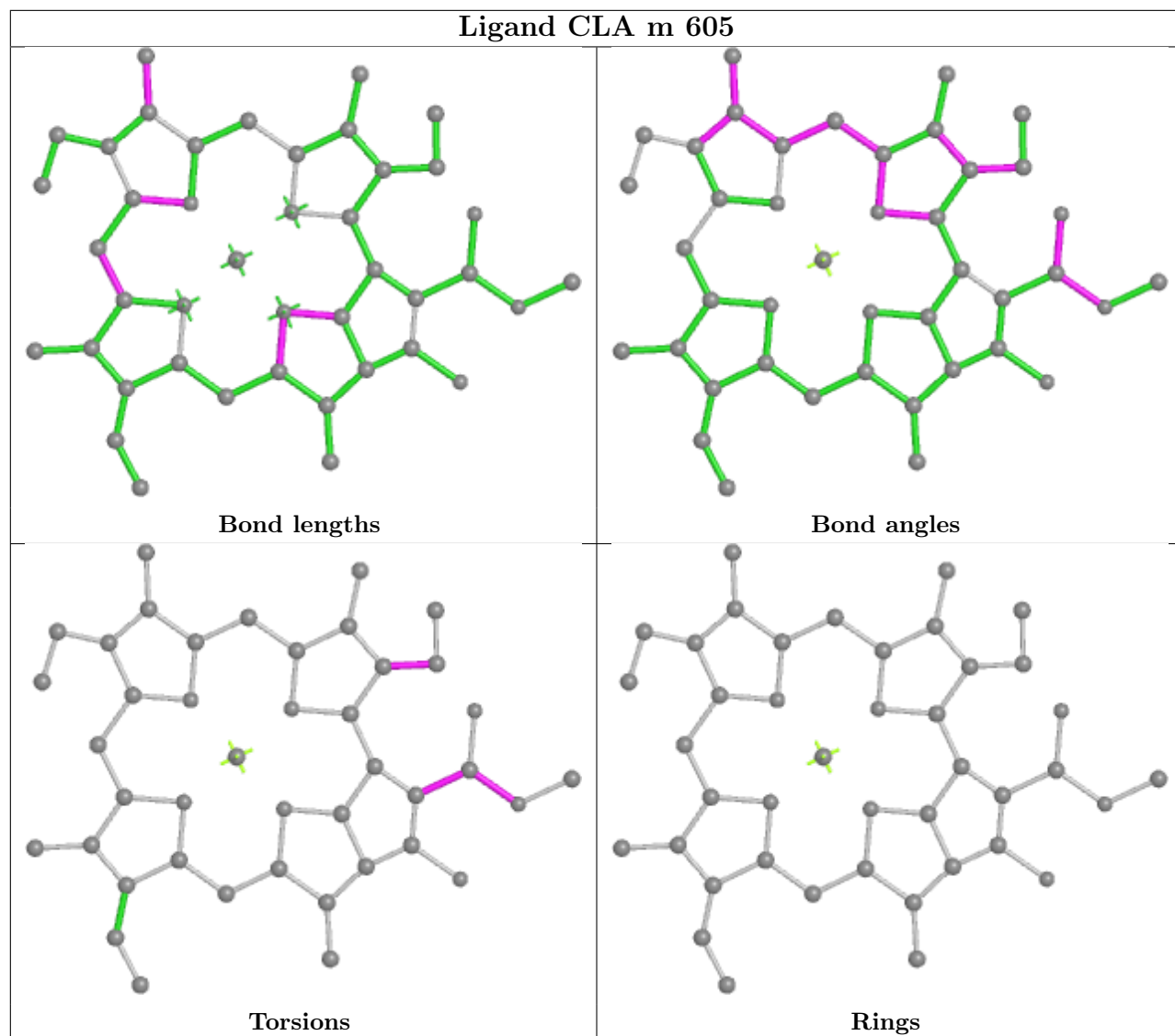
Bond angles



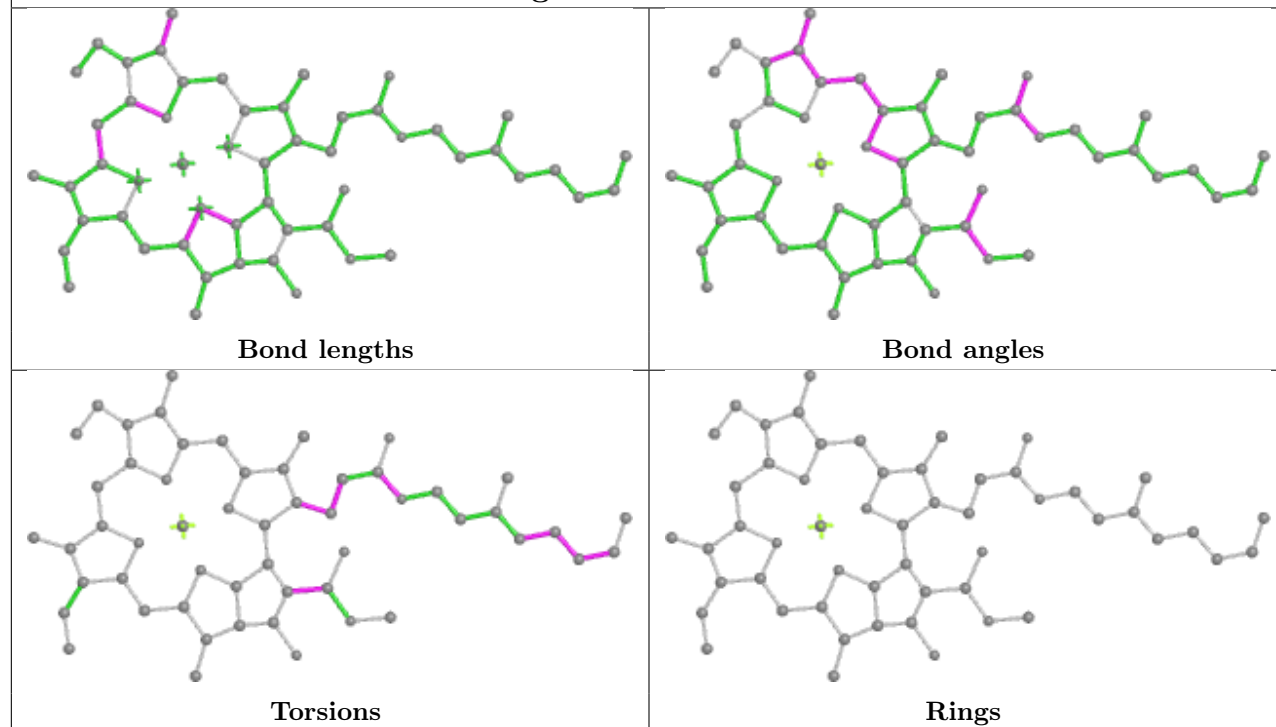
Torsions



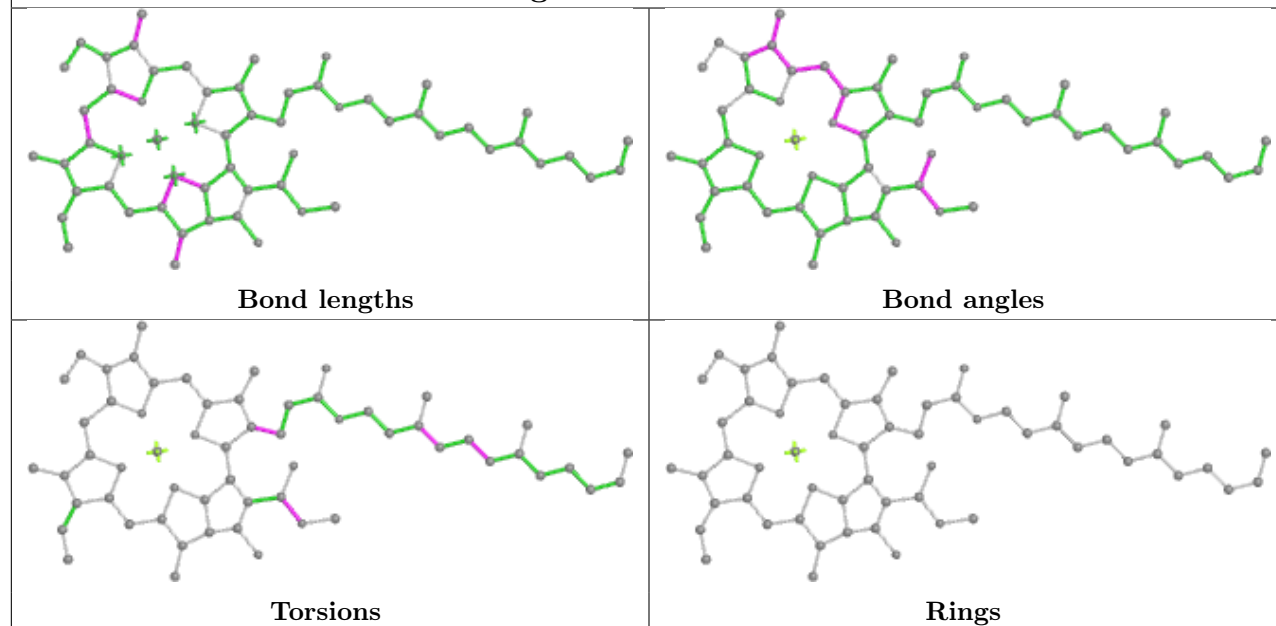
Rings



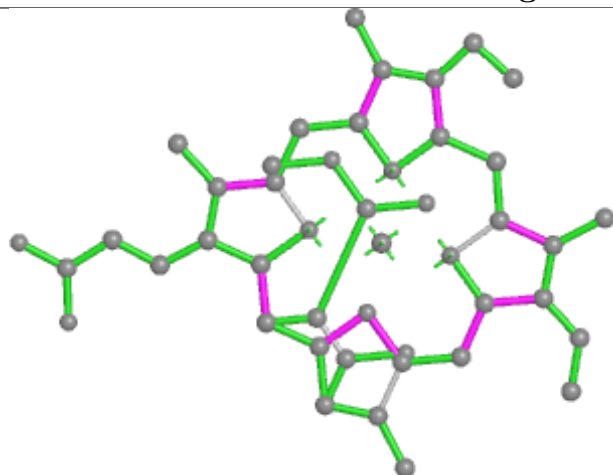
Ligand CLA A 811



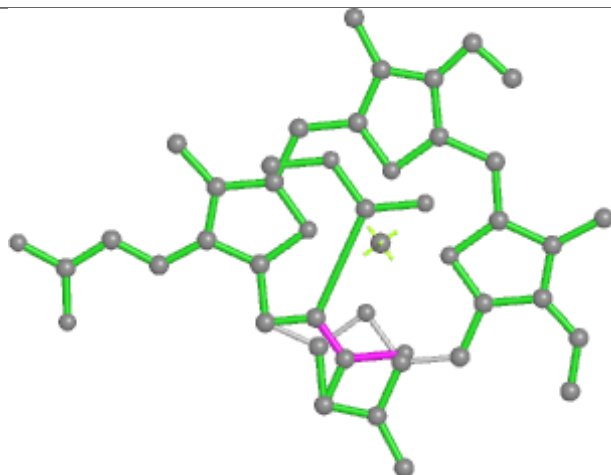
Ligand CLA m 603



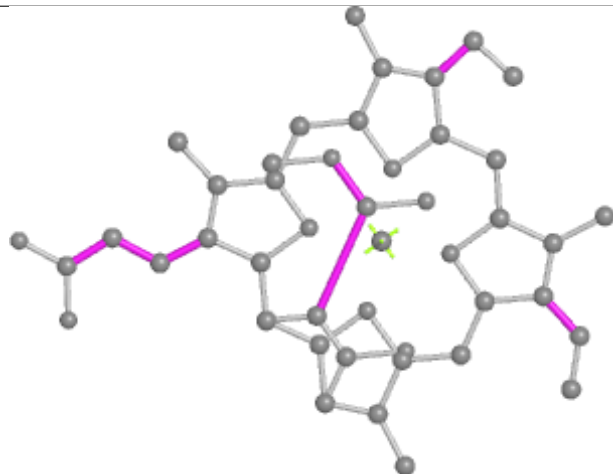
Ligand KC2 d 311



Bond lengths



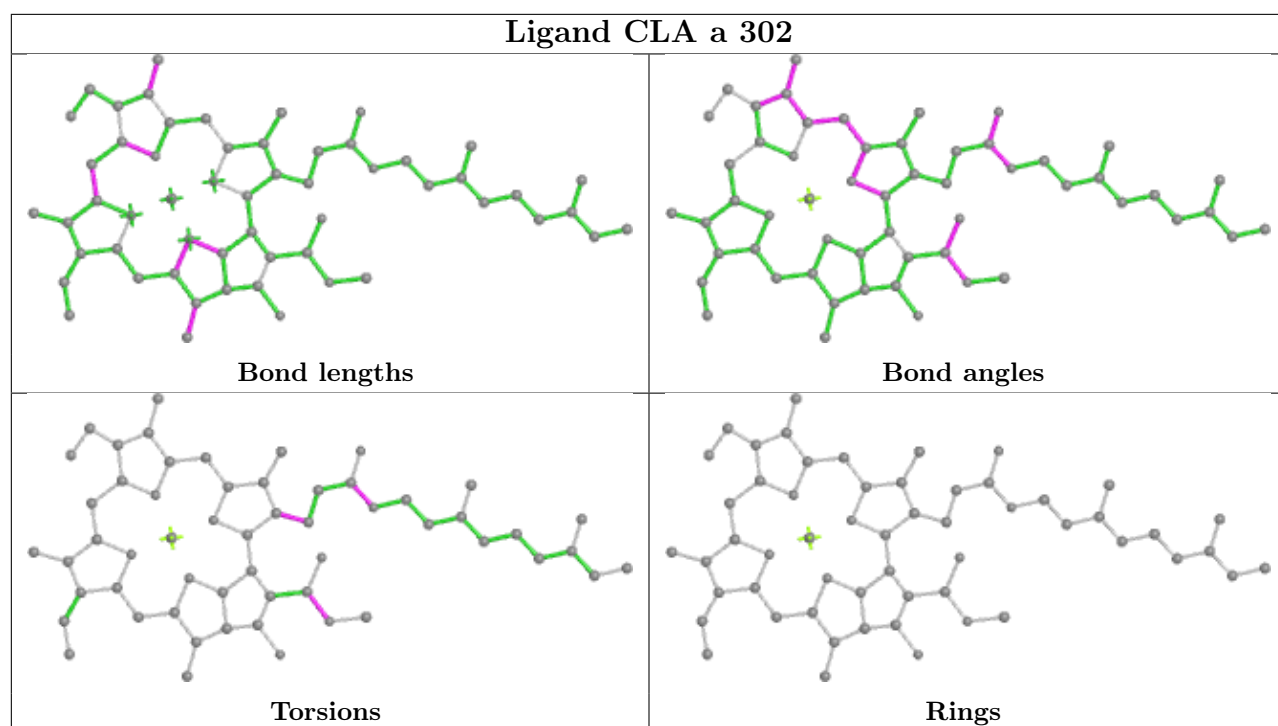
Bond angles



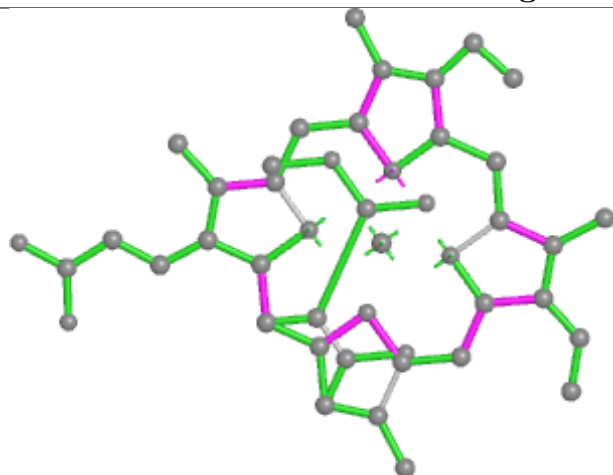
Torsions



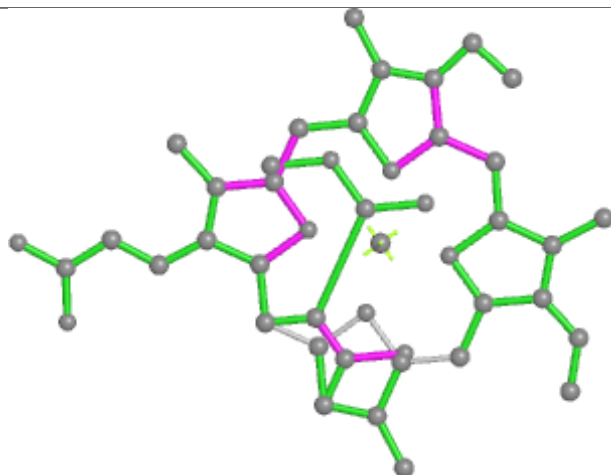
Rings



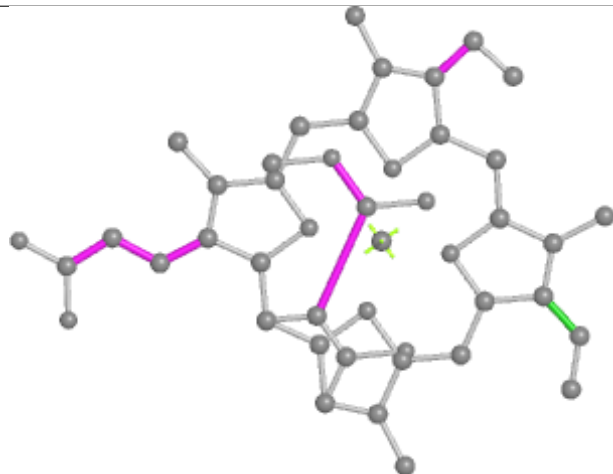
Ligand KC2 d 312



Bond lengths



Bond angles

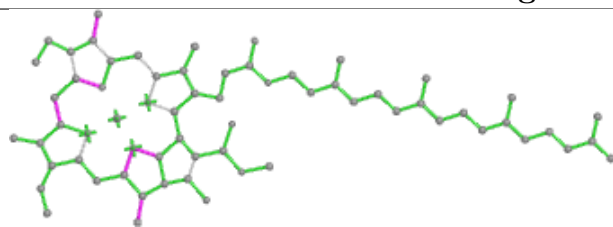


Torsions

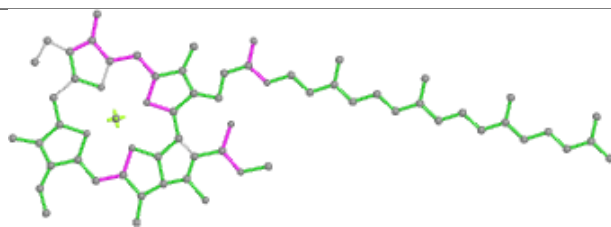


Rings

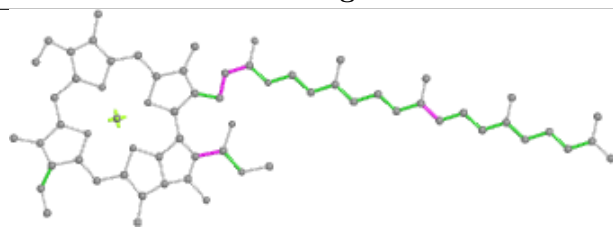
Ligand CLA a 304



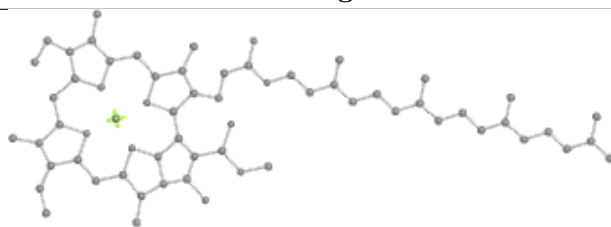
Bond lengths



Bond angles

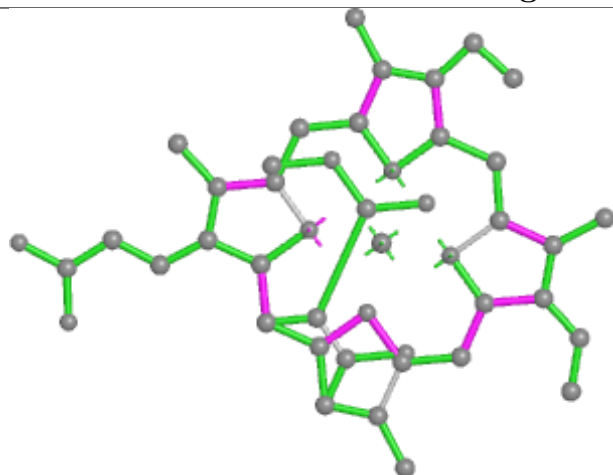


Torsions

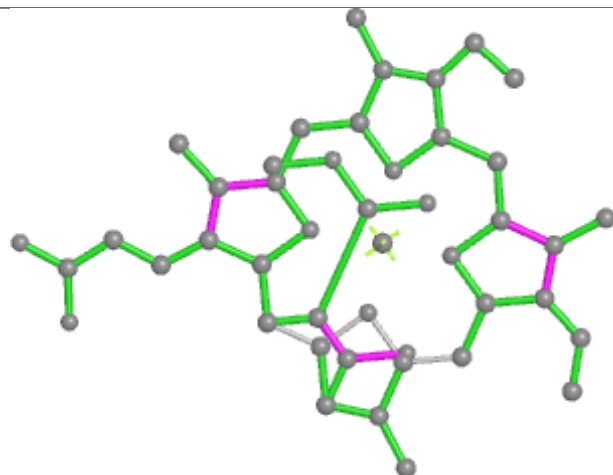


Rings

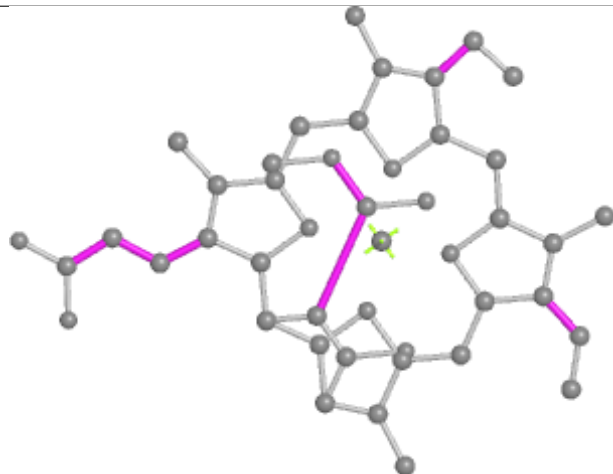
Ligand KC2 k 611



Bond lengths



Bond angles

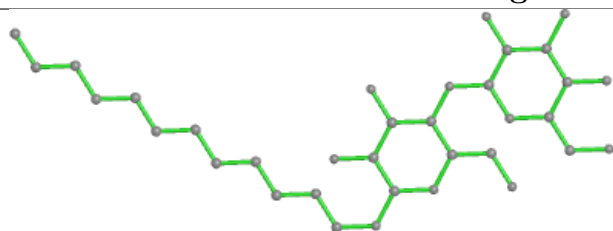


Torsions

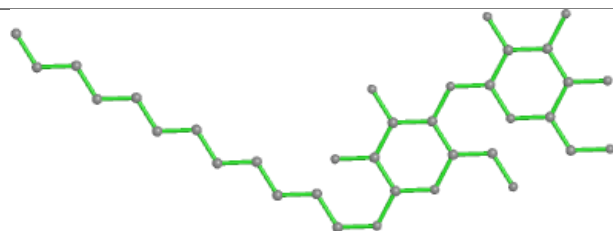


Rings

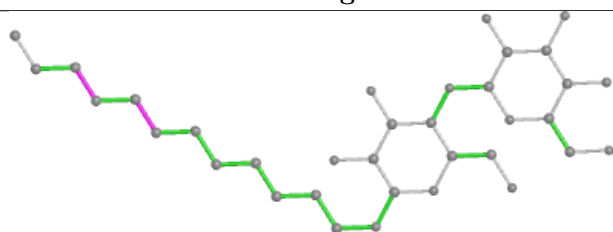
Ligand LMU B 852



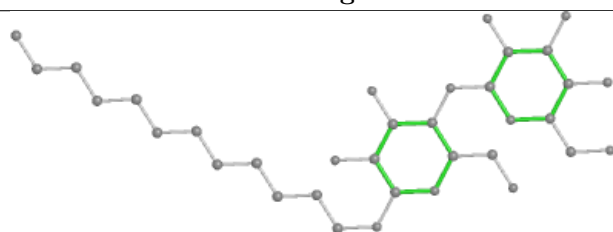
Bond lengths



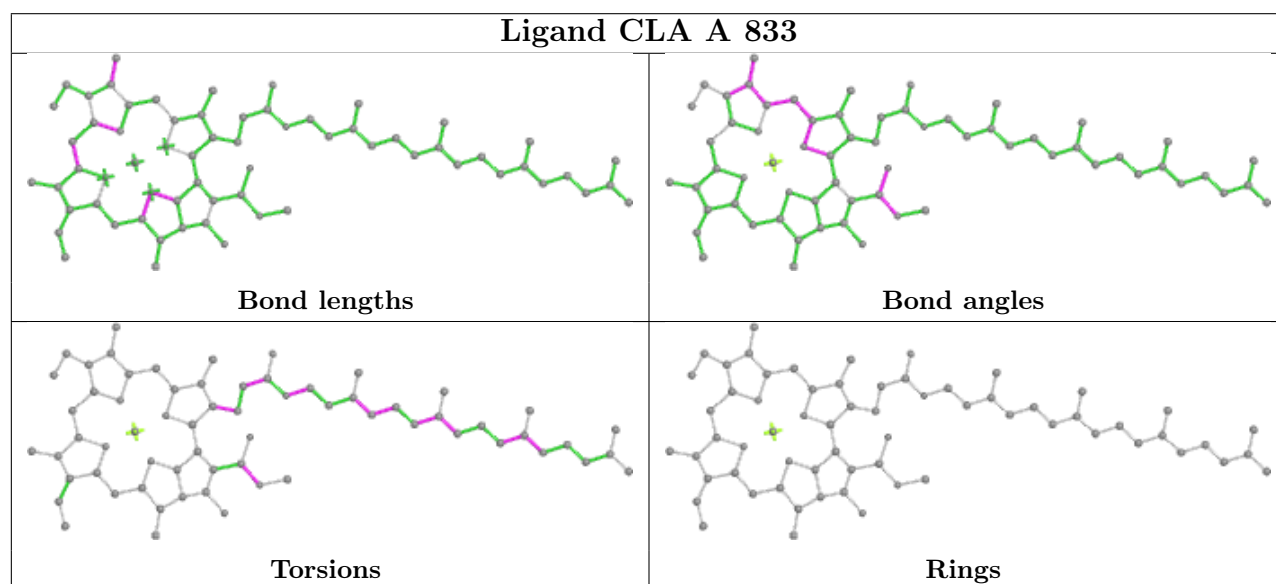
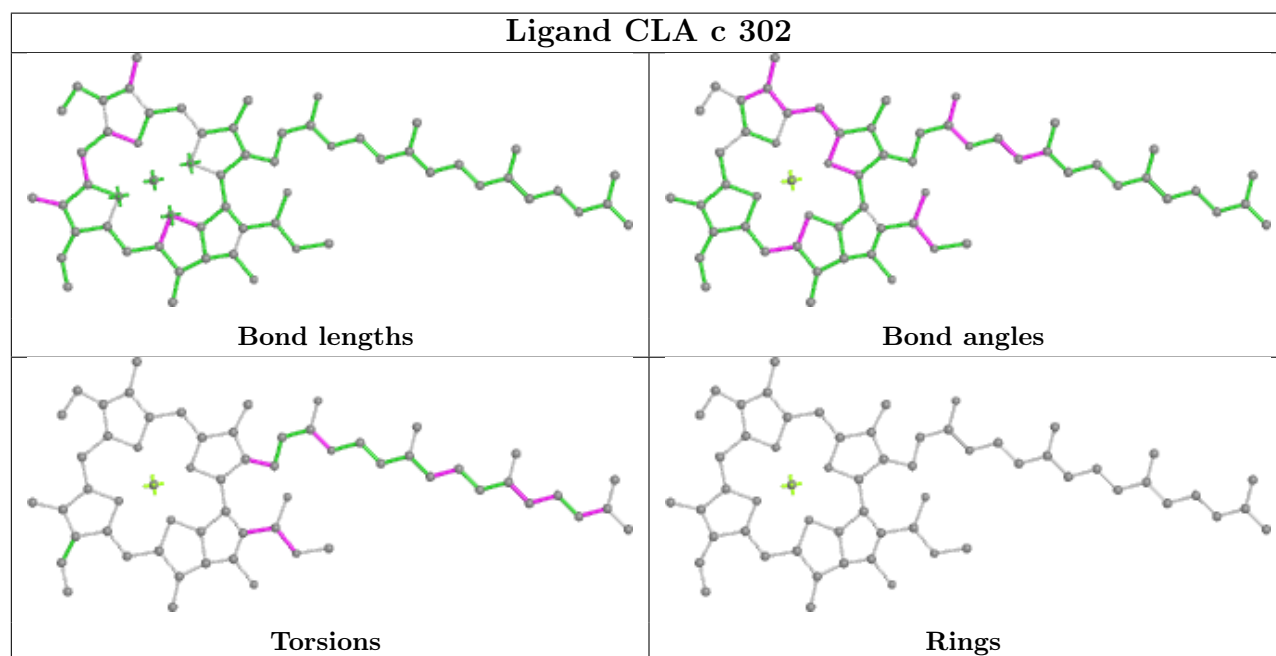
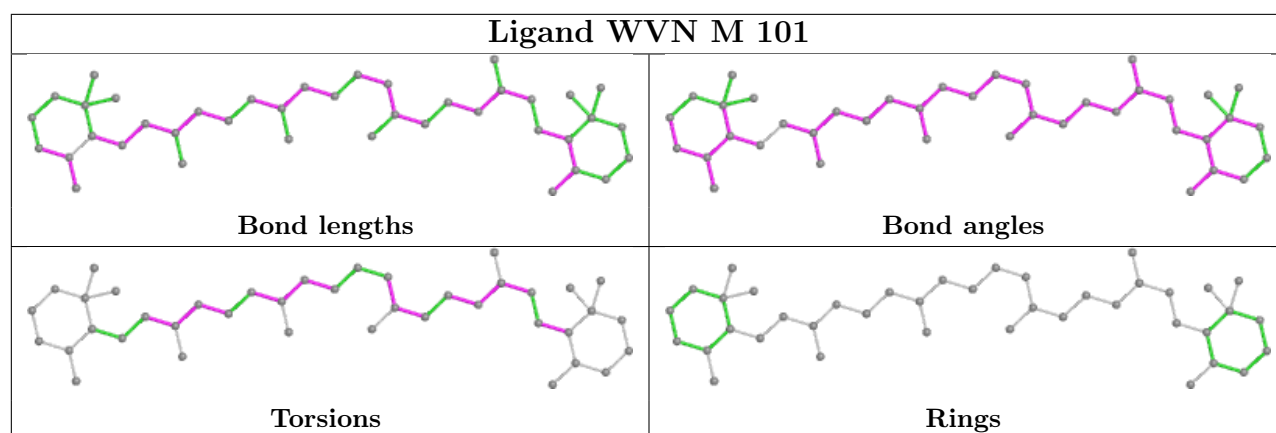
Bond angles

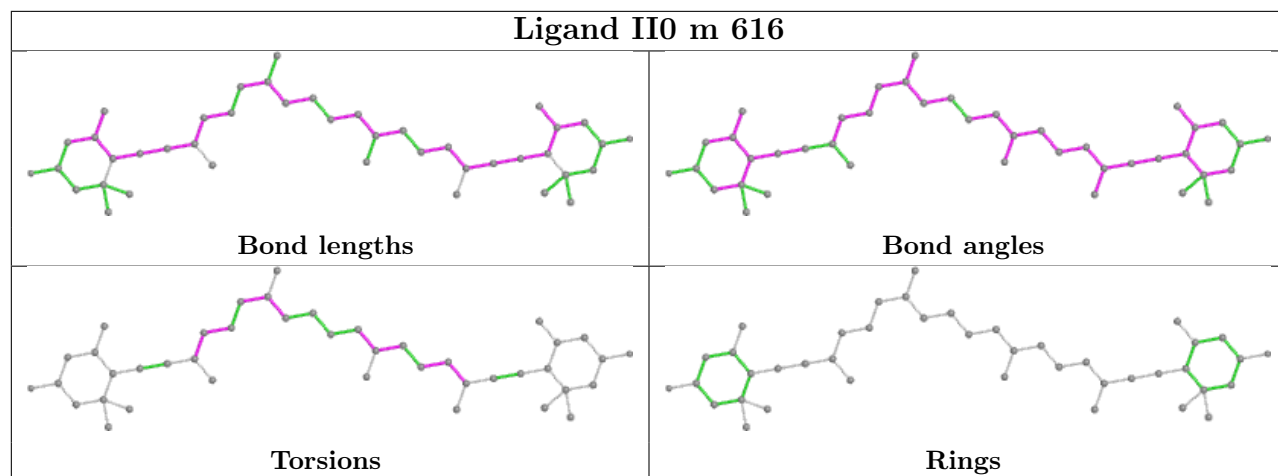
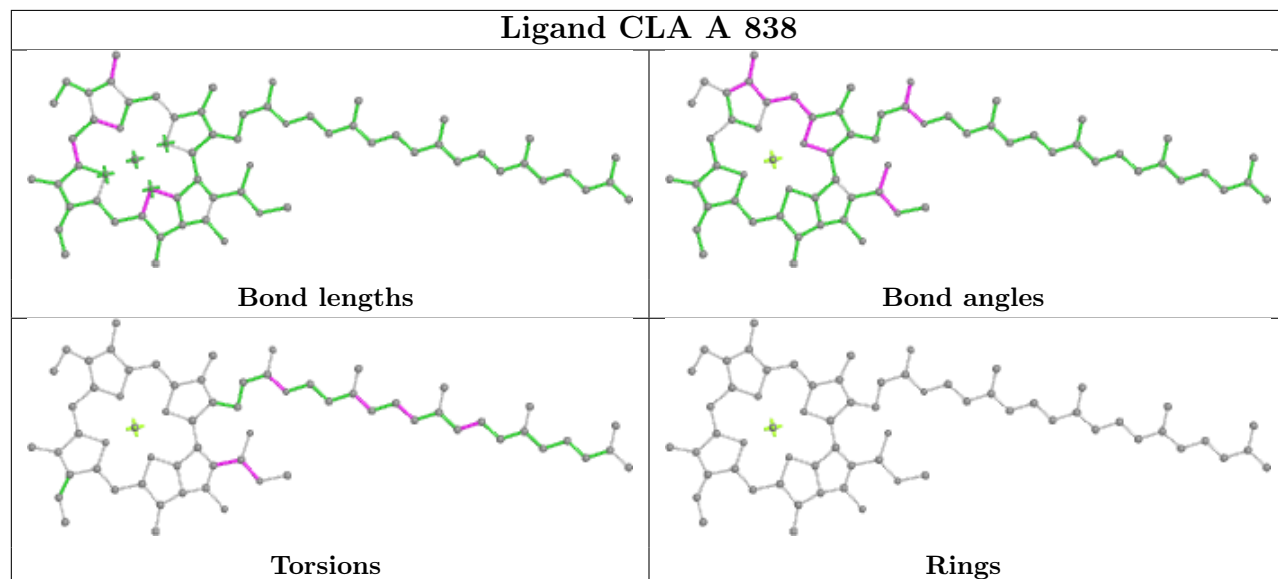
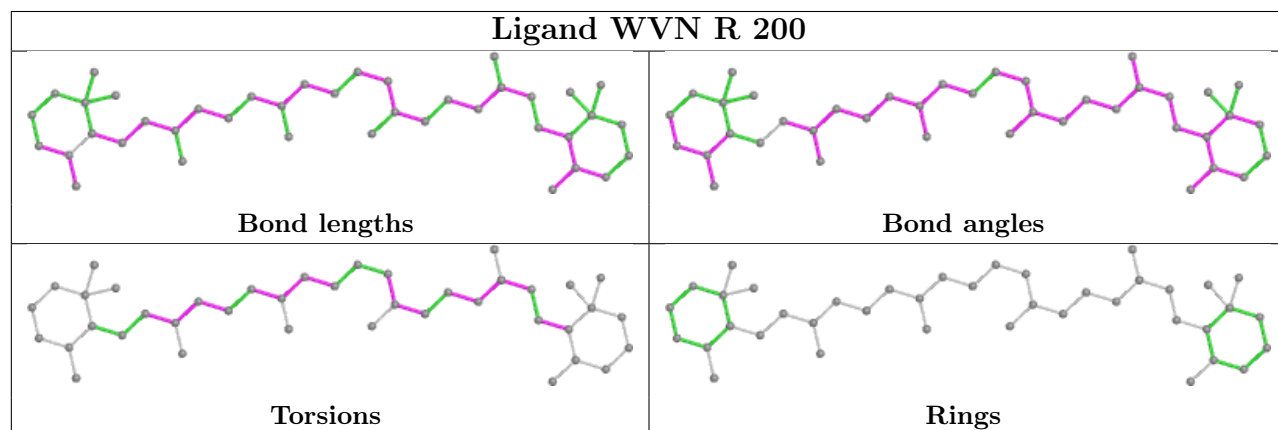


Torsions

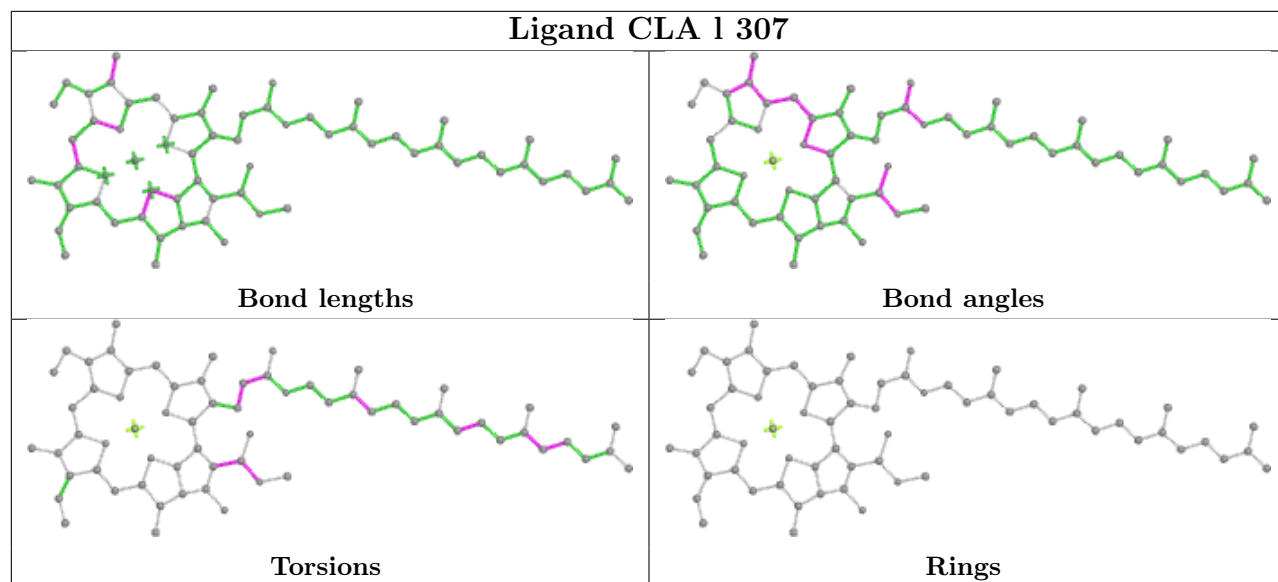


Rings

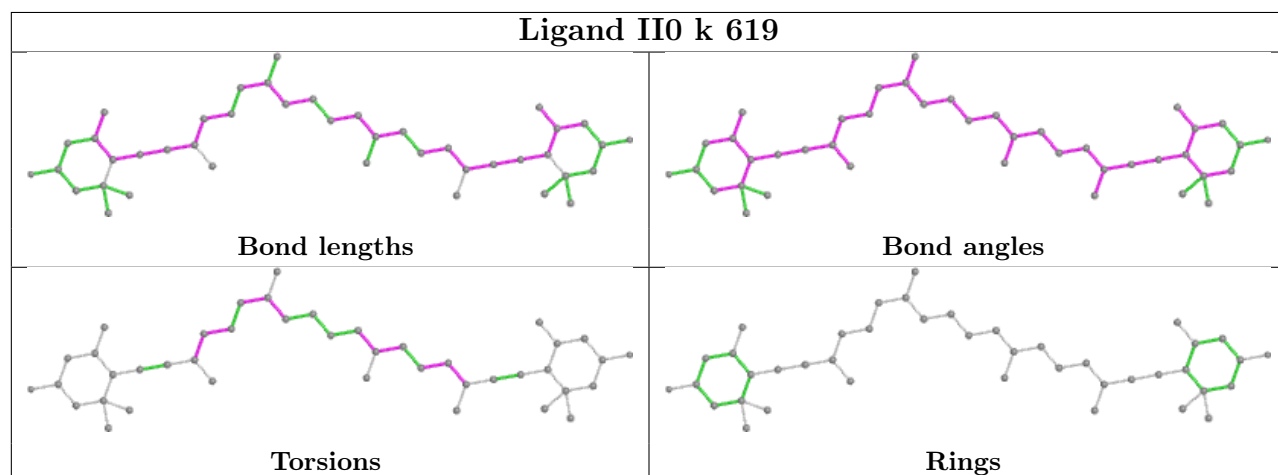


Ligand II0 m 616**Ligand CLA A 838****Ligand WVN R 200**

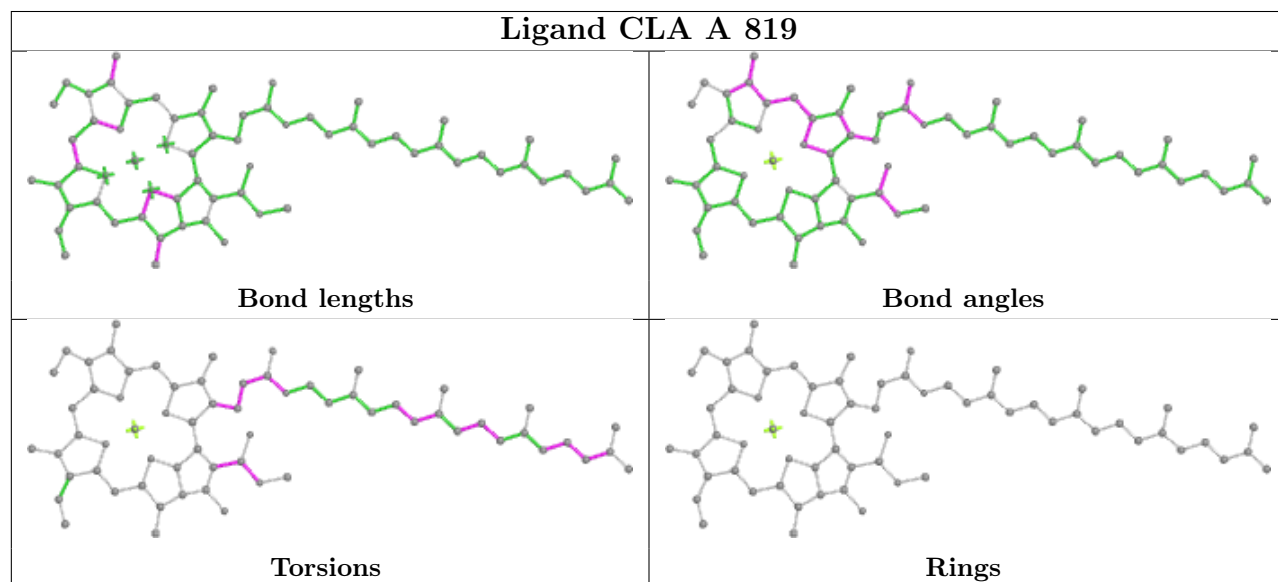
Ligand CLA I 307



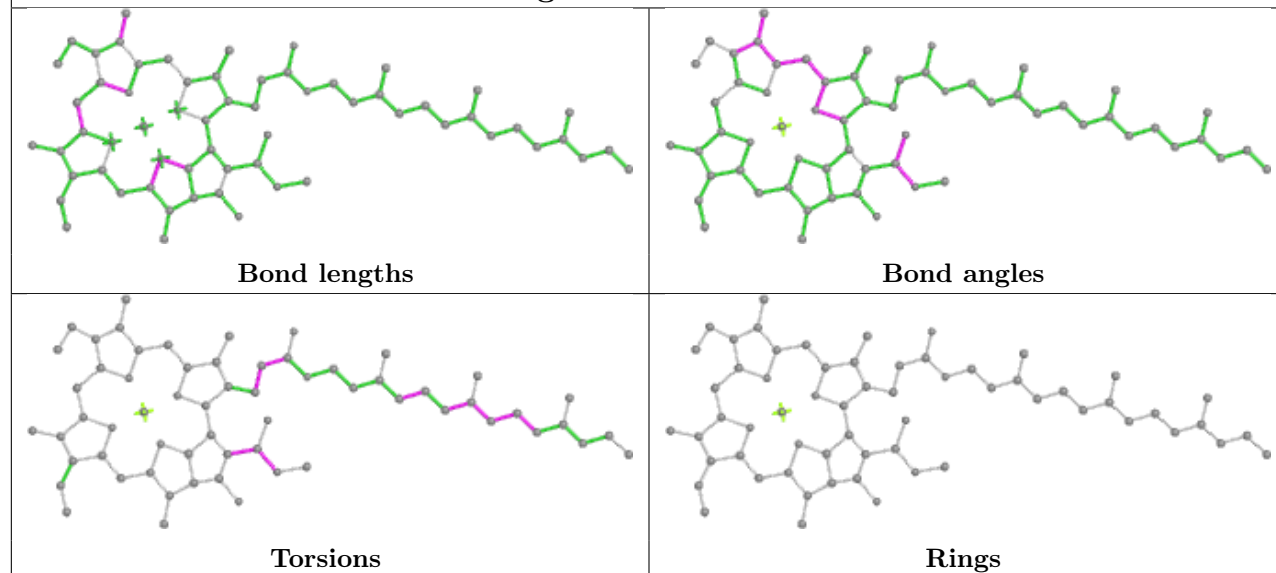
Ligand II0 k 619



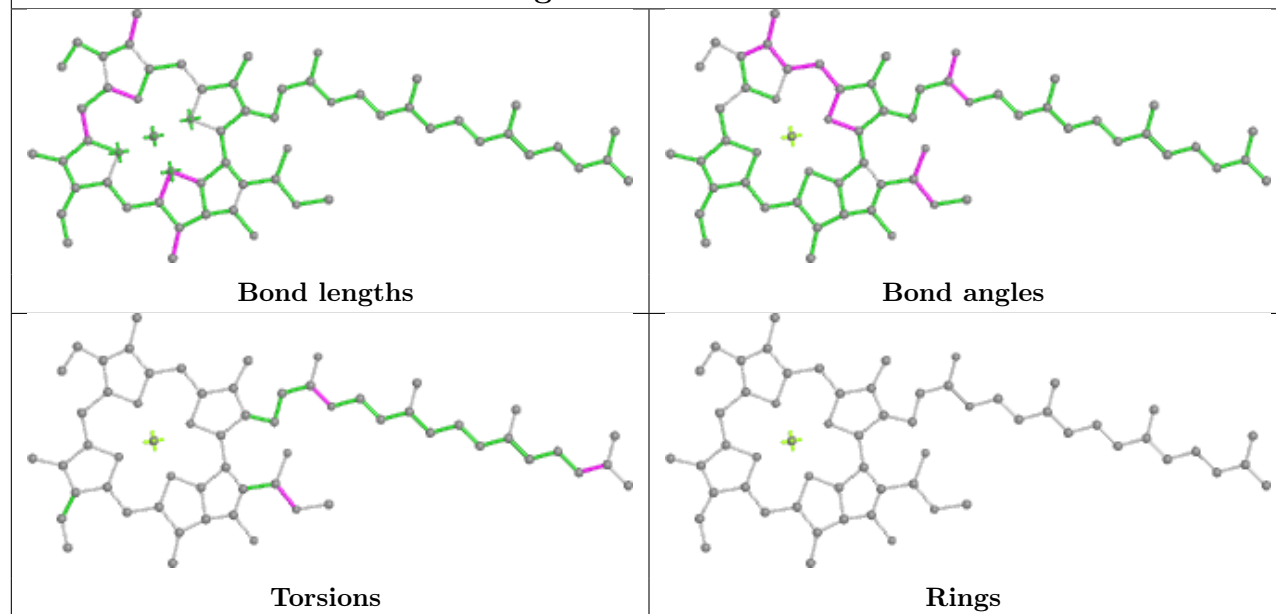
Ligand CLA A 819



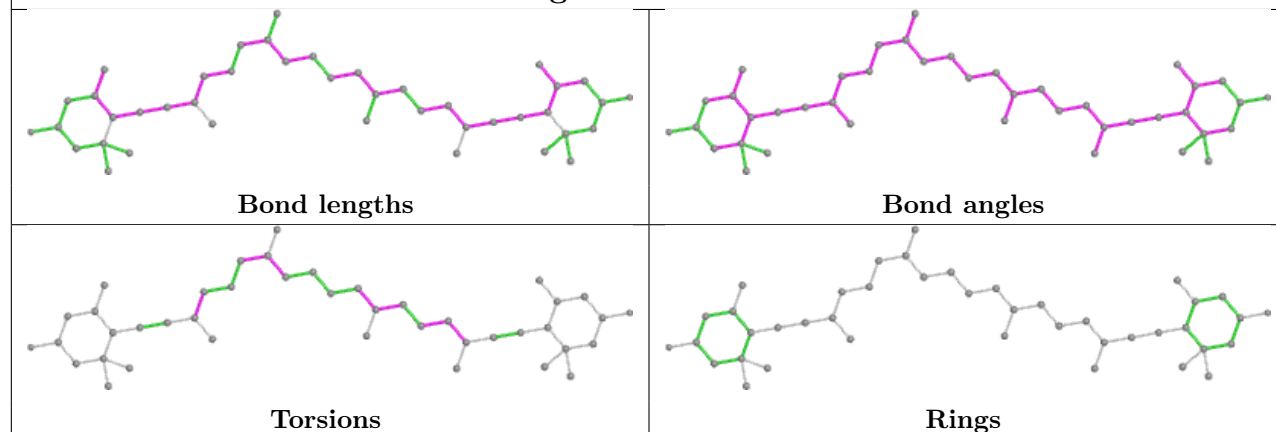
Ligand CLA c 304

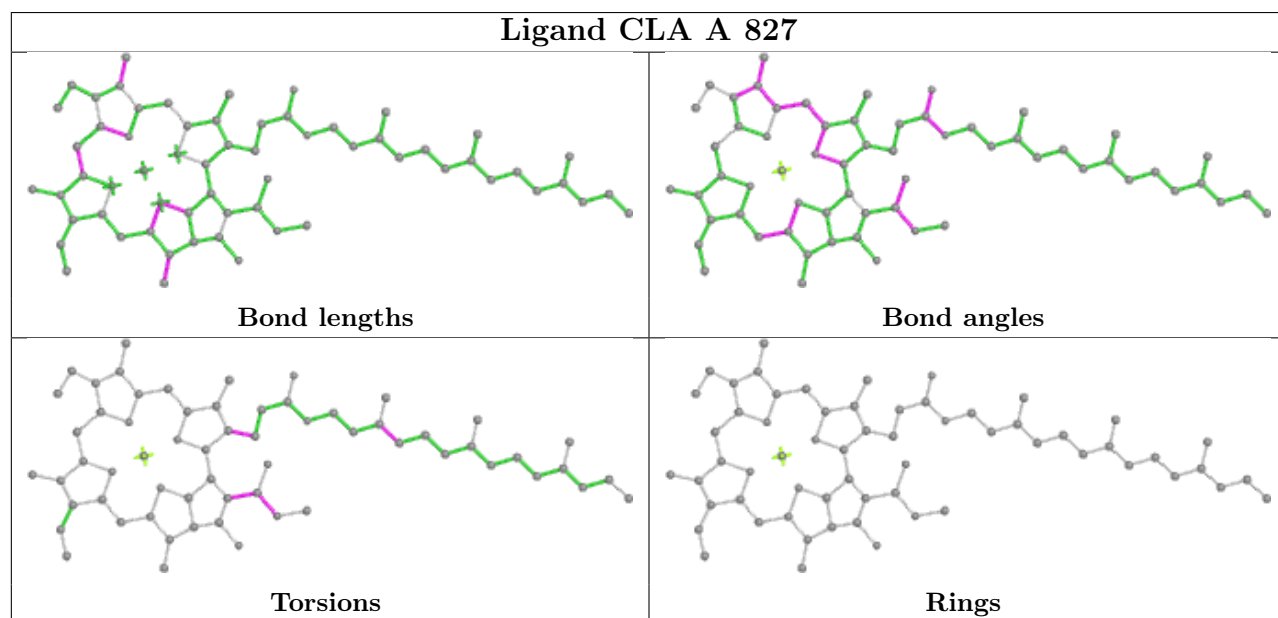
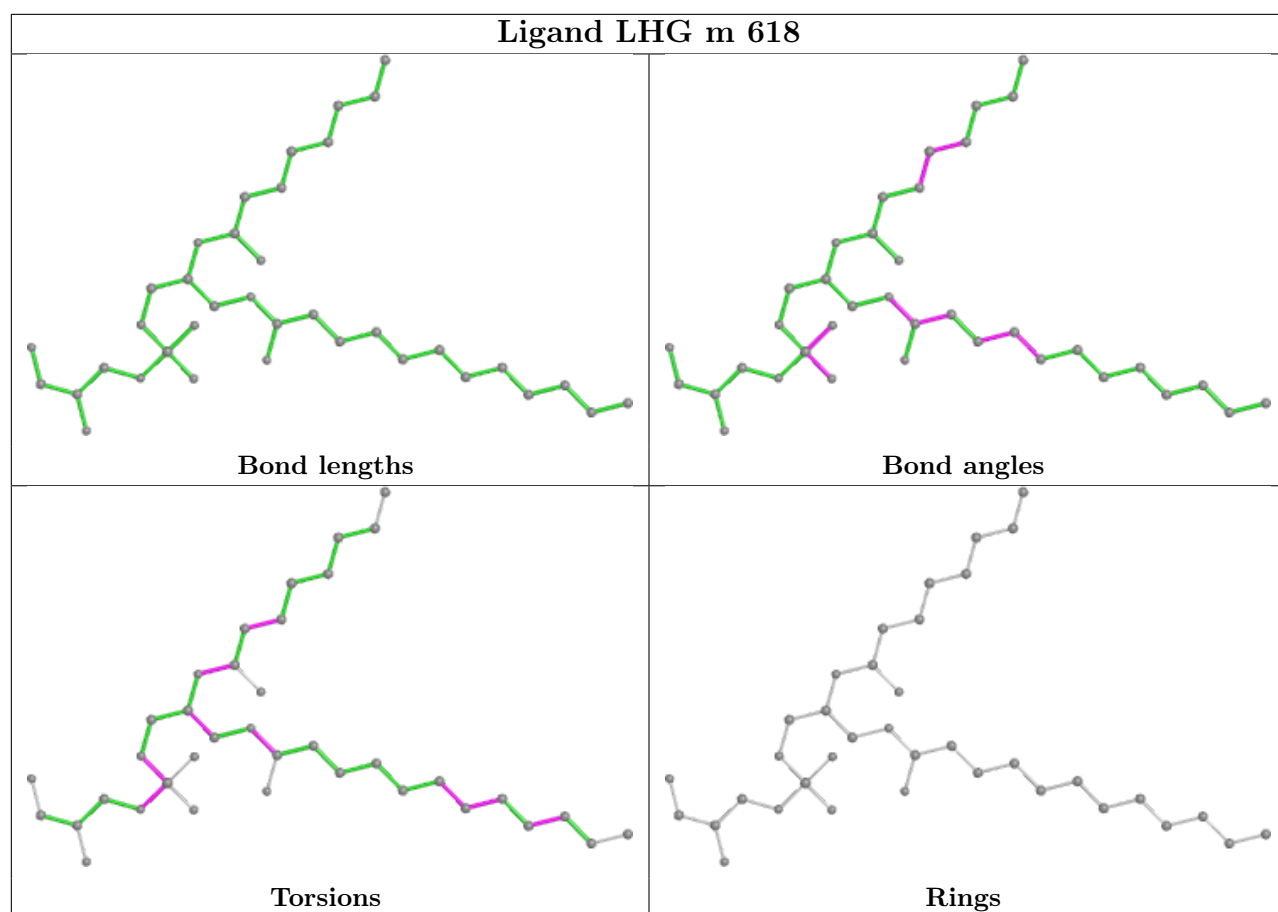


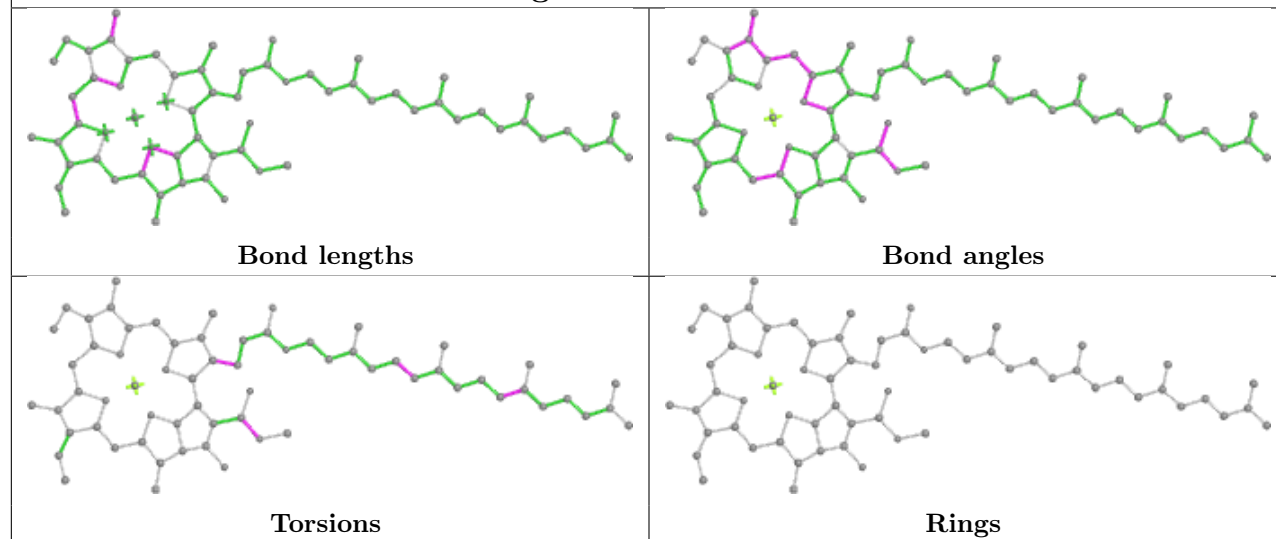
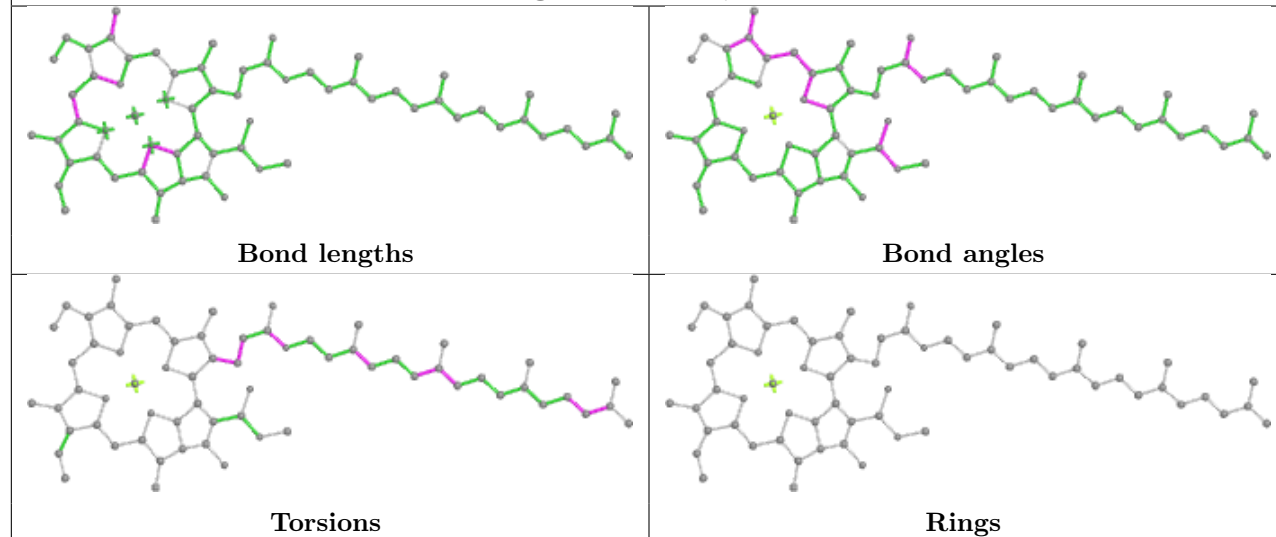
Ligand CLA L 204



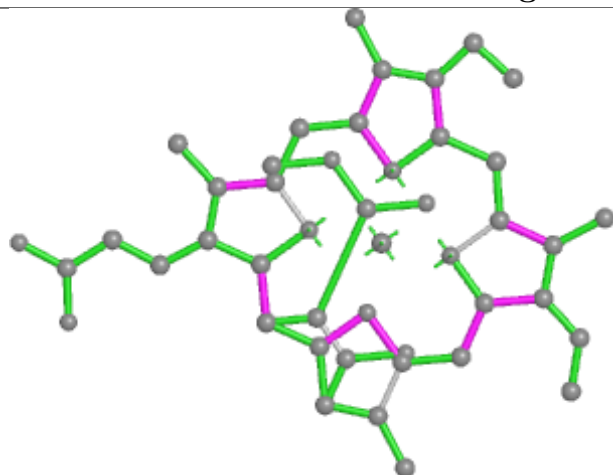
Ligand II0 b 314



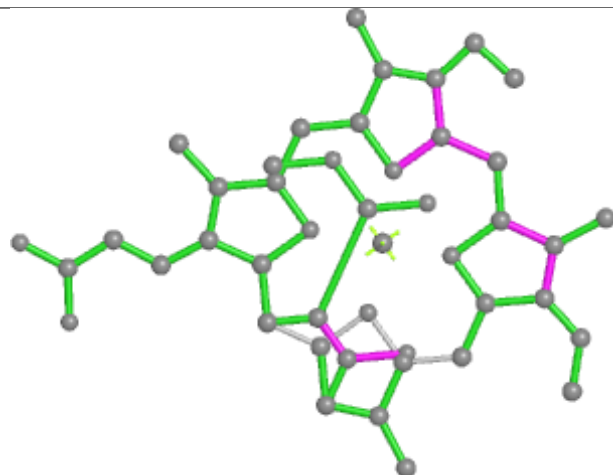


Ligand CLA A 832**Ligand CLA Q 302**

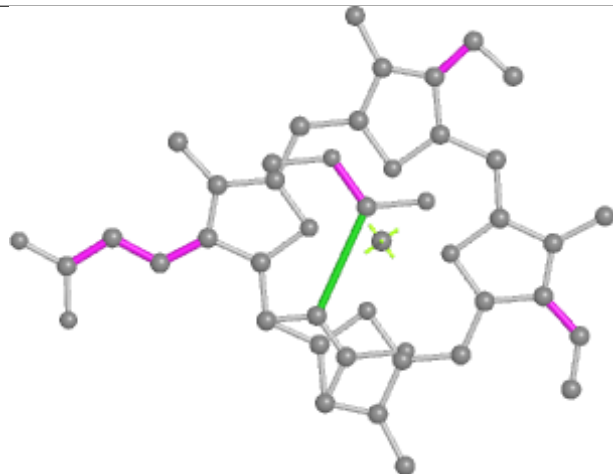
Ligand KC2 n 612



Bond lengths



Bond angles

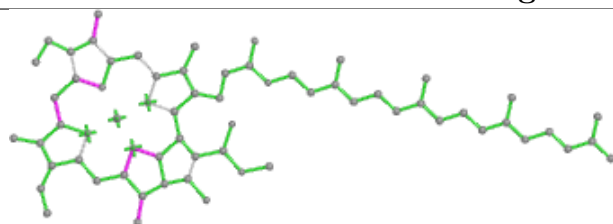


Torsions

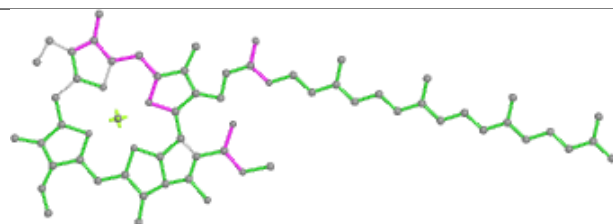


Rings

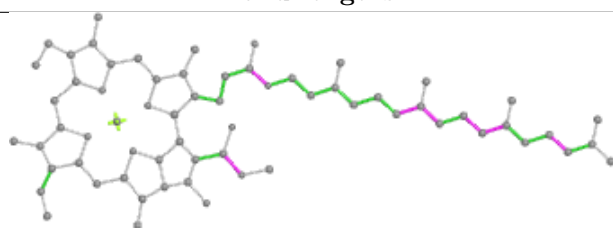
Ligand CLA a 310



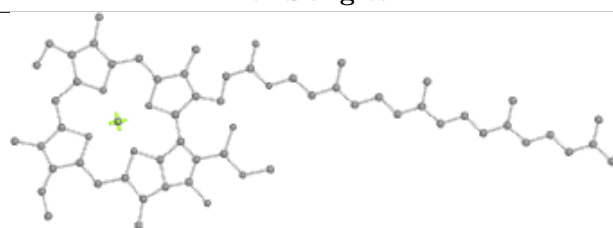
Bond lengths



Bond angles

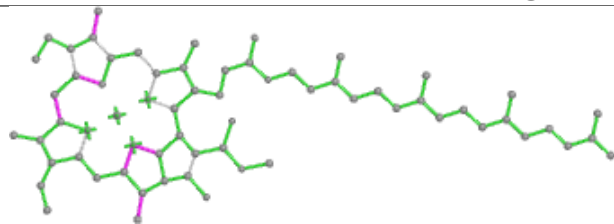


Torsions

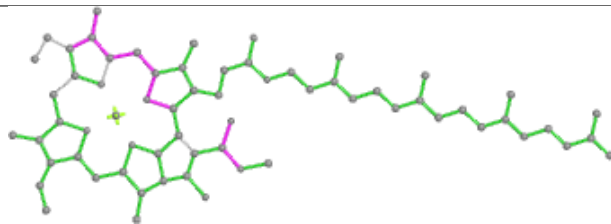


Rings

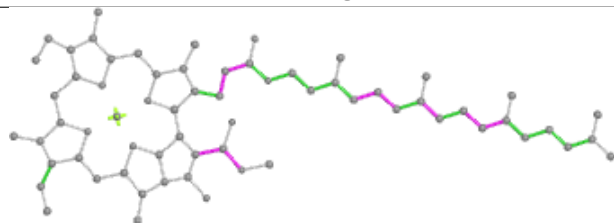
Ligand CLA i 304



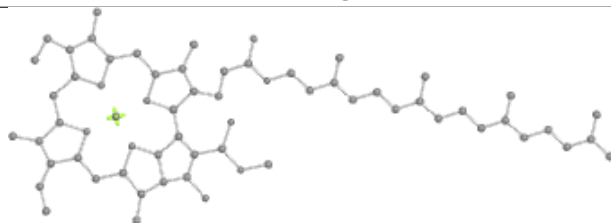
Bond lengths



Bond angles

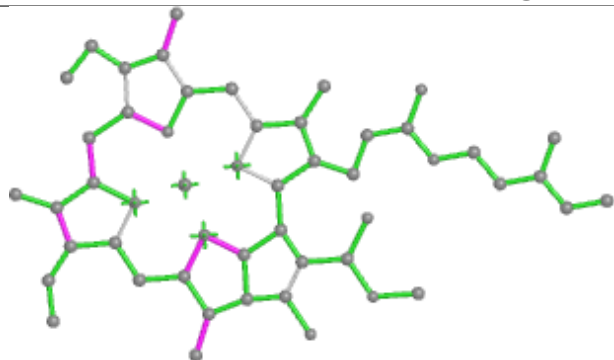


Torsions

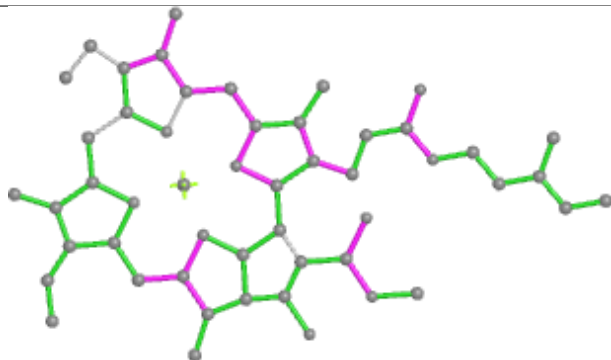


Rings

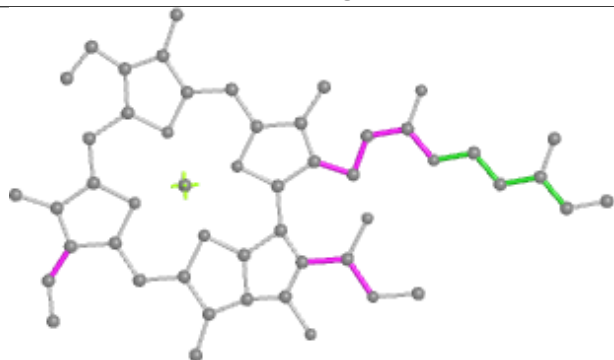
Ligand CLA k 607



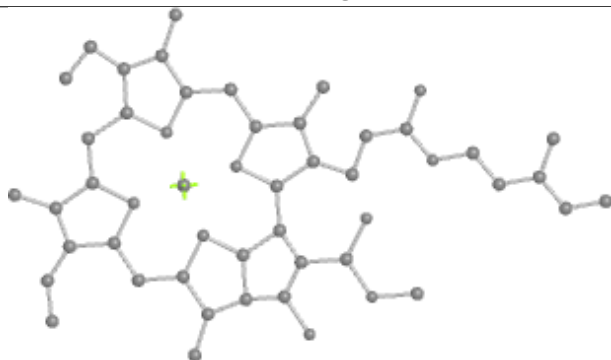
Bond lengths



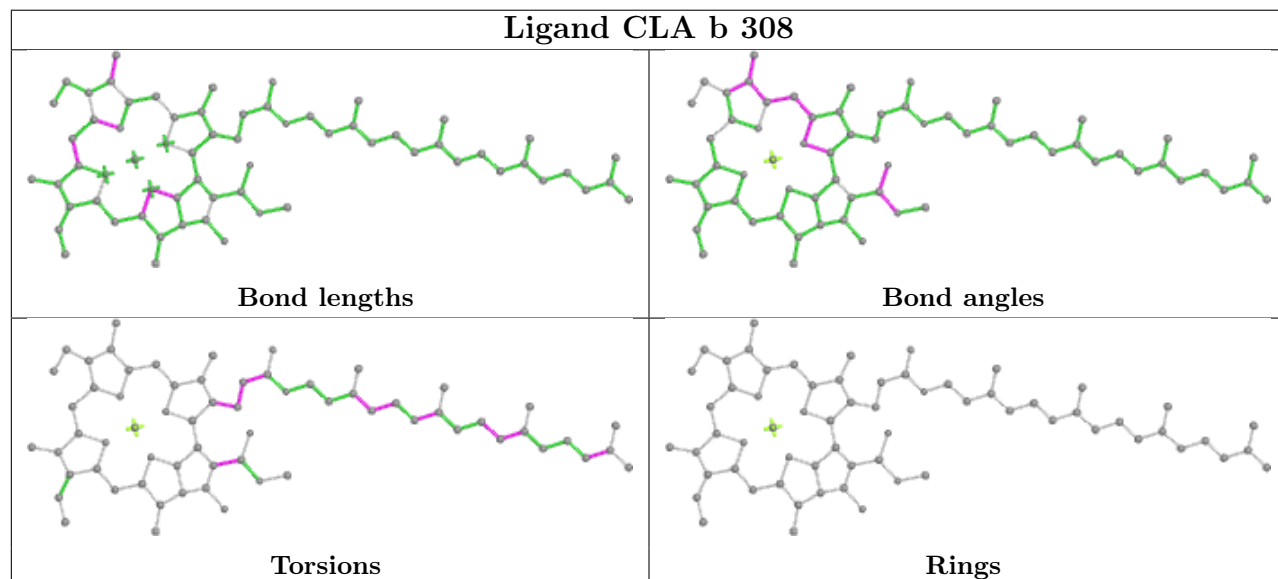
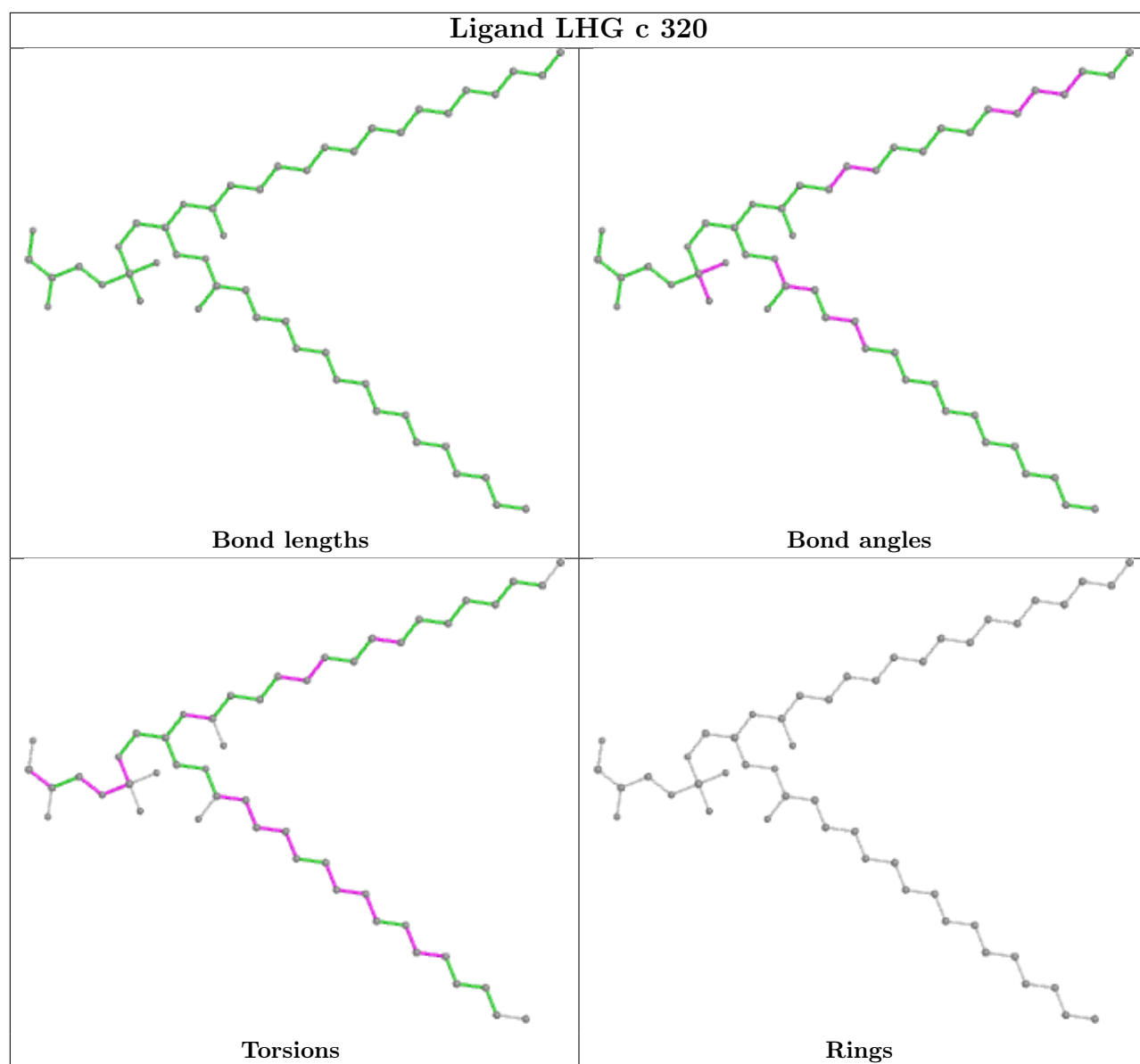
Bond angles

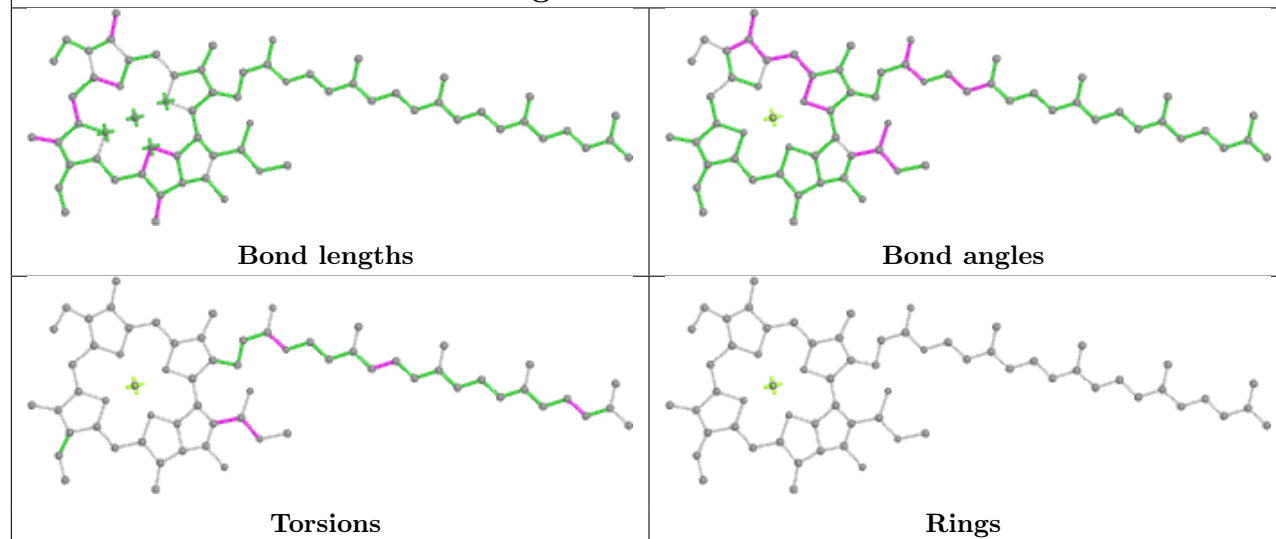
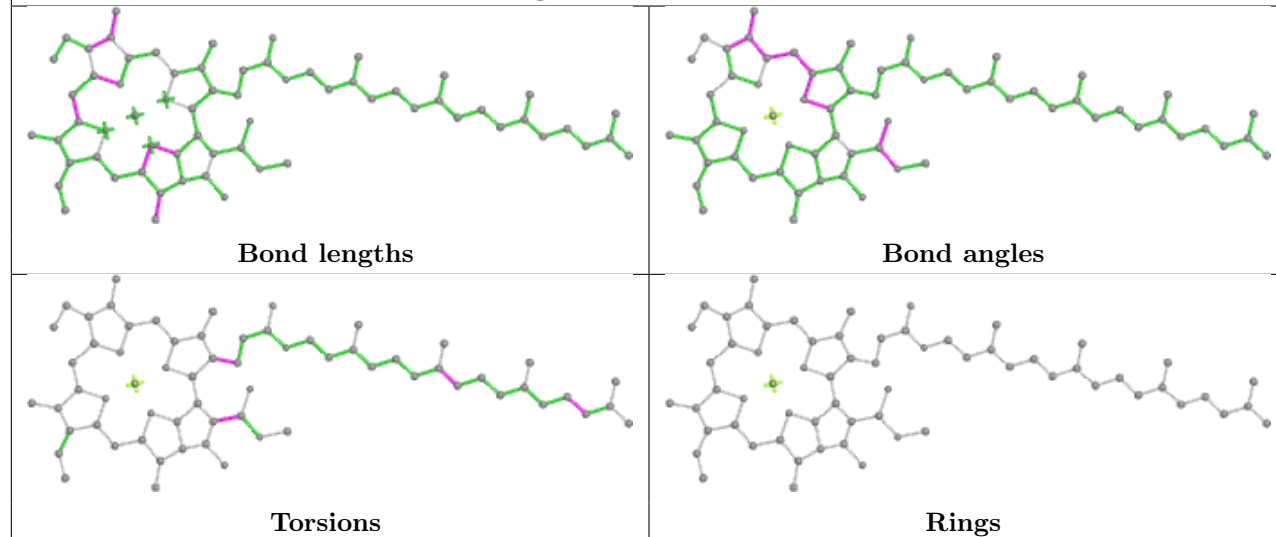
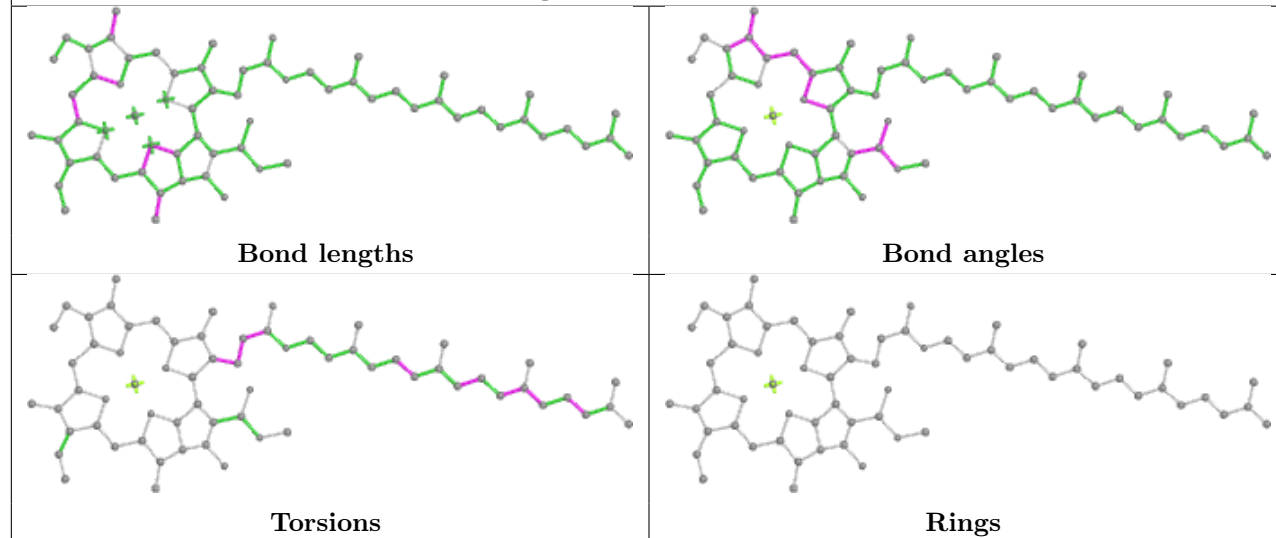


Torsions

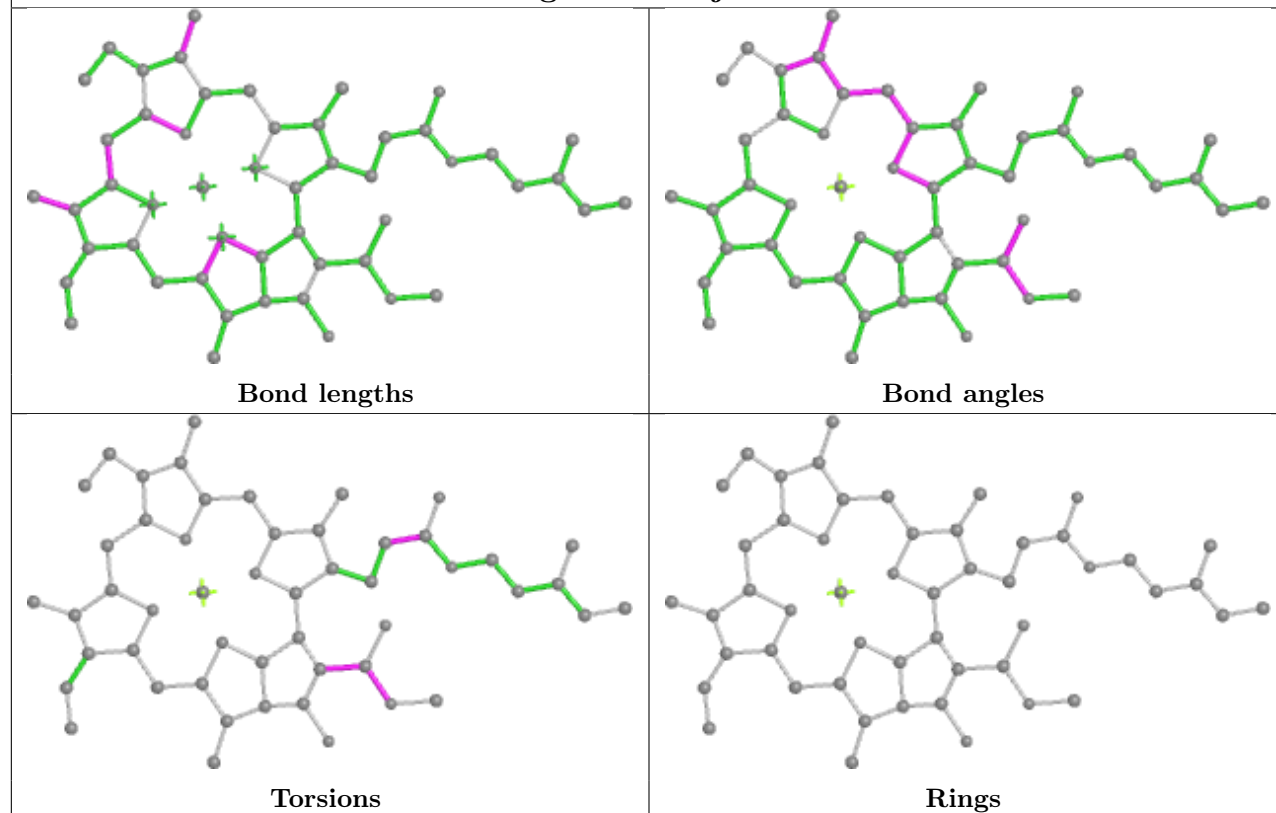


Rings

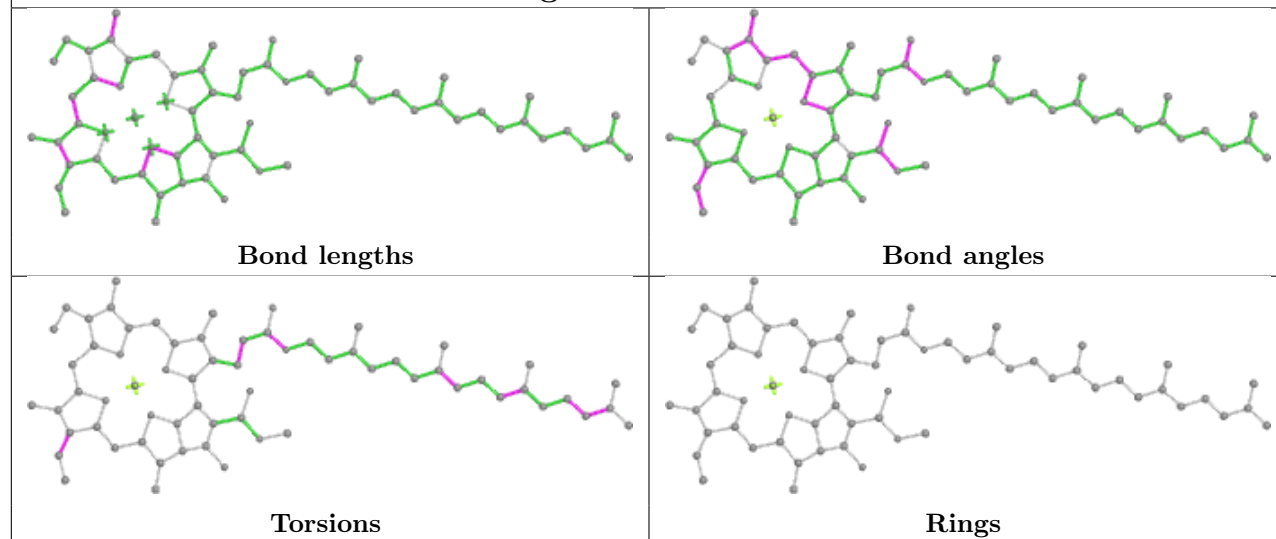


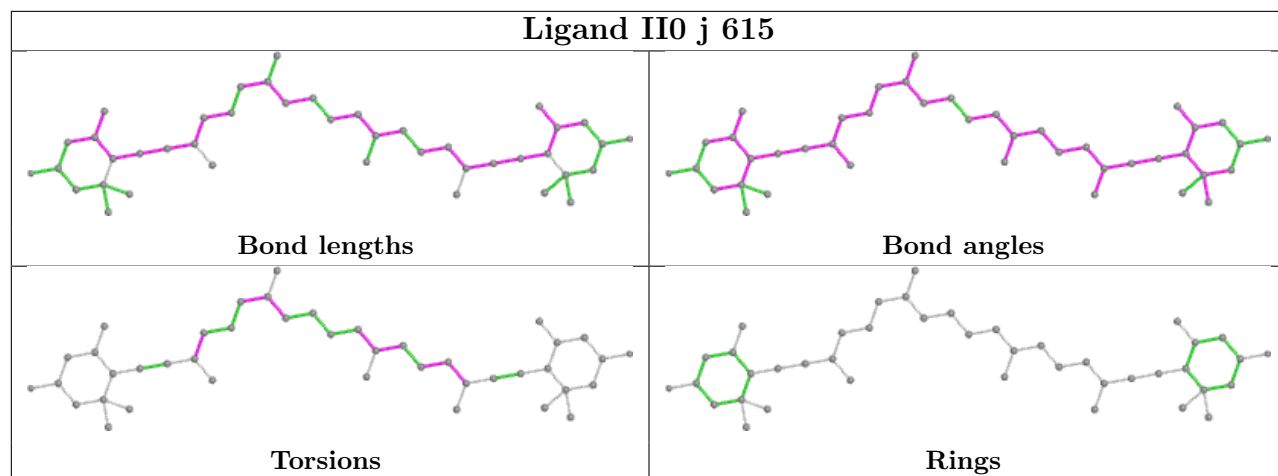
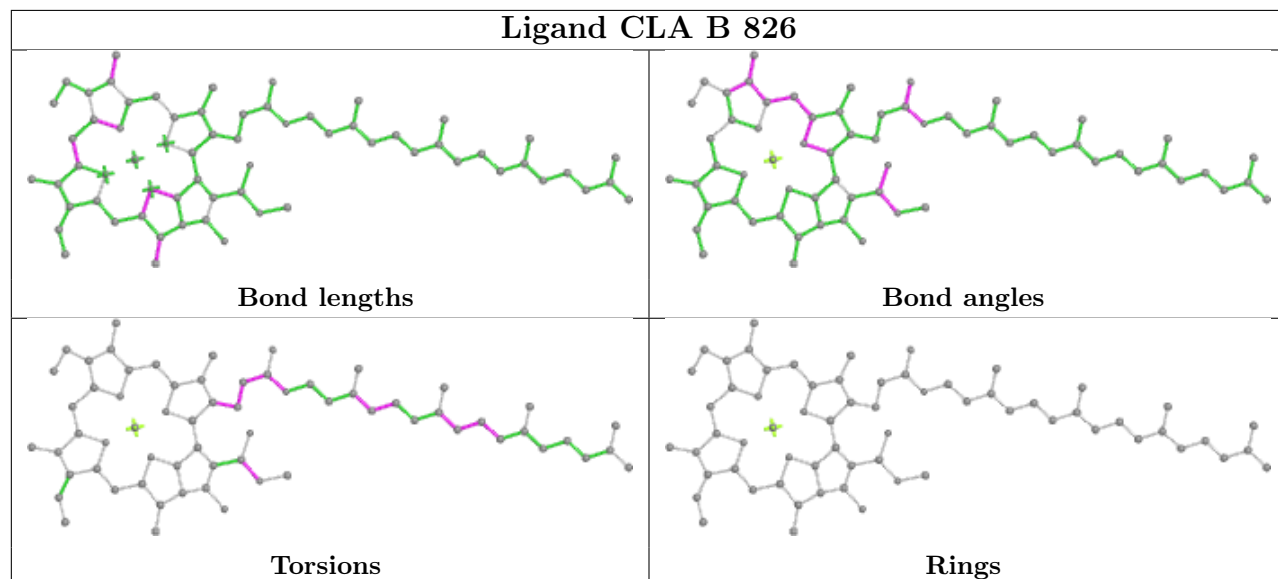
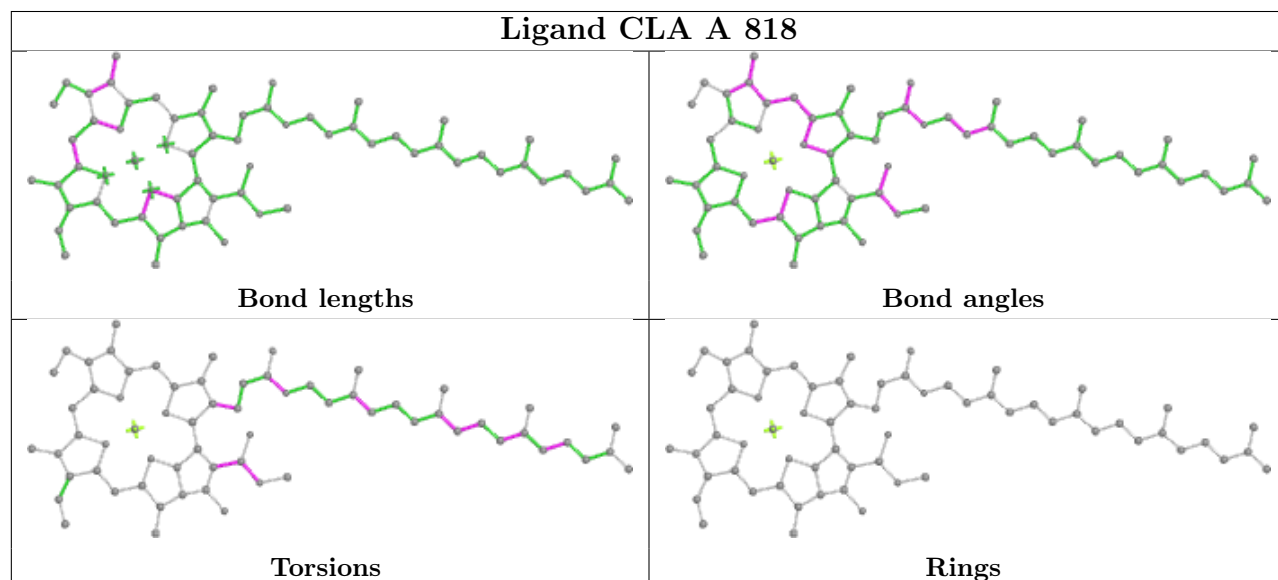
Ligand CLA B 808**Ligand CLA A 829****Ligand CLA a 306**

Ligand CLA j 603

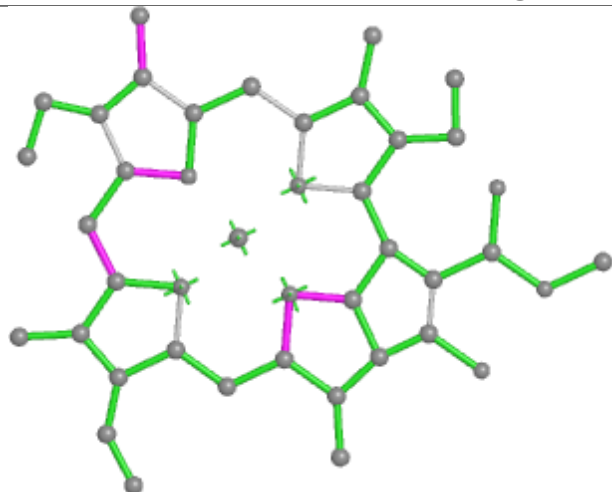


Ligand CLA i 311

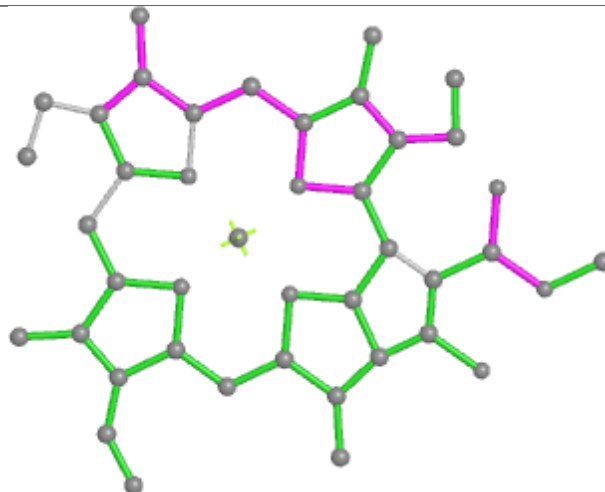


Ligand II0 j 615**Ligand CLA B 826****Ligand CLA A 818**

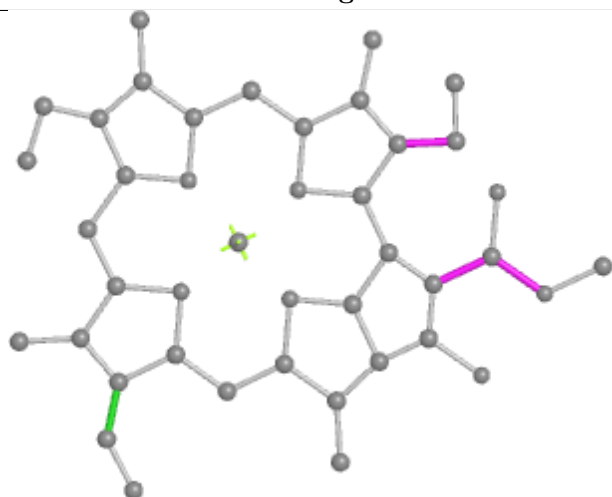
Ligand CLA m 601



Bond lengths



Bond angles

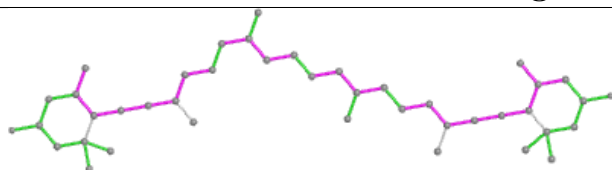


Torsions

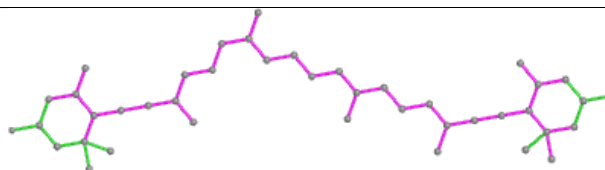


Rings

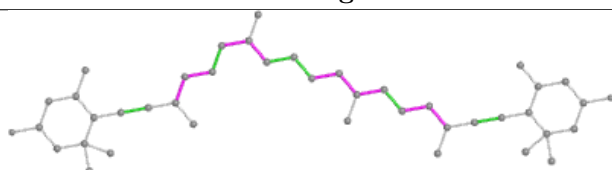
Ligand II0 d 301



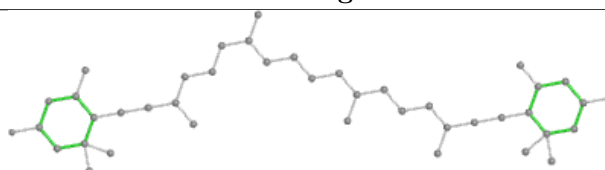
Bond lengths



Bond angles

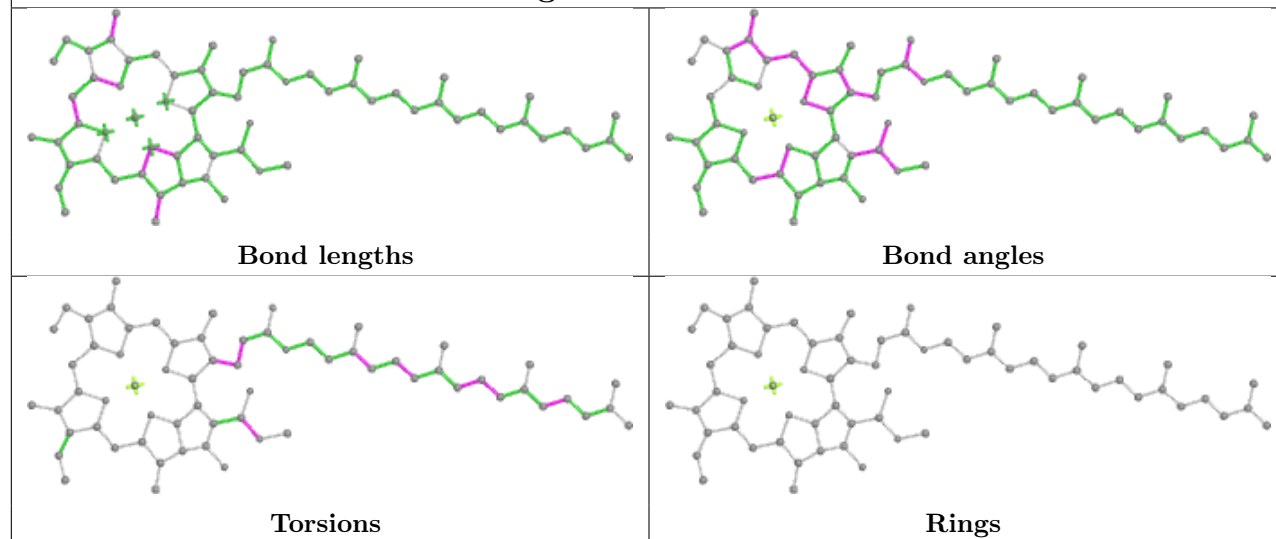


Torsions

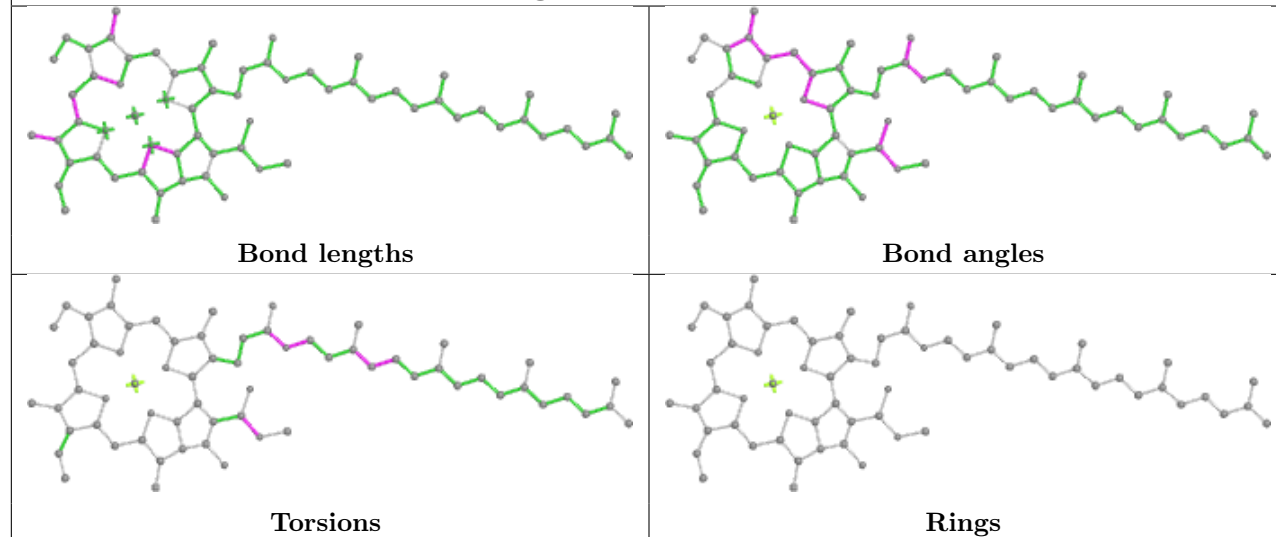


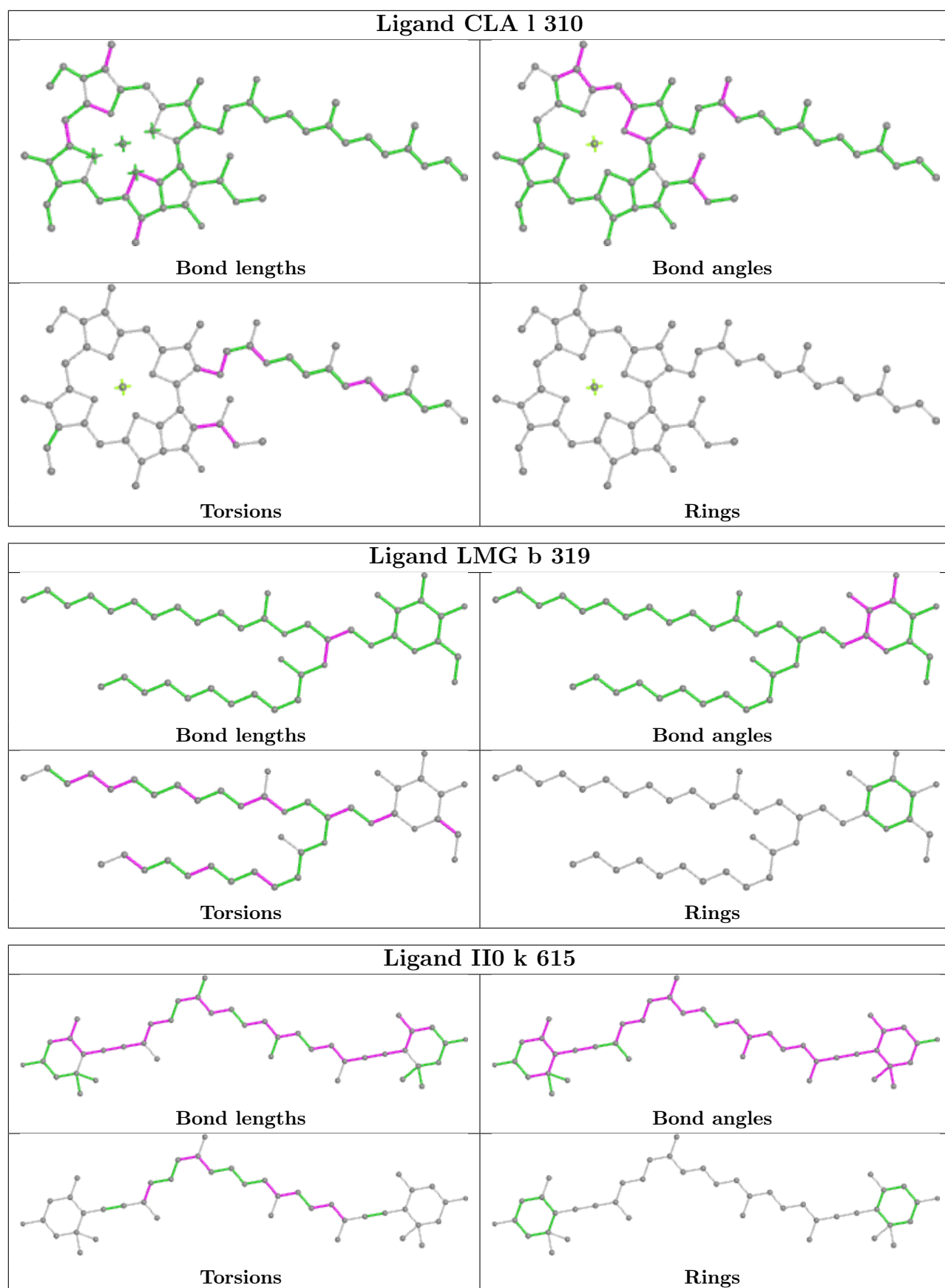
Rings

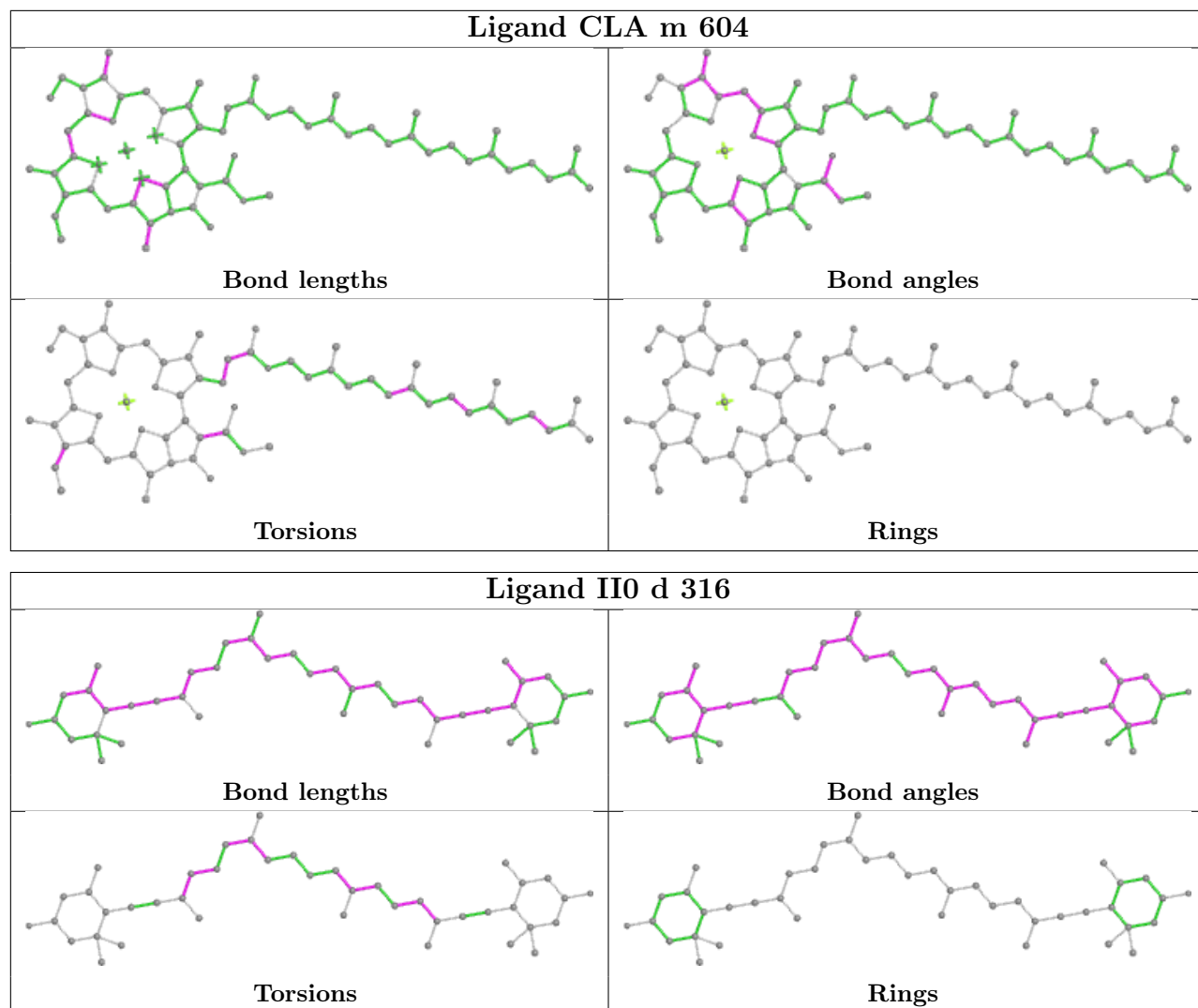
Ligand CLA s 406



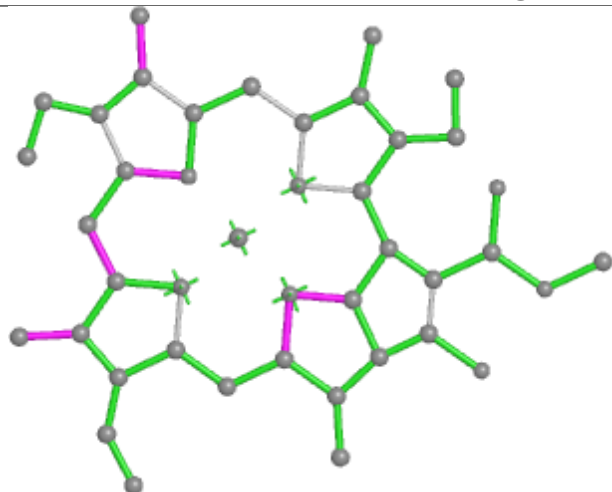
Ligand CLA A 820



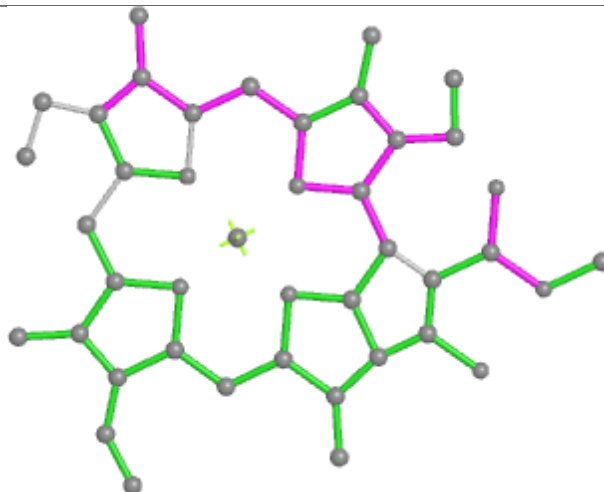




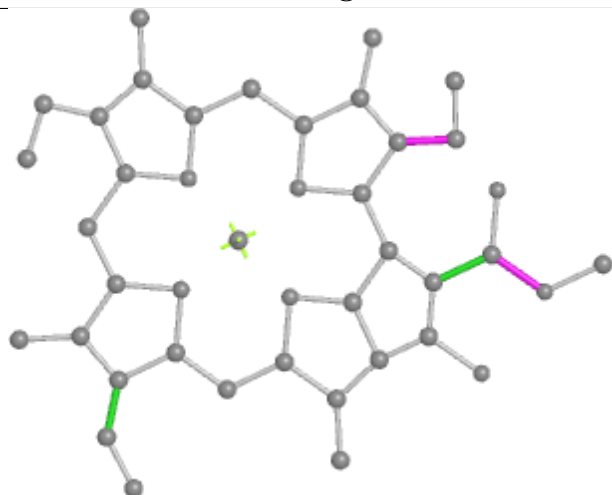
Ligand CLA K 101



Bond lengths



Bond angles

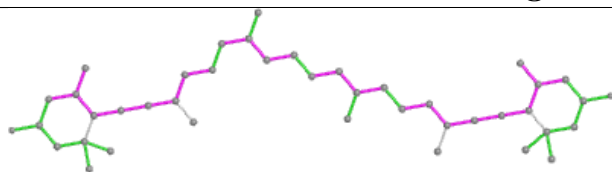


Torsions

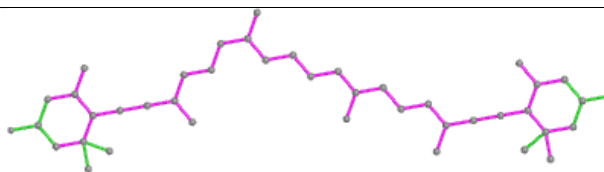


Rings

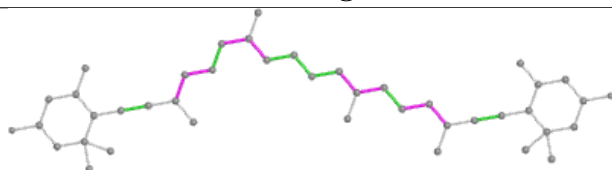
Ligand II0 m 619



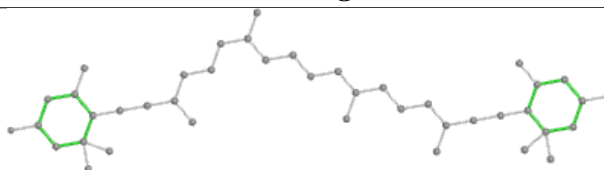
Bond lengths



Bond angles

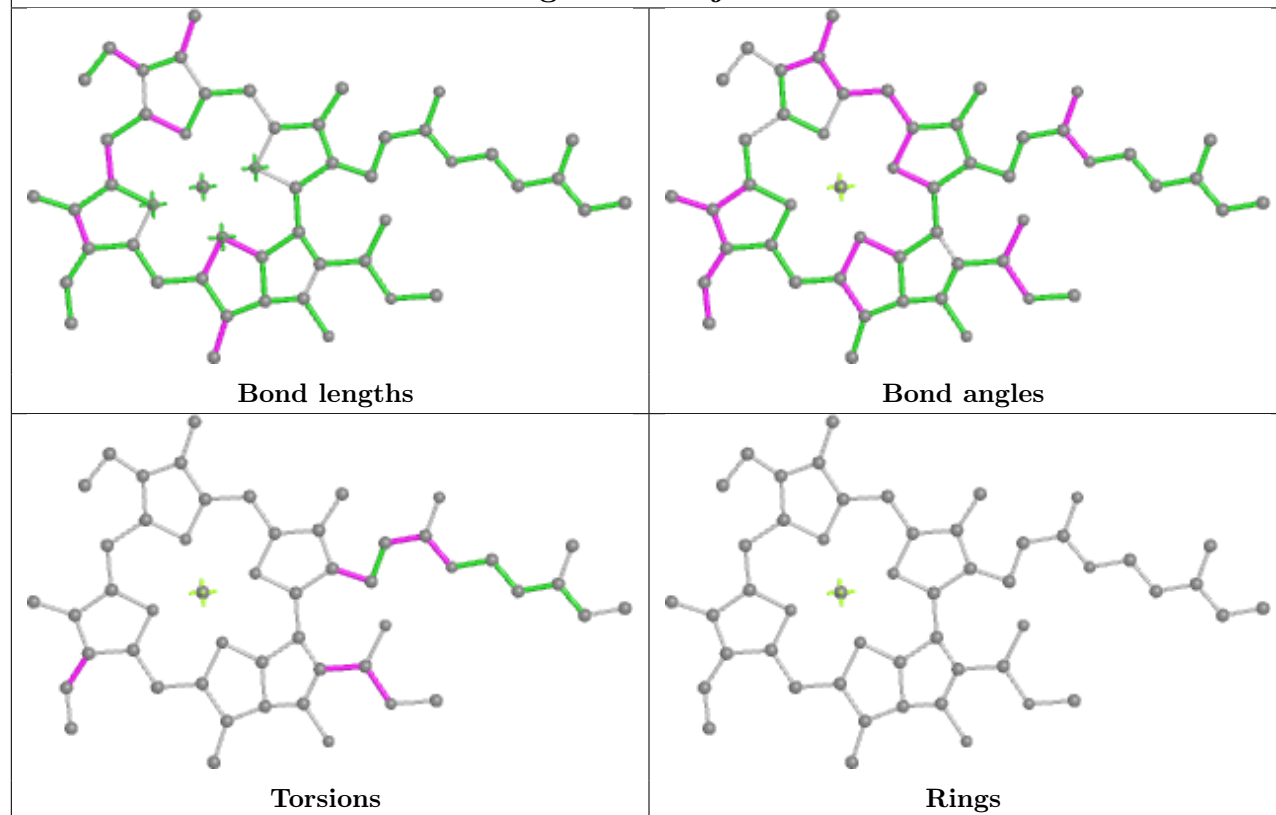


Torsions

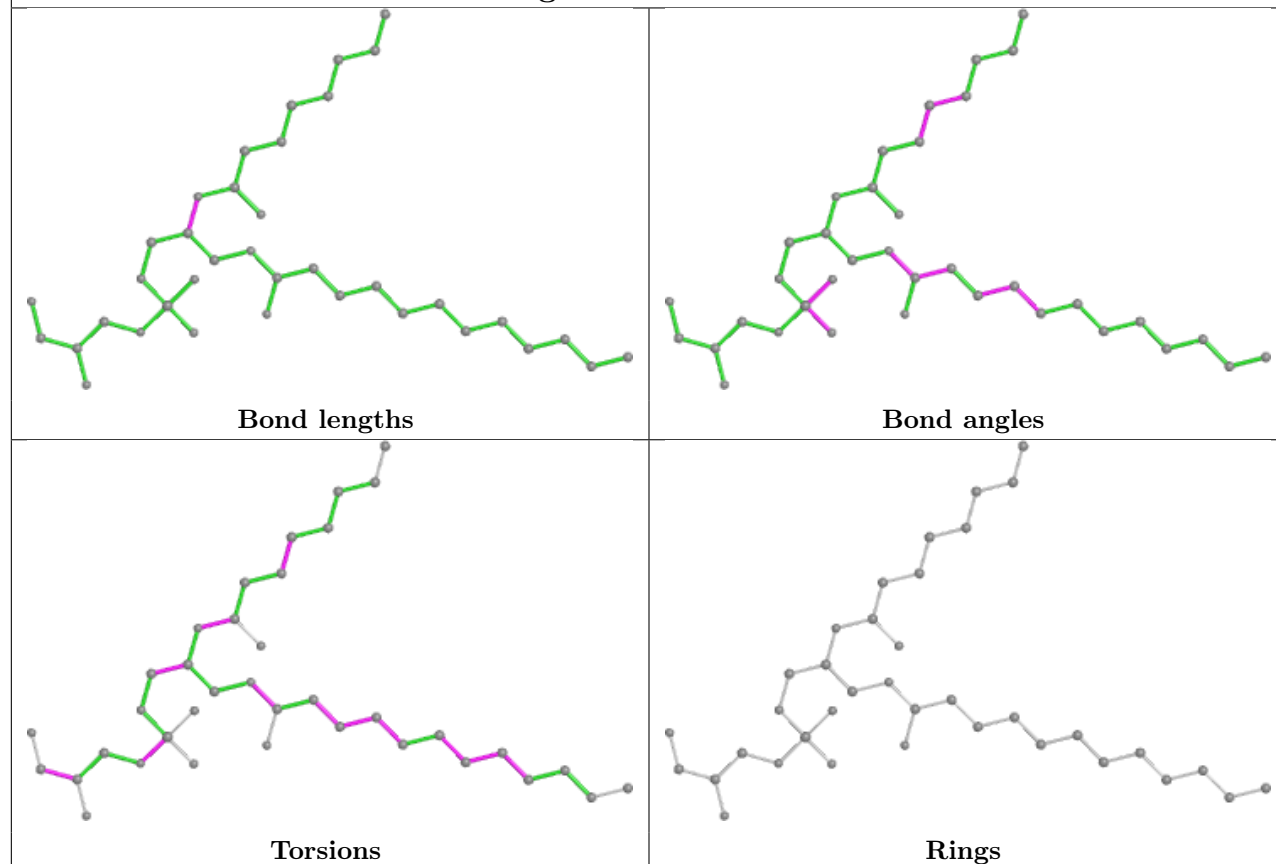


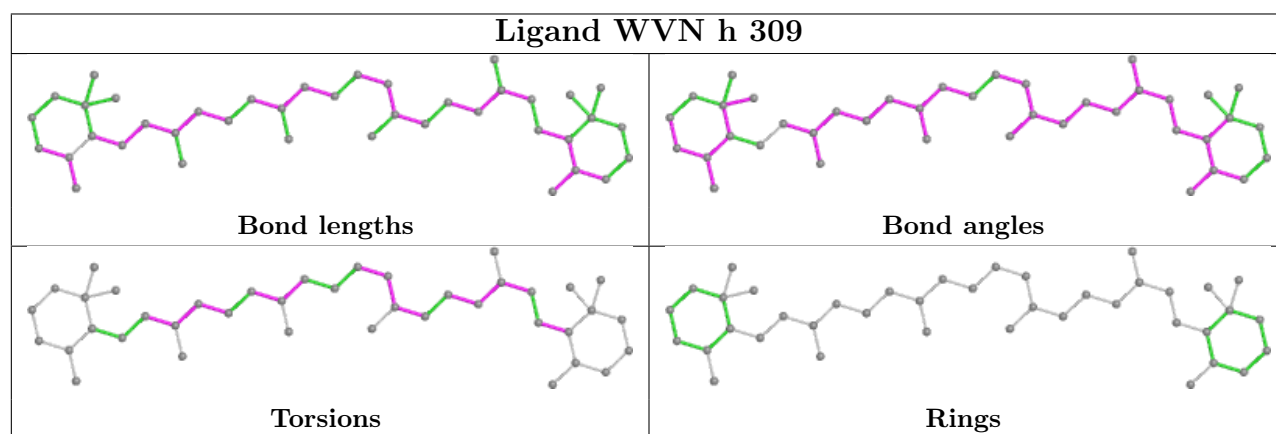
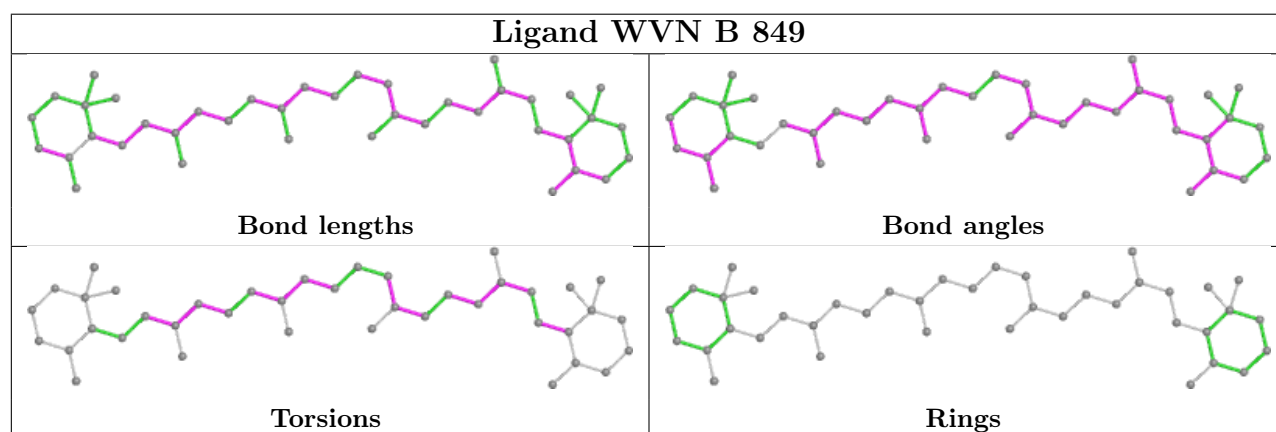
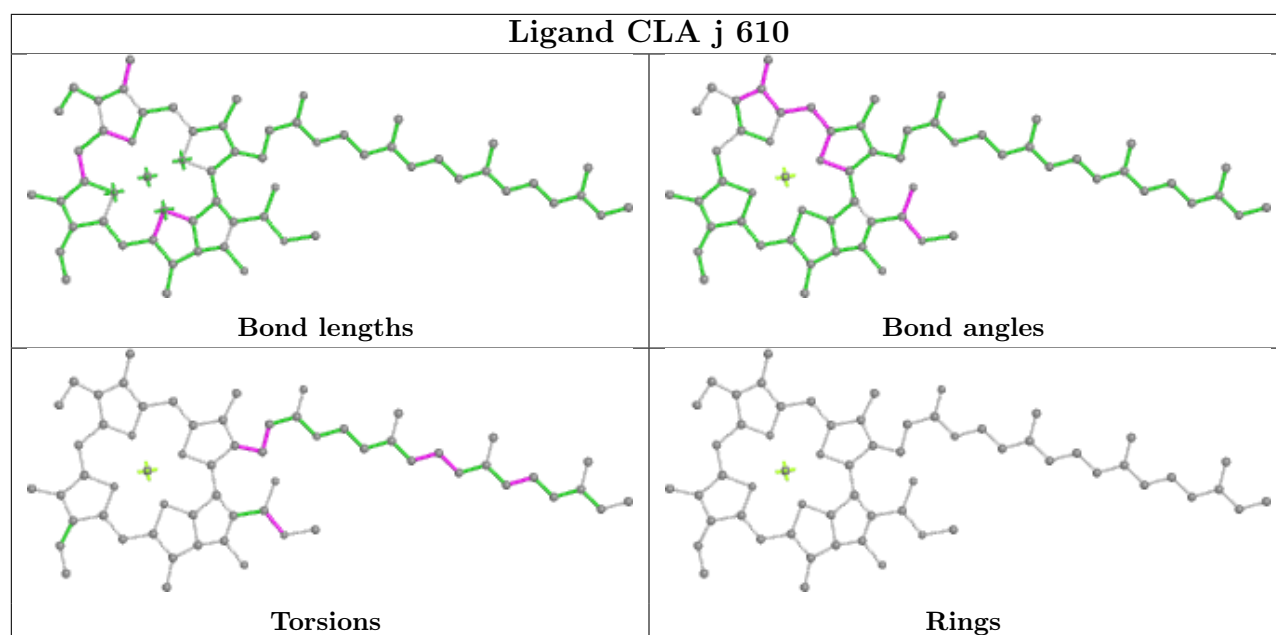
Rings

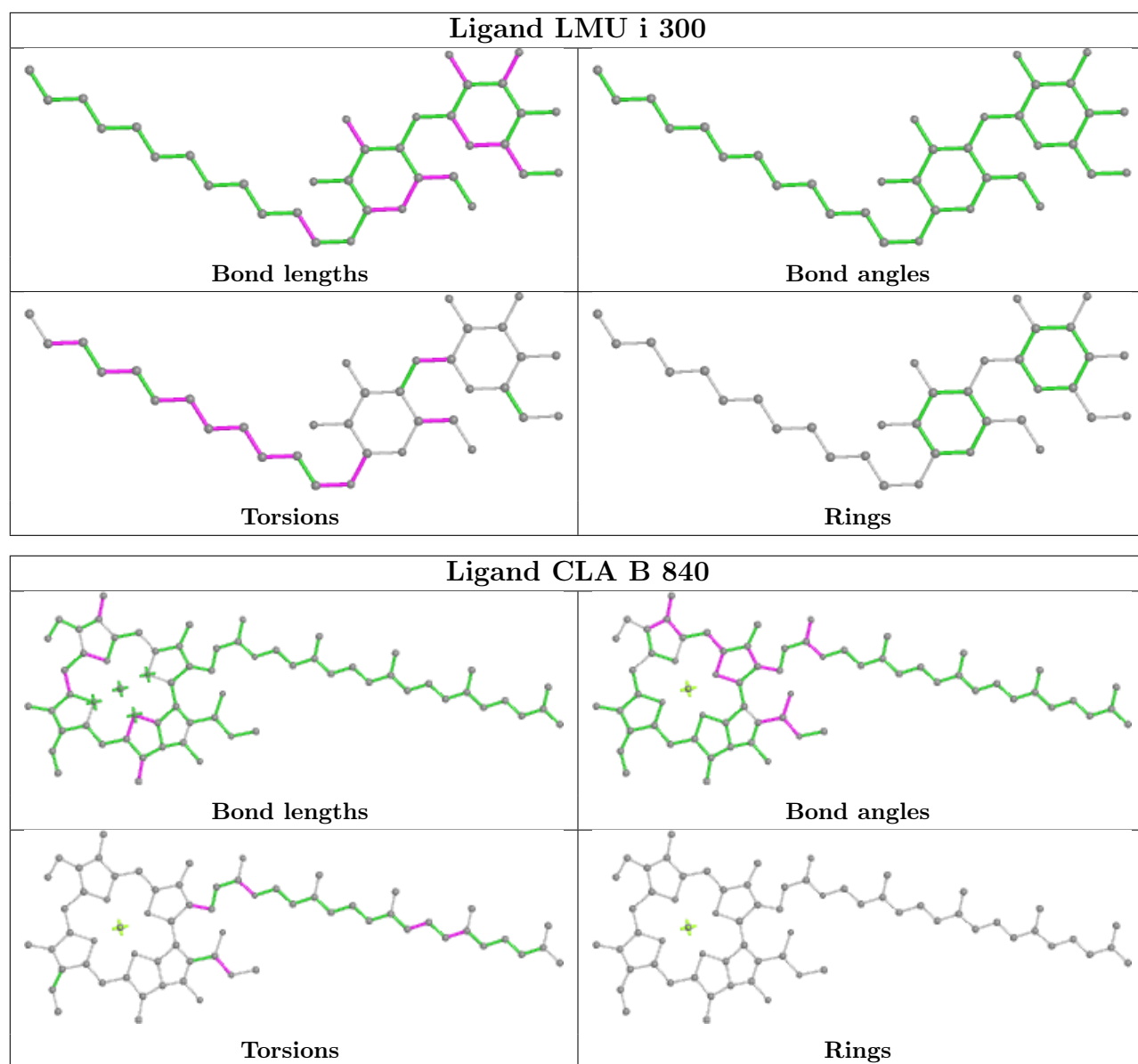
Ligand CLA j 607



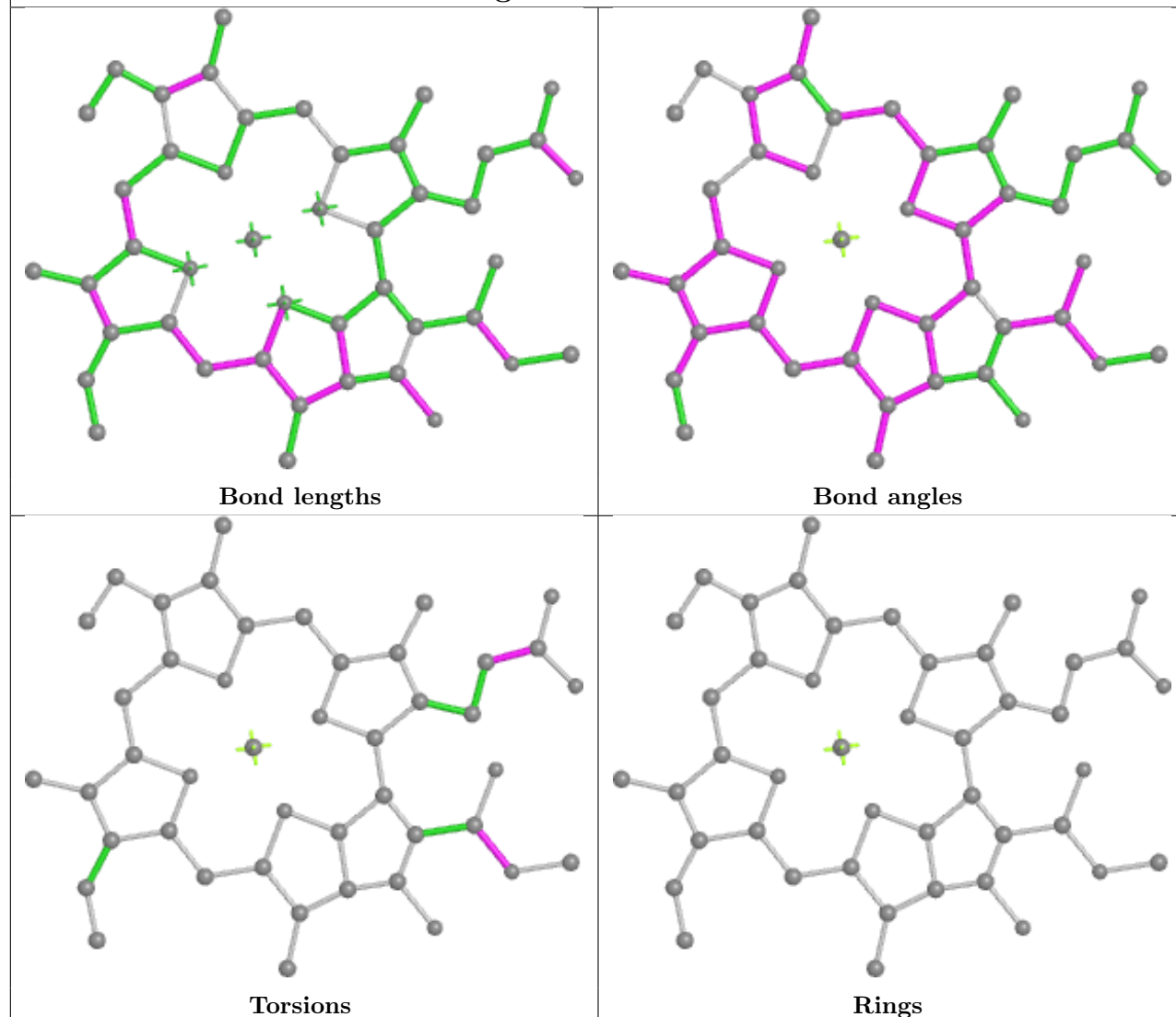
Ligand LHG i 317



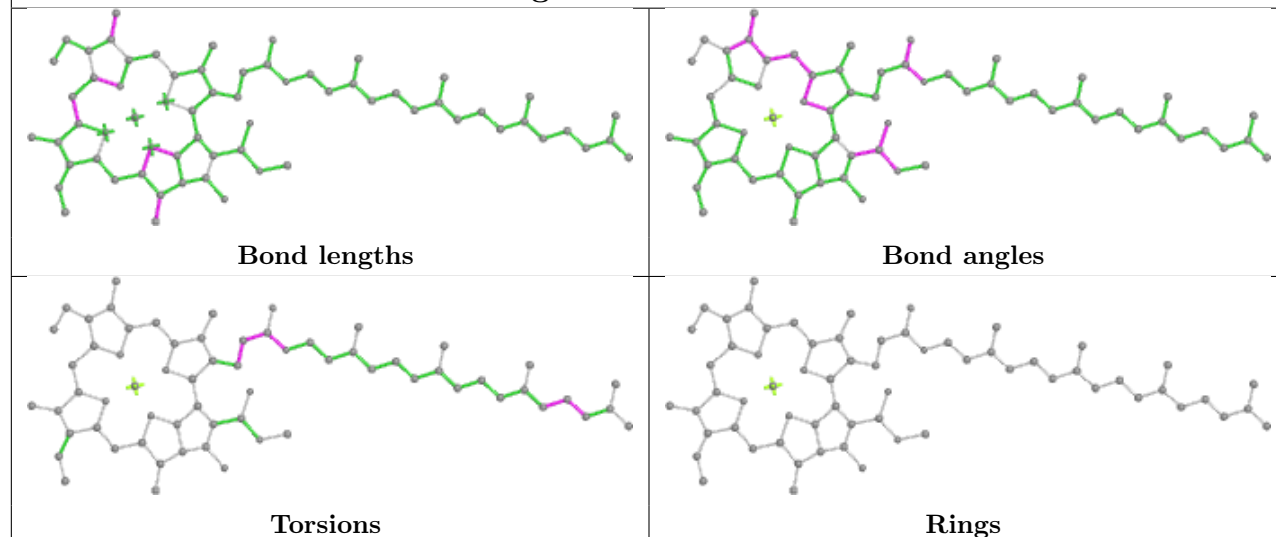


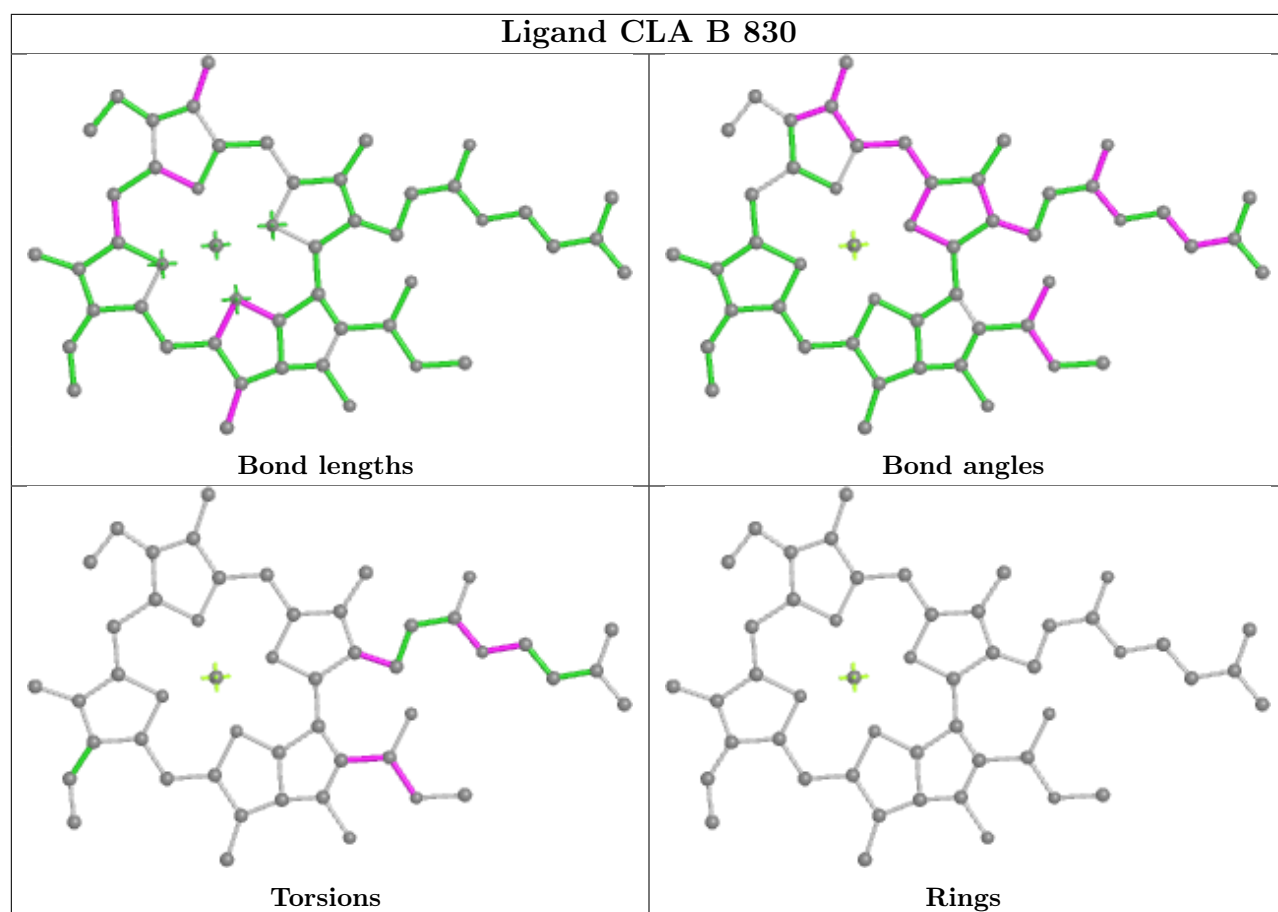


Ligand CLA c 309

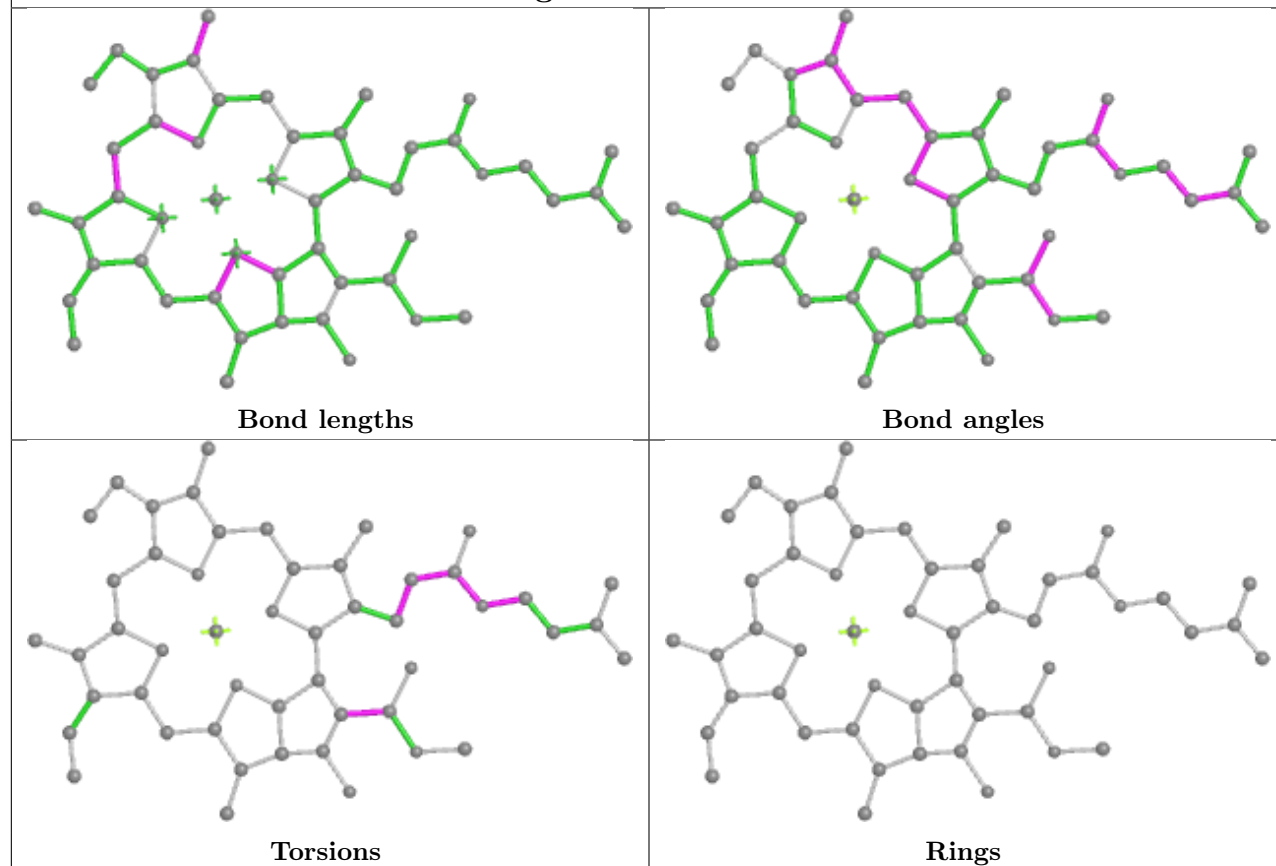


Ligand CLA A 802

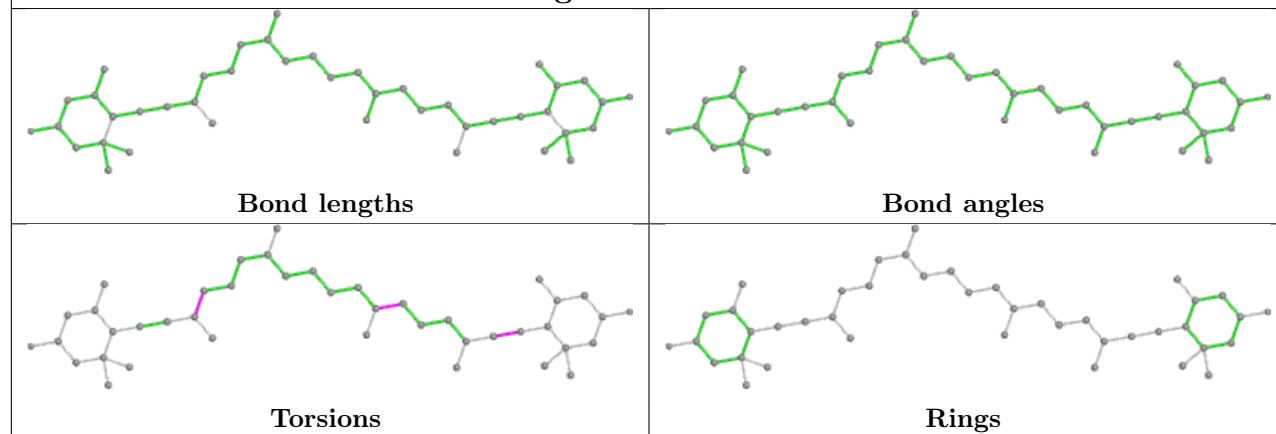


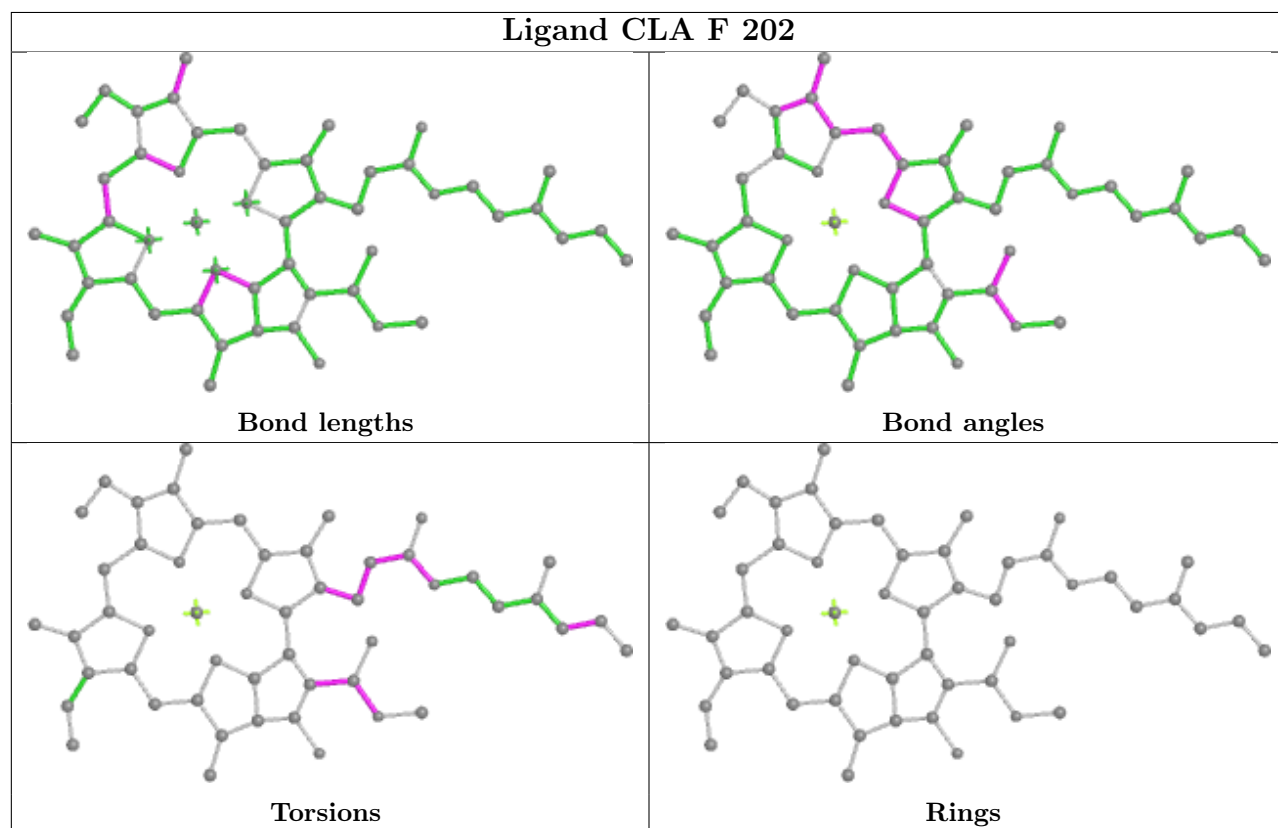
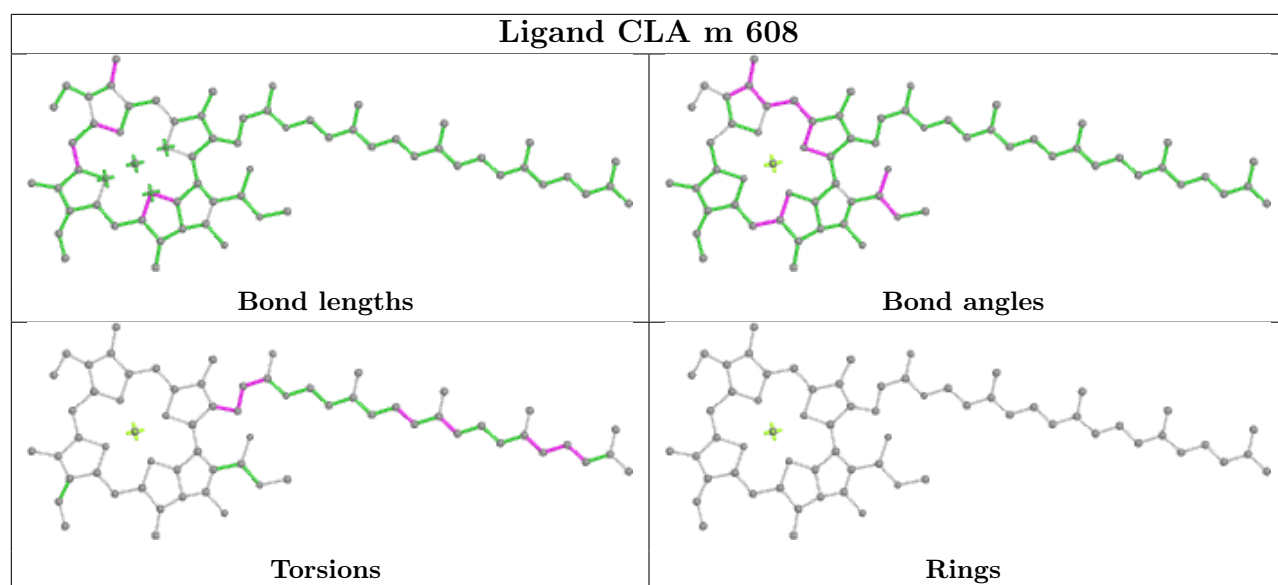


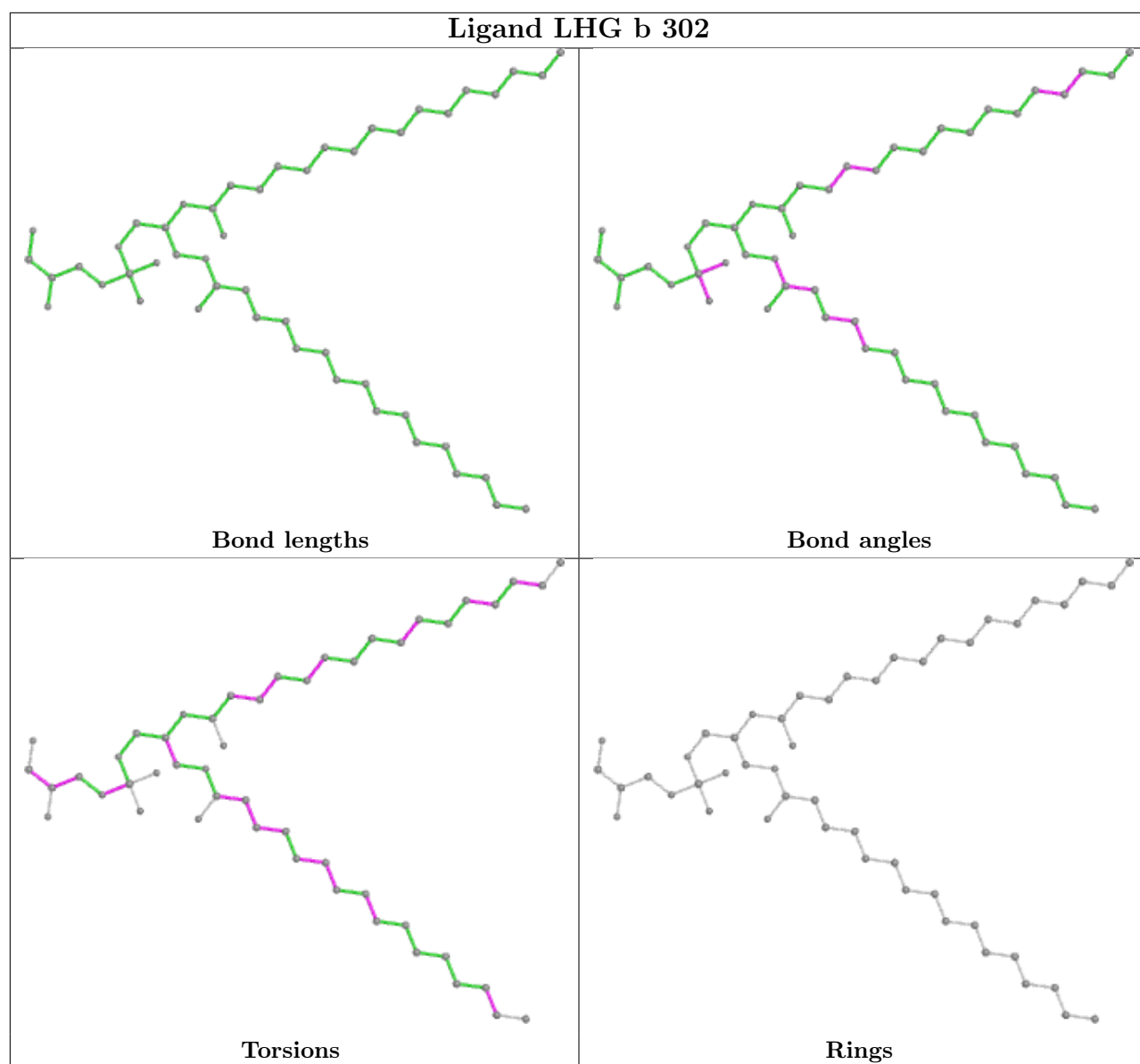
Ligand CLA h 303

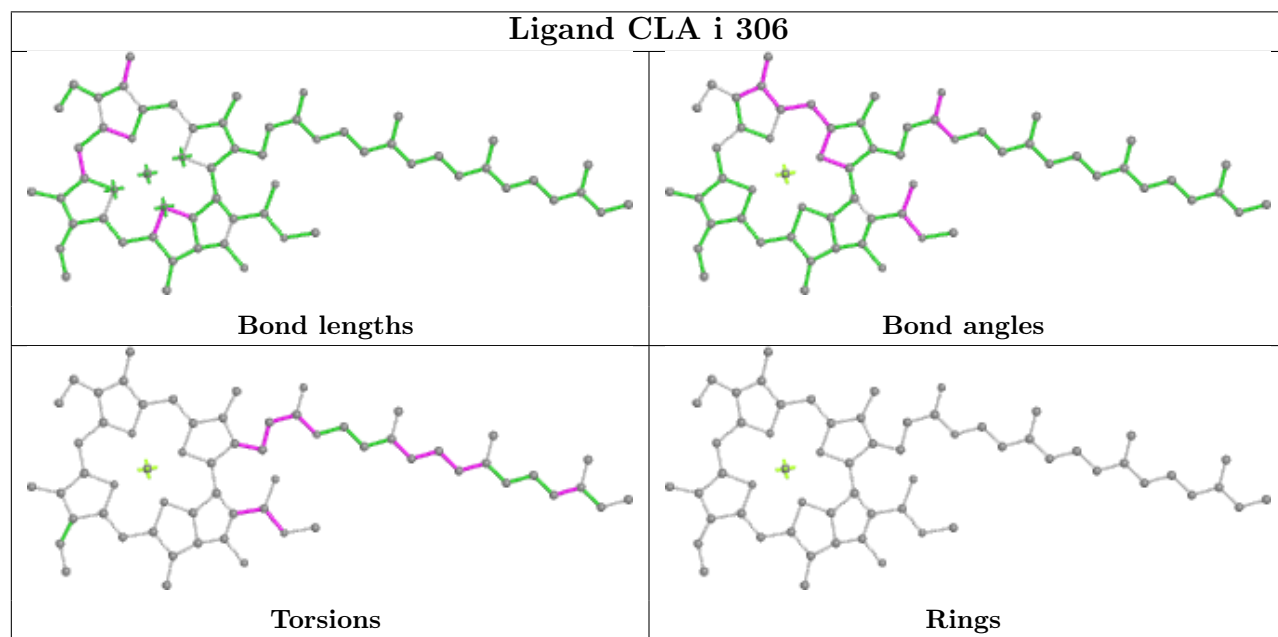
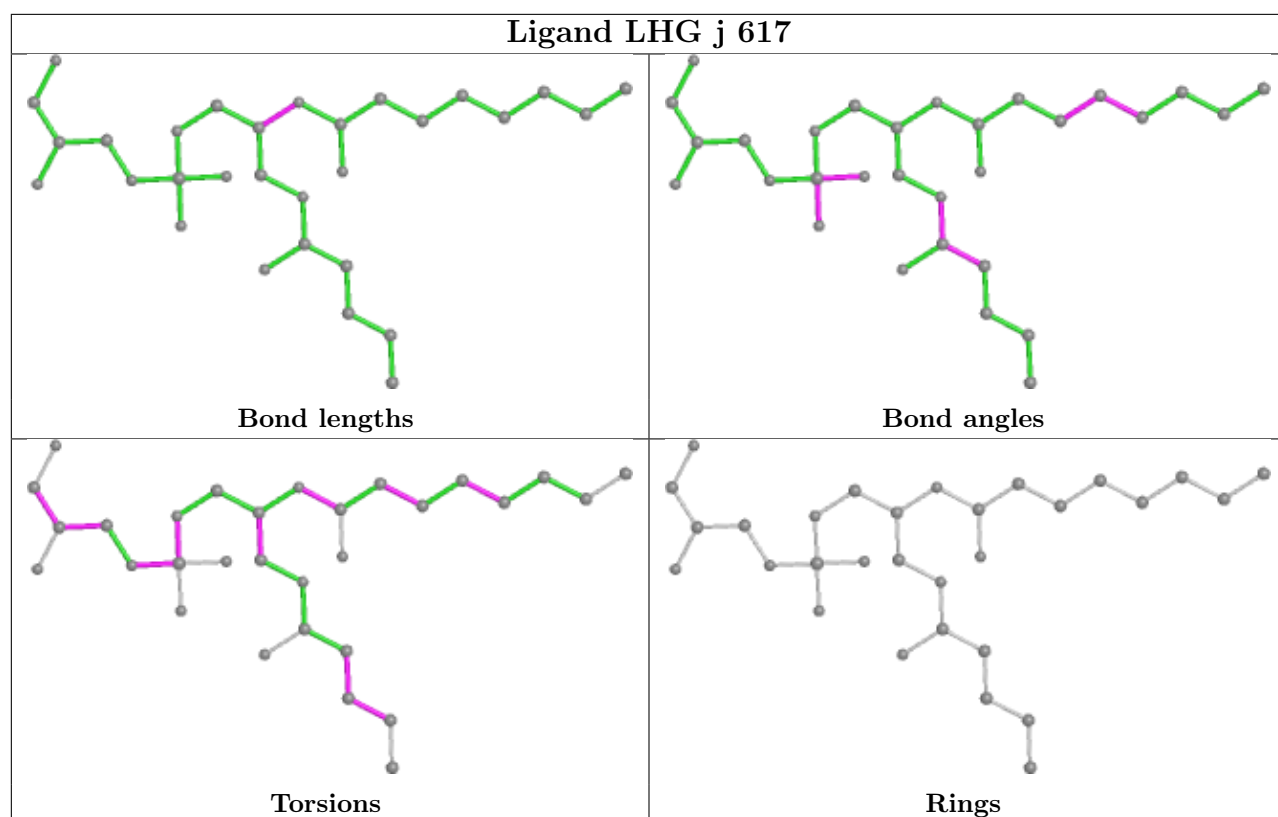


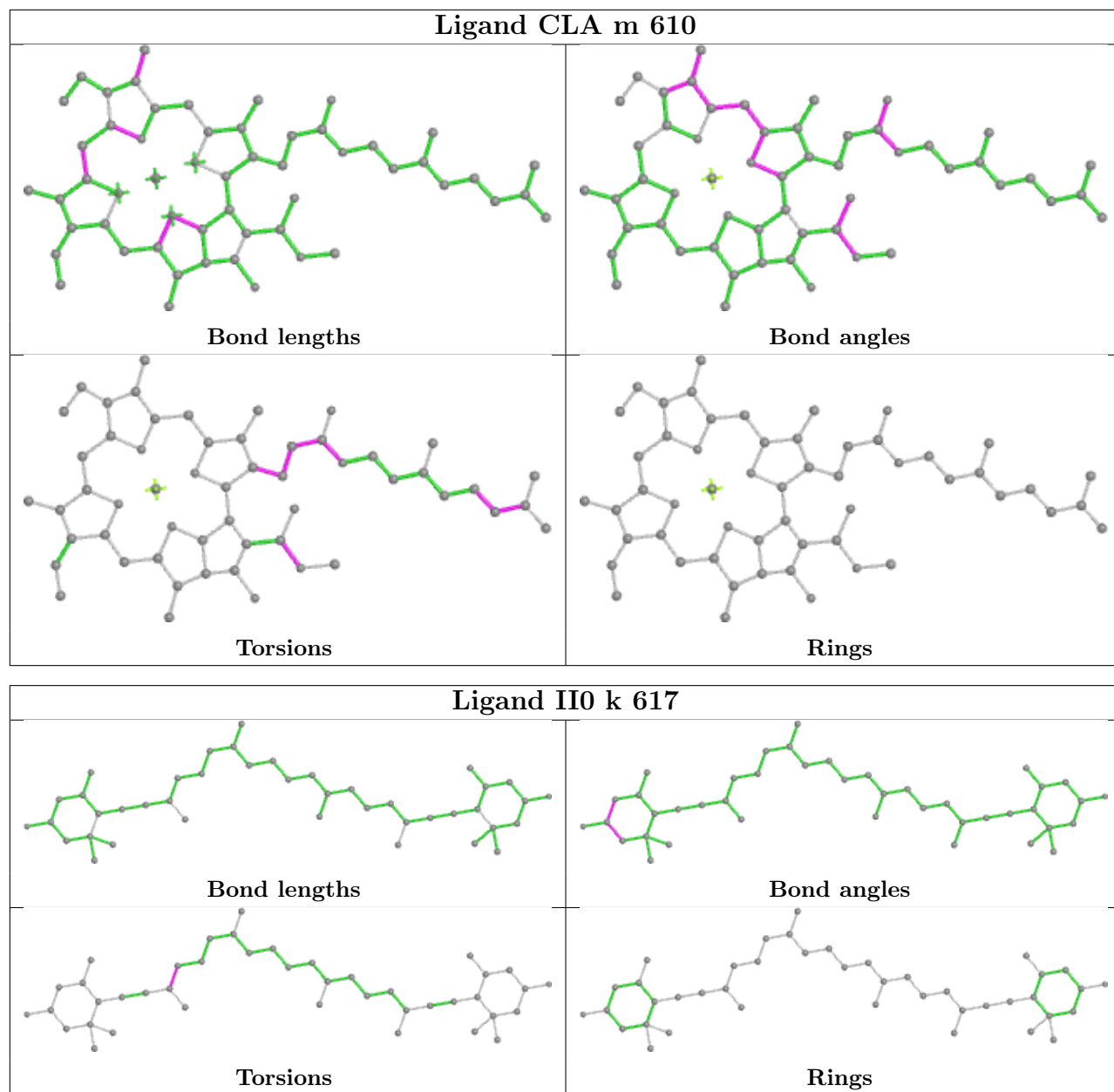
Ligand II0 l 317

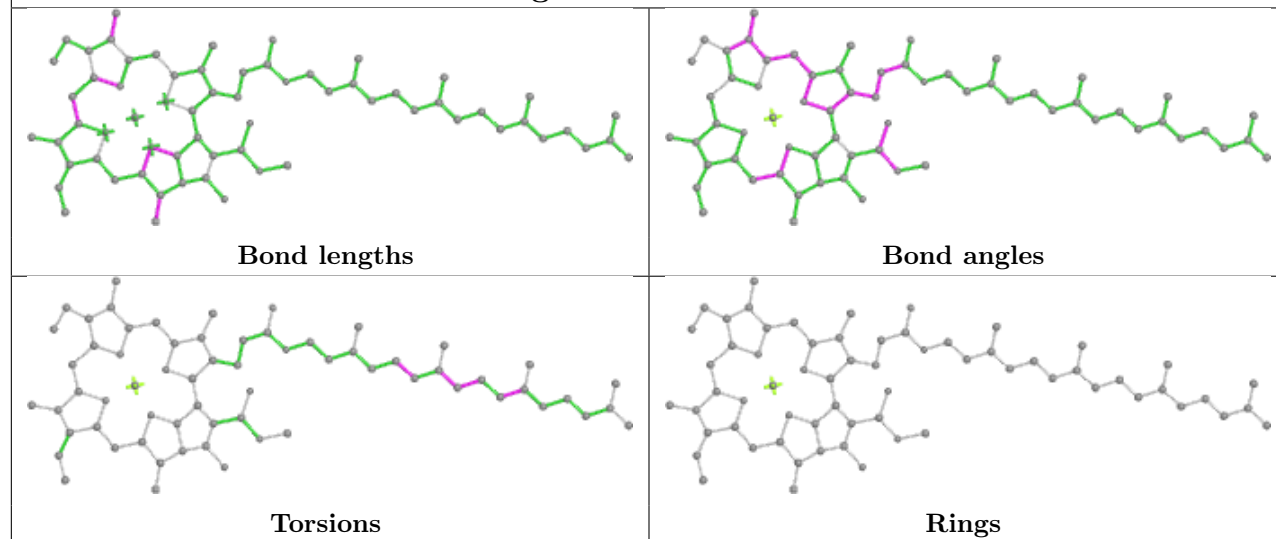
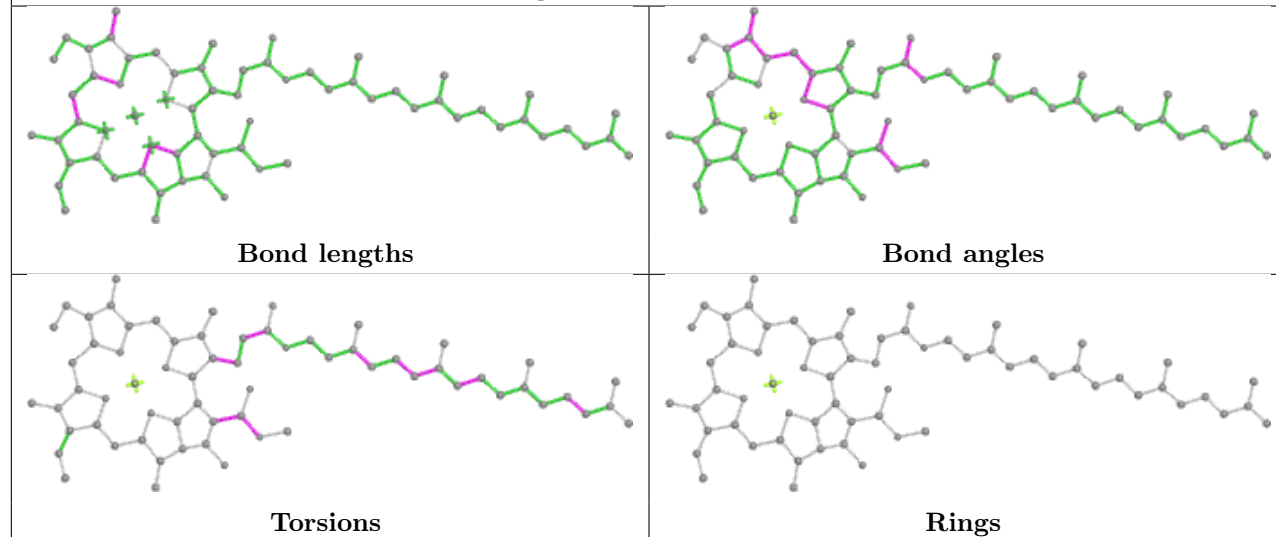




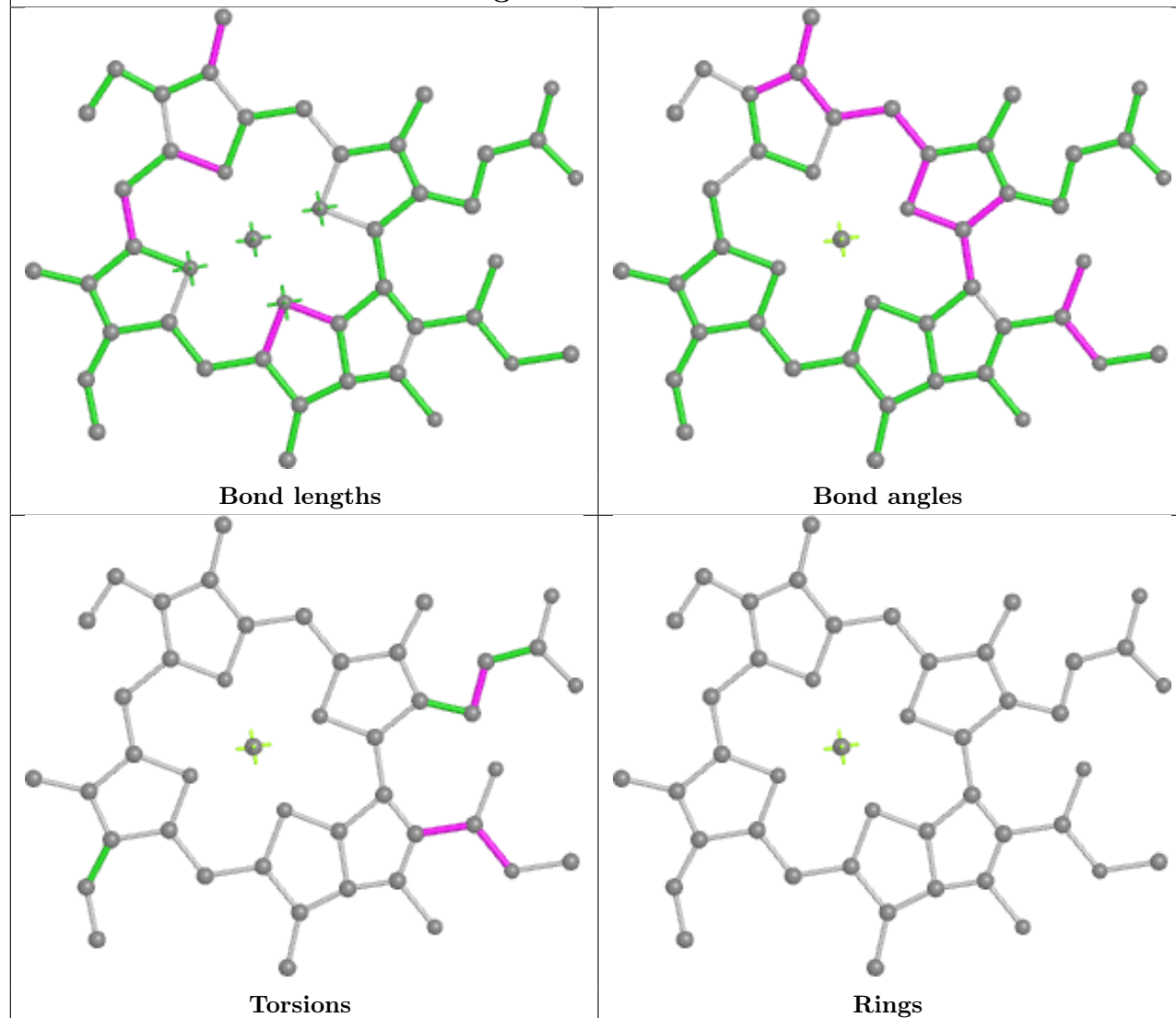




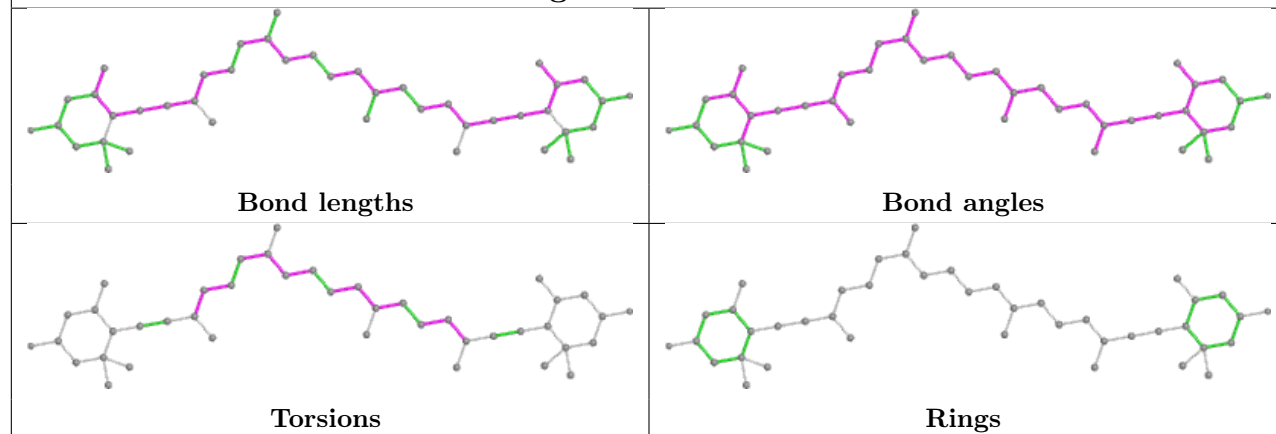


Ligand CLA A 825**Ligand CLA B 812**

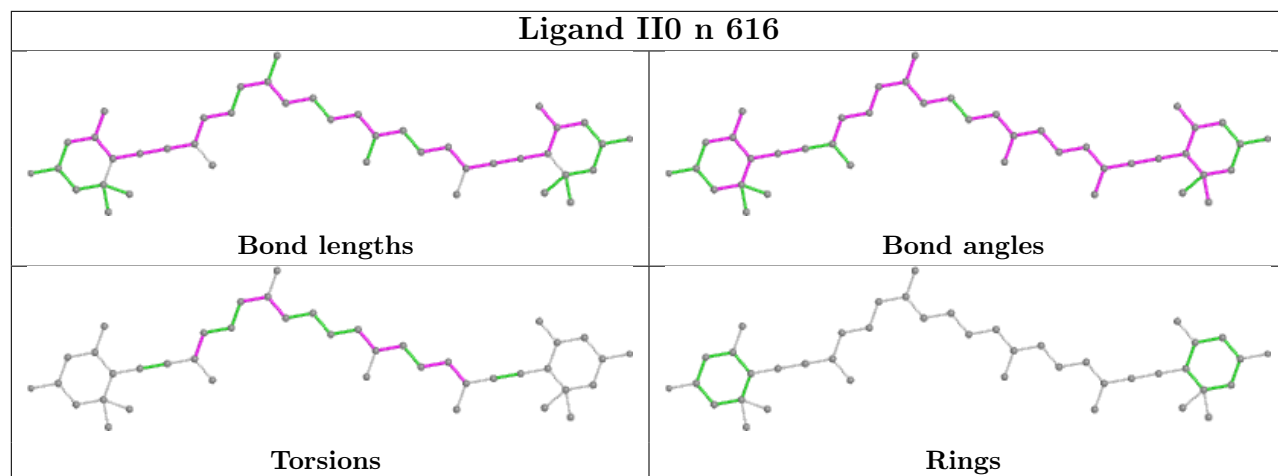
Ligand CLA k 605



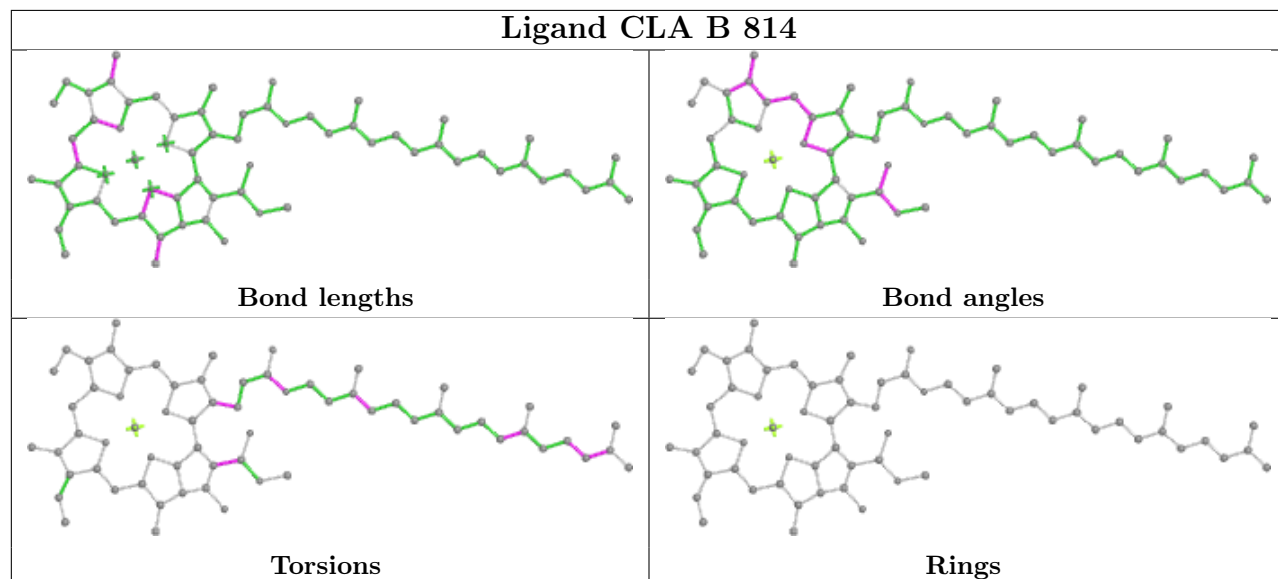
Ligand II0 h 311



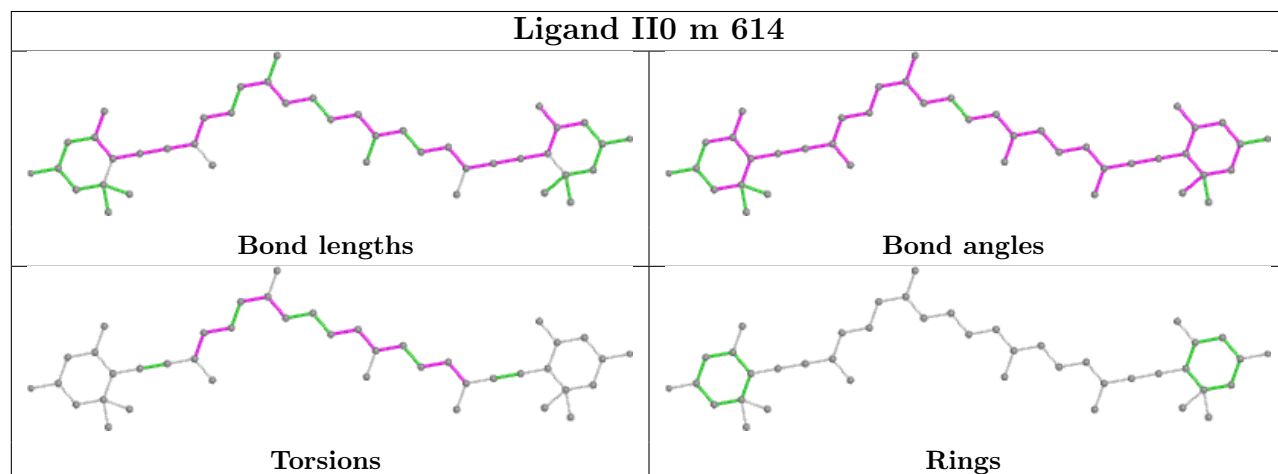
Ligand II0 n 616



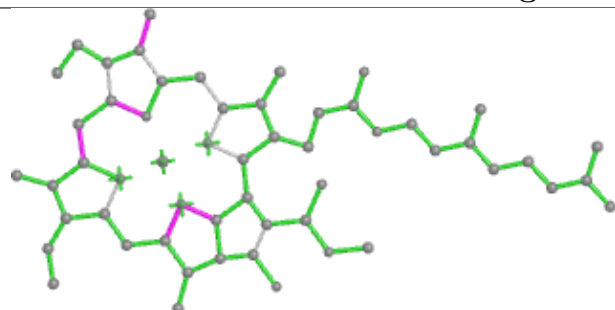
Ligand CLA B 814



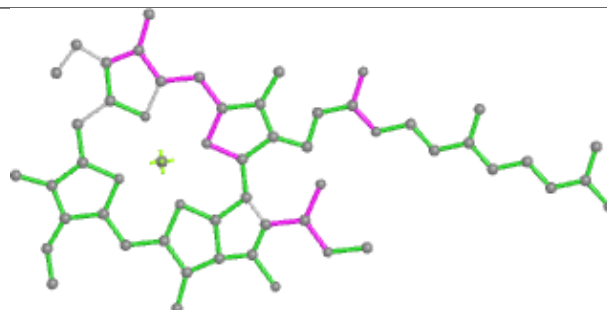
Ligand II0 m 614



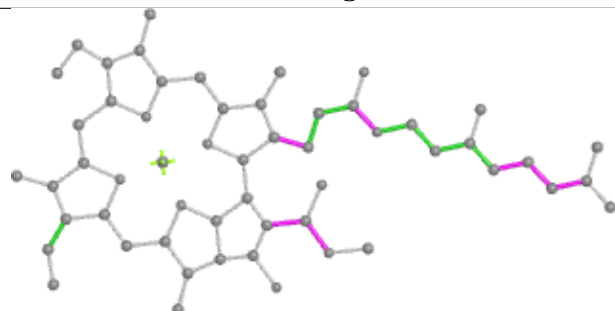
Ligand CLA b 304



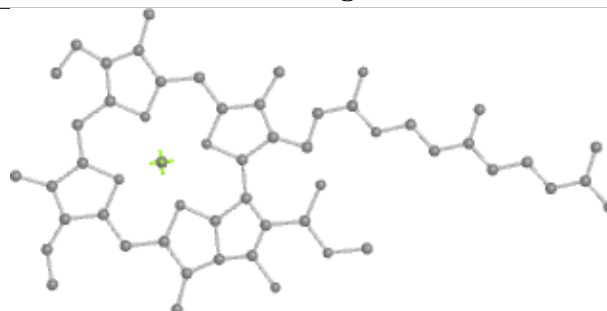
Bond lengths



Bond angles

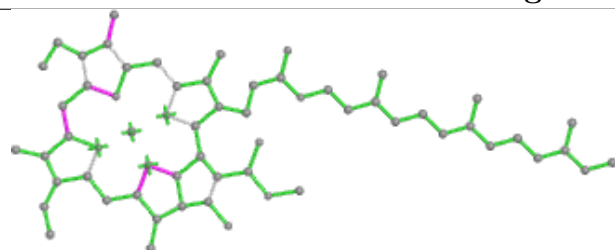


Torsions

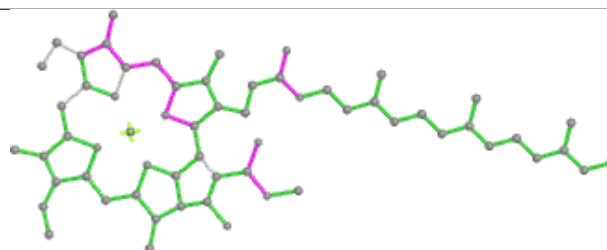


Rings

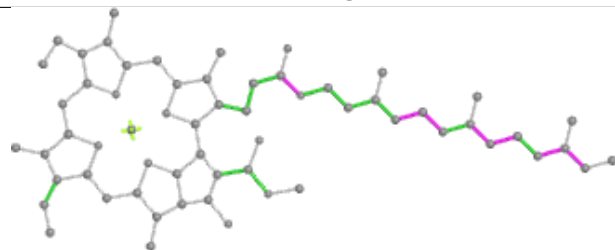
Ligand CLA l 311



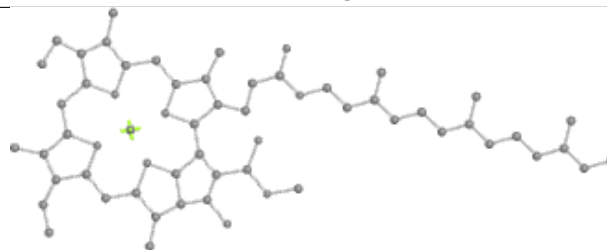
Bond lengths



Bond angles

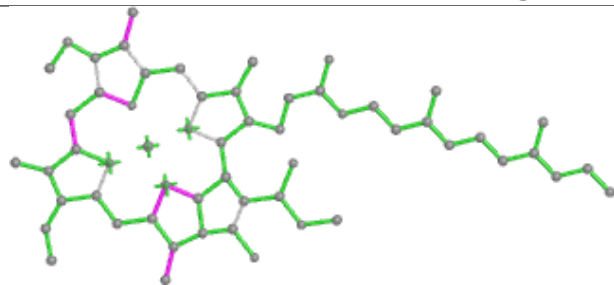


Torsions

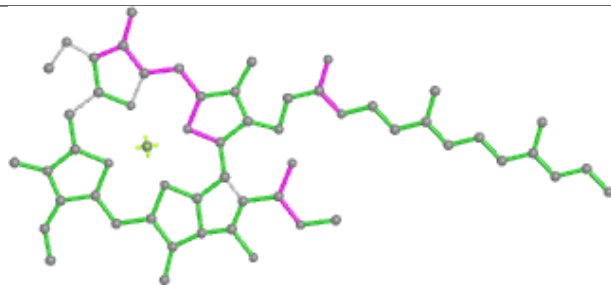


Rings

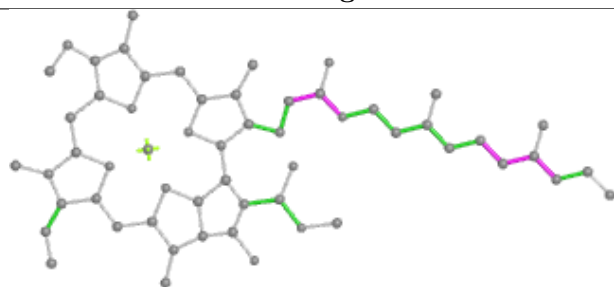
Ligand CLA B 839



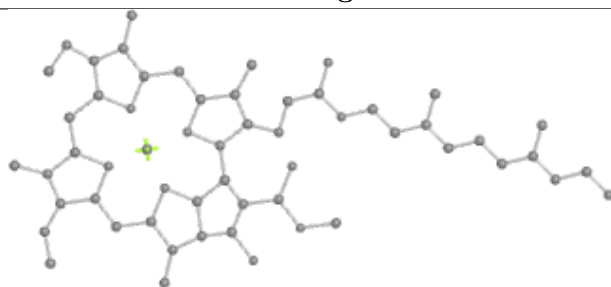
Bond lengths



Bond angles

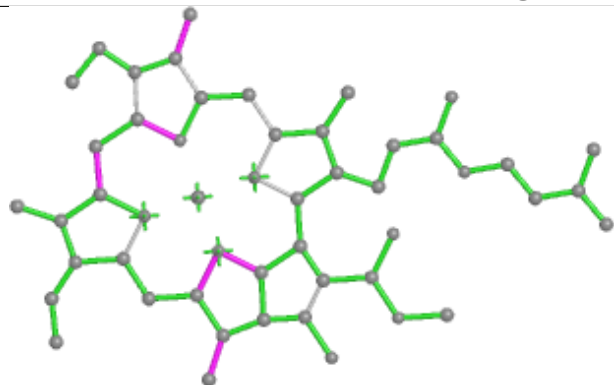


Torsions

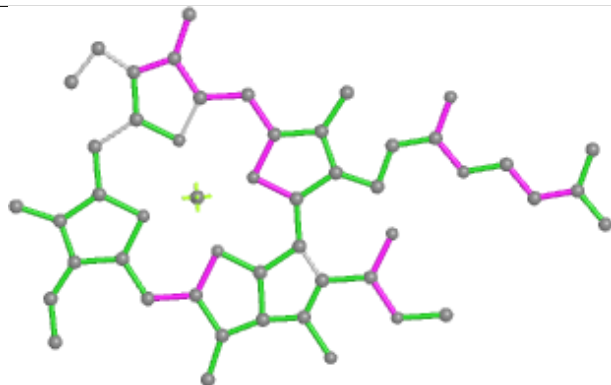


Rings

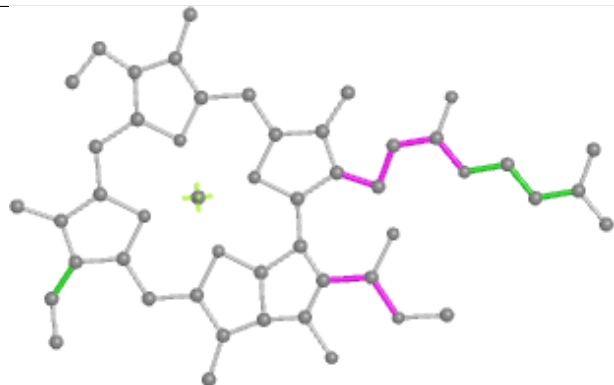
Ligand CLA B 828



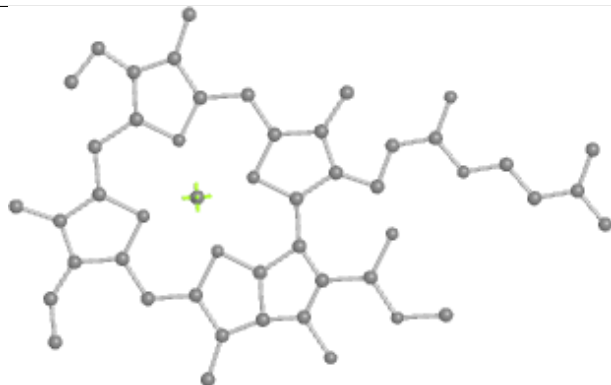
Bond lengths



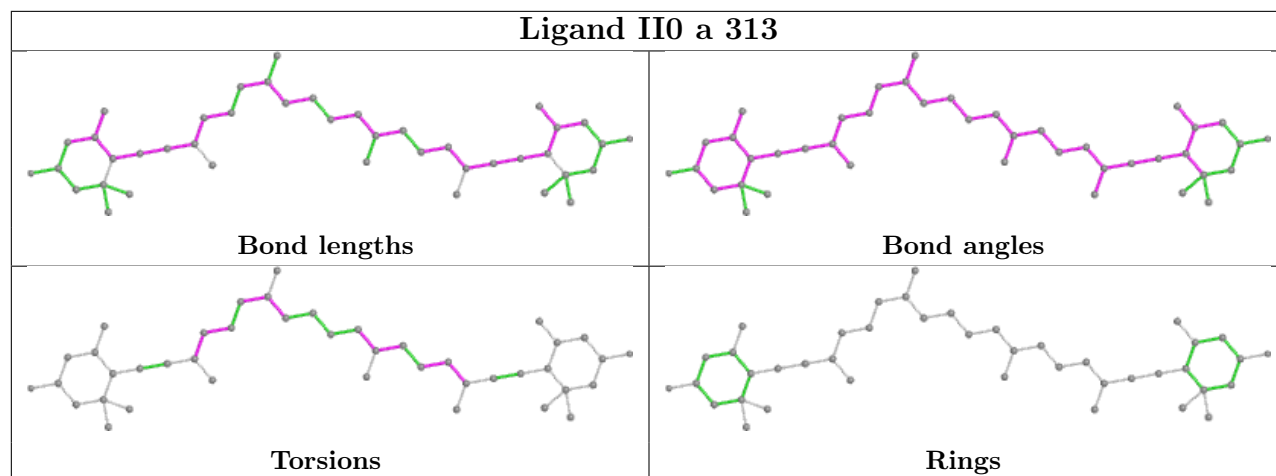
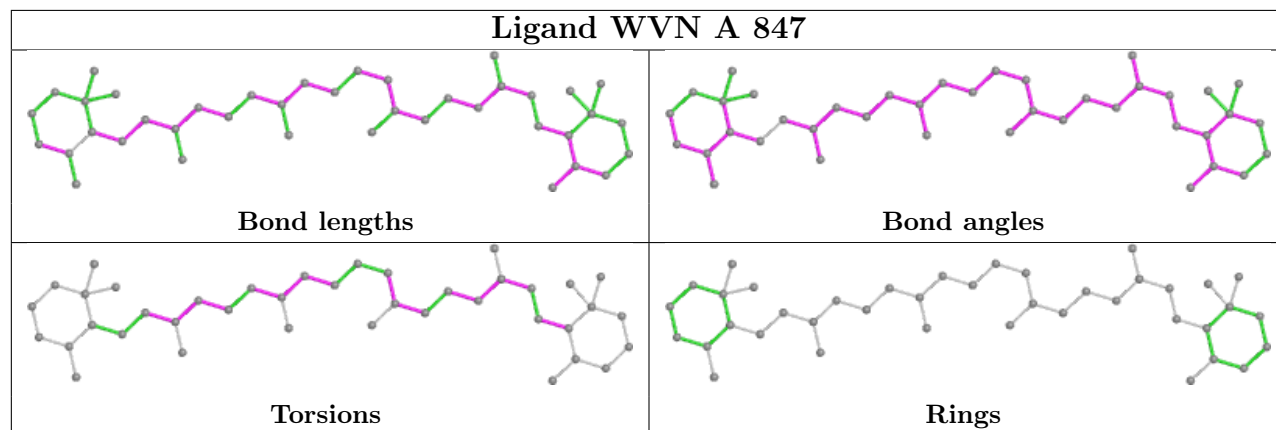
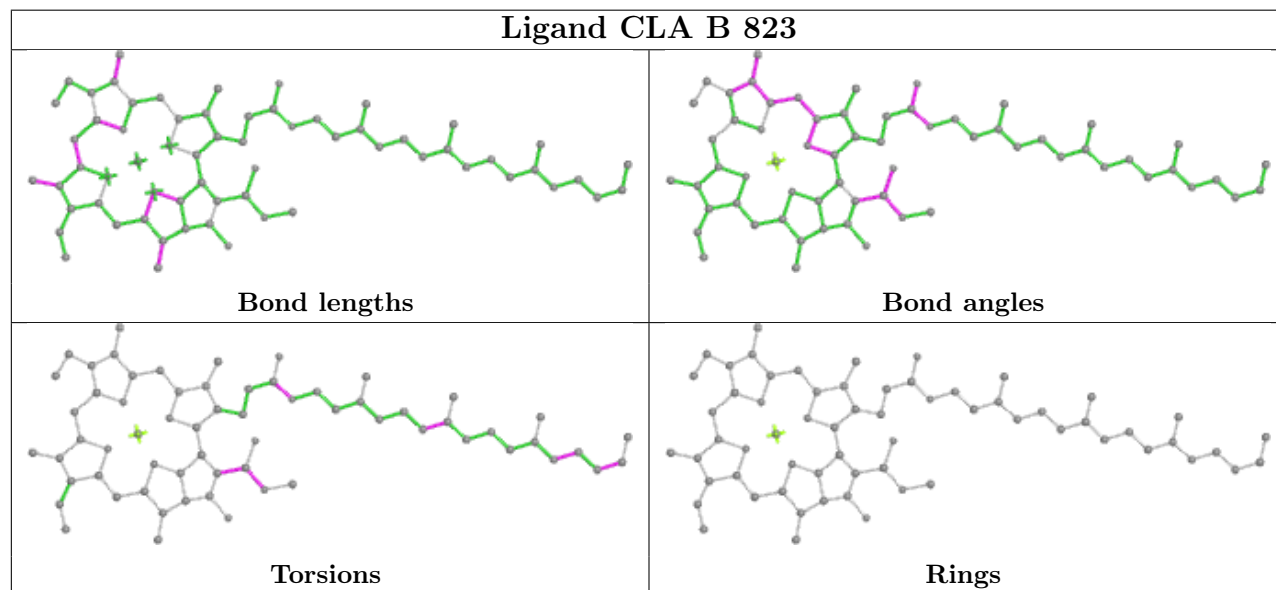
Bond angles



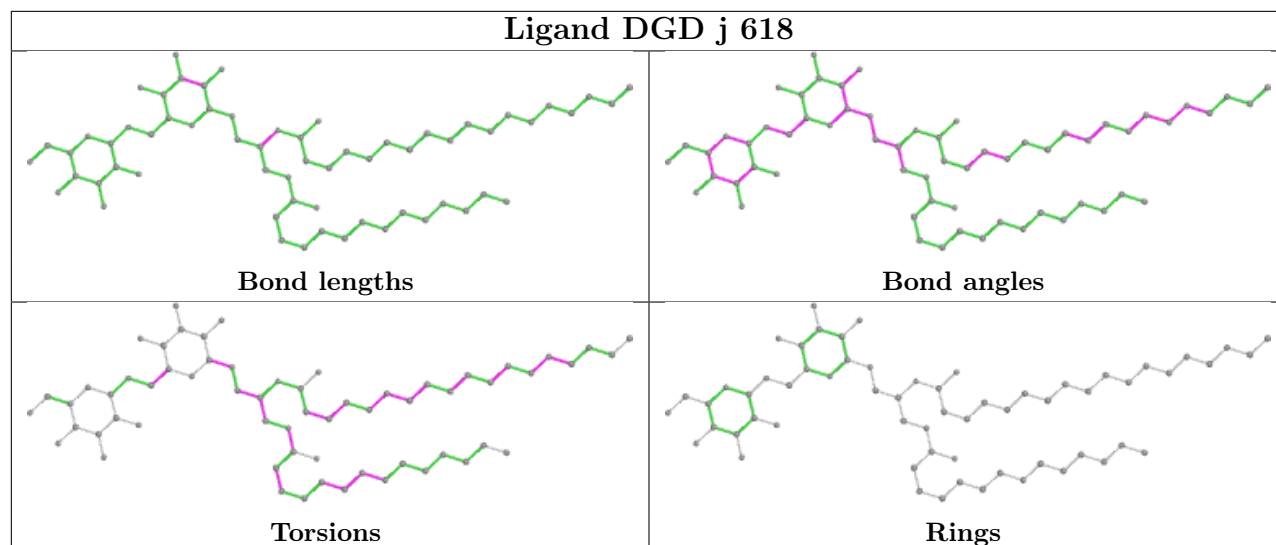
Torsions



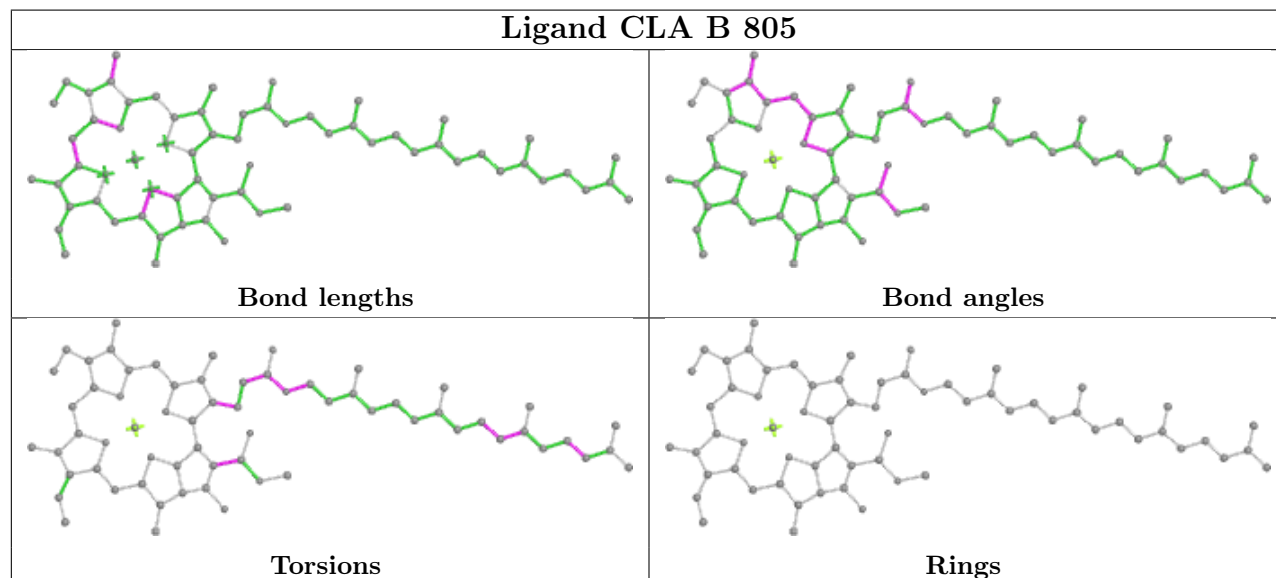
Rings

Ligand II0 a 313**Ligand WVN A 847****Ligand CLA B 823**

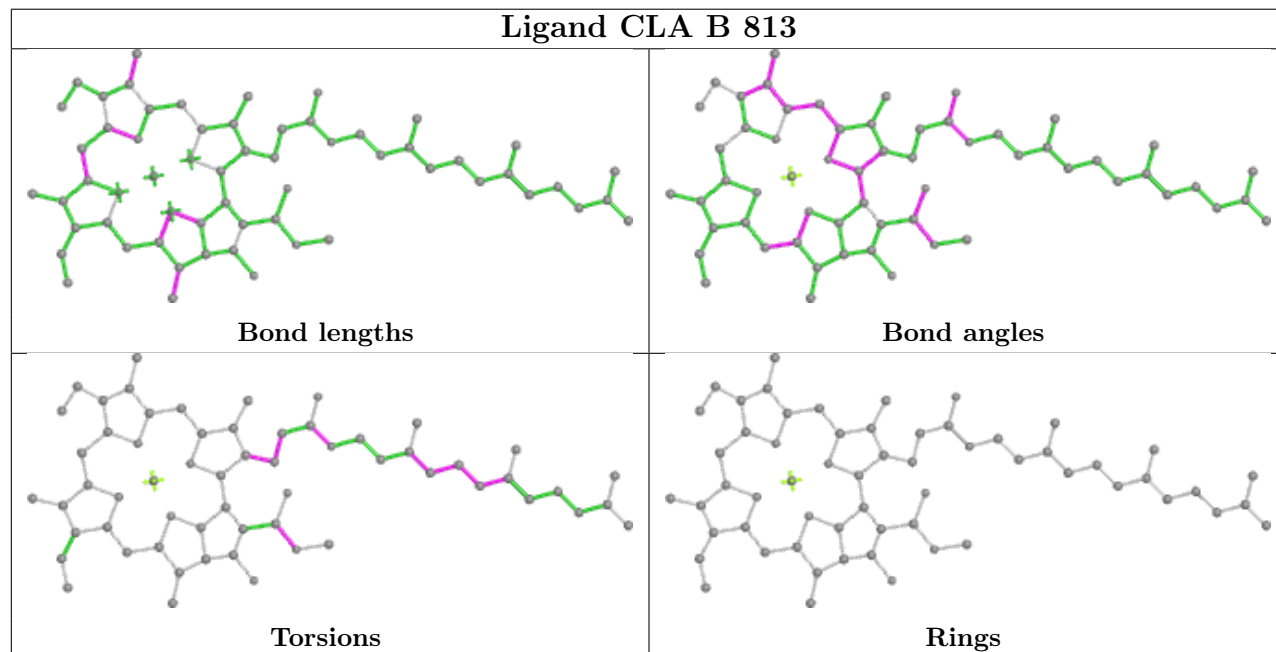
Ligand DGD j 618

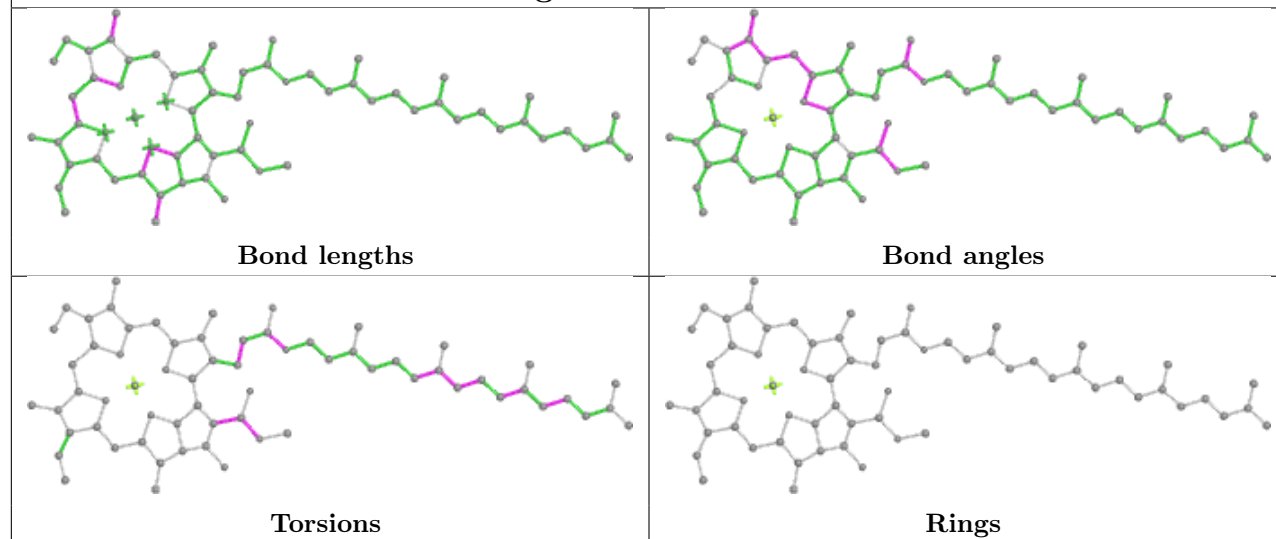
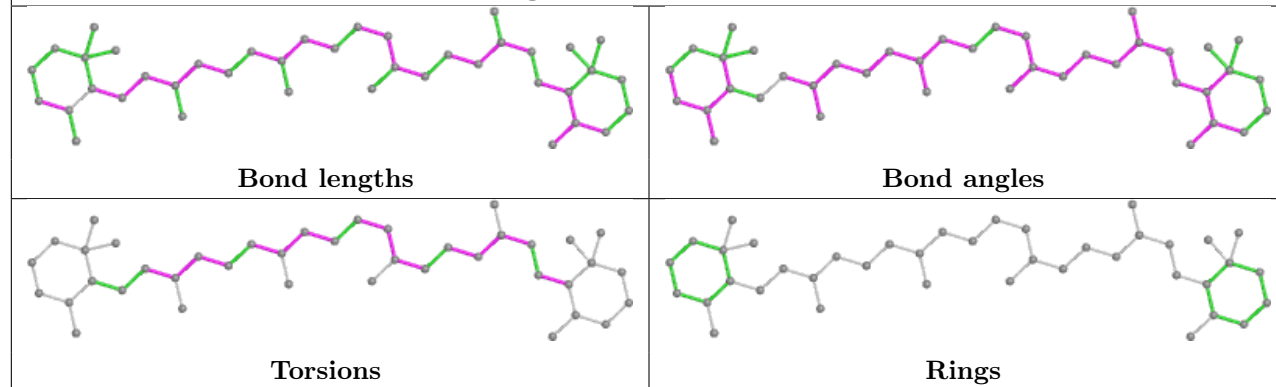


Ligand CLA B 805

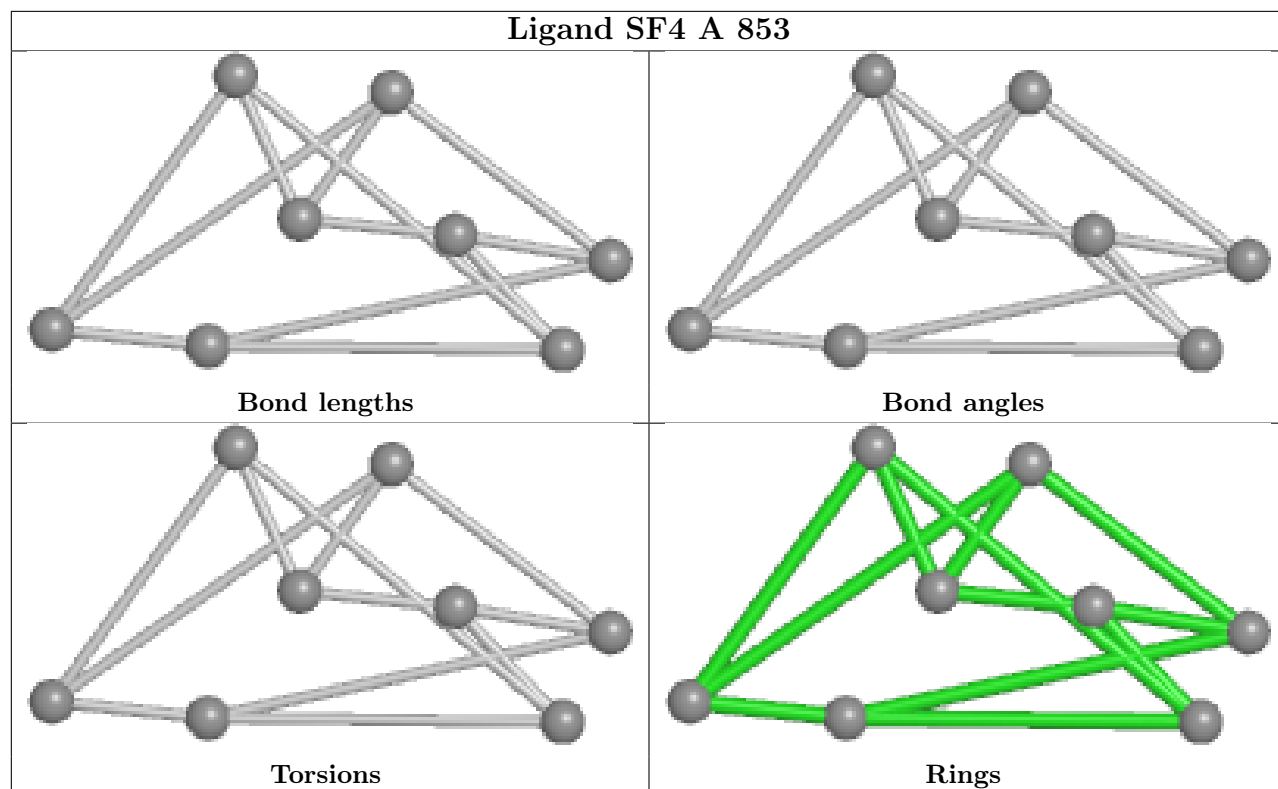


Ligand CLA B 813

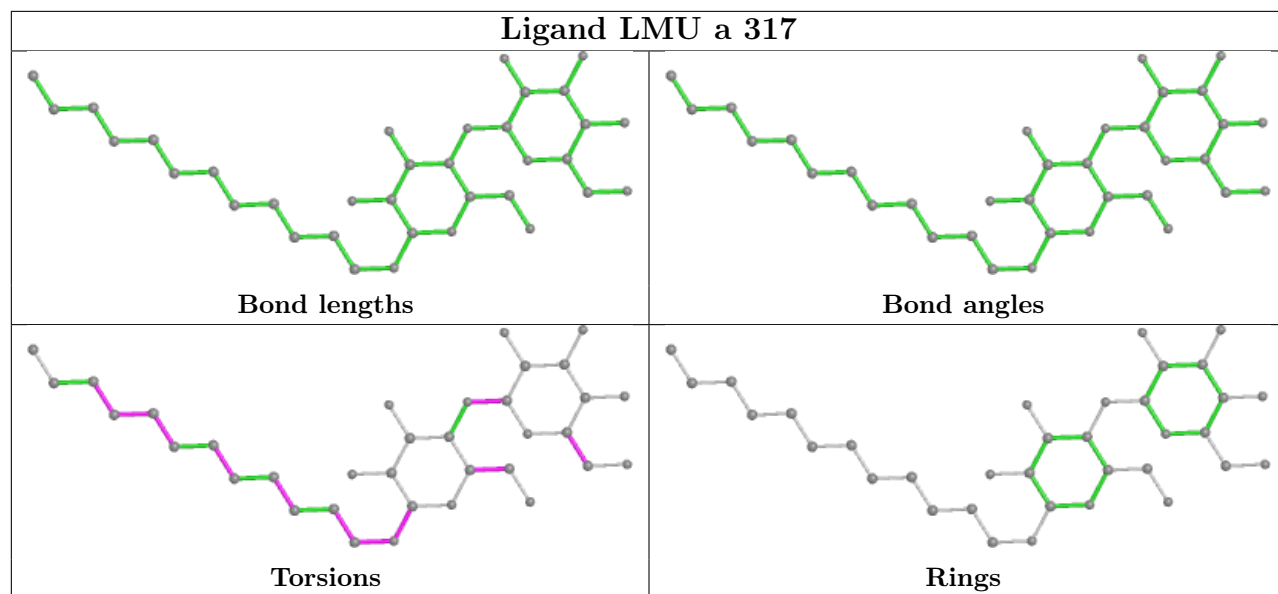


Ligand CLA b 306**Ligand WVN B 850**

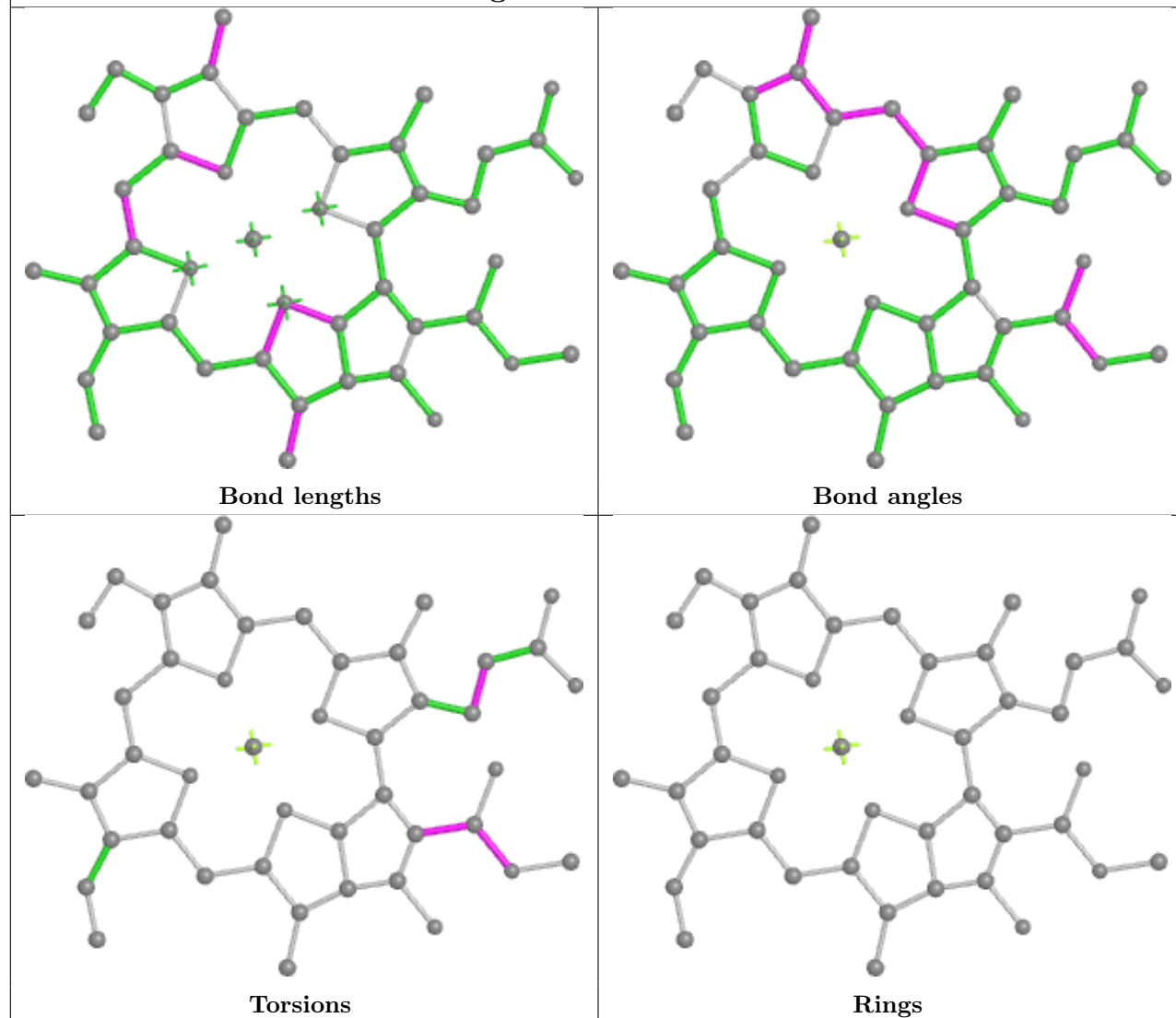
Ligand SF4 A 853



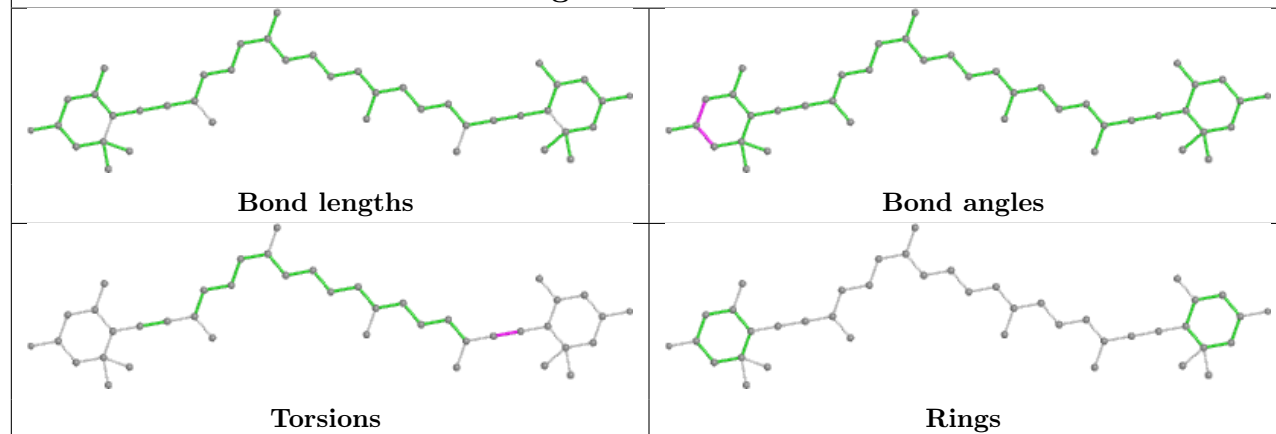
Ligand LMU a 317



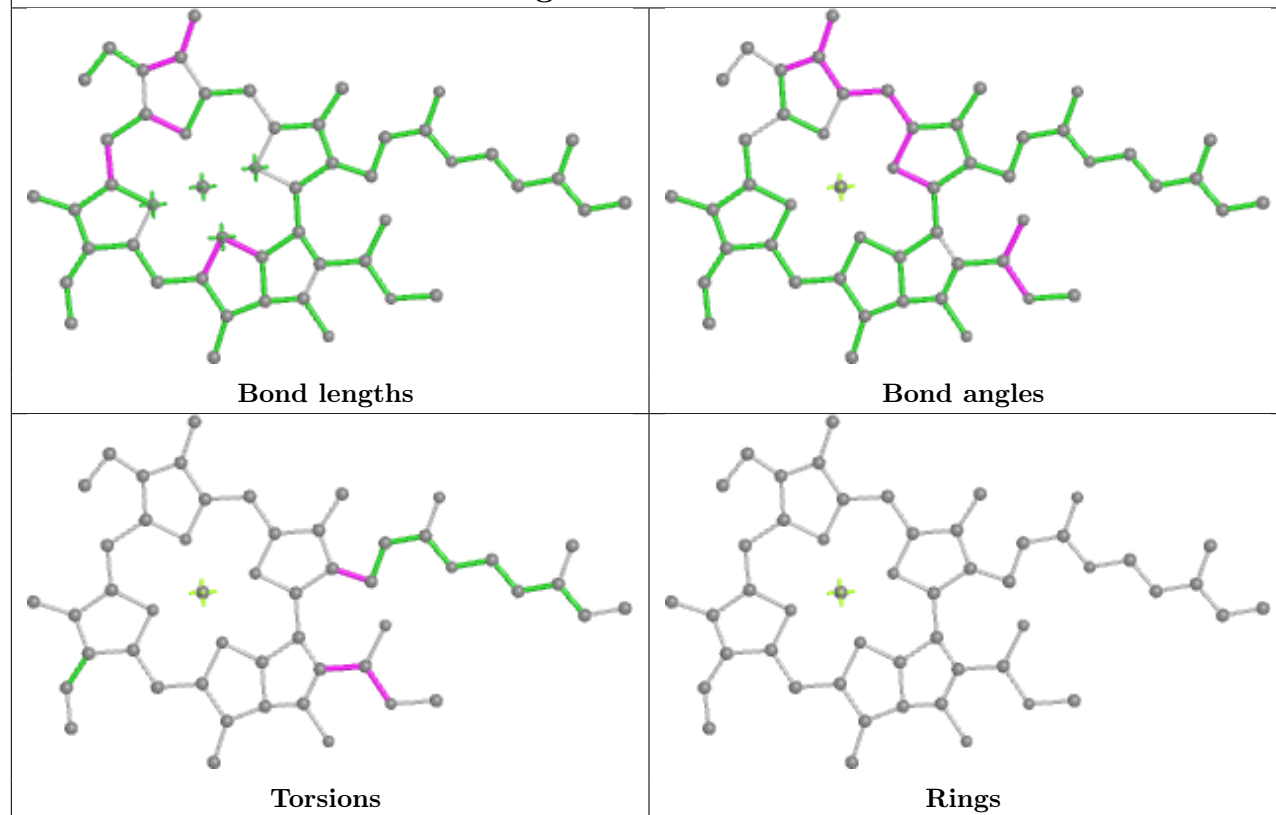
Ligand CLA A 815



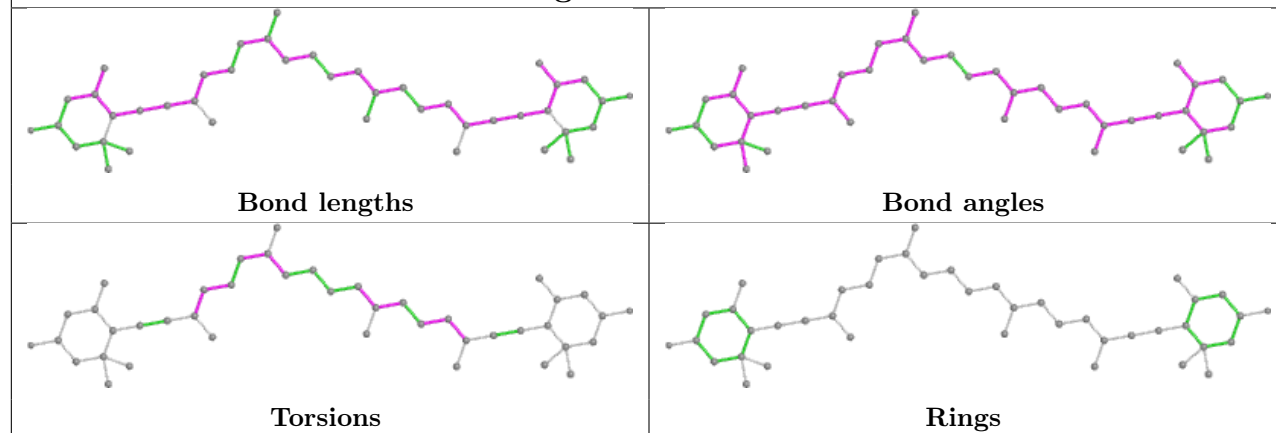
Ligand II0 c 314



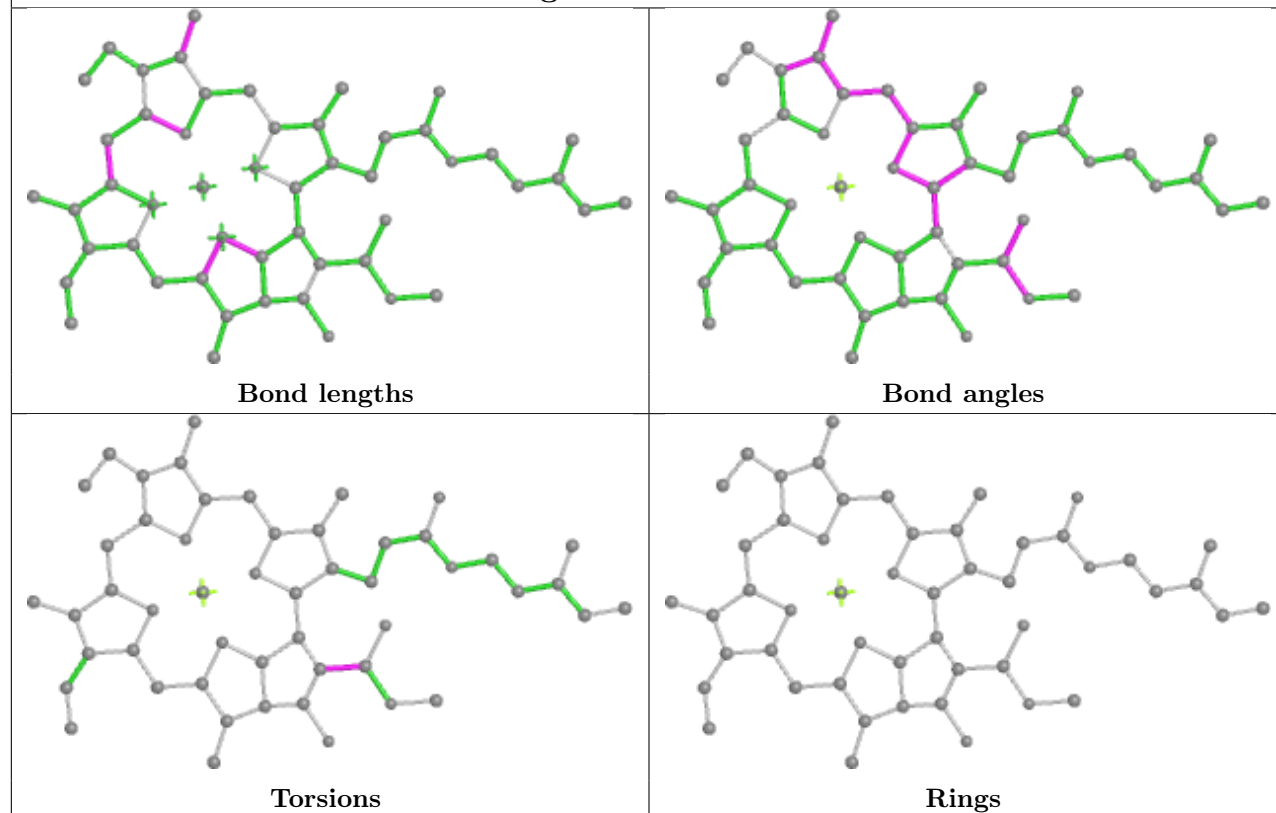
Ligand CLA k 603



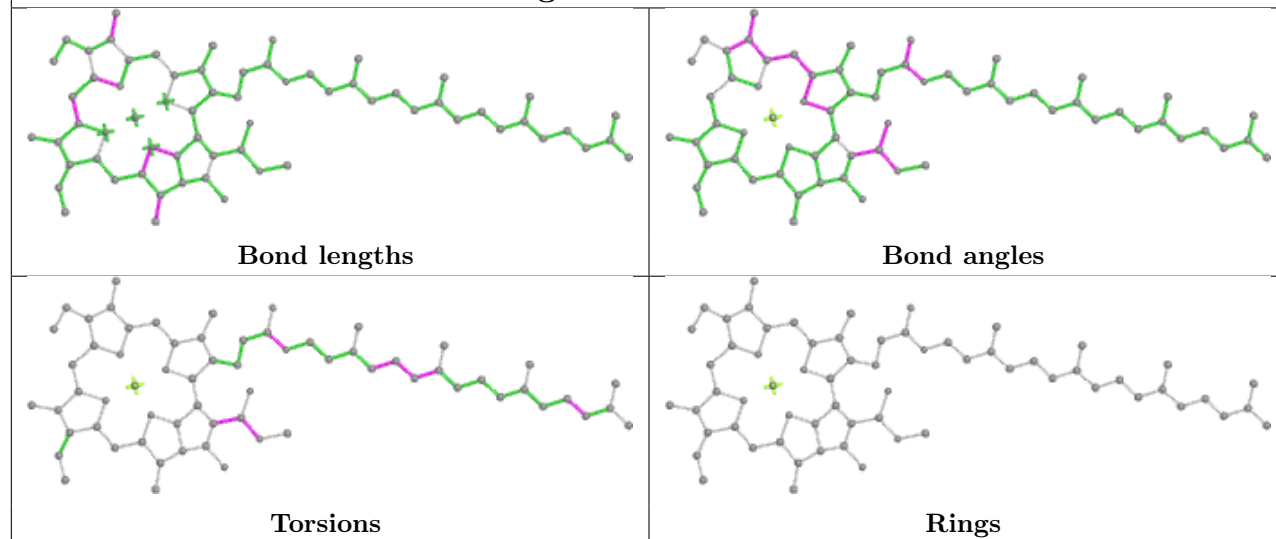
Ligand II0 i 314

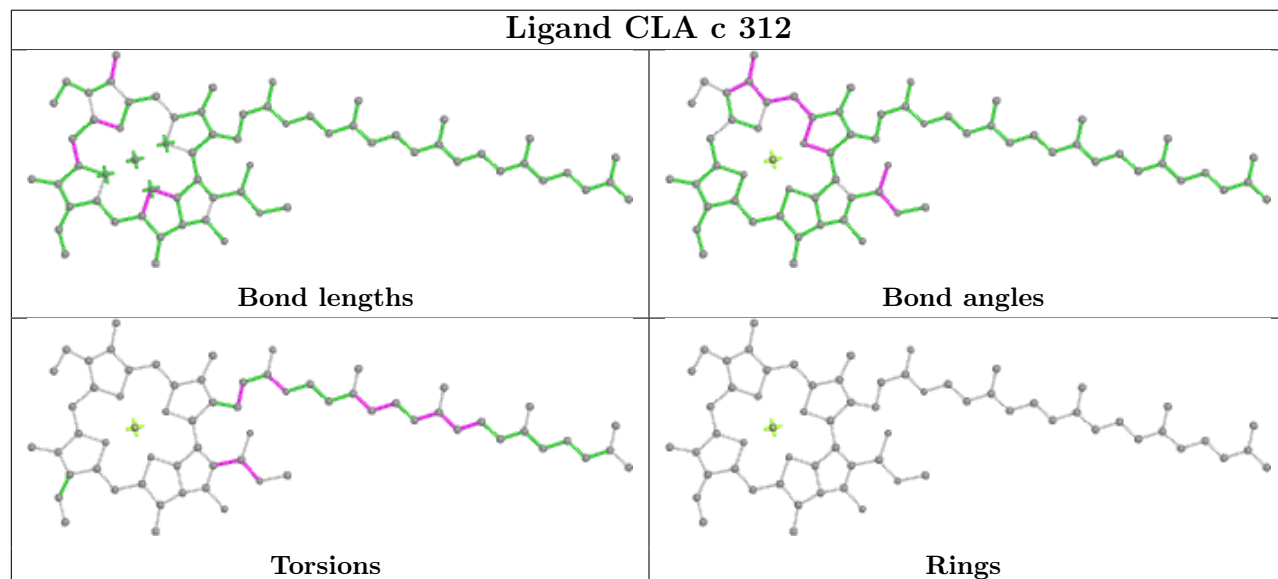
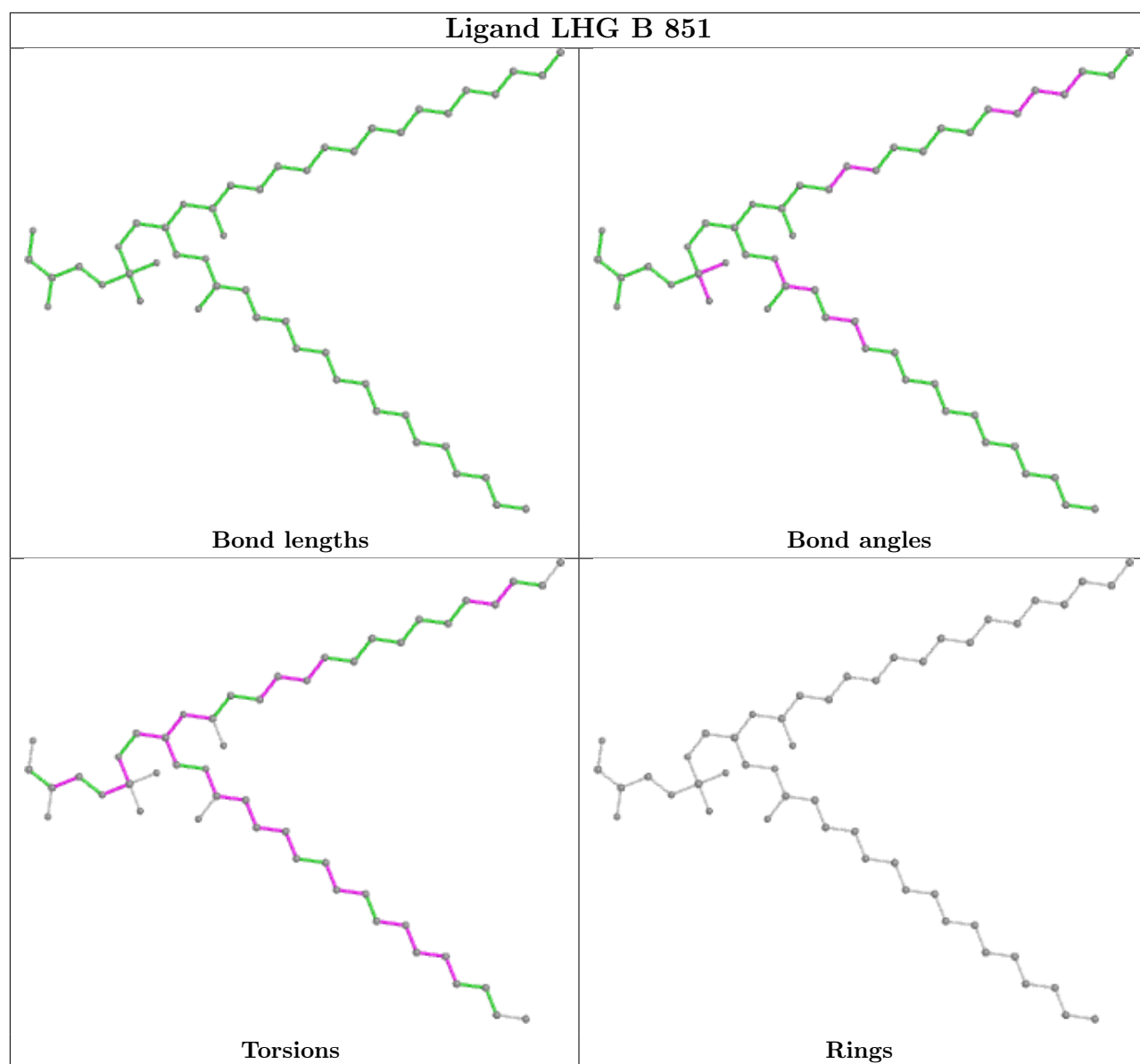


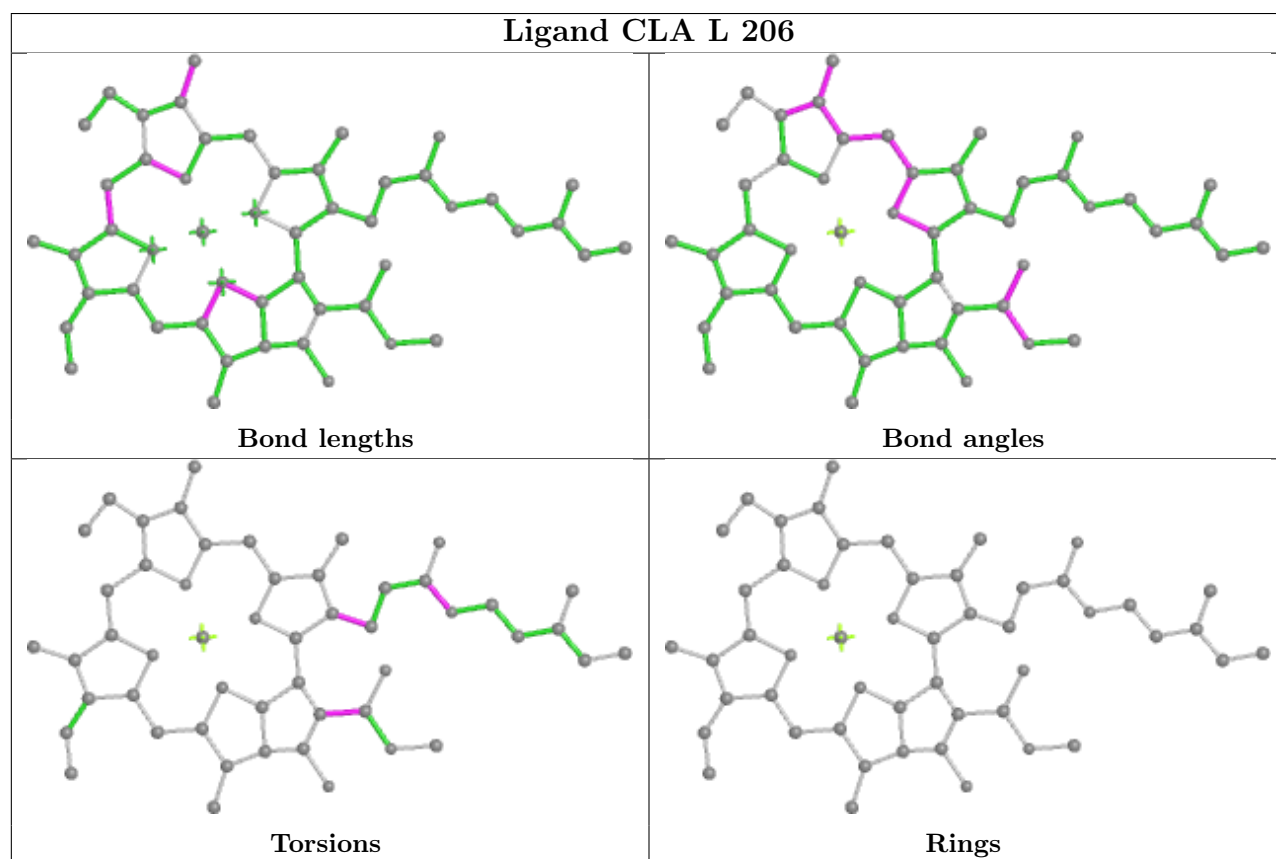
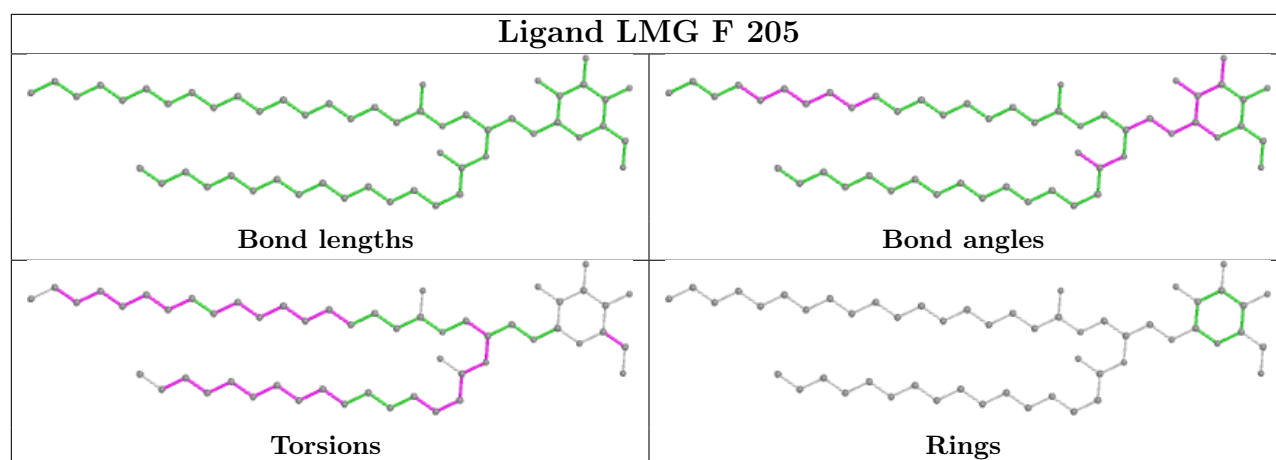
Ligand CLA l 306



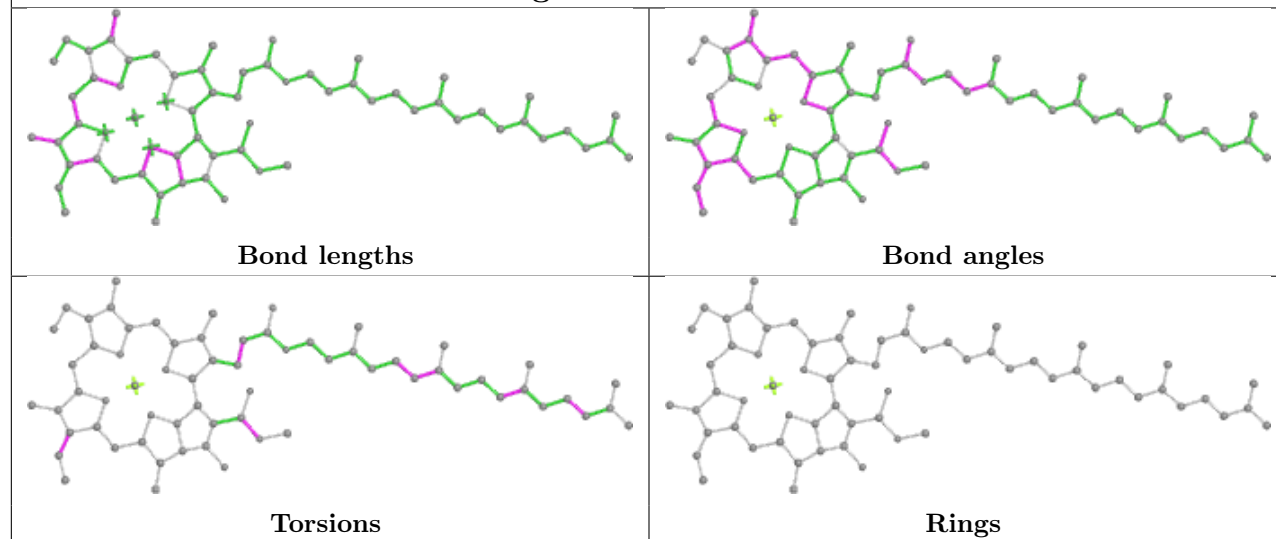
Ligand CLA s 403



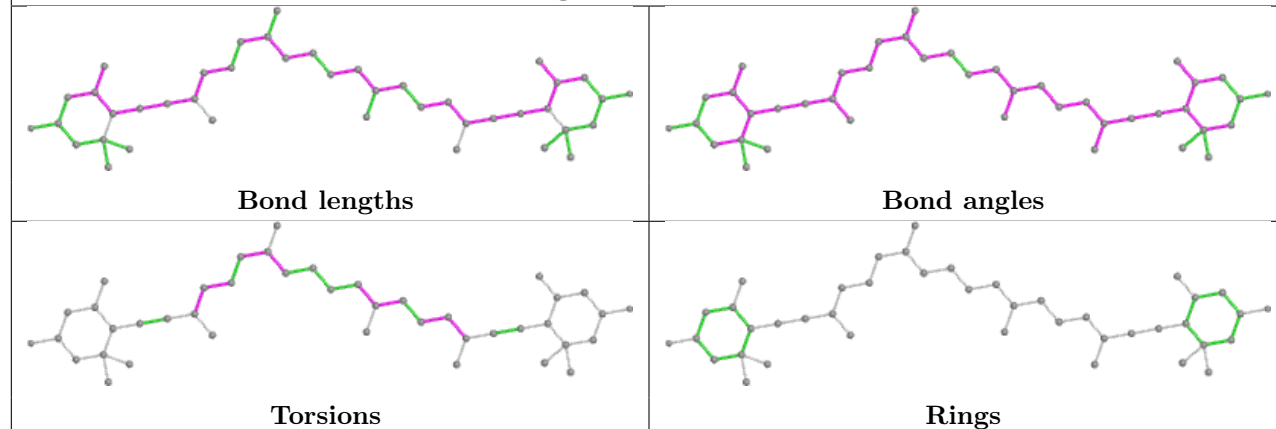




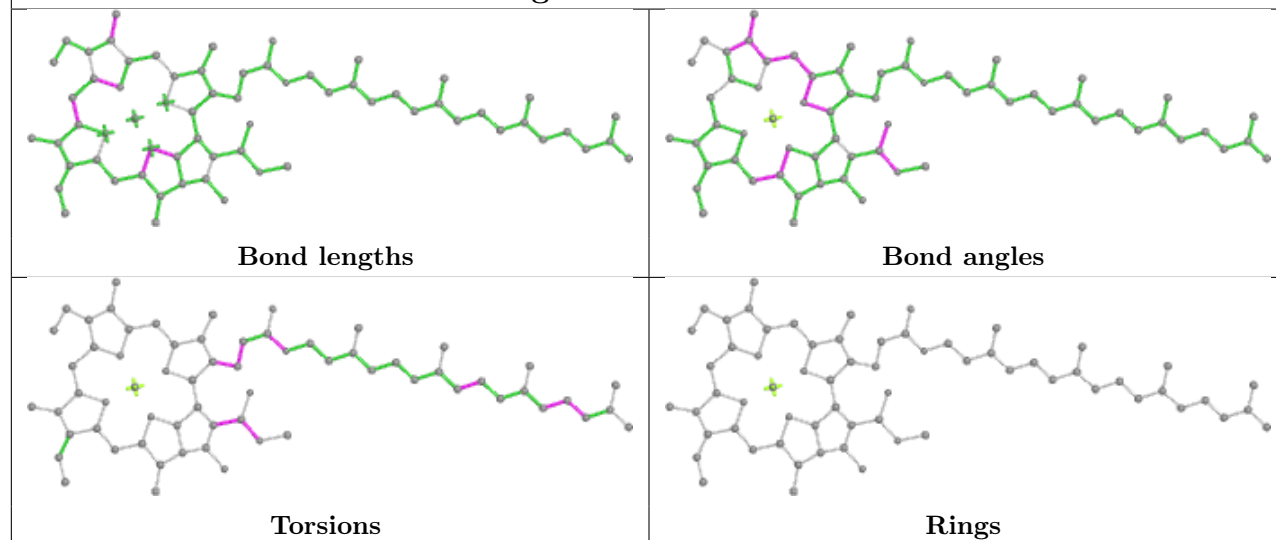
Ligand CLA B 804



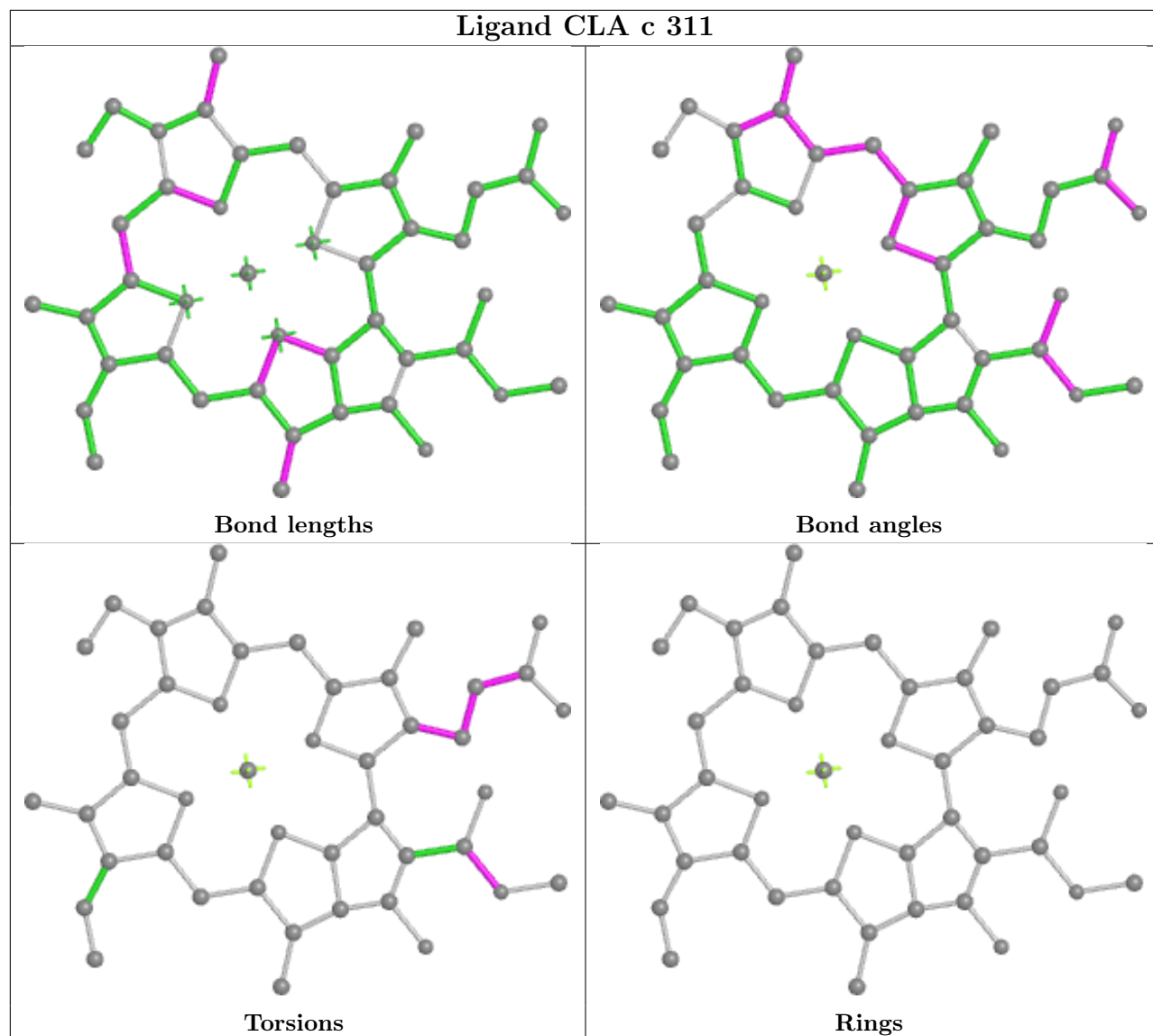
Ligand II0 i 313



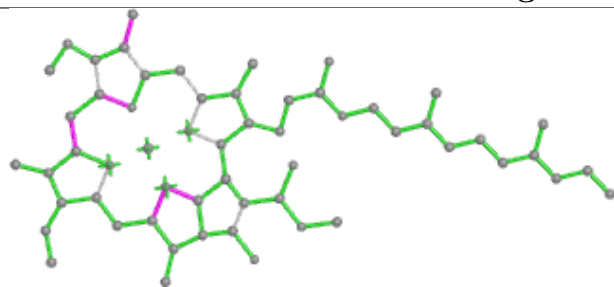
Ligand CLA A 807



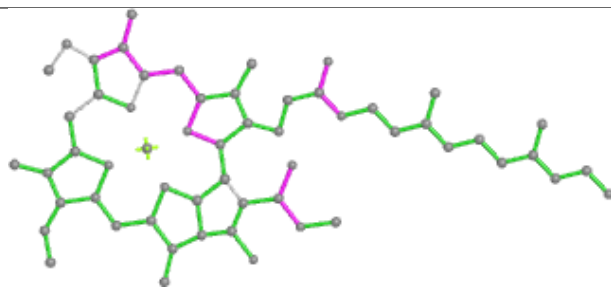
Ligand CLA c 311



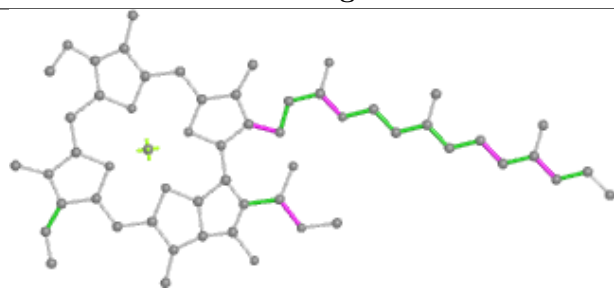
Ligand CLA k 609



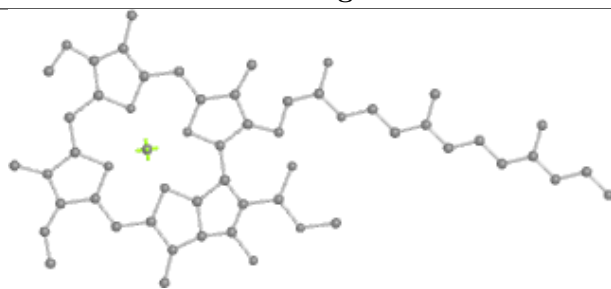
Bond lengths



Bond angles

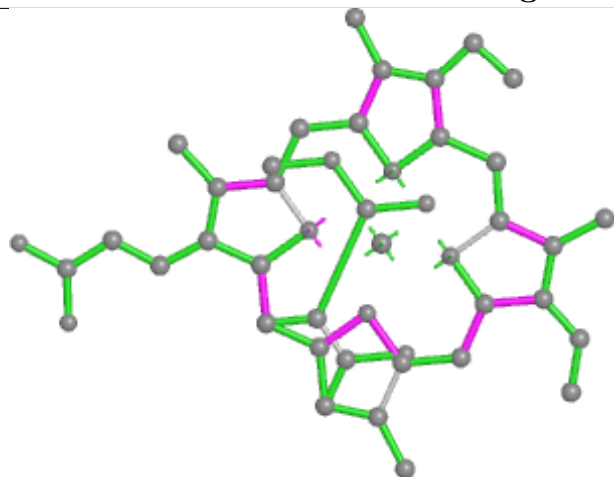


Torsions

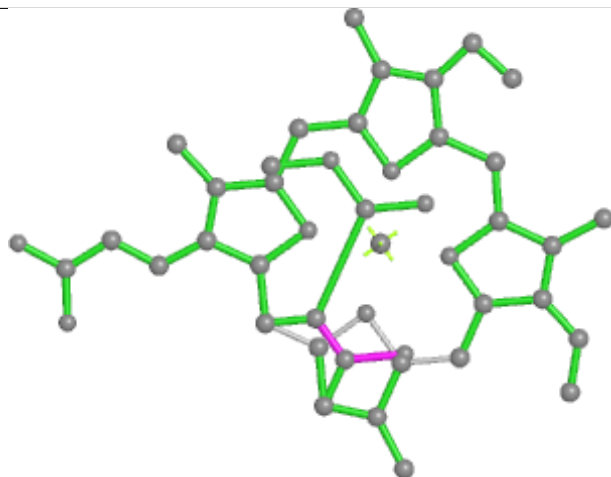


Rings

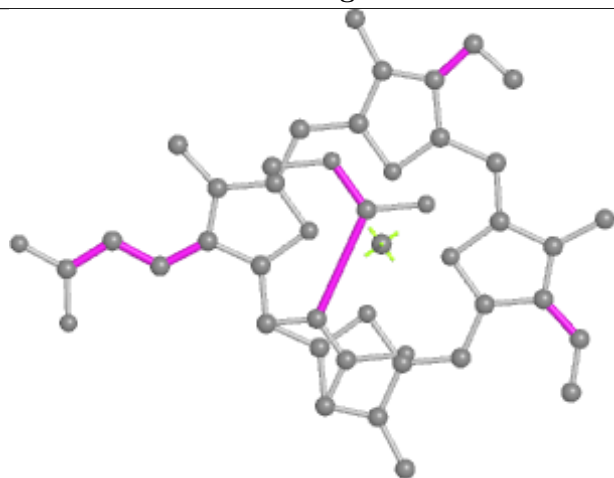
Ligand KC2 k 613



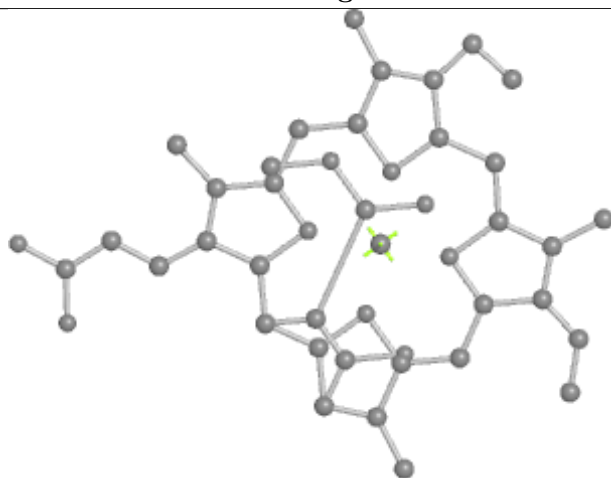
Bond lengths



Bond angles

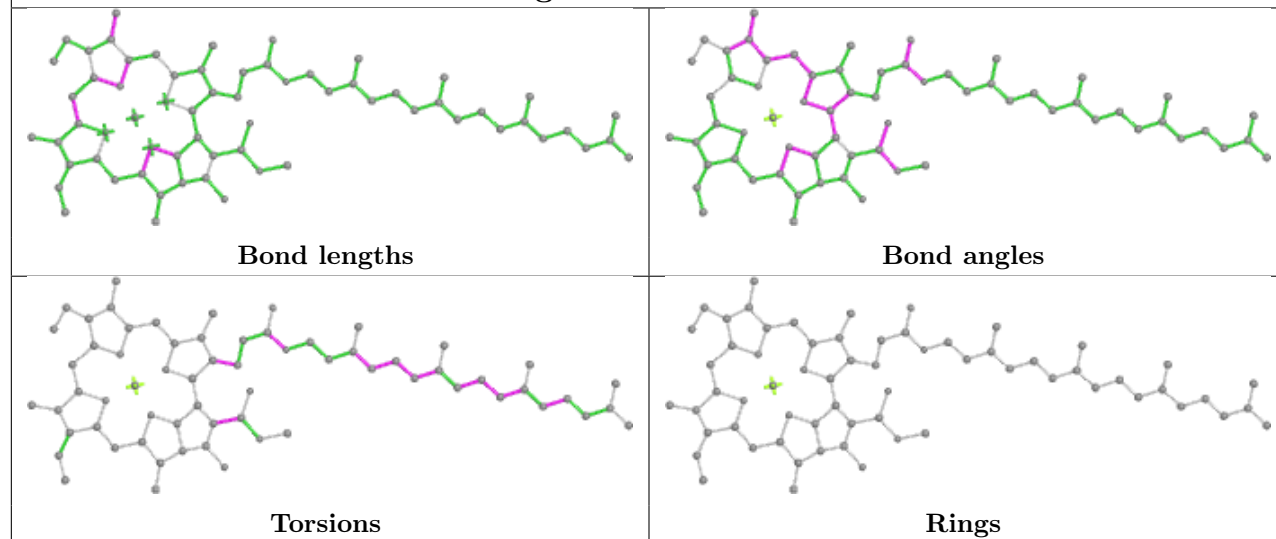


Torsions

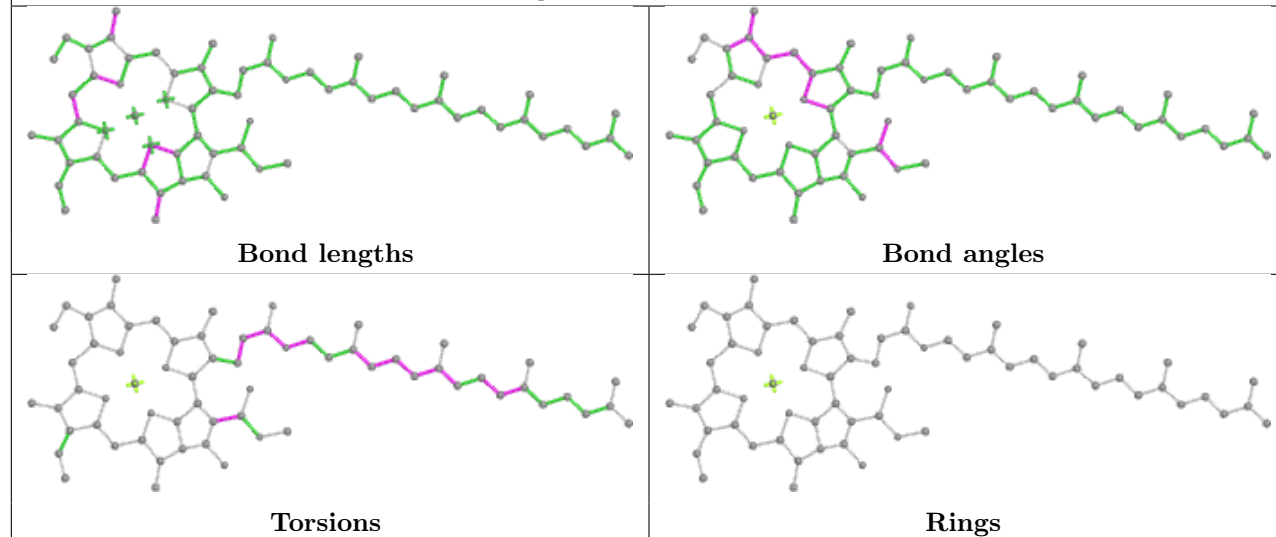


Rings

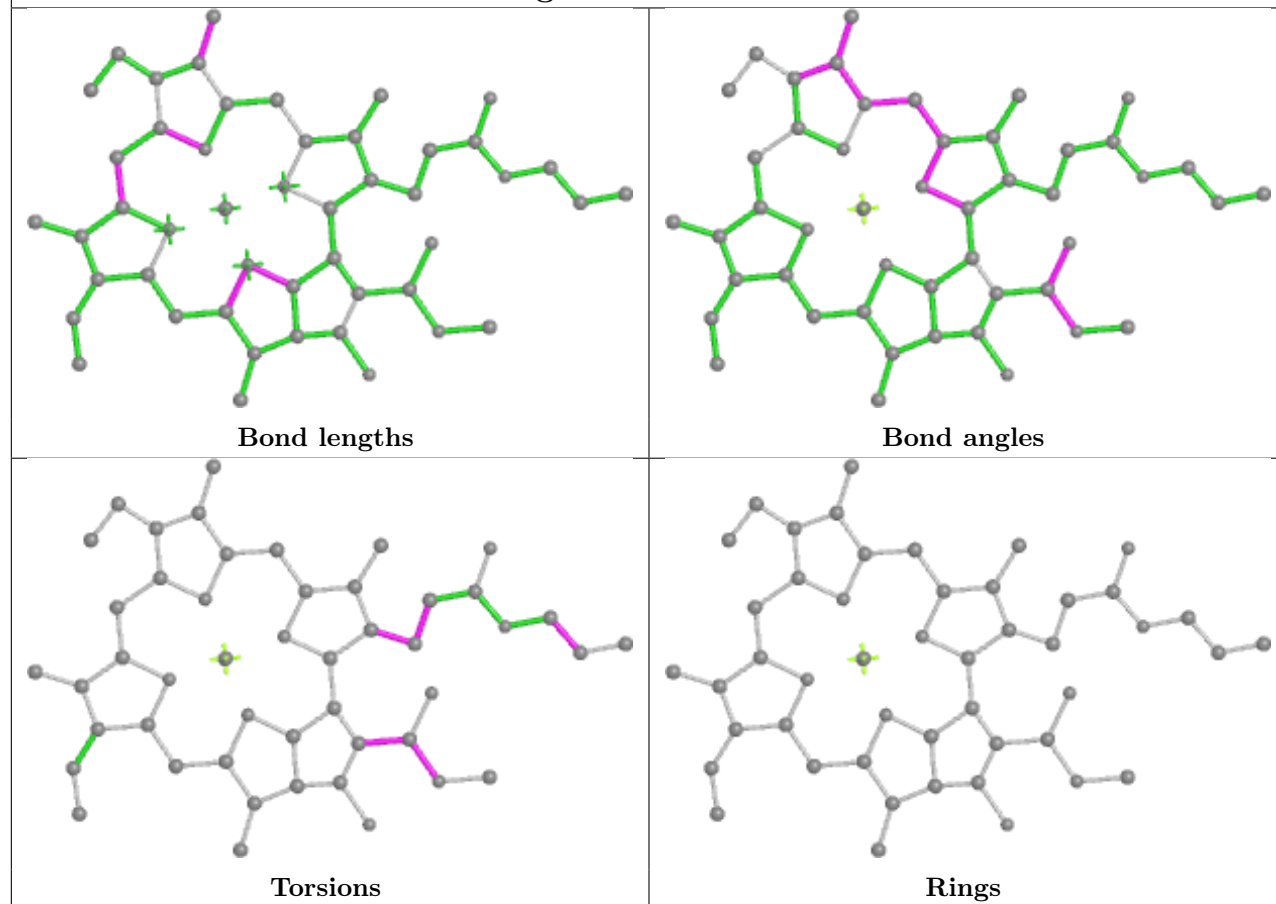
Ligand CLA n 608



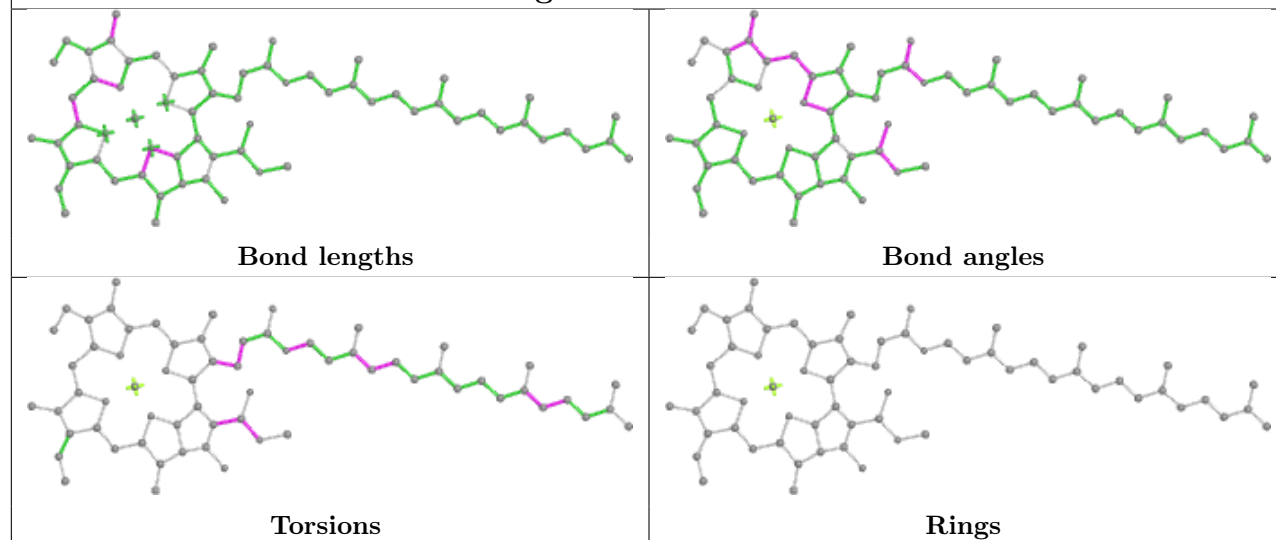
Ligand CLA B 801



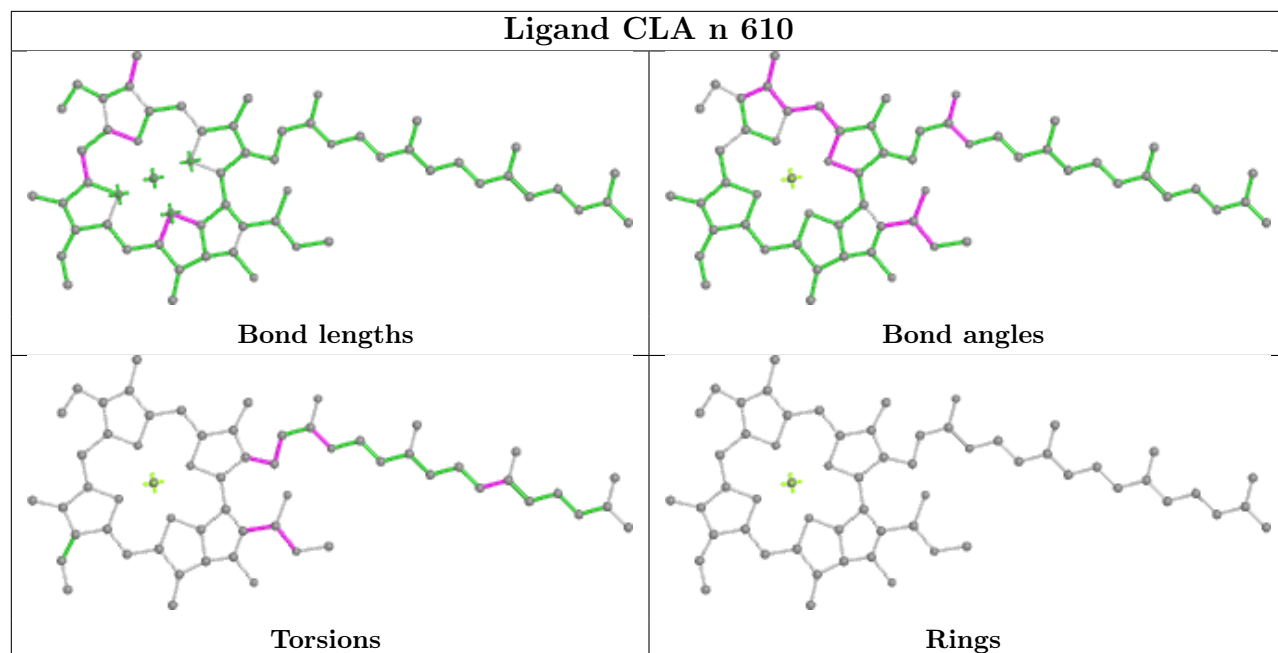
Ligand CLA a 311



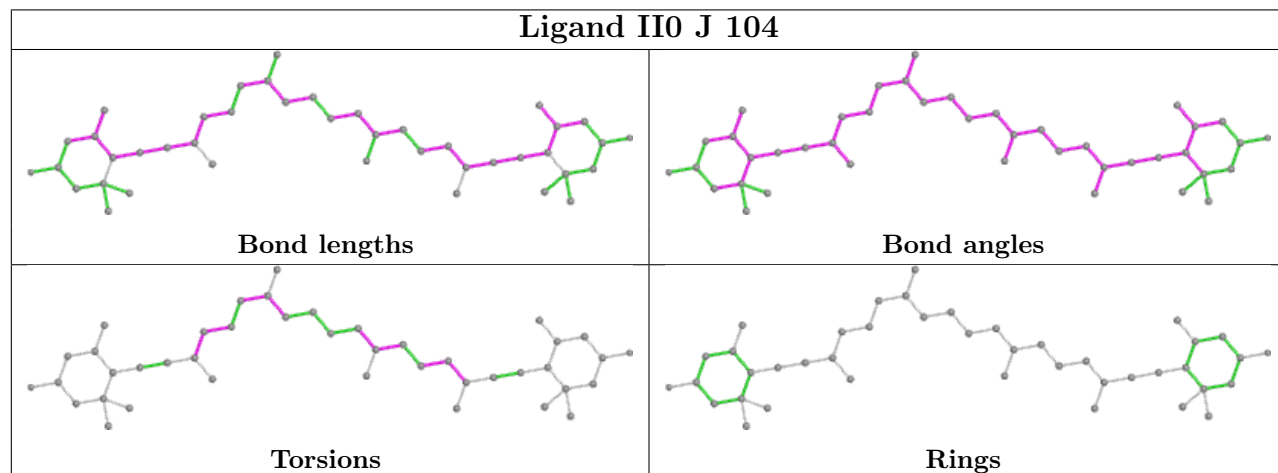
Ligand CLA n 609



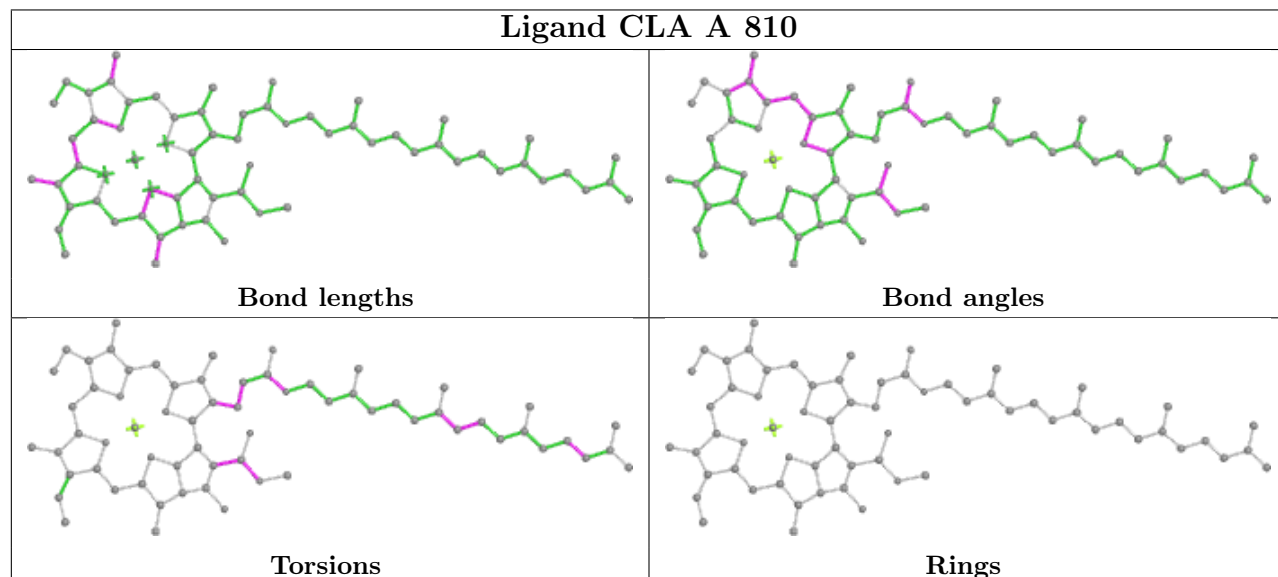
Ligand CLA n 610



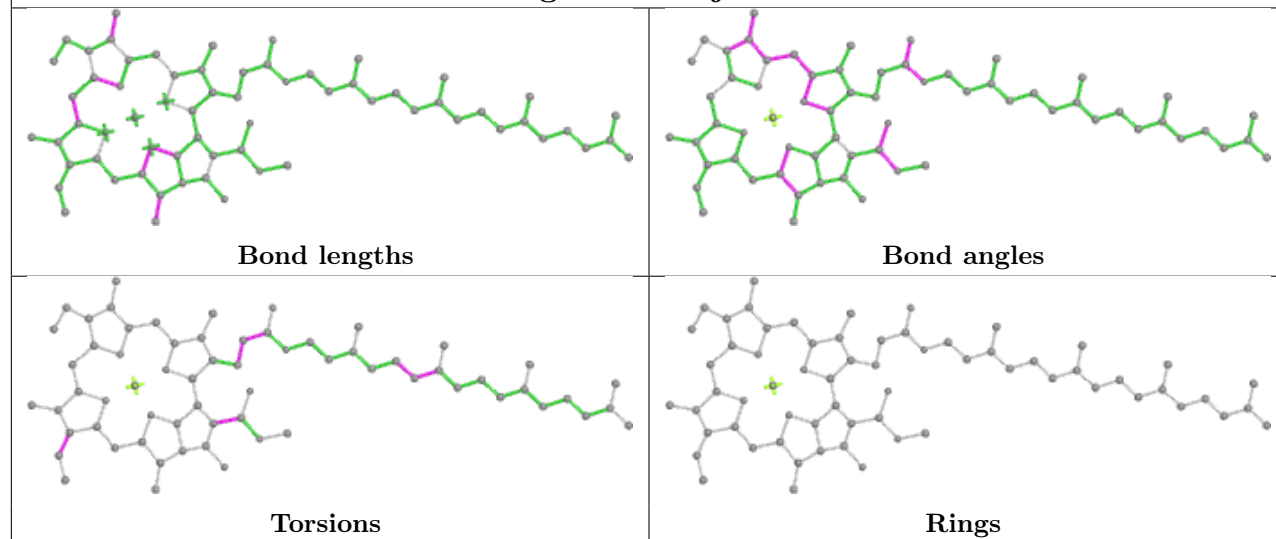
Ligand II0 J 104



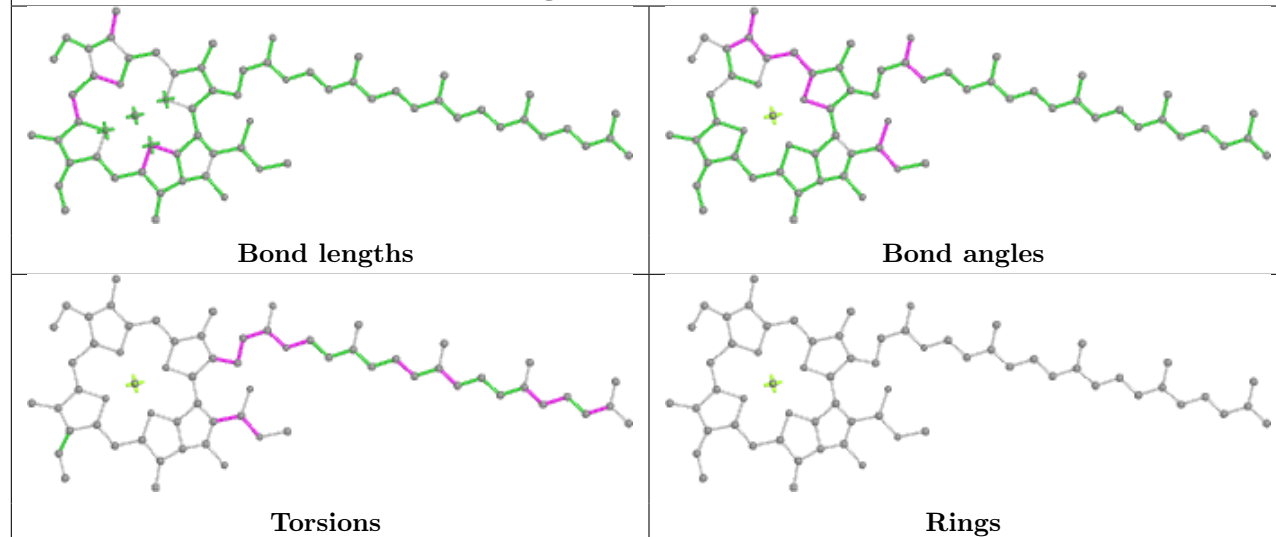
Ligand CLA A 810

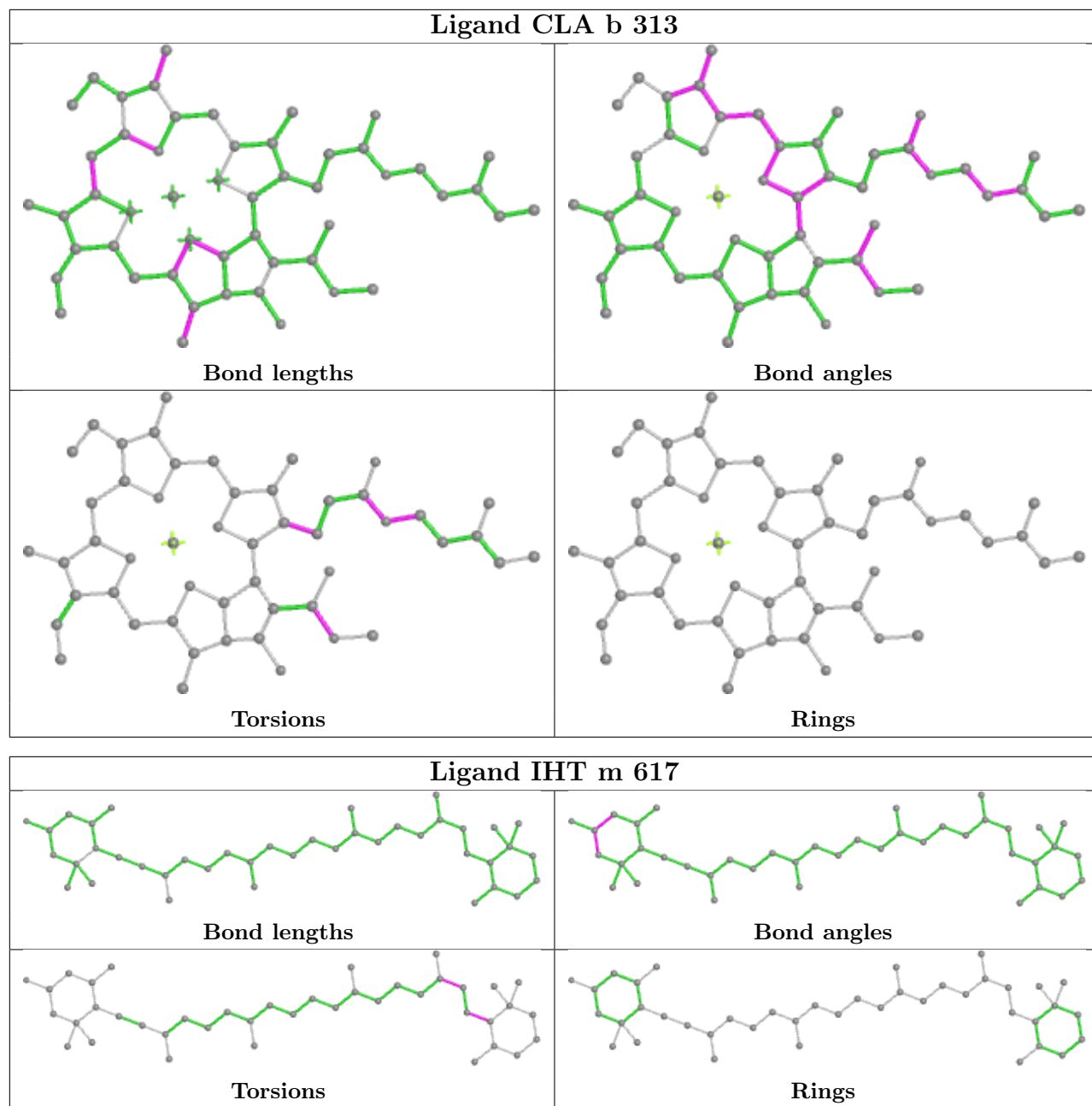


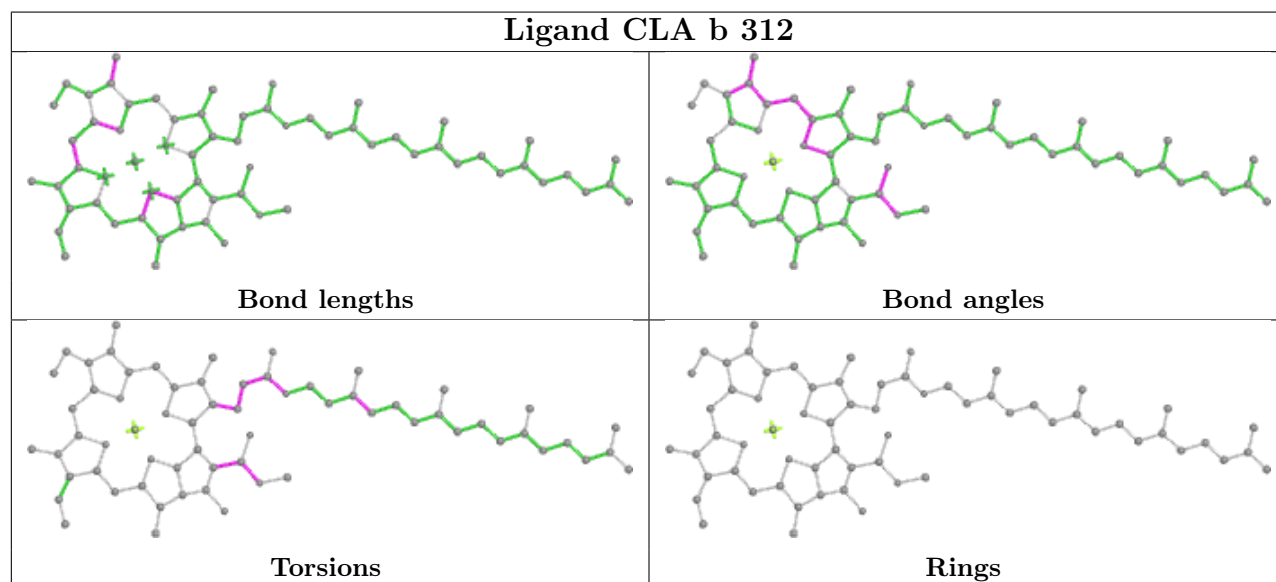
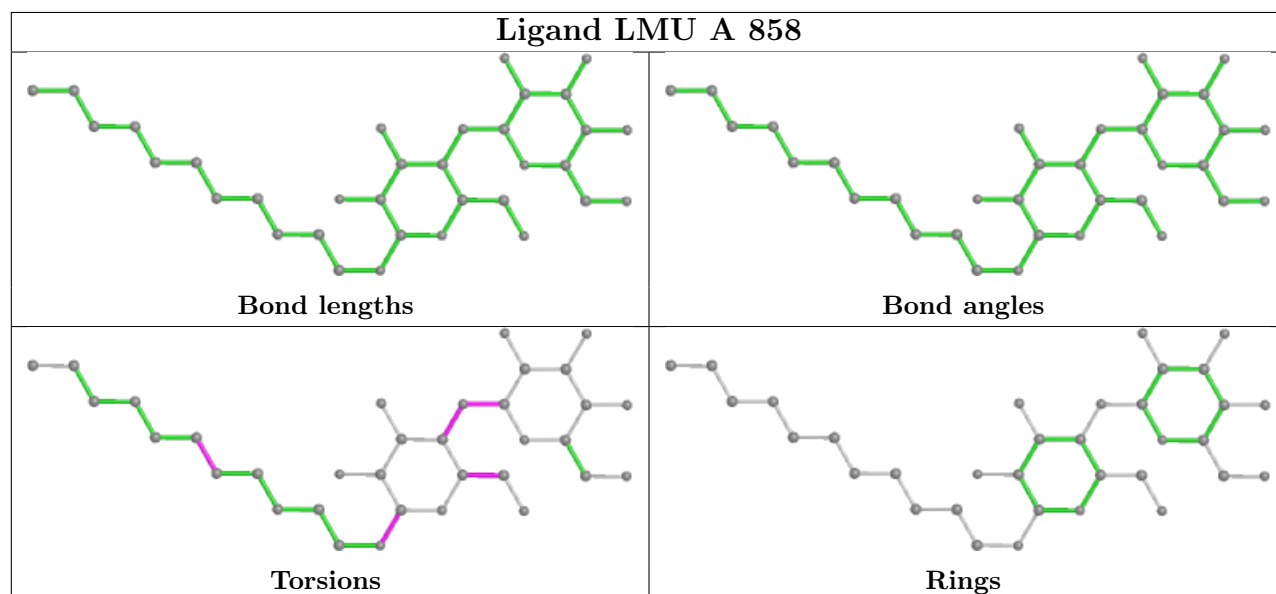
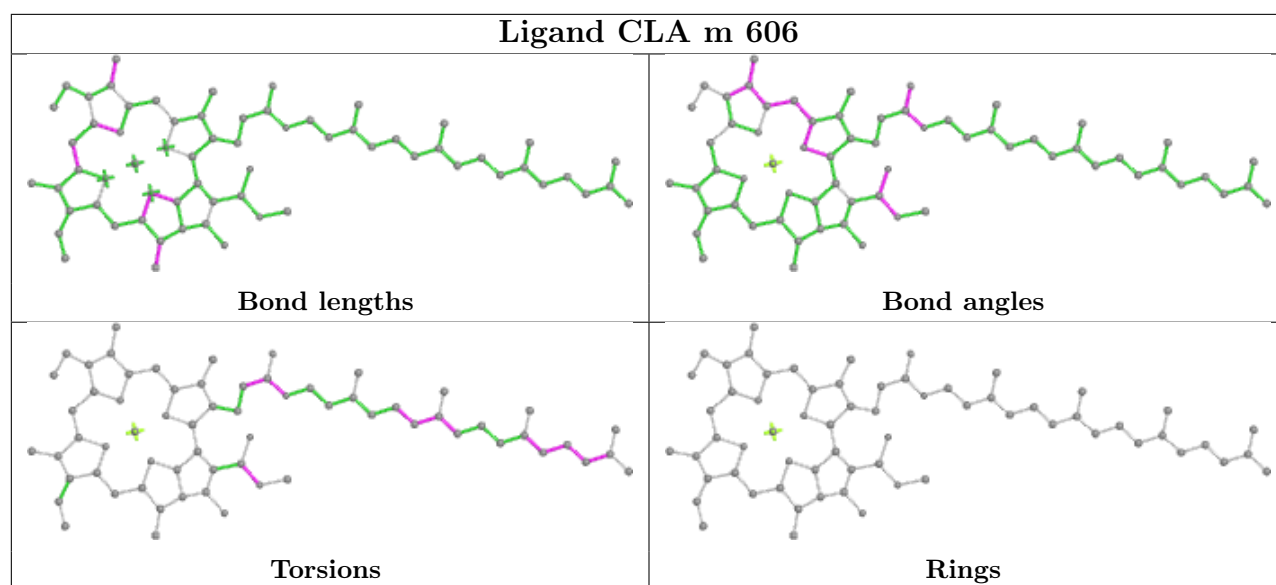
Ligand CLA j 604

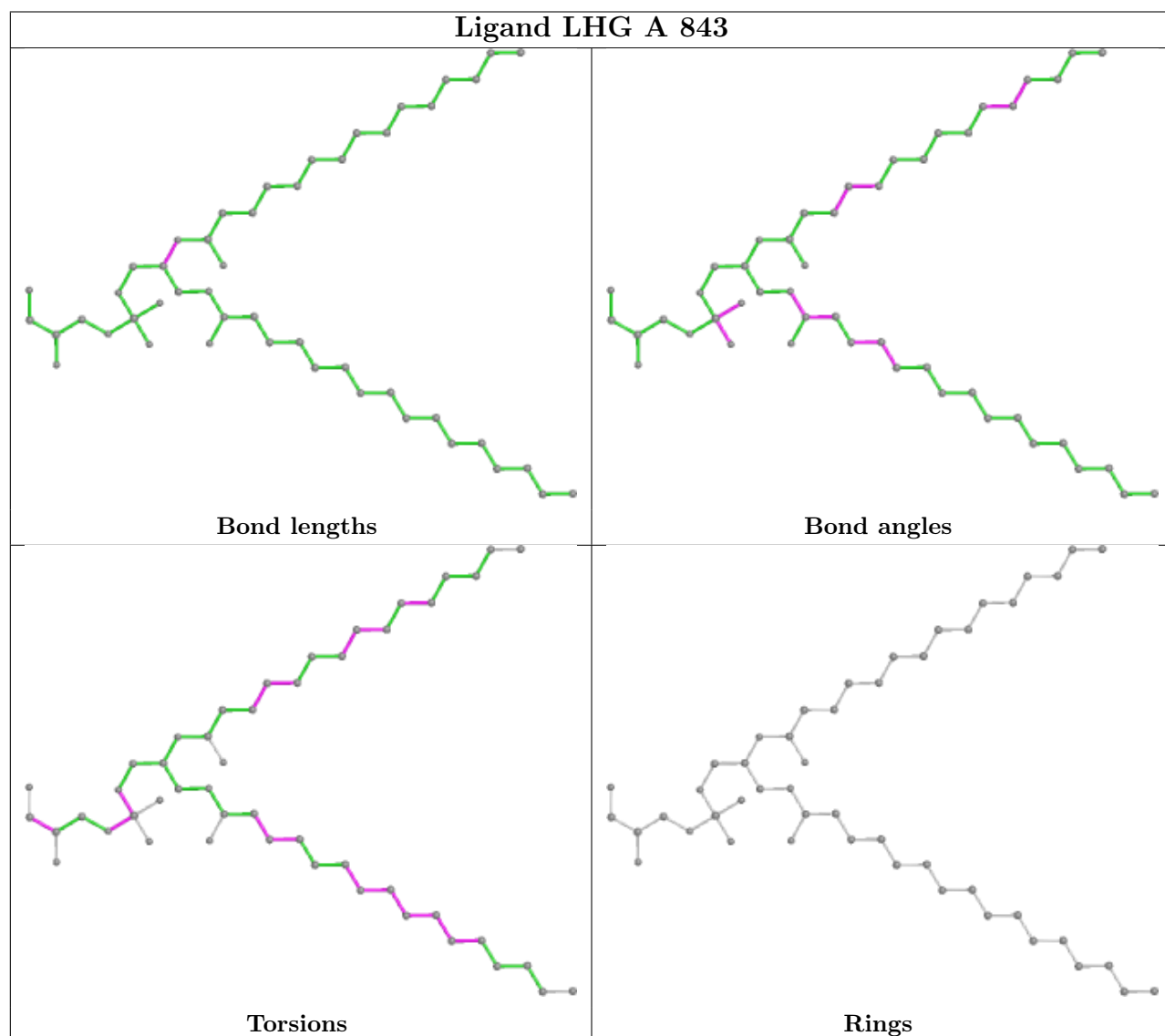
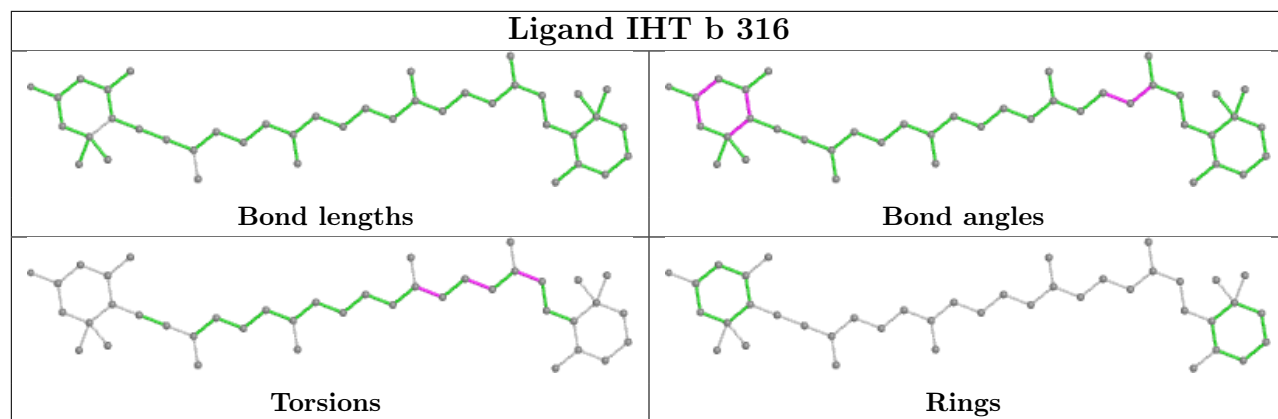


Ligand CLA i 301

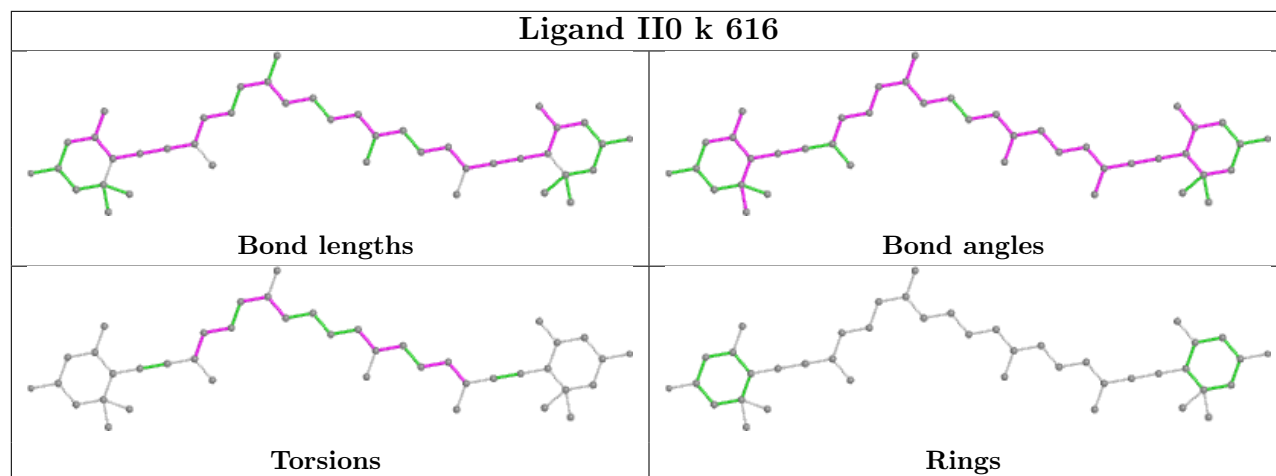




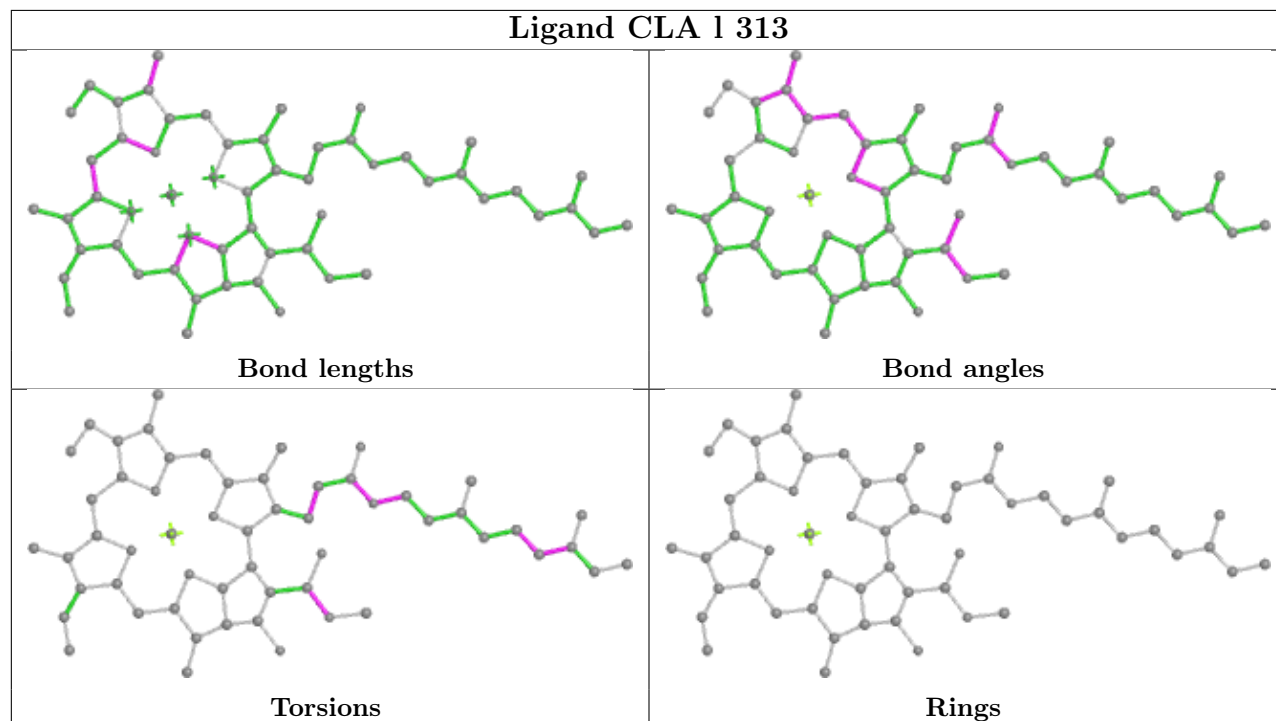




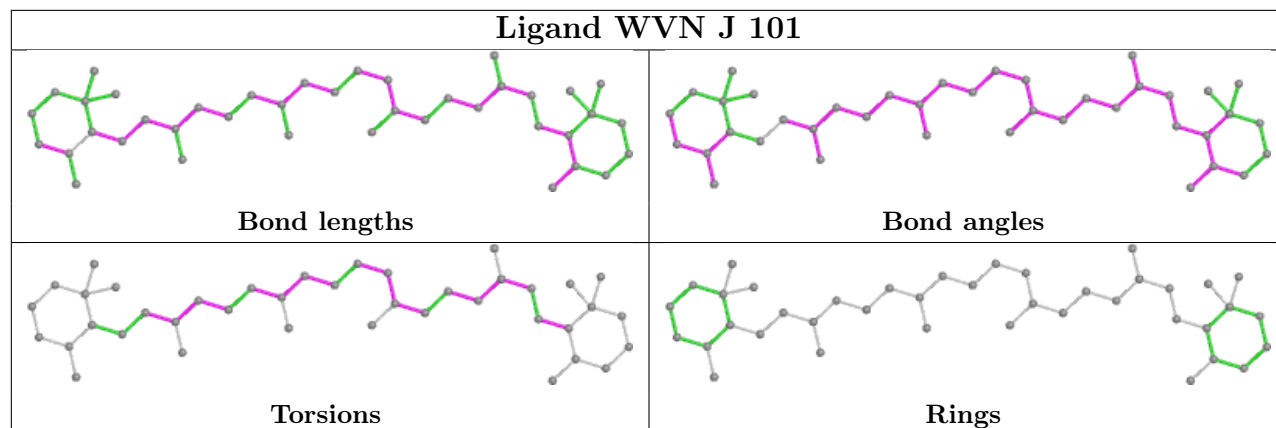
Ligand II0 k 616



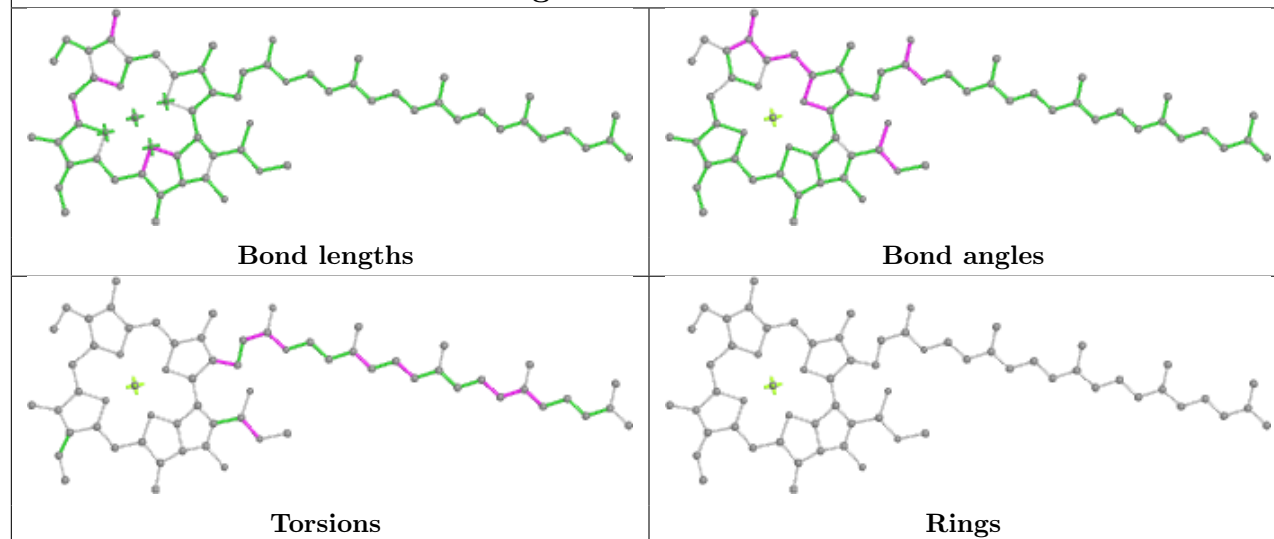
Ligand CLA l 313



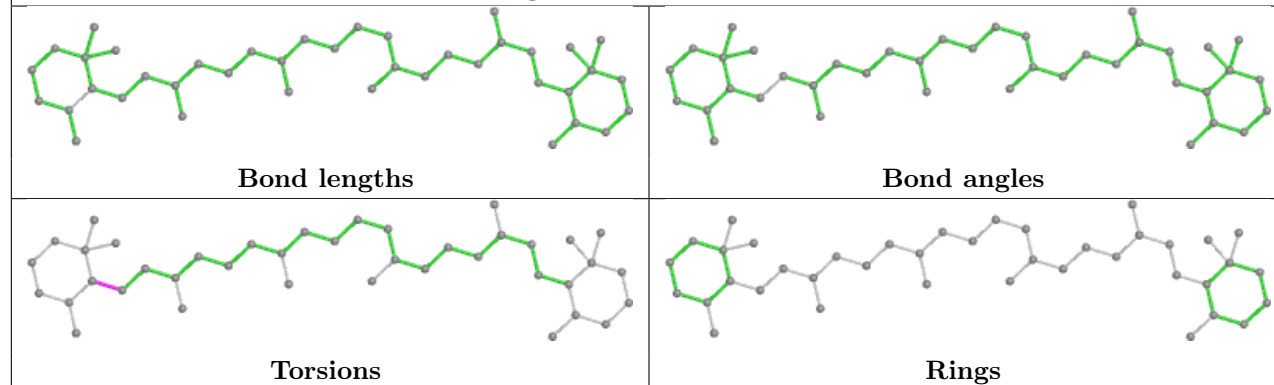
Ligand WVN J 101



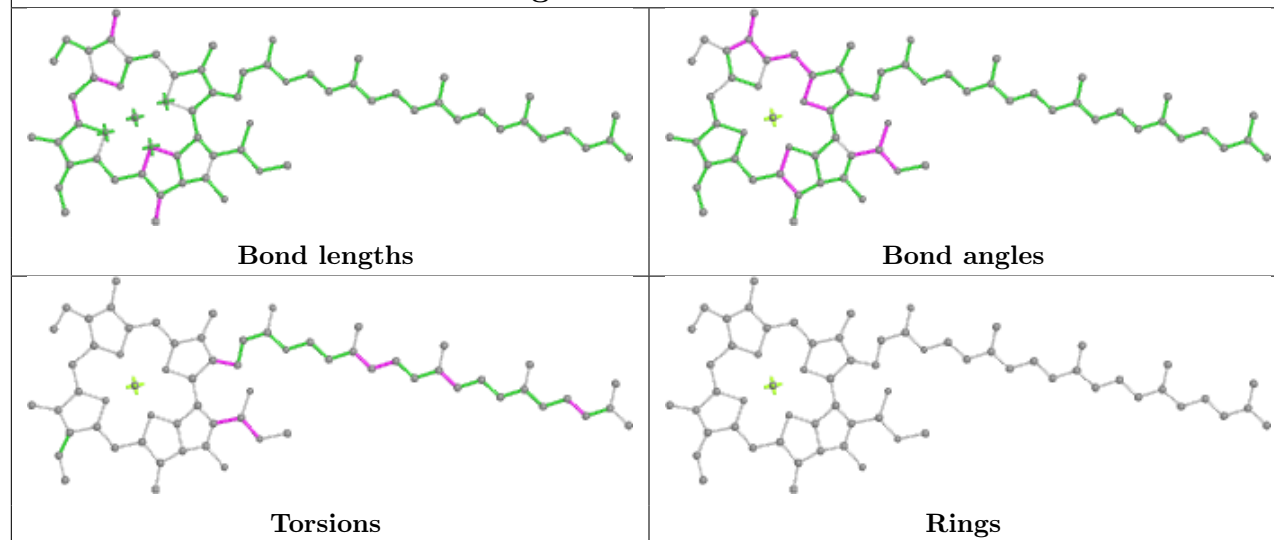
Ligand CLA B 816

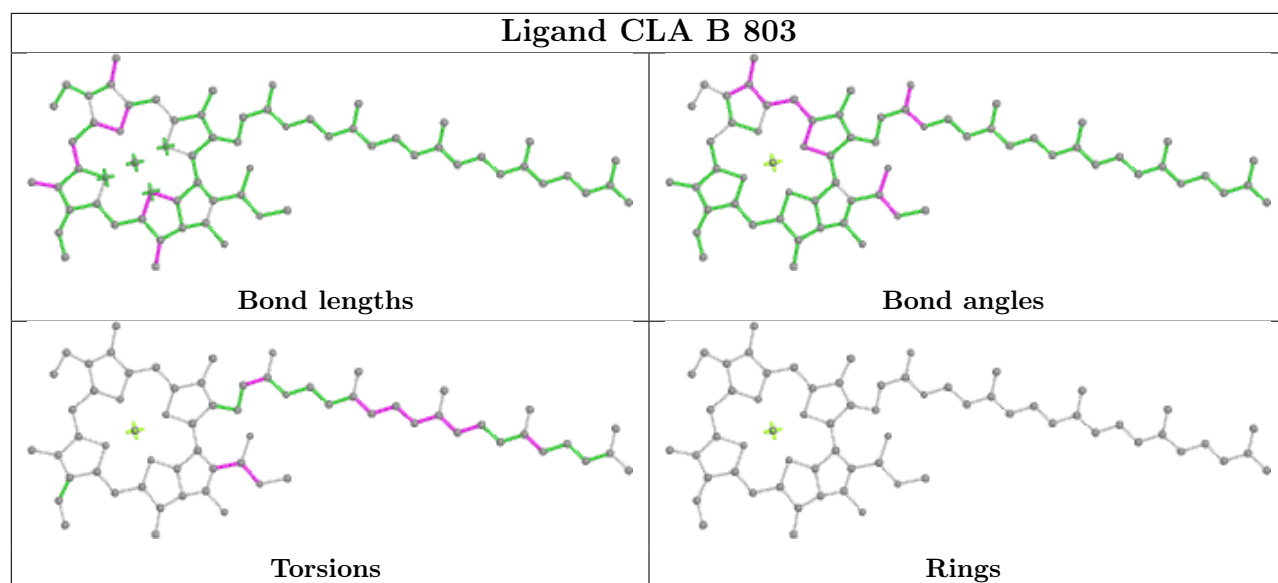
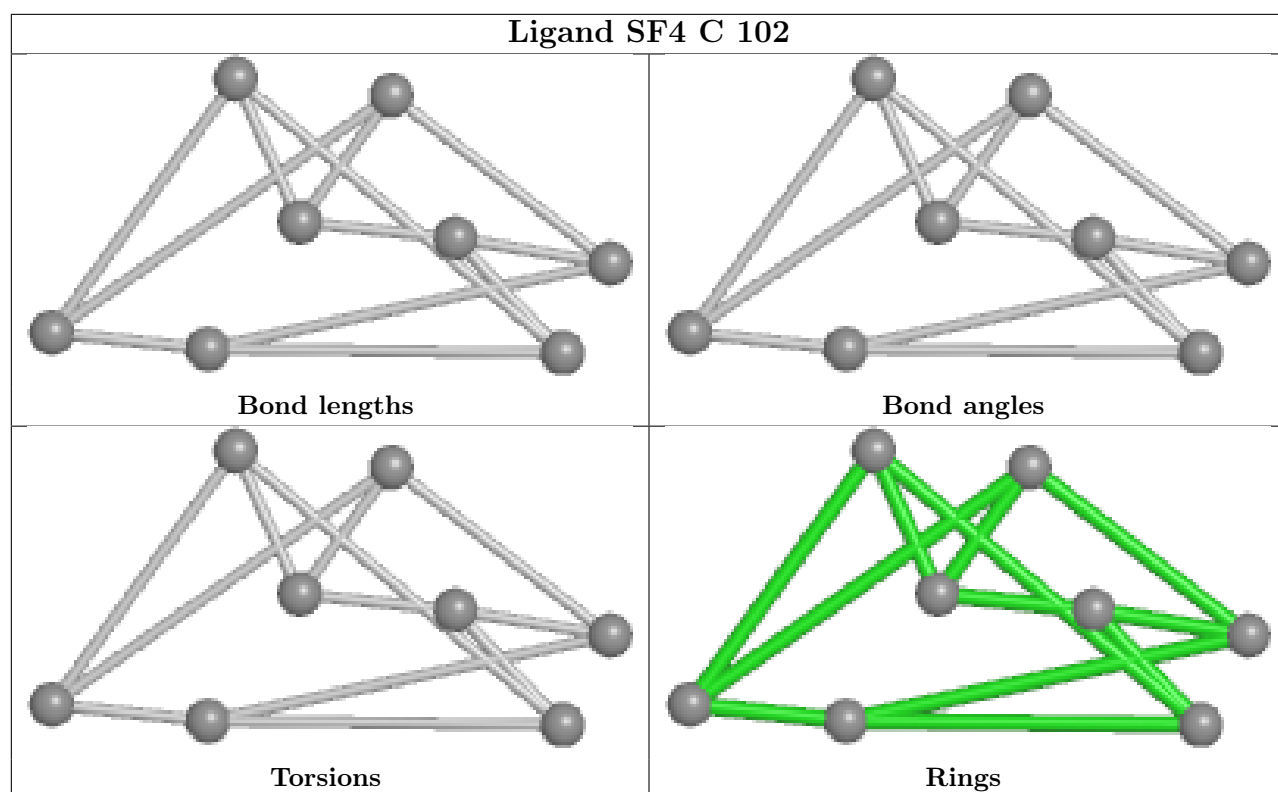


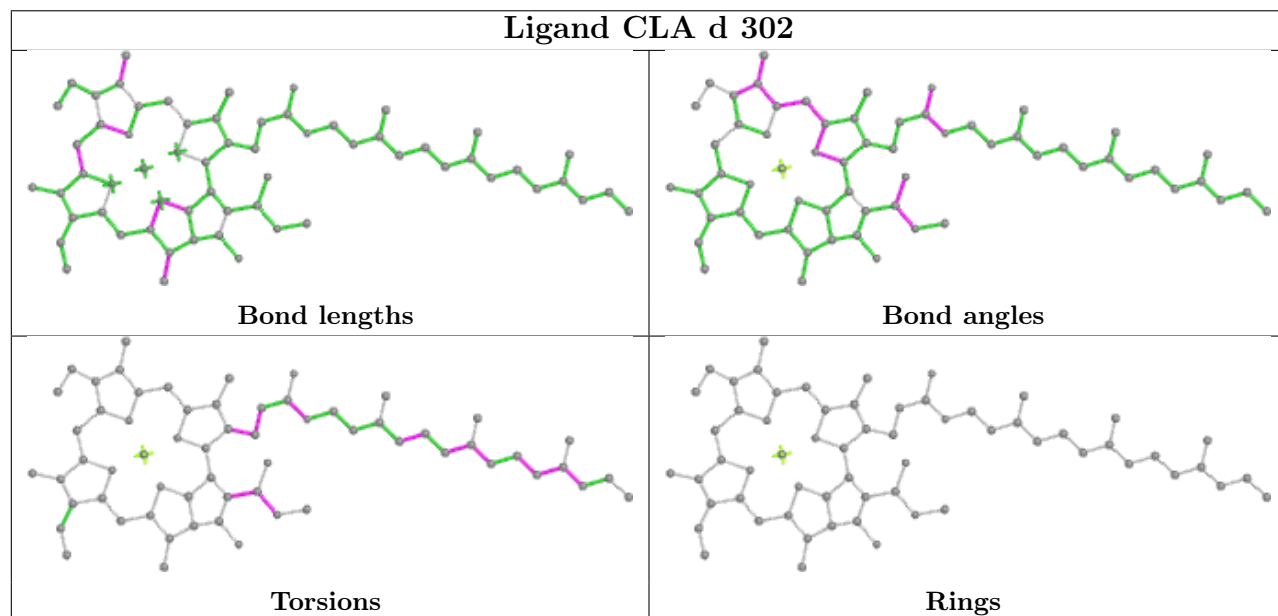
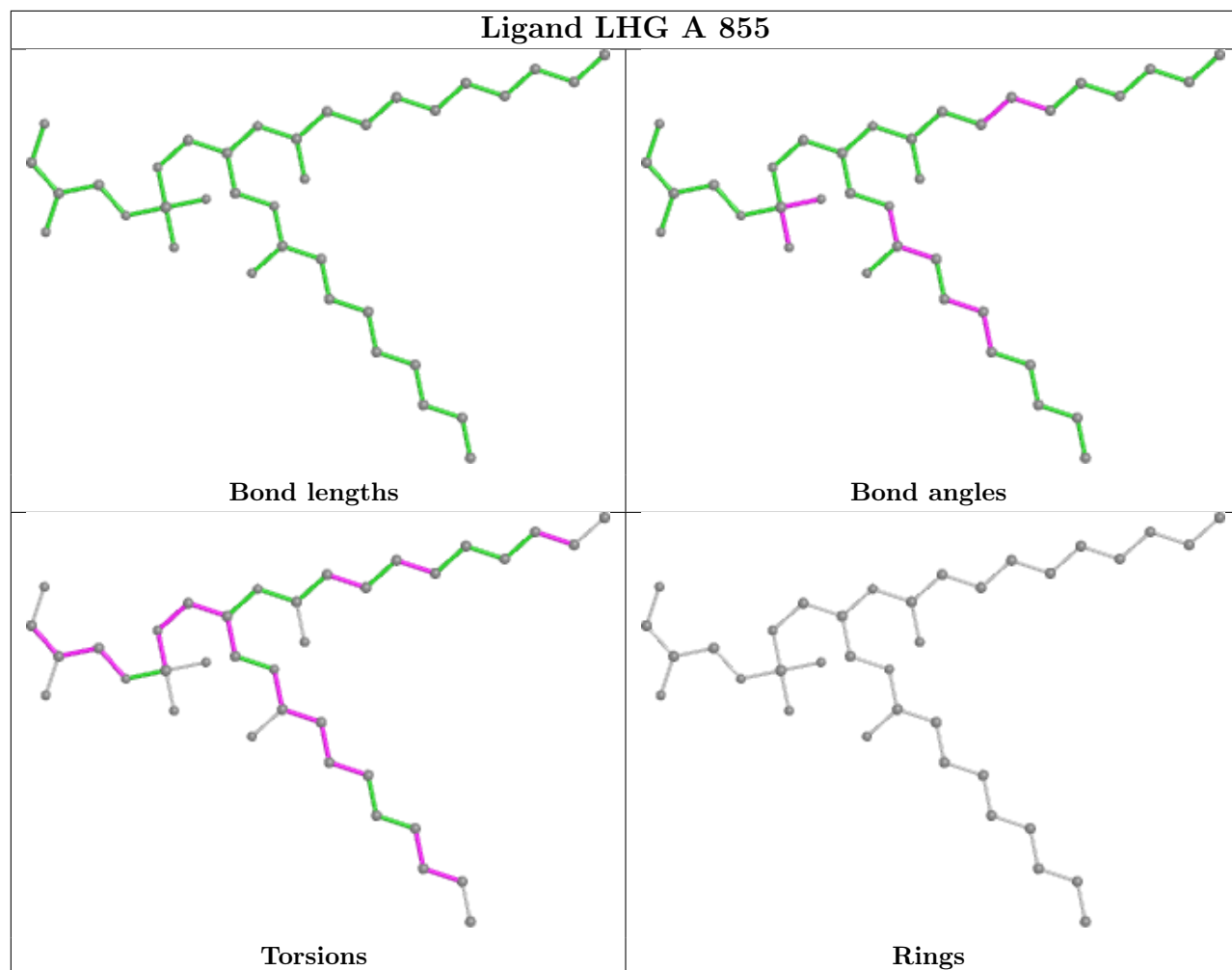
Ligand WVN B 845

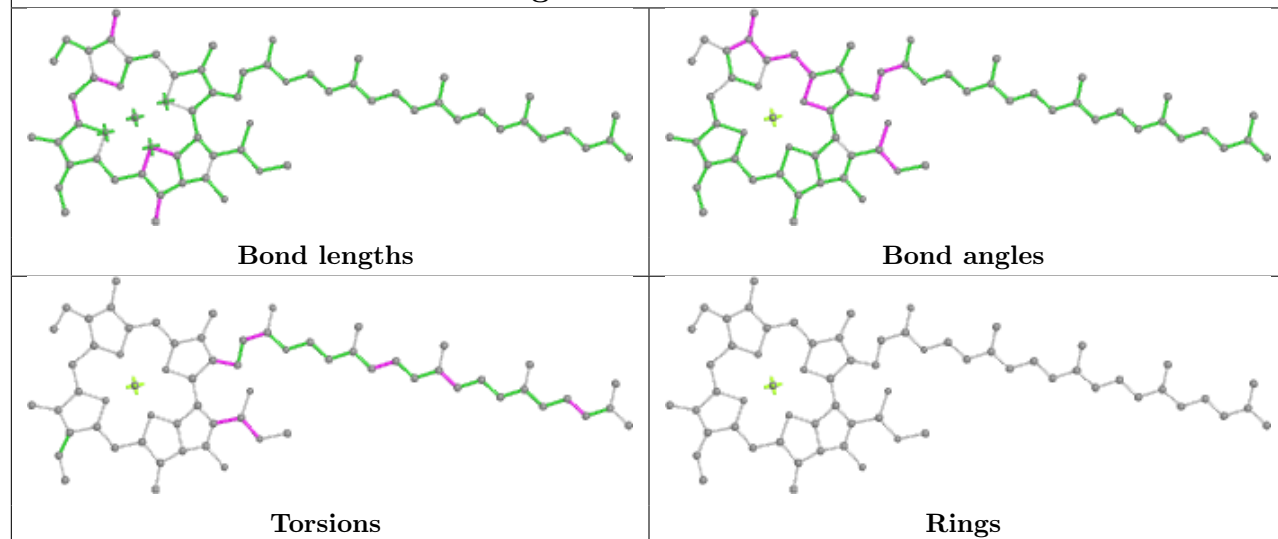
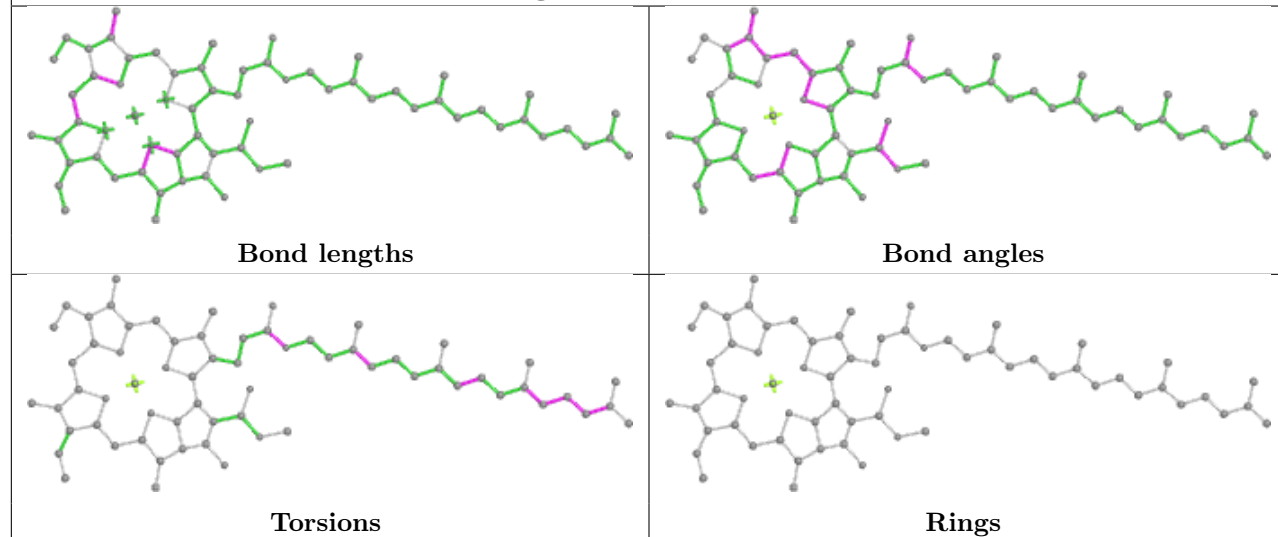


Ligand CLA A 840

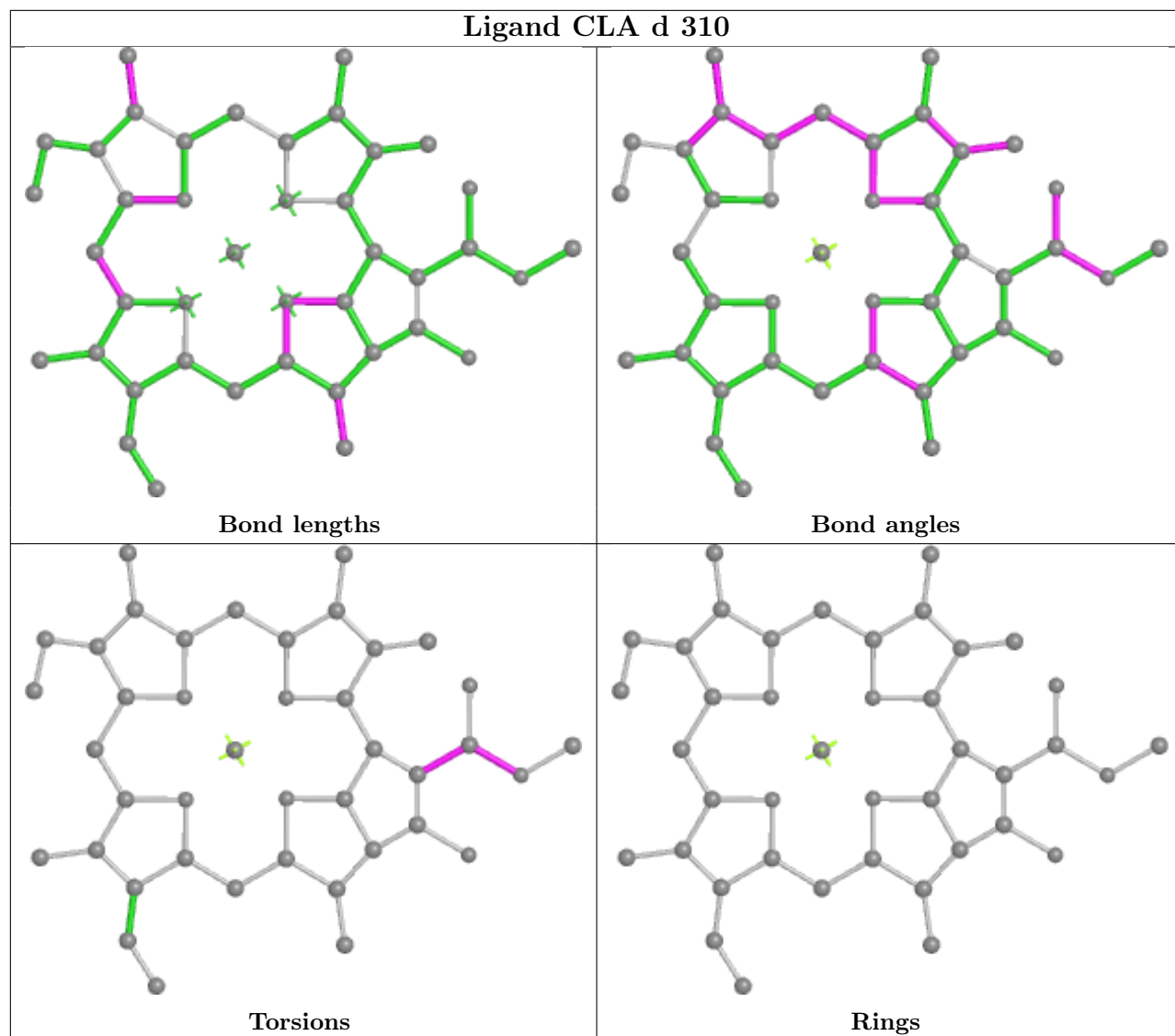


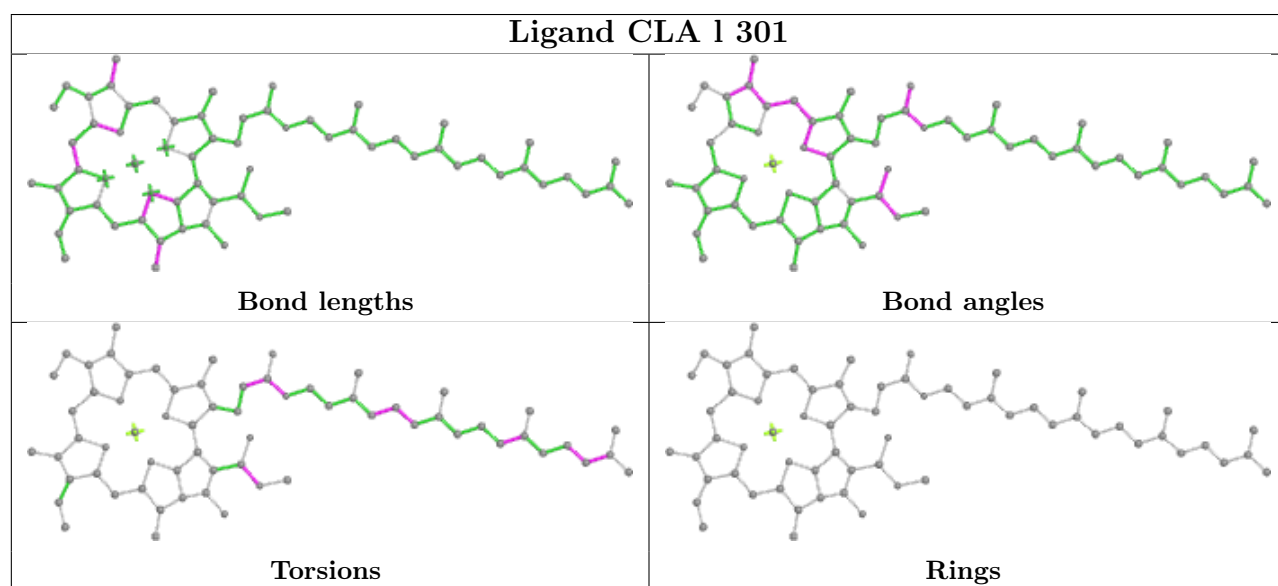
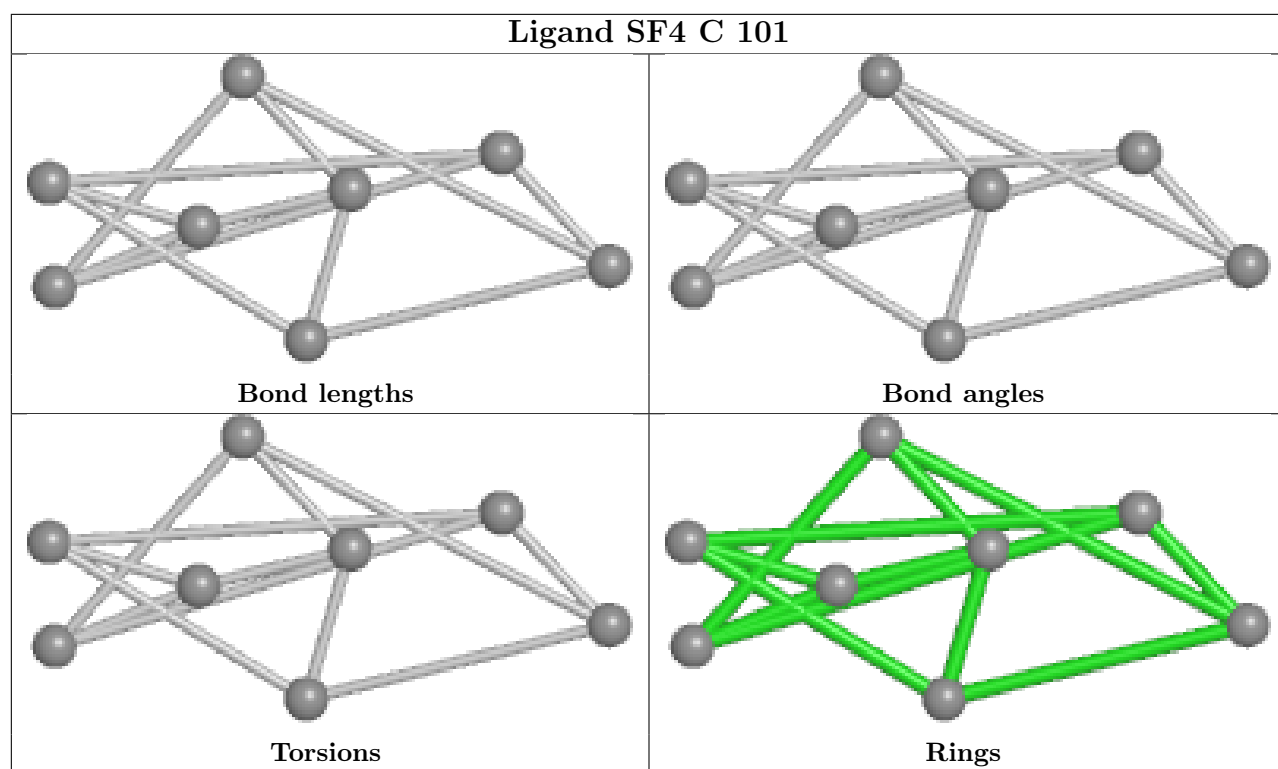




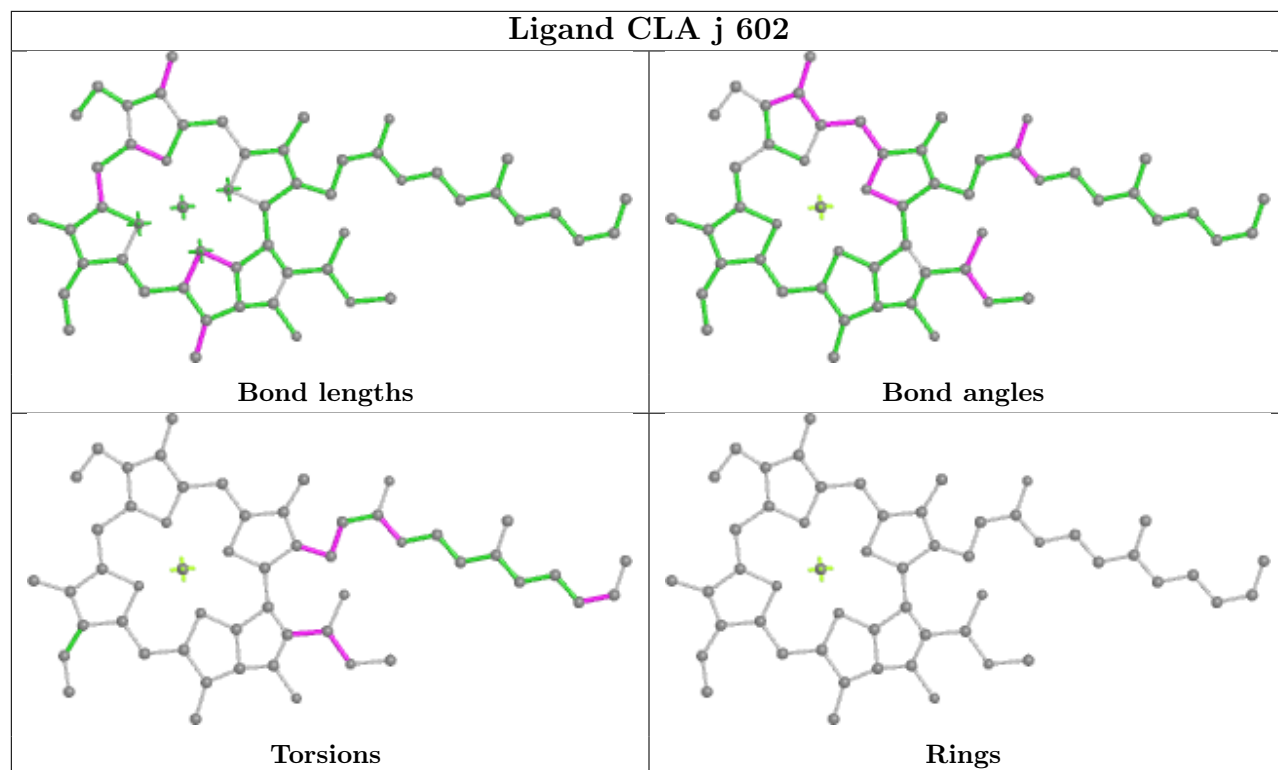
Ligand CLA A 836**Ligand CLA B 834**

Ligand CLA d 310

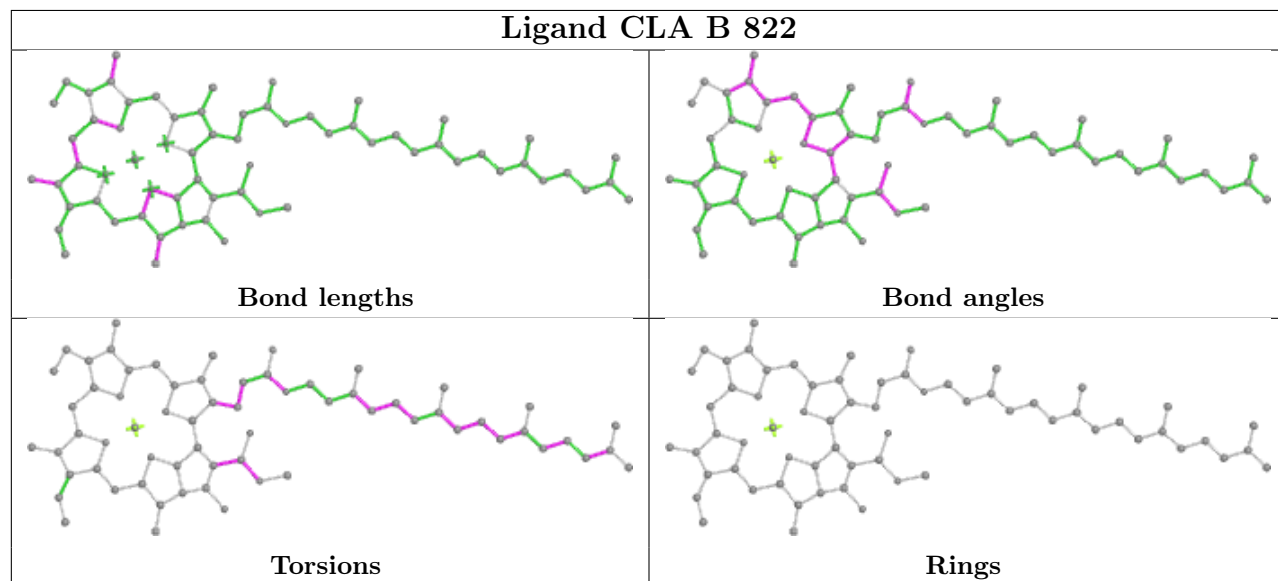




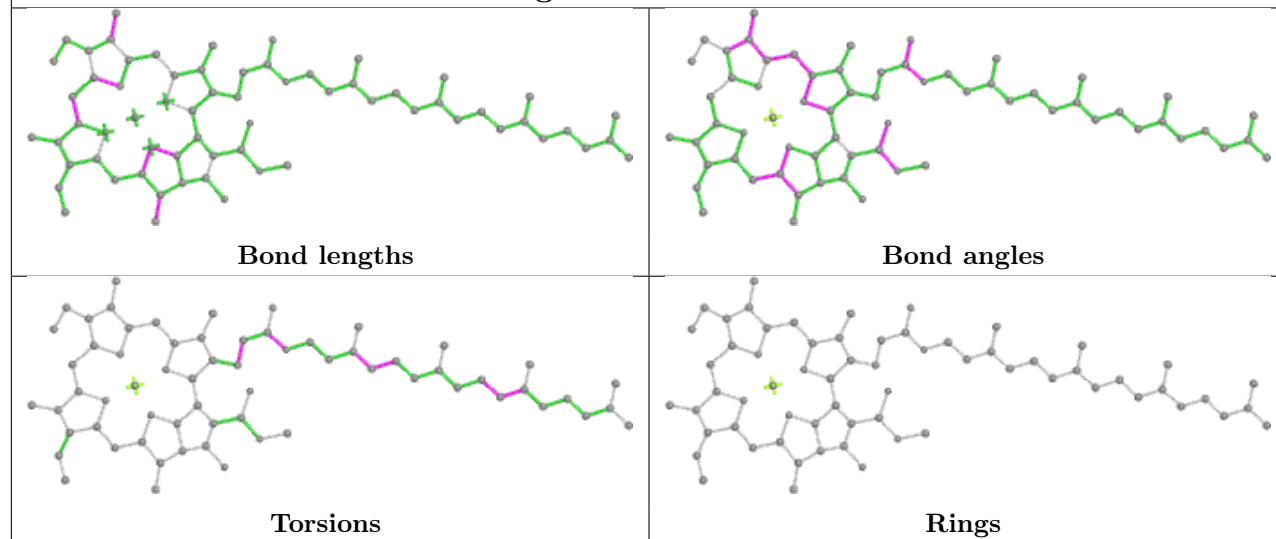
Ligand CLA j 602



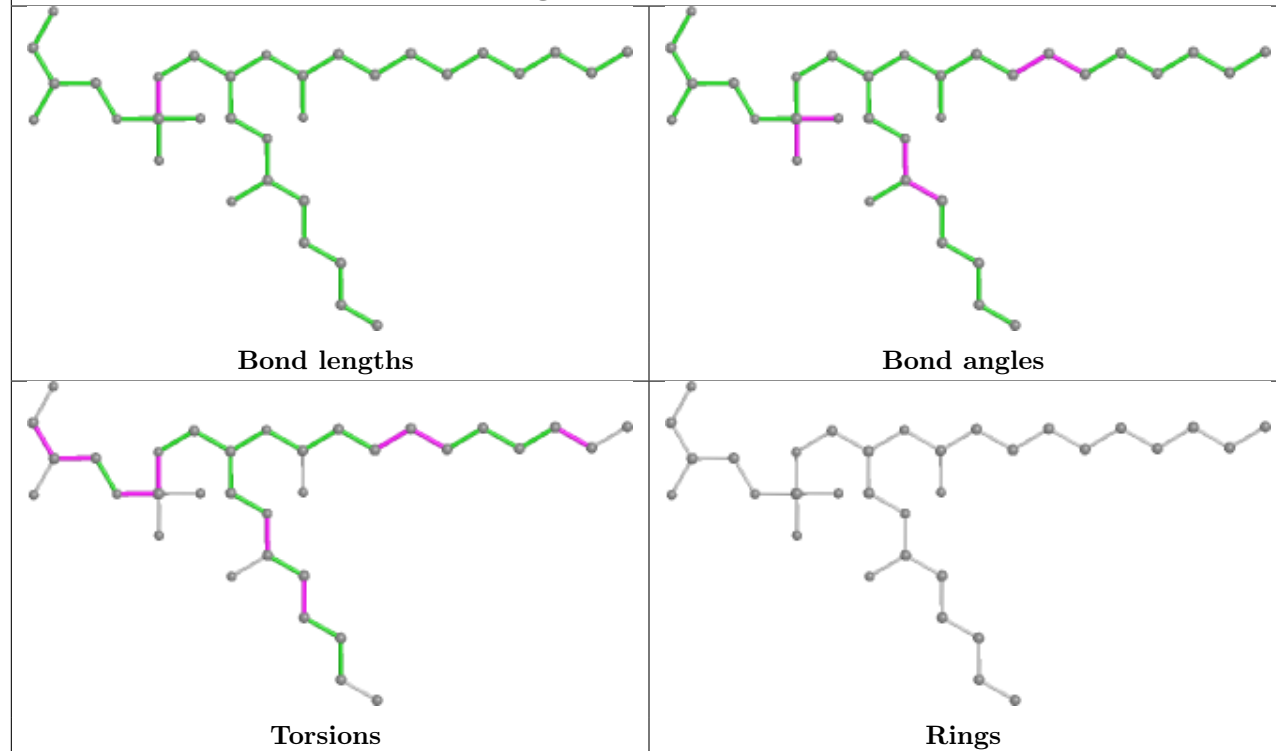
Ligand CLA B 822

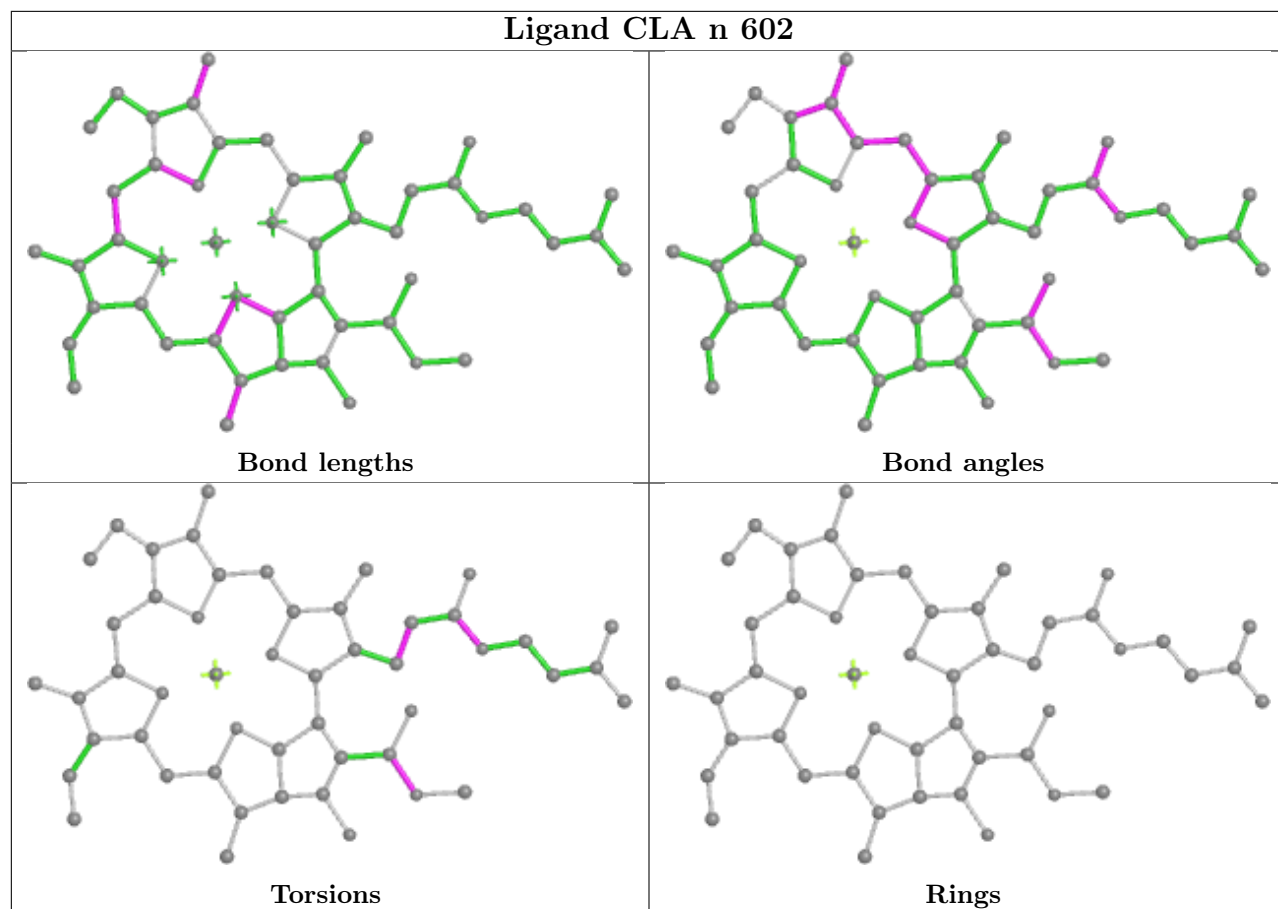


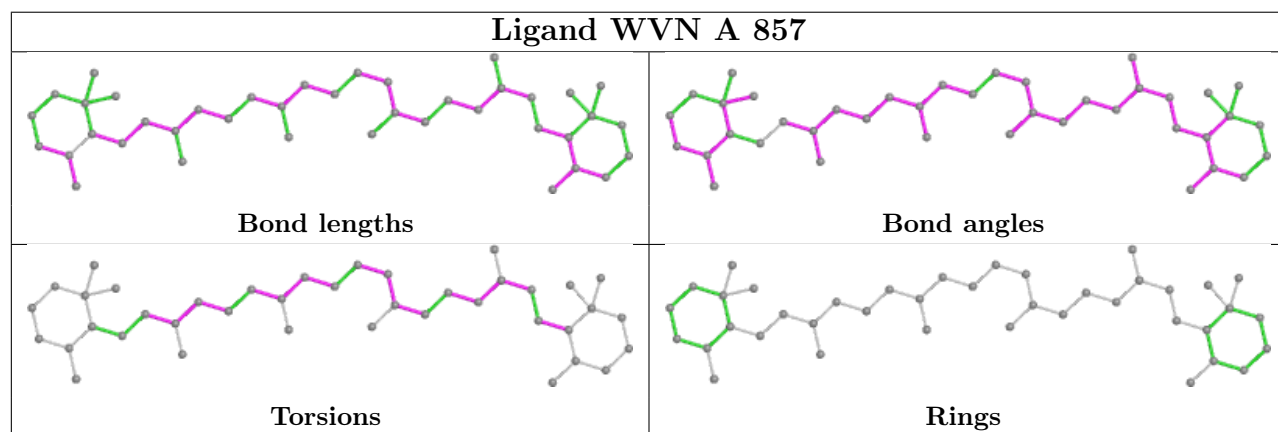
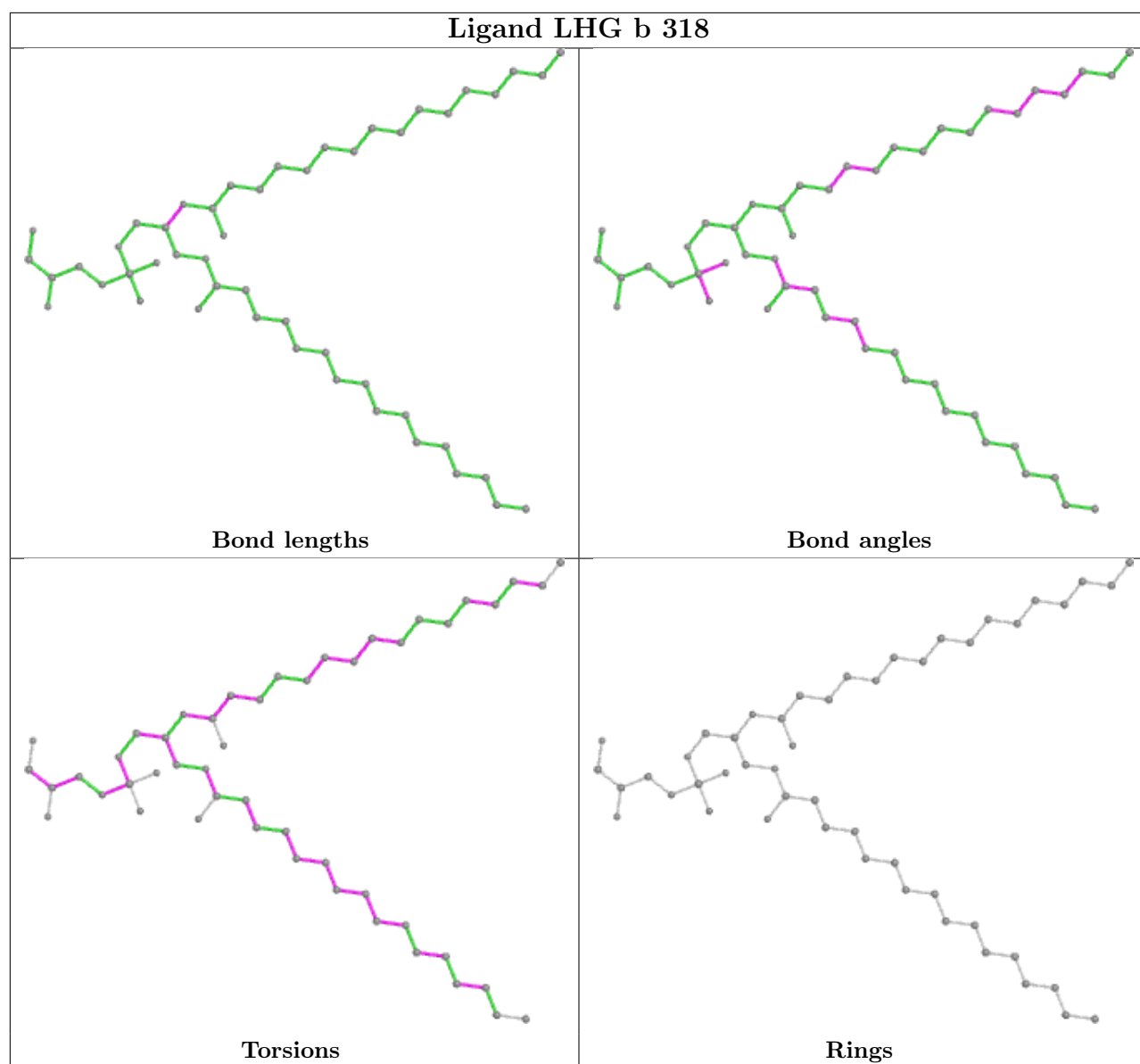
Ligand CLA h 306



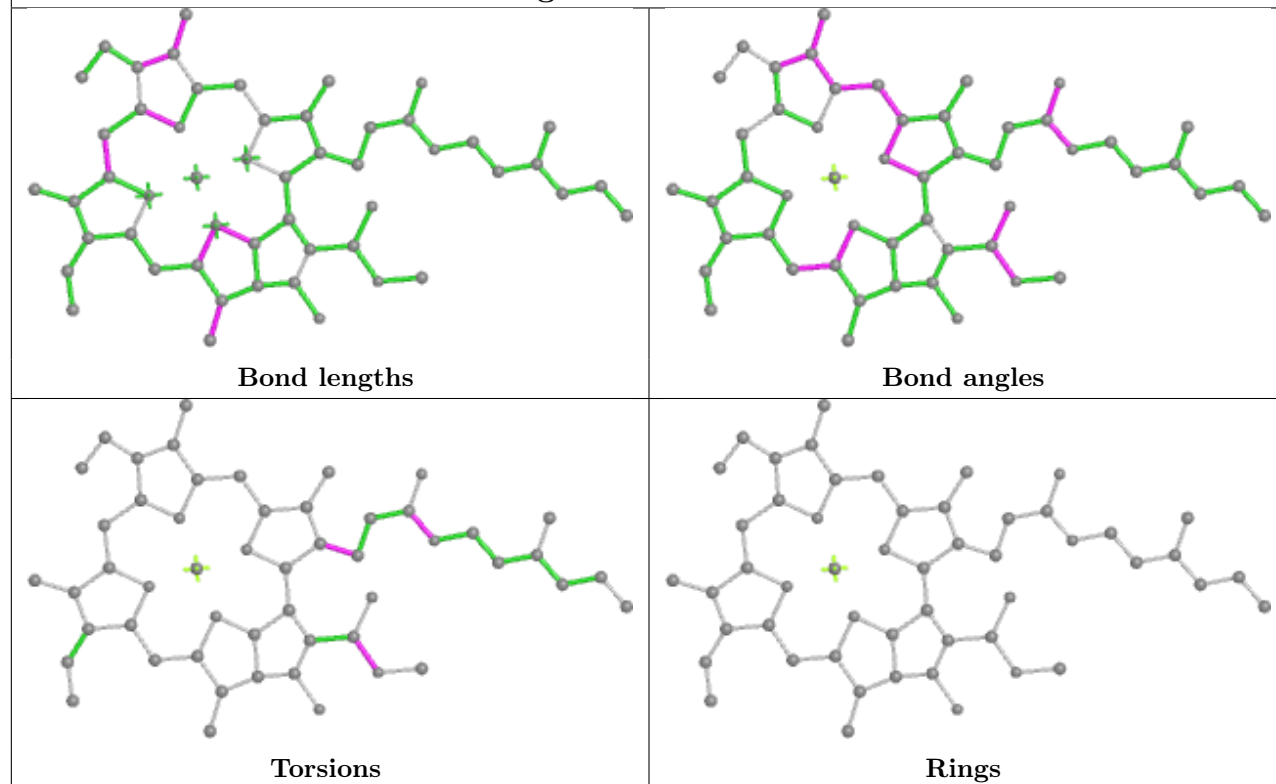
Ligand LHG J 105



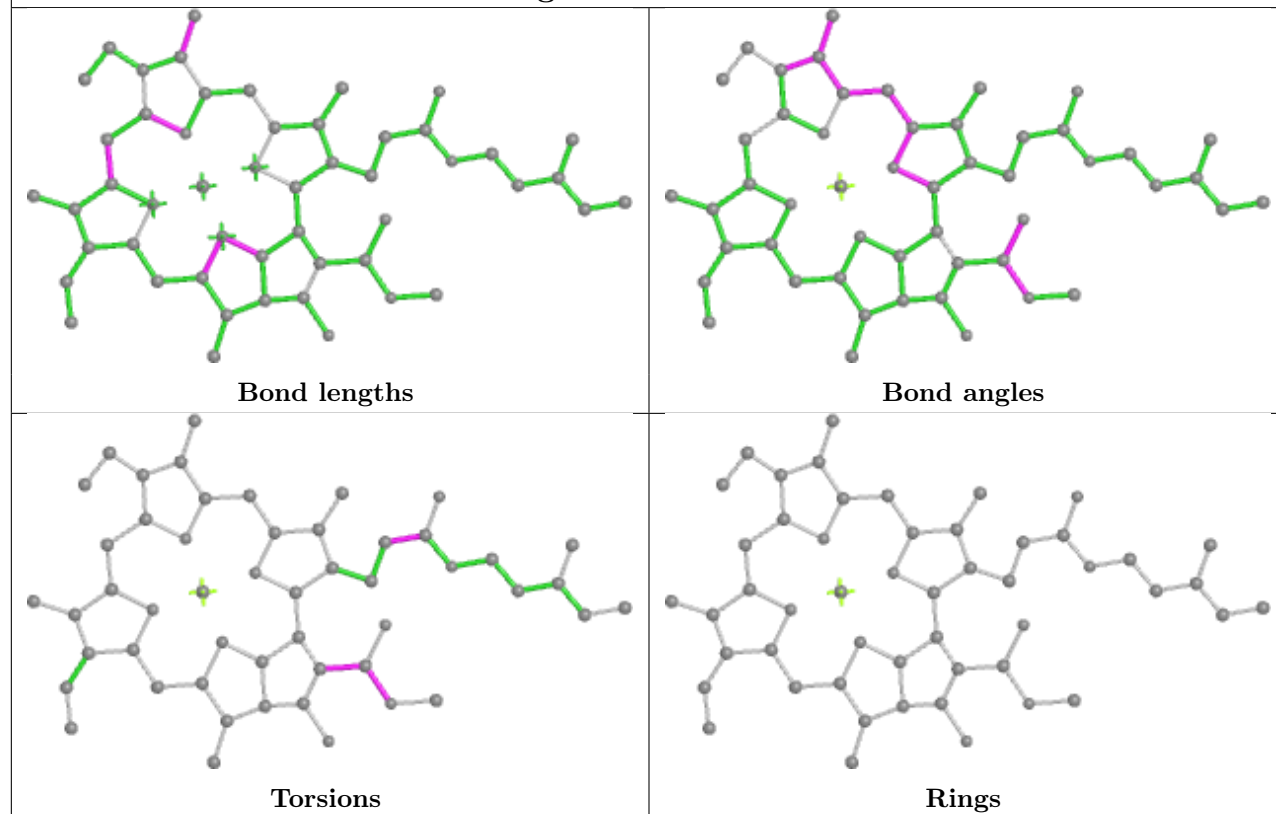




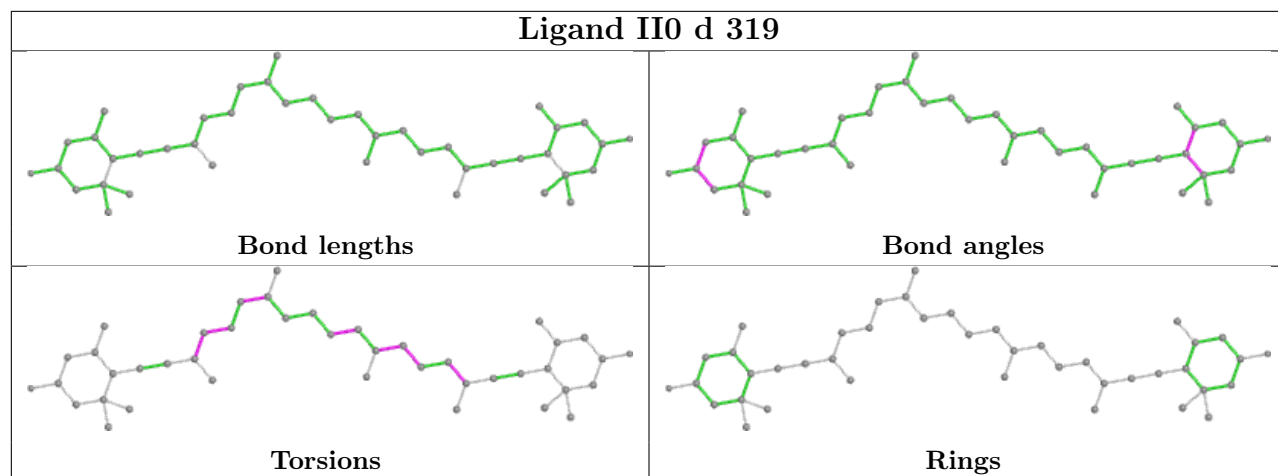
Ligand CLA c 306



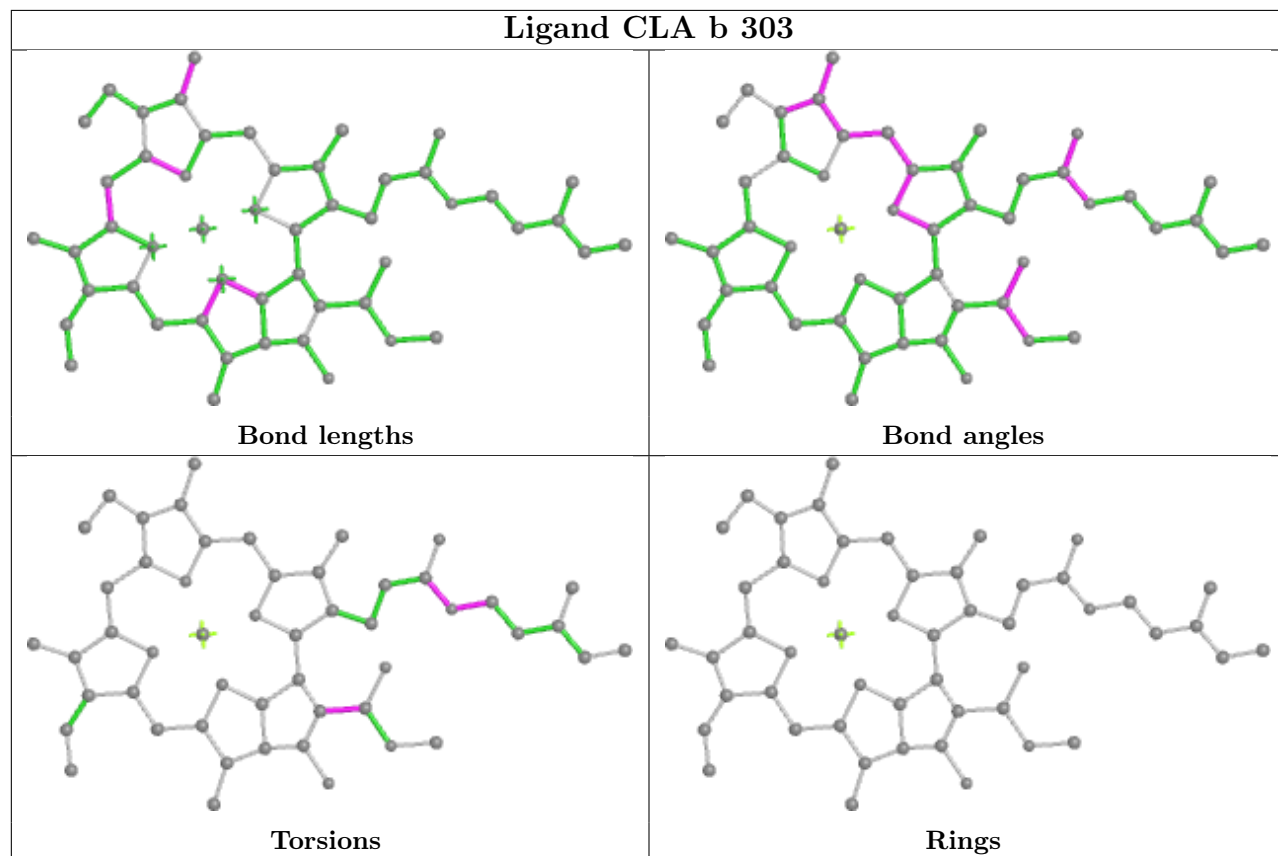
Ligand CLA c 303



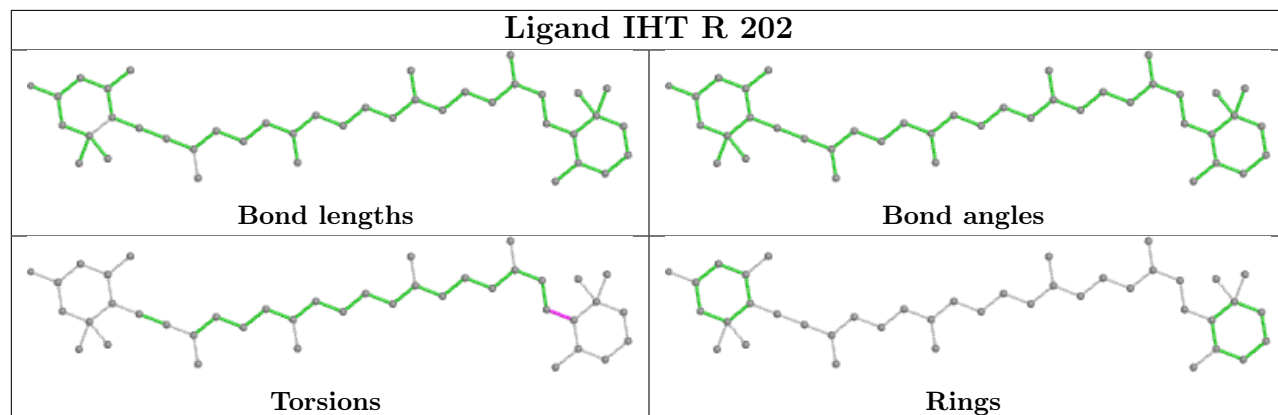
Ligand II0 d 319

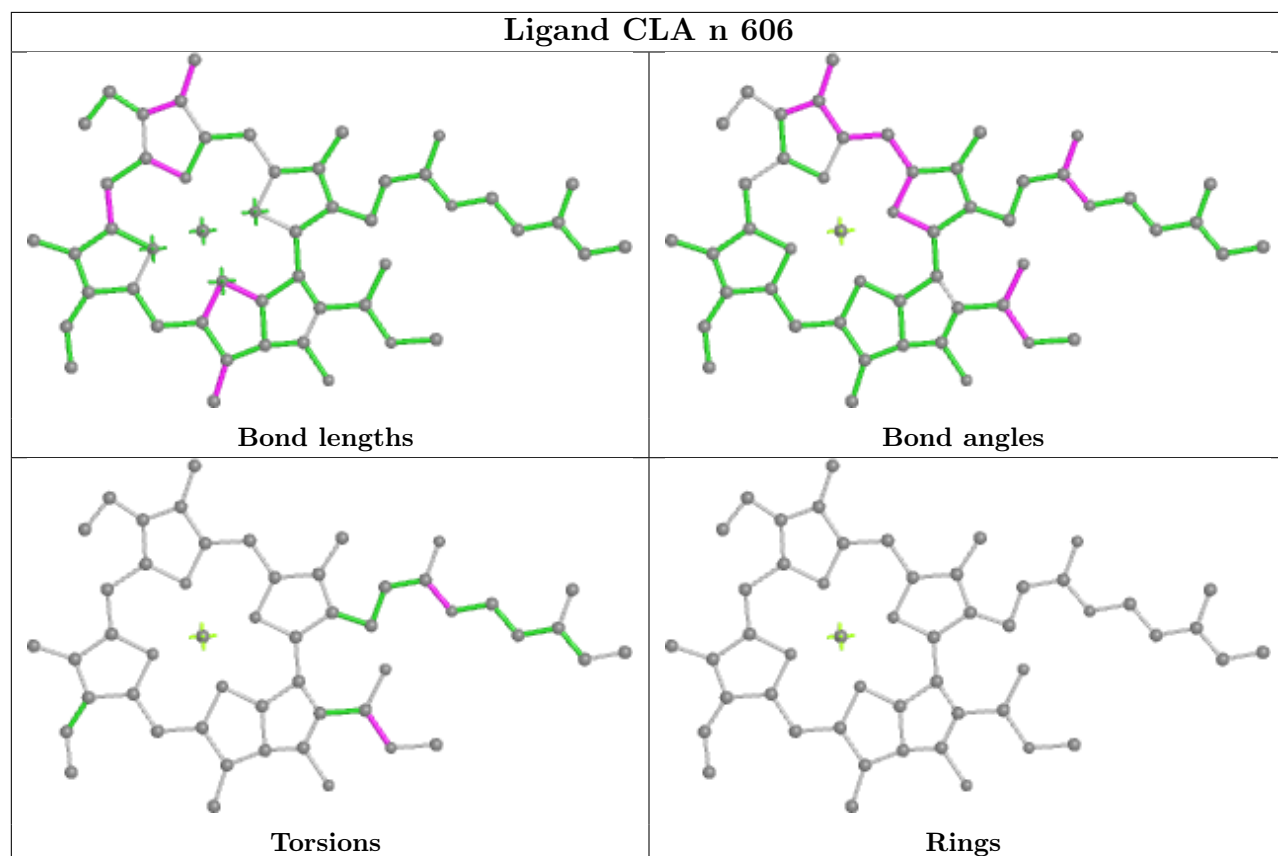
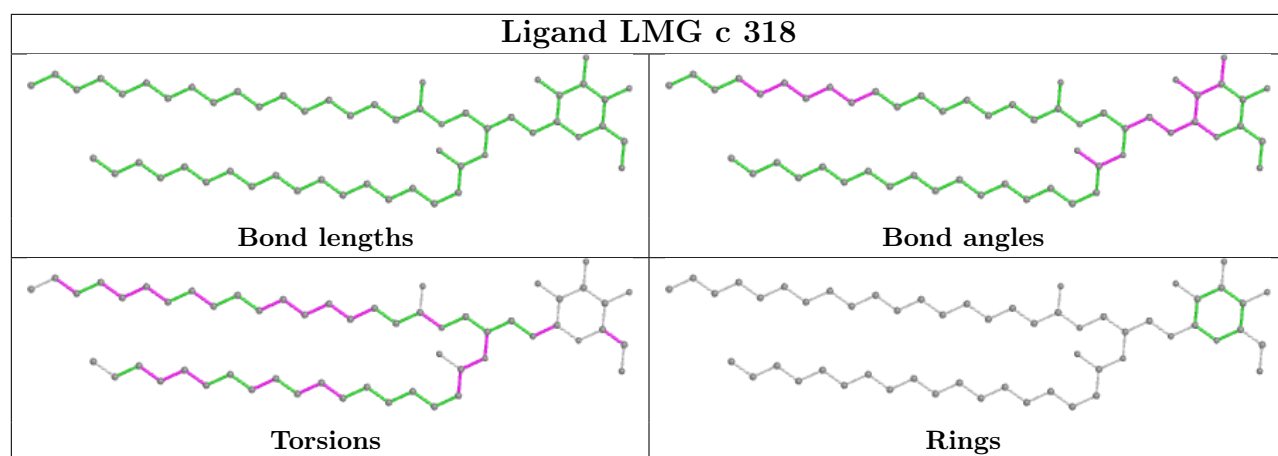


Ligand CLA b 303

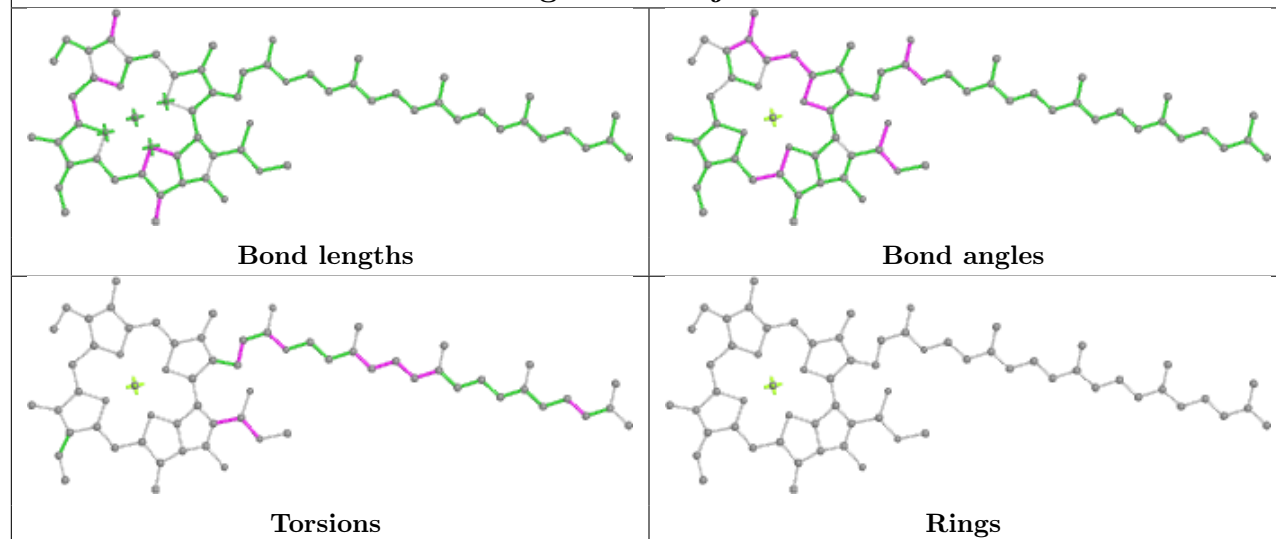


Ligand IHT R 202

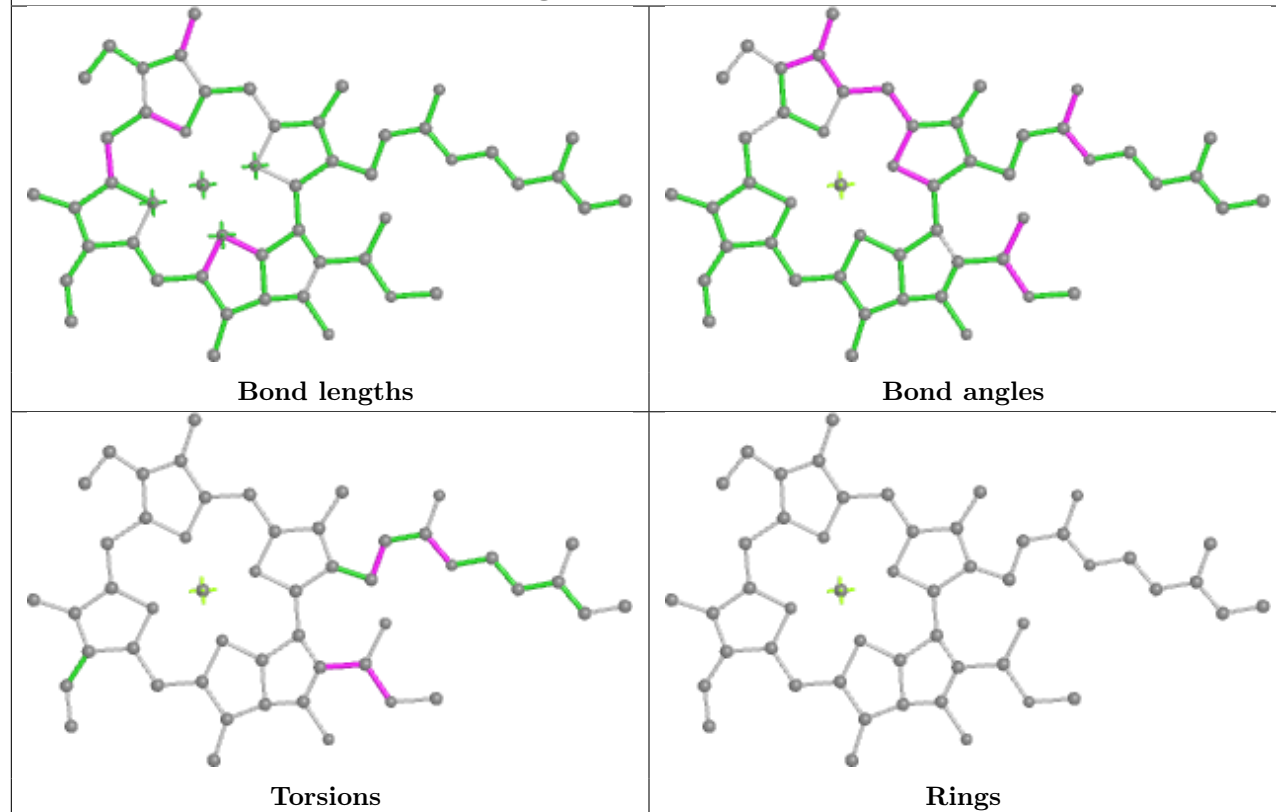




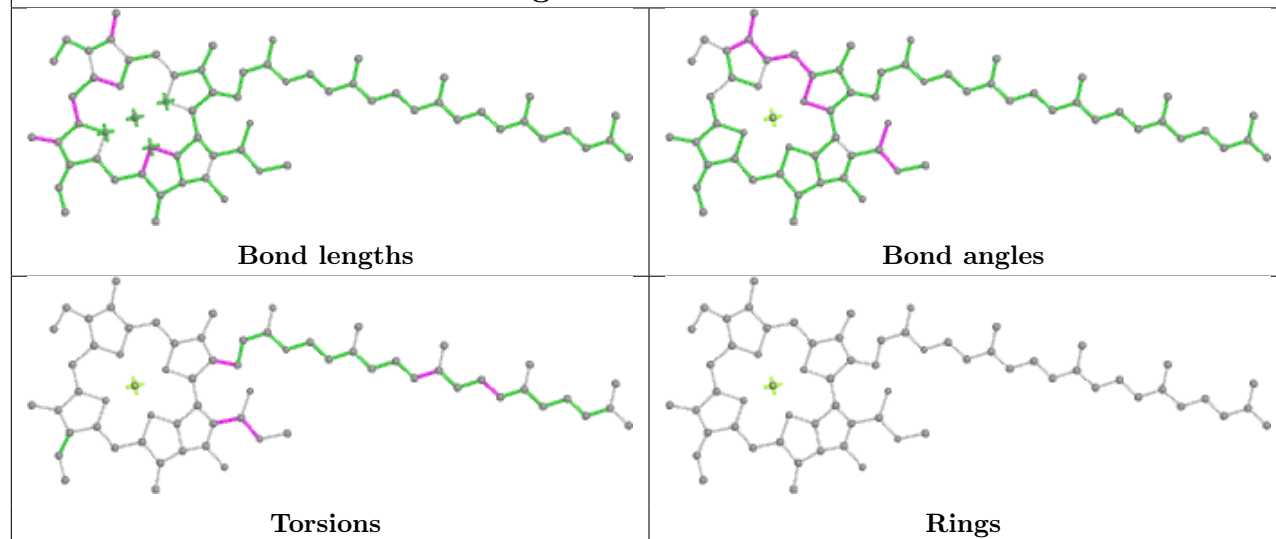
Ligand CLA j 613



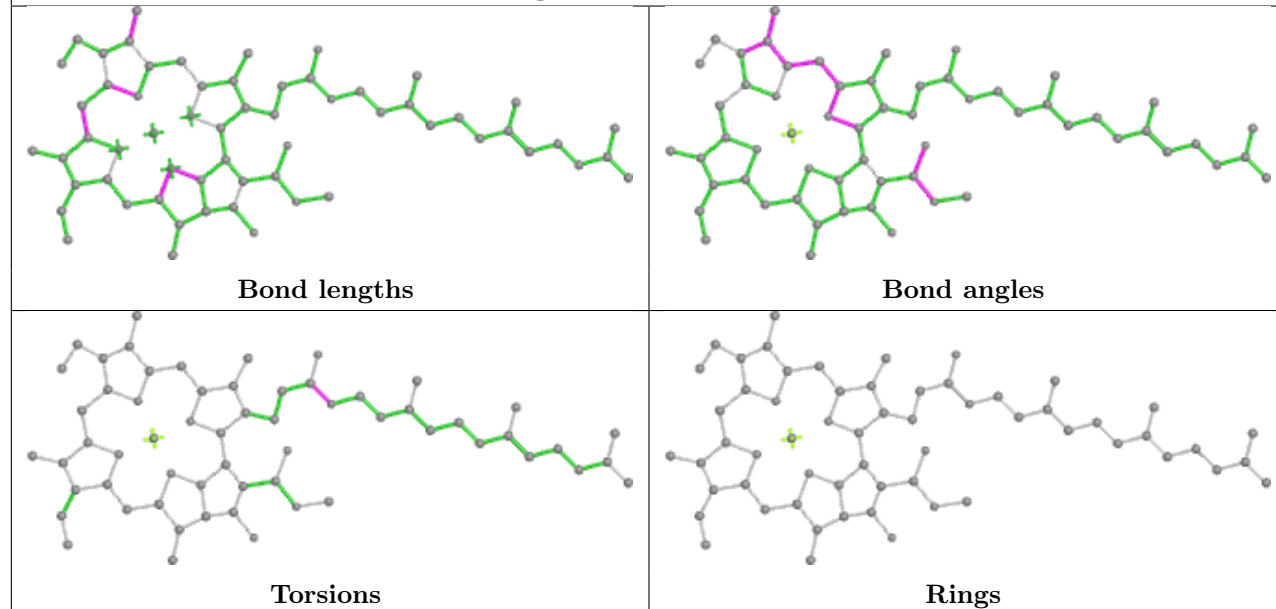
Ligand CLA d 305



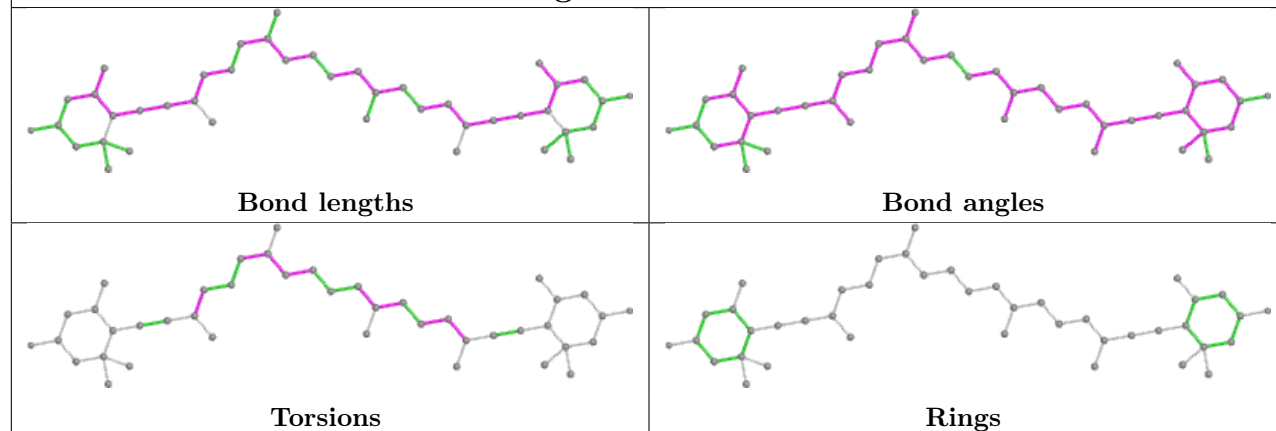
Ligand CLA B 824

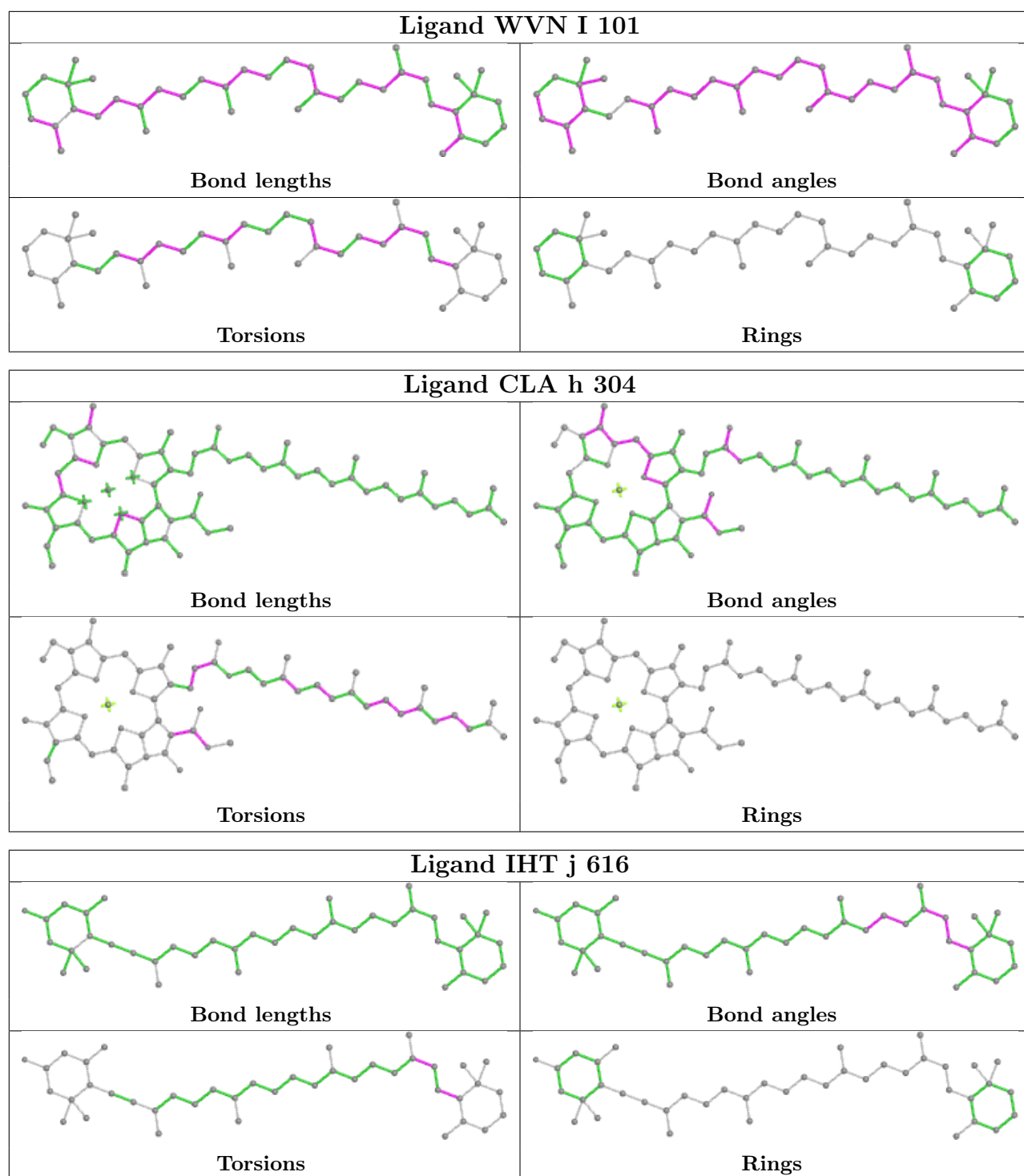


Ligand CLA A 839

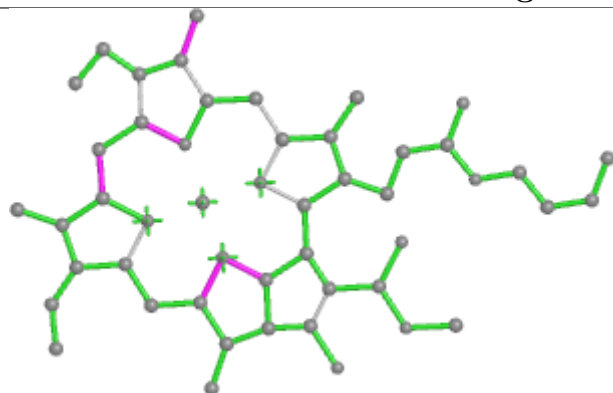


Ligand II0 I 314

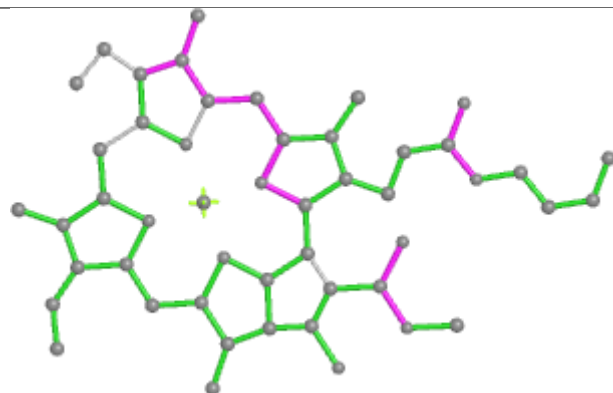




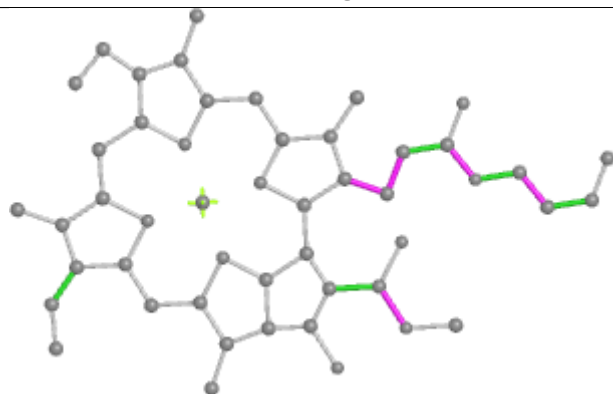
Ligand CLA L 202



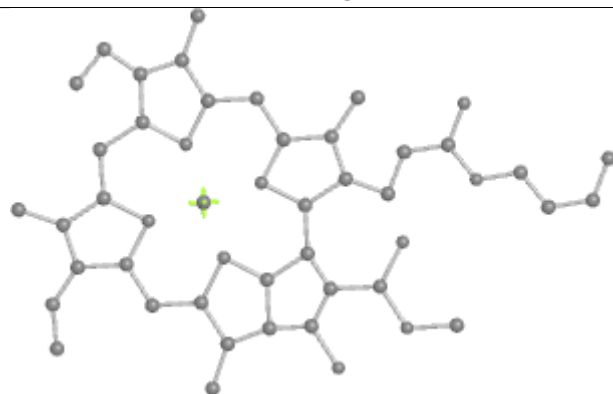
Bond lengths



Bond angles

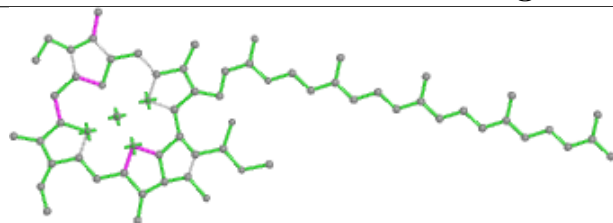


Torsions

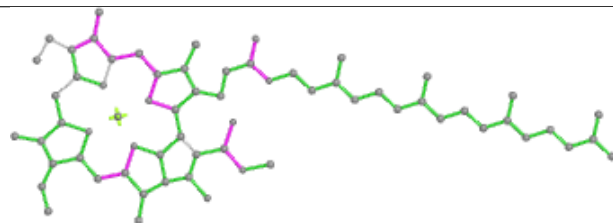


Rings

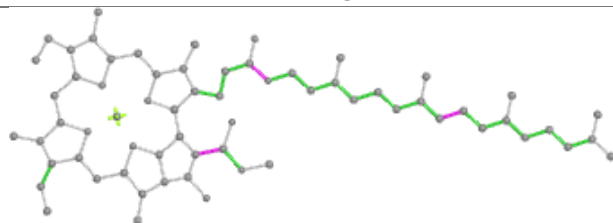
Ligand CLA L 203



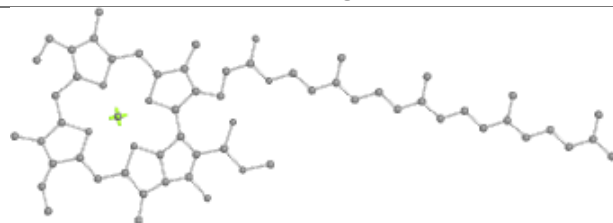
Bond lengths



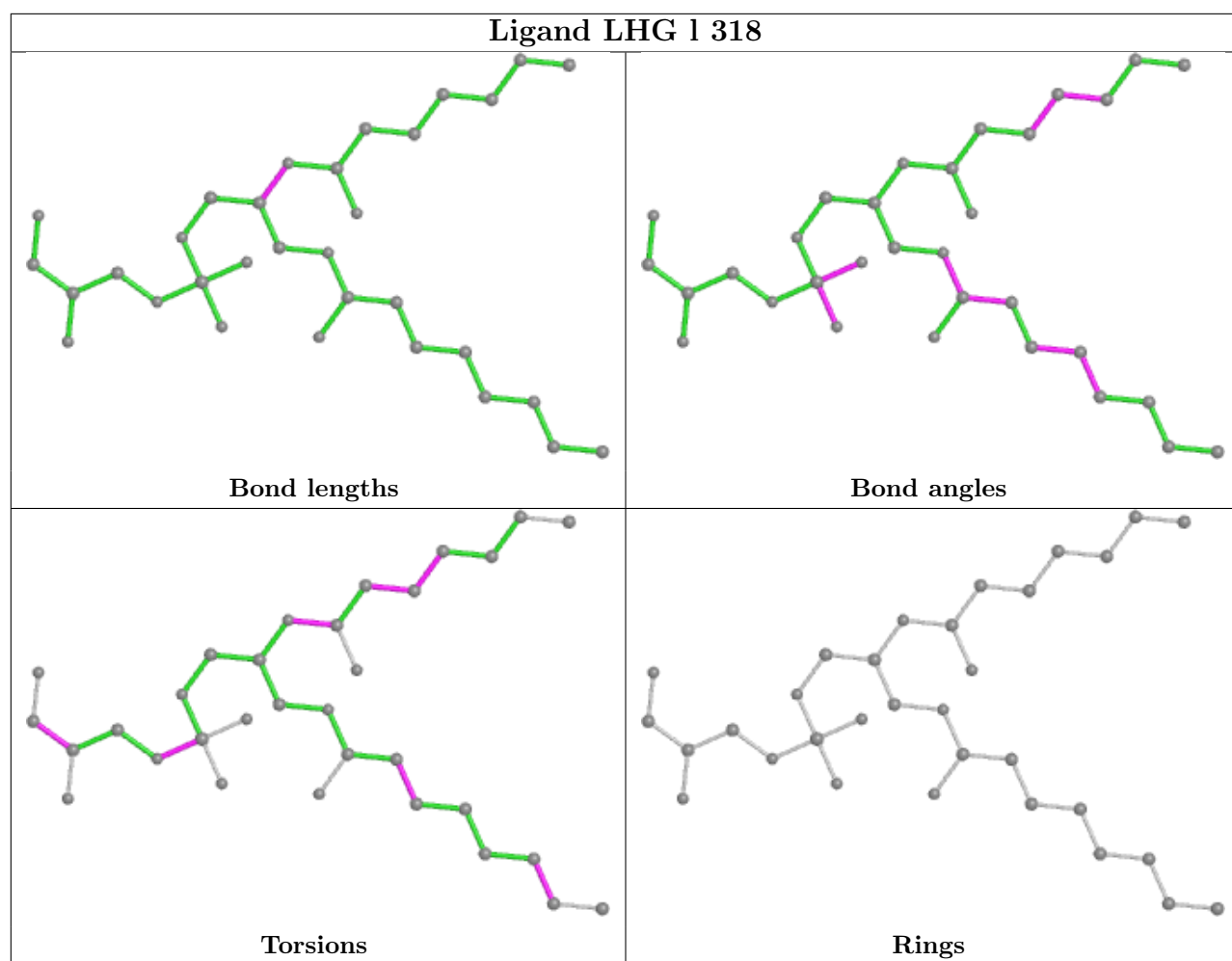
Bond angles



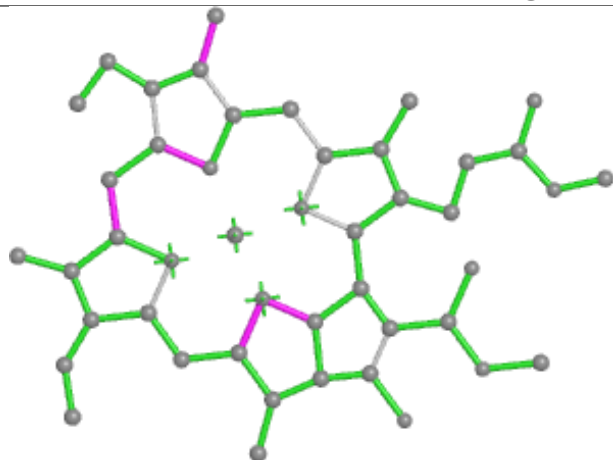
Torsions



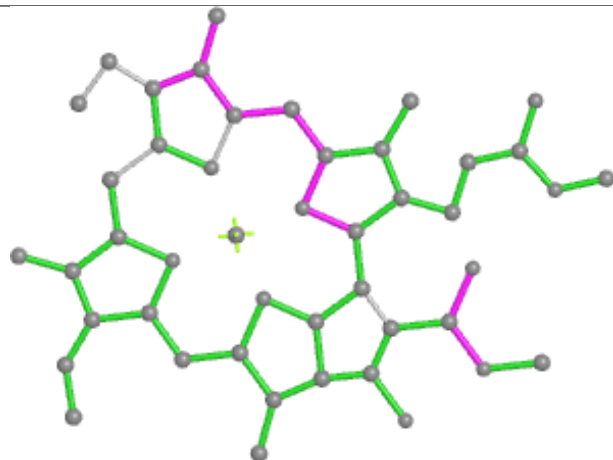
Rings



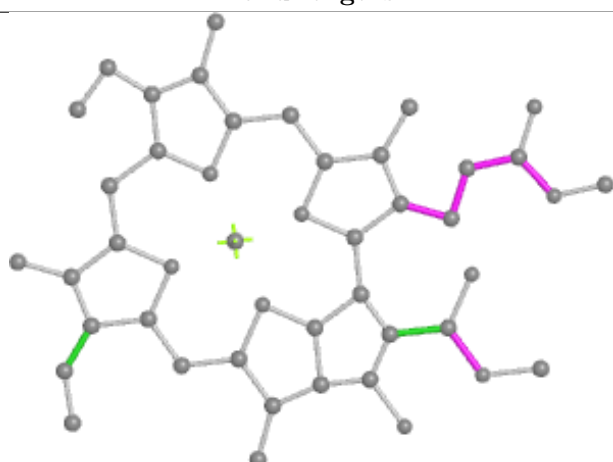
Ligand CLA i 308



Bond lengths



Bond angles

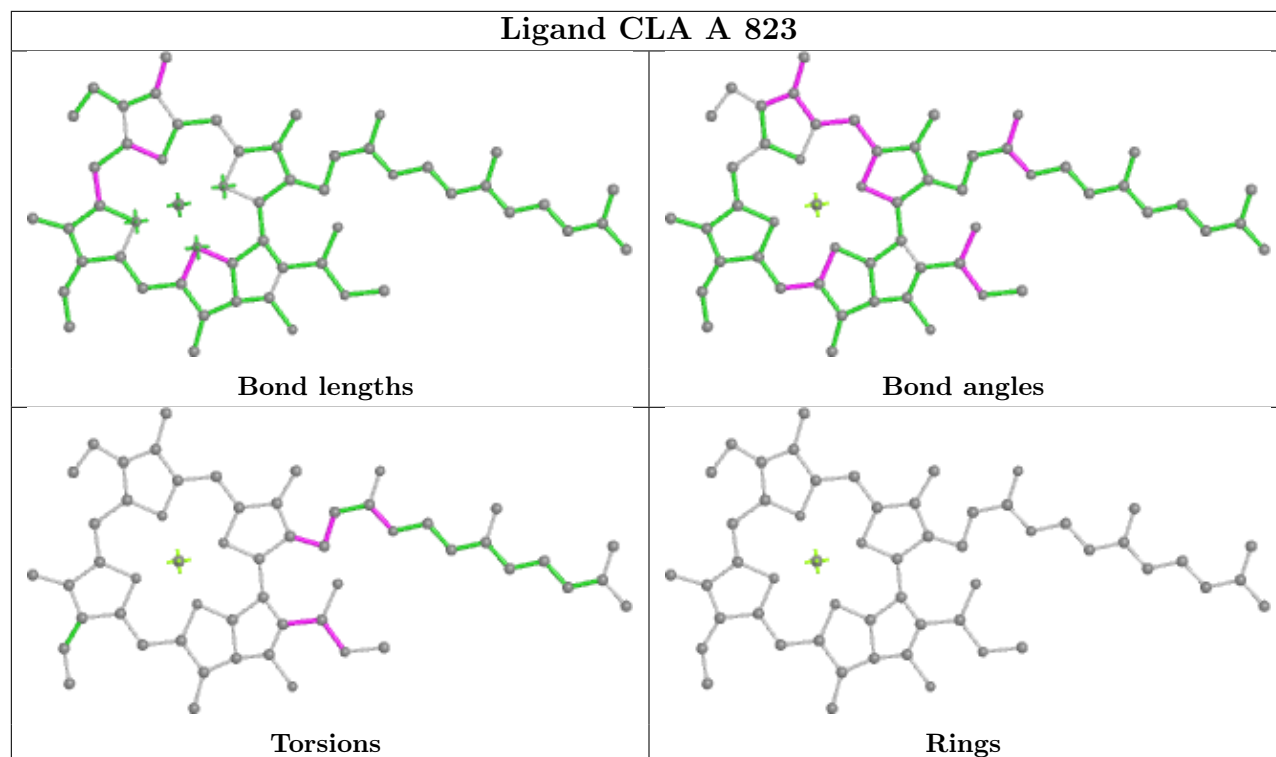


Torsions

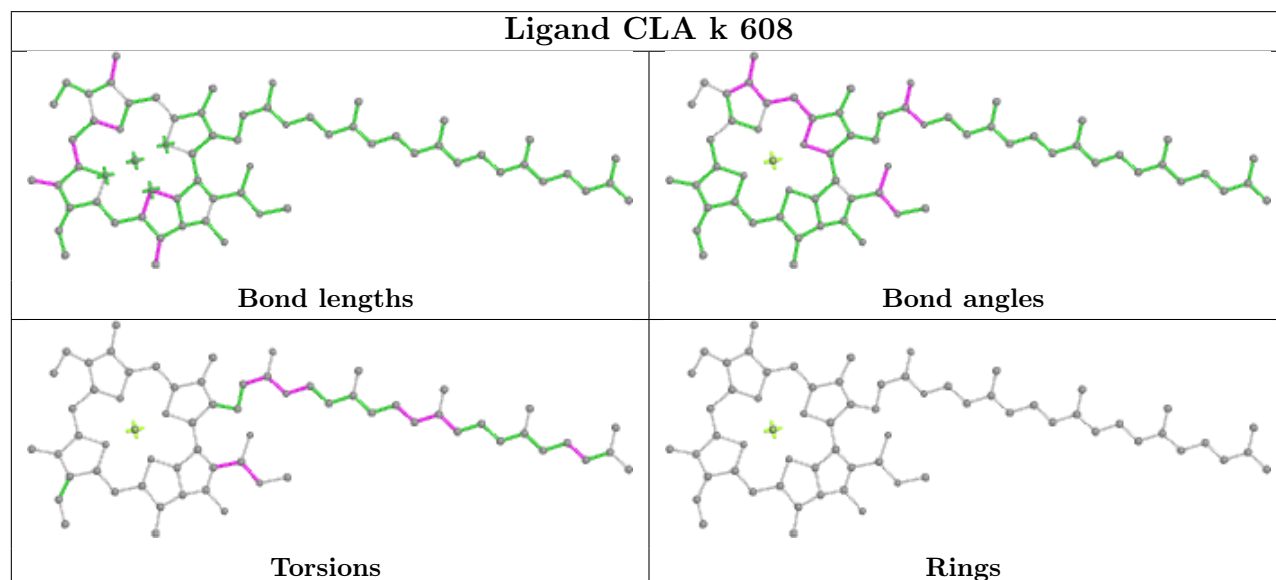


Rings

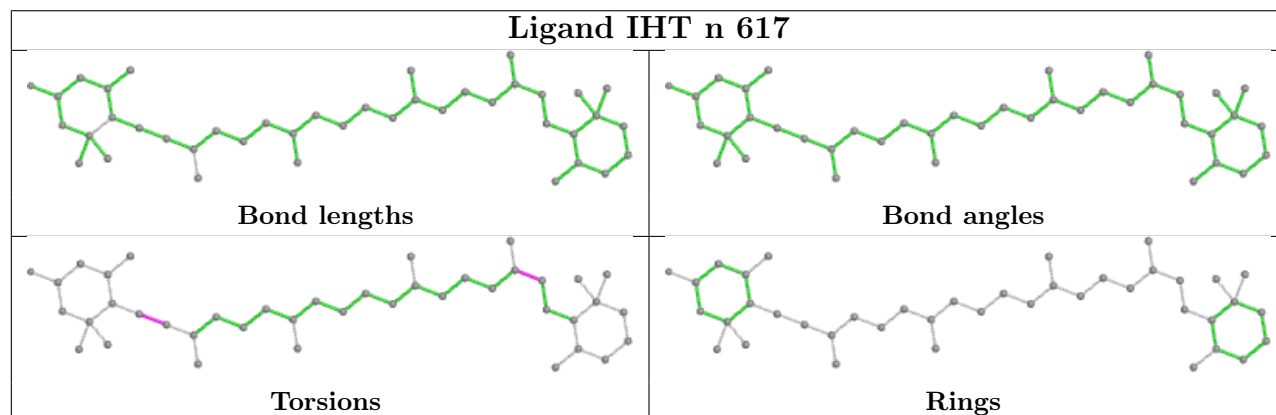
Ligand CLA A 823



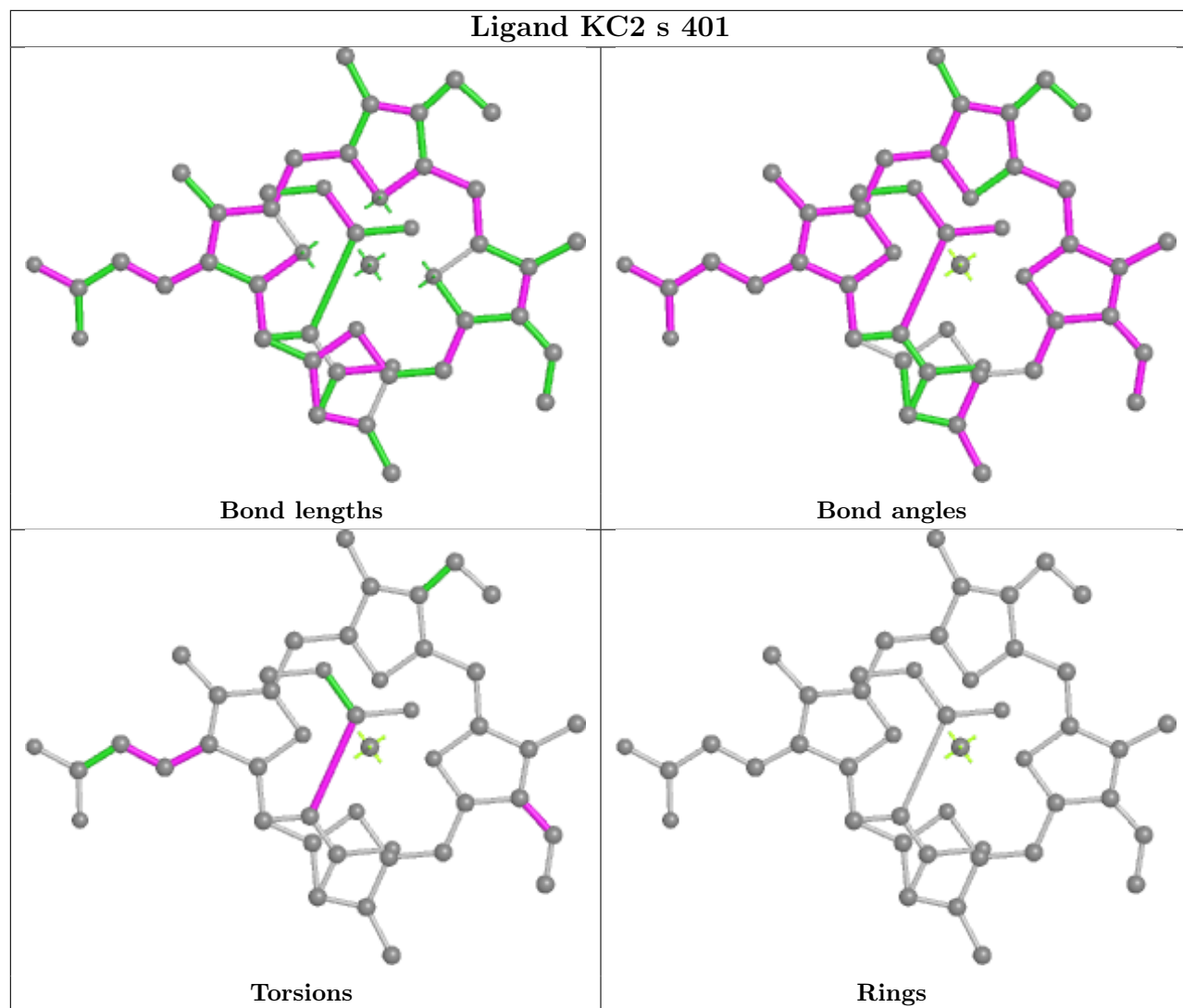
Ligand CLA k 608



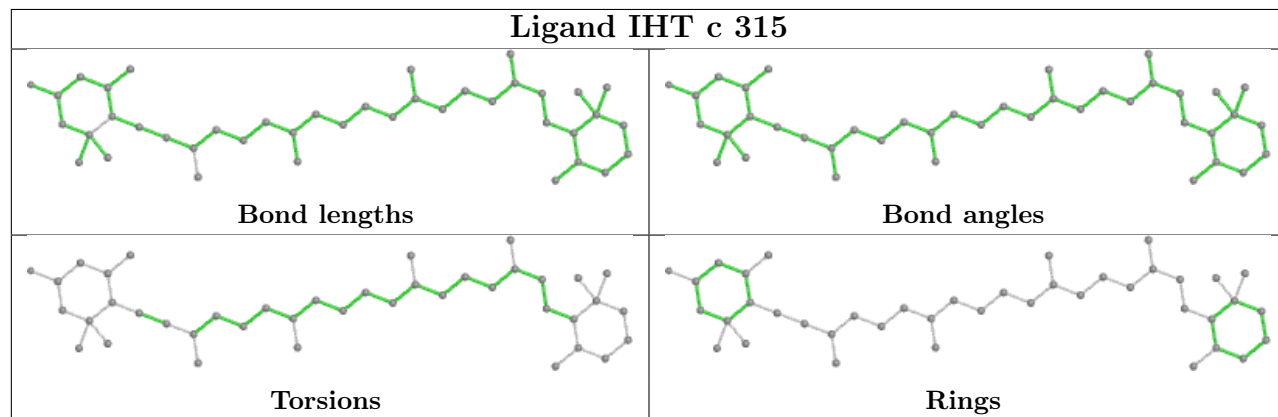
Ligand IHT n 617



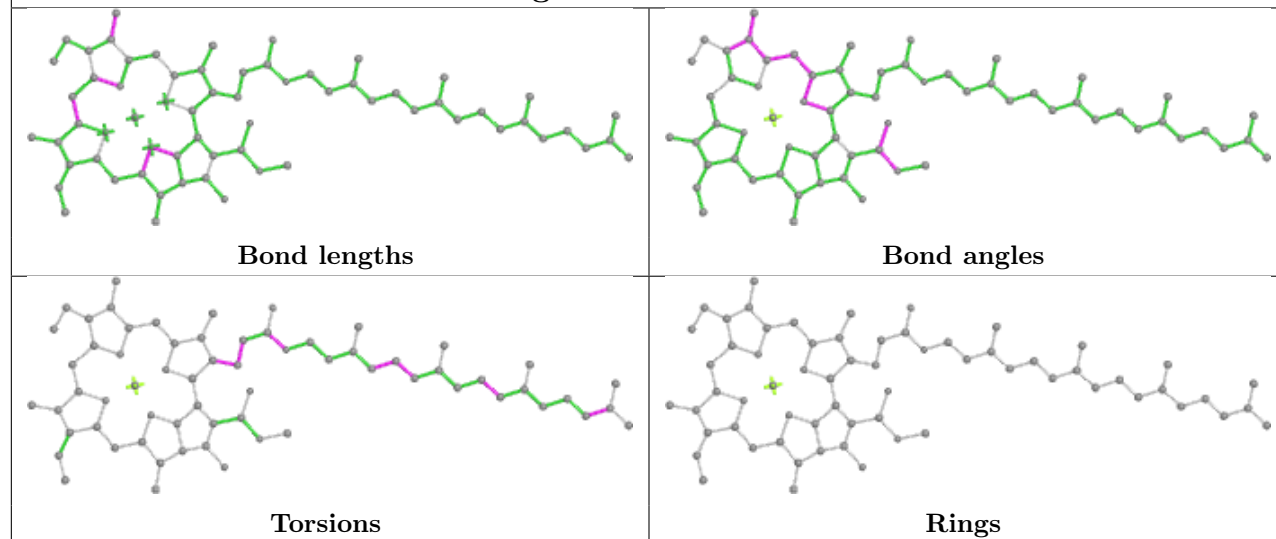
Ligand KC2 s 401



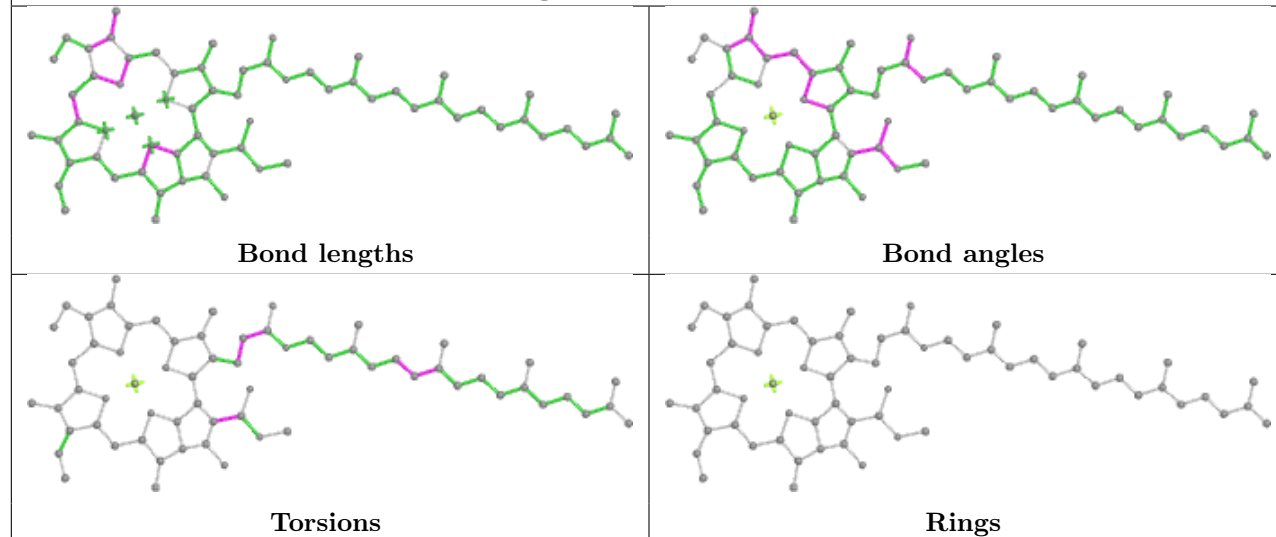
Ligand IHT c 315



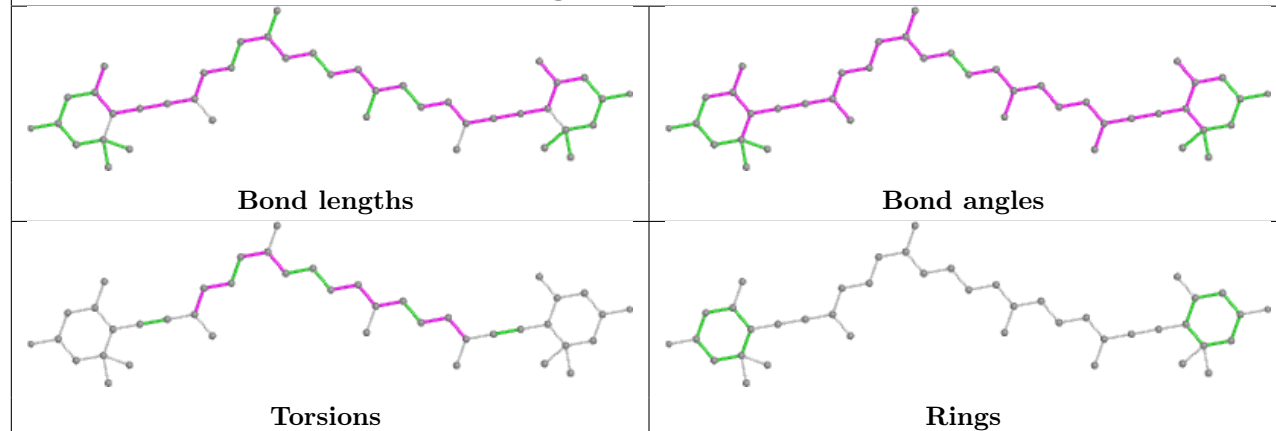
Ligand CLA B 817



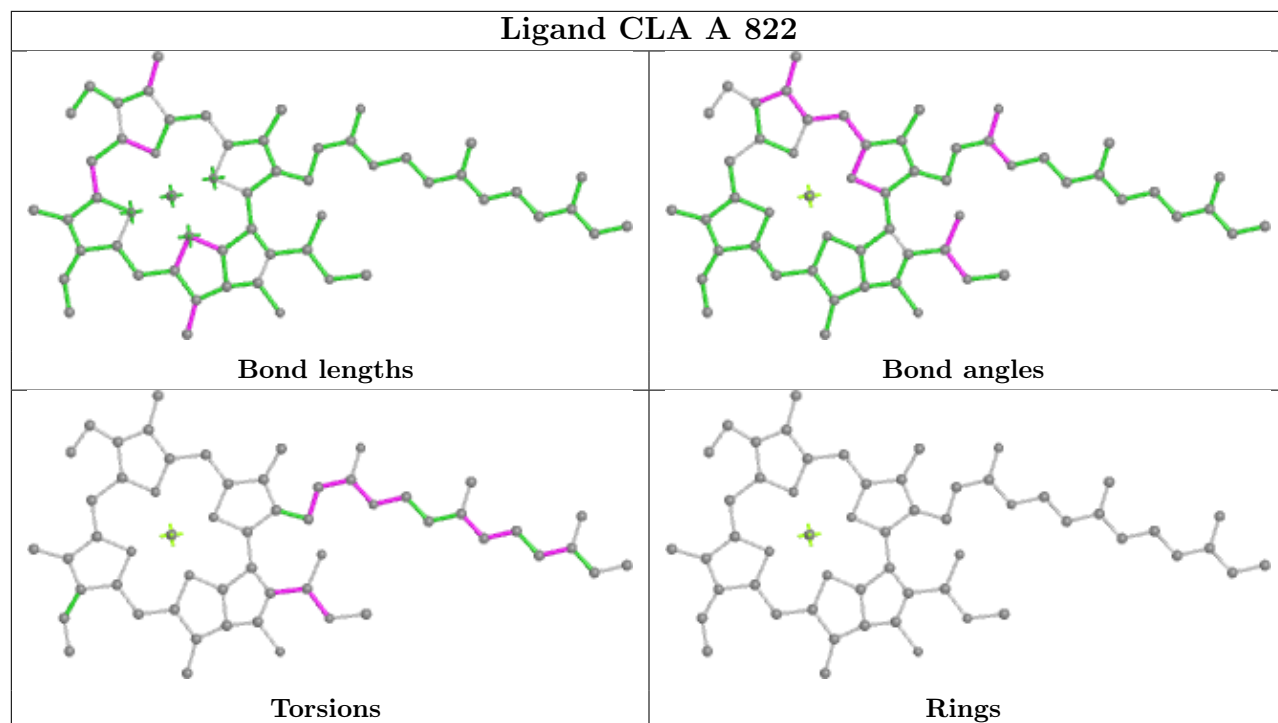
Ligand CLA k 604



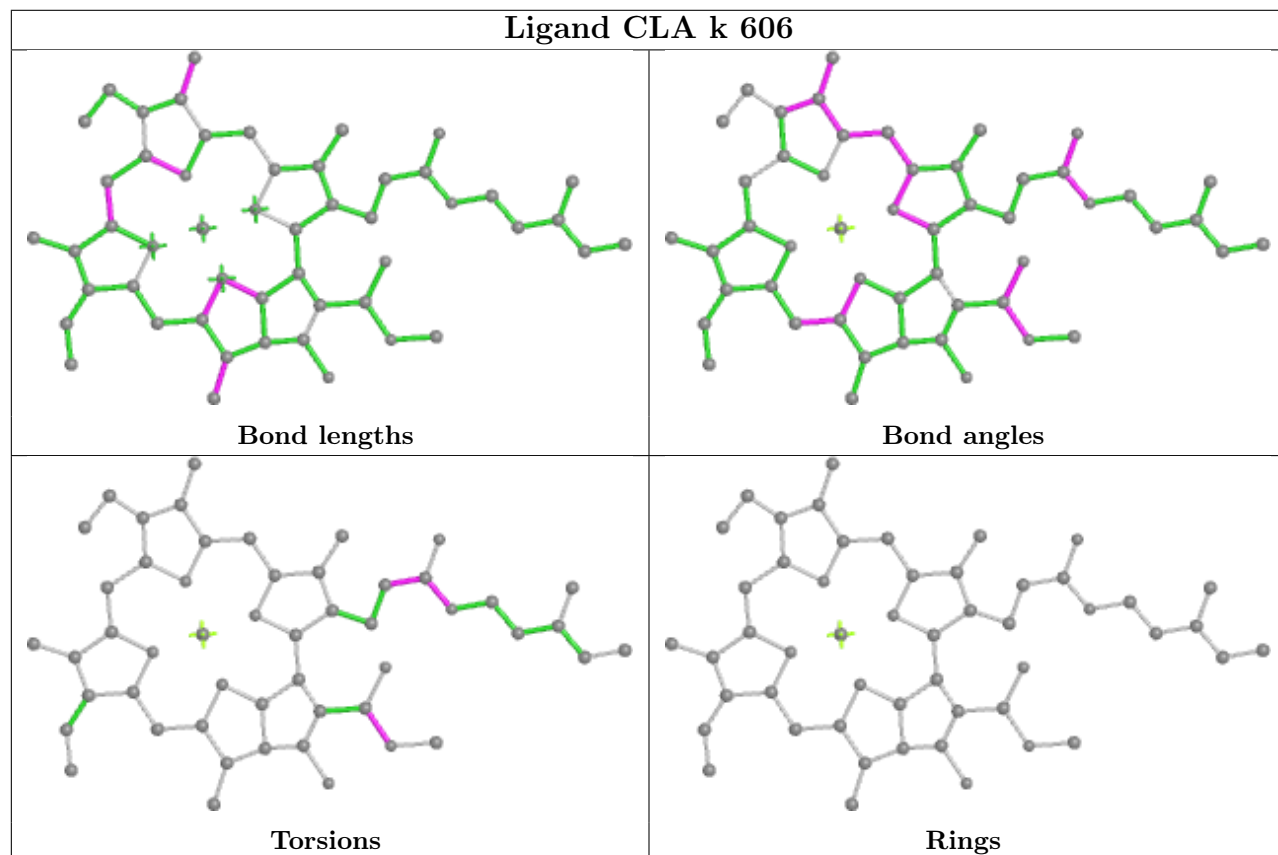
Ligand II0 b 315



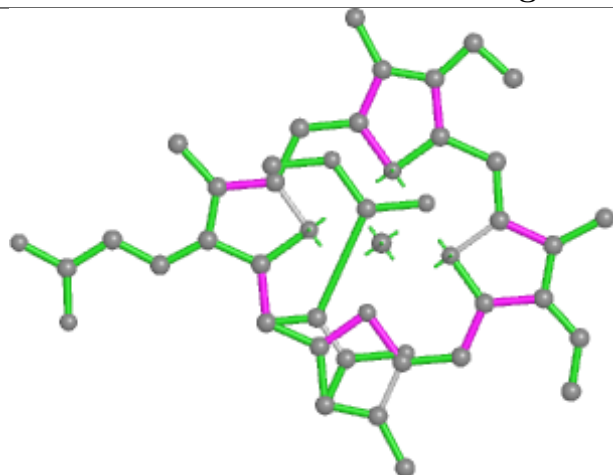
Ligand CLA A 822



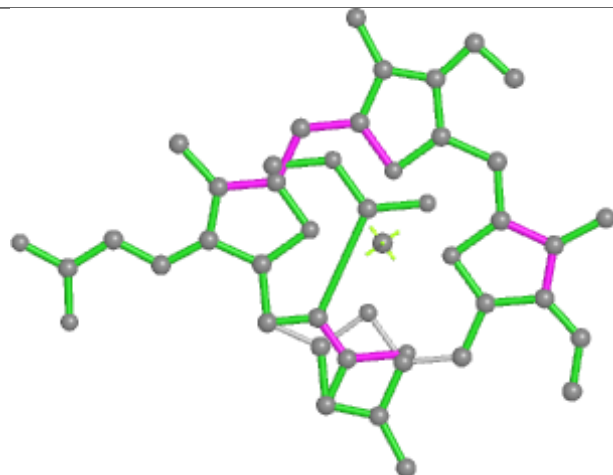
Ligand CLA k 606



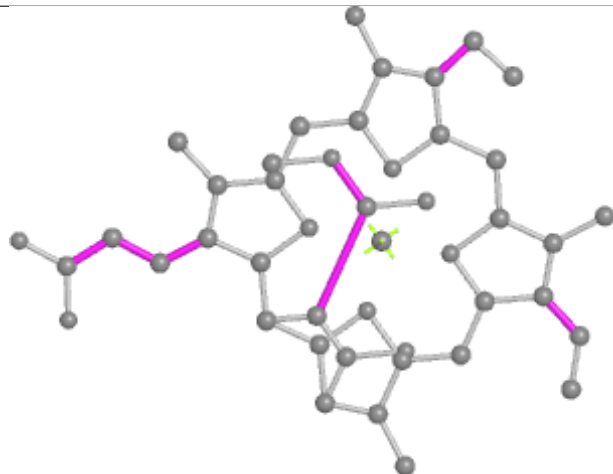
Ligand KC2 n 611



Bond lengths



Bond angles

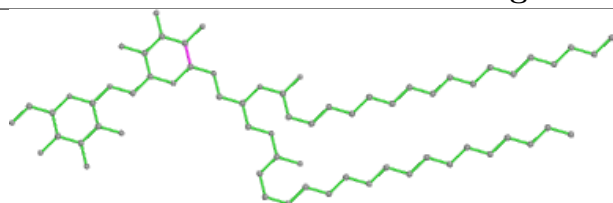


Torsions

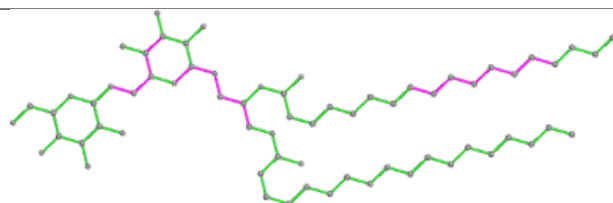


Rings

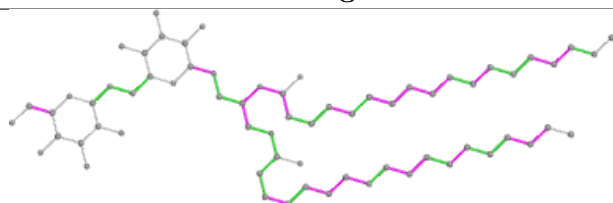
Ligand DGD B 844



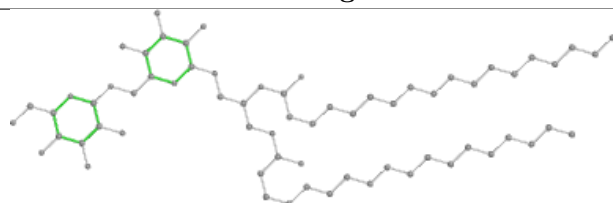
Bond lengths



Bond angles

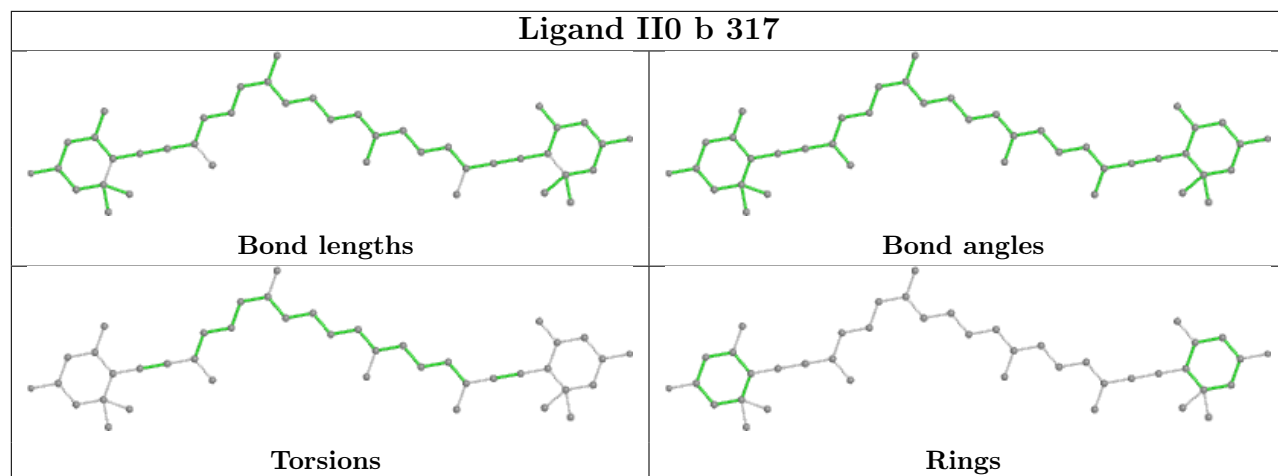


Torsions

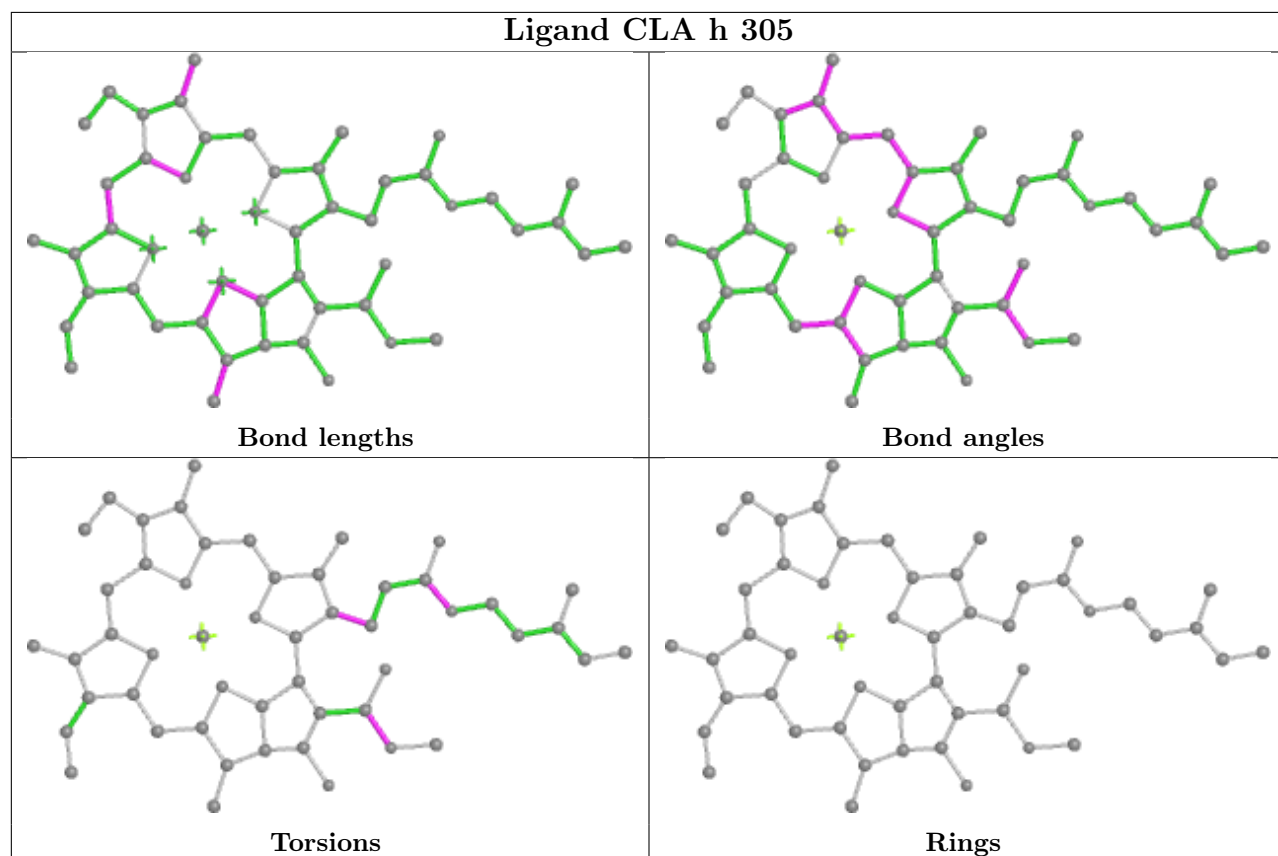


Rings

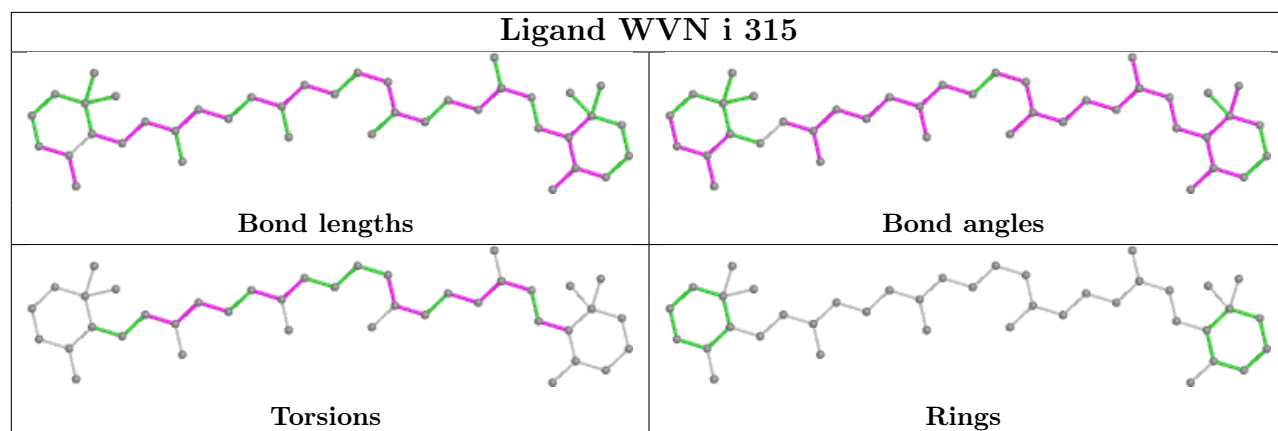
Ligand II0 b 317



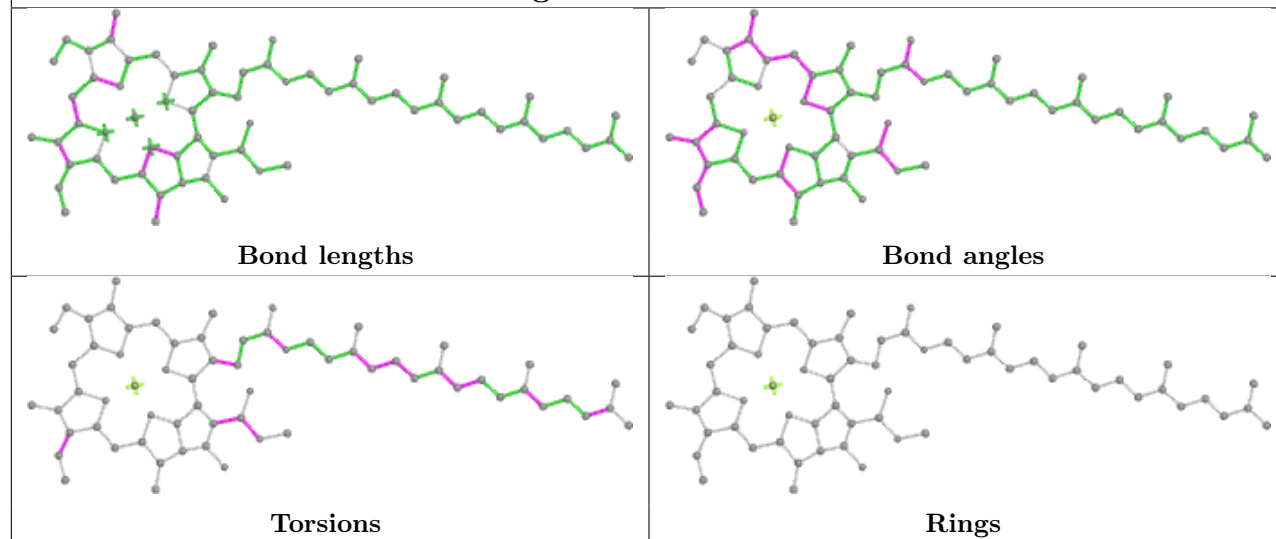
Ligand CLA h 305



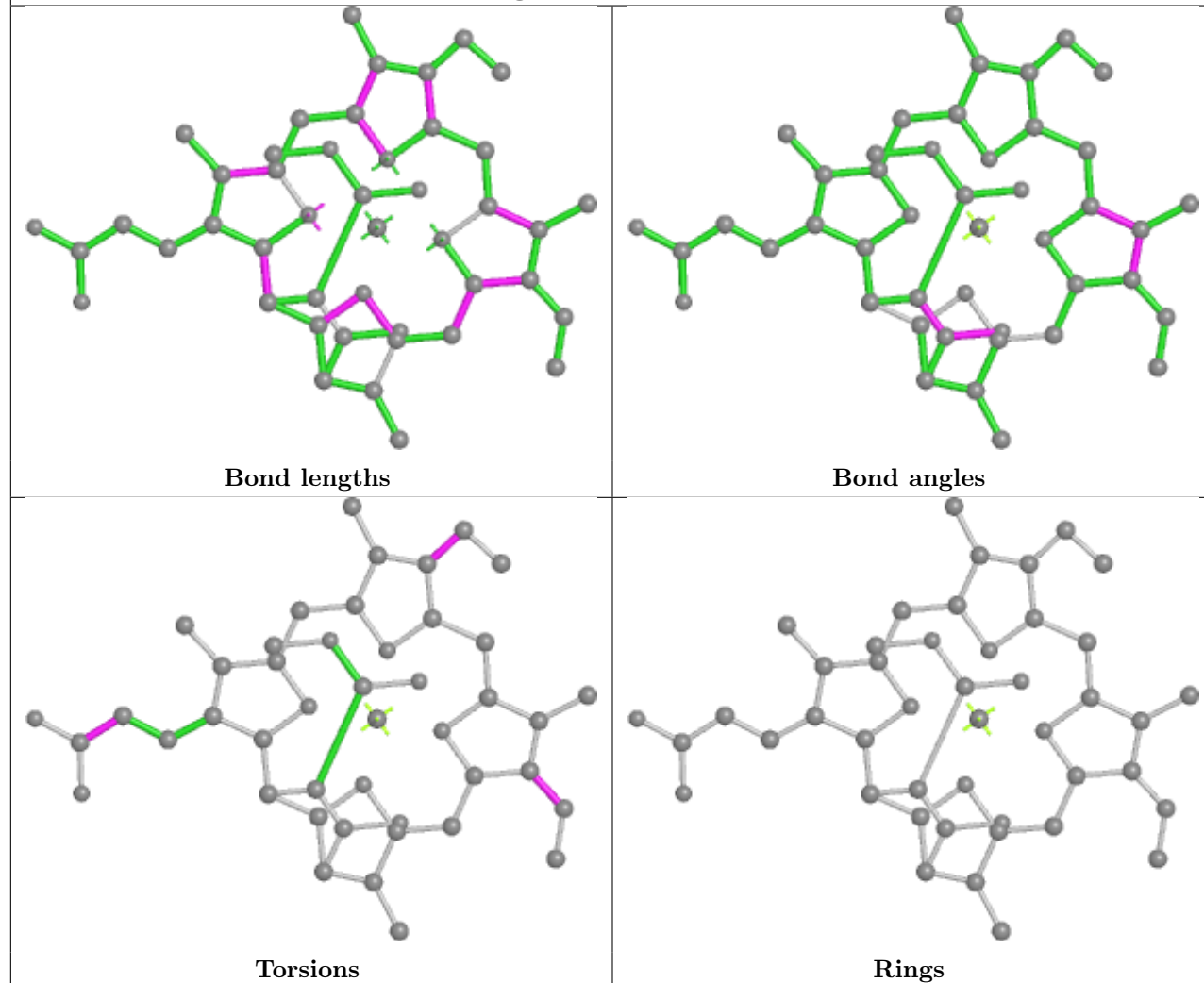
Ligand WVN i 315



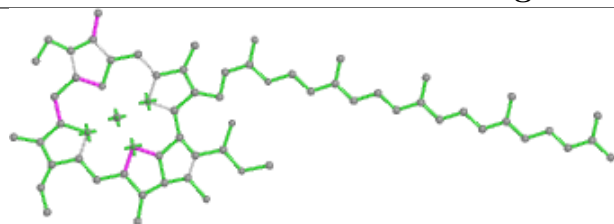
Ligand CLA B 819



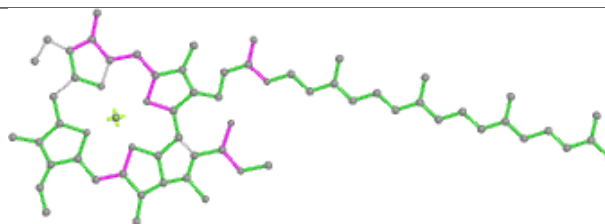
Ligand KC2 I 312



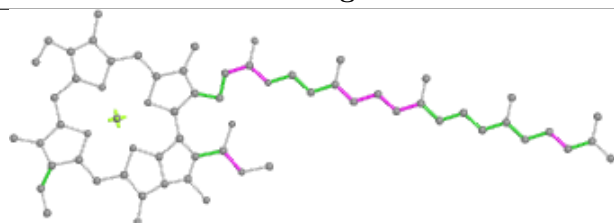
Ligand CLA B 806



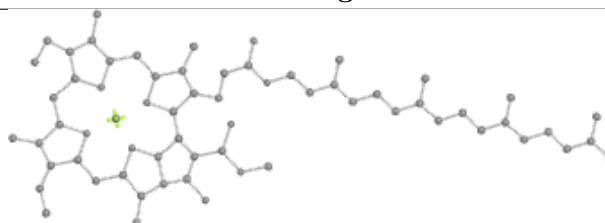
Bond lengths



Bond angles

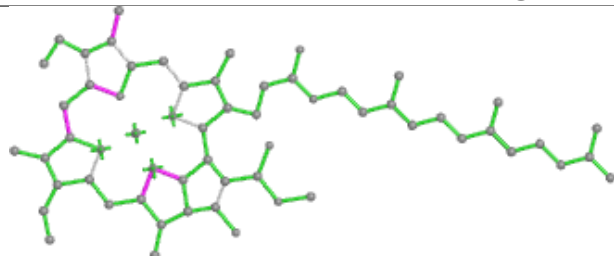


Torsions

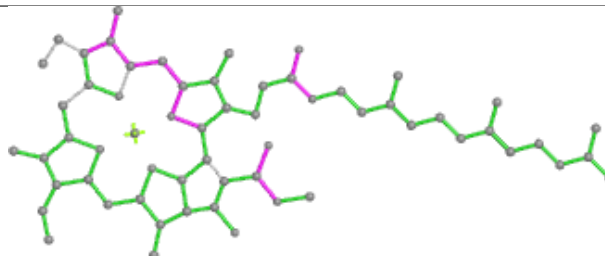


Rings

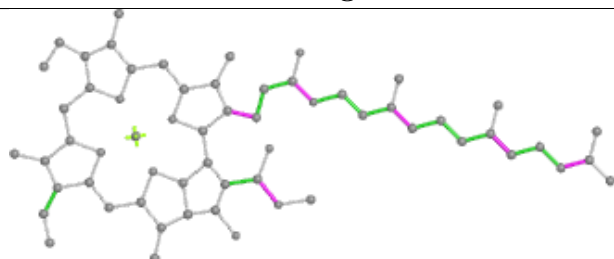
Ligand CLA m 609



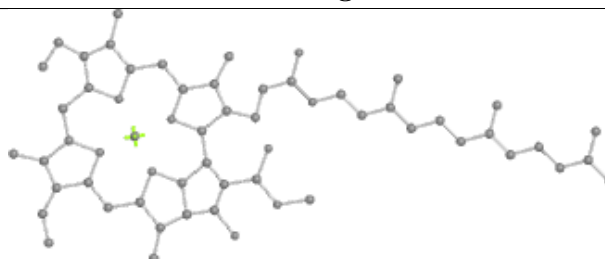
Bond lengths



Bond angles

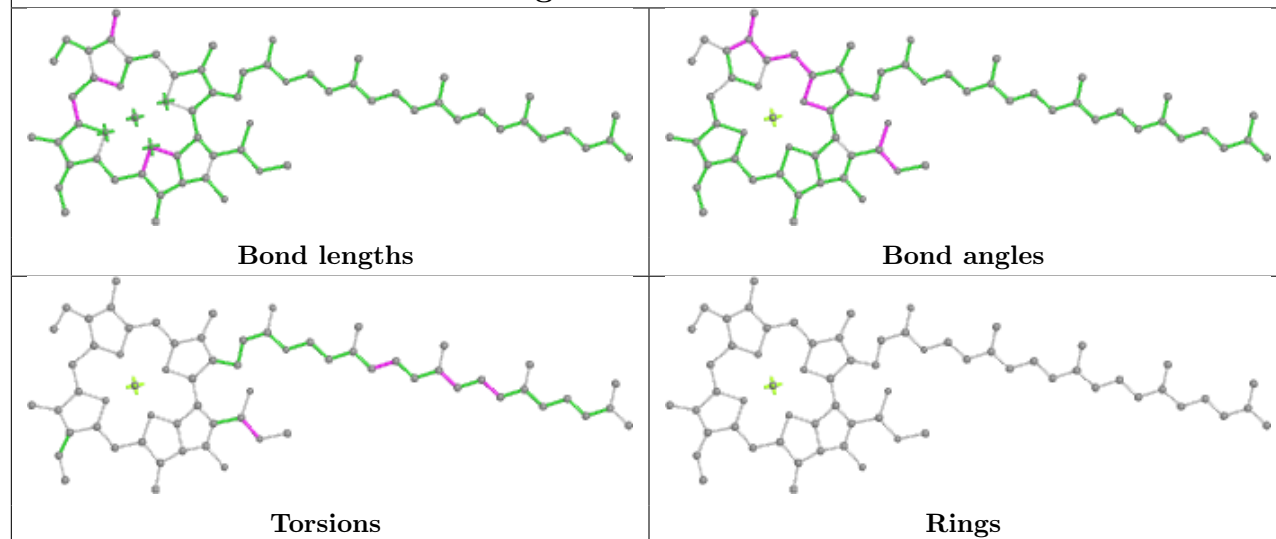


Torsions

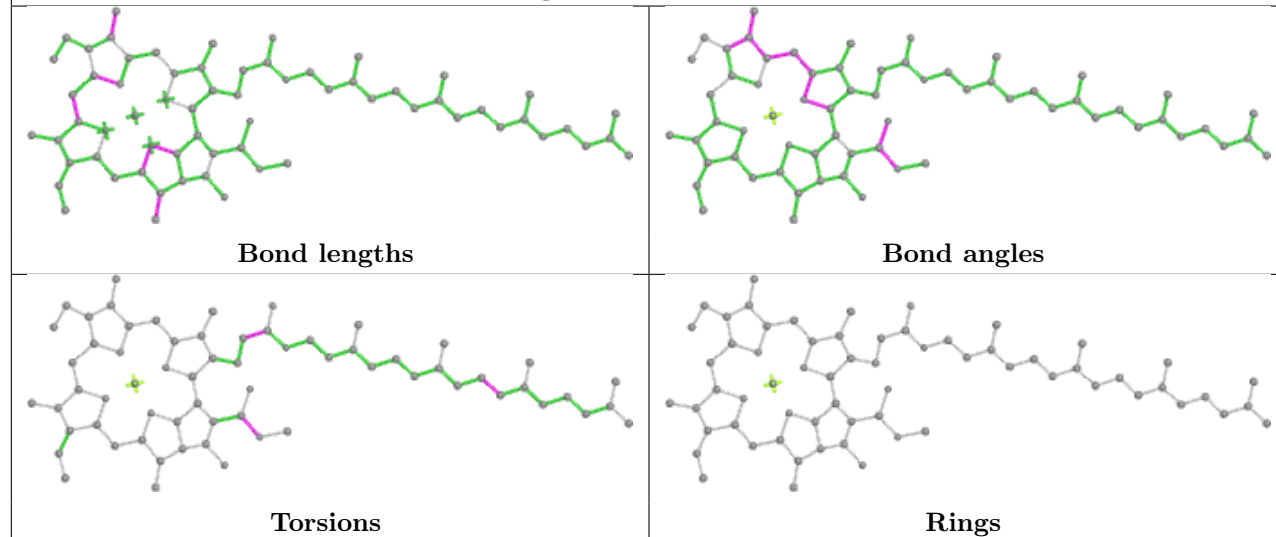


Rings

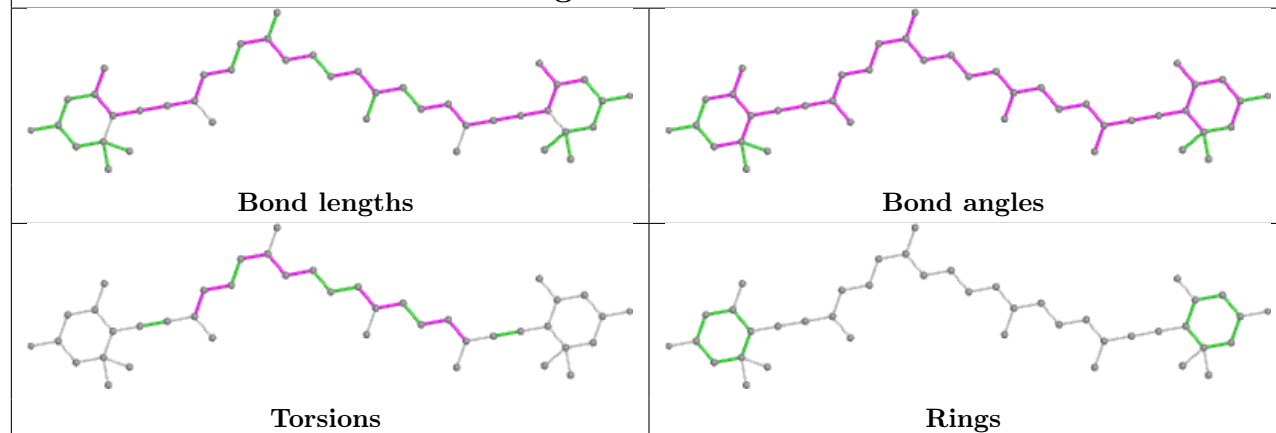
Ligand CLA b 309



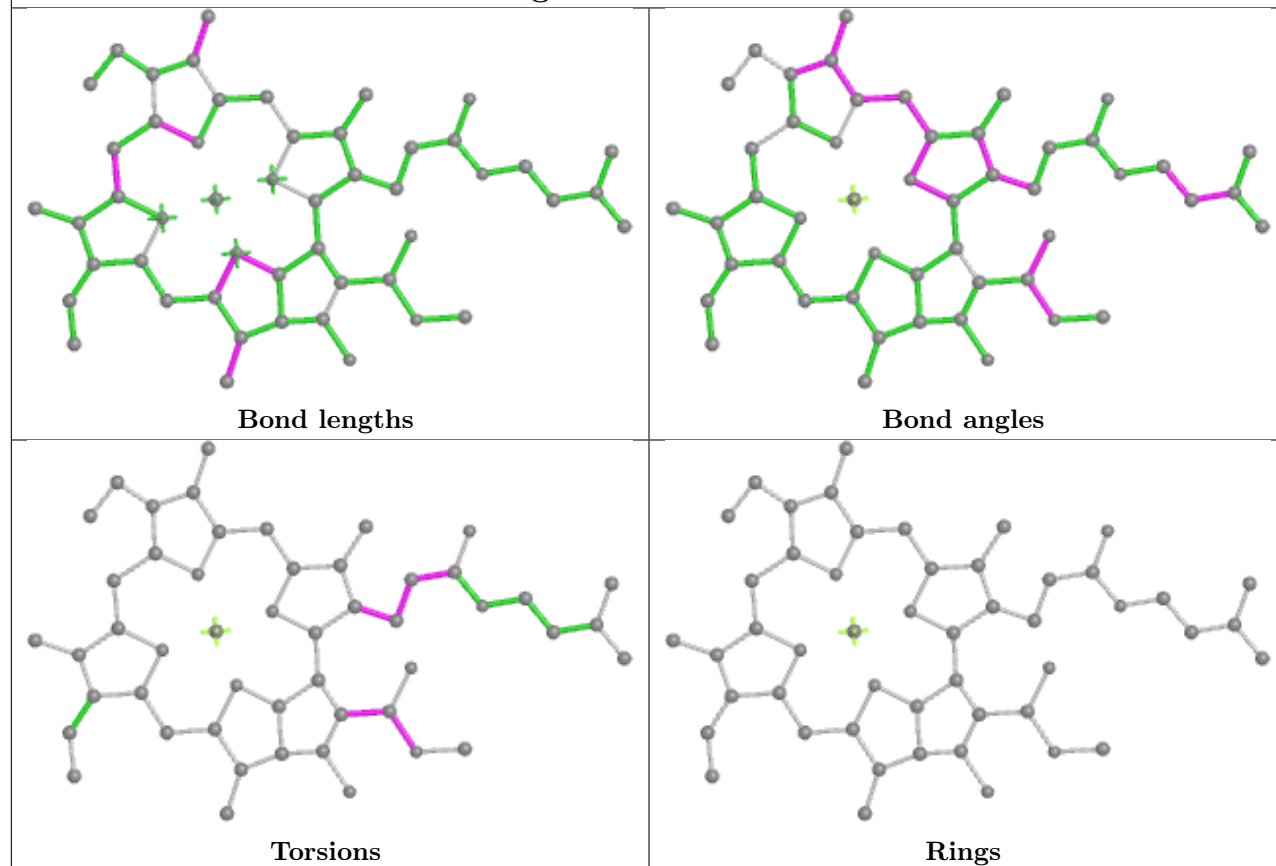
Ligand CLA c 305



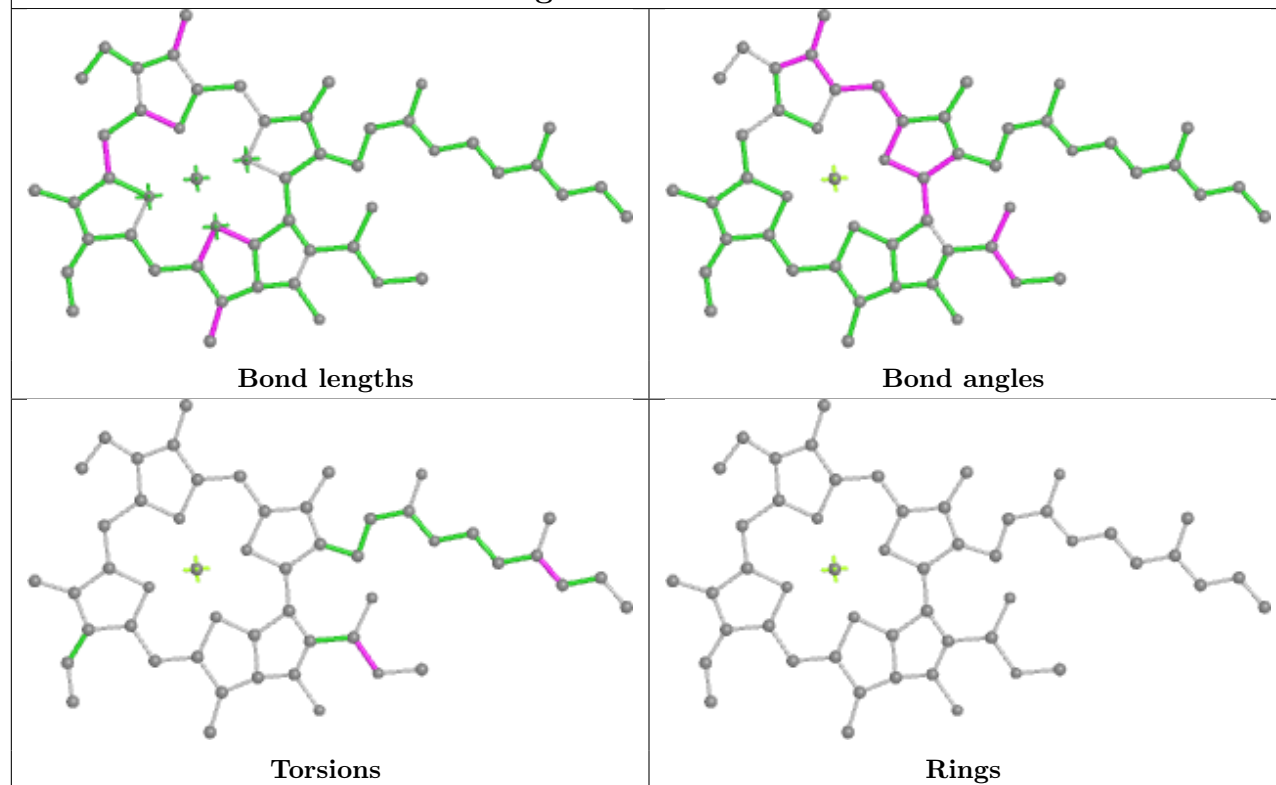
Ligand II0 i 319



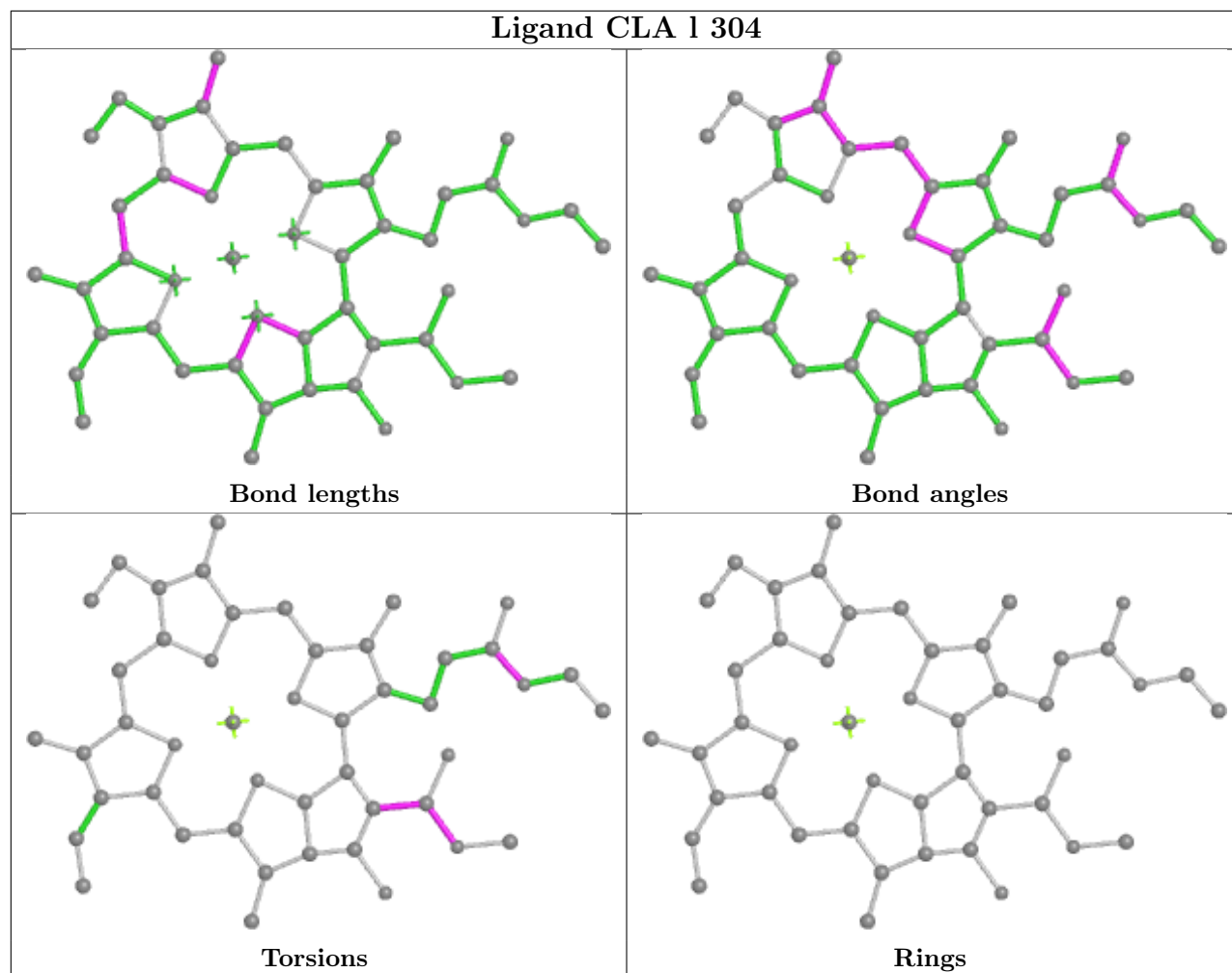
Ligand CLA A 814

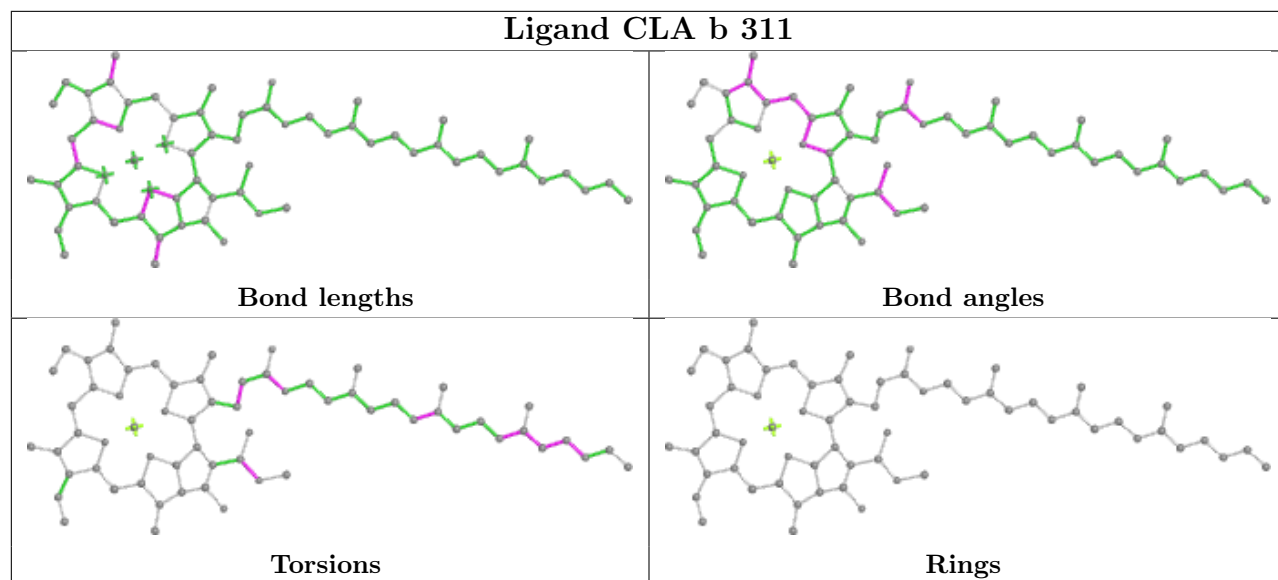
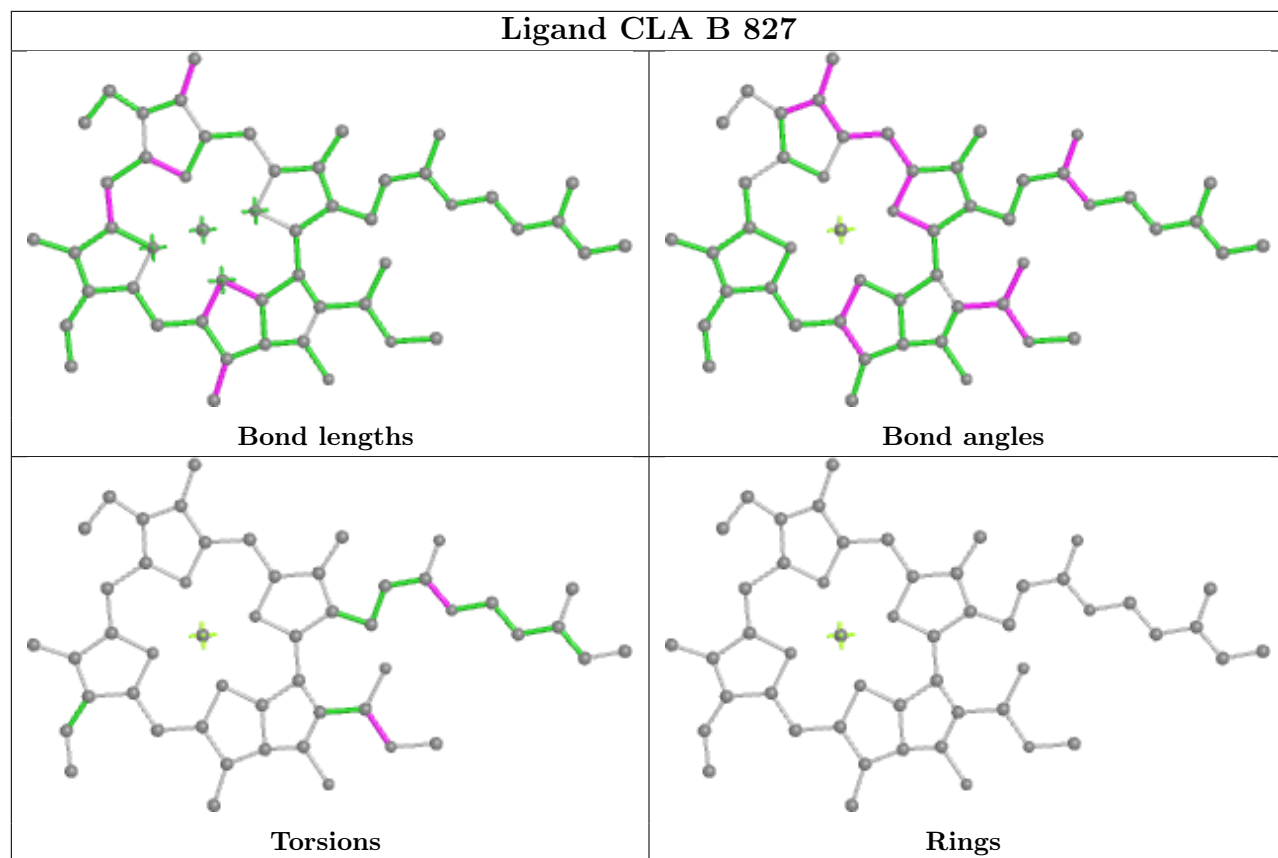


Ligand CLA b 305

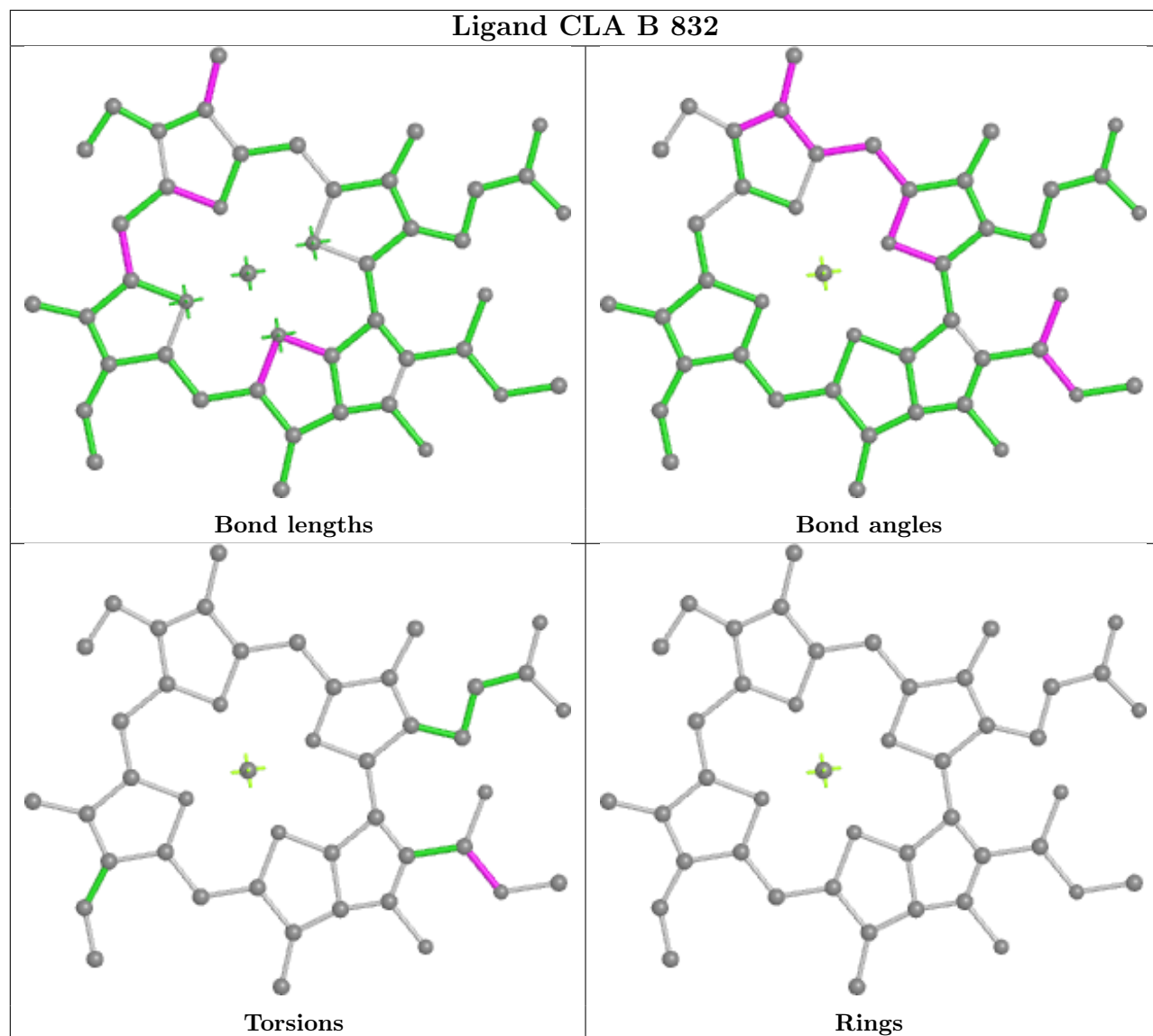


Ligand CLA 1 304

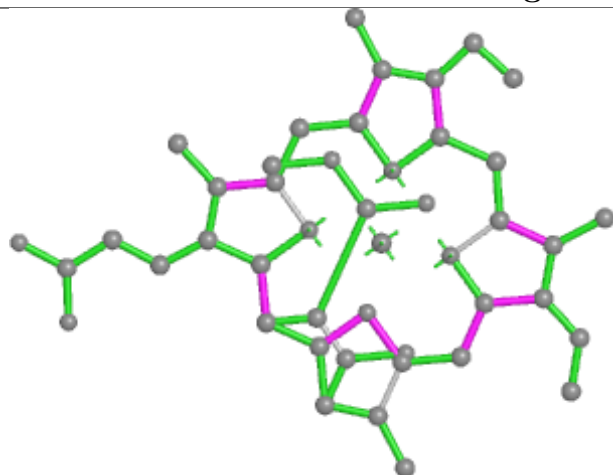




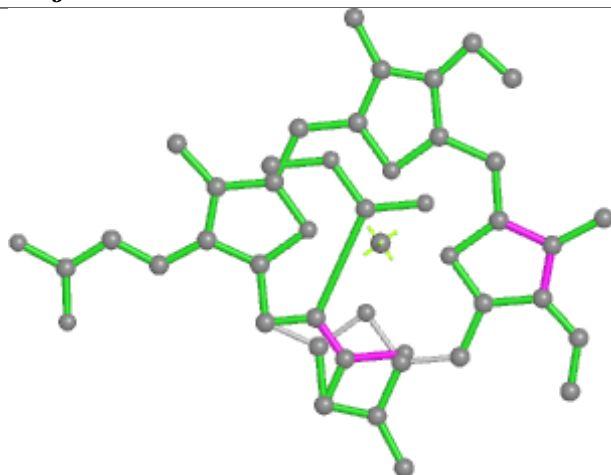
Ligand CLA B 832



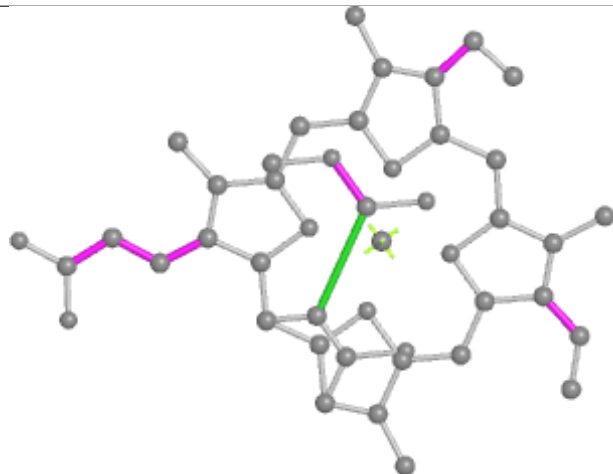
Ligand KC2 j 611



Bond lengths



Bond angles

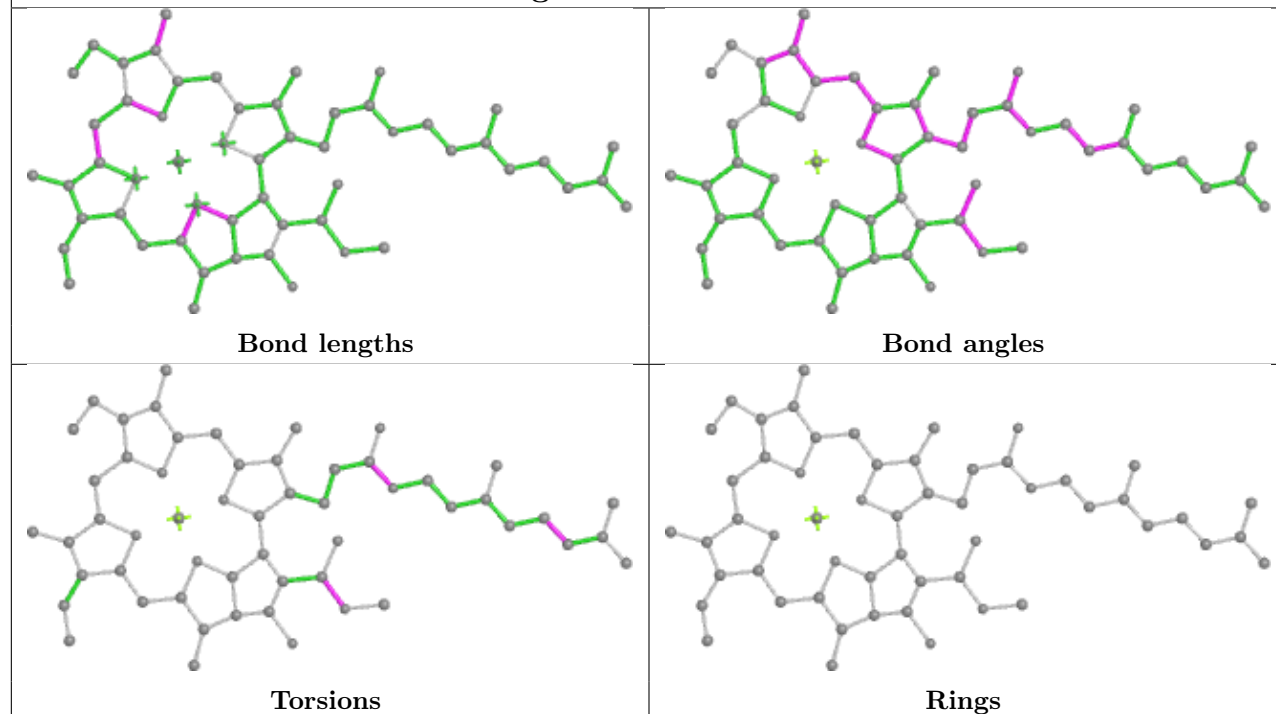


Torsions

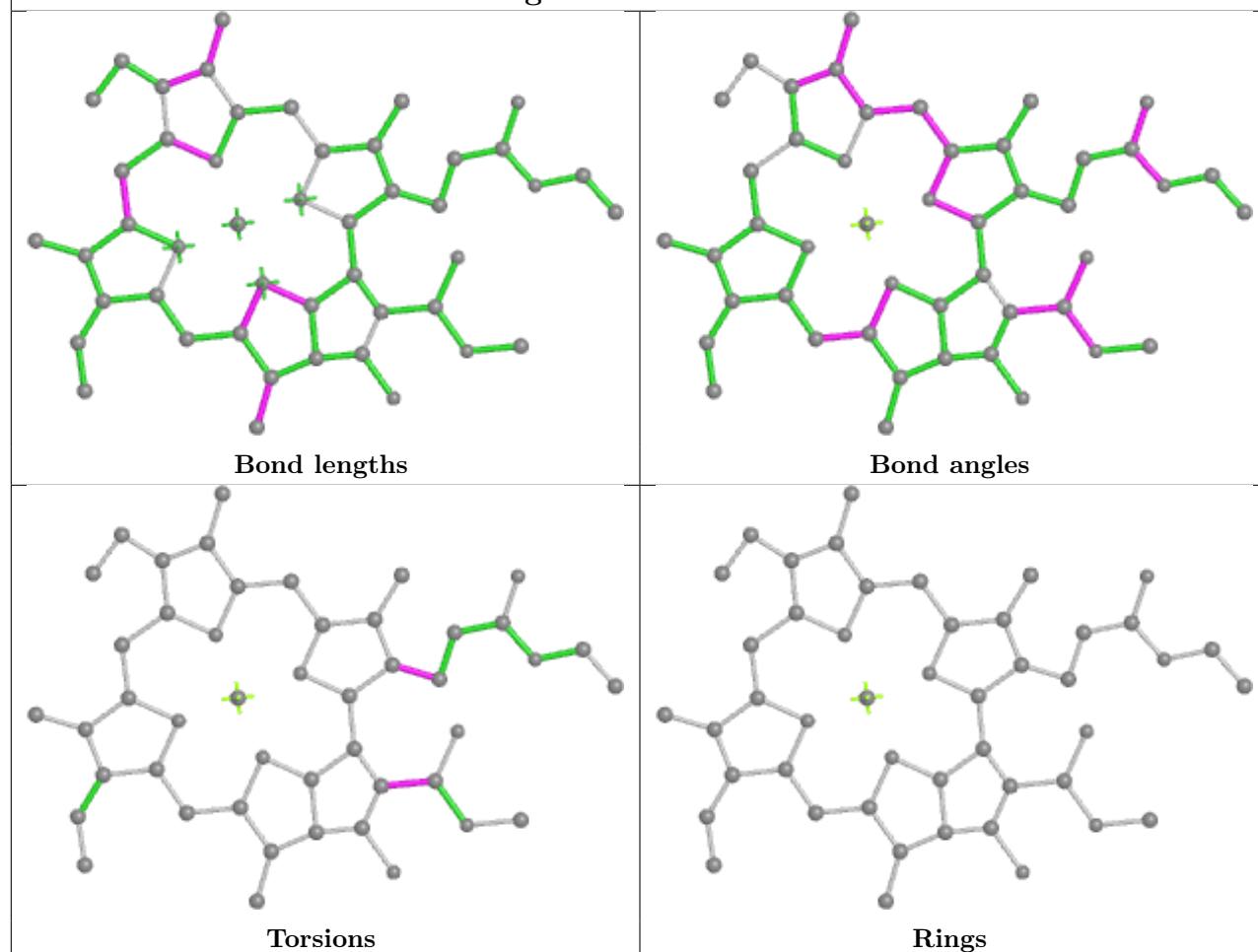


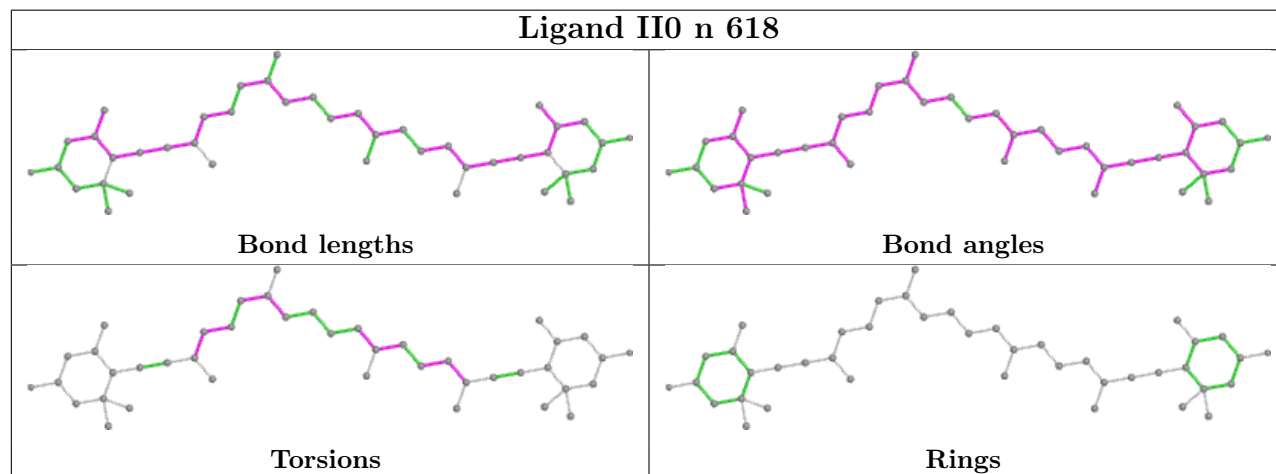
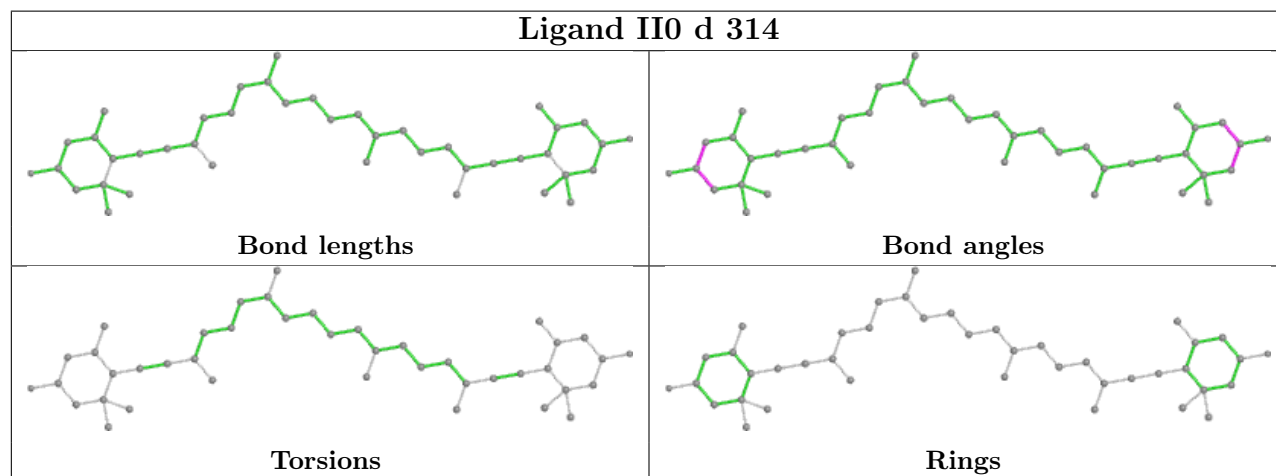
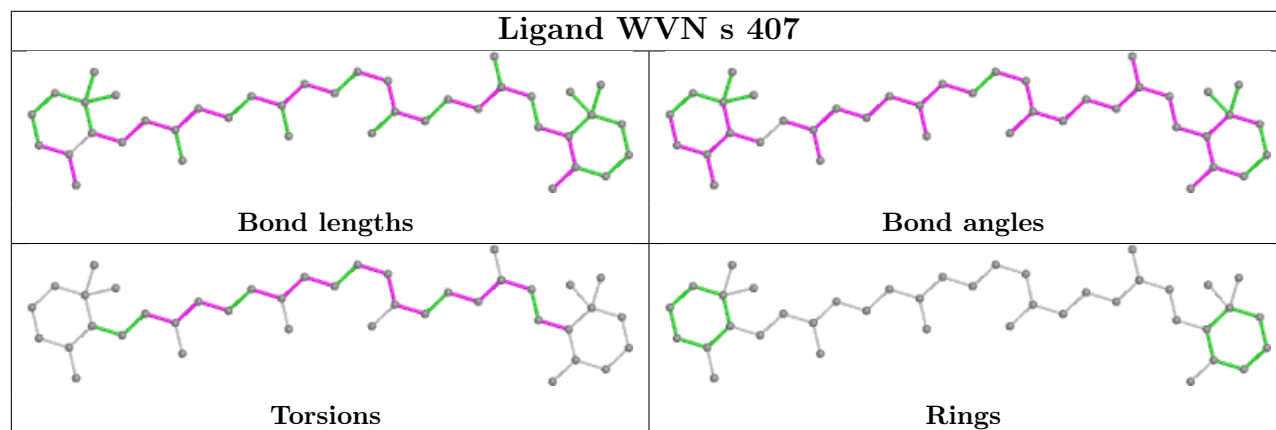
Rings

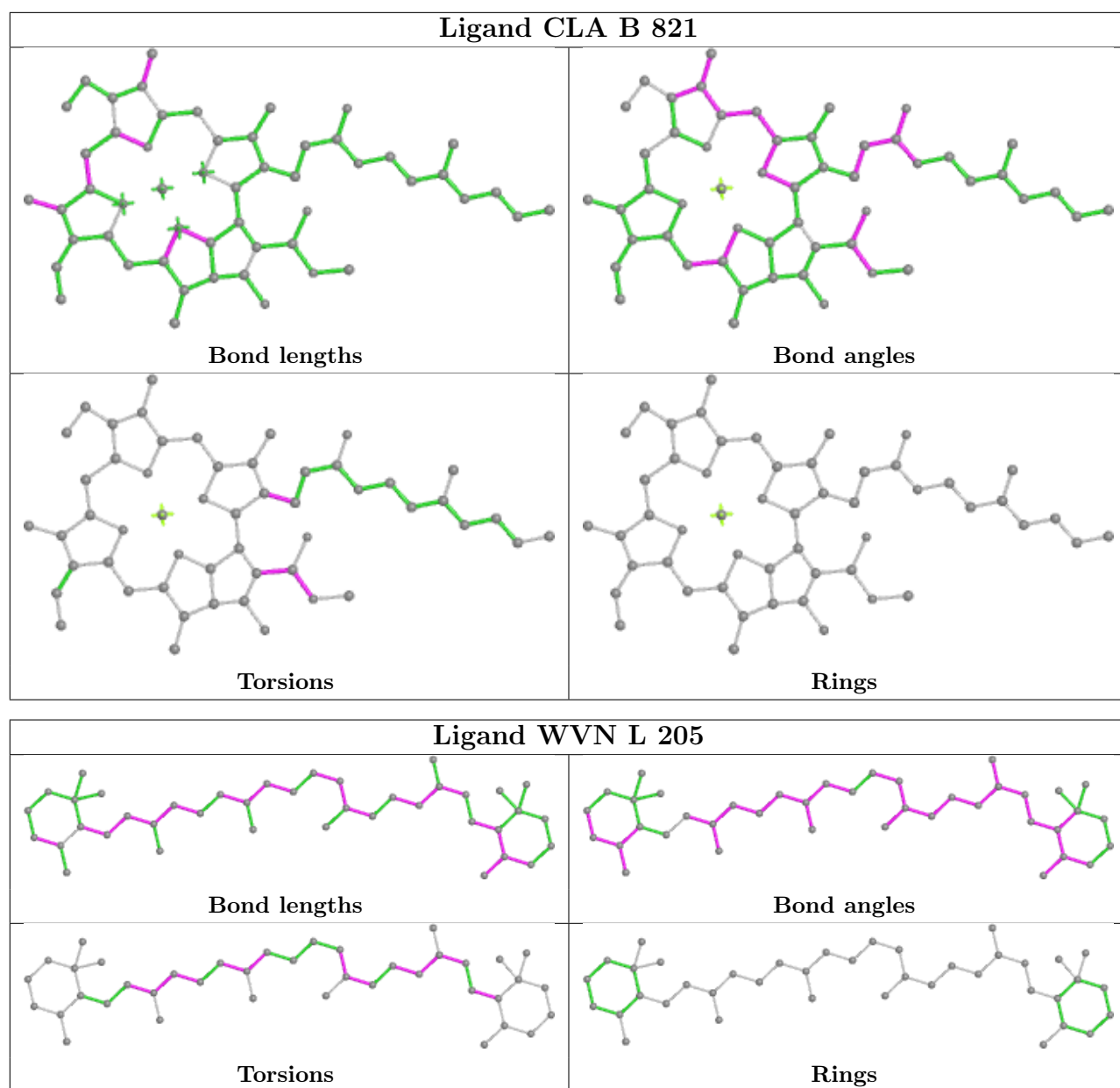
Ligand CLA R 201



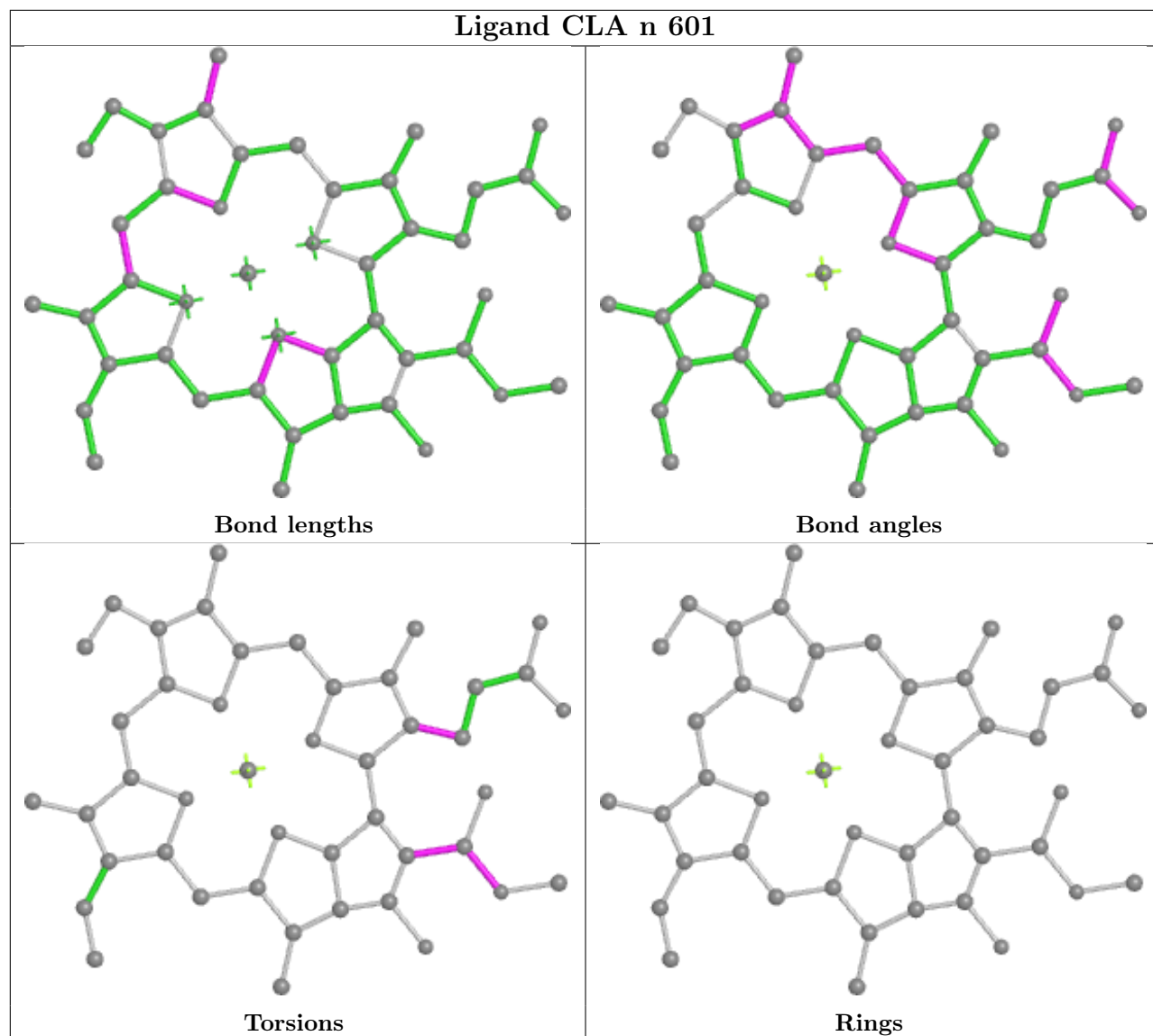
Ligand CLA B 835

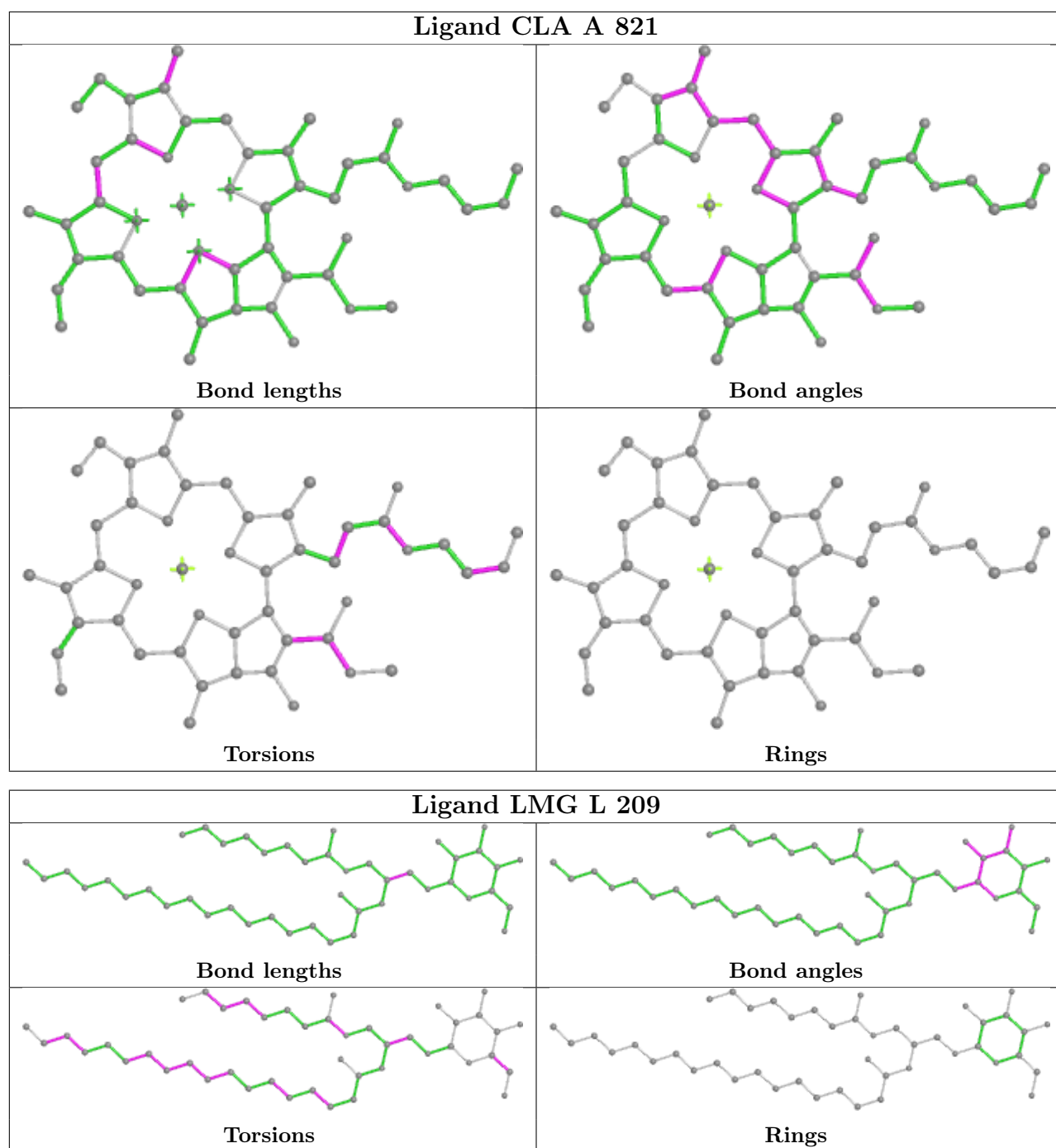




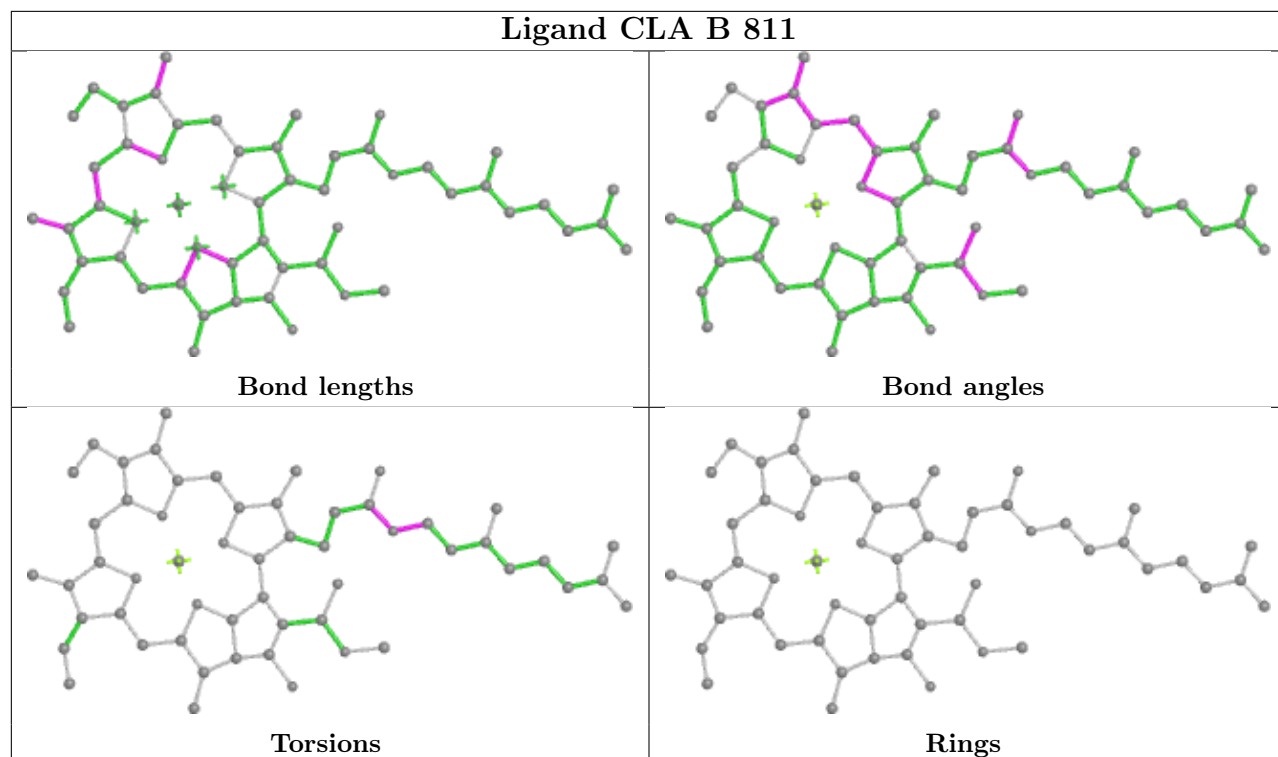


Ligand CLA n 601

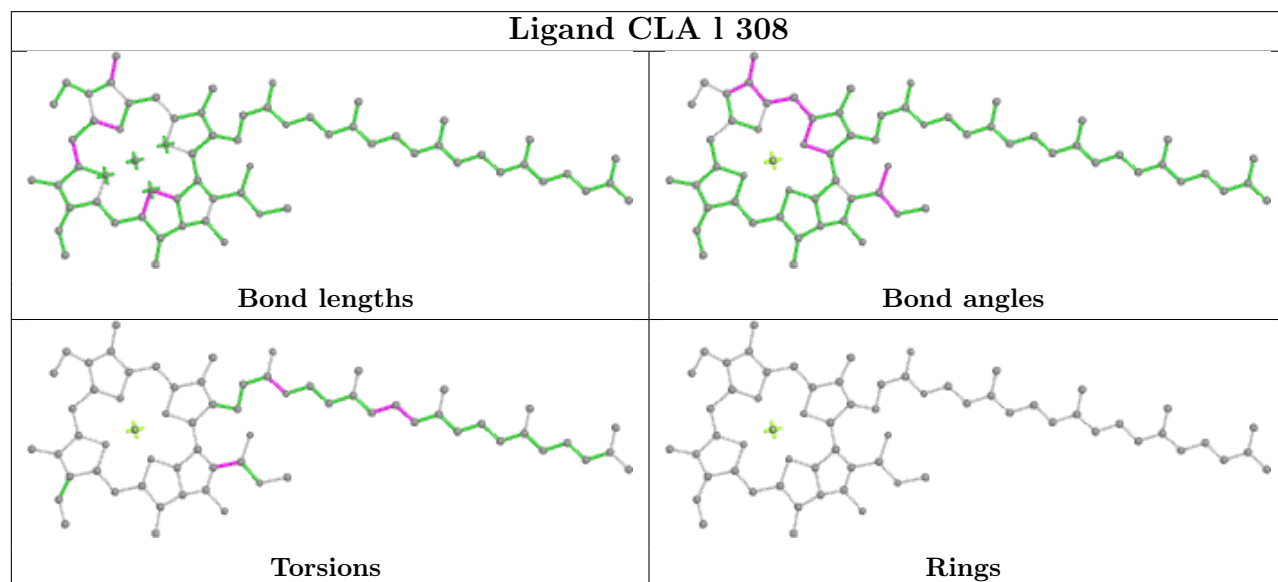




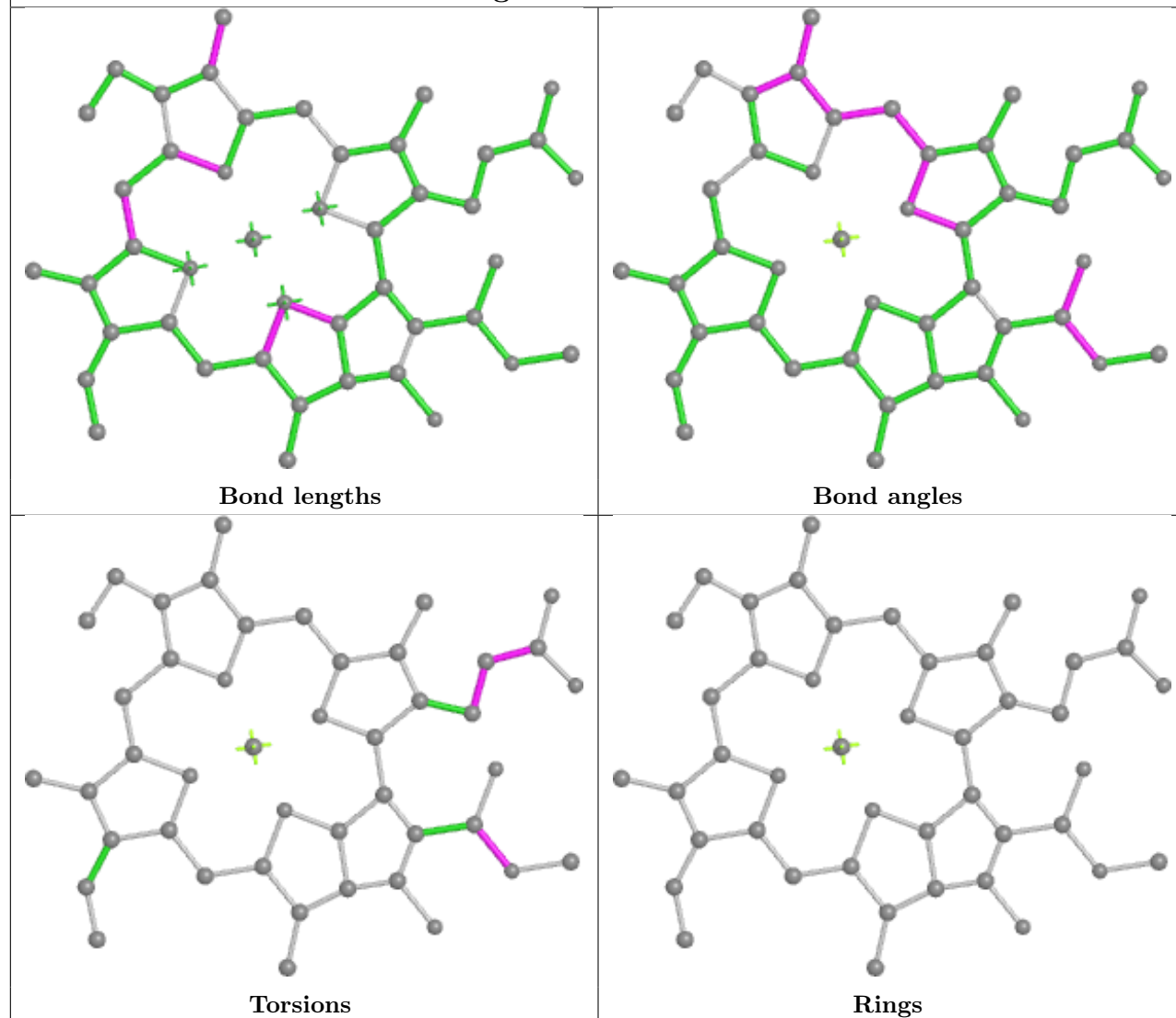
Ligand CLA B 811



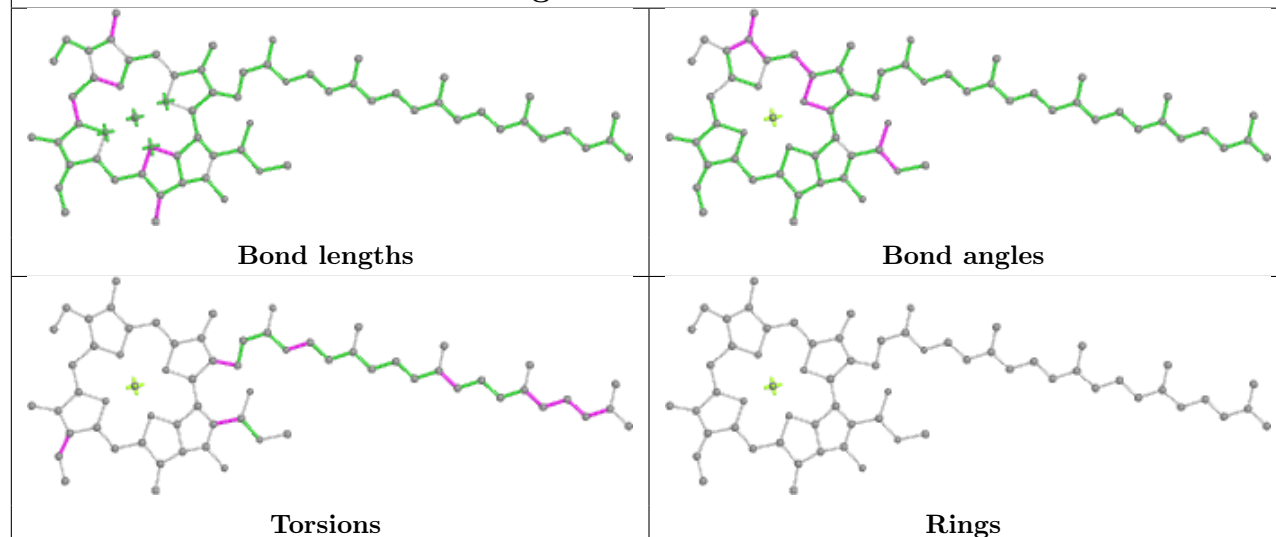
Ligand CLA I 308

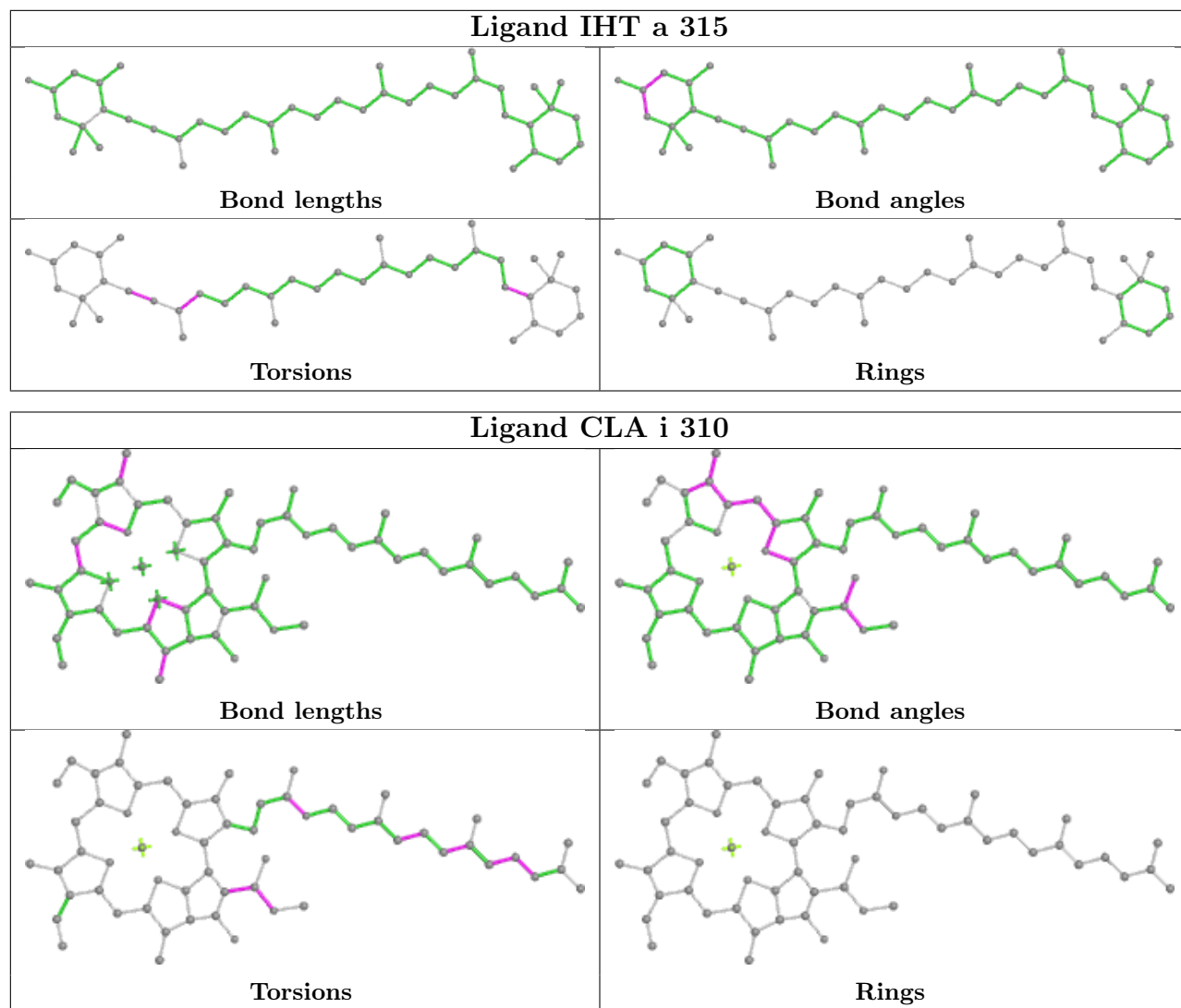


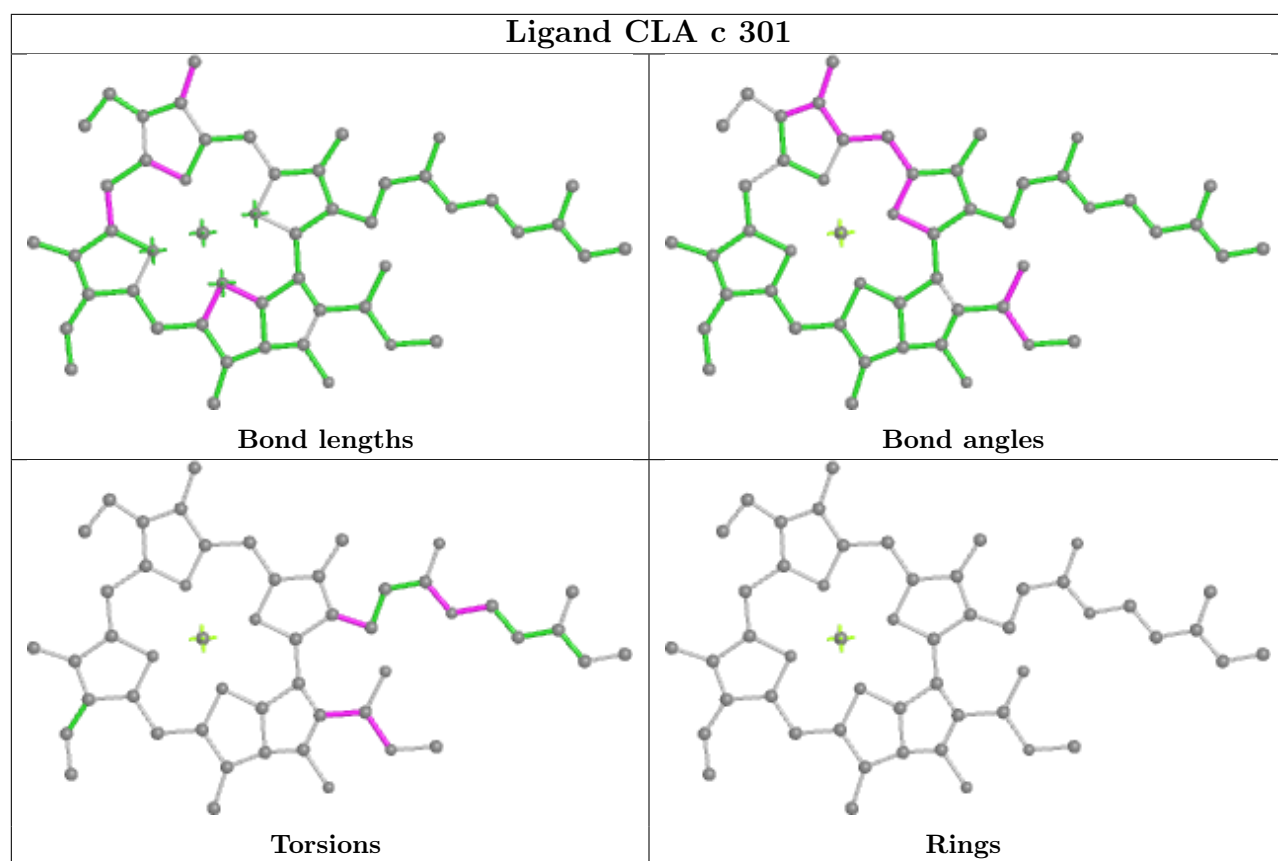
Ligand CLA d 318

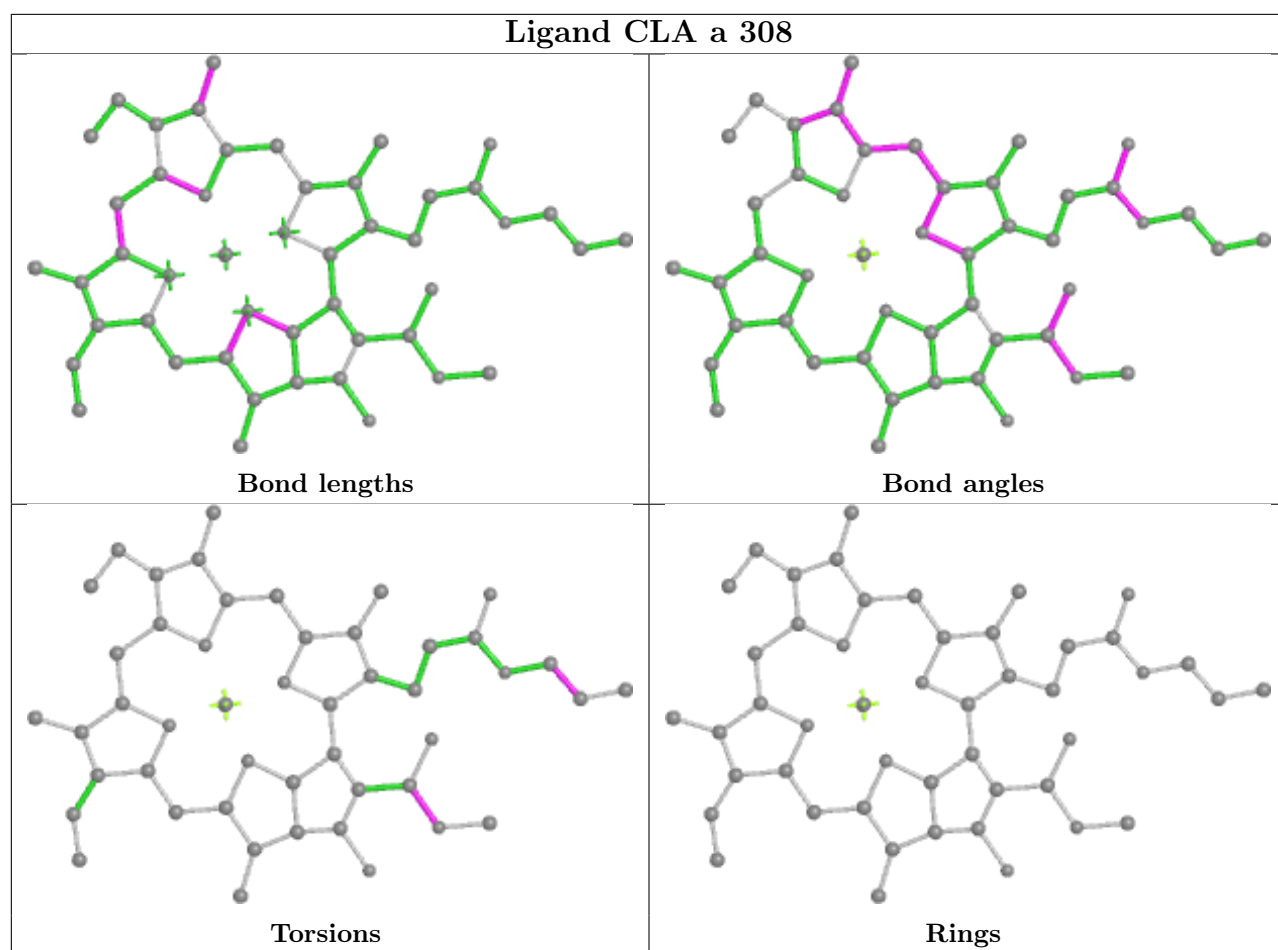


Ligand CLA B 837

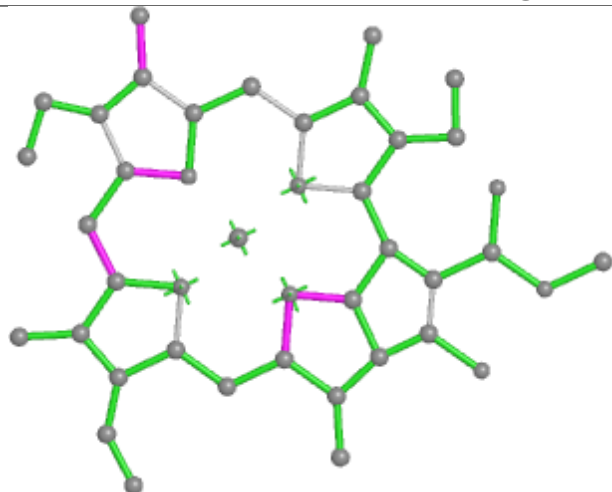




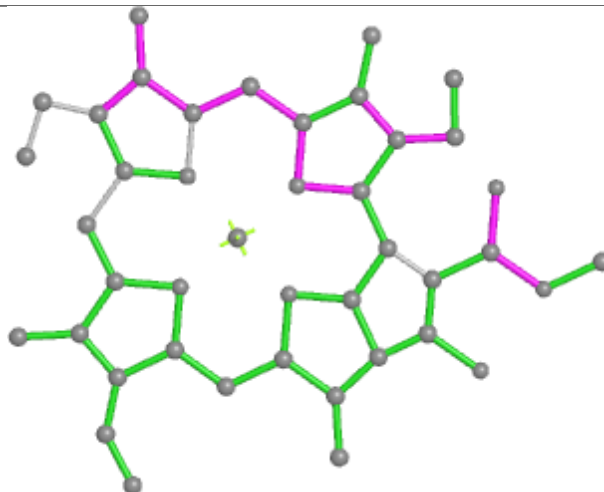




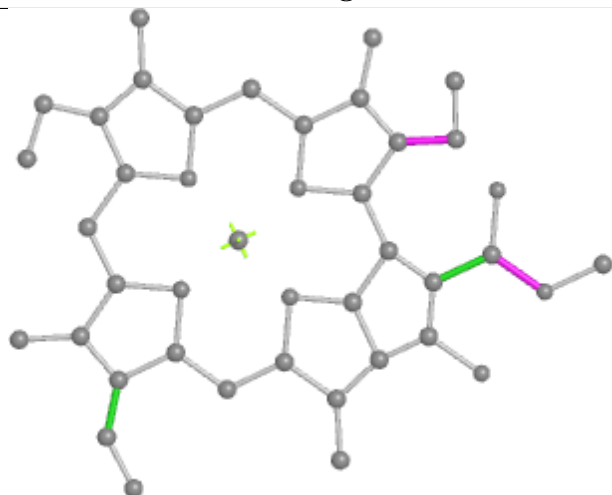
Ligand CLA J 103



Bond lengths



Bond angles

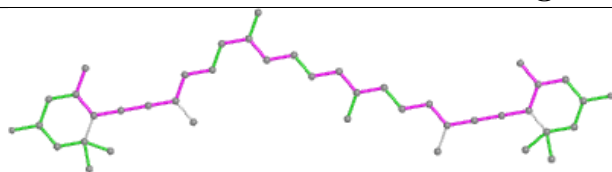


Torsions

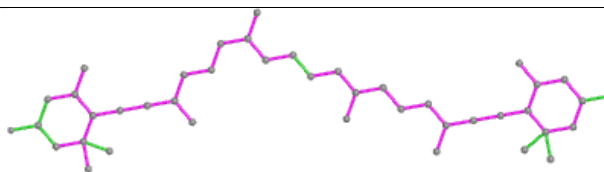


Rings

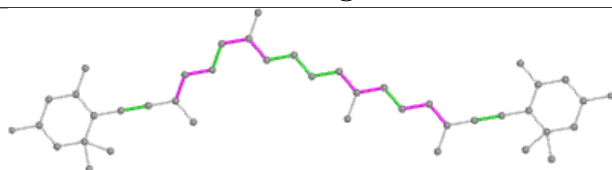
Ligand II0 1 302



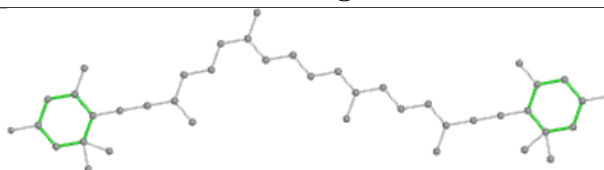
Bond lengths



Bond angles

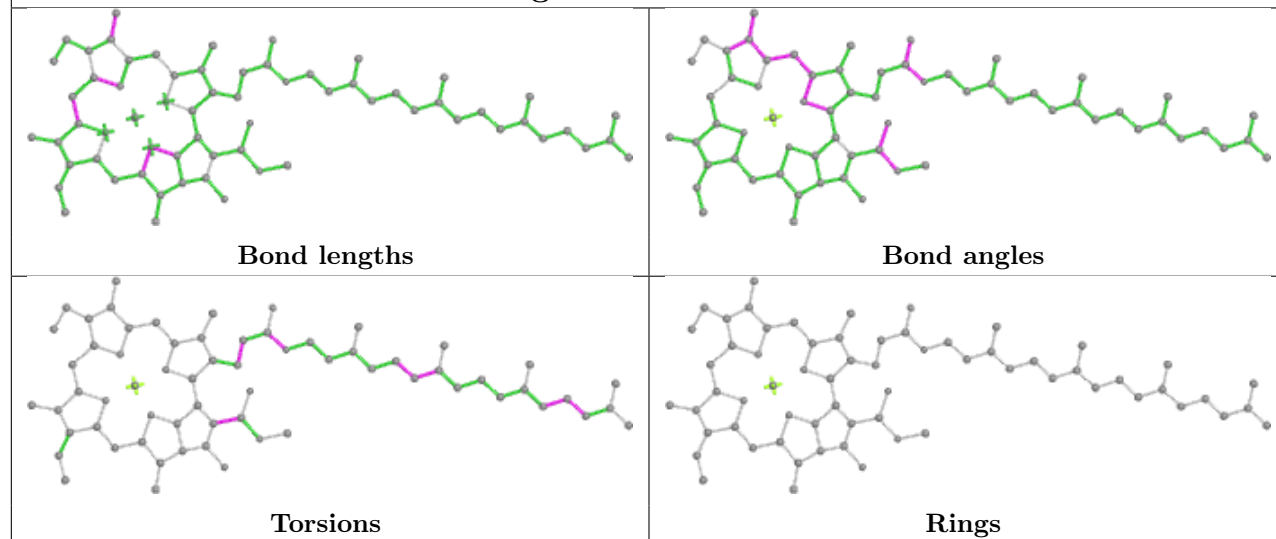


Torsions

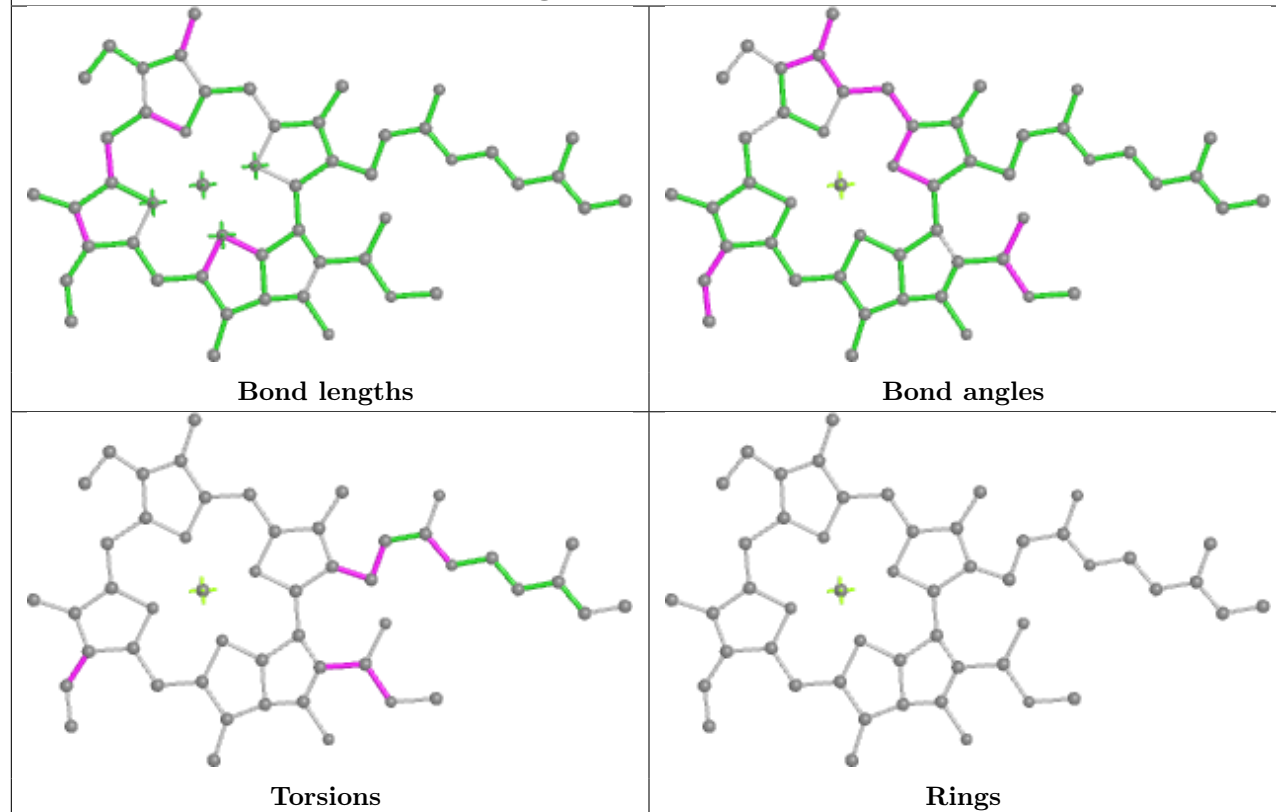


Rings

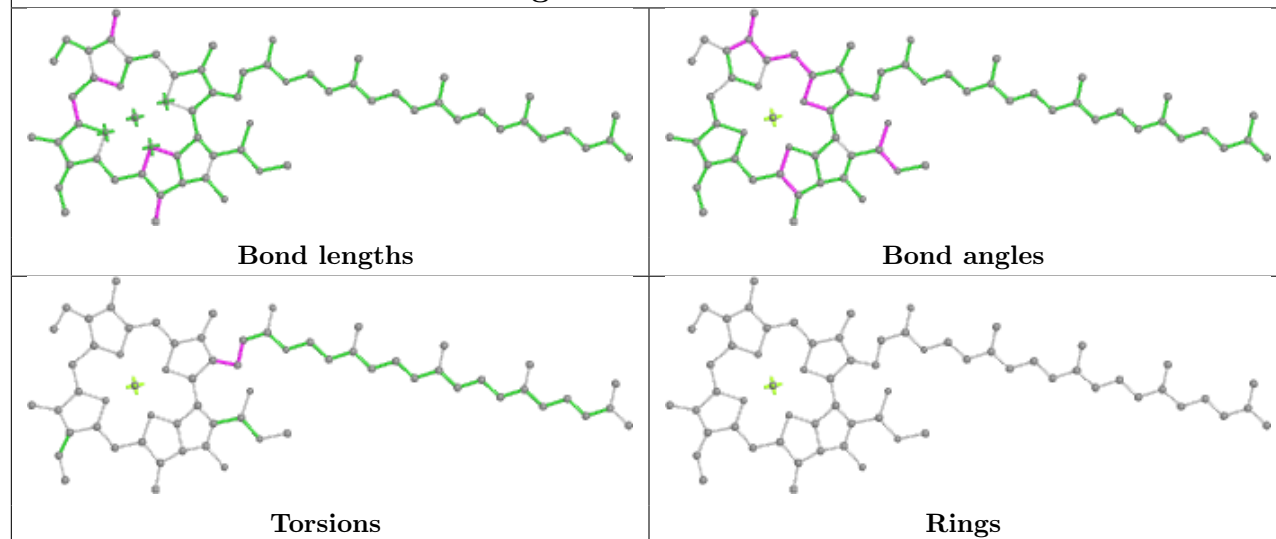
Ligand CLA A 835



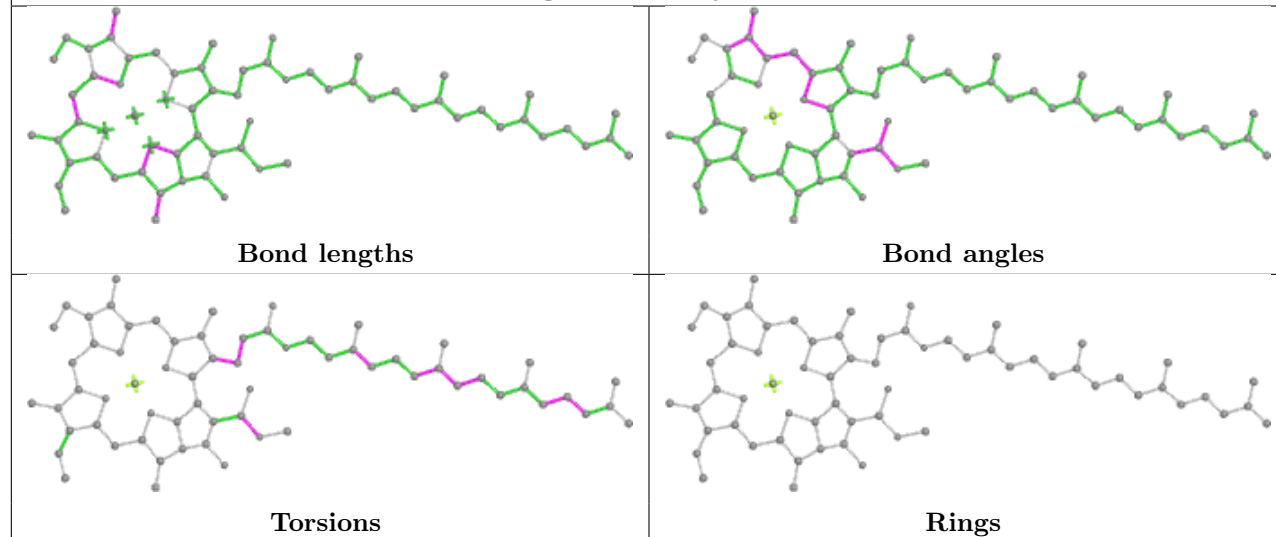
Ligand CLA k 614



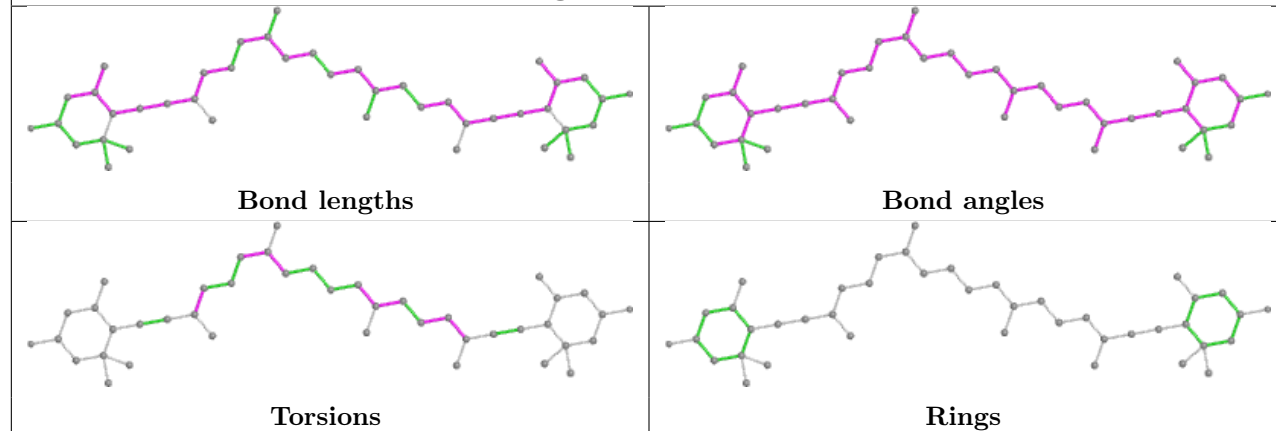
Ligand CLA A 851



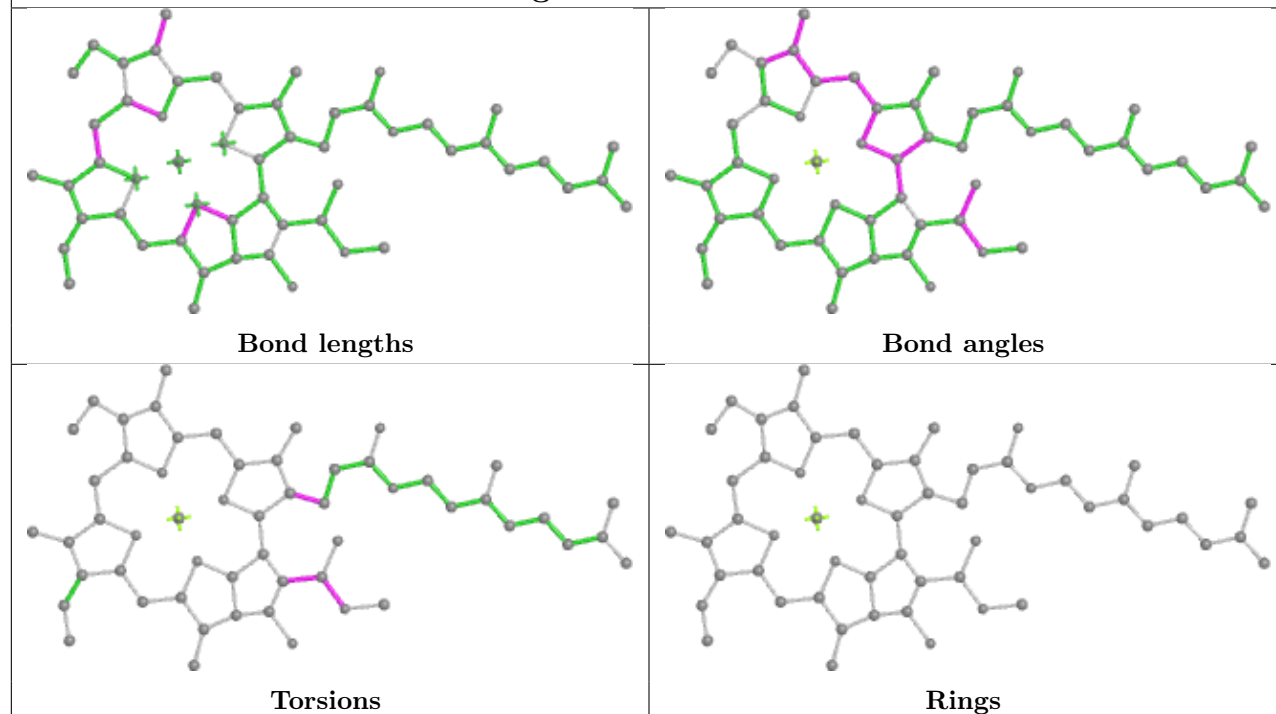
Ligand CLA j 601



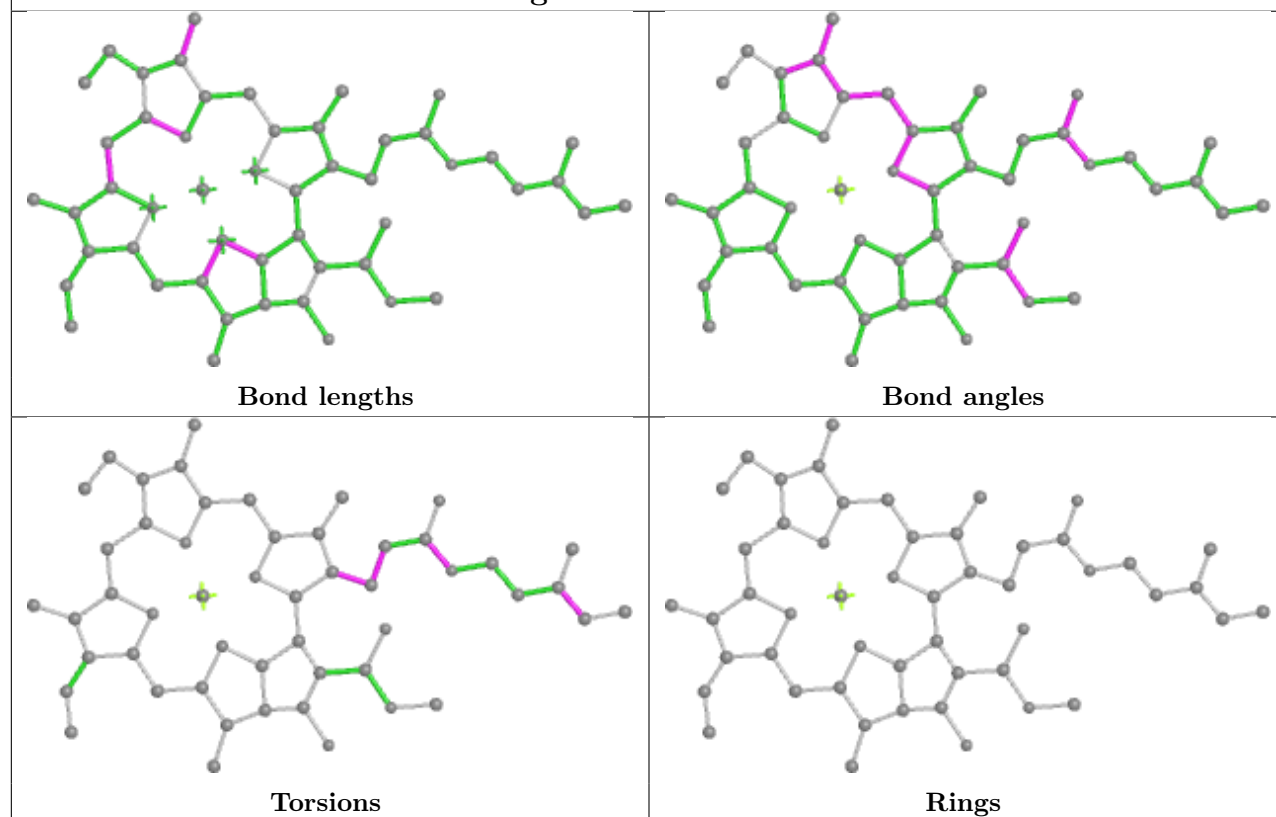
Ligand II0 c 313

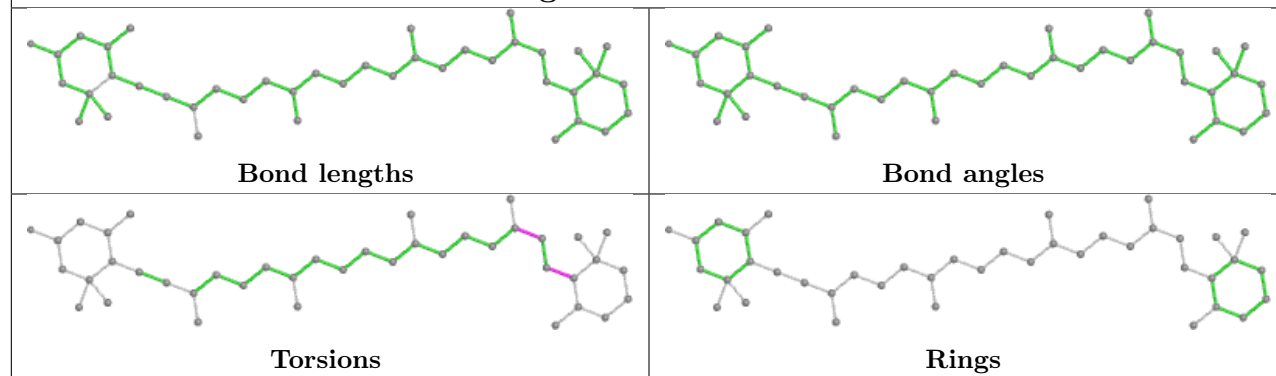
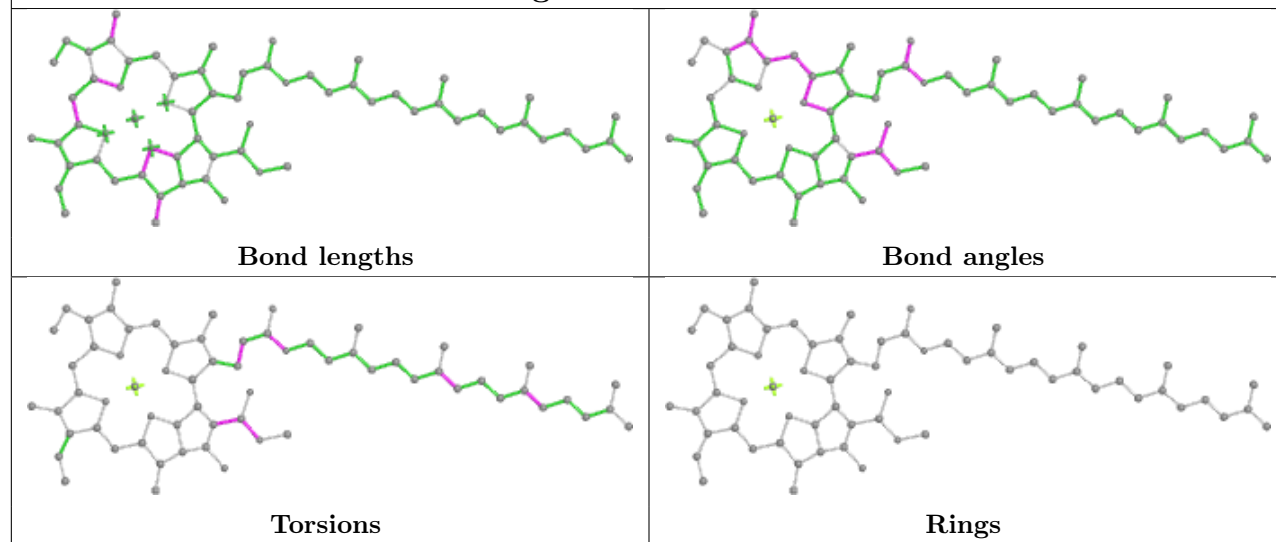


Ligand CLA B 833

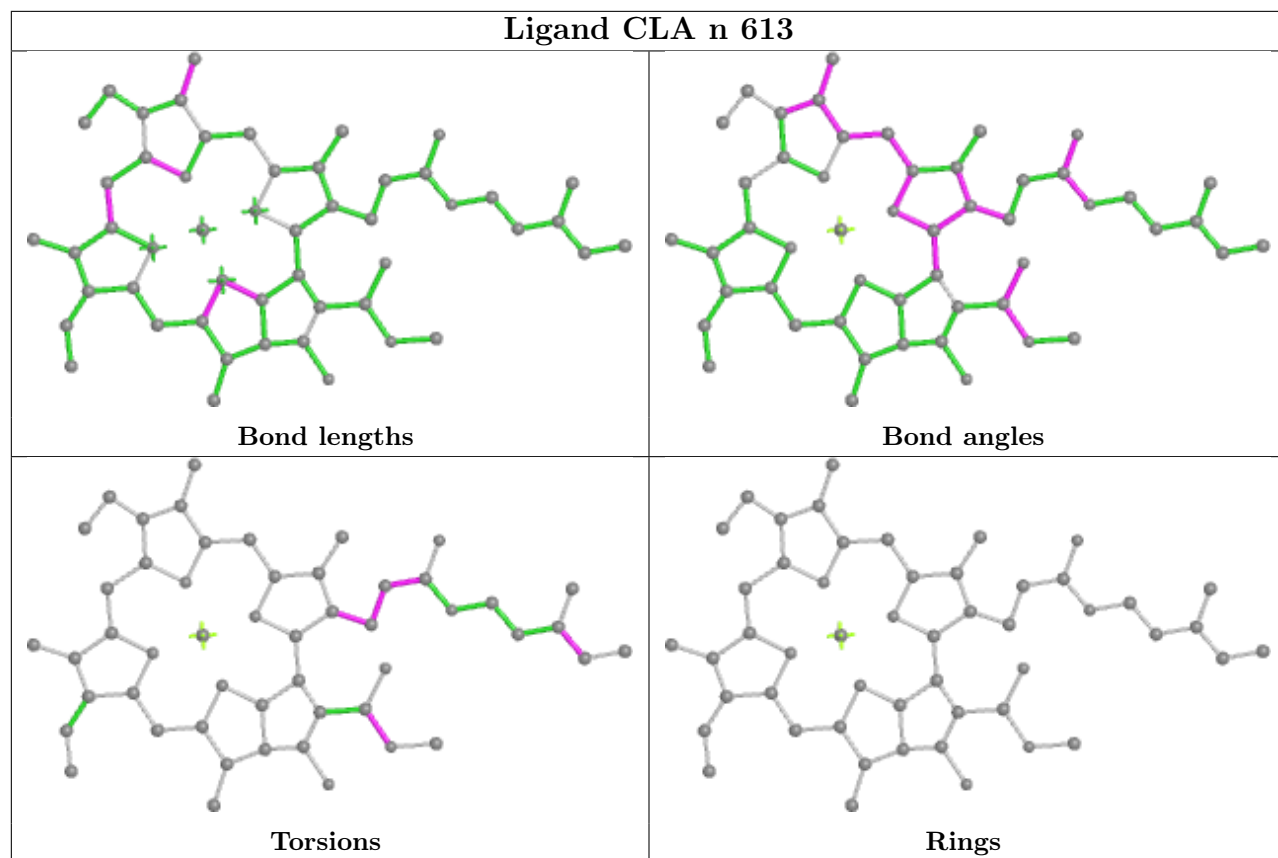


Ligand CLA m 607

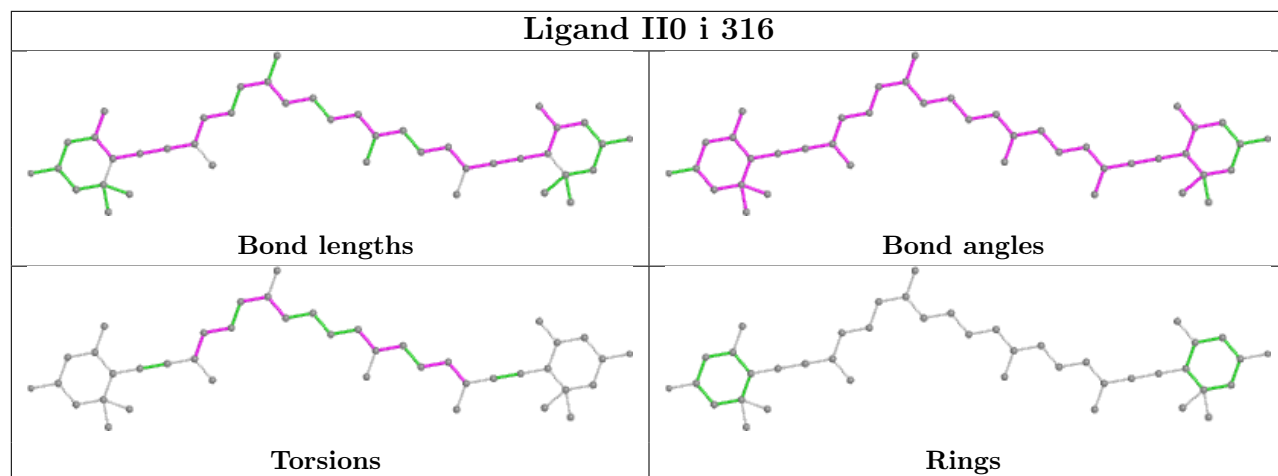


Ligand IHT b 301**Ligand CLA B 838**

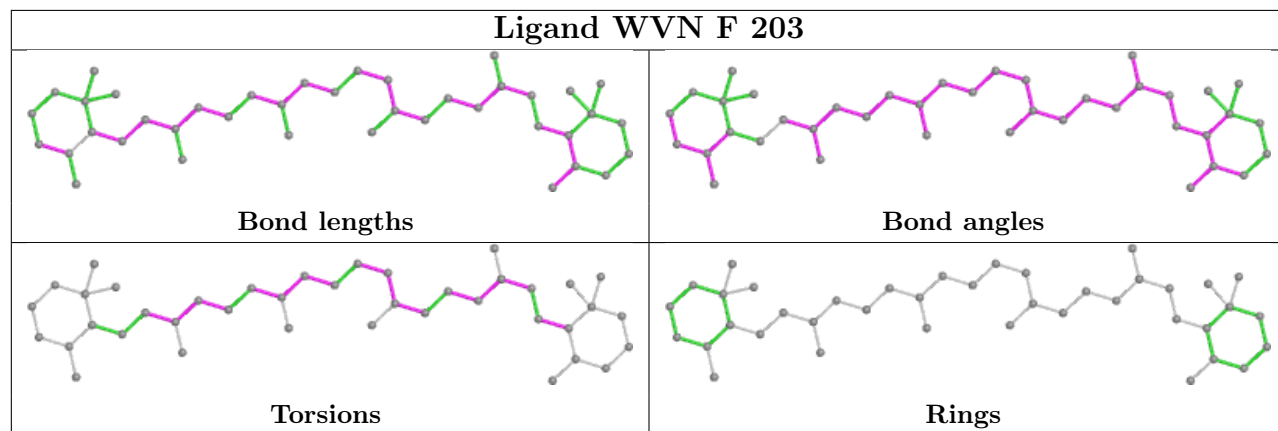
Ligand CLA n 613

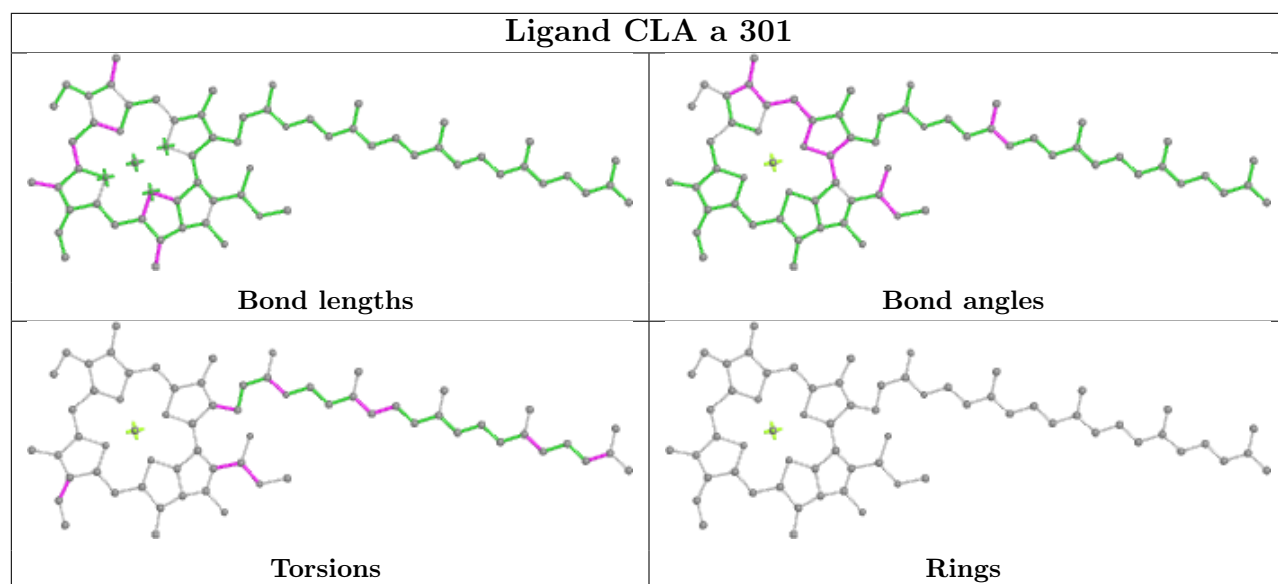
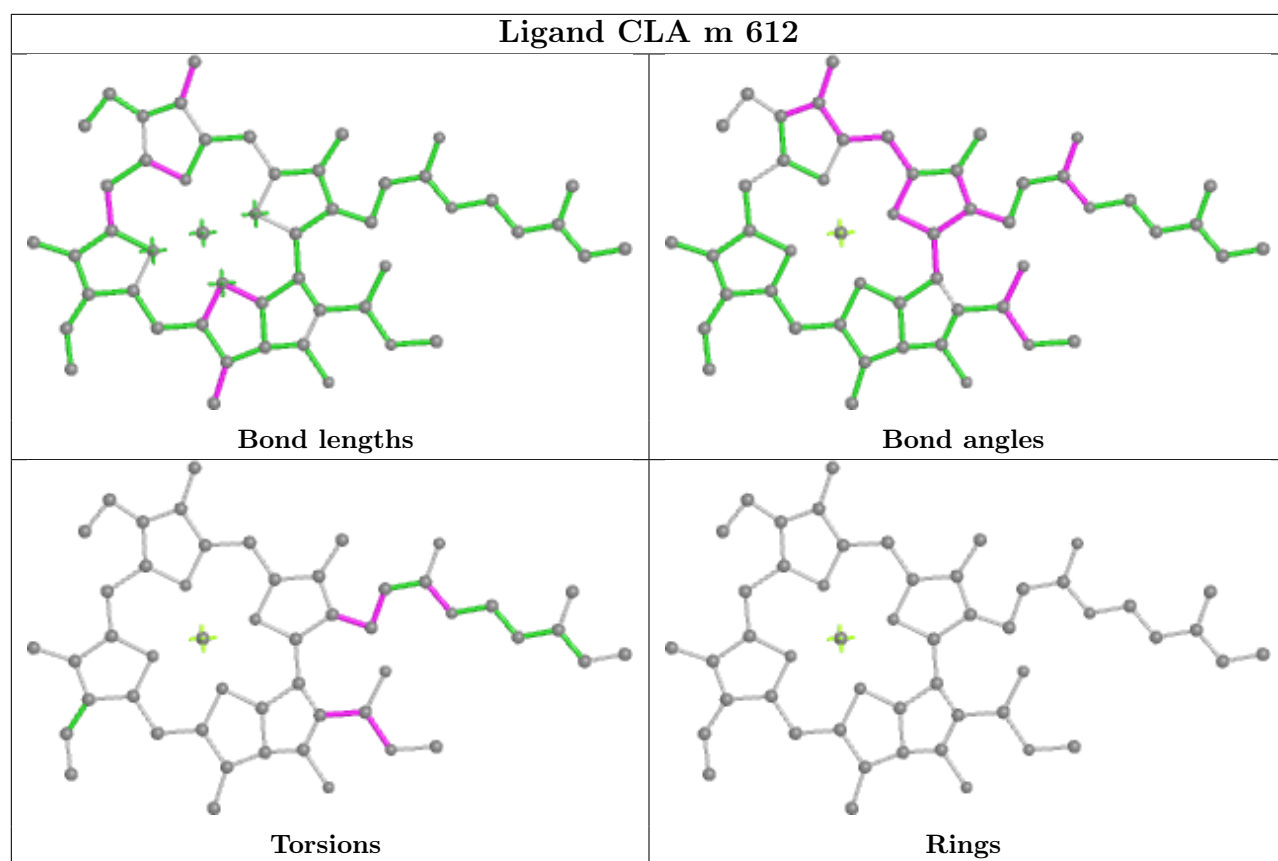


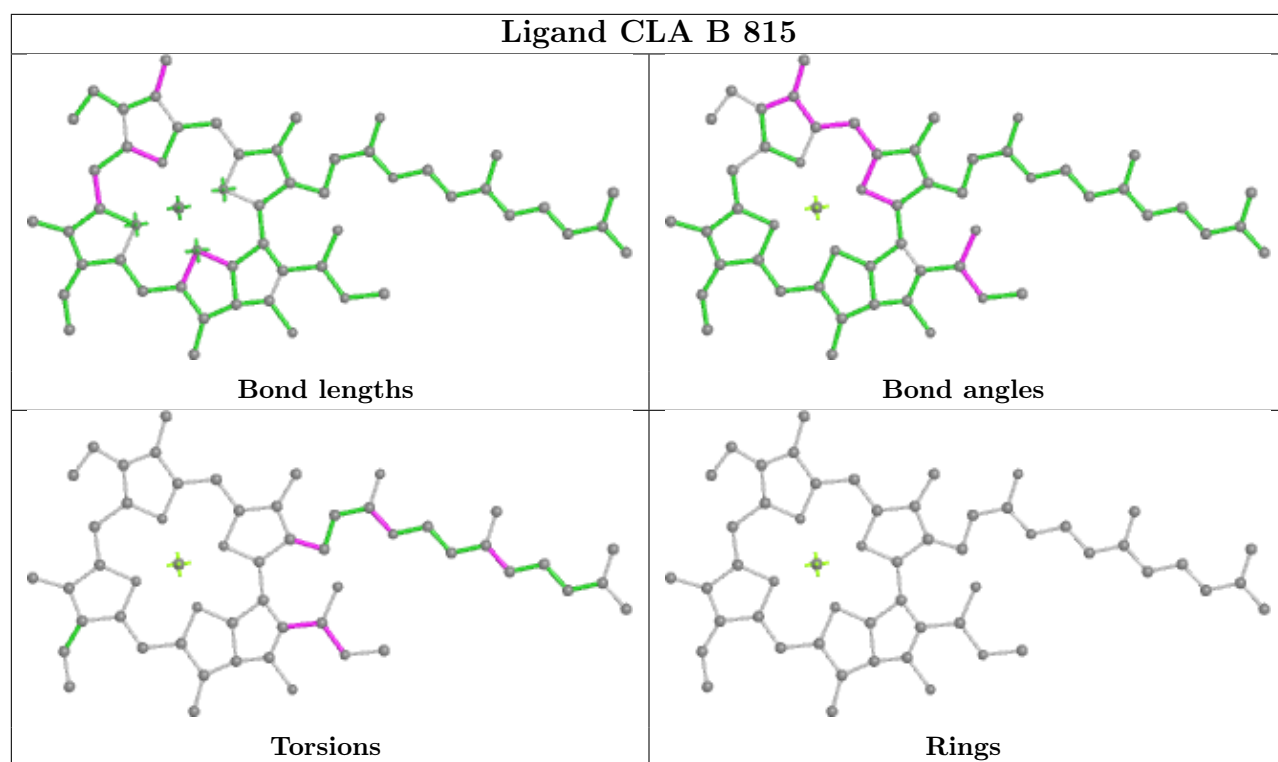
Ligand II0 i 316



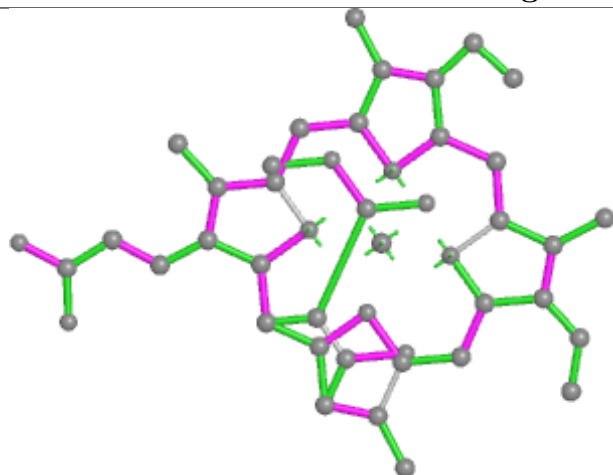
Ligand WVN F 203



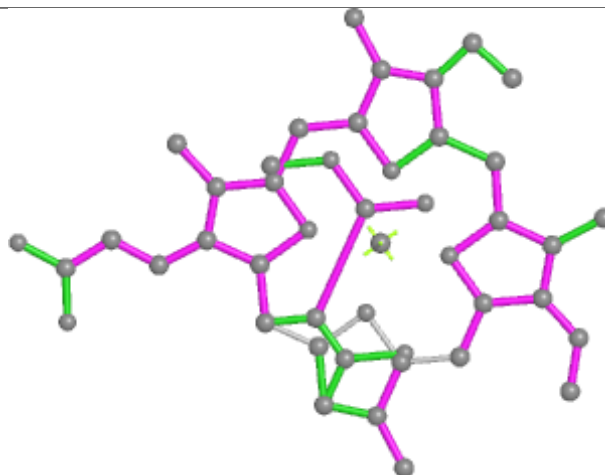




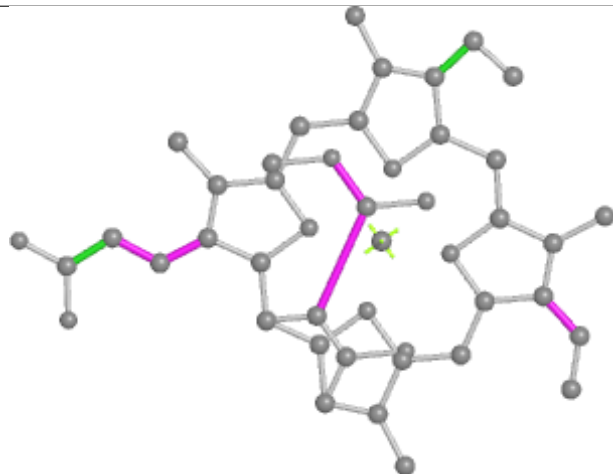
Ligand KC2 c 310



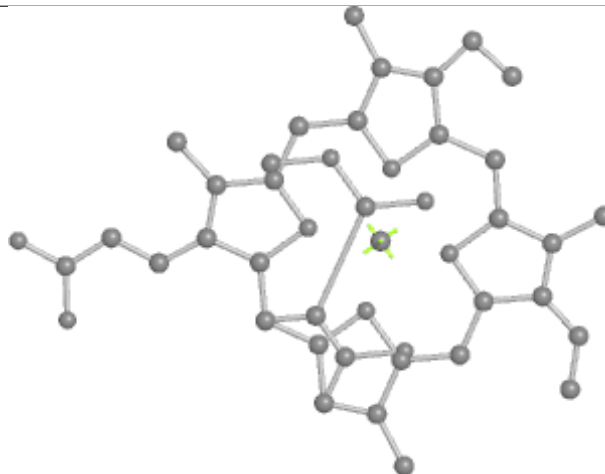
Bond lengths



Bond angles

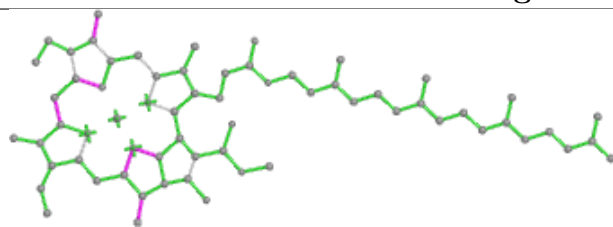


Torsions

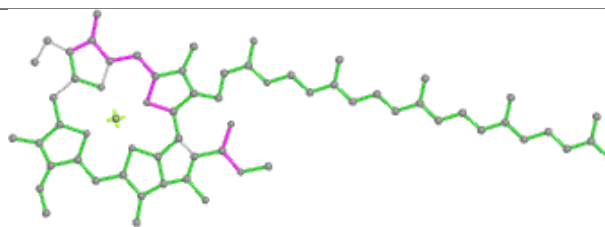


Rings

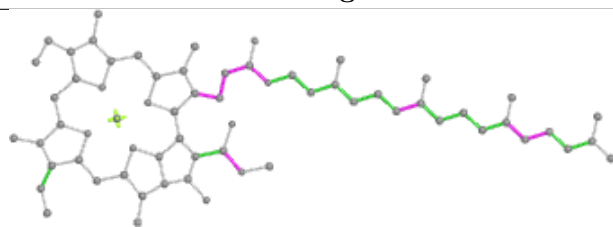
Ligand CLA A 837



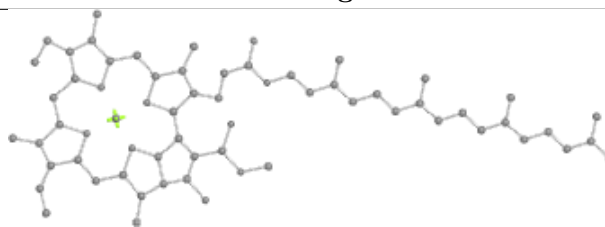
Bond lengths



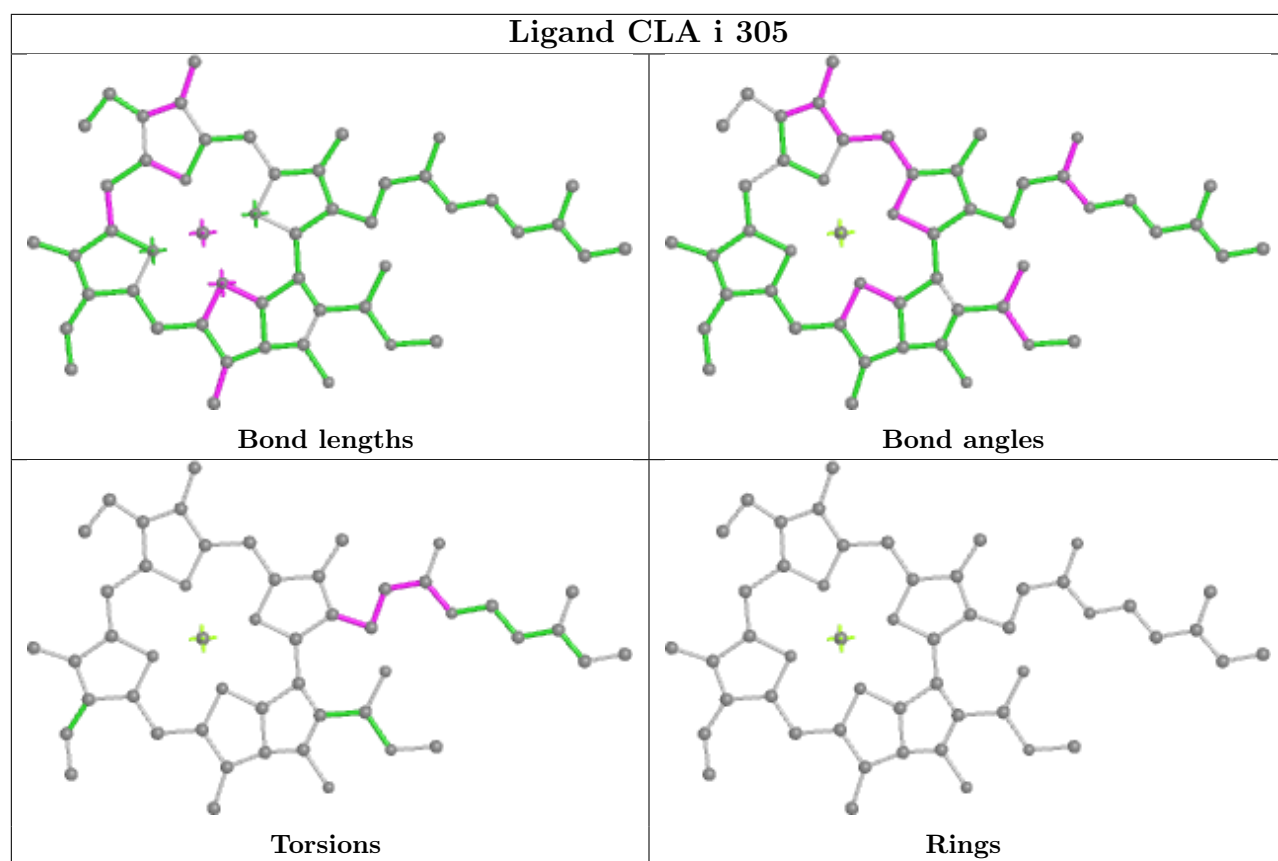
Bond angles

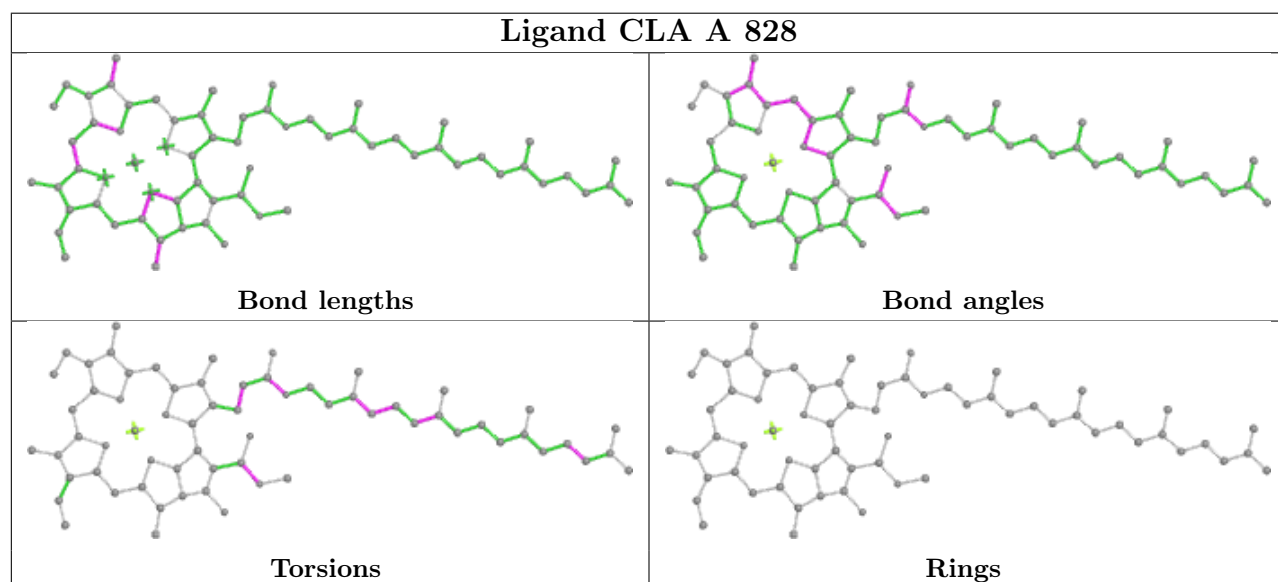
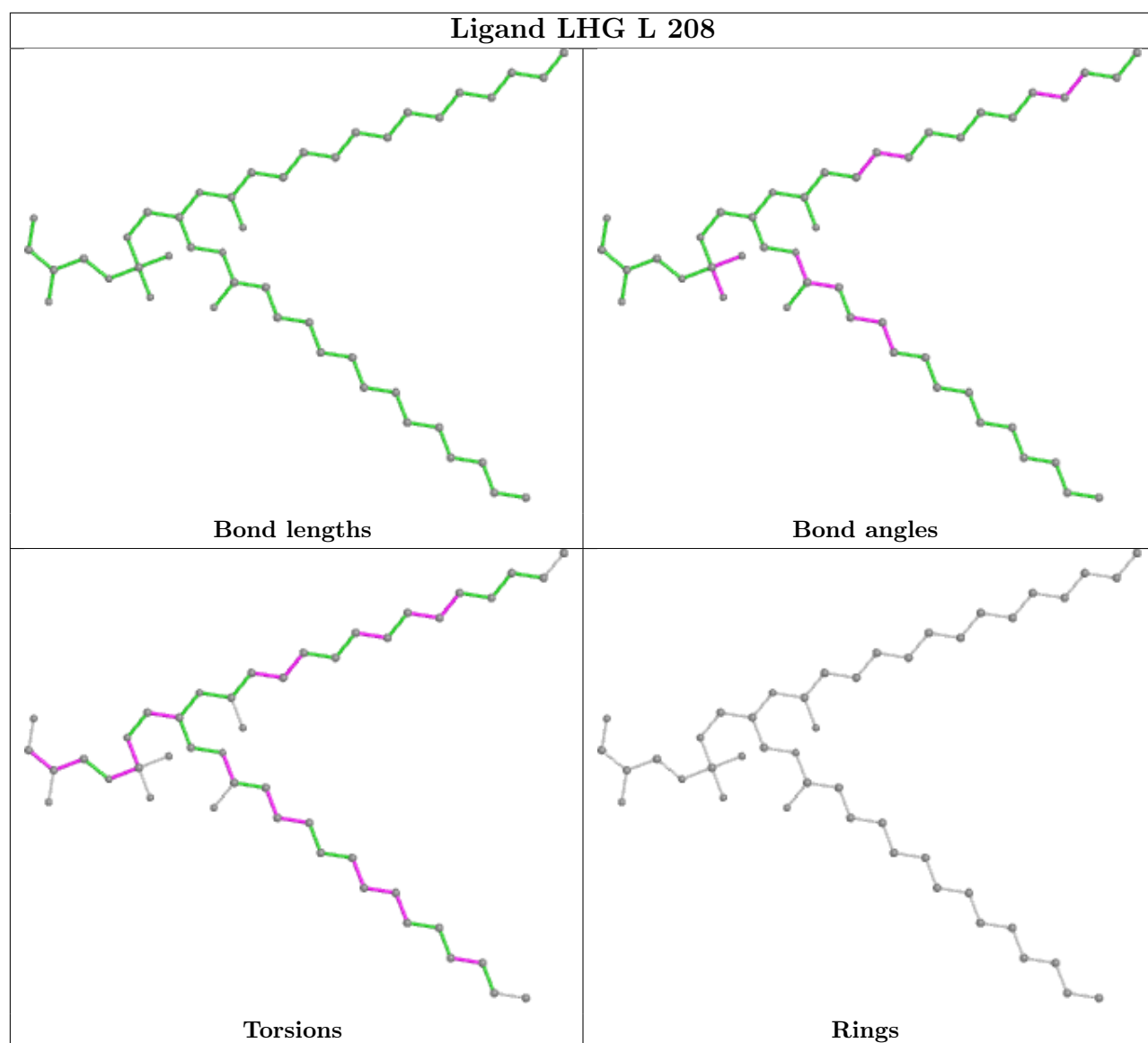


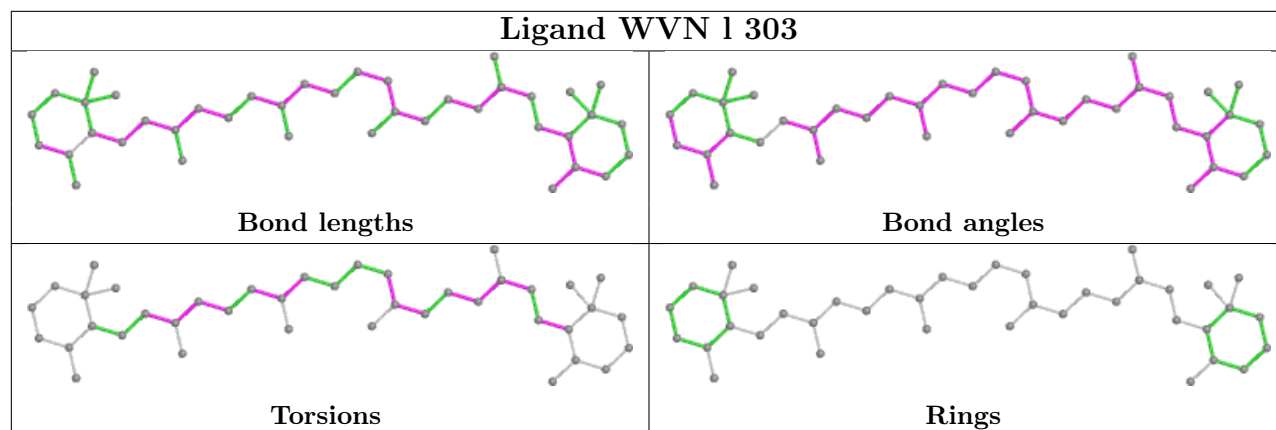
Torsions



Rings







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.

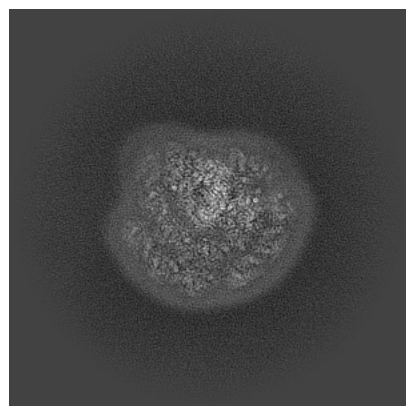
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62717. These allow visual inspection of the internal detail of the map and identification of artifacts.

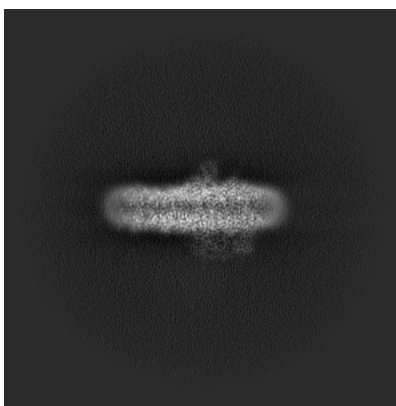
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

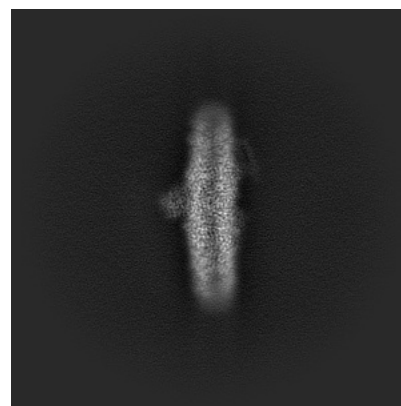
6.1.1 Primary map



X

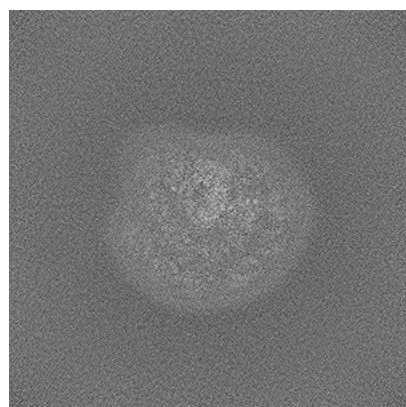


Y

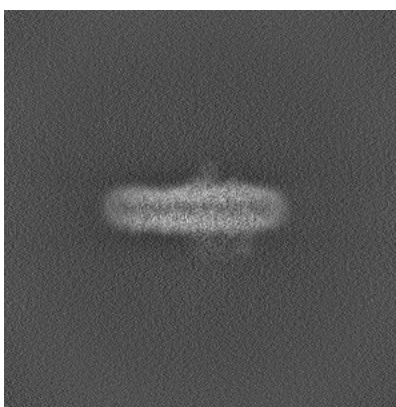


Z

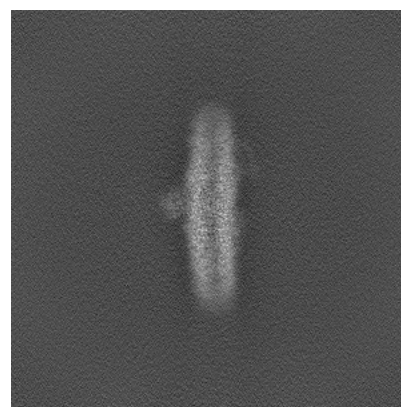
6.1.2 Raw map



X



Y

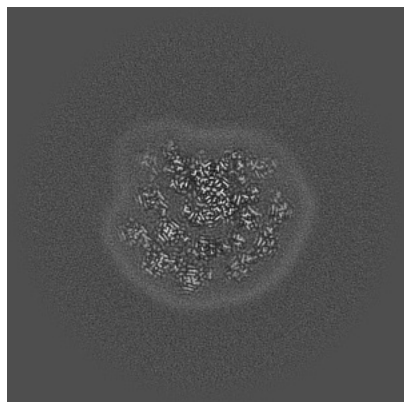


Z

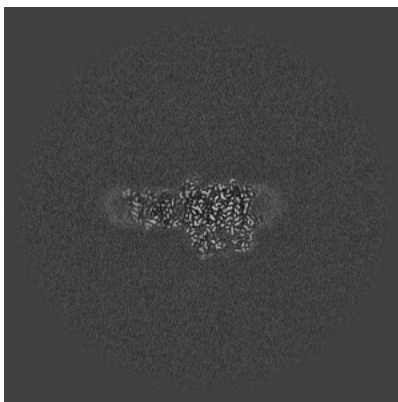
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

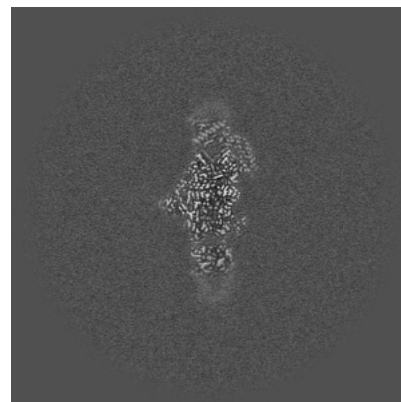
6.2.1 Primary map



X Index: 300

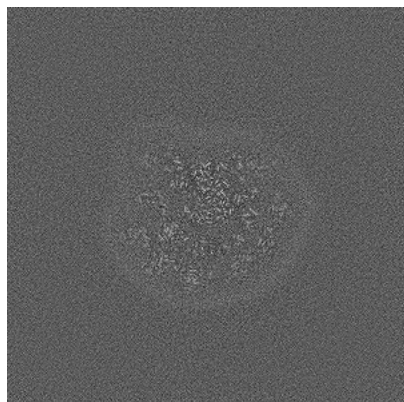


Y Index: 300

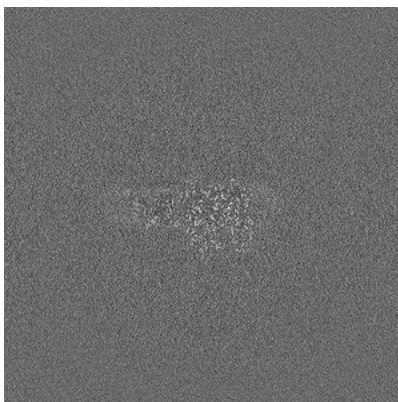


Z Index: 300

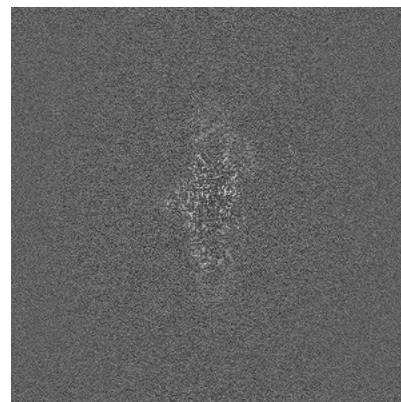
6.2.2 Raw map



X Index: 300



Y Index: 300

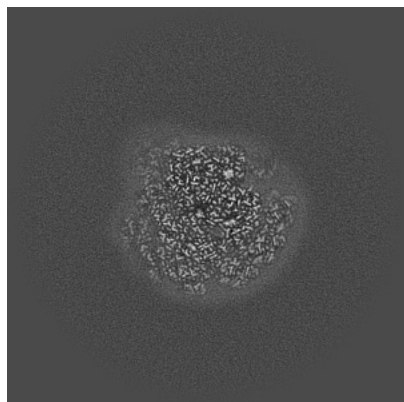


Z Index: 300

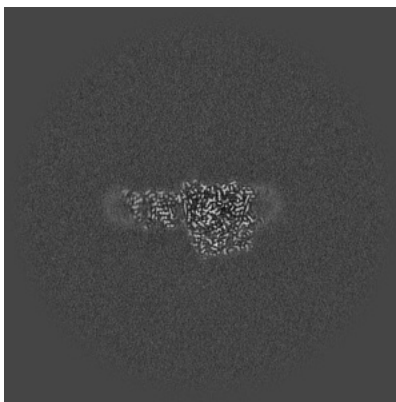
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

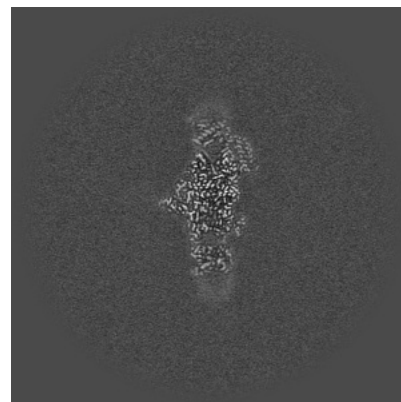
6.3.1 Primary map



X Index: 282

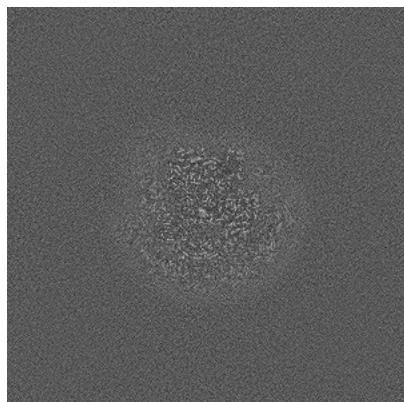


Y Index: 304

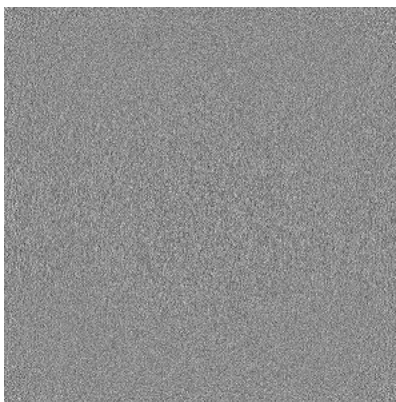


Z Index: 301

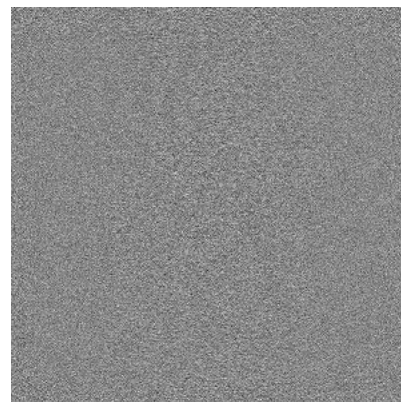
6.3.2 Raw map



X Index: 284



Y Index: 0

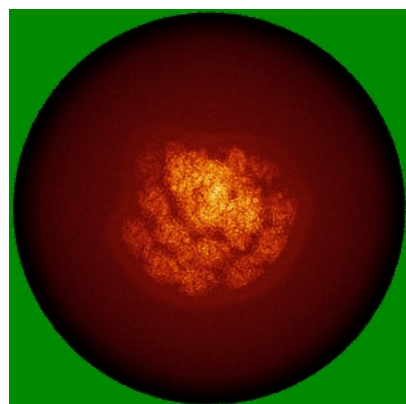


Z Index: 0

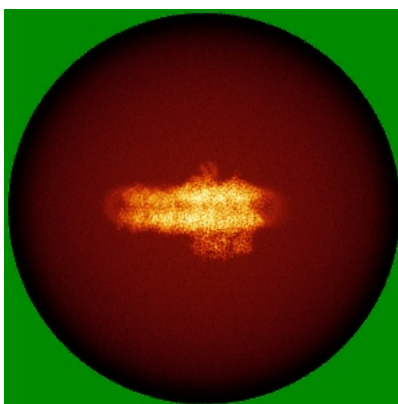
The images above show the largest variance slices of the map in three orthogonal directions.

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

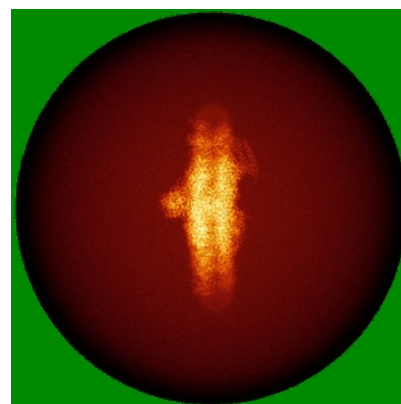
6.4.1 Primary map



X

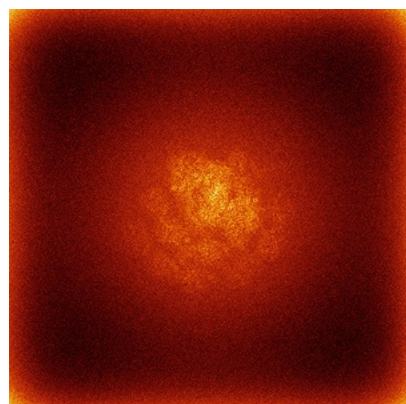


Y

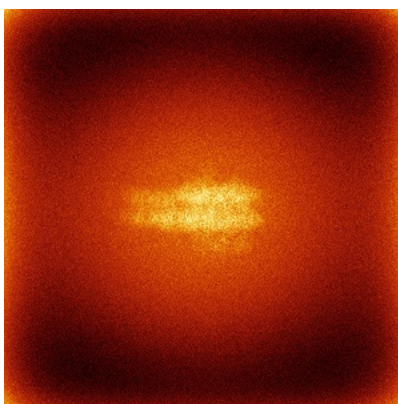


Z

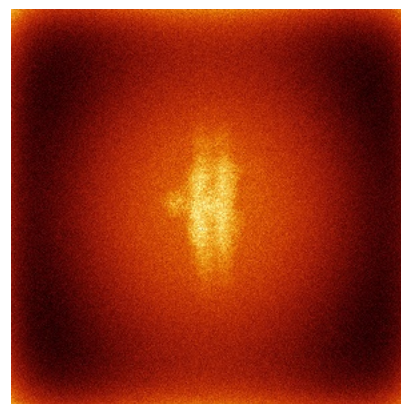
6.4.2 Raw map



X



Y

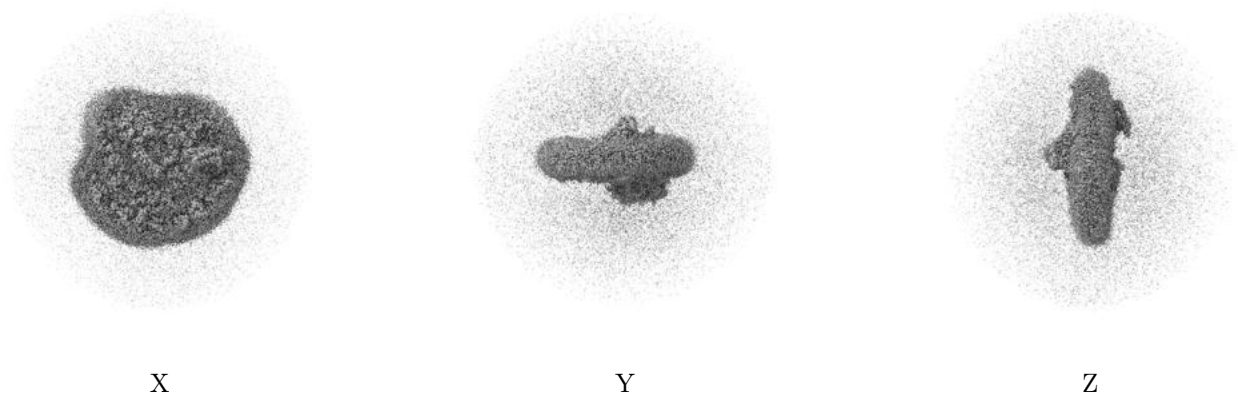


Z

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

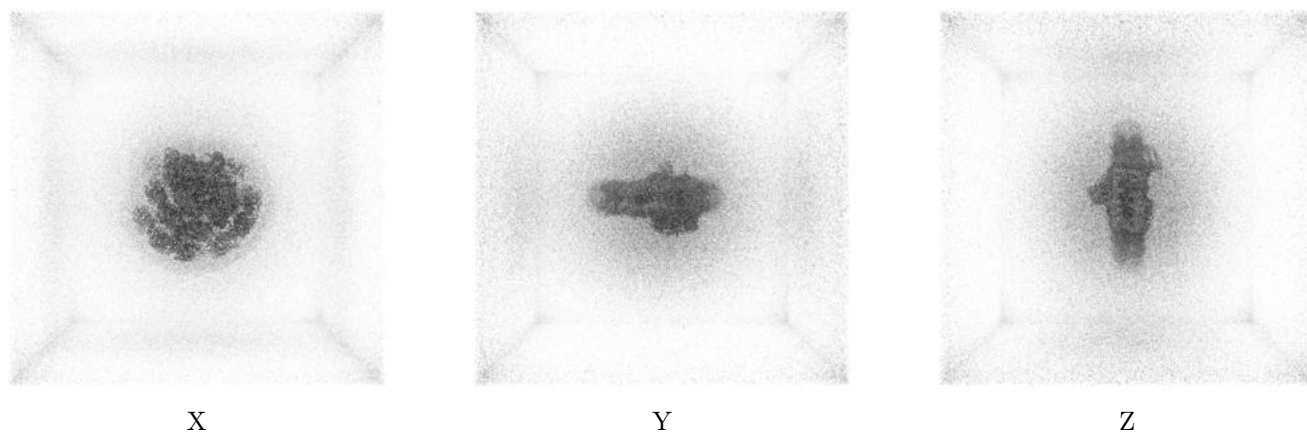
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

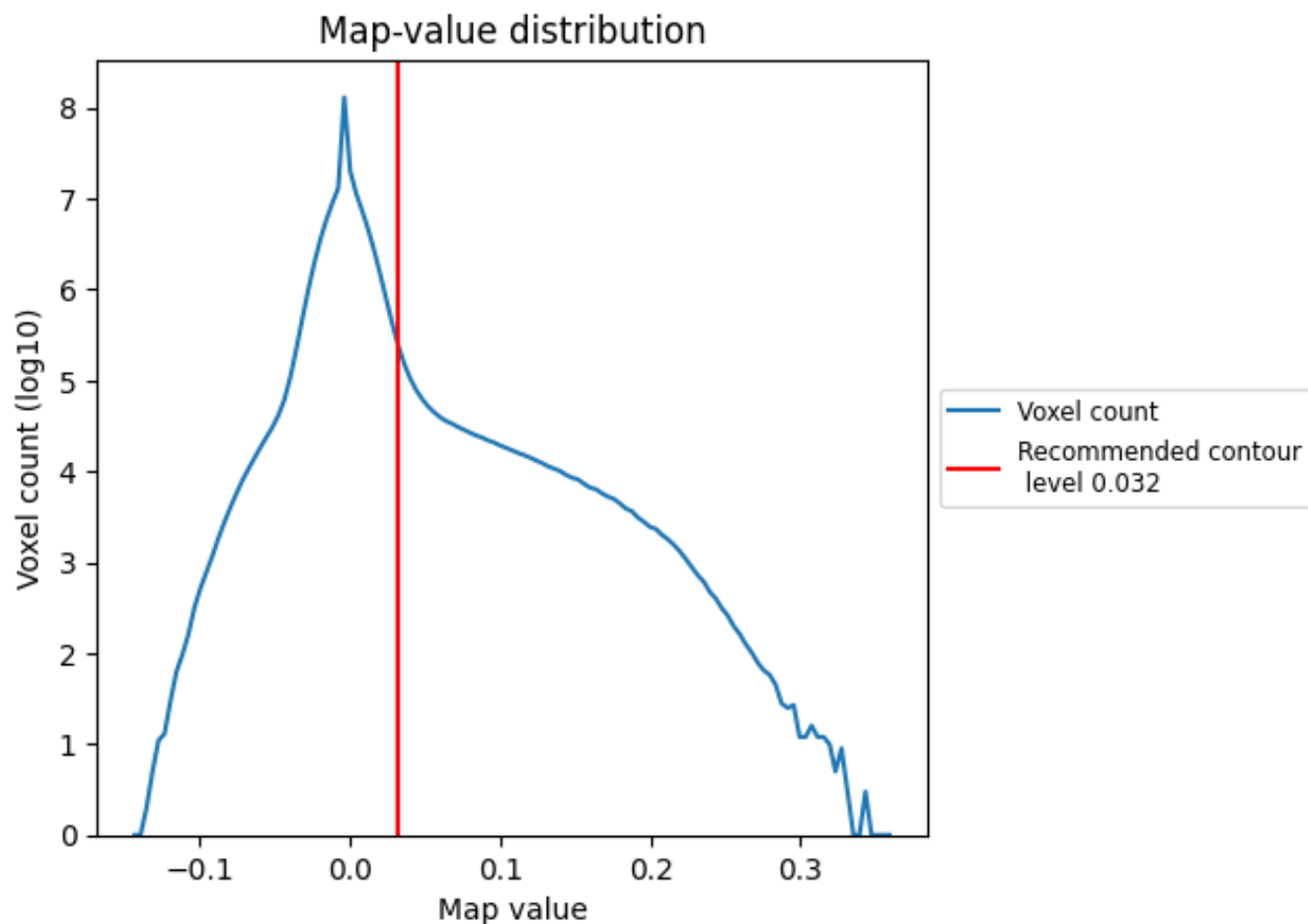
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

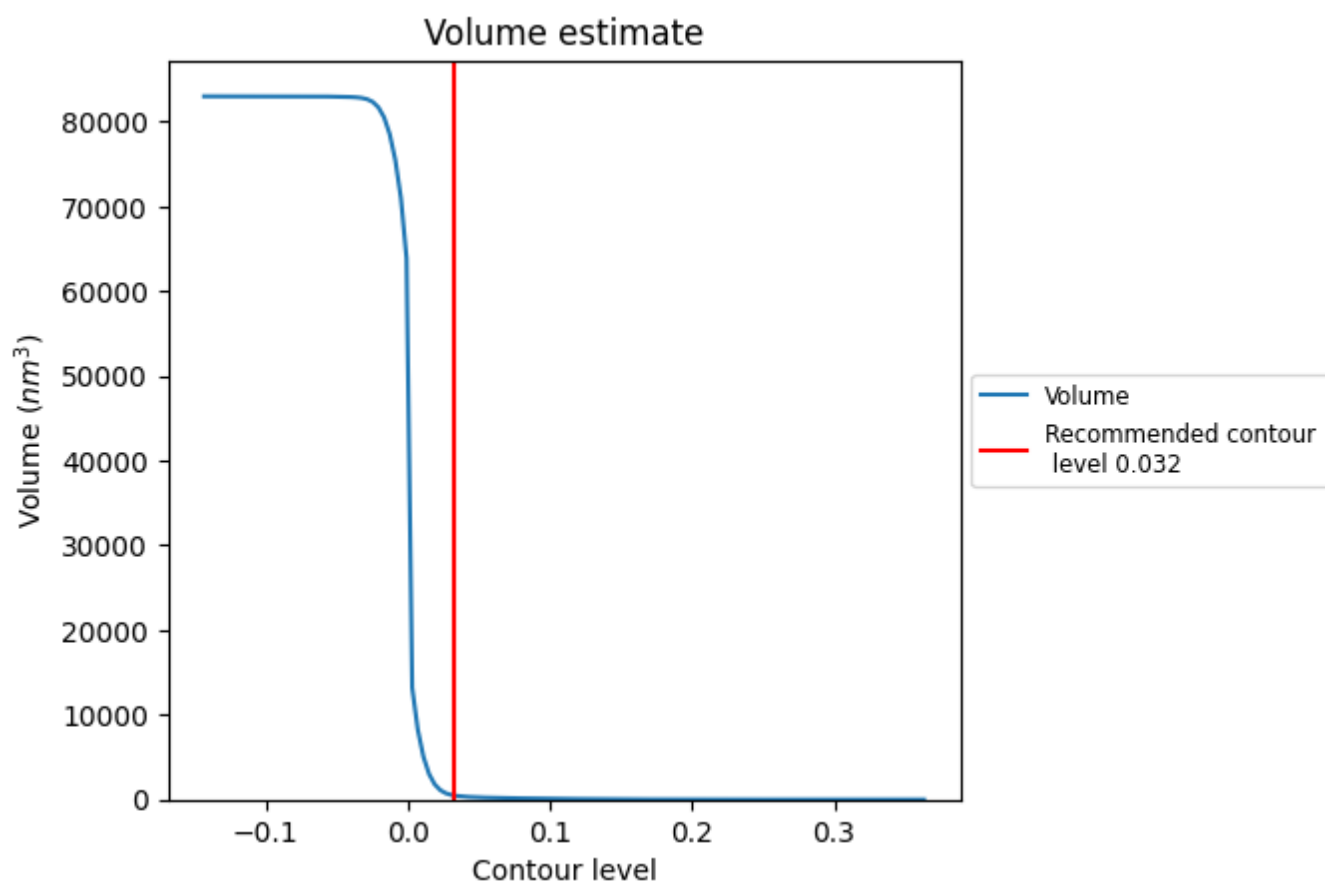
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

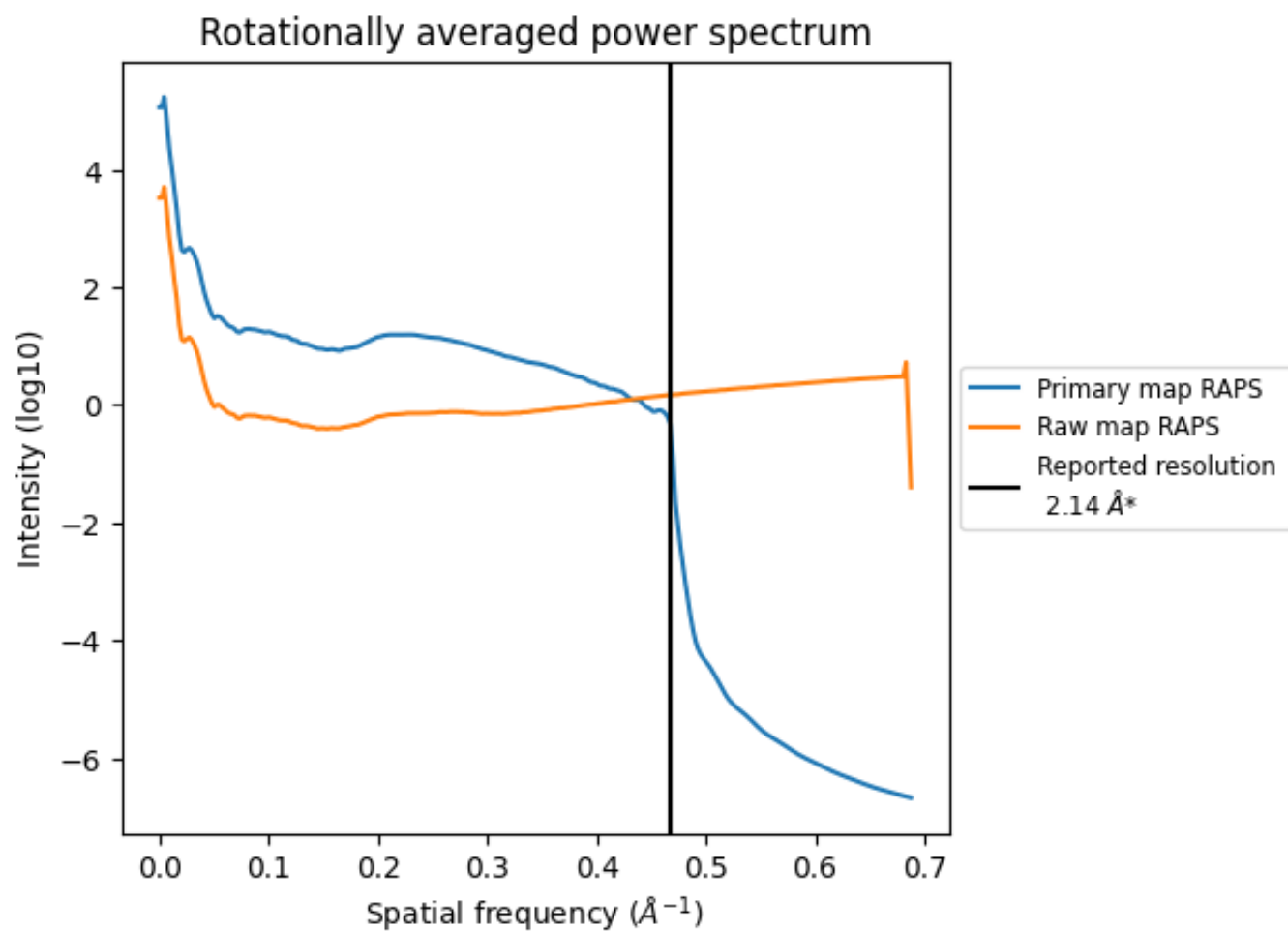
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 505 nm^3 ; this corresponds to an approximate mass of 456 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

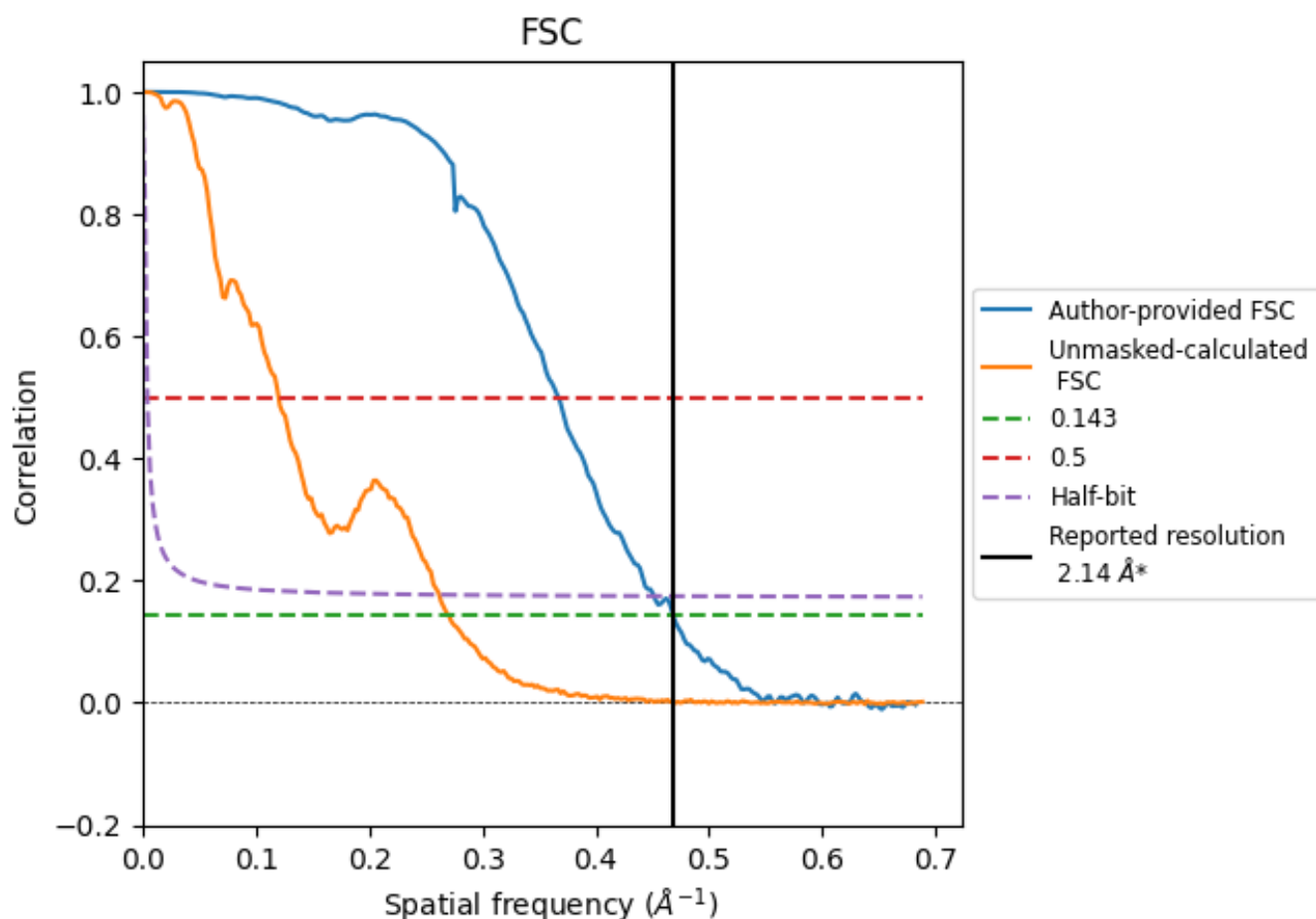


*Reported resolution corresponds to spatial frequency of 0.467 \AA^{-1}

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 0.467 \AA^{-1}

8.2 Resolution estimates [i](#)

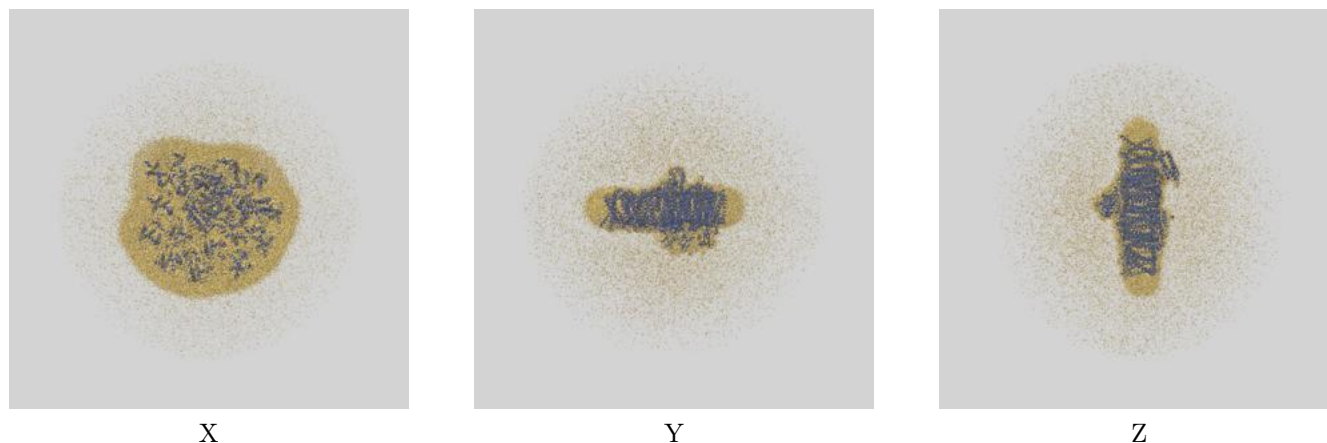
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.72	2.22
Unmasked-calculated*	3.70	8.31	3.82

*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 3.70 differs from the reported value 2.14 by more than 10 %

9 Map-model fit [i](#)

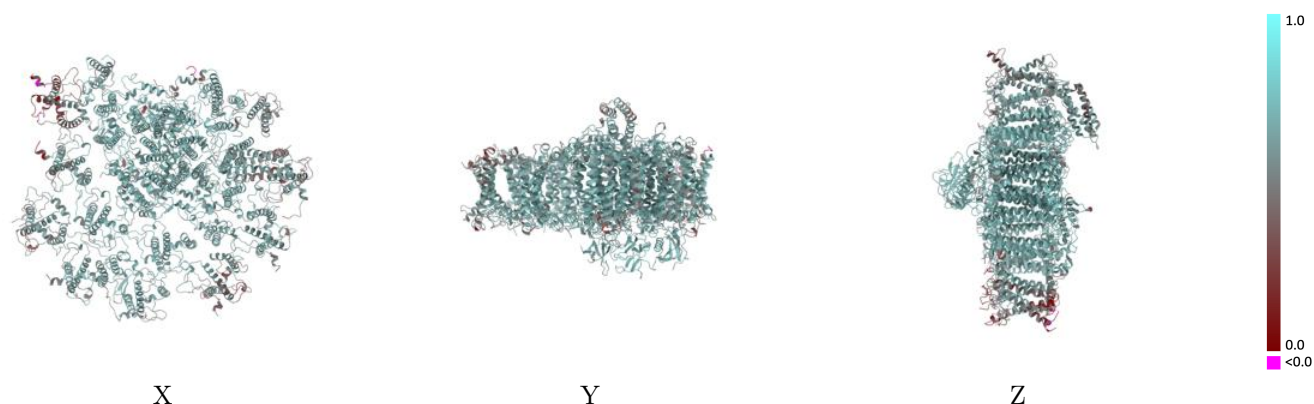
This section contains information regarding the fit between EMDB map EMD-62717 and PDB model 9L0K. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



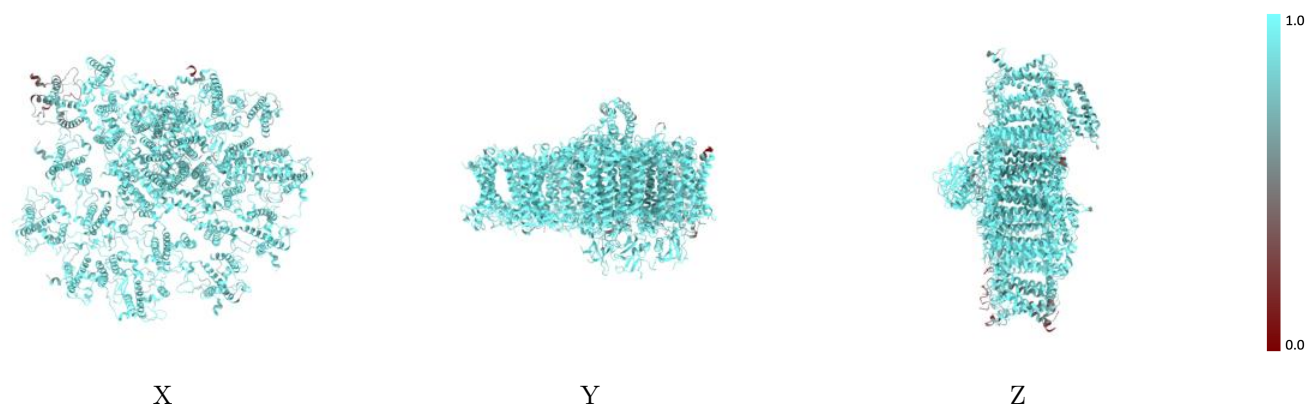
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



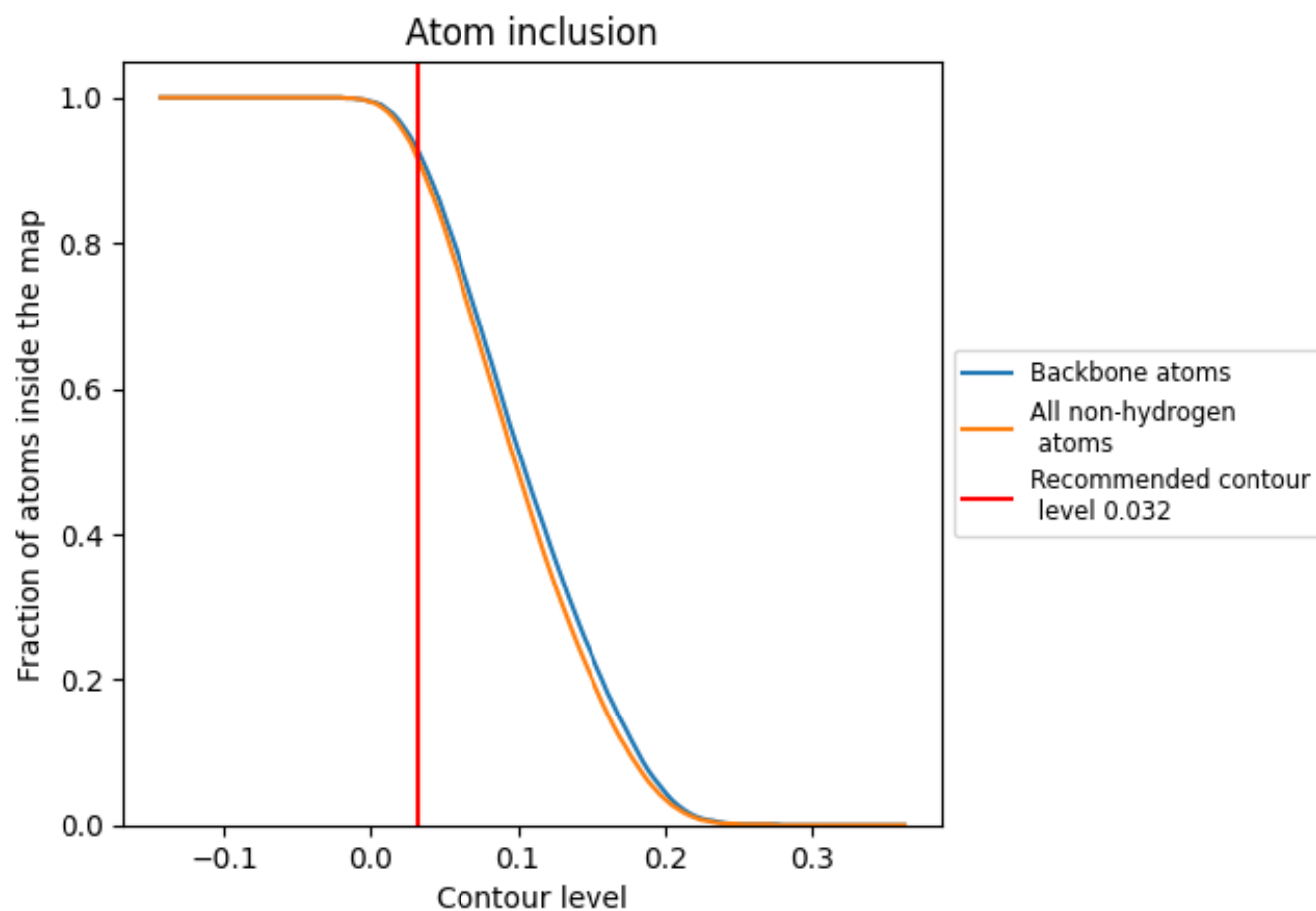
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.5980
A	 0.9610	 0.6550
B	 0.9750	 0.6640
C	 0.9950	 0.6790
D	 0.9640	 0.6460
E	 0.9450	 0.6280
F	 0.9520	 0.6390
I	 0.9660	 0.6490
J	 0.9700	 0.6370
K	 0.8450	 0.5340
L	 0.8130	 0.5460
M	 0.9400	 0.6280
Q	 0.8540	 0.5510
R	 0.9550	 0.6290
a	 0.9590	 0.6410
b	 0.9530	 0.6350
c	 0.8870	 0.5640
d	 0.6340	 0.3600
h	 0.8380	 0.5340
i	 0.8560	 0.5200
j	 0.8970	 0.5690
k	 0.8590	 0.4960
l	 0.9280	 0.5910
m	 0.9200	 0.5910
n	 0.8520	 0.5260
s	 0.9320	 0.6120

