



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 02:53 AM UTC

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:

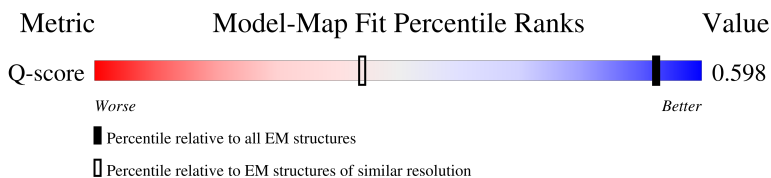
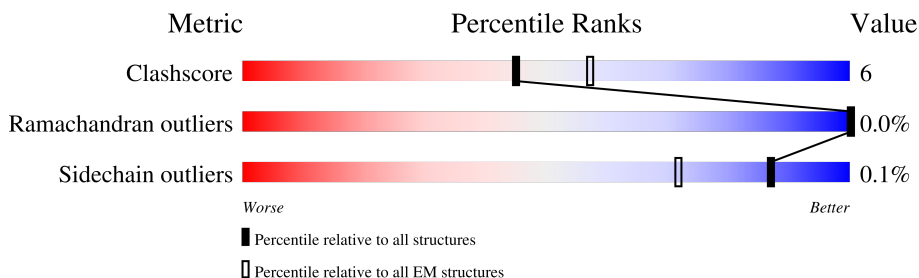
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



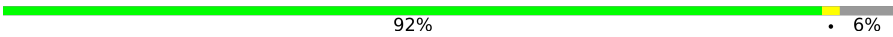
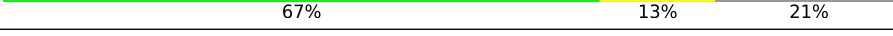
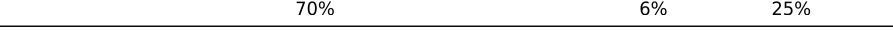
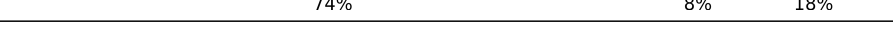
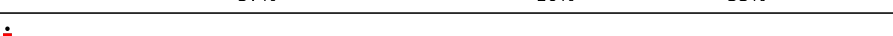
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2493 (1.66 - 2.64)

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	
2	B	734	
3	C	81	
4	D	141	

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	188	
7	I	36	
8	J	42	
9	L	153	
10	M	30	
11	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	405	-	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		

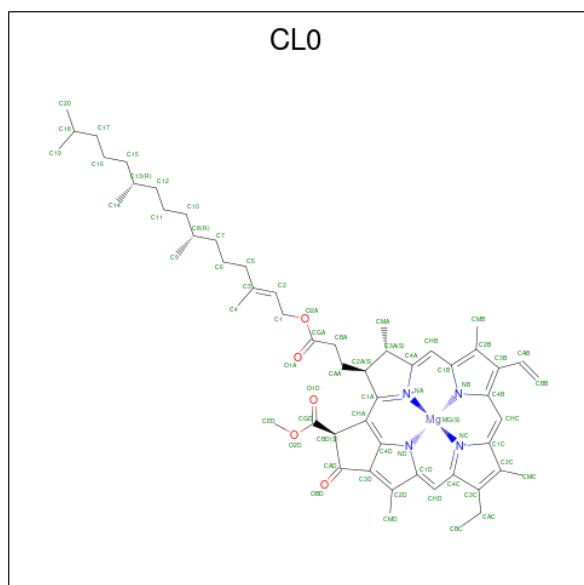
- Molecule 23 is a protein called ACPI-n.

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

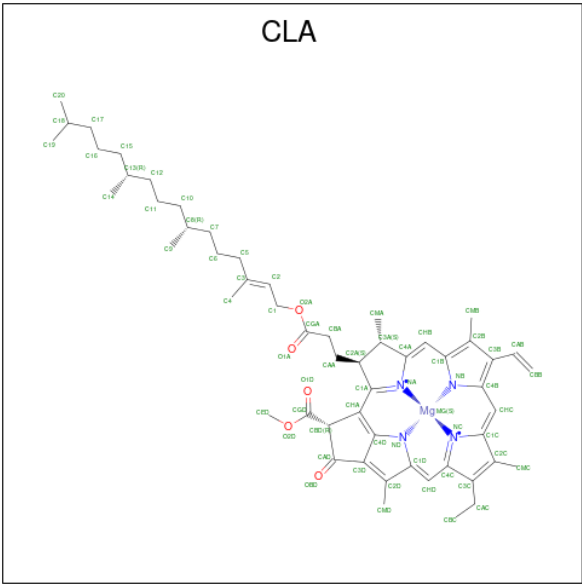
- Molecule 24 is a protein called PsaQ.

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).



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

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

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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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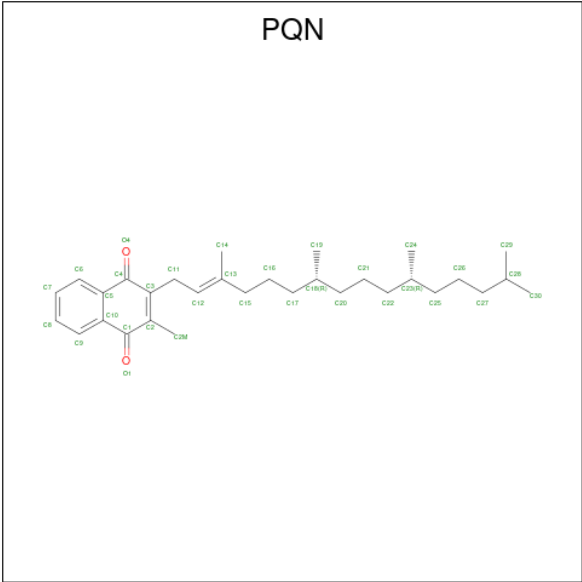
Mol	Chain	Residues	Atoms					AltConf
26	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	j	1	Total 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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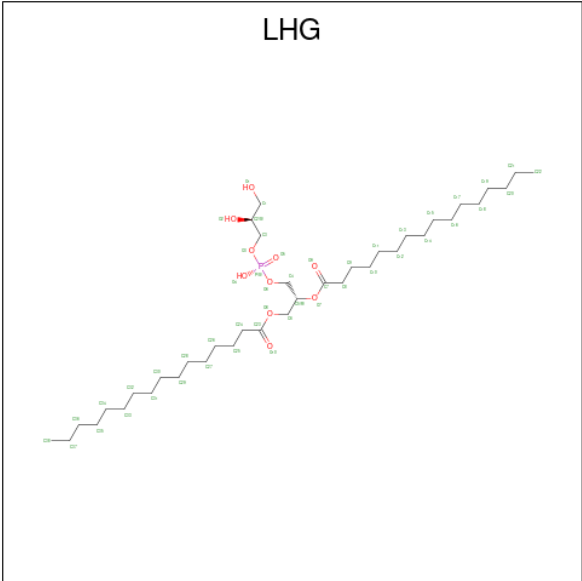
Mol	Chain	Residues	Atoms					AltConf
26	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			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).



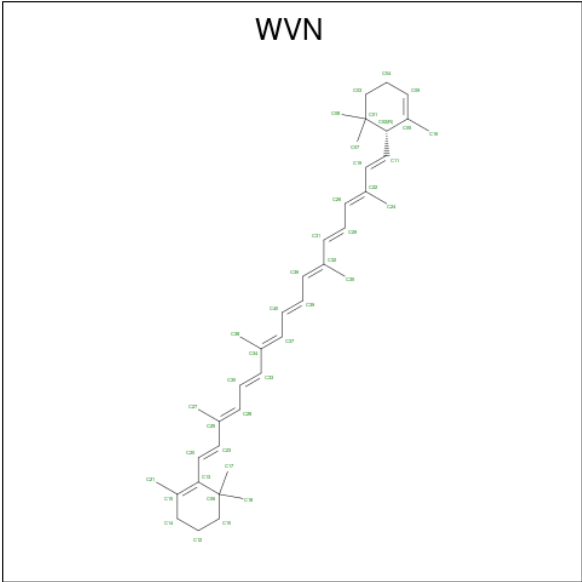
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	37	10	1	

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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).



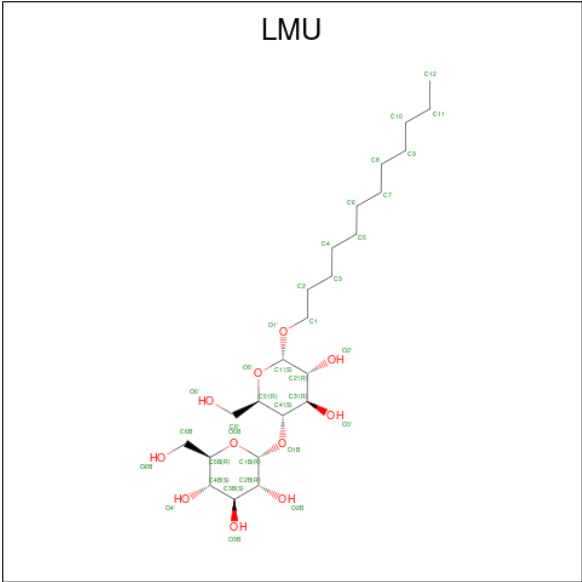
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
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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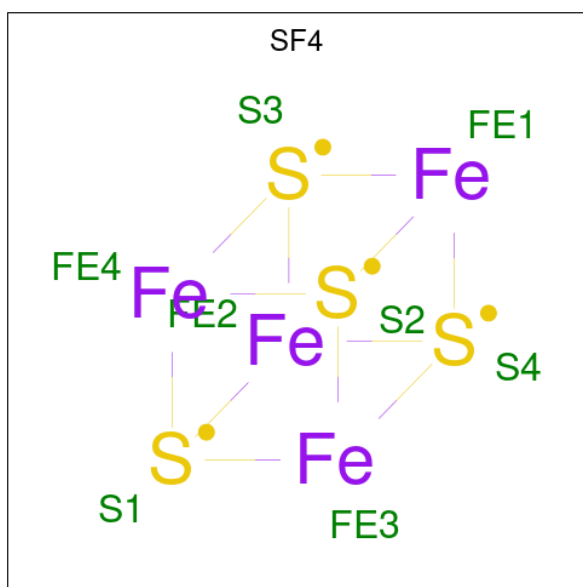
Mol	Chain	Residues	Atoms	AltConf
29	I	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	M	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	s	1	Total C 40 40	0
29	s	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	l	1	Total C 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: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



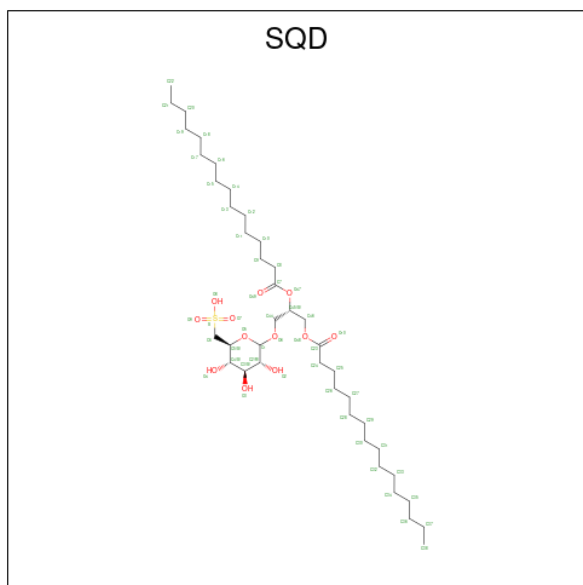
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			35	24	11	
30	A	1	Total	C	O	0
			34	23	11	
30	B	1	Total	C	O	0
			35	24	11	
30	a	1	Total	C	O	0
			35	24	11	
30	i	1	Total	C	O	0
			35	24	11	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



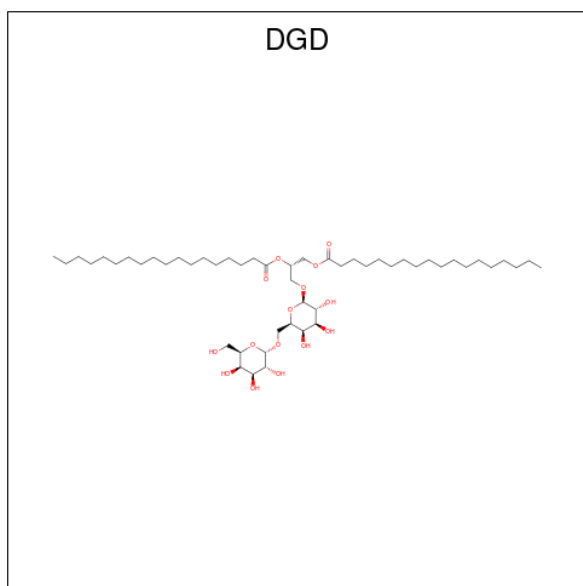
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



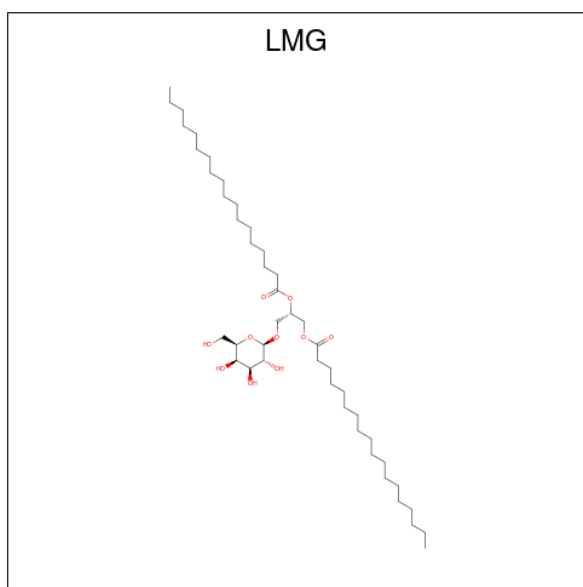
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			54	41	12	1	

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



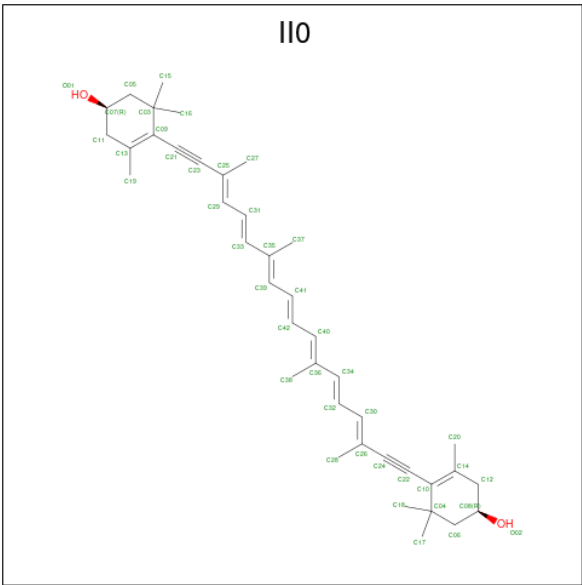
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O		0
			66	51	15		
33	j	1	Total	C	O		0
			62	47	15		

- 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: $C_{40}H_{52}O_2$) (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 42	C 40	O 2	0
35	d	1	Total 42	C 40	O 2	0
35	d	1	Total 42	C 40	O 2	0
35	d	1	Total 42	C 40	O 2	0
35	d	1	Total 42	C 40	O 2	0
35	d	1	Total 42	C 40	O 2	0
35	n	1	Total 42	C 40	O 2	0
35	n	1	Total 42	C 40	O 2	0
35	n	1	Total 42	C 40	O 2	0
35	n	1	Total 42	C 40	O 2	0

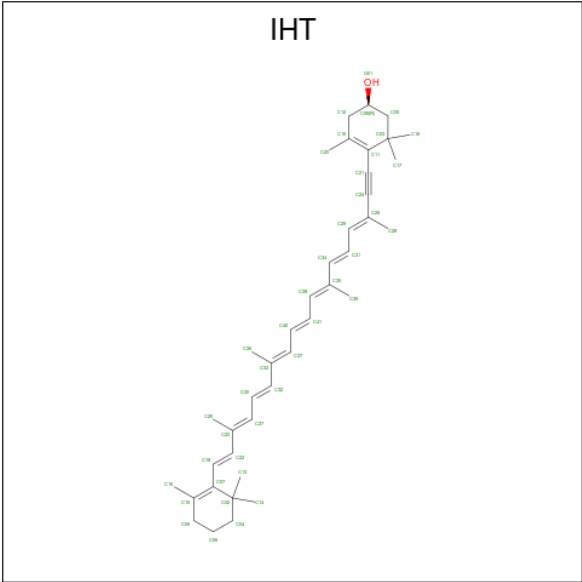
- ## KC2



Continued from previous page...

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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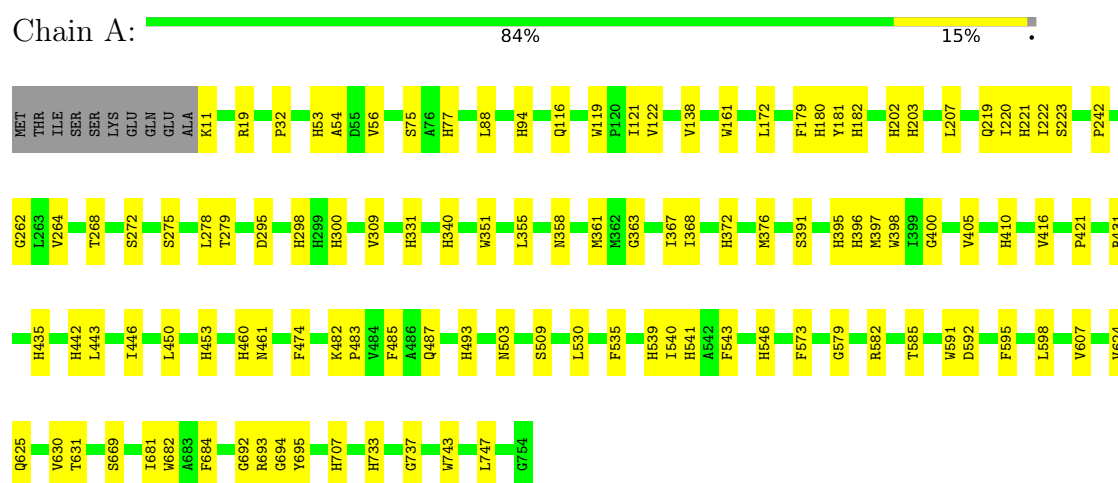
Continued from previous page...

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

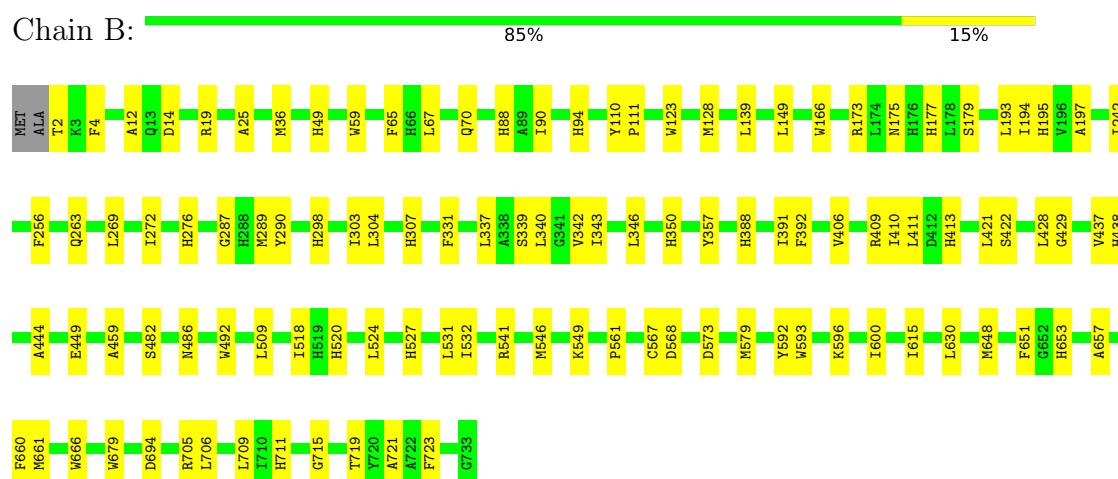
3 Residue-property plots

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.

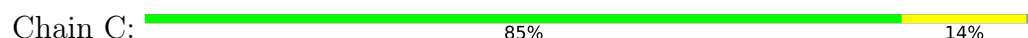
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- 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%



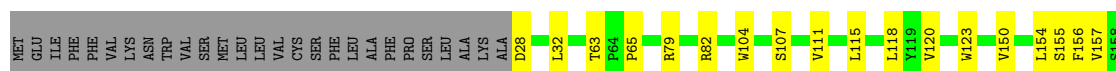
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 92% 6%



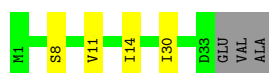
- Molecule 6: Photosystem I reaction center subunit III

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%



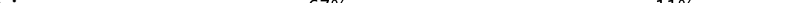
- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 6% 90% 8%

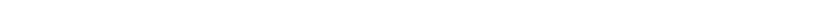


- Molecule 10: Photosystem I reaction center subunit XII

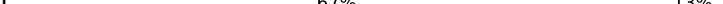
A diagram of a protein structure represented as a horizontal bar. The bar is divided into segments by vertical lines. The segments are labeled from left to right: M1, I7, L13, A21, L28, Y29, and Q30. The segments for M1, I7, L13, A21, and L28 are yellow, while the segments for Y29 and Q30 are green.

- Chain K: 

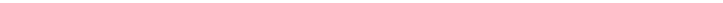
MET	ASN	ALA	ASP	LEU	LEU	ILE	ALA	LEU	V10	P11	Q12	T13	W16	I32	K42	GLY	THR	GLY	PRO	SER	LEU	PRO	ILE	SER	G52	S53	S54	A55	G56	F57	L62	S65	L80	S81	Y82	V83	L86	SER
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- Chain s:  47% . 49%

[illegible]

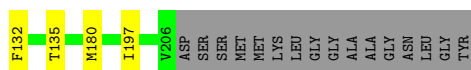
- Chain c:  67% 13% 21%

MET	LEU	ARG	THR	ALA	LEU	ILE	ALA	CYS	VAL	ALA	SER	ALA	SER	ALA	PHE	ALA	PRO	GLY	PHE	ALA	PRO	MET	ALA	LYS	SER	ARG	SER	SER	VAL	ALA	SER	SER	MET	ARG	MET	GLN	GLU	GLY	D43	F44	S45	A46	A47	V48	F49	F50		V65		G89		G98		Q102		P111	F115
M113		Q125		T149		R154	E155		D158		L166		H183	A194	R195		M188		H196		V200	T201	K202	Q203		L206	E207	Q208	L209		F212	LYS	SER	SER	LEU	ALA																					

- Chain a:  72% 7% 21%

[illegible]

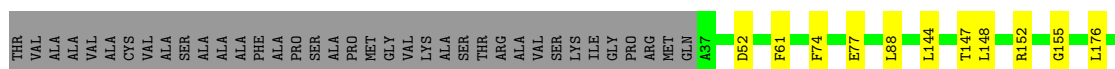
- Chain b:  70% 6% 25%



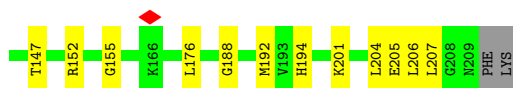
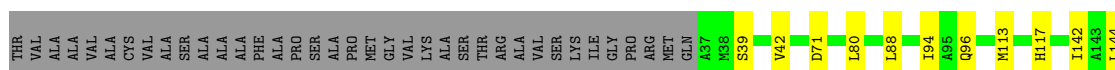
Chain h:



Chain m:



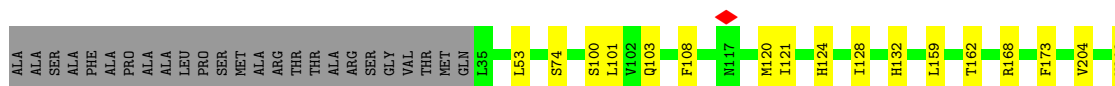
Chain j:

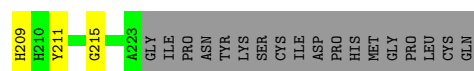


Chain 1:



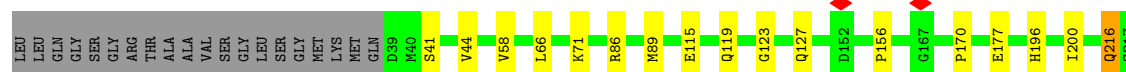
Chain k:





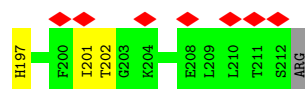
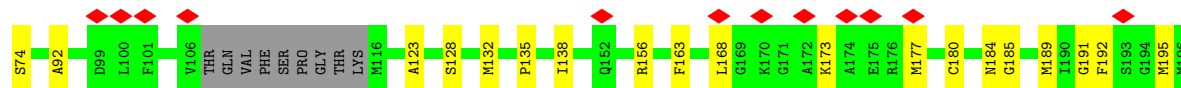
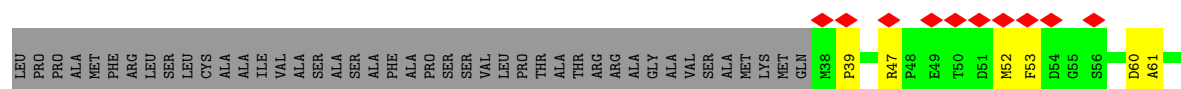
- Molecule 20: ACPI-i

Chain i: 81% 8% 10%



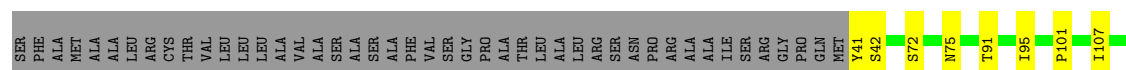
- Molecule 21: ACPI-d

Chain d: 13% 63% 13% 24%



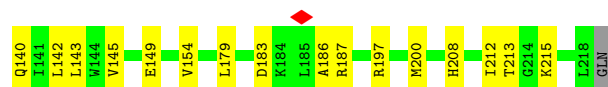
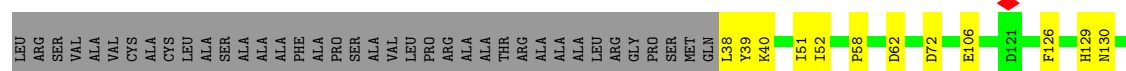
- Molecule 22: PsaR

Chain R: 57% 10% 33%



- Molecule 23: ACPI-n

Chain n: 70% 13% 18%



- 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	ALA	VAL	PRO	ALA	ILE	ALA	GLY	ALA	SER	LEU	ASP	PRO	LYS	THR	GLY	PHE
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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 ($\text{\AA}$)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.727, 0.727, 0.727	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, SF4, WVN, LHG, LMU, DGD, KC2, CLA, IHT, II0, PQN, LMG, SQD

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%)	9	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%)	55	61
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%)	76	81
20	i	142/156 (91%)	141 (99%)	1 (1%)	76	81
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%)	87	92

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	$\# Z > 2$
26	CLA	A	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
28	LHG	A	843	-	47,47,48	0.63	1 (2%)	50,53,54	1.25	5 (10%)
26	CLA	B	836	38	69,73,73	1.19	8 (11%)	82,113,113	1.29	7 (8%)
29	WVN	A	845	-	40,41,41	4.59	21 (52%)	51,56,56	6.26	33 (64%)
26	CLA	J	103	8	46,50,73	1.43	7 (15%)	53,85,113	1.47	4 (7%)
36	KC2	k	611	19	49,53,53	1.40	7 (14%)	60,89,89	0.99	2 (3%)
26	CLA	B	827	2	55,59,73	1.33	8 (14%)	64,96,113	1.48	8 (12%)
26	CLA	c	312	13	69,73,73	1.18	7 (10%)	82,113,113	1.23	4 (4%)
26	CLA	B	837	2	69,73,73	1.20	6 (8%)	82,113,113	1.22	4 (4%)
26	CLA	n	607	23	69,73,73	1.17	8 (11%)	82,113,113	1.17	6 (7%)
29	WVN	A	847	-	40,41,41	4.36	19 (47%)	51,56,56	6.85	35 (68%)
26	CLA	b	304	15	59,63,73	1.26	6 (10%)	70,101,113	1.41	9 (12%)
26	CLA	a	311	14	52,56,73	1.35	6 (11%)	61,92,113	1.37	4 (6%)
36	KC2	k	613	-	49,53,53	1.40	7 (14%)	60,89,89	0.89	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMU	a	317	-	36,36,36	0.19	0	47,47,47	0.47	0
26	CLA	d	303	21	55,59,73	1.32	7 (12%)	64,96,113	1.42	7 (10%)
26	CLA	k	601	19	55,59,73	1.33	7 (12%)	64,96,113	1.43	6 (9%)
35	II0	k	620	-	39,43,43	5.70	22 (56%)	48,60,60	8.12	27 (56%)
29	WVN	B	845	-	40,41,41	0.14	0	51,56,56	0.44	0
37	IHT	n	617	-	40,42,42	0.22	0	52,58,58	0.55	0
26	CLA	k	607	19	55,59,73	1.32	6 (10%)	64,96,113	1.39	7 (10%)
35	II0	b	314	-	39,43,43	5.67	20 (51%)	48,60,60	8.08	29 (60%)
37	IHT	b	316	-	40,42,42	0.27	0	52,58,58	0.75	1 (1%)
26	CLA	L	202	9	53,57,73	1.34	8 (15%)	61,93,113	1.41	5 (8%)
26	CLA	k	606	19	55,59,73	1.31	6 (10%)	64,96,113	1.38	5 (7%)
26	CLA	A	810	1	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
26	CLA	A	833	1	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
26	CLA	d	310	21	45,49,73	1.42	6 (13%)	54,84,113	1.45	5 (9%)
26	CLA	A	851	38	69,73,73	1.18	8 (11%)	82,113,113	1.21	4 (4%)
26	CLA	a	304	38	69,73,73	1.17	6 (8%)	82,113,113	1.28	6 (7%)
27	PQN	B	843	-	34,34,34	3.08	13 (38%)	43,45,45	1.95	6 (13%)
26	CLA	k	614	19	55,59,73	1.33	7 (12%)	64,96,113	1.41	4 (6%)
35	II0	h	311	-	39,43,43	5.62	20 (51%)	48,60,60	8.16	28 (58%)
26	CLA	b	307	15	65,69,73	1.21	7 (10%)	77,108,113	1.28	5 (6%)
26	CLA	b	312	15	69,73,73	1.17	6 (8%)	82,113,113	1.25	4 (4%)
26	CLA	k	608	19	69,73,73	1.18	9 (13%)	82,113,113	1.21	5 (6%)
26	CLA	n	608	-	69,73,73	1.18	8 (11%)	82,113,113	1.19	9 (10%)
36	KC2	s	404	-	49,53,53	1.49	8 (16%)	60,89,89	0.83	0
26	CLA	A	822	1	60,64,73	1.27	7 (11%)	71,102,113	1.36	5 (7%)
28	LHG	s	409	-	32,32,48	0.82	3 (9%)	35,37,54	1.65	4 (11%)
28	LHG	L	208	-	44,44,48	0.65	2 (4%)	47,50,54	1.28	5 (10%)
35	II0	a	316	-	39,43,43	5.98	22 (56%)	48,60,60	8.19	29 (60%)
26	CLA	b	309	34	69,73,73	1.18	6 (8%)	82,113,113	1.28	4 (4%)
26	CLA	i	311	20	69,73,73	1.18	6 (8%)	82,113,113	1.28	6 (7%)
29	WVN	K	102	-	40,41,41	4.40	18 (45%)	51,56,56	6.64	34 (66%)
26	CLA	B	814	2	69,73,73	1.16	6 (8%)	82,113,113	1.24	6 (7%)
26	CLA	m	603	17	63,67,73	1.24	8 (12%)	74,105,113	1.28	5 (6%)
26	CLA	k	609	19	61,65,73	1.28	7 (11%)	72,103,113	1.37	5 (6%)
26	CLA	c	301	13	55,59,73	1.31	5 (9%)	64,96,113	1.41	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	F	205	-	53,53,55	0.74	0	61,61,63	1.34	8 (13%)
26	CLA	a	301	14	69,73,73	1.19	8 (11%)	82,113,113	1.35	5 (6%)
26	CLA	n	601	23	49,53,73	1.40	8 (16%)	58,89,113	1.44	5 (8%)
26	CLA	A	812	1	69,73,73	1.18	6 (8%)	82,113,113	1.28	4 (4%)
34	LMG	F	206	-	41,41,55	0.85	0	49,49,63	1.26	3 (6%)
26	CLA	A	836	1	69,73,73	1.19	7 (10%)	82,113,113	1.30	4 (4%)
26	CLA	A	830	1	64,68,73	1.23	8 (12%)	76,107,113	1.30	4 (5%)
26	CLA	L	203	9	69,73,73	1.17	8 (11%)	82,113,113	1.34	8 (9%)
26	CLA	A	837	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
28	LHG	A	855	-	35,35,48	0.70	0	38,41,54	1.28	4 (10%)
26	CLA	n	603	23	55,59,73	1.34	7 (12%)	64,96,113	1.38	7 (10%)
26	CLA	A	824	38	69,73,73	1.18	7 (10%)	82,113,113	1.35	6 (7%)
26	CLA	A	828	1	69,73,73	1.18	6 (8%)	82,113,113	1.24	5 (6%)
26	CLA	B	804	-	69,73,73	1.18	10 (14%)	82,113,113	1.61	11 (13%)
26	CLA	n	604	23	64,68,73	1.21	5 (7%)	76,107,113	1.44	7 (9%)
26	CLA	R	201	22	59,63,73	1.30	7 (11%)	70,101,113	1.48	7 (10%)
26	CLA	h	302	16	54,58,73	1.33	8 (14%)	64,95,113	1.43	8 (12%)
26	CLA	h	313	38	69,73,73	1.18	8 (11%)	82,113,113	1.23	7 (8%)
26	CLA	d	308	21	50,54,73	1.38	7 (14%)	59,90,113	1.33	4 (6%)
34	LMG	c	318	-	55,55,55	0.70	0	63,63,63	1.38	9 (14%)
26	CLA	k	604	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	7 (8%)
26	CLA	A	825	38	69,73,73	1.17	7 (10%)	82,113,113	1.29	9 (10%)
26	CLA	B	812	2	69,73,73	1.19	8 (11%)	82,113,113	1.32	7 (8%)
26	CLA	L	206	-	55,59,73	1.32	7 (12%)	64,96,113	1.34	4 (6%)
26	CLA	m	610	28	59,63,73	1.28	7 (11%)	70,101,113	1.36	5 (7%)
26	CLA	d	305	-	55,59,73	1.33	6 (10%)	64,96,113	1.42	6 (9%)
26	CLA	j	610	28	65,69,73	1.22	7 (10%)	77,108,113	1.31	4 (5%)
35	II0	J	104	-	39,43,43	5.71	20 (51%)	48,60,60	8.19	28 (58%)
26	CLA	i	301	20	69,73,73	1.19	7 (10%)	82,113,113	1.29	5 (6%)
26	CLA	A	841	1	69,73,73	1.19	6 (8%)	82,113,113	1.37	11 (13%)
26	CLA	h	305	16	55,59,73	1.32	7 (12%)	64,96,113	1.33	7 (10%)
26	CLA	a	303	14	55,59,73	1.34	9 (16%)	64,96,113	1.46	7 (10%)
26	CLA	B	811	2	59,63,73	1.29	7 (11%)	70,101,113	1.31	5 (7%)
26	CLA	d	304	-	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
26	CLA	h	304	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	j	605	17	49,53,73	1.42	7 (14%)	58,89,113	1.55	6 (10%)
26	CLA	j	613	17	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
26	CLA	d	306	21	55,59,73	1.34	7 (12%)	64,96,113	1.39	4 (6%)
36	KC2	i	309	20	49,53,53	1.39	7 (14%)	60,89,89	1.07	3 (5%)
26	CLA	h	307	16	61,65,73	1.26	6 (9%)	72,103,113	1.39	6 (8%)
26	CLA	B	823	38	68,72,73	1.18	8 (11%)	80,111,113	1.26	7 (8%)
35	II0	k	617	-	39,43,43	0.21	0	48,60,60	0.35	0
29	WVN	B	846	-	40,41,41	4.36	20 (50%)	51,56,56	6.70	35 (68%)
29	WVN	B	848	-	40,41,41	4.47	19 (47%)	51,56,56	6.48	34 (66%)
26	CLA	A	815	38	49,53,73	1.40	8 (16%)	58,89,113	1.49	5 (8%)
26	CLA	F	201	38	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
26	CLA	c	306	13	56,60,73	1.31	8 (14%)	65,97,113	1.28	5 (7%)
36	KC2	l	312	18	49,53,53	1.41	8 (16%)	60,89,89	0.94	1 (1%)
26	CLA	a	302	14	60,64,73	1.24	7 (11%)	71,102,113	1.34	7 (9%)
26	CLA	A	838	1	69,73,73	1.19	5 (7%)	82,113,113	1.25	5 (6%)
29	WVN	s	407	-	40,41,41	4.44	20 (50%)	51,56,56	6.75	34 (66%)
26	CLA	B	821	2	57,61,73	1.30	7 (12%)	67,98,113	1.31	7 (10%)
26	CLA	A	803	1	59,63,73	1.30	7 (11%)	70,101,113	1.32	7 (10%)
26	CLA	j	602	17	58,62,73	1.27	7 (12%)	68,99,113	1.38	7 (10%)
32	SQD	A	854	-	52,54,54	0.93	3 (5%)	62,65,65	1.64	12 (19%)
37	IHT	a	315	-	40,42,42	0.24	0	52,58,58	0.49	0
26	CLA	B	809	2	69,73,73	1.20	8 (11%)	82,113,113	1.30	4 (4%)
26	CLA	a	305	14	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
26	CLA	B	841	2	69,73,73	1.19	7 (10%)	82,113,113	1.31	5 (6%)
26	CLA	m	607	17	55,59,73	1.32	8 (14%)	64,96,113	1.30	5 (7%)
35	II0	h	310	-	26,28,43	5.64	13 (50%)	30,37,60	8.69	20 (66%)
26	CLA	B	819	2	69,73,73	1.23	7 (10%)	82,113,113	1.40	10 (12%)
29	WVN	B	847	-	40,41,41	4.49	21 (52%)	51,56,56	6.32	34 (66%)
36	KC2	i	318	20	49,53,53	1.40	7 (14%)	60,89,89	0.88	0
26	CLA	B	803	2	69,73,73	1.16	7 (10%)	82,113,113	1.21	7 (8%)
26	CLA	j	606	17	55,59,73	1.34	7 (12%)	64,96,113	1.43	5 (7%)
36	KC2	j	611	17	49,53,53	1.37	6 (12%)	60,89,89	0.95	2 (3%)
29	WVN	I	101	-	40,41,41	4.32	19 (47%)	51,56,56	6.58	34 (66%)
26	CLA	A	805	1	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
35	II0	i	312	-	39,43,43	5.91	21 (53%)	48,60,60	8.11	30 (62%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	832	38	49,53,73	1.41	7 (14%)	58,89,113	1.50	4 (6%)
26	CLA	B	833	2	59,63,73	1.29	7 (11%)	70,101,113	1.39	8 (11%)
26	CLA	i	308	28	50,54,73	1.37	6 (12%)	59,90,113	1.42	4 (6%)
26	CLA	A	808	1	69,73,73	1.19	6 (8%)	82,113,113	1.32	6 (7%)
31	SF4	C	101	3	0,12,12	-	-	-	-	-
34	LMG	L	209	-	45,45,55	0.82	2 (4%)	53,53,63	1.23	3 (5%)
35	II0	n	615	-	39,43,43	5.80	20 (51%)	48,60,60	8.09	28 (58%)
29	WVN	F	203	-	40,41,41	4.42	18 (45%)	51,56,56	6.42	34 (66%)
29	WVN	h	309	-	40,41,41	4.46	20 (50%)	51,56,56	6.39	35 (68%)
26	CLA	s	402	12	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
26	CLA	j	607	17	55,59,73	1.34	6 (10%)	64,96,113	1.48	11 (17%)
26	CLA	A	826	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
26	CLA	B	810	2	69,73,73	1.18	6 (8%)	82,113,113	1.21	6 (7%)
35	II0	i	314	-	39,43,43	5.94	21 (53%)	48,60,60	8.17	29 (60%)
26	CLA	c	309	-	49,53,73	2.36	18 (36%)	58,89,113	4.53	27 (46%)
26	CLA	A	811	1	58,62,73	1.30	7 (12%)	68,99,113	1.33	5 (7%)
29	WVN	l	316	-	40,41,41	4.50	20 (50%)	51,56,56	6.60	33 (64%)
26	CLA	A	813	1	60,64,73	1.28	7 (11%)	71,102,113	1.36	7 (9%)
29	WVN	A	857	-	40,41,41	4.47	20 (50%)	51,56,56	6.60	33 (64%)
34	LMG	Q	301	-	38,38,55	0.85	0	46,46,63	1.24	4 (8%)
26	CLA	B	806	2	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
26	CLA	b	305	15	56,60,73	1.31	6 (10%)	65,97,113	1.41	8 (12%)
35	II0	i	319	-	39,43,43	5.89	21 (53%)	48,60,60	7.91	28 (58%)
26	CLA	i	310	-	64,68,73	1.23	6 (9%)	76,107,113	1.36	4 (5%)
26	CLA	B	822	38	69,73,73	1.20	9 (13%)	82,113,113	1.37	8 (9%)
26	CLA	l	313	18	60,64,73	1.28	6 (10%)	71,102,113	1.41	5 (7%)
26	CLA	B	840	2	69,73,73	1.18	7 (10%)	82,113,113	1.32	7 (8%)
37	IHT	R	202	-	40,42,42	0.21	0	52,58,58	0.35	0
26	CLA	n	605	23	55,59,73	1.33	6 (10%)	64,96,113	1.42	5 (7%)
26	CLA	j	608	17	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
26	CLA	a	306	14	69,73,73	1.19	7 (10%)	82,113,113	1.22	5 (6%)
26	CLA	A	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
26	CLA	l	304	18	51,55,73	1.37	7 (13%)	60,91,113	1.41	5 (8%)
26	CLA	i	303	20	69,73,73	1.19	7 (10%)	82,113,113	1.26	8 (9%)
29	WVN	A	846	-	40,41,41	4.46	20 (50%)	51,56,56	6.67	34 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	h	308	16	55,59,73	1.33	7 (12%)	64,96,113	1.42	6 (9%)
26	CLA	B	807	2	69,73,73	1.15	6 (8%)	82,113,113	1.26	6 (7%)
26	CLA	i	304	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
36	KC2	d	311	-	49,53,53	1.38	6 (12%)	60,89,89	1.04	2 (3%)
26	CLA	i	306	20	65,69,73	1.22	8 (12%)	77,108,113	1.24	5 (6%)
36	KC2	s	401	12	49,53,53	2.93	21 (42%)	60,89,89	3.98	35 (58%)
26	CLA	m	602	17	64,68,73	1.21	8 (12%)	76,107,113	1.42	7 (9%)
26	CLA	c	307	13	50,54,73	1.37	6 (12%)	59,90,113	1.36	6 (10%)
26	CLA	d	309	21	45,49,73	1.43	7 (15%)	54,84,113	1.51	6 (11%)
26	CLA	j	609	17	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
36	KC2	k	612	19	49,53,53	1.41	7 (14%)	60,89,89	0.84	1 (1%)
28	LHG	b	318	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
26	CLA	A	809	1	60,64,73	1.26	7 (11%)	71,102,113	1.31	5 (7%)
29	WVN	B	853	-	40,41,41	4.45	21 (52%)	51,56,56	6.54	34 (66%)
29	WVN	L	201	-	40,41,41	4.42	20 (50%)	51,56,56	6.68	36 (70%)
35	II0	k	619	-	39,43,43	5.69	21 (53%)	48,60,60	8.11	29 (60%)
26	CLA	n	610	-	64,68,73	1.23	7 (10%)	76,107,113	1.35	6 (7%)
26	CLA	d	302	21	66,70,73	1.20	8 (12%)	78,109,113	1.28	5 (6%)
26	CLA	A	832	1	69,73,73	1.18	6 (8%)	82,113,113	1.25	4 (4%)
26	CLA	j	604	17	69,73,73	1.17	6 (8%)	82,113,113	1.34	7 (8%)
26	CLA	B	842	28	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
30	LMU	i	300	-	36,36,36	1.78	9 (25%)	47,47,47	0.88	0
26	CLA	B	830	2	54,58,73	1.32	7 (12%)	64,95,113	1.36	7 (10%)
26	CLA	i	305	20	55,59,73	1.38	7 (12%)	64,96,113	1.59	10 (15%)
26	CLA	m	609	17	64,68,73	1.22	7 (10%)	76,107,113	1.29	6 (7%)
29	WVN	R	200	-	40,41,41	4.50	20 (50%)	51,56,56	6.61	31 (60%)
30	LMU	B	852	-	36,36,36	0.24	0	47,47,47	0.38	0
26	CLA	A	834	1	64,68,73	1.21	6 (9%)	76,107,113	1.35	7 (9%)
28	LHG	A	844	-	26,26,48	0.83	1 (3%)	29,32,54	1.31	3 (10%)
26	CLA	j	612	-	55,59,73	1.32	7 (12%)	64,96,113	1.42	5 (7%)
27	PQN	A	842	-	34,34,34	3.08	13 (38%)	43,45,45	2.03	6 (13%)
26	CLA	l	301	18	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
28	LHG	n	619	-	42,42,48	0.67	1 (2%)	45,48,54	1.23	4 (8%)
26	CLA	B	813	2	64,68,73	1.23	7 (10%)	76,107,113	1.37	7 (9%)
35	II0	n	616	-	39,43,43	5.93	22 (56%)	48,60,60	8.05	28 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	d	318	-	49,53,73	1.40	5 (10%)	58,89,113	1.47	4 (6%)
26	CLA	c	302	13	64,68,73	1.23	7 (10%)	76,107,113	1.28	6 (7%)
29	WVN	F	204	-	40,41,41	0.17	0	51,56,56	0.48	0
26	CLA	m	608	17	69,73,73	1.19	7 (10%)	82,113,113	1.22	4 (4%)
35	II0	n	614	-	39,43,43	0.19	0	48,60,60	0.45	0
26	CLA	k	605	19	49,53,73	1.41	8 (16%)	58,89,113	1.47	5 (8%)
26	CLA	a	309	14	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
35	II0	k	615	-	39,43,43	6.06	21 (53%)	48,60,60	7.80	29 (60%)
26	CLA	A	856	38	69,73,73	1.17	5 (7%)	82,113,113	1.32	6 (7%)
26	CLA	m	613	17	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
35	II0	c	314	-	39,43,43	0.29	0	48,60,60	0.32	0
35	II0	b	315	-	39,43,43	5.77	21 (53%)	48,60,60	7.79	24 (50%)
26	CLA	k	602	19	69,73,73	1.15	7 (10%)	82,113,113	1.34	4 (4%)
26	CLA	l	309	18	69,73,73	1.18	7 (10%)	82,113,113	1.25	7 (8%)
30	LMU	A	850	-	36,36,36	1.76	9 (25%)	47,47,47	1.03	2 (4%)
28	LHG	m	618	26	36,36,48	0.71	1 (2%)	39,42,54	1.26	4 (10%)
26	CLA	A	820	38	69,73,73	1.18	7 (10%)	82,113,113	1.31	5 (6%)
26	CLA	c	303	13	55,59,73	1.33	7 (12%)	64,96,113	1.39	6 (9%)
26	CLA	h	301	38	69,73,73	1.19	9 (13%)	82,113,113	3.22	7 (8%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
35	II0	c	313	-	39,43,43	5.82	21 (53%)	48,60,60	8.15	29 (60%)
37	IHT	j	616	-	40,42,42	0.24	0	52,58,58	0.85	3 (5%)
28	LHG	l	318	26	31,31,48	0.78	2 (6%)	34,37,54	1.31	4 (11%)
28	LHG	b	302	26	48,48,48	0.61	0	51,54,54	1.25	5 (9%)
33	DGD	B	844	-	67,67,67	0.87	2 (2%)	81,81,81	1.43	9 (11%)
35	II0	b	317	-	39,43,43	0.40	0	48,60,60	0.31	0
35	II0	m	616	-	39,43,43	6.10	22 (56%)	48,60,60	7.79	27 (56%)
26	CLA	B	839	2	61,65,73	1.25	6 (9%)	72,103,113	1.31	5 (6%)
26	CLA	K	101	11	46,50,73	1.43	8 (17%)	53,85,113	1.47	5 (9%)
26	CLA	l	311	28	65,69,73	1.22	7 (10%)	77,108,113	1.33	5 (6%)
26	CLA	n	606	23	55,59,73	1.34	7 (12%)	64,96,113	1.32	4 (6%)
26	CLA	B	805	2	69,73,73	1.15	5 (7%)	82,113,113	1.38	6 (7%)
26	CLA	m	604	17	69,73,73	1.18	6 (8%)	82,113,113	1.35	6 (7%)
29	WVN	J	101	-	40,41,41	4.42	18 (45%)	51,56,56	6.53	34 (66%)
28	LHG	J	105	26	32,32,48	0.76	2 (6%)	35,38,54	1.29	3 (8%)
26	CLA	A	818	1	69,73,73	1.17	7 (10%)	82,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	l	307	18	69,73,73	1.16	6 (8%)	82,113,113	1.34	7 (8%)
26	CLA	A	817	1	69,73,73	1.19	9 (13%)	82,113,113	1.27	6 (7%)
28	LHG	L	207	-	46,46,48	0.66	2 (4%)	49,52,54	1.30	6 (12%)
35	II0	l	317	-	39,43,43	0.21	0	48,60,60	0.25	0
26	CLA	F	202	6	56,60,73	1.32	6 (10%)	65,97,113	1.35	4 (6%)
26	CLA	A	804	1	69,73,73	1.16	7 (10%)	82,113,113	1.33	5 (6%)
33	DGD	j	618	-	63,63,67	0.97	2 (3%)	77,77,81	1.53	12 (15%)
28	LHG	c	320	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
26	CLA	A	840	38	69,73,73	1.20	8 (11%)	82,113,113	1.33	7 (8%)
26	CLA	a	307	14	69,73,73	1.18	9 (13%)	82,113,113	1.23	4 (4%)
26	CLA	A	819	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	7 (8%)
26	CLA	m	605	17	46,50,73	1.42	5 (10%)	53,85,113	1.47	4 (7%)
26	CLA	A	816	1	69,73,73	1.16	8 (11%)	82,113,113	1.43	9 (10%)
29	WVN	B	849	-	40,41,41	4.53	19 (47%)	51,56,56	6.32	32 (62%)
26	CLA	B	824	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
35	II0	j	615	-	39,43,43	5.87	22 (56%)	48,60,60	8.12	28 (58%)
28	LHG	j	617	26	29,29,48	0.80	2 (6%)	32,35,54	1.31	3 (9%)
37	IHT	b	301	-	40,42,42	0.30	0	52,58,58	0.47	0
29	WVN	M	101	-	40,41,41	4.44	20 (50%)	51,56,56	6.54	36 (70%)
34	LMG	c	319	26	43,43,55	0.82	1 (2%)	51,51,63	1.25	4 (7%)
26	CLA	B	815	2	59,63,73	1.28	8 (13%)	70,101,113	1.33	5 (7%)
26	CLA	A	827	1	66,70,73	1.22	6 (9%)	78,109,113	1.33	8 (10%)
26	CLA	Q	302	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
26	CLA	B	834	2	69,73,73	1.16	7 (10%)	82,113,113	1.34	5 (6%)
26	CLA	s	408	38	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
26	CLA	k	610	-	55,59,73	1.33	7 (12%)	64,96,113	1.42	7 (10%)
26	CLA	h	303	16	54,58,73	1.32	7 (12%)	64,95,113	1.39	6 (9%)
26	CLA	l	310	18	61,65,73	1.25	8 (13%)	72,103,113	1.34	6 (8%)
26	CLA	c	304	13	66,70,73	1.20	6 (9%)	78,109,113	1.38	4 (5%)
35	II0	d	315	-	39,43,43	5.87	22 (56%)	48,60,60	8.24	27 (56%)
26	CLA	B	829	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	7 (8%)
25	CL0	A	801	-	58,73,73	0.94	4 (6%)	60,113,113	1.78	9 (15%)
26	CLA	b	311	15	68,72,73	1.20	7 (10%)	80,111,113	1.30	5 (6%)
26	CLA	B	820	2	69,73,73	1.17	7 (10%)	82,113,113	1.24	4 (4%)
26	CLA	n	602	23	54,58,73	1.30	7 (12%)	64,95,113	1.45	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	KC2	c	310	13	49,53,53	2.95	21 (42%)	60,89,89	3.93	34 (56%)
26	CLA	i	307	20	69,73,73	1.18	9 (13%)	82,113,113	1.25	4 (4%)
26	CLA	n	609	23	69,73,73	1.17	6 (8%)	82,113,113	1.20	6 (7%)
26	CLA	j	603	17	55,59,73	1.31	7 (12%)	64,96,113	1.41	5 (7%)
26	CLA	A	806	1	64,68,73	1.23	7 (10%)	76,107,113	1.29	5 (6%)
35	II0	k	616	-	39,43,43	5.98	22 (56%)	48,60,60	7.87	28 (58%)
26	CLA	m	601	17	46,50,73	1.42	7 (15%)	53,85,113	1.44	4 (7%)
29	WVN	i	315	-	40,41,41	4.53	21 (52%)	51,56,56	6.70	32 (62%)
26	CLA	A	821	1	53,57,73	1.34	5 (9%)	61,93,113	1.47	6 (9%)
26	CLA	c	311	-	49,53,73	1.40	7 (14%)	58,89,113	1.47	6 (10%)
26	CLA	l	308	18	69,73,73	1.19	7 (10%)	82,113,113	1.27	4 (4%)
26	CLA	c	305	13	69,73,73	1.19	8 (11%)	82,113,113	1.23	4 (4%)
29	WVN	A	848	-	40,41,41	4.43	20 (50%)	51,56,56	6.56	34 (66%)
35	II0	n	618	-	39,43,43	5.92	22 (56%)	48,60,60	8.14	28 (58%)
36	KC2	n	612	-	49,53,53	1.43	8 (16%)	60,89,89	1.03	3 (5%)
26	CLA	B	828	2	54,58,73	1.34	8 (14%)	64,95,113	1.36	6 (9%)
26	CLA	i	302	20	69,73,73	1.16	9 (13%)	82,113,113	1.34	6 (7%)
26	CLA	s	403	12	69,73,73	1.18	8 (11%)	82,113,113	1.33	6 (7%)
35	II0	i	313	-	39,43,43	5.88	21 (53%)	48,60,60	7.88	28 (58%)
29	WVN	B	850	-	40,41,41	4.48	19 (47%)	51,56,56	6.36	33 (64%)
26	CLA	m	606	17	69,73,73	1.19	8 (11%)	82,113,113	1.24	5 (6%)
26	CLA	l	305	18	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
35	II0	l	314	-	39,43,43	5.74	22 (56%)	48,60,60	8.23	28 (58%)
26	CLA	B	825	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	7 (8%)
26	CLA	b	313	28	55,59,73	1.33	6 (10%)	64,96,113	1.44	9 (14%)
26	CLA	B	838	2	69,73,73	1.17	6 (8%)	82,113,113	1.30	7 (8%)
36	KC2	m	611	17	49,53,53	1.39	6 (12%)	60,89,89	0.98	3 (5%)
34	LMG	n	620	-	51,51,55	0.82	2 (3%)	59,59,63	1.24	5 (8%)
26	CLA	k	603	19	55,59,73	1.32	7 (12%)	64,96,113	1.30	7 (10%)
35	II0	l	315	-	39,43,43	5.86	21 (53%)	48,60,60	7.92	26 (54%)
35	II0	d	319	-	39,43,43	0.28	0	48,60,60	0.65	0
26	CLA	B	801	38	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
35	II0	a	313	-	39,43,43	5.82	21 (53%)	48,60,60	7.98	29 (60%)
26	CLA	B	835	2	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
35	II0	h	312	-	39,43,43	5.89	22 (56%)	48,60,60	8.14	28 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	II0	m	619	-	39,43,43	5.97	22 (56%)	48,60,60	8.11	28 (58%)
26	CLA	b	308	15	69,73,73	1.17	7 (10%)	82,113,113	1.28	5 (6%)
36	KC2	d	312	-	49,53,53	1.46	9 (18%)	60,89,89	1.22	6 (10%)
26	CLA	s	406	38	69,73,73	1.18	7 (10%)	82,113,113	1.33	9 (10%)
28	LHG	i	317	26	36,36,48	0.71	1 (2%)	39,42,54	1.27	4 (10%)
28	LHG	c	317	-	36,36,48	0.72	1 (2%)	39,42,54	1.28	5 (12%)
26	CLA	B	817	2	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
35	II0	i	316	-	39,43,43	5.82	21 (53%)	48,60,60	8.21	30 (62%)
35	II0	d	314	-	39,43,43	0.18	0	48,60,60	0.32	0
36	KC2	n	611	23	49,53,53	1.39	6 (12%)	60,89,89	1.11	4 (6%)
35	II0	d	301	-	39,43,43	5.75	21 (53%)	48,60,60	8.04	28 (58%)
29	WVN	s	405	-	40,41,41	4.48	19 (47%)	51,56,56	6.45	31 (60%)
34	LMG	b	319	-	42,42,55	0.87	2 (4%)	50,50,63	1.20	4 (8%)
26	CLA	l	306	18	55,59,73	1.31	6 (10%)	64,96,113	1.45	7 (10%)
37	IHT	m	617	-	40,42,42	0.25	0	52,58,58	0.51	0
30	LMU	A	858	-	35,35,36	0.20	0	46,46,47	0.52	0
26	CLA	A	829	1	69,73,73	1.20	7 (10%)	82,113,113	1.27	4 (4%)
26	CLA	B	826	2	69,73,73	1.18	7 (10%)	82,113,113	1.21	6 (7%)
29	WVN	l	303	-	40,41,41	4.44	19 (47%)	51,56,56	6.50	34 (66%)
26	CLA	n	613	23	55,59,73	1.31	6 (10%)	64,96,113	1.32	6 (9%)
28	LHG	A	849	-	26,26,48	0.69	0	28,29,54	1.44	4 (14%)
26	CLA	A	807	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
26	CLA	j	601	17	69,73,73	1.18	8 (11%)	82,113,113	1.31	5 (6%)
26	CLA	b	303	15	55,59,73	1.32	7 (12%)	64,96,113	1.42	5 (7%)
26	CLA	d	307	21	49,53,73	1.41	8 (16%)	58,89,113	1.36	4 (6%)
31	SF4	A	853	1,2	0,12,12	-	-	-	-	-
35	II0	c	316	-	39,43,43	5.98	22 (56%)	48,60,60	8.19	27 (56%)
26	CLA	c	308	13	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
35	II0	d	317	-	39,43,43	5.84	22 (56%)	48,60,60	8.18	27 (56%)
35	II0	m	614	-	39,43,43	5.90	21 (53%)	48,60,60	8.09	28 (58%)
26	CLA	B	831	38	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
35	II0	a	312	-	39,43,43	5.77	20 (51%)	48,60,60	8.06	28 (58%)
26	CLA	d	313	21	55,59,73	1.31	7 (12%)	64,96,113	1.45	8 (12%)
26	CLA	h	306	16	69,73,73	1.20	8 (11%)	82,113,113	1.28	5 (6%)
26	CLA	L	204	38	64,68,73	1.24	7 (10%)	76,107,113	1.32	6 (7%)
37	IHT	c	315	-	40,42,42	0.52	0	52,58,58	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	a	310	14	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
28	LHG	B	851	26	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
26	CLA	A	814	1	54,58,73	1.32	7 (12%)	64,95,113	1.40	9 (14%)
26	CLA	A	823	1	59,63,73	1.28	6 (10%)	70,101,113	1.37	5 (7%)
26	CLA	a	308	28	52,56,73	1.35	9 (17%)	61,92,113	1.43	5 (8%)
26	CLA	m	612	38	55,59,73	1.32	8 (14%)	64,96,113	1.44	7 (10%)
26	CLA	B	818	38	69,73,73	1.18	8 (11%)	82,113,113	1.30	9 (10%)
29	WVN	L	205	-	40,41,41	4.48	20 (50%)	51,56,56	6.42	33 (64%)
35	II0	a	314	-	39,43,43	5.74	21 (53%)	48,60,60	8.16	28 (58%)
26	CLA	B	802	38	69,73,73	1.17	5 (7%)	82,113,113	1.24	6 (7%)
26	CLA	A	835	1	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
26	CLA	A	852	1	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
35	II0	m	615	-	39,43,43	5.95	21 (53%)	48,60,60	8.15	30 (62%)
26	CLA	B	808	2	69,73,73	1.16	7 (10%)	82,113,113	1.40	7 (8%)
29	WVN	J	102	-	40,41,41	4.50	20 (50%)	51,56,56	6.52	31 (60%)
26	CLA	b	310	15	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
35	II0	l	302	-	39,43,43	6.04	20 (51%)	48,60,60	8.15	29 (60%)
26	CLA	b	306	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
35	II0	j	614	-	39,43,43	5.86	22 (56%)	48,60,60	8.20	27 (56%)
35	II0	d	316	-	39,43,43	5.92	22 (56%)	48,60,60	7.97	28 (58%)
35	II0	k	618	-	39,43,43	0.21	0	48,60,60	0.49	0
26	CLA	A	839	1	64,68,73	1.23	8 (12%)	76,107,113	1.32	7 (9%)
26	CLA	B	816	2	69,73,73	1.20	8 (11%)	82,113,113	1.24	5 (6%)

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
26	CLA	A	802	-	1/1/15/20	7/39/115/115	-
28	LHG	A	843	-	-	18/52/52/53	-
26	CLA	B	836	38	1/1/15/20	14/39/115/115	-
29	WVN	A	845	-	-	16/29/63/63	0/2/2/2
26	CLA	J	103	8	1/1/10/20	5/12/88/115	-
36	KC2	k	611	19	-	13/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	827	2	1/1/12/20	4/23/99/115	-
26	CLA	c	312	13	1/1/15/20	15/39/115/115	-
26	CLA	B	837	2	1/1/15/20	15/39/115/115	-
26	CLA	n	607	23	1/1/15/20	11/39/115/115	-
29	WVN	A	847	-	-	17/29/63/63	0/2/2/2
26	CLA	b	304	15	1/1/13/20	13/27/103/115	-
26	CLA	a	311	14	1/1/11/20	8/19/95/115	-
36	KC2	k	613	-	-	11/15/71/71	-
30	LMU	a	317	-	-	14/21/61/61	0/2/2/2
26	CLA	d	303	21	1/1/12/20	8/23/99/115	-
26	CLA	k	601	19	1/1/12/20	7/23/99/115	-
35	II0	k	620	-	-	13/21/67/67	0/2/2/2
29	WVN	B	845	-	-	2/29/63/63	0/2/2/2
37	IHT	n	617	-	-	3/25/65/65	0/2/2/2
26	CLA	k	607	19	1/1/12/20	10/23/99/115	-
35	II0	b	314	-	-	10/21/67/67	0/2/2/2
37	IHT	b	316	-	-	5/25/65/65	0/2/2/2
26	CLA	L	202	9	1/1/11/20	12/20/96/115	-
26	CLA	k	606	19	1/1/12/20	7/23/99/115	-
26	CLA	A	810	1	1/1/15/20	12/39/115/115	-
26	CLA	A	833	1	1/1/15/20	18/39/115/115	-
26	CLA	d	310	21	1/1/10/20	4/10/86/115	-
26	CLA	A	851	38	1/1/15/20	3/39/115/115	-
26	CLA	a	304	38	1/1/15/20	6/39/115/115	-
27	PQN	B	843	-	-	7/23/43/43	0/2/2/2
26	CLA	k	614	19	1/1/12/20	11/23/99/115	-
35	II0	h	311	-	-	14/21/67/67	0/2/2/2
26	CLA	b	307	15	1/1/14/20	10/35/111/115	-
26	CLA	b	312	15	1/1/15/20	13/39/115/115	-
26	CLA	k	608	19	1/1/15/20	15/39/115/115	-
26	CLA	n	608	-	1/1/15/20	15/39/115/115	-
36	KC2	s	404	-	-	1/15/71/71	-
26	CLA	A	822	1	1/1/13/20	17/29/105/115	-
28	LHG	s	409	-	-	15/34/34/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	L	208	-	-	21/49/49/53	-
35	II0	a	316	-	-	10/21/67/67	0/2/2/2
26	CLA	b	309	34	1/1/15/20	8/39/115/115	-
26	CLA	i	311	20	1/1/15/20	14/39/115/115	-
29	WVN	K	102	-	-	17/29/63/63	0/2/2/2
26	CLA	B	814	2	1/1/15/20	10/39/115/115	-
26	CLA	m	603	17	1/1/13/20	9/32/108/115	-
26	CLA	k	609	19	1/1/13/20	11/30/106/115	-
26	CLA	c	301	13	1/1/12/20	10/23/99/115	-
34	LMG	F	205	-	-	28/48/68/70	0/1/1/1
26	CLA	a	301	14	1/1/15/20	19/39/115/115	-
26	CLA	n	601	23	1/1/11/20	6/15/91/115	-
26	CLA	A	812	1	1/1/15/20	12/39/115/115	-
34	LMG	F	206	-	-	13/36/56/70	0/1/1/1
26	CLA	A	836	1	1/1/15/20	9/39/115/115	-
26	CLA	A	830	1	1/1/14/20	12/33/109/115	-
26	CLA	L	203	9	1/1/15/20	3/39/115/115	-
26	CLA	A	837	1	1/1/15/20	16/39/115/115	-
28	LHG	A	855	-	-	23/40/40/53	-
26	CLA	n	603	23	1/1/12/20	8/23/99/115	-
26	CLA	A	824	38	1/1/15/20	10/39/115/115	-
26	CLA	A	828	1	1/1/15/20	11/39/115/115	-
26	CLA	B	804	-	1/1/15/20	12/39/115/115	-
26	CLA	n	604	23	1/1/14/20	12/33/109/115	-
26	CLA	R	201	22	1/1/13/20	7/27/103/115	-
26	CLA	h	302	16	1/1/12/20	6/21/97/115	-
26	CLA	h	313	38	1/1/15/20	2/39/115/115	-
26	CLA	d	308	21	1/1/11/20	11/17/93/115	-
34	LMG	c	318	-	-	24/50/70/70	0/1/1/1
26	CLA	k	604	-	-	8/39/115/115	-
26	CLA	A	825	38	1/1/15/20	6/39/115/115	-
26	CLA	B	812	2	1/1/15/20	12/39/115/115	-
26	CLA	L	206	-	1/1/12/20	5/23/99/115	-
26	CLA	m	610	28	1/1/13/20	14/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	d	305	-	1/1/12/20	5/23/99/115	-
26	CLA	j	610	28	1/1/14/20	10/35/111/115	-
35	II0	J	104	-	-	12/21/67/67	0/2/2/2
26	CLA	i	301	20	1/1/15/20	22/39/115/115	-
26	CLA	A	841	1	1/1/15/20	13/39/115/115	-
26	CLA	h	305	16	1/1/12/20	6/23/99/115	-
26	CLA	a	303	14	1/1/12/20	4/23/99/115	-
26	CLA	B	811	2	1/1/13/20	5/27/103/115	-
26	CLA	d	304	-	1/1/11/20	8/15/91/115	-
26	CLA	h	304	-	1/1/15/20	16/39/115/115	-
26	CLA	j	605	17	1/1/11/20	10/15/91/115	-
26	CLA	j	613	17	1/1/15/20	12/39/115/115	-
26	CLA	d	306	21	1/1/12/20	7/23/99/115	-
36	KC2	i	309	20	-	11/15/71/71	-
26	CLA	h	307	16	1/1/13/20	8/30/106/115	-
26	CLA	B	823	38	1/1/14/20	11/38/114/115	-
35	II0	k	617	-	-	2/21/67/67	0/2/2/2
29	WVN	B	846	-	-	15/29/63/63	0/2/2/2
29	WVN	B	848	-	-	17/29/63/63	0/2/2/2
26	CLA	A	815	38	1/1/11/20	3/15/91/115	-
26	CLA	F	201	38	1/1/15/20	17/39/115/115	-
26	CLA	c	306	13	1/1/12/20	8/24/100/115	-
36	KC2	l	312	18	-	7/15/71/71	-
26	CLA	a	302	14	1/1/13/20	5/29/105/115	-
26	CLA	A	838	1	1/1/15/20	10/39/115/115	-
29	WVN	s	407	-	-	18/29/63/63	0/2/2/2
26	CLA	B	821	2	1/1/12/20	6/25/101/115	-
26	CLA	A	803	1	1/1/13/20	4/27/103/115	-
26	CLA	j	602	17	1/1/12/20	7/26/102/115	-
32	SQD	A	854	-	-	19/49/69/69	0/1/1/1
37	IHT	a	315	-	-	4/25/65/65	0/2/2/2
26	CLA	B	809	2	1/1/15/20	8/39/115/115	-
26	CLA	a	305	14	1/1/11/20	7/15/91/115	-
26	CLA	B	841	2	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	m	607	17	1/1/12/20	9/23/99/115	-
35	II0	h	310	-	-	11/17/40/67	0/1/1/2
26	CLA	B	819	2	1/1/15/20	18/39/115/115	-
29	WVN	B	847	-	-	16/29/63/63	0/2/2/2
36	KC2	i	318	20	-	11/15/71/71	-
26	CLA	B	803	2	1/1/15/20	16/39/115/115	-
26	CLA	j	606	17	1/1/12/20	7/23/99/115	-
36	KC2	j	611	17	-	11/15/71/71	-
29	WVN	I	101	-	-	17/29/63/63	0/2/2/2
26	CLA	A	805	1	1/1/15/20	14/39/115/115	-
35	II0	i	312	-	-	12/21/67/67	0/2/2/2
26	CLA	B	832	38	1/1/11/20	4/15/91/115	-
26	CLA	B	833	2	1/1/13/20	4/27/103/115	-
26	CLA	i	308	28	1/1/11/20	8/17/93/115	-
26	CLA	A	808	1	1/1/15/20	8/39/115/115	-
34	LMG	L	209	-	-	18/40/60/70	0/1/1/1
35	II0	n	615	-	-	11/21/67/67	0/2/2/2
31	SF4	C	101	3	-	-	0/6/5/5
29	WVN	F	203	-	-	17/29/63/63	0/2/2/2
29	WVN	h	309	-	-	19/29/63/63	0/2/2/2
26	CLA	s	402	12	1/1/15/20	19/39/115/115	-
26	CLA	j	607	17	1/1/12/20	11/23/99/115	-
26	CLA	A	826	1	1/1/15/20	11/39/115/115	-
26	CLA	B	810	2	1/1/15/20	15/39/115/115	-
35	II0	i	314	-	-	13/21/67/67	0/2/2/2
26	CLA	c	309	-	-	4/15/91/115	-
26	CLA	A	811	1	1/1/12/20	8/26/102/115	-
29	WVN	l	316	-	-	17/29/63/63	0/2/2/2
26	CLA	A	813	1	1/1/13/20	8/29/105/115	-
29	WVN	A	857	-	-	19/29/63/63	0/2/2/2
34	LMG	Q	301	-	-	16/33/53/70	0/1/1/1
26	CLA	B	806	2	1/1/15/20	14/39/115/115	-
26	CLA	b	305	15	1/1/12/20	4/24/100/115	-
35	II0	i	319	-	-	12/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	i	310	-	1/1/14/20	11/33/109/115	-
26	CLA	B	822	38	1/1/15/20	19/39/115/115	-
26	CLA	l	313	18	1/1/13/20	11/29/105/115	-
26	CLA	B	840	2	1/1/15/20	10/39/115/115	-
37	IHT	R	202	-	-	2/25/65/65	0/2/2/2
26	CLA	n	605	23	1/1/12/20	10/23/99/115	-
26	CLA	j	608	17	1/1/11/20	8/15/91/115	-
26	CLA	a	306	14	1/1/15/20	14/39/115/115	-
26	CLA	A	831	1	1/1/15/20	13/39/115/115	-
26	CLA	l	304	18	1/1/11/20	7/18/94/115	-
26	CLA	i	303	20	1/1/15/20	7/39/115/115	-
29	WVN	A	846	-	-	16/29/63/63	0/2/2/2
26	CLA	h	308	16	1/1/12/20	8/23/99/115	-
26	CLA	B	807	2	1/1/15/20	7/39/115/115	-
26	CLA	i	304	-	1/1/15/20	13/39/115/115	-
36	KC2	d	311	-	-	13/15/71/71	-
26	CLA	i	306	20	1/1/14/20	16/35/111/115	-
36	KC2	s	401	12	-	4/15/71/71	-
26	CLA	m	602	17	1/1/14/20	12/33/109/115	-
26	CLA	c	307	13	1/1/11/20	7/17/93/115	-
26	CLA	d	309	21	1/1/10/20	4/10/86/115	-
26	CLA	j	609	17	1/1/15/20	17/39/115/115	-
36	KC2	k	612	19	-	9/15/71/71	-
28	LHG	b	318	-	-	31/53/53/53	-
26	CLA	A	809	1	1/1/13/20	13/29/105/115	-
29	WVN	B	853	-	-	20/29/63/63	0/2/2/2
29	WVN	L	201	-	-	16/29/63/63	0/2/2/2
35	II0	k	619	-	-	10/21/67/67	0/2/2/2
26	CLA	n	610	-	1/1/14/20	14/33/109/115	-
26	CLA	d	302	21	1/1/14/20	17/36/112/115	-
26	CLA	A	832	1	1/1/15/20	8/39/115/115	-
26	CLA	j	604	17	1/1/15/20	8/39/115/115	-
26	CLA	B	842	28	1/1/15/20	9/39/115/115	-
30	LMU	i	300	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	830	2	1/1/12/20	9/21/97/115	-
26	CLA	i	305	20	1/1/12/20	9/23/99/115	-
26	CLA	m	609	17	1/1/14/20	13/33/109/115	-
29	WVN	R	200	-	-	17/29/63/63	0/2/2/2
30	LMU	B	852	-	-	3/21/61/61	0/2/2/2
26	CLA	A	834	1	1/1/14/20	6/33/109/115	-
28	LHG	A	844	-	-	7/31/31/53	-
26	CLA	j	612	-	1/1/12/20	9/23/99/115	-
27	PQN	A	842	-	-	10/23/43/43	0/2/2/2
26	CLA	l	301	18	1/1/15/20	14/39/115/115	-
28	LHG	n	619	-	-	22/47/47/53	-
26	CLA	B	813	2	1/1/14/20	13/33/109/115	-
35	II0	n	616	-	-	13/21/67/67	0/2/2/2
26	CLA	d	318	-	1/1/11/20	9/15/91/115	-
26	CLA	c	302	13	-	14/33/109/115	-
29	WVN	F	204	-	-	6/29/63/63	0/2/2/2
26	CLA	m	608	17	1/1/15/20	14/39/115/115	-
35	II0	n	614	-	-	1/21/67/67	0/2/2/2
26	CLA	k	605	19	1/1/11/20	5/15/91/115	-
26	CLA	a	309	14	1/1/15/20	12/39/115/115	-
35	II0	k	615	-	-	13/21/67/67	0/2/2/2
26	CLA	A	856	38	1/1/15/20	13/39/115/115	-
26	CLA	m	613	17	1/1/15/20	11/39/115/115	-
35	II0	c	314	-	-	1/21/67/67	0/2/2/2
35	II0	b	315	-	-	13/21/67/67	0/2/2/2
26	CLA	k	602	19	1/1/15/20	16/39/115/115	-
26	CLA	l	309	18	1/1/15/20	6/39/115/115	-
30	LMU	A	850	-	-	13/21/61/61	0/2/2/2
28	LHG	m	618	26	-	12/41/41/53	-
26	CLA	A	820	38	1/1/15/20	10/39/115/115	-
26	CLA	c	303	13	1/1/12/20	4/23/99/115	-
26	CLA	h	301	38	1/1/15/20	11/39/115/115	-
31	SF4	C	102	3	-	-	0/6/5/5
35	II0	c	313	-	-	12/21/67/67	0/2/2/2
37	IHT	j	616	-	-	2/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	l	318	26	-	9/36/36/53	-
28	LHG	b	302	26	-	22/53/53/53	-
33	DGD	B	844	-	-	27/55/95/95	0/2/2/2
35	II0	b	317	-	-	1/21/67/67	0/2/2/2
35	II0	m	616	-	-	12/21/67/67	0/2/2/2
26	CLA	B	839	2	1/1/13/20	11/30/106/115	-
26	CLA	K	101	11	1/1/10/20	6/12/88/115	-
26	CLA	l	311	28	1/1/14/20	13/35/111/115	-
26	CLA	n	606	23	-	6/23/99/115	-
26	CLA	B	805	2	1/1/15/20	11/39/115/115	-
26	CLA	m	604	17	1/1/15/20	9/39/115/115	-
29	WVN	J	101	-	-	19/29/63/63	0/2/2/2
28	LHG	J	105	26	-	13/37/37/53	-
26	CLA	A	818	1	1/1/15/20	14/39/115/115	-
26	CLA	l	307	18	1/1/15/20	11/39/115/115	-
26	CLA	A	817	1	1/1/15/20	13/39/115/115	-
28	LHG	L	207	-	-	20/51/51/53	-
35	II0	l	317	-	-	3/21/67/67	0/2/2/2
26	CLA	F	202	6	1/1/12/20	12/24/100/115	-
26	CLA	A	804	1	1/1/15/20	6/39/115/115	-
33	DGD	j	618	-	-	23/51/91/95	0/2/2/2
28	LHG	c	320	-	-	20/53/53/53	-
26	CLA	A	840	38	1/1/15/20	11/39/115/115	-
26	CLA	a	307	14	1/1/15/20	15/39/115/115	-
26	CLA	A	819	1	1/1/15/20	19/39/115/115	-
26	CLA	m	605	17	1/1/10/20	8/12/88/115	-
26	CLA	A	816	1	1/1/15/20	19/39/115/115	-
29	WVN	B	849	-	-	17/29/63/63	0/2/2/2
26	CLA	B	824	2	1/1/15/20	9/39/115/115	-
35	II0	j	615	-	-	10/21/67/67	0/2/2/2
28	LHG	j	617	26	-	16/34/34/53	-
37	IHT	b	301	-	-	3/25/65/65	0/2/2/2
29	WVN	M	101	-	-	18/29/63/63	0/2/2/2
34	LMG	c	319	26	-	21/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	815	2	1/1/13/20	8/27/103/115	-
26	CLA	A	827	1	1/1/14/20	6/36/112/115	-
26	CLA	Q	302	-	1/1/15/20	15/39/115/115	-
26	CLA	B	834	2	1/1/15/20	13/39/115/115	-
26	CLA	s	408	38	1/1/15/20	11/39/115/115	-
26	CLA	k	610	-	1/1/12/20	12/23/99/115	-
26	CLA	h	303	16	1/1/12/20	8/21/97/115	-
26	CLA	l	310	18	1/1/13/20	10/30/106/115	-
26	CLA	c	304	13	1/1/14/20	12/36/112/115	-
35	II0	d	315	-	-	12/21/67/67	0/2/2/2
26	CLA	B	829	2	1/1/15/20	11/39/115/115	-
25	CL0	A	801	-	2/2/20/25	14/37/135/135	-
26	CLA	b	311	15	1/1/14/20	14/38/114/115	-
26	CLA	B	820	2	1/1/15/20	9/39/115/115	-
26	CLA	n	602	23	1/1/12/20	6/21/97/115	-
36	KC2	c	310	13	-	7/15/71/71	-
26	CLA	i	307	20	1/1/15/20	12/39/115/115	-
26	CLA	n	609	23	1/1/15/20	11/39/115/115	-
26	CLA	j	603	17	1/1/12/20	3/23/99/115	-
26	CLA	A	806	1	1/1/14/20	6/33/109/115	-
35	II0	k	616	-	-	10/21/67/67	0/2/2/2
26	CLA	m	601	17	1/1/10/20	7/12/88/115	-
29	WVN	i	315	-	-	15/29/63/63	0/2/2/2
26	CLA	A	821	1	1/1/11/20	8/20/96/115	-
26	CLA	c	311	-	1/1/11/20	6/15/91/115	-
26	CLA	l	308	18	1/1/15/20	7/39/115/115	-
26	CLA	c	305	13	1/1/15/20	6/39/115/115	-
29	WVN	A	848	-	-	18/29/63/63	0/2/2/2
35	II0	n	618	-	-	11/21/67/67	0/2/2/2
36	KC2	n	612	-	-	13/15/71/71	-
26	CLA	B	828	2	1/1/12/20	10/21/97/115	-
26	CLA	i	302	20	1/1/15/20	18/39/115/115	-
26	CLA	s	403	12	1/1/15/20	11/39/115/115	-
35	II0	i	313	-	-	13/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	WVN	B	850	-	-	18/29/63/63	0/2/2/2
26	CLA	m	606	17	1/1/15/20	19/39/115/115	-
26	CLA	l	305	18	1/1/15/20	15/39/115/115	-
35	II0	l	314	-	-	12/21/67/67	0/2/2/2
26	CLA	B	825	2	1/1/15/20	16/39/115/115	-
26	CLA	b	313	28	1/1/12/20	7/23/99/115	-
26	CLA	B	838	2	1/1/15/20	10/39/115/115	-
36	KC2	m	611	17	-	9/15/71/71	-
34	LMG	n	620	-	-	15/46/66/70	0/1/1/1
26	CLA	k	603	19	1/1/12/20	5/23/99/115	-
35	II0	l	315	-	-	11/21/67/67	0/2/2/2
35	II0	d	319	-	-	11/21/67/67	0/2/2/2
26	CLA	B	801	38	1/1/15/20	17/39/115/115	-
35	II0	a	313	-	-	11/21/67/67	0/2/2/2
26	CLA	B	835	2	-	4/18/94/115	-
35	II0	h	312	-	-	11/21/67/67	0/2/2/2
35	II0	m	619	-	-	11/21/67/67	0/2/2/2
26	CLA	b	308	15	1/1/15/20	15/39/115/115	-
36	KC2	d	312	-	-	11/15/71/71	-
26	CLA	s	406	38	1/1/15/20	10/39/115/115	-
28	LHG	i	317	26	-	17/41/41/53	-
28	LHG	c	317	-	-	19/41/41/53	-
26	CLA	B	817	2	1/1/15/20	10/39/115/115	-
35	II0	i	316	-	-	13/21/67/67	0/2/2/2
35	II0	d	314	-	-	0/21/67/67	0/2/2/2
36	KC2	n	611	23	-	11/15/71/71	-
35	II0	d	301	-	-	10/21/67/67	0/2/2/2
29	WVN	s	405	-	-	16/29/63/63	0/2/2/2
34	LMG	b	319	-	-	16/37/57/70	0/1/1/1
26	CLA	l	306	18	1/1/12/20	2/23/99/115	-
37	IHT	m	617	-	-	4/25/65/65	0/2/2/2
30	LMU	A	858	-	-	6/20/60/61	0/2/2/2
26	CLA	A	829	1	1/1/15/20	6/39/115/115	-
26	CLA	B	826	2	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	WVN	l	303	-	-	16/29/63/63	0/2/2/2
26	CLA	n	613	23	1/1/12/20	10/23/99/115	-
28	LHG	A	849	-	-	12/27/27/53	-
26	CLA	A	807	1	1/1/15/20	13/39/115/115	-
26	CLA	j	601	17	1/1/15/20	14/39/115/115	-
26	CLA	b	303	15	1/1/12/20	7/23/99/115	-
26	CLA	d	307	21	1/1/11/20	10/15/91/115	-
31	SF4	A	853	1,2	-	-	0/6/5/5
35	II0	c	316	-	-	13/21/67/67	0/2/2/2
26	CLA	c	308	13	1/1/15/20	18/39/115/115	-
35	II0	d	317	-	-	13/21/67/67	0/2/2/2
35	II0	m	614	-	-	13/21/67/67	0/2/2/2
26	CLA	B	831	38	1/1/15/20	11/39/115/115	-
35	II0	a	312	-	-	11/21/67/67	0/2/2/2
26	CLA	d	313	21	1/1/12/20	7/23/99/115	-
26	CLA	h	306	16	1/1/15/20	7/39/115/115	-
26	CLA	L	204	38	1/1/14/20	6/33/109/115	-
37	IHT	c	315	-	-	0/25/65/65	0/2/2/2
26	CLA	a	310	14	-	15/39/115/115	-
28	LHG	B	851	26	-	30/53/53/53	-
26	CLA	A	814	1	1/1/12/20	7/21/97/115	-
26	CLA	A	823	1	1/1/13/20	9/27/103/115	-
26	CLA	a	308	28	1/1/11/20	5/19/95/115	-
26	CLA	m	612	38	1/1/12/20	8/23/99/115	-
26	CLA	B	818	38	1/1/15/20	12/39/115/115	-
29	WVN	L	205	-	-	16/29/63/63	0/2/2/2
35	II0	a	314	-	-	14/21/67/67	0/2/2/2
26	CLA	B	802	38	1/1/15/20	11/39/115/115	-
26	CLA	A	835	1	1/1/15/20	12/39/115/115	-
26	CLA	A	852	1	1/1/15/20	11/39/115/115	-
35	II0	m	615	-	-	11/21/67/67	0/2/2/2
26	CLA	B	808	2	1/1/15/20	10/39/115/115	-
29	WVN	J	102	-	-	19/29/63/63	0/2/2/2
26	CLA	b	310	15	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	II0	l	302	-	-	11/21/67/67	0/2/2/2
26	CLA	b	306	-	1/1/15/20	16/39/115/115	-
35	II0	j	614	-	-	13/21/67/67	0/2/2/2
35	II0	d	316	-	-	13/21/67/67	0/2/2/2
35	II0	k	618	-	-	1/21/67/67	0/2/2/2
26	CLA	A	839	1	1/1/14/20	2/33/109/115	-
26	CLA	B	816	2	1/1/15/20	18/39/115/115	-

All (3061) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	615	II0	C14-C10	20.92	1.58	1.35
35	m	616	II0	C13-C09	19.96	1.57	1.35
35	h	310	II0	C13-C09	19.91	1.57	1.35
35	h	312	II0	C13-C09	19.76	1.56	1.35
35	c	316	II0	C14-C10	19.71	1.56	1.35
35	m	615	II0	C14-C10	19.61	1.56	1.35
35	k	616	II0	C14-C10	19.60	1.56	1.35
35	n	616	II0	C14-C10	19.60	1.56	1.35
35	a	316	II0	C13-C09	19.57	1.56	1.35
35	i	314	II0	C13-C09	19.50	1.56	1.35
35	l	302	II0	C14-C10	19.49	1.56	1.35
35	i	312	II0	C14-C10	19.48	1.56	1.35
35	j	614	II0	C13-C09	19.44	1.56	1.35
35	j	615	II0	C14-C10	19.43	1.56	1.35
35	d	317	II0	C14-C10	19.38	1.56	1.35
35	m	619	II0	C14-C10	19.35	1.56	1.35
35	a	313	II0	C13-C09	19.26	1.56	1.35
35	i	319	II0	C13-C09	19.19	1.56	1.35
35	i	313	II0	C14-C10	19.15	1.56	1.35
35	l	302	II0	C13-C09	19.12	1.56	1.35
35	d	315	II0	C13-C09	19.05	1.56	1.35
35	a	316	II0	C14-C10	19.04	1.56	1.35
35	c	316	II0	C13-C09	18.99	1.56	1.35
35	m	615	II0	C13-C09	18.98	1.56	1.35
35	c	313	II0	C14-C10	18.94	1.56	1.35
35	d	316	II0	C13-C09	18.90	1.55	1.35
35	a	312	II0	C13-C09	18.89	1.55	1.35
35	m	619	II0	C13-C09	18.87	1.55	1.35
35	l	315	II0	C14-C10	18.83	1.55	1.35
35	n	618	II0	C13-C09	18.83	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	616	II0	C14-C10	18.83	1.55	1.35
35	k	616	II0	C13-C09	18.80	1.55	1.35
35	n	618	II0	C14-C10	18.77	1.55	1.35
35	i	316	II0	C14-C10	18.77	1.55	1.35
35	m	614	II0	C13-C09	18.76	1.55	1.35
35	i	314	II0	C14-C10	18.73	1.55	1.35
35	d	316	II0	C14-C10	18.72	1.55	1.35
35	d	315	II0	C14-C10	18.65	1.55	1.35
35	m	614	II0	C14-C10	18.50	1.55	1.35
35	d	301	II0	C14-C10	18.49	1.55	1.35
35	n	615	II0	C13-C09	18.48	1.55	1.35
35	a	314	II0	C14-C10	18.47	1.55	1.35
35	i	312	II0	C13-C09	18.42	1.55	1.35
35	l	314	II0	C14-C10	18.18	1.55	1.35
35	i	316	II0	C13-C09	18.15	1.55	1.35
35	J	104	II0	C13-C09	18.11	1.55	1.35
35	n	616	II0	C13-C09	18.05	1.55	1.35
35	k	620	II0	C14-C10	18.01	1.55	1.35
35	l	315	II0	C13-C09	17.99	1.54	1.35
35	i	319	II0	C14-C10	17.97	1.54	1.35
35	k	615	II0	C13-C09	17.90	1.54	1.35
35	j	615	II0	C13-C09	17.86	1.54	1.35
35	l	314	II0	C13-C09	17.85	1.54	1.35
35	n	615	II0	C14-C10	17.84	1.54	1.35
35	b	315	II0	C14-C10	17.82	1.54	1.35
35	c	313	II0	C13-C09	17.79	1.54	1.35
35	k	619	II0	C14-C10	17.73	1.54	1.35
35	j	614	II0	C14-C10	17.73	1.54	1.35
35	a	312	II0	C14-C10	17.73	1.54	1.35
35	h	312	II0	C14-C10	17.71	1.54	1.35
35	i	313	II0	C13-C09	17.71	1.54	1.35
35	J	104	II0	C14-C10	17.67	1.54	1.35
35	k	620	II0	C13-C09	17.66	1.54	1.35
35	b	314	II0	C14-C10	17.65	1.54	1.35
35	a	313	II0	C14-C10	17.52	1.54	1.35
35	k	619	II0	C13-C09	17.52	1.54	1.35
35	b	314	II0	C13-C09	17.45	1.54	1.35
35	d	317	II0	C13-C09	17.42	1.54	1.35
35	b	315	II0	C13-C09	17.41	1.54	1.35
35	h	311	II0	C13-C09	17.39	1.54	1.35
35	d	301	II0	C13-C09	17.37	1.54	1.35
35	h	311	II0	C14-C10	17.29	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	314	II0	C13-C09	17.22	1.54	1.35
29	A	845	WVN	C15-C13	13.35	1.56	1.34
29	L	201	WVN	C15-C13	13.22	1.56	1.34
29	i	315	WVN	C15-C13	13.08	1.56	1.34
29	B	846	WVN	C15-C13	12.93	1.56	1.34
29	A	848	WVN	C15-C13	12.90	1.56	1.34
29	B	849	WVN	C15-C13	12.88	1.56	1.34
29	R	200	WVN	C15-C13	12.86	1.56	1.34
29	J	102	WVN	C15-C13	12.83	1.56	1.34
29	A	857	WVN	C15-C13	12.80	1.56	1.34
29	B	847	WVN	C15-C13	12.79	1.56	1.34
29	M	101	WVN	C15-C13	12.79	1.56	1.34
29	h	309	WVN	C15-C13	12.74	1.55	1.34
29	s	405	WVN	C15-C13	12.58	1.55	1.34
29	B	850	WVN	C15-C13	12.56	1.55	1.34
29	L	205	WVN	C15-C13	12.56	1.55	1.34
29	A	846	WVN	C15-C13	12.53	1.55	1.34
29	l	303	WVN	C15-C13	12.53	1.55	1.34
29	s	407	WVN	C15-C13	12.49	1.55	1.34
29	B	853	WVN	C15-C13	12.41	1.55	1.34
29	B	848	WVN	C15-C13	12.36	1.55	1.34
29	l	316	WVN	C09-C05	12.30	1.56	1.32
29	l	316	WVN	C15-C13	12.27	1.55	1.34
29	B	850	WVN	C09-C05	12.26	1.56	1.32
29	A	845	WVN	C09-C05	12.25	1.56	1.32
29	J	101	WVN	C15-C13	12.19	1.55	1.34
29	J	101	WVN	C09-C05	12.17	1.55	1.32
29	F	203	WVN	C09-C05	12.14	1.55	1.32
29	L	205	WVN	C09-C05	12.14	1.55	1.32
29	B	848	WVN	C09-C05	12.14	1.55	1.32
29	B	853	WVN	C09-C05	12.13	1.55	1.32
29	h	309	WVN	C09-C05	12.12	1.55	1.32
29	J	102	WVN	C09-C05	12.11	1.55	1.32
29	s	405	WVN	C09-C05	12.10	1.55	1.32
29	l	303	WVN	C09-C05	12.06	1.55	1.32
29	K	102	WVN	C15-C13	12.05	1.54	1.34
29	B	849	WVN	C09-C05	12.05	1.55	1.32
29	I	101	WVN	C09-C05	12.02	1.55	1.32
29	K	102	WVN	C09-C05	12.02	1.55	1.32
29	A	847	WVN	C15-C13	12.01	1.54	1.34
29	M	101	WVN	C09-C05	11.93	1.55	1.32
29	s	407	WVN	C09-C05	11.92	1.55	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	203	WVN	C15-C13	11.89	1.54	1.34
29	L	201	WVN	C09-C05	11.89	1.55	1.32
29	B	847	WVN	C09-C05	11.89	1.55	1.32
29	A	848	WVN	C09-C05	11.87	1.55	1.32
29	A	846	WVN	C09-C05	11.85	1.55	1.32
29	R	200	WVN	C09-C05	11.84	1.55	1.32
29	i	315	WVN	C09-C05	11.82	1.55	1.32
29	I	101	WVN	C15-C13	11.81	1.54	1.34
29	A	857	WVN	C09-C05	11.74	1.55	1.32
29	B	846	WVN	C09-C05	11.59	1.54	1.32
29	A	847	WVN	C09-C05	11.38	1.54	1.32
35	i	316	II0	C29-C25	9.32	1.56	1.37
35	i	319	II0	C29-C25	9.30	1.56	1.37
27	A	842	PQN	C12-C13	9.25	1.54	1.33
35	i	313	II0	C29-C25	9.22	1.56	1.37
27	B	843	PQN	C12-C13	9.19	1.54	1.33
35	c	316	II0	C29-C25	9.17	1.56	1.37
35	m	616	II0	C29-C25	9.16	1.56	1.37
35	l	302	II0	C29-C25	9.13	1.56	1.37
35	d	301	II0	C29-C25	9.13	1.56	1.37
35	a	314	II0	C29-C25	9.10	1.56	1.37
35	n	616	II0	C29-C25	9.09	1.55	1.37
35	k	615	II0	C22-C10	9.09	1.59	1.42
35	l	315	II0	C29-C25	9.08	1.55	1.37
35	n	615	II0	C29-C25	9.06	1.55	1.37
35	b	315	II0	C29-C25	9.06	1.55	1.37
35	n	618	II0	C29-C25	9.06	1.55	1.37
35	h	311	II0	C29-C25	9.06	1.55	1.37
35	m	614	II0	C29-C25	9.05	1.55	1.37
35	k	620	II0	C29-C25	9.04	1.55	1.37
35	d	317	II0	C29-C25	9.04	1.55	1.37
35	k	619	II0	C29-C25	9.03	1.55	1.37
35	J	104	II0	C29-C25	9.02	1.55	1.37
35	j	614	II0	C29-C25	8.99	1.55	1.37
35	i	314	II0	C29-C25	8.98	1.55	1.37
35	j	615	II0	C29-C25	8.98	1.55	1.37
35	h	312	II0	C29-C25	8.98	1.55	1.37
35	a	312	II0	C29-C25	8.94	1.55	1.37
35	b	314	II0	C29-C25	8.92	1.55	1.37
35	m	619	II0	C29-C25	8.92	1.55	1.37
35	m	615	II0	C29-C25	8.91	1.55	1.37
35	d	315	II0	C29-C25	8.90	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	302	II0	C30-C26	8.90	1.55	1.37
35	l	314	II0	C29-C25	8.87	1.55	1.37
35	d	316	II0	C29-C25	8.84	1.55	1.37
35	a	313	II0	C29-C25	8.83	1.55	1.37
35	l	315	II0	C30-C26	8.83	1.55	1.37
35	c	313	II0	C29-C25	8.83	1.55	1.37
35	h	310	II0	C29-C25	8.81	1.55	1.37
35	a	316	II0	C29-C25	8.76	1.55	1.37
35	h	311	II0	C30-C26	8.75	1.55	1.37
35	i	312	II0	C29-C25	8.74	1.55	1.37
35	b	315	II0	C30-C26	8.74	1.55	1.37
35	m	614	II0	C30-C26	8.73	1.55	1.37
35	k	615	II0	C29-C25	8.71	1.55	1.37
35	m	619	II0	C30-C26	8.68	1.55	1.37
26	c	309	CLA	C1D-ND	8.68	1.49	1.37
35	m	616	II0	C30-C26	8.66	1.55	1.37
35	n	615	II0	C30-C26	8.65	1.55	1.37
35	k	616	II0	C29-C25	8.64	1.55	1.37
35	c	313	II0	C30-C26	8.63	1.55	1.37
35	b	314	II0	C30-C26	8.62	1.55	1.37
35	j	614	II0	C30-C26	8.61	1.54	1.37
35	a	316	II0	C30-C26	8.60	1.54	1.37
35	d	301	II0	C30-C26	8.60	1.54	1.37
35	a	313	II0	C30-C26	8.58	1.54	1.37
35	k	619	II0	C30-C26	8.57	1.54	1.37
35	h	312	II0	C30-C26	8.57	1.54	1.37
35	j	615	II0	C30-C26	8.56	1.54	1.37
35	i	313	II0	C39-C35	8.56	1.55	1.35
35	a	314	II0	C30-C26	8.56	1.54	1.37
35	l	315	II0	C39-C35	8.55	1.55	1.35
35	b	315	II0	C40-C36	8.54	1.55	1.35
35	n	618	II0	C30-C26	8.53	1.54	1.37
35	b	314	II0	C39-C35	8.53	1.55	1.35
35	m	616	II0	C39-C35	8.53	1.55	1.35
35	a	313	II0	C40-C36	8.51	1.55	1.35
35	n	616	II0	C30-C26	8.50	1.54	1.37
35	m	615	II0	C30-C26	8.50	1.54	1.37
35	k	616	II0	C30-C26	8.49	1.54	1.37
27	B	843	PQN	O1-C1	8.45	1.40	1.23
35	i	313	II0	C40-C36	8.45	1.55	1.35
35	d	315	II0	C39-C35	8.44	1.55	1.35
35	l	315	II0	C40-C36	8.43	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	842	PQN	O1-C1	8.41	1.40	1.23
35	b	315	II0	C39-C35	8.41	1.55	1.35
35	i	312	II0	C39-C35	8.41	1.55	1.35
27	B	843	PQN	O4-C4	8.40	1.40	1.23
35	l	302	II0	C40-C36	8.39	1.55	1.35
35	i	319	II0	C30-C26	8.39	1.54	1.37
35	k	616	II0	C39-C35	8.38	1.55	1.35
35	m	614	II0	C39-C35	8.38	1.55	1.35
35	a	313	II0	C39-C35	8.38	1.55	1.35
35	i	312	II0	C40-C36	8.38	1.55	1.35
35	d	316	II0	C39-C35	8.35	1.55	1.35
35	k	616	II0	C40-C36	8.34	1.55	1.35
35	d	317	II0	C30-C26	8.34	1.54	1.37
35	n	615	II0	C39-C35	8.34	1.55	1.35
35	d	317	II0	C39-C35	8.34	1.55	1.35
35	l	302	II0	C39-C35	8.34	1.55	1.35
35	b	314	II0	C40-C36	8.33	1.55	1.35
35	k	620	II0	C30-C26	8.33	1.54	1.37
27	A	842	PQN	O4-C4	8.33	1.40	1.23
35	k	615	II0	C39-C35	8.33	1.55	1.35
35	i	319	II0	C22-C10	8.32	1.58	1.42
35	d	316	II0	C30-C26	8.32	1.54	1.37
35	h	310	II0	C40-C36	8.31	1.55	1.35
35	k	616	II0	C21-C09	8.31	1.58	1.42
35	c	313	II0	C40-C36	8.30	1.55	1.35
35	l	314	II0	C39-C35	8.30	1.55	1.35
35	b	315	II0	C22-C10	8.29	1.58	1.42
35	i	314	II0	C30-C26	8.29	1.54	1.37
35	i	314	II0	C39-C35	8.29	1.55	1.35
35	l	314	II0	C30-C26	8.28	1.54	1.37
35	a	316	II0	C39-C35	8.28	1.55	1.35
35	i	313	II0	C30-C26	8.28	1.54	1.37
35	J	104	II0	C39-C35	8.28	1.54	1.35
35	J	104	II0	C30-C26	8.28	1.54	1.37
35	m	619	II0	C40-C36	8.28	1.54	1.35
35	c	313	II0	C39-C35	8.28	1.54	1.35
35	j	614	II0	C40-C36	8.28	1.54	1.35
35	k	619	II0	C40-C36	8.27	1.54	1.35
35	n	615	II0	C40-C36	8.27	1.54	1.35
35	k	615	II0	C30-C26	8.26	1.54	1.37
35	a	312	II0	C30-C26	8.26	1.54	1.37
35	n	616	II0	C39-C35	8.26	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	619	II0	C39-C35	8.25	1.54	1.35
35	d	317	II0	C40-C36	8.25	1.54	1.35
29	A	845	WVN	C28-C25	8.25	1.54	1.35
35	i	316	II0	C30-C26	8.25	1.54	1.37
35	h	312	II0	C39-C35	8.25	1.54	1.35
35	i	316	II0	C39-C35	8.25	1.54	1.35
35	k	619	II0	C39-C35	8.25	1.54	1.35
35	j	615	II0	C39-C35	8.25	1.54	1.35
35	d	315	II0	C30-C26	8.25	1.54	1.37
29	L	205	WVN	C26-C22	8.24	1.54	1.35
35	k	620	II0	C40-C36	8.24	1.54	1.35
35	i	319	II0	C39-C35	8.24	1.54	1.35
35	h	310	II0	C39-C35	8.23	1.54	1.35
29	s	407	WVN	C26-C22	8.22	1.54	1.35
35	i	312	II0	C30-C26	8.22	1.54	1.37
35	c	316	II0	C30-C26	8.22	1.54	1.37
35	n	618	II0	C39-C35	8.22	1.54	1.35
29	F	203	WVN	C26-C22	8.22	1.54	1.35
29	s	405	WVN	C37-C34	8.21	1.54	1.35
29	l	316	WVN	C37-C34	8.21	1.54	1.35
29	A	845	WVN	C26-C22	8.20	1.54	1.35
35	m	614	II0	C40-C36	8.20	1.54	1.35
35	h	312	II0	C40-C36	8.20	1.54	1.35
35	d	316	II0	C40-C36	8.19	1.54	1.35
35	a	314	II0	C40-C36	8.19	1.54	1.35
35	m	615	II0	C39-C35	8.19	1.54	1.35
35	a	312	II0	C39-C35	8.18	1.54	1.35
29	B	849	WVN	C28-C25	8.18	1.54	1.35
35	h	311	II0	C39-C35	8.18	1.54	1.35
35	J	104	II0	C40-C36	8.18	1.54	1.35
35	m	616	II0	C40-C36	8.18	1.54	1.35
35	j	615	II0	C40-C36	8.18	1.54	1.35
35	l	314	II0	C40-C36	8.17	1.54	1.35
35	k	615	II0	C40-C36	8.17	1.54	1.35
35	i	319	II0	C40-C36	8.17	1.54	1.35
35	a	312	II0	C40-C36	8.16	1.54	1.35
35	k	620	II0	C39-C35	8.16	1.54	1.35
29	J	102	WVN	C37-C34	8.16	1.54	1.35
35	n	618	II0	C40-C36	8.16	1.54	1.35
35	i	316	II0	C40-C36	8.15	1.54	1.35
29	J	101	WVN	C26-C22	8.15	1.54	1.35
35	a	316	II0	C40-C36	8.15	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	316	WVN	C26-C22	8.15	1.54	1.35
35	d	315	II0	C40-C36	8.14	1.54	1.35
35	d	301	II0	C40-C36	8.14	1.54	1.35
35	n	616	II0	C40-C36	8.14	1.54	1.35
29	A	857	WVN	C28-C25	8.12	1.54	1.35
35	c	316	II0	C39-C35	8.12	1.54	1.35
35	a	314	II0	C39-C35	8.12	1.54	1.35
35	d	301	II0	C39-C35	8.11	1.54	1.35
35	i	314	II0	C40-C36	8.11	1.54	1.35
29	B	849	WVN	C26-C22	8.11	1.54	1.35
29	K	102	WVN	C37-C34	8.10	1.54	1.35
35	j	614	II0	C39-C35	8.10	1.54	1.35
29	i	315	WVN	C37-C34	8.09	1.54	1.35
29	B	849	WVN	C37-C34	8.08	1.54	1.35
29	A	847	WVN	C26-C22	8.08	1.54	1.35
35	l	302	II0	C21-C09	8.08	1.57	1.42
29	h	309	WVN	C26-C22	8.08	1.54	1.35
29	B	850	WVN	C37-C34	8.06	1.54	1.35
29	l	303	WVN	C26-C22	8.05	1.54	1.35
35	d	316	II0	C21-C09	8.05	1.57	1.42
29	B	848	WVN	C28-C25	8.05	1.54	1.35
29	B	850	WVN	C26-C22	8.05	1.54	1.35
29	A	857	WVN	C37-C34	8.04	1.54	1.35
35	a	316	II0	C21-C09	8.04	1.57	1.42
35	m	615	II0	C40-C36	8.04	1.54	1.35
29	B	848	WVN	C37-C34	8.04	1.54	1.35
35	h	311	II0	C40-C36	8.03	1.54	1.35
29	M	101	WVN	C37-C34	8.02	1.54	1.35
29	s	405	WVN	C26-C22	8.02	1.54	1.35
29	B	847	WVN	C26-C22	8.02	1.54	1.35
29	K	102	WVN	C26-C22	8.01	1.54	1.35
29	A	846	WVN	C37-C34	8.01	1.54	1.35
29	A	845	WVN	C37-C34	8.01	1.54	1.35
35	m	619	II0	C22-C10	8.00	1.57	1.42
35	c	316	II0	C22-C10	8.00	1.57	1.42
29	R	200	WVN	C26-C22	8.00	1.54	1.35
29	A	847	WVN	C37-C34	7.99	1.54	1.35
29	B	847	WVN	C37-C34	7.99	1.54	1.35
29	B	848	WVN	C26-C22	7.99	1.54	1.35
35	n	615	II0	C21-C09	7.99	1.57	1.42
29	L	205	WVN	C37-C34	7.99	1.54	1.35
29	A	846	WVN	C26-C22	7.99	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	302	II0	C22-C10	7.99	1.57	1.42
35	c	316	II0	C40-C36	7.98	1.54	1.35
29	s	407	WVN	C37-C34	7.98	1.54	1.35
29	R	200	WVN	C37-C34	7.98	1.54	1.35
29	R	200	WVN	C28-C25	7.97	1.54	1.35
29	B	846	WVN	C28-C25	7.97	1.54	1.35
29	A	857	WVN	C26-C22	7.97	1.54	1.35
29	B	850	WVN	C28-C25	7.96	1.54	1.35
29	J	101	WVN	C37-C34	7.95	1.54	1.35
29	F	203	WVN	C28-C25	7.95	1.54	1.35
29	A	848	WVN	C37-C34	7.94	1.54	1.35
35	d	317	II0	C22-C10	7.94	1.57	1.42
29	B	853	WVN	C26-C22	7.94	1.54	1.35
29	J	102	WVN	C28-C25	7.93	1.54	1.35
35	n	616	II0	C22-C10	7.93	1.57	1.42
29	i	315	WVN	C28-C25	7.93	1.54	1.35
29	B	853	WVN	C37-C34	7.93	1.54	1.35
29	A	846	WVN	C28-C25	7.93	1.54	1.35
29	B	847	WVN	C28-C25	7.92	1.54	1.35
29	L	205	WVN	C28-C25	7.92	1.54	1.35
35	i	313	II0	C22-C10	7.92	1.57	1.42
35	j	615	II0	C22-C10	7.92	1.57	1.42
29	F	203	WVN	C36-C32	7.92	1.54	1.35
29	l	316	WVN	C36-C32	7.91	1.54	1.35
29	M	101	WVN	C26-C22	7.91	1.54	1.35
29	l	303	WVN	C37-C34	7.91	1.54	1.35
29	i	315	WVN	C26-C22	7.90	1.54	1.35
29	K	102	WVN	C28-C25	7.90	1.54	1.35
29	h	309	WVN	C37-C34	7.90	1.54	1.35
35	i	312	II0	C22-C10	7.90	1.57	1.42
29	A	847	WVN	C28-C25	7.89	1.54	1.35
29	L	201	WVN	C37-C34	7.88	1.54	1.35
35	i	319	II0	C21-C09	7.88	1.57	1.42
35	m	615	II0	C22-C10	7.88	1.57	1.42
35	i	314	II0	C21-C09	7.88	1.57	1.42
29	J	102	WVN	C36-C32	7.88	1.54	1.35
29	B	853	WVN	C28-C25	7.88	1.54	1.35
29	l	303	WVN	C28-C25	7.88	1.54	1.35
29	B	846	WVN	C37-C34	7.87	1.54	1.35
29	L	201	WVN	C26-C22	7.86	1.54	1.35
35	h	310	II0	C21-C09	7.86	1.57	1.42
29	M	101	WVN	C28-C25	7.86	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	407	WVN	C28-C25	7.86	1.54	1.35
29	I	101	WVN	C37-C34	7.85	1.54	1.35
35	m	614	II0	C21-C09	7.85	1.57	1.42
29	h	309	WVN	C28-C25	7.85	1.53	1.35
29	J	102	WVN	C26-C22	7.84	1.53	1.35
29	F	203	WVN	C37-C34	7.84	1.53	1.35
29	s	405	WVN	C28-C25	7.83	1.53	1.35
29	B	846	WVN	C26-C22	7.83	1.53	1.35
35	i	314	II0	C22-C10	7.83	1.57	1.42
35	m	616	II0	C21-C09	7.83	1.57	1.42
35	k	616	II0	C22-C10	7.81	1.57	1.42
35	n	618	II0	C22-C10	7.81	1.57	1.42
29	J	101	WVN	C28-C25	7.81	1.53	1.35
35	h	312	II0	C21-C09	7.81	1.57	1.42
29	I	101	WVN	C26-C22	7.80	1.53	1.35
35	m	616	II0	C22-C10	7.80	1.57	1.42
35	a	316	II0	C22-C10	7.79	1.57	1.42
29	M	101	WVN	C36-C32	7.78	1.53	1.35
35	m	619	II0	C21-C09	7.78	1.57	1.42
29	B	848	WVN	C36-C32	7.76	1.53	1.35
29	A	848	WVN	C26-C22	7.76	1.53	1.35
29	B	847	WVN	C36-C32	7.76	1.53	1.35
29	R	200	WVN	C36-C32	7.75	1.53	1.35
35	c	313	II0	C22-C10	7.75	1.57	1.42
35	d	316	II0	C22-C10	7.75	1.57	1.42
29	L	201	WVN	C28-C25	7.75	1.53	1.35
29	l	316	WVN	C28-C25	7.74	1.53	1.35
35	i	316	II0	C21-C09	7.74	1.57	1.42
29	A	848	WVN	C28-C25	7.73	1.53	1.35
35	j	614	II0	C21-C09	7.73	1.57	1.42
29	I	101	WVN	C28-C25	7.73	1.53	1.35
29	A	845	WVN	C36-C32	7.72	1.53	1.35
29	B	849	WVN	C36-C32	7.72	1.53	1.35
29	A	857	WVN	C36-C32	7.71	1.53	1.35
35	a	314	II0	C22-C10	7.71	1.57	1.42
29	s	405	WVN	C36-C32	7.70	1.53	1.35
29	A	847	WVN	C36-C32	7.70	1.53	1.35
35	J	104	II0	C21-C09	7.69	1.57	1.42
29	J	101	WVN	C36-C32	7.69	1.53	1.35
35	m	614	II0	C22-C10	7.69	1.57	1.42
29	L	205	WVN	C36-C32	7.68	1.53	1.35
29	i	315	WVN	C36-C32	7.68	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	848	WVN	C36-C32	7.67	1.53	1.35
35	l	315	II0	C21-C09	7.67	1.57	1.42
29	A	846	WVN	C36-C32	7.66	1.53	1.35
35	l	314	II0	C22-C10	7.66	1.57	1.42
35	d	301	II0	C22-C10	7.65	1.56	1.42
35	d	315	II0	C22-C10	7.65	1.56	1.42
29	h	309	WVN	C36-C32	7.63	1.53	1.35
29	s	407	WVN	C36-C32	7.63	1.53	1.35
35	a	313	II0	C21-C09	7.63	1.56	1.42
29	l	303	WVN	C36-C32	7.62	1.53	1.35
35	b	314	II0	C21-C09	7.61	1.56	1.42
35	h	312	II0	C22-C10	7.61	1.56	1.42
35	k	620	II0	C21-C09	7.61	1.56	1.42
35	a	312	II0	C21-C09	7.60	1.56	1.42
29	B	853	WVN	C36-C32	7.60	1.53	1.35
29	B	850	WVN	C36-C32	7.60	1.53	1.35
35	k	619	II0	C21-C09	7.59	1.56	1.42
29	L	201	WVN	C36-C32	7.58	1.53	1.35
35	d	317	II0	C21-C09	7.58	1.56	1.42
35	n	616	II0	C21-C09	7.58	1.56	1.42
35	c	316	II0	C21-C09	7.57	1.56	1.42
35	b	315	II0	C21-C09	7.57	1.56	1.42
35	i	312	II0	C21-C09	7.56	1.56	1.42
35	n	615	II0	C22-C10	7.55	1.56	1.42
35	n	618	II0	C21-C09	7.54	1.56	1.42
35	l	315	II0	C22-C10	7.54	1.56	1.42
29	K	102	WVN	C36-C32	7.52	1.53	1.35
35	i	316	II0	C22-C10	7.51	1.56	1.42
35	i	313	II0	C21-C09	7.50	1.56	1.42
35	k	620	II0	C22-C10	7.50	1.56	1.42
35	l	314	II0	C21-C09	7.50	1.56	1.42
29	I	101	WVN	C36-C32	7.49	1.53	1.35
35	c	313	II0	C21-C09	7.47	1.56	1.42
35	k	619	II0	C22-C10	7.47	1.56	1.42
35	m	615	II0	C21-C09	7.47	1.56	1.42
35	k	615	II0	C21-C09	7.46	1.56	1.42
35	h	311	II0	C22-C10	7.45	1.56	1.42
35	j	615	II0	C21-C09	7.44	1.56	1.42
35	j	614	II0	C22-C10	7.41	1.56	1.42
29	B	846	WVN	C36-C32	7.41	1.52	1.35
35	a	313	II0	C22-C10	7.41	1.56	1.42
35	a	314	II0	C21-C09	7.40	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	315	II0	C21-C09	7.39	1.56	1.42
35	d	301	II0	C21-C09	7.39	1.56	1.42
35	J	104	II0	C22-C10	7.38	1.56	1.42
35	h	311	II0	C21-C09	7.35	1.56	1.42
35	a	312	II0	C22-C10	7.30	1.56	1.42
35	b	314	II0	C22-C10	7.24	1.56	1.42
36	s	401	KC2	C2A-C3A	6.86	1.51	1.37
36	c	310	KC2	C2A-C3A	6.68	1.50	1.37
36	c	310	KC2	CBA-CAA	6.43	1.52	1.33
35	i	313	II0	C24-C22	6.43	1.38	1.20
35	i	314	II0	C24-C22	6.41	1.38	1.20
35	m	619	II0	C24-C22	6.38	1.38	1.20
35	d	317	II0	C24-C22	6.37	1.38	1.20
35	l	302	II0	C24-C22	6.35	1.38	1.20
35	j	615	II0	C24-C22	6.35	1.38	1.20
36	s	401	KC2	CBA-CAA	6.35	1.52	1.33
35	b	315	II0	C24-C22	6.35	1.38	1.20
35	k	615	II0	C24-C22	6.34	1.38	1.20
35	m	616	II0	C24-C22	6.29	1.38	1.20
35	c	316	II0	C24-C22	6.29	1.37	1.20
35	k	616	II0	C24-C22	6.28	1.37	1.20
35	n	618	II0	C24-C22	6.27	1.37	1.20
35	m	615	II0	C24-C22	6.26	1.37	1.20
35	i	319	II0	C24-C22	6.25	1.37	1.20
35	n	616	II0	C23-C21	6.25	1.37	1.20
35	h	312	II0	C24-C22	6.20	1.37	1.20
35	a	314	II0	C24-C22	6.15	1.37	1.20
35	i	312	II0	C24-C22	6.15	1.37	1.20
35	a	316	II0	C23-C21	6.13	1.37	1.20
35	d	316	II0	C23-C21	6.12	1.37	1.20
35	n	616	II0	C24-C22	6.12	1.37	1.20
35	i	314	II0	C23-C21	6.11	1.37	1.20
35	k	616	II0	C23-C21	6.10	1.37	1.20
35	m	614	II0	C24-C22	6.09	1.37	1.20
35	a	313	II0	C24-C22	6.08	1.37	1.20
35	m	616	II0	C23-C21	6.08	1.37	1.20
35	i	313	II0	C23-C21	6.08	1.37	1.20
35	d	316	II0	C24-C22	6.07	1.37	1.20
35	l	314	II0	C24-C22	6.06	1.37	1.20
35	j	614	II0	C24-C22	6.03	1.37	1.20
35	k	620	II0	C24-C22	6.02	1.37	1.20
35	c	313	II0	C24-C22	6.02	1.37	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	315	II0	C23-C21	6.02	1.37	1.20
35	d	301	II0	C24-C22	6.02	1.37	1.20
35	d	315	II0	C24-C22	5.99	1.37	1.20
35	a	316	II0	C24-C22	5.99	1.37	1.20
35	d	317	II0	C23-C21	5.99	1.37	1.20
35	J	104	II0	C24-C22	5.99	1.37	1.20
35	n	615	II0	C24-C22	5.98	1.37	1.20
35	i	316	II0	C24-C22	5.97	1.37	1.20
35	n	615	II0	C23-C21	5.97	1.37	1.20
35	i	312	II0	C23-C21	5.96	1.37	1.20
35	i	316	II0	C23-C21	5.95	1.37	1.20
35	k	619	II0	C24-C22	5.95	1.37	1.20
35	h	311	II0	C23-C21	5.94	1.37	1.20
35	h	311	II0	C24-C22	5.94	1.37	1.20
35	a	312	II0	C24-C22	5.92	1.36	1.20
35	l	315	II0	C24-C22	5.91	1.36	1.20
35	k	615	II0	C23-C21	5.90	1.36	1.20
35	a	314	II0	C23-C21	5.89	1.36	1.20
35	l	315	II0	C23-C21	5.89	1.36	1.20
35	d	301	II0	C23-C21	5.89	1.36	1.20
35	b	314	II0	C24-C22	5.88	1.36	1.20
35	b	314	II0	C23-C21	5.88	1.36	1.20
35	k	620	II0	C23-C21	5.87	1.36	1.20
35	m	614	II0	C23-C21	5.86	1.36	1.20
35	k	619	II0	C23-C21	5.86	1.36	1.20
35	J	104	II0	C23-C21	5.85	1.36	1.20
36	s	401	KC2	C3B-C2B	5.84	1.49	1.37
35	c	316	II0	C23-C21	5.84	1.36	1.20
35	l	314	II0	C23-C21	5.82	1.36	1.20
35	a	312	II0	C23-C21	5.82	1.36	1.20
35	j	615	II0	C23-C21	5.82	1.36	1.20
36	c	310	KC2	O2A-CGA	5.81	1.45	1.30
35	i	319	II0	C23-C21	5.79	1.36	1.20
35	c	313	II0	C23-C21	5.79	1.36	1.20
35	m	615	II0	C23-C21	5.78	1.36	1.20
35	j	614	II0	C23-C21	5.78	1.36	1.20
35	h	310	II0	C23-C21	5.77	1.36	1.20
35	m	619	II0	C23-C21	5.77	1.36	1.20
35	l	302	II0	C23-C21	5.77	1.36	1.20
35	a	313	II0	C23-C21	5.75	1.36	1.20
35	d	315	II0	C23-C21	5.75	1.36	1.20
35	h	312	II0	C23-C21	5.75	1.36	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	s	401	KC2	O2A-CGA	5.72	1.45	1.30
35	n	618	II0	C23-C21	5.72	1.36	1.20
36	c	310	KC2	C3B-C2B	5.43	1.48	1.37
29	l	316	WVN	C19-C22	5.29	1.57	1.46
35	m	616	II0	C33-C35	5.27	1.57	1.46
29	B	850	WVN	C19-C22	5.21	1.57	1.46
29	l	316	WVN	C31-C32	5.19	1.57	1.46
29	B	849	WVN	C19-C22	5.19	1.57	1.46
29	B	848	WVN	C19-C22	5.18	1.57	1.46
29	A	846	WVN	C19-C22	5.13	1.56	1.46
29	i	315	WVN	C19-C22	5.13	1.56	1.46
36	c	310	KC2	C3C-C2C	5.13	1.47	1.37
29	s	407	WVN	C19-C22	5.12	1.56	1.46
29	A	845	WVN	C02-C11	5.12	1.57	1.50
29	R	200	WVN	C19-C22	5.12	1.56	1.46
29	B	853	WVN	C19-C22	5.10	1.56	1.46
29	B	847	WVN	C19-C22	5.09	1.56	1.46
29	A	845	WVN	C19-C22	5.08	1.56	1.46
29	l	303	WVN	C19-C22	5.07	1.56	1.46
29	B	847	WVN	C31-C32	5.06	1.56	1.46
29	L	205	WVN	C19-C22	5.05	1.56	1.46
29	F	203	WVN	C19-C22	5.05	1.56	1.46
29	K	102	WVN	C19-C22	5.05	1.56	1.46
29	A	857	WVN	C19-C22	5.03	1.56	1.46
29	K	102	WVN	C31-C32	5.03	1.56	1.46
29	B	850	WVN	C31-C32	5.03	1.56	1.46
29	J	102	WVN	C19-C22	5.02	1.56	1.46
36	c	310	KC2	C1A-NA	-5.02	1.27	1.38
29	B	849	WVN	C31-C32	5.01	1.56	1.46
36	s	401	KC2	C1A-NA	-5.01	1.27	1.38
29	R	200	WVN	C31-C32	5.01	1.56	1.46
29	B	848	WVN	C31-C32	4.99	1.56	1.46
29	i	315	WVN	C31-C32	4.98	1.56	1.46
29	A	848	WVN	C19-C22	4.98	1.56	1.46
29	J	101	WVN	C19-C22	4.98	1.56	1.46
29	s	405	WVN	C19-C22	4.98	1.56	1.46
29	h	309	WVN	C19-C22	4.98	1.56	1.46
29	l	316	WVN	C39-C36	4.97	1.58	1.43
29	h	309	WVN	C31-C32	4.95	1.56	1.46
29	A	845	WVN	C31-C32	4.95	1.56	1.46
29	A	846	WVN	C31-C32	4.95	1.56	1.46
29	M	101	WVN	C31-C32	4.93	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	203	WVN	C31-C32	4.93	1.56	1.46
29	L	205	WVN	C31-C32	4.91	1.56	1.46
29	s	405	WVN	C31-C32	4.91	1.56	1.46
29	A	857	WVN	C31-C32	4.91	1.56	1.46
29	l	303	WVN	C31-C32	4.91	1.56	1.46
29	B	853	WVN	C31-C32	4.90	1.56	1.46
29	J	102	WVN	C39-C36	4.90	1.58	1.43
29	A	847	WVN	C31-C32	4.88	1.56	1.46
29	s	407	WVN	C31-C32	4.88	1.56	1.46
29	l	316	WVN	C02-C11	4.87	1.57	1.50
29	A	847	WVN	C19-C22	4.86	1.56	1.46
29	I	101	WVN	C19-C22	4.85	1.56	1.46
36	c	310	KC2	CHD-C4C	4.85	1.48	1.38
29	l	316	WVN	C40-C37	4.84	1.58	1.43
35	i	313	II0	C41-C39	4.84	1.58	1.43
35	b	315	II0	C42-C40	4.83	1.58	1.43
35	b	315	II0	C41-C39	4.82	1.58	1.43
29	J	101	WVN	C31-C32	4.81	1.56	1.46
35	b	314	II0	C31-C29	4.81	1.58	1.43
29	A	848	WVN	C02-C11	4.81	1.57	1.50
35	l	302	II0	C31-C29	4.81	1.58	1.43
35	b	314	II0	C41-C39	4.81	1.58	1.43
29	i	315	WVN	C39-C36	4.81	1.58	1.43
35	n	615	II0	C31-C29	4.80	1.58	1.43
29	A	847	WVN	C39-C36	4.80	1.58	1.43
29	B	850	WVN	C39-C36	4.80	1.58	1.43
29	B	849	WVN	C39-C36	4.79	1.58	1.43
35	b	315	II0	C31-C29	4.79	1.58	1.43
29	A	857	WVN	C39-C36	4.78	1.58	1.43
36	s	401	KC2	C3C-C2C	4.78	1.46	1.37
35	k	619	II0	C31-C29	4.78	1.58	1.43
29	A	846	WVN	C39-C36	4.78	1.58	1.43
35	m	619	II0	C31-C29	4.78	1.58	1.43
29	B	848	WVN	C39-C36	4.77	1.58	1.43
35	k	620	II0	C31-C29	4.77	1.58	1.43
29	A	845	WVN	C39-C36	4.77	1.58	1.43
29	R	200	WVN	C39-C36	4.77	1.58	1.43
29	i	315	WVN	C02-C11	4.77	1.57	1.50
29	K	102	WVN	C39-C36	4.77	1.58	1.43
29	B	847	WVN	C39-C36	4.77	1.58	1.43
29	J	102	WVN	C31-C32	4.77	1.56	1.46
29	M	101	WVN	C39-C36	4.77	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	102	WVN	C40-C37	4.76	1.57	1.43
26	c	309	CLA	O2D-CGD	4.76	1.44	1.33
35	m	614	II0	C31-C29	4.76	1.57	1.43
35	i	313	II0	C31-C29	4.76	1.57	1.43
35	m	616	II0	C31-C29	4.76	1.57	1.43
35	J	104	II0	C31-C29	4.75	1.57	1.43
35	m	616	II0	C41-C39	4.75	1.57	1.43
29	L	205	WVN	C39-C36	4.75	1.57	1.43
29	F	203	WVN	C39-C36	4.74	1.57	1.43
35	a	313	II0	C31-C29	4.74	1.57	1.43
35	l	315	II0	C41-C39	4.74	1.57	1.43
29	B	853	WVN	C02-C11	4.74	1.57	1.50
35	n	618	II0	C31-C29	4.73	1.57	1.43
29	s	405	WVN	C39-C36	4.73	1.57	1.43
36	c	310	KC2	O2D-CGD	4.73	1.44	1.33
29	B	847	WVN	C02-C11	4.73	1.57	1.50
29	I	101	WVN	C31-C32	4.72	1.56	1.46
35	l	315	II0	C31-C29	4.72	1.57	1.43
29	R	200	WVN	C02-C11	4.72	1.57	1.50
35	n	615	II0	C41-C39	4.72	1.57	1.43
35	m	616	II0	C27-C25	4.72	1.54	1.50
35	m	614	II0	C41-C39	4.72	1.57	1.43
35	b	314	II0	C33-C35	4.71	1.56	1.46
35	j	614	II0	C31-C29	4.71	1.57	1.43
35	k	619	II0	C41-C39	4.71	1.57	1.43
29	I	101	WVN	C02-C11	4.70	1.57	1.50
29	s	407	WVN	C39-C36	4.70	1.57	1.43
35	i	316	II0	C31-C29	4.70	1.57	1.43
35	i	319	II0	C31-C29	4.70	1.57	1.43
35	k	615	II0	C41-C39	4.70	1.57	1.43
29	B	850	WVN	C40-C37	4.70	1.57	1.43
29	J	102	WVN	C02-C11	4.70	1.57	1.50
35	d	317	II0	C41-C39	4.69	1.57	1.43
35	h	312	II0	C31-C29	4.69	1.57	1.43
35	a	314	II0	C31-C29	4.69	1.57	1.43
35	d	301	II0	C31-C29	4.69	1.57	1.43
35	i	313	II0	C42-C40	4.69	1.57	1.43
35	m	619	II0	C41-C39	4.69	1.57	1.43
35	a	313	II0	C41-C39	4.69	1.57	1.43
35	d	317	II0	C31-C29	4.69	1.57	1.43
29	J	101	WVN	C39-C36	4.69	1.57	1.43
35	i	312	II0	C41-C39	4.69	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	853	WVN	C39-C36	4.69	1.57	1.43
29	B	849	WVN	C40-C37	4.68	1.57	1.43
29	l	303	WVN	C39-C36	4.68	1.57	1.43
35	a	312	II0	C31-C29	4.68	1.57	1.43
29	i	315	WVN	C40-C37	4.68	1.57	1.43
29	L	201	WVN	C31-C32	4.68	1.56	1.46
35	a	314	II0	C33-C35	4.68	1.56	1.46
35	d	315	II0	C41-C39	4.68	1.57	1.43
35	d	316	II0	C41-C39	4.68	1.57	1.43
35	i	319	II0	C41-C39	4.67	1.57	1.43
35	j	615	II0	C31-C29	4.67	1.57	1.43
35	m	615	II0	C31-C29	4.67	1.57	1.43
26	c	309	CLA	C3D-C4D	-4.67	1.33	1.44
29	h	309	WVN	C39-C36	4.67	1.57	1.43
35	l	302	II0	C32-C30	4.67	1.57	1.43
35	h	311	II0	C31-C29	4.67	1.57	1.43
36	s	401	KC2	CHD-C4C	4.67	1.47	1.38
35	k	619	II0	C33-C35	4.67	1.55	1.46
35	J	104	II0	C41-C39	4.67	1.57	1.43
35	i	314	II0	C31-C29	4.66	1.57	1.43
29	A	857	WVN	C40-C37	4.66	1.57	1.43
35	l	302	II0	C42-C40	4.66	1.57	1.43
29	L	201	WVN	C19-C22	4.66	1.55	1.46
35	a	316	II0	C31-C29	4.66	1.57	1.43
35	i	314	II0	C41-C39	4.65	1.57	1.43
35	l	314	II0	C31-C29	4.65	1.57	1.43
35	n	616	II0	C41-C39	4.65	1.57	1.43
35	l	314	II0	C41-C39	4.65	1.57	1.43
35	c	313	II0	C41-C39	4.65	1.57	1.43
35	j	615	II0	C41-C39	4.64	1.57	1.43
35	n	618	II0	C41-C39	4.64	1.57	1.43
35	i	316	II0	C41-C39	4.64	1.57	1.43
29	A	847	WVN	C40-C37	4.64	1.57	1.43
35	d	301	II0	C33-C35	4.64	1.55	1.46
29	R	200	WVN	C40-C37	4.63	1.57	1.43
35	c	316	II0	C31-C29	4.63	1.57	1.43
29	A	857	WVN	C02-C11	4.63	1.57	1.50
35	a	312	II0	C41-C39	4.63	1.57	1.43
35	n	618	II0	C32-C30	4.63	1.57	1.43
35	h	312	II0	C41-C39	4.63	1.57	1.43
35	a	316	II0	C41-C39	4.63	1.57	1.43
35	h	311	II0	C32-C30	4.63	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	846	WVN	C39-C36	4.63	1.57	1.43
35	c	313	II0	C31-C29	4.63	1.57	1.43
35	j	614	II0	C41-C39	4.62	1.57	1.43
29	A	846	WVN	C40-C37	4.62	1.57	1.43
29	B	847	WVN	C40-C37	4.62	1.57	1.43
29	M	101	WVN	C19-C22	4.62	1.55	1.46
35	d	316	II0	C31-C29	4.62	1.57	1.43
35	h	311	II0	C41-C39	4.62	1.57	1.43
35	n	616	II0	C31-C29	4.61	1.57	1.43
29	A	848	WVN	C39-C36	4.61	1.57	1.43
35	b	315	II0	C32-C30	4.61	1.57	1.43
29	A	845	WVN	C40-C37	4.61	1.57	1.43
29	F	203	WVN	C02-C11	4.61	1.57	1.50
29	s	405	WVN	C40-C37	4.61	1.57	1.43
35	n	615	II0	C42-C40	4.61	1.57	1.43
35	k	620	II0	C41-C39	4.61	1.57	1.43
35	k	616	II0	C41-C39	4.61	1.57	1.43
35	d	315	II0	C31-C29	4.61	1.57	1.43
29	M	101	WVN	C40-C37	4.60	1.57	1.43
29	L	201	WVN	C39-C36	4.60	1.57	1.43
35	a	313	II0	C42-C40	4.60	1.57	1.43
35	m	614	II0	C42-C40	4.60	1.57	1.43
35	m	614	II0	C32-C30	4.60	1.57	1.43
29	A	846	WVN	C02-C11	4.60	1.57	1.50
35	a	314	II0	C41-C39	4.59	1.57	1.43
35	m	619	II0	C32-C30	4.59	1.57	1.43
35	i	313	II0	C33-C35	4.59	1.55	1.46
29	B	848	WVN	C02-C11	4.59	1.57	1.50
35	m	616	II0	C42-C40	4.59	1.57	1.43
35	b	314	II0	C42-C40	4.58	1.57	1.43
35	l	315	II0	C32-C30	4.58	1.57	1.43
29	l	316	WVN	C29-C26	4.58	1.57	1.43
29	K	102	WVN	C40-C37	4.58	1.57	1.43
35	a	313	II0	C32-C30	4.58	1.57	1.43
29	I	101	WVN	C39-C36	4.58	1.57	1.43
29	B	848	WVN	C40-C37	4.58	1.57	1.43
35	d	301	II0	C41-C39	4.58	1.57	1.43
29	L	205	WVN	C40-C37	4.57	1.57	1.43
35	d	317	II0	C42-C40	4.57	1.57	1.43
35	c	316	II0	C41-C39	4.57	1.57	1.43
29	J	101	WVN	C02-C11	4.56	1.57	1.50
29	h	309	WVN	C02-C11	4.56	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	302	II0	C33-C35	4.56	1.55	1.46
29	J	101	WVN	C40-C37	4.56	1.57	1.43
35	m	619	II0	C42-C40	4.56	1.57	1.43
29	F	203	WVN	C40-C37	4.56	1.57	1.43
35	i	312	II0	C31-C29	4.56	1.57	1.43
35	a	314	II0	C32-C30	4.56	1.57	1.43
35	n	615	II0	C32-C30	4.56	1.57	1.43
35	a	316	II0	C32-C30	4.56	1.57	1.43
36	s	401	KC2	O2D-CGD	4.55	1.44	1.33
35	i	319	II0	C42-C40	4.55	1.57	1.43
35	l	302	II0	C41-C39	4.55	1.57	1.43
35	h	310	II0	C31-C29	4.55	1.57	1.43
35	m	619	II0	C33-C35	4.55	1.55	1.46
35	h	310	II0	C41-C39	4.55	1.57	1.43
35	m	614	II0	C33-C35	4.55	1.55	1.46
29	B	849	WVN	C23-C25	4.54	1.55	1.46
35	m	615	II0	C41-C39	4.54	1.57	1.43
35	i	312	II0	C42-C40	4.54	1.57	1.43
35	m	616	II0	C32-C30	4.54	1.57	1.43
29	l	303	WVN	C02-C11	4.54	1.57	1.50
29	B	849	WVN	C02-C11	4.54	1.57	1.50
35	J	104	II0	C42-C40	4.54	1.57	1.43
35	a	316	II0	C42-C40	4.53	1.57	1.43
35	j	614	II0	C33-C35	4.53	1.55	1.46
29	B	853	WVN	C40-C37	4.53	1.57	1.43
35	c	313	II0	C32-C30	4.53	1.57	1.43
35	n	616	II0	C32-C30	4.53	1.57	1.43
29	L	205	WVN	C02-C11	4.53	1.57	1.50
29	A	848	WVN	C31-C32	4.53	1.55	1.46
35	l	315	II0	C33-C35	4.53	1.55	1.46
35	h	312	II0	C32-C30	4.53	1.57	1.43
35	j	614	II0	C42-C40	4.53	1.57	1.43
35	d	301	II0	C32-C30	4.53	1.57	1.43
35	c	313	II0	C42-C40	4.53	1.57	1.43
35	k	616	II0	C31-C29	4.53	1.57	1.43
29	s	407	WVN	C40-C37	4.53	1.57	1.43
35	d	316	II0	C32-C30	4.52	1.57	1.43
26	c	309	CLA	O2A-CGA	4.52	1.45	1.30
35	k	615	II0	C42-C40	4.52	1.57	1.43
29	h	309	WVN	C40-C37	4.52	1.57	1.43
35	k	619	II0	C32-C30	4.52	1.57	1.43
35	k	619	II0	C42-C40	4.52	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	316	II0	C42-C40	4.52	1.57	1.43
29	F	203	WVN	C23-C25	4.52	1.55	1.46
35	i	313	II0	C32-C30	4.52	1.57	1.43
35	j	615	II0	C32-C30	4.52	1.57	1.43
35	d	317	II0	C32-C30	4.51	1.57	1.43
29	l	303	WVN	C40-C37	4.51	1.57	1.43
35	k	615	II0	C31-C29	4.50	1.57	1.43
35	l	314	II0	C42-C40	4.50	1.57	1.43
35	d	301	II0	C42-C40	4.49	1.57	1.43
35	d	315	II0	C42-C40	4.49	1.57	1.43
35	i	319	II0	C32-C30	4.49	1.57	1.43
35	i	316	II0	C42-C40	4.49	1.57	1.43
35	k	616	II0	C32-C30	4.49	1.57	1.43
29	B	846	WVN	C40-C37	4.49	1.57	1.43
35	n	618	II0	C42-C40	4.49	1.57	1.43
29	A	845	WVN	C30-C28	4.49	1.57	1.43
29	s	407	WVN	C29-C26	4.49	1.57	1.43
35	j	614	II0	C32-C30	4.49	1.57	1.43
29	A	845	WVN	C23-C25	4.49	1.55	1.46
29	B	850	WVN	C29-C26	4.48	1.57	1.43
35	k	616	II0	C42-C40	4.48	1.57	1.43
35	a	312	II0	C42-C40	4.48	1.57	1.43
35	b	315	II0	C33-C35	4.48	1.55	1.46
35	h	310	II0	C42-C40	4.48	1.57	1.43
35	m	615	II0	C32-C30	4.48	1.57	1.43
29	A	846	WVN	C23-C25	4.48	1.55	1.46
29	s	405	WVN	C02-C11	4.48	1.56	1.50
29	s	407	WVN	C02-C11	4.48	1.56	1.50
35	h	311	II0	C33-C35	4.47	1.55	1.46
35	j	615	II0	C42-C40	4.47	1.57	1.43
35	n	616	II0	C42-C40	4.47	1.57	1.43
29	L	201	WVN	C40-C37	4.47	1.57	1.43
29	J	102	WVN	C30-C28	4.47	1.57	1.43
35	h	312	II0	C42-C40	4.47	1.57	1.43
35	k	615	II0	C32-C30	4.47	1.57	1.43
29	K	102	WVN	C29-C26	4.46	1.57	1.43
35	a	314	II0	C42-C40	4.46	1.57	1.43
29	B	849	WVN	C30-C28	4.46	1.57	1.43
35	k	620	II0	C32-C30	4.46	1.57	1.43
35	i	314	II0	C32-C30	4.46	1.57	1.43
29	A	845	WVN	C29-C26	4.46	1.57	1.43
29	I	101	WVN	C40-C37	4.46	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	i	314	II0	C42-C40	4.46	1.57	1.43
36	c	310	KC2	CHC-C4B	4.45	1.47	1.38
29	L	205	WVN	C23-C25	4.45	1.55	1.46
35	l	314	II0	C32-C30	4.45	1.57	1.43
29	L	205	WVN	C29-C26	4.45	1.57	1.43
29	B	846	WVN	C30-C28	4.44	1.57	1.43
35	i	312	II0	C32-C30	4.44	1.57	1.43
29	R	200	WVN	C30-C28	4.44	1.57	1.43
35	i	316	II0	C32-C30	4.44	1.57	1.43
29	B	848	WVN	C29-C26	4.44	1.57	1.43
29	B	847	WVN	C30-C28	4.44	1.57	1.43
35	k	620	II0	C42-C40	4.44	1.57	1.43
29	B	846	WVN	C31-C32	4.44	1.55	1.46
35	c	316	II0	C32-C30	4.44	1.56	1.43
29	A	848	WVN	C40-C37	4.44	1.56	1.43
35	d	315	II0	C32-C30	4.44	1.56	1.43
35	J	104	II0	C32-C30	4.43	1.56	1.43
35	b	314	II0	C32-C30	4.43	1.56	1.43
29	A	847	WVN	C29-C26	4.43	1.56	1.43
29	s	405	WVN	C30-C28	4.43	1.56	1.43
29	F	203	WVN	C29-C26	4.42	1.56	1.43
29	l	303	WVN	C29-C26	4.42	1.56	1.43
29	i	315	WVN	C30-C28	4.42	1.56	1.43
29	B	848	WVN	C23-C25	4.42	1.55	1.46
29	B	853	WVN	C23-C25	4.42	1.55	1.46
35	a	312	II0	C32-C30	4.42	1.56	1.43
35	h	311	II0	C42-C40	4.42	1.56	1.43
29	B	853	WVN	C29-C26	4.41	1.56	1.43
29	A	847	WVN	C23-C25	4.41	1.55	1.46
29	A	846	WVN	C29-C26	4.41	1.56	1.43
35	c	316	II0	C42-C40	4.41	1.56	1.43
29	L	205	WVN	C30-C28	4.41	1.56	1.43
29	l	316	WVN	C30-C28	4.41	1.56	1.43
29	i	315	WVN	C29-C26	4.41	1.56	1.43
29	B	850	WVN	C23-C25	4.41	1.55	1.46
29	R	200	WVN	C29-C26	4.41	1.56	1.43
29	B	847	WVN	C29-C26	4.41	1.56	1.43
29	B	850	WVN	C02-C11	4.40	1.56	1.50
29	A	857	WVN	C30-C28	4.40	1.56	1.43
29	B	849	WVN	C29-C26	4.40	1.56	1.43
29	B	847	WVN	C23-C25	4.40	1.55	1.46
29	B	848	WVN	C30-C28	4.40	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	203	WVN	C30-C28	4.40	1.56	1.43
29	s	405	WVN	C29-C26	4.40	1.56	1.43
29	h	309	WVN	C29-C26	4.40	1.56	1.43
35	m	615	II0	C42-C40	4.40	1.56	1.43
29	M	101	WVN	C23-C25	4.39	1.55	1.46
29	i	315	WVN	C23-C25	4.39	1.55	1.46
29	A	847	WVN	C02-C11	4.39	1.56	1.50
29	A	846	WVN	C30-C28	4.39	1.56	1.43
29	A	857	WVN	C29-C26	4.39	1.56	1.43
29	J	101	WVN	C29-C26	4.38	1.56	1.43
35	l	315	II0	C42-C40	4.38	1.56	1.43
29	A	857	WVN	C23-C25	4.37	1.55	1.46
29	J	101	WVN	C23-C25	4.37	1.55	1.46
35	n	615	II0	C33-C35	4.37	1.55	1.46
29	l	303	WVN	C30-C28	4.36	1.56	1.43
29	M	101	WVN	C30-C28	4.36	1.56	1.43
29	K	102	WVN	C30-C28	4.36	1.56	1.43
29	K	102	WVN	C23-C25	4.36	1.55	1.46
29	J	102	WVN	C23-C25	4.36	1.55	1.46
29	A	847	WVN	C30-C28	4.36	1.56	1.43
35	k	620	II0	C33-C35	4.36	1.55	1.46
35	l	314	II0	C33-C35	4.36	1.55	1.46
29	s	405	WVN	C23-C25	4.35	1.55	1.46
29	h	309	WVN	C30-C28	4.35	1.56	1.43
29	K	102	WVN	C02-C11	4.35	1.56	1.50
35	h	312	II0	C33-C35	4.35	1.55	1.46
35	J	104	II0	C33-C35	4.34	1.55	1.46
26	i	305	CLA	C1D-ND	4.34	1.43	1.37
29	B	853	WVN	C30-C28	4.34	1.56	1.43
35	i	316	II0	C33-C35	4.33	1.55	1.46
29	s	407	WVN	C30-C28	4.33	1.56	1.43
29	B	850	WVN	C30-C28	4.33	1.56	1.43
29	R	200	WVN	C23-C25	4.33	1.55	1.46
29	J	101	WVN	C30-C28	4.33	1.56	1.43
35	a	316	II0	C33-C35	4.32	1.55	1.46
35	d	315	II0	C33-C35	4.32	1.55	1.46
35	i	319	II0	C33-C35	4.32	1.55	1.46
29	J	102	WVN	C29-C26	4.32	1.56	1.43
35	c	316	II0	C33-C35	4.31	1.55	1.46
30	i	300	LMU	O5'-C5'	4.31	1.54	1.44
35	d	317	II0	C33-C35	4.31	1.55	1.46
35	n	618	II0	C33-C35	4.30	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	615	II0	C33-C35	4.30	1.55	1.46
29	L	201	WVN	C02-C11	4.30	1.56	1.50
35	i	314	II0	C33-C35	4.29	1.55	1.46
36	s	401	KC2	CHB-C1B	4.29	1.46	1.38
36	c	310	KC2	CHB-C1B	4.29	1.46	1.38
35	a	313	II0	C33-C35	4.29	1.55	1.46
29	l	303	WVN	C23-C25	4.28	1.55	1.46
29	L	201	WVN	C30-C28	4.28	1.56	1.43
30	A	850	LMU	O5'-C5'	4.28	1.54	1.44
35	a	312	II0	C33-C35	4.28	1.55	1.46
35	d	316	II0	C33-C35	4.28	1.55	1.46
29	L	201	WVN	C29-C26	4.27	1.56	1.43
29	B	846	WVN	C19-C22	4.27	1.55	1.46
35	n	616	II0	C33-C35	4.26	1.55	1.46
29	h	309	WVN	C23-C25	4.26	1.55	1.46
35	l	302	II0	C34-C36	4.26	1.55	1.46
29	M	101	WVN	C29-C26	4.26	1.56	1.43
35	b	315	II0	C34-C36	4.25	1.55	1.46
29	A	848	WVN	C30-C28	4.25	1.56	1.43
35	c	313	II0	C33-C35	4.25	1.55	1.46
35	l	315	II0	C34-C36	4.24	1.55	1.46
29	I	101	WVN	C30-C28	4.22	1.56	1.43
35	j	615	II0	C33-C35	4.22	1.55	1.46
29	I	101	WVN	C29-C26	4.21	1.56	1.43
29	s	407	WVN	C23-C25	4.21	1.55	1.46
29	B	846	WVN	C23-C25	4.21	1.55	1.46
29	A	848	WVN	C23-C25	4.20	1.55	1.46
29	A	848	WVN	C29-C26	4.20	1.56	1.43
29	I	101	WVN	C23-C25	4.20	1.54	1.46
29	L	201	WVN	C23-C25	4.20	1.54	1.46
29	M	101	WVN	C02-C11	4.20	1.56	1.50
26	A	827	CLA	C1D-ND	4.19	1.43	1.37
29	J	102	WVN	C33-C34	4.19	1.54	1.46
35	i	312	II0	C33-C35	4.19	1.54	1.46
35	a	313	II0	C34-C36	4.18	1.54	1.46
29	B	850	WVN	C33-C34	4.18	1.54	1.46
29	R	200	WVN	C33-C34	4.17	1.54	1.46
29	B	846	WVN	C29-C26	4.17	1.56	1.43
29	B	849	WVN	C33-C34	4.17	1.54	1.46
29	l	316	WVN	C23-C25	4.17	1.54	1.46
35	h	310	II0	C33-C35	4.15	1.54	1.46
35	m	619	II0	C34-C36	4.14	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	312	KC2	C3B-C4B	-4.14	1.38	1.46
30	i	300	LMU	O5B-C5B	4.14	1.54	1.44
36	c	310	KC2	C1D-ND	4.13	1.43	1.37
35	m	614	II0	C34-C36	4.13	1.54	1.46
35	n	618	II0	C34-C36	4.12	1.54	1.46
29	i	315	WVN	C33-C34	4.12	1.54	1.46
30	A	850	LMU	O5B-C5B	4.12	1.54	1.44
35	n	615	II0	C34-C36	4.12	1.54	1.46
36	m	611	KC2	C3B-C4B	-4.11	1.38	1.46
35	d	317	II0	C34-C36	4.11	1.54	1.46
29	A	845	WVN	C33-C34	4.10	1.54	1.46
35	i	313	II0	C34-C36	4.09	1.54	1.46
35	a	312	II0	C34-C36	4.09	1.54	1.46
36	s	404	KC2	C3B-C4B	-4.08	1.38	1.46
29	s	405	WVN	C33-C34	4.08	1.54	1.46
35	k	616	II0	C33-C35	4.08	1.54	1.46
26	k	604	CLA	C1D-ND	4.08	1.43	1.37
29	A	846	WVN	C33-C34	4.07	1.54	1.46
29	B	853	WVN	C33-C34	4.07	1.54	1.46
29	l	303	WVN	C33-C34	4.06	1.54	1.46
29	B	847	WVN	C33-C34	4.05	1.54	1.46
35	m	615	II0	C33-C35	4.05	1.54	1.46
36	k	613	KC2	C3B-C4B	-4.05	1.39	1.46
26	c	309	CLA	C3C-C2C	4.05	1.45	1.36
29	K	102	WVN	C33-C34	4.04	1.54	1.46
35	j	615	II0	C34-C36	4.04	1.54	1.46
29	L	205	WVN	C33-C34	4.04	1.54	1.46
29	l	316	WVN	C33-C34	4.04	1.54	1.46
26	B	825	CLA	C1D-ND	4.04	1.43	1.37
36	k	612	KC2	C3B-C4B	-4.03	1.39	1.46
29	B	848	WVN	C33-C34	4.03	1.54	1.46
36	s	401	KC2	CHC-C4B	4.03	1.46	1.38
36	k	611	KC2	C3B-C4B	-4.02	1.39	1.46
36	s	401	KC2	C4B-NB	-4.02	1.32	1.37
26	k	609	CLA	C1D-ND	4.02	1.43	1.37
36	i	318	KC2	C3B-C4B	-4.01	1.39	1.46
29	A	847	WVN	C33-C34	4.00	1.54	1.46
35	n	616	II0	C27-C25	4.00	1.53	1.50
35	m	616	II0	C34-C36	4.00	1.54	1.46
35	k	615	II0	C34-C36	4.00	1.54	1.46
29	A	857	WVN	C33-C34	4.00	1.54	1.46
35	a	316	II0	C34-C36	3.99	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	620	II0	C34-C36	3.98	1.54	1.46
36	j	611	KC2	C3B-C4B	-3.98	1.39	1.46
35	d	301	II0	C34-C36	3.98	1.54	1.46
29	M	101	WVN	C33-C34	3.97	1.54	1.46
35	c	313	II0	C34-C36	3.97	1.54	1.46
35	k	616	II0	C34-C36	3.97	1.54	1.46
35	h	312	II0	C34-C36	3.97	1.54	1.46
29	h	309	WVN	C33-C34	3.96	1.54	1.46
35	i	319	II0	C34-C36	3.96	1.54	1.46
29	F	203	WVN	C33-C34	3.96	1.54	1.46
26	B	816	CLA	C1D-ND	3.95	1.43	1.37
35	k	619	II0	C34-C36	3.95	1.54	1.46
35	J	104	II0	C34-C36	3.94	1.54	1.46
35	i	316	II0	C34-C36	3.94	1.54	1.46
29	J	101	WVN	C33-C34	3.93	1.54	1.46
35	i	312	II0	C34-C36	3.93	1.54	1.46
36	d	312	KC2	C3B-C4B	-3.93	1.39	1.46
35	i	314	II0	C34-C36	3.92	1.54	1.46
36	n	611	KC2	C3B-C4B	-3.92	1.39	1.46
35	a	314	II0	C34-C36	3.92	1.54	1.46
36	l	312	KC2	C1B-C2B	-3.91	1.37	1.45
35	d	315	II0	C34-C36	3.91	1.54	1.46
35	n	616	II0	C34-C36	3.91	1.54	1.46
26	A	817	CLA	C1D-ND	3.90	1.43	1.37
29	i	315	WVN	C20-C13	3.90	1.58	1.45
29	B	846	WVN	C02-C11	3.90	1.56	1.50
36	s	404	KC2	C1B-C2B	-3.90	1.37	1.45
35	h	310	II0	C34-C36	3.89	1.54	1.46
26	A	841	CLA	C1D-ND	3.89	1.43	1.37
36	i	309	KC2	C3B-C4B	-3.89	1.39	1.46
35	d	316	II0	C34-C36	3.88	1.54	1.46
35	c	316	II0	C34-C36	3.88	1.54	1.46
29	B	846	WVN	C33-C34	3.88	1.54	1.46
36	n	612	KC2	C3B-C4B	-3.88	1.39	1.46
35	h	311	II0	C34-C36	3.87	1.54	1.46
36	d	311	KC2	C3B-C4B	-3.87	1.39	1.46
29	L	201	WVN	C33-C34	3.87	1.54	1.46
35	l	314	II0	C34-C36	3.86	1.54	1.46
26	n	606	CLA	C1D-ND	3.86	1.42	1.37
36	s	401	KC2	C1B-NB	-3.85	1.32	1.37
26	n	608	CLA	C1D-ND	3.85	1.42	1.37
35	m	615	II0	C34-C36	3.85	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	848	WVN	C33-C34	3.83	1.54	1.46
36	d	312	KC2	C1B-C2B	-3.83	1.37	1.45
35	j	614	II0	C34-C36	3.83	1.54	1.46
29	s	407	WVN	C33-C34	3.83	1.54	1.46
26	A	823	CLA	C1D-ND	3.83	1.42	1.37
36	c	310	KC2	C1B-NB	-3.83	1.32	1.37
35	b	314	II0	C34-C36	3.80	1.54	1.46
29	I	101	WVN	C33-C34	3.80	1.54	1.46
26	A	821	CLA	C1D-ND	3.79	1.42	1.37
26	k	604	CLA	C4B-NB	3.79	1.42	1.37
29	s	405	WVN	C20-C13	3.77	1.58	1.45
26	l	313	CLA	C1D-ND	3.76	1.42	1.37
36	c	310	KC2	CHC-C1C	3.75	1.47	1.39
26	h	306	CLA	C1D-ND	3.75	1.42	1.37
29	R	200	WVN	C20-C13	3.75	1.57	1.45
26	a	303	CLA	C1D-ND	3.74	1.42	1.37
29	A	848	WVN	C20-C13	3.74	1.57	1.45
26	A	812	CLA	C1D-ND	3.74	1.42	1.37
35	k	615	II0	C20-C14	3.72	1.56	1.50
26	B	837	CLA	C1D-ND	3.72	1.42	1.37
26	m	610	CLA	C1D-ND	3.72	1.42	1.37
26	K	101	CLA	C1D-ND	3.71	1.42	1.37
26	j	606	CLA	C1D-ND	3.71	1.42	1.37
26	R	201	CLA	C1D-ND	3.71	1.42	1.37
26	B	832	CLA	C1D-ND	3.71	1.42	1.37
26	m	601	CLA	C1D-ND	3.71	1.42	1.37
26	n	603	CLA	C1D-ND	3.71	1.42	1.37
36	k	612	KC2	C1B-C2B	-3.71	1.38	1.45
26	j	605	CLA	C1D-ND	3.71	1.42	1.37
36	n	612	KC2	C1B-C2B	-3.71	1.38	1.45
26	d	306	CLA	C1D-ND	3.70	1.42	1.37
26	j	610	CLA	C1D-ND	3.70	1.42	1.37
26	c	302	CLA	C1D-ND	3.70	1.42	1.37
26	B	833	CLA	C1D-ND	3.70	1.42	1.37
26	c	303	CLA	C1D-ND	3.70	1.42	1.37
26	B	815	CLA	C1D-ND	3.70	1.42	1.37
36	n	611	KC2	C1B-C2B	-3.70	1.38	1.45
26	b	304	CLA	C1D-ND	3.69	1.42	1.37
26	A	840	CLA	C1D-ND	3.69	1.42	1.37
26	j	607	CLA	C1D-ND	3.69	1.42	1.37
26	d	303	CLA	C1D-ND	3.68	1.42	1.37
26	a	309	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	834	CLA	C1D-ND	3.68	1.42	1.37
26	B	812	CLA	C1D-ND	3.68	1.42	1.37
26	B	824	CLA	C1D-ND	3.68	1.42	1.37
26	j	608	CLA	C1D-ND	3.68	1.42	1.37
26	A	838	CLA	C1D-ND	3.67	1.42	1.37
36	m	611	KC2	C4A-C3A	-3.67	1.37	1.44
26	d	305	CLA	C1D-ND	3.67	1.42	1.37
26	A	836	CLA	C1D-ND	3.67	1.42	1.37
36	i	318	KC2	C1B-C2B	-3.67	1.38	1.45
26	k	610	CLA	C1D-ND	3.67	1.42	1.37
26	A	835	CLA	C1D-ND	3.67	1.42	1.37
26	n	609	CLA	C1D-ND	3.67	1.42	1.37
26	B	805	CLA	C1D-ND	3.67	1.42	1.37
26	A	826	CLA	C1D-ND	3.67	1.42	1.37
26	b	312	CLA	C1D-ND	3.67	1.42	1.37
26	i	301	CLA	C1D-ND	3.66	1.42	1.37
26	n	613	CLA	C1D-ND	3.66	1.42	1.37
26	B	811	CLA	C1D-ND	3.66	1.42	1.37
36	d	311	KC2	C1B-C2B	-3.66	1.38	1.45
26	F	202	CLA	C1D-ND	3.66	1.42	1.37
36	i	309	KC2	C1B-C2B	-3.65	1.38	1.45
26	a	308	CLA	C1D-ND	3.65	1.42	1.37
26	c	307	CLA	C1D-ND	3.65	1.42	1.37
26	B	803	CLA	C1D-ND	3.65	1.42	1.37
26	l	308	CLA	C1D-ND	3.65	1.42	1.37
26	h	307	CLA	C1D-ND	3.64	1.42	1.37
36	k	613	KC2	C1B-C2B	-3.64	1.38	1.45
26	d	318	CLA	C1D-ND	3.64	1.42	1.37
26	A	803	CLA	C4B-NB	3.64	1.42	1.37
26	a	306	CLA	C1D-ND	3.64	1.42	1.37
26	k	601	CLA	C1D-ND	3.64	1.42	1.37
36	m	611	KC2	C1B-C2B	-3.64	1.38	1.45
26	d	310	CLA	C1D-ND	3.64	1.42	1.37
26	i	307	CLA	C1D-ND	3.64	1.42	1.37
26	A	811	CLA	C1D-ND	3.64	1.42	1.37
26	A	837	CLA	C1D-ND	3.64	1.42	1.37
26	B	831	CLA	C1D-ND	3.64	1.42	1.37
26	A	808	CLA	C1D-ND	3.64	1.42	1.37
26	m	603	CLA	C1D-ND	3.64	1.42	1.37
26	m	613	CLA	C1D-ND	3.64	1.42	1.37
36	s	404	KC2	C4A-C3A	-3.63	1.37	1.44
26	k	605	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j	613	CLA	C1D-ND	3.63	1.42	1.37
26	A	818	CLA	C1D-ND	3.63	1.42	1.37
26	i	310	CLA	C1D-ND	3.63	1.42	1.37
26	B	841	CLA	C1D-ND	3.63	1.42	1.37
26	A	822	CLA	C1D-ND	3.63	1.42	1.37
26	A	824	CLA	C1D-ND	3.63	1.42	1.37
26	B	806	CLA	C1D-ND	3.63	1.42	1.37
26	c	301	CLA	C1D-ND	3.63	1.42	1.37
26	b	311	CLA	C1D-ND	3.63	1.42	1.37
26	A	832	CLA	C1D-ND	3.63	1.42	1.37
36	l	312	KC2	C4A-C3A	-3.62	1.37	1.44
26	F	201	CLA	C1D-ND	3.62	1.42	1.37
26	h	308	CLA	C1D-ND	3.62	1.42	1.37
26	B	838	CLA	C1D-ND	3.62	1.42	1.37
26	b	303	CLA	C1D-ND	3.61	1.42	1.37
26	A	806	CLA	C1D-ND	3.61	1.42	1.37
26	a	310	CLA	C1D-ND	3.61	1.42	1.37
26	i	306	CLA	C1D-ND	3.61	1.42	1.37
26	B	820	CLA	C1D-ND	3.61	1.42	1.37
26	i	303	CLA	C1D-ND	3.61	1.42	1.37
26	m	607	CLA	C1D-ND	3.61	1.42	1.37
26	B	821	CLA	C1D-ND	3.61	1.42	1.37
26	J	103	CLA	C1D-ND	3.61	1.42	1.37
26	b	307	CLA	C1D-ND	3.61	1.42	1.37
26	B	835	CLA	C4B-NB	3.61	1.42	1.37
26	B	828	CLA	C1D-ND	3.61	1.42	1.37
36	j	611	KC2	C1B-C2B	-3.61	1.38	1.45
26	b	309	CLA	C1D-ND	3.61	1.42	1.37
26	l	307	CLA	C1D-ND	3.60	1.42	1.37
26	B	810	CLA	C1D-ND	3.60	1.42	1.37
26	c	312	CLA	C1D-ND	3.60	1.42	1.37
26	B	819	CLA	C1D-ND	3.60	1.42	1.37
26	i	308	CLA	C1D-ND	3.60	1.42	1.37
26	a	304	CLA	C1D-ND	3.60	1.42	1.37
26	A	814	CLA	C1D-ND	3.60	1.42	1.37
26	n	601	CLA	C1D-ND	3.59	1.42	1.37
36	k	611	KC2	C1B-C2B	-3.59	1.38	1.45
26	B	840	CLA	C1D-ND	3.59	1.42	1.37
26	h	305	CLA	C1D-ND	3.59	1.42	1.37
26	m	608	CLA	C1D-ND	3.59	1.42	1.37
26	k	614	CLA	C1D-ND	3.59	1.42	1.37
26	d	309	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	815	CLA	C1D-ND	3.59	1.42	1.37
26	B	817	CLA	C1D-ND	3.59	1.42	1.37
26	s	402	CLA	C1D-ND	3.59	1.42	1.37
26	m	604	CLA	C1D-ND	3.59	1.42	1.37
26	a	311	CLA	C1D-ND	3.59	1.42	1.37
26	L	204	CLA	C1D-ND	3.58	1.42	1.37
26	d	307	CLA	C1D-ND	3.58	1.42	1.37
26	d	313	CLA	C1D-ND	3.58	1.42	1.37
26	n	605	CLA	C1D-ND	3.58	1.42	1.37
26	L	206	CLA	C1D-ND	3.58	1.42	1.37
26	l	304	CLA	C1D-ND	3.58	1.42	1.37
26	d	304	CLA	C1D-ND	3.58	1.42	1.37
26	A	852	CLA	C1D-ND	3.58	1.42	1.37
26	B	835	CLA	C1D-ND	3.58	1.42	1.37
26	c	306	CLA	C1D-ND	3.58	1.42	1.37
26	i	304	CLA	C1D-ND	3.58	1.42	1.37
26	A	830	CLA	C1D-ND	3.58	1.42	1.37
26	s	408	CLA	C1D-ND	3.58	1.42	1.37
26	n	610	CLA	C1D-ND	3.57	1.42	1.37
36	i	309	KC2	C4A-C3A	-3.57	1.37	1.44
26	A	820	CLA	C1D-ND	3.57	1.42	1.37
36	m	611	KC2	C1C-C2C	-3.57	1.37	1.44
26	L	202	CLA	C1D-ND	3.57	1.42	1.37
26	l	301	CLA	C1D-ND	3.57	1.42	1.37
26	B	808	CLA	C1D-ND	3.57	1.42	1.37
26	L	203	CLA	C1D-ND	3.57	1.42	1.37
26	c	304	CLA	C1D-ND	3.56	1.42	1.37
26	A	813	CLA	C1D-ND	3.56	1.42	1.37
26	l	306	CLA	C1D-ND	3.56	1.42	1.37
26	j	601	CLA	C1D-ND	3.56	1.42	1.37
26	A	851	CLA	C1D-ND	3.56	1.42	1.37
26	m	612	CLA	C1D-ND	3.56	1.42	1.37
26	b	313	CLA	C1D-ND	3.56	1.42	1.37
26	d	308	CLA	C1D-ND	3.56	1.42	1.37
26	A	809	CLA	C1D-ND	3.56	1.42	1.37
26	A	829	CLA	C1D-ND	3.56	1.42	1.37
26	B	834	CLA	C1D-ND	3.56	1.42	1.37
26	s	406	CLA	C1D-ND	3.56	1.42	1.37
26	h	303	CLA	C1D-ND	3.56	1.42	1.37
26	h	304	CLA	C1D-ND	3.55	1.42	1.37
26	B	829	CLA	C1D-ND	3.55	1.42	1.37
26	Q	302	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	807	CLA	C1D-ND	3.55	1.42	1.37
26	A	831	CLA	C1D-ND	3.55	1.42	1.37
26	d	302	CLA	C1D-ND	3.55	1.42	1.37
26	A	833	CLA	C1D-ND	3.55	1.42	1.37
26	B	802	CLA	C1D-ND	3.55	1.42	1.37
26	l	311	CLA	C1D-ND	3.55	1.42	1.37
26	j	603	CLA	C1D-ND	3.55	1.42	1.37
26	j	609	CLA	C1D-ND	3.55	1.42	1.37
26	B	827	CLA	C1D-ND	3.54	1.42	1.37
26	b	306	CLA	C1D-ND	3.54	1.42	1.37
26	h	302	CLA	C1D-ND	3.54	1.42	1.37
26	i	311	CLA	C1D-ND	3.54	1.42	1.37
26	m	605	CLA	C1D-ND	3.54	1.42	1.37
26	m	606	CLA	C1D-ND	3.54	1.42	1.37
36	s	401	KC2	C1D-ND	3.54	1.42	1.37
26	A	805	CLA	C1D-ND	3.54	1.42	1.37
26	h	301	CLA	C1D-ND	3.54	1.42	1.37
26	B	839	CLA	C1D-ND	3.53	1.42	1.37
26	c	305	CLA	C1D-ND	3.53	1.42	1.37
26	h	313	CLA	C1D-ND	3.53	1.42	1.37
26	B	807	CLA	C1D-ND	3.53	1.42	1.37
26	A	828	CLA	C1D-ND	3.53	1.42	1.37
26	k	608	CLA	C1D-ND	3.52	1.42	1.37
26	a	305	CLA	C1D-ND	3.52	1.42	1.37
26	B	813	CLA	C1D-ND	3.52	1.42	1.37
26	b	305	CLA	C1D-ND	3.52	1.42	1.37
26	k	607	CLA	C1D-ND	3.52	1.42	1.37
27	A	842	PQN	C11-C3	3.52	1.57	1.51
26	l	305	CLA	C1D-ND	3.52	1.42	1.37
27	A	842	PQN	C11-C12	3.52	1.56	1.50
26	l	310	CLA	C1D-ND	3.51	1.42	1.37
26	A	810	CLA	C1D-ND	3.51	1.42	1.37
26	A	816	CLA	C1D-ND	3.51	1.42	1.37
26	b	308	CLA	C1D-ND	3.51	1.42	1.37
26	A	839	CLA	C1D-ND	3.51	1.42	1.37
26	A	804	CLA	C1D-ND	3.51	1.42	1.37
26	c	311	CLA	C1D-ND	3.51	1.42	1.37
36	i	318	KC2	C4A-C3A	-3.51	1.37	1.44
26	B	809	CLA	C1D-ND	3.51	1.42	1.37
26	a	301	CLA	C1D-ND	3.50	1.42	1.37
26	A	819	CLA	C1D-ND	3.50	1.42	1.37
26	B	836	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	607	CLA	C1D-ND	3.49	1.42	1.37
26	R	201	CLA	C4B-NB	3.49	1.42	1.37
26	A	825	CLA	C1D-ND	3.48	1.42	1.37
29	B	846	WVN	C20-C13	3.48	1.57	1.45
36	c	310	KC2	C1A-CHA	3.47	1.49	1.40
26	j	604	CLA	C1D-ND	3.47	1.42	1.37
26	b	310	CLA	C1D-ND	3.47	1.42	1.37
26	j	612	CLA	C1D-ND	3.47	1.42	1.37
26	n	604	CLA	C1D-ND	3.47	1.42	1.37
26	m	609	CLA	C1D-ND	3.46	1.42	1.37
36	j	611	KC2	C4A-C3A	-3.46	1.37	1.44
26	k	606	CLA	C1D-ND	3.46	1.42	1.37
36	k	612	KC2	C4A-C3A	-3.46	1.37	1.44
26	B	801	CLA	C1D-ND	3.45	1.42	1.37
26	s	403	CLA	C1D-ND	3.45	1.42	1.37
26	n	603	CLA	C4B-NB	3.45	1.42	1.37
36	n	612	KC2	C4A-C3A	-3.45	1.37	1.44
26	B	826	CLA	C1D-ND	3.45	1.42	1.37
26	l	309	CLA	C1D-ND	3.45	1.42	1.37
26	n	602	CLA	C1D-ND	3.45	1.42	1.37
26	B	822	CLA	C1D-ND	3.43	1.42	1.37
26	j	602	CLA	C1D-ND	3.42	1.42	1.37
36	k	611	KC2	C4A-C3A	-3.42	1.37	1.44
26	k	603	CLA	C4B-NB	3.42	1.42	1.37
26	a	307	CLA	C1D-ND	3.42	1.42	1.37
26	A	856	CLA	C1D-ND	3.41	1.42	1.37
27	B	843	PQN	C11-C3	3.41	1.57	1.51
35	d	316	II0	C27-C25	3.41	1.53	1.50
26	A	803	CLA	C1D-ND	3.40	1.42	1.37
27	B	843	PQN	C11-C12	3.40	1.55	1.50
29	A	845	WVN	C20-C13	3.39	1.56	1.45
26	k	603	CLA	C1D-ND	3.39	1.42	1.37
36	k	613	KC2	C4A-C3A	-3.38	1.37	1.44
26	n	606	CLA	C4B-NB	3.38	1.42	1.37
26	B	842	CLA	C1D-ND	3.37	1.42	1.37
36	l	312	KC2	C1C-C2C	-3.37	1.37	1.44
26	n	608	CLA	C4B-NB	3.36	1.42	1.37
36	s	404	KC2	C1C-C2C	-3.36	1.37	1.44
26	m	602	CLA	C1D-ND	3.36	1.42	1.37
26	B	814	CLA	C1D-ND	3.35	1.42	1.37
26	a	302	CLA	C1D-ND	3.35	1.42	1.37
26	c	308	CLA	C1D-ND	3.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	836	CLA	C4B-NB	3.33	1.42	1.37
27	B	843	PQN	C2-C1	-3.32	1.40	1.47
26	B	830	CLA	C1D-ND	3.32	1.42	1.37
26	k	602	CLA	C1D-ND	3.32	1.42	1.37
26	i	302	CLA	C1D-ND	3.32	1.42	1.37
26	a	310	CLA	C4B-NB	3.32	1.42	1.37
29	B	848	WVN	C20-C13	3.31	1.56	1.45
36	s	401	KC2	C1A-CHA	3.31	1.48	1.40
36	k	613	KC2	C1C-C2C	-3.31	1.37	1.44
26	B	817	CLA	C4B-NB	3.31	1.42	1.37
26	h	307	CLA	C4B-NB	3.31	1.42	1.37
26	i	306	CLA	C4B-NB	3.30	1.42	1.37
36	d	311	KC2	C4A-C3A	-3.30	1.37	1.44
36	n	611	KC2	C4A-C3A	-3.30	1.37	1.44
36	d	312	KC2	C4A-C3A	-3.30	1.37	1.44
26	A	838	CLA	C4B-NB	3.29	1.42	1.37
29	R	200	WVN	C19-C11	3.29	1.39	1.32
29	B	847	WVN	C20-C13	3.29	1.56	1.45
36	s	401	KC2	CHC-C1C	3.29	1.46	1.39
26	B	832	CLA	C4B-NB	3.29	1.42	1.37
26	B	818	CLA	C1D-ND	3.28	1.42	1.37
26	B	823	CLA	C1D-ND	3.28	1.42	1.37
26	A	837	CLA	C4B-NB	3.28	1.42	1.37
26	B	810	CLA	C4B-NB	3.27	1.42	1.37
29	A	846	WVN	C20-C13	3.27	1.56	1.45
35	i	313	II0	C27-C25	3.27	1.53	1.50
26	l	313	CLA	C4B-NB	3.26	1.42	1.37
29	i	315	WVN	C19-C11	3.26	1.39	1.32
29	B	853	WVN	C20-C13	3.26	1.56	1.45
26	c	312	CLA	C4B-NB	3.26	1.42	1.37
26	a	306	CLA	C4B-NB	3.26	1.42	1.37
29	J	102	WVN	C20-C13	3.25	1.56	1.45
35	n	618	II0	C20-C14	3.25	1.56	1.50
26	A	832	CLA	C4B-NB	3.25	1.42	1.37
26	A	828	CLA	C4B-NB	3.25	1.42	1.37
26	A	829	CLA	C4B-NB	3.24	1.42	1.37
26	j	601	CLA	C4B-NB	3.24	1.42	1.37
26	b	310	CLA	C4B-NB	3.24	1.42	1.37
26	J	103	CLA	C4B-NB	3.24	1.42	1.37
26	n	613	CLA	C4B-NB	3.24	1.42	1.37
26	F	202	CLA	C4B-NB	3.24	1.42	1.37
29	B	849	WVN	C20-C13	3.23	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	857	WVN	C19-C11	3.23	1.39	1.32
26	A	813	CLA	C4B-NB	3.23	1.42	1.37
26	l	301	CLA	C4B-NB	3.23	1.42	1.37
29	A	857	WVN	C20-C13	3.23	1.56	1.45
26	A	852	CLA	C4B-NB	3.23	1.42	1.37
26	c	302	CLA	C4B-NB	3.23	1.42	1.37
26	B	813	CLA	C4B-NB	3.23	1.42	1.37
29	s	407	WVN	C19-C11	3.23	1.39	1.32
29	M	101	WVN	C20-C13	3.22	1.56	1.45
26	d	310	CLA	C4B-NB	3.22	1.42	1.37
26	i	301	CLA	C4B-NB	3.22	1.42	1.37
26	A	811	CLA	C4B-NB	3.22	1.42	1.37
26	K	101	CLA	C4B-NB	3.22	1.42	1.37
26	n	610	CLA	C4B-NB	3.22	1.42	1.37
26	F	201	CLA	C4B-NB	3.22	1.42	1.37
26	h	304	CLA	C4B-NB	3.21	1.42	1.37
26	B	840	CLA	C4B-NB	3.21	1.42	1.37
26	s	402	CLA	C4B-NB	3.21	1.42	1.37
26	B	811	CLA	C4B-NB	3.20	1.42	1.37
26	b	312	CLA	C4B-NB	3.20	1.42	1.37
26	j	613	CLA	C4B-NB	3.20	1.42	1.37
36	n	612	KC2	C1C-C2C	-3.20	1.38	1.44
26	d	306	CLA	C4B-NB	3.20	1.42	1.37
26	L	206	CLA	C4B-NB	3.20	1.42	1.37
26	i	303	CLA	C4B-NB	3.20	1.42	1.37
26	a	311	CLA	C4B-NB	3.20	1.42	1.37
26	m	601	CLA	C4B-NB	3.20	1.42	1.37
26	A	851	CLA	C4B-NB	3.19	1.42	1.37
26	B	841	CLA	C4B-NB	3.19	1.42	1.37
26	A	840	CLA	C4B-NB	3.19	1.42	1.37
29	h	309	WVN	C20-C13	3.19	1.56	1.45
26	B	820	CLA	C4B-NB	3.19	1.42	1.37
26	b	311	CLA	C4B-NB	3.19	1.42	1.37
26	L	202	CLA	C4B-NB	3.19	1.42	1.37
26	A	833	CLA	C4B-NB	3.18	1.42	1.37
26	A	806	CLA	C4B-NB	3.18	1.42	1.37
26	l	304	CLA	C4B-NB	3.18	1.42	1.37
26	d	313	CLA	C4B-NB	3.18	1.42	1.37
26	B	826	CLA	C4B-NB	3.18	1.42	1.37
26	h	301	CLA	C4B-NB	3.18	1.42	1.37
26	A	830	CLA	C4B-NB	3.18	1.42	1.37
26	B	828	CLA	C4B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	846	WVN	C19-C11	3.18	1.39	1.32
26	L	204	CLA	C4B-NB	3.18	1.42	1.37
27	A	842	PQN	C2-C1	-3.18	1.40	1.47
29	A	847	WVN	C20-C13	3.18	1.55	1.45
26	k	614	CLA	C4B-NB	3.18	1.42	1.37
32	A	854	SQD	O48-C23	3.18	1.42	1.33
26	m	609	CLA	C4B-NB	3.18	1.42	1.37
26	a	309	CLA	C4B-NB	3.17	1.42	1.37
26	A	802	CLA	C1D-ND	3.17	1.42	1.37
26	B	804	CLA	C1D-ND	3.17	1.42	1.37
26	b	306	CLA	C4B-NB	3.17	1.42	1.37
26	A	809	CLA	C4B-NB	3.17	1.42	1.37
26	m	606	CLA	C4B-NB	3.17	1.42	1.37
26	k	610	CLA	C4B-NB	3.17	1.42	1.37
36	s	404	KC2	C3C-C4C	-3.17	1.38	1.44
26	b	305	CLA	C4B-NB	3.17	1.42	1.37
26	i	311	CLA	C4B-NB	3.17	1.42	1.37
29	A	847	WVN	C19-C11	3.17	1.39	1.32
26	B	838	CLA	C4B-NB	3.16	1.42	1.37
26	c	305	CLA	C4B-NB	3.16	1.42	1.37
26	j	612	CLA	C4B-NB	3.16	1.42	1.37
26	d	309	CLA	C4B-NB	3.16	1.42	1.37
36	k	612	KC2	C1C-C2C	-3.16	1.38	1.44
26	b	303	CLA	C4B-NB	3.16	1.42	1.37
26	A	815	CLA	C4B-NB	3.16	1.42	1.37
26	A	820	CLA	C4B-NB	3.15	1.42	1.37
26	B	834	CLA	C4B-NB	3.15	1.42	1.37
26	h	308	CLA	C4B-NB	3.15	1.42	1.37
26	j	605	CLA	C4B-NB	3.15	1.42	1.37
36	m	611	KC2	C3C-C4C	-3.15	1.38	1.44
29	J	101	WVN	C20-C13	3.15	1.55	1.45
26	s	408	CLA	C4B-NB	3.15	1.42	1.37
29	K	102	WVN	C20-C13	3.15	1.55	1.45
29	L	201	WVN	C20-C13	3.15	1.55	1.45
26	c	303	CLA	C4B-NB	3.15	1.42	1.37
26	l	311	CLA	C4B-NB	3.15	1.42	1.37
26	B	833	CLA	C4B-NB	3.14	1.42	1.37
26	B	819	CLA	C4B-NB	3.14	1.42	1.37
26	B	802	CLA	C4B-NB	3.14	1.42	1.37
26	l	306	CLA	C4B-NB	3.14	1.42	1.37
26	i	308	CLA	C4B-NB	3.14	1.42	1.37
36	i	318	KC2	C1C-C2C	-3.14	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	310	KC2	C4B-NB	-3.14	1.33	1.37
26	B	839	CLA	C4B-NB	3.14	1.42	1.37
29	L	205	WVN	C20-C13	3.14	1.55	1.45
36	j	611	KC2	C1C-C2C	-3.14	1.38	1.44
26	h	303	CLA	C4B-NB	3.14	1.42	1.37
26	k	609	CLA	C4B-NB	3.14	1.42	1.37
26	B	837	CLA	C4B-NB	3.13	1.42	1.37
35	d	315	II0	C19-C13	3.13	1.55	1.50
29	F	203	WVN	C20-C13	3.13	1.55	1.45
36	c	310	KC2	OBD-CAD	3.13	1.27	1.22
29	l	316	WVN	C20-C13	3.13	1.55	1.45
26	B	830	CLA	C4B-NB	3.13	1.42	1.37
36	k	611	KC2	C1C-C2C	-3.12	1.38	1.44
26	d	303	CLA	C4B-NB	3.12	1.42	1.37
26	a	305	CLA	C4B-NB	3.12	1.42	1.37
29	s	407	WVN	C20-C13	3.12	1.55	1.45
26	A	816	CLA	C4B-NB	3.12	1.42	1.37
26	d	308	CLA	C4B-NB	3.12	1.42	1.37
35	d	316	II0	C20-C14	3.12	1.55	1.50
26	B	816	CLA	C4B-NB	3.11	1.42	1.37
26	m	605	CLA	C4B-NB	3.11	1.42	1.37
26	d	302	CLA	C4B-NB	3.11	1.42	1.37
36	j	611	KC2	C3C-C4C	-3.11	1.38	1.44
26	a	308	CLA	C4B-NB	3.11	1.42	1.37
26	d	307	CLA	C4B-NB	3.11	1.41	1.37
29	l	316	WVN	C19-C11	3.11	1.39	1.32
26	B	814	CLA	C4B-NB	3.11	1.41	1.37
26	c	306	CLA	C4B-NB	3.11	1.41	1.37
26	A	823	CLA	C4B-NB	3.11	1.41	1.37
26	A	819	CLA	C4B-NB	3.11	1.41	1.37
26	j	610	CLA	C4B-NB	3.11	1.41	1.37
26	B	808	CLA	C4B-NB	3.11	1.41	1.37
26	B	827	CLA	C4B-NB	3.11	1.41	1.37
29	B	847	WVN	C19-C11	3.11	1.39	1.32
26	B	806	CLA	C4B-NB	3.11	1.41	1.37
26	h	313	CLA	C4B-NB	3.11	1.41	1.37
26	m	613	CLA	C4B-NB	3.10	1.41	1.37
36	s	404	KC2	MG-NA	3.10	2.13	2.06
26	s	406	CLA	C4B-NB	3.10	1.41	1.37
26	m	607	CLA	C4B-NB	3.10	1.41	1.37
26	h	302	CLA	C4B-NB	3.10	1.41	1.37
26	d	304	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	848	WVN	C19-C11	3.10	1.39	1.32
26	B	815	CLA	C4B-NB	3.10	1.41	1.37
36	i	309	KC2	C1C-C2C	-3.10	1.38	1.44
26	n	601	CLA	C4B-NB	3.10	1.41	1.37
26	A	821	CLA	C4B-NB	3.10	1.41	1.37
29	B	850	WVN	C19-C11	3.09	1.39	1.32
26	A	831	CLA	C4B-NB	3.09	1.41	1.37
35	a	312	II0	C19-C13	3.09	1.55	1.50
26	d	305	CLA	C4B-NB	3.09	1.41	1.37
26	B	809	CLA	C4B-NB	3.09	1.41	1.37
26	a	303	CLA	C4B-NB	3.09	1.41	1.37
26	a	304	CLA	C4B-NB	3.09	1.41	1.37
26	B	822	CLA	C4B-NB	3.08	1.41	1.37
26	L	203	CLA	C4B-NB	3.08	1.41	1.37
26	s	403	CLA	C4B-NB	3.08	1.41	1.37
26	b	307	CLA	C4B-NB	3.08	1.41	1.37
36	l	312	KC2	C3C-C4C	-3.08	1.39	1.44
26	d	318	CLA	C4B-NB	3.08	1.41	1.37
36	d	312	KC2	C3C-C4C	-3.08	1.39	1.44
26	j	608	CLA	C4B-NB	3.08	1.41	1.37
36	n	611	KC2	C3C-C4C	-3.08	1.39	1.44
26	B	829	CLA	C4B-NB	3.08	1.41	1.37
26	c	304	CLA	C4B-NB	3.08	1.41	1.37
26	m	610	CLA	C4B-NB	3.08	1.41	1.37
26	m	603	CLA	C4B-NB	3.07	1.41	1.37
36	s	401	KC2	OBD-CAD	3.07	1.27	1.22
26	h	306	CLA	C4B-NB	3.07	1.41	1.37
26	k	605	CLA	C4B-NB	3.07	1.41	1.37
29	B	850	WVN	C20-C13	3.07	1.55	1.45
26	A	841	CLA	C4B-NB	3.07	1.41	1.37
26	A	856	CLA	C4B-NB	3.07	1.41	1.37
26	A	804	CLA	C4B-NB	3.07	1.41	1.37
26	A	822	CLA	C4B-NB	3.07	1.41	1.37
26	a	307	CLA	C4B-NB	3.07	1.41	1.37
26	n	607	CLA	C4B-NB	3.07	1.41	1.37
26	A	805	CLA	C4B-NB	3.07	1.41	1.37
26	n	605	CLA	C4B-NB	3.07	1.41	1.37
26	l	309	CLA	C4B-NB	3.07	1.41	1.37
26	c	309	CLA	CHC-C1C	3.07	1.44	1.38
26	B	801	CLA	C4B-NB	3.07	1.41	1.37
26	b	313	CLA	C4B-NB	3.07	1.41	1.37
27	B	843	PQN	C3-C4	-3.07	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	405	WVN	C19-C11	3.06	1.39	1.32
26	j	603	CLA	C4B-NB	3.06	1.41	1.37
26	m	608	CLA	C4B-NB	3.06	1.41	1.37
29	I	101	WVN	C20-C13	3.06	1.55	1.45
29	F	203	WVN	C19-C11	3.06	1.39	1.32
26	Q	302	CLA	C4B-NB	3.06	1.41	1.37
35	l	302	II0	C20-C14	3.06	1.55	1.50
36	i	318	KC2	C3C-C4C	-3.06	1.39	1.44
36	n	612	KC2	C3C-C4C	-3.05	1.39	1.44
26	B	821	CLA	C4B-NB	3.05	1.41	1.37
26	l	310	CLA	C4B-NB	3.05	1.41	1.37
29	A	845	WVN	C19-C11	3.05	1.39	1.32
26	j	606	CLA	C4B-NB	3.05	1.41	1.37
29	l	303	WVN	C20-C13	3.05	1.55	1.45
26	i	307	CLA	C4B-NB	3.05	1.41	1.37
26	B	803	CLA	C1B-C2B	3.05	1.50	1.43
26	A	808	CLA	C4B-NB	3.05	1.41	1.37
26	a	301	CLA	C4B-NB	3.05	1.41	1.37
26	A	839	CLA	C4B-NB	3.05	1.41	1.37
35	n	616	II0	C20-C14	3.04	1.55	1.50
26	c	311	CLA	C4B-NB	3.04	1.41	1.37
26	B	842	CLA	C4B-NB	3.04	1.41	1.37
26	j	609	CLA	C4B-NB	3.04	1.41	1.37
26	B	836	CLA	C4B-NB	3.04	1.41	1.37
26	m	612	CLA	C4B-NB	3.04	1.41	1.37
26	i	310	CLA	C4B-NB	3.04	1.41	1.37
26	B	831	CLA	C4B-NB	3.03	1.41	1.37
26	n	604	CLA	C4B-NB	3.03	1.41	1.37
35	n	618	II0	C19-C13	3.03	1.55	1.50
27	B	843	PQN	C3-C2	3.03	1.40	1.35
36	i	309	KC2	C3C-C4C	-3.03	1.39	1.44
26	k	608	CLA	C4B-NB	3.03	1.41	1.37
36	k	611	KC2	C3C-C4C	-3.03	1.39	1.44
36	d	311	KC2	C3C-C4C	-3.03	1.39	1.44
36	n	611	KC2	C1C-C2C	-3.03	1.38	1.44
26	A	817	CLA	C4B-NB	3.02	1.41	1.37
26	A	810	CLA	C4B-NB	3.02	1.41	1.37
26	A	827	CLA	C4B-NB	3.02	1.41	1.37
26	A	818	CLA	C4B-NB	3.02	1.41	1.37
26	k	607	CLA	C4B-NB	3.02	1.41	1.37
26	c	301	CLA	C4B-NB	3.02	1.41	1.37
26	b	309	CLA	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	311	KC2	C1C-C2C	-3.02	1.38	1.44
26	k	606	CLA	C4B-NB	3.01	1.41	1.37
26	k	601	CLA	C4B-NB	3.01	1.41	1.37
26	i	304	CLA	C4B-NB	3.01	1.41	1.37
26	h	305	CLA	C4B-NB	3.01	1.41	1.37
35	k	616	II0	C20-C14	3.01	1.55	1.50
27	A	842	PQN	C3-C4	-3.01	1.39	1.47
26	c	308	CLA	C4B-NB	3.01	1.41	1.37
26	A	814	CLA	C4B-NB	3.01	1.41	1.37
35	c	316	II0	C19-C13	3.01	1.55	1.50
35	h	312	II0	C19-C13	3.00	1.55	1.50
26	B	818	CLA	C4B-NB	3.00	1.41	1.37
36	c	310	KC2	CHD-C1D	3.00	1.46	1.39
35	i	312	II0	C20-C14	3.00	1.55	1.50
36	k	613	KC2	C3C-C4C	-3.00	1.39	1.44
26	B	805	CLA	C4B-NB	3.00	1.41	1.37
35	m	615	II0	C19-C13	3.00	1.55	1.50
26	A	835	CLA	C4B-NB	3.00	1.41	1.37
26	B	823	CLA	C4B-NB	3.00	1.41	1.37
35	a	316	II0	C20-C14	2.99	1.55	1.50
26	A	802	CLA	C4B-NB	2.99	1.41	1.37
26	l	308	CLA	C4B-NB	2.99	1.41	1.37
35	m	616	II0	C19-C13	2.99	1.55	1.50
36	s	401	KC2	CHD-C1D	2.99	1.46	1.39
35	d	317	II0	C20-C14	2.98	1.55	1.50
29	J	102	WVN	C19-C11	2.98	1.39	1.32
35	j	615	II0	C20-C14	2.98	1.55	1.50
29	B	849	WVN	C19-C11	2.98	1.39	1.32
35	i	316	II0	C20-C14	2.98	1.55	1.50
35	d	301	II0	C20-C14	2.98	1.55	1.50
29	L	205	WVN	C19-C11	2.98	1.39	1.32
26	B	824	CLA	C4B-NB	2.98	1.41	1.37
26	c	307	CLA	C4B-NB	2.97	1.41	1.37
35	a	313	II0	C19-C13	2.97	1.55	1.50
26	b	308	CLA	C4B-NB	2.97	1.41	1.37
26	A	807	CLA	C4B-NB	2.97	1.41	1.37
29	A	848	WVN	C19-C11	2.97	1.39	1.32
29	B	853	WVN	C19-C11	2.97	1.39	1.32
26	i	302	CLA	C4B-NB	2.97	1.41	1.37
35	c	316	II0	C20-C14	2.96	1.55	1.50
35	j	614	II0	C19-C13	2.96	1.55	1.50
35	m	615	II0	C20-C14	2.96	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	612	KC2	C3C-C4C	-2.96	1.39	1.44
26	n	609	CLA	C4B-NB	2.96	1.41	1.37
26	A	824	CLA	C4B-NB	2.95	1.41	1.37
29	l	303	WVN	C19-C11	2.95	1.39	1.32
26	m	604	CLA	C4B-NB	2.94	1.41	1.37
35	k	615	II0	C27-C25	2.94	1.52	1.50
35	m	614	II0	C19-C13	2.94	1.55	1.50
27	A	842	PQN	C3-C2	2.94	1.40	1.35
26	j	602	CLA	C4B-NB	2.94	1.41	1.37
25	A	801	CL0	MG-ND	-2.93	2.00	2.05
29	K	102	WVN	C19-C11	2.93	1.39	1.32
35	i	319	II0	C19-C13	2.93	1.55	1.50
26	B	804	CLA	C4B-NB	2.93	1.41	1.37
29	h	309	WVN	C19-C11	2.93	1.39	1.32
29	J	101	WVN	C19-C11	2.93	1.39	1.32
26	A	812	CLA	C4B-NB	2.92	1.41	1.37
26	A	804	CLA	C1B-C2B	2.92	1.50	1.43
36	d	312	KC2	MG-ND	-2.92	2.00	2.05
26	B	803	CLA	C4B-NB	2.92	1.41	1.37
26	B	825	CLA	C4B-NB	2.92	1.41	1.37
36	d	312	KC2	C1C-C2C	-2.91	1.38	1.44
26	l	307	CLA	C4B-NB	2.90	1.41	1.37
26	j	604	CLA	C4B-NB	2.90	1.41	1.37
26	m	602	CLA	C4B-NB	2.89	1.41	1.37
26	B	837	CLA	C1B-C2B	2.89	1.49	1.43
35	c	313	II0	C20-C14	2.88	1.55	1.50
26	B	832	CLA	C1B-C2B	2.87	1.49	1.43
26	A	825	CLA	C4B-NB	2.87	1.41	1.37
26	A	826	CLA	C4B-NB	2.87	1.41	1.37
35	d	315	II0	C20-C14	2.87	1.55	1.50
27	B	843	PQN	C10-C1	-2.85	1.42	1.48
32	A	854	SQD	O47-C7	2.85	1.42	1.34
26	b	311	CLA	C1B-C2B	2.85	1.49	1.43
26	B	807	CLA	C4B-NB	2.84	1.41	1.37
35	m	619	II0	C20-C14	2.84	1.55	1.50
26	a	310	CLA	C1B-C2B	2.84	1.49	1.43
26	A	835	CLA	C1B-C2B	2.84	1.49	1.43
26	i	301	CLA	C1B-C2B	2.84	1.49	1.43
26	B	812	CLA	C4B-NB	2.84	1.41	1.37
35	m	616	II0	C20-C14	2.83	1.55	1.50
26	d	308	CLA	C1B-C2B	2.83	1.49	1.43
35	d	316	II0	C12-C14	2.83	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	310	II0	C19-C13	2.82	1.55	1.50
35	l	302	II0	C19-C13	2.82	1.55	1.50
26	b	303	CLA	C1B-C2B	2.82	1.49	1.43
26	c	308	CLA	C1B-C2B	2.82	1.49	1.43
35	m	619	II0	C19-C13	2.81	1.55	1.50
26	c	309	CLA	CHB-C4A	-2.81	1.30	1.37
26	c	311	CLA	C1B-C2B	2.81	1.49	1.43
26	L	204	CLA	C1B-C2B	2.81	1.49	1.43
26	A	833	CLA	C1B-C2B	2.81	1.49	1.43
26	k	601	CLA	C1B-C2B	2.81	1.49	1.43
36	s	401	KC2	CHB-C4A	-2.80	1.32	1.39
35	m	616	II0	C11-C13	2.80	1.55	1.51
26	A	809	CLA	C1B-C2B	2.80	1.49	1.43
26	K	101	CLA	C1B-C2B	2.80	1.49	1.43
26	l	313	CLA	C1B-C2B	2.80	1.49	1.43
26	n	605	CLA	C1B-C2B	2.80	1.49	1.43
35	i	314	II0	C20-C14	2.80	1.55	1.50
26	B	805	CLA	C1B-C2B	2.80	1.49	1.43
26	d	318	CLA	C1B-C2B	2.80	1.49	1.43
26	A	823	CLA	C1B-C2B	2.79	1.49	1.43
26	m	605	CLA	C1B-C2B	2.79	1.49	1.43
35	i	314	II0	C19-C13	2.79	1.55	1.50
26	b	309	CLA	C1B-C2B	2.79	1.49	1.43
26	Q	302	CLA	C1B-C2B	2.79	1.49	1.43
26	A	824	CLA	C1B-C2B	2.79	1.49	1.43
29	M	101	WVN	C19-C11	2.79	1.38	1.32
26	n	601	CLA	C1B-C2B	2.79	1.49	1.43
26	B	804	CLA	C1B-C2B	2.79	1.49	1.43
26	a	305	CLA	C1B-C2B	2.79	1.49	1.43
26	A	816	CLA	C1B-C2B	2.79	1.49	1.43
26	l	308	CLA	C1B-C2B	2.78	1.49	1.43
26	a	301	CLA	C1B-C2B	2.78	1.49	1.43
26	n	602	CLA	C1B-C2B	2.78	1.49	1.43
26	k	614	CLA	C1B-C2B	2.78	1.49	1.43
26	j	601	CLA	C1B-C2B	2.78	1.49	1.43
26	s	408	CLA	C1B-C2B	2.78	1.49	1.43
33	j	618	DGD	C3D-C2D	2.78	1.59	1.52
26	h	307	CLA	C1B-C2B	2.78	1.49	1.43
26	j	606	CLA	C1B-C2B	2.78	1.49	1.43
26	B	814	CLA	C1B-C2B	2.78	1.49	1.43
26	l	307	CLA	C1B-C2B	2.78	1.49	1.43
26	B	834	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	841	CLA	C1B-C2B	2.78	1.49	1.43
29	I	101	WVN	C19-C11	2.78	1.38	1.32
35	k	616	II0	C19-C13	2.77	1.55	1.50
35	i	319	II0	C20-C14	2.77	1.55	1.50
26	n	613	CLA	C1B-C2B	2.77	1.49	1.43
30	i	300	LMU	C6B-C5B	-2.77	1.42	1.51
26	k	602	CLA	C1B-C2B	2.77	1.49	1.43
26	A	806	CLA	C1B-C2B	2.77	1.49	1.43
26	d	307	CLA	C1B-C2B	2.77	1.49	1.43
26	j	605	CLA	C1B-C2B	2.77	1.49	1.43
35	a	314	II0	C20-C14	2.77	1.55	1.50
35	i	312	II0	C19-C13	2.77	1.55	1.50
26	A	830	CLA	C1B-C2B	2.76	1.49	1.43
26	b	313	CLA	C1B-C2B	2.76	1.49	1.43
26	b	304	CLA	C1B-C2B	2.76	1.49	1.43
26	B	812	CLA	C1B-C2B	2.76	1.49	1.43
26	B	807	CLA	C1B-C2B	2.76	1.49	1.43
26	k	606	CLA	C1B-C2B	2.76	1.49	1.43
26	k	608	CLA	C1B-C2B	2.76	1.49	1.43
26	d	305	CLA	C1B-C2B	2.76	1.49	1.43
30	A	850	LMU	C6B-C5B	-2.76	1.42	1.51
26	A	810	CLA	C1B-C2B	2.76	1.49	1.43
26	n	610	CLA	C1B-C2B	2.76	1.49	1.43
26	B	813	CLA	C1B-C2B	2.76	1.49	1.43
26	a	311	CLA	C1B-C2B	2.76	1.49	1.43
26	h	306	CLA	C1B-C2B	2.76	1.49	1.43
35	d	316	II0	C19-C13	2.76	1.55	1.50
26	B	831	CLA	C1B-C2B	2.76	1.49	1.43
26	c	305	CLA	C1B-C2B	2.75	1.49	1.43
35	a	316	II0	C19-C13	2.75	1.55	1.50
26	A	829	CLA	CMB-C2B	-2.75	1.45	1.50
26	h	308	CLA	C1B-C2B	2.75	1.49	1.43
26	m	608	CLA	C1B-C2B	2.75	1.49	1.43
25	A	801	CL0	CHB-C1B	2.75	1.44	1.39
26	L	206	CLA	C1B-C2B	2.75	1.49	1.43
26	i	305	CLA	C1B-C2B	2.75	1.49	1.43
35	m	614	II0	C20-C14	2.75	1.55	1.50
26	A	826	CLA	C1B-C2B	2.75	1.49	1.43
26	i	308	CLA	C1B-C2B	2.75	1.49	1.43
26	B	815	CLA	C1B-C2B	2.75	1.49	1.43
26	i	310	CLA	C1B-C2B	2.75	1.49	1.43
26	j	608	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	618	II0	C12-C14	2.75	1.55	1.51
26	c	309	CLA	CHD-C4C	2.75	1.45	1.39
26	B	811	CLA	C1B-C2B	2.75	1.49	1.43
26	i	304	CLA	C1B-C2B	2.74	1.49	1.43
26	d	313	CLA	C1B-C2B	2.74	1.49	1.43
26	a	309	CLA	C1B-C2B	2.74	1.49	1.43
26	m	602	CLA	C1B-C2B	2.74	1.49	1.43
26	j	610	CLA	C1B-C2B	2.74	1.49	1.43
26	B	809	CLA	C1B-C2B	2.74	1.49	1.43
26	b	312	CLA	C1B-C2B	2.74	1.49	1.43
26	B	835	CLA	C1B-C2B	2.74	1.49	1.43
35	l	315	II0	C20-C14	2.74	1.55	1.50
26	a	302	CLA	C4B-NB	2.74	1.41	1.37
26	n	602	CLA	C4B-NB	2.74	1.41	1.37
26	A	821	CLA	C1B-C2B	2.74	1.49	1.43
35	h	312	II0	C28-C26	2.74	1.52	1.50
26	B	839	CLA	C1B-C2B	2.74	1.49	1.43
26	A	815	CLA	C1B-C2B	2.74	1.49	1.43
26	d	306	CLA	C1B-C2B	2.74	1.49	1.43
26	m	603	CLA	C1B-C2B	2.73	1.49	1.43
35	d	301	II0	C12-C14	2.73	1.55	1.51
26	l	304	CLA	C1B-C2B	2.73	1.49	1.43
35	a	313	II0	C11-C13	2.73	1.55	1.51
26	l	311	CLA	C1B-C2B	2.73	1.49	1.43
26	d	304	CLA	C1B-C2B	2.73	1.49	1.43
26	B	838	CLA	C1B-C2B	2.73	1.49	1.43
26	B	801	CLA	C1B-C2B	2.73	1.49	1.43
26	B	810	CLA	C1B-C2B	2.73	1.49	1.43
26	h	302	CLA	C1B-C2B	2.73	1.49	1.43
26	b	308	CLA	C1B-C2B	2.73	1.49	1.43
26	c	309	CLA	CHD-C1D	2.73	1.43	1.38
26	A	832	CLA	C1B-C2B	2.73	1.49	1.43
26	h	301	CLA	C1B-C2B	2.73	1.49	1.43
26	B	806	CLA	C1B-C2B	2.73	1.49	1.43
26	A	822	CLA	C1B-C2B	2.73	1.49	1.43
26	c	301	CLA	C1B-C2B	2.73	1.49	1.43
26	A	856	CLA	C1B-C2B	2.73	1.49	1.43
26	n	609	CLA	C1B-C2B	2.73	1.49	1.43
26	L	203	CLA	C1B-C2B	2.72	1.49	1.43
26	k	604	CLA	C1B-C2B	2.72	1.49	1.43
26	c	312	CLA	C1B-C2B	2.72	1.49	1.43
26	m	612	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	304	CLA	C1B-C2B	2.72	1.49	1.43
26	i	311	CLA	C1B-C2B	2.72	1.49	1.43
26	j	603	CLA	C1B-C2B	2.72	1.49	1.43
26	j	609	CLA	C1B-C2B	2.72	1.49	1.43
26	m	601	CLA	C1B-C2B	2.72	1.49	1.43
26	b	306	CLA	C1B-C2B	2.72	1.49	1.43
26	a	302	CLA	C1B-C2B	2.72	1.49	1.43
26	A	805	CLA	C1B-C2B	2.72	1.49	1.43
26	l	301	CLA	C1B-C2B	2.72	1.49	1.43
26	k	610	CLA	C1B-C2B	2.72	1.49	1.43
26	m	610	CLA	C1B-C2B	2.72	1.49	1.43
29	A	848	WVN	C21-C15	2.71	1.55	1.50
35	c	316	II0	C11-C13	2.71	1.55	1.51
26	h	303	CLA	C1B-C2B	2.71	1.49	1.43
26	a	308	CLA	C1B-C2B	2.71	1.49	1.43
26	c	307	CLA	C1B-C2B	2.71	1.49	1.43
26	d	310	CLA	C1B-C2B	2.71	1.49	1.43
26	B	830	CLA	C1B-C2B	2.71	1.49	1.43
26	s	403	CLA	C1B-C2B	2.71	1.49	1.43
29	A	845	WVN	C21-C15	2.71	1.55	1.50
26	B	820	CLA	C1B-C2B	2.71	1.49	1.43
26	i	305	CLA	C4B-NB	2.71	1.41	1.37
26	A	814	CLA	C1B-C2B	2.71	1.49	1.43
35	k	615	II0	C12-C14	2.71	1.55	1.51
26	k	605	CLA	C1B-C2B	2.71	1.49	1.43
26	j	613	CLA	C1B-C2B	2.70	1.49	1.43
26	m	607	CLA	C1B-C2B	2.70	1.49	1.43
26	d	309	CLA	C1B-C2B	2.70	1.49	1.43
26	b	304	CLA	C4B-NB	2.70	1.41	1.37
26	a	304	CLA	C1B-C2B	2.70	1.49	1.43
26	c	304	CLA	C1B-C2B	2.70	1.49	1.43
26	A	811	CLA	C1B-C2B	2.70	1.49	1.43
26	j	612	CLA	C1B-C2B	2.70	1.49	1.43
26	A	831	CLA	C1B-C2B	2.70	1.49	1.43
26	R	201	CLA	C1B-C2B	2.70	1.49	1.43
26	A	838	CLA	C1B-C2B	2.70	1.49	1.43
35	k	620	II0	C20-C14	2.70	1.55	1.50
26	A	837	CLA	C1B-C2B	2.70	1.49	1.43
35	i	312	II0	C11-C13	2.69	1.55	1.51
26	B	824	CLA	C1B-C2B	2.69	1.49	1.43
26	i	307	CLA	C1B-C2B	2.69	1.49	1.43
35	l	314	II0	C20-C14	2.69	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	602	CLA	C4B-NB	2.69	1.41	1.37
26	B	816	CLA	C1B-C2B	2.69	1.49	1.43
26	m	609	CLA	C1B-C2B	2.69	1.49	1.43
26	l	305	CLA	C1B-C2B	2.69	1.49	1.43
26	A	812	CLA	C1B-C2B	2.69	1.49	1.43
26	A	828	CLA	C1B-C2B	2.69	1.49	1.43
26	B	828	CLA	C1B-C2B	2.68	1.49	1.43
26	B	808	CLA	C1B-C2B	2.68	1.49	1.43
26	c	306	CLA	C1B-C2B	2.68	1.49	1.43
26	A	820	CLA	C1B-C2B	2.68	1.49	1.43
26	F	202	CLA	C1B-C2B	2.68	1.49	1.43
26	m	613	CLA	C1B-C2B	2.68	1.49	1.43
35	i	316	II0	C19-C13	2.68	1.55	1.50
35	n	616	II0	C19-C13	2.68	1.55	1.50
26	b	310	CLA	C1B-C2B	2.68	1.49	1.43
26	A	836	CLA	C1B-C2B	2.68	1.49	1.43
36	k	611	KC2	MG-NA	2.68	2.12	2.06
29	i	315	WVN	C21-C15	2.67	1.55	1.50
35	h	311	II0	C20-C14	2.67	1.55	1.50
26	k	607	CLA	C1B-C2B	2.67	1.49	1.43
26	A	808	CLA	C1B-C2B	2.67	1.49	1.43
35	b	315	II0	C20-C14	2.67	1.55	1.50
26	B	840	CLA	C1B-C2B	2.67	1.49	1.43
35	n	618	II0	C11-C13	2.67	1.55	1.51
26	d	302	CLA	C1B-C2B	2.67	1.49	1.43
26	n	603	CLA	C1B-C2B	2.67	1.49	1.43
26	a	306	CLA	C1B-C2B	2.67	1.49	1.43
26	m	604	CLA	C1B-C2B	2.67	1.49	1.43
26	L	202	CLA	C1B-C2B	2.67	1.49	1.43
26	B	825	CLA	C1B-C2B	2.66	1.49	1.43
26	c	302	CLA	C1B-C2B	2.66	1.49	1.43
26	s	406	CLA	C1B-C2B	2.66	1.49	1.43
26	b	307	CLA	C1B-C2B	2.66	1.49	1.43
26	n	604	CLA	C1B-C2B	2.66	1.49	1.43
26	i	302	CLA	C1B-C2B	2.66	1.49	1.43
26	A	852	CLA	C1B-C2B	2.66	1.49	1.43
26	B	826	CLA	C1B-C2B	2.66	1.49	1.43
27	A	842	PQN	C9-C10	2.66	1.44	1.39
35	b	315	II0	C28-C26	2.66	1.52	1.50
26	B	819	CLA	C1B-C2B	2.65	1.49	1.43
26	A	834	CLA	C1B-C2B	2.65	1.49	1.43
26	B	821	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	614	II0	C28-C26	2.65	1.52	1.50
25	A	801	CL0	MG-NB	-2.65	2.00	2.05
35	c	313	II0	C12-C14	2.65	1.55	1.51
26	n	606	CLA	C1B-C2B	2.65	1.49	1.43
29	M	101	WVN	C21-C15	2.64	1.55	1.50
36	c	310	KC2	CHB-C4A	-2.64	1.33	1.39
26	m	606	CLA	C1B-C2B	2.64	1.49	1.43
25	A	801	CL0	C3B-C4B	-2.64	1.38	1.41
30	i	300	LMU	C6'-C5'	-2.64	1.42	1.51
35	k	619	II0	C19-C13	2.64	1.55	1.50
26	A	803	CLA	CHC-C1C	2.64	1.43	1.38
35	k	615	II0	C19-C13	2.64	1.55	1.50
26	i	303	CLA	C1B-C2B	2.64	1.49	1.43
26	A	829	CLA	C1B-C2B	2.63	1.49	1.43
26	c	309	CLA	OBD-CAD	2.63	1.27	1.22
35	h	311	II0	C19-C13	2.63	1.55	1.50
26	j	607	CLA	C1B-C2B	2.63	1.49	1.43
29	h	309	WVN	C21-C15	2.63	1.55	1.50
35	j	614	II0	C20-C14	2.63	1.55	1.50
26	A	825	CLA	C3B-C4B	2.63	1.50	1.42
29	L	201	WVN	C21-C15	2.63	1.55	1.50
35	l	302	II0	C28-C26	2.63	1.52	1.50
29	B	849	WVN	C21-C15	2.63	1.55	1.50
26	l	310	CLA	C1B-C2B	2.63	1.49	1.43
29	R	200	WVN	C21-C15	2.63	1.55	1.50
26	c	303	CLA	C1B-C2B	2.63	1.49	1.43
26	a	307	CLA	C1B-C2B	2.63	1.49	1.43
26	j	604	CLA	C1B-C2B	2.63	1.49	1.43
26	A	834	CLA	C4B-NB	2.63	1.41	1.37
26	k	609	CLA	C1B-C2B	2.62	1.49	1.43
35	h	312	II0	C20-C14	2.62	1.55	1.50
26	B	841	CLA	C3B-C4B	2.62	1.50	1.42
26	F	201	CLA	C1B-C2B	2.62	1.49	1.43
29	L	201	WVN	C19-C11	2.62	1.38	1.32
26	h	313	CLA	C1B-C2B	2.62	1.49	1.43
35	J	104	II0	C20-C14	2.62	1.55	1.50
29	J	102	WVN	C21-C15	2.62	1.55	1.50
35	b	314	II0	C20-C14	2.62	1.55	1.50
35	n	615	II0	C19-C13	2.62	1.55	1.50
35	j	615	II0	C19-C13	2.61	1.55	1.50
36	n	612	KC2	MG-ND	-2.60	2.00	2.05
26	B	823	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	807	CLA	C1B-C2B	2.60	1.49	1.43
29	l	303	WVN	C21-C15	2.60	1.55	1.50
35	d	301	II0	C19-C13	2.60	1.55	1.50
35	c	316	II0	C27-C25	2.60	1.52	1.50
35	a	312	II0	C11-C13	2.60	1.55	1.51
30	A	850	LMU	C6'-C5'	-2.60	1.43	1.51
35	a	312	II0	C20-C14	2.59	1.55	1.50
35	l	314	II0	C19-C13	2.59	1.55	1.50
26	d	303	CLA	C1B-C2B	2.59	1.49	1.43
35	m	619	II0	C11-C13	2.59	1.55	1.51
35	k	615	II0	C11-C13	2.59	1.55	1.51
26	B	833	CLA	C1B-C2B	2.59	1.49	1.43
35	i	313	II0	C20-C14	2.59	1.55	1.50
26	A	818	CLA	C1B-C2B	2.59	1.49	1.43
26	B	818	CLA	C3B-C4B	2.59	1.50	1.42
26	J	103	CLA	C1B-C2B	2.58	1.49	1.43
26	k	603	CLA	C3B-C4B	2.58	1.50	1.42
26	A	819	CLA	C1B-C2B	2.58	1.49	1.43
26	l	309	CLA	C1B-C2B	2.58	1.49	1.43
26	i	306	CLA	C1B-C2B	2.58	1.49	1.43
26	A	817	CLA	C1B-C2B	2.58	1.49	1.43
26	j	607	CLA	C4B-NB	2.57	1.41	1.37
26	j	602	CLA	C1B-C2B	2.57	1.49	1.43
26	a	303	CLA	C1B-C2B	2.57	1.49	1.43
35	j	614	II0	C11-C13	2.56	1.55	1.51
26	B	818	CLA	CHC-C1C	2.56	1.43	1.38
29	B	846	WVN	C21-C15	2.56	1.55	1.50
35	j	614	II0	C28-C26	2.56	1.52	1.50
26	B	827	CLA	CMD-C2D	-2.55	1.45	1.50
27	A	842	PQN	C10-C1	-2.55	1.43	1.48
26	F	201	CLA	C3B-C4B	2.55	1.50	1.42
26	i	305	CLA	MG-ND	-2.55	2.00	2.05
26	A	827	CLA	C1B-C2B	2.55	1.49	1.43
26	A	803	CLA	C3B-C4B	2.55	1.50	1.42
29	B	847	WVN	C21-C15	2.55	1.55	1.50
35	c	313	II0	C19-C13	2.55	1.55	1.50
26	h	305	CLA	C1B-C2B	2.55	1.49	1.43
35	d	301	II0	C27-C25	2.55	1.52	1.50
35	a	313	II0	C20-C14	2.55	1.55	1.50
35	k	619	II0	C20-C14	2.55	1.55	1.50
26	B	817	CLA	C1B-C2B	2.55	1.49	1.43
35	h	312	II0	C11-C13	2.55	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	402	CLA	C1B-C2B	2.55	1.49	1.43
26	A	813	CLA	C1B-C2B	2.54	1.49	1.43
26	B	836	CLA	C1B-C2B	2.54	1.49	1.43
29	B	850	WVN	C21-C15	2.54	1.55	1.50
29	L	205	WVN	C21-C15	2.54	1.55	1.50
26	n	608	CLA	C1B-C2B	2.54	1.49	1.43
35	n	616	II0	C12-C14	2.53	1.55	1.51
26	l	306	CLA	C1B-C2B	2.53	1.49	1.43
35	a	316	II0	C28-C26	2.53	1.52	1.50
26	B	802	CLA	C1B-C2B	2.53	1.49	1.43
35	i	312	II0	C27-C25	2.53	1.52	1.50
26	A	802	CLA	C1B-C2B	2.52	1.49	1.43
26	B	833	CLA	C3B-C4B	2.52	1.50	1.42
29	B	846	WVN	C19-C11	2.52	1.38	1.32
26	B	842	CLA	C1B-C2B	2.52	1.49	1.43
35	m	616	II0	C28-C26	2.52	1.52	1.50
26	A	851	CLA	C1B-C2B	2.52	1.49	1.43
26	B	822	CLA	C1B-C2B	2.52	1.49	1.43
29	s	405	WVN	C21-C15	2.52	1.54	1.50
26	m	609	CLA	C3B-C4B	2.51	1.50	1.42
35	i	319	II0	C12-C14	2.51	1.54	1.51
26	b	312	CLA	C3B-C4B	2.51	1.50	1.42
26	B	819	CLA	C3B-C4B	2.51	1.50	1.42
35	a	314	II0	C19-C13	2.51	1.54	1.50
26	B	819	CLA	CHC-C1C	2.51	1.43	1.38
35	m	615	II0	C11-C13	2.50	1.54	1.51
29	A	846	WVN	C21-C15	2.50	1.54	1.50
26	A	839	CLA	C1B-C2B	2.50	1.49	1.43
35	d	317	II0	C19-C13	2.50	1.54	1.50
35	d	301	II0	C28-C26	2.49	1.52	1.50
35	b	314	II0	C19-C13	2.49	1.54	1.50
35	l	315	II0	C28-C26	2.49	1.52	1.50
26	b	305	CLA	C3B-C4B	2.49	1.50	1.42
35	j	614	II0	C12-C14	2.49	1.54	1.51
35	j	615	II0	C28-C26	2.49	1.52	1.50
26	j	602	CLA	C3B-C4B	2.49	1.50	1.42
26	B	809	CLA	CMB-C2B	-2.48	1.45	1.50
35	j	615	II0	C11-C13	2.48	1.54	1.51
35	l	314	II0	C11-C13	2.48	1.54	1.51
35	b	314	II0	C28-C26	2.48	1.52	1.50
29	i	315	WVN	C14-C15	2.48	1.55	1.51
35	J	104	II0	C19-C13	2.48	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	823	CLA	CHC-C1C	2.47	1.43	1.38
35	m	614	II0	C12-C14	2.47	1.54	1.51
26	F	202	CLA	C3B-C4B	2.47	1.49	1.42
29	A	857	WVN	C21-C15	2.47	1.54	1.50
26	A	806	CLA	C3B-C4B	2.46	1.49	1.42
26	c	307	CLA	C3B-C4B	2.46	1.49	1.42
29	s	407	WVN	C21-C15	2.46	1.54	1.50
26	j	602	CLA	CHC-C1C	2.46	1.43	1.38
35	n	616	II0	C28-C26	2.46	1.52	1.50
26	l	309	CLA	C3B-C4B	2.46	1.49	1.42
26	A	825	CLA	C1B-C2B	2.45	1.48	1.43
35	a	314	II0	C27-C25	2.45	1.52	1.50
35	a	314	II0	C28-C26	2.45	1.52	1.50
35	l	315	II0	C11-C13	2.45	1.54	1.51
35	n	615	II0	C20-C14	2.45	1.54	1.50
29	I	101	WVN	C21-C15	2.45	1.54	1.50
26	B	827	CLA	CMB-C2B	-2.45	1.45	1.50
26	c	312	CLA	C3B-C4B	2.45	1.49	1.42
27	B	843	PQN	C5-C4	-2.45	1.43	1.48
26	l	306	CLA	C3B-C4B	2.45	1.49	1.42
26	B	829	CLA	C1B-C2B	2.45	1.48	1.43
29	A	845	WVN	C14-C15	2.45	1.55	1.51
26	A	813	CLA	CHC-C1C	2.45	1.43	1.38
26	l	309	CLA	CMD-C2D	-2.45	1.45	1.50
26	A	827	CLA	C3B-C4B	2.45	1.49	1.42
26	A	840	CLA	C1B-C2B	2.44	1.48	1.43
26	B	821	CLA	C3B-C4B	2.44	1.49	1.42
26	a	306	CLA	C3B-C4B	2.44	1.49	1.42
35	i	316	II0	C12-C14	2.44	1.54	1.51
26	n	608	CLA	C3B-C4B	2.44	1.49	1.42
26	B	842	CLA	CHC-C1C	2.44	1.43	1.38
26	m	602	CLA	CHC-C1C	2.44	1.43	1.38
26	B	842	CLA	C3B-C4B	2.44	1.49	1.42
35	i	313	II0	C19-C13	2.44	1.54	1.50
26	m	609	CLA	CHC-C1C	2.44	1.43	1.38
35	d	315	II0	C11-C13	2.44	1.54	1.51
26	B	838	CLA	C3B-C4B	2.44	1.49	1.42
36	k	612	KC2	MG-NA	2.43	2.12	2.06
26	a	304	CLA	C3B-C4B	2.43	1.49	1.42
35	c	316	II0	C12-C14	2.43	1.54	1.51
26	B	802	CLA	C3B-C4B	2.43	1.49	1.42
26	s	406	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	305	CLA	C1B-C2B	2.43	1.48	1.43
33	j	618	DGD	O2G-C2G	-2.43	1.40	1.46
26	A	825	CLA	CHC-C1C	2.43	1.43	1.38
26	J	103	CLA	C3B-C4B	2.43	1.49	1.42
35	l	315	II0	C19-C13	2.43	1.54	1.50
26	m	601	CLA	C3B-C4B	2.43	1.49	1.42
26	l	309	CLA	CHC-C1C	2.42	1.43	1.38
26	h	301	CLA	C3B-C4B	2.42	1.49	1.42
26	B	829	CLA	C3B-C4B	2.42	1.49	1.42
26	k	609	CLA	C3B-C4B	2.42	1.49	1.42
26	j	612	CLA	C3B-C4B	2.42	1.49	1.42
26	A	803	CLA	C1B-C2B	2.42	1.48	1.43
26	l	310	CLA	C3B-C4B	2.41	1.49	1.42
26	b	303	CLA	C3B-C4B	2.41	1.49	1.42
26	k	603	CLA	CHC-C1C	2.41	1.43	1.38
26	A	840	CLA	C3B-C4B	2.41	1.49	1.42
35	b	315	II0	C19-C13	2.41	1.54	1.50
26	h	302	CLA	C3B-C4B	2.41	1.49	1.42
26	B	841	CLA	CHC-C1C	2.41	1.43	1.38
26	n	607	CLA	C1B-C2B	2.41	1.48	1.43
26	A	839	CLA	C3B-C4B	2.41	1.49	1.42
29	B	848	WVN	C21-C15	2.41	1.54	1.50
26	B	822	CLA	C3B-C4B	2.41	1.49	1.42
27	B	843	PQN	C10-C5	-2.41	1.36	1.40
35	c	313	II0	C11-C13	2.41	1.54	1.51
26	A	817	CLA	CHC-C1C	2.41	1.43	1.38
26	h	304	CLA	C3B-C4B	2.40	1.49	1.42
26	B	841	CLA	C1B-C2B	2.40	1.48	1.43
26	i	301	CLA	C3B-C4B	2.40	1.49	1.42
26	B	814	CLA	C3B-C4B	2.40	1.49	1.42
26	j	604	CLA	C3B-C4B	2.40	1.49	1.42
26	K	101	CLA	C3B-C4B	2.40	1.49	1.42
26	a	302	CLA	C3B-C4B	2.40	1.49	1.42
30	A	850	LMU	O5'-C1'	2.40	1.48	1.41
26	n	609	CLA	C3B-C4B	2.40	1.49	1.42
26	b	306	CLA	C3B-C4B	2.40	1.49	1.42
26	L	206	CLA	C3B-C4B	2.40	1.49	1.42
26	A	838	CLA	C3B-C4B	2.40	1.49	1.42
26	B	823	CLA	C3B-C4B	2.40	1.49	1.42
26	c	303	CLA	C3B-C4B	2.40	1.49	1.42
26	h	302	CLA	CHC-C1C	2.40	1.43	1.38
35	k	620	II0	C12-C14	2.40	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	618	II0	C28-C26	2.39	1.52	1.50
26	A	841	CLA	C3B-C4B	2.39	1.49	1.42
26	A	813	CLA	C3B-C4B	2.39	1.49	1.42
26	B	827	CLA	C1B-C2B	2.39	1.48	1.43
26	j	610	CLA	C3B-C4B	2.39	1.49	1.42
26	k	603	CLA	C1B-C2B	2.39	1.48	1.43
29	K	102	WVN	C21-C15	2.39	1.54	1.50
26	B	834	CLA	CHC-C1C	2.39	1.43	1.38
26	a	307	CLA	C3B-C4B	2.39	1.49	1.42
26	l	311	CLA	C3B-C4B	2.39	1.49	1.42
26	j	608	CLA	C3B-C4B	2.39	1.49	1.42
26	d	305	CLA	C3B-C4B	2.39	1.49	1.42
26	b	307	CLA	C3B-C4B	2.39	1.49	1.42
26	l	310	CLA	CHC-C1C	2.39	1.43	1.38
26	d	309	CLA	C3B-C4B	2.39	1.49	1.42
26	s	406	CLA	CHC-C1C	2.39	1.43	1.38
26	A	805	CLA	C3B-C4B	2.39	1.49	1.42
26	B	802	CLA	CHC-C1C	2.39	1.43	1.38
26	B	834	CLA	C3B-C4B	2.39	1.49	1.42
26	B	835	CLA	C3B-C4B	2.38	1.49	1.42
26	B	839	CLA	C3B-C4B	2.38	1.49	1.42
26	j	601	CLA	C3B-C4B	2.38	1.49	1.42
26	h	305	CLA	CHC-C1C	2.38	1.43	1.38
26	A	820	CLA	C3B-C4B	2.38	1.49	1.42
35	k	616	II0	C28-C26	2.38	1.52	1.50
26	i	303	CLA	C3B-C4B	2.38	1.49	1.42
26	h	313	CLA	C3B-C4B	2.38	1.49	1.42
26	h	308	CLA	C3B-C4B	2.38	1.49	1.42
35	J	104	II0	C11-C13	2.38	1.54	1.51
26	l	301	CLA	C3B-C4B	2.38	1.49	1.42
35	l	315	II0	C12-C14	2.38	1.54	1.51
26	L	202	CLA	C3B-C4B	2.38	1.49	1.42
26	A	856	CLA	C3B-C4B	2.38	1.49	1.42
26	c	309	CLA	CHB-C1B	2.38	1.44	1.39
26	j	603	CLA	C3B-C4B	2.38	1.49	1.42
26	B	833	CLA	CHC-C1C	2.38	1.43	1.38
26	A	814	CLA	C3B-C4B	2.37	1.49	1.42
35	a	314	II0	C12-C14	2.37	1.54	1.51
26	j	608	CLA	CHC-C1C	2.37	1.43	1.38
26	d	309	CLA	CHC-C1C	2.37	1.43	1.38
26	A	812	CLA	C3B-C4B	2.37	1.49	1.42
35	m	615	II0	C28-C26	2.37	1.52	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	619	II0	C27-C25	2.37	1.52	1.50
26	m	602	CLA	C3B-C4B	2.37	1.49	1.42
26	m	604	CLA	C3B-C4B	2.37	1.49	1.42
26	d	313	CLA	C3B-C4B	2.37	1.49	1.42
36	c	310	KC2	C1D-C2D	2.37	1.48	1.43
26	L	204	CLA	C3B-C4B	2.37	1.49	1.42
26	i	306	CLA	C3B-C4B	2.37	1.49	1.42
34	n	620	LMG	C4-C5	2.37	1.58	1.53
26	A	839	CLA	CHC-C1C	2.37	1.43	1.38
26	b	310	CLA	C3B-C4B	2.37	1.49	1.42
26	i	310	CLA	C3B-C4B	2.37	1.49	1.42
26	n	610	CLA	C3B-C4B	2.37	1.49	1.42
26	B	811	CLA	C3B-C4B	2.36	1.49	1.42
26	l	304	CLA	C3B-C4B	2.36	1.49	1.42
26	c	309	CLA	C4B-NB	-2.36	1.34	1.37
26	i	305	CLA	C3B-C4B	2.36	1.49	1.42
26	n	604	CLA	C3B-C4B	2.36	1.49	1.42
26	a	305	CLA	C3B-C4B	2.36	1.49	1.42
26	d	302	CLA	C3B-C4B	2.36	1.49	1.42
26	n	607	CLA	CMD-C2D	-2.36	1.45	1.50
26	A	837	CLA	C3B-C4B	2.36	1.49	1.42
26	B	831	CLA	C3B-C4B	2.36	1.49	1.42
26	B	815	CLA	CHC-C1C	2.36	1.43	1.38
26	c	309	CLA	CHC-C4B	2.36	1.44	1.39
26	B	807	CLA	C3B-C4B	2.36	1.49	1.42
26	B	810	CLA	C3B-C4B	2.36	1.49	1.42
26	B	823	CLA	CMD-C2D	-2.36	1.45	1.50
26	A	802	CLA	CHC-C1C	2.36	1.43	1.38
26	B	836	CLA	C3B-C4B	2.36	1.49	1.42
26	j	613	CLA	C3B-C4B	2.36	1.49	1.42
26	B	821	CLA	CHC-C1C	2.36	1.43	1.38
26	d	302	CLA	CHC-C1C	2.36	1.43	1.38
26	B	815	CLA	C3B-C4B	2.36	1.49	1.42
26	m	605	CLA	C3B-C4B	2.36	1.49	1.42
26	c	308	CLA	C3B-C4B	2.35	1.49	1.42
26	A	811	CLA	C3B-C4B	2.35	1.49	1.42
26	A	810	CLA	C3B-C4B	2.35	1.49	1.42
26	B	830	CLA	C3B-C4B	2.35	1.49	1.42
26	i	307	CLA	C3B-C4B	2.35	1.49	1.42
26	c	309	CLA	C1B-C2B	2.35	1.48	1.43
35	k	620	II0	C19-C13	2.35	1.54	1.50
26	B	806	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	i	304	CLA	C3B-C4B	2.35	1.49	1.42
26	j	606	CLA	C3B-C4B	2.35	1.49	1.42
26	a	307	CLA	CHC-C1C	2.35	1.43	1.38
26	A	826	CLA	C3B-C4B	2.35	1.49	1.42
26	m	606	CLA	C3B-C4B	2.35	1.49	1.42
26	A	827	CLA	CHC-C1C	2.35	1.43	1.38
29	B	853	WVN	C21-C15	2.35	1.54	1.50
26	A	816	CLA	C3B-C4B	2.35	1.49	1.42
26	h	305	CLA	C3B-C4B	2.35	1.49	1.42
26	h	303	CLA	C3B-C4B	2.35	1.49	1.42
27	A	842	PQN	C6-C5	2.35	1.43	1.39
26	c	307	CLA	CHC-C1C	2.35	1.43	1.38
26	l	313	CLA	C3B-C4B	2.35	1.49	1.42
26	B	817	CLA	C3B-C4B	2.35	1.49	1.42
35	n	618	II0	C27-C25	2.35	1.52	1.50
26	a	304	CLA	CHC-C1C	2.35	1.43	1.38
26	h	306	CLA	C3B-C4B	2.35	1.49	1.42
26	b	305	CLA	CHC-C1C	2.35	1.43	1.38
26	A	821	CLA	C3B-C4B	2.34	1.49	1.42
26	n	609	CLA	CHC-C1C	2.34	1.43	1.38
26	c	311	CLA	C3B-C4B	2.34	1.49	1.42
26	n	605	CLA	C3B-C4B	2.34	1.49	1.42
26	j	607	CLA	C3C-C2C	2.34	1.41	1.36
26	A	819	CLA	C3B-C4B	2.34	1.49	1.42
26	h	307	CLA	C3B-C4B	2.34	1.49	1.42
35	a	313	II0	C28-C26	2.34	1.52	1.50
26	J	103	CLA	CHC-C1C	2.34	1.43	1.38
26	B	829	CLA	CHC-C1C	2.34	1.43	1.38
29	A	847	WVN	C21-C15	2.34	1.54	1.50
26	A	817	CLA	C3B-C4B	2.34	1.49	1.42
26	B	830	CLA	CHC-C1C	2.34	1.43	1.38
26	B	822	CLA	CHC-C1C	2.34	1.43	1.38
26	d	308	CLA	C3B-C4B	2.34	1.49	1.42
26	a	311	CLA	C3B-C4B	2.34	1.49	1.42
26	a	308	CLA	C3B-C4B	2.34	1.49	1.42
26	k	608	CLA	C3B-C4B	2.34	1.49	1.42
26	n	603	CLA	C3B-C4B	2.34	1.49	1.42
26	A	805	CLA	CHC-C1C	2.34	1.43	1.38
26	b	306	CLA	CHC-C1C	2.34	1.43	1.38
26	d	304	CLA	C3B-C4B	2.34	1.49	1.42
26	m	612	CLA	C3B-C4B	2.34	1.49	1.42
29	B	847	WVN	C14-C15	2.33	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	309	CLA	C1D-C2D	2.33	1.50	1.45
27	B	843	PQN	C9-C10	2.33	1.43	1.39
36	n	612	KC2	C1A-CHA	2.33	1.46	1.40
26	c	303	CLA	CHC-C1C	2.33	1.43	1.38
26	m	610	CLA	C3B-C4B	2.33	1.49	1.42
26	c	308	CLA	CHC-C1C	2.33	1.43	1.38
26	a	309	CLA	C3B-C4B	2.33	1.49	1.42
26	B	826	CLA	C3B-C4B	2.33	1.49	1.42
26	h	304	CLA	CHC-C1C	2.33	1.43	1.38
26	A	802	CLA	C3B-C4B	2.33	1.49	1.42
30	A	850	LMU	O3'-C3'	2.33	1.48	1.43
26	A	822	CLA	C3B-C4B	2.33	1.49	1.42
26	L	204	CLA	CHC-C1C	2.33	1.43	1.38
26	L	203	CLA	C3B-C4B	2.33	1.49	1.42
26	j	605	CLA	C3B-C4B	2.33	1.49	1.42
26	A	807	CLA	C3B-C4B	2.32	1.49	1.42
26	s	402	CLA	C3B-C4B	2.32	1.49	1.42
26	m	608	CLA	C3B-C4B	2.32	1.49	1.42
29	A	846	WVN	C06-C13	2.32	1.56	1.53
26	s	403	CLA	C3B-C4B	2.32	1.49	1.42
35	l	314	II0	C12-C14	2.32	1.54	1.51
26	d	303	CLA	C3B-C4B	2.32	1.49	1.42
26	l	305	CLA	C4B-NB	2.32	1.40	1.37
29	J	102	WVN	C14-C15	2.32	1.55	1.51
26	k	610	CLA	C3B-C4B	2.32	1.49	1.42
35	h	312	II0	C27-C25	2.32	1.52	1.50
26	m	605	CLA	CHC-C1C	2.32	1.43	1.38
26	d	305	CLA	CHC-C1C	2.32	1.43	1.38
26	B	838	CLA	CHC-C1C	2.32	1.43	1.38
26	k	606	CLA	C3B-C4B	2.32	1.49	1.42
26	d	310	CLA	C3B-C4B	2.32	1.49	1.42
26	k	608	CLA	CHC-C1C	2.32	1.43	1.38
26	c	302	CLA	C3B-C4B	2.32	1.49	1.42
35	d	317	II0	C27-C25	2.32	1.52	1.50
26	A	851	CLA	C3B-C4B	2.32	1.49	1.42
26	L	206	CLA	CHC-C1C	2.31	1.43	1.38
26	i	308	CLA	C3B-C4B	2.31	1.49	1.42
26	A	841	CLA	CHC-C1C	2.31	1.43	1.38
26	k	614	CLA	C3B-C4B	2.31	1.49	1.42
26	d	318	CLA	C3B-C4B	2.31	1.49	1.42
26	A	840	CLA	CHC-C1C	2.31	1.43	1.38
26	Q	302	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	822	CLA	CMD-C2D	-2.31	1.46	1.50
26	A	809	CLA	C3B-C4B	2.31	1.49	1.42
26	k	605	CLA	C3B-C4B	2.31	1.49	1.42
26	k	607	CLA	C3B-C4B	2.31	1.49	1.42
26	i	311	CLA	C3B-C4B	2.31	1.49	1.42
26	b	311	CLA	C3B-C4B	2.31	1.49	1.42
26	B	826	CLA	CMD-C2D	-2.31	1.46	1.50
26	s	403	CLA	CMD-C2D	-2.31	1.46	1.50
26	A	818	CLA	C3B-C4B	2.31	1.49	1.42
36	d	312	KC2	MG-NB	-2.31	2.01	2.05
26	i	302	CLA	CHC-C1C	2.31	1.43	1.38
26	s	403	CLA	CHC-C1C	2.31	1.43	1.38
26	A	815	CLA	C3B-C4B	2.31	1.49	1.42
26	A	828	CLA	C3B-C4B	2.31	1.49	1.42
26	c	301	CLA	C3B-C4B	2.31	1.49	1.42
26	n	601	CLA	C3B-C4B	2.31	1.49	1.42
26	m	613	CLA	C3B-C4B	2.31	1.49	1.42
26	A	856	CLA	CHC-C1C	2.31	1.43	1.38
26	a	302	CLA	CMD-C2D	-2.31	1.46	1.50
35	k	616	II0	C27-C25	2.31	1.52	1.50
26	j	612	CLA	CHC-C1C	2.30	1.43	1.38
26	a	310	CLA	CMD-C2D	-2.30	1.46	1.50
26	b	313	CLA	C3B-C4B	2.30	1.49	1.42
26	B	831	CLA	CHC-C1C	2.30	1.43	1.38
26	l	311	CLA	CHC-C1C	2.30	1.43	1.38
29	J	101	WVN	C21-C15	2.30	1.54	1.50
26	B	803	CLA	CMD-C2D	-2.30	1.46	1.50
26	m	608	CLA	CHC-C1C	2.30	1.43	1.38
26	c	309	CLA	C3D-C2D	2.30	1.45	1.39
36	i	318	KC2	MG-NA	2.30	2.11	2.06
26	A	832	CLA	C3B-C4B	2.30	1.49	1.42
26	n	607	CLA	C3B-C4B	2.30	1.49	1.42
26	B	825	CLA	C3B-C4B	2.30	1.49	1.42
26	s	408	CLA	C3B-C4B	2.30	1.49	1.42
26	h	313	CLA	CHC-C1C	2.30	1.43	1.38
26	B	824	CLA	C3B-C4B	2.30	1.49	1.42
26	B	836	CLA	CMD-C2D	-2.30	1.46	1.50
26	A	852	CLA	C3B-C4B	2.30	1.49	1.42
26	j	609	CLA	C3B-C4B	2.30	1.49	1.42
26	i	302	CLA	C3B-C4B	2.30	1.49	1.42
26	R	201	CLA	C3B-C4B	2.30	1.49	1.42
29	B	850	WVN	C14-C15	2.29	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	304	CLA	CHC-C1C	2.29	1.43	1.38
26	i	305	CLA	CHC-C1C	2.29	1.43	1.38
26	B	807	CLA	CHC-C1C	2.29	1.43	1.38
26	B	813	CLA	C3B-C4B	2.29	1.49	1.42
26	i	310	CLA	CHC-C1C	2.29	1.43	1.38
26	b	309	CLA	C3B-C4B	2.29	1.49	1.42
26	k	601	CLA	C3B-C4B	2.29	1.49	1.42
26	B	816	CLA	CMB-C2B	-2.29	1.46	1.50
26	A	831	CLA	C3B-C4B	2.29	1.49	1.42
26	A	833	CLA	C3B-C4B	2.29	1.49	1.42
26	B	805	CLA	C3B-C4B	2.29	1.49	1.42
26	B	810	CLA	CHC-C1C	2.29	1.43	1.38
26	m	604	CLA	CHC-C1C	2.29	1.43	1.38
26	B	827	CLA	C3B-C4B	2.29	1.49	1.42
35	h	312	II0	C12-C14	2.29	1.54	1.51
26	i	304	CLA	CHC-C1C	2.29	1.43	1.38
36	i	318	KC2	C1A-CHA	2.28	1.46	1.40
35	k	616	II0	C11-C13	2.28	1.54	1.51
26	B	816	CLA	CHC-C1C	2.28	1.43	1.38
33	B	844	DGD	C1D-C2D	2.28	1.59	1.52
26	d	308	CLA	CHC-C1C	2.28	1.43	1.38
30	i	300	LMU	C2-C1	2.28	1.60	1.51
26	h	308	CLA	CHC-C1C	2.28	1.43	1.38
35	m	615	II0	C12-C14	2.28	1.54	1.51
26	B	808	CLA	C3B-C4B	2.28	1.49	1.42
26	m	607	CLA	C3B-C4B	2.28	1.49	1.42
26	a	310	CLA	C3B-C4B	2.28	1.49	1.42
26	j	605	CLA	CHC-C1C	2.28	1.43	1.38
35	k	619	II0	C12-C14	2.28	1.54	1.51
26	c	304	CLA	C3B-C4B	2.28	1.49	1.42
26	i	303	CLA	CHC-C1C	2.28	1.43	1.38
35	m	619	II0	C12-C14	2.28	1.54	1.51
26	c	306	CLA	C3B-C4B	2.28	1.49	1.42
26	l	305	CLA	MG-NB	-2.28	2.01	2.05
26	k	609	CLA	CHC-C1C	2.28	1.43	1.38
27	A	842	PQN	C10-C5	-2.28	1.37	1.40
29	F	203	WVN	C21-C15	2.28	1.54	1.50
26	B	801	CLA	CMB-C2B	-2.28	1.46	1.50
35	d	317	II0	C12-C14	2.28	1.54	1.51
26	B	813	CLA	CHC-C1C	2.28	1.43	1.38
35	J	104	II0	C12-C14	2.28	1.54	1.51
26	B	832	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	816	CLA	CHC-C1C	2.27	1.43	1.38
26	n	604	CLA	CHC-C1C	2.27	1.43	1.38
35	k	619	II0	C28-C26	2.27	1.52	1.50
29	h	309	WVN	C14-C15	2.27	1.55	1.51
26	A	802	CLA	CMD-C2D	-2.27	1.46	1.50
35	j	615	II0	C12-C14	2.27	1.54	1.51
26	n	607	CLA	CHC-C1C	2.27	1.43	1.38
36	s	401	KC2	CAA-C2A	2.27	1.53	1.46
29	l	316	WVN	C21-C15	2.27	1.54	1.50
26	L	203	CLA	CHC-C1C	2.27	1.43	1.38
26	k	606	CLA	CHC-C1C	2.27	1.43	1.38
26	B	826	CLA	CHC-C1C	2.27	1.43	1.38
26	B	836	CLA	CHC-C1C	2.27	1.43	1.38
26	A	810	CLA	CHC-C1C	2.27	1.43	1.38
26	B	811	CLA	CHC-C1C	2.27	1.43	1.38
26	A	823	CLA	C3B-C4B	2.27	1.49	1.42
28	A	843	LHG	O7-C5	-2.27	1.41	1.46
35	a	313	II0	C12-C14	2.27	1.54	1.51
26	a	301	CLA	C3B-C4B	2.27	1.49	1.42
26	A	807	CLA	CHC-C1C	2.27	1.43	1.38
26	i	307	CLA	CHC-C1C	2.27	1.43	1.38
35	k	616	II0	C12-C14	2.26	1.54	1.51
26	b	307	CLA	CHC-C1C	2.26	1.43	1.38
29	A	848	WVN	C16-C05	2.26	1.54	1.50
29	A	857	WVN	C14-C15	2.26	1.55	1.51
26	A	828	CLA	CHC-C1C	2.26	1.43	1.38
26	B	806	CLA	CHC-C1C	2.26	1.43	1.38
26	a	311	CLA	CHC-C1C	2.26	1.43	1.38
35	j	615	II0	C27-C25	2.26	1.52	1.50
35	b	315	II0	C12-C14	2.26	1.54	1.51
26	m	613	CLA	CHC-C1C	2.26	1.43	1.38
26	j	609	CLA	CHC-C1C	2.26	1.43	1.38
30	i	300	LMU	O5'-C1'	2.26	1.47	1.41
26	A	840	CLA	CMD-C2D	-2.26	1.46	1.50
26	i	308	CLA	CHC-C1C	2.26	1.43	1.38
26	n	610	CLA	CHC-C1C	2.26	1.43	1.38
26	i	306	CLA	CHC-C1C	2.26	1.43	1.38
26	Q	302	CLA	CHC-C1C	2.26	1.43	1.38
26	a	302	CLA	CHC-C1C	2.26	1.43	1.38
36	l	312	KC2	C1A-CHA	2.26	1.46	1.40
26	k	602	CLA	C3B-C4B	2.26	1.49	1.42
26	B	818	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	812	CLA	C3B-C4B	2.25	1.49	1.42
26	A	820	CLA	CHC-C1C	2.25	1.43	1.38
35	c	313	II0	C28-C26	2.25	1.52	1.50
35	i	314	II0	C12-C14	2.25	1.54	1.51
26	a	309	CLA	CHC-C1C	2.25	1.43	1.38
26	n	608	CLA	CHC-C1C	2.25	1.43	1.38
36	j	611	KC2	C1A-CHA	2.25	1.46	1.40
35	d	315	II0	C27-C25	2.25	1.52	1.50
26	d	313	CLA	CHC-C1C	2.25	1.43	1.38
26	n	613	CLA	C3B-C4B	2.25	1.49	1.42
26	A	814	CLA	CHC-C1C	2.25	1.43	1.38
26	l	304	CLA	CHC-C1C	2.25	1.43	1.38
30	i	300	LMU	O3'-C3'	2.25	1.48	1.43
26	l	308	CLA	C3B-C4B	2.25	1.49	1.42
36	i	309	KC2	C1A-CHA	2.25	1.46	1.40
26	A	813	CLA	CMD-C2D	-2.25	1.46	1.50
26	A	821	CLA	CHC-C1C	2.25	1.43	1.38
36	d	312	KC2	C1A-CHA	2.25	1.46	1.40
26	A	838	CLA	CHC-C1C	2.25	1.43	1.38
26	j	613	CLA	CHC-C1C	2.25	1.43	1.38
35	h	310	II0	C11-C13	2.25	1.54	1.51
26	i	302	CLA	CMC-C2C	-2.25	1.46	1.50
30	A	850	LMU	O5B-C1B	2.24	1.47	1.41
26	A	819	CLA	CHC-C1C	2.24	1.43	1.38
26	B	840	CLA	C3B-C4B	2.24	1.49	1.42
26	d	307	CLA	C3B-C4B	2.24	1.49	1.42
29	B	849	WVN	C14-C15	2.24	1.55	1.51
26	l	307	CLA	C3B-C4B	2.24	1.49	1.42
26	j	607	CLA	CMD-C2D	-2.24	1.46	1.50
26	B	825	CLA	CHC-C1C	2.24	1.43	1.38
26	A	833	CLA	CHC-C1C	2.24	1.43	1.38
26	A	852	CLA	CHC-C1C	2.24	1.43	1.38
26	d	306	CLA	CMB-C2B	-2.24	1.46	1.50
26	B	817	CLA	CHC-C1C	2.24	1.43	1.38
30	A	850	LMU	C2-C1	2.24	1.60	1.51
26	A	808	CLA	C3B-C4B	2.24	1.49	1.42
26	d	310	CLA	CHC-C1C	2.24	1.43	1.38
26	b	313	CLA	CHC-C1C	2.24	1.43	1.38
26	k	605	CLA	CHC-C1C	2.24	1.43	1.38
28	l	318	LHG	O7-C5	-2.24	1.41	1.46
26	A	835	CLA	C3B-C4B	2.24	1.49	1.42
26	B	837	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	305	CLA	CMD-C2D	-2.23	1.46	1.50
36	k	611	KC2	C1A-CHA	2.23	1.46	1.40
26	l	306	CLA	CHC-C1C	2.23	1.43	1.38
26	d	303	CLA	CHC-C1C	2.23	1.43	1.38
29	B	846	WVN	C14-C15	2.23	1.55	1.51
30	i	300	LMU	O5B-C1B	2.23	1.47	1.41
26	a	308	CLA	CHC-C1C	2.23	1.43	1.38
26	b	309	CLA	CHC-C1C	2.23	1.43	1.38
26	b	308	CLA	C3B-C4B	2.23	1.49	1.42
26	j	604	CLA	CHC-C1C	2.23	1.43	1.38
26	A	824	CLA	C3B-C4B	2.23	1.49	1.42
26	c	302	CLA	CHC-C1C	2.23	1.43	1.38
35	l	302	II0	C12-C14	2.23	1.54	1.51
29	s	405	WVN	C14-C15	2.23	1.55	1.51
26	B	801	CLA	C3B-C4B	2.23	1.49	1.42
36	k	613	KC2	C1A-CHA	2.23	1.46	1.40
26	l	308	CLA	CHC-C1C	2.23	1.43	1.38
35	d	316	II0	C28-C26	2.23	1.52	1.50
26	B	819	CLA	C3C-C2C	2.23	1.41	1.36
26	i	310	CLA	CMD-C2D	-2.23	1.46	1.50
26	A	830	CLA	CMD-C2D	-2.23	1.46	1.50
26	A	806	CLA	CHC-C1C	2.23	1.42	1.38
26	h	303	CLA	CHC-C1C	2.23	1.42	1.38
26	a	310	CLA	CHC-C1C	2.22	1.42	1.38
26	k	607	CLA	CHC-C1C	2.22	1.42	1.38
26	a	303	CLA	C3B-C4B	2.22	1.49	1.42
35	n	615	II0	C28-C26	2.22	1.52	1.50
28	n	619	LHG	O7-C5	-2.22	1.41	1.46
26	A	836	CLA	C3B-C4B	2.22	1.49	1.42
26	B	828	CLA	CMB-C2B	-2.22	1.46	1.50
35	d	315	II0	C12-C14	2.22	1.54	1.51
35	n	615	II0	C12-C14	2.22	1.54	1.51
26	h	306	CLA	CHC-C1C	2.22	1.42	1.38
35	h	311	II0	C27-C25	2.22	1.52	1.50
26	F	202	CLA	CHC-C1C	2.22	1.42	1.38
36	n	611	KC2	C1A-CHA	2.22	1.46	1.40
26	A	811	CLA	CHC-C1C	2.22	1.42	1.38
26	j	603	CLA	CHC-C1C	2.22	1.42	1.38
26	d	306	CLA	C3B-C4B	2.22	1.49	1.42
35	i	319	II0	C28-C26	2.22	1.52	1.50
35	a	312	II0	C12-C14	2.22	1.54	1.51
36	k	613	KC2	MG-NA	2.22	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	207	LHG	O7-C5	-2.22	1.41	1.46
28	b	318	LHG	O7-C5	-2.22	1.41	1.46
35	i	312	II0	C12-C14	2.22	1.54	1.51
26	k	607	CLA	CMD-C2D	-2.22	1.46	1.50
26	c	312	CLA	CHC-C1C	2.22	1.42	1.38
26	c	306	CLA	CHC-C1C	2.22	1.42	1.38
26	b	304	CLA	C3B-C4B	2.22	1.49	1.42
29	L	205	WVN	C14-C15	2.22	1.55	1.51
26	B	828	CLA	C3B-C4B	2.22	1.49	1.42
36	d	311	KC2	C1A-CHA	2.22	1.46	1.40
26	c	305	CLA	CMD-C2D	-2.21	1.46	1.50
26	k	602	CLA	CMD-C2D	-2.21	1.46	1.50
26	A	817	CLA	MG-NB	-2.21	2.01	2.05
35	m	616	II0	C12-C14	2.21	1.54	1.51
26	B	828	CLA	CHC-C1C	2.21	1.42	1.38
29	A	847	WVN	C14-C15	2.21	1.55	1.51
29	l	303	WVN	C14-C15	2.21	1.55	1.51
26	n	601	CLA	CHC-C1C	2.21	1.42	1.38
26	l	313	CLA	CHC-C1C	2.21	1.42	1.38
26	n	603	CLA	CHC-C1C	2.21	1.42	1.38
26	c	305	CLA	CMB-C2B	-2.21	1.46	1.50
29	i	315	WVN	C06-C13	2.21	1.56	1.53
26	B	824	CLA	CMC-C2C	-2.21	1.46	1.50
26	B	816	CLA	C3B-C4B	2.21	1.49	1.42
35	m	619	II0	C28-C26	2.21	1.52	1.50
35	i	313	II0	C12-C14	2.21	1.54	1.51
29	A	848	WVN	C14-C15	2.21	1.55	1.51
35	j	614	II0	C27-C25	2.21	1.52	1.50
26	A	835	CLA	CHC-C1C	2.21	1.42	1.38
36	s	404	KC2	C1A-CHA	2.21	1.46	1.40
35	i	319	II0	C27-C25	2.21	1.52	1.50
26	A	831	CLA	CHC-C1C	2.21	1.42	1.38
26	B	824	CLA	CHC-C1C	2.21	1.42	1.38
26	c	311	CLA	CHC-C1C	2.20	1.42	1.38
26	B	842	CLA	CMD-C2D	-2.20	1.46	1.50
26	n	605	CLA	CHC-C1C	2.20	1.42	1.38
26	l	305	CLA	CHC-C1C	2.20	1.42	1.38
35	a	316	II0	C27-C25	2.20	1.52	1.50
26	A	804	CLA	C3B-C4B	2.20	1.49	1.42
26	j	601	CLA	CHC-C1C	2.20	1.42	1.38
26	B	820	CLA	CMD-C2D	-2.20	1.46	1.50
26	h	301	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	408	CLA	CHC-C1C	2.20	1.42	1.38
26	m	606	CLA	CHC-C1C	2.20	1.42	1.38
28	c	317	LHG	O7-C5	-2.20	1.41	1.46
26	A	812	CLA	CHC-C1C	2.20	1.42	1.38
26	m	603	CLA	CMD-C2D	-2.20	1.46	1.50
27	A	842	PQN	C5-C4	-2.20	1.43	1.48
29	A	846	WVN	C14-C15	2.20	1.55	1.51
26	k	601	CLA	CHC-C1C	2.20	1.42	1.38
26	n	607	CLA	MG-NB	-2.20	2.01	2.05
35	d	315	II0	C28-C26	2.20	1.52	1.50
26	j	610	CLA	CHC-C1C	2.19	1.42	1.38
26	A	804	CLA	CMD-C2D	-2.19	1.46	1.50
26	b	311	CLA	CHC-C1C	2.19	1.42	1.38
26	k	610	CLA	CHC-C1C	2.19	1.42	1.38
26	d	318	CLA	CHC-C1C	2.19	1.42	1.38
26	B	820	CLA	C3B-C4B	2.19	1.49	1.42
29	B	853	WVN	C16-C05	2.19	1.54	1.50
29	R	200	WVN	C14-C15	2.19	1.55	1.51
26	A	832	CLA	CHC-C1C	2.19	1.42	1.38
26	n	602	CLA	C3B-C4B	2.19	1.49	1.42
29	B	853	WVN	C14-C15	2.19	1.55	1.51
26	s	402	CLA	CMB-C2B	-2.19	1.46	1.50
26	m	607	CLA	CHC-C1C	2.19	1.42	1.38
26	i	302	CLA	CMD-C2D	-2.19	1.46	1.50
26	B	840	CLA	CHC-C1C	2.19	1.42	1.38
26	k	614	CLA	CHC-C1C	2.19	1.42	1.38
28	s	409	LHG	P-O6	2.19	1.67	1.60
26	B	818	CLA	CMB-C2B	-2.19	1.46	1.50
26	B	839	CLA	CHC-C1C	2.19	1.42	1.38
26	a	305	CLA	CHC-C1C	2.19	1.42	1.38
26	m	612	CLA	CHC-C1C	2.18	1.42	1.38
26	B	832	CLA	CMB-C2B	-2.18	1.46	1.50
26	i	311	CLA	CHC-C1C	2.18	1.42	1.38
26	A	826	CLA	CMC-C2C	-2.18	1.46	1.50
26	B	830	CLA	CMD-C2D	-2.18	1.46	1.50
26	R	201	CLA	CHC-C1C	2.18	1.42	1.38
26	A	802	CLA	MG-NB	-2.18	2.01	2.05
35	l	314	II0	C28-C26	2.18	1.52	1.50
26	A	805	CLA	CMD-C2D	-2.18	1.46	1.50
36	c	310	KC2	C4A-C3A	2.18	1.48	1.44
26	A	822	CLA	CMD-C2D	-2.18	1.46	1.50
34	n	620	LMG	C7-C8	2.18	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	m	619	II0	C27-C25	2.18	1.52	1.50
26	B	840	CLA	CMB-C2B	-2.18	1.46	1.50
26	b	310	CLA	CHC-C1C	2.18	1.42	1.38
26	l	307	CLA	CHC-C1C	2.18	1.42	1.38
26	s	406	CLA	CMD-C2D	-2.18	1.46	1.50
36	k	612	KC2	C1A-CHA	2.18	1.45	1.40
35	b	314	II0	C12-C14	2.18	1.54	1.51
26	d	307	CLA	CMD-C2D	-2.18	1.46	1.50
26	L	202	CLA	CHC-C1C	2.17	1.42	1.38
26	m	603	CLA	C3B-C4B	2.17	1.49	1.42
26	B	818	CLA	MG-NB	-2.17	2.01	2.05
26	B	809	CLA	CMC-C2C	-2.17	1.46	1.50
26	F	201	CLA	CHC-C1C	2.17	1.42	1.38
26	n	602	CLA	CMD-C2D	-2.17	1.46	1.50
26	a	306	CLA	CHC-C1C	2.17	1.42	1.38
26	B	804	CLA	C3B-C4B	2.17	1.49	1.42
26	m	610	CLA	CHC-C1C	2.17	1.42	1.38
26	B	835	CLA	CMD-C2D	-2.17	1.46	1.50
26	A	822	CLA	CHC-C1C	2.17	1.42	1.38
26	b	311	CLA	CMD-C2D	-2.17	1.46	1.50
29	I	101	WVN	C16-C05	2.17	1.54	1.50
26	A	851	CLA	CHC-C1C	2.17	1.42	1.38
26	c	305	CLA	C3B-C4B	2.17	1.49	1.42
28	j	617	LHG	O7-C5	-2.17	1.41	1.46
26	B	814	CLA	CMD-C2D	-2.17	1.46	1.50
26	l	309	CLA	MG-NB	-2.17	2.01	2.05
34	b	319	LMG	O7-C8	-2.16	1.41	1.46
26	B	818	CLA	C1B-C2B	2.16	1.48	1.43
26	m	601	CLA	CHC-C1C	2.16	1.42	1.38
26	k	604	CLA	C3B-C4B	2.16	1.49	1.42
26	A	829	CLA	MG-NB	-2.16	2.01	2.05
26	c	304	CLA	CHC-C1C	2.16	1.42	1.38
26	j	606	CLA	CHC-C1C	2.16	1.42	1.38
26	A	834	CLA	MG-NB	-2.16	2.01	2.05
26	s	402	CLA	CHC-C1C	2.16	1.42	1.38
26	b	308	CLA	CHC-C1C	2.16	1.42	1.38
26	B	836	CLA	CMB-C2B	-2.16	1.46	1.50
29	B	846	WVN	C06-C13	2.16	1.56	1.53
26	B	837	CLA	CMB-C2B	-2.16	1.46	1.50
26	B	842	CLA	MG-NB	-2.16	2.01	2.05
26	l	305	CLA	C3B-C4B	2.16	1.49	1.42
26	k	602	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	304	CLA	CHC-C1C	2.16	1.42	1.38
28	i	317	LHG	O7-C5	-2.16	1.41	1.46
26	B	842	CLA	CMC-C2C	-2.16	1.46	1.50
26	k	608	CLA	CMC-C2C	-2.16	1.46	1.50
26	i	302	CLA	MG-NB	-2.16	2.01	2.05
26	h	306	CLA	CMD-C2D	-2.15	1.46	1.50
26	b	310	CLA	CMD-C2D	-2.15	1.46	1.50
26	B	801	CLA	CHC-C1C	2.15	1.42	1.38
26	B	804	CLA	CHC-C1C	2.15	1.42	1.38
26	B	825	CLA	CMD-C2D	-2.15	1.46	1.50
26	a	306	CLA	CMD-C2D	-2.15	1.46	1.50
26	k	608	CLA	CMD-C2D	-2.15	1.46	1.50
26	A	809	CLA	CHC-C1C	2.15	1.42	1.38
26	n	602	CLA	CHC-C1C	2.15	1.42	1.38
35	l	314	II0	C27-C25	2.15	1.52	1.50
26	A	830	CLA	C3B-C4B	2.15	1.49	1.42
29	L	201	WVN	C14-C15	2.15	1.55	1.51
26	a	301	CLA	CHC-C1C	2.15	1.42	1.38
35	d	317	II0	C28-C26	2.15	1.52	1.50
26	B	821	CLA	CMC-C2C	-2.15	1.46	1.50
26	B	804	CLA	C4C-C3C	2.15	1.48	1.45
26	A	836	CLA	CHC-C1C	2.15	1.42	1.38
26	B	808	CLA	CHC-C1C	2.15	1.42	1.38
26	k	606	CLA	CMD-C2D	-2.15	1.46	1.50
26	B	822	CLA	CMB-C2B	-2.15	1.46	1.50
26	c	311	CLA	CMD-C2D	-2.15	1.46	1.50
26	A	837	CLA	CHC-C1C	2.15	1.42	1.38
26	A	817	CLA	CMC-C2C	-2.15	1.46	1.50
26	A	833	CLA	CMB-C2B	-2.15	1.46	1.50
26	h	313	CLA	CMD-C2D	-2.15	1.46	1.50
26	A	815	CLA	CHC-C1C	2.15	1.42	1.38
26	h	301	CLA	CHC-C1C	2.15	1.42	1.38
26	B	823	CLA	MG-NB	-2.15	2.01	2.05
26	h	302	CLA	CMC-C2C	-2.15	1.46	1.50
26	n	606	CLA	CMD-C2D	-2.15	1.46	1.50
26	A	834	CLA	CHC-C1C	2.15	1.42	1.38
26	B	807	CLA	MG-NB	-2.15	2.01	2.05
26	A	840	CLA	CMB-C2B	-2.15	1.46	1.50
26	B	809	CLA	C3B-C4B	2.15	1.49	1.42
26	d	306	CLA	CMD-C2D	-2.15	1.46	1.50
26	A	830	CLA	CHC-C1C	2.14	1.42	1.38
26	a	303	CLA	CMB-C2B	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	824	CLA	CMD-C2D	-2.14	1.46	1.50
26	b	313	CLA	CMD-C2D	-2.14	1.46	1.50
26	B	804	CLA	CMC-C2C	-2.14	1.46	1.50
26	n	606	CLA	MG-NB	-2.14	2.01	2.05
26	A	808	CLA	CMD-C2D	-2.14	1.46	1.50
26	B	809	CLA	MG-NB	-2.14	2.01	2.05
26	A	820	CLA	CMB-C2B	-2.14	1.46	1.50
29	A	857	WVN	C16-C05	2.14	1.54	1.50
26	A	834	CLA	C3B-C4B	2.13	1.49	1.42
26	a	301	CLA	CMC-C2C	-2.13	1.46	1.50
26	A	823	CLA	CHC-C1C	2.13	1.42	1.38
26	B	822	CLA	CMC-C2C	-2.13	1.46	1.50
29	B	853	WVN	C06-C13	2.13	1.56	1.53
26	B	801	CLA	CMD-C2D	-2.13	1.46	1.50
26	B	836	CLA	MG-NB	-2.13	2.01	2.05
26	A	828	CLA	CMD-C2D	-2.13	1.46	1.50
26	m	603	CLA	MG-NB	-2.13	2.01	2.05
26	m	603	CLA	CHC-C1C	2.13	1.42	1.38
26	a	307	CLA	MG-NB	-2.13	2.01	2.05
26	n	606	CLA	C3B-C4B	2.13	1.48	1.42
26	c	305	CLA	CHC-C1C	2.13	1.42	1.38
26	m	606	CLA	CMB-C2B	-2.13	1.46	1.50
26	B	812	CLA	CHC-C1C	2.13	1.42	1.38
29	A	845	WVN	C16-C05	2.13	1.54	1.50
26	A	818	CLA	CHC-C1C	2.13	1.42	1.38
26	A	818	CLA	CMB-C2B	-2.13	1.46	1.50
26	j	602	CLA	MG-NB	-2.13	2.01	2.05
26	j	607	CLA	MG-NB	-2.13	2.01	2.05
26	c	306	CLA	CMD-C2D	-2.12	1.46	1.50
26	m	606	CLA	MG-NB	-2.12	2.01	2.05
26	d	313	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	814	CLA	CHC-C1C	2.12	1.42	1.38
35	a	316	II0	C11-C13	2.12	1.54	1.51
26	a	301	CLA	CMD-C2D	-2.12	1.46	1.50
26	m	604	CLA	CMD-C2D	-2.12	1.46	1.50
26	d	310	CLA	CMD-C2D	-2.12	1.46	1.50
26	a	302	CLA	MG-NB	-2.12	2.01	2.05
26	m	612	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	813	CLA	CMD-C2D	-2.12	1.46	1.50
26	a	310	CLA	CMB-C2B	-2.12	1.46	1.50
26	A	829	CLA	CMD-C2D	-2.12	1.46	1.50
26	A	839	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	319	LMG	C7-C8	2.12	1.57	1.50
26	A	825	CLA	CMD-C2D	-2.12	1.46	1.50
26	A	837	CLA	CMB-C2B	-2.12	1.46	1.50
30	i	300	LMU	O3B-C3B	2.12	1.48	1.43
26	a	307	CLA	CMB-C2B	-2.12	1.46	1.50
26	A	830	CLA	CMB-C2B	-2.11	1.46	1.50
26	B	835	CLA	CHC-C1C	2.11	1.42	1.38
26	i	301	CLA	CHC-C1C	2.11	1.42	1.38
36	m	611	KC2	C1A-CHA	2.11	1.45	1.40
26	B	805	CLA	CHC-C1C	2.11	1.42	1.38
35	i	314	II0	C27-C25	2.11	1.52	1.50
26	A	852	CLA	CMB-C2B	-2.11	1.46	1.50
28	J	105	LHG	O7-C5	-2.11	1.41	1.46
26	h	307	CLA	CHC-C1C	2.11	1.42	1.38
26	k	602	CLA	MG-NB	-2.11	2.01	2.05
29	l	316	WVN	C06-C13	2.11	1.56	1.53
26	B	815	CLA	MG-NB	-2.11	2.01	2.05
26	d	307	CLA	CHC-C1C	2.11	1.42	1.38
36	s	401	KC2	C4A-C3A	2.11	1.48	1.44
26	c	302	CLA	CMC-C2C	-2.11	1.46	1.50
26	A	837	CLA	CMD-C2D	-2.10	1.46	1.50
26	J	103	CLA	CMB-C2B	-2.10	1.46	1.50
26	A	836	CLA	CMD-C2D	-2.10	1.46	1.50
26	B	808	CLA	CMD-C2D	-2.10	1.46	1.50
26	s	403	CLA	MG-NB	-2.10	2.01	2.05
26	c	309	CLA	C1B-NB	-2.10	1.35	1.37
26	A	815	CLA	CMD-C2D	-2.10	1.46	1.50
28	s	409	LHG	O7-C5	-2.10	1.41	1.46
26	c	303	CLA	MG-NB	-2.10	2.01	2.05
26	B	839	CLA	CMD-C2D	-2.10	1.46	1.50
26	h	302	CLA	CMD-C2D	-2.10	1.46	1.50
35	d	317	II0	C11-C13	2.10	1.54	1.51
30	A	850	LMU	O3B-C3B	2.10	1.48	1.43
26	A	825	CLA	MG-NB	-2.10	2.01	2.05
26	B	828	CLA	MG-NB	-2.10	2.01	2.05
26	A	839	CLA	CMB-C2B	-2.10	1.46	1.50
26	i	305	CLA	CMD-C2D	-2.09	1.46	1.50
26	l	308	CLA	MG-NB	-2.09	2.01	2.05
26	j	613	CLA	CMD-C2D	-2.09	1.46	1.50
36	c	310	KC2	CBD-CAD	-2.09	1.47	1.56
26	B	809	CLA	CMD-C2D	-2.09	1.46	1.50
26	d	308	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	200	WVN	C16-C05	2.09	1.54	1.50
26	a	304	CLA	CMD-C2D	-2.09	1.46	1.50
26	A	804	CLA	CHC-C1C	2.09	1.42	1.38
26	c	304	CLA	CMB-C2B	-2.09	1.46	1.50
26	n	609	CLA	MG-NB	-2.09	2.01	2.05
26	B	820	CLA	CMB-C2B	-2.09	1.46	1.50
26	j	604	CLA	CMD-C2D	-2.09	1.46	1.50
26	K	101	CLA	CMC-C2C	-2.09	1.46	1.50
28	m	618	LHG	O7-C5	-2.09	1.41	1.46
26	B	808	CLA	CMC-C2C	-2.09	1.46	1.50
26	n	603	CLA	CMC-C2C	-2.09	1.46	1.50
26	l	310	CLA	MG-NB	-2.09	2.01	2.05
26	B	804	CLA	CMB-C2B	-2.09	1.46	1.50
26	i	304	CLA	CMD-C2D	-2.09	1.46	1.50
26	B	811	CLA	CMC-C2C	-2.09	1.46	1.50
26	B	828	CLA	CMD-C2D	-2.09	1.46	1.50
26	j	601	CLA	CMD-C2D	-2.09	1.46	1.50
35	i	316	II0	C27-C25	2.09	1.52	1.50
29	M	101	WVN	C14-C15	2.09	1.54	1.51
29	i	315	WVN	C16-C05	2.09	1.54	1.50
26	b	310	CLA	CMB-C2B	-2.08	1.46	1.50
26	b	310	CLA	CMC-C2C	-2.08	1.46	1.50
26	d	302	CLA	CMD-C2D	-2.08	1.46	1.50
26	c	308	CLA	CMD-C2D	-2.08	1.46	1.50
26	l	310	CLA	CMD-C2D	-2.08	1.46	1.50
26	b	304	CLA	MG-NB	-2.08	2.01	2.05
26	A	810	CLA	CMC-C2C	-2.08	1.46	1.50
26	b	311	CLA	CMB-C2B	-2.08	1.46	1.50
26	B	819	CLA	CMD-C2D	-2.08	1.46	1.50
26	b	307	CLA	CMD-C2D	-2.08	1.46	1.50
26	A	826	CLA	CMB-C2B	-2.08	1.46	1.50
26	m	602	CLA	CMC-C2C	-2.08	1.46	1.50
26	A	852	CLA	MG-NB	-2.08	2.01	2.05
35	i	313	II0	C11-C13	2.08	1.54	1.51
26	a	303	CLA	MG-NB	-2.08	2.01	2.05
26	A	815	CLA	CMB-C2B	-2.08	1.46	1.50
26	B	837	CLA	CMD-C2D	-2.08	1.46	1.50
26	d	307	CLA	CMB-C2B	-2.08	1.46	1.50
26	B	829	CLA	MG-NB	-2.08	2.01	2.05
26	c	309	CLA	MG-NB	2.08	2.09	2.05
26	A	808	CLA	CMB-C2B	-2.08	1.46	1.50
26	A	810	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	826	CLA	CHC-C1C	2.08	1.42	1.38
26	B	823	CLA	CMC-C2C	-2.08	1.46	1.50
26	m	613	CLA	CMB-C2B	-2.08	1.46	1.50
26	B	840	CLA	CMD-C2D	-2.08	1.46	1.50
26	k	609	CLA	CMB-C2B	-2.08	1.46	1.50
26	b	308	CLA	MG-NB	-2.08	2.01	2.05
26	h	313	CLA	CMB-C2B	-2.08	1.46	1.50
26	L	204	CLA	CMD-C2D	-2.08	1.46	1.50
26	A	831	CLA	CMD-C2D	-2.08	1.46	1.50
26	B	826	CLA	MG-NB	-2.08	2.01	2.05
26	l	301	CLA	CMD-C2D	-2.08	1.46	1.50
35	h	311	II0	C12-C14	2.08	1.54	1.51
26	K	101	CLA	CHC-C1C	2.07	1.42	1.38
26	A	816	CLA	CMD-C2D	-2.07	1.46	1.50
26	m	606	CLA	CMD-C2D	-2.07	1.46	1.50
26	n	602	CLA	MG-NB	-2.07	2.01	2.05
26	B	803	CLA	CHC-C1C	2.07	1.42	1.38
26	A	802	CLA	CMB-C2B	-2.07	1.46	1.50
36	s	404	KC2	C1B-NB	-2.07	1.35	1.37
26	j	612	CLA	CMD-C2D	-2.07	1.46	1.50
26	b	306	CLA	CMD-C2D	-2.07	1.46	1.50
26	j	602	CLA	CMD-C2D	-2.07	1.46	1.50
26	A	840	CLA	MG-NB	-2.07	2.01	2.05
26	c	307	CLA	CMD-C2D	-2.07	1.46	1.50
35	m	614	II0	C27-C25	2.07	1.52	1.50
26	A	819	CLA	CMD-C2D	-2.07	1.46	1.50
26	s	402	CLA	CMD-C2D	-2.07	1.46	1.50
35	d	316	II0	C11-C13	2.07	1.54	1.51
28	J	105	LHG	P-O6	2.07	1.67	1.59
26	L	202	CLA	CMB-C2B	-2.07	1.46	1.50
26	A	814	CLA	CMD-C2D	-2.07	1.46	1.50
26	h	307	CLA	CMB-C2B	-2.07	1.46	1.50
26	n	613	CLA	CHC-C1C	2.07	1.42	1.38
26	B	824	CLA	CMB-C2B	-2.07	1.46	1.50
26	A	803	CLA	CMD-C2D	-2.07	1.46	1.50
26	F	201	CLA	CMD-C2D	-2.07	1.46	1.50
26	h	305	CLA	CMB-C2B	-2.06	1.46	1.50
35	n	616	II0	C11-C13	2.06	1.54	1.51
26	F	201	CLA	CMB-C2B	-2.06	1.46	1.50
26	j	606	CLA	CMB-C2B	-2.06	1.46	1.50
26	A	837	CLA	MG-NB	-2.06	2.01	2.05
26	i	307	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	201	CLA	MG-NB	-2.06	2.01	2.05
26	j	603	CLA	CMC-C2C	-2.06	1.46	1.50
26	j	609	CLA	MG-NB	-2.06	2.01	2.05
29	l	316	WVN	C16-C05	2.06	1.54	1.50
26	B	835	CLA	CMB-C2B	-2.06	1.46	1.50
26	A	816	CLA	MG-NB	-2.06	2.01	2.05
26	B	803	CLA	CMC-C2C	-2.06	1.46	1.50
26	B	830	CLA	CMB-C2B	-2.06	1.46	1.50
26	b	305	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	838	CLA	CMD-C2D	-2.06	1.46	1.50
26	k	605	CLA	CMB-C2B	-2.06	1.46	1.50
28	A	844	LHG	O7-C5	-2.06	1.41	1.46
26	d	309	CLA	MG-NB	-2.06	2.01	2.05
26	B	806	CLA	MG-NB	-2.06	2.01	2.05
26	s	408	CLA	CMB-C2B	-2.06	1.46	1.50
26	A	827	CLA	CMD-C2D	-2.06	1.46	1.50
26	j	601	CLA	CMB-C2B	-2.06	1.46	1.50
26	A	805	CLA	MG-NB	-2.06	2.01	2.05
29	M	101	WVN	C16-C05	2.06	1.54	1.50
26	m	613	CLA	CMD-C2D	-2.06	1.46	1.50
26	c	305	CLA	MG-NB	-2.06	2.01	2.05
26	k	608	CLA	MG-NB	-2.06	2.01	2.05
35	k	620	II0	C11-C13	2.06	1.54	1.51
26	c	306	CLA	MG-NB	-2.06	2.01	2.05
26	A	809	CLA	CMD-C2D	-2.06	1.46	1.50
26	A	851	CLA	CMD-C2D	-2.06	1.46	1.50
26	A	852	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	812	CLA	MG-NB	-2.06	2.01	2.05
36	i	309	KC2	C1B-NB	-2.06	1.35	1.37
26	A	820	CLA	CMC-C2C	-2.05	1.46	1.50
26	a	309	CLA	CMD-C2D	-2.05	1.46	1.50
26	a	301	CLA	MG-NB	-2.05	2.01	2.05
26	h	303	CLA	CMB-C2B	-2.05	1.46	1.50
26	m	602	CLA	MG-NB	-2.05	2.01	2.05
26	B	806	CLA	CMD-C2D	-2.05	1.46	1.50
26	i	307	CLA	CMB-C2B	-2.05	1.46	1.50
26	m	608	CLA	CMD-C2D	-2.05	1.46	1.50
26	k	605	CLA	CMD-C2D	-2.05	1.46	1.50
29	h	309	WVN	C16-C05	2.05	1.54	1.50
26	A	813	CLA	CMB-C2B	-2.05	1.46	1.50
35	k	620	II0	C28-C26	2.05	1.52	1.50
26	a	309	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	601	CLA	CMD-C2D	-2.05	1.46	1.50
26	l	301	CLA	CHC-C1C	2.05	1.42	1.38
26	B	801	CLA	MG-NB	-2.05	2.01	2.05
29	A	845	WVN	C06-C13	2.05	1.56	1.53
29	B	848	WVN	C06-C13	2.05	1.56	1.53
26	B	817	CLA	CMB-C2B	-2.05	1.46	1.50
26	n	601	CLA	CMB-C2B	-2.05	1.46	1.50
26	i	304	CLA	MG-NB	-2.05	2.01	2.05
26	A	841	CLA	CMD-C2D	-2.05	1.46	1.50
26	m	603	CLA	CMB-C2B	-2.05	1.46	1.50
26	i	307	CLA	CMD-C2D	-2.05	1.46	1.50
26	n	608	CLA	CMD-C2D	-2.05	1.46	1.50
26	h	302	CLA	MG-NB	-2.05	2.01	2.05
26	d	303	CLA	MG-NB	-2.05	2.01	2.05
26	B	832	CLA	CHC-C1C	2.05	1.42	1.38
26	A	817	CLA	CMD-C2D	-2.05	1.46	1.50
26	B	829	CLA	CMC-C2C	-2.05	1.46	1.50
34	L	209	LMG	C7-C8	2.05	1.57	1.50
26	B	827	CLA	MG-NB	-2.05	2.01	2.05
26	A	824	CLA	CHC-C1C	2.05	1.42	1.38
26	A	815	CLA	MG-NB	-2.05	2.01	2.05
26	B	804	CLA	CMD-C2D	-2.05	1.46	1.50
26	h	301	CLA	CMC-C2C	-2.05	1.46	1.50
26	m	607	CLA	CMB-C2B	-2.05	1.46	1.50
26	m	609	CLA	CMD-C2D	-2.05	1.46	1.50
35	i	316	II0	C28-C26	2.05	1.52	1.50
26	m	601	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	308	CLA	MG-NB	-2.04	2.01	2.05
26	l	304	CLA	CMB-C2B	-2.04	1.46	1.50
26	n	605	CLA	CMD-C2D	-2.04	1.46	1.50
26	j	612	CLA	MG-NB	-2.04	2.01	2.05
26	A	824	CLA	CMB-C2B	-2.04	1.46	1.50
35	a	316	II0	C12-C14	2.04	1.54	1.51
26	B	804	CLA	C3D-C4D	2.04	1.48	1.44
26	B	815	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	807	CLA	CMB-C2B	-2.04	1.46	1.50
26	b	312	CLA	CMB-C2B	-2.04	1.46	1.50
34	c	319	LMG	O7-C8	-2.04	1.41	1.46
26	A	829	CLA	C3B-C4B	2.04	1.48	1.42
26	A	809	CLA	CMB-C2B	-2.04	1.46	1.50
26	j	609	CLA	CMC-C2C	-2.04	1.46	1.50
26	L	204	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	812	CLA	CMD-C2D	-2.04	1.46	1.50
26	a	306	CLA	CMB-C2B	-2.04	1.46	1.50
29	B	847	WVN	C16-C05	2.04	1.54	1.50
26	j	603	CLA	CMD-C2D	-2.04	1.46	1.50
26	Q	302	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	830	CLA	MG-NB	-2.04	2.01	2.05
26	i	306	CLA	MG-NB	-2.04	2.01	2.05
26	d	307	CLA	MG-NB	-2.04	2.01	2.05
26	B	815	CLA	CMC-C2C	-2.04	1.46	1.50
36	d	312	KC2	C1B-NB	-2.04	1.35	1.37
26	h	301	CLA	MG-NB	-2.04	2.01	2.05
26	B	841	CLA	CMC-C2C	-2.04	1.46	1.50
26	L	202	CLA	MG-NB	-2.04	2.01	2.05
26	L	206	CLA	CMD-C2D	-2.04	1.46	1.50
29	L	201	WVN	C16-C05	2.04	1.54	1.50
26	i	301	CLA	CMB-C2B	-2.04	1.46	1.50
26	m	612	CLA	MG-NB	-2.04	2.01	2.05
26	A	818	CLA	CMD-C2D	-2.04	1.46	1.50
26	K	101	CLA	CMB-C2B	-2.04	1.46	1.50
26	a	308	CLA	CMD-C2D	-2.04	1.46	1.50
26	l	305	CLA	CMB-C2B	-2.04	1.46	1.50
26	i	306	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	836	CLA	MG-NB	-2.04	2.01	2.05
26	a	308	CLA	CMB-C2B	-2.04	1.46	1.50
26	b	303	CLA	CMD-C2D	-2.04	1.46	1.50
26	k	609	CLA	CMC-C2C	-2.04	1.46	1.50
26	n	610	CLA	CMD-C2D	-2.04	1.46	1.50
26	J	103	CLA	MG-NB	-2.04	2.01	2.05
27	B	843	PQN	C6-C5	2.04	1.43	1.39
26	b	308	CLA	CMC-C2C	-2.04	1.46	1.50
29	s	407	WVN	C16-C05	2.04	1.54	1.50
26	d	302	CLA	MG-NB	-2.03	2.01	2.05
26	B	812	CLA	CMB-C2B	-2.03	1.46	1.50
26	l	304	CLA	CMD-C2D	-2.03	1.46	1.50
26	i	311	CLA	CMD-C2D	-2.03	1.46	1.50
34	L	209	LMG	O7-C8	-2.03	1.41	1.46
26	a	303	CLA	CHC-C1C	2.03	1.42	1.38
26	A	819	CLA	CMB-C2B	-2.03	1.46	1.50
36	s	401	KC2	CBD-CAD	-2.03	1.47	1.56
26	A	823	CLA	CMD-C2D	-2.03	1.46	1.50
26	B	812	CLA	CMC-C2C	-2.03	1.46	1.50
26	b	309	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	807	CLA	MG-NB	-2.03	2.01	2.05
28	L	207	LHG	P-O6	2.03	1.67	1.59
26	k	604	CLA	MG-NB	-2.03	2.01	2.05
26	k	605	CLA	MG-NB	-2.03	2.01	2.05
28	L	208	LHG	O7-C5	-2.03	1.41	1.46
28	j	617	LHG	P-O6	2.03	1.67	1.59
26	A	835	CLA	CMB-C2B	-2.03	1.46	1.50
26	a	307	CLA	CMD-C2D	-2.03	1.46	1.50
26	h	301	CLA	CMB-C2B	-2.03	1.46	1.50
26	l	307	CLA	CMC-C2C	-2.03	1.46	1.50
26	i	306	CLA	CMB-C2B	-2.03	1.46	1.50
26	B	831	CLA	MG-NB	-2.03	2.01	2.05
26	h	313	CLA	MG-NB	-2.03	2.01	2.05
26	B	829	CLA	CMD-C2D	-2.03	1.46	1.50
26	l	306	CLA	CMD-C2D	-2.03	1.46	1.50
26	k	603	CLA	CMD-C2D	-2.03	1.46	1.50
26	l	311	CLA	CMD-C2D	-2.03	1.46	1.50
26	A	811	CLA	CMD-C2D	-2.03	1.46	1.50
26	c	303	CLA	CMD-C2D	-2.03	1.46	1.50
26	a	303	CLA	CMC-C2C	-2.03	1.46	1.50
26	l	301	CLA	CMB-C2B	-2.03	1.46	1.50
26	n	601	CLA	CMD-C2D	-2.03	1.46	1.50
26	k	604	CLA	CHC-C1C	2.03	1.42	1.38
26	B	810	CLA	CMD-C2D	-2.03	1.46	1.50
26	l	305	CLA	CMD-C2D	-2.03	1.46	1.50
26	A	819	CLA	MG-NB	-2.03	2.01	2.05
26	c	302	CLA	MG-NB	-2.03	2.01	2.05
26	A	807	CLA	CMD-C2D	-2.03	1.46	1.50
26	B	833	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	834	CLA	CMD-C2D	-2.03	1.46	1.50
26	R	201	CLA	CMB-C2B	-2.03	1.46	1.50
26	A	816	CLA	CMC-C2C	-2.03	1.46	1.50
26	m	601	CLA	CMB-C2B	-2.03	1.46	1.50
26	m	607	CLA	CMD-C2D	-2.03	1.46	1.50
29	s	407	WVN	C14-C15	2.03	1.54	1.51
35	i	314	II0	C11-C13	2.03	1.54	1.51
26	n	601	CLA	MG-NB	-2.03	2.01	2.05
26	k	603	CLA	CMB-C2B	-2.03	1.46	1.50
26	m	609	CLA	MG-NB	-2.03	2.01	2.05
26	k	604	CLA	CMB-C2B	-2.03	1.46	1.50
35	k	620	II0	C27-C25	2.03	1.52	1.50
26	h	306	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	841	CLA	CMB-C2B	-2.03	1.46	1.50
26	F	202	CLA	CMD-C2D	-2.03	1.46	1.50
26	A	851	CLA	MG-NB	-2.03	2.01	2.05
26	L	206	CLA	CMB-C2B	-2.03	1.46	1.50
26	A	806	CLA	CMD-C2D	-2.03	1.46	1.50
26	h	304	CLA	CMD-C2D	-2.03	1.46	1.50
26	s	402	CLA	MG-NB	-2.03	2.01	2.05
26	l	308	CLA	CMB-C2B	-2.03	1.46	1.50
26	i	303	CLA	CMD-C2D	-2.03	1.46	1.50
26	i	308	CLA	CMD-C2D	-2.03	1.46	1.50
26	n	610	CLA	CMB-C2B	-2.03	1.46	1.50
26	l	311	CLA	CMB-C2B	-2.02	1.46	1.50
26	A	803	CLA	CMC-C2C	-2.02	1.46	1.50
26	A	831	CLA	CMB-C2B	-2.02	1.46	1.50
26	B	831	CLA	CMD-C2D	-2.02	1.46	1.50
26	h	306	CLA	CMB-C2B	-2.02	1.46	1.50
26	B	816	CLA	MG-NB	-2.02	2.01	2.05
26	d	309	CLA	CMD-C2D	-2.02	1.46	1.50
26	n	608	CLA	CMC-C2C	-2.02	1.46	1.50
26	A	814	CLA	MG-NB	-2.02	2.01	2.05
26	A	839	CLA	CMD-C2D	-2.02	1.46	1.50
26	c	306	CLA	CMB-C2B	-2.02	1.46	1.50
26	A	833	CLA	CMD-C2D	-2.02	1.46	1.50
26	i	302	CLA	CMB-C2B	-2.02	1.46	1.50
26	B	820	CLA	CHC-C1C	2.02	1.42	1.38
26	n	606	CLA	CMB-C2B	-2.02	1.46	1.50
26	n	613	CLA	CMD-C2D	-2.02	1.46	1.50
28	L	208	LHG	P-O6	2.02	1.67	1.59
33	B	844	DGD	O1G-C1G	-2.02	1.40	1.45
26	j	609	CLA	CMB-C2B	-2.02	1.46	1.50
26	d	305	CLA	CMD-C2D	-2.02	1.46	1.50
26	R	201	CLA	CMD-C2D	-2.02	1.46	1.50
32	A	854	SQD	O2-C2	-2.02	1.38	1.43
26	k	614	CLA	C3C-C2C	2.02	1.41	1.36
26	a	303	CLA	CMD-C2D	-2.02	1.46	1.50
26	c	312	CLA	CMD-C2D	-2.02	1.46	1.50
26	Q	302	CLA	MG-NB	-2.02	2.01	2.05
35	b	315	II0	C11-C13	2.02	1.54	1.51
26	B	827	CLA	CMC-C2C	-2.02	1.46	1.50
26	m	607	CLA	CMC-C2C	-2.02	1.46	1.50
26	k	608	CLA	CMB-C2B	-2.02	1.46	1.50
26	d	303	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	601	CLA	MG-NB	-2.02	2.01	2.05
26	B	811	CLA	CMD-C2D	-2.02	1.46	1.50
36	l	312	KC2	C1B-NB	-2.02	1.35	1.37
26	c	308	CLA	CMC-C2C	-2.02	1.46	1.50
26	a	305	CLA	CMB-C2B	-2.02	1.46	1.50
26	h	308	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	816	CLA	CMD-C2D	-2.02	1.46	1.50
26	B	821	CLA	CMD-C2D	-2.02	1.46	1.50
29	B	847	WVN	C06-C13	2.02	1.56	1.53
26	A	817	CLA	CMB-C2B	-2.02	1.46	1.50
26	A	835	CLA	CMD-C2D	-2.02	1.46	1.50
26	a	305	CLA	CMD-C2D	-2.02	1.46	1.50
28	l	318	LHG	P-O6	2.02	1.67	1.59
26	d	313	CLA	CMC-C2C	-2.02	1.46	1.50
26	L	202	CLA	CMD-C2D	-2.02	1.46	1.50
26	m	612	CLA	CMB-C2B	-2.02	1.46	1.50
26	K	101	CLA	CMD-C2D	-2.02	1.46	1.50
26	l	310	CLA	CMB-C2B	-2.02	1.46	1.50
26	B	834	CLA	CMC-C2C	-2.02	1.46	1.50
26	m	602	CLA	CMD-C2D	-2.02	1.46	1.50
26	k	610	CLA	CMB-C2B	-2.02	1.46	1.50
26	B	817	CLA	CMD-C2D	-2.01	1.46	1.50
26	b	303	CLA	CMB-C2B	-2.01	1.46	1.50
26	h	308	CLA	CMB-C2B	-2.01	1.46	1.50
26	A	822	CLA	CMB-C2B	-2.01	1.46	1.50
29	J	102	WVN	C06-C13	2.01	1.56	1.53
26	a	308	CLA	MG-NB	-2.01	2.01	2.05
35	c	316	II0	C28-C26	2.01	1.52	1.50
26	A	835	CLA	CMC-C2C	-2.01	1.46	1.50
26	A	851	CLA	CMB-C2B	-2.01	1.46	1.50
26	m	608	CLA	CMB-C2B	-2.01	1.46	1.50
28	c	320	LHG	O7-C5	-2.01	1.41	1.46
26	B	803	CLA	C3B-C4B	2.01	1.48	1.42
28	s	409	LHG	P-O3	2.01	1.62	1.54
26	B	822	CLA	MG-NB	-2.01	2.01	2.05
26	k	614	CLA	CMD-C2D	-2.01	1.46	1.50
26	d	306	CLA	CHC-C1C	2.01	1.42	1.38
26	L	203	CLA	CMD-C2D	-2.01	1.46	1.50
26	d	302	CLA	CMC-C2C	-2.01	1.46	1.50
26	B	813	CLA	CMB-C2B	-2.01	1.46	1.50
26	a	308	CLA	CMC-C2C	-2.01	1.46	1.50
26	A	832	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	307	CLA	CMC-C2C	-2.01	1.46	1.50
26	j	608	CLA	CMD-C2D	-2.01	1.46	1.50
26	A	806	CLA	CMB-C2B	-2.01	1.46	1.50
26	s	406	CLA	MG-NB	-2.01	2.01	2.05
26	k	610	CLA	CMD-C2D	-2.01	1.46	1.50
26	i	301	CLA	CMD-C2D	-2.01	1.46	1.50
26	j	605	CLA	CMD-C2D	-2.01	1.46	1.50
26	j	606	CLA	CMD-C2D	-2.01	1.46	1.50
26	j	609	CLA	CMD-C2D	-2.01	1.46	1.50
26	c	301	CLA	CMD-C2D	-2.01	1.46	1.50
26	d	304	CLA	CMB-C2B	-2.01	1.46	1.50
26	d	304	CLA	MG-NB	-2.01	2.01	2.05
26	d	308	CLA	CMD-C2D	-2.01	1.46	1.50
26	B	833	CLA	CMD-C2D	-2.01	1.46	1.50
26	i	303	CLA	CMB-C2B	-2.01	1.46	1.50
29	L	205	WVN	C16-C05	2.01	1.54	1.50
26	A	811	CLA	CMB-C2B	-2.01	1.46	1.50
26	s	403	CLA	CMB-C2B	-2.01	1.46	1.50
26	m	610	CLA	CMD-C2D	-2.01	1.46	1.50
26	j	610	CLA	CMD-C2D	-2.01	1.46	1.50
26	L	203	CLA	CMC-C2C	-2.01	1.46	1.50
26	B	825	CLA	MG-NB	-2.01	2.01	2.05
26	B	832	CLA	CMD-C2D	-2.01	1.46	1.50
26	m	610	CLA	CMB-C2B	-2.01	1.46	1.50
26	b	312	CLA	CHC-C1C	2.01	1.42	1.38
26	s	408	CLA	CMD-C2D	-2.01	1.46	1.50
26	j	601	CLA	MG-NB	-2.01	2.01	2.05
26	A	804	CLA	CMC-C2C	-2.00	1.46	1.50
26	a	311	CLA	CMD-C2D	-2.00	1.46	1.50
26	L	203	CLA	MG-NB	-2.00	2.01	2.05
26	b	303	CLA	CHC-C1C	2.00	1.42	1.38
26	h	303	CLA	CMD-C2D	-2.00	1.46	1.50
26	j	610	CLA	CMB-C2B	-2.00	1.46	1.50
26	c	312	CLA	CMB-C2B	-2.00	1.46	1.50
26	h	304	CLA	CMB-C2B	-2.00	1.46	1.50
36	n	612	KC2	C1B-NB	-2.00	1.35	1.37
26	A	826	CLA	CMD-C2D	-2.00	1.46	1.50
26	n	608	CLA	CMB-C2B	-2.00	1.46	1.50
26	A	826	CLA	MG-NB	-2.00	2.01	2.05
26	A	802	CLA	CMC-C2C	-2.00	1.46	1.50
26	n	607	CLA	CMB-C2B	-2.00	1.46	1.50
26	j	608	CLA	MG-NB	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	312	KC2	MG-NA	2.00	2.11	2.06
26	n	603	CLA	CMB-C2B	-2.00	1.46	1.50
26	c	311	CLA	CMC-C2C	-2.00	1.46	1.50
26	b	307	CLA	CMB-C2B	-2.00	1.46	1.50
26	j	605	CLA	CMB-C2B	-2.00	1.46	1.50
26	i	307	CLA	MG-NB	-2.00	2.01	2.05
26	l	313	CLA	CMD-C2D	-2.00	1.46	1.50

All (3469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	312	II0	C23-C21-C09	-28.33	109.52	175.48
35	c	316	II0	C23-C21-C09	-28.31	109.55	175.48
35	n	618	II0	C23-C21-C09	-28.10	110.04	175.48
35	h	310	II0	C23-C21-C09	-27.96	110.38	175.48
35	j	614	II0	C23-C21-C09	-27.65	111.10	175.48
35	b	315	II0	C23-C21-C09	-27.55	111.33	175.48
35	k	615	II0	C23-C21-C09	-27.55	111.33	175.48
35	J	104	II0	C23-C21-C09	-27.49	111.46	175.48
35	d	315	II0	C23-C21-C09	-27.47	111.52	175.48
35	l	314	II0	C23-C21-C09	-27.40	111.68	175.48
35	l	302	II0	C23-C21-C09	-27.34	111.81	175.48
35	i	312	II0	C24-C22-C10	-27.32	111.86	175.48
35	c	313	II0	C24-C22-C10	-27.27	111.98	175.48
35	a	316	II0	C23-C21-C09	-27.24	112.05	175.48
35	m	615	II0	C24-C22-C10	-27.23	112.08	175.48
35	l	314	II0	C24-C22-C10	-27.14	112.28	175.48
35	i	314	II0	C23-C21-C09	-27.10	112.38	175.48
35	m	615	II0	C23-C21-C09	-27.09	112.41	175.48
35	k	620	II0	C23-C21-C09	-27.05	112.50	175.48
35	d	317	II0	C23-C21-C09	-27.02	112.56	175.48
35	d	315	II0	C24-C22-C10	-27.00	112.62	175.48
35	n	615	II0	C23-C21-C09	-27.00	112.62	175.48
35	j	615	II0	C23-C21-C09	-26.96	112.72	175.48
35	i	319	II0	C23-C21-C09	-26.93	112.78	175.48
35	i	316	II0	C24-C22-C10	-26.92	112.79	175.48
35	k	616	II0	C24-C22-C10	-26.92	112.79	175.48
35	h	312	II0	C23-C21-C09	-26.90	112.85	175.48
35	m	619	II0	C23-C21-C09	-26.90	112.85	175.48
35	l	315	II0	C23-C21-C09	-26.85	112.96	175.48
35	a	314	II0	C24-C22-C10	-26.80	113.08	175.48
35	j	615	II0	C24-C22-C10	-26.77	113.15	175.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	n	616	II0	C23-C21-C09	-26.77	113.15	175.48
35	b	314	II0	C23-C21-C09	-26.74	113.22	175.48
35	c	316	II0	C24-C22-C10	-26.73	113.25	175.48
35	m	614	II0	C23-C21-C09	-26.69	113.33	175.48
35	m	616	II0	C23-C21-C09	-26.69	113.34	175.48
35	m	614	II0	C24-C22-C10	-26.67	113.39	175.48
35	c	313	II0	C23-C21-C09	-26.66	113.40	175.48
35	h	311	II0	C23-C21-C09	-26.65	113.44	175.48
35	a	313	II0	C23-C21-C09	-26.63	113.48	175.48
35	n	616	II0	C24-C22-C10	-26.59	113.56	175.48
35	i	316	II0	C23-C21-C09	-26.56	113.63	175.48
35	h	312	II0	C24-C22-C10	-26.52	113.73	175.48
35	d	301	II0	C24-C22-C10	-26.50	113.78	175.48
35	a	314	II0	C21-C23-C25	-26.49	86.20	176.23
35	a	312	II0	C23-C21-C09	-26.49	113.80	175.48
35	n	615	II0	C24-C22-C10	-26.48	113.81	175.48
35	i	313	II0	C23-C21-C09	-26.43	113.93	175.48
35	m	615	II0	C21-C23-C25	-26.42	86.44	176.23
35	d	317	II0	C24-C22-C10	-26.41	113.99	175.48
35	k	619	II0	C24-C22-C10	-26.40	114.02	175.48
35	n	618	II0	C24-C22-C10	-26.38	114.05	175.48
35	a	312	II0	C21-C23-C25	-26.34	86.72	176.23
35	a	314	II0	C23-C21-C09	-26.33	114.17	175.48
35	c	313	II0	C21-C23-C25	-26.32	86.80	176.23
35	h	311	II0	C24-C22-C10	-26.31	114.22	175.48
35	d	315	II0	C21-C23-C25	-26.29	86.91	176.23
35	j	614	II0	C24-C22-C10	-26.28	114.28	175.48
35	k	619	II0	C23-C21-C09	-26.28	114.29	175.48
35	h	312	II0	C21-C23-C25	-26.26	87.00	176.23
35	a	313	II0	C21-C23-C25	-26.25	87.02	176.23
35	m	619	II0	C24-C22-C10	-26.22	114.44	175.48
35	i	314	II0	C24-C22-C10	-26.19	114.51	175.48
35	l	315	II0	C24-C22-C10	-26.17	114.53	175.48
35	d	301	II0	C23-C21-C09	-26.14	114.61	175.48
35	j	615	II0	C21-C23-C25	-26.11	87.51	176.23
35	d	301	II0	C21-C23-C25	-26.09	87.56	176.23
35	a	316	II0	C24-C22-C10	-26.07	114.78	175.48
35	k	619	II0	C21-C23-C25	-26.06	87.68	176.23
35	d	316	II0	C24-C22-C10	-26.03	114.87	175.48
35	J	104	II0	C24-C22-C10	-25.96	115.03	175.48
35	m	619	II0	C21-C23-C25	-25.94	88.08	176.23
35	i	313	II0	C24-C22-C10	-25.93	115.11	175.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	314	II0	C24-C22-C10	-25.90	115.17	175.48
35	j	614	II0	C21-C23-C25	-25.90	88.22	176.23
35	l	314	II0	C21-C23-C25	-25.85	88.39	176.23
35	i	314	II0	C21-C23-C25	-25.81	88.52	176.23
35	a	313	II0	C24-C22-C10	-25.81	115.38	175.48
35	h	310	II0	C21-C23-C25	-25.78	88.63	176.23
35	l	302	II0	C24-C22-C10	-25.70	115.65	175.48
35	l	315	II0	C21-C23-C25	-25.66	89.05	176.23
35	k	616	II0	C23-C21-C09	-25.66	115.74	175.48
35	m	616	II0	C24-C22-C10	-25.65	115.76	175.48
35	a	316	II0	C21-C23-C25	-25.61	89.21	176.23
35	d	317	II0	C21-C23-C25	-25.55	89.40	176.23
35	h	311	II0	C21-C23-C25	-25.55	89.42	176.23
35	a	312	II0	C24-C22-C10	-25.52	116.06	175.48
35	k	620	II0	C21-C23-C25	-25.38	89.98	176.23
35	d	316	II0	C23-C21-C09	-25.37	116.40	175.48
35	b	314	II0	C21-C23-C25	-25.30	90.25	176.23
35	n	618	II0	C21-C23-C25	-25.30	90.27	176.23
35	k	620	II0	C24-C22-C10	-25.13	116.97	175.48
35	m	614	II0	C21-C23-C25	-25.04	91.15	176.23
35	l	302	II0	C21-C23-C25	-25.03	91.19	176.23
35	i	316	II0	C21-C23-C25	-25.00	91.27	176.23
35	n	615	II0	C21-C23-C25	-25.00	91.28	176.23
35	i	319	II0	C21-C23-C25	-24.87	91.70	176.23
35	J	104	II0	C21-C23-C25	-24.44	93.19	176.23
35	k	615	II0	C21-C23-C25	-23.80	95.34	176.23
35	k	616	II0	C21-C23-C25	-23.73	95.59	176.23
35	d	316	II0	C21-C23-C25	-23.64	95.89	176.23
35	i	313	II0	C21-C23-C25	-23.60	96.03	176.23
35	n	616	II0	C21-C23-C25	-23.50	96.38	176.23
35	m	616	II0	C21-C23-C25	-23.26	97.19	176.23
35	i	312	II0	C21-C23-C25	-23.19	97.43	176.23
35	c	316	II0	C21-C23-C25	-23.17	97.51	176.23
35	b	315	II0	C21-C23-C25	-22.57	99.53	176.23
35	i	319	II0	C24-C22-C10	-22.39	123.34	175.48
35	b	315	II0	C24-C22-C10	-22.10	124.01	175.48
35	k	615	II0	C24-C22-C10	-21.27	125.94	175.48
26	h	301	CLA	O2A-CGA-O1A	-19.99	73.62	123.63
29	s	407	WVN	C20-C23-C25	18.74	153.96	126.23
29	B	848	WVN	C20-C23-C25	18.64	153.82	126.23
29	l	316	WVN	C20-C23-C25	18.51	153.62	126.23
29	A	845	WVN	C20-C23-C25	18.32	153.34	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	102	WVN	C20-C23-C25	18.26	153.25	126.23
26	c	309	CLA	C1D-ND-C4D	-18.22	93.53	106.31
29	A	848	WVN	C20-C23-C25	18.16	153.10	126.23
29	L	201	WVN	C20-C23-C25	18.03	152.91	126.23
29	B	853	WVN	C20-C23-C25	17.96	152.80	126.23
29	R	200	WVN	C20-C23-C25	17.95	152.78	126.23
29	K	102	WVN	C20-C23-C25	17.89	152.70	126.23
29	L	205	WVN	C20-C23-C25	17.87	152.68	126.23
29	B	846	WVN	C20-C23-C25	17.86	152.66	126.23
29	i	315	WVN	C20-C23-C25	17.72	152.46	126.23
29	A	857	WVN	C20-C23-C25	17.71	152.43	126.23
29	B	849	WVN	C20-C23-C25	17.63	152.31	126.23
29	M	101	WVN	C20-C23-C25	17.63	152.31	126.23
29	h	309	WVN	C20-C23-C25	17.49	152.11	126.23
29	A	847	WVN	C20-C23-C25	17.45	152.04	126.23
29	J	101	WVN	C20-C23-C25	17.37	151.93	126.23
29	A	846	WVN	C20-C23-C25	17.18	151.65	126.23
29	s	405	WVN	C20-C23-C25	16.96	151.32	126.23
29	l	303	WVN	C20-C23-C25	16.94	151.29	126.23
29	A	847	WVN	C04-C09-C05	-16.85	108.75	124.83
29	B	850	WVN	C20-C23-C25	16.62	150.83	126.23
29	F	203	WVN	C20-C23-C25	16.57	150.75	126.23
29	B	847	WVN	C20-C23-C25	16.52	150.68	126.23
29	I	101	WVN	C20-C23-C25	16.32	150.38	126.23
29	i	315	WVN	C04-C09-C05	-15.20	110.32	124.83
29	A	857	WVN	C04-C09-C05	-15.11	110.40	124.83
26	h	301	CLA	O2A-CGA-CBA	15.09	157.84	111.83
29	A	846	WVN	C04-C09-C05	-14.86	110.65	124.83
29	s	407	WVN	C04-C09-C05	-14.66	110.84	124.83
35	h	310	II0	C31-C33-C35	-14.62	86.29	126.36
35	i	316	II0	C31-C33-C35	-14.50	86.61	126.36
35	n	616	II0	C31-C33-C35	-14.32	87.10	126.36
35	a	316	II0	C31-C33-C35	-14.31	87.13	126.36
35	d	315	II0	C31-C33-C35	-14.30	87.15	126.36
29	B	846	WVN	C21-C15-C13	-14.28	108.91	124.48
35	d	316	II0	C31-C33-C35	-14.27	87.22	126.36
29	s	407	WVN	C21-C15-C13	-14.26	108.92	124.48
35	n	615	II0	C31-C33-C35	-14.21	87.40	126.36
29	M	101	WVN	C04-C09-C05	-14.14	111.33	124.83
35	i	319	II0	C31-C33-C35	-14.09	87.73	126.36
35	i	314	II0	C31-C33-C35	-14.01	87.95	126.36
29	A	847	WVN	C21-C15-C13	-13.98	109.23	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	h	311	II0	C31-C33-C35	-13.88	88.29	126.36
35	n	618	II0	C31-C33-C35	-13.85	88.39	126.36
35	h	312	II0	C31-C33-C35	-13.85	88.39	126.36
35	i	312	II0	C31-C33-C35	-13.84	88.40	126.36
35	d	317	II0	C31-C33-C35	-13.84	88.42	126.36
35	c	316	II0	C31-C33-C35	-13.80	88.53	126.36
35	J	104	II0	C31-C33-C35	-13.78	88.58	126.36
29	R	200	WVN	C04-C09-C05	-13.73	111.73	124.83
29	L	201	WVN	C04-C09-C05	-13.69	111.76	124.83
29	B	850	WVN	C11-C19-C22	13.69	155.77	126.32
35	m	614	II0	C31-C33-C35	-13.54	89.23	126.36
29	l	316	WVN	C21-C15-C13	-13.51	109.74	124.48
35	k	615	II0	C31-C33-C35	-13.49	89.39	126.36
35	m	619	II0	C31-C33-C35	-13.43	89.53	126.36
35	k	616	II0	C31-C33-C35	-13.41	89.58	126.36
29	A	848	WVN	C04-C09-C05	-13.33	112.11	124.83
35	l	302	II0	C31-C33-C35	-13.31	89.86	126.36
35	l	302	II0	C42-C40-C36	-13.27	108.67	127.28
35	i	313	II0	C31-C33-C35	-13.25	90.02	126.36
35	k	620	II0	C31-C33-C35	-13.25	90.04	126.36
35	j	615	II0	C31-C33-C35	-13.18	90.22	126.36
29	K	102	WVN	C21-C15-C13	-13.11	110.17	124.48
35	c	313	II0	C31-C33-C35	-13.11	90.43	126.36
29	B	853	WVN	C21-C15-C13	-13.02	110.28	124.48
35	j	614	II0	C31-C33-C35	-13.00	90.72	126.36
29	L	205	WVN	C21-C15-C13	-12.99	110.31	124.48
35	b	314	II0	C31-C33-C35	-12.99	90.74	126.36
35	b	315	II0	C31-C33-C35	-12.95	90.86	126.36
35	a	314	II0	C31-C33-C35	-12.93	90.91	126.36
35	l	314	II0	C31-C33-C35	-12.93	90.92	126.36
29	B	850	WVN	C21-C15-C13	-12.91	110.40	124.48
35	k	619	II0	C31-C33-C35	-12.87	91.06	126.36
35	m	615	II0	C31-C33-C35	-12.87	91.07	126.36
29	i	315	WVN	C11-C19-C22	12.86	153.98	126.32
29	l	316	WVN	C11-C19-C22	12.74	153.74	126.32
29	A	857	WVN	C11-C19-C22	12.74	153.73	126.32
29	l	303	WVN	C21-C15-C13	-12.60	110.73	124.48
29	h	309	WVN	C21-C15-C13	-12.59	110.74	124.48
35	d	301	II0	C31-C33-C35	-12.52	92.04	126.36
29	F	203	WVN	C11-C19-C22	12.51	153.22	126.32
29	s	405	WVN	C21-C15-C13	-12.47	110.88	124.48
29	A	845	WVN	C11-C19-C22	12.45	153.10	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	846	WVN	C40-C37-C34	-12.41	109.88	127.28
29	s	405	WVN	C11-C19-C22	12.37	152.94	126.32
35	a	312	II0	C31-C33-C35	-12.37	92.46	126.36
29	R	200	WVN	C11-C19-C22	12.33	152.84	126.32
29	A	848	WVN	C29-C26-C22	-12.31	110.01	127.28
29	l	303	WVN	C11-C19-C22	12.30	152.79	126.32
29	J	101	WVN	C11-C19-C22	12.26	152.69	126.32
29	B	847	WVN	C21-C15-C13	-12.26	111.11	124.48
35	h	311	II0	C42-C40-C36	-12.21	110.16	127.28
29	L	205	WVN	C11-C19-C22	12.19	152.54	126.32
29	A	846	WVN	C11-C19-C22	12.17	152.50	126.32
35	a	313	II0	C31-C33-C35	-12.17	93.00	126.36
29	L	201	WVN	C11-C19-C22	12.14	152.43	126.32
35	m	619	II0	C42-C40-C36	-12.12	110.29	127.28
29	A	846	WVN	C21-C15-C13	-12.03	111.35	124.48
29	F	203	WVN	C21-C15-C13	-12.03	111.36	124.48
29	B	853	WVN	C11-C19-C22	12.02	152.17	126.32
29	J	102	WVN	C11-C19-C22	12.00	152.13	126.32
29	J	102	WVN	C21-C15-C13	-11.95	111.45	124.48
29	h	309	WVN	C11-C19-C22	11.94	152.00	126.32
29	A	857	WVN	C21-C15-C13	-11.90	111.49	124.48
35	k	620	II0	C42-C40-C36	-11.90	110.59	127.28
35	l	315	II0	C31-C33-C35	-11.87	93.82	126.36
29	B	848	WVN	C21-C15-C13	-11.82	111.58	124.48
29	A	845	WVN	C39-C36-C32	-11.81	110.72	127.28
29	K	102	WVN	C04-C09-C05	-11.76	113.61	124.83
35	a	314	II0	C42-C40-C36	-11.74	110.81	127.28
29	R	200	WVN	C21-C15-C13	-11.73	111.69	124.48
29	I	101	WVN	C21-C15-C13	-11.70	111.72	124.48
29	J	101	WVN	C21-C15-C13	-11.70	111.72	124.48
29	B	849	WVN	C21-C15-C13	-11.67	111.75	124.48
35	m	616	II0	C41-C39-C35	-11.64	110.95	127.28
29	A	847	WVN	C39-C36-C32	-11.62	110.98	127.28
35	b	314	II0	C42-C40-C36	-11.61	110.99	127.28
29	A	848	WVN	C21-C15-C13	-11.60	111.83	124.48
29	B	849	WVN	C11-C19-C22	11.59	151.25	126.32
29	i	315	WVN	C40-C37-C34	-11.57	111.05	127.28
29	B	850	WVN	C40-C37-C34	-11.57	111.05	127.28
29	l	316	WVN	C40-C37-C34	-11.55	111.08	127.28
29	B	848	WVN	C11-C19-C22	11.54	151.14	126.32
29	B	849	WVN	C40-C37-C34	-11.46	111.21	127.28
29	B	846	WVN	C11-C19-C22	11.44	150.94	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	407	WVN	C39-C36-C32	-11.44	111.24	127.28
29	i	315	WVN	C21-C15-C13	-11.43	112.01	124.48
29	M	101	WVN	C39-C36-C32	-11.43	111.25	127.28
29	s	407	WVN	C29-C26-C22	-11.42	111.26	127.28
29	B	848	WVN	C40-C37-C34	-11.42	111.27	127.28
29	K	102	WVN	C11-C19-C22	11.39	150.81	126.32
29	A	847	WVN	C11-C19-C22	11.38	150.79	126.32
29	I	101	WVN	C11-C19-C22	11.37	150.79	126.32
29	l	303	WVN	C39-C36-C32	-11.35	111.36	127.28
35	j	614	II0	C42-C40-C36	-11.34	111.37	127.28
29	B	847	WVN	C39-C36-C32	-11.34	111.37	127.28
36	c	310	KC2	CMA-C3A-C4A	-11.27	107.42	125.03
36	s	401	KC2	CMA-C3A-C4A	-11.27	107.42	125.03
35	i	316	II0	C42-C40-C36	-11.27	111.48	127.28
29	B	847	WVN	C11-C19-C22	11.25	150.52	126.32
29	K	102	WVN	C40-C37-C34	-11.25	111.51	127.28
29	A	857	WVN	C29-C26-C22	-11.24	111.51	127.28
29	J	101	WVN	C39-C36-C32	-11.22	111.54	127.28
29	A	857	WVN	C40-C37-C34	-11.19	111.59	127.28
29	s	405	WVN	C04-C09-C05	-11.18	114.16	124.83
29	h	309	WVN	C40-C37-C34	-11.18	111.60	127.28
29	A	845	WVN	C21-C15-C13	-11.14	112.33	124.48
29	A	848	WVN	C30-C28-C25	-11.12	111.68	127.28
29	J	101	WVN	C30-C28-C25	-11.10	111.71	127.28
35	h	312	II0	C42-C40-C36	-11.10	111.71	127.28
35	a	316	II0	C42-C40-C36	-11.08	111.74	127.28
29	A	847	WVN	C29-C26-C22	-11.08	111.74	127.28
29	B	853	WVN	C04-C09-C05	-11.08	114.25	124.83
29	s	405	WVN	C39-C36-C32	-11.07	111.75	127.28
29	L	201	WVN	C40-C37-C34	-11.07	111.76	127.28
29	B	849	WVN	C39-C36-C32	-11.05	111.78	127.28
35	J	104	II0	C42-C40-C36	-11.02	111.82	127.28
29	i	315	WVN	C39-C36-C32	-11.01	111.84	127.28
35	k	619	II0	C42-C40-C36	-11.01	111.84	127.28
29	M	101	WVN	C21-C15-C13	-10.99	112.49	124.48
29	L	205	WVN	C39-C36-C32	-10.96	111.91	127.28
35	a	312	II0	C42-C40-C36	-10.95	111.92	127.28
29	B	853	WVN	C30-C28-C25	-10.95	111.92	127.28
29	J	101	WVN	C04-C09-C05	-10.94	114.38	124.83
35	d	317	II0	C42-C40-C36	-10.94	111.94	127.28
35	m	616	II0	C31-C33-C35	-10.91	96.44	126.36
29	K	102	WVN	C29-C26-C22	-10.85	112.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	407	WVN	C11-C19-C22	10.85	149.66	126.32
35	m	614	II0	C42-C40-C36	-10.82	112.10	127.28
29	F	203	WVN	C30-C28-C25	-10.81	112.11	127.28
29	F	203	WVN	C04-C09-C05	-10.81	114.51	124.83
29	R	200	WVN	C40-C37-C34	-10.81	112.12	127.28
29	L	205	WVN	C40-C37-C34	-10.80	112.13	127.28
29	L	201	WVN	C30-C28-C25	-10.77	112.18	127.28
35	i	314	II0	C42-C40-C36	-10.77	112.18	127.28
29	I	101	WVN	C39-C36-C32	-10.76	112.19	127.28
35	n	616	II0	C42-C40-C36	-10.74	112.21	127.28
29	R	200	WVN	C39-C36-C32	-10.72	112.24	127.28
35	d	316	II0	C42-C40-C36	-10.71	112.25	127.28
29	L	201	WVN	C39-C36-C32	-10.71	112.25	127.28
29	M	101	WVN	C30-C28-C25	-10.71	112.25	127.28
29	I	101	WVN	C40-C37-C34	-10.70	112.28	127.28
29	L	201	WVN	C21-C15-C13	-10.69	112.82	124.48
29	B	846	WVN	C30-C33-C34	10.68	155.66	126.36
35	n	615	II0	C42-C40-C36	-10.68	112.30	127.28
29	J	102	WVN	C30-C28-C25	-10.66	112.32	127.28
29	L	205	WVN	C04-C09-C05	-10.65	114.66	124.83
29	A	847	WVN	C30-C28-C25	-10.63	112.36	127.28
29	J	102	WVN	C29-C26-C22	-10.62	112.38	127.28
35	d	315	II0	C42-C40-C36	-10.61	112.40	127.28
29	B	848	WVN	C29-C26-C22	-10.60	112.42	127.28
29	B	848	WVN	C04-C09-C05	-10.58	114.73	124.83
29	K	102	WVN	C30-C28-C25	-10.57	112.45	127.28
29	A	846	WVN	C40-C37-C34	-10.56	112.46	127.28
29	i	315	WVN	C29-C26-C22	-10.54	112.50	127.28
29	L	201	WVN	C29-C26-C22	-10.53	112.50	127.28
29	l	303	WVN	C40-C37-C34	-10.53	112.51	127.28
29	B	853	WVN	C39-C36-C32	-10.53	112.51	127.28
35	d	301	II0	C42-C40-C36	-10.52	112.52	127.28
29	J	102	WVN	C04-C09-C05	-10.52	114.79	124.83
29	R	200	WVN	C30-C28-C25	-10.51	112.54	127.28
35	c	316	II0	C41-C39-C35	-10.50	112.55	127.28
29	l	303	WVN	C04-C09-C05	-10.50	114.81	124.83
29	B	849	WVN	C29-C26-C22	-10.50	112.56	127.28
29	B	849	WVN	C04-C09-C05	-10.49	114.81	124.83
29	B	853	WVN	C29-C26-C22	-10.49	112.56	127.28
29	A	846	WVN	C30-C28-C25	-10.49	112.57	127.28
29	B	847	WVN	C30-C28-C25	-10.48	112.58	127.28
29	B	850	WVN	C29-C26-C22	-10.48	112.59	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	315	II0	C42-C40-C36	-10.47	112.59	127.28
29	B	853	WVN	C40-C37-C34	-10.46	112.61	127.28
29	M	101	WVN	C11-C19-C22	10.46	148.81	126.32
29	B	847	WVN	C40-C37-C34	-10.45	112.62	127.28
29	A	845	WVN	C40-C37-C34	-10.43	112.65	127.28
35	i	319	II0	C42-C40-C36	-10.43	112.65	127.28
29	l	316	WVN	C29-C26-C22	-10.39	112.71	127.28
29	l	316	WVN	C30-C33-C34	10.32	154.67	126.36
29	l	303	WVN	C30-C28-C25	-10.31	112.81	127.28
29	h	309	WVN	C30-C28-C25	-10.29	112.85	127.28
29	J	102	WVN	C29-C31-C32	10.28	154.56	126.36
29	A	848	WVN	C11-C19-C22	10.27	148.42	126.32
35	b	315	II0	C27-C25-C29	-10.27	104.23	124.18
35	m	616	II0	C42-C40-C36	-10.24	112.92	127.28
29	A	846	WVN	C39-C36-C32	-10.23	112.93	127.28
29	B	850	WVN	C04-C09-C05	-10.23	115.07	124.83
29	A	846	WVN	C29-C26-C22	-10.19	112.98	127.28
29	I	101	WVN	C29-C26-C22	-10.19	112.98	127.28
29	h	309	WVN	C29-C26-C22	-10.19	112.99	127.28
29	s	405	WVN	C30-C28-C25	-10.19	112.99	127.28
29	B	847	WVN	C29-C26-C22	-10.15	113.04	127.28
29	A	845	WVN	C04-C09-C05	-10.14	115.15	124.83
29	R	200	WVN	C29-C26-C22	-10.13	113.06	127.28
35	c	316	II0	C42-C40-C36	-10.12	113.09	127.28
26	h	301	CLA	O1A-CGA-CBA	-10.11	84.22	123.78
29	s	407	WVN	C30-C28-C25	-10.11	113.10	127.28
29	B	846	WVN	C30-C28-C25	-10.11	113.10	127.28
29	J	102	WVN	C39-C36-C32	-10.10	113.11	127.28
29	s	407	WVN	C40-C37-C34	-10.08	113.14	127.28
25	A	801	CL0	C1B-CHB-C4A	10.07	127.80	121.32
35	d	316	II0	C32-C34-C36	10.05	153.92	126.36
35	d	317	II0	C32-C34-C36	10.03	153.85	126.36
35	i	316	II0	C32-C34-C36	10.01	153.81	126.36
29	B	846	WVN	C29-C26-C22	-9.99	113.26	127.28
29	A	857	WVN	C39-C36-C32	-9.99	113.27	127.28
29	M	101	WVN	C29-C26-C22	-9.97	113.29	127.28
29	i	315	WVN	C30-C28-C25	-9.97	113.29	127.28
35	i	312	II0	C32-C34-C36	9.95	153.63	126.36
29	B	847	WVN	C04-C09-C05	-9.93	115.35	124.83
29	J	102	WVN	C40-C37-C34	-9.93	113.36	127.28
29	A	847	WVN	C40-C37-C34	-9.90	113.39	127.28
29	F	203	WVN	C40-C37-C34	-9.90	113.39	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	850	WVN	C30-C28-C25	-9.90	113.39	127.28
35	j	615	II0	C42-C40-C36	-9.89	113.41	127.28
29	I	101	WVN	C06-C13-C15	-9.88	109.14	122.64
29	B	853	WVN	C29-C31-C32	9.86	153.40	126.36
29	I	101	WVN	C04-C09-C05	-9.85	115.43	124.83
29	i	315	WVN	C29-C31-C32	9.83	153.31	126.36
35	l	314	II0	C42-C40-C36	-9.81	113.51	127.28
29	B	846	WVN	C02-C11-C19	-9.81	109.31	124.58
29	F	203	WVN	C29-C26-C22	-9.81	113.52	127.28
29	A	845	WVN	C29-C26-C22	-9.80	113.53	127.28
29	l	303	WVN	C30-C33-C34	9.80	153.24	126.36
29	l	316	WVN	C29-C31-C32	9.79	153.22	126.36
29	L	201	WVN	C02-C11-C19	-9.79	109.35	124.58
29	K	102	WVN	C30-C33-C34	9.77	153.16	126.36
29	B	847	WVN	C30-C33-C34	9.77	153.16	126.36
29	l	316	WVN	C30-C28-C25	-9.77	113.58	127.28
29	l	303	WVN	C29-C26-C22	-9.75	113.60	127.28
29	h	309	WVN	C30-C33-C34	9.74	153.07	126.36
29	M	101	WVN	C29-C31-C32	9.74	153.06	126.36
29	B	848	WVN	C30-C28-C25	-9.74	113.62	127.28
35	i	313	II0	C32-C34-C36	9.73	153.05	126.36
29	L	205	WVN	C30-C28-C25	-9.72	113.64	127.28
35	m	615	II0	C42-C40-C36	-9.71	113.67	127.28
26	c	309	CLA	C4A-NA-C1A	-9.71	102.25	106.68
29	F	203	WVN	C06-C13-C15	-9.70	109.38	122.64
29	A	848	WVN	C40-C37-C34	-9.70	113.67	127.28
35	i	312	II0	C42-C40-C36	-9.68	113.71	127.28
35	k	615	II0	C42-C40-C36	-9.67	113.72	127.28
29	h	309	WVN	C04-C09-C05	-9.65	115.62	124.83
29	s	405	WVN	C29-C26-C22	-9.64	113.76	127.28
29	A	846	WVN	C30-C33-C34	9.64	152.79	126.36
35	h	311	II0	C41-C39-C35	-9.63	113.78	127.28
29	s	405	WVN	C30-C33-C34	9.63	152.76	126.36
29	R	200	WVN	C29-C31-C32	9.63	152.76	126.36
35	n	616	II0	C32-C34-C36	9.62	152.75	126.36
29	l	303	WVN	C29-C31-C32	9.62	152.75	126.36
29	L	201	WVN	C30-C33-C34	9.59	152.67	126.36
35	c	316	II0	C32-C34-C36	9.59	152.67	126.36
29	A	847	WVN	C30-C33-C34	9.58	152.63	126.36
35	l	302	II0	C37-C35-C39	-9.58	107.30	122.82
29	s	405	WVN	C29-C31-C32	9.58	152.63	126.36
35	m	616	II0	C32-C34-C36	9.56	152.57	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	848	WVN	C30-C33-C34	9.56	152.57	126.36
29	l	316	WVN	C39-C36-C32	-9.55	113.89	127.28
35	l	302	II0	C41-C39-C35	-9.53	113.91	127.28
29	I	101	WVN	C30-C33-C34	9.53	152.49	126.36
35	a	313	II0	C42-C40-C36	-9.52	113.93	127.28
29	B	850	WVN	C29-C31-C32	9.51	152.43	126.36
35	i	314	II0	C32-C34-C36	9.50	152.41	126.36
35	l	314	II0	C32-C34-C36	9.50	152.41	126.36
29	I	101	WVN	C30-C28-C25	-9.50	113.96	127.28
35	c	313	II0	C42-C40-C36	-9.50	113.96	127.28
29	A	845	WVN	C30-C33-C34	9.50	152.40	126.36
29	I	101	WVN	C29-C31-C32	9.49	152.40	126.36
35	d	315	II0	C32-C34-C36	9.49	152.39	126.36
29	L	205	WVN	C30-C33-C34	9.49	152.38	126.36
29	h	309	WVN	C39-C36-C32	-9.49	113.97	127.28
35	c	313	II0	C32-C34-C36	9.48	152.37	126.36
29	M	101	WVN	C30-C33-C34	9.48	152.37	126.36
29	A	846	WVN	C29-C31-C32	9.48	152.35	126.36
29	L	205	WVN	C29-C31-C32	9.46	152.29	126.36
35	a	313	II0	C32-C34-C36	9.45	152.29	126.36
29	B	848	WVN	C29-C31-C32	9.45	152.28	126.36
35	k	616	II0	C32-C34-C36	9.45	152.27	126.36
29	F	203	WVN	C39-C36-C32	-9.44	114.04	127.28
35	d	316	II0	C27-C25-C29	-9.43	105.87	124.18
35	k	615	II0	C32-C34-C36	9.43	152.21	126.36
35	i	319	II0	C32-C34-C36	9.41	152.17	126.36
35	m	614	II0	C32-C34-C36	9.41	152.16	126.36
29	R	200	WVN	C30-C33-C34	9.40	152.14	126.36
29	A	857	WVN	C29-C31-C32	9.40	152.13	126.36
29	s	407	WVN	C30-C33-C34	9.40	152.13	126.36
29	B	848	WVN	C39-C36-C32	-9.38	114.13	127.28
35	l	315	II0	C38-C36-C40	-9.35	107.67	122.82
35	l	315	II0	C38-C36-C34	-9.34	103.81	118.09
35	a	316	II0	C41-C39-C35	-9.32	114.21	127.28
29	h	309	WVN	C29-C31-C32	9.31	151.89	126.36
29	J	101	WVN	C29-C26-C22	-9.31	114.23	127.28
35	J	104	II0	C32-C34-C36	9.29	151.85	126.36
29	A	848	WVN	C39-C36-C32	-9.28	114.26	127.28
29	B	853	WVN	C30-C33-C34	9.28	151.80	126.36
35	n	618	II0	C41-C39-C35	-9.28	114.27	127.28
29	B	846	WVN	C04-C09-C05	-9.27	115.99	124.83
29	J	101	WVN	C30-C33-C34	9.26	151.76	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	310	KC2	C1D-ND-C4D	-9.26	99.82	106.31
29	B	849	WVN	C30-C28-C25	-9.25	114.31	127.28
35	h	311	II0	C32-C34-C36	9.24	151.70	126.36
29	K	102	WVN	C29-C31-C32	9.24	151.69	126.36
35	k	620	II0	C32-C34-C36	9.23	151.68	126.36
35	k	619	II0	C37-C35-C39	-9.23	107.86	122.82
29	J	101	WVN	C40-C37-C34	-9.21	114.37	127.28
35	d	301	II0	C32-C34-C36	9.20	151.60	126.36
35	b	314	II0	C32-C34-C36	9.20	151.59	126.36
35	n	615	II0	C41-C39-C35	-9.19	114.39	127.28
29	J	101	WVN	C29-C31-C32	9.19	151.55	126.36
35	j	615	II0	C32-C34-C36	9.18	151.52	126.36
35	a	314	II0	C37-C35-C39	-9.16	107.97	122.82
29	J	102	WVN	C30-C33-C34	9.16	151.49	126.36
35	a	314	II0	C32-C34-C36	9.16	151.48	126.36
35	h	310	II0	C41-C39-C35	-9.16	114.43	127.28
29	A	845	WVN	C29-C31-C32	9.15	151.46	126.36
35	n	618	II0	C32-C34-C36	9.14	151.44	126.36
29	M	101	WVN	C40-C37-C34	-9.14	114.46	127.28
35	m	615	II0	C32-C34-C36	9.13	151.40	126.36
29	L	201	WVN	C29-C31-C32	9.13	151.40	126.36
35	m	614	II0	C41-C39-C35	-9.11	114.51	127.28
35	n	616	II0	C41-C39-C35	-9.09	114.53	127.28
29	B	848	WVN	C30-C33-C34	9.08	151.27	126.36
29	B	847	WVN	C29-C31-C32	9.07	151.23	126.36
29	F	203	WVN	C30-C33-C34	9.07	151.22	126.36
29	A	857	WVN	C30-C33-C34	9.06	151.20	126.36
35	a	316	II0	C32-C34-C36	9.02	151.09	126.36
29	B	846	WVN	C39-C36-C32	-9.01	114.64	127.28
29	A	848	WVN	C29-C31-C32	9.00	151.03	126.36
35	a	312	II0	C32-C34-C36	8.98	150.99	126.36
35	j	614	II0	C32-C34-C36	8.97	150.95	126.36
29	K	102	WVN	C39-C36-C32	-8.96	114.71	127.28
35	i	314	II0	C41-C39-C35	-8.95	114.72	127.28
35	h	312	II0	C32-C34-C36	8.94	150.89	126.36
35	n	618	II0	C42-C40-C36	-8.94	114.74	127.28
35	i	319	II0	C41-C39-C35	-8.93	114.75	127.28
35	l	314	II0	C41-C39-C35	-8.93	114.76	127.28
35	j	614	II0	C37-C35-C39	-8.92	108.36	122.82
29	I	101	WVN	C14-C15-C13	-8.92	110.65	122.70
29	B	846	WVN	C29-C31-C32	8.92	150.82	126.36
35	i	316	II0	C41-C39-C35	-8.92	114.77	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	314	II0	C41-C39-C35	-8.91	114.78	127.28
35	d	317	II0	C41-C39-C35	-8.88	114.82	127.28
35	k	615	II0	C27-C25-C29	-8.88	106.93	124.18
35	c	316	II0	C37-C35-C39	-8.87	108.45	122.82
35	h	310	II0	C42-C40-C36	-8.86	114.85	127.28
35	l	315	II0	C41-C39-C35	-8.84	114.88	127.28
35	k	619	II0	C32-C34-C36	8.83	150.56	126.36
29	A	848	WVN	C24-C22-C26	-8.82	108.52	122.82
29	F	203	WVN	C29-C31-C32	8.82	150.56	126.36
35	l	302	II0	C38-C36-C40	-8.82	108.53	122.82
29	B	849	WVN	C29-C31-C32	8.80	150.51	126.36
35	k	620	II0	C37-C35-C39	-8.78	108.59	122.82
29	i	315	WVN	C30-C33-C34	8.78	150.43	126.36
29	B	849	WVN	C38-C34-C37	-8.76	108.63	122.82
35	k	619	II0	C20-C14-C10	-8.75	107.81	124.16
29	K	102	WVN	C35-C32-C36	-8.74	108.66	122.82
29	l	316	WVN	C38-C34-C37	-8.74	108.66	122.82
29	J	102	WVN	C27-C25-C28	-8.74	108.66	122.82
29	B	849	WVN	C30-C33-C34	8.72	150.27	126.36
35	m	619	II0	C32-C34-C36	8.71	150.25	126.36
29	J	101	WVN	C06-C13-C15	-8.69	110.76	122.64
35	J	104	II0	C41-C39-C35	-8.69	115.09	127.28
35	n	615	II0	C32-C34-C36	8.68	150.17	126.36
29	M	101	WVN	C02-C05-C09	-8.68	110.79	121.47
35	d	301	II0	C37-C35-C39	-8.68	108.76	122.82
36	s	401	KC2	CMA-C3A-C2A	-8.67	107.44	128.43
35	J	104	II0	C27-C25-C29	-8.66	107.35	124.18
29	B	850	WVN	C39-C36-C32	-8.65	115.14	127.28
29	i	315	WVN	C38-C34-C37	-8.65	108.80	122.82
29	A	857	WVN	C24-C22-C26	-8.63	108.83	122.82
36	c	310	KC2	C2A-C3A-C4A	-8.63	99.93	106.41
35	k	620	II0	C20-C14-C10	-8.61	108.06	124.16
29	L	205	WVN	C29-C26-C22	-8.61	115.21	127.28
35	b	315	II0	C22-C24-C26	-8.60	147.00	176.23
36	s	401	KC2	C1D-ND-C4D	-8.58	100.29	106.31
29	A	845	WVN	C35-C32-C36	-8.57	108.92	122.82
35	i	313	II0	C42-C40-C36	-8.57	115.26	127.28
29	B	850	WVN	C30-C33-C34	8.57	149.86	126.36
29	B	846	WVN	C38-C34-C37	-8.56	108.95	122.82
29	A	857	WVN	C30-C28-C25	-8.54	115.30	127.28
35	j	615	II0	C41-C39-C35	-8.53	115.31	127.28
35	k	616	II0	C19-C13-C09	-8.52	108.23	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	850	WVN	C27-C25-C28	-8.52	109.02	122.82
29	B	846	WVN	C24-C22-C19	-8.51	105.08	118.09
35	m	619	II0	C41-C39-C35	-8.51	115.35	127.28
29	R	200	WVN	C38-C34-C37	-8.50	109.04	122.82
35	k	615	II0	C38-C36-C40	-8.50	109.04	122.82
26	c	309	CLA	C2C-C1C-NC	8.48	118.89	109.98
35	a	312	II0	C41-C39-C35	-8.48	115.39	127.28
35	j	614	II0	C41-C39-C35	-8.47	115.39	127.28
26	c	309	CLA	C2B-C1B-NB	8.45	119.09	110.33
29	l	316	WVN	C24-C22-C26	-8.44	109.14	122.82
29	B	850	WVN	C24-C22-C26	-8.43	109.16	122.82
29	A	846	WVN	C02-C05-C09	-8.43	111.10	121.47
29	A	848	WVN	C27-C25-C28	-8.41	109.19	122.82
29	B	849	WVN	C35-C32-C36	-8.40	109.21	122.82
29	i	315	WVN	C35-C32-C36	-8.39	109.22	122.82
35	m	614	II0	C38-C36-C40	-8.39	109.23	122.82
35	d	317	II0	C38-C36-C40	-8.39	109.23	122.82
35	a	316	II0	C38-C36-C40	-8.38	109.23	122.82
35	n	615	II0	C20-C14-C10	-8.38	108.49	124.16
35	m	615	II0	C33-C35-C39	-8.38	105.83	119.01
29	l	316	WVN	C04-C09-C05	-8.38	116.83	124.83
35	i	319	II0	C38-C36-C40	-8.38	109.25	122.82
29	s	405	WVN	C35-C32-C36	-8.37	109.25	122.82
29	K	102	WVN	C24-C22-C26	-8.36	109.27	122.82
35	j	614	II0	C20-C14-C10	-8.36	108.53	124.16
29	A	846	WVN	C27-C25-C28	-8.36	109.28	122.82
35	h	312	II0	C41-C39-C35	-8.35	115.56	127.28
35	d	316	II0	C41-C39-C35	-8.35	115.57	127.28
29	s	407	WVN	C02-C05-C09	-8.35	111.20	121.47
29	J	101	WVN	C35-C32-C36	-8.34	109.30	122.82
35	k	615	II0	C41-C39-C35	-8.34	115.58	127.28
35	i	316	II0	C38-C36-C40	-8.34	109.31	122.82
35	h	311	II0	C37-C35-C39	-8.33	109.31	122.82
29	M	101	WVN	C27-C25-C28	-8.33	109.32	122.82
35	i	313	II0	C19-C13-C09	-8.32	108.61	124.16
29	A	847	WVN	C29-C31-C32	8.31	149.16	126.36
35	h	311	II0	C38-C36-C40	-8.31	109.35	122.82
27	A	842	PQN	C11-C12-C13	-8.31	112.51	126.83
29	i	315	WVN	C24-C22-C26	-8.31	109.36	122.82
29	l	316	WVN	C38-C34-C33	-8.31	105.40	118.09
29	B	853	WVN	C35-C32-C36	-8.30	109.38	122.82
29	L	205	WVN	C38-C34-C37	-8.29	109.38	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	853	WVN	C27-C25-C28	-8.29	109.39	122.82
35	m	614	II0	C37-C35-C39	-8.29	109.39	122.82
29	F	203	WVN	C14-C15-C13	-8.29	111.51	122.70
29	L	201	WVN	C38-C34-C37	-8.29	109.39	122.82
27	B	843	PQN	C11-C12-C13	-8.28	112.56	126.83
29	B	850	WVN	C35-C32-C36	-8.28	109.40	122.82
35	a	312	II0	C37-C35-C39	-8.28	109.40	122.82
36	s	401	KC2	C2A-C3A-C4A	-8.28	100.19	106.41
29	A	846	WVN	C35-C32-C36	-8.28	109.41	122.82
29	B	850	WVN	C38-C34-C37	-8.28	109.41	122.82
29	A	847	WVN	C27-C25-C28	-8.28	109.41	122.82
29	J	102	WVN	C24-C22-C26	-8.27	109.41	122.82
29	l	303	WVN	C35-C32-C36	-8.27	109.41	122.82
35	n	616	II0	C38-C36-C40	-8.27	109.42	122.82
29	s	405	WVN	C06-C13-C15	-8.27	111.34	122.64
29	l	303	WVN	C38-C34-C37	-8.26	109.43	122.82
29	J	102	WVN	C35-C32-C31	-8.26	105.47	118.09
29	h	309	WVN	C27-C25-C28	-8.26	109.44	122.82
29	B	847	WVN	C38-C34-C37	-8.24	109.46	122.82
29	I	101	WVN	C27-C25-C28	-8.24	109.46	122.82
29	s	405	WVN	C40-C37-C34	-8.24	115.72	127.28
35	b	315	II0	C37-C35-C39	-8.24	109.47	122.82
35	l	302	II0	C32-C34-C36	8.23	148.93	126.36
29	B	848	WVN	C24-C22-C26	-8.23	109.48	122.82
35	c	316	II0	C38-C36-C40	-8.23	109.48	122.82
29	A	846	WVN	C38-C34-C37	-8.23	109.48	122.82
35	n	618	II0	C38-C36-C40	-8.23	109.49	122.82
29	A	845	WVN	C38-C34-C37	-8.23	109.49	122.82
35	a	314	II0	C38-C36-C40	-8.22	109.49	122.82
35	m	619	II0	C37-C35-C39	-8.22	109.49	122.82
35	J	104	II0	C20-C14-C10	-8.22	108.79	124.16
35	d	301	II0	C33-C35-C39	-8.22	106.09	119.01
29	R	200	WVN	C24-C22-C26	-8.21	109.51	122.82
29	A	847	WVN	C35-C32-C36	-8.21	109.51	122.82
29	A	857	WVN	C38-C34-C37	-8.21	109.52	122.82
35	i	319	II0	C22-C24-C26	-8.21	148.34	176.23
29	s	407	WVN	C29-C31-C32	8.21	148.86	126.36
29	A	846	WVN	C24-C22-C26	-8.20	109.53	122.82
29	s	405	WVN	C27-C25-C28	-8.20	109.53	122.82
35	J	104	II0	C38-C36-C40	-8.20	109.53	122.82
35	c	313	II0	C41-C39-C35	-8.19	115.79	127.28
29	h	309	WVN	C38-C34-C37	-8.19	109.54	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	203	WVN	C38-C34-C37	-8.19	109.54	122.82
35	n	618	II0	C37-C35-C39	-8.19	109.55	122.82
29	R	200	WVN	C27-C25-C28	-8.19	109.56	122.82
35	l	315	II0	C37-C35-C39	-8.18	109.56	122.82
29	A	845	WVN	C30-C28-C25	-8.18	115.80	127.28
29	l	316	WVN	C27-C25-C28	-8.18	109.57	122.82
35	i	314	II0	C38-C36-C40	-8.17	109.57	122.82
29	K	102	WVN	C27-C25-C28	-8.17	109.58	122.82
29	s	407	WVN	C35-C32-C36	-8.15	109.62	122.82
29	I	101	WVN	C35-C32-C36	-8.14	109.62	122.82
29	B	848	WVN	C38-C34-C37	-8.14	109.63	122.82
35	d	315	II0	C41-C39-C35	-8.13	115.88	127.28
35	b	315	II0	C38-C36-C34	-8.13	105.67	118.09
35	b	315	II0	C38-C36-C40	-8.12	109.65	122.82
29	l	316	WVN	C35-C32-C36	-8.11	109.67	122.82
29	l	303	WVN	C27-C25-C28	-8.11	109.68	122.82
29	s	405	WVN	C02-C05-C09	-8.10	111.50	121.47
29	J	101	WVN	C27-C25-C28	-8.10	109.70	122.82
35	i	319	II0	C37-C35-C39	-8.10	109.70	122.82
29	B	853	WVN	C24-C22-C26	-8.09	109.70	122.82
29	L	201	WVN	C27-C25-C28	-8.09	109.71	122.82
35	k	619	II0	C19-C13-C09	-8.09	109.03	124.16
29	R	200	WVN	C35-C32-C36	-8.09	109.71	122.82
29	B	847	WVN	C35-C32-C36	-8.09	109.71	122.82
36	c	310	KC2	CMA-C3A-C2A	-8.09	108.86	128.43
35	b	314	II0	C20-C14-C10	-8.07	109.08	124.16
29	L	201	WVN	C35-C32-C36	-8.07	109.75	122.82
29	i	315	WVN	C06-C13-C15	-8.06	111.63	122.64
29	L	205	WVN	C35-C32-C36	-8.05	109.78	122.82
35	k	616	II0	C27-C25-C29	-8.05	108.55	124.18
29	I	101	WVN	C24-C22-C26	-8.04	109.78	122.82
35	b	314	II0	C38-C36-C34	-8.03	105.82	118.09
29	K	102	WVN	C38-C34-C37	-8.03	109.81	122.82
35	b	314	II0	C27-C25-C29	-8.02	108.59	124.18
35	i	312	II0	C27-C25-C29	-8.02	108.61	124.18
29	s	405	WVN	C02-C11-C19	-8.02	112.11	124.58
29	A	857	WVN	C35-C32-C36	-8.01	109.83	122.82
35	a	313	II0	C33-C35-C39	-8.01	106.41	119.01
35	k	619	II0	C38-C36-C40	-8.00	109.85	122.82
35	a	313	II0	C20-C14-C10	-8.00	109.21	124.16
35	a	312	II0	C20-C14-C10	-7.99	109.22	124.16
35	d	315	II0	C38-C36-C40	-7.98	109.89	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	J	104	II0	C37-C35-C39	-7.97	109.90	122.82
35	a	312	II0	C33-C35-C39	-7.97	106.47	119.01
35	i	313	II0	C28-C26-C30	-7.97	108.70	124.18
26	c	309	CLA	CMD-C2D-C1D	7.96	138.75	124.73
29	B	846	WVN	C02-C05-C09	-7.94	111.70	121.47
35	k	616	II0	C41-C39-C35	-7.93	116.16	127.28
29	B	853	WVN	C38-C34-C37	-7.92	109.98	122.82
35	d	317	II0	C37-C35-C39	-7.92	109.98	122.82
29	A	848	WVN	C06-C13-C15	-7.92	111.81	122.64
29	A	847	WVN	C38-C34-C37	-7.92	109.99	122.82
29	B	847	WVN	C27-C25-C28	-7.92	109.99	122.82
29	h	309	WVN	C35-C32-C36	-7.92	109.99	122.82
35	b	315	II0	C32-C34-C36	7.91	148.06	126.36
35	j	615	II0	C37-C35-C39	-7.91	110.01	122.82
35	l	314	II0	C37-C35-C39	-7.90	110.02	122.82
35	c	313	II0	C19-C13-C09	-7.89	109.41	124.16
35	a	313	II0	C37-C35-C39	-7.89	110.03	122.82
29	i	315	WVN	C27-C25-C28	-7.89	110.04	122.82
35	k	615	II0	C28-C26-C30	-7.88	108.88	124.18
35	d	301	II0	C38-C36-C40	-7.87	110.06	122.82
35	k	616	II0	C33-C35-C39	-7.87	106.63	119.01
35	a	316	II0	C37-C35-C39	-7.87	110.06	122.82
35	k	620	II0	C41-C39-C35	-7.87	116.24	127.28
35	m	619	II0	C38-C36-C40	-7.86	110.07	122.82
35	l	314	II0	C19-C13-C09	-7.86	109.46	124.16
35	n	615	II0	C38-C36-C40	-7.86	110.08	122.82
29	I	101	WVN	C38-C34-C37	-7.84	110.12	122.82
29	B	847	WVN	C24-C22-C26	-7.83	110.12	122.82
29	R	200	WVN	C06-C13-C15	-7.83	111.93	122.64
29	L	205	WVN	C27-C25-C28	-7.82	110.15	122.82
35	a	316	II0	C27-C25-C29	-7.81	109.00	124.18
35	i	314	II0	C28-C26-C30	-7.81	109.01	124.18
35	k	615	II0	C19-C13-C09	-7.80	109.57	124.16
35	b	314	II0	C19-C13-C09	-7.80	109.58	124.16
35	m	616	II0	C38-C36-C40	-7.80	110.18	122.82
35	k	620	II0	C28-C26-C30	-7.78	109.07	124.18
35	h	312	II0	C37-C35-C39	-7.78	110.22	122.82
35	j	614	II0	C38-C36-C40	-7.78	110.22	122.82
35	i	313	II0	C37-C35-C39	-7.77	110.22	122.82
35	m	615	II0	C41-C39-C35	-7.77	116.38	127.28
35	j	615	II0	C19-C13-C09	-7.77	109.63	124.16
29	J	102	WVN	C38-C34-C37	-7.76	110.24	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	832	CLA	C4A-NA-C1A	7.76	110.22	106.68
26	l	313	CLA	C4A-NA-C1A	7.76	110.22	106.68
26	B	805	CLA	C4A-NA-C1A	7.76	110.22	106.68
35	d	301	II0	C41-C39-C35	-7.76	116.40	127.28
35	l	302	II0	C22-C24-C26	-7.76	149.88	176.23
29	s	407	WVN	C27-C25-C28	-7.74	110.28	122.82
35	b	314	II0	C37-C35-C39	-7.73	110.29	122.82
35	l	314	II0	C38-C36-C40	-7.73	110.29	122.82
35	d	316	II0	C38-C36-C40	-7.73	110.29	122.82
29	B	848	WVN	C35-C32-C36	-7.72	110.30	122.82
35	b	314	II0	C38-C36-C40	-7.72	110.31	122.82
35	k	615	II0	C37-C35-C39	-7.72	110.31	122.82
35	i	313	II0	C41-C39-C35	-7.71	116.46	127.28
29	l	303	WVN	C02-C11-C19	-7.71	112.58	124.58
35	k	620	II0	C38-C36-C40	-7.71	110.32	122.82
29	s	407	WVN	C38-C34-C37	-7.71	110.32	122.82
29	M	101	WVN	C24-C22-C26	-7.70	110.34	122.82
35	h	312	II0	C20-C14-C10	-7.70	109.77	124.16
29	s	407	WVN	C24-C22-C26	-7.70	110.35	122.82
35	j	615	II0	C38-C36-C40	-7.70	110.35	122.82
35	a	314	II0	C19-C13-C09	-7.68	109.80	124.16
29	J	101	WVN	C38-C34-C37	-7.68	110.38	122.82
35	i	314	II0	C37-C35-C39	-7.67	110.39	122.82
35	k	616	II0	C42-C40-C36	-7.67	116.52	127.28
29	M	101	WVN	C19-C22-C26	-7.67	106.95	119.01
35	n	615	II0	C37-C35-C39	-7.66	110.41	122.82
35	h	311	II0	C20-C14-C10	-7.65	109.85	124.16
29	B	846	WVN	C35-C32-C36	-7.65	110.42	122.82
29	J	101	WVN	C02-C11-C19	-7.64	112.69	124.58
35	c	313	II0	C37-C35-C39	-7.63	110.45	122.82
29	L	201	WVN	C24-C22-C26	-7.63	110.45	122.82
35	d	317	II0	C28-C26-C30	-7.62	109.38	124.18
29	h	309	WVN	C24-C22-C26	-7.62	110.47	122.82
35	i	316	II0	C28-C26-C30	-7.61	109.41	124.18
35	i	316	II0	C37-C35-C39	-7.60	110.50	122.82
26	k	602	CLA	C4A-NA-C1A	7.59	110.14	106.68
29	K	102	WVN	C02-C05-C09	-7.59	112.14	121.47
35	n	616	II0	C37-C35-C39	-7.57	110.55	122.82
29	l	303	WVN	C24-C22-C26	-7.57	110.55	122.82
35	h	312	II0	C38-C36-C40	-7.57	110.56	122.82
35	d	315	II0	C28-C26-C30	-7.56	109.49	124.18
29	F	203	WVN	C27-C25-C28	-7.55	110.58	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	316	II0	C28-C26-C30	-7.55	109.52	124.18
29	M	101	WVN	C38-C34-C37	-7.54	110.60	122.82
35	J	104	II0	C28-C26-C30	-7.54	109.54	124.18
29	s	405	WVN	C24-C22-C26	-7.54	110.61	122.82
29	J	102	WVN	C35-C32-C36	-7.53	110.61	122.82
26	c	309	CLA	C3D-C4D-ND	7.53	122.22	109.99
29	I	101	WVN	C23-C25-C28	-7.52	107.18	119.01
29	A	847	WVN	C02-C05-C09	-7.52	112.22	121.47
29	I	101	WVN	C19-C22-C26	-7.51	107.20	119.01
29	B	846	WVN	C27-C25-C28	-7.51	110.65	122.82
35	k	620	II0	C19-C13-C09	-7.51	110.13	124.16
35	i	312	II0	C28-C26-C30	-7.50	109.60	124.18
26	B	834	CLA	C4A-NA-C1A	7.50	110.10	106.68
26	i	305	CLA	C4A-NA-C1A	7.50	110.10	106.68
35	l	302	II0	C27-C25-C29	-7.50	109.62	124.18
26	c	304	CLA	C4A-NA-C1A	7.49	110.10	106.68
35	j	614	II0	C33-C35-C39	-7.48	107.24	119.01
29	I	101	WVN	C02-C11-C19	-7.48	112.94	124.58
35	d	301	II0	C19-C13-C09	-7.48	110.18	124.16
26	B	808	CLA	C4A-NA-C1A	7.47	110.09	106.68
29	A	847	WVN	C06-C13-C15	-7.47	112.44	122.64
29	i	315	WVN	C02-C05-C09	-7.46	112.28	121.47
29	M	101	WVN	C35-C32-C36	-7.46	110.72	122.82
35	c	316	II0	C28-C26-C30	-7.46	109.69	124.18
35	m	615	II0	C37-C35-C39	-7.45	110.75	122.82
35	m	616	II0	C37-C35-C39	-7.44	110.76	122.82
36	c	310	KC2	CMD-C2D-C1D	7.44	136.74	125.42
29	F	203	WVN	C02-C11-C19	-7.42	113.03	124.58
35	b	314	II0	C22-C24-C26	-7.41	151.06	176.23
35	m	614	II0	C27-C25-C29	-7.40	109.80	124.18
29	A	848	WVN	C31-C32-C36	-7.40	107.37	119.01
35	h	310	II0	C37-C35-C39	-7.39	110.84	122.82
29	B	848	WVN	C14-C15-C13	-7.39	112.72	122.70
35	l	314	II0	C28-C26-C30	-7.38	109.85	124.18
29	J	101	WVN	C14-C15-C13	-7.37	112.74	122.70
35	d	316	II0	C22-C24-C26	-7.37	151.19	176.23
26	j	605	CLA	C4A-NA-C1A	7.37	110.04	106.68
35	k	620	II0	C33-C35-C39	-7.36	107.44	119.01
35	b	315	II0	C19-C13-C09	-7.35	110.41	124.16
29	A	848	WVN	C38-C34-C37	-7.35	110.91	122.82
35	j	614	II0	C38-C36-C34	-7.34	106.87	118.09
29	K	102	WVN	C06-C13-C15	-7.34	112.61	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	314	II0	C33-C35-C39	-7.34	107.47	119.01
35	k	620	II0	C22-C24-C26	-7.33	151.31	176.23
26	A	852	CLA	C4A-NA-C1A	7.33	110.03	106.68
29	R	200	WVN	C02-C05-C09	-7.33	112.44	121.47
29	J	102	WVN	C27-C25-C23	-7.32	106.91	118.09
26	l	307	CLA	C4A-NA-C1A	7.31	110.01	106.68
35	h	311	II0	C19-C13-C09	-7.30	110.52	124.16
29	B	849	WVN	C24-C22-C26	-7.30	111.00	122.82
35	j	614	II0	C22-C24-C26	-7.29	151.46	176.23
26	L	203	CLA	C4A-NA-C1A	7.29	110.00	106.68
35	l	314	II0	C33-C35-C39	-7.28	107.56	119.01
35	a	312	II0	C22-C24-C26	-7.28	151.49	176.23
35	b	315	II0	C41-C39-C35	-7.28	117.07	127.28
29	A	847	WVN	C24-C22-C26	-7.27	111.03	122.82
35	a	312	II0	C28-C26-C30	-7.27	110.05	124.18
29	L	205	WVN	C02-C11-C19	-7.27	113.26	124.58
26	a	310	CLA	C4A-NA-C1A	7.27	110.00	106.68
29	J	102	WVN	C02-C11-C19	-7.24	113.31	124.58
35	a	312	II0	C38-C36-C40	-7.24	111.08	122.82
35	i	316	II0	C27-C25-C29	-7.23	110.15	124.18
35	m	619	II0	C22-C24-C26	-7.22	151.69	176.23
35	m	615	II0	C38-C36-C40	-7.22	111.12	122.82
29	B	848	WVN	C27-C25-C28	-7.22	111.12	122.82
35	c	313	II0	C38-C36-C40	-7.22	111.13	122.82
35	i	313	II0	C22-C24-C26	-7.21	151.73	176.23
26	A	835	CLA	C4A-NA-C1A	7.19	109.96	106.68
35	i	319	II0	C27-C25-C29	-7.19	110.22	124.18
35	d	301	II0	C22-C24-C26	-7.19	151.81	176.23
26	A	816	CLA	C4A-NA-C1A	7.19	109.96	106.68
35	a	316	II0	C22-C24-C26	-7.18	151.82	176.23
29	i	315	WVN	C02-C11-C19	-7.18	113.40	124.58
26	A	824	CLA	C4A-NA-C1A	7.17	109.95	106.68
35	i	313	II0	C27-C25-C29	-7.16	110.27	124.18
35	m	619	II0	C27-C25-C29	-7.16	110.28	124.18
35	d	315	II0	C27-C25-C29	-7.16	110.28	124.18
35	d	316	II0	C37-C35-C39	-7.16	111.22	122.82
35	n	615	II0	C27-C25-C29	-7.15	110.28	124.18
29	A	848	WVN	C33-C34-C37	-7.15	107.77	119.01
35	c	313	II0	C33-C35-C39	-7.15	107.77	119.01
35	i	312	II0	C38-C36-C40	-7.15	111.24	122.82
29	A	845	WVN	C24-C22-C26	-7.14	111.24	122.82
35	J	104	II0	C22-C24-C26	-7.14	151.96	176.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	311	CLA	C4A-NA-C1A	7.14	109.94	106.68
35	k	620	II0	C27-C25-C29	-7.14	110.31	124.18
35	m	616	II0	C27-C25-C29	-7.14	110.31	124.18
35	i	312	II0	C41-C39-C35	-7.14	117.27	127.28
26	A	804	CLA	C4A-NA-C1A	7.14	109.94	106.68
29	B	846	WVN	C27-C25-C23	-7.12	107.21	118.09
35	k	615	II0	C22-C24-C26	-7.12	152.05	176.23
26	A	815	CLA	C4A-NA-C1A	7.11	109.92	106.68
35	i	312	II0	C33-C35-C39	-7.11	107.82	119.01
29	K	102	WVN	C14-C15-C13	-7.11	113.10	122.70
35	k	619	II0	C41-C39-C35	-7.09	117.33	127.28
26	B	840	CLA	C4A-NA-C1A	7.09	109.91	106.68
35	n	618	II0	C28-C26-C30	-7.08	110.43	124.18
26	j	601	CLA	C4A-NA-C1A	7.07	109.91	106.68
35	c	316	II0	C27-C25-C29	-7.07	110.44	124.18
35	h	311	II0	C27-C25-C29	-7.07	110.45	124.18
35	k	619	II0	C33-C35-C39	-7.07	107.90	119.01
35	m	616	II0	C22-C24-C26	-7.06	152.22	176.23
36	s	401	KC2	C1A-C2A-C3A	-7.06	100.79	107.28
29	B	846	WVN	C19-C22-C26	-7.05	107.93	119.01
35	k	619	II0	C22-C24-C26	-7.04	152.30	176.23
26	B	807	CLA	C4A-NA-C1A	7.04	109.89	106.68
26	s	403	CLA	C4A-NA-C1A	7.03	109.89	106.68
35	m	619	II0	C33-C35-C39	-7.03	107.96	119.01
35	a	313	II0	C41-C39-C35	-7.02	117.43	127.28
29	B	846	WVN	C35-C32-C31	-7.02	107.37	118.09
26	b	303	CLA	C4A-NA-C1A	7.01	109.88	106.68
26	n	610	CLA	C4A-NA-C1A	7.01	109.88	106.68
26	b	312	CLA	C4A-NA-C1A	7.01	109.88	106.68
26	B	804	CLA	CAC-C3C-C4C	7.01	133.91	124.79
26	B	838	CLA	C4A-NA-C1A	7.00	109.87	106.68
29	B	849	WVN	C27-C25-C28	-7.00	111.48	122.82
26	a	304	CLA	C4A-NA-C1A	7.00	109.87	106.68
26	B	822	CLA	C4A-NA-C1A	6.99	109.87	106.68
26	A	836	CLA	C4A-NA-C1A	6.99	109.87	106.68
26	i	310	CLA	C4A-NA-C1A	6.99	109.87	106.68
35	l	315	II0	C33-C35-C39	-6.99	108.02	119.01
35	m	619	II0	C19-C13-C09	-6.98	111.10	124.16
29	L	201	WVN	C19-C22-C26	-6.98	108.03	119.01
35	J	104	II0	C19-C13-C09	-6.98	111.11	124.16
29	A	847	WVN	C24-C22-C19	-6.98	107.42	118.09
35	m	614	II0	C20-C14-C10	-6.98	111.11	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	856	CLA	C4A-NA-C1A	6.97	109.86	106.68
26	K	101	CLA	C4A-NA-C1A	6.96	109.86	106.68
29	s	407	WVN	C24-C22-C19	-6.96	107.45	118.09
29	J	101	WVN	C02-C05-C09	-6.96	112.90	121.47
35	a	314	II0	C22-C24-C26	-6.96	152.57	176.23
26	m	613	CLA	C4A-NA-C1A	6.96	109.85	106.68
29	I	101	WVN	C31-C32-C36	-6.96	108.07	119.01
35	a	313	II0	C22-C24-C26	-6.95	152.60	176.23
26	a	301	CLA	C4A-NA-C1A	6.95	109.85	106.68
26	Q	302	CLA	C4A-NA-C1A	6.95	109.85	106.68
26	i	301	CLA	C4A-NA-C1A	6.94	109.85	106.68
29	A	847	WVN	C35-C32-C31	-6.94	107.48	118.09
35	n	616	II0	C22-C24-C26	-6.94	152.64	176.23
26	A	837	CLA	C4A-NA-C1A	6.93	109.84	106.68
26	B	809	CLA	C4A-NA-C1A	6.93	109.84	106.68
26	k	610	CLA	C4A-NA-C1A	6.92	109.84	106.68
35	d	317	II0	C22-C24-C26	-6.92	152.71	176.23
26	A	820	CLA	C4A-NA-C1A	6.92	109.84	106.68
26	a	309	CLA	C4A-NA-C1A	6.92	109.84	106.68
26	h	303	CLA	C4A-NA-C1A	6.92	109.83	106.68
35	b	314	II0	C41-C39-C35	-6.92	117.58	127.28
26	h	308	CLA	C4A-NA-C1A	6.91	109.83	106.68
35	b	315	II0	C20-C14-C10	-6.91	111.25	124.16
35	i	316	II0	C22-C24-C26	-6.91	152.76	176.23
26	A	808	CLA	C4A-NA-C1A	6.90	109.83	106.68
26	A	822	CLA	C4A-NA-C1A	6.90	109.83	106.68
35	d	301	II0	C20-C14-C10	-6.90	111.27	124.16
35	n	616	II0	C27-C25-C29	-6.89	110.79	124.18
26	d	318	CLA	C4A-NA-C1A	6.89	109.82	106.68
29	K	102	WVN	C24-C22-C19	-6.89	107.56	118.09
29	A	846	WVN	C14-C15-C13	-6.89	113.40	122.70
29	l	316	WVN	C02-C11-C19	-6.89	113.86	124.58
26	m	604	CLA	C4A-NA-C1A	6.88	109.82	106.68
29	A	857	WVN	C02-C05-C09	-6.88	113.00	121.47
35	n	618	II0	C19-C13-C09	-6.87	111.32	124.16
26	a	308	CLA	C4A-NA-C1A	6.87	109.81	106.68
26	c	311	CLA	C4A-NA-C1A	6.87	109.81	106.68
26	h	302	CLA	C4A-NA-C1A	6.87	109.81	106.68
26	l	301	CLA	C4A-NA-C1A	6.86	109.81	106.68
29	F	203	WVN	C24-C22-C26	-6.86	111.71	122.82
35	b	315	II0	C28-C26-C30	-6.85	110.87	124.18
26	c	309	CLA	C4D-CHA-C1A	-6.85	113.07	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	835	CLA	C4A-NA-C1A	6.85	109.80	106.68
29	B	847	WVN	C02-C05-C09	-6.85	113.05	121.47
26	A	823	CLA	C4A-NA-C1A	6.84	109.80	106.68
26	j	612	CLA	C4A-NA-C1A	6.84	109.80	106.68
35	h	310	II0	C33-C35-C39	-6.84	108.25	119.01
35	d	315	II0	C37-C35-C39	-6.83	111.74	122.82
35	i	314	II0	C22-C24-C26	-6.83	153.03	176.23
26	b	313	CLA	C4A-NA-C1A	6.82	109.79	106.68
26	B	841	CLA	C4A-NA-C1A	6.82	109.79	106.68
26	b	308	CLA	C4A-NA-C1A	6.82	109.79	106.68
35	d	315	II0	C22-C24-C26	-6.82	153.06	176.23
35	h	311	II0	C22-C24-C26	-6.82	153.06	176.23
26	h	304	CLA	C4A-NA-C1A	6.81	109.79	106.68
35	d	317	II0	C19-C13-C09	-6.81	111.43	124.16
35	h	312	II0	C27-C25-C29	-6.80	110.97	124.18
35	l	314	II0	C20-C14-C10	-6.80	111.45	124.16
29	h	309	WVN	C02-C11-C19	-6.80	114.00	124.58
26	j	606	CLA	C4A-NA-C1A	6.79	109.78	106.68
26	A	806	CLA	C4A-NA-C1A	6.79	109.78	106.68
26	i	302	CLA	C4A-NA-C1A	6.79	109.78	106.68
29	F	203	WVN	C02-C05-C09	-6.79	113.12	121.47
26	A	802	CLA	C4A-NA-C1A	6.78	109.77	106.68
26	A	821	CLA	C4A-NA-C1A	6.78	109.77	106.68
35	i	316	II0	C19-C13-C09	-6.78	111.48	124.16
35	k	616	II0	C22-C24-C26	-6.78	153.19	176.23
35	c	316	II0	C22-C24-C26	-6.78	153.21	176.23
26	h	307	CLA	C4A-NA-C1A	6.77	109.77	106.68
29	J	101	WVN	C33-C34-C37	-6.77	108.37	119.01
35	n	618	II0	C27-C25-C29	-6.77	111.04	124.18
29	l	303	WVN	C20-C13-C15	-6.76	105.98	121.56
35	c	313	II0	C20-C14-C10	-6.76	111.52	124.16
35	a	314	II0	C20-C14-C10	-6.76	111.52	124.16
35	d	316	II0	C20-C14-C10	-6.75	111.53	124.16
26	i	307	CLA	C4A-NA-C1A	6.75	109.76	106.68
29	J	101	WVN	C24-C22-C26	-6.75	111.88	122.82
29	A	848	WVN	C35-C32-C36	-6.75	111.89	122.82
26	A	810	CLA	C4A-NA-C1A	6.74	109.76	106.68
35	l	315	II0	C32-C34-C36	6.74	144.86	126.36
35	d	317	II0	C27-C25-C29	-6.74	111.08	124.18
35	n	618	II0	C22-C24-C26	-6.74	153.32	176.23
35	i	314	II0	C27-C25-C29	-6.74	111.08	124.18
26	B	814	CLA	C4A-NA-C1A	6.74	109.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	405	WVN	C38-C34-C37	-6.74	111.90	122.82
26	L	202	CLA	C4A-NA-C1A	6.74	109.75	106.68
26	i	304	CLA	C4A-NA-C1A	6.74	109.75	106.68
29	R	200	WVN	C02-C11-C19	-6.73	114.11	124.58
26	d	304	CLA	C4A-NA-C1A	6.73	109.75	106.68
26	m	605	CLA	C4A-NA-C1A	6.72	109.74	106.68
26	A	812	CLA	C4A-NA-C1A	6.72	109.74	106.68
26	A	826	CLA	C4A-NA-C1A	6.72	109.74	106.68
26	c	301	CLA	C4A-NA-C1A	6.72	109.74	106.68
35	h	310	II0	C38-C36-C40	-6.71	111.95	122.82
29	B	850	WVN	C20-C13-C15	-6.70	106.12	121.56
29	s	405	WVN	C27-C25-C23	-6.70	107.85	118.09
26	l	311	CLA	C4A-NA-C1A	6.70	109.74	106.68
26	s	408	CLA	C4A-NA-C1A	6.70	109.73	106.68
29	B	850	WVN	C38-C34-C33	-6.70	107.86	118.09
26	A	829	CLA	C4A-NA-C1A	6.70	109.73	106.68
35	i	319	II0	C28-C26-C30	-6.69	111.19	124.18
35	i	312	II0	C22-C24-C26	-6.68	153.52	176.23
35	j	615	II0	C33-C35-C39	-6.68	108.50	119.01
26	k	609	CLA	C4A-NA-C1A	6.68	109.73	106.68
35	l	314	II0	C22-C24-C26	-6.68	153.53	176.23
35	d	316	II0	C19-C13-C09	-6.68	111.67	124.16
29	A	848	WVN	C35-C32-C31	-6.68	107.89	118.09
26	b	306	CLA	C4A-NA-C1A	6.68	109.72	106.68
26	d	305	CLA	C4A-NA-C1A	6.68	109.72	106.68
35	n	616	II0	C19-C13-C09	-6.68	111.68	124.16
35	n	615	II0	C22-C24-C26	-6.67	153.55	176.23
26	b	309	CLA	C4A-NA-C1A	6.67	109.72	106.68
26	A	811	CLA	C4A-NA-C1A	6.66	109.72	106.68
26	B	811	CLA	C4A-NA-C1A	6.66	109.72	106.68
26	n	605	CLA	C4A-NA-C1A	6.66	109.72	106.68
35	m	614	II0	C22-C24-C26	-6.66	153.60	176.23
26	B	820	CLA	C4A-NA-C1A	6.66	109.72	106.68
26	m	609	CLA	C4A-NA-C1A	6.66	109.72	106.68
26	k	601	CLA	C4A-NA-C1A	6.66	109.72	106.68
26	A	809	CLA	C4A-NA-C1A	6.66	109.72	106.68
35	l	315	II0	C22-C24-C26	-6.65	153.62	176.23
35	a	313	II0	C27-C25-C29	-6.65	111.26	124.18
26	j	610	CLA	C4A-NA-C1A	6.65	109.71	106.68
26	j	613	CLA	C4A-NA-C1A	6.65	109.71	106.68
26	d	306	CLA	C4A-NA-C1A	6.65	109.71	106.68
26	A	838	CLA	C4A-NA-C1A	6.65	109.71	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	304	CLA	C4A-NA-C1A	6.65	109.71	106.68
35	a	313	II0	C38-C36-C40	-6.65	112.05	122.82
26	B	801	CLA	C4A-NA-C1A	6.64	109.71	106.68
26	A	830	CLA	C4A-NA-C1A	6.64	109.71	106.68
35	h	311	II0	C33-C35-C39	-6.64	108.57	119.01
35	d	316	II0	C38-C36-C34	-6.63	107.95	118.09
35	k	619	II0	C27-C25-C29	-6.63	111.30	124.18
29	s	407	WVN	C35-C32-C31	-6.63	107.96	118.09
35	a	312	II0	C19-C13-C09	-6.63	111.76	124.16
26	n	604	CLA	C4A-NA-C1A	6.63	109.70	106.68
29	F	203	WVN	C35-C32-C31	-6.63	107.96	118.09
26	i	308	CLA	C4A-NA-C1A	6.63	109.70	106.68
35	j	615	II0	C27-C25-C29	-6.63	111.31	124.18
26	k	604	CLA	C4A-NA-C1A	6.63	109.70	106.68
26	n	602	CLA	C4A-NA-C1A	6.63	109.70	106.68
35	i	319	II0	C20-C14-C10	-6.63	111.77	124.16
26	l	308	CLA	C4A-NA-C1A	6.62	109.70	106.68
35	l	315	II0	C19-C13-C09	-6.62	111.79	124.16
26	A	833	CLA	C4A-NA-C1A	6.62	109.70	106.68
26	j	604	CLA	C4A-NA-C1A	6.62	109.70	106.68
35	n	615	II0	C19-C13-C09	-6.61	111.80	124.16
29	K	102	WVN	C02-C11-C19	-6.61	114.29	124.58
35	j	615	II0	C22-C24-C26	-6.61	153.76	176.23
26	B	813	CLA	C4A-NA-C1A	6.61	109.69	106.68
29	A	846	WVN	C06-C13-C15	-6.61	113.61	122.64
26	h	301	CLA	C4A-NA-C1A	6.61	109.69	106.68
26	m	601	CLA	C4A-NA-C1A	6.61	109.69	106.68
29	A	845	WVN	C27-C25-C28	-6.60	112.12	122.82
26	A	818	CLA	C4A-NA-C1A	6.60	109.69	106.68
26	m	602	CLA	C4A-NA-C1A	6.60	109.69	106.68
26	B	812	CLA	C4A-NA-C1A	6.60	109.69	106.68
26	m	610	CLA	C4A-NA-C1A	6.60	109.69	106.68
26	L	204	CLA	C4A-NA-C1A	6.60	109.69	106.68
35	m	614	II0	C19-C13-C09	-6.59	111.83	124.16
29	A	857	WVN	C27-C25-C28	-6.59	112.14	122.82
35	i	312	II0	C37-C35-C39	-6.59	112.14	122.82
35	l	302	II0	C38-C36-C34	-6.59	108.03	118.09
35	j	614	II0	C19-C13-C09	-6.58	111.85	124.16
35	l	315	II0	C28-C26-C30	-6.58	111.39	124.18
29	L	201	WVN	C31-C32-C36	-6.58	108.66	119.01
29	B	846	WVN	C24-C22-C26	-6.58	112.15	122.82
36	s	401	KC2	CMD-C2D-C1D	6.58	135.44	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	847	WVN	C02-C11-C19	-6.58	114.34	124.58
35	i	313	II0	C38-C36-C40	-6.58	112.16	122.82
29	L	201	WVN	C23-C25-C28	-6.57	108.67	119.01
35	c	313	II0	C27-C25-C29	-6.57	111.42	124.18
26	J	103	CLA	C4A-NA-C1A	6.57	109.68	106.68
26	c	308	CLA	C4A-NA-C1A	6.57	109.67	106.68
29	L	205	WVN	C24-C22-C26	-6.57	112.18	122.82
35	a	313	II0	C19-C13-C09	-6.56	111.89	124.16
29	B	850	WVN	C27-C25-C23	-6.56	108.06	118.09
29	M	101	WVN	C24-C22-C19	-6.56	108.07	118.09
29	L	205	WVN	C20-C13-C15	-6.56	106.45	121.56
29	F	203	WVN	C35-C32-C36	-6.55	112.20	122.82
26	a	305	CLA	C4A-NA-C1A	6.55	109.67	106.68
26	B	831	CLA	C4A-NA-C1A	6.55	109.67	106.68
26	n	601	CLA	C4A-NA-C1A	6.54	109.66	106.68
35	k	616	II0	C38-C36-C40	-6.54	112.22	122.82
26	k	605	CLA	C4A-NA-C1A	6.53	109.66	106.68
35	k	619	II0	C38-C36-C34	-6.53	108.11	118.09
26	A	819	CLA	C4A-NA-C1A	6.53	109.66	106.68
26	j	609	CLA	C4A-NA-C1A	6.53	109.66	106.68
26	b	310	CLA	C4A-NA-C1A	6.53	109.66	106.68
26	c	309	CLA	C3C-C4C-NC	6.53	118.79	110.43
26	h	306	CLA	C4A-NA-C1A	6.52	109.66	106.68
26	L	206	CLA	C4A-NA-C1A	6.52	109.65	106.68
26	c	309	CLA	C3B-C2B-C1B	-6.52	99.48	107.17
29	A	857	WVN	C23-C25-C28	-6.52	108.76	119.01
29	l	303	WVN	C02-C05-C09	-6.51	113.46	121.47
26	d	313	CLA	C4A-NA-C1A	6.51	109.65	106.68
29	K	102	WVN	C31-C32-C36	-6.51	108.77	119.01
35	m	615	II0	C19-C13-C09	-6.51	111.99	124.16
29	l	316	WVN	C27-C25-C23	-6.50	108.15	118.09
26	B	839	CLA	C4A-NA-C1A	6.50	109.64	106.68
26	c	309	CLA	C2D-C1D-ND	6.49	116.55	110.13
36	c	310	KC2	C1A-C2A-C3A	-6.49	101.31	107.28
26	A	827	CLA	C4A-NA-C1A	6.49	109.64	106.68
35	k	615	II0	C38-C36-C34	-6.49	108.17	118.09
35	l	314	II0	C27-C25-C29	-6.49	111.58	124.18
26	A	831	CLA	C4A-NA-C1A	6.49	109.64	106.68
35	m	615	II0	C22-C24-C26	-6.48	154.21	176.23
29	M	101	WVN	C33-C34-C37	-6.48	108.82	119.01
35	c	313	II0	C22-C24-C26	-6.47	154.23	176.23
26	A	841	CLA	C4A-NA-C1A	6.46	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	316	WVN	C20-C13-C15	-6.46	106.67	121.56
35	n	618	II0	C33-C35-C39	-6.46	108.85	119.01
29	i	315	WVN	C38-C34-C33	-6.46	108.22	118.09
26	l	310	CLA	C4A-NA-C1A	6.46	109.63	106.68
26	F	202	CLA	C4A-NA-C1A	6.45	109.62	106.68
35	a	312	II0	C27-C25-C29	-6.45	111.65	124.18
26	j	603	CLA	C4A-NA-C1A	6.45	109.62	106.68
26	A	828	CLA	C4A-NA-C1A	6.44	109.62	106.68
29	B	846	WVN	C38-C34-C33	-6.44	108.24	118.09
29	s	407	WVN	C33-C34-C37	-6.44	108.87	119.01
35	c	316	II0	C33-C35-C39	-6.44	108.88	119.01
35	h	312	II0	C33-C35-C39	-6.44	108.88	119.01
26	A	807	CLA	C4A-NA-C1A	6.44	109.62	106.68
26	a	303	CLA	C4A-NA-C1A	6.43	109.61	106.68
29	A	848	WVN	C19-C22-C26	-6.43	108.89	119.01
26	b	304	CLA	C4A-NA-C1A	6.43	109.61	106.68
29	A	846	WVN	C02-C11-C19	-6.43	114.58	124.58
29	B	849	WVN	C35-C32-C31	-6.42	108.28	118.09
35	h	310	II0	C30-C32-C34	-6.42	112.37	125.28
26	b	307	CLA	C4A-NA-C1A	6.42	109.61	106.68
29	l	303	WVN	C27-C25-C23	-6.42	108.28	118.09
26	B	836	CLA	C4A-NA-C1A	6.41	109.60	106.68
29	A	845	WVN	C27-C25-C23	-6.41	108.30	118.09
29	F	203	WVN	C24-C22-C19	-6.40	108.30	118.09
35	h	310	II0	C27-C25-C29	-6.40	111.75	124.18
35	k	616	II0	C37-C35-C39	-6.40	112.45	122.82
35	d	315	II0	C20-C14-C10	-6.40	112.20	124.16
35	i	319	II0	C33-C35-C39	-6.39	108.96	119.01
29	R	200	WVN	C27-C25-C23	-6.39	108.33	118.09
35	l	315	II0	C27-C25-C29	-6.39	111.78	124.18
35	i	314	II0	C33-C35-C39	-6.39	108.97	119.01
29	h	309	WVN	C23-C25-C28	-6.38	108.97	119.01
35	d	316	II0	C37-C35-C33	-6.38	108.33	118.09
26	i	311	CLA	C4A-NA-C1A	6.38	109.59	106.68
26	d	302	CLA	C4A-NA-C1A	6.38	109.59	106.68
29	s	407	WVN	C23-C25-C28	-6.38	108.98	119.01
35	k	615	II0	C37-C35-C33	-6.38	108.35	118.09
29	I	101	WVN	C33-C34-C37	-6.37	108.98	119.01
26	k	606	CLA	C4A-NA-C1A	6.37	109.59	106.68
35	c	316	II0	C19-C13-C09	-6.37	112.25	124.16
35	k	615	II0	C33-C35-C39	-6.37	108.99	119.01
35	m	615	II0	C27-C25-C29	-6.37	111.81	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	319	II0	C38-C36-C34	-6.37	108.36	118.09
35	n	616	II0	C28-C26-C30	-6.37	111.82	124.18
35	a	313	II0	C28-C26-C30	-6.36	111.82	124.18
35	k	616	II0	C28-C26-C30	-6.36	111.82	124.18
29	l	316	WVN	C14-C15-C13	-6.36	114.11	122.70
29	s	407	WVN	C27-C25-C23	-6.35	108.38	118.09
26	A	839	CLA	C4A-NA-C1A	6.35	109.58	106.68
26	F	201	CLA	C4A-NA-C1A	6.35	109.58	106.68
35	i	314	II0	C20-C14-C10	-6.35	112.29	124.16
35	J	104	II0	C33-C35-C39	-6.34	109.03	119.01
29	B	850	WVN	C31-C32-C36	-6.34	109.03	119.01
29	B	849	WVN	C02-C05-C09	-6.34	113.67	121.47
35	b	314	II0	C33-C35-C39	-6.34	109.04	119.01
35	i	313	II0	C20-C14-C10	-6.34	112.31	124.16
29	B	853	WVN	C02-C11-C19	-6.34	114.72	124.58
26	B	827	CLA	C4A-NA-C1A	6.33	109.57	106.68
26	k	608	CLA	C4A-NA-C1A	6.33	109.57	106.68
36	s	401	KC2	C3B-C2B-C1B	-6.33	101.05	107.05
29	A	857	WVN	C24-C22-C19	-6.33	108.41	118.09
29	B	848	WVN	C27-C25-C23	-6.33	108.42	118.09
26	A	805	CLA	C4A-NA-C1A	6.33	109.57	106.68
29	J	101	WVN	C19-C22-C26	-6.33	109.05	119.01
26	B	815	CLA	C4A-NA-C1A	6.33	109.57	106.68
29	l	316	WVN	C35-C32-C31	-6.33	108.42	118.09
29	L	205	WVN	C02-C05-C09	-6.32	113.69	121.47
26	c	312	CLA	C4A-NA-C1A	6.32	109.56	106.68
35	i	316	II0	C33-C35-C39	-6.32	109.06	119.01
26	B	825	CLA	C4A-NA-C1A	6.32	109.56	106.68
35	c	313	II0	C28-C26-C30	-6.32	111.91	124.18
35	k	619	II0	C28-C26-C30	-6.32	111.91	124.18
35	j	614	II0	C27-C25-C29	-6.32	111.91	124.18
35	l	315	II0	C42-C40-C36	-6.31	118.42	127.28
26	B	824	CLA	C4A-NA-C1A	6.31	109.56	106.68
29	A	847	WVN	C14-C15-C13	-6.31	114.17	122.70
35	a	314	II0	C28-C26-C30	-6.31	111.92	124.18
26	a	311	CLA	C4A-NA-C1A	6.31	109.56	106.68
35	d	317	II0	C33-C35-C39	-6.30	109.09	119.01
26	B	816	CLA	C4A-NA-C1A	6.30	109.56	106.68
35	m	614	II0	C28-C26-C30	-6.30	111.94	124.18
26	c	305	CLA	C4A-NA-C1A	6.30	109.55	106.68
29	s	405	WVN	C33-C34-C37	-6.30	109.10	119.01
35	l	314	II0	C38-C36-C34	-6.29	108.48	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	405	WVN	C19-C22-C26	-6.29	109.11	119.01
35	j	615	II0	C28-C26-C30	-6.29	111.96	124.18
35	h	312	II0	C22-C24-C26	-6.28	154.89	176.23
29	L	201	WVN	C33-C34-C37	-6.28	109.14	119.01
29	B	850	WVN	C24-C22-C19	-6.28	108.50	118.09
26	a	302	CLA	C4A-NA-C1A	6.27	109.54	106.68
26	B	842	CLA	C4A-NA-C1A	6.27	109.54	106.68
35	h	312	II0	C19-C13-C09	-6.27	112.44	124.16
29	A	845	WVN	C24-C22-C19	-6.26	108.52	118.09
35	m	615	II0	C34-C36-C40	-6.26	109.16	119.01
35	i	316	II0	C20-C14-C10	-6.26	112.46	124.16
35	a	316	II0	C28-C26-C30	-6.26	112.02	124.18
35	i	312	II0	C38-C36-C34	-6.26	108.53	118.09
26	h	313	CLA	C4A-NA-C1A	6.26	109.53	106.68
35	n	616	II0	C37-C35-C33	-6.25	108.53	118.09
26	c	302	CLA	C4A-NA-C1A	6.25	109.53	106.68
35	c	313	II0	C38-C36-C34	-6.24	108.56	118.09
35	l	315	II0	C20-C14-C10	-6.24	112.50	124.16
29	h	309	WVN	C20-C13-C15	-6.23	107.20	121.56
35	b	315	II0	C33-C35-C39	-6.23	109.21	119.01
29	A	848	WVN	C23-C25-C28	-6.23	109.22	119.01
29	l	303	WVN	C19-C22-C26	-6.22	109.23	119.01
29	B	849	WVN	C02-C11-C19	-6.22	114.91	124.58
29	s	407	WVN	C23-C20-C13	-6.22	110.39	127.00
26	R	201	CLA	C4A-NA-C1A	6.21	109.51	106.68
29	A	845	WVN	C35-C32-C31	-6.21	108.60	118.09
35	h	310	II0	C19-C13-C09	-6.21	112.55	124.16
35	n	615	II0	C28-C26-C30	-6.21	112.12	124.18
35	h	311	II0	C28-C26-C30	-6.20	112.13	124.18
29	B	853	WVN	C14-C15-C13	-6.20	114.32	122.70
29	s	407	WVN	C20-C13-C15	-6.20	107.27	121.56
26	B	803	CLA	C4A-NA-C1A	6.19	109.50	106.68
36	s	401	KC2	O2D-CGD-CBD	6.19	122.05	111.23
35	n	616	II0	C20-C14-C10	-6.19	112.59	124.16
29	L	205	WVN	C19-C22-C26	-6.19	109.28	119.01
29	J	102	WVN	C38-C34-C33	-6.18	108.64	118.09
35	J	104	II0	C38-C36-C34	-6.18	108.65	118.09
35	m	614	II0	C33-C35-C39	-6.18	109.29	119.01
29	B	848	WVN	C02-C05-C09	-6.17	113.87	121.47
35	m	615	II0	C28-C26-C30	-6.17	112.19	124.18
26	A	834	CLA	C4A-NA-C1A	6.17	109.50	106.68
26	d	309	CLA	C4A-NA-C1A	6.17	109.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	313	II0	C33-C35-C39	-6.17	109.31	119.01
35	i	312	II0	C19-C13-C09	-6.16	112.64	124.16
35	a	316	II0	C19-C13-C09	-6.16	112.64	124.16
29	B	847	WVN	C24-C22-C19	-6.16	108.68	118.09
35	m	616	II0	C20-C14-C10	-6.16	112.65	124.16
35	d	301	II0	C28-C26-C30	-6.16	112.22	124.18
26	n	603	CLA	C4A-NA-C1A	6.15	109.49	106.68
29	B	848	WVN	C02-C11-C19	-6.15	115.00	124.58
26	B	828	CLA	C4A-NA-C1A	6.15	109.48	106.68
36	s	401	KC2	CHB-C4A-C3A	-6.15	115.32	125.03
26	A	840	CLA	C4A-NA-C1A	6.15	109.48	106.68
29	A	857	WVN	C35-C32-C31	-6.15	108.70	118.09
26	B	826	CLA	C4A-NA-C1A	6.14	109.48	106.68
29	J	101	WVN	C24-C22-C19	-6.14	108.71	118.09
29	i	315	WVN	C35-C32-C31	-6.14	108.71	118.09
35	n	618	II0	C20-C14-C10	-6.14	112.68	124.16
26	A	814	CLA	C4A-NA-C1A	6.14	109.48	106.68
29	R	200	WVN	C14-C15-C13	-6.14	114.41	122.70
26	B	806	CLA	C4A-NA-C1A	6.14	109.48	106.68
35	n	615	II0	C38-C36-C34	-6.13	108.72	118.09
29	l	316	WVN	C23-C20-C13	-6.13	110.62	127.00
26	i	306	CLA	C4A-NA-C1A	6.13	109.47	106.68
29	l	303	WVN	C33-C34-C37	-6.12	109.38	119.01
35	m	619	II0	C28-C26-C30	-6.12	112.29	124.18
29	L	205	WVN	C24-C22-C19	-6.12	108.74	118.09
29	B	846	WVN	C31-C32-C36	-6.12	109.39	119.01
29	L	201	WVN	C35-C32-C31	-6.11	108.75	118.09
26	c	303	CLA	C4A-NA-C1A	6.11	109.47	106.68
26	B	804	CLA	C4A-NA-C1A	6.11	109.47	106.68
26	m	608	CLA	C4A-NA-C1A	6.11	109.47	106.68
35	m	616	II0	C28-C26-C30	-6.10	112.33	124.18
29	B	847	WVN	C27-C25-C23	-6.10	108.77	118.09
35	h	312	II0	C28-C26-C30	-6.09	112.34	124.18
26	B	817	CLA	C4A-NA-C1A	6.09	109.46	106.68
35	i	319	II0	C19-C13-C09	-6.09	112.77	124.16
35	i	316	II0	C38-C36-C34	-6.09	108.78	118.09
29	h	309	WVN	C31-C32-C36	-6.09	109.44	119.01
35	n	616	II0	C33-C35-C39	-6.08	109.44	119.01
26	k	614	CLA	C4A-NA-C1A	6.08	109.45	106.68
35	j	614	II0	C28-C26-C30	-6.08	112.37	124.18
35	l	302	II0	C28-C26-C30	-6.07	112.38	124.18
26	l	306	CLA	C4A-NA-C1A	6.07	109.45	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	316	II0	C33-C35-C39	-6.07	109.46	119.01
29	J	101	WVN	C35-C32-C31	-6.07	108.81	118.09
26	d	303	CLA	C4A-NA-C1A	6.07	109.45	106.68
35	d	315	II0	C38-C36-C34	-6.07	108.82	118.09
26	a	307	CLA	C4A-NA-C1A	6.07	109.45	106.68
35	d	315	II0	C19-C13-C09	-6.07	112.82	124.16
29	l	316	WVN	C24-C22-C19	-6.06	108.83	118.09
26	a	306	CLA	C4A-NA-C1A	6.06	109.44	106.68
35	c	316	II0	C34-C36-C40	-6.06	109.48	119.01
26	j	608	CLA	C4A-NA-C1A	6.05	109.44	106.68
26	d	310	CLA	C4A-NA-C1A	6.05	109.44	106.68
35	k	616	II0	C34-C36-C40	-6.05	109.50	119.01
26	l	309	CLA	C4A-NA-C1A	6.04	109.44	106.68
35	m	619	II0	C20-C14-C10	-6.04	112.86	124.16
29	A	857	WVN	C27-C25-C23	-6.04	108.86	118.09
29	B	850	WVN	C02-C11-C19	-6.04	115.19	124.58
29	i	315	WVN	C23-C25-C28	-6.03	109.52	119.01
35	i	314	II0	C37-C35-C33	-6.03	108.88	118.09
26	j	602	CLA	C4A-NA-C1A	6.03	109.43	106.68
26	B	837	CLA	C4A-NA-C1A	6.02	109.43	106.68
29	s	405	WVN	C24-C22-C19	-6.02	108.89	118.09
29	J	102	WVN	C02-C05-C09	-6.02	114.07	121.47
36	c	310	KC2	CHB-C4A-C3A	-6.02	115.53	125.03
29	L	205	WVN	C23-C25-C28	-6.01	109.55	119.01
29	B	848	WVN	C35-C32-C31	-6.01	108.91	118.09
35	i	314	II0	C19-C13-C09	-6.01	112.93	124.16
35	d	315	II0	C33-C35-C39	-6.00	109.56	119.01
29	A	857	WVN	C38-C34-C33	-6.00	108.92	118.09
26	c	309	CLA	C3B-C4B-NB	6.00	115.89	110.53
35	j	615	II0	C20-C14-C10	-6.00	112.95	124.16
29	s	405	WVN	C14-C15-C13	-5.98	114.62	122.70
35	d	301	II0	C27-C25-C29	-5.98	112.56	124.18
29	l	316	WVN	C23-C25-C28	-5.98	109.60	119.01
26	m	612	CLA	C4A-NA-C1A	5.98	109.41	106.68
26	A	803	CLA	C4A-NA-C1A	5.98	109.41	106.68
35	d	317	II0	C38-C36-C34	-5.97	108.96	118.09
35	c	316	II0	C20-C14-C10	-5.97	113.00	124.16
26	d	307	CLA	C4A-NA-C1A	5.97	109.40	106.68
29	B	849	WVN	C38-C34-C33	-5.96	108.98	118.09
29	J	102	WVN	C19-C22-C26	-5.96	109.63	119.01
29	K	102	WVN	C38-C34-C33	-5.95	108.99	118.09
29	F	203	WVN	C27-C25-C23	-5.95	109.00	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	317	II0	C20-C14-C10	-5.95	113.04	124.16
35	l	302	II0	C19-C13-C09	-5.95	113.04	124.16
26	m	606	CLA	C4A-NA-C1A	5.95	109.39	106.68
26	n	609	CLA	C4A-NA-C1A	5.95	109.39	106.68
29	F	203	WVN	C38-C34-C33	-5.94	109.01	118.09
29	s	407	WVN	C38-C34-C33	-5.94	109.01	118.09
35	m	614	II0	C38-C36-C34	-5.94	109.02	118.09
26	A	832	CLA	C4A-NA-C1A	5.94	109.39	106.68
29	B	847	WVN	C35-C32-C31	-5.94	109.02	118.09
29	B	849	WVN	C27-C25-C23	-5.93	109.02	118.09
26	A	817	CLA	C4A-NA-C1A	5.93	109.39	106.68
26	m	607	CLA	C4A-NA-C1A	5.93	109.39	106.68
29	I	101	WVN	C38-C34-C33	-5.93	109.03	118.09
35	b	314	II0	C28-C26-C30	-5.93	112.66	124.18
26	d	308	CLA	C4A-NA-C1A	5.93	109.38	106.68
29	L	201	WVN	C27-C25-C23	-5.93	109.03	118.09
29	B	853	WVN	C20-C13-C15	-5.93	107.91	121.56
29	K	102	WVN	C23-C25-C28	-5.92	109.69	119.01
29	B	848	WVN	C06-C13-C15	-5.92	114.55	122.64
29	M	101	WVN	C14-C15-C13	-5.91	114.72	122.70
29	A	847	WVN	C38-C34-C33	-5.91	109.06	118.09
35	m	616	II0	C19-C13-C09	-5.90	113.13	124.16
29	J	101	WVN	C38-C34-C33	-5.90	109.07	118.09
26	n	606	CLA	C4A-NA-C1A	5.90	109.37	106.68
35	h	310	II0	C34-C36-C40	-5.90	109.73	119.01
29	A	848	WVN	C14-C15-C13	-5.90	114.73	122.70
35	j	615	II0	C37-C35-C33	-5.89	109.09	118.09
29	B	853	WVN	C19-C22-C26	-5.89	109.74	119.01
29	B	853	WVN	C06-C13-C15	-5.89	114.59	122.64
35	a	316	II0	C38-C36-C34	-5.88	109.10	118.09
35	d	317	II0	C37-C35-C33	-5.88	109.10	118.09
35	a	316	II0	C20-C14-C10	-5.87	113.18	124.16
35	h	311	II0	C38-C36-C34	-5.86	109.13	118.09
29	A	847	WVN	C33-C34-C37	-5.85	109.80	119.01
29	B	849	WVN	C24-C22-C19	-5.84	109.16	118.09
29	h	309	WVN	C35-C32-C31	-5.84	109.17	118.09
26	B	833	CLA	C4A-NA-C1A	5.84	109.34	106.68
26	s	406	CLA	C4A-NA-C1A	5.84	109.34	106.68
35	m	616	II0	C38-C36-C34	-5.83	109.19	118.09
26	B	810	CLA	C4A-NA-C1A	5.82	109.34	106.68
29	s	405	WVN	C38-C34-C33	-5.82	109.20	118.09
29	h	309	WVN	C27-C25-C23	-5.82	109.20	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	303	WVN	C24-C22-C19	-5.81	109.21	118.09
29	F	203	WVN	C33-C34-C37	-5.81	109.86	119.01
29	A	848	WVN	C27-C25-C23	-5.81	109.21	118.09
35	h	310	II0	C38-C36-C34	-5.81	109.22	118.09
29	L	205	WVN	C27-C25-C23	-5.81	109.22	118.09
35	m	616	II0	C31-C29-C25	-5.80	110.37	126.61
35	k	616	II0	C20-C14-C10	-5.80	113.31	124.16
29	B	846	WVN	C23-C25-C28	-5.80	109.88	119.01
29	A	848	WVN	C38-C34-C33	-5.80	109.22	118.09
35	l	302	II0	C20-C14-C10	-5.80	113.31	124.16
29	s	405	WVN	C35-C32-C31	-5.80	109.23	118.09
35	a	316	II0	C37-C35-C33	-5.80	109.23	118.09
35	m	615	II0	C20-C14-C10	-5.80	113.33	124.16
29	B	853	WVN	C35-C32-C31	-5.79	109.24	118.09
26	m	603	CLA	C4A-NA-C1A	5.79	109.32	106.68
29	A	845	WVN	C02-C11-C19	-5.79	115.57	124.58
29	h	309	WVN	C19-C22-C26	-5.77	109.93	119.01
26	B	802	CLA	C4A-NA-C1A	5.76	109.31	106.68
29	B	853	WVN	C31-C32-C36	-5.76	109.95	119.01
29	A	847	WVN	C27-C25-C23	-5.76	109.29	118.09
29	J	102	WVN	C23-C20-C13	-5.76	111.62	127.00
35	i	312	II0	C20-C14-C10	-5.76	113.40	124.16
29	M	101	WVN	C23-C25-C28	-5.76	109.96	119.01
35	a	314	II0	C27-C25-C29	-5.75	113.01	124.18
29	A	857	WVN	C06-C13-C15	-5.75	114.78	122.64
35	n	616	II0	C38-C36-C34	-5.75	109.31	118.09
29	i	315	WVN	C27-C25-C23	-5.74	109.31	118.09
29	A	846	WVN	C35-C32-C31	-5.74	109.31	118.09
35	a	314	II0	C38-C36-C34	-5.74	109.32	118.09
29	M	101	WVN	C35-C32-C31	-5.74	109.32	118.09
35	c	316	II0	C38-C36-C34	-5.74	109.32	118.09
29	A	846	WVN	C31-C32-C36	-5.74	109.99	119.01
29	B	849	WVN	C23-C25-C28	-5.73	109.99	119.01
35	i	316	II0	C37-C35-C33	-5.73	109.34	118.09
29	h	309	WVN	C33-C34-C37	-5.73	110.00	119.01
35	d	315	II0	C37-C35-C33	-5.72	109.34	118.09
35	a	313	II0	C38-C36-C34	-5.72	109.35	118.09
29	i	315	WVN	C24-C22-C19	-5.72	109.35	118.09
35	b	315	II0	C37-C35-C33	-5.72	109.35	118.09
29	J	102	WVN	C06-C13-C15	-5.72	114.82	122.64
29	A	857	WVN	C14-C15-C13	-5.72	114.98	122.70
35	i	313	II0	C38-C36-C34	-5.72	109.36	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	830	CLA	C4A-NA-C1A	5.71	109.29	106.68
35	i	312	II0	C37-C35-C33	-5.71	109.36	118.09
29	R	200	WVN	C24-C22-C19	-5.71	109.37	118.09
29	K	102	WVN	C27-C25-C23	-5.71	109.37	118.09
35	J	104	II0	C37-C35-C33	-5.71	109.37	118.09
29	l	303	WVN	C23-C25-C28	-5.70	110.04	119.01
29	B	847	WVN	C33-C34-C37	-5.70	110.05	119.01
26	i	303	CLA	C4A-NA-C1A	5.70	109.28	106.68
29	A	847	WVN	C23-C25-C28	-5.70	110.05	119.01
26	s	402	CLA	C4A-NA-C1A	5.69	109.28	106.68
29	B	848	WVN	C23-C20-C13	-5.69	111.81	127.00
26	n	613	CLA	C4A-NA-C1A	5.68	109.27	106.68
29	B	848	WVN	C31-C32-C36	-5.68	110.07	119.01
35	c	316	II0	C31-C29-C25	-5.68	110.71	126.61
29	M	101	WVN	C38-C34-C33	-5.68	109.41	118.09
28	s	409	LHG	O4-P-O5	5.68	132.96	110.83
29	A	857	WVN	C31-C32-C36	-5.67	110.09	119.01
29	B	850	WVN	C35-C32-C31	-5.66	109.44	118.09
29	B	853	WVN	C33-C34-C37	-5.66	110.11	119.01
26	c	309	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
29	L	201	WVN	C24-C22-C19	-5.65	109.46	118.09
29	B	848	WVN	C24-C22-C19	-5.65	109.46	118.09
29	A	845	WVN	C38-C34-C33	-5.65	109.46	118.09
36	c	310	KC2	C3B-C2B-C1B	-5.65	101.70	107.05
29	L	205	WVN	C33-C34-C37	-5.64	110.14	119.01
35	d	316	II0	C33-C35-C39	-5.64	110.14	119.01
29	B	849	WVN	C06-C13-C15	-5.64	114.93	122.64
29	B	848	WVN	C23-C25-C28	-5.64	110.14	119.01
35	d	301	II0	C38-C36-C34	-5.63	109.48	118.09
29	A	847	WVN	C20-C13-C15	-5.63	108.60	121.56
29	h	309	WVN	C38-C34-C33	-5.61	109.51	118.09
29	J	101	WVN	C31-C32-C36	-5.61	110.18	119.01
29	A	846	WVN	C24-C22-C19	-5.61	109.52	118.09
29	A	846	WVN	C33-C34-C37	-5.61	110.18	119.01
35	h	312	II0	C38-C36-C34	-5.61	109.52	118.09
29	h	309	WVN	C24-C22-C19	-5.61	109.52	118.09
29	A	846	WVN	C38-C34-C33	-5.61	109.52	118.09
35	i	314	II0	C38-C36-C34	-5.60	109.53	118.09
26	l	305	CLA	C4A-NA-C1A	5.60	109.23	106.68
29	J	101	WVN	C23-C25-C28	-5.60	110.20	119.01
29	R	200	WVN	C19-C22-C26	-5.60	110.20	119.01
29	M	101	WVN	C27-C25-C23	-5.60	109.54	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	303	WVN	C31-C32-C36	-5.60	110.21	119.01
35	n	618	II0	C38-C36-C34	-5.59	109.54	118.09
29	I	101	WVN	C35-C32-C31	-5.59	109.55	118.09
29	l	303	WVN	C35-C32-C31	-5.59	109.55	118.09
35	c	313	II0	C37-C35-C33	-5.58	109.56	118.09
26	c	307	CLA	C4A-NA-C1A	5.58	109.22	106.68
29	R	200	WVN	C35-C32-C31	-5.57	109.58	118.09
29	A	845	WVN	C19-C22-C26	-5.57	110.25	119.01
29	B	847	WVN	C38-C34-C33	-5.56	109.59	118.09
26	B	823	CLA	C4A-NA-C1A	5.56	109.22	106.68
29	s	405	WVN	C31-C32-C36	-5.55	110.28	119.01
29	B	848	WVN	C38-C34-C33	-5.55	109.61	118.09
35	i	319	II0	C37-C35-C33	-5.54	109.62	118.09
29	F	203	WVN	C31-C32-C36	-5.53	110.31	119.01
29	A	846	WVN	C19-C22-C26	-5.53	110.31	119.01
29	R	200	WVN	C38-C34-C33	-5.51	109.67	118.09
29	B	853	WVN	C24-C22-C19	-5.50	109.69	118.09
29	L	205	WVN	C35-C32-C31	-5.50	109.69	118.09
35	n	615	II0	C33-C35-C39	-5.50	110.36	119.01
35	n	618	II0	C37-C35-C33	-5.49	109.70	118.09
29	J	102	WVN	C24-C22-C19	-5.49	109.70	118.09
35	J	104	II0	C31-C29-C25	-5.48	111.27	126.61
29	K	102	WVN	C20-C13-C15	-5.48	108.94	121.56
26	A	825	CLA	C4A-NA-C1A	5.48	109.18	106.68
29	i	315	WVN	C19-C22-C26	-5.48	110.40	119.01
29	A	846	WVN	C23-C25-C28	-5.46	110.42	119.01
35	n	616	II0	C34-C36-C40	-5.46	110.43	119.01
29	L	205	WVN	C38-C34-C33	-5.45	109.75	118.09
26	c	306	CLA	C4A-NA-C1A	5.45	109.17	106.68
35	c	313	II0	C34-C36-C40	-5.45	110.44	119.01
35	a	313	II0	C37-C35-C33	-5.45	109.77	118.09
29	A	845	WVN	C33-C34-C37	-5.44	110.46	119.01
29	B	847	WVN	C02-C11-C19	-5.44	116.12	124.58
35	i	314	II0	C34-C36-C40	-5.43	110.47	119.01
29	R	200	WVN	C31-C32-C36	-5.43	110.47	119.01
29	B	853	WVN	C27-C25-C23	-5.43	109.80	118.09
26	A	813	CLA	C4A-NA-C1A	5.42	109.15	106.68
29	L	201	WVN	C23-C20-C13	-5.41	112.53	127.00
26	B	818	CLA	C4A-NA-C1A	5.41	109.15	106.68
35	b	315	II0	C32-C30-C26	-5.41	111.47	126.61
29	L	205	WVN	C23-C20-C13	-5.40	112.57	127.00
27	B	843	PQN	C15-C13-C12	-5.39	109.06	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	302	II0	C33-C35-C39	-5.39	110.53	119.01
29	J	101	WVN	C27-C25-C23	-5.39	109.86	118.09
29	B	849	WVN	C19-C22-C26	-5.38	110.54	119.01
29	B	847	WVN	C20-C13-C15	-5.38	109.17	121.56
36	s	401	KC2	C3A-C4A-NA	5.38	117.11	110.45
26	B	819	CLA	C4A-NA-C1A	5.37	109.13	106.68
35	k	620	II0	C38-C36-C34	-5.37	109.89	118.09
35	j	615	II0	C38-C36-C34	-5.37	109.89	118.09
26	b	305	CLA	C4A-NA-C1A	5.37	109.13	106.68
29	s	405	WVN	C23-C25-C28	-5.36	110.58	119.01
35	n	618	II0	C34-C36-C40	-5.36	110.58	119.01
29	B	853	WVN	C38-C34-C33	-5.35	109.91	118.09
29	R	200	WVN	C23-C25-C28	-5.35	110.59	119.01
29	A	845	WVN	C23-C25-C28	-5.35	110.59	119.01
29	B	853	WVN	C23-C25-C28	-5.35	110.59	119.01
29	s	407	WVN	C02-C11-C19	-5.34	116.26	124.58
29	F	203	WVN	C19-C22-C26	-5.34	110.60	119.01
36	s	401	KC2	C1A-NA-C4A	-5.34	104.24	106.68
29	J	102	WVN	C14-C15-C13	-5.34	115.49	122.70
29	A	845	WVN	C23-C20-C13	-5.34	112.73	127.00
35	m	619	II0	C38-C36-C34	-5.33	109.94	118.09
35	d	315	II0	C34-C36-C40	-5.33	110.62	119.01
29	I	101	WVN	C24-C22-C19	-5.33	109.95	118.09
35	n	615	II0	C37-C35-C33	-5.33	109.95	118.09
26	B	821	CLA	C4A-NA-C1A	5.32	109.11	106.68
27	A	842	PQN	C14-C13-C12	-5.31	109.99	123.63
26	c	309	CLA	C1D-CHD-C4C	-5.31	114.73	126.02
35	h	310	II0	C37-C35-C33	-5.31	109.98	118.09
35	a	313	II0	C29-C31-C33	-5.31	107.82	123.20
35	j	615	II0	C34-C36-C40	-5.30	110.67	119.01
35	l	314	II0	C34-C36-C40	-5.30	110.67	119.01
29	L	201	WVN	C38-C34-C33	-5.30	109.99	118.09
27	A	842	PQN	C15-C13-C12	-5.30	109.28	121.17
29	B	847	WVN	C23-C25-C28	-5.29	110.69	119.01
35	h	312	II0	C37-C35-C33	-5.29	110.01	118.09
35	m	615	II0	C38-C36-C34	-5.29	110.01	118.09
29	A	846	WVN	C27-C25-C23	-5.28	110.02	118.09
35	i	312	II0	C34-C36-C40	-5.28	110.71	119.01
29	M	101	WVN	C23-C20-C13	-5.27	112.92	127.00
29	A	846	WVN	C20-C13-C15	-5.26	109.44	121.56
29	K	102	WVN	C33-C34-C37	-5.25	110.75	119.01
29	B	849	WVN	C14-C15-C13	-5.25	115.61	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	n	616	II0	C31-C29-C25	-5.24	111.95	126.61
35	k	616	II0	C38-C36-C34	-5.24	110.08	118.09
29	A	857	WVN	C23-C20-C13	-5.23	113.02	127.00
29	B	848	WVN	C19-C22-C26	-5.23	110.78	119.01
36	c	310	KC2	C2D-C1D-ND	5.22	115.74	110.33
29	I	101	WVN	C20-C13-C15	-5.22	109.54	121.56
35	i	313	II0	C37-C35-C33	-5.22	110.12	118.09
29	I	101	WVN	C27-C25-C23	-5.21	110.13	118.09
26	c	309	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
29	M	101	WVN	C02-C11-C19	-5.20	116.49	124.58
36	c	310	KC2	C3A-C4A-NA	5.20	116.88	110.45
29	A	848	WVN	C02-C05-C09	-5.19	115.08	121.47
35	b	314	II0	C31-C29-C25	-5.19	112.09	126.61
27	B	843	PQN	C14-C13-C12	-5.19	110.30	123.63
36	c	310	KC2	C3D-C4D-ND	5.19	117.43	110.20
35	l	314	II0	C32-C30-C26	-5.18	112.11	126.61
29	A	848	WVN	C02-C11-C19	-5.18	116.51	124.58
29	l	303	WVN	C38-C34-C33	-5.18	110.17	118.09
36	c	310	KC2	C2B-C1B-NB	5.17	115.24	110.13
36	s	401	KC2	C2A-C1A-NA	5.15	117.60	109.34
35	d	315	II0	C32-C30-C26	-5.13	112.25	126.61
29	i	315	WVN	C14-C15-C13	-5.13	115.77	122.70
35	l	315	II0	C29-C31-C33	-5.13	108.34	123.20
35	i	313	II0	C34-C36-C40	-5.12	110.95	119.01
29	R	200	WVN	C33-C34-C37	-5.12	110.96	119.01
35	k	615	II0	C32-C30-C26	-5.11	112.31	126.61
35	J	104	II0	C32-C30-C26	-5.11	112.31	126.61
35	a	312	II0	C32-C30-C26	-5.10	112.35	126.61
29	L	205	WVN	C31-C32-C36	-5.10	110.99	119.01
35	l	314	II0	C37-C35-C33	-5.09	110.31	118.09
29	l	303	WVN	C23-C20-C13	-5.08	113.42	127.00
35	k	620	II0	C37-C35-C33	-5.08	110.32	118.09
26	B	829	CLA	C4A-NA-C1A	5.08	109.00	106.68
35	c	316	II0	C32-C30-C26	-5.08	112.40	126.61
29	B	848	WVN	C33-C34-C37	-5.08	111.02	119.01
35	a	312	II0	C38-C36-C34	-5.05	110.37	118.09
35	d	301	II0	C34-C36-C40	-5.05	111.07	119.01
35	k	620	II0	C32-C30-C26	-5.05	112.49	126.61
36	s	401	KC2	C2B-C1B-NB	5.05	115.12	110.13
29	A	857	WVN	C19-C22-C26	-5.04	111.08	119.01
29	L	201	WVN	C06-C13-C15	-5.04	115.75	122.64
26	n	608	CLA	C4A-NA-C1A	5.03	108.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	316	II0	C37-C35-C33	-5.03	110.41	118.09
35	d	316	II0	C32-C30-C26	-5.01	112.59	126.61
35	k	616	II0	C29-C31-C33	-5.01	108.69	123.20
36	s	401	KC2	C2D-C1D-ND	5.00	115.51	110.33
26	A	851	CLA	C4A-NA-C1A	4.99	108.96	106.68
26	c	309	CLA	CHD-C1D-ND	-4.99	117.78	124.80
35	m	615	II0	C29-C31-C33	-4.99	108.74	123.20
35	h	312	II0	C34-C36-C40	-4.99	111.16	119.01
29	J	102	WVN	C33-C34-C37	-4.99	111.17	119.01
29	K	102	WVN	C35-C32-C31	-4.98	110.47	118.09
29	B	850	WVN	C23-C20-C13	-4.98	113.69	127.00
35	m	615	II0	C37-C35-C33	-4.98	110.48	118.09
36	s	401	KC2	C3D-C4D-ND	4.98	117.14	110.20
36	c	310	KC2	O2D-CGD-CBD	4.97	119.92	111.23
35	i	316	II0	C32-C30-C26	-4.97	112.71	126.61
29	h	309	WVN	C02-C05-C09	-4.97	115.36	121.47
29	F	203	WVN	C20-C13-C15	-4.96	110.12	121.56
35	l	302	II0	C37-C35-C33	-4.96	110.51	118.09
35	a	312	II0	C29-C31-C33	-4.95	108.85	123.20
29	J	101	WVN	C20-C13-C15	-4.95	110.16	121.56
29	M	101	WVN	C20-C13-C15	-4.95	110.16	121.56
35	a	314	II0	C34-C36-C40	-4.95	111.23	119.01
35	d	317	II0	C32-C30-C26	-4.95	112.77	126.61
35	b	315	II0	C20-C14-C12	-4.95	105.33	114.42
29	A	847	WVN	C16-C05-C09	-4.94	105.76	122.37
36	c	310	KC2	C2A-C1A-NA	4.93	117.23	109.34
35	i	319	II0	C20-C14-C12	-4.92	105.38	114.42
35	a	316	II0	C31-C29-C25	-4.91	112.86	126.61
35	m	614	II0	C37-C35-C33	-4.91	110.58	118.09
29	B	853	WVN	C23-C20-C13	-4.91	113.88	127.00
35	k	616	II0	C19-C13-C11	-4.91	105.39	114.42
35	i	319	II0	C34-C36-C40	-4.90	111.30	119.01
26	h	305	CLA	C4A-NA-C1A	4.90	108.91	106.68
35	a	312	II0	C37-C35-C33	-4.89	110.61	118.09
26	k	603	CLA	C4A-NA-C1A	4.88	108.91	106.68
29	B	849	WVN	C23-C20-C13	-4.87	113.99	127.00
29	K	102	WVN	C23-C20-C13	-4.87	114.00	127.00
29	i	315	WVN	C31-C32-C36	-4.86	111.37	119.01
35	d	316	II0	C34-C36-C40	-4.86	111.37	119.01
36	s	401	KC2	C4C-C3C-C2C	-4.85	102.82	107.28
29	L	201	WVN	C14-C15-C13	-4.85	116.15	122.70
36	s	401	KC2	C3C-C2C-C1C	-4.85	102.77	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	313	II0	C32-C30-C26	-4.85	113.04	126.61
35	i	312	II0	C29-C31-C33	-4.85	109.15	123.20
29	B	846	WVN	C20-C13-C15	-4.84	110.40	121.56
35	i	312	II0	C32-C30-C26	-4.84	113.07	126.61
36	c	310	KC2	C4C-C3C-C2C	-4.82	102.85	107.28
35	a	316	II0	C34-C36-C40	-4.81	111.44	119.01
35	J	104	II0	C34-C36-C40	-4.81	111.45	119.01
29	B	847	WVN	C19-C22-C26	-4.80	111.46	119.01
29	h	309	WVN	C23-C20-C13	-4.78	114.22	127.00
29	A	857	WVN	C02-C11-C19	-4.78	117.14	124.58
29	A	847	WVN	C23-C20-C13	-4.77	114.24	127.00
35	b	315	II0	C31-C29-C25	-4.77	113.28	126.61
29	l	303	WVN	C14-C15-C13	-4.75	116.28	122.70
35	b	315	II0	C12-C14-C10	-4.74	110.63	120.50
29	B	846	WVN	C33-C34-C37	-4.74	111.55	119.01
35	a	313	II0	C34-C36-C40	-4.74	111.56	119.01
26	c	309	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
35	k	616	II0	C37-C35-C33	-4.72	110.88	118.09
35	i	313	II0	C20-C14-C12	-4.71	105.75	114.42
29	K	102	WVN	C19-C22-C26	-4.71	111.59	119.01
35	k	615	II0	C20-C14-C12	-4.71	105.76	114.42
35	i	319	II0	C12-C14-C10	-4.70	110.72	120.50
35	i	316	II0	C34-C36-C40	-4.70	111.62	119.01
29	A	847	WVN	C19-C22-C26	-4.70	111.62	119.01
35	d	317	II0	C11-C13-C09	-4.69	110.74	120.50
35	k	620	II0	C34-C36-C40	-4.69	111.63	119.01
35	k	615	II0	C12-C14-C10	-4.68	110.75	120.50
36	c	310	KC2	C1A-NA-C4A	-4.68	104.54	106.68
26	c	309	CLA	CHB-C1B-NB	-4.68	117.03	124.05
29	F	203	WVN	C23-C25-C28	-4.67	111.66	119.01
26	B	819	CLA	CBC-CAC-C3C	4.67	125.07	112.42
26	k	607	CLA	C4A-NA-C1A	4.66	108.81	106.68
35	d	317	II0	C34-C36-C40	-4.64	111.70	119.01
35	c	313	II0	C29-C31-C33	-4.64	109.76	123.20
35	a	312	II0	C34-C36-C40	-4.64	111.72	119.01
29	B	847	WVN	C31-C32-C36	-4.64	111.72	119.01
29	A	845	WVN	C20-C13-C15	-4.63	110.88	121.56
29	B	850	WVN	C19-C22-C26	-4.63	111.73	119.01
36	s	401	KC2	CBC-CAC-C3C	-4.61	104.49	127.53
29	l	316	WVN	C19-C22-C26	-4.61	111.76	119.01
35	i	314	II0	C32-C30-C26	-4.60	113.73	126.61
29	B	850	WVN	C23-C25-C28	-4.60	111.77	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	847	WVN	C14-C15-C13	-4.60	116.49	122.70
29	B	850	WVN	C14-C15-C13	-4.59	116.50	122.70
35	h	312	II0	C32-C30-C26	-4.59	113.76	126.61
35	l	315	II0	C37-C35-C33	-4.59	111.08	118.09
35	l	315	II0	C11-C13-C09	-4.58	110.96	120.50
29	A	848	WVN	C16-C05-C09	-4.58	106.97	122.37
35	l	302	II0	C05-C03-C09	4.58	118.52	109.49
26	R	201	CLA	CAA-C2A-C3A	-4.58	100.62	113.00
29	B	847	WVN	C06-C13-C15	-4.57	116.39	122.64
35	m	619	II0	C20-C14-C12	-4.56	106.03	114.42
29	l	316	WVN	C16-C05-C09	-4.56	107.05	122.37
35	k	615	II0	C34-C36-C40	-4.55	111.85	119.01
29	B	849	WVN	C20-C13-C15	-4.55	111.08	121.56
29	l	316	WVN	C31-C32-C36	-4.54	111.87	119.01
29	s	407	WVN	C14-C15-C13	-4.54	116.57	122.70
35	c	316	II0	C20-C14-C12	-4.54	106.08	114.42
35	k	619	II0	C37-C35-C33	-4.52	111.18	118.09
29	A	857	WVN	C33-C34-C37	-4.51	111.91	119.01
29	A	857	WVN	C20-C13-C15	-4.51	111.17	121.56
29	B	847	WVN	C16-C05-C09	-4.51	107.23	122.37
29	h	309	WVN	C14-C15-C13	-4.50	116.62	122.70
36	c	310	KC2	CHC-C1C-C2C	-4.50	117.93	125.03
35	h	311	II0	C37-C35-C33	-4.49	111.22	118.09
29	I	101	WVN	C16-C05-C09	-4.49	107.27	122.37
35	b	315	II0	C11-C13-C09	-4.48	111.17	120.50
29	A	847	WVN	C31-C32-C36	-4.48	111.96	119.01
29	L	205	WVN	C14-C15-C13	-4.47	116.66	122.70
35	k	615	II0	C29-C31-C33	-4.47	110.24	123.20
35	l	314	II0	C29-C31-C33	-4.46	110.28	123.20
35	d	315	II0	C31-C29-C25	-4.46	114.14	126.61
29	l	316	WVN	C10-C06-C13	4.45	116.91	110.44
28	s	409	LHG	O3-P-O6	-4.45	95.07	106.67
29	J	102	WVN	C31-C32-C36	-4.45	112.01	119.01
35	d	317	II0	C20-C14-C12	-4.45	106.24	114.42
28	m	618	LHG	O4-P-O5	4.44	133.09	112.44
28	A	849	LHG	O4-P-O5	4.43	133.06	112.44
28	J	105	LHG	O4-P-O5	4.43	133.05	112.44
29	B	847	WVN	C23-C20-C13	-4.42	115.18	127.00
29	B	849	WVN	C31-C32-C36	-4.42	112.05	119.01
35	n	618	II0	C32-C30-C26	-4.42	114.24	126.61
35	l	302	II0	C31-C29-C25	-4.42	114.25	126.61
29	h	309	WVN	C16-C05-C09	-4.42	107.52	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	n	619	LHG	O4-P-O5	4.42	133.00	112.44
28	i	317	LHG	O4-P-O5	4.42	132.99	112.44
28	c	317	LHG	O4-P-O5	4.42	132.99	112.44
28	b	302	LHG	O4-P-O5	4.42	132.98	112.44
28	B	851	LHG	O4-P-O5	4.41	132.98	112.44
28	A	844	LHG	O4-P-O5	4.41	132.97	112.44
35	n	615	II0	C20-C14-C12	-4.41	106.31	114.42
35	k	619	II0	C34-C36-C40	-4.41	112.07	119.01
28	b	318	LHG	O4-P-O5	4.41	132.96	112.44
28	L	208	LHG	O4-P-O5	4.41	132.95	112.44
29	I	101	WVN	C02-C05-C09	-4.40	116.05	121.47
35	m	614	II0	C34-C36-C40	-4.40	112.08	119.01
35	h	311	II0	C34-C36-C40	-4.40	112.09	119.01
28	c	320	LHG	O4-P-O5	4.40	132.92	112.44
35	m	614	II0	C31-C29-C25	-4.40	114.31	126.61
28	A	843	LHG	O4-P-O5	4.40	132.90	112.44
28	L	207	LHG	O4-P-O5	4.40	132.90	112.44
28	A	855	LHG	O4-P-O5	4.40	132.89	112.44
28	j	617	LHG	O4-P-O5	4.39	132.87	112.44
28	l	318	LHG	O4-P-O5	4.39	132.86	112.44
29	A	846	WVN	C23-C20-C13	-4.38	115.29	127.00
36	s	401	KC2	CHC-C1C-C2C	-4.38	118.11	125.03
35	n	616	II0	C20-C14-C12	-4.37	106.39	114.42
35	i	319	II0	C32-C30-C26	-4.37	114.39	126.61
35	j	615	II0	C29-C31-C33	-4.36	110.56	123.20
33	j	618	DGD	O3G-C3G-C2G	-4.35	100.23	110.82
35	m	616	II0	C34-C36-C40	-4.34	112.19	119.01
29	s	407	WVN	C31-C32-C36	-4.34	112.19	119.01
29	B	848	WVN	C20-C13-C15	-4.33	111.59	121.56
35	l	315	II0	C32-C30-C26	-4.33	114.51	126.61
29	A	845	WVN	C31-C32-C36	-4.30	112.25	119.01
29	B	846	WVN	C06-C13-C15	-4.29	116.78	122.64
35	m	616	II0	C20-C14-C12	-4.29	106.54	114.42
29	J	102	WVN	C20-C13-C15	-4.29	111.68	121.56
35	h	311	II0	C11-C13-C09	-4.28	111.59	120.50
35	h	310	II0	C19-C13-C11	-4.27	106.56	114.42
29	F	203	WVN	C23-C20-C13	-4.27	115.59	127.00
35	j	614	II0	C19-C13-C11	-4.26	106.58	114.42
29	J	102	WVN	C16-C05-C09	-4.25	108.08	122.37
29	B	846	WVN	C16-C05-C09	-4.25	108.08	122.37
29	L	205	WVN	C16-C05-C09	-4.25	108.10	122.37
35	m	615	II0	C32-C30-C26	-4.24	114.75	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	313	II0	C31-C29-C25	-4.24	114.75	126.61
35	l	302	II0	C20-C14-C12	-4.24	106.63	114.42
29	I	101	WVN	C26-C29-C31	-4.23	110.94	123.20
26	c	309	CLA	O2D-CGD-CBD	4.22	118.61	111.23
26	i	305	CLA	C1D-ND-C4D	-4.22	103.35	106.31
35	a	316	II0	C19-C13-C11	-4.22	106.66	114.42
29	L	201	WVN	C16-C05-C09	-4.22	108.19	122.37
35	a	312	II0	C20-C14-C12	-4.22	106.67	114.42
29	B	848	WVN	C16-C05-C09	-4.22	108.20	122.37
29	I	101	WVN	C23-C20-C13	-4.21	115.74	127.00
35	J	104	II0	C19-C13-C11	-4.21	106.67	114.42
35	m	616	II0	C19-C13-C11	-4.21	106.68	114.42
26	n	607	CLA	C4A-NA-C1A	4.21	108.60	106.68
29	B	849	WVN	C33-C34-C37	-4.21	112.39	119.01
36	c	310	KC2	C3C-C2C-C1C	-4.21	103.25	106.41
35	k	619	II0	C32-C30-C26	-4.21	114.84	126.61
29	A	845	WVN	C16-C05-C09	-4.20	108.24	122.37
29	M	101	WVN	C31-C32-C36	-4.20	112.40	119.01
35	j	614	II0	C32-C30-C26	-4.20	114.87	126.61
35	m	615	II0	C20-C14-C12	-4.19	106.71	114.42
35	m	619	II0	C32-C30-C26	-4.19	114.89	126.61
29	J	101	WVN	C23-C20-C13	-4.19	115.82	127.00
29	s	407	WVN	C19-C22-C26	-4.18	112.44	119.01
35	a	316	II0	C06-C04-C10	4.18	117.72	109.49
29	B	849	WVN	C16-C05-C09	-4.18	108.33	122.37
35	m	619	II0	C37-C35-C33	-4.18	111.71	118.09
36	c	310	KC2	CBC-CAC-C3C	-4.17	106.69	127.53
29	B	850	WVN	C16-C05-C09	-4.17	108.37	122.37
29	B	846	WVN	C28-C30-C33	-4.16	111.13	123.20
35	a	314	II0	C11-C13-C09	-4.16	111.84	120.50
35	l	302	II0	C06-C04-C10	4.16	117.69	109.49
29	h	309	WVN	C06-C13-C15	-4.15	116.97	122.64
32	A	854	SQD	C4-C3-C2	4.15	118.11	110.83
29	l	303	WVN	C16-C05-C09	-4.14	108.44	122.37
29	A	845	WVN	C06-C13-C15	-4.14	116.97	122.64
35	d	301	II0	C32-C30-C26	-4.14	115.02	126.61
35	n	615	II0	C32-C30-C26	-4.14	115.02	126.61
32	A	854	SQD	O5-C5-C4	4.14	117.16	109.70
35	d	317	II0	C29-C31-C33	-4.13	111.22	123.20
29	A	857	WVN	C16-C05-C09	-4.13	108.49	122.37
35	i	313	II0	C19-C13-C11	-4.12	106.84	114.42
35	n	616	II0	C32-C30-C26	-4.12	115.09	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	844	DGD	O6D-C1D-O3G	-4.12	100.31	110.04
29	i	315	WVN	C16-C05-C09	-4.12	108.54	122.37
35	a	314	II0	C32-C30-C26	-4.11	115.12	126.61
29	R	200	WVN	C16-C05-C09	-4.10	108.58	122.37
29	B	848	WVN	C10-C06-C13	4.10	116.40	110.44
29	M	101	WVN	C06-C13-C15	-4.10	117.03	122.64
35	i	319	II0	C05-C03-C09	4.10	117.56	109.49
35	h	311	II0	C31-C29-C25	-4.09	115.17	126.61
35	k	619	II0	C20-C14-C12	-4.09	106.91	114.42
29	I	101	WVN	C28-C30-C33	-4.08	111.38	123.20
29	J	102	WVN	C23-C25-C28	-4.08	112.60	119.01
35	d	301	II0	C11-C13-C09	-4.08	112.02	120.50
35	h	310	II0	C29-C31-C33	-4.07	111.39	123.20
29	F	203	WVN	C16-C05-C09	-4.07	108.68	122.37
36	s	401	KC2	C2C-C1C-NC	4.06	115.48	110.45
35	b	315	II0	C29-C31-C33	-4.05	111.46	123.20
35	i	314	II0	C29-C31-C33	-4.05	111.46	123.20
35	c	313	II0	C32-C30-C26	-4.05	115.28	126.61
35	j	614	II0	C37-C35-C33	-4.04	111.91	118.09
29	A	848	WVN	C28-C30-C33	-4.04	111.49	123.20
35	n	616	II0	C11-C13-C09	-4.03	112.11	120.50
35	i	312	II0	C11-C13-C09	-4.03	112.11	120.50
35	d	316	II0	C19-C13-C11	-4.03	107.01	114.42
35	n	615	II0	C31-C29-C25	-4.03	115.35	126.61
35	h	312	II0	C19-C13-C11	-4.03	107.02	114.42
35	m	616	II0	C29-C31-C33	-4.02	111.54	123.20
29	B	853	WVN	C02-C05-C09	-4.02	116.52	121.47
35	n	618	II0	C29-C31-C33	-4.02	111.55	123.20
35	i	312	II0	C06-C04-C10	4.02	117.41	109.49
35	i	316	II0	C31-C29-C25	-4.02	115.37	126.61
35	k	615	II0	C31-C29-C25	-4.01	115.38	126.61
35	i	316	II0	C11-C13-C09	-4.00	112.17	120.50
35	j	615	II0	C20-C14-C12	-4.00	107.06	114.42
29	B	853	WVN	C16-C05-C09	-4.00	108.92	122.37
35	k	616	II0	C32-C30-C26	-4.00	115.42	126.61
29	J	102	WVN	C26-C29-C31	-4.00	111.61	123.20
35	b	314	II0	C32-C30-C26	-4.00	115.42	126.61
29	B	846	WVN	C26-C29-C31	-4.00	111.61	123.20
35	k	616	II0	C20-C14-C12	-4.00	107.07	114.42
35	j	614	II0	C34-C36-C40	-3.98	112.74	119.01
29	l	303	WVN	C06-C13-C15	-3.97	117.20	122.64
35	m	614	II0	C32-C30-C26	-3.97	115.50	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i	315	WVN	C33-C34-C37	-3.97	112.77	119.01
35	h	311	II0	C32-C30-C26	-3.97	115.52	126.61
26	m	612	CLA	CAA-C2A-C3A	-3.96	102.28	113.00
26	B	804	CLA	CBC-CAC-C3C	3.96	123.17	112.42
35	h	312	II0	C20-C14-C12	-3.96	107.13	114.42
35	a	316	II0	C32-C30-C26	-3.96	115.52	126.61
29	L	201	WVN	C28-C30-C33	-3.96	111.72	123.20
26	j	607	CLA	C4A-NA-C1A	3.96	108.49	106.68
29	B	850	WVN	C06-C13-C15	-3.96	117.22	122.64
29	l	316	WVN	C28-C30-C33	-3.96	111.73	123.20
35	n	615	II0	C34-C36-C40	-3.95	112.80	119.01
29	J	101	WVN	C16-C05-C09	-3.94	109.11	122.37
35	l	302	II0	C32-C30-C26	-3.94	115.58	126.61
29	L	205	WVN	C06-C13-C15	-3.94	117.25	122.64
35	d	316	II0	C29-C31-C33	-3.93	111.81	123.20
35	i	319	II0	C31-C29-C25	-3.93	115.62	126.61
26	l	305	CLA	O2D-CGD-O1D	-3.93	116.21	123.85
35	j	615	II0	C32-C30-C26	-3.92	115.65	126.61
35	m	619	II0	C34-C36-C40	-3.92	112.85	119.01
35	d	315	II0	C29-C31-C33	-3.91	111.86	123.20
35	k	620	II0	C19-C13-C11	-3.91	107.23	114.42
26	B	818	CLA	C3B-C4B-NB	-3.91	107.04	110.53
29	h	309	WVN	C28-C30-C33	-3.91	111.88	123.20
35	m	616	II0	C32-C30-C26	-3.91	115.68	126.61
29	M	101	WVN	C01-C02-C11	-3.90	108.34	112.83
29	A	848	WVN	C26-C29-C31	-3.90	111.91	123.20
29	s	407	WVN	C16-C05-C09	-3.89	109.29	122.37
29	M	101	WVN	C16-C05-C09	-3.89	109.31	122.37
29	s	405	WVN	C16-C05-C09	-3.87	109.36	122.37
26	c	309	CLA	C2A-C1A-CHA	-3.87	117.15	123.87
35	h	312	II0	C31-C29-C25	-3.87	115.79	126.61
35	i	312	II0	C19-C13-C11	-3.87	107.31	114.42
35	i	316	II0	C05-C03-C09	3.86	117.11	109.49
35	b	314	II0	C37-C35-C33	-3.86	112.19	118.09
29	l	316	WVN	C06-C13-C15	-3.86	117.36	122.64
26	B	804	CLA	CAC-C3C-C2C	-3.85	120.49	127.56
32	A	854	SQD	O9-S-O7	-3.85	101.32	113.82
35	i	312	II0	C30-C32-C34	-3.84	112.07	123.20
35	b	314	II0	C11-C13-C09	-3.84	112.52	120.50
29	A	846	WVN	C16-C05-C09	-3.83	109.49	122.37
29	L	201	WVN	C20-C13-C15	-3.83	112.73	121.56
32	A	854	SQD	C1-O5-C5	3.83	121.20	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	310	KC2	CHD-C1D-ND	-3.83	118.31	124.05
29	B	850	WVN	C33-C34-C37	-3.83	112.99	119.01
35	h	312	II0	C29-C31-C33	-3.82	112.14	123.20
35	k	620	II0	C31-C29-C25	-3.82	115.94	126.61
35	l	302	II0	C19-C13-C11	-3.81	107.41	114.42
35	i	314	II0	C31-C29-C25	-3.81	115.95	126.61
35	d	301	II0	C29-C31-C33	-3.81	112.16	123.20
29	B	846	WVN	C23-C20-C13	-3.79	116.86	127.00
29	K	102	WVN	C16-C05-C09	-3.79	109.62	122.37
35	d	317	II0	C31-C29-C25	-3.79	116.00	126.61
35	n	615	II0	C19-C13-C11	-3.79	107.46	114.42
32	A	854	SQD	O47-C7-C8	3.78	119.67	111.48
35	i	319	II0	C19-C13-C11	-3.78	107.46	114.42
36	c	310	KC2	C4B-C3B-C2B	-3.78	103.53	106.81
26	A	840	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
35	i	314	II0	C19-C13-C11	-3.78	107.48	114.42
29	B	853	WVN	C26-C29-C31	-3.77	112.26	123.20
29	K	102	WVN	C28-C30-C33	-3.77	112.27	123.20
35	n	616	II0	C29-C31-C33	-3.77	112.29	123.20
35	j	614	II0	C20-C14-C12	-3.76	107.51	114.42
27	A	842	PQN	C14-C13-C15	-3.76	108.71	115.23
35	c	313	II0	C20-C14-C12	-3.75	107.52	114.42
29	M	101	WVN	C26-C29-C31	-3.75	112.33	123.20
35	i	319	II0	C29-C31-C33	-3.74	112.35	123.20
35	j	615	II0	C31-C29-C25	-3.74	116.14	126.61
35	a	316	II0	C05-C03-C09	3.74	116.86	109.49
35	J	104	II0	C20-C14-C12	-3.74	107.55	114.42
35	b	314	II0	C20-C14-C12	-3.73	107.56	114.42
35	n	615	II0	C05-C03-C09	3.72	116.83	109.49
35	k	620	II0	C29-C31-C33	-3.72	112.41	123.20
35	k	620	II0	C11-C13-C09	-3.72	112.76	120.50
35	a	313	II0	C32-C30-C26	-3.71	116.23	126.61
29	l	303	WVN	C26-C29-C31	-3.71	112.46	123.20
35	k	616	II0	C30-C32-C34	-3.71	112.46	123.20
35	a	313	II0	C20-C14-C12	-3.70	107.61	114.42
35	c	316	II0	C30-C32-C34	-3.70	112.49	123.20
35	i	314	II0	C20-C14-C12	-3.69	107.63	114.42
33	B	844	DGD	O3G-C3G-C2G	-3.69	101.84	110.82
35	j	615	II0	C11-C13-C09	-3.69	112.83	120.50
29	B	846	WVN	C14-C15-C13	-3.68	117.74	122.70
35	J	104	II0	C11-C13-C09	-3.67	112.85	120.50
35	a	316	II0	C29-C31-C33	-3.67	112.55	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	201	WVN	C26-C29-C31	-3.67	112.58	123.20
33	j	618	DGD	O6D-C1D-O3G	-3.67	101.38	110.04
29	s	407	WVN	C28-C30-C33	-3.67	112.58	123.20
35	j	614	II0	C31-C29-C25	-3.66	116.36	126.61
33	j	618	DGD	C1E-O6E-C5E	3.66	120.86	113.72
35	l	315	II0	C20-C14-C12	-3.66	107.70	114.42
35	i	316	II0	C29-C31-C33	-3.65	112.62	123.20
36	d	312	KC2	CHD-C1D-ND	-3.65	118.58	124.05
35	j	614	II0	C29-C31-C33	-3.65	112.64	123.20
35	c	313	II0	C11-C13-C09	-3.64	112.92	120.50
29	i	315	WVN	C26-C29-C31	-3.64	112.67	123.20
29	L	205	WVN	C26-C29-C31	-3.63	112.67	123.20
35	d	315	II0	C20-C14-C12	-3.63	107.74	114.42
35	l	314	II0	C30-C32-C34	-3.63	112.70	123.20
29	J	101	WVN	C28-C30-C33	-3.62	112.72	123.20
29	A	846	WVN	C28-C30-C33	-3.62	112.72	123.20
35	n	616	II0	C06-C04-C10	3.61	116.61	109.49
29	s	407	WVN	C06-C13-C15	-3.61	117.70	122.64
35	l	314	II0	C11-C13-C09	-3.61	112.98	120.50
36	s	401	KC2	C1D-CHD-C4C	-3.61	117.76	126.25
26	s	406	CLA	CAA-C2A-C3A	-3.61	103.25	113.00
26	B	827	CLA	CMB-C2B-C1B	-3.61	119.93	125.42
35	d	315	II0	C30-C32-C34	-3.61	112.75	123.20
35	n	616	II0	C30-C32-C34	-3.60	112.77	123.20
35	d	316	II0	C30-C32-C34	-3.60	112.77	123.20
29	l	303	WVN	C28-C30-C33	-3.60	112.77	123.20
35	k	619	II0	C29-C31-C33	-3.60	112.78	123.20
35	d	316	II0	C31-C29-C25	-3.59	116.56	126.61
29	A	848	WVN	C01-C02-C11	-3.59	108.70	112.83
26	i	302	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
26	s	406	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
35	l	314	II0	C12-C14-C10	-3.58	113.05	120.50
29	A	847	WVN	C28-C30-C33	-3.57	112.85	123.20
35	m	616	II0	C30-C32-C34	-3.57	112.85	123.20
35	b	314	II0	C34-C36-C40	-3.57	113.40	119.01
29	B	847	WVN	C28-C30-C33	-3.57	112.87	123.20
29	M	101	WVN	C28-C30-C33	-3.56	112.87	123.20
35	k	620	II0	C20-C14-C12	-3.56	107.87	114.42
36	s	401	KC2	C4B-C3B-C2B	-3.56	103.73	106.81
35	J	104	II0	C29-C31-C33	-3.55	112.91	123.20
35	k	619	II0	C31-C29-C25	-3.54	116.71	126.61
35	h	311	II0	C12-C14-C10	-3.54	113.14	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	316	II0	C29-C31-C33	-3.53	112.96	123.20
35	a	316	II0	C20-C14-C12	-3.53	107.93	114.42
25	A	801	CL0	C3D-C4D-CHA	3.53	113.90	108.54
35	m	619	II0	C31-C29-C25	-3.53	116.75	126.61
35	n	618	II0	C31-C29-C25	-3.53	116.75	126.61
35	k	615	II0	C11-C13-C09	-3.52	113.17	120.50
35	b	314	II0	C30-C32-C34	-3.51	113.02	123.20
29	L	205	WVN	C28-C30-C33	-3.50	113.05	123.20
35	i	313	II0	C29-C31-C33	-3.49	113.08	123.20
29	B	847	WVN	C10-C06-C13	3.49	115.50	110.44
35	h	310	II0	C05-C03-C09	3.48	116.35	109.49
26	c	309	CLA	C4C-C3C-C2C	-3.48	101.82	106.89
29	A	845	WVN	C21-C15-C14	-3.48	106.18	113.60
29	B	848	WVN	C26-C29-C31	-3.48	113.13	123.20
26	s	403	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
29	A	857	WVN	C28-C30-C33	-3.47	113.15	123.20
35	d	317	II0	C06-C04-C10	3.47	116.32	109.49
29	s	405	WVN	C26-C29-C31	-3.46	113.18	123.20
35	m	619	II0	C06-C04-C10	3.46	116.30	109.49
35	i	316	II0	C30-C32-C34	-3.46	113.18	123.20
35	l	314	II0	C31-C29-C25	-3.45	116.97	126.61
26	c	309	CLA	CHC-C1C-C2C	-3.44	117.19	126.95
29	s	405	WVN	C28-C30-C33	-3.43	113.26	123.20
35	d	317	II0	C30-C32-C34	-3.43	113.26	123.20
26	l	306	CLA	CMB-C2B-C1B	-3.43	120.20	125.42
29	A	846	WVN	C26-C29-C31	-3.43	113.27	123.20
35	m	614	II0	C19-C13-C11	-3.43	108.12	114.42
26	d	313	CLA	CAA-C2A-C3A	-3.42	103.75	113.00
26	i	305	CLA	C3B-C4B-NB	-3.42	107.47	110.53
29	B	847	WVN	C26-C29-C31	-3.42	113.29	123.20
29	L	201	WVN	C02-C05-C09	-3.42	117.26	121.47
35	J	104	II0	C30-C32-C34	-3.42	113.30	123.20
26	s	402	CLA	CAA-C2A-C3A	-3.42	103.76	113.00
36	s	401	KC2	O2D-CGD-O1D	-3.41	117.20	123.85
25	A	801	CL0	C1C-CHC-C4B	3.41	128.28	116.07
26	A	817	CLA	C3B-C4B-NB	-3.41	107.49	110.53
35	b	314	II0	C29-C31-C33	-3.41	113.33	123.20
26	B	808	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
35	m	619	II0	C19-C13-C11	-3.40	108.17	114.42
26	i	302	CLA	O2D-CGD-CBD	3.40	117.17	111.23
35	h	310	II0	C31-C29-C25	-3.39	117.12	126.61
35	m	615	II0	C30-C32-C34	-3.38	113.39	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R	200	WVN	C26-C29-C31	-3.38	113.41	123.20
35	k	619	II0	C11-C13-C09	-3.38	113.47	120.50
35	i	314	II0	C30-C32-C34	-3.38	113.42	123.20
36	c	310	KC2	C2C-C1C-NC	3.37	114.63	110.45
35	m	619	II0	C29-C31-C33	-3.37	113.42	123.20
36	s	401	KC2	CHD-C1D-ND	-3.37	118.99	124.05
35	i	312	II0	C20-C14-C12	-3.37	108.23	114.42
29	B	846	WVN	C21-C15-C14	-3.37	106.42	113.60
35	h	310	II0	C15-C03-C09	-3.36	104.50	110.52
35	b	315	II0	C19-C13-C11	-3.36	108.25	114.42
35	m	614	II0	C05-C03-C09	3.36	116.10	109.49
35	i	313	II0	C30-C32-C34	-3.36	113.48	123.20
26	d	309	CLA	CAA-C2A-C3A	-3.36	108.54	116.23
29	B	853	WVN	C28-C30-C33	-3.35	113.48	123.20
26	B	840	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
26	k	607	CLA	CAA-C2A-C3A	-3.35	103.95	113.00
35	m	615	II0	C19-C13-C11	-3.35	108.26	114.42
29	A	857	WVN	C26-C29-C31	-3.35	113.51	123.20
27	B	843	PQN	C14-C13-C15	-3.35	109.42	115.23
35	a	314	II0	C29-C31-C33	-3.34	113.51	123.20
35	i	316	II0	C19-C13-C11	-3.34	108.28	114.42
29	R	200	WVN	C28-C30-C33	-3.34	113.52	123.20
35	n	615	II0	C11-C13-C09	-3.34	113.56	120.50
35	h	311	II0	C20-C14-C12	-3.33	108.29	114.42
35	h	312	II0	C05-C03-C09	3.33	116.05	109.49
35	l	302	II0	C29-C31-C33	-3.33	113.55	123.20
35	m	614	II0	C29-C31-C33	-3.32	113.57	123.20
35	k	615	II0	C30-C32-C34	-3.32	113.57	123.20
36	c	310	KC2	C1D-CHD-C4C	-3.32	118.44	126.25
35	c	313	II0	C31-C29-C25	-3.32	117.34	126.61
26	j	612	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
35	i	316	II0	C20-C14-C12	-3.30	108.34	114.42
35	a	314	II0	C12-C14-C10	-3.30	113.62	120.50
26	i	302	CLA	C3B-C4B-NB	-3.30	107.58	110.53
29	i	315	WVN	C10-C06-C13	3.30	115.24	110.44
35	m	614	II0	C20-C14-C12	-3.30	108.36	114.42
35	h	311	II0	C29-C31-C33	-3.29	113.67	123.20
35	j	615	II0	C06-C04-C10	3.28	115.96	109.49
26	B	838	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
26	k	609	CLA	C3B-C4B-NB	-3.27	107.61	110.53
26	A	816	CLA	CBA-CAA-C2A	3.27	123.52	113.79
35	a	313	II0	C30-C32-C34	-3.27	113.73	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	316	II0	C05-C03-C09	3.27	115.93	109.49
26	B	829	CLA	CMB-C2B-C1B	-3.26	120.45	125.42
29	A	845	WVN	C14-C15-C13	-3.26	118.30	122.70
36	c	310	KC2	CAA-C2A-C1A	-3.26	110.35	124.64
29	h	309	WVN	C26-C29-C31	-3.26	113.75	123.20
35	a	312	II0	C31-C29-C25	-3.26	117.50	126.61
26	c	309	CLA	CMB-C2B-C1B	3.26	130.38	125.42
26	l	305	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
35	k	616	II0	C06-C04-C10	3.25	115.89	109.49
35	i	314	II0	C05-C03-C09	3.24	115.88	109.49
26	A	802	CLA	CMB-C2B-C1B	-3.24	120.48	125.42
35	h	312	II0	C12-C14-C10	-3.24	113.75	120.50
29	R	200	WVN	C20-C13-C15	-3.24	114.09	121.56
35	m	614	II0	C11-C13-C09	-3.23	113.77	120.50
35	m	614	II0	C30-C32-C34	-3.23	113.83	123.20
29	A	848	WVN	C24-C22-C19	-3.23	113.15	118.09
35	d	301	II0	C30-C32-C34	-3.23	113.85	123.20
29	A	845	WVN	C28-C30-C33	-3.23	113.85	123.20
35	c	313	II0	C30-C32-C34	-3.23	113.85	123.20
26	B	841	CLA	C3B-C4B-NB	-3.23	107.65	110.53
26	A	832	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
35	m	615	II0	C06-C04-C10	3.22	115.84	109.49
26	i	310	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
29	B	850	WVN	C26-C29-C31	-3.22	113.87	123.20
26	m	602	CLA	C3B-C4B-NB	-3.22	107.66	110.53
35	n	618	II0	C20-C14-C12	-3.22	108.50	114.42
29	K	102	WVN	C26-C29-C31	-3.22	113.88	123.20
29	J	101	WVN	C26-C29-C31	-3.21	113.90	123.20
35	k	619	II0	C19-C13-C11	-3.21	108.52	114.42
26	m	610	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
35	b	314	II0	C19-C13-C11	-3.20	108.53	114.42
35	a	314	II0	C20-C14-C12	-3.20	108.54	114.42
35	n	615	II0	C29-C31-C33	-3.20	113.94	123.20
26	B	803	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
26	j	607	CLA	CMC-C2C-C1C	-3.20	120.04	125.03
35	a	316	II0	C30-C32-C34	-3.19	113.94	123.20
36	c	310	KC2	CAA-CBA-CGA	-3.19	110.81	127.05
35	d	301	II0	C37-C35-C33	-3.19	113.21	118.09
35	k	620	II0	C30-C32-C34	-3.19	113.97	123.20
26	d	306	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
26	c	304	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
35	a	313	II0	C12-C14-C10	-3.18	113.89	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	301	II0	C20-C14-C12	-3.18	108.58	114.42
29	B	848	WVN	C28-C30-C33	-3.18	113.99	123.20
29	l	316	WVN	C26-C29-C31	-3.17	114.00	123.20
35	l	314	II0	C20-C14-C12	-3.17	108.59	114.42
26	j	602	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
35	j	615	II0	C30-C32-C34	-3.17	114.03	123.20
26	h	305	CLA	CMB-C2B-C1B	-3.17	120.60	125.42
35	a	312	II0	C30-C32-C34	-3.17	114.03	123.20
35	l	314	II0	C19-C13-C11	-3.17	108.60	114.42
35	a	314	II0	C30-C32-C34	-3.16	114.03	123.20
29	s	407	WVN	C10-C06-C13	3.16	115.03	110.44
26	n	604	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
26	j	610	CLA	O2D-CGD-O1D	-3.16	117.71	123.85
26	b	304	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
26	n	610	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
26	b	305	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
26	A	825	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
29	A	845	WVN	C26-C29-C31	-3.13	114.12	123.20
26	k	604	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
29	s	407	WVN	C01-C02-C11	-3.13	109.23	112.83
26	j	607	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
26	B	805	CLA	CHB-C4A-NA	3.13	128.91	124.40
30	A	850	LMU	C2'-C3'-C4'	3.13	116.78	109.68
32	A	854	SQD	O7-S-C6	3.12	111.42	106.76
26	A	813	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
26	m	602	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
35	i	316	II0	C15-C03-C09	-3.11	104.94	110.52
35	h	312	II0	C30-C32-C34	-3.11	114.19	123.20
29	B	846	WVN	C40-C39-C36	-3.11	117.16	123.52
35	d	316	II0	C20-C14-C12	-3.09	108.73	114.42
35	m	614	II0	C12-C14-C10	-3.09	114.06	120.50
26	j	601	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
26	B	842	CLA	C3B-C4B-NB	-3.09	107.77	110.53
35	d	316	II0	C06-C04-C10	3.09	115.57	109.49
35	a	314	II0	C37-C35-C33	-3.08	113.38	118.09
29	i	315	WVN	C28-C30-C33	-3.08	114.27	123.20
25	A	801	CL0	C1A-CHA-C4D	3.08	124.12	118.98
26	B	823	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
35	k	615	II0	C06-C04-C10	3.08	115.55	109.49
35	m	616	II0	C37-C35-C33	-3.07	113.39	118.09
26	B	841	CLA	CHB-C4A-NA	3.07	128.83	124.40
29	B	850	WVN	C28-C30-C33	-3.07	114.31	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	612	CLA	C3B-C4B-NB	-3.07	107.79	110.53
26	B	829	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
26	B	827	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
26	m	604	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
26	n	604	CLA	CBA-CAA-C2A	3.06	122.89	113.79
26	i	304	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
26	B	802	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
35	k	619	II0	C30-C32-C34	-3.05	114.37	123.20
35	m	616	II0	C33-C35-C39	-3.05	114.22	119.01
35	n	616	II0	C19-C13-C11	-3.04	108.82	114.42
35	k	620	II0	C42-C41-C39	-3.04	117.30	123.52
26	B	810	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
35	j	614	II0	C30-C32-C34	-3.04	114.40	123.20
26	s	402	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
26	A	807	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
28	L	207	LHG	O8-C23-C24	3.03	121.08	111.83
26	A	839	CLA	C3B-C4B-NB	-3.03	107.83	110.53
26	B	833	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
35	m	615	II0	C31-C29-C25	-3.03	118.14	126.61
26	B	822	CLA	CHB-C4A-NA	3.03	128.77	124.40
35	a	312	II0	C19-C13-C11	-3.02	108.86	114.42
35	c	316	II0	C19-C13-C11	-3.02	108.86	114.42
26	i	301	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
35	d	315	II0	C12-C14-C10	-3.02	114.21	120.50
26	k	610	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
35	m	619	II0	C05-C03-C09	3.02	115.43	109.49
26	i	308	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
26	d	302	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
35	n	618	II0	C19-C13-C11	-3.01	108.89	114.42
35	d	301	II0	C06-C04-C10	3.01	115.42	109.49
26	m	609	CLA	C3B-C4B-NB	-3.01	107.84	110.53
26	a	302	CLA	CMB-C2B-C1B	-3.01	120.84	125.42
26	j	602	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
26	B	828	CLA	C3B-C4B-NB	-3.01	107.85	110.53
26	B	823	CLA	C3B-C4B-NB	-3.01	107.85	110.53
26	n	601	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
26	h	304	CLA	C3B-C4B-NB	-3.00	107.85	110.53
35	h	311	II0	C19-C13-C11	-3.00	108.90	114.42
26	A	816	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
35	c	313	II0	C19-C13-C11	-3.00	108.90	114.42
26	A	810	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
26	m	606	CLA	O2D-CGD-O1D	-3.00	118.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	832	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
26	l	311	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
32	A	854	SQD	O9-S-C6	3.00	111.23	106.76
35	j	614	II0	C42-C41-C39	-3.00	117.39	123.52
26	m	601	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
35	a	316	II0	C12-C14-C10	-2.99	114.28	120.50
26	h	307	CLA	CAA-C2A-C3A	-2.99	104.93	113.00
27	A	842	PQN	C2M-C2-C3	-2.98	119.54	124.45
26	B	804	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
35	c	316	II0	C06-C04-C10	2.98	115.36	109.49
26	c	301	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
34	b	319	LMG	O6-C1-O1	-2.98	103.01	110.04
35	m	616	II0	C06-C04-C10	2.98	115.36	109.49
35	l	302	II0	C11-C13-C09	-2.98	114.30	120.50
26	a	306	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
35	n	618	II0	C06-C04-C10	2.98	115.35	109.49
35	a	314	II0	C19-C13-C11	-2.97	108.95	114.42
26	d	308	CLA	C3B-C4B-NB	-2.97	107.88	110.53
35	j	614	II0	C06-C04-C10	2.97	115.35	109.49
26	b	304	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
29	F	203	WVN	C28-C30-C33	-2.97	114.60	123.20
26	R	201	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	A	848	WVN	C20-C13-C15	-2.97	114.72	121.56
26	A	818	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	B	849	WVN	C26-C29-C31	-2.97	114.60	123.20
35	h	311	II0	C30-C32-C34	-2.97	114.60	123.20
26	a	307	CLA	C3B-C4B-NB	-2.96	107.88	110.53
26	k	601	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
26	d	303	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
26	h	301	CLA	C3B-C4B-NB	-2.96	107.89	110.53
36	l	312	KC2	C3C-C2C-C1C	2.96	108.63	106.41
29	F	203	WVN	C26-C29-C31	-2.95	114.64	123.20
26	k	609	CLA	CHB-C4A-NA	2.95	128.66	124.40
26	k	606	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
26	A	856	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
26	A	806	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
26	A	818	CLA	CHB-C4A-NA	2.94	128.65	124.40
28	j	617	LHG	O8-C23-C24	2.94	120.81	111.83
26	a	308	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
26	c	308	CLA	C3B-C4B-NB	-2.94	107.91	110.53
26	A	824	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
29	B	849	WVN	C28-C30-C33	-2.94	114.69	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	306	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	j	608	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	a	301	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	d	312	KC2	C1D-CHD-C4C	-2.93	119.35	126.25
26	n	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
26	A	830	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
26	L	202	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
26	A	840	CLA	C3B-C4B-NB	-2.93	107.92	110.53
26	d	309	CLA	C3B-C4B-NB	-2.93	107.92	110.53
35	b	314	II0	C12-C14-C10	-2.92	114.41	120.50
35	i	319	II0	C11-C13-C09	-2.92	114.42	120.50
26	B	805	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
26	A	802	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
28	A	844	LHG	O8-C23-C24	2.92	120.01	111.15
26	c	307	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
26	h	302	CLA	C3B-C4B-NB	-2.92	107.93	110.53
26	n	604	CLA	CHB-C4A-NA	2.92	128.61	124.40
26	a	303	CLA	CHB-C4A-NA	2.91	128.60	124.40
26	s	403	CLA	C3B-C4B-NB	-2.91	107.93	110.53
26	l	309	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	j	603	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
26	A	851	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
35	j	615	II0	C19-C13-C11	-2.91	109.07	114.42
26	j	605	CLA	CHB-C4A-NA	2.91	128.60	124.40
26	B	807	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
26	B	833	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
35	i	312	II0	C31-C29-C25	-2.91	118.48	126.61
26	A	831	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
26	j	604	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
26	A	834	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
26	d	308	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
26	A	836	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	B	819	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	l	307	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	B	802	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
26	A	822	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	k	605	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	l	304	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	k	608	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
29	B	853	WVN	C21-C15-C14	-2.90	107.42	113.60
26	A	819	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
35	m	615	II0	C05-C03-C09	2.89	115.19	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	313	II0	C06-C04-C10	2.89	115.19	109.49
26	l	308	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	F	201	CLA	C3B-C4B-NB	-2.89	107.95	110.53
26	B	808	CLA	O2A-CGA-O1A	-2.89	116.40	123.63
35	d	301	II0	C19-C13-C11	-2.89	109.11	114.42
26	c	302	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	B	820	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
35	k	615	II0	C19-C13-C11	-2.89	109.11	114.42
35	i	313	II0	C11-C13-C09	-2.89	114.49	120.50
26	d	318	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
29	A	845	WVN	C02-C05-C09	-2.88	117.92	121.47
26	b	303	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
26	J	103	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	c	305	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
26	B	816	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	l	310	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	A	842	PQN	C11-C3-C2	-2.88	119.95	124.89
26	a	309	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
26	h	304	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
26	d	309	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
26	L	203	CLA	CHB-C4A-NA	2.88	128.55	124.40
26	R	201	CLA	CBA-CAA-C2A	2.88	122.35	113.79
26	l	309	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	l	310	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	c	308	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
26	m	605	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
26	B	815	CLA	C3B-C4B-NB	-2.87	107.96	110.53
26	K	101	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
26	B	835	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
29	A	847	WVN	C10-C06-C13	2.87	114.61	110.44
26	B	818	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	b	307	CLA	C3B-C4B-NB	-2.87	107.97	110.53
26	a	303	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	B	822	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	m	603	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	k	607	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
29	B	853	WVN	C01-C02-C11	-2.87	109.53	112.83
26	B	812	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
34	Q	301	LMG	O6-C1-O1	-2.87	103.27	110.04
26	A	815	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	B	836	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
36	c	310	KC2	CHD-C4C-NC	2.87	128.63	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	607	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	A	804	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	B	813	CLA	CHB-C4A-NA	2.86	128.53	124.40
26	L	204	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	n	609	CLA	C3B-C4B-NB	-2.86	107.98	110.53
26	a	305	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	d	313	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	A	835	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
26	A	813	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
26	A	841	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
26	l	311	CLA	C3B-C4B-NB	-2.85	107.98	110.53
26	b	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	m	612	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	J	103	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	b	305	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	a	306	CLA	C3B-C4B-NB	-2.85	107.98	110.53
29	l	316	WVN	C33-C34-C37	-2.85	114.53	119.01
26	n	606	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	k	603	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	k	602	CLA	CHB-C4A-NA	2.85	128.51	124.40
26	A	823	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	A	821	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	b	309	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	l	301	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	A	814	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	b	313	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	k	614	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	B	808	CLA	CHB-C4A-NA	2.85	128.51	124.40
28	b	302	LHG	O8-C23-C24	2.84	120.51	111.83
26	c	312	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
26	j	605	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	a	311	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
35	n	618	II0	C05-C03-C09	2.84	115.08	109.49
26	h	308	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	j	609	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
26	A	828	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
35	i	314	II0	C12-C14-C10	-2.83	114.61	120.50
26	c	303	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	m	604	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	l	307	CLA	CHB-C4A-NA	2.83	128.48	124.40
26	h	308	CLA	C3B-C4B-NB	-2.83	108.00	110.53
26	m	613	CLA	CHB-C4A-NA	2.83	128.48	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	613	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
26	A	837	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
26	d	304	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
26	A	812	CLA	CHB-C4A-NA	2.82	128.47	124.40
26	c	304	CLA	CHB-C4A-NA	2.82	128.47	124.40
26	j	602	CLA	C3B-C4B-NB	-2.82	108.01	110.53
26	d	302	CLA	C3B-C4B-NB	-2.82	108.01	110.53
26	b	311	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	c	306	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	j	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
35	J	104	II0	C12-C14-C10	-2.82	114.64	120.50
26	j	607	CLA	CMC-C2C-C3C	2.82	133.77	126.15
35	d	301	II0	C42-C41-C39	-2.82	117.76	123.52
26	k	605	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
26	m	608	CLA	C3B-C4B-NB	-2.82	108.02	110.53
35	m	616	II0	C12-C14-C10	-2.81	114.64	120.50
33	B	844	DGD	CDB-CCB-CBB	-2.81	100.14	114.37
29	L	201	WVN	C08-C01-C02	-2.81	105.28	109.55
26	A	820	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	A	808	CLA	CHB-C4A-NA	2.81	128.46	124.40
26	l	306	CLA	CHB-C4A-NA	2.81	128.46	124.40
26	B	839	CLA	C3B-C4B-NB	-2.81	108.02	110.53
26	B	829	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	A	809	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	a	310	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	B	848	WVN	C17-C06-C13	-2.81	105.84	110.24
26	h	303	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
26	m	601	CLA	C3B-C4B-NB	-2.81	108.03	110.53
26	k	602	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
26	n	603	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
32	A	854	SQD	C44-O6-C1	2.80	119.81	113.80
26	B	815	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
26	n	605	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
35	d	315	II0	C19-C13-C11	-2.80	109.27	114.42
28	J	105	LHG	O8-C23-C24	2.80	120.38	111.83
26	A	803	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
35	n	615	II0	C30-C32-C34	-2.80	115.08	123.20
26	l	306	CLA	CMB-C2B-C3B	2.80	133.14	126.55
26	B	828	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
26	a	307	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
35	i	319	II0	C30-C32-C34	-2.80	115.09	123.20
26	B	809	CLA	O2D-CGD-O1D	-2.80	118.40	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	n	611	KC2	CHD-C1D-ND	-2.80	119.85	124.05
35	a	312	II0	C12-C14-C10	-2.80	114.68	120.50
26	L	203	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
26	j	608	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	A	826	CLA	CHB-C4A-NA	2.80	128.44	124.40
26	A	827	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
26	A	823	CLA	CHB-C4A-NA	2.80	128.43	124.40
26	B	817	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	A	816	CLA	CHB-C4A-NA	2.79	128.43	124.40
26	d	307	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	F	202	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	b	306	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	j	610	CLA	C3B-C4B-NB	-2.79	108.04	110.53
36	d	311	KC2	CHD-C1D-ND	-2.79	119.86	124.05
26	B	813	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	B	801	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	A	803	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	j	604	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	h	307	CLA	CHB-C4A-NA	2.79	128.42	124.40
26	i	304	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	m	607	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
26	A	805	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
26	B	834	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
26	F	202	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
26	A	833	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
26	b	313	CLA	CHB-C4A-NA	2.78	128.41	124.40
29	B	847	WVN	C21-C15-C14	-2.78	107.67	113.60
37	j	616	IHT	C18-C22-C23	2.78	130.35	126.23
26	F	201	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	a	302	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
35	d	301	II0	C31-C29-C25	-2.78	118.84	126.61
26	B	819	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	B	826	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	j	601	CLA	C3B-C4B-NB	-2.78	108.05	110.53
28	m	618	LHG	O8-C23-C24	2.78	120.30	111.83
29	K	102	WVN	C21-C15-C14	-2.77	107.68	113.60
26	k	609	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
26	n	608	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	B	824	CLA	CHB-C4A-NA	2.77	128.40	124.40
26	d	310	CLA	CAA-C2A-C3A	-2.77	109.87	116.23
26	l	313	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
26	A	827	CLA	CHB-C4A-NA	2.77	128.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	818	CLA	CHB-C4A-NA	2.77	128.40	124.40
29	L	201	WVN	C21-C15-C14	-2.77	107.69	113.60
26	d	305	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
26	B	834	CLA	CHB-C4A-NA	2.77	128.39	124.40
26	n	609	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
26	A	831	CLA	CHB-C4A-NA	2.76	128.39	124.40
26	h	307	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
29	J	101	WVN	C21-C15-C14	-2.76	107.70	113.60
26	i	310	CLA	CHB-C4A-NA	2.76	128.39	124.40
26	A	811	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
35	i	314	II0	C06-C04-C10	2.76	114.93	109.49
26	b	312	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
26	A	817	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
26	c	311	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
28	c	320	LHG	O8-C23-C24	2.76	120.25	111.83
26	m	602	CLA	CBC-CAC-C3C	2.76	119.90	112.42
26	A	824	CLA	CHB-C4A-NA	2.76	128.38	124.40
26	A	824	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
26	B	834	CLA	C3B-C4B-NB	-2.76	108.07	110.53
26	B	824	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
26	A	839	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
26	B	825	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
26	m	605	CLA	C3B-C4B-NB	-2.76	108.07	110.53
26	j	609	CLA	C3B-C4B-NB	-2.75	108.07	110.53
28	l	318	LHG	O8-C23-C24	2.75	120.23	111.83
26	i	307	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
26	A	805	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
26	a	308	CLA	C3B-C4B-NB	-2.75	108.07	110.53
35	d	315	II0	C06-C04-C10	2.75	114.91	109.49
26	B	830	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
26	b	307	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
26	i	303	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
26	b	305	CLA	CHB-C4A-NA	2.75	128.37	124.40
35	i	316	II0	C12-C14-C10	-2.75	114.78	120.50
26	i	306	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	j	606	CLA	CHB-C4A-NA	2.75	128.36	124.40
26	j	605	CLA	C3B-C4B-NB	-2.75	108.08	110.53
26	s	408	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	i	310	CLA	C3B-C4B-NB	-2.75	108.08	110.53
35	c	316	II0	C11-C13-C09	-2.75	114.79	120.50
26	A	834	CLA	CMB-C2B-C1B	-2.75	121.24	125.42
26	A	851	CLA	O2D-CGD-O1D	-2.74	118.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	606	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	n	602	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
35	a	312	II0	C05-C03-C09	2.74	114.89	109.49
26	s	403	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	j	604	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	B	839	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	j	605	CLA	C2A-C1A-CHA	2.74	128.62	123.87
34	L	209	LMG	O6-C1-O1	-2.74	103.57	110.04
26	l	313	CLA	CHB-C4A-NA	2.74	128.35	124.40
26	m	613	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
26	B	832	CLA	CHB-C4A-NA	2.74	128.35	124.40
26	c	311	CLA	CHB-C4A-NA	2.74	128.35	124.40
34	F	205	LMG	O6-C1-O1	-2.74	103.58	110.04
26	A	836	CLA	CHB-C4A-NA	2.74	128.35	124.40
26	B	808	CLA	O2D-CGD-CBD	2.73	116.01	111.23
26	h	302	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
26	A	816	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
26	A	856	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	i	311	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
26	b	310	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	n	604	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
26	i	307	CLA	C3B-C4B-NB	-2.73	108.09	110.53
26	A	816	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
35	J	104	II0	C05-C03-C09	2.73	114.86	109.49
26	m	604	CLA	CHB-C4A-NA	2.73	128.33	124.40
26	k	614	CLA	CBC-CAC-C3C	2.73	119.81	112.42
26	B	836	CLA	C3B-C4B-NB	-2.73	108.10	110.53
26	B	806	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
26	s	406	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	B	842	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
34	c	318	LMG	O1-C7-C8	-2.72	104.19	110.82
26	L	202	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	k	608	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	B	816	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
26	m	606	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	A	813	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	n	605	CLA	CHB-C4A-NA	2.72	128.32	124.40
26	s	403	CLA	O2D-CGD-CBD	2.72	115.98	111.23
35	c	316	II0	C05-C03-C09	2.72	114.84	109.49
35	d	315	II0	C11-C13-C09	-2.72	114.84	120.50
26	m	610	CLA	CHB-C4A-NA	2.72	128.32	124.40
26	A	802	CLA	C3B-C4B-NB	-2.72	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	814	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
26	Q	302	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
26	B	821	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	A	841	CLA	CHB-C4A-NA	2.71	128.31	124.40
26	B	829	CLA	CMB-C2B-C3B	2.71	132.93	126.55
26	A	806	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	A	838	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
26	d	318	CLA	CHB-C4A-NA	2.71	128.31	124.40
26	A	829	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
26	B	838	CLA	O2D-CGD-CBD	2.71	115.96	111.23
26	A	825	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	n	610	CLA	CHB-C4A-NA	2.71	128.30	124.40
26	B	819	CLA	CMB-C2B-C1B	-2.70	121.30	125.42
36	s	401	KC2	CAA-CBA-CGA	-2.70	113.30	127.05
26	c	307	CLA	CMB-C2B-C1B	-2.70	121.30	125.42
26	l	308	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	h	306	CLA	CHB-C4A-NA	2.70	128.30	124.40
26	B	812	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	c	317	LHG	O8-C23-C24	2.70	120.07	111.83
26	b	313	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	n	602	CLA	CHB-C4A-NA	2.70	128.29	124.40
35	k	620	II0	C06-C04-C10	2.70	114.80	109.49
26	B	811	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
33	B	844	DGD	O5D-C6D-C5D	-2.70	103.34	109.42
26	h	305	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
26	b	303	CLA	CHB-C4A-NA	2.70	128.29	124.40
26	B	830	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	a	301	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	A	834	CLA	CHB-C4A-NA	2.69	128.29	124.40
26	n	608	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
26	k	605	CLA	CHB-C4A-NA	2.69	128.28	124.40
26	l	305	CLA	O2D-CGD-CBD	2.69	115.93	111.23
26	i	301	CLA	CHB-C4A-NA	2.69	128.28	124.40
26	L	206	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	i	303	CLA	CHB-C4A-NA	2.69	128.28	124.40
35	n	618	II0	C12-C14-C10	-2.69	114.90	120.50
26	Q	302	CLA	CHB-C4A-NA	2.69	128.28	124.40
26	A	826	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
26	j	612	CLA	CHB-C4A-NA	2.69	128.28	124.40
26	A	833	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	B	806	CLA	C3B-C4B-NB	-2.68	108.13	110.53
26	a	304	CLA	CHB-C4A-NA	2.68	128.27	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	308	CLA	CHB-C4A-NA	2.68	128.27	124.40
34	c	318	LMG	O1-C1-C2	-2.68	104.20	108.27
26	i	307	CLA	CHB-C4A-NA	2.68	128.26	124.40
36	i	309	KC2	CHD-C1D-ND	-2.68	120.03	124.05
29	s	405	WVN	C20-C13-C15	-2.68	115.39	121.56
26	A	820	CLA	CHB-C4A-NA	2.67	128.26	124.40
26	h	306	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
26	j	602	CLA	CMB-C2B-C3B	2.67	132.84	126.55
26	i	308	CLA	C3B-C4B-NB	-2.67	108.14	110.53
35	m	619	II0	C30-C32-C34	-2.67	115.46	123.20
26	A	835	CLA	CHB-C4A-NA	2.67	128.25	124.40
26	l	304	CLA	C3B-C4B-NB	-2.67	108.15	110.53
26	J	103	CLA	CHB-C4A-NA	2.67	128.25	124.40
29	i	315	WVN	C17-C06-C13	-2.67	106.06	110.24
26	m	609	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
26	m	612	CLA	CHB-C4A-NA	2.67	128.25	124.40
26	d	304	CLA	C3B-C4B-NB	-2.67	108.15	110.53
35	n	618	II0	C30-C32-C34	-2.67	115.47	123.20
26	j	601	CLA	CHB-C4A-NA	2.67	128.25	124.40
26	B	821	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
26	a	309	CLA	CHB-C4A-NA	2.67	128.25	124.40
26	j	610	CLA	CHB-C4A-NA	2.66	128.25	124.40
26	Q	302	CLA	C3B-C4B-NB	-2.66	108.15	110.53
26	B	831	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
26	d	304	CLA	CHB-C4A-NA	2.66	128.25	124.40
26	A	807	CLA	C3B-C4B-NB	-2.66	108.15	110.53
26	k	601	CLA	C3B-C4B-NB	-2.66	108.15	110.53
26	n	610	CLA	C3B-C4B-NB	-2.66	108.15	110.53
26	l	306	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
26	h	305	CLA	CHB-C4A-NA	2.66	128.24	124.40
26	l	311	CLA	CHB-C4A-NA	2.66	128.24	124.40
26	a	304	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	B	841	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	h	304	CLA	CHB-C4A-NA	2.66	128.24	124.40
26	m	612	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	A	852	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	n	605	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	F	202	CLA	CHB-C4A-NA	2.66	128.24	124.40
26	n	604	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	k	601	CLA	CHB-C4A-NA	2.66	128.23	124.40
26	b	308	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
26	n	607	CLA	CMB-C2B-C1B	-2.66	121.37	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	835	CLA	C3B-C4B-NB	-2.65	108.16	110.53
26	L	206	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
28	J	105	LHG	C11-C10-C9	-2.65	100.95	114.37
26	s	408	CLA	CHB-C4A-NA	2.65	128.23	124.40
26	b	309	CLA	CHB-C4A-NA	2.65	128.23	124.40
26	l	305	CLA	CMB-C2B-C3B	2.65	132.79	126.55
28	A	855	LHG	O8-C23-C24	2.65	119.92	111.83
26	i	305	CLA	CHB-C4A-NA	2.65	128.23	124.40
26	b	304	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	h	306	CLA	C3B-C4B-NB	-2.65	108.16	110.53
35	l	315	II0	C12-C14-C10	-2.65	114.98	120.50
26	l	301	CLA	CHB-C4A-NA	2.65	128.22	124.40
29	A	857	WVN	C21-C15-C14	-2.65	107.95	113.60
26	h	308	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	h	313	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
26	A	812	CLA	C3B-C4B-NB	-2.65	108.17	110.53
26	A	819	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	m	602	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	k	610	CLA	CHB-C4A-NA	2.65	128.22	124.40
35	k	619	II0	C05-C03-C09	2.65	114.70	109.49
35	a	313	II0	C19-C13-C11	-2.64	109.56	114.42
26	m	610	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	A	822	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	m	613	CLA	C3B-C4B-NB	-2.64	108.17	110.53
29	J	102	WVN	C28-C30-C33	-2.64	115.54	123.20
34	n	620	LMG	O6-C1-O1	-2.64	103.80	110.04
26	B	807	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	d	305	CLA	CHB-C4A-NA	2.64	128.21	124.40
35	d	317	II0	C19-C13-C11	-2.64	109.57	114.42
29	l	316	WVN	C12-C14-C15	-2.64	109.36	114.06
26	s	406	CLA	O2D-CGD-CBD	2.64	115.84	111.23
26	d	302	CLA	CHB-C4A-NA	2.64	128.20	124.40
26	n	613	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
26	d	305	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	s	409	LHG	O8-C23-C24	2.63	119.86	111.83
26	j	609	CLA	CHB-C4A-NA	2.63	128.20	124.40
26	B	824	CLA	C3B-C4B-NB	-2.63	108.18	110.53
26	L	204	CLA	C3B-C4B-NB	-2.63	108.18	110.53
29	A	847	WVN	C26-C29-C31	-2.63	115.58	123.20
26	A	830	CLA	C3B-C4B-NB	-2.63	108.19	110.53
26	s	402	CLA	CAA-CBA-CGA	-2.63	105.75	113.21
26	A	809	CLA	CHB-C4A-NA	2.63	128.19	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	802	CLA	O2A-CGA-O1A	-2.62	117.06	123.63
26	A	834	CLA	C3B-C4B-NB	-2.62	108.19	110.53
26	b	308	CLA	CHB-C4A-NA	2.62	128.19	124.40
35	a	316	II0	C15-C03-C09	-2.62	105.82	110.52
26	A	851	CLA	CMB-C2B-C3B	2.62	132.72	126.55
26	a	311	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	i	306	CLA	C3B-C4B-NB	-2.62	108.19	110.53
26	R	201	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	c	308	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	k	606	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	B	839	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	B	805	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
36	c	310	KC2	CHD-C4C-C3C	-2.62	117.10	125.91
26	A	852	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	m	608	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	m	608	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
26	l	304	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	B	838	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	b	311	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	B	816	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	B	842	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
26	B	802	CLA	CMB-C2B-C3B	2.61	132.69	126.55
26	a	304	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	B	827	CLA	CMB-C2B-C3B	2.61	132.68	126.55
26	A	807	CLA	CHB-C4A-NA	2.61	128.16	124.40
26	A	802	CLA	CMB-C2B-C3B	2.61	132.68	126.55
26	B	806	CLA	CHB-C4A-NA	2.61	128.16	124.40
26	l	310	CLA	CHB-C4A-NA	2.61	128.16	124.40
26	s	408	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	d	303	CLA	CHB-C4A-NA	2.60	128.16	124.40
33	B	844	DGD	C3D-C4D-C5D	-2.60	105.51	110.23
26	h	301	CLA	CHB-C4A-NA	2.60	128.16	124.40
26	A	841	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
26	A	852	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	b	305	CLA	CMB-C2B-C3B	2.60	132.67	126.55
25	A	801	CL0	C4D-CHA-CBD	-2.60	106.34	108.97
26	B	831	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	i	308	CLA	CHB-C4A-NA	2.60	128.15	124.40
26	b	304	CLA	CMB-C2B-C3B	2.60	132.66	126.55
26	A	820	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	b	309	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	L	206	CLA	CHB-C4A-NA	2.60	128.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	812	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
26	A	834	CLA	CMB-C2B-C3B	2.59	132.65	126.55
26	n	601	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	B	837	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
28	L	208	LHG	O8-C23-C24	2.59	119.73	111.83
26	B	822	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	A	821	CLA	CHB-C4A-NA	2.59	128.14	124.40
26	B	833	CLA	CMB-C2B-C3B	2.59	132.64	126.55
26	B	840	CLA	C3B-C4B-NB	-2.59	108.22	110.53
33	j	618	DGD	CDB-CCB-CBB	-2.59	101.30	114.37
26	A	826	CLA	C3B-C4B-NB	-2.58	108.22	110.53
26	b	308	CLA	C3B-C4B-NB	-2.58	108.22	110.53
26	i	301	CLA	C3B-C4B-NB	-2.58	108.22	110.53
26	j	606	CLA	C3B-C4B-NB	-2.58	108.23	110.53
29	A	848	WVN	C10-C06-C13	2.58	114.19	110.44
26	m	609	CLA	CHB-C4A-NA	2.58	128.12	124.40
26	A	804	CLA	CHB-C4A-NA	2.58	128.12	124.40
26	A	840	CLA	CHB-C4A-NA	2.58	128.12	124.40
35	k	619	II0	C42-C41-C39	-2.58	118.25	123.52
26	A	856	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	h	305	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	B	831	CLA	CHB-C4A-NA	2.58	128.12	124.40
26	d	318	CLA	C3B-C4B-NB	-2.58	108.23	110.53
35	a	313	II0	C05-C03-C09	2.57	114.56	109.49
26	c	303	CLA	CHB-C4A-NA	2.57	128.12	124.40
26	A	841	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
26	d	313	CLA	C2A-C1A-CHA	2.57	128.33	123.87
26	b	303	CLA	C3B-C4B-NB	-2.57	108.23	110.53
26	d	310	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
26	B	803	CLA	C3B-C4B-NB	-2.57	108.23	110.53
28	c	320	LHG	C11-C10-C9	-2.57	101.37	114.37
26	m	604	CLA	CMB-C2B-C3B	2.57	132.60	126.55
26	j	613	CLA	CHB-C4A-NA	2.57	128.11	124.40
29	A	847	WVN	C21-C15-C14	-2.57	108.12	113.60
26	a	301	CLA	CHB-C4A-NA	2.56	128.10	124.40
29	K	102	WVN	C40-C39-C36	-2.56	118.27	123.52
26	B	840	CLA	CHB-C4A-NA	2.56	128.10	124.40
35	b	314	II0	C42-C41-C39	-2.56	118.28	123.52
26	n	603	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	j	607	CLA	C2D-C1D-ND	-2.56	107.59	110.13
26	B	838	CLA	C3B-C4B-NB	-2.56	108.25	110.53
26	A	822	CLA	C3B-C4B-NB	-2.56	108.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	822	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
26	i	311	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	j	603	CLA	CHB-C4A-NA	2.55	128.09	124.40
35	m	615	II0	C42-C41-C39	-2.55	118.29	123.52
26	B	808	CLA	C1-C2-C3	-2.55	122.01	126.20
26	A	819	CLA	C3B-C4B-NB	-2.55	108.25	110.53
26	A	832	CLA	CHB-C4A-NA	2.55	128.09	124.40
35	m	619	II0	C42-C41-C39	-2.55	118.30	123.52
26	A	811	CLA	C3B-C4B-NB	-2.55	108.25	110.53
26	h	307	CLA	C3B-C4B-NB	-2.55	108.25	110.53
26	b	312	CLA	CHB-C4A-NA	2.55	128.08	124.40
26	l	309	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
26	m	606	CLA	CHB-C4A-NA	2.55	128.08	124.40
28	L	208	LHG	C11-C10-C9	-2.55	101.47	114.37
26	L	202	CLA	CHB-C4A-NA	2.55	128.08	124.40
29	l	316	WVN	C21-C15-C14	-2.55	108.17	113.60
26	A	841	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
26	B	811	CLA	C3B-C4B-NB	-2.55	108.26	110.53
26	a	302	CLA	CMB-C2B-C3B	2.54	132.53	126.55
26	i	304	CLA	CHB-C4A-NA	2.54	128.07	124.40
26	n	601	CLA	CHB-C4A-NA	2.54	128.07	124.40
36	j	611	KC2	CHD-C1D-ND	-2.54	120.23	124.05
26	A	838	CLA	CHB-C4A-NA	2.54	128.07	124.40
29	I	101	WVN	C06-C13-C20	-2.54	108.76	115.65
28	b	302	LHG	C11-C10-C9	-2.54	101.52	114.37
36	n	611	KC2	C3C-C2C-C1C	2.54	108.32	106.41
26	a	310	CLA	CHB-C4A-NA	2.54	128.06	124.40
26	i	302	CLA	CHB-C4A-NA	2.54	128.06	124.40
26	m	605	CLA	CHB-C4A-NA	2.54	128.06	124.40
26	k	602	CLA	C3B-C4B-NB	-2.53	108.27	110.53
26	c	301	CLA	CHB-C4A-NA	2.53	128.06	124.40
26	m	603	CLA	CHB-C4A-NA	2.53	128.06	124.40
26	B	801	CLA	C3B-C4B-NB	-2.53	108.27	110.53
28	A	843	LHG	O8-C23-C24	2.53	119.56	111.83
35	i	312	II0	C42-C41-C39	-2.53	118.34	123.52
26	A	805	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	a	302	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	B	805	CLA	CMB-C2B-C3B	2.53	132.50	126.55
26	K	101	CLA	CHB-C4A-NA	2.53	128.05	124.40
28	n	619	LHG	O8-C23-C24	2.53	119.55	111.83
35	a	314	II0	C31-C29-C25	-2.53	119.54	126.61
26	a	305	CLA	C3B-C4B-NB	-2.53	108.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	810	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	b	306	CLA	CHB-C4A-NA	2.53	128.04	124.40
26	k	610	CLA	C3B-C4B-NB	-2.52	108.28	110.53
26	b	311	CLA	C3B-C4B-NB	-2.52	108.28	110.53
26	A	806	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	j	604	CLA	CMB-C2B-C3B	2.52	132.48	126.55
28	B	851	LHG	O8-C23-C24	2.52	119.52	111.83
27	B	843	PQN	C11-C3-C2	-2.52	120.57	124.89
26	b	305	CLA	C3B-C4B-NB	-2.52	108.28	110.53
28	A	844	LHG	C11-C10-C9	-2.52	101.63	114.37
36	s	401	KC2	CBA-CAA-C2A	-2.52	115.34	125.45
26	c	302	CLA	C1-C2-C3	-2.52	122.07	126.20
26	B	833	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	k	610	CLA	C2A-C1A-CHA	2.51	128.23	123.87
26	B	804	CLA	CHD-C4C-C3C	2.51	128.44	124.77
26	s	406	CLA	CHB-C4A-NA	2.51	128.03	124.40
26	d	303	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
26	h	302	CLA	CHB-C4A-NA	2.51	128.03	124.40
28	A	843	LHG	C11-C10-C9	-2.51	101.68	114.37
28	i	317	LHG	C11-C10-C9	-2.51	101.68	114.37
35	l	315	II0	C19-C13-C11	-2.51	109.81	114.42
29	A	846	WVN	C10-C06-C13	2.51	114.08	110.44
26	j	603	CLA	CMB-C2B-C3B	2.51	132.45	126.55
26	h	305	CLA	CMB-C2B-C3B	2.51	132.44	126.55
35	d	316	II0	C11-C13-C09	-2.50	115.29	120.50
26	a	311	CLA	C3B-C4B-NB	-2.50	108.29	110.53
26	A	833	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	B	814	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	A	803	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
26	B	804	CLA	CHB-C4A-NA	2.50	128.01	124.40
35	l	315	II0	C31-C29-C25	-2.50	119.62	126.61
26	l	305	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
36	d	312	KC2	CHC-C4B-C3B	2.50	129.42	125.21
26	c	307	CLA	C3B-C4B-NB	-2.50	108.30	110.53
29	M	101	WVN	C21-C15-C14	-2.50	108.27	113.60
26	A	815	CLA	CHB-C4A-NA	2.50	128.00	124.40
28	j	617	LHG	C11-C10-C9	-2.49	101.76	114.37
29	B	850	WVN	C02-C05-C09	-2.49	118.40	121.47
26	B	822	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
26	B	836	CLA	CHB-C4A-NA	2.49	128.00	124.40
26	c	309	CLA	CAC-C3C-C4C	2.49	128.03	124.79
28	b	318	LHG	O8-C23-C24	2.49	119.43	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	814	CLA	CHB-C4A-NA	2.49	127.99	124.40
26	A	839	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	c	317	LHG	C11-C10-C9	-2.49	101.79	114.37
28	l	318	LHG	C11-C10-C9	-2.49	101.79	114.37
35	h	311	II0	C06-C04-C10	2.49	114.39	109.49
35	k	616	II0	C31-C29-C25	-2.49	119.66	126.61
26	j	608	CLA	CHB-C4A-NA	2.49	127.99	124.40
29	F	203	WVN	C39-C40-C37	-2.49	118.43	123.52
26	n	602	CLA	CMB-C2B-C3B	2.48	132.39	126.55
26	A	810	CLA	C3B-C4B-NB	-2.48	108.31	110.53
28	m	618	LHG	C11-C10-C9	-2.48	101.83	114.37
26	a	305	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	l	305	CLA	CHB-C4A-NA	2.48	127.98	124.40
36	s	401	KC2	CAA-C2A-C1A	-2.48	113.78	124.64
26	l	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	A	840	CLA	O1D-CGD-CBD	2.48	129.40	124.52
26	B	842	CLA	CHB-C4A-NA	2.47	127.97	124.40
29	B	849	WVN	C21-C15-C14	-2.47	108.32	113.60
35	i	314	II0	C11-C13-C09	-2.47	115.35	120.50
28	i	317	LHG	O8-C23-C24	2.47	119.37	111.83
26	A	805	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	A	849	LHG	C20-C19-C18	-2.47	101.89	114.37
35	k	619	II0	C06-C04-C10	2.47	114.35	109.49
26	d	309	CLA	CMA-C3A-C2A	-2.47	110.57	116.23
26	A	808	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
26	m	601	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	j	602	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	c	310	KC2	CMB-C2B-C1B	2.46	129.06	124.73
35	a	313	II0	C42-C41-C39	-2.46	118.48	123.52
25	A	801	CL0	C4C-CHD-C1D	2.46	124.87	116.07
26	B	836	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
26	A	814	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
36	s	401	KC2	CHD-C4C-C3C	-2.46	117.63	125.91
26	n	607	CLA	CMB-C2B-C3B	2.46	132.33	126.55
26	a	307	CLA	CHB-C4A-NA	2.46	127.94	124.40
30	A	850	LMU	C1'-C2'-C3'	2.45	115.17	110.01
26	h	303	CLA	C3B-C4B-NB	-2.45	108.34	110.53
29	M	101	WVN	C39-C40-C37	-2.45	118.50	123.52
28	A	849	LHG	C11-C10-C9	-2.45	101.98	114.37
26	b	310	CLA	C3B-C4B-NB	-2.45	108.34	110.53
26	k	606	CLA	C3B-C4B-NB	-2.45	108.34	110.53
28	L	207	LHG	C11-C10-C9	-2.45	101.98	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	811	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	c	301	CLA	C3B-C4B-NB	-2.45	108.34	110.53
35	m	615	II0	C11-C13-C09	-2.45	115.41	120.50
26	A	839	CLA	CMB-C2B-C1B	-2.45	121.70	125.42
26	d	313	CLA	CHB-C4A-NA	2.44	127.93	124.40
26	l	313	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	A	825	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
34	F	206	LMG	O6-C1-O1	-2.44	104.27	110.04
26	c	311	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	A	818	CLA	C1-C2-C3	-2.44	122.20	126.20
26	A	809	CLA	C3B-C4B-NB	-2.44	108.36	110.53
26	h	303	CLA	C1-C2-C3	-2.44	122.82	126.76
25	A	801	CL0	C3C-C4C-NC	-2.43	108.70	114.65
26	F	201	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	d	309	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	B	805	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
27	B	843	PQN	C2M-C2-C3	-2.43	120.45	124.45
34	c	318	LMG	C40-C39-C38	-2.43	102.08	114.37
26	c	304	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	A	838	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	B	813	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	d	306	CLA	CHB-C4A-NA	2.43	127.90	124.40
26	c	312	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	A	811	CLA	CHB-C4A-NA	2.42	127.90	124.40
29	A	846	WVN	C01-C02-C11	-2.42	110.04	112.83
26	B	815	CLA	CHB-C4A-NA	2.42	127.89	124.40
26	K	101	CLA	C2A-C1A-CHA	2.42	128.06	123.87
26	n	609	CLA	CHB-C4A-NA	2.42	127.89	124.40
26	a	306	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	A	801	CL0	CHA-C1A-C2A	-2.42	127.64	133.31
29	R	200	WVN	C10-C06-C13	2.41	113.95	110.44
26	A	817	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	s	402	CLA	CHB-C4A-NA	2.41	127.88	124.40
35	l	315	II0	C06-C04-C10	2.41	114.25	109.49
26	A	821	CLA	C3B-C4B-NB	-2.41	108.38	110.53
26	B	810	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	A	855	LHG	C11-C10-C9	-2.41	102.17	114.37
26	k	607	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
28	b	318	LHG	C20-C19-C18	-2.41	102.18	114.37
26	B	822	CLA	C2A-C1A-CHA	2.41	128.05	123.87
26	A	803	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	A	828	CLA	CHB-C4A-NA	2.41	127.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	312	II0	C11-C13-C09	-2.41	115.49	120.50
34	F	205	LMG	C40-C39-C38	-2.40	102.22	114.37
26	c	305	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	b	318	LHG	C11-C10-C9	-2.40	102.24	114.37
29	A	845	WVN	C10-C06-C13	2.40	113.92	110.44
26	B	830	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
28	L	207	LHG	C20-C19-C18	-2.40	102.25	114.37
26	a	303	CLA	C3B-C4B-NB	-2.40	108.39	110.53
35	n	618	II0	C11-C13-C09	-2.40	115.51	120.50
35	a	314	II0	C42-C41-C39	-2.40	118.62	123.52
26	A	837	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	l	309	CLA	CHB-C4A-NA	2.39	127.86	124.40
26	b	313	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
33	j	618	DGD	O2D-C2D-C1D	-2.39	104.37	110.08
35	b	314	II0	C06-C04-C10	2.39	114.20	109.49
35	m	616	II0	C05-C03-C09	2.39	114.20	109.49
26	B	820	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	h	303	CLA	CHB-C4A-NA	2.39	127.85	124.40
34	Q	301	LMG	O7-C10-O9	-2.39	118.12	123.70
26	h	313	CLA	CHB-C4A-NA	2.39	127.84	124.40
26	l	307	CLA	C3B-C4B-NB	-2.39	108.40	110.53
26	B	825	CLA	CHB-C4A-NA	2.39	127.84	124.40
35	n	615	II0	C12-C14-C10	-2.39	115.53	120.50
26	A	823	CLA	C3B-C4B-NB	-2.38	108.40	110.53
32	A	854	SQD	O48-C23-C24	2.38	119.11	111.83
26	A	821	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
26	h	313	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
26	d	306	CLA	O2D-CGD-CBD	2.38	115.39	111.23
36	c	310	KC2	CBA-CAA-C2A	-2.38	115.90	125.45
26	a	302	CLA	C3B-C4B-NB	-2.38	108.41	110.53
26	k	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
26	i	305	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
28	B	851	LHG	C11-C10-C9	-2.37	102.36	114.37
29	A	857	WVN	C07-C01-C02	2.37	113.14	109.55
36	m	611	KC2	C2A-C3A-C4A	2.37	108.19	106.41
29	s	407	WVN	C21-C15-C14	-2.37	108.54	113.60
26	c	308	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	L	204	CLA	CHB-C4A-NA	2.37	127.82	124.40
29	A	847	WVN	C01-C02-C11	-2.37	110.10	112.83
26	B	826	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	c	302	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	c	307	CLA	CMB-C2B-C3B	2.37	132.12	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	833	CLA	C2A-C1A-CHA	2.37	127.98	123.87
26	A	827	CLA	C3B-C4B-NB	-2.37	108.42	110.53
35	j	615	II0	C12-C14-C10	-2.37	115.57	120.50
32	A	854	SQD	O6-C1-C2	2.37	111.87	108.27
26	A	825	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	B	830	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	B	801	CLA	CHB-C4A-NA	2.37	127.81	124.40
26	d	308	CLA	CHB-C4A-NA	2.37	127.81	124.40
28	c	320	LHG	C20-C19-C18	-2.36	102.41	114.37
26	n	603	CLA	C2A-C1A-CHA	2.36	127.97	123.87
26	n	602	CLA	C3B-C4B-NB	-2.36	108.42	110.53
36	n	612	KC2	CHD-C1D-ND	-2.36	120.50	124.05
26	d	310	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	s	406	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
26	A	816	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
29	s	405	WVN	C10-C06-C13	2.36	113.87	110.44
26	R	201	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
26	A	818	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
26	A	814	CLA	C3B-C4B-NB	-2.36	108.42	110.53
26	m	603	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	M	101	WVN	C10-C06-C13	2.36	113.86	110.44
34	n	620	LMG	C38-C37-C36	-2.36	102.45	114.37
26	c	312	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	b	313	CLA	C2A-C1A-CHA	2.36	127.95	123.87
26	B	812	CLA	C3B-C4B-NB	-2.35	108.43	110.53
26	B	809	CLA	CHB-C4A-NA	2.35	127.80	124.40
33	B	844	DGD	CFB-CEB-CDB	-2.35	102.47	114.37
34	F	205	LMG	O1-C7-C8	-2.35	105.09	110.82
35	i	316	II0	C06-C04-C10	2.35	114.12	109.49
26	B	826	CLA	CHB-C4A-NA	2.35	127.80	124.40
26	c	303	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	n	619	LHG	C11-C10-C9	-2.35	102.49	114.37
36	k	611	KC2	C2A-C3A-C4A	2.35	108.17	106.41
36	n	612	KC2	C3C-C2C-C1C	2.35	108.17	106.41
28	B	851	LHG	C20-C19-C18	-2.35	102.50	114.37
26	k	614	CLA	CHB-C4A-NA	2.35	127.79	124.40
26	B	842	CLA	CMB-C2B-C3B	2.34	132.06	126.55
26	B	814	CLA	C3B-C4B-NB	-2.34	108.44	110.53
26	A	805	CLA	CMB-C2B-C3B	2.34	132.06	126.55
26	B	823	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	k	604	CLA	CHC-C4B-NB	2.34	127.56	124.05
26	A	816	CLA	CMB-C2B-C3B	2.34	132.05	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	301	II0	C12-C14-C10	-2.34	115.64	120.50
26	B	803	CLA	CHC-C4B-NB	2.34	127.55	124.05
26	a	310	CLA	C3B-C4B-NB	-2.34	108.44	110.53
26	i	306	CLA	CHB-C4A-NA	2.34	127.77	124.40
26	n	613	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
26	h	301	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
29	A	846	WVN	C21-C15-C14	-2.33	108.62	113.60
33	j	618	DGD	O6E-C5E-C4E	2.33	113.90	109.70
35	i	313	II0	C05-C03-C09	2.33	114.08	109.49
26	A	831	CLA	C3B-C4B-NB	-2.33	108.45	110.53
34	c	318	LMG	O6-C1-O1	-2.33	104.54	110.04
26	c	303	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
26	B	817	CLA	CHB-C4A-NA	2.33	127.76	124.40
26	B	810	CLA	CHB-C4A-NA	2.33	127.76	124.40
26	B	834	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
26	b	304	CLA	O2D-CGD-CBD	2.32	115.29	111.23
26	m	607	CLA	CHB-C4A-NA	2.32	127.75	124.40
35	b	314	II0	C05-C03-C09	2.32	114.07	109.49
35	k	615	II0	C17-C04-C10	-2.32	106.36	110.52
28	b	302	LHG	C20-C19-C18	-2.32	102.63	114.37
26	l	309	CLA	O1D-CGD-CBD	2.32	129.10	124.52
26	B	820	CLA	O2D-CGD-CBD	2.32	115.29	111.23
26	i	303	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
26	A	815	CLA	C3B-C4B-NB	-2.32	108.46	110.53
26	A	841	CLA	C3B-C4B-NB	-2.32	108.46	110.53
26	B	804	CLA	C3B-C4B-NB	-2.32	108.46	110.53
34	c	318	LMG	C38-C37-C36	-2.32	102.66	114.37
26	n	608	CLA	C2A-C1A-CHA	2.32	127.89	123.87
36	s	401	KC2	CMC-C2C-C1C	2.32	128.65	125.03
35	a	313	II0	C11-C13-C09	-2.31	115.68	120.50
26	B	841	CLA	C2A-C1A-CHA	2.31	127.88	123.87
26	k	607	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
36	d	312	KC2	C1A-NA-C4A	2.31	107.73	106.68
26	l	301	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	B	825	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
26	A	832	CLA	C3B-C4B-NB	-2.31	108.47	110.53
35	c	313	II0	C05-C03-C09	2.31	114.04	109.49
35	i	312	II0	C05-C03-C09	2.31	114.03	109.49
26	B	828	CLA	CHB-C4A-NA	2.31	127.73	124.40
29	h	309	WVN	C06-C13-C20	-2.30	109.40	115.65
26	A	830	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	B	853	WVN	C10-C06-C13	2.30	113.78	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	819	CLA	CMB-C2B-C3B	2.30	131.96	126.55
29	h	309	WVN	C07-C01-C02	2.30	113.03	109.55
26	B	818	CLA	CHB-C1B-NB	2.30	127.50	124.05
26	A	814	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
29	K	102	WVN	C06-C13-C20	-2.30	109.42	115.65
26	L	203	CLA	C3B-C4B-NB	-2.30	108.48	110.53
26	j	607	CLA	CBC-CAC-C3C	2.30	118.64	112.42
37	j	616	IHT	C27-C30-C32	2.29	129.85	123.20
35	m	619	II0	C12-C14-C10	-2.29	115.72	120.50
26	k	607	CLA	CHB-C4A-NA	2.29	127.71	124.40
35	j	615	II0	C05-C03-C09	2.29	114.01	109.49
26	A	825	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
35	j	614	II0	C12-C14-C10	-2.29	115.73	120.50
26	s	402	CLA	C1-C2-C3	-2.29	122.45	126.20
26	A	808	CLA	C2A-C1A-CHA	2.29	127.84	123.87
26	k	604	CLA	CHB-C4A-NA	2.29	127.70	124.40
26	A	815	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
26	A	813	CLA	CHB-C4A-NA	2.29	127.70	124.40
26	m	612	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
26	B	837	CLA	CHB-C4A-NA	2.28	127.70	124.40
29	l	303	WVN	C06-C13-C20	-2.28	109.46	115.65
25	A	801	CL0	C4D-ND-C1D	2.28	106.95	105.22
26	B	818	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
26	i	301	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
26	i	305	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
35	n	616	II0	C17-C04-C10	-2.28	106.43	110.52
34	c	319	LMG	O6-C1-O1	-2.28	104.66	110.04
26	A	803	CLA	CMB-C2B-C3B	2.28	131.91	126.55
26	d	303	CLA	CMB-C2B-C3B	2.28	131.91	126.55
26	k	608	CLA	CHB-C4A-NA	2.28	127.69	124.40
26	A	804	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
26	n	604	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
26	c	306	CLA	C3B-C4B-NB	-2.28	108.50	110.53
26	a	303	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
26	d	307	CLA	CHB-C4A-NA	2.28	127.68	124.40
26	B	817	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
26	L	202	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
26	b	312	CLA	C3B-C4B-NB	-2.27	108.50	110.53
26	A	802	CLA	CHB-C4A-NA	2.27	127.67	124.40
26	B	808	CLA	C3B-C4B-NB	-2.27	108.51	110.53
26	B	815	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
36	c	310	KC2	O2D-CGD-O1D	-2.27	119.44	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	j	618	DGD	CFB-CEB-CDB	-2.27	102.91	114.37
26	l	310	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
26	A	824	CLA	C2A-C1A-CHA	2.27	127.80	123.87
26	c	309	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
28	A	843	LHG	C27-C26-C25	-2.26	102.93	114.37
26	B	810	CLA	O2D-CGD-CBD	2.26	115.19	111.23
26	k	603	CLA	CHB-C1B-C2B	-2.26	120.86	127.43
29	s	407	WVN	C26-C29-C31	-2.26	116.66	123.20
28	b	318	LHG	C27-C26-C25	-2.26	102.96	114.37
35	h	312	II0	C42-C41-C39	-2.25	118.91	123.52
26	b	307	CLA	CHB-C4A-NA	2.25	127.65	124.40
32	A	854	SQD	C3-C4-C5	2.25	114.32	110.23
26	k	607	CLA	CMB-C2B-C3B	2.25	131.85	126.55
26	n	603	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
26	B	821	CLA	CHB-C4A-NA	2.25	127.65	124.40
26	R	201	CLA	C1-C2-C3	-2.25	122.51	126.20
29	B	846	WVN	C07-C01-C02	2.25	112.96	109.55
26	a	302	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
26	a	306	CLA	O2D-CGD-CBD	2.25	115.17	111.23
26	A	813	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
28	A	843	LHG	C18-C17-C16	-2.25	102.99	114.37
26	n	608	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
36	m	611	KC2	C3C-C2C-C1C	2.25	108.10	106.41
35	k	615	II0	C08-C12-C14	2.25	117.78	112.18
26	h	307	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
26	m	606	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
26	A	824	CLA	CMB-C2B-C3B	2.25	131.84	126.55
26	B	829	CLA	CHB-C4A-NA	2.25	127.64	124.40
35	a	312	II0	C42-C41-C39	-2.25	118.92	123.52
26	B	825	CLA	C3B-C4B-NB	-2.25	108.52	110.53
26	c	309	CLA	CMC-C2C-C1C	2.24	128.54	125.03
26	A	806	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
35	i	313	II0	C12-C14-C10	-2.24	115.83	120.50
26	k	609	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	l	305	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	b	313	CLA	C1-C2-C3	-2.24	122.52	126.20
34	F	205	LMG	C38-C37-C36	-2.24	103.03	114.37
34	c	318	LMG	C42-C41-C40	-2.24	103.03	114.37
26	c	302	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	B	821	CLA	CAA-CBA-CGA	-2.24	106.84	113.21
28	b	302	LHG	C27-C26-C25	-2.24	103.06	114.37
36	m	611	KC2	CHD-C1D-ND	-2.24	120.69	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	825	CLA	CMB-C2B-C3B	2.24	131.81	126.55
26	B	832	CLA	C3B-C4B-NB	-2.24	108.53	110.53
34	c	319	LMG	O1-C7-C8	-2.24	105.38	110.82
26	A	841	CLA	CMB-C2B-C3B	2.24	131.81	126.55
29	A	848	WVN	C39-C40-C37	-2.24	118.94	123.52
26	h	303	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
35	a	313	II0	C31-C29-C25	-2.23	120.36	126.61
35	l	314	II0	C06-C04-C10	2.23	113.89	109.49
26	l	306	CLA	C2A-C1A-CHA	2.23	127.74	123.87
26	i	305	CLA	CHC-C4B-NB	2.23	127.40	124.05
26	k	603	CLA	CHB-C1B-NB	2.23	127.40	124.05
26	B	827	CLA	CHB-C4A-NA	2.23	127.62	124.40
36	n	612	KC2	CHC-C4B-C3B	2.23	128.97	125.21
26	B	839	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
35	m	614	II0	C06-C04-C10	2.23	113.88	109.49
26	B	821	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
26	B	812	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
26	h	302	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
35	l	314	II0	C05-C03-C09	2.23	113.88	109.49
26	l	309	CLA	CMB-C2B-C3B	2.23	131.79	126.55
26	B	838	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
35	a	316	II0	C11-C13-C09	-2.22	115.87	120.50
26	l	310	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
35	d	317	II0	C12-C14-C10	-2.22	115.88	120.50
26	m	612	CLA	C2A-C1A-CHA	2.22	127.72	123.87
26	n	613	CLA	C2A-C1A-CHA	2.22	127.72	123.87
26	j	607	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
26	B	804	CLA	C1-C2-C3	-2.22	122.56	126.20
35	a	314	II0	C06-C04-C10	2.22	113.86	109.49
26	a	303	CLA	C2A-C1A-CHA	2.22	127.72	123.87
26	B	826	CLA	C3B-C4B-NB	-2.22	108.55	110.53
34	b	319	LMG	O2-C2-C1	-2.22	104.79	110.08
35	i	312	II0	C12-C14-C10	-2.22	115.88	120.50
33	B	844	DGD	CBB-CAB-C9B	-2.22	103.15	114.37
26	m	609	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
29	L	201	WVN	C03-C04-C09	-2.22	108.35	112.07
35	k	616	II0	C12-C14-C10	-2.22	115.89	120.50
26	A	802	CLA	O1D-CGD-CBD	2.22	128.89	124.52
26	B	812	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
28	L	208	LHG	C18-C17-C16	-2.21	103.18	114.37
26	b	304	CLA	C3B-C4B-NB	-2.21	108.55	110.53
26	A	825	CLA	CAA-CBA-CGA	-2.21	106.92	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	s	409	LHG	C27-C26-C25	-2.21	103.18	114.37
26	A	856	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
26	B	835	CLA	O2D-CGD-CBD	2.21	115.09	111.23
28	B	851	LHG	C27-C26-C25	-2.21	103.20	114.37
26	A	822	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
26	B	807	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
26	B	836	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
34	F	205	LMG	C42-C41-C40	-2.21	103.21	114.37
28	c	320	LHG	C27-C26-C25	-2.21	103.21	114.37
26	c	309	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
26	A	808	CLA	C3B-C4B-NB	-2.20	108.56	110.53
36	j	611	KC2	C3C-C2C-C1C	2.20	108.06	106.41
26	i	311	CLA	C3B-C4B-NB	-2.20	108.56	110.53
26	B	818	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
34	F	205	LMG	O3-C3-C2	-2.20	105.19	110.38
35	i	314	II0	C15-C03-C09	-2.20	106.58	110.52
26	j	604	CLA	C3B-C4B-NB	-2.20	108.56	110.53
26	B	816	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
29	L	205	WVN	C21-C15-C14	-2.20	108.90	113.60
26	B	835	CLA	CHB-C4A-NA	2.20	127.58	124.40
34	c	318	LMG	O2-C2-C1	-2.20	104.83	110.08
26	A	827	CLA	CMB-C2B-C3B	2.20	131.72	126.55
26	A	817	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
26	B	828	CLA	C1-C2-C3	-2.20	123.20	126.76
29	B	846	WVN	C10-C06-C13	2.20	113.63	110.44
26	a	309	CLA	C2A-C1A-CHA	2.20	127.68	123.87
35	m	615	II0	C12-C14-C10	-2.20	115.92	120.50
26	d	310	CLA	C3B-C4B-NB	-2.20	108.57	110.53
26	a	303	CLA	C3A-C2A-C1A	2.20	104.63	101.34
26	h	313	CLA	C3B-C4B-NB	-2.20	108.57	110.53
26	k	606	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
34	c	318	LMG	O3-C3-C2	-2.19	105.20	110.38
34	c	319	LMG	O2-C2-C1	-2.19	104.85	110.08
26	a	301	CLA	C2A-C1A-CHA	2.19	127.67	123.87
26	c	302	CLA	C3B-C4B-NB	-2.19	108.57	110.53
28	L	207	LHG	C18-C17-C16	-2.19	103.29	114.37
29	M	101	WVN	C06-C13-C20	-2.19	109.71	115.65
29	i	315	WVN	C20-C13-C15	-2.19	116.51	121.56
26	d	302	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
35	i	312	II0	C17-C04-C10	-2.19	106.60	110.52
28	L	208	LHG	C27-C26-C25	-2.19	103.31	114.37
26	A	840	CLA	CMB-C2B-C1B	-2.19	122.09	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	810	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
26	B	829	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
26	A	837	CLA	C3B-C4B-NB	-2.19	108.58	110.53
36	k	611	KC2	C3C-C2C-C1C	2.19	108.05	106.41
26	k	608	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
34	L	209	LMG	O3-C3-C2	-2.19	105.22	110.38
32	A	854	SQD	O8-S-C6	2.18	110.19	105.97
26	n	608	CLA	C1D-ND-C4D	-2.18	104.78	106.31
26	s	402	CLA	C3B-C4B-NB	-2.18	108.58	110.53
28	A	855	LHG	C27-C26-C25	-2.18	103.33	114.37
33	j	618	DGD	CAB-C9B-C8B	-2.18	103.34	114.37
34	F	205	LMG	O2-C2-C1	-2.18	104.88	110.08
36	s	401	KC2	CHD-C4C-NC	2.18	127.60	124.31
28	i	317	LHG	C27-C26-C25	-2.18	103.34	114.37
26	c	307	CLA	CHB-C4A-NA	2.18	127.55	124.40
28	n	619	LHG	C27-C26-C25	-2.18	103.35	114.37
26	A	819	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
26	B	825	CLA	CMB-C2B-C3B	2.18	131.68	126.55
35	i	316	II0	C42-C41-C39	-2.18	119.06	123.52
35	d	316	II0	C12-C14-C10	-2.18	115.97	120.50
34	b	319	LMG	O3-C3-C2	-2.18	105.25	110.38
26	B	803	CLA	CHB-C4A-NA	2.17	127.54	124.40
26	A	818	CLA	C3B-C4B-NB	-2.17	108.59	110.53
26	m	602	CLA	O2D-CGD-CBD	2.17	115.03	111.23
29	B	848	WVN	C21-C15-C14	-2.17	108.97	113.60
34	F	206	LMG	O2-C2-C1	-2.17	104.90	110.08
26	n	610	CLA	O2D-CGD-CBD	2.17	115.03	111.23
26	b	311	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
34	Q	301	LMG	O3-C3-C2	-2.17	105.26	110.38
26	A	814	CLA	C1-C2-C3	-2.17	123.25	126.76
29	J	101	WVN	C39-C40-C37	-2.17	119.08	123.52
35	k	615	II0	C05-C03-C09	2.17	113.76	109.49
37	j	616	IHT	C22-C18-C07	-2.17	121.21	127.00
34	n	620	LMG	O3-C3-C2	-2.17	105.27	110.38
26	A	809	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	i	302	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	j	613	CLA	C3B-C4B-NB	-2.17	108.60	110.53
26	i	306	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	B	802	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
26	B	813	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
26	b	304	CLA	C1-C2-C3	-2.16	122.65	126.20
26	m	609	CLA	O2A-CGA-O1A	-2.16	118.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	306	CLA	CHB-C4A-NA	2.16	127.52	124.40
36	c	310	KC2	CHB-C4A-NA	2.16	127.58	124.23
26	B	823	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	n	613	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	A	841	CLA	C2A-C1A-CHA	2.16	127.62	123.87
26	i	311	CLA	CBC-CAC-C3C	2.16	118.27	112.42
26	i	303	CLA	C2A-C1A-CHA	2.16	127.61	123.87
34	F	206	LMG	O3-C3-C2	-2.16	105.29	110.38
34	b	319	LMG	O1-C1-C2	-2.16	105.00	108.27
26	h	302	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	A	819	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	A	835	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	B	809	CLA	C3B-C4B-NB	-2.16	108.61	110.53
29	F	203	WVN	C06-C13-C20	-2.16	109.81	115.65
26	l	313	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
29	A	848	WVN	C23-C20-C13	-2.15	121.25	127.00
26	k	610	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
28	A	849	LHG	C18-C17-C16	-2.15	103.50	114.37
28	L	207	LHG	C27-C26-C25	-2.15	103.50	114.37
36	s	401	KC2	C2A-C1A-CHA	-2.15	120.14	128.96
34	n	620	LMG	O2-C2-C1	-2.15	104.96	110.08
26	A	813	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
26	A	836	CLA	CAA-CBA-CGA	-2.15	107.12	113.21
26	n	608	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
26	c	309	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
26	A	814	CLA	CMB-C2B-C3B	2.14	131.59	126.55
36	s	401	KC2	CHB-C4A-NA	2.14	127.55	124.23
26	n	602	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
26	d	305	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
35	k	619	II0	C12-C14-C10	-2.14	116.05	120.50
26	A	827	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
36	i	309	KC2	C3C-C2C-C1C	2.14	108.02	106.41
26	B	819	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
26	j	607	CLA	CHB-C4A-NA	2.14	127.48	124.40
35	l	302	II0	C34-C36-C40	-2.14	115.65	119.01
26	B	813	CLA	C2A-C1A-CHA	2.14	127.58	123.87
28	m	618	LHG	C27-C26-C25	-2.14	103.57	114.37
37	b	316	IHT	C30-C27-C23	2.13	130.27	127.28
26	A	820	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
28	b	318	LHG	C18-C17-C16	-2.13	103.58	114.37
26	A	816	CLA	C3B-C4B-NB	-2.13	108.62	110.53
26	B	840	CLA	CAA-C2A-C3A	-2.13	107.23	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	313	II0	C12-C14-C10	-2.13	116.06	120.50
26	B	827	CLA	O2D-CGD-CBD	2.13	114.96	111.23
26	B	842	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	m	607	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	A	817	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	A	819	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
36	c	310	KC2	C2A-C1A-CHA	-2.13	120.23	128.96
26	F	201	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
35	n	616	II0	C05-C03-C09	2.13	113.68	109.49
26	m	604	CLA	C3B-C4B-NB	-2.13	108.63	110.53
26	c	308	CLA	C1-C2-C3	-2.12	122.72	126.20
26	A	803	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
26	A	826	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
26	B	838	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
29	I	101	WVN	C40-C39-C36	-2.12	119.18	123.52
26	m	610	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	B	804	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	L	205	WVN	C10-C06-C13	2.12	113.52	110.44
36	c	310	KC2	C3D-C2D-C1D	-2.12	99.64	106.40
35	h	312	II0	C15-C03-C09	-2.12	106.72	110.52
35	h	310	II0	C42-C41-C39	-2.12	119.19	123.52
26	i	303	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
35	h	311	II0	C42-C41-C39	-2.12	119.19	123.52
35	a	313	II0	C06-C04-C10	2.12	113.66	109.49
26	B	807	CLA	C3B-C4B-NB	-2.11	108.64	110.53
26	n	606	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	B	825	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	B	827	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	B	840	CLA	O2D-CGD-CBD	2.11	114.92	111.23
26	n	607	CLA	C3B-C4B-NB	-2.11	108.64	110.53
26	j	602	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
36	d	312	KC2	CHB-C4A-C3A	2.11	128.36	125.03
26	k	604	CLA	O2D-CGD-CBD	2.11	114.92	111.23
35	l	315	II0	C18-C04-C10	-2.11	106.74	110.52
29	l	303	WVN	C39-C40-C37	-2.11	119.20	123.52
26	B	827	CLA	CHB-C1B-NB	2.11	127.21	124.05
26	c	305	CLA	C3B-C4B-NB	-2.11	108.65	110.53
36	i	309	KC2	CHC-C4B-C3B	2.11	128.76	125.21
35	c	313	II0	C42-C41-C39	-2.11	119.21	123.52
34	n	620	LMG	O1-C1-C2	-2.11	105.07	108.27
26	B	840	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
26	a	309	CLA	C3B-C4B-NB	-2.11	108.65	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	310	CLA	C2A-C1A-CHA	2.10	127.52	123.87
26	j	607	CLA	CMB-C2B-C3B	2.10	131.50	126.55
26	l	307	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
26	n	603	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
33	j	618	DGD	O5D-C6D-C5D	-2.10	104.68	109.42
26	k	601	CLA	O2D-CGD-CBD	2.10	114.91	111.23
34	F	205	LMG	O7-C10-O9	-2.10	118.80	123.70
26	j	606	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
35	J	104	II0	C42-C41-C39	-2.10	119.22	123.52
26	c	303	CLA	CMB-C2B-C3B	2.10	131.48	126.55
26	d	307	CLA	C3B-C4B-NB	-2.10	108.66	110.53
26	A	829	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
26	B	828	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
26	h	313	CLA	CMB-C2B-C3B	2.10	131.48	126.55
26	A	827	CLA	CHD-C1D-ND	-2.10	121.85	124.80
26	i	305	CLA	CHB-C1B-NB	2.10	127.19	124.05
26	s	406	CLA	CMB-C2B-C3B	2.09	131.48	126.55
26	A	807	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
26	B	837	CLA	C3B-C4B-NB	-2.09	108.66	110.53
26	a	310	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
26	B	817	CLA	CMB-C2B-C3B	2.09	131.47	126.55
26	n	606	CLA	CHB-C4A-NA	2.09	127.42	124.40
26	L	204	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
26	A	808	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
26	B	814	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
26	B	823	CLA	O2D-CGD-CBD	2.09	114.88	111.23
28	c	317	LHG	C5-O7-C7	-2.09	112.80	117.80
34	c	319	LMG	O3-C3-C2	-2.09	105.45	110.38
26	B	824	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
26	s	406	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
26	b	307	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
26	l	311	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
33	B	844	DGD	CAB-C9B-C8B	-2.08	103.83	114.37
29	B	850	WVN	C06-C13-C20	-2.08	110.00	115.65
26	m	602	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	i	303	CLA	C3B-C4B-NB	-2.08	108.67	110.53
26	A	823	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
33	j	618	DGD	C3G-C2G-C1G	-2.08	106.93	111.78
26	A	831	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
34	c	318	LMG	O7-C10-O9	-2.08	118.84	123.70
26	A	856	CLA	C2A-C1A-CHA	2.08	127.48	123.87
35	i	319	II0	C42-C41-C39	-2.08	119.26	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	831	CLA	C1-C2-C3	-2.08	122.79	126.20
26	a	304	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	b	303	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	A	828	CLA	C3B-C4B-NB	-2.08	108.67	110.53
26	s	402	CLA	C2A-C1A-CHA	2.08	127.48	123.87
26	d	303	CLA	C2A-C1A-CHA	2.08	127.48	123.87
26	j	607	CLA	C1D-ND-C4D	2.08	107.77	106.31
26	A	839	CLA	CMB-C2B-C3B	2.08	131.44	126.55
36	s	401	KC2	O2A-CGA-O1A	-2.08	118.47	122.70
26	A	834	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
26	B	819	CLA	CMC-C2C-C1C	-2.08	121.79	125.03
34	L	209	LMG	O2-C2-C1	-2.08	105.13	110.08
36	d	312	KC2	C3C-C2C-C1C	2.08	107.97	106.41
26	A	828	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
33	j	618	DGD	C5B-C4B-C3B	-2.08	103.87	114.37
29	J	101	WVN	C06-C13-C20	-2.08	110.02	115.65
28	c	317	LHG	C27-C26-C25	-2.08	103.88	114.37
26	n	605	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
28	c	320	LHG	C18-C17-C16	-2.07	103.88	114.37
26	h	304	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	k	604	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	B	833	CLA	C3B-C4B-NB	-2.07	108.68	110.53
26	n	610	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
36	c	310	KC2	CHC-C1C-NC	2.07	127.44	124.23
26	B	818	CLA	CMB-C2B-C3B	2.07	131.42	126.55
26	B	812	CLA	C1-C2-C3	-2.07	122.80	126.20
29	B	850	WVN	C21-C15-C14	-2.07	109.18	113.60
26	B	804	CLA	CHC-C1C-NC	2.07	127.43	124.31
26	A	841	CLA	CHA-C1A-NA	-2.07	121.70	126.39
26	k	605	CLA	C2A-C1A-CHA	2.07	127.46	123.87
26	B	823	CLA	C1-C2-C3	-2.07	122.81	126.20
28	B	851	LHG	C18-C17-C16	-2.07	103.91	114.37
26	c	311	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
26	j	604	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	c	306	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	j	601	CLA	O2D-CGD-CBD	2.06	114.84	111.23
26	b	306	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	B	835	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	A	841	CLA	C1-C2-C3	-2.06	122.82	126.20
26	B	802	CLA	CHB-C4A-NA	2.06	127.38	124.40
26	l	307	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
26	B	821	CLA	C1-C2-C3	-2.06	122.82	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	313	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
26	j	613	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
33	B	844	DGD	C3G-C2G-C1G	-2.06	106.98	111.78
26	n	608	CLA	C1-C2-C3	-2.06	122.82	126.20
26	B	803	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	L	203	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
29	A	847	WVN	C39-C40-C37	-2.06	119.31	123.52
26	n	603	CLA	CHA-C1A-NA	-2.06	121.73	126.39
26	B	822	CLA	CMB-C2B-C3B	2.06	131.39	126.55
26	a	304	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
26	b	310	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
26	n	613	CLA	CHB-C4A-NA	2.05	127.36	124.40
26	B	830	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	B	833	CLA	CHA-C1A-NA	-2.05	121.74	126.39
26	B	811	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	Q	302	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	a	308	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	d	313	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	B	836	CLA	CMB-C2B-C3B	2.05	131.38	126.55
26	A	838	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
34	Q	301	LMG	O2-C2-C1	-2.05	105.19	110.08
26	A	840	CLA	C1-C2-C3	-2.05	122.84	126.20
26	B	806	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	m	603	CLA	C1-C2-C3	-2.05	122.84	126.20
26	i	311	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
36	n	611	KC2	CHB-C4A-C3A	2.05	128.26	125.03
26	A	811	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
26	B	826	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
26	B	803	CLA	O1D-CGD-CBD	2.05	128.55	124.52
26	B	819	CLA	CHB-C4A-NA	2.04	127.35	124.40
26	A	805	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	b	304	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	A	852	CLA	C1-C2-C3	-2.04	122.85	126.20
35	n	615	II0	C06-C04-C10	2.04	113.51	109.49
26	j	609	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	d	305	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	h	306	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	A	804	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
36	k	612	KC2	CMD-C2D-C1D	2.04	128.53	125.42
26	n	609	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
35	l	302	II0	C12-C14-C10	-2.04	116.25	120.50
26	A	827	CLA	O2A-CGA-O1A	-2.04	118.53	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	301	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
36	n	611	KC2	CHC-C4B-C3B	2.04	128.65	125.21
26	b	305	CLA	C2A-C1A-CHA	2.04	127.40	123.87
26	s	403	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	L	201	WVN	C07-C01-C02	2.04	112.63	109.55
26	b	313	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
29	l	303	WVN	C21-C15-C14	-2.04	109.25	113.60
36	d	311	KC2	C3C-C2C-C1C	2.04	107.94	106.41
26	L	203	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
26	j	607	CLA	CHC-C4B-NB	2.04	127.10	124.05
36	s	401	KC2	C3D-C2D-C1D	-2.04	99.90	106.40
26	n	608	CLA	CHA-C1A-NA	-2.03	121.78	126.39
26	l	304	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
26	n	609	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
26	B	813	CLA	CHA-C1A-NA	-2.03	121.79	126.39
26	h	308	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
36	s	401	KC2	CHC-C4B-C3B	-2.03	121.78	125.21
36	k	613	KC2	C3C-C2C-C1C	2.03	107.94	106.41
26	B	807	CLA	CMB-C2B-C3B	2.03	131.33	126.55
26	n	607	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
33	j	618	DGD	C4E-C3E-C2E	-2.03	107.26	110.83
35	k	616	II0	C15-C03-C09	2.03	114.16	110.52
26	c	301	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	F	201	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
26	l	307	CLA	C1-C2-C3	-2.03	122.87	126.20
26	h	302	CLA	C1-C2-C3	-2.03	123.48	126.76
26	k	603	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
26	b	308	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	k	604	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
26	L	203	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
26	K	101	CLA	C3B-C4B-NB	-2.03	108.72	110.53
26	B	818	CLA	C1-C2-C3	-2.03	122.87	126.20
26	A	807	CLA	O2D-CGD-CBD	2.03	114.78	111.23
26	b	313	CLA	CHA-C1A-NA	-2.03	121.80	126.39
26	h	308	CLA	C2A-C1A-CHA	2.03	127.38	123.87
35	l	302	II0	C30-C32-C34	-2.02	117.33	123.20
29	h	309	WVN	C21-C15-C14	-2.02	109.28	113.60
26	k	601	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	A	829	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	B	810	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	i	304	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
26	A	814	CLA	O2A-CGA-O1A	-2.02	118.57	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	302	II0	C15-C03-C09	-2.02	106.90	110.52
29	B	847	WVN	C18-C06-C13	-2.02	107.07	110.24
29	h	309	WVN	C40-C39-C36	-2.02	119.39	123.52
28	l	318	LHG	C27-C26-C25	-2.02	104.16	114.37
29	I	101	WVN	C07-C01-C02	2.02	112.60	109.55
26	d	303	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	B	830	CLA	C1-C2-C3	-2.02	123.50	126.76
26	k	610	CLA	CHA-C1A-NA	-2.02	121.82	126.39
26	j	605	CLA	CHA-C1A-NA	-2.02	121.82	126.39
26	L	203	CLA	O2D-CGD-CBD	2.01	114.75	111.23
26	B	819	CLA	CAC-C3C-C2C	2.01	131.26	127.56
26	A	837	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
26	l	306	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
35	m	615	II0	C17-C04-C10	-2.01	106.91	110.52
26	B	814	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
26	j	612	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
26	L	204	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
26	A	839	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
35	c	313	II0	C06-C04-C10	2.01	113.45	109.49
29	F	203	WVN	C21-C15-C14	-2.01	109.31	113.60
26	h	313	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	A	825	CLA	O2D-CGD-CBD	2.01	114.74	111.23
26	k	603	CLA	C2A-C1A-CHA	2.01	127.35	123.87
29	L	201	WVN	C10-C12-C14	2.01	115.69	111.28
26	A	821	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
26	c	311	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
26	m	607	CLA	C3B-C4B-NB	-2.01	108.74	110.53
26	i	303	CLA	CMB-C2B-C3B	2.01	131.27	126.55
26	i	305	CLA	CMB-C2B-C1B	-2.01	122.37	125.42
26	h	302	CLA	CMB-C2B-C3B	2.00	131.27	126.55
26	h	305	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
26	n	601	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
35	k	616	II0	C42-C41-C39	-2.00	119.42	123.52
26	i	305	CLA	CAC-C3C-C4C	2.00	127.40	124.79
26	b	305	CLA	CHB-C1B-NB	2.00	127.05	124.05
26	d	313	CLA	CMB-C2B-C3B	2.00	131.26	126.55

All (214) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	801	CL0	ND
25	A	801	CL0	NA

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Mol	Chain	Res	Type	Atom
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
26	A	852	CLA	ND

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Mol	Chain	Res	Type	Atom
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
26	B	842	CLA	ND

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Mol	Chain	Res	Type	Atom
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
26	b	313	CLA	ND

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Mol	Chain	Res	Type	Atom
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
26	i	301	CLA	ND

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Mol	Chain	Res	Type	Atom
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
26	n	610	CLA	ND

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

All (3936) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CL0	C1-C2-C3-C4
26	A	804	CLA	CAD-CBD-CGD-O1D
26	A	804	CLA	CAD-CBD-CGD-O2D
26	A	807	CLA	CHA-CBD-CGD-O1D
26	A	807	CLA	CHA-CBD-CGD-O2D
26	A	809	CLA	CBD-CGD-O2D-CED
26	A	810	CLA	CBD-CGD-O2D-CED
26	A	811	CLA	C4B-C3B-CAB-CBB
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	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	819	CLA	CBD-CGD-O2D-CED
26	A	822	CLA	C2B-C3B-CAB-CBB
26	A	822	CLA	C4B-C3B-CAB-CBB
26	A	822	CLA	CAD-CBD-CGD-O2D
26	A	823	CLA	C1A-C2A-CAA-CBA
26	A	823	CLA	C3A-C2A-CAA-CBA
26	A	827	CLA	C1A-C2A-CAA-CBA
26	A	827	CLA	C3A-C2A-CAA-CBA
26	A	830	CLA	CHA-CBD-CGD-O2D
26	A	833	CLA	C2B-C3B-CAB-CBB
26	A	833	CLA	C4B-C3B-CAB-CBB
26	A	835	CLA	C2B-C3B-CAB-CBB
26	A	835	CLA	C4B-C3B-CAB-CBB
26	A	837	CLA	C1A-C2A-CAA-CBA
26	A	837	CLA	C3A-C2A-CAA-CBA
26	A	837	CLA	C2B-C3B-CAB-CBB
26	A	837	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	A	838	CLA	C4B-C3B-CAB-CBB
26	A	840	CLA	C2B-C3B-CAB-CBB
26	A	840	CLA	C4B-C3B-CAB-CBB
26	A	841	CLA	C1A-C2A-CAA-CBA
26	B	801	CLA	C2B-C3B-CAB-CBB
26	B	801	CLA	C4B-C3B-CAB-CBB
26	B	802	CLA	CAD-CBD-CGD-O1D
26	B	802	CLA	CAD-CBD-CGD-O2D
26	B	802	CLA	C2-C3-C5-C6
26	B	802	CLA	C4-C3-C5-C6
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	808	CLA	CHA-CBD-CGD-O1D
26	B	808	CLA	CHA-CBD-CGD-O2D
26	B	811	CLA	C2B-C3B-CAB-CBB
26	B	811	CLA	C4B-C3B-CAB-CBB
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	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	822	CLA	CHA-CBD-CGD-O1D
26	B	822	CLA	CHA-CBD-CGD-O2D
26	B	823	CLA	CHA-CBD-CGD-O1D
26	B	823	CLA	CHA-CBD-CGD-O2D
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	828	CLA	C4B-C3B-CAB-CBB
26	B	829	CLA	C1A-C2A-CAA-CBA
26	B	830	CLA	C1A-C2A-CAA-CBA
26	B	832	CLA	C4B-C3B-CAB-CBB

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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	838	CLA	CHA-CBD-CGD-O1D
26	B	838	CLA	CHA-CBD-CGD-O2D
26	B	839	CLA	C6-C7-C8-C9
26	B	840	CLA	C3A-C2A-CAA-CBA
26	B	840	CLA	C4B-C3B-CAB-CBB
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	202	CLA	C4B-C3B-CAB-CBB
26	L	202	CLA	CHA-CBD-CGD-O2D
26	L	204	CLA	CBD-CGD-O2D-CED
26	L	206	CLA	C2B-C3B-CAB-CBB
26	L	206	CLA	C4B-C3B-CAB-CBB
26	K	101	CLA	C3A-C2A-CAA-CBA
26	s	402	CLA	C1A-C2A-CAA-CBA
26	s	402	CLA	C2B-C3B-CAB-CBB
26	s	402	CLA	C4B-C3B-CAB-CBB
26	s	403	CLA	CBD-CGD-O2D-CED
26	s	406	CLA	C1A-C2A-CAA-CBA
26	s	408	CLA	C2B-C3B-CAB-CBB
26	s	408	CLA	C4B-C3B-CAB-CBB
26	c	301	CLA	C1A-C2A-CAA-CBA
26	c	301	CLA	CHA-CBD-CGD-O2D
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	CAD-CBD-CGD-O1D
26	c	303	CLA	CAD-CBD-CGD-O2D
26	c	306	CLA	C4B-C3B-CAB-CBB
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	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	a	304	CLA	CAD-CBD-CGD-O2D
26	a	305	CLA	C4B-C3B-CAB-CBB
26	a	306	CLA	C1A-C2A-CAA-CBA
26	a	306	CLA	C3A-C2A-CAA-CBA
26	a	308	CLA	C2B-C3B-CAB-CBB
26	a	308	CLA	C4B-C3B-CAB-CBB
26	a	308	CLA	CBD-CGD-O2D-CED
26	a	309	CLA	CHA-CBD-CGD-O1D
26	a	309	CLA	CHA-CBD-CGD-O2D
26	a	311	CLA	C1A-C2A-CAA-CBA
26	a	311	CLA	C3A-C2A-CAA-CBA
26	a	311	CLA	CBD-CGD-O2D-CED
26	b	303	CLA	CHA-CBD-CGD-O2D
26	b	304	CLA	C1A-C2A-CAA-CBA
26	b	304	CLA	C3A-C2A-CAA-CBA
26	b	304	CLA	CHA-CBD-CGD-O2D
26	b	305	CLA	CBD-CGD-O2D-CED
26	b	306	CLA	CAD-CBD-CGD-O1D
26	b	306	CLA	CAD-CBD-CGD-O2D
26	b	307	CLA	C4B-C3B-CAB-CBB
26	b	310	CLA	C4B-C3B-CAB-CBB
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	303	CLA	C4B-C3B-CAB-CBB
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	h	307	CLA	C2B-C3B-CAB-CBB
26	h	307	CLA	C4B-C3B-CAB-CBB
26	h	308	CLA	C4B-C3B-CAB-CBB
26	m	602	CLA	C1A-C2A-CAA-CBA
26	m	602	CLA	C3A-C2A-CAA-CBA
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	CAD-CBD-CGD-O1D
26	m	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	m	605	CLA	C1A-C2A-CAA-CBA
26	m	605	CLA	C3A-C2A-CAA-CBA
26	m	606	CLA	C2B-C3B-CAB-CBB
26	m	606	CLA	C4B-C3B-CAB-CBB
26	m	607	CLA	C2B-C3B-CAB-CBB
26	m	607	CLA	C4B-C3B-CAB-CBB
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	610	CLA	C4B-C3B-CAB-CBB
26	m	612	CLA	CBD-CGD-O2D-CED
26	m	613	CLA	C2B-C3B-CAB-CBB
26	m	613	CLA	C4B-C3B-CAB-CBB
26	m	613	CLA	CBD-CGD-O2D-CED
26	l	304	CLA	C2B-C3B-CAB-CBB
26	l	304	CLA	C4B-C3B-CAB-CBB
26	l	305	CLA	C1A-C2A-CAA-CBA
26	l	305	CLA	C3A-C2A-CAA-CBA
26	l	305	CLA	CHA-CBD-CGD-O2D
26	l	307	CLA	CBD-CGD-O2D-CED
26	l	309	CLA	C1A-C2A-CAA-CBA
26	l	309	CLA	C3A-C2A-CAA-CBA
26	l	311	CLA	C4B-C3B-CAB-CBB
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	CAD-CBD-CGD-O2D
26	k	608	CLA	CHA-CBD-CGD-O1D
26	k	608	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	C2B-C3B-CAB-CBB
26	k	610	CLA	C4B-C3B-CAB-CBB
26	k	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	302	CLA	CHA-CBD-CGD-O1D
26	i	302	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	305	CLA	C4B-C3B-CAB-CBB
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	604	CLA	CAD-CBD-CGD-O1D
26	j	604	CLA	CAD-CBD-CGD-O2D
26	j	605	CLA	C1A-C2A-CAA-CBA
26	j	605	CLA	CHA-CBD-CGD-O1D
26	j	605	CLA	CHA-CBD-CGD-O2D
26	j	606	CLA	C4B-C3B-CAB-CBB
26	j	607	CLA	CHA-CBD-CGD-O1D
26	j	607	CLA	CHA-CBD-CGD-O2D
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	610	CLA	C4B-C3B-CAB-CBB
26	j	612	CLA	C4B-C3B-CAB-CBB
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	CBD-CGD-O2D-CED
26	d	306	CLA	C2B-C3B-CAB-CBB
26	d	306	CLA	C4B-C3B-CAB-CBB
26	d	306	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	C4B-C3B-CAB-CBB
26	d	309	CLA	CBD-CGD-O2D-CED
26	d	310	CLA	C2B-C3B-CAB-CBB
26	d	310	CLA	C4B-C3B-CAB-CBB
26	d	318	CLA	CHA-CBD-CGD-O2D
26	d	318	CLA	CBD-CGD-O2D-CED
26	n	603	CLA	C1A-C2A-CAA-CBA
26	n	603	CLA	C2B-C3B-CAB-CBB
26	n	603	CLA	C4B-C3B-CAB-CBB
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	606	CLA	C2B-C3B-CAB-CBB
26	n	606	CLA	C4B-C3B-CAB-CBB
26	n	608	CLA	C3A-C2A-CAA-CBA
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	610	CLA	C4B-C3B-CAB-CBB
26	n	610	CLA	CHA-CBD-CGD-O1D
26	n	610	CLA	CHA-CBD-CGD-O2D
26	n	613	CLA	C1A-C2A-CAA-CBA
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	843	LHG	C4-O6-P-O3
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	A	855	LHG	C4-O6-P-O3
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
28	J	105	LHG	C4-O6-P-O3
28	L	207	LHG	C2-C3-O3-P
28	L	207	LHG	C3-O3-P-O4
28	L	207	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	L	207	LHG	C4-O6-P-O3
28	L	207	LHG	C4-O6-P-O4
28	L	208	LHG	C3-O3-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	C3-O3-P-O6
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	C3-O3-P-O6
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	C3-O3-P-O6
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	C4-O6-P-O3
28	b	318	LHG	C8-C7-O7-C5
28	m	618	LHG	C3-O3-P-O6
28	m	618	LHG	O7-C5-C6-O8
28	l	318	LHG	C3-O3-P-O6
28	i	317	LHG	C3-O3-P-O6
28	i	317	LHG	C8-C7-O7-C5
28	j	617	LHG	C3-O3-P-O6
28	j	617	LHG	C4-O6-P-O3
28	j	617	LHG	C4-O6-P-O5
28	n	619	LHG	O1-C1-C2-C3
28	n	619	LHG	C3-O3-P-O6
28	n	619	LHG	O9-C7-O7-C5
28	n	619	LHG	C8-C7-O7-C5
29	A	845	WVN	C05-C02-C11-C19
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

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Mol	Chain	Res	Type	Atoms
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	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
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-C36
29	A	848	WVN	C31-C32-C36-C39
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	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

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Mol	Chain	Res	Type	Atoms
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
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	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-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

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Mol	Chain	Res	Type	Atoms
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
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	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-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

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Mol	Chain	Res	Type	Atoms
29	L	201	WVN	C24-C22-C26-C29
29	L	201	WVN	C20-C23-C25-C27
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	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	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	C24-C22-C26-C29
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	C24-C22-C26-C29
29	l	303	WVN	C27-C25-C28-C30
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
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

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Mol	Chain	Res	Type	Atoms
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'
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	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
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

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Mol	Chain	Res	Type	Atoms
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	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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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-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	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
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

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Mol	Chain	Res	Type	Atoms
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
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	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

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Mol	Chain	Res	Type	Atoms
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	C2A-CAA-CBA-CGA
36	m	611	KC2	C3A-C2A-CAA-CBA
36	m	611	KC2	C2C-C3C-CAC-CBC
36	m	611	KC2	C4C-C3C-CAC-CBC
36	m	611	KC2	C2A-CAA-CBA-CGA
36	l	312	KC2	C2B-C3B-CAB-CBB
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	611	KC2	CHA-CBD-CGD-O1D
36	k	611	KC2	CHA-CBD-CGD-O2D
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

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Mol	Chain	Res	Type	Atoms
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	C3A-C2A-CAA-CBA
36	i	318	KC2	C2B-C3B-CAB-CBB
36	i	318	KC2	CBD-CGD-O2D-CED
36	i	318	KC2	O1D-CGD-O2D-CED
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	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	311	KC2	CHA-CBD-CGD-O1D
36	d	311	KC2	CHA-CBD-CGD-O2D
36	d	312	KC2	C3A-C2A-CAA-CBA
36	d	312	KC2	CHA-CBD-CGD-O1D
36	d	312	KC2	CHA-CBD-CGD-O2D
36	n	611	KC2	C1A-C2A-CAA-CBA
36	n	611	KC2	C3A-C2A-CAA-CBA
36	n	611	KC2	C2B-C3B-CAB-CBB
36	n	611	KC2	C2C-C3C-CAC-CBC
36	n	611	KC2	C2A-CAA-CBA-CGA
36	n	611	KC2	CBD-CGD-O2D-CED
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	C24-C26-C29-C31
37	b	316	IHT	C18-C22-C23-C27
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

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Mol	Chain	Res	Type	Atoms
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
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	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	312	CLA	CBD-CGD-O2D-CED
26	m	603	CLA	CBD-CGD-O2D-CED
26	l	301	CLA	CBD-CGD-O2D-CED
26	i	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	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
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	B	819	CLA	C4C-C3C-CAC-CBC
26	h	302	CLA	O1D-CGD-O2D-CED
26	m	602	CLA	O1D-CGD-O2D-CED
30	a	317	LMU	O5B-C1B-O1B-C4'
30	i	300	LMU	O5B-C1B-O1B-C4'
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	c	303	CLA	O1D-CGD-O2D-CED
26	b	312	CLA	O1D-CGD-O2D-CED
26	j	601	CLA	O1D-CGD-O2D-CED
26	n	613	CLA	O1D-CGD-O2D-CED
36	d	311	KC2	O1D-CGD-O2D-CED
36	d	312	KC2	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	b	306	CLA	CBD-CGD-O2D-CED
26	l	309	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

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Mol	Chain	Res	Type	Atoms
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
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	804	CLA	O1D-CGD-O2D-CED
26	J	103	CLA	O1D-CGD-O2D-CED
26	s	403	CLA	O1D-CGD-O2D-CED
26	a	311	CLA	O1D-CGD-O2D-CED
26	m	612	CLA	O1D-CGD-O2D-CED
26	m	613	CLA	O1D-CGD-O2D-CED
26	j	613	CLA	O1D-CGD-O2D-CED
26	d	309	CLA	O1D-CGD-O2D-CED
36	j	611	KC2	O1D-CGD-O2D-CED
26	B	819	CLA	O1D-CGD-O2D-CED
26	c	306	CLA	O1D-CGD-O2D-CED
26	c	312	CLA	O1D-CGD-O2D-CED
26	h	304	CLA	O1D-CGD-O2D-CED
26	k	602	CLA	O1D-CGD-O2D-CED
26	k	610	CLA	O1D-CGD-O2D-CED
26	j	612	CLA	O1D-CGD-O2D-CED
26	d	318	CLA	O1D-CGD-O2D-CED
33	j	618	DGD	O6D-C5D-C6D-O5D
26	A	822	CLA	CBD-CGD-O2D-CED
26	k	607	CLA	CBD-CGD-O2D-CED
26	i	307	CLA	CBD-CGD-O2D-CED
26	j	610	CLA	CBD-CGD-O2D-CED
26	R	201	CLA	CBD-CGD-O2D-CED
26	A	803	CLA	O1A-CGA-O2A-C1
26	n	610	CLA	O1A-CGA-O2A-C1
28	c	317	LHG	O9-C7-O7-C5
28	c	320	LHG	O9-C7-O7-C5
28	b	318	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
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	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
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	A	804	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	813	CLA	CBD-CGD-O2D-CED
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	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
34	c	319	LMG	C11-C10-O7-C8
26	B	819	CLA	C2C-C3C-CAC-CBC
26	A	814	CLA	O1D-CGD-O2D-CED
26	B	832	CLA	O1D-CGD-O2D-CED
26	a	308	CLA	O1D-CGD-O2D-CED
26	l	307	CLA	O1D-CGD-O2D-CED
26	A	809	CLA	O1A-CGA-O2A-C1
26	b	311	CLA	O1D-CGD-O2D-CED
36	l	312	KC2	CAA-CBA-CGA-O1A
36	l	312	KC2	CAA-CBA-CGA-O2A
36	k	612	KC2	CAA-CBA-CGA-O2A
36	j	611	KC2	CAA-CBA-CGA-O1A
36	j	611	KC2	CAA-CBA-CGA-O2A
36	d	312	KC2	CAA-CBA-CGA-O2A
26	B	801	CLA	C4-C3-C5-C6
26	B	816	CLA	C4-C3-C5-C6
26	n	607	CLA	C4-C3-C5-C6
26	B	816	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	n	607	CLA	C2-C3-C5-C6
26	n	609	CLA	C2-C3-C5-C6
26	B	842	CLA	O1D-CGD-O2D-CED
26	l	301	CLA	O1D-CGD-O2D-CED
26	B	822	CLA	C2A-CAA-CBA-CGA
26	j	601	CLA	C2A-CAA-CBA-CGA
26	d	308	CLA	C2A-CAA-CBA-CGA
26	n	613	CLA	C2A-CAA-CBA-CGA
26	l	311	CLA	O1A-CGA-O2A-C1
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
27	A	842	PQN	C11-C12-C13-C14
27	B	843	PQN	C11-C12-C13-C14
26	l	310	CLA	CBD-CGD-O2D-CED
26	k	603	CLA	CBD-CGD-O2D-CED
30	a	317	LMU	O5B-C5B-C6B-O6B
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

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Mol	Chain	Res	Type	Atoms
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
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
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

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Mol	Chain	Res	Type	Atoms
26	d	305	CLA	O1A-CGA-O2A-C1
26	B	828	CLA	O1D-CGD-O2D-CED
26	j	607	CLA	C2C-C3C-CAC-CBC
26	A	832	CLA	O1D-CGD-O2D-CED
26	a	305	CLA	O1D-CGD-O2D-CED
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
26	n	604	CLA	C3-C5-C6-C7
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
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	821	CLA	O1D-CGD-O2D-CED
26	i	301	CLA	O1D-CGD-O2D-CED
26	d	313	CLA	O1D-CGD-O2D-CED
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
34	F	206	LMG	O6-C5-C6-O5
34	L	209	LMG	O6-C5-C6-O5
26	A	819	CLA	O1A-CGA-O2A-C1
26	L	206	CLA	O1A-CGA-O2A-C1
26	h	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	A	831	CLA	O1D-CGD-O2D-CED
26	d	302	CLA	O1D-CGD-O2D-CED
30	a	317	LMU	C4B-C5B-C6B-O6B
34	L	209	LMG	C4-C5-C6-O5
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	i	308	CLA	O1D-CGD-O2D-CED
26	s	403	CLA	O1A-CGA-O2A-C1
26	n	602	CLA	O1A-CGA-O2A-C1
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	836	CLA	CBD-CGD-O2D-CED
26	k	606	CLA	CBD-CGD-O2D-CED
26	i	302	CLA	CBD-CGD-O2D-CED
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	828	CLA	CBA-CGA-O2A-C1
26	R	201	CLA	CBA-CGA-O2A-C1
28	i	317	LHG	C24-C23-O8-C6
36	n	612	KC2	CAA-CBA-CGA-O1A
25	A	801	CL0	C4-C3-C5-C6
26	a	301	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	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
26	A	807	CLA	CBD-CGD-O2D-CED
26	i	306	CLA	CBD-CGD-O2D-CED
26	n	602	CLA	CBD-CGD-O2D-CED
33	B	844	DGD	O6E-C5E-C6E-O5E
30	a	317	LMU	O1'-C1-C2-C3
26	l	309	CLA	O1D-CGD-O2D-CED
26	A	820	CLA	O1A-CGA-O2A-C1
26	A	837	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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
30	i	300	LMU	O5'-C1'-O1'-C1
34	Q	301	LMG	O6-C1-O1-C7
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
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
36	k	612	KC2	CAA-CBA-CGA-O1A
36	d	311	KC2	CAA-CBA-CGA-O1A
36	d	312	KC2	CAA-CBA-CGA-O1A
36	n	611	KC2	CAA-CBA-CGA-O2A
26	c	301	CLA	O1A-CGA-O2A-C1
34	L	209	LMG	O10-C28-O8-C9
34	n	620	LMG	O6-C5-C6-O5
26	b	306	CLA	O1D-CGD-O2D-CED
26	B	826	CLA	CBD-CGD-O2D-CED
26	a	301	CLA	CBD-CGD-O2D-CED
26	b	309	CLA	CBD-CGD-O2D-CED
26	k	605	CLA	CBD-CGD-O2D-CED
34	F	206	LMG	C4-C5-C6-O5
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

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Mol	Chain	Res	Type	Atoms
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	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
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	822	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	812	CLA	CBD-CGD-O2D-CED
26	a	310	CLA	CBD-CGD-O2D-CED
34	n	620	LMG	C4-C5-C6-O5
26	b	307	CLA	O1D-CGD-O2D-CED
26	m	605	CLA	O1D-CGD-O2D-CED
26	k	607	CLA	O1D-CGD-O2D-CED
26	i	307	CLA	O1D-CGD-O2D-CED
26	j	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	j	610	CLA	O1D-CGD-O2D-CED
26	R	201	CLA	O1D-CGD-O2D-CED
26	B	821	CLA	O1D-CGD-O2D-CED
36	k	613	KC2	CAA-CBA-CGA-O2A
36	n	611	KC2	CAA-CBA-CGA-O1A
36	n	612	KC2	CAA-CBA-CGA-O2A
26	m	602	CLA	C4-C3-C5-C6
26	m	602	CLA	C2-C3-C5-C6
26	B	803	CLA	C3-C5-C6-C7
26	s	402	CLA	C3-C5-C6-C7
26	B	823	CLA	CBD-CGD-O2D-CED
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
33	B	844	DGD	C4E-C5E-C6E-O5E
26	A	804	CLA	O1D-CGD-O2D-CED
26	i	304	CLA	O1D-CGD-O2D-CED
30	i	300	LMU	C2'-C1'-O1'-C1
32	A	854	SQD	C2-C1-O6-C44
33	B	844	DGD	C2D-C1D-O3G-C3G
34	Q	301	LMG	C2-C1-O1-C7
28	L	208	LHG	O2-C2-C3-O3
26	B	830	CLA	O1D-CGD-O2D-CED
26	h	305	CLA	O1D-CGD-O2D-CED
26	l	305	CLA	CBA-CGA-O2A-C1
26	A	806	CLA	CBD-CGD-O2D-CED
26	n	605	CLA	CBD-CGD-O2D-CED
26	c	307	CLA	O1D-CGD-O2D-CED
29	A	845	WVN	C11-C19-C22-C24
29	A	846	WVN	C20-C23-C25-C27
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	848	WVN	C29-C31-C32-C35
29	A	848	WVN	C30-C33-C34-C38
29	A	857	WVN	C20-C23-C25-C27
29	A	857	WVN	C29-C31-C32-C35

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Mol	Chain	Res	Type	Atoms
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	848	WVN	C20-C23-C25-C27
29	B	849	WVN	C20-C23-C25-C27
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	203	WVN	C30-C33-C34-C38
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	C20-C23-C25-C27
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	K	102	WVN	C30-C33-C34-C38
29	s	405	WVN	C20-C23-C25-C27
29	s	407	WVN	C11-C19-C22-C24
29	s	407	WVN	C20-C23-C25-C27
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	303	WVN	C11-C19-C22-C24
29	l	303	WVN	C29-C31-C32-C35
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	310	II0	C32-C34-C36-C38
35	h	312	II0	C32-C34-C36-C38
35	l	314	II0	C32-C34-C36-C38
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	314	II0	C32-C34-C36-C38
35	j	614	II0	C31-C33-C35-C37
35	j	615	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
35	d	301	II0	C31-C33-C35-C37
35	d	319	II0	C31-C33-C35-C37
35	d	319	II0	C32-C34-C36-C38
35	n	616	II0	C32-C34-C36-C38
37	b	301	IHT	C18-C22-C23-C25
37	b	316	IHT	C18-C22-C23-C25
37	b	316	IHT	C30-C32-C33-C36
37	m	617	IHT	C18-C22-C23-C25
37	n	617	IHT	C18-C22-C23-C25
30	A	850	LMU	O5'-C5'-C6'-O6'
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	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	I	101	WVN	C30-C33-C34-C37
29	J	101	WVN	C11-C19-C22-C26
29	J	102	WVN	C20-C23-C25-C28
29	L	201	WVN	C30-C33-C34-C37
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	C20-C23-C25-C28
29	R	200	WVN	C11-C19-C22-C26
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
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

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Mol	Chain	Res	Type	Atoms
35	k	616	II0	C32-C34-C36-C40
35	i	316	II0	C31-C33-C35-C39
35	i	316	II0	C32-C34-C36-C40
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	319	II0	C31-C33-C35-C39
35	n	615	II0	C31-C33-C35-C39
35	n	616	II0	C31-C33-C35-C39
37	b	301	IHT	C18-C22-C23-C27
37	b	316	IHT	C30-C32-C33-C37
37	m	617	IHT	C18-C22-C23-C27
26	A	837	CLA	C2A-CAA-CBA-CGA
26	B	841	CLA	C2A-CAA-CBA-CGA
26	F	202	CLA	C3-C5-C6-C7
26	s	402	CLA	C2A-CAA-CBA-CGA
26	h	302	CLA	C2A-CAA-CBA-CGA
26	m	610	CLA	O1D-CGD-O2D-CED
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
36	c	310	KC2	CBD-CGD-O2D-CED
33	B	844	DGD	C2B-C1B-O2G-C2G
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
33	B	844	DGD	O1G-C1G-C2G-O2G
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	A	834	CLA	C5-C6-C7-C8
26	s	408	CLA	C15-C16-C17-C18
26	B	831	CLA	C2-C1-O2A-CGA
26	h	301	CLA	C2-C1-O2A-CGA
26	A	813	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	841	CLA	O1D-CGD-O2D-CED
26	h	308	CLA	O1D-CGD-O2D-CED
26	l	304	CLA	O1D-CGD-O2D-CED
26	n	610	CLA	O1D-CGD-O2D-CED
28	c	317	LHG	C28-C29-C30-C31
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	j	617	LHG	C23-C24-C25-C26
26	A	823	CLA	O1D-CGD-O2D-CED
26	j	608	CLA	O1D-CGD-O2D-CED
26	j	610	CLA	C5-C6-C7-C8
26	B	815	CLA	CBD-CGD-O2D-CED
26	n	607	CLA	CBD-CGD-O2D-CED
26	F	201	CLA	C6-C7-C8-C10
26	A	836	CLA	O1D-CGD-O2D-CED
26	n	604	CLA	CBA-CGA-O2A-C1
36	k	613	KC2	CAA-CBA-CGA-O1A
36	i	309	KC2	CAA-CBA-CGA-O2A
26	k	614	CLA	C2C-C3C-CAC-CBC
28	A	849	LHG	C7-C8-C9-C10
28	i	317	LHG	C23-C24-C25-C26
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
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

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Mol	Chain	Res	Type	Atoms
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
26	B	805	CLA	O1A-CGA-O2A-C1
26	m	601	CLA	O1D-CGD-O2D-CED
26	a	307	CLA	C15-C16-C17-C18
34	c	319	LMG	C4-C5-C6-O5
28	J	105	LHG	C23-C24-C25-C26
28	L	208	LHG	C23-C24-C25-C26
28	b	302	LHG	C7-C8-C9-C10
28	b	302	LHG	C23-C24-C25-C26
28	l	318	LHG	C7-C8-C9-C10
34	c	319	LMG	C28-C29-C30-C31
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
26	k	608	CLA	CBD-CGD-O2D-CED
26	A	817	CLA	C13-C15-C16-C17
26	B	820	CLA	C15-C16-C17-C18
26	b	304	CLA	C5-C6-C7-C8
26	n	608	CLA	C5-C6-C7-C8
26	j	607	CLA	C4C-C3C-CAC-CBC
26	A	807	CLA	C2A-CAA-CBA-CGA
26	A	815	CLA	C2A-CAA-CBA-CGA
26	A	821	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	608	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	d	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	807	CLA	C15-C16-C17-C18
26	A	818	CLA	C13-C15-C16-C17
26	B	834	CLA	C8-C10-C11-C12
26	B	836	CLA	C10-C11-C12-C13
26	B	836	CLA	C15-C16-C17-C18
26	F	201	CLA	C13-C15-C16-C17
26	s	406	CLA	C8-C10-C11-C12
26	s	408	CLA	C8-C10-C11-C12
26	b	306	CLA	C8-C10-C11-C12
26	b	306	CLA	C13-C15-C16-C17
26	l	307	CLA	C13-C15-C16-C17
26	k	608	CLA	C15-C16-C17-C18
27	A	842	PQN	C20-C21-C22-C23
27	B	843	PQN	C15-C16-C17-C18
28	B	851	LHG	C23-C24-C25-C26
28	b	318	LHG	C23-C24-C25-C26
28	j	617	LHG	C7-C8-C9-C10
28	n	619	LHG	C23-C24-C25-C26
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	b	308	CLA	C3-C5-C6-C7
26	s	402	CLA	O1D-CGD-O2D-CED
26	c	301	CLA	O1D-CGD-O2D-CED
30	A	858	LMU	O5B-C1B-O1B-C4'
30	A	858	LMU	C5'-C4'-O1B-C1B
26	A	812	CLA	C13-C15-C16-C17
26	A	819	CLA	C13-C15-C16-C17
26	A	826	CLA	C5-C6-C7-C8
26	A	831	CLA	C13-C15-C16-C17
26	A	841	CLA	C5-C6-C7-C8
26	A	852	CLA	C15-C16-C17-C18
26	B	808	CLA	C15-C16-C17-C18
26	B	822	CLA	C13-C15-C16-C17
26	F	201	CLA	C8-C10-C11-C12
26	s	402	CLA	C10-C11-C12-C13
26	h	304	CLA	C15-C16-C17-C18
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	k	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	i	301	CLA	C5-C6-C7-C8
26	n	608	CLA	C10-C11-C12-C13
28	L	207	LHG	O2-C2-C3-O3
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	k	602	CLA	O1A-CGA-O2A-C1
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
30	a	317	LMU	O5'-C5'-C6'-O6'
26	B	808	CLA	C3-C5-C6-C7
26	n	608	CLA	C3-C5-C6-C7
26	B	813	CLA	O1D-CGD-O2D-CED
26	c	304	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	B	817	CLA	C10-C11-C12-C13
26	B	834	CLA	C13-C15-C16-C17
26	L	203	CLA	C8-C10-C11-C12
26	s	406	CLA	C10-C11-C12-C13
26	c	308	CLA	C15-C16-C17-C18
26	c	312	CLA	C8-C10-C11-C12
26	a	306	CLA	C5-C6-C7-C8
26	j	610	CLA	C8-C10-C11-C12
26	B	816	CLA	CBD-CGD-O2D-CED
30	i	300	LMU	O5'-C5'-C6'-O6'
26	B	822	CLA	O1D-CGD-O2D-CED
26	B	833	CLA	O1D-CGD-O2D-CED
26	a	302	CLA	O1D-CGD-O2D-CED
26	A	816	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	A	838	CLA	C5-C6-C7-C8
26	A	840	CLA	C15-C16-C17-C18
26	B	816	CLA	C5-C6-C7-C8
26	h	304	CLA	C13-C15-C16-C17
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	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	c	309	CLA	CBD-CGD-O2D-CED
34	F	205	LMG	C11-C10-O7-C8
34	c	318	LMG	C11-C10-O7-C8
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	B	806	CLA	O1A-CGA-O2A-C1
26	m	609	CLA	O1A-CGA-O2A-C1
26	l	305	CLA	O1A-CGA-O2A-C1
26	B	802	CLA	O1D-CGD-O2D-CED
26	B	802	CLA	C3-C5-C6-C7
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
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

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Mol	Chain	Res	Type	Atoms
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
26	B	805	CLA	C10-C11-C12-C13
34	c	319	LMG	O9-C10-O7-C8
28	L	207	LHG	C1-C2-C3-O3
28	b	302	LHG	C1-C2-C3-O3
26	A	851	CLA	C2A-CAA-CBA-CGA
26	s	406	CLA	C2A-CAA-CBA-CGA
26	h	303	CLA	C2A-CAA-CBA-CGA
26	m	607	CLA	C2A-CAA-CBA-CGA
26	k	614	CLA	C2A-CAA-CBA-CGA
26	i	307	CLA	C2A-CAA-CBA-CGA
26	d	305	CLA	C2A-CAA-CBA-CGA
26	B	823	CLA	CBA-CGA-O2A-C1
26	Q	302	CLA	CBA-CGA-O2A-C1
28	A	855	LHG	C24-C23-O8-C6
26	A	810	CLA	C8-C10-C11-C12
26	A	835	CLA	C13-C15-C16-C17
26	B	816	CLA	C10-C11-C12-C13
26	h	301	CLA	C13-C15-C16-C17
26	m	610	CLA	C5-C6-C7-C8
35	c	316	II0	C27-C25-C29-C31
35	k	620	II0	C28-C26-C30-C32
26	l	313	CLA	O1D-CGD-O2D-CED
26	A	813	CLA	C5-C6-C7-C8
26	A	852	CLA	C8-C10-C11-C12
26	B	810	CLA	C13-C15-C16-C17
26	s	402	CLA	C15-C16-C17-C18
26	m	606	CLA	C15-C16-C17-C18
26	A	819	CLA	C15-C16-C17-C18
26	B	810	CLA	C15-C16-C17-C18
26	B	818	CLA	C8-C10-C11-C12
26	B	822	CLA	C10-C11-C12-C13
26	B	825	CLA	C13-C15-C16-C17
26	B	829	CLA	C5-C6-C7-C8
26	m	602	CLA	C8-C10-C11-C12
26	l	313	CLA	C5-C6-C7-C8
26	d	302	CLA	C10-C11-C12-C13
27	A	842	PQN	C23-C25-C26-C27
26	B	801	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	i	302	CLA	C4-C3-C5-C6
26	B	837	CLA	C13-C15-C16-C17
26	m	606	CLA	C5-C6-C7-C8
26	n	608	CLA	C13-C15-C16-C17
26	l	305	CLA	O1D-CGD-O2D-CED
26	k	606	CLA	O1D-CGD-O2D-CED
26	d	308	CLA	O1D-CGD-O2D-CED
30	A	850	LMU	C2'-C1'-O1'-C1
33	j	618	DGD	C2D-C1D-O3G-C3G
34	b	319	LMG	C2-C1-O1-C7
26	A	812	CLA	C15-C16-C17-C18
26	b	308	CLA	C10-C11-C12-C13
28	j	617	LHG	O2-C2-C3-O3
28	n	619	LHG	O2-C2-C3-O3
26	L	204	CLA	CBA-CGA-O2A-C1
26	c	302	CLA	CBA-CGA-O2A-C1
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	l	310	CLA	O1A-CGA-O2A-C1
26	i	306	CLA	O1A-CGA-O2A-C1
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
26	i	302	CLA	O1D-CGD-O2D-CED
26	c	304	CLA	C10-C11-C12-C13
29	A	845	WVN	C30-C33-C34-C38
29	B	849	WVN	C30-C33-C34-C38
29	B	850	WVN	C11-C19-C22-C24
29	F	204	WVN	C20-C23-C25-C27
29	J	102	WVN	C30-C33-C34-C38

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Mol	Chain	Res	Type	Atoms
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	s	405	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
35	i	312	II0	C32-C34-C36-C38
37	j	616	IHT	C18-C22-C23-C25
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	846	WVN	C30-C33-C34-C37
29	B	847	WVN	C30-C33-C34-C37
29	B	850	WVN	C29-C31-C32-C36
29	F	204	WVN	C20-C23-C25-C28
29	I	101	WVN	C29-C31-C32-C36
29	J	101	WVN	C29-C31-C32-C36
29	M	101	WVN	C11-C19-C22-C26
29	i	315	WVN	C11-C19-C22-C26
29	R	200	WVN	C20-C23-C25-C28
29	R	200	WVN	C29-C31-C32-C36
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	d	317	II0	C32-C34-C36-C40
35	n	618	II0	C32-C34-C36-C40
37	j	616	IHT	C18-C22-C23-C27
37	n	617	IHT	C18-C22-C23-C27
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	A	802	CLA	C2A-CAA-CBA-CGA
26	A	828	CLA	C2A-CAA-CBA-CGA
26	F	202	CLA	C2A-CAA-CBA-CGA
26	c	307	CLA	C2A-CAA-CBA-CGA
26	c	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	h	304	CLA	C2A-CAA-CBA-CGA
26	m	612	CLA	C2A-CAA-CBA-CGA
26	k	610	CLA	C2A-CAA-CBA-CGA
26	A	819	CLA	C8-C10-C11-C12
26	A	856	CLA	C15-C16-C17-C18
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
26	A	818	CLA	CBD-CGD-O2D-CED
34	c	318	LMG	C7-C8-O7-C10
29	A	847	WVN	C22-C26-C29-C31
35	i	312	II0	C25-C29-C31-C33
26	A	856	CLA	C16-C17-C18-C19
26	B	836	CLA	O1D-CGD-O2D-CED
25	A	801	CL0	O1A-CGA-O2A-C1
26	A	823	CLA	O1A-CGA-O2A-C1
26	j	609	CLA	O1A-CGA-O2A-C1
26	l	308	CLA	C3-C5-C6-C7
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
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

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Mol	Chain	Res	Type	Atoms
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
30	A	850	LMU	O5'-C1'-O1'-C1
33	j	618	DGD	O6D-C1D-O3G-C3G
34	c	318	LMG	O6-C1-O1-C7
34	b	319	LMG	O6-C1-O1-C7
28	j	617	LHG	C8-C7-O7-C5
26	m	602	CLA	C2C-C3C-CAC-CBC
26	s	402	CLA	C13-C15-C16-C17
26	h	301	CLA	C5-C6-C7-C8
26	i	306	CLA	O1D-CGD-O2D-CED
28	A	855	LHG	O7-C5-C6-O8
26	n	603	CLA	O1D-CGD-O2D-CED
26	A	813	CLA	CBA-CGA-O2A-C1
26	l	309	CLA	CBA-CGA-O2A-C1
26	j	613	CLA	CBA-CGA-O2A-C1
26	A	808	CLA	C15-C16-C17-C18
26	a	310	CLA	C15-C16-C17-C18
26	F	201	CLA	CBD-CGD-O2D-CED
26	A	807	CLA	O1D-CGD-O2D-CED
26	B	801	CLA	C2-C1-O2A-CGA
26	m	609	CLA	C11-C12-C13-C15
26	i	301	CLA	C16-C17-C18-C20
26	c	304	CLA	C8-C10-C11-C12
26	m	604	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	L	202	CLA	O1D-CGD-O2D-CED
34	c	319	LMG	O6-C5-C6-O5
28	L	207	LHG	C27-C28-C29-C30
28	L	207	LHG	C30-C31-C32-C33
28	s	409	LHG	C32-C33-C34-C35
30	i	300	LMU	C1-C2-C3-C4
28	B	851	LHG	C24-C25-C26-C27
28	m	618	LHG	C27-C28-C29-C30
32	A	854	SQD	C11-C10-C9-C8
33	B	844	DGD	C7B-C8B-C9B-CAB
34	F	205	LMG	C16-C17-C18-C19
26	m	613	CLA	C13-C15-C16-C17
26	m	613	CLA	C15-C16-C17-C18
28	L	207	LHG	C25-C26-C27-C28
34	c	319	LMG	C29-C30-C31-C32
34	Q	301	LMG	C30-C31-C32-C33
26	A	822	CLA	O1A-CGA-O2A-C1
26	d	313	CLA	O1A-CGA-O2A-C1
26	B	838	CLA	O1D-CGD-O2D-CED
26	A	817	CLA	CBA-CGA-O2A-C1
26	F	201	CLA	CBA-CGA-O2A-C1
26	l	313	CLA	CBA-CGA-O2A-C1
28	L	208	LHG	C13-C14-C15-C16
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
28	c	320	LHG	C32-C33-C34-C35
28	b	302	LHG	C27-C28-C29-C30
28	n	619	LHG	C28-C29-C30-C31
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
26	b	310	CLA	C10-C11-C12-C13
26	A	808	CLA	C4B-C3B-CAB-CBB
26	A	823	CLA	C4B-C3B-CAB-CBB
26	A	830	CLA	C4B-C3B-CAB-CBB
26	A	832	CLA	C4B-C3B-CAB-CBB
26	A	852	CLA	C4B-C3B-CAB-CBB
26	B	803	CLA	C4B-C3B-CAB-CBB
26	B	818	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	B	830	CLA	C4B-C3B-CAB-CBB
26	B	837	CLA	C4B-C3B-CAB-CBB
26	B	839	CLA	C4B-C3B-CAB-CBB
26	J	103	CLA	C4B-C3B-CAB-CBB
26	K	101	CLA	C4B-C3B-CAB-CBB
26	c	305	CLA	C4B-C3B-CAB-CBB
26	c	312	CLA	C4B-C3B-CAB-CBB
26	a	310	CLA	C4B-C3B-CAB-CBB
26	b	309	CLA	C4B-C3B-CAB-CBB
26	b	313	CLA	C4B-C3B-CAB-CBB
26	m	601	CLA	C4B-C3B-CAB-CBB
26	m	612	CLA	C4B-C3B-CAB-CBB
26	l	308	CLA	C4B-C3B-CAB-CBB
26	k	601	CLA	C4B-C3B-CAB-CBB
26	k	604	CLA	C4B-C3B-CAB-CBB
26	k	605	CLA	C4B-C3B-CAB-CBB
26	k	609	CLA	C4B-C3B-CAB-CBB
26	i	301	CLA	C4B-C3B-CAB-CBB
26	i	302	CLA	C4B-C3B-CAB-CBB
26	i	306	CLA	C4B-C3B-CAB-CBB
26	i	310	CLA	C4B-C3B-CAB-CBB
26	j	601	CLA	C4B-C3B-CAB-CBB
26	j	605	CLA	C4B-C3B-CAB-CBB
26	j	609	CLA	C4B-C3B-CAB-CBB
26	d	318	CLA	C4B-C3B-CAB-CBB
26	n	605	CLA	C4B-C3B-CAB-CBB
26	n	608	CLA	C4B-C3B-CAB-CBB
26	Q	302	CLA	C4B-C3B-CAB-CBB
28	c	317	LHG	C27-C28-C29-C30
33	j	618	DGD	C6A-C7A-C8A-C9A
34	L	209	LMG	C18-C19-C20-C21
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	610	CLA	C6-C7-C8-C10
26	n	602	CLA	O1D-CGD-O2D-CED
26	A	821	CLA	O1A-CGA-O2A-C1
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	i	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	n	619	LHG	C11-C10-C9-C8
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	b	310	CLA	C13-C15-C16-C17
26	l	307	CLA	C8-C10-C11-C12
26	B	807	CLA	C11-C10-C8-C7
26	s	403	CLA	C6-C7-C8-C10
26	j	601	CLA	C11-C10-C8-C7
27	A	842	PQN	C17-C18-C20-C21
34	F	205	LMG	C31-C32-C33-C34
30	A	858	LMU	C3'-C4'-O1B-C1B
26	B	812	CLA	C8-C10-C11-C12
26	B	826	CLA	C10-C11-C12-C13
28	s	409	LHG	C29-C30-C31-C32
28	i	317	LHG	C24-C25-C26-C27
26	A	826	CLA	O1A-CGA-O2A-C1
26	m	613	CLA	C3-C5-C6-C7
26	n	607	CLA	C3-C5-C6-C7
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
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
28	L	208	LHG	C14-C15-C16-C17
32	A	854	SQD	C11-C12-C13-C14
26	A	820	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	F	205	LMG	C33-C34-C35-C36
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	B	834	CLA	C16-C17-C18-C20
26	B	823	CLA	O1A-CGA-O2A-C1
26	Q	302	CLA	O1A-CGA-O2A-C1
28	B	851	LHG	O10-C23-O8-C6
34	n	620	LMG	C31-C32-C33-C34
28	A	843	LHG	C24-C25-C26-C27
34	c	319	LMG	C16-C17-C18-C19
26	n	606	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
28	B	851	LHG	C9-C10-C11-C12
28	B	851	LHG	C32-C33-C34-C35
26	B	819	CLA	C3-C5-C6-C7
26	B	841	CLA	C3-C5-C6-C7
28	A	855	LHG	C23-C24-C25-C26
28	L	207	LHG	C23-C24-C25-C26
28	c	320	LHG	C23-C24-C25-C26
28	B	851	LHG	C27-C28-C29-C30
28	c	320	LHG	C24-C25-C26-C27
28	b	318	LHG	C26-C27-C28-C29
28	l	318	LHG	C11-C10-C9-C8
30	A	850	LMU	C5-C6-C7-C8
30	a	317	LMU	C11-C10-C9-C8
30	i	300	LMU	C2-C3-C4-C5
34	c	319	LMG	C30-C31-C32-C33
26	c	302	CLA	O1A-CGA-O2A-C1
28	b	302	LHG	C26-C27-C28-C29
30	i	300	LMU	C7-C8-C9-C10
32	A	854	SQD	C16-C17-C18-C19
33	B	844	DGD	CEB-CFB-CGB-CHB
34	Q	301	LMG	C15-C16-C17-C18
28	s	409	LHG	C27-C28-C29-C30
34	c	318	LMG	C18-C19-C20-C21
26	a	307	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	b	304	CLA	O1D-CGD-O2D-CED
34	F	206	LMG	C16-C17-C18-C19
34	n	620	LMG	C37-C38-C39-C40
26	A	816	CLA	C16-C17-C18-C19
26	A	856	CLA	C16-C17-C18-C20
26	L	204	CLA	O1A-CGA-O2A-C1
26	A	808	CLA	C2B-C3B-CAB-CBB
26	A	811	CLA	C2B-C3B-CAB-CBB
26	A	838	CLA	C2B-C3B-CAB-CBB
26	B	818	CLA	C2B-C3B-CAB-CBB
26	B	828	CLA	C2B-C3B-CAB-CBB
26	B	832	CLA	C2B-C3B-CAB-CBB
26	B	837	CLA	C2B-C3B-CAB-CBB
26	B	839	CLA	C2B-C3B-CAB-CBB
26	B	840	CLA	C2B-C3B-CAB-CBB
26	J	103	CLA	C2B-C3B-CAB-CBB
26	L	202	CLA	C2B-C3B-CAB-CBB
26	K	101	CLA	C2B-C3B-CAB-CBB
26	c	306	CLA	C2B-C3B-CAB-CBB
26	c	312	CLA	C2B-C3B-CAB-CBB
26	a	305	CLA	C2B-C3B-CAB-CBB
26	b	307	CLA	C2B-C3B-CAB-CBB
26	b	310	CLA	C2B-C3B-CAB-CBB
26	h	303	CLA	C2B-C3B-CAB-CBB
26	h	308	CLA	C2B-C3B-CAB-CBB
26	m	601	CLA	C2B-C3B-CAB-CBB
26	m	610	CLA	C2B-C3B-CAB-CBB
26	l	311	CLA	C2B-C3B-CAB-CBB
26	k	604	CLA	C2B-C3B-CAB-CBB
26	k	609	CLA	C2B-C3B-CAB-CBB
26	i	301	CLA	C2B-C3B-CAB-CBB
26	i	305	CLA	C2B-C3B-CAB-CBB
26	i	306	CLA	C2B-C3B-CAB-CBB
26	j	601	CLA	C2B-C3B-CAB-CBB
26	j	606	CLA	C2B-C3B-CAB-CBB
26	j	610	CLA	C2B-C3B-CAB-CBB
26	j	612	CLA	C2B-C3B-CAB-CBB
26	d	308	CLA	C2B-C3B-CAB-CBB
26	n	610	CLA	C2B-C3B-CAB-CBB
29	B	846	WVN	C15-C13-C20-C23
29	B	850	WVN	C15-C13-C20-C23
29	L	205	WVN	C06-C13-C20-C23

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Mol	Chain	Res	Type	Atoms
29	l	316	WVN	C15-C13-C20-C23
29	i	315	WVN	C06-C13-C20-C23
37	m	617	IHT	C02-C07-C18-C22
28	L	208	LHG	C11-C10-C9-C8
28	L	208	LHG	C27-C28-C29-C30
26	B	820	CLA	CBD-CGD-O2D-CED
26	j	607	CLA	CBD-CGD-O2D-CED
26	A	837	CLA	O1D-CGD-O2D-CED
26	i	305	CLA	CBA-CGA-O2A-C1
26	j	606	CLA	CBA-CGA-O2A-C1
26	n	603	CLA	CBA-CGA-O2A-C1
26	i	307	CLA	C3-C5-C6-C7
28	A	849	LHG	C11-C10-C9-C8
34	c	319	LMG	C10-C11-C12-C13
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	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
33	j	618	DGD	C4D-C5D-C6D-O5D
28	A	843	LHG	C11-C10-C9-C8
34	n	620	LMG	C29-C30-C31-C32
26	A	809	CLA	C4-C3-C5-C6
26	h	304	CLA	C4-C3-C5-C6
28	b	318	LHG	C12-C13-C14-C15
34	c	319	LMG	C31-C32-C33-C34
26	B	814	CLA	C15-C16-C17-C18
26	i	307	CLA	C5-C6-C7-C8
26	i	302	CLA	C2-C3-C5-C6
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
26	l	301	CLA	CBA-CGA-O2A-C1
26	k	607	CLA	CBA-CGA-O2A-C1
26	b	309	CLA	C3-C5-C6-C7
26	A	824	CLA	C14-C13-C15-C16
28	A	855	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
28	L	208	LHG	C32-C33-C34-C35
32	A	854	SQD	C9-C10-C11-C12
26	k	609	CLA	C5-C6-C7-C8
34	c	319	LMG	C18-C19-C20-C21
28	A	843	LHG	C30-C31-C32-C33
30	a	317	LMU	C6-C7-C8-C9
34	c	319	LMG	C2-C1-O1-C7
26	A	833	CLA	CBD-CGD-O2D-CED
26	a	309	CLA	CBD-CGD-O2D-CED
26	A	809	CLA	C5-C6-C7-C8
26	A	856	CLA	C13-C15-C16-C17
26	i	310	CLA	C10-C11-C12-C13
28	A	843	LHG	C31-C32-C33-C34
28	l	318	LHG	C23-C24-C25-C26
34	c	318	LMG	O6-C5-C6-O5
28	n	619	LHG	C29-C30-C31-C32
34	F	205	LMG	C32-C33-C34-C35
26	B	837	CLA	C15-C16-C17-C18
26	m	608	CLA	C13-C15-C16-C17
26	A	816	CLA	C3-C5-C6-C7
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	301	CLA	C16-C17-C18-C19
26	i	301	CLA	C16-C17-C18-C19
26	Q	302	CLA	C16-C17-C18-C19
28	n	619	LHG	C7-C8-C9-C10
26	b	310	CLA	C5-C6-C7-C8
28	j	617	LHG	O9-C7-O7-C5
28	A	843	LHG	C9-C10-C11-C12
28	s	409	LHG	C24-C25-C26-C27
34	L	209	LMG	C23-C24-C25-C26
26	m	602	CLA	C4C-C3C-CAC-CBC
26	B	822	CLA	O1A-CGA-O2A-C1
26	i	310	CLA	C8-C10-C11-C12
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

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Mol	Chain	Res	Type	Atoms
35	i	316	II0	C32-C34-C36-C38
35	d	316	II0	C32-C34-C36-C38
35	n	618	II0	C32-C34-C36-C38
34	Q	301	LMG	C31-C32-C33-C34
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	A	808	CLA	C2A-CAA-CBA-CGA
26	Q	302	CLA	C2A-CAA-CBA-CGA
26	A	816	CLA	C16-C17-C18-C20
28	A	843	LHG	C28-C29-C30-C31
28	b	302	LHG	C24-C25-C26-C27
32	A	854	SQD	C12-C13-C14-C15
34	c	318	LMG	C23-C24-C25-C26
26	A	809	CLA	C2-C3-C5-C6
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
28	c	317	LHG	C30-C31-C32-C33
33	B	844	DGD	C4A-C5A-C6A-C7A
34	F	205	LMG	C17-C18-C19-C20
26	b	309	CLA	O1D-CGD-O2D-CED
26	l	311	CLA	C5-C6-C7-C8
34	c	318	LMG	C22-C23-C24-C25
34	c	319	LMG	C32-C33-C34-C35
26	F	202	CLA	O1A-CGA-O2A-C1
26	b	304	CLA	O1A-CGA-O2A-C1
34	F	206	LMG	C17-C18-C19-C20
34	c	318	LMG	C30-C31-C32-C33
26	k	614	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	L	208	LHG	C28-C29-C30-C31
28	A	855	LHG	C24-C25-C26-C27
28	n	619	LHG	C30-C31-C32-C33
33	B	844	DGD	C2A-C3A-C4A-C5A
26	A	835	CLA	C5-C6-C7-C8
26	B	841	CLA	C15-C16-C17-C18
26	l	301	CLA	C15-C16-C17-C18
36	c	310	KC2	C4C-C3C-CAC-CBC
36	l	312	KC2	C4B-C3B-CAB-CBB
36	l	312	KC2	C4C-C3C-CAC-CBC
36	k	613	KC2	C2A-CAA-CBA-CGA
36	i	318	KC2	C4B-C3B-CAB-CBB
36	n	611	KC2	C4B-C3B-CAB-CBB
26	c	302	CLA	C11-C12-C13-C15
26	B	827	CLA	O1A-CGA-O2A-C1
26	j	607	CLA	O1A-CGA-O2A-C1
26	n	603	CLA	O1A-CGA-O2A-C1
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	h	304	CLA	C8-C10-C11-C12
26	i	307	CLA	C13-C15-C16-C17
26	j	601	CLA	C8-C10-C11-C12
27	A	842	PQN	C18-C20-C21-C22
26	B	826	CLA	O1D-CGD-O2D-CED
26	a	301	CLA	O1D-CGD-O2D-CED
33	B	844	DGD	CBA-CCA-CDA-CEA
33	j	618	DGD	C4A-C5A-C6A-C7A
34	b	319	LMG	C14-C15-C16-C17
26	A	840	CLA	C3-C5-C6-C7
26	A	841	CLA	C3-C5-C6-C7
34	c	319	LMG	O1-C7-C8-O7
28	j	617	LHG	C9-C10-C11-C12
30	A	850	LMU	C4'-C5'-C6'-O6'
26	B	823	CLA	O1D-CGD-O2D-CED
26	k	605	CLA	O1D-CGD-O2D-CED
26	j	606	CLA	O1A-CGA-O2A-C1
34	F	205	LMG	C18-C19-C20-C21
26	B	836	CLA	C13-C15-C16-C17
34	b	319	LMG	O6-C5-C6-O5
28	b	318	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	n	619	LHG	C32-C33-C34-C35
33	j	618	DGD	C4B-C5B-C6B-C7B
26	a	301	CLA	C16-C17-C18-C20
26	A	807	CLA	C8-C10-C11-C12
30	A	850	LMU	C2-C3-C4-C5
26	B	803	CLA	C4-C3-C5-C6
26	h	304	CLA	C2-C3-C5-C6
28	j	617	LHG	C1-C2-C3-O3
26	A	814	CLA	C2A-CAA-CBA-CGA
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
36	n	612	KC2	CBD-CGD-O2D-CED
26	k	614	CLA	C4C-C3C-CAC-CBC
26	B	812	CLA	O1D-CGD-O2D-CED
30	A	850	LMU	C7-C8-C9-C10
26	A	838	CLA	C8-C10-C11-C12
26	c	308	CLA	C10-C11-C12-C13
35	c	313	II0	C28-C26-C30-C32
35	h	310	II0	C27-C25-C29-C31
35	h	312	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
28	A	849	LHG	C9-C10-C11-C12
28	B	851	LHG	C28-C29-C30-C31
28	n	619	LHG	C27-C28-C29-C30
34	F	205	LMG	C30-C31-C32-C33
30	A	858	LMU	O5'-C5'-C6'-O6'
26	a	310	CLA	O1D-CGD-O2D-CED
26	n	605	CLA	O1D-CGD-O2D-CED
28	A	855	LHG	O1-C1-C2-O2
28	L	207	LHG	O1-C1-C2-O2
28	j	617	LHG	O1-C1-C2-O2
26	m	606	CLA	O1A-CGA-O2A-C1
26	m	612	CLA	O1A-CGA-O2A-C1
26	l	301	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	826	CLA	C3-C5-C6-C7
28	B	851	LHG	C31-C32-C33-C34
36	m	611	KC2	CAA-CBA-CGA-O1A
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
34	F	205	LMG	O6-C5-C6-O5
33	B	844	DGD	C8A-C9A-CAA-CBA
33	B	844	DGD	CAB-CBB-CCB-CDB
28	L	207	LHG	C32-C33-C34-C35
26	A	806	CLA	O1A-CGA-O2A-C1
26	k	607	CLA	O1A-CGA-O2A-C1
26	i	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	851	LHG	O6-C4-C5-C6
28	c	317	LHG	O6-C4-C5-C6
28	b	302	LHG	C29-C30-C31-C32
34	n	620	LMG	C17-C18-C19-C20
28	A	843	LHG	C23-C24-C25-C26
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	837	CLA	C6-C7-C8-C10
26	A	841	CLA	C11-C10-C8-C7
26	A	841	CLA	C11-C12-C13-C15
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
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	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	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

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Mol	Chain	Res	Type	Atoms
28	n	619	LHG	C24-C25-C26-C27
26	B	810	CLA	C16-C17-C18-C20
26	A	831	CLA	O1A-CGA-O2A-C1
26	h	307	CLA	O1A-CGA-O2A-C1
36	k	611	KC2	CAA-CBA-CGA-O1A
26	A	802	CLA	C15-C16-C17-C18
26	s	403	CLA	C5-C6-C7-C8
26	k	604	CLA	C5-C6-C7-C8
28	c	317	LHG	C7-C8-C9-C10
33	j	618	DGD	CDB-CEB-CFB-CGB
34	F	205	LMG	C20-C21-C22-C23
26	m	603	CLA	C4-C3-C5-C6
26	A	826	CLA	C2-C3-C5-C6
26	B	803	CLA	C2-C3-C5-C6
26	B	834	CLA	C2-C3-C5-C6
26	m	603	CLA	C2-C3-C5-C6
26	A	819	CLA	C10-C11-C12-C13
26	d	305	CLA	CBD-CGD-O2D-CED
26	d	310	CLA	CBD-CGD-O2D-CED
28	l	318	LHG	C8-C7-O7-C5
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	d	318	CLA	C2A-CAA-CBA-CGA
26	A	816	CLA	C6-C7-C8-C9
26	A	816	CLA	C11-C10-C8-C9
26	B	801	CLA	C11-C10-C8-C9
26	B	818	CLA	C11-C12-C13-C14
26	B	819	CLA	C14-C13-C15-C16
26	B	829	CLA	C14-C13-C15-C16
26	B	831	CLA	C11-C10-C8-C9
26	B	838	CLA	C14-C13-C15-C16
26	B	841	CLA	C6-C7-C8-C9
26	c	304	CLA	C11-C10-C8-C9
26	a	304	CLA	C11-C10-C8-C9
26	a	306	CLA	C14-C13-C15-C16
26	b	308	CLA	C6-C7-C8-C9
26	b	311	CLA	C14-C13-C15-C16
26	h	304	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
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	i	301	CLA	C14-C13-C15-C16
26	j	601	CLA	C11-C10-C8-C9
26	j	609	CLA	C14-C13-C15-C16
26	j	613	CLA	C6-C7-C8-C9
26	Q	302	CLA	C11-C10-C8-C9
27	A	842	PQN	C19-C18-C20-C21
27	A	842	PQN	C21-C22-C23-C24
33	B	844	DGD	CEA-CFA-CGA-CHA
35	l	315	II0	C26-C30-C32-C34
26	A	806	CLA	O1D-CGD-O2D-CED
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
26	b	307	CLA	C14-C13-C15-C16
28	A	844	LHG	C4-C5-C6-O8
28	A	855	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
28	b	302	LHG	O2-C2-C3-O3
26	B	810	CLA	C16-C17-C18-C19
34	F	205	LMG	C38-C39-C40-C41
26	A	828	CLA	C15-C16-C17-C18
26	b	311	CLA	C13-C15-C16-C17
28	B	851	LHG	C25-C26-C27-C28
28	L	208	LHG	C7-C8-C9-C10
26	n	607	CLA	O1D-CGD-O2D-CED
26	k	614	CLA	O1A-CGA-O2A-C1
26	A	826	CLA	C4-C3-C5-C6
26	B	834	CLA	C4-C3-C5-C6
27	A	842	PQN	C14-C13-C15-C16
26	A	828	CLA	C2-C3-C5-C6
28	b	318	LHG	C25-C26-C27-C28
26	B	819	CLA	CBA-CGA-O2A-C1
26	A	852	CLA	C13-C15-C16-C17
26	B	812	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
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	i	311	CLA	C16-C17-C18-C20
29	A	848	WVN	C11-C19-C22-C26
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	m	619	II0	C31-C33-C35-C39
35	d	319	II0	C32-C34-C36-C40
26	B	839	CLA	C5-C6-C7-C8
28	b	318	LHG	C30-C31-C32-C33
26	B	801	CLA	C5-C6-C7-C8
26	B	836	CLA	C8-C10-C11-C12
32	A	854	SQD	C14-C15-C16-C17
26	l	304	CLA	CBA-CGA-O2A-C1
26	k	606	CLA	CBA-CGA-O2A-C1
36	m	611	KC2	CAA-CBA-CGA-O2A
33	B	844	DGD	C3G-C2G-O2G-C1B
34	F	205	LMG	C9-C8-O7-C10
34	Q	301	LMG	C7-C8-O7-C10
26	A	837	CLA	C13-C15-C16-C17
29	A	847	WVN	C32-C36-C39-C40
35	d	315	II0	C36-C40-C42-C41
26	B	837	CLA	C16-C17-C18-C20
30	a	317	LMU	C4-C5-C6-C7
34	F	205	LMG	C15-C16-C17-C18
26	F	201	CLA	C5-C6-C7-C8
26	B	815	CLA	O1D-CGD-O2D-CED
29	B	848	WVN	C31-C32-C36-C39
35	j	614	II0	C33-C35-C39-C41
35	j	614	II0	C34-C36-C40-C42
28	i	317	LHG	C25-C26-C27-C28
28	L	208	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
26	k	608	CLA	O1D-CGD-O2D-CED
26	B	817	CLA	CBA-CGA-O2A-C1
34	L	209	LMG	C17-C18-C19-C20
34	b	319	LMG	C33-C34-C35-C36
30	a	317	LMU	C4'-C5'-C6'-O6'
26	A	856	CLA	C4-C3-C5-C6
28	B	851	LHG	C11-C10-C9-C8
28	L	207	LHG	C11-C10-C9-C8
28	c	320	LHG	C25-C26-C27-C28
34	n	620	LMG	C19-C20-C21-C22
33	B	844	DGD	C6B-C7B-C8B-C9B
26	B	818	CLA	CBA-CGA-O2A-C1
26	s	402	CLA	CBA-CGA-O2A-C1
33	B	844	DGD	C5A-C6A-C7A-C8A
36	c	310	KC2	O1D-CGD-O2D-CED
26	A	856	CLA	CAA-CBA-CGA-O2A
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
28	A	855	LHG	C28-C29-C30-C31
34	F	205	LMG	C22-C23-C24-C25
36	k	611	KC2	CAA-CBA-CGA-O2A
26	i	306	CLA	C5-C6-C7-C8
28	j	617	LHG	C24-C25-C26-C27
28	L	208	LHG	C29-C30-C31-C32
26	h	306	CLA	O1A-CGA-O2A-C1
28	L	207	LHG	C12-C13-C14-C15
28	i	317	LHG	C27-C28-C29-C30
26	B	820	CLA	CBA-CGA-O2A-C1
26	k	608	CLA	CBA-CGA-O2A-C1
26	A	816	CLA	CBD-CGD-O2D-CED
28	m	618	LHG	C8-C7-O7-C5
34	Q	301	LMG	C17-C18-C19-C20
33	j	618	DGD	C6B-C7B-C8B-C9B
34	b	319	LMG	C17-C18-C19-C20
26	B	816	CLA	O1D-CGD-O2D-CED
26	B	814	CLA	C16-C17-C18-C20
26	s	402	CLA	C16-C17-C18-C19
26	l	301	CLA	C16-C17-C18-C20
26	A	828	CLA	C4-C3-C5-C6
26	A	833	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	A	841	CLA	C4-C3-C5-C6
26	b	305	CLA	C4-C3-C5-C6
26	A	838	CLA	C2-C3-C5-C6
26	l	307	CLA	C2-C3-C5-C6
26	B	808	CLA	CBA-CGA-O2A-C1
26	L	202	CLA	CBA-CGA-O2A-C1
26	b	306	CLA	CBA-CGA-O2A-C1
28	L	208	LHG	C11-C12-C13-C14
34	L	209	LMG	C16-C17-C18-C19
28	A	843	LHG	O1-C1-C2-O2
28	l	318	LHG	O1-C1-C2-O2
35	c	314	II0	C10-C22-C24-C26
37	n	617	IHT	C11-C21-C24-C26
26	A	805	CLA	C6-C7-C8-C9
26	A	816	CLA	C14-C13-C15-C16
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	841	CLA	C11-C10-C8-C9
26	A	841	CLA	C11-C12-C13-C14
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	813	CLA	C6-C7-C8-C9
26	B	818	CLA	C11-C10-C8-C9
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-C12-C13-C14
26	B	837	CLA	C14-C13-C15-C16
26	s	403	CLA	C6-C7-C8-C9
26	a	301	CLA	C14-C13-C15-C16
26	a	306	CLA	C11-C12-C13-C14
26	a	309	CLA	C6-C7-C8-C9
26	a	310	CLA	C6-C7-C8-C9
26	b	306	CLA	C6-C7-C8-C9
26	b	306	CLA	C11-C10-C8-C9
26	b	306	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	b	309	CLA	C11-C10-C8-C9
26	b	310	CLA	C11-C10-C8-C9
26	k	608	CLA	C6-C7-C8-C9
26	i	304	CLA	C11-C12-C13-C14
26	d	302	CLA	C11-C12-C13-C14
26	B	804	CLA	C15-C16-C17-C18
26	B	822	CLA	C5-C6-C7-C8
26	A	809	CLA	C4B-C3B-CAB-CBB
26	A	810	CLA	C4B-C3B-CAB-CBB
26	A	812	CLA	C4B-C3B-CAB-CBB
26	A	818	CLA	C4B-C3B-CAB-CBB
26	A	831	CLA	C4B-C3B-CAB-CBB
26	B	804	CLA	C4B-C3B-CAB-CBB
26	B	808	CLA	C4B-C3B-CAB-CBB
26	B	809	CLA	C4B-C3B-CAB-CBB
26	B	810	CLA	C4B-C3B-CAB-CBB
26	B	821	CLA	C4B-C3B-CAB-CBB
26	B	824	CLA	C4B-C3B-CAB-CBB
26	B	831	CLA	C4B-C3B-CAB-CBB
26	B	834	CLA	C4B-C3B-CAB-CBB
26	B	835	CLA	C4B-C3B-CAB-CBB
26	F	202	CLA	C4B-C3B-CAB-CBB
26	s	403	CLA	C4B-C3B-CAB-CBB
26	c	302	CLA	C4B-C3B-CAB-CBB
26	c	308	CLA	C4B-C3B-CAB-CBB
26	a	301	CLA	C4B-C3B-CAB-CBB
26	a	306	CLA	C4B-C3B-CAB-CBB
26	a	307	CLA	C4B-C3B-CAB-CBB
26	a	311	CLA	C4B-C3B-CAB-CBB
26	b	306	CLA	C4B-C3B-CAB-CBB
26	b	308	CLA	C4B-C3B-CAB-CBB
26	b	311	CLA	C4B-C3B-CAB-CBB
26	h	304	CLA	C4B-C3B-CAB-CBB
26	h	306	CLA	C4B-C3B-CAB-CBB
26	m	603	CLA	C4B-C3B-CAB-CBB
26	m	605	CLA	C4B-C3B-CAB-CBB
26	m	608	CLA	C4B-C3B-CAB-CBB
26	l	301	CLA	C4B-C3B-CAB-CBB
26	k	606	CLA	C4B-C3B-CAB-CBB
26	k	608	CLA	C4B-C3B-CAB-CBB
26	i	307	CLA	C4B-C3B-CAB-CBB
26	i	308	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	i	311	CLA	C4B-C3B-CAB-CBB
26	j	613	CLA	C4B-C3B-CAB-CBB
26	d	302	CLA	C4B-C3B-CAB-CBB
26	d	304	CLA	C4B-C3B-CAB-CBB
26	d	307	CLA	C4B-C3B-CAB-CBB
26	d	309	CLA	C4B-C3B-CAB-CBB
26	R	201	CLA	C4B-C3B-CAB-CBB
26	n	601	CLA	C4B-C3B-CAB-CBB
28	B	851	LHG	C33-C34-C35-C36
26	h	304	CLA	C10-C11-C12-C13
28	c	317	LHG	C5-C6-O8-C23
26	i	311	CLA	C16-C17-C18-C19
26	b	306	CLA	C2A-CAA-CBA-CGA
34	F	205	LMG	C41-C42-C43-C44
28	J	105	LHG	C13-C14-C15-C16
28	A	844	LHG	O6-C4-C5-C6
28	i	317	LHG	O6-C4-C5-C6
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	833	CLA	C11-C10-C8-C7
26	A	837	CLA	C12-C13-C15-C16
26	A	840	CLA	C11-C10-C8-C7
26	B	804	CLA	C6-C7-C8-C10
26	B	813	CLA	C6-C7-C8-C10
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	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	m	606	CLA	C6-C7-C8-C10
26	m	606	CLA	C12-C13-C15-C16
26	m	613	CLA	C11-C10-C8-C7
26	l	311	CLA	C11-C12-C13-C15
26	l	313	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	k	602	CLA	C11-C10-C8-C7
26	k	609	CLA	C11-C10-C8-C7
26	i	304	CLA	C11-C10-C8-C7
26	i	304	CLA	C11-C12-C13-C15
26	i	311	CLA	C11-C12-C13-C15
26	j	609	CLA	C12-C13-C15-C16
26	j	613	CLA	C6-C7-C8-C10
34	c	318	LMG	C42-C43-C44-C45
28	A	855	LHG	C7-C8-C9-C10
25	A	801	CL0	C16-C17-C18-C20
26	B	818	CLA	C16-C17-C18-C20
26	A	810	CLA	C3A-C2A-CAA-CBA
26	A	820	CLA	C4-C3-C5-C6
26	A	852	CLA	C4-C3-C5-C6
26	F	202	CLA	C3A-C2A-CAA-CBA
26	b	312	CLA	C4-C3-C5-C6
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	n	608	CLA	C4-C3-C5-C6
26	Q	302	CLA	C3A-C2A-CAA-CBA
26	c	309	CLA	O1D-CGD-O2D-CED
26	B	813	CLA	C2-C3-C5-C6
26	i	311	CLA	C2C-C3C-CAC-CBC
34	F	205	LMG	C40-C41-C42-C43
26	A	811	CLA	O1A-CGA-O2A-C1
26	B	819	CLA	O1A-CGA-O2A-C1
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
35	c	316	II0	C32-C34-C36-C38
34	L	209	LMG	C30-C31-C32-C33
26	s	402	CLA	O1A-CGA-O2A-C1
26	l	304	CLA	O1A-CGA-O2A-C1
29	l	316	WVN	C30-C33-C34-C37
35	c	316	II0	C31-C33-C35-C39
28	A	855	LHG	C9-C10-C11-C12
34	L	209	LMG	C19-C20-C21-C22
34	n	620	LMG	C14-C15-C16-C17
26	B	810	CLA	CBA-CGA-O2A-C1
26	B	834	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	m	618	LHG	C4-C5-C6-O8
28	j	617	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
28	l	318	LHG	C27-C28-C29-C30
26	B	814	CLA	C16-C17-C18-C19
26	s	402	CLA	C16-C17-C18-C20
28	b	302	LHG	C10-C11-C12-C13
26	k	606	CLA	O1A-CGA-O2A-C1
34	b	319	LMG	C34-C35-C36-C37
26	A	836	CLA	C15-C16-C17-C18
26	A	822	CLA	C4-C3-C5-C6
26	A	838	CLA	C4-C3-C5-C6
26	B	813	CLA	C4-C3-C5-C6
26	B	814	CLA	C4-C3-C5-C6
26	l	307	CLA	C4-C3-C5-C6
27	B	843	PQN	C14-C13-C15-C16
26	A	820	CLA	C2-C3-C5-C6
26	b	305	CLA	C2-C3-C5-C6
26	n	608	CLA	C2-C3-C5-C6
26	B	817	CLA	O1A-CGA-O2A-C1
26	d	308	CLA	CBA-CGA-O2A-C1
26	j	607	CLA	O1D-CGD-O2D-CED
26	m	606	CLA	C16-C17-C18-C19
26	l	305	CLA	C16-C17-C18-C19
28	B	851	LHG	O6-C4-C5-O7
26	F	202	CLA	C2B-C3B-CAB-CBB
26	a	306	CLA	C2B-C3B-CAB-CBB
26	l	301	CLA	C2B-C3B-CAB-CBB
37	a	315	IHT	C02-C07-C18-C22
37	R	202	IHT	C02-C07-C18-C22
26	A	818	CLA	O1D-CGD-O2D-CED
26	l	311	CLA	C14-C13-C15-C16
30	A	858	LMU	C4-C5-C6-C7
34	c	318	LMG	O10-C28-O8-C9
26	B	805	CLA	C15-C16-C17-C18
26	B	810	CLA	C10-C11-C12-C13
34	n	620	LMG	C34-C35-C36-C37
33	j	618	DGD	C8B-C9B-CAB-CBB
26	B	818	CLA	C16-C17-C18-C19
26	l	301	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	B	839	CLA	CAA-CBA-CGA-O2A
26	m	606	CLA	CAA-CBA-CGA-O2A
26	B	801	CLA	C2A-CAA-CBA-CGA
26	i	308	CLA	C2A-CAA-CBA-CGA
26	l	308	CLA	C5-C6-C7-C8
33	j	618	DGD	O2G-C2G-C3G-O3G
34	F	206	LMG	O7-C8-C9-O8
26	F	201	CLA	O1D-CGD-O2D-CED
26	B	819	CLA	C5-C6-C7-C8
26	A	802	CLA	C13-C15-C16-C17
26	A	852	CLA	C2-C3-C5-C6
34	b	319	LMG	C11-C12-C13-C14
25	A	801	CL0	C1-C2-C3-C5
26	m	602	CLA	CBA-CGA-O2A-C1
28	n	619	LHG	C33-C34-C35-C36
26	b	307	CLA	C3-C5-C6-C7
26	A	837	CLA	C6-C7-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
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
34	F	205	LMG	C37-C38-C39-C40
34	c	318	LMG	C15-C16-C17-C18
26	l	305	CLA	C16-C17-C18-C20
26	L	202	CLA	O2A-C1-C2-C3
26	J	103	CLA	C1A-C2A-CAA-CBA
26	K	101	CLA	C1A-C2A-CAA-CBA
26	m	601	CLA	C1A-C2A-CAA-CBA
34	F	205	LMG	C42-C43-C44-C45
28	L	208	LHG	O1-C1-C2-O2
26	B	815	CLA	C4-C3-C5-C6
26	b	312	CLA	C2-C3-C5-C6
28	B	851	LHG	C1-C2-C3-O3
34	L	209	LMG	C11-C12-C13-C14
34	c	318	LMG	C16-C17-C18-C19
29	F	203	WVN	C35-C32-C36-C39
25	A	801	CL0	C8-C10-C11-C12
28	b	302	LHG	C35-C36-C37-C38
28	A	855	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	m	606	CLA	C16-C17-C18-C20
28	A	849	LHG	C14-C15-C16-C17
34	c	318	LMG	C31-C32-C33-C34
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
28	A	843	LHG	C27-C28-C29-C30
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	B	803	CLA	C12-C13-C15-C16
26	B	806	CLA	C6-C7-C8-C10
26	B	812	CLA	C6-C7-C8-C10
26	B	836	CLA	C6-C7-C8-C10
26	c	308	CLA	C6-C7-C8-C10
26	c	312	CLA	C11-C10-C8-C7
26	a	307	CLA	C12-C13-C15-C16
26	b	311	CLA	C11-C12-C13-C15
26	l	305	CLA	C6-C7-C8-C10
26	l	311	CLA	C11-C10-C8-C7
26	i	302	CLA	C12-C13-C15-C16
26	i	307	CLA	C6-C7-C8-C10
26	i	311	CLA	C11-C10-C8-C7
26	j	604	CLA	C6-C7-C8-C10
26	j	609	CLA	C11-C10-C8-C7
26	Q	302	CLA	C11-C10-C8-C7
30	A	850	LMU	C6-C7-C8-C9
26	B	803	CLA	C8-C10-C11-C12
26	B	804	CLA	C5-C6-C7-C8
34	Q	301	LMG	O6-C5-C6-O5
29	A	847	WVN	C30-C33-C34-C37
29	A	848	WVN	C20-C23-C25-C28
29	B	849	WVN	C29-C31-C32-C36
29	J	101	WVN	C30-C33-C34-C37
29	M	101	WVN	C20-C23-C25-C28
29	l	316	WVN	C29-C31-C32-C36
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	A	816	CLA	CBA-CGA-O2A-C1
26	B	842	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	j	602	CLA	CBA-CGA-O2A-C1
28	b	318	LHG	C11-C12-C13-C14
30	i	300	LMU	C4-C5-C6-C7
26	B	818	CLA	O1A-CGA-O2A-C1
26	m	602	CLA	O1A-CGA-O2A-C1
26	B	834	CLA	C15-C16-C17-C18
26	m	604	CLA	C2A-CAA-CBA-CGA
26	j	604	CLA	C2A-CAA-CBA-CGA
26	A	833	CLA	O1D-CGD-O2D-CED
30	i	300	LMU	C4'-C5'-C6'-O6'
30	A	850	LMU	C11-C10-C9-C8
30	B	852	LMU	C11-C10-C9-C8
26	B	812	CLA	C4-C3-C5-C6
26	b	306	CLA	O1A-CGA-O2A-C1
26	k	608	CLA	O1A-CGA-O2A-C1
26	B	814	CLA	C2-C3-C5-C6
26	B	815	CLA	C2-C3-C5-C6
36	i	318	KC2	C2C-C3C-CAC-CBC
36	d	312	KC2	C2B-C3B-CAB-CBB
26	A	812	CLA	C3-C5-C6-C7
26	A	828	CLA	CBA-CGA-O2A-C1
34	F	206	LMG	C28-C29-C30-C31
28	c	317	LHG	C11-C10-C9-C8
34	F	205	LMG	C34-C35-C36-C37
34	n	620	LMG	C38-C39-C40-C41
26	B	820	CLA	O1A-CGA-O2A-C1
26	L	202	CLA	O1A-CGA-O2A-C1
26	A	813	CLA	C3-C5-C6-C7
26	A	810	CLA	C15-C16-C17-C18
26	l	311	CLA	C8-C10-C11-C12
26	j	609	CLA	C15-C16-C17-C18
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	j	609	CLA	C10-C11-C12-C13
28	A	855	LHG	O6-C4-C5-O7
28	i	317	LHG	O6-C4-C5-O7
34	c	318	LMG	C38-C39-C40-C41
33	B	844	DGD	C6A-C7A-C8A-C9A
28	b	302	LHG	C4-C5-C6-O8
34	L	209	LMG	O1-C7-C8-C9
34	n	620	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	m	611	KC2	C4B-C3B-CAB-CBB
36	n	611	KC2	C4C-C3C-CAC-CBC
36	n	612	KC2	C4B-C3B-CAB-CBB
26	B	837	CLA	C16-C17-C18-C19
28	i	317	LHG	C28-C29-C30-C31
28	s	409	LHG	C34-C35-C36-C37
28	n	619	LHG	O10-C23-O8-C6
36	n	612	KC2	O1D-CGD-O2D-CED
26	A	807	CLA	CBA-CGA-O2A-C1
26	B	829	CLA	C15-C16-C17-C18
26	B	825	CLA	C4-C3-C5-C6
26	A	823	CLA	C2A-CAA-CBA-CGA
26	A	802	CLA	CAA-CBA-CGA-O2A
26	B	812	CLA	C2-C3-C5-C6
26	A	805	CLA	C15-C16-C17-C18
28	m	618	LHG	C30-C31-C32-C33
26	A	826	CLA	C3-C5-C6-C7
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	A	817	CLA	C11-C12-C13-C14
26	A	833	CLA	C14-C13-C15-C16
26	c	304	CLA	C6-C7-C8-C9
26	b	311	CLA	C11-C12-C13-C14
26	i	311	CLA	C11-C10-C8-C9
26	i	311	CLA	C11-C12-C13-C14
26	j	604	CLA	C6-C7-C8-C9
33	B	844	DGD	CDB-CEB-CFB-CGB
33	j	618	DGD	C5A-C6A-C7A-C8A
26	B	810	CLA	O1A-CGA-O2A-C1
28	L	208	LHG	C24-C25-C26-C27
29	A	857	WVN	C02-C11-C19-C22
29	B	850	WVN	C02-C11-C19-C22
28	b	318	LHG	C27-C28-C29-C30
34	c	318	LMG	C39-C40-C41-C42
26	a	309	CLA	O1D-CGD-O2D-CED
26	h	303	CLA	C2-C1-O2A-CGA
35	j	614	II0	C36-C40-C42-C41
26	B	841	CLA	C16-C17-C18-C19
26	A	807	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	c	320	LHG	C2-C3-O3-P
34	F	206	LMG	C13-C14-C15-C16
34	L	209	LMG	C32-C33-C34-C35
26	B	836	CLA	C4-C3-C5-C6
28	n	619	LHG	C1-C2-C3-O3
26	j	610	CLA	C2A-CAA-CBA-CGA
34	L	209	LMG	C31-C32-C33-C34
32	A	854	SQD	C25-C26-C27-C28
26	A	816	CLA	O1A-CGA-O2A-C1
28	J	105	LHG	C9-C10-C11-C12
34	c	318	LMG	C21-C22-C23-C24
34	c	319	LMG	C11-C12-C13-C14
28	A	843	LHG	C12-C13-C14-C15
26	R	201	CLA	C5-C6-C7-C8
35	a	314	II0	C27-C25-C29-C31
35	h	312	II0	C27-C25-C29-C31
35	k	617	II0	C27-C25-C29-C31
35	i	316	II0	C27-C25-C29-C31
26	B	820	CLA	O1D-CGD-O2D-CED
26	j	602	CLA	O1A-CGA-O2A-C1
26	A	824	CLA	CBA-CGA-O2A-C1
26	d	305	CLA	O1D-CGD-O2D-CED
26	m	606	CLA	C13-C15-C16-C17
26	A	811	CLA	C3-C5-C6-C7
26	a	308	CLA	O2A-C1-C2-C3
26	a	311	CLA	O2A-C1-C2-C3
26	A	829	CLA	C15-C16-C17-C18
26	A	806	CLA	C4B-C3B-CAB-CBB
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	B	841	CLA	C4B-C3B-CAB-CBB
26	F	201	CLA	C4B-C3B-CAB-CBB
26	F	202	CLA	C1A-C2A-CAA-CBA
26	L	206	CLA	C1A-C2A-CAA-CBA
26	c	301	CLA	C4B-C3B-CAB-CBB
26	b	303	CLA	C4B-C3B-CAB-CBB
26	b	308	CLA	C1A-C2A-CAA-CBA
26	b	312	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	h	301	CLA	C4B-C3B-CAB-CBB
26	i	302	CLA	C1A-C2A-CAA-CBA
26	j	602	CLA	C1A-C2A-CAA-CBA
26	d	313	CLA	C1A-C2A-CAA-CBA
26	B	805	CLA	CAA-CBA-CGA-O2A
29	s	407	WVN	C11-C19-C22-C26
26	i	311	CLA	C4C-C3C-CAC-CBC
26	B	807	CLA	C2A-CAA-CBA-CGA
26	A	816	CLA	O1D-CGD-O2D-CED
28	L	208	LHG	O6-C4-C5-C6
26	m	607	CLA	C2-C3-C5-C6
26	k	610	CLA	C2-C3-C5-C6
26	n	613	CLA	C2-C3-C5-C6
26	B	813	CLA	C5-C6-C7-C8
34	b	319	LMG	C30-C31-C32-C33
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	810	CLA	C11-C10-C8-C7
26	B	814	CLA	C11-C12-C13-C15
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	s	408	CLA	C6-C7-C8-C10
26	c	312	CLA	C6-C7-C8-C10
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	i	306	CLA	C11-C12-C13-C15
26	i	310	CLA	C6-C7-C8-C10
27	B	843	PQN	C21-C22-C23-C25
26	A	808	CLA	C16-C17-C18-C19
26	B	842	CLA	O1A-CGA-O2A-C1
26	h	307	CLA	CAA-CBA-CGA-O2A
26	B	834	CLA	O1A-CGA-O2A-C1
26	B	806	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	L	204	CLA	C11-C12-C13-C14
30	i	300	LMU	C5-C6-C7-C8
27	A	842	PQN	C15-C16-C17-C18
26	A	824	CLA	O1A-CGA-O2A-C1
26	A	828	CLA	O1A-CGA-O2A-C1
28	A	844	LHG	O6-C4-C5-O7
28	c	317	LHG	O6-C4-C5-O7
26	A	818	CLA	C11-C12-C13-C14
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	l	311	CLA	C11-C12-C13-C14
26	l	313	CLA	C6-C7-C8-C9
26	j	609	CLA	C11-C10-C8-C9
27	B	843	PQN	C21-C22-C23-C24
26	A	807	CLA	O1A-CGA-O2A-C1
28	L	207	LHG	C24-C25-C26-C27
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	b	308	CLA	C16-C17-C18-C19
26	s	406	CLA	C5-C6-C7-C8
26	i	302	CLA	C13-C15-C16-C17
26	A	821	CLA	C1-C2-C3-C4
36	m	611	KC2	C1A-C2A-CAA-CBA
36	i	309	KC2	C1A-C2A-CAA-CBA
36	i	318	KC2	C1A-C2A-CAA-CBA
36	j	611	KC2	C1A-C2A-CAA-CBA
36	d	311	KC2	C1A-C2A-CAA-CBA
36	d	312	KC2	C1A-C2A-CAA-CBA
36	n	612	KC2	C1A-C2A-CAA-CBA
34	c	318	LMG	C33-C34-C35-C36
33	j	618	DGD	C1B-C2B-C3B-C4B
26	B	808	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
34	c	319	LMG	C33-C34-C35-C36
28	B	851	LHG	C4-C5-C6-O8
28	c	317	LHG	C4-C5-C6-O8
28	b	318	LHG	C4-C5-C6-O8
34	F	205	LMG	C7-C8-C9-O8
28	b	318	LHG	C19-C20-C21-C22
28	i	317	LHG	C29-C30-C31-C32
26	B	836	CLA	C2-C3-C5-C6
26	A	814	CLA	CAD-CBD-CGD-O2D
26	A	826	CLA	CAD-CBD-CGD-O2D
26	A	835	CLA	CAD-CBD-CGD-O2D
26	B	805	CLA	CAD-CBD-CGD-O2D
26	c	302	CLA	CAD-CBD-CGD-O2D
26	l	307	CLA	CAD-CBD-CGD-O2D
26	i	301	CLA	CAD-CBD-CGD-O2D
28	c	320	LHG	C28-C29-C30-C31
34	c	319	LMG	O6-C1-O1-C7
26	c	302	CLA	C8-C10-C11-C12
26	c	308	CLA	C13-C15-C16-C17
32	A	854	SQD	C7-C8-C9-C10
26	A	808	CLA	C16-C17-C18-C20
26	b	308	CLA	C2A-CAA-CBA-CGA
26	i	311	CLA	C15-C16-C17-C18
33	j	618	DGD	C5B-C6B-C7B-C8B
26	A	814	CLA	CAD-CBD-CGD-O1D
26	A	822	CLA	CAD-CBD-CGD-O1D
26	A	825	CLA	CHA-CBD-CGD-O1D
26	A	826	CLA	CAD-CBD-CGD-O1D
26	A	829	CLA	CHA-CBD-CGD-O1D
26	A	829	CLA	CHA-CBD-CGD-O2D
26	A	830	CLA	CHA-CBD-CGD-O1D
26	A	835	CLA	CAD-CBD-CGD-O1D
26	B	805	CLA	CAD-CBD-CGD-O1D
26	L	202	CLA	CHA-CBD-CGD-O1D
26	c	301	CLA	CHA-CBD-CGD-O1D
26	c	302	CLA	CAD-CBD-CGD-O1D
26	a	301	CLA	CHA-CBD-CGD-O1D
26	a	301	CLA	CHA-CBD-CGD-O2D
26	a	303	CLA	CHA-CBD-CGD-O1D
26	a	303	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	a	304	CLA	CAD-CBD-CGD-O1D
26	a	310	CLA	CHA-CBD-CGD-O1D
26	b	303	CLA	CHA-CBD-CGD-O1D
26	b	304	CLA	CHA-CBD-CGD-O1D
26	b	308	CLA	CHA-CBD-CGD-O1D
26	b	308	CLA	CHA-CBD-CGD-O2D
26	m	601	CLA	CHA-CBD-CGD-O1D
26	m	601	CLA	CHA-CBD-CGD-O2D
26	m	605	CLA	CHA-CBD-CGD-O1D
26	m	605	CLA	CHA-CBD-CGD-O2D
26	m	607	CLA	CHA-CBD-CGD-O1D
26	m	607	CLA	CHA-CBD-CGD-O2D
26	l	305	CLA	CHA-CBD-CGD-O1D
26	l	306	CLA	CHA-CBD-CGD-O1D
26	l	306	CLA	CHA-CBD-CGD-O2D
26	l	307	CLA	CAD-CBD-CGD-O1D
26	k	604	CLA	CAD-CBD-CGD-O1D
26	i	301	CLA	CAD-CBD-CGD-O1D
26	j	608	CLA	CHA-CBD-CGD-O1D
26	j	608	CLA	CHA-CBD-CGD-O2D
26	d	303	CLA	CHA-CBD-CGD-O1D
26	d	303	CLA	CHA-CBD-CGD-O2D
26	d	307	CLA	CHA-CBD-CGD-O1D
26	d	307	CLA	CHA-CBD-CGD-O2D
26	d	318	CLA	CHA-CBD-CGD-O1D
26	n	605	CLA	CHA-CBD-CGD-O1D
26	n	605	CLA	CHA-CBD-CGD-O2D
26	n	607	CLA	CHA-CBD-CGD-O1D
26	n	607	CLA	CHA-CBD-CGD-O2D
28	A	843	LHG	C4-O6-P-O5
28	A	844	LHG	C3-O3-P-O5
28	A	855	LHG	C4-O6-P-O5
28	B	851	LHG	C3-O3-P-O6
28	B	851	LHG	C4-O6-P-O3
28	J	105	LHG	C3-O3-P-O5
28	J	105	LHG	C4-O6-P-O5
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

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Mol	Chain	Res	Type	Atoms
28	j	617	LHG	C3-O3-P-O5
28	n	619	LHG	C3-O3-P-O5
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
36	l	312	KC2	CHA-CBD-CGD-O1D
36	l	312	KC2	CHA-CBD-CGD-O2D
36	n	612	KC2	CHA-CBD-CGD-O1D
36	n	612	KC2	CHA-CBD-CGD-O2D
28	J	105	LHG	C11-C10-C9-C8
33	B	844	DGD	C3B-C4B-C5B-C6B
26	B	837	CLA	C2C-C3C-CAC-CBC
26	A	806	CLA	C2B-C3B-CAB-CBB
26	A	823	CLA	C2B-C3B-CAB-CBB
26	A	830	CLA	C2B-C3B-CAB-CBB
26	A	832	CLA	C2B-C3B-CAB-CBB
26	A	852	CLA	C2B-C3B-CAB-CBB
26	B	803	CLA	C2B-C3B-CAB-CBB
26	B	830	CLA	C2B-C3B-CAB-CBB
26	B	835	CLA	C2B-C3B-CAB-CBB
26	c	301	CLA	C2B-C3B-CAB-CBB
26	c	305	CLA	C2B-C3B-CAB-CBB
26	a	303	CLA	C2B-C3B-CAB-CBB
26	a	310	CLA	C2B-C3B-CAB-CBB
26	b	303	CLA	C2B-C3B-CAB-CBB
26	b	308	CLA	C2B-C3B-CAB-CBB
26	b	309	CLA	C2B-C3B-CAB-CBB
26	b	313	CLA	C2B-C3B-CAB-CBB
26	h	301	CLA	C2B-C3B-CAB-CBB
26	m	608	CLA	C2B-C3B-CAB-CBB
26	m	612	CLA	C2B-C3B-CAB-CBB
26	l	308	CLA	C2B-C3B-CAB-CBB
26	k	601	CLA	C2B-C3B-CAB-CBB
26	k	605	CLA	C2B-C3B-CAB-CBB
26	i	302	CLA	C2B-C3B-CAB-CBB
26	i	310	CLA	C2B-C3B-CAB-CBB
26	j	605	CLA	C2B-C3B-CAB-CBB
26	j	609	CLA	C2B-C3B-CAB-CBB
26	d	302	CLA	C2B-C3B-CAB-CBB
26	d	318	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	n	601	CLA	C2B-C3B-CAB-CBB
26	n	605	CLA	C2B-C3B-CAB-CBB
26	n	608	CLA	C2B-C3B-CAB-CBB
26	Q	302	CLA	C2B-C3B-CAB-CBB
26	B	825	CLA	C2-C3-C5-C6
28	s	409	LHG	C4-O6-P-O5
30	a	317	LMU	C2-C3-C4-C5
28	c	320	LHG	C29-C30-C31-C32
34	F	205	LMG	C39-C40-C41-C42
34	b	319	LMG	C35-C36-C37-C38
28	i	317	LHG	C11-C10-C9-C8
26	m	609	CLA	C4-C3-C5-C6
32	A	854	SQD	C19-C20-C21-C22
35	d	319	II0	C30-C32-C34-C36
26	n	613	CLA	CAA-CBA-CGA-O2A
26	A	841	CLA	C2-C3-C5-C6
26	B	806	CLA	C2-C3-C5-C6
29	i	315	WVN	C25-C28-C30-C33
26	s	406	CLA	O1D-CGD-O2D-CED
26	i	304	CLA	C10-C11-C12-C13
34	F	205	LMG	C21-C22-C23-C24
33	B	844	DGD	C5B-C6B-C7B-C8B
26	l	301	CLA	C5-C6-C7-C8
26	Q	302	CLA	C15-C16-C17-C18
26	A	809	CLA	C6-C7-C8-C9
26	A	833	CLA	C11-C10-C8-C9
26	A	840	CLA	C11-C10-C8-C9
26	B	825	CLA	C6-C7-C8-C9
26	B	836	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	C14-C13-C15-C16
26	l	311	CLA	C11-C10-C8-C9
26	i	302	CLA	C14-C13-C15-C16
26	Q	302	CLA	C6-C7-C8-C9
26	A	832	CLA	C11-C12-C13-C15
26	A	833	CLA	C12-C13-C15-C16
26	i	302	CLA	C6-C7-C8-C10
26	B	812	CLA	C5-C6-C7-C8
29	A	847	WVN	C33-C34-C37-C40
29	A	857	WVN	C31-C32-C36-C39
28	m	618	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	b	318	LHG	C29-C30-C31-C32
30	A	858	LMU	O5'-C1'-O1'-C1
26	s	408	CLA	CBD-CGD-O2D-CED
36	i	309	KC2	CBD-CGD-O2D-CED
26	B	829	CLA	C4-C3-C5-C6
26	A	856	CLA	C2-C3-C5-C6
28	c	320	LHG	C9-C10-C11-C12
26	B	841	CLA	C16-C17-C18-C20
28	A	855	LHG	C2-C3-O3-P
34	n	620	LMG	O1-C7-C8-O7
29	R	200	WVN	C32-C36-C39-C40
35	l	314	II0	C35-C39-C41-C42
26	b	308	CLA	C16-C17-C18-C20
26	A	822	CLA	C2A-CAA-CBA-CGA
26	A	835	CLA	C2A-CAA-CBA-CGA
26	l	310	CLA	C2A-CAA-CBA-CGA
26	B	819	CLA	C8-C10-C11-C12
28	b	302	LHG	C11-C10-C9-C8
26	a	301	CLA	C2C-C3C-CAC-CBC
33	B	844	DGD	C9A-CAA-CBA-CCA
26	k	608	CLA	C5-C6-C7-C8
34	b	319	LMG	O1-C7-C8-C9
28	c	317	LHG	C11-C12-C13-C14
26	k	606	CLA	CAA-CBA-CGA-O2A
26	k	607	CLA	CAA-CBA-CGA-O2A
29	B	847	WVN	C20-C23-C25-C28
26	B	803	CLA	C5-C6-C7-C8
26	a	307	CLA	C8-C10-C11-C12
26	B	817	CLA	C5-C6-C7-C8
26	A	809	CLA	C2A-CAA-CBA-CGA
26	B	828	CLA	C2A-CAA-CBA-CGA
26	c	304	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
29	A	857	WVN	C32-C36-C39-C40
26	s	408	CLA	O1D-CGD-O2D-CED
36	k	612	KC2	C2C-C3C-CAC-CBC
28	b	318	LHG	O1-C1-C2-O2
35	n	614	II0	C09-C21-C23-C25
26	A	831	CLA	C14-C13-C15-C16
26	B	810	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	B	814	CLA	C11-C12-C13-C14
26	B	842	CLA	C11-C10-C8-C9
26	c	312	CLA	C6-C7-C8-C9
26	m	608	CLA	C11-C10-C8-C9
26	A	807	CLA	C4B-C3B-CAB-CBB
26	A	820	CLA	C4B-C3B-CAB-CBB
26	A	829	CLA	C4B-C3B-CAB-CBB
26	c	304	CLA	C4B-C3B-CAB-CBB
26	a	309	CLA	C4B-C3B-CAB-CBB
26	n	604	CLA	C4B-C3B-CAB-CBB
26	n	613	CLA	C4B-C3B-CAB-CBB
26	A	824	CLA	C13-C15-C16-C17
26	a	309	CLA	C15-C16-C17-C18
26	B	810	CLA	C8-C10-C11-C12
26	A	803	CLA	C6-C7-C8-C10
26	B	819	CLA	C16-C17-C18-C20
26	k	602	CLA	C15-C16-C17-C18
26	j	606	CLA	CAA-CBA-CGA-O2A
26	j	607	CLA	CAA-CBA-CGA-O2A
28	A	843	LHG	C32-C33-C34-C35
28	A	849	LHG	C13-C14-C15-C16
26	A	822	CLA	C2-C3-C5-C6
26	A	833	CLA	C2-C3-C5-C6
26	A	856	CLA	CAA-CBA-CGA-O1A
26	B	802	CLA	C5-C6-C7-C8
36	k	611	KC2	C4C-C3C-CAC-CBC
36	i	309	KC2	C4C-C3C-CAC-CBC
36	i	318	KC2	C4C-C3C-CAC-CBC
36	d	311	KC2	C4B-C3B-CAB-CBB
36	d	312	KC2	C4B-C3B-CAB-CBB
34	n	620	LMG	C23-C24-C25-C26
26	A	825	CLA	C11-C12-C13-C15
26	A	841	CLA	C6-C7-C8-C10
33	j	618	DGD	C2B-C3B-C4B-C5B
26	A	833	CLA	C3-C5-C6-C7
26	d	310	CLA	O1D-CGD-O2D-CED
26	k	608	CLA	CAA-CBA-CGA-O2A
26	L	204	CLA	C11-C12-C13-C15
26	i	301	CLA	C13-C15-C16-C17
26	B	812	CLA	C3A-C2A-CAA-CBA
26	s	402	CLA	C3A-C2A-CAA-CBA
26	s	406	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	d	313	CLA	C3A-C2A-CAA-CBA
26	n	613	CLA	C3A-C2A-CAA-CBA
26	Q	302	CLA	C4-C3-C5-C6
36	i	309	KC2	O1D-CGD-O2D-CED
26	A	841	CLA	CAA-CBA-CGA-O2A
26	B	825	CLA	C2A-CAA-CBA-CGA
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	B	801	CLA	C10-C11-C12-C13
26	A	830	CLA	CBD-CGD-O2D-CED
26	b	313	CLA	C2-C1-O2A-CGA
26	m	613	CLA	C2-C1-O2A-CGA
26	l	313	CLA	C2-C1-O2A-CGA
26	d	308	CLA	O1A-CGA-O2A-C1
28	A	849	LHG	C12-C13-C14-C15
34	L	209	LMG	C20-C21-C22-C23
26	n	613	CLA	C4-C3-C5-C6
26	d	304	CLA	CAA-CBA-CGA-O2A
26	b	309	CLA	C10-C11-C12-C13
26	A	817	CLA	CAA-CBA-CGA-O2A
28	B	851	LHG	C30-C31-C32-C33
28	L	208	LHG	C1-C2-C3-O3
26	n	609	CLA	C13-C15-C16-C17
26	A	810	CLA	C11-C10-C8-C9
26	A	835	CLA	C6-C7-C8-C9
26	B	819	CLA	C11-C10-C8-C9
26	B	829	CLA	C6-C7-C8-C9
26	B	834	CLA	C14-C13-C15-C16
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
26	n	610	CLA	C6-C7-C8-C9
26	s	406	CLA	C13-C15-C16-C17
26	s	406	CLA	CBD-CGD-O2D-CED
28	b	318	LHG	C24-C23-O8-C6
26	k	607	CLA	C2C-C3C-CAC-CBC
35	l	315	II0	C28-C26-C30-C32
26	j	605	CLA	CAA-CBA-CGA-O2A
29	A	857	WVN	C34-C37-C40-C39
29	B	849	WVN	C32-C36-C39-C40

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Mol	Chain	Res	Type	Atoms
35	a	313	II0	C25-C29-C31-C33
26	A	830	CLA	O1D-CGD-O2D-CED
28	c	317	LHG	C9-C10-C11-C12
26	A	811	CLA	C2A-CAA-CBA-CGA
26	B	826	CLA	C2A-CAA-CBA-CGA
26	c	312	CLA	C2A-CAA-CBA-CGA
26	a	307	CLA	C2A-CAA-CBA-CGA
26	h	306	CLA	C2A-CAA-CBA-CGA
26	i	303	CLA	O1D-CGD-O2D-CED
26	a	310	CLA	C10-C11-C12-C13
28	A	843	LHG	C15-C16-C17-C18
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
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
26	d	318	CLA	CAA-CBA-CGA-O1A
26	d	318	CLA	CAA-CBA-CGA-O2A
26	A	832	CLA	C5-C6-C7-C8
26	A	807	CLA	C2B-C3B-CAB-CBB
26	A	810	CLA	C2B-C3B-CAB-CBB
26	A	817	CLA	C2B-C3B-CAB-CBB
26	A	819	CLA	C2B-C3B-CAB-CBB
26	A	826	CLA	C2B-C3B-CAB-CBB
26	A	828	CLA	C2B-C3B-CAB-CBB
26	A	831	CLA	C2B-C3B-CAB-CBB
26	A	836	CLA	C2B-C3B-CAB-CBB
26	A	856	CLA	C2B-C3B-CAB-CBB
26	B	804	CLA	C2B-C3B-CAB-CBB
26	B	806	CLA	C2B-C3B-CAB-CBB
26	B	808	CLA	C2B-C3B-CAB-CBB
26	B	809	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	B	810	CLA	C2B-C3B-CAB-CBB
26	B	831	CLA	C2B-C3B-CAB-CBB
26	B	834	CLA	C2B-C3B-CAB-CBB
26	B	836	CLA	C2B-C3B-CAB-CBB
26	B	841	CLA	C2B-C3B-CAB-CBB
26	F	201	CLA	C2B-C3B-CAB-CBB
26	s	403	CLA	C2B-C3B-CAB-CBB
26	c	308	CLA	C2B-C3B-CAB-CBB
26	a	301	CLA	C2B-C3B-CAB-CBB
26	a	307	CLA	C2B-C3B-CAB-CBB
26	a	311	CLA	C2B-C3B-CAB-CBB
26	b	306	CLA	C2B-C3B-CAB-CBB
26	b	311	CLA	C2B-C3B-CAB-CBB
26	b	312	CLA	C2B-C3B-CAB-CBB
26	h	304	CLA	C2B-C3B-CAB-CBB
26	h	306	CLA	C2B-C3B-CAB-CBB
26	m	603	CLA	C2B-C3B-CAB-CBB
26	m	605	CLA	C2B-C3B-CAB-CBB
26	l	310	CLA	C2B-C3B-CAB-CBB
26	l	313	CLA	C2B-C3B-CAB-CBB
26	k	608	CLA	C2B-C3B-CAB-CBB
26	k	614	CLA	C2B-C3B-CAB-CBB
26	i	308	CLA	C2B-C3B-CAB-CBB
26	j	608	CLA	C2B-C3B-CAB-CBB
26	j	613	CLA	C2B-C3B-CAB-CBB
26	d	304	CLA	C2B-C3B-CAB-CBB
26	d	307	CLA	C2B-C3B-CAB-CBB
26	R	201	CLA	C2B-C3B-CAB-CBB
26	n	604	CLA	C2B-C3B-CAB-CBB
26	n	613	CLA	C2B-C3B-CAB-CBB
29	l	303	WVN	C15-C13-C20-C23
37	a	315	IHT	C10-C07-C18-C22
37	m	617	IHT	C10-C07-C18-C22
37	R	202	IHT	C10-C07-C18-C22
26	c	309	CLA	CAA-CBA-CGA-O2A
28	A	855	LHG	C13-C14-C15-C16
26	A	802	CLA	CBA-CGA-O2A-C1
26	c	305	CLA	C10-C11-C12-C13
26	j	601	CLA	C4-C3-C5-C6
34	F	205	LMG	C10-C11-C12-C13
29	s	407	WVN	C22-C26-C29-C31
26	A	826	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
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	F	201	CLA	C12-C13-C15-C16
26	m	606	CLA	C11-C10-C8-C7
26	m	608	CLA	C12-C13-C15-C16
26	l	307	CLA	C12-C13-C15-C16
26	k	602	CLA	C6-C7-C8-C10
26	d	302	CLA	C6-C7-C8-C10
26	n	610	CLA	C6-C7-C8-C10
28	b	318	LHG	C28-C29-C30-C31
26	A	812	CLA	C2A-CAA-CBA-CGA
34	F	206	LMG	O1-C7-C8-O7
28	b	302	LHG	C17-C18-C19-C20
26	b	304	CLA	C3-C5-C6-C7
26	i	302	CLA	C3-C5-C6-C7
28	b	318	LHG	C13-C14-C15-C16
28	B	851	LHG	C17-C18-C19-C20
26	b	307	CLA	C12-C13-C15-C16
26	l	311	CLA	C12-C13-C15-C16
26	c	311	CLA	CBD-CGD-O2D-CED
26	i	303	CLA	CBD-CGD-O2D-CED
26	c	305	CLA	CAA-CBA-CGA-O2A
26	i	301	CLA	CAA-CBA-CGA-O2A
26	A	825	CLA	C5-C6-C7-C8
26	B	826	CLA	C8-C10-C11-C12
34	F	206	LMG	C19-C20-C21-C22
26	c	311	CLA	O1D-CGD-O2D-CED
28	b	318	LHG	C34-C35-C36-C37
26	c	309	CLA	CAA-CBA-CGA-O1A
26	A	822	CLA	C6-C7-C8-C9
26	B	816	CLA	C14-C13-C15-C16
26	d	302	CLA	C6-C7-C8-C9
26	B	823	CLA	C16-C17-C18-C19
27	B	843	PQN	C20-C21-C22-C23
26	B	837	CLA	C4C-C3C-CAC-CBC
28	c	320	LHG	C10-C11-C12-C13
28	m	618	LHG	C24-C23-O8-C6
26	B	807	CLA	C4-C3-C5-C6
26	B	822	CLA	C4-C3-C5-C6
26	j	601	CLA	C2-C3-C5-C6
26	Q	302	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	j	605	CLA	CAA-CBA-CGA-O1A
26	d	307	CLA	CAA-CBA-CGA-O2A
26	A	802	CLA	O1A-CGA-O2A-C1
28	m	618	LHG	C28-C29-C30-C31
26	j	613	CLA	C5-C6-C7-C8
26	B	817	CLA	C16-C17-C18-C20
26	i	306	CLA	CAA-CBA-CGA-O2A
28	s	409	LHG	C25-C26-C27-C28
26	B	822	CLA	C8-C10-C11-C12
28	J	105	LHG	O1-C1-C2-O2
35	l	317	II0	C10-C22-C24-C26
28	b	318	LHG	O6-C4-C5-O7
26	A	827	CLA	C4-C3-C5-C6
26	s	406	CLA	C4-C3-C5-C6
26	d	304	CLA	CAA-CBA-CGA-O1A
26	A	827	CLA	C2-C3-C5-C6
26	B	819	CLA	C16-C17-C18-C19
26	A	817	CLA	C4B-C3B-CAB-CBB
26	A	819	CLA	C4B-C3B-CAB-CBB
26	A	826	CLA	C4B-C3B-CAB-CBB
26	A	828	CLA	C4B-C3B-CAB-CBB
26	A	856	CLA	C4B-C3B-CAB-CBB
26	B	806	CLA	C4B-C3B-CAB-CBB
26	B	815	CLA	C4B-C3B-CAB-CBB
26	B	836	CLA	C4B-C3B-CAB-CBB
26	m	609	CLA	C4B-C3B-CAB-CBB
26	l	310	CLA	C4B-C3B-CAB-CBB
26	l	313	CLA	C4B-C3B-CAB-CBB
26	k	614	CLA	C4B-C3B-CAB-CBB
26	i	303	CLA	C4B-C3B-CAB-CBB
26	j	608	CLA	C4B-C3B-CAB-CBB
26	n	609	CLA	C4B-C3B-CAB-CBB
26	A	825	CLA	C8-C10-C11-C12
26	c	312	CLA	O1A-CGA-O2A-C1
34	F	205	LMG	C19-C20-C21-C22
26	j	602	CLA	C6-C7-C8-C9
26	j	605	CLA	CBD-CGD-O2D-CED
26	B	803	CLA	CAA-CBA-CGA-O2A
26	b	311	CLA	C15-C16-C17-C18
26	A	804	CLA	O1A-CGA-O2A-C1
26	A	819	CLA	C16-C17-C18-C19
26	A	819	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	J	105	LHG	C1-C2-C3-O3
29	B	847	WVN	C24-C22-C26-C29
26	a	301	CLA	C4C-C3C-CAC-CBC
26	k	607	CLA	C4C-C3C-CAC-CBC
28	c	320	LHG	C31-C32-C33-C34
28	n	619	LHG	C34-C35-C36-C37
26	A	840	CLA	C4-C3-C5-C6
25	A	801	CL0	CAA-CBA-CGA-O2A
26	A	817	CLA	O1D-CGD-O2D-CED
28	A	855	LHG	C5-C4-O6-P
26	A	822	CLA	C6-C7-C8-C10
26	B	834	CLA	C12-C13-C15-C16
26	B	839	CLA	C6-C7-C8-C10
26	A	838	CLA	O1D-CGD-O2D-CED
26	B	830	CLA	O1A-CGA-O2A-C1
26	B	816	CLA	C11-C12-C13-C14
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	i	310	CLA	C6-C7-C8-C9
26	A	811	CLA	C6-C7-C8-C9
34	F	206	LMG	C8-C7-O1-C1
34	b	319	LMG	C8-C7-O1-C1
34	Q	301	LMG	C8-C7-O1-C1
30	i	300	LMU	C9-C10-C11-C12
26	n	607	CLA	C8-C10-C11-C12
26	A	852	CLA	C2A-CAA-CBA-CGA
26	a	304	CLA	C2A-CAA-CBA-CGA
26	n	610	CLA	C2A-CAA-CBA-CGA
25	A	801	CL0	C2-C1-O2A-CGA
26	A	852	CLA	C2-C1-O2A-CGA
26	B	811	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	A	828	CLA	C3-C5-C6-C7
26	a	302	CLA	CBA-CGA-O2A-C1
26	A	812	CLA	C3A-C2A-CAA-CBA
26	A	824	CLA	C3A-C2A-CAA-CBA
26	B	826	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	B	839	CLA	CAA-CBA-CGA-O1A
26	m	609	CLA	C2-C3-C5-C6
30	B	852	LMU	C6-C7-C8-C9
34	F	205	LMG	C11-C12-C13-C14
26	j	605	CLA	O1D-CGD-O2D-CED
26	B	830	CLA	CBA-CGA-O2A-C1
26	B	842	CLA	CAA-CBA-CGA-O2A
30	a	317	LMU	C2'-C1'-O1'-C1
28	b	318	LHG	C17-C18-C19-C20
26	A	817	CLA	CBD-CGD-O2D-CED
34	L	209	LMG	C24-C25-C26-C27
28	c	320	LHG	C27-C28-C29-C30
26	d	307	CLA	CAA-CBA-CGA-O1A
26	A	819	CLA	C2A-CAA-CBA-CGA
26	B	829	CLA	C2-C3-C5-C6
26	c	312	CLA	CBA-CGA-O2A-C1
26	B	806	CLA	CBD-CGD-O2D-CED
30	a	317	LMU	O5'-C1'-O1'-C1
26	A	803	CLA	C5-C6-C7-C8
26	m	604	CLA	C10-C11-C12-C13
28	b	302	LHG	C14-C15-C16-C17
36	k	612	KC2	C4C-C3C-CAC-CBC
26	B	806	CLA	O1D-CGD-O2D-CED
26	m	606	CLA	CAA-CBA-CGA-O1A
34	F	205	LMG	C35-C36-C37-C38
26	b	308	CLA	C4-C3-C5-C6
26	a	306	CLA	C2A-CAA-CBA-CGA
26	m	604	CLA	C4C-C3C-CAC-CBC
26	s	402	CLA	CAA-CBA-CGA-O2A
29	B	847	WVN	C22-C26-C29-C31
29	F	203	WVN	C34-C37-C40-C39
35	i	319	II0	C35-C39-C41-C42
28	c	320	LHG	C13-C14-C15-C16
26	d	303	CLA	O1A-CGA-O2A-C1
26	F	202	CLA	CAA-CBA-CGA-O2A
30	A	850	LMU	C9-C10-C11-C12
30	i	300	LMU	C3-C4-C5-C6
26	A	805	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
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	839	CLA	C11-C10-C8-C9
26	m	609	CLA	C11-C10-C8-C9
26	l	301	CLA	C11-C12-C13-C14
26	j	609	CLA	C11-C12-C13-C14
26	d	302	CLA	C14-C13-C15-C16
26	A	819	CLA	C16-C17-C18-C20
26	A	819	CLA	CAA-CBA-CGA-O2A
26	d	308	CLA	CAA-CBA-CGA-O2A
34	n	620	LMG	O8-C28-C29-C30
30	a	317	LMU	C7-C8-C9-C10
29	A	847	WVN	C11-C19-C22-C26
26	m	608	CLA	C5-C6-C7-C8
35	b	314	II0	C23-C25-C29-C31
26	A	824	CLA	C11-C12-C13-C15
26	B	816	CLA	C12-C13-C15-C16
26	B	822	CLA	C11-C10-C8-C7
26	B	829	CLA	C6-C7-C8-C10
26	B	842	CLA	C11-C12-C13-C15
26	a	307	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	k	604	CLA	C6-C7-C8-C10
26	n	608	CLA	C11-C12-C13-C15
28	c	317	LHG	C23-C24-C25-C26
26	A	809	CLA	C2B-C3B-CAB-CBB
26	A	812	CLA	C2B-C3B-CAB-CBB
26	A	818	CLA	C2B-C3B-CAB-CBB
26	A	820	CLA	C2B-C3B-CAB-CBB
26	A	821	CLA	C2B-C3B-CAB-CBB
26	A	829	CLA	C2B-C3B-CAB-CBB
26	B	816	CLA	C2B-C3B-CAB-CBB
26	B	821	CLA	C2B-C3B-CAB-CBB
26	B	824	CLA	C2B-C3B-CAB-CBB
26	B	826	CLA	C2B-C3B-CAB-CBB
26	c	302	CLA	C2B-C3B-CAB-CBB
26	c	304	CLA	C2B-C3B-CAB-CBB
26	a	309	CLA	C2B-C3B-CAB-CBB
26	b	304	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	k	602	CLA	C2B-C3B-CAB-CBB
26	k	603	CLA	C2B-C3B-CAB-CBB
26	k	606	CLA	C2B-C3B-CAB-CBB
26	i	307	CLA	C2B-C3B-CAB-CBB
26	i	311	CLA	C2B-C3B-CAB-CBB
26	d	309	CLA	C2B-C3B-CAB-CBB
26	n	609	CLA	C2B-C3B-CAB-CBB
29	B	848	WVN	C06-C13-C20-C23
29	J	102	WVN	C06-C13-C20-C23
37	b	301	IHT	C02-C07-C18-C22
34	c	318	LMG	C40-C41-C42-C43
32	A	854	SQD	O49-C7-O47-C45
26	A	833	CLA	C2-C1-O2A-CGA
26	B	830	CLA	C2-C1-O2A-CGA
26	A	822	CLA	CAA-CBA-CGA-O2A
26	l	305	CLA	C8-C10-C11-C12
26	A	804	CLA	CBA-CGA-O2A-C1
26	B	822	CLA	C16-C17-C18-C19
26	n	604	CLA	CAA-CBA-CGA-O2A
26	A	818	CLA	C2-C3-C5-C6
26	j	604	CLA	C5-C6-C7-C8
26	h	303	CLA	CAA-CBA-CGA-O2A
26	n	605	CLA	CAA-CBA-CGA-O2A
26	B	823	CLA	C13-C15-C16-C17
26	h	306	CLA	C10-C11-C12-C13
30	a	317	LMU	C2B-C1B-O1B-C4'
28	L	207	LHG	C28-C29-C30-C31
26	A	830	CLA	C8-C10-C11-C12
28	A	843	LHG	C29-C30-C31-C32
26	B	806	CLA	CAA-CBA-CGA-O2A
26	B	820	CLA	CAA-CBA-CGA-O2A
26	b	312	CLA	CAA-CBA-CGA-O2A
26	h	304	CLA	CAA-CBA-CGA-O2A
26	m	610	CLA	CAA-CBA-CGA-O2A
28	L	207	LHG	O10-C23-O8-C6
32	A	854	SQD	C4-C5-C6-S
26	B	817	CLA	C16-C17-C18-C19
26	A	838	CLA	CBD-CGD-O2D-CED
26	a	309	CLA	CAA-CBA-CGA-O2A
32	A	854	SQD	C17-C18-C19-C20
26	B	817	CLA	C2A-CAA-CBA-CGA
26	A	837	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	A	854	SQD	O47-C7-C8-C9
35	b	317	II0	C10-C22-C24-C26
34	F	206	LMG	O10-C28-O8-C9
26	a	306	CLA	C8-C10-C11-C12
26	l	305	CLA	C13-C15-C16-C17
26	B	810	CLA	C11-C12-C13-C14
26	s	402	CLA	C11-C10-C8-C9
26	b	308	CLA	C11-C12-C13-C14
26	l	307	CLA	C14-C13-C15-C16
33	j	618	DGD	CCB-CDB-CEB-CFB
26	B	806	CLA	C15-C16-C17-C18
26	h	301	CLA	CAA-CBA-CGA-O2A
28	c	320	LHG	O8-C23-C24-C25
34	c	318	LMG	O7-C10-C11-C12
28	J	105	LHG	O2-C2-C3-O3
33	B	844	DGD	C8B-C9B-CAB-CBB
26	A	821	CLA	C4B-C3B-CAB-CBB
26	A	836	CLA	C4B-C3B-CAB-CBB
26	B	816	CLA	C4B-C3B-CAB-CBB
26	B	822	CLA	C1A-C2A-CAA-CBA
26	B	823	CLA	C4B-C3B-CAB-CBB
26	B	826	CLA	C4B-C3B-CAB-CBB
26	a	309	CLA	C1A-C2A-CAA-CBA
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	n	609	CLA	O1D-CGD-O2D-CED
26	A	818	CLA	C4-C3-C5-C6
26	i	306	CLA	C4-C3-C5-C6
26	B	806	CLA	C5-C6-C7-C8
26	B	816	CLA	CAA-CBA-CGA-O2A
26	c	307	CLA	CAA-CBA-CGA-O2A
26	k	610	CLA	CAA-CBA-CGA-O2A
28	A	849	LHG	O7-C7-C8-C9
28	b	302	LHG	O8-C23-C24-C25
26	c	312	CLA	C2-C3-C5-C6
35	b	314	II0	C31-C33-C35-C39
35	l	314	II0	C31-C33-C35-C39
35	l	317	II0	C32-C34-C36-C40
35	a	314	II0	C35-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
35	d	315	II0	C35-C39-C41-C42
26	B	824	CLA	CBD-CGD-O2D-CED
28	b	318	LHG	C10-C11-C12-C13
26	d	303	CLA	CBA-CGA-O2A-C1
34	b	319	LMG	C29-C28-O8-C9
26	A	818	CLA	C8-C10-C11-C12
26	s	408	CLA	C5-C6-C7-C8
26	B	801	CLA	CAA-CBA-CGA-O2A
26	c	308	CLA	CAA-CBA-CGA-O2A
26	m	608	CLA	CAA-CBA-CGA-O2A
26	i	305	CLA	CAA-CBA-CGA-O2A
26	L	202	CLA	C2A-CAA-CBA-CGA
26	a	302	CLA	O1A-CGA-O2A-C1
26	A	811	CLA	C5-C6-C7-C8
33	B	844	DGD	O2G-C1B-C2B-C3B
34	b	319	LMG	O8-C28-C29-C30
34	L	209	LMG	C13-C14-C15-C16
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	F	201	CLA	C2-C1-O2A-CGA
26	c	308	CLA	C2-C1-O2A-CGA
26	A	805	CLA	C12-C13-C15-C16
26	A	833	CLA	C6-C7-C8-C10
26	B	824	CLA	C6-C7-C8-C10
26	B	838	CLA	C11-C10-C8-C7
26	c	308	CLA	C12-C13-C15-C16
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	d	302	CLA	C11-C10-C8-C7
28	B	851	LHG	C18-C19-C20-C21
34	c	318	LMG	C32-C33-C34-C35
28	B	851	LHG	C6-C5-O7-C7
28	s	409	LHG	O7-C7-C8-C9
28	b	302	LHG	C19-C20-C21-C22
26	i	305	CLA	C2A-CAA-CBA-CGA
26	n	609	CLA	C2A-CAA-CBA-CGA
26	B	824	CLA	O1D-CGD-O2D-CED
26	A	830	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	A	813	CLA	C3A-C2A-CAA-CBA
26	A	819	CLA	C3A-C2A-CAA-CBA
26	B	829	CLA	C3A-C2A-CAA-CBA
26	k	607	CLA	C3A-C2A-CAA-CBA
28	J	105	LHG	O10-C23-O8-C6
26	A	805	CLA	C16-C17-C18-C19
26	A	812	CLA	CAA-CBA-CGA-O2A
26	j	604	CLA	CAA-CBA-CGA-O2A
29	A	857	WVN	C33-C34-C37-C40
26	A	835	CLA	C15-C16-C17-C18
28	s	409	LHG	O10-C23-C24-C25
34	b	319	LMG	O10-C28-C29-C30
30	A	850	LMU	O5B-C5B-C6B-O6B
34	c	318	LMG	C29-C30-C31-C32
26	B	826	CLA	CAA-CBA-CGA-O2A
28	b	318	LHG	O7-C7-C8-C9
34	Q	301	LMG	C29-C30-C31-C32
26	j	604	CLA	C4C-C3C-CAC-CBC
26	A	802	CLA	CAA-CBA-CGA-O1A
26	B	806	CLA	CAA-CBA-CGA-O1A
26	b	312	CLA	CAA-CBA-CGA-O1A
28	b	318	LHG	O9-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
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	C11-C12-C13-C14
26	A	822	CLA	CAA-CBA-CGA-O1A
26	B	820	CLA	CAA-CBA-CGA-O1A
26	n	605	CLA	CAA-CBA-CGA-O1A
28	A	855	LHG	O10-C23-C24-C25
28	s	409	LHG	O9-C7-C8-C9
28	b	302	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	A	805	CLA	C5-C6-C7-C8
26	c	312	CLA	C4-C3-C5-C6
26	n	610	CLA	C4-C3-C5-C6
26	h	301	CLA	CAA-CBA-CGA-O1A
26	m	610	CLA	CAA-CBA-CGA-O1A
26	d	308	CLA	CAA-CBA-CGA-O1A
36	s	404	KC2	C3A-C2A-CAA-CBA
36	k	611	KC2	C1A-C2A-CAA-CBA
36	k	612	KC2	C3A-C2A-CAA-CBA
33	j	618	DGD	CAB-CBB-CCB-CDB
26	A	837	CLA	CAA-CBA-CGA-O1A
26	s	402	CLA	CAA-CBA-CGA-O1A
26	h	303	CLA	CAA-CBA-CGA-O1A
26	i	305	CLA	CAA-CBA-CGA-O1A
34	c	319	LMG	C20-C21-C22-C23
28	B	851	LHG	C10-C11-C12-C13
26	F	202	CLA	CAA-CBA-CGA-O1A
28	A	849	LHG	O9-C7-C8-C9
28	n	619	LHG	C31-C32-C33-C34
33	B	844	DGD	CFA-CGA-CHA-CIA
26	a	309	CLA	CAA-CBA-CGA-O1A
28	A	855	LHG	O8-C23-C24-C25
28	s	409	LHG	O8-C23-C24-C25
26	d	313	CLA	C2A-CAA-CBA-CGA
26	A	819	CLA	CAA-CBA-CGA-O1A
26	B	816	CLA	CAA-CBA-CGA-O1A
26	c	307	CLA	CAA-CBA-CGA-O1A
26	c	308	CLA	CAA-CBA-CGA-O1A
27	B	843	PQN	C25-C26-C27-C28
26	B	812	CLA	CAA-CBA-CGA-O2A
26	i	304	CLA	CAA-CBA-CGA-O2A
28	B	851	LHG	O8-C23-C24-C25
28	c	320	LHG	O10-C23-C24-C25
26	A	805	CLA	CAD-CBD-CGD-O2D
26	A	824	CLA	CAD-CBD-CGD-O2D
26	B	835	CLA	CAD-CBD-CGD-O2D
26	B	841	CLA	CAD-CBD-CGD-O2D
26	a	305	CLA	CAD-CBD-CGD-O2D
26	l	304	CLA	CAD-CBD-CGD-O2D
26	l	308	CLA	CAD-CBD-CGD-O2D
26	n	602	CLA	CAD-CBD-CGD-O2D
36	c	310	KC2	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	A	816	CLA	C13-C15-C16-C17
26	B	841	CLA	C5-C6-C7-C8
34	c	318	LMG	C36-C37-C38-C39
26	B	828	CLA	CAA-CBA-CGA-O2A
26	j	603	CLA	CAA-CBA-CGA-O2A
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	m	608	CLA	CAA-CBA-CGA-O1A
26	A	820	CLA	C2-C1-O2A-CGA
26	A	822	CLA	C2-C1-O2A-CGA
26	b	303	CLA	C2-C1-O2A-CGA
26	k	608	CLA	C2-C1-O2A-CGA
26	i	301	CLA	C2-C1-O2A-CGA
26	c	311	CLA	CAA-CBA-CGA-O2A
26	h	304	CLA	CAA-CBA-CGA-O1A
26	k	610	CLA	CAA-CBA-CGA-O1A
32	A	854	SQD	O49-C7-C8-C9
26	c	304	CLA	CAA-CBA-CGA-O2A
26	m	604	CLA	CAA-CBA-CGA-O2A
26	i	301	CLA	C8-C10-C11-C12
26	B	826	CLA	CAA-CBA-CGA-O1A
26	n	604	CLA	CAA-CBA-CGA-O1A
30	B	852	LMU	C4-C5-C6-C7
26	A	808	CLA	CAA-CBA-CGA-O2A
26	A	833	CLA	CAA-CBA-CGA-O2A
26	B	809	CLA	CAA-CBA-CGA-O2A
26	a	304	CLA	CAA-CBA-CGA-O2A
26	A	805	CLA	C10-C11-C12-C13
26	a	306	CLA	C13-C15-C16-C17
28	L	207	LHG	C8-C7-O7-C5
26	A	812	CLA	CAA-CBA-CGA-O1A
28	m	618	LHG	C29-C30-C31-C32
26	a	306	CLA	CAA-CBA-CGA-O2A
26	h	308	CLA	CAA-CBA-CGA-O2A
26	l	301	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
26	A	802	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	843	LHG	1	0
26	B	836	CLA	4	0
26	J	103	CLA	1	0
26	B	827	CLA	3	0
26	c	312	CLA	2	0
26	B	837	CLA	5	0
26	n	607	CLA	3	0
26	b	304	CLA	1	0
26	a	311	CLA	1	0
26	k	607	CLA	1	0
35	b	314	II0	1	0
26	L	202	CLA	1	0
26	A	810	CLA	2	0
26	A	833	CLA	3	0
26	A	851	CLA	2	0
26	a	304	CLA	1	0
27	B	843	PQN	2	0
26	k	614	CLA	1	0
26	b	307	CLA	1	0
26	b	312	CLA	4	0
26	k	608	CLA	1	0
26	n	608	CLA	6	0
36	s	404	KC2	1	0
26	A	822	CLA	4	0
28	s	409	LHG	3	0
26	b	309	CLA	6	0
26	i	311	CLA	3	0
26	B	814	CLA	5	0
26	m	603	CLA	1	0
26	k	609	CLA	3	0
26	c	301	CLA	2	0
34	F	205	LMG	1	0
26	a	301	CLA	7	0
26	A	812	CLA	4	0
34	F	206	LMG	1	0
26	A	836	CLA	6	0
26	A	830	CLA	3	0
26	L	203	CLA	4	0
26	A	837	CLA	7	0
28	A	855	LHG	2	0
26	A	824	CLA	2	0
26	A	828	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	804	CLA	3	0
26	n	604	CLA	1	0
26	R	201	CLA	4	0
26	h	313	CLA	3	0
26	d	308	CLA	1	0
26	k	604	CLA	2	0
26	A	825	CLA	2	0
26	B	812	CLA	3	0
26	L	206	CLA	1	0
26	m	610	CLA	2	0
26	j	610	CLA	3	0
26	i	301	CLA	1	0
26	A	841	CLA	7	0
26	h	305	CLA	2	0
26	a	303	CLA	1	0
26	B	811	CLA	2	0
26	d	304	CLA	1	0
26	h	304	CLA	2	0
26	j	613	CLA	2	0
26	d	306	CLA	1	0
26	h	307	CLA	2	0
26	B	823	CLA	4	0
26	A	815	CLA	1	0
26	F	201	CLA	2	0
26	c	306	CLA	1	0
26	A	838	CLA	2	0
26	B	821	CLA	3	0
26	A	803	CLA	4	0
26	B	809	CLA	1	0
26	B	841	CLA	2	0
26	m	607	CLA	2	0
26	B	819	CLA	3	0
26	B	803	CLA	4	0
26	A	805	CLA	6	0
26	B	832	CLA	1	0
26	B	833	CLA	3	0
26	A	808	CLA	1	0
34	L	209	LMG	2	0
26	s	402	CLA	2	0
26	j	607	CLA	1	0
26	A	826	CLA	2	0
26	B	810	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	309	CLA	1	0
26	A	811	CLA	1	0
34	Q	301	LMG	3	0
26	B	806	CLA	2	0
35	i	319	II0	1	0
26	B	822	CLA	5	0
26	l	313	CLA	3	0
26	B	840	CLA	4	0
26	j	608	CLA	2	0
26	a	306	CLA	1	0
26	A	831	CLA	4	0
26	l	304	CLA	1	0
26	h	308	CLA	1	0
26	B	807	CLA	4	0
26	i	304	CLA	1	0
26	i	306	CLA	1	0
36	s	401	KC2	1	0
26	m	602	CLA	5	0
26	c	307	CLA	1	0
26	j	609	CLA	1	0
28	b	318	LHG	1	0
26	A	809	CLA	1	0
26	n	610	CLA	2	0
26	d	302	CLA	3	0
26	A	832	CLA	4	0
26	j	604	CLA	2	0
26	B	842	CLA	4	0
30	i	300	LMU	2	0
26	B	830	CLA	4	0
26	m	609	CLA	1	0
30	B	852	LMU	1	0
26	A	834	CLA	1	0
28	A	844	LHG	2	0
27	A	842	PQN	4	0
26	l	301	CLA	3	0
28	n	619	LHG	1	0
26	B	813	CLA	1	0
26	c	302	CLA	1	0
26	m	608	CLA	2	0
35	n	614	II0	1	0
26	k	605	CLA	1	0
26	A	856	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	m	613	CLA	5	0
26	k	602	CLA	2	0
26	l	309	CLA	4	0
26	c	303	CLA	1	0
26	h	301	CLA	6	0
31	C	102	SF4	1	0
28	b	302	LHG	2	0
33	B	844	DGD	6	0
26	B	839	CLA	1	0
26	B	805	CLA	1	0
26	m	604	CLA	1	0
26	A	818	CLA	5	0
26	A	817	CLA	2	0
26	F	202	CLA	2	0
26	A	804	CLA	4	0
33	j	618	DGD	3	0
28	c	320	LHG	4	0
26	A	840	CLA	2	0
26	a	307	CLA	1	0
26	A	819	CLA	1	0
26	A	816	CLA	4	0
26	B	824	CLA	2	0
37	b	301	IHT	1	0
34	c	319	LMG	1	0
26	B	815	CLA	3	0
26	A	827	CLA	7	0
26	B	834	CLA	3	0
26	k	610	CLA	1	0
26	c	304	CLA	2	0
26	B	829	CLA	1	0
25	A	801	CL0	4	0
26	b	311	CLA	1	0
26	B	820	CLA	2	0
26	i	307	CLA	1	0
26	n	609	CLA	2	0
26	j	603	CLA	3	0
26	A	806	CLA	1	0
26	m	601	CLA	2	0
26	l	308	CLA	2	0
26	c	305	CLA	1	0
26	B	828	CLA	4	0
26	l	305	CLA	3	0

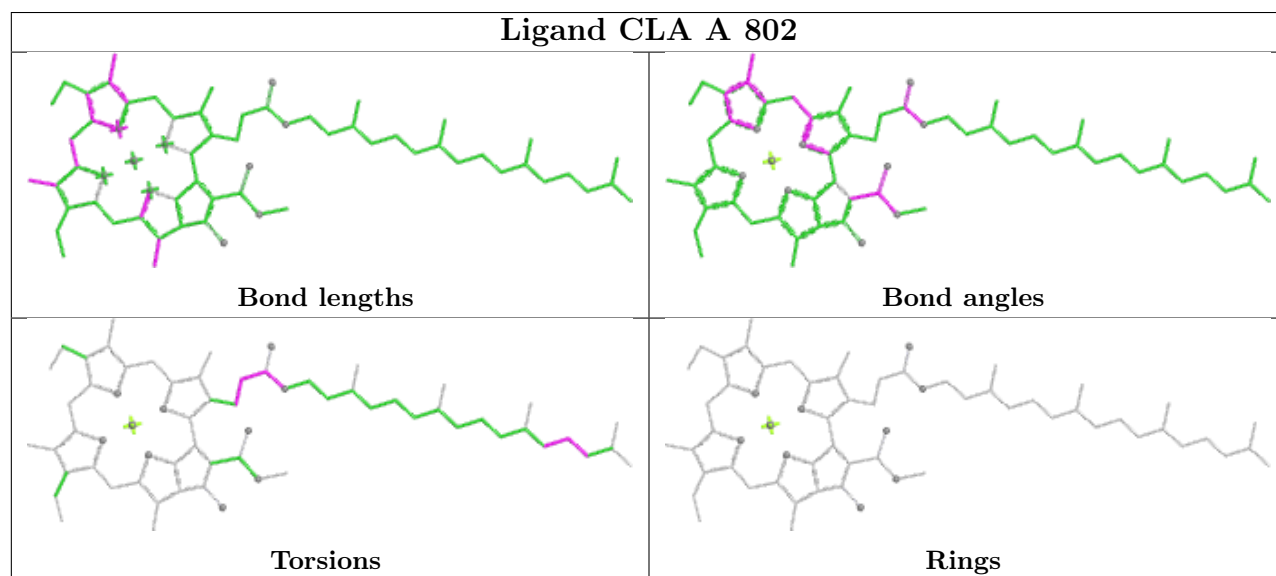
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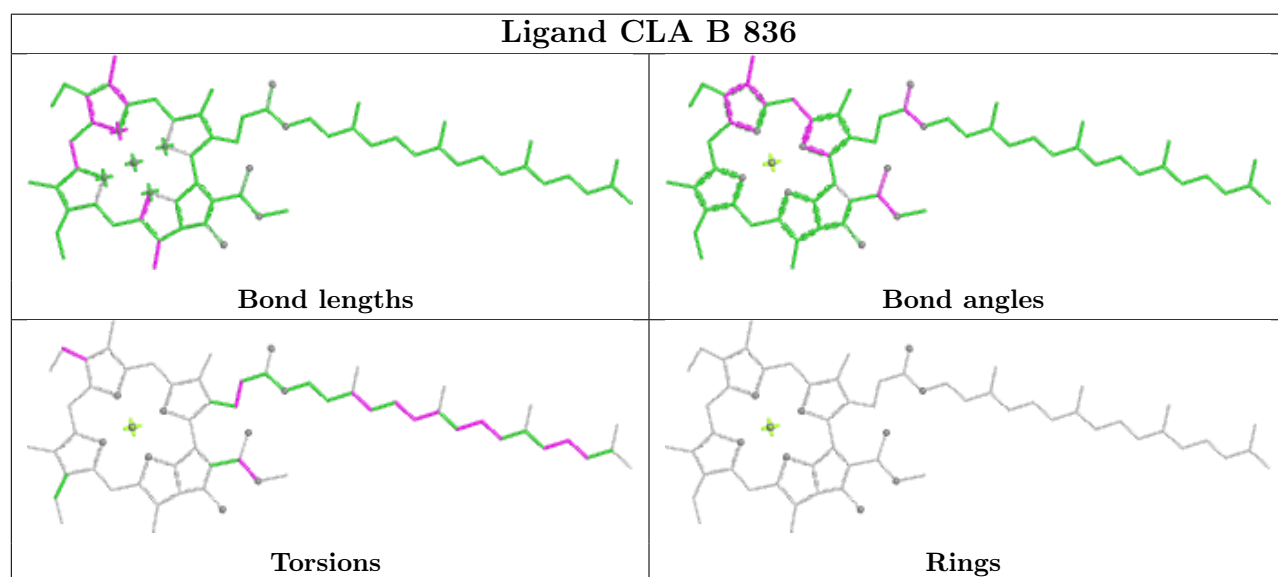
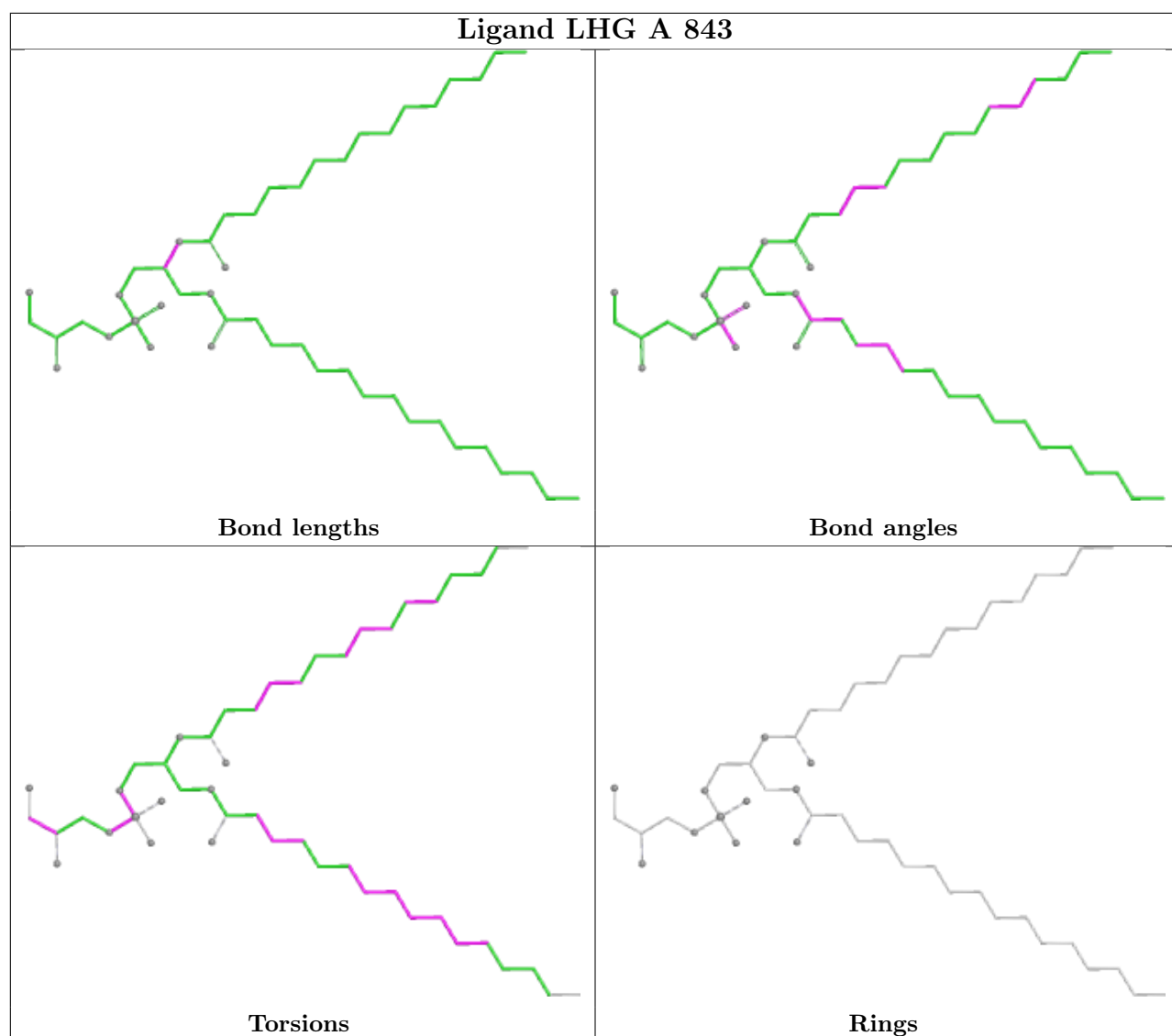
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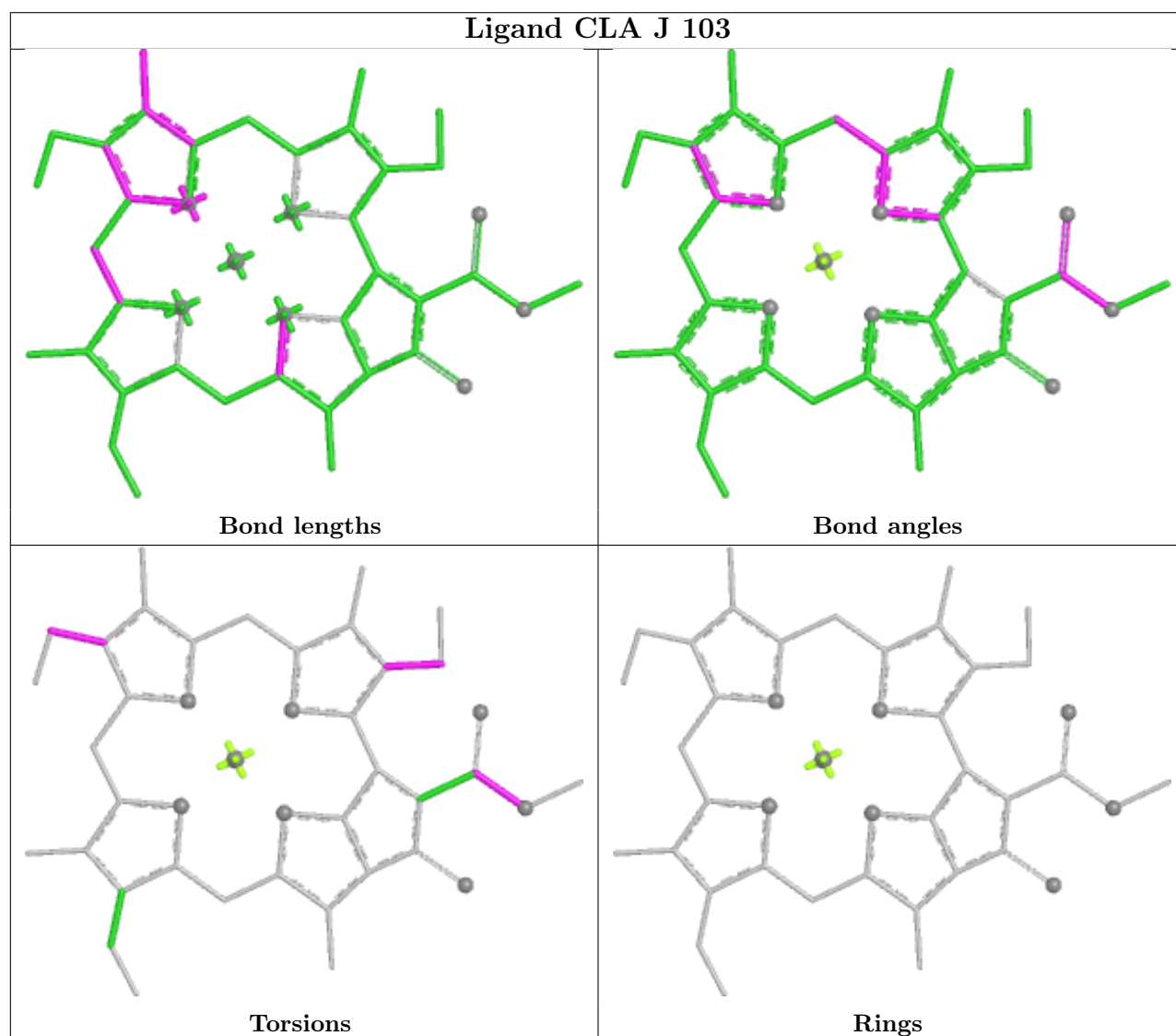
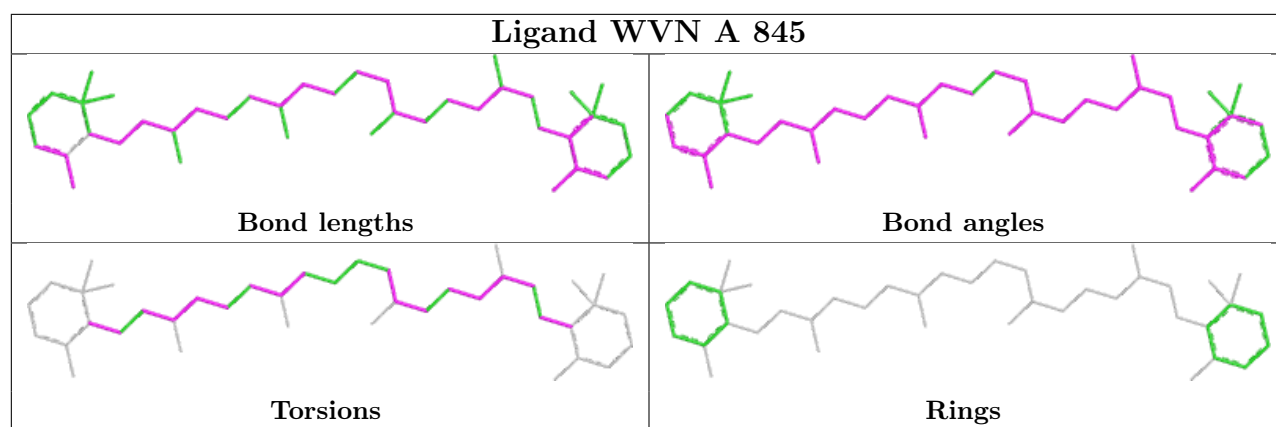
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	825	CLA	5	0
26	b	313	CLA	1	0
26	B	838	CLA	2	0
34	n	620	LMG	3	0
26	k	603	CLA	1	0
35	d	319	II0	1	0
26	B	801	CLA	3	0
26	B	835	CLA	3	0
36	d	312	KC2	3	0
26	s	406	CLA	3	0
26	B	817	CLA	6	0
36	n	611	KC2	1	0
34	b	319	LMG	1	0
26	l	306	CLA	3	0
30	A	858	LMU	2	0
26	A	829	CLA	7	0
26	B	826	CLA	3	0
26	n	613	CLA	2	0
28	A	849	LHG	2	0
26	A	807	CLA	1	0
26	c	308	CLA	3	0
26	B	831	CLA	3	0
26	d	313	CLA	4	0
26	h	306	CLA	1	0
26	L	204	CLA	3	0
26	a	310	CLA	1	0
28	B	851	LHG	2	0
26	A	814	CLA	2	0
26	A	823	CLA	4	0
26	a	308	CLA	1	0
26	B	818	CLA	2	0
26	B	802	CLA	3	0
26	A	835	CLA	4	0
26	A	852	CLA	3	0
26	B	808	CLA	4	0
26	b	310	CLA	5	0
26	b	306	CLA	3	0
26	A	839	CLA	2	0
26	B	816	CLA	2	0

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

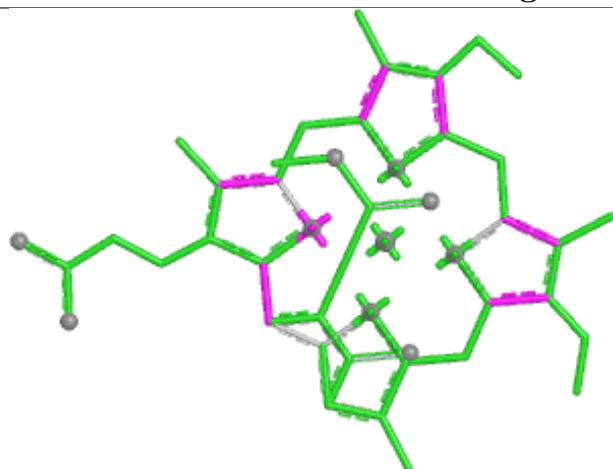
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



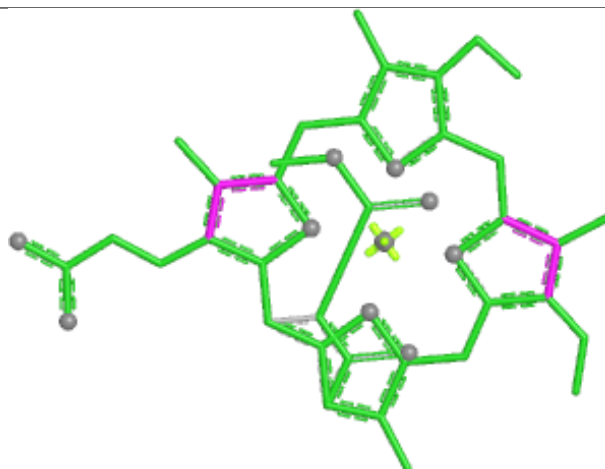




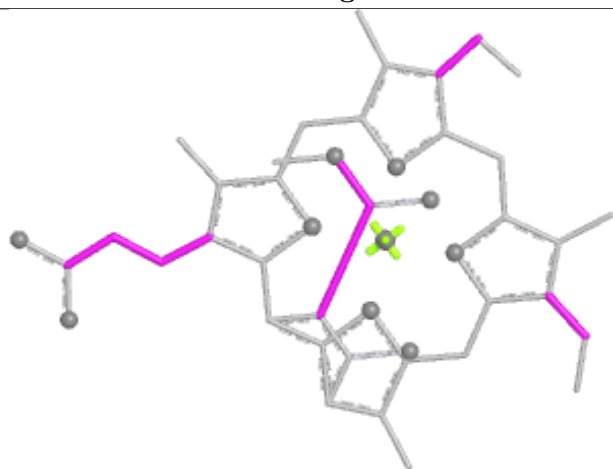
Ligand KC2 k 611



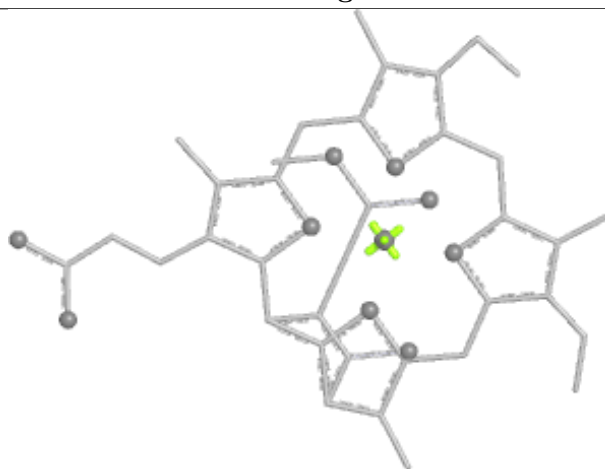
Bond lengths



Bond angles

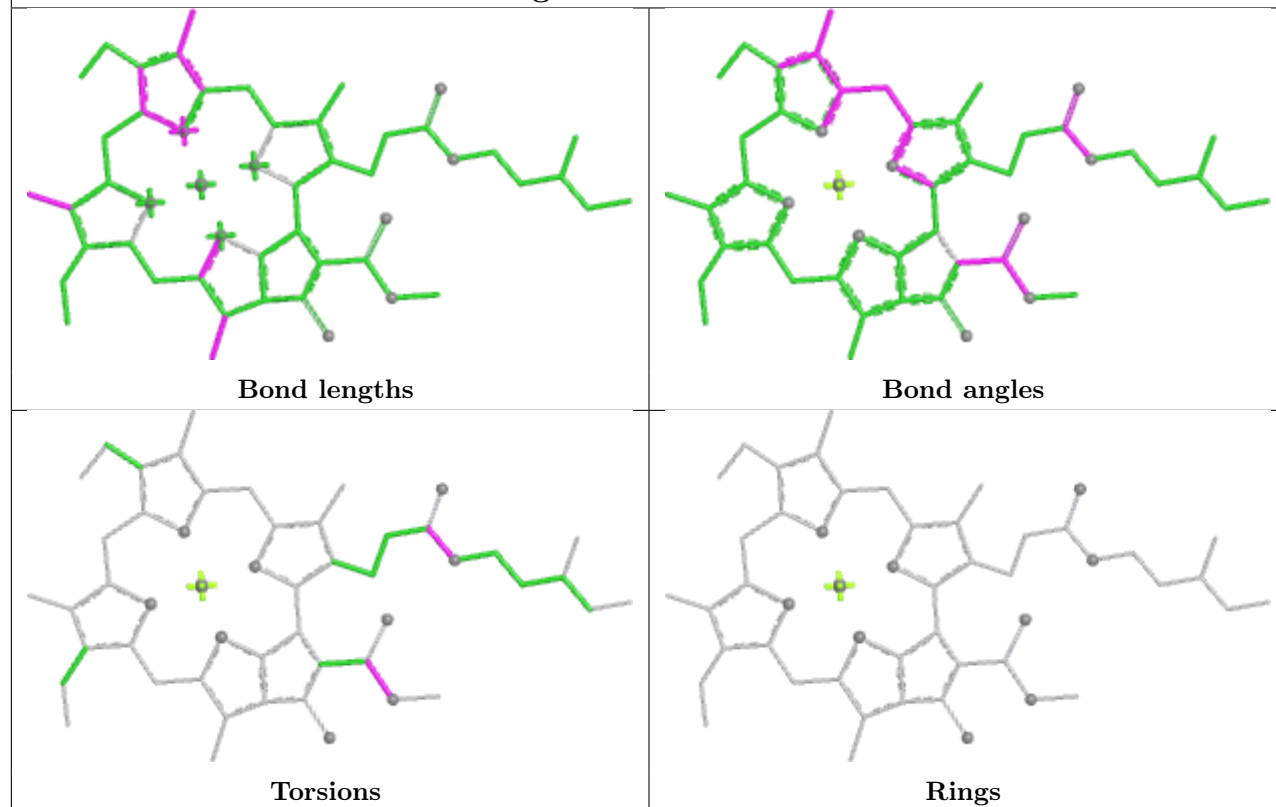


Torsions

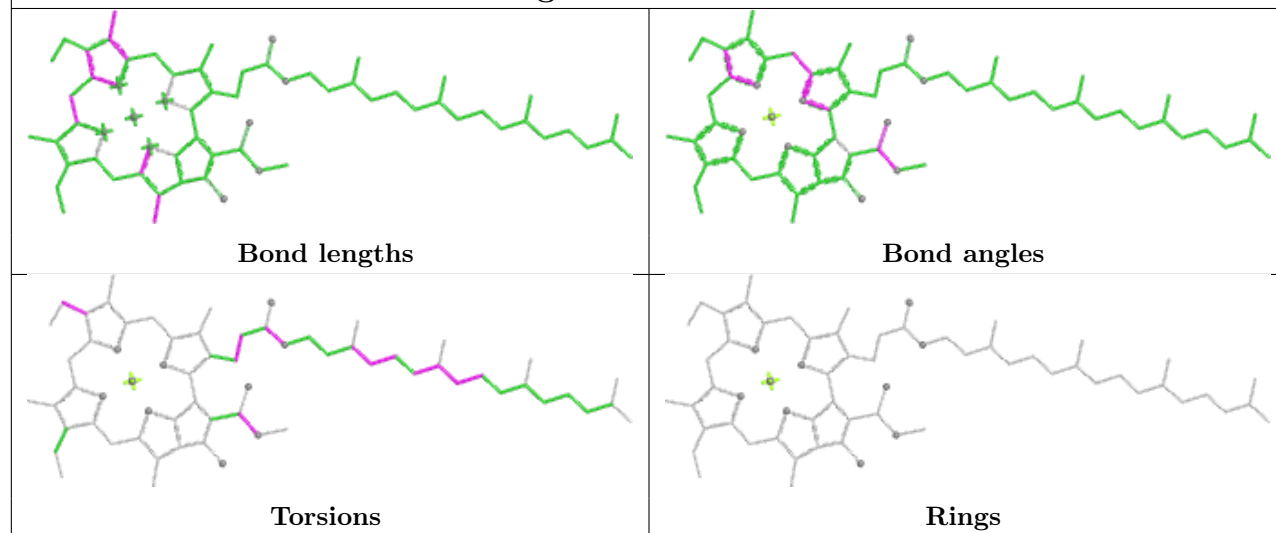


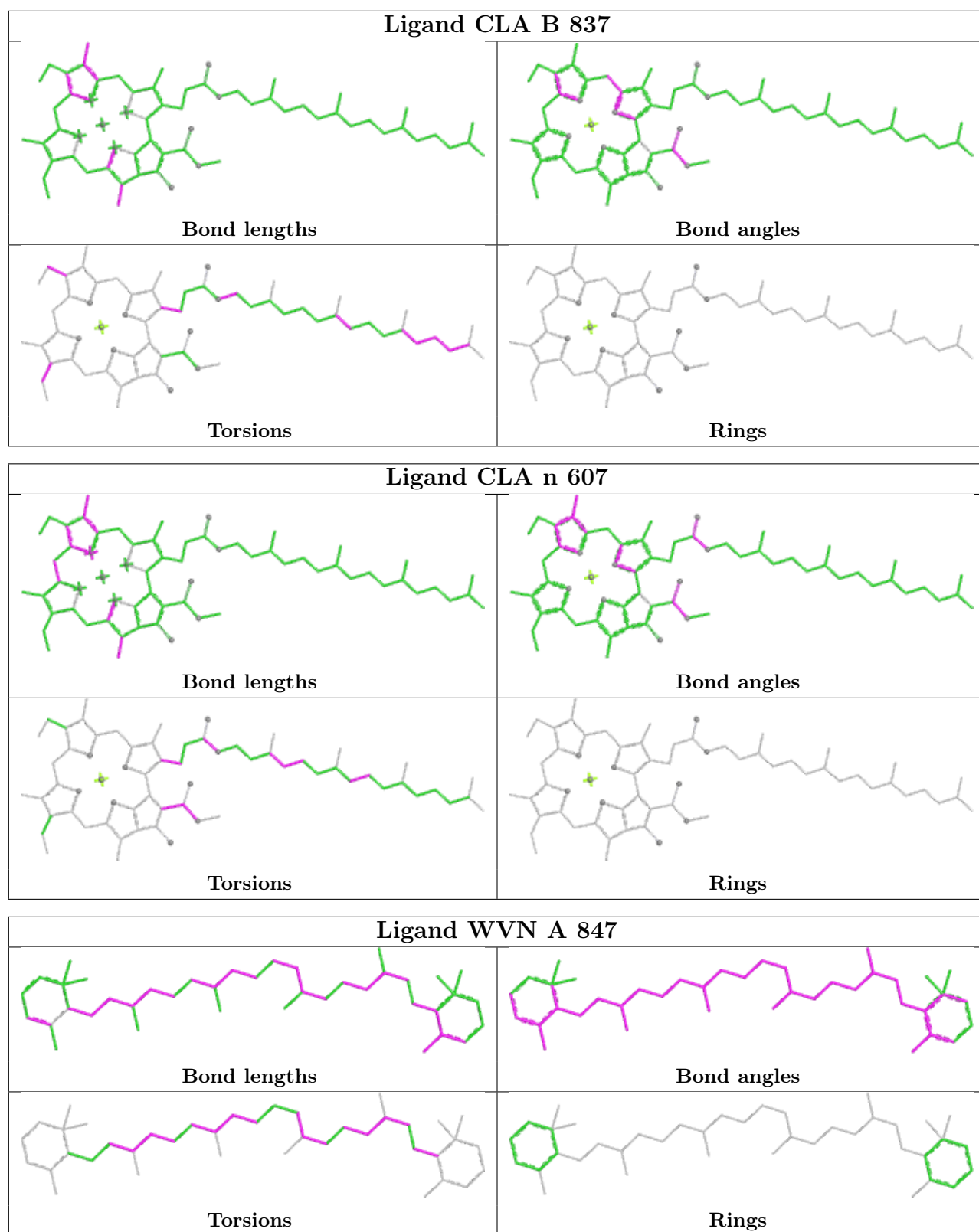
Rings

Ligand CLA B 827

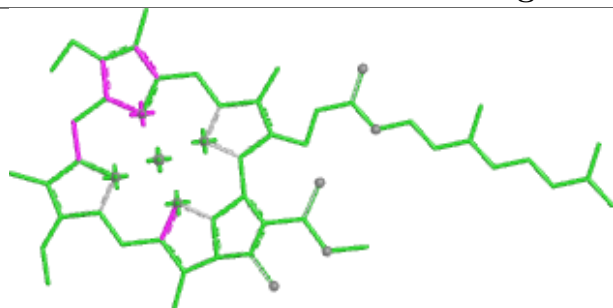


Ligand CLA c 312

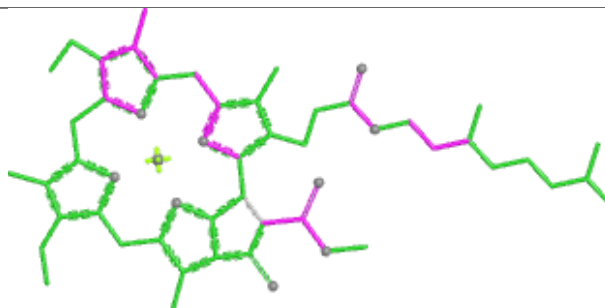




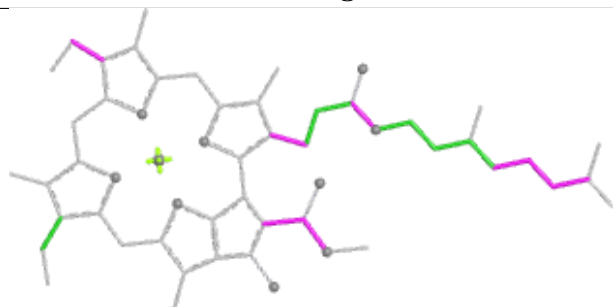
Ligand CLA b 304



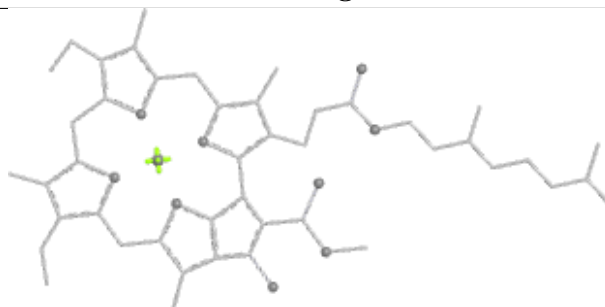
Bond lengths



Bond angles

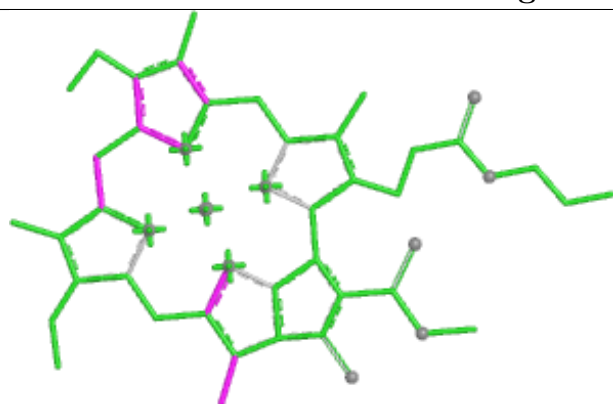


Torsions

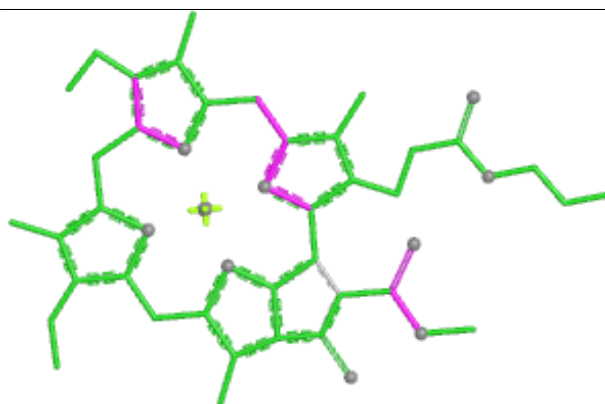


Rings

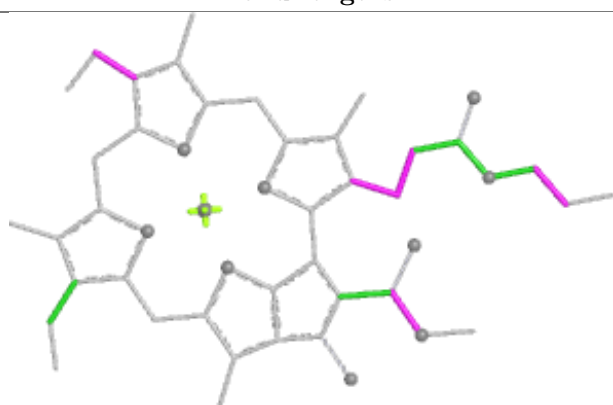
Ligand CLA a 311



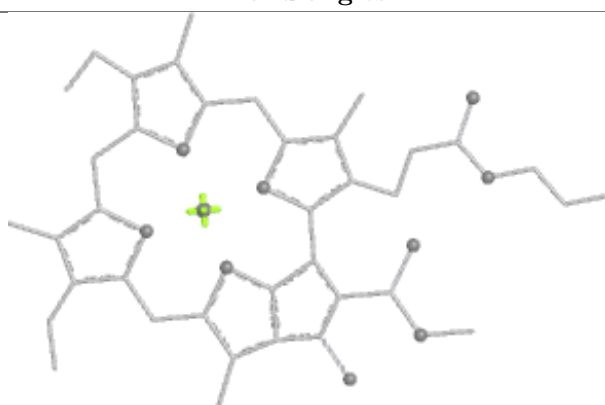
Bond lengths



Bond angles

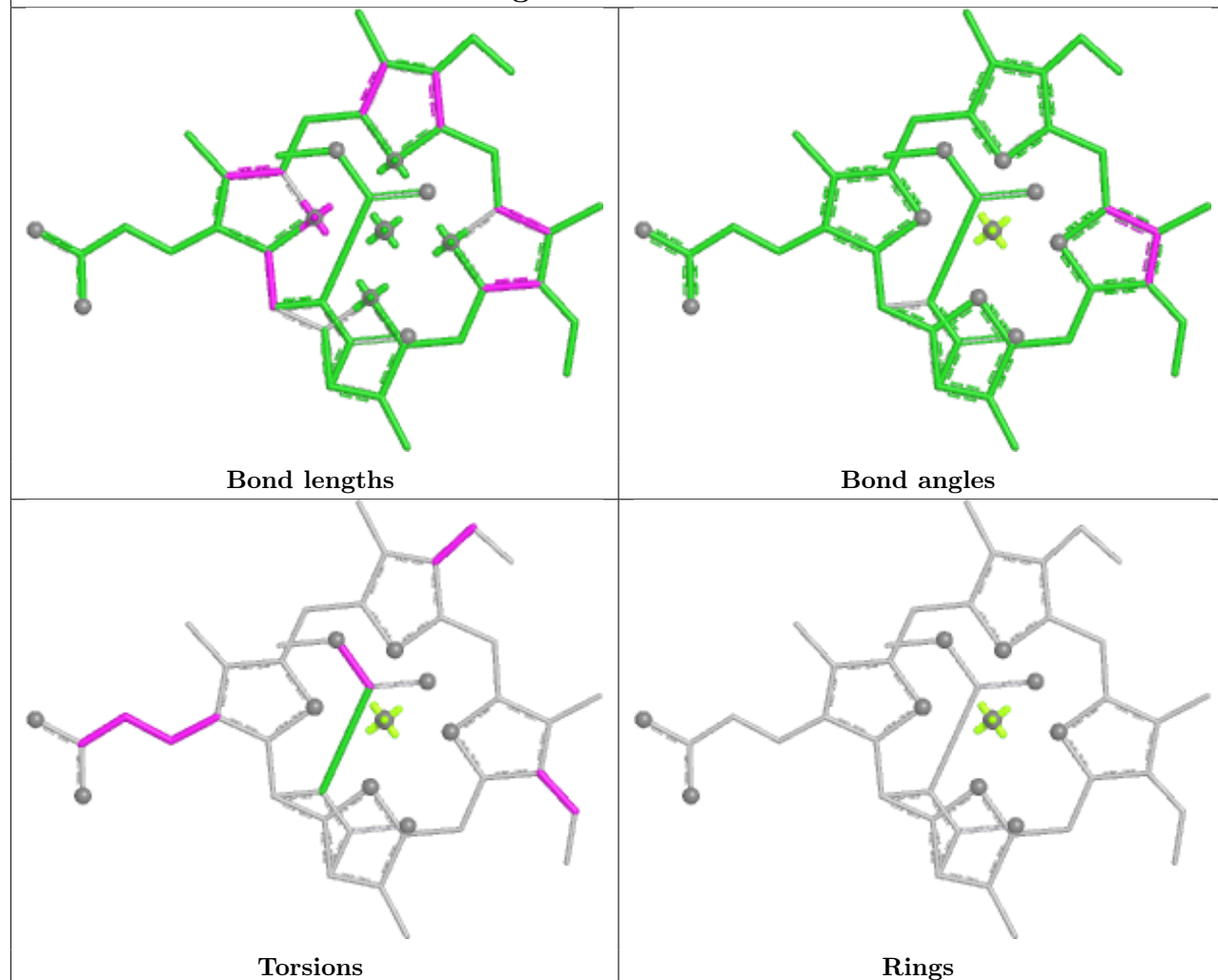


Torsions

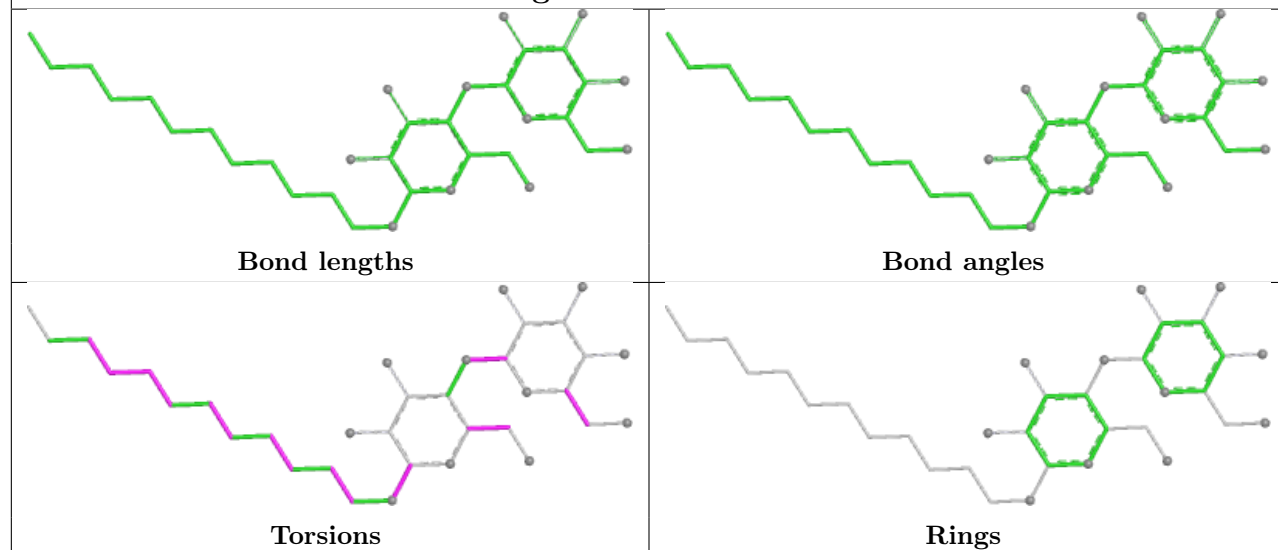


Rings

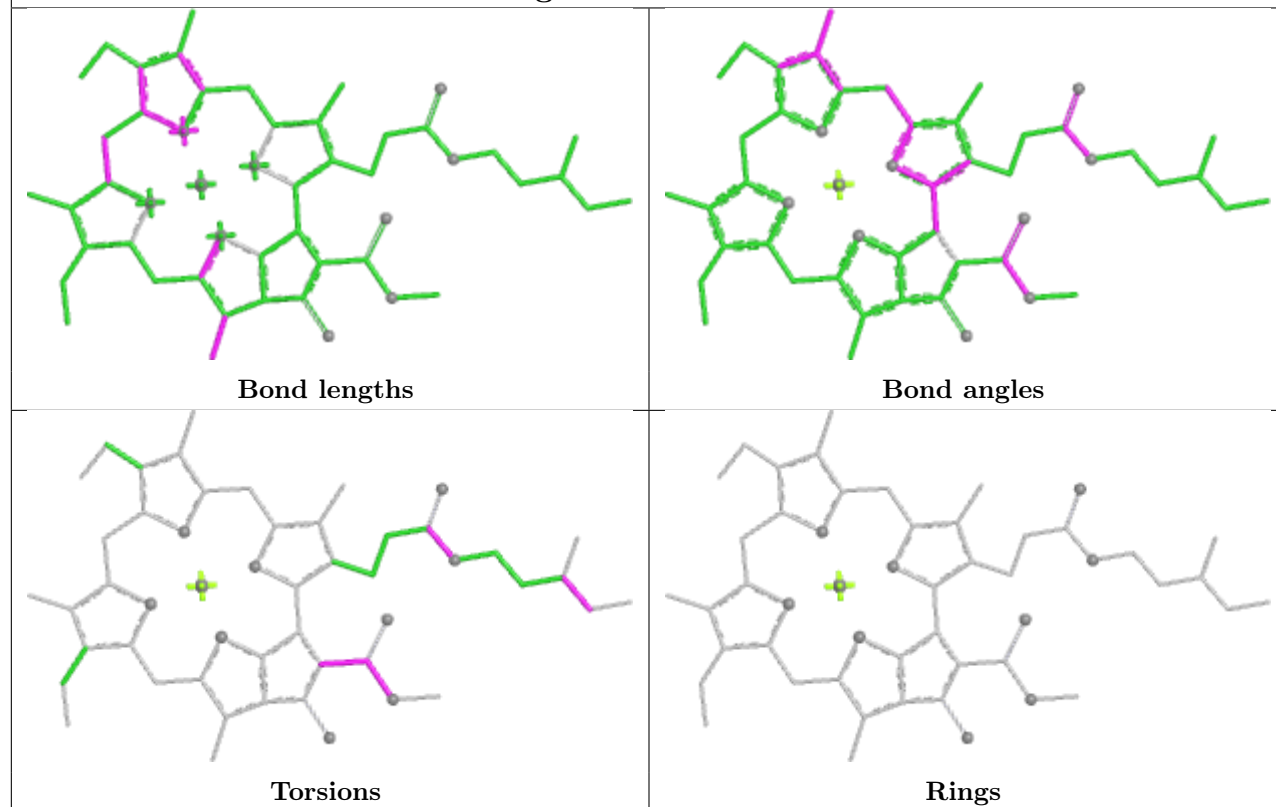
Ligand KC2 k 613



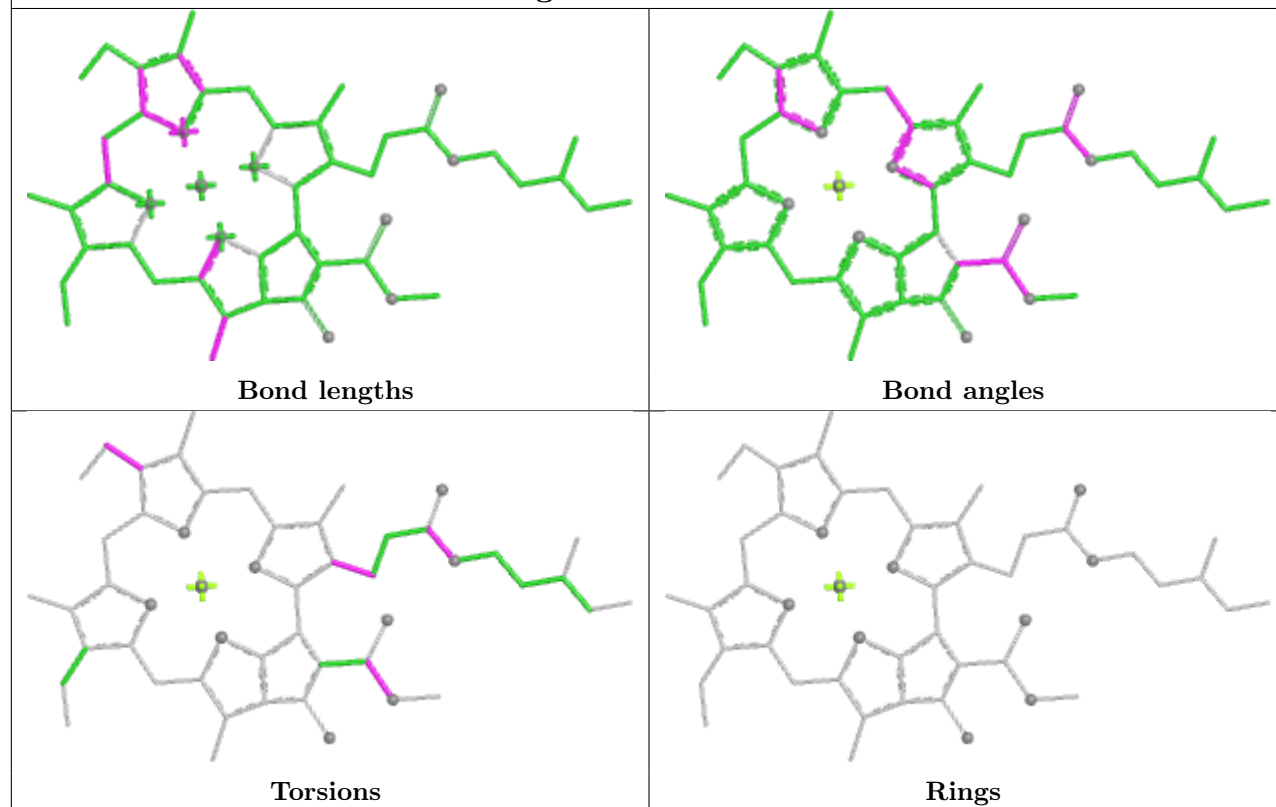
Ligand LMU a 317

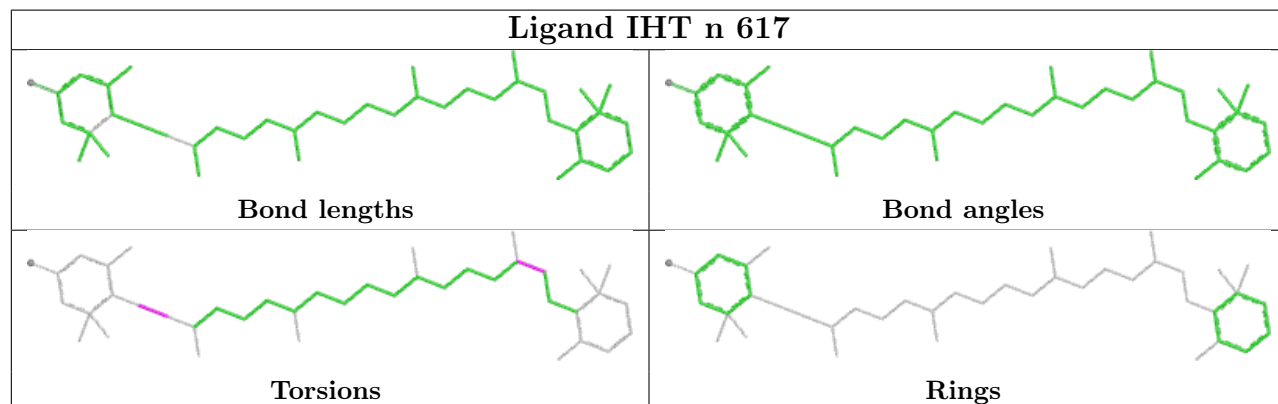
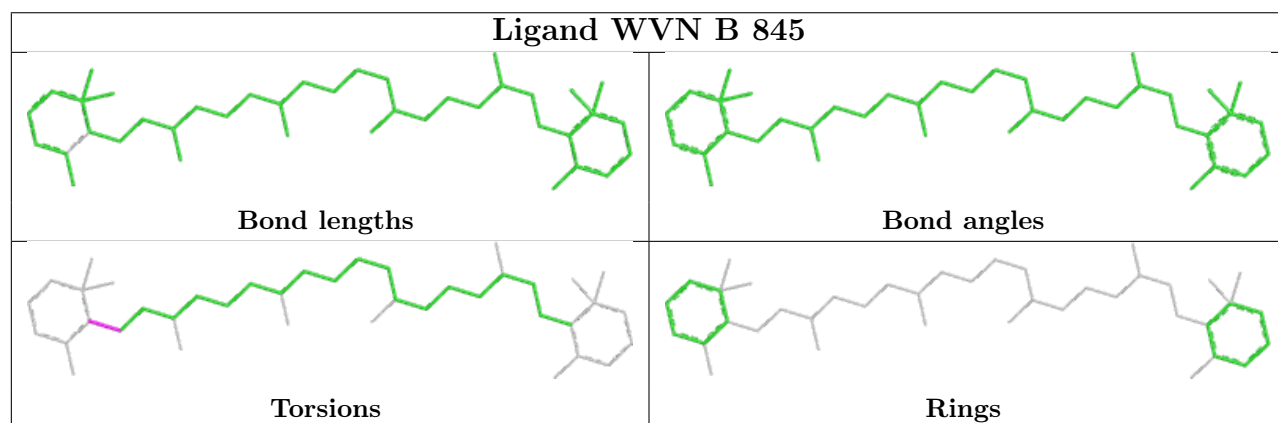
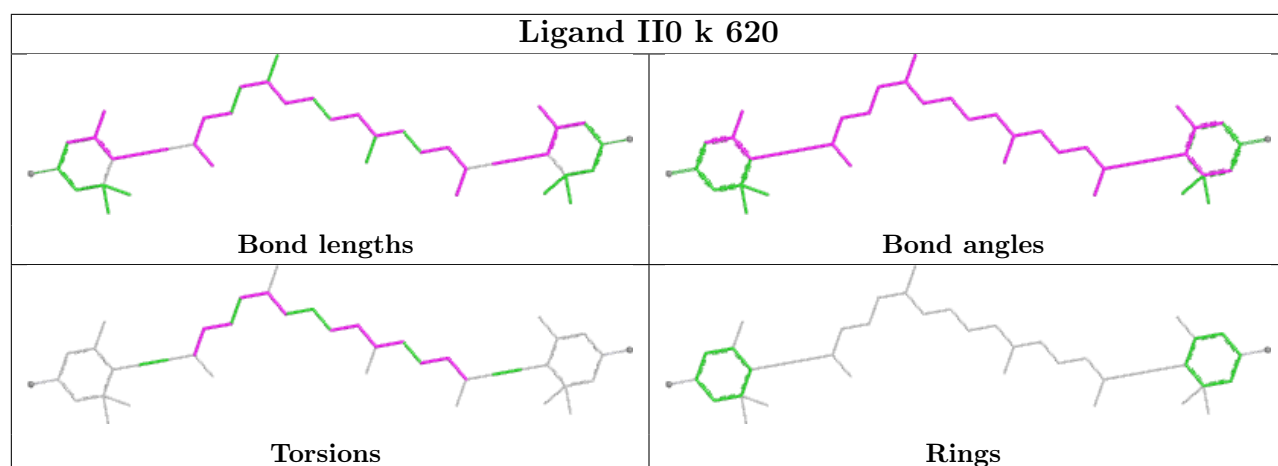


Ligand CLA d 303

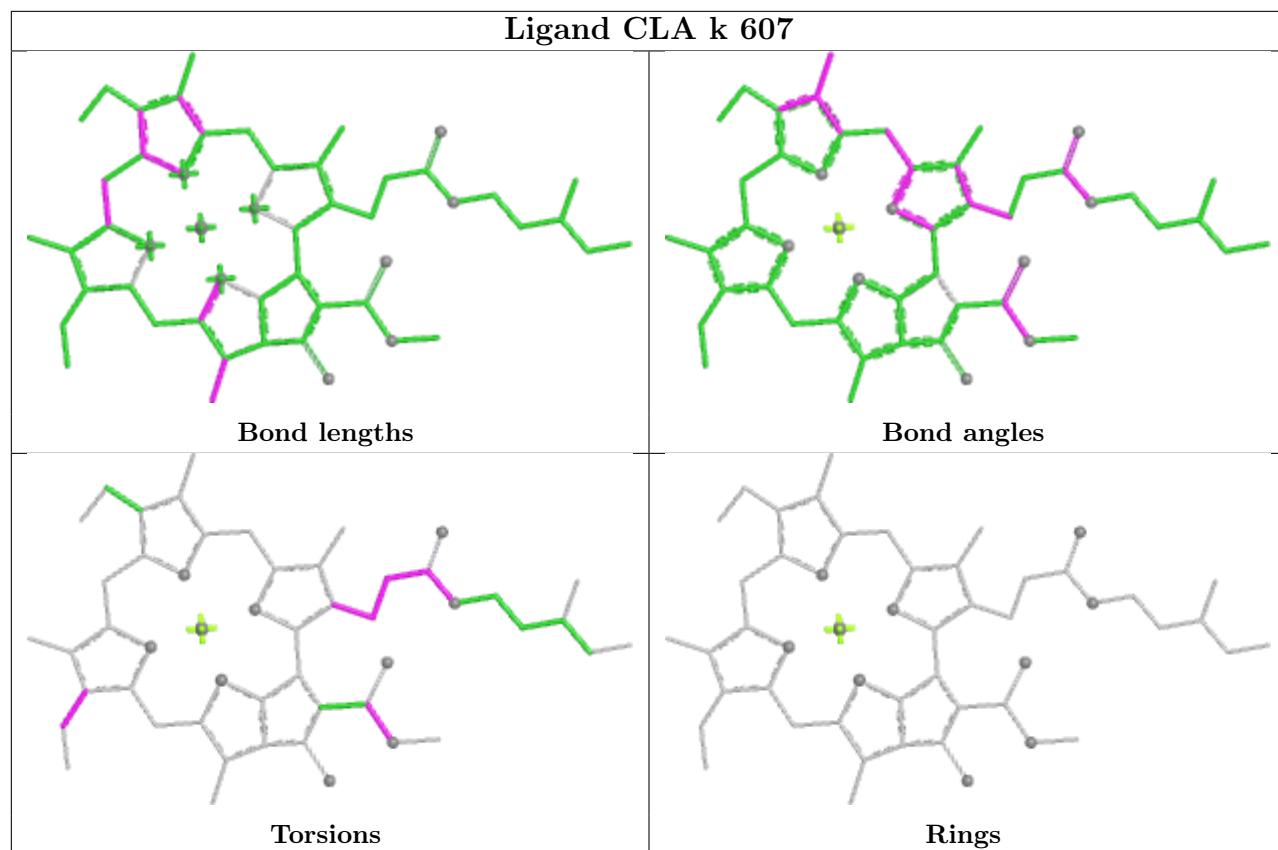


Ligand CLA k 601

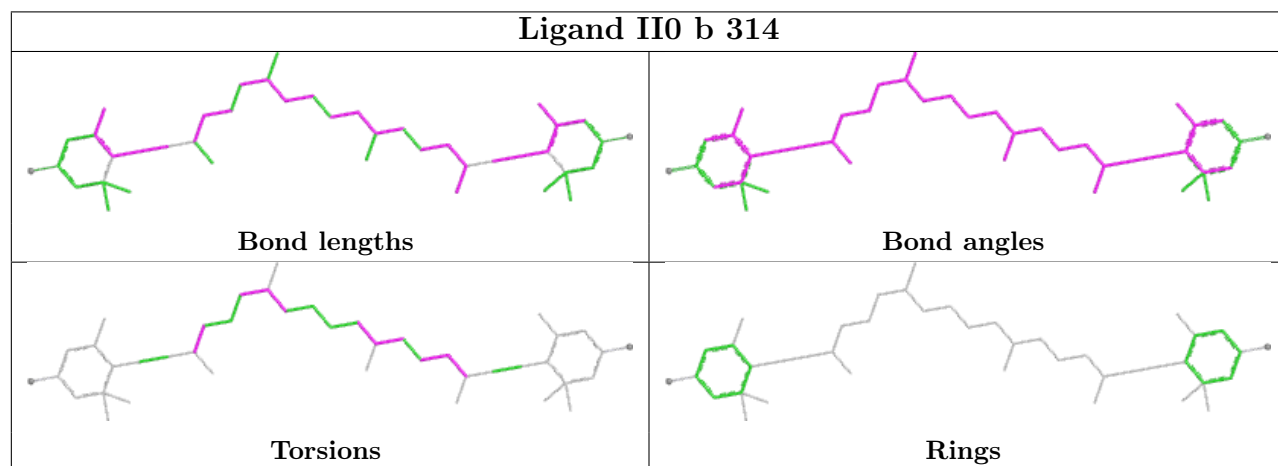




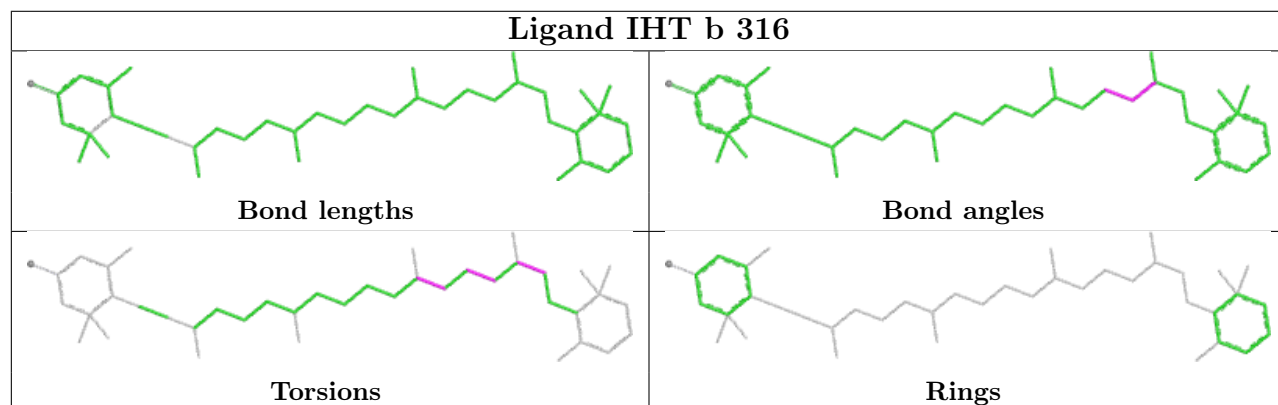
Ligand CLA k 607



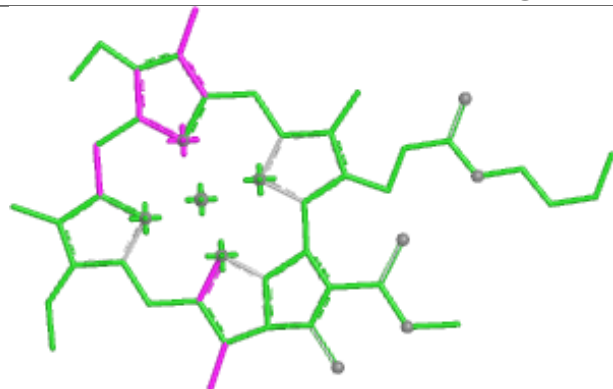
Ligand II0 b 314



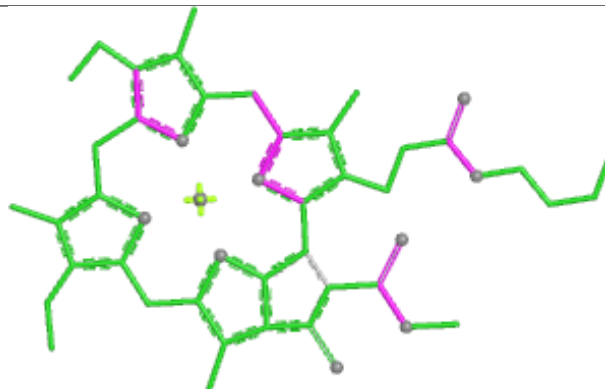
Ligand IHT b 316



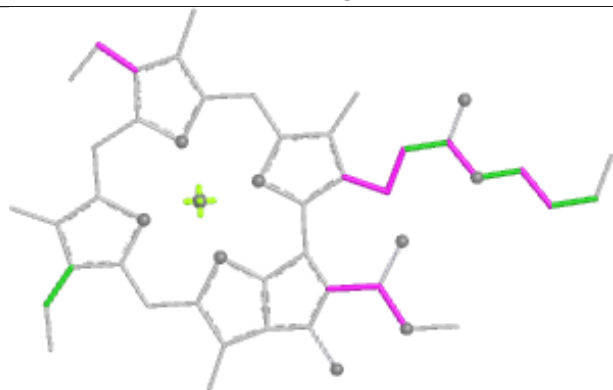
Ligand CLA L 202



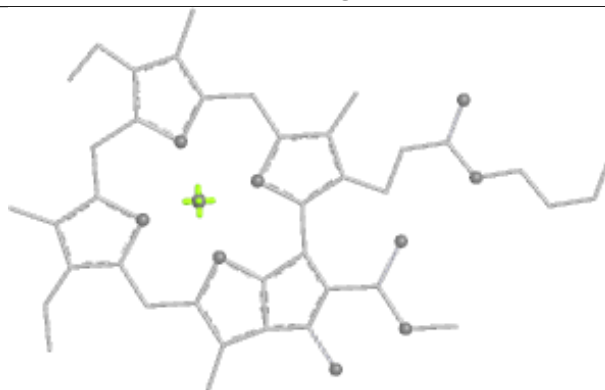
Bond lengths



Bond angles

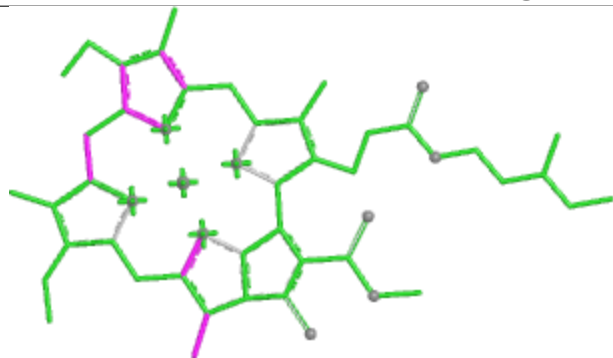


Torsions

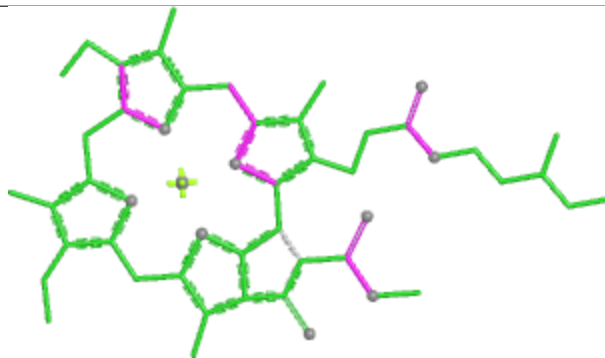


Rings

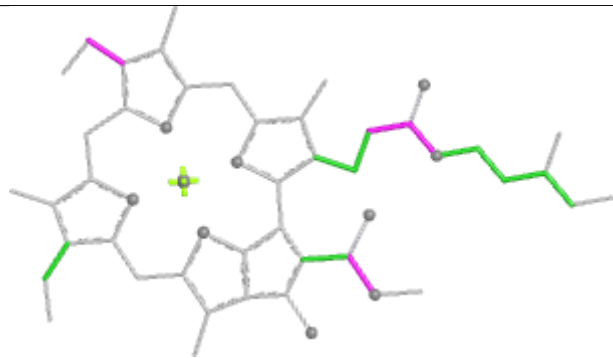
Ligand CLA k 606



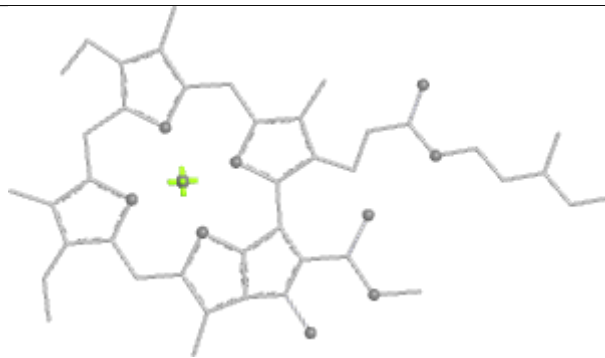
Bond lengths



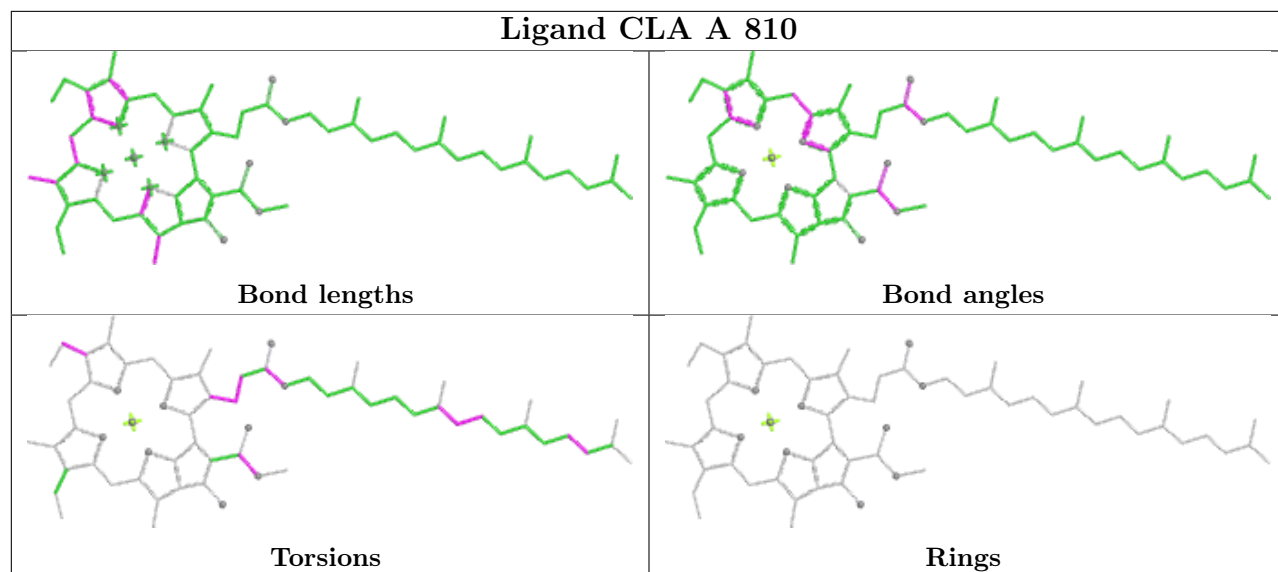
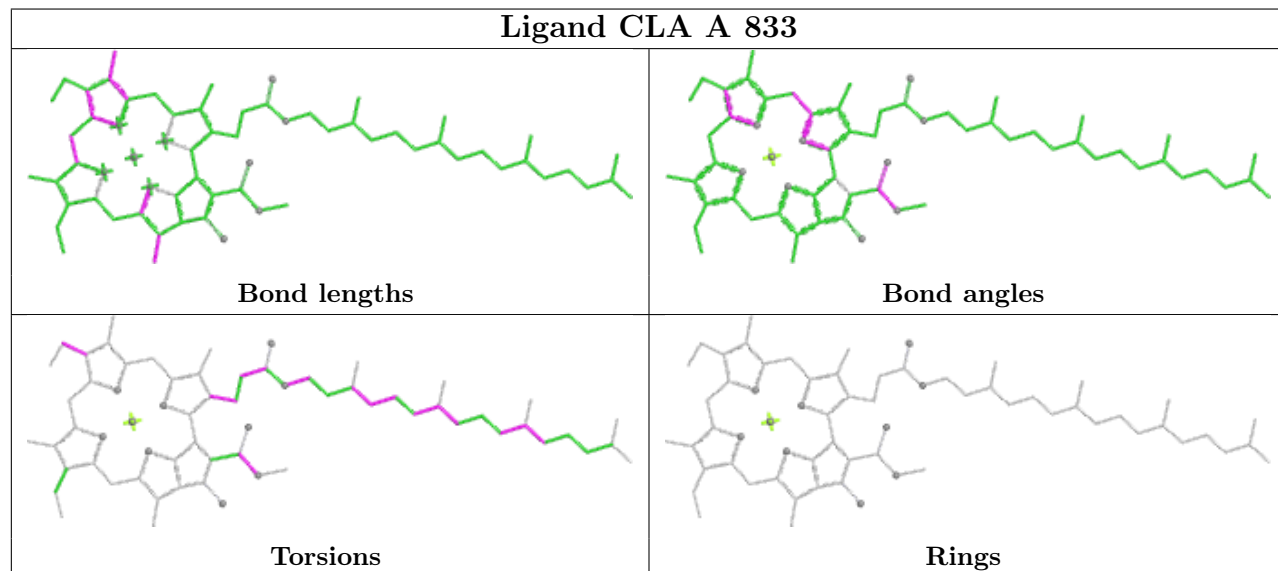
Bond angles



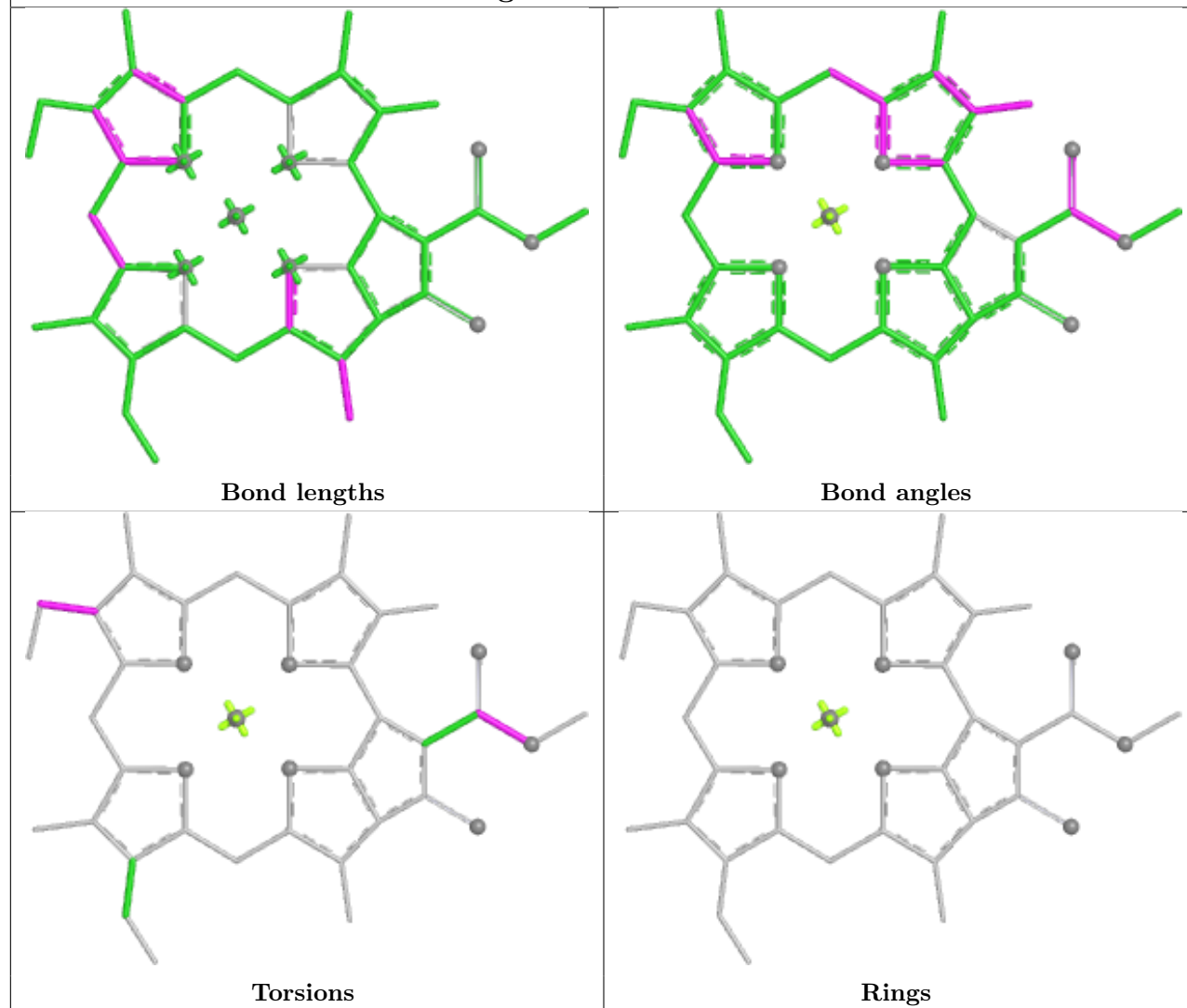
Torsions



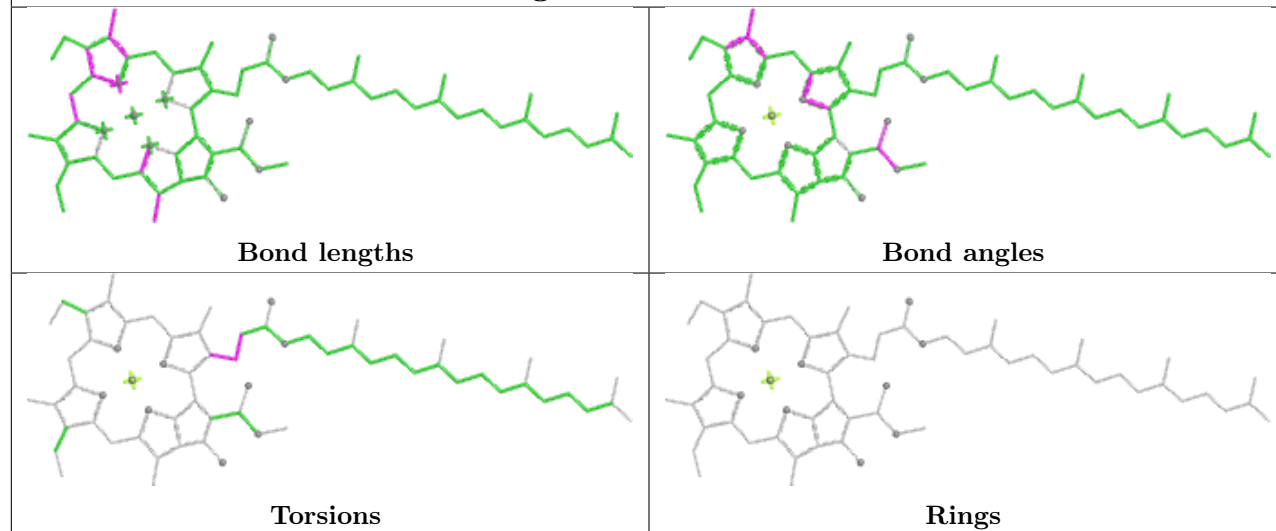
Rings

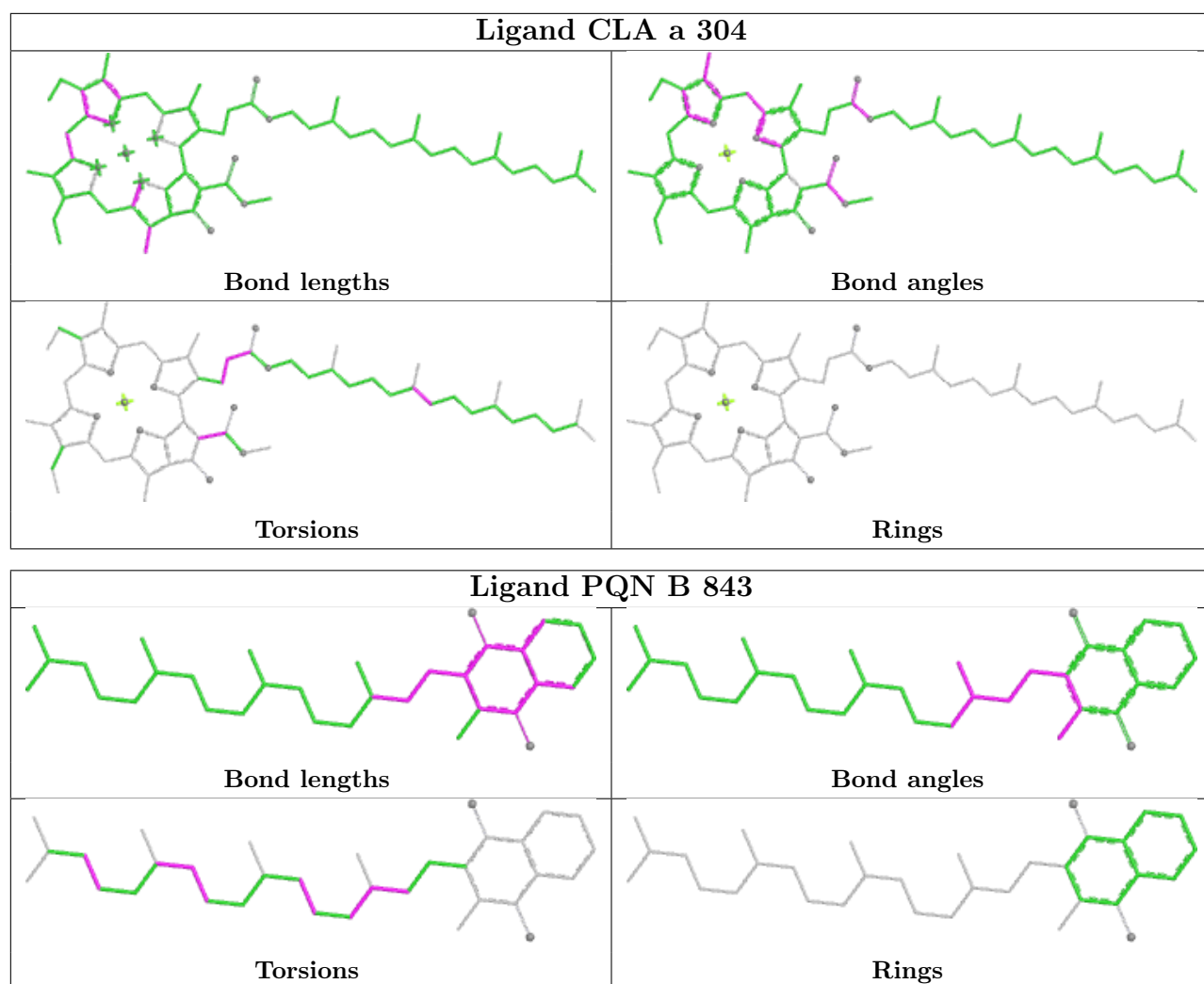
Ligand CLA A 810**Ligand CLA A 833**

Ligand CLA d 310

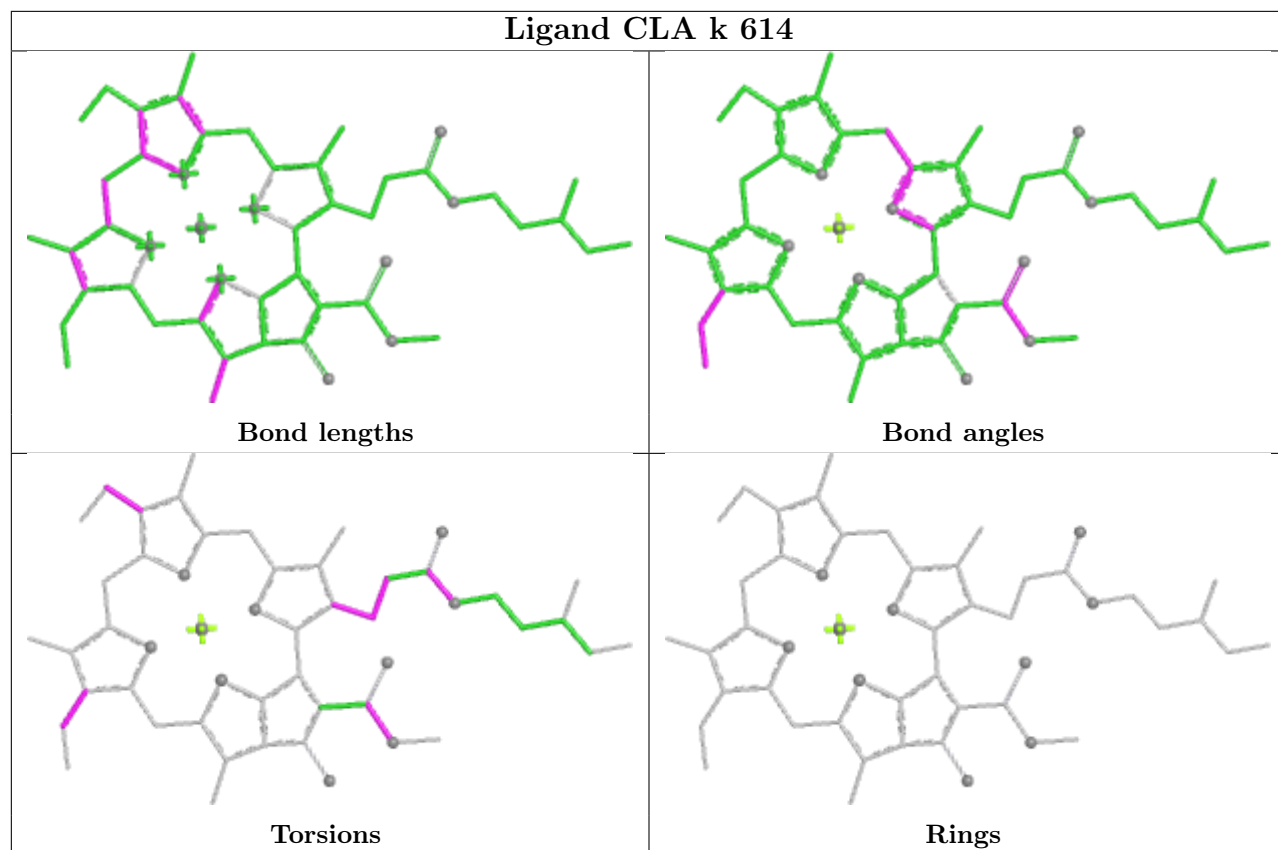


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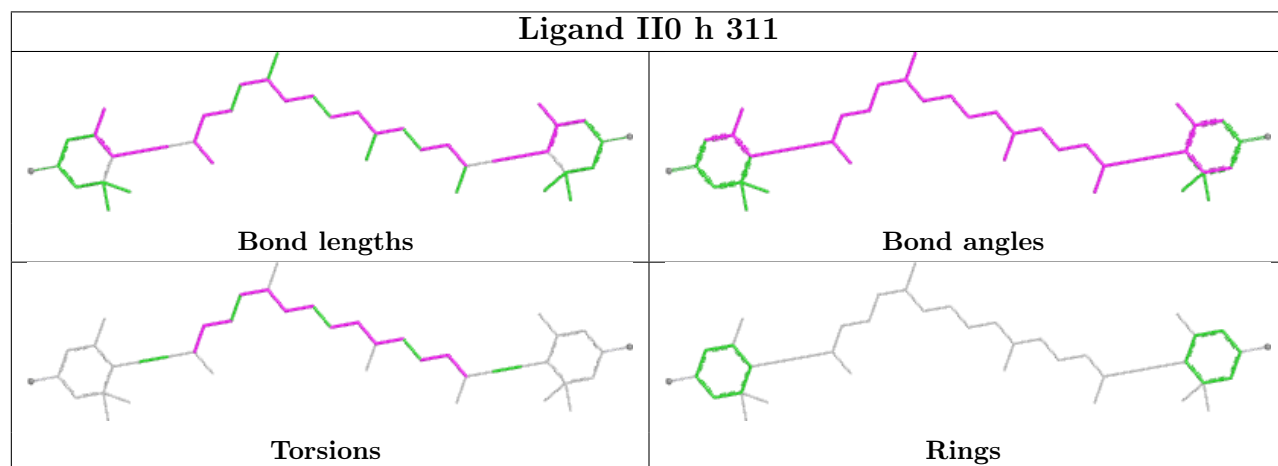




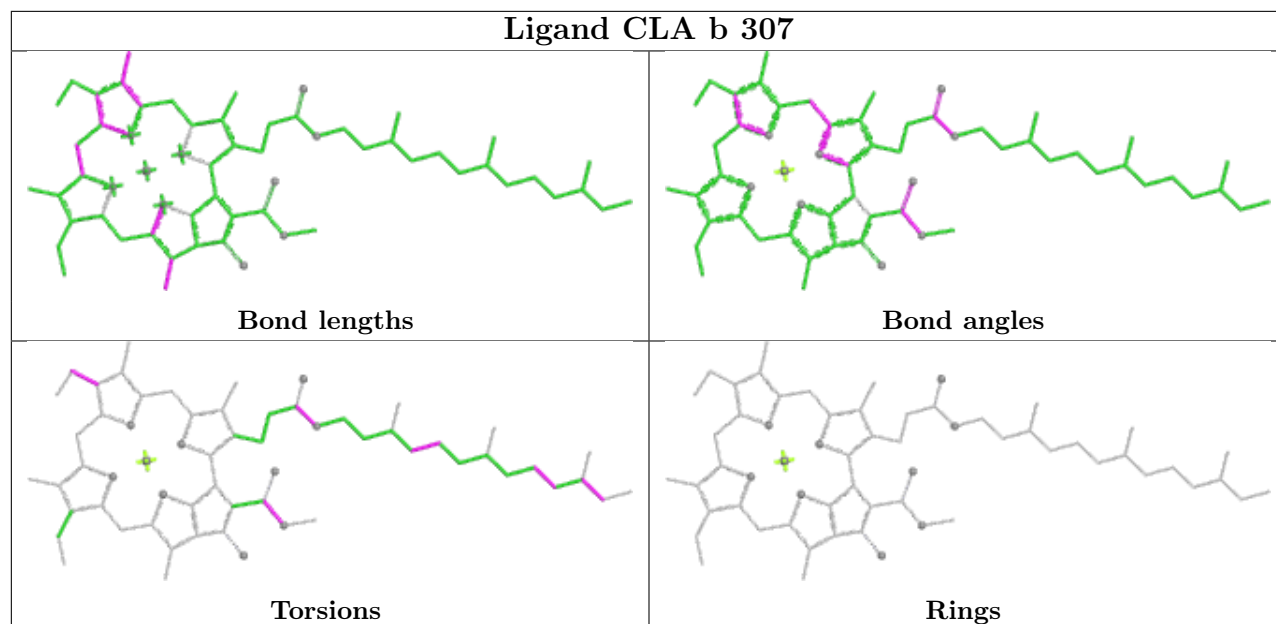
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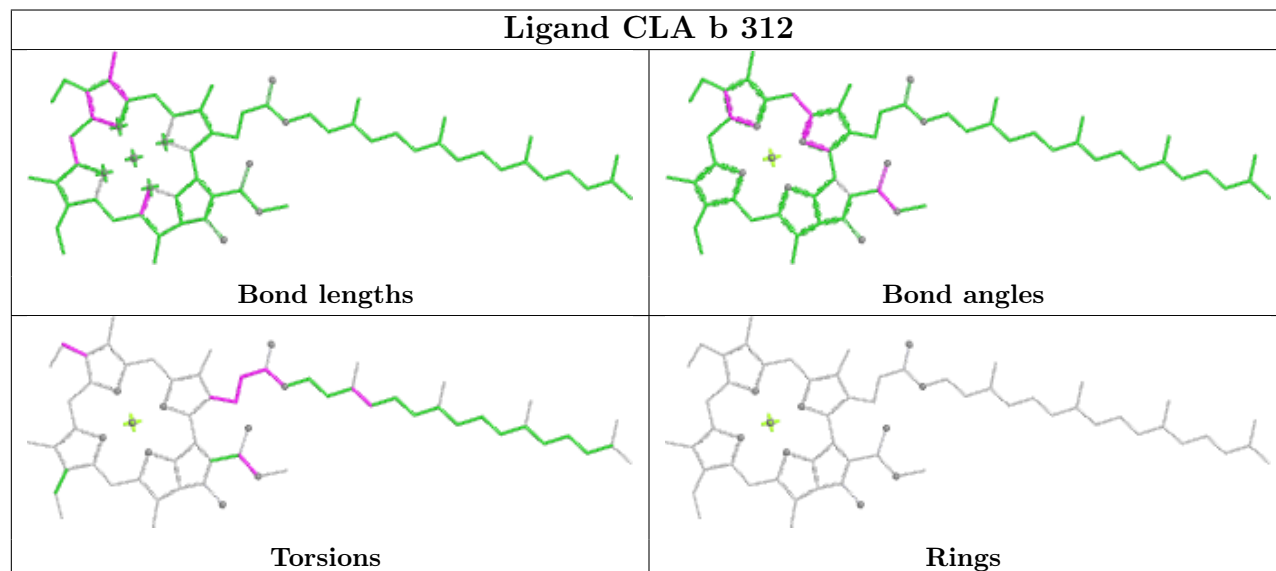
Ligand II0 h 311



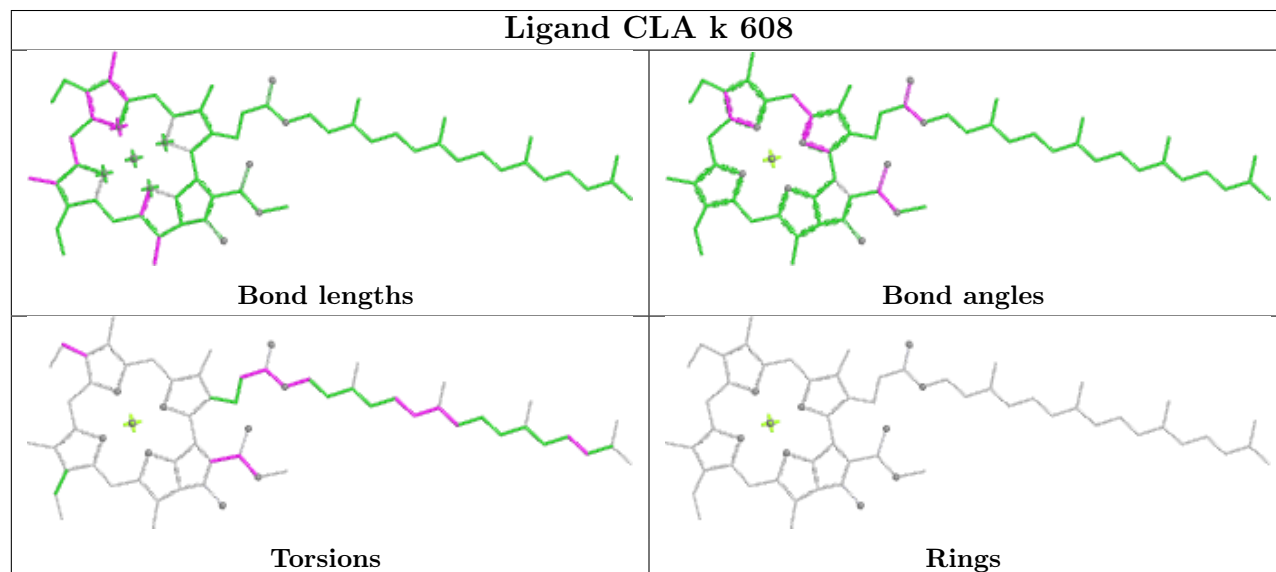
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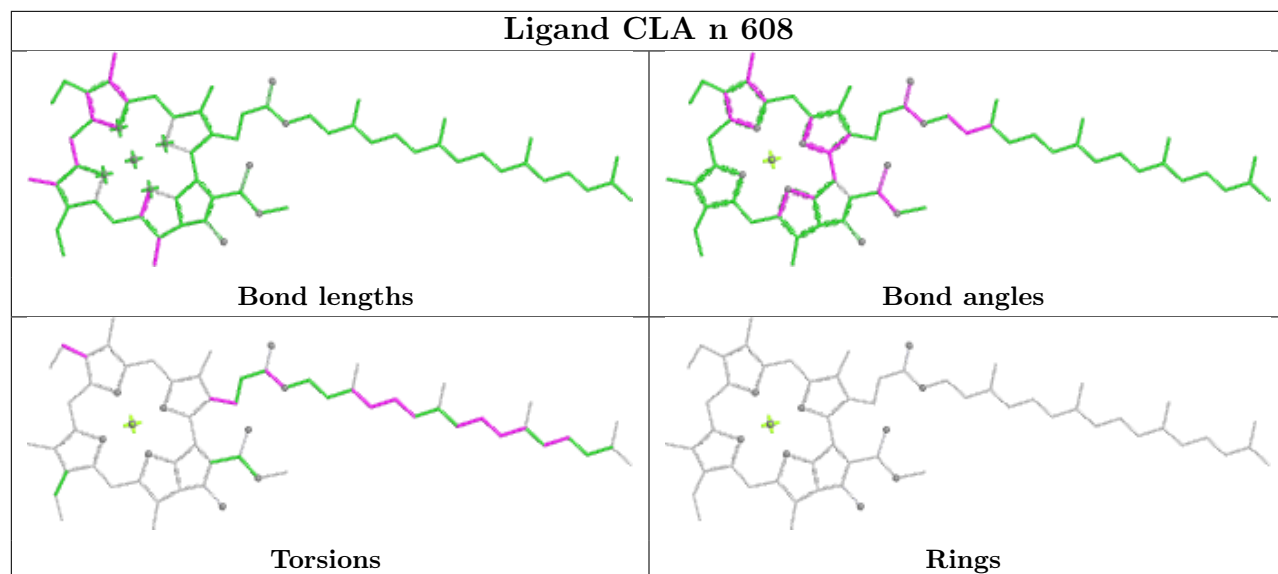
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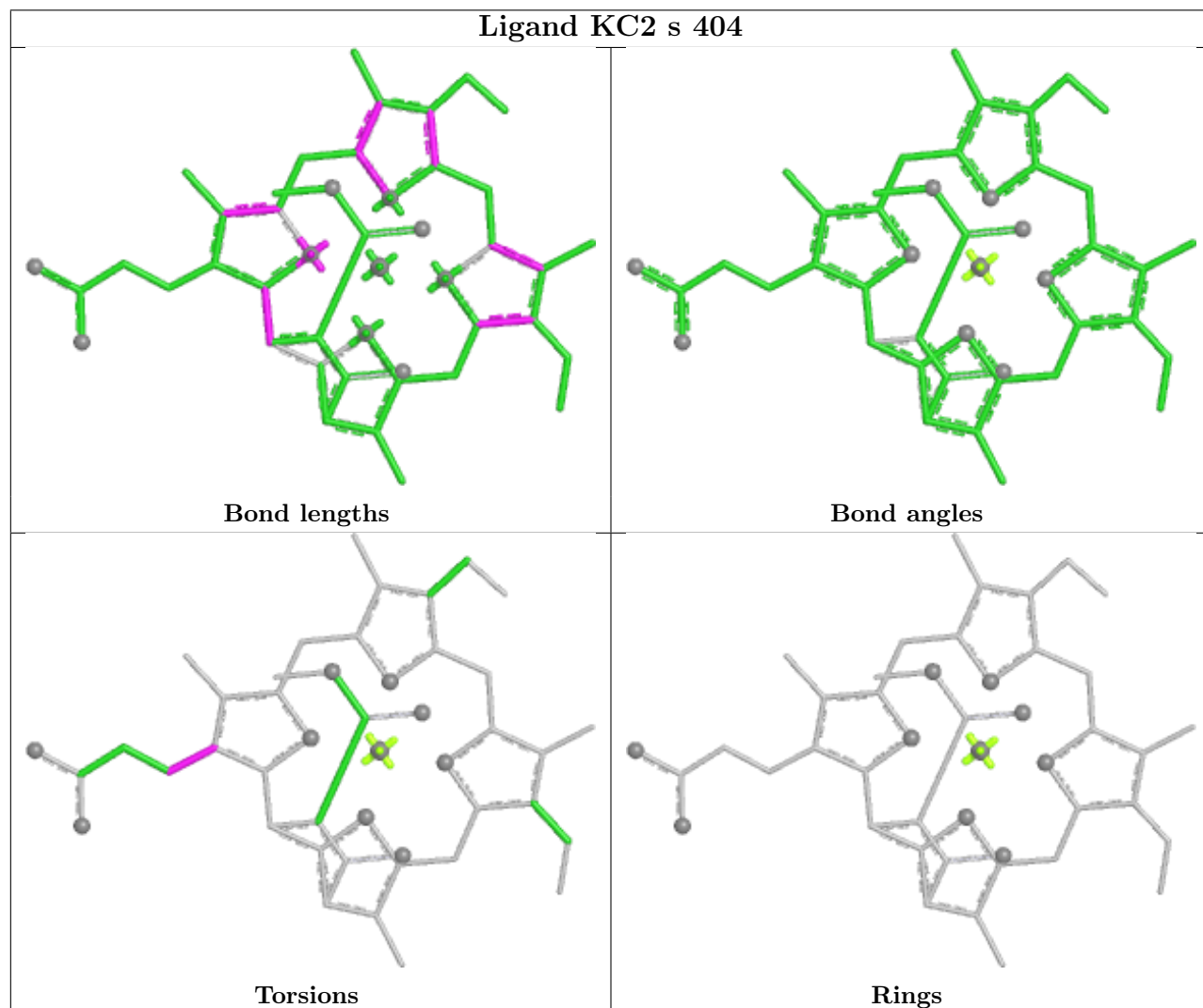
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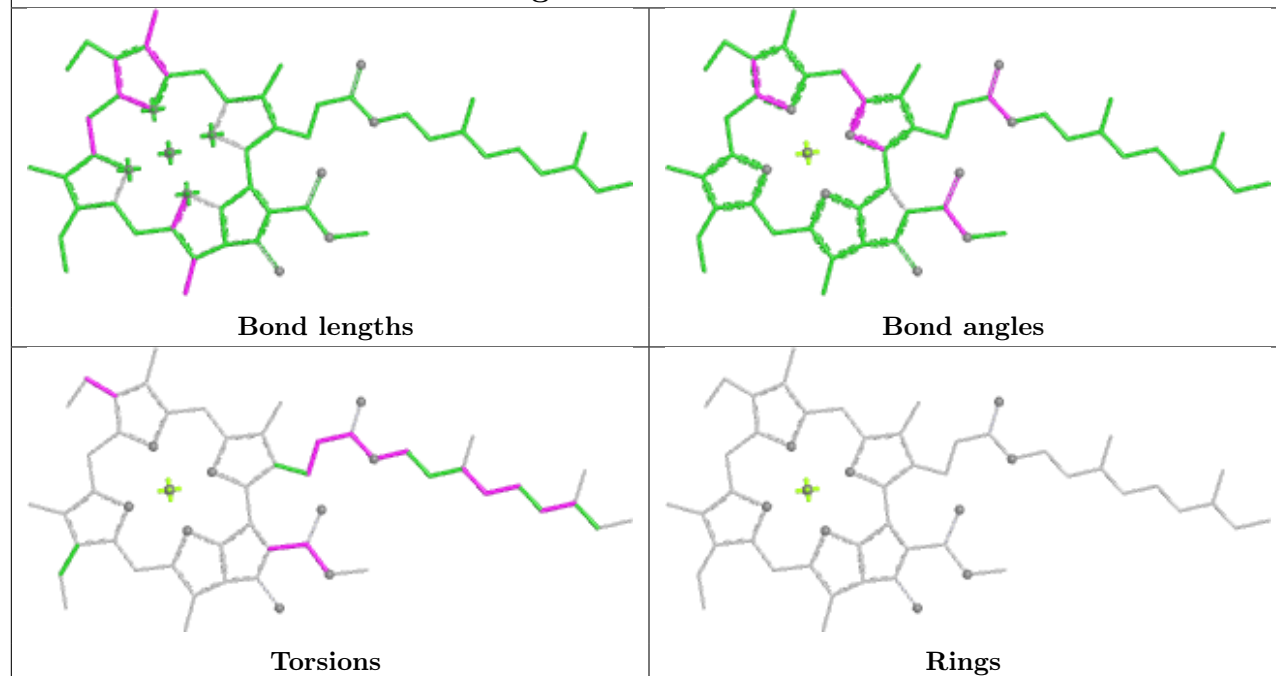
Ligand CLA n 608



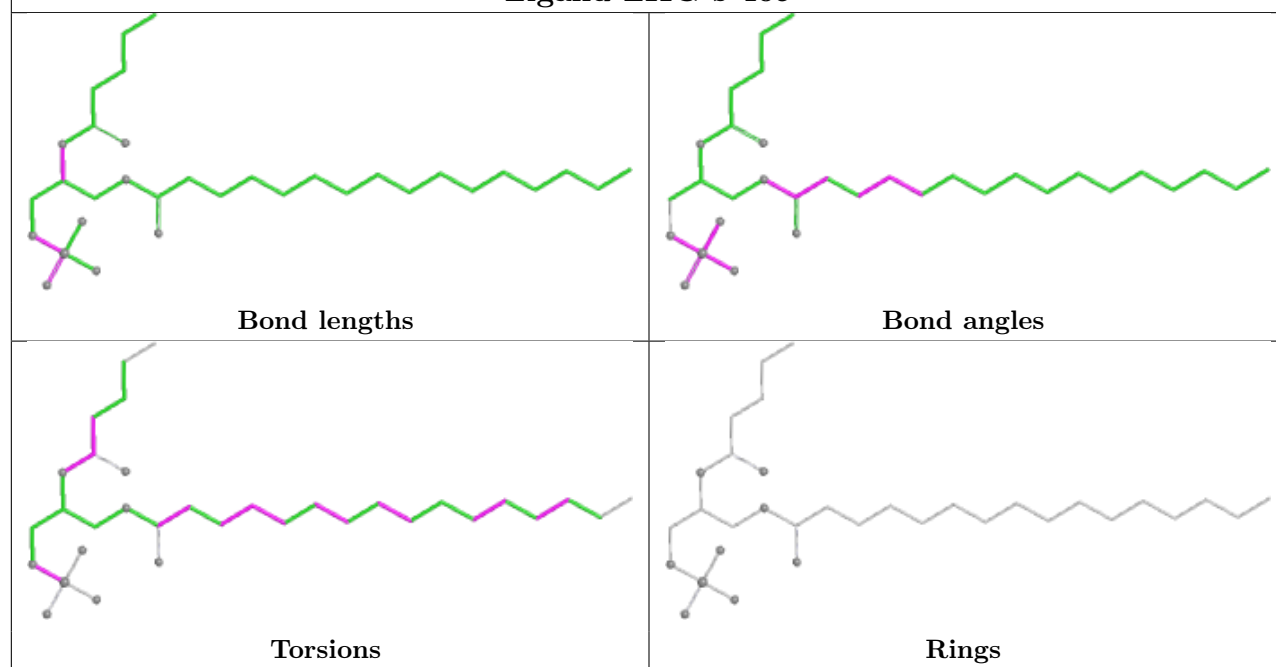
Ligand KC2 s 404



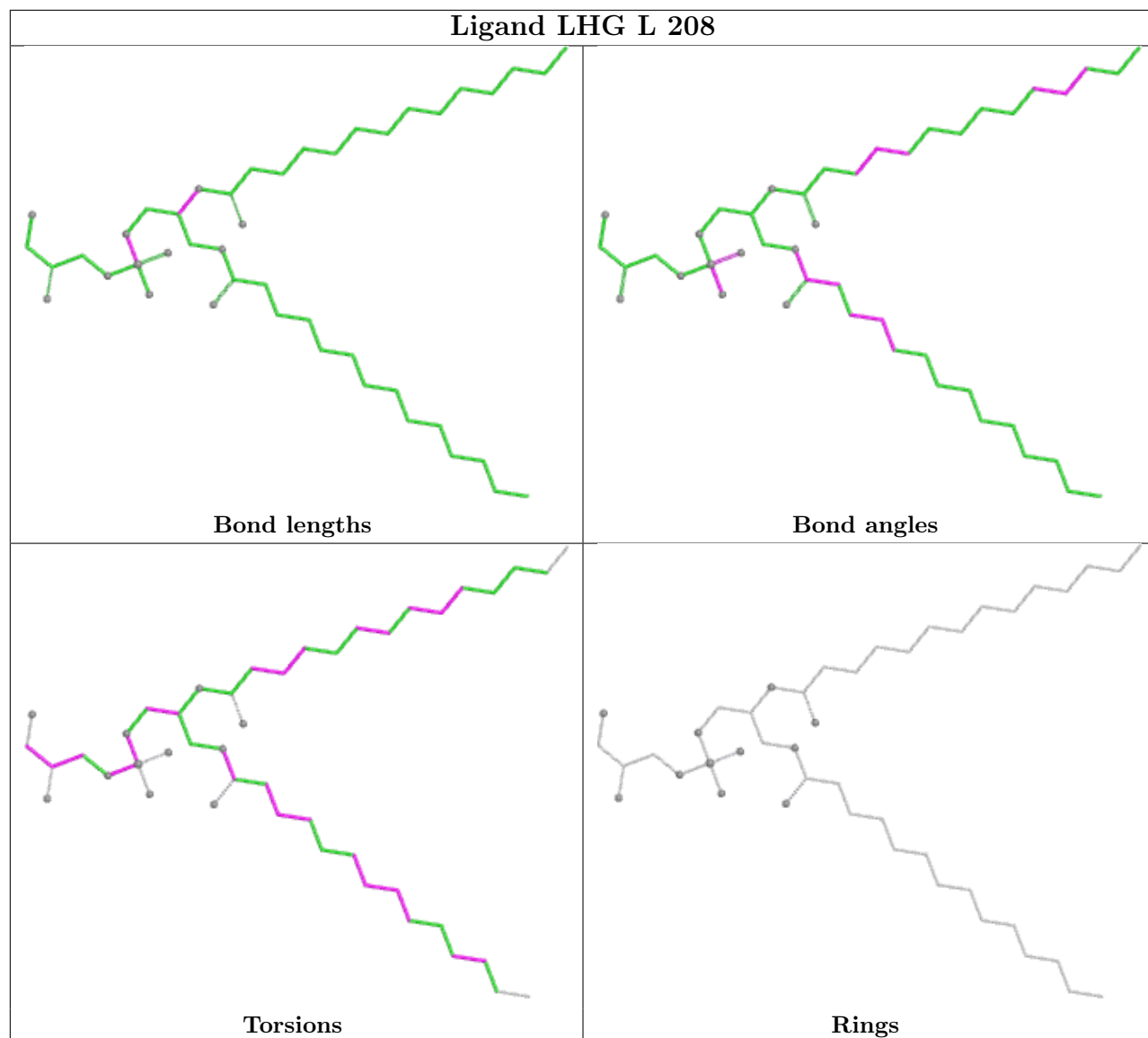
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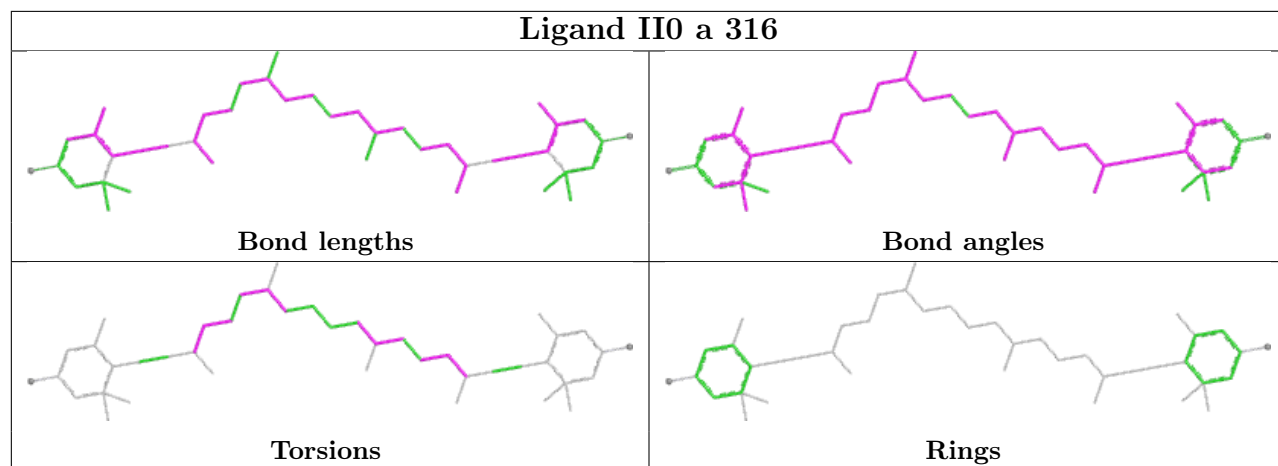
Ligand LHG s 409

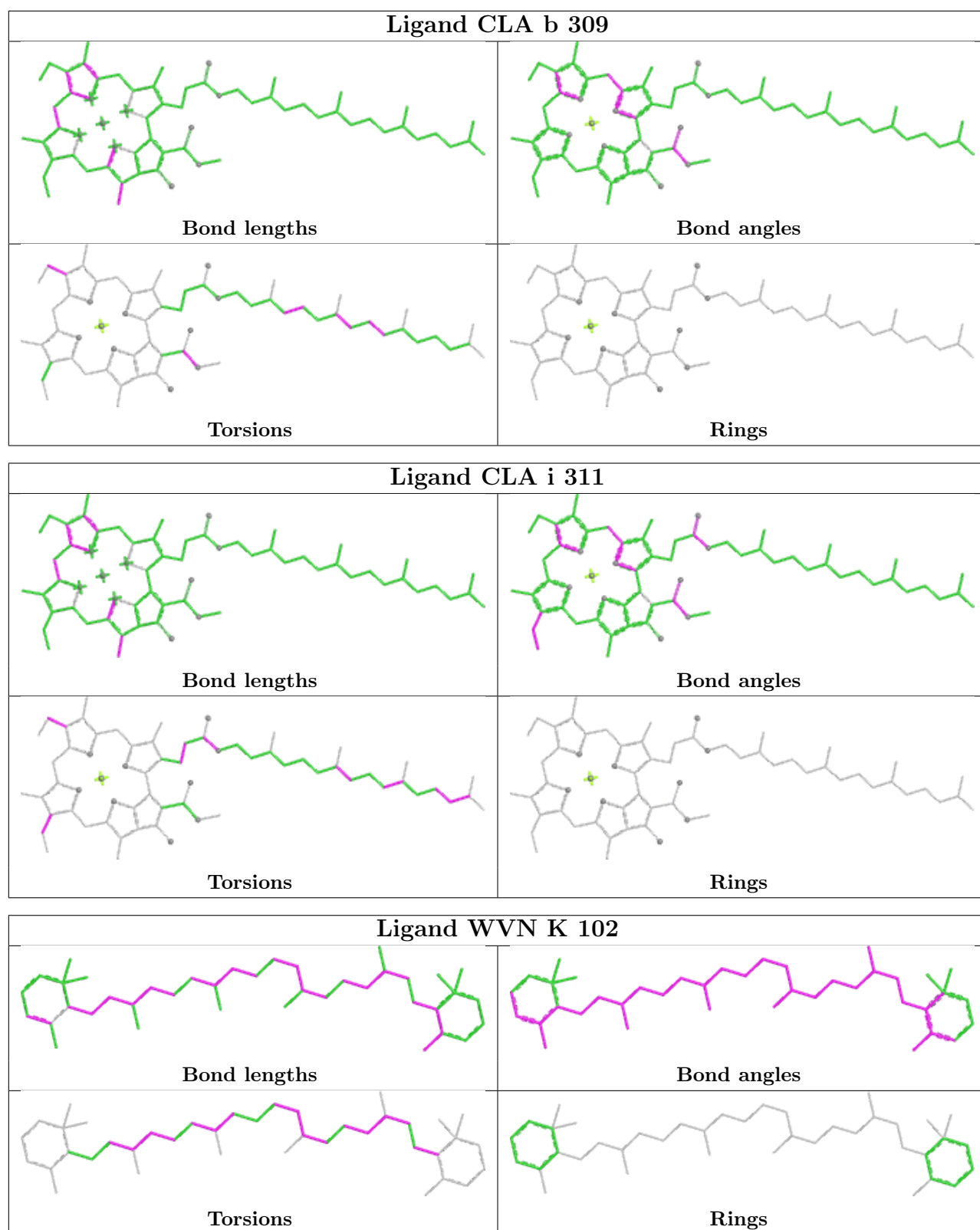


Ligand LHG L 208

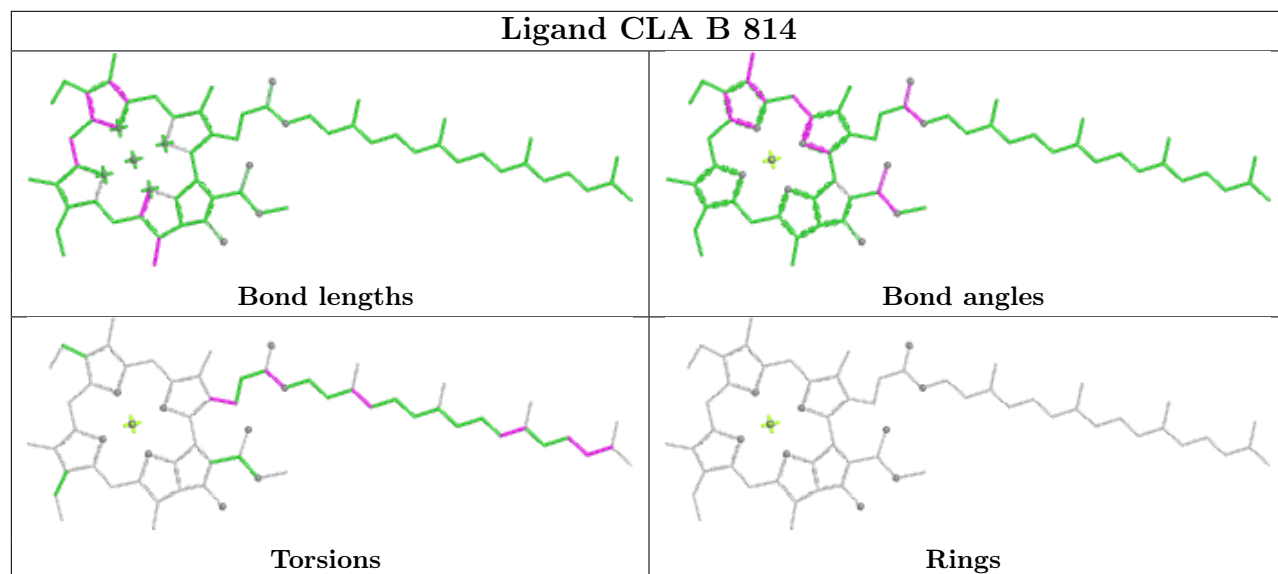


Ligand II0 a 316

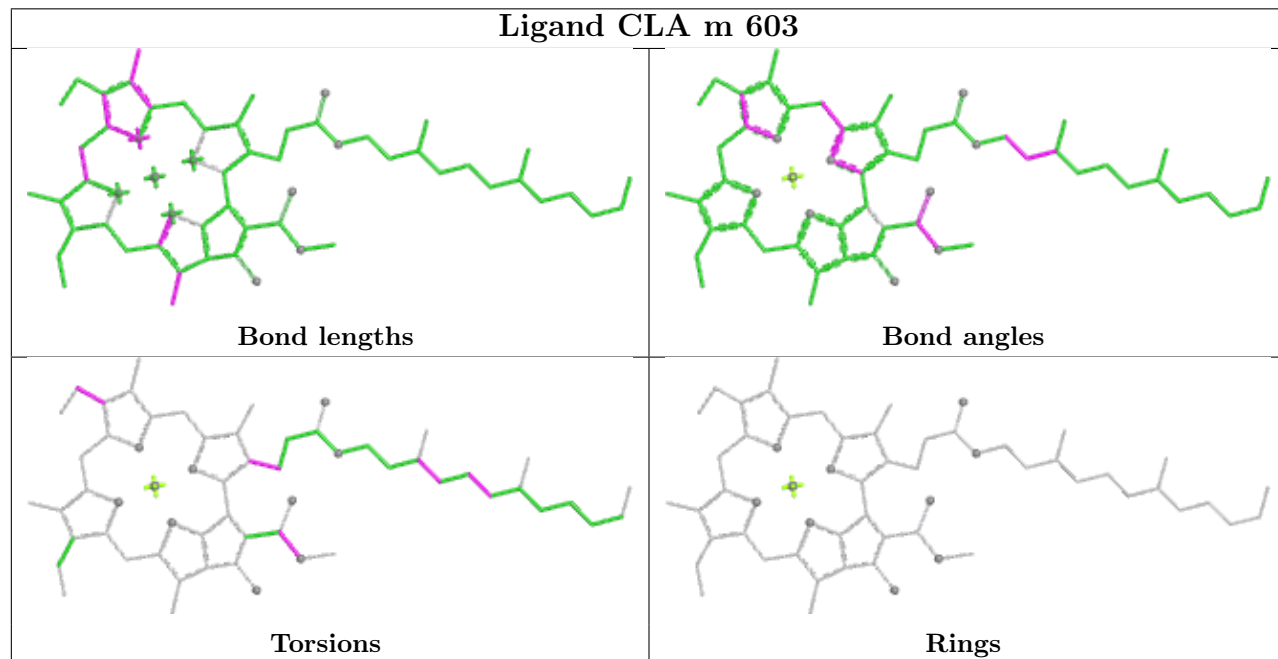




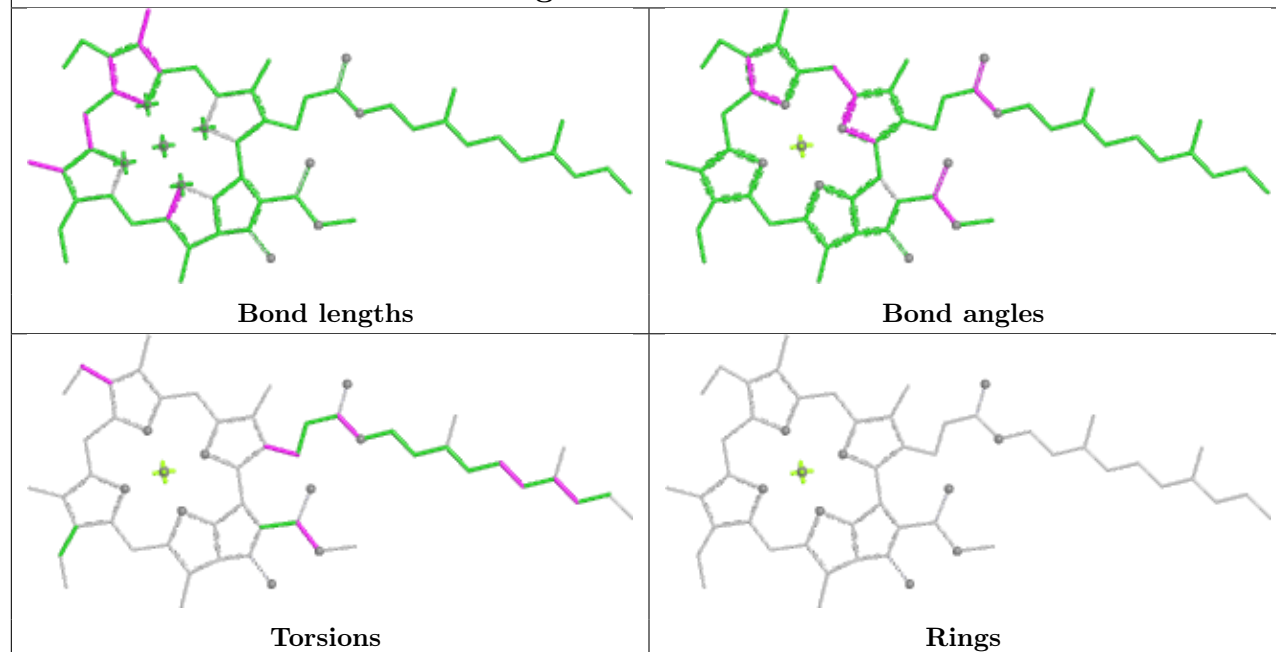
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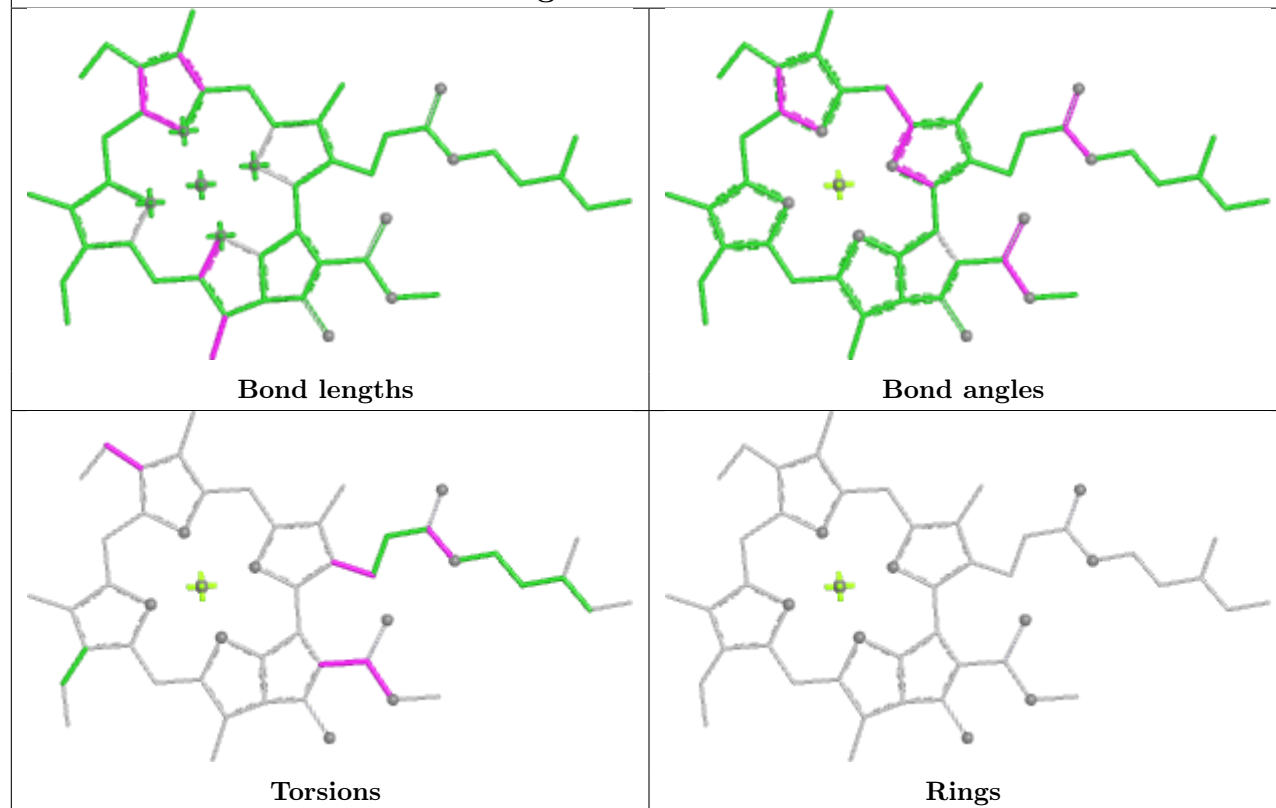
Ligand CLA m 603

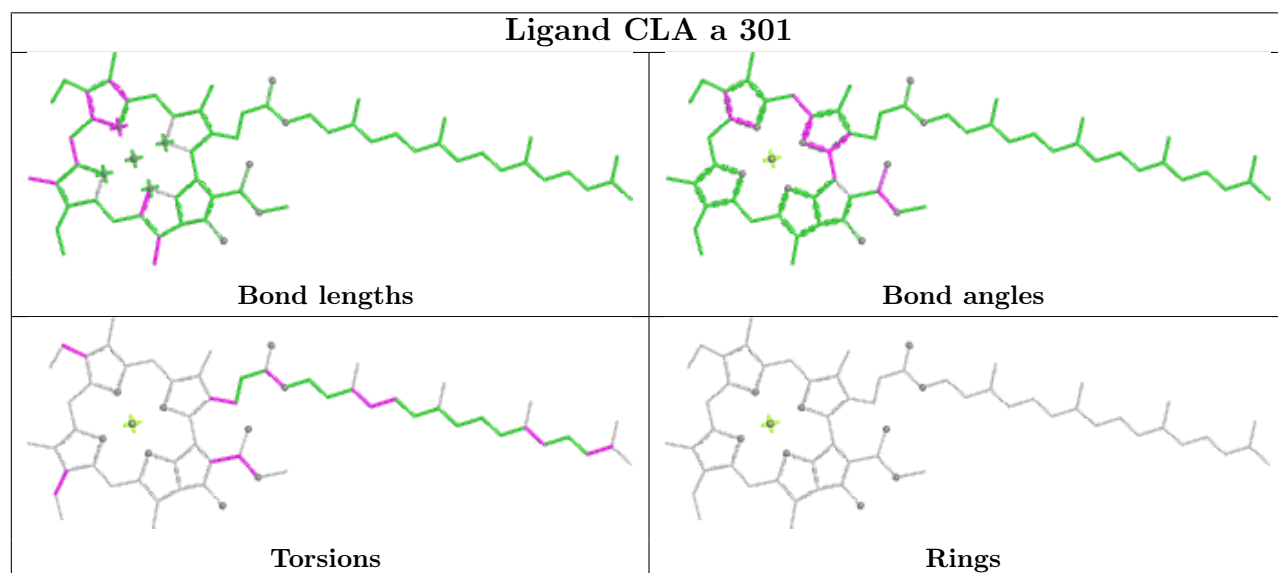
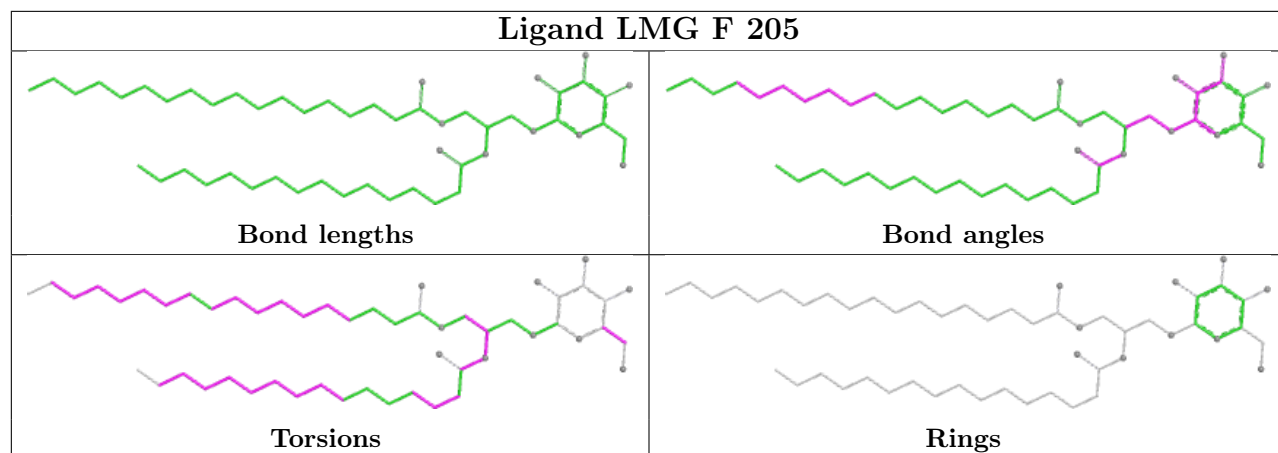


Ligand CLA k 609

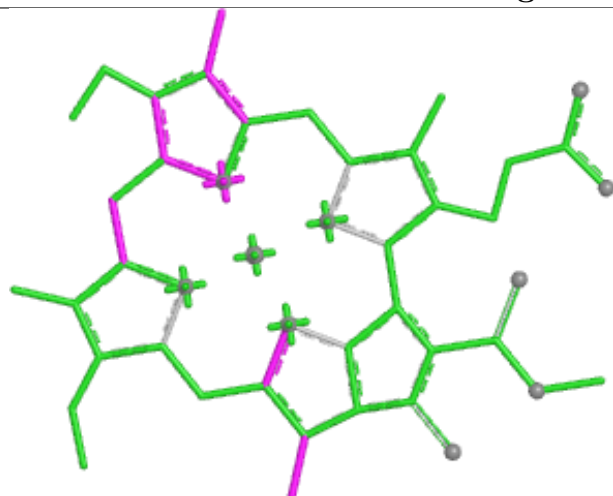


Ligand CLA c 301

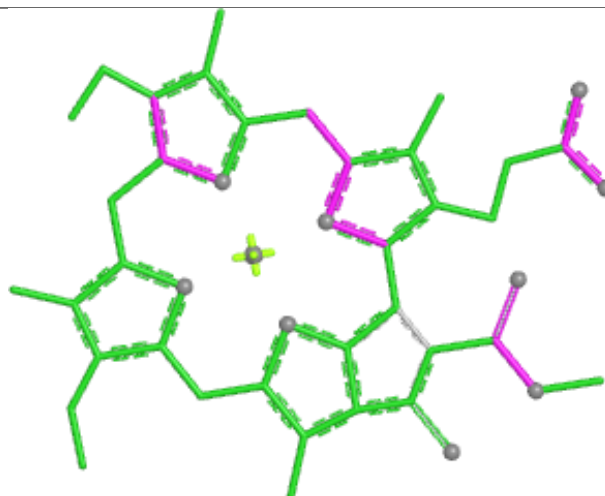




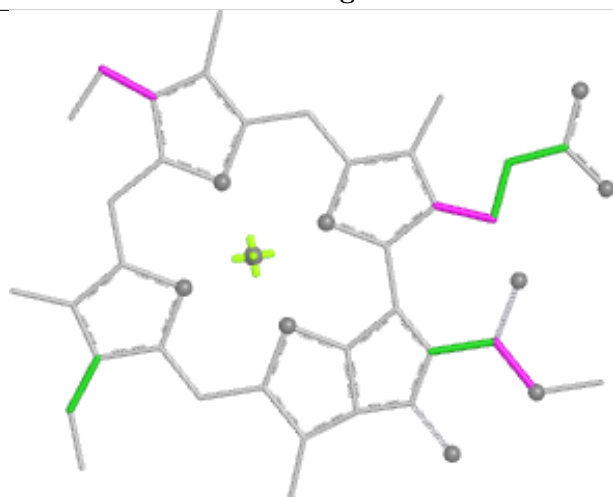
Ligand CLA n 601



Bond lengths



Bond angles

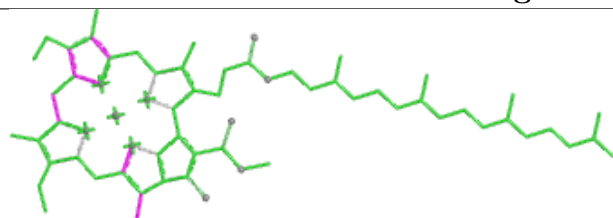


Torsions

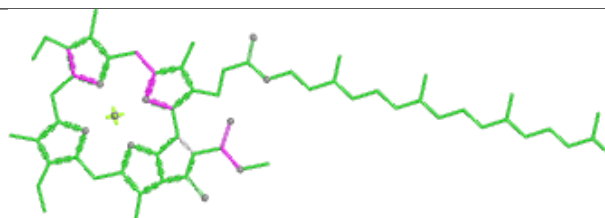


Rings

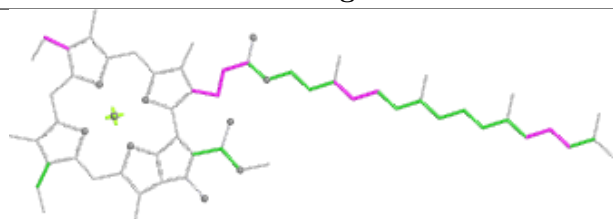
Ligand CLA A 812



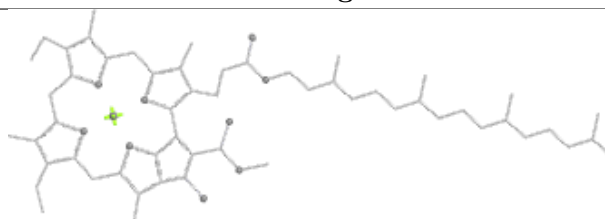
Bond lengths



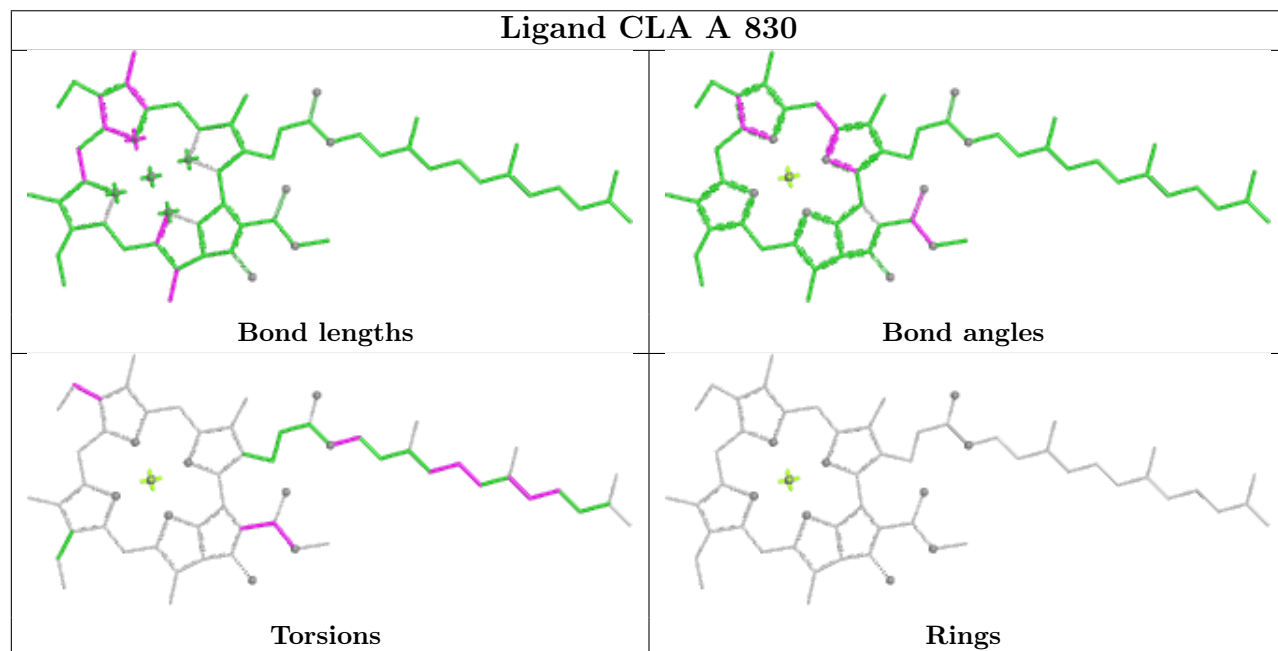
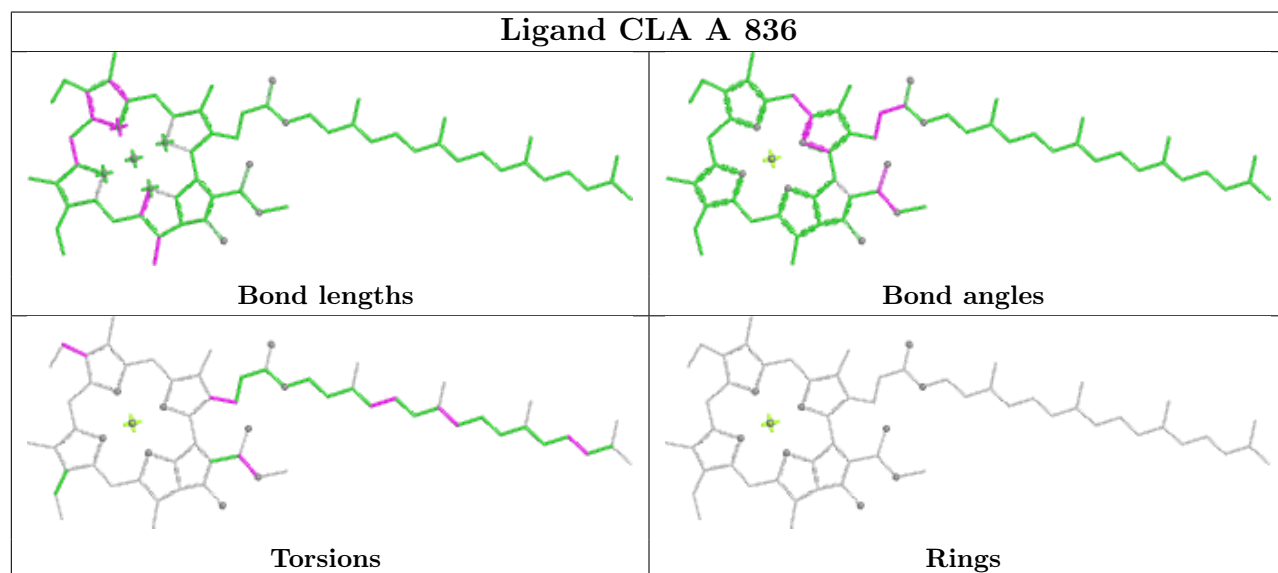
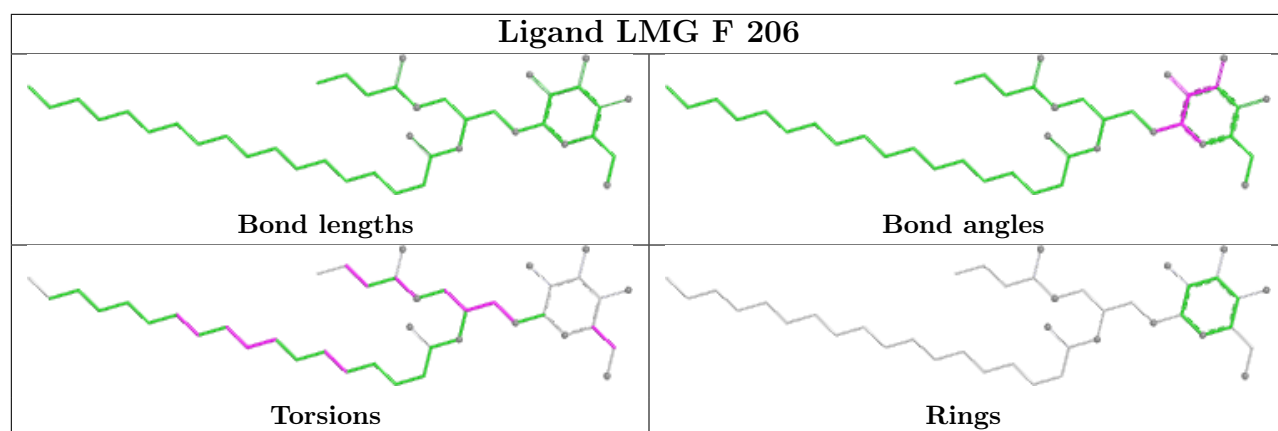
Bond angles

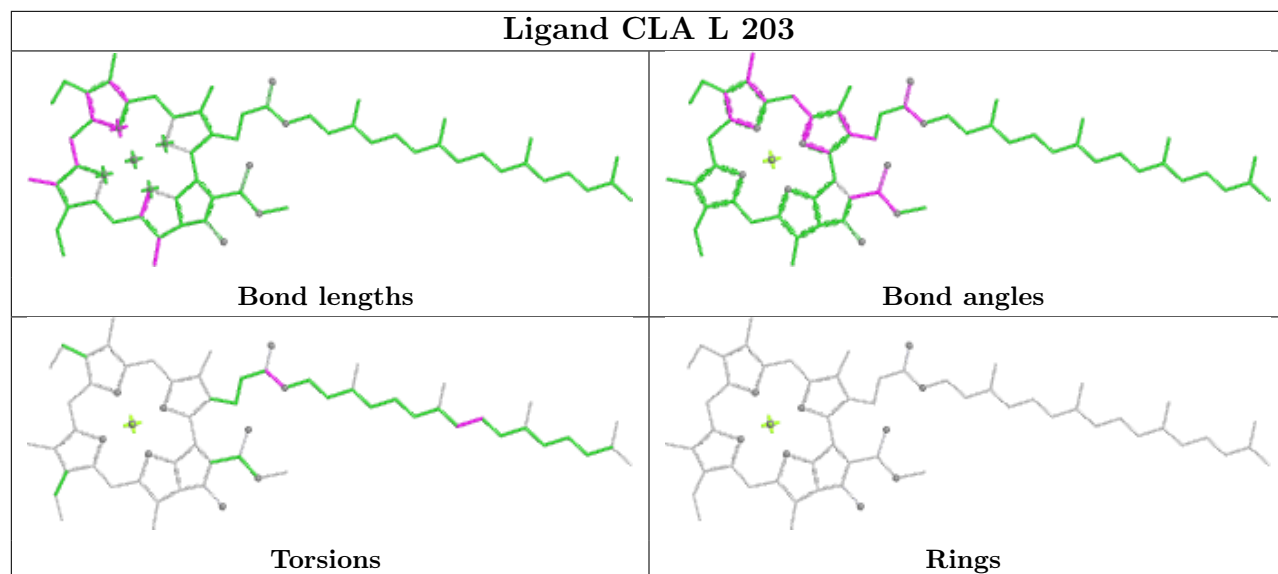
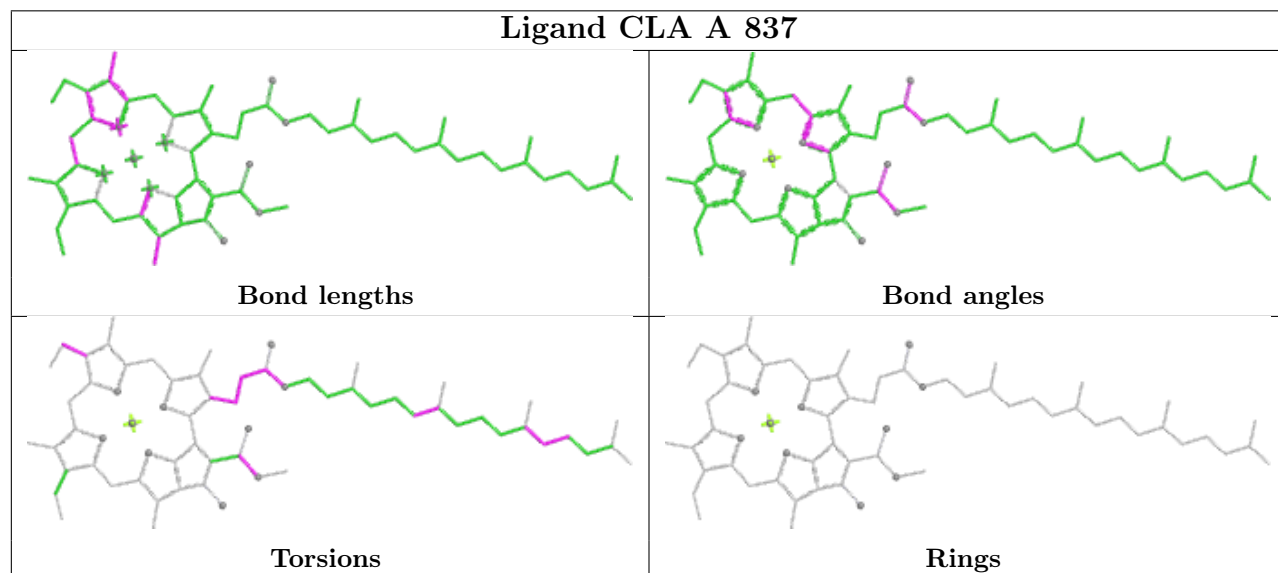


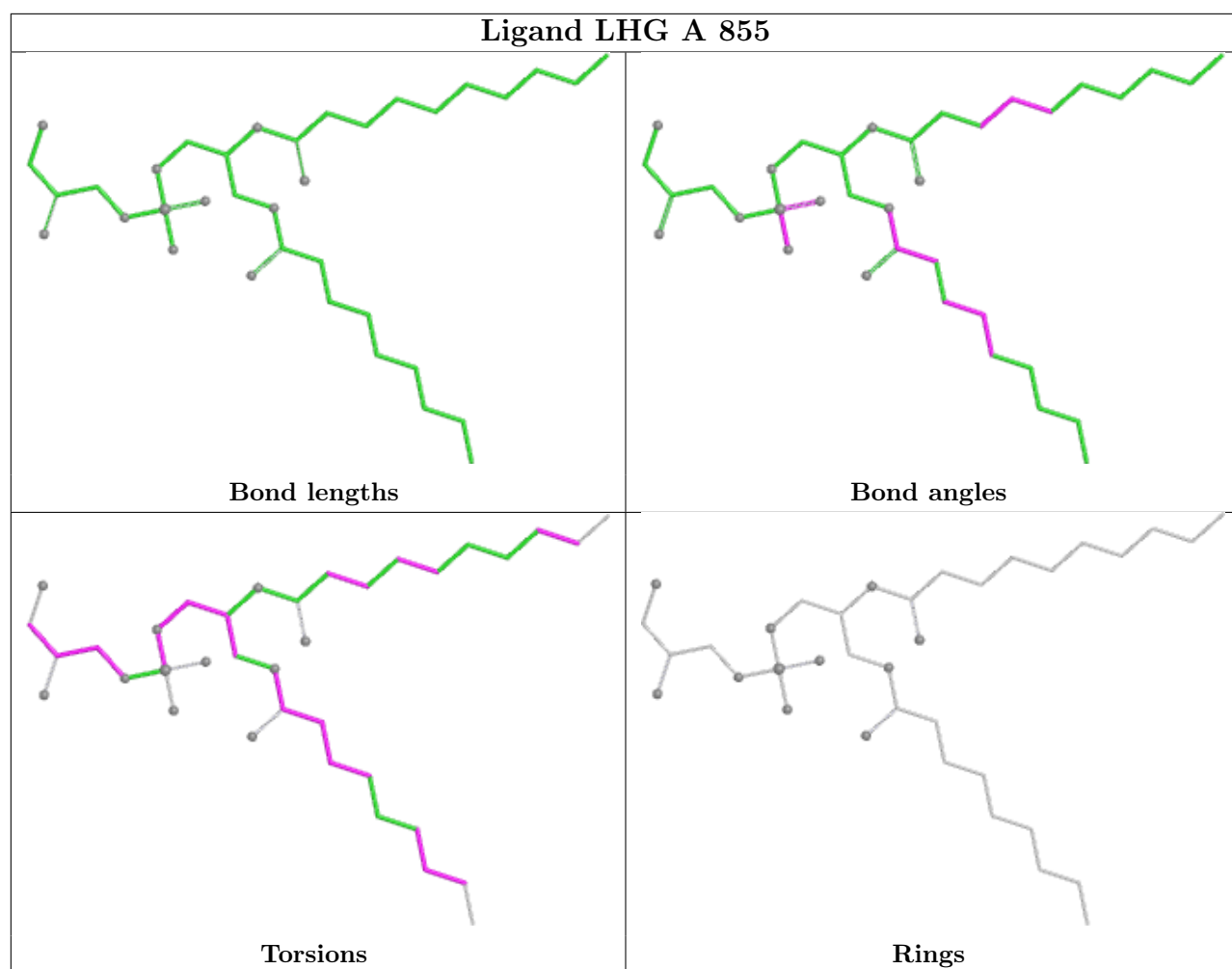
Torsions



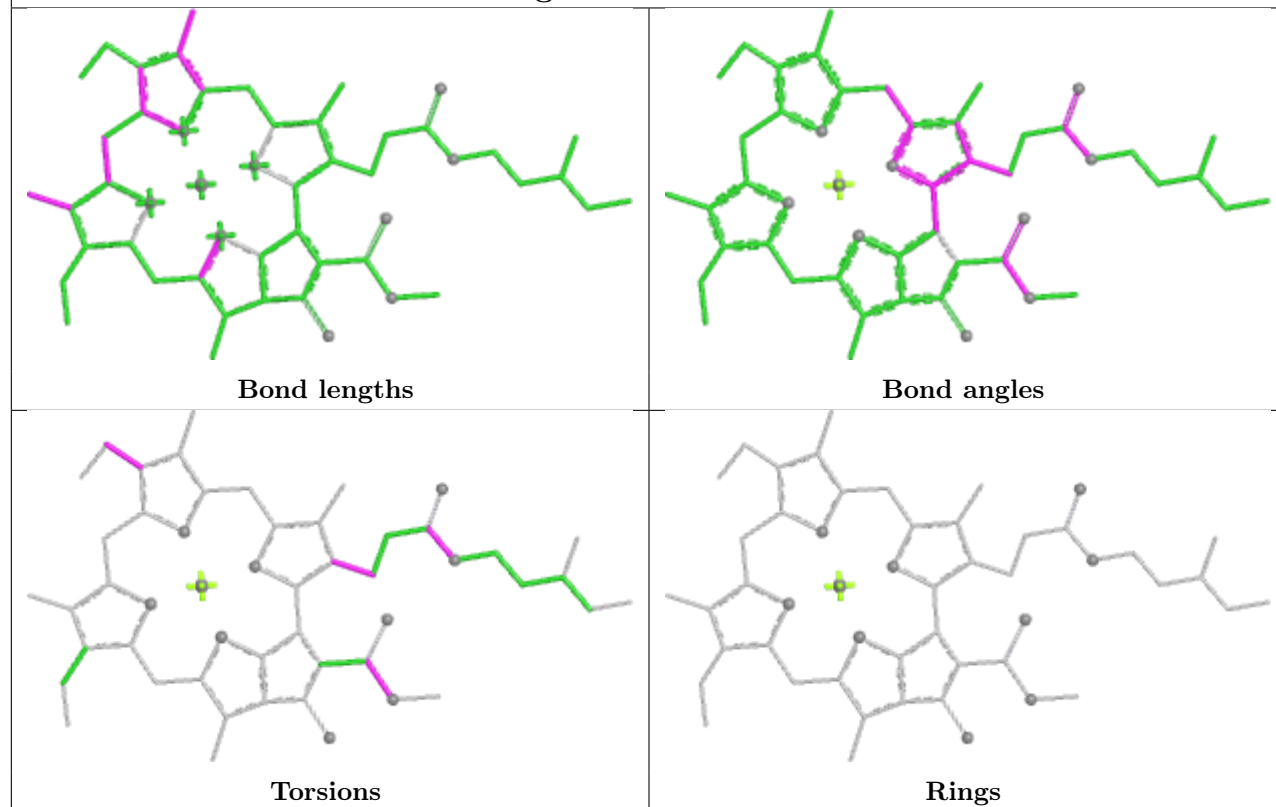
Rings



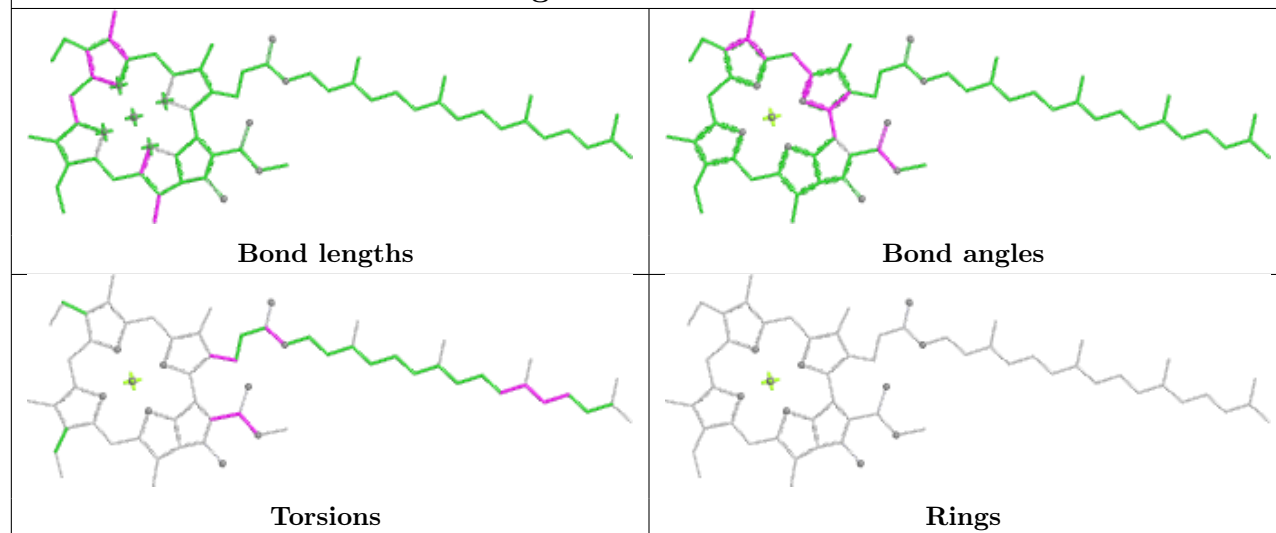
Ligand CLA L 203**Ligand CLA A 837**

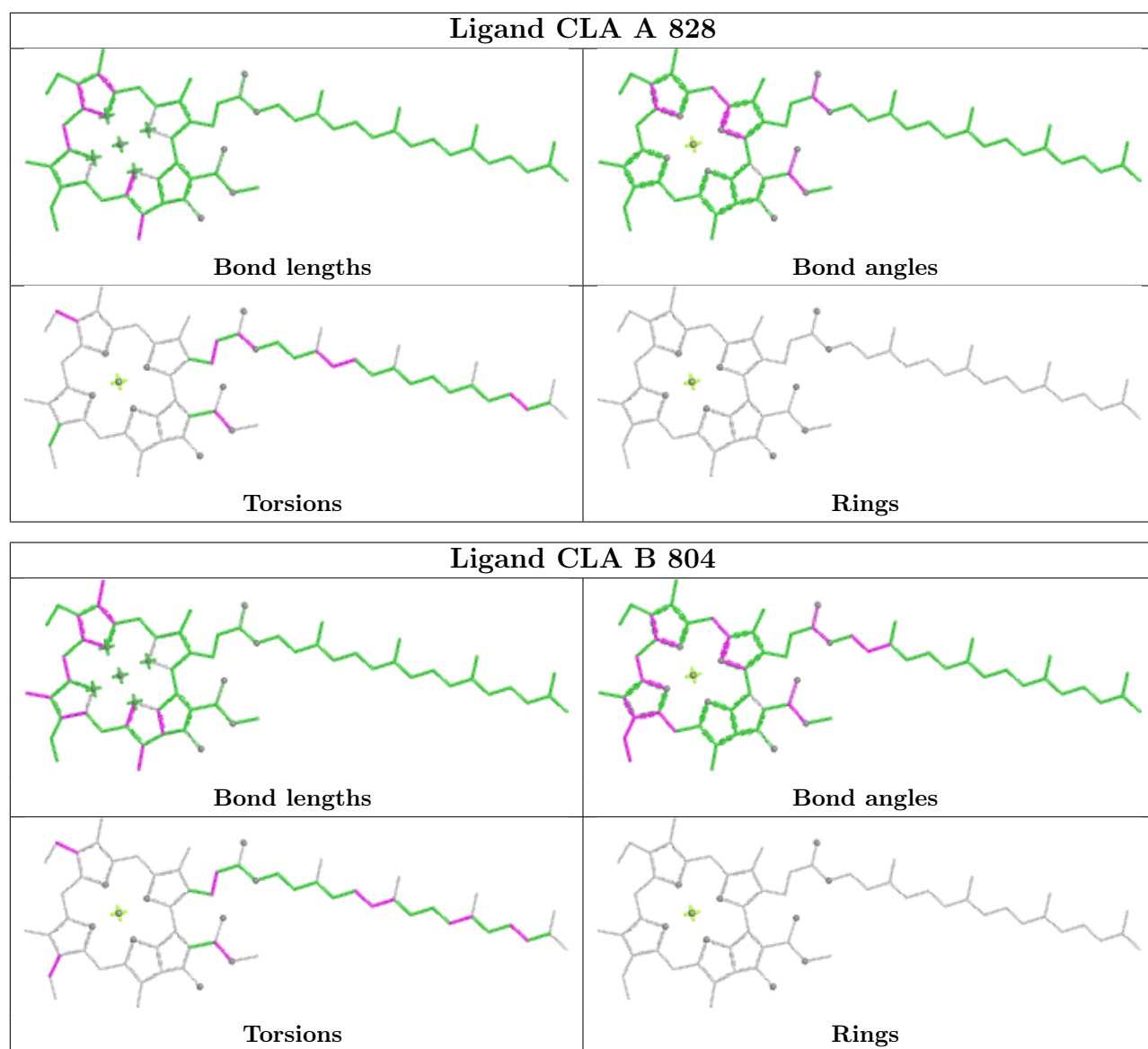


Ligand CLA n 603

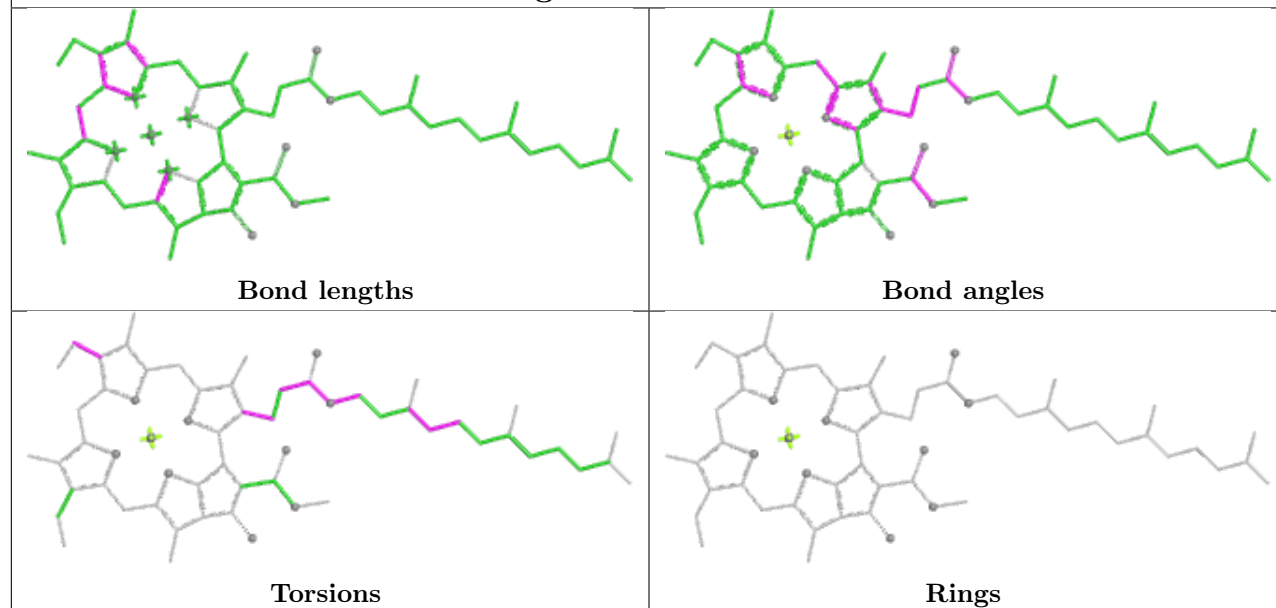


Ligand CLA A 824

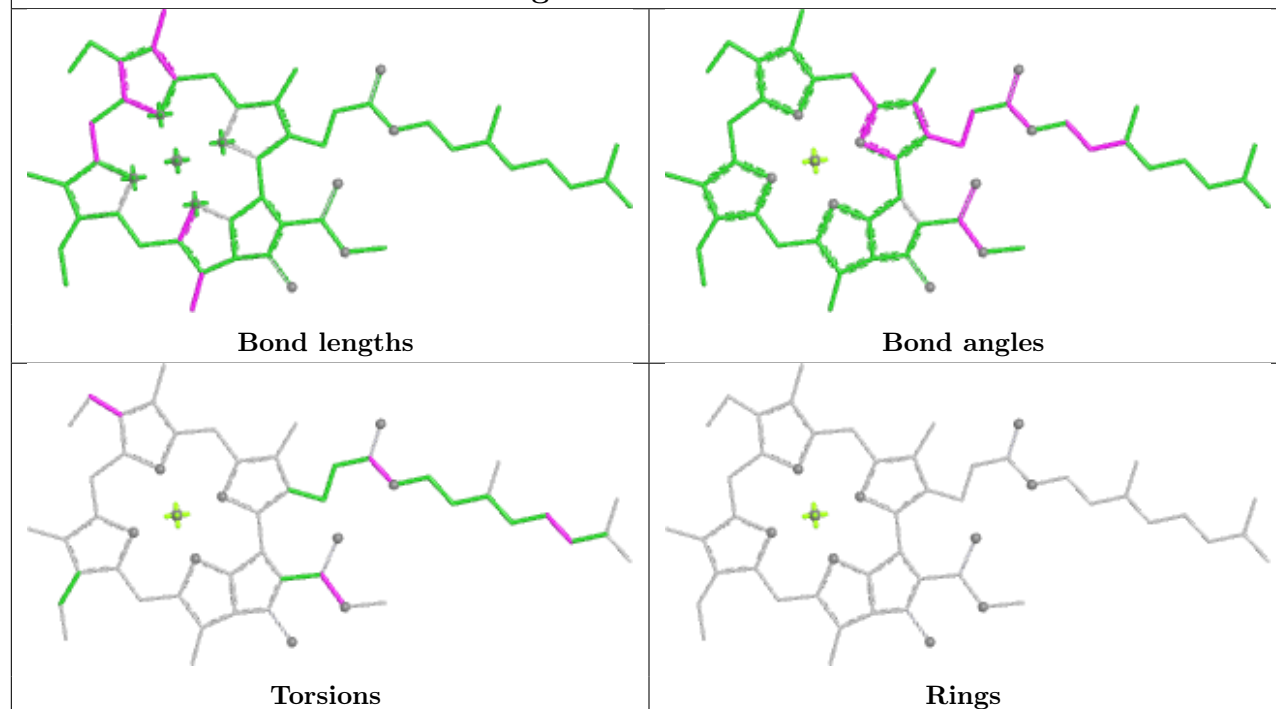




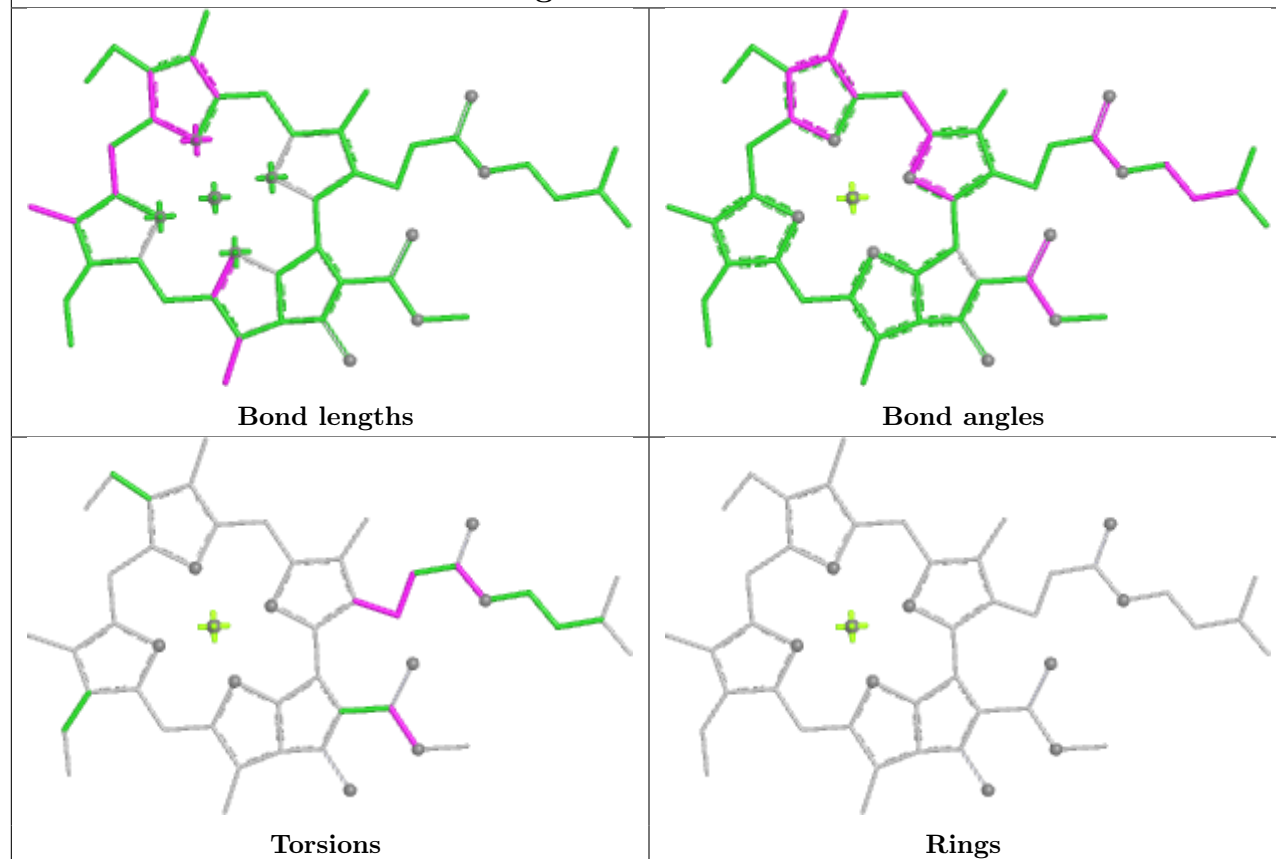
Ligand CLA n 604



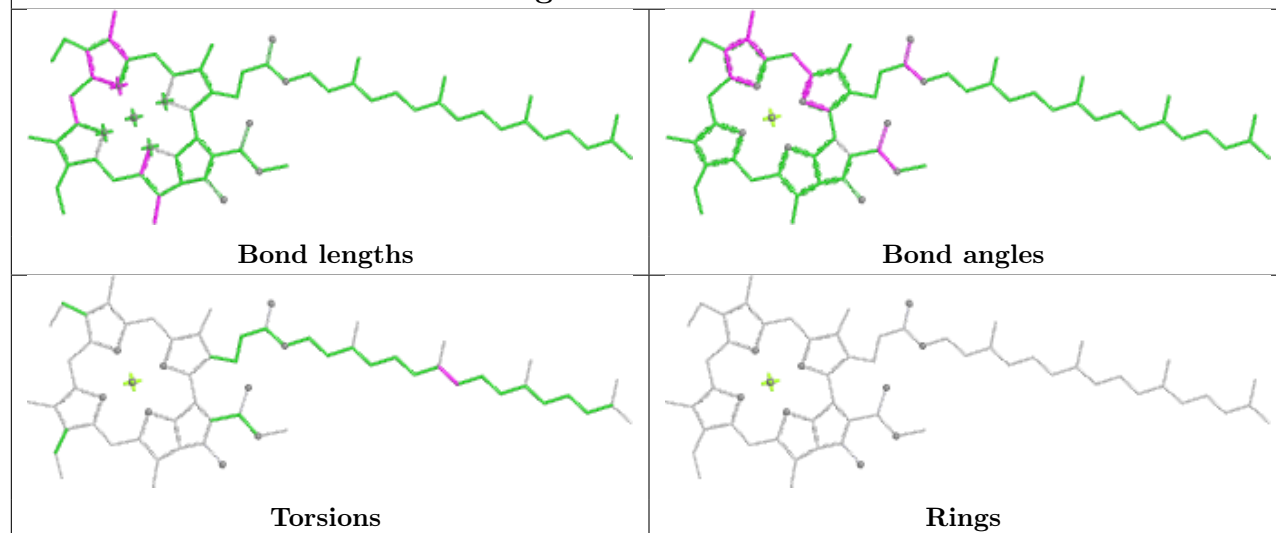
Ligand CLA R 201



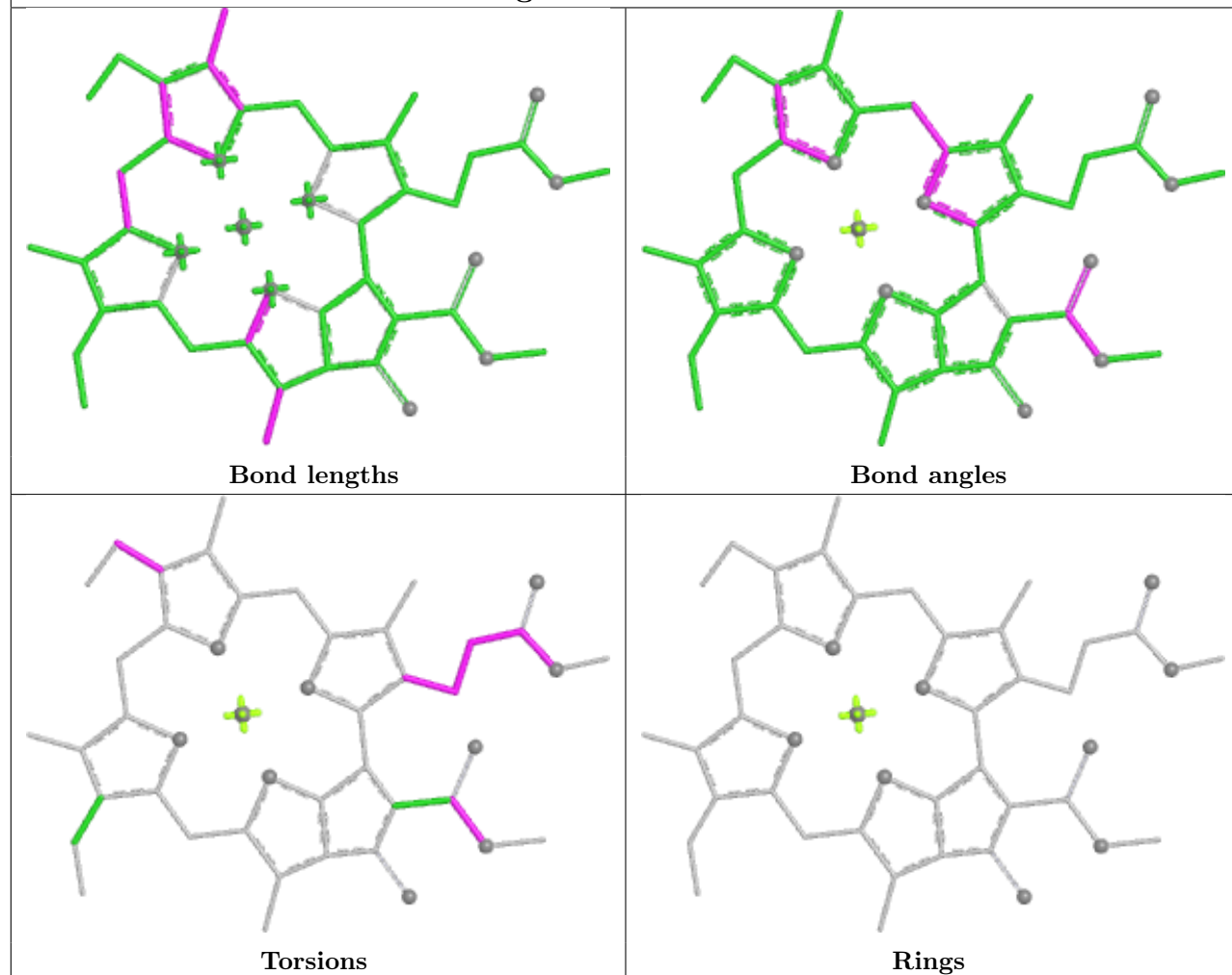
Ligand CLA h 302



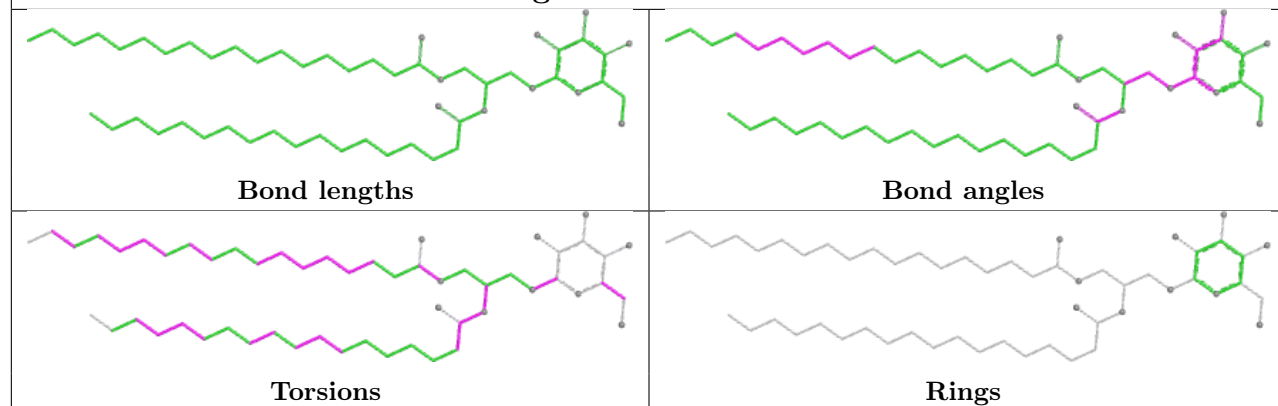
Ligand CLA h 313

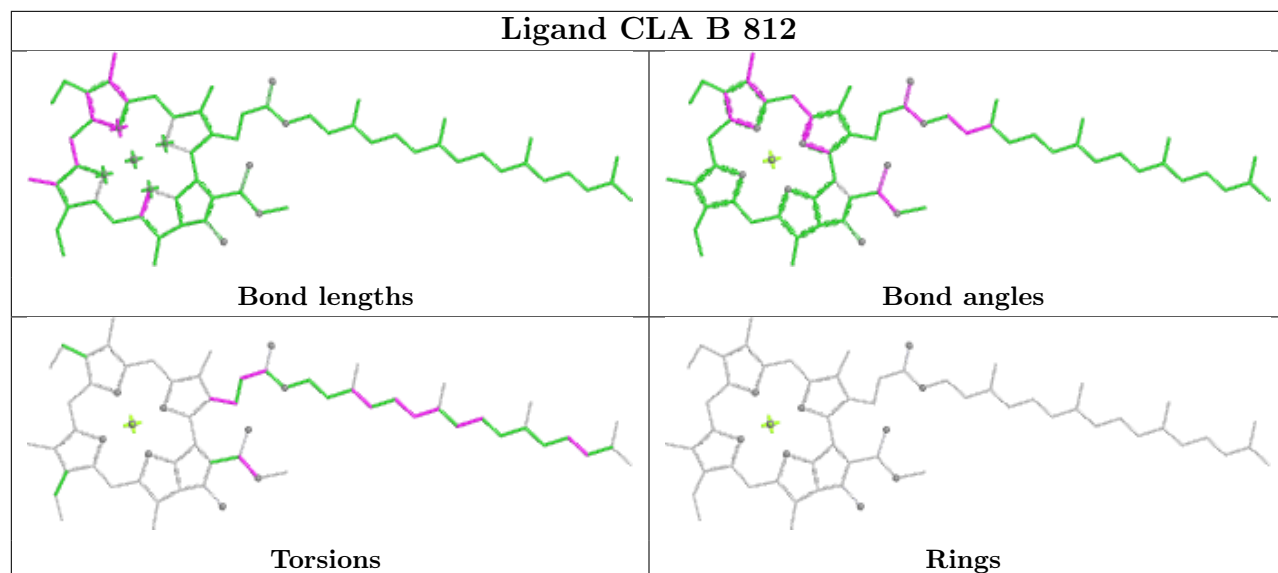
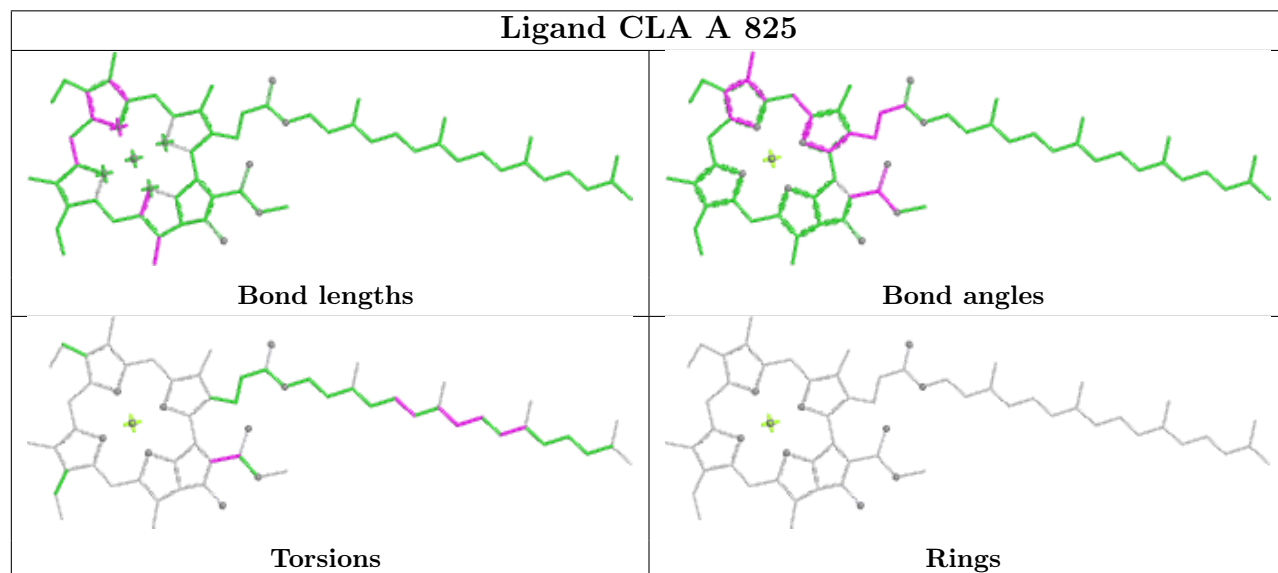
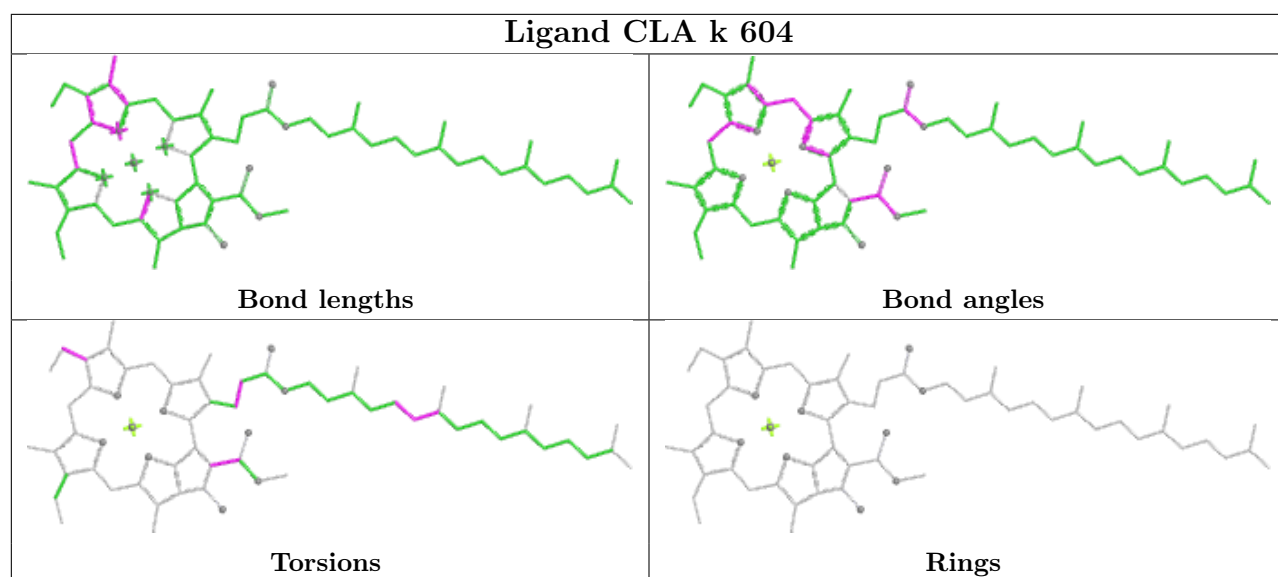


Ligand CLA d 308

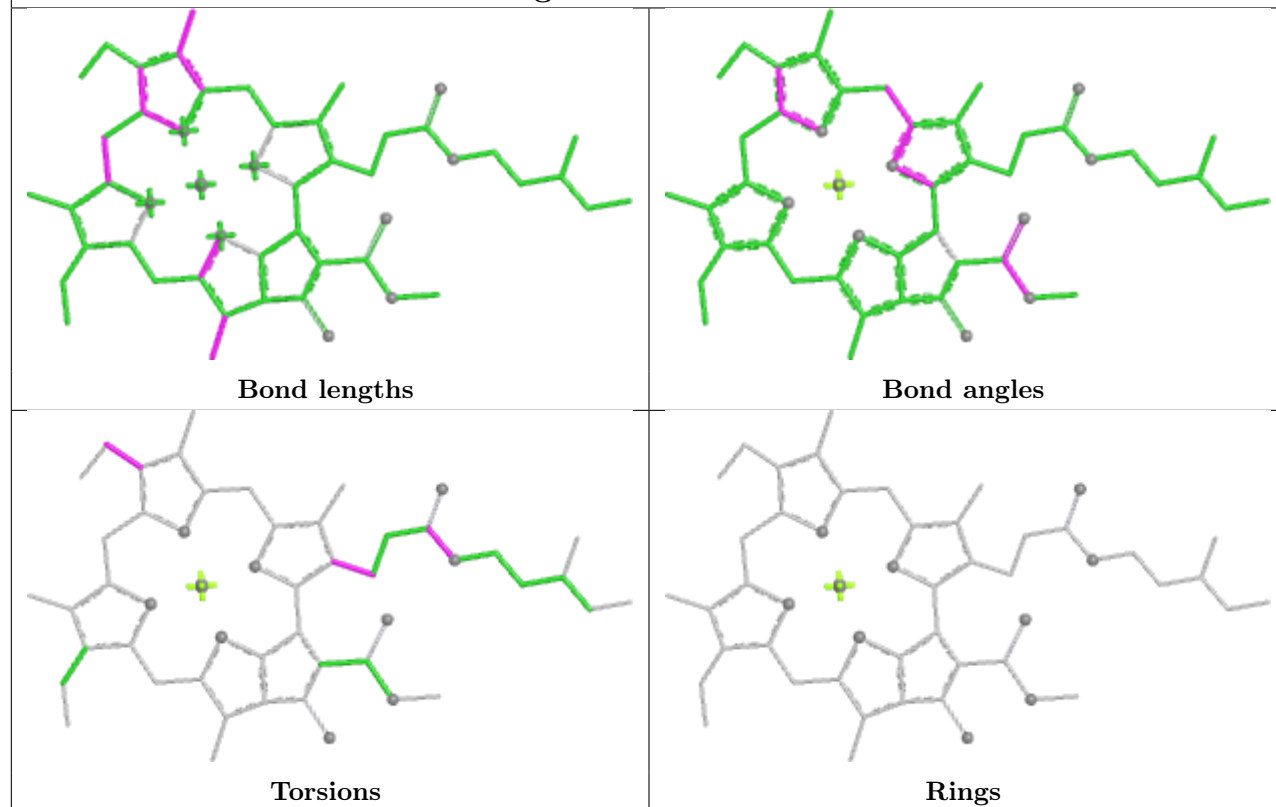


Ligand LMG c 318

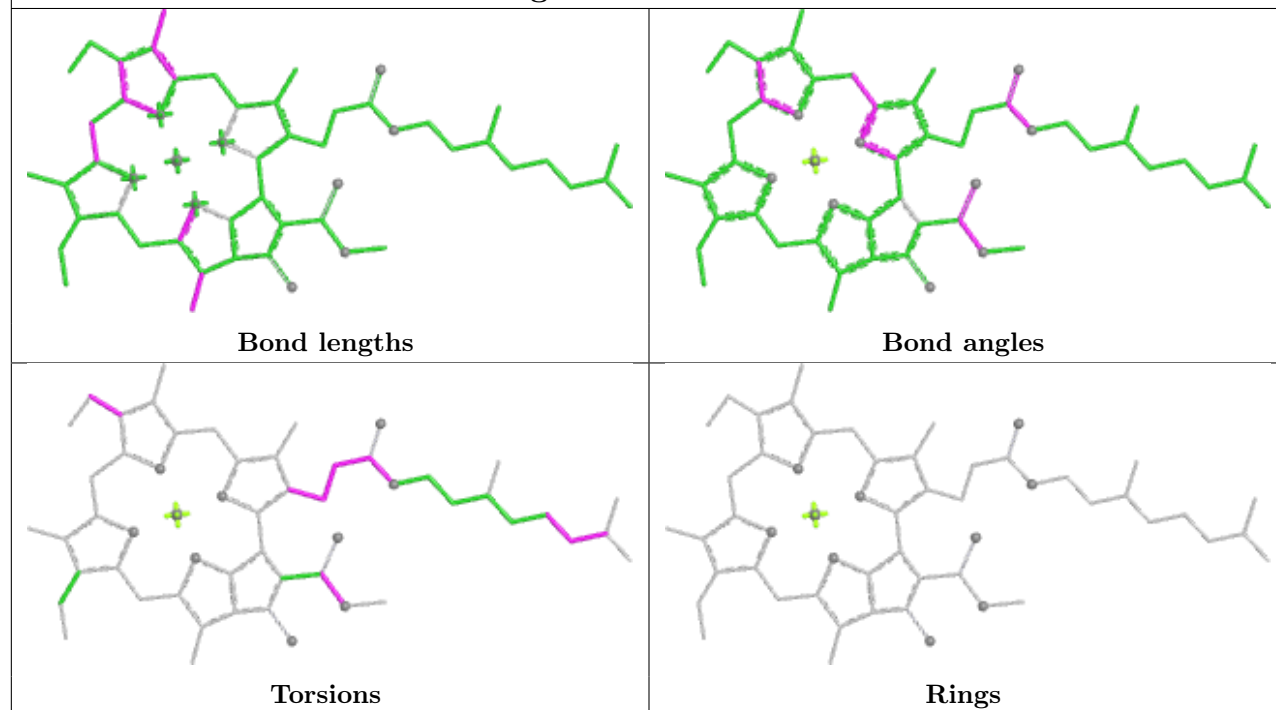




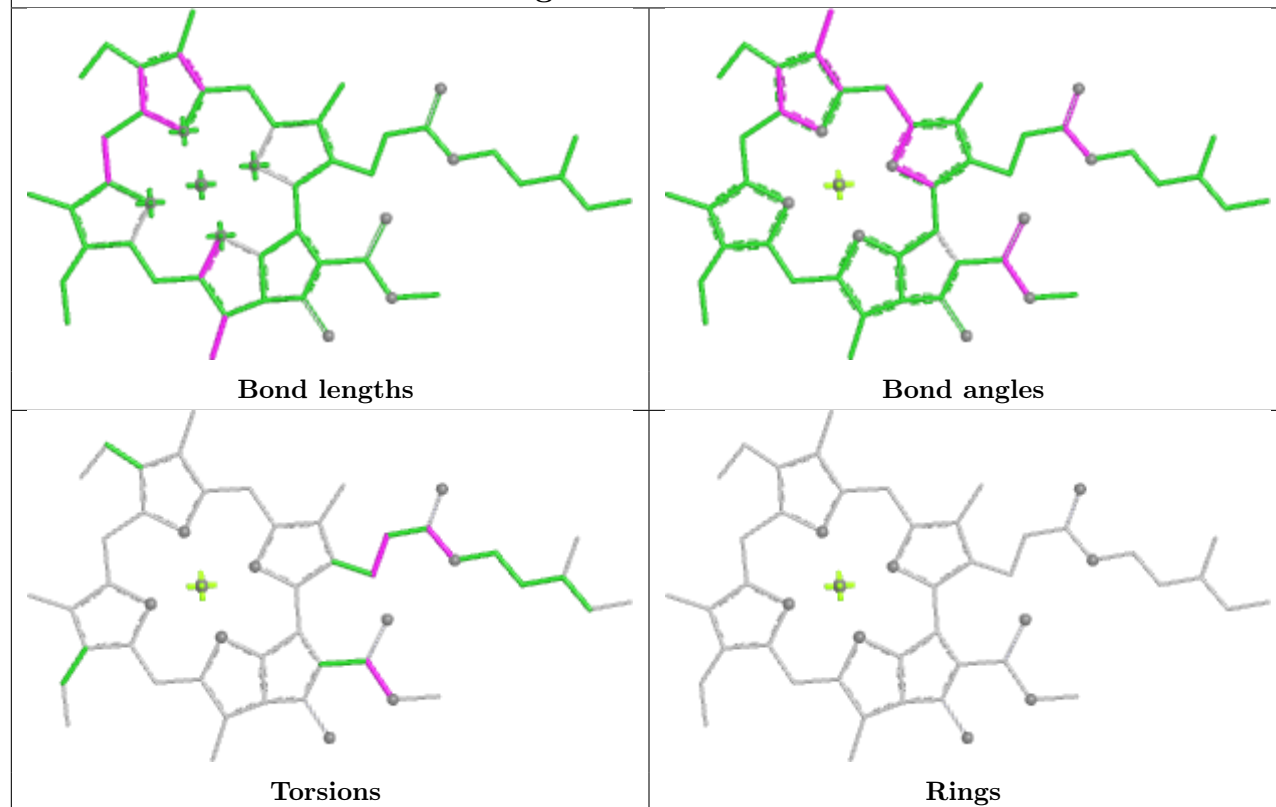
Ligand CLA L 206



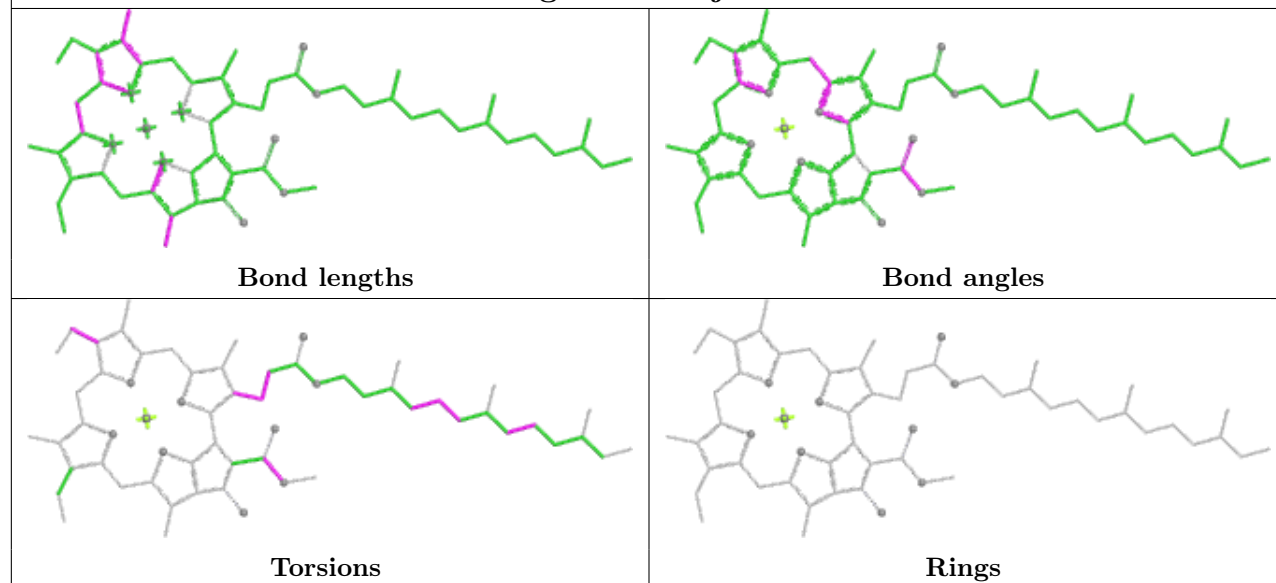
Ligand CLA m 610



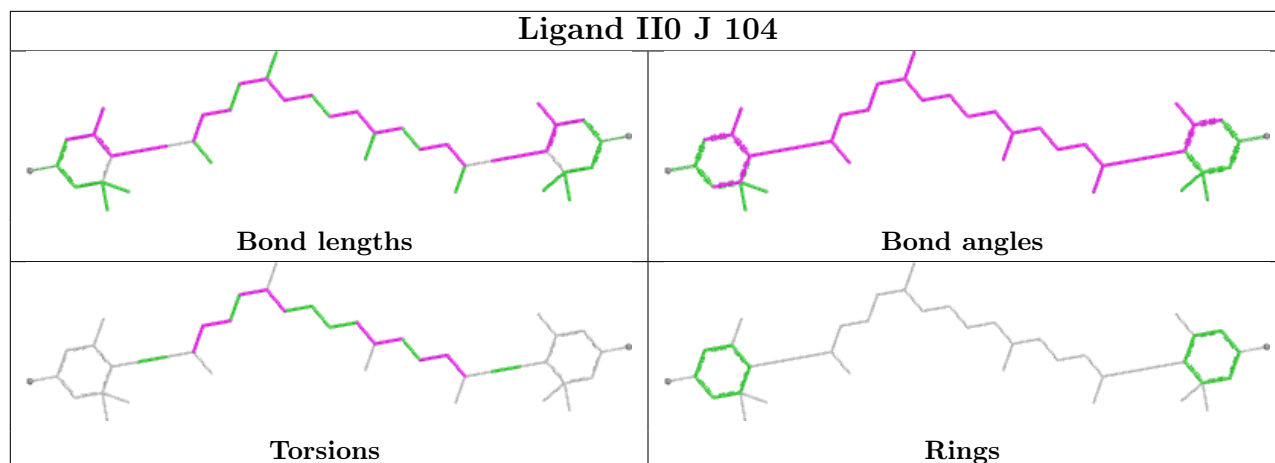
Ligand CLA d 305



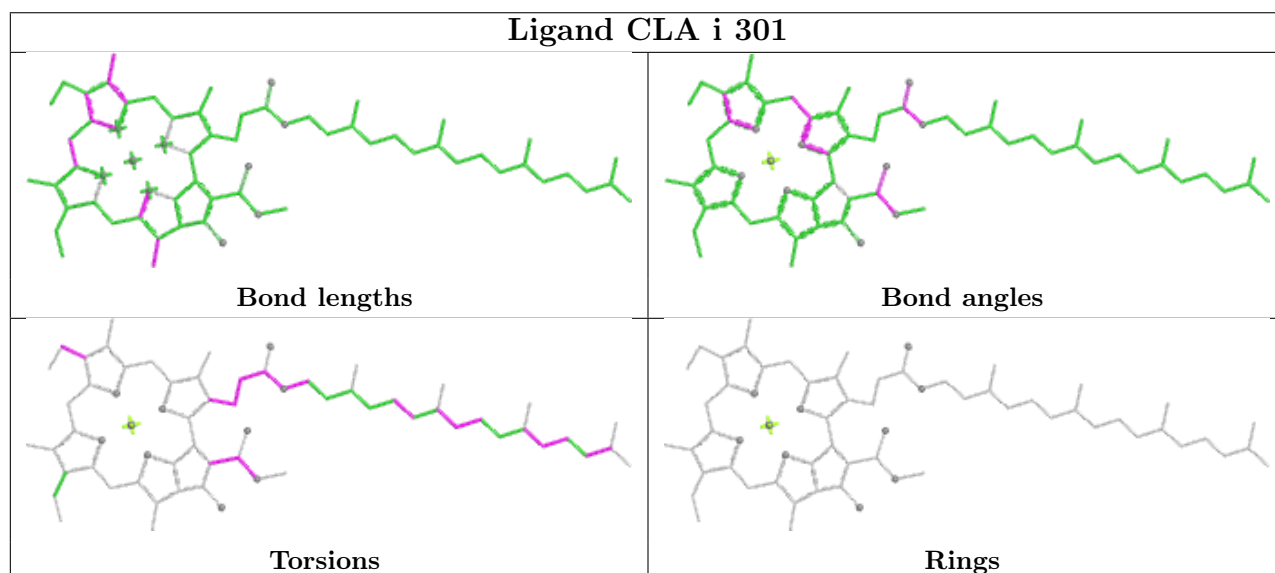
Ligand CLA j 610



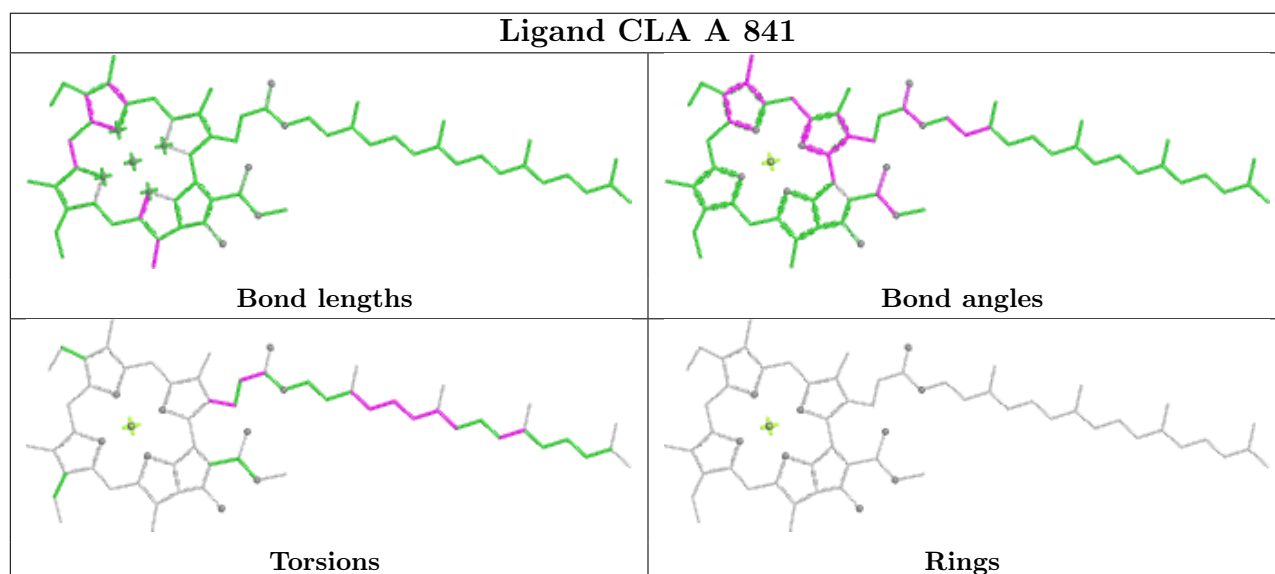
Ligand II0 J 104



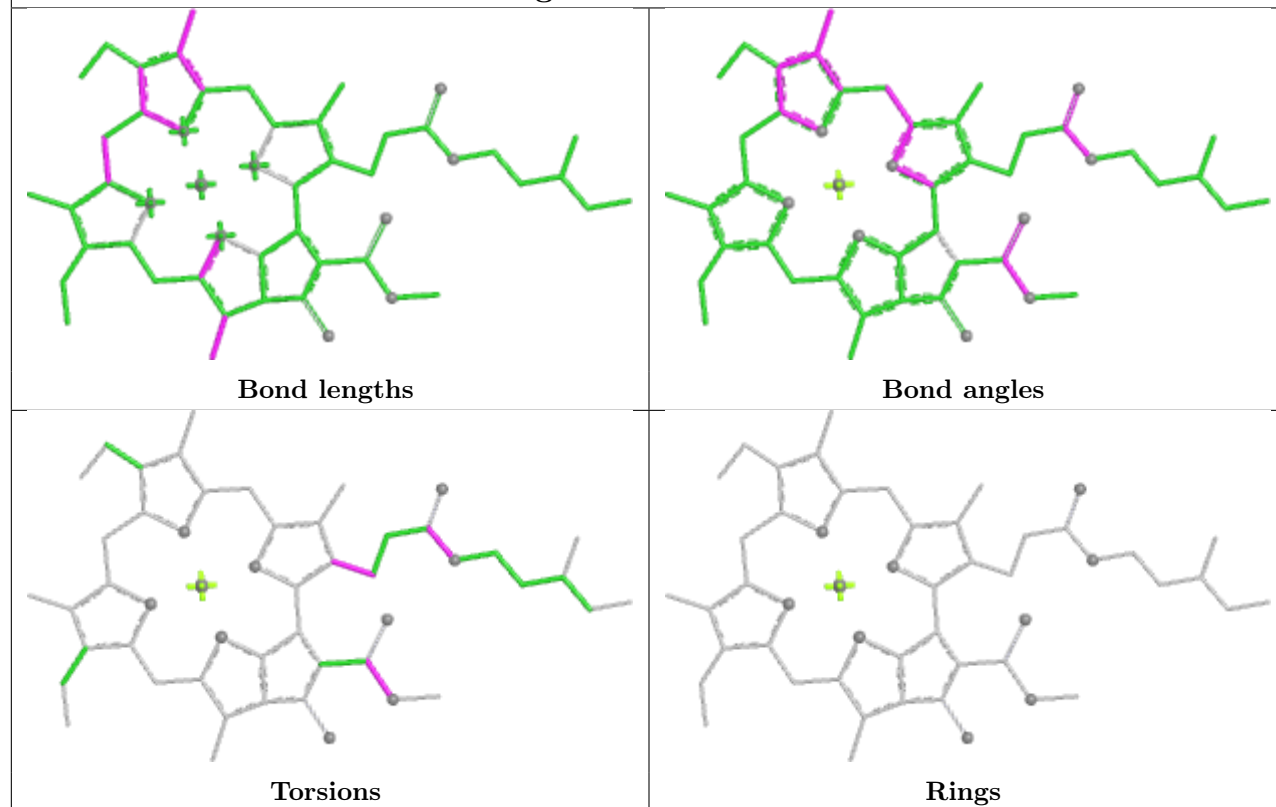
Ligand CLA i 301



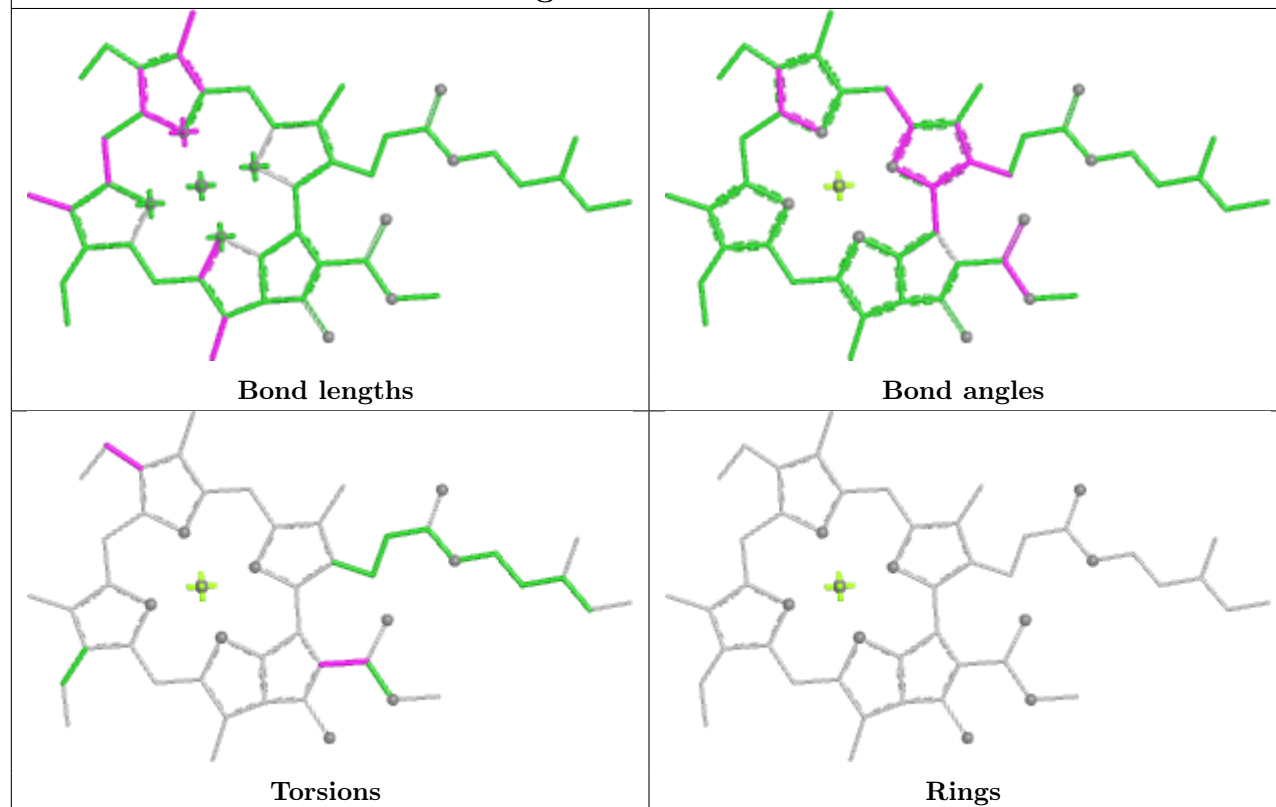
Ligand CLA A 841

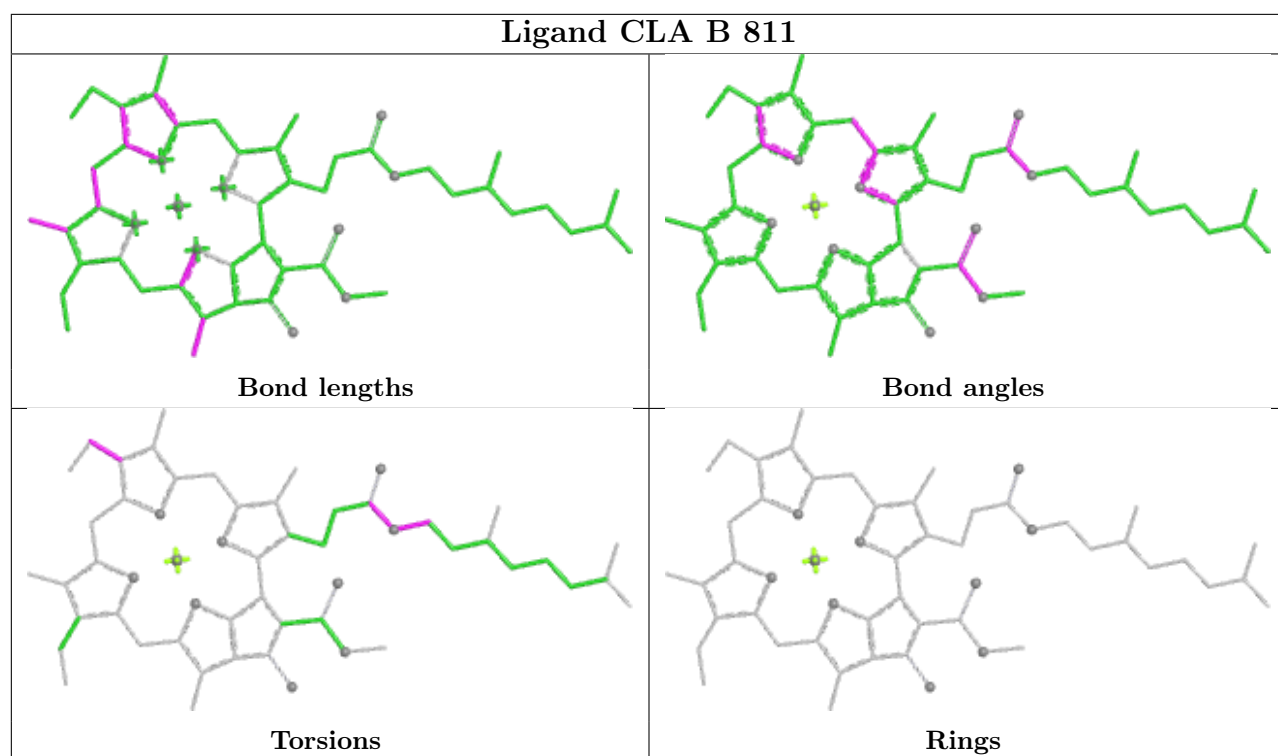


Ligand CLA h 305

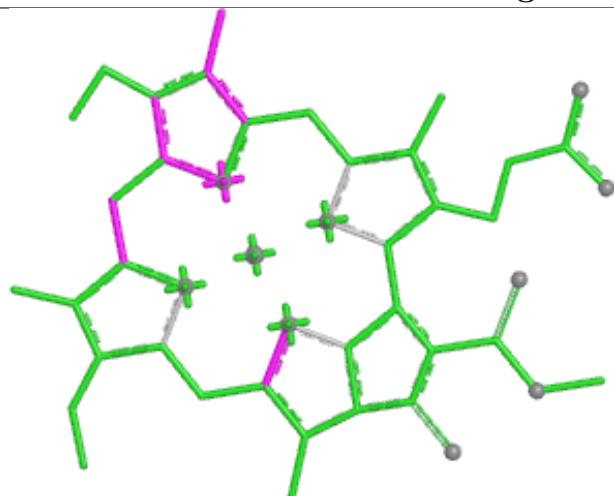


Ligand CLA a 303

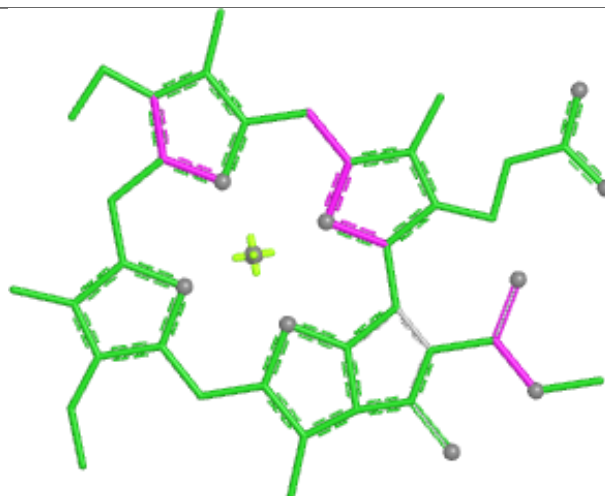




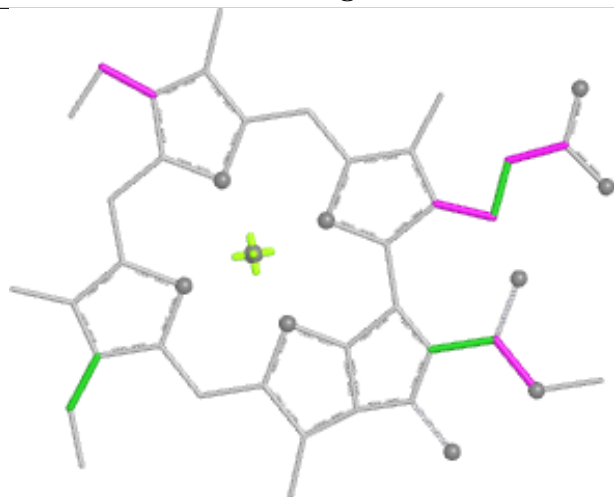
Ligand CLA d 304



Bond lengths



Bond angles

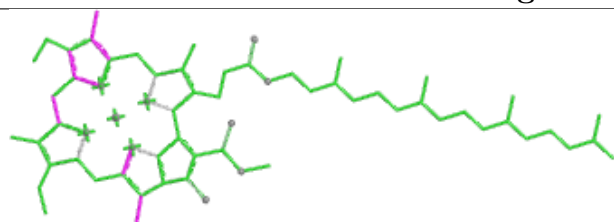


Torsions

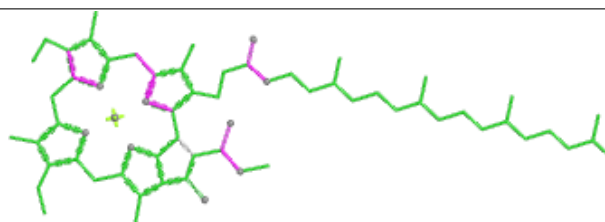


Rings

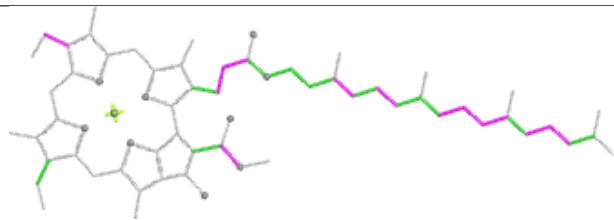
Ligand CLA h 304



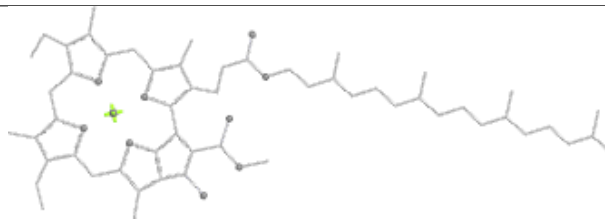
Bond lengths



Bond angles

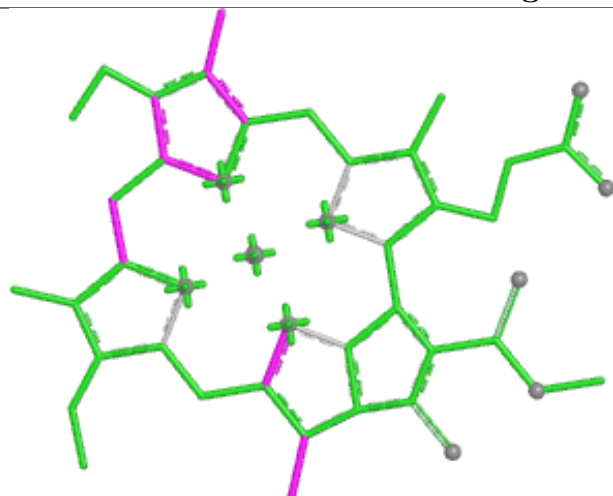


Torsions

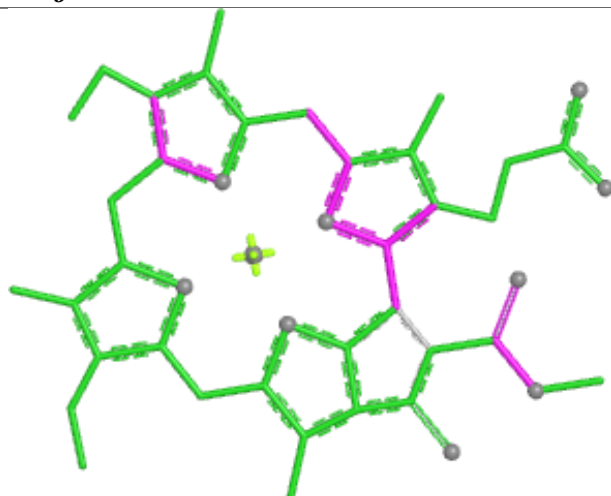


Rings

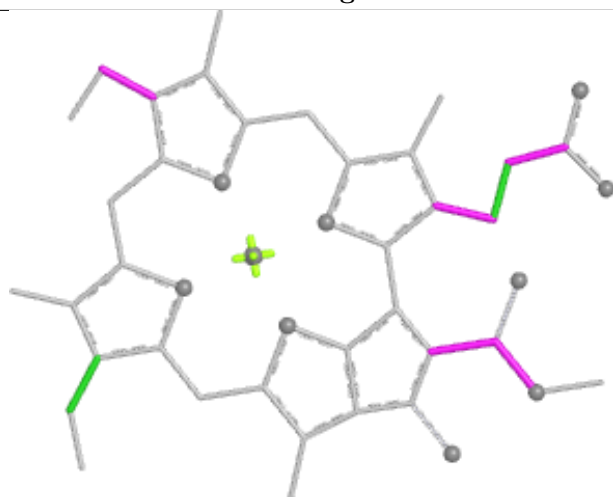
Ligand CLA j 605



Bond lengths



Bond angles

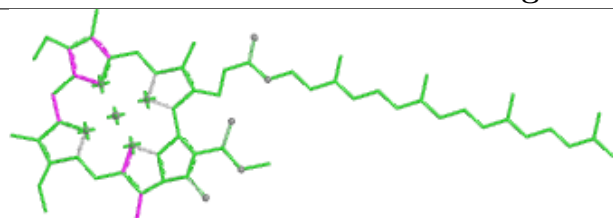


Torsions

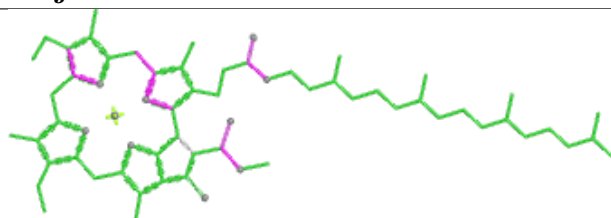


Rings

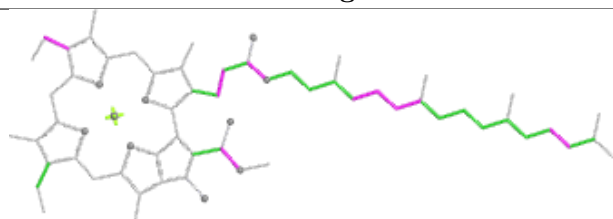
Ligand CLA j 613



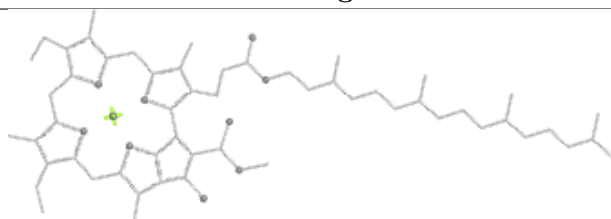
Bond lengths



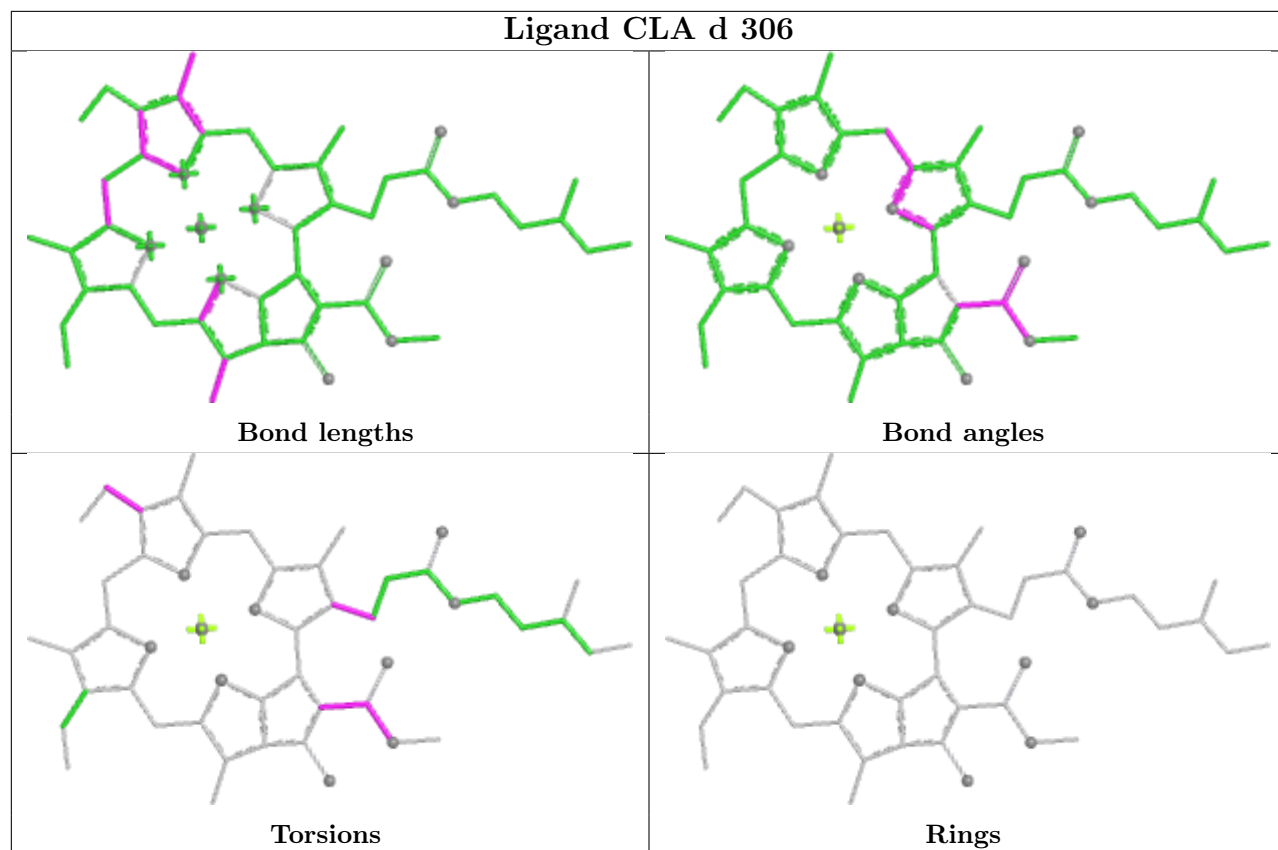
Bond angles



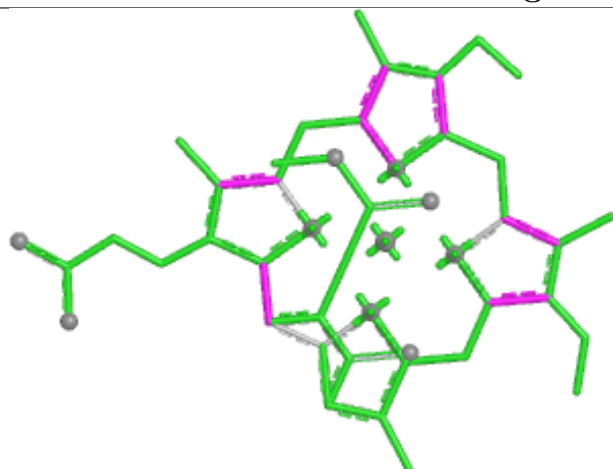
Torsions



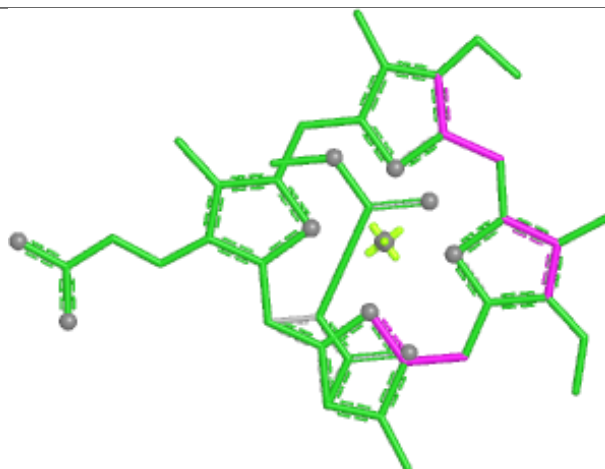
Rings



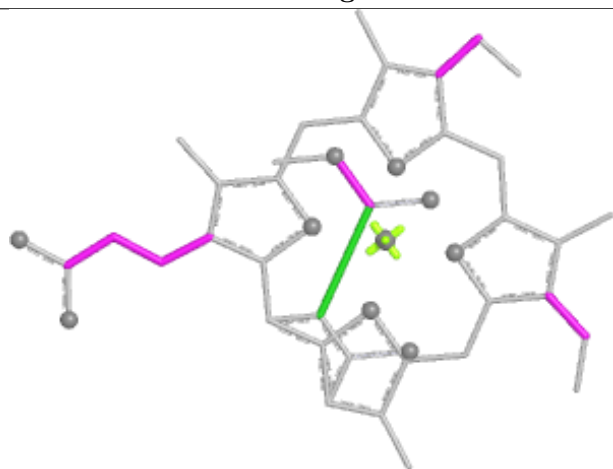
Ligand KC2 i 309



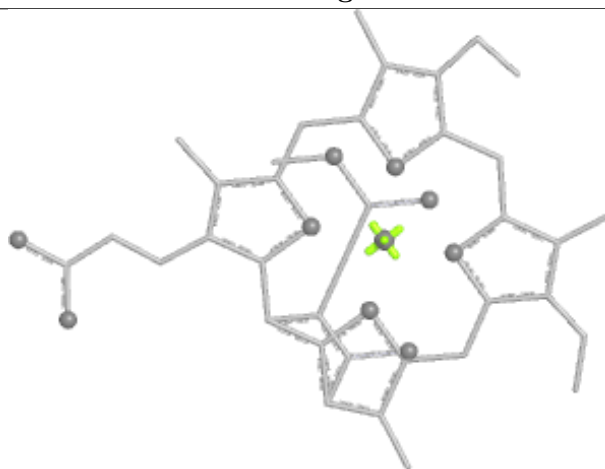
Bond lengths



Bond angles

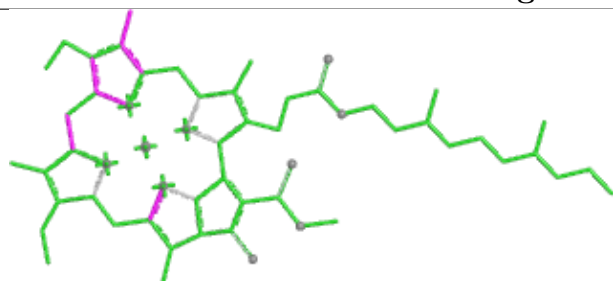


Torsions

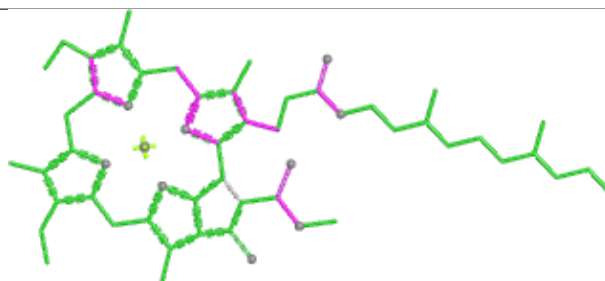


Rings

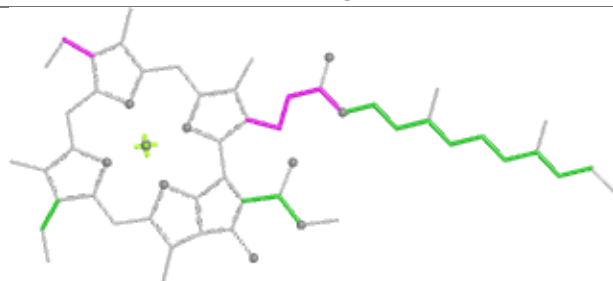
Ligand CLA h 307



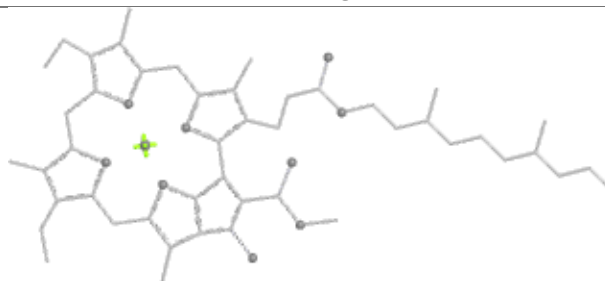
Bond lengths



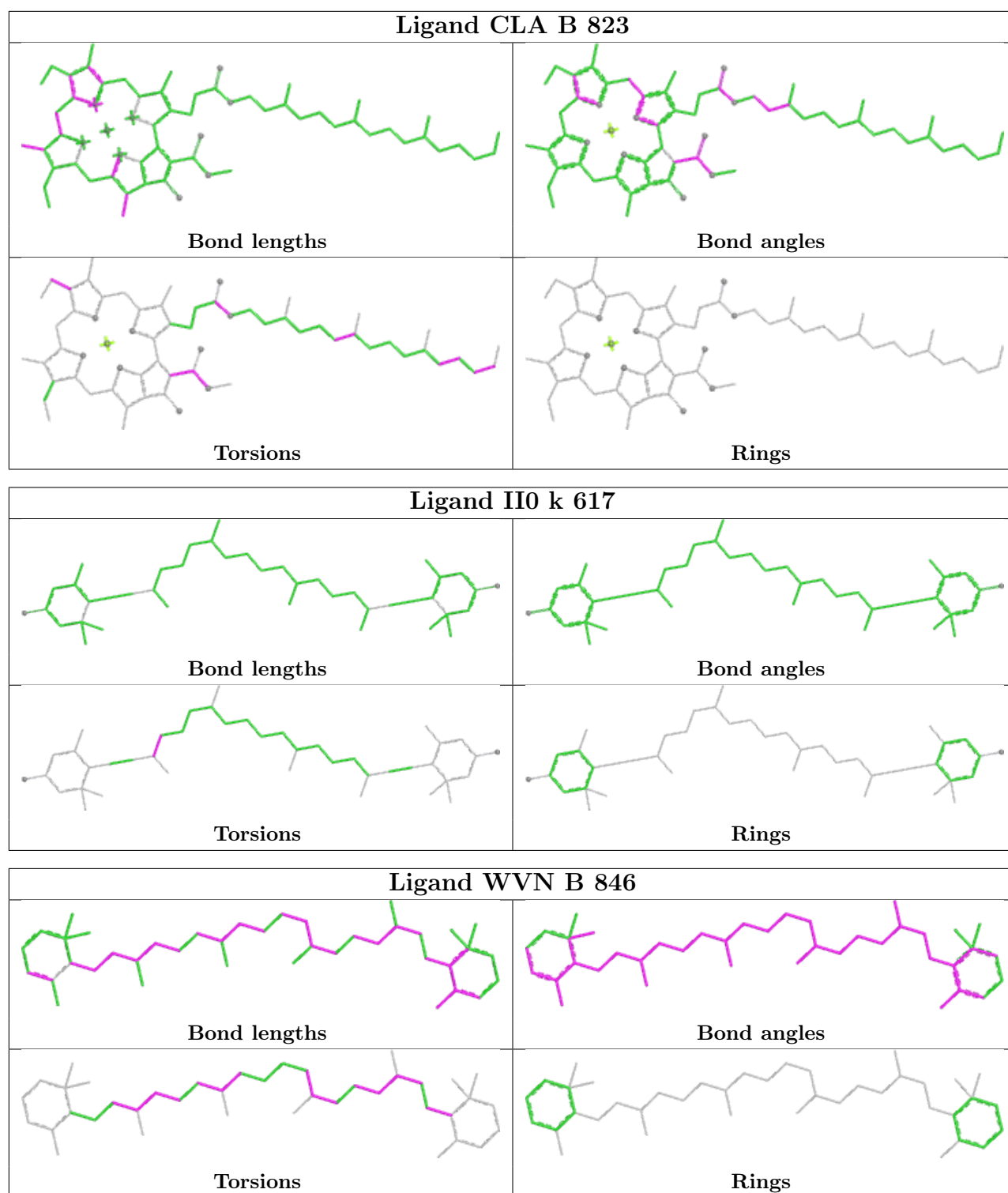
Bond angles

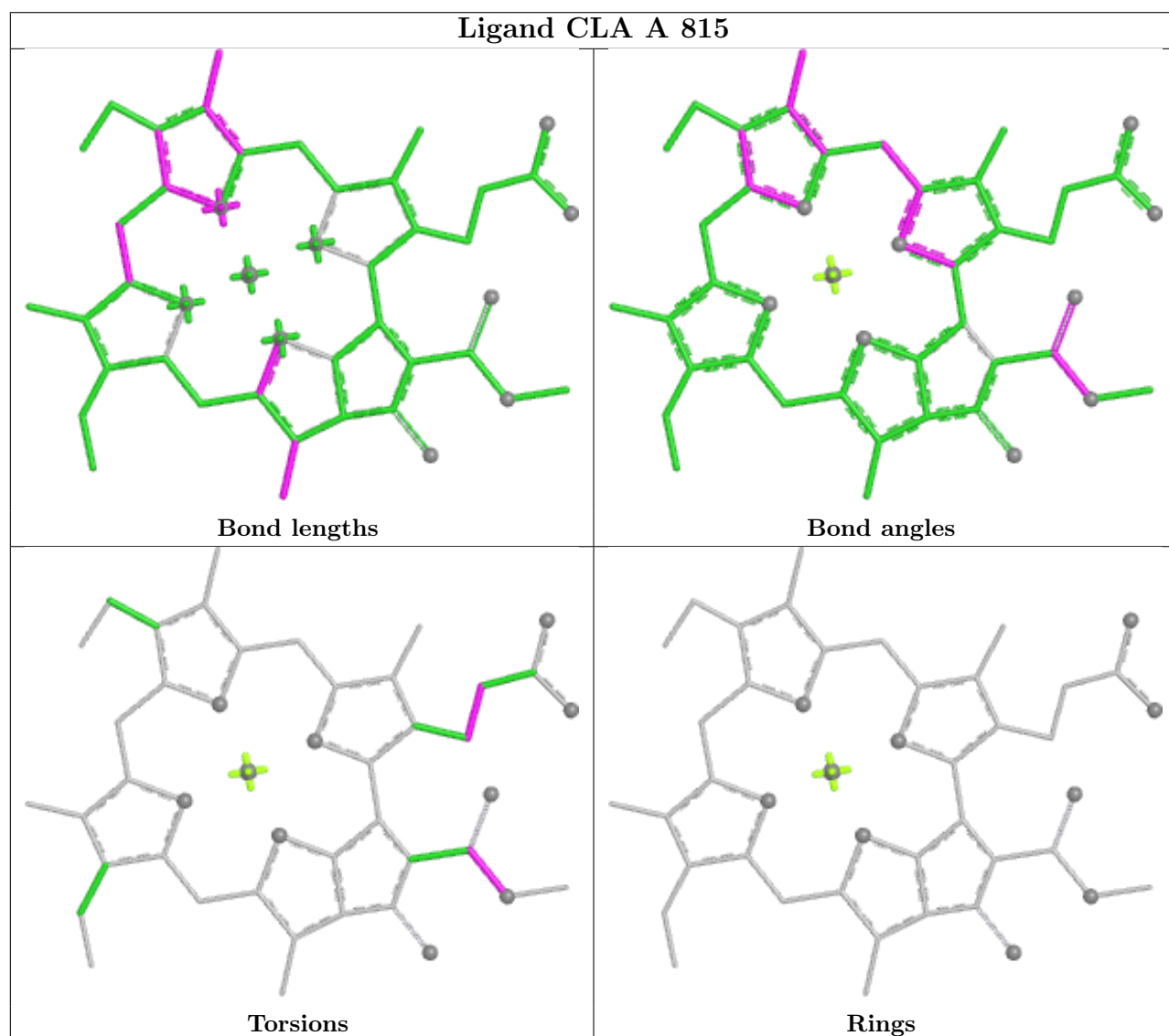
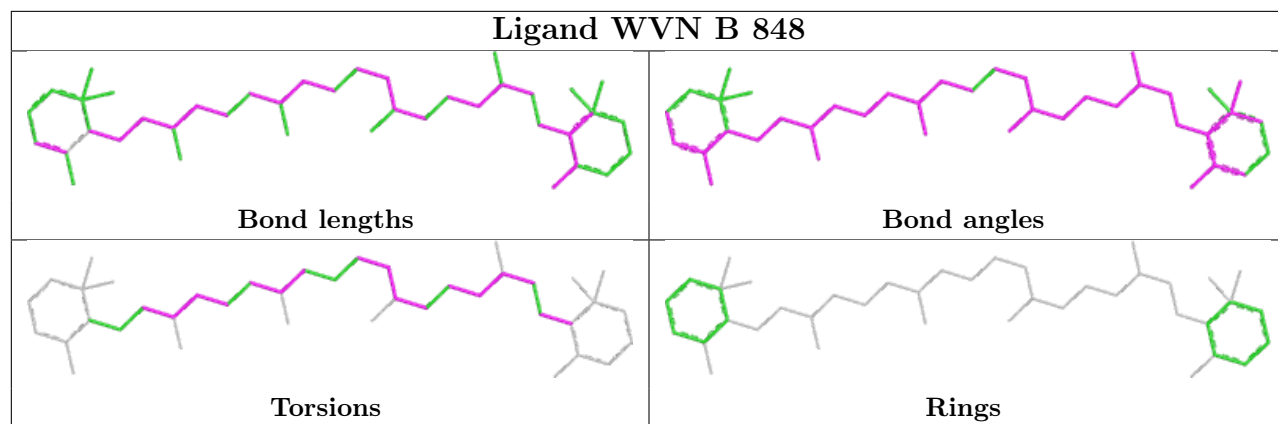


Torsions

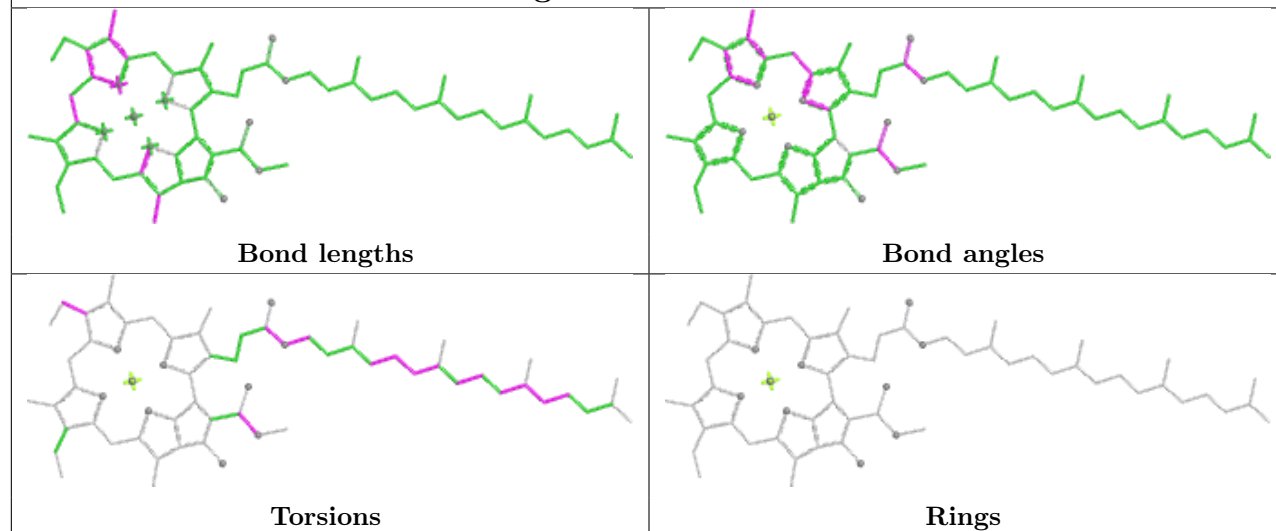


Rings

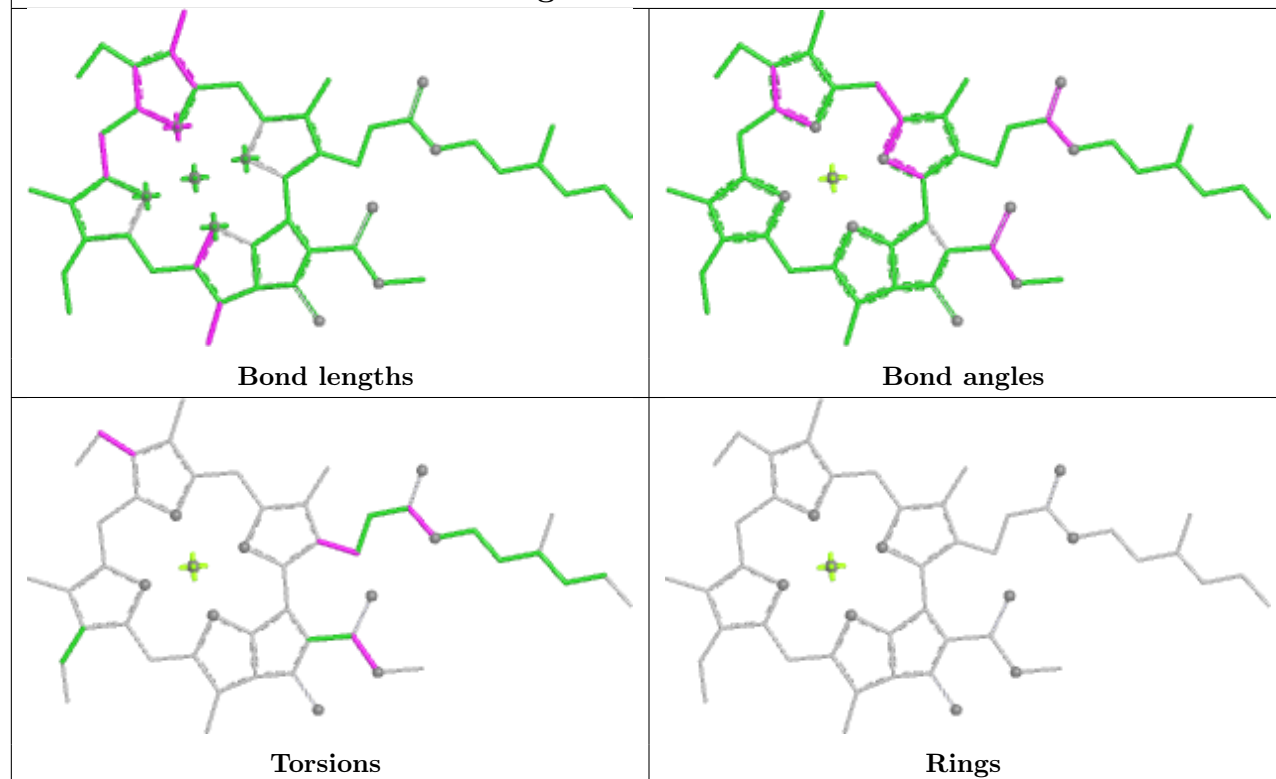




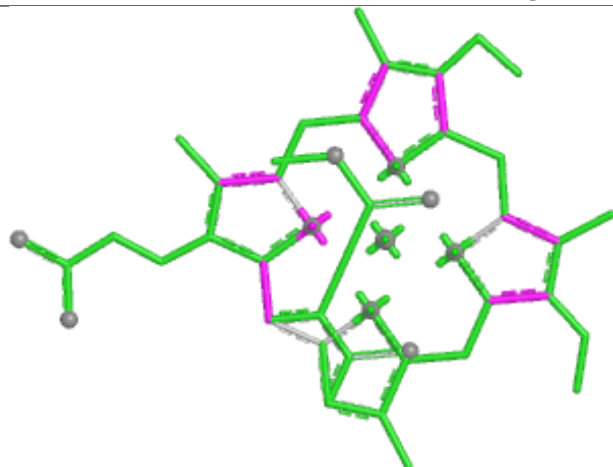
Ligand CLA F 201



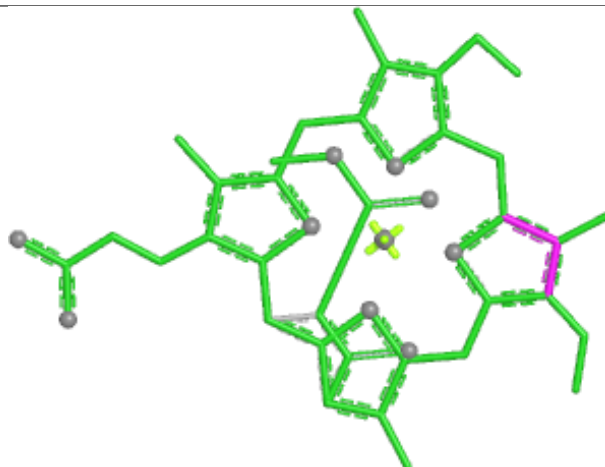
Ligand CLA c 306



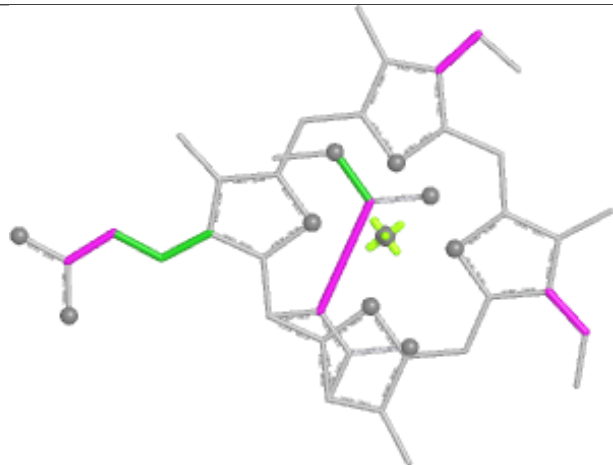
Ligand KC2 l 312



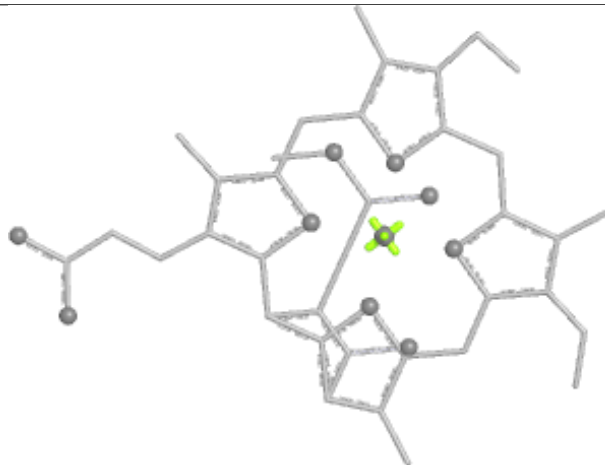
Bond lengths



Bond angles

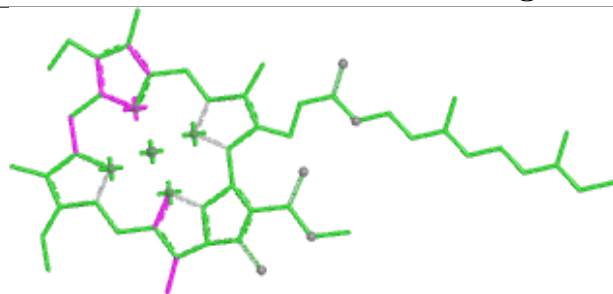


Torsions

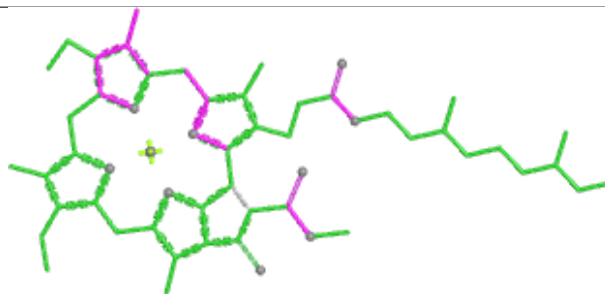


Rings

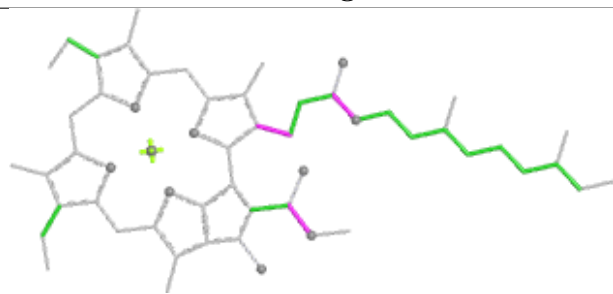
Ligand CLA a 302



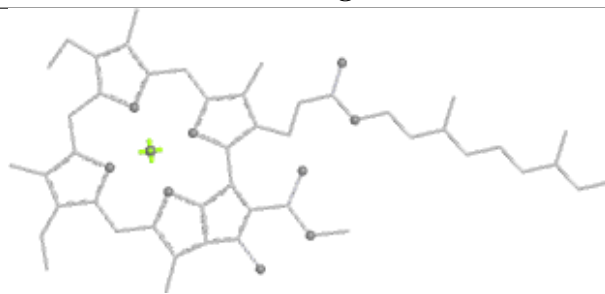
Bond lengths



Bond angles

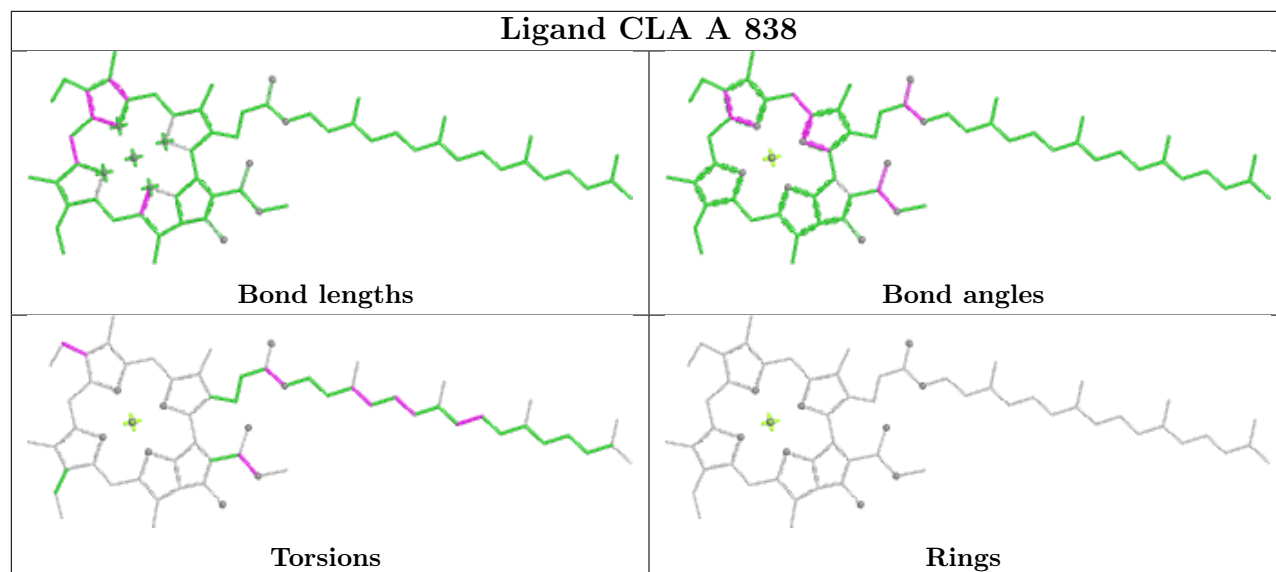


Torsions

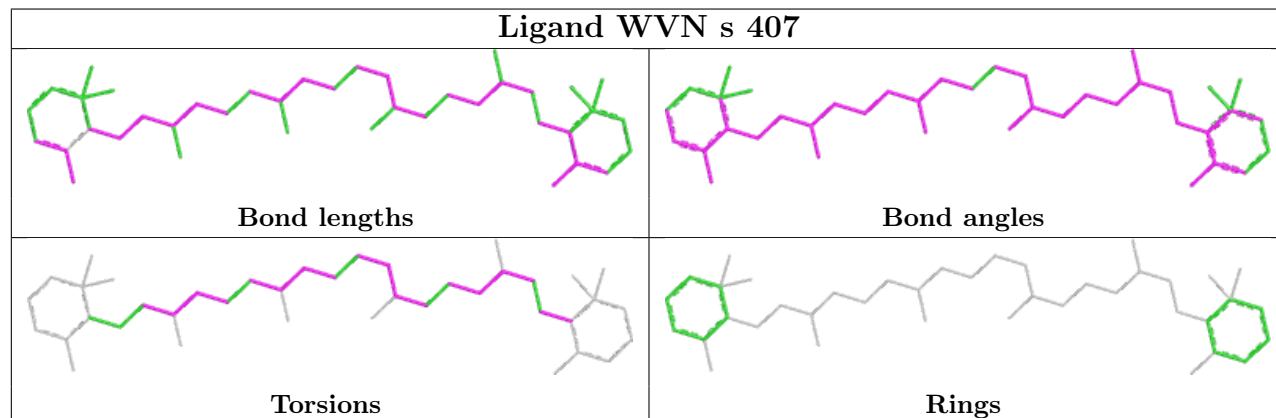


Rings

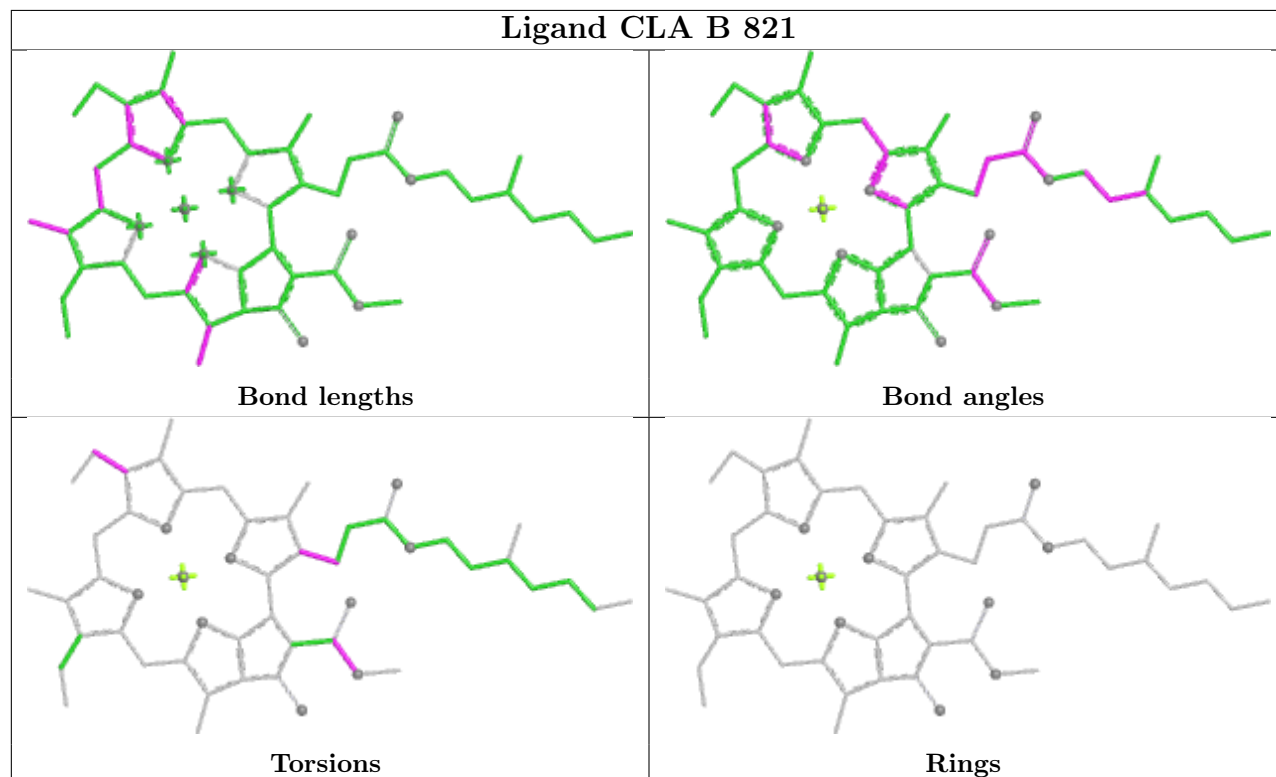
Ligand CLA A 838



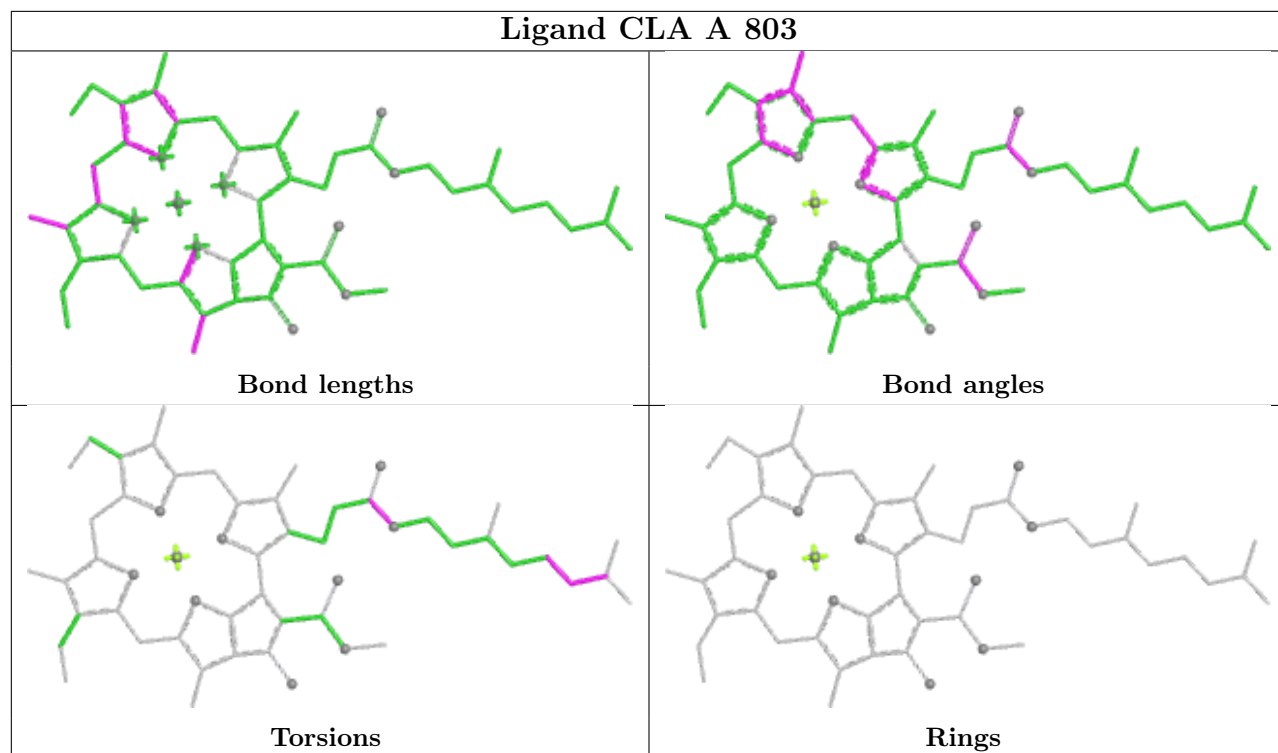
Ligand WVN s 407



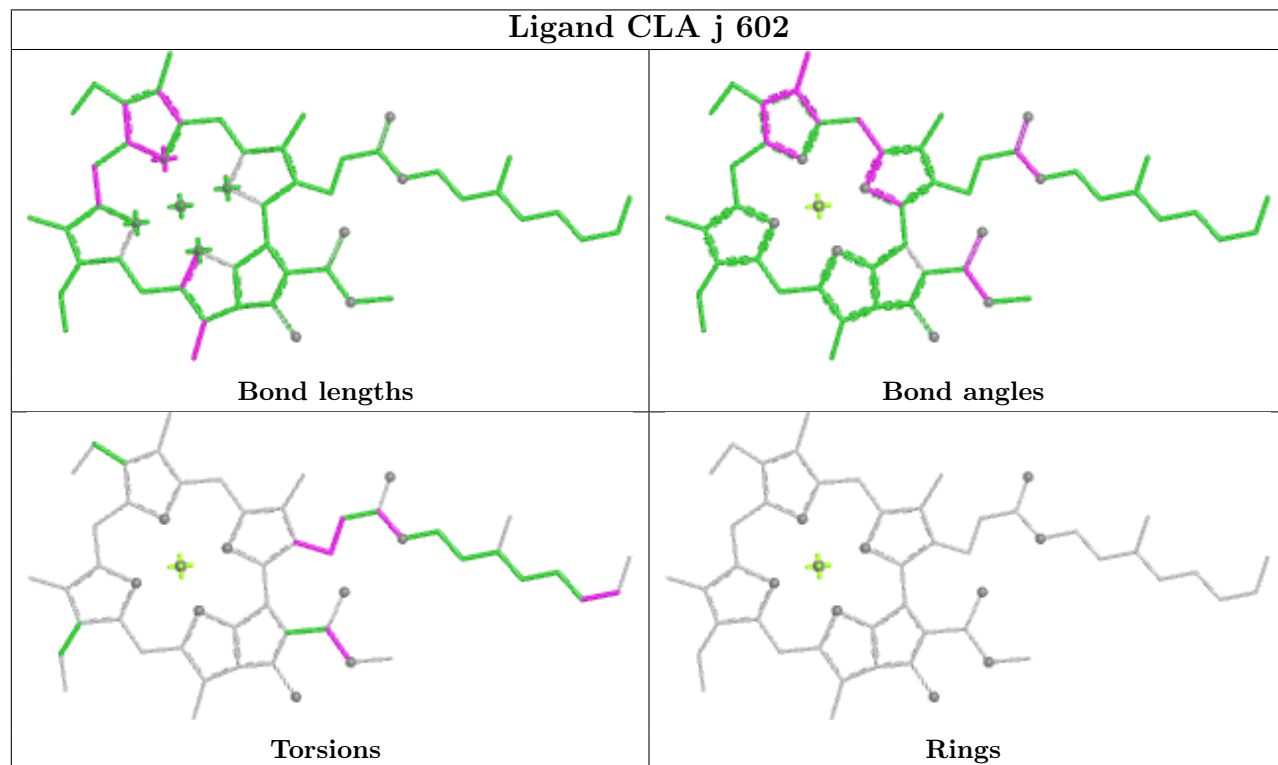
Ligand CLA B 821

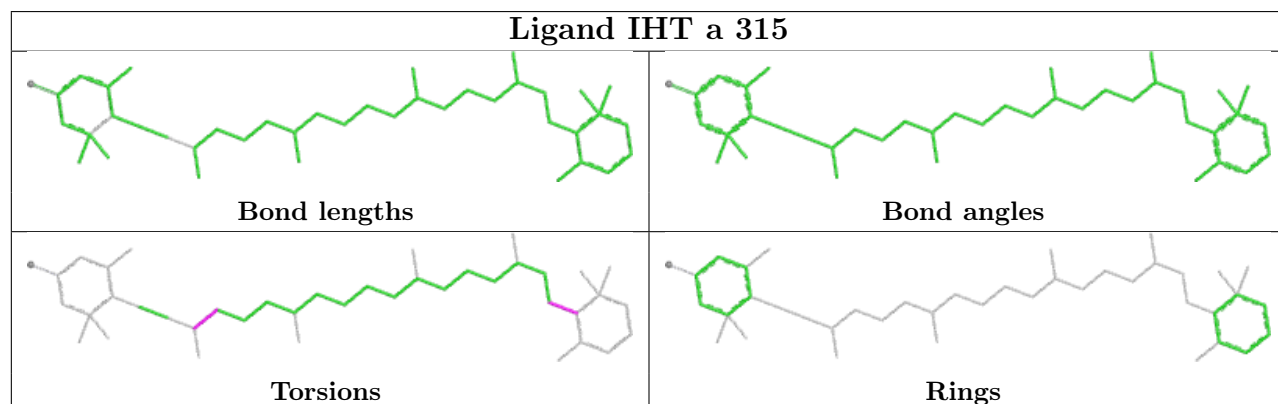
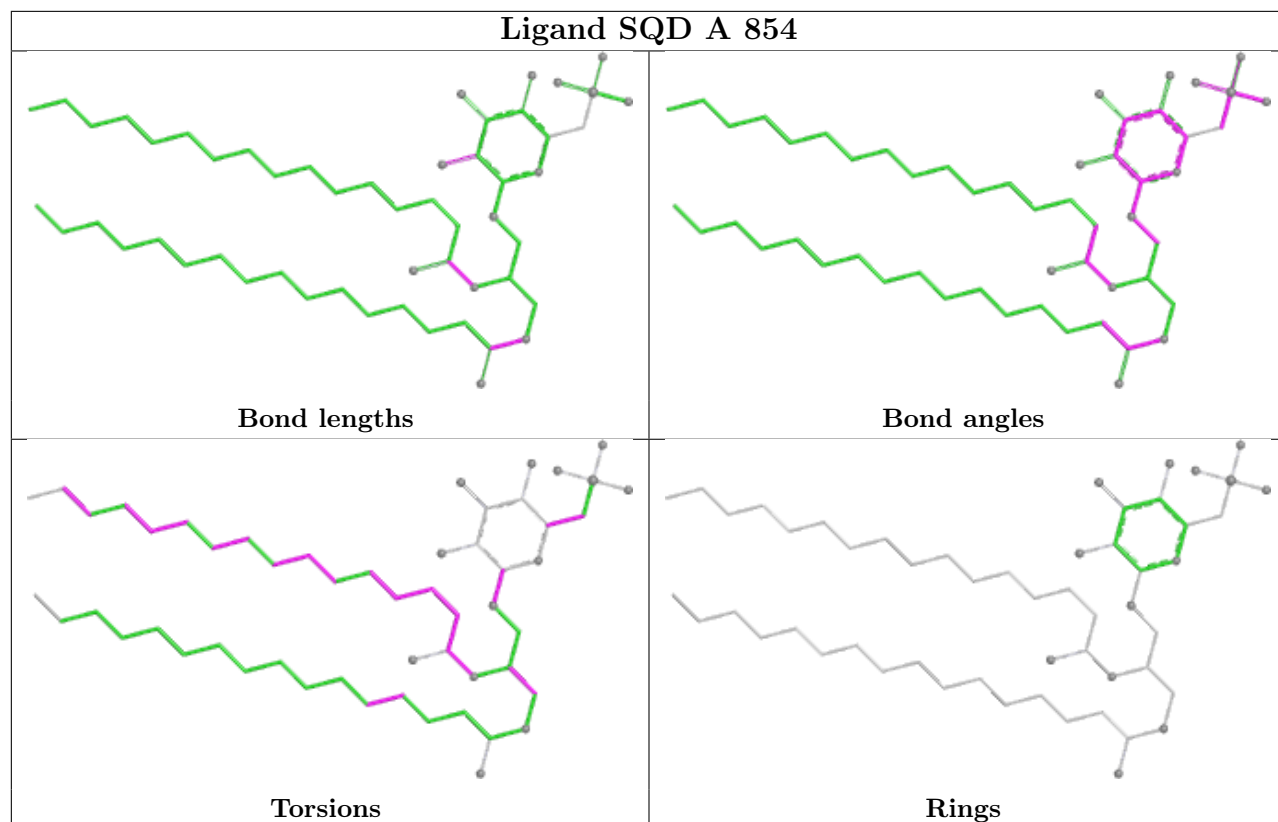


Ligand CLA A 803

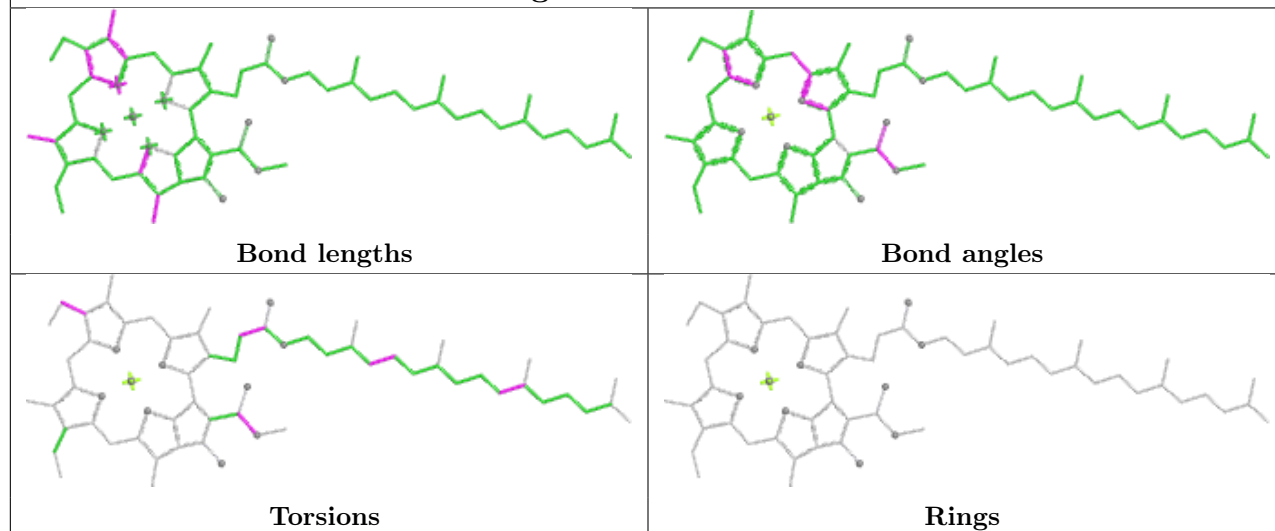


Ligand CLA j 602

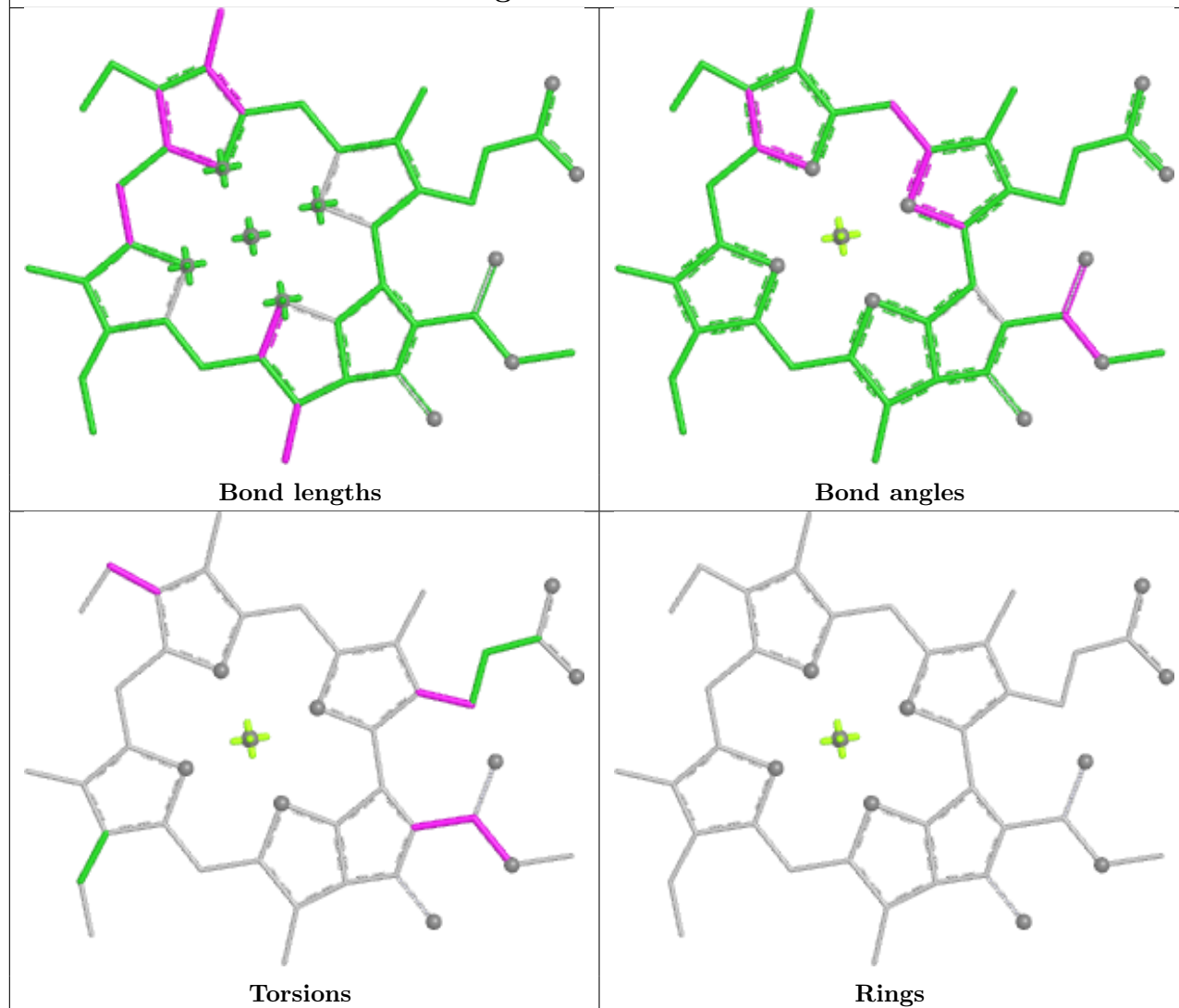


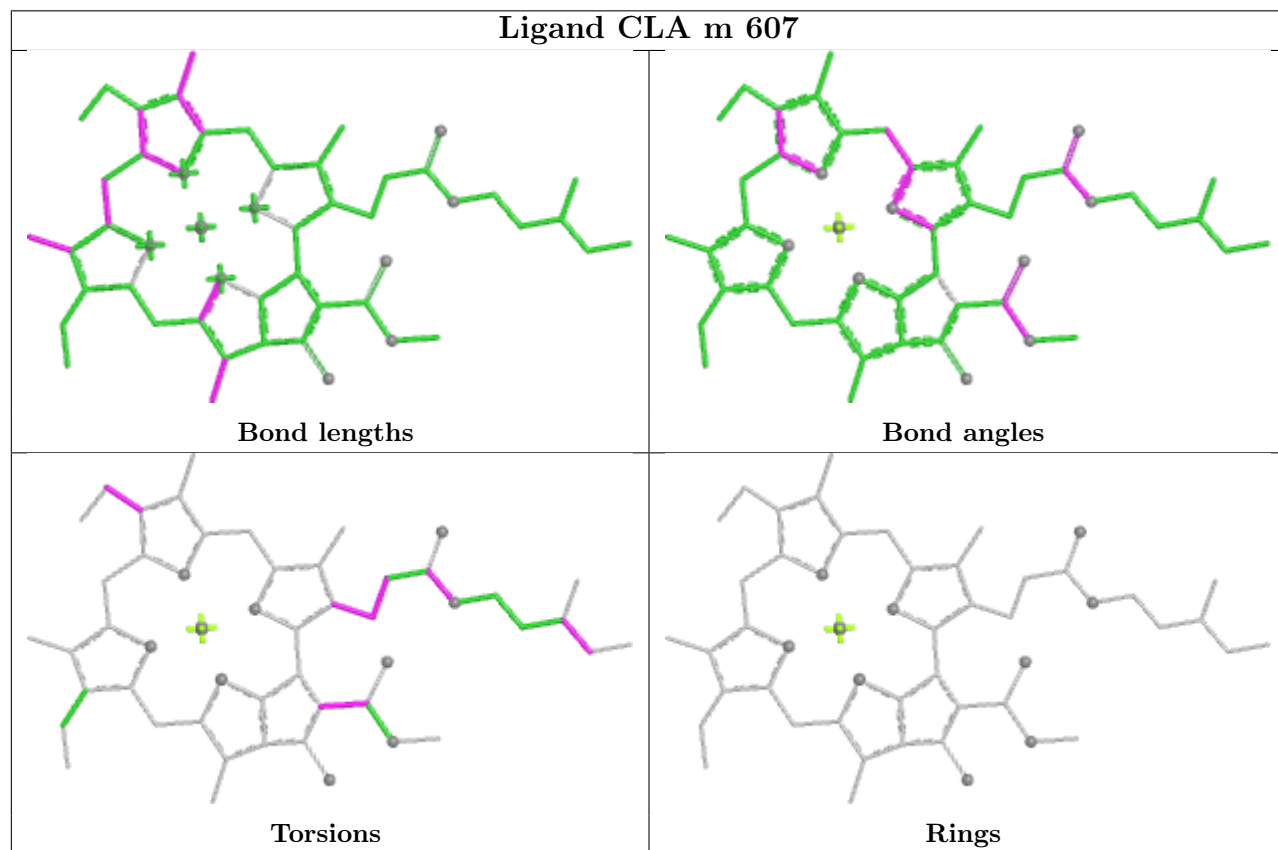
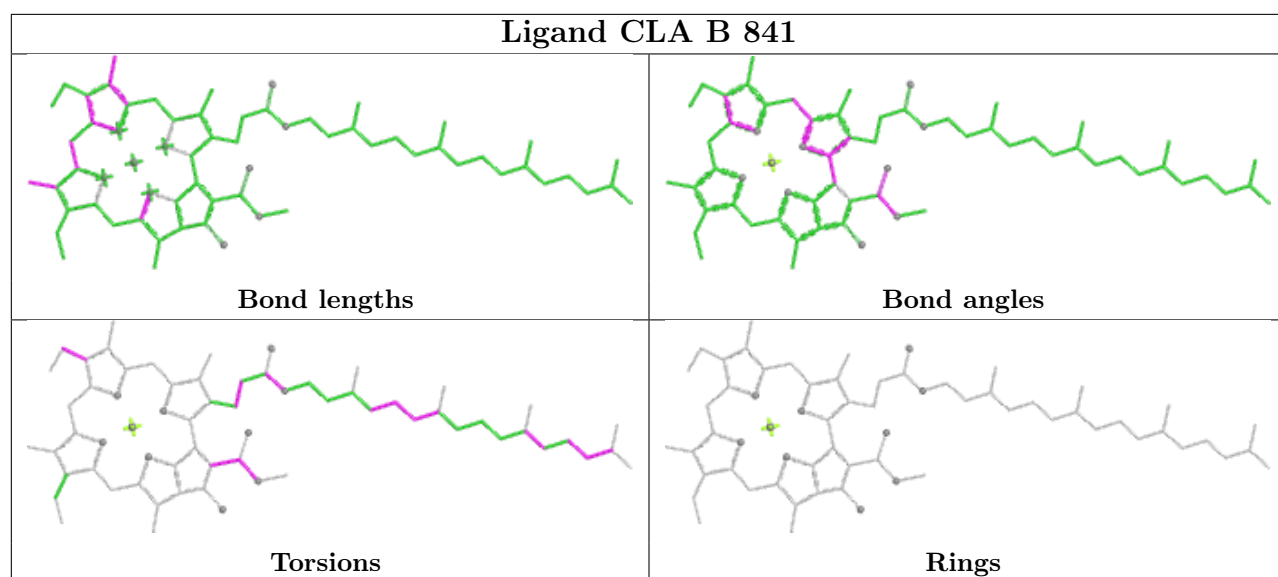


Ligand CLA B 809

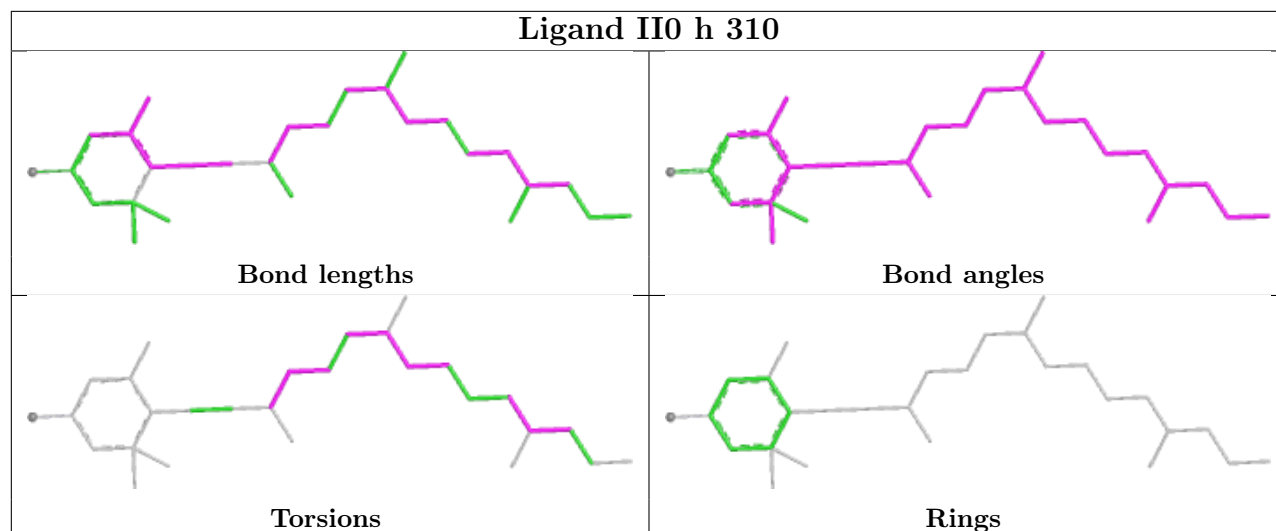


Ligand CLA a 305

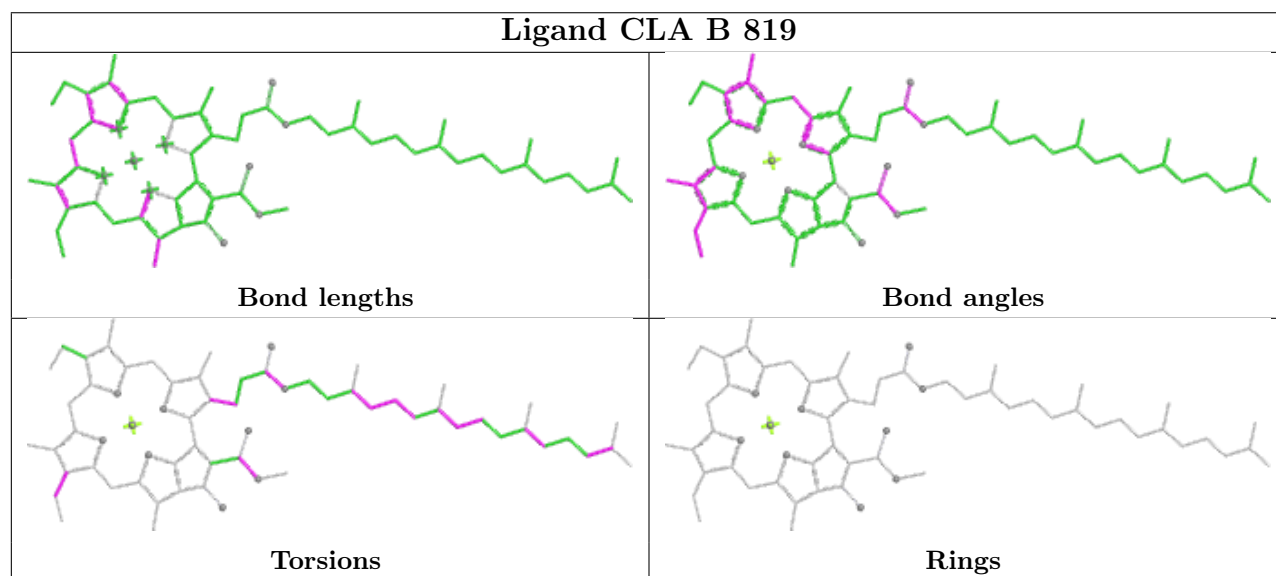




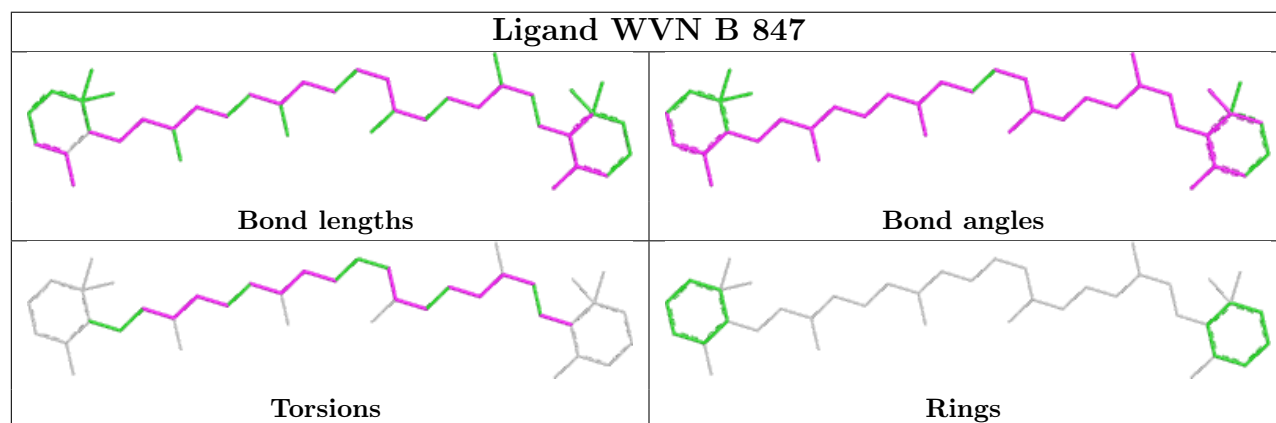
Ligand II0 h 310



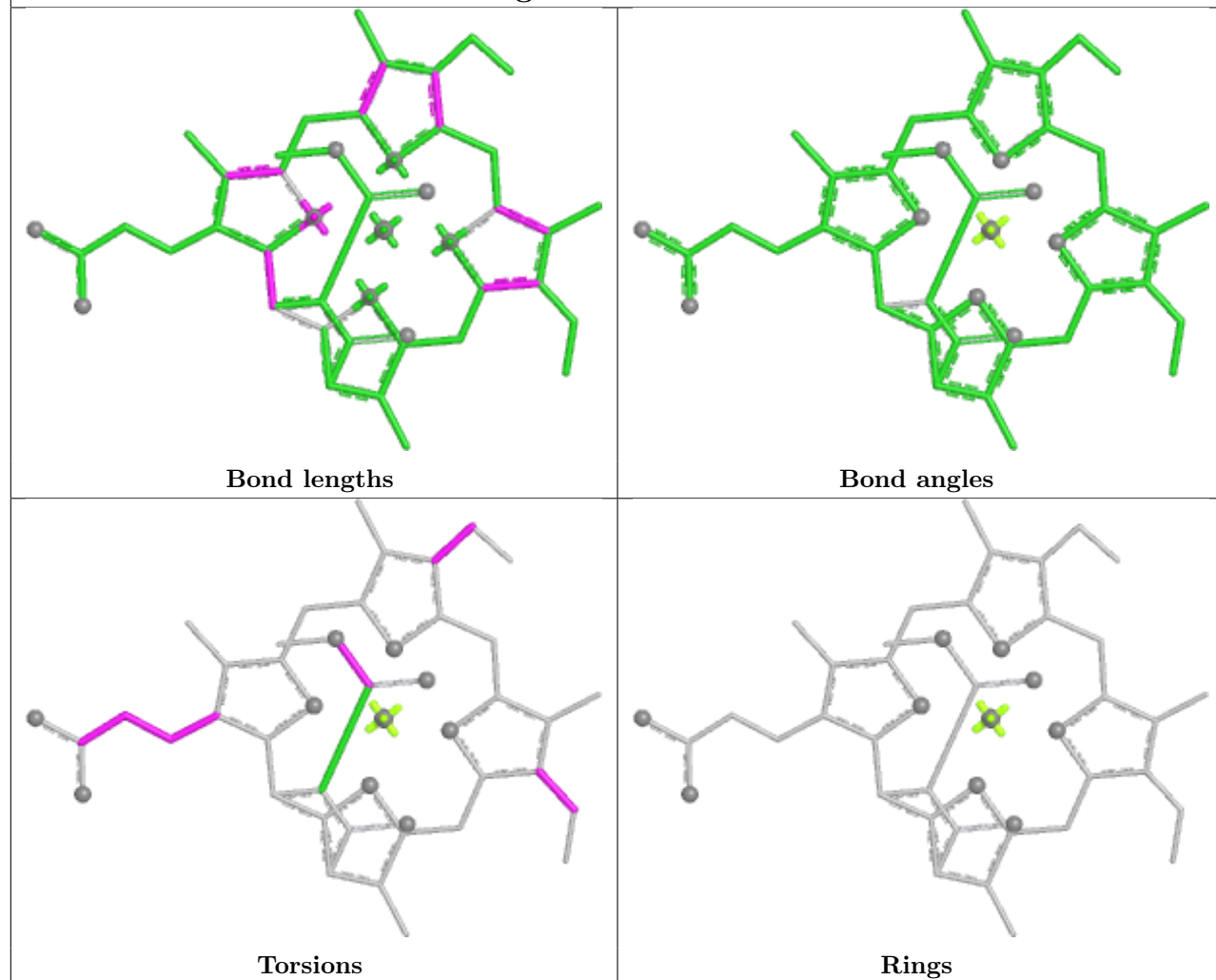
Ligand CLA B 819



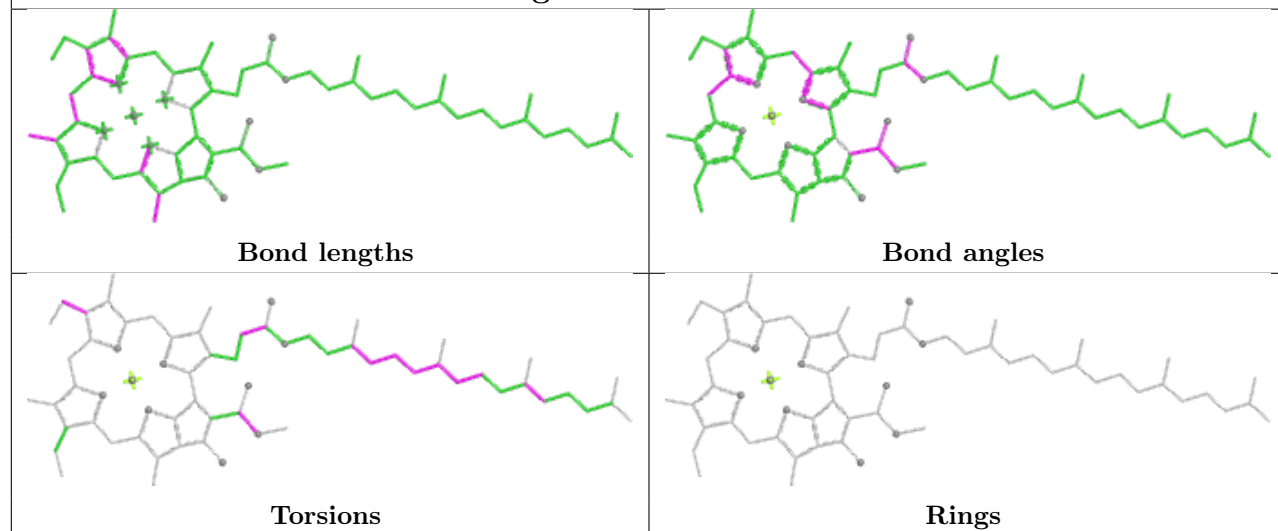
Ligand WVN B 847

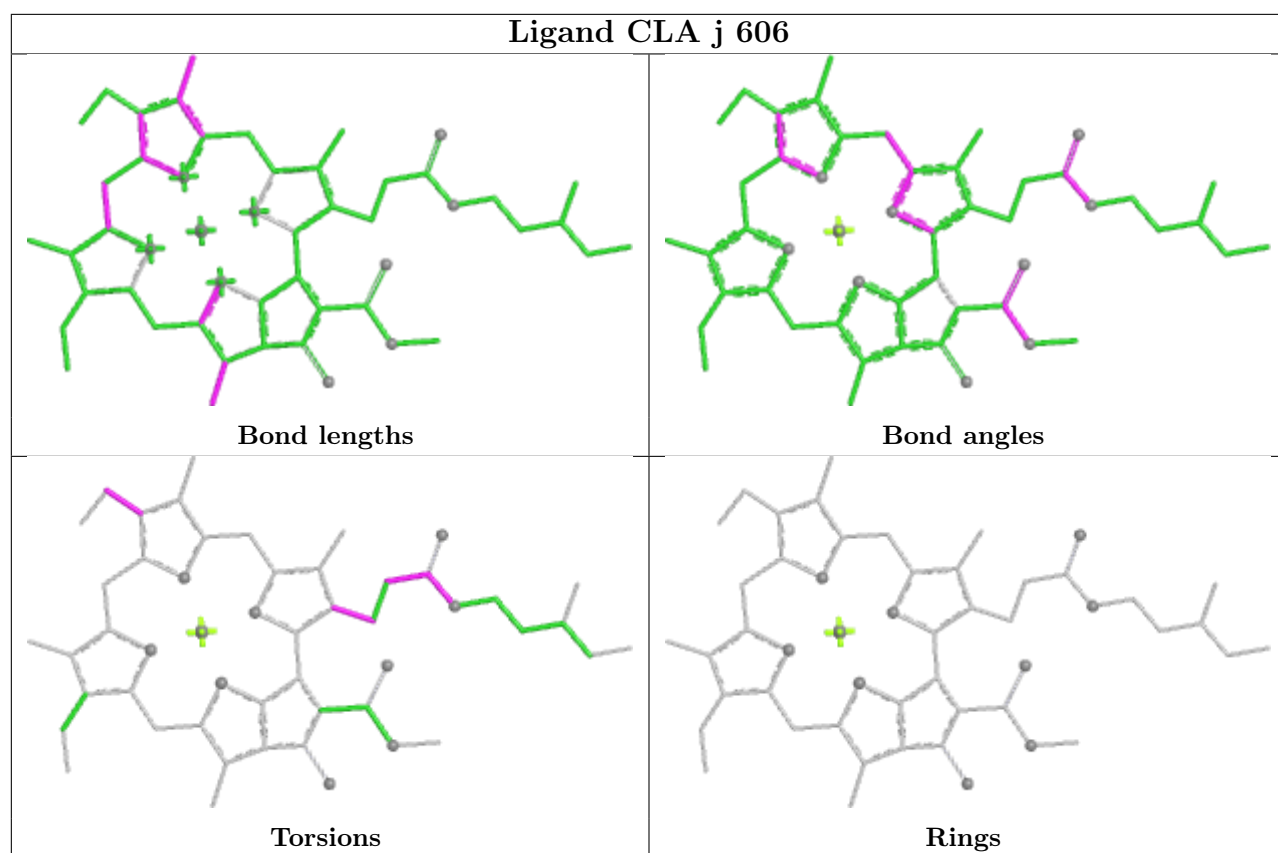


Ligand KC2 i 318

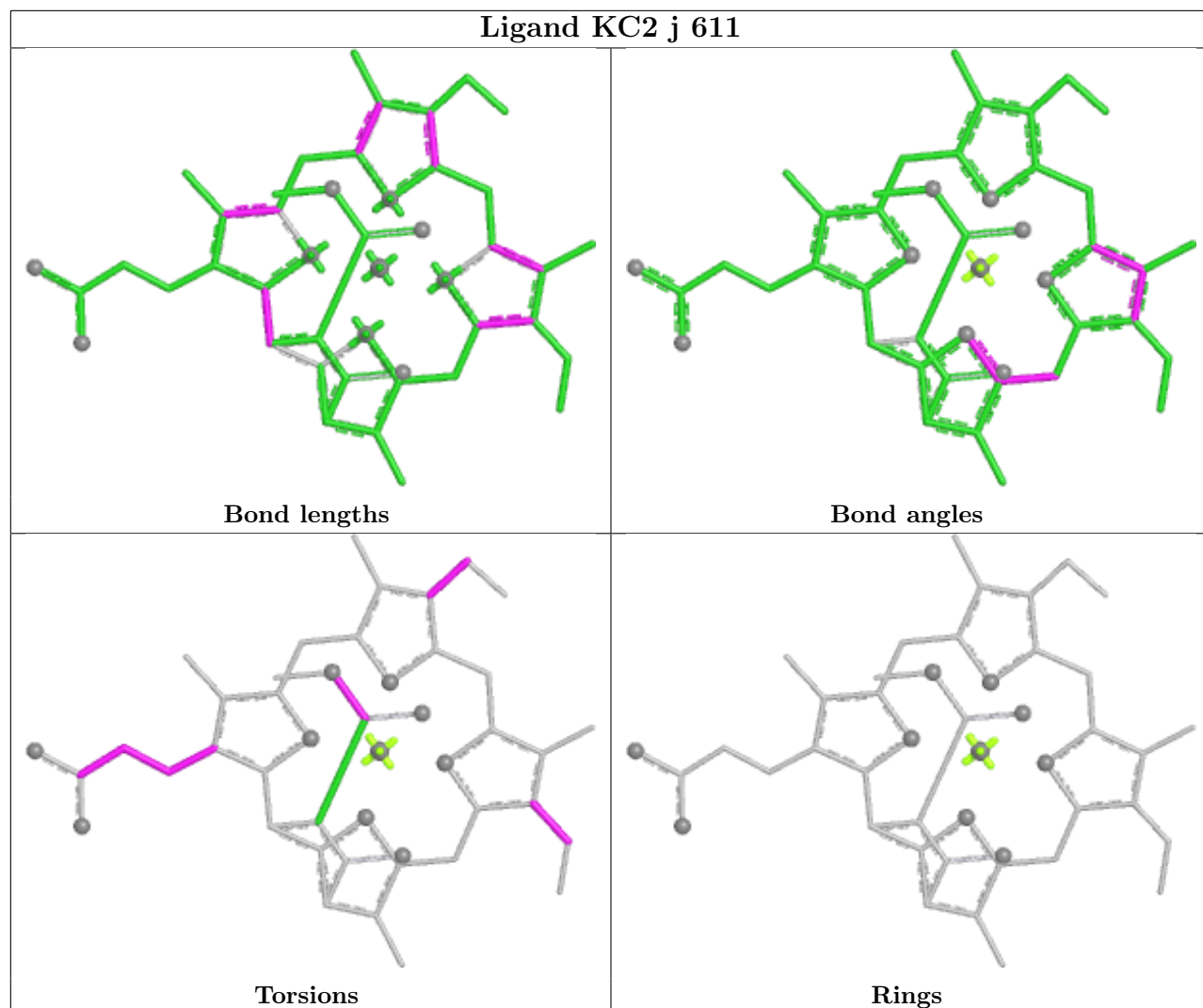


Ligand CLA B 803

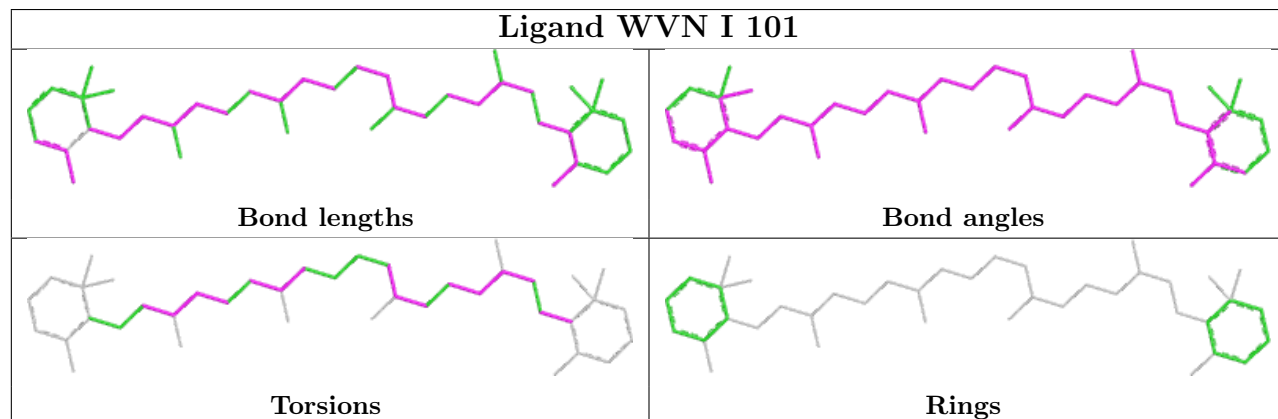


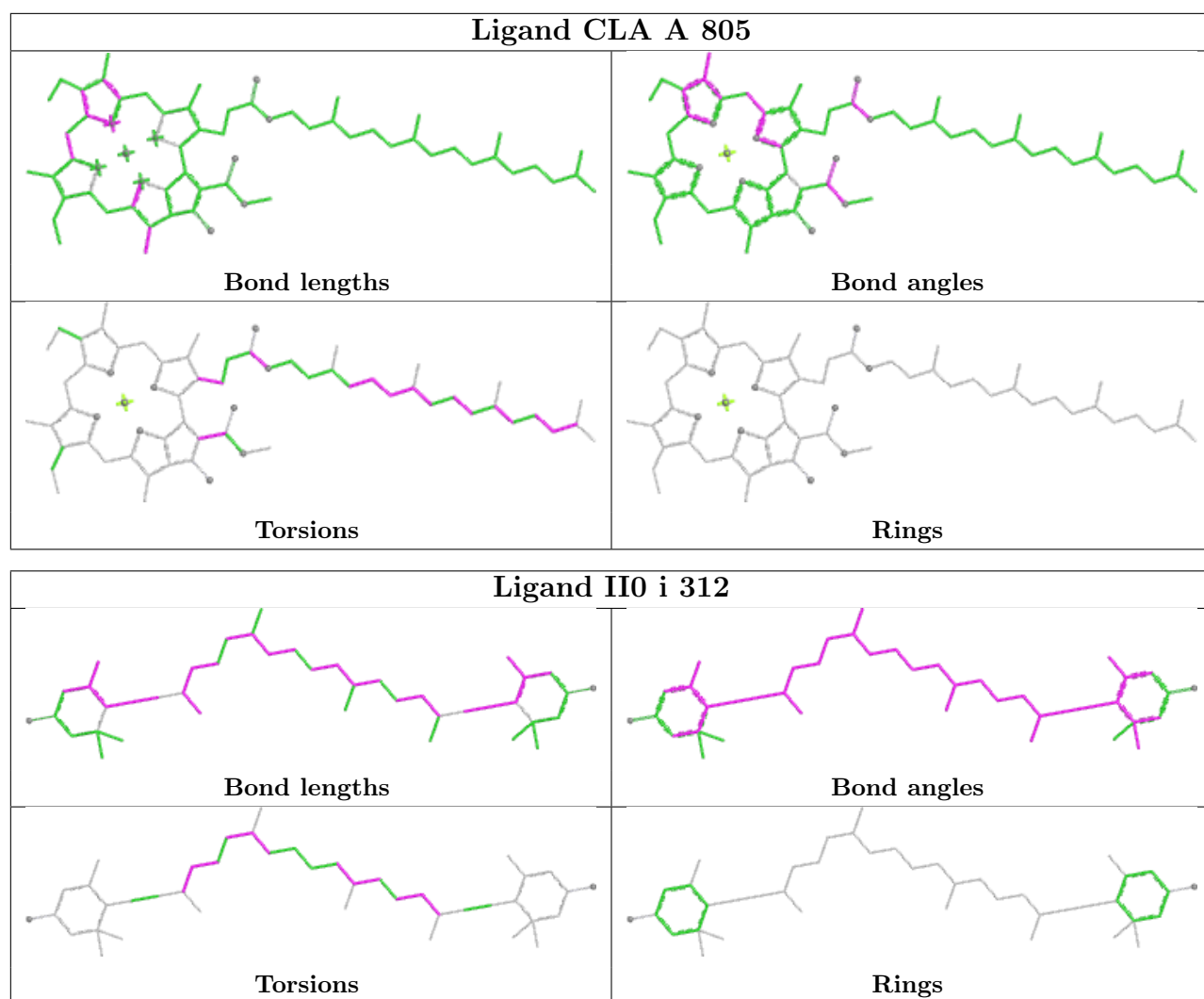


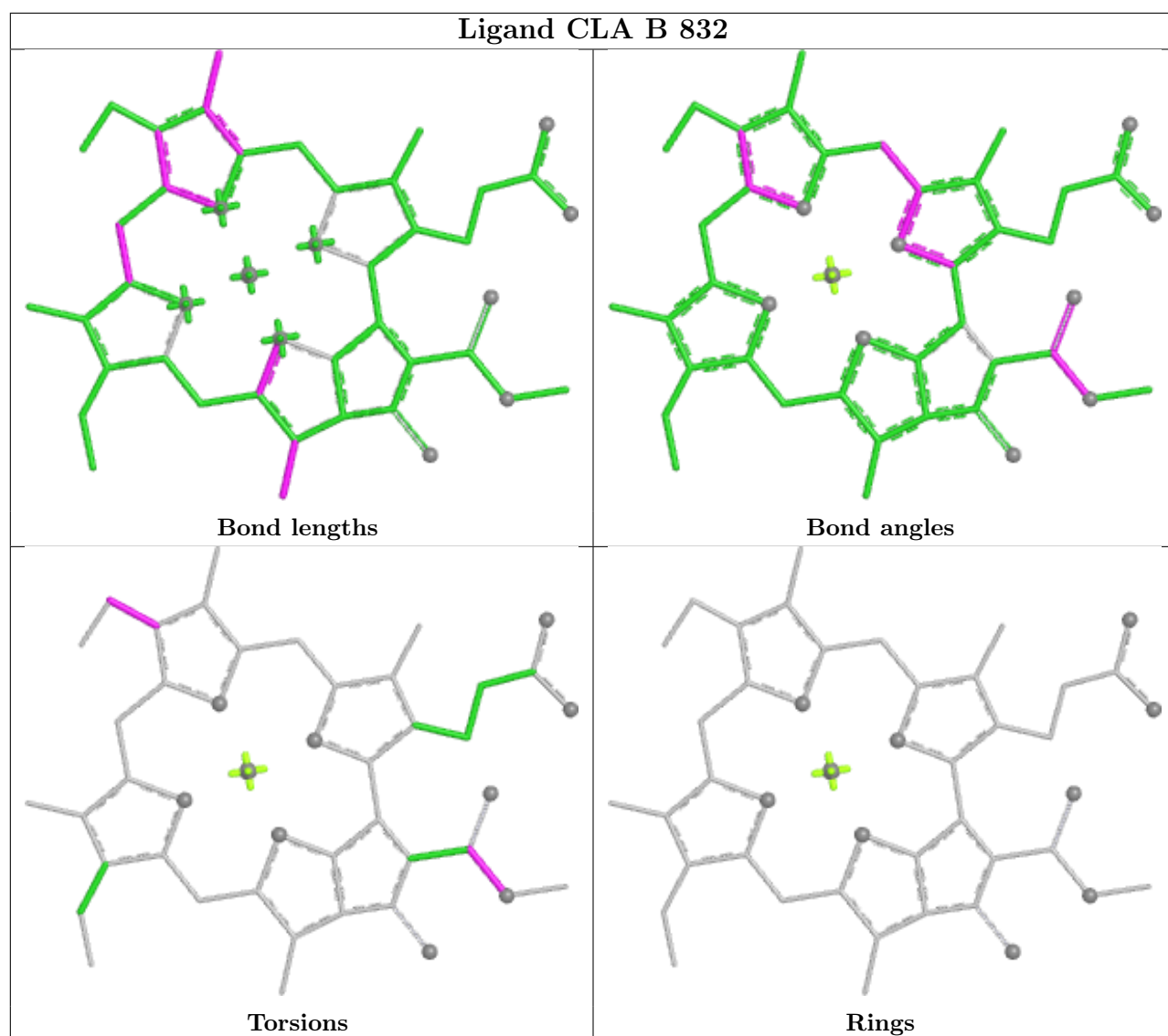
Ligand KC2 j 611

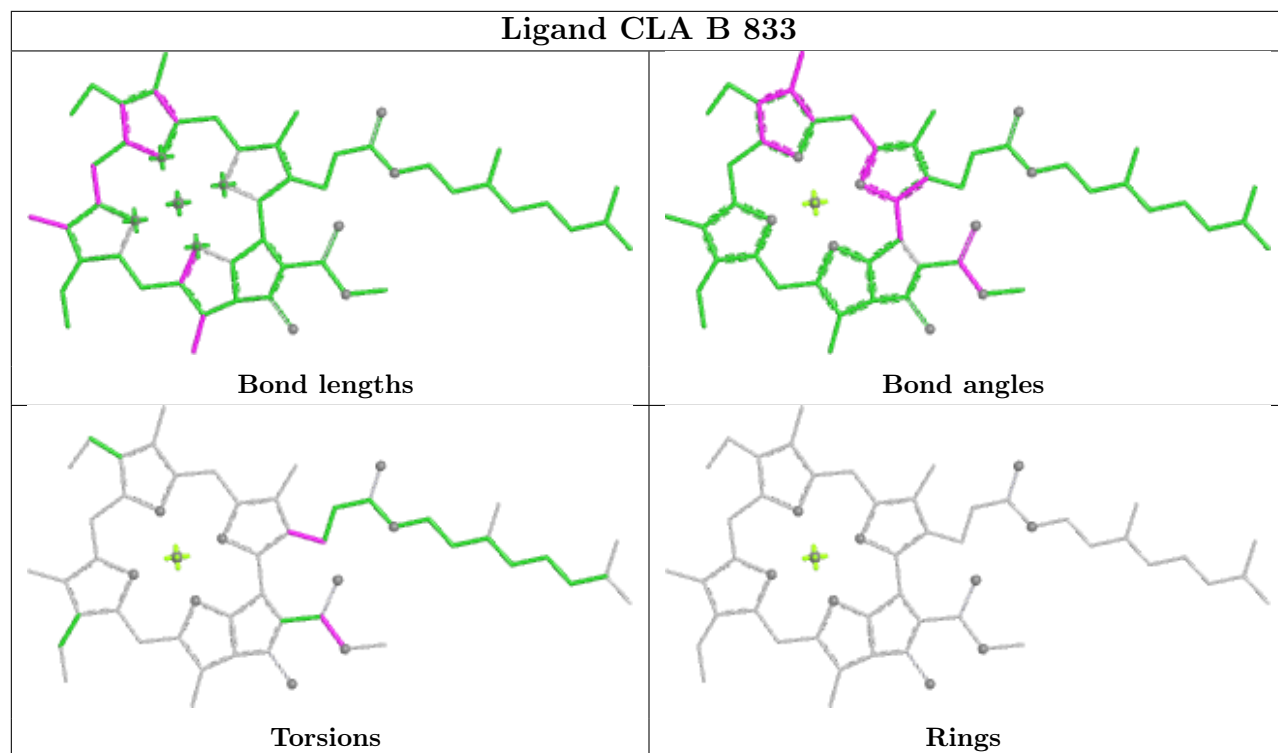


Ligand WVN I 101

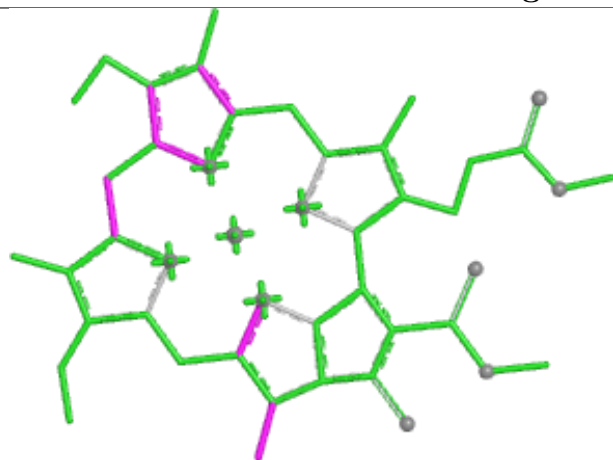




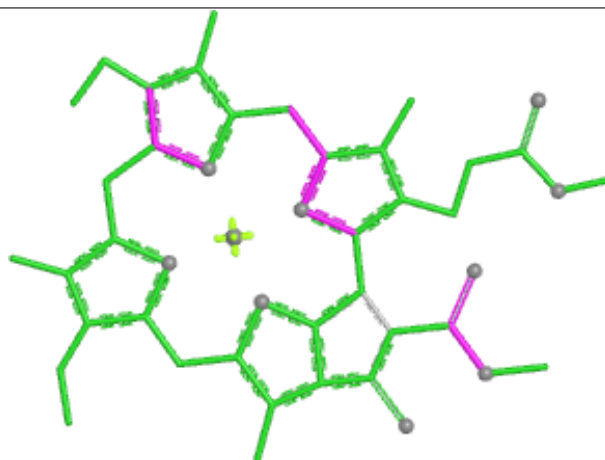




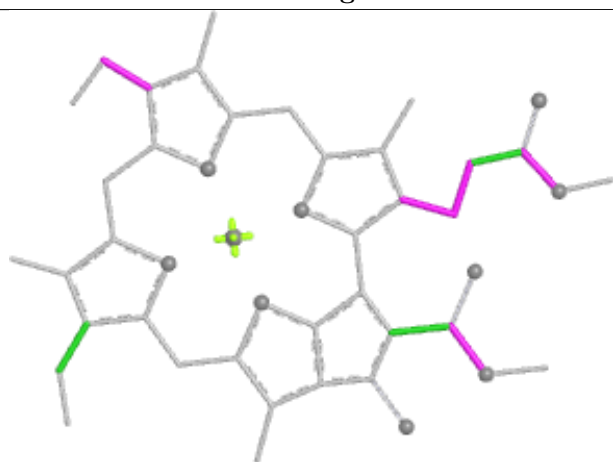
Ligand CLA i 308



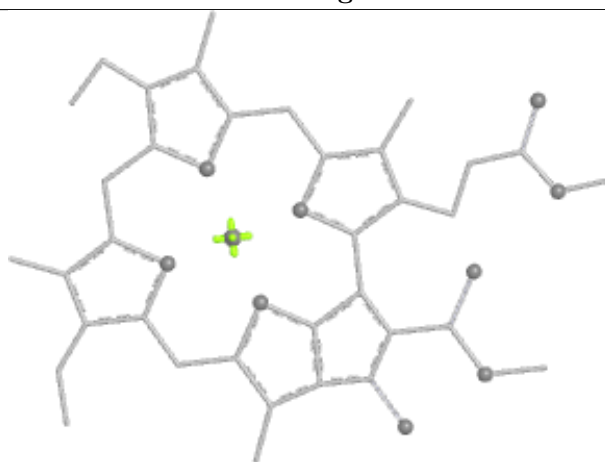
Bond lengths



Bond angles

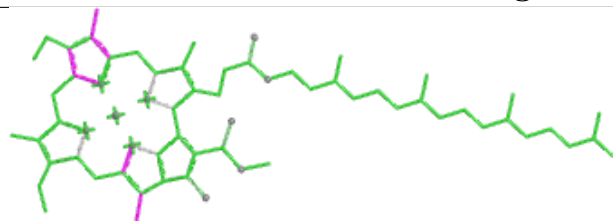


Torsions

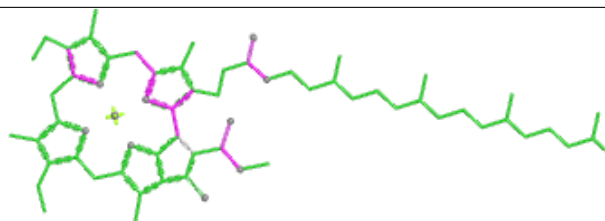


Rings

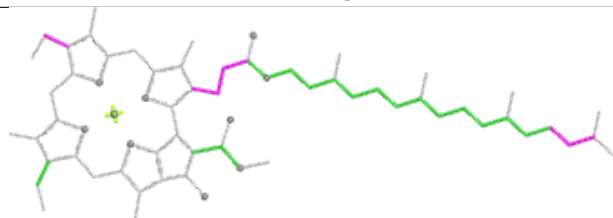
Ligand CLA A 808



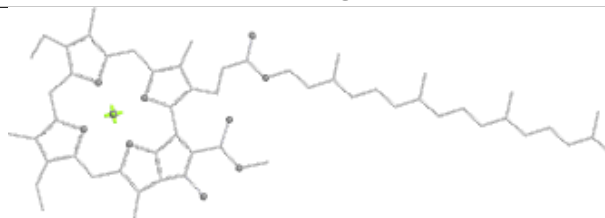
Bond lengths



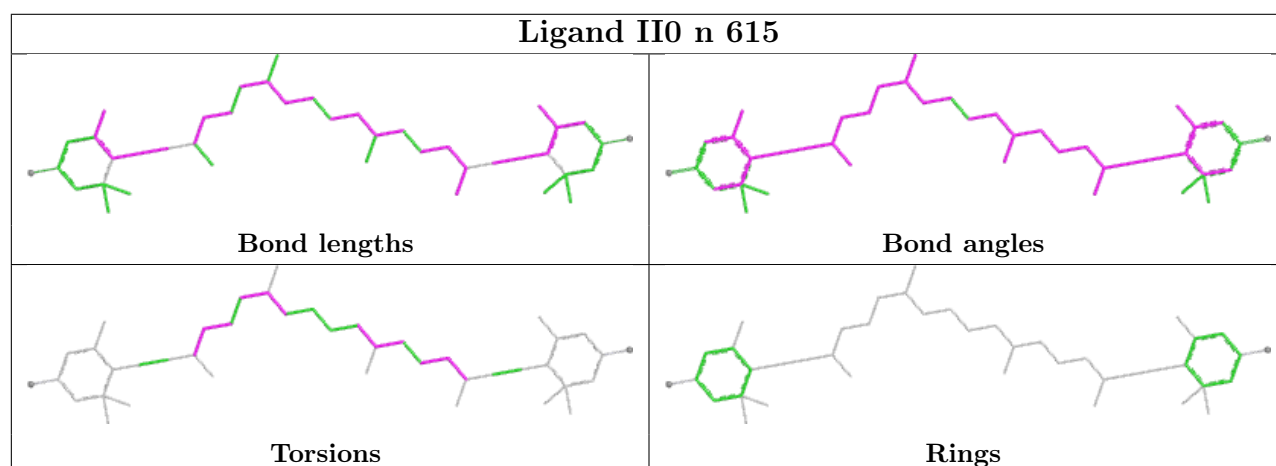
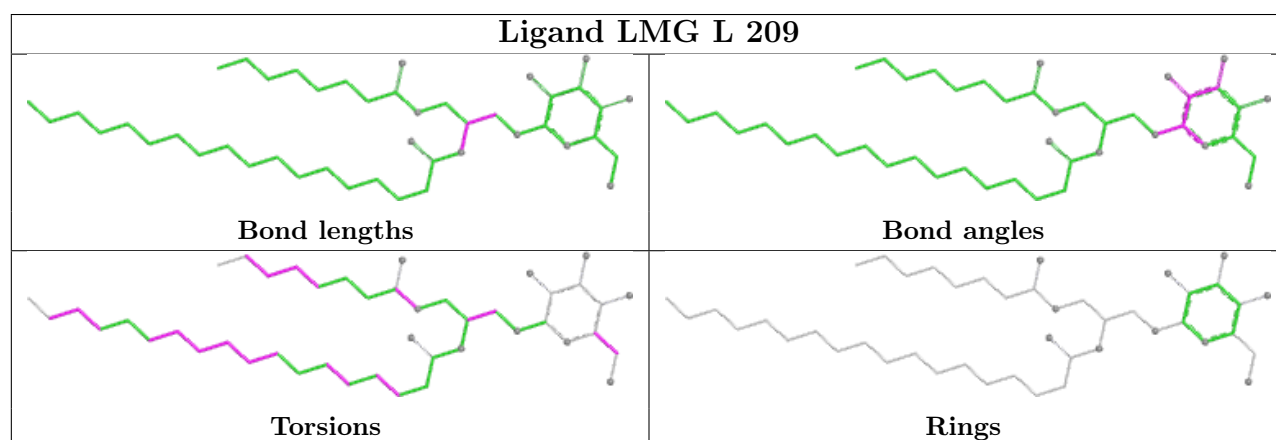
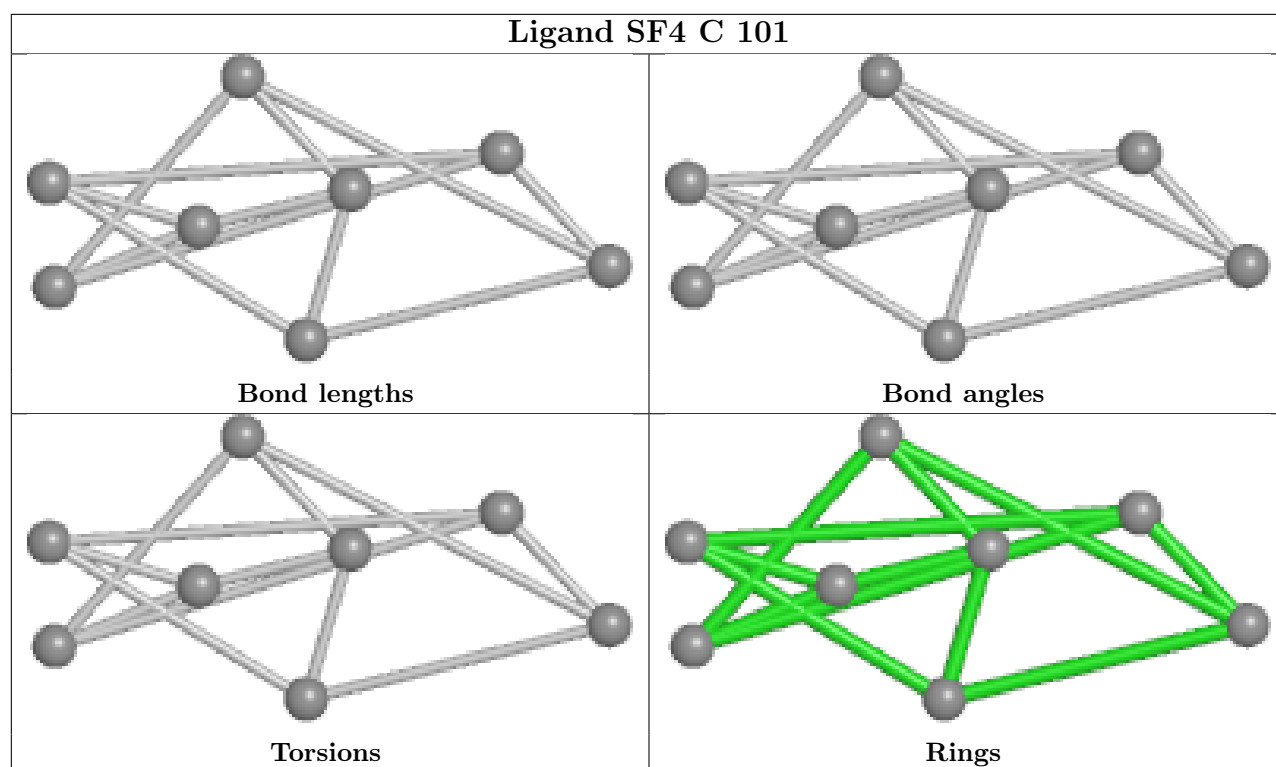
Bond angles

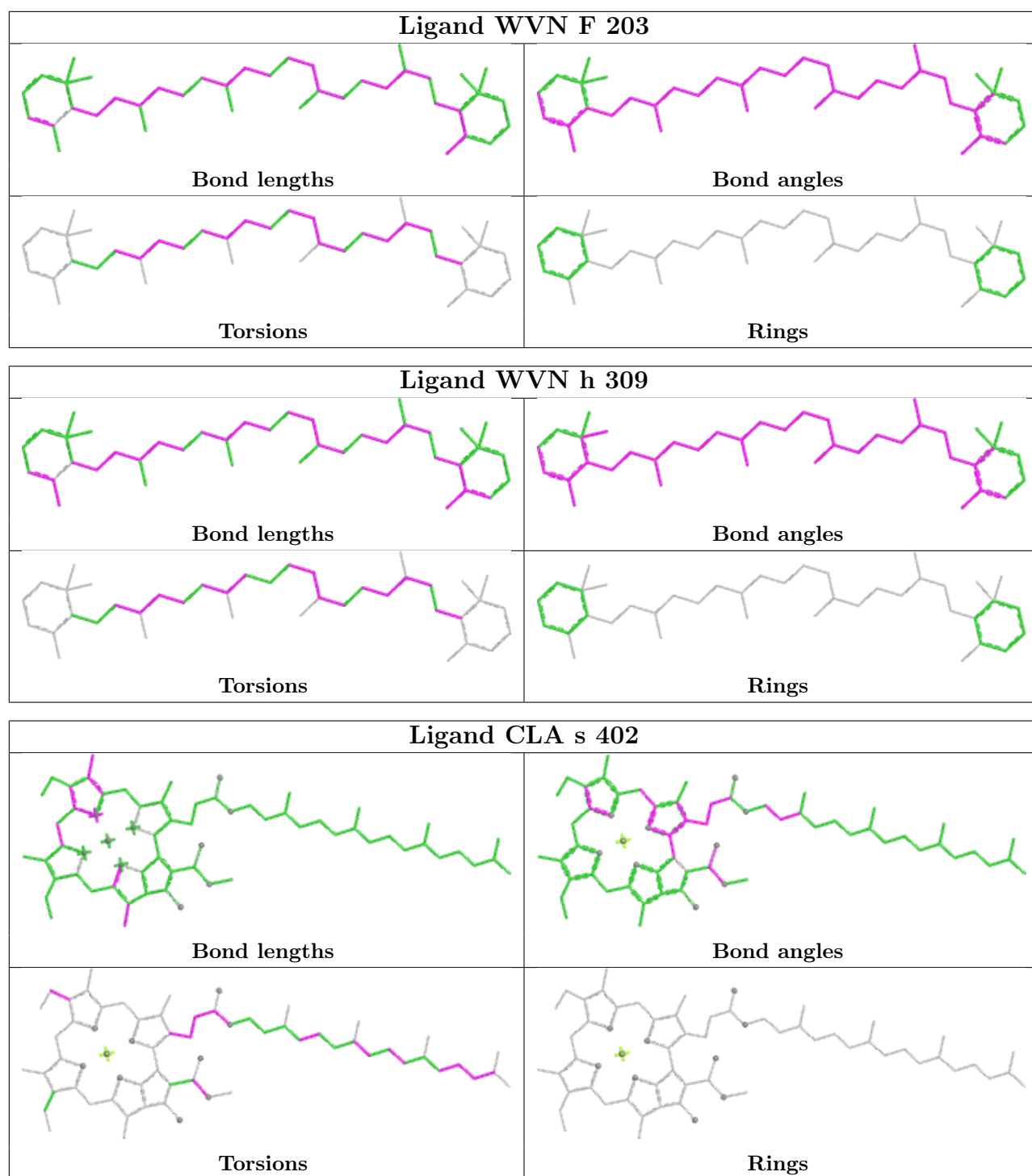


Torsions

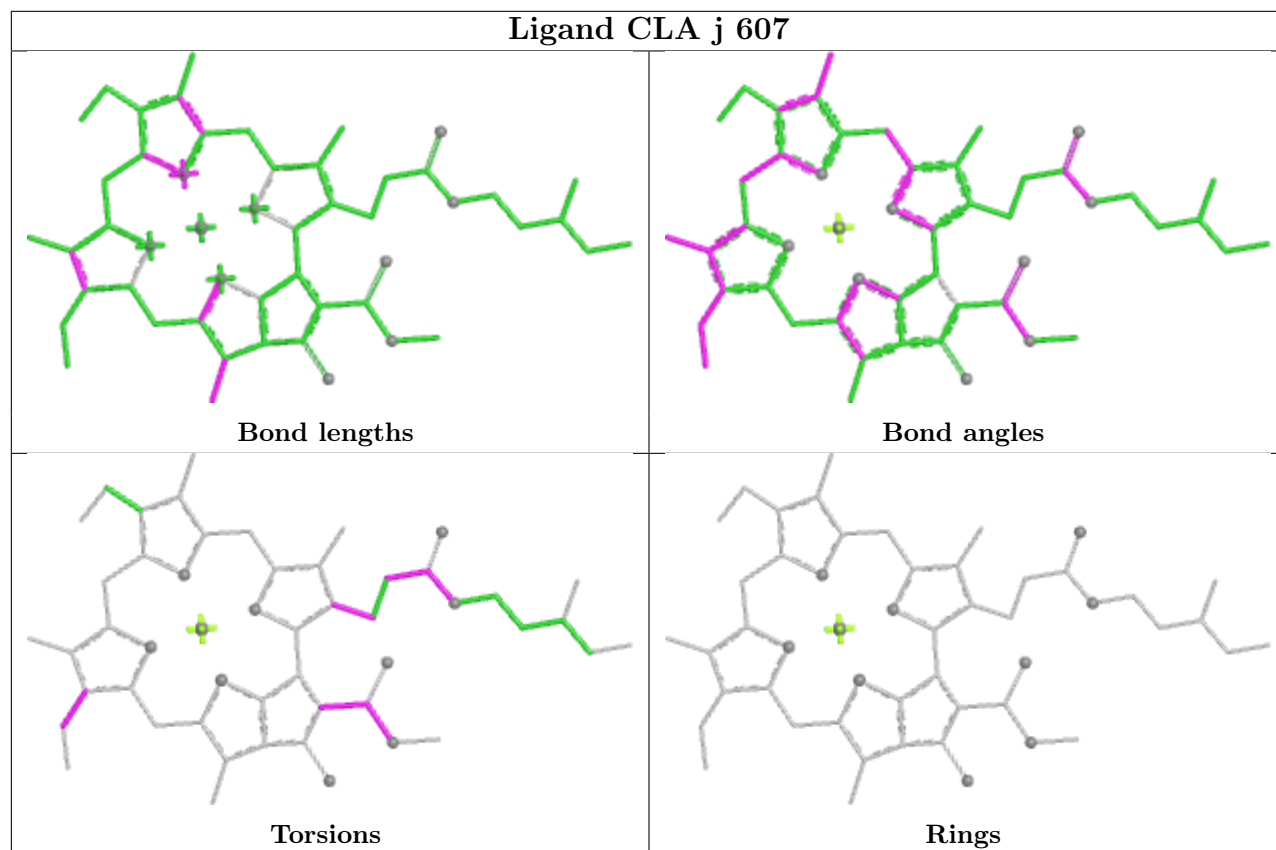


Rings

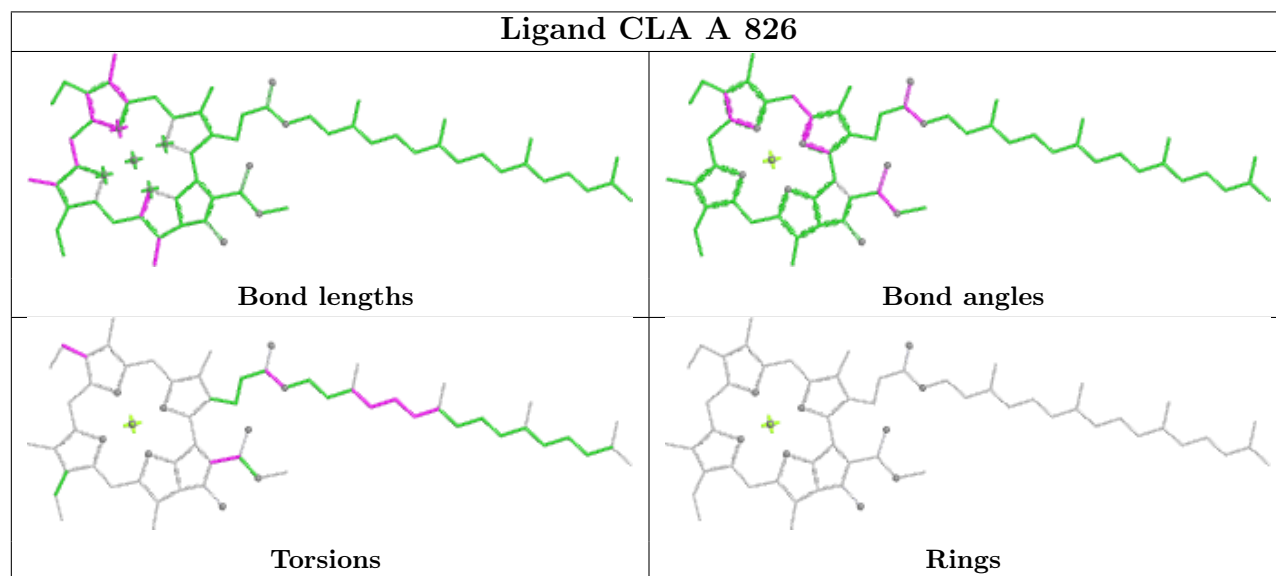


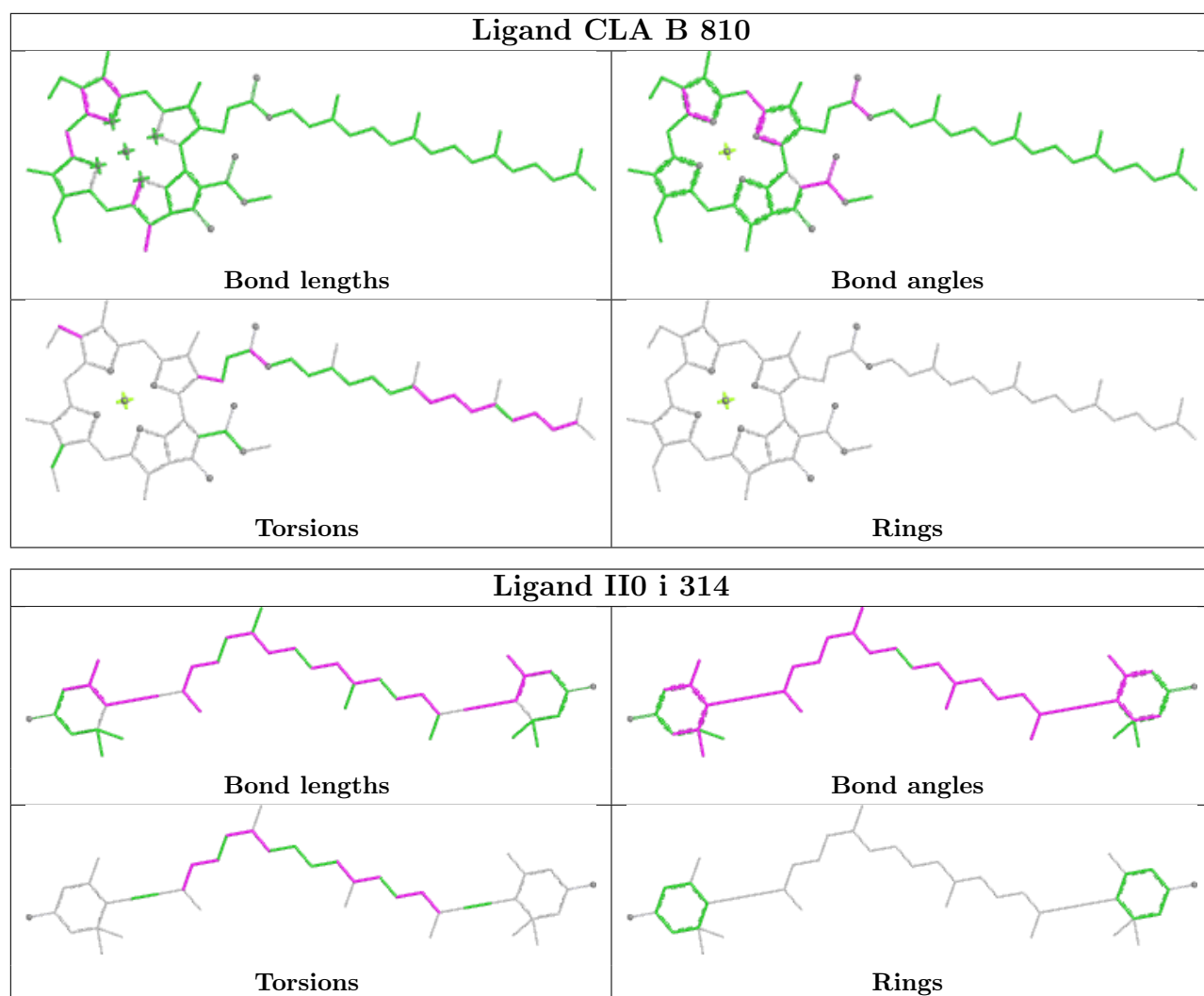


Ligand CLA j 607

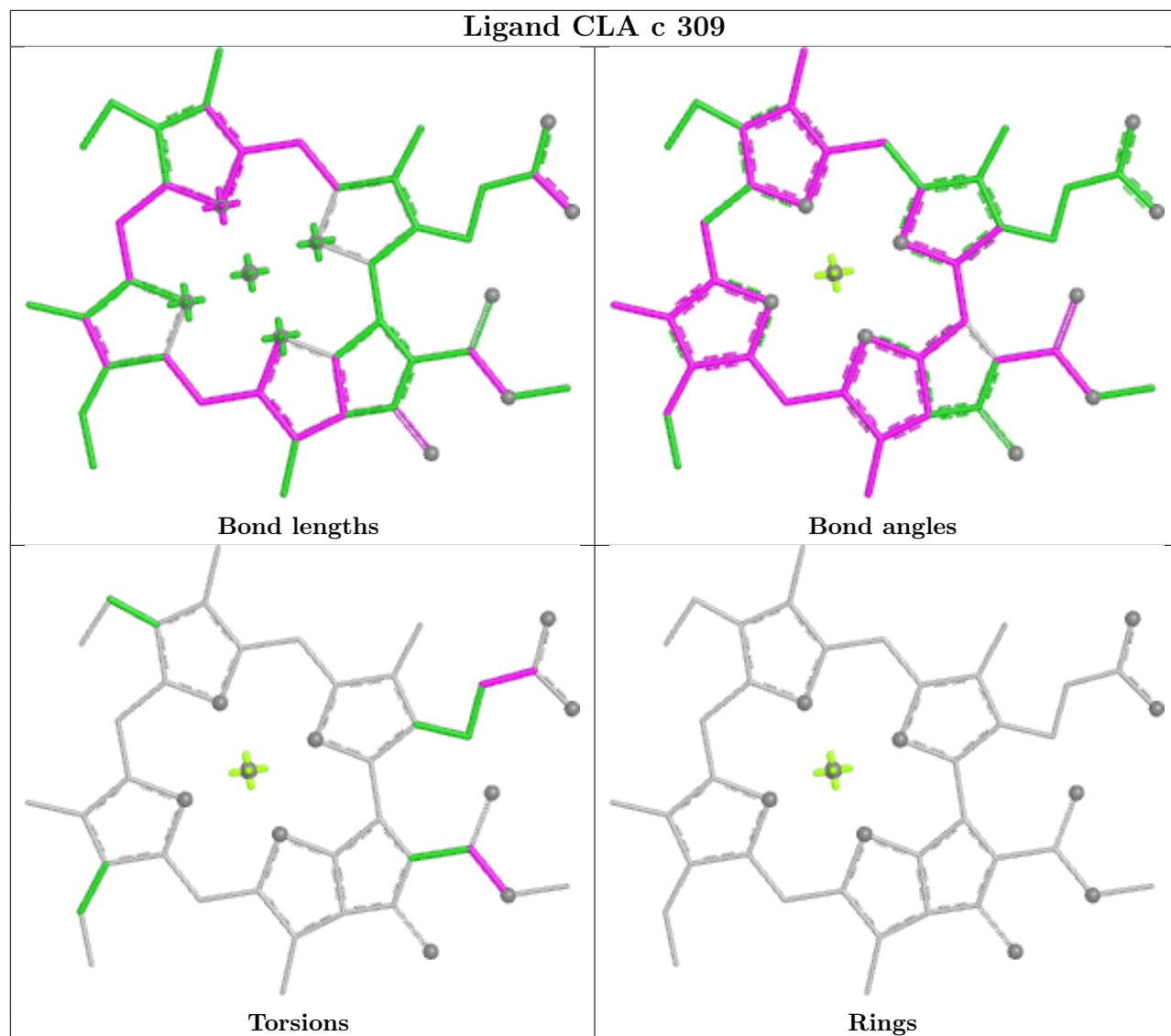


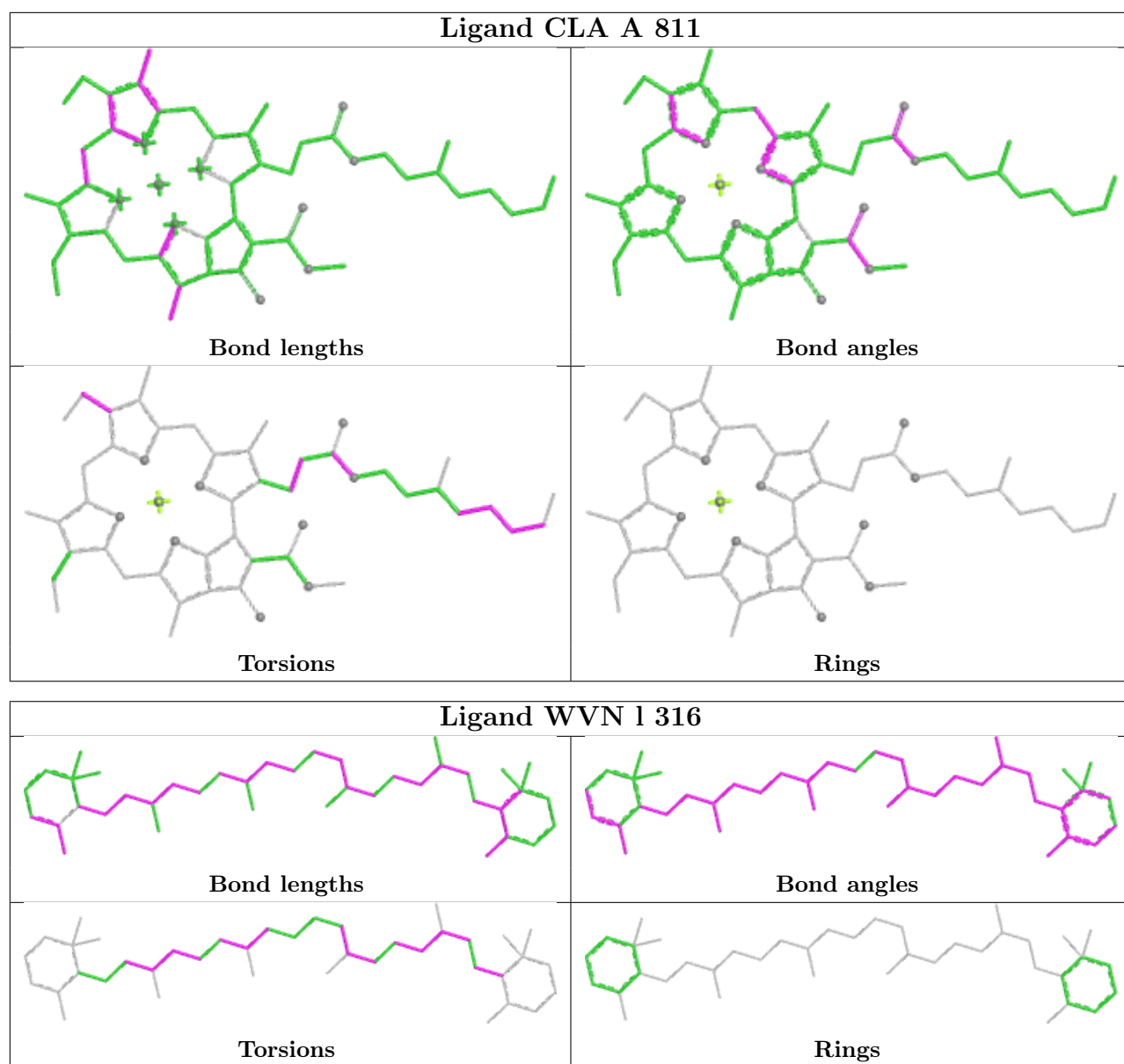
Ligand CLA A 826

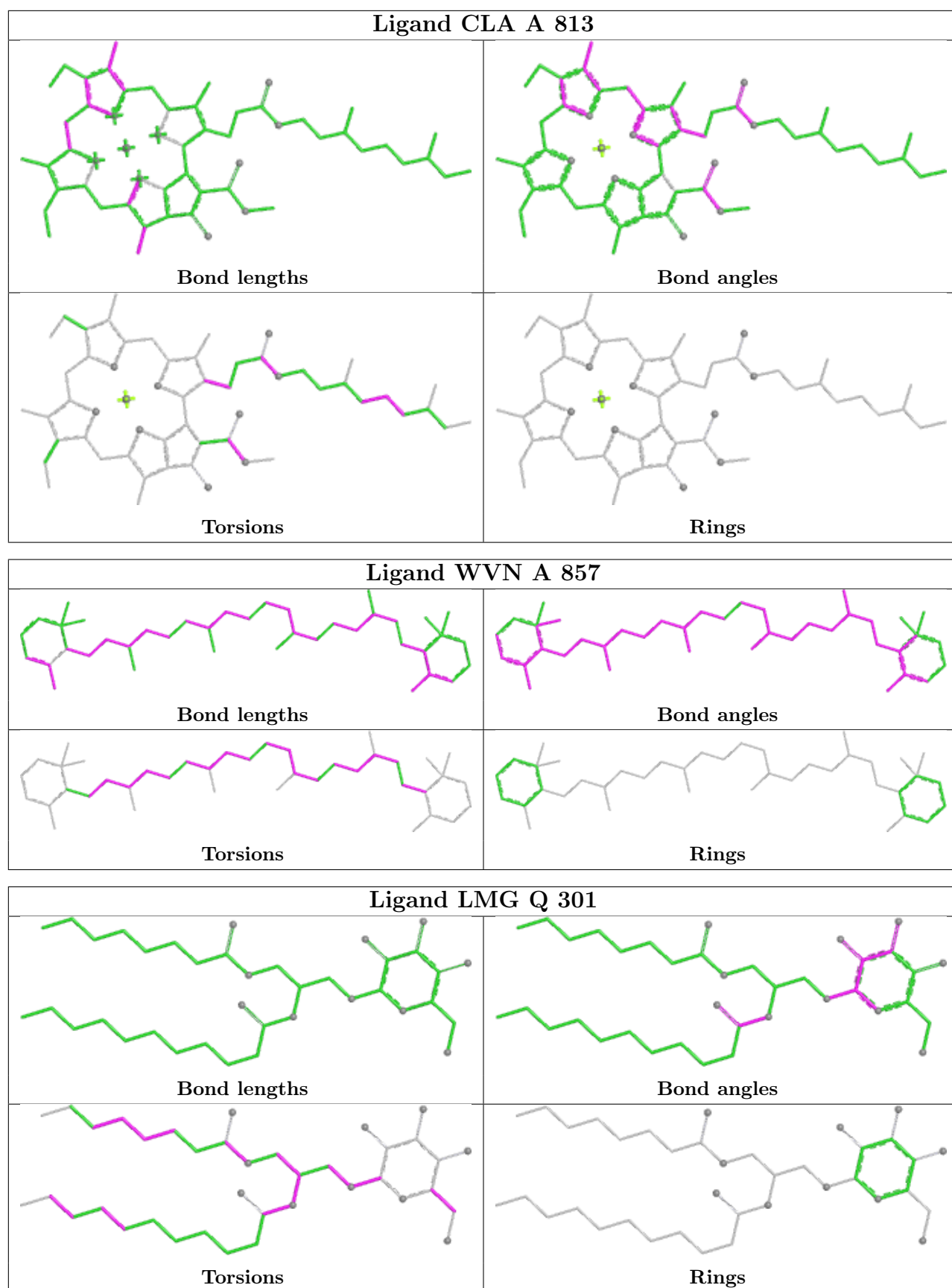


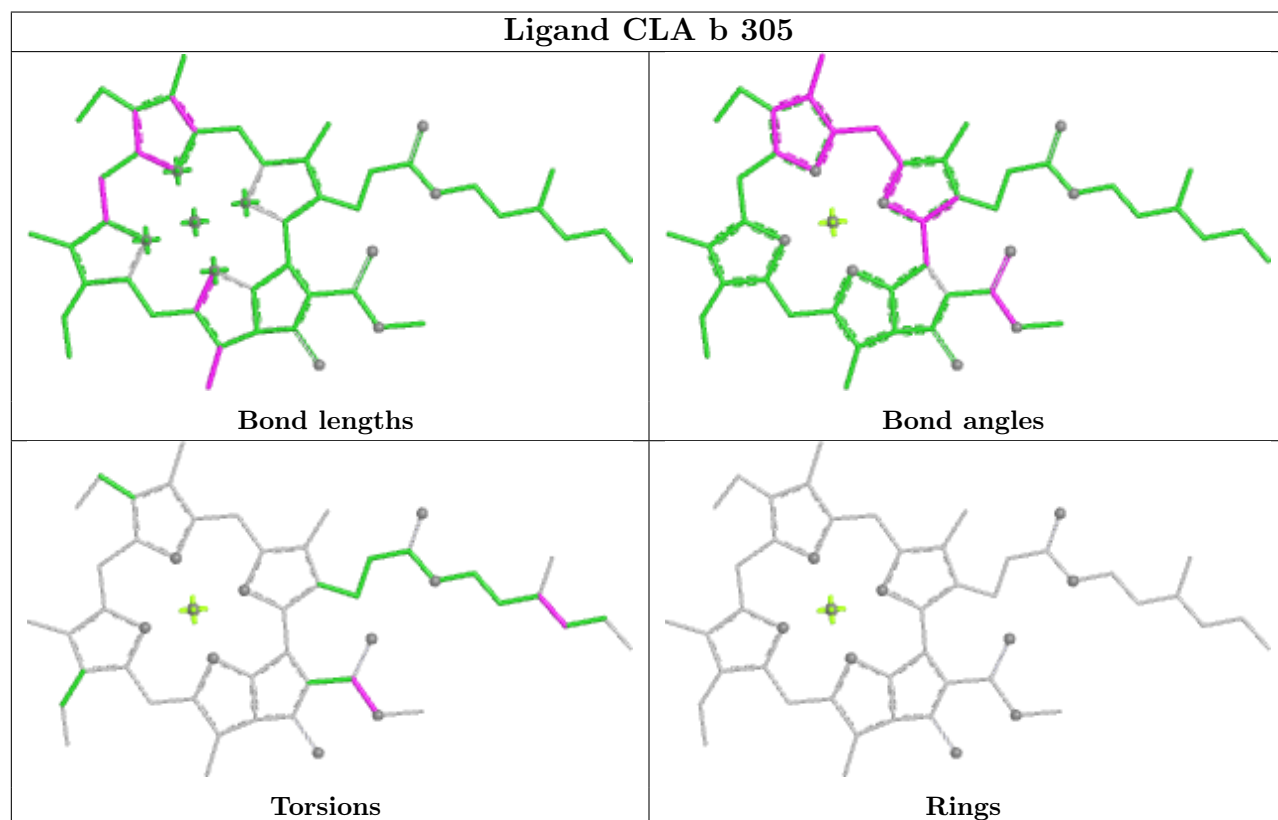
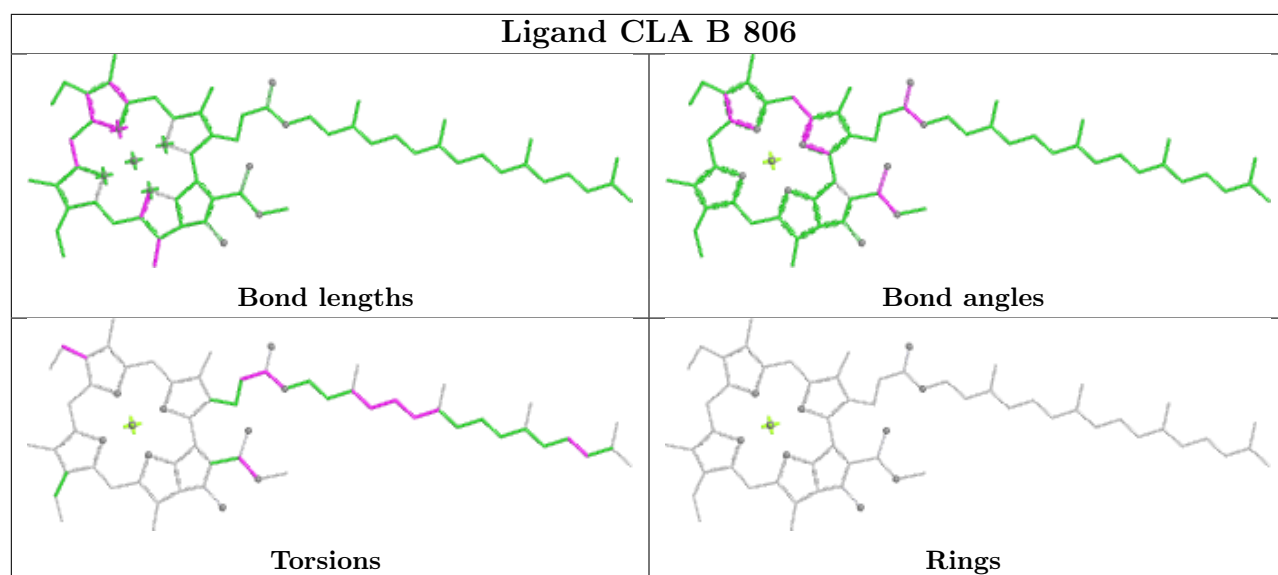


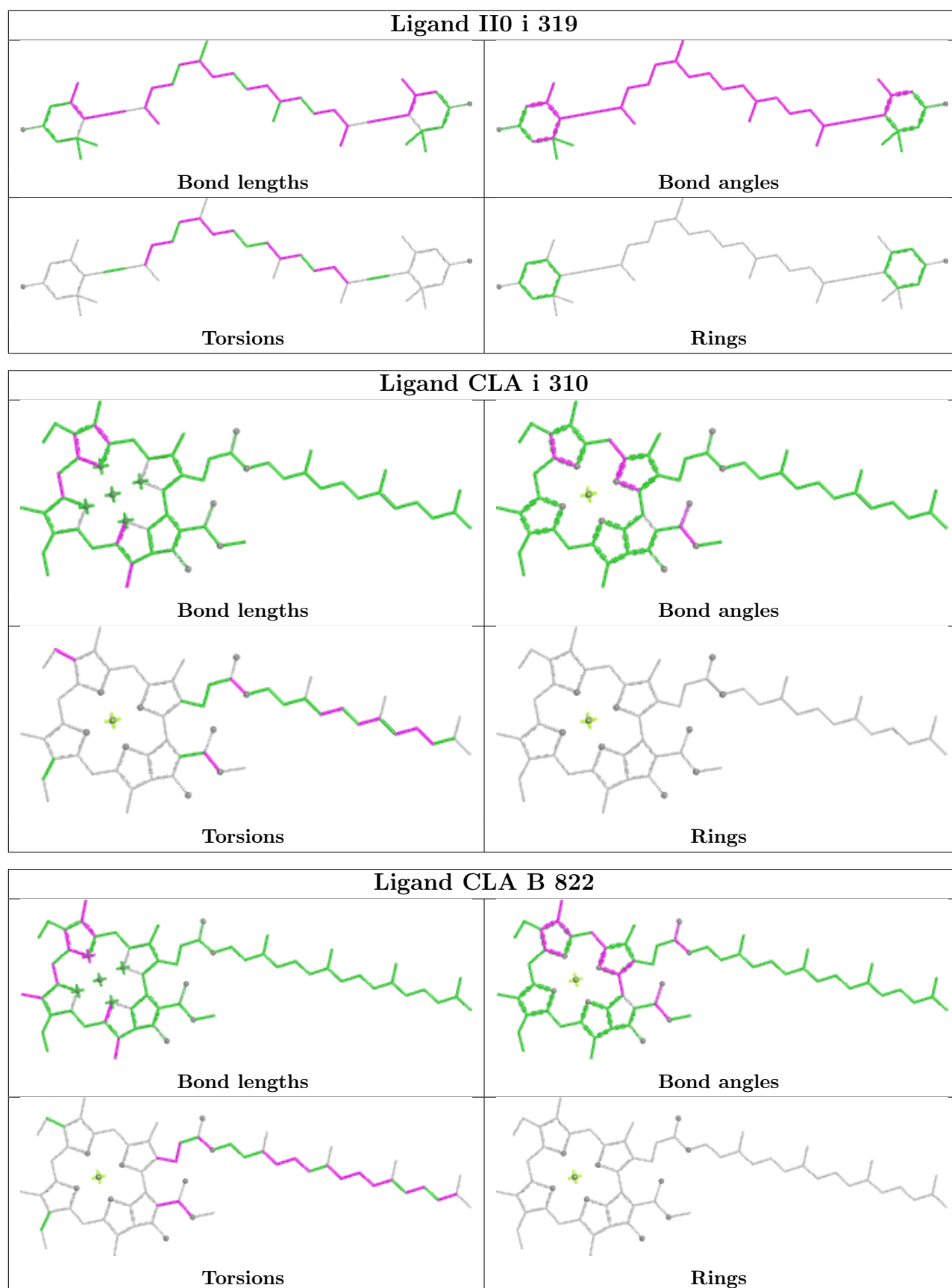
Ligand CLA c 309



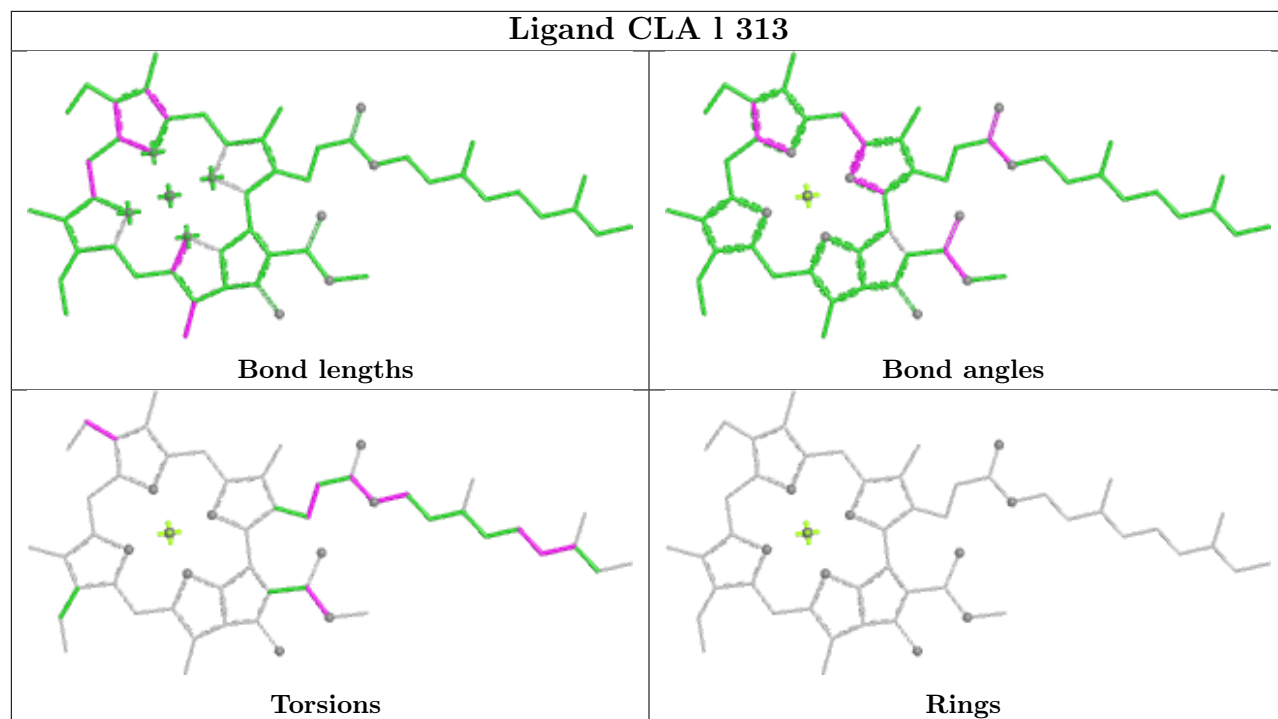




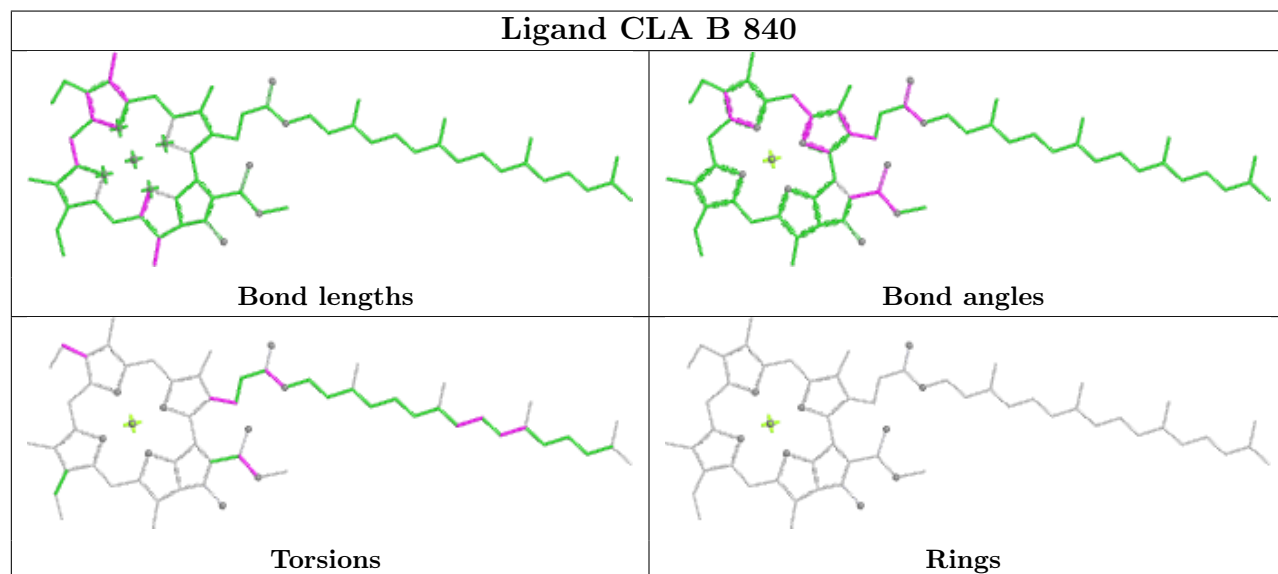




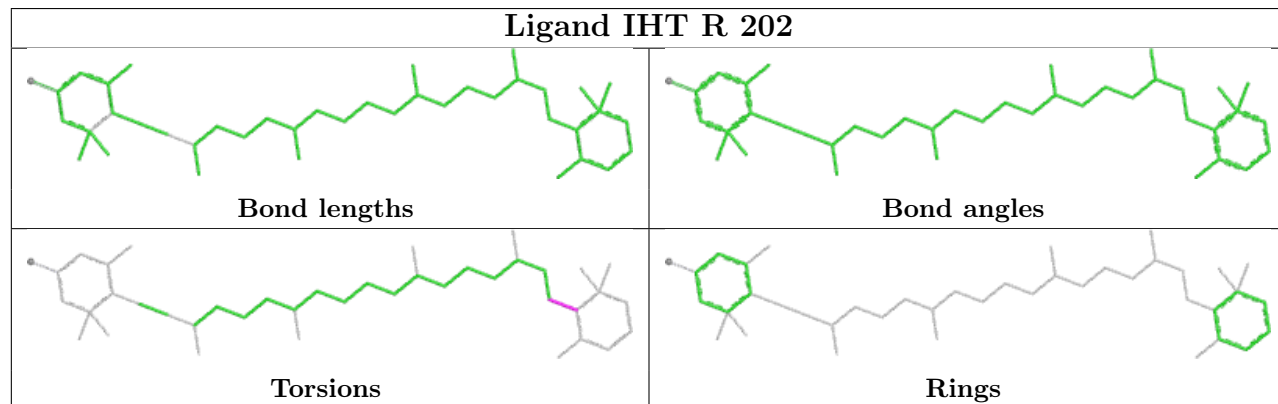
Ligand CLA I 313

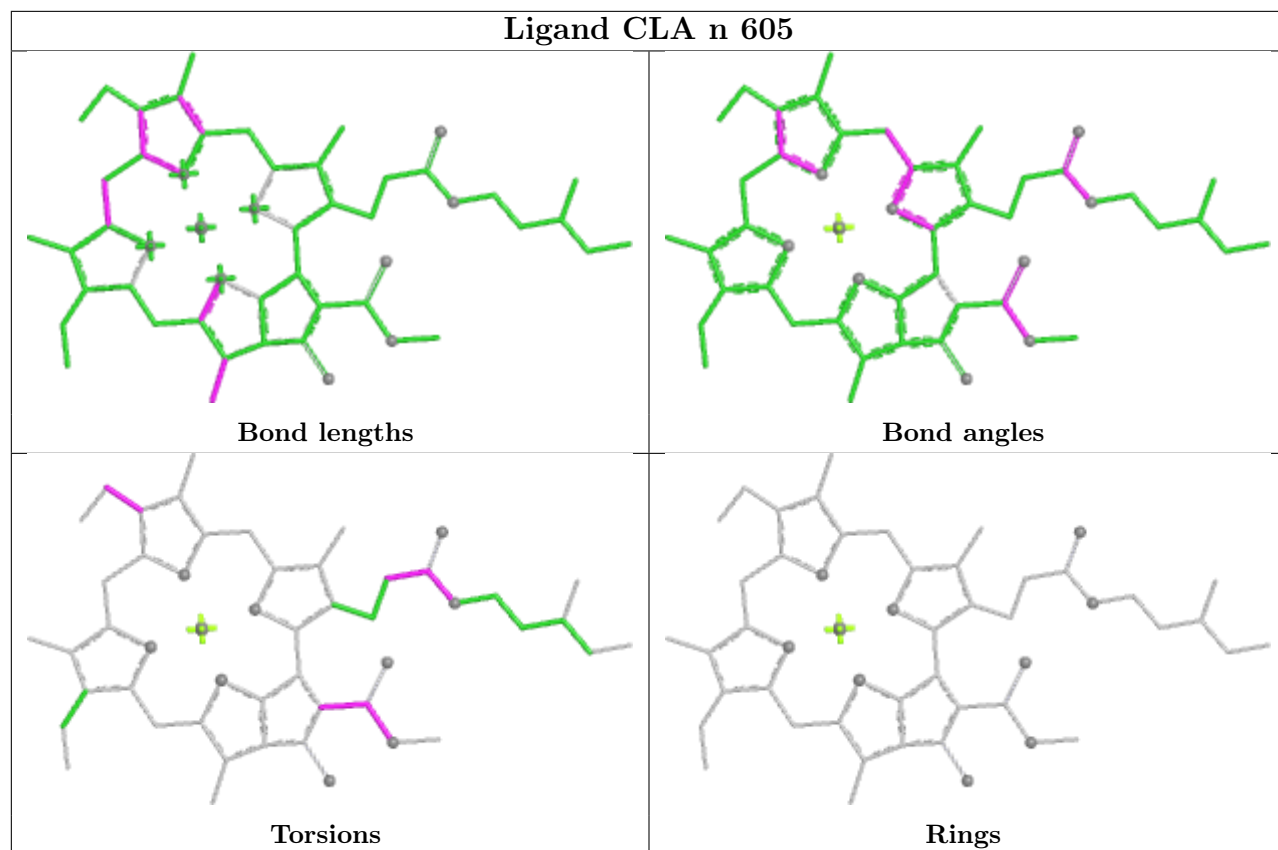


Ligand CLA B 840

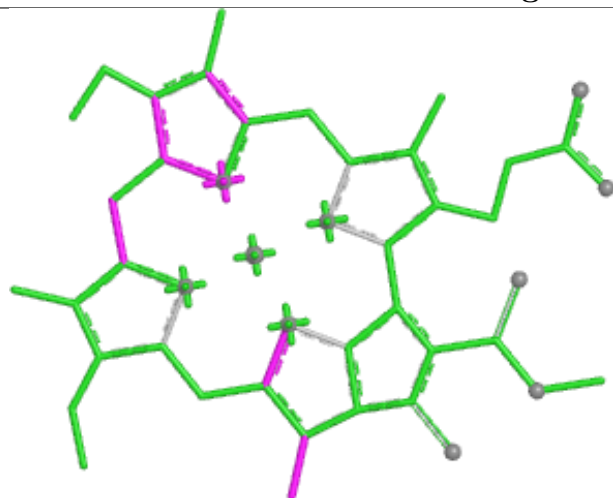


Ligand IHT R 202

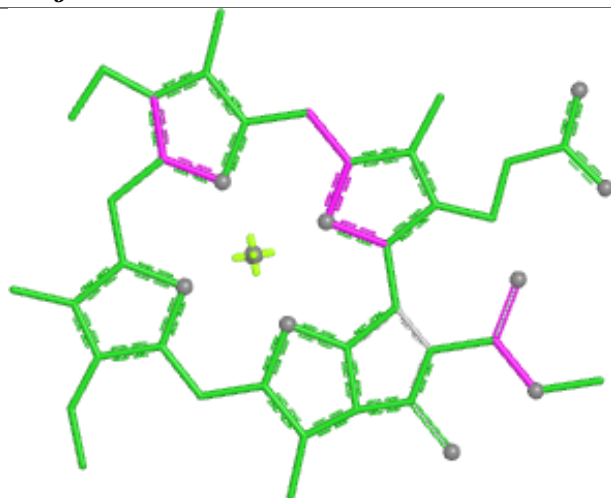




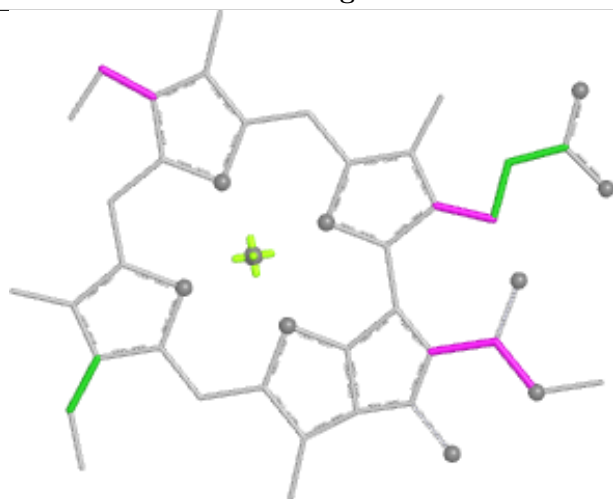
Ligand CLA j 608



Bond lengths



Bond angles

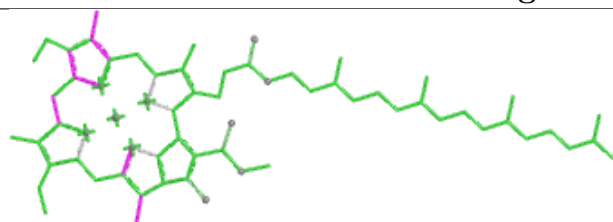


Torsions

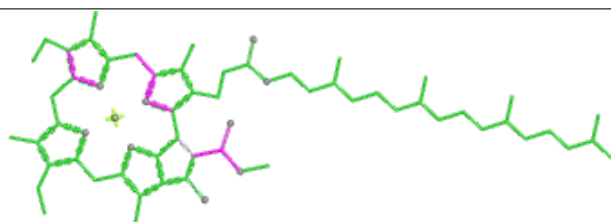


Rings

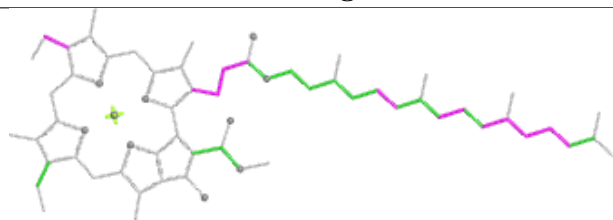
Ligand CLA a 306



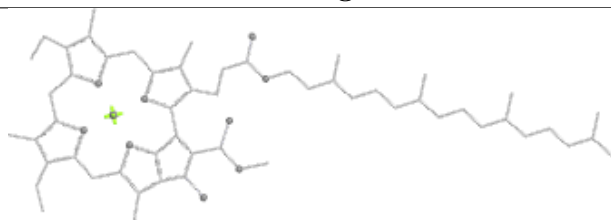
Bond lengths



Bond angles

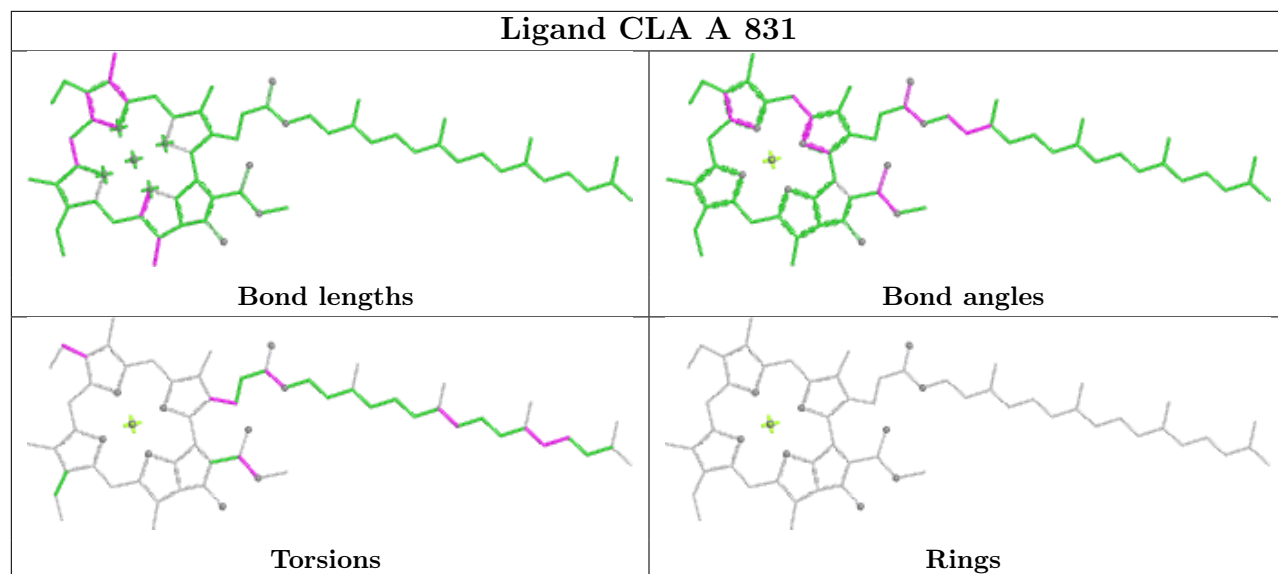


Torsions

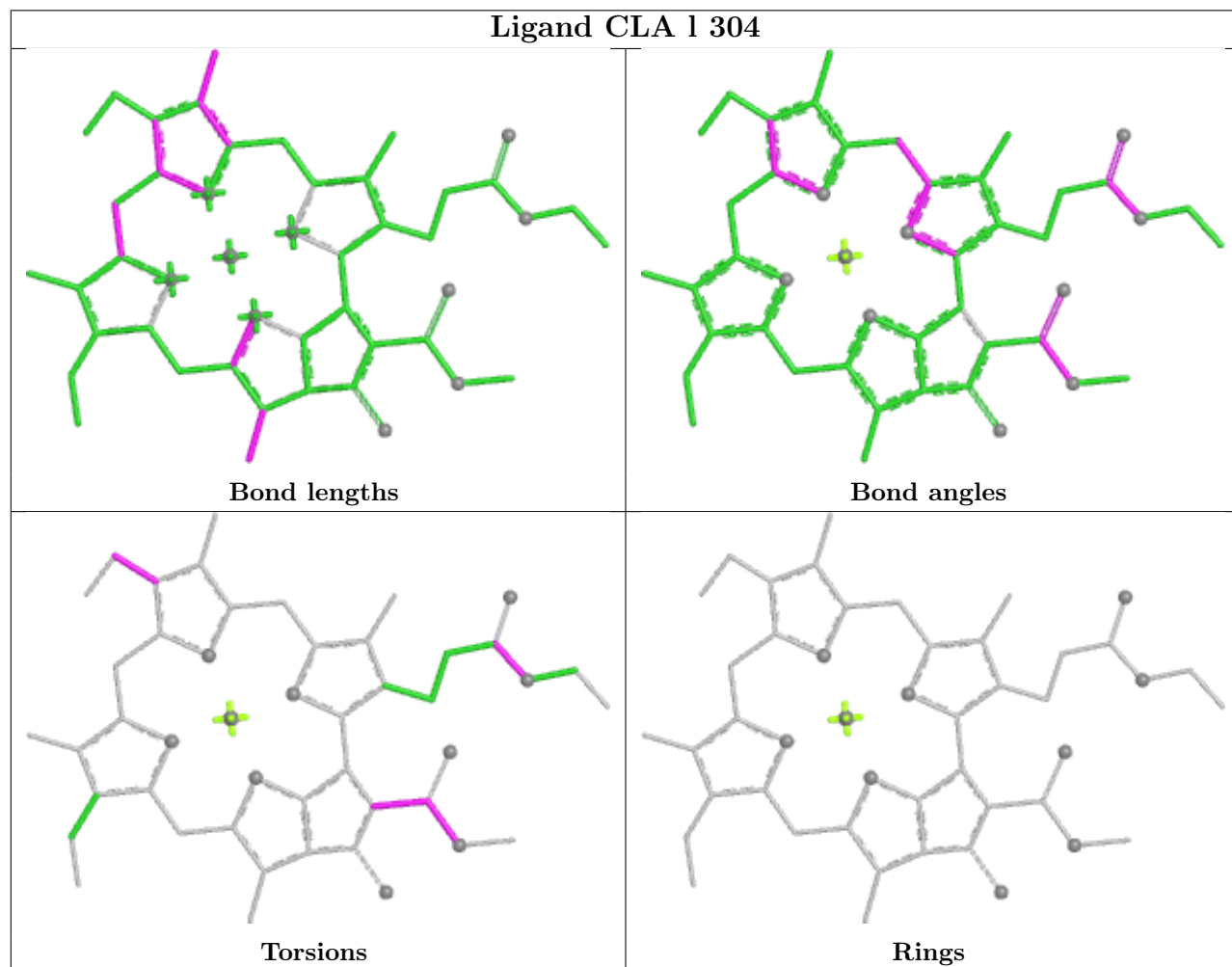


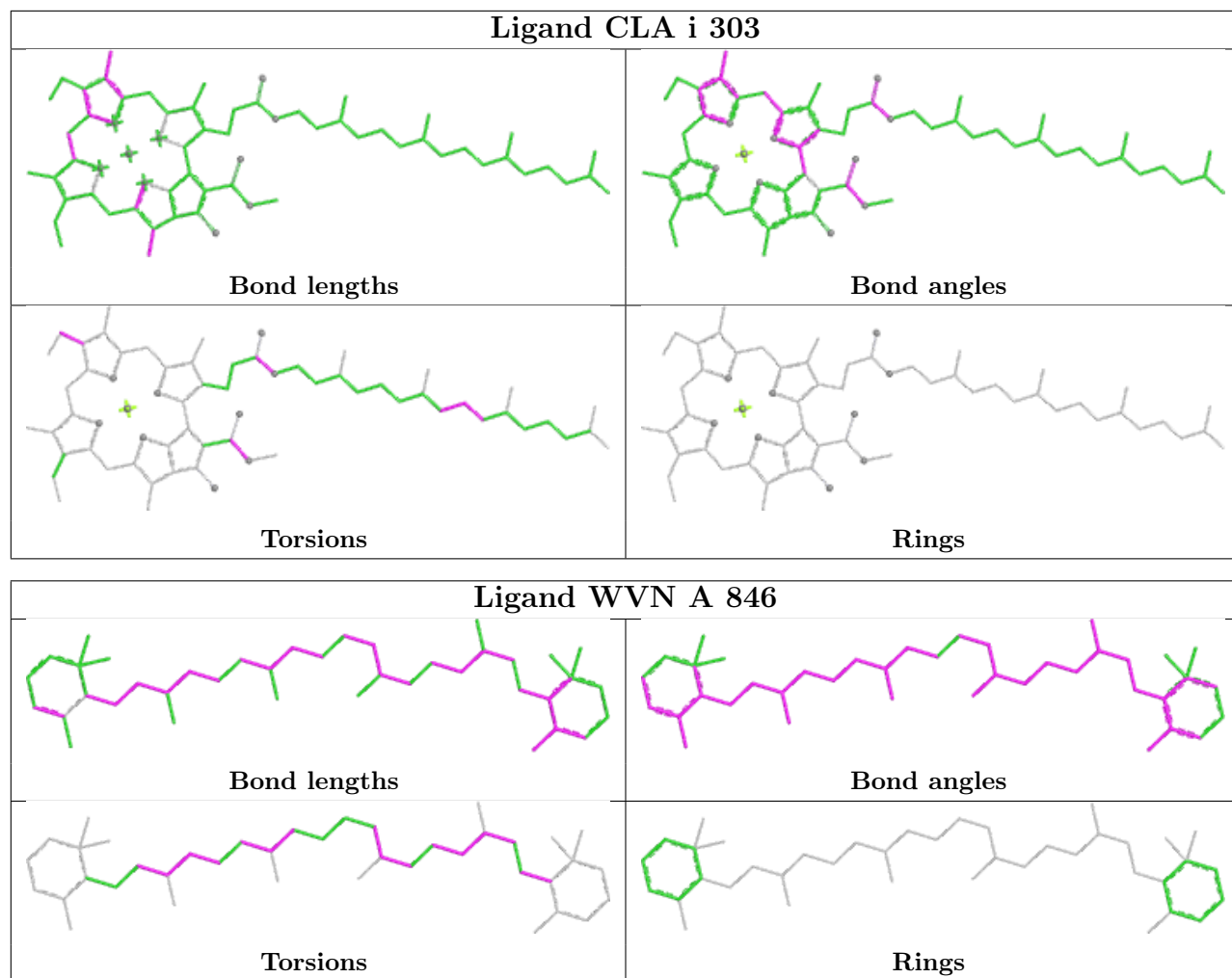
Rings

Ligand CLA A 831

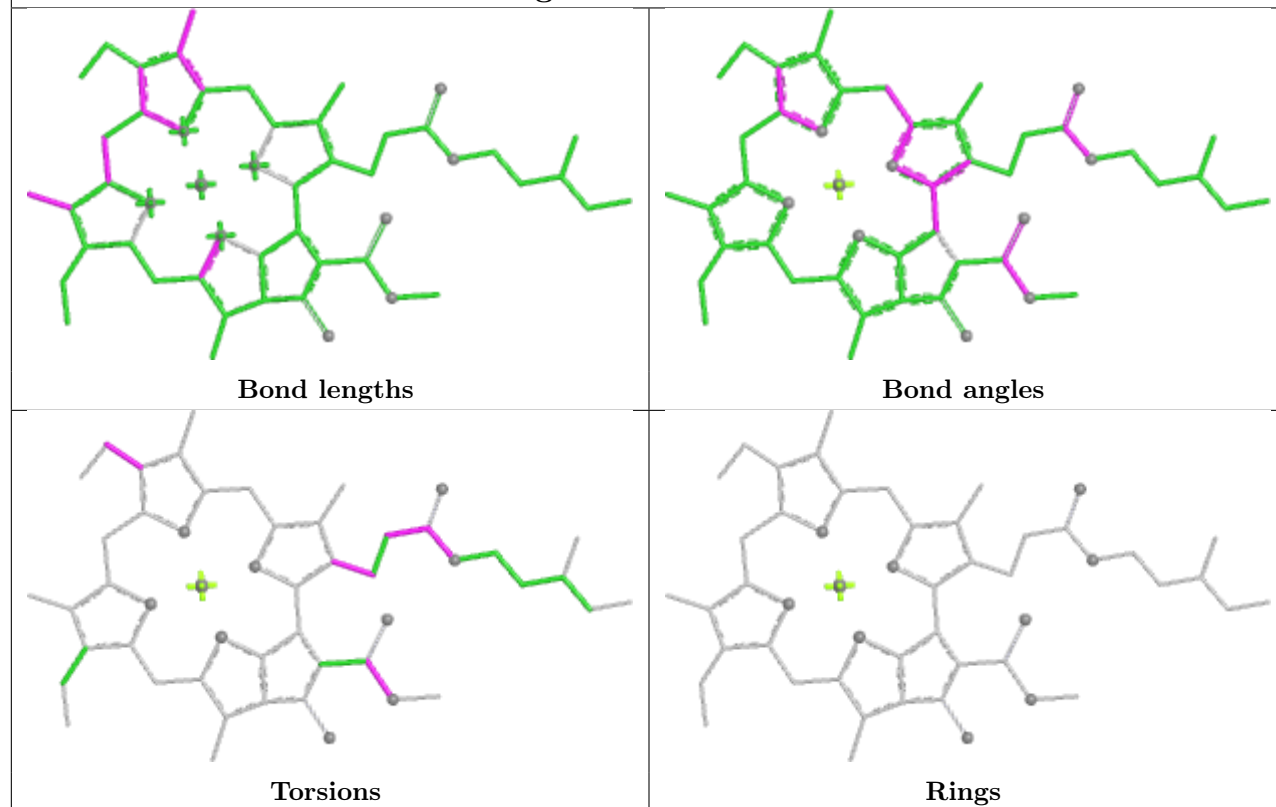


Ligand CLA I 304

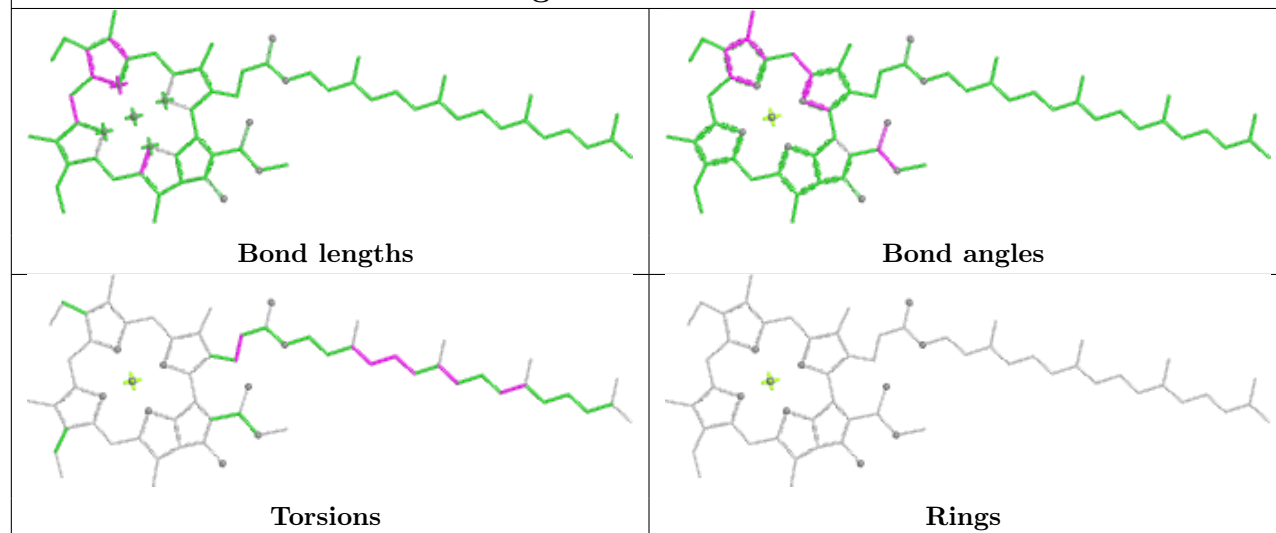




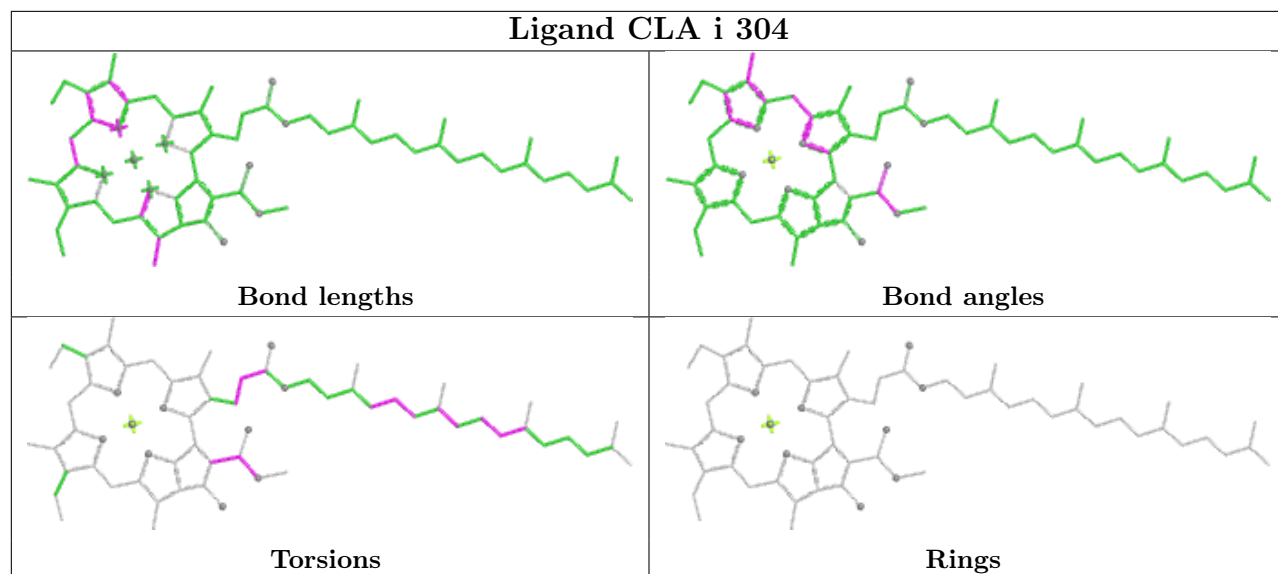
Ligand CLA h 308



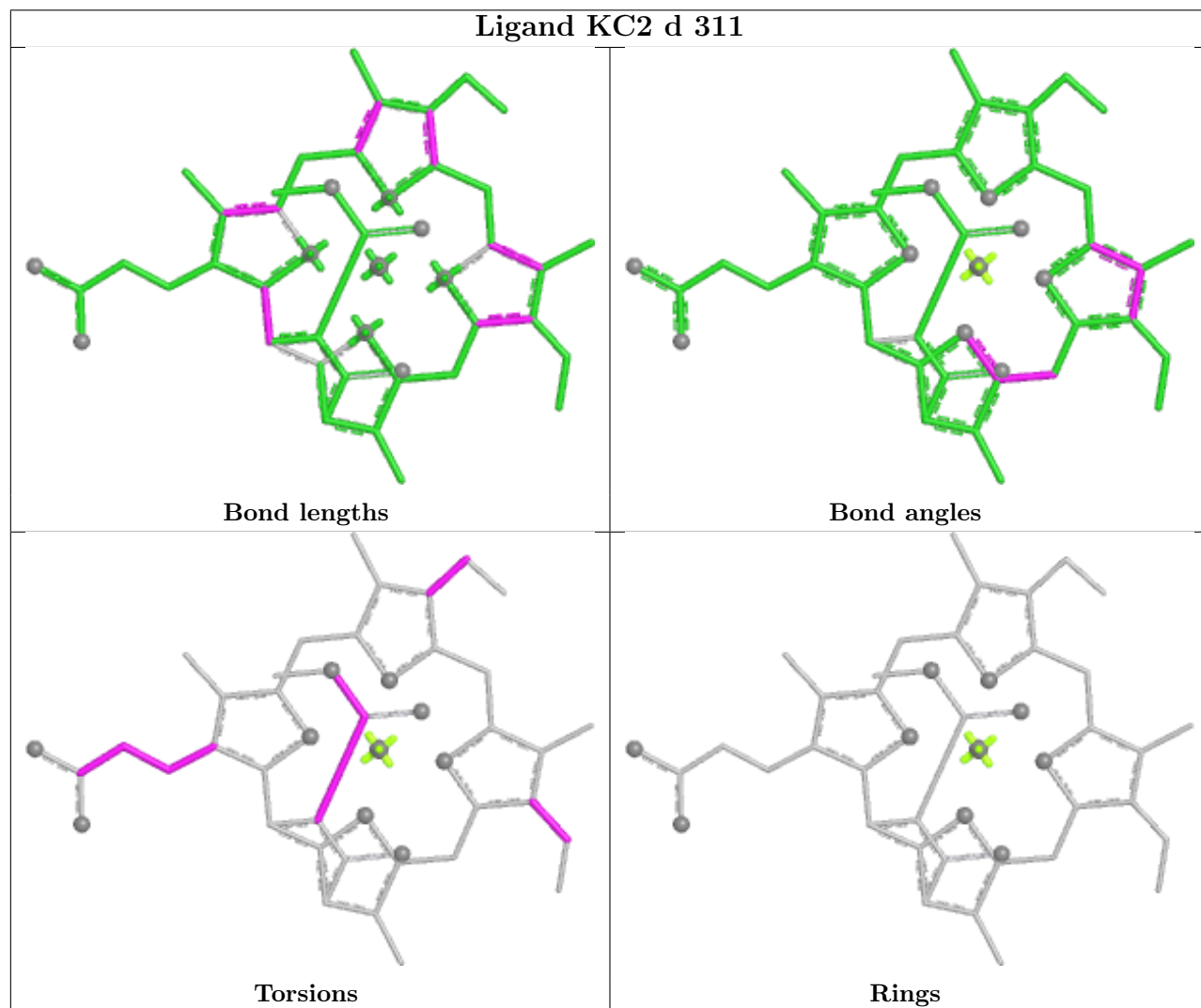
Ligand CLA B 807



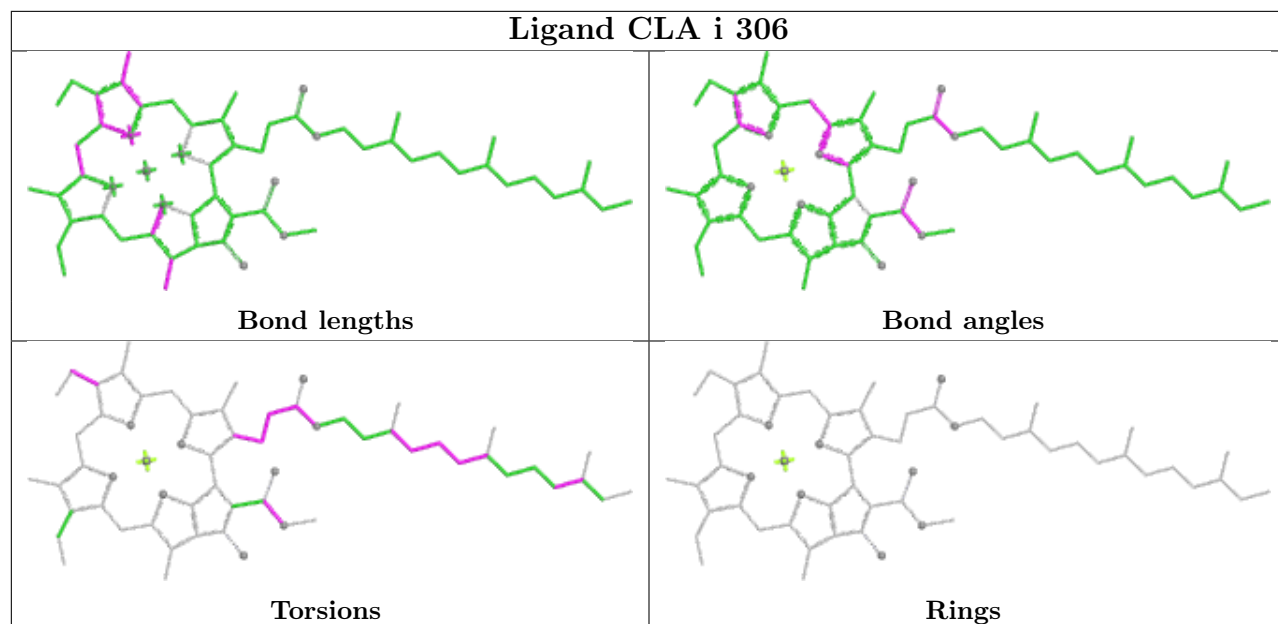
Ligand CLA i 304



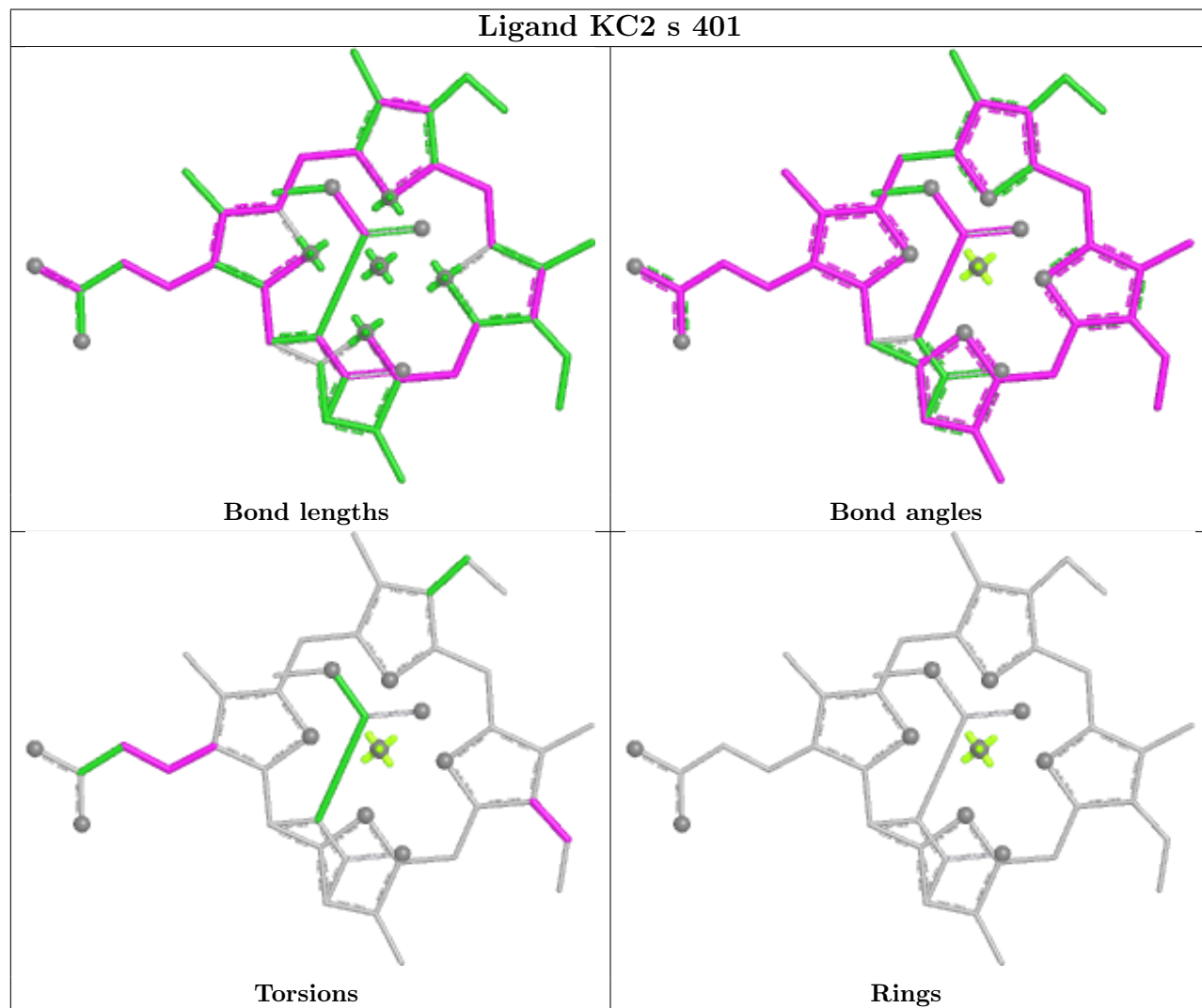
Ligand KC2 d 311

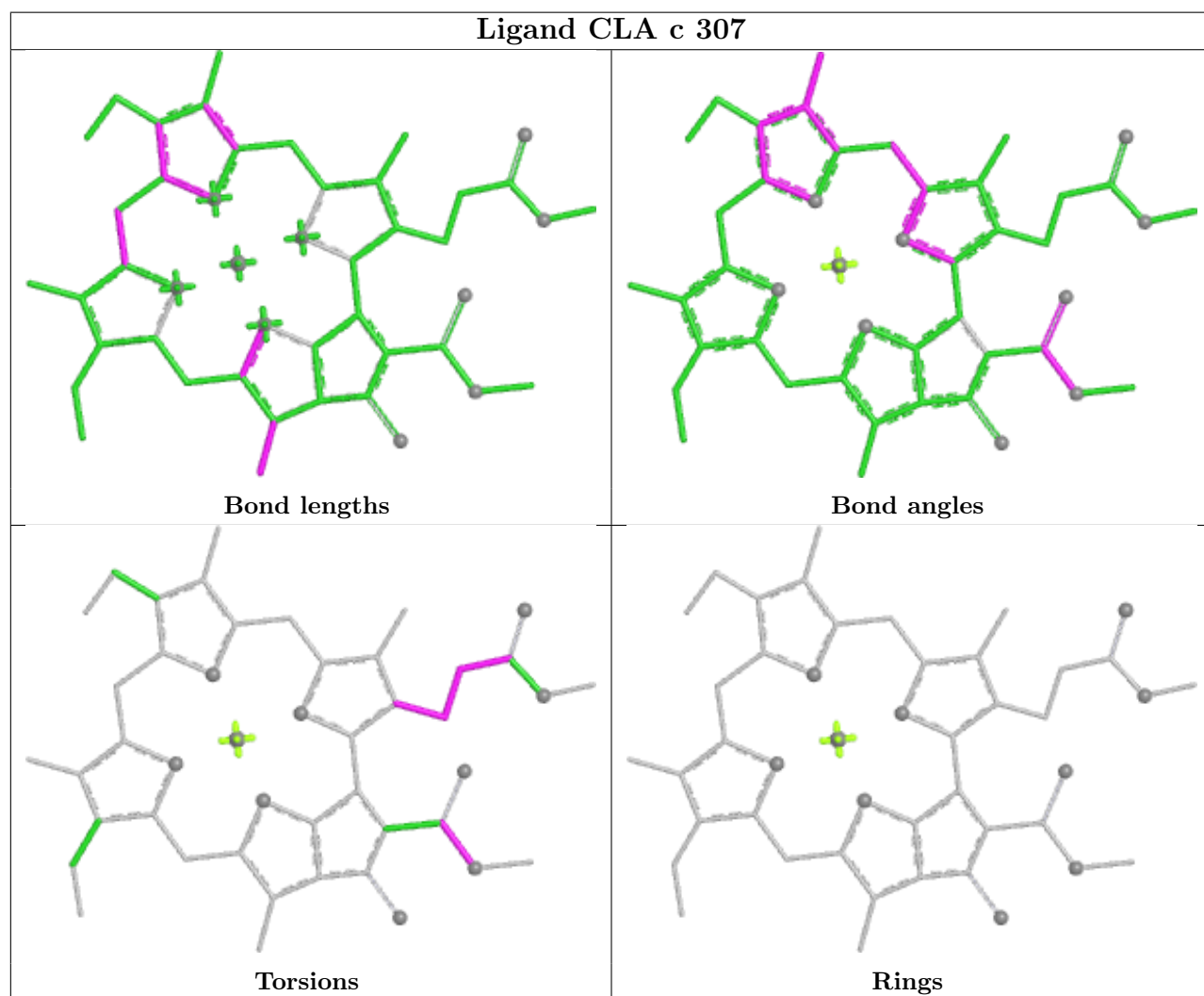
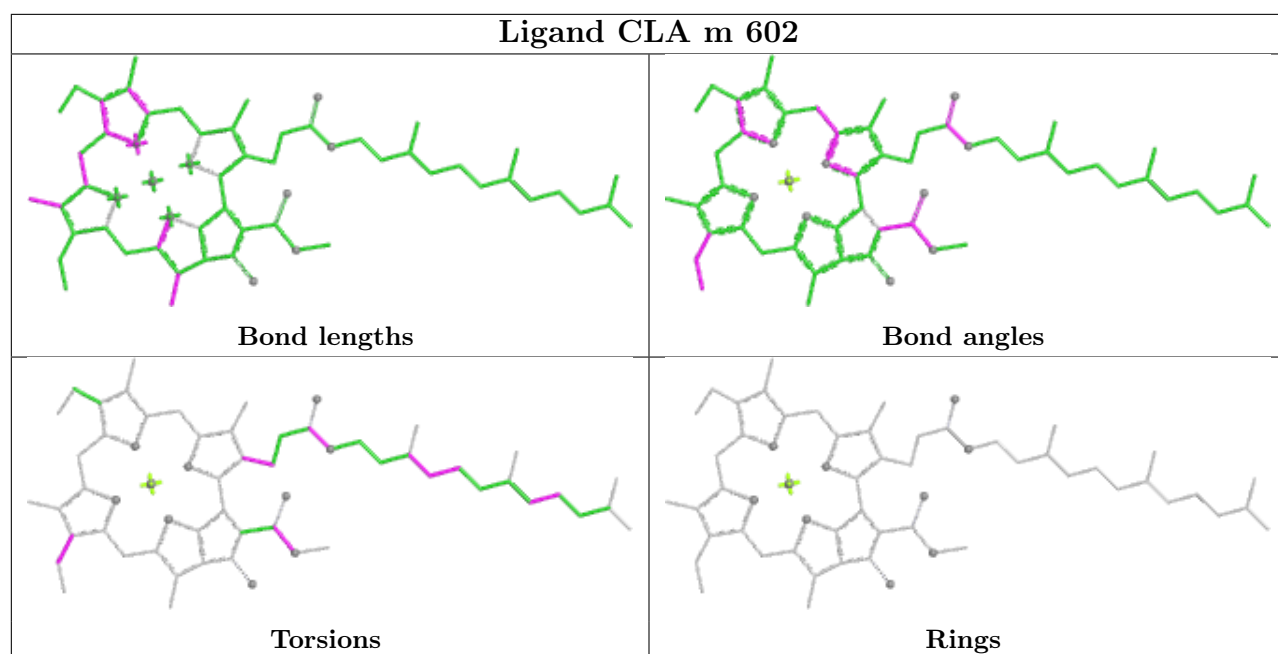


Ligand CLA i 306

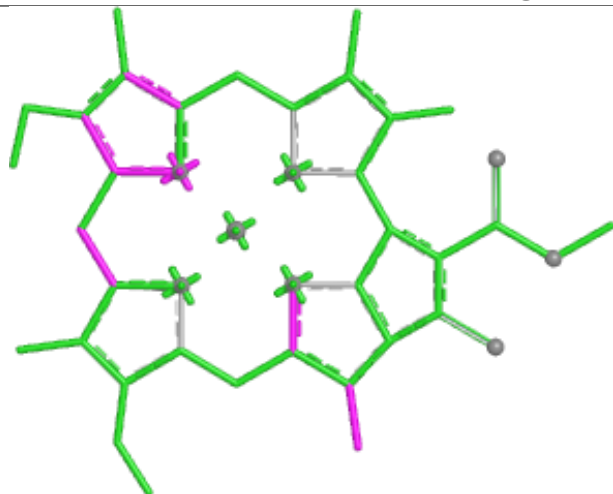


Ligand KC2 s 401

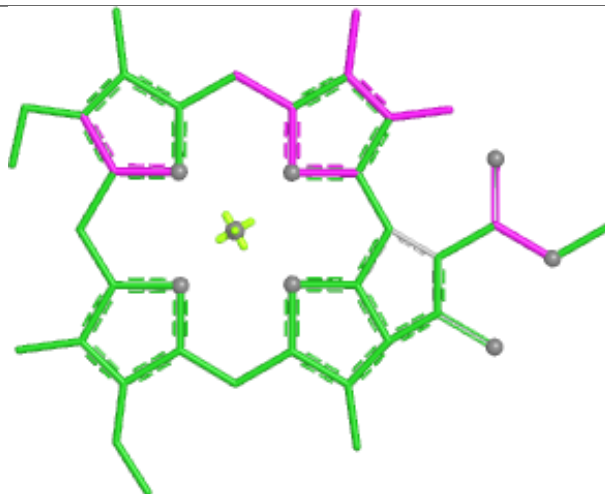




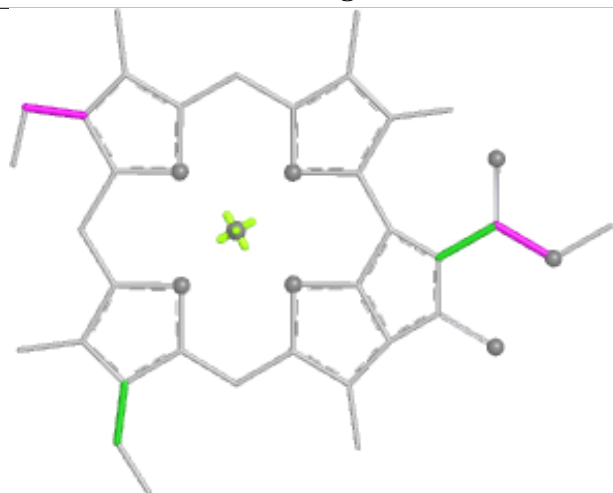
Ligand CLA d 309



Bond lengths



Bond angles

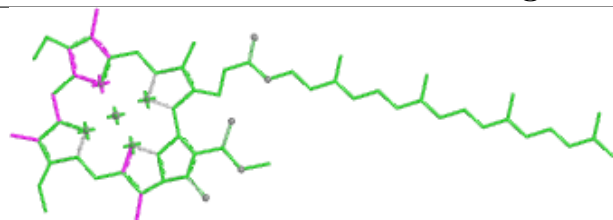


Torsions

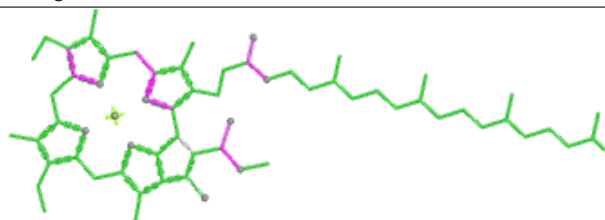


Rings

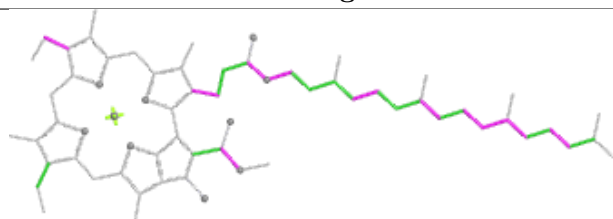
Ligand CLA j 609



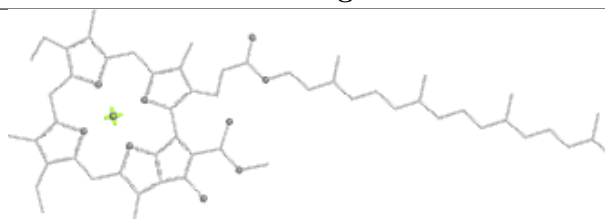
Bond lengths



Bond angles

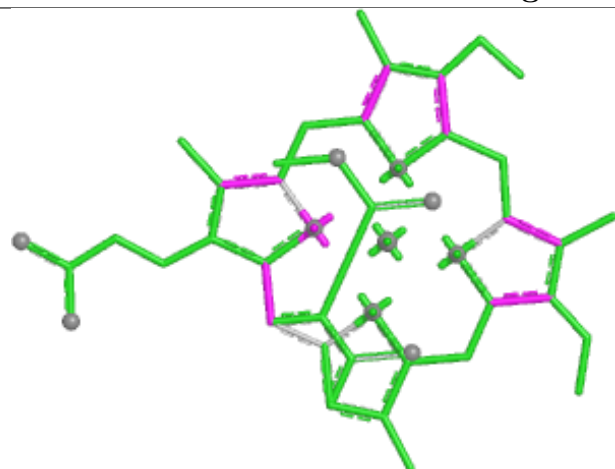


Torsions

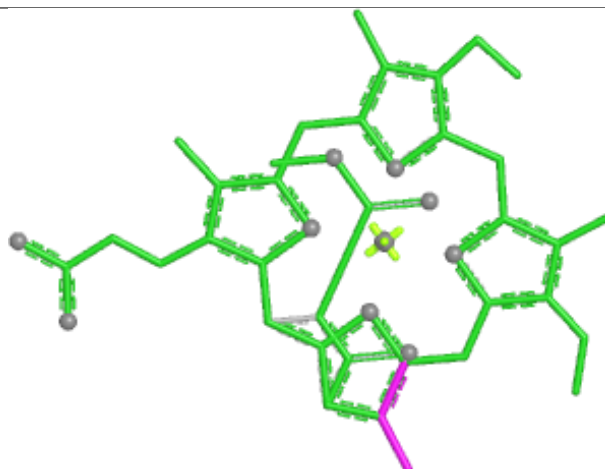


Rings

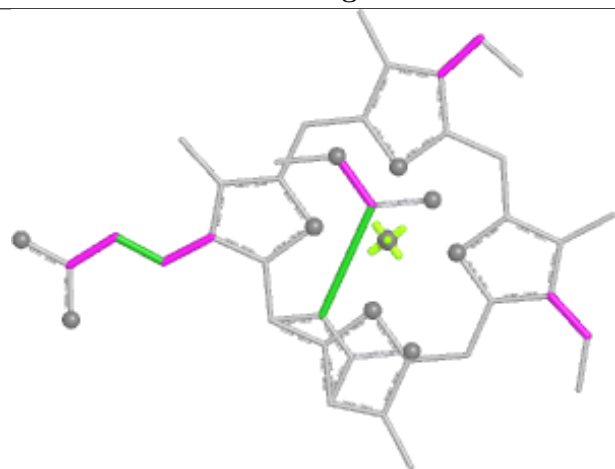
Ligand KC2 k 612



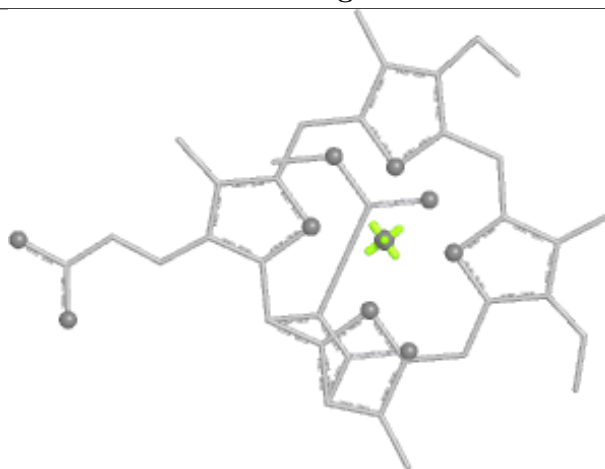
Bond lengths



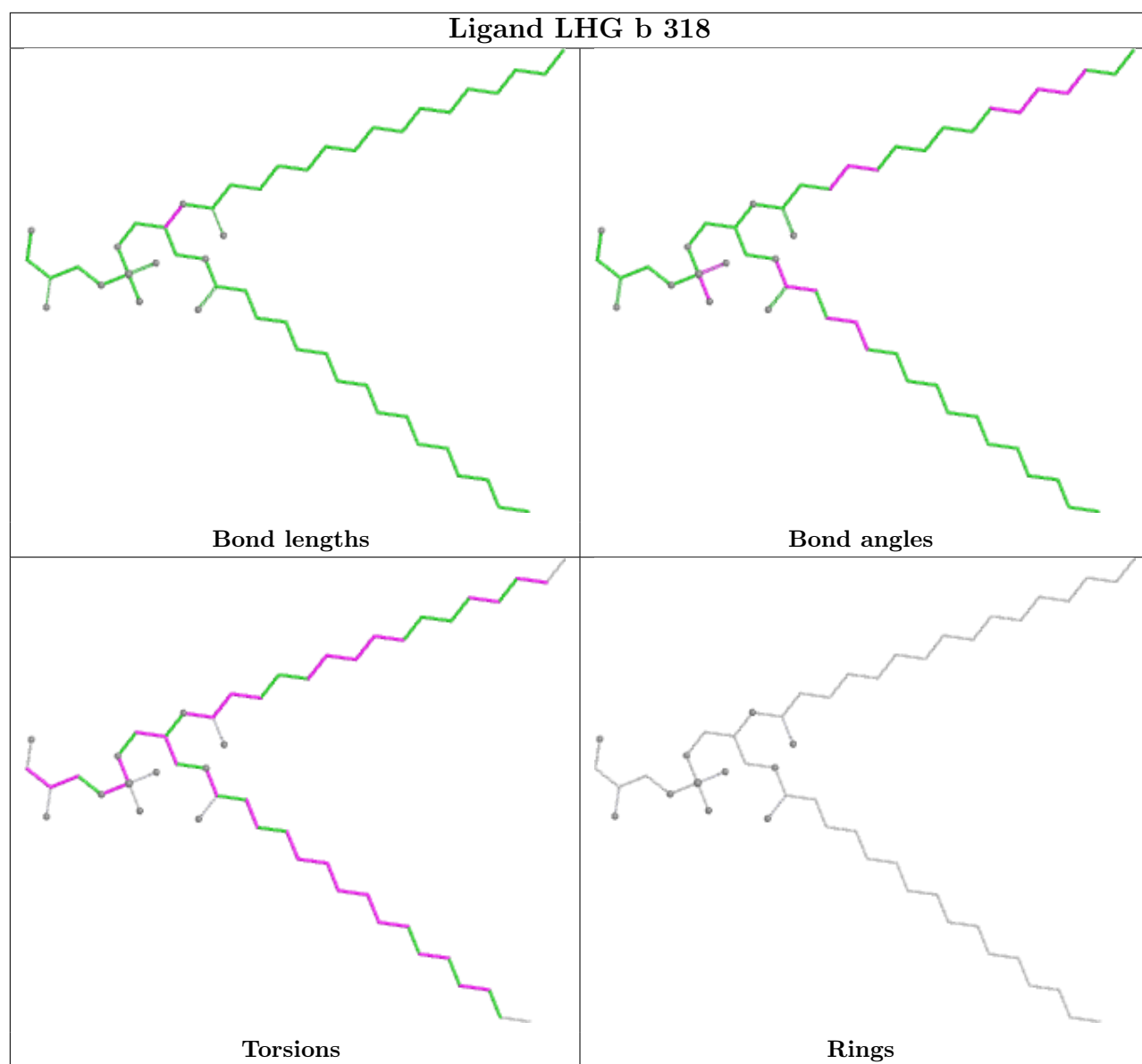
Bond angles

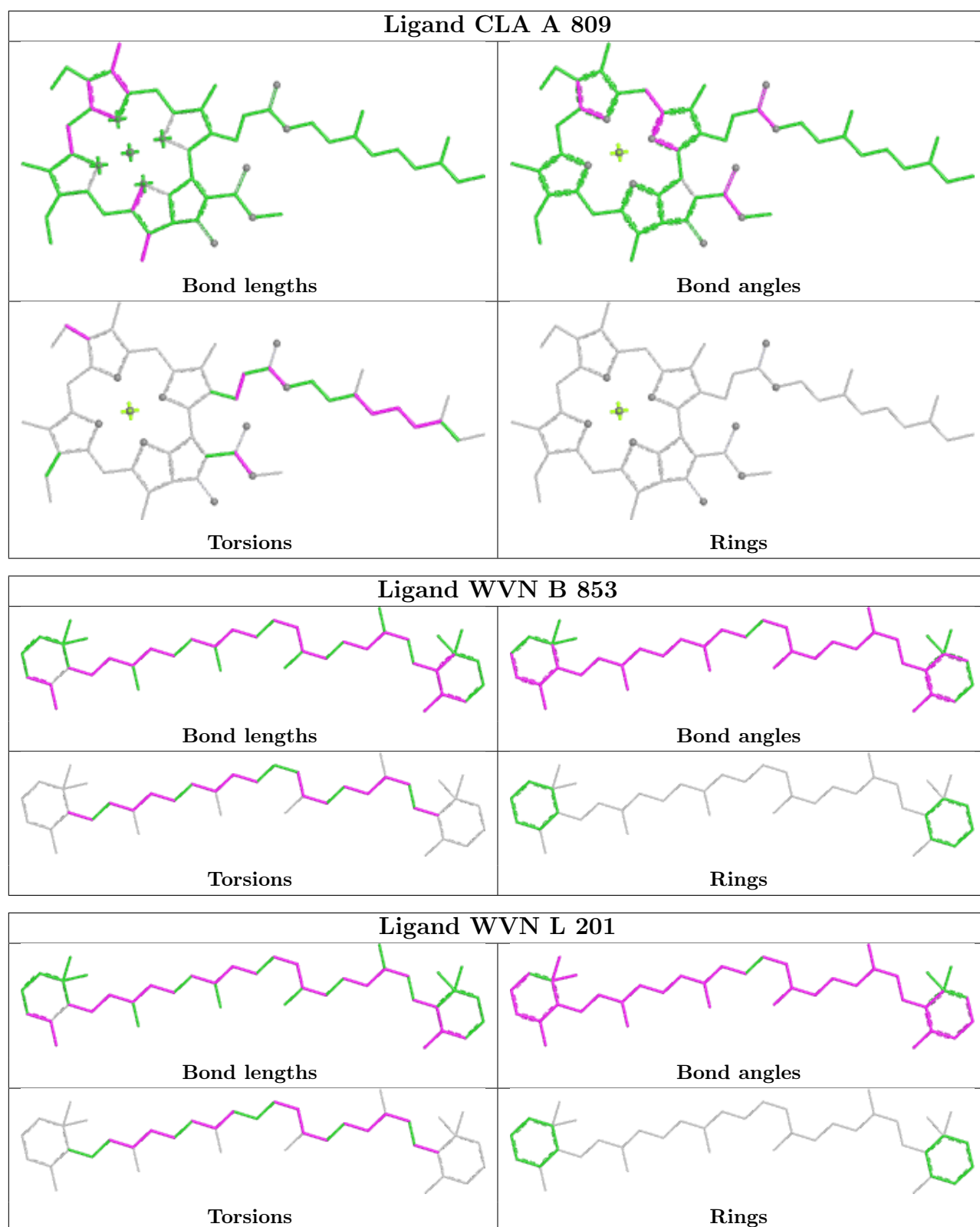


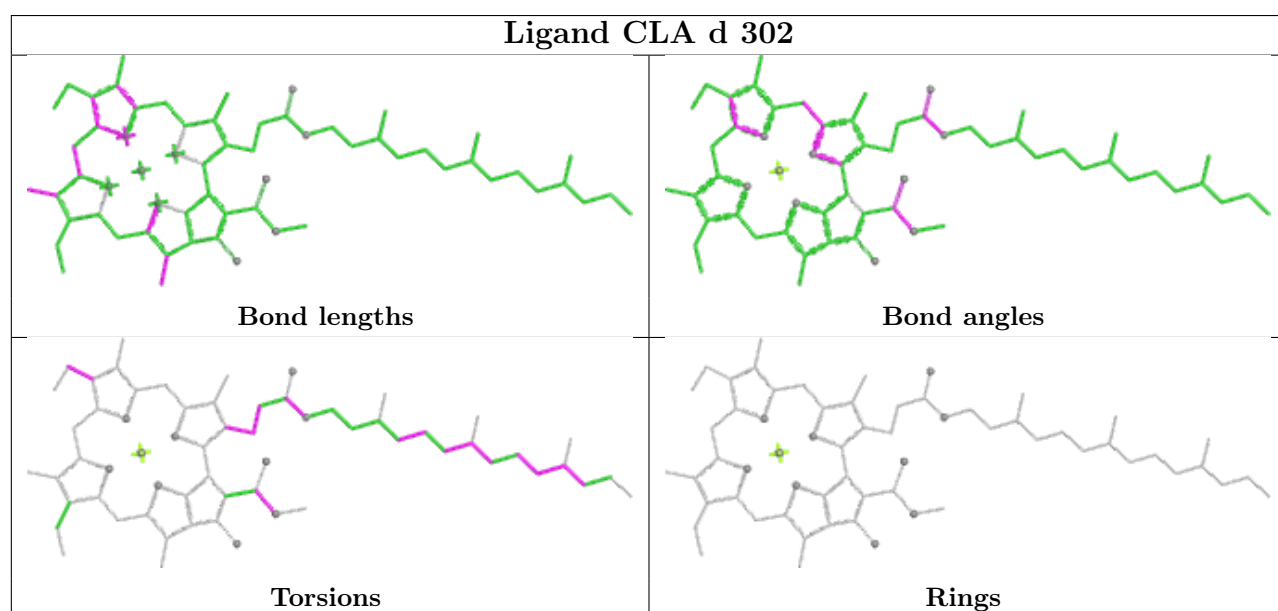
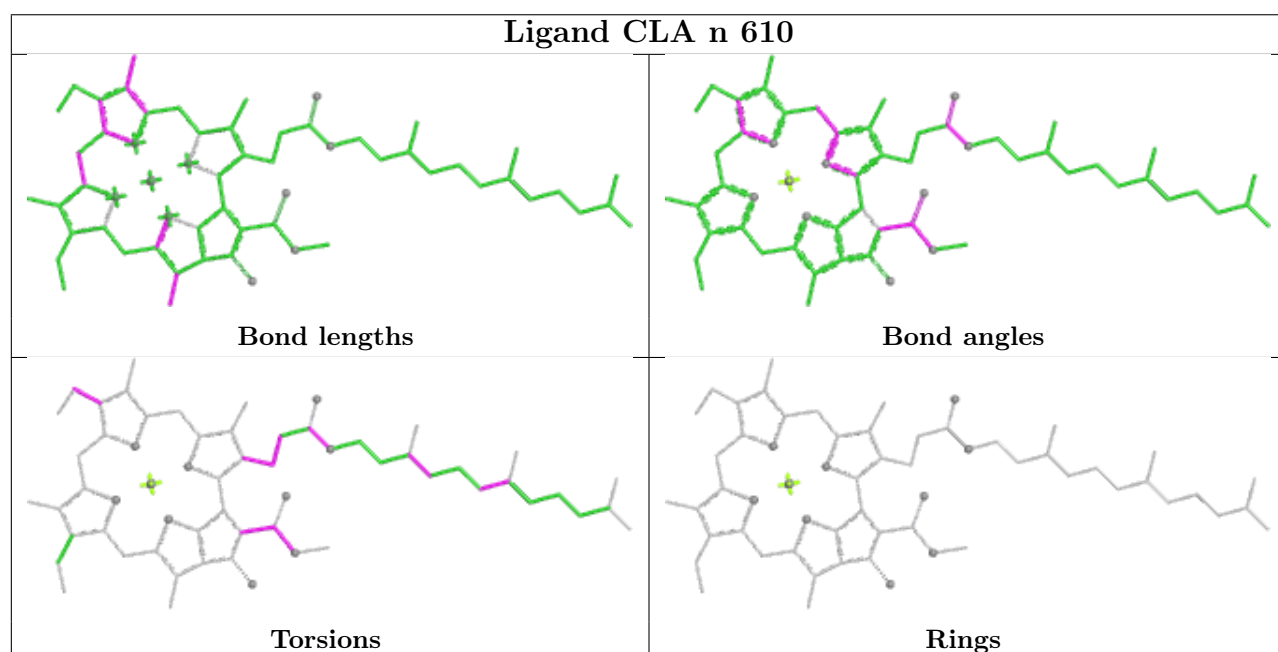
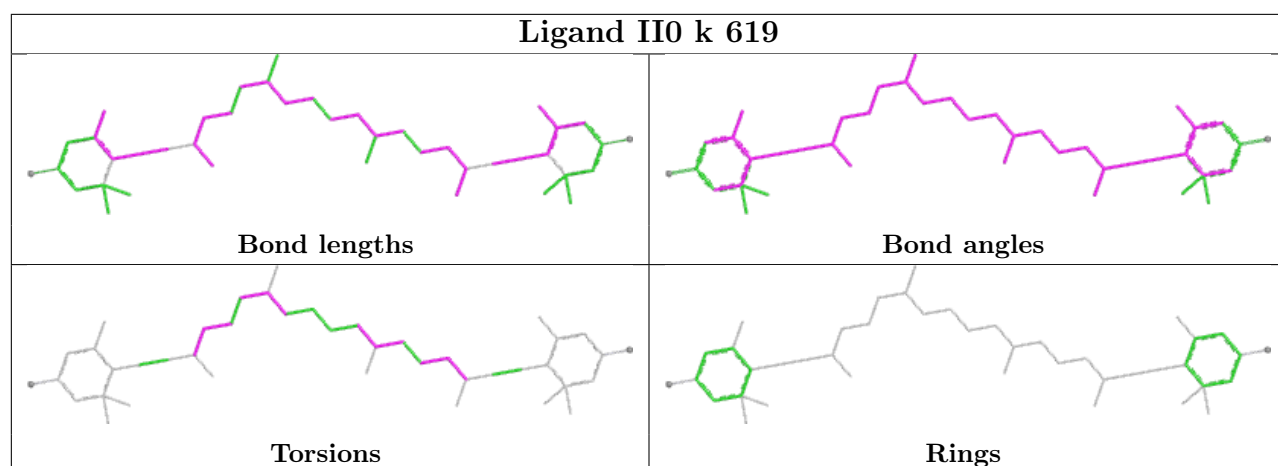
Torsions

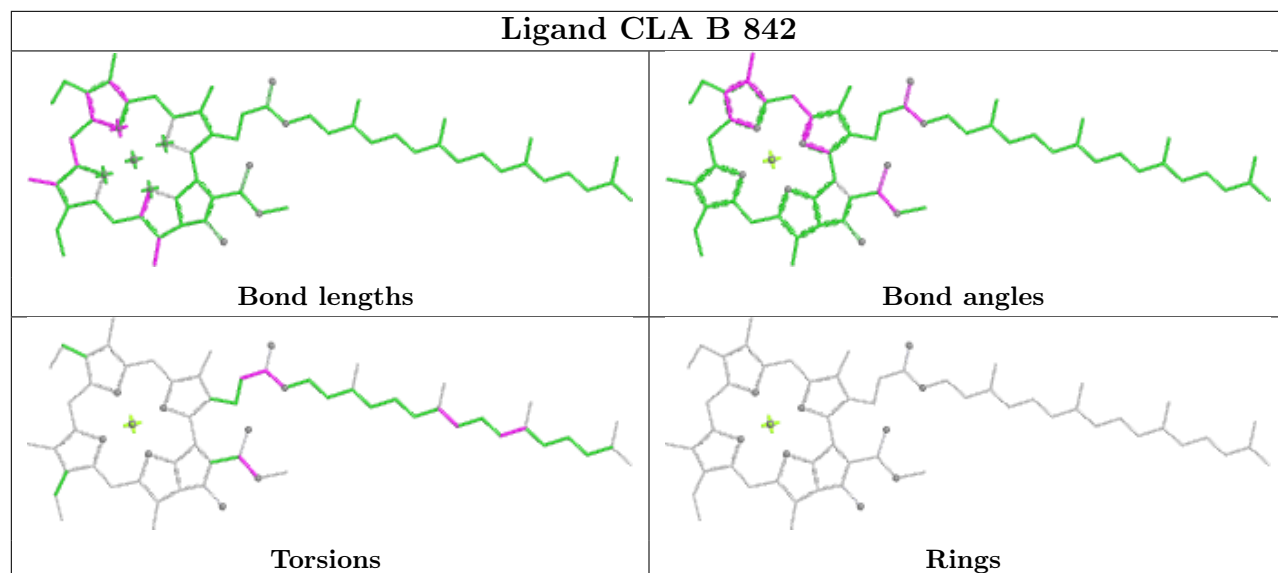
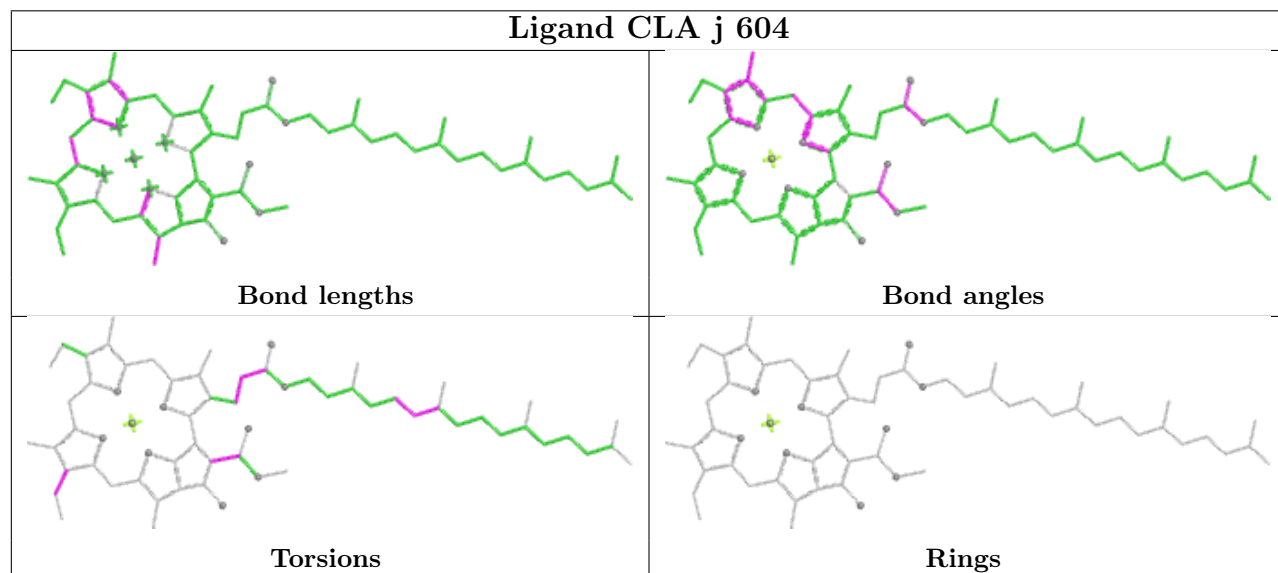
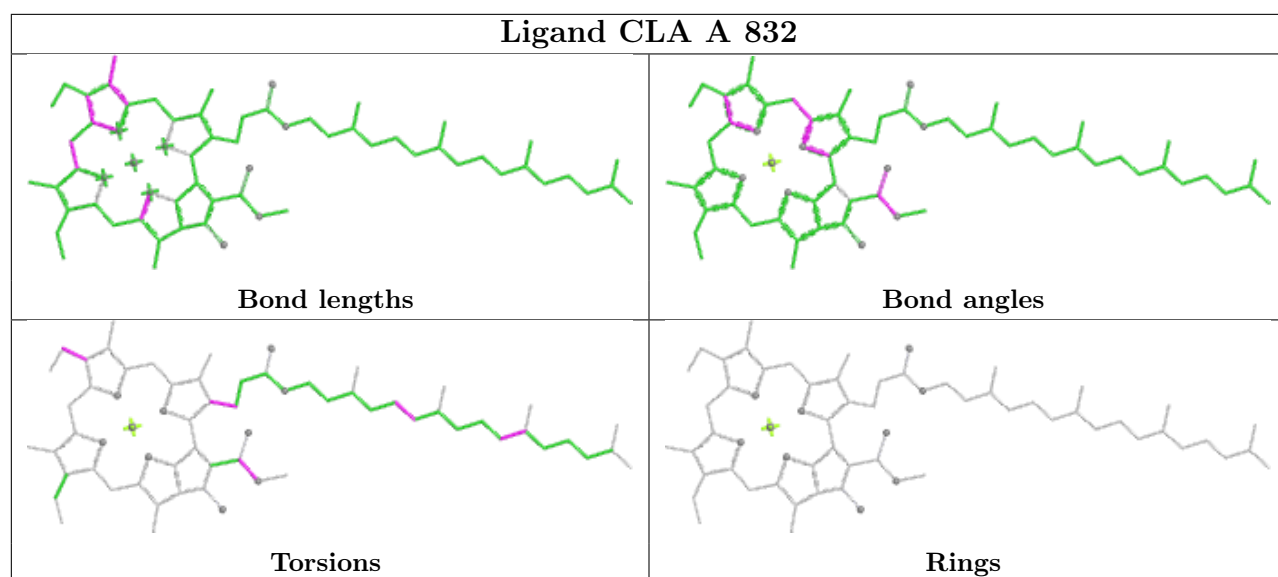


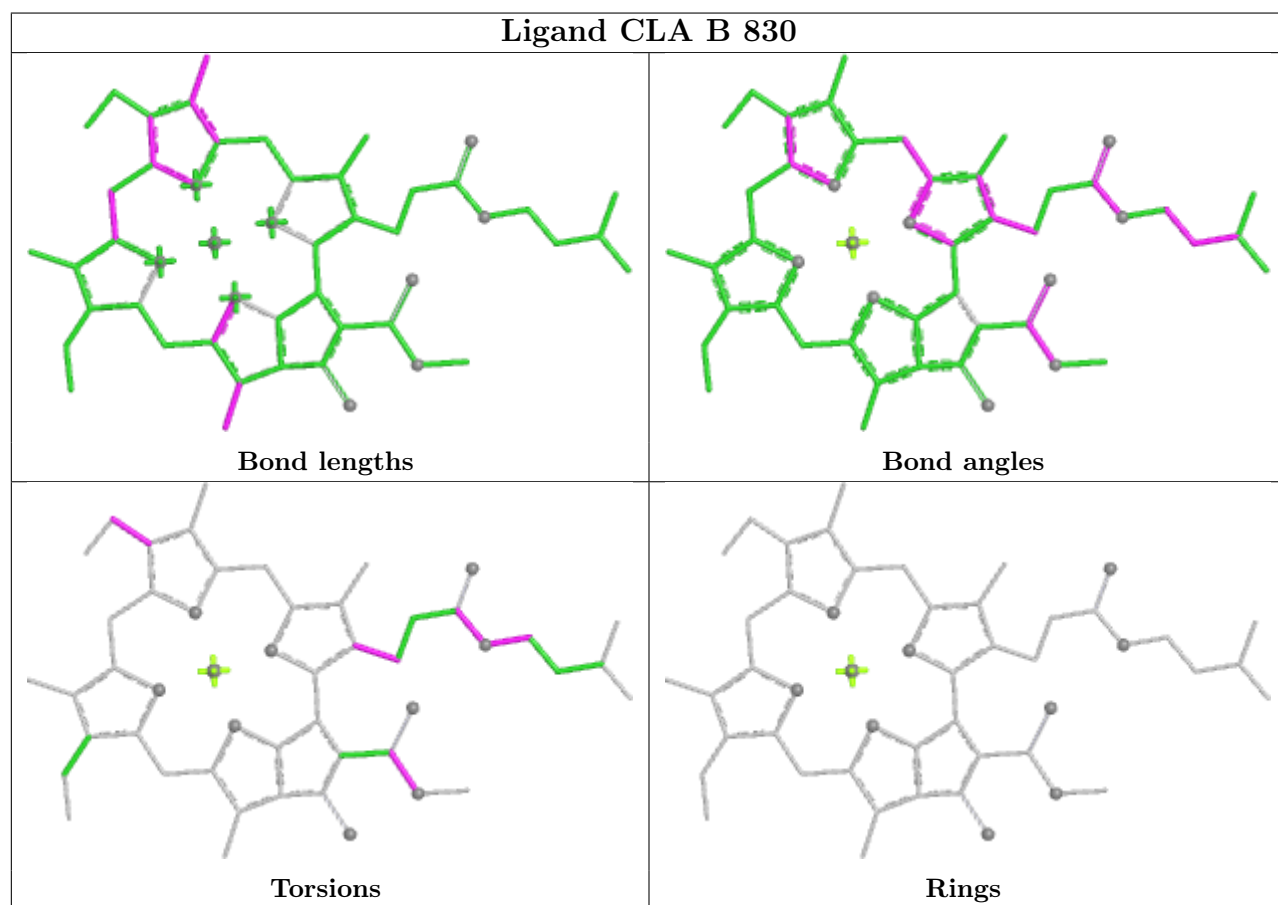
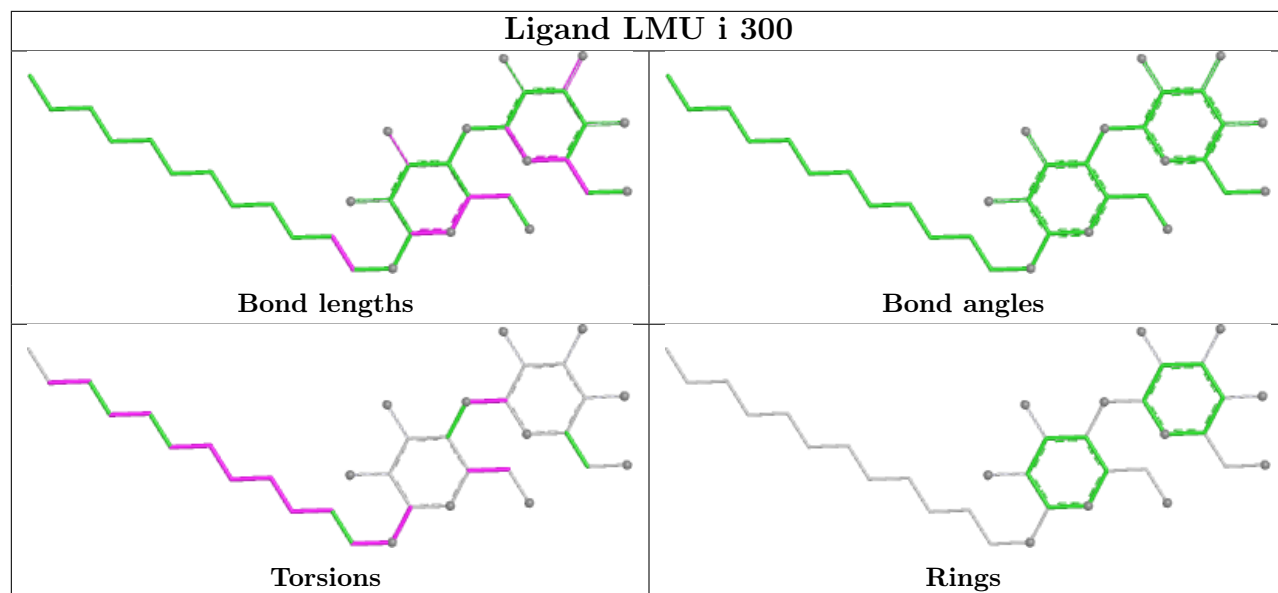
Rings



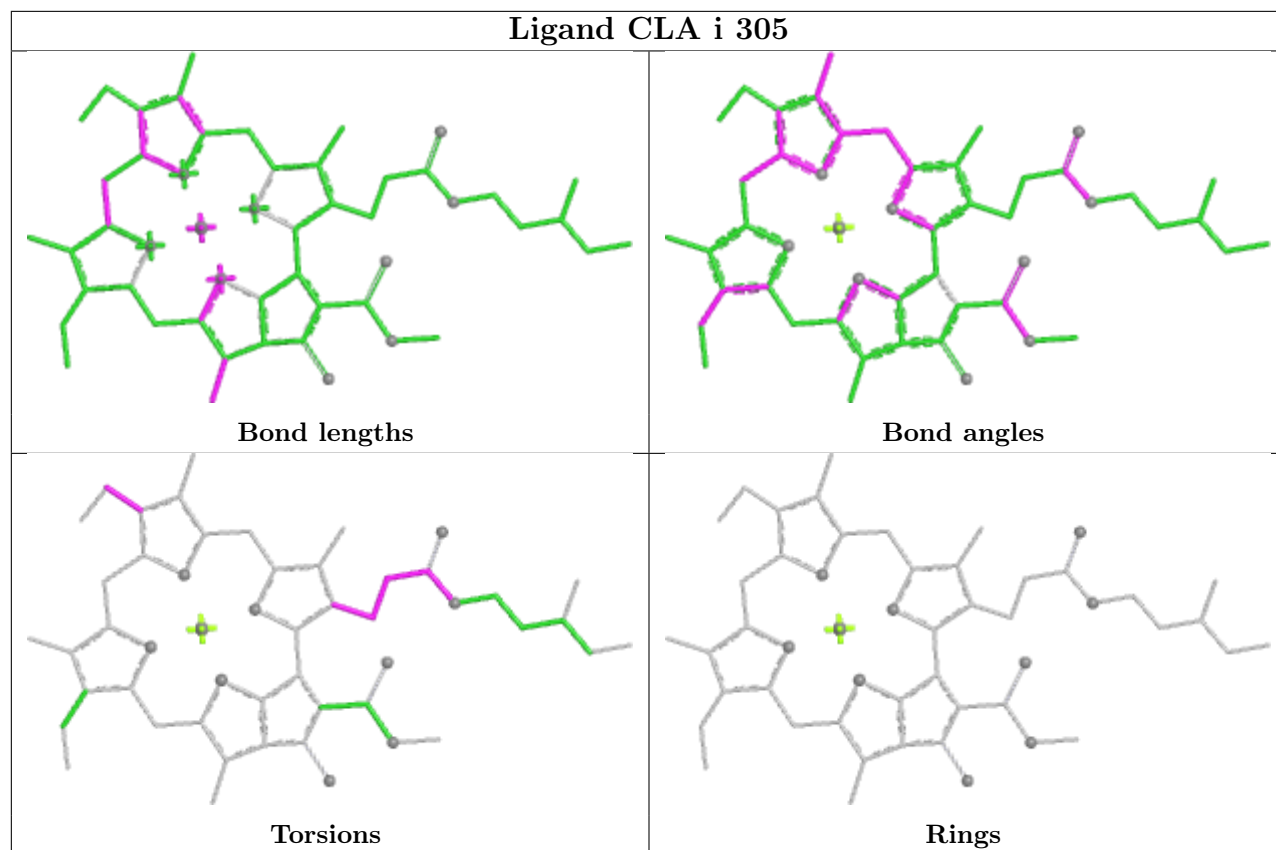




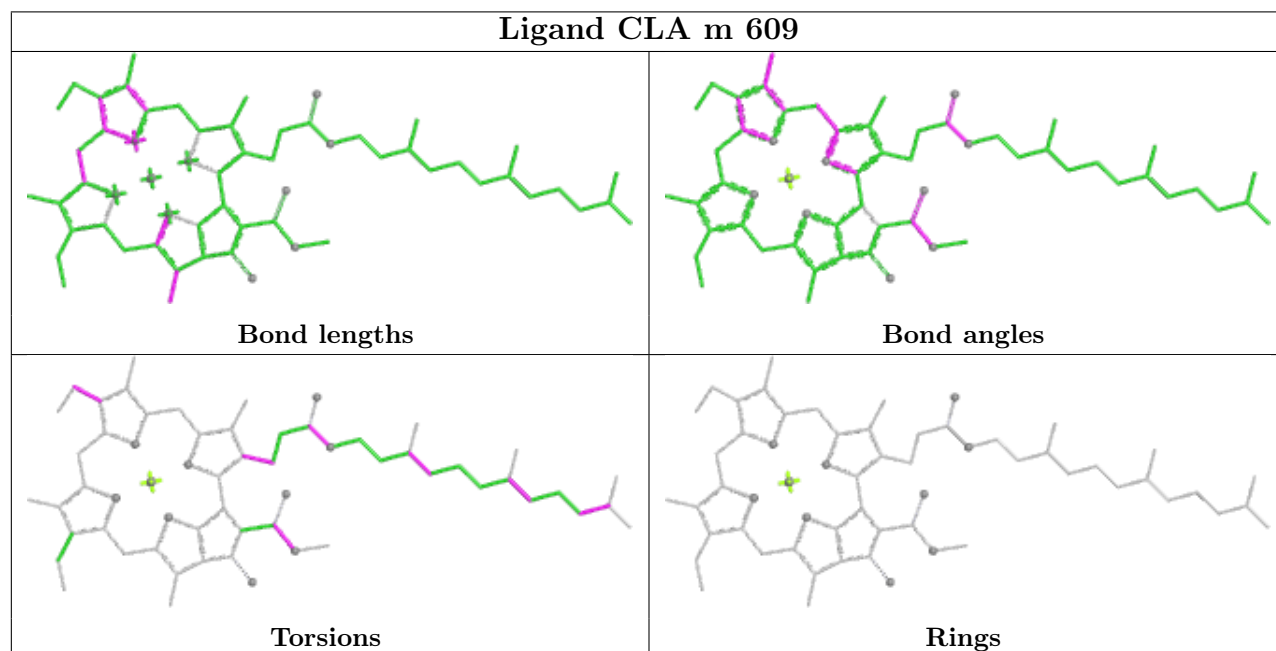


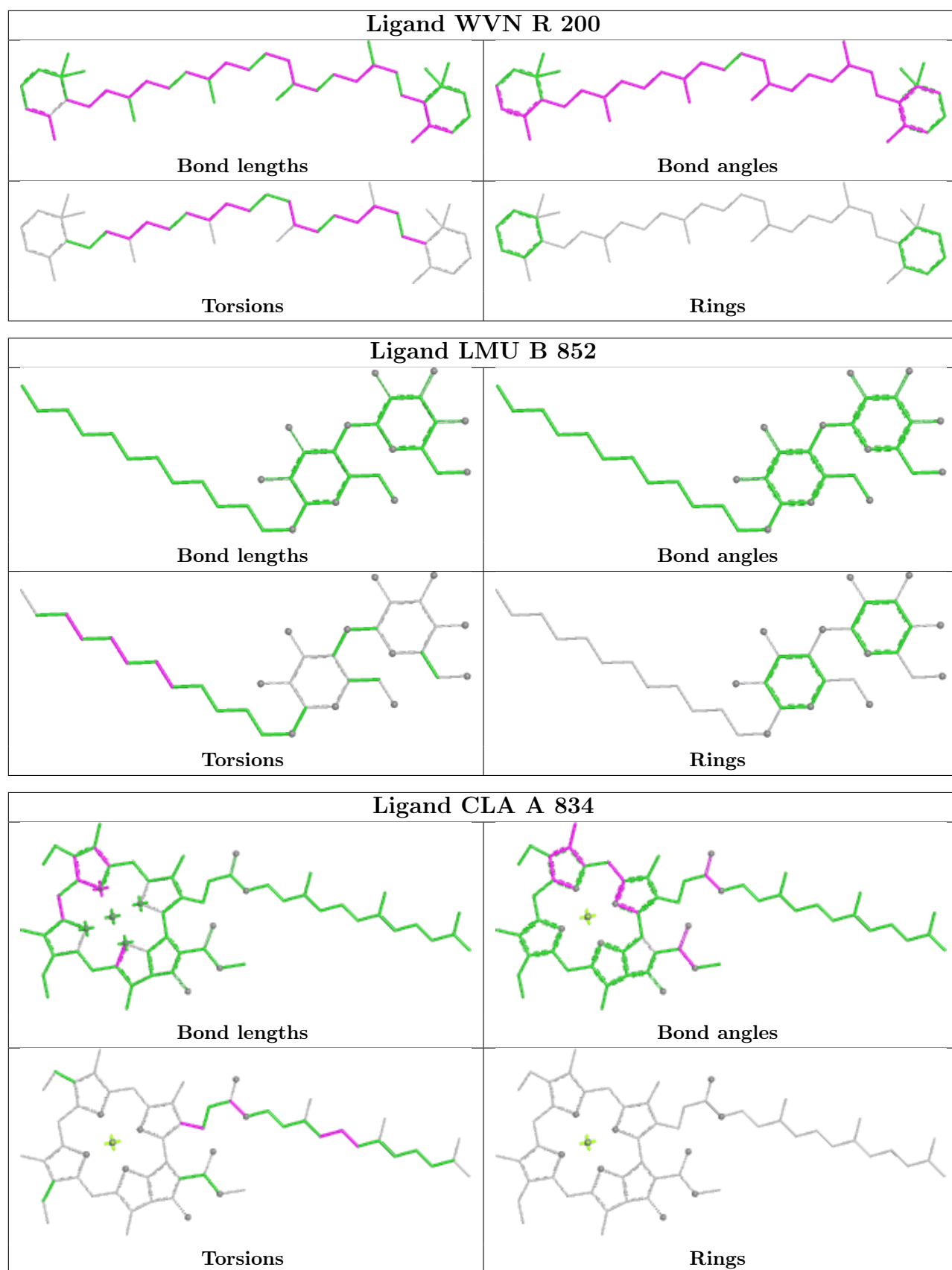


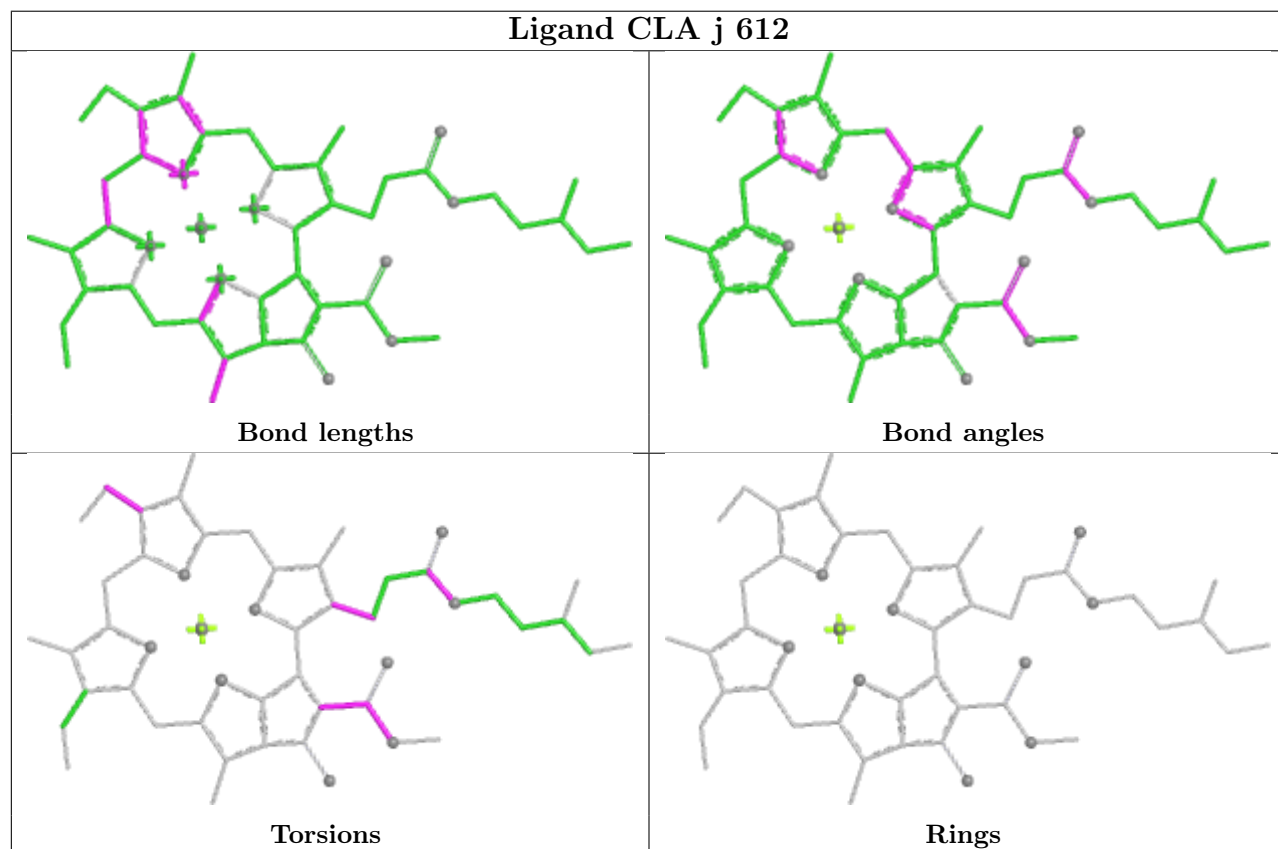
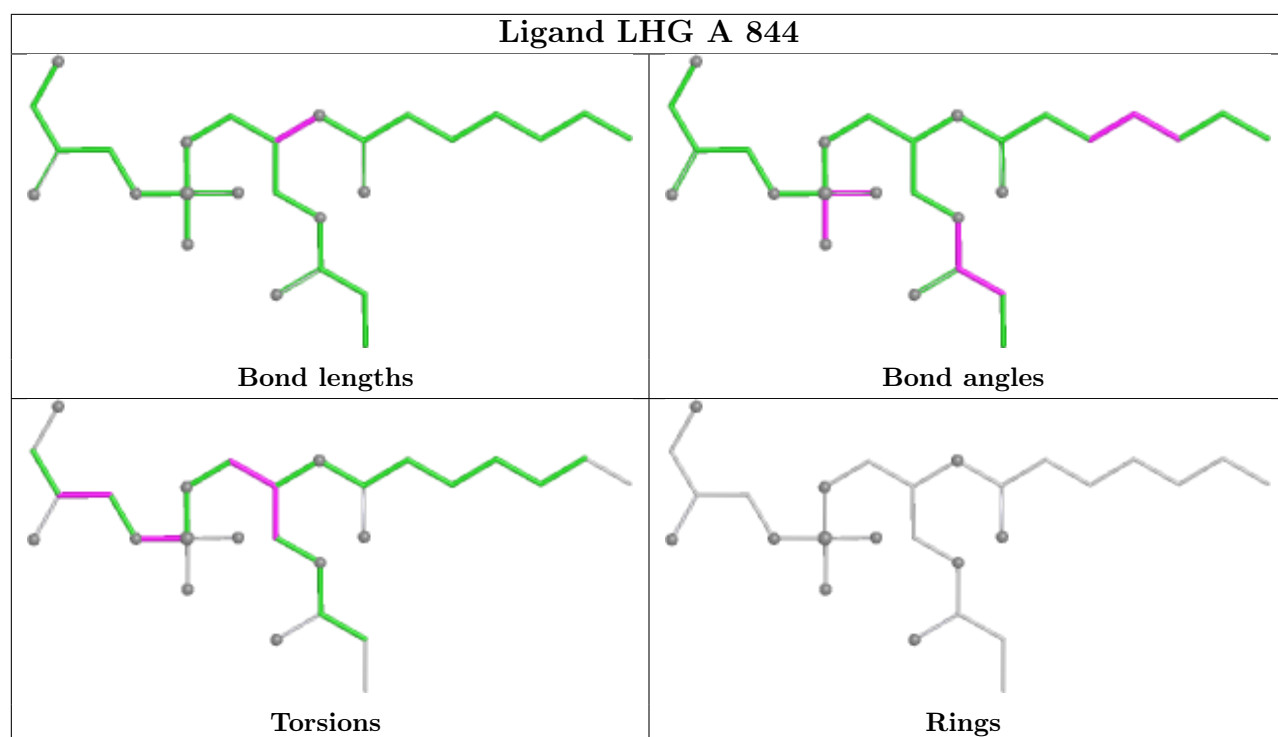
Ligand CLA i 305

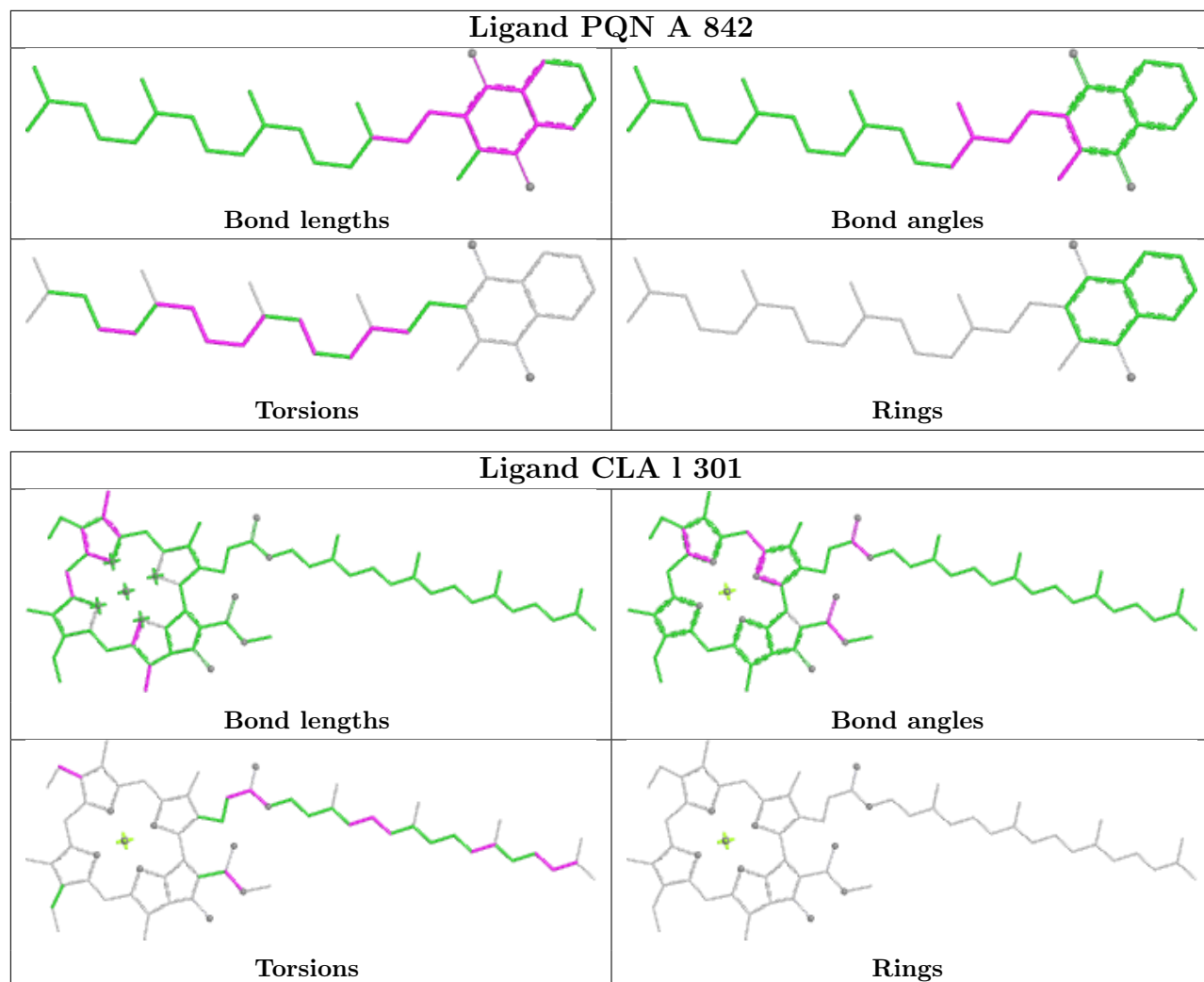


Ligand CLA m 609

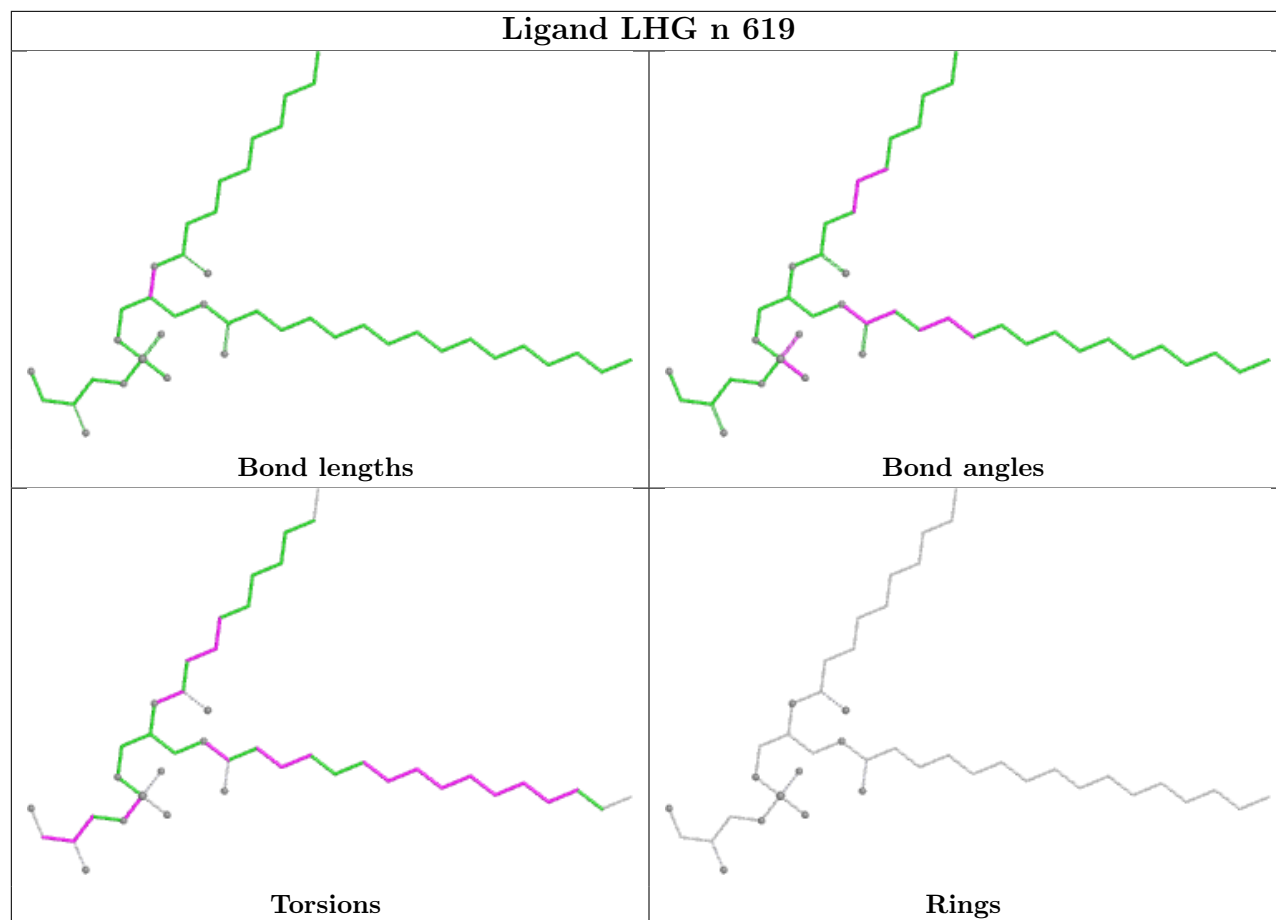




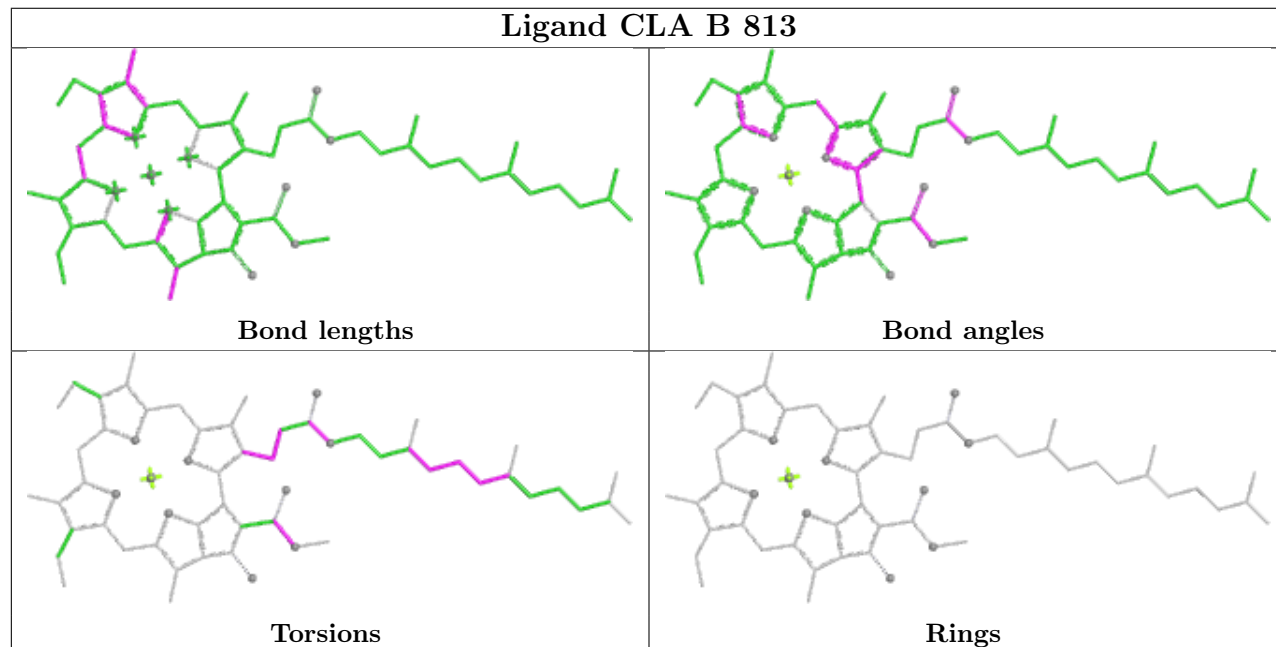




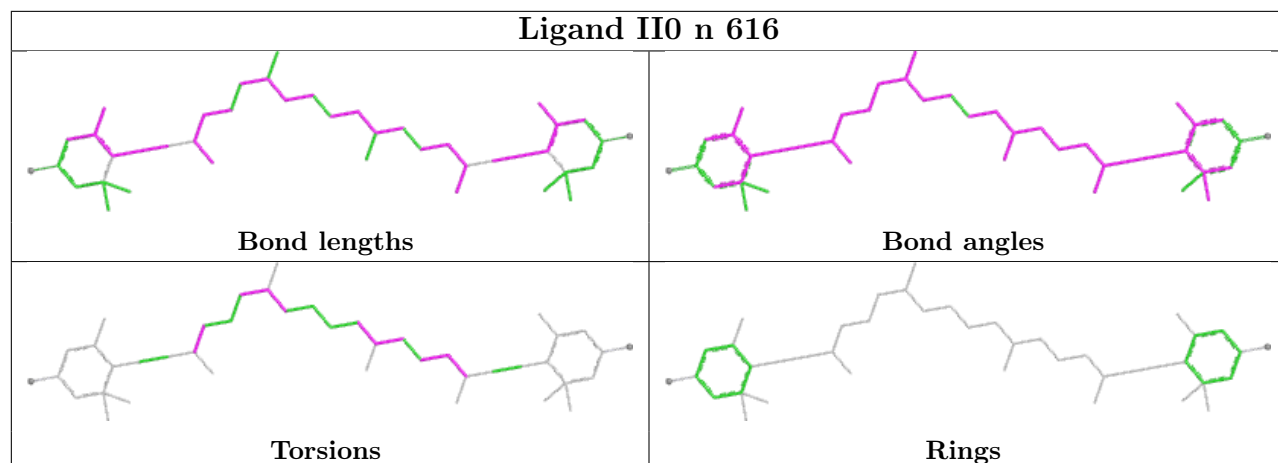
Ligand LHG n 619



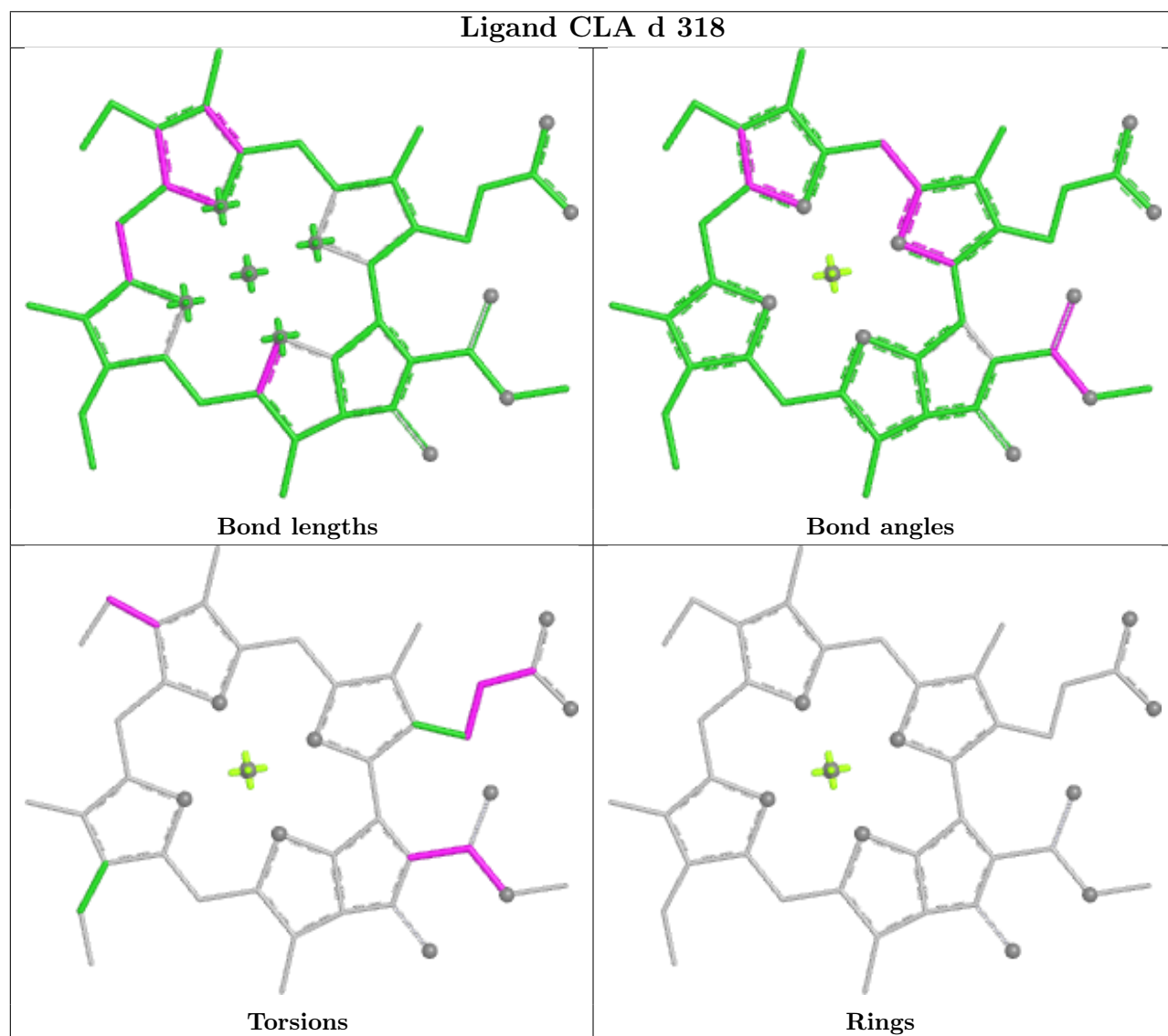
Ligand CLA B 813



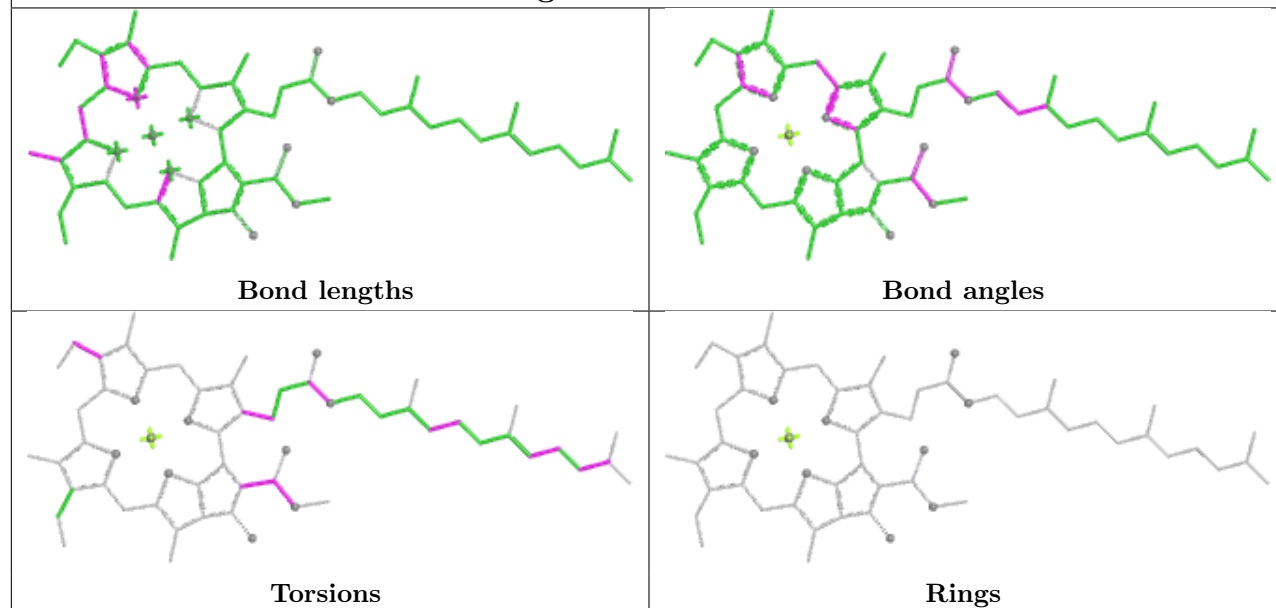
Ligand II0 n 616



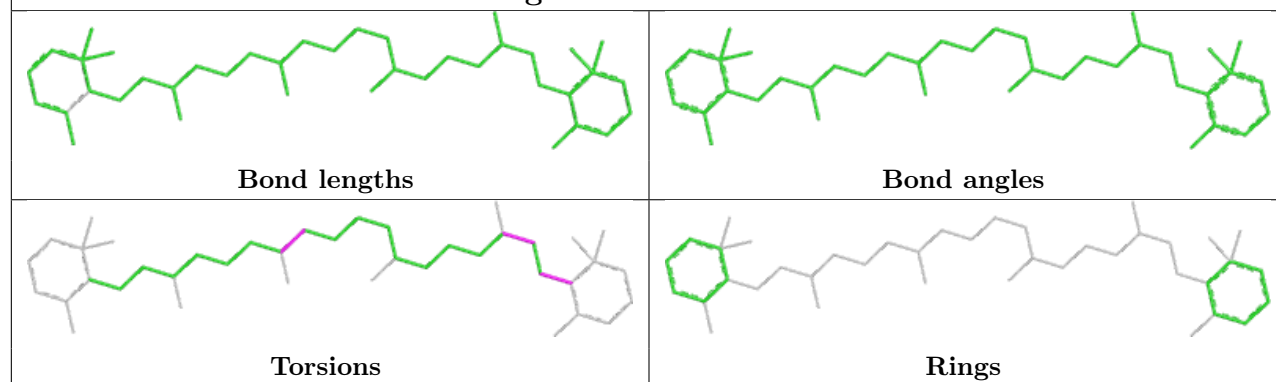
Ligand CLA d 318



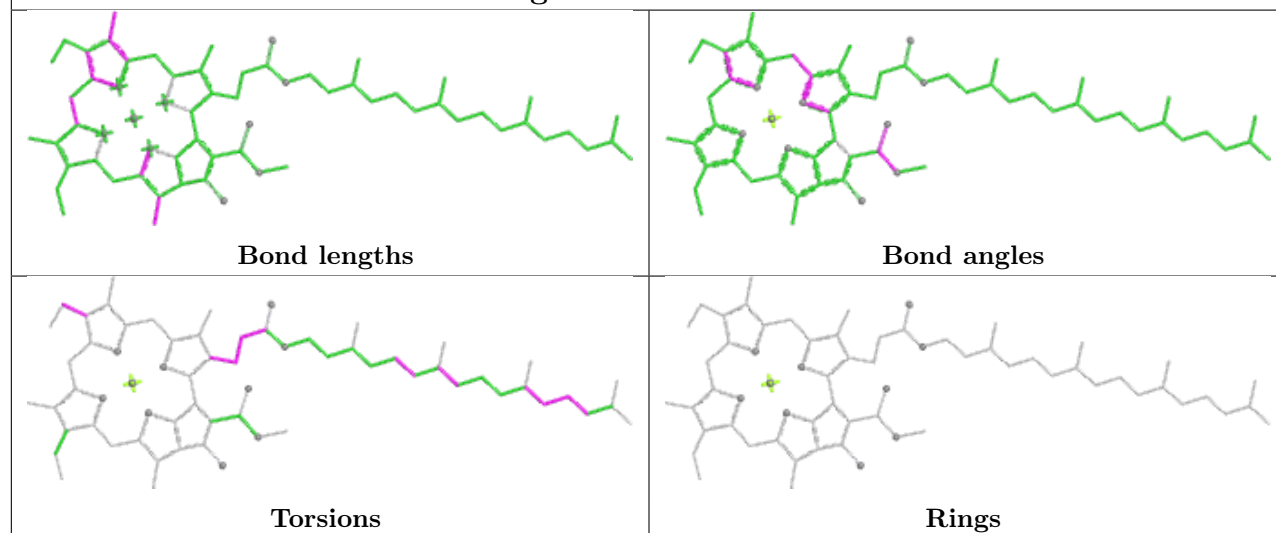
Ligand CLA c 302



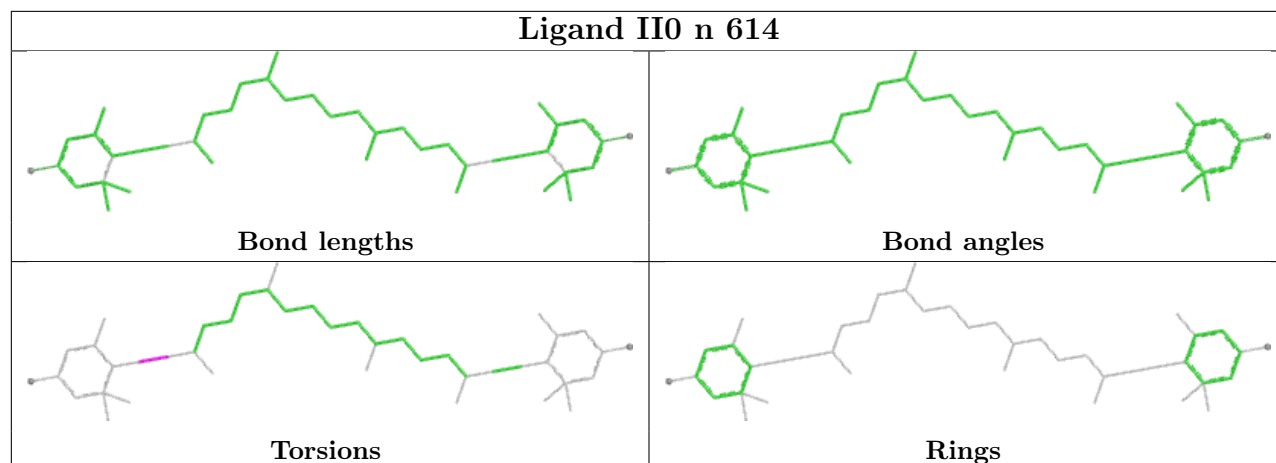
Ligand WVN F 204



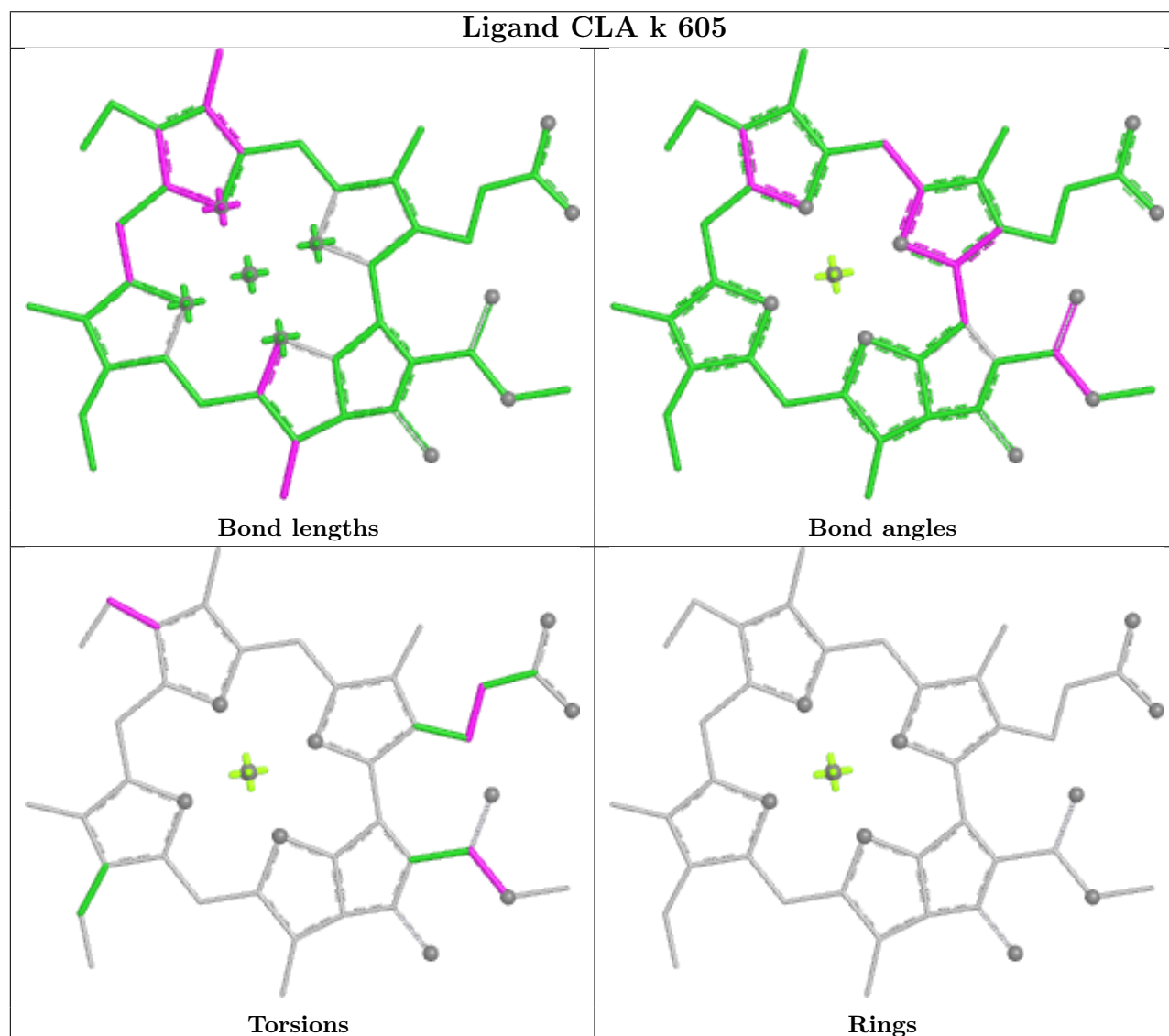
Ligand CLA m 608



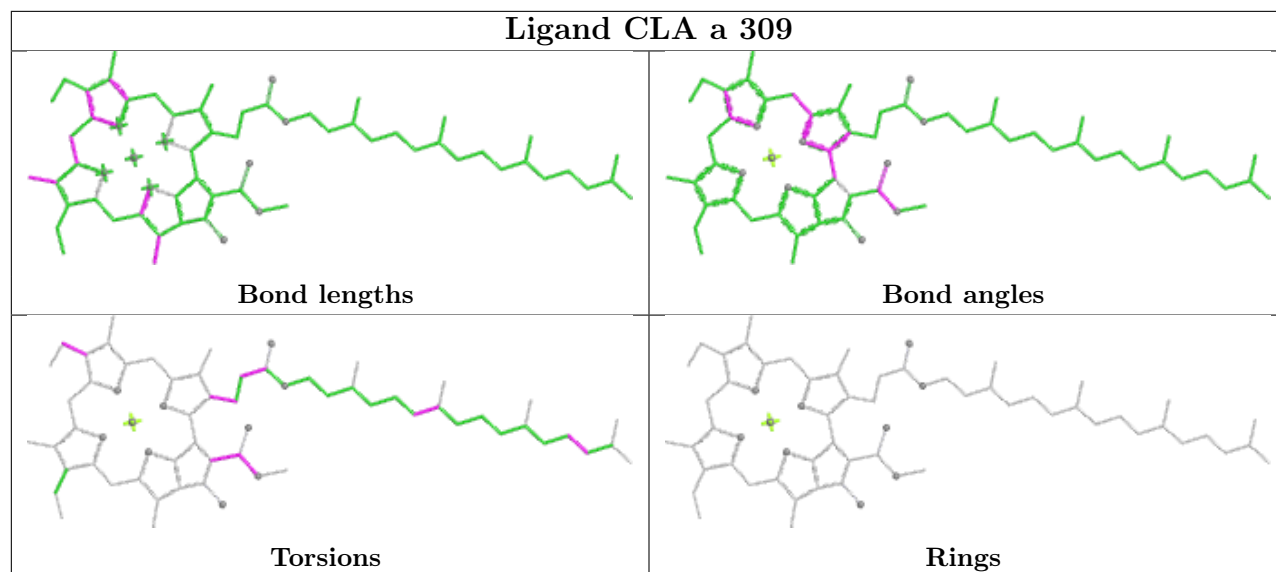
Ligand II0 n 614



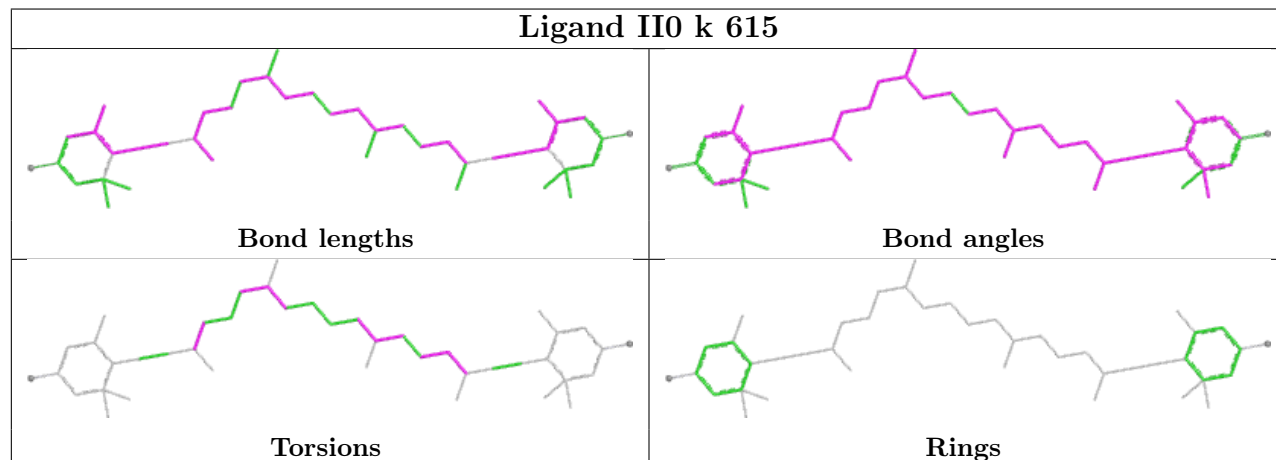
Ligand CLA k 605



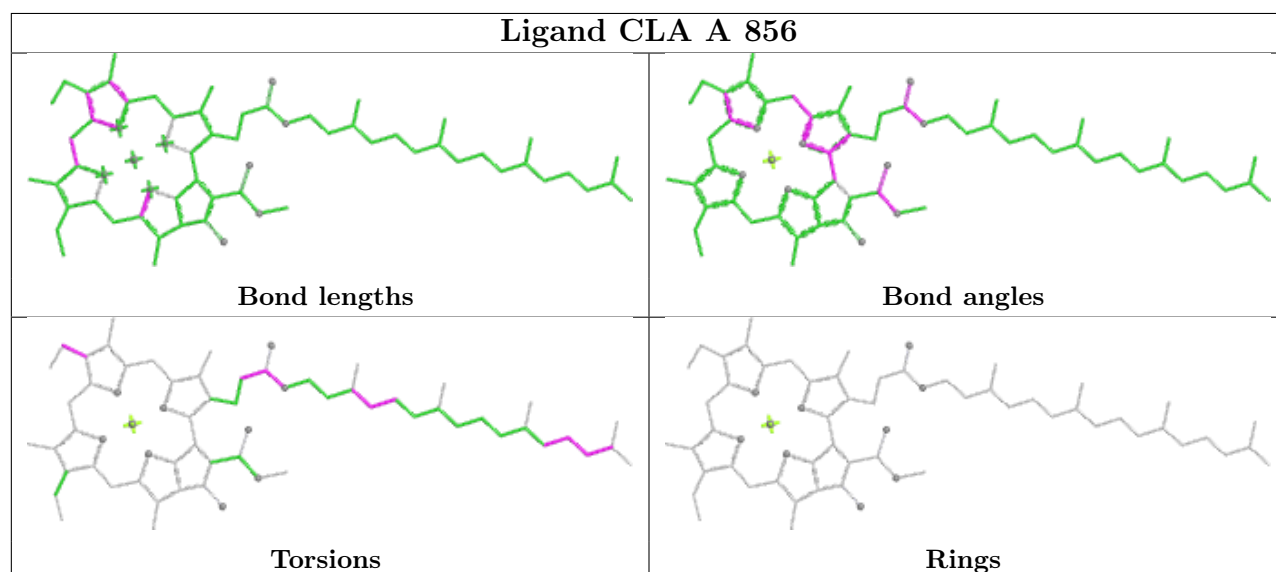
Ligand CLA a 309

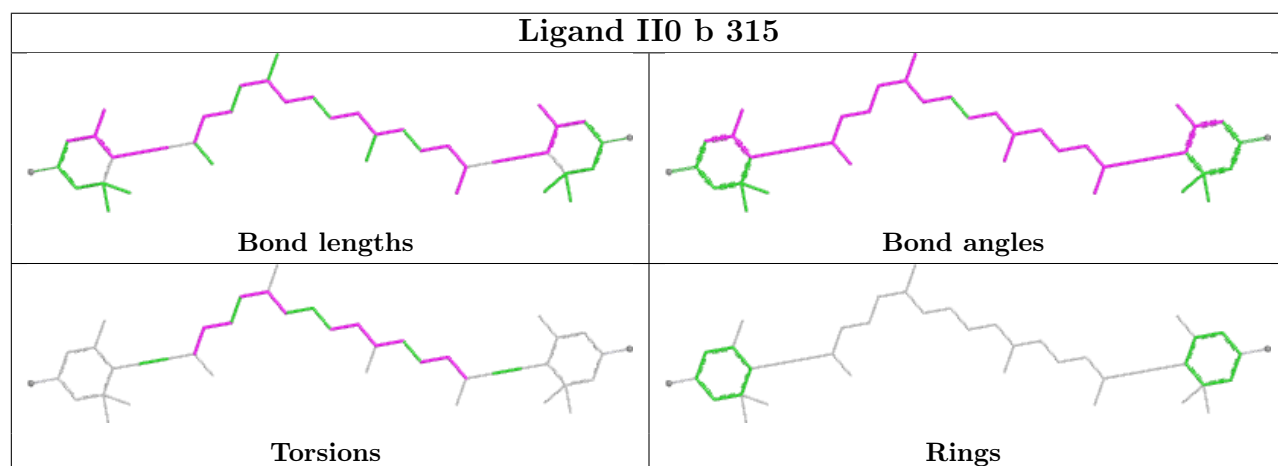
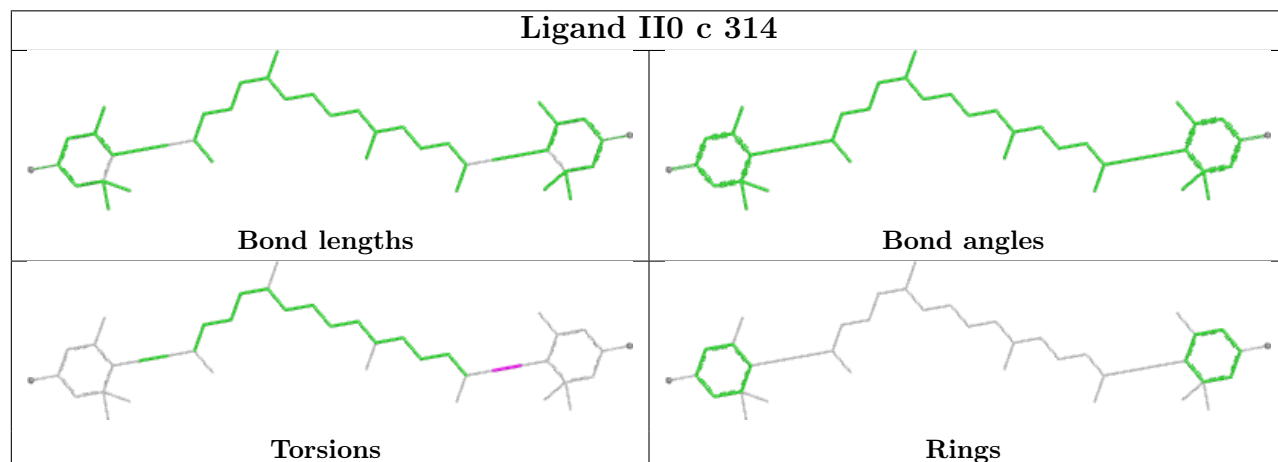
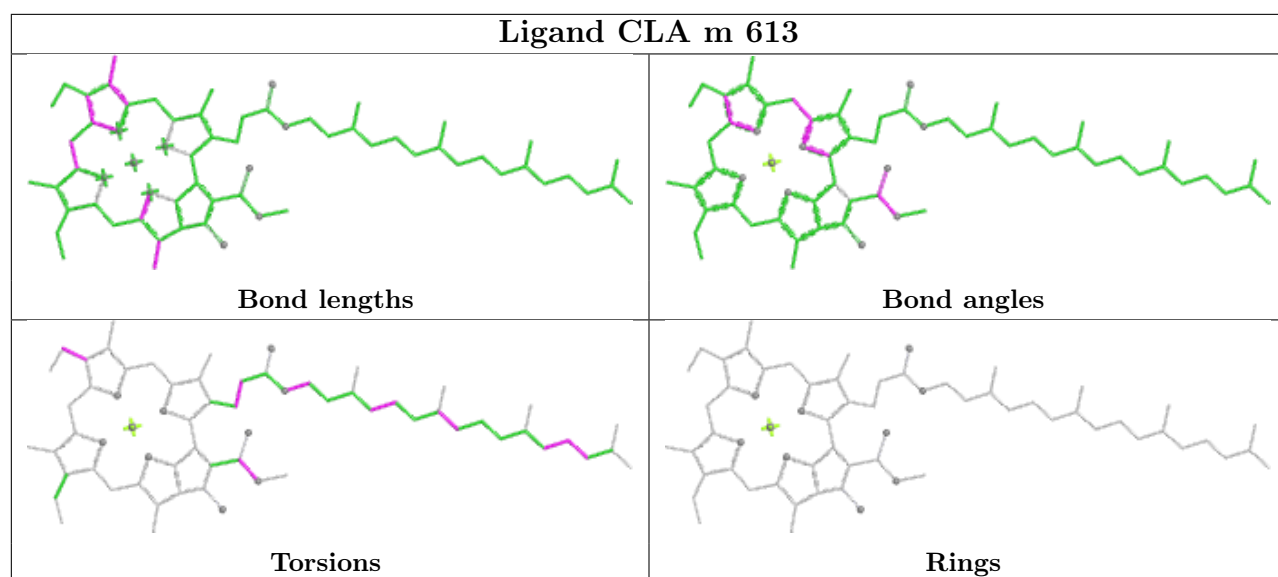


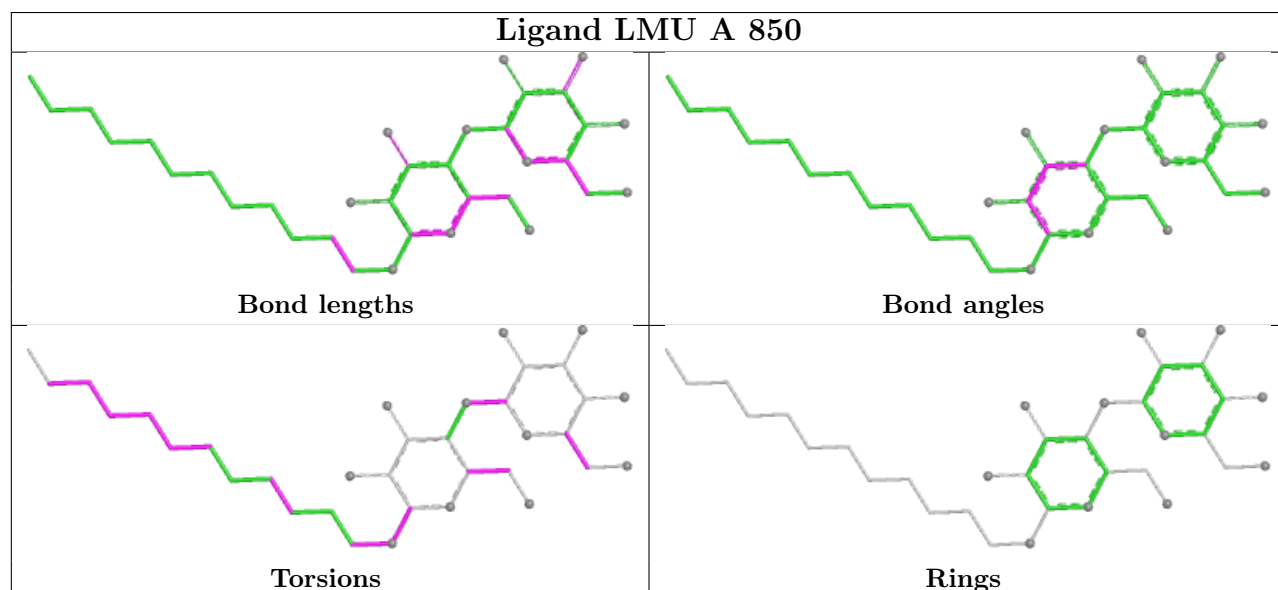
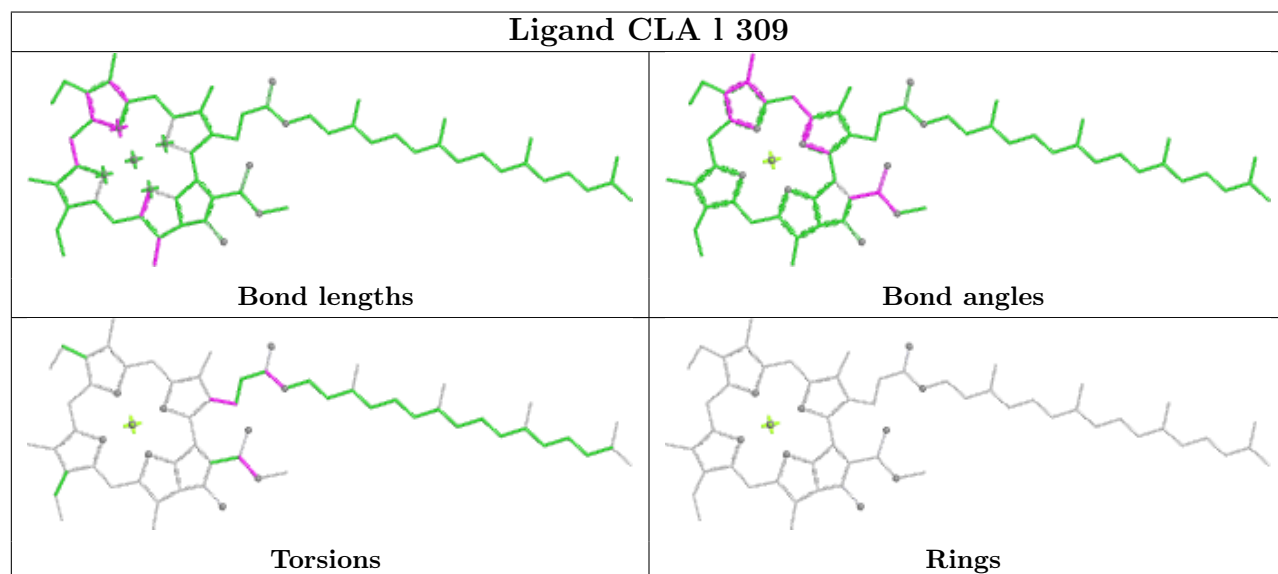
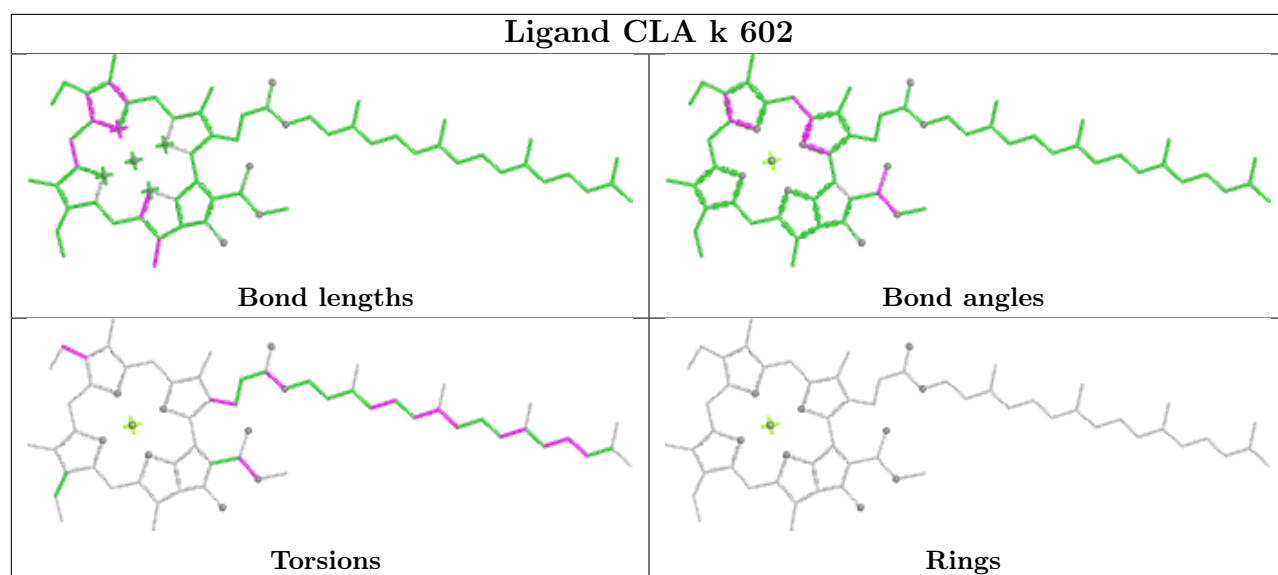
Ligand II0 k 615

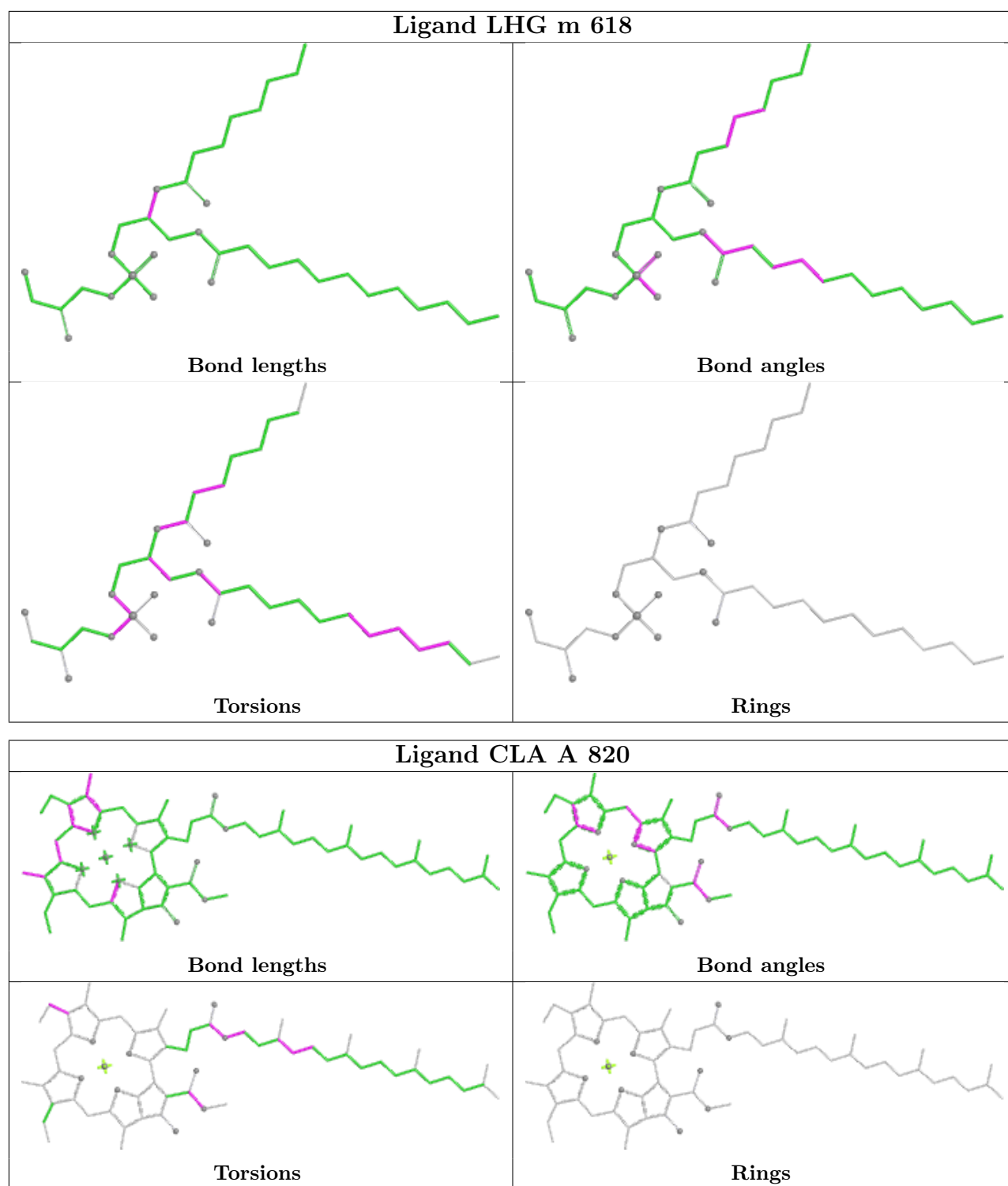


Ligand CLA A 856

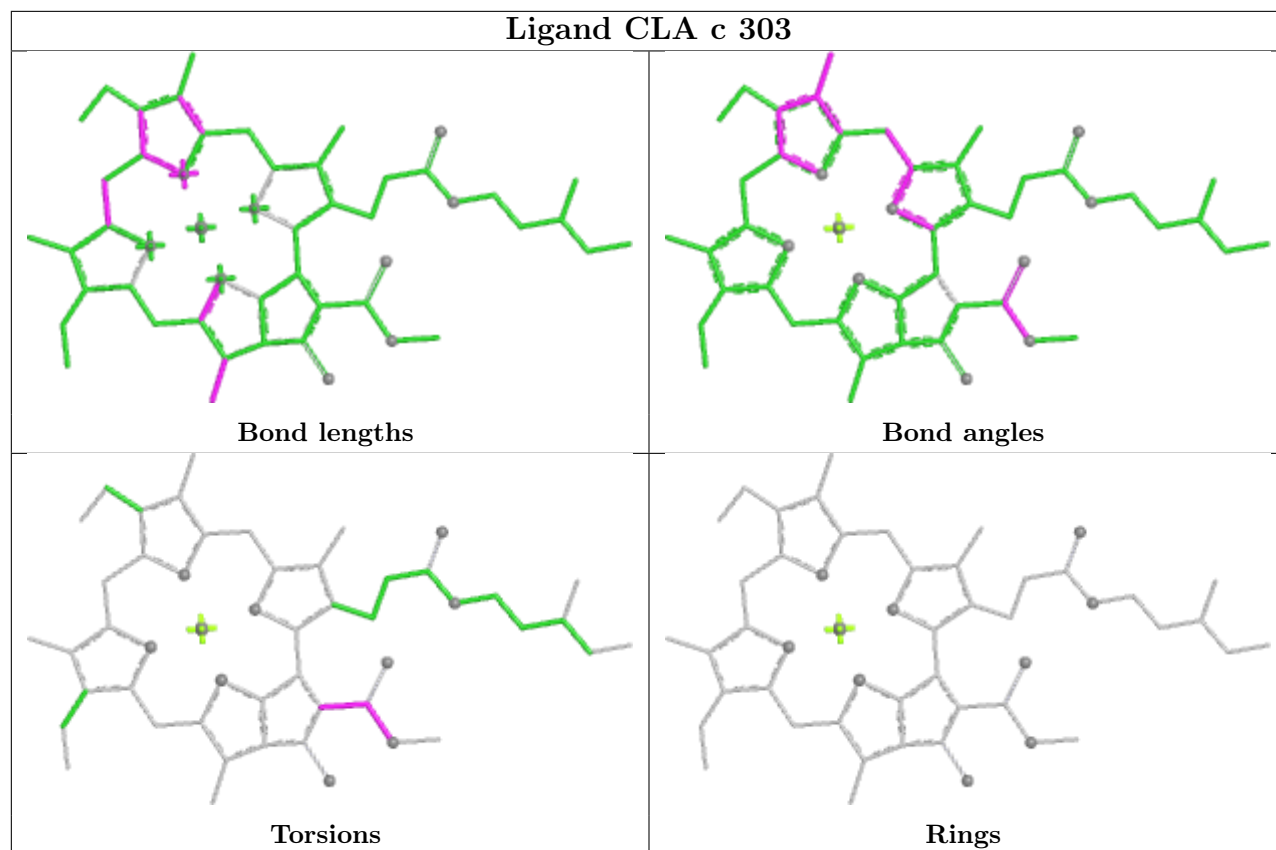




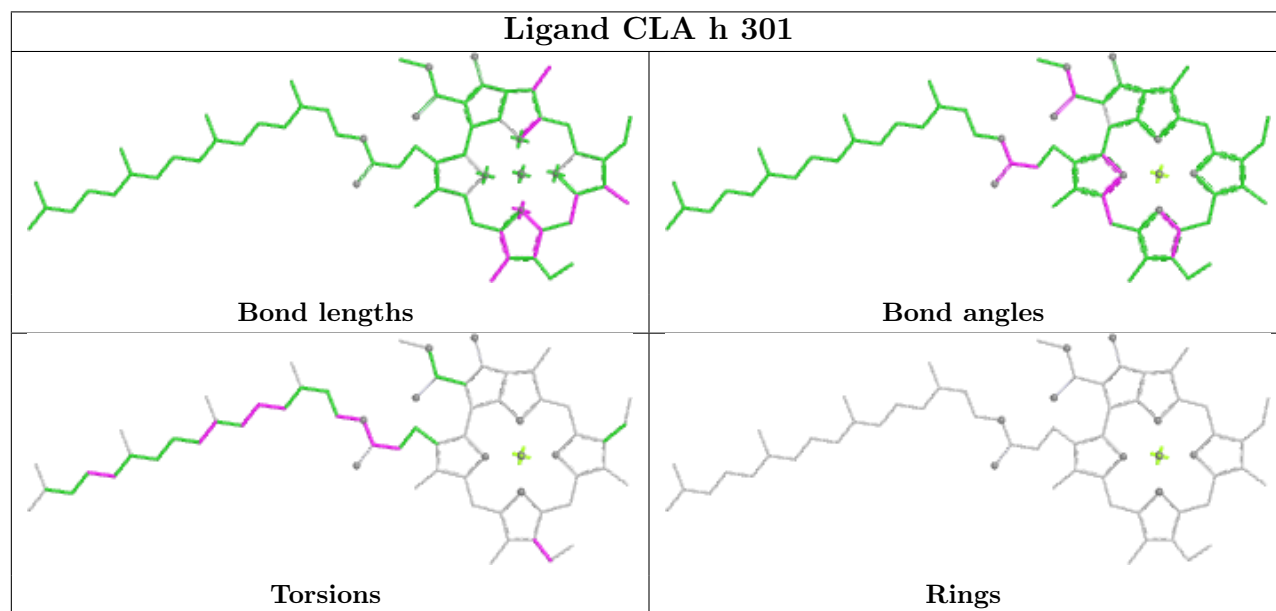


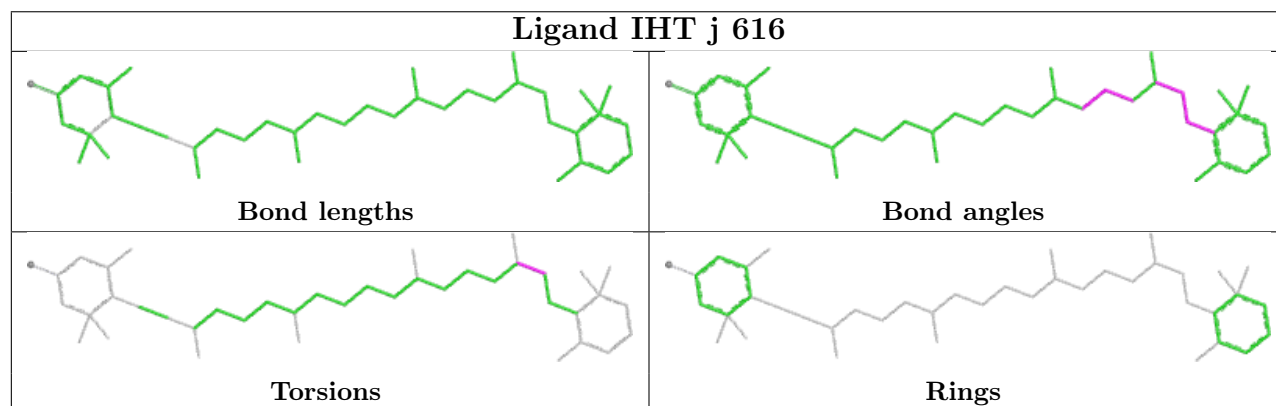
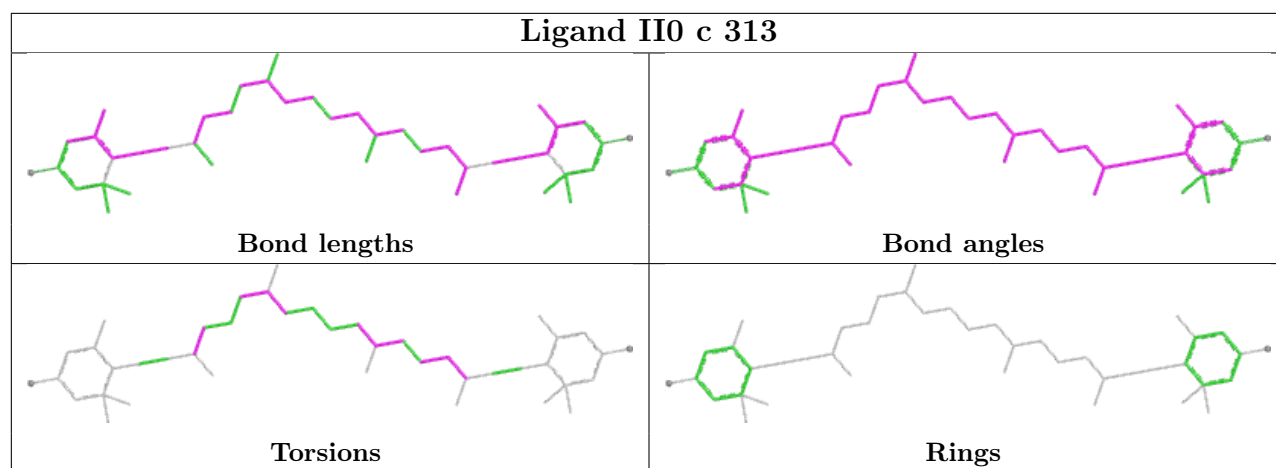
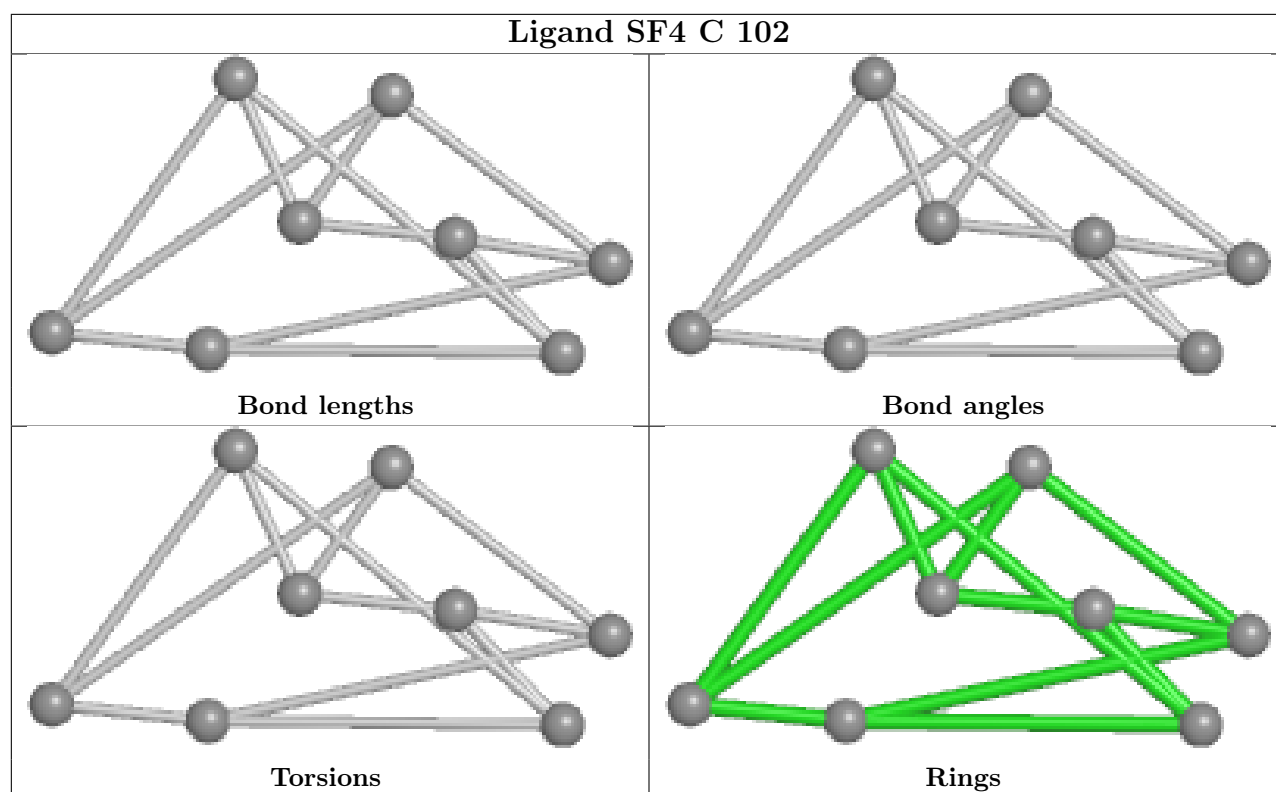


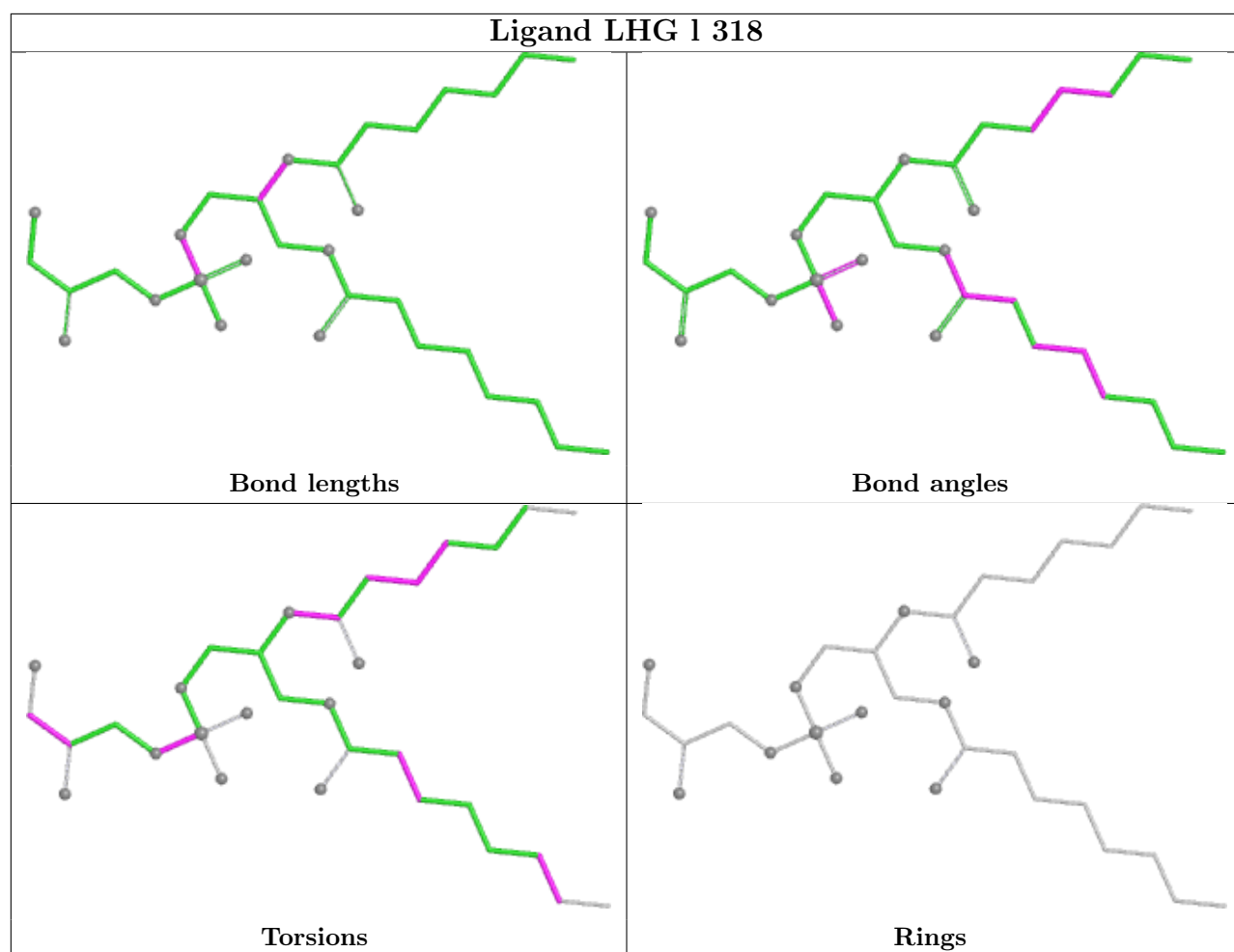
Ligand CLA c 303

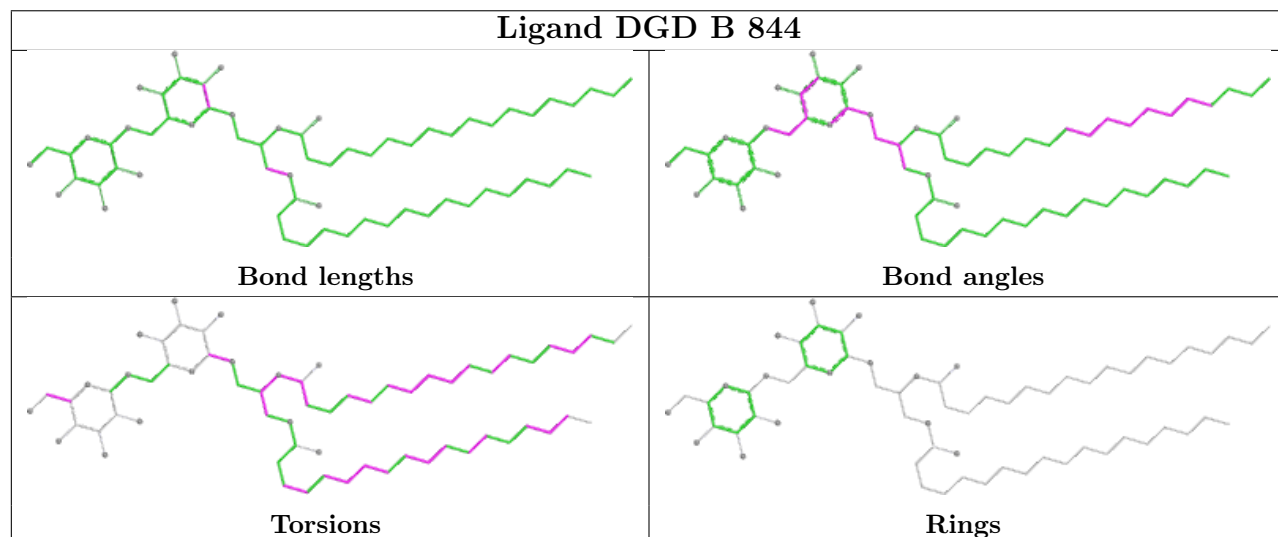
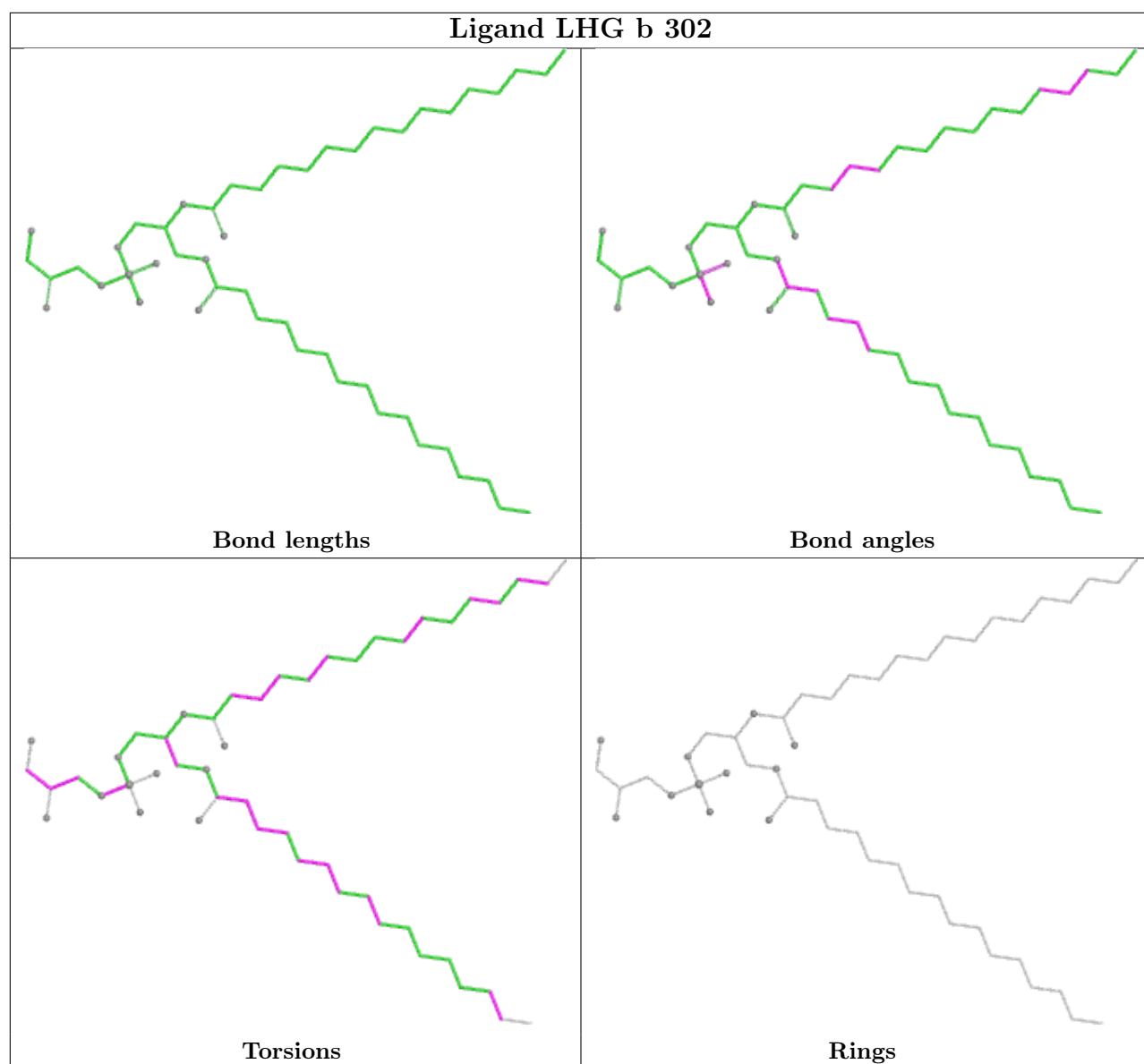


Ligand CLA h 301

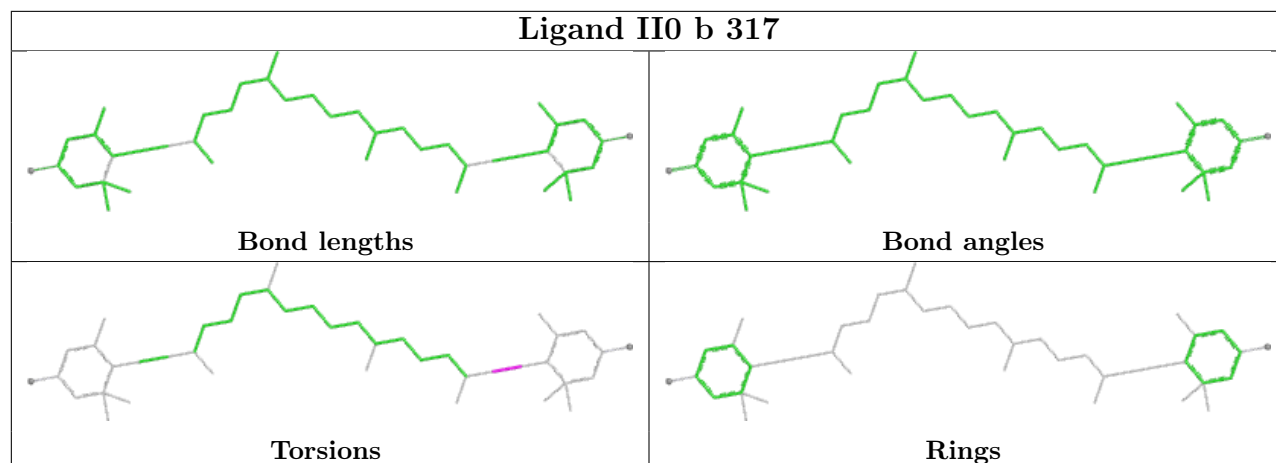




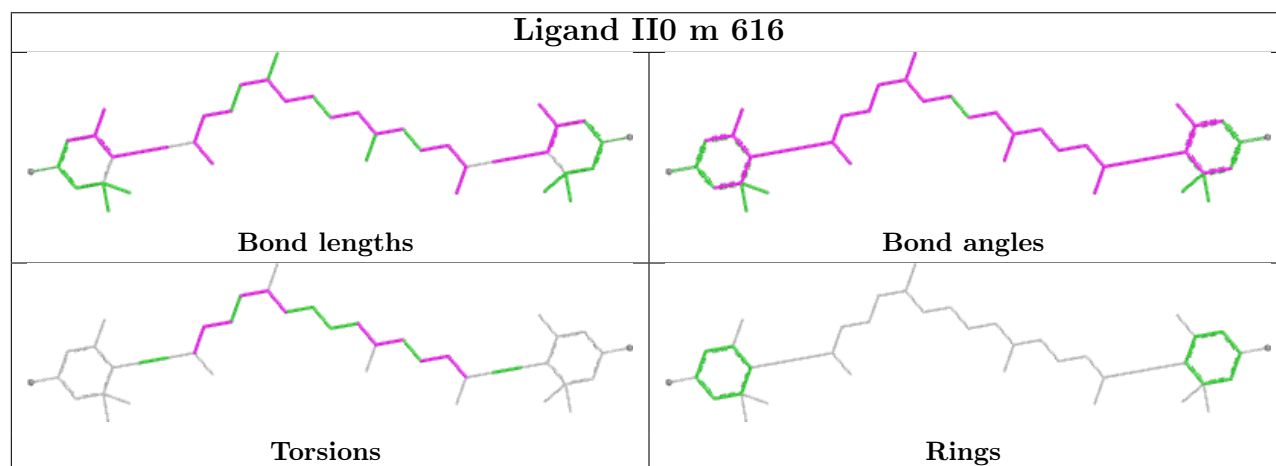




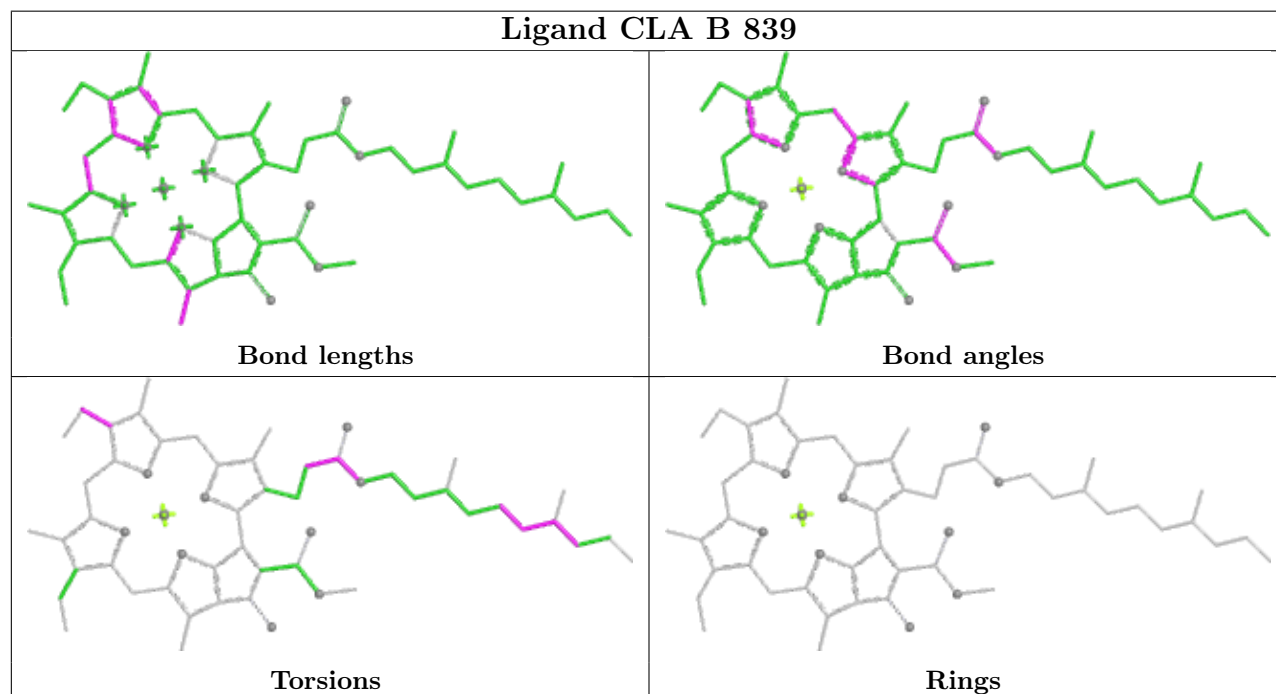
Ligand II0 b 317



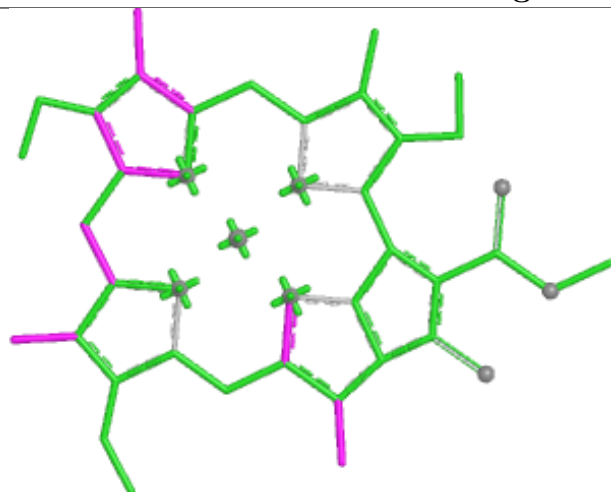
Ligand II0 m 616



Ligand CLA B 839



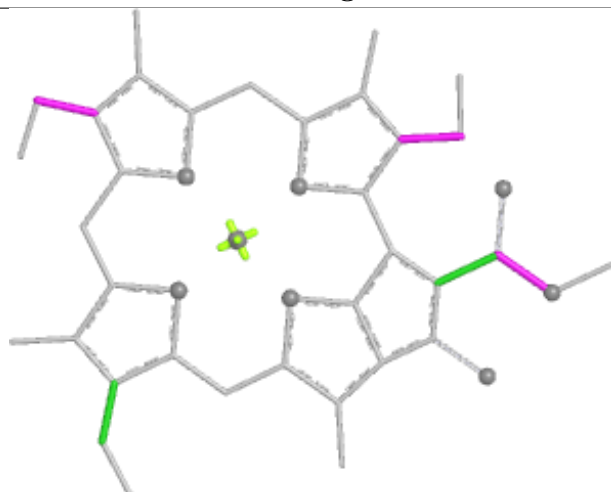
Ligand CLA K 101



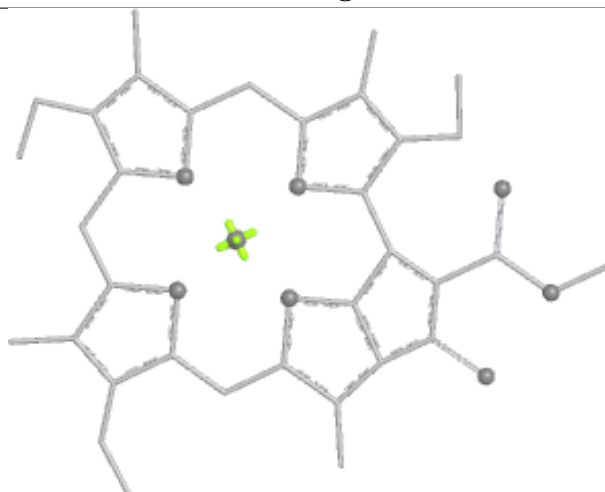
Bond lengths



Bond angles

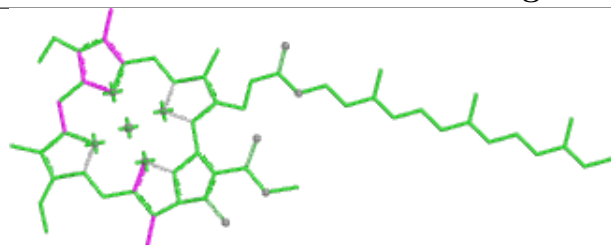


Torsions

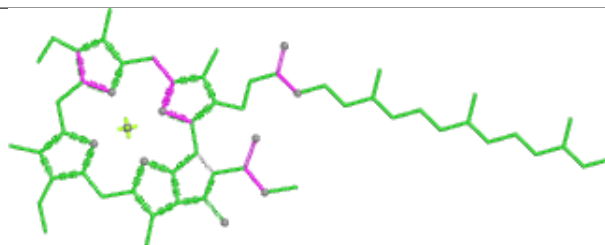


Rings

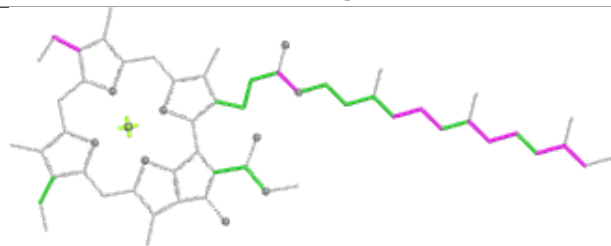
Ligand CLA I 311



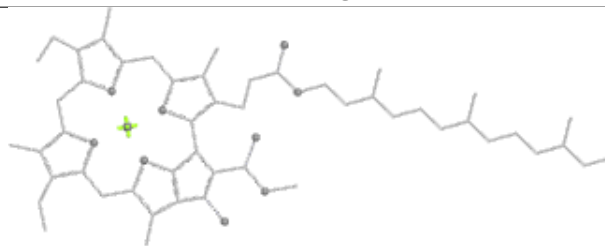
Bond lengths



Bond angles

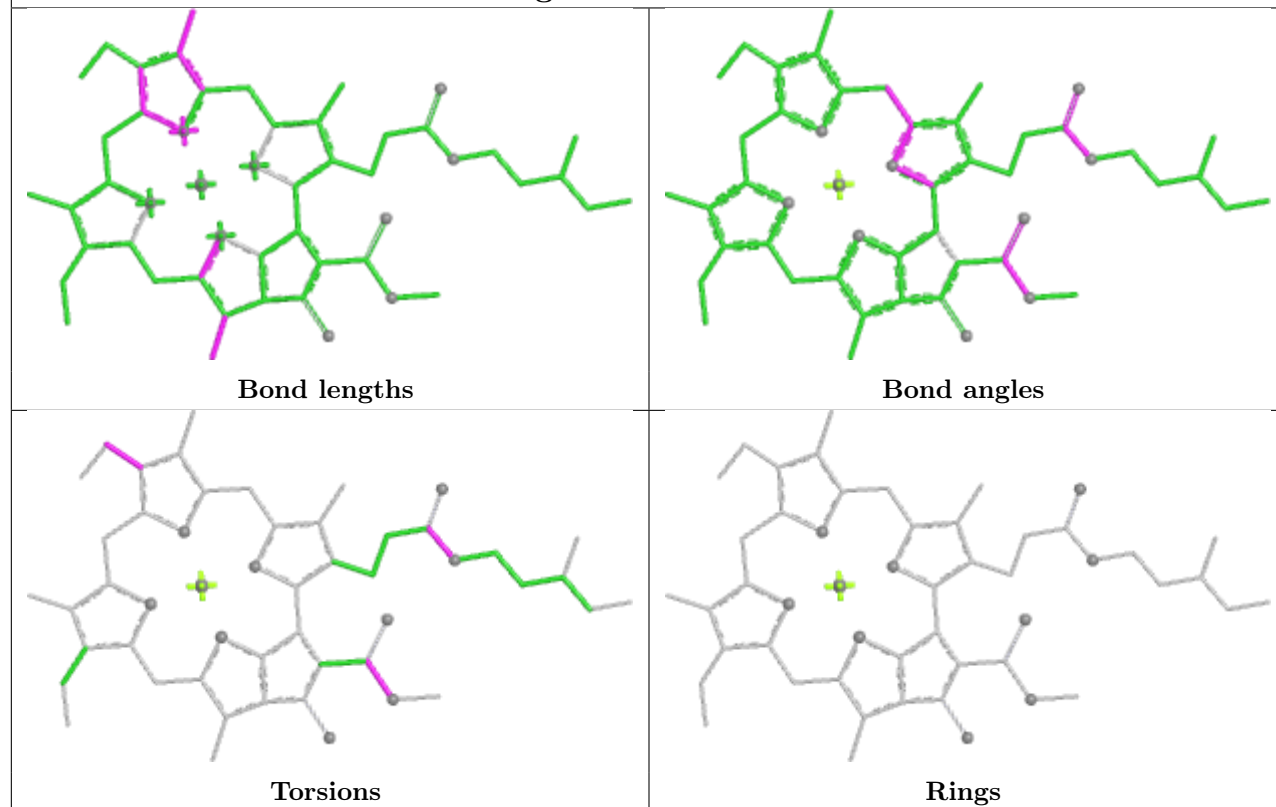


Torsions

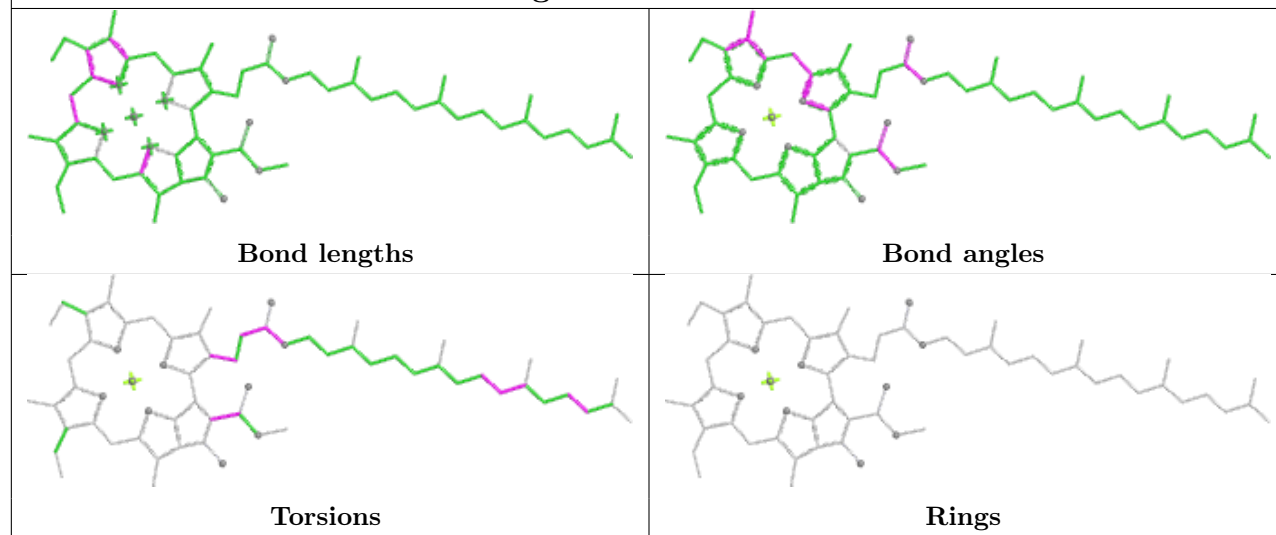


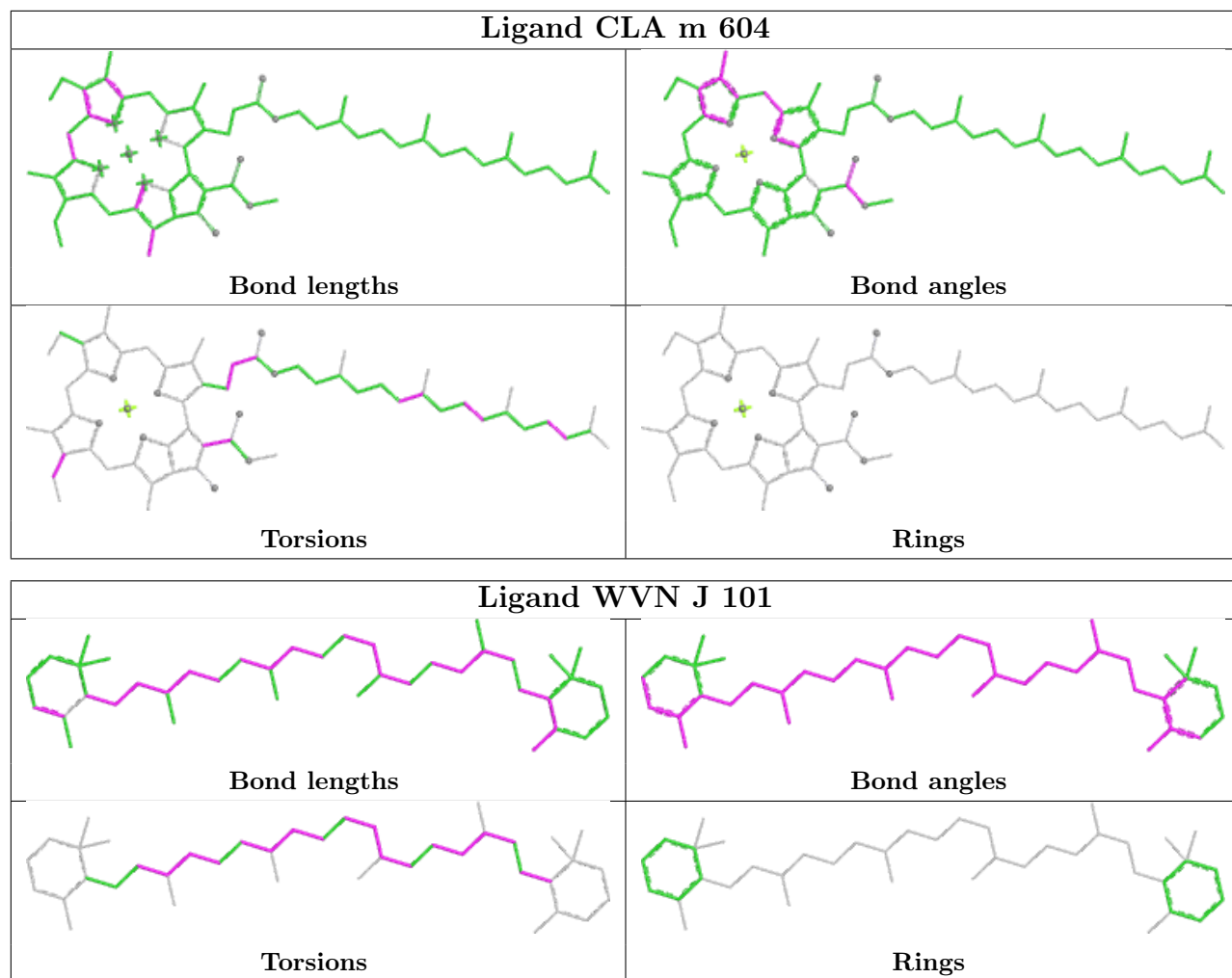
Rings

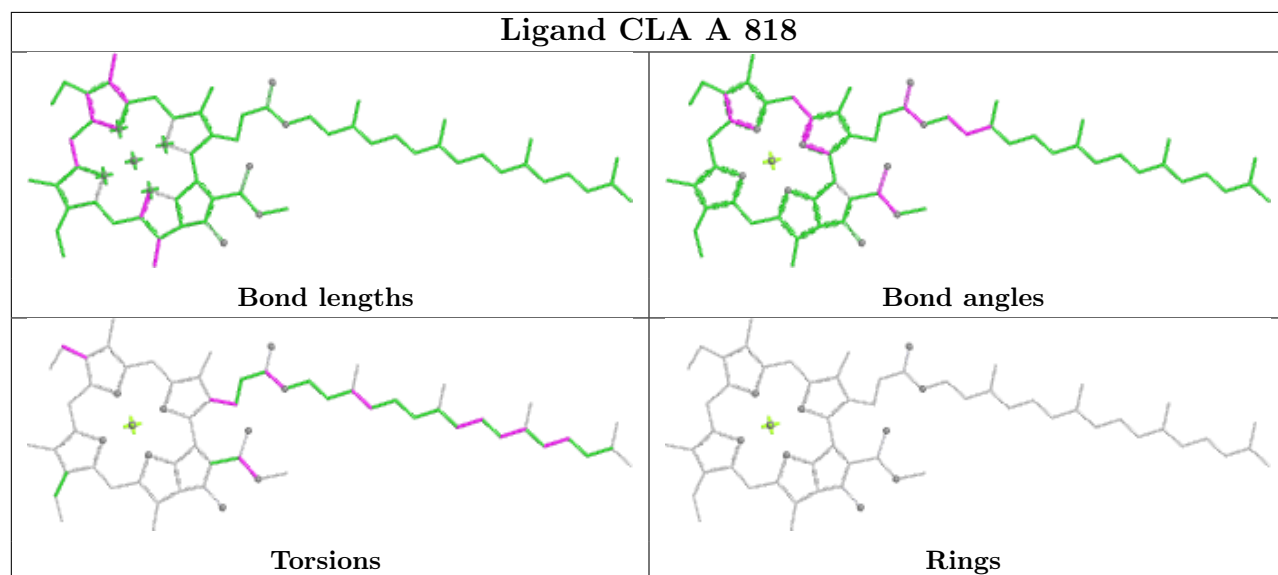
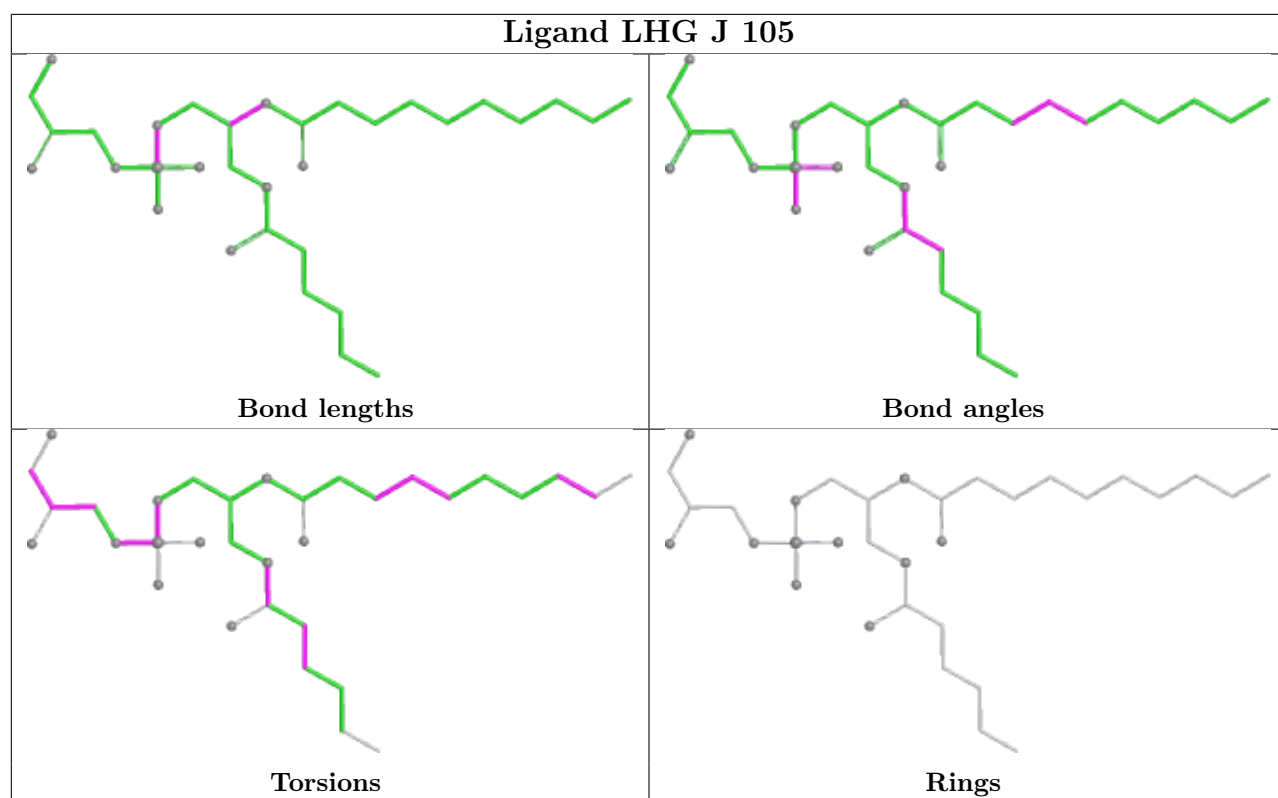
Ligand CLA n 606

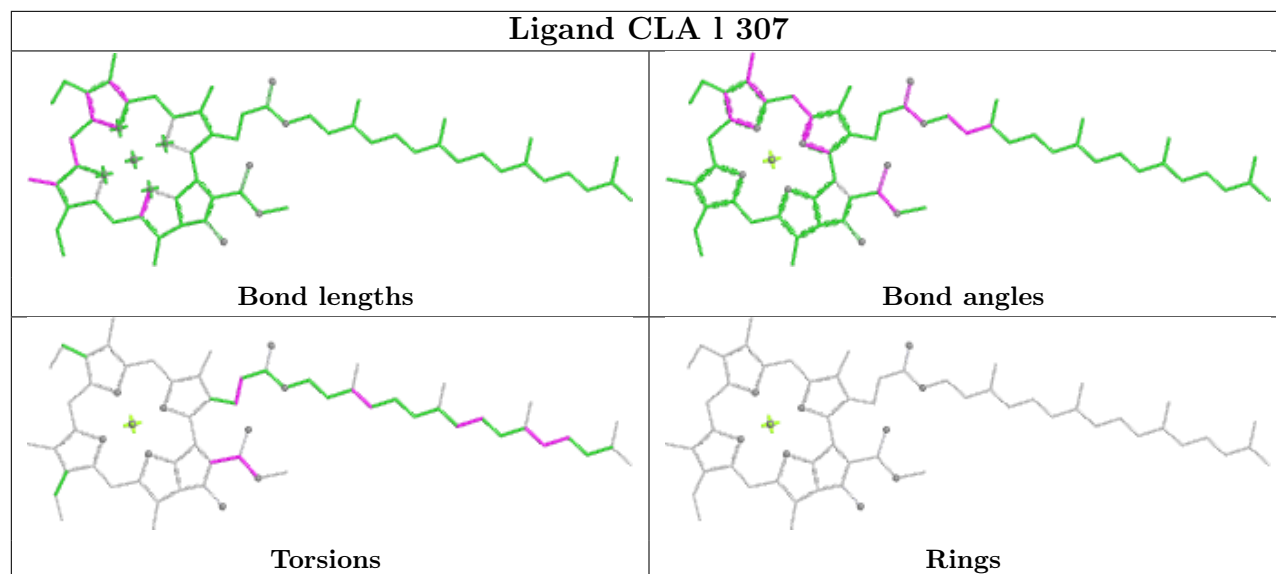
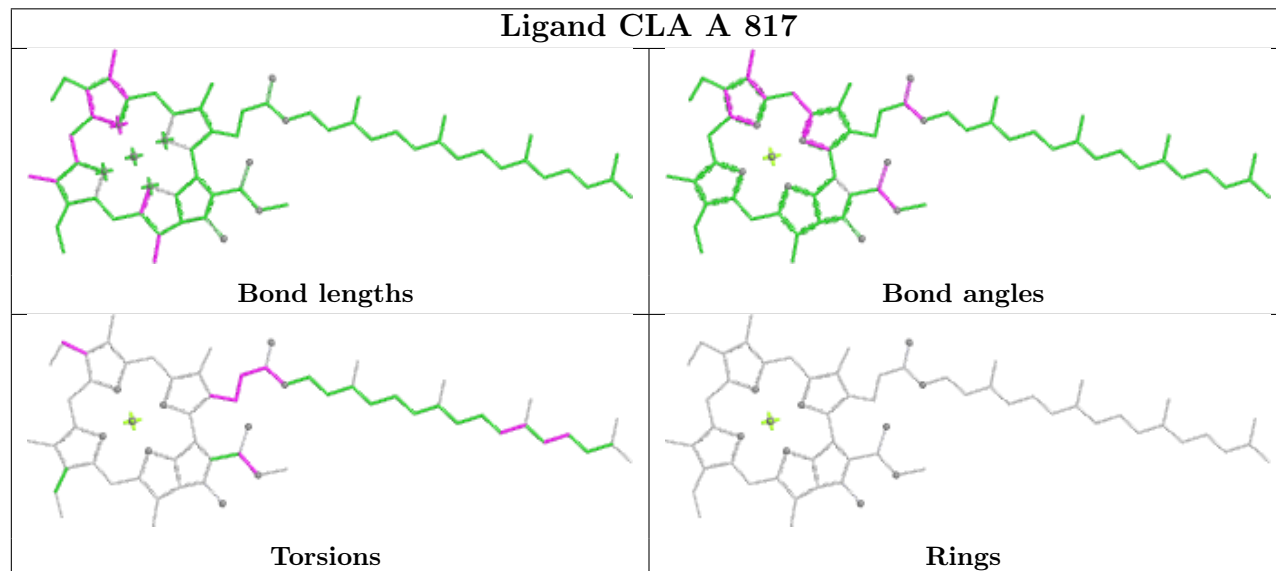


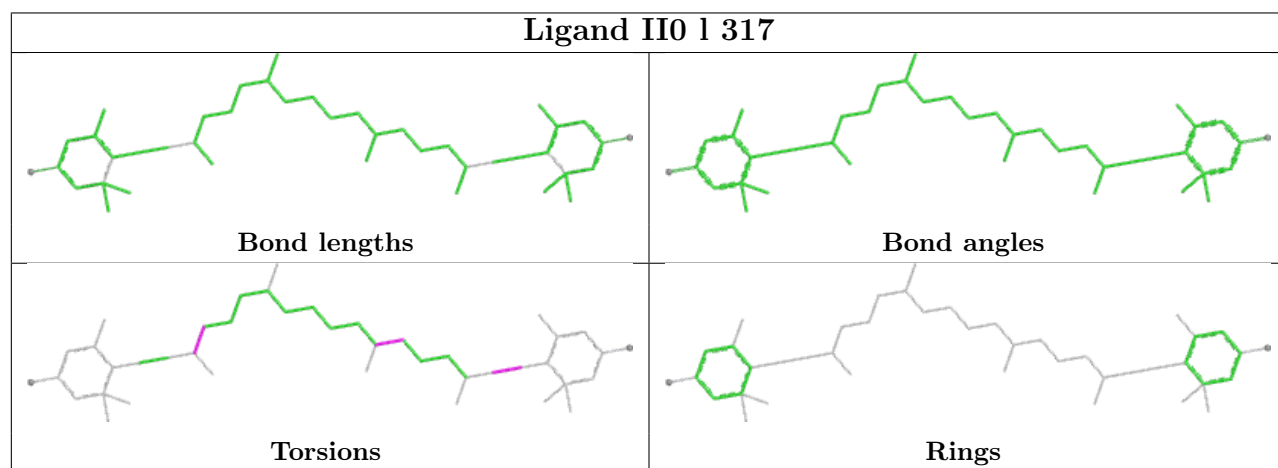
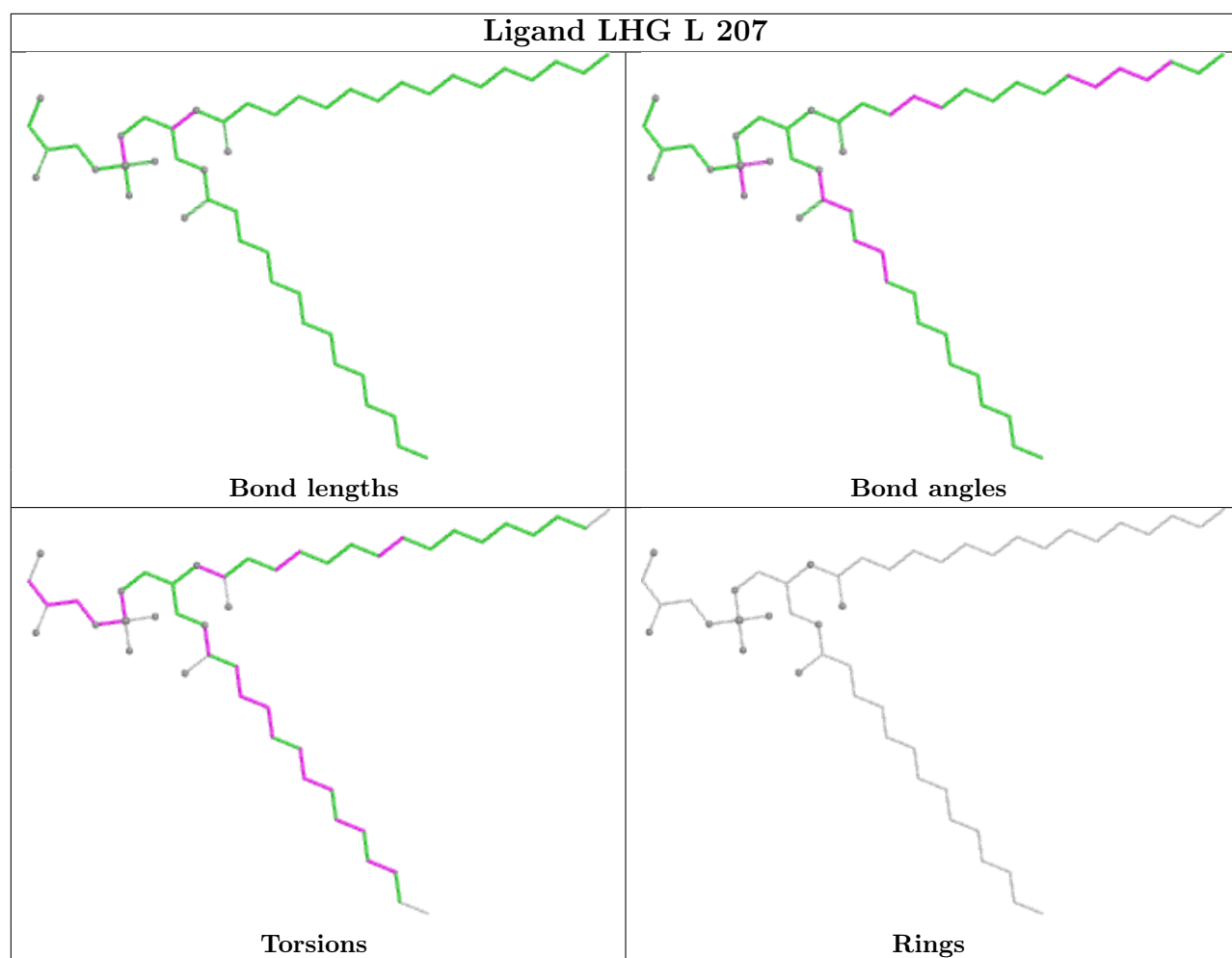
Ligand CLA B 805



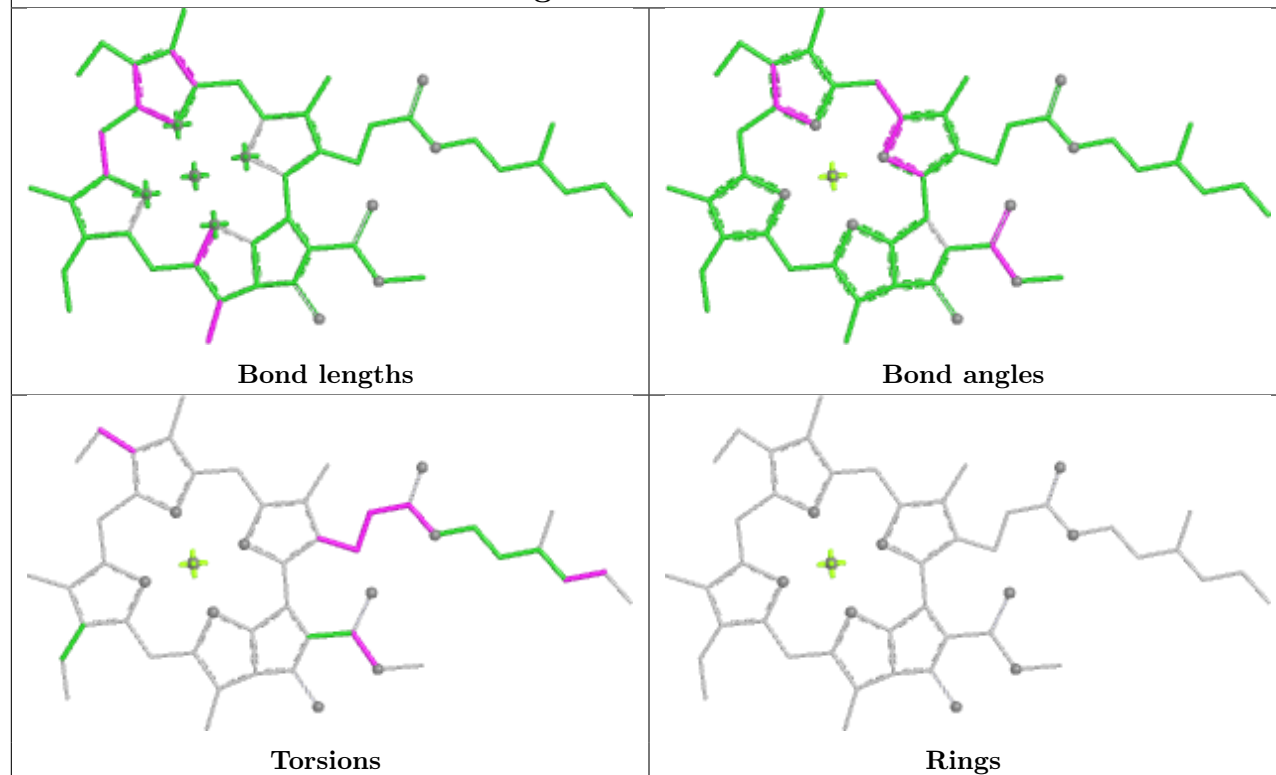




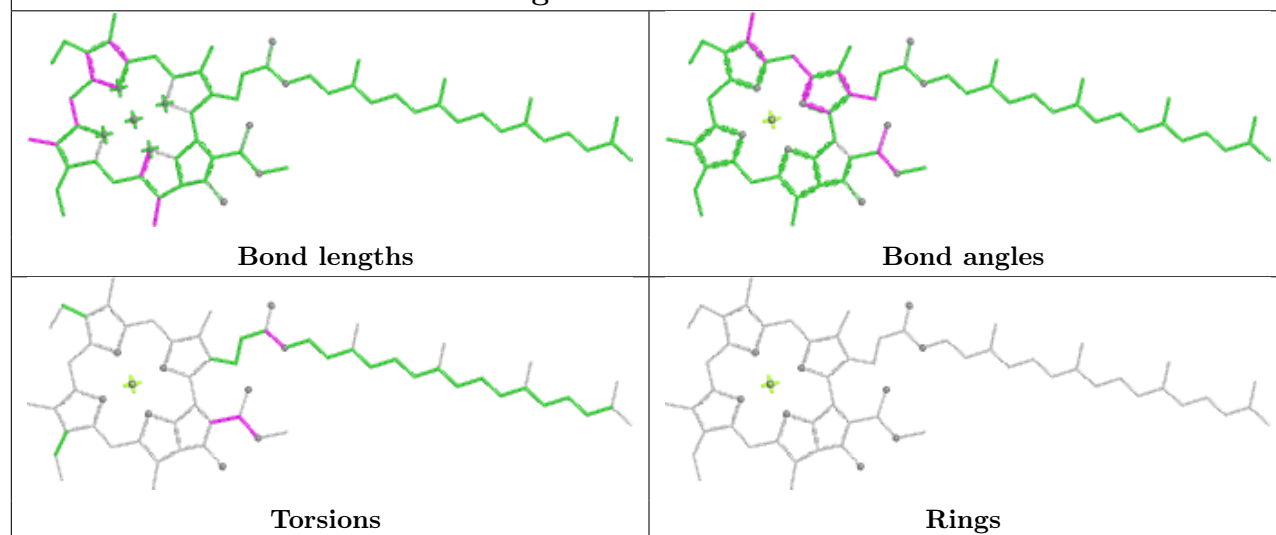
Ligand CLA I 307**Ligand CLA A 817**

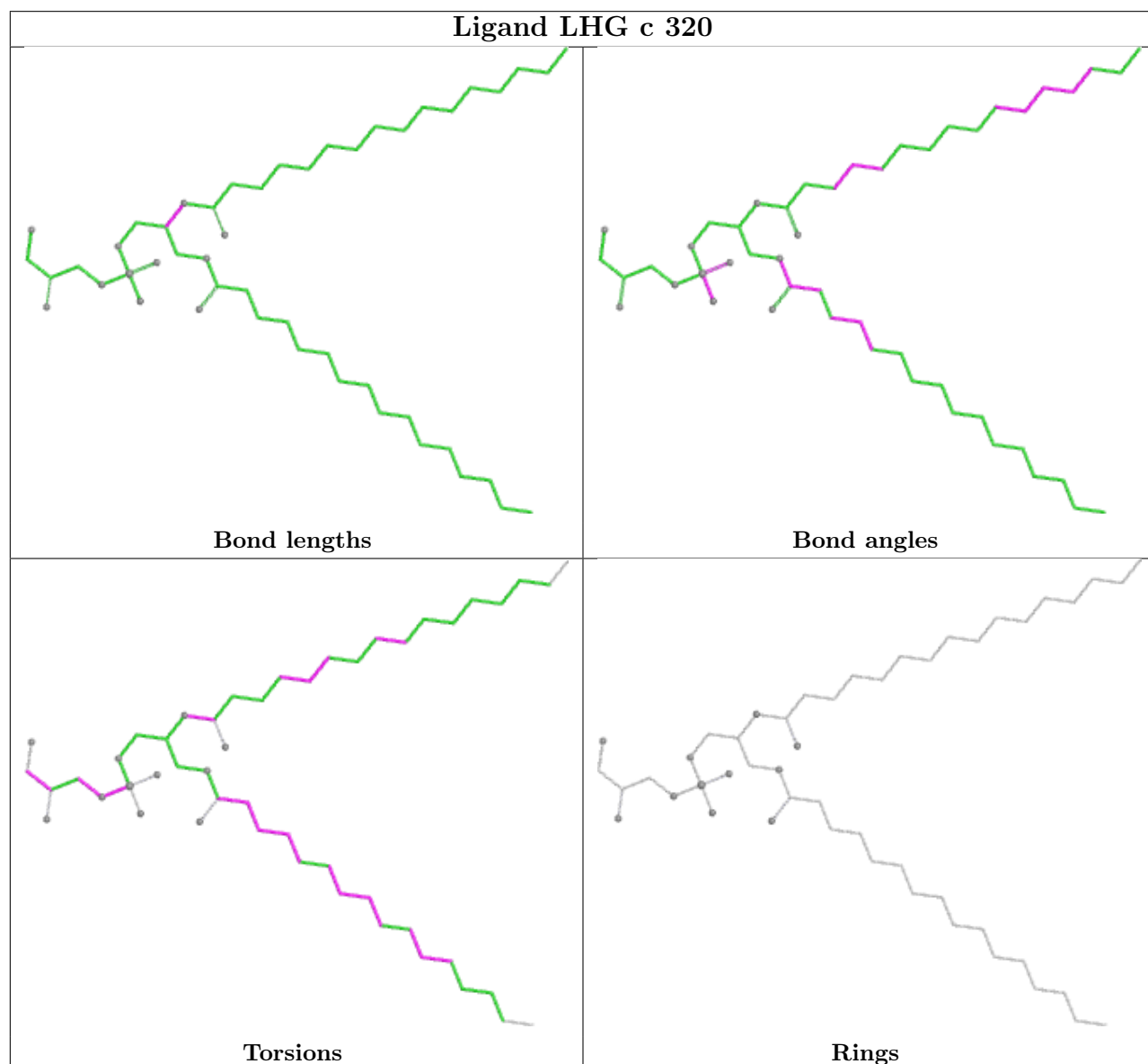
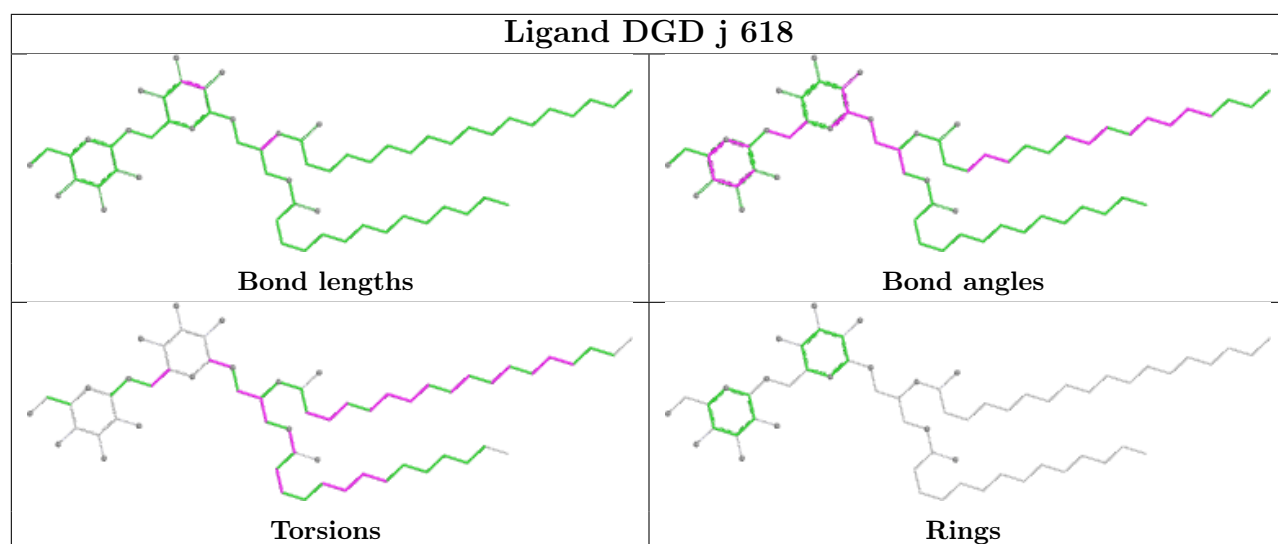


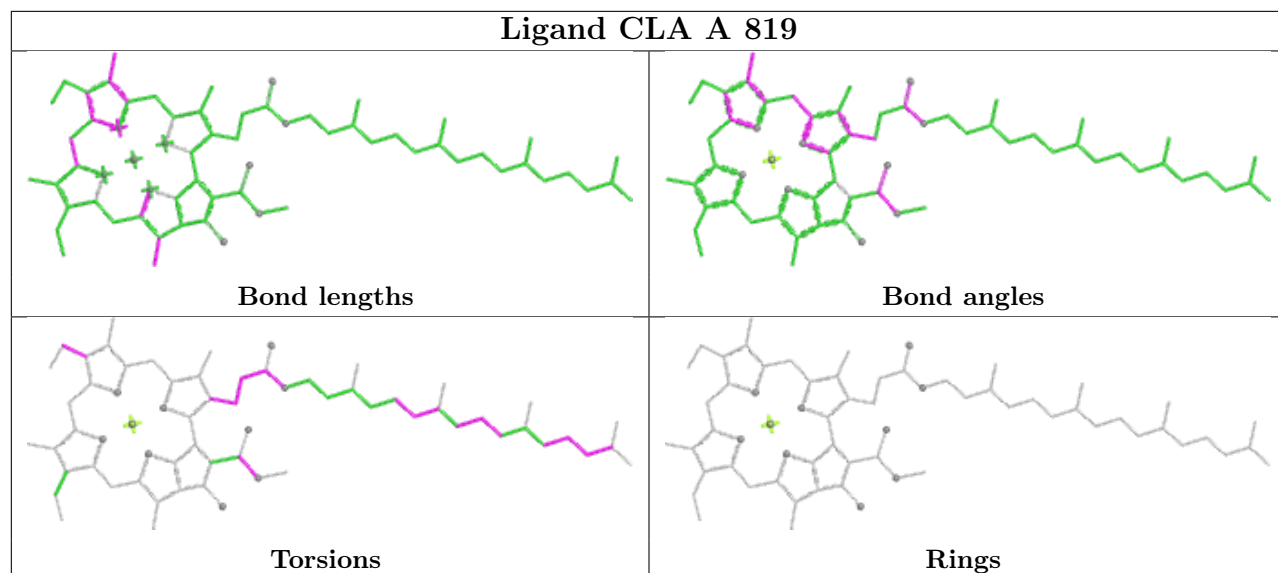
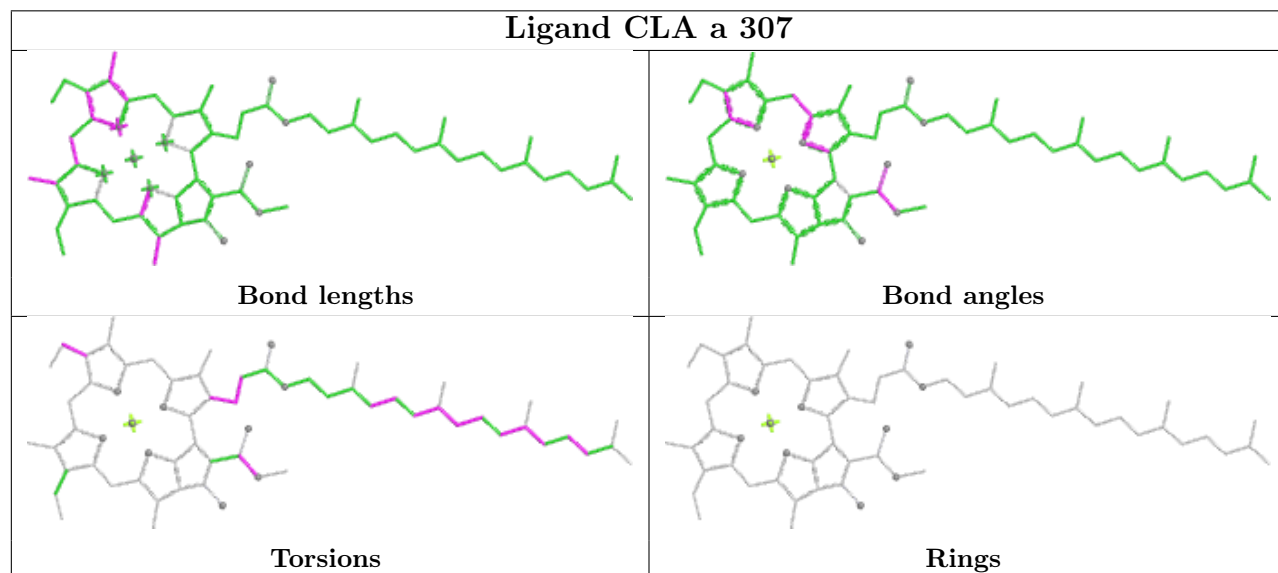
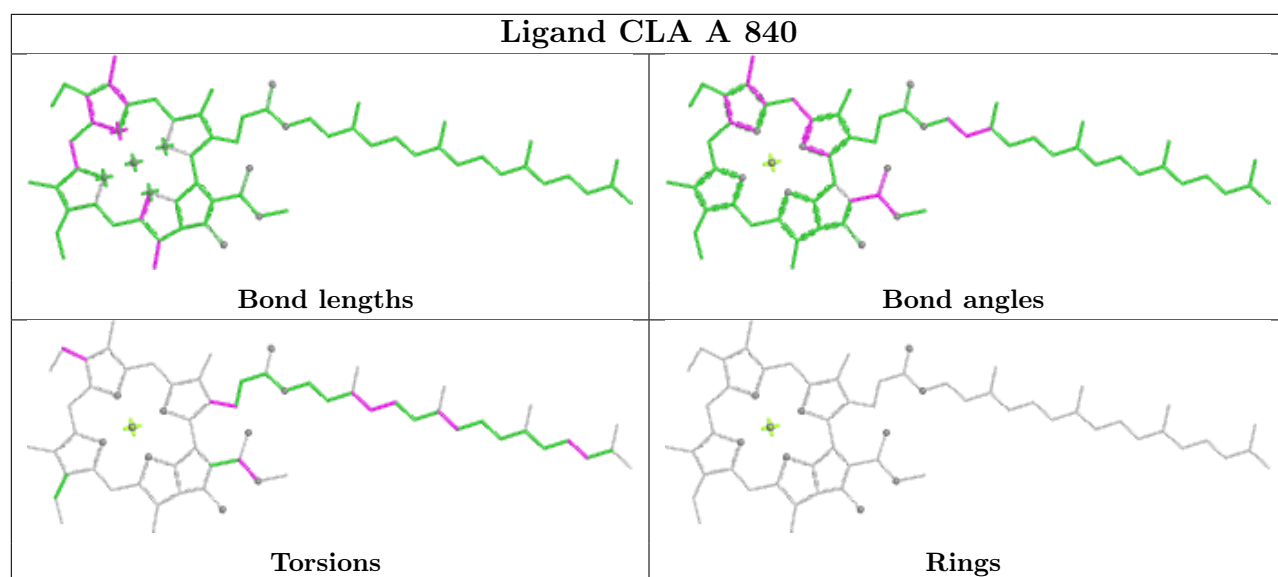
Ligand CLA F 202



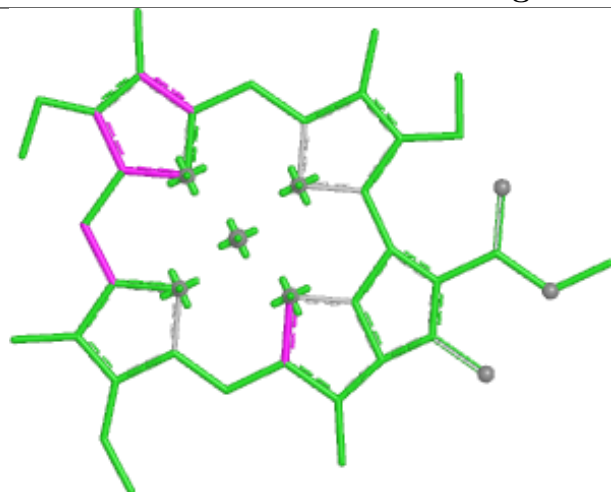
Ligand CLA A 804



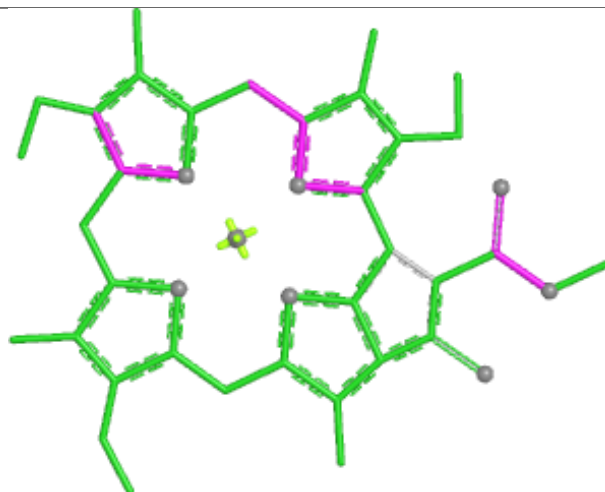




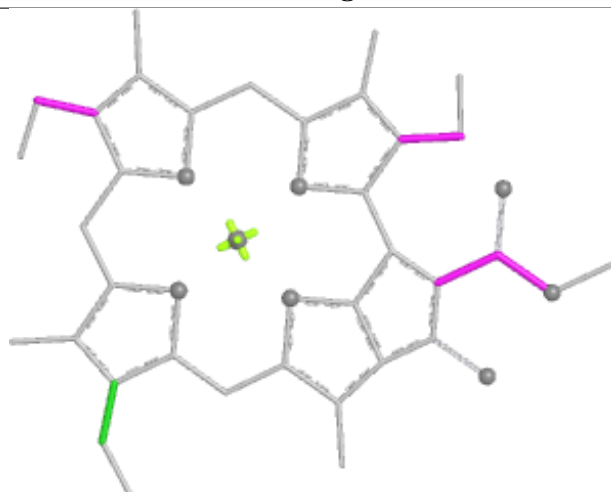
Ligand CLA m 605



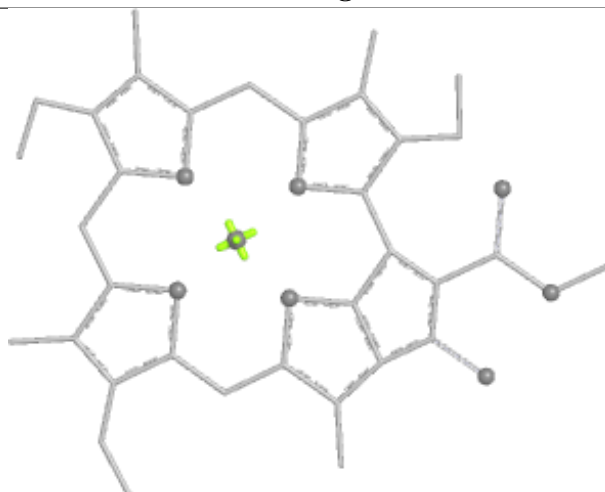
Bond lengths



Bond angles

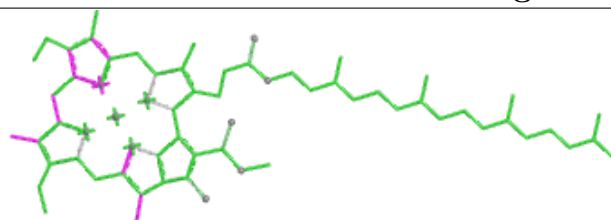


Torsions

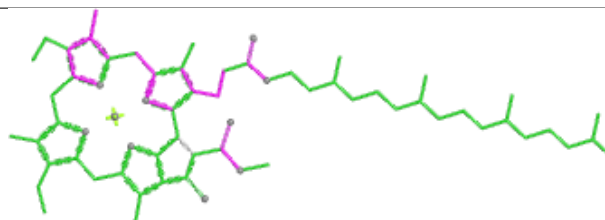


Rings

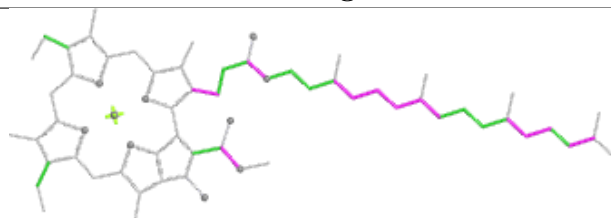
Ligand CLA A 816



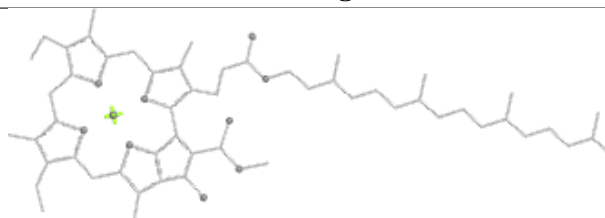
Bond lengths



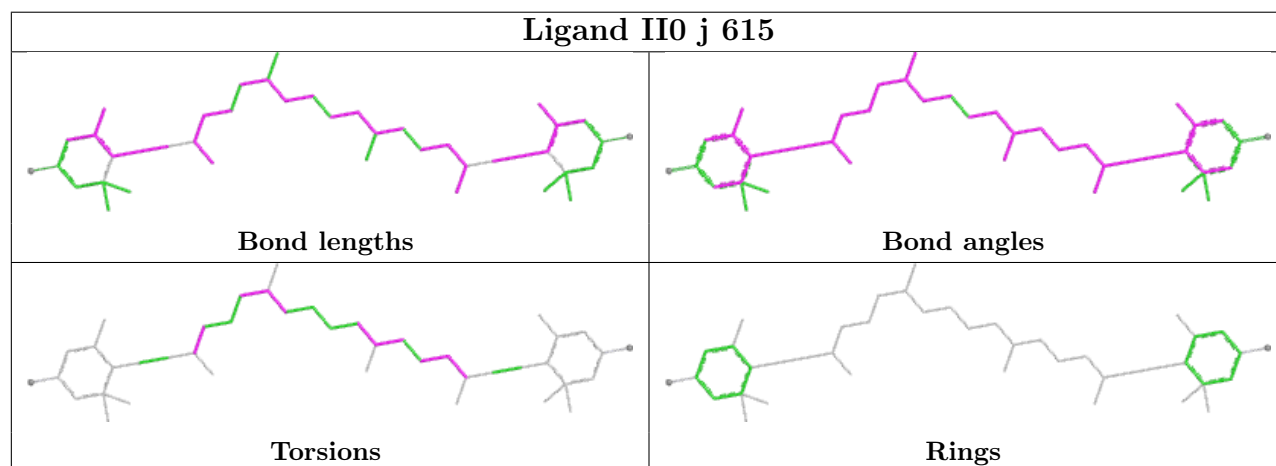
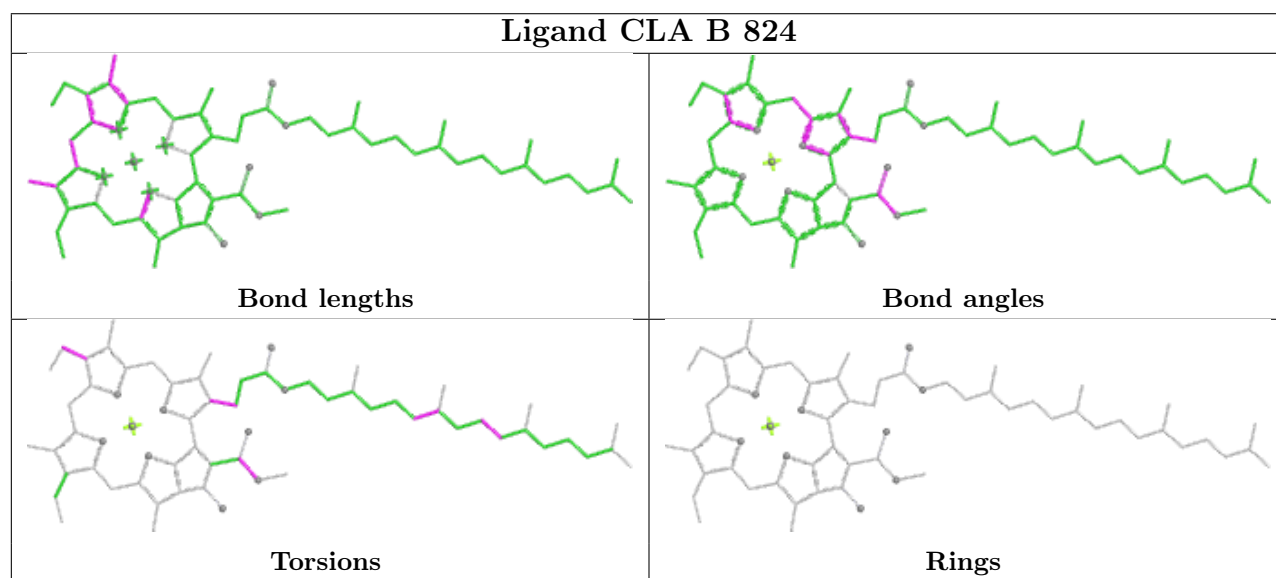
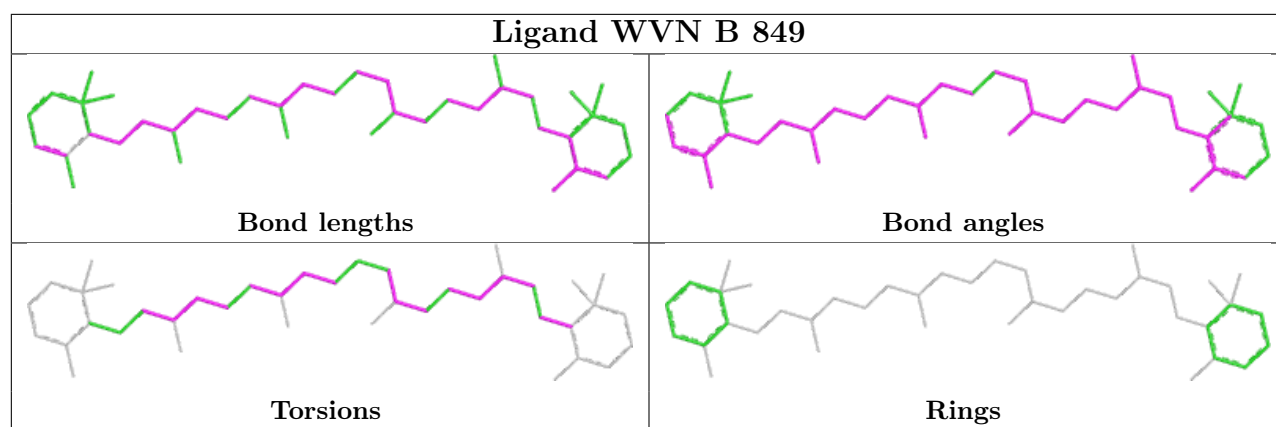
Bond angles

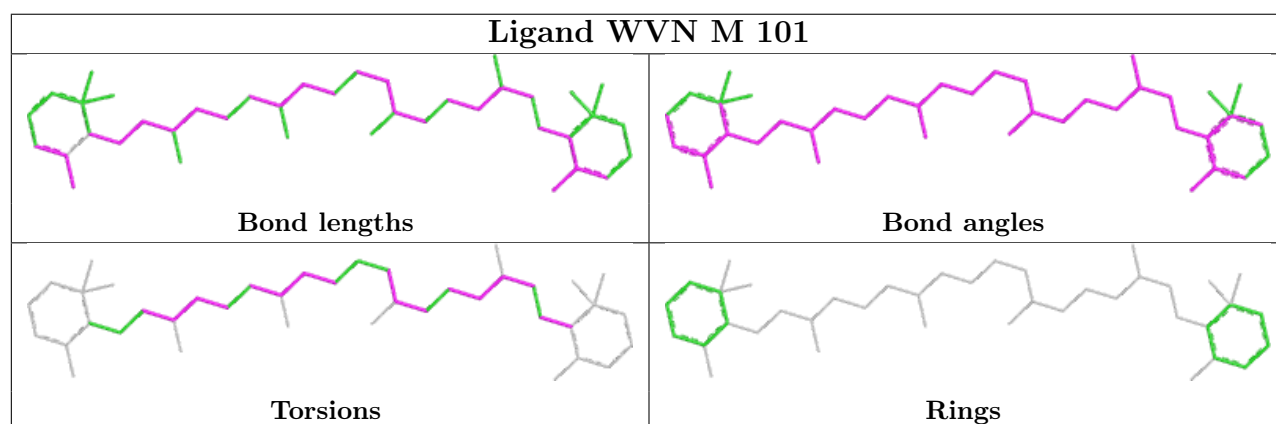
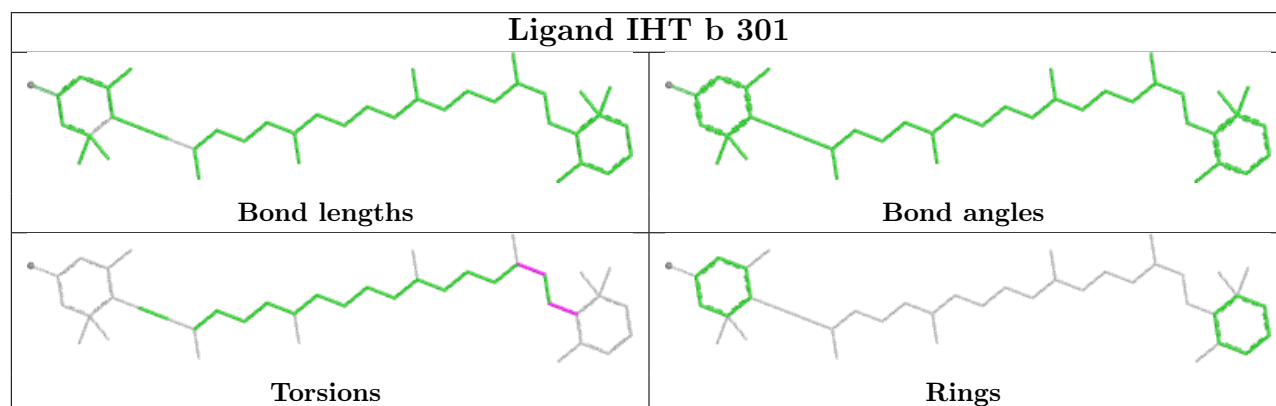
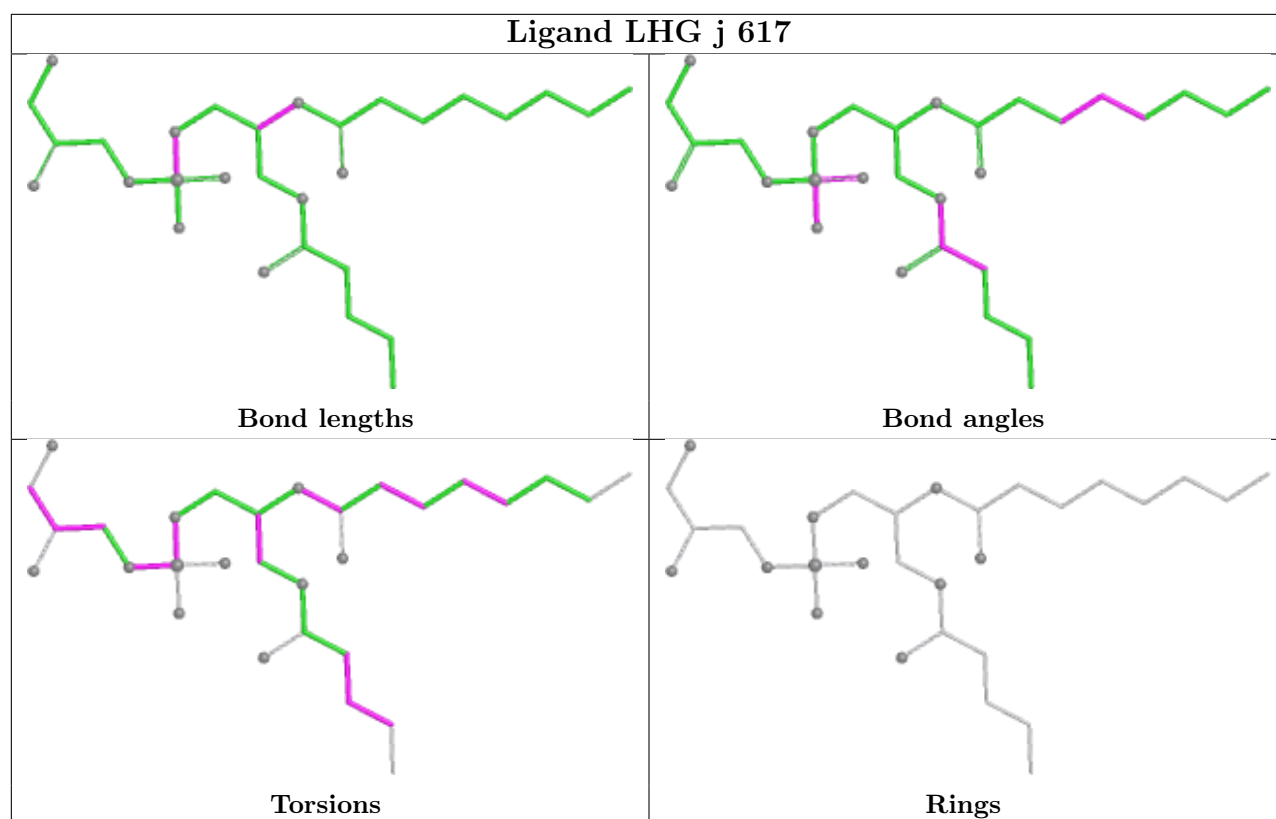


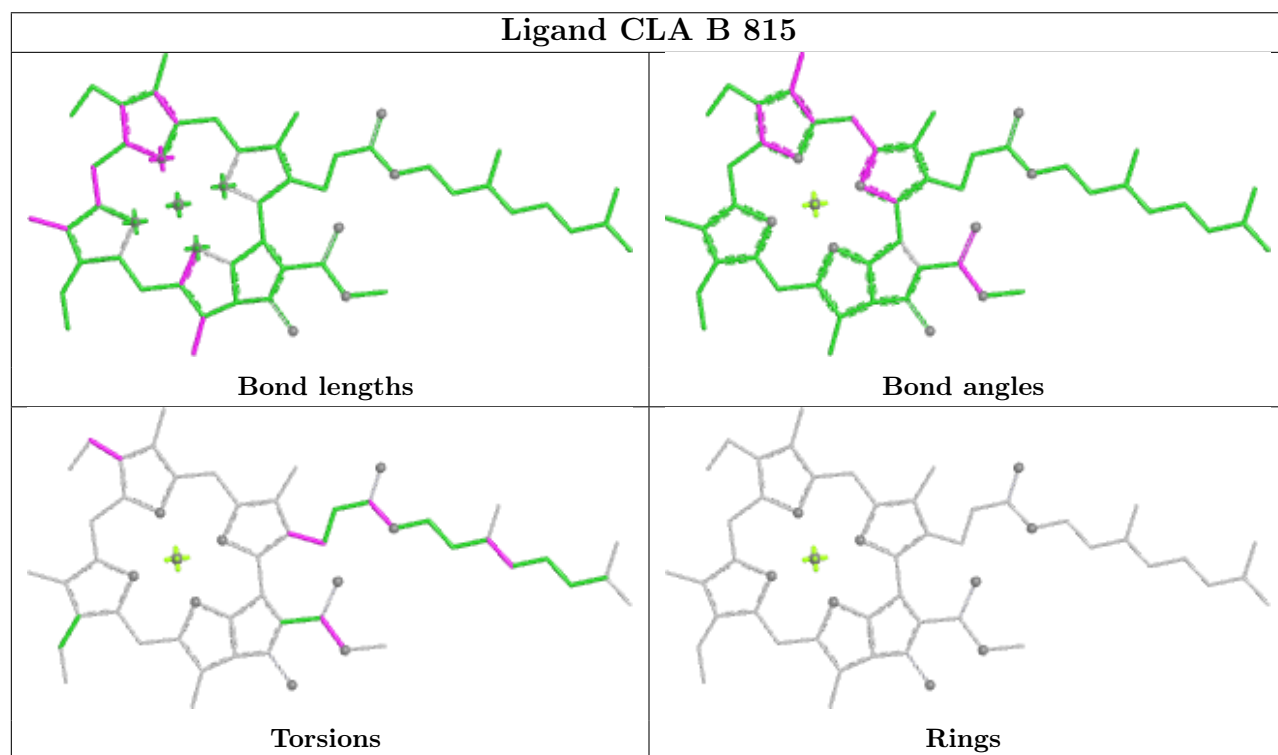
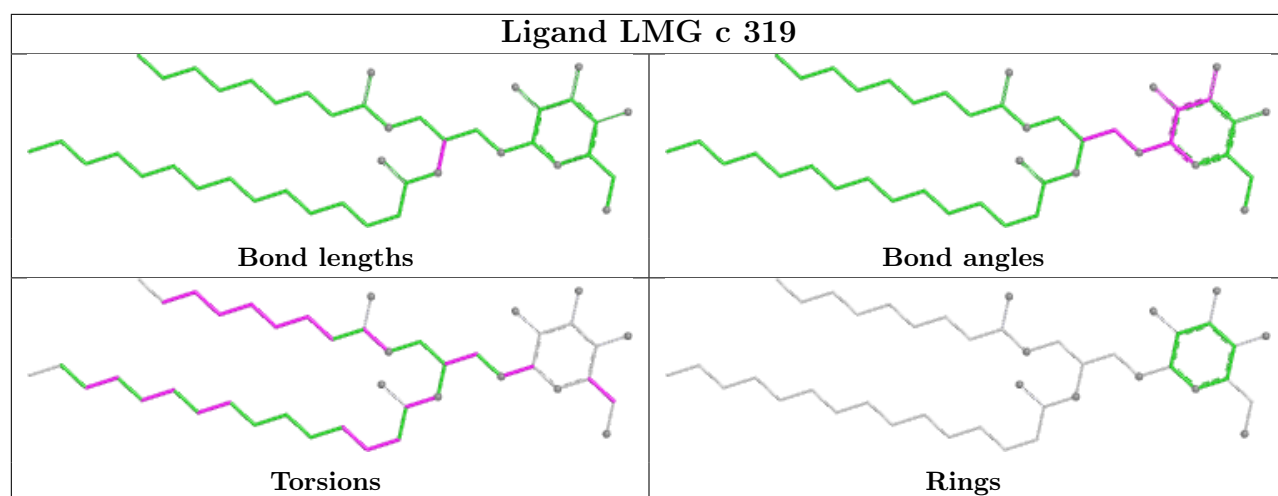
Torsions



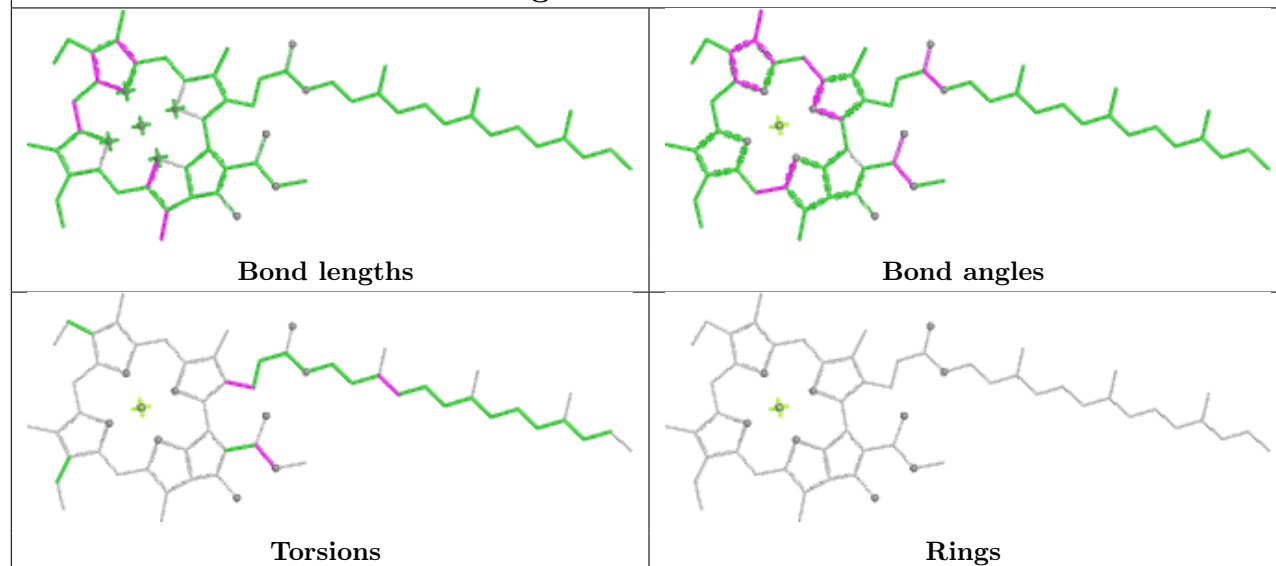
Rings



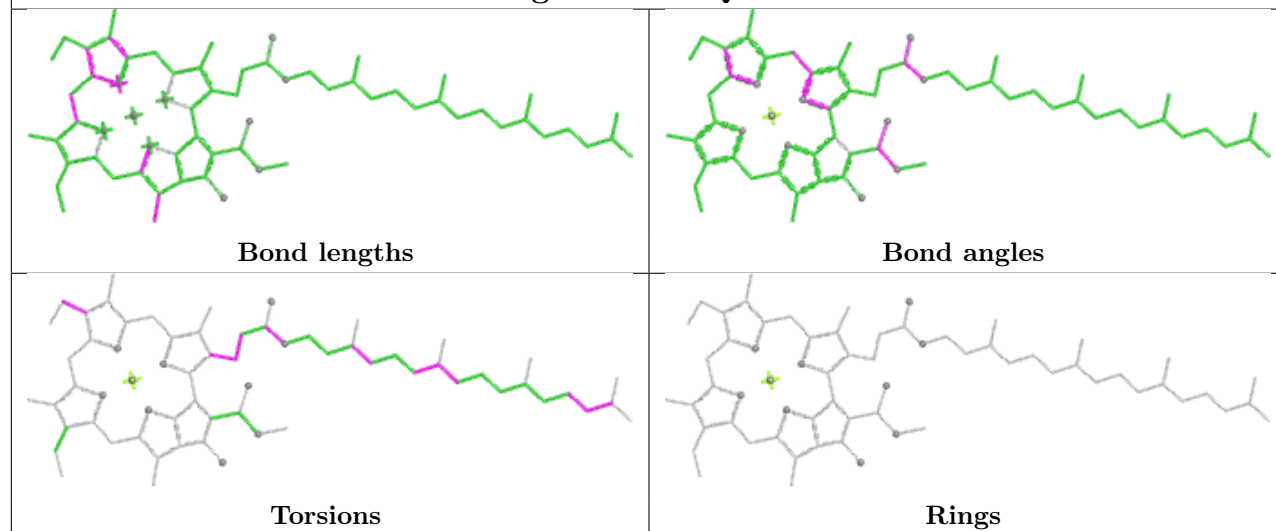




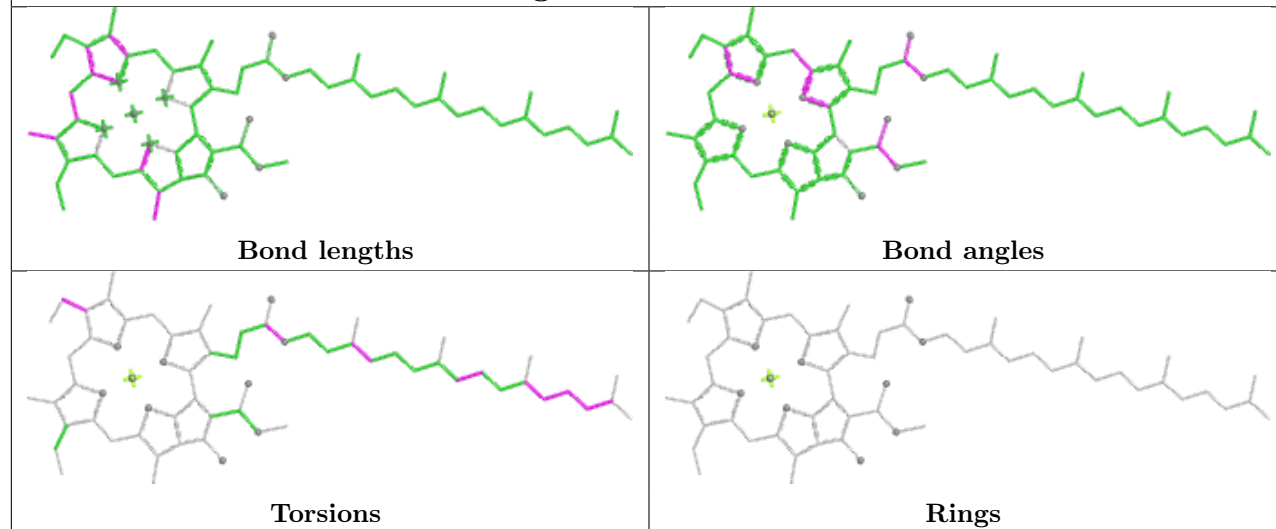
Ligand CLA A 827



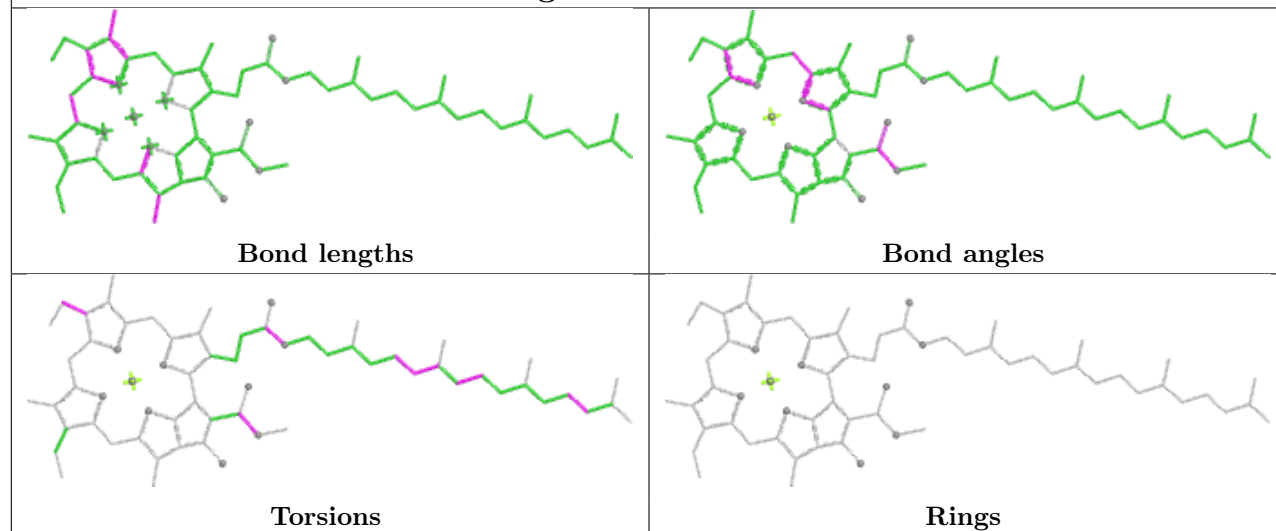
Ligand CLA Q 302



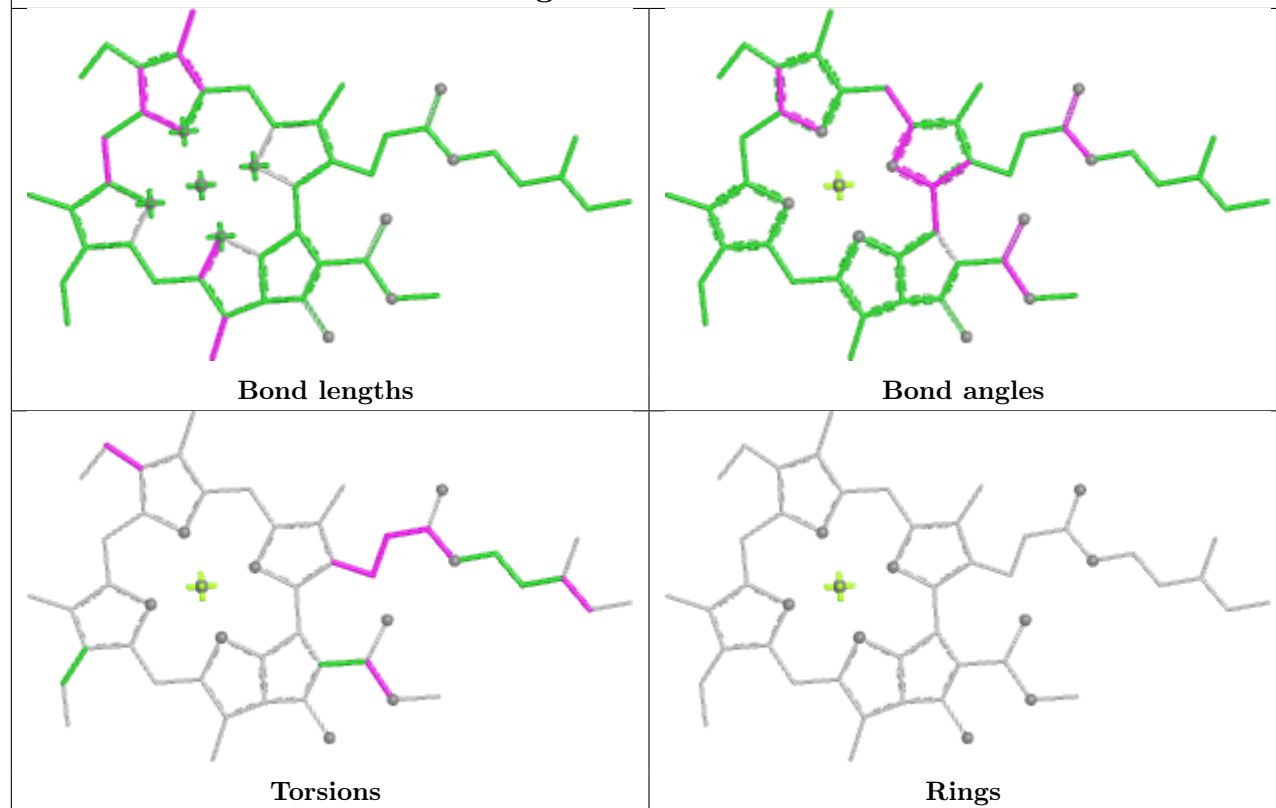
Ligand CLA B 834



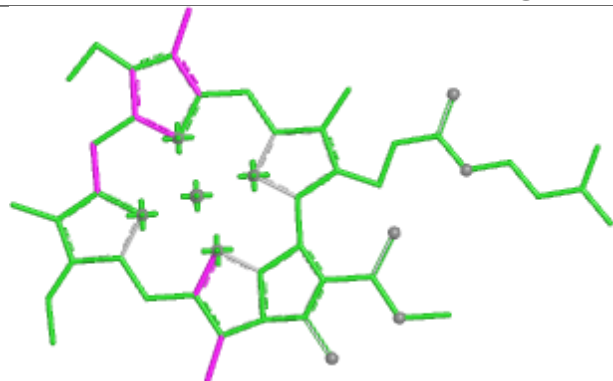
Ligand CLA s 408



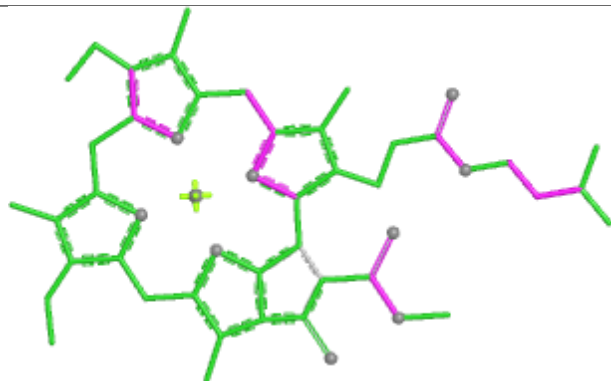
Ligand CLA k 610



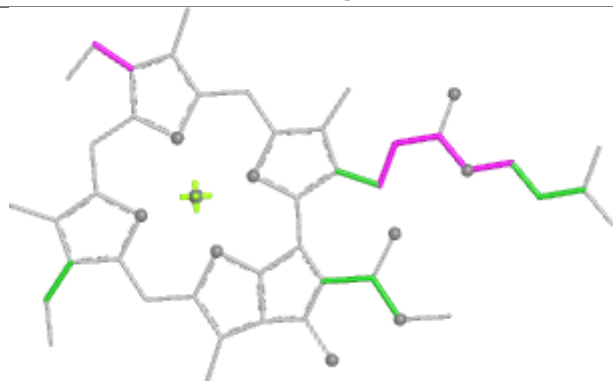
Ligand CLA h 303



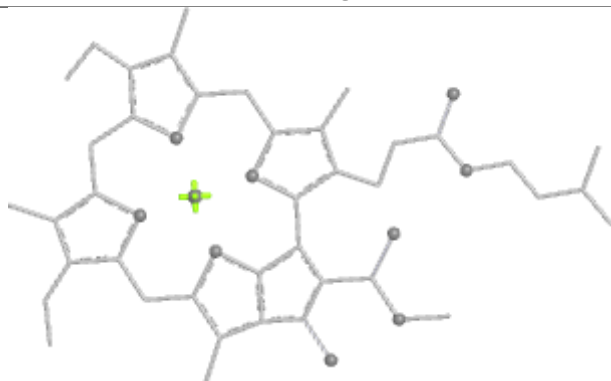
Bond lengths



Bond angles

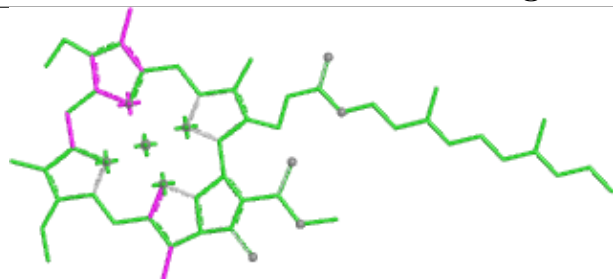


Torsions

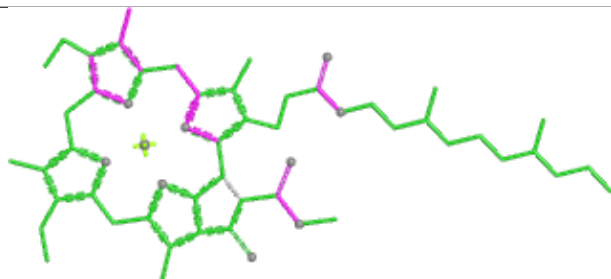


Rings

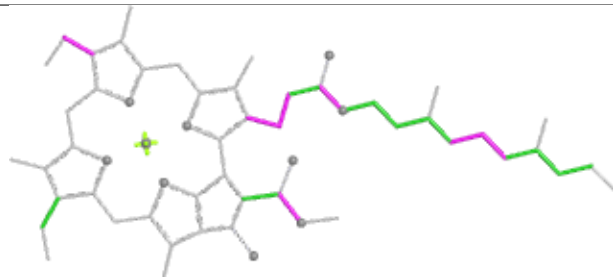
Ligand CLA l 310



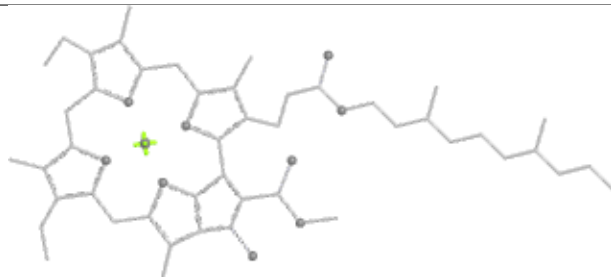
Bond lengths



Bond angles

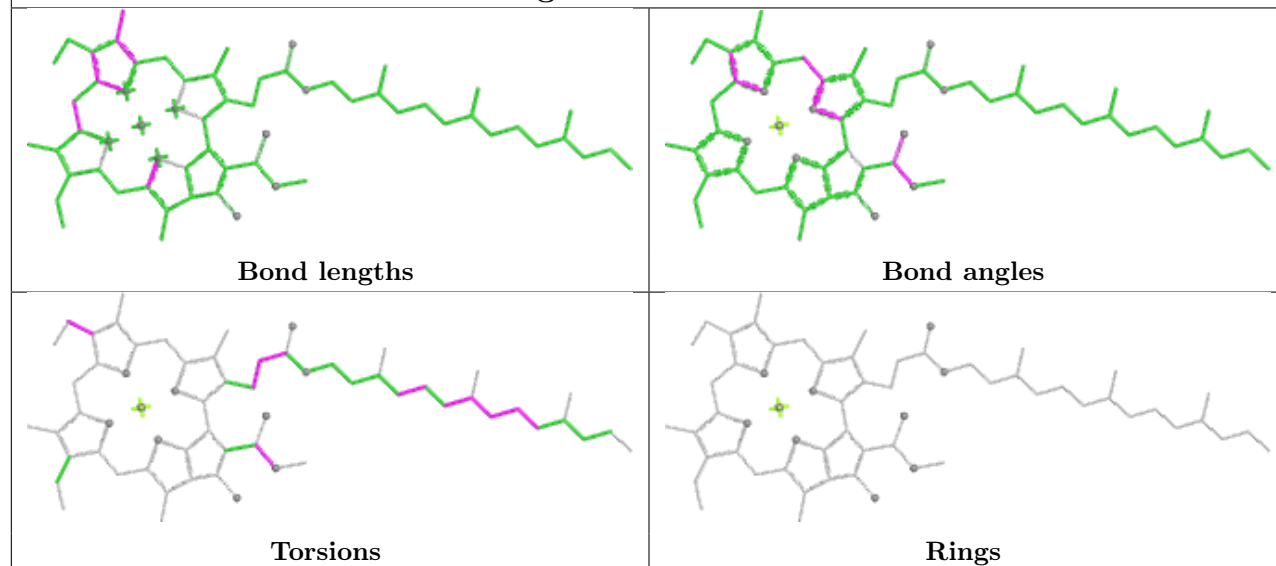


Torsions

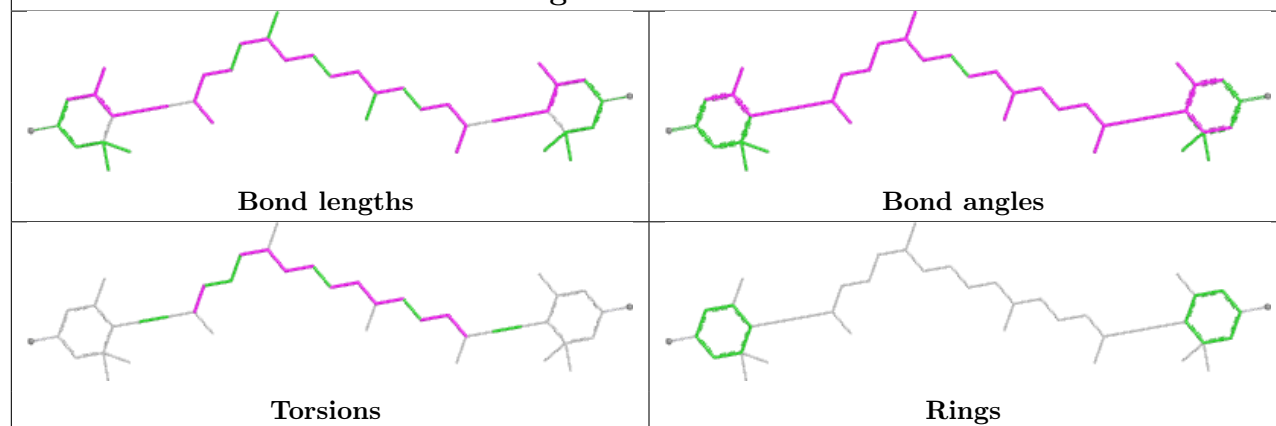


Rings

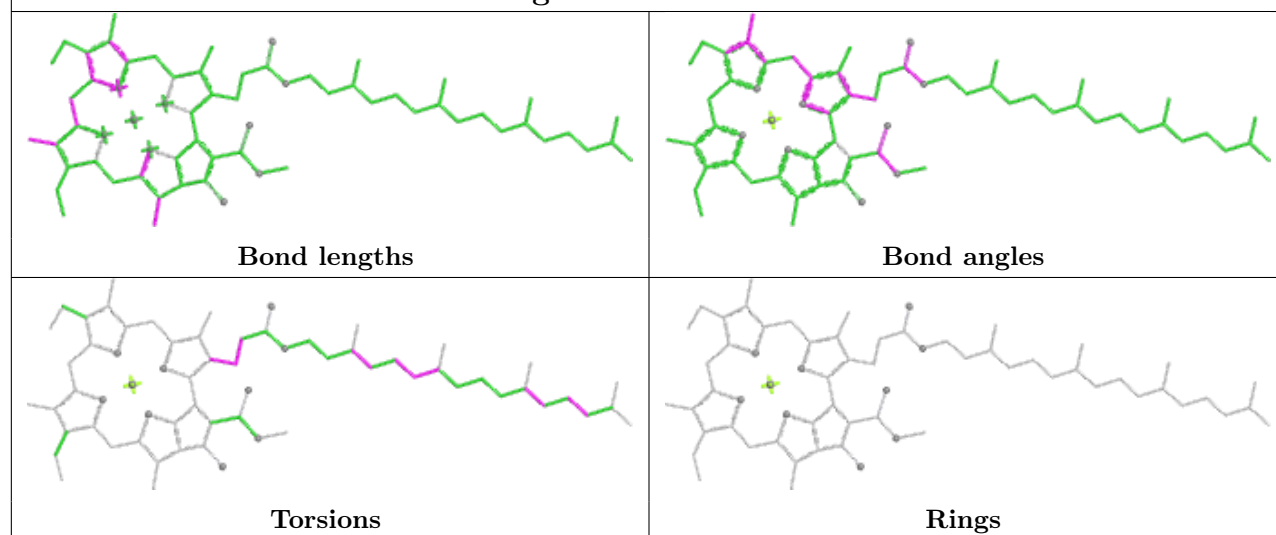
Ligand CLA c 304

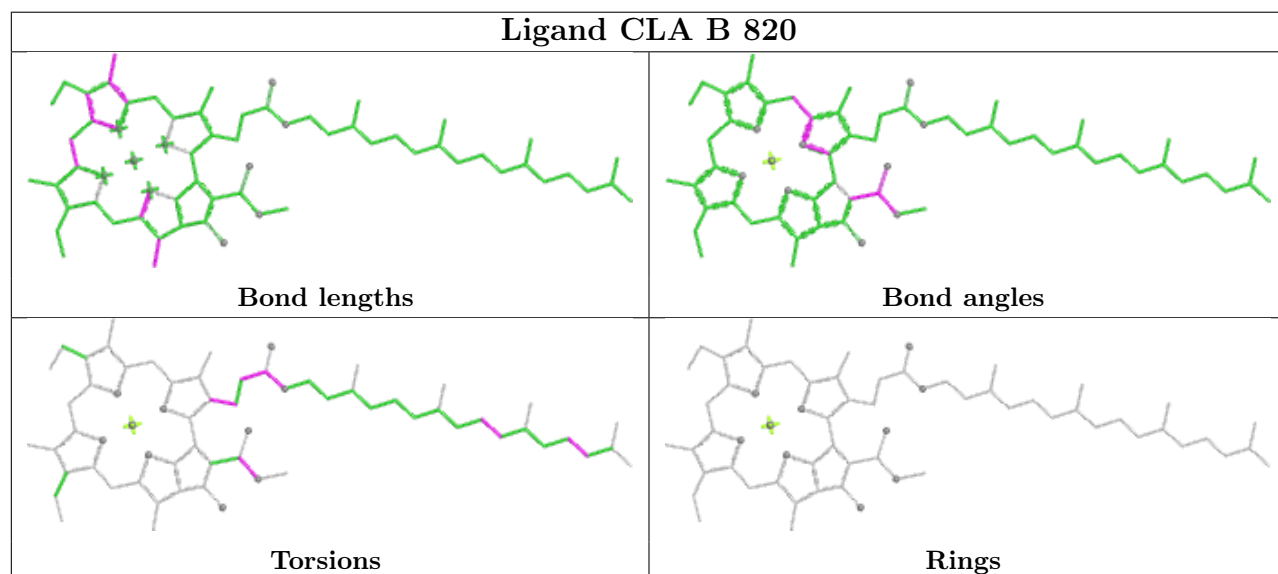
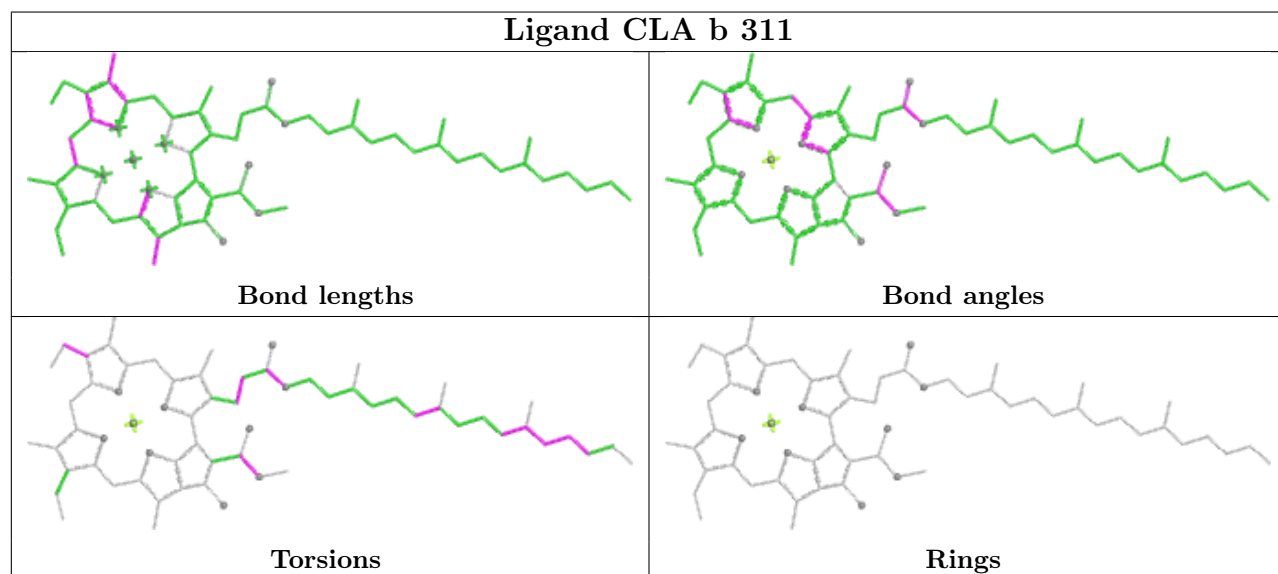
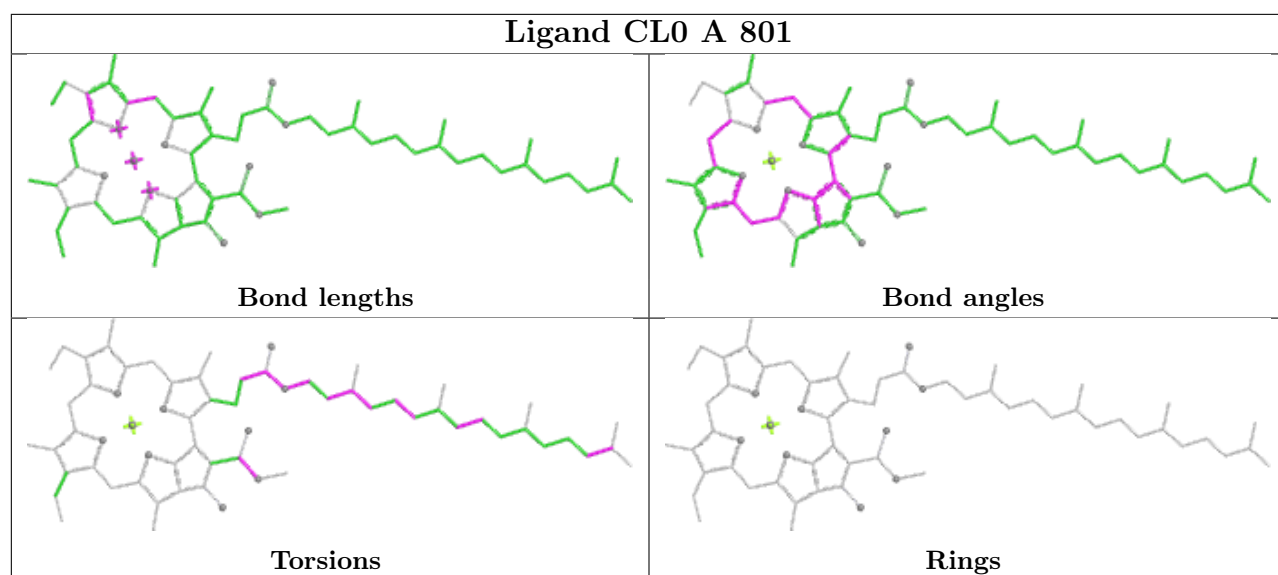


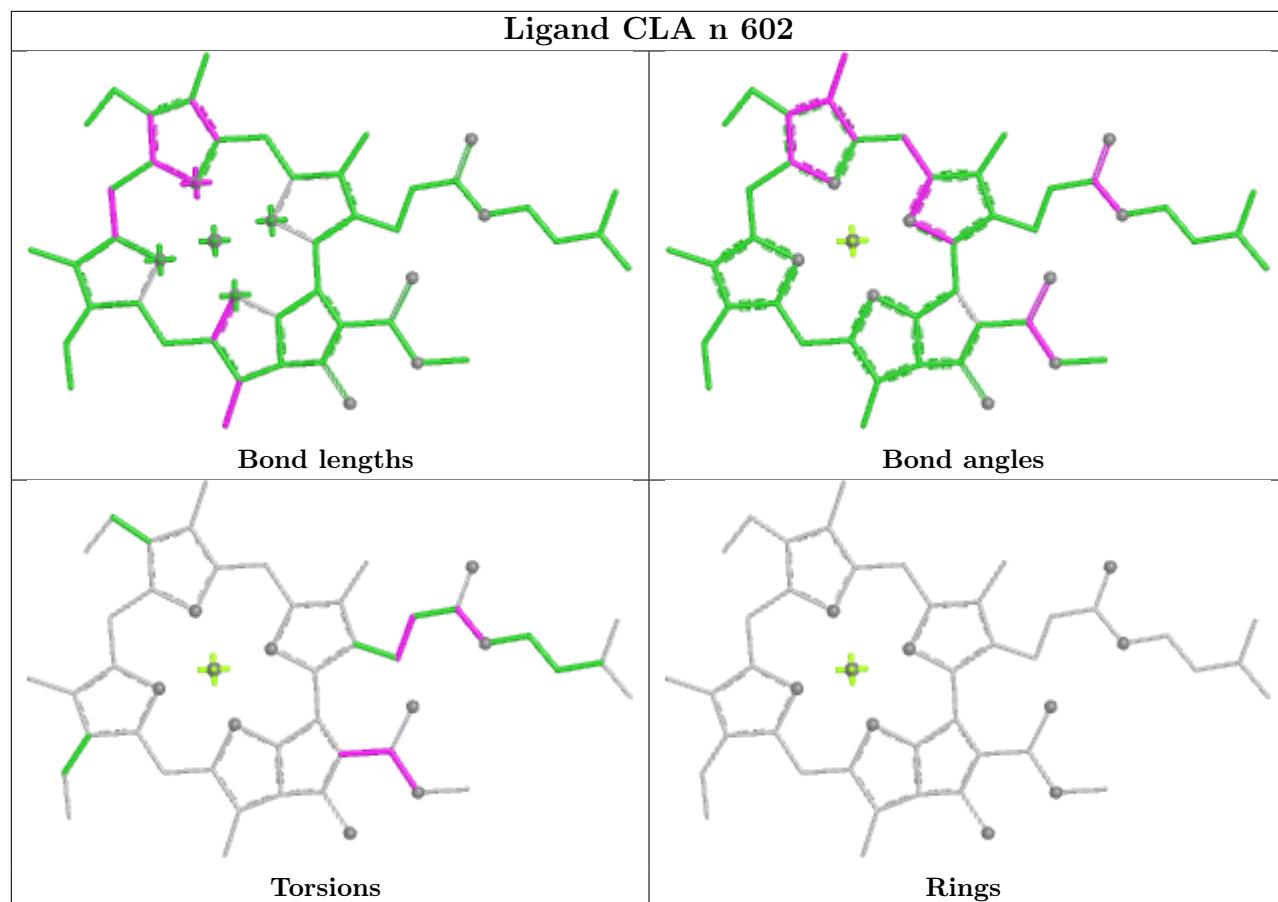
Ligand II0 d 315



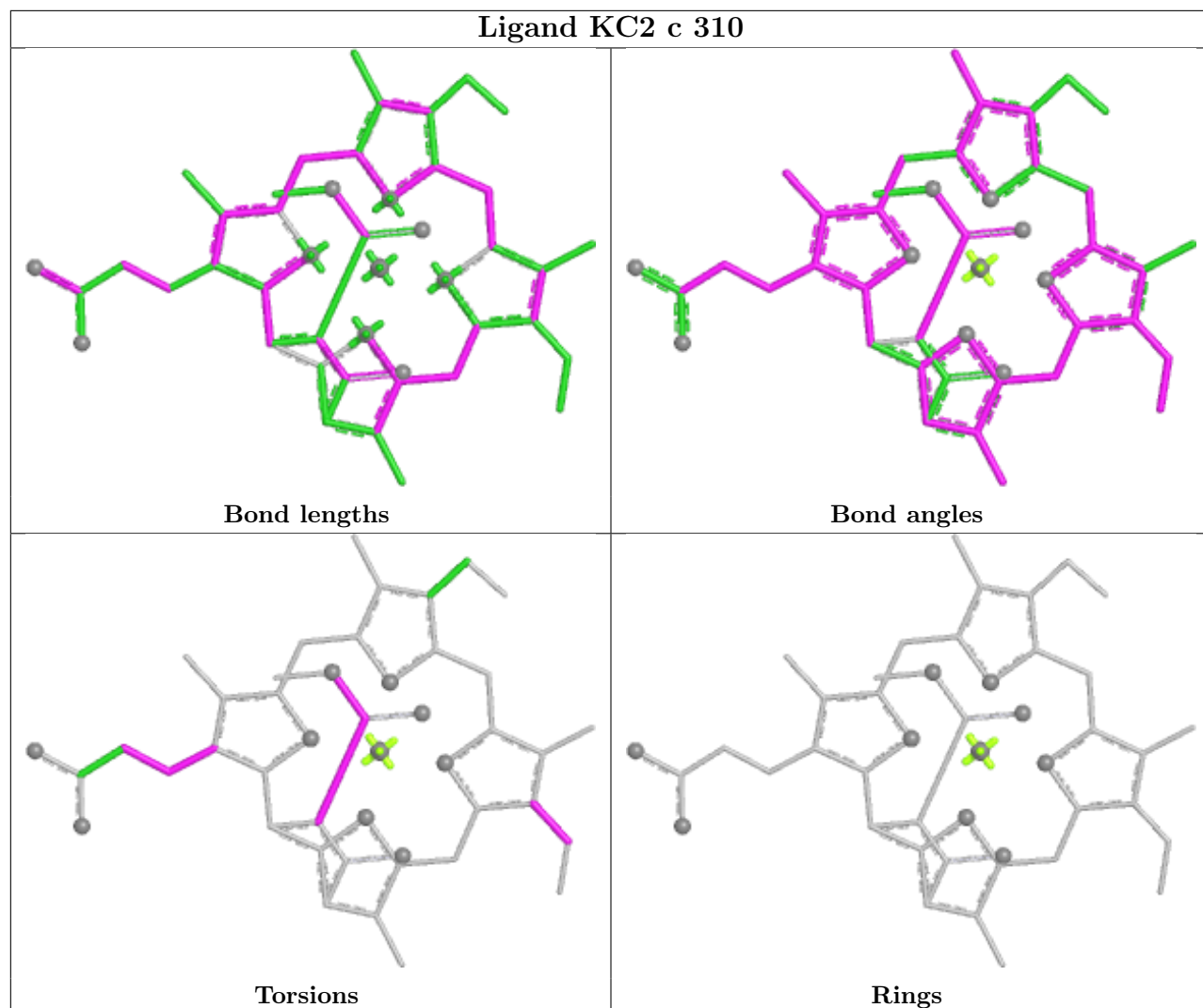
Ligand CLA B 829



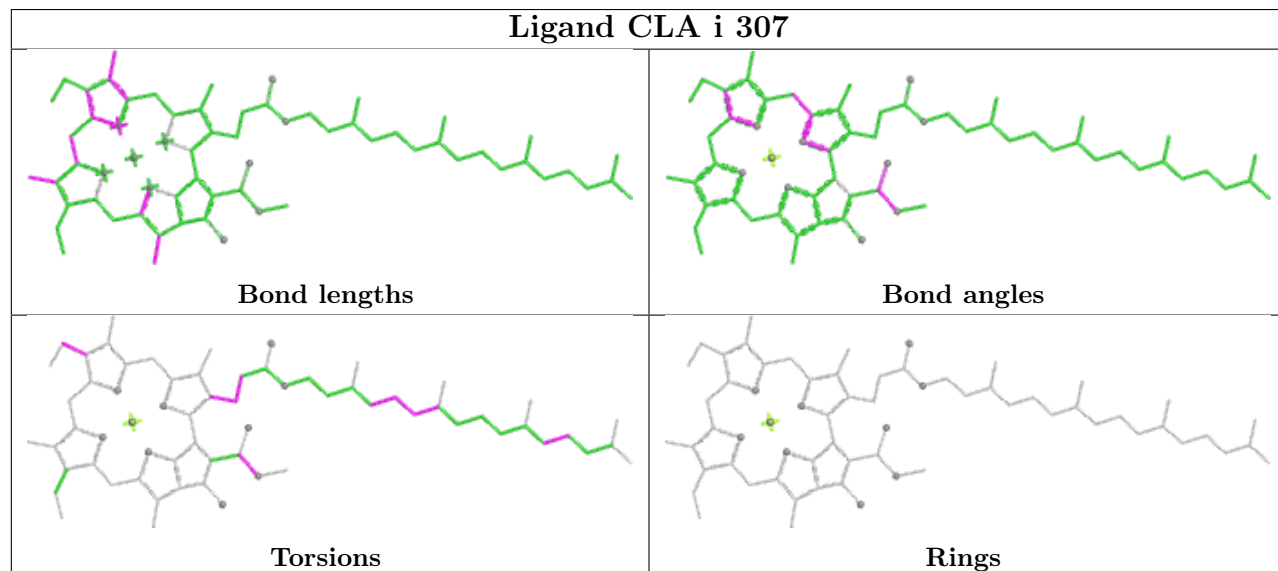




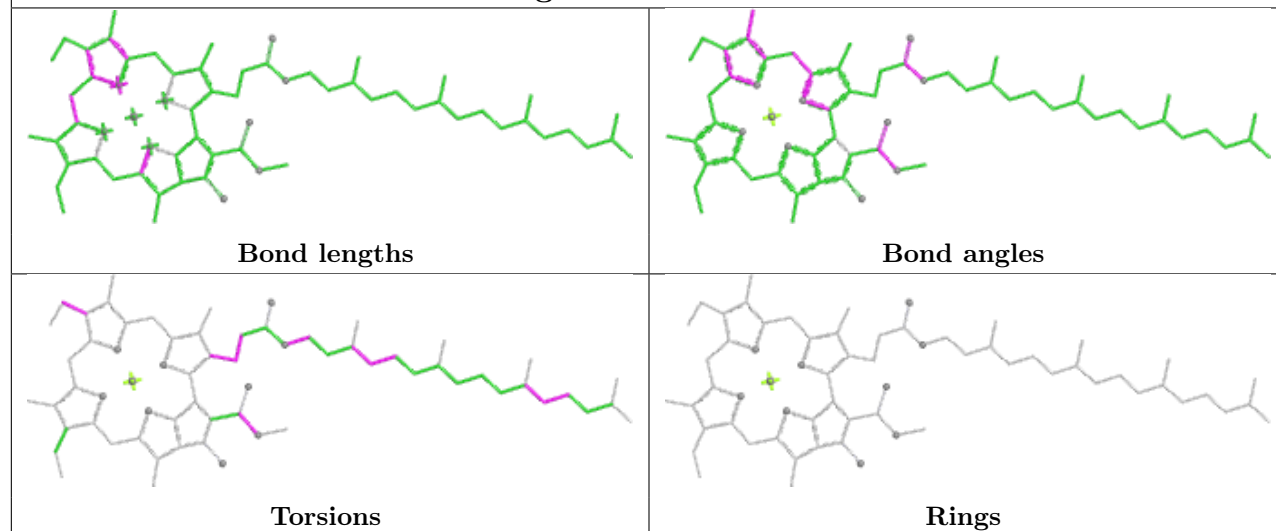
Ligand KC2 c 310



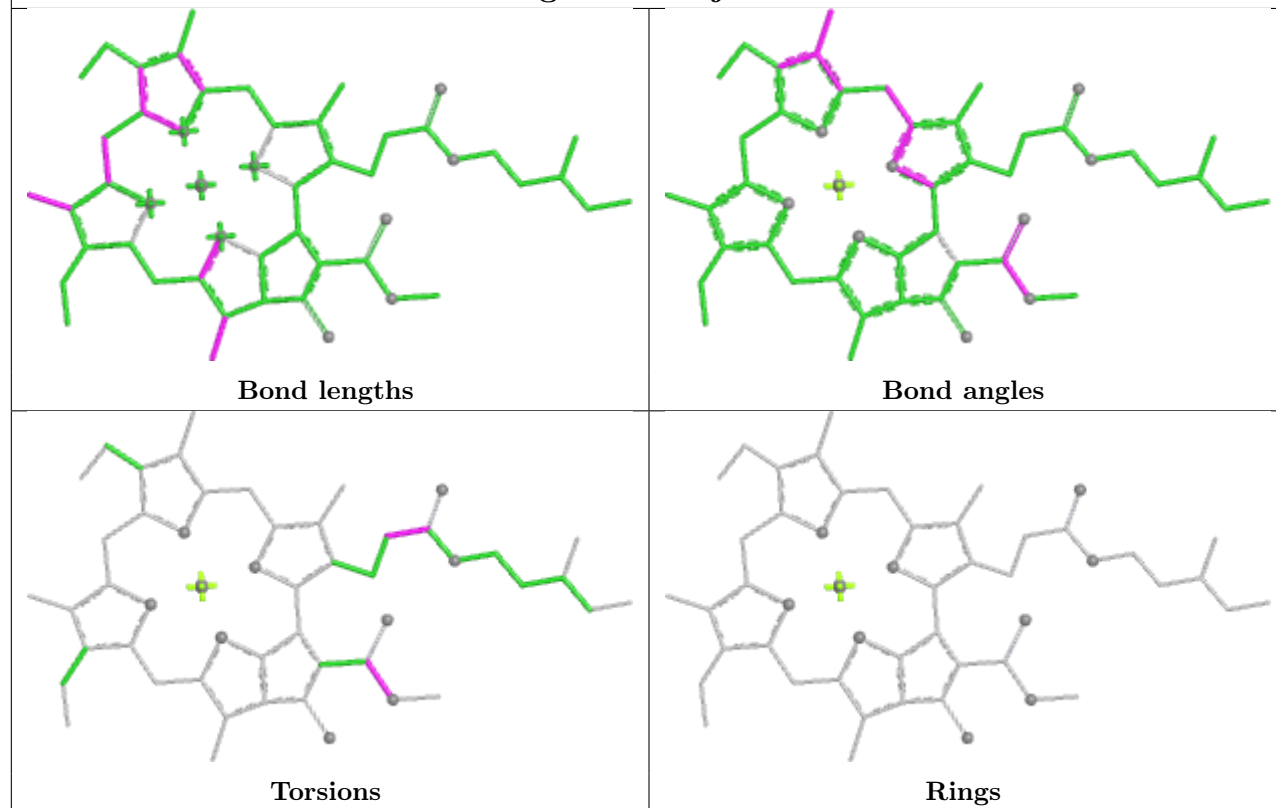
Ligand CLA i 307

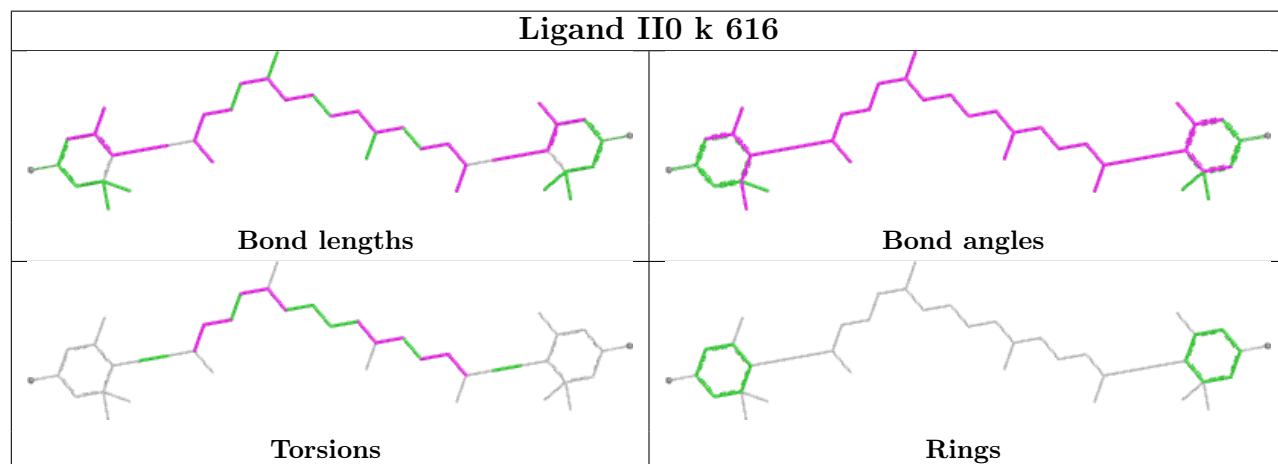
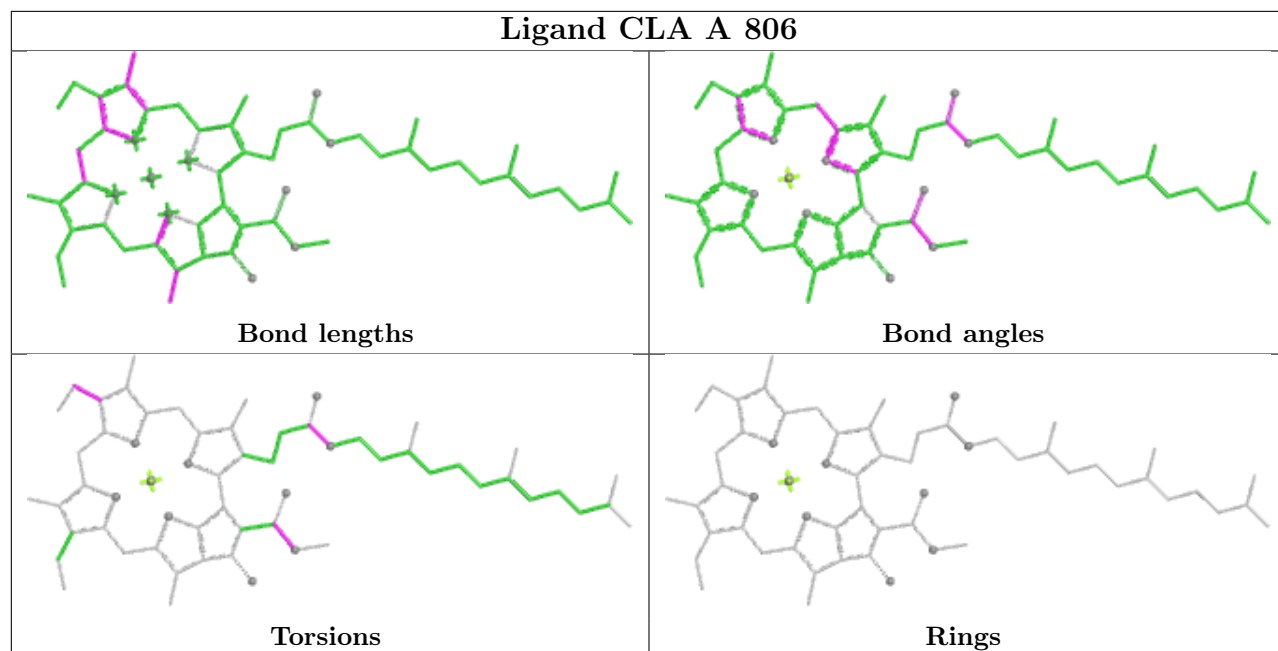


Ligand CLA n 609

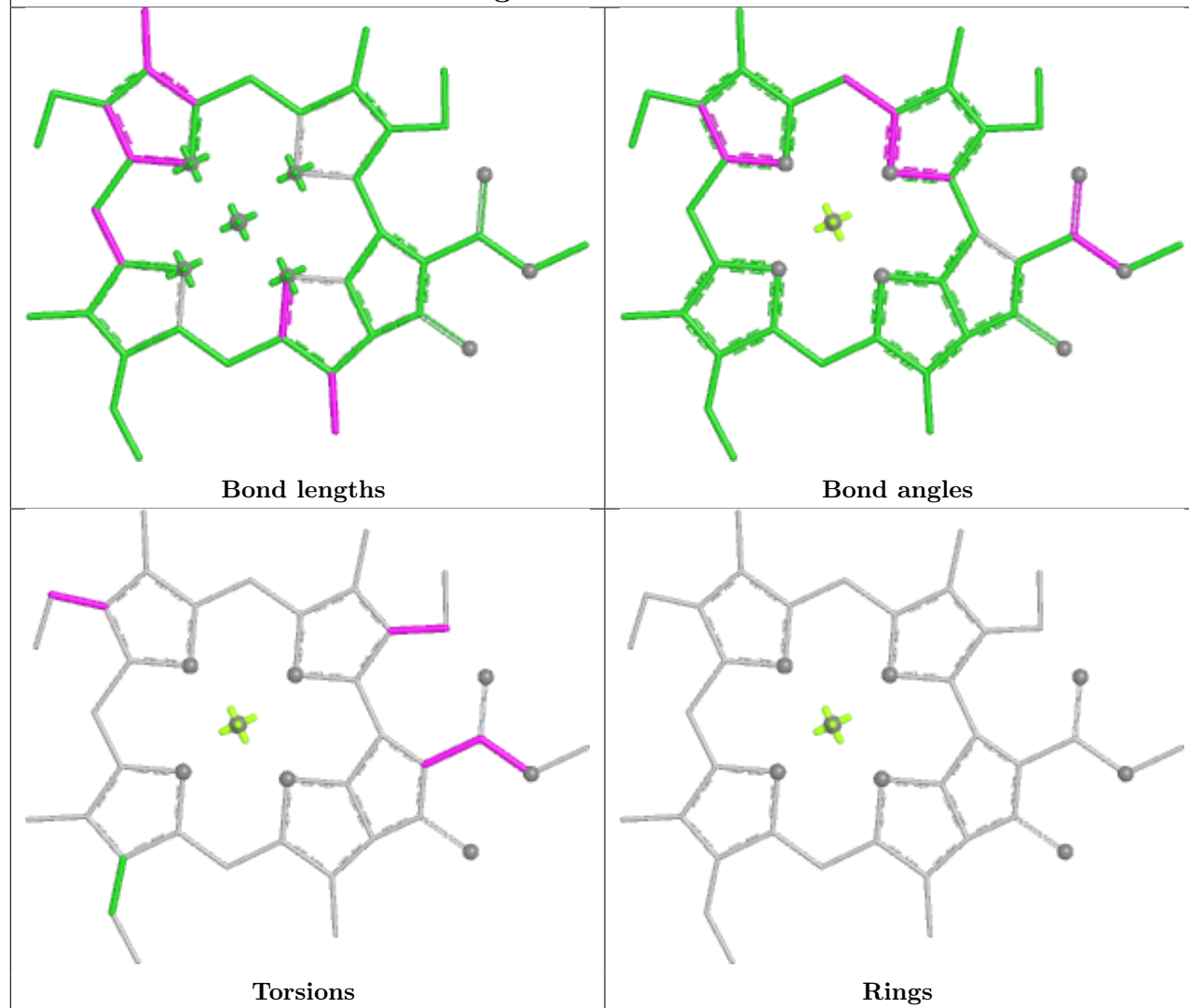


Ligand CLA j 603

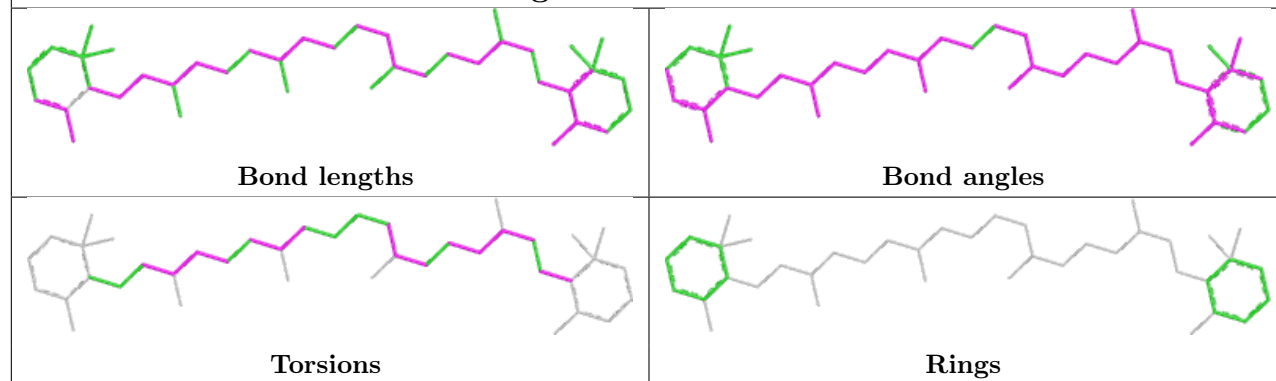




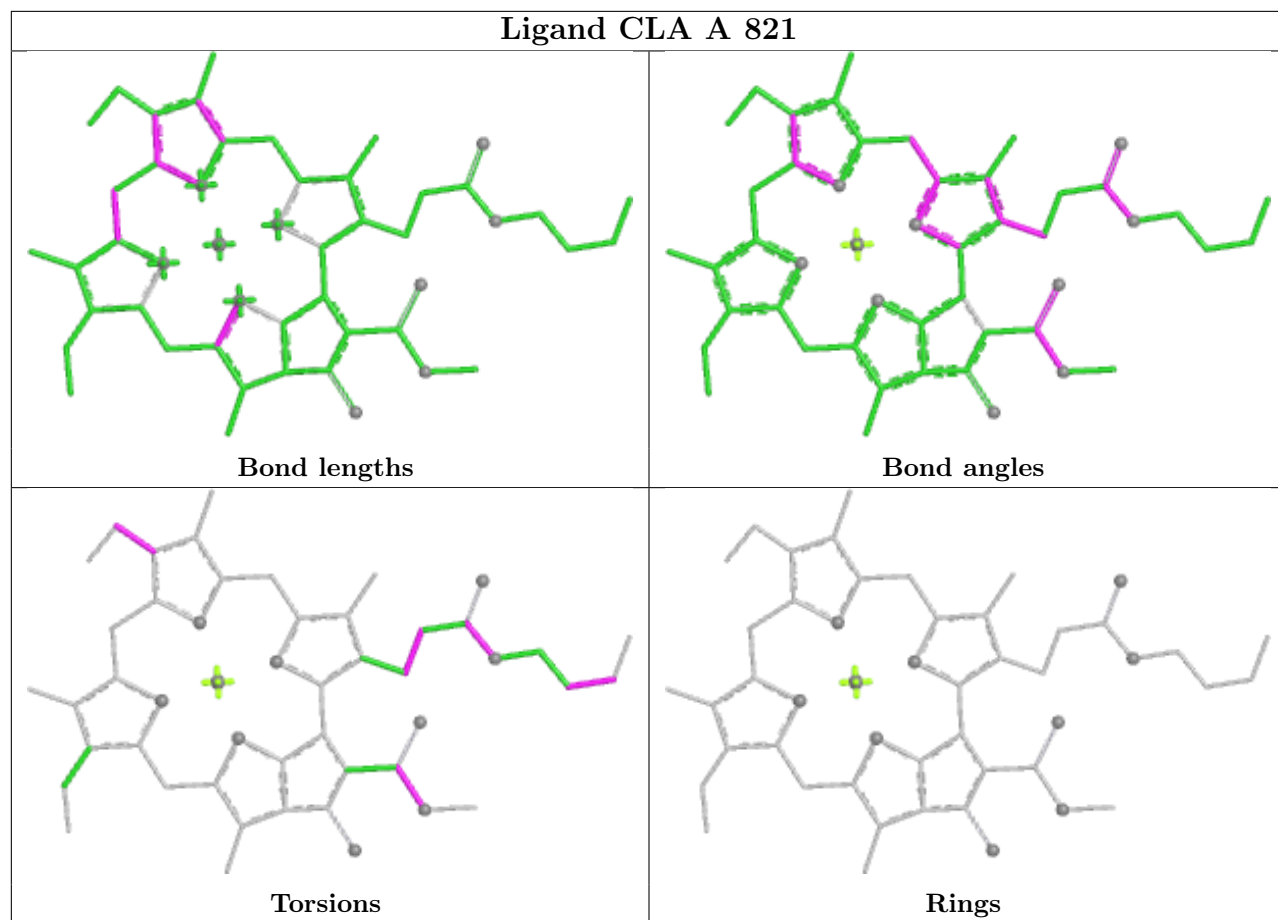
Ligand CLA m 601



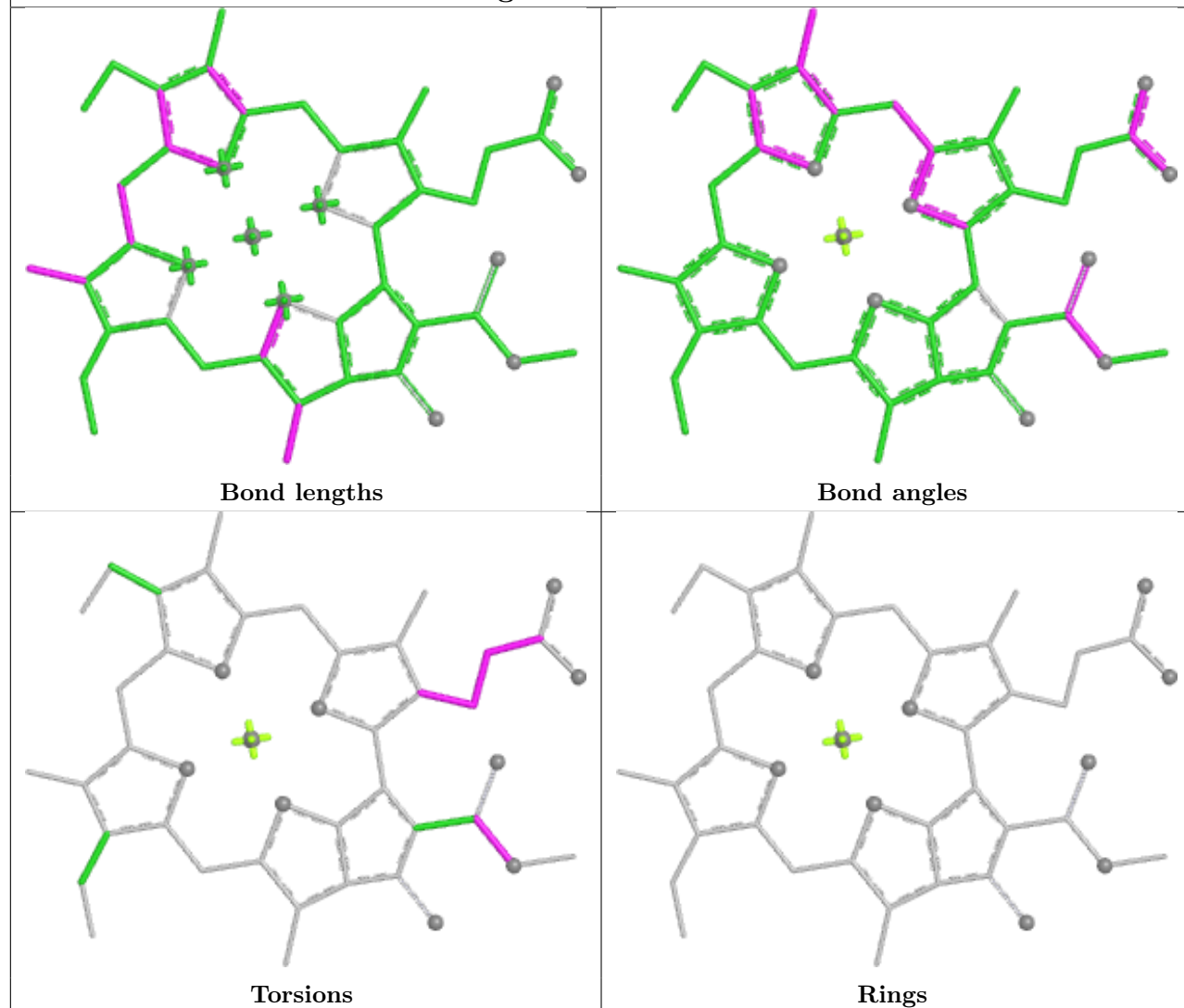
Ligand WVN i 315



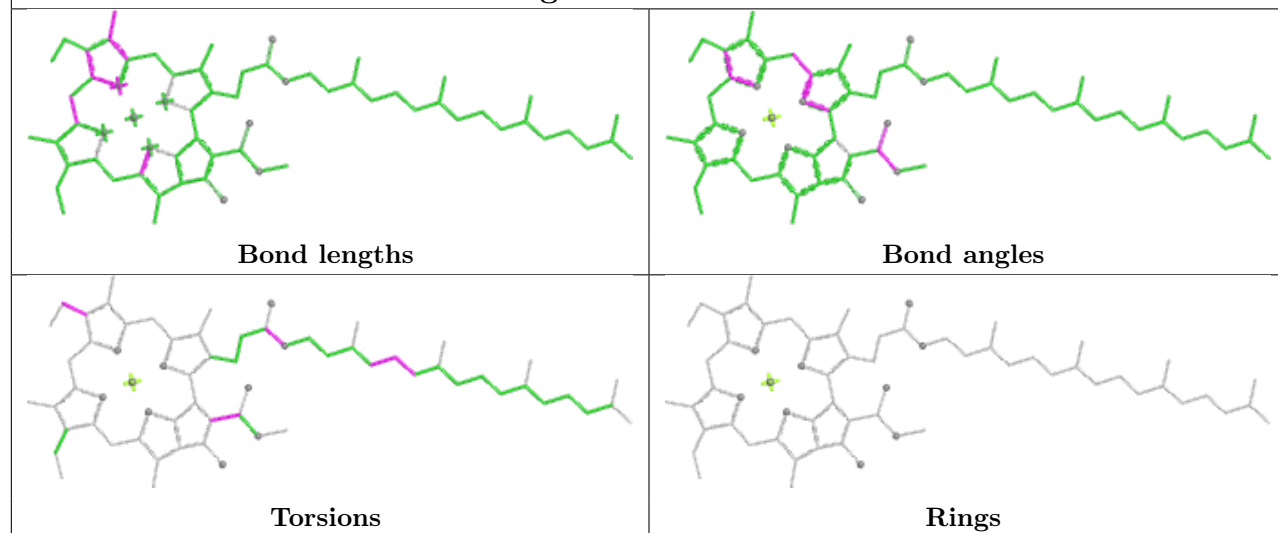
Ligand CLA A 821

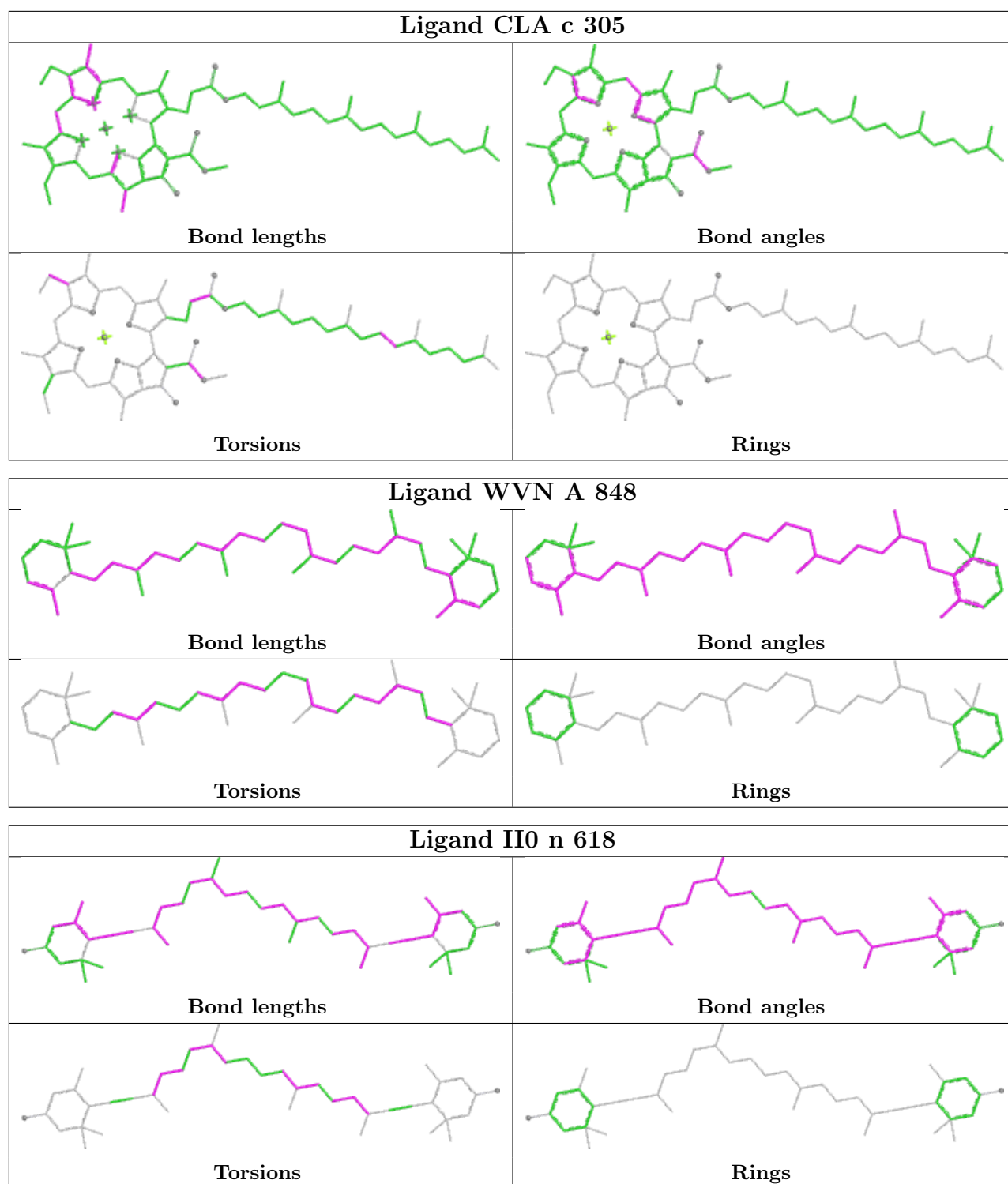


Ligand CLA c 311

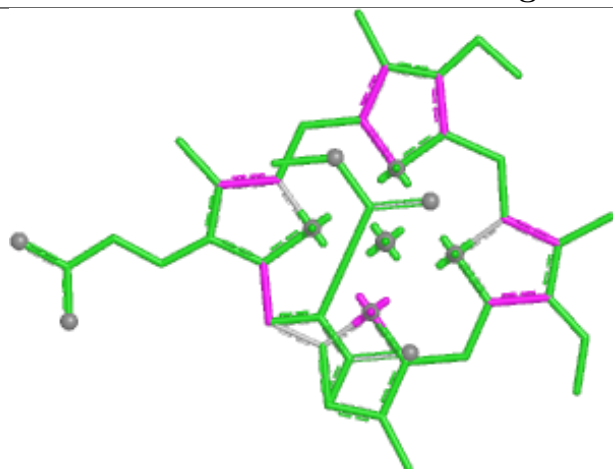


Ligand CLA l 308

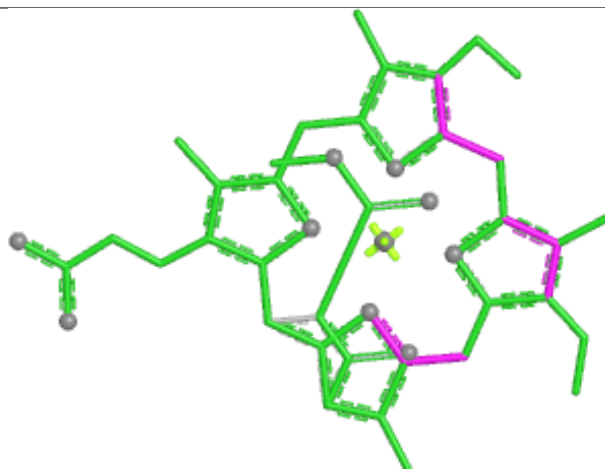




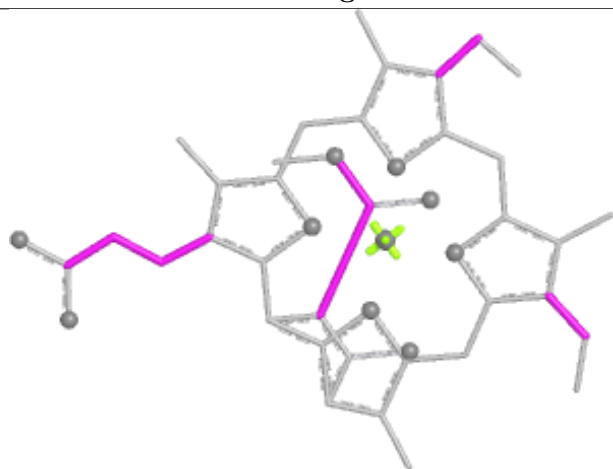
Ligand KC2 n 612



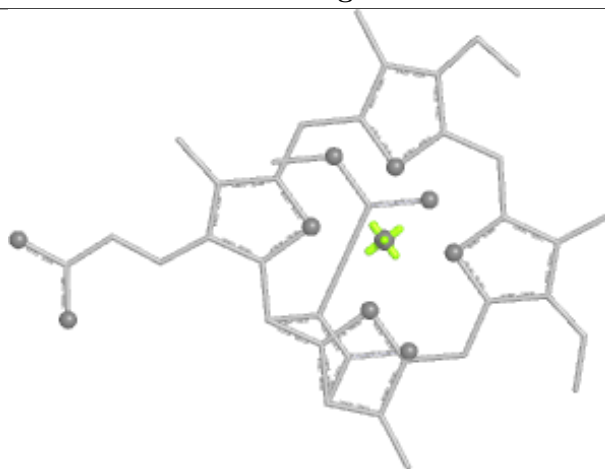
Bond lengths



Bond angles

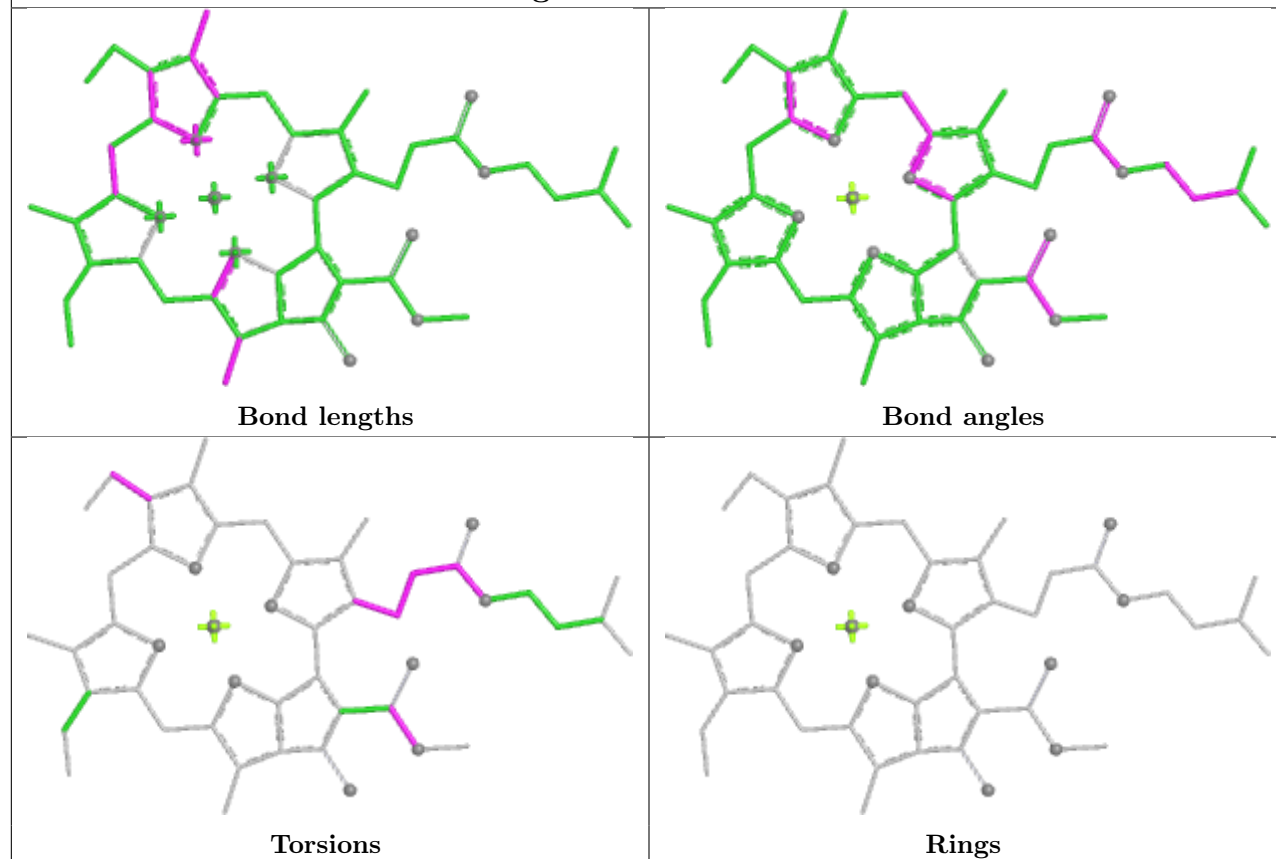


Torsions

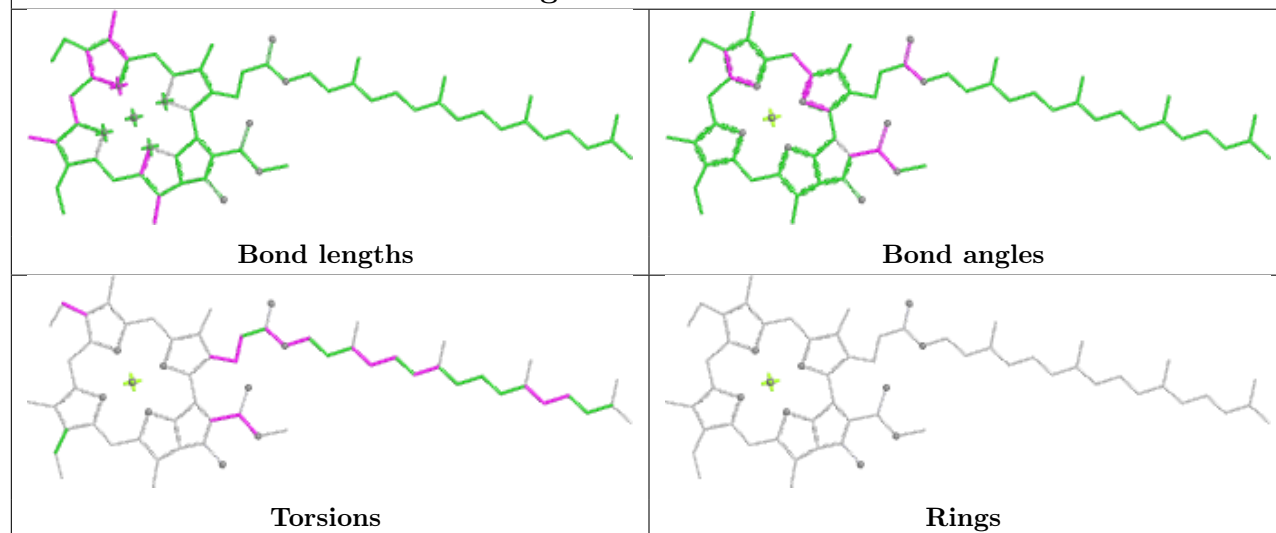


Rings

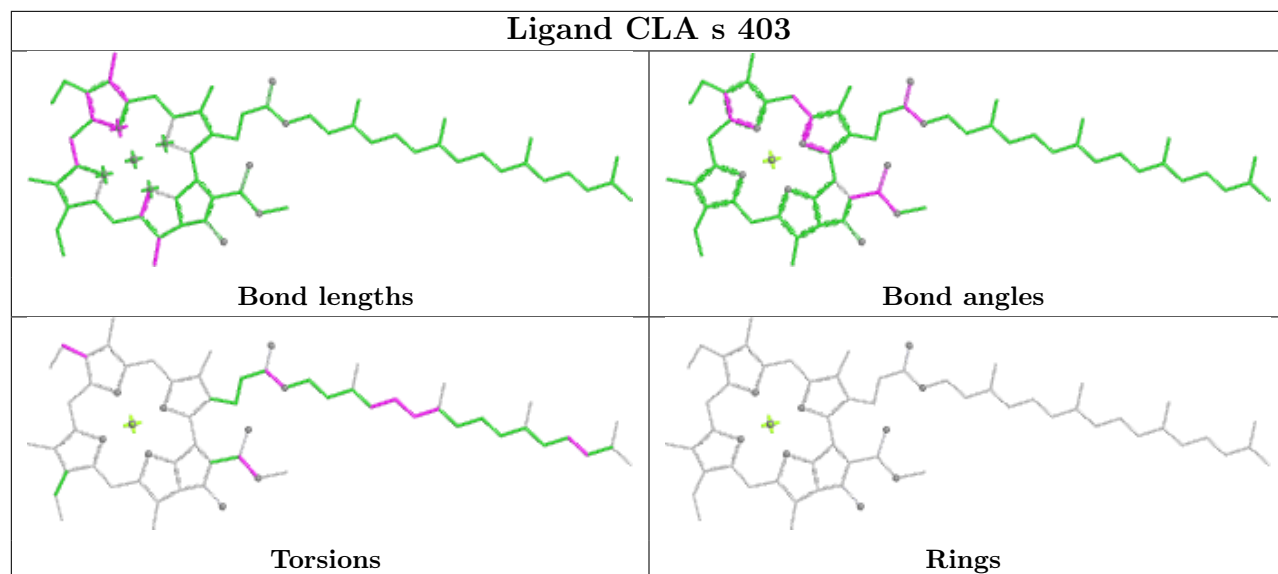
Ligand CLA B 828



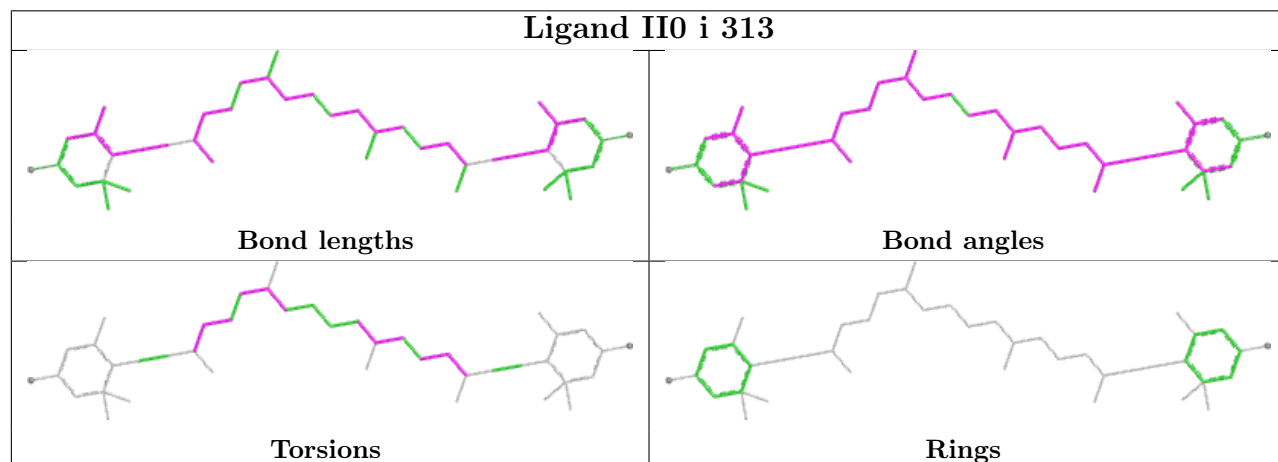
Ligand CLA i 302



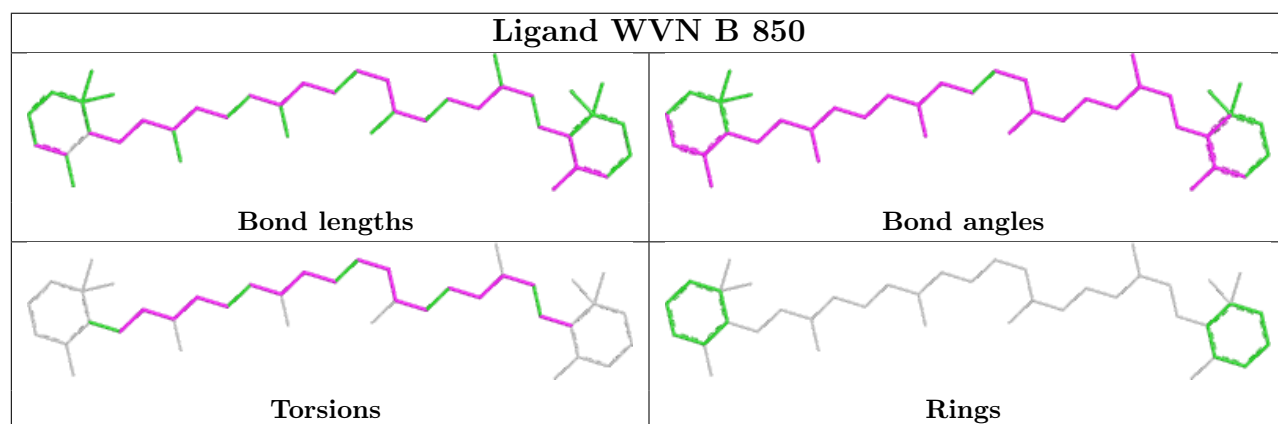
Ligand CLA s 403

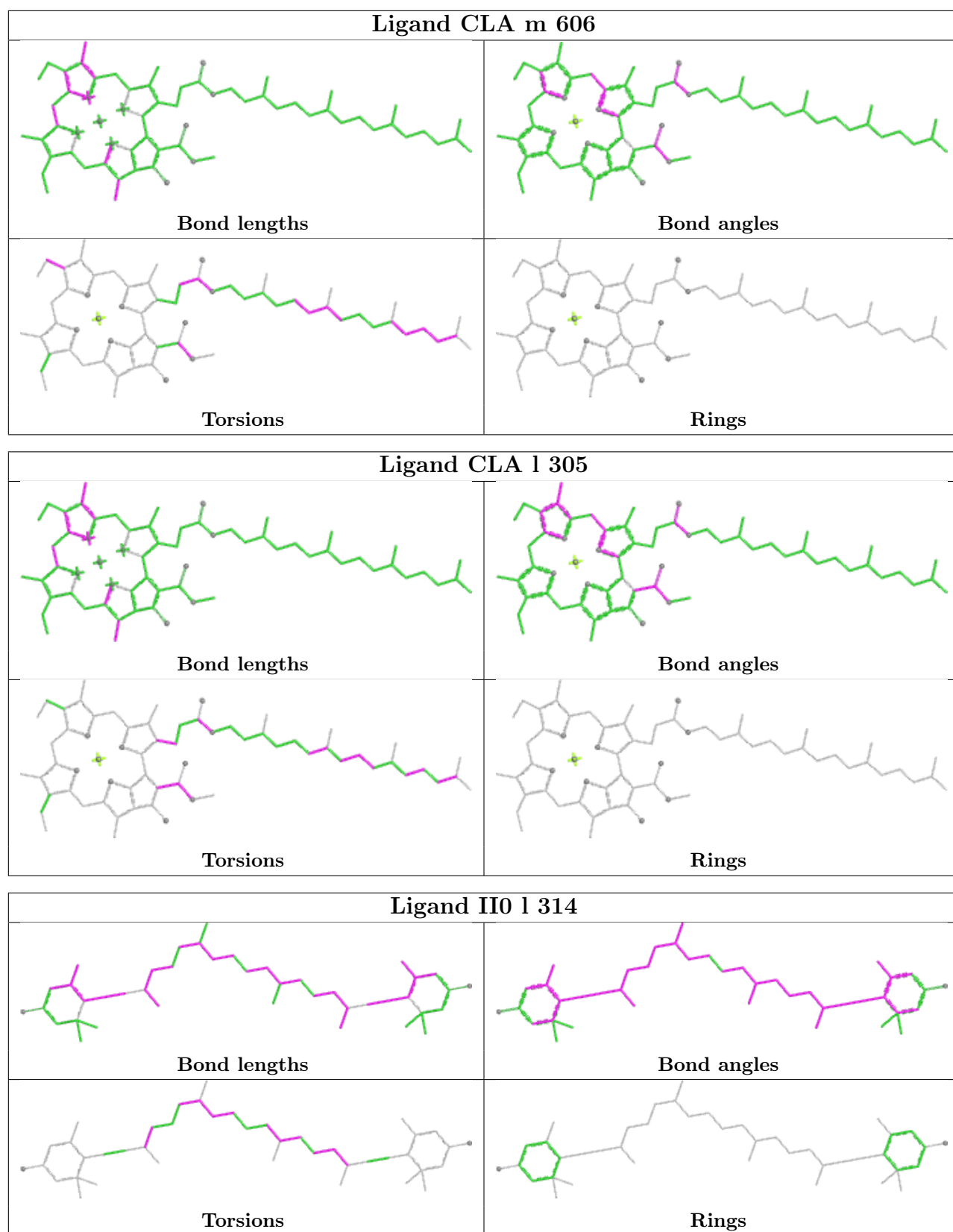


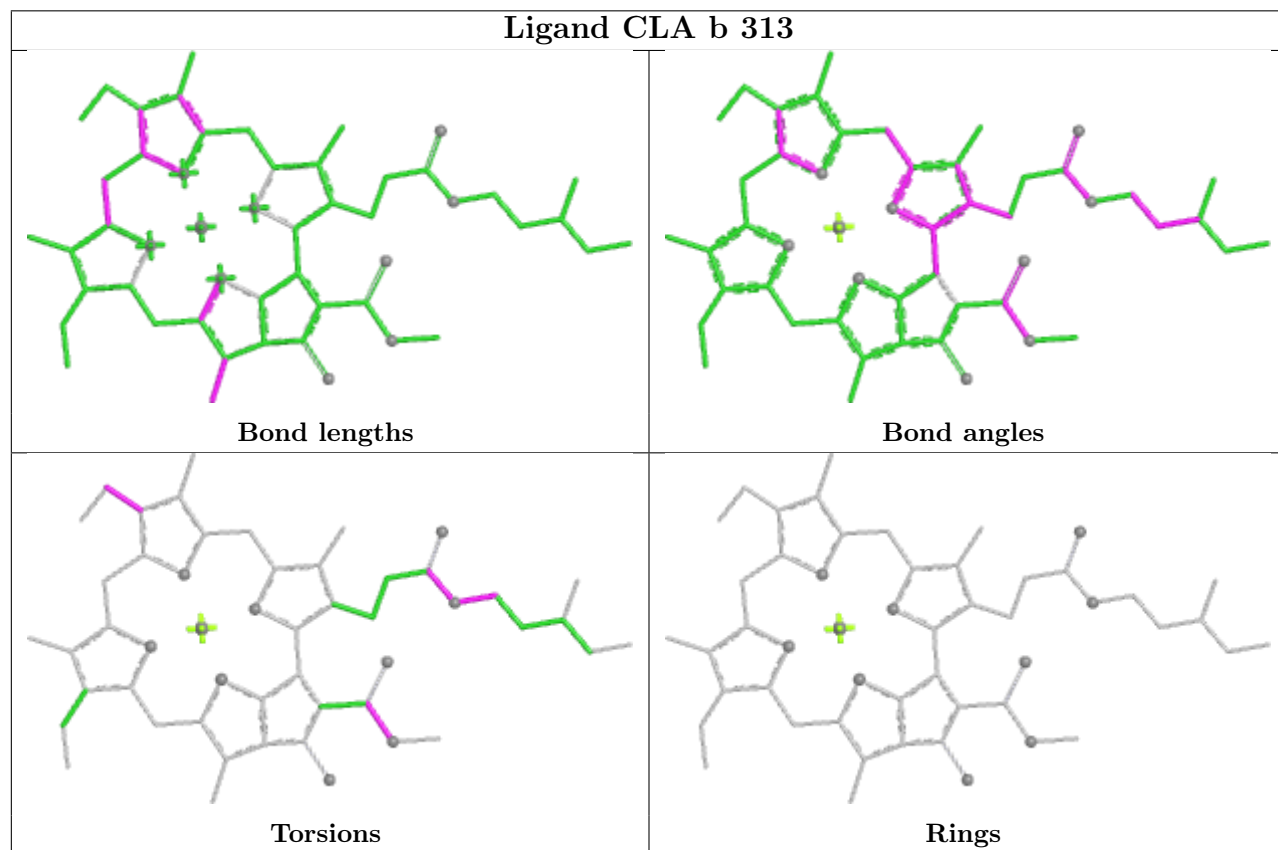
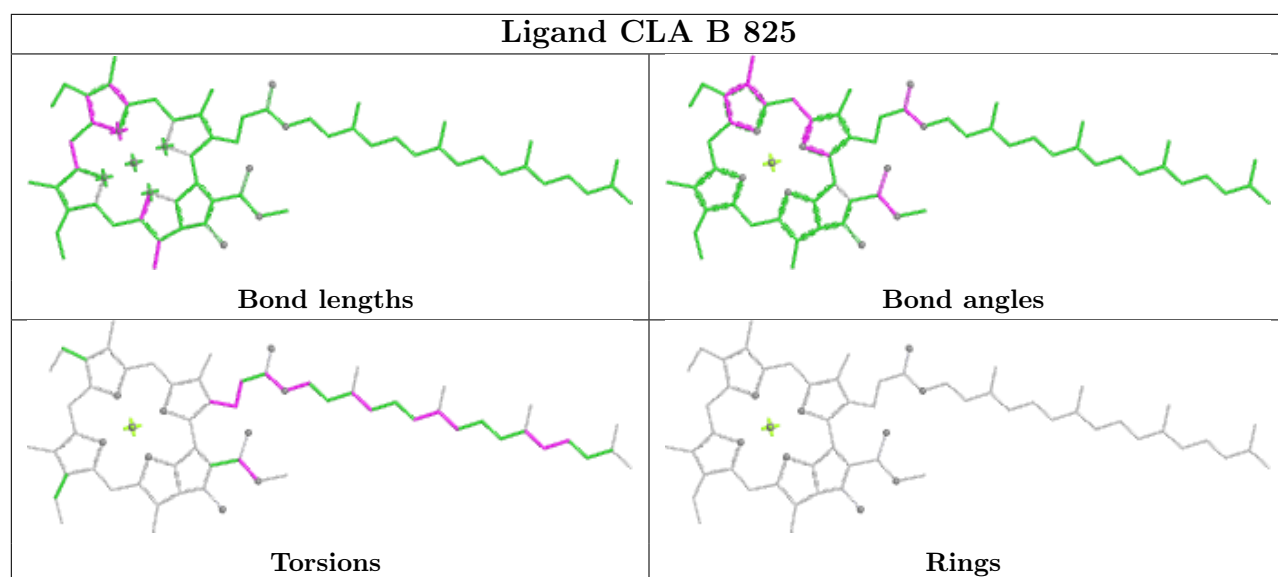
Ligand II0 i 313



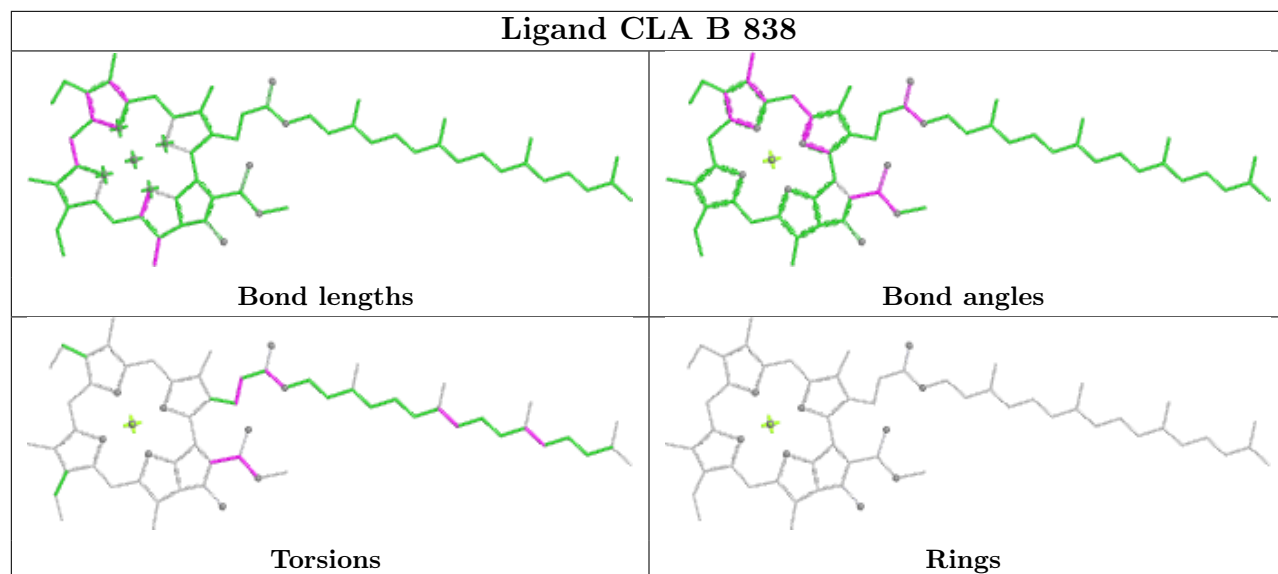
Ligand WVN B 850



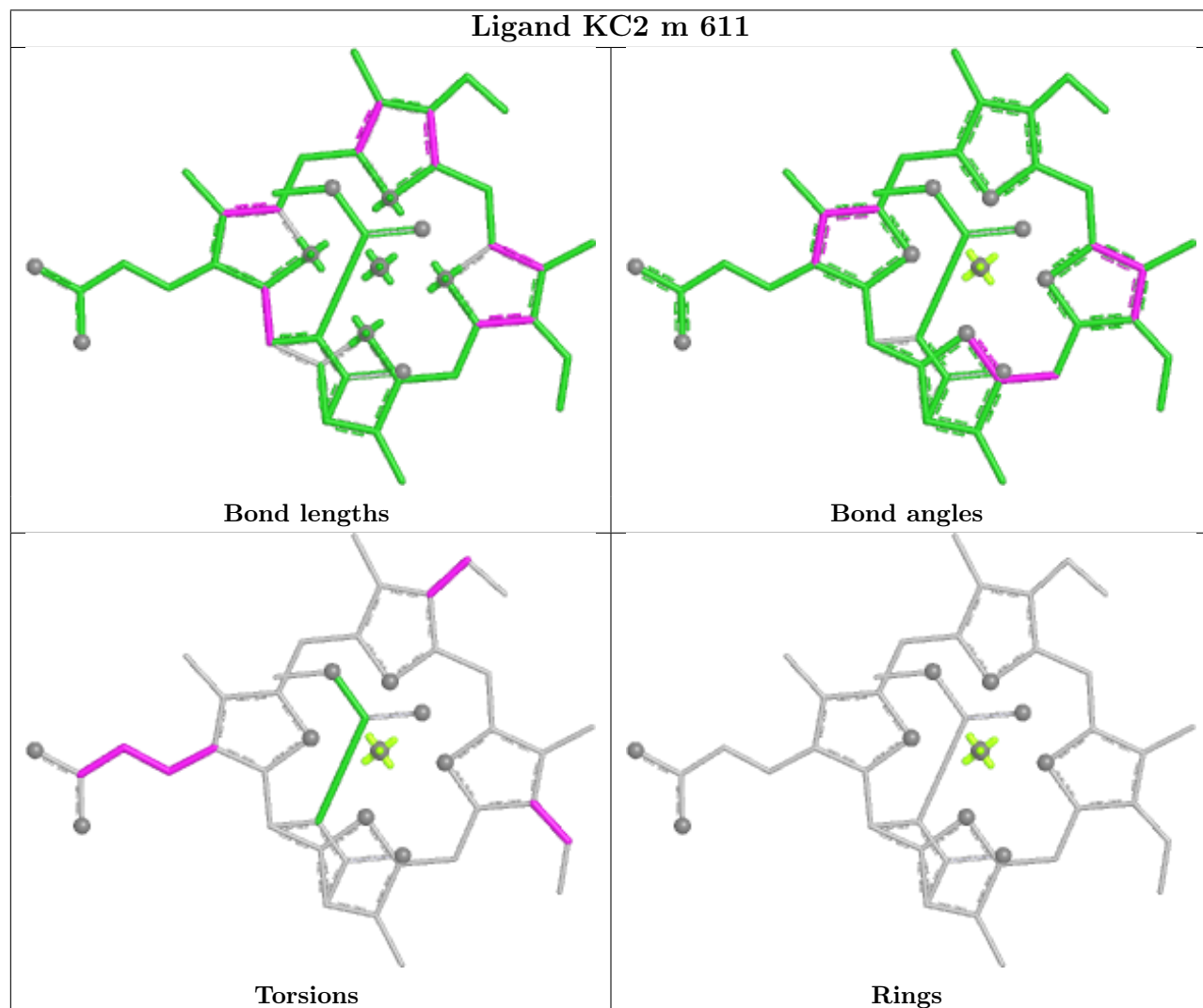


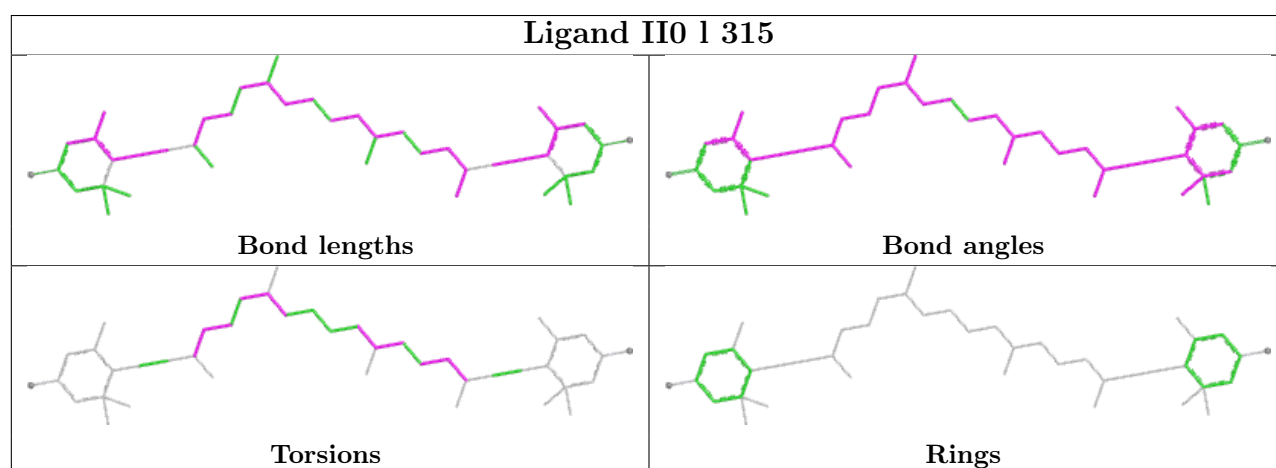
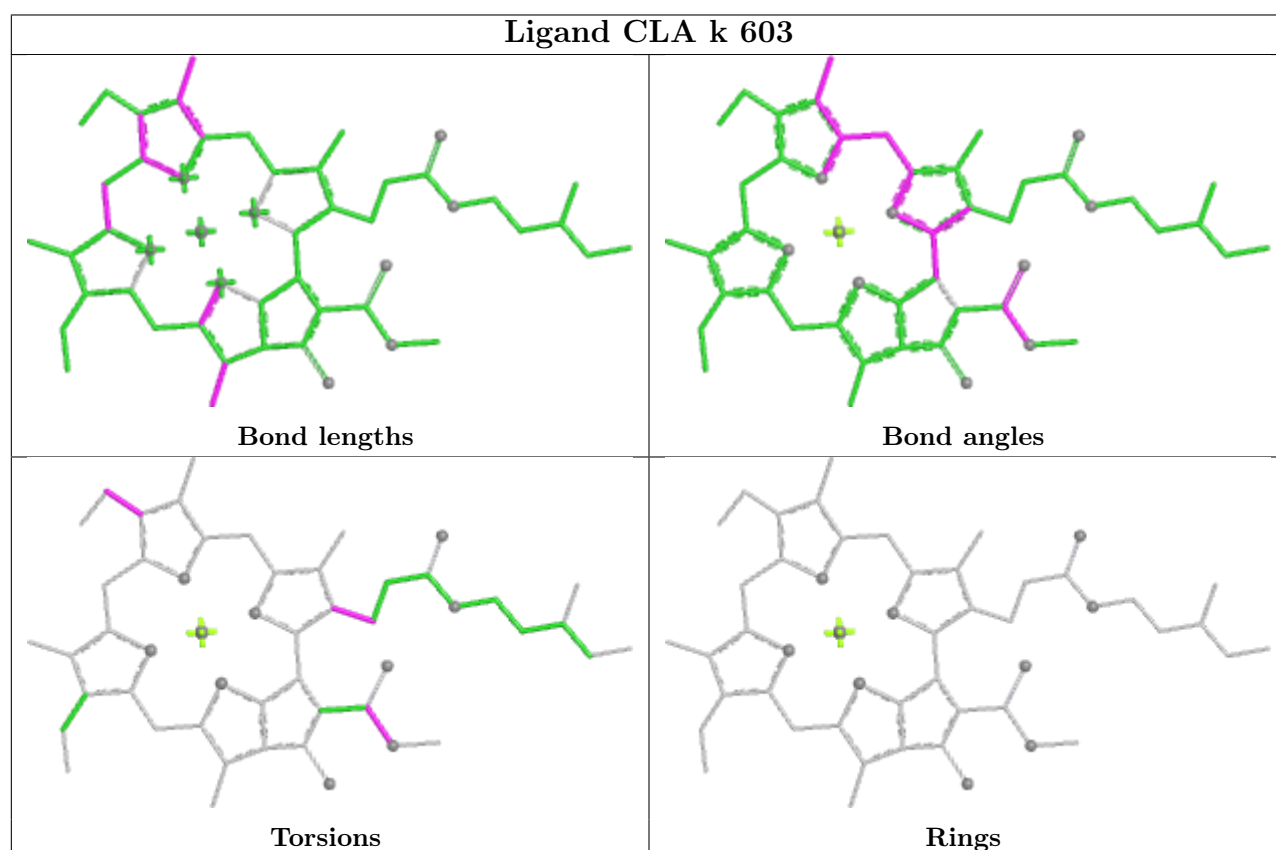
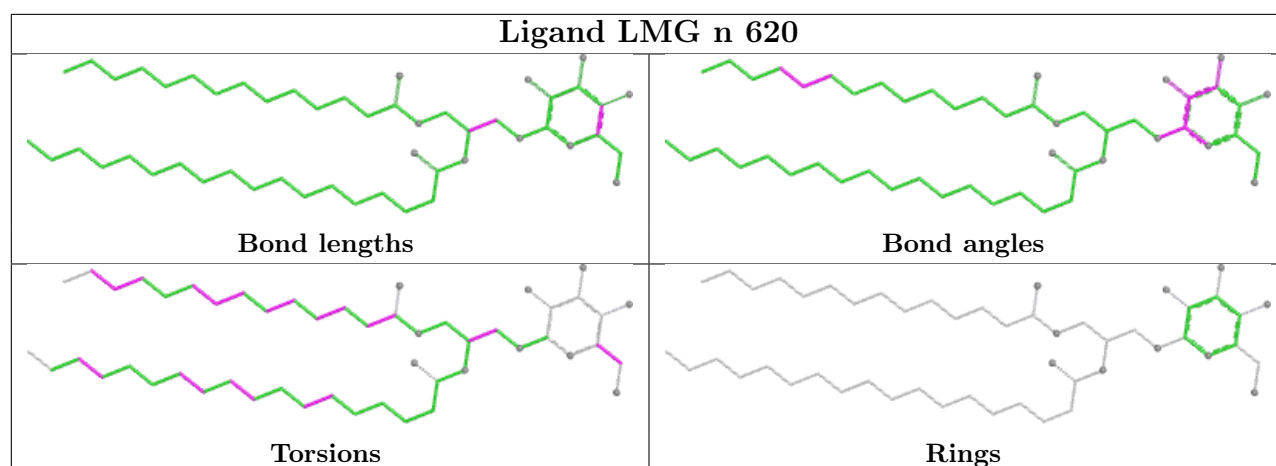


Ligand CLA B 838

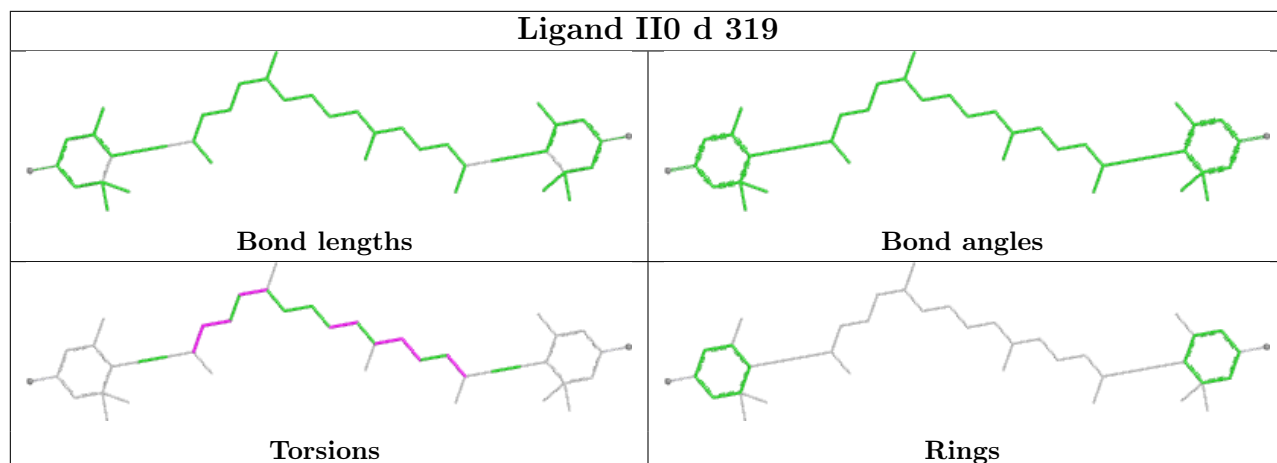


Ligand KC2 m 611

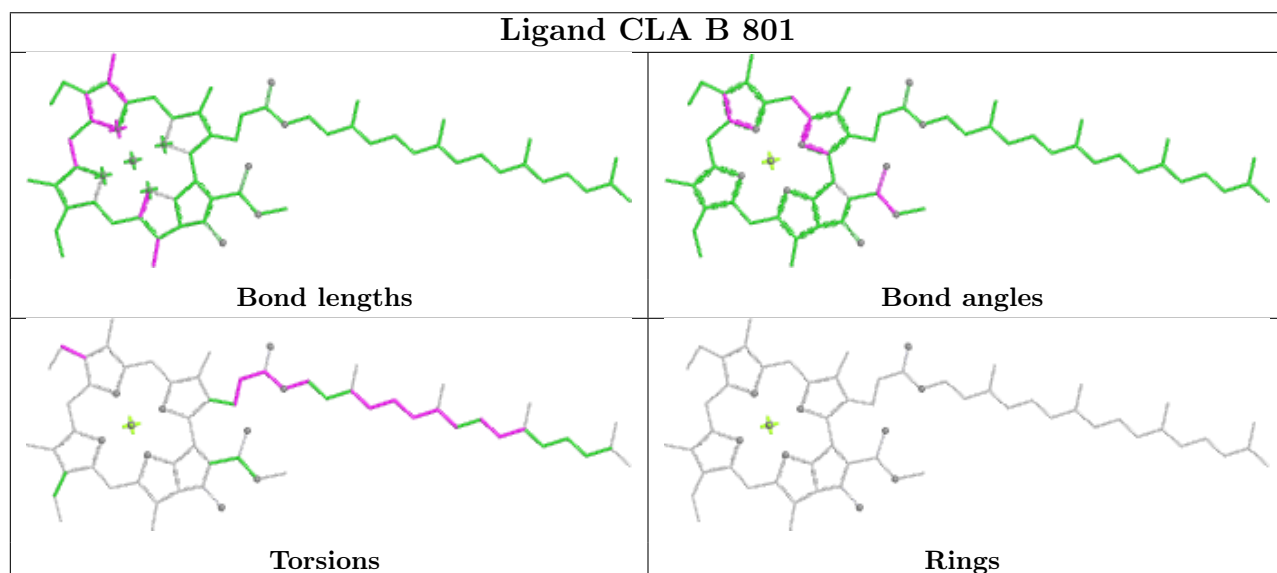




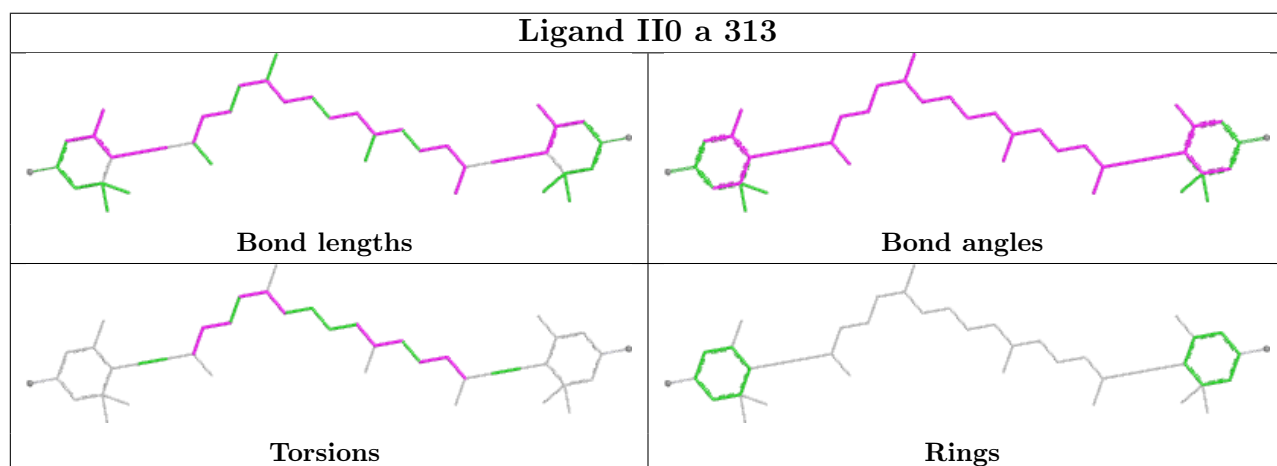
Ligand II0 d 319



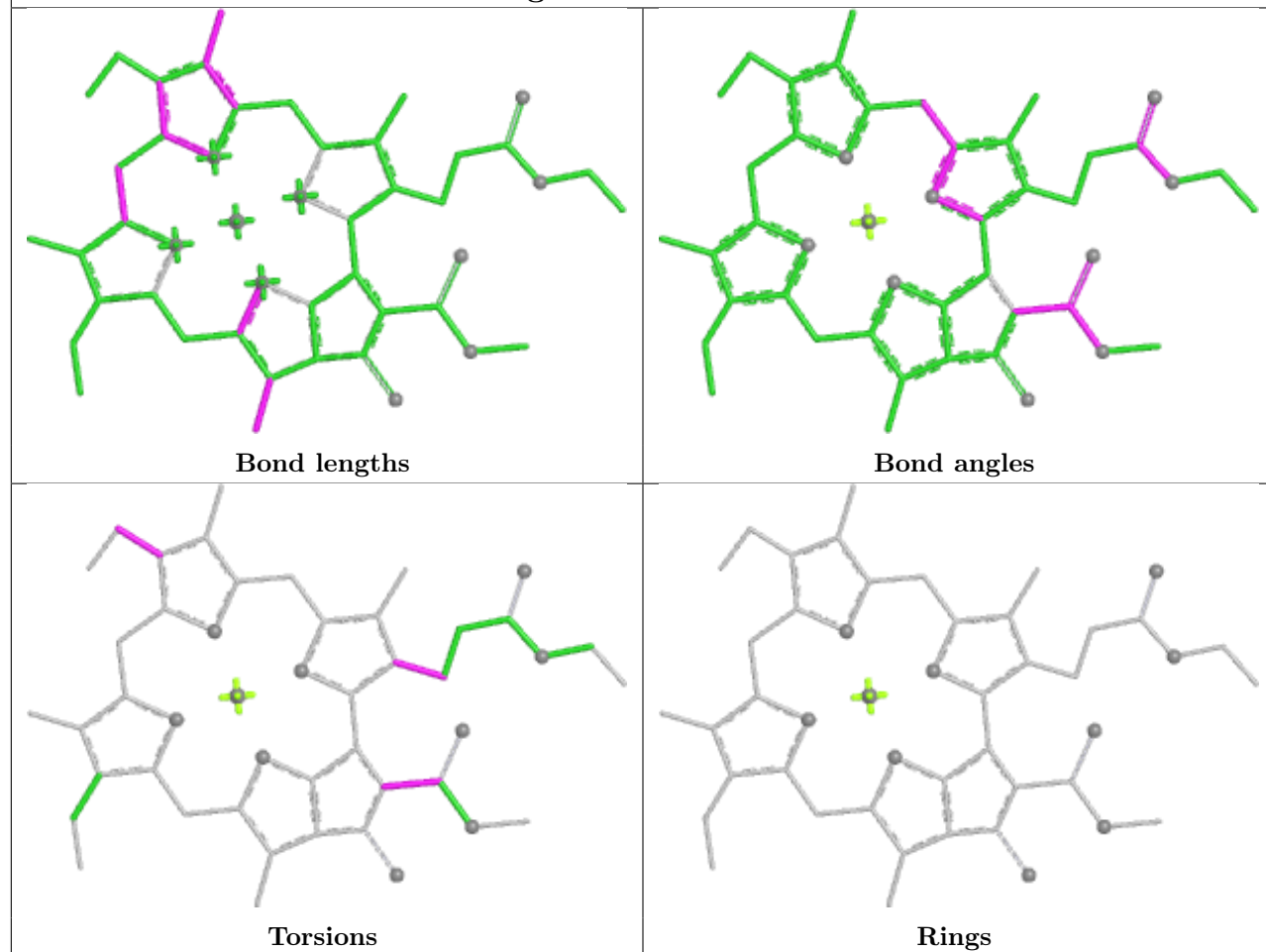
Ligand CLA B 801



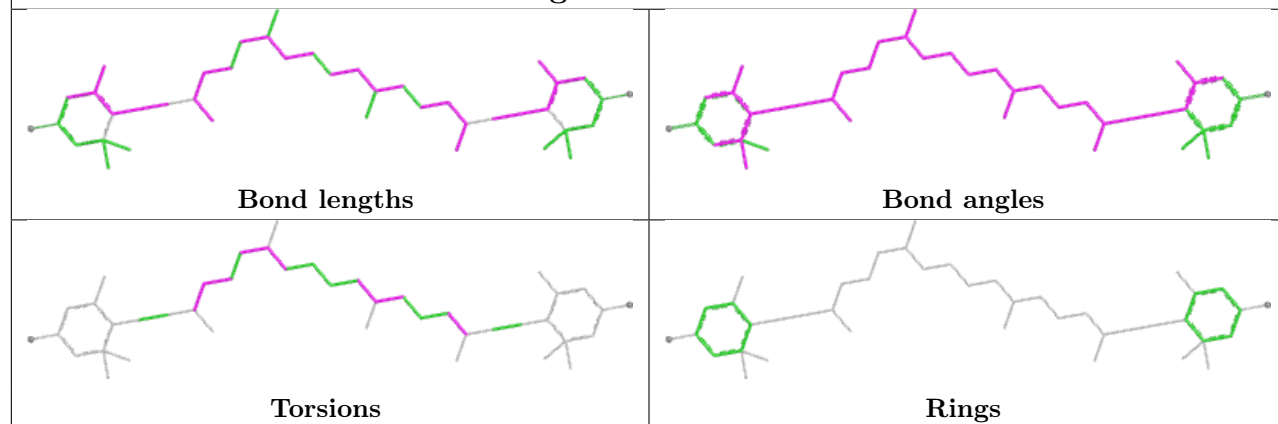
Ligand II0 a 313

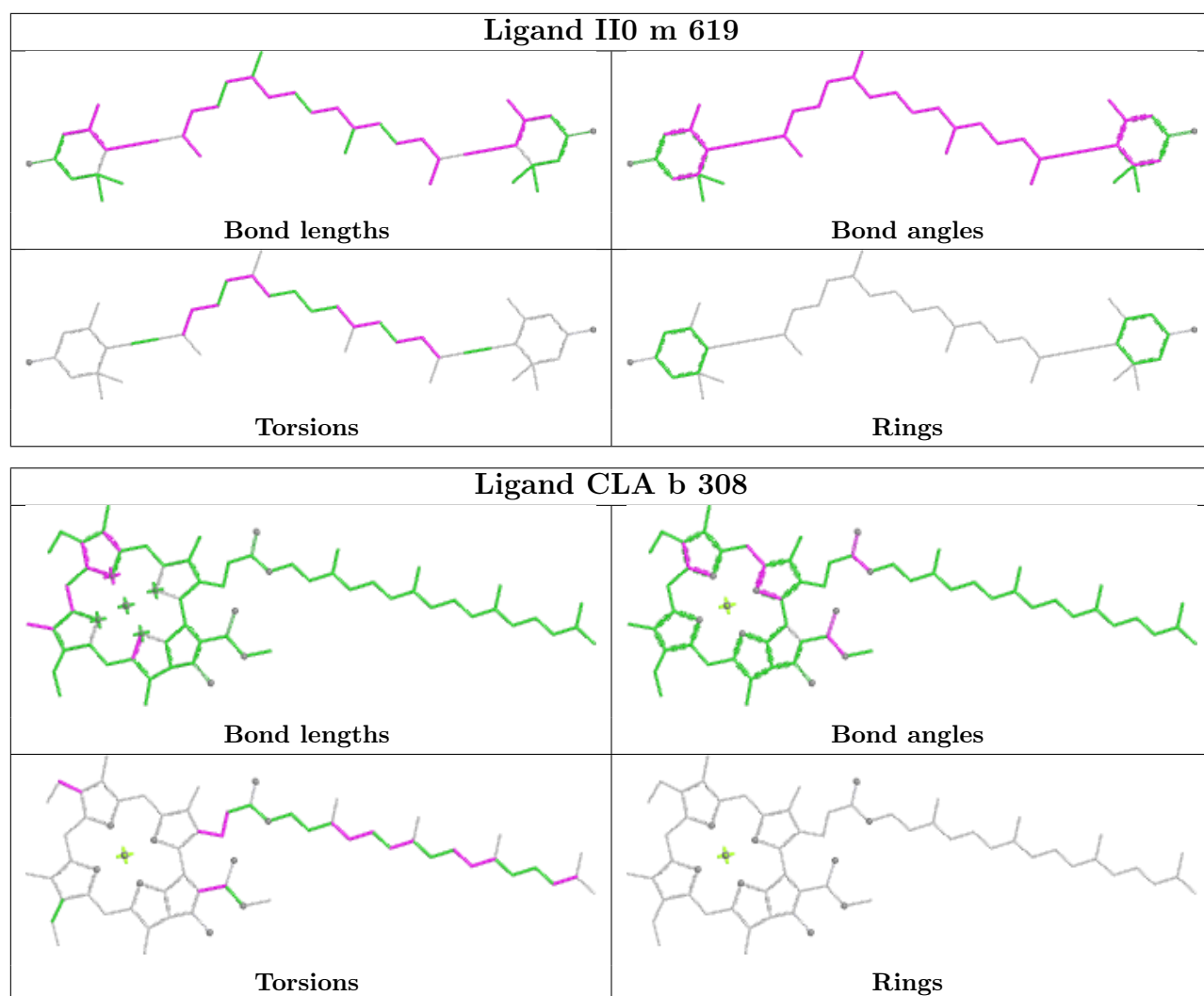


Ligand CLA B 835

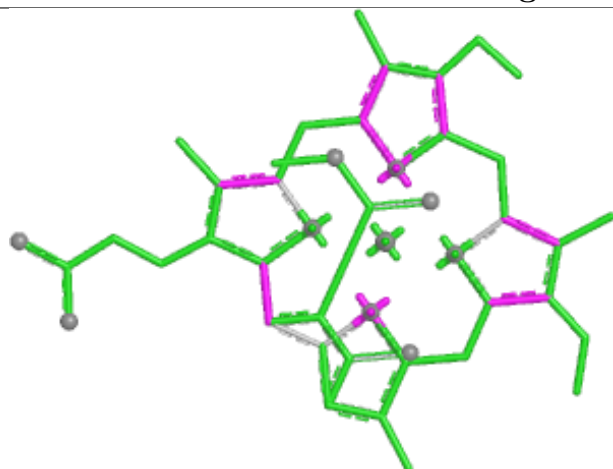


Ligand II0 h 312

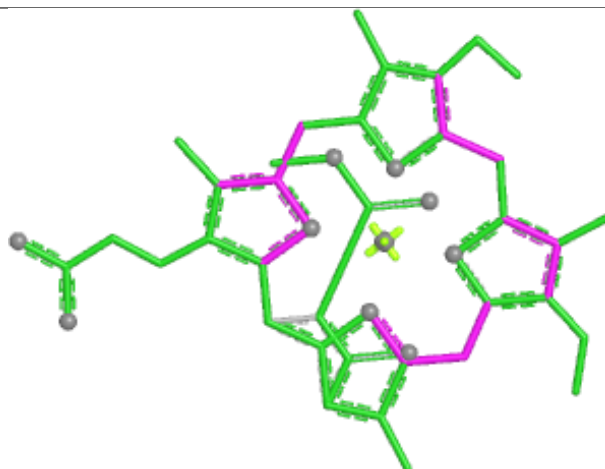




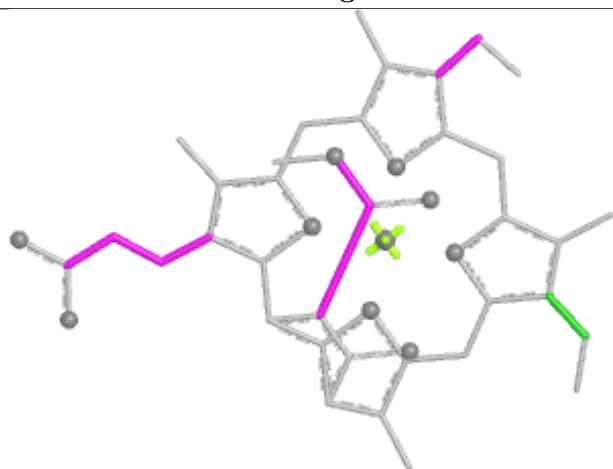
Ligand KC2 d 312



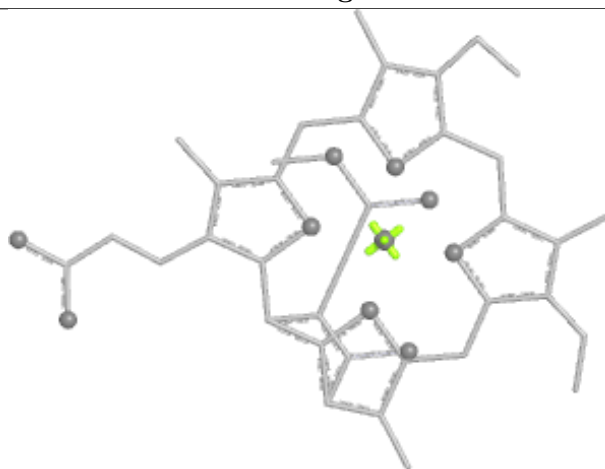
Bond lengths



Bond angles

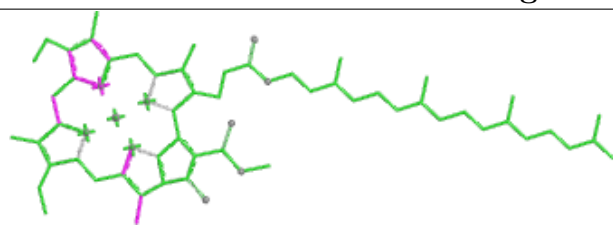


Torsions

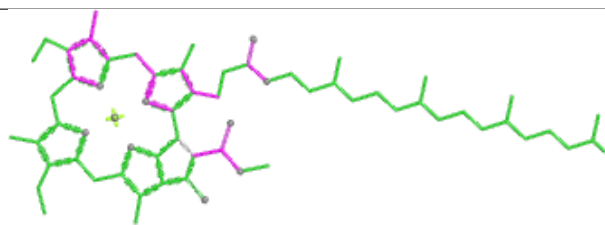


Rings

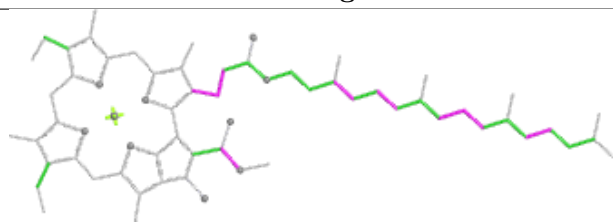
Ligand CLA s 406



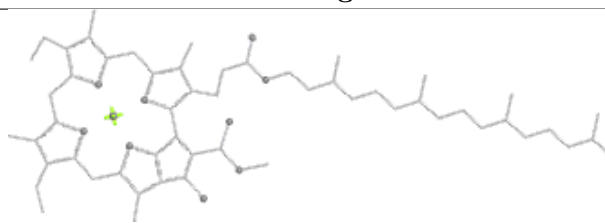
Bond lengths



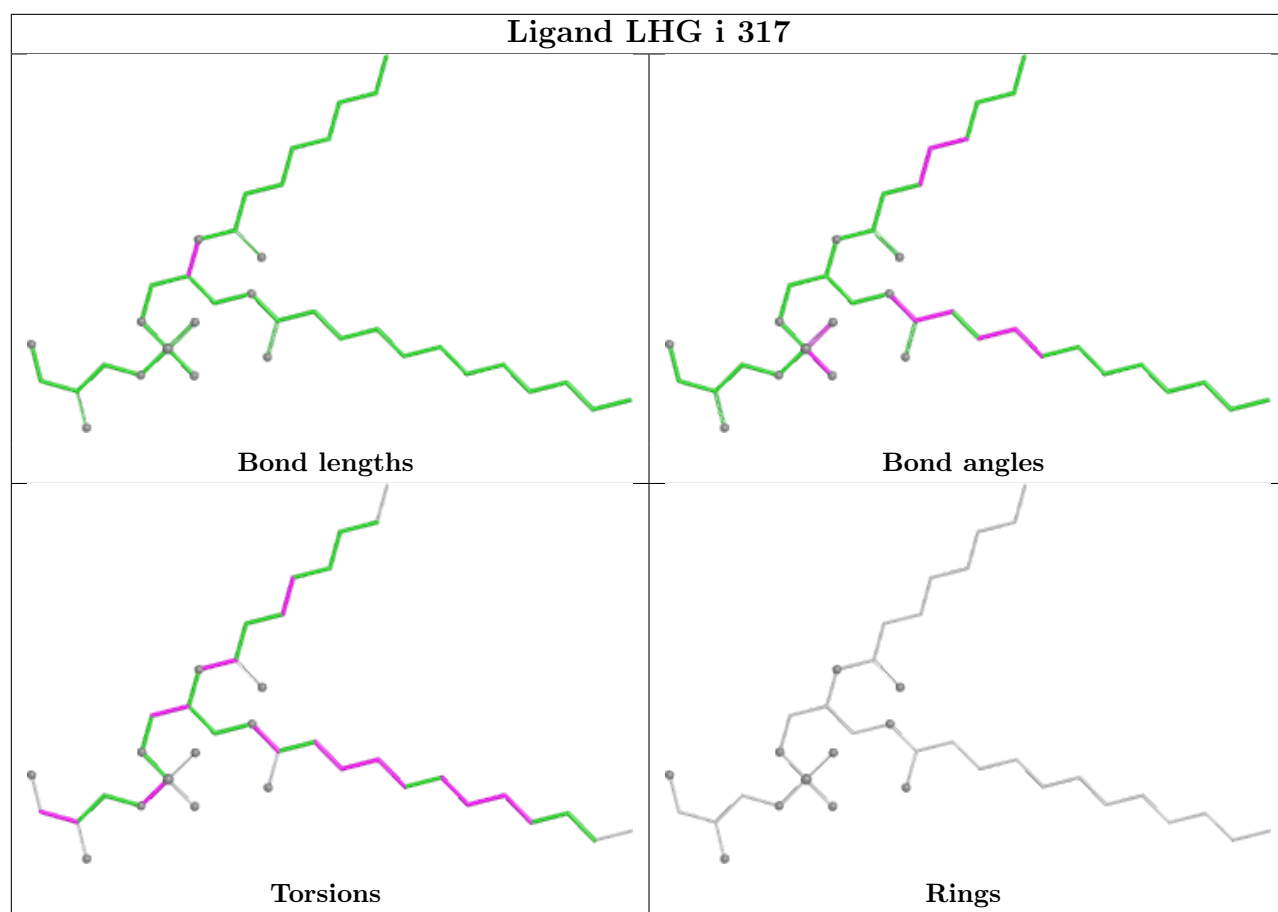
Bond angles

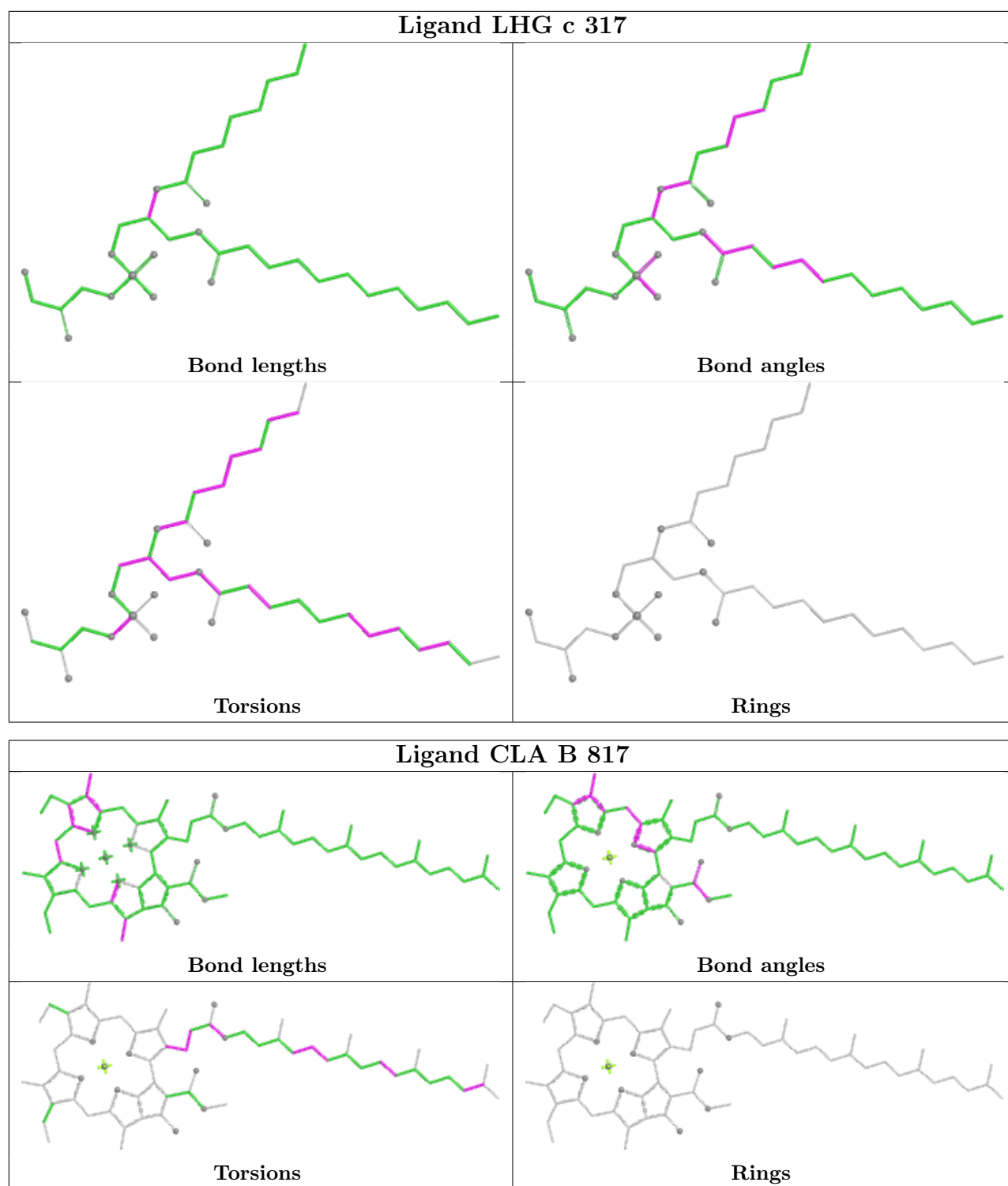


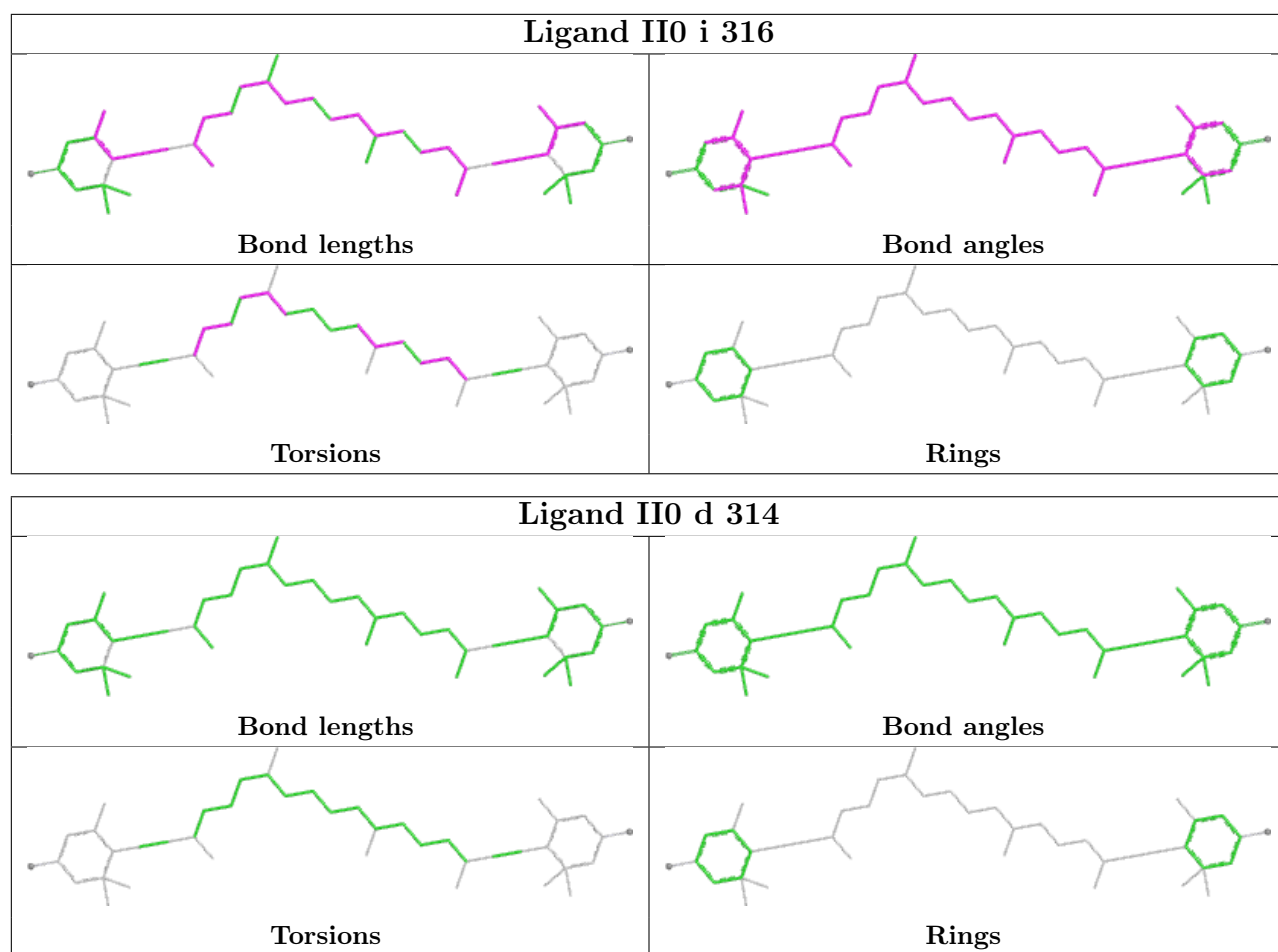
Torsions



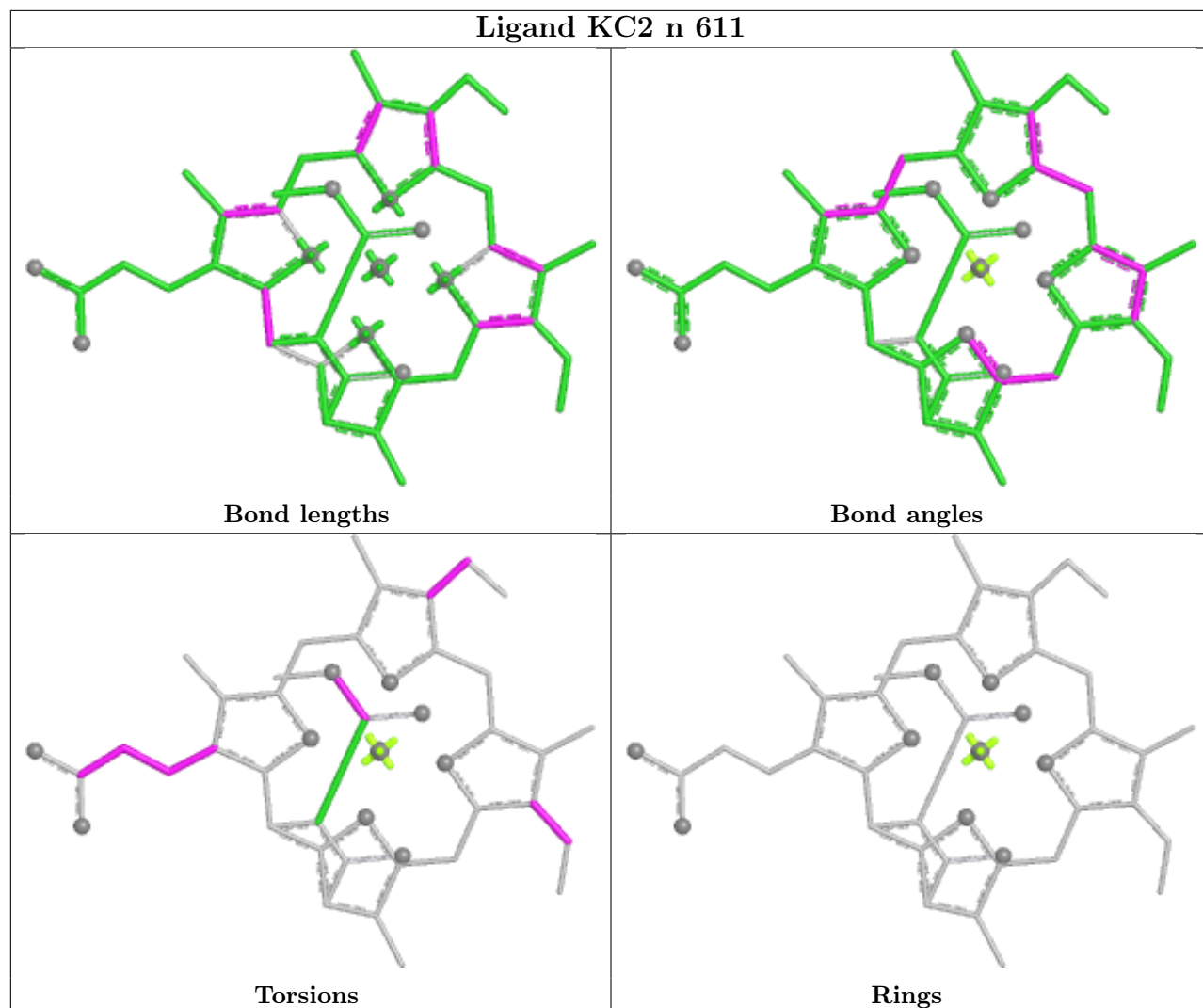
Rings



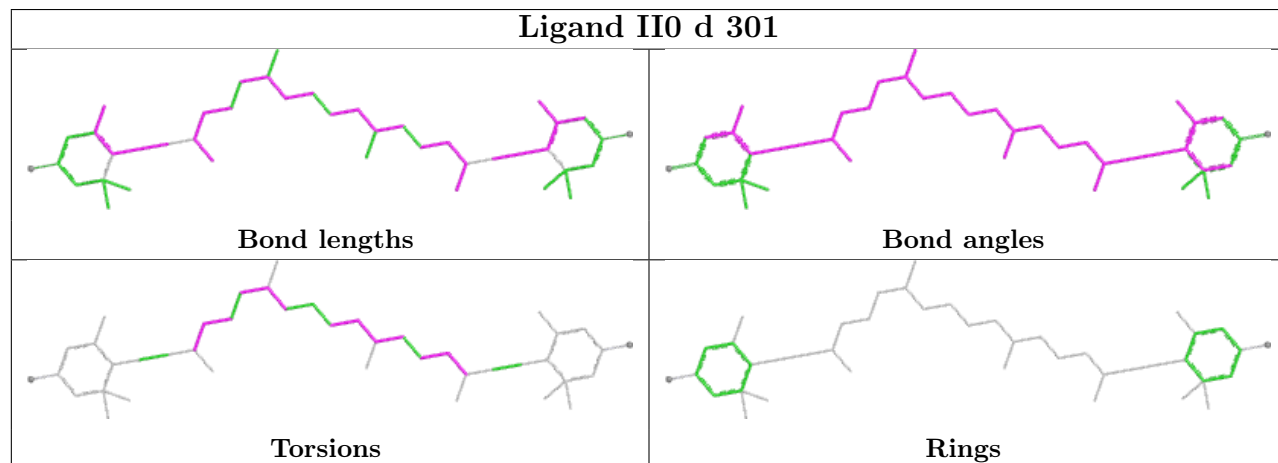


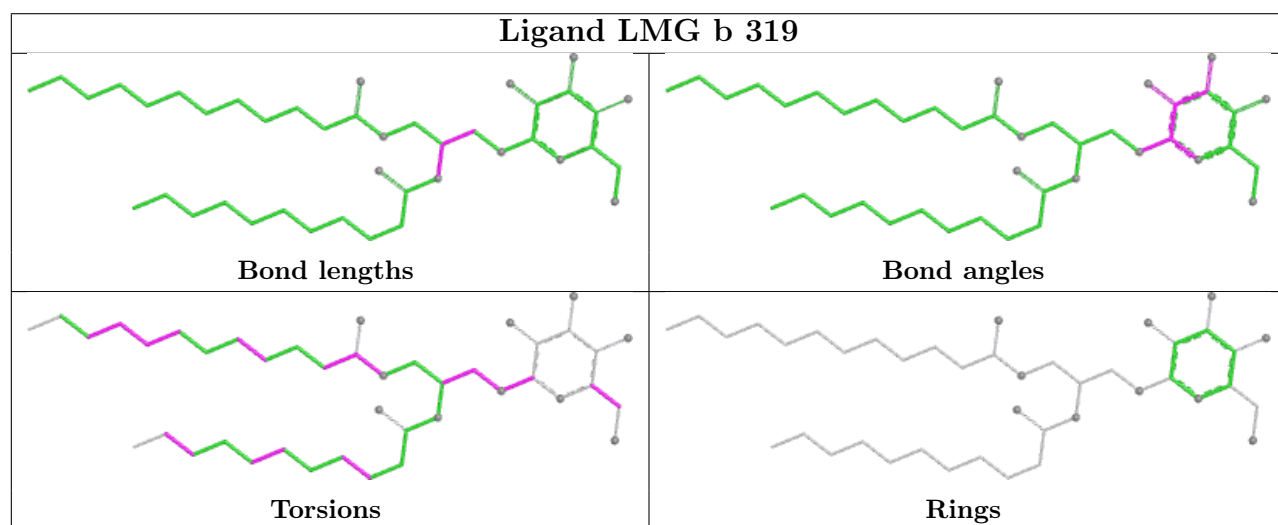
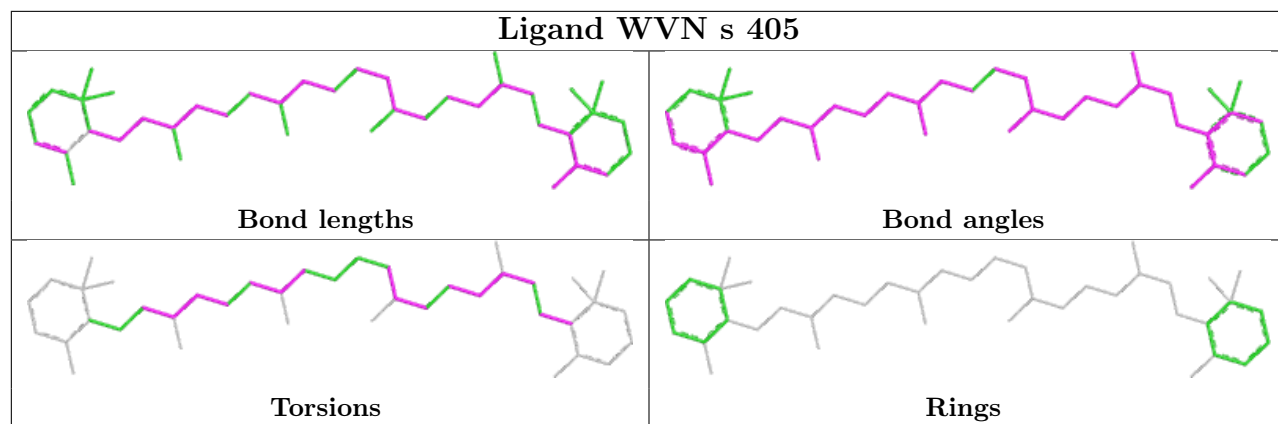


Ligand KC2 n 611

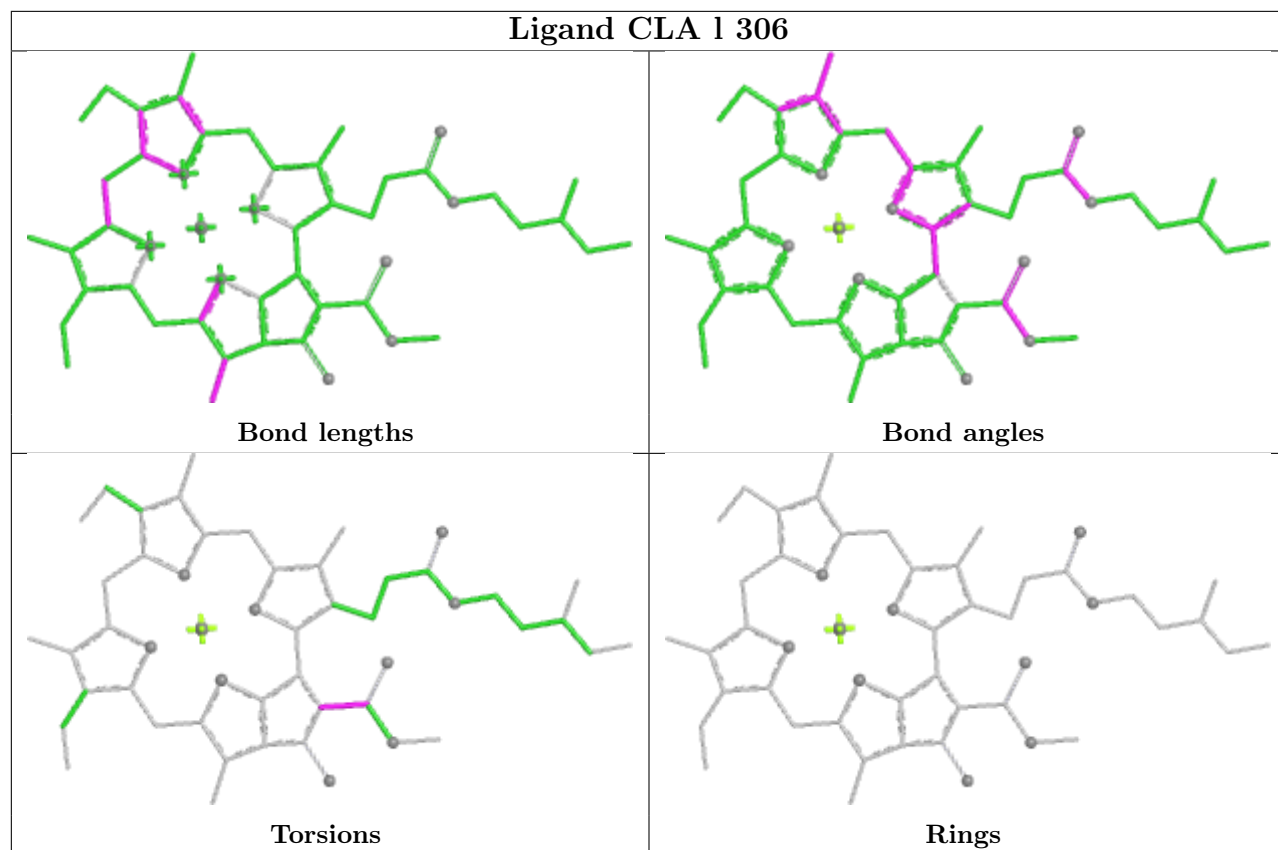


Ligand II0 d 301

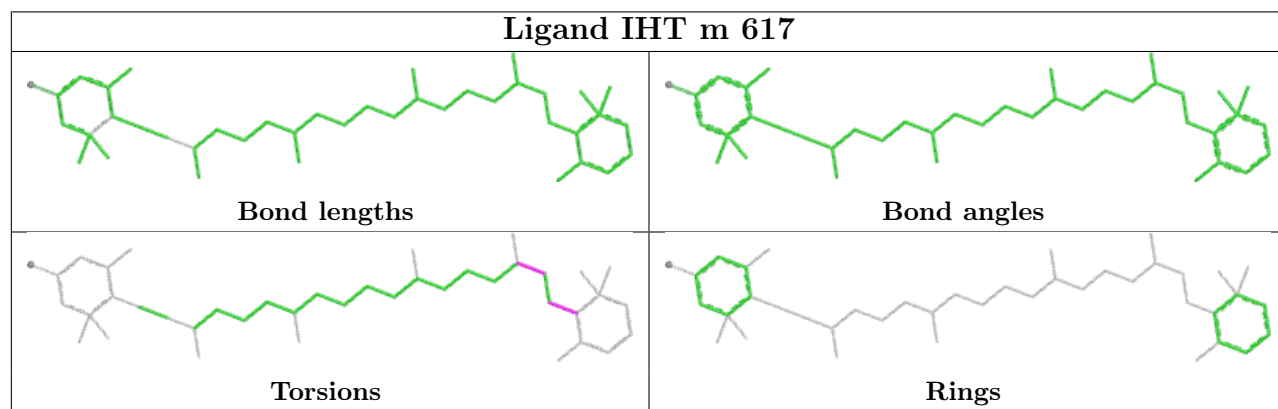


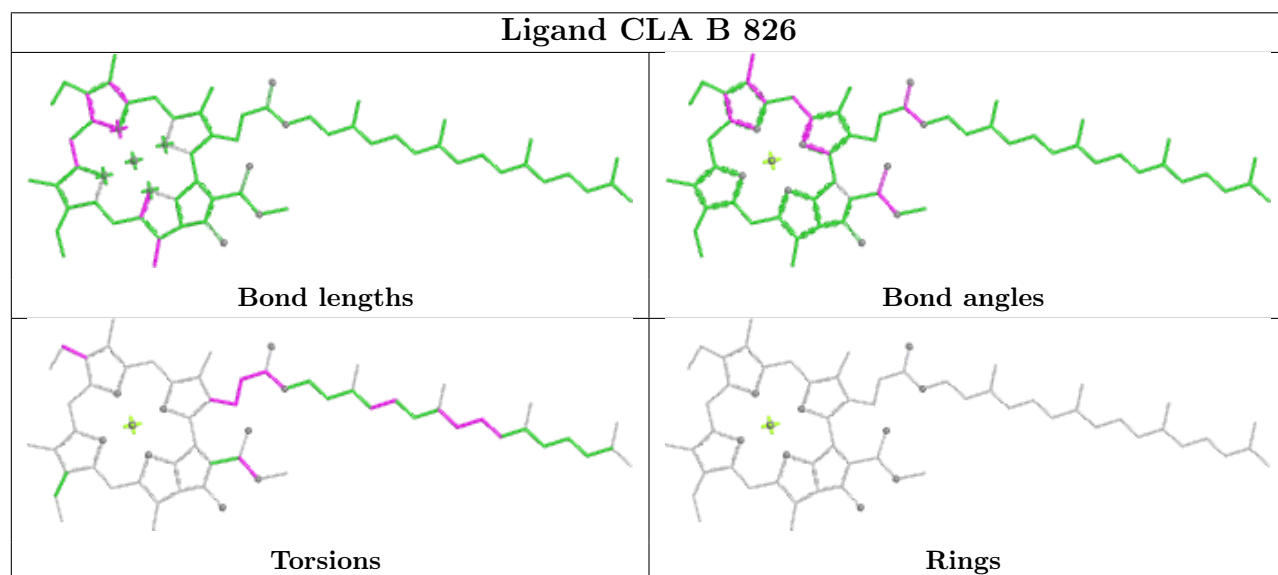
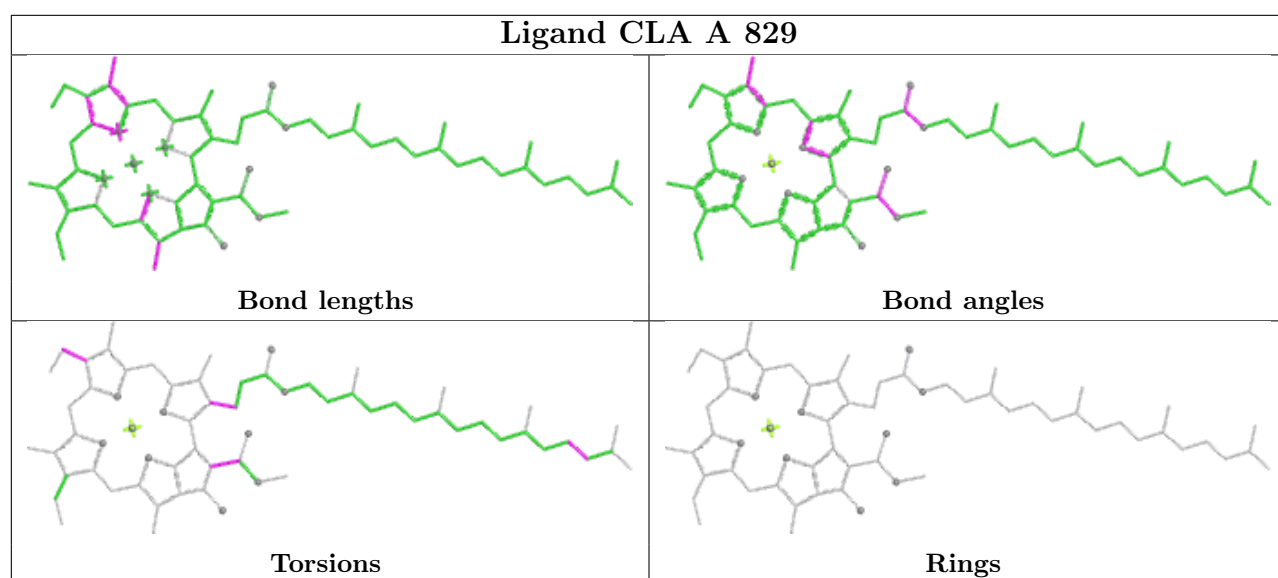
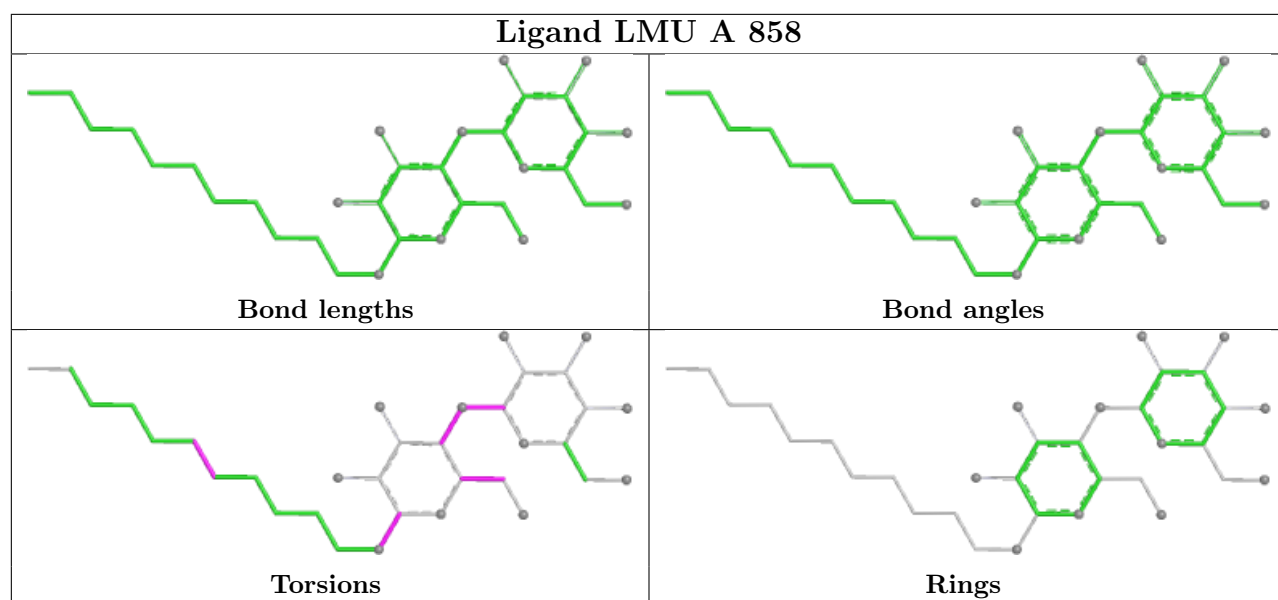


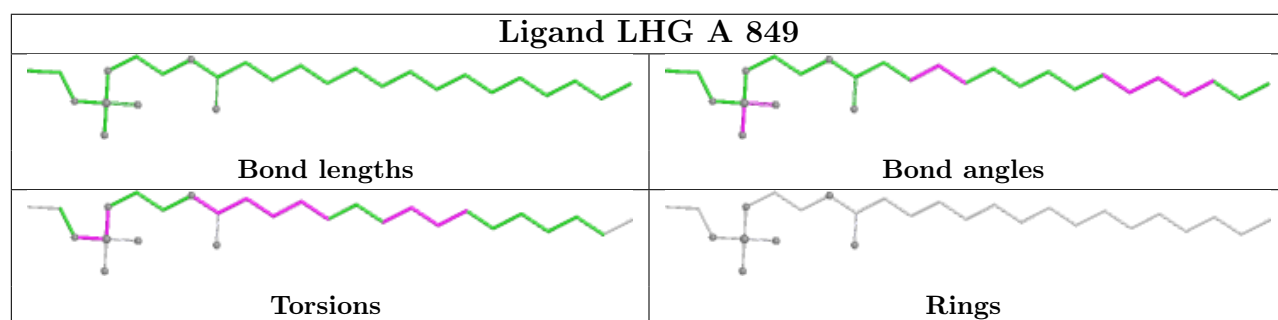
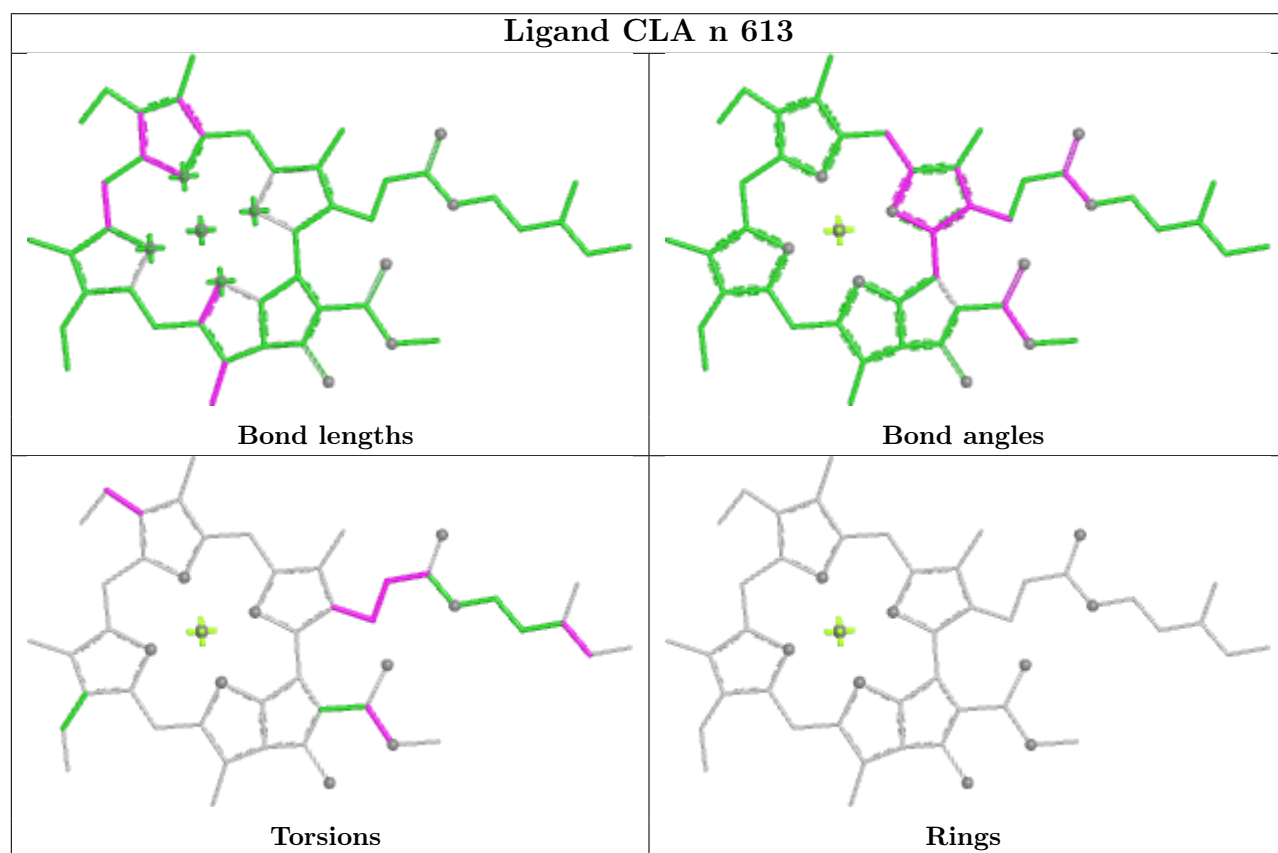
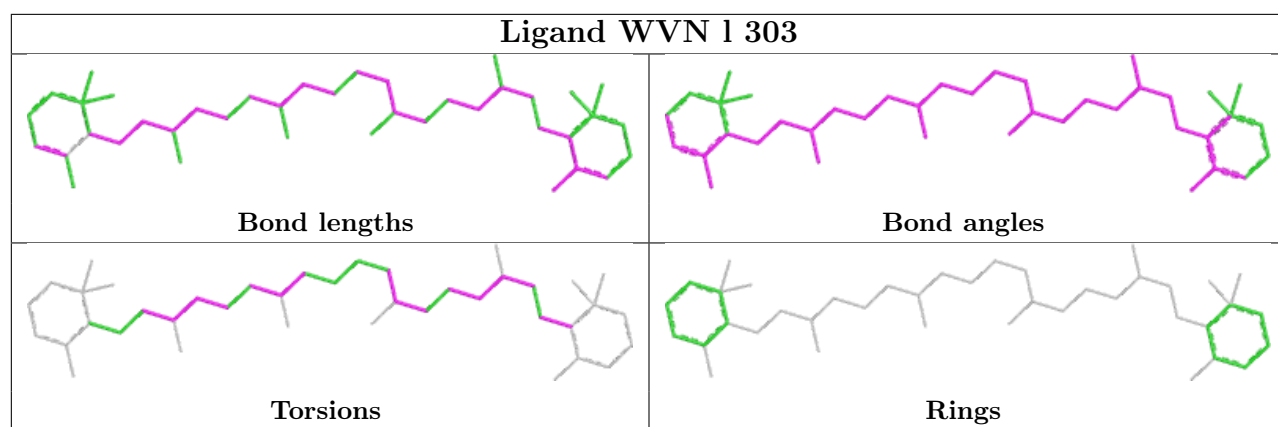
Ligand CLA l 306



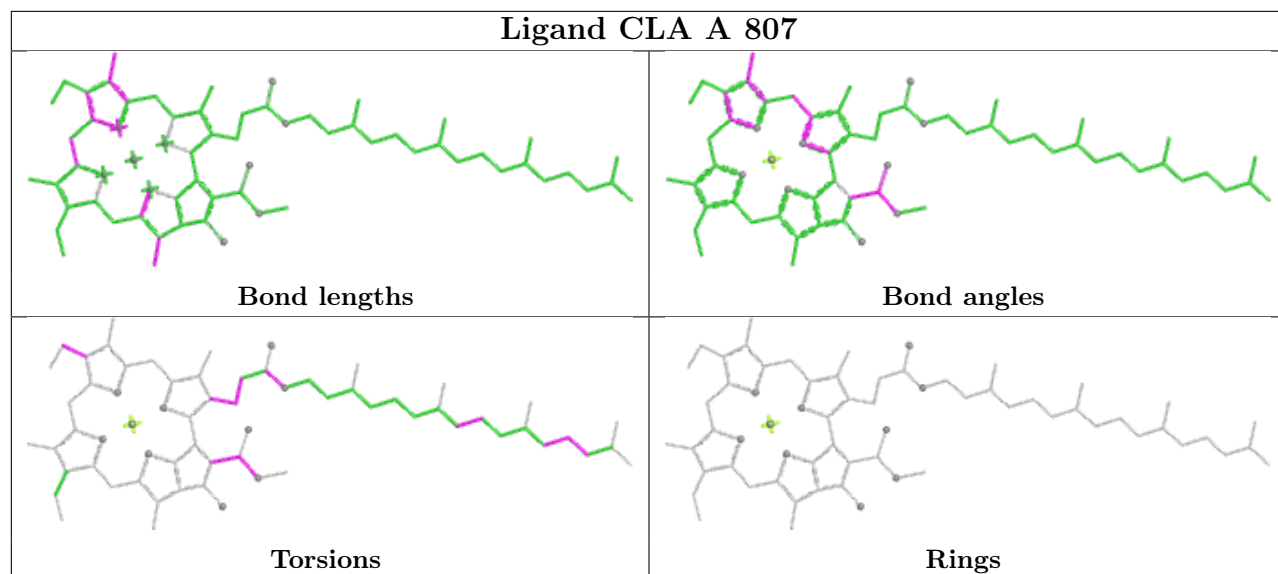
Ligand IHT m 617



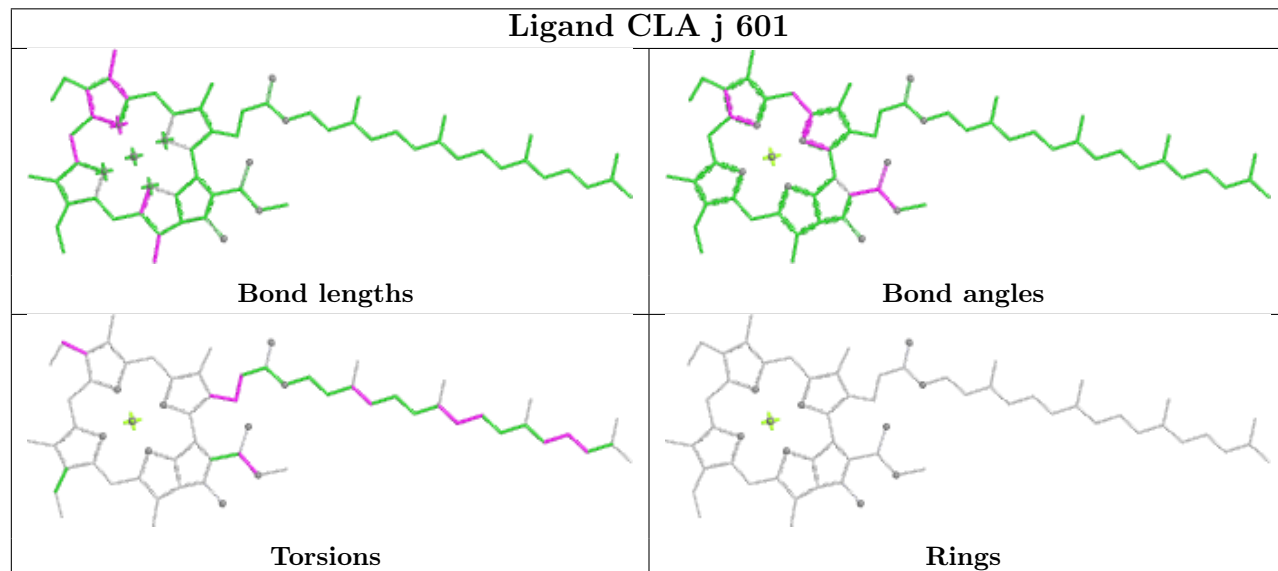




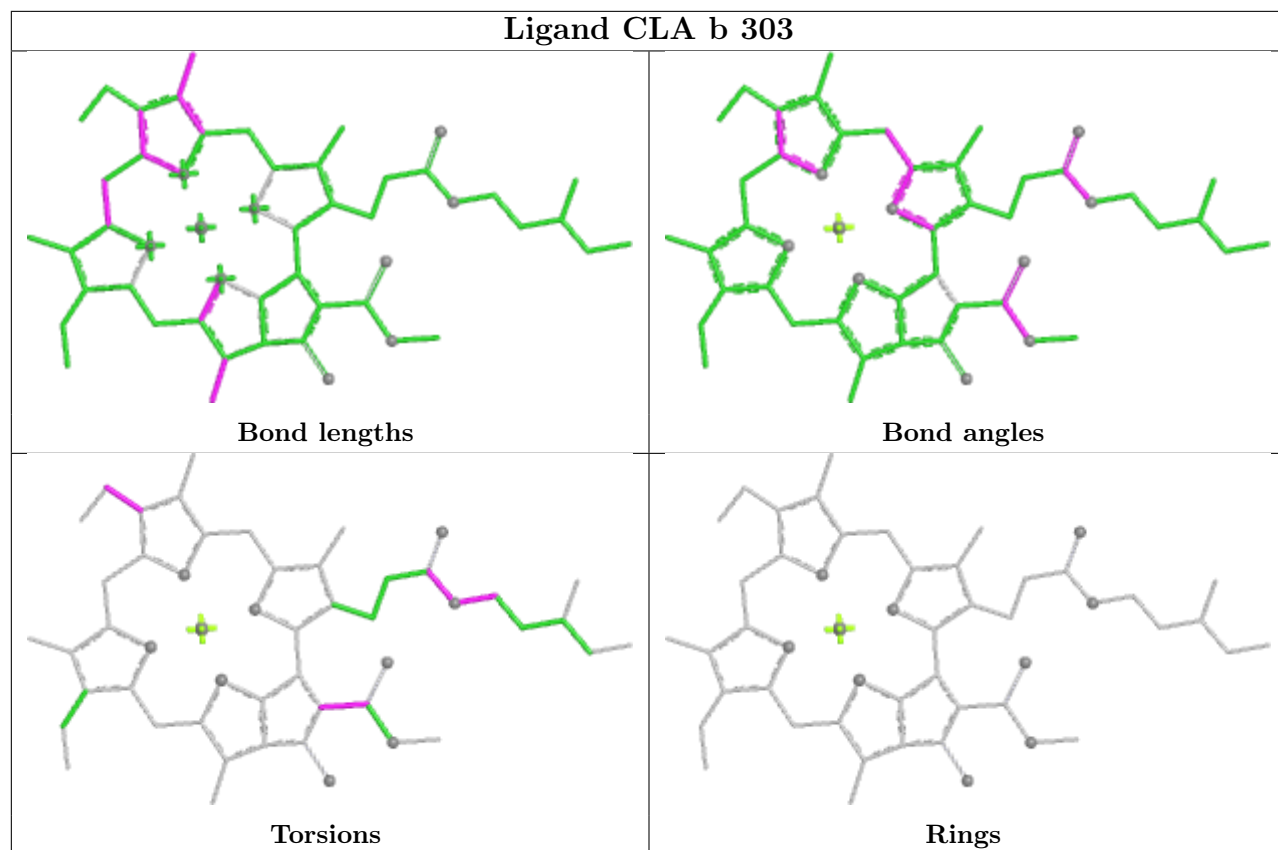
Ligand CLA A 807



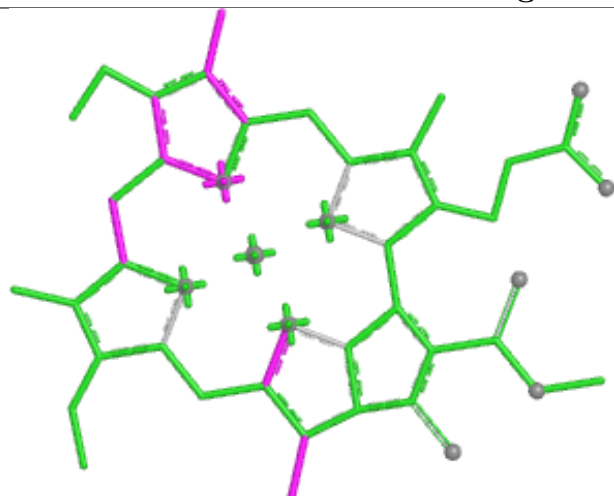
Ligand CLA j 601



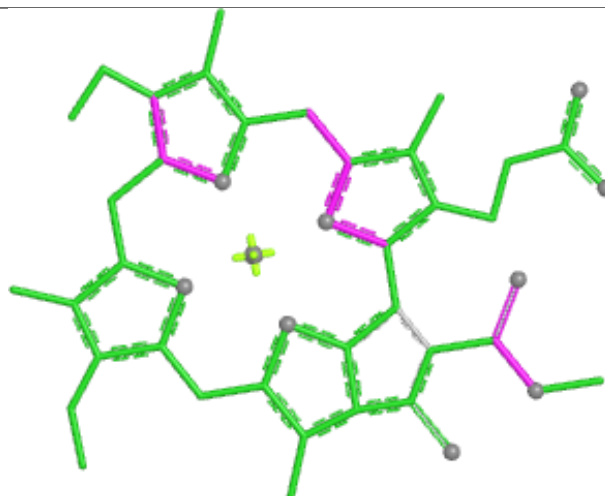
Ligand CLA b 303



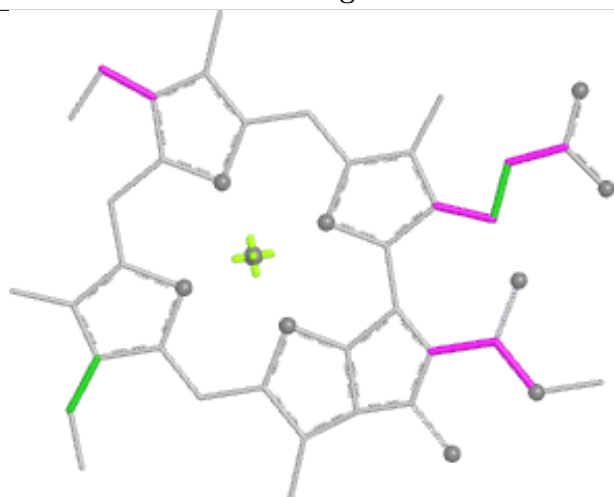
Ligand CLA d 307



Bond lengths



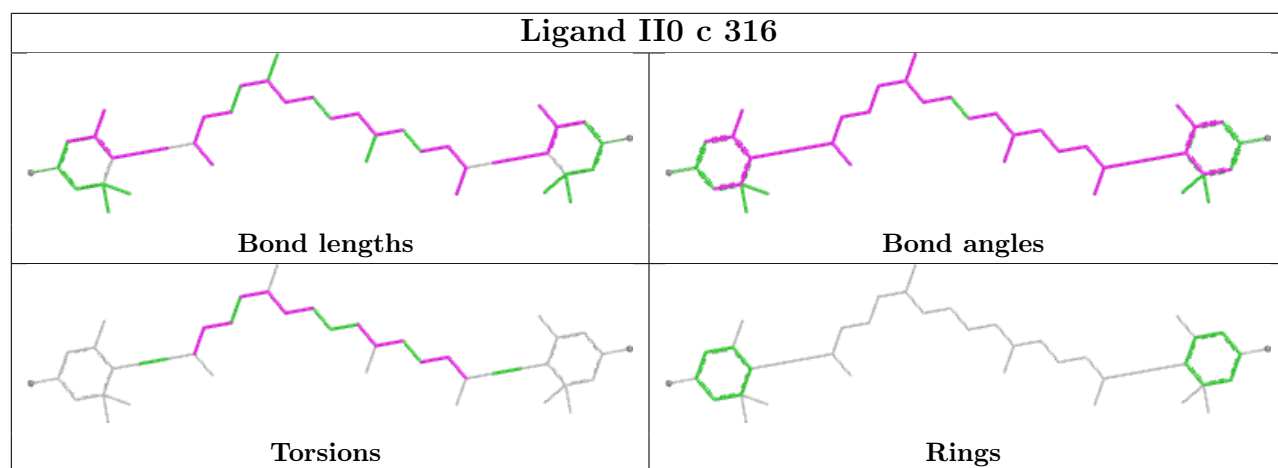
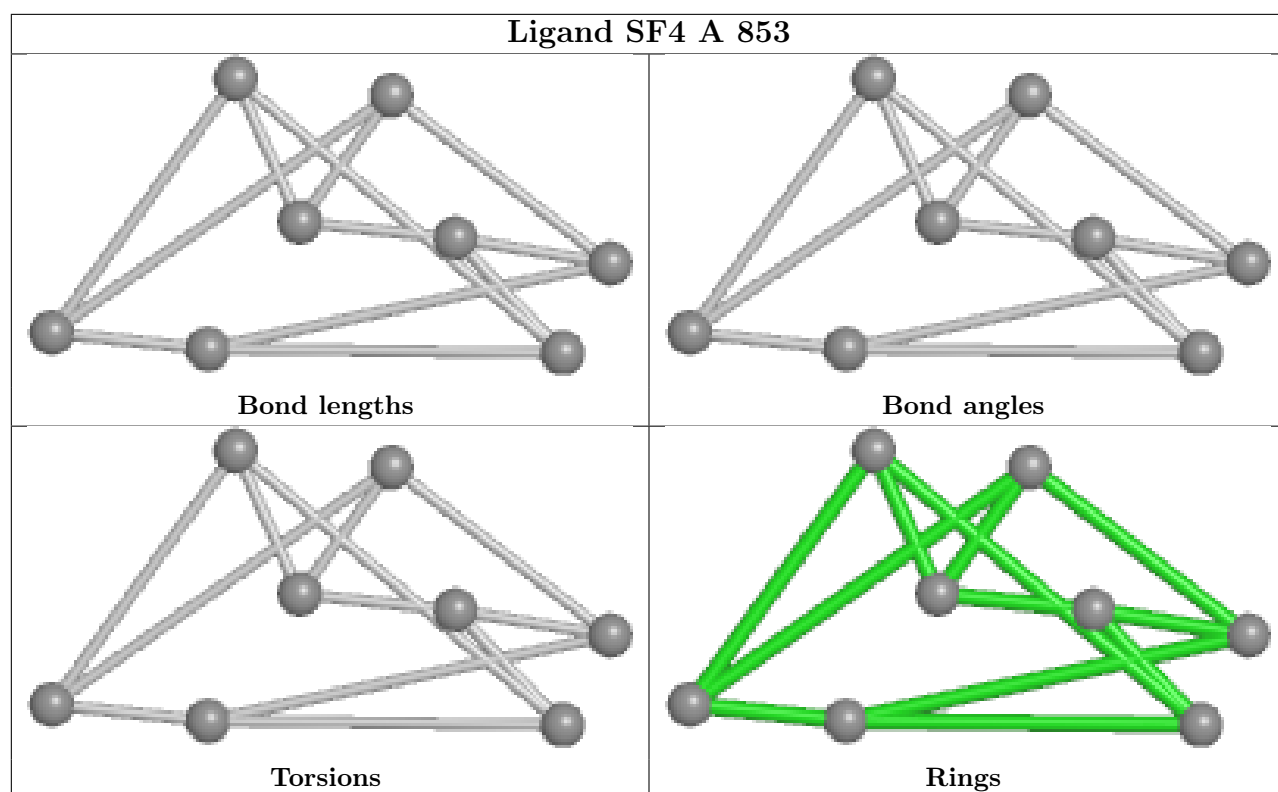
Bond angles



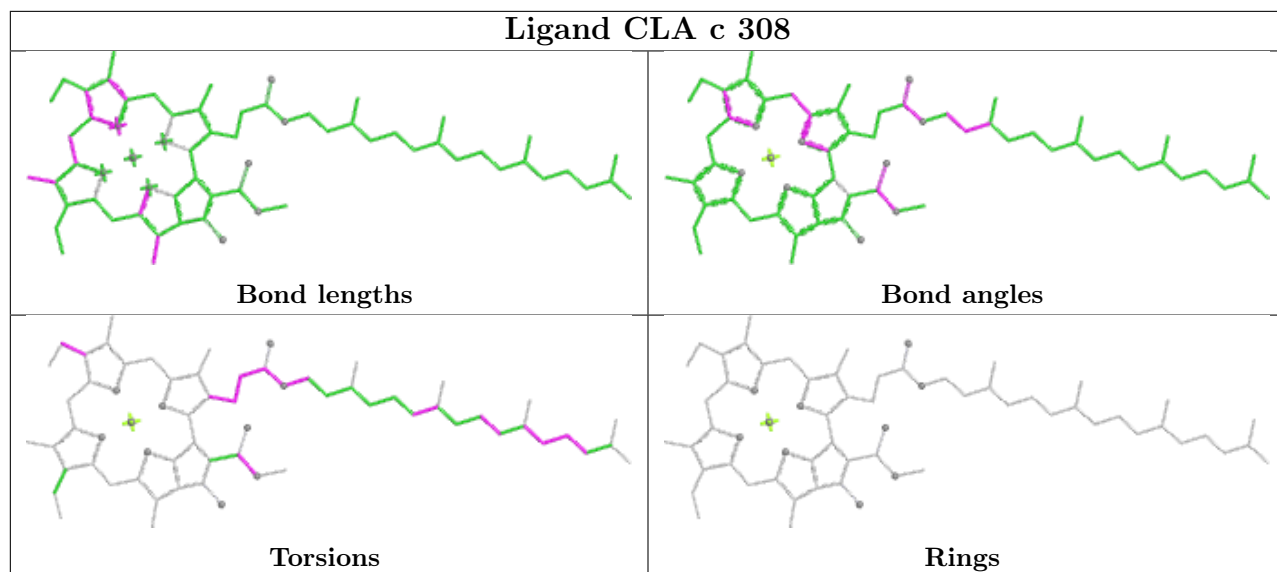
Torsions



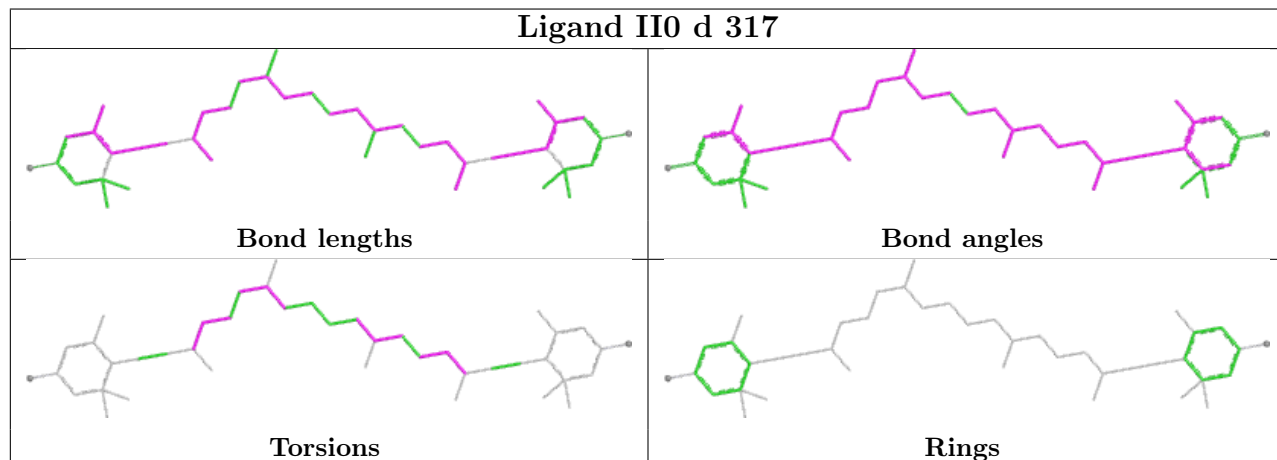
Rings



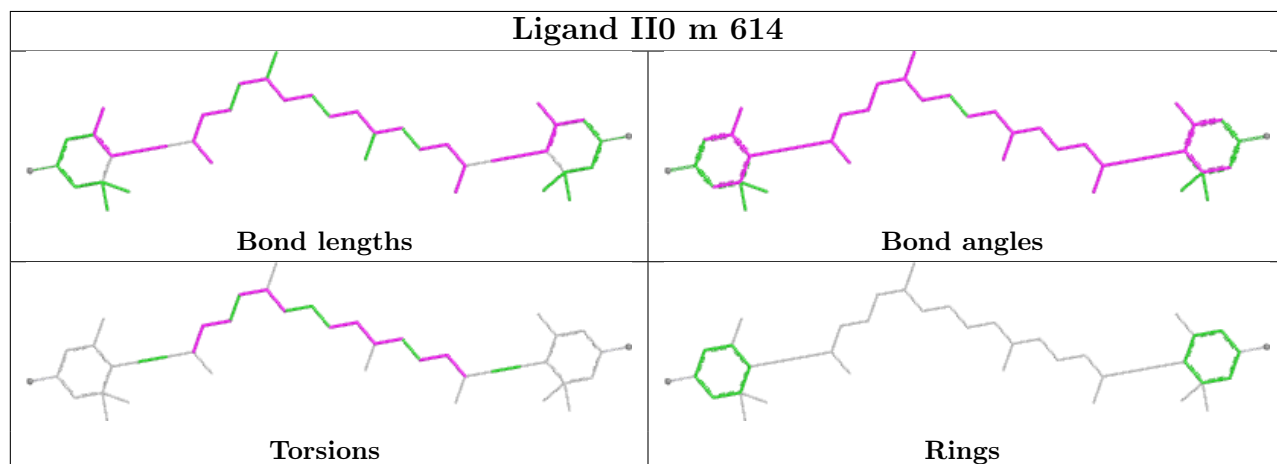
Ligand CLA c 308

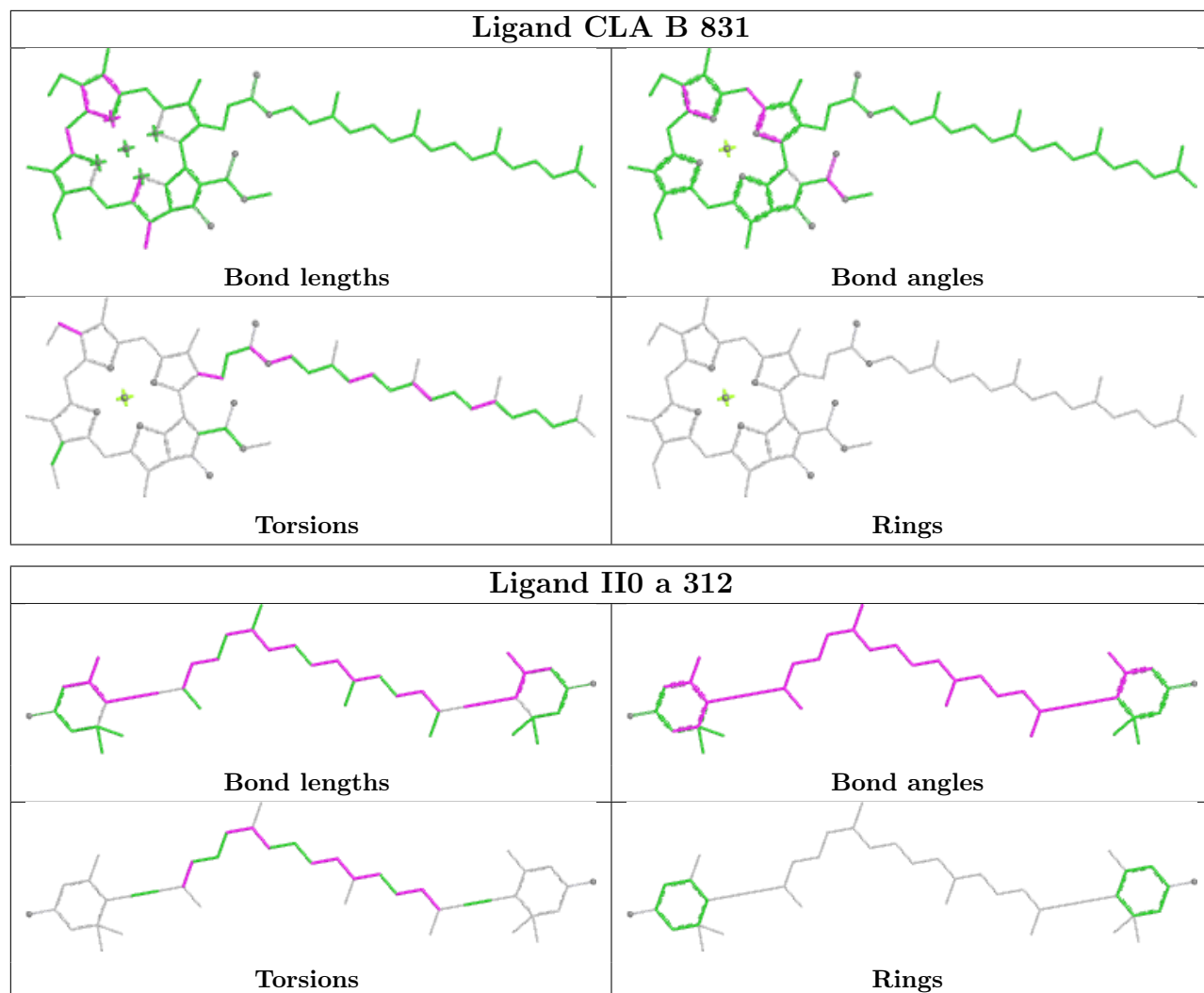


Ligand II0 d 317

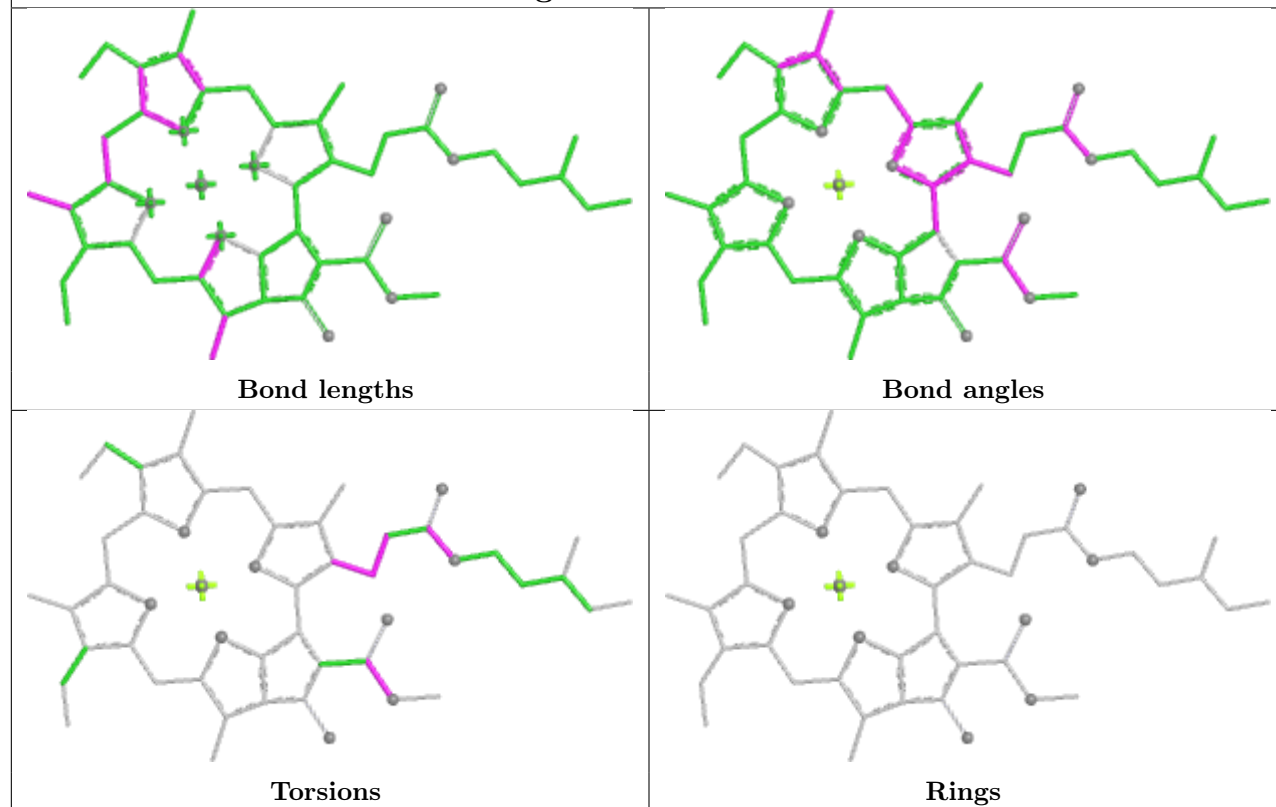


Ligand II0 m 614

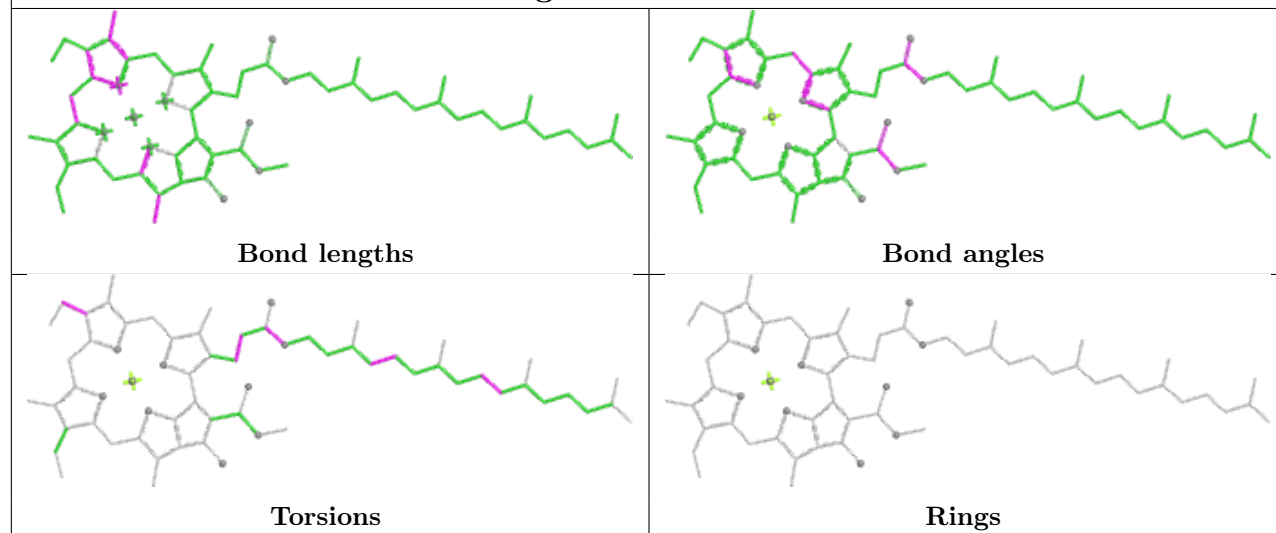




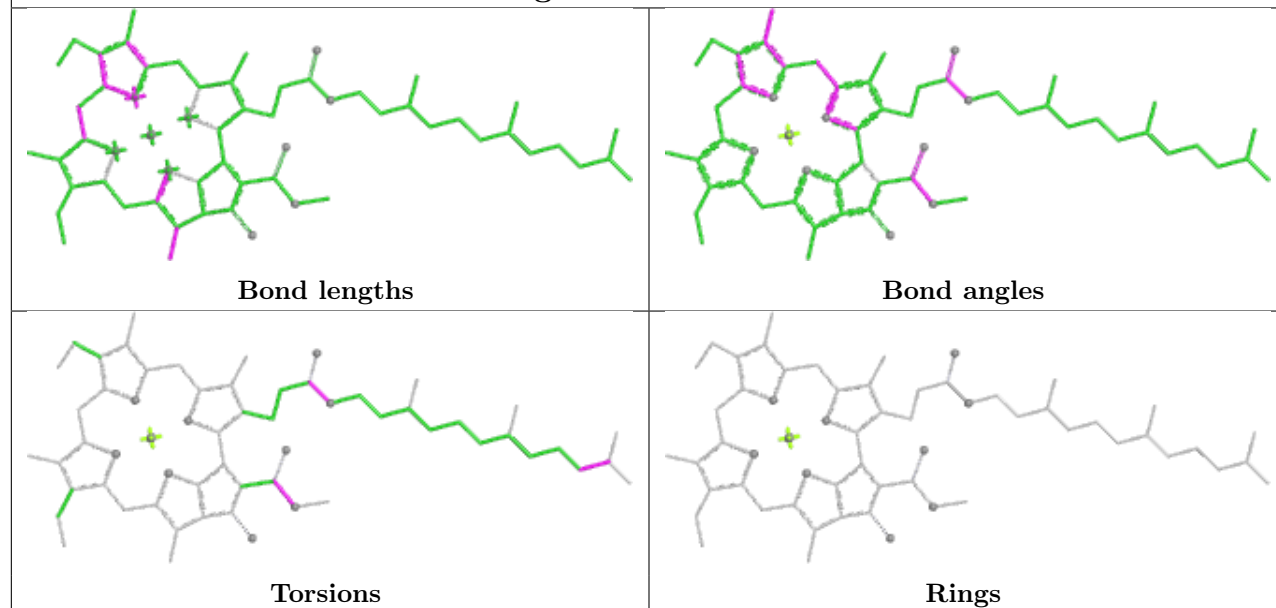
Ligand CLA d 313



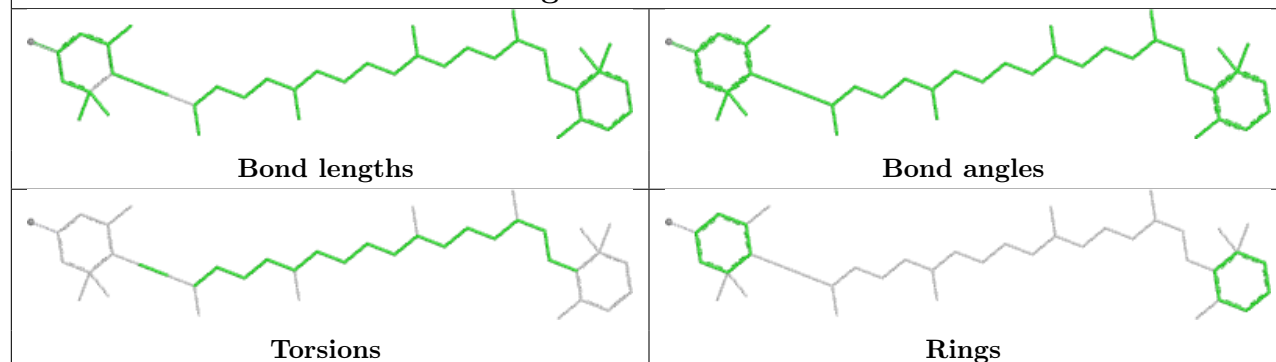
Ligand CLA h 306



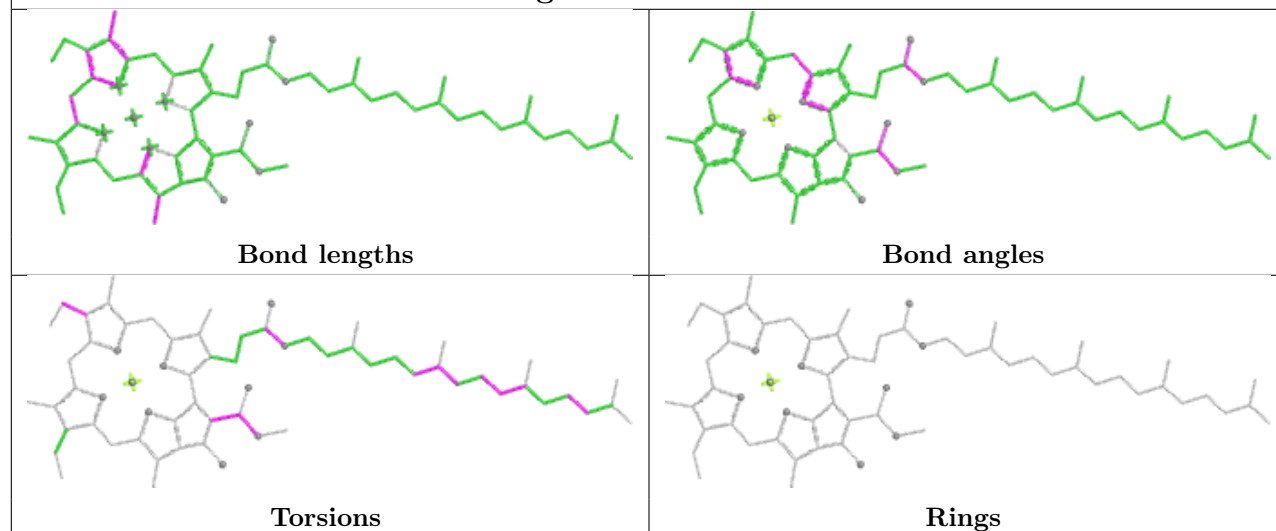
Ligand CLA L 204

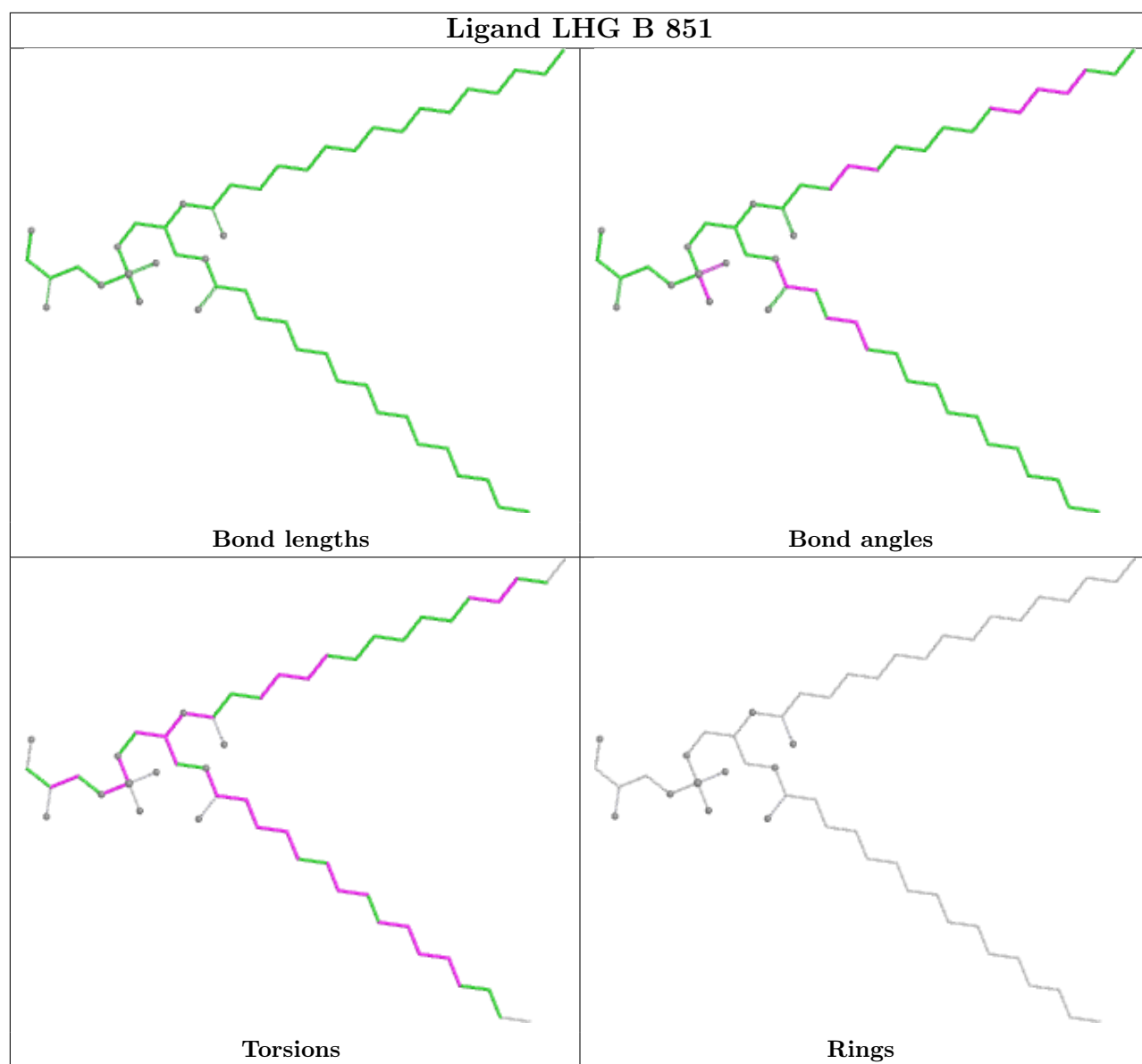


Ligand IHT c 315

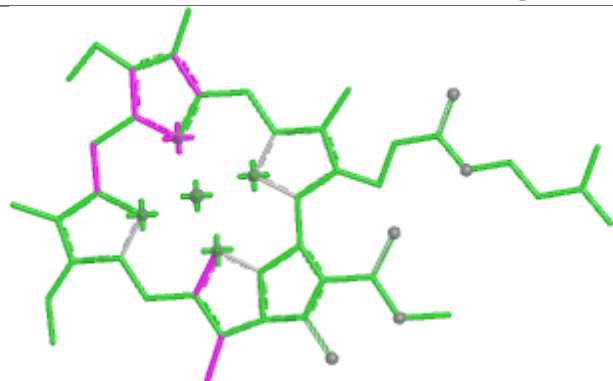


Ligand CLA a 310

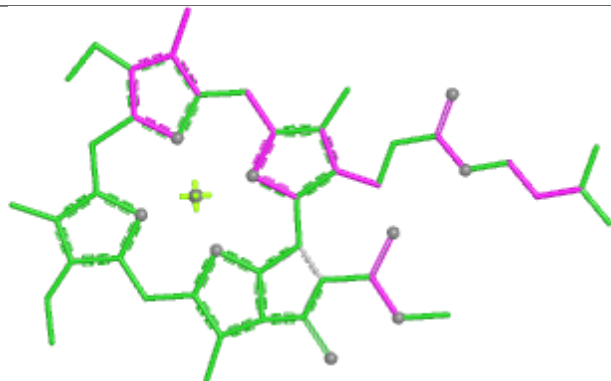




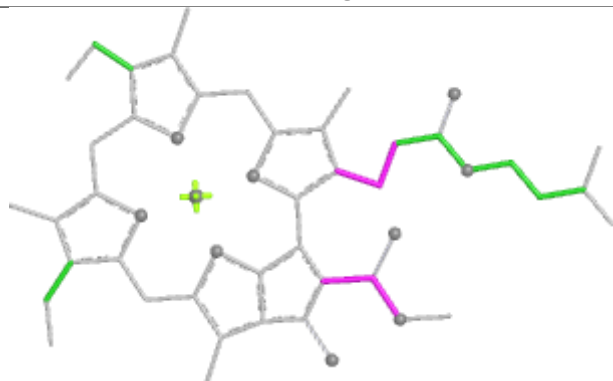
Ligand CLA A 814



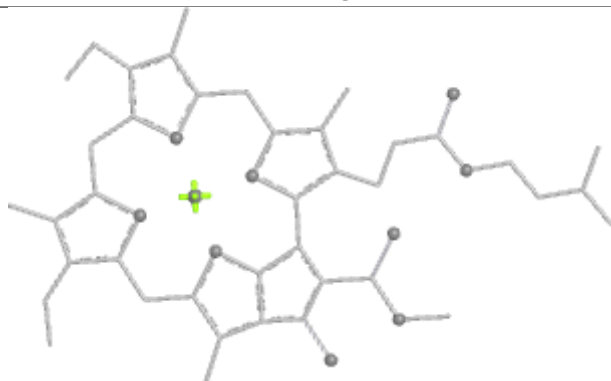
Bond lengths



Bond angles

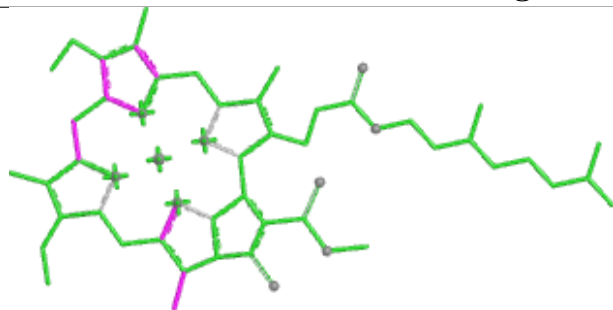


Torsions

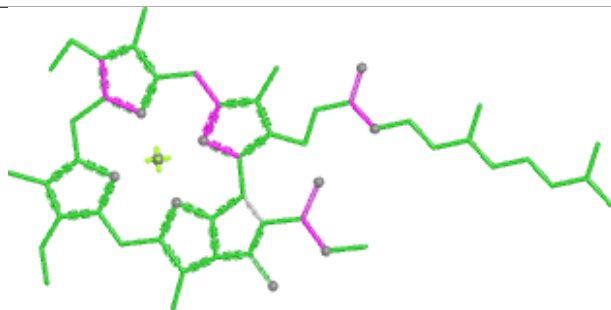


Rings

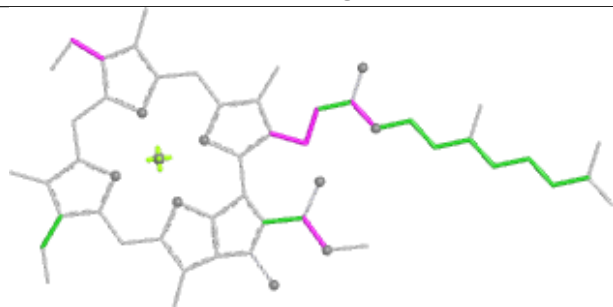
Ligand CLA A 823



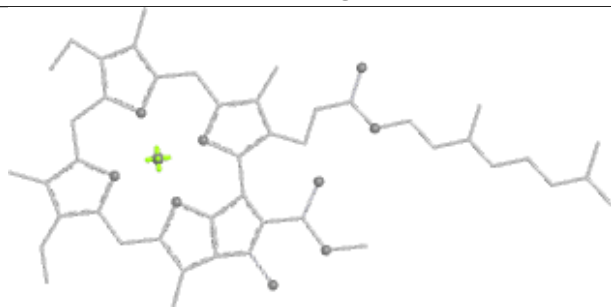
Bond lengths



Bond angles

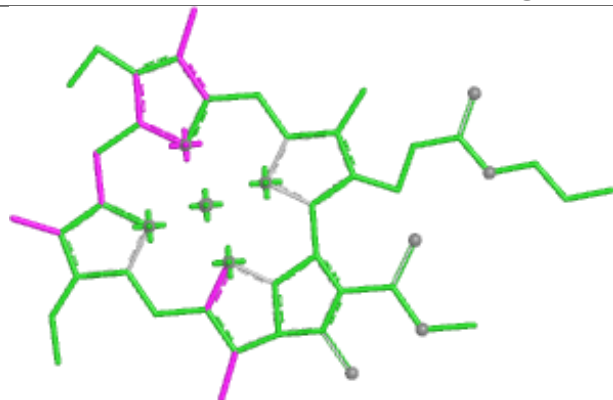


Torsions

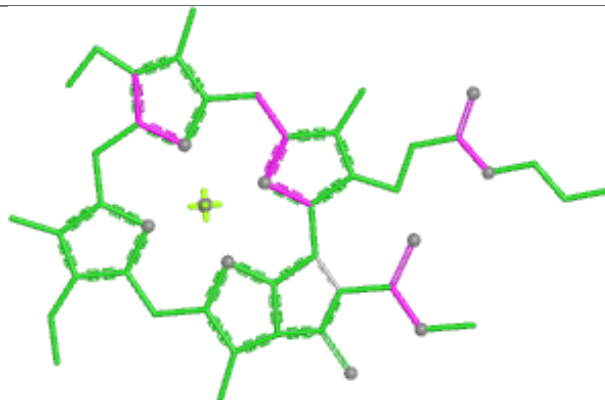


Rings

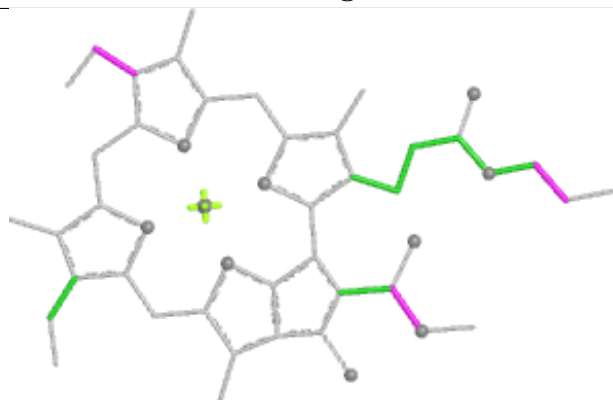
Ligand CLA a 308



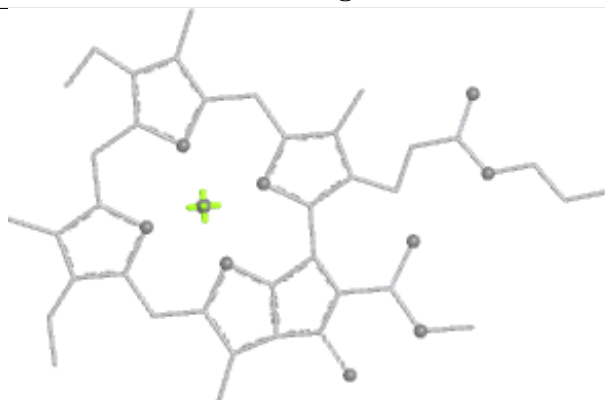
Bond lengths



Bond angles

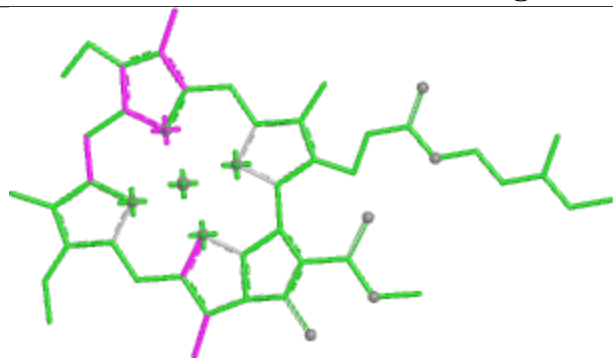


Torsions

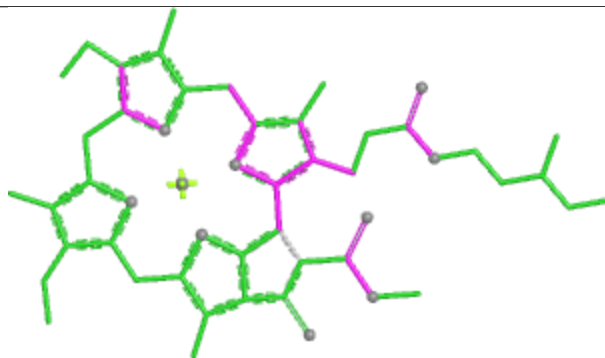


Rings

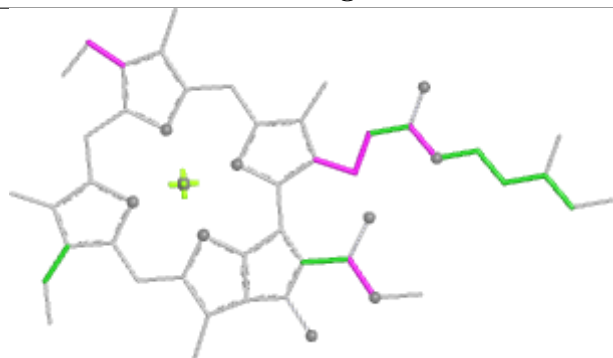
Ligand CLA m 612



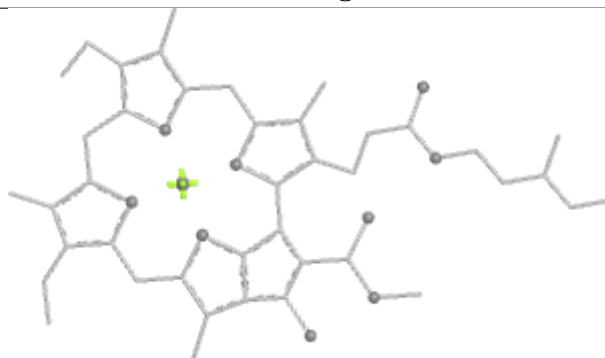
Bond lengths



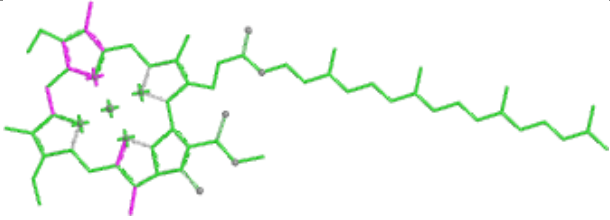
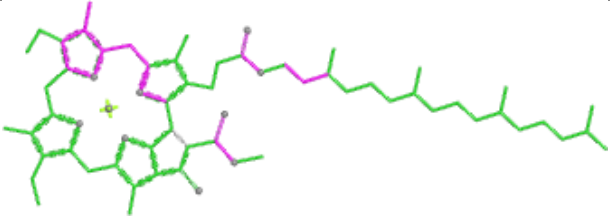
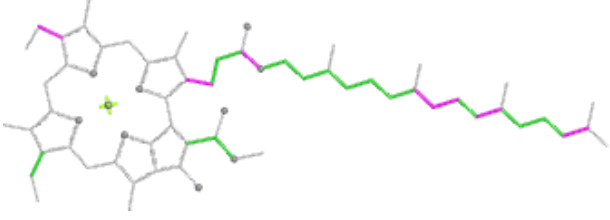
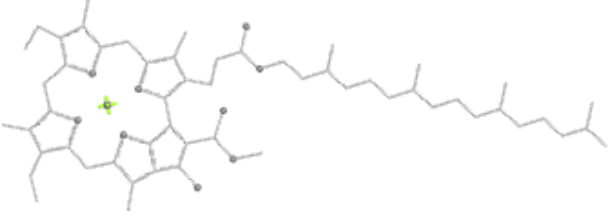
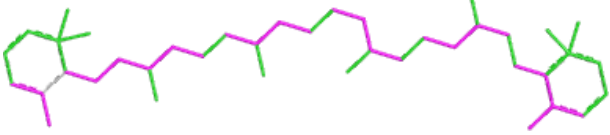
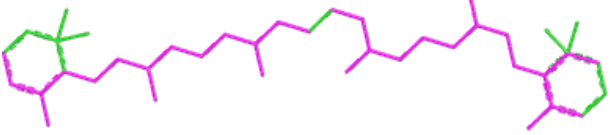
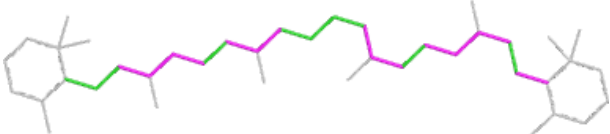
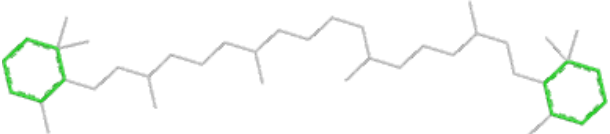
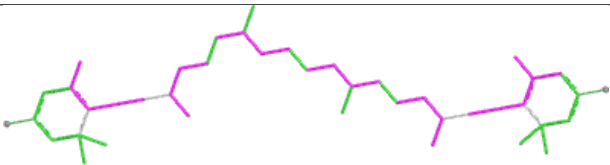
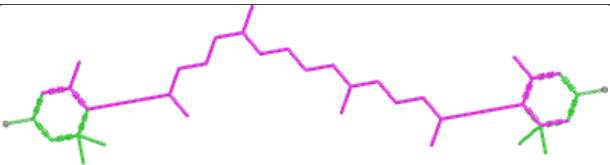
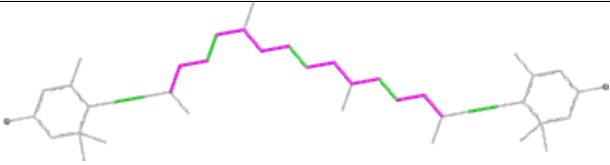
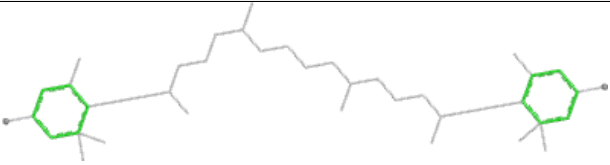
Bond angles

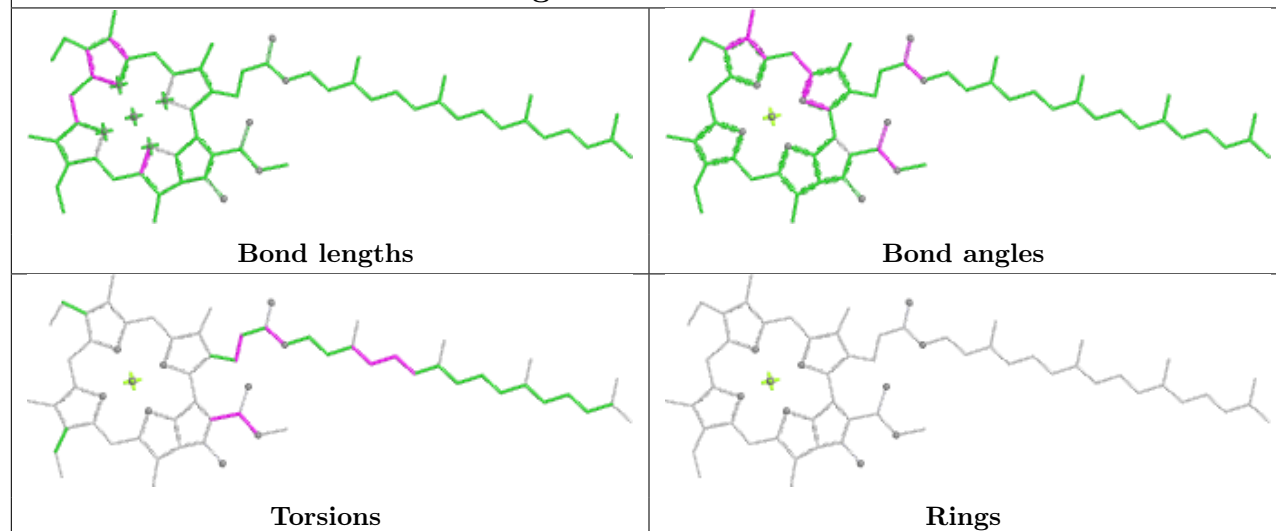
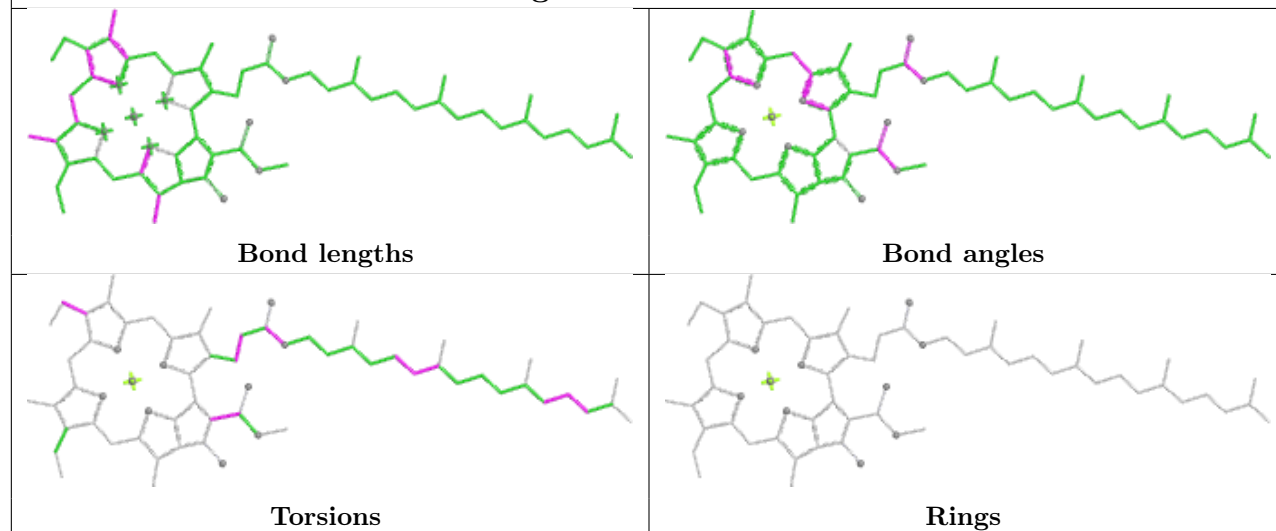
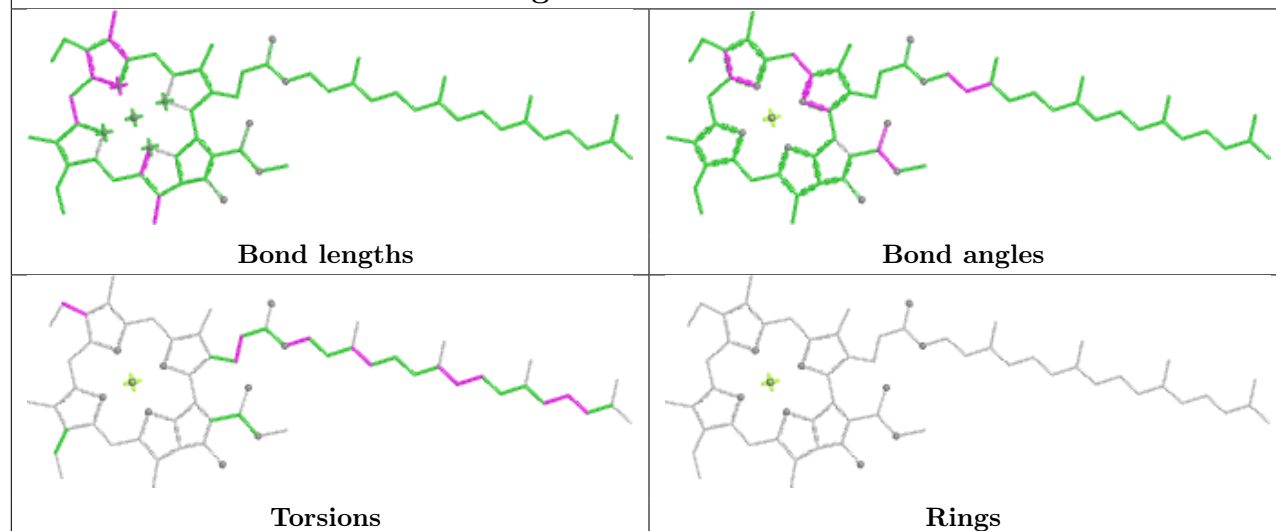


Torsions

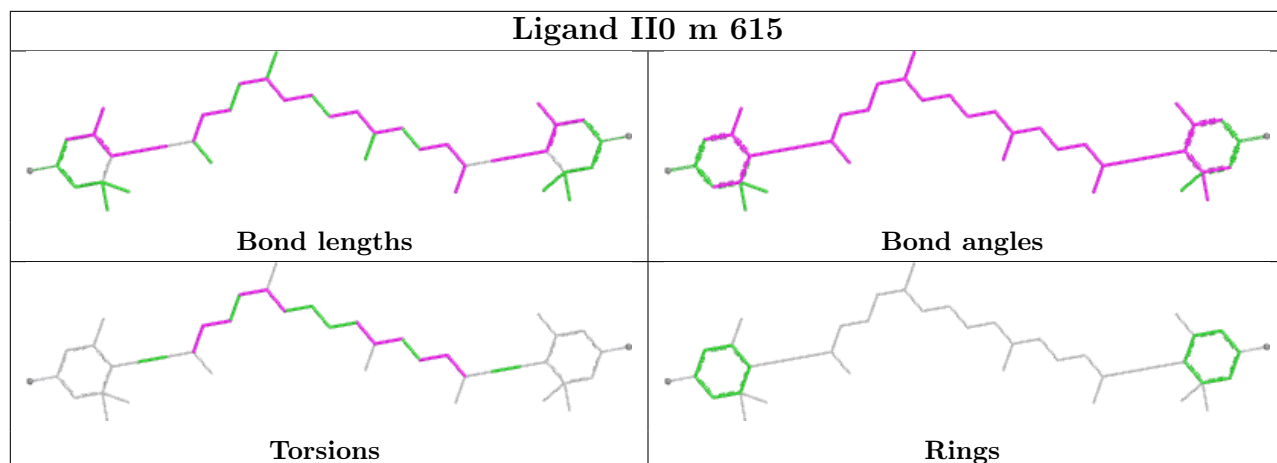


Rings

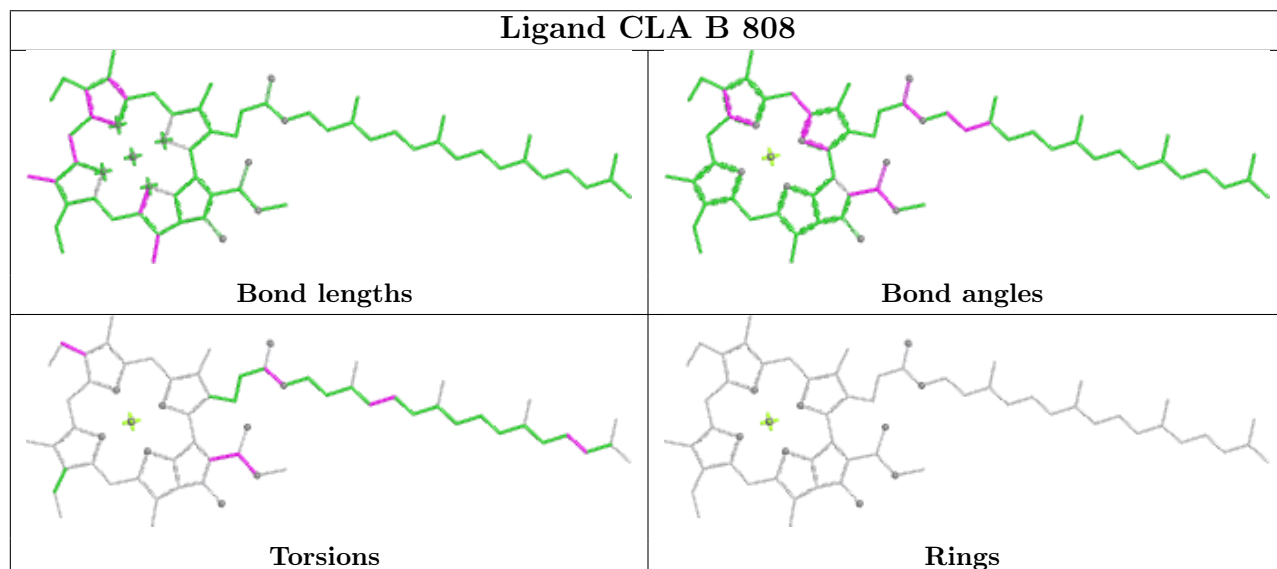
Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN L 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 a 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 802**Ligand CLA A 835****Ligand CLA A 852**

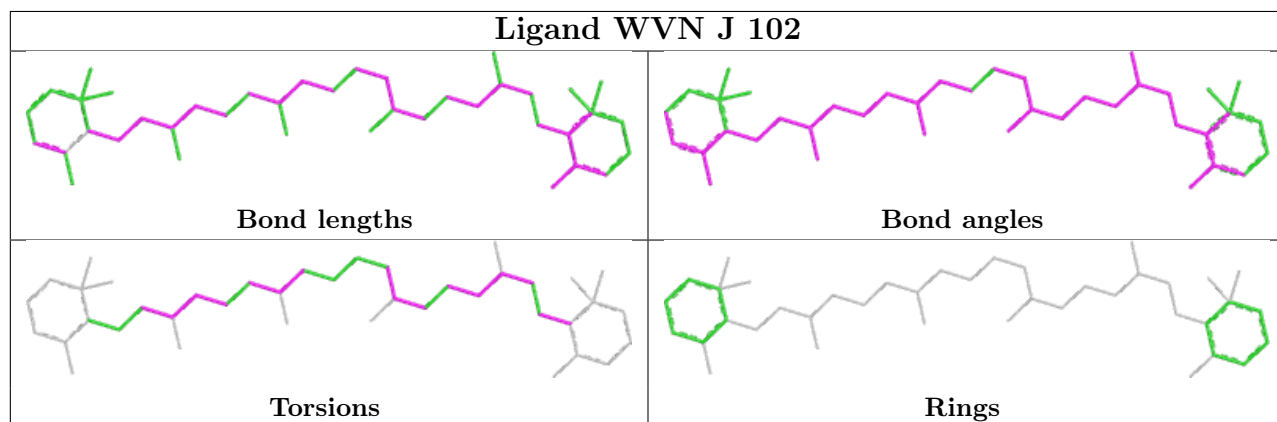
Ligand II0 m 615



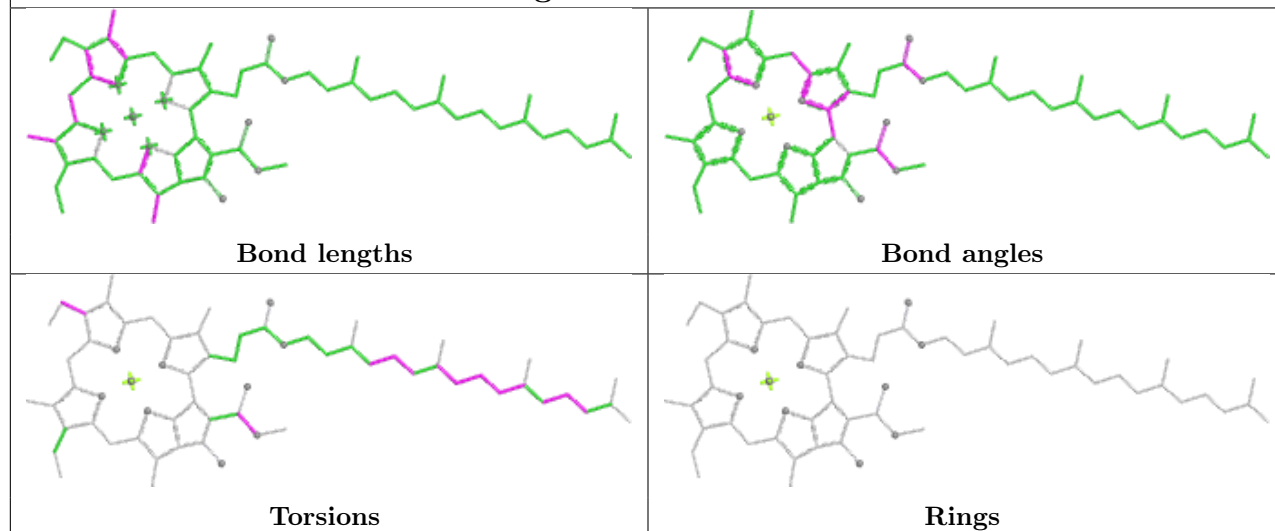
Ligand CLA B 808



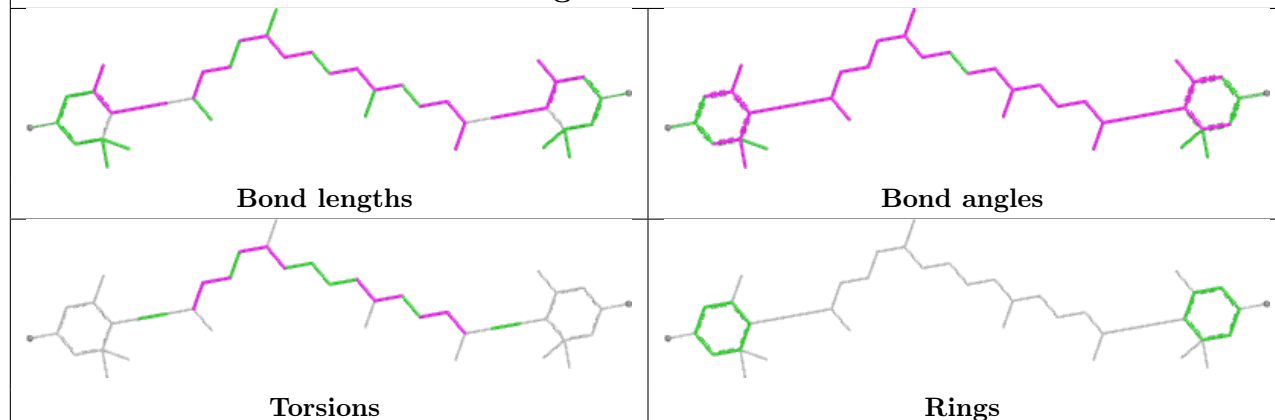
Ligand WVN J 102



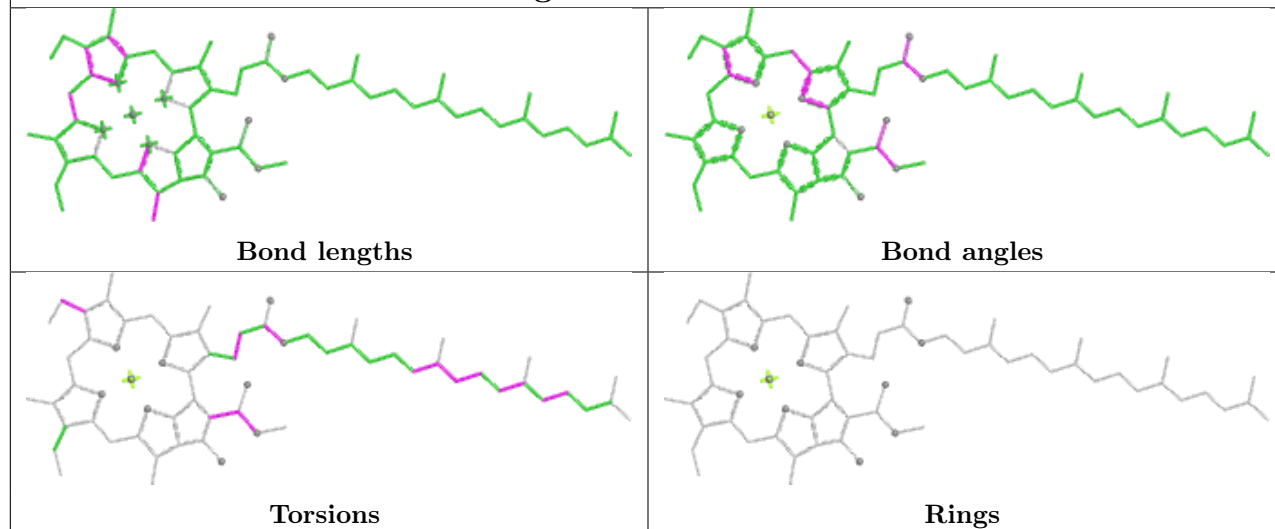
Ligand CLA b 310

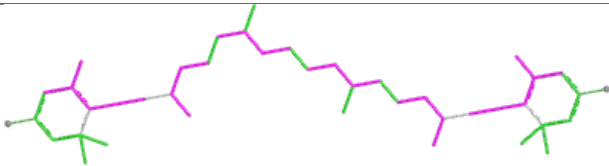
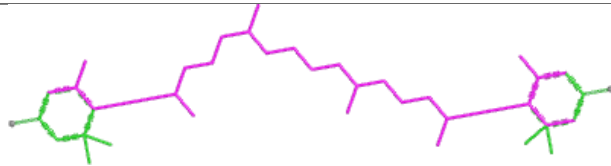
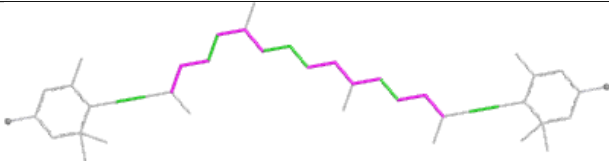
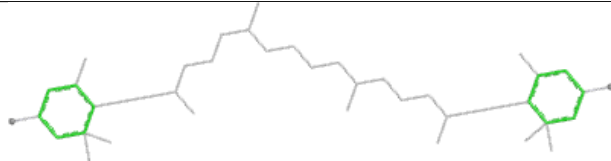


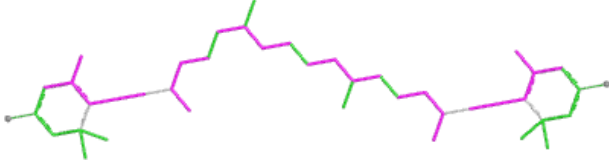
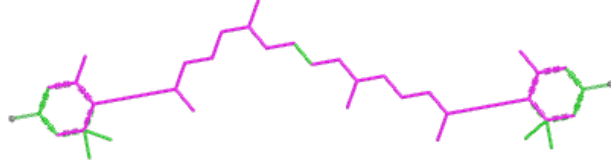
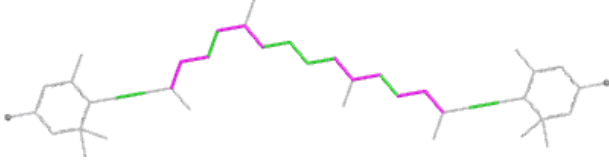
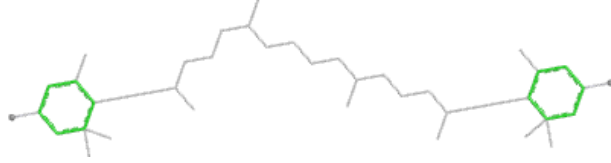
Ligand II0 l 302

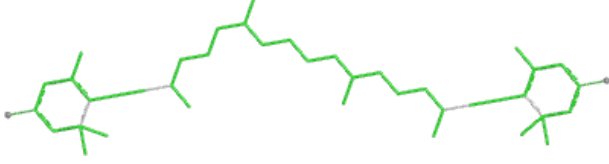
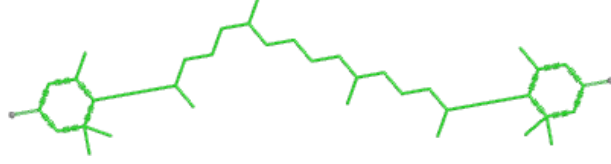
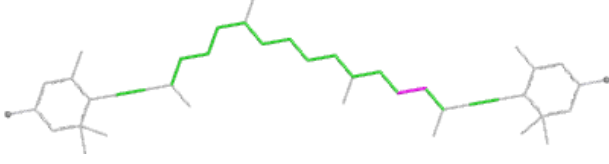
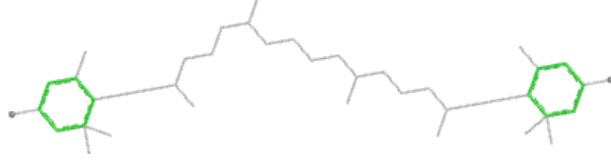


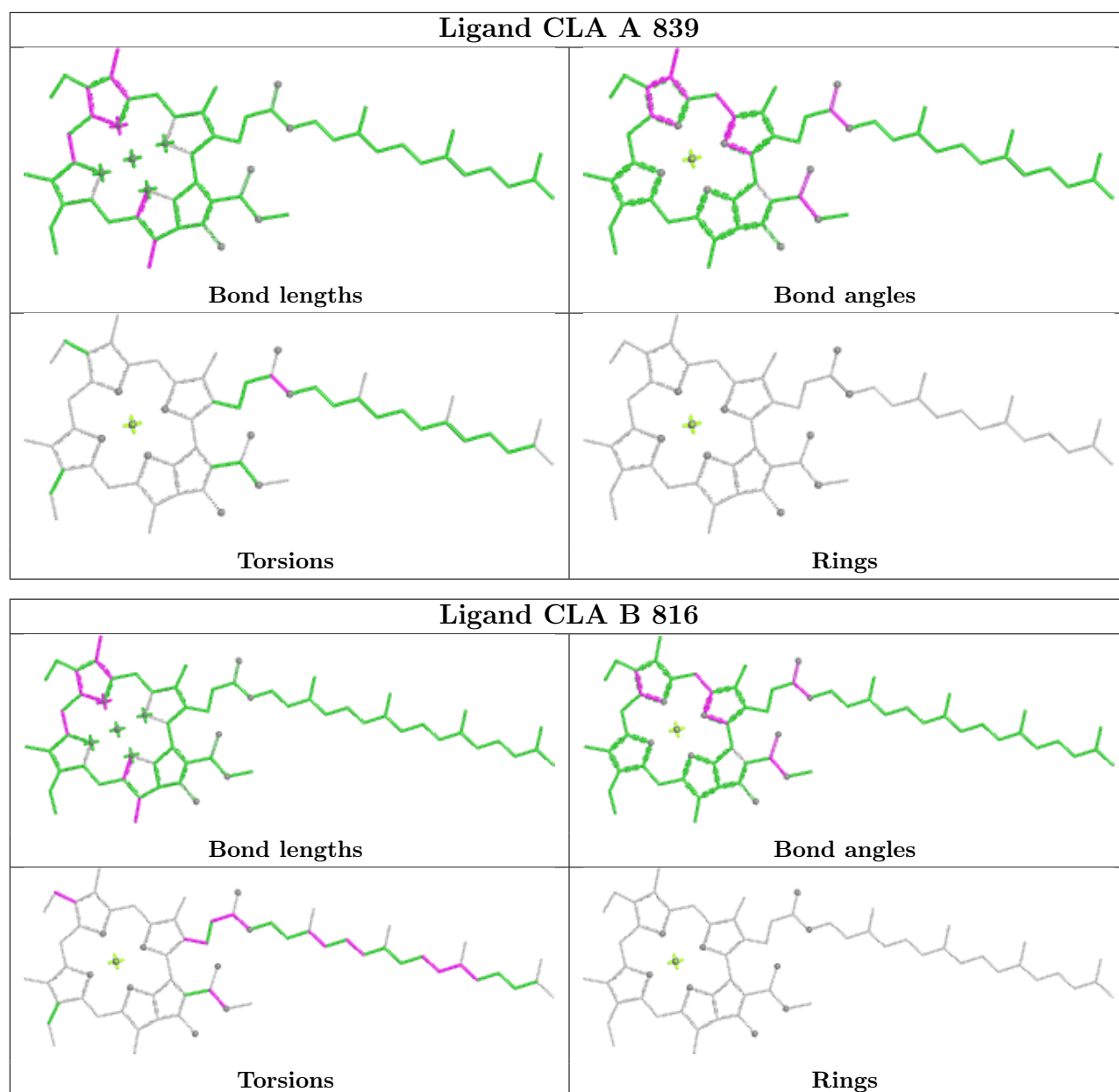
Ligand CLA b 306



Ligand II0 j 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 d 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 k 618	
	
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.

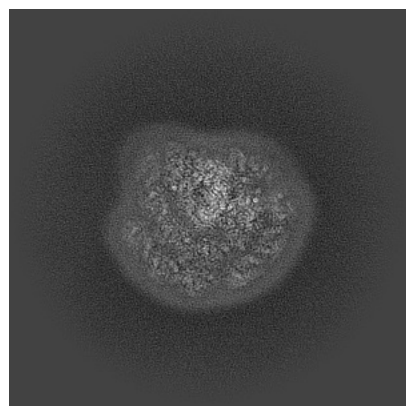
6 Map visualisation [i](#)

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.

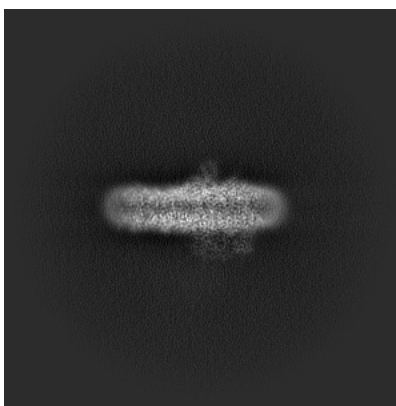
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

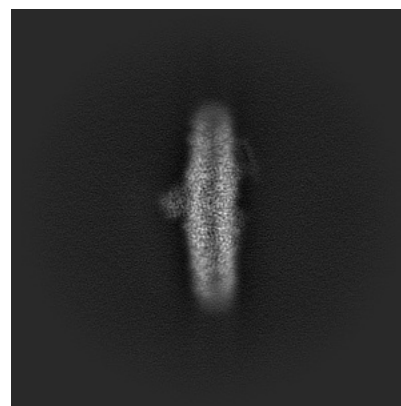
6.1.1 Primary map



X

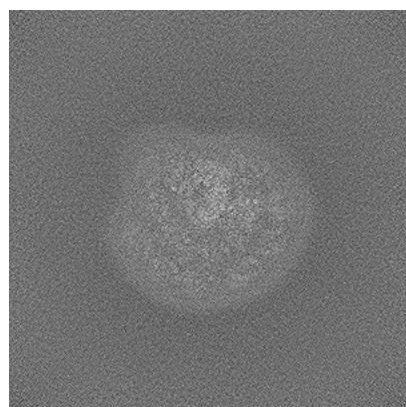


Y

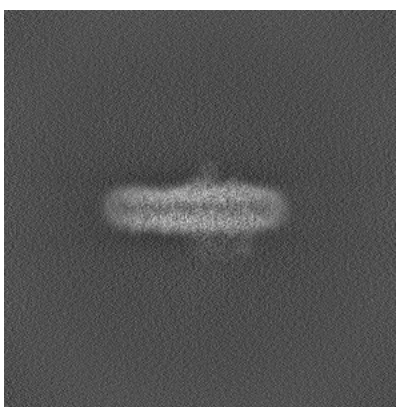


Z

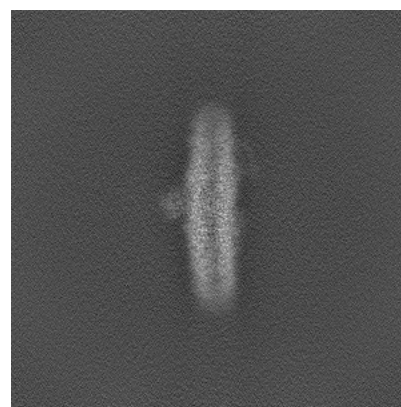
6.1.2 Raw map



X



Y

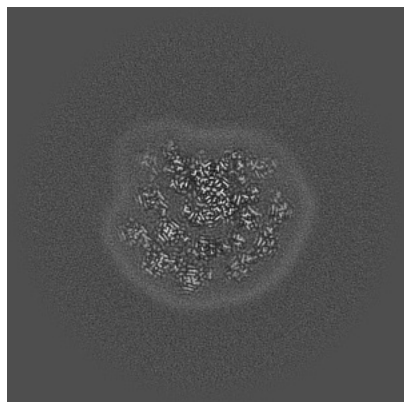


Z

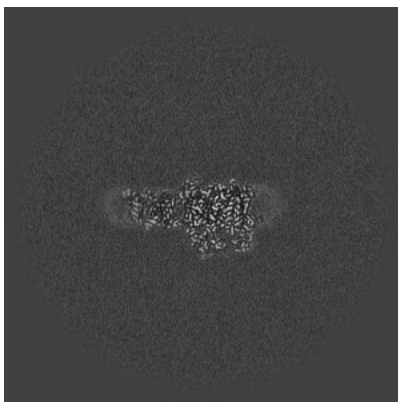
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

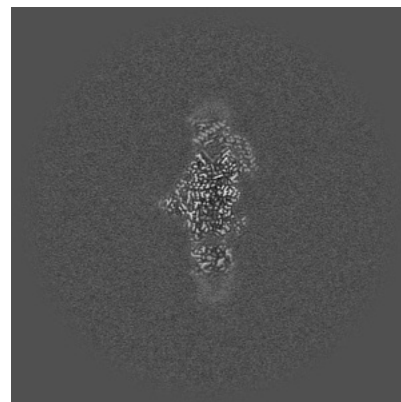
6.2.1 Primary map



X Index: 300

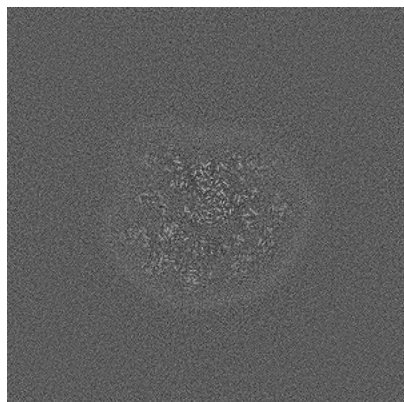


Y Index: 300

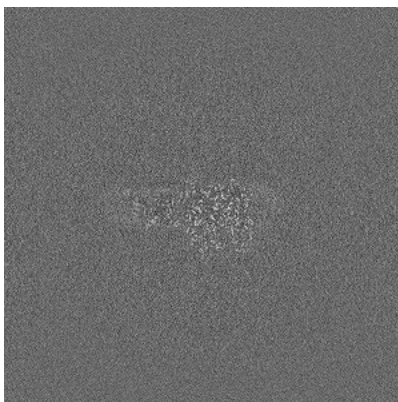


Z Index: 300

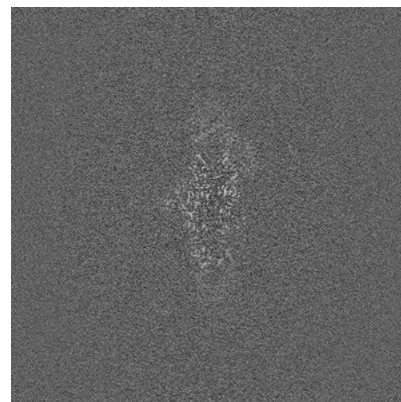
6.2.2 Raw map



X Index: 300



Y Index: 300

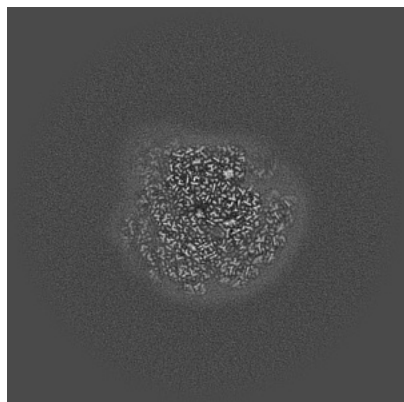


Z Index: 300

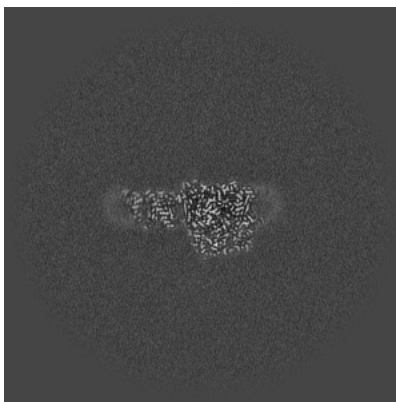
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

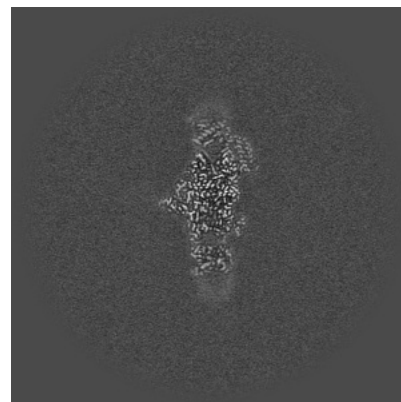
6.3.1 Primary map



X Index: 282

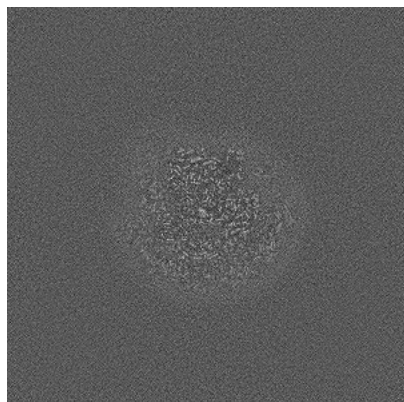


Y Index: 304

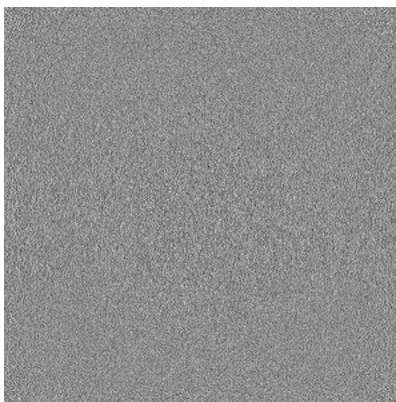


Z Index: 301

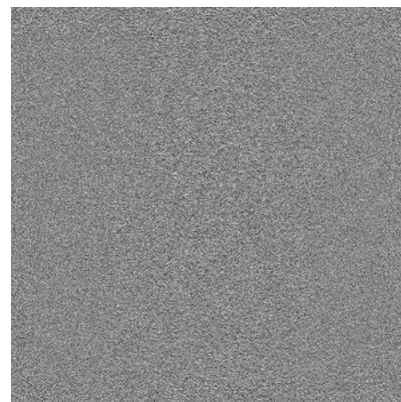
6.3.2 Raw map



X Index: 284



Y Index: 0

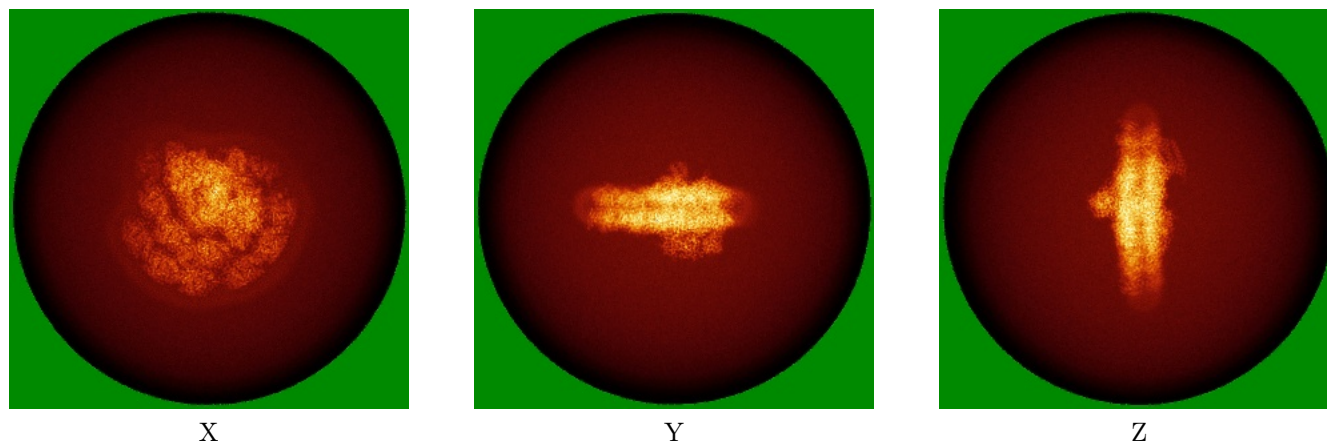


Z Index: 0

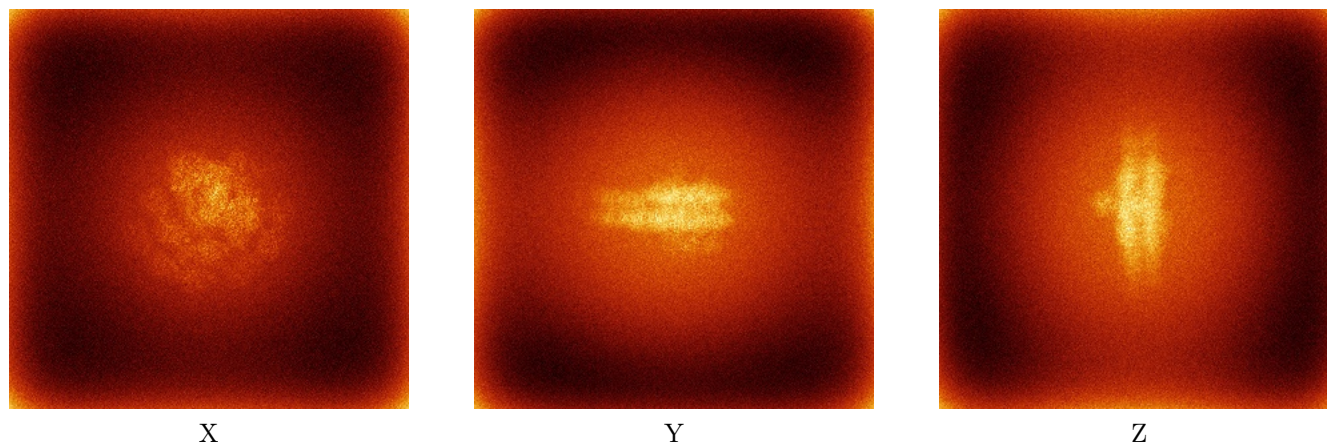
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



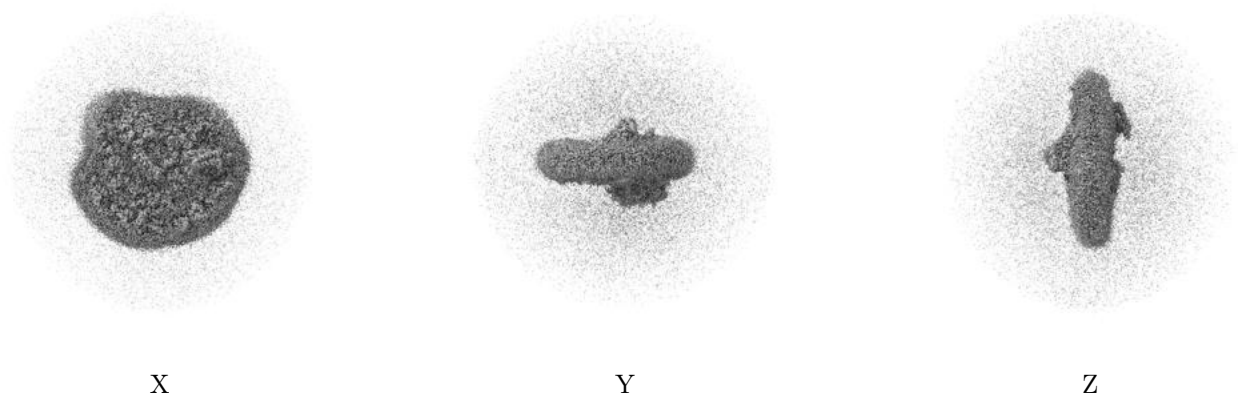
6.4.2 Raw map



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

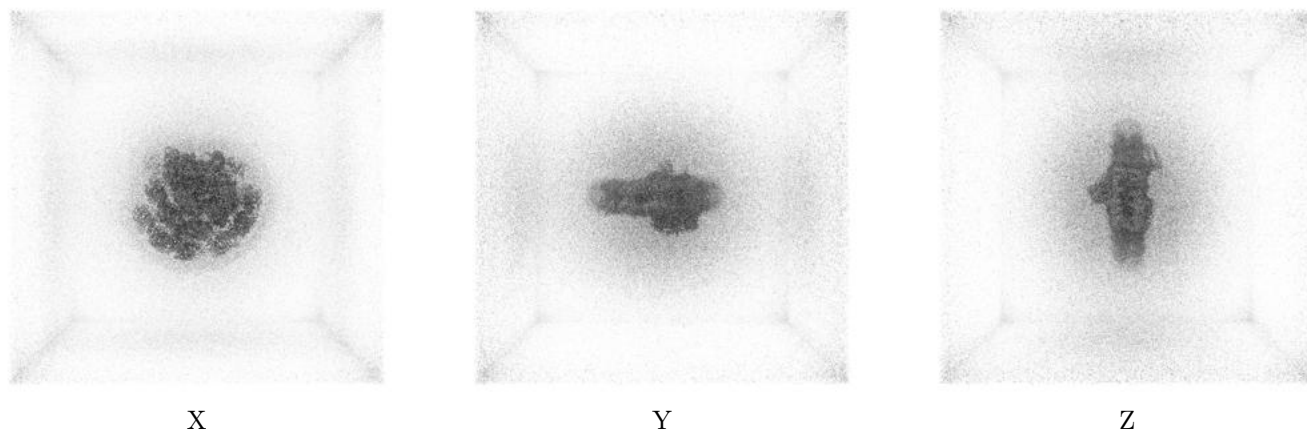
6.5 Orthogonal surface views [i](#)

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.

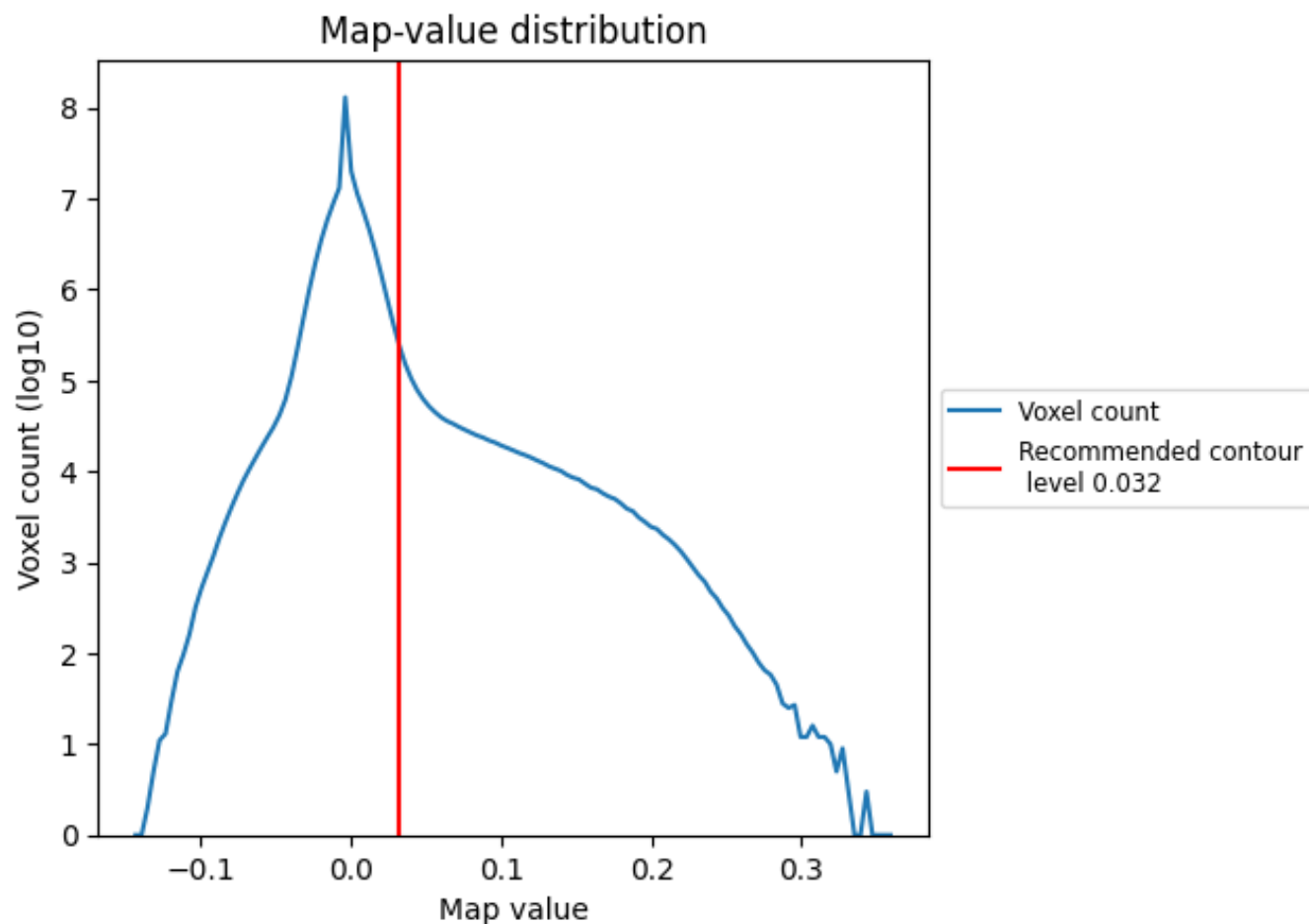
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

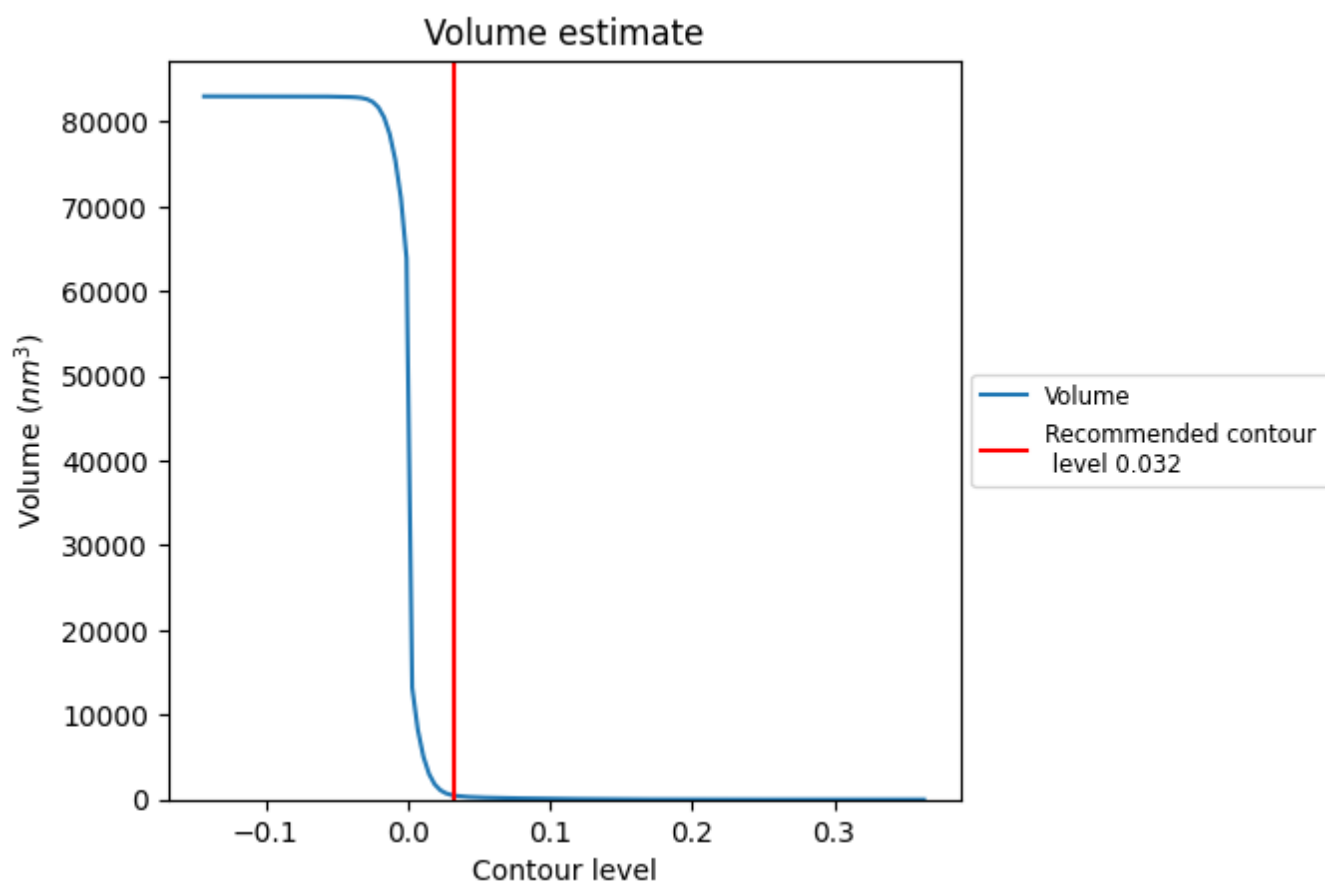
This section contains the results of statistical analysis of the map.

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.

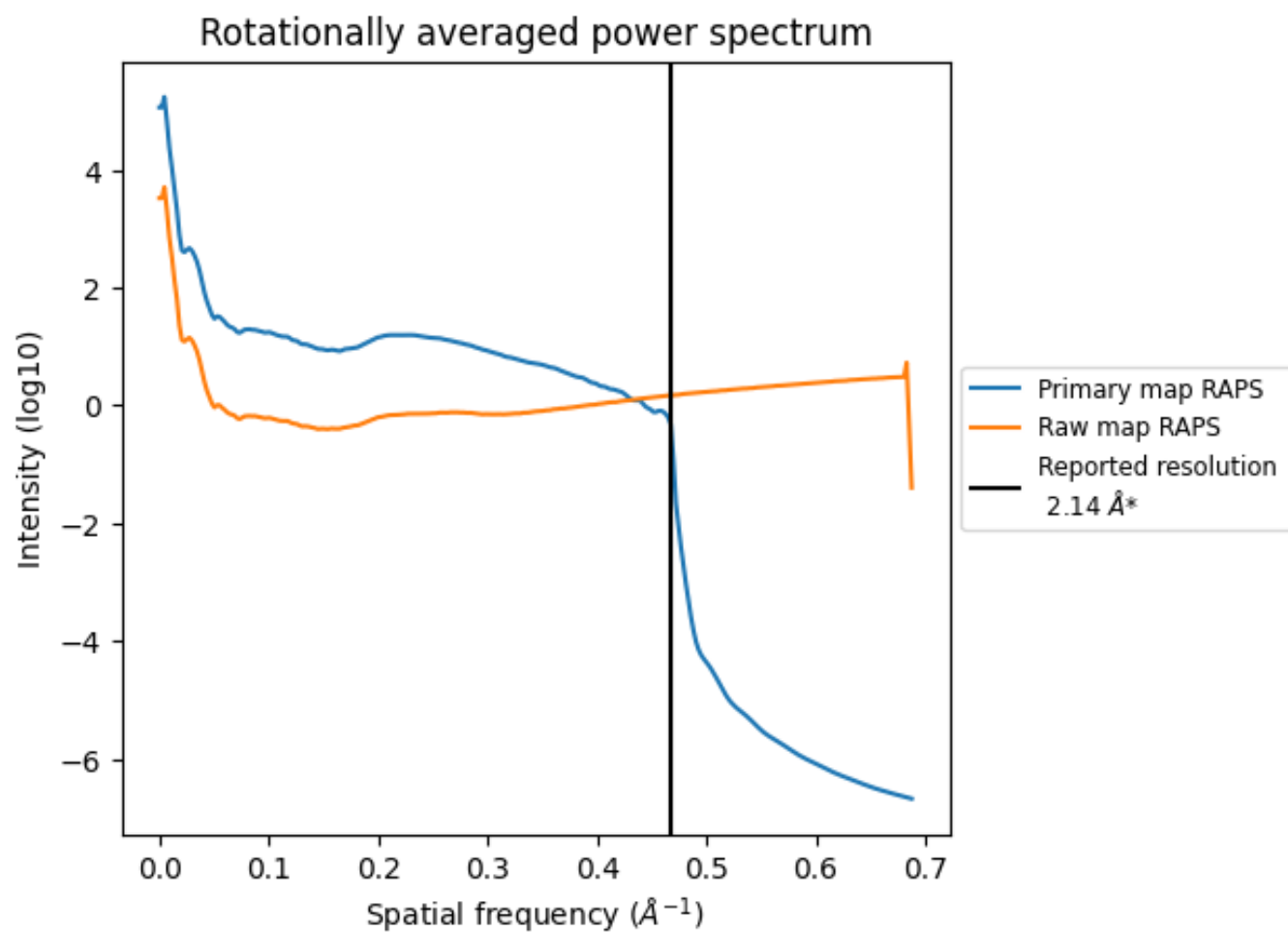
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 505 nm³; 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](#)

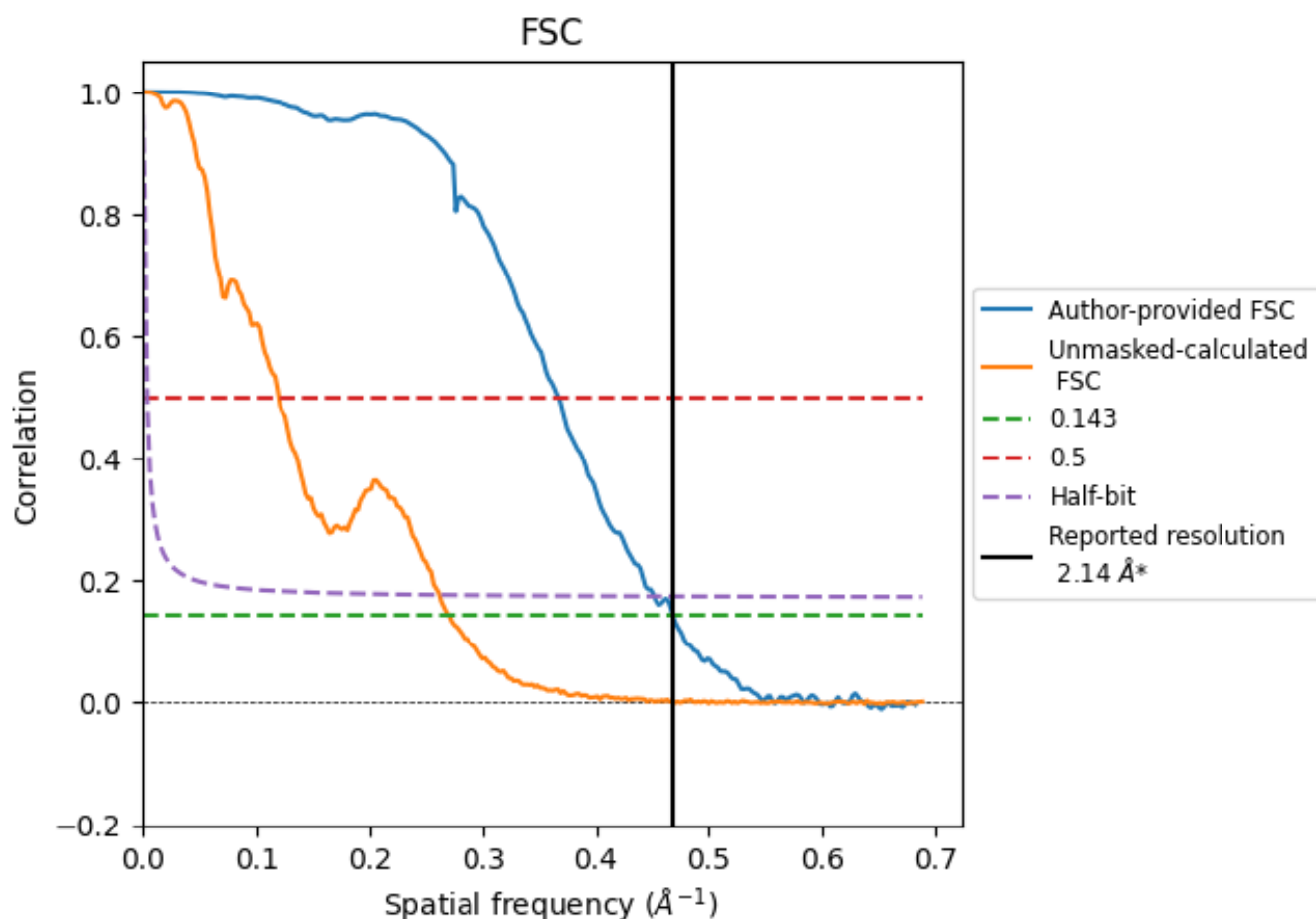


*Reported resolution corresponds to spatial frequency of 0.467 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

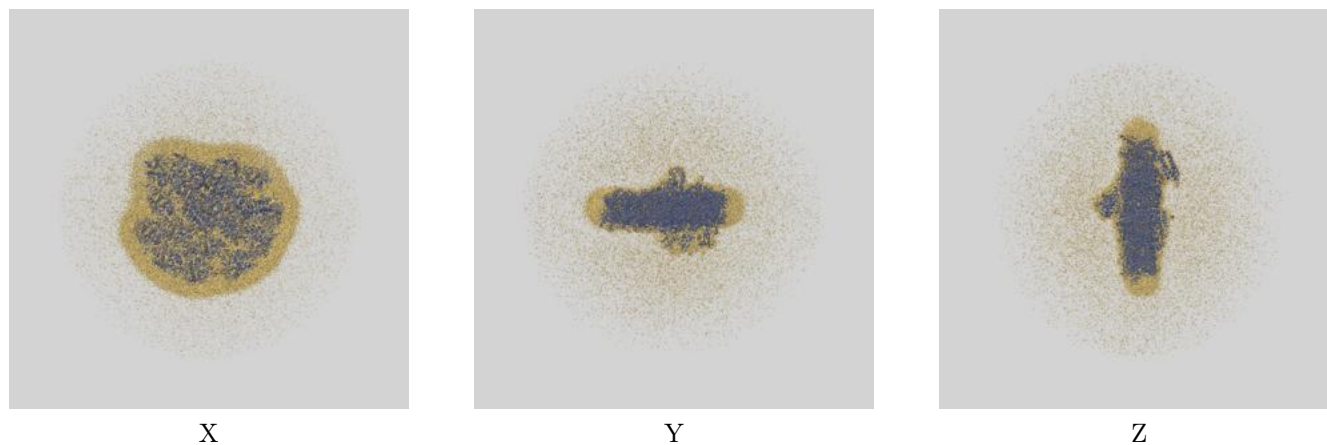
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.72	2.22
Unmasked-calculated*	3.70	8.31	3.82

*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](#)

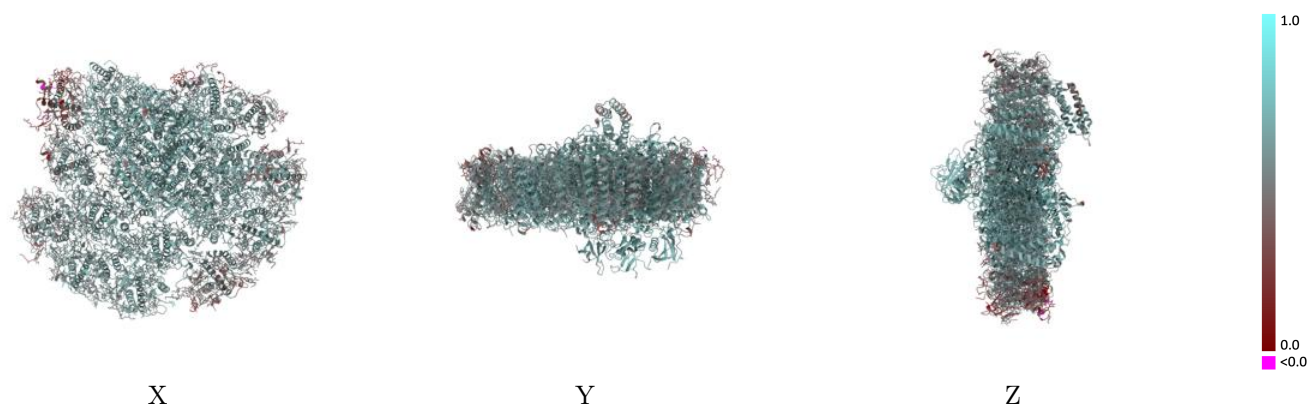
This section contains information regarding the fit between EMDB map EMD-62717 and PDB model 9L0K. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



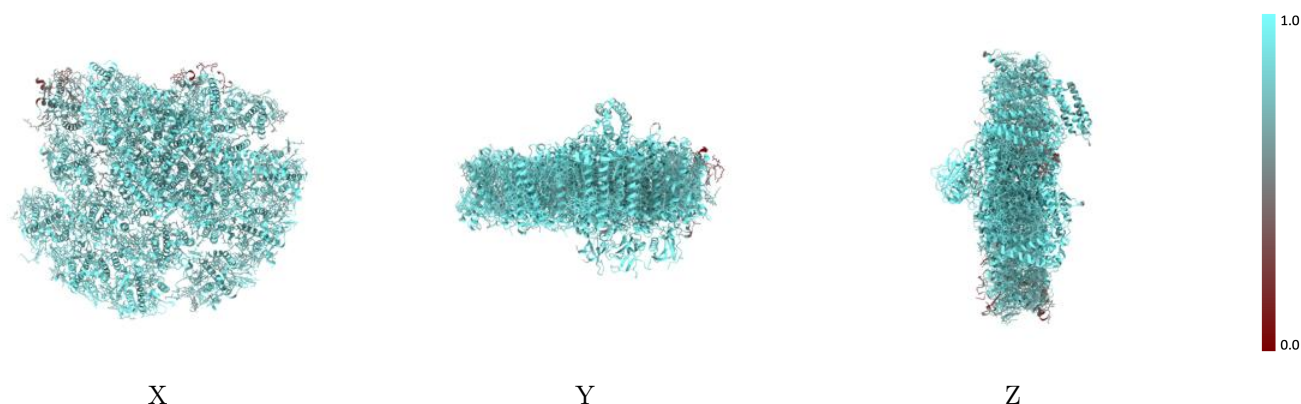
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



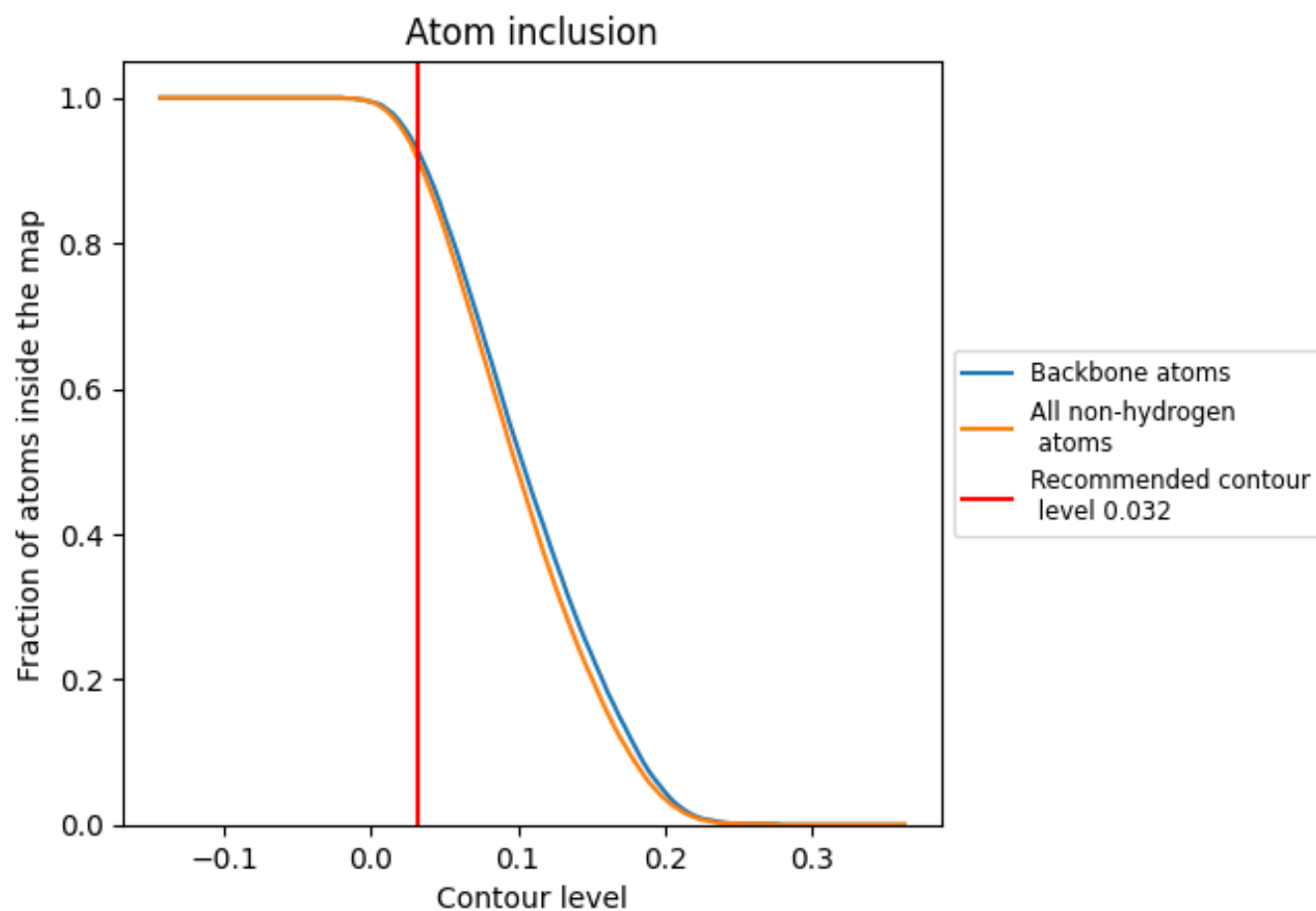
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

