



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 01:59 AM JST

PDB ID : 9KZ9 / pdb_00009kz9
EMDB ID : EMD-62656
Title : Cryo-EM structure of PSI-ACPI from Rhodomonas sp. NIES-2332 at 2.08 angstroms resolution
Authors : Zhang, W.Y.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-10
Resolution : 2.08 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

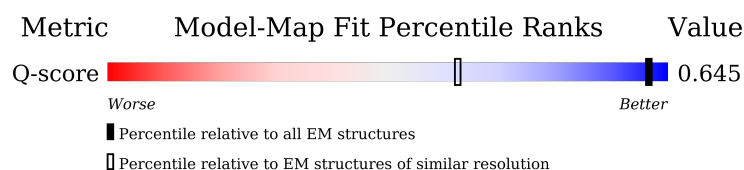
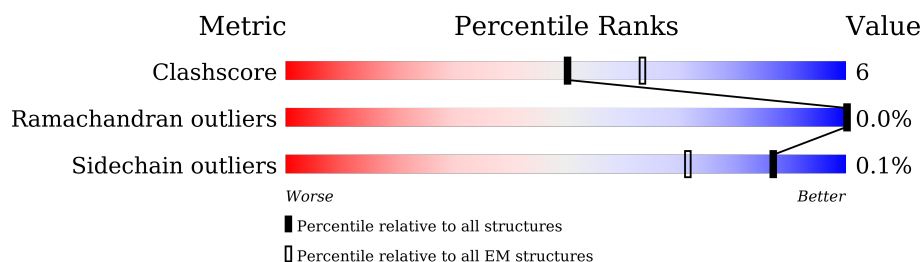
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.08 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.



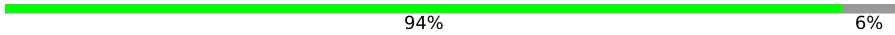
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1976 (1.58 - 2.58)

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	33	
8	J	42	
9	L	153	
10	M	30	
11	O	153	
12	K	86	
13	s	302	
14	c	215	
15	a	217	
16	b	236	
17	h	229	
18	f	212	
18	j	212	
18	m	212	
19	e	210	
20	l	175	
21	k	232	
22	i	200	
23	d	219	
24	g	216	
25	R	135	
26	n	220	
27	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
32	WVN	A	844	-	X	-	-
32	WVN	A	845	-	X	-	-
32	WVN	A	846	-	X	-	-
32	WVN	A	847	-	X	-	-
32	WVN	A	854	-	X	-	-
32	WVN	B	847	-	X	-	-
32	WVN	B	848	-	X	-	-
32	WVN	B	849	-	X	-	-
32	WVN	F	204	-	X	-	-
32	WVN	F	205	-	X	-	-
32	WVN	F	207	-	X	-	-
32	WVN	I	101	-	X	-	-
32	WVN	J	101	-	X	-	-
32	WVN	K	103	-	X	-	-
32	WVN	L	201	-	X	-	-
32	WVN	L	205	-	X	-	-
32	WVN	L	206	-	X	-	-
32	WVN	M	101	-	X	-	-
32	WVN	R	201	-	X	-	-
32	WVN	R	202	-	X	-	-
32	WVN	e	315	-	X	-	-
32	WVN	h	308	-	X	-	-
32	WVN	i	315	-	X	-	-
32	WVN	l	302	-	X	-	-
32	WVN	l	316	-	X	-	-
32	WVN	s	407	-	X	-	-
38	II0	h	309	-	X	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 61938 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 PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	95	Total	C	N	O	S	0	0
			714	480	107	124	3		

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

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

- Molecule 13 is a protein called ACPI-s.

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

- Molecule 14 is a protein called ACPI-c.

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

- Molecule 15 is a protein called ACPI-a.

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

- Molecule 16 is a protein called ACPI-b.

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

- Molecule 17 is a protein called ACPI-h.

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

- Molecule 18 is a protein called ACPI-m,f,j.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	174	Total	C	N	O	S	0	0
			1313	850	217	238	8		
18	f	174	Total	C	N	O	S	0	0
			1306	846	215	237	8		
18	j	173	Total	C	N	O	S	0	0
			1302	841	216	237	8		

- Molecule 19 is a protein called ACPI-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	166	Total	C	N	O	S	0	0
			1268	822	209	228	9		

- Molecule 20 is a protein called ACPI-l.

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

- Molecule 21 is a protein called ACPI-k.

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

- Molecule 22 is a protein called ACPI-i.

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

- Molecule 23 is a protein called ACPI-d.

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

- Molecule 24 is a protein called ACPI-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	216	Total	C	N	O	S	0	0
			1608	1047	265	285	11		

- Molecule 25 is a protein called PsaR.

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

- Molecule 26 is a protein called ACPI-n.

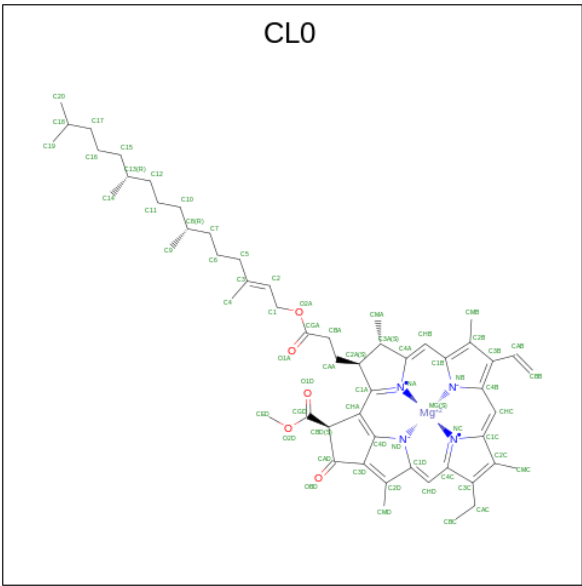
Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	181	Total	C	N	O	S	0	0
			1343	862	226	245	10		

- Molecule 27 is a protein called PsaQ.

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

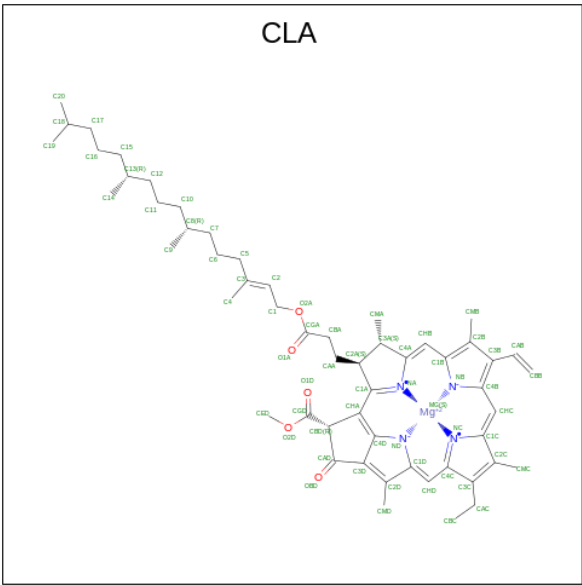
- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅)

(labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	m	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
29	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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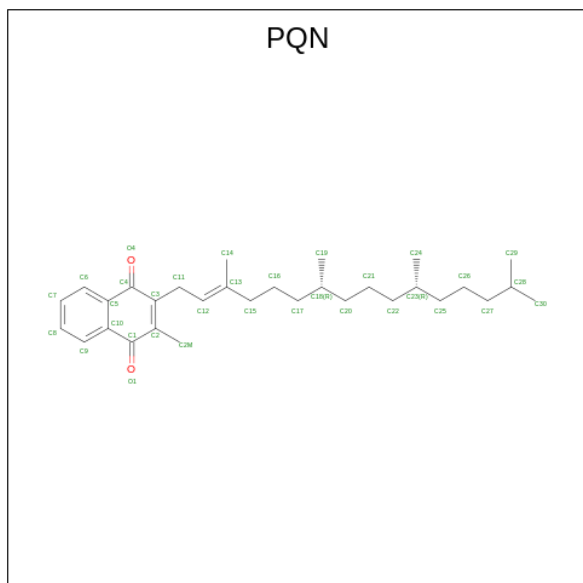
Mol	Chain	Residues	Atoms					AltConf
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	g	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 60	C 50	Mg 1	N 4	O 5	0

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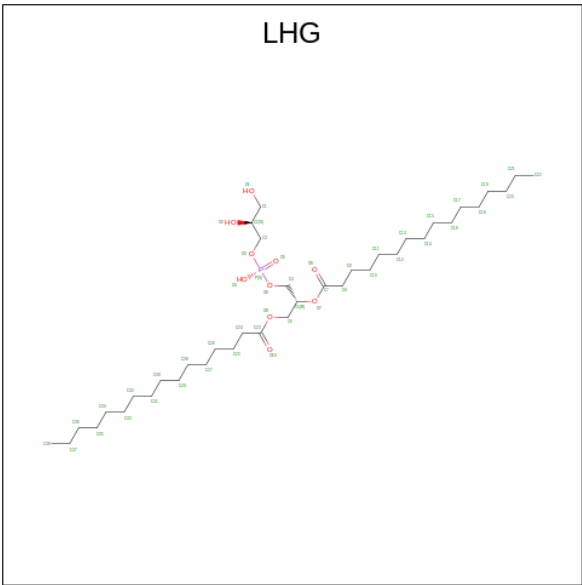
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



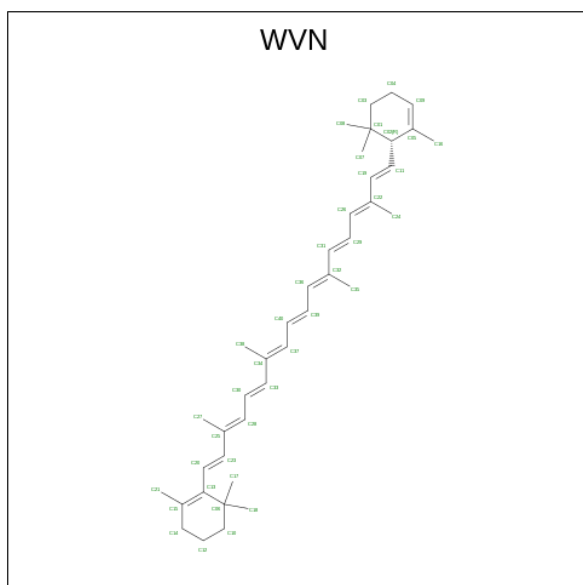
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			48	37	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			27	20	6	1	
31	J	1	Total	C	O	P	0
			33	22	10	1	
31	L	1	Total	C	O	P	0
			47	36	10	1	
31	L	1	Total	C	O	P	0
			36	25	10	1	
31	s	1	Total	C	O	P	0
			33	24	8	1	
31	c	1	Total	C	O	P	0
			37	26	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	b	1	Total	C	O	P	0
			49	38	10	1	
31	m	1	Total	C	O	P	0
			37	26	10	1	
31	e	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	l	1	Total	C	O	P	0
			32	21	10	1	
31	f	1	Total	C	O	P	0
			49	38	10	1	
31	f	1	Total	C	O	P	0
			37	26	10	1	
31	i	1	Total	C	O	P	0
			37	26	10	1	
31	j	1	Total	C	O	P	0
			30	19	10	1	
31	g	1	Total	C	O	P	0
			45	34	10	1	
31	g	1	Total	C	O	P	0
			37	26	10	1	
31	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 32 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
32	A	1	Total	C	0
			40	40	
32	A	1	Total	C	0
			40	40	

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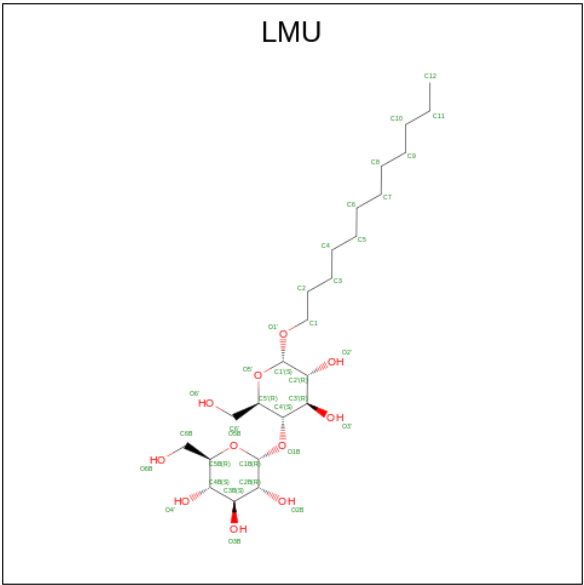
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	I	1	Total C 40 40	0
32	J	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	M	1	Total C 40 40	0
32	K	1	Total C 40 40	0
32	s	1	Total C 40 40	0
32	s	1	Total C 40 40	0
32	h	1	Total C 40 40	0

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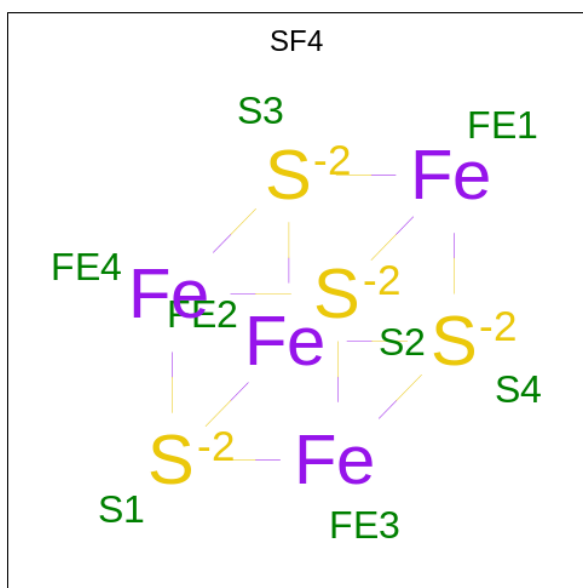
Mol	Chain	Residues	Atoms	AltConf
32	e	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	R	1	Total C 40 40	0
32	R	1	Total C 40 40	0

- Molecule 33 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



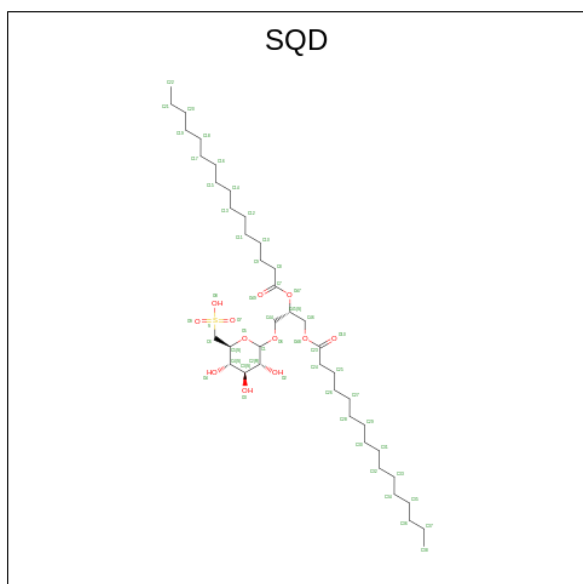
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 35 24 11	0
33	A	1	Total C O 34 23 11	0
33	B	1	Total C O 35 24 11	0
33	a	1	Total C O 35 24 11	0
33	i	1	Total C O 35 24 11	0

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



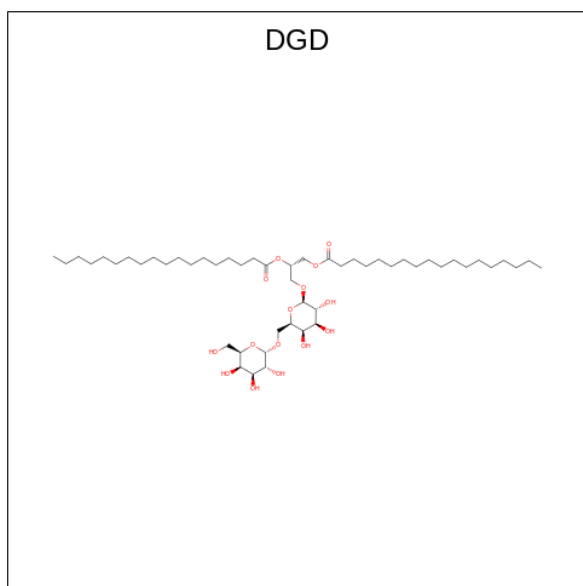
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$) (labeled as "Ligand of Interest" by depositor).



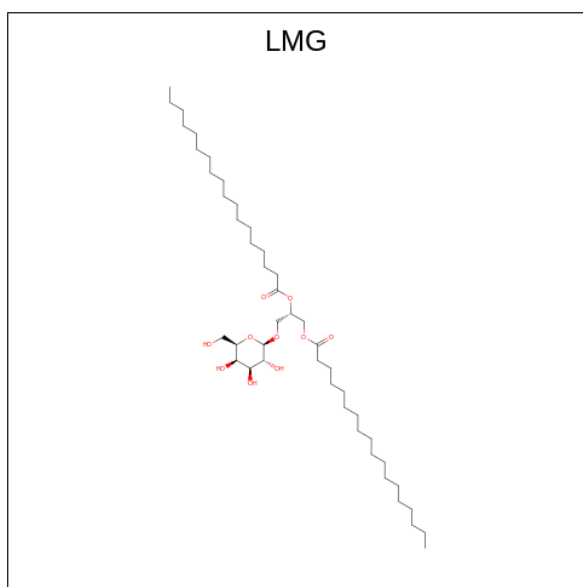
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



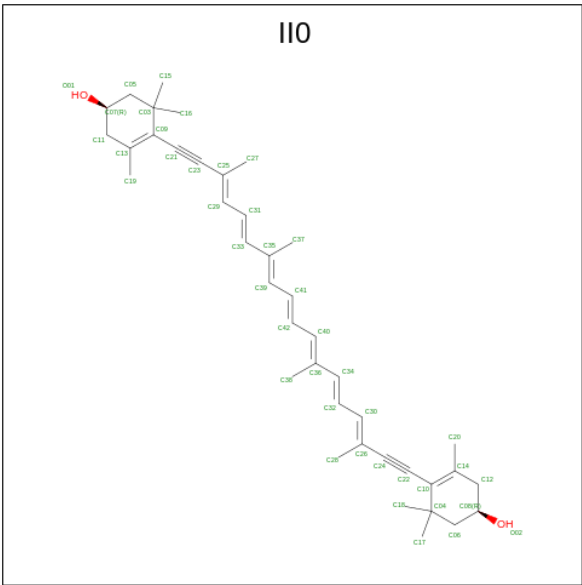
Mol	Chain	Residues	Atoms				AltConf
36	B	1	Total	C	O		0
			66	51	15		
36	j	1	Total	C	O		0
			62	47	15		

- Molecule 37 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
37	F	1	Total	C	O	0
			53	43	10	
37	F	1	Total	C	O	0
			41	31	10	
37	L	1	Total	C	O	0
			45	35	10	
37	O	1	Total	C	O	0
			26	16	10	
37	c	1	Total	C	O	0
			55	45	10	
37	c	1	Total	C	O	0
			43	33	10	
37	b	1	Total	C	O	0
			42	32	10	
37	n	1	Total	C	O	0
			51	41	10	
37	Q	1	Total	C	O	0
			38	28	10	

- Molecule 38 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	J	1	Total	C	O	0
			42	40	2	
38	O	1	Total	C	O	0
			42	40	2	
38	c	1	Total	C	O	0
			42	40	2	
38	c	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	h	1	Total	C	O	0
			28	27	1	
38	h	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
38	h	1	Total	C	O	0
			42	40	2	
38	m	1	Total	C	O	0
			42	40	2	
38	m	1	Total	C	O	0
			42	40	2	
38	m	1	Total	C	O	0
			42	40	2	
38	m	1	Total	C	O	0
			42	40	2	
38	e	1	Total	C	O	0
			42	40	2	
38	e	1	Total	C	O	0
			42	40	2	
38	e	1	Total	C	O	0
			42	40	2	
38	e	1	Total	C	O	0
			42	40	2	
38	l	1	Total	C	O	0
			42	40	2	
38	l	1	Total	C	O	0
			42	40	2	
38	l	1	Total	C	O	0
			42	40	2	
38	l	1	Total	C	O	0
			42	40	2	
38	k	1	Total	C	O	0
			42	40	2	
38	k	1	Total	C	O	0
			42	40	2	
38	k	1	Total	C	O	0
			42	40	2	
38	k	1	Total	C	O	0
			42	40	2	
38	k	1	Total	C	O	0
			42	40	2	
38	k	1	Total	C	O	0
			42	40	2	
38	f	1	Total	C	O	0
			42	40	2	
38	f	1	Total	C	O	0
			42	40	2	

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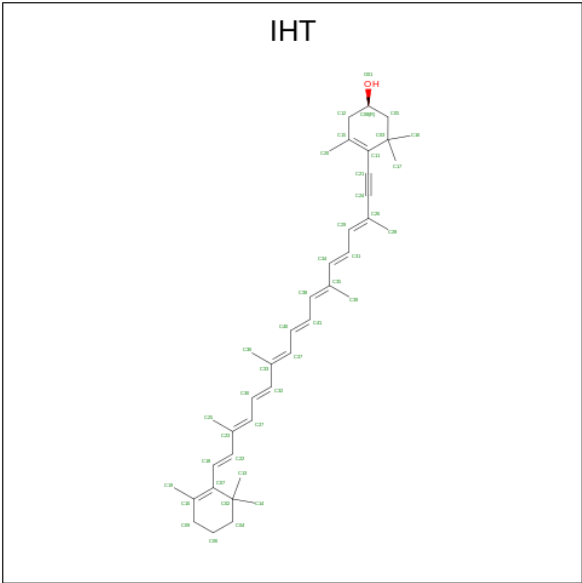
Mol	Chain	Residues	Atoms			AltConf
38	f	1	Total 42	C 40	O 2	0
38	f	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	d	1	Total 42	C 40	O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

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

- Molecule 39 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
39	O	1	Total	C	O	0
			41	40	1	
39	c	1	Total	C	O	0
			41	40	1	
39	c	1	Total	C	O	0
			41	40	1	
39	a	1	Total	C	O	0
			41	40	1	
39	b	1	Total	C	O	0
			41	40	1	
39	m	1	Total	C	O	0
			41	40	1	
39	f	1	Total	C	O	0
			41	40	1	
39	j	1	Total	C	O	0
			41	40	1	

Continued on next page...

Mol	Chain	Residues	Atoms			AltConf
39	g	1	Total 41	C 40	O 1	0
39	g	1	Total 41	C 40	O 1	0
39	R	1	Total 41	C 40	O 1	0
39	n	1	Total 41	C 40	O 1	0

- ## KC2

Mol	Chain	Residues	Atoms					AltConf
40	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	k	1	Total 45	C 35	Mg 1	N 4	O 5	0



WORLD WIDE
PDB
PROTEIN DATA BANK

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	126	Total 126	O 126	0
41	B	150	Total 150	O 150	0
41	C	22	Total 22	O 22	0
41	D	15	Total 15	O 15	0
41	E	6	Total 6	O 6	0
41	F	14	Total 14	O 14	0

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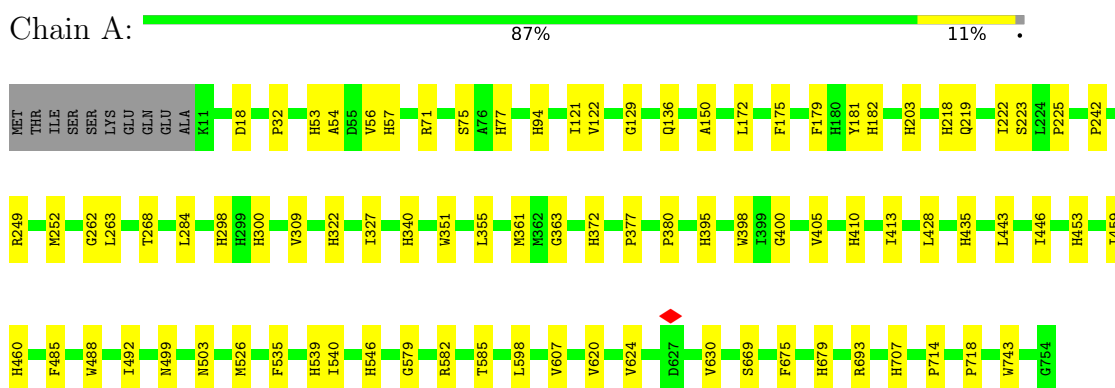
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Mol	Chain	Residues	Atoms		AltConf
41	J	2	Total 2	O 2	0
41	L	15	Total 15	O 15	0
41	M	2	Total 2	O 2	0
41	O	5	Total 5	O 5	0
41	K	2	Total 2	O 2	0
41	s	7	Total 7	O 7	0
41	c	2	Total 2	O 2	0
41	a	16	Total 16	O 16	0
41	b	21	Total 21	O 21	0
41	h	9	Total 9	O 9	0
41	m	1	Total 1	O 1	0
41	e	3	Total 3	O 3	0
41	f	1	Total 1	O 1	0
41	g	1	Total 1	O 1	0
41	R	1	Total 1	O 1	0
41	n	1	Total 1	O 1	0

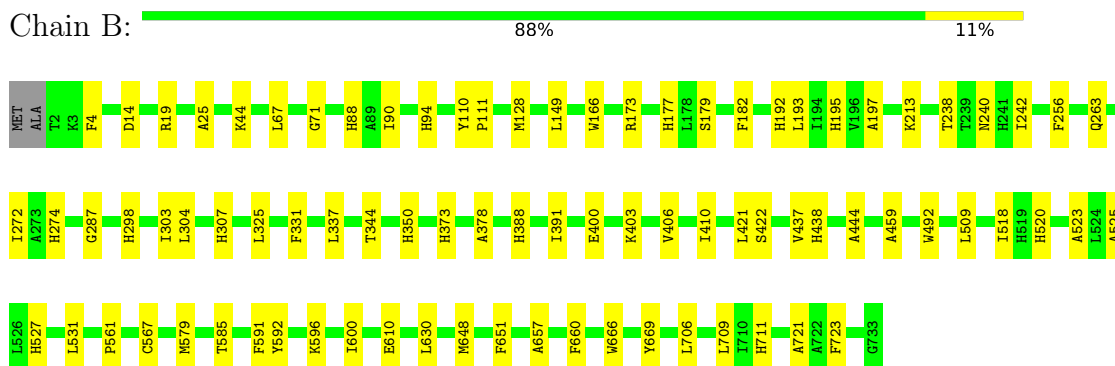
3 Residue-property plots

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.

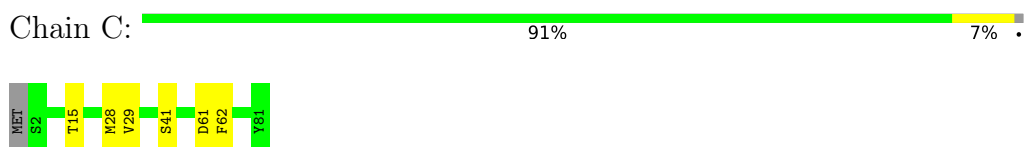
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

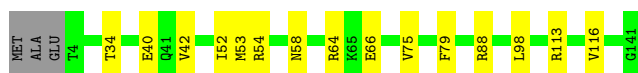


- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II





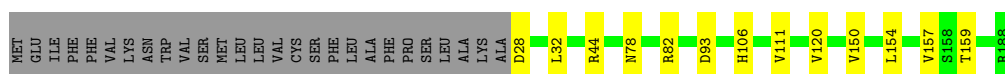
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 94% 6%



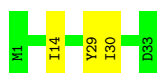
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 79% 7% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 91% 9%



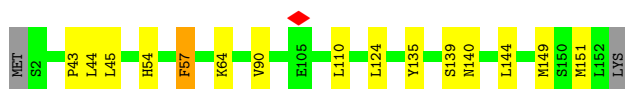
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 79% 21%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 89% 9% ..



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 90% 10%

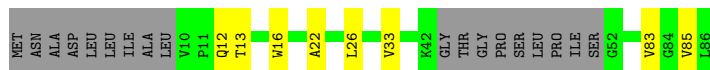


- Molecule 11: PsaO

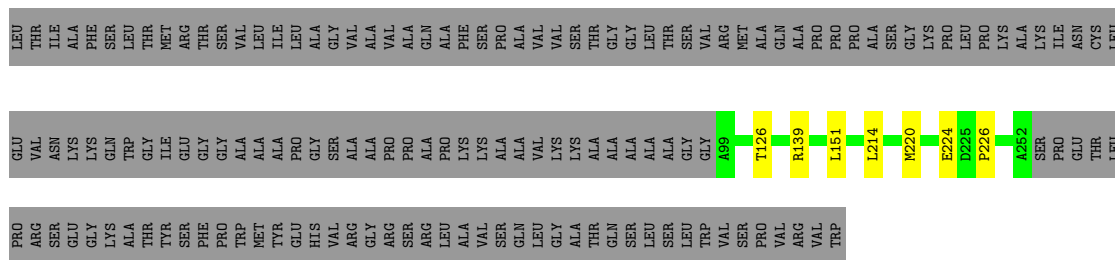
Chain O: 56% 5% 38%



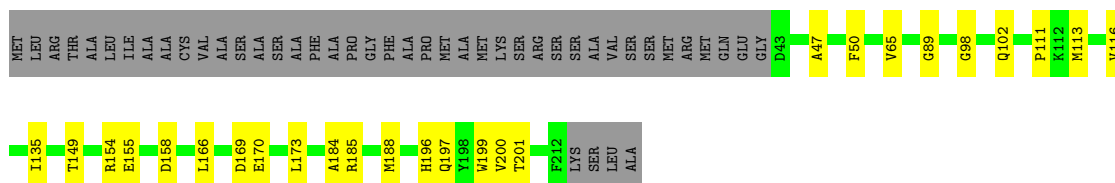
- Molecule 12: Photosystem I reaction center subunit PsaK



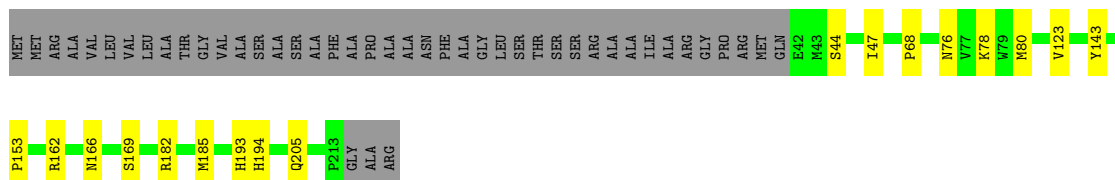
- Molecule 13: ACPI-s



- Molecule 14: ACPI-c

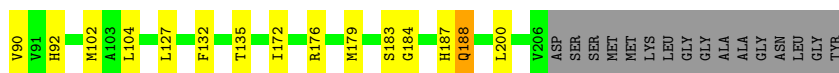
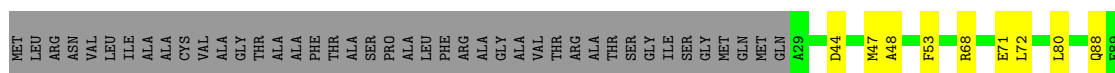


- Molecule 15: ACPI-a



- Molecule 16: ACPI-b





• Molecule 17: ACPI-h

Chain h: 66% 29%



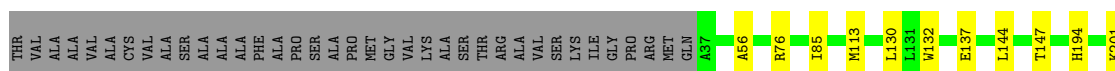
• Molecule 18: ACPI-m,f,j

Chain m: 79% 18%



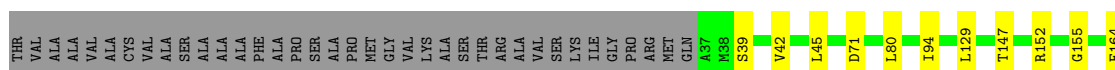
• Molecule 18: ACPI-m,f,j

Chain f: 76% 6% 18%



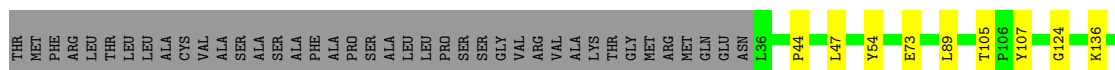
• Molecule 18: ACPI-m,f,j

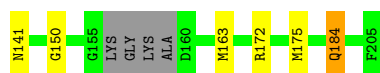
Chain j: 70% 11% 18%



• Molecule 19: ACPI-e

Chain e: 72% 7% 21%





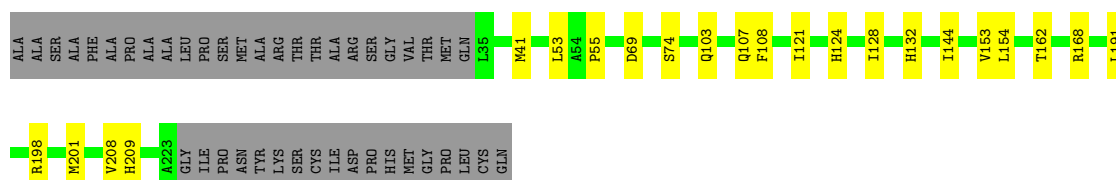
- Molecule 20: ACPI-I

Chain l: 87% 13%



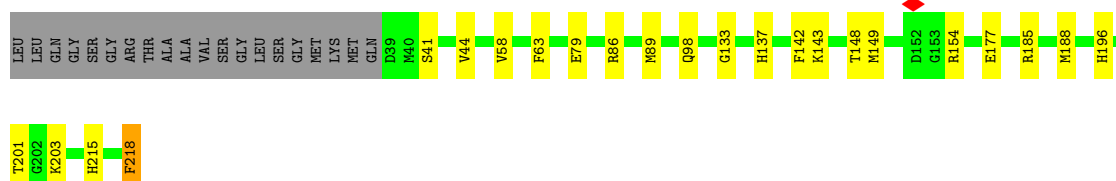
- Molecule 21: ACPI-k

Chain k: 72% 9% 19%



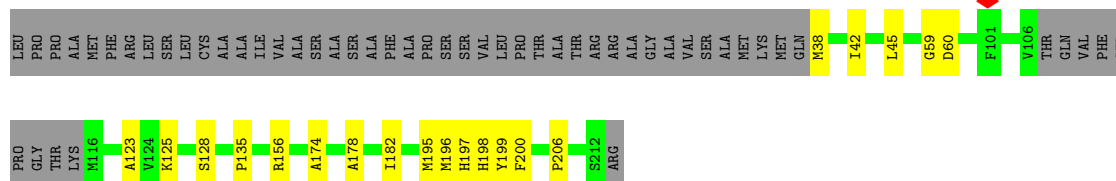
- Molecule 22: ACPI-i

Chain i: 78% 11% 10%



- Molecule 23: ACPI-d

Chain d: 67% 9% 24%



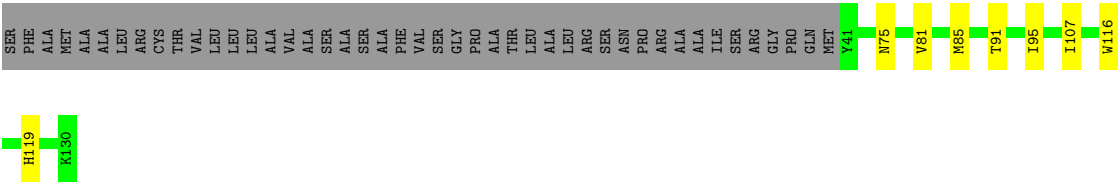
- Molecule 24: ACPI-g

Chain g: 86% 14%



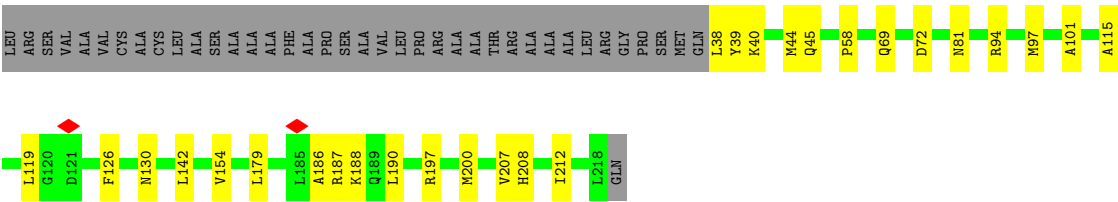
- Molecule 25: Psar

Chain R: 61% 6% 33%



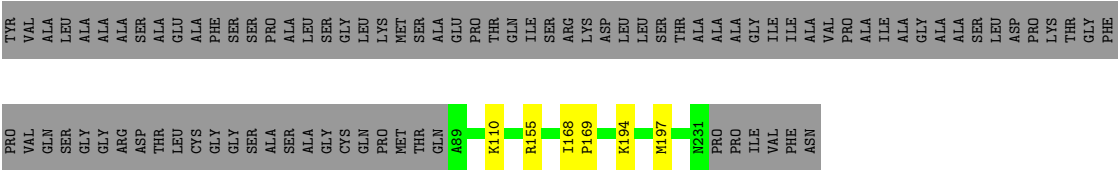
• Molecule 26: ACPI-n

Chain n: 70% 13% 18%



• Molecule 27: PsaQ

Chain Q: 59% 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38563	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	0.439	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.24	0/6020	0.46	0/8205
2	B	0.25	0/6055	0.50	0/8266
3	C	0.17	0/601	0.48	0/813
4	D	0.16	0/1100	0.43	0/1488
5	E	0.16	0/492	0.34	0/666
6	F	0.22	0/1291	0.43	0/1750
7	I	0.25	0/262	0.55	0/358
8	J	0.21	0/364	0.48	0/495
9	L	0.22	0/1188	0.46	0/1616
10	M	0.17	0/233	0.37	0/315
11	O	0.23	0/741	0.49	0/1016
12	K	0.22	0/489	0.48	0/664
13	s	0.17	0/1177	0.42	0/1591
14	c	0.23	0/1401	0.48	0/1896
15	a	0.22	0/1372	0.42	0/1858
16	b	0.27	0/1360	0.49	0/1834
17	h	0.20	0/1228	0.44	0/1671
18	f	0.24	0/1334	0.51	1/1797 (0.1%)
18	j	0.24	0/1329	0.49	0/1789
18	m	0.21	0/1341	0.44	0/1805
19	e	0.20	0/1303	0.48	0/1764
20	l	0.21	0/1365	0.44	0/1845
21	k	0.24	0/1445	0.55	0/1954
22	i	0.28	0/1400	0.56	0/1891
23	d	0.27	0/1259	0.57	0/1700
24	g	0.25	0/1650	0.51	0/2238
25	R	0.22	0/687	0.49	0/940
26	n	0.21	0/1371	0.52	0/1847
27	Q	0.21	0/1053	0.46	0/1418
All	All	0.23	0/40911	0.48	1/55490 (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
11	O	0	1
16	b	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	f	113	MET	CB-CA-C	-5.69	109.49	117.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	666	TRP	Peptide
3	C	61	ASP	Peptide
11	O	86	PHE	Peptide
16	b	188	GLN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5826	0	5682	74	0
2	B	5832	0	5643	71	0
3	C	592	0	567	3	0
4	D	1075	0	1074	9	0
5	E	484	0	486	0	0
6	F	1257	0	1266	11	0
7	I	255	0	270	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	351	0	344	8	0
9	L	1158	0	1170	13	0
10	M	232	0	265	4	0
11	O	714	0	703	6	0
12	K	482	0	511	6	0
13	s	1146	0	1095	6	0
14	c	1362	0	1338	17	0
15	a	1331	0	1284	13	0
16	b	1332	0	1336	21	0
17	h	1201	0	1228	7	0
18	f	1306	0	1311	9	0
18	j	1302	0	1316	17	0
18	m	1313	0	1326	6	0
19	e	1268	0	1244	12	0
20	l	1333	0	1311	17	0
21	k	1412	0	1429	17	0
22	i	1363	0	1322	16	0
23	d	1231	0	1237	14	0
24	g	1608	0	1638	21	0
25	R	666	0	655	6	0
26	n	1343	0	1356	22	0
27	Q	1041	0	1071	7	0
28	A	65	0	72	5	0
29	A	2533	0	2645	83	0
29	B	2592	0	2717	81	0
29	F	182	0	187	5	0
29	J	42	0	31	0	0
29	K	107	0	103	3	0
29	L	225	0	208	6	0
29	O	182	0	187	2	0
29	Q	65	0	72	1	0
29	R	55	0	49	5	0
29	a	638	0	629	19	0
29	b	724	0	735	30	0
29	c	607	0	560	15	0
29	d	529	0	417	7	0
29	e	587	0	588	15	0
29	f	700	0	695	14	0
29	g	765	0	763	22	0
29	h	454	0	429	10	0
29	i	608	0	622	10	0
29	j	669	0	623	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	603	0	548	12	0
29	l	597	0	601	11	0
29	m	680	0	655	20	0
29	n	614	0	570	22	0
29	s	195	0	216	4	0
30	A	33	0	46	4	0
30	B	33	0	46	1	0
31	A	102	0	128	3	0
31	J	33	0	36	3	0
31	L	83	0	108	2	0
31	a	98	0	148	3	0
31	b	49	0	72	1	0
31	c	86	0	118	4	0
31	e	37	0	44	0	0
31	f	86	0	118	3	0
31	g	82	0	104	1	0
31	i	37	0	44	2	0
31	j	30	0	28	0	0
31	l	32	0	34	0	0
31	m	37	0	44	1	0
31	n	43	0	59	3	0
31	s	33	0	40	3	0
32	A	200	0	0	0	0
32	B	200	0	0	1	0
32	F	120	0	0	0	0
32	I	40	0	0	0	0
32	J	40	0	0	0	0
32	K	40	0	0	0	0
32	L	120	0	0	0	0
32	M	40	0	0	0	0
32	R	80	0	0	0	0
32	e	40	0	0	0	0
32	h	40	0	0	0	0
32	i	40	0	0	0	0
32	l	80	0	0	0	0
32	s	80	0	0	0	0
33	A	69	0	87	3	0
33	B	35	0	46	1	0
33	a	35	0	46	0	0
33	i	35	0	46	0	0
34	A	8	0	0	0	0
34	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	54	0	78	0	0
36	B	66	0	96	4	0
36	j	62	0	84	3	0
37	F	94	0	134	4	0
37	L	45	0	61	0	0
37	O	26	0	22	0	0
37	Q	38	0	46	4	0
37	b	42	0	54	2	0
37	c	98	0	141	4	0
37	n	51	0	75	2	0
38	J	42	0	0	0	0
38	O	42	0	0	0	0
38	a	168	0	0	0	0
38	b	168	0	0	2	0
38	c	84	0	0	0	0
38	d	252	0	0	0	0
38	e	168	0	0	0	0
38	f	168	0	0	0	0
38	g	168	0	0	2	0
38	h	112	0	0	0	0
38	i	168	0	0	0	0
38	j	126	0	0	0	0
38	k	252	0	0	1	0
38	l	168	0	0	0	0
38	m	168	0	0	0	0
38	n	168	0	0	4	0
39	O	41	0	0	0	0
39	R	41	0	0	0	0
39	a	41	0	0	0	0
39	b	41	0	0	1	0
39	c	82	0	0	0	0
39	f	41	0	0	0	0
39	g	82	0	0	5	0
39	j	41	0	0	0	0
39	m	41	0	0	0	0
39	n	41	0	0	1	0
40	c	45	0	0	0	0
40	d	90	0	0	1	0
40	e	45	0	0	0	0
40	f	45	0	0	1	0
40	g	135	0	0	5	0
40	i	90	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	j	45	0	0	0	0
40	k	135	0	0	0	0
40	l	45	0	0	3	0
40	m	45	0	0	0	0
40	n	90	0	0	1	0
40	s	90	0	0	2	0
41	A	126	0	0	1	0
41	B	150	0	0	1	0
41	C	22	0	0	0	0
41	D	15	0	0	0	0
41	E	6	0	0	0	0
41	F	14	0	0	0	0
41	J	2	0	0	0	0
41	K	2	0	0	0	0
41	L	15	0	0	0	0
41	M	2	0	0	0	0
41	O	5	0	0	0	0
41	R	1	0	0	0	0
41	a	16	0	0	1	0
41	b	21	0	0	0	0
41	c	2	0	0	0	0
41	e	3	0	0	0	0
41	f	1	0	0	0	0
41	g	1	0	0	0	0
41	h	9	0	0	0	0
41	m	1	0	0	0	0
41	n	1	0	0	0	0
41	s	7	0	0	0	0
All	All	61938	0	56633	661	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 (661) 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)
22:i:218:PHE:CE1	22:i:218:PHE:CE2	2.33	1.07
29:g:316:CLA:H111	39:g:324:IHT:C36	2.07	0.84
14:c:98:GLY:O	14:c:102:GLN:HB3	1.79	0.83
2:B:373:HIS:HE1	29:B:825:CLA:ND	1.77	0.81
1:A:410:HIS:HE1	29:A:829:CLA:NA	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:HIS:HE1	29:A:827:CLA:ND	1.81	0.76
20:l:174:VAL:HG11	40:l:311:KC2:CAA	2.17	0.74
29:B:842:CLA:HBB2	29:R:203:CLA:H11	1.68	0.73
1:A:53:HIS:HE1	29:A:840:CLA:ND	1.89	0.71
29:g:316:CLA:C11	39:g:324:IHT:C36	2.69	0.70
2:B:438:HIS:HE1	29:B:830:CLA:NA	1.90	0.70
29:g:316:CLA:C12	39:g:324:IHT:C36	2.70	0.69
2:B:388:HIS:HE1	29:B:827:CLA:NA	1.91	0.69
29:c:303:CLA:HAC1	29:c:306:CLA:HAB	1.74	0.69
29:g:304:CLA:H62	29:g:305:CLA:HBB	1.75	0.68
9:L:151:MET:HB3	11:O:87:PRO:HG3	1.74	0.68
29:b:313:CLA:HAA1	31:b:318:LHG:HC62	1.74	0.68
14:c:197:GLN:OE1	29:c:311:CLA:NA	2.28	0.67
29:h:306:CLA:HBB2	29:h:307:CLA:HBB2	1.76	0.67
1:A:94:HIS:HE1	29:A:806:CLA:NA	1.94	0.65
1:A:443:LEU:HD22	29:A:836:CLA:HBB1	1.79	0.65
18:m:183:ARG:HB3	29:m:602:CLA:HBC3	1.79	0.65
1:A:446:ILE:HD11	29:A:835:CLA:HBB2	1.77	0.64
1:A:460:HIS:HE1	29:A:832:CLA:NA	1.93	0.64
29:n:609:CLA:HAB	38:n:614:II0:C32	2.28	0.64
20:l:53:LEU:HB3	20:l:74:ARG:HH21	1.62	0.63
29:j:309:CLA:HED2	29:j:309:CLA:H2A	1.79	0.62
21:k:103:GLN:OE1	29:k:604:CLA:NA	2.32	0.62
21:k:74:SER:HB3	29:k:602:CLA:HBA1	1.81	0.62
29:B:840:CLA:H2	29:B:840:CLA:HED2	1.80	0.62
20:l:54:ALA:O	20:l:74:ARG:NH2	2.33	0.61
7:I:29:TYR:HH	10:M:29:TYR:HH	1.48	0.60
15:a:162:ARG:NH2	21:k:53:LEU:O	2.33	0.60
18:j:129:LEU:HB2	29:j:308:CLA:HBC1	1.83	0.60
26:n:179:LEU:HD22	29:n:609:CLA:H2	1.84	0.60
29:l:310:CLA:H142	40:l:311:KC2:CMA	2.32	0.60
16:b:68:ARG:NH1	16:b:71:GLU:OE1	2.35	0.59
29:b:309:CLA:H193	29:m:613:CLA:H121	1.85	0.59
26:n:142:LEU:HD23	37:n:620:LMG:H291	1.85	0.58
13:s:126:THR:OG1	13:s:139:ARG:NH1	2.37	0.58
4:D:42:VAL:HG22	4:D:52:ILE:HG12	1.85	0.58
29:B:821:CLA:HAB	29:B:828:CLA:HMD2	1.84	0.58
1:A:693:ARG:H	2:B:567:CYS:HB2	1.67	0.58
6:F:120:VAL:HG13	29:F:202:CLA:HAA1	1.83	0.58
12:K:22:ALA:HB1	29:e:311:CLA:H142	1.86	0.58
2:B:182:PHE:HZ	29:B:822:CLA:H11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:79:GLU:HG2	22:i:149:MET:HE1	1.84	0.57
18:j:71:ASP:HB2	36:j:319:DGD:HD3	1.87	0.57
2:B:192:HIS:HE1	29:B:813:CLA:NA	1.95	0.57
26:n:126:PHE:O	26:n:130:ASN:ND2	2.37	0.56
29:n:610:CLA:HBA2	29:n:610:CLA:HED2	1.86	0.56
1:A:435:HIS:CE1	29:A:830:CLA:ND	2.72	0.56
29:A:850:CLA:H91	29:B:804:CLA:H101	1.87	0.56
9:L:44:LEU:HD23	24:g:71:PRO:HD3	1.86	0.56
19:e:124:GLY:HA3	29:e:305:CLA:HBC2	1.86	0.56
23:d:135:PRO:HG2	29:d:306:CLA:HBC2	1.85	0.56
16:b:48:ALA:O	16:b:68:ARG:NH2	2.39	0.56
4:D:40:GLU:HG2	4:D:54:ARG:HA	1.87	0.56
1:A:57:HIS:HE1	29:A:803:CLA:NC	2.04	0.56
2:B:307:HIS:HE1	29:B:820:CLA:ND	2.03	0.56
1:A:222:ILE:HD12	1:A:242:PRO:HB3	1.88	0.56
31:L:208:LHG:H252	29:g:302:CLA:C4D	2.09	0.56
24:g:66:VAL:HG11	29:g:304:CLA:H42	1.87	0.56
8:J:42:MET:HA	31:J:104:LHG:HC11	1.89	0.55
1:A:262:GLY:HA3	29:A:814:CLA:H42	1.88	0.55
1:A:707:HIS:HE1	29:A:851:CLA:ND	2.04	0.55
2:B:67:LEU:HD12	2:B:71:GLY:HA3	1.88	0.55
20:l:191:HIS:CD2	29:l:301:CLA:NA	2.73	0.55
29:a:302:CLA:H51	29:a:309:CLA:HBB2	1.88	0.55
29:l:305:CLA:H2	29:l:305:CLA:HED2	1.87	0.55
2:B:14:ASP:HB3	2:B:19:ARG:HB2	1.88	0.55
29:B:817:CLA:H192	29:B:831:CLA:H11	1.87	0.55
16:b:102:MET:HE3	16:b:104:LEU:HB2	1.87	0.55
29:A:837:CLA:H101	8:J:17:THR:HG23	1.89	0.55
9:L:64:LYS:HE2	31:L:209:LHG:HC61	1.89	0.55
29:b:310:CLA:H152	29:m:602:CLA:H121	1.87	0.55
20:l:74:ARG:NH1	20:l:77:GLU:OE1	2.40	0.55
6:F:159:THR:HG22	16:b:135:THR:HB	1.89	0.55
22:i:196:HIS:CD2	29:i:312:CLA:NA	2.75	0.55
4:D:34:THR:HA	4:D:58:ASN:O	2.07	0.54
19:e:136:LYS:HB3	19:e:141:ASN:HB3	1.89	0.54
29:A:824:CLA:HBA1	29:A:828:CLA:H193	1.89	0.54
18:j:147:THR:OG1	18:j:152:ARG:NH1	2.37	0.54
1:A:340:HIS:CD2	29:A:823:CLA:ND	2.75	0.54
16:b:88:GLN:OE1	29:b:305:CLA:NA	2.41	0.54
29:A:835:CLA:H191	29:L:203:CLA:H71	1.90	0.54
20:l:203:GLN:NE2	29:l:312:CLA:O1D	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:g:115:VAL:HB	24:g:119:SER:HB3	1.89	0.54
23:d:174:ALA:O	23:d:178:ALA:N	2.38	0.54
24:g:244:VAL:HA	24:g:248:LEU:HB2	1.89	0.54
2:B:610:GLU:OE1	6:F:44:ARG:NH2	2.41	0.54
2:B:721:ALA:HB2	29:B:825:CLA:HBB1	1.90	0.54
18:j:192:MET:HG2	18:j:203:PRO:HB3	1.90	0.54
26:n:197:ARG:HA	26:n:200:MET:HE3	1.89	0.54
21:k:144:ILE:HB	29:k:607:CLA:HBC1	1.89	0.54
18:f:194:HIS:CD2	29:f:613:CLA:NA	2.75	0.54
14:c:196:HIS:CD2	29:c:312:CLA:NA	2.76	0.53
29:a:302:CLA:H161	29:l:301:CLA:H121	1.89	0.53
2:B:238:THR:HG22	2:B:240:ASN:H	1.74	0.53
26:n:187:ARG:HH22	40:n:611:KC2:CAD	2.20	0.53
29:B:828:CLA:HAB	29:B:835:CLA:HBB2	1.91	0.53
33:B:850:LMU:H123	29:j:309:CLA:HAC2	1.91	0.53
18:m:194:HIS:CD2	29:m:613:CLA:NA	2.75	0.53
27:Q:168:ILE:HG22	37:Q:301:LMG:H292	1.91	0.53
21:k:209:HIS:CD2	29:k:614:CLA:NA	2.75	0.53
2:B:298:HIS:HB3	2:B:303:ILE:HD11	1.90	0.53
22:i:185:ARG:HA	22:i:188:MET:HE3	1.90	0.53
1:A:56:VAL:HG21	29:A:803:CLA:C2D	2.38	0.53
29:A:840:CLA:HMA1	29:A:840:CLA:H2	1.91	0.53
22:i:215:HIS:HA	29:j:306:CLA:CAA	2.39	0.53
4:D:40:GLU:HA	4:D:53:MET:O	2.09	0.52
29:h:304:CLA:HMA2	29:h:305:CLA:HBC1	1.91	0.52
18:f:56:ALA:O	18:f:76:ARG:NH2	2.41	0.52
24:g:156:ILE:HG22	29:g:310:CLA:H42	1.91	0.52
29:A:822:CLA:HBB2	29:A:836:CLA:H18	1.91	0.52
2:B:523:ALA:HB2	29:B:834:CLA:HMA1	1.92	0.52
24:g:206:VAL:HG11	39:g:320:IHT:C29	2.39	0.52
1:A:675:PHE:O	1:A:679:HIS:ND1	2.36	0.52
29:A:840:CLA:H11	30:A:841:PQN:H211	1.91	0.52
2:B:173:ARG:HB2	29:B:812:CLA:HBC2	1.92	0.52
29:B:834:CLA:H191	6:F:111:VAL:HG13	1.92	0.52
29:B:842:CLA:HMC2	29:R:203:CLA:H3A	1.91	0.52
1:A:395:HIS:HE1	29:A:827:CLA:C1D	2.23	0.52
6:F:28:ASP:N	6:F:32:LEU:O	2.43	0.52
18:j:201:LYS:HE3	18:j:205:GLU:HG2	1.91	0.52
29:A:850:CLA:H143	29:B:840:CLA:HBC3	1.92	0.52
2:B:195:HIS:HE1	29:B:814:CLA:NA	2.03	0.52
13:s:220:MET:HE1	29:m:607:CLA:H2A	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:170:ARG:NH2	40:l:311:KC2:O2A	2.44	0.51
29:a:307:CLA:H111	29:a:307:CLA:H171	1.91	0.51
24:g:227:LYS:HE2	40:g:315:KC2:O1A	2.09	0.51
2:B:657:ALA:O	2:B:660:PHE:HB2	2.11	0.51
17:h:142:VAL:O	17:h:146:SER:OG	2.22	0.51
29:A:851:CLA:H162	29:F:201:CLA:H52	1.91	0.51
19:e:163:MET:HG3	29:e:307:CLA:HBB	1.92	0.51
1:A:485:PHE:HB3	29:A:834:CLA:H2	1.91	0.51
2:B:94:HIS:HE1	29:B:840:CLA:NB	2.03	0.51
20:l:40:MET:HG3	20:l:43:LEU:HD12	1.91	0.51
1:A:225:PRO:HD3	1:A:252:MET:HE1	1.93	0.51
29:n:610:CLA:H72	29:n:610:CLA:HAA1	1.93	0.51
14:c:50:PHE:HB2	23:d:156:ARG:HD2	1.91	0.51
25:R:81:VAL:HG12	25:R:85:MET:HE2	1.91	0.51
14:c:111:PRO:HG2	14:c:113:MET:HE1	1.92	0.51
20:l:104:ASN:ND2	20:l:105:GLY:O	2.44	0.51
21:k:128:ILE:O	21:k:132:HIS:N	2.43	0.51
6:F:82:ARG:HH21	8:J:36:ASP:HB2	1.75	0.51
1:A:182:HIS:HE1	29:A:810:CLA:NA	2.08	0.51
14:c:89:GLY:HA3	14:c:184:ALA:HB1	1.93	0.50
2:B:527:HIS:CD2	29:B:835:CLA:NB	2.80	0.50
26:n:39:TYR:HA	26:n:186:ALA:HB3	1.94	0.50
18:m:147:THR:OG1	18:m:152:ARG:NH1	2.44	0.50
19:e:73:GLU:OE1	19:e:150:GLY:N	2.45	0.50
26:n:81:ASN:ND2	31:n:619:LHG:O4	2.42	0.50
29:A:803:CLA:HBD	29:A:810:CLA:H2	1.94	0.50
2:B:388:HIS:HA	2:B:391:ILE:HD12	1.94	0.50
2:B:421:LEU:HD13	2:B:531:LEU:HA	1.94	0.50
2:B:648:MET:O	2:B:651:PHE:HB3	2.12	0.50
29:d:302:CLA:H151	29:d:313:CLA:HBB2	1.94	0.50
29:A:829:CLA:H102	29:A:837:CLA:HAA2	1.93	0.50
18:j:39:SER:OG	18:j:42:VAL:O	2.28	0.50
24:g:190:LYS:O	24:g:194:ASN:ND2	2.33	0.50
2:B:177:HIS:CD2	29:B:812:CLA:NB	2.79	0.50
1:A:32:PRO:HB3	29:A:840:CLA:HAC1	1.94	0.50
1:A:459:ILE:HG22	29:A:832:CLA:HBC2	1.94	0.50
29:B:829:CLA:HAB	29:B:841:CLA:H203	1.93	0.50
2:B:579:MET:HG3	2:B:709:LEU:HD21	1.92	0.50
31:s:408:LHG:H272	29:m:607:CLA:HMB1	1.94	0.50
29:F:202:CLA:H101	29:F:202:CLA:H2	1.93	0.50
18:j:194:HIS:CD2	29:j:314:CLA:NA	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:VAL:HG22	1:A:630:VAL:HG22	1.94	0.49
2:B:337:LEU:HD21	29:B:827:CLA:HAB	1.94	0.49
31:c:320:LHG:H272	29:b:312:CLA:HBA1	1.94	0.49
15:a:182:ARG:HA	15:a:185:MET:HE3	1.94	0.49
2:B:4:PHE:HB2	7:I:30:ILE:HA	1.93	0.49
2:B:437:VAL:HG12	29:B:830:CLA:HAC1	1.94	0.49
19:e:47:LEU:HB3	19:e:54:TYR:HE1	1.77	0.49
29:B:808:CLA:HAB	29:B:809:CLA:HAA2	1.92	0.49
1:A:57:HIS:HE1	29:A:803:CLA:C1C	2.26	0.49
3:C:29:VAL:HG12	4:D:113:ARG:HB3	1.94	0.49
23:d:60:ASP:OD1	23:d:60:ASP:N	2.46	0.49
29:k:602:CLA:HBA2	29:k:602:CLA:H3A	1.54	0.49
23:d:198:HIS:NE2	40:d:312:KC2:NA	2.61	0.49
18:m:183:ARG:HA	18:m:186:MET:HE3	1.94	0.49
29:l:304:CLA:H2A	29:l:304:CLA:HED2	1.95	0.49
15:a:194:HIS:HE1	29:a:311:CLA:NB	2.09	0.49
37:c:318:LMG:H182	29:b:311:CLA:H13	1.95	0.49
16:b:47:MET:HB3	16:b:68:ARG:HH21	1.78	0.48
29:f:607:CLA:H3A	29:f:607:CLA:HBA2	1.46	0.48
29:d:302:CLA:HBA2	29:d:302:CLA:H3A	1.48	0.48
2:B:25:ALA:HB2	36:B:844:DGD:HA52	1.95	0.48
37:c:318:LMG:H111	29:b:311:CLA:H203	1.95	0.48
29:f:610:CLA:H92	40:f:611:KC2:CED	2.43	0.48
27:Q:155:ARG:NH2	37:Q:301:LMG:O2	2.46	0.48
1:A:77:HIS:CE1	29:A:804:CLA:ND	2.81	0.48
1:A:372:HIS:CD2	29:A:826:CLA:NC	2.80	0.48
1:A:460:HIS:HE1	29:A:832:CLA:C1A	2.26	0.48
2:B:213:LYS:HD3	27:Q:169:PRO:HB3	1.95	0.48
20:l:40:MET:HE1	20:l:59:PHE:HA	1.96	0.48
29:j:309:CLA:H3A	29:j:309:CLA:HBA2	1.62	0.48
1:A:203:HIS:CD2	29:A:812:CLA:NB	2.81	0.48
1:A:669:SER:HB2	2:B:444:ALA:HB1	1.95	0.48
31:s:408:LHG:H261	29:m:607:CLA:H2	1.96	0.48
24:g:123:THR:HG22	24:g:127:MET:HE2	1.96	0.48
1:A:179:PHE:CE1	33:A:855:LMU:H6E	2.49	0.48
20:l:139:LEU:HG	29:l:308:CLA:HMA1	1.96	0.48
29:i:302:CLA:H43	31:i:317:LHG:H262	1.94	0.48
1:A:351:TRP:HB3	29:A:804:CLA:HAC1	1.95	0.48
29:B:826:CLA:H143	32:B:845:WVN:C40	2.42	0.48
18:j:94:ILE:HG23	18:j:204:LEU:HD11	1.96	0.48
8:J:12:ALA:O	8:J:16:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:224:GLU:OE2	16:b:92:HIS:NE2	2.47	0.48
1:A:218:HIS:HE1	29:A:813:CLA:NA	2.02	0.48
29:B:824:CLA:H191	29:B:842:CLA:H152	1.95	0.48
9:L:57[B]:PHE:HZ	29:L:203:CLA:HBB1	1.77	0.48
9:L:90:VAL:HG21	9:L:124:LEU:HD13	1.95	0.48
18:f:137:GLU:HG2	29:f:608:CLA:C4B	2.44	0.48
29:c:308:CLA:H3A	29:c:308:CLA:HBA2	1.56	0.48
29:f:601:CLA:H3A	29:f:601:CLA:HBA2	1.57	0.48
29:A:811:CLA:HBB2	29:A:819:CLA:H141	1.96	0.48
29:B:817:CLA:H3A	29:B:817:CLA:HBA2	1.64	0.48
6:F:154:LEU:HA	6:F:157:VAL:HG22	1.96	0.48
14:c:200:VAL:HG23	14:c:201:THR:HG23	1.95	0.48
29:b:305:CLA:H101	29:b:306:CLA:H172	1.96	0.48
27:Q:169:PRO:HG3	37:Q:301:LMG:HC2	1.95	0.48
2:B:88:HIS:CD2	29:B:808:CLA:NA	2.82	0.47
2:B:706:LEU:HD23	36:B:844:DGD:HA21	1.96	0.47
15:a:44:SER:OG	15:a:47:ILE:O	2.30	0.47
19:e:105:THR:HG22	19:e:107:TYR:H	1.77	0.47
18:f:132:TRP:CZ2	29:f:606:CLA:HBB1	2.49	0.47
29:f:613:CLA:H62	29:f:613:CLA:H41	1.63	0.47
1:A:219:GLN:HA	1:A:223:SER:HB2	1.95	0.47
1:A:546:HIS:CD2	29:A:836:CLA:NB	2.82	0.47
29:A:816:CLA:H62	29:A:816:CLA:H41	1.54	0.47
29:A:817:CLA:HAC1	29:A:833:CLA:H42	1.95	0.47
29:B:807:CLA:H12	7:I:14:ILE:HG13	1.96	0.47
37:F:206:LMG:H432	31:J:104:LHG:H262	1.95	0.47
22:i:133:GLY:O	22:i:137:HIS:ND1	2.32	0.47
29:i:302:CLA:HBA2	29:i:302:CLA:H3A	1.43	0.47
23:d:197:HIS:O	23:d:200:PHE:HB2	2.14	0.47
29:n:609:CLA:H93	38:n:614:II0:C30	2.44	0.47
29:B:801:CLA:H41	29:B:801:CLA:H61	1.55	0.47
14:c:169:ASP:OD1	14:c:169:ASP:N	2.46	0.47
29:c:302:CLA:H3A	29:c:302:CLA:HBA2	1.55	0.47
21:k:41:MET:HG2	21:k:191:LEU:HD21	1.95	0.47
23:d:123:ALA:HB1	23:d:128:SER:HB3	1.95	0.47
26:n:200:MET:SD	29:n:602:CLA:HAB	2.54	0.47
1:A:361:MET:HG3	29:A:824:CLA:HBB	1.96	0.47
29:j:310:CLA:H3A	29:j:310:CLA:HBA2	1.49	0.47
29:d:304:CLA:H3A	29:d:304:CLA:HBA2	1.62	0.47
1:A:363:GLY:HA2	1:A:400:GLY:HA2	1.97	0.47
31:J:104:LHG:H112	29:b:313:CLA:HBC1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:610:CLA:H3A	29:f:610:CLA:HBA2	1.55	0.47
29:g:304:CLA:H3A	29:g:304:CLA:HBA2	1.61	0.47
2:B:518:ILE:HD13	29:B:803:CLA:H141	1.97	0.47
29:B:831:CLA:H61	29:B:831:CLA:H2	1.60	0.47
29:c:311:CLA:HBA2	29:c:311:CLA:H3A	1.38	0.47
19:e:172:ARG:HB3	29:e:302:CLA:HBC3	1.96	0.47
23:d:195:MET:HB3	23:d:206:PRO:HG3	1.97	0.47
29:g:316:CLA:NA	39:g:324:IHT:C39	2.78	0.47
1:A:309:VAL:HG11	29:A:816:CLA:H162	1.96	0.47
29:h:305:CLA:H61	29:h:305:CLA:H2	1.64	0.47
29:l:309:CLA:H2A	29:l:309:CLA:HED3	1.96	0.47
29:g:304:CLA:H151	29:g:304:CLA:H111	1.61	0.47
29:A:851:CLA:HAA2	29:B:829:CLA:HMB1	1.96	0.47
23:d:125:LYS:HD2	23:d:125:LYS:HA	1.73	0.47
30:A:841:PQN:H171	29:F:201:CLA:HAB	1.97	0.47
20:l:193:GLN:NE2	20:l:200:THR:OG1	2.41	0.47
23:d:38:MET:SD	23:d:38:MET:N	2.88	0.47
1:A:54:ALA:HB2	31:A:842:LHG:HC82	1.96	0.47
28:A:801:CL0:H29	28:A:801:CL0:H40	1.96	0.47
2:B:509:LEU:HD22	2:B:600:ILE:HD13	1.96	0.47
29:g:311:CLA:H3A	29:g:311:CLA:HBA2	1.78	0.47
8:J:41:PRO:HG2	29:b:313:CLA:HMD3	1.96	0.46
21:k:198:ARG:HA	21:k:201:MET:HE3	1.97	0.46
23:d:197:HIS:CD2	29:d:313:CLA:NA	2.82	0.46
1:A:535:PHE:HA	29:A:835:CLA:HED1	1.96	0.46
14:c:166:LEU:HD13	29:c:308:CLA:H42	1.96	0.46
21:k:103:GLN:O	21:k:107:GLN:NE2	2.46	0.46
24:g:128:GLU:HG2	24:g:136:ALA:HA	1.96	0.46
26:n:101:ALA:HB2	38:n:614:II0:C38	2.44	0.46
1:A:540:ILE:HD12	28:A:801:CL0:H63	1.96	0.46
29:A:818:CLA:HAB	29:A:818:CLA:H8	1.96	0.46
2:B:373:HIS:HE1	29:B:825:CLA:C1D	2.28	0.46
29:L:204:CLA:H43	29:L:207:CLA:HBA1	1.97	0.46
2:B:110:TYR:HB3	17:h:121:TRP:HB3	1.97	0.46
29:B:814:CLA:H161	29:B:814:CLA:H122	1.71	0.46
15:a:143:TYR:HE2	31:a:301:LHG:H112	1.79	0.46
15:a:166:ASN:HB3	15:a:169:SER:HB2	1.97	0.46
29:d:307:CLA:HBA1	29:d:307:CLA:H3A	1.59	0.46
24:g:196:ARG:HA	24:g:199:MET:HE3	1.98	0.46
29:n:608:CLA:H11	31:n:619:LHG:H102	1.97	0.46
29:B:821:CLA:H2A	29:B:821:CLA:HED3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:78:LYS:HG3	15:a:153:PRO:HG3	1.97	0.46
29:e:307:CLA:H162	29:e:307:CLA:H141	1.75	0.46
24:g:251:ILE:HG21	40:g:315:KC2:OBD	2.15	0.46
2:B:438:HIS:HE1	29:B:830:CLA:C1A	2.28	0.46
29:F:203:CLA:HBA1	29:F:203:CLA:H3A	1.52	0.46
14:c:185:ARG:HA	14:c:188:MET:HE3	1.96	0.46
18:f:85:ILE:HD12	29:f:608:CLA:HMD3	1.98	0.46
18:j:199:THR:HB	18:j:201:LYS:HG3	1.97	0.46
29:j:311:CLA:H3A	29:j:311:CLA:HBA2	1.50	0.46
26:n:69:GLN:NE2	38:n:616:II0:O02	2.46	0.46
29:B:806:CLA:H112	29:B:806:CLA:H152	1.76	0.46
17:h:117:LEU:HD13	29:h:301:CLA:H92	1.97	0.46
17:h:157:GLN:NE2	29:h:304:CLA:OBD	2.48	0.46
29:e:302:CLA:H203	31:f:619:LHG:H161	1.97	0.46
22:i:142:PHE:HB3	40:i:318:KC2:CBC	2.46	0.46
26:n:207:VAL:HG11	39:n:617:IHT:C29	2.46	0.46
29:e:307:CLA:H3A	29:e:307:CLA:H2	1.98	0.46
29:i:307:CLA:H3A	29:i:307:CLA:HBA2	1.65	0.46
1:A:284:LEU:HD21	1:A:377:PRO:HD2	1.98	0.45
2:B:350:HIS:CD2	29:B:824:CLA:NC	2.84	0.45
29:B:819:CLA:H92	25:R:75:ASN:HB3	1.97	0.45
14:c:47:ALA:HB2	14:c:65:VAL:HB	1.98	0.45
16:b:176:ARG:HA	16:b:179:MET:HE3	1.98	0.45
29:c:308:CLA:H142	29:c:308:CLA:H111	1.85	0.45
15:a:123:VAL:HG21	29:a:305:CLA:HAA2	1.97	0.45
29:b:307:CLA:H143	29:b:312:CLA:HAB	1.98	0.45
18:j:188:GLY:HA2	29:j:313:CLA:HBB1	1.98	0.45
29:A:822:CLA:HAB	29:O:201:CLA:HAB	1.98	0.45
2:B:596:LYS:NZ	41:B:928:HOH:O	2.49	0.45
12:K:83:VAL:HG23	12:K:85:VAL:HG23	1.97	0.45
29:c:312:CLA:H62	29:c:312:CLA:H2	1.72	0.45
29:e:305:CLA:H2	29:e:305:CLA:H62	1.78	0.45
29:i:304:CLA:HBC1	29:i:307:CLA:H122	1.97	0.45
29:i:312:CLA:H102	29:i:312:CLA:H62	1.76	0.45
29:A:823:CLA:HMB1	31:A:843:LHG:HC41	1.98	0.45
24:g:214:LYS:HB3	24:g:218:GLN:HB2	1.97	0.45
29:a:302:CLA:H41	29:a:302:CLA:H62	1.55	0.45
37:b:319:LMG:H361	29:m:608:CLA:HMB1	1.97	0.45
21:k:154:LEU:HD13	29:j:302:CLA:HBC1	1.98	0.45
29:j:314:CLA:H61	29:j:314:CLA:H2	1.67	0.45
29:n:607:CLA:H122	29:n:607:CLA:H8	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:808:CLA:HAB	29:B:830:CLA:HMD2	1.98	0.45
2:B:307:HIS:HE1	29:B:820:CLA:C4D	2.30	0.45
4:D:64:ARG:NH2	4:D:66:GLU:OE1	2.47	0.45
21:k:124:HIS:HE1	29:k:607:CLA:NA	2.15	0.45
1:A:18:ASP:OD2	1:A:71:ARG:NH2	2.46	0.45
2:B:179:SER:HB3	2:B:287:GLY:HA3	1.98	0.45
29:B:841:CLA:H2	29:B:841:CLA:H62	1.74	0.45
3:C:41:SER:HB2	4:D:116:VAL:H	1.81	0.45
40:s:404:KC2:CBC	29:a:309:CLA:HAB	2.46	0.45
2:B:192:HIS:HE1	29:B:813:CLA:C1A	2.29	0.45
2:B:630:LEU:HD22	2:B:723:PHE:HA	1.98	0.45
29:c:308:CLA:H61	29:c:308:CLA:H41	1.58	0.45
27:Q:169:PRO:HD3	37:Q:301:LMG:HC92	1.99	0.45
1:A:582:ARG:NH1	41:A:916:HOH:O	2.50	0.45
4:D:75:VAL:HA	4:D:79:PHE:HD2	1.81	0.45
29:b:312:CLA:H3A	29:b:312:CLA:HBA2	1.37	0.45
2:B:256:PHE:HD2	2:B:492:TRP:HB3	1.83	0.44
29:B:807:CLA:H93	29:B:807:CLA:H61	1.85	0.44
29:B:840:CLA:H143	29:h:301:CLA:HBB2	1.99	0.44
29:s:402:CLA:H141	29:s:402:CLA:H161	1.81	0.44
14:c:116:VAL:HG11	14:c:199:TRP:HE1	1.82	0.44
1:A:322:HIS:HB3	1:A:327:ILE:HD11	1.98	0.44
2:B:193:LEU:HA	2:B:197:ALA:HB3	1.99	0.44
2:B:520:HIS:HE1	29:B:834:CLA:ND	2.15	0.44
29:a:307:CLA:H171	29:a:307:CLA:H91	1.99	0.44
18:f:130:LEU:HD11	29:f:608:CLA:H172	1.99	0.44
24:g:128:GLU:OE1	24:g:139:HIS:ND1	2.45	0.44
29:n:610:CLA:H62	29:n:610:CLA:H41	1.77	0.44
1:A:582:ARG:HH11	1:A:585:THR:HG21	1.82	0.44
2:B:195:HIS:HE1	29:B:814:CLA:C1A	2.30	0.44
2:B:242:ILE:HG23	2:B:263[A]:GLN:HE22	1.82	0.44
2:B:525:ALA:HB1	2:B:585:THR:HB	1.99	0.44
29:B:805:CLA:HBA1	29:B:805:CLA:H3A	1.58	0.44
3:C:15:THR:HG22	3:C:28:MET:HG3	2.00	0.44
22:i:143:LYS:HB3	22:i:148:THR:HG22	1.98	0.44
24:g:239:TRP:NE1	29:g:302:CLA:OBD	2.45	0.44
1:A:499:ASN:HD21	11:O:65:LEU:HB2	1.83	0.44
12:K:26:LEU:HD22	29:e:311:CLA:H121	1.98	0.44
29:b:312:CLA:H102	29:b:312:CLA:H62	1.73	0.44
29:m:602:CLA:H3A	29:m:602:CLA:HBA2	1.54	0.44
26:n:208:HIS:CD2	29:n:613:CLA:NA	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n:607:CLA:H61	29:n:607:CLA:H41	1.59	0.44
29:B:823:CLA:C2B	29:B:835:CLA:H3A	2.47	0.44
4:D:88:ARG:HB2	4:D:98:LEU:HD11	1.99	0.44
29:a:311:CLA:H102	29:b:306:CLA:HBB1	1.99	0.44
29:b:309:CLA:H43	26:n:154:VAL:HG11	2.00	0.44
29:b:312:CLA:H62	29:b:312:CLA:H2	1.69	0.44
29:e:304:CLA:H161	29:e:304:CLA:H122	1.79	0.44
26:n:119:LEU:HD21	29:n:604:CLA:HAA1	1.99	0.44
29:B:838:CLA:H52	29:B:838:CLA:H11	1.72	0.44
12:K:33:VAL:HG21	29:e:306:CLA:H43	1.98	0.44
25:R:91:THR:O	25:R:95:ILE:HG12	2.18	0.44
1:A:121:ILE:HG13	1:A:122:VAL:HG13	2.00	0.44
1:A:175:PHE:CE2	33:A:855:LMU:H71	2.52	0.44
29:A:826:CLA:HED1	29:A:833:CLA:HAB	1.99	0.44
29:A:840:CLA:H41	29:A:840:CLA:H62	1.79	0.44
37:c:318:LMG:HC71	29:b:302:CLA:HBD	2.00	0.44
29:a:307:CLA:H2A	29:a:307:CLA:HED2	2.00	0.44
21:k:108:PHE:HE2	29:k:604:CLA:H42	1.82	0.44
24:g:74:GLY:O	24:g:77:LYS:HB2	2.18	0.44
2:B:406:VAL:O	2:B:410:ILE:HG12	2.17	0.44
29:h:306:CLA:H2	29:h:306:CLA:H61	1.67	0.44
29:m:602:CLA:H61	29:m:602:CLA:H41	1.56	0.44
20:l:40:MET:HG2	20:l:43:LEU:HB2	2.00	0.44
29:f:602:CLA:H143	29:f:602:CLA:H162	1.84	0.44
29:f:602:CLA:H3A	29:f:602:CLA:HBA2	1.53	0.44
26:n:188:LYS:HA	26:n:188:LYS:HD3	1.86	0.44
1:A:268:THR:HB	12:K:16:TRP:HB2	1.98	0.44
29:A:817:CLA:HBA2	29:A:817:CLA:H3A	1.56	0.44
29:B:820:CLA:H122	29:B:820:CLA:H162	1.73	0.44
16:b:80:LEU:HD13	29:b:305:CLA:H91	2.00	0.44
29:l:308:CLA:HBA2	29:l:308:CLA:H3A	1.61	0.44
29:k:602:CLA:H202	29:k:602:CLA:H162	1.83	0.44
29:B:807:CLA:HBB	29:B:808:CLA:HMB3	1.99	0.43
7:I:29:TYR:OH	10:M:29:TYR:OH	2.24	0.43
20:l:82:ARG:HA	20:l:85:MET:HE3	1.98	0.43
2:B:711:HIS:HE1	29:B:837:CLA:C4D	2.31	0.43
29:a:307:CLA:HAB	29:R:203:CLA:H61	1.99	0.43
29:m:603:CLA:HBA1	29:m:603:CLA:H3A	1.67	0.43
22:i:41:SER:OG	22:i:44:VAL:O	2.35	0.43
2:B:669:TYR:OH	29:B:804:CLA:OBD	2.28	0.43
40:s:401:KC2:C4C	40:s:404:KC2:CMA	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:205:GLN:NE2	41:a:404:HOH:O	2.51	0.43
29:i:306:CLA:HBA2	29:i:306:CLA:H3A	1.47	0.43
1:A:300:HIS:HE1	29:A:818:CLA:NA	2.14	0.43
29:A:818:CLA:H3A	29:A:818:CLA:HBA2	1.67	0.43
2:B:128:MET:HE3	29:B:813:CLA:HMA2	2.01	0.43
37:F:206:LMG:H331	16:b:127:LEU:HD22	2.00	0.43
13:s:151:LEU:HD23	37:b:319:LMG:H342	2.00	0.43
14:c:135:ILE:HG21	29:c:307:CLA:HBC2	2.00	0.43
29:b:309:CLA:H102	29:n:608:CLA:H203	2.00	0.43
22:i:98:GLN:OE1	29:i:305:CLA:NA	2.51	0.43
29:n:607:CLA:H141	31:n:619:LHG:H331	1.99	0.43
1:A:263:LEU:HD12	29:A:814:CLA:H12	2.01	0.43
1:A:298:HIS:HE1	29:A:816:CLA:C4D	2.32	0.43
29:m:613:CLA:H2A	29:m:613:CLA:HED2	2.00	0.43
19:e:172:ARG:HA	19:e:175:MET:HE3	2.01	0.43
29:e:301:CLA:H3A	29:e:301:CLA:HBA2	1.51	0.43
20:l:132:PHE:HA	20:l:139:LEU:HD11	2.00	0.43
29:f:613:CLA:H43	29:g:323:CLA:H3A	1.99	0.43
22:i:58:VAL:HG11	22:i:177:GLU:HB3	2.01	0.43
18:j:183:ARG:HA	18:j:186:MET:HE3	2.00	0.43
26:n:38:LEU:HB3	26:n:39:TYR:H	1.76	0.43
26:n:212:ILE:HG22	29:n:613:CLA:HED3	1.99	0.43
1:A:410:HIS:HA	1:A:413:ILE:HD12	2.00	0.43
9:L:43:PRO:HB3	9:L:110:LEU:HD23	2.00	0.43
26:n:94:ARG:HA	26:n:97:MET:HE3	2.00	0.43
29:Q:302:CLA:H162	29:Q:302:CLA:H121	1.87	0.43
1:A:179:PHE:HE1	33:A:855:LMU:H6E	1.82	0.43
2:B:256:PHE:CD1	29:B:816:CLA:HBB1	2.54	0.43
2:B:591:PHE:HE2	29:B:803:CLA:H72	1.84	0.43
29:c:308:CLA:H112	29:c:308:CLA:H71	1.85	0.43
29:a:302:CLA:HBC2	16:b:132:PHE:HZ	1.83	0.43
18:j:80:LEU:HD13	18:j:155:GLY:HA3	2.01	0.43
29:n:610:CLA:H91	29:n:610:CLA:H111	1.86	0.43
2:B:400:GLU:HA	2:B:403:LYS:HE3	2.00	0.43
26:n:58:PRO:HG3	26:n:72:ASP:HB3	2.01	0.43
29:B:815:CLA:H93	25:R:107:ILE:HG13	2.00	0.43
29:B:817:CLA:H142	29:B:817:CLA:H112	1.78	0.43
29:a:307:CLA:H111	29:a:307:CLA:H91	1.75	0.43
29:b:303:CLA:HBA2	29:b:303:CLA:H3A	1.54	0.43
29:k:608:CLA:H93	29:k:608:CLA:H111	1.90	0.43
18:j:164:PHE:HD2	29:j:310:CLA:H11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:78:ASN:OD1	6:F:82:ARG:NH1	2.52	0.43
13:s:226:PRO:HG3	16:b:90:VAL:HG22	2.00	0.43
31:a:301:LHG:HC92	29:a:307:CLA:HBA1	2.01	0.43
20:l:180:ARG:HA	20:l:183:MET:HE3	2.00	0.43
21:k:121:ILE:HD11	21:k:208:VAL:HG22	1.99	0.43
1:A:607:VAL:HG21	28:A:801:CL0:H69	2.00	0.42
29:A:838:CLA:H43	29:K:101:CLA:H71	2.00	0.42
29:B:838:CLA:H8	29:B:838:CLA:H122	1.69	0.42
15:a:143:TYR:HH	31:a:301:LHG:H02	1.55	0.42
29:b:306:CLA:H171	38:b:317:II0:C40	2.49	0.42
1:A:526:MET:HG2	1:A:620:VAL:HG13	2.00	0.42
2:B:274:HIS:HE1	29:B:815:CLA:C4D	2.32	0.42
6:F:150:VAL:HG21	37:F:208:LMG:H112	2.01	0.42
29:a:308:CLA:H192	29:a:308:CLA:H161	1.87	0.42
29:m:603:CLA:H61	29:m:603:CLA:H2	1.77	0.42
29:A:835:CLA:H51	29:A:835:CLA:H11	1.81	0.42
2:B:44:LYS:HD2	10:M:28:LEU:HD23	2.01	0.42
9:L:57[B]:PHE:CZ	29:L:203:CLA:HBB1	2.54	0.42
9:L:140:ASN:HB3	29:g:309:CLA:HAA2	2.01	0.42
29:K:101:CLA:H11	29:K:101:CLA:H51	1.91	0.42
31:s:408:LHG:H242	29:m:607:CLA:HMB3	2.01	0.42
14:c:197:GLN:HA	14:c:200:VAL:HG22	2.01	0.42
31:c:320:LHG:H152	31:c:320:LHG:H182	1.85	0.42
29:b:305:CLA:H143	29:b:305:CLA:H161	1.90	0.42
19:e:184:GLN:HE21	19:e:184:GLN:HB2	1.69	0.42
2:B:304:LEU:HD11	29:B:822:CLA:HMC3	2.01	0.42
6:F:106:HIS:HA	8:J:42:MET:HE1	2.01	0.42
17:h:154:PHE:HB2	17:h:157:GLN:HB2	2.00	0.42
29:k:603:CLA:H3A	29:k:603:CLA:HBA1	1.75	0.42
23:d:42:ILE:HD12	23:d:45:LEU:HD13	2.00	0.42
29:A:802:CLA:H3A	29:A:802:CLA:C2	2.50	0.42
29:A:822:CLA:H62	29:A:822:CLA:H41	1.73	0.42
16:b:88:GLN:HG2	29:b:305:CLA:C1D	2.50	0.42
17:h:81:ARG:HA	17:h:84:MET:HE3	2.01	0.42
18:f:201:LYS:NZ	18:f:209:ASN:O	2.48	0.42
1:A:405:VAL:HG11	1:A:598:LEU:HG	2.02	0.42
2:B:325:LEU:HD13	2:B:331:PHE:HD2	1.84	0.42
29:B:816:CLA:H3A	29:B:816:CLA:HBA2	1.45	0.42
29:s:402:CLA:H142	29:s:402:CLA:H61	2.02	0.42
29:c:305:CLA:C4B	29:b:311:CLA:H2	2.50	0.42
29:a:303:CLA:H102	29:a:303:CLA:H62	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:175:MET:SD	29:e:302:CLA:HAB	2.59	0.42
18:f:144:LEU:HA	18:f:147:THR:HG22	2.01	0.42
18:j:45:LEU:HD23	18:j:45:LEU:HA	1.90	0.42
29:g:304:CLA:H91	29:g:304:CLA:H112	1.86	0.42
1:A:398:TRP:HB3	29:A:827:CLA:HMC3	2.02	0.42
1:A:428:LEU:HD13	29:A:823:CLA:C1C	2.50	0.42
1:A:579:GLY:HA2	2:B:561:PRO:HD3	2.01	0.42
29:A:827:CLA:H122	29:A:827:CLA:H8	1.85	0.42
29:A:837:CLA:H171	8:J:24:ALA:HB2	2.01	0.42
2:B:325:LEU:HD13	2:B:331:PHE:CD2	2.54	0.42
2:B:518:ILE:HG12	2:B:592:TYR:HB2	2.01	0.42
29:s:406:CLA:H43	29:m:613:CLA:H112	2.02	0.42
29:m:610:CLA:H41	29:m:610:CLA:H62	1.70	0.42
22:i:63:PHE:HE1	29:i:302:CLA:HBC3	1.84	0.42
22:i:149:MET:HE3	22:i:154:ARG:HH22	1.84	0.42
36:j:319:DGD:HBN1	36:j:319:DGD:HGB2	1.79	0.42
2:B:90:ILE:HB	2:B:111:PRO:HB2	2.01	0.42
9:L:149:MET:HE3	9:L:149:MET:HB3	1.94	0.42
29:c:301:CLA:H2	31:c:316:LHG:HC61	2.00	0.42
29:h:301:CLA:H143	29:h:301:CLA:H161	1.91	0.42
29:l:306:CLA:H111	29:l:306:CLA:H152	1.88	0.42
29:g:312:CLA:HBD	40:g:313:KC2:OBD	2.19	0.42
27:Q:194:LYS:O	27:Q:197:MET:HB2	2.19	0.42
29:B:806:CLA:H192	29:B:806:CLA:H161	1.88	0.42
29:B:822:CLA:H62	29:B:822:CLA:H41	1.77	0.42
11:O:59:LEU:HA	11:O:60:PRO:HD3	1.93	0.42
13:s:214:LEU:HD21	29:b:306:CLA:H61	2.01	0.42
16:b:72:LEU:HD23	16:b:72:LEU:HA	1.91	0.42
29:l:301:CLA:H12	29:l:301:CLA:H52	1.79	0.42
24:g:88:ARG:HA	24:g:91:MET:HE3	2.01	0.42
28:A:801:CL0:H49	28:A:801:CL0:H41	1.77	0.42
29:A:838:CLA:H112	29:A:838:CLA:H91	1.81	0.42
29:A:851:CLA:OBD	2:B:422:SER:OG	2.29	0.42
29:B:825:CLA:HBC3	36:B:844:DGD:HBV2	2.01	0.42
9:L:135:TYR:O	9:L:139:SER:OG	2.29	0.42
29:h:312:CLA:H62	29:h:312:CLA:H41	1.87	0.42
29:e:302:CLA:H3A	29:e:302:CLA:HBA2	1.42	0.42
31:f:619:LHG:H152	31:f:619:LHG:H121	1.79	0.42
22:i:137:HIS:NE2	40:i:318:KC2:NA	2.68	0.42
1:A:503:ASN:HB2	29:A:838:CLA:HED2	2.01	0.41
29:B:834:CLA:H91	29:B:834:CLA:H111	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:m:186:MET:SD	29:m:602:CLA:HAB	2.60	0.41
31:m:619:LHG:H241	31:m:619:LHG:H271	1.83	0.41
26:n:40:LYS:HB2	26:n:44:MET:HB2	2.02	0.41
30:B:843:PQN:H222	30:B:843:PQN:H261	1.81	0.41
37:F:206:LMG:H132	15:a:68:PRO:HB2	2.03	0.41
14:c:149:THR:OG1	14:c:154:ARG:NH1	2.50	0.41
15:a:193:HIS:CD2	29:a:312:CLA:NA	2.87	0.41
18:m:88:LEU:HB3	29:m:604:CLA:HAB	2.01	0.41
20:l:140:THR:OG1	20:l:143:ASP:OD1	2.28	0.41
18:f:132:TRP:CH2	29:f:606:CLA:HBB1	2.55	0.41
29:g:305:CLA:HBA1	29:g:305:CLA:H3A	1.86	0.41
29:g:312:CLA:H11	29:g:312:CLA:H51	1.85	0.41
1:A:488:TRP:CE2	1:A:492:ILE:HD11	2.54	0.41
29:B:812:CLA:H2	29:B:812:CLA:H62	1.69	0.41
29:B:840:CLA:H141	29:B:840:CLA:H161	1.83	0.41
9:L:144:LEU:HD11	31:g:301:LHG:HC91	2.02	0.41
29:O:202:CLA:H143	29:O:202:CLA:H111	1.83	0.41
1:A:75:SER:OG	1:A:181:TYR:HB2	2.20	0.41
1:A:129:GLY:O	1:A:136:GLN:HA	2.19	0.41
1:A:428:LEU:HB3	29:A:823:CLA:HMC2	2.01	0.41
1:A:453:HIS:HE1	29:A:831:CLA:NA	2.12	0.41
30:A:841:PQN:H262	30:A:841:PQN:H222	1.71	0.41
29:B:819:CLA:H41	29:B:819:CLA:H62	1.75	0.41
11:O:73:THR:HG22	31:f:619:LHG:H241	2.02	0.41
29:s:403:CLA:H142	29:s:403:CLA:H111	1.83	0.41
16:b:53:PHE:HE1	29:b:302:CLA:HBC3	1.85	0.41
29:g:311:CLA:H143	29:g:311:CLA:H161	1.91	0.41
29:n:603:CLA:HMC3	29:n:607:CLA:HBB2	2.01	0.41
1:A:150:ALA:HB2	1:A:380:PRO:HD2	2.02	0.41
1:A:539:HIS:HE1	29:A:835:CLA:ND	2.16	0.41
1:A:743:TRP:NE1	29:A:827:CLA:O1A	2.43	0.41
11:O:69:LYS:HB3	11:O:73:THR:OG1	2.20	0.41
29:k:609:CLA:HBA2	29:k:609:CLA:H3A	1.58	0.41
23:d:196:MET:O	23:d:199:TYR:HB3	2.20	0.41
1:A:355:LEU:HD11	29:A:829:CLA:HBB1	2.02	0.41
29:A:832:CLA:H2A	29:A:832:CLA:HED2	2.01	0.41
14:c:170:GLU:O	14:c:173:LEU:N	2.53	0.41
16:b:187:HIS:HB2	29:b:311:CLA:HBC3	2.02	0.41
29:b:310:CLA:HBB1	38:b:314:II0:C42	2.50	0.41
29:d:313:CLA:H2A	29:d:313:CLA:HED2	2.02	0.41
2:B:272:ILE:HG23	29:B:817:CLA:HMA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:ALA:HB1	29:B:833:CLA:HBD	2.03	0.41
29:B:819:CLA:H3A	29:B:819:CLA:HBA2	1.58	0.41
16:b:184:GLY:O	16:b:188:GLN:HG3	2.20	0.41
19:e:44:PRO:HG2	19:e:47:LEU:HD22	2.02	0.41
24:g:247:VAL:HG11	29:g:302:CLA:H12	2.02	0.41
29:A:804:CLA:HBA1	29:A:804:CLA:H3A	1.79	0.41
6:F:93:ASP:OD1	6:F:93:ASP:N	2.52	0.41
29:c:303:CLA:H52	29:c:303:CLA:HED3	2.02	0.41
17:h:128:ILE:HD11	17:h:132:ARG:HG2	2.03	0.41
31:i:317:LHG:HC82	31:i:317:LHG:H111	1.93	0.41
29:R:203:CLA:H11	29:R:203:CLA:H51	1.85	0.41
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.96	0.41
1:A:714:PRO:HG2	1:A:718:PRO:HD3	2.02	0.41
29:A:804:CLA:H152	29:A:804:CLA:H111	1.93	0.41
29:A:833:CLA:H61	29:A:833:CLA:H41	1.85	0.41
29:B:825:CLA:H141	36:B:844:DGD:HAV1	2.02	0.41
9:L:45:LEU:HD13	24:g:70:LEU:HD21	2.03	0.41
11:O:53:TRP:CH2	11:O:106:GLY:HA3	2.56	0.41
14:c:155:GLU:HB2	14:c:158:ASP:HB2	2.03	0.41
37:c:317:LMG:H212	31:c:320:LHG:H341	2.03	0.41
29:m:610:CLA:H3A	29:m:610:CLA:HBA2	1.71	0.41
21:k:208:VAL:HG21	38:k:618:II0:C28	2.51	0.41
29:i:308:CLA:H3A	29:i:308:CLA:HBA2	1.70	0.41
18:j:198:ILE:HG13	29:j:314:CLA:HED3	2.03	0.41
24:g:174:ASP:OD1	38:g:317:II0:O01	2.39	0.41
24:g:208:HIS:NE2	40:g:314:KC2:NA	2.69	0.41
25:R:116:TRP:HE1	29:R:203:CLA:C3B	2.34	0.41
29:n:608:CLA:HBB2	37:n:620:LMG:H342	2.03	0.41
27:Q:110:LYS:HD2	27:Q:110:LYS:HA	1.79	0.41
29:A:803:CLA:H61	29:A:803:CLA:H41	1.85	0.41
29:A:810:CLA:H91	29:A:810:CLA:H111	1.82	0.41
30:A:841:PQN:H112	30:A:841:PQN:H142	1.86	0.41
2:B:166:TRP:CZ2	29:B:810:CLA:HBB	2.55	0.41
2:B:344:THR:HG23	2:B:378:ALA:HB2	2.03	0.41
29:B:819:CLA:H193	21:k:153:VAL:HG11	2.02	0.41
12:K:12:GLN:NE2	12:K:13:THR:O	2.54	0.41
19:e:89:LEU:HD23	19:e:89:LEU:HA	1.88	0.41
1:A:94:HIS:HE1	29:A:806:CLA:C1A	2.33	0.40
1:A:249:ARG:HH22	29:A:814:CLA:H2	1.86	0.40
29:a:305:CLA:H161	29:a:305:CLA:H141	1.90	0.40
16:b:200:LEU:HD23	16:b:200:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:312:CLA:H162	29:b:312:CLA:H141	1.87	0.40
29:h:305:CLA:HBA2	29:h:305:CLA:H3A	1.73	0.40
29:n:609:CLA:H143	29:n:609:CLA:H111	1.91	0.40
29:A:820:CLA:H102	29:A:820:CLA:H61	1.86	0.40
2:B:298:HIS:HE1	29:B:819:CLA:C4A	2.35	0.40
8:J:22:PHE:CZ	8:J:26:PHE:HE2	2.39	0.40
29:K:101:CLA:H143	29:K:101:CLA:H161	1.90	0.40
16:b:71:GLU:HG2	16:b:172:ILE:HD11	2.04	0.40
22:i:201:THR:HB	22:i:203:LYS:HD2	2.03	0.40
26:n:115:ALA:HA	29:n:605:CLA:HBC3	2.02	0.40
9:L:54:HIS:HE1	29:L:203:CLA:C4D	2.34	0.40
29:L:202:CLA:HED2	29:L:202:CLA:H2A	2.03	0.40
29:b:310:CLA:H171	29:m:602:CLA:H101	2.04	0.40
21:k:162:THR:OG1	21:k:168:ARG:NH1	2.45	0.40
25:R:116:TRP:HA	25:R:119:HIS:HD1	1.85	0.40
29:A:835:CLA:H112	29:A:835:CLA:H151	1.92	0.40
2:B:149:LEU:HD22	10:M:21:ALA:HA	2.03	0.40
29:B:831:CLA:H101	29:B:832:CLA:HBB1	2.02	0.40
29:a:308:CLA:H101	29:a:310:CLA:H8	2.04	0.40
29:e:306:CLA:H71	29:e:306:CLA:H111	1.82	0.40
23:d:59:GLY:HA3	23:d:182:ILE:HG21	2.03	0.40
29:g:304:CLA:H41	29:g:305:CLA:HBA1	2.03	0.40
40:g:314:KC2:CAA	40:g:315:KC2:C1C	2.99	0.40
29:n:608:CLA:H3A	29:n:608:CLA:HBA2	1.54	0.40
28:A:801:CL0:H70	28:A:801:CL0:H61	1.92	0.40
29:A:827:CLA:H142	29:A:829:CLA:H162	2.04	0.40
29:A:838:CLA:H141	29:A:838:CLA:H162	1.95	0.40
31:A:848:LHG:H111	31:A:848:LHG:H142	1.81	0.40
15:a:76:ASN:O	15:a:80:MET:HG2	2.21	0.40
16:b:44:ASP:N	16:b:44:ASP:OD1	2.53	0.40
16:b:183:SER:HB3	39:b:316:IHT:C40	2.52	0.40
21:k:55:PRO:HD2	21:k:69:ASP:HB3	2.03	0.40
29:k:610:CLA:H3A	29:k:610:CLA:HBA2	1.40	0.40
22:i:86:ARG:HA	22:i:89:MET:HE3	2.04	0.40
18:j:42:VAL:HG11	18:j:45:LEU:HD12	2.04	0.40
18:j:170:THR:HG22	18:j:173:ARG:HH21	1.86	0.40
29:j:304:CLA:H12	36:j:319:DGD:HG12	2.04	0.40
29:j:304:CLA:HBA1	29:j:304:CLA:H3A	1.83	0.40
29:g:306:CLA:H92	38:g:321:II0:C33	2.51	0.40
26:n:45:GLN:NE2	26:n:190:LEU:HD22	2.37	0.40
29:n:604:CLA:H41	29:n:604:CLA:H62	1.72	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	5
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	31/33 (94%)	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	O	93/153 (61%)	92 (99%)	0	1 (1%)	11	7
12	K	64/86 (74%)	64 (100%)	0	0	100	100
13	s	152/302 (50%)	151 (99%)	1 (1%)	0	100	100
14	c	168/215 (78%)	168 (100%)	0	0	100	100
15	a	170/217 (78%)	170 (100%)	0	0	100	100
16	b	176/236 (75%)	176 (100%)	0	0	100	100
17	h	160/229 (70%)	160 (100%)	0	0	100	100
18	f	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
18	j	171/212 (81%)	170 (99%)	1 (1%)	0	100	100
18	m	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
19	e	162/210 (77%)	162 (100%)	0	0	100	100
20	l	173/175 (99%)	173 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	k	187/232 (81%)	185 (99%)	2 (1%)	0	100	100
22	i	178/200 (89%)	177 (99%)	1 (1%)	0	100	100
23	d	162/219 (74%)	161 (99%)	1 (1%)	0	100	100
24	g	214/216 (99%)	214 (100%)	0	0	100	100
25	R	88/135 (65%)	88 (100%)	0	0	100	100
26	n	179/220 (81%)	179 (100%)	0	0	100	100
27	Q	141/233 (60%)	140 (99%)	1 (1%)	0	100	100
All	All	5134/6132 (84%)	5121 (100%)	11 (0%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
11	O	87	PRO

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	27/27 (100%)	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	62
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	74/117 (63%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	51/65 (78%)	51 (100%)	0	100	100
13	s	119/228 (52%)	119 (100%)	0	100	100
14	c	139/171 (81%)	139 (100%)	0	100	100
15	a	139/167 (83%)	139 (100%)	0	100	100
16	b	136/174 (78%)	136 (100%)	0	100	100
17	h	124/167 (74%)	124 (100%)	0	100	100
18	f	134/161 (83%)	134 (100%)	0	100	100
18	j	135/161 (84%)	135 (100%)	0	100	100
18	m	136/161 (84%)	136 (100%)	0	100	100
19	e	130/164 (79%)	129 (99%)	1 (1%)	73	80
20	l	136/137 (99%)	136 (100%)	0	100	100
21	k	143/178 (80%)	143 (100%)	0	100	100
22	i	142/156 (91%)	141 (99%)	1 (1%)	76	82
23	d	125/165 (76%)	125 (100%)	0	100	100
24	g	169/170 (99%)	169 (100%)	0	100	100
25	R	72/104 (69%)	72 (100%)	0	100	100
26	n	141/167 (84%)	141 (100%)	0	100	100
27	Q	106/169 (63%)	106 (100%)	0	100	100
All	All	4135/4806 (86%)	4131 (100%)	4 (0%)	87	93

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	e	184	GLN
22	i	218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	640	GLN
2	B	40	ASN
2	B	75	GLN
2	B	486	ASN

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Mol	Chain	Res	Type
2	B	490	ASN
3	C	16	GLN
5	E	19	GLN
13	s	138	HIS
13	s	141	ASN
13	s	146	HIS
13	s	170	GLN
13	s	240	HIS
15	a	166	ASN
16	b	100	GLN
18	m	175	GLN
18	m	181	ASN
19	e	65	ASN
20	l	193	GLN
20	l	198	GLN
20	l	211	ASN
18	f	175	GLN
18	f	181	ASN
22	i	183	ASN
22	i	216	GLN
18	j	181	ASN
24	g	80	GLN
24	g	135	GLN
24	g	218	GLN
26	n	50	ASN
26	n	195	ASN
27	Q	109	ASN
27	Q	220	GLN
27	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

419 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$
29	CLA	k	608	21	69,73,73	1.24	10 (14%)	83,113,113	1.24	5 (6%)
32	WVN	e	315	-	40,41,41	5.74	19 (47%)	50,56,56	6.26	31 (62%)
29	CLA	A	840	1	69,73,73	1.22	8 (11%)	83,113,113	1.35	8 (9%)
37	LMG	L	210	29	45,45,55	0.82	0	53,53,63	1.24	3 (5%)
38	II0	b	301	-	39,43,43	6.40	22 (56%)	50,60,60	6.77	29 (58%)
38	II0	i	314	-	39,43,43	6.60	22 (56%)	50,60,60	6.55	28 (56%)
29	CLA	B	810	2	69,73,73	1.23	7 (10%)	83,113,113	1.24	8 (9%)
32	WVN	I	101	-	40,41,41	5.69	19 (47%)	50,56,56	6.28	32 (64%)
29	CLA	d	309	23	45,49,73	1.50	8 (17%)	54,84,113	1.58	7 (12%)
40	KC2	n	612	26	49,53,53	1.57	9 (18%)	62,89,89	1.08	2 (3%)
31	LHG	A	848	-	26,26,48	0.68	0	28,29,54	1.44	4 (14%)
29	CLA	B	826	2	69,73,73	1.24	9 (13%)	83,113,113	1.25	9 (10%)
29	CLA	a	304	15	55,59,73	1.38	7 (12%)	66,96,113	1.40	5 (7%)
29	CLA	L	204	9,41	64,68,73	1.30	9 (14%)	77,107,113	1.38	6 (7%)
40	KC2	i	310	22	49,53,53	3.07	21 (42%)	62,89,89	4.23	32 (51%)
38	II0	i	313	-	39,43,43	6.26	21 (53%)	50,60,60	7.02	30 (60%)
28	CL0	A	801	-	69,73,73	1.42	10 (14%)	83,113,113	0.81	3 (3%)
39	IHT	f	617	-	40,42,42	0.21	0	53,58,58	0.70	2 (3%)
33	LMU	B	850	-	36,36,36	0.21	0	47,47,47	0.40	0
29	CLA	h	305	17	69,73,73	1.25	9 (13%)	83,113,113	1.33	5 (6%)
38	II0	k	615	-	39,43,43	6.42	22 (56%)	50,60,60	6.71	31 (62%)
31	LHG	j	318	29	29,29,48	0.80	1 (3%)	32,35,54	1.28	3 (9%)
29	CLA	e	306	19	69,73,73	1.24	7 (10%)	83,113,113	1.24	7 (8%)
29	CLA	a	308	15	69,73,73	1.23	9 (13%)	83,113,113	1.32	7 (8%)
29	CLA	B	821	2	57,61,73	1.38	8 (14%)	68,98,113	1.36	6 (8%)
29	CLA	B	807	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	d	307	23	49,53,73	1.49	8 (16%)	59,89,113	1.43	7 (11%)
32	WVN	B	846	-	40,41,41	5.64	20 (50%)	50,56,56	6.25	29 (58%)
29	CLA	m	610	31	59,63,73	1.35	6 (10%)	71,101,113	1.37	5 (7%)
29	CLA	R	203	25	59,63,73	1.36	8 (13%)	71,101,113	1.53	10 (14%)
39	IHT	j	317	-	40,42,42	0.27	0	53,58,58	0.78	3 (5%)
29	CLA	B	814	2	69,73,73	1.22	8 (11%)	83,113,113	1.29	5 (6%)
29	CLA	a	311	15	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
29	CLA	B	813	2	64,68,73	1.29	8 (12%)	77,107,113	1.40	6 (7%)
38	II0	m	618	-	39,43,43	6.48	21 (53%)	50,60,60	6.77	30 (60%)
32	WVN	M	101	-	40,41,41	5.76	19 (47%)	50,56,56	6.44	33 (66%)
29	CLA	J	102	8	46,50,73	1.50	8 (17%)	55,85,113	1.50	6 (10%)
29	CLA	g	306	24	69,73,73	1.26	9 (13%)	83,113,113	1.57	13 (15%)
39	IHT	g	320	-	40,42,42	0.17	0	53,58,58	0.57	2 (3%)
31	LHG	c	316	29	36,36,48	0.73	1 (2%)	39,42,54	1.25	5 (12%)
29	CLA	n	608	26	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
29	CLA	c	304	14	66,70,73	1.26	8 (12%)	79,109,113	1.40	7 (8%)
36	DGD	B	844	-	67,67,67	0.89	4 (5%)	81,81,81	1.43	9 (11%)
39	IHT	R	204	-	40,42,42	0.21	0	53,58,58	0.52	1 (1%)
38	II0	n	616	-	39,43,43	6.27	21 (53%)	50,60,60	6.97	30 (60%)
29	CLA	A	816	1	69,73,73	1.21	8 (11%)	83,113,113	1.44	8 (9%)
29	CLA	g	311	38,24	69,73,73	1.22	8 (11%)	83,113,113	1.43	10 (12%)
29	CLA	A	828	1	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
29	CLA	a	303	15	60,64,73	1.31	8 (13%)	72,102,113	1.36	7 (9%)
29	CLA	i	309	31	50,54,73	1.45	8 (16%)	60,90,113	1.47	4 (6%)
29	CLA	L	203	9	69,73,73	1.21	8 (11%)	83,113,113	1.37	9 (10%)
38	II0	n	614	-	39,43,43	0.28	0	50,60,60	0.88	3 (6%)
31	LHG	J	104	29	32,32,48	0.75	2 (6%)	35,38,54	1.24	3 (8%)
38	II0	k	619	-	39,43,43	6.21	22 (56%)	50,60,60	6.96	28 (56%)
29	CLA	A	833	1	69,73,73	1.23	7 (10%)	83,113,113	1.32	6 (7%)
29	CLA	m	601	18	46,50,73	1.51	8 (17%)	55,85,113	1.48	7 (12%)
40	KC2	k	612	21	49,53,53	1.58	8 (16%)	62,89,89	0.98	3 (4%)
29	CLA	l	306	20	69,73,73	1.24	9 (13%)	83,113,113	1.32	5 (6%)
37	LMG	n	620	-	51,51,55	0.87	2 (3%)	59,59,63	1.24	5 (8%)
29	CLA	c	303	14	55,59,73	1.39	9 (16%)	66,96,113	1.45	7 (10%)
29	CLA	O	202	41	69,73,73	1.24	9 (13%)	83,113,113	1.35	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	KC2	g	315	40	49,53,53	3.06	21 (42%)	62,89,89	4.07	35 (56%)
38	II0	g	317	29	39,43,43	6.51	21 (53%)	50,60,60	6.92	29 (58%)
29	CLA	m	606	18	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
29	CLA	l	310	31	65,69,73	1.29	8 (12%)	78,108,113	1.31	5 (6%)
29	CLA	l	303	20	51,55,73	1.43	8 (15%)	61,91,113	1.42	5 (8%)
29	CLA	b	302	16	55,59,73	1.40	7 (12%)	66,96,113	1.44	5 (7%)
29	CLA	m	604	18	69,73,73	1.25	8 (11%)	83,113,113	1.36	7 (8%)
29	CLA	A	851	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
29	CLA	i	307	22	65,69,73	1.30	9 (13%)	78,108,113	1.21	6 (7%)
40	KC2	n	611	-	49,53,53	3.06	22 (44%)	62,89,89	4.18	33 (53%)
29	CLA	g	307	24	55,59,73	1.41	8 (14%)	66,96,113	1.45	6 (9%)
38	II0	k	620	-	39,43,43	6.13	21 (53%)	50,60,60	6.85	28 (56%)
38	II0	J	103	-	39,43,43	6.12	21 (53%)	50,60,60	6.85	30 (60%)
29	CLA	j	306	18	49,53,73	1.49	9 (18%)	59,89,113	1.60	6 (10%)
29	CLA	j	310	18	69,73,73	1.24	9 (13%)	83,113,113	1.31	4 (4%)
29	CLA	c	311	14	49,53,73	1.47	6 (12%)	59,89,113	1.57	5 (8%)
38	II0	l	317	-	39,43,43	0.21	0	50,60,60	0.40	0
39	IHT	n	617	-	40,42,42	0.18	0	53,58,58	0.58	0
29	CLA	B	841	2	69,73,73	1.28	8 (11%)	83,113,113	1.35	9 (10%)
29	CLA	A	824	41	69,73,73	1.24	8 (11%)	83,113,113	1.34	10 (12%)
29	CLA	n	613	26	55,59,73	1.41	7 (12%)	66,96,113	1.31	7 (10%)
29	CLA	i	305	22	69,73,73	1.26	7 (10%)	83,113,113	1.36	7 (8%)
29	CLA	n	602	26	54,58,73	1.40	8 (14%)	65,95,113	1.45	8 (12%)
29	CLA	g	305	24,39	69,73,73	1.25	8 (11%)	83,113,113	1.32	5 (6%)
29	CLA	e	308	31	50,54,73	1.46	8 (16%)	60,90,113	1.42	4 (6%)
29	CLA	B	812	2	69,73,73	1.26	9 (13%)	83,113,113	1.32	9 (10%)
32	WVN	B	845	-	40,41,41	0.36	0	50,56,56	1.10	4 (8%)
39	IHT	a	316	-	40,42,42	0.20	0	53,58,58	0.51	0
37	LMG	F	208	-	41,41,55	0.89	0	49,49,63	1.26	3 (6%)
29	CLA	B	825	2	69,73,73	1.23	8 (11%)	83,113,113	1.30	9 (10%)
29	CLA	L	207	41	55,59,73	1.40	9 (16%)	66,96,113	1.39	5 (7%)
29	CLA	c	308	14	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
38	II0	a	314	-	39,43,43	6.39	21 (53%)	50,60,60	6.58	27 (54%)
39	IHT	b	316	-	40,42,42	0.21	0	53,58,58	0.78	1 (1%)
29	CLA	F	201	41	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	809	2	69,73,73	1.28	9 (13%)	83,113,113	1.37	6 (7%)
29	CLA	A	822	1	60,64,73	1.33	9 (15%)	72,102,113	1.38	7 (9%)
29	CLA	i	306	22	55,59,73	1.41	7 (12%)	66,96,113	1.44	5 (7%)
38	II0	i	316	-	39,43,43	6.26	21 (53%)	50,60,60	6.93	30 (60%)
29	CLA	i	302	22	69,73,73	1.24	7 (10%)	83,113,113	1.33	6 (7%)
29	CLA	j	303	18	58,62,73	1.34	8 (13%)	69,99,113	1.41	8 (11%)
29	CLA	A	802	-	69,73,73	1.22	10 (14%)	83,113,113	1.36	9 (10%)
38	II0	j	301	-	39,43,43	6.34	21 (53%)	50,60,60	6.89	28 (56%)
37	LMG	c	317	-	55,55,55	0.72	0	63,63,63	1.41	7 (11%)
29	CLA	d	310	23	45,49,73	1.53	8 (17%)	54,84,113	1.53	6 (11%)
29	CLA	n	609	26	69,73,73	1.24	10 (14%)	83,113,113	1.30	6 (7%)
39	IHT	g	324	29	40,42,42	0.17	0	53,58,58	0.79	2 (3%)
29	CLA	d	303	23	55,59,73	1.38	9 (16%)	66,96,113	1.48	8 (12%)
29	CLA	h	301	41	69,73,73	1.26	9 (13%)	83,113,113	3.23	8 (9%)
32	WVN	F	207	-	40,41,41	5.72	20 (50%)	50,56,56	6.18	29 (58%)
30	PQN	B	843	-	34,34,34	2.81	9 (26%)	42,45,45	1.94	4 (9%)
29	CLA	B	822	41	69,73,73	1.26	10 (14%)	83,113,113	1.52	10 (12%)
29	CLA	K	102	12	46,50,73	1.54	7 (15%)	55,85,113	1.57	9 (16%)
29	CLA	B	805	2	69,73,73	1.21	6 (8%)	83,113,113	1.37	7 (8%)
33	LMU	i	301	-	36,36,36	1.75	12 (33%)	47,47,47	0.93	1 (2%)
37	LMG	Q	301	-	38,38,55	0.88	0	46,46,63	1.22	3 (6%)
29	CLA	B	804	-	69,73,73	1.23	9 (13%)	83,113,113	1.54	9 (10%)
29	CLA	A	811	1	58,62,73	1.38	9 (15%)	69,99,113	1.34	5 (7%)
29	CLA	B	827	2	55,59,73	1.41	10 (18%)	66,96,113	1.51	8 (12%)
29	CLA	l	308	20	69,73,73	1.24	8 (11%)	83,113,113	1.27	7 (8%)
29	CLA	b	313	31	55,59,73	1.40	8 (14%)	66,96,113	1.51	9 (13%)
33	LMU	A	855	-	35,35,36	0.17	0	46,46,47	0.29	0
29	CLA	B	820	2	69,73,73	1.23	8 (11%)	83,113,113	1.28	6 (7%)
33	LMU	a	319	-	36,36,36	0.15	0	47,47,47	0.25	0
32	WVN	B	848	-	40,41,41	5.58	19 (47%)	50,56,56	6.31	34 (68%)
33	LMU	A	849	-	36,36,36	1.75	11 (30%)	47,47,47	1.02	4 (8%)
32	WVN	L	205	-	40,41,41	5.72	19 (47%)	50,56,56	6.10	31 (62%)
38	II0	b	314	-	39,43,43	6.12	19 (48%)	50,60,60	6.77	29 (58%)
29	CLA	l	312	20	60,64,73	1.34	10 (16%)	72,102,113	1.38	5 (6%)
32	WVN	A	854	-	40,41,41	5.69	19 (47%)	50,56,56	6.32	33 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	a	317	-	39,43,43	6.38	20 (51%)	50,60,60	6.83	31 (62%)
29	CLA	c	309	31	49,53,73	1.48	8 (16%)	59,89,113	1.44	5 (8%)
29	CLA	a	309	31	52,56,73	1.43	10 (19%)	62,92,113	1.44	4 (6%)
29	CLA	c	302	14	64,68,73	1.29	8 (12%)	77,107,113	1.33	6 (7%)
29	CLA	j	308	18	55,59,73	1.36	8 (14%)	66,96,113	1.47	9 (13%)
38	II0	k	617	-	39,43,43	0.27	0	50,60,60	0.77	2 (4%)
29	CLA	B	837	2	69,73,73	1.23	7 (10%)	83,113,113	1.31	5 (6%)
29	CLA	b	303	16	59,63,73	1.32	9 (15%)	71,101,113	1.46	9 (12%)
31	LHG	s	408	29	32,32,48	0.80	2 (6%)	36,37,54	1.61	4 (11%)
38	II0	n	618	-	39,43,43	6.47	22 (56%)	50,60,60	6.73	33 (66%)
40	KC2	c	310	14	49,53,53	2.99	21 (42%)	62,89,89	4.22	33 (53%)
29	CLA	s	403	13	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
34	SF4	A	852	2,1	0,12,12	-	-	-	-	-
29	CLA	B	802	41	69,73,73	1.22	7 (10%)	83,113,113	1.29	8 (9%)
29	CLA	m	602	18	64,68,73	1.30	9 (14%)	77,107,113	1.52	15 (19%)
29	CLA	n	607	26	69,73,73	1.24	9 (13%)	83,113,113	1.23	8 (9%)
31	LHG	L	208	-	46,46,48	0.66	2 (4%)	49,52,54	1.35	7 (14%)
32	WVN	s	407	-	40,41,41	5.72	19 (47%)	50,56,56	6.53	32 (64%)
29	CLA	h	312	41	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
29	CLA	m	603	18	63,67,73	1.28	8 (12%)	75,105,113	1.36	6 (8%)
32	WVN	B	849	-	40,41,41	5.67	20 (50%)	50,56,56	6.02	31 (62%)
29	CLA	B	836	41	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
29	CLA	c	307	14	50,54,73	1.45	8 (16%)	60,90,113	1.41	7 (11%)
29	CLA	f	609	18	69,73,73	1.23	10 (14%)	83,113,113	1.35	7 (8%)
29	CLA	B	829	2	69,73,73	1.24	8 (11%)	83,113,113	1.35	9 (10%)
40	KC2	s	404	-	49,53,53	3.04	20 (40%)	62,89,89	3.98	32 (51%)
29	CLA	h	307	17	55,59,73	1.40	8 (14%)	66,96,113	1.45	7 (10%)
38	II0	f	616	-	39,43,43	6.35	20 (51%)	50,60,60	6.73	28 (56%)
29	CLA	l	304	20	69,73,73	1.22	7 (10%)	83,113,113	1.40	9 (10%)
29	CLA	A	823	1	59,63,73	1.35	7 (11%)	71,101,113	1.46	7 (9%)
32	WVN	L	201	-	40,41,41	5.71	19 (47%)	50,56,56	6.23	32 (64%)
29	CLA	A	817	1	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
29	CLA	m	612	41	55,59,73	1.39	9 (16%)	66,96,113	1.47	8 (12%)
29	CLA	k	602	21	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
29	CLA	n	601	26	49,53,73	1.47	8 (16%)	59,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	d	308	23	50,54,73	1.44	8 (16%)	60,90,113	1.38	4 (6%)
29	CLA	k	603	21	55,59,73	1.39	9 (16%)	66,96,113	1.41	8 (12%)
38	II0	e	313	-	39,43,43	6.27	21 (53%)	50,60,60	6.65	30 (60%)
38	II0	e	312	-	39,43,43	6.22	22 (56%)	50,60,60	6.80	30 (60%)
29	CLA	A	810	1	69,73,73	1.23	8 (11%)	83,113,113	1.22	5 (6%)
38	II0	l	313	-	39,43,43	6.31	21 (53%)	50,60,60	6.85	30 (60%)
39	IHT	O	204	-	40,42,42	0.22	0	53,58,58	0.31	0
29	CLA	A	815	41	49,53,73	1.45	8 (16%)	59,89,113	1.63	9 (15%)
29	CLA	g	323	31	59,63,73	1.37	9 (15%)	71,101,113	1.48	8 (11%)
29	CLA	O	201	31	56,60,73	1.37	10 (17%)	67,97,113	1.39	8 (11%)
29	CLA	b	306	41	69,73,73	1.24	8 (11%)	83,113,113	1.36	8 (9%)
31	LHG	c	320	-	48,48,48	0.59	0	51,54,54	1.25	6 (11%)
31	LHG	b	318	29	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
29	CLA	k	605	21	49,53,73	1.48	6 (12%)	59,89,113	1.57	6 (10%)
29	CLA	k	614	21	55,59,73	1.42	7 (12%)	66,96,113	1.46	8 (12%)
29	CLA	j	309	18	49,53,73	1.49	8 (16%)	59,89,113	1.45	6 (10%)
38	II0	b	317	-	39,43,43	0.22	0	50,60,60	0.91	2 (4%)
29	CLA	h	302	17	54,58,73	1.40	9 (16%)	65,95,113	1.47	7 (10%)
29	CLA	B	842	31	69,73,73	1.25	8 (11%)	83,113,113	1.33	8 (9%)
29	CLA	g	310	24	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
29	CLA	Q	302	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	4 (4%)
29	CLA	m	605	18	46,50,73	1.51	7 (15%)	55,85,113	1.56	6 (10%)
40	KC2	g	313	-	49,53,53	3.03	21 (42%)	62,89,89	4.09	35 (56%)
29	CLA	B	835	2	51,55,73	1.45	8 (15%)	61,91,113	1.39	6 (9%)
29	CLA	e	302	19	69,73,73	1.23	8 (11%)	83,113,113	1.30	8 (9%)
29	CLA	g	303	24	46,50,73	1.51	9 (19%)	55,85,113	1.46	5 (9%)
29	CLA	i	311	-	64,68,73	1.29	8 (12%)	77,107,113	1.32	5 (6%)
38	II0	l	315	-	39,43,43	6.55	22 (56%)	50,60,60	6.79	33 (66%)
38	II0	m	615	-	39,43,43	6.44	21 (53%)	50,60,60	6.66	33 (66%)
31	LHG	a	301	29	48,48,48	0.61	0	51,54,54	1.23	6 (11%)
29	CLA	A	830	1	64,68,73	1.30	8 (12%)	77,107,113	1.37	8 (10%)
29	CLA	O	206	11	69,73,73	1.25	10 (14%)	83,113,113	1.33	4 (4%)
38	II0	g	318	-	39,43,43	6.34	21 (53%)	50,60,60	6.66	30 (60%)
31	LHG	g	301	29	44,44,48	0.63	0	47,50,54	1.25	5 (10%)
29	CLA	k	610	-	55,59,73	1.41	8 (14%)	66,96,113	1.47	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	c	314	-	39,43,43	0.21	0	50,60,60	0.55	1 (2%)
29	CLA	n	606	26	55,59,73	1.40	8 (14%)	66,96,113	1.41	5 (7%)
29	CLA	j	304	18	55,59,73	1.39	9 (16%)	66,96,113	1.46	6 (9%)
35	SQD	A	853	-	53,54,54	0.92	4 (7%)	62,65,65	1.74	12 (19%)
29	CLA	j	313	-	55,59,73	1.39	9 (16%)	66,96,113	1.42	5 (7%)
29	CLA	A	832	1	69,73,73	1.22	6 (8%)	83,113,113	1.31	9 (10%)
40	KC2	f	611	-	49,53,53	2.98	20 (40%)	62,89,89	4.14	35 (56%)
37	LMG	O	205	-	26,26,55	1.07	1 (3%)	34,34,63	1.30	6 (17%)
29	CLA	A	829	1	69,73,73	1.28	10 (14%)	83,113,113	1.31	9 (10%)
38	II0	d	314	-	39,43,43	0.21	0	50,60,60	0.72	1 (2%)
29	CLA	A	834	1	64,68,73	1.29	8 (12%)	77,107,113	1.36	7 (9%)
29	CLA	B	808	2	69,73,73	1.22	7 (10%)	83,113,113	1.42	8 (9%)
29	CLA	i	303	22	69,73,73	1.24	8 (11%)	83,113,113	1.34	6 (7%)
29	CLA	B	803	2	69,73,73	1.22	9 (13%)	83,113,113	1.29	6 (7%)
29	CLA	i	308	22	69,73,73	1.22	7 (10%)	83,113,113	1.31	6 (7%)
29	CLA	k	606	21	55,59,73	1.40	9 (16%)	66,96,113	1.38	6 (9%)
29	CLA	A	807	1	69,73,73	1.22	8 (11%)	83,113,113	1.33	7 (8%)
29	CLA	s	406	41	69,73,73	1.26	9 (13%)	83,113,113	1.37	10 (12%)
37	LMG	F	206	-	53,53,55	0.75	0	61,61,63	1.33	7 (11%)
40	KC2	d	311	-	49,53,53	3.07	22 (44%)	62,89,89	4.18	36 (58%)
38	II0	k	618	-	39,43,43	0.27	0	50,60,60	0.76	1 (2%)
29	CLA	a	312	15	52,56,73	1.42	7 (13%)	62,92,113	1.40	4 (6%)
29	CLA	A	838	1	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
29	CLA	f	612	41	55,59,73	1.37	8 (14%)	66,96,113	1.45	5 (7%)
29	CLA	s	402	13	69,73,73	1.27	9 (13%)	83,113,113	1.33	10 (12%)
32	WVN	K	103	-	40,41,41	5.63	19 (47%)	50,56,56	6.57	33 (66%)
29	CLA	k	609	21	61,65,73	1.35	10 (16%)	73,103,113	1.36	5 (6%)
31	LHG	A	843	29	26,26,48	0.89	1 (3%)	29,32,54	1.32	3 (10%)
29	CLA	A	839	1	64,68,73	1.29	8 (12%)	77,107,113	1.35	9 (11%)
29	CLA	b	309	37	69,73,73	1.24	8 (11%)	83,113,113	1.30	4 (4%)
29	CLA	e	305	19	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
29	CLA	m	613	18	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
29	CLA	e	310	41	59,63,73	1.34	8 (13%)	71,101,113	1.43	6 (8%)
30	PQN	A	841	-	34,34,34	2.80	10 (29%)	42,45,45	1.98	5 (11%)
32	WVN	l	302	-	40,41,41	5.67	19 (47%)	50,56,56	6.11	31 (62%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	g	308	24	55,59,73	1.40	7 (12%)	66,96,113	1.36	7 (10%)
38	II0	f	618	-	39,43,43	6.44	20 (51%)	50,60,60	6.82	32 (64%)
31	LHG	n	619	-	42,42,48	0.65	0	45,48,54	1.20	4 (8%)
29	CLA	A	806	1	64,68,73	1.31	7 (10%)	77,107,113	1.33	7 (9%)
29	CLA	m	608	18	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
29	CLA	F	202	41	69,73,73	1.27	9 (13%)	83,113,113	1.24	5 (6%)
29	CLA	A	831	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	6 (7%)
29	CLA	e	307	19	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
32	WVN	h	308	-	40,41,41	5.77	20 (50%)	50,56,56	6.26	34 (68%)
38	II0	e	316	-	39,43,43	0.22	0	50,60,60	0.78	2 (4%)
32	WVN	B	847	-	40,41,41	5.69	20 (50%)	50,56,56	6.11	31 (62%)
31	LHG	e	317	29	36,36,48	0.71	1 (2%)	39,42,54	1.21	4 (10%)
29	CLA	e	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
38	II0	b	315	-	39,43,43	6.18	19 (48%)	50,60,60	6.52	27 (54%)
29	CLA	c	312	14	69,73,73	1.25	8 (11%)	83,113,113	1.26	4 (4%)
29	CLA	k	604	21	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
37	LMG	c	318	29	43,43,55	0.91	0	51,51,63	1.23	5 (9%)
29	CLA	B	801	41	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
29	CLA	f	607	18	69,73,73	1.27	8 (11%)	83,113,113	1.22	7 (8%)
38	II0	f	614	-	39,43,43	6.26	22 (56%)	50,60,60	6.82	28 (56%)
40	KC2	i	318	22	49,53,53	3.13	23 (46%)	62,89,89	4.08	34 (54%)
29	CLA	a	306	15	49,53,73	1.48	9 (18%)	59,89,113	1.56	8 (13%)
29	CLA	f	610	31	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
29	CLA	f	601	18	51,55,73	1.44	9 (17%)	61,91,113	1.46	4 (6%)
38	II0	d	315	-	39,43,43	6.50	22 (56%)	50,60,60	6.45	29 (58%)
29	CLA	d	302	23	66,70,73	1.27	8 (12%)	79,109,113	1.33	7 (8%)
29	CLA	g	302	-	69,73,73	1.26	7 (10%)	83,113,113	1.33	7 (8%)
29	CLA	j	311	31	65,69,73	1.29	8 (12%)	78,108,113	1.32	5 (6%)
31	LHG	a	318	29	48,48,48	0.63	0	51,54,54	1.25	6 (11%)
29	CLA	e	303	19	55,59,73	1.38	8 (14%)	66,96,113	1.45	6 (9%)
32	WVN	s	405	-	40,41,41	5.67	19 (47%)	50,56,56	6.29	29 (58%)
40	KC2	k	613	-	49,53,53	1.56	9 (18%)	62,89,89	0.99	0
29	CLA	B	816	2	69,73,73	1.24	9 (13%)	83,113,113	1.40	12 (14%)
29	CLA	k	601	21	55,59,73	1.41	8 (14%)	66,96,113	1.47	7 (10%)
31	LHG	L	209	-	35,35,48	0.68	0	38,41,54	1.27	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	833	2	59,63,73	1.35	8 (13%)	71,101,113	1.38	7 (9%)
32	WVN	A	845	-	40,41,41	5.63	20 (50%)	50,56,56	6.71	32 (64%)
29	CLA	m	609	18	64,68,73	1.27	8 (12%)	77,107,113	1.35	6 (7%)
37	LMG	b	319	-	42,42,55	0.89	2 (4%)	50,50,63	1.21	4 (8%)
29	CLA	L	202	9	53,57,73	1.42	8 (15%)	62,93,113	1.45	5 (8%)
29	CLA	g	304	24	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
29	CLA	A	805	1	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
29	CLA	A	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.37	13 (15%)
38	II0	m	616	-	39,43,43	6.40	22 (56%)	50,60,60	6.76	31 (62%)
32	WVN	F	204	-	40,41,41	5.61	19 (47%)	50,56,56	6.18	33 (66%)
29	CLA	B	818	41	69,73,73	1.26	9 (13%)	83,113,113	1.31	7 (8%)
40	KC2	j	312	18	49,53,53	3.02	20 (40%)	62,89,89	4.16	36 (58%)
29	CLA	A	821	1	53,57,73	1.41	6 (11%)	62,93,113	1.46	7 (11%)
29	CLA	e	311	19	69,73,73	1.26	8 (11%)	83,113,113	1.29	8 (9%)
29	CLA	A	825	41	69,73,73	1.25	8 (11%)	83,113,113	1.31	11 (13%)
29	CLA	f	613	18	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
38	II0	m	614	-	39,43,43	6.42	22 (56%)	50,60,60	6.79	28 (56%)
31	LHG	f	619	-	48,48,48	0.60	0	51,54,54	1.23	6 (11%)
29	CLA	A	850	41	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
29	CLA	m	607	18,31	55,59,73	1.40	7 (12%)	66,96,113	1.35	7 (10%)
31	LHG	A	842	-	47,47,48	0.66	1 (2%)	50,53,54	1.25	5 (10%)
29	CLA	A	814	1	54,58,73	1.38	7 (12%)	65,95,113	1.44	6 (9%)
29	CLA	h	303	17,37	54,58,73	1.41	9 (16%)	65,95,113	1.47	7 (10%)
32	WVN	i	315	-	40,41,41	5.77	20 (50%)	50,56,56	6.06	31 (62%)
38	II0	d	316	-	39,43,43	6.43	22 (56%)	50,60,60	6.81	30 (60%)
29	CLA	n	610	-	64,68,73	1.31	8 (12%)	77,107,113	1.37	7 (9%)
38	II0	i	319	-	39,43,43	6.38	21 (53%)	50,60,60	6.55	30 (60%)
29	CLA	A	837	1	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
29	CLA	i	304	22	69,73,73	1.23	7 (10%)	83,113,113	1.32	4 (4%)
29	CLA	A	804	1	69,73,73	1.22	8 (11%)	83,113,113	1.42	10 (12%)
31	LHG	f	620	29	36,36,48	0.70	1 (2%)	39,42,54	1.19	4 (10%)
29	CLA	n	603	26	55,59,73	1.39	9 (16%)	66,96,113	1.37	6 (9%)
29	CLA	A	827	1	66,70,73	1.26	7 (10%)	79,109,113	1.39	8 (10%)
32	WVN	R	202	-	40,41,41	5.74	19 (47%)	50,56,56	6.39	32 (64%)
29	CLA	A	820	41	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	d	318	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	6 (10%)
29	CLA	d	313	23	55,59,73	1.39	8 (14%)	66,96,113	1.47	10 (15%)
29	CLA	h	306	17	61,65,73	1.33	6 (9%)	73,103,113	1.38	6 (8%)
29	CLA	j	302	18,31	69,73,73	1.25	8 (11%)	83,113,113	1.31	4 (4%)
29	CLA	e	301	19	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
39	IHT	c	319	-	40,42,42	0.20	0	53,58,58	0.69	1 (1%)
29	CLA	c	301	14	55,59,73	1.40	5 (9%)	66,96,113	1.43	4 (6%)
31	LHG	l	318	29	31,31,48	0.76	0	34,37,54	1.27	4 (11%)
38	II0	g	321	-	39,43,43	0.23	0	50,60,60	0.47	0
29	CLA	A	826	1	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
29	CLA	B	830	2	54,58,73	1.38	7 (12%)	65,95,113	1.47	8 (12%)
39	IHT	c	315	-	40,42,42	0.20	0	53,58,58	0.79	2 (3%)
29	CLA	B	832	41	49,53,73	1.48	8 (16%)	59,89,113	1.50	5 (8%)
38	II0	j	316	-	39,43,43	6.31	22 (56%)	50,60,60	6.74	30 (60%)
29	CLA	a	307	15	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)
38	II0	g	319	-	39,43,43	6.12	22 (56%)	50,60,60	6.94	29 (58%)
38	II0	e	314	-	39,43,43	6.43	22 (56%)	50,60,60	6.92	30 (60%)
38	II0	l	314	-	39,43,43	6.44	22 (56%)	50,60,60	6.69	26 (52%)
38	II0	a	315	-	39,43,43	6.15	21 (53%)	50,60,60	7.01	31 (62%)
29	CLA	B	824	2	69,73,73	1.23	8 (11%)	83,113,113	1.31	6 (7%)
29	CLA	K	101	41	69,73,73	1.23	7 (10%)	83,113,113	1.39	8 (9%)
32	WVN	R	201	-	40,41,41	5.60	19 (47%)	50,56,56	6.21	34 (68%)
29	CLA	n	605	26	55,59,73	1.40	8 (14%)	66,96,113	1.46	5 (7%)
29	CLA	A	836	1	69,73,73	1.25	8 (11%)	83,113,113	1.39	7 (8%)
29	CLA	B	839	2	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
29	CLA	g	316	24	61,65,73	1.35	7 (11%)	73,103,113	1.29	5 (6%)
29	CLA	b	310	16	69,73,73	1.25	8 (11%)	83,113,113	1.24	6 (7%)
38	II0	n	615	-	39,43,43	6.32	22 (56%)	50,60,60	6.86	28 (56%)
32	WVN	L	206	-	40,41,41	5.58	20 (50%)	50,56,56	6.50	31 (62%)
38	II0	k	616	-	39,43,43	6.42	22 (56%)	50,60,60	6.80	30 (60%)
29	CLA	g	309	24	69,73,73	1.22	8 (11%)	83,113,113	1.37	7 (8%)
29	CLA	f	603	18	55,59,73	1.37	9 (16%)	66,96,113	1.46	7 (10%)
40	KC2	e	309	-	49,53,53	3.08	22 (44%)	62,89,89	4.09	34 (54%)
29	CLA	B	806	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
31	LHG	m	619	29	36,36,48	0.70	0	39,42,54	1.22	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	O	203	-	39,43,43	0.19	0	50,60,60	1.05	4 (8%)
29	CLA	B	831	41	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
29	CLA	A	813	1	60,64,73	1.34	9 (15%)	72,102,113	1.43	11 (15%)
29	CLA	d	305	23	55,59,73	1.42	7 (12%)	66,96,113	1.42	7 (10%)
29	CLA	j	314	18	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
34	SF4	C	101	3	0,12,12	-	-	-	-	-
38	II0	h	311	-	39,43,43	6.31	22 (56%)	50,60,60	6.75	27 (54%)
31	LHG	i	317	29	36,36,48	0.66	0	39,42,54	1.22	4 (10%)
29	CLA	B	811	2	59,63,73	1.35	9 (15%)	71,101,113	1.35	6 (8%)
29	CLA	i	312	22	69,73,73	1.25	7 (10%)	83,113,113	1.39	7 (8%)
29	CLA	A	812	1	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
29	CLA	l	309	20	61,65,73	1.32	9 (14%)	73,103,113	1.38	5 (6%)
29	CLA	g	312	31	58,62,73	1.36	8 (13%)	69,99,113	1.38	4 (5%)
40	KC2	k	611	-	49,53,53	3.10	22 (44%)	62,89,89	4.14	35 (56%)
32	WVN	l	316	-	40,41,41	5.84	19 (47%)	50,56,56	6.14	31 (62%)
40	KC2	m	611	18	49,53,53	3.03	20 (40%)	62,89,89	4.18	34 (54%)
29	CLA	b	308	16	69,73,73	1.22	8 (11%)	83,113,113	1.33	8 (9%)
29	CLA	B	823	41	68,72,73	1.24	8 (11%)	81,111,113	1.33	8 (9%)
32	WVN	J	101	-	40,41,41	5.70	19 (47%)	50,56,56	6.24	29 (58%)
38	II0	j	315	-	39,43,43	6.20	22 (56%)	50,60,60	6.96	30 (60%)
29	CLA	F	203	6	56,60,73	1.40	8 (14%)	67,97,113	1.39	6 (8%)
31	LHG	g	322	29	36,36,48	0.73	1 (2%)	39,42,54	1.23	4 (10%)
40	KC2	l	311	-	49,53,53	3.09	21 (42%)	62,89,89	3.97	32 (51%)
29	CLA	f	604	18	69,73,73	1.26	7 (10%)	83,113,113	1.46	8 (9%)
40	KC2	s	401	13	49,53,53	2.96	20 (40%)	62,89,89	4.03	35 (56%)
29	CLA	f	605	18	49,53,73	1.50	8 (16%)	59,89,113	1.51	7 (11%)
32	WVN	A	847	-	40,41,41	5.79	19 (47%)	50,56,56	5.80	32 (64%)
29	CLA	l	307	20	69,73,73	1.26	7 (10%)	83,113,113	1.34	6 (7%)
39	IHT	m	617	-	40,42,42	0.18	0	53,58,58	0.43	1 (1%)
38	II0	f	615	-	39,43,43	6.35	22 (56%)	50,60,60	6.70	29 (58%)
32	WVN	A	844	-	40,41,41	5.76	20 (50%)	50,56,56	6.18	33 (66%)
29	CLA	B	840	2	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
38	II0	d	317	-	39,43,43	6.40	21 (53%)	50,60,60	6.75	27 (54%)
29	CLA	B	815	2	59,63,73	1.32	9 (15%)	71,101,113	1.40	8 (11%)
29	CLA	A	808	29,1	69,73,73	1.25	9 (13%)	83,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	834	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
29	CLA	l	301	20	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
29	CLA	A	803	29,1	59,63,73	1.37	8 (13%)	71,101,113	1.35	9 (12%)
29	CLA	b	304	16	56,60,73	1.38	8 (14%)	67,97,113	1.44	8 (11%)
29	CLA	b	307	16	65,69,73	1.28	9 (13%)	78,108,113	1.30	6 (7%)
40	KC2	d	312	23	49,53,53	1.58	8 (16%)	62,89,89	1.17	4 (6%)
29	CLA	A	835	1	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
29	CLA	b	312	16	69,73,73	1.25	6 (8%)	83,113,113	1.23	5 (6%)
29	CLA	A	809	1	60,64,73	1.32	8 (13%)	72,102,113	1.31	5 (6%)
29	CLA	d	306	23	55,59,73	1.40	9 (16%)	66,96,113	1.41	6 (9%)
40	KC2	g	314	24,40	49,53,53	3.07	21 (42%)	62,89,89	3.89	33 (53%)
29	CLA	a	310	15	69,73,73	1.24	10 (14%)	83,113,113	1.31	4 (4%)
29	CLA	j	307	18	55,59,73	1.40	8 (14%)	66,96,113	1.42	5 (7%)
29	CLA	b	305	16	69,73,73	1.24	7 (10%)	83,113,113	1.32	5 (6%)
32	WVN	F	205	-	40,41,41	5.26	16 (40%)	50,56,56	6.25	36 (72%)
29	CLA	l	305	20	55,59,73	1.38	8 (14%)	66,96,113	1.49	6 (9%)
29	CLA	B	819	2	69,73,73	1.31	9 (13%)	83,113,113	1.53	11 (13%)
29	CLA	c	305	14	69,73,73	1.27	8 (11%)	83,113,113	1.28	4 (4%)
36	DGD	j	319	18	63,63,67	1.01	5 (7%)	77,77,81	1.57	11 (14%)
29	CLA	B	828	2	54,58,73	1.40	9 (16%)	65,95,113	1.39	7 (10%)
38	II0	d	319	-	39,43,43	0.21	0	50,60,60	0.76	1 (2%)
29	CLA	B	838	2	69,73,73	1.23	8 (11%)	83,113,113	1.32	7 (8%)
29	CLA	d	304	23	49,53,73	1.49	7 (14%)	59,89,113	1.59	5 (8%)
29	CLA	n	604	26	64,68,73	1.29	8 (12%)	77,107,113	1.49	10 (12%)
38	II0	h	310	-	39,43,43	6.09	21 (53%)	50,60,60	6.91	29 (58%)
29	CLA	a	302	15	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
29	CLA	f	606	18	55,59,73	1.39	7 (12%)	66,96,113	1.39	6 (9%)
38	II0	h	309	-	26,28,43	6.25	13 (50%)	31,37,60	6.82	19 (61%)
34	SF4	C	102	3	0,12,12	-	-	-	-	-
29	CLA	f	608	18	69,73,73	1.26	7 (10%)	83,113,113	1.36	7 (8%)
29	CLA	b	311	16	68,72,73	1.26	6 (8%)	81,111,113	1.55	6 (7%)
29	CLA	j	305	18	69,73,73	1.25	7 (10%)	83,113,113	1.37	10 (12%)
29	CLA	h	304	17	55,59,73	1.36	6 (10%)	66,96,113	1.43	6 (9%)
29	CLA	c	306	14	56,60,73	1.38	9 (16%)	67,97,113	1.35	6 (8%)
38	II0	d	301	-	39,43,43	6.16	22 (56%)	50,60,60	6.99	29 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	k	607	21	55,59,73	1.39	7 (12%)	66,96,113	1.45	9 (13%)
38	II0	c	313	-	39,43,43	6.30	21 (53%)	50,60,60	6.91	29 (58%)
38	II0	a	313	-	39,43,43	6.29	21 (53%)	50,60,60	6.71	29 (58%)
32	WVN	A	846	-	40,41,41	5.64	19 (47%)	50,56,56	6.45	32 (64%)
29	CLA	f	602	18	69,73,73	1.22	9 (13%)	83,113,113	1.38	7 (8%)
29	CLA	A	818	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	9 (10%)
29	CLA	a	305	41	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
29	CLA	B	817	2	69,73,73	1.24	9 (13%)	83,113,113	1.25	8 (9%)

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
29	CLA	k	608	21	-	11/39/115/115	-
32	WVN	e	315	-	-	16/29/63/63	0/2/2/2
29	CLA	A	840	1	-	16/39/115/115	-
37	LMG	L	210	29	-	20/40/60/70	0/1/1/1
38	II0	b	301	-	-	13/21/67/67	0/2/2/2
38	II0	i	314	-	-	10/21/67/67	0/2/2/2
29	CLA	B	810	2	-	10/39/115/115	-
32	WVN	I	101	-	-	18/29/63/63	0/2/2/2
29	CLA	d	309	23	-	4/10/86/115	-
40	KC2	n	612	26	-	12/15/71/71	-
31	LHG	A	848	-	-	14/27/27/53	-
29	CLA	B	826	2	-	9/39/115/115	-
29	CLA	a	304	15	-	2/23/99/115	-
29	CLA	L	204	9,41	-	4/33/109/115	-
40	KC2	i	310	22	-	10/15/71/71	-
38	II0	i	313	-	-	11/21/67/67	0/2/2/2
28	CL0	A	801	-	-	11/39/115/115	-
39	IHT	f	617	-	-	2/25/65/65	0/2/2/2
33	LMU	B	850	-	-	4/21/61/61	0/2/2/2
29	CLA	h	305	17	-	12/39/115/115	-
38	II0	k	615	-	-	14/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	j	318	29	-	13/34/34/53	-
29	CLA	e	306	19	-	16/39/115/115	-
29	CLA	a	308	15	-	11/39/115/115	-
29	CLA	B	821	2	-	7/25/101/115	-
29	CLA	B	807	2	-	8/39/115/115	-
29	CLA	d	307	23	-	8/15/91/115	-
32	WVN	B	846	-	-	15/29/63/63	0/2/2/2
29	CLA	m	610	31	-	18/27/103/115	-
29	CLA	R	203	25	-	7/27/103/115	-
39	IHT	j	317	-	-	2/25/65/65	0/2/2/2
29	CLA	B	814	2	-	10/39/115/115	-
29	CLA	a	311	15	-	13/39/115/115	-
29	CLA	B	813	2	-	13/33/109/115	-
38	II0	m	618	-	-	13/21/67/67	0/2/2/2
32	WVN	M	101	-	-	17/29/63/63	0/2/2/2
29	CLA	J	102	8	-	5/12/88/115	-
29	CLA	g	306	24	-	12/39/115/115	-
39	IHT	g	320	-	-	5/25/65/65	0/2/2/2
31	LHG	c	316	29	-	19/41/41/53	-
29	CLA	n	608	26	-	18/39/115/115	-
29	CLA	c	304	14	-	16/36/112/115	-
36	DGD	B	844	-	-	28/55/95/95	0/2/2/2
39	IHT	R	204	-	-	1/25/65/65	0/2/2/2
38	II0	n	616	-	-	10/21/67/67	0/2/2/2
29	CLA	A	816	1	-	16/39/115/115	-
29	CLA	g	311	38,24	-	19/39/115/115	-
29	CLA	A	828	1	-	9/39/115/115	-
29	CLA	a	303	15	-	6/29/105/115	-
29	CLA	i	309	31	-	8/17/93/115	-
29	CLA	L	203	9	-	6/39/115/115	-
38	II0	n	614	-	-	10/21/67/67	0/2/2/2
31	LHG	J	104	29	-	16/37/37/53	-
38	II0	k	619	-	-	11/21/67/67	0/2/2/2
29	CLA	A	833	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	m	601	18	-	6/12/88/115	-
40	KC2	k	612	21	-	9/15/71/71	-
29	CLA	l	306	20	-	19/39/115/115	-
37	LMG	n	620	-	-	18/46/66/70	0/1/1/1
29	CLA	c	303	14	-	6/23/99/115	-
29	CLA	O	202	41	-	10/39/115/115	-
40	KC2	g	315	40	-	7/15/71/71	-
38	II0	g	317	29	-	9/21/67/67	0/2/2/2
29	CLA	m	606	18	-	17/39/115/115	-
29	CLA	l	310	31	-	14/35/111/115	-
29	CLA	l	303	20	-	8/18/94/115	-
29	CLA	b	302	16	-	6/23/99/115	-
29	CLA	m	604	18	-	12/39/115/115	-
29	CLA	A	851	1	-	14/39/115/115	-
29	CLA	i	307	22	-	10/35/111/115	-
40	KC2	n	611	-	-	5/15/71/71	-
29	CLA	g	307	24	-	13/23/99/115	-
38	II0	k	620	-	-	13/21/67/67	0/2/2/2
38	II0	J	103	-	-	14/21/67/67	0/2/2/2
29	CLA	j	306	18	-	10/15/91/115	-
29	CLA	j	310	18	-	15/39/115/115	-
29	CLA	c	311	14	-	9/15/91/115	-
38	II0	l	317	-	-	1/21/67/67	0/2/2/2
39	IHT	n	617	-	-	6/25/65/65	0/2/2/2
29	CLA	B	841	2	-	20/39/115/115	-
29	CLA	A	824	41	-	10/39/115/115	-
29	CLA	n	613	26	-	10/23/99/115	-
29	CLA	i	305	22	-	15/39/115/115	-
29	CLA	n	602	26	-	5/21/97/115	-
29	CLA	g	305	24,39	-	5/39/115/115	-
29	CLA	e	308	31	-	3/17/93/115	-
29	CLA	B	812	2	-	13/39/115/115	-
32	WVN	B	845	-	-	6/29/63/63	0/2/2/2
39	IHT	a	316	-	-	5/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	F	208	-	-	13/36/56/70	0/1/1/1
29	CLA	B	825	2	-	18/39/115/115	-
29	CLA	L	207	41	-	10/23/99/115	-
29	CLA	c	308	14	-	15/39/115/115	-
38	II0	a	314	-	-	10/21/67/67	0/2/2/2
39	IHT	b	316	-	-	8/25/65/65	0/2/2/2
29	CLA	F	201	41	-	16/39/115/115	-
29	CLA	B	809	2	-	9/39/115/115	-
29	CLA	A	822	1	-	15/29/105/115	-
29	CLA	i	306	22	-	9/23/99/115	-
38	II0	i	316	-	-	12/21/67/67	0/2/2/2
29	CLA	i	302	22	-	20/39/115/115	-
29	CLA	j	303	18	-	9/26/102/115	-
29	CLA	A	802	-	-	10/39/115/115	-
38	II0	j	301	-	-	14/21/67/67	0/2/2/2
37	LMG	c	317	-	-	21/50/70/70	0/1/1/1
29	CLA	d	310	23	-	6/10/86/115	-
29	CLA	n	609	26	-	13/39/115/115	-
39	IHT	g	324	29	-	7/25/65/65	0/2/2/2
29	CLA	d	303	23	-	7/23/99/115	-
29	CLA	h	301	41	-	11/39/115/115	-
32	WVN	F	207	-	-	18/29/63/63	0/2/2/2
30	PQN	B	843	-	-	8/23/43/43	0/2/2/2
29	CLA	B	822	41	-	18/39/115/115	-
29	CLA	K	102	12	-	6/12/88/115	-
29	CLA	B	805	2	-	13/39/115/115	-
33	LMU	i	301	-	-	13/21/61/61	0/2/2/2
37	LMG	Q	301	-	-	16/33/53/70	0/1/1/1
29	CLA	B	804	-	-	10/39/115/115	-
29	CLA	A	811	1	-	7/26/102/115	-
29	CLA	B	827	2	-	5/23/99/115	-
29	CLA	l	308	20	-	6/39/115/115	-
29	CLA	b	313	31	-	7/23/99/115	-
33	LMU	A	855	-	-	17/20/60/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	820	2	-	13/39/115/115	-
33	LMU	a	319	-	-	13/21/61/61	0/2/2/2
32	WVN	B	848	-	-	15/29/63/63	0/2/2/2
33	LMU	A	849	-	-	16/21/61/61	0/2/2/2
32	WVN	L	205	-	-	16/29/63/63	0/2/2/2
38	II0	b	314	-	-	13/21/67/67	0/2/2/2
29	CLA	l	312	20	-	10/29/105/115	-
32	WVN	A	854	-	-	19/29/63/63	0/2/2/2
38	II0	a	317	-	-	13/21/67/67	0/2/2/2
29	CLA	c	309	31	-	6/15/91/115	-
29	CLA	a	309	31	-	7/19/95/115	-
29	CLA	c	302	14	-	16/33/109/115	-
29	CLA	j	308	18	-	9/23/99/115	-
38	II0	k	617	-	-	4/21/67/67	0/2/2/2
29	CLA	B	837	2	-	17/39/115/115	-
29	CLA	b	303	16	-	11/27/103/115	-
31	LHG	s	408	29	-	12/34/34/53	-
38	II0	n	618	-	-	10/21/67/67	0/2/2/2
40	KC2	c	310	14	-	10/15/71/71	-
29	CLA	s	403	13	-	10/39/115/115	-
34	SF4	A	852	2,1	-	-	0/6/5/5
29	CLA	B	802	41	-	12/39/115/115	-
29	CLA	m	602	18	-	13/33/109/115	-
29	CLA	n	607	26	-	12/39/115/115	-
31	LHG	L	208	-	-	19/51/51/53	-
32	WVN	s	407	-	-	14/29/63/63	0/2/2/2
29	CLA	h	312	41	-	8/39/115/115	-
29	CLA	m	603	18	-	7/32/108/115	-
32	WVN	B	849	-	-	14/29/63/63	0/2/2/2
29	CLA	B	836	41	-	15/39/115/115	-
29	CLA	c	307	14	-	9/17/93/115	-
29	CLA	f	609	18	-	11/39/115/115	-
29	CLA	B	829	2	-	8/39/115/115	-
40	KC2	s	404	-	-	2/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	h	307	17	-	7/23/99/115	-
38	II0	f	616	-	-	12/21/67/67	0/2/2/2
29	CLA	l	304	20	-	14/39/115/115	-
29	CLA	A	823	1	-	11/27/103/115	-
32	WVN	L	201	-	-	22/29/63/63	0/2/2/2
29	CLA	A	817	1	-	12/39/115/115	-
29	CLA	m	612	41	-	11/23/99/115	-
29	CLA	k	602	21	-	19/39/115/115	-
29	CLA	n	601	26	-	7/15/91/115	-
29	CLA	d	308	23	-	9/17/93/115	-
29	CLA	k	603	21	-	0/23/99/115	-
38	II0	e	313	-	-	13/21/67/67	0/2/2/2
38	II0	e	312	-	-	14/21/67/67	0/2/2/2
29	CLA	A	810	1	-	19/39/115/115	-
38	II0	l	313	-	-	12/21/67/67	0/2/2/2
39	IHT	O	204	-	-	4/25/65/65	0/2/2/2
29	CLA	A	815	41	-	7/15/91/115	-
29	CLA	g	323	31	-	9/27/103/115	-
29	CLA	O	201	31	-	9/24/100/115	-
29	CLA	b	306	41	-	15/39/115/115	-
31	LHG	c	320	-	-	23/53/53/53	-
31	LHG	b	318	29	-	27/53/53/53	-
29	CLA	k	605	21	-	7/15/91/115	-
29	CLA	k	614	21	-	13/23/99/115	-
29	CLA	j	309	18	-	6/15/91/115	-
38	II0	b	317	-	-	9/21/67/67	0/2/2/2
29	CLA	h	302	17	-	6/21/97/115	-
29	CLA	B	842	31	-	7/39/115/115	-
29	CLA	g	310	24	-	16/39/115/115	-
29	CLA	Q	302	-	-	21/39/115/115	-
29	CLA	m	605	18	-	7/12/88/115	-
40	KC2	g	313	-	-	8/15/71/71	-
29	CLA	B	835	2	-	3/18/94/115	-
29	CLA	e	302	19	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	g	303	24	-	7/12/88/115	-
29	CLA	i	311	-	-	13/33/109/115	-
38	II0	l	315	-	-	11/21/67/67	0/2/2/2
38	II0	m	615	-	-	12/21/67/67	0/2/2/2
31	LHG	a	301	29	-	22/53/53/53	-
29	CLA	A	830	1	-	7/33/109/115	-
29	CLA	O	206	11	-	11/39/115/115	-
38	II0	g	318	-	-	13/21/67/67	0/2/2/2
31	LHG	g	301	29	-	24/49/49/53	-
29	CLA	k	610	-	-	10/23/99/115	-
38	II0	c	314	-	-	4/21/67/67	0/2/2/2
29	CLA	n	606	26	-	5/23/99/115	-
29	CLA	j	304	18	-	7/23/99/115	-
35	SQD	A	853	-	-	19/49/69/69	0/1/1/1
29	CLA	j	313	-	-	12/23/99/115	-
29	CLA	A	832	1	-	8/39/115/115	-
40	KC2	f	611	-	-	8/15/71/71	-
37	LMG	O	205	-	-	10/21/41/70	0/1/1/1
29	CLA	A	829	1	-	8/39/115/115	-
38	II0	d	314	-	-	3/21/67/67	0/2/2/2
29	CLA	A	834	1	-	8/33/109/115	-
29	CLA	B	808	2	-	7/39/115/115	-
29	CLA	i	303	22	-	18/39/115/115	-
29	CLA	B	803	2	-	17/39/115/115	-
29	CLA	i	308	22	-	19/39/115/115	-
29	CLA	k	606	21	-	7/23/99/115	-
29	CLA	A	807	1	-	7/39/115/115	-
29	CLA	s	406	41	-	12/39/115/115	-
37	LMG	F	206	-	-	31/48/68/70	0/1/1/1
40	KC2	d	311	-	-	12/15/71/71	-
38	II0	k	618	-	-	5/21/67/67	0/2/2/2
29	CLA	a	312	15	-	8/19/95/115	-
29	CLA	A	838	1	-	11/39/115/115	-
29	CLA	f	612	41	-	12/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	402	13	-	23/39/115/115	-
32	WVN	K	103	-	-	14/29/63/63	0/2/2/2
29	CLA	k	609	21	-	10/30/106/115	-
31	LHG	A	843	29	-	6/31/31/53	-
29	CLA	A	839	1	-	3/33/109/115	-
29	CLA	b	309	37	-	5/39/115/115	-
29	CLA	e	305	19	-	10/39/115/115	-
29	CLA	m	613	18	-	17/39/115/115	-
29	CLA	e	310	41	-	9/27/103/115	-
30	PQN	A	841	-	-	10/23/43/43	0/2/2/2
32	WVN	l	302	-	-	16/29/63/63	0/2/2/2
29	CLA	g	308	24	-	7/23/99/115	-
38	II0	f	618	-	-	12/21/67/67	0/2/2/2
31	LHG	n	619	-	-	20/47/47/53	-
29	CLA	A	806	1	-	5/33/109/115	-
29	CLA	m	608	18	-	12/39/115/115	-
29	CLA	F	202	41	-	15/39/115/115	-
29	CLA	A	831	1	-	15/39/115/115	-
29	CLA	e	307	19	-	15/39/115/115	-
32	WVN	h	308	-	-	18/29/63/63	0/2/2/2
38	II0	e	316	-	-	13/21/67/67	0/2/2/2
32	WVN	B	847	-	-	14/29/63/63	0/2/2/2
31	LHG	e	317	29	-	21/41/41/53	-
29	CLA	e	304	-	-	16/39/115/115	-
38	II0	b	315	-	-	10/21/67/67	0/2/2/2
29	CLA	c	312	14	-	12/39/115/115	-
29	CLA	k	604	21	-	12/39/115/115	-
37	LMG	c	318	29	-	21/38/58/70	0/1/1/1
29	CLA	B	801	41	-	17/39/115/115	-
29	CLA	f	607	18	-	15/39/115/115	-
38	II0	f	614	-	-	11/21/67/67	0/2/2/2
40	KC2	i	318	22	-	8/15/71/71	-
29	CLA	a	306	15	-	9/15/91/115	-
29	CLA	f	610	31	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	f	601	18	-	6/18/94/115	-
38	II0	d	315	-	-	11/21/67/67	0/2/2/2
29	CLA	d	302	23	-	17/36/112/115	-
29	CLA	g	302	-	-	17/39/115/115	-
29	CLA	j	311	31	-	15/35/111/115	-
31	LHG	a	318	29	-	27/53/53/53	-
29	CLA	e	303	19	-	6/23/99/115	-
32	WVN	s	405	-	-	14/29/63/63	0/2/2/2
40	KC2	k	613	-	-	9/15/71/71	-
29	CLA	B	816	2	-	17/39/115/115	-
29	CLA	k	601	21	-	7/23/99/115	-
31	LHG	L	209	-	-	23/40/40/53	-
29	CLA	B	833	2	-	5/27/103/115	-
32	WVN	A	845	-	-	17/29/63/63	0/2/2/2
29	CLA	m	609	18	-	17/33/109/115	-
37	LMG	b	319	-	-	17/37/57/70	0/1/1/1
29	CLA	L	202	9	-	8/20/96/115	-
29	CLA	g	304	24	-	20/39/115/115	-
29	CLA	A	805	1	-	10/39/115/115	-
29	CLA	A	819	1	-	19/39/115/115	-
38	II0	m	616	-	-	11/21/67/67	0/2/2/2
32	WVN	F	204	-	-	14/29/63/63	0/2/2/2
29	CLA	B	818	41	-	14/39/115/115	-
40	KC2	j	312	18	-	8/15/71/71	-
29	CLA	A	821	1	-	6/20/96/115	-
29	CLA	e	311	19	-	18/39/115/115	-
29	CLA	A	825	41	-	6/39/115/115	-
29	CLA	f	613	18	-	16/39/115/115	-
38	II0	m	614	-	-	13/21/67/67	0/2/2/2
31	LHG	f	619	-	-	18/53/53/53	-
29	CLA	A	850	41	-	3/39/115/115	-
29	CLA	m	607	18,31	-	3/23/99/115	-
31	LHG	A	842	-	-	23/52/52/53	-
29	CLA	A	814	1	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	h	303	17,37	-	8/21/97/115	-
32	WVN	i	315	-	-	18/29/63/63	0/2/2/2
38	II0	d	316	-	-	11/21/67/67	0/2/2/2
29	CLA	n	610	-	-	16/33/109/115	-
38	II0	i	319	-	-	12/21/67/67	0/2/2/2
29	CLA	A	837	1	-	13/39/115/115	-
29	CLA	i	304	22	-	7/39/115/115	-
29	CLA	A	804	1	-	5/39/115/115	-
31	LHG	f	620	29	-	21/41/41/53	-
29	CLA	n	603	26	-	11/23/99/115	-
29	CLA	A	827	1	-	7/36/112/115	-
32	WVN	R	202	-	-	15/29/63/63	0/2/2/2
29	CLA	A	820	41	-	7/39/115/115	-
29	CLA	d	318	-	-	8/15/91/115	-
29	CLA	d	313	23	-	10/23/99/115	-
29	CLA	h	306	17	-	12/30/106/115	-
29	CLA	j	302	18,31	-	16/39/115/115	-
29	CLA	e	301	19	-	10/15/91/115	-
39	IHT	c	319	-	-	8/25/65/65	0/2/2/2
29	CLA	c	301	14	-	11/23/99/115	-
31	LHG	l	318	29	-	12/36/36/53	-
38	II0	g	321	-	-	3/21/67/67	0/2/2/2
29	CLA	A	826	1	-	9/39/115/115	-
29	CLA	B	830	2	-	7/21/97/115	-
39	IHT	c	315	-	-	6/25/65/65	0/2/2/2
29	CLA	B	832	41	-	4/15/91/115	-
38	II0	j	316	-	-	13/21/67/67	0/2/2/2
29	CLA	a	307	15	-	15/39/115/115	-
38	II0	g	319	-	-	13/21/67/67	0/2/2/2
38	II0	e	314	-	-	11/21/67/67	0/2/2/2
38	II0	l	314	-	-	11/21/67/67	0/2/2/2
38	II0	a	315	-	-	11/21/67/67	0/2/2/2
29	CLA	B	824	2	-	3/39/115/115	-
29	CLA	K	101	41	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	WVN	R	201	-	-	18/29/63/63	0/2/2/2
29	CLA	n	605	26	-	11/23/99/115	-
29	CLA	A	836	1	-	10/39/115/115	-
29	CLA	B	839	2	-	10/30/106/115	-
29	CLA	g	316	24	-	10/30/106/115	-
29	CLA	b	310	16	-	13/39/115/115	-
38	II0	n	615	-	-	12/21/67/67	0/2/2/2
32	WVN	L	206	-	-	17/29/63/63	0/2/2/2
38	II0	k	616	-	-	12/21/67/67	0/2/2/2
29	CLA	g	309	24	-	12/39/115/115	-
29	CLA	f	603	18	-	6/23/99/115	-
40	KC2	e	309	-	-	9/15/71/71	-
29	CLA	B	806	2	-	16/39/115/115	-
31	LHG	m	619	29	-	13/41/41/53	-
38	II0	O	203	-	-	4/21/67/67	0/2/2/2
29	CLA	B	831	41	-	9/39/115/115	-
29	CLA	A	813	1	-	9/29/105/115	-
29	CLA	d	305	23	-	5/23/99/115	-
29	CLA	j	314	18	-	12/39/115/115	-
38	II0	h	311	-	-	12/21/67/67	0/2/2/2
34	SF4	C	101	3	-	-	0/6/5/5
31	LHG	i	317	29	-	16/41/41/53	-
29	CLA	B	811	2	-	3/27/103/115	-
29	CLA	i	312	22	-	16/39/115/115	-
29	CLA	A	812	1	-	10/39/115/115	-
29	CLA	l	309	20	-	10/30/106/115	-
29	CLA	g	312	31	-	5/26/102/115	-
40	KC2	k	611	-	-	8/15/71/71	-
32	WVN	l	316	-	-	19/29/63/63	0/2/2/2
40	KC2	m	611	18	-	7/15/71/71	-
29	CLA	b	308	16	-	11/39/115/115	-
29	CLA	B	823	41	-	8/38/114/115	-
32	WVN	J	101	-	-	17/29/63/63	0/2/2/2
38	II0	j	315	-	-	11/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	F	203	6	-	10/24/100/115	-
31	LHG	g	322	29	-	17/41/41/53	-
40	KC2	l	311	-	-	6/15/71/71	-
29	CLA	f	604	18	-	13/39/115/115	-
40	KC2	s	401	13	-	7/15/71/71	-
29	CLA	f	605	18	-	6/15/91/115	-
32	WVN	A	847	-	-	18/29/63/63	0/2/2/2
29	CLA	l	307	20	-	7/39/115/115	-
39	IHT	m	617	-	-	2/25/65/65	0/2/2/2
38	II0	f	615	-	-	12/21/67/67	0/2/2/2
32	WVN	A	844	-	-	18/29/63/63	0/2/2/2
29	CLA	B	840	2	-	7/39/115/115	-
38	II0	d	317	-	-	13/21/67/67	0/2/2/2
29	CLA	B	815	2	-	3/27/103/115	-
29	CLA	A	808	29,1	-	10/39/115/115	-
29	CLA	B	834	2	-	11/39/115/115	-
29	CLA	l	301	20	-	11/39/115/115	-
29	CLA	A	803	29,1	-	8/27/103/115	-
29	CLA	b	304	16	-	2/24/100/115	-
29	CLA	b	307	16	-	8/35/111/115	-
40	KC2	d	312	23	-	12/15/71/71	-
29	CLA	A	835	1	-	14/39/115/115	-
29	CLA	b	312	16	-	17/39/115/115	-
29	CLA	A	809	1	-	11/29/105/115	-
29	CLA	d	306	23	-	8/23/99/115	-
40	KC2	g	314	24,40	-	10/15/71/71	-
29	CLA	a	310	15	-	11/39/115/115	-
29	CLA	j	307	18	-	5/23/99/115	-
29	CLA	b	305	16	-	15/39/115/115	-
32	WVN	F	205	-	-	21/29/63/63	0/2/2/2
29	CLA	l	305	20	-	0/23/99/115	-
29	CLA	B	819	2	-	18/39/115/115	-
29	CLA	c	305	14	-	7/39/115/115	-
36	DGD	j	319	18	-	23/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	828	2	-	10/21/97/115	-
38	II0	d	319	-	-	7/21/67/67	0/2/2/2
29	CLA	B	838	2	-	13/39/115/115	-
29	CLA	d	304	23	-	10/15/91/115	-
29	CLA	n	604	26	-	13/33/109/115	-
38	II0	h	310	-	-	11/21/67/67	0/2/2/2
29	CLA	a	302	15	-	11/39/115/115	-
29	CLA	f	606	18	-	6/23/99/115	-
38	II0	h	309	-	-	12/17/40/67	0/1/1/2
34	SF4	C	102	3	-	-	0/6/5/5
29	CLA	f	608	18	-	7/39/115/115	-
29	CLA	b	311	16	-	14/38/114/115	-
29	CLA	j	305	18	-	12/39/115/115	-
29	CLA	h	304	17	-	6/23/99/115	-
29	CLA	c	306	14	-	9/24/100/115	-
38	II0	d	301	-	-	14/21/67/67	0/2/2/2
29	CLA	k	607	21	-	8/23/99/115	-
38	II0	c	313	-	-	12/21/67/67	0/2/2/2
38	II0	a	313	-	-	12/21/67/67	0/2/2/2
32	WVN	A	846	-	-	15/29/63/63	0/2/2/2
29	CLA	f	602	18	-	18/39/115/115	-
29	CLA	A	818	1	-	15/39/115/115	-
29	CLA	a	305	41	-	8/39/115/115	-
29	CLA	B	817	2	-	13/39/115/115	-

All (4074) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	615	II0	C14-C10	20.53	1.57	1.34
38	g	317	II0	C13-C09	20.15	1.57	1.34
38	l	315	II0	C13-C09	20.10	1.57	1.34
38	d	315	II0	C14-C10	19.87	1.57	1.34
38	e	314	II0	C13-C09	19.81	1.57	1.34
38	h	311	II0	C13-C09	19.74	1.56	1.34
38	a	313	II0	C13-C09	19.69	1.56	1.34
38	h	309	II0	C13-C09	19.61	1.56	1.34
38	f	616	II0	C13-C09	19.58	1.56	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	b	301	II0	C14-C10	19.57	1.56	1.34
38	a	314	II0	C13-C09	19.55	1.56	1.34
38	i	314	II0	C14-C10	19.48	1.56	1.34
38	n	618	II0	C13-C09	19.41	1.56	1.34
38	m	614	II0	C13-C09	19.39	1.56	1.34
38	d	317	II0	C14-C10	19.36	1.56	1.34
38	f	615	II0	C14-C10	19.33	1.56	1.34
38	n	615	II0	C13-C09	19.29	1.56	1.34
38	i	314	II0	C13-C09	19.29	1.56	1.34
38	m	615	II0	C14-C10	19.20	1.56	1.34
38	f	618	II0	C13-C09	19.15	1.56	1.34
38	j	316	II0	C14-C10	19.13	1.56	1.34
38	d	316	II0	C14-C10	19.13	1.56	1.34
38	k	616	II0	C14-C10	19.12	1.56	1.34
38	n	616	II0	C14-C10	19.11	1.56	1.34
38	m	618	II0	C13-C09	19.07	1.56	1.34
38	g	318	II0	C14-C10	19.06	1.56	1.34
38	m	618	II0	C14-C10	19.05	1.56	1.34
38	f	618	II0	C14-C10	18.98	1.56	1.34
38	l	314	II0	C14-C10	18.96	1.56	1.34
38	m	616	II0	C14-C10	18.94	1.56	1.34
38	n	618	II0	C14-C10	18.94	1.56	1.34
38	a	317	II0	C13-C09	18.90	1.56	1.34
38	i	313	II0	C14-C10	18.87	1.56	1.34
38	m	614	II0	C14-C10	18.87	1.55	1.34
38	m	615	II0	C13-C09	18.85	1.55	1.34
38	d	316	II0	C13-C09	18.84	1.55	1.34
38	l	315	II0	C14-C10	18.83	1.55	1.34
38	a	317	II0	C14-C10	18.79	1.55	1.34
38	j	315	II0	C13-C09	18.79	1.55	1.34
38	g	317	II0	C14-C10	18.77	1.55	1.34
38	j	301	II0	C14-C10	18.69	1.55	1.34
38	j	301	II0	C13-C09	18.65	1.55	1.34
38	e	312	II0	C13-C09	18.58	1.55	1.34
38	i	319	II0	C13-C09	18.57	1.55	1.34
38	m	616	II0	C13-C09	18.56	1.55	1.34
38	e	314	II0	C14-C10	18.53	1.55	1.34
38	d	315	II0	C13-C09	18.51	1.55	1.34
38	i	316	II0	C14-C10	18.50	1.55	1.34
38	b	301	II0	C13-C09	18.49	1.55	1.34
38	f	614	II0	C14-C10	18.40	1.55	1.34
38	l	313	II0	C14-C10	18.38	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	e	313	II0	C14-C10	18.36	1.55	1.34
38	c	313	II0	C14-C10	18.35	1.55	1.34
38	d	301	II0	C14-C10	18.30	1.55	1.34
38	k	616	II0	C13-C09	18.15	1.55	1.34
38	a	315	II0	C14-C10	18.12	1.55	1.34
38	k	619	II0	C13-C09	18.07	1.55	1.34
38	c	313	II0	C13-C09	17.95	1.54	1.34
38	i	316	II0	C13-C09	17.91	1.54	1.34
38	i	319	II0	C14-C10	17.79	1.54	1.34
38	h	310	II0	C13-C09	17.76	1.54	1.34
38	l	314	II0	C13-C09	17.74	1.54	1.34
38	d	301	II0	C13-C09	17.68	1.54	1.34
38	k	619	II0	C14-C10	17.65	1.54	1.34
38	b	314	II0	C13-C09	17.61	1.54	1.34
38	f	614	II0	C13-C09	17.59	1.54	1.34
38	f	615	II0	C13-C09	17.55	1.54	1.34
38	k	620	II0	C14-C10	17.55	1.54	1.34
38	b	315	II0	C13-C09	17.54	1.54	1.34
38	g	318	II0	C13-C09	17.53	1.54	1.34
38	h	311	II0	C14-C10	17.52	1.54	1.34
38	g	319	II0	C13-C09	17.51	1.54	1.34
38	n	616	II0	C13-C09	17.51	1.54	1.34
38	J	103	II0	C13-C09	17.50	1.54	1.34
38	e	313	II0	C13-C09	17.48	1.54	1.34
38	k	615	II0	C13-C09	17.44	1.54	1.34
38	i	313	II0	C13-C09	17.43	1.54	1.34
38	k	620	II0	C13-C09	17.41	1.54	1.34
38	l	313	II0	C13-C09	17.40	1.54	1.34
38	d	317	II0	C13-C09	17.39	1.54	1.34
38	n	615	II0	C14-C10	17.36	1.54	1.34
38	b	315	II0	C14-C10	17.33	1.54	1.34
38	j	316	II0	C13-C09	17.28	1.54	1.34
38	a	315	II0	C13-C09	17.21	1.54	1.34
38	j	315	II0	C14-C10	17.20	1.54	1.34
38	J	103	II0	C14-C10	17.16	1.54	1.34
38	b	314	II0	C14-C10	17.16	1.54	1.34
38	a	314	II0	C14-C10	17.13	1.54	1.34
38	g	319	II0	C14-C10	17.12	1.54	1.34
38	h	310	II0	C14-C10	17.09	1.54	1.34
38	f	616	II0	C14-C10	17.08	1.54	1.34
38	e	312	II0	C14-C10	17.06	1.53	1.34
38	a	313	II0	C14-C10	17.04	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	315	WVN	C26-C22	15.44	1.56	1.35
32	M	101	WVN	C26-C22	15.43	1.56	1.35
32	A	847	WVN	C26-C22	15.39	1.56	1.35
32	h	308	WVN	C26-C22	15.36	1.56	1.35
32	L	205	WVN	C26-C22	15.23	1.56	1.35
32	l	316	WVN	C26-C22	15.17	1.55	1.35
32	s	407	WVN	C26-C22	15.10	1.55	1.35
32	i	315	WVN	C26-C22	15.06	1.55	1.35
38	i	314	II0	C40-C36	15.02	1.55	1.35
32	A	844	WVN	C26-C22	15.00	1.55	1.35
32	L	201	WVN	C26-C22	14.97	1.55	1.35
32	s	405	WVN	C26-C22	14.96	1.55	1.35
38	a	314	II0	C40-C36	14.89	1.55	1.35
32	J	101	WVN	C26-C22	14.88	1.55	1.35
38	l	314	II0	C40-C36	14.85	1.55	1.35
32	A	854	WVN	C26-C22	14.85	1.55	1.35
32	B	849	WVN	C26-C22	14.85	1.55	1.35
32	B	847	WVN	C26-C22	14.84	1.55	1.35
32	R	202	WVN	C26-C22	14.82	1.55	1.35
32	K	103	WVN	C26-C22	14.81	1.55	1.35
32	l	302	WVN	C26-C22	14.77	1.55	1.35
32	R	201	WVN	C26-C22	14.77	1.55	1.35
32	I	101	WVN	C26-C22	14.75	1.55	1.35
32	B	848	WVN	C26-C22	14.71	1.55	1.35
32	A	846	WVN	C26-C22	14.68	1.55	1.35
38	d	317	II0	C40-C36	14.60	1.55	1.35
32	F	207	WVN	C26-C22	14.58	1.55	1.35
32	L	206	WVN	C26-C22	14.55	1.55	1.35
32	A	845	WVN	C26-C22	14.55	1.55	1.35
38	i	319	II0	C40-C36	14.54	1.55	1.35
38	k	616	II0	C40-C36	14.46	1.55	1.35
32	l	316	WVN	C37-C34	14.43	1.54	1.35
32	F	204	WVN	C26-C22	14.43	1.54	1.35
38	g	318	II0	C40-C36	14.42	1.54	1.35
38	e	313	II0	C40-C36	14.40	1.54	1.35
38	d	315	II0	C40-C36	14.38	1.54	1.35
38	l	313	II0	C40-C36	14.35	1.54	1.35
38	c	313	II0	C40-C36	14.32	1.54	1.35
38	m	615	II0	C40-C36	14.32	1.54	1.35
32	B	846	WVN	C26-C22	14.32	1.54	1.35
38	m	618	II0	C40-C36	14.31	1.54	1.35
38	i	313	II0	C40-C36	14.29	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	f	614	II0	C40-C36	14.27	1.54	1.35
38	h	309	II0	C40-C36	14.27	1.54	1.35
38	f	616	II0	C40-C36	14.25	1.54	1.35
38	e	312	II0	C40-C36	14.22	1.54	1.35
38	m	616	II0	C40-C36	14.21	1.54	1.35
38	n	618	II0	C40-C36	14.20	1.54	1.35
32	s	407	WVN	C37-C34	14.19	1.54	1.35
38	g	317	II0	C40-C36	14.18	1.54	1.35
32	A	847	WVN	C37-C34	14.18	1.54	1.35
32	R	202	WVN	C37-C34	14.16	1.54	1.35
38	J	103	II0	C40-C36	14.16	1.54	1.35
38	j	316	II0	C40-C36	14.16	1.54	1.35
38	a	313	II0	C40-C36	14.16	1.54	1.35
38	f	615	II0	C40-C36	14.15	1.54	1.35
38	i	316	II0	C40-C36	14.13	1.54	1.35
32	e	315	WVN	C37-C34	14.12	1.54	1.35
38	l	314	II0	C39-C35	14.11	1.54	1.35
32	B	846	WVN	C37-C34	14.11	1.54	1.35
38	b	315	II0	C40-C36	14.10	1.54	1.35
38	n	616	II0	C40-C36	14.10	1.54	1.35
32	M	101	WVN	C37-C34	14.09	1.54	1.35
38	g	319	II0	C40-C36	14.09	1.54	1.35
32	A	846	WVN	C37-C34	14.09	1.54	1.35
32	F	207	WVN	C36-C32	14.08	1.54	1.35
32	I	101	WVN	C37-C34	14.08	1.54	1.35
32	L	201	WVN	C37-C34	14.08	1.54	1.35
32	A	854	WVN	C37-C34	14.07	1.54	1.35
32	F	204	WVN	C36-C32	14.07	1.54	1.35
38	a	317	II0	C40-C36	14.06	1.54	1.35
32	R	202	WVN	C36-C32	14.05	1.54	1.35
32	e	315	WVN	C36-C32	14.05	1.54	1.35
32	K	103	WVN	C37-C34	14.04	1.54	1.35
38	b	301	II0	C40-C36	14.03	1.54	1.35
38	n	615	II0	C40-C36	14.02	1.54	1.35
32	l	316	WVN	C36-C32	14.00	1.54	1.35
32	s	405	WVN	C37-C34	13.99	1.54	1.35
38	l	315	II0	C40-C36	13.98	1.54	1.35
38	a	315	II0	C40-C36	13.98	1.54	1.35
38	b	314	II0	C40-C36	13.98	1.54	1.35
38	f	618	II0	C40-C36	13.98	1.54	1.35
38	k	620	II0	C40-C36	13.98	1.54	1.35
32	J	101	WVN	C37-C34	13.96	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	207	WVN	C37-C34	13.96	1.54	1.35
38	h	311	II0	C40-C36	13.96	1.54	1.35
32	A	847	WVN	C36-C32	13.96	1.54	1.35
38	e	314	II0	C40-C36	13.95	1.54	1.35
32	M	101	WVN	C36-C32	13.95	1.54	1.35
32	A	846	WVN	C28-C25	13.90	1.54	1.35
32	h	308	WVN	C37-C34	13.90	1.54	1.35
38	d	316	II0	C40-C36	13.89	1.54	1.35
32	l	316	WVN	C28-C25	13.88	1.54	1.35
38	k	615	II0	C40-C36	13.88	1.54	1.35
38	j	301	II0	C40-C36	13.87	1.54	1.35
32	L	205	WVN	C37-C34	13.87	1.54	1.35
32	A	854	WVN	C36-C32	13.86	1.54	1.35
38	h	310	II0	C40-C36	13.86	1.54	1.35
32	B	846	WVN	C28-C25	13.85	1.54	1.35
38	j	315	II0	C40-C36	13.84	1.54	1.35
32	B	847	WVN	C37-C34	13.84	1.54	1.35
32	L	205	WVN	C36-C32	13.83	1.54	1.35
32	A	844	WVN	C37-C34	13.83	1.54	1.35
38	m	614	II0	C40-C36	13.83	1.54	1.35
32	i	315	WVN	C36-C32	13.81	1.54	1.35
32	s	405	WVN	C36-C32	13.81	1.54	1.35
38	a	314	II0	C39-C35	13.81	1.54	1.35
32	F	204	WVN	C37-C34	13.80	1.54	1.35
32	i	315	WVN	C37-C34	13.80	1.54	1.35
32	F	205	WVN	C37-C34	13.79	1.54	1.35
32	A	845	WVN	C37-C34	13.79	1.54	1.35
32	l	302	WVN	C37-C34	13.79	1.54	1.35
32	A	844	WVN	C36-C32	13.78	1.54	1.35
32	B	849	WVN	C37-C34	13.77	1.54	1.35
32	I	101	WVN	C36-C32	13.77	1.54	1.35
38	g	318	II0	C39-C35	13.77	1.54	1.35
38	d	316	II0	C39-C35	13.76	1.54	1.35
32	R	201	WVN	C36-C32	13.75	1.54	1.35
32	h	308	WVN	C36-C32	13.74	1.54	1.35
38	k	619	II0	C40-C36	13.73	1.54	1.35
38	m	615	II0	C39-C35	13.73	1.54	1.35
38	j	316	II0	C39-C35	13.73	1.54	1.35
32	B	848	WVN	C36-C32	13.72	1.54	1.35
38	b	315	II0	C39-C35	13.72	1.54	1.35
32	A	845	WVN	C36-C32	13.70	1.53	1.35
32	l	302	WVN	C28-C25	13.69	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	206	WVN	C37-C34	13.69	1.53	1.35
32	R	201	WVN	C37-C34	13.69	1.53	1.35
32	A	846	WVN	C36-C32	13.68	1.53	1.35
38	f	615	II0	C39-C35	13.67	1.53	1.35
32	R	202	WVN	C28-C25	13.67	1.53	1.35
38	i	314	II0	C39-C35	13.67	1.53	1.35
32	s	407	WVN	C36-C32	13.67	1.53	1.35
32	K	103	WVN	C36-C32	13.66	1.53	1.35
32	I	101	WVN	C28-C25	13.65	1.53	1.35
32	F	205	WVN	C36-C32	13.64	1.53	1.35
32	B	849	WVN	C36-C32	13.63	1.53	1.35
32	i	315	WVN	C28-C25	13.62	1.53	1.35
32	L	201	WVN	C36-C32	13.61	1.53	1.35
32	B	847	WVN	C28-C25	13.59	1.53	1.35
32	L	201	WVN	C28-C25	13.58	1.53	1.35
38	c	313	II0	C39-C35	13.58	1.53	1.35
32	A	847	WVN	C28-C25	13.58	1.53	1.35
32	B	848	WVN	C37-C34	13.57	1.53	1.35
32	B	847	WVN	C36-C32	13.57	1.53	1.35
38	k	616	II0	C39-C35	13.57	1.53	1.35
38	d	301	II0	C40-C36	13.56	1.53	1.35
38	a	313	II0	C39-C35	13.55	1.53	1.35
32	s	407	WVN	C28-C25	13.54	1.53	1.35
32	h	308	WVN	C28-C25	13.53	1.53	1.35
32	J	101	WVN	C36-C32	13.52	1.53	1.35
38	m	614	II0	C39-C35	13.52	1.53	1.35
38	n	615	II0	C39-C35	13.51	1.53	1.35
32	F	205	WVN	C28-C25	13.51	1.53	1.35
38	b	314	II0	C39-C35	13.50	1.53	1.35
38	m	616	II0	C39-C35	13.50	1.53	1.35
38	e	312	II0	C39-C35	13.47	1.53	1.35
38	f	614	II0	C39-C35	13.47	1.53	1.35
38	f	618	II0	C39-C35	13.47	1.53	1.35
32	A	844	WVN	C28-C25	13.46	1.53	1.35
32	l	302	WVN	C36-C32	13.46	1.53	1.35
32	A	854	WVN	C28-C25	13.46	1.53	1.35
32	F	207	WVN	C28-C25	13.44	1.53	1.35
38	e	313	II0	C39-C35	13.44	1.53	1.35
38	i	319	II0	C39-C35	13.43	1.53	1.35
32	F	205	WVN	C26-C22	13.42	1.53	1.35
38	J	103	II0	C39-C35	13.42	1.53	1.35
38	d	317	II0	C39-C35	13.41	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	620	II0	C39-C35	13.39	1.53	1.35
32	J	101	WVN	C28-C25	13.39	1.53	1.35
32	s	405	WVN	C28-C25	13.39	1.53	1.35
38	l	315	II0	C39-C35	13.39	1.53	1.35
38	a	317	II0	C39-C35	13.38	1.53	1.35
38	f	616	II0	C39-C35	13.37	1.53	1.35
32	B	849	WVN	C28-C25	13.35	1.53	1.35
38	g	317	II0	C39-C35	13.35	1.53	1.35
32	e	315	WVN	C28-C25	13.34	1.53	1.35
38	g	319	II0	C39-C35	13.33	1.53	1.35
38	l	313	II0	C39-C35	13.32	1.53	1.35
38	e	314	II0	C39-C35	13.32	1.53	1.35
38	k	619	II0	C39-C35	13.32	1.53	1.35
32	A	844	WVN	C15-C13	13.31	1.57	1.34
32	L	206	WVN	C36-C32	13.31	1.53	1.35
32	B	846	WVN	C36-C32	13.30	1.53	1.35
38	n	618	II0	C39-C35	13.30	1.53	1.35
38	m	618	II0	C39-C35	13.29	1.53	1.35
38	d	315	II0	C39-C35	13.29	1.53	1.35
32	M	101	WVN	C28-C25	13.28	1.53	1.35
38	i	313	II0	C39-C35	13.27	1.53	1.35
32	A	845	WVN	C28-C25	13.27	1.53	1.35
32	L	205	WVN	C28-C25	13.25	1.53	1.35
38	b	301	II0	C39-C35	13.25	1.53	1.35
38	k	615	II0	C39-C35	13.24	1.53	1.35
38	n	616	II0	C39-C35	13.22	1.53	1.35
32	K	103	WVN	C28-C25	13.22	1.53	1.35
38	j	301	II0	C39-C35	13.20	1.53	1.35
38	h	311	II0	C39-C35	13.20	1.53	1.35
38	j	315	II0	C39-C35	13.18	1.53	1.35
38	h	310	II0	C39-C35	13.15	1.53	1.35
32	R	201	WVN	C28-C25	13.12	1.53	1.35
32	B	848	WVN	C28-C25	13.10	1.53	1.35
32	F	204	WVN	C28-C25	13.09	1.53	1.35
38	d	301	II0	C39-C35	13.07	1.53	1.35
32	L	206	WVN	C28-C25	13.07	1.53	1.35
38	a	315	II0	C39-C35	13.06	1.53	1.35
38	i	316	II0	C39-C35	13.03	1.53	1.35
32	B	849	WVN	C15-C13	12.88	1.56	1.34
32	F	207	WVN	C15-C13	12.83	1.56	1.34
38	h	309	II0	C39-C35	12.82	1.52	1.35
32	L	201	WVN	C15-C13	12.80	1.56	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	315	WVN	C15-C13	12.61	1.56	1.34
32	h	308	WVN	C15-C13	12.59	1.56	1.34
32	B	847	WVN	C15-C13	12.49	1.56	1.34
32	A	847	WVN	C15-C13	12.48	1.56	1.34
32	A	854	WVN	C15-C13	12.46	1.56	1.34
32	l	302	WVN	C15-C13	12.36	1.55	1.34
32	M	101	WVN	C15-C13	12.36	1.55	1.34
32	R	202	WVN	C15-C13	12.24	1.55	1.34
32	L	205	WVN	C15-C13	12.23	1.55	1.34
32	l	316	WVN	C15-C13	12.20	1.55	1.34
32	B	846	WVN	C15-C13	12.17	1.55	1.34
32	s	407	WVN	C15-C13	12.16	1.55	1.34
32	A	845	WVN	C15-C13	12.10	1.55	1.34
32	R	201	WVN	C15-C13	12.08	1.55	1.34
32	J	101	WVN	C15-C13	12.04	1.55	1.34
32	L	206	WVN	C15-C13	12.01	1.55	1.34
32	B	848	WVN	C15-C13	11.95	1.55	1.34
32	s	405	WVN	C15-C13	11.95	1.55	1.34
32	A	846	WVN	C15-C13	11.91	1.55	1.34
32	e	315	WVN	C15-C13	11.90	1.55	1.34
32	K	103	WVN	C15-C13	11.70	1.54	1.34
32	F	204	WVN	C15-C13	11.57	1.54	1.34
32	R	201	WVN	C09-C05	11.55	1.55	1.32
32	L	206	WVN	C09-C05	11.54	1.55	1.32
32	J	101	WVN	C09-C05	11.41	1.55	1.32
32	I	101	WVN	C09-C05	11.40	1.55	1.32
32	L	205	WVN	C09-C05	11.38	1.55	1.32
32	F	207	WVN	C09-C05	11.34	1.55	1.32
32	F	204	WVN	C09-C05	11.32	1.55	1.32
32	l	316	WVN	C09-C05	11.32	1.55	1.32
32	A	844	WVN	C09-C05	11.30	1.55	1.32
32	K	103	WVN	C09-C05	11.28	1.54	1.32
32	A	847	WVN	C09-C05	11.27	1.54	1.32
32	B	848	WVN	C09-C05	11.27	1.54	1.32
32	l	302	WVN	C09-C05	11.26	1.54	1.32
32	B	849	WVN	C09-C05	11.26	1.54	1.32
32	h	308	WVN	C09-C05	11.24	1.54	1.32
32	I	101	WVN	C15-C13	11.22	1.53	1.34
32	s	405	WVN	C09-C05	11.21	1.54	1.32
32	i	315	WVN	C09-C05	11.20	1.54	1.32
32	M	101	WVN	C09-C05	11.09	1.54	1.32
32	B	847	WVN	C09-C05	11.07	1.54	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	846	WVN	C09-C05	11.05	1.54	1.32
32	e	315	WVN	C09-C05	11.01	1.54	1.32
32	s	407	WVN	C09-C05	10.99	1.54	1.32
32	A	845	WVN	C09-C05	10.99	1.54	1.32
32	A	854	WVN	C09-C05	10.96	1.54	1.32
32	R	202	WVN	C09-C05	10.91	1.54	1.32
32	F	205	WVN	C15-C13	10.90	1.53	1.34
32	L	201	WVN	C09-C05	10.87	1.54	1.32
32	F	205	WVN	C09-C05	10.59	1.53	1.32
32	A	846	WVN	C09-C05	10.50	1.53	1.32
38	l	314	II0	C29-C25	8.79	1.55	1.37
38	k	619	II0	C29-C25	8.74	1.55	1.37
38	i	314	II0	C29-C25	8.74	1.55	1.37
38	l	314	II0	C30-C26	8.70	1.55	1.37
38	n	618	II0	C29-C25	8.69	1.55	1.37
38	a	314	II0	C29-C25	8.64	1.55	1.37
38	i	319	II0	C29-C25	8.64	1.55	1.37
38	l	313	II0	C29-C25	8.63	1.55	1.37
38	d	317	II0	C29-C25	8.63	1.55	1.37
38	m	616	II0	C29-C25	8.62	1.55	1.37
38	g	317	II0	C29-C25	8.62	1.55	1.37
38	f	615	II0	C29-C25	8.62	1.55	1.37
38	l	313	II0	C30-C26	8.61	1.55	1.37
40	s	404	KC2	C2A-C3A	8.61	1.54	1.37
38	e	314	II0	C29-C25	8.59	1.55	1.37
38	n	615	II0	C29-C25	8.59	1.55	1.37
38	i	316	II0	C29-C25	8.58	1.55	1.37
38	j	315	II0	C29-C25	8.57	1.55	1.37
38	f	616	II0	C21-C09	8.57	1.60	1.42
38	m	614	II0	C29-C25	8.55	1.55	1.37
38	c	313	II0	C29-C25	8.55	1.55	1.37
38	l	315	II0	C29-C25	8.55	1.54	1.37
38	f	618	II0	C29-C25	8.53	1.54	1.37
38	g	318	II0	C29-C25	8.53	1.54	1.37
38	h	310	II0	C29-C25	8.52	1.54	1.37
40	g	314	KC2	C2A-C3A	8.51	1.54	1.37
38	j	316	II0	C29-C25	8.51	1.54	1.37
38	a	313	II0	C29-C25	8.50	1.54	1.37
38	k	616	II0	C29-C25	8.50	1.54	1.37
38	m	618	II0	C29-C25	8.49	1.54	1.37
38	f	614	II0	C29-C25	8.47	1.54	1.37
38	d	317	II0	C30-C26	8.46	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	m	615	II0	C29-C25	8.45	1.54	1.37
38	m	618	II0	C30-C26	8.45	1.54	1.37
38	f	618	II0	C30-C26	8.45	1.54	1.37
38	d	315	II0	C30-C26	8.43	1.54	1.37
38	m	615	II0	C30-C26	8.43	1.54	1.37
38	a	317	II0	C29-C25	8.41	1.54	1.37
38	k	615	II0	C30-C26	8.41	1.54	1.37
38	b	301	II0	C30-C26	8.41	1.54	1.37
38	f	615	II0	C30-C26	8.41	1.54	1.37
38	k	619	II0	C30-C26	8.41	1.54	1.37
38	e	312	II0	C30-C26	8.40	1.54	1.37
38	j	316	II0	C30-C26	8.40	1.54	1.37
38	m	616	II0	C30-C26	8.40	1.54	1.37
38	f	614	II0	C30-C26	8.39	1.54	1.37
38	n	616	II0	C30-C26	8.38	1.54	1.37
38	g	319	II0	C30-C26	8.38	1.54	1.37
38	c	313	II0	C30-C26	8.36	1.54	1.37
38	j	301	II0	C29-C25	8.36	1.54	1.37
38	d	315	II0	C29-C25	8.36	1.54	1.37
38	g	319	II0	C29-C25	8.35	1.54	1.37
38	a	315	II0	C29-C25	8.35	1.54	1.37
30	B	843	PQN	C12-C13	8.35	1.53	1.33
30	A	841	PQN	C12-C13	8.34	1.53	1.33
38	J	103	II0	C29-C25	8.34	1.54	1.37
38	b	315	II0	C29-C25	8.34	1.54	1.37
38	h	311	II0	C30-C26	8.33	1.54	1.37
38	a	315	II0	C30-C26	8.33	1.54	1.37
38	i	313	II0	C30-C26	8.33	1.54	1.37
38	i	319	II0	C30-C26	8.33	1.54	1.37
38	m	614	II0	C30-C26	8.33	1.54	1.37
38	g	317	II0	C30-C26	8.32	1.54	1.37
38	b	314	II0	C30-C26	8.32	1.54	1.37
38	n	615	II0	C30-C26	8.31	1.54	1.37
38	d	316	II0	C30-C26	8.30	1.54	1.37
38	i	313	II0	C29-C25	8.30	1.54	1.37
38	a	317	II0	C30-C26	8.30	1.54	1.37
38	f	616	II0	C30-C26	8.30	1.54	1.37
38	g	318	II0	C30-C26	8.30	1.54	1.37
38	l	315	II0	C21-C09	8.28	1.59	1.42
38	J	103	II0	C30-C26	8.27	1.54	1.37
38	k	620	II0	C29-C25	8.27	1.54	1.37
38	b	314	II0	C29-C25	8.27	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	620	II0	C30-C26	8.27	1.54	1.37
38	h	311	II0	C29-C25	8.26	1.54	1.37
38	i	316	II0	C30-C26	8.26	1.54	1.37
38	n	618	II0	C30-C26	8.25	1.54	1.37
38	d	316	II0	C29-C25	8.25	1.54	1.37
38	b	315	II0	C30-C26	8.25	1.54	1.37
38	l	315	II0	C30-C26	8.24	1.54	1.37
38	a	314	II0	C30-C26	8.23	1.54	1.37
38	i	314	II0	C30-C26	8.22	1.54	1.37
38	n	616	II0	C29-C25	8.21	1.54	1.37
38	e	314	II0	C30-C26	8.21	1.54	1.37
38	h	310	II0	C30-C26	8.21	1.54	1.37
38	j	301	II0	C30-C26	8.20	1.54	1.37
38	d	301	II0	C30-C26	8.19	1.54	1.37
38	k	616	II0	C30-C26	8.17	1.54	1.37
38	b	301	II0	C29-C25	8.17	1.54	1.37
38	a	313	II0	C30-C26	8.16	1.54	1.37
38	e	312	II0	C29-C25	8.15	1.54	1.37
38	j	315	II0	C30-C26	8.14	1.54	1.37
38	e	313	II0	C30-C26	8.13	1.54	1.37
38	k	615	II0	C29-C25	8.11	1.54	1.37
40	l	311	KC2	C2A-C3A	8.10	1.53	1.37
38	f	616	II0	C29-C25	8.08	1.54	1.37
38	d	301	II0	C29-C25	8.08	1.54	1.37
38	e	313	II0	C29-C25	8.08	1.53	1.37
38	k	615	II0	C22-C10	8.07	1.59	1.42
40	k	611	KC2	C2A-C3A	8.07	1.53	1.37
38	h	309	II0	C29-C25	8.05	1.53	1.37
30	B	843	PQN	O1-C1	7.94	1.40	1.23
38	d	315	II0	C22-C10	7.89	1.59	1.42
40	i	318	KC2	C2A-C3A	7.88	1.53	1.37
30	B	843	PQN	O4-C4	7.84	1.39	1.23
40	n	611	KC2	C2A-C3A	7.83	1.53	1.37
30	A	841	PQN	O4-C4	7.83	1.39	1.23
30	A	841	PQN	O1-C1	7.82	1.39	1.23
40	d	311	KC2	C2A-C3A	7.60	1.52	1.37
40	g	313	KC2	C2A-C3A	7.59	1.52	1.37
38	k	616	II0	C21-C09	7.52	1.58	1.42
40	j	312	KC2	C2A-C3A	7.50	1.52	1.37
40	i	310	KC2	C2A-C3A	7.47	1.52	1.37
38	i	319	II0	C22-C10	7.43	1.58	1.42
40	m	611	KC2	C2A-C3A	7.43	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	e	309	KC2	C2A-C3A	7.41	1.52	1.37
40	g	315	KC2	C2A-C3A	7.40	1.52	1.37
38	b	315	II0	C22-C10	7.32	1.57	1.42
40	f	611	KC2	C2A-C3A	7.24	1.51	1.37
38	i	314	II0	C22-C10	7.21	1.57	1.42
38	m	618	II0	C22-C10	7.20	1.57	1.42
32	i	315	WVN	C02-C11	7.20	1.60	1.50
38	i	314	II0	C21-C09	7.19	1.57	1.42
38	d	317	II0	C22-C10	7.18	1.57	1.42
38	e	313	II0	C22-C10	7.12	1.57	1.42
38	g	318	II0	C22-C10	7.08	1.57	1.42
38	b	301	II0	C22-C10	7.08	1.57	1.42
38	n	618	II0	C22-C10	7.07	1.57	1.42
38	k	616	II0	C22-C10	7.07	1.57	1.42
32	l	316	WVN	C02-C11	7.06	1.60	1.50
38	j	301	II0	C22-C10	7.03	1.57	1.42
38	m	615	II0	C22-C10	7.02	1.57	1.42
38	g	317	II0	C21-C09	7.02	1.57	1.42
38	l	315	II0	C22-C10	7.01	1.57	1.42
38	l	313	II0	C22-C10	7.00	1.57	1.42
38	f	618	II0	C22-C10	6.98	1.57	1.42
38	d	316	II0	C22-C10	6.98	1.57	1.42
32	I	101	WVN	C02-C11	6.98	1.60	1.50
32	A	844	WVN	C02-C11	6.94	1.60	1.50
38	l	314	II0	C24-C26	6.91	1.55	1.42
38	n	616	II0	C22-C10	6.89	1.56	1.42
40	c	310	KC2	C2A-C3A	6.89	1.51	1.37
38	i	313	II0	C22-C10	6.88	1.56	1.42
38	g	317	II0	C22-C10	6.87	1.56	1.42
38	f	615	II0	C22-C10	6.87	1.56	1.42
38	e	314	II0	C22-C10	6.86	1.56	1.42
38	a	317	II0	C22-C10	6.86	1.56	1.42
32	h	308	WVN	C02-C11	6.86	1.60	1.50
38	e	314	II0	C21-C09	6.85	1.56	1.42
38	m	616	II0	C22-C10	6.84	1.56	1.42
38	m	618	II0	C21-C09	6.83	1.56	1.42
38	a	315	II0	C22-C10	6.83	1.56	1.42
40	s	401	KC2	C2A-C3A	6.83	1.51	1.37
38	j	316	II0	C22-C10	6.83	1.56	1.42
38	d	301	II0	C22-C10	6.81	1.56	1.42
38	l	314	II0	C22-C10	6.80	1.56	1.42
32	A	847	WVN	C02-C11	6.80	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	m	614	II0	C22-C10	6.80	1.56	1.42
38	l	313	II0	C24-C26	6.79	1.55	1.42
38	h	311	II0	C24-C26	6.79	1.55	1.42
38	f	618	II0	C21-C09	6.79	1.56	1.42
38	m	618	II0	C24-C26	6.75	1.55	1.42
38	c	313	II0	C22-C10	6.75	1.56	1.42
32	e	315	WVN	C02-C11	6.73	1.60	1.50
38	f	614	II0	C22-C10	6.73	1.56	1.42
38	e	313	II0	C24-C26	6.71	1.55	1.42
38	b	315	II0	C24-C26	6.69	1.55	1.42
38	a	313	II0	C21-C09	6.68	1.56	1.42
38	n	618	II0	C21-C09	6.67	1.56	1.42
38	k	619	II0	C22-C10	6.67	1.56	1.42
38	h	311	II0	C22-C10	6.67	1.56	1.42
38	a	314	II0	C24-C26	6.67	1.55	1.42
32	A	845	WVN	C02-C11	6.67	1.60	1.50
38	n	615	II0	C21-C09	6.66	1.56	1.42
38	j	301	II0	C21-C09	6.65	1.56	1.42
32	s	407	WVN	C02-C11	6.65	1.60	1.50
38	i	319	II0	C21-C09	6.65	1.56	1.42
38	d	317	II0	C24-C26	6.65	1.55	1.42
38	i	319	II0	C24-C26	6.64	1.55	1.42
32	M	101	WVN	C02-C11	6.64	1.60	1.50
38	f	616	II0	C22-C10	6.62	1.56	1.42
38	m	614	II0	C21-C09	6.61	1.56	1.42
38	i	316	II0	C22-C10	6.61	1.56	1.42
38	k	620	II0	C22-C10	6.60	1.56	1.42
38	n	615	II0	C22-C10	6.60	1.56	1.42
40	i	318	KC2	CBA-CAA	6.60	1.53	1.33
38	h	310	II0	C22-C10	6.60	1.56	1.42
38	n	618	II0	C24-C26	6.60	1.55	1.42
38	i	314	II0	C24-C26	6.59	1.55	1.42
38	j	315	II0	C22-C10	6.59	1.56	1.42
40	i	310	KC2	CBA-CAA	6.59	1.53	1.33
40	g	314	KC2	CBA-CAA	6.58	1.53	1.33
38	h	309	II0	C21-C09	6.58	1.56	1.42
38	a	314	II0	C22-C10	6.58	1.56	1.42
32	R	202	WVN	C02-C11	6.57	1.59	1.50
38	m	616	II0	C21-C09	6.57	1.56	1.42
38	h	311	II0	C21-C09	6.57	1.56	1.42
38	a	314	II0	C21-C09	6.57	1.56	1.42
32	K	103	WVN	C02-C11	6.56	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	m	614	II0	C24-C26	6.56	1.55	1.42
38	a	317	II0	C21-C09	6.56	1.56	1.42
38	k	616	II0	C24-C26	6.55	1.55	1.42
38	f	614	II0	C24-C26	6.55	1.55	1.42
38	e	312	II0	C22-C10	6.55	1.56	1.42
38	b	301	II0	C24-C26	6.55	1.55	1.42
38	d	316	II0	C24-C26	6.54	1.55	1.42
38	i	316	II0	C21-C09	6.54	1.56	1.42
38	d	316	II0	C21-C09	6.54	1.56	1.42
38	k	619	II0	C21-C09	6.53	1.56	1.42
40	k	611	KC2	CBA-CAA	6.52	1.52	1.33
38	m	618	II0	C23-C25	6.52	1.55	1.42
38	e	312	II0	C24-C26	6.52	1.55	1.42
38	f	616	II0	C24-C26	6.52	1.55	1.42
38	e	312	II0	C21-C09	6.52	1.56	1.42
38	b	301	II0	C21-C09	6.51	1.56	1.42
40	j	312	KC2	CBA-CAA	6.50	1.52	1.33
38	g	319	II0	C22-C10	6.49	1.56	1.42
38	m	616	II0	C24-C26	6.49	1.55	1.42
32	J	101	WVN	C02-C11	6.49	1.59	1.50
38	b	314	II0	C22-C10	6.48	1.56	1.42
40	g	315	KC2	CBA-CAA	6.48	1.52	1.33
38	k	619	II0	C24-C26	6.47	1.55	1.42
38	d	315	II0	C24-C26	6.47	1.55	1.42
40	l	311	KC2	CBA-CAA	6.47	1.52	1.33
38	g	317	II0	C24-C26	6.47	1.55	1.42
38	l	315	II0	C24-C26	6.46	1.55	1.42
32	F	207	WVN	C02-C11	6.46	1.59	1.50
40	n	611	KC2	CBA-CAA	6.46	1.52	1.33
38	g	318	II0	C24-C26	6.46	1.55	1.42
38	e	314	II0	C24-C26	6.45	1.55	1.42
38	m	615	II0	C21-C09	6.45	1.56	1.42
32	L	205	WVN	C02-C11	6.45	1.59	1.50
38	a	315	II0	C24-C26	6.44	1.54	1.42
32	L	201	WVN	C02-C11	6.44	1.59	1.50
38	m	615	II0	C24-C26	6.44	1.54	1.42
38	j	301	II0	C24-C26	6.43	1.54	1.42
38	n	615	II0	C24-C26	6.42	1.54	1.42
38	f	615	II0	C24-C26	6.42	1.54	1.42
38	l	313	II0	C21-C09	6.42	1.55	1.42
38	j	315	II0	C21-C09	6.41	1.55	1.42
38	i	313	II0	C21-C09	6.41	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	i	316	II0	C24-C26	6.41	1.54	1.42
38	g	319	II0	C24-C26	6.41	1.54	1.42
32	B	848	WVN	C02-C11	6.41	1.59	1.50
40	g	313	KC2	CBA-CAA	6.41	1.52	1.33
38	c	313	II0	C21-C09	6.41	1.55	1.42
38	d	315	II0	C21-C09	6.40	1.55	1.42
38	j	316	II0	C24-C26	6.39	1.54	1.42
38	j	315	II0	C24-C26	6.39	1.54	1.42
40	e	309	KC2	CBA-CAA	6.39	1.52	1.33
38	f	615	II0	C21-C09	6.39	1.55	1.42
38	d	317	II0	C23-C25	6.38	1.54	1.42
38	k	620	II0	C24-C26	6.38	1.54	1.42
38	d	317	II0	C21-C09	6.38	1.55	1.42
38	f	618	II0	C24-C26	6.37	1.54	1.42
38	J	103	II0	C21-C09	6.37	1.55	1.42
38	b	314	II0	C24-C26	6.36	1.54	1.42
38	n	616	II0	C21-C09	6.36	1.55	1.42
38	d	301	II0	C24-C26	6.35	1.54	1.42
40	s	404	KC2	CBA-CAA	6.35	1.52	1.33
32	l	302	WVN	C02-C11	6.35	1.59	1.50
40	m	611	KC2	CBA-CAA	6.35	1.52	1.33
38	J	103	II0	C22-C10	6.34	1.55	1.42
38	c	313	II0	C24-C26	6.34	1.54	1.42
38	a	313	II0	C22-C10	6.34	1.55	1.42
38	n	615	II0	C23-C25	6.34	1.54	1.42
38	a	317	II0	C24-C26	6.34	1.54	1.42
38	b	314	II0	C21-C09	6.34	1.55	1.42
38	i	319	II0	C23-C25	6.33	1.54	1.42
32	J	101	WVN	C19-C22	6.33	1.59	1.45
38	n	616	II0	C24-C26	6.32	1.54	1.42
40	c	310	KC2	CBA-CAA	6.32	1.52	1.33
38	h	310	II0	C24-C26	6.32	1.54	1.42
40	s	401	KC2	CBA-CAA	6.31	1.52	1.33
40	f	611	KC2	CBA-CAA	6.31	1.52	1.33
40	d	311	KC2	CBA-CAA	6.31	1.52	1.33
38	g	319	II0	C21-C09	6.30	1.55	1.42
38	g	317	II0	C23-C25	6.29	1.54	1.42
32	B	847	WVN	C02-C11	6.29	1.59	1.50
38	k	615	II0	C24-C26	6.28	1.54	1.42
32	A	854	WVN	C02-C11	6.28	1.59	1.50
38	d	301	II0	C21-C09	6.28	1.55	1.42
38	k	620	II0	C21-C09	6.27	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	i	313	II0	C24-C26	6.27	1.54	1.42
32	L	206	WVN	C02-C11	6.27	1.59	1.50
32	B	849	WVN	C02-C11	6.27	1.59	1.50
38	j	316	II0	C21-C09	6.27	1.55	1.42
38	f	618	II0	C23-C25	6.26	1.54	1.42
38	k	615	II0	C21-C09	6.26	1.55	1.42
32	F	204	WVN	C02-C11	6.25	1.59	1.50
38	a	313	II0	C24-C26	6.25	1.54	1.42
38	l	314	II0	C21-C09	6.25	1.55	1.42
32	s	405	WVN	C02-C11	6.24	1.59	1.50
38	l	315	II0	C23-C25	6.24	1.54	1.42
38	h	310	II0	C21-C09	6.23	1.55	1.42
38	f	614	II0	C21-C09	6.23	1.55	1.42
38	e	313	II0	C21-C09	6.23	1.55	1.42
38	J	103	II0	C24-C26	6.22	1.54	1.42
32	A	846	WVN	C02-C11	6.20	1.59	1.50
38	g	318	II0	C21-C09	6.20	1.55	1.42
38	j	301	II0	C23-C25	6.20	1.54	1.42
38	l	313	II0	C23-C25	6.20	1.54	1.42
38	J	103	II0	C23-C25	6.19	1.54	1.42
38	f	616	II0	C23-C25	6.18	1.54	1.42
38	b	314	II0	C23-C25	6.17	1.54	1.42
38	a	317	II0	C23-C25	6.17	1.54	1.42
38	c	313	II0	C23-C25	6.16	1.54	1.42
38	b	315	II0	C21-C09	6.14	1.55	1.42
38	k	619	II0	C23-C25	6.14	1.54	1.42
38	i	316	II0	C23-C25	6.14	1.54	1.42
38	a	315	II0	C21-C09	6.14	1.55	1.42
38	d	301	II0	C23-C25	6.12	1.54	1.42
38	n	618	II0	C23-C25	6.12	1.54	1.42
32	L	205	WVN	C19-C22	6.12	1.59	1.45
38	k	616	II0	C23-C25	6.12	1.54	1.42
38	i	314	II0	C23-C25	6.11	1.54	1.42
38	f	615	II0	C23-C25	6.10	1.54	1.42
38	m	616	II0	C23-C25	6.10	1.54	1.42
38	d	315	II0	C23-C25	6.08	1.54	1.42
38	k	620	II0	C23-C25	6.07	1.54	1.42
38	a	315	II0	C23-C25	6.06	1.54	1.42
38	g	318	II0	C23-C25	6.06	1.54	1.42
38	b	315	II0	C23-C25	6.06	1.54	1.42
32	M	101	WVN	C19-C22	6.06	1.59	1.45
38	j	315	II0	C23-C25	6.05	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	316	II0	C23-C25	6.04	1.54	1.42
38	b	301	II0	C23-C25	6.04	1.54	1.42
38	a	314	II0	C23-C25	6.04	1.54	1.42
38	f	614	II0	C23-C25	6.04	1.54	1.42
38	i	313	II0	C23-C25	6.04	1.54	1.42
38	e	312	II0	C23-C25	6.03	1.54	1.42
38	e	314	II0	C23-C25	6.03	1.54	1.42
38	g	319	II0	C23-C25	6.01	1.54	1.42
32	l	316	WVN	C19-C22	6.01	1.58	1.45
38	j	316	II0	C23-C25	6.01	1.54	1.42
38	l	314	II0	C23-C25	6.01	1.54	1.42
38	a	313	II0	C23-C25	6.00	1.54	1.42
38	n	616	II0	C23-C25	5.99	1.54	1.42
38	h	309	II0	C23-C25	5.98	1.54	1.42
38	m	614	II0	C23-C25	5.98	1.54	1.42
40	i	310	KC2	O2A-CGA	5.98	1.45	1.30
38	e	313	II0	C24-C22	5.97	1.37	1.20
38	k	616	II0	C24-C22	5.97	1.37	1.20
38	j	301	II0	C24-C22	5.96	1.37	1.20
38	i	314	II0	C24-C22	5.95	1.37	1.20
38	d	317	II0	C24-C22	5.95	1.37	1.20
40	i	318	KC2	O2A-CGA	5.93	1.45	1.30
38	j	316	II0	C24-C22	5.93	1.37	1.20
38	k	615	II0	C24-C22	5.93	1.37	1.20
32	R	202	WVN	C19-C22	5.92	1.58	1.45
38	h	310	II0	C23-C25	5.92	1.53	1.42
38	m	616	II0	C24-C22	5.91	1.37	1.20
38	l	315	II0	C24-C22	5.90	1.37	1.20
38	h	311	II0	C23-C25	5.90	1.53	1.42
38	d	315	II0	C24-C22	5.90	1.37	1.20
38	i	319	II0	C24-C22	5.88	1.37	1.20
38	g	318	II0	C24-C22	5.88	1.37	1.20
38	m	618	II0	C24-C22	5.88	1.37	1.20
38	m	615	II0	C23-C25	5.88	1.53	1.42
40	f	611	KC2	O2A-CGA	5.88	1.45	1.30
32	B	846	WVN	C02-C11	5.87	1.58	1.50
38	f	618	II0	C24-C22	5.87	1.37	1.20
32	i	315	WVN	C19-C22	5.87	1.58	1.45
40	k	611	KC2	O2A-CGA	5.87	1.45	1.30
38	k	615	II0	C23-C25	5.87	1.53	1.42
38	f	615	II0	C24-C22	5.87	1.37	1.20
38	b	301	II0	C24-C22	5.86	1.37	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	b	315	II0	C24-C22	5.86	1.37	1.20
40	e	309	KC2	O2A-CGA	5.86	1.45	1.30
38	e	313	II0	C23-C25	5.85	1.53	1.42
38	l	313	II0	C24-C22	5.83	1.37	1.20
40	d	311	KC2	O2A-CGA	5.82	1.45	1.30
32	A	845	WVN	C19-C22	5.81	1.58	1.45
38	n	618	II0	C24-C22	5.81	1.37	1.20
38	a	314	II0	C24-C22	5.80	1.37	1.20
40	j	312	KC2	O2A-CGA	5.80	1.45	1.30
38	m	615	II0	C24-C22	5.79	1.37	1.20
38	l	314	II0	C24-C22	5.78	1.37	1.20
40	d	311	KC2	C1A-NA	-5.78	1.26	1.38
40	c	310	KC2	O2A-CGA	5.78	1.45	1.30
40	c	310	KC2	C3B-C2B	5.78	1.49	1.37
40	n	611	KC2	O2A-CGA	5.77	1.45	1.30
40	g	315	KC2	C3C-C2C	5.77	1.49	1.37
40	m	611	KC2	O2A-CGA	5.76	1.45	1.30
38	f	616	II0	C24-C22	5.75	1.37	1.20
40	l	311	KC2	C3B-C2B	5.75	1.48	1.37
40	s	401	KC2	O2A-CGA	5.75	1.45	1.30
38	g	317	II0	C24-C22	5.75	1.37	1.20
40	g	314	KC2	O2A-CGA	5.74	1.45	1.30
38	f	614	II0	C24-C22	5.74	1.37	1.20
40	g	315	KC2	O2A-CGA	5.74	1.45	1.30
38	h	311	II0	C24-C22	5.73	1.37	1.20
40	c	310	KC2	C1A-NA	-5.73	1.26	1.38
32	R	201	WVN	C02-C11	5.72	1.58	1.50
40	g	313	KC2	O2A-CGA	5.71	1.45	1.30
32	K	103	WVN	C19-C22	5.71	1.58	1.45
38	m	614	II0	C24-C22	5.70	1.36	1.20
40	l	311	KC2	O2A-CGA	5.69	1.45	1.30
32	e	315	WVN	C19-C22	5.69	1.58	1.45
32	h	308	WVN	C19-C22	5.69	1.58	1.45
38	e	312	II0	C24-C22	5.68	1.36	1.20
38	a	315	II0	C24-C22	5.67	1.36	1.20
32	s	407	WVN	C19-C22	5.67	1.58	1.45
38	h	310	II0	C24-C22	5.66	1.36	1.20
38	n	616	II0	C24-C22	5.65	1.36	1.20
38	c	313	II0	C24-C22	5.64	1.36	1.20
38	d	316	II0	C24-C22	5.64	1.36	1.20
40	i	310	KC2	C1A-NA	-5.64	1.27	1.38
38	n	615	II0	C24-C22	5.63	1.36	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	i	313	II0	C24-C22	5.63	1.36	1.20
40	i	318	KC2	C3B-C2B	5.62	1.48	1.37
38	g	319	II0	C24-C22	5.62	1.36	1.20
38	i	316	II0	C24-C22	5.61	1.36	1.20
38	k	619	II0	C24-C22	5.60	1.36	1.20
38	e	314	II0	C24-C22	5.60	1.36	1.20
38	k	620	II0	C24-C22	5.59	1.36	1.20
40	e	309	KC2	C1A-NA	-5.59	1.27	1.38
40	m	611	KC2	C3B-C2B	5.59	1.48	1.37
40	m	611	KC2	C1A-NA	-5.59	1.27	1.38
38	J	103	II0	C24-C22	5.59	1.36	1.20
38	j	315	II0	C24-C22	5.59	1.36	1.20
38	a	317	II0	C24-C22	5.58	1.36	1.20
40	g	315	KC2	C3B-C2B	5.57	1.48	1.37
38	b	314	II0	C24-C22	5.56	1.36	1.20
38	d	301	II0	C24-C22	5.55	1.36	1.20
32	F	204	WVN	C19-C22	5.54	1.57	1.45
40	g	313	KC2	C3B-C2B	5.52	1.48	1.37
40	e	309	KC2	C3B-C2B	5.52	1.48	1.37
38	a	313	II0	C24-C22	5.52	1.36	1.20
40	g	313	KC2	C1A-NA	-5.50	1.27	1.38
40	f	611	KC2	C1A-NA	-5.50	1.27	1.38
40	k	611	KC2	C3B-C2B	5.50	1.48	1.37
32	A	846	WVN	C19-C22	5.49	1.57	1.45
40	g	314	KC2	C3B-C2B	5.48	1.48	1.37
38	j	301	II0	C23-C21	5.48	1.36	1.20
40	i	310	KC2	C3B-C2B	5.46	1.48	1.37
40	n	611	KC2	C1A-NA	-5.46	1.27	1.38
38	l	315	II0	C23-C21	5.46	1.36	1.20
40	j	312	KC2	C1A-NA	-5.45	1.27	1.38
40	s	401	KC2	C1A-NA	-5.43	1.27	1.38
40	i	318	KC2	C1A-NA	-5.42	1.27	1.38
38	f	618	II0	C23-C21	5.41	1.36	1.20
40	j	312	KC2	C3B-C2B	5.41	1.48	1.37
40	n	611	KC2	C3B-C2B	5.40	1.48	1.37
38	m	618	II0	C23-C21	5.39	1.36	1.20
40	s	401	KC2	C3B-C2B	5.39	1.48	1.37
32	B	846	WVN	C19-C22	5.36	1.57	1.45
32	I	101	WVN	C19-C22	5.36	1.57	1.45
40	f	611	KC2	C3B-C2B	5.35	1.48	1.37
32	s	405	WVN	C19-C22	5.35	1.57	1.45
40	s	404	KC2	O2A-CGA	5.35	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	a	317	II0	C23-C21	5.35	1.35	1.20
40	l	311	KC2	C3C-C2C	5.34	1.48	1.37
38	g	317	II0	C23-C21	5.34	1.35	1.20
38	k	616	II0	C23-C21	5.34	1.35	1.20
40	k	611	KC2	C1A-NA	-5.34	1.27	1.38
38	i	319	II0	C23-C21	5.32	1.35	1.20
40	i	318	KC2	C1D-ND	5.32	1.44	1.37
32	A	847	WVN	C19-C22	5.31	1.57	1.45
40	e	309	KC2	C3C-C2C	5.30	1.48	1.37
40	d	311	KC2	C3B-C2B	5.30	1.48	1.37
32	B	847	WVN	C19-C22	5.30	1.57	1.45
32	B	848	WVN	C19-C22	5.29	1.57	1.45
40	i	318	KC2	C3C-C2C	5.28	1.48	1.37
40	g	315	KC2	C1A-NA	-5.27	1.27	1.38
40	s	404	KC2	C3C-C2C	5.26	1.47	1.37
32	l	316	WVN	C33-C34	5.25	1.57	1.45
40	s	404	KC2	C1A-NA	-5.24	1.27	1.38
38	f	616	II0	C23-C21	5.24	1.35	1.20
38	d	317	II0	C23-C21	5.23	1.35	1.20
32	l	302	WVN	C19-C22	5.22	1.57	1.45
38	n	616	II0	C23-C21	5.22	1.35	1.20
40	d	311	KC2	O2D-CGD	5.20	1.45	1.33
38	h	309	II0	C23-C21	5.20	1.35	1.20
40	d	311	KC2	C3C-C2C	5.19	1.47	1.37
38	n	615	II0	C23-C21	5.19	1.35	1.20
40	i	310	KC2	C3C-C2C	5.19	1.47	1.37
38	a	313	II0	C23-C21	5.17	1.35	1.20
40	j	312	KC2	C3C-C2C	5.16	1.47	1.37
38	b	314	II0	C23-C21	5.16	1.35	1.20
40	n	611	KC2	C3C-C2C	5.15	1.47	1.37
32	A	844	WVN	C19-C22	5.15	1.57	1.45
38	i	316	II0	C23-C21	5.15	1.35	1.20
38	k	619	II0	C23-C21	5.14	1.35	1.20
38	f	615	II0	C23-C21	5.14	1.35	1.20
38	J	103	II0	C23-C21	5.14	1.35	1.20
38	m	616	II0	C23-C21	5.13	1.35	1.20
40	k	611	KC2	C3C-C2C	5.13	1.47	1.37
38	l	314	II0	C23-C21	5.12	1.35	1.20
32	F	207	WVN	C19-C22	5.11	1.56	1.45
38	e	313	II0	C34-C36	5.11	1.56	1.45
38	k	620	II0	C23-C21	5.11	1.35	1.20
38	l	313	II0	C23-C21	5.11	1.35	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	g	319	II0	C23-C21	5.11	1.35	1.20
32	B	846	WVN	C33-C34	5.10	1.56	1.45
38	b	315	II0	C23-C21	5.09	1.35	1.20
38	i	313	II0	C23-C21	5.09	1.35	1.20
38	n	618	II0	C23-C21	5.08	1.35	1.20
38	j	315	II0	C23-C21	5.08	1.35	1.20
38	e	314	II0	C23-C21	5.07	1.35	1.20
40	i	318	KC2	O2D-CGD	5.07	1.45	1.33
38	c	313	II0	C23-C21	5.07	1.35	1.20
38	h	311	II0	C23-C21	5.07	1.35	1.20
38	j	316	II0	C23-C21	5.06	1.35	1.20
38	d	315	II0	C23-C21	5.05	1.35	1.20
38	a	314	II0	C23-C21	5.04	1.35	1.20
38	d	301	II0	C23-C21	5.04	1.35	1.20
40	l	311	KC2	C1A-NA	-5.04	1.28	1.38
32	L	201	WVN	C19-C22	5.03	1.56	1.45
40	e	309	KC2	C1D-ND	5.03	1.44	1.37
38	f	614	II0	C23-C21	5.03	1.35	1.20
38	a	315	II0	C23-C21	5.03	1.35	1.20
32	B	849	WVN	C19-C22	5.02	1.56	1.45
38	g	318	II0	C23-C21	5.01	1.34	1.20
40	s	404	KC2	C3B-C2B	5.00	1.47	1.37
40	s	401	KC2	C3C-C2C	5.00	1.47	1.37
38	i	314	II0	C23-C21	4.99	1.34	1.20
40	k	611	KC2	O2D-CGD	4.99	1.45	1.33
40	i	310	KC2	O2D-CGD	4.99	1.45	1.33
40	g	313	KC2	C3C-C2C	4.99	1.47	1.37
38	e	312	II0	C23-C21	4.98	1.34	1.20
40	g	315	KC2	O2D-CGD	4.98	1.45	1.33
40	m	611	KC2	C3C-C2C	4.97	1.47	1.37
32	I	101	WVN	C33-C34	4.97	1.56	1.45
40	e	309	KC2	O2D-CGD	4.97	1.45	1.33
38	e	313	II0	C23-C21	4.97	1.34	1.20
38	d	316	II0	C23-C21	4.97	1.34	1.20
38	d	315	II0	C34-C36	4.96	1.56	1.45
38	d	317	II0	C34-C36	4.96	1.56	1.45
38	b	301	II0	C23-C21	4.96	1.34	1.20
40	c	310	KC2	O2D-CGD	4.96	1.45	1.33
40	c	310	KC2	C3C-C2C	4.95	1.47	1.37
38	k	615	II0	C23-C21	4.95	1.34	1.20
32	R	201	WVN	C19-C22	4.94	1.56	1.45
38	m	614	II0	C23-C21	4.94	1.34	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	h	310	II0	C23-C21	4.94	1.34	1.20
32	L	206	WVN	C19-C22	4.94	1.56	1.45
40	f	611	KC2	C3C-C2C	4.94	1.47	1.37
38	i	319	II0	C34-C36	4.93	1.56	1.45
38	m	615	II0	C23-C21	4.92	1.34	1.20
40	e	309	KC2	CHD-C4C	4.89	1.48	1.38
40	k	611	KC2	C1D-ND	4.89	1.43	1.37
32	L	201	WVN	C33-C34	4.88	1.56	1.45
32	s	407	WVN	C33-C34	4.88	1.56	1.45
40	g	314	KC2	C1A-NA	-4.87	1.28	1.38
38	l	313	II0	C34-C36	4.87	1.56	1.45
40	s	401	KC2	O2D-CGD	4.86	1.45	1.33
40	g	314	KC2	C3C-C2C	4.85	1.47	1.37
40	d	311	KC2	C1D-ND	4.85	1.43	1.37
40	d	312	KC2	C4D-ND	-4.85	1.31	1.37
40	m	611	KC2	O2D-CGD	4.85	1.45	1.33
40	i	318	KC2	CHD-C4C	4.84	1.48	1.38
40	l	311	KC2	O2D-CGD	4.84	1.45	1.33
32	B	847	WVN	C33-C34	4.84	1.56	1.45
40	g	315	KC2	CHD-C4C	4.81	1.48	1.38
40	s	404	KC2	O2D-CGD	4.81	1.44	1.33
28	A	801	CL0	MG-NA	4.80	2.17	2.06
40	j	312	KC2	O2D-CGD	4.80	1.44	1.33
40	m	611	KC2	CHD-C4C	4.78	1.48	1.38
38	i	314	II0	C34-C36	4.77	1.56	1.45
40	n	611	KC2	O2D-CGD	4.77	1.44	1.33
40	m	611	KC2	C1D-ND	4.76	1.43	1.37
40	n	612	KC2	C4D-ND	-4.76	1.31	1.37
32	J	101	WVN	C33-C34	4.75	1.56	1.45
40	c	310	KC2	CHD-C4C	4.74	1.48	1.38
38	l	314	II0	C34-C36	4.72	1.56	1.45
32	A	846	WVN	C33-C34	4.72	1.56	1.45
32	l	302	WVN	C33-C34	4.72	1.56	1.45
40	i	318	KC2	CHB-C1B	4.71	1.47	1.38
40	k	611	KC2	CHC-C4B	4.71	1.47	1.38
40	g	315	KC2	C1D-ND	4.71	1.43	1.37
40	n	611	KC2	CHD-C4C	4.69	1.48	1.38
40	g	313	KC2	O2D-CGD	4.69	1.44	1.33
40	i	310	KC2	CHD-C4C	4.69	1.48	1.38
40	g	313	KC2	CHD-C4C	4.68	1.48	1.38
38	l	314	II0	C32-C30	4.68	1.57	1.43
40	j	312	KC2	CHD-C4C	4.67	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	i	310	KC2	C1D-ND	4.67	1.43	1.37
40	s	401	KC2	CHD-C4C	4.67	1.48	1.38
38	i	314	II0	C32-C30	4.67	1.57	1.43
40	j	312	KC2	C1D-ND	4.67	1.43	1.37
32	F	204	WVN	C33-C34	4.66	1.56	1.45
40	d	311	KC2	CHD-C4C	4.66	1.48	1.38
40	l	311	KC2	C1D-ND	4.64	1.43	1.37
40	g	315	KC2	CHC-C4B	4.64	1.47	1.38
40	c	310	KC2	CHC-C4B	4.63	1.47	1.38
40	k	611	KC2	CHD-C4C	4.63	1.47	1.38
40	g	314	KC2	CHD-C4C	4.62	1.47	1.38
32	A	854	WVN	C19-C22	4.61	1.55	1.45
40	i	318	KC2	CHC-C4B	4.60	1.47	1.38
40	g	314	KC2	O2D-CGD	4.60	1.44	1.33
38	a	314	II0	C32-C30	4.58	1.57	1.43
40	e	309	KC2	CHB-C1B	4.56	1.47	1.38
33	A	849	LMU	O5'-C5'	4.55	1.55	1.44
38	m	618	II0	C32-C30	4.54	1.57	1.43
32	h	308	WVN	C29-C26	4.53	1.57	1.43
40	k	612	KC2	C4D-ND	-4.53	1.31	1.37
28	A	801	CL0	MG-NC	4.53	2.17	2.06
40	n	611	KC2	C1D-ND	4.52	1.43	1.37
32	l	316	WVN	C29-C26	4.51	1.57	1.43
40	f	611	KC2	CHD-C4C	4.50	1.47	1.38
40	i	310	KC2	CHC-C4B	4.50	1.47	1.38
32	I	101	WVN	C29-C26	4.50	1.57	1.43
40	f	611	KC2	O2D-CGD	4.50	1.44	1.33
40	g	314	KC2	CHB-C1B	4.49	1.47	1.38
38	f	615	II0	C32-C30	4.49	1.57	1.43
38	f	618	II0	C32-C30	4.49	1.57	1.43
32	M	101	WVN	C29-C26	4.49	1.57	1.43
38	m	615	II0	C32-C30	4.49	1.57	1.43
38	l	313	II0	C32-C30	4.48	1.57	1.43
38	b	301	II0	C32-C30	4.48	1.57	1.43
38	k	615	II0	C32-C30	4.47	1.57	1.43
38	i	319	II0	C32-C30	4.47	1.57	1.43
29	K	102	CLA	C1D-ND	4.47	1.43	1.37
40	f	611	KC2	C1D-ND	4.47	1.43	1.37
40	g	313	KC2	C1D-ND	4.46	1.43	1.37
32	i	315	WVN	C29-C26	4.46	1.57	1.43
40	g	313	KC2	CHB-C1B	4.46	1.47	1.38
40	e	309	KC2	CHC-C4B	4.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	a	314	II0	C34-C36	4.45	1.55	1.45
33	i	301	LMU	O5'-C5'	4.44	1.55	1.44
38	j	316	II0	C32-C30	4.44	1.57	1.43
38	m	614	II0	C32-C30	4.43	1.57	1.43
38	g	318	II0	C32-C30	4.43	1.57	1.43
32	e	315	WVN	C29-C26	4.43	1.57	1.43
38	b	315	II0	C32-C30	4.43	1.57	1.43
40	f	611	KC2	CHB-C1B	4.42	1.47	1.38
38	e	313	II0	C32-C30	4.42	1.57	1.43
38	d	317	II0	C32-C30	4.42	1.57	1.43
38	k	619	II0	C32-C30	4.41	1.57	1.43
32	A	854	WVN	C29-C26	4.41	1.57	1.43
38	n	618	II0	C32-C30	4.41	1.57	1.43
32	M	101	WVN	C31-C32	4.40	1.55	1.45
40	s	404	KC2	CHD-C4C	4.40	1.47	1.38
32	I	101	WVN	C31-C32	4.40	1.55	1.45
40	l	311	KC2	CHD-C4C	4.40	1.47	1.38
28	A	801	CL0	C4C-C3C	-4.39	1.37	1.45
40	k	613	KC2	C4D-ND	-4.39	1.31	1.37
33	A	849	LMU	O5B-C5B	4.39	1.55	1.44
40	s	401	KC2	CHB-C1B	4.39	1.46	1.38
40	m	611	KC2	CHC-C4B	4.39	1.46	1.38
28	A	801	CL0	C1C-C2C	-4.39	1.36	1.44
38	n	615	II0	C32-C30	4.38	1.57	1.43
38	c	313	II0	C32-C30	4.38	1.57	1.43
38	d	316	II0	C32-C30	4.38	1.57	1.43
32	l	316	WVN	C31-C32	4.38	1.55	1.45
38	b	314	II0	C32-C30	4.38	1.57	1.43
40	k	611	KC2	CHB-C1B	4.38	1.46	1.38
32	L	205	WVN	C29-C26	4.38	1.57	1.43
38	f	614	II0	C32-C30	4.37	1.57	1.43
38	a	317	II0	C32-C30	4.37	1.57	1.43
40	c	310	KC2	CHB-C1B	4.37	1.46	1.38
38	m	616	II0	C32-C30	4.37	1.57	1.43
32	A	847	WVN	C29-C26	4.37	1.57	1.43
38	d	315	II0	C32-C30	4.36	1.57	1.43
38	k	616	II0	C32-C30	4.36	1.57	1.43
40	n	611	KC2	CHC-C4B	4.36	1.46	1.38
38	g	317	II0	C32-C30	4.36	1.57	1.43
38	i	313	II0	C32-C30	4.36	1.57	1.43
40	j	312	KC2	CHB-C1B	4.36	1.46	1.38
33	i	301	LMU	O5B-C5B	4.34	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	h	308	WVN	C31-C32	4.34	1.55	1.45
38	d	317	II0	C31-C29	4.34	1.56	1.43
38	h	310	II0	C32-C30	4.34	1.56	1.43
32	A	847	WVN	C31-C32	4.34	1.55	1.45
38	e	312	II0	C32-C30	4.34	1.56	1.43
40	d	311	KC2	CHB-C1B	4.33	1.46	1.38
40	d	311	KC2	CHC-C4B	4.33	1.46	1.38
40	l	311	KC2	CHB-C1B	4.32	1.46	1.38
32	L	206	WVN	C29-C26	4.32	1.56	1.43
38	J	103	II0	C32-C30	4.32	1.56	1.43
38	f	616	II0	C32-C30	4.32	1.56	1.43
38	i	314	II0	C31-C29	4.32	1.56	1.43
40	m	611	KC2	CHB-C1B	4.31	1.46	1.38
38	h	311	II0	C32-C30	4.30	1.56	1.43
38	k	620	II0	C32-C30	4.30	1.56	1.43
40	s	404	KC2	C1B-NB	-4.30	1.32	1.37
38	l	315	II0	C32-C30	4.30	1.56	1.43
38	e	314	II0	C32-C30	4.29	1.56	1.43
38	a	315	II0	C32-C30	4.29	1.56	1.43
40	s	404	KC2	CHB-C1B	4.29	1.46	1.38
38	d	316	II0	C31-C29	4.29	1.56	1.43
38	g	319	II0	C32-C30	4.28	1.56	1.43
38	g	317	II0	C31-C29	4.28	1.56	1.43
38	n	616	II0	C32-C30	4.28	1.56	1.43
38	j	301	II0	C32-C30	4.28	1.56	1.43
32	B	847	WVN	C29-C26	4.28	1.56	1.43
40	g	313	KC2	CHC-C4B	4.27	1.46	1.38
32	e	315	WVN	C31-C32	4.27	1.55	1.45
38	a	313	II0	C32-C30	4.27	1.56	1.43
38	k	616	II0	C31-C29	4.27	1.56	1.43
29	A	827	CLA	C1D-ND	4.27	1.43	1.37
40	s	401	KC2	C4B-NB	-4.27	1.32	1.37
32	F	207	WVN	C29-C26	4.27	1.56	1.43
40	f	611	KC2	C4B-NB	-4.26	1.32	1.37
32	L	201	WVN	C29-C26	4.26	1.56	1.43
32	A	844	WVN	C29-C26	4.26	1.56	1.43
38	i	316	II0	C32-C30	4.26	1.56	1.43
38	j	315	II0	C32-C30	4.25	1.56	1.43
32	K	103	WVN	C29-C26	4.25	1.56	1.43
38	d	301	II0	C32-C30	4.25	1.56	1.43
40	s	404	KC2	C1D-ND	4.24	1.43	1.37
38	l	314	II0	C31-C29	4.24	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	R	201	WVN	C29-C26	4.23	1.56	1.43
32	l	302	WVN	C29-C26	4.23	1.56	1.43
32	R	202	WVN	C29-C26	4.23	1.56	1.43
32	s	407	WVN	C29-C26	4.23	1.56	1.43
32	l	316	WVN	C39-C36	4.23	1.56	1.43
38	l	315	II0	C31-C29	4.23	1.56	1.43
38	l	313	II0	C31-C29	4.23	1.56	1.43
38	m	618	II0	C34-C36	4.23	1.55	1.45
38	a	317	II0	C31-C29	4.23	1.56	1.43
38	m	616	II0	C31-C29	4.22	1.56	1.43
40	g	315	KC2	CHB-C1B	4.22	1.46	1.38
32	K	103	WVN	C31-C32	4.22	1.55	1.45
40	s	404	KC2	CHC-C4B	4.21	1.46	1.38
40	s	401	KC2	CHC-C4B	4.21	1.46	1.38
32	s	405	WVN	C29-C26	4.21	1.56	1.43
40	c	310	KC2	C1D-ND	4.20	1.43	1.37
32	L	205	WVN	C31-C32	4.20	1.55	1.45
32	J	101	WVN	C29-C26	4.20	1.56	1.43
38	k	619	II0	C31-C29	4.20	1.56	1.43
30	B	843	PQN	C2-C1	-4.20	1.39	1.48
38	i	316	II0	C31-C29	4.20	1.56	1.43
40	g	313	KC2	C4B-NB	-4.20	1.32	1.37
38	i	313	II0	C31-C29	4.19	1.56	1.43
32	e	315	WVN	C39-C36	4.19	1.56	1.43
38	j	316	II0	C31-C29	4.19	1.56	1.43
38	c	313	II0	C31-C29	4.19	1.56	1.43
32	F	207	WVN	C39-C36	4.18	1.56	1.43
32	R	202	WVN	C39-C36	4.18	1.56	1.43
38	i	319	II0	C31-C29	4.18	1.56	1.43
38	a	317	II0	C34-C36	4.18	1.54	1.45
38	j	301	II0	C31-C29	4.18	1.56	1.43
32	A	847	WVN	C39-C36	4.18	1.56	1.43
38	a	314	II0	C31-C29	4.18	1.56	1.43
32	A	854	WVN	C31-C32	4.17	1.54	1.45
32	B	849	WVN	C29-C26	4.17	1.56	1.43
38	n	618	II0	C31-C29	4.17	1.56	1.43
38	b	301	II0	C31-C29	4.17	1.56	1.43
38	l	314	II0	C33-C35	4.17	1.54	1.45
40	f	611	KC2	C1B-NB	-4.16	1.32	1.37
38	h	310	II0	C31-C29	4.16	1.56	1.43
32	M	101	WVN	C39-C36	4.16	1.56	1.43
38	m	618	II0	C31-C29	4.16	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	845	WVN	C29-C26	4.15	1.56	1.43
38	n	615	II0	C31-C29	4.15	1.56	1.43
38	a	314	II0	C42-C40	4.15	1.56	1.43
38	e	314	II0	C31-C29	4.15	1.56	1.43
40	n	611	KC2	C4B-NB	-4.15	1.32	1.37
40	i	310	KC2	CHB-C1B	4.15	1.46	1.38
32	R	202	WVN	C31-C32	4.15	1.54	1.45
32	s	407	WVN	C31-C32	4.14	1.54	1.45
40	i	310	KC2	C1B-NB	-4.14	1.32	1.37
38	d	315	II0	C31-C29	4.14	1.56	1.43
38	k	619	II0	C34-C36	4.14	1.54	1.45
40	l	311	KC2	C1B-NB	-4.13	1.32	1.37
38	g	318	II0	C31-C29	4.13	1.56	1.43
32	A	854	WVN	C33-C34	4.13	1.54	1.45
38	b	315	II0	C31-C29	4.13	1.56	1.43
32	L	206	WVN	C33-C34	4.13	1.54	1.45
38	m	615	II0	C31-C29	4.13	1.56	1.43
32	B	848	WVN	C29-C26	4.12	1.56	1.43
32	F	204	WVN	C29-C26	4.12	1.56	1.43
38	J	103	II0	C31-C29	4.12	1.56	1.43
38	e	312	II0	C31-C29	4.12	1.56	1.43
38	j	315	II0	C31-C29	4.12	1.56	1.43
38	f	615	II0	C31-C29	4.12	1.56	1.43
38	m	614	II0	C31-C29	4.11	1.56	1.43
38	k	620	II0	C31-C29	4.11	1.56	1.43
38	i	314	II0	C33-C35	4.11	1.54	1.45
38	b	314	II0	C31-C29	4.11	1.56	1.43
32	B	847	WVN	C31-C32	4.11	1.54	1.45
38	i	314	II0	C42-C40	4.11	1.56	1.43
29	d	304	CLA	C1D-ND	4.11	1.42	1.37
32	i	315	WVN	C39-C36	4.11	1.56	1.43
32	I	101	WVN	C39-C36	4.10	1.56	1.43
38	h	311	II0	C31-C29	4.10	1.56	1.43
38	k	615	II0	C31-C29	4.10	1.56	1.43
40	s	401	KC2	C1B-NB	-4.10	1.32	1.37
32	F	207	WVN	C31-C32	4.10	1.54	1.45
38	f	614	II0	C31-C29	4.10	1.56	1.43
40	g	314	KC2	CHC-C4B	4.09	1.46	1.38
32	J	101	WVN	C39-C36	4.09	1.56	1.43
38	a	313	II0	C31-C29	4.09	1.56	1.43
40	l	311	KC2	CHC-C4B	4.09	1.46	1.38
32	l	316	WVN	C40-C37	4.09	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	846	WVN	C29-C26	4.09	1.56	1.43
38	a	315	II0	C31-C29	4.09	1.56	1.43
30	A	841	PQN	C2-C1	-4.09	1.39	1.48
38	n	616	II0	C31-C29	4.08	1.56	1.43
38	g	317	II0	C33-C35	4.08	1.54	1.45
40	j	312	KC2	C4B-NB	-4.08	1.32	1.37
38	f	618	II0	C31-C29	4.08	1.56	1.43
32	F	207	WVN	C30-C28	4.08	1.56	1.43
32	s	407	WVN	C39-C36	4.08	1.56	1.43
32	K	103	WVN	C39-C36	4.08	1.56	1.43
40	s	401	KC2	C1D-ND	4.07	1.42	1.37
38	g	318	II0	C34-C36	4.07	1.54	1.45
40	d	311	KC2	C4B-NB	-4.07	1.32	1.37
40	j	312	KC2	CHC-C4B	4.07	1.46	1.38
32	i	315	WVN	C31-C32	4.07	1.54	1.45
40	l	311	KC2	C4B-NB	-4.07	1.32	1.37
38	g	319	II0	C31-C29	4.07	1.56	1.43
32	B	847	WVN	C39-C36	4.07	1.56	1.43
38	d	316	II0	C33-C35	4.07	1.54	1.45
32	B	846	WVN	C39-C36	4.06	1.56	1.43
32	A	844	WVN	C39-C36	4.06	1.56	1.43
32	F	204	WVN	C39-C36	4.06	1.56	1.43
32	L	201	WVN	C39-C36	4.06	1.56	1.43
40	n	611	KC2	C1B-NB	-4.05	1.32	1.37
32	A	846	WVN	C30-C28	4.05	1.56	1.43
32	A	845	WVN	C31-C32	4.05	1.54	1.45
32	R	201	WVN	C31-C32	4.05	1.54	1.45
32	l	316	WVN	C30-C28	4.05	1.56	1.43
32	s	405	WVN	C39-C36	4.05	1.56	1.43
32	h	308	WVN	C39-C36	4.05	1.56	1.43
32	e	315	WVN	C40-C37	4.05	1.56	1.43
40	g	314	KC2	C1B-NB	-4.04	1.32	1.37
40	g	314	KC2	C1D-ND	4.04	1.42	1.37
38	j	301	II0	C33-C35	4.04	1.54	1.45
32	R	202	WVN	C33-C34	4.04	1.54	1.45
32	L	205	WVN	C39-C36	4.04	1.56	1.43
32	F	207	WVN	C40-C37	4.03	1.55	1.43
29	c	311	CLA	C1D-ND	4.03	1.42	1.37
32	R	202	WVN	C30-C28	4.03	1.55	1.43
32	A	854	WVN	C39-C36	4.03	1.55	1.43
32	R	202	WVN	C40-C37	4.03	1.55	1.43
38	a	314	II0	C41-C39	4.03	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	845	WVN	C39-C36	4.03	1.55	1.43
32	A	846	WVN	C39-C36	4.03	1.55	1.43
32	A	844	WVN	C31-C32	4.03	1.54	1.45
38	f	618	II0	C34-C36	4.03	1.54	1.45
40	g	313	KC2	C1B-NB	-4.03	1.32	1.37
38	l	315	II0	C33-C35	4.03	1.54	1.45
32	A	854	WVN	C23-C25	4.03	1.54	1.45
38	m	615	II0	C34-C36	4.02	1.54	1.45
32	A	847	WVN	C40-C37	4.02	1.55	1.43
32	B	849	WVN	C33-C34	4.02	1.54	1.45
38	g	318	II0	C33-C35	4.02	1.54	1.45
29	f	608	CLA	C1D-ND	4.02	1.42	1.37
29	d	318	CLA	C1D-ND	4.02	1.42	1.37
29	A	823	CLA	C1D-ND	4.01	1.42	1.37
38	l	313	II0	C42-C40	4.01	1.55	1.43
32	B	849	WVN	C23-C25	4.01	1.54	1.45
38	m	618	II0	C33-C35	4.01	1.54	1.45
40	n	611	KC2	CHB-C1B	4.01	1.46	1.38
38	h	309	II0	C31-C29	4.01	1.55	1.43
38	l	314	II0	C41-C39	4.01	1.55	1.43
38	n	615	II0	C33-C35	4.01	1.54	1.45
40	m	611	KC2	C4B-NB	-4.01	1.32	1.37
32	L	206	WVN	C39-C36	4.01	1.55	1.43
38	d	317	II0	C33-C35	4.00	1.54	1.45
40	k	612	KC2	C3B-C4B	-4.00	1.38	1.46
32	h	308	WVN	C30-C28	4.00	1.55	1.43
32	B	849	WVN	C39-C36	4.00	1.55	1.43
32	R	202	WVN	C23-C25	4.00	1.54	1.45
38	k	616	II0	C34-C36	3.99	1.54	1.45
38	e	313	II0	C31-C29	3.99	1.55	1.43
38	d	316	II0	C42-C40	3.99	1.55	1.43
32	L	205	WVN	C23-C25	3.99	1.54	1.45
32	e	315	WVN	C33-C34	3.99	1.54	1.45
38	b	314	II0	C34-C36	3.99	1.54	1.45
32	J	101	WVN	C31-C32	3.98	1.54	1.45
38	f	615	II0	C34-C36	3.98	1.54	1.45
38	f	616	II0	C31-C29	3.98	1.55	1.43
40	g	314	KC2	C4B-NB	-3.98	1.32	1.37
32	s	405	WVN	C33-C34	3.98	1.54	1.45
38	i	314	II0	C41-C39	3.98	1.55	1.43
38	g	318	II0	C42-C40	3.97	1.55	1.43
32	F	204	WVN	C30-C28	3.97	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	204	WVN	C23-C25	3.97	1.54	1.45
38	b	315	II0	C33-C35	3.97	1.54	1.45
38	c	313	II0	C42-C40	3.97	1.55	1.43
32	L	206	WVN	C31-C32	3.97	1.54	1.45
38	a	314	II0	C33-C35	3.97	1.54	1.45
32	A	847	WVN	C30-C28	3.97	1.55	1.43
32	F	204	WVN	C31-C32	3.97	1.54	1.45
29	l	307	CLA	C1D-ND	3.96	1.42	1.37
29	d	310	CLA	C1D-ND	3.96	1.42	1.37
38	d	301	II0	C31-C29	3.96	1.55	1.43
29	i	309	CLA	C1D-ND	3.96	1.42	1.37
38	b	301	II0	C42-C40	3.96	1.55	1.43
38	a	317	II0	C33-C35	3.96	1.54	1.45
32	B	846	WVN	C30-C28	3.96	1.55	1.43
32	I	101	WVN	C40-C37	3.96	1.55	1.43
38	k	615	II0	C42-C40	3.96	1.55	1.43
32	B	848	WVN	C39-C36	3.96	1.55	1.43
32	s	405	WVN	C30-C28	3.96	1.55	1.43
32	L	205	WVN	C33-C34	3.96	1.54	1.45
32	R	201	WVN	C39-C36	3.96	1.55	1.43
38	j	316	II0	C34-C36	3.96	1.54	1.45
29	B	816	CLA	C1D-ND	3.96	1.42	1.37
38	m	616	II0	C42-C40	3.96	1.55	1.43
40	f	611	KC2	CHC-C4B	3.95	1.46	1.38
32	F	207	WVN	C23-C25	3.95	1.54	1.45
32	L	201	WVN	C31-C32	3.95	1.54	1.45
32	s	405	WVN	C40-C37	3.95	1.55	1.43
32	h	308	WVN	C40-C37	3.95	1.55	1.43
38	g	317	II0	C42-C40	3.95	1.55	1.43
38	j	316	II0	C33-C35	3.95	1.54	1.45
32	l	302	WVN	C39-C36	3.94	1.55	1.43
38	J	103	II0	C33-C35	3.94	1.54	1.45
29	i	305	CLA	C1D-ND	3.94	1.42	1.37
38	i	313	II0	C42-C40	3.94	1.55	1.43
32	s	405	WVN	C31-C32	3.94	1.54	1.45
38	f	614	II0	C42-C40	3.94	1.55	1.43
32	i	315	WVN	C30-C28	3.94	1.55	1.43
32	l	302	WVN	C31-C32	3.93	1.54	1.45
38	j	316	II0	C42-C40	3.93	1.55	1.43
38	n	618	II0	C34-C36	3.93	1.54	1.45
38	f	616	II0	C42-C40	3.93	1.55	1.43
32	L	201	WVN	C30-C28	3.93	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	619	II0	C33-C35	3.93	1.54	1.45
38	h	309	II0	C34-C36	3.93	1.54	1.45
32	i	315	WVN	C33-C34	3.93	1.54	1.45
38	k	615	II0	C34-C36	3.93	1.54	1.45
38	g	319	II0	C42-C40	3.93	1.55	1.43
38	a	317	II0	C42-C40	3.93	1.55	1.43
38	f	614	II0	C34-C36	3.93	1.54	1.45
38	d	316	II0	C34-C36	3.92	1.54	1.45
38	i	319	II0	C42-C40	3.92	1.55	1.43
40	n	612	KC2	C3B-C4B	-3.92	1.39	1.46
32	B	846	WVN	C40-C37	3.92	1.55	1.43
38	J	103	II0	C42-C40	3.92	1.55	1.43
32	A	854	WVN	C30-C28	3.92	1.55	1.43
38	d	317	II0	C42-C40	3.92	1.55	1.43
38	m	615	II0	C33-C35	3.92	1.54	1.45
32	J	101	WVN	C30-C28	3.92	1.55	1.43
32	B	846	WVN	C29-C26	3.92	1.55	1.43
32	M	101	WVN	C40-C37	3.92	1.55	1.43
38	e	314	II0	C33-C35	3.92	1.54	1.45
29	B	825	CLA	C1D-ND	3.91	1.42	1.37
40	k	613	KC2	C3B-C4B	-3.91	1.39	1.46
29	k	610	CLA	C1D-ND	3.91	1.42	1.37
32	e	315	WVN	C30-C28	3.91	1.55	1.43
38	b	315	II0	C34-C36	3.91	1.54	1.45
38	e	313	II0	C42-C40	3.91	1.55	1.43
32	B	848	WVN	C31-C32	3.91	1.54	1.45
32	F	205	WVN	C30-C28	3.91	1.55	1.43
32	A	844	WVN	C23-C25	3.91	1.54	1.45
38	f	618	II0	C42-C40	3.91	1.55	1.43
38	k	616	II0	C33-C35	3.91	1.54	1.45
32	A	854	WVN	C40-C37	3.91	1.55	1.43
32	J	101	WVN	C40-C37	3.91	1.55	1.43
38	n	615	II0	C34-C36	3.91	1.54	1.45
38	m	618	II0	C42-C40	3.91	1.55	1.43
38	i	316	II0	C34-C36	3.91	1.54	1.45
38	m	616	II0	C33-C35	3.90	1.54	1.45
40	c	310	KC2	C1B-NB	-3.90	1.33	1.37
32	L	201	WVN	C40-C37	3.90	1.55	1.43
38	n	616	II0	C42-C40	3.90	1.55	1.43
38	k	616	II0	C42-C40	3.90	1.55	1.43
32	B	847	WVN	C23-C25	3.90	1.54	1.45
38	n	618	II0	C42-C40	3.90	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	849	WVN	C30-C28	3.90	1.55	1.43
32	L	205	WVN	C30-C28	3.90	1.55	1.43
38	k	620	II0	C42-C40	3.90	1.55	1.43
29	b	311	CLA	C1D-ND	3.90	1.42	1.37
32	B	847	WVN	C30-C28	3.90	1.55	1.43
32	A	847	WVN	C23-C25	3.90	1.54	1.45
32	A	846	WVN	C40-C37	3.90	1.55	1.43
38	h	309	II0	C42-C40	3.90	1.55	1.43
32	I	101	WVN	C30-C28	3.89	1.55	1.43
29	n	610	CLA	C1D-ND	3.89	1.42	1.37
38	c	313	II0	C34-C36	3.89	1.54	1.45
32	A	844	WVN	C40-C37	3.89	1.55	1.43
38	m	614	II0	C42-C40	3.89	1.55	1.43
38	f	615	II0	C42-C40	3.89	1.55	1.43
29	n	608	CLA	C1D-ND	3.89	1.42	1.37
38	k	620	II0	C33-C35	3.89	1.54	1.45
29	k	601	CLA	C1D-ND	3.89	1.42	1.37
32	A	847	WVN	C33-C34	3.89	1.54	1.45
40	e	309	KC2	C4B-NB	-3.89	1.33	1.37
38	a	313	II0	C42-C40	3.88	1.55	1.43
38	b	301	II0	C33-C35	3.88	1.54	1.45
38	f	616	II0	C33-C35	3.88	1.54	1.45
32	A	844	WVN	C30-C28	3.88	1.55	1.43
38	l	313	II0	C41-C39	3.88	1.55	1.43
29	h	306	CLA	C1D-ND	3.88	1.42	1.37
32	s	405	WVN	C23-C25	3.88	1.54	1.45
32	s	407	WVN	C40-C37	3.88	1.55	1.43
40	i	318	KC2	CHC-C1C	3.88	1.48	1.39
38	c	313	II0	C33-C35	3.88	1.54	1.45
32	A	845	WVN	C40-C37	3.88	1.55	1.43
38	l	315	II0	C34-C36	3.88	1.54	1.45
32	L	205	WVN	C40-C37	3.88	1.55	1.43
29	B	835	CLA	C1D-ND	3.87	1.42	1.37
38	f	618	II0	C33-C35	3.87	1.54	1.45
32	B	847	WVN	C40-C37	3.87	1.55	1.43
38	g	317	II0	C34-C36	3.87	1.54	1.45
32	L	201	WVN	C23-C25	3.87	1.54	1.45
32	l	302	WVN	C30-C28	3.87	1.55	1.43
38	n	615	II0	C42-C40	3.87	1.55	1.43
38	k	619	II0	C42-C40	3.87	1.55	1.43
32	B	846	WVN	C23-C25	3.87	1.54	1.45
38	m	616	II0	C41-C39	3.87	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	c	310	KC2	CHC-C1C	3.87	1.48	1.39
38	b	315	II0	C42-C40	3.87	1.55	1.43
40	d	312	KC2	C3B-C4B	-3.87	1.39	1.46
32	B	849	WVN	C31-C32	3.87	1.54	1.45
38	j	301	II0	C42-C40	3.87	1.55	1.43
29	d	305	CLA	C1D-ND	3.87	1.42	1.37
38	f	616	II0	C34-C36	3.86	1.54	1.45
38	m	616	II0	C34-C36	3.86	1.54	1.45
38	e	312	II0	C42-C40	3.86	1.55	1.43
32	L	206	WVN	C40-C37	3.86	1.55	1.43
29	A	836	CLA	C1D-ND	3.86	1.42	1.37
32	i	315	WVN	C23-C25	3.86	1.54	1.45
29	n	613	CLA	C1D-ND	3.86	1.42	1.37
40	m	611	KC2	C1B-NB	-3.86	1.33	1.37
38	f	614	II0	C41-C39	3.86	1.55	1.43
38	d	315	II0	C42-C40	3.86	1.55	1.43
32	A	846	WVN	C23-C25	3.86	1.54	1.45
38	i	319	II0	C33-C35	3.86	1.54	1.45
38	e	312	II0	C41-C39	3.86	1.55	1.43
38	b	314	II0	C33-C35	3.86	1.54	1.45
32	M	101	WVN	C30-C28	3.86	1.55	1.43
38	c	313	II0	C41-C39	3.85	1.55	1.43
38	l	313	II0	C33-C35	3.85	1.54	1.45
32	F	204	WVN	C40-C37	3.85	1.55	1.43
29	f	604	CLA	C1D-ND	3.85	1.42	1.37
38	e	314	II0	C42-C40	3.85	1.55	1.43
29	d	303	CLA	C1D-ND	3.85	1.42	1.37
32	A	844	WVN	C33-C34	3.85	1.54	1.45
38	m	614	II0	C41-C39	3.85	1.55	1.43
38	d	316	II0	C41-C39	3.85	1.55	1.43
38	f	615	II0	C33-C35	3.85	1.54	1.45
40	k	611	KC2	CHC-C1C	3.85	1.48	1.39
32	i	315	WVN	C40-C37	3.85	1.55	1.43
32	B	848	WVN	C33-C34	3.85	1.54	1.45
38	g	319	II0	C33-C35	3.85	1.54	1.45
32	A	845	WVN	C23-C25	3.85	1.54	1.45
29	e	306	CLA	C1D-ND	3.85	1.42	1.37
29	e	310	CLA	C1D-ND	3.85	1.42	1.37
29	f	607	CLA	C1D-ND	3.85	1.42	1.37
38	e	313	II0	C33-C35	3.84	1.54	1.45
32	F	205	WVN	C40-C37	3.84	1.55	1.43
32	s	407	WVN	C30-C28	3.84	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	m	615	II0	C42-C40	3.84	1.55	1.43
38	j	301	II0	C41-C39	3.84	1.55	1.43
32	J	101	WVN	C23-C25	3.84	1.54	1.45
29	m	610	CLA	C1D-ND	3.84	1.42	1.37
29	g	303	CLA	C1D-ND	3.84	1.42	1.37
29	k	605	CLA	C1D-ND	3.84	1.42	1.37
29	m	601	CLA	C1D-ND	3.84	1.42	1.37
40	j	312	KC2	C1B-NB	-3.84	1.33	1.37
38	i	313	II0	C34-C36	3.83	1.54	1.45
38	b	314	II0	C42-C40	3.83	1.55	1.43
38	j	316	II0	C41-C39	3.83	1.55	1.43
29	m	605	CLA	C1D-ND	3.83	1.42	1.37
38	g	317	II0	C41-C39	3.83	1.55	1.43
29	c	309	CLA	C1D-ND	3.83	1.42	1.37
40	k	612	KC2	C4A-C3A	-3.83	1.37	1.44
38	h	310	II0	C42-C40	3.83	1.55	1.43
38	e	312	II0	C34-C36	3.82	1.54	1.45
29	b	302	CLA	C1D-ND	3.82	1.42	1.37
38	J	103	II0	C34-C36	3.82	1.54	1.45
38	h	311	II0	C42-C40	3.82	1.55	1.43
29	e	311	CLA	C1D-ND	3.82	1.42	1.37
38	n	618	II0	C33-C35	3.82	1.54	1.45
29	i	302	CLA	C1D-ND	3.82	1.42	1.37
38	m	614	II0	C33-C35	3.82	1.54	1.45
32	A	846	WVN	C31-C32	3.82	1.54	1.45
38	i	319	II0	C41-C39	3.82	1.55	1.43
38	h	311	II0	C33-C35	3.82	1.54	1.45
29	e	307	CLA	C1D-ND	3.82	1.42	1.37
29	m	607	CLA	C1D-ND	3.82	1.42	1.37
32	R	201	WVN	C40-C37	3.82	1.55	1.43
38	f	615	II0	C41-C39	3.82	1.55	1.43
38	m	614	II0	C34-C36	3.82	1.54	1.45
32	A	845	WVN	C33-C34	3.82	1.54	1.45
32	K	103	WVN	C40-C37	3.81	1.55	1.43
29	j	306	CLA	C1D-ND	3.81	1.42	1.37
38	e	313	II0	C41-C39	3.81	1.55	1.43
38	k	615	II0	C41-C39	3.81	1.55	1.43
38	a	317	II0	C41-C39	3.81	1.55	1.43
38	m	615	II0	C41-C39	3.81	1.55	1.43
29	h	305	CLA	C1D-ND	3.81	1.42	1.37
38	d	315	II0	C33-C35	3.81	1.54	1.45
38	g	319	II0	C34-C36	3.81	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	312	CLA	C1D-ND	3.81	1.42	1.37
38	i	316	II0	C42-C40	3.81	1.55	1.43
29	e	305	CLA	C1D-ND	3.81	1.42	1.37
38	k	619	II0	C41-C39	3.81	1.55	1.43
29	d	306	CLA	C1D-ND	3.81	1.42	1.37
38	l	315	II0	C42-C40	3.81	1.55	1.43
29	i	306	CLA	C1D-ND	3.81	1.42	1.37
32	A	845	WVN	C30-C28	3.80	1.55	1.43
29	k	609	CLA	C1D-ND	3.80	1.42	1.37
29	c	301	CLA	C1D-ND	3.80	1.42	1.37
38	J	103	II0	C41-C39	3.80	1.55	1.43
29	j	302	CLA	C1D-ND	3.80	1.42	1.37
32	R	201	WVN	C30-C28	3.80	1.55	1.43
40	i	310	KC2	CHC-C1C	3.80	1.47	1.39
29	O	206	CLA	C1D-ND	3.80	1.42	1.37
29	A	834	CLA	C1D-ND	3.80	1.42	1.37
29	g	312	CLA	C1D-ND	3.80	1.42	1.37
38	d	317	II0	C41-C39	3.80	1.55	1.43
29	j	314	CLA	C1D-ND	3.80	1.42	1.37
38	h	310	II0	C33-C35	3.80	1.54	1.45
38	f	618	II0	C41-C39	3.80	1.55	1.43
29	A	835	CLA	C1D-ND	3.80	1.42	1.37
38	g	318	II0	C41-C39	3.79	1.55	1.43
32	l	302	WVN	C40-C37	3.79	1.55	1.43
29	B	824	CLA	C1D-ND	3.79	1.42	1.37
29	h	307	CLA	C1D-ND	3.79	1.42	1.37
29	e	304	CLA	C1D-ND	3.79	1.42	1.37
29	R	203	CLA	C1D-ND	3.79	1.42	1.37
29	d	302	CLA	C1D-ND	3.79	1.42	1.37
38	i	313	II0	C41-C39	3.79	1.55	1.43
32	L	206	WVN	C30-C28	3.79	1.55	1.43
38	l	315	II0	C41-C39	3.79	1.55	1.43
29	l	301	CLA	C1D-ND	3.79	1.42	1.37
29	l	310	CLA	C1D-ND	3.79	1.42	1.37
38	e	314	II0	C34-C36	3.79	1.54	1.45
29	B	832	CLA	C1D-ND	3.79	1.42	1.37
38	k	620	II0	C34-C36	3.78	1.54	1.45
29	A	817	CLA	C1D-ND	3.78	1.42	1.37
29	e	308	CLA	C1D-ND	3.78	1.42	1.37
32	F	205	WVN	C39-C36	3.78	1.55	1.43
32	M	101	WVN	C23-C25	3.78	1.54	1.45
38	a	315	II0	C42-C40	3.78	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	f	616	II0	C41-C39	3.78	1.55	1.43
38	a	313	II0	C33-C35	3.78	1.54	1.45
38	j	315	II0	C34-C36	3.78	1.54	1.45
29	g	323	CLA	C1D-ND	3.78	1.42	1.37
32	F	207	WVN	C33-C34	3.78	1.54	1.45
32	B	848	WVN	C30-C28	3.78	1.55	1.43
29	A	837	CLA	C1D-ND	3.78	1.42	1.37
38	b	301	II0	C41-C39	3.78	1.55	1.43
38	k	616	II0	C41-C39	3.77	1.55	1.43
29	c	307	CLA	C1D-ND	3.77	1.42	1.37
29	j	304	CLA	C1D-ND	3.77	1.42	1.37
29	l	312	CLA	C1D-ND	3.77	1.42	1.37
29	a	309	CLA	C1D-ND	3.77	1.42	1.37
38	n	616	II0	C34-C36	3.77	1.54	1.45
29	m	604	CLA	C1D-ND	3.77	1.42	1.37
40	n	611	KC2	CHC-C1C	3.77	1.47	1.39
29	A	803	CLA	C4B-NB	3.77	1.42	1.37
29	B	838	CLA	C1D-ND	3.77	1.42	1.37
32	h	308	WVN	C23-C25	3.77	1.54	1.45
29	n	601	CLA	C1D-ND	3.77	1.42	1.37
38	e	314	II0	C41-C39	3.77	1.55	1.43
40	g	315	KC2	CHC-C1C	3.77	1.47	1.39
38	h	310	II0	C34-C36	3.76	1.54	1.45
38	i	313	II0	C33-C35	3.76	1.54	1.45
29	h	301	CLA	C1D-ND	3.76	1.42	1.37
32	I	101	WVN	C23-C25	3.76	1.54	1.45
29	e	303	CLA	C1D-ND	3.76	1.42	1.37
29	k	604	CLA	C1D-ND	3.76	1.42	1.37
29	b	305	CLA	C1D-ND	3.76	1.42	1.37
38	f	614	II0	C33-C35	3.76	1.54	1.45
29	f	601	CLA	C1D-ND	3.76	1.42	1.37
38	b	315	II0	C41-C39	3.75	1.55	1.43
29	A	807	CLA	C1D-ND	3.75	1.42	1.37
29	k	614	CLA	C1D-ND	3.75	1.42	1.37
38	k	620	II0	C41-C39	3.75	1.55	1.43
38	a	315	II0	C34-C36	3.75	1.54	1.45
29	s	402	CLA	C1D-ND	3.75	1.42	1.37
29	d	307	CLA	C1D-ND	3.75	1.42	1.37
38	n	615	II0	C41-C39	3.75	1.55	1.43
32	B	848	WVN	C40-C37	3.75	1.55	1.43
29	F	203	CLA	C1D-ND	3.75	1.42	1.37
40	k	613	KC2	C4A-C3A	-3.75	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	n	616	II0	C41-C39	3.75	1.55	1.43
29	A	811	CLA	C1D-ND	3.75	1.42	1.37
32	B	849	WVN	C40-C37	3.75	1.55	1.43
29	g	306	CLA	C1D-ND	3.75	1.42	1.37
38	d	315	II0	C41-C39	3.75	1.55	1.43
29	l	306	CLA	C1D-ND	3.74	1.42	1.37
38	j	315	II0	C33-C35	3.74	1.54	1.45
40	d	312	KC2	C1B-C2B	-3.74	1.37	1.45
29	F	202	CLA	C1D-ND	3.74	1.42	1.37
38	a	315	II0	C41-C39	3.74	1.55	1.43
38	j	315	II0	C42-C40	3.74	1.55	1.43
29	e	301	CLA	C1D-ND	3.74	1.42	1.37
29	l	303	CLA	C1D-ND	3.74	1.42	1.37
29	a	304	CLA	C1D-ND	3.74	1.42	1.37
29	j	309	CLA	C1D-ND	3.74	1.42	1.37
38	a	313	II0	C41-C39	3.74	1.55	1.43
38	g	319	II0	C41-C39	3.73	1.55	1.43
32	M	101	WVN	C33-C34	3.73	1.54	1.45
29	l	308	CLA	C1D-ND	3.73	1.42	1.37
38	n	618	II0	C41-C39	3.73	1.55	1.43
32	R	201	WVN	C23-C25	3.73	1.54	1.45
38	b	301	II0	C34-C36	3.73	1.54	1.45
38	j	301	II0	C34-C36	3.73	1.54	1.45
29	b	309	CLA	C1D-ND	3.73	1.42	1.37
29	k	606	CLA	C1D-ND	3.73	1.42	1.37
32	h	308	WVN	C33-C34	3.73	1.54	1.45
38	k	615	II0	C33-C35	3.73	1.54	1.45
29	A	822	CLA	C1D-ND	3.73	1.42	1.37
29	d	313	CLA	C1D-ND	3.73	1.42	1.37
29	n	606	CLA	C1D-ND	3.73	1.42	1.37
38	a	315	II0	C33-C35	3.73	1.54	1.45
29	B	815	CLA	C1D-ND	3.73	1.42	1.37
29	f	609	CLA	C1D-ND	3.73	1.42	1.37
32	l	316	WVN	C23-C25	3.73	1.53	1.45
32	K	103	WVN	C30-C28	3.72	1.55	1.43
32	B	848	WVN	C23-C25	3.72	1.53	1.45
40	e	309	KC2	CHC-C1C	3.72	1.47	1.39
29	B	806	CLA	C1D-ND	3.72	1.42	1.37
40	g	315	KC2	C1B-NB	-3.72	1.33	1.37
29	A	812	CLA	C1D-ND	3.72	1.42	1.37
38	i	316	II0	C33-C35	3.72	1.53	1.45
29	a	305	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	611	KC2	C1B-NB	-3.72	1.33	1.37
38	d	301	II0	C34-C36	3.72	1.53	1.45
29	j	311	CLA	C1D-ND	3.72	1.42	1.37
38	m	618	II0	C41-C39	3.72	1.55	1.43
29	j	307	CLA	C1D-ND	3.72	1.42	1.37
29	B	833	CLA	C1D-ND	3.71	1.42	1.37
29	s	406	CLA	C1D-ND	3.71	1.42	1.37
29	k	608	CLA	C1D-ND	3.71	1.42	1.37
32	e	315	WVN	C23-C25	3.71	1.53	1.45
29	J	102	CLA	C1D-ND	3.71	1.42	1.37
29	f	605	CLA	C1D-ND	3.71	1.42	1.37
29	g	305	CLA	C1D-ND	3.71	1.42	1.37
29	B	811	CLA	C1D-ND	3.71	1.42	1.37
29	A	851	CLA	C1D-ND	3.71	1.42	1.37
40	d	311	KC2	C1B-NB	-3.71	1.33	1.37
29	B	812	CLA	C1D-ND	3.71	1.42	1.37
40	g	315	KC2	C4B-NB	-3.71	1.33	1.37
29	a	311	CLA	C1D-ND	3.71	1.42	1.37
38	a	313	II0	C34-C36	3.71	1.53	1.45
29	L	204	CLA	C1D-ND	3.71	1.42	1.37
29	h	303	CLA	C1D-ND	3.71	1.42	1.37
29	g	316	CLA	C1D-ND	3.71	1.42	1.37
38	l	314	II0	C42-C40	3.71	1.54	1.43
29	c	303	CLA	C1D-ND	3.70	1.42	1.37
29	j	305	CLA	C1D-ND	3.70	1.42	1.37
32	F	205	WVN	C29-C26	3.70	1.54	1.43
29	m	609	CLA	C1D-ND	3.70	1.42	1.37
29	i	312	CLA	C1D-ND	3.70	1.42	1.37
29	m	608	CLA	C1D-ND	3.70	1.42	1.37
29	d	309	CLA	C1D-ND	3.70	1.42	1.37
29	A	814	CLA	C1D-ND	3.70	1.42	1.37
38	d	301	II0	C42-C40	3.70	1.54	1.43
32	F	205	WVN	C19-C22	3.70	1.53	1.45
29	B	810	CLA	C1D-ND	3.70	1.42	1.37
32	l	302	WVN	C23-C25	3.70	1.53	1.45
29	L	202	CLA	C1D-ND	3.69	1.42	1.37
29	A	840	CLA	C1D-ND	3.69	1.42	1.37
29	f	613	CLA	C1D-ND	3.69	1.42	1.37
38	b	314	II0	C41-C39	3.69	1.54	1.43
29	g	308	CLA	C1D-ND	3.69	1.42	1.37
40	i	310	KC2	C4B-NB	-3.69	1.33	1.37
29	A	837	CLA	C4B-NB	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	j	315	II0	C41-C39	3.69	1.54	1.43
29	c	302	CLA	C1D-ND	3.69	1.42	1.37
29	i	308	CLA	C1D-ND	3.69	1.42	1.37
29	A	813	CLA	C1D-ND	3.68	1.42	1.37
29	m	606	CLA	C1D-ND	3.68	1.42	1.37
29	B	803	CLA	C1D-ND	3.68	1.42	1.37
29	m	613	CLA	C1D-ND	3.68	1.42	1.37
38	e	312	II0	C33-C35	3.68	1.53	1.45
29	k	607	CLA	C1D-ND	3.68	1.42	1.37
29	c	312	CLA	C1D-ND	3.68	1.42	1.37
29	A	824	CLA	C1D-ND	3.68	1.42	1.37
29	m	603	CLA	C1D-ND	3.68	1.42	1.37
29	f	606	CLA	C1D-ND	3.68	1.42	1.37
29	g	307	CLA	C1D-ND	3.68	1.42	1.37
29	A	839	CLA	C1D-ND	3.67	1.42	1.37
29	B	821	CLA	C1D-ND	3.67	1.42	1.37
29	O	202	CLA	C1D-ND	3.67	1.42	1.37
38	i	316	II0	C41-C39	3.67	1.54	1.43
29	n	604	CLA	C1D-ND	3.67	1.42	1.37
29	g	309	CLA	C1D-ND	3.67	1.42	1.37
38	h	310	II0	C41-C39	3.67	1.54	1.43
38	n	616	II0	C33-C35	3.67	1.53	1.45
40	d	311	KC2	CHC-C1C	3.67	1.47	1.39
32	B	846	WVN	C31-C32	3.67	1.53	1.45
29	B	829	CLA	C1D-ND	3.66	1.42	1.37
29	n	603	CLA	C1D-ND	3.66	1.42	1.37
29	B	841	CLA	C4B-NB	3.66	1.42	1.37
29	B	841	CLA	C3B-C4B	3.66	1.51	1.42
29	F	201	CLA	C1D-ND	3.66	1.42	1.37
29	a	307	CLA	C1D-ND	3.66	1.42	1.37
29	A	821	CLA	C1D-ND	3.66	1.42	1.37
29	A	838	CLA	C1D-ND	3.66	1.42	1.37
29	j	310	CLA	C1D-ND	3.66	1.42	1.37
40	c	310	KC2	C4B-NB	-3.66	1.33	1.37
32	L	206	WVN	C23-C25	3.66	1.53	1.45
40	l	311	KC2	CHC-C1C	3.66	1.47	1.39
29	i	311	CLA	C1D-ND	3.66	1.42	1.37
32	F	205	WVN	C33-C34	3.66	1.53	1.45
40	k	613	KC2	C1B-C2B	-3.65	1.38	1.45
29	l	305	CLA	C1D-ND	3.65	1.42	1.37
40	k	612	KC2	C1B-C2B	-3.65	1.38	1.45
29	A	830	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	h	302	CLA	C1D-ND	3.65	1.42	1.37
29	g	310	CLA	C1D-ND	3.65	1.42	1.37
29	a	302	CLA	C1D-ND	3.65	1.42	1.37
29	B	822	CLA	C1D-ND	3.65	1.42	1.37
32	K	103	WVN	C23-C25	3.65	1.53	1.45
29	n	607	CLA	C1D-ND	3.65	1.42	1.37
29	A	806	CLA	C1D-ND	3.65	1.42	1.37
29	B	805	CLA	C1D-ND	3.65	1.42	1.37
29	n	605	CLA	C1D-ND	3.64	1.42	1.37
29	B	839	CLA	C1D-ND	3.64	1.42	1.37
29	d	308	CLA	C1D-ND	3.64	1.42	1.37
32	R	201	WVN	C33-C34	3.64	1.53	1.45
29	B	819	CLA	C1D-ND	3.64	1.42	1.37
32	K	103	WVN	C33-C34	3.64	1.53	1.45
29	b	306	CLA	C1D-ND	3.63	1.42	1.37
29	i	303	CLA	C1D-ND	3.63	1.42	1.37
38	h	309	II0	C41-C39	3.63	1.54	1.43
29	c	308	CLA	C1D-ND	3.63	1.42	1.37
29	B	840	CLA	C1D-ND	3.63	1.42	1.37
29	B	837	CLA	C1D-ND	3.63	1.42	1.37
29	b	304	CLA	C1D-ND	3.63	1.42	1.37
29	h	304	CLA	C1D-ND	3.63	1.42	1.37
29	h	312	CLA	C1D-ND	3.63	1.42	1.37
38	d	301	II0	C41-C39	3.62	1.54	1.43
32	s	407	WVN	C23-C25	3.62	1.53	1.45
29	g	304	CLA	C1D-ND	3.62	1.42	1.37
38	h	311	II0	C34-C36	3.62	1.53	1.45
40	m	611	KC2	CHC-C1C	3.62	1.47	1.39
29	b	313	CLA	C1D-ND	3.62	1.42	1.37
38	h	311	II0	C41-C39	3.62	1.54	1.43
29	c	304	CLA	C1D-ND	3.62	1.42	1.37
40	d	312	KC2	C4A-C3A	-3.61	1.37	1.44
29	b	307	CLA	C1D-ND	3.61	1.42	1.37
29	l	309	CLA	C1D-ND	3.61	1.42	1.37
29	B	807	CLA	C1D-ND	3.61	1.42	1.37
29	L	207	CLA	C1D-ND	3.61	1.42	1.37
29	i	304	CLA	C1D-ND	3.61	1.42	1.37
29	m	612	CLA	C1D-ND	3.61	1.42	1.37
29	b	310	CLA	C1D-ND	3.61	1.42	1.37
29	B	834	CLA	C1D-ND	3.60	1.42	1.37
29	j	308	CLA	C1D-ND	3.60	1.42	1.37
40	n	612	KC2	C4A-C3A	-3.60	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	603	CLA	C1D-ND	3.60	1.42	1.37
29	n	602	CLA	C1D-ND	3.60	1.42	1.37
29	a	312	CLA	C1D-ND	3.60	1.42	1.37
29	Q	302	CLA	C1D-ND	3.60	1.42	1.37
29	A	831	CLA	C1D-ND	3.60	1.42	1.37
29	A	826	CLA	C1D-ND	3.59	1.42	1.37
29	B	831	CLA	C1D-ND	3.59	1.42	1.37
29	l	304	CLA	C1D-ND	3.59	1.42	1.37
29	A	803	CLA	C1D-ND	3.59	1.42	1.37
29	a	303	CLA	C1D-ND	3.59	1.42	1.37
29	j	313	CLA	C1D-ND	3.59	1.42	1.37
29	i	307	CLA	C1D-ND	3.59	1.42	1.37
29	B	817	CLA	C1D-ND	3.59	1.42	1.37
29	b	310	CLA	C4B-NB	3.59	1.42	1.37
29	A	832	CLA	C1D-ND	3.59	1.42	1.37
29	O	201	CLA	C1D-ND	3.58	1.42	1.37
29	A	805	CLA	C1D-ND	3.58	1.42	1.37
29	B	828	CLA	C1D-ND	3.58	1.42	1.37
29	A	815	CLA	C1D-ND	3.58	1.42	1.37
40	k	611	KC2	C4B-NB	-3.58	1.33	1.37
29	A	819	CLA	C1D-ND	3.58	1.42	1.37
29	i	307	CLA	C4B-NB	3.58	1.42	1.37
29	a	308	CLA	C1D-ND	3.57	1.42	1.37
29	c	306	CLA	C1D-ND	3.57	1.42	1.37
29	f	608	CLA	C4B-NB	3.57	1.42	1.37
38	d	301	II0	C33-C35	3.57	1.53	1.45
40	n	612	KC2	C1B-C2B	-3.57	1.38	1.45
29	f	610	CLA	C1D-ND	3.57	1.42	1.37
29	n	609	CLA	C1D-ND	3.57	1.42	1.37
29	B	835	CLA	C4B-NB	3.57	1.42	1.37
40	s	404	KC2	C4A-C3A	3.57	1.51	1.44
29	A	809	CLA	C1D-ND	3.57	1.42	1.37
29	B	820	CLA	C1D-ND	3.56	1.42	1.37
38	h	309	II0	C33-C35	3.56	1.53	1.45
29	e	302	CLA	C1D-ND	3.56	1.42	1.37
29	B	813	CLA	C1D-ND	3.56	1.42	1.37
29	g	316	CLA	C4B-NB	3.55	1.42	1.37
29	A	829	CLA	C1D-ND	3.55	1.42	1.37
29	A	820	CLA	C1D-ND	3.55	1.42	1.37
40	l	311	KC2	C1A-CHA	3.54	1.50	1.40
29	B	808	CLA	C1D-ND	3.54	1.42	1.37
29	b	303	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	315	WVN	C20-C13	3.53	1.57	1.45
29	A	808	CLA	C1D-ND	3.53	1.42	1.37
29	A	818	CLA	C1D-ND	3.53	1.42	1.37
29	f	612	CLA	C1D-ND	3.53	1.42	1.37
29	k	603	CLA	C1D-ND	3.53	1.42	1.37
29	A	850	CLA	C1D-ND	3.52	1.42	1.37
29	k	609	CLA	C4B-NB	3.51	1.42	1.37
29	s	403	CLA	C1D-ND	3.50	1.42	1.37
29	m	602	CLA	C1D-ND	3.50	1.42	1.37
29	B	836	CLA	C1D-ND	3.50	1.42	1.37
29	A	825	CLA	C1D-ND	3.50	1.42	1.37
29	c	305	CLA	C1D-ND	3.50	1.42	1.37
40	e	309	KC2	C1B-NB	-3.50	1.33	1.37
29	i	305	CLA	C4B-NB	3.50	1.42	1.37
40	s	401	KC2	CHC-C1C	3.49	1.47	1.39
29	A	810	CLA	C1D-ND	3.49	1.42	1.37
29	k	614	CLA	C4B-NB	3.49	1.42	1.37
29	B	814	CLA	C1D-ND	3.48	1.42	1.37
32	R	202	WVN	C20-C13	3.48	1.57	1.45
40	n	612	KC2	C1C-C2C	-3.48	1.37	1.44
40	i	310	KC2	OBD-CAD	3.47	1.28	1.22
29	B	802	CLA	C1D-ND	3.47	1.42	1.37
29	B	842	CLA	C1D-ND	3.47	1.42	1.37
40	g	314	KC2	C1A-CHA	3.47	1.49	1.40
32	A	847	WVN	C20-C13	3.47	1.57	1.45
29	a	306	CLA	C1D-ND	3.46	1.42	1.37
40	s	404	KC2	C4B-NB	-3.46	1.33	1.37
29	g	302	CLA	C4D-ND	-3.46	1.32	1.37
29	n	610	CLA	C4B-NB	3.44	1.42	1.37
29	A	833	CLA	C1D-ND	3.44	1.42	1.37
40	m	611	KC2	OBD-CAD	3.44	1.28	1.22
29	B	818	CLA	C1D-ND	3.44	1.42	1.37
29	b	312	CLA	C4B-NB	3.44	1.42	1.37
29	R	203	CLA	C4B-NB	3.43	1.42	1.37
40	s	404	KC2	C1A-CHA	3.43	1.49	1.40
29	g	302	CLA	C1D-ND	3.43	1.42	1.37
40	i	318	KC2	C4B-NB	-3.43	1.33	1.37
29	g	311	CLA	C1D-ND	3.43	1.42	1.37
29	s	402	CLA	C4B-NB	3.42	1.42	1.37
29	b	305	CLA	C4B-NB	3.42	1.42	1.37
40	f	611	KC2	OBD-CAD	3.42	1.28	1.22
29	d	310	CLA	C4B-NB	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	s	404	KC2	CHC-C1C	3.42	1.47	1.39
29	b	308	CLA	C1D-ND	3.42	1.42	1.37
29	B	823	CLA	C1D-ND	3.42	1.42	1.37
29	B	809	CLA	C1D-ND	3.41	1.42	1.37
29	l	301	CLA	C4B-NB	3.41	1.42	1.37
29	k	602	CLA	C1D-ND	3.41	1.42	1.37
29	A	804	CLA	C1D-ND	3.40	1.42	1.37
29	F	203	CLA	C4B-NB	3.40	1.42	1.37
32	s	405	WVN	C20-C13	3.40	1.57	1.45
29	d	305	CLA	C4B-NB	3.40	1.42	1.37
29	a	307	CLA	C4B-NB	3.40	1.42	1.37
38	k	615	II0	C20-C14	3.39	1.56	1.50
29	e	311	CLA	C4B-NB	3.39	1.42	1.37
40	k	612	KC2	C1C-C2C	-3.39	1.38	1.44
40	i	318	KC2	OBD-CAD	3.39	1.28	1.22
29	F	202	CLA	C3B-C4B	3.39	1.50	1.42
29	f	602	CLA	C1D-ND	3.39	1.42	1.37
29	a	310	CLA	C1D-ND	3.39	1.41	1.37
29	A	816	CLA	C1D-ND	3.39	1.41	1.37
29	d	306	CLA	C4B-NB	3.39	1.41	1.37
29	n	603	CLA	C4B-NB	3.38	1.41	1.37
32	e	315	WVN	C20-C13	3.38	1.57	1.45
29	e	305	CLA	C4B-NB	3.38	1.41	1.37
40	e	309	KC2	CHD-C1D	3.38	1.47	1.39
29	A	850	CLA	C4D-ND	-3.38	1.33	1.37
29	A	806	CLA	C4B-NB	3.38	1.41	1.37
40	k	613	KC2	C1C-C2C	-3.38	1.38	1.44
29	a	311	CLA	C4B-NB	3.37	1.41	1.37
29	A	838	CLA	C4B-NB	3.37	1.41	1.37
29	B	804	CLA	C4D-ND	-3.37	1.33	1.37
40	g	315	KC2	C1A-CHA	3.37	1.49	1.40
29	f	605	CLA	C4B-NB	3.36	1.41	1.37
29	B	820	CLA	C4B-NB	3.36	1.41	1.37
29	j	303	CLA	C1D-ND	3.36	1.41	1.37
29	A	813	CLA	C4B-NB	3.36	1.41	1.37
29	B	827	CLA	C1D-ND	3.35	1.41	1.37
29	A	828	CLA	C1D-ND	3.35	1.41	1.37
40	f	611	KC2	CHC-C1C	3.35	1.46	1.39
40	k	611	KC2	C1A-CHA	3.35	1.49	1.40
29	B	801	CLA	C4B-NB	3.35	1.41	1.37
29	B	821	CLA	C4D-ND	-3.34	1.33	1.37
29	B	827	CLA	C4B-NB	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	d	311	KC2	OBD-CAD	3.34	1.28	1.22
29	A	811	CLA	C4B-NB	3.34	1.41	1.37
29	c	305	CLA	C4B-NB	3.34	1.41	1.37
29	d	307	CLA	C4B-NB	3.34	1.41	1.37
40	n	611	KC2	OBD-CAD	3.34	1.28	1.22
29	n	613	CLA	C4B-NB	3.33	1.41	1.37
29	K	101	CLA	C1D-ND	3.33	1.41	1.37
29	L	207	CLA	C4B-NB	3.33	1.41	1.37
40	g	314	KC2	CHC-C1C	3.33	1.46	1.39
40	k	611	KC2	OBD-CAD	3.33	1.28	1.22
29	A	829	CLA	C4B-NB	3.33	1.41	1.37
29	j	314	CLA	C4B-NB	3.33	1.41	1.37
40	j	312	KC2	OBD-CAD	3.33	1.28	1.22
29	B	830	CLA	C1D-ND	3.33	1.41	1.37
29	g	308	CLA	C4B-NB	3.33	1.41	1.37
29	a	312	CLA	C4B-NB	3.33	1.41	1.37
29	d	304	CLA	C4B-NB	3.33	1.41	1.37
29	m	601	CLA	C4B-NB	3.32	1.41	1.37
29	b	302	CLA	C4B-NB	3.32	1.41	1.37
40	e	309	KC2	OBD-CAD	3.32	1.28	1.22
29	B	819	CLA	C4B-NB	3.32	1.41	1.37
40	l	311	KC2	OBD-CAD	3.31	1.28	1.22
29	l	310	CLA	C4B-NB	3.31	1.41	1.37
29	k	603	CLA	C4B-NB	3.31	1.41	1.37
29	g	303	CLA	C4B-NB	3.31	1.41	1.37
29	B	810	CLA	C4B-NB	3.31	1.41	1.37
29	a	307	CLA	C3B-C4B	3.31	1.50	1.42
29	n	608	CLA	C4B-NB	3.31	1.41	1.37
29	c	301	CLA	C4B-NB	3.30	1.41	1.37
29	d	318	CLA	C4B-NB	3.30	1.41	1.37
29	B	839	CLA	C4B-NB	3.30	1.41	1.37
29	A	819	CLA	C4D-ND	-3.30	1.33	1.37
29	B	837	CLA	C4B-NB	3.30	1.41	1.37
29	A	818	CLA	C4D-ND	-3.30	1.33	1.37
29	A	825	CLA	C4D-ND	-3.30	1.33	1.37
40	i	318	KC2	C1A-CHA	3.30	1.49	1.40
40	i	318	KC2	CHD-C1D	3.30	1.46	1.39
29	i	306	CLA	C4B-NB	3.30	1.41	1.37
40	g	313	KC2	CHC-C1C	3.30	1.46	1.39
32	h	308	WVN	C20-C13	3.29	1.56	1.45
29	c	312	CLA	C4B-NB	3.29	1.41	1.37
29	d	308	CLA	C4B-NB	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	834	CLA	C4B-NB	3.29	1.41	1.37
29	A	838	CLA	C4D-ND	-3.29	1.33	1.37
29	h	301	CLA	C4B-NB	3.29	1.41	1.37
40	s	401	KC2	C1A-CHA	3.29	1.49	1.40
29	g	302	CLA	C4B-NB	3.29	1.41	1.37
29	e	301	CLA	C4B-NB	3.29	1.41	1.37
29	l	303	CLA	C4B-NB	3.29	1.41	1.37
29	j	306	CLA	C4B-NB	3.29	1.41	1.37
29	B	832	CLA	C4B-NB	3.29	1.41	1.37
29	d	313	CLA	C4B-NB	3.28	1.41	1.37
29	f	606	CLA	C4B-NB	3.28	1.41	1.37
29	A	822	CLA	C4B-NB	3.28	1.41	1.37
29	h	303	CLA	C4B-NB	3.28	1.41	1.37
29	Q	302	CLA	C4B-NB	3.28	1.41	1.37
29	F	202	CLA	C4B-NB	3.28	1.41	1.37
40	j	312	KC2	CHC-C1C	3.28	1.46	1.39
29	B	811	CLA	C4B-NB	3.28	1.41	1.37
29	A	817	CLA	C4D-ND	-3.27	1.33	1.37
29	b	311	CLA	C4D-ND	-3.27	1.33	1.37
29	j	304	CLA	C4B-NB	3.27	1.41	1.37
29	j	313	CLA	C4B-NB	3.27	1.41	1.37
29	f	601	CLA	C4B-NB	3.27	1.41	1.37
32	A	844	WVN	C20-C13	3.27	1.56	1.45
32	A	854	WVN	C19-C11	3.27	1.40	1.32
29	m	613	CLA	C4B-NB	3.27	1.41	1.37
29	a	310	CLA	C4D-ND	-3.27	1.33	1.37
40	g	313	KC2	CHD-C1D	3.27	1.46	1.39
29	k	606	CLA	C4B-NB	3.27	1.41	1.37
29	f	604	CLA	C4B-NB	3.27	1.41	1.37
40	d	312	KC2	C1C-C2C	-3.26	1.38	1.44
29	B	841	CLA	C4D-ND	-3.26	1.33	1.37
29	h	307	CLA	C4B-NB	3.26	1.41	1.37
29	i	302	CLA	C4B-NB	3.26	1.41	1.37
29	B	801	CLA	C1D-ND	3.26	1.41	1.37
29	g	307	CLA	C4B-NB	3.26	1.41	1.37
29	L	203	CLA	C1D-ND	3.26	1.41	1.37
29	n	604	CLA	C4B-NB	3.26	1.41	1.37
29	A	834	CLA	C4D-ND	-3.25	1.33	1.37
29	k	605	CLA	C4B-NB	3.25	1.41	1.37
29	O	206	CLA	C4B-NB	3.25	1.41	1.37
29	B	828	CLA	C4D-ND	-3.25	1.33	1.37
29	g	312	CLA	C4B-NB	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g	323	CLA	C4B-NB	3.25	1.41	1.37
29	B	842	CLA	C4D-ND	-3.25	1.33	1.37
29	l	306	CLA	C4B-NB	3.25	1.41	1.37
29	c	309	CLA	C4B-NB	3.24	1.41	1.37
29	g	305	CLA	C4B-NB	3.24	1.41	1.37
29	j	302	CLA	C4B-NB	3.24	1.41	1.37
29	A	831	CLA	C4B-NB	3.24	1.41	1.37
29	i	311	CLA	C4B-NB	3.24	1.41	1.37
29	n	606	CLA	C4B-NB	3.24	1.41	1.37
29	j	309	CLA	C4B-NB	3.24	1.41	1.37
29	A	829	CLA	C4D-ND	-3.24	1.33	1.37
29	B	818	CLA	C4B-NB	3.24	1.41	1.37
29	e	308	CLA	C4B-NB	3.24	1.41	1.37
29	j	311	CLA	C4B-NB	3.24	1.41	1.37
29	c	303	CLA	C4B-NB	3.23	1.41	1.37
29	J	102	CLA	C4B-NB	3.23	1.41	1.37
29	B	833	CLA	C4D-ND	-3.23	1.33	1.37
29	B	813	CLA	C4B-NB	3.23	1.41	1.37
29	n	601	CLA	C4B-NB	3.23	1.41	1.37
32	B	846	WVN	C20-C13	3.23	1.56	1.45
30	B	843	PQN	C10-C1	-3.23	1.42	1.48
29	A	835	CLA	C4B-NB	3.23	1.41	1.37
29	F	201	CLA	C4B-NB	3.23	1.41	1.37
29	B	838	CLA	C4B-NB	3.23	1.41	1.37
29	A	809	CLA	C4B-NB	3.22	1.41	1.37
29	m	607	CLA	C4B-NB	3.22	1.41	1.37
29	A	830	CLA	C4B-NB	3.22	1.41	1.37
29	c	311	CLA	C4B-NB	3.22	1.41	1.37
29	B	841	CLA	C1D-ND	3.22	1.41	1.37
29	f	603	CLA	C4B-NB	3.22	1.41	1.37
29	A	836	CLA	C4B-NB	3.22	1.41	1.37
29	B	819	CLA	C4D-ND	-3.22	1.33	1.37
29	l	307	CLA	C4B-NB	3.22	1.41	1.37
29	A	833	CLA	C4B-NB	3.22	1.41	1.37
30	B	843	PQN	C3-C4	-3.21	1.39	1.47
40	e	309	KC2	C1A-CHA	3.21	1.49	1.40
29	B	811	CLA	C3B-C4B	3.21	1.50	1.42
29	f	604	CLA	C4D-ND	-3.21	1.33	1.37
29	s	406	CLA	C4B-NB	3.21	1.41	1.37
29	A	810	CLA	C4B-NB	3.21	1.41	1.37
29	B	806	CLA	C4D-ND	-3.21	1.33	1.37
29	i	307	CLA	C3B-C4B	3.21	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	809	CLA	C4B-NB	3.21	1.41	1.37
29	n	605	CLA	C4B-NB	3.21	1.41	1.37
29	A	830	CLA	C4D-ND	-3.21	1.33	1.37
29	F	202	CLA	C4D-ND	-3.20	1.33	1.37
29	A	832	CLA	C4B-NB	3.20	1.41	1.37
29	k	610	CLA	C4B-NB	3.20	1.41	1.37
29	h	306	CLA	C4B-NB	3.20	1.41	1.37
29	g	304	CLA	C4B-NB	3.20	1.41	1.37
29	B	828	CLA	C4B-NB	3.20	1.41	1.37
29	f	607	CLA	C4B-NB	3.19	1.41	1.37
29	A	821	CLA	C4D-ND	-3.19	1.33	1.37
29	a	303	CLA	C4D-ND	-3.19	1.33	1.37
29	g	323	CLA	C4D-ND	-3.19	1.33	1.37
40	d	311	KC2	CHD-C1D	3.19	1.46	1.39
40	i	310	KC2	CHD-C1D	3.19	1.46	1.39
29	A	851	CLA	C4B-NB	3.19	1.41	1.37
29	b	307	CLA	C4B-NB	3.19	1.41	1.37
29	B	840	CLA	C4D-ND	-3.19	1.33	1.37
29	c	306	CLA	C4B-NB	3.19	1.41	1.37
29	L	202	CLA	C4B-NB	3.19	1.41	1.37
29	g	305	CLA	C4D-ND	-3.18	1.33	1.37
40	k	611	KC2	CHD-C1D	3.18	1.46	1.39
29	b	308	CLA	C4D-ND	-3.18	1.33	1.37
29	l	301	CLA	C3B-C4B	3.18	1.50	1.42
29	b	311	CLA	C4B-NB	3.18	1.41	1.37
29	m	606	CLA	C4B-NB	3.18	1.41	1.37
29	j	308	CLA	C4D-ND	-3.18	1.33	1.37
29	B	831	CLA	C4D-ND	-3.18	1.33	1.37
29	m	610	CLA	C4B-NB	3.18	1.41	1.37
29	l	312	CLA	C4B-NB	3.18	1.41	1.37
29	f	613	CLA	C4B-NB	3.18	1.41	1.37
29	B	815	CLA	C4B-NB	3.18	1.41	1.37
29	h	312	CLA	C4D-ND	-3.18	1.33	1.37
40	n	611	KC2	C1A-CHA	3.18	1.49	1.40
29	m	605	CLA	C4B-NB	3.18	1.41	1.37
29	A	808	CLA	C4B-NB	3.17	1.41	1.37
29	B	804	CLA	C1D-ND	3.17	1.41	1.37
29	B	817	CLA	C4B-NB	3.17	1.41	1.37
29	A	821	CLA	C4B-NB	3.17	1.41	1.37
29	j	303	CLA	C4D-ND	-3.17	1.33	1.37
29	i	304	CLA	C4B-NB	3.17	1.41	1.37
40	f	611	KC2	C1A-CHA	3.17	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	313	KC2	OBD-CAD	3.17	1.27	1.22
29	s	403	CLA	C4B-NB	3.17	1.41	1.37
29	a	306	CLA	C4B-NB	3.17	1.41	1.37
29	B	835	CLA	C4D-ND	-3.16	1.33	1.37
40	g	314	KC2	OBD-CAD	3.16	1.27	1.22
29	j	305	CLA	C4B-NB	3.16	1.41	1.37
29	K	101	CLA	C4D-ND	-3.16	1.33	1.37
40	g	315	KC2	OBD-CAD	3.16	1.27	1.22
29	j	307	CLA	C4B-NB	3.16	1.41	1.37
29	m	612	CLA	C4B-NB	3.16	1.41	1.37
29	k	608	CLA	C4B-NB	3.16	1.41	1.37
29	B	826	CLA	C1D-ND	3.16	1.41	1.37
29	e	303	CLA	C4B-NB	3.16	1.41	1.37
29	A	827	CLA	C4B-NB	3.16	1.41	1.37
29	h	302	CLA	C4B-NB	3.15	1.41	1.37
29	A	810	CLA	C4D-ND	-3.15	1.33	1.37
29	L	204	CLA	C4D-ND	-3.15	1.33	1.37
29	A	802	CLA	C1D-ND	3.15	1.41	1.37
29	B	814	CLA	C4B-NB	3.15	1.41	1.37
29	B	817	CLA	C4D-ND	-3.15	1.33	1.37
29	B	836	CLA	C4D-ND	-3.15	1.33	1.37
29	A	806	CLA	C3B-C4B	3.15	1.50	1.42
29	A	828	CLA	C4B-NB	3.15	1.41	1.37
29	i	312	CLA	C4B-NB	3.15	1.41	1.37
29	a	311	CLA	C4D-ND	-3.15	1.33	1.37
29	h	305	CLA	C4B-NB	3.15	1.41	1.37
29	j	310	CLA	C4B-NB	3.15	1.41	1.37
29	A	811	CLA	C4D-ND	-3.15	1.33	1.37
29	f	610	CLA	C4B-NB	3.14	1.41	1.37
29	i	305	CLA	C4D-ND	-3.14	1.33	1.37
29	b	306	CLA	C4B-NB	3.14	1.41	1.37
40	g	314	KC2	CHD-C1D	3.14	1.46	1.39
29	b	305	CLA	C4D-ND	-3.14	1.33	1.37
29	i	312	CLA	C4D-ND	-3.14	1.33	1.37
29	A	818	CLA	C4B-NB	3.14	1.41	1.37
29	a	305	CLA	C4D-ND	-3.14	1.33	1.37
29	k	607	CLA	C4B-NB	3.14	1.41	1.37
29	a	304	CLA	C4B-NB	3.14	1.41	1.37
29	b	310	CLA	C3B-C4B	3.14	1.50	1.42
40	l	311	KC2	C4A-C3A	3.14	1.50	1.44
40	l	311	KC2	CHD-C1D	3.13	1.46	1.39
29	B	807	CLA	C4D-ND	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	602	CLA	C4D-ND	-3.13	1.33	1.37
29	F	203	CLA	C3B-C4B	3.13	1.50	1.42
29	A	838	CLA	C3B-C4B	3.13	1.50	1.42
29	e	304	CLA	C4B-NB	3.13	1.41	1.37
29	n	607	CLA	C4B-NB	3.13	1.41	1.37
29	A	819	CLA	C4B-NB	3.13	1.41	1.37
32	L	206	WVN	C19-C11	3.13	1.39	1.32
29	A	804	CLA	C4B-NB	3.13	1.41	1.37
29	A	820	CLA	C4B-NB	3.13	1.41	1.37
29	A	823	CLA	C4B-NB	3.13	1.41	1.37
29	m	608	CLA	C4B-NB	3.12	1.41	1.37
29	B	840	CLA	C4B-NB	3.12	1.41	1.37
29	h	312	CLA	C4B-NB	3.12	1.41	1.37
29	m	601	CLA	C3B-C4B	3.12	1.50	1.42
29	k	601	CLA	C4B-NB	3.12	1.41	1.37
40	f	611	KC2	CHD-C1D	3.12	1.46	1.39
29	B	809	CLA	C4D-ND	-3.12	1.33	1.37
29	B	830	CLA	C4B-NB	3.12	1.41	1.37
29	l	304	CLA	C4D-ND	-3.12	1.33	1.37
29	B	819	CLA	C3B-C4B	3.12	1.50	1.42
29	l	305	CLA	C4B-NB	3.12	1.41	1.37
29	b	307	CLA	C4D-ND	-3.12	1.33	1.37
29	A	825	CLA	C4B-NB	3.12	1.41	1.37
29	a	312	CLA	C4D-ND	-3.12	1.33	1.37
29	i	309	CLA	C4B-NB	3.12	1.41	1.37
40	m	611	KC2	C1A-CHA	3.12	1.48	1.40
29	d	309	CLA	C4B-NB	3.12	1.41	1.37
29	A	816	CLA	C4B-NB	3.11	1.41	1.37
29	h	304	CLA	C4D-ND	-3.11	1.33	1.37
29	B	829	CLA	C4B-NB	3.11	1.41	1.37
29	g	306	CLA	C4D-ND	-3.11	1.33	1.37
29	n	607	CLA	C4D-ND	-3.11	1.33	1.37
29	a	309	CLA	C4B-NB	3.11	1.41	1.37
29	e	307	CLA	C4B-NB	3.11	1.41	1.37
29	B	811	CLA	C4D-ND	-3.11	1.33	1.37
29	A	832	CLA	C4D-ND	-3.11	1.33	1.37
29	n	609	CLA	C4D-ND	-3.11	1.33	1.37
40	s	401	KC2	OBD-CAD	3.11	1.27	1.22
29	B	808	CLA	C4B-NB	3.11	1.41	1.37
29	A	833	CLA	C4D-ND	-3.11	1.33	1.37
29	k	603	CLA	C3B-C4B	3.11	1.50	1.42
29	a	305	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	k	604	CLA	C4B-NB	3.10	1.41	1.37
29	g	310	CLA	C4B-NB	3.10	1.41	1.37
29	m	602	CLA	C4D-ND	-3.10	1.33	1.37
29	a	310	CLA	C4B-NB	3.10	1.41	1.37
29	B	842	CLA	C4B-NB	3.10	1.41	1.37
29	A	806	CLA	C4D-ND	-3.10	1.33	1.37
29	A	808	CLA	C4D-ND	-3.10	1.33	1.37
29	B	826	CLA	C4B-NB	3.10	1.41	1.37
29	s	406	CLA	C4D-ND	-3.10	1.33	1.37
29	c	302	CLA	C4D-ND	-3.10	1.33	1.37
29	L	203	CLA	C4D-ND	-3.10	1.33	1.37
29	B	805	CLA	C4B-NB	3.10	1.41	1.37
29	B	836	CLA	C4B-NB	3.10	1.41	1.37
29	b	312	CLA	C4D-ND	-3.10	1.33	1.37
29	B	812	CLA	C4D-ND	-3.10	1.33	1.37
29	n	609	CLA	C4B-NB	3.10	1.41	1.37
29	A	827	CLA	C3B-C4B	3.10	1.50	1.42
29	B	802	CLA	C4B-NB	3.09	1.41	1.37
29	B	821	CLA	C4B-NB	3.09	1.41	1.37
29	A	835	CLA	C4D-ND	-3.09	1.33	1.37
29	F	203	CLA	C4D-ND	-3.09	1.33	1.37
29	l	309	CLA	C4B-NB	3.09	1.41	1.37
29	A	807	CLA	C4D-ND	-3.09	1.33	1.37
40	j	312	KC2	C1A-CHA	3.09	1.48	1.40
29	A	826	CLA	C4D-ND	-3.09	1.33	1.37
29	B	818	CLA	C4D-ND	-3.09	1.33	1.37
29	f	609	CLA	C4D-ND	-3.09	1.33	1.37
29	g	311	CLA	C4B-NB	3.09	1.41	1.37
29	c	304	CLA	C4D-ND	-3.09	1.33	1.37
29	B	822	CLA	C4D-ND	-3.09	1.33	1.37
29	g	311	CLA	C3B-C4B	3.08	1.50	1.42
29	c	304	CLA	C4B-NB	3.08	1.41	1.37
29	b	313	CLA	C4B-NB	3.08	1.41	1.37
29	A	837	CLA	C3B-C4B	3.08	1.50	1.42
29	A	825	CLA	C3B-C4B	3.08	1.50	1.42
29	L	207	CLA	C4D-ND	-3.08	1.33	1.37
30	A	841	PQN	C3-C4	-3.08	1.39	1.47
29	e	306	CLA	C4B-NB	3.08	1.41	1.37
29	L	204	CLA	C4B-NB	3.08	1.41	1.37
29	c	308	CLA	C4B-NB	3.07	1.41	1.37
29	b	306	CLA	C4D-ND	-3.07	1.33	1.37
29	l	308	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	309	CLA	C4D-ND	-3.07	1.33	1.37
29	b	304	CLA	C4B-NB	3.07	1.41	1.37
40	g	313	KC2	C1A-CHA	3.07	1.48	1.40
29	R	203	CLA	C4D-ND	-3.07	1.33	1.37
32	F	205	WVN	C31-C32	3.07	1.52	1.45
29	h	302	CLA	C4D-ND	-3.07	1.33	1.37
40	i	310	KC2	C1A-CHA	3.07	1.48	1.40
29	O	202	CLA	C4D-ND	-3.07	1.33	1.37
29	k	602	CLA	C4D-ND	-3.07	1.33	1.37
29	g	307	CLA	C4D-ND	-3.07	1.33	1.37
29	A	824	CLA	C4B-NB	3.07	1.41	1.37
29	a	302	CLA	C4B-NB	3.06	1.41	1.37
29	A	805	CLA	C4D-ND	-3.06	1.33	1.37
29	A	814	CLA	C4B-NB	3.06	1.41	1.37
29	f	607	CLA	C4D-ND	-3.06	1.33	1.37
40	g	315	KC2	CHD-C1D	3.06	1.46	1.39
29	B	831	CLA	C4B-NB	3.06	1.41	1.37
29	m	603	CLA	C4B-NB	3.06	1.41	1.37
29	j	305	CLA	C4D-ND	-3.06	1.33	1.37
32	F	205	WVN	C23-C25	3.06	1.52	1.45
29	F	201	CLA	C3B-C4B	3.06	1.49	1.42
29	J	102	CLA	C3B-C4B	3.06	1.49	1.42
29	A	850	CLA	C4B-NB	3.06	1.41	1.37
29	B	801	CLA	C4D-ND	-3.05	1.33	1.37
29	f	608	CLA	C3B-C4B	3.05	1.49	1.42
29	c	307	CLA	C4B-NB	3.05	1.41	1.37
29	B	806	CLA	C4B-NB	3.05	1.41	1.37
29	B	829	CLA	C4D-ND	-3.05	1.33	1.37
40	m	611	KC2	CHD-C1D	3.05	1.46	1.39
40	s	404	KC2	CHD-C1D	3.05	1.46	1.39
29	A	802	CLA	C4B-NB	3.05	1.41	1.37
29	k	609	CLA	C3B-C4B	3.05	1.49	1.42
29	B	809	CLA	CMB-C2B	-3.05	1.44	1.50
29	m	604	CLA	C4B-NB	3.05	1.41	1.37
29	B	833	CLA	C3B-C4B	3.05	1.49	1.42
29	A	820	CLA	C4D-ND	-3.04	1.33	1.37
29	h	306	CLA	C4D-ND	-3.04	1.33	1.37
29	m	607	CLA	C4D-ND	-3.04	1.33	1.37
32	l	302	WVN	C20-C13	3.04	1.55	1.45
29	n	602	CLA	C4D-ND	-3.04	1.33	1.37
29	A	840	CLA	C4B-NB	3.04	1.41	1.37
29	B	825	CLA	C4B-NB	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	829	CLA	CMB-C2B	-3.04	1.44	1.50
29	i	303	CLA	C4B-NB	3.04	1.41	1.37
32	B	847	WVN	C20-C13	3.04	1.55	1.45
32	A	854	WVN	C20-C13	3.04	1.55	1.45
29	A	823	CLA	C4D-ND	-3.04	1.33	1.37
29	g	309	CLA	C4D-ND	-3.04	1.33	1.37
29	A	804	CLA	C4D-ND	-3.04	1.33	1.37
29	A	815	CLA	C4D-ND	-3.04	1.33	1.37
29	h	301	CLA	C4D-ND	-3.04	1.33	1.37
29	B	823	CLA	C4B-NB	3.03	1.41	1.37
29	K	101	CLA	C4B-NB	3.03	1.41	1.37
29	l	308	CLA	C4D-ND	-3.03	1.33	1.37
29	h	305	CLA	C4D-ND	-3.03	1.33	1.37
29	j	313	CLA	C3B-C4B	3.03	1.49	1.42
29	B	826	CLA	C4D-ND	-3.03	1.33	1.37
29	h	303	CLA	C4D-ND	-3.03	1.33	1.37
29	B	822	CLA	C4B-NB	3.03	1.41	1.37
40	c	310	KC2	OBD-CAD	3.03	1.27	1.22
29	F	201	CLA	C4D-ND	-3.03	1.33	1.37
29	c	308	CLA	C4D-ND	-3.03	1.33	1.37
29	e	307	CLA	C4D-ND	-3.03	1.33	1.37
29	L	203	CLA	C4B-NB	3.03	1.41	1.37
29	m	608	CLA	C4D-ND	-3.03	1.33	1.37
29	A	839	CLA	C4B-NB	3.03	1.41	1.37
29	B	827	CLA	C4D-ND	-3.03	1.33	1.37
29	d	309	CLA	C4D-ND	-3.02	1.33	1.37
32	B	849	WVN	C20-C13	3.02	1.55	1.45
29	g	308	CLA	C3B-C4B	3.02	1.49	1.42
29	f	612	CLA	C4B-NB	3.02	1.41	1.37
29	c	306	CLA	C4D-ND	-3.02	1.33	1.37
29	f	612	CLA	C4D-ND	-3.02	1.33	1.37
29	O	202	CLA	C4B-NB	3.02	1.41	1.37
29	k	602	CLA	C4B-NB	3.02	1.41	1.37
29	B	803	CLA	C4B-NB	3.01	1.41	1.37
29	c	307	CLA	C4D-ND	-3.01	1.33	1.37
29	e	310	CLA	C4B-NB	3.01	1.41	1.37
40	j	312	KC2	CHD-C1D	3.01	1.46	1.39
29	B	824	CLA	C4D-ND	-3.01	1.33	1.37
29	A	839	CLA	C4D-ND	-3.01	1.33	1.37
29	A	809	CLA	C4D-ND	-3.01	1.33	1.37
32	F	207	WVN	C20-C13	3.01	1.55	1.45
29	b	303	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	i	301	LMU	C6'-C5'	-3.01	1.41	1.51
29	b	304	CLA	C3B-C4B	3.01	1.49	1.42
29	A	831	CLA	C4D-ND	-3.01	1.33	1.37
29	m	613	CLA	C4D-ND	-3.01	1.33	1.37
29	B	833	CLA	C4B-NB	3.01	1.41	1.37
29	c	305	CLA	C4D-ND	-3.00	1.33	1.37
29	j	310	CLA	C4D-ND	-3.00	1.33	1.37
29	d	302	CLA	C4B-NB	3.00	1.41	1.37
29	A	828	CLA	C4D-ND	-3.00	1.33	1.37
29	A	817	CLA	C4B-NB	3.00	1.41	1.37
29	B	832	CLA	C4D-ND	-3.00	1.33	1.37
29	b	302	CLA	C3B-C4B	3.00	1.49	1.42
29	B	830	CLA	C4D-ND	-3.00	1.33	1.37
29	A	802	CLA	C3B-C4B	3.00	1.49	1.42
29	g	308	CLA	C4D-ND	-3.00	1.33	1.37
29	n	604	CLA	C4D-ND	-3.00	1.33	1.37
29	B	832	CLA	C3B-C4B	3.00	1.49	1.42
29	B	839	CLA	C4D-ND	-3.00	1.33	1.37
29	l	312	CLA	C4D-ND	-3.00	1.33	1.37
29	B	808	CLA	C4D-ND	-3.00	1.33	1.37
29	c	312	CLA	C4D-ND	-3.00	1.33	1.37
29	m	604	CLA	C4D-ND	-3.00	1.33	1.37
29	B	818	CLA	C3B-C4B	3.00	1.49	1.42
29	B	802	CLA	C4D-ND	-3.00	1.33	1.37
29	b	309	CLA	C4D-ND	-3.00	1.33	1.37
29	A	836	CLA	C4D-ND	-2.99	1.33	1.37
29	s	403	CLA	C4D-ND	-2.99	1.33	1.37
29	A	814	CLA	C4D-ND	-2.99	1.33	1.37
40	i	318	KC2	C1B-NB	-2.99	1.34	1.37
40	c	310	KC2	C1A-CHA	2.99	1.48	1.40
29	h	301	CLA	C3B-C4B	2.99	1.49	1.42
29	L	202	CLA	C4D-ND	-2.99	1.33	1.37
29	k	604	CLA	C4D-ND	-2.99	1.33	1.37
32	A	845	WVN	C20-C13	2.99	1.55	1.45
29	B	813	CLA	C4D-ND	-2.99	1.33	1.37
29	c	309	CLA	C4D-ND	-2.99	1.33	1.37
29	m	609	CLA	C4D-ND	-2.99	1.33	1.37
29	j	311	CLA	C4D-ND	-2.99	1.33	1.37
29	j	309	CLA	C4D-ND	-2.99	1.33	1.37
29	d	310	CLA	C4D-ND	-2.99	1.33	1.37
29	g	316	CLA	C4D-ND	-2.99	1.33	1.37
29	c	301	CLA	C3B-C4B	2.99	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	815	CLA	C4B-NB	2.99	1.41	1.37
29	c	302	CLA	C4B-NB	2.99	1.41	1.37
29	B	834	CLA	C4D-ND	-2.99	1.33	1.37
29	e	310	CLA	C4D-ND	-2.99	1.33	1.37
29	e	302	CLA	C4D-ND	-2.98	1.33	1.37
29	k	607	CLA	C4D-ND	-2.98	1.33	1.37
29	m	602	CLA	C4B-NB	2.98	1.41	1.37
29	l	310	CLA	C4D-ND	-2.98	1.33	1.37
29	a	308	CLA	C4B-NB	2.98	1.41	1.37
29	i	308	CLA	C4D-ND	-2.98	1.33	1.37
38	n	618	II0	C20-C14	2.98	1.55	1.50
29	g	312	CLA	C4D-ND	-2.98	1.33	1.37
29	B	805	CLA	C4D-ND	-2.98	1.33	1.37
29	l	301	CLA	C4D-ND	-2.98	1.33	1.37
29	m	612	CLA	C4D-ND	-2.97	1.33	1.37
29	k	614	CLA	C4D-ND	-2.97	1.33	1.37
29	j	305	CLA	C3B-C4B	2.97	1.49	1.42
29	j	307	CLA	C3B-C4B	2.97	1.49	1.42
29	O	206	CLA	C4D-ND	-2.97	1.33	1.37
29	g	304	CLA	C4D-ND	-2.97	1.33	1.37
29	f	603	CLA	C4D-ND	-2.97	1.33	1.37
29	B	835	CLA	C3B-C4B	2.97	1.49	1.42
29	j	314	CLA	C4D-ND	-2.97	1.33	1.37
29	A	805	CLA	C4B-NB	2.97	1.41	1.37
29	a	302	CLA	C4D-ND	-2.97	1.33	1.37
29	g	302	CLA	C3B-C4B	2.97	1.49	1.42
29	j	313	CLA	C4D-ND	-2.97	1.33	1.37
40	g	314	KC2	C4A-C3A	2.96	1.50	1.44
32	B	848	WVN	C20-C13	2.96	1.55	1.45
29	A	812	CLA	C4D-ND	-2.96	1.33	1.37
29	b	308	CLA	C4B-NB	2.96	1.41	1.37
33	A	849	LMU	C6'-C5'	-2.96	1.41	1.51
35	A	853	SQD	O48-C23	2.96	1.42	1.33
29	g	316	CLA	C3B-C4B	2.96	1.49	1.42
29	B	825	CLA	C4D-ND	-2.96	1.33	1.37
29	O	201	CLA	C4D-ND	-2.95	1.33	1.37
29	B	814	CLA	C4D-ND	-2.95	1.33	1.37
29	j	309	CLA	C3B-C4B	2.95	1.49	1.42
29	g	311	CLA	C4D-ND	-2.95	1.33	1.37
29	e	308	CLA	C4D-ND	-2.95	1.33	1.37
29	i	303	CLA	C4D-ND	-2.95	1.33	1.37
29	d	313	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	810	CLA	C4D-ND	-2.95	1.33	1.37
29	n	613	CLA	C4D-ND	-2.95	1.33	1.37
29	s	406	CLA	C3B-C4B	2.95	1.49	1.42
29	A	816	CLA	C4D-ND	-2.95	1.33	1.37
29	a	306	CLA	C4D-ND	-2.95	1.33	1.37
29	j	304	CLA	C4D-ND	-2.95	1.33	1.37
29	B	803	CLA	C1B-C2B	2.95	1.50	1.43
29	B	842	CLA	C3B-C4B	2.95	1.49	1.42
32	M	101	WVN	C20-C13	2.95	1.55	1.45
40	c	310	KC2	CHD-C1D	2.95	1.46	1.39
29	b	312	CLA	C3B-C4B	2.94	1.49	1.42
29	n	604	CLA	C3B-C4B	2.94	1.49	1.42
29	s	402	CLA	C3B-C4B	2.94	1.49	1.42
29	B	823	CLA	C4D-ND	-2.94	1.33	1.37
29	A	812	CLA	C4B-NB	2.94	1.41	1.37
29	l	309	CLA	C4D-ND	-2.94	1.33	1.37
29	f	606	CLA	C4D-ND	-2.94	1.33	1.37
29	f	610	CLA	C4D-ND	-2.94	1.33	1.37
29	c	307	CLA	C3B-C4B	2.94	1.49	1.42
29	k	603	CLA	C4D-ND	-2.94	1.33	1.37
29	n	606	CLA	C3B-C4B	2.94	1.49	1.42
29	A	802	CLA	C4D-ND	-2.94	1.33	1.37
29	a	308	CLA	C4D-ND	-2.94	1.33	1.37
29	j	306	CLA	C3B-C4B	2.94	1.49	1.42
29	B	837	CLA	C4D-ND	-2.94	1.33	1.37
29	m	610	CLA	C4D-ND	-2.94	1.33	1.37
32	l	316	WVN	C20-C13	2.94	1.55	1.45
29	i	307	CLA	C4D-ND	-2.94	1.33	1.37
29	A	837	CLA	C4D-ND	-2.94	1.33	1.37
32	R	201	WVN	C20-C13	2.94	1.55	1.45
29	b	309	CLA	C4B-NB	2.94	1.41	1.37
29	h	307	CLA	C4D-ND	-2.94	1.33	1.37
29	f	605	CLA	C4D-ND	-2.94	1.33	1.37
30	B	843	PQN	C5-C4	-2.93	1.42	1.48
29	c	303	CLA	C3B-C4B	2.93	1.49	1.42
36	j	319	DGD	C3D-C2D	2.93	1.59	1.52
29	d	303	CLA	C4B-NB	2.93	1.41	1.37
29	k	609	CLA	C4D-ND	-2.93	1.33	1.37
29	B	816	CLA	C4B-NB	2.93	1.41	1.37
29	A	813	CLA	C3B-C4B	2.93	1.49	1.42
29	e	311	CLA	C3B-C4B	2.93	1.49	1.42
29	d	302	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	834	CLA	C3B-C4B	2.93	1.49	1.42
29	d	305	CLA	C3B-C4B	2.93	1.49	1.42
32	L	201	WVN	C20-C13	2.93	1.55	1.45
29	h	302	CLA	C3B-C4B	2.93	1.49	1.42
29	n	602	CLA	C4B-NB	2.93	1.41	1.37
29	c	301	CLA	C4D-ND	-2.93	1.33	1.37
29	d	304	CLA	C4D-ND	-2.93	1.33	1.37
29	g	310	CLA	C4D-ND	-2.93	1.33	1.37
29	m	606	CLA	C4D-ND	-2.92	1.33	1.37
32	I	101	WVN	C20-C13	2.92	1.55	1.45
29	e	302	CLA	C4B-NB	2.92	1.41	1.37
29	e	301	CLA	C3B-C4B	2.92	1.49	1.42
29	l	303	CLA	C3B-C4B	2.92	1.49	1.42
29	A	839	CLA	C3B-C4B	2.92	1.49	1.42
29	a	305	CLA	C3B-C4B	2.92	1.49	1.42
29	A	820	CLA	C3B-C4B	2.92	1.49	1.42
29	K	102	CLA	C4B-NB	2.92	1.41	1.37
32	i	315	WVN	C19-C11	2.92	1.39	1.32
29	k	610	CLA	C3B-C4B	2.92	1.49	1.42
29	A	803	CLA	C4D-ND	-2.92	1.33	1.37
29	g	323	CLA	C3B-C4B	2.91	1.49	1.42
29	B	838	CLA	C4D-ND	-2.91	1.33	1.37
29	J	102	CLA	C4D-ND	-2.91	1.33	1.37
40	n	611	KC2	CHD-C1D	2.91	1.45	1.39
29	l	306	CLA	C4D-ND	-2.91	1.33	1.37
29	f	613	CLA	C4D-ND	-2.91	1.33	1.37
29	A	813	CLA	C4D-ND	-2.91	1.33	1.37
29	A	811	CLA	C3B-C4B	2.91	1.49	1.42
29	b	311	CLA	C1B-C2B	2.91	1.50	1.43
29	h	304	CLA	C4B-NB	2.91	1.41	1.37
38	d	316	II0	C20-C14	2.91	1.55	1.50
40	k	612	KC2	C3C-C4C	-2.91	1.39	1.44
29	O	201	CLA	C4B-NB	2.91	1.41	1.37
29	k	608	CLA	C4D-ND	-2.91	1.33	1.37
29	B	839	CLA	C3B-C4B	2.91	1.49	1.42
29	A	851	CLA	C4D-ND	-2.91	1.33	1.37
29	j	302	CLA	C3B-C4B	2.90	1.49	1.42
40	d	312	KC2	C3C-C4C	-2.90	1.39	1.44
29	B	815	CLA	C3B-C4B	2.90	1.49	1.42
29	A	824	CLA	C4D-ND	-2.90	1.33	1.37
29	m	601	CLA	C4D-ND	-2.90	1.33	1.37
29	b	304	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j	302	CLA	C4D-ND	-2.90	1.33	1.37
29	L	207	CLA	C3B-C4B	2.90	1.49	1.42
29	Q	302	CLA	C3B-C4B	2.90	1.49	1.42
29	l	303	CLA	C4D-ND	-2.90	1.33	1.37
29	i	305	CLA	C3B-C4B	2.90	1.49	1.42
29	B	824	CLA	C4B-NB	2.90	1.41	1.37
29	n	608	CLA	C3B-C4B	2.90	1.49	1.42
29	m	609	CLA	C4B-NB	2.90	1.41	1.37
40	n	612	KC2	C3C-C4C	-2.90	1.39	1.44
29	g	303	CLA	C4D-ND	-2.90	1.33	1.37
29	a	307	CLA	C4D-ND	-2.89	1.33	1.37
29	c	303	CLA	C4D-ND	-2.89	1.33	1.37
29	b	302	CLA	C4D-ND	-2.89	1.33	1.37
29	e	304	CLA	C4D-ND	-2.89	1.33	1.37
29	e	308	CLA	C3B-C4B	2.89	1.49	1.42
29	K	102	CLA	C1B-C2B	2.89	1.50	1.43
29	n	610	CLA	C3B-C4B	2.89	1.49	1.42
29	j	308	CLA	C4B-NB	2.89	1.41	1.37
29	j	306	CLA	C4D-ND	-2.89	1.33	1.37
29	e	305	CLA	C4D-ND	-2.89	1.33	1.37
32	J	101	WVN	C20-C13	2.89	1.55	1.45
29	g	312	CLA	C3B-C4B	2.89	1.49	1.42
29	k	606	CLA	C3B-C4B	2.88	1.49	1.42
29	f	606	CLA	C3B-C4B	2.88	1.49	1.42
29	n	610	CLA	C4D-ND	-2.88	1.33	1.37
32	A	846	WVN	C20-C13	2.88	1.55	1.45
29	A	826	CLA	C4B-NB	2.88	1.41	1.37
29	f	607	CLA	C3B-C4B	2.88	1.49	1.42
29	h	306	CLA	C3B-C4B	2.88	1.49	1.42
29	d	308	CLA	C4D-ND	-2.88	1.33	1.37
29	s	402	CLA	C4D-ND	-2.88	1.33	1.37
29	B	838	CLA	C3B-C4B	2.88	1.49	1.42
29	c	311	CLA	C4D-ND	-2.88	1.33	1.37
29	i	302	CLA	C3B-C4B	2.88	1.49	1.42
29	j	311	CLA	C3B-C4B	2.88	1.49	1.42
40	n	611	KC2	CHB-C4A	-2.88	1.32	1.39
29	L	202	CLA	C3B-C4B	2.88	1.49	1.42
29	m	610	CLA	C3B-C4B	2.88	1.49	1.42
29	m	605	CLA	C4D-ND	-2.88	1.33	1.37
29	f	601	CLA	C3B-C4B	2.88	1.49	1.42
32	F	207	WVN	C21-C15	2.88	1.55	1.50
29	l	310	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	821	CLA	C3B-C4B	2.87	1.49	1.42
32	L	205	WVN	C20-C13	2.87	1.55	1.45
29	A	826	CLA	C3B-C4B	2.87	1.49	1.42
32	s	407	WVN	C20-C13	2.87	1.55	1.45
29	g	303	CLA	C3B-C4B	2.87	1.49	1.42
40	k	613	KC2	C3C-C4C	-2.87	1.39	1.44
29	b	307	CLA	C3B-C4B	2.87	1.49	1.42
40	d	311	KC2	C1A-CHA	2.87	1.48	1.40
40	i	318	KC2	C4A-C3A	2.87	1.50	1.44
32	K	103	WVN	C20-C13	2.87	1.55	1.45
40	g	314	KC2	C3C-C4C	2.87	1.50	1.44
29	j	303	CLA	C4B-NB	2.87	1.41	1.37
29	n	603	CLA	C3B-C4B	2.87	1.49	1.42
29	B	807	CLA	C4B-NB	2.86	1.41	1.37
29	A	822	CLA	C4D-ND	-2.86	1.33	1.37
29	g	307	CLA	C3B-C4B	2.86	1.49	1.42
29	i	309	CLA	C4D-ND	-2.86	1.33	1.37
29	e	306	CLA	C3B-C4B	2.86	1.49	1.42
29	m	605	CLA	C3B-C4B	2.86	1.49	1.42
32	F	204	WVN	C20-C13	2.86	1.55	1.45
29	B	816	CLA	C4D-ND	-2.86	1.33	1.37
29	c	309	CLA	C3B-C4B	2.86	1.49	1.42
29	B	804	CLA	C4B-NB	2.86	1.41	1.37
29	f	609	CLA	C4B-NB	2.86	1.41	1.37
29	j	307	CLA	C4D-ND	-2.86	1.33	1.37
29	n	605	CLA	C4D-ND	-2.86	1.33	1.37
32	e	315	WVN	C19-C11	2.86	1.39	1.32
29	a	303	CLA	C4B-NB	2.85	1.41	1.37
29	i	306	CLA	C3B-C4B	2.85	1.49	1.42
32	i	315	WVN	C21-C15	2.85	1.55	1.50
29	m	603	CLA	C4D-ND	-2.85	1.33	1.37
29	m	604	CLA	C3B-C4B	2.85	1.49	1.42
29	i	302	CLA	C4D-ND	-2.85	1.33	1.37
29	i	306	CLA	C4D-ND	-2.85	1.33	1.37
29	B	822	CLA	C3B-C4B	2.85	1.49	1.42
29	f	601	CLA	C4D-ND	-2.85	1.33	1.37
29	e	310	CLA	C3B-C4B	2.85	1.49	1.42
29	d	307	CLA	C3B-C4B	2.85	1.49	1.42
29	m	606	CLA	C3B-C4B	2.85	1.49	1.42
29	B	803	CLA	C4D-ND	-2.85	1.33	1.37
29	h	307	CLA	C3B-C4B	2.85	1.49	1.42
29	f	605	CLA	C3B-C4B	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	602	CLA	C4B-NB	2.84	1.41	1.37
29	d	303	CLA	C4D-ND	-2.84	1.33	1.37
29	l	308	CLA	C3B-C4B	2.84	1.49	1.42
29	Q	302	CLA	C4D-ND	-2.84	1.33	1.37
29	i	311	CLA	C4D-ND	-2.84	1.33	1.37
29	A	840	CLA	C4D-ND	-2.84	1.33	1.37
29	n	601	CLA	C4D-ND	-2.84	1.33	1.37
29	B	829	CLA	C3B-C4B	2.84	1.49	1.42
29	n	606	CLA	C4D-ND	-2.84	1.33	1.37
29	i	311	CLA	C3B-C4B	2.84	1.49	1.42
29	l	307	CLA	C4D-ND	-2.84	1.33	1.37
29	L	204	CLA	C3B-C4B	2.84	1.49	1.42
38	k	615	II0	C12-C14	2.84	1.55	1.51
29	A	807	CLA	C4B-NB	2.83	1.41	1.37
29	A	803	CLA	C3B-C4B	2.83	1.49	1.42
29	k	601	CLA	C3B-C4B	2.83	1.49	1.42
29	A	812	CLA	C3B-C4B	2.83	1.49	1.42
40	s	404	KC2	OBD-CAD	2.83	1.27	1.22
29	B	802	CLA	C3B-C4B	2.83	1.49	1.42
29	i	308	CLA	C4B-NB	2.83	1.41	1.37
29	a	306	CLA	C3B-C4B	2.83	1.49	1.42
29	i	303	CLA	C3B-C4B	2.83	1.49	1.42
29	k	601	CLA	C4D-ND	-2.83	1.33	1.37
29	h	303	CLA	C3B-C4B	2.83	1.49	1.42
29	B	812	CLA	C4B-NB	2.83	1.41	1.37
29	k	610	CLA	C4D-ND	-2.83	1.33	1.37
29	K	101	CLA	C3B-C4B	2.83	1.49	1.42
29	B	827	CLA	CMD-C2D	-2.83	1.44	1.50
29	d	310	CLA	C3B-C4B	2.83	1.49	1.42
28	A	801	CL0	MG-ND	-2.83	2.00	2.05
29	e	305	CLA	C3B-C4B	2.83	1.49	1.42
40	s	401	KC2	CHD-C1D	2.83	1.45	1.39
29	n	601	CLA	C3B-C4B	2.83	1.49	1.42
29	n	609	CLA	C3B-C4B	2.83	1.49	1.42
29	B	826	CLA	C3B-C4B	2.82	1.49	1.42
29	A	822	CLA	C3B-C4B	2.82	1.49	1.42
29	s	403	CLA	C3B-C4B	2.82	1.49	1.42
29	B	804	CLA	C3B-C4B	2.82	1.49	1.42
29	n	605	CLA	C3B-C4B	2.82	1.49	1.42
29	f	604	CLA	C3B-C4B	2.82	1.49	1.42
29	e	301	CLA	C4D-ND	-2.82	1.33	1.37
29	l	304	CLA	C4B-NB	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	841	PQN	C3-C2	2.82	1.40	1.35
29	b	306	CLA	C3B-C4B	2.82	1.49	1.42
29	l	312	CLA	C3B-C4B	2.82	1.49	1.42
29	d	308	CLA	C3B-C4B	2.82	1.49	1.42
29	f	610	CLA	C3B-C4B	2.82	1.49	1.42
29	f	612	CLA	C3B-C4B	2.81	1.49	1.42
35	A	853	SQD	O47-C7	2.81	1.42	1.34
29	B	825	CLA	C3B-C4B	2.81	1.49	1.42
29	k	608	CLA	C3B-C4B	2.81	1.49	1.42
29	d	304	CLA	C3B-C4B	2.81	1.49	1.42
32	A	844	WVN	C21-C15	2.81	1.55	1.50
29	k	606	CLA	C4D-ND	-2.81	1.33	1.37
29	j	314	CLA	C3B-C4B	2.81	1.49	1.42
29	g	305	CLA	C3B-C4B	2.81	1.49	1.42
29	A	835	CLA	C3B-C4B	2.81	1.49	1.42
29	R	203	CLA	C3B-C4B	2.81	1.49	1.42
29	j	310	CLA	C3B-C4B	2.81	1.49	1.42
29	e	306	CLA	C4D-ND	-2.81	1.33	1.37
30	B	843	PQN	C3-C2	2.80	1.40	1.35
29	B	815	CLA	C4D-ND	-2.80	1.33	1.37
29	n	613	CLA	C3B-C4B	2.80	1.49	1.42
29	l	307	CLA	C3B-C4B	2.80	1.49	1.42
29	n	608	CLA	C4D-ND	-2.80	1.33	1.37
29	f	613	CLA	C3B-C4B	2.80	1.49	1.42
29	i	304	CLA	C4D-ND	-2.80	1.33	1.37
29	K	102	CLA	C3B-C4B	2.80	1.49	1.42
29	A	805	CLA	C3B-C4B	2.80	1.49	1.42
29	e	302	CLA	C3B-C4B	2.80	1.49	1.42
32	L	206	WVN	C20-C13	2.80	1.55	1.45
29	a	309	CLA	C3B-C4B	2.80	1.49	1.42
29	k	614	CLA	C3B-C4B	2.80	1.49	1.42
29	m	607	CLA	C3B-C4B	2.80	1.49	1.42
32	B	847	WVN	C21-C15	2.80	1.55	1.50
29	A	824	CLA	C3B-C4B	2.80	1.49	1.42
32	B	849	WVN	C21-C15	2.80	1.55	1.50
29	O	206	CLA	C3B-C4B	2.80	1.49	1.42
29	b	303	CLA	C4B-NB	2.79	1.41	1.37
29	l	305	CLA	C3B-C4B	2.79	1.49	1.42
29	b	309	CLA	C3B-C4B	2.79	1.49	1.42
29	l	305	CLA	C4D-ND	-2.79	1.33	1.37
29	B	837	CLA	C3B-C4B	2.79	1.49	1.42
29	A	817	CLA	C3B-C4B	2.79	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	824	CLA	C3B-C4B	2.79	1.49	1.42
29	c	308	CLA	C3B-C4B	2.79	1.49	1.42
29	l	309	CLA	C3B-C4B	2.79	1.49	1.42
29	d	308	CLA	C1B-C2B	2.79	1.49	1.43
29	b	313	CLA	C4D-ND	-2.79	1.33	1.37
29	A	818	CLA	C3B-C4B	2.79	1.49	1.42
29	a	304	CLA	C3B-C4B	2.79	1.49	1.42
29	e	307	CLA	C3B-C4B	2.79	1.49	1.42
29	A	828	CLA	C3B-C4B	2.79	1.49	1.42
29	l	306	CLA	C3B-C4B	2.79	1.49	1.42
29	f	603	CLA	C3B-C4B	2.79	1.49	1.42
40	i	310	KC2	CHB-C4A	-2.79	1.32	1.39
29	A	807	CLA	C3B-C4B	2.78	1.49	1.42
29	g	310	CLA	C3B-C4B	2.78	1.49	1.42
29	m	608	CLA	C3B-C4B	2.78	1.49	1.42
29	B	813	CLA	C1B-C2B	2.78	1.49	1.43
32	s	405	WVN	C21-C15	2.78	1.55	1.50
29	d	305	CLA	C4D-ND	-2.78	1.33	1.37
29	B	836	CLA	C3B-C4B	2.78	1.49	1.42
29	m	612	CLA	C3B-C4B	2.78	1.49	1.42
29	a	308	CLA	C3B-C4B	2.78	1.49	1.42
30	A	841	PQN	C10-C1	-2.77	1.42	1.48
32	h	308	WVN	C21-C15	2.77	1.55	1.50
29	i	309	CLA	C3B-C4B	2.77	1.49	1.42
32	M	101	WVN	C21-C15	2.77	1.55	1.50
29	a	310	CLA	C3B-C4B	2.77	1.49	1.42
29	b	305	CLA	C3B-C4B	2.77	1.49	1.42
32	A	854	WVN	C16-C05	2.77	1.55	1.50
29	m	602	CLA	C3B-C4B	2.77	1.49	1.42
29	e	303	CLA	C3B-C4B	2.77	1.49	1.42
29	A	814	CLA	C3B-C4B	2.77	1.49	1.42
29	O	201	CLA	C3B-C4B	2.76	1.49	1.42
29	B	831	CLA	C3B-C4B	2.76	1.49	1.42
32	l	302	WVN	C21-C15	2.76	1.55	1.50
29	A	821	CLA	C3B-C4B	2.76	1.49	1.42
29	A	851	CLA	C3B-C4B	2.76	1.49	1.42
29	B	823	CLA	C3B-C4B	2.76	1.49	1.42
29	h	312	CLA	C3B-C4B	2.76	1.49	1.42
29	k	605	CLA	C3B-C4B	2.76	1.49	1.42
29	e	304	CLA	C3B-C4B	2.76	1.49	1.42
38	n	618	II0	C19-C13	2.76	1.55	1.50
29	A	810	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	312	CLA	C3B-C4B	2.76	1.49	1.42
29	k	604	CLA	C3B-C4B	2.76	1.49	1.42
29	j	304	CLA	C3B-C4B	2.75	1.49	1.42
29	A	804	CLA	C3B-C4B	2.75	1.49	1.42
29	g	306	CLA	C4B-NB	2.75	1.41	1.37
29	B	828	CLA	C3B-C4B	2.75	1.49	1.42
29	B	816	CLA	C3B-C4B	2.75	1.49	1.42
29	A	831	CLA	C1B-C2B	2.75	1.49	1.43
38	d	316	II0	C12-C14	2.75	1.55	1.51
29	n	603	CLA	C4D-ND	-2.74	1.33	1.37
29	A	808	CLA	C3B-C4B	2.74	1.49	1.42
29	A	834	CLA	C3B-C4B	2.74	1.49	1.42
29	b	308	CLA	C3B-C4B	2.74	1.49	1.42
32	L	201	WVN	C21-C15	2.74	1.55	1.50
38	d	301	II0	C20-C14	2.74	1.55	1.50
29	b	310	CLA	C4D-ND	-2.74	1.33	1.37
29	A	809	CLA	C3B-C4B	2.74	1.49	1.42
29	B	801	CLA	C3B-C4B	2.74	1.49	1.42
29	d	313	CLA	C3B-C4B	2.74	1.49	1.42
29	m	613	CLA	C1B-C2B	2.74	1.49	1.43
29	a	304	CLA	C4D-ND	-2.73	1.33	1.37
29	O	206	CLA	C1B-C2B	2.73	1.49	1.43
29	B	807	CLA	C1B-C2B	2.73	1.49	1.43
29	k	605	CLA	C4D-ND	-2.73	1.33	1.37
29	a	302	CLA	C3B-C4B	2.73	1.49	1.42
29	g	304	CLA	C3B-C4B	2.73	1.49	1.42
29	e	311	CLA	C4D-ND	-2.73	1.33	1.37
29	e	303	CLA	C4D-ND	-2.73	1.33	1.37
29	B	801	CLA	CMB-C2B	-2.73	1.45	1.50
29	A	836	CLA	C1B-C2B	2.73	1.49	1.43
38	l	315	II0	C11-C13	2.73	1.55	1.51
29	A	823	CLA	C3B-C4B	2.73	1.49	1.42
38	d	301	II0	C12-C14	2.73	1.55	1.51
29	d	302	CLA	C3B-C4B	2.73	1.49	1.42
29	b	313	CLA	C1B-C2B	2.73	1.49	1.43
29	k	605	CLA	C1B-C2B	2.73	1.49	1.43
29	i	306	CLA	C1B-C2B	2.73	1.49	1.43
29	g	309	CLA	C4B-NB	2.73	1.41	1.37
32	A	847	WVN	C21-C15	2.73	1.55	1.50
40	e	309	KC2	C4A-C3A	2.73	1.49	1.44
29	g	316	CLA	C1B-C2B	2.73	1.49	1.43
29	A	827	CLA	C4D-ND	-2.73	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	203	CLA	C3B-C4B	2.72	1.49	1.42
29	B	827	CLA	CMB-C2B	-2.72	1.45	1.50
29	j	303	CLA	C3B-C4B	2.72	1.49	1.42
29	b	305	CLA	C1B-C2B	2.72	1.49	1.43
29	a	303	CLA	C3B-C4B	2.72	1.49	1.42
29	B	810	CLA	C3B-C4B	2.72	1.49	1.42
29	d	306	CLA	C3B-C4B	2.72	1.49	1.42
29	B	812	CLA	C3B-C4B	2.72	1.49	1.42
29	k	602	CLA	C3B-C4B	2.72	1.49	1.42
29	d	318	CLA	C4D-ND	-2.72	1.34	1.37
40	g	315	KC2	C4A-C3A	2.72	1.49	1.44
29	g	306	CLA	C3B-C4B	2.71	1.49	1.42
29	B	820	CLA	C3B-C4B	2.71	1.49	1.42
29	A	814	CLA	C1B-C2B	2.71	1.49	1.43
29	h	305	CLA	C3B-C4B	2.71	1.49	1.42
40	d	311	KC2	C4A-C3A	2.71	1.49	1.44
29	n	602	CLA	C3B-C4B	2.71	1.49	1.42
29	d	304	CLA	C1B-C2B	2.71	1.49	1.43
38	d	315	II0	C20-C14	2.71	1.55	1.50
29	l	309	CLA	C1B-C2B	2.70	1.49	1.43
29	d	318	CLA	C3B-C4B	2.70	1.49	1.42
29	A	804	CLA	C1B-C2B	2.70	1.49	1.43
38	n	618	II0	C12-C14	2.70	1.55	1.51
29	k	607	CLA	C1B-C2B	2.70	1.49	1.43
29	A	832	CLA	C3B-C4B	2.69	1.49	1.42
29	c	302	CLA	C3B-C4B	2.69	1.49	1.42
29	A	816	CLA	C1B-C2B	2.69	1.49	1.43
29	B	817	CLA	C3B-C4B	2.69	1.49	1.42
29	d	313	CLA	C1B-C2B	2.69	1.49	1.43
29	n	601	CLA	C1B-C2B	2.69	1.49	1.43
29	A	819	CLA	C3B-C4B	2.69	1.49	1.42
29	i	302	CLA	C1B-C2B	2.69	1.49	1.43
29	e	310	CLA	C1B-C2B	2.69	1.49	1.43
29	i	312	CLA	C3B-C4B	2.69	1.49	1.42
29	e	305	CLA	C1B-C2B	2.68	1.49	1.43
29	i	309	CLA	C1B-C2B	2.68	1.49	1.43
29	B	814	CLA	C1B-C2B	2.68	1.49	1.43
29	a	302	CLA	C1B-C2B	2.68	1.49	1.43
29	B	804	CLA	CMC-C2C	-2.68	1.45	1.50
29	B	806	CLA	C3B-C4B	2.68	1.49	1.42
29	c	304	CLA	C3B-C4B	2.68	1.49	1.42
29	e	306	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	205	WVN	C19-C11	2.68	1.38	1.32
29	A	840	CLA	C3B-C4B	2.68	1.49	1.42
29	O	202	CLA	C3B-C4B	2.68	1.49	1.42
29	h	306	CLA	C1B-C2B	2.68	1.49	1.43
29	B	820	CLA	C4D-ND	-2.68	1.34	1.37
29	A	810	CLA	C1B-C2B	2.68	1.49	1.43
29	B	827	CLA	C3B-C4B	2.68	1.49	1.42
29	B	840	CLA	C3B-C4B	2.67	1.49	1.42
32	R	202	WVN	C19-C11	2.67	1.38	1.32
30	A	841	PQN	C5-C4	-2.67	1.43	1.48
29	A	834	CLA	C4B-NB	2.67	1.41	1.37
29	A	815	CLA	C3B-C4B	2.67	1.49	1.42
29	c	311	CLA	C1B-C2B	2.67	1.49	1.43
29	a	311	CLA	C3B-C4B	2.67	1.49	1.42
28	A	801	CL0	MG-NB	-2.67	2.00	2.05
29	m	603	CLA	C3B-C4B	2.67	1.49	1.42
29	B	814	CLA	C3B-C4B	2.67	1.49	1.42
32	B	846	WVN	C21-C15	2.67	1.55	1.50
29	O	202	CLA	C1B-C2B	2.67	1.49	1.43
38	i	316	II0	C20-C14	2.67	1.55	1.50
38	g	317	II0	C12-C14	2.67	1.55	1.51
38	n	618	II0	C11-C13	2.67	1.55	1.51
29	l	304	CLA	C1B-C2B	2.67	1.49	1.43
29	d	303	CLA	C3B-C4B	2.67	1.49	1.42
29	A	816	CLA	C3B-C4B	2.67	1.49	1.42
29	c	309	CLA	C1B-C2B	2.67	1.49	1.43
40	s	404	KC2	CHB-C4A	-2.67	1.33	1.39
29	d	306	CLA	C4D-ND	-2.67	1.34	1.37
40	c	310	KC2	CHB-C4A	-2.67	1.33	1.39
29	c	302	CLA	C1B-C2B	2.67	1.49	1.43
29	e	304	CLA	C1B-C2B	2.67	1.49	1.43
29	B	830	CLA	C3B-C4B	2.67	1.49	1.42
40	l	311	KC2	C2A-C1A	2.66	1.52	1.44
29	i	308	CLA	C3B-C4B	2.66	1.49	1.42
29	c	311	CLA	C3B-C4B	2.66	1.49	1.42
29	c	308	CLA	C1B-C2B	2.66	1.49	1.43
38	e	314	II0	C19-C13	2.66	1.55	1.50
29	B	820	CLA	C1B-C2B	2.66	1.49	1.43
29	c	301	CLA	C1B-C2B	2.66	1.49	1.43
29	e	308	CLA	C1B-C2B	2.66	1.49	1.43
38	l	315	II0	C20-C14	2.66	1.55	1.50
29	n	613	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	305	CLA	C1B-C2B	2.66	1.49	1.43
29	n	608	CLA	C1B-C2B	2.66	1.49	1.43
29	n	610	CLA	C1B-C2B	2.66	1.49	1.43
29	k	601	CLA	C1B-C2B	2.66	1.49	1.43
29	j	311	CLA	C1B-C2B	2.66	1.49	1.43
29	B	807	CLA	C3B-C4B	2.66	1.49	1.42
29	B	810	CLA	C1B-C2B	2.66	1.49	1.43
29	i	303	CLA	C1B-C2B	2.65	1.49	1.43
29	B	808	CLA	C3B-C4B	2.65	1.49	1.42
29	f	602	CLA	C3B-C4B	2.65	1.49	1.42
29	B	813	CLA	C3B-C4B	2.65	1.49	1.42
29	b	302	CLA	C1B-C2B	2.65	1.49	1.43
29	b	303	CLA	C3B-C4B	2.65	1.49	1.42
29	s	403	CLA	C1B-C2B	2.65	1.49	1.43
32	A	846	WVN	C16-C05	2.65	1.55	1.50
29	a	309	CLA	C1B-C2B	2.65	1.49	1.43
29	d	318	CLA	C1B-C2B	2.65	1.49	1.43
29	d	302	CLA	C1B-C2B	2.65	1.49	1.43
29	g	307	CLA	C1B-C2B	2.65	1.49	1.43
29	b	312	CLA	C1B-C2B	2.65	1.49	1.43
29	d	305	CLA	C1B-C2B	2.65	1.49	1.43
29	c	306	CLA	C3B-C4B	2.65	1.49	1.42
32	R	202	WVN	C16-C05	2.65	1.55	1.50
29	L	207	CLA	C1B-C2B	2.65	1.49	1.43
29	a	306	CLA	C1B-C2B	2.65	1.49	1.43
40	n	611	KC2	C4A-C3A	2.64	1.49	1.44
38	d	315	II0	C19-C13	2.64	1.55	1.50
29	K	102	CLA	C4D-ND	-2.64	1.34	1.37
29	b	313	CLA	C3B-C4B	2.64	1.48	1.42
32	R	202	WVN	C21-C15	2.64	1.55	1.50
29	B	805	CLA	C1B-C2B	2.64	1.49	1.43
40	m	611	KC2	CHB-C4A	-2.64	1.33	1.39
29	c	312	CLA	C1B-C2B	2.64	1.49	1.43
29	a	303	CLA	C1B-C2B	2.64	1.49	1.43
38	d	316	II0	C19-C13	2.64	1.55	1.50
29	d	310	CLA	C1B-C2B	2.64	1.49	1.43
29	i	311	CLA	C1B-C2B	2.64	1.49	1.43
29	l	312	CLA	C1B-C2B	2.64	1.49	1.43
29	j	302	CLA	C1B-C2B	2.64	1.49	1.43
29	n	602	CLA	C1B-C2B	2.64	1.49	1.43
29	g	309	CLA	C3B-C4B	2.64	1.48	1.42
38	n	616	II0	C12-C14	2.64	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	805	CLA	C3B-C4B	2.64	1.48	1.42
29	m	609	CLA	C1B-C2B	2.64	1.49	1.43
32	A	845	WVN	C16-C05	2.64	1.55	1.50
29	d	306	CLA	C1B-C2B	2.64	1.49	1.43
38	e	312	II0	C19-C13	2.63	1.55	1.50
29	f	601	CLA	C1B-C2B	2.63	1.49	1.43
29	i	305	CLA	C1B-C2B	2.63	1.49	1.43
29	A	850	CLA	C3B-C4B	2.63	1.48	1.42
29	A	831	CLA	C3B-C4B	2.63	1.48	1.42
29	A	809	CLA	C1B-C2B	2.63	1.49	1.43
29	k	614	CLA	C1B-C2B	2.63	1.49	1.43
29	b	311	CLA	C3B-C4B	2.63	1.48	1.42
29	A	835	CLA	C1B-C2B	2.63	1.49	1.43
38	m	615	II0	C19-C13	2.63	1.55	1.50
32	i	315	WVN	C16-C05	2.63	1.55	1.50
29	l	308	CLA	C1B-C2B	2.63	1.49	1.43
29	e	301	CLA	C1B-C2B	2.63	1.49	1.43
38	n	616	II0	C20-C14	2.62	1.55	1.50
29	B	830	CLA	C1B-C2B	2.62	1.49	1.43
29	B	840	CLA	C1B-C2B	2.62	1.49	1.43
29	i	312	CLA	C1B-C2B	2.62	1.49	1.43
29	f	612	CLA	C1B-C2B	2.62	1.49	1.43
29	m	609	CLA	C3B-C4B	2.62	1.48	1.42
29	c	305	CLA	C3B-C4B	2.62	1.48	1.42
40	g	315	KC2	CHB-C4A	-2.62	1.33	1.39
29	m	610	CLA	C1B-C2B	2.62	1.49	1.43
29	i	304	CLA	C3B-C4B	2.62	1.48	1.42
32	F	204	WVN	C19-C11	2.62	1.38	1.32
29	A	826	CLA	C1B-C2B	2.62	1.49	1.43
29	h	305	CLA	C1B-C2B	2.62	1.49	1.43
29	g	303	CLA	C1B-C2B	2.62	1.49	1.43
32	F	205	WVN	C02-C11	2.62	1.54	1.50
29	B	838	CLA	C1B-C2B	2.62	1.49	1.43
29	d	307	CLA	C1B-C2B	2.62	1.49	1.43
29	l	310	CLA	C1B-C2B	2.62	1.49	1.43
32	F	205	WVN	C20-C13	2.62	1.54	1.45
29	e	302	CLA	C1B-C2B	2.62	1.49	1.43
32	K	103	WVN	C21-C15	2.62	1.55	1.50
38	e	314	II0	C20-C14	2.62	1.55	1.50
29	a	311	CLA	C1B-C2B	2.62	1.49	1.43
38	f	618	II0	C20-C14	2.62	1.55	1.50
38	i	314	II0	C19-C13	2.62	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	314	KC2	C2A-C1A	2.62	1.52	1.44
32	s	407	WVN	C19-C11	2.62	1.38	1.32
29	Q	302	CLA	C1B-C2B	2.62	1.49	1.43
38	d	317	II0	C20-C14	2.62	1.55	1.50
40	i	310	KC2	C4A-C3A	2.62	1.49	1.44
29	f	609	CLA	C1B-C2B	2.61	1.49	1.43
29	k	608	CLA	C1B-C2B	2.61	1.49	1.43
38	j	316	II0	C20-C14	2.61	1.55	1.50
29	B	819	CLA	CHC-C1C	2.61	1.43	1.38
38	n	615	II0	C19-C13	2.61	1.55	1.50
29	A	832	CLA	C1B-C2B	2.61	1.49	1.43
29	B	808	CLA	C1B-C2B	2.61	1.49	1.43
29	i	304	CLA	C1B-C2B	2.61	1.49	1.43
40	j	312	KC2	C4A-C3A	2.61	1.49	1.44
29	g	312	CLA	C1B-C2B	2.61	1.49	1.43
29	j	303	CLA	C1B-C2B	2.61	1.49	1.43
38	h	311	II0	C19-C13	2.61	1.55	1.50
29	A	830	CLA	C1B-C2B	2.61	1.49	1.43
29	l	303	CLA	C1B-C2B	2.61	1.49	1.43
29	d	309	CLA	C1B-C2B	2.61	1.49	1.43
29	f	608	CLA	C4D-ND	-2.61	1.34	1.37
29	B	839	CLA	C1B-C2B	2.61	1.49	1.43
32	s	407	WVN	C16-C05	2.61	1.55	1.50
29	n	606	CLA	C1B-C2B	2.61	1.49	1.43
29	A	805	CLA	C1B-C2B	2.61	1.49	1.43
29	c	305	CLA	CMB-C2B	-2.61	1.45	1.50
29	j	308	CLA	C1B-C2B	2.61	1.49	1.43
29	A	833	CLA	C3B-C4B	2.60	1.48	1.42
29	l	307	CLA	C1B-C2B	2.60	1.49	1.43
29	n	605	CLA	C1B-C2B	2.60	1.49	1.43
38	c	313	II0	C12-C14	2.60	1.55	1.51
29	B	831	CLA	C1B-C2B	2.60	1.49	1.43
29	B	837	CLA	C1B-C2B	2.60	1.49	1.43
29	h	304	CLA	C3B-C4B	2.60	1.48	1.42
40	d	311	KC2	CHB-C4A	-2.60	1.33	1.39
29	g	323	CLA	C1B-C2B	2.60	1.49	1.43
29	m	605	CLA	C1B-C2B	2.59	1.49	1.43
38	m	615	II0	C20-C14	2.59	1.55	1.50
29	h	304	CLA	C1B-C2B	2.59	1.49	1.43
29	g	305	CLA	C1B-C2B	2.59	1.49	1.43
29	c	312	CLA	C3B-C4B	2.59	1.48	1.42
29	m	613	CLA	C3B-C4B	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	610	CLA	C1B-C2B	2.59	1.49	1.43
29	h	303	CLA	C1B-C2B	2.59	1.49	1.43
29	k	610	CLA	C1B-C2B	2.59	1.49	1.43
29	K	101	CLA	C1B-C2B	2.59	1.49	1.43
29	A	840	CLA	C1B-C2B	2.59	1.49	1.43
29	f	602	CLA	C1B-C2B	2.59	1.49	1.43
29	B	821	CLA	C1B-C2B	2.59	1.49	1.43
29	h	307	CLA	C1B-C2B	2.59	1.49	1.43
40	s	401	KC2	CHB-C4A	-2.59	1.33	1.39
29	j	304	CLA	C1B-C2B	2.58	1.49	1.43
32	A	845	WVN	C19-C11	2.58	1.38	1.32
29	b	303	CLA	C1B-C2B	2.58	1.49	1.43
29	B	826	CLA	CMD-C2D	-2.58	1.45	1.50
29	b	309	CLA	C1B-C2B	2.58	1.49	1.43
29	L	204	CLA	C1B-C2B	2.58	1.49	1.43
29	j	313	CLA	C1B-C2B	2.58	1.49	1.43
29	f	605	CLA	C1B-C2B	2.58	1.49	1.43
32	A	846	WVN	C21-C15	2.58	1.55	1.50
29	k	606	CLA	C1B-C2B	2.58	1.49	1.43
32	L	206	WVN	C21-C15	2.58	1.55	1.50
29	g	310	CLA	C1B-C2B	2.57	1.49	1.43
40	k	611	KC2	C4A-C3A	2.57	1.49	1.44
29	a	312	CLA	C1B-C2B	2.57	1.49	1.43
29	A	833	CLA	CMB-C2B	-2.57	1.45	1.50
29	A	828	CLA	C1B-C2B	2.57	1.49	1.43
29	l	306	CLA	C1B-C2B	2.57	1.49	1.43
29	g	302	CLA	C1B-C2B	2.57	1.49	1.43
38	m	614	II0	C12-C14	2.57	1.55	1.51
32	J	101	WVN	C19-C11	2.57	1.38	1.32
29	m	603	CLA	C1B-C2B	2.57	1.49	1.43
29	A	821	CLA	C1B-C2B	2.57	1.49	1.43
29	g	308	CLA	C1B-C2B	2.57	1.49	1.43
32	M	101	WVN	C16-C05	2.56	1.55	1.50
29	B	834	CLA	C1B-C2B	2.56	1.49	1.43
29	f	609	CLA	C3B-C4B	2.56	1.48	1.42
32	l	316	WVN	C19-C11	2.56	1.38	1.32
33	i	301	LMU	C6B-C5B	-2.56	1.43	1.51
29	n	607	CLA	C3B-C4B	2.56	1.48	1.42
29	A	851	CLA	C1B-C2B	2.56	1.49	1.43
29	k	607	CLA	C3B-C4B	2.56	1.48	1.42
29	a	310	CLA	C1B-C2B	2.56	1.49	1.43
29	A	823	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	307	CLA	C4D-ND	-2.56	1.34	1.37
30	B	843	PQN	C10-C5	-2.56	1.36	1.40
29	A	808	CLA	C1B-C2B	2.55	1.49	1.43
29	h	302	CLA	C1B-C2B	2.55	1.49	1.43
29	B	828	CLA	C1B-C2B	2.55	1.49	1.43
29	f	603	CLA	C1B-C2B	2.55	1.49	1.43
29	A	830	CLA	C3B-C4B	2.55	1.48	1.42
29	f	607	CLA	C1B-C2B	2.55	1.49	1.43
38	f	615	II0	C20-C14	2.55	1.55	1.50
29	A	819	CLA	C1B-C2B	2.55	1.49	1.43
29	b	307	CLA	C1B-C2B	2.55	1.49	1.43
29	n	609	CLA	C1B-C2B	2.54	1.49	1.43
29	A	836	CLA	C3B-C4B	2.54	1.48	1.42
29	A	837	CLA	C1B-C2B	2.54	1.49	1.43
29	B	806	CLA	C1B-C2B	2.54	1.49	1.43
29	k	604	CLA	C1B-C2B	2.54	1.49	1.43
29	n	603	CLA	C1B-C2B	2.54	1.49	1.43
38	j	315	II0	C19-C13	2.54	1.55	1.50
29	c	307	CLA	C1B-C2B	2.54	1.49	1.43
38	b	301	II0	C20-C14	2.54	1.55	1.50
29	k	602	CLA	C1B-C2B	2.54	1.49	1.43
40	e	309	KC2	CHB-C4A	-2.54	1.33	1.39
29	B	835	CLA	C1B-C2B	2.54	1.49	1.43
32	K	103	WVN	C19-C11	2.54	1.38	1.32
40	k	613	KC2	MG-NA	2.54	2.12	2.06
29	d	309	CLA	C3B-C4B	2.54	1.48	1.42
29	A	826	CLA	CMC-C2C	-2.53	1.45	1.50
32	A	844	WVN	C16-C05	2.53	1.55	1.50
29	a	304	CLA	C1B-C2B	2.53	1.49	1.43
29	m	612	CLA	C1B-C2B	2.53	1.49	1.43
29	f	606	CLA	C1B-C2B	2.53	1.49	1.43
32	s	405	WVN	C19-C11	2.53	1.38	1.32
29	A	818	CLA	CMB-C2B	-2.53	1.45	1.50
29	F	203	CLA	C1B-C2B	2.53	1.49	1.43
29	B	823	CLA	C1B-C2B	2.53	1.49	1.43
29	b	308	CLA	C1B-C2B	2.53	1.49	1.43
40	f	611	KC2	CHB-C4A	-2.53	1.33	1.39
29	A	824	CLA	C1B-C2B	2.52	1.49	1.43
38	m	616	II0	C19-C13	2.52	1.55	1.50
38	c	313	II0	C20-C14	2.52	1.55	1.50
29	B	804	CLA	C1B-C2B	2.52	1.49	1.43
40	e	309	KC2	C1D-C2D	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	815	CLA	C1B-C2B	2.52	1.49	1.43
38	m	618	II0	C20-C14	2.52	1.55	1.50
29	e	307	CLA	C1B-C2B	2.52	1.49	1.43
29	B	825	CLA	C1B-C2B	2.52	1.49	1.43
32	A	847	WVN	C16-C05	2.52	1.55	1.50
29	A	822	CLA	C1B-C2B	2.52	1.49	1.43
29	B	820	CLA	CMD-C2D	-2.52	1.45	1.50
29	e	311	CLA	C1B-C2B	2.52	1.49	1.43
29	l	301	CLA	C1B-C2B	2.52	1.49	1.43
29	m	608	CLA	C1B-C2B	2.52	1.49	1.43
33	A	849	LMU	O5B-C1B	2.51	1.48	1.41
32	L	205	WVN	C21-C15	2.51	1.55	1.50
29	m	601	CLA	C1B-C2B	2.51	1.49	1.43
29	i	311	CLA	CMD-C2D	-2.51	1.45	1.50
38	f	614	II0	C12-C14	2.51	1.55	1.51
38	e	312	II0	C11-C13	2.51	1.55	1.51
38	e	314	II0	C12-C14	2.51	1.55	1.51
29	m	606	CLA	C1B-C2B	2.51	1.49	1.43
29	f	608	CLA	CHC-C1C	2.51	1.43	1.38
32	s	407	WVN	C21-C15	2.51	1.55	1.50
29	A	839	CLA	C1B-C2B	2.51	1.49	1.43
29	c	304	CLA	C1B-C2B	2.51	1.49	1.43
32	J	101	WVN	C21-C15	2.51	1.55	1.50
29	i	308	CLA	C1B-C2B	2.51	1.49	1.43
29	L	203	CLA	C1B-C2B	2.51	1.49	1.43
40	j	312	KC2	CHB-C4A	-2.51	1.33	1.39
29	B	824	CLA	C1B-C2B	2.51	1.49	1.43
29	A	833	CLA	C1B-C2B	2.51	1.49	1.43
32	A	845	WVN	C21-C15	2.51	1.55	1.50
38	m	614	II0	C20-C14	2.51	1.55	1.50
33	A	849	LMU	O3'-C3'	2.51	1.48	1.43
29	j	307	CLA	C1B-C2B	2.51	1.49	1.43
33	A	849	LMU	C6B-C5B	-2.51	1.43	1.51
32	I	101	WVN	C16-C05	2.51	1.55	1.50
29	j	306	CLA	C1B-C2B	2.51	1.49	1.43
30	A	841	PQN	C10-C5	-2.50	1.36	1.40
40	g	314	KC2	CHB-C4A	-2.50	1.33	1.39
32	R	201	WVN	C21-C15	2.50	1.55	1.50
29	g	309	CLA	C1B-C2B	2.50	1.49	1.43
38	i	313	II0	C20-C14	2.50	1.55	1.50
29	L	202	CLA	C1B-C2B	2.50	1.49	1.43
28	A	801	CL0	C1D-C2D	-2.50	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	612	KC2	MG-NA	2.50	2.12	2.06
29	l	304	CLA	C3B-C4B	2.50	1.48	1.42
32	h	308	WVN	C19-C11	2.49	1.38	1.32
29	h	301	CLA	C1B-C2B	2.49	1.49	1.43
29	B	801	CLA	CMD-C2D	-2.49	1.45	1.50
38	m	614	II0	C19-C13	2.49	1.55	1.50
33	i	301	LMU	C3'-C2'	-2.49	1.46	1.52
29	b	306	CLA	C1B-C2B	2.49	1.49	1.43
38	a	317	II0	C20-C14	2.49	1.55	1.50
29	j	314	CLA	C1B-C2B	2.49	1.49	1.43
33	A	849	LMU	O2'-C2'	2.48	1.48	1.43
29	f	613	CLA	C1B-C2B	2.48	1.49	1.43
37	n	620	LMG	C4-C5	2.48	1.58	1.53
40	g	313	KC2	C4A-C3A	2.48	1.49	1.44
29	A	803	CLA	CHC-C1C	2.48	1.43	1.38
31	A	842	LHG	O7-C5	-2.48	1.40	1.46
32	R	201	WVN	C16-C05	2.48	1.55	1.50
29	A	806	CLA	C1B-C2B	2.48	1.49	1.43
29	A	812	CLA	C1B-C2B	2.48	1.49	1.43
38	a	315	II0	C12-C14	2.48	1.54	1.51
40	g	313	KC2	CHB-C4A	-2.48	1.33	1.39
29	i	307	CLA	C1B-C2B	2.48	1.49	1.43
29	e	303	CLA	C1B-C2B	2.48	1.49	1.43
29	f	604	CLA	C1B-C2B	2.48	1.49	1.43
29	j	309	CLA	C1B-C2B	2.48	1.49	1.43
33	i	301	LMU	O3'-C3'	2.48	1.48	1.43
32	F	204	WVN	C21-C15	2.48	1.55	1.50
38	m	616	II0	C20-C14	2.48	1.55	1.50
32	l	316	WVN	C16-C05	2.48	1.55	1.50
29	B	812	CLA	C1B-C2B	2.48	1.49	1.43
29	c	305	CLA	C1B-C2B	2.47	1.49	1.43
29	m	604	CLA	C1B-C2B	2.47	1.49	1.43
29	A	829	CLA	C3B-C4B	2.47	1.48	1.42
32	l	316	WVN	C21-C15	2.47	1.55	1.50
38	k	619	II0	C19-C13	2.47	1.55	1.50
29	j	310	CLA	C1B-C2B	2.47	1.49	1.43
38	n	615	II0	C11-C13	2.47	1.54	1.51
29	m	602	CLA	C1B-C2B	2.46	1.49	1.43
40	m	611	KC2	C4A-C3A	2.46	1.49	1.44
38	k	616	II0	C20-C14	2.46	1.55	1.50
29	R	203	CLA	C1B-C2B	2.46	1.49	1.43
38	g	318	II0	C20-C14	2.46	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	807	CLA	C1B-C2B	2.46	1.49	1.43
40	s	404	KC2	C2A-C1A	2.46	1.52	1.44
29	F	201	CLA	C1B-C2B	2.46	1.49	1.43
40	k	611	KC2	CHB-C4A	-2.46	1.33	1.39
38	l	314	II0	C12-C14	2.46	1.54	1.51
38	j	301	II0	C20-C14	2.46	1.55	1.50
32	e	315	WVN	C16-C05	2.46	1.55	1.50
32	J	101	WVN	C16-C05	2.45	1.55	1.50
38	a	314	II0	C19-C13	2.45	1.55	1.50
38	e	313	II0	C20-C14	2.45	1.54	1.50
29	B	821	CLA	CMC-C2C	-2.45	1.45	1.50
29	d	303	CLA	C1B-C2B	2.45	1.49	1.43
38	a	313	II0	C19-C13	2.45	1.54	1.50
32	L	201	WVN	C16-C05	2.45	1.55	1.50
32	M	101	WVN	C19-C11	2.45	1.38	1.32
29	a	305	CLA	C1B-C2B	2.44	1.49	1.43
29	A	811	CLA	C1B-C2B	2.44	1.49	1.43
29	J	102	CLA	C1B-C2B	2.44	1.49	1.43
33	i	301	LMU	O5B-C1B	2.44	1.48	1.41
38	g	317	II0	C20-C14	2.44	1.54	1.50
38	b	301	II0	C11-C13	2.44	1.54	1.51
32	F	204	WVN	C16-C05	2.44	1.55	1.50
29	A	825	CLA	C1B-C2B	2.44	1.49	1.43
28	A	801	CL0	C3D-C4D	-2.43	1.38	1.44
32	e	315	WVN	C21-C15	2.43	1.54	1.50
40	n	611	KC2	C2A-C1A	2.43	1.52	1.44
29	B	841	CLA	CHC-C1C	2.43	1.43	1.38
38	i	314	II0	C12-C14	2.43	1.54	1.51
29	h	312	CLA	C1B-C2B	2.43	1.49	1.43
40	i	318	KC2	CHB-C4A	-2.43	1.33	1.39
38	l	314	II0	C20-C14	2.43	1.54	1.50
38	n	616	II0	C19-C13	2.43	1.54	1.50
29	B	824	CLA	CMC-C2C	-2.43	1.45	1.50
33	A	849	LMU	O5'-C1'	2.43	1.48	1.41
29	k	609	CLA	C1B-C2B	2.43	1.49	1.43
29	g	306	CLA	C3C-C2C	2.43	1.41	1.36
38	i	316	II0	C12-C14	2.43	1.54	1.51
29	n	607	CLA	C1B-C2B	2.43	1.49	1.43
29	h	302	CLA	CMC-C2C	-2.43	1.45	1.50
29	B	832	CLA	C1B-C2B	2.42	1.49	1.43
29	n	604	CLA	C1B-C2B	2.42	1.49	1.43
29	b	310	CLA	C1B-C2B	2.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	815	CLA	C1B-C2B	2.42	1.49	1.43
38	a	315	II0	C20-C14	2.42	1.54	1.50
36	j	319	DGD	O2G-C2G	-2.42	1.40	1.46
40	k	611	KC2	C2A-C1A	2.42	1.52	1.44
29	B	836	CLA	C1B-C2B	2.41	1.48	1.43
29	B	822	CLA	C1B-C2B	2.41	1.48	1.43
29	k	603	CLA	CHC-C1C	2.41	1.43	1.38
29	b	313	CLA	CMD-C2D	-2.41	1.45	1.50
29	g	311	CLA	C1B-C2B	2.41	1.48	1.43
40	l	311	KC2	CHB-C4A	-2.41	1.33	1.39
29	d	307	CLA	CMD-C2D	-2.41	1.45	1.50
29	A	829	CLA	MG-NB	-2.41	2.01	2.05
38	b	301	II0	C12-C14	2.41	1.54	1.51
29	B	811	CLA	C1B-C2B	2.41	1.48	1.43
29	s	406	CLA	C1B-C2B	2.40	1.48	1.43
29	j	305	CLA	C1B-C2B	2.40	1.48	1.43
29	B	826	CLA	C1B-C2B	2.40	1.48	1.43
29	O	201	CLA	C1B-C2B	2.40	1.48	1.43
29	B	842	CLA	CHC-C1C	2.40	1.43	1.38
29	B	823	CLA	CMD-C2D	-2.40	1.45	1.50
29	s	403	CLA	CMD-C2D	-2.40	1.45	1.50
32	L	205	WVN	C16-C05	2.39	1.55	1.50
38	b	301	II0	C19-C13	2.39	1.54	1.50
29	F	202	CLA	C1B-C2B	2.39	1.48	1.43
29	A	813	CLA	CHC-C1C	2.38	1.43	1.38
32	B	846	WVN	C16-C05	2.38	1.55	1.50
29	O	201	CLA	CMD-C2D	-2.38	1.45	1.50
29	c	306	CLA	C1B-C2B	2.38	1.48	1.43
32	I	101	WVN	C19-C11	2.38	1.37	1.32
40	s	401	KC2	C4A-C3A	2.38	1.49	1.44
38	f	614	II0	C20-C14	2.38	1.54	1.50
29	B	803	CLA	C3B-C4B	2.38	1.48	1.42
40	i	310	KC2	C1D-C2D	2.37	1.48	1.43
38	i	319	II0	C20-C14	2.37	1.54	1.50
40	c	310	KC2	C4A-C3A	2.37	1.49	1.44
29	g	304	CLA	C1B-C2B	2.37	1.48	1.43
29	A	817	CLA	C1B-C2B	2.37	1.48	1.43
29	B	809	CLA	C3B-C4B	2.37	1.48	1.42
38	l	315	II0	C19-C13	2.37	1.54	1.50
29	B	829	CLA	C1B-C2B	2.37	1.48	1.43
38	l	313	II0	C12-C14	2.37	1.54	1.51
32	B	848	WVN	C19-C11	2.37	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	f	611	KC2	C4A-C3A	2.37	1.49	1.44
32	B	848	WVN	C21-C15	2.37	1.54	1.50
38	j	301	II0	C19-C13	2.37	1.54	1.50
32	B	848	WVN	C16-C05	2.37	1.55	1.50
38	i	319	II0	C12-C14	2.36	1.54	1.51
32	A	854	WVN	C21-C15	2.36	1.54	1.50
29	s	402	CLA	C1B-C2B	2.36	1.48	1.43
29	c	303	CLA	C1B-C2B	2.36	1.48	1.43
29	A	828	CLA	CMD-C2D	-2.36	1.45	1.50
40	c	310	KC2	C1D-C2D	2.36	1.48	1.43
29	B	819	CLA	C3C-C2C	2.36	1.41	1.36
29	A	825	CLA	CHC-C1C	2.36	1.43	1.38
38	a	317	II0	C19-C13	2.36	1.54	1.50
29	A	827	CLA	C1B-C2B	2.36	1.48	1.43
40	d	311	KC2	C1D-C2D	2.36	1.48	1.43
29	g	306	CLA	CMB-C2B	-2.36	1.45	1.50
29	m	607	CLA	C1B-C2B	2.36	1.48	1.43
29	B	809	CLA	MG-NB	-2.36	2.01	2.05
40	m	611	KC2	C1D-C2D	2.35	1.48	1.43
29	B	802	CLA	C1B-C2B	2.35	1.48	1.43
29	B	819	CLA	C1B-C2B	2.35	1.48	1.43
29	B	818	CLA	CMB-C2B	-2.35	1.45	1.50
29	a	308	CLA	C1B-C2B	2.35	1.48	1.43
29	A	838	CLA	C1B-C2B	2.35	1.48	1.43
29	g	306	CLA	C1B-C2B	2.35	1.48	1.43
32	s	405	WVN	C16-C05	2.35	1.55	1.50
40	i	318	KC2	C1D-C2D	2.35	1.48	1.43
29	l	305	CLA	CMC-C2C	-2.35	1.45	1.50
38	k	620	II0	C20-C14	2.35	1.54	1.50
37	n	620	LMG	C7-C8	2.35	1.57	1.50
32	h	308	WVN	C16-C05	2.34	1.55	1.50
38	d	317	II0	C12-C14	2.34	1.54	1.51
29	j	309	CLA	CHC-C1C	2.34	1.43	1.38
29	f	608	CLA	C1B-C2B	2.34	1.48	1.43
29	d	303	CLA	MG-NB	-2.34	2.01	2.05
29	a	307	CLA	C1B-C2B	2.34	1.48	1.43
29	B	818	CLA	CHC-C1C	2.34	1.43	1.38
40	k	611	KC2	C1D-C2D	2.33	1.48	1.43
29	k	603	CLA	C1B-C2B	2.33	1.48	1.43
38	i	314	II0	C20-C14	2.33	1.54	1.50
32	l	302	WVN	C19-C11	2.33	1.37	1.32
29	f	607	CLA	CMD-C2D	-2.33	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	311	CLA	CMD-C2D	-2.33	1.45	1.50
29	A	803	CLA	C1B-C2B	2.33	1.48	1.43
29	c	306	CLA	CMB-C2B	-2.33	1.45	1.50
29	A	802	CLA	CHC-C1C	2.33	1.43	1.38
37	b	319	LMG	O7-C8	-2.33	1.40	1.46
29	j	308	CLA	C3B-C4B	2.33	1.48	1.42
29	A	813	CLA	C1B-C2B	2.32	1.48	1.43
29	B	836	CLA	CMD-C2D	-2.32	1.45	1.50
40	i	318	KC2	C1C-C2C	2.32	1.49	1.44
29	B	817	CLA	C1B-C2B	2.32	1.48	1.43
29	A	830	CLA	CMD-C2D	-2.32	1.45	1.50
29	B	833	CLA	CHC-C1C	2.32	1.43	1.38
29	f	613	CLA	CMD-C2D	-2.32	1.45	1.50
29	g	316	CLA	CHC-C1C	2.32	1.43	1.38
38	m	616	II0	C12-C14	2.31	1.54	1.51
38	J	103	II0	C20-C14	2.31	1.54	1.50
29	f	610	CLA	CMD-C2D	-2.31	1.45	1.50
38	f	615	II0	C19-C13	2.31	1.54	1.50
29	B	822	CLA	CMD-C2D	-2.31	1.45	1.50
32	l	302	WVN	C16-C05	2.31	1.54	1.50
32	I	101	WVN	C21-C15	2.31	1.54	1.50
29	c	307	CLA	CHC-C1C	2.31	1.43	1.38
38	j	315	II0	C12-C14	2.31	1.54	1.51
38	d	301	II0	C19-C13	2.31	1.54	1.50
38	g	318	II0	C19-C13	2.30	1.54	1.50
38	k	616	II0	C19-C13	2.30	1.54	1.50
29	A	817	CLA	CMC-C2C	-2.30	1.45	1.50
40	g	313	KC2	C1D-C2D	2.30	1.48	1.43
32	A	844	WVN	C19-C11	2.30	1.37	1.32
29	A	820	CLA	C1B-C2B	2.29	1.48	1.43
38	k	615	II0	C19-C13	2.29	1.54	1.50
29	m	602	CLA	C3C-C2C	2.29	1.41	1.36
29	A	850	CLA	MG-NB	-2.29	2.01	2.05
29	A	827	CLA	CHC-C1C	2.29	1.43	1.38
38	k	620	II0	C12-C14	2.29	1.54	1.51
38	n	615	II0	C12-C14	2.29	1.54	1.51
29	j	306	CLA	CHC-C1C	2.29	1.43	1.38
32	B	847	WVN	C16-C05	2.28	1.54	1.50
29	A	834	CLA	C1B-C2B	2.28	1.48	1.43
29	b	304	CLA	C1B-C2B	2.28	1.48	1.43
29	A	834	CLA	MG-NB	-2.28	2.01	2.05
29	B	813	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	817	CLA	MG-NB	-2.28	2.01	2.05
32	B	847	WVN	C19-C11	2.28	1.37	1.32
38	d	315	II0	C12-C14	2.28	1.54	1.51
29	K	102	CLA	CMC-C2C	-2.28	1.46	1.50
33	i	301	LMU	O2'-C2'	2.28	1.48	1.43
29	B	808	CLA	CMD-C2D	-2.28	1.46	1.50
29	A	830	CLA	CMB-C2B	-2.27	1.46	1.50
29	s	403	CLA	CHC-C1C	2.27	1.43	1.38
29	j	310	CLA	CHC-C1C	2.27	1.43	1.38
38	j	315	II0	C11-C13	2.27	1.54	1.51
29	B	812	CLA	MG-NB	-2.27	2.01	2.05
29	a	305	CLA	CHC-C1C	2.27	1.43	1.38
29	B	801	CLA	C1B-C2B	2.27	1.48	1.43
38	e	312	II0	C20-C14	2.27	1.54	1.50
36	B	844	DGD	C1D-C2D	2.27	1.59	1.52
29	B	803	CLA	CMC-C2C	-2.27	1.46	1.50
32	B	849	WVN	C16-C05	2.27	1.54	1.50
38	d	316	II0	C11-C13	2.27	1.54	1.51
29	B	822	CLA	CMC-C2C	-2.27	1.46	1.50
29	B	809	CLA	C1B-C2B	2.27	1.48	1.43
29	B	801	CLA	MG-NB	-2.27	2.01	2.05
29	B	803	CLA	CMD-C2D	-2.26	1.46	1.50
29	s	406	CLA	CHC-C1C	2.26	1.43	1.38
38	h	310	II0	C19-C13	2.26	1.54	1.50
29	A	820	CLA	CMB-C2B	-2.26	1.46	1.50
29	B	842	CLA	MG-NB	-2.26	2.01	2.05
29	h	302	CLA	CHC-C1C	2.26	1.43	1.38
38	m	614	II0	C11-C13	2.26	1.54	1.51
40	f	611	KC2	C1D-C2D	2.26	1.48	1.43
38	h	310	II0	C20-C14	2.26	1.54	1.50
38	i	319	II0	C19-C13	2.26	1.54	1.50
38	f	616	II0	C19-C13	2.25	1.54	1.50
29	B	842	CLA	C1B-C2B	2.25	1.48	1.43
29	a	302	CLA	CMD-C2D	-2.25	1.46	1.50
38	h	311	II0	C12-C14	2.25	1.54	1.51
38	g	319	II0	C20-C14	2.25	1.54	1.50
29	B	804	CLA	CHC-C1C	2.25	1.43	1.38
29	n	606	CLA	CHC-C1C	2.25	1.43	1.38
36	j	319	DGD	O1G-C1G	-2.25	1.40	1.45
38	k	619	II0	C12-C14	2.25	1.54	1.51
29	c	303	CLA	CHC-C1C	2.25	1.43	1.38
29	B	817	CLA	MG-NB	-2.24	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	i	301	LMU	O5'-C1'	2.24	1.47	1.41
32	F	207	WVN	C16-C05	2.24	1.54	1.50
29	b	304	CLA	CHC-C1C	2.24	1.43	1.38
29	s	402	CLA	CMD-C2D	-2.24	1.46	1.50
32	F	207	WVN	C19-C11	2.24	1.37	1.32
29	d	309	CLA	MG-NB	-2.24	2.01	2.05
29	A	850	CLA	CMB-C2B	-2.24	1.46	1.50
29	B	821	CLA	CHC-C1C	2.24	1.43	1.38
29	i	307	CLA	CHC-C1C	2.24	1.43	1.38
29	g	311	CLA	CHC-C1C	2.24	1.43	1.38
29	A	802	CLA	MG-NB	-2.24	2.01	2.05
29	i	305	CLA	CHC-C1C	2.23	1.43	1.38
29	h	312	CLA	CMD-C2D	-2.23	1.46	1.50
29	n	602	CLA	CMD-C2D	-2.23	1.46	1.50
29	B	812	CLA	CMB-C2B	-2.23	1.46	1.50
29	A	804	CLA	CMC-C2C	-2.23	1.46	1.50
29	A	850	CLA	C1B-C2B	2.23	1.48	1.43
29	k	602	CLA	MG-NB	-2.23	2.01	2.05
29	b	310	CLA	CHC-C1C	2.23	1.43	1.38
29	n	607	CLA	MG-NB	-2.23	2.01	2.05
29	O	201	CLA	CMC-C2C	-2.23	1.46	1.50
29	d	313	CLA	CMC-C2C	-2.23	1.46	1.50
29	B	802	CLA	CHC-C1C	2.23	1.43	1.38
29	f	605	CLA	CHC-C1C	2.23	1.43	1.38
38	g	319	II0	C12-C14	2.23	1.54	1.51
32	A	847	WVN	C19-C11	2.23	1.37	1.32
29	i	311	CLA	CHC-C1C	2.22	1.43	1.38
29	j	307	CLA	CHC-C1C	2.22	1.43	1.38
29	k	614	CLA	C3C-C2C	2.22	1.41	1.36
29	n	607	CLA	CMD-C2D	-2.22	1.46	1.50
29	A	817	CLA	CHC-C1C	2.22	1.43	1.38
29	n	602	CLA	CHC-C1C	2.22	1.43	1.38
38	a	313	II0	C20-C14	2.22	1.54	1.50
29	B	816	CLA	C1B-C2B	2.22	1.48	1.43
29	j	303	CLA	CMD-C2D	-2.22	1.46	1.50
29	B	816	CLA	CHC-C1C	2.22	1.43	1.38
40	j	312	KC2	C1D-C2D	2.22	1.48	1.43
29	j	314	CLA	CMD-C2D	-2.22	1.46	1.50
29	k	606	CLA	CHC-C1C	2.22	1.43	1.38
29	B	833	CLA	C1B-C2B	2.22	1.48	1.43
38	e	314	II0	C11-C13	2.22	1.54	1.51
29	a	308	CLA	MG-NB	-2.22	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	843	LHG	O7-C5	-2.22	1.41	1.46
31	b	318	LHG	O7-C5	-2.22	1.41	1.46
29	l	304	CLA	MG-NB	-2.21	2.01	2.05
29	g	302	CLA	CHC-C1C	2.21	1.43	1.38
33	A	849	LMU	O3B-C3B	2.21	1.48	1.43
38	m	618	II0	C19-C13	2.21	1.54	1.50
29	A	822	CLA	CMD-C2D	-2.21	1.46	1.50
29	B	830	CLA	CMD-C2D	-2.21	1.46	1.50
29	c	303	CLA	CMC-C2C	-2.21	1.46	1.50
29	f	602	CLA	MG-NB	-2.21	2.01	2.05
29	L	207	CLA	CHC-C1C	2.21	1.43	1.38
36	j	319	DGD	O6D-C5D	-2.21	1.39	1.44
29	j	313	CLA	CHC-C1C	2.21	1.43	1.38
29	c	305	CLA	MG-NB	-2.21	2.01	2.05
38	f	614	II0	C19-C13	2.21	1.54	1.50
29	f	606	CLA	CHC-C1C	2.21	1.43	1.38
29	A	817	CLA	CMD-C2D	-2.21	1.46	1.50
29	B	808	CLA	CMC-C2C	-2.21	1.46	1.50
29	A	802	CLA	CMD-C2D	-2.21	1.46	1.50
29	F	201	CLA	CHC-C1C	2.21	1.43	1.38
29	O	201	CLA	CMB-C2B	-2.21	1.46	1.50
29	m	605	CLA	CHC-C1C	2.21	1.43	1.38
29	k	608	CLA	CHC-C1C	2.21	1.43	1.38
29	g	304	CLA	CHC-C1C	2.21	1.43	1.38
38	h	309	II0	C19-C13	2.20	1.54	1.50
29	B	825	CLA	CMD-C2D	-2.20	1.46	1.50
29	A	806	CLA	CMB-C2B	-2.20	1.46	1.50
29	F	201	CLA	CMD-C2D	-2.20	1.46	1.50
38	i	316	II0	C19-C13	2.20	1.54	1.50
31	J	104	LHG	O7-C5	-2.20	1.41	1.46
29	e	311	CLA	CHC-C1C	2.20	1.43	1.38
29	n	604	CLA	CHC-C1C	2.20	1.43	1.38
29	A	802	CLA	C1B-C2B	2.20	1.48	1.43
29	L	202	CLA	CMB-C2B	-2.20	1.46	1.50
29	a	307	CLA	CMD-C2D	-2.20	1.46	1.50
29	l	312	CLA	CMD-C2D	-2.20	1.46	1.50
29	B	833	CLA	MG-NB	-2.20	2.01	2.05
29	m	608	CLA	CHC-C1C	2.20	1.43	1.38
32	B	849	WVN	C19-C11	2.20	1.37	1.32
29	h	303	CLA	CHC-C1C	2.20	1.43	1.38
29	A	829	CLA	CMD-C2D	-2.20	1.46	1.50
29	e	310	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	h	311	II0	C20-C14	2.20	1.54	1.50
29	g	307	CLA	CHC-C1C	2.20	1.43	1.38
29	A	808	CLA	CMD-C2D	-2.20	1.46	1.50
29	B	830	CLA	CMB-C2B	-2.20	1.46	1.50
29	s	402	CLA	CMB-C2B	-2.20	1.46	1.50
38	k	615	II0	C11-C13	2.20	1.54	1.51
29	R	203	CLA	CHC-C1C	2.20	1.43	1.38
31	j	318	LHG	O7-C5	-2.20	1.41	1.46
38	f	615	II0	C12-C14	2.19	1.54	1.51
29	b	307	CLA	CHC-C1C	2.19	1.43	1.38
40	k	612	KC2	C1A-CHA	2.19	1.46	1.40
40	k	613	KC2	C1A-CHA	2.19	1.46	1.40
29	A	804	CLA	CMD-C2D	-2.19	1.46	1.50
29	j	305	CLA	CHC-C1C	2.19	1.43	1.38
29	B	838	CLA	CHC-C1C	2.19	1.43	1.38
29	A	813	CLA	CMD-C2D	-2.19	1.46	1.50
29	B	817	CLA	CMB-C2B	-2.19	1.46	1.50
29	d	306	CLA	CMB-C2B	-2.19	1.46	1.50
29	B	807	CLA	MG-NB	-2.19	2.01	2.05
29	b	304	CLA	MG-NB	-2.19	2.01	2.05
29	B	829	CLA	MG-NB	-2.19	2.01	2.05
38	e	313	II0	C11-C13	2.19	1.54	1.51
29	k	602	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	839	CLA	CHC-C1C	2.19	1.43	1.38
29	l	308	CLA	CHC-C1C	2.19	1.43	1.38
29	B	814	CLA	CMD-C2D	-2.19	1.46	1.50
29	B	811	CLA	CMC-C2C	-2.19	1.46	1.50
29	B	841	CLA	C1B-C2B	2.19	1.48	1.43
38	b	314	II0	C19-C13	2.19	1.54	1.50
29	m	603	CLA	CMD-C2D	-2.19	1.46	1.50
29	B	837	CLA	CMB-C2B	-2.19	1.46	1.50
38	i	314	II0	C11-C13	2.19	1.54	1.51
29	A	815	CLA	MG-NB	-2.19	2.01	2.05
29	c	312	CLA	MG-NB	-2.19	2.01	2.05
29	j	303	CLA	MG-NB	-2.19	2.01	2.05
29	n	602	CLA	MG-NB	-2.18	2.01	2.05
29	a	308	CLA	CMB-C2B	-2.18	1.46	1.50
29	B	816	CLA	MG-NB	-2.18	2.01	2.05
29	B	832	CLA	CHC-C1C	2.18	1.43	1.38
29	b	303	CLA	MG-NB	-2.18	2.01	2.05
38	f	614	II0	C11-C13	2.18	1.54	1.51
29	J	102	CLA	CHC-C1C	2.18	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	834	CLA	CHC-C1C	2.18	1.43	1.38
29	j	304	CLA	CMC-C2C	-2.18	1.46	1.50
29	A	833	CLA	CMD-C2D	-2.18	1.46	1.50
29	h	301	CLA	CMD-C2D	-2.18	1.46	1.50
38	c	313	II0	C11-C13	2.18	1.54	1.51
29	h	312	CLA	MG-NB	-2.18	2.01	2.05
38	f	618	II0	C19-C13	2.18	1.54	1.50
29	A	834	CLA	CMD-C2D	-2.18	1.46	1.50
29	b	310	CLA	CMD-C2D	-2.18	1.46	1.50
33	i	301	LMU	O3B-C3B	2.18	1.48	1.43
29	b	308	CLA	CHC-C1C	2.18	1.42	1.38
29	l	310	CLA	CHC-C1C	2.18	1.42	1.38
29	B	836	CLA	CMB-C2B	-2.18	1.46	1.50
38	g	319	II0	C19-C13	2.18	1.54	1.50
29	l	306	CLA	CHC-C1C	2.18	1.42	1.38
29	Q	302	CLA	CHC-C1C	2.18	1.42	1.38
29	k	609	CLA	CMB-C2B	-2.17	1.46	1.50
29	B	834	CLA	CHC-C1C	2.17	1.42	1.38
29	d	305	CLA	CHC-C1C	2.17	1.42	1.38
29	A	837	CLA	CMD-C2D	-2.17	1.46	1.50
29	A	811	CLA	MG-NB	-2.17	2.01	2.05
29	B	818	CLA	MG-NB	-2.17	2.01	2.05
32	K	103	WVN	C16-C05	2.17	1.54	1.50
29	e	306	CLA	CHC-C1C	2.17	1.42	1.38
29	e	307	CLA	CHC-C1C	2.17	1.42	1.38
29	A	838	CLA	CMB-C2B	-2.17	1.46	1.50
29	s	402	CLA	CHC-C1C	2.17	1.42	1.38
29	i	303	CLA	CHC-C1C	2.17	1.42	1.38
29	m	602	CLA	MG-NB	-2.17	2.01	2.05
29	j	304	CLA	MG-NB	-2.17	2.01	2.05
29	d	308	CLA	CHC-C1C	2.17	1.42	1.38
29	A	816	CLA	MG-NB	-2.17	2.01	2.05
38	m	615	II0	C12-C14	2.17	1.54	1.51
29	h	312	CLA	CMB-C2B	-2.17	1.46	1.50
29	l	312	CLA	CHC-C1C	2.17	1.42	1.38
29	n	609	CLA	CHC-C1C	2.17	1.42	1.38
29	B	816	CLA	CMB-C2B	-2.17	1.46	1.50
29	A	807	CLA	CHC-C1C	2.16	1.42	1.38
29	B	826	CLA	MG-NB	-2.16	2.01	2.05
29	b	307	CLA	CMD-C2D	-2.16	1.46	1.50
29	m	604	CLA	CMD-C2D	-2.16	1.46	1.50
29	A	829	CLA	C1B-C2B	2.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	818	CLA	C1B-C2B	2.16	1.48	1.43
29	L	204	CLA	CHC-C1C	2.16	1.42	1.38
37	O	205	LMG	O7-C8	-2.16	1.41	1.46
29	A	818	CLA	MG-NB	-2.16	2.01	2.05
32	L	206	WVN	C16-C05	2.16	1.54	1.50
29	B	815	CLA	CHC-C1C	2.16	1.42	1.38
29	m	606	CLA	CHC-C1C	2.16	1.42	1.38
29	d	302	CLA	CMD-C2D	-2.16	1.46	1.50
29	c	309	CLA	CHC-C1C	2.16	1.42	1.38
38	i	313	II0	C11-C13	2.16	1.54	1.51
29	A	836	CLA	MG-NB	-2.16	2.01	2.05
29	B	812	CLA	CMC-C2C	-2.16	1.46	1.50
29	B	836	CLA	MG-NB	-2.16	2.01	2.05
29	j	311	CLA	CHC-C1C	2.16	1.42	1.38
29	s	403	CLA	CMC-C2C	-2.16	1.46	1.50
29	b	311	CLA	CMB-C2B	-2.16	1.46	1.50
38	k	620	II0	C19-C13	2.16	1.54	1.50
38	a	314	II0	C12-C14	2.16	1.54	1.51
29	h	312	CLA	CHC-C1C	2.16	1.42	1.38
29	m	602	CLA	CHC-C1C	2.16	1.42	1.38
38	m	618	II0	C11-C13	2.16	1.54	1.51
29	O	201	CLA	MG-NB	-2.16	2.01	2.05
29	i	306	CLA	CHC-C1C	2.16	1.42	1.38
29	B	814	CLA	CMB-C2B	-2.16	1.46	1.50
40	g	315	KC2	C1D-C2D	2.16	1.48	1.43
29	j	308	CLA	MG-NB	-2.16	2.01	2.05
29	B	826	CLA	CHC-C1C	2.16	1.42	1.38
29	L	203	CLA	CHC-C1C	2.15	1.42	1.38
29	k	606	CLA	CMD-C2D	-2.15	1.46	1.50
29	B	831	CLA	CMD-C2D	-2.15	1.46	1.50
29	A	820	CLA	CHC-C1C	2.15	1.42	1.38
29	e	305	CLA	CHC-C1C	2.15	1.42	1.38
29	A	823	CLA	CMB-C2B	-2.15	1.46	1.50
29	A	810	CLA	CMD-C2D	-2.15	1.46	1.50
29	f	602	CLA	CMD-C2D	-2.15	1.46	1.50
36	j	319	DGD	C4D-C3D	2.15	1.57	1.52
29	b	303	CLA	CMC-C2C	-2.15	1.46	1.50
29	B	842	CLA	CMD-C2D	-2.15	1.46	1.50
29	m	608	CLA	MG-NB	-2.15	2.01	2.05
29	k	603	CLA	MG-NB	-2.15	2.01	2.05
29	a	305	CLA	CMD-C2D	-2.15	1.46	1.50
29	n	605	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j	314	CLA	CHC-C1C	2.15	1.42	1.38
29	n	601	CLA	CHC-C1C	2.15	1.42	1.38
38	l	314	II0	C19-C13	2.15	1.54	1.50
29	c	303	CLA	MG-NB	-2.15	2.01	2.05
29	c	308	CLA	CHC-C1C	2.15	1.42	1.38
29	c	306	CLA	MG-NB	-2.15	2.01	2.05
29	B	832	CLA	CMB-C2B	-2.15	1.46	1.50
29	m	606	CLA	CMB-C2B	-2.15	1.46	1.50
29	B	818	CLA	CMD-C2D	-2.15	1.46	1.50
29	g	304	CLA	CMB-C2B	-2.15	1.46	1.50
29	B	829	CLA	CHC-C1C	2.14	1.42	1.38
29	g	312	CLA	CHC-C1C	2.14	1.42	1.38
29	n	603	CLA	CHC-C1C	2.14	1.42	1.38
29	A	802	CLA	CMB-C2B	-2.14	1.46	1.50
29	s	402	CLA	MG-NB	-2.14	2.01	2.05
29	B	825	CLA	CHC-C1C	2.14	1.42	1.38
29	g	310	CLA	CHC-C1C	2.14	1.42	1.38
29	a	311	CLA	CHC-C1C	2.14	1.42	1.38
32	B	846	WVN	C19-C11	2.14	1.37	1.32
38	j	301	II0	C12-C14	2.14	1.54	1.51
31	s	408	LHG	P-O6	2.14	1.67	1.60
29	B	823	CLA	MG-NB	-2.14	2.01	2.05
29	B	817	CLA	CHC-C1C	2.14	1.42	1.38
29	B	836	CLA	CHC-C1C	2.14	1.42	1.38
29	m	612	CLA	MG-NB	-2.14	2.01	2.05
29	B	809	CLA	CMD-C2D	-2.14	1.46	1.50
29	B	816	CLA	CMD-C2D	-2.14	1.46	1.50
29	B	831	CLA	CHC-C1C	2.14	1.42	1.38
29	B	828	CLA	CMB-C2B	-2.14	1.46	1.50
38	j	316	II0	C11-C13	2.14	1.54	1.51
29	A	802	CLA	CMC-C2C	-2.14	1.46	1.50
29	e	308	CLA	CHC-C1C	2.14	1.42	1.38
29	d	307	CLA	MG-NB	-2.14	2.01	2.05
38	e	312	II0	C12-C14	2.14	1.54	1.51
29	B	813	CLA	CHC-C1C	2.14	1.42	1.38
29	A	831	CLA	MG-NB	-2.14	2.01	2.05
29	A	827	CLA	CMD-C2D	-2.14	1.46	1.50
29	f	604	CLA	CMB-C2B	-2.14	1.46	1.50
31	e	317	LHG	P-O6	2.14	1.68	1.59
38	j	315	II0	C20-C14	2.14	1.54	1.50
29	B	804	CLA	CMD-C2D	-2.14	1.46	1.50
29	g	303	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	607	CLA	CMB-C2B	-2.13	1.46	1.50
29	A	825	CLA	MG-NB	-2.13	2.01	2.05
29	c	304	CLA	MG-NB	-2.13	2.01	2.05
29	g	309	CLA	CMC-C2C	-2.13	1.46	1.50
29	s	406	CLA	MG-NB	-2.13	2.01	2.05
29	f	603	CLA	MG-NB	-2.13	2.01	2.05
29	B	828	CLA	CHC-C1C	2.13	1.42	1.38
29	A	803	CLA	CMD-C2D	-2.13	1.46	1.50
29	f	609	CLA	MG-NB	-2.13	2.01	2.05
29	i	309	CLA	CHC-C1C	2.13	1.42	1.38
29	c	304	CLA	CMB-C2B	-2.13	1.46	1.50
29	B	815	CLA	MG-NB	-2.13	2.01	2.05
29	F	202	CLA	MG-NB	-2.13	2.01	2.05
29	B	809	CLA	C1B-NB	-2.13	1.35	1.37
29	e	301	CLA	CHC-C1C	2.13	1.42	1.38
38	J	103	II0	C12-C14	2.13	1.54	1.51
38	j	316	II0	C12-C14	2.13	1.54	1.51
29	A	850	CLA	CHC-C1C	2.13	1.42	1.38
29	A	808	CLA	CMB-C2B	-2.13	1.46	1.50
38	J	103	II0	C11-C13	2.13	1.54	1.51
29	h	301	CLA	CHC-C1C	2.13	1.42	1.38
29	A	816	CLA	CMD-C2D	-2.13	1.46	1.50
29	F	202	CLA	CHC-C1C	2.13	1.42	1.38
29	B	827	CLA	MG-NB	-2.13	2.01	2.05
29	n	613	CLA	CHC-C1C	2.13	1.42	1.38
38	g	319	II0	C11-C13	2.13	1.54	1.51
29	n	608	CLA	CHC-C1C	2.13	1.42	1.38
29	B	822	CLA	CMB-C2B	-2.13	1.46	1.50
29	B	840	CLA	CMC-C2C	-2.13	1.46	1.50
29	c	308	CLA	CMC-C2C	-2.13	1.46	1.50
29	j	305	CLA	CMD-C2D	-2.13	1.46	1.50
38	k	619	II0	C20-C14	2.13	1.54	1.50
29	k	601	CLA	CHC-C1C	2.13	1.42	1.38
32	L	201	WVN	C19-C11	2.13	1.37	1.32
37	b	319	LMG	C7-C8	2.13	1.57	1.50
29	n	603	CLA	MG-NB	-2.13	2.01	2.05
29	A	824	CLA	CHC-C1C	2.12	1.42	1.38
29	B	822	CLA	CHC-C1C	2.12	1.42	1.38
29	B	802	CLA	MG-NB	-2.12	2.01	2.05
29	g	304	CLA	MG-NB	-2.12	2.01	2.05
29	f	612	CLA	CMD-C2D	-2.12	1.46	1.50
29	g	323	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	828	CLA	CMC-C2C	-2.12	1.46	1.50
29	B	806	CLA	CMD-C2D	-2.12	1.46	1.50
29	L	204	CLA	CMD-C2D	-2.12	1.46	1.50
29	c	306	CLA	CMD-C2D	-2.12	1.46	1.50
29	d	306	CLA	CMD-C2D	-2.12	1.46	1.50
29	m	604	CLA	CHC-C1C	2.12	1.42	1.38
29	f	610	CLA	MG-NB	-2.12	2.01	2.05
29	O	202	CLA	MG-NB	-2.12	2.01	2.05
29	i	307	CLA	CMB-C2B	-2.12	1.46	1.50
29	k	602	CLA	CHC-C1C	2.12	1.42	1.38
29	n	609	CLA	MG-NB	-2.12	2.01	2.05
29	B	828	CLA	CMD-C2D	-2.12	1.46	1.50
29	f	603	CLA	CHC-C1C	2.12	1.42	1.38
29	j	303	CLA	CHC-C1C	2.12	1.42	1.38
38	g	317	II0	C19-C13	2.12	1.54	1.50
40	d	311	KC2	C3D-C2D	2.12	1.49	1.42
32	B	849	WVN	C14-C15	2.12	1.55	1.51
38	f	616	II0	C20-C14	2.12	1.54	1.50
29	e	307	CLA	MG-NB	-2.12	2.01	2.05
29	g	311	CLA	CMD-C2D	-2.12	1.46	1.50
29	B	822	CLA	MG-NB	-2.12	2.01	2.05
29	e	302	CLA	CHC-C1C	2.12	1.42	1.38
29	g	304	CLA	CMD-C2D	-2.12	1.46	1.50
38	k	616	II0	C11-C13	2.12	1.54	1.51
40	d	311	KC2	C1C-C2C	2.12	1.48	1.44
29	A	808	CLA	MG-NB	-2.12	2.01	2.05
29	a	310	CLA	MG-NB	-2.12	2.01	2.05
29	k	605	CLA	CHC-C1C	2.12	1.42	1.38
29	A	823	CLA	CMD-C2D	-2.12	1.46	1.50
29	g	323	CLA	CHC-C1C	2.11	1.42	1.38
29	j	310	CLA	MG-NB	-2.11	2.01	2.05
38	f	615	II0	C11-C13	2.11	1.54	1.51
29	A	820	CLA	CMD-C2D	-2.11	1.46	1.50
29	m	607	CLA	CMB-C2B	-2.11	1.46	1.50
29	a	303	CLA	MG-NB	-2.11	2.01	2.05
38	a	313	II0	C12-C14	2.11	1.54	1.51
29	c	302	CLA	CMD-C2D	-2.11	1.46	1.50
29	n	603	CLA	CMC-C2C	-2.11	1.46	1.50
29	s	403	CLA	MG-NB	-2.11	2.01	2.05
29	k	604	CLA	CHC-C1C	2.11	1.42	1.38
29	d	306	CLA	MG-NB	-2.11	2.01	2.05
31	c	316	LHG	P-O6	2.11	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	i	303	CLA	CMD-C2D	-2.11	1.46	1.50
29	e	308	CLA	CMD-C2D	-2.11	1.46	1.50
29	A	818	CLA	CMD-C2D	-2.11	1.46	1.50
29	c	302	CLA	MG-NB	-2.11	2.01	2.05
29	m	609	CLA	MG-NB	-2.11	2.01	2.05
29	i	303	CLA	MG-NB	-2.11	2.01	2.05
29	d	303	CLA	CHC-C1C	2.11	1.42	1.38
29	O	202	CLA	CMB-C2B	-2.11	1.46	1.50
29	n	613	CLA	CMD-C2D	-2.11	1.46	1.50
29	F	201	CLA	MG-NB	-2.11	2.01	2.05
29	b	304	CLA	CMD-C2D	-2.11	1.46	1.50
32	A	845	WVN	C06-C13	2.11	1.56	1.53
38	d	315	II0	C11-C13	2.11	1.54	1.51
29	e	302	CLA	MG-NB	-2.11	2.01	2.05
29	l	312	CLA	CMC-C2C	-2.11	1.46	1.50
29	A	821	CLA	CHC-C1C	2.11	1.42	1.38
29	A	835	CLA	CHC-C1C	2.11	1.42	1.38
35	A	853	SQD	O2-C2	-2.11	1.38	1.43
29	k	607	CLA	CMD-C2D	-2.11	1.46	1.50
29	b	308	CLA	MG-NB	-2.11	2.01	2.05
29	A	804	CLA	CHC-C1C	2.11	1.42	1.38
29	A	805	CLA	CHC-C1C	2.11	1.42	1.38
29	a	310	CLA	CHC-C1C	2.11	1.42	1.38
29	m	608	CLA	CMB-C2B	-2.11	1.46	1.50
29	g	311	CLA	CMC-C2C	-2.11	1.46	1.50
29	c	302	CLA	CHC-C1C	2.11	1.42	1.38
29	f	603	CLA	CMD-C2D	-2.11	1.46	1.50
29	f	612	CLA	MG-NB	-2.11	2.01	2.05
32	i	315	WVN	C14-C15	2.11	1.55	1.51
29	e	303	CLA	CHC-C1C	2.11	1.42	1.38
29	A	809	CLA	CMD-C2D	-2.11	1.46	1.50
29	A	822	CLA	CHC-C1C	2.11	1.42	1.38
38	m	616	II0	C11-C13	2.10	1.54	1.51
29	a	304	CLA	CMD-C2D	-2.10	1.46	1.50
38	k	616	II0	C12-C14	2.10	1.54	1.51
29	A	851	CLA	CMD-C2D	-2.10	1.46	1.50
28	A	801	CL0	C1B-C2B	-2.10	1.38	1.43
29	A	816	CLA	CMC-C2C	-2.10	1.46	1.50
29	A	836	CLA	CMD-C2D	-2.10	1.46	1.50
29	a	312	CLA	CMD-C2D	-2.10	1.46	1.50
29	a	303	CLA	CHC-C1C	2.10	1.42	1.38
29	B	806	CLA	MG-NB	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	812	CLA	CMC-C2C	-2.10	1.46	1.50
29	a	304	CLA	MG-NB	-2.10	2.01	2.05
29	A	819	CLA	CHC-C1C	2.10	1.42	1.38
29	B	807	CLA	CMD-C2D	-2.10	1.46	1.50
38	h	310	II0	C12-C14	2.10	1.54	1.51
29	a	312	CLA	CHC-C1C	2.10	1.42	1.38
29	m	612	CLA	CHC-C1C	2.10	1.42	1.38
29	b	303	CLA	CMD-C2D	-2.10	1.46	1.50
29	R	203	CLA	MG-NB	-2.10	2.01	2.05
29	B	840	CLA	CMD-C2D	-2.10	1.46	1.50
29	A	812	CLA	CMB-C2B	-2.10	1.46	1.50
29	A	805	CLA	MG-NB	-2.10	2.01	2.05
40	n	612	KC2	C1A-CHA	2.10	1.46	1.40
29	A	839	CLA	MG-NB	-2.10	2.01	2.05
29	A	812	CLA	MG-NB	-2.10	2.01	2.05
29	i	311	CLA	MG-NB	-2.10	2.01	2.05
29	B	829	CLA	CMB-C2B	-2.10	1.46	1.50
29	O	206	CLA	CMD-C2D	-2.10	1.46	1.50
29	A	820	CLA	MG-NB	-2.10	2.01	2.05
29	i	308	CLA	MG-NB	-2.10	2.01	2.05
38	i	313	II0	C12-C14	2.10	1.54	1.51
29	A	837	CLA	CMB-C2B	-2.10	1.46	1.50
29	B	831	CLA	MG-NB	-2.10	2.01	2.05
29	d	302	CLA	CHC-C1C	2.10	1.42	1.38
29	B	827	CLA	C1B-NB	-2.10	1.35	1.37
29	A	815	CLA	CMB-C2B	-2.10	1.46	1.50
29	h	307	CLA	CHC-C1C	2.10	1.42	1.38
29	b	309	CLA	CMD-C2D	-2.10	1.46	1.50
29	d	307	CLA	CHC-C1C	2.10	1.42	1.38
29	J	102	CLA	MG-NB	-2.10	2.01	2.05
29	A	810	CLA	CHC-C1C	2.10	1.42	1.38
40	c	310	KC2	C1C-C2C	2.09	1.48	1.44
28	A	801	CL0	CHB-C1B	2.09	1.44	1.39
29	A	831	CLA	CMB-C2B	-2.09	1.46	1.50
29	j	304	CLA	CMD-C2D	-2.09	1.46	1.50
38	g	318	II0	C11-C13	2.09	1.54	1.51
38	a	315	II0	C19-C13	2.09	1.54	1.50
29	K	101	CLA	CHC-C1C	2.09	1.42	1.38
29	b	305	CLA	CHC-C1C	2.09	1.42	1.38
29	g	310	CLA	CMD-C2D	-2.09	1.46	1.50
29	g	305	CLA	CHC-C1C	2.09	1.42	1.38
29	L	203	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	303	CLA	MG-NB	-2.09	2.01	2.05
29	B	823	CLA	CHC-C1C	2.09	1.42	1.38
31	g	322	LHG	O7-C5	-2.09	1.41	1.46
29	F	202	CLA	CMB-C2B	-2.09	1.46	1.50
29	A	830	CLA	MG-NB	-2.09	2.01	2.05
29	B	812	CLA	CMD-C2D	-2.09	1.46	1.50
29	f	608	CLA	CMD-C2D	-2.09	1.46	1.50
29	s	406	CLA	CMD-C2D	-2.09	1.46	1.50
38	k	619	II0	C11-C13	2.09	1.54	1.51
29	f	613	CLA	CHC-C1C	2.09	1.42	1.38
29	g	303	CLA	CMD-C2D	-2.09	1.46	1.50
29	B	819	CLA	MG-NB	-2.09	2.01	2.05
40	n	611	KC2	C1C-C2C	2.09	1.48	1.44
29	A	820	CLA	CMC-C2C	-2.09	1.46	1.50
38	l	313	II0	C20-C14	2.09	1.54	1.50
29	g	306	CLA	MG-NB	-2.09	2.01	2.05
29	k	608	CLA	MG-NB	-2.09	2.01	2.05
29	a	303	CLA	CMD-C2D	-2.09	1.46	1.50
29	n	609	CLA	CMC-C2C	-2.09	1.46	1.50
29	i	307	CLA	MG-NB	-2.09	2.01	2.05
29	a	309	CLA	CMC-C2C	-2.09	1.46	1.50
40	n	612	KC2	C1B-NB	-2.09	1.35	1.37
29	L	202	CLA	MG-NB	-2.09	2.01	2.05
29	k	604	CLA	MG-NB	-2.09	2.01	2.05
29	A	839	CLA	CMD-C2D	-2.09	1.46	1.50
29	L	202	CLA	CMD-C2D	-2.09	1.46	1.50
29	O	202	CLA	CMD-C2D	-2.09	1.46	1.50
29	O	206	CLA	CMB-C2B	-2.09	1.46	1.50
29	A	808	CLA	CMC-C2C	-2.09	1.46	1.50
29	e	304	CLA	CMD-C2D	-2.08	1.46	1.50
29	k	602	CLA	CMC-C2C	-2.08	1.46	1.50
29	j	313	CLA	CMD-C2D	-2.08	1.46	1.50
29	g	305	CLA	CMD-C2D	-2.08	1.46	1.50
29	L	204	CLA	MG-NB	-2.08	2.01	2.05
29	A	811	CLA	CMB-C2B	-2.08	1.46	1.50
29	l	303	CLA	CHC-C1C	2.08	1.42	1.38
29	j	309	CLA	MG-NB	-2.08	2.01	2.05
32	F	207	WVN	C14-C15	2.08	1.55	1.51
29	d	318	CLA	CMD-C2D	-2.08	1.46	1.50
29	n	601	CLA	CMD-C2D	-2.08	1.46	1.50
29	g	316	CLA	CMD-C2D	-2.08	1.46	1.50
29	g	323	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	824	CLA	CHC-C1C	2.08	1.42	1.38
29	a	302	CLA	CHC-C1C	2.08	1.42	1.38
29	a	306	CLA	MG-NB	-2.08	2.01	2.05
38	a	314	II0	C11-C13	2.08	1.54	1.51
29	b	308	CLA	CMC-C2C	-2.08	1.46	1.50
29	g	309	CLA	CMD-C2D	-2.08	1.46	1.50
38	l	313	II0	C11-C13	2.08	1.54	1.51
29	k	614	CLA	CHC-C1C	2.08	1.42	1.38
32	A	844	WVN	C06-C13	2.08	1.56	1.53
29	l	310	CLA	MG-NB	-2.08	2.01	2.05
29	k	606	CLA	MG-NB	-2.08	2.01	2.05
29	j	313	CLA	MG-NB	-2.08	2.01	2.05
29	d	302	CLA	MG-NB	-2.08	2.01	2.05
29	L	203	CLA	CMC-C2C	-2.08	1.46	1.50
29	A	812	CLA	CMD-C2D	-2.08	1.46	1.50
29	i	307	CLA	CMD-C2D	-2.08	1.46	1.50
29	B	835	CLA	CMB-C2B	-2.08	1.46	1.50
29	c	311	CLA	CMC-C2C	-2.08	1.46	1.50
29	f	605	CLA	MG-NB	-2.08	2.01	2.05
29	B	821	CLA	CMD-C2D	-2.08	1.46	1.50
29	l	301	CLA	CMB-C2B	-2.08	1.46	1.50
38	d	317	II0	C19-C13	2.08	1.54	1.50
29	A	828	CLA	CHC-C1C	2.08	1.42	1.38
32	B	846	WVN	C06-C13	2.08	1.56	1.53
29	A	831	CLA	CMD-C2D	-2.08	1.46	1.50
29	l	306	CLA	CMD-C2D	-2.08	1.46	1.50
40	i	310	KC2	C2A-C1A	2.08	1.50	1.44
40	n	611	KC2	C1D-C2D	2.08	1.48	1.43
29	a	311	CLA	CMB-C2B	-2.08	1.46	1.50
29	g	305	CLA	MG-NB	-2.08	2.01	2.05
32	R	201	WVN	C19-C11	2.08	1.37	1.32
29	c	305	CLA	CMD-C2D	-2.08	1.46	1.50
29	j	306	CLA	CMD-C2D	-2.08	1.46	1.50
40	s	401	KC2	C2A-C1A	2.08	1.50	1.44
38	n	615	II0	C20-C14	2.08	1.54	1.50
29	c	308	CLA	MG-NB	-2.08	2.01	2.05
29	B	839	CLA	CMB-C2B	-2.08	1.46	1.50
35	A	853	SQD	O4-C4	-2.08	1.38	1.43
29	B	834	CLA	CMC-C2C	-2.07	1.46	1.50
29	A	819	CLA	CMB-C2B	-2.07	1.46	1.50
29	B	835	CLA	MG-NB	-2.07	2.01	2.05
29	n	610	CLA	CHC-C1C	2.07	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	309	CLA	MG-NB	-2.07	2.01	2.05
29	A	819	CLA	CMD-C2D	-2.07	1.46	1.50
29	B	838	CLA	CMD-C2D	-2.07	1.46	1.50
29	k	608	CLA	CMC-C2C	-2.07	1.46	1.50
29	i	312	CLA	C3C-C2C	2.07	1.41	1.36
29	e	303	CLA	CMD-C2D	-2.07	1.46	1.50
29	e	302	CLA	CMD-C2D	-2.07	1.46	1.50
29	m	603	CLA	CHC-C1C	2.07	1.42	1.38
29	a	309	CLA	CMB-C2B	-2.07	1.46	1.50
29	b	312	CLA	CMB-C2B	-2.07	1.46	1.50
29	Q	302	CLA	CMD-C2D	-2.07	1.46	1.50
29	m	603	CLA	MG-NB	-2.07	2.01	2.05
29	A	850	CLA	CMD-C2D	-2.07	1.46	1.50
29	m	613	CLA	CMD-C2D	-2.07	1.46	1.50
29	A	812	CLA	CHC-C1C	2.07	1.42	1.38
29	j	307	CLA	CMD-C2D	-2.07	1.46	1.50
29	k	609	CLA	CHC-C1C	2.07	1.42	1.38
29	b	310	CLA	CMB-C2B	-2.07	1.46	1.50
29	d	309	CLA	CMD-C2D	-2.07	1.46	1.50
38	b	315	II0	C12-C14	2.07	1.54	1.51
29	h	305	CLA	MG-NB	-2.07	2.01	2.05
29	l	309	CLA	MG-NB	-2.07	2.01	2.05
29	B	813	CLA	CMC-C2C	-2.07	1.46	1.50
29	B	810	CLA	CHC-C1C	2.07	1.42	1.38
29	j	310	CLA	CMC-C2C	-2.07	1.46	1.50
40	d	312	KC2	C1B-NB	-2.07	1.35	1.37
29	B	804	CLA	MG-NB	-2.07	2.01	2.05
29	d	309	CLA	CHC-C1C	2.07	1.42	1.38
29	g	308	CLA	CHC-C1C	2.07	1.42	1.38
29	n	605	CLA	MG-NB	-2.07	2.01	2.05
29	B	806	CLA	CHC-C1C	2.07	1.42	1.38
29	B	824	CLA	CMB-C2B	-2.07	1.46	1.50
29	m	602	CLA	CMD-C2D	-2.07	1.46	1.50
29	A	805	CLA	CMD-C2D	-2.07	1.46	1.50
29	A	835	CLA	CMD-C2D	-2.07	1.46	1.50
29	B	811	CLA	CMD-C2D	-2.07	1.46	1.50
29	f	610	CLA	CHC-C1C	2.06	1.42	1.38
29	a	310	CLA	CMD-C2D	-2.06	1.46	1.50
31	f	620	LHG	P-O6	2.06	1.67	1.59
29	L	207	CLA	CMD-C2D	-2.06	1.46	1.50
29	A	840	CLA	CMD-C2D	-2.06	1.46	1.50
29	b	305	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	301	CLA	CMD-C2D	-2.06	1.46	1.50
29	m	613	CLA	MG-NB	-2.06	2.01	2.05
29	B	811	CLA	CMB-C2B	-2.06	1.46	1.50
40	i	318	KC2	CAA-C2A	2.06	1.52	1.46
29	n	608	CLA	CMB-C2B	-2.06	1.46	1.50
29	j	311	CLA	MG-NB	-2.06	2.01	2.05
29	j	309	CLA	CMD-C2D	-2.06	1.46	1.50
40	d	312	KC2	C1A-CHA	2.06	1.46	1.40
29	A	824	CLA	MG-NB	-2.06	2.01	2.05
29	f	601	CLA	CMD-C2D	-2.06	1.46	1.50
29	j	308	CLA	CMD-C2D	-2.06	1.46	1.50
29	k	608	CLA	CMD-C2D	-2.06	1.46	1.50
29	l	307	CLA	CHC-C1C	2.06	1.42	1.38
36	B	844	DGD	O6D-C5D	-2.06	1.39	1.44
29	h	304	CLA	CMD-C2D	-2.06	1.46	1.50
29	A	807	CLA	MG-NB	-2.06	2.01	2.05
29	i	309	CLA	MG-NB	-2.06	2.01	2.05
38	e	313	II0	C19-C13	2.06	1.54	1.50
29	a	309	CLA	CMD-C2D	-2.06	1.46	1.50
29	c	312	CLA	CMB-C2B	-2.06	1.46	1.50
29	g	323	CLA	MG-NB	-2.06	2.01	2.05
29	B	832	CLA	CMD-C2D	-2.06	1.46	1.50
29	l	305	CLA	CMD-C2D	-2.06	1.46	1.50
38	j	316	II0	C19-C13	2.06	1.54	1.50
31	L	208	LHG	O7-C5	-2.06	1.41	1.46
29	A	838	CLA	CHC-C1C	2.06	1.42	1.38
29	O	201	CLA	CHC-C1C	2.06	1.42	1.38
29	A	809	CLA	CMC-C2C	-2.06	1.46	1.50
29	m	612	CLA	CMD-C2D	-2.06	1.46	1.50
29	A	826	CLA	CMB-C2B	-2.06	1.46	1.50
29	A	829	CLA	CMC-C2C	-2.06	1.46	1.50
29	h	307	CLA	CMC-C2C	-2.06	1.46	1.50
29	i	305	CLA	CMD-C2D	-2.06	1.46	1.50
29	g	312	CLA	MG-NB	-2.06	2.01	2.05
40	e	309	KC2	C3D-C2D	2.05	1.49	1.42
29	B	811	CLA	CHC-C1C	2.05	1.42	1.38
29	B	839	CLA	CHC-C1C	2.05	1.42	1.38
29	g	303	CLA	CMB-C2B	-2.05	1.46	1.50
29	g	310	CLA	CMB-C2B	-2.05	1.46	1.50
29	f	604	CLA	CMD-C2D	-2.05	1.46	1.50
29	B	840	CLA	CMB-C2B	-2.05	1.46	1.50
29	j	302	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	308	CLA	MG-NB	-2.05	2.01	2.05
29	f	601	CLA	CHC-C1C	2.05	1.42	1.38
29	A	815	CLA	CMD-C2D	-2.05	1.46	1.50
29	k	602	CLA	CMB-C2B	-2.05	1.46	1.50
29	B	834	CLA	MG-NB	-2.05	2.01	2.05
29	K	102	CLA	MG-NB	-2.05	2.01	2.05
29	A	836	CLA	CMB-C2B	-2.05	1.46	1.50
29	B	837	CLA	CMD-C2D	-2.05	1.46	1.50
29	m	607	CLA	CMD-C2D	-2.05	1.46	1.50
29	n	609	CLA	CMB-C2B	-2.05	1.46	1.50
29	b	307	CLA	CMB-C2B	-2.05	1.46	1.50
29	f	609	CLA	CMC-C2C	-2.05	1.46	1.50
29	A	811	CLA	CHC-C1C	2.05	1.42	1.38
29	e	305	CLA	MG-NB	-2.05	2.01	2.05
29	f	610	CLA	CMB-C2B	-2.05	1.46	1.50
29	g	307	CLA	CMD-C2D	-2.05	1.46	1.50
29	f	612	CLA	CHC-C1C	2.05	1.42	1.38
29	h	307	CLA	MG-NB	-2.05	2.01	2.05
33	i	301	LMU	C3B-C2B	-2.05	1.47	1.52
29	B	820	CLA	MG-NB	-2.05	2.01	2.05
29	b	313	CLA	MG-NB	-2.05	2.01	2.05
29	i	302	CLA	MG-NB	-2.05	2.01	2.05
29	j	307	CLA	CMB-C2B	-2.05	1.46	1.50
29	b	307	CLA	MG-NB	-2.05	2.01	2.05
29	g	310	CLA	MG-NB	-2.05	2.01	2.05
29	m	601	CLA	MG-NB	-2.05	2.01	2.05
29	A	822	CLA	MG-NB	-2.05	2.01	2.05
29	B	819	CLA	CMD-C2D	-2.05	1.46	1.50
29	l	304	CLA	CMD-C2D	-2.05	1.46	1.50
29	f	601	CLA	CMB-C2B	-2.05	1.46	1.50
29	A	826	CLA	CHC-C1C	2.05	1.42	1.38
29	K	101	CLA	MG-NB	-2.05	2.01	2.05
29	b	309	CLA	CHC-C1C	2.05	1.42	1.38
29	R	203	CLA	CMC-C2C	-2.05	1.46	1.50
29	f	601	CLA	MG-NB	-2.04	2.01	2.05
29	d	304	CLA	CHC-C1C	2.04	1.42	1.38
29	c	304	CLA	CMD-C2D	-2.04	1.46	1.50
29	a	306	CLA	CHC-C1C	2.04	1.42	1.38
31	L	208	LHG	P-O6	2.04	1.67	1.59
29	e	304	CLA	CMB-C2B	-2.04	1.46	1.50
29	f	609	CLA	CMD-C2D	-2.04	1.46	1.50
33	i	301	LMU	O2B-C2B	2.04	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	312	CLA	MG-NB	-2.04	2.01	2.05
29	b	303	CLA	CHC-C1C	2.04	1.42	1.38
29	h	302	CLA	CMD-C2D	-2.04	1.46	1.50
29	B	801	CLA	CMC-C2C	-2.04	1.46	1.50
29	c	309	CLA	CMB-C2B	-2.04	1.46	1.50
29	j	302	CLA	MG-NB	-2.04	2.01	2.05
29	A	813	CLA	MG-NB	-2.04	2.01	2.05
29	B	803	CLA	MG-NB	-2.04	2.01	2.05
29	d	318	CLA	CHC-C1C	2.04	1.42	1.38
29	B	805	CLA	CMD-C2D	-2.04	1.46	1.50
29	e	310	CLA	MG-NB	-2.04	2.01	2.05
29	a	310	CLA	CMB-C2B	-2.04	1.46	1.50
29	k	610	CLA	CMD-C2D	-2.04	1.46	1.50
29	a	307	CLA	CMB-C2B	-2.04	1.46	1.50
29	k	609	CLA	CMC-C2C	-2.04	1.46	1.50
29	m	610	CLA	CHC-C1C	2.04	1.42	1.38
29	l	309	CLA	CHC-C1C	2.04	1.42	1.38
29	g	303	CLA	MG-NB	-2.04	2.01	2.05
33	A	849	LMU	C3'-C2'	-2.04	1.47	1.52
29	f	602	CLA	CMC-C2C	-2.04	1.46	1.50
29	e	301	CLA	MG-NB	-2.04	2.01	2.05
29	e	311	CLA	MG-NB	-2.04	2.01	2.05
29	d	305	CLA	MG-NB	-2.04	2.01	2.05
29	A	832	CLA	CMB-C2B	-2.04	1.46	1.50
29	B	817	CLA	CMD-C2D	-2.04	1.46	1.50
29	F	202	CLA	CMD-C2D	-2.04	1.46	1.50
32	A	846	WVN	C19-C11	2.04	1.37	1.32
29	d	310	CLA	CHC-C1C	2.04	1.42	1.38
29	i	312	CLA	CMD-C2D	-2.04	1.46	1.50
29	d	313	CLA	CMB-C2B	-2.04	1.46	1.50
29	O	206	CLA	CHC-C1C	2.04	1.42	1.38
29	a	302	CLA	CMB-C2B	-2.04	1.46	1.50
29	l	310	CLA	CMB-C2B	-2.04	1.46	1.50
29	A	814	CLA	CMD-C2D	-2.04	1.46	1.50
29	A	826	CLA	CMD-C2D	-2.04	1.46	1.50
29	B	841	CLA	CMD-C2D	-2.04	1.46	1.50
29	g	302	CLA	CMD-C2D	-2.04	1.46	1.50
29	m	604	CLA	MG-NB	-2.04	2.01	2.05
29	A	851	CLA	CMB-C2B	-2.04	1.46	1.50
29	j	302	CLA	CMB-C2B	-2.04	1.46	1.50
29	e	304	CLA	MG-NB	-2.04	2.01	2.05
29	B	827	CLA	C1B-C2B	2.04	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	807	CLA	CMD-C2D	-2.04	1.46	1.50
29	A	817	CLA	CMB-C2B	-2.04	1.46	1.50
29	l	306	CLA	CMC-C2C	-2.04	1.46	1.50
29	j	306	CLA	CMC-C2C	-2.04	1.46	1.50
29	A	811	CLA	CMD-C2D	-2.04	1.46	1.50
29	c	306	CLA	CMC-C2C	-2.04	1.46	1.50
29	c	312	CLA	CMD-C2D	-2.04	1.46	1.50
29	n	603	CLA	CMD-C2D	-2.04	1.46	1.50
29	l	305	CLA	CHC-C1C	2.04	1.42	1.38
29	d	306	CLA	CHC-C1C	2.04	1.42	1.38
32	h	308	WVN	C06-C13	2.04	1.56	1.53
29	k	608	CLA	CMB-C2B	-2.04	1.46	1.50
38	h	311	II0	C11-C13	2.04	1.54	1.51
29	b	306	CLA	MG-NB	-2.03	2.01	2.05
29	k	601	CLA	MG-NB	-2.03	2.01	2.05
40	n	612	KC2	MG-ND	-2.03	2.01	2.05
29	b	302	CLA	CMD-C2D	-2.03	1.46	1.50
29	h	305	CLA	CMC-C2C	-2.03	1.46	1.50
29	k	609	CLA	CMD-C2D	-2.03	1.46	1.50
29	l	303	CLA	CMB-C2B	-2.03	1.46	1.50
29	i	309	CLA	CMD-C2D	-2.03	1.46	1.50
40	e	309	KC2	C3C-C4C	2.03	1.48	1.44
31	J	104	LHG	P-O6	2.03	1.67	1.59
29	g	308	CLA	CMD-C2D	-2.03	1.46	1.50
29	A	803	CLA	MG-NB	-2.03	2.01	2.05
29	A	829	CLA	C1B-NB	-2.03	1.35	1.37
29	b	313	CLA	CMB-C2B	-2.03	1.46	1.50
29	O	206	CLA	CMC-C2C	-2.03	1.46	1.50
29	d	304	CLA	CMD-C2D	-2.03	1.46	1.50
29	i	304	CLA	CMD-C2D	-2.03	1.46	1.50
29	f	607	CLA	MG-NB	-2.03	2.01	2.05
29	m	606	CLA	CMD-C2D	-2.03	1.46	1.50
29	m	613	CLA	CMB-C2B	-2.03	1.46	1.50
29	i	308	CLA	CMC-C2C	-2.03	1.46	1.50
32	B	847	WVN	C06-C13	2.03	1.56	1.53
29	B	815	CLA	CMD-C2D	-2.03	1.46	1.50
29	l	308	CLA	CMD-C2D	-2.03	1.46	1.50
29	g	306	CLA	CMD-C2D	-2.03	1.46	1.50
29	A	828	CLA	MG-NB	-2.03	2.01	2.05
29	B	810	CLA	CMD-C2D	-2.03	1.46	1.50
29	f	605	CLA	CMD-C2D	-2.03	1.46	1.50
29	B	840	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	313	KC2	C2A-C1A	2.03	1.50	1.44
29	a	302	CLA	MG-NB	-2.03	2.01	2.05
29	h	303	CLA	MG-NB	-2.03	2.01	2.05
29	i	302	CLA	CMD-C2D	-2.03	1.46	1.50
40	g	315	KC2	C1C-C2C	2.03	1.48	1.44
29	d	308	CLA	CMB-C2B	-2.03	1.46	1.50
29	d	313	CLA	CHC-C1C	2.03	1.42	1.38
29	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
29	a	309	CLA	CHC-C1C	2.03	1.42	1.38
29	h	301	CLA	CMB-C2B	-2.03	1.46	1.50
29	h	305	CLA	CMD-C2D	-2.03	1.46	1.50
29	F	203	CLA	CHC-C1C	2.03	1.42	1.38
29	A	809	CLA	CMB-C2B	-2.03	1.46	1.50
29	j	313	CLA	CMC-C2C	-2.03	1.46	1.50
29	d	310	CLA	CMD-C2D	-2.03	1.46	1.50
29	n	604	CLA	CMB-C2B	-2.03	1.46	1.50
29	L	207	CLA	CMB-C2B	-2.03	1.46	1.50
29	d	308	CLA	MG-NB	-2.03	2.01	2.05
29	n	607	CLA	CHC-C1C	2.03	1.42	1.38
29	m	601	CLA	CMB-C2B	-2.03	1.46	1.50
29	A	824	CLA	CMD-C2D	-2.02	1.46	1.50
29	h	303	CLA	CMB-C2B	-2.02	1.46	1.50
38	l	314	II0	C11-C13	2.02	1.54	1.51
29	h	302	CLA	MG-NB	-2.02	2.01	2.05
29	a	305	CLA	CMC-C2C	-2.02	1.46	1.50
29	b	306	CLA	CMB-C2B	-2.02	1.46	1.50
29	k	601	CLA	CMD-C2D	-2.02	1.46	1.50
29	g	307	CLA	MG-NB	-2.02	2.01	2.05
29	n	604	CLA	MG-NB	-2.02	2.01	2.05
29	A	813	CLA	CMB-C2B	-2.02	1.46	1.50
29	j	304	CLA	CHC-C1C	2.02	1.42	1.38
29	A	835	CLA	CMB-C2B	-2.02	1.46	1.50
29	l	309	CLA	CMB-C2B	-2.02	1.46	1.50
29	f	606	CLA	CMB-C2B	-2.02	1.46	1.50
29	A	851	CLA	MG-NB	-2.02	2.01	2.05
29	A	822	CLA	CMB-C2B	-2.02	1.46	1.50
29	F	203	CLA	CMD-C2D	-2.02	1.46	1.50
29	A	810	CLA	CMC-C2C	-2.02	1.46	1.50
29	l	309	CLA	CMD-C2D	-2.02	1.46	1.50
29	k	606	CLA	CMB-C2B	-2.02	1.46	1.50
29	b	309	CLA	MG-NB	-2.02	2.01	2.05
40	k	613	KC2	MG-ND	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	307	CLA	CMD-C2D	-2.02	1.46	1.50
29	n	605	CLA	CMD-C2D	-2.02	1.46	1.50
29	m	606	CLA	MG-NB	-2.02	2.01	2.05
29	n	610	CLA	MG-NB	-2.02	2.01	2.05
29	A	818	CLA	C1B-C2B	2.02	1.48	1.43
29	g	312	CLA	CMD-C2D	-2.02	1.46	1.50
29	B	828	CLA	MG-NB	-2.02	2.01	2.05
29	F	201	CLA	CMB-C2B	-2.02	1.46	1.50
29	k	604	CLA	CMB-C2B	-2.02	1.46	1.50
29	A	819	CLA	MG-NB	-2.02	2.01	2.05
29	B	839	CLA	CMD-C2D	-2.02	1.46	1.50
29	A	851	CLA	CHC-C1C	2.02	1.42	1.38
29	O	202	CLA	CHC-C1C	2.02	1.42	1.38
29	e	311	CLA	CMD-C2D	-2.02	1.46	1.50
29	b	306	CLA	CMD-C2D	-2.02	1.46	1.50
29	f	613	CLA	MG-NB	-2.02	2.01	2.05
29	b	302	CLA	CMB-C2B	-2.02	1.46	1.50
29	h	303	CLA	CMD-C2D	-2.02	1.46	1.50
29	i	304	CLA	CMB-C2B	-2.02	1.46	1.50
29	A	806	CLA	CMD-C2D	-2.02	1.46	1.50
29	e	301	CLA	CMD-C2D	-2.02	1.46	1.50
29	k	604	CLA	CMD-C2D	-2.02	1.46	1.50
29	O	206	CLA	MG-NB	-2.02	2.01	2.05
29	k	607	CLA	CMB-C2B	-2.02	1.46	1.50
29	f	603	CLA	CMC-C2C	-2.02	1.46	1.50
29	f	609	CLA	CMB-C2B	-2.02	1.46	1.50
29	n	606	CLA	MG-NB	-2.02	2.01	2.05
29	A	818	CLA	C3C-C2C	2.02	1.41	1.36
29	B	820	CLA	CMB-C2B	-2.02	1.46	1.50
29	a	306	CLA	CMD-C2D	-2.02	1.46	1.50
29	m	608	CLA	CMD-C2D	-2.02	1.46	1.50
29	m	605	CLA	CMB-C2B	-2.02	1.46	1.50
29	B	825	CLA	MG-NB	-2.02	2.01	2.05
29	J	102	CLA	CMB-C2B	-2.01	1.46	1.50
29	A	825	CLA	CMD-C2D	-2.01	1.46	1.50
29	e	305	CLA	CMD-C2D	-2.01	1.46	1.50
29	B	827	CLA	CMC-C2C	-2.01	1.46	1.50
29	i	306	CLA	CMD-C2D	-2.01	1.46	1.50
29	d	303	CLA	CMC-C2C	-2.01	1.46	1.50
29	k	610	CLA	CHC-C1C	2.01	1.42	1.38
40	k	611	KC2	C1C-C2C	2.01	1.48	1.44
29	L	207	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	m	601	CLA	CMD-C2D	-2.01	1.46	1.50
29	h	305	CLA	CHC-C1C	2.01	1.42	1.38
29	e	304	CLA	CHC-C1C	2.01	1.42	1.38
40	i	318	KC2	C3D-C2D	2.01	1.49	1.42
29	l	303	CLA	MG-NB	-2.01	2.01	2.05
29	k	609	CLA	MG-NB	-2.01	2.01	2.05
29	Q	302	CLA	MG-NB	-2.01	2.01	2.05
29	B	834	CLA	CMD-C2D	-2.01	1.46	1.50
29	n	607	CLA	CMB-C2B	-2.01	1.46	1.50
38	l	315	II0	C12-C14	2.01	1.54	1.51
36	B	844	DGD	C3D-C2D	2.01	1.57	1.52
29	A	814	CLA	CHC-C1C	2.01	1.42	1.38
29	B	803	CLA	CHC-C1C	2.01	1.42	1.38
29	a	306	CLA	CMB-C2B	-2.01	1.46	1.50
29	a	311	CLA	CMC-C2C	-2.01	1.46	1.50
29	e	305	CLA	CMB-C2B	-2.01	1.46	1.50
29	n	609	CLA	CMD-C2D	-2.01	1.46	1.50
29	a	308	CLA	CHC-C1C	2.01	1.42	1.38
29	A	838	CLA	CMD-C2D	-2.01	1.46	1.50
29	c	309	CLA	MG-NB	-2.01	2.01	2.05
29	a	307	CLA	CHC-C1C	2.01	1.42	1.38
36	B	844	DGD	O1G-C1G	-2.01	1.40	1.45
29	j	314	CLA	MG-NB	-2.01	2.01	2.05
30	A	841	PQN	C9-C10	2.01	1.43	1.39
29	e	307	CLA	CMD-C2D	-2.01	1.46	1.50
29	k	610	CLA	CMB-C2B	-2.01	1.46	1.50
29	j	310	CLA	CMB-C2B	-2.01	1.46	1.50
29	d	303	CLA	CMD-C2D	-2.01	1.46	1.50
29	g	309	CLA	MG-NB	-2.01	2.01	2.05
38	d	301	II0	C11-C13	2.01	1.54	1.51
29	A	840	CLA	CHC-C1C	2.01	1.42	1.38
29	j	311	CLA	CMD-C2D	-2.01	1.46	1.50
29	f	602	CLA	CHC-C1C	2.01	1.42	1.38
29	a	310	CLA	CMC-C2C	-2.01	1.46	1.50
31	s	408	LHG	O7-C5	-2.01	1.41	1.46
29	l	307	CLA	MG-NB	-2.01	2.01	2.05
29	l	312	CLA	CMB-C2B	-2.01	1.46	1.50
29	k	603	CLA	CMC-C2C	-2.01	1.46	1.50
29	F	203	CLA	CMB-C2B	-2.01	1.46	1.50
29	c	303	CLA	CMD-C2D	-2.01	1.46	1.50
29	h	301	CLA	MG-NB	-2.01	2.01	2.05
29	e	306	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	204	CLA	CMB-C2B	-2.01	1.46	1.50
29	m	609	CLA	CHC-C1C	2.01	1.42	1.38
29	n	610	CLA	CMB-C2B	-2.01	1.46	1.50
29	m	609	CLA	CMD-C2D	-2.01	1.46	1.50
29	m	612	CLA	CMB-C2B	-2.01	1.46	1.50
29	l	308	CLA	MG-NB	-2.00	2.01	2.05
29	n	601	CLA	MG-NB	-2.00	2.01	2.05
29	B	841	CLA	CMB-C2B	-2.00	1.46	1.50
29	B	807	CLA	CMC-C2C	-2.00	1.46	1.50
29	c	307	CLA	MG-NB	-2.00	2.01	2.05
29	a	305	CLA	MG-NB	-2.00	2.01	2.05
29	f	609	CLA	CHC-C1C	2.00	1.42	1.38
33	A	849	LMU	O2B-C2B	2.00	1.47	1.43
29	d	310	CLA	CMB-C2B	-2.00	1.46	1.50
29	j	306	CLA	MG-NB	-2.00	2.01	2.05
29	B	835	CLA	CMD-C2D	-2.00	1.46	1.50
29	s	406	CLA	CMB-C2B	-2.00	1.46	1.50
29	k	603	CLA	CMD-C2D	-2.00	1.46	1.50
29	B	838	CLA	CMC-C2C	-2.00	1.46	1.50
29	A	840	CLA	MG-NB	-2.00	2.01	2.05
29	B	826	CLA	MG-ND	-2.00	2.01	2.05
29	h	306	CLA	MG-NB	-2.00	2.01	2.05
29	e	310	CLA	CHC-C1C	2.00	1.42	1.38
40	l	311	KC2	CAA-C2A	2.00	1.52	1.46
29	l	306	CLA	MG-NB	-2.00	2.01	2.05
32	L	206	WVN	C14-C15	2.00	1.54	1.51
29	a	308	CLA	CMD-C2D	-2.00	1.46	1.50
29	j	308	CLA	CMC-C2C	-2.00	1.46	1.50
29	n	606	CLA	CMD-C2D	-2.00	1.46	1.50
29	A	828	CLA	CMB-C2B	-2.00	1.46	1.50
29	B	807	CLA	CMB-C2B	-2.00	1.46	1.50
29	B	815	CLA	CMC-C2C	-2.00	1.46	1.50
29	B	814	CLA	MG-NB	-2.00	2.01	2.05

All (4755) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	e	314	II0	C24-C22-C10	-25.41	111.10	175.43
38	i	313	II0	C24-C22-C10	-25.20	111.61	175.43
38	m	615	II0	C23-C21-C09	-24.97	112.20	175.43
38	m	616	II0	C23-C21-C09	-24.96	112.23	175.43
38	m	615	II0	C24-C22-C10	-24.96	112.24	175.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	e	312	II0	C23-C21-C09	-24.95	112.25	175.43
38	i	316	II0	C23-C21-C09	-24.94	112.27	175.43
38	k	615	II0	C23-C21-C09	-24.94	112.28	175.43
38	e	313	II0	C23-C21-C09	-24.93	112.30	175.43
38	m	618	II0	C23-C21-C09	-24.92	112.33	175.43
38	a	317	II0	C23-C21-C09	-24.91	112.35	175.43
38	a	314	II0	C23-C21-C09	-24.91	112.36	175.43
38	j	315	II0	C23-C21-C09	-24.91	112.37	175.43
38	i	319	II0	C23-C21-C09	-24.91	112.37	175.43
38	i	313	II0	C23-C21-C09	-24.90	112.37	175.43
38	n	615	II0	C23-C21-C09	-24.89	112.40	175.43
38	k	619	II0	C23-C21-C09	-24.89	112.41	175.43
38	m	614	II0	C23-C21-C09	-24.88	112.43	175.43
38	f	618	II0	C23-C21-C09	-24.88	112.43	175.43
38	n	616	II0	C23-C21-C09	-24.88	112.44	175.43
38	j	301	II0	C23-C21-C09	-24.87	112.45	175.43
38	n	618	II0	C23-C21-C09	-24.87	112.45	175.43
38	b	301	II0	C23-C21-C09	-24.87	112.46	175.43
38	a	315	II0	C24-C22-C10	-24.86	112.47	175.43
38	a	313	II0	C23-C21-C09	-24.86	112.47	175.43
38	d	316	II0	C23-C21-C09	-24.84	112.52	175.43
38	j	316	II0	C23-C21-C09	-24.84	112.52	175.43
38	d	315	II0	C23-C21-C09	-24.84	112.53	175.43
38	h	311	II0	C23-C21-C09	-24.84	112.54	175.43
38	h	309	II0	C23-C21-C09	-24.83	112.55	175.43
38	l	313	II0	C23-C21-C09	-24.83	112.57	175.43
38	g	317	II0	C24-C22-C10	-24.81	112.60	175.43
38	g	319	II0	C23-C21-C09	-24.81	112.62	175.43
38	c	313	II0	C23-C21-C09	-24.80	112.64	175.43
38	b	314	II0	C23-C21-C09	-24.80	112.64	175.43
38	d	301	II0	C23-C21-C09	-24.79	112.66	175.43
38	h	310	II0	C23-C21-C09	-24.79	112.66	175.43
38	f	615	II0	C23-C21-C09	-24.79	112.67	175.43
38	k	620	II0	C23-C21-C09	-24.78	112.69	175.43
38	J	103	II0	C23-C21-C09	-24.77	112.70	175.43
38	f	614	II0	C23-C21-C09	-24.76	112.75	175.43
38	l	314	II0	C23-C21-C09	-24.75	112.76	175.43
38	d	317	II0	C23-C21-C09	-24.73	112.80	175.43
38	e	314	II0	C23-C21-C09	-24.73	112.81	175.43
38	g	318	II0	C23-C21-C09	-24.73	112.82	175.43
38	n	616	II0	C24-C22-C10	-24.72	112.83	175.43
38	c	313	II0	C24-C22-C10	-24.72	112.84	175.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	d	301	II0	C24-C22-C10	-24.71	112.86	175.43
38	l	313	II0	C24-C22-C10	-24.71	112.86	175.43
38	g	317	II0	C23-C21-C09	-24.71	112.86	175.43
38	b	315	II0	C23-C21-C09	-24.71	112.86	175.43
38	i	316	II0	C24-C22-C10	-24.66	112.98	175.43
38	a	315	II0	C23-C21-C09	-24.64	113.03	175.43
38	k	616	II0	C24-C22-C10	-24.63	113.06	175.43
38	g	318	II0	C24-C22-C10	-24.49	113.42	175.43
38	f	615	II0	C24-C22-C10	-24.48	113.45	175.43
38	i	314	II0	C23-C21-C09	-24.44	113.55	175.43
38	k	616	II0	C23-C21-C09	-24.37	113.74	175.43
38	j	301	II0	C24-C22-C10	-24.35	113.78	175.43
38	l	315	II0	C24-C22-C10	-24.32	113.84	175.43
38	j	316	II0	C24-C22-C10	-24.15	114.29	175.43
38	m	614	II0	C24-C22-C10	-24.09	114.43	175.43
38	h	310	II0	C24-C22-C10	-24.04	114.57	175.43
38	l	315	II0	C23-C21-C09	-24.01	114.64	175.43
38	j	315	II0	C24-C22-C10	-23.99	114.68	175.43
38	k	619	II0	C24-C22-C10	-23.99	114.69	175.43
38	e	313	II0	C24-C22-C10	-23.97	114.74	175.43
38	f	618	II0	C24-C22-C10	-23.96	114.77	175.43
38	f	616	II0	C23-C21-C09	-23.95	114.80	175.43
38	d	316	II0	C24-C22-C10	-23.91	114.89	175.43
38	d	317	II0	C24-C22-C10	-23.86	115.02	175.43
38	i	314	II0	C24-C22-C10	-23.85	115.04	175.43
38	m	618	II0	C24-C22-C10	-23.84	115.06	175.43
38	h	311	II0	C24-C22-C10	-23.79	115.20	175.43
38	n	615	II0	C24-C22-C10	-23.76	115.27	175.43
38	a	317	II0	C24-C22-C10	-23.72	115.36	175.43
38	n	618	II0	C24-C22-C10	-23.66	115.51	175.43
38	b	301	II0	C24-C22-C10	-23.65	115.54	175.43
38	f	614	II0	C24-C22-C10	-23.44	116.08	175.43
38	e	312	II0	C24-C22-C10	-23.30	116.42	175.43
38	g	319	II0	C24-C22-C10	-23.22	116.63	175.43
38	a	313	II0	C24-C22-C10	-23.04	117.08	175.43
38	m	616	II0	C24-C22-C10	-23.04	117.10	175.43
38	f	616	II0	C24-C22-C10	-22.98	117.24	175.43
38	b	314	II0	C24-C22-C10	-22.92	117.40	175.43
38	J	103	II0	C24-C22-C10	-22.78	117.76	175.43
38	k	620	II0	C24-C22-C10	-22.68	118.01	175.43
38	a	314	II0	C24-C22-C10	-22.38	118.77	175.43
38	l	314	II0	C24-C22-C10	-22.33	118.88	175.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	301	CLA	O2A-CGA-O1A	-20.72	71.29	123.59
38	d	315	II0	C24-C22-C10	-20.55	123.41	175.43
38	i	319	II0	C24-C22-C10	-20.01	124.77	175.43
32	l	316	WVN	C20-C23-C25	19.93	156.35	126.23
38	b	315	II0	C24-C22-C10	-19.75	125.42	175.43
38	k	615	II0	C24-C22-C10	-19.57	125.89	175.43
32	h	308	WVN	C20-C23-C25	18.06	153.53	126.23
32	K	103	WVN	C20-C23-C25	17.36	152.47	126.23
32	A	844	WVN	C20-C23-C25	17.09	152.05	126.23
32	s	407	WVN	C20-C23-C25	17.03	151.96	126.23
32	R	201	WVN	C20-C23-C25	16.83	151.66	126.23
32	A	845	WVN	C20-C23-C25	16.69	151.46	126.23
32	M	101	WVN	C20-C23-C25	16.65	151.39	126.23
32	A	846	WVN	C04-C09-C05	-16.19	109.33	124.85
32	L	206	WVN	C20-C23-C25	16.18	150.69	126.23
32	B	848	WVN	C20-C23-C25	16.15	150.64	126.23
32	L	205	WVN	C20-C23-C25	16.14	150.62	126.23
32	F	205	WVN	C04-C09-C05	-16.05	109.46	124.85
32	F	207	WVN	C20-C23-C25	16.02	150.45	126.23
32	J	101	WVN	C20-C23-C25	15.97	150.37	126.23
32	F	205	WVN	C20-C23-C25	15.94	150.32	126.23
32	B	849	WVN	C20-C23-C25	15.88	150.23	126.23
32	A	854	WVN	C20-C23-C25	15.77	150.06	126.23
32	e	315	WVN	C20-C23-C25	15.72	149.99	126.23
32	l	302	WVN	C20-C23-C25	15.62	149.84	126.23
32	I	101	WVN	C20-C23-C25	15.62	149.83	126.23
32	F	204	WVN	C20-C23-C25	15.61	149.82	126.23
32	A	854	WVN	C04-C09-C05	-15.54	109.95	124.85
32	L	201	WVN	C20-C23-C25	15.47	149.60	126.23
32	R	202	WVN	C04-C09-C05	-15.43	110.06	124.85
32	A	845	WVN	C04-C09-C05	-15.42	110.06	124.85
32	L	201	WVN	C04-C09-C05	-15.07	110.40	124.85
32	s	407	WVN	C04-C09-C05	-14.99	110.48	124.85
32	s	407	WVN	C21-C15-C13	-14.97	107.72	124.53
32	B	847	WVN	C20-C23-C25	14.66	148.38	126.23
32	R	202	WVN	C20-C23-C25	14.66	148.38	126.23
32	i	315	WVN	C20-C23-C25	14.50	148.14	126.23
32	M	101	WVN	C04-C09-C05	-14.46	110.99	124.85
29	h	301	CLA	O2A-CGA-CBA	14.38	157.03	111.91
38	a	315	II0	C32-C34-C36	-14.36	86.06	126.42
32	A	844	WVN	C30-C33-C34	-14.35	86.11	126.42
38	g	317	II0	C32-C34-C36	-14.29	86.27	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	K	103	WVN	C30-C33-C34	-14.26	86.35	126.42
32	L	206	WVN	C30-C33-C34	-14.15	86.66	126.42
38	e	312	II0	C32-C34-C36	-14.07	86.90	126.42
38	l	315	II0	C32-C34-C36	-14.06	86.91	126.42
32	A	847	WVN	C20-C23-C25	14.06	147.48	126.23
38	k	616	II0	C32-C34-C36	-14.05	86.96	126.42
32	A	846	WVN	C20-C23-C25	14.01	147.41	126.23
38	i	316	II0	C32-C34-C36	-14.00	87.08	126.42
32	s	405	WVN	C30-C33-C34	-13.98	87.15	126.42
32	B	846	WVN	C40-C37-C34	-13.86	107.53	127.31
38	d	316	II0	C32-C34-C36	-13.85	87.51	126.42
38	g	319	II0	C32-C34-C36	-13.82	87.59	126.42
38	a	314	II0	C32-C34-C36	-13.75	87.78	126.42
38	c	313	II0	C32-C34-C36	-13.73	87.83	126.42
38	i	313	II0	C32-C34-C36	-13.72	87.87	126.42
38	n	616	II0	C32-C34-C36	-13.71	87.90	126.42
32	L	205	WVN	C30-C33-C34	-13.70	87.92	126.42
38	l	314	II0	C41-C39-C35	-13.69	107.77	127.31
38	m	616	II0	C32-C34-C36	-13.63	88.12	126.42
38	J	103	II0	C32-C34-C36	-13.56	88.32	126.42
38	k	615	II0	C32-C34-C36	-13.53	88.40	126.42
38	k	619	II0	C32-C34-C36	-13.53	88.40	126.42
38	f	618	II0	C32-C34-C36	-13.50	88.50	126.42
38	f	614	II0	C32-C34-C36	-13.48	88.54	126.42
38	a	317	II0	C32-C34-C36	-13.45	88.63	126.42
32	A	845	WVN	C30-C33-C34	-13.38	88.84	126.42
38	a	313	II0	C32-C34-C36	-13.37	88.85	126.42
38	g	318	II0	C32-C34-C36	-13.32	88.99	126.42
32	e	315	WVN	C04-C09-C05	-13.29	112.11	124.85
38	j	315	II0	C32-C34-C36	-13.27	89.14	126.42
38	e	314	II0	C32-C34-C36	-13.26	89.16	126.42
38	n	618	II0	C32-C34-C36	-13.15	89.47	126.42
38	d	301	II0	C32-C34-C36	-13.13	89.54	126.42
38	k	620	II0	C32-C34-C36	-13.12	89.55	126.42
32	M	101	WVN	C30-C33-C34	-13.11	89.58	126.42
38	f	616	II0	C32-C34-C36	-13.04	89.79	126.42
32	L	205	WVN	C21-C15-C13	-13.02	109.90	124.53
38	j	301	II0	C32-C34-C36	-13.00	89.89	126.42
32	B	846	WVN	C20-C23-C25	12.93	145.78	126.23
32	B	846	WVN	C21-C15-C13	-12.90	110.05	124.53
38	n	615	II0	C32-C34-C36	-12.86	90.29	126.42
38	g	317	II0	C41-C39-C35	-12.81	109.02	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	848	WVN	C30-C33-C34	-12.80	90.46	126.42
32	s	405	WVN	C20-C23-C25	12.79	145.56	126.23
38	n	615	II0	C41-C39-C35	-12.76	109.10	127.31
32	L	206	WVN	C21-C15-C13	-12.71	110.25	124.53
38	f	618	II0	C41-C39-C35	-12.70	109.18	127.31
32	R	202	WVN	C30-C33-C34	-12.68	90.79	126.42
32	L	201	WVN	C40-C37-C34	-12.65	109.25	127.31
38	k	619	II0	C20-C14-C10	-12.64	107.17	124.35
32	R	201	WVN	C21-C15-C13	-12.64	110.34	124.53
32	F	205	WVN	C21-C15-C13	-12.62	110.36	124.53
32	l	316	WVN	C21-C15-C13	-12.60	110.38	124.53
32	A	846	WVN	C21-C15-C13	-12.54	110.44	124.53
32	A	844	WVN	C39-C36-C32	-12.51	109.45	127.31
32	F	207	WVN	C30-C33-C34	-12.50	91.31	126.42
32	A	854	WVN	C30-C33-C34	-12.49	91.34	126.42
32	A	847	WVN	C30-C33-C34	-12.49	91.34	126.42
38	l	315	II0	C41-C39-C35	-12.43	109.57	127.31
32	R	201	WVN	C30-C33-C34	-12.42	91.53	126.42
32	B	846	WVN	C30-C28-C25	-12.39	109.62	127.31
32	L	206	WVN	C39-C36-C32	-12.38	109.65	127.31
38	e	314	II0	C41-C39-C35	-12.35	109.68	127.31
32	I	101	WVN	C21-C15-C13	-12.34	110.67	124.53
38	l	314	II0	C38-C36-C40	-12.31	105.68	122.92
38	j	316	II0	C32-C34-C36	-12.28	91.93	126.42
38	b	301	II0	C32-C34-C36	-12.25	92.01	126.42
32	s	405	WVN	C39-C36-C32	-12.24	109.84	127.31
38	h	310	II0	C41-C39-C35	-12.22	109.87	127.31
32	F	204	WVN	C24-C22-C26	-12.20	105.83	122.92
38	b	314	II0	C32-C34-C36	-12.20	92.14	126.42
38	b	315	II0	C32-C34-C36	-12.20	92.16	126.42
38	f	615	II0	C32-C34-C36	-12.18	92.20	126.42
32	A	846	WVN	C40-C37-C34	-12.15	109.97	127.31
38	d	316	II0	C41-C39-C35	-12.13	110.00	127.31
38	m	614	II0	C32-C34-C36	-12.12	92.37	126.42
32	h	308	WVN	C21-C15-C13	-12.11	110.93	124.53
32	l	316	WVN	C40-C37-C34	-12.07	110.08	127.31
38	c	313	II0	C19-C13-C09	-12.03	108.00	124.35
38	h	311	II0	C32-C34-C36	-12.03	92.63	126.42
38	h	310	II0	C32-C34-C36	-12.02	92.65	126.42
40	g	313	KC2	CMA-C3A-C4A	-11.99	106.78	125.04
32	s	407	WVN	C39-C36-C32	-11.98	110.21	127.31
32	K	103	WVN	C04-C09-C05	-11.95	113.40	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	309	II0	C41-C39-C35	-11.94	110.26	127.31
38	j	315	II0	C41-C39-C35	-11.92	110.31	127.31
32	i	315	WVN	C04-C09-C05	-11.91	113.43	124.85
38	g	319	II0	C41-C39-C35	-11.91	110.31	127.31
38	n	615	II0	C20-C14-C10	-11.90	108.18	124.35
32	l	302	WVN	C21-C15-C13	-11.88	111.19	124.53
32	h	308	WVN	C30-C33-C34	-11.88	93.05	126.42
38	f	614	II0	C41-C39-C35	-11.86	110.38	127.31
40	m	611	KC2	CMA-C3A-C4A	-11.86	106.98	125.04
32	i	315	WVN	C30-C33-C34	-11.85	93.12	126.42
38	j	315	II0	C20-C14-C10	-11.85	108.25	124.35
32	R	202	WVN	C21-C15-C13	-11.84	111.23	124.53
32	s	405	WVN	C21-C15-C13	-11.77	111.31	124.53
38	k	620	II0	C20-C14-C10	-11.75	108.38	124.35
38	m	615	II0	C32-C34-C36	-11.75	93.40	126.42
38	a	313	II0	C41-C39-C35	-11.75	110.54	127.31
38	b	314	II0	C20-C14-C10	-11.75	108.39	124.35
32	K	103	WVN	C21-C15-C13	-11.73	111.36	124.53
38	k	620	II0	C41-C39-C35	-11.72	110.58	127.31
38	i	319	II0	C41-C39-C35	-11.72	110.59	127.31
40	f	611	KC2	CMA-C3A-C4A	-11.71	107.21	125.04
38	l	314	II0	C32-C34-C36	-11.71	93.53	126.42
32	e	315	WVN	C30-C33-C34	-11.70	93.54	126.42
32	B	849	WVN	C39-C36-C32	-11.67	110.65	127.31
40	s	404	KC2	C2A-C3A-C4A	-11.67	97.83	106.49
32	B	847	WVN	C21-C15-C13	-11.65	111.45	124.53
38	m	614	II0	C41-C39-C35	-11.63	110.72	127.31
32	l	302	WVN	C39-C36-C32	-11.61	110.74	127.31
32	s	405	WVN	C30-C28-C25	-11.60	110.75	127.31
32	A	845	WVN	C21-C15-C13	-11.58	111.53	124.53
32	A	845	WVN	C24-C22-C26	-11.58	106.71	122.92
40	j	312	KC2	CMA-C3A-C4A	-11.57	107.42	125.04
38	k	620	II0	C19-C13-C09	-11.56	108.64	124.35
32	B	849	WVN	C30-C33-C34	-11.53	94.02	126.42
38	m	618	II0	C32-C34-C36	-11.53	94.03	126.42
38	i	313	II0	C19-C13-C09	-11.51	108.71	124.35
38	a	317	II0	C41-C39-C35	-11.51	110.89	127.31
32	B	848	WVN	C21-C15-C13	-11.50	111.61	124.53
40	c	310	KC2	CMA-C3A-C4A	-11.49	107.53	125.04
32	B	847	WVN	C40-C37-C34	-11.45	110.97	127.31
32	A	854	WVN	C21-C15-C13	-11.43	111.69	124.53
32	A	845	WVN	C39-C36-C32	-11.43	111.00	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	i	313	II0	C41-C39-C35	-11.42	111.01	127.31
38	j	316	II0	C19-C13-C09	-11.42	108.83	124.35
38	e	313	II0	C19-C13-C09	-11.40	108.86	124.35
38	f	616	II0	C41-C39-C35	-11.38	111.07	127.31
32	A	847	WVN	C39-C36-C32	-11.36	111.10	127.31
32	R	201	WVN	C39-C36-C32	-11.35	111.11	127.31
38	k	615	II0	C19-C13-C09	-11.32	108.96	124.35
38	k	615	II0	C41-C39-C35	-11.31	111.17	127.31
40	k	611	KC2	CMA-C3A-C4A	-11.30	107.82	125.04
38	f	614	II0	C19-C13-C09	-11.30	108.99	124.35
38	d	315	II0	C41-C39-C35	-11.26	111.24	127.31
38	n	618	II0	C41-C39-C35	-11.26	111.25	127.31
32	J	101	WVN	C29-C26-C22	-11.25	111.25	127.31
32	M	101	WVN	C29-C26-C22	-11.24	111.27	127.31
32	F	207	WVN	C39-C36-C32	-11.20	111.32	127.31
38	l	313	II0	C19-C13-C09	-11.20	109.14	124.35
38	d	315	II0	C42-C40-C36	-11.19	111.33	127.31
32	B	847	WVN	C29-C26-C22	-11.18	111.36	127.31
38	a	315	II0	C41-C39-C35	-11.16	111.39	127.31
38	d	301	II0	C19-C13-C09	-11.15	109.20	124.35
32	K	103	WVN	C29-C26-C22	-11.14	111.41	127.31
32	l	302	WVN	C04-C09-C05	-11.14	114.17	124.85
40	n	611	KC2	CMA-C3A-C4A	-11.13	108.09	125.04
32	J	101	WVN	C21-C15-C13	-11.12	112.04	124.53
38	J	103	II0	C20-C14-C10	-11.09	109.28	124.35
32	i	315	WVN	C39-C36-C32	-11.08	111.50	127.31
32	R	202	WVN	C24-C22-C26	-11.07	107.42	122.92
32	J	101	WVN	C40-C37-C34	-11.07	111.52	127.31
32	A	846	WVN	C39-C36-C32	-11.06	111.52	127.31
38	J	103	II0	C19-C13-C09	-11.03	109.35	124.35
38	a	314	II0	C20-C14-C10	-11.03	109.36	124.35
40	s	401	KC2	CMA-C3A-C4A	-11.03	108.25	125.04
40	i	310	KC2	CMA-C3A-C4A	-11.02	108.25	125.04
32	e	315	WVN	C21-C15-C13	-11.01	112.17	124.53
40	e	309	KC2	CMA-C3A-C4A	-10.98	108.31	125.04
38	h	311	II0	C41-C39-C35	-10.98	111.64	127.31
38	a	315	II0	C19-C13-C09	-10.96	109.46	124.35
38	J	103	II0	C41-C39-C35	-10.94	111.69	127.31
38	b	301	II0	C41-C39-C35	-10.93	111.71	127.31
38	a	313	II0	C20-C14-C10	-10.93	109.50	124.35
32	s	405	WVN	C04-C09-C05	-10.92	114.38	124.85
32	K	103	WVN	C24-C22-C26	-10.91	107.64	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	b	315	II0	C19-C13-C09	-10.91	109.53	124.35
32	i	315	WVN	C21-C15-C13	-10.90	112.29	124.53
38	c	313	II0	C41-C39-C35	-10.89	111.77	127.31
38	d	315	II0	C32-C34-C36	-10.88	95.84	126.42
32	F	204	WVN	C21-C15-C13	-10.88	112.31	124.53
32	M	101	WVN	C21-C15-C13	-10.87	112.32	124.53
38	a	314	II0	C41-C39-C35	-10.86	111.81	127.31
38	e	312	II0	C20-C14-C10	-10.85	109.61	124.35
38	g	319	II0	C20-C14-C10	-10.83	109.63	124.35
38	d	317	II0	C32-C34-C36	-10.83	96.00	126.42
32	F	204	WVN	C29-C26-C22	-10.82	111.86	127.31
32	K	103	WVN	C30-C28-C25	-10.82	111.87	127.31
32	s	407	WVN	C30-C33-C34	-10.80	96.08	126.42
38	g	319	II0	C19-C13-C09	-10.79	109.69	124.35
32	B	847	WVN	C39-C36-C32	-10.78	111.92	127.31
40	g	315	KC2	CMA-C3A-C4A	-10.78	108.63	125.04
32	B	846	WVN	C19-C22-C26	-10.78	102.41	118.94
32	I	101	WVN	C40-C37-C34	-10.74	111.98	127.31
38	n	616	II0	C41-C39-C35	-10.73	111.99	127.31
40	d	311	KC2	CMA-C3A-C4A	-10.72	108.71	125.04
38	i	316	II0	C41-C39-C35	-10.71	112.03	127.31
38	l	313	II0	C41-C39-C35	-10.69	112.05	127.31
32	B	848	WVN	C04-C09-C05	-10.68	114.61	124.85
32	B	849	WVN	C21-C15-C13	-10.67	112.55	124.53
32	h	308	WVN	C24-C22-C26	-10.64	108.02	122.92
40	i	310	KC2	C2A-C3A-C4A	-10.64	98.59	106.49
32	B	846	WVN	C04-C09-C05	-10.63	114.65	124.85
32	M	101	WVN	C39-C36-C32	-10.62	112.15	127.31
32	B	848	WVN	C39-C36-C32	-10.62	112.16	127.31
38	m	618	II0	C38-C36-C40	-10.61	108.06	122.92
32	L	206	WVN	C40-C37-C34	-10.61	112.17	127.31
32	L	206	WVN	C35-C32-C36	-10.60	108.07	122.92
38	g	318	II0	C19-C13-C09	-10.60	109.95	124.35
38	d	301	II0	C41-C39-C35	-10.59	112.20	127.31
32	R	202	WVN	C39-C36-C32	-10.59	112.20	127.31
32	I	101	WVN	C04-C09-C05	-10.59	114.70	124.85
38	i	319	II0	C32-C34-C36	-10.58	96.68	126.42
32	F	207	WVN	C21-C15-C13	-10.58	112.64	124.53
38	d	317	II0	C42-C40-C36	-10.58	112.21	127.31
29	b	311	CLA	C4A-NA-C1A	10.58	111.46	106.71
32	l	316	WVN	C29-C26-C22	-10.57	112.22	127.31
38	d	317	II0	C19-C13-C09	-10.57	109.99	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	616	II0	C41-C39-C35	-10.54	112.26	127.31
32	L	201	WVN	C30-C33-C34	-10.53	96.83	126.42
32	L	201	WVN	C21-C15-C13	-10.51	112.72	124.53
32	L	206	WVN	C27-C25-C28	-10.50	108.21	122.92
40	i	318	KC2	CMA-C3A-C4A	-10.50	109.05	125.04
32	A	847	WVN	C21-C15-C13	-10.50	112.74	124.53
32	J	101	WVN	C24-C22-C26	-10.49	108.22	122.92
32	l	302	WVN	C40-C37-C34	-10.46	112.39	127.31
32	B	847	WVN	C30-C28-C25	-10.44	112.41	127.31
32	s	407	WVN	C40-C37-C34	-10.44	112.41	127.31
38	h	311	II0	C20-C14-C10	-10.43	110.18	124.35
32	L	206	WVN	C38-C34-C37	-10.43	108.32	122.92
32	L	205	WVN	C39-C36-C32	-10.40	112.47	127.31
32	L	205	WVN	C04-C09-C05	-10.40	114.88	124.85
32	h	308	WVN	C04-C09-C05	-10.40	114.88	124.85
38	k	619	II0	C41-C39-C35	-10.40	112.47	127.31
40	g	314	KC2	C2A-C3A-C4A	-10.39	98.78	106.49
38	l	313	II0	C32-C34-C36	-10.37	97.30	126.42
32	B	846	WVN	C30-C33-C34	-10.35	97.34	126.42
32	B	847	WVN	C04-C09-C05	-10.35	114.93	124.85
32	h	308	WVN	C39-C36-C32	-10.35	112.55	127.31
32	B	847	WVN	C24-C22-C26	-10.33	108.45	122.92
38	d	317	II0	C41-C39-C35	-10.33	112.57	127.31
38	f	616	II0	C20-C14-C10	-10.33	110.32	124.35
32	i	315	WVN	C29-C26-C22	-10.29	112.62	127.31
32	B	849	WVN	C04-C09-C05	-10.28	114.99	124.85
32	A	844	WVN	C04-C09-C05	-10.28	115.00	124.85
32	F	204	WVN	C40-C37-C34	-10.27	112.65	127.31
38	k	615	II0	C38-C36-C40	-10.26	108.55	122.92
32	F	207	WVN	C04-C09-C05	-10.25	115.03	124.85
32	J	101	WVN	C30-C28-C25	-10.22	112.73	127.31
38	m	615	II0	C41-C39-C35	-10.20	112.75	127.31
32	L	205	WVN	C29-C26-C22	-10.20	112.75	127.31
38	l	313	II0	C42-C40-C36	-10.20	112.75	127.31
38	k	619	II0	C19-C13-C09	-10.19	110.50	124.35
32	L	201	WVN	C30-C28-C25	-10.19	112.77	127.31
32	A	846	WVN	C30-C33-C34	-10.19	97.80	126.42
32	L	206	WVN	C24-C22-C26	-10.18	108.67	122.92
40	g	315	KC2	C2A-C3A-C4A	-10.17	98.94	106.49
32	F	205	WVN	C29-C31-C32	10.17	154.98	126.42
32	J	101	WVN	C39-C36-C32	-10.16	112.80	127.31
32	e	315	WVN	C39-C36-C32	-10.16	112.82	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	n	611	KC2	C2A-C3A-C4A	-10.15	98.96	106.49
32	I	101	WVN	C29-C26-C22	-10.14	112.83	127.31
38	b	315	II0	C41-C39-C35	-10.13	112.85	127.31
32	I	101	WVN	C24-C22-C26	-10.13	108.74	122.92
38	m	618	II0	C42-C40-C36	-10.12	112.86	127.31
32	F	204	WVN	C04-C09-C05	-10.10	115.16	124.85
32	A	844	WVN	C21-C15-C13	-10.10	113.19	124.53
38	m	618	II0	C37-C35-C39	-10.10	108.78	122.92
32	J	101	WVN	C30-C33-C34	-10.09	98.06	126.42
38	j	316	II0	C41-C39-C35	-10.09	112.91	127.31
38	b	314	II0	C19-C13-C09	-10.08	110.65	124.35
32	I	101	WVN	C39-C36-C32	-10.08	112.92	127.31
38	h	310	II0	C19-C13-C09	-10.07	110.66	124.35
32	I	101	WVN	C06-C13-C15	-10.07	108.44	122.61
38	k	619	II0	C38-C36-C40	-10.06	108.83	122.92
32	F	205	WVN	C30-C28-C25	-10.05	112.97	127.31
38	k	615	II0	C31-C33-C35	10.05	154.65	126.42
32	A	845	WVN	C30-C28-C25	-10.04	112.97	127.31
32	s	407	WVN	C35-C32-C36	-10.04	108.86	122.92
32	I	101	WVN	C30-C28-C25	-10.00	113.03	127.31
38	a	317	II0	C37-C35-C39	-9.99	108.92	122.92
38	f	615	II0	C41-C39-C35	-9.99	113.06	127.31
40	g	314	KC2	CMA-C3A-C4A	-9.98	109.83	125.04
32	A	846	WVN	C30-C28-C25	-9.98	113.06	127.31
40	d	311	KC2	C2A-C3A-C4A	-9.97	99.09	106.49
32	A	854	WVN	C24-C22-C26	-9.97	108.95	122.92
32	h	308	WVN	C29-C31-C32	9.97	154.42	126.42
32	M	101	WVN	C29-C31-C32	9.94	154.34	126.42
38	j	301	II0	C37-C35-C39	-9.93	109.02	122.92
32	F	204	WVN	C06-C13-C15	-9.91	108.66	122.61
32	I	101	WVN	C30-C33-C34	-9.89	98.62	126.42
38	j	301	II0	C41-C39-C35	-9.89	113.19	127.31
32	i	315	WVN	C35-C32-C36	-9.87	109.10	122.92
38	l	315	II0	C37-C35-C39	-9.87	109.10	122.92
32	l	302	WVN	C30-C33-C34	-9.86	98.71	126.42
32	L	206	WVN	C29-C31-C32	9.86	154.11	126.42
38	h	311	II0	C31-C33-C35	9.86	154.10	126.42
40	i	318	KC2	C2A-C3A-C4A	-9.85	99.18	106.49
32	A	845	WVN	C29-C31-C32	9.85	154.09	126.42
40	k	611	KC2	C2A-C3A-C4A	-9.84	99.19	106.49
32	B	847	WVN	C30-C33-C34	-9.84	98.79	126.42
32	R	202	WVN	C29-C26-C22	-9.83	113.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	101	WVN	C04-C09-C05	-9.83	115.43	124.85
32	I	101	WVN	C29-C31-C32	9.82	154.01	126.42
38	h	310	II0	C20-C14-C10	-9.81	111.01	124.35
38	e	313	II0	C41-C39-C35	-9.81	113.31	127.31
32	F	205	WVN	C30-C33-C34	9.81	153.97	126.42
32	F	207	WVN	C24-C22-C26	-9.81	109.19	122.92
32	s	405	WVN	C35-C32-C36	-9.78	109.22	122.92
32	I	101	WVN	C35-C32-C36	-9.77	109.23	122.92
38	e	312	II0	C31-C33-C35	9.77	153.87	126.42
32	M	101	WVN	C24-C22-C26	-9.77	109.24	122.92
32	A	846	WVN	C24-C22-C26	-9.76	109.25	122.92
29	h	301	CLA	O1A-CGA-CBA	-9.74	85.74	123.73
32	l	316	WVN	C38-C34-C37	-9.73	109.29	122.92
40	l	311	KC2	C2A-C3A-C4A	-9.73	99.27	106.49
32	F	207	WVN	C38-C34-C37	-9.73	109.30	122.92
38	h	310	II0	C37-C35-C39	-9.73	109.30	122.92
40	c	310	KC2	C1D-ND-C4D	-9.72	99.43	106.33
32	s	405	WVN	C02-C05-C09	-9.72	109.52	121.47
32	A	854	WVN	C39-C36-C32	-9.71	113.45	127.31
38	b	301	II0	C19-C13-C09	-9.70	111.17	124.35
32	F	204	WVN	C30-C33-C34	-9.70	99.17	126.42
32	F	207	WVN	C29-C26-C22	-9.69	113.47	127.31
38	b	301	II0	C37-C35-C39	-9.69	109.34	122.92
40	d	311	KC2	C1D-ND-C4D	-9.69	99.45	106.33
38	g	317	II0	C37-C35-C39	-9.69	109.35	122.92
38	i	316	II0	C37-C35-C39	-9.69	109.36	122.92
40	e	309	KC2	C2A-C3A-C4A	-9.68	99.30	106.49
38	i	319	II0	C37-C35-C39	-9.68	109.36	122.92
38	k	616	II0	C41-C39-C35	-9.67	113.51	127.31
38	b	314	II0	C41-C39-C35	-9.66	113.52	127.31
38	g	318	II0	C41-C39-C35	-9.66	113.52	127.31
32	A	846	WVN	C29-C26-C22	-9.66	113.52	127.31
32	J	101	WVN	C35-C32-C36	-9.66	109.39	122.92
38	i	319	II0	C42-C40-C36	-9.66	113.53	127.31
38	n	616	II0	C31-C33-C35	9.65	153.53	126.42
32	l	316	WVN	C29-C31-C32	9.65	153.53	126.42
32	B	849	WVN	C38-C34-C37	-9.64	109.42	122.92
32	L	201	WVN	C39-C36-C32	-9.64	113.56	127.31
32	F	205	WVN	C40-C37-C34	-9.64	113.56	127.31
32	F	204	WVN	C27-C25-C28	-9.63	109.44	122.92
32	e	315	WVN	C27-C25-C28	-9.63	109.44	122.92
38	n	616	II0	C37-C35-C39	-9.62	109.45	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	d	316	II0	C37-C35-C39	-9.62	109.45	122.92
38	a	317	II0	C31-C33-C35	9.61	153.42	126.42
38	k	619	II0	C37-C35-C39	-9.61	109.46	122.92
40	m	611	KC2	C2A-C3A-C4A	-9.61	99.36	106.49
32	s	405	WVN	C27-C25-C28	-9.61	109.46	122.92
32	l	302	WVN	C35-C32-C36	-9.60	109.47	122.92
32	A	845	WVN	C35-C32-C36	-9.60	109.47	122.92
32	K	103	WVN	C35-C32-C36	-9.59	109.48	122.92
38	d	301	II0	C20-C14-C10	-9.59	111.31	124.35
38	g	319	II0	C37-C35-C39	-9.59	109.49	122.92
38	h	309	II0	C31-C33-C35	9.58	153.34	126.42
38	f	618	II0	C37-C35-C39	-9.58	109.51	122.92
38	f	615	II0	C19-C13-C09	-9.57	111.34	124.35
38	i	313	II0	C37-C35-C39	-9.57	109.52	122.92
38	k	615	II0	C37-C35-C39	-9.55	109.54	122.92
32	R	202	WVN	C02-C05-C09	-9.55	109.72	121.47
40	m	611	KC2	C1D-ND-C4D	-9.55	99.55	106.33
32	A	844	WVN	C38-C34-C37	-9.54	109.56	122.92
38	h	309	II0	C37-C35-C39	-9.53	109.57	122.92
32	i	315	WVN	C29-C31-C32	9.53	153.20	126.42
38	i	316	II0	C19-C13-C09	-9.53	111.41	124.35
38	i	314	II0	C41-C39-C35	-9.52	113.72	127.31
38	a	315	II0	C20-C14-C10	-9.52	111.41	124.35
38	e	312	II0	C19-C13-C09	-9.50	111.44	124.35
32	A	845	WVN	C27-C25-C28	-9.49	109.63	122.92
38	e	314	II0	C20-C14-C10	-9.49	111.46	124.35
32	B	846	WVN	C38-C34-C37	-9.48	109.64	122.92
38	d	301	II0	C38-C36-C40	-9.48	109.65	122.92
38	c	313	II0	C20-C14-C10	-9.46	111.49	124.35
38	d	317	II0	C37-C35-C39	-9.46	109.67	122.92
32	L	206	WVN	C29-C26-C22	-9.45	113.82	127.31
32	F	207	WVN	C29-C31-C32	9.45	152.96	126.42
38	j	315	II0	C37-C35-C39	-9.44	109.69	122.92
38	g	317	II0	C19-C13-C09	-9.44	111.52	124.35
38	g	317	II0	C20-C14-C10	-9.44	111.52	124.35
38	f	614	II0	C20-C14-C10	-9.43	111.53	124.35
40	c	310	KC2	C2A-C3A-C4A	-9.42	99.50	106.49
32	A	844	WVN	C35-C32-C36	-9.42	109.73	122.92
32	B	849	WVN	C33-C34-C37	-9.42	104.49	118.94
32	K	103	WVN	C27-C25-C28	-9.41	109.74	122.92
38	j	315	II0	C19-C13-C09	-9.40	111.58	124.35
38	l	313	II0	C20-C14-C10	-9.40	111.58	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	n	618	II0	C37-C35-C39	-9.39	109.76	122.92
32	M	101	WVN	C30-C28-C25	-9.39	113.91	127.31
38	i	314	II0	C42-C40-C36	-9.39	113.91	127.31
32	F	207	WVN	C27-C25-C28	-9.39	109.77	122.92
32	B	849	WVN	C35-C32-C36	-9.38	109.78	122.92
32	e	315	WVN	C14-C15-C13	-9.37	109.13	122.73
32	B	846	WVN	C24-C22-C26	-9.37	109.80	122.92
32	l	316	WVN	C30-C33-C34	-9.37	100.09	126.42
38	l	313	II0	C37-C35-C39	-9.36	109.81	122.92
38	m	614	II0	C20-C14-C10	-9.36	111.63	124.35
38	i	314	II0	C32-C34-C36	-9.34	100.17	126.42
38	i	313	II0	C31-C33-C35	9.34	152.64	126.42
32	A	844	WVN	C29-C26-C22	-9.33	113.99	127.31
32	R	201	WVN	C33-C34-C37	-9.33	104.62	118.94
32	s	407	WVN	C30-C28-C25	-9.33	114.00	127.31
38	b	301	II0	C31-C33-C35	9.32	152.59	126.42
32	L	205	WVN	C35-C32-C36	-9.31	109.88	122.92
32	R	201	WVN	C29-C31-C32	9.31	152.58	126.42
32	A	847	WVN	C04-C09-C05	-9.31	115.92	124.85
38	g	319	II0	C31-C33-C35	9.31	152.57	126.42
38	J	103	II0	C31-C33-C35	9.31	152.57	126.42
32	M	101	WVN	C27-C25-C28	-9.30	109.89	122.92
32	L	206	WVN	C24-C22-C19	-9.30	103.42	118.08
32	B	847	WVN	C35-C32-C36	-9.28	109.92	122.92
32	B	848	WVN	C19-C22-C26	-9.28	104.70	118.94
38	m	615	II0	C34-C36-C40	-9.28	104.70	118.94
32	e	315	WVN	C35-C32-C36	-9.27	109.93	122.92
40	k	611	KC2	C1D-ND-C4D	-9.27	99.75	106.33
32	h	308	WVN	C35-C32-C36	-9.26	109.95	122.92
38	d	315	II0	C38-C36-C40	-9.26	109.95	122.92
40	g	313	KC2	C2A-C3A-C4A	-9.26	99.62	106.49
32	l	316	WVN	C04-C09-C05	-9.25	115.98	124.85
38	j	301	II0	C31-C33-C35	9.25	152.41	126.42
32	B	848	WVN	C38-C34-C37	-9.25	109.96	122.92
32	e	315	WVN	C38-C34-C37	-9.25	109.96	122.92
38	n	616	II0	C03-C09-C13	-9.25	109.57	122.63
38	k	620	II0	C37-C35-C39	-9.25	109.97	122.92
40	e	309	KC2	C1D-ND-C4D	-9.24	99.77	106.33
38	l	314	II0	C19-C13-C09	-9.23	111.81	124.35
38	d	317	II0	C31-C33-C35	9.23	152.34	126.42
32	A	846	WVN	C35-C32-C36	-9.23	110.00	122.92
38	m	616	II0	C19-C13-C09	-9.22	111.81	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	L	205	WVN	C38-C34-C37	-9.21	110.02	122.92
38	b	314	II0	C31-C33-C35	9.20	152.27	126.42
38	k	616	II0	C19-C13-C09	-9.20	111.84	124.35
32	M	101	WVN	C35-C32-C36	-9.19	110.05	122.92
38	k	619	II0	C31-C33-C35	9.19	152.24	126.42
32	F	205	WVN	C35-C32-C36	-9.19	110.05	122.92
38	e	314	II0	C37-C35-C39	-9.19	110.05	122.92
32	A	846	WVN	C19-C22-C26	-9.18	104.85	118.94
38	J	103	II0	C37-C35-C39	-9.18	110.06	122.92
32	L	201	WVN	C29-C31-C32	9.18	152.19	126.42
32	B	846	WVN	C39-C36-C32	-9.18	114.22	127.31
32	e	315	WVN	C29-C31-C32	9.18	152.19	126.42
38	n	615	II0	C19-C13-C09	-9.16	111.90	124.35
38	e	313	II0	C42-C40-C36	-9.14	114.26	127.31
32	l	302	WVN	C24-C22-C26	-9.14	110.13	122.92
32	F	207	WVN	C35-C32-C36	-9.13	110.13	122.92
32	A	854	WVN	C29-C31-C32	9.12	152.04	126.42
38	d	315	II0	C37-C35-C39	-9.12	110.14	122.92
32	h	308	WVN	C29-C26-C22	-9.12	114.29	127.31
32	F	205	WVN	C29-C26-C22	-9.12	114.30	127.31
40	f	611	KC2	C2A-C3A-C4A	-9.12	99.72	106.49
32	A	845	WVN	C38-C34-C37	-9.11	110.17	122.92
38	f	615	II0	C34-C36-C40	-9.09	104.99	118.94
38	m	614	II0	C37-C35-C39	-9.09	110.19	122.92
38	a	317	II0	C38-C36-C40	-9.08	110.20	122.92
32	B	846	WVN	C29-C26-C22	-9.08	114.35	127.31
32	A	844	WVN	C29-C31-C32	9.08	151.93	126.42
38	l	314	II0	C37-C35-C39	-9.08	110.20	122.92
32	L	201	WVN	C35-C32-C36	-9.08	110.21	122.92
38	m	616	II0	C31-C33-C35	9.07	151.90	126.42
32	A	854	WVN	C35-C32-C36	-9.06	110.23	122.92
38	i	316	II0	C31-C33-C35	9.06	151.87	126.42
32	s	407	WVN	C24-C22-C26	-9.05	110.24	122.92
32	s	407	WVN	C27-C25-C28	-9.05	110.25	122.92
38	i	314	II0	C37-C35-C39	-9.04	110.26	122.92
38	m	614	II0	C38-C36-C40	-9.04	110.26	122.92
32	i	315	WVN	C24-C22-C26	-9.03	110.27	122.92
32	A	847	WVN	C29-C26-C22	-9.02	114.44	127.31
32	i	315	WVN	C38-C34-C37	-9.02	110.29	122.92
32	K	103	WVN	C29-C31-C32	9.01	151.74	126.42
38	j	301	II0	C38-C36-C40	-9.01	110.30	122.92
32	s	405	WVN	C29-C26-C22	-9.01	114.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	i	310	KC2	C1D-ND-C4D	-9.01	99.94	106.33
32	B	848	WVN	C29-C31-C32	9.01	151.72	126.42
32	l	302	WVN	C29-C31-C32	9.00	151.70	126.42
38	b	315	II0	C20-C14-C10	-9.00	112.12	124.35
38	k	616	II0	C31-C33-C35	9.00	151.70	126.42
38	a	315	II0	C37-C35-C39	-9.00	110.32	122.92
32	L	201	WVN	C29-C26-C22	-9.00	114.47	127.31
38	c	313	II0	C37-C35-C39	-8.99	110.32	122.92
32	B	848	WVN	C24-C22-C26	-8.99	110.33	122.92
32	F	204	WVN	C39-C36-C32	-8.99	114.48	127.31
32	L	201	WVN	C38-C34-C37	-8.99	110.33	122.92
38	j	316	II0	C34-C36-C40	-8.98	105.16	118.94
32	i	315	WVN	C33-C34-C37	-8.97	105.17	118.94
32	A	846	WVN	C38-C34-C37	-8.97	110.35	122.92
38	j	315	II0	C31-C33-C35	8.96	151.59	126.42
32	L	205	WVN	C29-C31-C32	8.95	151.57	126.42
32	R	202	WVN	C27-C25-C28	-8.95	110.38	122.92
38	h	310	II0	C34-C36-C40	-8.95	105.21	118.94
32	h	308	WVN	C27-C25-C28	-8.94	110.39	122.92
38	n	618	II0	C31-C33-C35	8.94	151.54	126.42
38	m	616	II0	C37-C35-C39	-8.94	110.41	122.92
32	R	201	WVN	C35-C32-C36	-8.93	110.41	122.92
38	d	317	II0	C38-C36-C40	-8.93	110.42	122.92
38	n	616	II0	C19-C13-C09	-8.92	112.23	124.35
32	h	308	WVN	C24-C22-C19	-8.92	104.02	118.08
40	n	611	KC2	C1D-ND-C4D	-8.91	100.00	106.33
38	f	614	II0	C37-C35-C39	-8.91	110.44	122.92
38	d	315	II0	C19-C13-C09	-8.91	112.25	124.35
32	A	847	WVN	C27-C25-C28	-8.90	110.45	122.92
32	R	201	WVN	C04-C09-C05	-8.89	116.32	124.85
40	s	401	KC2	C2A-C3A-C4A	-8.89	99.89	106.49
38	a	314	II0	C37-C35-C39	-8.88	110.48	122.92
32	A	854	WVN	C29-C26-C22	-8.88	114.64	127.31
38	h	311	II0	C38-C36-C40	-8.88	110.49	122.92
40	g	313	KC2	C1D-ND-C4D	-8.86	100.04	106.33
32	h	308	WVN	C38-C34-C37	-8.86	110.52	122.92
32	l	316	WVN	C35-C32-C36	-8.85	110.53	122.92
40	j	312	KC2	C2A-C3A-C4A	-8.85	99.92	106.49
32	s	405	WVN	C24-C22-C26	-8.84	110.54	122.92
32	B	848	WVN	C33-C34-C37	-8.83	105.40	118.94
38	d	301	II0	C42-C40-C36	-8.82	114.73	127.31
38	h	310	II0	C38-C36-C40	-8.81	110.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	f	611	KC2	C1D-ND-C4D	-8.80	100.08	106.33
32	R	202	WVN	C38-C34-C37	-8.80	110.59	122.92
32	I	101	WVN	C27-C25-C28	-8.80	110.60	122.92
32	J	101	WVN	C38-C34-C37	-8.79	110.60	122.92
32	s	407	WVN	C38-C34-C37	-8.79	110.61	122.92
38	a	313	II0	C37-C35-C39	-8.79	110.61	122.92
40	i	318	KC2	C1D-ND-C4D	-8.78	100.10	106.33
32	s	407	WVN	C29-C26-C22	-8.77	114.79	127.31
38	d	301	II0	C31-C33-C35	8.77	151.04	126.42
32	F	204	WVN	C30-C28-C25	-8.76	114.80	127.31
32	R	201	WVN	C29-C26-C22	-8.76	114.80	127.31
32	l	316	WVN	C24-C22-C26	-8.76	110.65	122.92
32	R	201	WVN	C27-C25-C28	-8.76	110.65	122.92
32	s	405	WVN	C38-C34-C37	-8.76	110.66	122.92
32	B	846	WVN	C27-C25-C28	-8.75	110.66	122.92
40	j	312	KC2	C1D-ND-C4D	-8.75	100.12	106.33
32	B	849	WVN	C29-C26-C22	-8.74	114.83	127.31
38	b	314	II0	C34-C36-C40	-8.73	105.54	118.94
38	n	618	II0	C19-C13-C09	-8.73	112.48	124.35
32	A	845	WVN	C02-C05-C09	-8.73	110.73	121.47
32	R	202	WVN	C29-C31-C32	8.72	150.91	126.42
38	e	314	II0	C38-C36-C40	-8.71	110.72	122.92
40	d	311	KC2	C2D-C1D-ND	8.71	116.07	110.23
38	h	310	II0	C31-C33-C35	8.71	150.88	126.42
38	f	616	II0	C37-C35-C39	-8.70	110.73	122.92
40	n	611	KC2	C2D-C1D-ND	8.70	116.06	110.23
32	l	316	WVN	C39-C36-C32	-8.69	114.91	127.31
38	n	618	II0	C38-C36-C40	-8.69	110.76	122.92
38	i	314	II0	C20-C14-C10	-8.68	112.55	124.35
32	l	302	WVN	C29-C26-C22	-8.68	114.93	127.31
32	A	847	WVN	C35-C32-C36	-8.67	110.78	122.92
38	e	313	II0	C31-C33-C35	8.66	150.76	126.42
32	F	205	WVN	C24-C22-C26	-8.66	110.79	122.92
38	l	315	II0	C38-C36-C40	-8.66	110.79	122.92
38	m	618	II0	C31-C33-C35	8.66	150.73	126.42
32	F	205	WVN	C27-C25-C28	-8.66	110.80	122.92
38	m	614	II0	C19-C13-C09	-8.65	112.59	124.35
32	R	202	WVN	C35-C32-C36	-8.65	110.80	122.92
32	B	846	WVN	C35-C32-C36	-8.65	110.80	122.92
32	B	848	WVN	C35-C32-C36	-8.65	110.81	122.92
38	j	301	II0	C19-C13-C09	-8.65	112.60	124.35
38	b	314	II0	C38-C36-C40	-8.63	110.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	L	201	WVN	C27-C25-C28	-8.62	110.84	122.92
38	d	316	II0	C19-C13-C09	-8.62	112.63	124.35
38	i	316	II0	C20-C14-C10	-8.62	112.64	124.35
32	B	847	WVN	C38-C34-C37	-8.62	110.85	122.92
38	m	618	II0	C41-C39-C35	-8.61	115.02	127.31
32	B	849	WVN	C27-C25-C28	-8.61	110.86	122.92
38	j	315	II0	C34-C36-C40	-8.61	105.73	118.94
40	s	401	KC2	CMA-C3A-C2A	-8.61	107.23	128.30
38	k	616	II0	C37-C35-C39	-8.60	110.88	122.92
38	m	614	II0	C34-C36-C40	-8.59	105.75	118.94
32	J	101	WVN	C27-C25-C28	-8.57	110.92	122.92
32	s	407	WVN	C29-C31-C32	8.57	150.48	126.42
40	c	310	KC2	C2D-C1D-ND	8.57	115.97	110.23
40	l	311	KC2	CMA-C3A-C4A	-8.56	112.00	125.04
38	d	301	II0	C37-C35-C39	-8.55	110.95	122.92
38	e	312	II0	C42-C40-C36	-8.54	115.12	127.31
38	m	618	II0	C19-C13-C09	-8.54	112.74	124.35
38	l	313	II0	C31-C33-C35	8.54	150.40	126.42
32	B	847	WVN	C02-C05-C09	-8.54	110.97	121.47
38	k	620	II0	C38-C36-C40	-8.54	110.97	122.92
32	B	847	WVN	C27-C25-C28	-8.53	110.97	122.92
32	s	405	WVN	C29-C31-C32	8.53	150.37	126.42
38	m	616	II0	C20-C14-C10	-8.52	112.78	124.35
38	d	316	II0	C31-C33-C35	8.51	150.32	126.42
38	b	315	II0	C34-C36-C40	-8.51	105.88	118.94
38	f	616	II0	C19-C13-C09	-8.50	112.79	124.35
32	A	845	WVN	C19-C22-C26	-8.50	105.90	118.94
32	A	844	WVN	C27-C25-C28	-8.50	111.02	122.92
38	f	618	II0	C38-C36-C40	-8.50	111.02	122.92
38	e	313	II0	C37-C35-C39	-8.49	111.02	122.92
32	L	205	WVN	C30-C28-C25	-8.49	115.19	127.31
38	n	615	II0	C37-C35-C39	-8.49	111.03	122.92
32	e	315	WVN	C24-C22-C26	-8.49	111.03	122.92
40	l	311	KC2	C1D-ND-C4D	-8.49	100.31	106.33
32	F	207	WVN	C30-C28-C25	-8.48	115.20	127.31
38	i	319	II0	C19-C13-C09	-8.48	112.82	124.35
38	n	615	II0	C38-C36-C40	-8.48	111.04	122.92
38	i	319	II0	C20-C14-C10	-8.48	112.83	124.35
32	F	207	WVN	C40-C37-C34	-8.47	115.22	127.31
38	j	301	II0	C20-C14-C10	-8.47	112.84	124.35
32	R	202	WVN	C19-C22-C26	-8.47	105.95	118.94
38	e	312	II0	C41-C39-C35	-8.47	115.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	854	WVN	C27-C25-C28	-8.46	111.07	122.92
38	e	312	II0	C38-C36-C40	-8.46	111.07	122.92
32	L	205	WVN	C27-C25-C28	-8.46	111.07	122.92
38	e	313	II0	C32-C34-C36	-8.45	102.67	126.42
32	s	407	WVN	C19-C22-C26	-8.44	105.99	118.94
38	d	301	II0	C34-C36-C40	-8.43	106.00	118.94
32	L	206	WVN	C30-C28-C25	-8.42	115.29	127.31
32	B	848	WVN	C27-C25-C28	-8.41	111.14	122.92
38	i	319	II0	C31-C33-C35	8.40	150.01	126.42
38	l	314	II0	C20-C14-C10	-8.40	112.94	124.35
38	i	319	II0	C38-C36-C40	-8.39	111.17	122.92
40	g	315	KC2	C1D-ND-C4D	-8.38	100.38	106.33
32	l	302	WVN	C19-C22-C26	-8.38	106.09	118.94
32	A	854	WVN	C38-C34-C37	-8.37	111.19	122.92
40	s	401	KC2	C1D-ND-C4D	-8.36	100.40	106.33
32	M	101	WVN	C24-C22-C19	-8.36	104.91	118.08
38	b	315	II0	C31-C33-C35	8.36	149.89	126.42
38	i	316	II0	C38-C36-C40	-8.35	111.22	122.92
38	a	317	II0	C19-C13-C09	-8.35	113.00	124.35
32	A	844	WVN	C40-C37-C34	-8.34	115.40	127.31
32	L	205	WVN	C24-C22-C26	-8.34	111.24	122.92
38	k	620	II0	C31-C33-C35	8.34	149.85	126.42
38	n	615	II0	C34-C36-C40	-8.34	106.14	118.94
40	m	611	KC2	C2D-C1D-ND	8.34	115.82	110.23
38	b	301	II0	C38-C36-C40	-8.33	111.25	122.92
38	n	616	II0	C20-C14-C10	-8.33	113.02	124.35
32	i	315	WVN	C23-C25-C28	-8.32	106.17	118.94
40	s	404	KC2	C1D-ND-C4D	-8.32	100.43	106.33
38	i	316	II0	C42-C40-C36	-8.31	115.45	127.31
32	R	201	WVN	C24-C22-C26	-8.31	111.28	122.92
38	d	316	II0	C38-C36-C40	-8.31	111.28	122.92
32	A	847	WVN	C38-C34-C37	-8.31	111.28	122.92
32	I	101	WVN	C14-C15-C13	-8.30	110.67	122.73
32	J	101	WVN	C29-C31-C32	8.28	149.69	126.42
32	A	854	WVN	C24-C22-C19	-8.28	105.03	118.08
32	B	846	WVN	C02-C05-C09	-8.28	111.28	121.47
32	s	405	WVN	C19-C22-C26	-8.28	106.23	118.94
38	h	309	II0	C42-C40-C36	-8.28	115.50	127.31
32	B	849	WVN	C29-C31-C32	8.26	149.62	126.42
38	l	315	II0	C20-C14-C10	-8.25	113.13	124.35
38	h	311	II0	C34-C36-C40	-8.24	106.29	118.94
32	K	103	WVN	C39-C36-C32	-8.24	115.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	j	312	KC2	C1A-C2A-C3A	-8.24	100.57	107.11
38	l	313	II0	C38-C36-C40	-8.23	111.40	122.92
32	I	101	WVN	C38-C34-C37	-8.22	111.41	122.92
38	f	615	II0	C38-C36-C40	-8.22	111.41	122.92
32	R	201	WVN	C38-C34-C37	-8.22	111.41	122.92
32	l	316	WVN	C30-C28-C25	-8.21	115.59	127.31
38	m	615	II0	C20-C14-C10	-8.21	113.19	124.35
32	F	204	WVN	C29-C31-C32	8.21	149.49	126.42
32	F	204	WVN	C14-C15-C13	-8.21	110.82	122.73
38	a	315	II0	C38-C36-C40	-8.19	111.45	122.92
38	m	616	II0	C38-C36-C40	-8.19	111.45	122.92
32	A	854	WVN	C33-C34-C37	-8.19	106.38	118.94
38	n	615	II0	C31-C33-C35	8.19	149.41	126.42
38	f	614	II0	C38-C36-C40	-8.18	111.46	122.92
38	e	313	II0	C20-C14-C10	-8.18	113.24	124.35
38	g	318	II0	C20-C14-C10	-8.17	113.25	124.35
38	b	315	II0	C38-C36-C40	-8.16	111.49	122.92
38	J	103	II0	C38-C36-C40	-8.16	111.49	122.92
32	B	848	WVN	C29-C26-C22	-8.15	115.67	127.31
38	m	615	II0	C38-C36-C40	-8.15	111.51	122.92
38	b	301	II0	C20-C14-C10	-8.14	113.28	124.35
32	L	206	WVN	C04-C09-C05	-8.14	117.05	124.85
38	c	313	II0	C31-C33-C35	8.13	149.27	126.42
38	i	313	II0	C38-C36-C40	-8.13	111.54	122.92
32	A	846	WVN	C29-C31-C32	8.13	149.24	126.42
29	d	304	CLA	C4A-NA-C1A	8.12	110.36	106.71
32	e	315	WVN	C30-C28-C25	-8.12	115.72	127.31
32	A	844	WVN	C24-C22-C26	-8.12	111.55	122.92
38	g	319	II0	C38-C36-C40	-8.12	111.55	122.92
38	j	316	II0	C20-C14-C10	-8.11	113.33	124.35
40	k	611	KC2	C2D-C1D-ND	8.11	115.67	110.23
38	j	315	II0	C38-C36-C40	-8.11	111.57	122.92
38	b	301	II0	C34-C36-C40	-8.10	106.51	118.94
38	d	317	II0	C20-C14-C10	-8.10	113.34	124.35
32	l	302	WVN	C02-C05-C09	-8.09	111.51	121.47
32	R	201	WVN	C30-C28-C25	-8.09	115.76	127.31
32	F	204	WVN	C19-C22-C26	-8.09	106.53	118.94
38	f	616	II0	C38-C36-C40	-8.08	111.60	122.92
32	A	847	WVN	C24-C22-C26	-8.08	111.61	122.92
38	j	316	II0	C38-C36-C40	-8.08	111.61	122.92
40	s	404	KC2	C2D-C1D-ND	8.08	115.65	110.23
32	K	103	WVN	C06-C13-C15	-8.07	111.24	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	846	WVN	C29-C31-C32	8.07	149.09	126.42
29	f	604	CLA	C4A-NA-C1A	8.07	110.33	106.71
38	f	615	II0	C37-C35-C39	-8.07	111.62	122.92
38	f	616	II0	C31-C33-C35	8.06	149.06	126.42
38	e	314	II0	C19-C13-C09	-8.06	113.39	124.35
32	L	205	WVN	C40-C37-C34	-8.06	115.81	127.31
32	l	302	WVN	C38-C34-C37	-8.06	111.64	122.92
38	d	316	II0	C20-C14-C10	-8.06	113.40	124.35
38	k	616	II0	C20-C14-C10	-8.05	113.41	124.35
38	a	317	II0	C20-C14-C10	-8.05	113.42	124.35
38	g	317	II0	C38-C36-C40	-8.04	111.66	122.92
38	m	618	II0	C20-C14-C10	-8.04	113.42	124.35
32	A	846	WVN	C27-C25-C28	-8.04	111.66	122.92
29	A	836	CLA	C4A-NA-C1A	8.03	110.32	106.71
38	h	311	II0	C37-C35-C39	-8.03	111.67	122.92
40	s	401	KC2	C2D-C1D-ND	8.03	115.61	110.23
32	A	854	WVN	C19-C22-C26	-8.02	106.63	118.94
40	i	310	KC2	C2D-C1D-ND	8.02	115.61	110.23
38	e	314	II0	C31-C33-C35	8.02	148.93	126.42
38	f	616	II0	C04-C10-C14	-8.01	111.32	122.63
38	i	314	II0	C19-C13-C09	-8.00	113.47	124.35
38	f	615	II0	C31-C33-C35	8.00	148.90	126.42
38	f	615	II0	C20-C14-C10	-8.00	113.47	124.35
29	B	808	CLA	C4A-NA-C1A	8.00	110.30	106.71
38	l	315	II0	C42-C40-C36	-8.00	115.90	127.31
38	e	312	II0	C37-C35-C39	-7.99	111.72	122.92
38	a	315	II0	C31-C33-C35	7.99	148.87	126.42
38	a	314	II0	C19-C13-C09	-7.98	113.50	124.35
38	k	615	II0	C42-C40-C36	-7.98	115.92	127.31
38	h	311	II0	C19-C13-C09	-7.98	113.51	124.35
38	f	618	II0	C31-C33-C35	7.97	148.82	126.42
40	l	311	KC2	C2D-C1D-ND	7.97	115.57	110.23
32	e	315	WVN	C06-C13-C15	-7.97	111.39	122.61
38	f	618	II0	C19-C13-C09	-7.96	113.53	124.35
38	d	315	II0	C31-C33-C35	7.96	148.77	126.42
38	i	314	II0	C19-C13-C11	-7.95	99.62	114.36
38	m	614	II0	C31-C33-C35	7.95	148.76	126.42
40	g	314	KC2	C1D-ND-C4D	-7.95	100.69	106.33
38	a	313	II0	C19-C13-C09	-7.95	113.55	124.35
40	g	315	KC2	C2D-C1D-ND	7.95	115.56	110.23
38	g	318	II0	C34-C36-C40	-7.94	106.76	118.94
30	B	843	PQN	C11-C12-C13	-7.94	113.58	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	846	WVN	C35-C32-C31	-7.93	105.58	118.08
32	A	845	WVN	C40-C37-C34	-7.93	116.00	127.31
38	i	313	II0	C20-C14-C10	-7.93	113.58	124.35
32	e	315	WVN	C33-C34-C37	-7.92	106.78	118.94
29	b	305	CLA	C4A-NA-C1A	7.92	110.27	106.71
32	B	848	WVN	C40-C37-C34	-7.91	116.02	127.31
32	L	201	WVN	C24-C22-C26	-7.89	111.86	122.92
38	l	314	II0	C42-C40-C36	-7.89	116.05	127.31
38	a	313	II0	C31-C33-C35	7.89	148.58	126.42
38	e	314	II0	C42-C40-C36	-7.89	116.05	127.31
40	c	310	KC2	CMA-C3A-C2A	-7.88	109.02	128.30
32	A	845	WVN	C29-C26-C22	-7.87	116.08	127.31
38	a	315	II0	C42-C40-C36	-7.87	116.08	127.31
32	B	847	WVN	C29-C31-C32	7.87	148.52	126.42
38	j	316	II0	C37-C35-C39	-7.87	111.90	122.92
32	M	101	WVN	C38-C34-C37	-7.86	111.91	122.92
38	n	618	II0	C20-C14-C10	-7.85	113.68	124.35
38	n	616	II0	C38-C36-C40	-7.85	111.92	122.92
38	f	618	II0	C20-C14-C10	-7.85	113.68	124.35
38	a	315	II0	C34-C36-C40	-7.85	106.90	118.94
32	i	315	WVN	C06-C13-C15	-7.84	111.57	122.61
38	f	614	II0	C37-C35-C33	-7.84	105.73	118.08
38	a	313	II0	C38-C36-C40	-7.82	111.97	122.92
38	m	615	II0	C31-C33-C35	7.81	148.37	126.42
38	h	309	II0	C19-C13-C09	-7.81	113.73	124.35
32	F	205	WVN	C38-C34-C37	-7.81	111.99	122.92
38	g	318	II0	C38-C36-C40	-7.80	112.00	122.92
32	J	101	WVN	C06-C13-C15	-7.80	111.63	122.61
38	i	319	II0	C04-C10-C14	-7.79	111.63	122.63
32	B	848	WVN	C30-C28-C25	-7.79	116.19	127.31
38	e	313	II0	C38-C36-C40	-7.79	112.01	122.92
38	a	314	II0	C37-C35-C33	-7.79	105.81	118.08
38	a	317	II0	C42-C40-C36	-7.79	116.20	127.31
29	A	815	CLA	C4A-NA-C1A	7.78	110.20	106.71
29	B	805	CLA	C4A-NA-C1A	7.78	110.20	106.71
38	c	313	II0	C38-C36-C40	-7.78	112.02	122.92
40	f	611	KC2	C2D-C1D-ND	7.78	115.45	110.23
32	B	849	WVN	C23-C25-C28	-7.77	107.02	118.94
38	b	314	II0	C37-C35-C39	-7.77	112.04	122.92
30	A	841	PQN	C11-C12-C13	-7.77	113.86	126.79
38	j	301	II0	C34-C36-C40	-7.76	107.03	118.94
29	O	206	CLA	C4A-NA-C1A	7.76	110.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	101	WVN	C19-C22-C26	-7.75	107.05	118.94
38	a	314	II0	C38-C36-C40	-7.75	112.07	122.92
38	n	616	II0	C42-C40-C36	-7.75	116.25	127.31
32	s	405	WVN	C40-C37-C34	-7.74	116.26	127.31
32	K	103	WVN	C40-C37-C34	-7.74	116.26	127.31
40	i	318	KC2	C2D-C1D-ND	7.74	115.42	110.23
32	A	846	WVN	C27-C25-C23	-7.73	105.89	118.08
38	i	313	II0	C42-C40-C36	-7.71	116.30	127.31
32	l	302	WVN	C27-C25-C28	-7.71	112.13	122.92
38	m	615	II0	C19-C13-C09	-7.70	113.88	124.35
40	g	313	KC2	C2D-C1D-ND	7.70	115.39	110.23
32	M	101	WVN	C33-C34-C37	-7.69	107.14	118.94
29	k	605	CLA	C4A-NA-C1A	7.69	110.16	106.71
29	A	804	CLA	C4A-NA-C1A	7.69	110.16	106.71
40	j	312	KC2	C2D-C1D-ND	7.68	115.38	110.23
40	e	309	KC2	C2D-C1D-ND	7.67	115.38	110.23
32	B	849	WVN	C40-C37-C34	-7.67	116.37	127.31
32	B	848	WVN	C02-C05-C09	-7.67	112.03	121.47
38	h	309	II0	C38-C36-C40	-7.67	112.18	122.92
32	B	848	WVN	C23-C25-C28	-7.67	107.18	118.94
38	i	314	II0	C31-C33-C35	7.66	147.93	126.42
32	e	315	WVN	C29-C26-C22	-7.66	116.38	127.31
38	k	616	II0	C38-C36-C40	-7.66	112.19	122.92
32	F	204	WVN	C35-C32-C36	-7.65	112.20	122.92
32	R	201	WVN	C19-C22-C26	-7.65	107.20	118.94
29	b	313	CLA	C4A-NA-C1A	7.64	110.14	106.71
29	B	834	CLA	C4A-NA-C1A	7.64	110.14	106.71
38	l	315	II0	C31-C33-C35	7.64	147.88	126.42
38	g	318	II0	C31-C33-C35	7.64	147.87	126.42
32	e	315	WVN	C19-C22-C26	-7.63	107.23	118.94
29	A	851	CLA	C4A-NA-C1A	7.63	110.14	106.71
29	e	304	CLA	C4A-NA-C1A	7.63	110.14	106.71
38	j	316	II0	C31-C33-C35	7.62	147.83	126.42
40	g	314	KC2	C2D-C1D-ND	7.62	115.34	110.23
40	n	611	KC2	C2B-C1B-NB	7.62	115.72	110.10
38	k	619	II0	C42-C40-C36	-7.61	116.44	127.31
38	d	317	II0	C03-C09-C13	-7.60	111.90	122.63
29	i	305	CLA	C4A-NA-C1A	7.60	110.12	106.71
40	f	611	KC2	CMA-C3A-C2A	-7.58	109.74	128.30
32	A	854	WVN	C23-C25-C28	-7.57	107.32	118.94
29	j	306	CLA	C4A-NA-C1A	7.56	110.11	106.71
38	k	620	II0	C34-C36-C40	-7.56	107.34	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	k	611	KC2	CMD-C2D-C1D	7.55	136.88	125.37
32	i	315	WVN	C27-C25-C28	-7.55	112.35	122.92
40	g	313	KC2	C1A-C2A-C3A	-7.54	101.13	107.11
32	A	844	WVN	C30-C28-C25	-7.54	116.55	127.31
29	B	822	CLA	C4A-NA-C1A	7.53	110.09	106.71
29	B	807	CLA	C4A-NA-C1A	7.52	110.09	106.71
40	l	311	KC2	C1A-C2A-C3A	-7.52	101.15	107.11
40	i	310	KC2	CMD-C2D-C1D	7.51	136.80	125.37
38	J	103	II0	C42-C40-C36	-7.50	116.61	127.31
32	l	302	WVN	C23-C25-C28	-7.49	107.44	118.94
29	s	403	CLA	C4A-NA-C1A	7.49	110.08	106.71
29	a	311	CLA	C4A-NA-C1A	7.48	110.07	106.71
32	B	849	WVN	C24-C22-C26	-7.48	112.44	122.92
38	b	315	II0	C04-C10-C14	-7.48	112.07	122.63
29	c	304	CLA	C4A-NA-C1A	7.47	110.06	106.71
40	c	310	KC2	CMD-C2D-C1D	7.47	136.74	125.37
32	K	103	WVN	C14-C15-C13	-7.46	111.90	122.73
32	B	847	WVN	C19-C22-C26	-7.46	107.49	118.94
29	B	804	CLA	C4A-NA-C1A	7.46	110.06	106.71
38	k	616	II0	C34-C36-C40	-7.45	107.50	118.94
38	f	616	II0	C34-C36-C40	-7.45	107.50	118.94
38	b	315	II0	C37-C35-C39	-7.45	112.48	122.92
40	i	318	KC2	C2B-C1B-NB	7.45	115.59	110.10
40	k	611	KC2	C1A-C2A-C3A	-7.44	101.21	107.11
32	K	103	WVN	C33-C34-C37	-7.42	107.55	118.94
38	m	615	II0	C37-C35-C39	-7.42	112.53	122.92
32	h	308	WVN	C40-C37-C34	-7.39	116.76	127.31
38	k	620	II0	C42-C40-C36	-7.38	116.78	127.31
29	f	612	CLA	C4A-NA-C1A	7.38	110.02	106.71
40	j	312	KC2	CMA-C3A-C2A	-7.38	110.24	128.30
32	s	405	WVN	C06-C13-C15	-7.38	112.22	122.61
40	i	318	KC2	CMD-C2D-C1D	7.37	136.60	125.37
38	h	310	II0	C42-C40-C36	-7.37	116.79	127.31
32	h	308	WVN	C30-C28-C25	-7.37	116.79	127.31
40	f	611	KC2	CMD-C2D-C1D	7.37	136.59	125.37
40	f	611	KC2	C1A-C2A-C3A	-7.37	101.27	107.11
29	c	311	CLA	C4A-NA-C1A	7.36	110.02	106.71
38	m	616	II0	C42-C40-C36	-7.36	116.80	127.31
38	j	301	II0	C03-C09-C13	-7.36	112.24	122.63
32	A	845	WVN	C33-C34-C37	-7.35	107.66	118.94
32	B	846	WVN	C27-C25-C23	-7.35	106.50	118.08
38	l	314	II0	C03-C09-C13	-7.34	112.27	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	618	II0	C34-C36-C40	-7.34	107.68	118.94
40	g	315	KC2	C2B-C1B-NB	7.34	115.51	110.10
40	i	310	KC2	C2B-C1B-NB	7.34	115.51	110.10
32	I	101	WVN	C24-C22-C19	-7.34	106.52	118.08
32	s	407	WVN	C02-C05-C09	-7.33	112.44	121.47
40	e	309	KC2	CMA-C3A-C2A	-7.33	110.36	128.30
38	e	314	II0	C34-C36-C40	-7.32	107.70	118.94
32	K	103	WVN	C19-C22-C26	-7.32	107.71	118.94
38	b	314	II0	C42-C40-C36	-7.32	116.87	127.31
32	K	103	WVN	C38-C34-C37	-7.31	112.69	122.92
29	B	813	CLA	C4A-NA-C1A	7.30	109.99	106.71
38	a	314	II0	C04-C10-C14	-7.30	112.33	122.63
32	R	202	WVN	C33-C34-C37	-7.30	107.74	118.94
38	j	301	II0	C42-C40-C36	-7.30	116.90	127.31
29	h	303	CLA	C4A-NA-C1A	7.29	109.98	106.71
29	n	610	CLA	C4A-NA-C1A	7.29	109.98	106.71
32	A	847	WVN	C29-C31-C32	7.28	146.86	126.42
32	A	847	WVN	C33-C34-C37	-7.28	107.77	118.94
29	a	302	CLA	C4A-NA-C1A	7.28	109.98	106.71
32	R	202	WVN	C06-C13-C15	-7.27	112.37	122.61
29	K	101	CLA	C4A-NA-C1A	7.27	109.97	106.71
29	B	838	CLA	C4A-NA-C1A	7.27	109.97	106.71
32	l	302	WVN	C30-C28-C25	-7.27	116.94	127.31
40	c	310	KC2	C2B-C1B-NB	7.26	115.46	110.10
29	k	610	CLA	C4A-NA-C1A	7.26	109.97	106.71
38	c	313	II0	C37-C35-C33	-7.25	106.66	118.08
38	n	616	II0	C34-C36-C40	-7.24	107.83	118.94
29	B	837	CLA	C4A-NA-C1A	7.24	109.96	106.71
40	c	310	KC2	C1A-C2A-C3A	-7.24	101.37	107.11
40	n	611	KC2	C1A-C2A-C3A	-7.23	101.37	107.11
29	a	305	CLA	C4A-NA-C1A	7.23	109.96	106.71
29	l	312	CLA	C4A-NA-C1A	7.23	109.96	106.71
38	f	615	II0	C03-C09-C13	-7.23	112.43	122.63
40	s	401	KC2	C1A-C2A-C3A	-7.22	101.38	107.11
32	M	101	WVN	C02-C05-C09	-7.22	112.59	121.47
38	l	315	II0	C34-C36-C40	-7.22	107.86	118.94
40	s	404	KC2	CBA-CAA-C2A	-7.21	97.79	125.27
38	m	614	II0	C37-C35-C33	-7.20	106.73	118.08
29	g	311	CLA	C4A-NA-C1A	7.20	109.94	106.71
40	d	311	KC2	C1A-C2A-C3A	-7.20	101.40	107.11
40	e	309	KC2	CMD-C2D-C1D	7.19	136.31	125.37
38	g	317	II0	C31-C33-C35	7.18	146.60	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	310	CLA	C4A-NA-C1A	7.18	109.93	106.71
32	l	316	WVN	C27-C25-C23	-7.18	106.77	118.08
29	l	306	CLA	C4A-NA-C1A	7.18	109.93	106.71
29	B	814	CLA	C4A-NA-C1A	7.18	109.93	106.71
32	A	847	WVN	C23-C25-C28	-7.17	107.93	118.94
40	d	311	KC2	CMA-C3A-C2A	-7.17	110.74	128.30
29	A	830	CLA	C4A-NA-C1A	7.17	109.93	106.71
32	h	308	WVN	C33-C34-C37	-7.17	107.94	118.94
40	n	611	KC2	CMD-C2D-C1D	7.16	136.28	125.37
32	J	101	WVN	C02-C05-C09	-7.16	112.66	121.47
38	d	316	II0	C34-C36-C40	-7.16	107.96	118.94
38	b	314	II0	C03-C09-C13	-7.16	112.53	122.63
40	g	313	KC2	CMA-C3A-C2A	-7.16	110.78	128.30
29	B	832	CLA	C4A-NA-C1A	7.16	109.92	106.71
40	m	611	KC2	C1A-C2A-C3A	-7.15	101.44	107.11
38	k	615	II0	C37-C35-C33	-7.15	106.81	118.08
29	b	308	CLA	C4A-NA-C1A	7.15	109.92	106.71
32	R	202	WVN	C30-C28-C25	-7.15	117.11	127.31
38	i	314	II0	C38-C36-C40	-7.14	112.92	122.92
29	A	835	CLA	C4A-NA-C1A	7.14	109.92	106.71
38	j	315	II0	C42-C40-C36	-7.14	117.12	127.31
29	A	838	CLA	C4A-NA-C1A	7.14	109.92	106.71
29	A	816	CLA	C4A-NA-C1A	7.13	109.91	106.71
29	L	204	CLA	C4A-NA-C1A	7.13	109.91	106.71
29	b	302	CLA	C4A-NA-C1A	7.13	109.91	106.71
29	L	203	CLA	C4A-NA-C1A	7.12	109.91	106.71
29	h	307	CLA	C4A-NA-C1A	7.12	109.91	106.71
29	g	302	CLA	C4A-NA-C1A	7.12	109.91	106.71
38	h	311	II0	C42-C40-C36	-7.12	117.14	127.31
29	m	610	CLA	C4A-NA-C1A	7.12	109.91	106.71
38	g	317	II0	C42-C40-C36	-7.12	117.15	127.31
29	A	823	CLA	C4A-NA-C1A	7.12	109.91	106.71
38	m	616	II0	C34-C36-C40	-7.12	108.02	118.94
38	k	619	II0	C34-C36-C40	-7.11	108.03	118.94
38	c	313	II0	C34-C36-C40	-7.11	108.04	118.94
32	B	849	WVN	C19-C22-C26	-7.10	108.04	118.94
40	m	611	KC2	C2B-C1B-NB	7.10	115.34	110.10
29	A	837	CLA	C4A-NA-C1A	7.10	109.90	106.71
40	m	611	KC2	CMA-C3A-C2A	-7.10	110.91	128.30
29	B	840	CLA	C4A-NA-C1A	7.10	109.90	106.71
40	i	310	KC2	CMA-C3A-C2A	-7.09	110.93	128.30
29	O	202	CLA	C4A-NA-C1A	7.09	109.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	F	204	WVN	C02-C05-C09	-7.09	112.74	121.47
32	A	847	WVN	C30-C28-C25	-7.09	117.19	127.31
29	A	833	CLA	C4A-NA-C1A	7.09	109.89	106.71
29	i	302	CLA	C4A-NA-C1A	7.09	109.89	106.71
40	g	314	KC2	C1A-C2A-C3A	-7.09	101.49	107.11
29	F	203	CLA	C4A-NA-C1A	7.08	109.89	106.71
29	b	312	CLA	C4A-NA-C1A	7.08	109.89	106.71
29	l	307	CLA	C4A-NA-C1A	7.07	109.89	106.71
29	j	313	CLA	C4A-NA-C1A	7.07	109.89	106.71
40	j	312	KC2	CMD-C2D-C1D	7.07	136.14	125.37
38	m	618	II0	C34-C36-C40	-7.07	108.09	118.94
29	f	605	CLA	C4A-NA-C1A	7.06	109.88	106.71
40	m	611	KC2	CMD-C2D-C1D	7.06	136.12	125.37
29	A	807	CLA	C4A-NA-C1A	7.06	109.88	106.71
29	i	312	CLA	C4A-NA-C1A	7.06	109.88	106.71
32	A	846	WVN	C35-C32-C31	-7.05	106.96	118.08
38	m	614	II0	C42-C40-C36	-7.05	117.24	127.31
32	e	315	WVN	C23-C25-C28	-7.05	108.13	118.94
32	e	315	WVN	C40-C37-C34	-7.04	117.26	127.31
29	a	310	CLA	C4A-NA-C1A	7.04	109.87	106.71
29	f	609	CLA	C4A-NA-C1A	7.04	109.87	106.71
38	e	312	II0	C37-C35-C33	-7.04	106.99	118.08
29	Q	302	CLA	C4A-NA-C1A	7.03	109.87	106.71
32	F	207	WVN	C35-C32-C31	-7.03	107.00	118.08
38	l	313	II0	C03-C09-C13	-7.03	112.71	122.63
29	a	309	CLA	C4A-NA-C1A	7.02	109.86	106.71
32	A	854	WVN	C40-C37-C34	-7.02	117.30	127.31
40	g	313	KC2	CMD-C2D-C1D	7.02	136.05	125.37
29	m	613	CLA	C4A-NA-C1A	7.01	109.86	106.71
38	k	616	II0	C37-C35-C33	-7.01	107.03	118.08
29	l	309	CLA	C4A-NA-C1A	7.01	109.86	106.71
29	B	803	CLA	C4A-NA-C1A	7.01	109.86	106.71
40	i	318	KC2	C1A-C2A-C3A	-7.00	101.55	107.11
32	R	201	WVN	C23-C25-C28	-7.00	108.19	118.94
40	g	315	KC2	CMD-C2D-C1D	7.00	136.03	125.37
29	f	601	CLA	C4A-NA-C1A	7.00	109.85	106.71
40	l	311	KC2	CMD-C2D-C1D	7.00	136.02	125.37
38	a	313	II0	C34-C36-C40	-6.99	108.21	118.94
38	l	313	II0	C37-C35-C33	-6.99	107.06	118.08
29	L	202	CLA	C4A-NA-C1A	6.99	109.85	106.71
29	l	301	CLA	C4A-NA-C1A	6.99	109.85	106.71
29	i	306	CLA	C4A-NA-C1A	6.99	109.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	d	311	KC2	CMD-C2D-C1D	6.98	136.00	125.37
32	A	847	WVN	C06-C13-C15	-6.98	112.78	122.61
29	f	602	CLA	C4A-NA-C1A	6.98	109.84	106.71
29	k	604	CLA	C4A-NA-C1A	6.98	109.84	106.71
29	A	831	CLA	C4A-NA-C1A	6.97	109.84	106.71
40	s	404	KC2	CMD-C2D-C1D	6.96	135.97	125.37
29	a	307	CLA	C4A-NA-C1A	6.96	109.83	106.71
38	l	314	II0	C37-C35-C33	-6.96	107.12	118.08
29	j	302	CLA	C4A-NA-C1A	6.96	109.83	106.71
38	g	319	II0	C34-C36-C40	-6.95	108.28	118.94
29	m	605	CLA	C4A-NA-C1A	6.95	109.83	106.71
32	F	205	WVN	C24-C22-C19	-6.95	107.13	118.08
29	B	825	CLA	C4A-NA-C1A	6.94	109.83	106.71
29	g	312	CLA	C4A-NA-C1A	6.94	109.83	106.71
40	d	311	KC2	C2B-C1B-NB	6.94	115.22	110.10
40	l	311	KC2	CMA-C3A-C2A	-6.94	111.32	128.30
40	e	309	KC2	C1A-C2A-C3A	-6.93	101.61	107.11
32	s	405	WVN	C35-C32-C31	-6.93	107.15	118.08
38	f	618	II0	C03-C09-C13	-6.93	112.85	122.63
29	n	604	CLA	C4A-NA-C1A	6.91	109.81	106.71
32	A	844	WVN	C33-C34-C37	-6.90	108.35	118.94
29	B	820	CLA	C4A-NA-C1A	6.90	109.81	106.71
29	h	302	CLA	C4A-NA-C1A	6.90	109.81	106.71
29	f	610	CLA	C4A-NA-C1A	6.90	109.81	106.71
32	L	205	WVN	C33-C34-C37	-6.89	108.37	118.94
38	f	618	II0	C42-C40-C36	-6.89	117.48	127.31
29	A	814	CLA	C4A-NA-C1A	6.88	109.80	106.71
38	h	310	II0	C04-C10-C14	-6.88	112.92	122.63
38	f	616	II0	C42-C40-C36	-6.88	117.50	127.31
32	M	101	WVN	C40-C37-C34	-6.87	117.50	127.31
29	A	824	CLA	C4A-NA-C1A	6.87	109.79	106.71
29	g	323	CLA	C4A-NA-C1A	6.87	109.79	106.71
38	a	317	II0	C34-C36-C40	-6.86	108.41	118.94
40	s	404	KC2	C1A-C2A-C3A	-6.86	101.67	107.11
40	i	310	KC2	C3A-C4A-NA	6.86	118.06	110.57
29	i	309	CLA	C4A-NA-C1A	6.86	109.79	106.71
29	i	308	CLA	C4A-NA-C1A	6.86	109.79	106.71
38	f	614	II0	C42-C40-C36	-6.86	117.52	127.31
32	h	308	WVN	C27-C25-C23	-6.86	107.27	118.08
29	c	301	CLA	C4A-NA-C1A	6.86	109.79	106.71
29	b	307	CLA	C4A-NA-C1A	6.86	109.79	106.71
29	l	304	CLA	C4A-NA-C1A	6.85	109.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	301	CLA	C4A-NA-C1A	6.85	109.78	106.71
29	A	826	CLA	C4A-NA-C1A	6.85	109.78	106.71
29	g	305	CLA	C4A-NA-C1A	6.85	109.78	106.71
32	A	847	WVN	C35-C32-C31	-6.84	107.30	118.08
29	L	207	CLA	C4A-NA-C1A	6.84	109.78	106.71
29	g	306	CLA	C4A-NA-C1A	6.83	109.78	106.71
29	A	827	CLA	C4A-NA-C1A	6.83	109.78	106.71
32	B	849	WVN	C35-C32-C31	-6.83	107.32	118.08
29	A	805	CLA	C4A-NA-C1A	6.82	109.77	106.71
38	i	313	II0	C03-C09-C13	-6.82	113.00	122.63
29	e	308	CLA	C4A-NA-C1A	6.82	109.77	106.71
38	g	318	II0	C03-C09-C13	-6.81	113.01	122.63
29	l	303	CLA	C4A-NA-C1A	6.81	109.77	106.71
29	e	305	CLA	C4A-NA-C1A	6.81	109.77	106.71
38	g	317	II0	C34-C36-C40	-6.81	108.50	118.94
29	B	831	CLA	C4A-NA-C1A	6.81	109.77	106.71
40	j	312	KC2	C2B-C1B-NB	6.80	115.12	110.10
29	A	821	CLA	C4A-NA-C1A	6.80	109.76	106.71
32	i	315	WVN	C40-C37-C34	-6.80	117.60	127.31
29	B	835	CLA	C4A-NA-C1A	6.80	109.76	106.71
29	g	307	CLA	C4A-NA-C1A	6.80	109.76	106.71
38	a	314	II0	C31-C33-C35	6.80	145.51	126.42
38	h	309	II0	C30-C32-C34	-6.80	111.93	125.34
40	s	404	KC2	O2D-CGD-CBD	6.79	123.33	111.27
29	m	609	CLA	C4A-NA-C1A	6.79	109.76	106.71
38	n	618	II0	C42-C40-C36	-6.78	117.63	127.31
29	d	305	CLA	C4A-NA-C1A	6.78	109.75	106.71
29	B	809	CLA	C4A-NA-C1A	6.78	109.75	106.71
40	n	611	KC2	CMA-C3A-C2A	-6.77	111.72	128.30
32	J	101	WVN	C35-C32-C31	-6.77	107.40	118.08
29	l	305	CLA	C4A-NA-C1A	6.77	109.75	106.71
40	i	318	KC2	CMA-C3A-C2A	-6.77	111.73	128.30
29	g	309	CLA	C4A-NA-C1A	6.76	109.75	106.71
40	n	611	KC2	C3A-C4A-NA	6.76	117.95	110.57
29	k	602	CLA	C4A-NA-C1A	6.75	109.74	106.71
29	h	305	CLA	C4A-NA-C1A	6.75	109.74	106.71
29	d	318	CLA	C4A-NA-C1A	6.75	109.74	106.71
32	F	207	WVN	C27-C25-C23	-6.75	107.45	118.08
29	A	808	CLA	C4A-NA-C1A	6.74	109.74	106.71
32	F	204	WVN	C35-C32-C31	-6.74	107.45	118.08
29	A	806	CLA	C4A-NA-C1A	6.74	109.74	106.71
32	l	302	WVN	C27-C25-C23	-6.74	107.46	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	603	CLA	C4A-NA-C1A	6.74	109.74	106.71
38	f	616	II0	C16-C03-C09	6.74	121.17	110.47
38	c	313	II0	C42-C40-C36	-6.73	117.70	127.31
38	f	614	II0	C31-C33-C35	6.73	145.33	126.42
29	j	311	CLA	C4A-NA-C1A	6.73	109.73	106.71
38	i	319	II0	C03-C09-C13	-6.73	113.13	122.63
38	i	313	II0	C34-C36-C40	-6.73	108.62	118.94
32	A	846	WVN	C06-C13-C15	-6.72	113.14	122.61
32	A	844	WVN	C23-C25-C28	-6.72	108.62	118.94
29	d	306	CLA	C4A-NA-C1A	6.72	109.73	106.71
29	d	302	CLA	C4A-NA-C1A	6.72	109.72	106.71
38	g	319	II0	C42-C40-C36	-6.71	117.73	127.31
32	F	204	WVN	C38-C34-C37	-6.71	113.53	122.92
29	b	309	CLA	C4A-NA-C1A	6.71	109.72	106.71
29	i	311	CLA	C4A-NA-C1A	6.71	109.72	106.71
32	A	847	WVN	C24-C22-C19	-6.71	107.51	118.08
40	i	310	KC2	C1A-C2A-C3A	-6.70	101.79	107.11
32	l	316	WVN	C27-C25-C28	-6.70	113.54	122.92
32	L	206	WVN	C27-C25-C23	-6.70	107.52	118.08
29	B	824	CLA	C4A-NA-C1A	6.69	109.71	106.71
29	m	604	CLA	C4A-NA-C1A	6.69	109.71	106.71
38	k	616	II0	C03-C09-C13	-6.69	113.19	122.63
29	l	310	CLA	C4A-NA-C1A	6.69	109.71	106.71
29	j	305	CLA	C4A-NA-C1A	6.69	109.71	106.71
29	n	606	CLA	C4A-NA-C1A	6.68	109.71	106.71
40	k	611	KC2	C2B-C1B-NB	6.68	115.02	110.10
38	a	313	II0	C42-C40-C36	-6.67	117.79	127.31
38	J	103	II0	C34-C36-C40	-6.67	108.71	118.94
32	h	308	WVN	C23-C25-C28	-6.66	108.72	118.94
32	L	206	WVN	C20-C13-C15	-6.66	105.32	121.46
40	g	313	KC2	C2B-C1B-NB	6.66	115.01	110.10
32	s	405	WVN	C27-C25-C23	-6.66	107.58	118.08
29	B	839	CLA	C4A-NA-C1A	6.66	109.70	106.71
40	g	314	KC2	C2B-C1B-NB	6.65	115.00	110.10
40	g	314	KC2	C3A-C4A-NA	6.65	117.83	110.57
40	s	401	KC2	C2B-C1B-NB	6.65	115.00	110.10
32	R	202	WVN	C35-C32-C31	-6.65	107.61	118.08
29	l	308	CLA	C4A-NA-C1A	6.64	109.69	106.71
29	n	601	CLA	C4A-NA-C1A	6.64	109.69	106.71
38	g	319	II0	C04-C10-C14	-6.64	113.25	122.63
40	g	315	KC2	CMA-C3A-C2A	-6.64	112.04	128.30
29	k	609	CLA	C4A-NA-C1A	6.64	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	609	CLA	C4A-NA-C1A	6.64	109.69	106.71
29	A	809	CLA	C4A-NA-C1A	6.64	109.69	106.71
29	A	822	CLA	C4A-NA-C1A	6.64	109.69	106.71
38	l	314	II0	C31-C33-C35	6.64	145.06	126.42
29	j	310	CLA	C4A-NA-C1A	6.63	109.69	106.71
29	n	605	CLA	C4A-NA-C1A	6.63	109.69	106.71
32	K	103	WVN	C23-C25-C28	-6.62	108.78	118.94
29	c	308	CLA	C4A-NA-C1A	6.62	109.68	106.71
29	j	307	CLA	C4A-NA-C1A	6.62	109.68	106.71
40	f	611	KC2	C2B-C1B-NB	6.62	114.98	110.10
29	k	608	CLA	C4A-NA-C1A	6.62	109.68	106.71
38	m	618	II0	C03-C09-C13	-6.62	113.29	122.63
29	h	312	CLA	C4A-NA-C1A	6.61	109.68	106.71
40	k	611	KC2	CHB-C4A-C3A	-6.61	114.66	124.98
38	i	316	II0	C03-C09-C13	-6.61	113.31	122.63
38	n	615	II0	C42-C40-C36	-6.60	117.89	127.31
29	j	303	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	B	836	CLA	C4A-NA-C1A	6.60	109.67	106.71
38	n	618	II0	C34-C36-C40	-6.60	108.81	118.94
29	B	830	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	k	601	CLA	C4A-NA-C1A	6.60	109.67	106.71
38	n	616	II0	C37-C35-C33	-6.59	107.69	118.08
40	n	611	KC2	CHB-C4A-C3A	-6.59	114.69	124.98
29	h	306	CLA	C4A-NA-C1A	6.59	109.67	106.71
38	g	318	II0	C37-C35-C39	-6.58	113.70	122.92
29	a	306	CLA	C4A-NA-C1A	6.58	109.67	106.71
29	a	312	CLA	C4A-NA-C1A	6.58	109.66	106.71
29	b	306	CLA	C4A-NA-C1A	6.58	109.66	106.71
29	c	309	CLA	C4A-NA-C1A	6.57	109.66	106.71
38	m	616	II0	C04-C10-C14	-6.57	113.36	122.63
29	g	303	CLA	C4A-NA-C1A	6.56	109.66	106.71
38	g	319	II0	C37-C35-C33	-6.56	107.74	118.08
32	s	407	WVN	C23-C25-C28	-6.55	108.89	118.94
38	e	312	II0	C34-C36-C40	-6.55	108.89	118.94
40	k	611	KC2	CMA-C3A-C2A	-6.55	112.27	128.30
32	R	202	WVN	C23-C25-C28	-6.55	108.90	118.94
29	e	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
40	g	315	KC2	C3B-C2B-C1B	-6.54	100.83	107.08
29	n	608	CLA	C4A-NA-C1A	6.54	109.64	106.71
29	A	812	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	m	601	CLA	C4A-NA-C1A	6.53	109.64	106.71
40	i	310	KC2	CHB-C4A-C3A	-6.53	114.77	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	841	PQN	C15-C13-C12	-6.53	107.90	121.12
29	a	303	CLA	C4A-NA-C1A	6.53	109.64	106.71
38	h	310	II0	C03-C09-C13	-6.52	113.42	122.63
40	e	309	KC2	C2B-C1B-NB	6.52	114.91	110.10
40	g	314	KC2	CHB-C4A-C3A	-6.52	114.79	124.98
29	h	301	CLA	C4A-NA-C1A	6.52	109.64	106.71
38	a	315	II0	C03-C09-C13	-6.52	113.43	122.63
38	j	316	II0	C03-C09-C13	-6.52	113.43	122.63
29	i	303	CLA	C4A-NA-C1A	6.52	109.64	106.71
32	i	315	WVN	C35-C32-C31	-6.51	107.82	118.08
29	h	304	CLA	C4A-NA-C1A	6.51	109.63	106.71
29	f	613	CLA	C4A-NA-C1A	6.51	109.63	106.71
38	f	614	II0	C34-C36-C40	-6.51	108.95	118.94
29	f	606	CLA	C4A-NA-C1A	6.50	109.63	106.71
38	J	103	II0	C03-C09-C13	-6.50	113.45	122.63
38	i	313	II0	C37-C35-C33	-6.50	107.83	118.08
38	e	313	II0	C03-C09-C13	-6.50	113.45	122.63
29	A	802	CLA	C4A-NA-C1A	6.50	109.63	106.71
29	j	304	CLA	C4A-NA-C1A	6.50	109.63	106.71
40	g	315	KC2	C4C-C3C-C2C	-6.50	101.96	107.11
29	m	606	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	n	602	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	A	810	CLA	C4A-NA-C1A	6.49	109.62	106.71
40	l	311	KC2	C2B-C1B-NB	6.48	114.88	110.10
29	B	811	CLA	C4A-NA-C1A	6.48	109.62	106.71
32	B	848	WVN	C14-C15-C13	-6.48	113.33	122.73
40	g	315	KC2	C1A-C2A-C3A	-6.48	101.97	107.11
29	B	815	CLA	C4A-NA-C1A	6.47	109.62	106.71
29	k	606	CLA	C4A-NA-C1A	6.47	109.62	106.71
29	A	817	CLA	C4A-NA-C1A	6.47	109.62	106.71
40	s	404	KC2	CMA-C3A-C4A	-6.47	115.18	125.04
29	e	302	CLA	C4A-NA-C1A	6.47	109.61	106.71
38	i	316	II0	C34-C36-C40	-6.47	109.01	118.94
40	n	611	KC2	C4C-C3C-C2C	-6.47	101.98	107.11
32	A	845	WVN	C06-C13-C15	-6.47	113.51	122.61
29	B	828	CLA	C4A-NA-C1A	6.46	109.61	106.71
38	a	315	II0	C37-C35-C33	-6.46	107.89	118.08
38	b	315	II0	C03-C09-C13	-6.46	113.51	122.63
40	n	611	KC2	C3B-C2B-C1B	-6.46	100.91	107.08
29	e	306	CLA	C4A-NA-C1A	6.45	109.61	106.71
38	g	319	II0	C03-C09-C13	-6.45	113.52	122.63
32	A	845	WVN	C35-C32-C31	-6.45	107.92	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	313	CLA	C4A-NA-C1A	6.44	109.60	106.71
29	A	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
32	A	846	WVN	C02-C05-C09	-6.44	113.55	121.47
32	s	407	WVN	C20-C13-C15	-6.43	105.88	121.46
29	g	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
32	R	202	WVN	C40-C37-C34	-6.43	118.14	127.31
29	A	811	CLA	C4A-NA-C1A	6.42	109.59	106.71
32	F	207	WVN	C38-C34-C33	-6.41	107.97	118.08
29	d	309	CLA	C4A-NA-C1A	6.41	109.59	106.71
29	c	305	CLA	C4A-NA-C1A	6.41	109.59	106.71
29	m	612	CLA	C4A-NA-C1A	6.41	109.59	106.71
38	d	301	II0	C37-C35-C33	-6.41	107.98	118.08
40	g	314	KC2	C4C-C3C-C2C	-6.40	102.03	107.11
29	J	102	CLA	C4A-NA-C1A	6.40	109.58	106.71
29	j	314	CLA	C4A-NA-C1A	6.40	109.58	106.71
40	k	611	KC2	C3A-C4A-NA	6.40	117.56	110.57
29	A	828	CLA	C4A-NA-C1A	6.40	109.58	106.71
29	B	823	CLA	C4A-NA-C1A	6.39	109.58	106.71
38	a	315	II0	C31-C29-C25	-6.39	108.03	126.58
29	m	608	CLA	C4A-NA-C1A	6.39	109.58	106.71
40	c	310	KC2	C3B-C2B-C1B	-6.38	100.98	107.08
40	g	315	KC2	CHB-C4A-C3A	-6.38	115.01	124.98
29	A	839	CLA	C4A-NA-C1A	6.37	109.57	106.71
40	s	404	KC2	C2B-C1B-NB	6.37	114.80	110.10
29	c	312	CLA	C4A-NA-C1A	6.37	109.57	106.71
29	B	801	CLA	C4A-NA-C1A	6.37	109.57	106.71
38	k	615	II0	C38-C36-C34	-6.36	108.05	118.08
38	a	313	II0	C04-C10-C14	-6.36	113.66	122.63
29	B	841	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	A	840	CLA	C4A-NA-C1A	6.35	109.56	106.71
38	h	309	II0	C34-C36-C40	-6.35	109.20	118.94
38	h	311	II0	C04-C10-C14	-6.34	113.68	122.63
32	F	205	WVN	C20-C13-C15	-6.34	106.11	121.46
32	L	206	WVN	C35-C32-C31	-6.33	108.10	118.08
40	m	611	KC2	C3B-C2B-C1B	-6.33	101.03	107.08
40	s	404	KC2	C4C-C3C-C2C	-6.33	102.09	107.11
38	J	103	II0	C04-C10-C14	-6.33	113.70	122.63
29	b	303	CLA	C4A-NA-C1A	6.33	109.55	106.71
29	A	819	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	g	310	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	R	203	CLA	C4A-NA-C1A	6.32	109.55	106.71
32	K	103	WVN	C38-C34-C33	-6.32	108.12	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s	404	KC2	C3A-C4A-NA	6.32	117.47	110.57
40	j	312	KC2	C3B-C2B-C1B	-6.31	101.05	107.08
38	i	314	II0	C37-C35-C33	-6.31	108.13	118.08
40	g	315	KC2	C3A-C4A-NA	6.31	117.46	110.57
32	A	847	WVN	C40-C37-C34	-6.30	118.31	127.31
32	l	302	WVN	C33-C34-C37	-6.30	109.28	118.94
32	l	316	WVN	C23-C20-C13	-6.28	109.55	127.20
29	d	308	CLA	C4A-NA-C1A	6.28	109.53	106.71
29	g	316	CLA	C4A-NA-C1A	6.28	109.53	106.71
38	k	616	II0	C42-C40-C36	-6.28	118.35	127.31
38	j	316	II0	C37-C35-C33	-6.28	108.19	118.08
40	d	311	KC2	C3B-C2B-C1B	-6.28	101.08	107.08
40	s	401	KC2	CMD-C2D-C1D	6.27	134.92	125.37
38	k	620	II0	C03-C09-C13	-6.27	113.78	122.63
32	B	847	WVN	C27-C25-C23	-6.27	108.19	118.08
32	B	847	WVN	C35-C32-C31	-6.27	108.20	118.08
32	F	207	WVN	C24-C22-C19	-6.26	108.21	118.08
30	B	843	PQN	C15-C13-C12	-6.26	108.45	121.12
32	L	201	WVN	C24-C22-C19	-6.26	108.22	118.08
40	s	404	KC2	CHB-C4A-C3A	-6.26	115.21	124.98
38	d	315	II0	C37-C35-C33	-6.25	108.22	118.08
32	F	207	WVN	C33-C34-C37	-6.25	109.35	118.94
38	b	301	II0	C42-C40-C36	-6.25	118.39	127.31
32	B	849	WVN	C02-C05-C09	-6.25	113.78	121.47
38	l	313	II0	C04-C10-C14	-6.24	113.82	122.63
32	F	207	WVN	C19-C22-C26	-6.24	109.37	118.94
38	k	615	II0	C03-C09-C13	-6.24	113.83	122.63
40	f	611	KC2	O2D-CGD-CBD	6.22	122.33	111.27
29	c	302	CLA	C4A-NA-C1A	6.22	109.50	106.71
38	k	619	II0	C03-C09-C13	-6.22	113.85	122.63
40	i	318	KC2	C3B-C2B-C1B	-6.22	101.14	107.08
38	a	314	II0	C34-C36-C40	-6.21	109.41	118.94
38	i	316	II0	C33-C35-C39	-6.21	109.41	118.94
29	B	810	CLA	C4A-NA-C1A	6.21	109.50	106.71
40	l	311	KC2	CHB-C4A-C3A	-6.21	115.28	124.98
32	h	308	WVN	C38-C34-C33	-6.21	108.30	118.08
32	R	202	WVN	C14-C15-C13	-6.21	113.72	122.73
29	a	308	CLA	C4A-NA-C1A	6.20	109.49	106.71
29	i	304	CLA	C4A-NA-C1A	6.19	109.49	106.71
29	g	308	CLA	C4A-NA-C1A	6.19	109.49	106.71
29	K	102	CLA	C4A-NA-C1A	6.19	109.49	106.71
38	k	615	II0	C34-C36-C40	-6.19	109.45	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	F	204	WVN	C27-C25-C23	-6.19	108.33	118.08
40	s	401	KC2	C3B-C2B-C1B	-6.18	101.17	107.08
40	l	311	KC2	C3A-C4A-NA	6.18	117.32	110.57
32	B	849	WVN	C30-C28-C25	-6.18	118.48	127.31
40	g	314	KC2	CMD-C2D-C1D	6.18	134.79	125.37
38	h	311	II0	C37-C35-C33	-6.18	108.33	118.08
38	j	301	II0	C04-C10-C14	-6.18	113.91	122.63
32	R	201	WVN	C40-C37-C34	-6.17	118.50	127.31
32	s	407	WVN	C27-C25-C23	-6.17	108.36	118.08
32	J	101	WVN	C14-C15-C13	-6.16	113.78	122.73
38	d	316	II0	C42-C40-C36	-6.16	118.52	127.31
38	d	301	II0	C33-C35-C39	-6.15	109.50	118.94
32	R	201	WVN	C35-C32-C31	-6.15	108.39	118.08
32	e	315	WVN	C35-C32-C31	-6.14	108.40	118.08
32	L	206	WVN	C33-C34-C37	-6.14	109.52	118.94
32	L	201	WVN	C27-C25-C23	-6.14	108.41	118.08
32	L	205	WVN	C20-C13-C15	-6.14	106.60	121.46
38	d	315	II0	C31-C29-C25	-6.13	108.77	126.58
38	f	615	II0	C37-C35-C33	-6.13	108.41	118.08
32	F	205	WVN	C14-C15-C13	-6.13	113.83	122.73
38	e	312	II0	C04-C10-C14	-6.13	113.97	122.63
32	i	315	WVN	C30-C28-C25	-6.13	118.56	127.31
29	e	307	CLA	C4A-NA-C1A	6.13	109.46	106.71
29	A	834	CLA	C4A-NA-C1A	6.13	109.46	106.71
38	f	618	II0	C37-C35-C33	-6.13	108.43	118.08
32	A	854	WVN	C30-C28-C25	-6.12	118.57	127.31
40	e	309	KC2	C3B-C2B-C1B	-6.12	101.23	107.08
29	B	812	CLA	C4A-NA-C1A	6.12	109.46	106.71
38	e	313	II0	C34-C36-C40	-6.11	109.56	118.94
40	m	611	KC2	CHB-C4A-C3A	-6.10	115.45	124.98
29	B	842	CLA	C4A-NA-C1A	6.10	109.45	106.71
40	l	311	KC2	C3B-C2B-C1B	-6.10	101.25	107.08
32	s	405	WVN	C14-C15-C13	-6.10	113.87	122.73
40	f	611	KC2	C3B-C2B-C1B	-6.09	101.26	107.08
40	i	310	KC2	C3B-C2B-C1B	-6.09	101.26	107.08
29	s	406	CLA	C4A-NA-C1A	6.09	109.44	106.71
32	M	101	WVN	C23-C25-C28	-6.09	109.60	118.94
32	L	206	WVN	C23-C25-C28	-6.09	109.60	118.94
29	a	304	CLA	C4A-NA-C1A	6.08	109.44	106.71
40	g	314	KC2	C3B-C2B-C1B	-6.08	101.27	107.08
38	a	315	II0	C04-C10-C14	-6.08	114.05	122.63
29	c	303	CLA	C4A-NA-C1A	6.06	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	d	311	KC2	CHB-C4A-C3A	-6.05	115.52	124.98
32	l	316	WVN	C20-C13-C15	-6.05	106.81	121.46
38	j	301	II0	C38-C36-C34	-6.05	108.55	118.08
29	m	603	CLA	C4A-NA-C1A	6.05	109.42	106.71
32	R	201	WVN	C20-C13-C15	-6.04	106.83	121.46
38	d	316	II0	C37-C35-C33	-6.04	108.56	118.08
40	i	310	KC2	O2D-CGD-CBD	6.04	121.99	111.27
32	A	845	WVN	C14-C15-C13	-6.04	113.97	122.73
32	A	845	WVN	C23-C25-C28	-6.03	109.69	118.94
38	m	618	II0	C37-C35-C33	-6.03	108.57	118.08
40	i	310	KC2	C4C-C3C-C2C	-6.03	102.33	107.11
40	j	312	KC2	CHB-C4A-C3A	-6.03	115.57	124.98
32	F	205	WVN	C35-C32-C31	-6.02	108.59	118.08
29	O	201	CLA	C4A-NA-C1A	6.01	109.41	106.71
40	g	313	KC2	C3B-C2B-C1B	-6.01	101.33	107.08
29	j	309	CLA	C4A-NA-C1A	6.01	109.41	106.71
40	g	313	KC2	CHB-C4A-C3A	-6.01	115.59	124.98
32	A	854	WVN	C06-C13-C15	-6.01	114.15	122.61
29	c	307	CLA	C4A-NA-C1A	6.01	109.41	106.71
29	n	603	CLA	C4A-NA-C1A	6.01	109.41	106.71
38	g	318	II0	C42-C40-C36	-6.01	118.74	127.31
29	d	310	CLA	C4A-NA-C1A	6.00	109.40	106.71
32	B	848	WVN	C06-C13-C15	-5.99	114.17	122.61
40	s	401	KC2	CHB-C4A-C3A	-5.99	115.63	124.98
40	i	318	KC2	CHB-C4A-C3A	-5.99	115.63	124.98
40	d	311	KC2	C3A-C4A-NA	5.98	117.11	110.57
40	k	611	KC2	C3B-C2B-C1B	-5.98	101.36	107.08
32	s	405	WVN	C33-C34-C37	-5.98	109.76	118.94
32	F	205	WVN	C39-C36-C32	-5.98	118.78	127.31
38	a	317	II0	C03-C09-C13	-5.98	114.20	122.63
40	m	611	KC2	C4C-C3C-C2C	-5.97	102.38	107.11
38	a	314	II0	C42-C40-C36	-5.96	118.80	127.31
32	L	201	WVN	C31-C32-C36	-5.96	109.79	118.94
29	B	806	CLA	C4A-NA-C1A	5.96	109.39	106.71
29	F	202	CLA	C4A-NA-C1A	5.96	109.39	106.71
38	n	618	II0	C38-C36-C34	-5.96	108.69	118.08
29	B	821	CLA	C4A-NA-C1A	5.95	109.38	106.71
40	f	611	KC2	CHB-C4A-C3A	-5.95	115.68	124.98
29	B	827	CLA	C4A-NA-C1A	5.95	109.38	106.71
29	m	602	CLA	C4A-NA-C1A	5.95	109.38	106.71
29	B	818	CLA	C4A-NA-C1A	5.95	109.38	106.71
40	c	310	KC2	CHD-C1D-ND	-5.95	117.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	844	WVN	C19-C22-C26	-5.94	109.83	118.94
32	L	201	WVN	C19-C22-C26	-5.94	109.83	118.94
40	c	310	KC2	CHB-C4A-C3A	-5.94	115.70	124.98
29	f	608	CLA	C4A-NA-C1A	5.93	109.37	106.71
40	m	611	KC2	CHD-C1D-ND	-5.93	117.98	124.26
40	i	318	KC2	C3A-C4A-NA	5.93	117.05	110.57
40	m	611	KC2	C3A-C4A-NA	5.93	117.04	110.57
29	A	832	CLA	C4A-NA-C1A	5.92	109.37	106.71
29	A	829	CLA	C4A-NA-C1A	5.92	109.37	106.71
32	A	847	WVN	C14-C15-C13	-5.91	114.15	122.73
29	j	308	CLA	C4A-NA-C1A	5.91	109.36	106.71
38	e	314	II0	C37-C35-C33	-5.91	108.76	118.08
32	L	201	WVN	C35-C32-C31	-5.91	108.77	118.08
29	d	303	CLA	C4A-NA-C1A	5.91	109.36	106.71
40	j	312	KC2	C3A-C4A-NA	5.90	117.01	110.57
40	g	313	KC2	C3A-C4A-NA	5.90	117.01	110.57
29	A	825	CLA	C4A-NA-C1A	5.89	109.36	106.71
32	K	103	WVN	C35-C32-C31	-5.89	108.79	118.08
32	B	848	WVN	C35-C32-C31	-5.89	108.79	118.08
32	F	205	WVN	C23-C25-C28	-5.89	109.90	118.94
38	i	314	II0	C03-C09-C13	-5.89	114.32	122.63
38	n	618	II0	C37-C35-C33	-5.89	108.80	118.08
29	b	310	CLA	C4A-NA-C1A	5.89	109.35	106.71
38	g	317	II0	C31-C29-C25	-5.88	109.50	126.58
32	l	316	WVN	C35-C32-C31	-5.88	108.81	118.08
38	m	616	II0	C03-C09-C13	-5.88	114.33	122.63
29	F	201	CLA	C4A-NA-C1A	5.87	109.34	106.71
38	a	313	II0	C37-C35-C33	-5.86	108.84	118.08
29	B	819	CLA	CBC-CAC-C3C	5.86	128.57	112.43
38	J	103	II0	C37-C35-C33	-5.85	108.86	118.08
29	B	816	CLA	C4A-NA-C1A	5.85	109.34	106.71
40	s	401	KC2	C3A-C4A-NA	5.85	116.96	110.57
32	B	849	WVN	C24-C22-C19	-5.85	108.86	118.08
40	e	309	KC2	CHB-C4A-C3A	-5.85	115.85	124.98
40	c	310	KC2	C3A-C4A-NA	5.84	116.95	110.57
38	h	309	II0	C37-C35-C33	-5.84	108.88	118.08
38	g	317	II0	C37-C35-C33	-5.84	108.88	118.08
40	f	611	KC2	C3A-C4A-NA	5.84	116.94	110.57
38	f	614	II0	C03-C09-C13	-5.83	114.40	122.63
32	A	844	WVN	C35-C32-C31	-5.83	108.89	118.08
38	f	616	II0	C37-C35-C33	-5.83	108.89	118.08
29	A	803	CLA	C4A-NA-C1A	5.82	109.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	l	311	KC2	O2D-CGD-CBD	5.81	121.60	111.27
29	B	817	CLA	C4A-NA-C1A	5.81	109.32	106.71
38	a	317	II0	C37-C35-C33	-5.81	108.92	118.08
38	k	620	II0	C37-C35-C33	-5.81	108.92	118.08
38	f	614	II0	C04-C10-C14	-5.81	114.44	122.63
40	e	309	KC2	C3A-C4A-NA	5.79	116.89	110.57
38	f	616	II0	C31-C29-C25	-5.79	109.78	126.58
32	J	101	WVN	C27-C25-C23	-5.79	108.96	118.08
32	M	101	WVN	C27-C25-C23	-5.79	108.96	118.08
29	B	802	CLA	C4A-NA-C1A	5.78	109.31	106.71
32	L	205	WVN	C02-C05-C09	-5.78	114.36	121.47
32	I	101	WVN	C23-C25-C28	-5.78	110.07	118.94
32	i	315	WVN	C24-C22-C19	-5.78	108.97	118.08
40	l	311	KC2	C4C-C3C-C2C	-5.76	102.54	107.11
38	e	312	II0	C33-C35-C39	-5.75	110.11	118.94
38	i	316	II0	C38-C36-C34	-5.75	109.02	118.08
32	I	101	WVN	C20-C13-C15	-5.75	107.53	121.46
29	e	303	CLA	C4A-NA-C1A	5.74	109.29	106.71
32	A	846	WVN	C20-C13-C15	-5.74	107.56	121.46
38	m	616	II0	C37-C35-C33	-5.74	109.04	118.08
38	i	319	II0	C37-C35-C33	-5.74	109.04	118.08
38	j	315	II0	C37-C35-C33	-5.73	109.04	118.08
38	m	616	II0	C38-C36-C34	-5.73	109.04	118.08
38	c	313	II0	C04-C10-C14	-5.73	114.54	122.63
31	s	408	LHG	O4-P-O5	5.72	133.06	110.68
29	A	818	CLA	C4A-NA-C1A	5.71	109.27	106.71
40	d	311	KC2	CHD-C1D-ND	-5.71	118.21	124.26
38	l	315	II0	C37-C35-C33	-5.71	109.08	118.08
32	F	207	WVN	C02-C05-C09	-5.70	114.45	121.47
38	k	616	II0	C19-C13-C11	-5.70	103.79	114.36
40	i	310	KC2	CHD-C1D-ND	-5.70	118.23	124.26
38	g	319	II0	C31-C29-C25	-5.69	110.05	126.58
32	A	844	WVN	C24-C22-C19	-5.69	109.12	118.08
38	h	309	II0	C38-C36-C34	-5.68	109.13	118.08
38	b	301	II0	C37-C35-C33	-5.67	109.14	118.08
29	n	613	CLA	C4A-NA-C1A	5.67	109.26	106.71
40	s	401	KC2	O2D-CGD-CBD	5.67	121.34	111.27
38	f	615	II0	C42-C40-C36	-5.67	119.22	127.31
32	A	854	WVN	C35-C32-C31	-5.66	109.16	118.08
38	m	615	II0	C37-C35-C33	-5.66	109.16	118.08
32	e	315	WVN	C27-C25-C23	-5.66	109.17	118.08
38	i	319	II0	C32-C30-C26	-5.65	110.16	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	306	CLA	C4A-NA-C1A	5.65	109.25	106.71
38	e	313	II0	C37-C35-C33	-5.63	109.20	118.08
32	R	201	WVN	C27-C25-C23	-5.62	109.22	118.08
32	h	308	WVN	C35-C32-C31	-5.62	109.23	118.08
32	l	302	WVN	C35-C32-C31	-5.60	109.25	118.08
40	g	314	KC2	CMA-C3A-C2A	-5.60	114.60	128.30
40	n	611	KC2	CHD-C1D-ND	-5.59	118.33	124.26
38	k	619	II0	C37-C35-C33	-5.59	109.27	118.08
32	e	315	WVN	C02-C05-C09	-5.59	114.60	121.47
40	i	310	KC2	C1A-NA-C4A	-5.58	104.20	106.71
38	e	313	II0	C04-C10-C14	-5.58	114.76	122.63
40	k	611	KC2	O2D-CGD-CBD	5.57	121.16	111.27
32	L	205	WVN	C27-C25-C23	-5.56	109.31	118.08
29	m	607	CLA	C4A-NA-C1A	5.56	109.21	106.71
40	j	312	KC2	C4C-C3C-C2C	-5.56	102.70	107.11
32	s	407	WVN	C35-C32-C31	-5.56	109.32	118.08
40	f	611	KC2	C4C-C3C-C2C	-5.55	102.71	107.11
32	l	302	WVN	C31-C32-C36	-5.55	110.43	118.94
38	d	301	II0	C03-C09-C13	-5.54	114.81	122.63
32	I	101	WVN	C35-C32-C31	-5.54	109.36	118.08
32	B	846	WVN	C14-C15-C13	-5.53	114.70	122.73
32	R	201	WVN	C24-C22-C19	-5.53	109.37	118.08
38	h	310	II0	C37-C35-C33	-5.53	109.37	118.08
29	B	829	CLA	C4A-NA-C1A	5.53	109.19	106.71
38	i	313	II0	C38-C36-C34	-5.52	109.37	118.08
32	B	848	WVN	C31-C32-C36	-5.52	110.46	118.94
40	c	310	KC2	C3D-C4D-ND	5.52	118.08	110.17
40	d	311	KC2	C4C-C3C-C2C	-5.51	102.74	107.11
32	K	103	WVN	C27-C25-C23	-5.51	109.40	118.08
32	M	101	WVN	C14-C15-C13	-5.51	114.73	122.73
38	d	317	II0	C37-C35-C33	-5.50	109.41	118.08
38	b	314	II0	C33-C35-C39	-5.50	110.51	118.94
40	d	311	KC2	C3D-C4D-ND	5.49	118.04	110.17
38	e	314	II0	C38-C36-C34	-5.49	109.43	118.08
38	n	615	II0	C37-C35-C33	-5.49	109.43	118.08
40	k	611	KC2	C4C-C3C-C2C	-5.48	102.76	107.11
38	b	314	II0	C04-C10-C14	-5.48	114.89	122.63
38	n	616	II0	C38-C36-C34	-5.48	109.44	118.08
38	n	615	II0	C04-C10-C14	-5.47	114.90	122.63
38	k	620	II0	C38-C36-C34	-5.47	109.46	118.08
32	A	847	WVN	C27-C25-C23	-5.47	109.46	118.08
29	s	402	CLA	C4A-NA-C1A	5.47	109.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	n	616	II0	C33-C35-C39	-5.47	110.55	118.94
38	j	315	II0	C04-C10-C14	-5.46	114.92	122.63
38	b	301	II0	C38-C36-C34	-5.46	109.47	118.08
38	i	316	II0	C37-C35-C33	-5.46	109.48	118.08
32	F	205	WVN	C27-C25-C23	-5.46	109.48	118.08
29	k	614	CLA	C4A-NA-C1A	5.45	109.16	106.71
38	e	314	II0	C04-C10-C14	-5.45	114.93	122.63
40	s	401	KC2	C4C-C3C-C2C	-5.45	102.79	107.11
38	f	614	II0	C38-C36-C34	-5.43	109.51	118.08
40	i	318	KC2	C4C-C3C-C2C	-5.43	102.80	107.11
29	f	607	CLA	C4A-NA-C1A	5.43	109.15	106.71
29	d	307	CLA	C4A-NA-C1A	5.43	109.15	106.71
40	e	309	KC2	CHD-C1D-ND	-5.43	118.51	124.26
38	d	316	II0	C27-C25-C23	-5.43	106.09	116.84
29	k	603	CLA	C4A-NA-C1A	5.42	109.14	106.71
38	g	318	II0	C37-C35-C33	-5.42	109.53	118.08
38	e	313	II0	C30-C32-C34	-5.42	106.30	123.22
29	A	813	CLA	C4A-NA-C1A	5.41	109.14	106.71
29	A	850	CLA	C4A-NA-C1A	5.40	109.14	106.71
38	j	301	II0	C33-C35-C39	-5.40	110.66	118.94
40	e	309	KC2	C3D-C4D-ND	5.40	117.91	110.17
32	l	302	WVN	C20-C13-C15	-5.39	108.40	121.46
32	A	847	WVN	C38-C34-C33	-5.37	109.62	118.08
29	k	607	CLA	C4A-NA-C1A	5.37	109.12	106.71
40	j	312	KC2	C2A-C1A-NA	5.36	118.00	109.40
32	L	205	WVN	C35-C32-C31	-5.36	109.63	118.08
38	c	313	II0	C38-C36-C34	-5.35	109.64	118.08
40	l	311	KC2	C3C-C2C-C1C	-5.35	102.52	106.49
38	j	315	II0	C03-C09-C13	-5.35	115.08	122.63
38	h	311	II0	C30-C32-C34	-5.35	106.53	123.22
38	k	616	II0	C04-C10-C14	-5.34	115.09	122.63
40	m	611	KC2	C3D-C4D-ND	5.34	117.83	110.17
38	j	301	II0	C37-C35-C33	-5.34	109.66	118.08
32	M	101	WVN	C38-C34-C33	-5.33	109.68	118.08
32	R	201	WVN	C06-C13-C15	-5.33	115.11	122.61
38	j	316	II0	C27-C25-C23	-5.33	106.28	116.84
32	A	847	WVN	C02-C05-C09	-5.32	114.92	121.47
29	i	307	CLA	C4A-NA-C1A	5.32	109.10	106.71
38	e	313	II0	C33-C35-C39	-5.32	110.78	118.94
38	d	317	II0	C04-C10-C14	-5.31	115.13	122.63
38	b	315	II0	C31-C29-C25	-5.31	111.15	126.58
32	B	848	WVN	C27-C25-C23	-5.31	109.71	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	c	313	II0	C03-C09-C13	-5.31	115.14	122.63
38	d	316	II0	C38-C36-C34	-5.30	109.72	118.08
32	R	202	WVN	C27-C25-C23	-5.30	109.73	118.08
38	d	301	II0	C31-C29-C25	-5.30	111.20	126.58
38	e	312	II0	C38-C36-C34	-5.30	109.73	118.08
38	b	314	II0	C37-C35-C33	-5.30	109.73	118.08
29	B	804	CLA	CAC-C3C-C4C	5.29	131.67	124.81
32	A	844	WVN	C27-C25-C23	-5.28	109.75	118.08
40	g	313	KC2	C4C-C3C-C2C	-5.28	102.92	107.11
29	n	607	CLA	C4A-NA-C1A	5.28	109.08	106.71
38	j	316	II0	C04-C10-C14	-5.28	115.18	122.63
40	c	310	KC2	C4C-C3C-C2C	-5.27	102.93	107.11
32	R	202	WVN	C38-C34-C33	-5.27	109.77	118.08
38	f	616	II0	C03-C09-C13	-5.27	115.19	122.63
40	k	611	KC2	CBA-CAA-C2A	-5.27	105.19	125.27
32	A	845	WVN	C38-C34-C33	-5.26	109.78	118.08
38	b	315	II0	C32-C30-C26	-5.26	111.30	126.58
32	B	847	WVN	C20-C13-C15	-5.26	108.72	121.46
38	J	103	II0	C38-C36-C34	-5.25	109.80	118.08
32	i	315	WVN	C14-C15-C13	-5.25	115.11	122.73
38	j	316	II0	C42-C40-C36	-5.25	119.82	127.31
29	B	826	CLA	C4A-NA-C1A	5.25	109.06	106.71
40	j	312	KC2	CHD-C1D-ND	-5.24	118.70	124.26
40	c	310	KC2	O2D-CGD-CBD	5.24	120.58	111.27
38	a	315	II0	C38-C36-C34	-5.24	109.82	118.08
32	K	103	WVN	C31-C32-C36	-5.24	110.90	118.94
38	k	615	II0	C28-C26-C24	-5.24	106.47	116.84
38	i	314	II0	C27-C25-C23	-5.23	106.48	116.84
32	L	201	WVN	C02-C05-C09	-5.23	115.04	121.47
38	l	315	II0	C04-C10-C14	-5.22	115.26	122.63
40	j	312	KC2	C1A-NA-C4A	-5.21	104.36	106.71
38	b	315	II0	C42-C40-C36	-5.21	119.88	127.31
38	d	317	II0	C33-C35-C39	-5.21	110.95	118.94
32	A	846	WVN	C14-C15-C13	-5.20	115.18	122.73
38	k	619	II0	C33-C35-C39	-5.20	110.96	118.94
38	i	314	II0	C28-C26-C24	-5.20	106.55	116.84
40	c	310	KC2	C2A-C1A-NA	5.19	117.73	109.40
40	e	309	KC2	C3C-C2C-C1C	-5.19	102.64	106.49
32	F	204	WVN	C33-C34-C37	-5.19	110.98	118.94
40	i	318	KC2	CHD-C1D-ND	-5.17	118.78	124.26
32	A	854	WVN	C31-C32-C36	-5.17	111.01	118.94
38	l	315	II0	C19-C13-C11	-5.17	104.78	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	L	201	WVN	C06-C13-C15	-5.16	115.34	122.61
38	b	301	II0	C33-C35-C39	-5.16	111.02	118.94
38	i	313	II0	C28-C26-C24	-5.15	106.64	116.84
38	l	315	II0	C38-C36-C34	-5.15	109.97	118.08
38	h	309	II0	C33-C35-C39	-5.15	111.05	118.94
38	h	309	II0	C31-C29-C25	-5.15	111.64	126.58
40	i	318	KC2	O2D-CGD-CBD	5.14	120.41	111.27
38	i	314	II0	C20-C14-C12	-5.14	104.83	114.36
40	k	611	KC2	CHD-C1D-ND	-5.14	118.81	124.26
32	F	204	WVN	C31-C32-C36	-5.14	111.06	118.94
40	g	313	KC2	CHD-C1D-ND	-5.14	118.82	124.26
40	f	611	KC2	CHD-C1D-ND	-5.13	118.82	124.26
32	s	405	WVN	C38-C34-C33	-5.13	109.99	118.08
40	s	404	KC2	C3B-C2B-C1B	-5.13	102.18	107.08
38	m	614	II0	C04-C10-C14	-5.13	115.39	122.63
40	g	313	KC2	O2D-CGD-CBD	5.13	120.38	111.27
40	c	310	KC2	C1A-NA-C4A	-5.12	104.40	106.71
40	g	313	KC2	C3D-C4D-ND	5.11	117.50	110.17
38	f	616	II0	C38-C36-C34	-5.11	110.02	118.08
32	A	844	WVN	C38-C34-C33	-5.11	110.03	118.08
38	g	319	II0	C38-C36-C34	-5.11	110.03	118.08
40	e	309	KC2	C4C-C3C-C2C	-5.10	103.06	107.11
38	k	615	II0	C31-C29-C25	-5.10	111.78	126.58
38	i	314	II0	C30-C32-C34	-5.09	107.34	123.22
38	l	315	II0	C03-C09-C13	-5.09	115.45	122.63
38	i	319	II0	C20-C14-C12	-5.08	104.95	114.36
38	g	317	II0	C38-C36-C34	-5.08	110.08	118.08
38	b	314	II0	C31-C29-C25	-5.07	111.85	126.58
40	g	315	KC2	CHD-C1D-ND	-5.07	118.89	124.26
40	k	611	KC2	C3D-C4D-ND	5.07	117.44	110.17
38	g	317	II0	C04-C10-C14	-5.07	115.47	122.63
40	d	311	KC2	C2A-C1A-NA	5.07	117.53	109.40
32	A	854	WVN	C02-C05-C09	-5.07	115.23	121.47
38	m	614	II0	C38-C36-C34	-5.07	110.09	118.08
40	j	312	KC2	C3D-C4D-ND	5.06	117.43	110.17
38	d	316	II0	C32-C30-C26	-5.06	111.88	126.58
29	b	304	CLA	C4A-NA-C1A	5.06	108.98	106.71
38	d	315	II0	C32-C30-C26	-5.06	111.89	126.58
30	A	841	PQN	C14-C13-C12	-5.05	110.71	123.68
32	K	103	WVN	C02-C05-C09	-5.05	115.25	121.47
38	m	615	II0	C28-C26-C24	-5.05	106.84	116.84
32	L	206	WVN	C19-C22-C26	-5.05	111.20	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	843	PQN	C14-C13-C12	-5.04	110.74	123.68
32	F	205	WVN	C06-C13-C15	-5.04	115.51	122.61
38	d	316	II0	C31-C29-C25	-5.04	111.95	126.58
38	b	315	II0	C37-C35-C33	-5.04	110.14	118.08
38	b	315	II0	C20-C14-C12	-5.04	105.03	114.36
38	b	315	II0	C12-C14-C10	-5.04	109.14	120.57
40	j	312	KC2	C3C-C2C-C1C	-5.03	102.76	106.49
32	F	205	WVN	C01-C02-C11	-5.02	106.35	112.70
32	L	205	WVN	C23-C25-C28	-5.02	111.24	118.94
38	f	614	II0	C31-C29-C25	-5.01	112.03	126.58
40	d	311	KC2	C3C-C2C-C1C	-5.01	102.77	106.49
38	f	618	II0	C28-C26-C24	-5.00	106.94	116.84
38	j	301	II0	C31-C29-C25	-5.00	112.07	126.58
40	e	309	KC2	C2A-C1A-NA	4.99	117.41	109.40
32	B	849	WVN	C06-C13-C15	-4.99	115.58	122.61
40	j	312	KC2	CHC-C1C-C2C	-4.99	117.19	124.98
40	i	318	KC2	C3C-C2C-C1C	-4.99	102.79	106.49
32	L	205	WVN	C38-C34-C33	-4.99	110.22	118.08
40	s	404	KC2	CHD-C1D-ND	-4.99	118.98	124.26
32	K	103	WVN	C20-C13-C15	-4.98	109.40	121.46
38	l	314	II0	C27-C25-C23	-4.98	106.98	116.84
40	i	310	KC2	C3D-C4D-ND	4.97	117.31	110.17
38	n	618	II0	C33-C35-C39	-4.97	111.31	118.94
40	g	313	KC2	C3C-C2C-C1C	-4.96	102.80	106.49
40	f	611	KC2	C3D-C4D-ND	4.96	117.29	110.17
32	F	207	WVN	C06-C13-C15	-4.96	115.63	122.61
38	d	317	II0	C20-C14-C12	-4.95	105.18	114.36
40	s	401	KC2	C3C-C2C-C1C	-4.95	102.81	106.49
32	A	845	WVN	C27-C25-C23	-4.95	110.28	118.08
38	k	620	II0	C31-C29-C25	-4.95	112.22	126.58
38	b	301	II0	C20-C14-C12	-4.94	105.20	114.36
32	I	101	WVN	C27-C25-C23	-4.94	110.30	118.08
38	h	310	II0	C30-C32-C34	-4.93	107.82	123.22
40	i	318	KC2	C2A-C1A-NA	4.93	117.31	109.40
38	d	301	II0	C38-C36-C34	-4.93	110.31	118.08
32	s	407	WVN	C23-C20-C13	-4.92	113.37	127.20
38	m	614	II0	C30-C32-C34	-4.92	107.85	123.22
40	m	611	KC2	C2A-C1A-NA	4.92	117.29	109.40
32	A	854	WVN	C27-C25-C23	-4.92	110.33	118.08
38	j	315	II0	C33-C35-C39	-4.91	111.40	118.94
38	k	620	II0	C04-C10-C14	-4.90	115.71	122.63
32	F	205	WVN	C02-C05-C09	-4.90	115.44	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	j	319	DGD	O3G-C3G-C2G	-4.90	99.09	110.90
40	i	310	KC2	C2A-C1A-NA	4.89	117.25	109.40
32	F	205	WVN	C38-C34-C33	-4.89	110.36	118.08
32	A	845	WVN	C20-C13-C15	-4.89	109.61	121.46
40	i	318	KC2	C3D-C4D-ND	4.89	117.18	110.17
40	f	611	KC2	C3C-C2C-C1C	-4.88	102.86	106.49
38	m	615	II0	C30-C32-C34	-4.87	108.01	123.22
38	n	616	II0	C31-C29-C25	-4.87	112.44	126.58
38	k	619	II0	C38-C36-C34	-4.87	110.41	118.08
32	i	315	WVN	C27-C25-C23	-4.87	110.41	118.08
32	i	315	WVN	C28-C30-C33	-4.87	108.03	123.22
40	j	312	KC2	O2D-CGD-CBD	4.86	119.91	111.27
32	L	206	WVN	C23-C20-C13	-4.86	113.55	127.20
32	A	844	WVN	C21-C15-C14	-4.86	104.28	113.62
32	R	201	WVN	C28-C30-C33	-4.86	108.05	123.22
40	e	309	KC2	CHC-C1C-C2C	-4.86	117.39	124.98
40	g	313	KC2	C2A-C1A-NA	4.85	117.19	109.40
38	f	618	II0	C38-C36-C34	-4.85	110.44	118.08
38	g	317	II0	C27-C25-C23	-4.84	107.25	116.84
40	g	314	KC2	CHC-C1C-C2C	-4.84	117.42	124.98
32	R	201	WVN	C38-C34-C33	-4.84	110.45	118.08
40	n	611	KC2	C1A-NA-C4A	-4.84	104.53	106.71
38	b	315	II0	C33-C35-C39	-4.83	111.53	118.94
38	b	301	II0	C31-C29-C25	-4.83	112.56	126.58
38	j	315	II0	C38-C36-C34	-4.83	110.47	118.08
38	a	317	II0	C31-C29-C25	-4.83	112.57	126.58
38	n	615	II0	C03-C09-C13	-4.82	115.83	122.63
32	J	101	WVN	C31-C32-C36	-4.82	111.54	118.94
32	e	315	WVN	C38-C34-C33	-4.82	110.48	118.08
32	M	101	WVN	C35-C32-C31	-4.82	110.48	118.08
38	h	310	II0	C33-C35-C39	-4.81	111.56	118.94
32	K	103	WVN	C23-C20-C13	-4.81	113.70	127.20
32	M	101	WVN	C20-C13-C15	-4.81	109.82	121.46
32	J	101	WVN	C23-C25-C28	-4.80	111.58	118.94
40	n	611	KC2	C3D-C4D-ND	4.79	117.05	110.17
40	f	611	KC2	C2A-C1A-NA	4.79	117.09	109.40
38	a	313	II0	C19-C13-C11	-4.79	105.49	114.36
29	B	819	CLA	C4A-NA-C1A	4.78	108.86	106.71
38	e	313	II0	C31-C29-C25	-4.78	112.70	126.58
40	d	311	KC2	O2D-CGD-CBD	4.78	119.75	111.27
40	s	404	KC2	C3C-C2C-C1C	-4.77	102.95	106.49
40	n	611	KC2	C2A-C1A-NA	4.75	117.03	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	615	II0	C20-C14-C12	-4.75	105.56	114.36
38	d	315	II0	C12-C14-C10	-4.75	109.79	120.57
38	b	301	II0	C03-C09-C13	-4.75	115.93	122.63
38	i	319	II0	C12-C14-C10	-4.74	109.80	120.57
38	d	315	II0	C20-C14-C12	-4.74	105.57	114.36
38	J	103	II0	C31-C29-C25	-4.74	112.82	126.58
40	l	311	KC2	C2C-C1C-NC	4.74	115.75	110.57
38	d	315	II0	C17-C04-C10	4.74	117.99	110.47
40	s	401	KC2	CHD-C1D-ND	-4.74	119.24	124.26
38	l	314	II0	C31-C29-C25	-4.73	112.84	126.58
38	e	314	II0	C32-C30-C26	-4.73	112.84	126.58
32	L	201	WVN	C23-C25-C28	-4.73	111.68	118.94
40	d	311	KC2	CBA-CAA-C2A	-4.73	107.24	125.27
40	m	611	KC2	CHC-C1C-C2C	-4.72	117.60	124.98
38	k	616	II0	C11-C13-C09	-4.72	109.85	120.57
38	h	311	II0	C31-C29-C25	-4.72	112.88	126.58
32	B	849	WVN	C27-C25-C23	-4.72	110.64	118.08
40	l	311	KC2	CHD-C1D-ND	-4.71	119.27	124.26
38	n	615	II0	C38-C36-C34	-4.71	110.66	118.08
40	g	313	KC2	CHC-C1C-C2C	-4.71	117.62	124.98
32	M	101	WVN	C23-C20-C13	-4.71	113.98	127.20
40	n	611	KC2	CBA-CAA-C2A	-4.71	107.32	125.27
40	g	315	KC2	C2A-C1A-NA	4.71	116.95	109.40
32	J	101	WVN	C20-C13-C15	-4.70	110.08	121.46
38	h	310	II0	C38-C36-C34	-4.70	110.67	118.08
40	s	401	KC2	C2A-C1A-NA	4.70	116.94	109.40
38	g	318	II0	C27-C25-C23	-4.70	107.53	116.84
40	s	401	KC2	C3D-C4D-ND	4.69	116.90	110.17
38	f	618	II0	C31-C29-C25	-4.69	112.96	126.58
32	B	846	WVN	C21-C15-C14	-4.69	104.61	113.62
40	g	315	KC2	C3C-C2C-C1C	-4.69	103.01	106.49
32	B	847	WVN	C33-C34-C37	-4.69	111.75	118.94
38	a	314	II0	C31-C29-C25	-4.69	112.97	126.58
40	j	312	KC2	C2C-C1C-NC	4.69	115.69	110.57
38	i	314	II0	C04-C10-C14	-4.68	116.03	122.63
32	l	316	WVN	C14-C15-C13	-4.67	115.95	122.73
38	f	615	II0	C28-C26-C24	-4.67	107.59	116.84
38	g	318	II0	C04-C10-C14	-4.67	116.04	122.63
32	e	315	WVN	C28-C30-C33	-4.66	108.67	123.22
32	A	846	WVN	C31-C32-C36	-4.66	111.79	118.94
32	B	845	WVN	C20-C23-C25	-4.66	119.19	126.23
38	k	616	II0	C27-C25-C23	-4.66	107.61	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	l	311	KC2	CHC-C1C-C2C	-4.66	117.70	124.98
38	h	309	II0	C03-C09-C13	-4.65	116.06	122.63
38	f	618	II0	C04-C10-C14	-4.65	116.06	122.63
29	R	203	CLA	CAA-C2A-C3A	-4.65	100.05	112.78
29	B	833	CLA	C4A-NA-C1A	4.65	108.80	106.71
38	l	315	II0	C27-C25-C23	-4.64	107.65	116.84
38	i	319	II0	C28-C26-C24	-4.64	107.65	116.84
32	R	201	WVN	C14-C15-C13	-4.64	116.00	122.73
38	b	301	II0	C04-C10-C14	-4.63	116.09	122.63
38	j	316	II0	C31-C29-C25	-4.63	113.13	126.58
40	g	314	KC2	CBA-CAA-C2A	-4.63	107.61	125.27
38	l	315	II0	C16-C03-C09	4.63	117.82	110.47
40	m	611	KC2	C2C-C1C-NC	4.63	115.63	110.57
38	b	301	II0	C28-C26-C24	-4.63	107.67	116.84
38	k	620	II0	C30-C32-C34	-4.63	108.77	123.22
32	L	205	WVN	C31-C32-C36	-4.62	111.85	118.94
38	a	317	II0	C38-C36-C34	-4.62	110.80	118.08
32	l	316	WVN	C16-C05-C09	-4.61	105.92	122.33
40	f	611	KC2	CHC-C1C-C2C	-4.61	117.77	124.98
32	R	201	WVN	C31-C32-C36	-4.61	111.86	118.94
38	g	318	II0	C28-C26-C24	-4.61	107.71	116.84
38	f	614	II0	C27-C25-C23	-4.61	107.71	116.84
32	F	204	WVN	C23-C25-C28	-4.61	111.87	118.94
38	e	314	II0	C19-C13-C11	-4.61	105.82	114.36
32	B	846	WVN	C06-C13-C15	-4.60	116.13	122.61
38	J	103	II0	C33-C35-C39	-4.60	111.88	118.94
32	h	308	WVN	C20-C13-C15	-4.60	110.33	121.46
38	i	316	II0	C32-C30-C26	-4.59	113.24	126.58
32	l	316	WVN	C31-C32-C36	-4.59	111.90	118.94
32	l	316	WVN	C24-C22-C19	-4.59	110.85	118.08
32	A	854	WVN	C14-C15-C13	-4.59	116.07	122.73
38	d	317	II0	C32-C30-C26	-4.58	113.28	126.58
40	e	309	KC2	O2D-CGD-CBD	4.58	119.40	111.27
32	K	103	WVN	C16-C05-C09	-4.58	106.05	122.33
40	s	401	KC2	CBC-CAC-C3C	-4.58	104.85	127.62
38	d	315	II0	C33-C35-C39	-4.57	111.92	118.94
40	s	404	KC2	C2C-C1C-NC	4.57	115.56	110.57
38	d	301	II0	C32-C30-C26	-4.57	113.30	126.58
40	k	611	KC2	C2A-C1A-NA	4.57	116.73	109.40
38	m	618	II0	C06-C04-C10	4.57	118.88	109.62
38	m	618	II0	C31-C29-C25	-4.57	113.32	126.58
40	m	611	KC2	C3C-C2C-C1C	-4.56	103.10	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	g	315	KC2	C1A-NA-C4A	-4.56	104.66	106.71
38	f	615	II0	C04-C10-C14	-4.55	116.21	122.63
38	i	313	II0	C33-C35-C39	-4.55	111.96	118.94
38	m	618	II0	C04-C10-C14	-4.55	116.21	122.63
38	a	313	II0	C38-C36-C34	-4.54	110.92	118.08
40	g	315	KC2	C3D-C4D-ND	4.54	116.68	110.17
40	g	314	KC2	C2C-C1C-NC	4.54	115.53	110.57
38	j	316	II0	C28-C26-C24	-4.53	107.86	116.84
32	F	207	WVN	C23-C20-C13	-4.53	114.49	127.20
38	a	315	II0	C33-C35-C39	-4.52	112.00	118.94
32	B	848	WVN	C23-C20-C13	-4.52	114.51	127.20
40	l	311	KC2	C3D-C4D-ND	4.51	116.63	110.17
32	l	302	WVN	C14-C15-C13	-4.51	116.19	122.73
32	L	205	WVN	C23-C20-C13	-4.50	114.55	127.20
38	a	313	II0	C30-C32-C34	-4.50	109.16	123.22
38	j	316	II0	C30-C32-C34	-4.50	109.16	123.22
38	f	615	II0	C30-C32-C34	-4.50	109.18	123.22
32	A	847	WVN	C28-C30-C33	-4.50	109.18	123.22
32	J	101	WVN	C33-C34-C37	-4.50	112.04	118.94
38	i	313	II0	C31-C29-C25	-4.50	113.53	126.58
38	k	619	II0	C19-C13-C11	-4.49	106.03	114.36
38	d	301	II0	C04-C10-C14	-4.49	116.29	122.63
40	e	309	KC2	C2C-C1C-NC	4.49	115.47	110.57
40	g	313	KC2	C2C-C1C-NC	4.49	115.47	110.57
38	d	301	II0	C30-C32-C34	-4.49	109.21	123.22
40	g	313	KC2	CBC-CAC-C3C	-4.49	105.29	127.62
38	e	312	II0	C31-C29-C25	-4.49	113.56	126.58
40	s	404	KC2	CHC-C1C-C2C	-4.48	117.98	124.98
32	L	201	WVN	C16-C05-C09	-4.48	106.39	122.33
38	j	301	II0	C30-C32-C34	-4.48	109.23	123.22
38	a	313	II0	C31-C29-C25	-4.48	113.57	126.58
32	l	316	WVN	C23-C25-C28	-4.47	112.08	118.94
38	g	318	II0	C31-C29-C25	-4.47	113.61	126.58
32	B	849	WVN	C28-C30-C33	-4.46	109.30	123.22
40	f	611	KC2	C2C-C1C-NC	4.46	115.44	110.57
32	e	315	WVN	C16-C05-C09	-4.45	106.49	122.33
32	h	308	WVN	C16-C05-C09	-4.44	106.52	122.33
40	k	611	KC2	C3C-C2C-C1C	-4.44	103.19	106.49
32	A	844	WVN	C06-C13-C15	-4.44	116.36	122.61
38	n	615	II0	C31-C29-C25	-4.44	113.69	126.58
38	m	615	II0	C31-C29-C25	-4.44	113.70	126.58
40	i	310	KC2	CBC-CAC-C3C	-4.43	105.56	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	I	101	WVN	C31-C32-C36	-4.43	112.14	118.94
40	f	611	KC2	CBC-CAC-C3C	-4.42	105.63	127.62
38	h	309	II0	C19-C13-C11	-4.42	106.17	114.36
38	b	315	II0	C38-C36-C34	-4.42	111.11	118.08
32	l	302	WVN	C28-C30-C33	-4.42	109.43	123.22
40	l	311	KC2	C2A-C1A-NA	4.42	116.48	109.40
32	A	844	WVN	C23-C20-C13	-4.41	114.80	127.20
40	l	311	KC2	CBA-CAA-C2A	-4.41	108.45	125.27
38	n	618	II0	C04-C10-C14	-4.41	116.40	122.63
40	s	404	KC2	C3D-C4D-ND	4.41	116.50	110.17
38	J	103	II0	C28-C26-C24	-4.41	108.10	116.84
38	h	311	II0	C19-C13-C11	-4.41	106.19	114.36
32	h	308	WVN	C28-C30-C33	-4.41	109.47	123.22
38	f	616	II0	C30-C32-C34	-4.40	109.48	123.22
38	g	317	II0	C19-C13-C11	-4.40	106.20	114.36
38	a	314	II0	C28-C26-C24	-4.40	108.13	116.84
32	A	845	WVN	C31-C32-C36	-4.40	112.19	118.94
40	n	611	KC2	C2C-C1C-NC	4.39	115.37	110.57
38	l	314	II0	C04-C10-C14	-4.39	116.43	122.63
38	m	615	II0	C27-C25-C23	-4.39	108.14	116.84
32	i	315	WVN	C16-C05-C09	-4.39	106.71	122.33
32	A	847	WVN	C16-C05-C09	-4.39	106.72	122.33
38	a	313	II0	C27-C25-C23	-4.39	108.15	116.84
40	i	318	KC2	C2C-C1C-NC	4.38	115.36	110.57
38	c	313	II0	C28-C26-C24	-4.38	108.16	116.84
38	k	620	II0	C33-C35-C39	-4.38	112.22	118.94
32	F	207	WVN	C23-C25-C28	-4.38	112.22	118.94
40	c	310	KC2	CBC-CAC-C3C	-4.37	105.88	127.62
32	F	207	WVN	C16-C05-C09	-4.37	106.80	122.33
32	h	308	WVN	C06-C13-C15	-4.37	116.46	122.61
38	f	616	II0	C33-C35-C39	-4.36	112.25	118.94
38	e	313	II0	C06-C04-C10	4.36	118.46	109.62
38	m	616	II0	C33-C35-C39	-4.36	112.25	118.94
31	s	408	LHG	O3-P-O6	-4.36	95.14	106.73
38	m	618	II0	C33-C35-C39	-4.36	112.26	118.94
32	B	847	WVN	C06-C13-C15	-4.36	116.48	122.61
32	B	849	WVN	C31-C32-C36	-4.35	112.26	118.94
40	g	315	KC2	O2D-CGD-CBD	4.35	119.00	111.27
32	J	101	WVN	C16-C05-C09	-4.35	106.85	122.33
38	m	616	II0	C31-C29-C25	-4.35	113.94	126.58
32	F	204	WVN	C16-C05-C09	-4.35	106.85	122.33
32	F	204	WVN	C28-C30-C33	-4.35	109.64	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	s	407	WVN	C31-C32-C36	-4.35	112.27	118.94
38	b	314	II0	C30-C32-C34	-4.34	109.66	123.22
40	g	314	KC2	C3D-C4D-ND	4.34	116.40	110.17
32	R	201	WVN	C23-C20-C13	-4.34	115.01	127.20
40	g	314	KC2	C2A-C1A-NA	4.34	116.36	109.40
38	k	616	II0	C31-C29-C25	-4.34	113.98	126.58
40	e	309	KC2	CBC-CAC-C3C	-4.34	106.03	127.62
38	d	315	II0	C03-C09-C13	-4.34	116.51	122.63
38	e	314	II0	C03-C09-C13	-4.34	116.51	122.63
32	B	848	WVN	C28-C30-C33	-4.34	109.69	123.22
32	i	315	WVN	C38-C34-C33	-4.33	111.25	118.08
38	e	312	II0	C03-C09-C13	-4.33	116.52	122.63
40	c	310	KC2	CAA-CBA-CGA	-4.33	105.02	127.26
38	d	316	II0	C03-C09-C13	-4.33	116.52	122.63
32	B	847	WVN	C23-C25-C28	-4.32	112.31	118.94
38	l	313	II0	C27-C25-C23	-4.32	108.28	116.84
38	f	618	II0	C06-C04-C10	4.32	118.37	109.62
38	n	616	II0	C11-C13-C09	-4.31	110.78	120.57
29	B	827	CLA	CMB-C2B-C1B	-4.31	118.81	125.37
38	m	615	II0	C04-C10-C14	-4.31	116.55	122.63
38	l	315	II0	C31-C29-C25	-4.31	114.07	126.58
38	g	317	II0	C05-C03-C09	4.30	118.34	109.62
38	a	314	II0	C27-C25-C23	-4.30	108.32	116.84
38	i	314	II0	C31-C29-C25	-4.30	114.09	126.58
40	s	404	KC2	CMA-C3A-C2A	-4.30	117.78	128.30
38	m	615	II0	C42-C40-C36	-4.30	121.18	127.31
38	n	615	II0	C30-C32-C34	-4.30	109.81	123.22
38	n	616	II0	C20-C14-C12	-4.29	106.40	114.36
38	l	314	II0	C28-C26-C24	-4.29	108.34	116.84
38	k	615	II0	C12-C14-C10	-4.29	110.83	120.57
40	m	611	KC2	CBC-CAC-C3C	-4.29	106.28	127.62
38	k	615	II0	C04-C10-C14	-4.28	116.58	122.63
32	J	101	WVN	C28-C30-C33	-4.28	109.85	123.22
32	F	205	WVN	C19-C22-C26	-4.28	112.37	118.94
38	d	315	II0	C27-C25-C23	-4.28	108.36	116.84
40	e	309	KC2	C1A-NA-C4A	-4.28	104.78	106.71
40	i	310	KC2	CBA-CAA-C2A	-4.28	108.97	125.27
38	j	315	II0	C32-C30-C26	-4.27	114.17	126.58
32	B	847	WVN	C14-C15-C13	-4.27	116.53	122.73
38	n	618	II0	C32-C30-C26	-4.26	114.20	126.58
40	d	311	KC2	C1A-NA-C4A	-4.26	104.79	106.71
32	h	308	WVN	C14-C15-C13	-4.26	116.55	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	615	II0	C03-C09-C13	-4.26	116.62	122.63
32	L	205	WVN	C16-C05-C09	-4.25	107.20	122.33
38	c	313	II0	C19-C13-C11	-4.25	106.48	114.36
32	A	846	WVN	C16-C05-C09	-4.25	107.21	122.33
32	F	204	WVN	C20-C13-C15	-4.25	111.17	121.46
38	J	103	II0	C30-C32-C34	-4.25	109.96	123.22
31	A	848	LHG	O4-P-O5	4.25	133.23	112.24
38	d	317	II0	C31-C29-C25	-4.24	114.26	126.58
31	a	301	LHG	O4-P-O5	4.24	133.20	112.24
40	m	611	KC2	C1D-CHD-C4C	-4.24	116.28	126.34
40	s	404	KC2	C4B-C3B-C2B	-4.24	103.27	106.75
38	l	313	II0	C34-C36-C40	-4.24	112.44	118.94
38	b	315	II0	C19-C13-C11	-4.24	106.51	114.36
38	i	319	II0	C31-C29-C25	-4.23	114.29	126.58
38	n	615	II0	C19-C13-C11	-4.23	106.51	114.36
38	m	618	II0	C20-C14-C12	-4.23	106.51	114.36
32	A	845	WVN	C23-C20-C13	-4.23	115.32	127.20
40	s	401	KC2	C1A-NA-C4A	-4.23	104.81	106.71
40	i	318	KC2	CBC-CAC-C3C	-4.23	106.59	127.62
40	i	310	KC2	CHC-C1C-C2C	-4.22	118.38	124.98
40	n	611	KC2	C3C-C2C-C1C	-4.22	103.35	106.49
31	c	320	LHG	O4-P-O5	4.22	133.12	112.24
38	f	615	II0	C31-C29-C25	-4.22	114.32	126.58
32	l	302	WVN	C24-C22-C19	-4.22	111.43	118.08
32	A	854	WVN	C16-C05-C09	-4.22	107.33	122.33
38	a	317	II0	C33-C35-C39	-4.22	112.47	118.94
40	g	315	KC2	C2C-C1C-NC	4.22	115.17	110.57
32	B	847	WVN	C28-C30-C33	-4.21	110.07	123.22
31	i	317	LHG	O4-P-O5	4.21	133.06	112.24
31	J	104	LHG	O4-P-O5	4.21	133.04	112.24
31	a	318	LHG	O4-P-O5	4.20	133.01	112.24
38	m	615	II0	C33-C35-C39	-4.20	112.50	118.94
31	L	209	LHG	O4-P-O5	4.20	132.99	112.24
31	n	619	LHG	O4-P-O5	4.20	132.99	112.24
38	n	616	II0	C30-C32-C34	-4.20	110.12	123.22
40	n	611	KC2	O2D-CGD-CBD	4.20	118.72	111.27
40	g	315	KC2	CHC-C1C-C2C	-4.19	118.43	124.98
40	s	401	KC2	C2C-C1C-NC	4.19	115.15	110.57
31	m	619	LHG	O4-P-O5	4.19	132.96	112.24
32	A	854	WVN	C20-C13-C15	-4.19	111.31	121.46
38	d	315	II0	C04-C10-C14	-4.19	116.72	122.63
38	m	614	II0	C19-C13-C11	-4.19	106.59	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	301	LHG	O4-P-O5	4.19	132.94	112.24
38	m	614	II0	C27-C25-C23	-4.18	108.55	116.84
32	I	101	WVN	C28-C30-C33	-4.18	110.16	123.22
40	s	404	KC2	C2A-C1A-NA	4.18	116.11	109.40
32	h	308	WVN	C31-C32-C36	-4.18	112.52	118.94
38	k	619	II0	C28-C26-C24	-4.18	108.56	116.84
31	l	318	LHG	O4-P-O5	4.18	132.91	112.24
38	e	314	II0	C30-C32-C34	-4.18	110.17	123.22
35	A	853	SQD	O7-S-C6	4.18	111.91	106.94
31	f	620	LHG	O4-P-O5	4.18	132.90	112.24
38	a	317	II0	C04-C10-C14	-4.18	116.73	122.63
40	k	611	KC2	CHC-C1C-C2C	-4.18	118.45	124.98
31	L	208	LHG	O4-P-O5	4.17	132.88	112.24
32	L	201	WVN	C23-C20-C13	-4.17	115.48	127.20
35	A	853	SQD	O47-C7-C8	4.17	120.50	111.50
31	f	619	LHG	O4-P-O5	4.17	132.87	112.24
40	m	611	KC2	C1A-NA-C4A	-4.17	104.83	106.71
31	b	318	LHG	O4-P-O5	4.17	132.87	112.24
40	d	311	KC2	C1D-CHD-C4C	-4.17	116.44	126.34
31	j	318	LHG	O4-P-O5	4.17	132.85	112.24
40	d	311	KC2	C2C-C1C-NC	4.16	115.12	110.57
38	m	616	II0	C27-C25-C23	-4.16	108.59	116.84
31	A	842	LHG	O4-P-O5	4.16	132.82	112.24
32	B	848	WVN	C20-C13-C15	-4.16	111.38	121.46
32	F	205	WVN	C33-C34-C37	-4.16	112.56	118.94
31	e	317	LHG	O4-P-O5	4.16	132.81	112.24
31	c	316	LHG	O4-P-O5	4.16	132.80	112.24
38	m	615	II0	C05-C03-C09	4.15	118.04	109.62
38	d	316	II0	C04-C10-C14	-4.15	116.77	122.63
40	g	315	KC2	CBA-CAA-C2A	-4.15	109.44	125.27
38	i	313	II0	C06-C04-C10	4.15	118.04	109.62
32	M	101	WVN	C28-C30-C33	-4.15	110.26	123.22
40	f	611	KC2	CBA-CAA-C2A	-4.15	109.44	125.27
31	g	322	LHG	O4-P-O5	4.15	132.76	112.24
40	s	401	KC2	CHC-C1C-C2C	-4.15	118.50	124.98
38	b	301	II0	C30-C32-C34	-4.15	110.27	123.22
31	A	843	LHG	O4-P-O5	4.15	132.75	112.24
32	i	315	WVN	C31-C32-C36	-4.15	112.58	118.94
32	F	205	WVN	C23-C20-C13	-4.14	115.56	127.20
40	n	611	KC2	C1D-CHD-C4C	-4.14	116.52	126.34
32	l	302	WVN	C06-C13-C15	-4.14	116.79	122.61
38	m	618	II0	C27-C25-C23	-4.13	108.65	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	d	311	KC2	CBC-CAC-C3C	-4.13	107.06	127.62
40	c	310	KC2	C3C-C2C-C1C	-4.13	103.42	106.49
38	m	614	II0	C20-C14-C12	-4.13	106.71	114.36
38	j	315	II0	C30-C32-C34	-4.12	110.37	123.22
32	e	315	WVN	C31-C32-C36	-4.11	112.63	118.94
38	c	313	II0	C27-C25-C23	-4.11	108.69	116.84
38	g	319	II0	C33-C35-C39	-4.11	112.64	118.94
38	i	319	II0	C33-C35-C39	-4.10	112.64	118.94
38	k	615	II0	C32-C30-C26	-4.10	114.66	126.58
38	m	614	II0	C31-C29-C25	-4.10	114.67	126.58
40	n	611	KC2	CHC-C1C-C2C	-4.10	118.57	124.98
32	s	407	WVN	C33-C34-C37	-4.10	112.65	118.94
40	i	318	KC2	C1A-NA-C4A	-4.10	104.86	106.71
38	b	315	II0	C28-C26-C24	-4.10	108.72	116.84
40	i	318	KC2	CBA-CAA-C2A	-4.10	109.66	125.27
40	m	611	KC2	O2D-CGD-CBD	4.09	118.54	111.27
36	B	844	DGD	O6D-C1D-O3G	-4.09	100.28	109.97
32	e	315	WVN	C21-C15-C14	-4.09	105.75	113.62
38	l	315	II0	C32-C30-C26	-4.09	114.71	126.58
38	f	615	II0	C33-C35-C39	-4.09	112.67	118.94
40	j	312	KC2	CBC-CAC-C3C	-4.08	107.30	127.62
32	F	205	WVN	C10-C06-C13	4.08	116.77	110.48
40	g	313	KC2	C4B-C3B-C2B	-4.08	103.40	106.75
38	h	310	II0	C27-C25-C23	-4.08	108.76	116.84
38	k	616	II0	C33-C35-C39	-4.08	112.68	118.94
35	A	853	SQD	C4-C3-C2	4.08	117.94	110.82
32	L	201	WVN	C14-C15-C13	-4.08	116.81	122.73
38	n	618	II0	C03-C09-C13	-4.08	116.88	122.63
38	g	317	II0	C32-C30-C26	-4.07	114.76	126.58
38	h	309	II0	C29-C31-C33	-4.07	110.51	123.22
38	e	314	II0	C31-C29-C25	-4.07	114.76	126.58
40	k	611	KC2	CBC-CAC-C3C	-4.07	107.37	127.62
38	f	615	II0	C27-C25-C23	-4.07	108.78	116.84
38	n	616	II0	C28-C26-C24	-4.06	108.79	116.84
38	f	614	II0	C32-C30-C26	-4.06	114.78	126.58
38	a	313	II0	C33-C35-C39	-4.06	112.71	118.94
38	d	315	II0	C28-C26-C24	-4.06	108.80	116.84
38	j	301	II0	C27-C25-C23	-4.06	108.80	116.84
40	g	314	KC2	CHD-C1D-ND	-4.06	119.96	124.26
32	I	101	WVN	C16-C05-C09	-4.05	107.91	122.33
38	m	616	II0	C20-C14-C12	-4.05	106.85	114.36
38	i	313	II0	C27-C25-C23	-4.05	108.82	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	618	II0	C20-C14-C12	-4.05	106.85	114.36
32	R	202	WVN	C28-C30-C33	-4.05	110.59	123.22
38	k	616	II0	C38-C36-C34	-4.05	111.70	118.08
38	d	316	II0	C06-C08-C12	4.05	115.84	110.30
40	j	312	KC2	C1D-CHD-C4C	-4.04	116.76	126.34
40	i	318	KC2	C1D-CHD-C4C	-4.03	116.77	126.34
32	A	845	WVN	C01-C02-C11	-4.03	107.60	112.70
32	s	405	WVN	C24-C22-C19	-4.03	111.72	118.08
32	M	101	WVN	C06-C13-C15	-4.03	116.94	122.61
38	k	619	II0	C27-C25-C23	-4.03	108.86	116.84
35	A	853	SQD	C1-O5-C5	4.03	121.60	113.69
38	n	615	II0	C28-C26-C24	-4.03	108.86	116.84
38	h	311	II0	C33-C35-C39	-4.03	112.76	118.94
29	m	612	CLA	CAA-C2A-C3A	-4.02	101.76	112.78
32	I	101	WVN	C02-C05-C09	-4.02	116.52	121.47
32	A	845	WVN	C26-C29-C31	-4.02	110.68	123.22
40	l	311	KC2	C4B-C3B-C2B	-4.01	103.46	106.75
38	c	313	II0	C31-C29-C25	-4.01	114.93	126.58
40	j	312	KC2	CBA-CAA-C2A	-4.01	110.00	125.27
38	m	618	II0	C28-C26-C24	-4.01	108.90	116.84
38	g	318	II0	C06-C04-C10	4.01	117.74	109.62
32	s	405	WVN	C31-C32-C36	-4.00	112.80	118.94
32	R	202	WVN	C31-C32-C36	-3.99	112.81	118.94
38	k	619	II0	C04-C10-C14	-3.99	116.99	122.63
38	l	315	II0	C20-C14-C12	-3.99	106.97	114.36
38	b	301	II0	C32-C30-C26	-3.99	115.00	126.58
38	k	615	II0	C29-C31-C33	-3.99	110.78	123.22
38	i	316	II0	C04-C10-C14	-3.99	117.01	122.63
38	l	313	II0	C31-C29-C25	-3.99	115.01	126.58
29	B	829	CLA	CAA-C2A-C3A	-3.98	101.87	112.78
38	f	615	II0	C20-C14-C12	-3.98	106.98	114.36
38	g	318	II0	C33-C35-C39	-3.98	112.83	118.94
38	a	317	II0	C05-C03-C09	3.98	117.69	109.62
38	a	317	II0	C06-C04-C10	3.97	117.67	109.62
38	d	317	II0	C27-C25-C23	-3.97	108.97	116.84
38	g	319	II0	C30-C32-C34	-3.97	110.82	123.22
38	a	313	II0	C28-C26-C24	-3.97	108.98	116.84
38	l	313	II0	C28-C26-C24	-3.97	108.98	116.84
38	n	615	II0	C20-C14-C12	-3.97	107.00	114.36
32	L	206	WVN	C38-C34-C33	-3.97	111.82	118.08
38	l	313	II0	C32-C30-C26	-3.97	115.06	126.58
38	a	317	II0	C28-C26-C24	-3.96	109.00	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	j	316	II0	C20-C14-C12	-3.96	107.02	114.36
38	i	316	II0	C31-C29-C25	-3.96	115.09	126.58
32	B	849	WVN	C16-C05-C09	-3.96	108.26	122.33
38	i	313	II0	C32-C30-C26	-3.96	115.10	126.58
40	i	310	KC2	C3C-C2C-C1C	-3.95	103.55	106.49
38	a	313	II0	C03-C09-C13	-3.95	117.05	122.63
38	k	616	II0	C28-C26-C24	-3.95	109.01	116.84
38	l	315	II0	C06-C04-C10	3.95	117.63	109.62
38	b	315	II0	C27-C25-C23	-3.95	109.02	116.84
38	l	314	II0	C20-C14-C12	-3.95	107.04	114.36
38	i	316	II0	C27-C25-C23	-3.95	109.02	116.84
38	d	316	II0	C28-C26-C24	-3.94	109.03	116.84
38	d	301	II0	C19-C13-C11	-3.94	107.05	114.36
40	c	310	KC2	CAA-C2A-C1A	-3.94	106.65	124.75
29	n	604	CLA	CAA-C2A-C3A	-3.94	102.00	112.78
32	L	205	WVN	C06-C13-C15	-3.93	117.07	122.61
32	B	849	WVN	C20-C13-C15	-3.93	111.94	121.46
38	l	315	II0	C19-C13-C09	-3.93	119.01	124.35
32	B	845	WVN	C23-C20-C13	3.93	138.24	127.20
32	L	206	WVN	C31-C32-C36	-3.93	112.92	118.94
38	n	618	II0	C31-C29-C25	-3.93	115.18	126.58
38	m	615	II0	C20-C14-C12	-3.93	107.08	114.36
32	I	101	WVN	C33-C34-C37	-3.92	112.92	118.94
38	h	311	II0	C20-C14-C12	-3.92	107.09	114.36
38	n	618	II0	C28-C26-C24	-3.92	109.08	116.84
40	f	611	KC2	C1A-NA-C4A	-3.92	104.94	106.71
38	g	317	II0	C20-C14-C12	-3.92	107.10	114.36
32	h	308	WVN	C02-C05-C09	-3.91	116.66	121.47
32	B	847	WVN	C24-C22-C19	-3.91	111.92	118.08
32	A	845	WVN	C28-C30-C33	-3.91	111.02	123.22
38	b	317	II0	C05-C07-C11	3.91	115.65	110.30
40	d	312	KC2	CHD-C1D-ND	-3.91	120.12	124.26
32	B	848	WVN	C10-C06-C13	3.90	116.49	110.48
40	l	311	KC2	C1D-CHD-C4C	-3.90	117.08	126.34
38	b	314	II0	C19-C13-C11	-3.90	107.12	114.36
38	n	615	II0	C32-C30-C26	-3.90	115.25	126.58
32	B	848	WVN	C38-C34-C33	-3.90	111.93	118.08
32	A	844	WVN	C20-C13-C15	-3.90	112.01	121.46
40	e	309	KC2	CBA-CAA-C2A	-3.90	110.40	125.27
38	k	615	II0	C33-C35-C39	-3.90	112.96	118.94
38	l	315	II0	C11-C13-C09	-3.90	111.73	120.57
38	a	317	II0	C27-C25-C23	-3.90	109.12	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	311	II0	C27-C25-C23	-3.90	109.12	116.84
40	i	318	KC2	CHC-C1C-C2C	-3.89	118.89	124.98
29	A	832	CLA	O2D-CGD-O1D	-3.89	116.22	123.84
38	d	315	II0	C20-C14-C10	-3.89	119.06	124.35
38	d	317	II0	C28-C26-C24	-3.89	109.13	116.84
36	j	319	DGD	C1E-O6E-C5E	3.89	121.31	113.69
40	n	611	KC2	CBC-CAC-C3C	-3.88	108.30	127.62
32	M	101	WVN	C16-C05-C09	-3.88	108.54	122.33
38	l	313	II0	C33-C35-C39	-3.87	113.00	118.94
40	i	310	KC2	C1D-CHD-C4C	-3.87	117.15	126.34
32	B	848	WVN	C26-C29-C31	-3.87	111.14	123.22
32	F	207	WVN	C20-C13-C15	-3.87	112.09	121.46
38	g	317	II0	C28-C26-C24	-3.87	109.18	116.84
40	f	611	KC2	C1D-CHD-C4C	-3.87	117.17	126.34
38	i	313	II0	C30-C32-C34	-3.86	111.16	123.22
32	F	204	WVN	C23-C20-C13	-3.86	116.35	127.20
32	J	101	WVN	C23-C20-C13	-3.86	116.36	127.20
32	B	849	WVN	C23-C20-C13	-3.86	116.36	127.20
40	c	310	KC2	CBA-CAA-C2A	-3.86	110.55	125.27
29	s	403	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
40	k	611	KC2	C1A-NA-C4A	-3.86	104.97	106.71
38	b	314	II0	C20-C14-C12	-3.85	107.22	114.36
32	L	205	WVN	C24-C22-C19	-3.85	112.01	118.08
38	k	619	II0	C20-C14-C12	-3.85	107.22	114.36
32	A	844	WVN	C31-C32-C36	-3.85	113.04	118.94
40	l	311	KC2	CBC-CAC-C3C	-3.84	108.50	127.62
32	A	854	WVN	C23-C20-C13	-3.84	116.41	127.20
40	e	309	KC2	C1D-CHD-C4C	-3.84	117.23	126.34
32	M	101	WVN	C31-C32-C36	-3.84	113.05	118.94
32	B	846	WVN	C26-C29-C31	-3.84	111.24	123.22
38	e	312	II0	C29-C31-C33	-3.83	111.25	123.22
38	l	313	II0	C30-C32-C34	-3.83	111.25	123.22
38	f	614	II0	C30-C32-C34	-3.83	111.25	123.22
29	k	607	CLA	CAA-C2A-C3A	-3.83	102.29	112.78
32	A	844	WVN	C16-C05-C09	-3.83	108.71	122.33
38	h	310	II0	C31-C29-C25	-3.83	115.47	126.58
38	e	314	II0	C27-C25-C23	-3.83	109.26	116.84
40	m	611	KC2	CBA-CAA-C2A	-3.82	110.70	125.27
38	n	616	II0	C04-C10-C14	-3.82	117.25	122.63
29	b	303	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
38	a	314	II0	C20-C14-C12	-3.81	107.29	114.36
38	n	618	II0	C27-C25-C23	-3.81	109.29	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	616	II0	C30-C32-C34	-3.81	111.32	123.22
29	s	402	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
38	h	311	II0	C03-C09-C13	-3.81	117.25	122.63
38	j	315	II0	C31-C29-C25	-3.81	115.51	126.58
38	b	314	II0	C38-C36-C34	-3.81	112.08	118.08
40	g	313	KC2	CBA-CAA-C2A	-3.81	110.76	125.27
38	f	614	II0	C28-C26-C24	-3.81	109.30	116.84
38	J	103	II0	C19-C13-C11	-3.80	107.31	114.36
40	g	313	KC2	C1A-NA-C4A	-3.80	105.00	106.71
32	L	206	WVN	C16-C05-C09	-3.80	108.81	122.33
38	i	316	II0	C11-C13-C09	-3.80	111.94	120.57
40	k	611	KC2	C2C-C1C-NC	3.80	114.72	110.57
38	m	615	II0	C06-C04-C10	3.80	117.32	109.62
38	h	311	II0	C29-C31-C33	-3.79	111.38	123.22
38	k	619	II0	C31-C29-C25	-3.79	115.57	126.58
38	c	313	II0	C30-C32-C34	-3.79	111.38	123.22
38	n	616	II0	C29-C31-C33	-3.79	111.38	123.22
40	g	314	KC2	C4B-C3B-C2B	-3.79	103.64	106.75
36	j	319	DGD	O6D-C1D-O3G	-3.79	101.00	109.97
38	a	317	II0	C32-C30-C26	-3.79	115.59	126.58
40	f	611	KC2	C4B-C3B-C2B	-3.78	103.64	106.75
38	i	313	II0	C04-C10-C14	-3.78	117.29	122.63
35	A	853	SQD	O9-S-O7	-3.78	100.87	113.95
32	s	405	WVN	C16-C05-C09	-3.78	108.90	122.33
32	B	847	WVN	C31-C32-C36	-3.77	113.15	118.94
32	L	201	WVN	C28-C30-C33	-3.77	111.44	123.22
32	L	206	WVN	C06-C13-C15	-3.77	117.30	122.61
38	h	311	II0	C05-C03-C09	3.77	117.26	109.62
38	a	313	II0	C05-C03-C09	3.77	117.26	109.62
38	a	315	II0	C27-C25-C23	-3.77	109.38	116.84
32	F	207	WVN	C28-C30-C33	-3.76	111.47	123.22
32	L	201	WVN	C20-C13-C15	-3.76	112.34	121.46
32	L	206	WVN	C14-C15-C13	-3.76	117.27	122.73
38	l	314	II0	C19-C13-C11	-3.76	107.39	114.36
38	g	317	II0	C03-C09-C13	-3.76	117.32	122.63
29	a	306	CLA	CAC-C3C-C4C	3.76	129.69	124.81
38	f	614	II0	C19-C13-C11	-3.76	107.40	114.36
38	e	312	II0	C30-C32-C34	-3.76	111.50	123.22
32	l	316	WVN	C06-C13-C15	-3.76	117.32	122.61
38	e	312	II0	C32-C30-C26	-3.75	115.68	126.58
38	d	316	II0	C20-C14-C12	-3.75	107.40	114.36
38	m	618	II0	C30-C32-C34	-3.75	111.50	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	j	315	II0	C19-C13-C11	-3.75	107.41	114.36
38	i	316	II0	C28-C26-C24	-3.75	109.42	116.84
38	g	319	II0	C28-C26-C24	-3.74	109.42	116.84
29	g	306	CLA	CBC-CAC-C3C	3.74	122.74	112.43
36	B	844	DGD	O5D-C6D-C5D	-3.74	102.13	109.05
38	e	312	II0	C27-C25-C23	-3.74	109.43	116.84
40	g	314	KC2	C1A-NA-C4A	-3.74	105.03	106.71
38	e	313	II0	C28-C26-C24	-3.74	109.44	116.84
38	e	314	II0	C05-C03-C09	3.74	117.19	109.62
38	b	301	II0	C27-C25-C23	-3.73	109.44	116.84
38	h	310	II0	C32-C30-C26	-3.73	115.74	126.58
32	i	315	WVN	C17-C06-C13	-3.73	104.25	110.30
38	h	310	II0	C28-C26-C24	-3.73	109.46	116.84
38	b	315	II0	C30-C32-C34	-3.72	111.60	123.22
38	j	315	II0	C27-C25-C23	-3.72	109.47	116.84
32	A	854	WVN	C28-C30-C33	-3.72	111.61	123.22
38	j	301	II0	C28-C26-C24	-3.72	109.47	116.84
32	K	103	WVN	C28-C30-C33	-3.72	111.62	123.22
40	n	612	KC2	CHD-C1D-ND	-3.72	120.32	124.26
38	m	614	II0	C28-C26-C24	-3.71	109.48	116.84
29	K	102	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
32	F	207	WVN	C31-C32-C36	-3.71	113.25	118.94
38	i	314	II0	C34-C36-C40	-3.71	113.25	118.94
38	d	317	II0	C34-C36-C40	-3.71	113.25	118.94
38	k	615	II0	C27-C25-C23	-3.71	109.49	116.84
38	j	301	II0	C32-C30-C26	-3.71	115.81	126.58
38	a	313	II0	C32-C30-C26	-3.70	115.83	126.58
38	j	315	II0	C28-C26-C24	-3.70	109.51	116.84
38	i	316	II0	C30-C32-C34	-3.70	111.68	123.22
32	B	848	WVN	C16-C05-C09	-3.69	109.20	122.33
38	j	301	II0	C20-C14-C12	-3.69	107.52	114.36
38	j	316	II0	C33-C35-C39	-3.69	113.28	118.94
38	f	614	II0	C20-C14-C12	-3.69	107.52	114.36
32	B	846	WVN	C20-C13-C15	-3.69	112.53	121.46
32	K	103	WVN	C01-C02-C11	-3.69	108.04	112.70
38	b	314	II0	C28-C26-C24	-3.68	109.54	116.84
38	b	315	II0	C41-C42-C40	-3.68	115.93	123.47
38	f	615	II0	C11-C13-C09	-3.68	112.22	120.57
32	B	847	WVN	C23-C20-C13	-3.68	116.87	127.20
32	s	407	WVN	C16-C05-C09	-3.68	109.25	122.33
38	j	301	II0	C19-C13-C11	-3.68	107.54	114.36
38	i	319	II0	C27-C25-C23	-3.68	109.56	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s	404	KC2	CBC-CAC-C3C	-3.68	109.33	127.62
38	a	314	II0	C05-C03-C09	3.67	117.07	109.62
29	A	802	CLA	CMB-C2B-C1B	-3.67	119.77	125.37
40	g	315	KC2	C1D-CHD-C4C	-3.67	117.62	126.34
32	i	315	WVN	C02-C05-C09	-3.67	116.95	121.47
29	g	306	CLA	CMC-C2C-C1C	-3.67	119.45	125.04
32	A	846	WVN	C01-C02-C05	3.67	117.99	111.42
38	l	315	II0	C28-C26-C24	-3.67	109.58	116.84
40	g	313	KC2	C1D-CHD-C4C	-3.66	117.65	126.34
38	l	315	II0	C30-C32-C34	-3.66	111.79	123.22
38	j	315	II0	C20-C14-C12	-3.66	107.57	114.36
38	d	315	II0	C30-C32-C34	-3.66	111.79	123.22
29	B	841	CLA	C3B-C4B-NB	-3.66	107.12	110.52
40	d	311	KC2	CHC-C1C-C2C	-3.65	119.27	124.98
39	b	316	IHT	C05-C08-C12	3.65	115.30	110.30
38	i	319	II0	C38-C36-C34	-3.65	112.33	118.08
40	s	401	KC2	C1D-CHD-C4C	-3.64	117.70	126.34
40	m	611	KC2	C4B-C3B-C2B	-3.64	103.76	106.75
38	m	615	II0	C41-C42-C40	-3.64	116.02	123.47
29	b	303	CLA	O2D-CGD-CBD	3.64	117.73	111.27
40	k	611	KC2	C4B-C3B-C2B	-3.63	103.77	106.75
32	R	201	WVN	C26-C29-C31	-3.63	111.89	123.22
38	k	620	II0	C27-C25-C23	-3.63	109.65	116.84
38	a	317	II0	C15-C03-C09	-3.63	104.70	110.47
38	g	318	II0	C38-C36-C34	-3.63	112.36	118.08
38	i	313	II0	C19-C13-C11	-3.63	107.64	114.36
40	k	611	KC2	C1D-CHD-C4C	-3.63	117.74	126.34
29	i	303	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
38	b	301	II0	C19-C13-C11	-3.62	107.65	114.36
40	c	310	KC2	CHC-C1C-C2C	-3.62	119.33	124.98
38	i	314	II0	C38-C36-C34	-3.61	112.38	118.08
32	l	302	WVN	C16-C05-C09	-3.61	109.48	122.33
38	k	620	II0	C28-C26-C24	-3.61	109.69	116.84
31	A	843	LHG	O8-C23-C24	3.61	120.85	111.38
38	m	616	II0	C32-C30-C26	-3.61	116.11	126.58
38	f	616	II0	C32-C30-C26	-3.61	116.11	126.58
38	d	316	II0	C33-C35-C39	-3.61	113.41	118.94
38	f	616	II0	C20-C14-C12	-3.60	107.68	114.36
38	l	313	II0	C20-C14-C12	-3.60	107.68	114.36
38	h	309	II0	C27-C25-C23	-3.60	109.71	116.84
38	k	620	II0	C32-C30-C26	-3.60	116.13	126.58
32	A	846	WVN	C33-C34-C37	-3.60	113.42	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	g	314	KC2	C3C-C2C-C1C	-3.60	103.82	106.49
40	g	315	KC2	CAA-CBA-CGA	-3.60	108.78	127.26
32	L	205	WVN	C14-C15-C13	-3.59	117.52	122.73
32	L	206	WVN	C26-C29-C31	-3.59	112.02	123.22
29	l	304	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
40	i	310	KC2	C4B-C3B-C2B	-3.59	103.81	106.75
38	n	615	II0	C33-C35-C39	-3.59	113.44	118.94
32	J	101	WVN	C21-C15-C14	-3.59	106.73	113.62
38	a	315	II0	C28-C26-C24	-3.58	109.74	116.84
38	k	615	II0	C06-C08-C12	3.58	115.21	110.30
40	j	312	KC2	C4B-C3B-C2B	-3.58	103.81	106.75
38	n	618	II0	C19-C13-C11	-3.58	107.73	114.36
32	A	846	WVN	C28-C30-C33	-3.57	112.06	123.22
38	d	301	II0	C28-C26-C24	-3.57	109.76	116.84
32	l	302	WVN	C26-C29-C31	-3.57	112.08	123.22
40	i	318	KC2	C4B-C3B-C2B	-3.57	103.82	106.75
38	m	614	II0	C03-C09-C13	-3.57	117.60	122.63
40	i	310	KC2	C2C-C1C-NC	3.56	114.46	110.57
38	g	319	II0	C32-C30-C26	-3.56	116.24	126.58
32	l	316	WVN	C28-C30-C33	-3.56	112.11	123.22
38	f	618	II0	C27-C25-C23	-3.56	109.80	116.84
38	k	619	II0	C32-C30-C26	-3.55	116.26	126.58
29	B	833	CLA	CMB-C2B-C1B	-3.55	119.96	125.37
38	n	616	II0	C32-C30-C26	-3.55	116.27	126.58
38	g	318	II0	C30-C32-C34	-3.55	112.14	123.22
38	m	614	II0	C33-C35-C39	-3.55	113.49	118.94
38	n	618	II0	C30-C32-C34	-3.55	112.14	123.22
38	i	314	II0	C33-C35-C39	-3.55	113.50	118.94
32	R	201	WVN	C21-C15-C14	-3.55	106.80	113.62
38	e	313	II0	C27-C25-C23	-3.55	109.81	116.84
32	F	205	WVN	C16-C05-C09	-3.54	109.72	122.33
38	b	314	II0	C32-C30-C26	-3.54	116.30	126.58
38	d	316	II0	C30-C32-C34	-3.54	112.18	123.22
32	h	308	WVN	C23-C20-C13	-3.54	117.27	127.20
38	c	313	II0	C33-C35-C39	-3.53	113.52	118.94
32	L	201	WVN	C33-C34-C37	-3.53	113.52	118.94
38	l	313	II0	C19-C13-C11	-3.53	107.81	114.36
38	m	618	II0	C32-C30-C26	-3.53	116.33	126.58
40	f	611	KC2	CAA-CBA-CGA	-3.53	109.12	127.26
38	g	319	II0	C27-C25-C23	-3.53	109.85	116.84
32	B	847	WVN	C16-C05-C09	-3.53	109.78	122.33
38	m	616	II0	C28-C26-C24	-3.52	109.86	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	819	CLA	CAC-C3C-C2C	3.52	133.54	127.53
32	L	205	WVN	C28-C30-C33	-3.52	112.24	123.22
32	s	407	WVN	C06-C13-C15	-3.51	117.66	122.61
40	n	611	KC2	C4B-C3B-C2B	-3.51	103.87	106.75
40	s	401	KC2	CBA-CAA-C2A	-3.51	111.89	125.27
38	i	319	II0	C05-C07-C11	3.51	115.11	110.30
38	a	314	II0	C38-C36-C34	-3.51	112.55	118.08
32	B	848	WVN	C17-C06-C13	-3.50	104.62	110.30
40	d	311	KC2	CAA-CBA-CGA	-3.50	109.26	127.26
40	e	309	KC2	C4B-C3B-C2B	-3.50	103.88	106.75
29	s	406	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
38	n	616	II0	C27-C25-C23	-3.50	109.91	116.84
32	A	846	WVN	C23-C25-C28	-3.49	113.58	118.94
38	a	314	II0	C19-C13-C11	-3.49	107.88	114.36
38	f	618	II0	C33-C35-C39	-3.49	113.58	118.94
38	k	616	II0	C20-C14-C12	-3.49	107.89	114.36
29	d	313	CLA	CAA-C2A-C3A	-3.49	103.22	112.78
30	A	841	PQN	C14-C13-C15	-3.49	109.40	115.27
38	d	316	II0	C19-C13-C11	-3.49	107.90	114.36
38	h	311	II0	C38-C36-C34	-3.49	112.59	118.08
32	B	846	WVN	C16-C05-C09	-3.48	109.94	122.33
29	A	834	CLA	CMB-C2B-C1B	-3.48	120.07	125.37
35	A	853	SQD	O5-C5-C4	3.48	116.01	109.69
38	a	314	II0	C03-C09-C13	-3.48	117.72	122.63
35	A	853	SQD	O9-S-C6	3.47	111.07	106.94
40	l	311	KC2	CAA-CBA-CGA	-3.47	109.44	127.26
40	s	404	KC2	C1D-CHD-C4C	-3.46	118.13	126.34
32	B	846	WVN	C31-C32-C36	-3.46	113.64	118.94
38	k	616	II0	C06-C04-C10	3.46	116.62	109.62
32	F	207	WVN	C14-C15-C13	-3.46	117.71	122.73
31	L	208	LHG	O8-C23-C24	3.45	122.75	111.91
29	g	306	CLA	CAC-C3C-C2C	3.45	133.43	127.53
40	i	310	KC2	O2D-CGD-O1D	-3.45	117.09	123.84
32	L	205	WVN	C19-C22-C26	-3.45	113.65	118.94
38	j	316	II0	C38-C36-C34	-3.45	112.64	118.08
38	f	618	II0	C19-C13-C11	-3.45	107.97	114.36
32	R	201	WVN	C39-C40-C37	-3.44	116.42	123.47
38	m	615	II0	C38-C36-C34	-3.44	112.65	118.08
38	e	314	II0	C33-C35-C39	-3.44	113.66	118.94
40	d	311	KC2	C4B-C3B-C2B	-3.44	103.93	106.75
38	d	316	II0	C05-C03-C09	3.44	116.59	109.62
32	s	407	WVN	C01-C02-C11	-3.44	108.36	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	816	CLA	CBA-CAA-C2A	3.44	124.00	113.86
38	d	317	II0	C30-C32-C34	-3.43	112.50	123.22
38	i	319	II0	C30-C32-C34	-3.43	112.51	123.22
37	c	317	LMG	O1-C7-C8	-3.43	102.62	110.90
32	R	201	WVN	C16-C05-C09	-3.43	110.13	122.33
29	g	304	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
38	j	315	II0	C29-C31-C33	-3.43	112.52	123.22
29	B	840	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
38	k	615	II0	C30-C32-C34	-3.42	112.53	123.22
40	e	309	KC2	CAA-C2A-C1A	-3.42	109.01	124.75
32	l	302	WVN	C23-C20-C13	-3.42	117.60	127.20
40	m	611	KC2	CAA-C2A-C1A	-3.42	109.03	124.75
29	f	608	CLA	CMB-C2B-C1B	-3.42	120.17	125.37
32	B	846	WVN	C28-C30-C33	-3.42	112.55	123.22
38	J	103	II0	C32-C30-C26	-3.42	116.66	126.58
38	n	615	II0	C41-C42-C40	-3.41	116.48	123.47
38	c	313	II0	C32-C30-C26	-3.41	116.68	126.58
38	d	315	II0	C34-C36-C40	-3.41	113.71	118.94
32	A	854	WVN	C38-C34-C33	-3.41	112.70	118.08
32	s	407	WVN	C28-C30-C33	-3.41	112.58	123.22
38	j	301	II0	C06-C04-C10	3.40	116.52	109.62
38	b	314	II0	C29-C31-C33	-3.40	112.61	123.22
38	f	615	II0	C06-C04-C10	3.39	116.49	109.62
29	d	309	CLA	CAA-C2A-C3A	-3.39	108.19	116.10
38	m	618	II0	C05-C07-C11	3.39	114.94	110.30
32	l	316	WVN	C01-C02-C05	3.39	117.48	111.42
38	d	316	II0	C41-C42-C40	-3.39	116.54	123.47
38	k	620	II0	C20-C14-C12	-3.38	108.08	114.36
40	s	401	KC2	C4B-C3B-C2B	-3.38	103.97	106.75
29	m	602	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
29	g	311	CLA	O2A-CGA-O1A	-3.38	115.07	123.59
38	d	315	II0	C19-C13-C11	-3.38	108.10	114.36
32	F	207	WVN	C26-C29-C31	-3.38	112.68	123.22
40	k	611	KC2	CAA-CBA-CGA	-3.37	109.92	127.26
38	e	312	II0	C28-C26-C24	-3.37	110.16	116.84
38	m	616	II0	C19-C13-C11	-3.37	108.11	114.36
29	A	813	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
38	a	315	II0	C19-C13-C11	-3.37	108.11	114.36
38	i	319	II0	C06-C08-C12	3.36	114.91	110.30
38	l	314	II0	C34-C36-C40	-3.36	113.78	118.94
38	n	618	II0	C20-C14-C12	-3.36	108.13	114.36
38	m	614	II0	C32-C30-C26	-3.36	116.83	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	616	II0	C28-C26-C24	-3.36	110.19	116.84
30	B	843	PQN	C14-C13-C15	-3.35	109.63	115.27
38	a	315	II0	C30-C32-C34	-3.35	112.76	123.22
38	b	314	II0	C27-C25-C23	-3.35	110.20	116.84
38	g	319	II0	C11-C13-C09	-3.35	112.97	120.57
29	i	303	CLA	O2D-CGD-CBD	3.34	117.21	111.27
40	c	310	KC2	CHD-C4C-NC	3.34	129.28	124.20
32	A	846	WVN	C21-C15-C14	-3.34	107.19	113.62
38	m	616	II0	C05-C07-C11	3.34	114.87	110.30
38	i	319	II0	C11-C13-C09	-3.34	113.00	120.57
38	m	614	II0	C41-C42-C40	-3.33	116.64	123.47
40	s	404	KC2	O2D-CGD-O1D	-3.33	117.32	123.84
29	g	323	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
38	i	316	II0	C05-C07-C11	3.33	114.86	110.30
38	j	316	II0	C41-C42-C40	-3.33	116.66	123.47
38	m	618	II0	C38-C36-C34	-3.33	112.83	118.08
29	b	304	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
38	h	309	II0	C05-C03-C09	3.32	116.36	109.62
38	k	616	II0	C15-C03-C09	3.32	115.75	110.47
32	L	201	WVN	C26-C29-C31	-3.32	112.86	123.22
29	d	303	CLA	CMB-C2B-C1B	-3.32	120.31	125.37
29	d	306	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
29	B	818	CLA	C3B-C4B-NB	-3.32	107.44	110.52
38	k	620	II0	C19-C13-C11	-3.31	108.21	114.36
29	A	829	CLA	CHB-C1B-NB	3.31	127.77	124.26
40	c	310	KC2	C1D-CHD-C4C	-3.31	118.48	126.34
32	A	846	WVN	C23-C20-C13	-3.31	117.91	127.20
32	s	405	WVN	C28-C30-C33	-3.31	112.89	123.22
38	e	313	II0	C19-C13-C11	-3.31	108.23	114.36
29	B	829	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
38	k	616	II0	C30-C32-C34	-3.31	112.90	123.22
38	a	315	II0	C32-C30-C26	-3.30	116.99	126.58
38	h	310	II0	C20-C14-C12	-3.30	108.24	114.36
38	l	315	II0	C33-C35-C39	-3.30	113.88	118.94
38	a	313	II0	C20-C14-C12	-3.30	108.24	114.36
32	A	847	WVN	C19-C22-C26	-3.30	113.88	118.94
36	B	844	DGD	O3G-C3G-C2G	-3.29	102.95	110.90
40	g	314	KC2	O2D-CGD-CBD	3.29	117.12	111.27
38	g	318	II0	C20-C14-C12	-3.29	108.26	114.36
38	f	616	II0	C12-C14-C10	-3.29	113.11	120.57
40	g	315	KC2	CBC-CAC-C3C	-3.29	111.27	127.62
38	l	314	II0	C30-C32-C34	-3.28	112.97	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	847	WVN	C10-C06-C13	3.28	115.53	110.48
38	l	313	II0	C11-C13-C09	-3.28	113.13	120.57
38	l	314	II0	C38-C36-C34	-3.28	112.92	118.08
38	g	318	II0	C19-C13-C11	-3.27	108.29	114.36
32	s	407	WVN	C21-C15-C14	-3.27	107.33	113.62
29	g	310	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
38	f	618	II0	C32-C30-C26	-3.27	117.09	126.58
38	d	301	II0	C29-C31-C33	-3.27	113.02	123.22
29	A	822	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
29	d	307	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
32	L	201	WVN	C01-C02-C05	3.26	117.25	111.42
40	c	310	KC2	C4B-C3B-C2B	-3.26	104.08	106.75
32	F	205	WVN	C26-C29-C31	-3.25	113.07	123.22
29	f	613	CLA	CMB-C2B-C1B	-3.25	120.42	125.37
29	a	307	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
29	B	827	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
38	g	317	II0	C30-C32-C34	-3.25	113.08	123.22
29	B	803	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
38	a	317	II0	C29-C31-C33	-3.24	113.09	123.22
38	e	314	II0	C20-C14-C12	-3.24	108.35	114.36
38	b	301	II0	C29-C31-C33	-3.24	113.10	123.22
38	e	314	II0	C28-C26-C24	-3.24	110.42	116.84
32	A	844	WVN	C02-C05-C09	-3.24	117.48	121.47
38	g	319	II0	C41-C42-C40	-3.24	116.84	123.47
38	i	313	II0	C29-C31-C33	-3.23	113.13	123.22
29	A	839	CLA	CMB-C2B-C1B	-3.23	120.44	125.37
38	j	315	II0	C41-C42-C40	-3.23	116.85	123.47
40	l	311	KC2	C1A-NA-C4A	-3.23	105.25	106.71
32	I	101	WVN	C23-C20-C13	-3.23	118.14	127.20
29	k	605	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
29	k	601	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
38	g	319	II0	C20-C14-C12	-3.21	108.40	114.36
29	B	827	CLA	CHB-C1B-NB	3.21	127.66	124.26
32	A	845	WVN	C16-C05-C09	-3.21	110.90	122.33
38	i	316	II0	C20-C14-C12	-3.21	108.40	114.36
38	b	301	II0	C06-C04-C10	3.21	116.13	109.62
32	e	315	WVN	C26-C29-C31	-3.21	113.20	123.22
29	B	838	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
32	B	849	WVN	C14-C15-C13	-3.21	118.07	122.73
32	A	854	WVN	C21-C15-C14	-3.21	107.45	113.62
32	e	315	WVN	C24-C22-C19	-3.21	113.02	118.08
29	F	201	CLA	C3B-C4B-NB	-3.21	107.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	842	CLA	C3B-C4B-NB	-3.20	107.54	110.52
29	A	835	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
29	B	819	CLA	C3B-C4B-NB	-3.20	107.55	110.52
29	e	303	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
29	c	303	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
32	B	847	WVN	C21-C15-C14	-3.20	107.47	113.62
29	B	802	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
38	a	315	II0	C12-C14-C10	-3.20	113.31	120.57
29	j	313	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
38	e	313	II0	C12-C14-C10	-3.20	113.31	120.57
32	R	201	WVN	C01-C02-C05	3.19	117.14	111.42
38	n	618	II0	C29-C31-C33	-3.19	113.26	123.22
32	s	405	WVN	C26-C29-C31	-3.19	113.26	123.22
38	g	319	II0	C19-C13-C11	-3.19	108.44	114.36
38	f	615	II0	C41-C42-C40	-3.19	116.94	123.47
40	g	314	KC2	CAA-CBA-CGA	-3.19	110.88	127.26
32	s	405	WVN	C23-C25-C28	-3.19	114.05	118.94
38	d	317	II0	C06-C04-C10	3.19	116.08	109.62
38	i	319	II0	C19-C13-C11	-3.19	108.45	114.36
40	j	312	KC2	CAA-CBA-CGA	-3.19	110.88	127.26
38	J	103	II0	C29-C31-C33	-3.19	113.27	123.22
38	i	316	II0	C29-C31-C33	-3.18	113.28	123.22
40	n	611	KC2	CAA-CBA-CGA	-3.18	110.90	127.26
29	i	305	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
29	A	824	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
40	i	318	KC2	CAA-CBA-CGA	-3.18	110.91	127.26
38	h	310	II0	C29-C31-C33	-3.18	113.29	123.22
38	a	313	II0	C41-C42-C40	-3.18	116.96	123.47
29	B	808	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
29	n	610	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
29	B	805	CLA	CHB-C4A-NA	3.18	128.90	124.51
32	R	202	WVN	C20-C13-C15	-3.17	113.77	121.46
38	k	615	II0	C19-C13-C11	-3.17	108.48	114.36
32	R	202	WVN	C01-C02-C11	-3.17	108.69	112.70
29	n	604	CLA	CBA-CAA-C2A	3.16	123.20	113.86
38	j	315	II0	C06-C04-C10	3.16	116.03	109.62
38	e	313	II0	C20-C14-C12	-3.16	108.50	114.36
32	s	407	WVN	C26-C29-C31	-3.16	113.36	123.22
38	b	301	II0	C05-C03-C09	3.16	116.02	109.62
40	c	310	KC2	C2C-C1C-NC	3.15	114.02	110.57
29	k	603	CLA	CMB-C2B-C1B	-3.15	120.57	125.37
38	e	312	II0	C19-C13-C11	-3.15	108.52	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	846	WVN	C10-C06-C13	3.15	115.33	110.48
29	f	612	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
32	B	849	WVN	C21-C15-C14	-3.15	107.57	113.62
32	I	101	WVN	C19-C22-C26	-3.14	114.11	118.94
29	b	311	CLA	CHB-C4A-NA	3.14	128.86	124.51
38	a	315	II0	C11-C13-C09	-3.14	113.43	120.57
38	h	310	II0	C19-C13-C11	-3.14	108.53	114.36
40	i	310	KC2	CAA-CBA-CGA	-3.14	111.11	127.26
29	k	614	CLA	CBC-CAC-C3C	3.13	121.07	112.43
38	i	319	II0	C34-C36-C40	-3.13	114.13	118.94
29	j	306	CLA	CHB-C4A-NA	3.13	128.84	124.51
40	i	310	KC2	CHD-C4C-NC	3.13	128.95	124.20
32	B	849	WVN	C26-C29-C31	-3.13	113.46	123.22
38	a	317	II0	C20-C14-C12	-3.13	108.56	114.36
38	f	618	II0	C05-C07-C11	3.13	114.58	110.30
38	d	317	II0	C11-C13-C09	-3.12	113.48	120.57
29	A	829	CLA	CMB-C2B-C1B	-3.12	120.62	125.37
32	R	202	WVN	C16-C05-C09	-3.12	111.24	122.33
38	j	316	II0	C19-C13-C11	-3.12	108.58	114.36
29	j	308	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
40	s	404	KC2	CMB-C2B-C1B	3.11	130.20	124.71
32	R	202	WVN	C26-C29-C31	-3.11	113.50	123.22
32	A	846	WVN	C26-C29-C31	-3.11	113.51	123.22
29	A	806	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
29	A	825	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
32	F	205	WVN	C06-C13-C20	-3.11	106.99	115.78
38	b	314	II0	C11-C13-C09	-3.11	113.52	120.57
38	i	314	II0	C06-C04-C10	3.11	115.91	109.62
29	m	602	CLA	CBC-CAC-C3C	3.10	120.99	112.43
32	L	201	WVN	C01-C02-C11	-3.10	108.78	112.70
29	d	304	CLA	CHB-C4A-NA	3.10	128.80	124.51
29	j	309	CLA	C3B-C4B-NB	-3.10	107.64	110.52
38	O	203	II0	C42-C41-C39	-3.10	117.13	123.47
32	A	844	WVN	C26-C29-C31	-3.10	113.55	123.22
29	s	402	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
38	a	317	II0	C30-C32-C34	-3.10	113.56	123.22
29	A	831	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
29	B	822	CLA	O2A-CGA-O1A	-3.09	115.79	123.59
38	f	616	II0	C27-C25-C23	-3.09	110.72	116.84
29	h	304	CLA	CHB-C4A-NA	3.09	128.78	124.51
32	F	205	WVN	C28-C30-C33	-3.08	113.60	123.22
40	m	611	KC2	CAA-CBA-CGA	-3.08	111.42	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	804	CLA	CBC-CAC-C3C	3.08	120.93	112.43
29	B	815	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
32	B	849	WVN	C39-C40-C37	-3.08	117.17	123.47
29	f	605	CLA	C3B-C4B-NB	-3.08	107.66	110.52
38	g	318	II0	C41-C42-C40	-3.07	117.17	123.47
38	j	316	II0	C06-C04-C10	3.07	115.85	109.62
29	i	307	CLA	C3B-C4B-NB	-3.07	107.66	110.52
29	B	840	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
29	g	306	CLA	CAC-C3C-C4C	-3.07	120.83	124.81
38	d	314	II0	C05-C07-C11	-3.07	106.10	110.30
40	d	311	KC2	CAA-C2A-C1A	-3.07	110.65	124.75
29	B	816	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
29	i	302	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
29	d	313	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
38	d	317	II0	C19-C13-C11	-3.06	108.68	114.36
40	g	315	KC2	C4B-C3B-C2B	-3.06	104.24	106.75
29	f	608	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
29	L	204	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
32	B	848	WVN	C39-C40-C37	-3.06	117.21	123.47
29	K	101	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
29	m	608	CLA	C3B-C4B-NB	-3.06	107.68	110.52
29	B	822	CLA	C4-C3-C2	-3.05	115.84	123.68
38	i	313	II0	C11-C13-C09	-3.05	113.64	120.57
38	h	310	II0	C12-C14-C10	-3.05	113.64	120.57
29	m	601	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
29	j	304	CLA	CMB-C2B-C1B	-3.05	120.72	125.37
29	s	406	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
38	n	614	II0	C03-C05-C07	3.05	120.53	113.64
38	f	616	II0	C19-C13-C11	-3.05	108.70	114.36
38	m	618	II0	C19-C13-C11	-3.05	108.71	114.36
29	A	810	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	A	826	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	g	305	CLA	CMB-C2B-C1B	-3.05	120.73	125.37
38	f	615	II0	C38-C36-C34	-3.05	113.28	118.08
38	g	317	II0	C33-C35-C39	-3.05	114.27	118.94
40	d	311	KC2	CMB-C2B-C1B	3.04	130.08	124.71
29	n	604	CLA	CHB-C4A-NA	3.04	128.72	124.51
35	A	853	SQD	C44-O6-C1	3.04	119.69	113.74
38	n	618	II0	C06-C04-C10	3.04	115.79	109.62
32	i	315	WVN	C10-C06-C13	3.04	115.17	110.48
40	e	309	KC2	CAA-CBA-CGA	-3.04	111.63	127.26
38	c	313	II0	C20-C14-C12	-3.04	108.72	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	619	II0	C30-C32-C34	-3.04	113.73	123.22
29	B	810	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	J	102	CLA	C3B-C4B-NB	-3.04	107.70	110.52
29	j	309	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
29	j	313	CLA	C3B-C4B-NB	-3.03	107.70	110.52
29	g	308	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
38	m	615	II0	C11-C13-C09	-3.03	113.69	120.57
29	B	807	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
29	g	306	CLA	CMC-C2C-C3C	3.02	134.32	126.12
29	A	817	CLA	C3B-C4B-NB	-3.02	107.71	110.52
29	c	304	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
35	A	853	SQD	O8-S-C6	3.02	110.55	105.74
29	e	302	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
29	A	811	CLA	C3B-C4B-NB	-3.02	107.72	110.52
29	k	610	CLA	CHB-C4A-NA	3.02	128.68	124.51
29	B	841	CLA	CHB-C4A-NA	3.01	128.68	124.51
29	n	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	B	828	CLA	C3B-C4B-NB	-3.01	107.72	110.52
29	a	308	CLA	CMB-C2B-C1B	-3.01	120.78	125.37
29	g	311	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
33	A	849	LMU	C2'-C3'-C4'	3.01	116.55	109.68
38	a	313	II0	C12-C14-C10	-3.01	113.74	120.57
29	B	817	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
29	B	820	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
40	g	315	KC2	CHD-C4C-NC	3.00	128.76	124.20
29	A	807	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
29	e	304	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
29	F	202	CLA	C3B-C4B-NB	-3.00	107.73	110.52
29	B	829	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
38	k	615	II0	C08-C12-C14	3.00	117.83	111.85
29	L	203	CLA	CHB-C4A-NA	3.00	128.66	124.51
29	A	829	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
29	A	803	CLA	C3B-C4B-NB	-3.00	107.73	110.52
29	A	803	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
38	n	618	II0	C08-C12-C14	2.99	117.82	111.85
38	k	615	II0	C06-C04-C10	2.99	115.69	109.62
29	l	306	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
29	j	308	CLA	CHC-C4B-NB	2.99	127.43	124.26
29	A	815	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
38	m	616	II0	C11-C13-C09	-2.99	113.78	120.57
29	i	311	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
38	a	315	II0	C20-C14-C12	-2.99	108.81	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	819	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
29	B	815	CLA	CMB-C2B-C1B	-2.99	120.81	125.37
38	d	317	II0	C29-C31-C33	-2.99	113.89	123.22
38	n	615	II0	C27-C25-C23	-2.99	110.92	116.84
38	h	310	II0	C11-C13-C09	-2.99	113.79	120.57
29	e	306	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
29	b	304	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
29	B	803	CLA	CHC-C4B-NB	2.98	127.41	124.26
29	A	818	CLA	CHB-C1B-NB	2.98	127.41	124.26
29	b	313	CLA	CHB-C4A-NA	2.98	128.63	124.51
29	f	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
29	f	613	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
29	d	302	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
29	B	833	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
38	a	317	II0	C19-C13-C11	-2.98	108.84	114.36
38	m	616	II0	C29-C31-C33	-2.98	113.93	123.22
29	B	835	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
32	J	101	WVN	C01-C02-C11	-2.97	108.94	112.70
32	I	101	WVN	C26-C29-C31	-2.97	113.95	123.22
38	g	319	II0	C12-C14-C10	-2.97	113.83	120.57
29	B	824	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
38	d	301	II0	C20-C14-C12	-2.97	108.86	114.36
29	m	603	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
29	k	610	CLA	C2A-C1A-CHA	2.97	129.05	123.86
29	m	603	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
29	A	823	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
29	j	303	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
29	m	604	CLA	CMB-C2B-C1B	-2.96	120.85	125.37
32	A	844	WVN	C01-C02-C05	2.96	116.73	111.42
29	F	202	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
40	j	312	KC2	CHB-C1B-NB	-2.96	121.73	124.45
29	a	302	CLA	CBA-CAA-C2A	2.96	122.60	113.86
38	g	319	II0	C05-C07-C11	2.96	114.35	110.30
29	g	311	CLA	CHB-C4A-NA	2.96	128.60	124.51
38	O	203	II0	C41-C42-C40	2.96	129.53	123.47
40	g	313	KC2	CAA-C2A-C1A	-2.96	111.15	124.75
29	c	301	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
40	i	318	KC2	CAA-C2A-C1A	-2.96	111.16	124.75
29	A	836	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	A	840	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	B	822	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	F	201	CLA	O2D-CGD-O1D	-2.96	118.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	808	CLA	CHB-C4A-NA	2.95	128.60	124.51
29	A	817	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
29	b	310	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
29	j	310	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
29	A	813	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	B	824	CLA	CHB-C4A-NA	2.95	128.59	124.51
29	e	304	CLA	CHB-C4A-NA	2.95	128.59	124.51
29	k	603	CLA	CHB-C1B-NB	2.95	127.38	124.26
29	g	309	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	A	823	CLA	CHB-C4A-NA	2.95	128.59	124.51
29	f	606	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	g	309	CLA	CHB-C4A-NA	2.95	128.59	124.51
29	l	309	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	k	608	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
29	g	309	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
37	b	319	LMG	O6-C1-O1	-2.94	103.01	109.97
29	l	305	CLA	CHB-C4A-NA	2.94	128.58	124.51
29	d	309	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
29	A	840	CLA	CHB-C4A-NA	2.94	128.57	124.51
29	k	609	CLA	CHB-C4A-NA	2.94	128.57	124.51
40	g	315	KC2	CAA-C2A-C1A	-2.93	111.26	124.75
29	B	819	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
29	B	822	CLA	O2A-C1-C2	-2.93	100.93	108.64
28	A	801	CL0	CHA-C1A-NA	-2.93	119.69	126.40
29	c	302	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
32	L	201	WVN	C21-C15-C14	-2.93	107.99	113.62
29	A	814	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	B	822	CLA	CHB-C4A-NA	2.93	128.56	124.51
29	k	602	CLA	C3B-C4B-NB	-2.93	107.80	110.52
38	k	616	II0	C41-C42-C40	-2.93	117.48	123.47
29	i	312	CLA	CHB-C4A-NA	2.93	128.56	124.51
38	h	309	II0	C15-C03-C09	-2.92	105.82	110.47
32	F	205	WVN	C12-C14-C15	-2.92	108.86	114.08
29	l	307	CLA	CHB-C4A-NA	2.92	128.56	124.51
29	i	308	CLA	CHB-C4A-NA	2.92	128.56	124.51
38	j	301	II0	C29-C31-C33	-2.92	114.10	123.22
38	e	312	II0	C20-C14-C12	-2.92	108.94	114.36
38	d	316	II0	C08-C12-C14	2.92	117.67	111.85
40	s	404	KC2	C1A-NA-C4A	-2.92	105.39	106.71
29	c	305	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	i	304	CLA	CHB-C4A-NA	2.92	128.55	124.51
29	B	811	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	826	CLA	CHB-C4A-NA	2.92	128.55	124.51
38	j	316	II0	C11-C13-C09	-2.92	113.95	120.57
38	a	315	II0	C05-C03-C09	2.92	115.53	109.62
37	Q	301	LMG	O6-C1-O1	-2.92	103.07	109.97
38	k	620	II0	C29-C31-C33	-2.91	114.12	123.22
29	A	827	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
29	n	601	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
29	B	826	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
38	j	315	II0	C05-C07-C11	2.91	114.29	110.30
29	A	837	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
29	b	307	CLA	C3B-C4B-NB	-2.91	107.81	110.52
29	A	816	CLA	CHB-C4A-NA	2.91	128.54	124.51
29	B	823	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	n	608	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
38	l	313	II0	C06-C08-C12	2.91	114.29	110.30
40	g	314	KC2	CHB-C1B-NB	-2.91	121.78	124.45
29	B	808	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
29	A	802	CLA	C3B-C4B-NB	-2.91	107.82	110.52
29	h	301	CLA	C3B-C4B-NB	-2.91	107.82	110.52
29	d	308	CLA	C3B-C4B-NB	-2.91	107.82	110.52
29	B	804	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	A	818	CLA	CMB-C2B-C1B	-2.91	120.94	125.37
29	A	811	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	A	839	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	B	816	CLA	C3B-C4B-NB	-2.91	107.82	110.52
32	F	204	WVN	C26-C29-C31	-2.91	114.15	123.22
38	J	103	II0	C27-C25-C23	-2.91	111.08	116.84
32	R	201	WVN	C02-C05-C09	-2.91	117.89	121.47
32	l	316	WVN	C21-C15-C14	-2.90	108.04	113.62
38	j	301	II0	C05-C03-C09	2.90	115.51	109.62
29	d	308	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	A	809	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	m	609	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
38	j	301	II0	C11-C13-C09	-2.90	113.98	120.57
29	B	825	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	B	832	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	n	609	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
32	B	846	WVN	C33-C34-C37	-2.90	114.49	118.94
29	n	606	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
38	d	301	II0	C27-C25-C23	-2.90	111.10	116.84
32	M	101	WVN	C21-C15-C14	-2.90	108.05	113.62
38	f	618	II0	C41-C42-C40	-2.90	117.54	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	310	CLA	C3B-C4B-NB	-2.90	107.83	110.52
40	g	314	KC2	C1D-CHD-C4C	-2.89	119.48	126.34
40	f	611	KC2	CAA-C2A-C1A	-2.89	111.45	124.75
29	A	805	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	e	302	CLA	CHB-C4A-NA	2.89	128.51	124.51
29	A	834	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	c	311	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	B	836	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
38	m	615	II0	C19-C13-C11	-2.89	109.01	114.36
29	L	207	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
38	a	314	II0	C12-C14-C10	-2.88	114.02	120.57
29	d	310	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
29	a	303	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
29	k	609	CLA	C3B-C4B-NB	-2.88	107.84	110.52
29	n	605	CLA	CAC-C3C-C4C	2.88	128.55	124.81
38	d	319	II0	C03-C09-C13	-2.88	118.57	122.63
29	f	603	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
38	e	316	II0	C06-C08-C12	2.88	114.25	110.30
38	b	315	II0	C11-C13-C09	-2.88	114.04	120.57
29	i	303	CLA	C3B-C4B-NB	-2.88	107.84	110.52
29	O	201	CLA	CMB-C2B-C1B	-2.88	120.99	125.37
29	b	305	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	c	302	CLA	CMB-C2B-C1B	-2.88	120.99	125.37
29	g	302	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
38	a	315	II0	C06-C08-C12	2.88	114.24	110.30
29	l	305	CLA	CMB-C2B-C1B	-2.88	120.99	125.37
29	f	609	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
40	g	315	KC2	CHD-C4C-C3C	-2.88	115.69	126.11
29	B	818	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	j	306	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	B	848	WVN	C24-C22-C19	-2.87	113.55	118.08
29	h	306	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
32	M	101	WVN	C26-C29-C31	-2.87	114.25	123.22
29	B	830	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	a	304	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	j	305	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	L	202	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	L	201	WVN	C08-C01-C02	-2.87	105.20	109.55
29	j	306	CLA	C3B-C4B-NB	-2.87	107.85	110.52
29	d	303	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	g	306	CLA	CHB-C4A-NA	2.87	128.48	124.51
29	A	850	CLA	CMB-C2B-C1B	-2.87	121.00	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	203	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
38	n	618	II0	C07-C11-C13	2.87	117.56	111.85
29	k	614	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
29	j	307	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
40	d	311	KC2	CHD-C4C-NC	2.86	128.55	124.20
29	g	316	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	B	842	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	k	605	CLA	CHB-C4A-NA	2.86	128.47	124.51
38	J	103	II0	C20-C14-C12	-2.86	109.05	114.36
29	a	308	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	n	609	CLA	C3B-C4B-NB	-2.86	107.86	110.52
38	e	314	II0	C06-C08-C12	2.86	114.22	110.30
40	l	311	KC2	O2D-CGD-O1D	-2.86	118.25	123.84
29	f	602	CLA	CMB-C2B-C1B	-2.86	121.01	125.37
29	a	307	CLA	C3B-C4B-NB	-2.86	107.86	110.52
29	m	612	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
29	A	840	CLA	CAA-C2A-C3A	-2.86	104.96	112.78
29	B	839	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
32	A	847	WVN	C18-C06-C13	-2.86	105.67	110.30
38	e	313	II0	C11-C13-C09	-2.86	114.09	120.57
40	f	611	KC2	O2D-CGD-O1D	-2.85	118.26	123.84
29	B	836	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	a	302	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	e	310	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	k	604	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	A	834	CLA	CMB-C2B-C3B	2.85	133.50	126.59
29	O	201	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	e	311	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	J	102	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	B	818	CLA	CHB-C1B-NB	2.85	127.28	124.26
29	j	304	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	d	309	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	d	318	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	B	832	CLA	CHB-C4A-NA	2.85	128.45	124.51
29	k	606	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	n	602	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	A	815	CLA	CHB-C4A-NA	2.84	128.45	124.51
29	O	202	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	n	603	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
32	A	844	WVN	C10-C06-C13	2.84	114.86	110.48
38	g	318	II0	C05-C03-C09	2.84	115.38	109.62
29	b	302	CLA	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	607	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	k	607	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
38	f	618	II0	C11-C13-C09	-2.84	114.12	120.57
29	c	308	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	m	605	CLA	CHB-C4A-NA	2.84	128.44	124.51
38	k	619	II0	C29-C31-C33	-2.84	114.36	123.22
29	e	303	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	d	303	CLA	CMB-C2B-C3B	2.84	133.46	126.59
29	n	607	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
32	L	205	WVN	C21-C15-C14	-2.84	108.17	113.62
29	j	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	i	304	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	B	805	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	g	302	CLA	CHB-C4A-NA	2.83	128.43	124.51
38	n	616	II0	C06-C04-C10	2.83	115.36	109.62
29	h	306	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	i	309	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	A	830	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	h	301	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	A	818	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	m	610	CLA	CHB-C4A-NA	2.83	128.43	124.51
29	c	306	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
29	l	301	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
29	K	101	CLA	CHB-C4A-NA	2.83	128.42	124.51
29	B	833	CLA	CMB-C2B-C3B	2.83	133.43	126.59
29	g	304	CLA	C3B-C4B-NB	-2.83	107.89	110.52
29	g	307	CLA	C3B-C4B-NB	-2.83	107.89	110.52
29	R	203	CLA	C1-C2-C3	-2.83	121.16	126.04
29	A	828	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
29	c	307	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
29	g	306	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
29	B	834	CLA	CHB-C4A-NA	2.82	128.42	124.51
40	i	310	KC2	CAA-C2A-C1A	-2.82	111.77	124.75
29	a	304	CLA	CHB-C4A-NA	2.82	128.41	124.51
29	c	311	CLA	CHB-C4A-NA	2.82	128.41	124.51
29	f	608	CLA	CMB-C2B-C3B	2.82	133.42	126.59
29	g	303	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
29	f	601	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
40	s	404	KC2	CAA-CBA-CGA	-2.82	112.78	127.26
29	B	819	CLA	CHB-C1B-NB	2.82	127.24	124.26
29	f	609	CLA	CHB-C4A-NA	2.82	128.41	124.51
32	A	844	WVN	C28-C30-C33	-2.82	114.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	833	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
40	s	401	KC2	O2D-CGD-O1D	-2.82	118.33	123.84
29	e	301	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
29	B	811	CLA	C3B-C4B-NB	-2.82	107.90	110.52
31	j	318	LHG	O8-C23-C24	2.82	120.74	111.91
32	A	847	WVN	C10-C06-C13	2.81	114.81	110.48
29	g	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	n	610	CLA	CHB-C4A-NA	2.81	128.40	124.51
38	c	313	II0	C41-C42-C40	-2.81	117.71	123.47
29	f	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	n	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	L	205	WVN	C26-C29-C31	-2.81	114.45	123.22
29	c	312	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
38	m	616	II0	C06-C04-C10	2.81	115.31	109.62
38	d	301	II0	C06-C04-C10	2.81	115.31	109.62
29	m	604	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
38	l	314	II0	C11-C13-C09	-2.81	114.20	120.57
29	l	310	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
29	m	605	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
32	A	844	WVN	C39-C40-C37	-2.81	117.73	123.47
29	j	306	CLA	C2A-C1A-CHA	2.80	128.76	123.86
29	m	612	CLA	C3B-C4B-NB	-2.80	107.92	110.52
38	k	615	II0	C41-C42-C40	-2.80	117.74	123.47
29	A	822	CLA	C3B-C4B-NB	-2.80	107.92	110.52
29	k	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
29	A	807	CLA	CHB-C4A-NA	2.80	128.38	124.51
32	A	847	WVN	C39-C40-C37	-2.80	117.74	123.47
29	c	309	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
29	h	304	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
38	f	615	II0	C19-C13-C11	-2.80	109.17	114.36
38	e	312	II0	C05-C03-C09	2.80	115.28	109.62
29	k	609	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
29	m	606	CLA	CHB-C4A-NA	2.79	128.38	124.51
38	g	317	II0	C41-C42-C40	-2.79	117.75	123.47
29	a	305	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
29	b	308	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
29	m	608	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	L	203	CLA	CHD-C1D-ND	-2.79	121.89	124.45
29	A	812	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	n	605	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	d	318	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	a	303	CLA	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	i	313	II0	C17-C04-C10	-2.79	106.03	110.47
29	A	802	CLA	CMB-C2B-C3B	2.79	133.34	126.59
29	s	403	CLA	O2D-CGD-CBD	2.79	116.22	111.27
29	B	813	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
32	l	302	WVN	C06-C13-C20	-2.79	107.89	115.78
29	A	827	CLA	CHD-C1D-ND	-2.79	121.89	124.45
32	K	103	WVN	C21-C15-C14	-2.79	108.26	113.62
40	c	310	KC2	CMC-C2C-C1C	2.79	129.28	125.04
29	h	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
32	K	103	WVN	C26-C29-C31	-2.79	114.52	123.22
29	l	309	CLA	CHB-C4A-NA	2.79	128.36	124.51
36	B	844	DGD	CDB-CCB-CBB	-2.79	100.28	114.42
29	A	820	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
38	g	319	II0	C29-C31-C33	-2.79	114.53	123.22
29	l	305	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
29	b	306	CLA	CHB-C4A-NA	2.78	128.36	124.51
29	i	306	CLA	CHB-C4A-NA	2.78	128.36	124.51
29	j	310	CLA	CHB-C4A-NA	2.78	128.36	124.51
38	l	315	II0	C15-C03-C09	-2.78	106.05	110.47
29	A	816	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	Q	302	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	g	312	CLA	C3B-C4B-NB	-2.78	107.93	110.52
29	k	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	f	604	CLA	CHB-C4A-NA	2.78	128.36	124.51
29	B	806	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	c	303	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	f	604	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	B	840	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	m	602	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	h	303	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	f	602	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	J	102	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	a	305	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	a	312	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	B	816	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
29	l	312	CLA	CHB-C4A-NA	2.77	128.35	124.51
29	j	303	CLA	CMB-C2B-C1B	-2.77	121.14	125.37
29	F	203	CLA	CHB-C4A-NA	2.77	128.35	124.51
29	i	302	CLA	CHB-C4A-NA	2.77	128.35	124.51
29	g	310	CLA	CHB-C4A-NA	2.77	128.35	124.51
40	g	313	KC2	CAA-CBA-CGA	-2.77	113.01	127.26
29	B	826	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	307	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	F	203	CLA	C3B-C4B-NB	-2.77	107.94	110.52
29	A	838	CLA	CHB-C4A-NA	2.77	128.34	124.51
29	g	312	CLA	CHB-C4A-NA	2.77	128.34	124.51
38	l	314	II0	C32-C30-C26	-2.77	118.53	126.58
29	B	802	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
37	c	317	LMG	O1-C1-C2	-2.77	103.98	108.30
29	b	304	CLA	CMB-C2B-C3B	2.77	133.30	126.59
38	f	618	II0	C30-C32-C34	-2.77	114.57	123.22
29	b	311	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	i	307	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	a	310	CLA	CHB-C4A-NA	2.77	128.34	124.51
29	B	828	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
32	J	101	WVN	C26-C29-C31	-2.77	114.58	123.22
40	j	312	KC2	O2D-CGD-O1D	-2.77	118.43	123.84
29	e	301	CLA	C3B-C4B-NB	-2.77	107.95	110.52
29	B	809	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
40	s	401	KC2	CAA-CBA-CGA	-2.77	113.05	127.26
31	l	318	LHG	O8-C23-C24	2.77	120.58	111.91
29	A	820	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
38	i	316	II0	C19-C13-C11	-2.76	109.23	114.36
29	m	602	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
29	n	606	CLA	C3B-C4B-NB	-2.76	107.95	110.52
38	e	313	II0	C29-C31-C33	-2.76	114.60	123.22
29	l	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	n	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	h	307	CLA	CHB-C4A-NA	2.76	128.33	124.51
29	i	312	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	O	206	CLA	CHB-C4A-NA	2.76	128.33	124.51
32	A	845	WVN	C21-C15-C14	-2.76	108.32	113.62
29	s	403	CLA	CHB-C4A-NA	2.76	128.32	124.51
38	m	615	II0	C07-C11-C13	-2.76	106.36	111.85
29	d	305	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
29	l	310	CLA	C3B-C4B-NB	-2.76	107.96	110.52
29	K	101	CLA	CAA-C2A-C3A	-2.75	105.23	112.78
29	A	836	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	B	816	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	s	402	CLA	CAA-CBA-CGA	-2.75	105.20	113.25
29	R	203	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
29	a	312	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
38	d	315	II0	C11-C13-C09	-2.75	114.32	120.57
29	a	311	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	e	309	KC2	CHD-C4C-NC	2.75	128.38	124.20
29	O	202	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	i	309	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	B	833	CLA	CHB-C1B-NB	2.75	127.17	124.26
38	J	103	II0	C12-C14-C10	-2.75	114.33	120.57
29	l	306	CLA	CHB-C4A-NA	2.75	128.31	124.51
29	l	301	CLA	CHB-C4A-NA	2.75	128.31	124.51
29	h	302	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
29	B	818	CLA	CHB-C4A-NA	2.75	128.31	124.51
38	b	301	II0	C41-C42-C40	-2.75	117.85	123.47
38	i	319	II0	C29-C31-C33	-2.75	114.65	123.22
29	f	601	CLA	CHB-C4A-NA	2.75	128.31	124.51
38	i	316	II0	C12-C14-C10	-2.74	114.34	120.57
29	A	835	CLA	C3B-C4B-NB	-2.74	107.97	110.52
29	A	804	CLA	CHB-C4A-NA	2.74	128.31	124.51
32	l	316	WVN	C10-C06-C13	2.74	114.70	110.48
29	f	608	CLA	CHB-C1B-NB	2.74	127.16	124.26
29	b	302	CLA	CHB-C4A-NA	2.74	128.30	124.51
29	e	310	CLA	CHB-C4A-NA	2.74	128.30	124.51
29	e	305	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
40	i	318	KC2	CHD-C4C-NC	2.74	128.36	124.20
29	f	609	CLA	C1-C2-C3	-2.74	121.30	126.04
38	a	314	II0	C15-C03-C09	-2.74	106.11	110.47
29	j	305	CLA	CHB-C4A-NA	2.74	128.30	124.51
29	k	604	CLA	CHB-C4A-NA	2.74	128.30	124.51
31	g	322	LHG	O8-C23-C24	2.74	120.51	111.91
29	l	303	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	g	307	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	m	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	d	304	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	g	312	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	c	307	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
29	B	841	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
29	k	608	CLA	C3B-C4B-NB	-2.74	107.98	110.52
38	h	310	II0	C41-C42-C40	-2.74	117.87	123.47
29	O	206	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
29	i	306	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
29	n	608	CLA	C3B-C4B-NB	-2.73	107.98	110.52
29	B	816	CLA	CBC-CAC-C3C	2.73	119.97	112.43
29	k	601	CLA	O2D-CGD-CBD	2.73	116.13	111.27
29	d	313	CLA	CHB-C4A-NA	2.73	128.29	124.51
29	h	305	CLA	CHB-C4A-NA	2.73	128.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	O	203	II0	C05-C07-C11	2.73	114.04	110.30
29	i	308	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	m	602	CLA	CAC-C3C-C2C	2.73	132.20	127.53
29	B	814	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	e	306	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
29	l	303	CLA	CHB-C4A-NA	2.73	128.29	124.51
29	b	309	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	Q	302	CLA	CHB-C4A-NA	2.73	128.28	124.51
29	m	605	CLA	CAA-C2A-C3A	-2.73	107.44	114.26
29	d	310	CLA	CAA-C2A-C3A	-2.73	109.73	116.10
29	L	202	CLA	C3B-C4B-NB	-2.73	107.98	110.52
32	A	847	WVN	C20-C13-C15	-2.73	114.86	121.46
29	d	303	CLA	CHB-C4A-NA	2.73	128.28	124.51
40	j	312	KC2	CHD-C4C-NC	2.73	128.34	124.20
38	d	315	II0	C38-C36-C34	-2.73	113.78	118.08
32	l	316	WVN	C33-C34-C37	-2.73	114.76	118.94
38	n	618	II0	C06-C08-C12	2.72	114.03	110.30
38	b	301	II0	C15-C03-C09	-2.72	106.14	110.47
29	B	808	CLA	O2D-CGD-CBD	2.72	116.11	111.27
29	B	820	CLA	O2D-CGD-CBD	2.72	116.11	111.27
29	b	303	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
29	k	610	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
38	J	103	II0	C11-C13-C09	-2.72	114.39	120.57
29	n	606	CLA	CHB-C4A-NA	2.72	128.28	124.51
32	L	206	WVN	C01-C02-C05	2.72	116.29	111.42
32	A	844	WVN	C14-C15-C13	-2.72	118.78	122.73
29	m	609	CLA	CHB-C4A-NA	2.72	128.27	124.51
38	a	317	II0	C12-C14-C10	-2.72	114.40	120.57
38	f	614	II0	C41-C42-C40	-2.72	117.91	123.47
29	a	306	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	B	819	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
40	f	611	KC2	CHD-C4C-NC	2.72	128.33	124.20
29	j	307	CLA	CHB-C4A-NA	2.72	128.27	124.51
39	j	317	IHT	C05-C08-C12	-2.72	106.58	110.30
29	s	406	CLA	C3B-C4B-NB	-2.72	108.00	110.52
29	A	827	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
29	j	305	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
29	g	323	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	f	606	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	F	203	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
29	f	612	CLA	CHB-C4A-NA	2.71	128.26	124.51
29	j	314	CLA	O2D-CGD-O1D	-2.71	118.54	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	615	II0	C11-C13-C09	-2.71	114.42	120.57
31	f	620	LHG	O8-C23-C24	2.71	120.41	111.91
40	i	318	KC2	CHB-C1B-NB	-2.71	121.96	124.45
32	e	315	WVN	C18-C06-C13	2.71	114.69	110.30
29	h	307	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	B	801	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	B	801	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
29	B	834	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	O	206	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	l	303	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	A	842	LHG	C11-C10-C9	-2.71	100.69	114.42
38	i	313	II0	C20-C14-C12	-2.71	109.34	114.36
29	m	606	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
38	f	616	II0	C41-C42-C40	-2.71	117.93	123.47
29	e	311	CLA	CHB-C4A-NA	2.71	128.25	124.51
29	n	602	CLA	CHB-C4A-NA	2.71	128.25	124.51
38	l	314	II0	C42-C41-C39	2.70	129.01	123.47
29	B	841	CLA	CHB-C1B-NB	2.70	127.12	124.26
29	h	303	CLA	C3B-C4B-NB	-2.70	108.01	110.52
29	m	605	CLA	C3B-C4B-NB	-2.70	108.01	110.52
29	c	304	CLA	CHB-C4A-NA	2.70	128.25	124.51
29	h	312	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
38	k	615	II0	C17-C04-C10	-2.70	106.17	110.47
29	A	802	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
29	B	813	CLA	CHB-C4A-NA	2.70	128.25	124.51
32	B	846	WVN	C40-C39-C36	-2.70	117.94	123.47
38	h	311	II0	C41-C42-C40	-2.70	117.94	123.47
29	b	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
29	e	305	CLA	CHB-C4A-NA	2.70	128.24	124.51
29	m	603	CLA	CHB-C4A-NA	2.70	128.24	124.51
38	a	315	II0	C16-C03-C09	-2.69	106.19	110.47
29	B	804	CLA	CAC-C3C-C2C	-2.69	122.92	127.53
29	c	303	CLA	CMB-C2B-C3B	2.69	133.11	126.59
38	c	313	II0	C05-C03-C09	2.69	115.08	109.62
29	f	605	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
38	e	314	II0	C41-C42-C40	-2.69	117.96	123.47
29	B	814	CLA	CHB-C4A-NA	2.69	128.23	124.51
29	A	851	CLA	C3B-C4B-NB	-2.69	108.02	110.52
40	j	312	KC2	CMB-C2B-C1B	2.69	129.46	124.71
29	A	851	CLA	CHB-C4A-NA	2.69	128.23	124.51
29	a	309	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	i	315	WVN	C39-C40-C37	-2.69	117.96	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	207	CLA	C3B-C4B-NB	-2.69	108.02	110.52
29	s	406	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
29	A	804	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
29	e	308	CLA	C3B-C4B-NB	-2.69	108.02	110.52
32	M	101	WVN	C39-C40-C37	-2.69	117.97	123.47
29	b	306	CLA	C3B-C4B-NB	-2.69	108.02	110.52
29	j	311	CLA	CHB-C4A-NA	2.69	128.23	124.51
29	e	307	CLA	C3B-C4B-NB	-2.69	108.02	110.52
29	b	309	CLA	CHB-C4A-NA	2.69	128.22	124.51
29	f	613	CLA	CMB-C2B-C3B	2.68	133.09	126.59
38	i	319	II0	C05-C03-C09	2.68	115.06	109.62
29	B	822	CLA	C5-C3-C2	2.68	126.55	121.12
29	A	825	CLA	C3B-C4B-NB	-2.68	108.03	110.52
29	i	311	CLA	C3B-C4B-NB	-2.68	108.03	110.52
29	g	307	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
29	k	606	CLA	CHB-C4A-NA	2.68	128.22	124.51
29	d	302	CLA	CHB-C4A-NA	2.68	128.22	124.51
40	i	310	KC2	CHD-C4C-C3C	-2.68	116.38	126.11
37	O	205	LMG	O6-C1-O1	-2.68	103.62	109.97
38	k	620	II0	C41-C42-C40	-2.68	117.98	123.47
29	j	304	CLA	CHB-C4A-NA	2.68	128.22	124.51
29	B	821	CLA	C3B-C4B-NB	-2.68	108.03	110.52
29	e	308	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
40	k	611	KC2	CHD-C4C-NC	2.68	128.27	124.20
29	m	612	CLA	CHB-C4A-NA	2.68	128.22	124.51
29	g	323	CLA	CHB-C4A-NA	2.68	128.22	124.51
38	k	619	II0	C06-C04-C10	2.68	115.05	109.62
29	j	302	CLA	CHB-C4A-NA	2.68	128.22	124.51
38	g	319	II0	C05-C03-C09	2.68	115.05	109.62
40	i	318	KC2	CMB-C2B-C1B	2.68	129.43	124.71
29	d	305	CLA	CHB-C4A-NA	2.68	128.21	124.51
29	g	311	CLA	C3B-C4B-NB	-2.68	108.03	110.52
29	A	818	CLA	CHB-C4A-NA	2.67	128.21	124.51
38	l	313	II0	C12-C14-C10	-2.67	114.50	120.57
29	l	304	CLA	CHB-C4A-NA	2.67	128.21	124.51
37	F	206	LMG	O6-C1-O1	-2.67	103.65	109.97
29	j	302	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
38	n	616	II0	C19-C13-C11	-2.67	109.41	114.36
29	m	608	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	k	606	CLA	C3B-C4B-NB	-2.67	108.04	110.52
40	n	611	KC2	CHD-C4C-C3C	-2.67	116.43	126.11
40	s	404	KC2	CHD-C4C-C3C	-2.67	116.43	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	827	CLA	CMB-C2B-C3B	2.67	133.05	126.59
29	d	306	CLA	O2D-CGD-CBD	2.67	116.01	111.27
38	b	314	II0	C06-C04-C10	2.67	115.03	109.62
29	h	302	CLA	CHB-C4A-NA	2.67	128.20	124.51
31	s	408	LHG	O8-C23-C24	2.67	120.28	111.91
29	f	601	CLA	C3B-C4B-NB	-2.67	108.04	110.52
29	B	834	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	B	837	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	A	824	CLA	CHB-C4A-NA	2.67	128.20	124.51
39	c	315	IHT	C05-C08-C12	2.67	113.95	110.30
29	A	820	CLA	CHB-C4A-NA	2.67	128.20	124.51
29	A	805	CLA	CHB-C4A-NA	2.66	128.20	124.51
29	n	603	CLA	CHB-C4A-NA	2.66	128.20	124.51
29	l	306	CLA	C3B-C4B-NB	-2.66	108.04	110.52
38	n	618	II0	C05-C03-C09	2.66	115.02	109.62
29	A	812	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	A	827	CLA	CHB-C4A-NA	2.66	128.20	124.51
40	c	310	KC2	CHD-C4C-C3C	-2.66	116.45	126.11
31	c	320	LHG	O8-C23-C24	2.66	120.26	111.91
29	A	813	CLA	C3B-C4B-NB	-2.66	108.05	110.52
29	f	612	CLA	C3B-C4B-NB	-2.66	108.05	110.52
40	l	311	KC2	CHD-C4C-C3C	-2.66	116.47	126.11
29	R	203	CLA	CHB-C4A-NA	2.66	128.19	124.51
29	s	403	CLA	C3B-C4B-NB	-2.66	108.05	110.52
38	d	301	II0	C41-C42-C40	-2.66	118.03	123.47
29	j	302	CLA	C3B-C4B-NB	-2.66	108.05	110.52
29	A	827	CLA	CMB-C2B-C3B	2.66	133.02	126.59
31	c	320	LHG	C11-C10-C9	-2.66	100.94	114.42
29	B	831	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
29	a	310	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
29	h	307	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
38	m	615	II0	C17-C04-C10	-2.65	106.25	110.47
29	b	308	CLA	C3B-C4B-NB	-2.65	108.05	110.52
29	c	308	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	a	307	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	f	603	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	A	816	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
29	b	308	CLA	CHB-C4A-NA	2.65	128.18	124.51
35	A	853	SQD	O6-C1-C2	2.65	112.44	108.30
29	B	815	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	k	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	L	207	CLA	CHB-C4A-NA	2.65	128.18	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	847	WVN	C01-C02-C05	2.65	116.16	111.42
39	c	315	IHT	C41-C40-C37	2.65	128.90	123.47
29	A	808	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
29	h	305	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
38	d	315	II0	C05-C03-C09	2.65	114.98	109.62
29	A	815	CLA	CMB-C2B-C1B	-2.65	121.34	125.37
31	e	317	LHG	O8-C23-C24	2.65	120.21	111.91
29	f	606	CLA	CHB-C4A-NA	2.65	128.17	124.51
29	m	613	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	L	203	CLA	C3B-C4B-NB	-2.64	108.06	110.52
29	l	310	CLA	CHB-C4A-NA	2.64	128.17	124.51
29	l	312	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
38	b	314	II0	C41-C42-C40	-2.64	118.06	123.47
29	A	835	CLA	CHB-C4A-NA	2.64	128.16	124.51
29	g	309	CLA	CMB-C2B-C3B	2.64	132.98	126.59
40	d	311	KC2	CHD-C4C-C3C	-2.64	116.54	126.11
29	B	807	CLA	CHB-C4A-NA	2.64	128.16	124.51
29	f	610	CLA	C3B-C4B-NB	-2.64	108.07	110.52
29	j	311	CLA	C3B-C4B-NB	-2.64	108.07	110.52
31	A	842	LHG	O8-C23-C24	2.64	120.19	111.91
29	A	823	CLA	CHD-C1D-ND	-2.64	122.03	124.45
29	g	303	CLA	C3B-C4B-NB	-2.64	108.07	110.52
29	b	304	CLA	CHB-C4A-NA	2.64	128.16	124.51
32	s	405	WVN	C39-C40-C37	-2.64	118.07	123.47
29	j	309	CLA	CHB-C4A-NA	2.63	128.16	124.51
29	m	607	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
40	d	311	KC2	CMC-C2C-C1C	2.63	129.05	125.04
29	B	841	CLA	CHD-C1D-ND	-2.63	122.03	124.45
29	b	304	CLA	CHB-C1B-NB	2.63	127.04	124.26
38	n	615	II0	C29-C31-C33	-2.63	115.00	123.22
40	l	311	KC2	CHD-C4C-NC	2.63	128.19	124.20
38	l	315	II0	C41-C42-C40	-2.63	118.09	123.47
29	A	831	CLA	C3B-C4B-NB	-2.63	108.08	110.52
29	K	101	CLA	C3B-C4B-NB	-2.63	108.08	110.52
29	R	203	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	B	803	CLA	C3B-C4B-NB	-2.63	108.08	110.52
29	m	604	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	k	601	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	A	804	CLA	CAA-CBA-CGA	-2.63	105.57	113.25
32	A	845	WVN	C39-C40-C37	-2.63	118.09	123.47
38	h	311	II0	C12-C14-C10	-2.63	114.61	120.57
29	m	602	CLA	CMC-C2C-C1C	-2.63	121.04	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	311	CLA	CHB-C4A-NA	2.63	128.14	124.51
29	j	313	CLA	CHB-C4A-NA	2.63	128.14	124.51
29	j	307	CLA	C3B-C4B-NB	-2.62	108.08	110.52
38	k	616	II0	C29-C31-C33	-2.62	115.03	123.22
29	B	811	CLA	CHB-C4A-NA	2.62	128.14	124.51
40	i	318	KC2	O2D-CGD-O1D	-2.62	118.71	123.84
29	A	813	CLA	CMB-C2B-C1B	-2.62	121.37	125.37
38	c	313	II0	C29-C31-C33	-2.62	115.03	123.22
29	i	311	CLA	CHB-C4A-NA	2.62	128.14	124.51
38	k	620	II0	C11-C13-C09	-2.62	114.62	120.57
40	c	310	KC2	C2A-C1A-CHA	-2.62	118.77	127.44
31	m	619	LHG	O8-C23-C24	2.62	120.13	111.91
29	g	316	CLA	C3B-C4B-NB	-2.62	108.08	110.52
29	Q	302	CLA	C3B-C4B-NB	-2.62	108.08	110.52
29	B	831	CLA	CHB-C4A-NA	2.62	128.13	124.51
38	m	618	II0	C29-C31-C33	-2.62	115.04	123.22
29	b	305	CLA	CHB-C4A-NA	2.62	128.13	124.51
29	A	820	CLA	CHB-C1B-NB	2.62	127.03	124.26
29	B	839	CLA	C3B-C4B-NB	-2.62	108.09	110.52
29	h	302	CLA	C3B-C4B-NB	-2.62	108.09	110.52
29	K	102	CLA	CHB-C4A-NA	2.62	128.13	124.51
29	h	306	CLA	CHB-C4A-NA	2.62	128.13	124.51
29	e	301	CLA	CHB-C4A-NA	2.62	128.13	124.51
29	i	312	CLA	CBC-CAC-C3C	2.62	119.64	112.43
29	B	822	CLA	C3B-C4B-NB	-2.62	108.09	110.52
29	A	833	CLA	CHB-C4A-NA	2.61	128.13	124.51
29	e	305	CLA	C3B-C4B-NB	-2.61	108.09	110.52
29	h	301	CLA	CHB-C4A-NA	2.61	128.13	124.51
29	e	303	CLA	CMB-C2B-C3B	2.61	132.92	126.59
40	i	318	KC2	CHD-C4C-C3C	-2.61	116.64	126.11
40	g	313	KC2	CHD-C4C-NC	2.61	128.17	124.20
29	B	839	CLA	CHB-C4A-NA	2.61	128.12	124.51
29	l	304	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
29	A	808	CLA	CHB-C4A-NA	2.61	128.12	124.51
38	i	316	II0	C05-C03-C09	2.61	114.91	109.62
29	B	840	CLA	C3B-C4B-NB	-2.61	108.09	110.52
40	e	309	KC2	CMB-C2B-C1B	2.61	129.31	124.71
38	f	618	II0	C29-C31-C33	-2.61	115.08	123.22
39	c	319	IHT	C41-C40-C37	2.61	128.81	123.47
29	A	836	CLA	CHC-C4B-NB	2.61	127.02	124.26
40	g	314	KC2	CBC-CAC-C3C	-2.61	114.66	127.62
29	i	303	CLA	CHB-C4A-NA	2.60	128.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	j	312	KC2	CAA-C2A-C1A	-2.60	112.77	124.75
29	A	822	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	a	306	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	L	204	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	B	821	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	B	842	CLA	CHB-C1B-NB	2.60	127.01	124.26
29	e	311	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	f	605	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	c	312	CLA	CHC-C4B-NB	2.60	127.01	124.26
29	B	830	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	B	824	CLA	C3B-C4B-NB	-2.60	108.11	110.52
29	l	308	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
29	c	303	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	k	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	i	305	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	k	607	CLA	CHC-C4B-NB	2.60	127.01	124.26
29	A	834	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	B	823	CLA	C3B-C4B-NB	-2.59	108.11	110.52
29	b	313	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	B	806	CLA	CHB-C4A-NA	2.59	128.10	124.51
29	j	303	CLA	CHB-C4A-NA	2.59	128.10	124.51
29	A	831	CLA	CHB-C4A-NA	2.59	128.10	124.51
31	f	619	LHG	O8-C23-C24	2.59	120.05	111.91
29	m	610	CLA	C3B-C4B-NB	-2.59	108.11	110.52
40	m	611	KC2	CHD-C4C-C3C	-2.59	116.72	126.11
38	m	618	II0	C11-C13-C09	-2.59	114.69	120.57
29	A	850	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	a	302	CLA	CHB-C4A-NA	2.59	128.09	124.51
29	B	832	CLA	C3B-C4B-NB	-2.59	108.11	110.52
38	m	614	II0	C05-C03-C09	2.59	114.87	109.62
29	B	829	CLA	CMB-C2B-C3B	2.59	132.86	126.59
29	d	307	CLA	C2D-C1D-ND	-2.59	108.20	110.10
29	b	312	CLA	CHB-C4A-NA	2.59	128.09	124.51
29	B	812	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
38	n	615	II0	C07-C11-C13	2.59	117.01	111.85
38	m	614	II0	C29-C31-C33	-2.59	115.15	123.22
29	B	812	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	f	613	CLA	CHB-C4A-NA	2.59	128.09	124.51
36	j	319	DGD	CDB-CCB-CBB	-2.58	101.30	114.42
29	e	307	CLA	CHB-C4A-NA	2.58	128.09	124.51
29	f	610	CLA	CHB-C4A-NA	2.58	128.09	124.51
29	B	808	CLA	CBA-CAA-C2A	2.58	121.49	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	m	607	CLA	CHB-C4A-NA	2.58	128.09	124.51
29	A	834	CLA	C3B-C4B-NB	-2.58	108.12	110.52
29	B	806	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	a	318	LHG	O8-C23-C24	2.58	120.01	111.91
29	g	303	CLA	CHB-C4A-NA	2.58	128.08	124.51
32	M	101	WVN	C10-C06-C13	2.58	114.45	110.48
29	A	820	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	g	301	LHG	C11-C10-C9	-2.58	101.33	114.42
29	A	826	CLA	C3B-C4B-NB	-2.58	108.12	110.52
38	d	316	II0	C11-C13-C09	-2.58	114.72	120.57
29	B	804	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	a	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	A	817	CLA	CHB-C4A-NA	2.58	128.08	124.51
38	k	617	II0	C06-C08-C12	2.58	113.83	110.30
38	d	317	II0	C38-C36-C34	-2.58	114.02	118.08
29	d	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
32	s	407	WVN	C14-C15-C13	-2.57	118.99	122.73
38	f	614	II0	C05-C03-C09	2.57	114.84	109.62
31	j	318	LHG	C11-C10-C9	-2.57	101.36	114.42
39	g	324	IHT	C18-C22-C23	-2.57	122.35	126.23
29	c	301	CLA	CHB-C4A-NA	2.57	128.07	124.51
29	n	601	CLA	CHB-C4A-NA	2.57	128.07	124.51
32	A	846	WVN	C03-C04-C09	-2.57	107.73	112.00
29	b	310	CLA	CHB-C4A-NA	2.57	128.07	124.51
29	f	607	CLA	C3B-C4B-NB	-2.57	108.13	110.52
38	J	103	II0	C05-C03-C09	2.57	114.83	109.62
31	J	104	LHG	O8-C23-C24	2.57	119.97	111.91
40	k	611	KC2	CMB-C2B-C1B	2.57	129.24	124.71
40	g	313	KC2	CHB-C1B-NB	-2.57	122.09	124.45
29	A	824	CLA	CMB-C2B-C1B	-2.57	121.46	125.37
29	B	838	CLA	CHB-C4A-NA	2.57	128.06	124.51
29	O	202	CLA	C3B-C4B-NB	-2.57	108.13	110.52
29	A	838	CLA	C3B-C4B-NB	-2.57	108.13	110.52
29	B	816	CLA	CHB-C1B-NB	2.57	126.97	124.26
29	k	603	CLA	CMB-C2B-C3B	2.57	132.80	126.59
38	l	315	II0	C12-C14-C10	-2.57	114.75	120.57
31	L	209	LHG	O8-C23-C24	2.57	119.96	111.91
29	A	818	CLA	CHD-C1D-ND	-2.57	122.10	124.45
29	a	305	CLA	C3B-C4B-NB	-2.57	108.14	110.52
32	F	205	WVN	C21-C15-C14	-2.56	108.69	113.62
38	a	317	II0	C11-C13-C09	-2.56	114.75	120.57
29	g	308	CLA	O2D-CGD-CBD	2.56	115.82	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	613	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
29	e	308	CLA	CHB-C4A-NA	2.56	128.06	124.51
29	j	314	CLA	CHB-C4A-NA	2.56	128.06	124.51
29	A	806	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	g	304	CLA	CHB-C4A-NA	2.56	128.05	124.51
37	L	210	LMG	O6-C1-O1	-2.56	103.92	109.97
29	g	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
38	e	314	II0	C29-C31-C33	-2.56	115.24	123.22
38	k	619	II0	C11-C13-C09	-2.56	114.77	120.57
29	k	607	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	f	608	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	B	838	CLA	C3B-C4B-NB	-2.55	108.14	110.52
29	h	312	CLA	C3B-C4B-NB	-2.55	108.15	110.52
38	n	614	II0	C06-C08-C12	-2.55	106.81	110.30
29	A	832	CLA	O2D-CGD-CBD	2.55	115.80	111.27
29	A	808	CLA	C3B-C4B-NB	-2.55	108.15	110.52
29	B	804	CLA	C3B-C4B-NB	-2.55	108.15	110.52
29	A	809	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	b	310	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	a	318	LHG	C11-C10-C9	-2.55	101.50	114.42
29	A	814	CLA	CHB-C4A-NA	2.55	128.03	124.51
38	c	314	II0	C05-C07-C11	-2.55	106.82	110.30
40	g	314	KC2	CMB-C2B-C1B	2.54	129.20	124.71
29	b	302	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	A	832	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	i	315	WVN	C01-C02-C05	2.54	115.97	111.42
29	e	302	CLA	C3B-C4B-NB	-2.54	108.16	110.52
38	f	615	II0	C05-C03-C09	2.54	114.77	109.62
38	n	618	II0	C41-C42-C40	-2.54	118.27	123.47
29	L	202	CLA	CHB-C4A-NA	2.54	128.02	124.51
32	l	316	WVN	C02-C05-C09	-2.54	118.34	121.47
29	A	839	CLA	CMB-C2B-C3B	2.54	132.73	126.59
31	m	619	LHG	C11-C10-C9	-2.54	101.54	114.42
29	d	307	CLA	O2D-CGD-CBD	2.54	115.78	111.27
29	h	306	CLA	C3B-C4B-NB	-2.54	108.16	110.52
38	a	314	II0	C05-C07-C11	-2.54	106.83	110.30
29	d	307	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	n	607	CLA	CHC-C4B-NB	2.54	126.94	124.26
29	f	610	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
29	R	203	CLA	CHC-C4B-NB	2.54	126.94	124.26
29	k	601	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	B	825	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	303	CLA	CHB-C4A-NA	2.53	128.01	124.51
40	s	401	KC2	CHD-C4C-NC	2.53	128.04	124.20
32	h	308	WVN	C26-C29-C31	-2.53	115.31	123.22
29	m	601	CLA	C3B-C4B-NB	-2.53	108.17	110.52
29	b	312	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
29	B	842	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
29	m	601	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	d	310	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	g	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	b	313	CLA	C2A-C1A-CHA	2.53	128.28	123.86
40	f	611	KC2	CHD-C4C-C3C	-2.53	116.95	126.11
38	e	312	II0	C12-C14-C10	-2.53	114.84	120.57
29	a	308	CLA	CHB-C4A-NA	2.53	128.00	124.51
29	A	806	CLA	C3B-C4B-NB	-2.52	108.17	110.52
29	R	203	CLA	CBA-CAA-C2A	2.52	121.31	113.86
29	B	838	CLA	O2D-CGD-CBD	2.52	115.75	111.27
29	B	836	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	A	807	CLA	C3B-C4B-NB	-2.52	108.17	110.52
32	R	202	WVN	C39-C40-C37	-2.52	118.31	123.47
40	f	611	KC2	CHB-C1B-NB	-2.52	122.14	124.45
29	B	841	CLA	CAC-C3C-C4C	2.52	128.08	124.81
29	b	310	CLA	CHB-C1B-NB	2.52	126.93	124.26
29	A	839	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	c	316	LHG	O8-C23-C24	2.52	119.81	111.91
40	k	611	KC2	O1D-CGD-CBD	-2.52	119.33	124.48
32	A	847	WVN	C31-C32-C36	-2.52	115.08	118.94
32	B	846	WVN	C23-C25-C28	-2.52	115.08	118.94
32	I	101	WVN	C01-C02-C05	2.52	115.93	111.42
32	h	308	WVN	C01-C02-C05	2.52	115.93	111.42
29	m	609	CLA	C3B-C4B-NB	-2.52	108.18	110.52
32	A	846	WVN	C38-C34-C33	-2.52	114.11	118.08
29	B	802	CLA	CMB-C2B-C3B	2.51	132.68	126.59
38	f	614	II0	C12-C14-C10	-2.51	114.86	120.57
29	m	606	CLA	C3B-C4B-NB	-2.51	108.18	110.52
38	m	615	II0	C29-C31-C33	-2.51	115.37	123.22
29	c	311	CLA	CAC-C3C-C4C	2.51	128.07	124.81
29	s	406	CLA	CHB-C4A-NA	2.51	127.99	124.51
29	e	303	CLA	CHB-C4A-NA	2.51	127.99	124.51
40	s	404	KC2	O1D-CGD-CBD	-2.51	119.34	124.48
32	s	405	WVN	C20-C13-C15	-2.51	115.38	121.46
29	n	608	CLA	C1-C2-C3	-2.51	121.70	126.04
32	B	849	WVN	C38-C34-C33	-2.51	114.12	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s	401	KC2	CHD-C4C-C3C	-2.51	117.01	126.11
29	g	308	CLA	C3B-C4B-NB	-2.51	108.19	110.52
29	A	817	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
29	n	609	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	B	812	CLA	C3B-C4B-NB	-2.51	108.19	110.52
29	A	802	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	k	608	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	b	308	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
29	A	851	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
31	g	322	LHG	C11-C10-C9	-2.51	101.70	114.42
35	A	853	SQD	O48-C23-C24	2.51	119.77	111.91
38	n	616	II0	C08-C12-C14	2.50	116.84	111.85
29	B	810	CLA	CHB-C4A-NA	2.50	127.97	124.51
38	n	615	II0	C05-C07-C11	2.50	113.73	110.30
40	m	611	KC2	CHD-C4C-NC	2.50	128.00	124.20
38	f	618	II0	C12-C14-C10	-2.50	114.89	120.57
39	j	317	IHT	C22-C18-C07	-2.50	120.17	127.20
29	g	305	CLA	CMB-C2B-C3B	2.50	132.65	126.59
29	e	304	CLA	C3B-C4B-NB	-2.50	108.19	110.52
39	g	324	IHT	C22-C18-C07	2.50	134.23	127.20
31	b	318	LHG	O8-C23-C24	2.50	119.75	111.91
32	F	205	WVN	C31-C32-C36	-2.50	115.11	118.94
29	d	306	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	c	309	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	L	208	LHG	C11-C10-C9	-2.50	101.76	114.42
29	d	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
40	j	312	KC2	CHD-C4C-C3C	-2.49	117.07	126.11
29	j	303	CLA	C3B-C4B-NB	-2.49	108.20	110.52
29	n	601	CLA	C3B-C4B-NB	-2.49	108.20	110.52
38	f	615	II0	C29-C31-C33	-2.49	115.43	123.22
38	l	313	II0	C29-C31-C33	-2.49	115.44	123.22
29	l	308	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
29	n	608	CLA	CHB-C4A-NA	2.49	127.95	124.51
38	b	315	II0	C29-C31-C33	-2.49	115.45	123.22
38	l	314	II0	C05-C03-C09	2.49	114.66	109.62
32	A	854	WVN	C26-C29-C31	-2.49	115.45	123.22
32	l	316	WVN	C26-C29-C31	-2.49	115.45	123.22
31	n	619	LHG	O8-C23-C24	2.49	119.72	111.91
29	i	306	CLA	C3B-C4B-NB	-2.49	108.21	110.52
37	c	317	LMG	C40-C39-C38	-2.49	101.80	114.42
29	a	306	CLA	C3B-C4B-NB	-2.49	108.21	110.52
38	f	614	II0	C33-C35-C39	-2.49	115.13	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	307	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	B	833	CLA	C3B-C4B-NB	-2.48	108.21	110.52
29	j	304	CLA	CMB-C2B-C3B	2.48	132.60	126.59
40	f	611	KC2	O1D-CGD-CBD	-2.48	119.41	124.48
38	n	614	II0	C05-C07-C11	2.48	113.70	110.30
40	s	404	KC2	CHD-C4C-NC	2.48	127.97	124.20
29	g	302	CLA	C3B-C4B-NB	-2.48	108.21	110.52
29	g	306	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
40	d	312	KC2	C3C-C2C-C1C	2.48	108.32	106.49
36	j	319	DGD	O6E-C5E-C4E	2.48	114.19	109.69
31	a	301	LHG	C11-C10-C9	-2.48	101.85	114.42
29	A	814	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
29	A	850	CLA	CMB-C2B-C3B	2.48	132.59	126.59
38	i	313	II0	C12-C14-C10	-2.47	114.95	120.57
29	B	831	CLA	C3B-C4B-NB	-2.47	108.22	110.52
29	n	604	CLA	C3B-C4B-NB	-2.47	108.22	110.52
29	j	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
38	i	314	II0	C05-C03-C09	2.47	114.63	109.62
29	B	820	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	c	305	CLA	C3B-C4B-NB	-2.47	108.22	110.52
29	A	840	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
29	A	840	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
29	A	812	CLA	C3B-C4B-NB	-2.47	108.22	110.52
29	a	303	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	A	819	CLA	C3B-C4B-NB	-2.47	108.23	110.52
29	A	819	CLA	CED-O2D-CGD	2.47	121.52	115.94
29	A	802	CLA	CHB-C1B-NB	2.47	126.87	124.26
38	a	317	II0	C41-C42-C40	-2.46	118.43	123.47
32	i	315	WVN	C26-C29-C31	-2.46	115.53	123.22
40	f	611	KC2	CMB-C2B-C1B	2.46	129.05	124.71
31	i	317	LHG	C11-C10-C9	-2.46	101.93	114.42
29	A	819	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	g	301	LHG	O8-C23-C24	2.46	119.62	111.91
29	c	308	CLA	C3B-C4B-NB	-2.46	108.23	110.52
29	A	830	CLA	CHB-C4A-NA	2.46	127.91	124.51
35	A	853	SQD	C3-C4-C5	2.46	114.62	110.24
31	A	848	LHG	C11-C10-C9	-2.46	101.96	114.42
29	i	309	CLA	C3B-C4B-NB	-2.46	108.24	110.52
29	B	812	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	J	104	LHG	C11-C10-C9	-2.45	101.97	114.42
29	h	303	CLA	C1-C2-C3	-2.45	122.78	126.75
40	k	611	KC2	CHD-C4C-C3C	-2.45	117.22	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	303	CLA	CMB-C2B-C3B	2.45	132.53	126.59
29	A	802	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
29	d	309	CLA	CMA-C3A-C2A	-2.45	110.38	116.10
37	F	206	LMG	C40-C39-C38	-2.45	101.98	114.42
29	l	309	CLA	C3B-C4B-NB	-2.45	108.24	110.52
29	B	809	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
40	d	311	KC2	O1D-CGD-CBD	-2.45	119.47	124.48
38	f	616	II0	C29-C31-C33	-2.45	115.57	123.22
40	s	401	KC2	CAA-C2A-C1A	-2.45	113.49	124.75
29	B	818	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
38	d	301	II0	C11-C13-C09	-2.45	115.01	120.57
29	a	309	CLA	C3B-C4B-NB	-2.45	108.24	110.52
29	e	304	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
29	b	309	CLA	C3B-C4B-NB	-2.45	108.25	110.52
29	B	837	CLA	CHB-C4A-NA	2.45	127.89	124.51
29	A	813	CLA	CHD-C1D-ND	-2.45	122.21	124.45
29	b	307	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
29	A	803	CLA	CHB-C4A-NA	2.44	127.89	124.51
29	b	304	CLA	C3B-C4B-NB	-2.44	108.25	110.52
29	h	305	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	i	317	LHG	O8-C23-C24	2.44	119.57	111.91
29	F	201	CLA	CHB-C1B-NB	2.44	126.84	124.26
38	k	616	II0	C06-C08-C12	-2.44	106.96	110.30
29	m	602	CLA	O2D-CGD-CBD	2.44	115.61	111.27
32	A	845	WVN	C10-C06-C13	2.44	114.24	110.48
38	k	615	II0	C05-C03-C09	2.44	114.56	109.62
38	e	314	II0	C12-C14-C10	-2.44	115.03	120.57
29	n	605	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	L	208	LHG	C20-C19-C18	-2.44	102.06	114.42
29	c	302	CLA	CMB-C2B-C3B	2.44	132.49	126.59
29	A	838	CLA	CHB-C1B-NB	2.44	126.83	124.26
29	l	304	CLA	C1-C2-C3	-2.43	121.83	126.04
29	F	202	CLA	CHB-C1B-NB	2.43	126.83	124.26
29	b	306	CLA	CAC-C3C-C4C	2.43	127.97	124.81
29	B	816	CLA	CHD-C1D-ND	-2.43	122.22	124.45
31	c	316	LHG	C11-C10-C9	-2.43	102.07	114.42
39	m	617	IHT	C05-C08-C12	-2.43	106.97	110.30
29	B	834	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
29	A	819	CLA	C1-C2-C3	-2.43	121.84	126.04
38	e	313	II0	C17-C04-C10	-2.43	106.61	110.47
29	A	821	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	A	835	CLA	O2A-CGA-O1A	-2.43	117.46	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	m	613	CLA	CHC-C4B-NB	2.43	126.83	124.26
32	F	204	WVN	C12-C14-C15	-2.43	109.74	114.08
29	m	613	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	B	815	CLA	CMB-C2B-C3B	2.43	132.47	126.59
29	e	310	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
29	c	303	CLA	CHB-C1B-NB	2.43	126.83	124.26
29	A	825	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
31	e	317	LHG	C11-C10-C9	-2.43	102.11	114.42
38	c	313	II0	C12-C14-C10	-2.43	115.06	120.57
29	A	838	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
29	c	307	CLA	C3B-C4B-NB	-2.43	108.27	110.52
29	m	602	CLA	C3B-C4B-NB	-2.43	108.27	110.52
31	a	301	LHG	O8-C23-C24	2.42	119.51	111.91
29	f	608	CLA	C3B-C4B-NB	-2.42	108.27	110.52
32	M	101	WVN	C01-C02-C11	-2.42	109.64	112.70
32	L	206	WVN	C28-C30-C33	-2.42	115.66	123.22
29	a	311	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
29	a	308	CLA	C3B-C4B-NB	-2.42	108.27	110.52
29	g	311	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
40	g	315	KC2	CHB-C1B-NB	-2.42	122.23	124.45
29	B	804	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
29	B	841	CLA	CBC-CAC-C3C	2.42	119.10	112.43
29	l	312	CLA	C3B-C4B-NB	-2.42	108.27	110.52
29	f	603	CLA	CMB-C2B-C3B	2.42	132.44	126.59
31	A	843	LHG	C11-C10-C9	-2.42	102.16	114.42
40	g	315	KC2	O2D-CGD-O1D	-2.42	119.11	123.84
31	b	318	LHG	C20-C19-C18	-2.42	102.16	114.42
29	g	308	CLA	CHB-C4A-NA	2.42	127.85	124.51
31	f	619	LHG	C20-C19-C18	-2.41	102.17	114.42
32	R	201	WVN	C10-C06-C13	2.41	114.20	110.48
38	l	313	II0	C05-C03-C09	2.41	114.51	109.62
31	b	318	LHG	C11-C10-C9	-2.41	102.17	114.42
29	l	305	CLA	CMB-C2B-C3B	2.41	132.43	126.59
29	A	816	CLA	CHC-C4B-NB	2.41	126.81	124.26
38	d	315	II0	C18-C04-C10	-2.41	106.63	110.47
38	k	619	II0	C41-C42-C40	-2.41	118.53	123.47
37	n	620	LMG	C38-C37-C36	-2.41	102.18	114.42
29	A	804	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
31	f	620	LHG	C11-C10-C9	-2.41	102.18	114.42
38	e	314	II0	C05-C07-C11	-2.41	107.00	110.30
29	B	801	CLA	CHB-C1B-NB	2.41	126.81	124.26
29	A	813	CLA	CHB-C4A-NA	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	402	CLA	C3B-C4B-NB	-2.41	108.28	110.52
40	e	309	KC2	CHB-C1B-NB	-2.41	122.24	124.45
29	B	813	CLA	CBA-CAA-C2A	2.41	120.97	113.86
29	i	308	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
38	a	314	II0	C30-C32-C34	-2.41	115.71	123.22
29	A	812	CLA	CMB-C2B-C1B	-2.41	121.71	125.37
29	k	604	CLA	C3B-C4B-NB	-2.40	108.28	110.52
29	j	305	CLA	C3B-C4B-NB	-2.40	108.28	110.52
29	B	833	CLA	CHB-C4A-NA	2.40	127.84	124.51
38	h	311	II0	C15-C03-C09	-2.40	106.65	110.47
38	g	317	II0	C15-C03-C09	-2.40	106.65	110.47
29	h	306	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
29	k	614	CLA	CHC-C4B-NB	2.40	126.80	124.26
29	m	603	CLA	CMB-C2B-C3B	2.40	132.40	126.59
38	j	301	II0	C12-C14-C10	-2.40	115.12	120.57
29	A	823	CLA	C2D-C1D-ND	-2.40	108.33	110.10
31	A	848	LHG	C20-C19-C18	-2.40	102.24	114.42
29	k	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	g	305	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	l	308	CLA	C3B-C4B-NB	-2.40	108.29	110.52
29	d	303	CLA	CHB-C1B-NB	2.40	126.80	124.26
29	f	602	CLA	CMB-C2B-C3B	2.40	132.40	126.59
40	n	611	KC2	CHD-C4C-NC	2.40	127.84	124.20
38	b	314	II0	C12-C14-C10	-2.40	115.13	120.57
31	l	318	LHG	C11-C10-C9	-2.40	102.25	114.42
29	B	819	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
29	m	604	CLA	CMB-C2B-C3B	2.40	132.39	126.59
40	n	611	KC2	O2D-CGD-O1D	-2.40	119.15	123.84
32	F	204	WVN	C01-C02-C11	-2.40	109.67	112.70
29	j	303	CLA	CMB-C2B-C3B	2.40	132.39	126.59
38	i	319	II0	C15-C03-C09	-2.40	106.66	110.47
29	n	610	CLA	C2A-C1A-CHA	2.40	128.05	123.86
29	b	303	CLA	C3B-C4B-NB	-2.40	108.29	110.52
40	e	309	KC2	CHD-C4C-C3C	-2.40	117.43	126.11
31	a	318	LHG	C20-C19-C18	-2.39	102.27	114.42
29	f	607	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	B	842	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	J	102	CLA	CHB-C1B-NB	2.39	126.79	124.26
29	O	201	CLA	C3B-C4B-NB	-2.39	108.30	110.52
29	s	402	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	B	829	CLA	CHB-C4A-NA	2.39	127.81	124.51
31	L	209	LHG	C11-C10-C9	-2.39	102.31	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	j	312	KC2	C2A-C1A-CHA	-2.39	119.55	127.44
29	B	826	CLA	CMB-C2B-C3B	2.39	132.37	126.59
40	g	314	KC2	CMC-C2C-C1C	2.38	128.67	125.04
38	j	316	II0	C05-C03-C09	2.38	114.45	109.62
36	j	319	DGD	O2D-C2D-C1D	-2.38	104.26	110.05
29	A	805	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
29	A	810	CLA	C3B-C4B-NB	-2.38	108.31	110.52
29	b	306	CLA	CHD-C1D-ND	-2.38	122.27	124.45
29	B	823	CLA	CHB-C4A-NA	2.38	127.80	124.51
38	e	316	II0	C04-C06-C08	2.38	119.02	113.64
29	B	802	CLA	C3B-C4B-NB	-2.38	108.31	110.52
38	i	314	II0	C17-C04-C10	-2.38	106.69	110.47
38	k	620	II0	C06-C04-C10	2.38	114.44	109.62
29	A	828	CLA	CHB-C4A-NA	2.38	127.80	124.51
29	A	811	CLA	CHB-C1B-NB	2.38	126.77	124.26
29	L	204	CLA	C3B-C4B-NB	-2.38	108.31	110.52
29	A	833	CLA	CHC-C4B-NB	2.38	126.77	124.26
37	O	205	LMG	O1-C7-C8	-2.38	105.17	110.90
29	f	609	CLA	C3B-C4B-NB	-2.37	108.31	110.52
37	c	317	LMG	O3-C3-C2	-2.37	104.86	110.35
37	n	620	LMG	O3-C3-C2	-2.37	104.86	110.35
29	c	302	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	g	316	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	A	821	CLA	C3B-C4B-NB	-2.37	108.31	110.52
38	J	103	II0	C15-C03-C09	-2.37	106.70	110.47
29	m	602	CLA	CMC-C2C-C3C	2.37	132.56	126.12
29	i	302	CLA	C3B-C4B-NB	-2.37	108.31	110.52
29	A	824	CLA	C2A-C1A-CHA	2.37	128.00	123.86
29	c	301	CLA	C3B-C4B-NB	-2.37	108.32	110.52
32	B	846	WVN	C17-C06-C13	2.37	114.14	110.30
38	m	615	II0	C16-C03-C09	-2.37	106.70	110.47
32	e	315	WVN	C39-C40-C37	-2.37	118.62	123.47
40	s	401	KC2	CMC-C2C-C1C	2.37	128.65	125.04
31	c	320	LHG	C20-C19-C18	-2.37	102.40	114.42
38	l	315	II0	C07-C11-C13	2.37	116.57	111.85
29	A	821	CLA	CHD-C1D-ND	-2.37	122.28	124.45
32	A	854	WVN	C39-C40-C37	-2.37	118.63	123.47
29	a	310	CLA	C3B-C4B-NB	-2.37	108.32	110.52
29	c	309	CLA	C3B-C4B-NB	-2.36	108.32	110.52
38	h	310	II0	C06-C04-C10	2.36	114.41	109.62
29	A	825	CLA	CHD-C1D-ND	-2.36	122.28	124.45
36	B	844	DGD	CFB-CEB-CDB	-2.36	102.45	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	620	II0	C05-C03-C09	2.36	114.40	109.62
29	c	305	CLA	CHB-C4A-NA	2.36	127.77	124.51
29	A	804	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
29	B	808	CLA	C3B-C4B-NB	-2.36	108.33	110.52
38	g	317	II0	C11-C13-C09	-2.36	115.22	120.57
29	c	304	CLA	C3B-C4B-NB	-2.36	108.33	110.52
29	a	305	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
37	Q	301	LMG	O7-C10-O9	-2.35	118.01	123.70
40	m	611	KC2	CMB-C2B-C1B	2.35	128.86	124.71
29	d	305	CLA	C3B-C4B-NB	-2.35	108.33	110.52
32	F	204	WVN	C06-C13-C20	-2.35	109.12	115.78
29	A	832	CLA	C3B-C4B-NB	-2.35	108.33	110.52
29	b	313	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
29	k	605	CLA	C3B-C4B-NB	-2.35	108.33	110.52
32	l	302	WVN	C21-C15-C14	-2.35	109.10	113.62
40	g	314	KC2	CAC-C3C-C4C	2.35	135.42	124.47
29	J	102	CLA	CAA-C2A-C3A	-2.35	108.39	114.26
29	A	837	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	A	833	CLA	C3B-C4B-NB	-2.35	108.34	110.52
29	O	201	CLA	CHB-C1B-NB	2.35	126.74	124.26
29	B	839	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
29	B	840	CLA	O2D-CGD-CBD	2.35	115.44	111.27
40	e	309	KC2	C2A-C1A-CHA	-2.35	119.68	127.44
29	K	102	CLA	C3B-C4B-NB	-2.35	108.34	110.52
38	J	103	II0	C41-C42-C40	-2.35	118.67	123.47
40	g	313	KC2	CHD-C4C-C3C	-2.35	117.60	126.11
29	F	202	CLA	CHB-C4A-NA	2.35	127.75	124.51
29	b	307	CLA	CHB-C4A-NA	2.35	127.75	124.51
29	d	310	CLA	C2D-C1D-ND	-2.34	108.38	110.10
29	A	805	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	B	837	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
29	f	604	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
38	m	616	II0	C16-C03-C09	-2.34	106.74	110.47
38	a	313	II0	C29-C31-C33	-2.34	115.91	123.22
31	n	619	LHG	C11-C10-C9	-2.34	102.54	114.42
38	e	313	II0	C05-C03-C09	2.34	114.36	109.62
29	a	311	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	d	313	CLA	C2A-C1A-CHA	2.34	127.95	123.86
29	A	811	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	a	307	CLA	CHB-C1B-NB	2.34	126.73	124.26
29	B	816	CLA	CMB-C2B-C3B	2.34	132.25	126.59
29	A	819	CLA	CAA-C2A-C3A	-2.34	106.37	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s	404	KC2	CAB-C3B-C4B	2.34	130.54	124.90
38	j	315	II0	C11-C13-C09	-2.34	115.27	120.57
29	B	840	CLA	O2A-C1-C2	-2.34	102.50	108.64
29	a	302	CLA	C3B-C4B-NB	-2.33	108.35	110.52
32	h	308	WVN	C21-C15-C14	-2.33	109.13	113.62
38	i	316	II0	C15-C03-C09	-2.33	106.76	110.47
29	B	805	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
29	h	312	CLA	CHB-C4A-NA	2.33	127.74	124.51
29	g	323	CLA	CBA-CAA-C2A	2.33	120.75	113.86
32	s	407	WVN	C38-C34-C33	-2.33	114.40	118.08
32	i	315	WVN	C18-C06-C13	2.33	114.08	110.30
29	B	822	CLA	C2A-C1A-CHA	2.33	127.94	123.86
29	A	803	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
29	B	828	CLA	CHB-C4A-NA	2.33	127.73	124.51
31	a	301	LHG	C20-C19-C18	-2.33	102.60	114.42
40	m	611	KC2	C2A-C1A-CHA	-2.33	119.74	127.44
29	i	302	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
29	A	806	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
38	m	614	II0	C08-C12-C14	2.33	116.49	111.85
31	L	209	LHG	C27-C26-C25	-2.33	102.61	114.42
38	i	314	II0	C07-C11-C13	2.33	116.49	111.85
29	A	815	CLA	C3B-C4B-NB	-2.33	108.36	110.52
29	B	827	CLA	C2D-C1D-ND	-2.32	108.39	110.10
29	a	305	CLA	CHD-C1D-ND	-2.32	122.32	124.45
40	g	314	KC2	CGD-CBD-CAD	-2.32	103.21	110.73
29	B	827	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
29	m	602	CLA	CAC-C3C-C4C	-2.32	121.80	124.81
29	h	302	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
29	l	304	CLA	O2D-CGD-CBD	2.32	115.39	111.27
29	g	323	CLA	CAA-C2A-C1A	2.32	119.58	111.97
29	A	825	CLA	CAA-C2A-C1A	-2.32	104.38	111.97
38	e	313	II0	C06-C08-C12	2.32	113.48	110.30
29	n	608	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
32	A	854	WVN	C07-C01-C03	-2.32	104.26	109.03
32	F	205	WVN	C40-C39-C36	-2.32	118.73	123.47
29	n	613	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
29	k	604	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
29	k	605	CLA	C2A-C1A-CHA	2.32	127.91	123.86
29	s	403	CLA	C3A-C2A-C1A	2.32	104.81	101.34
29	b	303	CLA	CMB-C2B-C3B	2.32	132.19	126.59
29	A	839	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	L	204	CLA	CMB-C2B-C1B	-2.31	121.84	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	607	CLA	C2D-C1D-ND	-2.31	108.40	110.10
38	k	618	II0	C41-C42-C40	2.31	128.21	123.47
40	d	311	KC2	C2A-C1A-CHA	-2.31	119.79	127.44
29	l	308	CLA	CHB-C4A-NA	2.31	127.71	124.51
29	a	303	CLA	C3B-C4B-NB	-2.31	108.37	110.52
38	d	317	II0	C05-C03-C09	2.31	114.31	109.62
29	B	842	CLA	CMB-C2B-C3B	2.31	132.19	126.59
29	m	602	CLA	CMB-C2B-C3B	2.31	132.19	126.59
29	A	816	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
29	a	308	CLA	CMB-C2B-C3B	2.31	132.18	126.59
29	K	101	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
29	A	809	CLA	C3B-C4B-NB	-2.31	108.37	110.52
36	B	844	DGD	O2D-C2D-C3D	-2.31	105.01	110.35
29	A	821	CLA	CHB-C4A-NA	2.31	127.71	124.51
37	b	319	LMG	O1-C1-C2	-2.31	104.70	108.30
29	B	823	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
32	A	854	WVN	C03-C04-C09	-2.31	108.17	112.00
38	g	318	II0	C12-C14-C10	-2.31	115.33	120.57
38	g	317	II0	C08-C12-C14	2.31	116.45	111.85
29	A	810	CLA	CHB-C4A-NA	2.31	127.70	124.51
29	a	308	CLA	CHB-C1B-NB	2.31	126.70	124.26
37	F	206	LMG	O1-C7-C8	-2.31	105.34	110.90
38	c	313	II0	C06-C08-C12	2.30	113.46	110.30
40	i	310	KC2	C2A-C1A-CHA	-2.30	119.83	127.44
29	B	817	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	s	406	CLA	CHB-C1B-NB	2.30	126.69	124.26
38	j	316	II0	C12-C14-C10	-2.30	115.35	120.57
29	f	606	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
40	c	310	KC2	O2D-CGD-O1D	-2.30	119.34	123.84
29	h	304	CLA	C3B-C4B-NB	-2.30	108.38	110.52
31	c	320	LHG	C27-C26-C25	-2.30	102.75	114.42
40	d	311	KC2	CHB-C1B-NB	-2.30	122.34	124.45
29	l	304	CLA	CMB-C2B-C3B	2.30	132.15	126.59
40	e	309	KC2	O2D-CGD-O1D	-2.30	119.35	123.84
32	F	204	WVN	C39-C40-C37	-2.30	118.77	123.47
38	a	315	II0	C41-C42-C40	-2.30	118.77	123.47
29	e	306	CLA	CMB-C2B-C3B	2.29	132.14	126.59
38	l	315	II0	C17-C04-C10	-2.29	106.82	110.47
29	K	101	CLA	CHD-C1D-ND	-2.29	122.35	124.45
29	m	612	CLA	C2A-C1A-CHA	2.29	127.87	123.86
29	n	607	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	d	318	CLA	C3B-C4B-NB	-2.29	108.39	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	849	LMU	C1'-C2'-C3'	2.29	114.77	110.00
29	m	608	CLA	CHD-C1D-ND	-2.29	122.35	124.45
29	B	831	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
29	B	835	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
32	K	103	WVN	C24-C22-C19	-2.29	114.47	118.08
29	f	613	CLA	C2D-C1D-ND	-2.29	108.42	110.10
29	h	307	CLA	C2A-C1A-CHA	2.29	127.86	123.86
29	B	825	CLA	CHD-C1D-ND	-2.29	122.35	124.45
29	l	307	CLA	C3B-C4B-NB	-2.29	108.39	110.52
29	c	306	CLA	CHB-C4A-NA	2.29	127.67	124.51
37	F	208	LMG	O6-C1-O1	-2.28	104.56	109.97
29	B	827	CLA	O2D-CGD-CBD	2.28	115.33	111.27
36	j	319	DGD	O5D-C6D-C5D	-2.28	104.82	109.05
29	c	307	CLA	CMB-C2B-C3B	2.28	132.12	126.59
38	n	618	II0	C05-C07-C11	2.28	113.43	110.30
38	d	316	II0	C29-C31-C33	-2.28	116.09	123.22
38	m	615	II0	C32-C30-C26	-2.28	119.95	126.58
38	i	313	II0	C05-C03-C09	2.28	114.25	109.62
40	g	315	KC2	CMB-C2B-C1B	2.28	128.74	124.71
29	B	836	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
36	j	319	DGD	CFB-CEB-CDB	-2.28	102.84	114.42
29	B	821	CLA	CHB-C4A-NA	2.28	127.66	124.51
37	c	317	LMG	C42-C41-C40	-2.28	102.86	114.42
29	A	825	CLA	CHB-C1B-NB	2.28	126.67	124.26
29	A	830	CLA	CHC-C4B-NB	2.28	126.67	124.26
38	m	614	II0	C06-C08-C12	2.28	113.42	110.30
29	A	807	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
29	A	830	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	B	819	CLA	CMC-C2C-C1C	-2.28	121.57	125.04
29	g	316	CLA	CBC-CAC-C3C	2.28	118.71	112.43
29	B	801	CLA	C2D-C1D-ND	-2.28	108.43	110.10
29	B	834	CLA	CHD-C1D-ND	-2.28	122.36	124.45
32	B	848	WVN	C18-C06-C13	2.28	113.99	110.30
29	B	802	CLA	O2D-CGD-CBD	2.28	115.31	111.27
29	B	826	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
40	n	612	KC2	CMD-C2D-C1D	2.27	128.83	125.37
31	f	619	LHG	C18-C17-C16	-2.27	102.88	114.42
38	d	301	II0	C05-C03-C09	2.27	114.23	109.62
29	m	610	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
29	B	811	CLA	CHB-C1B-NB	2.27	126.66	124.26
40	k	611	KC2	CHB-C4A-NA	2.27	127.78	124.20
29	B	819	CLA	CMB-C2B-C3B	2.27	132.09	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	j	316	II0	C32-C30-C26	-2.27	119.99	126.58
29	A	829	CLA	C2B-C1B-NB	-2.27	108.71	110.23
29	B	801	CLA	CHB-C4A-NA	2.27	127.65	124.51
29	B	807	CLA	O2D-CGD-CBD	2.27	115.30	111.27
29	k	607	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
32	h	308	WVN	C39-C40-C37	-2.27	118.83	123.47
29	A	818	CLA	C1-C2-C3	-2.27	122.12	126.04
38	e	312	II0	C06-C04-C10	2.27	114.21	109.62
36	B	844	DGD	C3D-C4D-C5D	-2.27	106.20	110.24
29	l	307	CLA	C2A-C1A-CHA	2.26	127.82	123.86
29	j	303	CLA	O2D-CGD-CBD	2.26	115.29	111.27
29	A	808	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
31	f	619	LHG	C11-C10-C9	-2.26	102.94	114.42
29	B	816	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
40	i	318	KC2	C2A-C1A-CHA	-2.26	119.96	127.44
29	s	402	CLA	C2D-C1D-ND	-2.26	108.44	110.10
29	f	604	CLA	C2D-C1D-ND	-2.26	108.44	110.10
29	d	309	CLA	CHC-C4B-NB	2.26	126.65	124.26
29	B	817	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
29	B	826	CLA	CHB-C4A-NA	2.26	127.63	124.51
29	B	830	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	K	102	CLA	CAA-C2A-C3A	-2.26	108.62	114.26
36	B	844	DGD	CBB-CAB-C9B	-2.26	102.97	114.42
32	s	407	WVN	C10-C06-C13	2.26	113.95	110.48
31	A	842	LHG	C18-C17-C16	-2.26	102.97	114.42
29	b	306	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
29	n	603	CLA	C3B-C4B-NB	-2.26	108.42	110.52
38	n	615	II0	C12-C14-C10	-2.25	115.45	120.57
29	A	803	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
38	f	615	II0	C17-C04-C10	-2.25	106.89	110.47
29	b	313	CLA	C3B-C4B-NB	-2.25	108.42	110.52
39	f	617	IHT	C22-C18-C07	-2.25	120.88	127.20
29	L	203	CLA	O2D-CGD-CBD	2.25	115.27	111.27
29	B	830	CLA	C2D-C1D-ND	-2.25	108.44	110.10
38	m	618	II0	C12-C14-C10	-2.25	115.46	120.57
29	A	837	CLA	C3B-C4B-NB	-2.25	108.43	110.52
36	j	319	DGD	O3G-C1D-C2D	-2.25	104.79	108.30
29	R	203	CLA	O2A-C1-C2	2.25	114.54	108.64
38	i	316	II0	C06-C04-C10	2.25	114.17	109.62
38	l	313	II0	C38-C36-C34	-2.25	114.54	118.08
29	k	614	CLA	CAC-C3C-C2C	2.25	131.37	127.53
29	B	815	CLA	C3B-C4B-NB	-2.25	108.43	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	614	II0	C11-C13-C09	-2.25	115.47	120.57
31	n	619	LHG	C27-C26-C25	-2.24	103.03	114.42
29	B	826	CLA	C3B-C4B-NB	-2.24	108.43	110.52
38	g	317	II0	C16-C03-C09	2.24	114.03	110.47
29	a	302	CLA	C2A-C1A-CHA	2.24	127.78	123.86
29	A	850	CLA	CHD-C1D-ND	-2.24	122.39	124.45
29	j	308	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
29	B	828	CLA	CHD-C1D-ND	-2.24	122.39	124.45
29	B	802	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
29	A	832	CLA	CHD-C1D-ND	-2.24	122.39	124.45
29	B	817	CLA	CHB-C4A-NA	2.24	127.61	124.51
38	k	616	II0	C12-C14-C10	-2.24	115.49	120.57
38	a	313	II0	C15-C03-C09	-2.24	106.91	110.47
29	A	803	CLA	CHB-C1B-NB	2.24	126.63	124.26
29	B	809	CLA	CHB-C1B-NB	2.24	126.63	124.26
32	L	206	WVN	C06-C13-C20	-2.24	109.44	115.78
40	n	611	KC2	C3D-C2D-C1D	-2.24	99.18	106.39
29	F	201	CLA	CHB-C4A-NA	2.24	127.61	124.51
29	l	304	CLA	CHC-C4B-NB	2.24	126.63	124.26
29	n	604	CLA	CHD-C1D-ND	-2.24	122.40	124.45
29	A	838	CLA	CHD-C1D-ND	-2.24	122.40	124.45
37	F	208	LMG	O3-C3-C2	-2.24	105.18	110.35
31	g	301	LHG	C27-C26-C25	-2.24	103.07	114.42
40	i	318	KC2	CMC-C2C-C1C	2.24	128.44	125.04
29	B	842	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
29	B	835	CLA	CHB-C4A-NA	2.23	127.60	124.51
28	A	801	CL0	C4D-CHA-C1A	2.23	123.97	121.25
40	n	611	KC2	CHB-C1B-C2B	-2.23	120.80	125.48
38	a	315	II0	C29-C31-C33	-2.23	116.25	123.22
31	A	842	LHG	C27-C26-C25	-2.23	103.09	114.42
29	h	312	CLA	CHB-C1B-NB	2.23	126.62	124.26
37	F	206	LMG	C42-C41-C40	-2.23	103.09	114.42
38	m	616	II0	C12-C14-C10	-2.23	115.50	120.57
29	l	304	CLA	C3B-C4B-NB	-2.23	108.44	110.52
29	B	808	CLA	CHC-C4B-NB	2.23	126.62	124.26
38	f	618	II0	C16-C03-C09	-2.23	106.92	110.47
29	j	305	CLA	CHB-C1B-NB	2.23	126.62	124.26
37	c	317	LMG	O2-C2-C1	-2.23	104.63	110.05
32	e	315	WVN	C07-C01-C02	2.23	112.92	109.55
29	d	306	CLA	C3B-C4B-NB	-2.23	108.45	110.52
29	i	303	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
38	b	317	II0	C41-C42-C40	2.23	128.04	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	204	IHT	C05-C08-C12	2.23	113.35	110.30
38	a	313	II0	C05-C07-C11	-2.23	107.26	110.30
32	L	205	WVN	C10-C06-C13	2.23	113.91	110.48
40	g	314	KC2	O2D-CGD-O1D	-2.23	119.49	123.84
40	k	611	KC2	CHB-C1B-NB	-2.23	122.41	124.45
29	m	606	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
31	L	208	LHG	O8-C23-O10	-2.22	117.98	123.59
29	k	610	CLA	CHA-C1A-NA	-2.22	121.30	126.40
29	B	823	CLA	C2D-C1D-ND	-2.22	108.47	110.10
29	O	201	CLA	CHB-C4A-NA	2.22	127.59	124.51
36	j	319	DGD	CAB-C9B-C8B	-2.22	103.14	114.42
29	g	307	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
38	m	616	II0	C05-C03-C09	2.22	114.12	109.62
29	A	815	CLA	CMB-C2B-C3B	2.22	131.97	126.59
29	A	830	CLA	C2D-C1D-ND	-2.22	108.47	110.10
29	b	308	CLA	CMB-C2B-C3B	2.22	131.97	126.59
29	j	305	CLA	CMB-C2B-C3B	2.22	131.97	126.59
29	b	307	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
32	L	206	WVN	C21-C15-C14	-2.22	109.35	113.62
29	A	824	CLA	C3B-C4B-NB	-2.22	108.45	110.52
37	F	208	LMG	O2-C2-C1	-2.22	104.65	110.05
29	d	306	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
40	k	611	KC2	O2D-CGD-O1D	-2.22	119.50	123.84
29	B	812	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
29	A	819	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
38	d	315	II0	C29-C31-C33	-2.22	116.30	123.22
29	K	101	CLA	O2D-CGD-CBD	2.22	115.21	111.27
29	f	606	CLA	CHD-C1D-ND	-2.22	122.42	124.45
29	n	613	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	c	308	CLA	C1-C2-C3	-2.22	122.21	126.04
31	a	301	LHG	C27-C26-C25	-2.22	103.17	114.42
29	O	201	CLA	CMB-C2B-C3B	2.22	131.96	126.59
38	l	314	II0	C06-C04-C10	2.21	114.11	109.62
37	b	319	LMG	O3-C3-C2	-2.21	105.23	110.35
29	b	311	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
29	j	303	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
37	c	317	LMG	C38-C37-C36	-2.21	103.19	114.42
29	n	607	CLA	CHB-C1B-NB	2.21	126.60	124.26
40	m	611	KC2	CHB-C1B-NB	-2.21	122.42	124.45
29	A	817	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
29	A	829	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
31	b	318	LHG	C18-C17-C16	-2.21	103.20	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	610	CLA	O2D-CGD-CBD	2.21	115.20	111.27
37	n	620	LMG	O6-C1-O1	-2.21	104.74	109.97
29	l	309	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
29	f	607	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
29	c	307	CLA	CHB-C4A-NA	2.21	127.57	124.51
29	A	835	CLA	O2D-CGD-CBD	2.21	115.19	111.27
29	A	813	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
29	K	102	CLA	CHC-C4B-NB	2.21	126.59	124.26
29	i	307	CLA	CHB-C1B-NB	2.21	126.59	124.26
29	B	837	CLA	C3B-C4B-NB	-2.21	108.47	110.52
29	k	609	CLA	CHB-C1B-NB	2.21	126.59	124.26
29	c	306	CLA	CHB-C1B-NB	2.21	126.59	124.26
29	n	610	CLA	C3B-C4B-NB	-2.21	108.47	110.52
37	Q	301	LMG	O3-C3-C2	-2.21	105.25	110.35
38	g	318	II0	C29-C31-C33	-2.20	116.34	123.22
38	g	318	II0	C17-C04-C10	-2.20	106.97	110.47
29	h	301	CLA	CHD-C1D-ND	-2.20	122.43	124.45
38	g	318	II0	C06-C08-C12	-2.20	107.29	110.30
40	s	404	KC2	C3D-C2D-C1D	-2.20	99.30	106.39
40	g	313	KC2	O2D-CGD-O1D	-2.20	119.53	123.84
31	A	848	LHG	C18-C17-C16	-2.20	103.25	114.42
37	L	210	LMG	O3-C3-C2	-2.20	105.26	110.35
29	n	602	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
40	n	611	KC2	CMC-C2C-C1C	2.20	128.39	125.04
29	m	604	CLA	C2D-C1D-ND	-2.20	108.48	110.10
29	s	402	CLA	C1-C2-C3	-2.20	122.24	126.04
38	d	301	II0	C12-C14-C10	-2.20	115.58	120.57
29	m	601	CLA	CHB-C1B-NB	2.20	126.58	124.26
29	A	803	CLA	CHD-C1D-ND	-2.20	122.43	124.45
29	m	606	CLA	CHD-C1D-ND	-2.20	122.43	124.45
29	j	307	CLA	CHD-C1D-ND	-2.20	122.43	124.45
32	F	205	WVN	C01-C02-C05	2.20	115.35	111.42
29	B	812	CLA	C1-C2-C3	-2.20	122.24	126.04
29	B	832	CLA	CHB-C1B-NB	2.20	126.58	124.26
32	B	847	WVN	C26-C29-C31	-2.20	116.36	123.22
29	b	303	CLA	C1-C2-C3	-2.20	122.24	126.04
29	d	303	CLA	CHC-C4B-NB	2.20	126.58	124.26
37	c	318	LMG	O2-C2-C1	-2.20	104.71	110.05
29	A	831	CLA	CHC-C4B-NB	2.20	126.58	124.26
37	O	205	LMG	O2-C2-C1	-2.19	104.71	110.05
29	A	813	CLA	CHB-C1B-NB	2.19	126.58	124.26
29	A	826	CLA	O2D-CGD-CBD	2.19	115.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	821	CLA	CHD-C1D-ND	-2.19	122.44	124.45
31	a	318	LHG	C27-C26-C25	-2.19	103.30	114.42
29	A	821	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
38	e	313	II0	C32-C30-C26	-2.19	120.22	126.58
29	i	311	CLA	C2D-C1D-ND	-2.19	108.49	110.10
32	B	848	WVN	C21-C15-C14	-2.19	109.41	113.62
29	m	605	CLA	C2A-C1A-CHA	2.19	127.69	123.86
32	I	101	WVN	C01-C02-C11	2.19	115.47	112.70
38	i	314	II0	C11-C13-C09	-2.19	115.61	120.57
29	A	832	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
29	a	305	CLA	CHB-C1B-NB	2.19	126.57	124.26
29	g	302	CLA	C2A-C1A-CHA	2.19	127.68	123.86
29	m	607	CLA	C2D-C1D-ND	-2.19	108.49	110.10
32	R	202	WVN	C18-C06-C13	-2.19	106.75	110.30
32	B	845	WVN	C28-C30-C33	-2.18	116.40	123.22
32	A	847	WVN	C21-C15-C14	-2.18	109.42	113.62
29	n	604	CLA	CMB-C2B-C1B	-2.18	122.04	125.37
29	B	815	CLA	CHB-C1B-NB	2.18	126.57	124.26
29	g	306	CLA	CHB-C1B-NB	2.18	126.57	124.26
32	M	101	WVN	C06-C13-C20	-2.18	109.60	115.78
37	O	205	LMG	O3-C3-C2	-2.18	105.30	110.35
29	B	826	CLA	CHB-C1B-NB	2.18	126.57	124.26
31	c	316	LHG	O8-C23-O10	-2.18	118.08	123.59
40	k	612	KC2	C4D-C3D-CAD	2.18	108.89	107.42
40	s	401	KC2	CHB-C1B-NB	-2.18	122.45	124.45
32	l	302	WVN	C39-C40-C37	-2.18	119.01	123.47
29	B	809	CLA	CHC-C4B-NB	2.18	126.56	124.26
29	j	314	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
38	e	314	II0	C18-C04-C10	-2.18	107.00	110.47
29	B	836	CLA	CHB-C1B-NB	2.18	126.56	124.26
29	d	318	CLA	C2A-C1A-CHA	2.18	127.67	123.86
40	j	312	KC2	O2A-CGA-O1A	-2.18	118.14	122.67
38	k	617	II0	C04-C10-C14	-2.18	119.56	122.63
31	s	408	LHG	C27-C26-C25	-2.18	103.38	114.42
29	k	606	CLA	CHD-C1D-ND	-2.18	122.45	124.45
38	m	615	II0	C12-C14-C10	-2.18	115.63	120.57
40	g	313	KC2	C2A-C1A-CHA	-2.17	120.25	127.44
29	B	805	CLA	C3B-C4B-NB	-2.17	108.50	110.52
29	A	806	CLA	CHB-C1B-NB	2.17	126.56	124.26
29	n	610	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
40	d	312	KC2	CHC-C4B-C3B	2.17	128.97	125.26
29	A	829	CLA	O2D-CGD-CBD	2.17	115.13	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	305	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
29	f	604	CLA	CHB-C1B-NB	2.17	126.56	124.26
40	g	315	KC2	C2A-C1A-CHA	-2.17	120.26	127.44
40	s	401	KC2	CMB-C2B-C1B	2.17	128.54	124.71
29	B	806	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
38	m	616	II0	C41-C42-C40	-2.17	119.03	123.47
38	d	316	II0	C06-C04-C10	2.17	114.01	109.62
38	f	614	II0	C06-C08-C12	2.17	113.27	110.30
37	F	206	LMG	C38-C37-C36	-2.17	103.42	114.42
38	f	618	II0	C05-C03-C09	2.17	114.01	109.62
29	m	604	CLA	C3B-C4B-NB	-2.17	108.50	110.52
29	j	314	CLA	CHD-C1D-ND	-2.17	122.46	124.45
40	d	312	KC2	CHC-C4B-NB	-2.17	122.46	124.45
32	h	308	WVN	C06-C13-C20	-2.17	109.65	115.78
29	B	826	CLA	C2D-C1D-ND	-2.17	108.51	110.10
39	f	617	IHT	C18-C22-C23	2.17	129.51	126.23
29	g	308	CLA	CHD-C1D-ND	-2.17	122.46	124.45
40	d	311	KC2	C3D-C2D-C1D	-2.17	99.41	106.39
38	m	615	II0	C06-C08-C12	-2.17	107.34	110.30
29	k	610	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
29	K	102	CLA	O1D-CGD-CBD	2.16	128.91	124.48
29	e	311	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
29	A	840	CLA	CMB-C2B-C3B	2.16	131.83	126.59
29	g	311	CLA	CMB-C2B-C3B	2.16	131.83	126.59
29	k	610	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	A	824	CLA	O2D-CGD-CBD	2.16	115.11	111.27
32	F	204	WVN	C24-C22-C19	-2.16	114.67	118.08
29	A	804	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
29	a	312	CLA	CHC-C4B-NB	2.16	126.54	124.26
31	L	208	LHG	C25-C24-C23	2.16	121.48	113.62
29	j	311	CLA	C4-C3-C5	2.16	118.90	115.27
29	B	828	CLA	CHB-C1B-NB	2.16	126.54	124.26
31	L	208	LHG	C18-C17-C16	-2.16	103.47	114.42
29	d	302	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	b	313	CLA	C1-C2-C3	-2.16	122.31	126.04
29	n	607	CLA	C2D-C1D-ND	-2.16	108.51	110.10
31	g	322	LHG	C27-C26-C25	-2.16	103.47	114.42
29	A	824	CLA	CMB-C2B-C3B	2.16	131.81	126.59
40	g	313	KC2	CMB-C2B-C1B	2.16	128.51	124.71
32	l	316	WVN	C19-C22-C26	-2.16	115.63	118.94
29	f	612	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
40	c	310	KC2	O1D-CGD-CBD	-2.16	120.07	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	822	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
29	B	816	CLA	C2D-C1D-ND	-2.16	108.52	110.10
29	d	302	CLA	C1-C2-C3	-2.15	122.32	126.04
40	g	315	KC2	C3D-C2D-C1D	-2.15	99.45	106.39
29	k	614	CLA	CMC-C2C-C1C	-2.15	121.76	125.04
29	B	810	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	j	305	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
29	s	406	CLA	CMB-C2B-C3B	2.15	131.80	126.59
40	g	313	KC2	O1D-CGD-CBD	-2.15	120.08	124.48
29	A	815	CLA	CHB-C1B-NB	2.15	126.53	124.26
29	e	303	CLA	CHB-C1B-NB	2.15	126.53	124.26
29	k	606	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
29	B	825	CLA	O2D-CGD-CBD	2.15	115.09	111.27
29	s	402	CLA	O2D-CGD-CBD	2.15	115.09	111.27
29	e	306	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
29	B	825	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	a	304	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	f	603	CLA	C3B-C4B-NB	-2.15	108.52	110.52
37	c	318	LMG	C1-O6-C5	-2.15	109.47	113.69
29	B	804	CLA	CMB-C2B-C3B	2.15	131.80	126.59
31	a	301	LHG	C18-C17-C16	-2.15	103.51	114.42
31	b	318	LHG	C27-C26-C25	-2.15	103.51	114.42
29	m	607	CLA	C3B-C4B-NB	-2.15	108.52	110.52
37	b	319	LMG	O2-C2-C1	-2.15	104.83	110.05
40	f	611	KC2	C2A-C1A-CHA	-2.15	120.33	127.44
40	i	310	KC2	C3D-C2D-C1D	-2.15	99.47	106.39
29	A	839	CLA	C1-C2-C3	-2.15	122.33	126.04
29	n	606	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	B	817	CLA	CHB-C1B-NB	2.15	126.53	124.26
38	e	312	II0	C11-C13-C09	-2.15	115.70	120.57
29	k	603	CLA	CHD-C1D-ND	-2.14	122.48	124.45
29	d	302	CLA	CMB-C2B-C1B	-2.14	122.10	125.37
29	g	310	CLA	O2D-CGD-CBD	2.14	115.08	111.27
29	B	809	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	e	310	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
29	g	311	CLA	CHB-C1B-NB	2.14	126.52	124.26
29	B	810	CLA	CHC-C4B-NB	2.14	126.52	124.26
29	B	830	CLA	C1-C2-C3	-2.14	123.29	126.75
29	e	302	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
29	B	813	CLA	C3B-C4B-NB	-2.14	108.53	110.52
40	e	309	KC2	CED-O2D-CGD	2.14	120.78	115.94
37	c	318	LMG	C1-C2-C3	-2.14	105.54	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	202	WVN	C10-C06-C13	2.14	113.77	110.48
29	m	612	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
29	k	601	CLA	CED-O2D-CGD	2.14	120.77	115.94
29	A	819	CLA	C1-O2A-CGA	2.14	122.05	116.44
29	R	203	CLA	C2A-C1A-CHA	2.14	127.59	123.86
29	j	305	CLA	CHD-C1D-ND	-2.14	122.49	124.45
38	f	615	II0	C06-C08-C12	-2.14	107.38	110.30
29	i	312	CLA	CHC-C4B-NB	2.14	126.52	124.26
29	B	830	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
29	i	305	CLA	C3B-C4B-NB	-2.13	108.53	110.52
38	n	618	II0	C15-C03-C09	-2.13	107.08	110.47
38	m	618	II0	C17-C04-C10	-2.13	107.08	110.47
29	g	306	CLA	C2D-C1D-ND	-2.13	108.53	110.10
29	A	824	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
29	B	803	CLA	C1D-ND-C4D	-2.13	104.82	106.33
29	i	308	CLA	CMB-C2B-C3B	2.13	131.75	126.59
29	B	816	CLA	O2D-CGD-CBD	2.13	115.06	111.27
29	A	840	CLA	C3B-C4B-NB	-2.13	108.54	110.52
31	e	317	LHG	C27-C26-C25	-2.13	103.61	114.42
37	F	206	LMG	O3-C3-C2	-2.13	105.42	110.35
29	K	102	CLA	CHA-C1A-NA	-2.13	121.52	126.40
38	j	316	II0	C17-C04-C10	-2.13	107.08	110.47
29	A	837	CLA	O2D-CGD-CBD	2.13	115.05	111.27
37	c	318	LMG	O3-C3-C2	-2.13	105.42	110.35
31	g	301	LHG	C18-C17-C16	-2.13	103.61	114.42
29	f	609	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	c	308	CLA	C4-C3-C5	2.13	118.85	115.27
29	i	307	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	f	602	CLA	C3B-C4B-NB	-2.13	108.54	110.52
38	k	616	II0	C17-C04-C10	-2.13	107.09	110.47
29	A	851	CLA	C1-C2-C3	-2.13	122.36	126.04
29	n	603	CLA	CHB-C1B-NB	2.13	126.51	124.26
29	B	838	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
38	m	618	II0	C05-C03-C09	2.13	113.93	109.62
29	e	311	CLA	C2A-C1A-CHA	2.12	127.57	123.86
29	B	829	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
29	A	813	CLA	CMB-C2B-C3B	2.12	131.73	126.59
38	i	313	II0	C41-C42-C40	-2.12	119.12	123.47
29	m	602	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
40	g	315	KC2	CED-O2D-CGD	2.12	120.74	115.94
29	A	826	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	A	808	CLA	C2A-C1A-CHA	2.12	127.57	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	312	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
29	d	304	CLA	C3B-C4B-NB	-2.12	108.55	110.52
32	K	103	WVN	C06-C13-C20	-2.12	109.78	115.78
29	e	302	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	A	851	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	j	313	CLA	CHB-C1B-NB	2.12	126.50	124.26
29	c	306	CLA	C3B-C4B-NB	-2.12	108.55	110.52
29	A	825	CLA	CHB-C4A-NA	2.12	127.44	124.51
29	k	607	CLA	C2D-C1D-ND	-2.12	108.54	110.10
29	B	823	CLA	O2D-CGD-CBD	2.12	115.03	111.27
29	a	305	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
40	l	311	KC2	O1D-CGD-CBD	-2.12	120.15	124.48
29	e	306	CLA	C3B-C4B-NB	-2.12	108.55	110.52
29	A	830	CLA	CHB-C1B-NB	2.12	126.50	124.26
29	A	814	CLA	CMB-C2B-C3B	2.12	131.71	126.59
38	h	310	II0	C05-C03-C09	2.12	113.91	109.62
29	f	605	CLA	C2A-C1A-CHA	2.11	127.56	123.86
29	B	810	CLA	CHD-C1D-ND	-2.11	122.51	124.45
29	B	841	CLA	C2A-C1A-CHA	2.11	127.55	123.86
29	l	307	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
29	b	313	CLA	C2D-C1D-ND	-2.11	108.55	110.10
29	A	823	CLA	C3B-C4B-NB	-2.11	108.56	110.52
29	n	603	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
29	c	312	CLA	CHB-C4A-NA	2.11	127.43	124.51
40	g	315	KC2	CHB-C4A-NA	2.11	127.53	124.20
29	n	613	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
38	g	318	II0	C11-C13-C09	-2.11	115.78	120.57
29	B	825	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
38	n	616	II0	C41-C42-C40	-2.11	119.15	123.47
38	e	312	II0	C15-C03-C09	-2.11	107.11	110.47
40	c	310	KC2	C3D-C2D-C1D	-2.11	99.59	106.39
29	g	323	CLA	C2A-C1A-CHA	2.11	127.55	123.86
29	b	306	CLA	CHB-C1B-NB	2.11	126.49	124.26
29	B	823	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
29	A	815	CLA	C3A-C2A-C1A	2.11	104.50	101.34
40	i	310	KC2	CED-O2D-CGD	2.11	120.71	115.94
40	k	611	KC2	C2A-C1A-CHA	-2.11	120.47	127.44
32	B	845	WVN	C30-C28-C25	2.11	130.32	127.31
29	A	817	CLA	CMB-C2B-C3B	2.11	131.69	126.59
31	f	619	LHG	C27-C26-C25	-2.11	103.72	114.42
29	A	819	CLA	CHB-C1B-NB	2.11	126.49	124.26
37	O	205	LMG	O1-C1-C2	-2.11	105.01	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	j	315	II0	C16-C03-C09	-2.11	107.12	110.47
29	A	815	CLA	CHD-C1D-ND	-2.11	122.52	124.45
29	B	824	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
29	g	302	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
29	l	310	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
29	f	605	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
29	F	203	CLA	C2A-C1A-CHA	2.11	127.54	123.86
40	i	318	KC2	C3D-C2D-C1D	-2.10	99.61	106.39
32	h	308	WVN	C10-C06-C13	2.10	113.72	110.48
29	f	605	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
29	h	304	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
29	a	307	CLA	O2D-CGD-CBD	2.10	115.00	111.27
29	A	827	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
29	m	609	CLA	CHC-C4B-NB	2.10	126.48	124.26
29	j	304	CLA	CHB-C1B-NB	2.10	126.48	124.26
40	m	611	KC2	CHB-C4A-NA	2.10	127.51	124.20
29	A	804	CLA	C3B-C4B-NB	-2.10	108.57	110.52
29	A	817	CLA	CAC-C3C-C4C	2.10	127.53	124.81
29	l	308	CLA	CMB-C2B-C3B	2.10	131.67	126.59
39	g	320	IHT	C41-C40-C37	-2.10	119.18	123.47
29	c	311	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
32	h	308	WVN	C07-C01-C02	2.10	112.72	109.55
29	d	303	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	B	805	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
29	j	309	CLA	CHB-C1B-NB	2.10	126.48	124.26
37	O	205	LMG	C1-C2-C3	-2.10	105.63	110.00
29	d	313	CLA	CAC-C3C-C4C	2.10	127.53	124.81
40	m	611	KC2	C3D-C2D-C1D	-2.10	99.64	106.39
29	B	828	CLA	CHC-C4B-NB	2.10	126.47	124.26
29	m	607	CLA	CHB-C1B-NB	2.10	126.47	124.26
29	n	607	CLA	C3B-C4B-NB	-2.09	108.57	110.52
29	i	304	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
31	f	620	LHG	C27-C26-C25	-2.09	103.80	114.42
29	g	303	CLA	CAA-C2A-C3A	-2.09	109.03	114.26
29	e	305	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	e	307	CLA	CHB-C1B-NB	2.09	126.47	124.26
40	l	311	KC2	C3D-C2D-C1D	-2.09	99.65	106.39
29	A	813	CLA	C2D-C1D-ND	-2.09	108.56	110.10
29	d	305	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
29	A	805	CLA	CMB-C2B-C3B	2.09	131.65	126.59
29	j	309	CLA	CHD-C1D-ND	-2.09	122.53	124.45
29	A	820	CLA	CMB-C2B-C3B	2.09	131.65	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	613	CLA	C2A-C1A-CHA	2.09	127.52	123.86
38	a	317	II0	C18-C04-C10	-2.09	107.14	110.47
29	B	811	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
29	i	306	CLA	CAC-C3C-C4C	2.09	127.52	124.81
38	J	103	II0	C06-C04-C10	2.09	113.86	109.62
31	m	619	LHG	C27-C26-C25	-2.09	103.82	114.42
29	n	607	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
40	g	314	KC2	CHC-C4B-C3B	-2.09	121.69	125.26
40	j	312	KC2	CHC-C4B-C3B	-2.09	121.69	125.26
29	A	825	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
37	n	620	LMG	O2-C2-C1	-2.09	104.98	110.05
29	g	302	CLA	CHD-C1D-ND	-2.09	122.54	124.45
33	A	849	LMU	O1B-C4'-C3'	2.09	112.83	107.28
29	A	822	CLA	O2D-CGD-CBD	2.09	114.97	111.27
29	B	821	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
29	h	302	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
29	B	803	CLA	CHB-C4A-NA	2.08	127.39	124.51
29	e	307	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
29	A	803	CLA	CMB-C2B-C3B	2.08	131.64	126.59
38	k	619	II0	C05-C03-C09	2.08	113.84	109.62
29	s	406	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	m	601	CLA	CAA-C2A-C3A	-2.08	109.05	114.26
38	n	618	II0	C12-C14-C10	-2.08	115.84	120.57
29	B	812	CLA	CMB-C2B-C3B	2.08	131.63	126.59
29	A	836	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
29	A	825	CLA	CMB-C2B-C3B	2.08	131.63	126.59
29	g	306	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
29	B	812	CLA	CHB-C1B-NB	2.08	126.46	124.26
29	k	605	CLA	O2D-CGD-CBD	2.08	114.97	111.27
29	B	805	CLA	CHC-C4B-NB	2.08	126.46	124.26
38	a	314	II0	C06-C04-C10	2.08	113.84	109.62
29	A	818	CLA	CMC-C2C-C3C	2.08	131.77	126.12
29	k	610	CLA	C1-C2-C3	-2.08	122.44	126.04
29	A	819	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	A	832	CLA	CHB-C1B-NB	2.08	126.46	124.26
29	k	604	CLA	CBC-CAC-C3C	2.08	118.17	112.43
29	k	614	CLA	CMC-C2C-C3C	2.08	131.76	126.12
29	j	308	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	A	827	CLA	C2B-C1B-NB	2.08	111.63	110.23
29	i	308	CLA	C3B-C4B-NB	-2.08	108.59	110.52
29	k	603	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
29	m	612	CLA	CAA-CBA-CGA	-2.08	107.18	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	804	CLA	CMB-C2B-C3B	2.08	131.62	126.59
29	m	609	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
28	A	801	CL0	C2A-C1A-CHA	2.08	127.49	123.86
29	e	304	CLA	C1-C2-C3	-2.08	122.45	126.04
29	m	602	CLA	CHD-C1D-ND	-2.08	122.55	124.45
29	A	807	CLA	CMB-C2B-C3B	2.08	131.62	126.59
29	A	830	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
29	c	306	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
29	j	314	CLA	CMB-C2B-C3B	2.07	131.61	126.59
29	A	850	CLA	C2D-C1D-ND	-2.07	108.58	110.10
29	b	308	CLA	CHB-C1B-NB	2.07	126.45	124.26
29	b	311	CLA	C3B-C4B-NB	-2.07	108.59	110.52
29	L	203	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
29	A	817	CLA	CHB-C1B-NB	2.07	126.45	124.26
29	e	306	CLA	CHB-C4A-NA	2.07	127.38	124.51
38	l	313	II0	C05-C07-C11	2.07	113.14	110.30
29	i	302	CLA	O2D-CGD-CBD	2.07	114.95	111.27
29	A	810	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
32	K	103	WVN	C39-C40-C37	-2.07	119.23	123.47
29	a	303	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	h	312	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	m	607	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	i	312	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	B	817	CLA	O2D-CGD-CBD	2.07	114.94	111.27
29	j	314	CLA	C2D-C1D-ND	-2.07	108.58	110.10
29	A	818	CLA	CMB-C2B-C3B	2.07	131.60	126.59
29	e	310	CLA	CMB-C2B-C3B	2.07	131.59	126.59
29	B	838	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	b	312	CLA	C3B-C4B-NB	-2.07	108.60	110.52
40	s	401	KC2	C3D-C2D-C1D	-2.07	99.73	106.39
29	A	832	CLA	CHC-C4B-NB	2.07	126.44	124.26
29	B	814	CLA	CHC-C4B-NB	2.07	126.44	124.26
29	m	603	CLA	CHB-C1B-NB	2.07	126.44	124.26
29	a	305	CLA	CMB-C2B-C3B	2.07	131.59	126.59
29	A	838	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
29	A	829	CLA	C3B-C4B-NB	-2.06	108.60	110.52
40	k	611	KC2	C3D-C2D-C1D	-2.06	99.74	106.39
37	L	210	LMG	O2-C2-C1	-2.06	105.03	110.05
29	n	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
29	g	306	CLA	C3B-C4B-NB	-2.06	108.60	110.52
29	i	305	CLA	CHD-C1D-ND	-2.06	122.56	124.45
29	m	601	CLA	O2D-CGD-CBD	2.06	114.93	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	824	CLA	O2D-CGD-CBD	2.06	114.93	111.27
29	b	307	CLA	CHB-C1B-NB	2.06	126.44	124.26
29	f	607	CLA	CHB-C1B-NB	2.06	126.44	124.26
29	a	306	CLA	CAC-C3C-C2C	-2.06	124.00	127.53
29	g	311	CLA	O1A-CGA-CBA	2.06	131.77	123.73
32	I	101	WVN	C07-C01-C02	2.06	112.67	109.55
29	g	311	CLA	CHD-C1D-ND	-2.06	122.56	124.45
40	f	611	KC2	C3D-C2D-C1D	-2.06	99.75	106.39
29	F	203	CLA	CHB-C1B-NB	2.06	126.44	124.26
29	A	834	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	B	819	CLA	C2D-C1D-ND	-2.06	108.59	110.10
29	b	305	CLA	CHC-C4B-NB	2.06	126.44	124.26
36	B	844	DGD	CAB-C9B-C8B	-2.06	103.97	114.42
29	B	817	CLA	CHD-C1D-ND	-2.06	122.56	124.45
31	l	318	LHG	C27-C26-C25	-2.06	103.98	114.42
29	A	831	CLA	C1-C2-C3	-2.06	122.48	126.04
29	A	839	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
29	m	613	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
38	l	315	II0	C29-C31-C33	-2.06	116.80	123.22
29	s	402	CLA	C2A-C1A-CHA	2.06	127.45	123.86
29	A	828	CLA	C3B-C4B-NB	-2.06	108.61	110.52
29	b	305	CLA	C3B-C4B-NB	-2.06	108.61	110.52
29	B	831	CLA	CHD-C1D-ND	-2.06	122.56	124.45
29	b	308	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
29	k	608	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	b	310	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	j	306	CLA	CHA-C1A-NA	-2.05	121.69	126.40
29	l	306	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	B	820	CLA	C2D-C1D-ND	-2.05	108.59	110.10
29	c	302	CLA	CED-O2D-CGD	2.05	120.58	115.94
29	L	203	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
40	k	611	KC2	CMC-C2C-C1C	2.05	128.16	125.04
29	B	829	CLA	C2A-C1A-CHA	2.05	127.45	123.86
29	h	307	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
29	B	825	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	l	301	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	n	602	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
37	c	318	LMG	O7-C10-O9	-2.05	118.75	123.70
29	h	303	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	A	836	CLA	C2A-C1A-CHA	2.05	127.44	123.86
29	A	821	CLA	CHB-C1B-NB	2.05	126.43	124.26
29	d	313	CLA	CHC-C4B-NB	2.05	126.43	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	311	II0	C32-C30-C26	-2.05	120.63	126.58
31	i	317	LHG	C27-C26-C25	-2.05	104.03	114.42
29	d	313	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	A	833	CLA	C4-C3-C5	2.05	118.71	115.27
40	d	311	KC2	CED-O2D-CGD	2.05	120.57	115.94
29	A	814	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
38	a	315	II0	C06-C04-C10	2.05	113.77	109.62
29	O	202	CLA	C1-C2-C3	-2.05	122.50	126.04
29	A	828	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
33	i	301	LMU	C4B-C3B-C2B	2.05	114.39	110.82
29	B	829	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	k	607	CLA	CBA-CAA-C2A	2.05	119.90	113.86
29	a	311	CLA	CHC-C4B-NB	2.05	126.42	124.26
29	l	301	CLA	C3B-C4B-NB	-2.04	108.62	110.52
29	A	824	CLA	CHA-C1A-NA	-2.04	121.72	126.40
40	m	611	KC2	O2D-CGD-O1D	-2.04	119.84	123.84
29	B	815	CLA	O2D-CGD-CBD	2.04	114.90	111.27
40	j	312	KC2	C3D-C2D-C1D	-2.04	99.81	106.39
29	n	602	CLA	CMB-C2B-C3B	2.04	131.53	126.59
29	A	804	CLA	C3A-C2A-C1A	2.04	104.40	101.34
29	A	829	CLA	CHC-C4B-NB	2.04	126.42	124.26
29	A	839	CLA	CHB-C1B-NB	2.04	126.42	124.26
29	f	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
38	b	314	II0	C05-C03-C09	2.04	113.75	109.62
40	j	312	KC2	CHB-C4A-NA	2.04	127.42	124.20
29	n	602	CLA	CHC-C4B-NB	2.04	126.42	124.26
32	B	847	WVN	C18-C06-C13	-2.04	106.99	110.30
29	A	819	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
38	b	301	II0	C11-C13-C09	-2.04	115.94	120.57
29	a	306	CLA	CBC-CAC-C3C	2.04	118.05	112.43
29	L	202	CLA	CHB-C1B-NB	2.04	126.42	124.26
29	k	602	CLA	CHB-C1B-NB	2.04	126.42	124.26
29	L	204	CLA	O2D-CGD-CBD	2.04	114.89	111.27
40	l	311	KC2	CHB-C1B-NB	-2.04	122.58	124.45
37	n	620	LMG	O1-C1-C2	-2.04	105.12	108.30
38	j	316	II0	C05-C07-C11	2.04	113.09	110.30
29	n	609	CLA	CHD-C1D-ND	-2.04	122.58	124.45
29	k	601	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	A	816	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	h	303	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	d	307	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
29	B	802	CLA	CHD-C1D-ND	-2.04	122.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	201	WVN	C17-C06-C13	2.04	113.60	110.30
29	j	308	CLA	C3C-C4C-NC	-2.04	108.29	110.57
29	f	603	CLA	CHB-C1B-NB	2.04	126.41	124.26
29	g	304	CLA	CHB-C1B-NB	2.04	126.41	124.26
29	B	835	CLA	O2D-CGD-CBD	2.04	114.89	111.27
29	A	809	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
40	s	401	KC2	CHB-C4A-NA	2.04	127.41	124.20
29	d	302	CLA	CMB-C2B-C3B	2.04	131.52	126.59
29	d	313	CLA	CBA-CAA-C2A	2.04	119.87	113.86
38	i	314	II0	C32-C30-C26	-2.04	120.67	126.58
29	e	311	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
40	k	612	KC2	CHD-C1D-ND	-2.03	122.10	124.26
38	l	315	II0	C05-C03-C09	2.03	113.74	109.62
29	b	303	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
29	k	607	CLA	C2A-C1A-CHA	2.03	127.41	123.86
32	R	202	WVN	C01-C02-C05	-2.03	107.77	111.42
29	l	312	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
32	I	101	WVN	C06-C13-C20	-2.03	110.03	115.78
29	s	406	CLA	O2D-CGD-CBD	2.03	114.88	111.27
29	i	305	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	l	301	CLA	CHB-C1B-NB	2.03	126.41	124.26
29	i	312	CLA	CMC-C2C-C3C	2.03	131.63	126.12
29	A	802	CLA	O1D-CGD-CBD	2.03	128.64	124.48
29	e	302	CLA	CMB-C2B-C3B	2.03	131.51	126.59
29	B	820	CLA	CHC-C4B-NB	2.03	126.41	124.26
29	n	604	CLA	C2A-C1A-CHA	2.03	127.41	123.86
40	s	401	KC2	O1D-CGD-CBD	-2.03	120.33	124.48
29	f	609	CLA	CHC-C4B-NB	2.03	126.41	124.26
40	g	313	KC2	CHB-C4A-NA	2.03	127.40	124.20
29	b	302	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
29	F	201	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
29	a	304	CLA	CHB-C1B-NB	2.03	126.40	124.26
29	A	828	CLA	C1-C2-C3	-2.03	122.54	126.04
29	B	810	CLA	O2D-CGD-CBD	2.03	114.87	111.27
38	l	313	II0	C18-C04-C10	-2.03	107.25	110.47
38	e	313	II0	C04-C06-C08	2.03	118.22	113.64
29	m	602	CLA	CHB-C1B-NB	2.03	126.40	124.26
38	f	618	II0	C17-C04-C10	-2.03	107.25	110.47
29	g	308	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
29	c	304	CLA	CMB-C2B-C1B	-2.02	122.28	125.37
39	j	317	IHT	C09-C10-C07	-2.02	119.79	122.73
31	c	320	LHG	C18-C17-C16	-2.02	104.15	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	311	CLA	CHB-C1B-NB	2.02	126.40	124.26
29	k	604	CLA	CHB-C1B-NB	2.02	126.40	124.26
29	j	305	CLA	C2D-C1D-ND	-2.02	108.61	110.10
31	a	318	LHG	C18-C17-C16	-2.02	104.16	114.42
29	A	836	CLA	O2D-CGD-CBD	2.02	114.86	111.27
38	a	314	II0	C41-C42-C40	-2.02	119.33	123.47
29	g	309	CLA	CHC-C4B-NB	2.02	126.40	124.26
29	l	303	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	A	851	CLA	CHC-C4B-NB	2.02	126.40	124.26
29	h	302	CLA	CMB-C2B-C3B	2.02	131.48	126.59
29	c	307	CLA	CHD-C1D-ND	-2.02	122.60	124.45
40	g	313	KC2	C3D-C2D-C1D	-2.02	99.88	106.39
30	A	841	PQN	C2M-C2-C3	-2.02	121.10	124.40
29	j	314	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
29	f	613	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	i	307	CLA	CHB-C4A-NA	2.02	127.30	124.51
29	j	308	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	c	304	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	a	306	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	A	822	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	b	313	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	A	822	CLA	C2D-C1D-ND	-2.02	108.62	110.10
29	c	304	CLA	CHB-C1B-NB	2.02	126.39	124.26
29	A	819	CLA	O2D-CGD-CBD	2.02	114.85	111.27
29	b	311	CLA	CHC-C4B-NB	2.02	126.39	124.26
29	i	305	CLA	CHB-C1B-NB	2.02	126.39	124.26
36	j	319	DGD	C4E-C3E-C2E	-2.02	107.30	110.82
40	l	311	KC2	CHB-C4A-NA	2.02	127.38	124.20
29	h	305	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	h	307	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
38	c	313	II0	C06-C04-C10	2.02	113.70	109.62
39	g	320	IHT	C40-C41-C38	2.02	127.60	123.47
29	a	307	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
29	f	610	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	B	835	CLA	C3B-C4B-NB	-2.01	108.65	110.52
29	d	313	CLA	O2D-CGD-CBD	2.01	114.85	111.27
29	d	304	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
29	j	308	CLA	CMB-C2B-C3B	2.01	131.46	126.59
29	A	823	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	g	309	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	l	308	CLA	CHD-C1D-ND	-2.01	122.61	124.45
40	d	311	KC2	CHB-C4A-NA	2.01	127.37	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	g	314	KC2	CHB-C4A-NA	2.01	127.37	124.20
37	F	206	LMG	O7-C10-O9	-2.01	118.84	123.70
29	e	302	CLA	CHD-C1D-ND	-2.01	122.61	124.45
31	c	316	LHG	C27-C26-C25	-2.01	104.22	114.42
29	A	825	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	d	305	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	n	613	CLA	CHD-C1D-ND	-2.01	122.61	124.45
38	O	203	II0	C03-C05-C07	2.01	118.18	113.64
40	f	611	KC2	CHB-C4A-NA	2.01	127.37	124.20
33	A	849	LMU	O3'-C3'-C2'	-2.01	105.70	110.35
29	K	102	CLA	C2A-C1A-CHA	2.01	127.37	123.86
38	f	616	II0	C05-C03-C09	2.01	113.69	109.62
29	B	818	CLA	C2D-C1D-ND	-2.01	108.62	110.10
29	L	207	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	B	814	CLA	C2A-C1A-CHA	2.01	127.37	123.86
29	d	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	h	304	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
38	e	312	II0	C07-C11-C13	2.01	115.85	111.85
40	k	612	KC2	CMD-C2D-C1D	2.01	128.42	125.37
29	f	604	CLA	C3A-C2A-C1A	2.00	104.34	101.34
40	n	611	KC2	CHB-C4A-NA	2.00	127.36	124.20
29	B	830	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
29	O	201	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	L	203	CLA	CHB-C1B-NB	2.00	126.38	124.26
29	g	323	CLA	CHA-C1A-NA	-2.00	121.81	126.40
29	A	806	CLA	O2D-CGD-CBD	2.00	114.83	111.27
29	b	304	CLA	O1D-CGD-CBD	2.00	128.58	124.48
29	l	305	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	n	609	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
40	e	309	KC2	C3D-C2D-C1D	-2.00	99.94	106.39
38	n	616	II0	C18-C04-C10	2.00	113.65	110.47
38	n	616	II0	C17-C04-C10	-2.00	107.28	110.47
29	B	813	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
29	c	309	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
29	B	810	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	f	604	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	c	303	CLA	C2A-C1A-CHA	2.00	127.36	123.86
29	A	807	CLA	CHB-C1B-NB	2.00	126.38	124.26
29	b	312	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
40	n	611	KC2	CMB-C2B-C1B	2.00	128.24	124.71
32	s	407	WVN	C18-C06-C13	2.00	113.55	110.30
32	F	204	WVN	C38-C34-C33	-2.00	114.92	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	301	CLA	CHD-C1D-ND	-2.00	122.61	124.45
29	B	825	CLA	CMB-C2B-C3B	2.00	131.43	126.59
29	d	318	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
38	j	315	II0	C12-C14-C10	-2.00	116.03	120.57

There are no chirality outliers.

All (4748) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	801	CL0	C2B-C3B-CAB-CBB
28	A	801	CL0	C4B-C3B-CAB-CBB
29	A	804	CLA	CHA-CBD-CGD-O1D
29	A	804	CLA	CHA-CBD-CGD-O2D
29	A	805	CLA	C1A-C2A-CAA-CBA
29	A	805	CLA	C3A-C2A-CAA-CBA
29	A	810	CLA	C1A-C2A-CAA-CBA
29	A	810	CLA	CBD-CGD-O2D-CED
29	A	812	CLA	C2-C3-C5-C6
29	A	812	CLA	C4-C3-C5-C6
29	A	813	CLA	C1A-C2A-CAA-CBA
29	A	814	CLA	C1A-C2A-CAA-CBA
29	A	815	CLA	CHA-CBD-CGD-O1D
29	A	815	CLA	CHA-CBD-CGD-O2D
29	A	815	CLA	CBD-CGD-O2D-CED
29	A	816	CLA	C1A-C2A-CAA-CBA
29	A	817	CLA	C3A-C2A-CAA-CBA
29	A	818	CLA	C1A-C2A-CAA-CBA
29	A	818	CLA	C3A-C2A-CAA-CBA
29	A	818	CLA	CHA-CBD-CGD-O1D
29	A	818	CLA	CHA-CBD-CGD-O2D
29	A	819	CLA	CBD-CGD-O2D-CED
29	A	822	CLA	C2B-C3B-CAB-CBB
29	A	822	CLA	C4B-C3B-CAB-CBB
29	A	823	CLA	C2B-C3B-CAB-CBB
29	A	823	CLA	C4B-C3B-CAB-CBB
29	A	823	CLA	CHA-CBD-CGD-O1D
29	A	823	CLA	CHA-CBD-CGD-O2D
29	A	823	CLA	C2-C3-C5-C6
29	A	823	CLA	C4-C3-C5-C6
29	A	827	CLA	CBD-CGD-O2D-CED
29	A	831	CLA	C2B-C3B-CAB-CBB
29	A	831	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	A	834	CLA	C1A-C2A-CAA-CBA
29	A	834	CLA	C3A-C2A-CAA-CBA
29	A	835	CLA	C4B-C3B-CAB-CBB
29	A	836	CLA	CHA-CBD-CGD-O1D
29	A	836	CLA	CHA-CBD-CGD-O2D
29	A	837	CLA	C1A-C2A-CAA-CBA
29	A	837	CLA	C3A-C2A-CAA-CBA
29	A	838	CLA	CHA-CBD-CGD-O1D
29	A	838	CLA	CHA-CBD-CGD-O2D
29	A	840	CLA	C1A-C2A-CAA-CBA
29	A	851	CLA	CHA-CBD-CGD-O1D
29	A	851	CLA	CHA-CBD-CGD-O2D
29	B	802	CLA	CHA-CBD-CGD-O1D
29	B	802	CLA	CHA-CBD-CGD-O2D
29	B	802	CLA	CAD-CBD-CGD-O1D
29	B	803	CLA	CHA-CBD-CGD-O1D
29	B	803	CLA	CHA-CBD-CGD-O2D
29	B	804	CLA	CBD-CGD-O2D-CED
29	B	805	CLA	C3A-C2A-CAA-CBA
29	B	813	CLA	C1A-C2A-CAA-CBA
29	B	817	CLA	C3A-C2A-CAA-CBA
29	B	818	CLA	C4B-C3B-CAB-CBB
29	B	819	CLA	C1A-C2A-CAA-CBA
29	B	819	CLA	C3A-C2A-CAA-CBA
29	B	819	CLA	C11-C10-C8-C9
29	B	821	CLA	CHA-CBD-CGD-O1D
29	B	826	CLA	C1A-C2A-CAA-CBA
29	B	828	CLA	C1A-C2A-CAA-CBA
29	B	828	CLA	C3A-C2A-CAA-CBA
29	B	829	CLA	C1A-C2A-CAA-CBA
29	B	836	CLA	C2B-C3B-CAB-CBB
29	B	836	CLA	C4B-C3B-CAB-CBB
29	B	837	CLA	C1A-C2A-CAA-CBA
29	B	840	CLA	C1A-C2A-CAA-CBA
29	F	201	CLA	C1A-C2A-CAA-CBA
29	F	201	CLA	C3A-C2A-CAA-CBA
29	F	203	CLA	C1A-C2A-CAA-CBA
29	F	203	CLA	C3A-C2A-CAA-CBA
29	L	202	CLA	C1A-C2A-CAA-CBA
29	L	202	CLA	C3A-C2A-CAA-CBA
29	L	204	CLA	CBD-CGD-O2D-CED
29	L	207	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	L	207	CLA	C4B-C3B-CAB-CBB
29	L	207	CLA	C2-C3-C5-C6
29	O	201	CLA	C1A-C2A-CAA-CBA
29	O	206	CLA	C4B-C3B-CAB-CBB
29	K	102	CLA	C4B-C3B-CAB-CBB
29	K	102	CLA	CBD-CGD-O2D-CED
29	s	402	CLA	C1A-C2A-CAA-CBA
29	s	402	CLA	C4B-C3B-CAB-CBB
29	s	402	CLA	CHA-CBD-CGD-O1D
29	s	402	CLA	CHA-CBD-CGD-O2D
29	s	406	CLA	C1A-C2A-CAA-CBA
29	s	406	CLA	C14-C13-C15-C16
29	c	301	CLA	C1A-C2A-CAA-CBA
29	c	302	CLA	C1A-C2A-CAA-CBA
29	c	302	CLA	C3A-C2A-CAA-CBA
29	c	302	CLA	CBD-CGD-O2D-CED
29	c	303	CLA	CBD-CGD-O2D-CED
29	c	305	CLA	C2B-C3B-CAB-CBB
29	c	305	CLA	C4B-C3B-CAB-CBB
29	c	305	CLA	CBD-CGD-O2D-CED
29	c	306	CLA	C4B-C3B-CAB-CBB
29	c	306	CLA	CBD-CGD-O2D-CED
29	c	307	CLA	C1A-C2A-CAA-CBA
29	c	307	CLA	C3A-C2A-CAA-CBA
29	c	308	CLA	C1A-C2A-CAA-CBA
29	c	308	CLA	C3A-C2A-CAA-CBA
29	c	308	CLA	C6-C7-C8-C9
29	c	311	CLA	C3A-C2A-CAA-CBA
29	c	311	CLA	CHA-CBD-CGD-O1D
29	c	311	CLA	CHA-CBD-CGD-O2D
29	c	311	CLA	CBD-CGD-O2D-CED
29	a	302	CLA	C1A-C2A-CAA-CBA
29	a	302	CLA	C3A-C2A-CAA-CBA
29	a	306	CLA	C4B-C3B-CAB-CBB
29	a	307	CLA	C1A-C2A-CAA-CBA
29	a	312	CLA	C1A-C2A-CAA-CBA
29	a	312	CLA	C3A-C2A-CAA-CBA
29	a	312	CLA	CBD-CGD-O2D-CED
29	b	303	CLA	C1A-C2A-CAA-CBA
29	b	303	CLA	C3A-C2A-CAA-CBA
29	b	305	CLA	CHA-CBD-CGD-O1D
29	b	305	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	b	305	CLA	CAD-CBD-CGD-O1D
29	b	305	CLA	CBD-CGD-O2D-CED
29	b	307	CLA	C12-C13-C15-C16
29	b	308	CLA	C11-C10-C8-C9
29	b	311	CLA	CBD-CGD-O2D-CED
29	b	312	CLA	C3A-C2A-CAA-CBA
29	b	312	CLA	C2A-CAA-CBA-CGA
29	h	302	CLA	CBD-CGD-O2D-CED
29	h	303	CLA	C2B-C3B-CAB-CBB
29	h	303	CLA	C4B-C3B-CAB-CBB
29	h	306	CLA	C1A-C2A-CAA-CBA
29	h	307	CLA	C4B-C3B-CAB-CBB
29	m	602	CLA	C1A-C2A-CAA-CBA
29	m	602	CLA	C3A-C2A-CAA-CBA
29	m	602	CLA	CHA-CBD-CGD-O1D
29	m	602	CLA	CHA-CBD-CGD-O2D
29	m	602	CLA	CBD-CGD-O2D-CED
29	m	603	CLA	CBD-CGD-O2D-CED
29	m	604	CLA	CHA-CBD-CGD-O1D
29	m	604	CLA	CHA-CBD-CGD-O2D
29	m	605	CLA	C1A-C2A-CAA-CBA
29	m	605	CLA	C3A-C2A-CAA-CBA
29	m	608	CLA	C1A-C2A-CAA-CBA
29	m	608	CLA	C3A-C2A-CAA-CBA
29	m	609	CLA	C3A-C2A-CAA-CBA
29	m	609	CLA	CBD-CGD-O2D-CED
29	m	610	CLA	C1A-C2A-CAA-CBA
29	m	610	CLA	C3A-C2A-CAA-CBA
29	m	610	CLA	C4B-C3B-CAB-CBB
29	m	613	CLA	C1A-C2A-CAA-CBA
29	m	613	CLA	CBD-CGD-O2D-CED
29	e	301	CLA	C1A-C2A-CAA-CBA
29	e	301	CLA	C3A-C2A-CAA-CBA
29	e	302	CLA	C1A-C2A-CAA-CBA
29	e	302	CLA	C3A-C2A-CAA-CBA
29	e	303	CLA	CBD-CGD-O2D-CED
29	e	305	CLA	C2B-C3B-CAB-CBB
29	e	305	CLA	C4B-C3B-CAB-CBB
29	e	307	CLA	CBD-CGD-O2D-CED
29	e	308	CLA	C4B-C3B-CAB-CBB
29	e	311	CLA	C2B-C3B-CAB-CBB
29	e	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	e	311	CLA	CBD-CGD-O2D-CED
29	l	304	CLA	C1A-C2A-CAA-CBA
29	l	304	CLA	C3A-C2A-CAA-CBA
29	l	306	CLA	CHA-CBD-CGD-O1D
29	l	306	CLA	CBD-CGD-O2D-CED
29	l	308	CLA	C1A-C2A-CAA-CBA
29	l	308	CLA	C3A-C2A-CAA-CBA
29	l	310	CLA	C4B-C3B-CAB-CBB
29	k	601	CLA	CBD-CGD-O2D-CED
29	k	602	CLA	C1A-C2A-CAA-CBA
29	k	602	CLA	C3A-C2A-CAA-CBA
29	k	602	CLA	C2B-C3B-CAB-CBB
29	k	602	CLA	C4B-C3B-CAB-CBB
29	k	604	CLA	CHA-CBD-CGD-O1D
29	k	604	CLA	CHA-CBD-CGD-O2D
29	k	609	CLA	C1A-C2A-CAA-CBA
29	k	609	CLA	C3A-C2A-CAA-CBA
29	k	609	CLA	CBD-CGD-O2D-CED
29	k	609	CLA	O1D-CGD-O2D-CED
29	k	610	CLA	C1A-C2A-CAA-CBA
29	k	610	CLA	C3A-C2A-CAA-CBA
29	k	610	CLA	C4B-C3B-CAB-CBB
29	k	610	CLA	CBD-CGD-O2D-CED
29	k	610	CLA	C2-C3-C5-C6
29	k	614	CLA	C1A-C2A-CAA-CBA
29	k	614	CLA	CBD-CGD-O2D-CED
29	f	601	CLA	C1A-C2A-CAA-CBA
29	f	601	CLA	C3A-C2A-CAA-CBA
29	f	602	CLA	C1A-C2A-CAA-CBA
29	f	602	CLA	C3A-C2A-CAA-CBA
29	f	602	CLA	C4-C3-C5-C6
29	f	603	CLA	C2-C3-C5-C6
29	f	606	CLA	C2B-C3B-CAB-CBB
29	f	606	CLA	C4B-C3B-CAB-CBB
29	f	607	CLA	C1A-C2A-CAA-CBA
29	f	607	CLA	C3A-C2A-CAA-CBA
29	f	608	CLA	CBD-CGD-O2D-CED
29	f	609	CLA	C6-C7-C8-C9
29	f	610	CLA	C1A-C2A-CAA-CBA
29	f	610	CLA	C3A-C2A-CAA-CBA
29	f	610	CLA	C4B-C3B-CAB-CBB
29	f	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	f	612	CLA	CHA-CBD-CGD-O2D
29	f	612	CLA	CAD-CBD-CGD-O1D
29	i	302	CLA	C1A-C2A-CAA-CBA
29	i	302	CLA	C3A-C2A-CAA-CBA
29	i	302	CLA	CHA-CBD-CGD-O1D
29	i	303	CLA	C2B-C3B-CAB-CBB
29	i	303	CLA	C4B-C3B-CAB-CBB
29	i	305	CLA	CHA-CBD-CGD-O1D
29	i	305	CLA	CHA-CBD-CGD-O2D
29	i	306	CLA	C1A-C2A-CAA-CBA
29	i	306	CLA	C3A-C2A-CAA-CBA
29	i	307	CLA	C1A-C2A-CAA-CBA
29	i	307	CLA	C3A-C2A-CAA-CBA
29	i	308	CLA	C1A-C2A-CAA-CBA
29	i	308	CLA	C3A-C2A-CAA-CBA
29	i	309	CLA	CBA-CGA-O2A-C1
29	i	309	CLA	O1A-CGA-O2A-C1
29	j	302	CLA	C1A-C2A-CAA-CBA
29	j	302	CLA	C3A-C2A-CAA-CBA
29	j	303	CLA	CHA-CBD-CGD-O1D
29	j	303	CLA	CHA-CBD-CGD-O2D
29	j	305	CLA	CHA-CBD-CGD-O1D
29	j	305	CLA	CHA-CBD-CGD-O2D
29	j	306	CLA	C1A-C2A-CAA-CBA
29	j	306	CLA	CBD-CGD-O2D-CED
29	j	310	CLA	C1A-C2A-CAA-CBA
29	j	310	CLA	C3A-C2A-CAA-CBA
29	j	310	CLA	CBD-CGD-O2D-CED
29	j	310	CLA	O1D-CGD-O2D-CED
29	j	311	CLA	C3A-C2A-CAA-CBA
29	j	313	CLA	CHA-CBD-CGD-O1D
29	j	313	CLA	CHA-CBD-CGD-O2D
29	j	313	CLA	CAD-CBD-CGD-O1D
29	j	313	CLA	CBD-CGD-O2D-CED
29	j	314	CLA	CBD-CGD-O2D-CED
29	d	302	CLA	C1A-C2A-CAA-CBA
29	d	302	CLA	C3A-C2A-CAA-CBA
29	d	302	CLA	CBD-CGD-O2D-CED
29	d	303	CLA	CBD-CGD-O2D-CED
29	d	304	CLA	C1A-C2A-CAA-CBA
29	d	304	CLA	CBD-CGD-O2D-CED
29	d	306	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	d	306	CLA	CHA-CBD-CGD-O1D
29	d	306	CLA	CHA-CBD-CGD-O2D
29	d	307	CLA	C1A-C2A-CAA-CBA
29	d	307	CLA	C3A-C2A-CAA-CBA
29	d	307	CLA	C4B-C3B-CAB-CBB
29	d	307	CLA	CHA-CBD-CGD-O1D
29	d	307	CLA	CHA-CBD-CGD-O2D
29	d	308	CLA	C1A-C2A-CAA-CBA
29	d	308	CLA	C3A-C2A-CAA-CBA
29	d	308	CLA	C4B-C3B-CAB-CBB
29	d	309	CLA	CBD-CGD-O2D-CED
29	d	310	CLA	C2B-C3B-CAB-CBB
29	d	310	CLA	C4B-C3B-CAB-CBB
29	d	310	CLA	CHA-CBD-CGD-O1D
29	d	310	CLA	CHA-CBD-CGD-O2D
29	d	318	CLA	C2B-C3B-CAB-CBB
29	d	318	CLA	C4B-C3B-CAB-CBB
29	g	302	CLA	C6-C7-C8-C9
29	g	303	CLA	C4B-C3B-CAB-CBB
29	g	304	CLA	C1A-C2A-CAA-CBA
29	g	304	CLA	C3A-C2A-CAA-CBA
29	g	304	CLA	C2B-C3B-CAB-CBB
29	g	304	CLA	C4B-C3B-CAB-CBB
29	g	306	CLA	CHA-CBD-CGD-O1D
29	g	307	CLA	C2-C3-C5-C6
29	g	310	CLA	CBD-CGD-O2D-CED
29	g	311	CLA	C1A-C2A-CAA-CBA
29	g	311	CLA	C3A-C2A-CAA-CBA
29	g	311	CLA	CHA-CBD-CGD-O1D
29	g	311	CLA	CHA-CBD-CGD-O2D
29	g	311	CLA	CBD-CGD-O2D-CED
29	g	312	CLA	C2B-C3B-CAB-CBB
29	g	312	CLA	C4B-C3B-CAB-CBB
29	g	316	CLA	C2B-C3B-CAB-CBB
29	g	316	CLA	C4B-C3B-CAB-CBB
29	g	316	CLA	CBD-CGD-O2D-CED
29	g	323	CLA	C1A-C2A-CAA-CBA
29	g	323	CLA	C3A-C2A-CAA-CBA
29	g	323	CLA	CBD-CGD-O2D-CED
29	n	601	CLA	C1A-C2A-CAA-CBA
29	n	601	CLA	CBD-CGD-O2D-CED
29	n	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	C2B-C3B-CAB-CBB
29	n	603	CLA	C4B-C3B-CAB-CBB
29	n	604	CLA	C1A-C2A-CAA-CBA
29	n	604	CLA	C2-C3-C5-C6
29	n	604	CLA	C4-C3-C5-C6
29	n	606	CLA	C4B-C3B-CAB-CBB
29	n	607	CLA	C4-C3-C5-C6
29	n	608	CLA	C1A-C2A-CAA-CBA
29	n	608	CLA	C3A-C2A-CAA-CBA
29	n	610	CLA	C1A-C2A-CAA-CBA
29	n	610	CLA	C3A-C2A-CAA-CBA
29	n	610	CLA	C4B-C3B-CAB-CBB
29	n	613	CLA	C1A-C2A-CAA-CBA
31	A	842	LHG	C3-O3-P-O5
31	A	843	LHG	C3-O3-P-O5
31	A	848	LHG	C4-O6-P-O5
31	A	848	LHG	O9-C7-O7-C5
31	J	104	LHG	C3-O3-P-O5
31	L	208	LHG	C2-C3-O3-P
31	L	208	LHG	C3-O3-P-O4
31	L	209	LHG	O1-C1-C2-C3
31	L	209	LHG	C4-O6-P-O3
31	L	209	LHG	C4-O6-P-O5
31	s	408	LHG	C4-O6-P-O3
31	s	408	LHG	C4-O6-P-O4
31	s	408	LHG	C8-C7-O7-C5
31	c	316	LHG	C3-O3-P-O5
31	c	316	LHG	O9-C7-O7-C5
31	c	316	LHG	C8-C7-O7-C5
31	c	320	LHG	O1-C1-C2-O2
31	c	320	LHG	C3-O3-P-O5
31	c	320	LHG	C8-C7-O7-C5
31	a	301	LHG	C1-C2-C3-O3
31	a	301	LHG	O2-C2-C3-O3
31	a	301	LHG	C3-O3-P-O4
31	a	301	LHG	O9-C7-O7-C5
31	a	318	LHG	O1-C1-C2-O2
31	a	318	LHG	O1-C1-C2-C3
31	a	318	LHG	C3-O3-P-O4
31	a	318	LHG	C3-O3-P-O5
31	b	318	LHG	O1-C1-C2-C3
31	b	318	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	b	318	LHG	C3-O3-P-O5
31	b	318	LHG	C3-O3-P-O6
31	b	318	LHG	C4-O6-P-O3
31	b	318	LHG	C8-C7-O7-C5
31	m	619	LHG	C3-O3-P-O5
31	m	619	LHG	O7-C5-C6-O8
31	e	317	LHG	C4-O6-P-O4
31	e	317	LHG	O9-C7-O7-C5
31	e	317	LHG	C8-C7-O7-C5
31	l	318	LHG	C3-O3-P-O6
31	f	619	LHG	C4-O6-P-O3
31	f	619	LHG	C4-O6-P-O4
31	f	619	LHG	O9-C7-O7-C5
31	f	619	LHG	C8-C7-O7-C5
31	f	620	LHG	C1-C2-C3-O3
31	f	620	LHG	C4-O6-P-O4
31	i	317	LHG	C3-O3-P-O5
31	i	317	LHG	C8-C7-O7-C5
31	j	318	LHG	C4-O6-P-O3
31	j	318	LHG	C4-O6-P-O5
31	g	301	LHG	C3-O3-P-O4
31	g	322	LHG	O9-C7-O7-C5
31	g	322	LHG	C8-C7-O7-C5
31	n	619	LHG	O9-C7-O7-C5
31	n	619	LHG	C8-C7-O7-C5
32	A	844	WVN	C19-C22-C26-C29
32	A	844	WVN	C20-C23-C25-C27
32	A	844	WVN	C20-C23-C25-C28
32	A	844	WVN	C27-C25-C28-C30
32	A	844	WVN	C25-C28-C30-C33
32	A	844	WVN	C29-C31-C32-C35
32	A	844	WVN	C29-C31-C32-C36
32	A	844	WVN	C35-C32-C36-C39
32	A	844	WVN	C38-C34-C37-C40
32	A	845	WVN	C15-C13-C20-C23
32	A	845	WVN	C19-C22-C26-C29
32	A	845	WVN	C24-C22-C26-C29
32	A	845	WVN	C27-C25-C28-C30
32	A	845	WVN	C35-C32-C36-C39
32	A	845	WVN	C30-C33-C34-C37
32	A	845	WVN	C30-C33-C34-C38
32	A	845	WVN	C38-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
32	A	846	WVN	C15-C13-C20-C23
32	A	846	WVN	C24-C22-C26-C29
32	A	846	WVN	C20-C23-C25-C28
32	A	846	WVN	C23-C25-C28-C30
32	A	846	WVN	C27-C25-C28-C30
32	A	846	WVN	C29-C31-C32-C36
32	A	846	WVN	C35-C32-C36-C39
32	A	846	WVN	C30-C33-C34-C37
32	A	846	WVN	C38-C34-C37-C40
32	A	847	WVN	C01-C02-C11-C19
32	A	847	WVN	C05-C02-C11-C19
32	A	847	WVN	C06-C13-C20-C23
32	A	847	WVN	C11-C19-C22-C26
32	A	847	WVN	C19-C22-C26-C29
32	A	847	WVN	C23-C25-C28-C30
32	A	847	WVN	C27-C25-C28-C30
32	A	847	WVN	C35-C32-C36-C39
32	A	847	WVN	C30-C33-C34-C37
32	A	847	WVN	C30-C33-C34-C38
32	A	847	WVN	C33-C34-C37-C40
32	A	854	WVN	C15-C13-C20-C23
32	A	854	WVN	C11-C19-C22-C24
32	A	854	WVN	C11-C19-C22-C26
32	A	854	WVN	C19-C22-C26-C29
32	A	854	WVN	C20-C23-C25-C27
32	A	854	WVN	C27-C25-C28-C30
32	A	854	WVN	C22-C26-C29-C31
32	A	854	WVN	C29-C31-C32-C35
32	A	854	WVN	C29-C31-C32-C36
32	A	854	WVN	C35-C32-C36-C39
32	A	854	WVN	C30-C33-C34-C38
32	A	854	WVN	C33-C34-C37-C40
32	B	845	WVN	C01-C02-C11-C19
32	B	845	WVN	C05-C02-C11-C19
32	B	845	WVN	C30-C33-C34-C37
32	B	846	WVN	C24-C22-C26-C29
32	B	846	WVN	C27-C25-C28-C30
32	B	846	WVN	C25-C28-C30-C33
32	B	846	WVN	C35-C32-C36-C39
32	B	846	WVN	C30-C33-C34-C37
32	B	846	WVN	C38-C34-C37-C40
32	B	847	WVN	C15-C13-C20-C23

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Mol	Chain	Res	Type	Atoms
32	B	847	WVN	C19-C22-C26-C29
32	B	847	WVN	C20-C23-C25-C27
32	B	847	WVN	C20-C23-C25-C28
32	B	847	WVN	C27-C25-C28-C30
32	B	847	WVN	C25-C28-C30-C33
32	B	847	WVN	C29-C31-C32-C36
32	B	847	WVN	C35-C32-C36-C39
32	B	847	WVN	C30-C33-C34-C37
32	B	847	WVN	C30-C33-C34-C38
32	B	847	WVN	C38-C34-C37-C40
32	B	847	WVN	C34-C37-C40-C39
32	B	848	WVN	C15-C13-C20-C23
32	B	848	WVN	C24-C22-C26-C29
32	B	848	WVN	C27-C25-C28-C30
32	B	848	WVN	C29-C31-C32-C35
32	B	848	WVN	C35-C32-C36-C39
32	B	848	WVN	C30-C33-C34-C38
32	B	848	WVN	C38-C34-C37-C40
32	B	849	WVN	C15-C13-C20-C23
32	B	849	WVN	C11-C19-C22-C24
32	B	849	WVN	C11-C19-C22-C26
32	B	849	WVN	C19-C22-C26-C29
32	B	849	WVN	C20-C23-C25-C28
32	B	849	WVN	C27-C25-C28-C30
32	B	849	WVN	C35-C32-C36-C39
32	B	849	WVN	C38-C34-C37-C40
32	F	204	WVN	C15-C13-C20-C23
32	F	204	WVN	C24-C22-C26-C29
32	F	204	WVN	C20-C23-C25-C27
32	F	204	WVN	C27-C25-C28-C30
32	F	204	WVN	C25-C28-C30-C33
32	F	204	WVN	C31-C32-C36-C39
32	F	204	WVN	C30-C33-C34-C37
32	F	204	WVN	C38-C34-C37-C40
32	F	205	WVN	C01-C02-C11-C19
32	F	205	WVN	C15-C13-C20-C23
32	F	205	WVN	C11-C19-C22-C24
32	F	205	WVN	C11-C19-C22-C26
32	F	205	WVN	C19-C22-C26-C29
32	F	205	WVN	C24-C22-C26-C29
32	F	205	WVN	C20-C23-C25-C28
32	F	205	WVN	C23-C25-C28-C30

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Mol	Chain	Res	Type	Atoms
32	F	205	WVN	C27-C25-C28-C30
32	F	205	WVN	C29-C31-C32-C35
32	F	205	WVN	C31-C32-C36-C39
32	F	205	WVN	C30-C33-C34-C38
32	F	205	WVN	C38-C34-C37-C40
32	F	207	WVN	C15-C13-C20-C23
32	F	207	WVN	C11-C19-C22-C24
32	F	207	WVN	C11-C19-C22-C26
32	F	207	WVN	C24-C22-C26-C29
32	F	207	WVN	C20-C23-C25-C27
32	F	207	WVN	C20-C23-C25-C28
32	F	207	WVN	C27-C25-C28-C30
32	F	207	WVN	C22-C26-C29-C31
32	F	207	WVN	C29-C31-C32-C36
32	F	207	WVN	C35-C32-C36-C39
32	F	207	WVN	C38-C34-C37-C40
32	I	101	WVN	C01-C02-C11-C19
32	I	101	WVN	C15-C13-C20-C23
32	I	101	WVN	C11-C19-C22-C26
32	I	101	WVN	C24-C22-C26-C29
32	I	101	WVN	C27-C25-C28-C30
32	I	101	WVN	C22-C26-C29-C31
32	I	101	WVN	C35-C32-C36-C39
32	I	101	WVN	C30-C33-C34-C37
32	I	101	WVN	C30-C33-C34-C38
32	I	101	WVN	C38-C34-C37-C40
32	J	101	WVN	C15-C13-C20-C23
32	J	101	WVN	C11-C19-C22-C26
32	J	101	WVN	C24-C22-C26-C29
32	J	101	WVN	C20-C23-C25-C27
32	J	101	WVN	C27-C25-C28-C30
32	J	101	WVN	C35-C32-C36-C39
32	J	101	WVN	C30-C33-C34-C37
32	J	101	WVN	C38-C34-C37-C40
32	J	101	WVN	C34-C37-C40-C39
32	L	201	WVN	C01-C02-C11-C19
32	L	201	WVN	C05-C02-C11-C19
32	L	201	WVN	C15-C13-C20-C23
32	L	201	WVN	C11-C19-C22-C24
32	L	201	WVN	C19-C22-C26-C29
32	L	201	WVN	C20-C23-C25-C27
32	L	201	WVN	C27-C25-C28-C30

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Mol	Chain	Res	Type	Atoms
32	L	201	WVN	C29-C31-C32-C35
32	L	201	WVN	C29-C31-C32-C36
32	L	201	WVN	C35-C32-C36-C39
32	L	201	WVN	C30-C33-C34-C37
32	L	201	WVN	C38-C34-C37-C40
32	L	201	WVN	C34-C37-C40-C39
32	L	205	WVN	C11-C19-C22-C26
32	L	205	WVN	C24-C22-C26-C29
32	L	205	WVN	C20-C23-C25-C28
32	L	205	WVN	C27-C25-C28-C30
32	L	205	WVN	C29-C31-C32-C36
32	L	205	WVN	C35-C32-C36-C39
32	L	205	WVN	C30-C33-C34-C37
32	L	205	WVN	C30-C33-C34-C38
32	L	205	WVN	C38-C34-C37-C40
32	L	206	WVN	C24-C22-C26-C29
32	L	206	WVN	C23-C25-C28-C30
32	L	206	WVN	C27-C25-C28-C30
32	L	206	WVN	C22-C26-C29-C31
32	L	206	WVN	C29-C31-C32-C35
32	L	206	WVN	C35-C32-C36-C39
32	L	206	WVN	C30-C33-C34-C38
32	L	206	WVN	C38-C34-C37-C40
32	M	101	WVN	C15-C13-C20-C23
32	M	101	WVN	C11-C19-C22-C24
32	M	101	WVN	C24-C22-C26-C29
32	M	101	WVN	C20-C23-C25-C27
32	M	101	WVN	C20-C23-C25-C28
32	M	101	WVN	C27-C25-C28-C30
32	M	101	WVN	C25-C28-C30-C33
32	M	101	WVN	C29-C31-C32-C35
32	M	101	WVN	C35-C32-C36-C39
32	M	101	WVN	C30-C33-C34-C37
32	M	101	WVN	C30-C33-C34-C38
32	M	101	WVN	C33-C34-C37-C40
32	M	101	WVN	C32-C36-C39-C40
32	K	103	WVN	C15-C13-C20-C23
32	K	103	WVN	C24-C22-C26-C29
32	K	103	WVN	C20-C23-C25-C28
32	K	103	WVN	C27-C25-C28-C30
32	K	103	WVN	C35-C32-C36-C39
32	K	103	WVN	C33-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
32	s	405	WVN	C20-C23-C25-C27
32	s	405	WVN	C27-C25-C28-C30
32	s	405	WVN	C25-C28-C30-C33
32	s	405	WVN	C35-C32-C36-C39
32	s	405	WVN	C33-C34-C37-C40
32	s	407	WVN	C15-C13-C20-C23
32	s	407	WVN	C24-C22-C26-C29
32	s	407	WVN	C27-C25-C28-C30
32	s	407	WVN	C29-C31-C32-C35
32	s	407	WVN	C35-C32-C36-C39
32	s	407	WVN	C30-C33-C34-C37
32	s	407	WVN	C38-C34-C37-C40
32	h	308	WVN	C15-C13-C20-C23
32	h	308	WVN	C11-C19-C22-C24
32	h	308	WVN	C24-C22-C26-C29
32	h	308	WVN	C20-C23-C25-C27
32	h	308	WVN	C27-C25-C28-C30
32	h	308	WVN	C29-C31-C32-C35
32	h	308	WVN	C35-C32-C36-C39
32	h	308	WVN	C30-C33-C34-C37
32	h	308	WVN	C33-C34-C37-C40
32	e	315	WVN	C19-C22-C26-C29
32	e	315	WVN	C23-C25-C28-C30
32	e	315	WVN	C27-C25-C28-C30
32	e	315	WVN	C29-C31-C32-C36
32	e	315	WVN	C35-C32-C36-C39
32	e	315	WVN	C33-C34-C37-C40
32	l	302	WVN	C20-C23-C25-C27
32	l	302	WVN	C20-C23-C25-C28
32	l	302	WVN	C27-C25-C28-C30
32	l	302	WVN	C29-C31-C32-C36
32	l	302	WVN	C35-C32-C36-C39
32	l	302	WVN	C30-C33-C34-C37
32	l	302	WVN	C30-C33-C34-C38
32	l	302	WVN	C38-C34-C37-C40
32	l	316	WVN	C01-C02-C11-C19
32	l	316	WVN	C19-C22-C26-C29
32	l	316	WVN	C24-C22-C26-C29
32	l	316	WVN	C20-C23-C25-C28
32	l	316	WVN	C27-C25-C28-C30
32	l	316	WVN	C29-C31-C32-C35
32	l	316	WVN	C35-C32-C36-C39

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Mol	Chain	Res	Type	Atoms
32	l	316	WVN	C30-C33-C34-C37
32	l	316	WVN	C30-C33-C34-C38
32	l	316	WVN	C38-C34-C37-C40
32	i	315	WVN	C19-C22-C26-C29
32	i	315	WVN	C24-C22-C26-C29
32	i	315	WVN	C23-C25-C28-C30
32	i	315	WVN	C29-C31-C32-C36
32	i	315	WVN	C35-C32-C36-C39
32	i	315	WVN	C38-C34-C37-C40
32	R	201	WVN	C01-C02-C11-C19
32	R	201	WVN	C15-C13-C20-C23
32	R	201	WVN	C24-C22-C26-C29
32	R	201	WVN	C27-C25-C28-C30
32	R	201	WVN	C35-C32-C36-C39
32	R	201	WVN	C30-C33-C34-C38
32	R	201	WVN	C33-C34-C37-C40
32	R	202	WVN	C06-C13-C20-C23
32	R	202	WVN	C11-C19-C22-C24
32	R	202	WVN	C24-C22-C26-C29
32	R	202	WVN	C27-C25-C28-C30
32	R	202	WVN	C25-C28-C30-C33
32	R	202	WVN	C35-C32-C36-C39
32	R	202	WVN	C30-C33-C34-C38
32	R	202	WVN	C33-C34-C37-C40
33	A	849	LMU	O5B-C1B-O1B-C4'
33	A	849	LMU	C2'-C1'-O1'-C1
33	A	849	LMU	C2-C1-O1'-C1'
33	A	855	LMU	C2'-C1'-O1'-C1
33	A	855	LMU	O5'-C1'-O1'-C1
33	A	855	LMU	C2-C1-O1'-C1'
33	a	319	LMU	O5B-C1B-O1B-C4'
33	i	301	LMU	C2'-C1'-O1'-C1
35	A	853	SQD	C2-C1-O6-C44
35	A	853	SQD	O5-C1-O6-C44
35	A	853	SQD	O5-C5-C6-S
36	B	844	DGD	O6D-C1D-O3G-C3G
37	c	317	LMG	O6-C1-O1-C7
37	c	318	LMG	C11-C10-O7-C8
37	Q	301	LMG	C2-C1-O1-C7
37	Q	301	LMG	O6-C1-O1-C7
37	Q	301	LMG	C11-C10-O7-C8
38	J	103	II0	C23-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
38	J	103	II0	C27-C25-C29-C31
38	J	103	II0	C31-C33-C35-C37
38	J	103	II0	C31-C33-C35-C39
38	J	103	II0	C32-C34-C36-C38
38	J	103	II0	C37-C35-C39-C41
38	J	103	II0	C34-C36-C40-C42
38	O	203	II0	C24-C26-C30-C32
38	c	313	II0	C23-C25-C29-C31
38	c	313	II0	C24-C26-C30-C32
38	c	313	II0	C28-C26-C30-C32
38	c	313	II0	C31-C33-C35-C37
38	c	313	II0	C31-C33-C35-C39
38	c	313	II0	C32-C34-C36-C38
38	c	313	II0	C37-C35-C39-C41
38	c	313	II0	C34-C36-C40-C42
38	c	314	II0	C32-C34-C36-C38
38	c	314	II0	C32-C34-C36-C40
38	a	313	II0	C23-C25-C29-C31
38	a	313	II0	C24-C26-C30-C32
38	a	313	II0	C31-C33-C35-C37
38	a	313	II0	C31-C33-C35-C39
38	a	313	II0	C32-C34-C36-C38
38	a	313	II0	C32-C34-C36-C40
38	a	313	II0	C37-C35-C39-C41
38	a	313	II0	C34-C36-C40-C42
38	a	314	II0	C23-C25-C29-C31
38	a	314	II0	C28-C26-C30-C32
38	a	314	II0	C25-C29-C31-C33
38	a	314	II0	C26-C30-C32-C34
38	a	314	II0	C32-C34-C36-C38
38	a	314	II0	C37-C35-C39-C41
38	a	314	II0	C34-C36-C40-C42
38	a	315	II0	C27-C25-C29-C31
38	a	315	II0	C24-C26-C30-C32
38	a	315	II0	C28-C26-C30-C32
38	a	315	II0	C26-C30-C32-C34
38	a	315	II0	C31-C33-C35-C39
38	a	315	II0	C37-C35-C39-C41
38	a	315	II0	C34-C36-C40-C42
38	a	317	II0	C23-C25-C29-C31
38	a	317	II0	C27-C25-C29-C31
38	a	317	II0	C24-C26-C30-C32

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Mol	Chain	Res	Type	Atoms
38	a	317	II0	C32-C34-C36-C38
38	a	317	II0	C37-C35-C39-C41
38	a	317	II0	C38-C36-C40-C42
38	b	301	II0	C23-C25-C29-C31
38	b	301	II0	C27-C25-C29-C31
38	b	301	II0	C24-C26-C30-C32
38	b	301	II0	C28-C26-C30-C32
38	b	301	II0	C31-C33-C35-C37
38	b	301	II0	C37-C35-C39-C41
38	b	301	II0	C34-C36-C40-C42
38	b	314	II0	C23-C25-C29-C31
38	b	314	II0	C27-C25-C29-C31
38	b	314	II0	C28-C26-C30-C32
38	b	314	II0	C25-C29-C31-C33
38	b	314	II0	C31-C33-C35-C39
38	b	314	II0	C37-C35-C39-C41
38	b	314	II0	C34-C36-C40-C42
38	b	315	II0	C23-C25-C29-C31
38	b	315	II0	C27-C25-C29-C31
38	b	315	II0	C28-C26-C30-C32
38	b	315	II0	C37-C35-C39-C41
38	b	315	II0	C34-C36-C40-C42
38	b	317	II0	C23-C25-C29-C31
38	b	317	II0	C31-C33-C35-C37
38	b	317	II0	C31-C33-C35-C39
38	h	309	II0	C23-C25-C29-C31
38	h	309	II0	C27-C25-C29-C31
38	h	309	II0	C31-C33-C35-C37
38	h	309	II0	C31-C33-C35-C39
38	h	309	II0	C32-C34-C36-C40
38	h	309	II0	C37-C35-C39-C41
38	h	309	II0	C34-C36-C40-C42
38	h	310	II0	C23-C25-C29-C31
38	h	310	II0	C24-C26-C30-C32
38	h	310	II0	C28-C26-C30-C32
38	h	310	II0	C32-C34-C36-C38
38	h	310	II0	C37-C35-C39-C41
38	h	310	II0	C34-C36-C40-C42
38	h	311	II0	C23-C25-C29-C31
38	h	311	II0	C27-C25-C29-C31
38	h	311	II0	C24-C26-C30-C32
38	h	311	II0	C31-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
38	h	311	II0	C32-C34-C36-C38
38	h	311	II0	C32-C34-C36-C40
38	h	311	II0	C37-C35-C39-C41
38	h	311	II0	C34-C36-C40-C42
38	m	614	II0	C23-C25-C29-C31
38	m	614	II0	C24-C26-C30-C32
38	m	614	II0	C31-C33-C35-C37
38	m	614	II0	C31-C33-C35-C39
38	m	614	II0	C32-C34-C36-C38
38	m	614	II0	C32-C34-C36-C40
38	m	614	II0	C37-C35-C39-C41
38	m	614	II0	C38-C36-C40-C42
38	m	615	II0	C23-C25-C29-C31
38	m	615	II0	C24-C26-C30-C32
38	m	615	II0	C28-C26-C30-C32
38	m	615	II0	C26-C30-C32-C34
38	m	615	II0	C31-C33-C35-C37
38	m	615	II0	C31-C33-C35-C39
38	m	615	II0	C32-C34-C36-C38
38	m	615	II0	C32-C34-C36-C40
38	m	615	II0	C37-C35-C39-C41
38	m	615	II0	C34-C36-C40-C42
38	m	616	II0	C23-C25-C29-C31
38	m	616	II0	C24-C26-C30-C32
38	m	616	II0	C28-C26-C30-C32
38	m	616	II0	C37-C35-C39-C41
38	m	616	II0	C34-C36-C40-C42
38	m	618	II0	C23-C25-C29-C31
38	m	618	II0	C27-C25-C29-C31
38	m	618	II0	C28-C26-C30-C32
38	m	618	II0	C31-C33-C35-C37
38	m	618	II0	C33-C35-C39-C41
38	m	618	II0	C37-C35-C39-C41
38	m	618	II0	C38-C36-C40-C42
38	e	312	II0	C23-C25-C29-C31
38	e	312	II0	C24-C26-C30-C32
38	e	312	II0	C28-C26-C30-C32
38	e	312	II0	C31-C33-C35-C37
38	e	312	II0	C32-C34-C36-C38
38	e	312	II0	C33-C35-C39-C41
38	e	312	II0	C34-C36-C40-C42
38	e	313	II0	C23-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
38	e	313	II0	C27-C25-C29-C31
38	e	313	II0	C24-C26-C30-C32
38	e	313	II0	C28-C26-C30-C32
38	e	313	II0	C31-C33-C35-C39
38	e	313	II0	C32-C34-C36-C38
38	e	313	II0	C32-C34-C36-C40
38	e	313	II0	C37-C35-C39-C41
38	e	313	II0	C38-C36-C40-C42
38	e	314	II0	C23-C25-C29-C31
38	e	314	II0	C24-C26-C30-C32
38	e	314	II0	C28-C26-C30-C32
38	e	314	II0	C31-C33-C35-C37
38	e	314	II0	C31-C33-C35-C39
38	e	314	II0	C32-C34-C36-C38
38	e	314	II0	C32-C34-C36-C40
38	e	314	II0	C37-C35-C39-C41
38	e	316	II0	C23-C25-C29-C31
38	e	316	II0	C24-C26-C30-C32
38	e	316	II0	C28-C26-C30-C32
38	e	316	II0	C31-C33-C35-C37
38	e	316	II0	C31-C33-C35-C39
38	e	316	II0	C32-C34-C36-C38
38	e	316	II0	C32-C34-C36-C40
38	l	313	II0	C23-C25-C29-C31
38	l	313	II0	C28-C26-C30-C32
38	l	313	II0	C31-C33-C35-C37
38	l	313	II0	C32-C34-C36-C40
38	l	313	II0	C37-C35-C39-C41
38	l	313	II0	C38-C36-C40-C42
38	l	314	II0	C23-C25-C29-C31
38	l	314	II0	C28-C26-C30-C32
38	l	314	II0	C25-C29-C31-C33
38	l	314	II0	C31-C33-C35-C37
38	l	314	II0	C31-C33-C35-C39
38	l	314	II0	C37-C35-C39-C41
38	l	314	II0	C38-C36-C40-C42
38	l	315	II0	C23-C25-C29-C31
38	l	315	II0	C28-C26-C30-C32
38	l	315	II0	C32-C34-C36-C38
38	l	315	II0	C32-C34-C36-C40
38	l	315	II0	C37-C35-C39-C41
38	l	315	II0	C38-C36-C40-C42

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Mol	Chain	Res	Type	Atoms
38	k	615	II0	C23-C25-C29-C31
38	k	615	II0	C27-C25-C29-C31
38	k	615	II0	C24-C26-C30-C32
38	k	615	II0	C25-C29-C31-C33
38	k	615	II0	C31-C33-C35-C39
38	k	615	II0	C32-C34-C36-C38
38	k	615	II0	C32-C34-C36-C40
38	k	615	II0	C37-C35-C39-C41
38	k	615	II0	C34-C36-C40-C42
38	k	615	II0	C38-C36-C40-C42
38	k	616	II0	C23-C25-C29-C31
38	k	616	II0	C28-C26-C30-C32
38	k	616	II0	C32-C34-C36-C38
38	k	616	II0	C32-C34-C36-C40
38	k	616	II0	C37-C35-C39-C41
38	k	616	II0	C34-C36-C40-C42
38	k	617	II0	C24-C26-C30-C32
38	k	618	II0	C23-C25-C29-C31
38	k	618	II0	C27-C25-C29-C31
38	k	618	II0	C32-C34-C36-C38
38	k	618	II0	C32-C34-C36-C40
38	k	619	II0	C23-C25-C29-C31
38	k	619	II0	C28-C26-C30-C32
38	k	619	II0	C31-C33-C35-C39
38	k	619	II0	C32-C34-C36-C38
38	k	619	II0	C32-C34-C36-C40
38	k	619	II0	C33-C35-C39-C41
38	k	619	II0	C37-C35-C39-C41
38	k	619	II0	C38-C36-C40-C42
38	k	620	II0	C23-C25-C29-C31
38	k	620	II0	C27-C25-C29-C31
38	k	620	II0	C28-C26-C30-C32
38	k	620	II0	C31-C33-C35-C37
38	k	620	II0	C31-C33-C35-C39
38	k	620	II0	C32-C34-C36-C38
38	k	620	II0	C32-C34-C36-C40
38	k	620	II0	C37-C35-C39-C41
38	k	620	II0	C34-C36-C40-C42
38	f	614	II0	C23-C25-C29-C31
38	f	614	II0	C27-C25-C29-C31
38	f	614	II0	C24-C26-C30-C32
38	f	614	II0	C28-C26-C30-C32

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Mol	Chain	Res	Type	Atoms
38	f	614	II0	C26-C30-C32-C34
38	f	614	II0	C37-C35-C39-C41
38	f	614	II0	C34-C36-C40-C42
38	f	615	II0	C23-C25-C29-C31
38	f	615	II0	C24-C26-C30-C32
38	f	615	II0	C28-C26-C30-C32
38	f	615	II0	C31-C33-C35-C37
38	f	615	II0	C31-C33-C35-C39
38	f	615	II0	C32-C34-C36-C38
38	f	615	II0	C32-C34-C36-C40
38	f	615	II0	C37-C35-C39-C41
38	f	615	II0	C34-C36-C40-C42
38	f	616	II0	C23-C25-C29-C31
38	f	616	II0	C27-C25-C29-C31
38	f	616	II0	C28-C26-C30-C32
38	f	616	II0	C31-C33-C35-C37
38	f	616	II0	C32-C34-C36-C38
38	f	616	II0	C32-C34-C36-C40
38	f	616	II0	C37-C35-C39-C41
38	f	616	II0	C34-C36-C40-C42
38	f	618	II0	C23-C25-C29-C31
38	f	618	II0	C27-C25-C29-C31
38	f	618	II0	C28-C26-C30-C32
38	f	618	II0	C31-C33-C35-C37
38	f	618	II0	C31-C33-C35-C39
38	f	618	II0	C32-C34-C36-C38
38	f	618	II0	C32-C34-C36-C40
38	f	618	II0	C37-C35-C39-C41
38	f	618	II0	C34-C36-C40-C42
38	i	313	II0	C23-C25-C29-C31
38	i	313	II0	C28-C26-C30-C32
38	i	313	II0	C31-C33-C35-C39
38	i	313	II0	C37-C35-C39-C41
38	i	313	II0	C34-C36-C40-C42
38	i	314	II0	C23-C25-C29-C31
38	i	314	II0	C24-C26-C30-C32
38	i	314	II0	C37-C35-C39-C41
38	i	314	II0	C38-C36-C40-C42
38	i	316	II0	C23-C25-C29-C31
38	i	316	II0	C24-C26-C30-C32
38	i	316	II0	C32-C34-C36-C40
38	i	316	II0	C37-C35-C39-C41

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Mol	Chain	Res	Type	Atoms
38	i	316	II0	C34-C36-C40-C42
38	i	319	II0	C23-C25-C29-C31
38	i	319	II0	C28-C26-C30-C32
38	i	319	II0	C25-C29-C31-C33
38	i	319	II0	C26-C30-C32-C34
38	i	319	II0	C31-C33-C35-C37
38	i	319	II0	C37-C35-C39-C41
38	i	319	II0	C38-C36-C40-C42
38	j	301	II0	C23-C25-C29-C31
38	j	301	II0	C27-C25-C29-C31
38	j	301	II0	C24-C26-C30-C32
38	j	301	II0	C31-C33-C35-C37
38	j	301	II0	C32-C34-C36-C38
38	j	301	II0	C37-C35-C39-C41
38	j	301	II0	C38-C36-C40-C42
38	j	315	II0	C23-C25-C29-C31
38	j	315	II0	C28-C26-C30-C32
38	j	315	II0	C25-C29-C31-C33
38	j	315	II0	C32-C34-C36-C38
38	j	315	II0	C32-C34-C36-C40
38	j	315	II0	C37-C35-C39-C41
38	j	315	II0	C34-C36-C40-C42
38	j	316	II0	C23-C25-C29-C31
38	j	316	II0	C24-C26-C30-C32
38	j	316	II0	C28-C26-C30-C32
38	j	316	II0	C31-C33-C35-C37
38	j	316	II0	C31-C33-C35-C39
38	j	316	II0	C32-C34-C36-C38
38	j	316	II0	C32-C34-C36-C40
38	j	316	II0	C37-C35-C39-C41
38	j	316	II0	C34-C36-C40-C42
38	d	301	II0	C23-C25-C29-C31
38	d	301	II0	C28-C26-C30-C32
38	d	301	II0	C31-C33-C35-C37
38	d	301	II0	C31-C33-C35-C39
38	d	301	II0	C32-C34-C36-C38
38	d	301	II0	C32-C34-C36-C40
38	d	301	II0	C37-C35-C39-C41
38	d	301	II0	C38-C36-C40-C42
38	d	314	II0	C26-C30-C32-C34
38	d	314	II0	C32-C34-C36-C38
38	d	314	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
38	d	315	II0	C27-C25-C29-C31
38	d	315	II0	C28-C26-C30-C32
38	d	315	II0	C31-C33-C35-C37
38	d	315	II0	C32-C34-C36-C40
38	d	315	II0	C37-C35-C39-C41
38	d	315	II0	C38-C36-C40-C42
38	d	316	II0	C23-C25-C29-C31
38	d	316	II0	C27-C25-C29-C31
38	d	316	II0	C28-C26-C30-C32
38	d	316	II0	C31-C33-C35-C37
38	d	316	II0	C32-C34-C36-C38
38	d	316	II0	C37-C35-C39-C41
38	d	316	II0	C34-C36-C40-C42
38	d	317	II0	C23-C25-C29-C31
38	d	317	II0	C27-C25-C29-C31
38	d	317	II0	C28-C26-C30-C32
38	d	317	II0	C26-C30-C32-C34
38	d	317	II0	C31-C33-C35-C39
38	d	317	II0	C32-C34-C36-C40
38	d	317	II0	C33-C35-C39-C41
38	d	317	II0	C37-C35-C39-C41
38	d	317	II0	C38-C36-C40-C42
38	d	319	II0	C23-C25-C29-C31
38	d	319	II0	C27-C25-C29-C31
38	d	319	II0	C32-C34-C36-C38
38	d	319	II0	C32-C34-C36-C40
38	g	317	II0	C23-C25-C29-C31
38	g	317	II0	C27-C25-C29-C31
38	g	317	II0	C28-C26-C30-C32
38	g	317	II0	C26-C30-C32-C34
38	g	317	II0	C32-C34-C36-C40
38	g	317	II0	C37-C35-C39-C41
38	g	317	II0	C34-C36-C40-C42
38	g	318	II0	C23-C25-C29-C31
38	g	318	II0	C28-C26-C30-C32
38	g	318	II0	C31-C33-C35-C37
38	g	318	II0	C31-C33-C35-C39
38	g	318	II0	C32-C34-C36-C38
38	g	318	II0	C32-C34-C36-C40
38	g	318	II0	C37-C35-C39-C41
38	g	318	II0	C34-C36-C40-C42
38	g	319	II0	C23-C25-C29-C31

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Mol	Chain	Res	Type	Atoms
38	g	319	II0	C24-C26-C30-C32
38	g	319	II0	C28-C26-C30-C32
38	g	319	II0	C37-C35-C39-C41
38	g	319	II0	C34-C36-C40-C42
38	g	321	II0	C26-C30-C32-C34
38	g	321	II0	C32-C34-C36-C38
38	g	321	II0	C32-C34-C36-C40
38	n	614	II0	C23-C25-C29-C31
38	n	614	II0	C27-C25-C29-C31
38	n	614	II0	C26-C30-C32-C34
38	n	614	II0	C31-C33-C35-C37
38	n	614	II0	C31-C33-C35-C39
38	n	614	II0	C32-C34-C36-C38
38	n	614	II0	C32-C34-C36-C40
38	n	615	II0	C23-C25-C29-C31
38	n	615	II0	C27-C25-C29-C31
38	n	615	II0	C28-C26-C30-C32
38	n	615	II0	C26-C30-C32-C34
38	n	615	II0	C31-C33-C35-C37
38	n	615	II0	C32-C34-C36-C38
38	n	615	II0	C32-C34-C36-C40
38	n	615	II0	C37-C35-C39-C41
38	n	615	II0	C34-C36-C40-C42
38	n	616	II0	C23-C25-C29-C31
38	n	616	II0	C27-C25-C29-C31
38	n	616	II0	C24-C26-C30-C32
38	n	616	II0	C31-C33-C35-C39
38	n	616	II0	C32-C34-C36-C38
38	n	616	II0	C32-C34-C36-C40
38	n	616	II0	C37-C35-C39-C41
38	n	616	II0	C34-C36-C40-C42
38	n	618	II0	C23-C25-C29-C31
38	n	618	II0	C28-C26-C30-C32
38	n	618	II0	C25-C29-C31-C33
38	n	618	II0	C26-C30-C32-C34
38	n	618	II0	C32-C34-C36-C40
38	n	618	II0	C37-C35-C39-C41
38	n	618	II0	C34-C36-C40-C42
39	O	204	IHT	C02-C07-C18-C22
39	O	204	IHT	C10-C07-C18-C22
39	O	204	IHT	C24-C26-C29-C31
39	c	315	IHT	C26-C29-C31-C34

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Mol	Chain	Res	Type	Atoms
39	c	315	IHT	C31-C34-C35-C38
39	c	315	IHT	C31-C34-C35-C39
39	c	319	IHT	C11-C21-C24-C26
39	c	319	IHT	C26-C29-C31-C34
39	c	319	IHT	C31-C34-C35-C38
39	c	319	IHT	C31-C34-C35-C39
39	a	316	IHT	C02-C07-C18-C22
39	a	316	IHT	C24-C26-C29-C31
39	a	316	IHT	C28-C26-C29-C31
39	b	316	IHT	C24-C26-C29-C31
39	b	316	IHT	C31-C34-C35-C38
39	b	316	IHT	C31-C34-C35-C39
39	f	617	IHT	C18-C22-C23-C25
39	f	617	IHT	C18-C22-C23-C27
39	j	317	IHT	C18-C22-C23-C25
39	j	317	IHT	C18-C22-C23-C27
39	g	320	IHT	C24-C26-C29-C31
39	g	320	IHT	C31-C34-C35-C38
39	g	320	IHT	C31-C34-C35-C39
39	g	324	IHT	C11-C21-C24-C26
39	g	324	IHT	C24-C26-C29-C31
39	g	324	IHT	C28-C26-C29-C31
39	n	617	IHT	C02-C07-C18-C22
39	n	617	IHT	C10-C07-C18-C22
39	n	617	IHT	C26-C29-C31-C34
39	n	617	IHT	C31-C34-C35-C38
40	s	401	KC2	C3A-C2A-CAA-CBA
40	s	401	KC2	C2C-C3C-CAC-CBC
40	s	401	KC2	C4C-C3C-CAC-CBC
40	s	401	KC2	C2A-CAA-CBA-CGA
40	s	404	KC2	C3A-C2A-CAA-CBA
40	c	310	KC2	C3A-C2A-CAA-CBA
40	c	310	KC2	C2C-C3C-CAC-CBC
40	c	310	KC2	C4C-C3C-CAC-CBC
40	c	310	KC2	C2A-CAA-CBA-CGA
40	c	310	KC2	CBD-CGD-O2D-CED
40	m	611	KC2	C3A-C2A-CAA-CBA
40	m	611	KC2	C2C-C3C-CAC-CBC
40	m	611	KC2	C4C-C3C-CAC-CBC
40	m	611	KC2	C2A-CAA-CBA-CGA
40	e	309	KC2	C3A-C2A-CAA-CBA
40	e	309	KC2	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
40	l	311	KC2	C3A-C2A-CAA-CBA
40	l	311	KC2	C2A-CAA-CBA-CGA
40	l	311	KC2	CHA-CBD-CGD-O2D
40	k	611	KC2	C3A-C2A-CAA-CBA
40	k	611	KC2	C2C-C3C-CAC-CBC
40	k	611	KC2	C4C-C3C-CAC-CBC
40	k	611	KC2	C2A-CAA-CBA-CGA
40	k	611	KC2	CBD-CGD-O2D-CED
40	k	612	KC2	C1A-C2A-CAA-CBA
40	k	612	KC2	C3A-C2A-CAA-CBA
40	k	612	KC2	C2B-C3B-CAB-CBB
40	k	612	KC2	C4B-C3B-CAB-CBB
40	k	612	KC2	C2C-C3C-CAC-CBC
40	k	613	KC2	C1A-C2A-CAA-CBA
40	k	613	KC2	C3A-C2A-CAA-CBA
40	k	613	KC2	C2C-C3C-CAC-CBC
40	k	613	KC2	C4C-C3C-CAC-CBC
40	k	613	KC2	C2A-CAA-CBA-CGA
40	f	611	KC2	C3A-C2A-CAA-CBA
40	f	611	KC2	C2C-C3C-CAC-CBC
40	f	611	KC2	C4C-C3C-CAC-CBC
40	f	611	KC2	C2A-CAA-CBA-CGA
40	i	310	KC2	C3A-C2A-CAA-CBA
40	i	310	KC2	C2C-C3C-CAC-CBC
40	i	310	KC2	C4C-C3C-CAC-CBC
40	i	310	KC2	C2A-CAA-CBA-CGA
40	i	318	KC2	C3A-C2A-CAA-CBA
40	i	318	KC2	C2C-C3C-CAC-CBC
40	i	318	KC2	C2A-CAA-CBA-CGA
40	i	318	KC2	CBD-CGD-O2D-CED
40	j	312	KC2	C3A-C2A-CAA-CBA
40	j	312	KC2	C2A-CAA-CBA-CGA
40	j	312	KC2	CBD-CGD-O2D-CED
40	d	311	KC2	C3A-C2A-CAA-CBA
40	d	311	KC2	C2A-CAA-CBA-CGA
40	d	311	KC2	CBD-CGD-O2D-CED
40	d	312	KC2	C1A-C2A-CAA-CBA
40	d	312	KC2	C3A-C2A-CAA-CBA
40	d	312	KC2	C2C-C3C-CAC-CBC
40	d	312	KC2	C4C-C3C-CAC-CBC
40	g	313	KC2	C2C-C3C-CAC-CBC
40	g	313	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
40	g	313	KC2	C2A-CAA-CBA-CGA
40	g	314	KC2	CAA-CBA-CGA-O2A
40	g	315	KC2	C3A-C2A-CAA-CBA
40	g	315	KC2	C2B-C3B-CAB-CBB
40	g	315	KC2	C2A-CAA-CBA-CGA
40	n	611	KC2	C2C-C3C-CAC-CBC
40	n	611	KC2	C4C-C3C-CAC-CBC
40	n	611	KC2	C2A-CAA-CBA-CGA
40	n	611	KC2	CAA-CBA-CGA-O1A
40	n	611	KC2	CAA-CBA-CGA-O2A
40	n	612	KC2	C1A-C2A-CAA-CBA
40	n	612	KC2	C3A-C2A-CAA-CBA
40	n	612	KC2	C2B-C3B-CAB-CBB
40	n	612	KC2	C4B-C3B-CAB-CBB
40	n	612	KC2	C2C-C3C-CAC-CBC
40	n	612	KC2	C4C-C3C-CAC-CBC
29	B	819	CLA	C4C-C3C-CAC-CBC
29	K	102	CLA	O1D-CGD-O2D-CED
29	c	302	CLA	O1D-CGD-O2D-CED
29	h	302	CLA	O1D-CGD-O2D-CED
29	m	602	CLA	O1D-CGD-O2D-CED
29	m	609	CLA	O1D-CGD-O2D-CED
29	d	303	CLA	O1D-CGD-O2D-CED
29	g	311	CLA	O1D-CGD-O2D-CED
29	n	601	CLA	O1D-CGD-O2D-CED
40	j	312	KC2	O1D-CGD-O2D-CED
29	B	819	CLA	C2C-C3C-CAC-CBC
29	g	306	CLA	C2C-C3C-CAC-CBC
29	A	810	CLA	O1D-CGD-O2D-CED
29	B	804	CLA	O1D-CGD-O2D-CED
29	F	201	CLA	O1D-CGD-O2D-CED
29	L	204	CLA	O1D-CGD-O2D-CED
29	c	308	CLA	O1D-CGD-O2D-CED
29	b	304	CLA	O1D-CGD-O2D-CED
29	e	306	CLA	O1D-CGD-O2D-CED
29	k	601	CLA	O1D-CGD-O2D-CED
29	k	610	CLA	O1D-CGD-O2D-CED
29	k	614	CLA	O1D-CGD-O2D-CED
29	f	608	CLA	O1D-CGD-O2D-CED
29	i	311	CLA	O1D-CGD-O2D-CED
29	g	310	CLA	O1D-CGD-O2D-CED
29	n	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
40	c	310	KC2	O1D-CGD-O2D-CED
40	k	611	KC2	O1D-CGD-O2D-CED
40	i	310	KC2	O1D-CGD-O2D-CED
40	i	318	KC2	O1D-CGD-O2D-CED
29	A	814	CLA	CBD-CGD-O2D-CED
29	A	822	CLA	CBD-CGD-O2D-CED
29	B	803	CLA	CBD-CGD-O2D-CED
29	B	825	CLA	CBD-CGD-O2D-CED
29	B	827	CLA	CBD-CGD-O2D-CED
29	B	832	CLA	CBD-CGD-O2D-CED
29	F	201	CLA	CBD-CGD-O2D-CED
29	J	102	CLA	CBD-CGD-O2D-CED
29	O	202	CLA	CBD-CGD-O2D-CED
29	s	402	CLA	CBD-CGD-O2D-CED
29	s	403	CLA	CBD-CGD-O2D-CED
29	c	308	CLA	CBD-CGD-O2D-CED
29	a	306	CLA	CBD-CGD-O2D-CED
29	b	304	CLA	CBD-CGD-O2D-CED
29	b	312	CLA	CBD-CGD-O2D-CED
29	m	605	CLA	CBD-CGD-O2D-CED
29	m	612	CLA	CBD-CGD-O2D-CED
29	e	304	CLA	CBD-CGD-O2D-CED
29	e	306	CLA	CBD-CGD-O2D-CED
29	e	310	CLA	CBD-CGD-O2D-CED
29	l	309	CLA	CBD-CGD-O2D-CED
29	l	312	CLA	CBD-CGD-O2D-CED
29	k	602	CLA	CBD-CGD-O2D-CED
29	f	612	CLA	CBD-CGD-O2D-CED
29	i	308	CLA	CBD-CGD-O2D-CED
29	i	311	CLA	CBD-CGD-O2D-CED
29	j	309	CLA	CBD-CGD-O2D-CED
29	d	318	CLA	CBD-CGD-O2D-CED
29	n	603	CLA	CBD-CGD-O2D-CED
29	n	613	CLA	CBD-CGD-O2D-CED
40	e	309	KC2	CBD-CGD-O2D-CED
40	l	311	KC2	CBD-CGD-O2D-CED
40	i	310	KC2	CBD-CGD-O2D-CED
40	g	314	KC2	CBD-CGD-O2D-CED
40	n	612	KC2	CBD-CGD-O2D-CED
29	a	311	CLA	O1A-CGA-O2A-C1
29	h	301	CLA	O1A-CGA-O2A-C1
29	n	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	i	317	LHG	O10-C23-O8-C6
37	c	318	LMG	O10-C28-O8-C9
33	i	301	LMU	O5B-C1B-O1B-C4'
29	g	306	CLA	C4C-C3C-CAC-CBC
29	A	815	CLA	O1D-CGD-O2D-CED
29	A	819	CLA	O1D-CGD-O2D-CED
29	A	827	CLA	O1D-CGD-O2D-CED
29	B	803	CLA	O1D-CGD-O2D-CED
29	J	102	CLA	O1D-CGD-O2D-CED
29	O	202	CLA	O1D-CGD-O2D-CED
29	s	403	CLA	O1D-CGD-O2D-CED
29	b	312	CLA	O1D-CGD-O2D-CED
29	g	323	CLA	O1D-CGD-O2D-CED
40	d	311	KC2	O1D-CGD-O2D-CED
29	m	602	CLA	C4C-C3C-CAC-CBC
33	A	855	LMU	O5B-C1B-O1B-C4'
29	c	303	CLA	O1D-CGD-O2D-CED
29	c	306	CLA	O1D-CGD-O2D-CED
29	c	311	CLA	O1D-CGD-O2D-CED
29	a	312	CLA	O1D-CGD-O2D-CED
29	m	603	CLA	O1D-CGD-O2D-CED
29	m	613	CLA	O1D-CGD-O2D-CED
29	e	303	CLA	O1D-CGD-O2D-CED
29	e	304	CLA	O1D-CGD-O2D-CED
29	l	306	CLA	O1D-CGD-O2D-CED
29	j	313	CLA	O1D-CGD-O2D-CED
29	j	314	CLA	O1D-CGD-O2D-CED
29	d	302	CLA	O1D-CGD-O2D-CED
29	d	309	CLA	O1D-CGD-O2D-CED
40	e	309	KC2	O1D-CGD-O2D-CED
29	B	811	CLA	CBA-CGA-O2A-C1
29	a	311	CLA	CBA-CGA-O2A-C1
37	Q	301	LMG	C29-C28-O8-C9
29	A	809	CLA	CBD-CGD-O2D-CED
29	A	831	CLA	CBD-CGD-O2D-CED
29	A	832	CLA	CBD-CGD-O2D-CED
29	B	819	CLA	CBD-CGD-O2D-CED
29	B	842	CLA	CBD-CGD-O2D-CED
29	L	202	CLA	CBD-CGD-O2D-CED
29	c	309	CLA	CBD-CGD-O2D-CED
29	c	312	CLA	CBD-CGD-O2D-CED
29	a	307	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	a	309	CLA	CBD-CGD-O2D-CED
29	b	303	CLA	CBD-CGD-O2D-CED
29	m	610	CLA	CBD-CGD-O2D-CED
29	l	304	CLA	CBD-CGD-O2D-CED
29	k	605	CLA	CBD-CGD-O2D-CED
29	k	606	CLA	CBD-CGD-O2D-CED
29	k	608	CLA	CBD-CGD-O2D-CED
29	f	613	CLA	CBD-CGD-O2D-CED
29	i	302	CLA	CBD-CGD-O2D-CED
29	i	305	CLA	CBD-CGD-O2D-CED
29	d	307	CLA	CBD-CGD-O2D-CED
29	d	313	CLA	CBD-CGD-O2D-CED
29	g	302	CLA	CBD-CGD-O2D-CED
29	g	308	CLA	CBD-CGD-O2D-CED
29	n	610	CLA	CBD-CGD-O2D-CED
40	d	312	KC2	CBD-CGD-O2D-CED
29	A	835	CLA	O1A-CGA-O2A-C1
29	A	839	CLA	O1A-CGA-O2A-C1
29	B	811	CLA	O1A-CGA-O2A-C1
29	B	813	CLA	O1A-CGA-O2A-C1
29	B	831	CLA	O1A-CGA-O2A-C1
29	b	307	CLA	O1A-CGA-O2A-C1
29	b	313	CLA	O1A-CGA-O2A-C1
29	h	302	CLA	O1A-CGA-O2A-C1
29	h	303	CLA	O1A-CGA-O2A-C1
29	m	610	CLA	O1A-CGA-O2A-C1
29	e	306	CLA	O1A-CGA-O2A-C1
29	e	311	CLA	O1A-CGA-O2A-C1
29	k	601	CLA	O1A-CGA-O2A-C1
29	f	602	CLA	O1A-CGA-O2A-C1
29	i	312	CLA	O1A-CGA-O2A-C1
29	g	311	CLA	O1A-CGA-O2A-C1
29	n	606	CLA	O1A-CGA-O2A-C1
29	n	608	CLA	O1A-CGA-O2A-C1
31	c	316	LHG	O10-C23-O8-C6
31	e	317	LHG	O10-C23-O8-C6
31	f	620	LHG	O10-C23-O8-C6
37	Q	301	LMG	O10-C28-O8-C9
29	e	307	CLA	O1D-CGD-O2D-CED
29	e	311	CLA	O1D-CGD-O2D-CED
29	d	304	CLA	O1D-CGD-O2D-CED
30	A	841	PQN	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
29	c	305	CLA	O1D-CGD-O2D-CED
29	b	305	CLA	O1D-CGD-O2D-CED
29	j	306	CLA	O1D-CGD-O2D-CED
29	d	318	CLA	O1D-CGD-O2D-CED
36	j	319	DGD	O6D-C5D-C6D-O5D
29	F	202	CLA	CBD-CGD-O2D-CED
29	c	304	CLA	CBD-CGD-O2D-CED
29	m	601	CLA	CBD-CGD-O2D-CED
29	i	309	CLA	CBD-CGD-O2D-CED
29	n	609	CLA	CBD-CGD-O2D-CED
29	b	311	CLA	O1D-CGD-O2D-CED
29	g	316	CLA	O1D-CGD-O2D-CED
31	s	408	LHG	O9-C7-O7-C5
31	c	320	LHG	O9-C7-O7-C5
31	b	318	LHG	O9-C7-O7-C5
31	f	620	LHG	O9-C7-O7-C5
31	i	317	LHG	O9-C7-O7-C5
36	B	844	DGD	O1B-C1B-O2G-C2G
37	F	206	LMG	O9-C10-O7-C8
37	c	317	LMG	O9-C10-O7-C8
37	Q	301	LMG	O9-C10-O7-C8
29	A	818	CLA	O1A-CGA-O2A-C1
31	g	301	LHG	O10-C23-O8-C6
33	A	855	LMU	C2B-C1B-O1B-C4'
29	A	805	CLA	C3-C5-C6-C7
29	A	816	CLA	C3-C5-C6-C7
29	A	834	CLA	C3-C5-C6-C7
29	B	806	CLA	C3-C5-C6-C7
29	B	809	CLA	C3-C5-C6-C7
29	B	817	CLA	C3-C5-C6-C7
29	B	819	CLA	C3-C5-C6-C7
29	F	202	CLA	C3-C5-C6-C7
29	K	101	CLA	C3-C5-C6-C7
29	c	302	CLA	C3-C5-C6-C7
29	c	304	CLA	C3-C5-C6-C7
29	b	308	CLA	C3-C5-C6-C7
29	b	310	CLA	C3-C5-C6-C7
29	m	602	CLA	C3-C5-C6-C7
29	e	306	CLA	C3-C5-C6-C7
29	l	301	CLA	C3-C5-C6-C7
29	l	309	CLA	C3-C5-C6-C7
29	l	310	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	k	602	CLA	C3-C5-C6-C7
29	f	607	CLA	C3-C5-C6-C7
29	f	609	CLA	C3-C5-C6-C7
29	f	613	CLA	C3-C5-C6-C7
29	i	305	CLA	C3-C5-C6-C7
29	i	311	CLA	C3-C5-C6-C7
29	g	311	CLA	C3-C5-C6-C7
29	n	609	CLA	C3-C5-C6-C7
29	b	302	CLA	CBA-CGA-O2A-C1
29	h	303	CLA	CBA-CGA-O2A-C1
29	m	610	CLA	CBA-CGA-O2A-C1
29	l	310	CLA	CBA-CGA-O2A-C1
29	k	601	CLA	CBA-CGA-O2A-C1
29	d	305	CLA	CBA-CGA-O2A-C1
29	g	311	CLA	CBA-CGA-O2A-C1
29	n	605	CLA	CBA-CGA-O2A-C1
29	n	606	CLA	CBA-CGA-O2A-C1
29	n	610	CLA	CBA-CGA-O2A-C1
31	A	848	LHG	C8-C7-O7-C5
31	f	620	LHG	C24-C23-O8-C6
37	c	318	LMG	C29-C28-O8-C9
29	m	602	CLA	C2C-C3C-CAC-CBC
31	a	301	LHG	C8-C7-O7-C5
29	A	814	CLA	O1D-CGD-O2D-CED
29	f	612	CLA	O1D-CGD-O2D-CED
29	n	603	CLA	O1D-CGD-O2D-CED
40	n	612	KC2	O1D-CGD-O2D-CED
29	B	821	CLA	CBD-CGD-O2D-CED
29	j	311	CLA	CBD-CGD-O2D-CED
29	d	308	CLA	CBD-CGD-O2D-CED
29	B	804	CLA	C2C-C3C-CAC-CBC
29	k	614	CLA	C2C-C3C-CAC-CBC
40	g	314	KC2	CAA-CBA-CGA-O1A
29	A	822	CLA	C4-C3-C5-C6
29	B	802	CLA	C4-C3-C5-C6
29	B	819	CLA	C4-C3-C5-C6
29	m	610	CLA	C4-C3-C5-C6
29	n	609	CLA	C4-C3-C5-C6
29	B	802	CLA	C2-C3-C5-C6
29	f	602	CLA	C2-C3-C5-C6
29	n	609	CLA	C2-C3-C5-C6
29	h	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	d	306	CLA	CBD-CGD-O2D-CED
29	A	815	CLA	C2A-CAA-CBA-CGA
29	B	829	CLA	C2A-CAA-CBA-CGA
29	B	836	CLA	C2A-CAA-CBA-CGA
29	O	201	CLA	C2A-CAA-CBA-CGA
29	s	406	CLA	C2A-CAA-CBA-CGA
29	a	312	CLA	C2A-CAA-CBA-CGA
29	h	302	CLA	C2A-CAA-CBA-CGA
29	h	303	CLA	C2A-CAA-CBA-CGA
29	m	610	CLA	C2A-CAA-CBA-CGA
29	l	312	CLA	C2A-CAA-CBA-CGA
29	k	605	CLA	C2A-CAA-CBA-CGA
29	k	614	CLA	C2A-CAA-CBA-CGA
29	j	302	CLA	C2A-CAA-CBA-CGA
29	f	607	CLA	O1A-CGA-O2A-C1
29	m	612	CLA	O1D-CGD-O2D-CED
29	B	831	CLA	C3-C5-C6-C7
29	s	403	CLA	C3-C5-C6-C7
29	a	308	CLA	C3-C5-C6-C7
29	h	305	CLA	C3-C5-C6-C7
29	n	604	CLA	C3-C5-C6-C7
29	A	809	CLA	CBA-CGA-O2A-C1
29	A	818	CLA	CBA-CGA-O2A-C1
29	A	819	CLA	CBA-CGA-O2A-C1
29	A	823	CLA	CBA-CGA-O2A-C1
29	A	834	CLA	CBA-CGA-O2A-C1
29	A	835	CLA	CBA-CGA-O2A-C1
29	A	837	CLA	CBA-CGA-O2A-C1
29	A	839	CLA	CBA-CGA-O2A-C1
29	B	813	CLA	CBA-CGA-O2A-C1
29	B	831	CLA	CBA-CGA-O2A-C1
29	b	307	CLA	CBA-CGA-O2A-C1
29	b	313	CLA	CBA-CGA-O2A-C1
29	h	302	CLA	CBA-CGA-O2A-C1
29	e	305	CLA	CBA-CGA-O2A-C1
29	e	306	CLA	CBA-CGA-O2A-C1
29	e	311	CLA	CBA-CGA-O2A-C1
29	l	307	CLA	CBA-CGA-O2A-C1
29	k	610	CLA	CBA-CGA-O2A-C1
29	f	602	CLA	CBA-CGA-O2A-C1
29	i	303	CLA	CBA-CGA-O2A-C1
29	i	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	d	306	CLA	CBA-CGA-O2A-C1
29	n	608	CLA	CBA-CGA-O2A-C1
31	i	317	LHG	C24-C23-O8-C6
31	g	301	LHG	C24-C23-O8-C6
37	c	318	LMG	O6-C5-C6-O5
33	A	855	LMU	C4'-C5'-C6'-O6'
29	m	605	CLA	O1D-CGD-O2D-CED
29	i	308	CLA	O1D-CGD-O2D-CED
30	A	841	PQN	C11-C12-C13-C14
30	B	843	PQN	C11-C12-C13-C14
29	k	604	CLA	CBD-CGD-O2D-CED
29	i	303	CLA	CBD-CGD-O2D-CED
29	B	825	CLA	O1D-CGD-O2D-CED
29	e	310	CLA	O1D-CGD-O2D-CED
29	l	312	CLA	O1D-CGD-O2D-CED
29	j	309	CLA	O1D-CGD-O2D-CED
37	c	318	LMG	O9-C10-O7-C8
29	A	809	CLA	O1A-CGA-O2A-C1
29	A	819	CLA	O1A-CGA-O2A-C1
29	A	823	CLA	O1A-CGA-O2A-C1
29	B	838	CLA	O1A-CGA-O2A-C1
29	i	303	CLA	O1A-CGA-O2A-C1
29	n	605	CLA	O1A-CGA-O2A-C1
31	L	209	LHG	O10-C23-O8-C6
37	L	210	LMG	O10-C28-O8-C9
40	g	314	KC2	O1D-CGD-O2D-CED
32	A	847	WVN	C22-C26-C29-C31
32	A	854	WVN	C25-C28-C30-C33
32	F	207	WVN	C25-C28-C30-C33
32	I	101	WVN	C25-C28-C30-C33
32	L	201	WVN	C22-C26-C29-C31
32	L	201	WVN	C25-C28-C30-C33
32	l	316	WVN	C25-C28-C30-C33
32	R	201	WVN	C25-C28-C30-C33
38	J	103	II0	C25-C29-C31-C33
38	c	314	II0	C26-C30-C32-C34
38	a	313	II0	C25-C29-C31-C33
38	b	314	II0	C26-C30-C32-C34
38	b	317	II0	C25-C29-C31-C33
38	b	317	II0	C35-C39-C41-C42
38	h	310	II0	C25-C29-C31-C33
38	m	614	II0	C25-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
38	m	615	II0	C25-C29-C31-C33
38	m	616	II0	C25-C29-C31-C33
38	m	618	II0	C25-C29-C31-C33
38	l	313	II0	C26-C30-C32-C34
38	l	315	II0	C25-C29-C31-C33
38	k	616	II0	C26-C30-C32-C34
38	k	620	II0	C25-C29-C31-C33
38	f	615	II0	C25-C29-C31-C33
38	i	313	II0	C26-C30-C32-C34
38	i	314	II0	C25-C29-C31-C33
38	j	301	II0	C26-C30-C32-C34
38	j	316	II0	C25-C29-C31-C33
38	d	301	II0	C25-C29-C31-C33
38	d	301	II0	C26-C30-C32-C34
38	d	315	II0	C36-C40-C42-C41
38	g	318	II0	C25-C29-C31-C33
39	b	316	IHT	C26-C29-C31-C34
37	L	210	LMG	O6-C5-C6-O5
29	A	808	CLA	CBD-CGD-O2D-CED
29	A	823	CLA	CBD-CGD-O2D-CED
29	A	824	CLA	CBD-CGD-O2D-CED
29	B	802	CLA	CBD-CGD-O2D-CED
29	B	830	CLA	CBD-CGD-O2D-CED
29	B	838	CLA	CBD-CGD-O2D-CED
29	a	308	CLA	CBD-CGD-O2D-CED
29	l	301	CLA	CBD-CGD-O2D-CED
29	j	304	CLA	CBD-CGD-O2D-CED
29	g	303	CLA	CBD-CGD-O2D-CED
29	g	309	CLA	CBD-CGD-O2D-CED
29	n	602	CLA	CBD-CGD-O2D-CED
40	g	313	KC2	CBD-CGD-O2D-CED
29	B	832	CLA	O1D-CGD-O2D-CED
31	A	843	LHG	O2-C2-C3-O3
31	b	318	LHG	O2-C2-C3-O3
31	f	620	LHG	O2-C2-C3-O3
31	n	619	LHG	O2-C2-C3-O3
29	A	809	CLA	C3-C5-C6-C7
29	e	302	CLA	C3-C5-C6-C7
29	i	307	CLA	C3-C5-C6-C7
29	g	310	CLA	C3-C5-C6-C7
29	A	803	CLA	CBA-CGA-O2A-C1
29	B	816	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	828	CLA	CBA-CGA-O2A-C1
29	k	609	CLA	CBA-CGA-O2A-C1
29	i	311	CLA	CBA-CGA-O2A-C1
29	d	313	CLA	CBA-CGA-O2A-C1
29	R	203	CLA	CBA-CGA-O2A-C1
31	c	316	LHG	C24-C23-O8-C6
31	e	317	LHG	C24-C23-O8-C6
29	b	302	CLA	O1A-CGA-O2A-C1
29	e	305	CLA	O1A-CGA-O2A-C1
29	l	307	CLA	O1A-CGA-O2A-C1
29	l	310	CLA	O1A-CGA-O2A-C1
29	d	305	CLA	O1A-CGA-O2A-C1
29	d	306	CLA	O1A-CGA-O2A-C1
29	k	602	CLA	O1D-CGD-O2D-CED
40	l	311	KC2	O1D-CGD-O2D-CED
29	A	817	CLA	CBD-CGD-O2D-CED
29	c	307	CLA	CBD-CGD-O2D-CED
29	b	310	CLA	CBD-CGD-O2D-CED
29	i	312	CLA	CBD-CGD-O2D-CED
33	A	855	LMU	O5B-C5B-C6B-O6B
37	O	205	LMG	O6-C5-C6-O5
33	A	849	LMU	O5'-C5'-C6'-O6'
37	n	620	LMG	O6-C5-C6-O5
29	s	402	CLA	O1D-CGD-O2D-CED
29	B	820	CLA	CBD-CGD-O2D-CED
29	B	801	CLA	C3-C5-C6-C7
29	B	813	CLA	C3-C5-C6-C7
29	h	301	CLA	C3-C5-C6-C7
29	l	307	CLA	C3-C5-C6-C7
29	B	838	CLA	CBA-CGA-O2A-C1
29	f	607	CLA	CBA-CGA-O2A-C1
36	B	844	DGD	O6E-C5E-C6E-O5E
40	i	318	KC2	CAA-CBA-CGA-O2A
29	A	803	CLA	O1A-CGA-O2A-C1
29	A	834	CLA	O1A-CGA-O2A-C1
29	A	837	CLA	O1A-CGA-O2A-C1
29	k	610	CLA	O1A-CGA-O2A-C1
29	i	311	CLA	O1A-CGA-O2A-C1
29	d	313	CLA	O1A-CGA-O2A-C1
29	R	203	CLA	O1A-CGA-O2A-C1
36	j	319	DGD	O1A-C1A-O1G-C1G
33	A	855	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
29	A	816	CLA	C4-C3-C5-C6
29	A	833	CLA	C4-C3-C5-C6
29	B	801	CLA	C4-C3-C5-C6
29	c	308	CLA	C4-C3-C5-C6
29	a	302	CLA	C4-C3-C5-C6
29	m	602	CLA	C4-C3-C5-C6
29	f	613	CLA	C4-C3-C5-C6
29	j	311	CLA	C4-C3-C5-C6
33	A	855	LMU	C4B-C5B-C6B-O6B
29	A	816	CLA	C2-C3-C5-C6
29	A	833	CLA	C2-C3-C5-C6
29	B	801	CLA	C2-C3-C5-C6
29	c	308	CLA	C2-C3-C5-C6
29	a	302	CLA	C2-C3-C5-C6
29	m	602	CLA	C2-C3-C5-C6
29	f	613	CLA	C2-C3-C5-C6
29	j	311	CLA	C2-C3-C5-C6
29	n	607	CLA	C2-C3-C5-C6
29	B	841	CLA	C2A-CAA-CBA-CGA
29	f	612	CLA	C2A-CAA-CBA-CGA
29	A	822	CLA	O1D-CGD-O2D-CED
29	l	309	CLA	O1D-CGD-O2D-CED
29	B	816	CLA	O1A-CGA-O2A-C1
29	B	828	CLA	O1A-CGA-O2A-C1
29	k	609	CLA	O1A-CGA-O2A-C1
33	i	301	LMU	O5'-C1'-O1'-C1
37	c	318	LMG	O6-C1-O1-C7
29	k	614	CLA	C4C-C3C-CAC-CBC
29	B	805	CLA	CBA-CGA-O2A-C1
29	B	839	CLA	CBA-CGA-O2A-C1
29	m	606	CLA	CBA-CGA-O2A-C1
29	f	610	CLA	CBA-CGA-O2A-C1
31	L	209	LHG	C24-C23-O8-C6
37	L	210	LMG	C29-C28-O8-C9
29	B	822	CLA	CBD-CGD-O2D-CED
29	c	301	CLA	CBD-CGD-O2D-CED
37	c	318	LMG	C4-C5-C6-O5
29	B	827	CLA	O1D-CGD-O2D-CED
29	a	306	CLA	O1D-CGD-O2D-CED
29	i	302	CLA	O1D-CGD-O2D-CED
40	m	611	KC2	CAA-CBA-CGA-O1A
40	m	611	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
40	e	309	KC2	CAA-CBA-CGA-O1A
40	k	613	KC2	CAA-CBA-CGA-O2A
40	f	611	KC2	CAA-CBA-CGA-O1A
40	f	611	KC2	CAA-CBA-CGA-O2A
40	i	310	KC2	CAA-CBA-CGA-O2A
40	i	318	KC2	CAA-CBA-CGA-O1A
40	j	312	KC2	CAA-CBA-CGA-O1A
40	j	312	KC2	CAA-CBA-CGA-O2A
40	d	312	KC2	CAA-CBA-CGA-O1A
40	n	612	KC2	CAA-CBA-CGA-O1A
37	L	210	LMG	C4-C5-C6-O5
29	A	809	CLA	O1D-CGD-O2D-CED
29	A	832	CLA	O1D-CGD-O2D-CED
29	a	309	CLA	O1D-CGD-O2D-CED
29	B	841	CLA	CBD-CGD-O2D-CED
29	k	608	CLA	O1D-CGD-O2D-CED
29	f	613	CLA	O1D-CGD-O2D-CED
31	c	320	LHG	C1-C2-C3-O3
29	f	610	CLA	O1A-CGA-O2A-C1
29	b	306	CLA	C3-C5-C6-C7
29	m	610	CLA	C3-C5-C6-C7
29	d	302	CLA	C3-C5-C6-C7
29	k	606	CLA	O1D-CGD-O2D-CED
29	A	805	CLA	CBA-CGA-O2A-C1
29	A	810	CLA	CBA-CGA-O2A-C1
29	A	820	CLA	CBA-CGA-O2A-C1
29	A	838	CLA	CBA-CGA-O2A-C1
29	B	802	CLA	CBA-CGA-O2A-C1
29	B	815	CLA	CBA-CGA-O2A-C1
29	L	203	CLA	CBA-CGA-O2A-C1
29	K	101	CLA	CBA-CGA-O2A-C1
29	a	302	CLA	CBA-CGA-O2A-C1
29	b	306	CLA	CBA-CGA-O2A-C1
29	b	312	CLA	CBA-CGA-O2A-C1
29	h	304	CLA	CBA-CGA-O2A-C1
29	h	307	CLA	CBA-CGA-O2A-C1
29	l	309	CLA	CBA-CGA-O2A-C1
29	f	613	CLA	CBA-CGA-O2A-C1
29	j	310	CLA	CBA-CGA-O2A-C1
29	j	313	CLA	CBA-CGA-O2A-C1
29	d	302	CLA	CBA-CGA-O2A-C1
29	g	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	g	323	CLA	CBA-CGA-O2A-C1
36	j	319	DGD	C2A-C1A-O1G-C1G
29	l	309	CLA	C5-C6-C7-C8
33	A	849	LMU	C4'-C5'-C6'-O6'
29	c	309	CLA	O1D-CGD-O2D-CED
32	F	205	WVN	C25-C28-C30-C33
32	M	101	WVN	C22-C26-C29-C31
32	s	407	WVN	C34-C37-C40-C39
32	h	308	WVN	C22-C26-C29-C31
32	h	308	WVN	C32-C36-C39-C40
32	l	302	WVN	C25-C28-C30-C33
32	l	316	WVN	C22-C26-C29-C31
32	i	315	WVN	C22-C26-C29-C31
38	c	313	II0	C25-C29-C31-C33
38	b	301	II0	C25-C29-C31-C33
38	b	301	II0	C26-C30-C32-C34
38	h	311	II0	C25-C29-C31-C33
38	m	618	II0	C35-C39-C41-C42
38	e	312	II0	C25-C29-C31-C33
38	e	312	II0	C26-C30-C32-C34
38	l	315	II0	C26-C30-C32-C34
38	k	619	II0	C25-C29-C31-C33
38	f	615	II0	C26-C30-C32-C34
38	f	616	II0	C25-C29-C31-C33
38	i	316	II0	C25-C29-C31-C33
38	j	315	II0	C26-C30-C32-C34
38	j	316	II0	C26-C30-C32-C34
38	n	615	II0	C25-C29-C31-C33
38	n	616	II0	C25-C29-C31-C33
39	g	320	IHT	C26-C29-C31-C34
31	c	316	LHG	C28-C29-C30-C31
29	A	812	CLA	C13-C15-C16-C17
29	A	819	CLA	C15-C16-C17-C18
29	B	812	CLA	C5-C6-C7-C8
33	i	301	LMU	O5'-C5'-C6'-O6'
37	n	620	LMG	C4-C5-C6-O5
40	c	310	KC2	CAA-CBA-CGA-O2A
40	k	612	KC2	CAA-CBA-CGA-O2A
40	k	613	KC2	CAA-CBA-CGA-O1A
40	i	310	KC2	CAA-CBA-CGA-O1A
40	d	311	KC2	CAA-CBA-CGA-O1A
40	d	311	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
40	g	313	KC2	CAA-CBA-CGA-O2A
29	i	312	CLA	C2C-C3C-CAC-CBC
36	B	844	DGD	C4E-C5E-C6E-O5E
29	B	820	CLA	C15-C16-C17-C18
29	K	101	CLA	C10-C11-C12-C13
29	K	101	CLA	C15-C16-C17-C18
29	b	311	CLA	C13-C15-C16-C17
31	c	320	LHG	O2-C2-C3-O3
29	m	613	CLA	C3-C5-C6-C7
36	B	844	DGD	C2D-C1D-O3G-C3G
37	c	318	LMG	C2-C1-O1-C7
37	c	318	LMG	O1-C7-C8-O7
29	K	101	CLA	O1A-CGA-O2A-C1
29	g	309	CLA	O1A-CGA-O2A-C1
29	g	323	CLA	O1A-CGA-O2A-C1
29	n	610	CLA	C4-C3-C5-C6
29	A	822	CLA	C2-C3-C5-C6
29	B	819	CLA	C2-C3-C5-C6
29	A	810	CLA	C11-C10-C8-C9
29	A	824	CLA	C14-C13-C15-C16
29	A	840	CLA	C6-C7-C8-C9
29	B	804	CLA	C11-C12-C13-C14
29	B	839	CLA	C6-C7-C8-C9
29	B	840	CLA	C11-C12-C13-C14
29	F	202	CLA	C14-C13-C15-C16
29	c	304	CLA	C6-C7-C8-C9
29	a	311	CLA	C11-C12-C13-C14
29	b	306	CLA	C11-C12-C13-C14
29	e	307	CLA	C14-C13-C15-C16
29	k	602	CLA	C11-C12-C13-C14
29	f	613	CLA	C11-C10-C8-C9
29	i	302	CLA	C11-C10-C8-C9
29	i	308	CLA	C11-C10-C8-C9
29	g	304	CLA	C6-C7-C8-C9
29	g	305	CLA	C11-C12-C13-C14
29	g	311	CLA	C14-C13-C15-C16
29	Q	302	CLA	C6-C7-C8-C9
29	A	831	CLA	O1D-CGD-O2D-CED
29	m	610	CLA	O1D-CGD-O2D-CED
29	k	605	CLA	O1D-CGD-O2D-CED
29	d	307	CLA	O1D-CGD-O2D-CED
29	B	836	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	n	608	CLA	CBD-CGD-O2D-CED
31	g	322	LHG	C29-C30-C31-C32
29	A	817	CLA	C13-C15-C16-C17
29	B	838	CLA	C15-C16-C17-C18
29	l	304	CLA	C10-C11-C12-C13
29	A	821	CLA	C2A-CAA-CBA-CGA
29	s	402	CLA	C2A-CAA-CBA-CGA
29	c	307	CLA	C2A-CAA-CBA-CGA
29	e	301	CLA	C2A-CAA-CBA-CGA
32	A	845	WVN	C11-C19-C22-C24
32	A	845	WVN	C20-C23-C25-C27
32	A	846	WVN	C11-C19-C22-C24
32	A	846	WVN	C30-C33-C34-C38
32	A	847	WVN	C20-C23-C25-C27
32	A	847	WVN	C29-C31-C32-C35
32	B	845	WVN	C30-C33-C34-C38
32	B	846	WVN	C11-C19-C22-C24
32	B	846	WVN	C20-C23-C25-C27
32	B	846	WVN	C30-C33-C34-C38
32	B	847	WVN	C11-C19-C22-C24
32	B	848	WVN	C11-C19-C22-C24
32	B	848	WVN	C20-C23-C25-C27
32	B	849	WVN	C20-C23-C25-C27
32	B	849	WVN	C29-C31-C32-C35
32	B	849	WVN	C30-C33-C34-C38
32	F	204	WVN	C11-C19-C22-C24
32	F	204	WVN	C29-C31-C32-C35
32	F	204	WVN	C30-C33-C34-C38
32	F	205	WVN	C20-C23-C25-C27
32	F	207	WVN	C30-C33-C34-C38
32	J	101	WVN	C30-C33-C34-C38
32	L	201	WVN	C30-C33-C34-C38
32	K	103	WVN	C20-C23-C25-C27
32	s	405	WVN	C11-C19-C22-C24
32	s	407	WVN	C20-C23-C25-C27
32	s	407	WVN	C30-C33-C34-C38
32	e	315	WVN	C30-C33-C34-C38
32	l	302	WVN	C11-C19-C22-C24
32	i	315	WVN	C29-C31-C32-C35
32	i	315	WVN	C30-C33-C34-C38
38	a	314	II0	C31-C33-C35-C37
38	a	317	II0	C31-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
38	b	301	II0	C32-C34-C36-C38
38	b	314	II0	C31-C33-C35-C37
38	b	314	II0	C32-C34-C36-C38
38	b	315	II0	C32-C34-C36-C38
38	h	310	II0	C31-C33-C35-C37
38	m	618	II0	C32-C34-C36-C38
38	l	313	II0	C32-C34-C36-C38
38	l	314	II0	C32-C34-C36-C38
38	k	615	II0	C31-C33-C35-C37
38	k	619	II0	C31-C33-C35-C37
38	f	614	II0	C32-C34-C36-C38
38	i	314	II0	C31-C33-C35-C37
38	d	317	II0	C31-C33-C35-C37
38	d	317	II0	C32-C34-C36-C38
38	g	317	II0	C31-C33-C35-C37
38	g	319	II0	C32-C34-C36-C38
38	n	616	II0	C31-C33-C35-C37
39	n	617	IHT	C31-C34-C35-C39
32	B	846	WVN	C29-C31-C32-C36
32	F	205	WVN	C29-C31-C32-C36
32	I	101	WVN	C20-C23-C25-C28
32	J	101	WVN	C29-C31-C32-C36
32	L	201	WVN	C11-C19-C22-C26
32	L	201	WVN	C20-C23-C25-C28
32	L	206	WVN	C11-C19-C22-C26
32	M	101	WVN	C11-C19-C22-C26
32	s	405	WVN	C29-C31-C32-C36
32	e	315	WVN	C20-C23-C25-C28
32	l	316	WVN	C29-C31-C32-C36
32	i	315	WVN	C20-C23-C25-C28
32	R	201	WVN	C11-C19-C22-C26
32	R	201	WVN	C20-C23-C25-C28
32	R	201	WVN	C29-C31-C32-C36
32	R	201	WVN	C30-C33-C34-C37
32	R	202	WVN	C30-C33-C34-C37
38	J	103	II0	C32-C34-C36-C40
38	c	313	II0	C32-C34-C36-C40
38	a	315	II0	C32-C34-C36-C40
38	b	315	II0	C31-C33-C35-C39
38	m	616	II0	C31-C33-C35-C39
38	m	616	II0	C32-C34-C36-C40
38	m	618	II0	C31-C33-C35-C39

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Mol	Chain	Res	Type	Atoms
38	e	312	II0	C32-C34-C36-C40
38	k	616	II0	C31-C33-C35-C39
38	f	616	II0	C31-C33-C35-C39
38	i	313	II0	C32-C34-C36-C40
38	i	316	II0	C31-C33-C35-C39
38	i	319	II0	C31-C33-C35-C39
38	j	301	II0	C32-C34-C36-C40
38	j	315	II0	C31-C33-C35-C39
38	d	316	II0	C31-C33-C35-C39
38	d	316	II0	C32-C34-C36-C40
38	n	618	II0	C31-C33-C35-C39
29	d	313	CLA	O1D-CGD-O2D-CED
31	J	104	LHG	C23-C24-C25-C26
31	n	619	LHG	C23-C24-C25-C26
29	A	805	CLA	O1A-CGA-O2A-C1
29	A	838	CLA	O1A-CGA-O2A-C1
29	a	302	CLA	O1A-CGA-O2A-C1
29	b	312	CLA	O1A-CGA-O2A-C1
29	h	307	CLA	O1A-CGA-O2A-C1
29	f	613	CLA	O1A-CGA-O2A-C1
29	j	310	CLA	O1A-CGA-O2A-C1
29	j	313	CLA	O1A-CGA-O2A-C1
29	A	828	CLA	C13-C15-C16-C17
29	B	836	CLA	C10-C11-C12-C13
29	c	308	CLA	C13-C15-C16-C17
29	c	312	CLA	C15-C16-C17-C18
29	a	308	CLA	C15-C16-C17-C18
29	a	311	CLA	C15-C16-C17-C18
29	m	603	CLA	C5-C6-C7-C8
29	i	308	CLA	C13-C15-C16-C17
29	i	311	CLA	C8-C10-C11-C12
29	g	302	CLA	C15-C16-C17-C18
29	g	311	CLA	C13-C15-C16-C17
29	g	302	CLA	O1D-CGD-O2D-CED
29	A	813	CLA	CBD-CGD-O2D-CED
40	c	310	KC2	CAA-CBA-CGA-O1A
40	e	309	KC2	CAA-CBA-CGA-O2A
40	d	312	KC2	CAA-CBA-CGA-O2A
40	g	313	KC2	CAA-CBA-CGA-O1A
40	g	315	KC2	CAA-CBA-CGA-O2A
40	n	612	KC2	CAA-CBA-CGA-O2A
29	j	314	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	A	822	CLA	CBA-CGA-O2A-C1
29	B	801	CLA	CBA-CGA-O2A-C1
29	B	822	CLA	CBA-CGA-O2A-C1
29	c	302	CLA	CBA-CGA-O2A-C1
29	n	607	CLA	CBA-CGA-O2A-C1
29	A	807	CLA	C15-C16-C17-C18
29	A	819	CLA	C10-C11-C12-C13
29	A	833	CLA	C8-C10-C11-C12
29	A	834	CLA	C5-C6-C7-C8
29	A	840	CLA	C5-C6-C7-C8
29	B	816	CLA	C10-C11-C12-C13
29	B	822	CLA	C5-C6-C7-C8
29	c	312	CLA	C8-C10-C11-C12
29	a	307	CLA	C15-C16-C17-C18
29	b	312	CLA	C5-C6-C7-C8
29	m	608	CLA	C5-C6-C7-C8
29	f	602	CLA	C13-C15-C16-C17
29	f	610	CLA	C8-C10-C11-C12
29	n	608	CLA	C8-C10-C11-C12
31	a	318	LHG	C23-C24-C25-C26
31	b	318	LHG	C23-C24-C25-C26
31	f	619	LHG	C7-C8-C9-C10
31	f	619	LHG	C23-C24-C25-C26
29	i	305	CLA	O1D-CGD-O2D-CED
29	A	837	CLA	CBD-CGD-O2D-CED
29	h	312	CLA	CBD-CGD-O2D-CED
29	B	804	CLA	C4C-C3C-CAC-CBC
33	a	319	LMU	O5'-C5'-C6'-O6'
29	A	807	CLA	C8-C10-C11-C12
29	A	810	CLA	C15-C16-C17-C18
29	A	818	CLA	C13-C15-C16-C17
29	A	831	CLA	C13-C15-C16-C17
29	A	838	CLA	C5-C6-C7-C8
29	B	805	CLA	C10-C11-C12-C13
29	B	813	CLA	C8-C10-C11-C12
29	B	836	CLA	C15-C16-C17-C18
29	F	202	CLA	C8-C10-C11-C12
29	b	307	CLA	C10-C11-C12-C13
29	b	310	CLA	C15-C16-C17-C18
29	e	302	CLA	C10-C11-C12-C13
29	e	307	CLA	C5-C6-C7-C8
29	e	311	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	l	312	CLA	C5-C6-C7-C8
29	k	602	CLA	C13-C15-C16-C17
29	f	610	CLA	C13-C15-C16-C17
29	i	302	CLA	C5-C6-C7-C8
29	j	302	CLA	C15-C16-C17-C18
29	g	304	CLA	C5-C6-C7-C8
29	n	608	CLA	C5-C6-C7-C8
29	n	608	CLA	C10-C11-C12-C13
29	Q	302	CLA	C5-C6-C7-C8
31	b	318	LHG	O1-C1-C2-O2
29	A	810	CLA	O1A-CGA-O2A-C1
29	b	306	CLA	O1A-CGA-O2A-C1
31	c	320	LHG	C23-C24-C25-C26
31	l	318	LHG	C7-C8-C9-C10
31	l	318	LHG	C23-C24-C25-C26
31	j	318	LHG	C7-C8-C9-C10
31	j	318	LHG	C23-C24-C25-C26
31	g	322	LHG	C23-C24-C25-C26
29	Q	302	CLA	CBD-CGD-O2D-CED
40	d	312	KC2	O1D-CGD-O2D-CED
29	A	809	CLA	C5-C6-C7-C8
29	A	835	CLA	C5-C6-C7-C8
29	B	801	CLA	C5-C6-C7-C8
29	B	816	CLA	C5-C6-C7-C8
29	s	403	CLA	C15-C16-C17-C18
29	c	302	CLA	C10-C11-C12-C13
29	a	307	CLA	C5-C6-C7-C8
29	b	305	CLA	C13-C15-C16-C17
29	e	304	CLA	C13-C15-C16-C17
29	e	307	CLA	C13-C15-C16-C17
29	i	304	CLA	C8-C10-C11-C12
29	g	304	CLA	C13-C15-C16-C17
30	B	843	PQN	C15-C16-C17-C18
29	c	312	CLA	O1D-CGD-O2D-CED
29	b	303	CLA	O1D-CGD-O2D-CED
29	n	610	CLA	O1D-CGD-O2D-CED
40	k	612	KC2	CAA-CBA-CGA-O1A
40	g	315	KC2	CAA-CBA-CGA-O1A
29	B	801	CLA	C2-C1-O2A-CGA
29	A	812	CLA	C15-C16-C17-C18
29	F	202	CLA	C13-C15-C16-C17
29	O	206	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	K	101	CLA	C13-C15-C16-C17
29	s	402	CLA	C10-C11-C12-C13
29	s	402	CLA	C15-C16-C17-C18
29	m	604	CLA	C15-C16-C17-C18
29	m	613	CLA	C13-C15-C16-C17
29	g	304	CLA	C10-C11-C12-C13
29	g	310	CLA	C5-C6-C7-C8
29	L	202	CLA	O1D-CGD-O2D-CED
31	c	316	LHG	C7-C8-C9-C10
37	c	318	LMG	C28-C29-C30-C31
29	d	310	CLA	CBD-CGD-O2D-CED
29	s	403	CLA	C10-C11-C12-C13
29	b	308	CLA	C13-C15-C16-C17
29	F	202	CLA	O1D-CGD-O2D-CED
29	n	609	CLA	O1D-CGD-O2D-CED
29	A	816	CLA	C12-C13-C15-C16
29	A	825	CLA	C11-C12-C13-C15
29	A	830	CLA	C11-C10-C8-C7
29	B	807	CLA	C12-C13-C15-C16
29	s	402	CLA	C11-C10-C8-C7
29	e	306	CLA	C11-C10-C8-C7
29	g	304	CLA	C11-C12-C13-C15
29	g	311	CLA	C12-C13-C15-C16
29	n	608	CLA	C6-C7-C8-C10
29	O	202	CLA	C3-C5-C6-C7
29	c	308	CLA	C3-C5-C6-C7
29	A	820	CLA	O1A-CGA-O2A-C1
29	B	802	CLA	O1A-CGA-O2A-C1
29	B	805	CLA	O1A-CGA-O2A-C1
29	L	203	CLA	O1A-CGA-O2A-C1
29	h	304	CLA	O1A-CGA-O2A-C1
32	A	844	WVN	C22-C26-C29-C31
32	A	846	WVN	C25-C28-C30-C33
32	A	846	WVN	C32-C36-C39-C40
32	B	848	WVN	C25-C28-C30-C33
32	L	205	WVN	C22-C26-C29-C31
32	L	205	WVN	C25-C28-C30-C33
32	R	201	WVN	C22-C26-C29-C31
38	c	313	II0	C26-C30-C32-C34
38	a	317	II0	C25-C29-C31-C33
38	b	315	II0	C25-C29-C31-C33
38	h	309	II0	C25-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
38	m	616	II0	C26-C30-C32-C34
38	m	618	II0	C26-C30-C32-C34
38	e	313	II0	C25-C29-C31-C33
38	e	316	II0	C36-C40-C42-C41
38	k	616	II0	C25-C29-C31-C33
38	k	619	II0	C26-C30-C32-C34
38	k	620	II0	C35-C39-C41-C42
38	f	614	II0	C25-C29-C31-C33
38	i	313	II0	C25-C29-C31-C33
38	j	301	II0	C25-C29-C31-C33
38	d	301	II0	C35-C39-C41-C42
38	d	315	II0	C26-C30-C32-C34
38	d	316	II0	C25-C29-C31-C33
38	d	317	II0	C25-C29-C31-C33
38	g	318	II0	C26-C30-C32-C34
39	c	315	IHT	C35-C38-C41-C40
39	c	319	IHT	C33-C37-C40-C41
29	B	825	CLA	CBA-CGA-O2A-C1
29	A	807	CLA	C2A-CAA-CBA-CGA
29	A	817	CLA	C2A-CAA-CBA-CGA
29	A	828	CLA	C2A-CAA-CBA-CGA
29	A	837	CLA	C2A-CAA-CBA-CGA
29	h	306	CLA	C2A-CAA-CBA-CGA
29	m	613	CLA	C2A-CAA-CBA-CGA
29	j	311	CLA	C2A-CAA-CBA-CGA
29	g	307	CLA	C2A-CAA-CBA-CGA
29	n	613	CLA	C2A-CAA-CBA-CGA
29	B	819	CLA	O1D-CGD-O2D-CED
29	B	842	CLA	O1D-CGD-O2D-CED
29	c	304	CLA	O1D-CGD-O2D-CED
29	a	307	CLA	O1D-CGD-O2D-CED
29	m	601	CLA	O1D-CGD-O2D-CED
29	l	304	CLA	O1D-CGD-O2D-CED
29	g	308	CLA	O1D-CGD-O2D-CED
29	m	606	CLA	C13-C15-C16-C17
29	m	608	CLA	C13-C15-C16-C17
29	l	307	CLA	C13-C15-C16-C17
29	i	305	CLA	C8-C10-C11-C12
29	B	815	CLA	O1A-CGA-O2A-C1
29	d	302	CLA	O1A-CGA-O2A-C1
29	B	816	CLA	CBD-CGD-O2D-CED
33	A	849	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
33	a	319	LMU	O5'-C1'-O1'-C1
29	B	837	CLA	C13-C15-C16-C17
29	g	302	CLA	C13-C15-C16-C17
29	n	608	CLA	C13-C15-C16-C17
29	i	309	CLA	O1D-CGD-O2D-CED
31	L	208	LHG	O2-C2-C3-O3
31	a	318	LHG	O2-C2-C3-O3
31	e	317	LHG	O2-C2-C3-O3
29	a	302	CLA	C3-C5-C6-C7
29	e	310	CLA	C3-C5-C6-C7
29	A	807	CLA	C13-C15-C16-C17
29	A	813	CLA	C5-C6-C7-C8
29	B	810	CLA	C8-C10-C11-C12
29	b	306	CLA	C8-C10-C11-C12
29	e	311	CLA	C15-C16-C17-C18
29	j	302	CLA	C13-C15-C16-C17
29	g	304	CLA	C8-C10-C11-C12
29	Q	302	CLA	C15-C16-C17-C18
29	F	203	CLA	CBA-CGA-O2A-C1
29	f	612	CLA	CBA-CGA-O2A-C1
31	J	104	LHG	C24-C23-O8-C6
29	B	822	CLA	O1A-CGA-O2A-C1
29	B	839	CLA	O1A-CGA-O2A-C1
29	m	606	CLA	O1A-CGA-O2A-C1
29	A	826	CLA	C5-C6-C7-C8
29	A	851	CLA	C8-C10-C11-C12
29	B	812	CLA	C15-C16-C17-C18
29	F	202	CLA	C5-C6-C7-C8
29	s	406	CLA	C8-C10-C11-C12
29	s	406	CLA	C13-C15-C16-C17
29	b	310	CLA	C8-C10-C11-C12
29	g	311	CLA	C5-C6-C7-C8
29	O	201	CLA	CBD-CGD-O2D-CED
29	j	308	CLA	CBD-CGD-O2D-CED
29	A	822	CLA	O1A-CGA-O2A-C1
29	B	801	CLA	O1A-CGA-O2A-C1
29	c	302	CLA	O1A-CGA-O2A-C1
29	l	309	CLA	O1A-CGA-O2A-C1
36	B	844	DGD	C2B-C1B-O2G-C2G
29	d	308	CLA	O1D-CGD-O2D-CED
29	B	814	CLA	C15-C16-C17-C18
29	B	817	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	B	820	CLA	C10-C11-C12-C13
29	B	834	CLA	C8-C10-C11-C12
29	O	202	CLA	C8-C10-C11-C12
29	c	312	CLA	C10-C11-C12-C13
29	a	307	CLA	C8-C10-C11-C12
29	b	310	CLA	C13-C15-C16-C17
29	m	608	CLA	C15-C16-C17-C18
29	e	310	CLA	C5-C6-C7-C8
29	l	306	CLA	C13-C15-C16-C17
31	A	842	LHG	C4-O6-P-O3
31	L	208	LHG	C3-O3-P-O6
31	c	320	LHG	C3-O3-P-O6
31	a	301	LHG	C3-O3-P-O6
31	a	318	LHG	C3-O3-P-O6
31	m	619	LHG	C3-O3-P-O6
31	e	317	LHG	C4-O6-P-O3
31	f	620	LHG	C3-O3-P-O6
31	f	620	LHG	C4-O6-P-O3
31	i	317	LHG	C3-O3-P-O6
31	g	301	LHG	C3-O3-P-O6
31	g	322	LHG	C3-O3-P-O6
31	n	619	LHG	C3-O3-P-O6
28	A	801	CL0	C3-C5-C6-C7
29	B	803	CLA	C3-C5-C6-C7
29	g	316	CLA	C3-C5-C6-C7
29	c	306	CLA	CBA-CGA-O2A-C1
29	h	306	CLA	CBA-CGA-O2A-C1
29	l	312	CLA	CBA-CGA-O2A-C1
29	i	302	CLA	CBA-CGA-O2A-C1
29	B	818	CLA	CBD-CGD-O2D-CED
29	l	303	CLA	CBD-CGD-O2D-CED
29	A	810	CLA	C8-C10-C11-C12
29	B	810	CLA	C13-C15-C16-C17
29	B	836	CLA	C13-C15-C16-C17
29	s	406	CLA	C5-C6-C7-C8
29	g	310	CLA	C15-C16-C17-C18
33	i	301	LMU	C4'-C5'-C6'-O6'
29	j	311	CLA	O1D-CGD-O2D-CED
31	e	317	LHG	C7-C8-C9-C10
29	B	821	CLA	O1D-CGD-O2D-CED
31	L	208	LHG	C1-C2-C3-O3
31	L	209	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	a	318	LHG	C1-C2-C3-O3
31	e	317	LHG	C1-C2-C3-O3
29	B	816	CLA	C4-C3-C5-C6
29	b	306	CLA	C4-C3-C5-C6
29	m	610	CLA	C2-C3-C5-C6
29	B	825	CLA	C13-C15-C16-C17
29	m	610	CLA	C5-C6-C7-C8
29	A	822	CLA	C2A-CAA-CBA-CGA
29	A	850	CLA	C2A-CAA-CBA-CGA
29	F	203	CLA	C2A-CAA-CBA-CGA
29	m	612	CLA	C2A-CAA-CBA-CGA
29	i	307	CLA	C2A-CAA-CBA-CGA
29	i	308	CLA	C2A-CAA-CBA-CGA
29	i	309	CLA	C2A-CAA-CBA-CGA
29	j	308	CLA	C2A-CAA-CBA-CGA
29	d	305	CLA	C2A-CAA-CBA-CGA
29	B	818	CLA	C16-C17-C18-C20
29	a	302	CLA	C16-C17-C18-C19
29	f	613	CLA	C16-C17-C18-C19
29	b	307	CLA	C3-C5-C6-C7
29	n	608	CLA	C3-C5-C6-C7
29	B	826	CLA	CBA-CGA-O2A-C1
29	B	841	CLA	CBA-CGA-O2A-C1
29	e	307	CLA	CBA-CGA-O2A-C1
29	l	308	CLA	CBA-CGA-O2A-C1
38	J	103	II0	C28-C26-C30-C32
38	a	313	II0	C27-C25-C29-C31
38	a	313	II0	C28-C26-C30-C32
38	a	314	II0	C27-C25-C29-C31
38	a	317	II0	C28-C26-C30-C32
38	m	614	II0	C28-C26-C30-C32
38	m	615	II0	C27-C25-C29-C31
38	m	616	II0	C27-C25-C29-C31
38	e	312	II0	C27-C25-C29-C31
38	e	316	II0	C27-C25-C29-C31
38	l	313	II0	C27-C25-C29-C31
38	k	615	II0	C28-C26-C30-C32
38	k	616	II0	C27-C25-C29-C31
38	i	313	II0	C27-C25-C29-C31
38	i	314	II0	C28-C26-C30-C32
38	i	316	II0	C28-C26-C30-C32
38	j	301	II0	C28-C26-C30-C32

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Mol	Chain	Res	Type	Atoms
38	j	316	II0	C27-C25-C29-C31
38	d	301	II0	C27-C25-C29-C31
38	g	319	II0	C27-C25-C29-C31
39	O	204	IHT	C28-C26-C29-C31
39	g	320	IHT	C28-C26-C29-C31
29	A	808	CLA	C15-C16-C17-C18
32	A	847	WVN	C32-C36-C39-C40
32	B	849	WVN	C25-C28-C30-C33
32	F	204	WVN	C32-C36-C39-C40
32	F	205	WVN	C22-C26-C29-C31
32	J	101	WVN	C32-C36-C39-C40
32	h	308	WVN	C25-C28-C30-C33
32	e	315	WVN	C22-C26-C29-C31
38	e	316	II0	C25-C29-C31-C33
38	l	313	II0	C25-C29-C31-C33
38	k	615	II0	C26-C30-C32-C34
38	i	314	II0	C26-C30-C32-C34
31	A	842	LHG	C30-C31-C32-C33
36	B	844	DGD	C7B-C8B-C9B-CAB
37	c	318	LMG	C18-C19-C20-C21
37	c	318	LMG	C29-C30-C31-C32
29	B	805	CLA	CBD-CGD-O2D-CED
29	f	601	CLA	CBD-CGD-O2D-CED
31	f	620	LHG	C8-C7-O7-C5
37	c	317	LMG	C11-C10-O7-C8
29	B	812	CLA	C8-C10-C11-C12
29	b	310	CLA	C10-C11-C12-C13
32	A	844	WVN	C24-C22-C26-C29
32	A	854	WVN	C24-C22-C26-C29
32	B	847	WVN	C24-C22-C26-C29
32	L	201	WVN	C24-C22-C26-C29
32	K	103	WVN	C38-C34-C37-C40
32	s	405	WVN	C24-C22-C26-C29
32	s	405	WVN	C38-C34-C37-C40
32	h	308	WVN	C38-C34-C37-C40
32	e	315	WVN	C38-C34-C37-C40
32	l	302	WVN	C24-C22-C26-C29
32	i	315	WVN	C27-C25-C28-C30
38	a	315	II0	C38-C36-C40-C42
38	b	314	II0	C38-C36-C40-C42
38	h	310	II0	C38-C36-C40-C42
38	e	312	II0	C37-C35-C39-C41

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Mol	Chain	Res	Type	Atoms
38	e	312	II0	C38-C36-C40-C42
38	e	314	II0	C38-C36-C40-C42
38	k	620	II0	C38-C36-C40-C42
38	f	618	II0	C38-C36-C40-C42
38	i	316	II0	C38-C36-C40-C42
38	j	315	II0	C38-C36-C40-C42
38	n	615	II0	C38-C36-C40-C42
31	s	408	LHG	C27-C28-C29-C30
31	a	301	LHG	C24-C25-C26-C27
31	a	301	LHG	C31-C32-C33-C34
31	b	318	LHG	C26-C27-C28-C29
31	l	318	LHG	C11-C10-C9-C8
31	f	619	LHG	C11-C10-C9-C8
31	f	619	LHG	C32-C33-C34-C35
31	g	322	LHG	C27-C28-C29-C30
33	A	855	LMU	C4-C5-C6-C7
35	A	853	SQD	C11-C10-C9-C8
35	A	853	SQD	C12-C13-C14-C15
36	j	319	DGD	C6B-C7B-C8B-C9B
37	c	317	LMG	C22-C23-C24-C25
37	c	318	LMG	C16-C17-C18-C19
37	Q	301	LMG	C31-C32-C33-C34
29	d	306	CLA	O1D-CGD-O2D-CED
40	g	314	KC2	C2A-CAA-CBA-CGA
29	B	810	CLA	C16-C17-C18-C20
29	B	834	CLA	C16-C17-C18-C20
29	c	302	CLA	C11-C12-C13-C14
29	b	303	CLA	C6-C7-C8-C9
29	i	303	CLA	C16-C17-C18-C19
29	L	207	CLA	CBA-CGA-O2A-C1
29	g	304	CLA	CBA-CGA-O2A-C1
29	i	312	CLA	C4C-C3C-CAC-CBC
31	J	104	LHG	C9-C10-C11-C12
31	s	408	LHG	C29-C30-C31-C32
31	s	408	LHG	C32-C33-C34-C35
36	j	319	DGD	C7B-C8B-C9B-CAB
29	h	301	CLA	O1D-CGD-O2D-CED
29	i	303	CLA	O1D-CGD-O2D-CED
31	L	208	LHG	C23-C24-C25-C26
31	A	842	LHG	C11-C10-C9-C8
31	A	842	LHG	C24-C25-C26-C27
31	L	208	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	f	619	LHG	C28-C29-C30-C31
33	A	849	LMU	C11-C10-C9-C8
37	Q	301	LMG	C15-C16-C17-C18
31	m	619	LHG	C27-C28-C29-C30
31	g	301	LHG	C10-C11-C12-C13
36	j	319	DGD	C6A-C7A-C8A-C9A
37	n	620	LMG	C36-C37-C38-C39
31	j	318	LHG	O2-C2-C3-O3
31	g	301	LHG	O2-C2-C3-O3
31	n	619	LHG	C11-C10-C9-C8
29	k	604	CLA	C3-C5-C6-C7
29	F	203	CLA	C3-C5-C6-C7
29	g	309	CLA	O1D-CGD-O2D-CED
40	g	313	KC2	O1D-CGD-O2D-CED
32	A	844	WVN	C33-C34-C37-C40
32	A	845	WVN	C33-C34-C37-C40
32	B	846	WVN	C33-C34-C37-C40
32	B	848	WVN	C19-C22-C26-C29
32	F	204	WVN	C33-C34-C37-C40
32	F	207	WVN	C33-C34-C37-C40
32	J	101	WVN	C19-C22-C26-C29
32	J	101	WVN	C33-C34-C37-C40
32	L	201	WVN	C33-C34-C37-C40
32	L	205	WVN	C33-C34-C37-C40
32	L	206	WVN	C19-C22-C26-C29
32	M	101	WVN	C19-C22-C26-C29
32	s	405	WVN	C19-C22-C26-C29
32	s	407	WVN	C19-C22-C26-C29
32	h	308	WVN	C23-C25-C28-C30
32	l	302	WVN	C19-C22-C26-C29
32	l	316	WVN	C33-C34-C37-C40
32	i	315	WVN	C33-C34-C37-C40
32	R	201	WVN	C19-C22-C26-C29
32	R	202	WVN	C23-C25-C28-C30
38	a	317	II0	C34-C36-C40-C42
38	b	314	II0	C33-C35-C39-C41
38	h	309	II0	C33-C35-C39-C41
38	m	614	II0	C34-C36-C40-C42
38	e	314	II0	C34-C36-C40-C42
38	l	313	II0	C34-C36-C40-C42
38	k	615	II0	C33-C35-C39-C41
38	k	616	II0	C33-C35-C39-C41

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Mol	Chain	Res	Type	Atoms
38	f	615	II0	C33-C35-C39-C41
38	j	301	II0	C33-C35-C39-C41
38	j	316	II0	C33-C35-C39-C41
38	d	315	II0	C34-C36-C40-C42
38	d	317	II0	C34-C36-C40-C42
31	A	842	LHG	C9-C10-C11-C12
31	A	842	LHG	C28-C29-C30-C31
31	f	620	LHG	C27-C28-C29-C30
37	F	206	LMG	C30-C31-C32-C33
37	F	206	LMG	C31-C32-C33-C34
29	B	841	CLA	C15-C16-C17-C18
29	l	306	CLA	C8-C10-C11-C12
29	B	826	CLA	O1A-CGA-O2A-C1
29	B	841	CLA	O1A-CGA-O2A-C1
29	i	302	CLA	O1A-CGA-O2A-C1
31	a	318	LHG	O10-C23-O8-C6
29	e	305	CLA	C16-C17-C18-C19
29	e	311	CLA	C16-C17-C18-C19
29	B	838	CLA	O1D-CGD-O2D-CED
29	k	604	CLA	O1D-CGD-O2D-CED
29	A	828	CLA	C4-C3-C5-C6
29	B	836	CLA	C4-C3-C5-C6
29	e	305	CLA	C4-C3-C5-C6
29	l	308	CLA	C4-C3-C5-C6
29	n	608	CLA	C4-C3-C5-C6
31	b	318	LHG	C12-C13-C14-C15
31	e	317	LHG	C27-C28-C29-C30
31	g	301	LHG	C27-C28-C29-C30
37	F	206	LMG	C40-C41-C42-C43
37	n	620	LMG	C29-C30-C31-C32
29	m	603	CLA	C2-C3-C5-C6
29	A	825	CLA	C11-C12-C13-C14
29	B	841	CLA	C6-C7-C8-C9
29	b	311	CLA	C11-C12-C13-C14
29	e	304	CLA	C6-C7-C8-C9
29	l	310	CLA	C11-C10-C8-C9
29	n	610	CLA	C6-C7-C8-C9
29	A	824	CLA	O1D-CGD-O2D-CED
29	f	602	CLA	CBD-CGD-O2D-CED
29	B	841	CLA	C2C-C3C-CAC-CBC
31	f	619	LHG	C24-C25-C26-C27
31	f	620	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
31	g	301	LHG	C11-C12-C13-C14
31	g	301	LHG	C14-C15-C16-C17
31	g	301	LHG	C28-C29-C30-C31
31	g	301	LHG	C32-C33-C34-C35
31	n	619	LHG	C29-C30-C31-C32
33	i	301	LMU	C2-C3-C4-C5
33	i	301	LMU	C4-C5-C6-C7
35	A	853	SQD	C16-C17-C18-C19
37	F	208	LMG	C16-C17-C18-C19
37	L	210	LMG	C30-C31-C32-C33
37	c	317	LMG	C18-C19-C20-C21
37	b	319	LMG	C35-C36-C37-C38
29	f	609	CLA	C15-C16-C17-C18
29	A	808	CLA	C2A-CAA-CBA-CGA
29	B	802	CLA	C2A-CAA-CBA-CGA
29	b	311	CLA	C2A-CAA-CBA-CGA
29	i	303	CLA	C2A-CAA-CBA-CGA
29	g	302	CLA	C2A-CAA-CBA-CGA
29	g	303	CLA	O1D-CGD-O2D-CED
29	B	825	CLA	O1A-CGA-O2A-C1
29	f	612	CLA	O1A-CGA-O2A-C1
29	n	607	CLA	O1A-CGA-O2A-C1
32	A	845	WVN	C29-C31-C32-C35
32	A	847	WVN	C11-C19-C22-C24
32	F	207	WVN	C29-C31-C32-C35
32	I	101	WVN	C11-C19-C22-C24
32	I	101	WVN	C29-C31-C32-C35
32	L	205	WVN	C11-C19-C22-C24
32	L	205	WVN	C29-C31-C32-C35
32	K	103	WVN	C11-C19-C22-C24
32	K	103	WVN	C29-C31-C32-C35
32	s	407	WVN	C11-C19-C22-C24
32	e	315	WVN	C11-C19-C22-C24
32	l	316	WVN	C11-C19-C22-C24
32	i	315	WVN	C11-C19-C22-C24
32	i	315	WVN	C20-C23-C25-C27
32	R	201	WVN	C20-C23-C25-C27
32	R	202	WVN	C20-C23-C25-C27
38	e	313	II0	C31-C33-C35-C37
38	l	315	II0	C31-C33-C35-C37
38	f	614	II0	C31-C33-C35-C37
38	i	314	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
38	i	316	II0	C32-C34-C36-C38
38	i	319	II0	C32-C34-C36-C38
38	d	315	II0	C32-C34-C36-C38
38	g	319	II0	C31-C33-C35-C37
38	n	618	II0	C32-C34-C36-C38
39	g	324	IHT	C30-C32-C33-C36
31	n	619	LHG	C31-C32-C33-C34
31	n	619	LHG	C32-C33-C34-C35
33	a	319	LMU	C3-C4-C5-C6
37	F	206	LMG	C32-C33-C34-C35
31	A	843	LHG	O1-C1-C2-C3
31	c	320	LHG	O1-C1-C2-C3
31	m	619	LHG	O1-C1-C2-C3
31	e	317	LHG	O1-C1-C2-C3
31	l	318	LHG	O1-C1-C2-C3
31	i	317	LHG	O1-C1-C2-C3
31	g	301	LHG	O1-C1-C2-C3
31	n	619	LHG	O1-C1-C2-C3
32	A	844	WVN	C11-C19-C22-C26
32	A	844	WVN	C30-C33-C34-C37
32	F	205	WVN	C30-C33-C34-C37
32	F	207	WVN	C30-C33-C34-C37
32	L	206	WVN	C20-C23-C25-C28
32	K	103	WVN	C30-C33-C34-C37
32	s	405	WVN	C30-C33-C34-C37
32	l	316	WVN	C11-C19-C22-C26
32	R	202	WVN	C20-C23-C25-C28
32	R	202	WVN	C29-C31-C32-C36
38	a	314	II0	C32-C34-C36-C40
38	b	301	II0	C31-C33-C35-C39
38	b	301	II0	C32-C34-C36-C40
38	h	310	II0	C31-C33-C35-C39
38	e	312	II0	C31-C33-C35-C39
38	l	313	II0	C31-C33-C35-C39
38	f	614	II0	C32-C34-C36-C40
38	i	314	II0	C32-C34-C36-C40
38	i	319	II0	C32-C34-C36-C40
38	g	319	II0	C31-C33-C35-C39
38	g	319	II0	C32-C34-C36-C40
38	n	615	II0	C31-C33-C35-C39
29	A	826	CLA	C3-C5-C6-C7
29	A	831	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	n	607	CLA	C3-C5-C6-C7
29	A	808	CLA	O1D-CGD-O2D-CED
29	A	835	CLA	C13-C15-C16-C17
37	F	206	LMG	C11-C10-O7-C8
31	g	301	LHG	C13-C14-C15-C16
33	A	849	LMU	C5-C6-C7-C8
37	c	318	LMG	C31-C32-C33-C34
31	L	209	LHG	C7-C8-C9-C10
31	g	301	LHG	C7-C8-C9-C10
31	J	104	LHG	C10-C11-C12-C13
31	c	316	LHG	C27-C28-C29-C30
31	f	619	LHG	C10-C11-C12-C13
31	g	301	LHG	C11-C10-C9-C8
33	A	855	LMU	C6-C7-C8-C9
37	c	317	LMG	C23-C24-C25-C26
37	c	318	LMG	C30-C31-C32-C33
29	A	808	CLA	C4B-C3B-CAB-CBB
29	A	832	CLA	C4B-C3B-CAB-CBB
29	A	833	CLA	C4B-C3B-CAB-CBB
29	A	851	CLA	C4B-C3B-CAB-CBB
29	B	801	CLA	C4B-C3B-CAB-CBB
29	B	808	CLA	C4B-C3B-CAB-CBB
29	B	821	CLA	C4B-C3B-CAB-CBB
29	B	828	CLA	C4B-C3B-CAB-CBB
29	B	839	CLA	C4B-C3B-CAB-CBB
29	F	201	CLA	C4B-C3B-CAB-CBB
29	L	202	CLA	C4B-C3B-CAB-CBB
29	a	309	CLA	C4B-C3B-CAB-CBB
29	b	306	CLA	C4B-C3B-CAB-CBB
29	b	307	CLA	C4B-C3B-CAB-CBB
29	b	313	CLA	C4B-C3B-CAB-CBB
29	h	306	CLA	C4B-C3B-CAB-CBB
29	m	606	CLA	C4B-C3B-CAB-CBB
29	m	607	CLA	C4B-C3B-CAB-CBB
29	m	612	CLA	C4B-C3B-CAB-CBB
29	e	301	CLA	C4B-C3B-CAB-CBB
29	e	304	CLA	C4B-C3B-CAB-CBB
29	l	303	CLA	C4B-C3B-CAB-CBB
29	k	606	CLA	C4B-C3B-CAB-CBB
29	k	608	CLA	C4B-C3B-CAB-CBB
29	f	601	CLA	C4B-C3B-CAB-CBB
29	f	605	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	i	302	CLA	C4B-C3B-CAB-CBB
29	i	306	CLA	C4B-C3B-CAB-CBB
29	i	309	CLA	C4B-C3B-CAB-CBB
29	j	302	CLA	C4B-C3B-CAB-CBB
29	j	307	CLA	C4B-C3B-CAB-CBB
29	j	311	CLA	C4B-C3B-CAB-CBB
29	j	313	CLA	C4B-C3B-CAB-CBB
29	g	323	CLA	C4B-C3B-CAB-CBB
29	n	601	CLA	C4B-C3B-CAB-CBB
29	n	608	CLA	C4B-C3B-CAB-CBB
29	n	613	CLA	C4B-C3B-CAB-CBB
28	A	801	CL0	C16-C17-C18-C19
29	B	834	CLA	C16-C17-C18-C19
29	K	101	CLA	C16-C17-C18-C19
29	b	303	CLA	C6-C7-C8-C10
29	e	310	CLA	C6-C7-C8-C10
29	f	613	CLA	C16-C17-C18-C20
37	L	210	LMG	O6-C1-O1-C7
29	A	810	CLA	C13-C15-C16-C17
31	a	318	LHG	C26-C27-C28-C29
31	a	318	LHG	C27-C28-C29-C30
33	A	855	LMU	C2-C3-C4-C5
36	B	844	DGD	CEA-CFA-CGA-CHA
37	F	206	LMG	C18-C19-C20-C21
36	j	319	DGD	C4D-C5D-C6D-O5D
29	B	833	CLA	CBD-CGD-O2D-CED
29	g	307	CLA	CBD-CGD-O2D-CED
31	b	318	LHG	C30-C31-C32-C33
33	A	849	LMU	C7-C8-C9-C10
35	A	853	SQD	C9-C10-C11-C12
37	F	206	LMG	C20-C21-C22-C23
37	Q	301	LMG	C30-C31-C32-C33
31	A	842	LHG	C23-C24-C25-C26
29	B	818	CLA	C8-C10-C11-C12
29	j	302	CLA	C8-C10-C11-C12
29	F	203	CLA	O1A-CGA-O2A-C1
29	c	306	CLA	O1A-CGA-O2A-C1
29	l	312	CLA	O1A-CGA-O2A-C1
31	L	208	LHG	C11-C10-C9-C8
31	a	301	LHG	C11-C10-C9-C8
31	i	317	LHG	C27-C28-C29-C30
33	a	319	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
36	j	319	DGD	C4A-C5A-C6A-C7A
37	F	206	LMG	C33-C34-C35-C36
37	n	620	LMG	C17-C18-C19-C20
37	n	620	LMG	C31-C32-C33-C34
29	A	851	CLA	C3-C5-C6-C7
29	B	806	CLA	CBA-CGA-O2A-C1
29	a	308	CLA	O1D-CGD-O2D-CED
29	n	602	CLA	O1D-CGD-O2D-CED
29	A	810	CLA	C3A-C2A-CAA-CBA
29	A	814	CLA	C3A-C2A-CAA-CBA
29	A	816	CLA	C3A-C2A-CAA-CBA
29	A	831	CLA	C3A-C2A-CAA-CBA
29	A	840	CLA	C3A-C2A-CAA-CBA
29	B	813	CLA	C3A-C2A-CAA-CBA
29	B	830	CLA	C3A-C2A-CAA-CBA
29	B	837	CLA	C3A-C2A-CAA-CBA
29	B	840	CLA	C3A-C2A-CAA-CBA
29	O	201	CLA	C3A-C2A-CAA-CBA
29	K	101	CLA	C3A-C2A-CAA-CBA
29	c	301	CLA	C3A-C2A-CAA-CBA
29	c	306	CLA	C3A-C2A-CAA-CBA
29	a	306	CLA	C3A-C2A-CAA-CBA
29	h	304	CLA	C3A-C2A-CAA-CBA
29	h	306	CLA	C3A-C2A-CAA-CBA
29	m	603	CLA	C3A-C2A-CAA-CBA
29	m	613	CLA	C3A-C2A-CAA-CBA
29	k	614	CLA	C3A-C2A-CAA-CBA
29	f	605	CLA	C3A-C2A-CAA-CBA
29	j	306	CLA	C3A-C2A-CAA-CBA
29	g	307	CLA	C3A-C2A-CAA-CBA
29	g	316	CLA	C3A-C2A-CAA-CBA
29	n	601	CLA	C3A-C2A-CAA-CBA
29	n	603	CLA	C3A-C2A-CAA-CBA
29	n	604	CLA	C3A-C2A-CAA-CBA
29	A	830	CLA	C8-C10-C11-C12
29	B	834	CLA	C13-C15-C16-C17
29	e	306	CLA	C8-C10-C11-C12
37	c	317	LMG	O6-C5-C6-O5
32	s	407	WVN	C25-C28-C30-C33
38	k	617	II0	C35-C39-C41-C42
39	c	315	IHT	C33-C37-C40-C41
33	i	301	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	J	104	LHG	C12-C13-C14-C15
31	s	408	LHG	C24-C25-C26-C27
31	c	320	LHG	C24-C25-C26-C27
31	f	620	LHG	C11-C10-C9-C8
37	b	319	LMG	C33-C34-C35-C36
29	l	301	CLA	O1D-CGD-O2D-CED
29	c	302	CLA	C11-C12-C13-C15
29	a	302	CLA	C16-C17-C18-C20
29	e	311	CLA	C16-C17-C18-C20
31	a	301	LHG	C27-C28-C29-C30
36	B	844	DGD	C2A-C3A-C4A-C5A
29	B	802	CLA	O1D-CGD-O2D-CED
37	F	208	LMG	C7-C8-C9-O8
29	k	607	CLA	CBD-CGD-O2D-CED
31	a	301	LHG	C9-C10-C11-C12
29	A	823	CLA	O1D-CGD-O2D-CED
29	B	802	CLA	C3-C5-C6-C7
29	c	312	CLA	C3-C5-C6-C7
31	f	620	LHG	C7-C8-C9-C10
31	g	322	LHG	C7-C8-C9-C10
37	Q	301	LMG	C28-C29-C30-C31
29	A	838	CLA	C4-C3-C5-C6
29	h	306	CLA	C4-C3-C5-C6
29	m	603	CLA	C4-C3-C5-C6
29	B	827	CLA	CBA-CGA-O2A-C1
29	i	304	CLA	CBA-CGA-O2A-C1
37	O	205	LMG	C4-C5-C6-O5
29	A	828	CLA	C2-C3-C5-C6
29	A	838	CLA	C2-C3-C5-C6
29	B	836	CLA	C2-C3-C5-C6
29	h	306	CLA	C2-C3-C5-C6
29	l	308	CLA	C2-C3-C5-C6
29	n	608	CLA	C2-C3-C5-C6
29	m	606	CLA	CBD-CGD-O2D-CED
37	F	206	LMG	C37-C38-C39-C40
29	j	304	CLA	O1D-CGD-O2D-CED
29	B	804	CLA	C2A-CAA-CBA-CGA
29	B	822	CLA	C2A-CAA-CBA-CGA
31	A	843	LHG	O1-C1-C2-O2
31	L	209	LHG	O1-C1-C2-O2
31	e	317	LHG	O1-C1-C2-O2
31	l	318	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	b	305	CLA	C8-C10-C11-C12
31	A	848	LHG	C11-C10-C9-C8
31	L	209	LHG	C24-C25-C26-C27
35	A	853	SQD	C14-C15-C16-C17
36	B	844	DGD	C8A-C9A-CAA-CBA
29	h	306	CLA	O1A-CGA-O2A-C1
29	l	308	CLA	O1A-CGA-O2A-C1
31	A	848	LHG	C7-C8-C9-C10
29	B	818	CLA	C16-C17-C18-C19
29	A	818	CLA	C2C-C3C-CAC-CBC
31	J	104	LHG	C11-C10-C9-C8
31	L	209	LHG	C9-C10-C11-C12
31	b	318	LHG	C29-C30-C31-C32
33	a	319	LMU	C1-C2-C3-C4
29	A	808	CLA	C2B-C3B-CAB-CBB
29	A	833	CLA	C2B-C3B-CAB-CBB
29	A	835	CLA	C2B-C3B-CAB-CBB
29	A	851	CLA	C2B-C3B-CAB-CBB
29	B	801	CLA	C2B-C3B-CAB-CBB
29	B	808	CLA	C2B-C3B-CAB-CBB
29	B	818	CLA	C2B-C3B-CAB-CBB
29	B	821	CLA	C2B-C3B-CAB-CBB
29	B	828	CLA	C2B-C3B-CAB-CBB
29	B	832	CLA	C2B-C3B-CAB-CBB
29	B	839	CLA	C2B-C3B-CAB-CBB
29	B	840	CLA	C2B-C3B-CAB-CBB
29	F	201	CLA	C2B-C3B-CAB-CBB
29	J	102	CLA	C2B-C3B-CAB-CBB
29	L	202	CLA	C2B-C3B-CAB-CBB
29	O	206	CLA	C2B-C3B-CAB-CBB
29	K	102	CLA	C2B-C3B-CAB-CBB
29	s	402	CLA	C2B-C3B-CAB-CBB
29	c	306	CLA	C2B-C3B-CAB-CBB
29	a	306	CLA	C2B-C3B-CAB-CBB
29	a	309	CLA	C2B-C3B-CAB-CBB
29	b	306	CLA	C2B-C3B-CAB-CBB
29	b	307	CLA	C2B-C3B-CAB-CBB
29	b	313	CLA	C2B-C3B-CAB-CBB
29	h	306	CLA	C2B-C3B-CAB-CBB
29	h	307	CLA	C2B-C3B-CAB-CBB
29	m	606	CLA	C2B-C3B-CAB-CBB
29	m	607	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	m	608	CLA	C2B-C3B-CAB-CBB
29	m	610	CLA	C2B-C3B-CAB-CBB
29	e	301	CLA	C2B-C3B-CAB-CBB
29	e	304	CLA	C2B-C3B-CAB-CBB
29	e	308	CLA	C2B-C3B-CAB-CBB
29	l	303	CLA	C2B-C3B-CAB-CBB
29	l	307	CLA	C2B-C3B-CAB-CBB
29	l	310	CLA	C2B-C3B-CAB-CBB
29	k	606	CLA	C2B-C3B-CAB-CBB
29	k	608	CLA	C2B-C3B-CAB-CBB
29	k	610	CLA	C2B-C3B-CAB-CBB
29	f	601	CLA	C2B-C3B-CAB-CBB
29	f	610	CLA	C2B-C3B-CAB-CBB
29	i	306	CLA	C2B-C3B-CAB-CBB
29	i	309	CLA	C2B-C3B-CAB-CBB
29	j	302	CLA	C2B-C3B-CAB-CBB
29	j	307	CLA	C2B-C3B-CAB-CBB
29	j	311	CLA	C2B-C3B-CAB-CBB
29	j	313	CLA	C2B-C3B-CAB-CBB
29	d	306	CLA	C2B-C3B-CAB-CBB
29	d	307	CLA	C2B-C3B-CAB-CBB
29	d	308	CLA	C2B-C3B-CAB-CBB
29	g	303	CLA	C2B-C3B-CAB-CBB
29	g	323	CLA	C2B-C3B-CAB-CBB
29	n	601	CLA	C2B-C3B-CAB-CBB
29	n	606	CLA	C2B-C3B-CAB-CBB
29	n	608	CLA	C2B-C3B-CAB-CBB
29	n	610	CLA	C2B-C3B-CAB-CBB
29	n	613	CLA	C2B-C3B-CAB-CBB
31	L	209	LHG	O2-C2-C3-O3
29	c	302	CLA	C8-C10-C11-C12
29	k	609	CLA	C5-C6-C7-C8
37	F	206	LMG	C16-C17-C18-C19
29	B	807	CLA	C3-C5-C6-C7
29	i	308	CLA	C3-C5-C6-C7
29	m	609	CLA	CBA-CGA-O2A-C1
31	L	208	LHG	C30-C31-C32-C33
31	a	301	LHG	C30-C31-C32-C33
37	F	206	LMG	C38-C39-C40-C41
37	L	210	LMG	C13-C14-C15-C16
37	b	319	LMG	C14-C15-C16-C17
29	e	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	g	304	CLA	O1A-CGA-O2A-C1
31	g	301	LHG	C23-C24-C25-C26
29	l	310	CLA	C5-C6-C7-C8
29	e	301	CLA	CBD-CGD-O2D-CED
31	A	843	LHG	C1-C2-C3-O3
31	j	318	LHG	C1-C2-C3-O3
37	F	206	LMG	O6-C5-C6-O5
29	B	831	CLA	C2-C1-O2A-CGA
29	b	313	CLA	C2-C1-O2A-CGA
29	h	301	CLA	C2-C1-O2A-CGA
29	h	303	CLA	C2-C1-O2A-CGA
31	a	301	LHG	C28-C29-C30-C31
29	A	816	CLA	C13-C15-C16-C17
29	A	819	CLA	C13-C15-C16-C17
29	A	828	CLA	C15-C16-C17-C18
29	A	837	CLA	C13-C15-C16-C17
29	B	822	CLA	C13-C15-C16-C17
29	B	836	CLA	C8-C10-C11-C12
29	i	304	CLA	C10-C11-C12-C13
29	L	207	CLA	O1A-CGA-O2A-C1
31	j	318	LHG	C9-C10-C11-C12
33	a	319	LMU	C11-C10-C9-C8
36	j	319	DGD	CDB-CEB-CFB-CGB
28	A	801	CL0	C16-C17-C18-C20
29	s	402	CLA	C3-C5-C6-C7
32	A	844	WVN	C15-C13-C20-C23
32	B	846	WVN	C15-C13-C20-C23
32	L	205	WVN	C15-C13-C20-C23
32	L	206	WVN	C15-C13-C20-C23
32	s	405	WVN	C06-C13-C20-C23
32	e	315	WVN	C06-C13-C20-C23
32	l	302	WVN	C06-C13-C20-C23
32	l	316	WVN	C15-C13-C20-C23
32	i	315	WVN	C06-C13-C20-C23
39	a	316	IHT	C10-C07-C18-C22
39	m	617	IHT	C02-C07-C18-C22
39	m	617	IHT	C10-C07-C18-C22
31	a	301	LHG	C32-C33-C34-C35
29	F	202	CLA	CBA-CGA-O2A-C1
29	h	301	CLA	CBA-CGA-O2A-C1
29	k	602	CLA	CBA-CGA-O2A-C1
31	a	301	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	a	309	CLA	O2A-C1-C2-C3
29	i	312	CLA	O1D-CGD-O2D-CED
31	a	301	LHG	C23-C24-C25-C26
33	A	855	LMU	C7-C8-C9-C10
37	c	317	LMG	C15-C16-C17-C18
29	c	305	CLA	C10-C11-C12-C13
29	f	613	CLA	C8-C10-C11-C12
29	b	310	CLA	O1D-CGD-O2D-CED
37	F	208	LMG	O6-C5-C6-O5
29	a	306	CLA	C2C-C3C-CAC-CBC
31	c	316	LHG	C9-C10-C11-C12
31	c	316	LHG	C30-C31-C32-C33
29	B	803	CLA	C4-C3-C5-C6
29	B	806	CLA	C4-C3-C5-C6
29	B	812	CLA	C4-C3-C5-C6
29	g	310	CLA	C4-C3-C5-C6
29	B	830	CLA	O1D-CGD-O2D-CED
29	A	816	CLA	C6-C7-C8-C10
29	A	831	CLA	C6-C7-C8-C10
29	A	833	CLA	C12-C13-C15-C16
29	A	840	CLA	C6-C7-C8-C10
29	B	801	CLA	C11-C10-C8-C7
29	B	806	CLA	C2-C3-C5-C6
29	B	812	CLA	C2-C3-C5-C6
29	B	813	CLA	C2-C3-C5-C6
29	B	813	CLA	C6-C7-C8-C10
29	B	816	CLA	C12-C13-C15-C16
29	B	819	CLA	C12-C13-C15-C16
29	B	829	CLA	C6-C7-C8-C10
29	B	839	CLA	C6-C7-C8-C10
29	B	841	CLA	C6-C7-C8-C10
29	F	202	CLA	C6-C7-C8-C10
29	s	403	CLA	C6-C7-C8-C10
29	a	311	CLA	C11-C12-C13-C15
29	b	311	CLA	C11-C12-C13-C15
29	m	608	CLA	C12-C13-C15-C16
29	e	304	CLA	C6-C7-C8-C10
29	e	305	CLA	C2-C3-C5-C6
29	e	306	CLA	C2-C3-C5-C6
29	l	310	CLA	C11-C10-C8-C7
29	k	608	CLA	C6-C7-C8-C10
29	f	613	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	i	308	CLA	C6-C7-C8-C10
29	j	305	CLA	C11-C12-C13-C15
29	d	302	CLA	C11-C12-C13-C15
29	d	302	CLA	C12-C13-C15-C16
29	g	302	CLA	C11-C12-C13-C15
29	g	309	CLA	C11-C10-C8-C7
29	g	310	CLA	C12-C13-C15-C16
29	n	610	CLA	C2-C3-C5-C6
29	Q	302	CLA	C2-C3-C5-C6
29	B	806	CLA	O1A-CGA-O2A-C1
29	B	827	CLA	O1A-CGA-O2A-C1
29	i	304	CLA	O1A-CGA-O2A-C1
31	L	208	LHG	C24-C25-C26-C27
35	A	853	SQD	C25-C26-C27-C28
29	b	303	CLA	C5-C6-C7-C8
29	m	613	CLA	C15-C16-C17-C18
29	j	314	CLA	C15-C16-C17-C18
32	J	101	WVN	C25-C28-C30-C33
32	R	201	WVN	C32-C36-C39-C40
38	J	103	II0	C26-C30-C32-C34
38	g	319	II0	C26-C30-C32-C34
29	B	810	CLA	C16-C17-C18-C19
29	B	814	CLA	C16-C17-C18-C20
29	e	305	CLA	C16-C17-C18-C20
29	i	303	CLA	C16-C17-C18-C20
28	A	801	CL0	CBA-CGA-O2A-C1
29	A	813	CLA	CBA-CGA-O2A-C1
29	A	817	CLA	CBA-CGA-O2A-C1
29	b	303	CLA	CBA-CGA-O2A-C1
29	k	606	CLA	CBA-CGA-O2A-C1
29	k	607	CLA	CBA-CGA-O2A-C1
29	j	303	CLA	CBA-CGA-O2A-C1
36	B	844	DGD	CEB-CFB-CGB-CHB
29	A	810	CLA	C2A-CAA-CBA-CGA
29	B	826	CLA	C2A-CAA-CBA-CGA
29	B	838	CLA	C2A-CAA-CBA-CGA
29	i	302	CLA	C2A-CAA-CBA-CGA
29	d	313	CLA	C2A-CAA-CBA-CGA
29	A	817	CLA	O1D-CGD-O2D-CED
29	B	829	CLA	C15-C16-C17-C18
29	m	602	CLA	C8-C10-C11-C12
29	f	608	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	i	303	CLA	C13-C15-C16-C17
29	g	302	CLA	C8-C10-C11-C12
29	A	818	CLA	C4C-C3C-CAC-CBC
31	L	208	LHG	C25-C26-C27-C28
31	c	320	LHG	C29-C30-C31-C32
31	e	317	LHG	C24-C25-C26-C27
33	A	849	LMU	C2-C3-C4-C5
31	c	320	LHG	C30-C31-C32-C33
37	L	210	LMG	C18-C19-C20-C21
29	c	307	CLA	O1D-CGD-O2D-CED
29	f	607	CLA	C15-C16-C17-C18
31	b	318	LHG	C25-C26-C27-C28
40	k	613	KC2	C2B-C3B-CAB-CBB
31	A	842	LHG	C31-C32-C33-C34
29	m	609	CLA	O1A-CGA-O2A-C1
29	k	602	CLA	O1A-CGA-O2A-C1
29	A	806	CLA	CBD-CGD-O2D-CED
29	A	836	CLA	CBD-CGD-O2D-CED
29	A	811	CLA	CBA-CGA-O2A-C1
29	m	612	CLA	CBA-CGA-O2A-C1
36	j	319	DGD	O6D-C1D-O3G-C3G
37	b	319	LMG	O6-C1-O1-C7
29	B	813	CLA	C5-C6-C7-C8
29	B	829	CLA	C5-C6-C7-C8
29	F	201	CLA	C15-C16-C17-C18
33	i	301	LMU	C7-C8-C9-C10
37	O	205	LMG	C11-C10-O7-C8
31	A	842	LHG	C32-C33-C34-C35
40	k	612	KC2	C4C-C3C-CAC-CBC
40	k	613	KC2	C4B-C3B-CAB-CBB
40	i	318	KC2	C4C-C3C-CAC-CBC
40	g	315	KC2	C4B-C3B-CAB-CBB
29	B	806	CLA	CBD-CGD-O2D-CED
29	A	840	CLA	C3-C5-C6-C7
29	R	203	CLA	C3-C5-C6-C7
31	b	318	LHG	C32-C33-C34-C35
36	j	319	DGD	C2D-C1D-O3G-C3G
31	J	104	LHG	O7-C5-C6-O8
31	L	209	LHG	O7-C5-C6-O8
31	a	318	LHG	O7-C5-C6-O8
33	B	850	LMU	O5'-C5'-C6'-O6'
36	B	844	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
37	c	317	LMG	C32-C33-C34-C35
31	A	848	LHG	C14-C15-C16-C17
37	b	319	LMG	O6-C5-C6-O5
29	B	813	CLA	C4-C3-C5-C6
29	B	817	CLA	C4-C3-C5-C6
29	e	306	CLA	C4-C3-C5-C6
29	Q	302	CLA	C4-C3-C5-C6
29	B	803	CLA	C2-C3-C5-C6
29	B	816	CLA	C2-C3-C5-C6
29	b	306	CLA	C2-C3-C5-C6
29	g	310	CLA	C2-C3-C5-C6
39	R	204	IHT	C11-C21-C24-C26
29	A	816	CLA	C6-C7-C8-C9
29	A	816	CLA	C14-C13-C15-C16
29	A	830	CLA	C11-C10-C8-C9
29	A	831	CLA	C6-C7-C8-C9
29	A	833	CLA	C14-C13-C15-C16
29	A	851	CLA	C11-C10-C8-C9
29	B	807	CLA	C14-C13-C15-C16
29	B	812	CLA	C6-C7-C8-C9
29	B	813	CLA	C6-C7-C8-C9
29	B	816	CLA	C14-C13-C15-C16
29	B	825	CLA	C6-C7-C8-C9
29	B	829	CLA	C6-C7-C8-C9
29	B	836	CLA	C6-C7-C8-C9
29	s	403	CLA	C6-C7-C8-C9
29	a	308	CLA	C14-C13-C15-C16
29	m	608	CLA	C14-C13-C15-C16
29	k	608	CLA	C6-C7-C8-C9
29	f	604	CLA	C14-C13-C15-C16
29	i	308	CLA	C6-C7-C8-C9
29	j	305	CLA	C11-C12-C13-C14
29	d	302	CLA	C11-C12-C13-C14
29	d	302	CLA	C14-C13-C15-C16
29	g	302	CLA	C11-C12-C13-C14
29	g	304	CLA	C14-C13-C15-C16
29	g	309	CLA	C11-C10-C8-C9
29	g	310	CLA	C14-C13-C15-C16
29	n	608	CLA	C6-C7-C8-C9
29	B	822	CLA	O1D-CGD-O2D-CED
31	L	208	LHG	C12-C13-C14-C15
36	B	844	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
37	F	208	LMG	C17-C18-C19-C20
29	A	819	CLA	C3-C5-C6-C7
29	L	202	CLA	C2A-CAA-CBA-CGA
29	i	305	CLA	C2A-CAA-CBA-CGA
29	i	312	CLA	C2A-CAA-CBA-CGA
29	n	602	CLA	C2A-CAA-CBA-CGA
32	A	844	WVN	C11-C19-C22-C24
32	K	103	WVN	C30-C33-C34-C38
32	s	405	WVN	C30-C33-C34-C38
32	l	316	WVN	C20-C23-C25-C27
38	i	313	II0	C31-C33-C35-C37
29	i	308	CLA	C8-C10-C11-C12
30	B	843	PQN	C20-C21-C22-C23
31	b	318	LHG	C13-C14-C15-C16
32	A	845	WVN	C29-C31-C32-C36
32	A	854	WVN	C20-C23-C25-C28
32	L	206	WVN	C29-C31-C32-C36
32	h	308	WVN	C11-C19-C22-C26
32	h	308	WVN	C20-C23-C25-C28
32	i	315	WVN	C11-C19-C22-C26
38	j	301	II0	C31-C33-C35-C39
29	F	202	CLA	O1A-CGA-O2A-C1
29	k	606	CLA	O1A-CGA-O2A-C1
29	A	808	CLA	C1A-C2A-CAA-CBA
29	A	817	CLA	C1A-C2A-CAA-CBA
29	A	827	CLA	C1A-C2A-CAA-CBA
29	A	831	CLA	C1A-C2A-CAA-CBA
29	B	805	CLA	C1A-C2A-CAA-CBA
29	B	815	CLA	C1A-C2A-CAA-CBA
29	B	817	CLA	C1A-C2A-CAA-CBA
29	B	825	CLA	C1A-C2A-CAA-CBA
29	B	830	CLA	C1A-C2A-CAA-CBA
29	B	835	CLA	C1A-C2A-CAA-CBA
29	O	202	CLA	C1A-C2A-CAA-CBA
29	c	306	CLA	C1A-C2A-CAA-CBA
29	c	309	CLA	C1A-C2A-CAA-CBA
29	c	311	CLA	C1A-C2A-CAA-CBA
29	a	303	CLA	C1A-C2A-CAA-CBA
29	a	306	CLA	C1A-C2A-CAA-CBA
29	b	312	CLA	C1A-C2A-CAA-CBA
29	h	302	CLA	C1A-C2A-CAA-CBA
29	h	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	h	307	CLA	C1A-C2A-CAA-CBA
29	m	603	CLA	C1A-C2A-CAA-CBA
29	m	609	CLA	C1A-C2A-CAA-CBA
29	m	612	CLA	C1A-C2A-CAA-CBA
29	e	306	CLA	C1A-C2A-CAA-CBA
29	e	308	CLA	C1A-C2A-CAA-CBA
29	f	605	CLA	C1A-C2A-CAA-CBA
29	f	613	CLA	C1A-C2A-CAA-CBA
29	i	309	CLA	C1A-C2A-CAA-CBA
29	i	311	CLA	C1A-C2A-CAA-CBA
29	j	308	CLA	C1A-C2A-CAA-CBA
29	j	311	CLA	C1A-C2A-CAA-CBA
29	j	313	CLA	C1A-C2A-CAA-CBA
29	g	307	CLA	C1A-C2A-CAA-CBA
29	g	316	CLA	C1A-C2A-CAA-CBA
29	n	607	CLA	C1A-C2A-CAA-CBA
29	n	609	CLA	C1A-C2A-CAA-CBA
29	B	837	CLA	C16-C17-C18-C20
29	i	302	CLA	C16-C17-C18-C19
31	j	318	LHG	C8-C7-O7-C5
38	e	313	II0	C26-C30-C32-C34
29	c	301	CLA	O1D-CGD-O2D-CED
29	b	310	CLA	C5-C6-C7-C8
31	g	301	LHG	C4-O6-P-O3
29	B	837	CLA	CBD-CGD-O2D-CED
29	g	309	CLA	C3-C5-C6-C7
33	A	849	LMU	C4B-C5B-C6B-O6B
29	B	810	CLA	C15-C16-C17-C18
29	B	812	CLA	C10-C11-C12-C13
29	e	304	CLA	C5-C6-C7-C8
29	A	821	CLA	CBA-CGA-O2A-C1
29	n	602	CLA	CBA-CGA-O2A-C1
29	n	604	CLA	CBA-CGA-O2A-C1
31	i	317	LHG	O6-C4-C5-C6
31	f	620	LHG	C25-C26-C27-C28
37	L	210	LMG	C16-C17-C18-C19
31	n	619	LHG	C27-C28-C29-C30
29	e	302	CLA	C15-C16-C17-C18
29	n	609	CLA	C15-C16-C17-C18
29	B	814	CLA	C16-C17-C18-C19
29	K	101	CLA	C16-C17-C18-C20
33	A	855	LMU	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
37	c	317	LMG	C30-C31-C32-C33
33	a	319	LMU	O5B-C5B-C6B-O6B
37	L	210	LMG	C19-C20-C21-C22
31	c	320	LHG	C32-C33-C34-C35
31	n	619	LHG	C1-C2-C3-O3
29	O	206	CLA	C2-C3-C5-C6
36	j	319	DGD	C8B-C9B-CAB-CBB
37	c	318	LMG	C32-C33-C34-C35
29	e	302	CLA	C8-C10-C11-C12
36	B	844	DGD	C5A-C6A-C7A-C8A
36	j	319	DGD	CCB-CDB-CEB-CFB
31	m	619	LHG	C8-C7-O7-C5
28	A	801	CL0	O1A-CGA-O2A-C1
29	A	817	CLA	O1A-CGA-O2A-C1
29	b	303	CLA	O1A-CGA-O2A-C1
29	j	303	CLA	O1A-CGA-O2A-C1
31	L	209	LHG	C27-C28-C29-C30
37	c	317	LMG	C31-C32-C33-C34
29	e	310	CLA	C6-C7-C8-C9
29	l	301	CLA	C16-C17-C18-C20
29	B	812	CLA	C3-C5-C6-C7
31	J	104	LHG	C4-C5-C6-O8
31	a	318	LHG	C4-C5-C6-O8
31	e	317	LHG	C4-C5-C6-O8
31	e	317	LHG	C10-C11-C12-C13
36	B	844	DGD	O1G-C1G-C2G-C3G
37	Q	301	LMG	C7-C8-C9-O8
29	b	306	CLA	C10-C11-C12-C13
29	A	811	CLA	C6-C7-C8-C9
36	B	844	DGD	C3B-C4B-C5B-C6B
37	n	620	LMG	C32-C33-C34-C35
29	A	813	CLA	O1A-CGA-O2A-C1
29	h	312	CLA	O1D-CGD-O2D-CED
29	B	816	CLA	C2C-C3C-CAC-CBC
31	l	318	LHG	C27-C28-C29-C30
35	A	853	SQD	C11-C12-C13-C14
37	F	206	LMG	C22-C23-C24-C25
29	B	820	CLA	O1D-CGD-O2D-CED
29	B	841	CLA	O1D-CGD-O2D-CED
29	B	837	CLA	C15-C16-C17-C18
29	R	203	CLA	C5-C6-C7-C8
29	l	310	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
38	l	314	II0	C27-C25-C29-C31
29	k	607	CLA	O1A-CGA-O2A-C1
29	c	307	CLA	CBA-CGA-O2A-C1
29	k	602	CLA	C15-C16-C17-C18
37	Q	301	LMG	C17-C18-C19-C20
31	m	619	LHG	O1-C1-C2-O2
31	g	301	LHG	O1-C1-C2-O2
31	n	619	LHG	O1-C1-C2-O2
38	a	317	II0	C26-C30-C32-C34
38	d	319	II0	C35-C39-C41-C42
31	f	619	LHG	C31-C32-C33-C34
29	A	811	CLA	O1A-CGA-O2A-C1
37	c	318	LMG	C11-C12-C13-C14
29	j	308	CLA	O1D-CGD-O2D-CED
29	B	839	CLA	C5-C6-C7-C8
32	A	854	WVN	C38-C34-C37-C40
29	A	818	CLA	C4-C3-C5-C6
29	F	202	CLA	C4-C3-C5-C6
29	O	206	CLA	C4-C3-C5-C6
29	e	304	CLA	C4-C3-C5-C6
29	F	202	CLA	C2-C3-C5-C6
29	A	813	CLA	O1D-CGD-O2D-CED
40	d	312	KC2	C2A-CAA-CBA-CGA
40	n	612	KC2	C2A-CAA-CBA-CGA
29	A	826	CLA	CBA-CGA-O2A-C1
29	k	614	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	CBA-CGA-O2A-C1
29	Q	302	CLA	CBA-CGA-O2A-C1
29	h	304	CLA	CBD-CGD-O2D-CED
29	n	604	CLA	CBD-CGD-O2D-CED
29	i	311	CLA	C10-C11-C12-C13
29	Q	302	CLA	O1D-CGD-O2D-CED
31	f	620	LHG	C6-C5-O7-C7
36	B	844	DGD	C3G-C2G-O2G-C1B
37	F	206	LMG	C9-C8-O7-C10
37	c	317	LMG	C7-C8-O7-C10
37	Q	301	LMG	C7-C8-O7-C10
29	n	608	CLA	O1D-CGD-O2D-CED
29	e	307	CLA	C2A-CAA-CBA-CGA
29	l	306	CLA	C2A-CAA-CBA-CGA
29	c	308	CLA	C10-C11-C12-C13
29	i	308	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	i	312	CLA	C15-C16-C17-C18
29	B	805	CLA	C2-C1-O2A-CGA
29	g	307	CLA	C2-C1-O2A-CGA
29	O	206	CLA	C3-C5-C6-C7
31	L	209	LHG	C28-C29-C30-C31
29	B	836	CLA	O1D-CGD-O2D-CED
29	f	602	CLA	C15-C16-C17-C18
29	j	311	CLA	C8-C10-C11-C12
31	s	408	LHG	C4-O6-P-O5
33	A	849	LMU	C6-C7-C8-C9
37	F	206	LMG	C17-C18-C19-C20
29	s	402	CLA	CBA-CGA-O2A-C1
29	c	308	CLA	CBA-CGA-O2A-C1
29	l	301	CLA	CBA-CGA-O2A-C1
29	l	304	CLA	CBA-CGA-O2A-C1
29	n	604	CLA	O1A-CGA-O2A-C1
29	F	201	CLA	C16-C17-C18-C20
29	e	307	CLA	C16-C17-C18-C19
29	i	302	CLA	C16-C17-C18-C20
29	b	306	CLA	C15-C16-C17-C18
29	e	306	CLA	C15-C16-C17-C18
29	g	302	CLA	C5-C6-C7-C8
31	l	318	LHG	O2-C2-C3-O3
33	a	319	LMU	C4'-C5'-C6'-O6'
29	m	612	CLA	O1A-CGA-O2A-C1
29	n	602	CLA	O1A-CGA-O2A-C1
32	e	315	WVN	C31-C32-C36-C39
37	L	210	LMG	C2-C1-O1-C7
31	j	318	LHG	C24-C25-C26-C27
37	c	318	LMG	C33-C34-C35-C36
36	B	844	DGD	O1G-C1G-C2G-O2G
37	F	208	LMG	O7-C8-C9-O8
37	L	210	LMG	O1-C7-C8-O7
37	L	210	LMG	C32-C33-C34-C35
37	c	317	LMG	C21-C22-C23-C24
29	g	302	CLA	C10-C11-C12-C13
29	A	821	CLA	O1A-CGA-O2A-C1
29	s	402	CLA	O1A-CGA-O2A-C1
29	l	301	CLA	O1A-CGA-O2A-C1
31	L	209	LHG	C13-C14-C15-C16
33	B	850	LMU	C2-C3-C4-C5
37	F	206	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	a	319	LMU	C6-C7-C8-C9
29	A	810	CLA	C6-C7-C8-C10
29	A	810	CLA	C11-C10-C8-C7
29	A	818	CLA	C11-C12-C13-C15
29	A	819	CLA	C6-C7-C8-C10
29	A	826	CLA	C6-C7-C8-C10
29	A	831	CLA	C11-C10-C8-C7
29	A	833	CLA	C11-C10-C8-C7
29	A	851	CLA	C11-C10-C8-C7
29	B	803	CLA	C6-C7-C8-C10
29	B	803	CLA	C11-C10-C8-C7
29	B	809	CLA	C11-C12-C13-C15
29	B	812	CLA	C6-C7-C8-C10
29	B	814	CLA	C11-C12-C13-C15
29	B	823	CLA	C6-C7-C8-C10
29	B	825	CLA	C6-C7-C8-C10
29	B	825	CLA	C11-C10-C8-C7
29	B	825	CLA	C12-C13-C15-C16
29	B	829	CLA	C12-C13-C15-C16
29	B	834	CLA	C12-C13-C15-C16
29	B	836	CLA	C6-C7-C8-C10
29	B	840	CLA	C11-C12-C13-C15
29	K	101	CLA	C11-C10-C8-C7
29	c	304	CLA	C6-C7-C8-C10
29	c	304	CLA	C11-C10-C8-C7
29	a	302	CLA	C12-C13-C15-C16
29	a	308	CLA	C12-C13-C15-C16
29	b	308	CLA	C6-C7-C8-C10
29	b	308	CLA	C11-C10-C8-C7
29	b	309	CLA	C11-C10-C8-C7
29	b	310	CLA	C11-C10-C8-C7
29	e	306	CLA	C12-C13-C15-C16
29	k	602	CLA	C11-C10-C8-C7
29	f	604	CLA	C12-C13-C15-C16
29	i	302	CLA	C12-C13-C15-C16
29	i	305	CLA	C11-C12-C13-C15
29	j	302	CLA	C11-C10-C8-C7
29	j	310	CLA	C11-C10-C8-C7
29	j	310	CLA	C12-C13-C15-C16
29	j	314	CLA	C6-C7-C8-C10
29	g	304	CLA	C12-C13-C15-C16
29	g	306	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	g	310	CLA	C11-C10-C8-C7
29	n	610	CLA	C6-C7-C8-C10
30	A	841	PQN	C22-C23-C25-C26
29	A	805	CLA	C11-C10-C8-C9
29	A	818	CLA	C11-C12-C13-C14
29	A	819	CLA	C6-C7-C8-C9
29	A	819	CLA	C11-C12-C13-C14
29	A	825	CLA	C11-C10-C8-C9
29	A	831	CLA	C11-C10-C8-C9
29	B	801	CLA	C11-C10-C8-C9
29	B	803	CLA	C6-C7-C8-C9
29	B	803	CLA	C11-C10-C8-C9
29	B	809	CLA	C11-C12-C13-C14
29	B	818	CLA	C11-C12-C13-C14
29	B	819	CLA	C14-C13-C15-C16
29	B	829	CLA	C14-C13-C15-C16
29	B	834	CLA	C14-C13-C15-C16
29	B	838	CLA	C14-C13-C15-C16
29	O	206	CLA	C11-C12-C13-C14
29	s	402	CLA	C6-C7-C8-C9
29	c	304	CLA	C11-C10-C8-C9
29	a	302	CLA	C14-C13-C15-C16
29	a	310	CLA	C6-C7-C8-C9
29	b	305	CLA	C11-C12-C13-C14
29	b	308	CLA	C6-C7-C8-C9
29	b	309	CLA	C11-C10-C8-C9
29	b	310	CLA	C11-C10-C8-C9
29	b	311	CLA	C14-C13-C15-C16
29	m	613	CLA	C11-C10-C8-C9
29	e	306	CLA	C14-C13-C15-C16
29	k	602	CLA	C11-C10-C8-C9
29	f	602	CLA	C11-C12-C13-C14
29	f	604	CLA	C11-C12-C13-C14
29	i	302	CLA	C14-C13-C15-C16
29	i	305	CLA	C11-C12-C13-C14
29	j	302	CLA	C11-C10-C8-C9
29	j	310	CLA	C11-C10-C8-C9
29	j	310	CLA	C14-C13-C15-C16
29	j	314	CLA	C6-C7-C8-C9
29	g	306	CLA	C14-C13-C15-C16
29	g	310	CLA	C11-C10-C8-C9
29	g	311	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	A	841	PQN	C19-C18-C20-C21
30	A	841	PQN	C21-C22-C23-C24
38	e	316	II0	C26-C30-C32-C34
38	k	617	II0	C36-C40-C42-C41
38	f	618	II0	C26-C30-C32-C34
31	g	322	LHG	C26-C27-C28-C29
37	F	206	LMG	C34-C35-C36-C37
29	g	312	CLA	CBA-CGA-O2A-C1
29	B	819	CLA	C5-C6-C7-C8
29	k	608	CLA	C15-C16-C17-C18
31	n	619	LHG	C28-C29-C30-C31
29	B	816	CLA	O1D-CGD-O2D-CED
32	A	844	WVN	C30-C33-C34-C38
32	R	201	WVN	C11-C19-C22-C24
38	b	315	II0	C31-C33-C35-C37
38	m	616	II0	C32-C34-C36-C38
38	k	616	II0	C31-C33-C35-C37
38	i	313	II0	C32-C34-C36-C38
38	i	316	II0	C31-C33-C35-C37
38	j	315	II0	C31-C33-C35-C37
38	n	618	II0	C31-C33-C35-C37
29	e	306	CLA	C16-C17-C18-C19
29	l	301	CLA	C16-C17-C18-C19
32	B	848	WVN	C20-C23-C25-C28
32	I	101	WVN	C29-C31-C32-C36
32	J	101	WVN	C20-C23-C25-C28
32	M	101	WVN	C29-C31-C32-C36
32	h	308	WVN	C29-C31-C32-C36
38	h	311	II0	C31-C33-C35-C39
39	g	324	IHT	C30-C32-C33-C37
29	B	816	CLA	C4C-C3C-CAC-CBC
36	B	844	DGD	C6B-C7B-C8B-C9B
37	F	208	LMG	C20-C21-C22-C23
29	A	820	CLA	C3-C5-C6-C7
29	d	310	CLA	O1D-CGD-O2D-CED
29	B	805	CLA	C15-C16-C17-C18
29	f	609	CLA	C5-C6-C7-C8
31	l	318	LHG	C8-C7-O7-C5
31	A	842	LHG	C13-C14-C15-C16
29	c	301	CLA	CBA-CGA-O2A-C1
29	h	305	CLA	CBA-CGA-O2A-C1
29	e	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	f	606	CLA	CBA-CGA-O2A-C1
29	j	314	CLA	CBA-CGA-O2A-C1
29	e	307	CLA	C8-C10-C11-C12
29	B	818	CLA	O1D-CGD-O2D-CED
31	A	842	LHG	C12-C13-C14-C15
36	B	844	DGD	CBA-CCA-CDA-CEA
29	A	837	CLA	O1D-CGD-O2D-CED
29	l	303	CLA	O1D-CGD-O2D-CED
29	A	809	CLA	C4B-C3B-CAB-CBB
29	A	811	CLA	C4B-C3B-CAB-CBB
29	A	830	CLA	C4B-C3B-CAB-CBB
29	B	803	CLA	C4B-C3B-CAB-CBB
29	B	820	CLA	C4B-C3B-CAB-CBB
29	B	830	CLA	C4B-C3B-CAB-CBB
29	B	832	CLA	C4B-C3B-CAB-CBB
29	B	840	CLA	C4B-C3B-CAB-CBB
29	J	102	CLA	C4B-C3B-CAB-CBB
29	s	403	CLA	C4B-C3B-CAB-CBB
29	a	311	CLA	C4B-C3B-CAB-CBB
29	b	309	CLA	C4B-C3B-CAB-CBB
29	b	311	CLA	C4B-C3B-CAB-CBB
29	h	301	CLA	C4B-C3B-CAB-CBB
29	m	605	CLA	C4B-C3B-CAB-CBB
29	m	608	CLA	C4B-C3B-CAB-CBB
29	m	613	CLA	C4B-C3B-CAB-CBB
29	l	306	CLA	C4B-C3B-CAB-CBB
29	l	307	CLA	C4B-C3B-CAB-CBB
29	k	601	CLA	C4B-C3B-CAB-CBB
29	k	605	CLA	C4B-C3B-CAB-CBB
29	i	304	CLA	C4B-C3B-CAB-CBB
29	i	311	CLA	C4B-C3B-CAB-CBB
29	i	312	CLA	C4B-C3B-CAB-CBB
29	j	309	CLA	C4B-C3B-CAB-CBB
29	d	309	CLA	C4B-C3B-CAB-CBB
29	d	313	CLA	C4B-C3B-CAB-CBB
29	g	307	CLA	C4B-C3B-CAB-CBB
29	g	310	CLA	C4B-C3B-CAB-CBB
29	n	605	CLA	C4B-C3B-CAB-CBB
29	n	607	CLA	C4B-C3B-CAB-CBB
29	n	609	CLA	C4B-C3B-CAB-CBB
29	Q	302	CLA	C4B-C3B-CAB-CBB
31	f	620	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	f	604	CLA	C4C-C3C-CAC-CBC
37	F	208	LMG	C13-C14-C15-C16
29	A	820	CLA	C4-C3-C5-C6
29	B	814	CLA	C4-C3-C5-C6
29	m	606	CLA	C4-C3-C5-C6
29	g	309	CLA	C4-C3-C5-C6
29	A	820	CLA	C2-C3-C5-C6
29	m	606	CLA	C2-C3-C5-C6
29	B	805	CLA	O1D-CGD-O2D-CED
29	c	304	CLA	C8-C10-C11-C12
29	a	303	CLA	C11-C10-C8-C9
29	b	307	CLA	C14-C13-C15-C16
37	F	206	LMG	O10-C28-O8-C9
29	O	201	CLA	O1D-CGD-O2D-CED
29	e	305	CLA	C3-C5-C6-C7
29	m	606	CLA	C16-C17-C18-C19
29	B	817	CLA	CBA-CGA-O2A-C1
31	a	318	LHG	C24-C23-O8-C6
37	c	317	LMG	C29-C28-O8-C9
37	b	319	LMG	C29-C28-O8-C9
37	F	206	LMG	C15-C16-C17-C18
37	Q	301	LMG	C29-C30-C31-C32
29	Q	302	CLA	O1A-CGA-O2A-C1
29	B	812	CLA	C3A-C2A-CAA-CBA
29	B	826	CLA	C3A-C2A-CAA-CBA
29	a	307	CLA	C3A-C2A-CAA-CBA
29	j	308	CLA	C3A-C2A-CAA-CBA
29	d	304	CLA	C3A-C2A-CAA-CBA
29	n	605	CLA	C3A-C2A-CAA-CBA
29	f	601	CLA	O1D-CGD-O2D-CED
32	K	103	WVN	C25-C28-C30-C33
38	b	317	II0	C36-C40-C42-C41
38	i	316	II0	C26-C30-C32-C34
31	A	842	LHG	C29-C30-C31-C32
31	c	320	LHG	C25-C26-C27-C28
30	A	841	PQN	C23-C25-C26-C27
33	A	855	LMU	C1-C2-C3-C4
29	e	307	CLA	C16-C17-C18-C20
29	a	307	CLA	CBA-CGA-O2A-C1
31	n	619	LHG	C24-C23-O8-C6
37	F	208	LMG	C29-C28-O8-C9
37	O	205	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
29	B	804	CLA	C5-C6-C7-C8
29	g	307	CLA	O1D-CGD-O2D-CED
31	L	209	LHG	C4-C5-C6-O8
35	A	853	SQD	C44-C45-C46-O48
36	j	319	DGD	C1G-C2G-C3G-O3G
37	c	318	LMG	O1-C7-C8-C9
31	L	209	LHG	C23-C24-C25-C26
31	c	320	LHG	C35-C36-C37-C38
31	a	318	LHG	C10-C11-C12-C13
29	A	812	CLA	C3-C5-C6-C7
29	f	602	CLA	C3-C5-C6-C7
29	c	304	CLA	C10-C11-C12-C13
30	B	843	PQN	C14-C13-C15-C16
29	m	606	CLA	O1D-CGD-O2D-CED
31	A	842	LHG	C3-O3-P-O6
31	A	848	LHG	C4-O6-P-O3
29	c	308	CLA	O1A-CGA-O2A-C1
33	B	850	LMU	C9-C10-C11-C12
29	k	610	CLA	C2A-CAA-CBA-CGA
29	e	311	CLA	C10-C11-C12-C13
33	B	850	LMU	C3-C4-C5-C6
37	c	317	LMG	C42-C43-C44-C45
31	f	620	LHG	O6-C4-C5-O7
31	g	301	LHG	O6-C4-C5-O7
33	A	849	LMU	O5B-C5B-C6B-O6B
29	e	303	CLA	CBA-CGA-O2A-C1
37	F	206	LMG	C11-C12-C13-C14
29	B	806	CLA	O1D-CGD-O2D-CED
29	A	826	CLA	O1A-CGA-O2A-C1
29	k	614	CLA	O1A-CGA-O2A-C1
29	n	603	CLA	O1A-CGA-O2A-C1
31	a	318	LHG	C7-C8-C9-C10
29	B	826	CLA	C10-C11-C12-C13
29	B	839	CLA	CAA-CBA-CGA-O2A
29	A	809	CLA	C2B-C3B-CAB-CBB
29	A	830	CLA	C2B-C3B-CAB-CBB
29	A	832	CLA	C2B-C3B-CAB-CBB
29	B	820	CLA	C2B-C3B-CAB-CBB
29	a	311	CLA	C2B-C3B-CAB-CBB
29	b	311	CLA	C2B-C3B-CAB-CBB
29	h	301	CLA	C2B-C3B-CAB-CBB
29	m	605	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	m	612	CLA	C2B-C3B-CAB-CBB
29	l	306	CLA	C2B-C3B-CAB-CBB
29	k	601	CLA	C2B-C3B-CAB-CBB
29	f	605	CLA	C2B-C3B-CAB-CBB
29	i	302	CLA	C2B-C3B-CAB-CBB
29	i	311	CLA	C2B-C3B-CAB-CBB
29	g	307	CLA	C2B-C3B-CAB-CBB
29	n	607	CLA	C2B-C3B-CAB-CBB
29	Q	302	CLA	C2B-C3B-CAB-CBB
29	B	803	CLA	C8-C10-C11-C12
29	B	819	CLA	C8-C10-C11-C12
29	B	817	CLA	O1A-CGA-O2A-C1
29	l	304	CLA	O1A-CGA-O2A-C1
31	m	619	LHG	O10-C23-O8-C6
31	e	317	LHG	O7-C5-C6-O8
35	A	853	SQD	O47-C45-C46-O48
37	b	319	LMG	O1-C7-C8-O7
37	n	620	LMG	O1-C7-C8-O7
29	a	310	CLA	CBD-CGD-O2D-CED
32	L	206	WVN	C25-C28-C30-C33
38	e	316	II0	C35-C39-C41-C42
29	B	837	CLA	O1D-CGD-O2D-CED
29	m	606	CLA	C16-C17-C18-C20
29	Q	302	CLA	C16-C17-C18-C20
29	j	310	CLA	C8-C10-C11-C12
29	F	201	CLA	C3-C5-C6-C7
30	A	841	PQN	C14-C13-C15-C16
29	A	851	CLA	C2-C1-O2A-CGA
29	B	811	CLA	C2-C1-O2A-CGA
29	m	610	CLA	C2-C1-O2A-CGA
29	l	312	CLA	C2-C1-O2A-CGA
29	f	613	CLA	C2-C1-O2A-CGA
29	B	814	CLA	C2-C3-C5-C6
36	B	844	DGD	C7A-C8A-C9A-CAA
29	A	840	CLA	C8-C10-C11-C12
29	O	206	CLA	C13-C15-C16-C17
29	A	824	CLA	C11-C12-C13-C14
29	A	825	CLA	C6-C7-C8-C9
29	A	840	CLA	C11-C12-C13-C14
29	B	807	CLA	C11-C10-C8-C9
29	B	818	CLA	C11-C10-C8-C9
29	B	826	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	B	836	CLA	C11-C10-C8-C9
29	B	837	CLA	C14-C13-C15-C16
29	K	101	CLA	C11-C10-C8-C9
29	c	312	CLA	C6-C7-C8-C9
29	a	311	CLA	C11-C10-C8-C9
29	f	608	CLA	C11-C12-C13-C14
29	i	312	CLA	C11-C10-C8-C9
29	g	305	CLA	C6-C7-C8-C9
29	a	309	CLA	CBA-CGA-O2A-C1
31	a	318	LHG	C24-C25-C26-C27
36	B	844	DGD	C4A-C5A-C6A-C7A
37	n	620	LMG	C14-C15-C16-C17
29	B	807	CLA	C5-C6-C7-C8
29	B	808	CLA	C15-C16-C17-C18
29	l	307	CLA	C5-C6-C7-C8
29	g	307	CLA	C4-C3-C5-C6
37	c	317	LMG	C39-C40-C41-C42
29	e	304	CLA	C2A-CAA-CBA-CGA
32	B	848	WVN	C06-C13-C20-C23
39	c	319	IHT	C02-C07-C18-C22
39	c	319	IHT	C10-C07-C18-C22
29	j	314	CLA	C13-C15-C16-C17
31	g	301	LHG	C29-C30-C31-C32
36	B	844	DGD	CDB-CEB-CFB-CGB
29	B	833	CLA	O1D-CGD-O2D-CED
32	h	308	WVN	C30-C33-C34-C38
32	e	315	WVN	C20-C23-C25-C27
29	f	606	CLA	O1A-CGA-O2A-C1
29	e	301	CLA	O1D-CGD-O2D-CED
29	A	806	CLA	CBA-CGA-O2A-C1
29	m	601	CLA	C1A-C2A-CAA-CBA
29	g	303	CLA	C1A-C2A-CAA-CBA
32	A	854	WVN	C30-C33-C34-C37
32	B	848	WVN	C30-C33-C34-C37
32	L	206	WVN	C30-C33-C34-C37
38	a	317	II0	C32-C34-C36-C40
38	d	319	II0	C31-C33-C35-C39
39	b	316	IHT	C18-C22-C23-C27
29	j	311	CLA	C10-C11-C12-C13
31	a	301	LHG	C25-C26-C27-C28
36	B	844	DGD	C9A-CAA-CBA-CCA
29	a	312	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	g	312	CLA	O1A-CGA-O2A-C1
37	Q	301	LMG	C32-C33-C34-C35
29	B	808	CLA	C3-C5-C6-C7
29	e	311	CLA	C3-C5-C6-C7
37	L	210	LMG	C23-C24-C25-C26
38	b	317	II0	C27-C25-C29-C31
38	h	311	II0	C28-C26-C30-C32
38	l	315	II0	C27-C25-C29-C31
38	k	617	II0	C28-C26-C30-C32
38	g	318	II0	C27-C25-C29-C31
39	b	316	IHT	C28-C26-C29-C31
29	c	308	CLA	C15-C16-C17-C18
29	f	609	CLA	C10-C11-C12-C13
29	k	607	CLA	O1D-CGD-O2D-CED
29	c	301	CLA	O1A-CGA-O2A-C1
29	e	310	CLA	O1A-CGA-O2A-C1
28	A	801	CL0	C5-C6-C7-C8
31	L	209	LHG	O6-C4-C5-C6
31	g	322	LHG	C28-C29-C30-C31
29	A	818	CLA	C2-C3-C5-C6
29	A	824	CLA	C11-C12-C13-C15
29	A	825	CLA	C11-C10-C8-C7
29	A	836	CLA	C11-C10-C8-C7
29	A	837	CLA	C12-C13-C15-C16
29	A	840	CLA	C11-C10-C8-C7
29	A	840	CLA	C11-C12-C13-C15
29	B	801	CLA	C6-C7-C8-C10
29	B	803	CLA	C12-C13-C15-C16
29	B	804	CLA	C6-C7-C8-C10
29	B	807	CLA	C11-C10-C8-C7
29	B	818	CLA	C11-C10-C8-C7
29	B	818	CLA	C11-C12-C13-C15
29	B	822	CLA	C11-C12-C13-C15
29	B	831	CLA	C11-C12-C13-C15
29	B	836	CLA	C11-C10-C8-C7
29	B	837	CLA	C12-C13-C15-C16
29	B	838	CLA	C12-C13-C15-C16
29	F	201	CLA	C12-C13-C15-C16
29	F	202	CLA	C12-C13-C15-C16
29	O	206	CLA	C11-C12-C13-C15
29	s	406	CLA	C12-C13-C15-C16
29	c	312	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
29	a	305	CLA	C11-C10-C8-C7
29	a	307	CLA	C12-C13-C15-C16
29	a	308	CLA	C11-C12-C13-C15
29	a	310	CLA	C6-C7-C8-C10
29	a	311	CLA	C11-C10-C8-C7
29	b	305	CLA	C6-C7-C8-C10
29	b	305	CLA	C11-C12-C13-C15
29	b	311	CLA	C12-C13-C15-C16
29	m	604	CLA	C6-C7-C8-C10
29	m	606	CLA	C11-C12-C13-C15
29	m	606	CLA	C12-C13-C15-C16
29	e	304	CLA	C2-C3-C5-C6
29	l	304	CLA	C6-C7-C8-C10
29	l	310	CLA	C11-C12-C13-C15
29	k	602	CLA	C11-C12-C13-C15
29	f	602	CLA	C11-C12-C13-C15
29	f	604	CLA	C11-C12-C13-C15
29	f	607	CLA	C11-C12-C13-C15
29	f	608	CLA	C11-C12-C13-C15
29	i	302	CLA	C11-C10-C8-C7
29	i	303	CLA	C11-C12-C13-C15
29	i	303	CLA	C12-C13-C15-C16
29	i	305	CLA	C11-C10-C8-C7
29	i	312	CLA	C11-C10-C8-C7
29	g	311	CLA	C11-C10-C8-C7
29	Q	302	CLA	C6-C7-C8-C10
30	A	841	PQN	C17-C18-C20-C21
30	A	841	PQN	C21-C22-C23-C25
31	J	104	LHG	O10-C23-O8-C6
29	d	302	CLA	C10-C11-C12-C13
32	s	405	WVN	C22-C26-C29-C31
32	e	315	WVN	C25-C28-C30-C33
32	l	302	WVN	C34-C37-C40-C39
32	R	202	WVN	C32-C36-C39-C40
38	b	314	II0	C35-C39-C41-C42
38	h	309	II0	C35-C39-C41-C42
38	h	311	II0	C26-C30-C32-C34
38	e	314	II0	C25-C29-C31-C33
38	l	314	II0	C26-C30-C32-C34
38	f	618	II0	C25-C29-C31-C33
38	i	319	II0	C36-C40-C42-C41
38	n	614	II0	C25-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
39	c	319	IHT	C35-C38-C41-C40
29	e	302	CLA	CBD-CGD-O2D-CED
29	F	201	CLA	C16-C17-C18-C19
29	e	305	CLA	C5-C6-C7-C8
29	m	608	CLA	C2A-CAA-CBA-CGA
32	R	202	WVN	C38-C34-C37-C40
31	n	619	LHG	C7-C8-C9-C10
29	m	609	CLA	C3-C5-C6-C7
31	s	408	LHG	C11-C10-C9-C8
29	B	837	CLA	C16-C17-C18-C19
29	A	851	CLA	C15-C16-C17-C18
29	b	311	CLA	CBA-CGA-O2A-C1
31	b	318	LHG	C24-C23-O8-C6
31	g	322	LHG	C11-C10-C9-C8
37	n	620	LMG	C19-C20-C21-C22
29	j	305	CLA	C5-C6-C7-C8
31	i	317	LHG	C29-C30-C31-C32
29	A	805	CLA	CAD-CBD-CGD-O2D
29	A	816	CLA	CAD-CBD-CGD-O2D
29	A	825	CLA	CAD-CBD-CGD-O2D
29	A	833	CLA	CAD-CBD-CGD-O2D
29	B	810	CLA	CAD-CBD-CGD-O2D
29	B	814	CLA	CAD-CBD-CGD-O2D
29	B	830	CLA	CAD-CBD-CGD-O2D
29	B	839	CLA	CAD-CBD-CGD-O2D
29	L	207	CLA	CAD-CBD-CGD-O2D
29	c	309	CLA	CAD-CBD-CGD-O2D
29	a	303	CLA	CAD-CBD-CGD-O2D
29	a	304	CLA	CAD-CBD-CGD-O2D
29	a	306	CLA	CAD-CBD-CGD-O2D
29	a	310	CLA	CAD-CBD-CGD-O2D
29	b	305	CLA	CAD-CBD-CGD-O2D
29	b	310	CLA	CAD-CBD-CGD-O2D
29	h	306	CLA	CAD-CBD-CGD-O2D
29	m	610	CLA	CAD-CBD-CGD-O2D
29	e	301	CLA	CAD-CBD-CGD-O2D
29	l	303	CLA	CAD-CBD-CGD-O2D
29	f	609	CLA	CAD-CBD-CGD-O2D
29	j	302	CLA	CAD-CBD-CGD-O2D
29	j	311	CLA	CAD-CBD-CGD-O2D
29	j	313	CLA	CAD-CBD-CGD-O2D
29	j	314	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	d	302	CLA	CAD-CBD-CGD-O2D
29	g	303	CLA	CAD-CBD-CGD-O2D
29	g	308	CLA	CAD-CBD-CGD-O2D
29	g	316	CLA	CAD-CBD-CGD-O2D
29	n	601	CLA	CAD-CBD-CGD-O2D
29	n	603	CLA	CAD-CBD-CGD-O2D
29	n	604	CLA	CAD-CBD-CGD-O2D
29	n	606	CLA	CAD-CBD-CGD-O2D
29	n	609	CLA	CAD-CBD-CGD-O2D
40	s	401	KC2	CAD-CBD-CGD-O2D
40	s	404	KC2	CAD-CBD-CGD-O2D
40	m	611	KC2	CAD-CBD-CGD-O2D
40	e	309	KC2	C2C-C3C-CAC-CBC
40	k	612	KC2	CAD-CBD-CGD-O2D
40	j	312	KC2	C2C-C3C-CAC-CBC
40	d	311	KC2	C2C-C3C-CAC-CBC
40	d	312	KC2	C2B-C3B-CAB-CBB
40	d	312	KC2	CAD-CBD-CGD-O2D
40	g	315	KC2	CAD-CBD-CGD-O2D
29	B	820	CLA	C8-C10-C11-C12
29	g	307	CLA	CBA-CGA-O2A-C1
29	A	840	CLA	C4-C3-C5-C6
29	e	306	CLA	C16-C17-C18-C20
37	b	319	LMG	C28-C29-C30-C31
31	L	209	LHG	C2-C3-O3-P
31	c	320	LHG	C2-C3-O3-P
31	m	619	LHG	C4-C5-C6-O8
31	g	322	LHG	C4-C5-C6-O8
37	F	206	LMG	C7-C8-C9-O8
37	O	205	LMG	C7-C8-C9-O8
37	b	319	LMG	O1-C7-C8-C9
29	h	305	CLA	O1A-CGA-O2A-C1
37	n	620	LMG	C37-C38-C39-C40
31	b	318	LHG	O6-C4-C5-O7
29	B	805	CLA	CAA-CBA-CGA-O2A
29	L	202	CLA	O2A-C1-C2-C3
29	A	830	CLA	C2A-CAA-CBA-CGA
29	B	817	CLA	C10-C11-C12-C13
29	f	604	CLA	C2C-C3C-CAC-CBC
37	b	319	LMG	C30-C31-C32-C33
29	k	602	CLA	C16-C17-C18-C20
29	Q	302	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	A	806	CLA	O1D-CGD-O2D-CED
29	A	814	CLA	CHA-CBD-CGD-O1D
29	A	822	CLA	CHA-CBD-CGD-O1D
29	A	822	CLA	CHA-CBD-CGD-O2D
29	A	829	CLA	CHA-CBD-CGD-O1D
29	A	829	CLA	CHA-CBD-CGD-O2D
29	B	808	CLA	CHA-CBD-CGD-O1D
29	B	808	CLA	CHA-CBD-CGD-O2D
29	B	821	CLA	CHA-CBD-CGD-O2D
29	B	822	CLA	CHA-CBD-CGD-O1D
29	B	822	CLA	CHA-CBD-CGD-O2D
29	B	823	CLA	CHA-CBD-CGD-O1D
29	B	823	CLA	CHA-CBD-CGD-O2D
29	c	302	CLA	CHA-CBD-CGD-O1D
29	c	302	CLA	CHA-CBD-CGD-O2D
29	c	303	CLA	CHA-CBD-CGD-O1D
29	c	303	CLA	CHA-CBD-CGD-O2D
29	a	305	CLA	CHA-CBD-CGD-O1D
29	a	305	CLA	CHA-CBD-CGD-O2D
29	b	303	CLA	CHA-CBD-CGD-O1D
29	b	303	CLA	CHA-CBD-CGD-O2D
29	b	312	CLA	CHA-CBD-CGD-O1D
29	m	601	CLA	CHA-CBD-CGD-O1D
29	m	612	CLA	CHA-CBD-CGD-O1D
29	m	612	CLA	CHA-CBD-CGD-O2D
29	l	306	CLA	CHA-CBD-CGD-O2D
29	k	605	CLA	CHA-CBD-CGD-O1D
29	f	602	CLA	CHA-CBD-CGD-O1D
29	f	604	CLA	CHA-CBD-CGD-O1D
29	f	604	CLA	CHA-CBD-CGD-O2D
29	i	302	CLA	CHA-CBD-CGD-O2D
29	i	303	CLA	CHA-CBD-CGD-O1D
29	i	303	CLA	CHA-CBD-CGD-O2D
29	j	308	CLA	CHA-CBD-CGD-O1D
29	j	308	CLA	CHA-CBD-CGD-O2D
29	d	304	CLA	CHA-CBD-CGD-O1D
29	d	304	CLA	CHA-CBD-CGD-O2D
29	d	313	CLA	CHA-CBD-CGD-O1D
29	d	313	CLA	CHA-CBD-CGD-O2D
29	g	306	CLA	CHA-CBD-CGD-O2D
29	g	310	CLA	CHA-CBD-CGD-O1D
29	g	310	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
40	l	311	KC2	CHA-CBD-CGD-O1D
40	k	611	KC2	CHA-CBD-CGD-O1D
40	k	611	KC2	CHA-CBD-CGD-O2D
29	c	305	CLA	C3-C5-C6-C7
29	j	303	CLA	CBD-CGD-O2D-CED
29	e	303	CLA	O1A-CGA-O2A-C1
29	j	314	CLA	O1A-CGA-O2A-C1
31	a	318	LHG	C35-C36-C37-C38
33	i	301	LMU	C1-C2-C3-C4
29	A	836	CLA	O1D-CGD-O2D-CED
29	a	310	CLA	O1D-CGD-O2D-CED
32	A	854	WVN	C31-C32-C36-C39
32	B	846	WVN	C19-C22-C26-C29
32	B	848	WVN	C31-C32-C36-C39
32	F	207	WVN	C23-C25-C28-C30
38	l	315	II0	C34-C36-C40-C42
38	j	301	II0	C34-C36-C40-C42
38	d	301	II0	C33-C35-C39-C41
31	g	322	LHG	O7-C5-C6-O8
36	j	319	DGD	O2G-C2G-C3G-O3G
37	O	205	LMG	O7-C8-C9-O8
37	Q	301	LMG	O7-C8-C9-O8
29	A	806	CLA	O1A-CGA-O2A-C1
29	a	307	CLA	O1A-CGA-O2A-C1
37	F	206	LMG	C41-C42-C43-C44
29	B	838	CLA	C16-C17-C18-C19
29	i	308	CLA	C16-C17-C18-C20
29	f	602	CLA	O1D-CGD-O2D-CED
37	F	208	LMG	C28-C29-C30-C31
37	O	205	LMG	C28-C29-C30-C31
29	f	602	CLA	C5-C6-C7-C8
29	j	311	CLA	C5-C6-C7-C8
31	A	842	LHG	C15-C16-C17-C18
29	B	817	CLA	C2-C3-C5-C6
38	c	314	II0	C10-C22-C24-C26
38	b	317	II0	C09-C21-C23-C25
38	b	317	II0	C10-C22-C24-C26
38	l	317	II0	C10-C22-C24-C26
38	n	614	II0	C09-C21-C23-C25
38	n	614	II0	C10-C22-C24-C26
39	b	316	IHT	C11-C21-C24-C26
39	n	617	IHT	C11-C21-C24-C26

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Mol	Chain	Res	Type	Atoms
29	A	805	CLA	C6-C7-C8-C9
29	A	836	CLA	C11-C10-C8-C9
29	A	837	CLA	C14-C13-C15-C16
29	B	822	CLA	C11-C12-C13-C14
29	B	831	CLA	C11-C12-C13-C14
29	F	201	CLA	C14-C13-C15-C16
29	k	609	CLA	C11-C10-C8-C9
29	i	303	CLA	C11-C12-C13-C14
29	i	305	CLA	C11-C10-C8-C9
37	n	620	LMG	C34-C35-C36-C37
29	A	824	CLA	C13-C15-C16-C17
35	A	853	SQD	C4-C5-C6-S
29	j	305	CLA	C4C-C3C-CAC-CBC
29	A	828	CLA	CBD-CGD-O2D-CED
29	k	607	CLA	CAA-CBA-CGA-O2A
32	I	101	WVN	C20-C23-C25-C27
32	L	205	WVN	C20-C23-C25-C27
32	L	206	WVN	C11-C19-C22-C24
32	e	315	WVN	C29-C31-C32-C35
38	a	315	II0	C32-C34-C36-C38
38	h	309	II0	C32-C34-C36-C38
38	g	317	II0	C32-C34-C36-C38
33	A	855	LMU	C3'-C4'-O1B-C1B
29	A	804	CLA	C15-C16-C17-C18
37	b	319	LMG	C11-C12-C13-C14
32	A	845	WVN	C20-C23-C25-C28
32	A	847	WVN	C20-C23-C25-C28
32	s	407	WVN	C20-C23-C25-C28
38	a	317	II0	C31-C33-C35-C39
29	a	311	CLA	C3-C5-C6-C7
29	A	803	CLA	C1A-C2A-CAA-CBA
29	A	807	CLA	C1A-C2A-CAA-CBA
29	A	820	CLA	C1A-C2A-CAA-CBA
29	A	832	CLA	C1A-C2A-CAA-CBA
29	A	833	CLA	C1A-C2A-CAA-CBA
29	B	809	CLA	C1A-C2A-CAA-CBA
29	B	814	CLA	C1A-C2A-CAA-CBA
29	B	818	CLA	C1A-C2A-CAA-CBA
29	B	820	CLA	C1A-C2A-CAA-CBA
29	B	827	CLA	C1A-C2A-CAA-CBA
29	K	101	CLA	C1A-C2A-CAA-CBA
31	i	317	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	A	808	CLA	C16-C17-C18-C19
29	A	808	CLA	C16-C17-C18-C20
29	O	202	CLA	C5-C6-C7-C8
32	B	849	WVN	C22-C26-C29-C31
32	J	101	WVN	C22-C26-C29-C31
38	g	319	II0	C36-C40-C42-C41
29	A	835	CLA	C15-C16-C17-C18
31	L	208	LHG	C4-O6-P-O3
31	g	322	LHG	C4-O6-P-O3
31	A	842	LHG	C27-C28-C29-C30
37	c	317	LMG	C33-C34-C35-C36
29	A	851	CLA	C4-C3-C5-C6
31	b	318	LHG	C2-C3-O3-P
29	n	604	CLA	O1D-CGD-O2D-CED
31	L	208	LHG	C28-C29-C30-C31
36	j	319	DGD	C2A-C3A-C4A-C5A
29	a	309	CLA	O1A-CGA-O2A-C1
29	A	837	CLA	C4B-C3B-CAB-CBB
29	A	838	CLA	C4B-C3B-CAB-CBB
29	B	835	CLA	C4B-C3B-CAB-CBB
29	B	837	CLA	C4B-C3B-CAB-CBB
29	F	203	CLA	C4B-C3B-CAB-CBB
29	c	301	CLA	C4B-C3B-CAB-CBB
29	b	302	CLA	C4B-C3B-CAB-CBB
29	b	310	CLA	C4B-C3B-CAB-CBB
29	k	609	CLA	C4B-C3B-CAB-CBB
29	f	607	CLA	C4B-C3B-CAB-CBB
29	g	308	CLA	C4B-C3B-CAB-CBB
31	A	842	LHG	C4-O6-P-O5
31	J	104	LHG	C4-O6-P-O5
31	c	320	LHG	C3-O3-P-O4
31	a	301	LHG	C3-O3-P-O5
31	b	318	LHG	C4-O6-P-O5
31	l	318	LHG	C3-O3-P-O5
31	f	620	LHG	C3-O3-P-O5
31	f	620	LHG	C4-O6-P-O5
31	j	318	LHG	C4-O6-P-O4
31	g	301	LHG	C4-O6-P-O5
31	g	322	LHG	C3-O3-P-O5
31	g	322	LHG	C4-O6-P-O4
31	n	619	LHG	C3-O3-P-O5
29	s	402	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	i	312	CLA	C16-C17-C18-C20
35	A	853	SQD	C7-C8-C9-C10
29	l	310	CLA	C8-C10-C11-C12
29	B	823	CLA	CBA-CGA-O2A-C1
29	l	303	CLA	CBA-CGA-O2A-C1
31	c	316	LHG	O6-C4-C5-C6
31	b	318	LHG	O6-C4-C5-C6
29	f	606	CLA	CAA-CBA-CGA-O2A
29	i	307	CLA	CAA-CBA-CGA-O2A
29	h	301	CLA	C5-C6-C7-C8
31	g	301	LHG	C9-C10-C11-C12
29	m	613	CLA	C16-C17-C18-C20
29	k	604	CLA	C4C-C3C-CAC-CBC
29	A	804	CLA	CAD-CBD-CGD-O1D
29	A	814	CLA	CAD-CBD-CGD-O1D
29	A	822	CLA	CAD-CBD-CGD-O1D
29	c	301	CLA	C2-C3-C5-C6
29	c	302	CLA	CAD-CBD-CGD-O1D
29	c	303	CLA	CAD-CBD-CGD-O1D
29	a	305	CLA	CAD-CBD-CGD-O1D
29	b	312	CLA	CAD-CBD-CGD-O1D
29	m	604	CLA	CAD-CBD-CGD-O1D
29	m	612	CLA	CAD-CBD-CGD-O1D
29	l	306	CLA	CAD-CBD-CGD-O1D
29	k	604	CLA	CAD-CBD-CGD-O1D
29	f	602	CLA	CAD-CBD-CGD-O1D
29	f	604	CLA	CAD-CBD-CGD-O1D
29	i	302	CLA	CAD-CBD-CGD-O1D
29	i	305	CLA	CAD-CBD-CGD-O1D
29	j	304	CLA	C2-C3-C5-C6
29	j	305	CLA	CAD-CBD-CGD-O1D
29	d	303	CLA	C2-C3-C5-C6
29	g	304	CLA	CAD-CBD-CGD-O1D
29	g	306	CLA	CAD-CBD-CGD-O1D
29	B	822	CLA	C10-C11-C12-C13
29	k	604	CLA	C5-C6-C7-C8
29	b	311	CLA	O1A-CGA-O2A-C1
29	l	303	CLA	O1A-CGA-O2A-C1
29	g	307	CLA	O1A-CGA-O2A-C1
37	c	317	LMG	C29-C30-C31-C32
29	i	306	CLA	CBA-CGA-O2A-C1
29	g	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	A	803	CLA	C6-C7-C8-C10
29	A	816	CLA	C11-C10-C8-C7
29	A	819	CLA	C12-C13-C15-C16
29	A	831	CLA	C12-C13-C15-C16
29	A	835	CLA	C6-C7-C8-C10
29	B	816	CLA	C11-C12-C13-C15
29	B	841	CLA	C12-C13-C15-C16
29	F	201	CLA	C11-C10-C8-C7
29	c	302	CLA	C6-C7-C8-C10
29	c	304	CLA	C12-C13-C15-C16
29	b	306	CLA	C11-C12-C13-C15
29	b	306	CLA	C12-C13-C15-C16
29	m	609	CLA	C11-C10-C8-C7
29	m	613	CLA	C11-C10-C8-C7
29	e	302	CLA	C11-C12-C13-C15
29	e	311	CLA	C12-C13-C15-C16
29	l	301	CLA	C12-C13-C15-C16
29	l	306	CLA	C12-C13-C15-C16
29	k	609	CLA	C11-C10-C8-C7
29	f	607	CLA	C11-C10-C8-C7
29	f	610	CLA	C11-C12-C13-C15
29	i	312	CLA	C11-C12-C13-C15
29	j	305	CLA	C6-C7-C8-C10
29	g	303	CLA	C3A-C2A-CAA-CBA
29	g	305	CLA	C11-C12-C13-C15
29	Q	302	CLA	C11-C10-C8-C7
30	B	843	PQN	C21-C22-C23-C25
31	L	209	LHG	O6-C4-C5-O7
31	i	317	LHG	O6-C4-C5-O7
32	A	844	WVN	C05-C02-C11-C19
32	B	846	WVN	C05-C02-C11-C19
32	F	205	WVN	C05-C02-C11-C19
32	I	101	WVN	C05-C02-C11-C19
32	l	316	WVN	C05-C02-C11-C19
32	R	201	WVN	C05-C02-C11-C19
31	c	316	LHG	C24-C25-C26-C27
38	a	315	II0	C35-C39-C41-C42
38	k	620	II0	C26-C30-C32-C34
29	s	402	CLA	C13-C15-C16-C17
30	A	841	PQN	C20-C21-C22-C23
29	A	820	CLA	C5-C6-C7-C8
29	m	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	j	314	CLA	C2A-CAA-CBA-CGA
29	d	318	CLA	C2A-CAA-CBA-CGA
29	B	817	CLA	C16-C17-C18-C20
29	B	821	CLA	C5-C6-C7-C8
29	j	302	CLA	C3-C5-C6-C7
29	n	613	CLA	CAA-CBA-CGA-O2A
36	j	319	DGD	O1G-C1G-C2G-O2G
37	F	206	LMG	O7-C8-C9-O8
37	F	206	LMG	C12-C13-C14-C15
31	L	208	LHG	C11-C12-C13-C14
31	j	318	LHG	C11-C12-C13-C14
33	A	855	LMU	C5'-C4'-O1B-C1B
37	n	620	LMG	C18-C19-C20-C21
29	h	306	CLA	CAA-CBA-CGA-O2A
29	B	838	CLA	C16-C17-C18-C20
29	A	832	CLA	C13-C15-C16-C17
29	B	806	CLA	C5-C6-C7-C8
29	B	841	CLA	C3-C5-C6-C7
33	A	849	LMU	C9-C10-C11-C12
36	B	844	DGD	C3A-C4A-C5A-C6A
29	i	306	CLA	O1A-CGA-O2A-C1
29	B	825	CLA	C4-C3-C5-C6
29	g	309	CLA	C2-C3-C5-C6
29	A	802	CLA	CAA-CBA-CGA-O2A
29	k	606	CLA	CAA-CBA-CGA-O2A
29	A	833	CLA	C11-C10-C8-C9
29	B	803	CLA	C14-C13-C15-C16
29	B	804	CLA	C6-C7-C8-C9
29	B	814	CLA	C11-C12-C13-C14
29	a	305	CLA	C11-C10-C8-C9
29	a	307	CLA	C14-C13-C15-C16
29	m	604	CLA	C6-C7-C8-C9
29	e	306	CLA	C11-C10-C8-C9
29	l	304	CLA	C6-C7-C8-C9
29	l	304	CLA	C14-C13-C15-C16
29	l	310	CLA	C11-C12-C13-C14
29	f	607	CLA	C11-C12-C13-C14
29	i	303	CLA	C14-C13-C15-C16
29	g	304	CLA	C11-C12-C13-C14
29	Q	302	CLA	C11-C10-C8-C9
29	h	304	CLA	O1D-CGD-O2D-CED
29	g	308	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	L	207	CLA	CBD-CGD-O2D-CED
31	L	208	LHG	C27-C28-C29-C30
29	l	312	CLA	C3-C5-C6-C7
29	K	101	CLA	C5-C6-C7-C8
29	B	806	CLA	C15-C16-C17-C18
38	k	618	II0	C30-C32-C34-C36
38	d	319	II0	C30-C32-C34-C36
32	L	206	WVN	C32-C36-C39-C40
38	f	616	II0	C26-C30-C32-C34
35	A	853	SQD	C17-C18-C19-C20
29	B	823	CLA	O1A-CGA-O2A-C1
37	c	318	LMG	C10-C11-C12-C13
29	A	828	CLA	O1D-CGD-O2D-CED
29	A	810	CLA	C2B-C3B-CAB-CBB
29	A	811	CLA	C2B-C3B-CAB-CBB
29	B	803	CLA	C2B-C3B-CAB-CBB
29	B	806	CLA	C2B-C3B-CAB-CBB
29	B	810	CLA	C2B-C3B-CAB-CBB
29	B	823	CLA	C2B-C3B-CAB-CBB
29	B	830	CLA	C2B-C3B-CAB-CBB
29	B	831	CLA	C2B-C3B-CAB-CBB
29	O	202	CLA	C2B-C3B-CAB-CBB
29	K	101	CLA	C2B-C3B-CAB-CBB
29	s	403	CLA	C2B-C3B-CAB-CBB
29	c	309	CLA	C2B-C3B-CAB-CBB
29	c	311	CLA	C2B-C3B-CAB-CBB
29	c	312	CLA	C2B-C3B-CAB-CBB
29	a	310	CLA	C2B-C3B-CAB-CBB
29	b	302	CLA	C2B-C3B-CAB-CBB
29	b	305	CLA	C2B-C3B-CAB-CBB
29	b	309	CLA	C2B-C3B-CAB-CBB
29	h	312	CLA	C2B-C3B-CAB-CBB
29	m	613	CLA	C2B-C3B-CAB-CBB
29	k	605	CLA	C2B-C3B-CAB-CBB
29	k	614	CLA	C2B-C3B-CAB-CBB
29	f	612	CLA	C2B-C3B-CAB-CBB
29	i	304	CLA	C2B-C3B-CAB-CBB
29	i	305	CLA	C2B-C3B-CAB-CBB
29	i	312	CLA	C2B-C3B-CAB-CBB
29	j	306	CLA	C2B-C3B-CAB-CBB
29	j	309	CLA	C2B-C3B-CAB-CBB
29	j	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	d	304	CLA	C2B-C3B-CAB-CBB
29	d	309	CLA	C2B-C3B-CAB-CBB
29	d	313	CLA	C2B-C3B-CAB-CBB
29	g	308	CLA	C2B-C3B-CAB-CBB
29	g	310	CLA	C2B-C3B-CAB-CBB
29	R	203	CLA	C2B-C3B-CAB-CBB
29	n	604	CLA	C2B-C3B-CAB-CBB
29	n	605	CLA	C2B-C3B-CAB-CBB
29	n	609	CLA	C2B-C3B-CAB-CBB
29	j	303	CLA	C6-C7-C8-C9
29	A	827	CLA	C3-C5-C6-C7
29	A	809	CLA	C4-C3-C5-C6
29	A	826	CLA	C4-C3-C5-C6
29	g	307	CLA	CAA-CBA-CGA-O2A
31	a	301	LHG	C17-C18-C19-C20
29	B	819	CLA	C13-C15-C16-C17
29	l	304	CLA	C16-C17-C18-C19
29	i	308	CLA	C16-C17-C18-C19
31	i	317	LHG	C25-C26-C27-C28
29	f	613	CLA	C10-C11-C12-C13
29	Q	302	CLA	C10-C11-C12-C13
29	A	821	CLA	C1-C2-C3-C4
31	a	318	LHG	C29-C30-C31-C32
29	A	822	CLA	C3-C5-C6-C7
29	i	302	CLA	CAA-CBA-CGA-O2A
31	e	317	LHG	C6-C5-O7-C7
31	f	619	LHG	O6-C4-C5-C6
29	A	802	CLA	C2A-CAA-CBA-CGA
29	B	801	CLA	C2A-CAA-CBA-CGA
29	e	302	CLA	C2A-CAA-CBA-CGA
29	k	607	CLA	C2A-CAA-CBA-CGA
29	f	604	CLA	C2A-CAA-CBA-CGA
29	f	607	CLA	C2A-CAA-CBA-CGA
29	g	306	CLA	C2A-CAA-CBA-CGA
29	A	816	CLA	C2-C1-O2A-CGA
29	A	833	CLA	C2-C1-O2A-CGA
29	B	822	CLA	C2-C1-O2A-CGA
29	m	602	CLA	C2-C1-O2A-CGA
29	m	613	CLA	C2-C1-O2A-CGA
29	j	307	CLA	C2-C1-O2A-CGA
29	n	609	CLA	C2-C1-O2A-CGA
33	A	849	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	c	317	LMG	C16-C17-C18-C19
29	s	402	CLA	C16-C17-C18-C20
29	m	613	CLA	C16-C17-C18-C19
36	j	319	DGD	CEB-CFB-CGB-CHB
29	B	809	CLA	C13-C15-C16-C17
29	L	207	CLA	O1D-CGD-O2D-CED
35	A	853	SQD	C24-C23-O48-C46
31	f	619	LHG	O6-C4-C5-O7
31	b	318	LHG	C28-C29-C30-C31
31	m	619	LHG	C29-C30-C31-C32
29	f	607	CLA	C4-C3-C5-C6
29	c	307	CLA	O1A-CGA-O2A-C1
29	e	302	CLA	O1D-CGD-O2D-CED
29	A	851	CLA	C2-C3-C5-C6
31	A	842	LHG	C10-C11-C12-C13
37	F	206	LMG	C21-C22-C23-C24
29	b	312	CLA	C8-C10-C11-C12
31	J	104	LHG	C24-C25-C26-C27
32	A	845	WVN	C23-C25-C28-C30
32	A	846	WVN	C19-C22-C26-C29
32	A	846	WVN	C33-C34-C37-C40
32	l	302	WVN	C33-C34-C37-C40
37	b	319	LMG	C2-C1-O1-C7
38	l	314	II0	C34-C36-C40-C42
38	g	318	II0	C33-C35-C39-C41
37	F	208	LMG	O1-C7-C8-O7
31	A	843	LHG	C3-O3-P-O6
31	A	848	LHG	C3-O3-P-O6
31	J	104	LHG	C3-O3-P-O6
31	c	316	LHG	C3-O3-P-O6
31	c	320	LHG	C4-O6-P-O3
31	j	318	LHG	C3-O3-P-O6
33	i	301	LMU	C11-C10-C9-C8
29	d	302	CLA	C13-C15-C16-C17
31	i	317	LHG	C24-C25-C26-C27
29	i	312	CLA	C16-C17-C18-C19
29	F	202	CLA	C10-C11-C12-C13
36	j	319	DGD	O1G-C1G-C2G-C3G
37	O	205	LMG	O1-C7-C8-C9
37	n	620	LMG	O1-C7-C8-C9
29	A	805	CLA	C6-C7-C8-C10
29	B	826	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	s	402	CLA	C6-C7-C8-C10
29	a	311	CLA	C12-C13-C15-C16
29	k	602	CLA	C6-C7-C8-C10
29	b	312	CLA	C3-C5-C6-C7
29	h	306	CLA	C3-C5-C6-C7
29	k	604	CLA	C2C-C3C-CAC-CBC
29	A	819	CLA	C14-C13-C15-C16
29	A	835	CLA	C6-C7-C8-C9
29	A	840	CLA	C11-C10-C8-C9
29	B	801	CLA	C6-C7-C8-C9
29	B	816	CLA	C11-C12-C13-C14
29	B	823	CLA	C6-C7-C8-C9
29	B	825	CLA	C11-C10-C8-C9
29	B	841	CLA	C14-C13-C15-C16
29	s	402	CLA	C11-C10-C8-C9
29	a	308	CLA	C11-C12-C13-C14
29	b	305	CLA	C6-C7-C8-C9
29	m	606	CLA	C11-C12-C13-C14
29	m	609	CLA	C11-C10-C8-C9
29	j	305	CLA	C6-C7-C8-C9
29	g	309	CLA	C14-C13-C15-C16
30	B	843	PQN	C21-C22-C23-C24
38	a	313	II0	C26-C30-C32-C34
38	h	309	II0	C36-C40-C42-C41
29	A	817	CLA	C8-C10-C11-C12
29	e	302	CLA	C13-C15-C16-C17
29	g	305	CLA	C10-C11-C12-C13
29	m	604	CLA	C4C-C3C-CAC-CBC
29	B	841	CLA	C16-C17-C18-C19
37	F	208	LMG	C18-C19-C20-C21
37	b	319	LMG	C17-C18-C19-C20
31	a	318	LHG	C11-C12-C13-C14
29	a	303	CLA	C11-C10-C8-C7
29	l	310	CLA	C12-C13-C15-C16
29	i	308	CLA	C5-C6-C7-C8
29	A	826	CLA	C2-C3-C5-C6
29	A	840	CLA	C2-C3-C5-C6
29	A	816	CLA	CBA-CGA-O2A-C1
29	O	201	CLA	CBA-CGA-O2A-C1
29	f	603	CLA	CBA-CGA-O2A-C1
40	g	314	KC2	C2B-C3B-CAB-CBB
29	c	306	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	A	816	CLA	O1A-CGA-O2A-C1
31	A	842	LHG	C24-C23-O8-C6
29	A	810	CLA	C4B-C3B-CAB-CBB
29	A	828	CLA	C4B-C3B-CAB-CBB
29	B	806	CLA	C4B-C3B-CAB-CBB
29	B	810	CLA	C4B-C3B-CAB-CBB
29	B	822	CLA	C4B-C3B-CAB-CBB
29	B	823	CLA	C4B-C3B-CAB-CBB
29	B	831	CLA	C4B-C3B-CAB-CBB
29	B	834	CLA	C4B-C3B-CAB-CBB
29	O	202	CLA	C4B-C3B-CAB-CBB
29	K	101	CLA	C4B-C3B-CAB-CBB
29	c	309	CLA	C4B-C3B-CAB-CBB
29	c	311	CLA	C4B-C3B-CAB-CBB
29	c	312	CLA	C4B-C3B-CAB-CBB
29	a	304	CLA	C4B-C3B-CAB-CBB
29	a	310	CLA	C4B-C3B-CAB-CBB
29	a	312	CLA	C4B-C3B-CAB-CBB
29	b	305	CLA	C4B-C3B-CAB-CBB
29	b	312	CLA	C4B-C3B-CAB-CBB
29	h	312	CLA	C4B-C3B-CAB-CBB
29	m	601	CLA	C4B-C3B-CAB-CBB
29	m	609	CLA	C4B-C3B-CAB-CBB
29	e	307	CLA	C4B-C3B-CAB-CBB
29	l	309	CLA	C4B-C3B-CAB-CBB
29	k	607	CLA	C4B-C3B-CAB-CBB
29	i	305	CLA	C4B-C3B-CAB-CBB
29	i	307	CLA	C4B-C3B-CAB-CBB
29	j	306	CLA	C4B-C3B-CAB-CBB
29	j	310	CLA	C4B-C3B-CAB-CBB
29	d	304	CLA	C4B-C3B-CAB-CBB
29	n	604	CLA	C4B-C3B-CAB-CBB
29	A	811	CLA	C2A-CAA-CBA-CGA
29	B	807	CLA	C2A-CAA-CBA-CGA
29	c	304	CLA	C2A-CAA-CBA-CGA
29	c	311	CLA	C2A-CAA-CBA-CGA
29	k	604	CLA	C2A-CAA-CBA-CGA
29	j	305	CLA	C2A-CAA-CBA-CGA
29	B	817	CLA	C16-C17-C18-C19
32	A	845	WVN	C22-C26-C29-C31
32	F	205	WVN	C32-C36-C39-C40
32	L	201	WVN	C32-C36-C39-C40

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Mol	Chain	Res	Type	Atoms
32	K	103	WVN	C32-C36-C39-C40
38	c	313	II0	C35-C39-C41-C42
38	i	319	II0	C35-C39-C41-C42
38	g	318	II0	C35-C39-C41-C42
31	l	318	LHG	O6-C4-C5-O7
29	O	201	CLA	O1A-CGA-O2A-C1
31	L	208	LHG	C16-C17-C18-C19
29	m	606	CLA	CAA-CBA-CGA-O2A
40	d	312	KC2	C4B-C3B-CAB-CBB
40	g	314	KC2	C4B-C3B-CAB-CBB
29	B	814	CLA	C3-C5-C6-C7
29	K	101	CLA	C4-C3-C5-C6
29	h	305	CLA	C4-C3-C5-C6
29	a	306	CLA	C4C-C3C-CAC-CBC
29	h	305	CLA	C2-C3-C5-C6
29	f	603	CLA	O1A-CGA-O2A-C1
31	A	848	LHG	C9-C10-C11-C12
29	e	302	CLA	C2-C1-O2A-CGA
29	g	304	CLA	C2-C1-O2A-CGA
29	A	802	CLA	C8-C10-C11-C12
29	i	307	CLA	C5-C6-C7-C8
38	O	203	II0	C28-C26-C30-C32
29	j	305	CLA	C2C-C3C-CAC-CBC
29	A	814	CLA	C2A-CAA-CBA-CGA
29	B	813	CLA	C2A-CAA-CBA-CGA
29	a	308	CLA	C2A-CAA-CBA-CGA
29	b	305	CLA	C2A-CAA-CBA-CGA
29	b	308	CLA	C2A-CAA-CBA-CGA
29	m	609	CLA	C2A-CAA-CBA-CGA
29	f	609	CLA	C2A-CAA-CBA-CGA
29	j	303	CLA	C2A-CAA-CBA-CGA
29	n	608	CLA	C2A-CAA-CBA-CGA
37	L	210	LMG	C20-C21-C22-C23
31	L	209	LHG	C5-C4-O6-P
29	A	827	CLA	C3A-C2A-CAA-CBA
29	B	809	CLA	C3A-C2A-CAA-CBA
29	B	816	CLA	C3A-C2A-CAA-CBA
29	s	402	CLA	C3A-C2A-CAA-CBA
29	s	406	CLA	C3A-C2A-CAA-CBA
29	d	313	CLA	C3A-C2A-CAA-CBA
29	n	613	CLA	C3A-C2A-CAA-CBA
29	e	301	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
38	e	316	II0	C10-C22-C24-C26
39	a	316	IHT	C11-C21-C24-C26
36	B	844	DGD	O2G-C1B-C2B-C3B
29	A	810	CLA	C6-C7-C8-C9
29	A	817	CLA	C11-C10-C8-C9
29	B	817	CLA	C14-C13-C15-C16
29	B	824	CLA	C14-C13-C15-C16
29	a	311	CLA	C14-C13-C15-C16
29	e	302	CLA	C11-C12-C13-C14
29	e	311	CLA	C14-C13-C15-C16
29	l	306	CLA	C14-C13-C15-C16
29	k	608	CLA	C11-C10-C8-C9
29	i	312	CLA	C11-C12-C13-C14
29	j	314	CLA	C11-C12-C13-C14
29	Q	302	CLA	C11-C12-C13-C14
30	B	843	PQN	C16-C17-C18-C19
29	B	841	CLA	C16-C17-C18-C20
29	m	609	CLA	C11-C12-C13-C14
29	l	304	CLA	C16-C17-C18-C20
29	l	301	CLA	C10-C11-C12-C13
31	m	619	LHG	C7-C8-C9-C10
32	B	845	WVN	C27-C25-C28-C30
32	F	205	WVN	C35-C32-C36-C39
38	O	203	II0	C37-C35-C39-C41
39	g	324	IHT	C25-C23-C27-C30
37	b	319	LMG	O9-C10-O7-C8
29	A	805	CLA	C15-C16-C17-C18
29	B	834	CLA	CBA-CGA-O2A-C1
37	n	620	LMG	O6-C1-O1-C7
31	a	318	LHG	C32-C33-C34-C35
39	b	316	IHT	C18-C22-C23-C25
29	f	604	CLA	C8-C10-C11-C12
29	A	803	CLA	C4-C3-C5-C6
29	B	820	CLA	C4-C3-C5-C6
29	A	812	CLA	C1A-C2A-CAA-CBA
29	A	829	CLA	C1A-C2A-CAA-CBA
29	A	850	CLA	C1A-C2A-CAA-CBA
29	B	812	CLA	C1A-C2A-CAA-CBA
29	B	816	CLA	C1A-C2A-CAA-CBA
29	B	824	CLA	C1A-C2A-CAA-CBA
29	L	207	CLA	C1A-C2A-CAA-CBA
29	a	311	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	m	607	CLA	C1A-C2A-CAA-CBA
29	e	311	CLA	C1A-C2A-CAA-CBA
29	l	303	CLA	C1A-C2A-CAA-CBA
29	l	309	CLA	C1A-C2A-CAA-CBA
29	l	310	CLA	C1A-C2A-CAA-CBA
29	k	601	CLA	C1A-C2A-CAA-CBA
29	j	303	CLA	C1A-C2A-CAA-CBA
29	d	318	CLA	C1A-C2A-CAA-CBA
29	n	605	CLA	C1A-C2A-CAA-CBA
29	A	804	CLA	C11-C10-C8-C7
29	B	806	CLA	C12-C13-C15-C16
29	B	819	CLA	C11-C10-C8-C7
29	K	101	CLA	C11-C12-C13-C15
29	b	308	CLA	C11-C12-C13-C15
29	b	311	CLA	C6-C7-C8-C10
29	b	312	CLA	C6-C7-C8-C10
29	i	303	CLA	C6-C7-C8-C10
29	i	311	CLA	C6-C7-C8-C10
29	d	302	CLA	C11-C10-C8-C7
29	g	304	CLA	C6-C7-C8-C10
29	g	306	CLA	C6-C7-C8-C10
29	d	303	CLA	O1A-CGA-O2A-C1
31	g	322	LHG	C30-C31-C32-C33
37	F	206	LMG	C39-C40-C41-C42
32	B	849	WVN	C32-C36-C39-C40
32	i	315	WVN	C25-C28-C30-C33
38	f	616	II0	C35-C39-C41-C42
38	g	319	II0	C25-C29-C31-C33
29	A	817	CLA	CAA-CBA-CGA-O2A
29	j	311	CLA	CAA-CBA-CGA-O2A
29	e	302	CLA	CBA-CGA-O2A-C1
29	e	301	CLA	CAA-CBA-CGA-O2A
33	i	301	LMU	C3-C4-C5-C6
29	A	802	CLA	C3-C5-C6-C7
29	A	813	CLA	C3-C5-C6-C7
29	A	851	CLA	C2A-CAA-CBA-CGA
29	B	825	CLA	C2A-CAA-CBA-CGA
29	B	828	CLA	C2A-CAA-CBA-CGA
29	h	305	CLA	C2A-CAA-CBA-CGA
29	n	610	CLA	C10-C11-C12-C13
31	b	318	LHG	C7-C8-C9-C10
31	e	317	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
28	A	801	CL0	CAA-CBA-CGA-O2A
29	k	608	CLA	C8-C10-C11-C12
29	d	303	CLA	CBA-CGA-O2A-C1
40	g	314	KC2	C3A-C2A-CAA-CBA
31	c	316	LHG	C11-C10-C9-C8
29	f	604	CLA	C13-C15-C16-C17
31	e	317	LHG	C30-C31-C32-C33
29	F	203	CLA	C4-C3-C5-C6
29	g	309	CLA	C15-C16-C17-C18
29	B	825	CLA	C2-C3-C5-C6
29	F	203	CLA	C2-C3-C5-C6
29	A	828	CLA	C2B-C3B-CAB-CBB
29	A	829	CLA	C2B-C3B-CAB-CBB
29	A	838	CLA	C2B-C3B-CAB-CBB
29	B	822	CLA	C2B-C3B-CAB-CBB
29	B	834	CLA	C2B-C3B-CAB-CBB
29	B	835	CLA	C2B-C3B-CAB-CBB
29	B	837	CLA	C2B-C3B-CAB-CBB
29	L	203	CLA	C2B-C3B-CAB-CBB
29	c	301	CLA	C2B-C3B-CAB-CBB
29	b	310	CLA	C2B-C3B-CAB-CBB
29	h	305	CLA	C2B-C3B-CAB-CBB
29	m	609	CLA	C2B-C3B-CAB-CBB
29	e	307	CLA	C2B-C3B-CAB-CBB
29	l	309	CLA	C2B-C3B-CAB-CBB
29	l	312	CLA	C2B-C3B-CAB-CBB
29	k	607	CLA	C2B-C3B-CAB-CBB
29	f	607	CLA	C2B-C3B-CAB-CBB
29	m	606	CLA	C15-C16-C17-C18
29	j	311	CLA	C3-C5-C6-C7
31	A	848	LHG	C5-C4-O6-P
38	O	203	II0	C33-C35-C39-C41
38	d	301	II0	C34-C36-C40-C42
31	m	619	LHG	C24-C23-O8-C6
29	c	305	CLA	CAA-CBA-CGA-O2A
29	B	841	CLA	C4C-C3C-CAC-CBC
32	B	846	WVN	C32-C36-C39-C40
38	b	301	II0	C35-C39-C41-C42
29	d	318	CLA	CAA-CBA-CGA-O1A
29	O	206	CLA	C10-C11-C12-C13
37	n	620	LMG	C38-C39-C40-C41
29	A	819	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	n	607	CLA	C8-C10-C11-C12
29	e	302	CLA	O1A-CGA-O2A-C1
31	J	104	LHG	C1-C2-C3-O3
29	j	306	CLA	CAA-CBA-CGA-O2A
29	d	318	CLA	CAA-CBA-CGA-O2A
29	F	201	CLA	C4-C3-C5-C6
29	B	825	CLA	C2-C1-O2A-CGA
29	B	837	CLA	C2-C1-O2A-CGA
29	b	302	CLA	C2-C1-O2A-CGA
29	j	308	CLA	C2-C1-O2A-CGA
31	a	318	LHG	C17-C18-C19-C20
29	B	825	CLA	C15-C16-C17-C18
29	A	835	CLA	C14-C13-C15-C16
29	e	307	CLA	C15-C16-C17-C18
29	L	207	CLA	C4-C3-C5-C6
29	j	304	CLA	C4-C3-C5-C6
31	n	619	LHG	C33-C34-C35-C36
37	O	205	LMG	O9-C10-O7-C8
29	n	610	CLA	C8-C10-C11-C12
29	a	307	CLA	C2A-CAA-CBA-CGA
29	l	309	CLA	C2A-CAA-CBA-CGA
32	A	845	WVN	C06-C13-C20-C23
39	c	315	IHT	C02-C07-C18-C22
29	i	308	CLA	CAA-CBA-CGA-O2A
37	L	210	LMG	O1-C7-C8-C9
29	A	832	CLA	C5-C6-C7-C8
36	B	844	DGD	C9B-CAB-CBB-CCB
38	m	614	II0	C26-C30-C32-C34
38	m	614	II0	C35-C39-C41-C42
31	g	301	LHG	C33-C34-C35-C36
29	j	302	CLA	C4-C3-C5-C6
29	g	316	CLA	C4-C3-C5-C6
29	J	102	CLA	C1A-C2A-CAA-CBA
37	b	319	LMG	C34-C35-C36-C37
29	A	809	CLA	C2-C3-C5-C6
29	B	810	CLA	C2-C3-C5-C6
36	B	844	DGD	C8B-C9B-CAB-CBB
29	A	818	CLA	C8-C10-C11-C12
29	B	840	CLA	C13-C15-C16-C17
37	F	208	LMG	C8-C7-O1-C1
31	A	848	LHG	C10-C11-C12-C13
29	A	802	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	A	840	CLA	CAA-CBA-CGA-O2A
29	l	306	CLA	C15-C16-C17-C18
29	f	608	CLA	C5-C6-C7-C8
29	n	609	CLA	C13-C15-C16-C17
31	c	316	LHG	O6-C4-C5-O7
31	n	619	LHG	O6-C4-C5-O7
37	L	210	LMG	C31-C32-C33-C34
29	j	303	CLA	O1D-CGD-O2D-CED
29	A	809	CLA	C2A-CAA-CBA-CGA
29	d	308	CLA	C2A-CAA-CBA-CGA
29	Q	302	CLA	C2A-CAA-CBA-CGA
29	j	308	CLA	CAA-CBA-CGA-O2A
31	c	320	LHG	C19-C20-C21-C22
29	A	803	CLA	C4B-C3B-CAB-CBB
29	B	809	CLA	C4B-C3B-CAB-CBB
29	B	842	CLA	C4B-C3B-CAB-CBB
29	h	305	CLA	C4B-C3B-CAB-CBB
29	l	312	CLA	C4B-C3B-CAB-CBB
29	k	614	CLA	C4B-C3B-CAB-CBB
29	f	609	CLA	C4B-C3B-CAB-CBB
29	f	612	CLA	C4B-C3B-CAB-CBB
29	R	203	CLA	C4B-C3B-CAB-CBB
29	d	305	CLA	CAA-CBA-CGA-O2A
29	L	203	CLA	C4-C3-C5-C6
29	L	204	CLA	C4-C3-C5-C6
29	m	613	CLA	C4-C3-C5-C6
29	i	303	CLA	C4-C3-C5-C6
29	i	307	CLA	C4-C3-C5-C6
29	g	302	CLA	C4-C3-C5-C6
29	A	818	CLA	C12-C13-C15-C16
29	B	806	CLA	C6-C7-C8-C10
29	B	820	CLA	C2-C3-C5-C6
29	B	841	CLA	C2-C3-C5-C6
29	l	304	CLA	C12-C13-C15-C16
29	l	306	CLA	C2-C3-C5-C6
29	A	829	CLA	CBA-CGA-O2A-C1
29	e	311	CLA	C5-C6-C7-C8
32	A	854	WVN	C32-C36-C39-C40
38	J	103	II0	C35-C39-C41-C42
37	O	205	LMG	O1-C7-C8-O7
37	F	206	LMG	C29-C28-O8-C9
29	j	306	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	B	842	CLA	CAA-CBA-CGA-O2A
29	s	406	CLA	CAA-CBA-CGA-O2A
33	A	849	LMU	C1-C2-C3-C4
31	a	318	LHG	C34-C35-C36-C37
28	A	801	CL0	C15-C16-C17-C18
36	j	319	DGD	CBA-CCA-CDA-CEA
29	i	307	CLA	CBA-CGA-O2A-C1
31	g	322	LHG	C24-C23-O8-C6
32	F	204	WVN	C35-C32-C36-C39
29	d	308	CLA	CAA-CBA-CGA-O2A
29	A	827	CLA	C4-C3-C5-C6
29	B	822	CLA	C4-C3-C5-C6
29	a	308	CLA	C4-C3-C5-C6
29	f	610	CLA	C4C-C3C-CAC-CBC
31	J	104	LHG	C4-O6-P-O3
29	b	312	CLA	C2-C3-C5-C6
29	f	607	CLA	C2-C3-C5-C6
31	c	320	LHG	O8-C23-C24-C25
29	A	816	CLA	C11-C10-C8-C9
29	A	831	CLA	C14-C13-C15-C16
29	B	806	CLA	C14-C13-C15-C16
29	B	808	CLA	C14-C13-C15-C16
29	B	825	CLA	C14-C13-C15-C16
29	F	201	CLA	C11-C10-C8-C9
29	c	302	CLA	C6-C7-C8-C9
29	c	304	CLA	C14-C13-C15-C16
29	b	306	CLA	C6-C7-C8-C9
29	b	308	CLA	C14-C13-C15-C16
29	b	311	CLA	C6-C7-C8-C9
29	m	606	CLA	C14-C13-C15-C16
29	k	602	CLA	C6-C7-C8-C9
29	f	607	CLA	C11-C10-C8-C9
29	f	610	CLA	C11-C12-C13-C14
29	i	311	CLA	C6-C7-C8-C9
31	f	619	LHG	C33-C34-C35-C36
31	e	317	LHG	C9-C10-C11-C12
29	A	812	CLA	C3A-C2A-CAA-CBA
29	A	815	CLA	C3A-C2A-CAA-CBA
29	A	819	CLA	C3A-C2A-CAA-CBA
29	A	850	CLA	C3A-C2A-CAA-CBA
29	B	824	CLA	C3A-C2A-CAA-CBA
29	h	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	e	311	CLA	C3A-C2A-CAA-CBA
29	j	309	CLA	C3A-C2A-CAA-CBA
29	Q	302	CLA	C3A-C2A-CAA-CBA
29	g	304	CLA	O1D-CGD-O2D-CED
29	A	829	CLA	O1A-CGA-O2A-C1
29	i	307	CLA	O1A-CGA-O2A-C1
29	B	801	CLA	CAA-CBA-CGA-O2A
29	A	806	CLA	CAD-CBD-CGD-O2D
29	A	812	CLA	CAD-CBD-CGD-O2D
29	A	821	CLA	CAD-CBD-CGD-O2D
29	A	834	CLA	CAD-CBD-CGD-O2D
29	A	835	CLA	CAD-CBD-CGD-O2D
29	B	802	CLA	CAD-CBD-CGD-O2D
29	B	813	CLA	CAD-CBD-CGD-O2D
29	B	819	CLA	CAD-CBD-CGD-O2D
29	B	828	CLA	CAD-CBD-CGD-O2D
29	a	308	CLA	CAD-CBD-CGD-O2D
29	b	308	CLA	CAD-CBD-CGD-O2D
29	h	307	CLA	CAD-CBD-CGD-O2D
29	h	312	CLA	CAD-CBD-CGD-O2D
29	m	613	CLA	CAD-CBD-CGD-O2D
29	e	302	CLA	CAD-CBD-CGD-O2D
29	e	303	CLA	CAD-CBD-CGD-O2D
29	e	310	CLA	CAD-CBD-CGD-O2D
29	k	602	CLA	CAD-CBD-CGD-O2D
29	k	614	CLA	CAD-CBD-CGD-O2D
29	f	603	CLA	CAD-CBD-CGD-O2D
29	f	606	CLA	CAD-CBD-CGD-O2D
29	f	612	CLA	CAD-CBD-CGD-O2D
29	f	613	CLA	CAD-CBD-CGD-O2D
29	i	311	CLA	CAD-CBD-CGD-O2D
29	d	305	CLA	CAD-CBD-CGD-O2D
29	g	302	CLA	CAD-CBD-CGD-O2D
29	R	203	CLA	CAD-CBD-CGD-O2D
40	d	311	KC2	C2B-C3B-CAB-CBB
40	g	314	KC2	CAD-CBD-CGD-O2D
40	n	612	KC2	CAD-CBD-CGD-O2D
29	A	835	CLA	C2A-CAA-CBA-CGA
29	s	406	CLA	CBD-CGD-O2D-CED
36	j	319	DGD	C7A-C8A-C9A-CAA
37	c	317	LMG	C38-C39-C40-C41
29	a	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	m	610	CLA	CAA-CBA-CGA-O2A
29	e	304	CLA	CAA-CBA-CGA-O2A
37	n	620	LMG	O8-C28-C29-C30
29	B	810	CLA	C4-C3-C5-C6
29	b	308	CLA	C4-C3-C5-C6
29	f	602	CLA	C16-C17-C18-C19
29	B	822	CLA	C3-C5-C6-C7
32	A	847	WVN	C29-C31-C32-C36
38	b	315	II0	C32-C34-C36-C40
38	h	310	II0	C32-C34-C36-C40
38	d	315	II0	C31-C33-C35-C39
31	c	316	LHG	C4-C5-C6-O8
29	A	812	CLA	CAA-CBA-CGA-O2A
29	s	402	CLA	CAA-CBA-CGA-O2A
29	A	827	CLA	O2A-C1-C2-C3
29	B	831	CLA	O2A-C1-C2-C3
29	B	841	CLA	O2A-C1-C2-C3
29	h	301	CLA	O2A-C1-C2-C3
29	m	610	CLA	O2A-C1-C2-C3
40	e	309	KC2	C4B-C3B-CAB-CBB
40	e	309	KC2	C4C-C3C-CAC-CBC
40	j	312	KC2	C4C-C3C-CAC-CBC
40	d	311	KC2	C4B-C3B-CAB-CBB
40	d	311	KC2	C4C-C3C-CAC-CBC
40	g	314	KC2	C4C-C3C-CAC-CBC
29	B	825	CLA	C10-C11-C12-C13
31	J	104	LHG	O2-C2-C3-O3
31	c	316	LHG	C11-C12-C13-C14
29	A	824	CLA	O1A-CGA-O2A-C1
29	A	802	CLA	CHA-CBD-CGD-O1D
29	A	802	CLA	CHA-CBD-CGD-O2D
29	A	803	CLA	CHA-CBD-CGD-O1D
29	A	807	CLA	CHA-CBD-CGD-O1D
29	A	807	CLA	CHA-CBD-CGD-O2D
29	A	810	CLA	CHA-CBD-CGD-O1D
29	A	810	CLA	CHA-CBD-CGD-O2D
29	A	814	CLA	CHA-CBD-CGD-O2D
29	A	819	CLA	CHA-CBD-CGD-O2D
29	A	832	CLA	CHA-CBD-CGD-O2D
29	A	835	CLA	CHA-CBD-CGD-O1D
29	B	812	CLA	CHA-CBD-CGD-O1D
29	B	833	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	B	837	CLA	CHA-CBD-CGD-O1D
29	B	837	CLA	CHA-CBD-CGD-O2D
29	B	842	CLA	CHA-CBD-CGD-O1D
29	F	203	CLA	CHA-CBD-CGD-O1D
29	K	102	CLA	CHA-CBD-CGD-O1D
29	K	102	CLA	CHA-CBD-CGD-O2D
29	c	301	CLA	CHA-CBD-CGD-O1D
29	c	301	CLA	CHA-CBD-CGD-O2D
29	a	307	CLA	CHA-CBD-CGD-O1D
29	a	307	CLA	CHA-CBD-CGD-O2D
29	b	302	CLA	CHA-CBD-CGD-O2D
29	b	312	CLA	CHA-CBD-CGD-O2D
29	m	601	CLA	CHA-CBD-CGD-O2D
29	m	605	CLA	CHA-CBD-CGD-O1D
29	l	304	CLA	CHA-CBD-CGD-O2D
29	k	605	CLA	CHA-CBD-CGD-O2D
29	k	608	CLA	CHA-CBD-CGD-O1D
29	f	605	CLA	CHA-CBD-CGD-O1D
29	f	605	CLA	CHA-CBD-CGD-O2D
29	f	608	CLA	CHA-CBD-CGD-O2D
29	i	304	CLA	CHA-CBD-CGD-O2D
29	i	308	CLA	CHA-CBD-CGD-O1D
29	j	306	CLA	CHA-CBD-CGD-O1D
29	j	306	CLA	CHA-CBD-CGD-O2D
29	d	303	CLA	CHA-CBD-CGD-O1D
29	d	303	CLA	CHA-CBD-CGD-O2D
29	n	603	CLA	CHA-CBD-CGD-O2D
29	n	605	CLA	CHA-CBD-CGD-O1D
29	n	605	CLA	CHA-CBD-CGD-O2D
29	n	607	CLA	CHA-CBD-CGD-O1D
29	n	610	CLA	CHA-CBD-CGD-O1D
29	n	610	CLA	CHA-CBD-CGD-O2D
32	I	101	WVN	C34-C37-C40-C39
38	d	316	II0	C26-C30-C32-C34
40	c	310	KC2	CHA-CBD-CGD-O1D
40	c	310	KC2	CHA-CBD-CGD-O2D
40	f	611	KC2	CHA-CBD-CGD-O1D
40	f	611	KC2	CHA-CBD-CGD-O2D
40	i	310	KC2	CHA-CBD-CGD-O1D
40	i	310	KC2	CHA-CBD-CGD-O2D
40	d	311	KC2	CHA-CBD-CGD-O1D
40	d	311	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
40	g	313	KC2	CHA-CBD-CGD-O2D
29	d	304	CLA	CAA-CBA-CGA-O2A
37	b	319	LMG	O8-C28-C29-C30
29	B	818	CLA	CBA-CGA-O2A-C1
29	g	316	CLA	C2-C3-C5-C6
35	A	853	SQD	C10-C11-C12-C13
29	e	304	CLA	C3-C5-C6-C7
29	A	829	CLA	C15-C16-C17-C18
29	B	839	CLA	CAA-CBA-CGA-O1A
31	a	301	LHG	O6-C4-C5-C6
31	g	301	LHG	O6-C4-C5-C6
32	B	845	WVN	C23-C25-C28-C30
32	F	207	WVN	C19-C22-C26-C29
32	L	201	WVN	C23-C25-C28-C30
38	e	313	II0	C34-C36-C40-C42
39	g	324	IHT	C22-C23-C27-C30
29	j	304	CLA	CAA-CBA-CGA-O2A
31	A	848	LHG	O7-C7-C8-C9
31	L	209	LHG	O8-C23-C24-C25
31	a	318	LHG	C33-C34-C35-C36
33	i	301	LMU	C6-C7-C8-C9
31	b	318	LHG	O7-C5-C6-O8
31	c	316	LHG	C23-C24-C25-C26
37	L	210	LMG	C24-C25-C26-C27
29	m	604	CLA	C10-C11-C12-C13
29	s	406	CLA	O1D-CGD-O2D-CED
29	A	831	CLA	C5-C6-C7-C8
29	B	806	CLA	CAA-CBA-CGA-O2A
29	B	820	CLA	CAA-CBA-CGA-O2A
29	B	837	CLA	CAA-CBA-CGA-O2A
29	m	608	CLA	CAA-CBA-CGA-O2A
29	k	604	CLA	CAA-CBA-CGA-O2A
29	g	302	CLA	CAA-CBA-CGA-O2A
29	g	311	CLA	C2A-CAA-CBA-CGA
29	d	304	CLA	CAA-CBA-CGA-O1A
29	A	838	CLA	C15-C16-C17-C18
29	f	604	CLA	C10-C11-C12-C13
29	g	309	CLA	C8-C10-C11-C12
29	B	805	CLA	CAA-CBA-CGA-O1A
29	A	822	CLA	CAA-CBA-CGA-O2A
29	h	303	CLA	CAA-CBA-CGA-O2A
29	n	605	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	A	842	LHG	C33-C34-C35-C36
29	A	824	CLA	C12-C13-C15-C16
29	B	805	CLA	C11-C12-C13-C15
29	B	838	CLA	C11-C10-C8-C7
29	L	203	CLA	C2-C3-C5-C6
29	L	204	CLA	C2-C3-C5-C6
29	c	308	CLA	C6-C7-C8-C10
29	f	609	CLA	C6-C7-C8-C10
29	g	305	CLA	C12-C13-C15-C16
29	m	609	CLA	C11-C12-C13-C15
31	a	318	LHG	O8-C23-C24-C25
29	A	826	CLA	C6-C7-C8-C9
29	B	838	CLA	C11-C10-C8-C9
29	F	202	CLA	C6-C7-C8-C9
29	K	101	CLA	C11-C12-C13-C14
29	c	312	CLA	C11-C10-C8-C9
29	a	307	CLA	C11-C12-C13-C14
29	b	306	CLA	C14-C13-C15-C16
29	h	305	CLA	C11-C12-C13-C14
29	h	312	CLA	C11-C10-C8-C9
29	d	302	CLA	C11-C10-C8-C9
29	g	306	CLA	C6-C7-C8-C9
31	f	620	LHG	C23-C24-C25-C26
31	c	316	LHG	C5-C6-O8-C23
31	c	320	LHG	O10-C23-C24-C25
29	A	836	CLA	C2B-C3B-CAB-CBB
29	B	809	CLA	C2B-C3B-CAB-CBB
29	B	842	CLA	C2B-C3B-CAB-CBB
29	a	303	CLA	C2B-C3B-CAB-CBB
29	a	312	CLA	C2B-C3B-CAB-CBB
29	f	609	CLA	C2B-C3B-CAB-CBB
29	j	304	CLA	C2B-C3B-CAB-CBB
31	f	619	LHG	C29-C30-C31-C32
29	A	840	CLA	C13-C15-C16-C17
31	s	408	LHG	O7-C7-C8-C9
37	L	210	LMG	C17-C18-C19-C20
29	j	302	CLA	O1A-CGA-O2A-C1
37	F	206	LMG	C29-C30-C31-C32
29	B	803	CLA	C5-C6-C7-C8
29	b	313	CLA	C2A-CAA-CBA-CGA
31	s	408	LHG	O9-C7-C8-C9
31	f	619	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	i	317	LHG	O9-C7-C8-C9
37	L	210	LMG	O10-C28-C29-C30
29	B	834	CLA	C15-C16-C17-C18
29	f	602	CLA	C16-C17-C18-C20
29	n	613	CLA	O1A-CGA-O2A-C1
31	A	842	LHG	O10-C23-C24-C25
29	A	824	CLA	CBA-CGA-O2A-C1
29	j	302	CLA	CBA-CGA-O2A-C1
29	A	834	CLA	C10-C11-C12-C13
29	n	605	CLA	C2C-C3C-CAC-CBC
36	j	319	DGD	C5A-C6A-C7A-C8A
29	A	802	CLA	C1A-C2A-CAA-CBA
29	A	815	CLA	C1A-C2A-CAA-CBA
29	A	819	CLA	C1A-C2A-CAA-CBA
29	A	821	CLA	C1A-C2A-CAA-CBA
29	A	823	CLA	C1A-C2A-CAA-CBA
29	A	839	CLA	C1A-C2A-CAA-CBA
29	B	822	CLA	C1A-C2A-CAA-CBA
29	B	833	CLA	C1A-C2A-CAA-CBA
29	h	305	CLA	C1A-C2A-CAA-CBA
29	f	609	CLA	C1A-C2A-CAA-CBA
29	j	307	CLA	C1A-C2A-CAA-CBA
29	j	309	CLA	C1A-C2A-CAA-CBA
29	Q	302	CLA	C1A-C2A-CAA-CBA
29	m	610	CLA	CAA-CBA-CGA-O1A
29	d	308	CLA	CAA-CBA-CGA-O1A
29	e	304	CLA	O1A-CGA-O2A-C1
29	m	609	CLA	C2-C1-O2A-CGA
29	j	310	CLA	C2-C1-O2A-CGA
29	g	311	CLA	C2-C1-O2A-CGA
37	F	208	LMG	C4-C5-C6-O5
29	e	304	CLA	CBA-CGA-O2A-C1
29	n	613	CLA	CBA-CGA-O2A-C1
29	s	402	CLA	CAA-CBA-CGA-O1A
29	h	303	CLA	CAA-CBA-CGA-O1A
31	b	318	LHG	O9-C7-C8-C9
29	A	802	CLA	C13-C15-C16-C17
29	k	608	CLA	C5-C6-C7-C8
29	a	305	CLA	C2A-CAA-CBA-CGA
29	i	306	CLA	C2A-CAA-CBA-CGA
29	d	302	CLA	C2A-CAA-CBA-CGA
29	g	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	806	CLA	CAA-CBA-CGA-O1A
29	B	820	CLA	CAA-CBA-CGA-O1A
29	a	310	CLA	CAA-CBA-CGA-O1A
29	A	824	CLA	C15-C16-C17-C18
29	g	311	CLA	C8-C10-C11-C12
29	B	841	CLA	C4-C3-C5-C6
29	l	306	CLA	C4-C3-C5-C6
29	B	801	CLA	CAA-CBA-CGA-O1A
29	K	101	CLA	C2-C3-C5-C6
29	g	302	CLA	C2-C3-C5-C6
29	A	817	CLA	C4B-C3B-CAB-CBB
29	A	829	CLA	C4B-C3B-CAB-CBB
29	B	817	CLA	C4B-C3B-CAB-CBB
29	c	304	CLA	C4B-C3B-CAB-CBB
31	A	848	LHG	C3-O3-P-O5
31	L	208	LHG	C4-O6-P-O4
31	c	320	LHG	C4-O6-P-O5
31	m	619	LHG	C4-O6-P-O4
31	j	318	LHG	C3-O3-P-O5
29	g	310	CLA	C16-C17-C18-C19
33	a	319	LMU	C9-C10-C11-C12
29	e	304	CLA	CAA-CBA-CGA-O1A
29	k	604	CLA	CAA-CBA-CGA-O1A
31	A	848	LHG	O9-C7-C8-C9
31	L	209	LHG	O10-C23-C24-C25
29	e	311	CLA	CAA-CBA-CGA-O2A
38	J	103	II0	C38-C36-C40-C42
31	a	301	LHG	C29-C30-C31-C32
31	a	318	LHG	C25-C26-C27-C28
40	s	401	KC2	CAA-CBA-CGA-O1A
29	b	313	CLA	C4C-C3C-CAC-CBC
29	B	838	CLA	C8-C10-C11-C12
29	a	305	CLA	C10-C11-C12-C13
29	h	305	CLA	C10-C11-C12-C13
29	A	812	CLA	CAA-CBA-CGA-O1A
29	j	304	CLA	CAA-CBA-CGA-O1A
29	B	834	CLA	O1A-CGA-O2A-C1
33	a	319	LMU	C4B-C5B-C6B-O6B
29	B	826	CLA	CAA-CBA-CGA-O2A
29	a	305	CLA	CAA-CBA-CGA-O2A
29	e	302	CLA	CAA-CBA-CGA-O2A
37	c	318	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	B	819	CLA	C16-C17-C18-C20
29	A	840	CLA	C2A-CAA-CBA-CGA
40	s	401	KC2	CAA-CBA-CGA-O2A
30	B	843	PQN	C25-C26-C27-C28
31	f	619	LHG	O9-C7-C8-C9
29	j	302	CLA	C2-C3-C5-C6
29	A	802	CLA	CAD-CBD-CGD-O1D
29	A	813	CLA	CAD-CBD-CGD-O1D
29	A	835	CLA	CAD-CBD-CGD-O1D
29	B	801	CLA	CAD-CBD-CGD-O1D
29	B	807	CLA	CAD-CBD-CGD-O1D
29	B	812	CLA	CAD-CBD-CGD-O1D
29	B	833	CLA	CAD-CBD-CGD-O1D
29	B	842	CLA	CAD-CBD-CGD-O1D
29	L	203	CLA	CAD-CBD-CGD-O1D
29	c	304	CLA	CAD-CBD-CGD-O1D
29	k	614	CLA	C2-C3-C5-C6
29	f	612	CLA	C2-C3-C5-C6
29	i	308	CLA	CAD-CBD-CGD-O1D
29	j	313	CLA	C2-C3-C5-C6
29	n	603	CLA	C2-C3-C5-C6
38	J	103	II0	C24-C26-C30-C32
38	m	618	II0	C24-C26-C30-C32
29	A	822	CLA	CAA-CBA-CGA-O1A
31	f	620	LHG	C24-C25-C26-C27
29	A	819	CLA	CAA-CBA-CGA-O2A
29	O	206	CLA	CAA-CBA-CGA-O2A
29	i	306	CLA	CAA-CBA-CGA-O2A
29	n	604	CLA	CAA-CBA-CGA-O2A
35	A	853	SQD	O47-C7-C8-C9
29	A	810	CLA	C11-C12-C13-C14
29	A	833	CLA	C6-C7-C8-C9
29	B	805	CLA	C11-C12-C13-C14
29	B	820	CLA	C11-C12-C13-C14
29	a	310	CLA	C11-C12-C13-C14
29	l	301	CLA	C14-C13-C15-C16
29	l	306	CLA	C11-C10-C8-C9
31	l	318	LHG	C25-C26-C27-C28
29	s	403	CLA	C5-C6-C7-C8
29	f	610	CLA	C15-C16-C17-C18
29	m	608	CLA	CAA-CBA-CGA-O1A
31	a	318	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
35	A	853	SQD	O49-C7-C8-C9
37	F	206	LMG	O9-C10-C11-C12
29	c	304	CLA	CAA-CBA-CGA-O2A
29	l	301	CLA	CAA-CBA-CGA-O2A
29	f	603	CLA	CAA-CBA-CGA-O2A
29	i	305	CLA	CAA-CBA-CGA-O2A
29	A	819	CLA	C5-C6-C7-C8
37	n	620	LMG	C16-C17-C18-C19
29	g	302	CLA	CAA-CBA-CGA-O1A
29	n	609	CLA	C2A-CAA-CBA-CGA
29	A	811	CLA	C5-C6-C7-C8
29	A	836	CLA	CAA-CBA-CGA-O2A
29	A	837	CLA	CAA-CBA-CGA-O2A
29	O	201	CLA	CAA-CBA-CGA-O2A
29	c	303	CLA	CAA-CBA-CGA-O2A
29	m	604	CLA	CAA-CBA-CGA-O2A
29	e	307	CLA	CAA-CBA-CGA-O2A
29	l	306	CLA	CAA-CBA-CGA-O2A
29	j	305	CLA	CAA-CBA-CGA-O2A
29	j	310	CLA	CAA-CBA-CGA-O2A
31	n	619	LHG	O7-C7-C8-C9
29	B	818	CLA	O1A-CGA-O2A-C1
29	j	307	CLA	O1A-CGA-O2A-C1
29	B	837	CLA	CAA-CBA-CGA-O1A
29	m	609	CLA	CAA-CBA-CGA-O1A
37	b	319	LMG	O10-C28-C29-C30
29	s	406	CLA	C4-C3-C5-C6
29	b	312	CLA	C4-C3-C5-C6
29	g	312	CLA	C4-C3-C5-C6
29	O	202	CLA	C15-C16-C17-C18
31	b	318	LHG	C34-C35-C36-C37
28	A	801	CL0	C11-C10-C8-C7
29	A	803	CLA	C2-C3-C5-C6
29	A	813	CLA	C3A-C2A-CAA-CBA
29	A	826	CLA	C11-C10-C8-C7
29	A	838	CLA	C11-C12-C13-C15
29	A	851	CLA	C11-C12-C13-C15
29	B	804	CLA	C11-C10-C8-C7
29	F	201	CLA	C2-C3-C5-C6
29	c	304	CLA	C11-C12-C13-C15
29	c	312	CLA	C11-C10-C8-C7
29	a	303	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
29	h	312	CLA	C11-C10-C8-C7
29	l	306	CLA	C11-C10-C8-C7
29	i	308	CLA	C11-C10-C8-C7
29	g	302	CLA	C6-C7-C8-C10
29	g	311	CLA	C6-C7-C8-C10
31	a	301	LHG	O6-C4-C5-O7
29	n	605	CLA	CAA-CBA-CGA-O1A
29	B	816	CLA	CAA-CBA-CGA-O2A
29	O	202	CLA	CAA-CBA-CGA-O2A
29	c	307	CLA	CAA-CBA-CGA-O2A
29	h	307	CLA	CAA-CBA-CGA-O2A
29	m	609	CLA	CAA-CBA-CGA-O2A
29	e	303	CLA	CAA-CBA-CGA-O2A
29	g	306	CLA	CAA-CBA-CGA-O2A
29	n	607	CLA	CAA-CBA-CGA-O2A
31	A	842	LHG	O8-C23-C24-C25
31	i	317	LHG	O7-C7-C8-C9
37	c	317	LMG	O7-C10-C11-C12
29	A	836	CLA	C3-C5-C6-C7
32	l	302	WVN	C11-C19-C22-C26
32	i	315	WVN	C30-C33-C34-C37
29	A	836	CLA	CAA-CBA-CGA-O1A
29	h	301	CLA	CAA-CBA-CGA-O1A
33	a	319	LMU	C2-C1-O1'-C1'
29	A	808	CLA	CAA-CBA-CGA-O2A
29	B	809	CLA	CAA-CBA-CGA-O2A
36	j	319	DGD	CAB-CBB-CCB-CDB
29	b	309	CLA	C10-C11-C12-C13
29	m	604	CLA	C13-C15-C16-C17
29	A	837	CLA	CAA-CBA-CGA-O1A
29	B	828	CLA	CAA-CBA-CGA-O1A
29	O	201	CLA	CAA-CBA-CGA-O1A
29	c	307	CLA	CAA-CBA-CGA-O1A
29	m	604	CLA	CAA-CBA-CGA-O1A
29	l	306	CLA	CAA-CBA-CGA-O1A
29	f	603	CLA	CAA-CBA-CGA-O1A
29	i	306	CLA	CAA-CBA-CGA-O1A
31	e	317	LHG	C31-C32-C33-C34
29	A	830	CLA	C5-C6-C7-C8
31	L	208	LHG	C31-C32-C33-C34
29	B	828	CLA	CAA-CBA-CGA-O2A
29	h	312	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	g	323	CLA	CAA-CBA-CGA-O2A
31	A	842	LHG	C17-C18-C19-C20
31	c	320	LHG	C10-C11-C12-C13
29	c	308	CLA	C8-C10-C11-C12
29	B	841	CLA	C5-C6-C7-C8
29	B	841	CLA	C13-C15-C16-C17
29	a	310	CLA	C15-C16-C17-C18
37	F	206	LMG	C10-C11-C12-C13
29	g	306	CLA	CAA-CBA-CGA-O1A
29	n	607	CLA	CAA-CBA-CGA-O1A
29	A	833	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

249 monomers are involved in 448 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	k	608	CLA	1	0
29	A	840	CLA	5	0
29	B	810	CLA	1	0
31	A	848	LHG	1	0
29	B	826	CLA	1	0
29	L	204	CLA	1	0
28	A	801	CL0	5	0
33	B	850	LMU	1	0
29	h	305	CLA	3	0
29	e	306	CLA	2	0
29	a	308	CLA	2	0
29	B	821	CLA	2	0
29	B	807	CLA	3	0
29	d	307	CLA	1	0
29	m	610	CLA	2	0
29	R	203	CLA	5	0
29	B	814	CLA	3	0
29	a	311	CLA	2	0
29	B	813	CLA	3	0
29	g	306	CLA	1	0
39	g	320	IHT	1	0
31	c	316	LHG	1	0
29	n	608	CLA	4	0
36	B	844	DGD	4	0
38	n	616	II0	1	0
29	A	816	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	g	311	CLA	2	0
29	A	828	CLA	1	0
29	a	303	CLA	1	0
29	L	203	CLA	4	0
38	n	614	II0	3	0
31	J	104	LHG	3	0
29	A	833	CLA	3	0
29	l	306	CLA	1	0
37	n	620	LMG	2	0
29	c	303	CLA	2	0
29	O	202	CLA	1	0
40	g	315	KC2	3	0
38	g	317	II0	1	0
29	l	310	CLA	1	0
29	b	302	CLA	2	0
29	m	604	CLA	1	0
29	A	851	CLA	4	0
29	i	307	CLA	2	0
40	n	611	KC2	1	0
29	j	306	CLA	1	0
29	j	310	CLA	2	0
29	c	311	CLA	2	0
39	n	617	IHT	1	0
29	B	841	CLA	2	0
29	A	824	CLA	2	0
29	n	613	CLA	2	0
29	i	305	CLA	1	0
29	n	602	CLA	1	0
29	g	305	CLA	3	0
29	B	812	CLA	3	0
32	B	845	WVN	1	0
37	F	208	LMG	1	0
29	B	825	CLA	5	0
29	L	207	CLA	1	0
29	c	308	CLA	5	0
39	b	316	IHT	1	0
29	F	201	CLA	2	0
29	B	809	CLA	1	0
29	A	822	CLA	3	0
29	i	306	CLA	1	0
29	i	302	CLA	3	0
29	A	802	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	c	317	LMG	1	0
29	n	609	CLA	4	0
39	g	324	IHT	4	0
29	h	301	CLA	3	0
30	B	843	PQN	1	0
29	B	822	CLA	3	0
29	B	805	CLA	1	0
37	Q	301	LMG	4	0
29	B	804	CLA	2	0
29	A	811	CLA	1	0
29	B	827	CLA	2	0
29	l	308	CLA	2	0
29	b	313	CLA	3	0
33	A	855	LMU	3	0
29	B	820	CLA	3	0
38	b	314	II0	1	0
29	l	312	CLA	1	0
29	a	309	CLA	2	0
29	c	302	CLA	1	0
29	j	308	CLA	1	0
29	B	837	CLA	1	0
29	b	303	CLA	1	0
31	s	408	LHG	3	0
29	s	403	CLA	1	0
29	m	602	CLA	6	0
29	n	607	CLA	4	0
31	L	208	LHG	1	0
29	h	312	CLA	1	0
29	m	603	CLA	2	0
29	c	307	CLA	1	0
29	B	829	CLA	2	0
40	s	404	KC2	2	0
29	h	307	CLA	1	0
29	l	304	CLA	1	0
29	A	823	CLA	4	0
29	A	817	CLA	2	0
29	k	602	CLA	3	0
29	k	603	CLA	1	0
29	A	810	CLA	3	0
29	g	323	CLA	1	0
29	O	201	CLA	1	0
29	b	306	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	320	LHG	3	0
31	b	318	LHG	1	0
29	k	614	CLA	1	0
29	j	309	CLA	3	0
38	b	317	II0	1	0
29	B	842	CLA	3	0
29	g	310	CLA	1	0
29	Q	302	CLA	1	0
40	g	313	KC2	1	0
29	B	835	CLA	3	0
29	e	302	CLA	4	0
31	a	301	LHG	3	0
29	A	830	CLA	1	0
31	g	301	LHG	1	0
29	k	610	CLA	1	0
29	j	304	CLA	2	0
29	j	313	CLA	1	0
29	A	832	CLA	4	0
40	f	611	KC2	1	0
29	A	829	CLA	4	0
29	A	834	CLA	1	0
29	B	808	CLA	3	0
29	B	803	CLA	2	0
29	i	308	CLA	1	0
29	s	406	CLA	1	0
37	F	206	LMG	3	0
38	k	618	II0	1	0
29	a	312	CLA	1	0
29	A	838	CLA	4	0
29	s	402	CLA	2	0
29	k	609	CLA	1	0
31	A	843	LHG	1	0
29	b	309	CLA	3	0
29	e	305	CLA	2	0
29	m	613	CLA	4	0
30	A	841	PQN	4	0
31	n	619	LHG	3	0
29	A	806	CLA	2	0
29	m	608	CLA	1	0
29	F	202	CLA	2	0
29	A	831	CLA	1	0
29	e	307	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	e	304	CLA	1	0
29	c	312	CLA	2	0
29	k	604	CLA	2	0
37	c	318	LMG	3	0
29	B	801	CLA	1	0
29	f	607	CLA	1	0
40	i	318	KC2	2	0
29	f	610	CLA	2	0
29	f	601	CLA	1	0
29	d	302	CLA	2	0
29	g	302	CLA	3	0
29	j	311	CLA	1	0
29	B	816	CLA	2	0
31	L	209	LHG	1	0
29	B	833	CLA	1	0
37	b	319	LMG	2	0
29	L	202	CLA	1	0
29	g	304	CLA	6	0
29	A	819	CLA	1	0
29	e	311	CLA	2	0
29	f	613	CLA	3	0
31	f	619	LHG	3	0
29	A	850	CLA	2	0
29	m	607	CLA	4	0
31	A	842	LHG	1	0
29	A	814	CLA	3	0
29	n	610	CLA	4	0
29	A	837	CLA	3	0
29	i	304	CLA	1	0
29	A	804	CLA	4	0
29	n	603	CLA	1	0
29	A	827	CLA	6	0
29	A	820	CLA	1	0
29	d	313	CLA	3	0
29	h	306	CLA	2	0
29	j	302	CLA	1	0
29	e	301	CLA	1	0
29	c	301	CLA	1	0
38	g	321	II0	1	0
29	A	826	CLA	2	0
29	B	830	CLA	4	0
29	B	832	CLA	1	0

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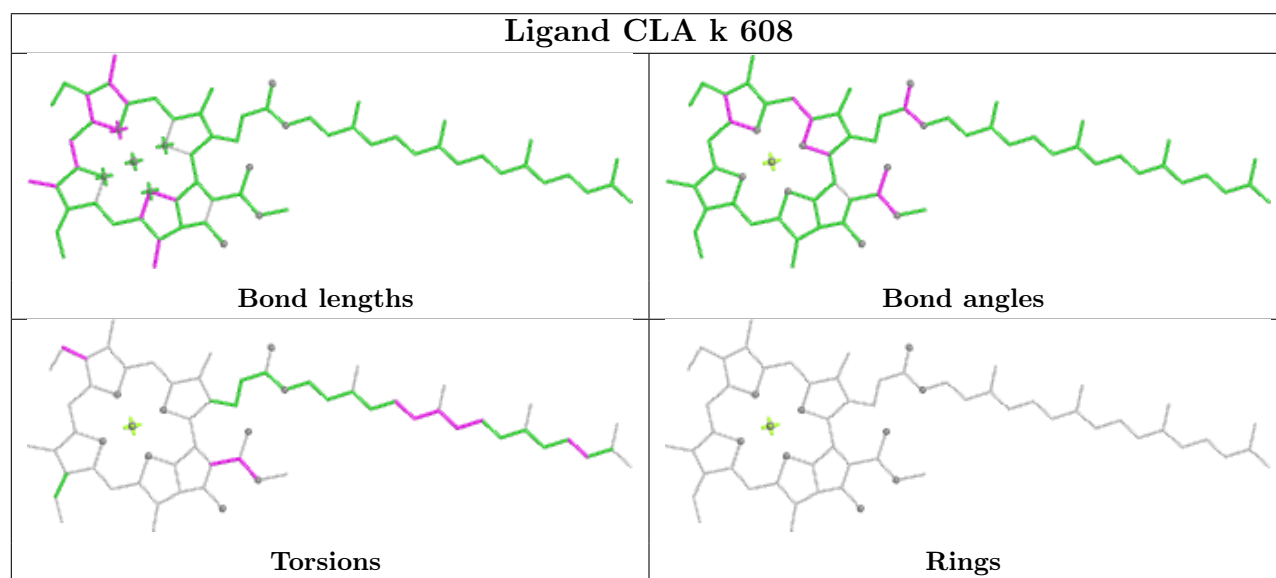
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29	B	824	CLA	2	0
29	K	101	CLA	3	0
29	n	605	CLA	1	0
29	A	836	CLA	3	0
29	g	316	CLA	4	0
29	b	310	CLA	3	0
29	g	309	CLA	1	0
29	B	806	CLA	2	0
31	m	619	LHG	1	0
29	B	831	CLA	3	0
29	A	813	CLA	1	0
29	j	314	CLA	3	0
31	i	317	LHG	2	0
29	i	312	CLA	2	0
29	A	812	CLA	1	0
29	l	309	CLA	1	0
29	g	312	CLA	2	0
29	B	823	CLA	1	0
29	F	203	CLA	1	0
40	l	311	KC2	3	0
40	s	401	KC2	1	0
29	B	840	CLA	5	0
29	B	815	CLA	2	0
29	A	808	CLA	1	0
29	B	834	CLA	4	0
29	l	301	CLA	3	0
29	A	803	CLA	5	0
29	b	307	CLA	1	0
40	d	312	KC2	1	0
29	A	835	CLA	6	0
29	b	312	CLA	6	0
29	d	306	CLA	1	0
40	g	314	KC2	2	0
29	a	310	CLA	1	0
29	b	305	CLA	5	0
29	l	305	CLA	1	0
29	B	819	CLA	5	0
29	c	305	CLA	1	0
36	j	319	DGD	3	0
29	B	828	CLA	2	0
29	B	838	CLA	2	0

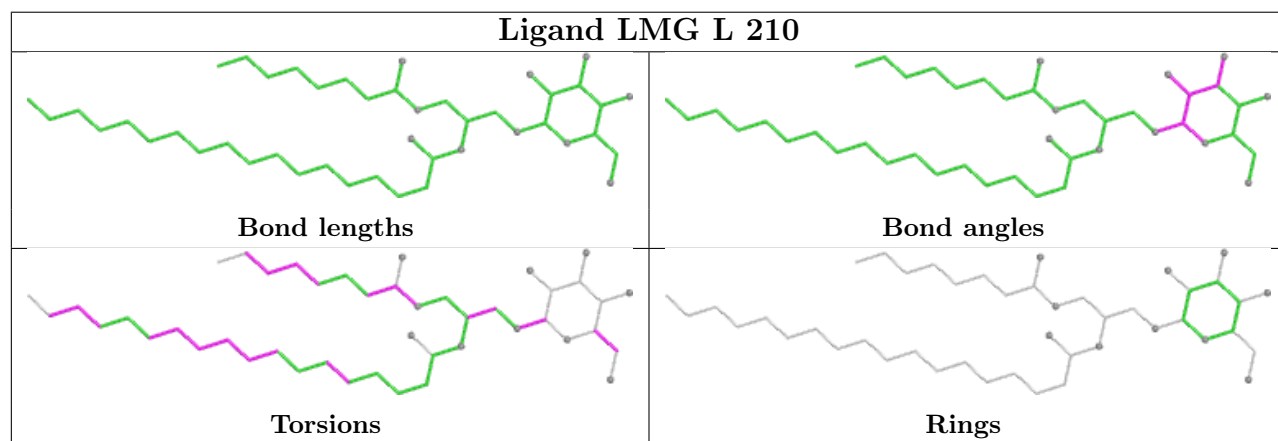
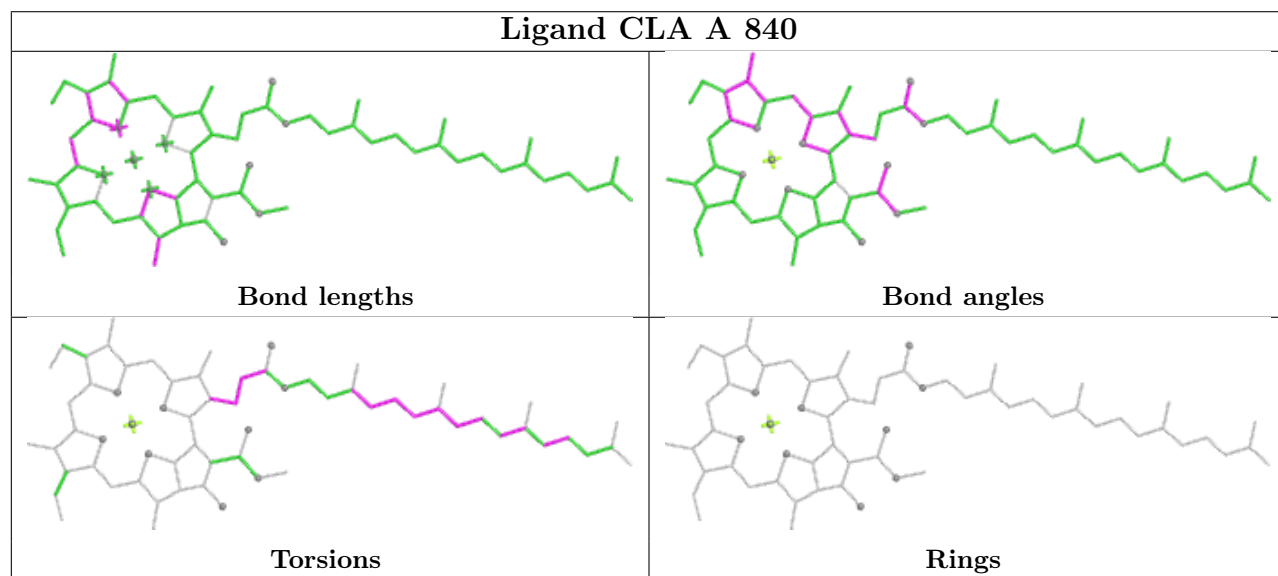
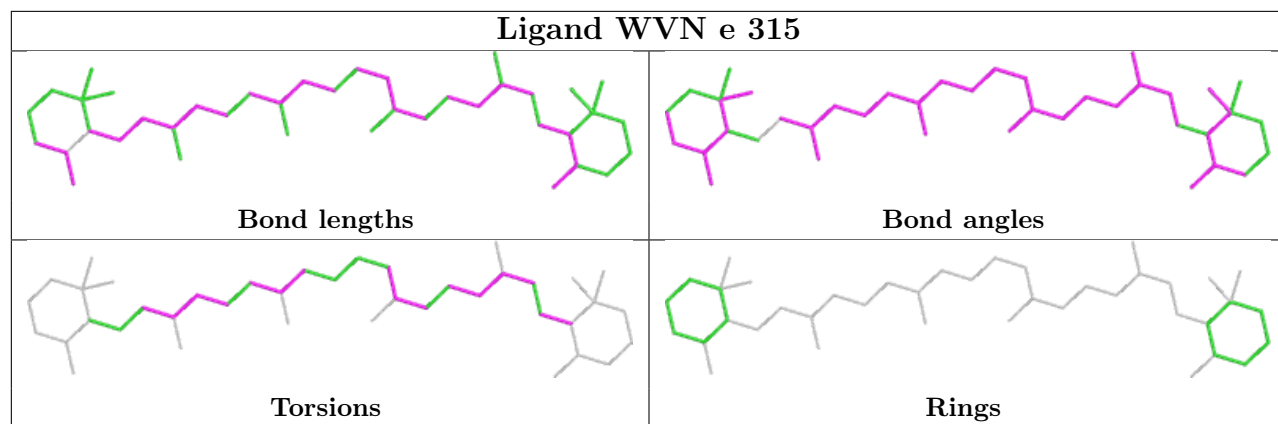
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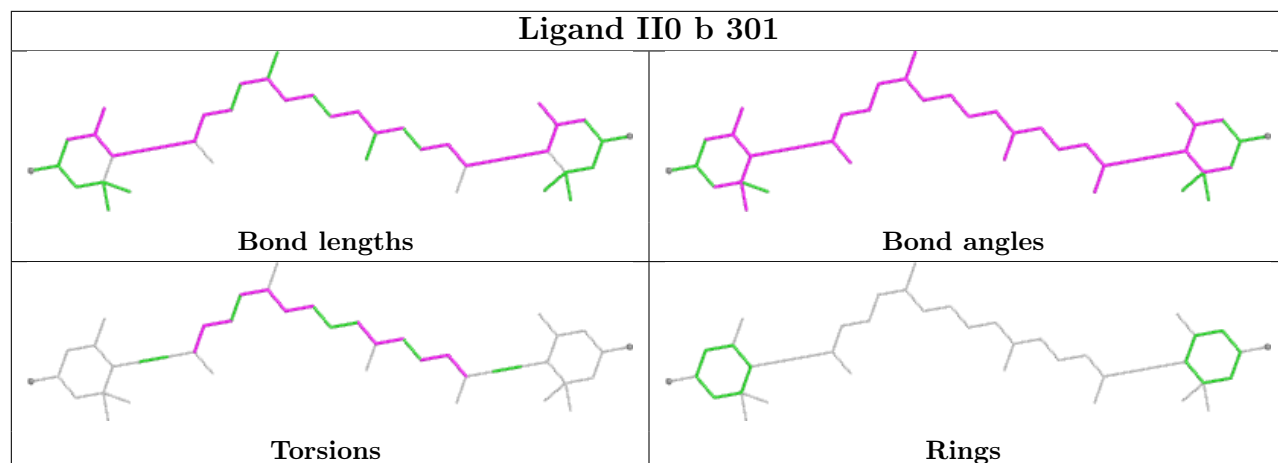
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	304	CLA	1	0
29	n	604	CLA	2	0
29	a	302	CLA	4	0
29	f	606	CLA	2	0
29	f	608	CLA	3	0
29	b	311	CLA	4	0
29	h	304	CLA	2	0
29	c	306	CLA	1	0
29	k	607	CLA	2	0
29	f	602	CLA	2	0
29	A	818	CLA	3	0
29	a	305	CLA	2	0
29	B	817	CLA	4	0

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

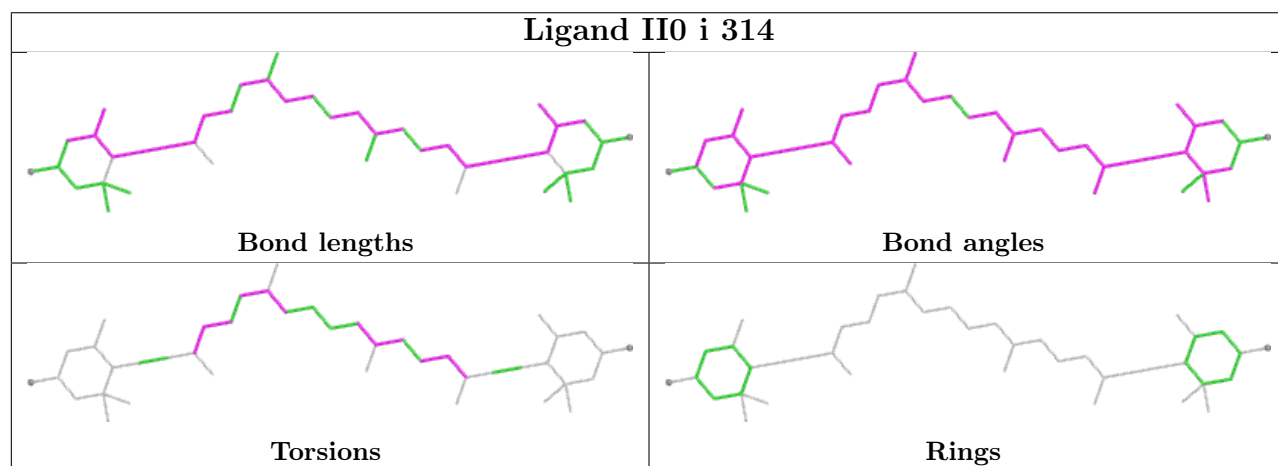




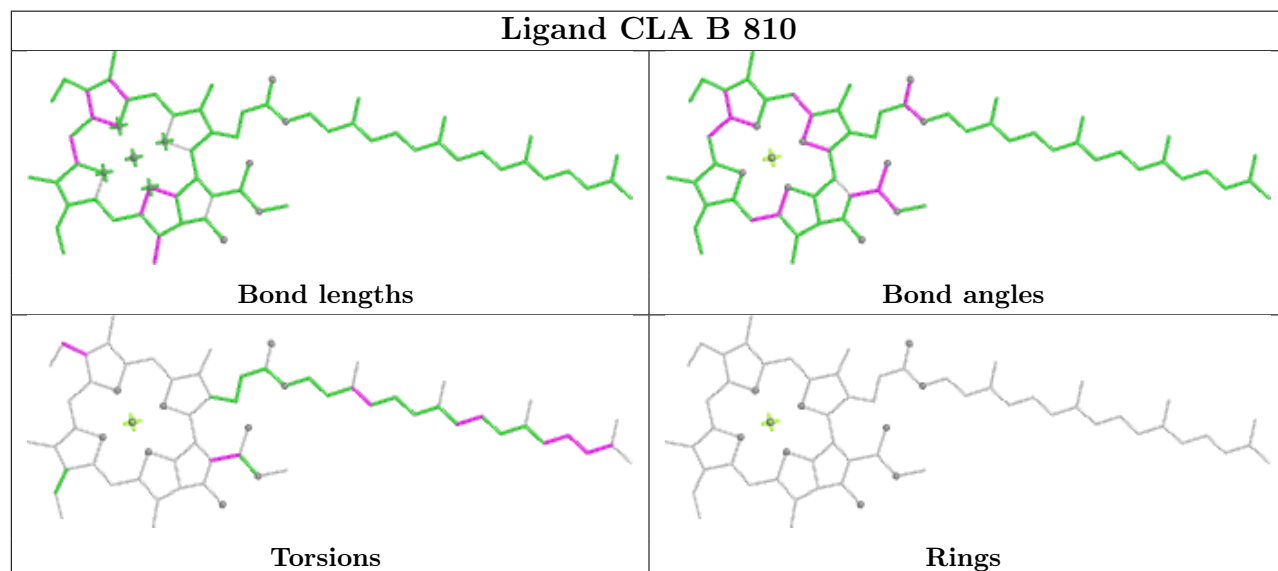
Ligand II0 b 301

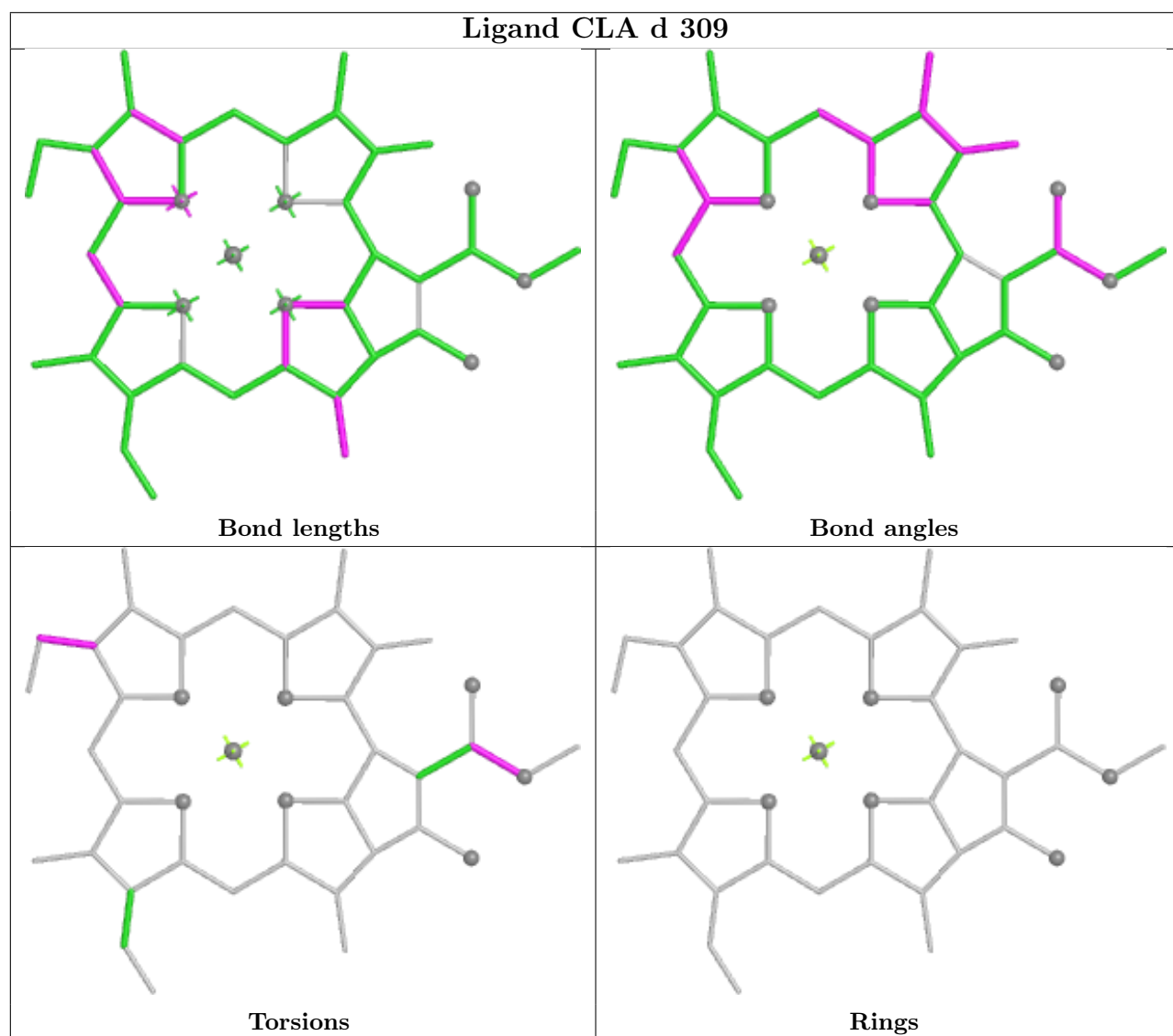
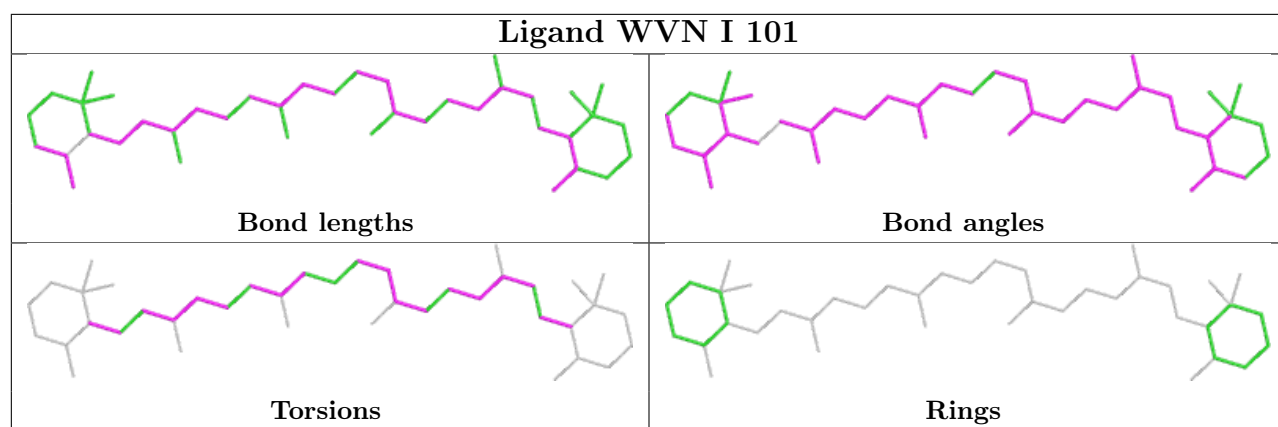


Ligand II0 i 314

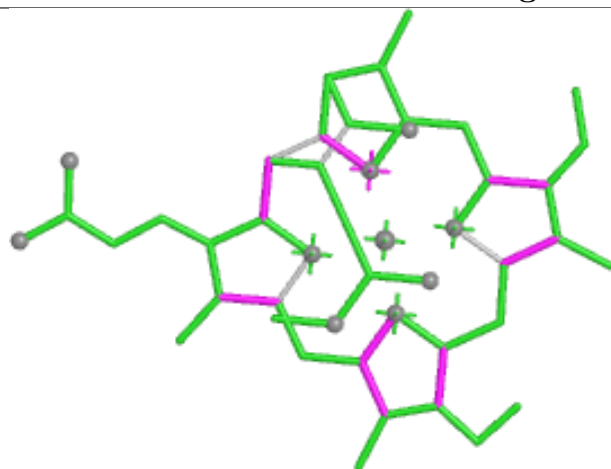


Ligand CLA B 810

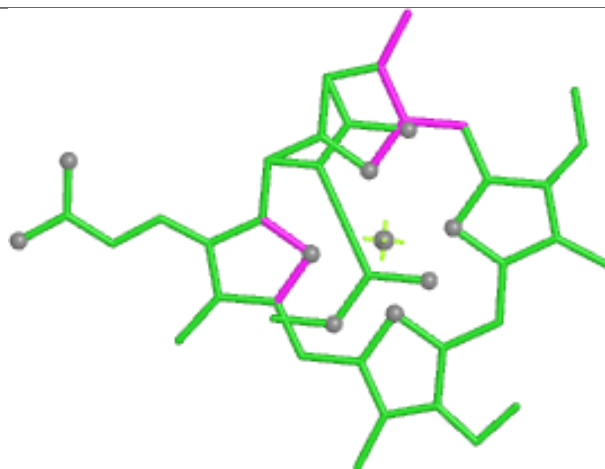




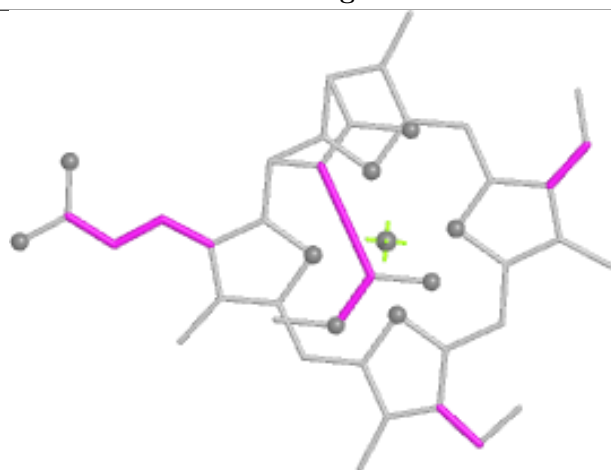
Ligand KC2 n 612



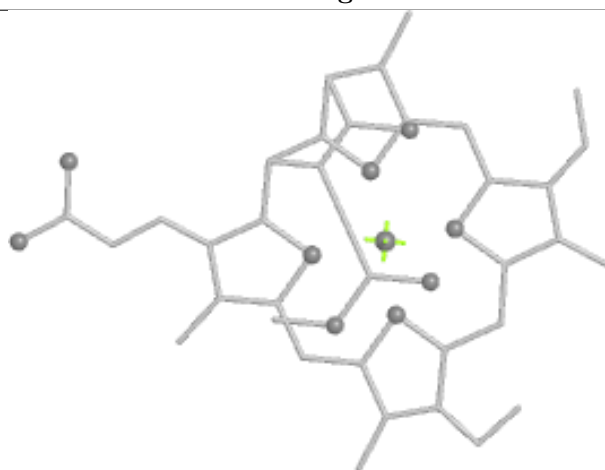
Bond lengths



Bond angles



Torsions



Rings

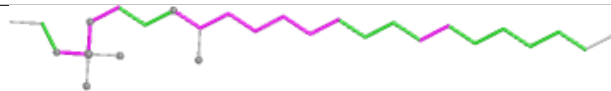
Ligand LHG A 848



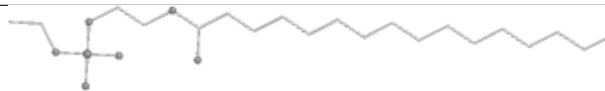
Bond lengths



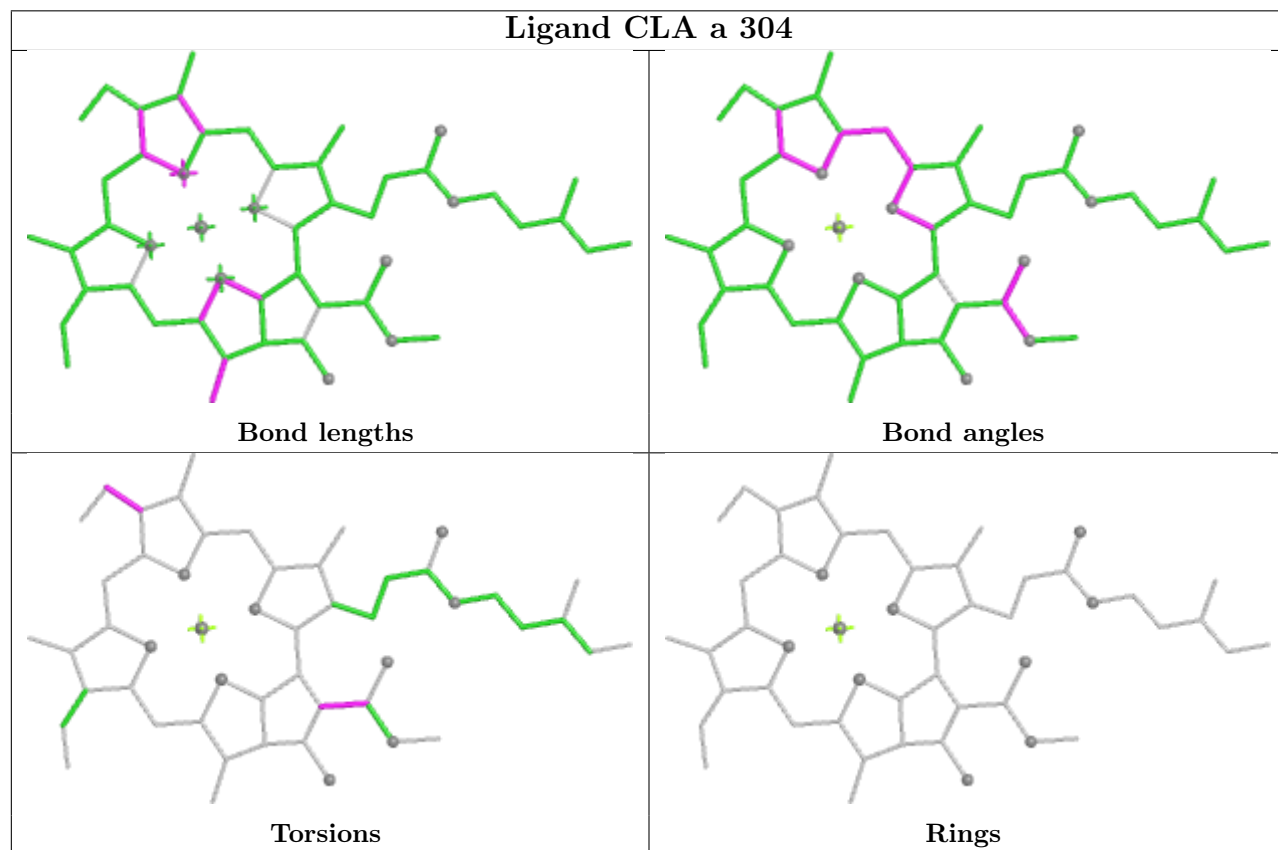
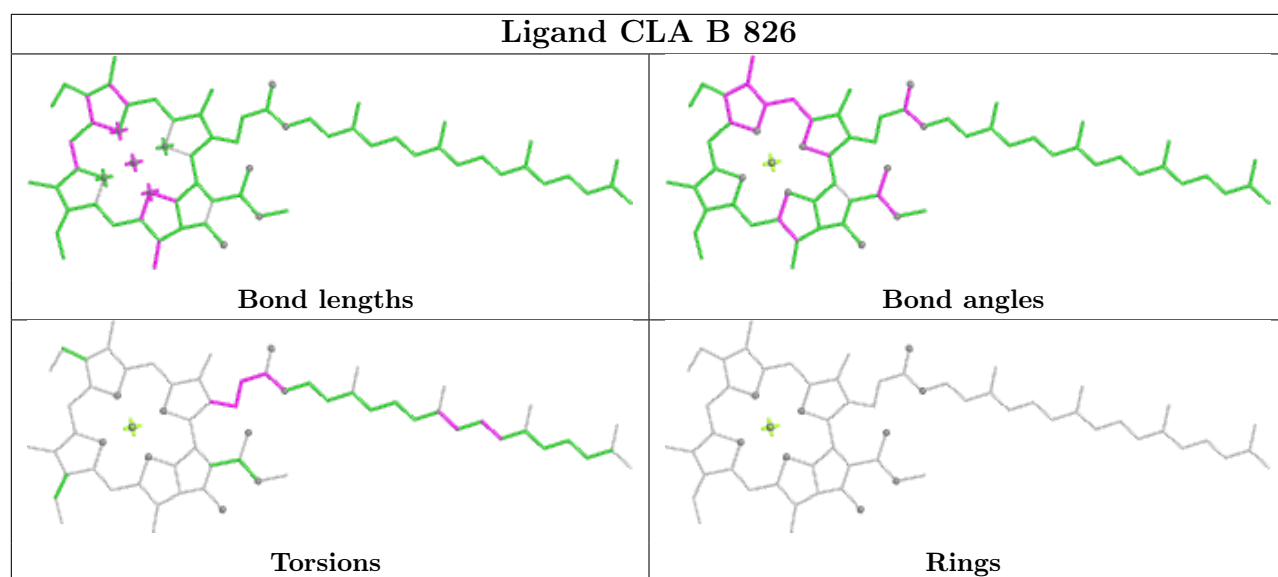
Bond angles



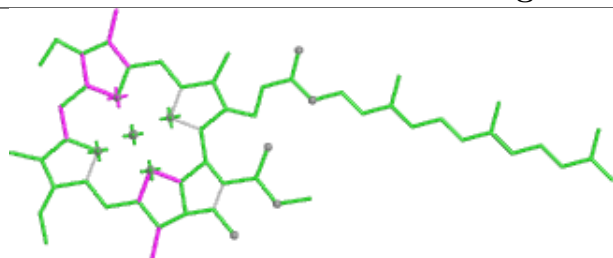
Torsions



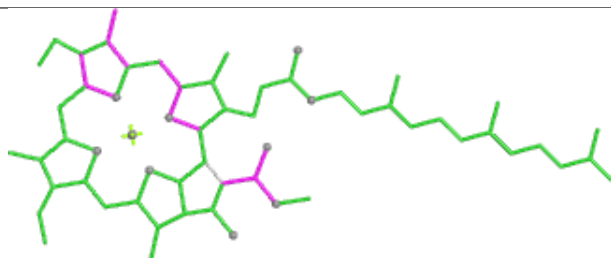
Rings



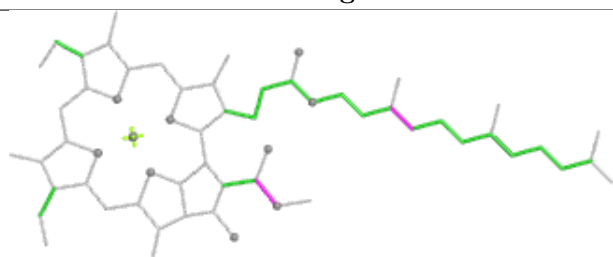
Ligand CLA L 204



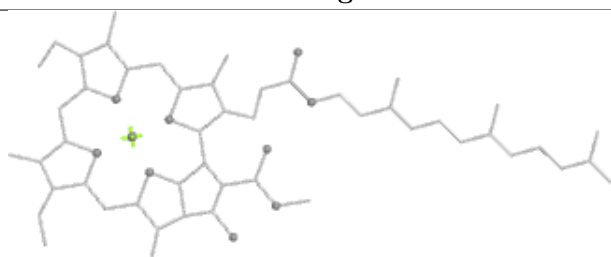
Bond lengths



Bond angles

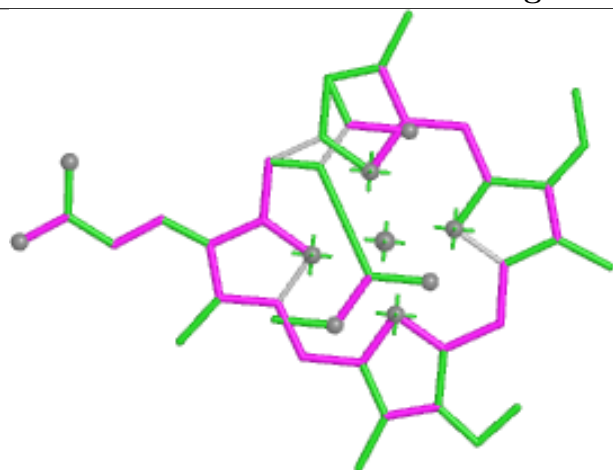


Torsions

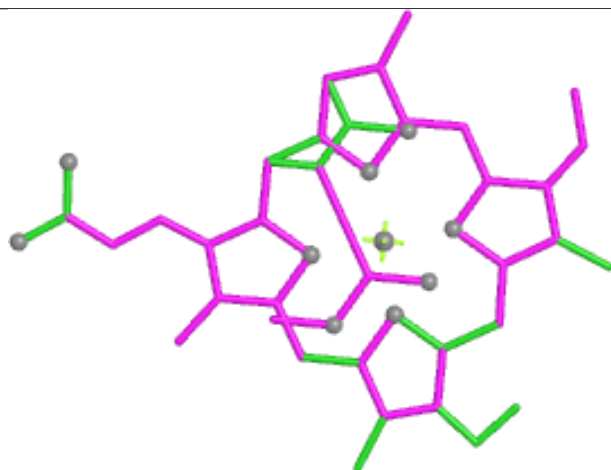


Rings

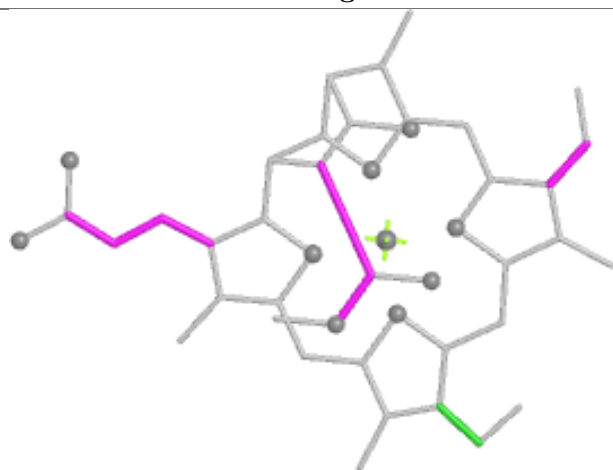
Ligand KC2 i 310



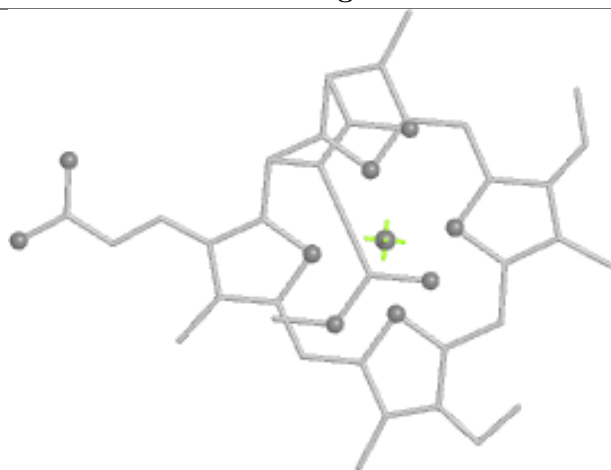
Bond lengths



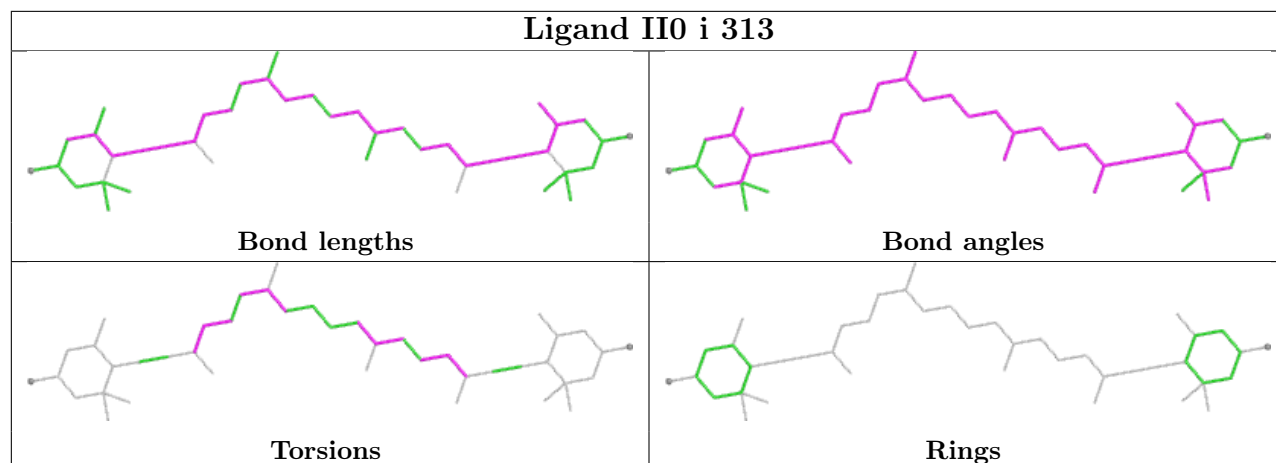
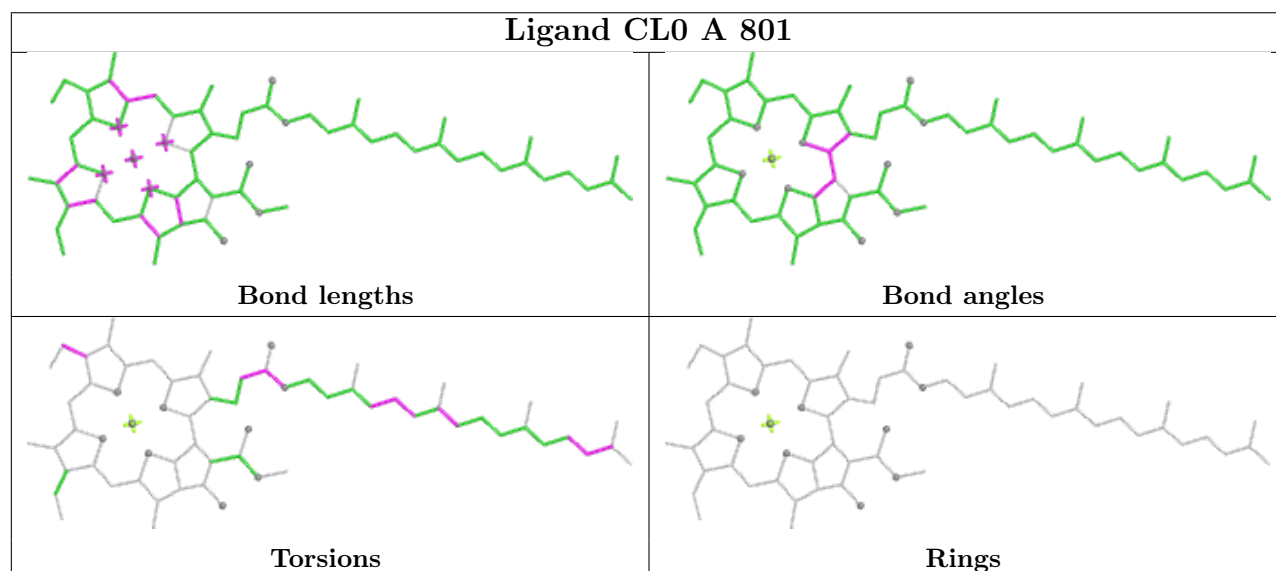
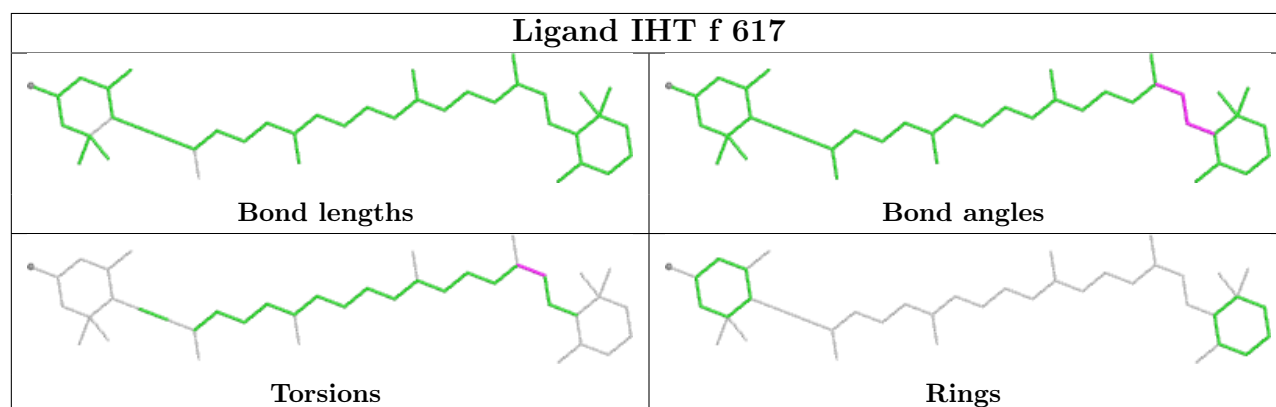
Bond angles

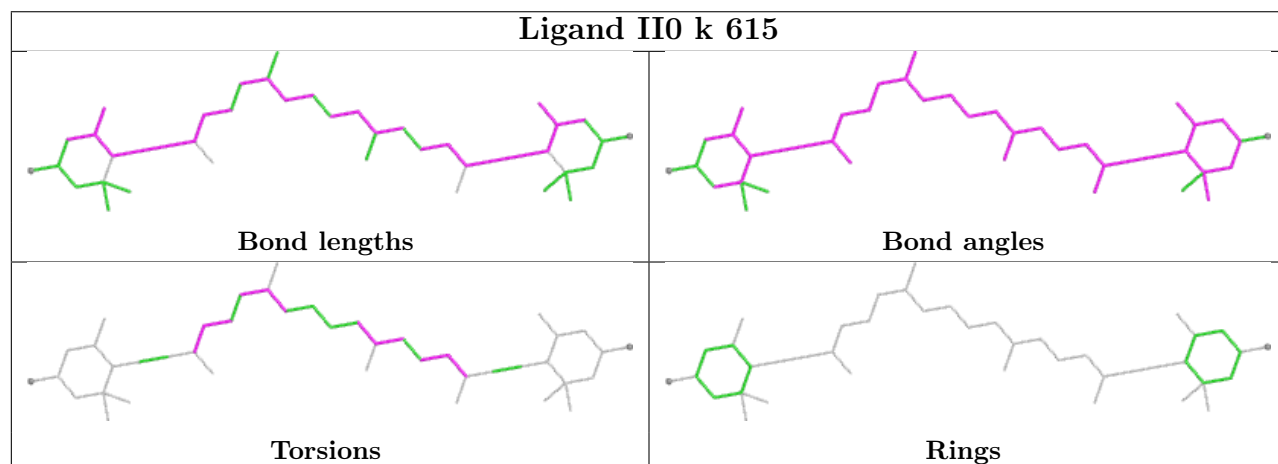
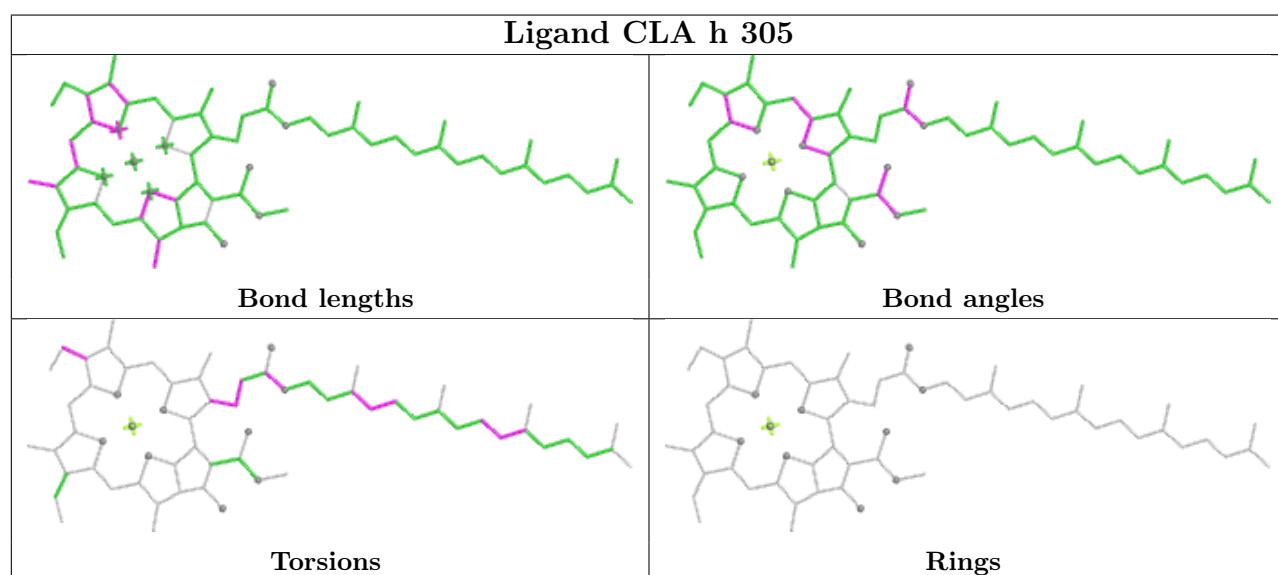
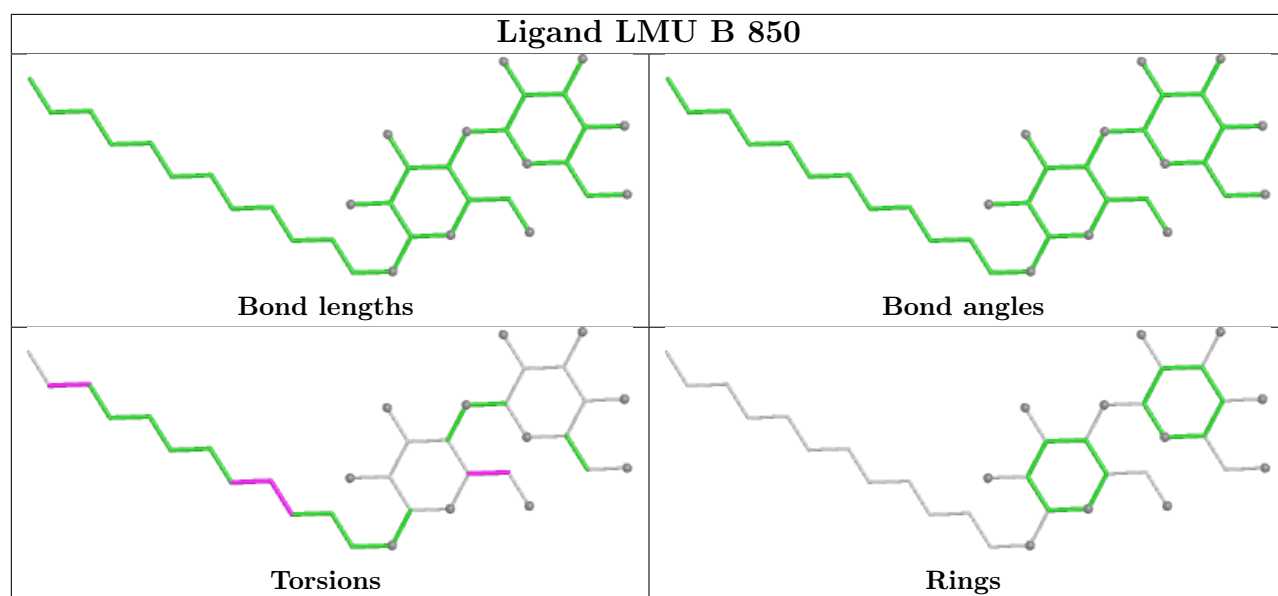


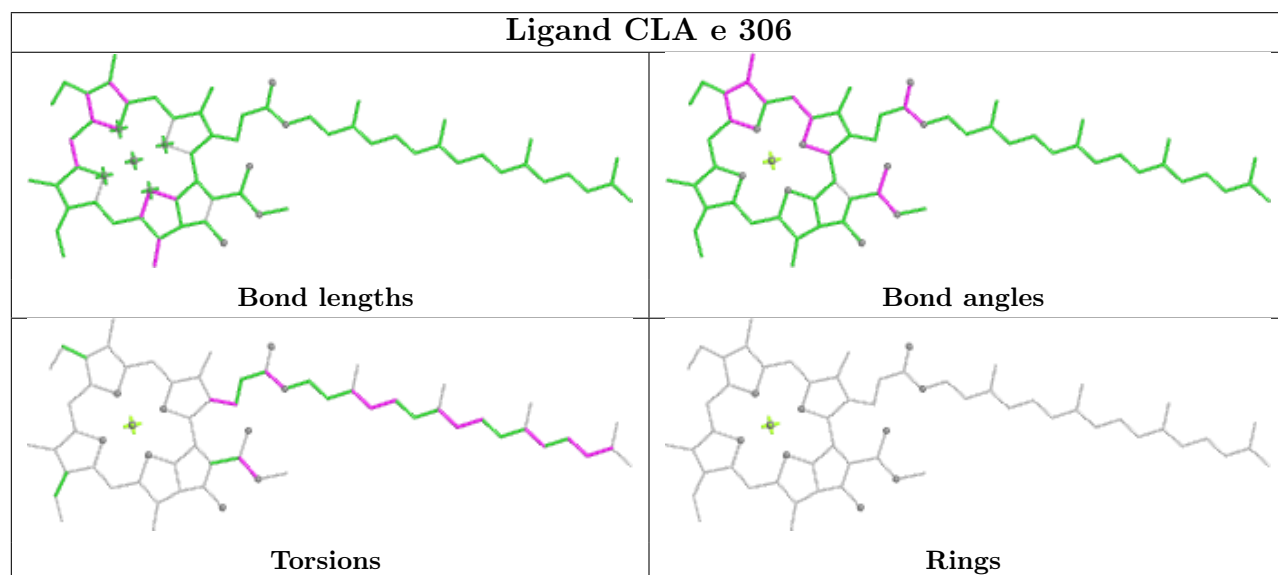
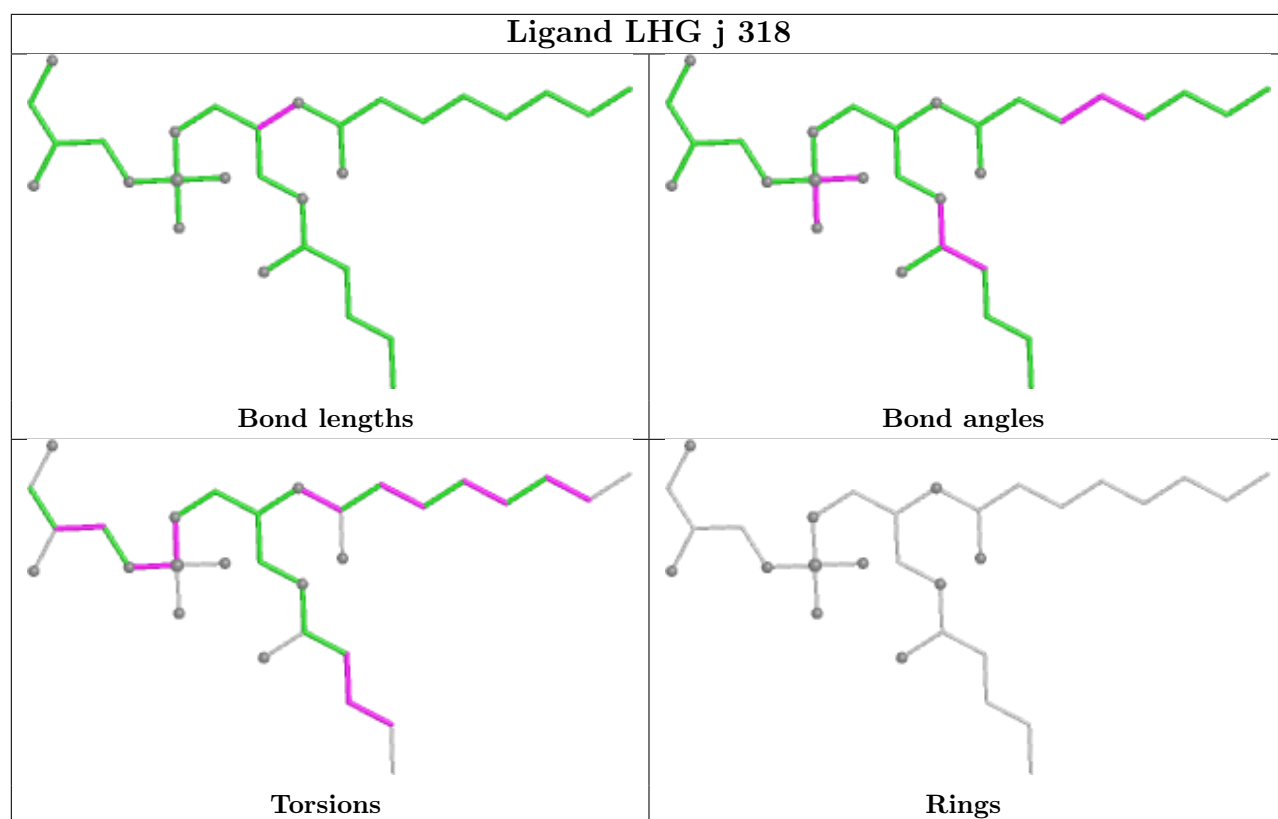
Torsions



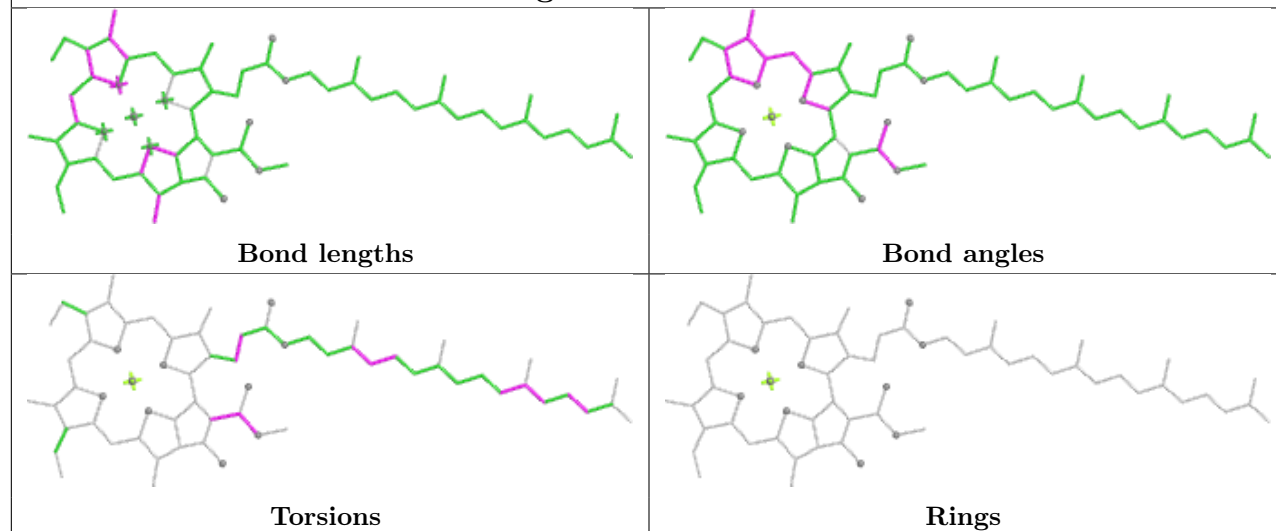
Rings

Ligand II0 i 313**Ligand CL0 A 801****Ligand IHT f 617**

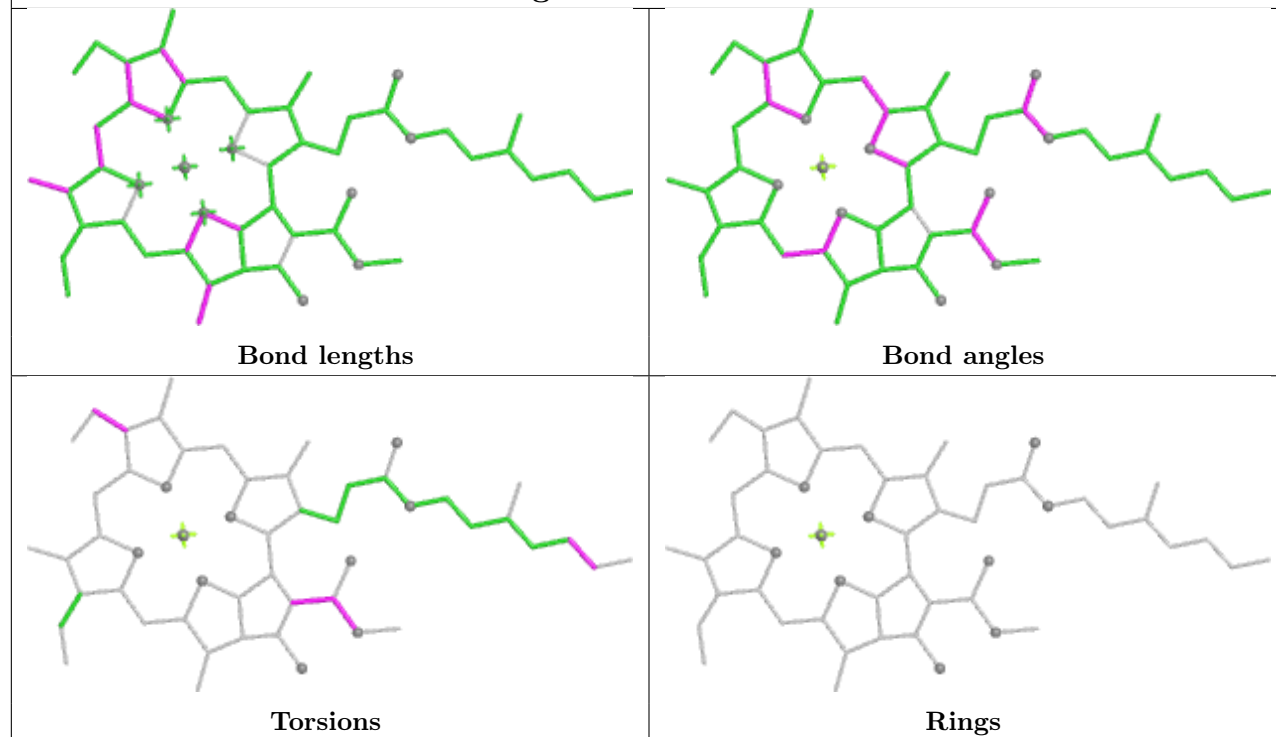




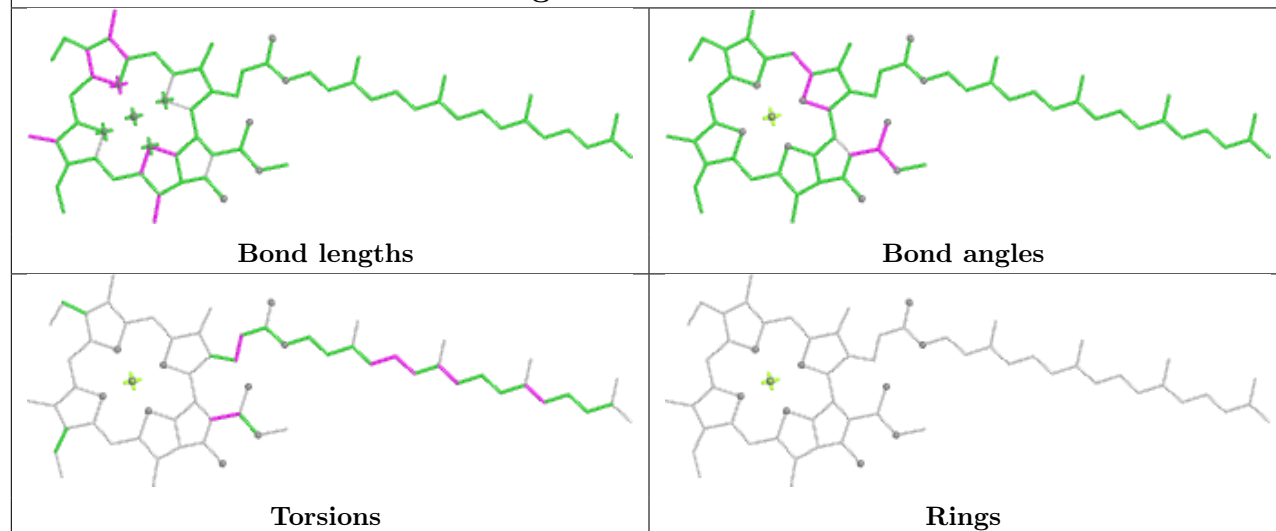
Ligand CLA a 308



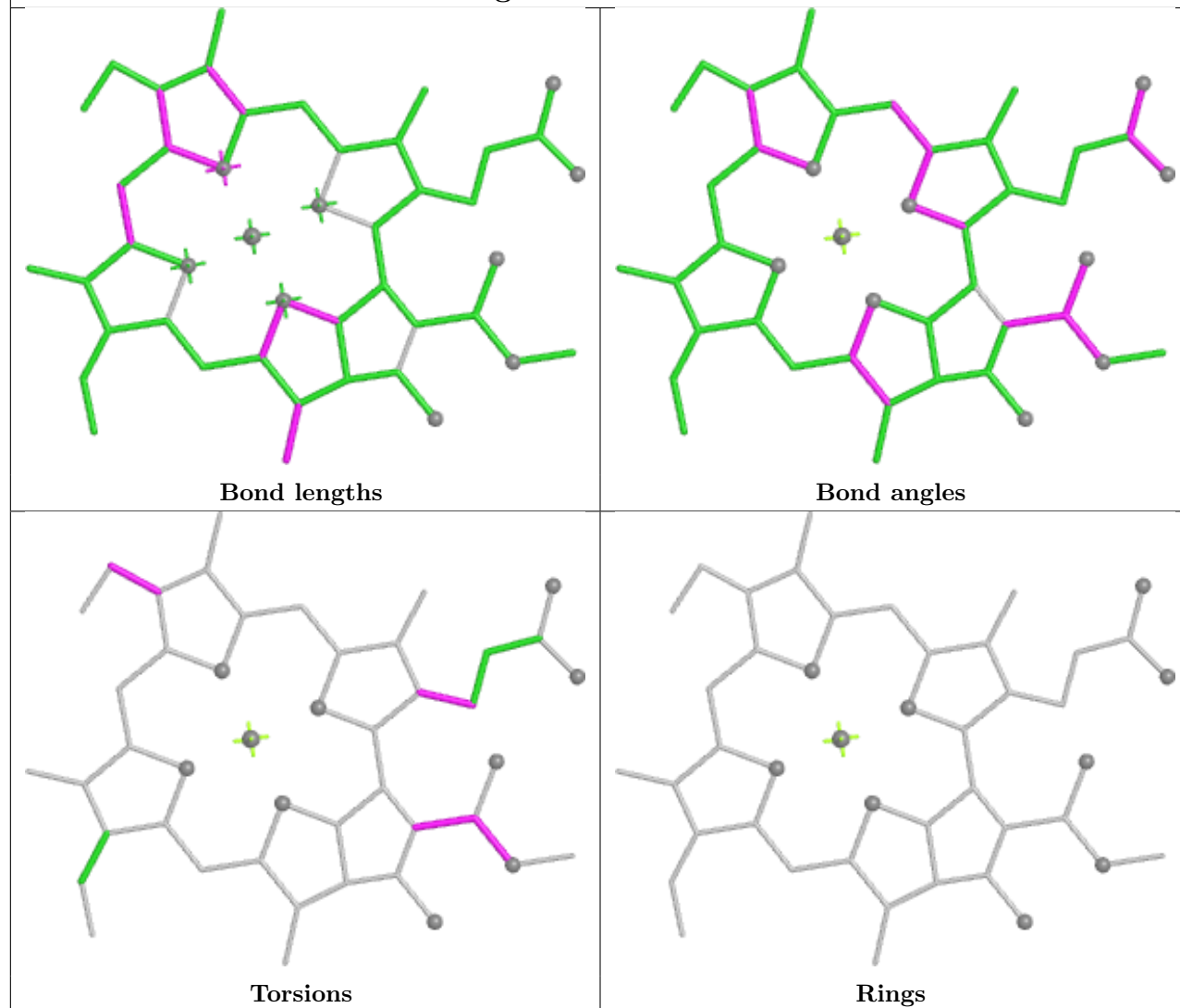
Ligand CLA B 821

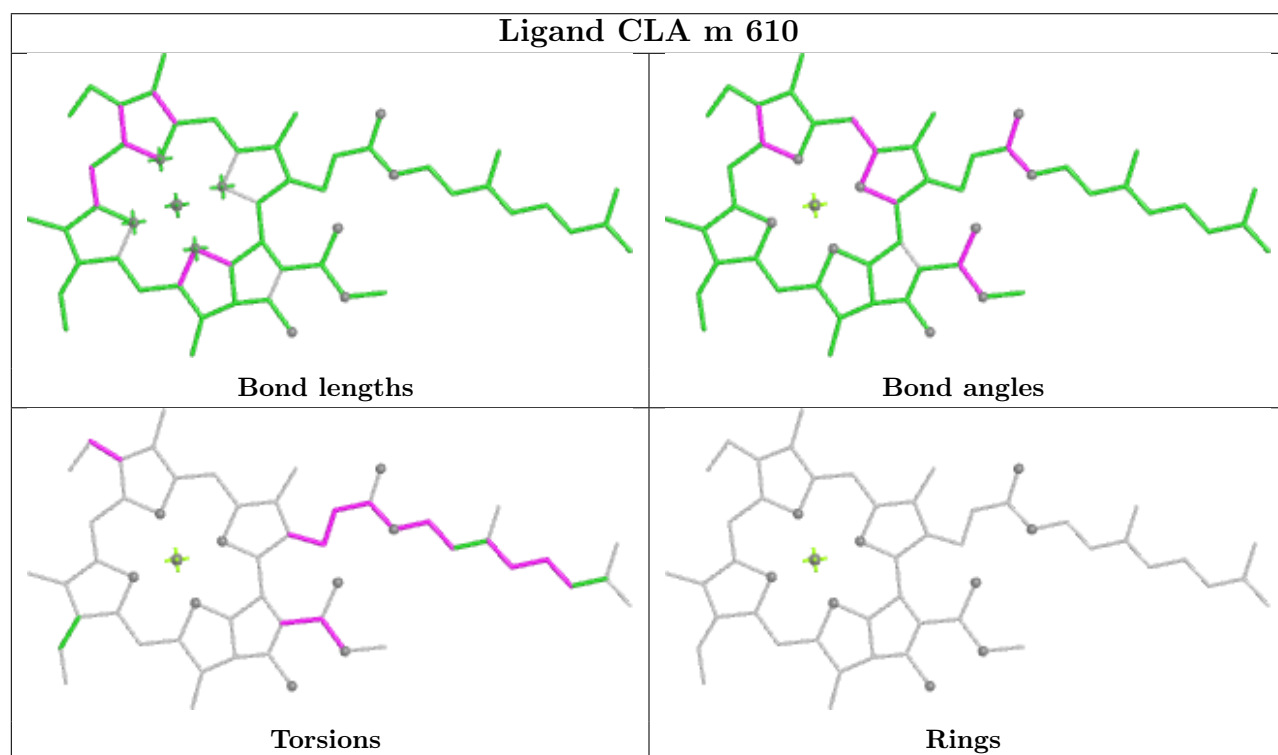
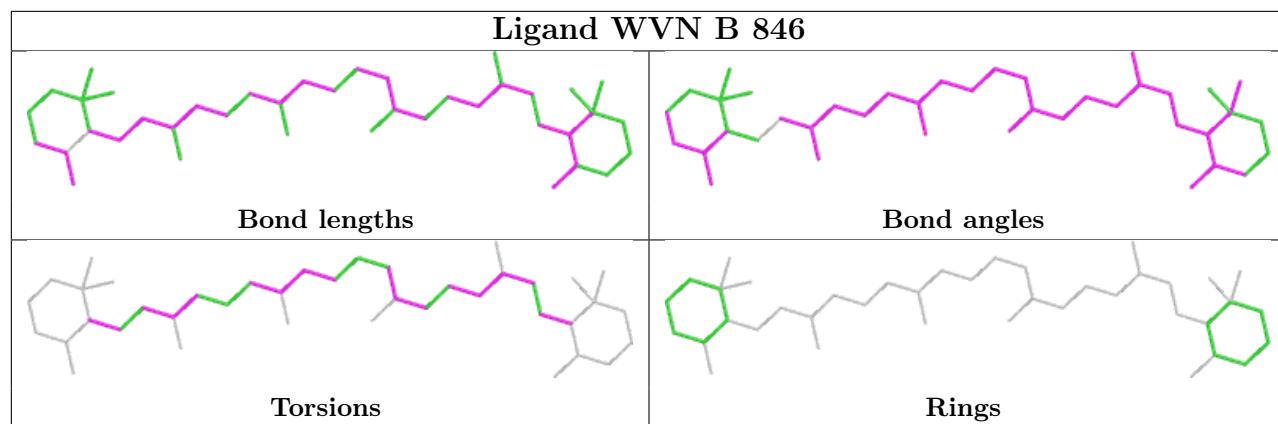


Ligand CLA B 807

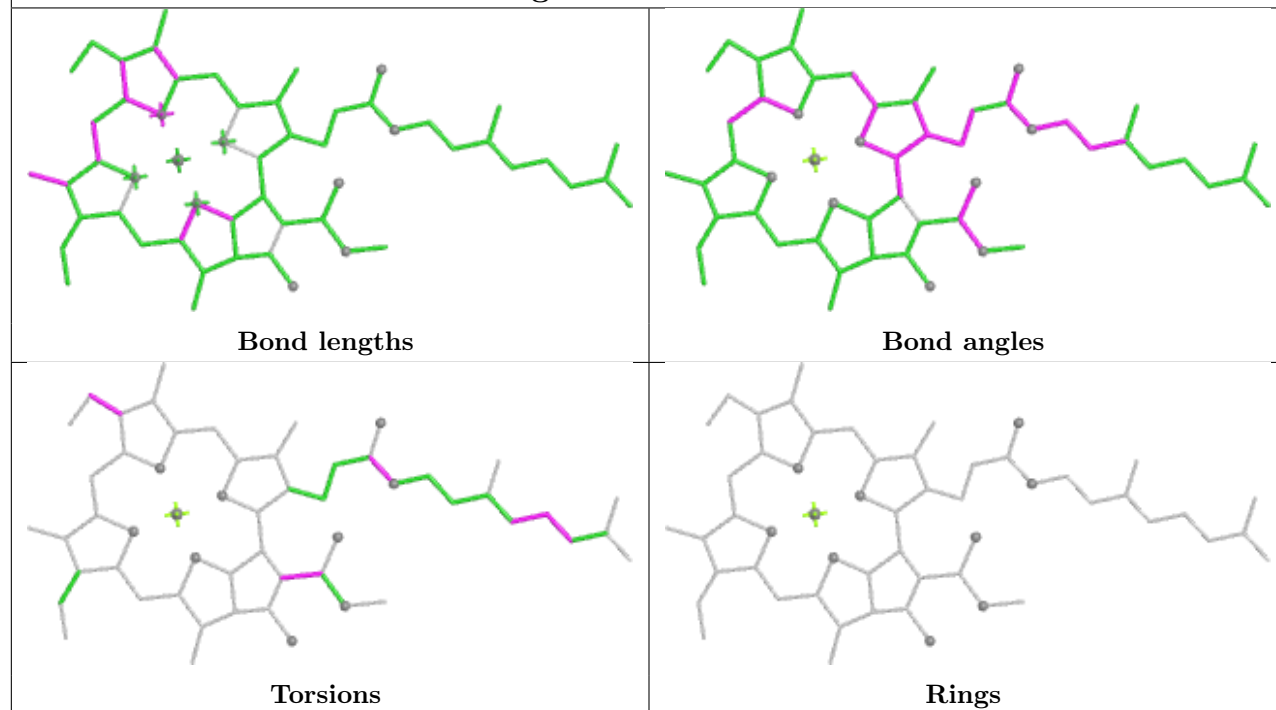


Ligand CLA d 307

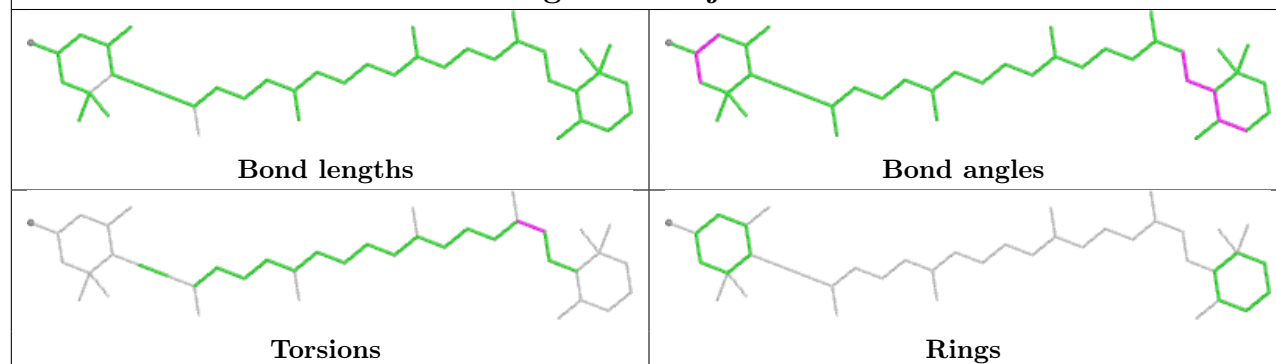




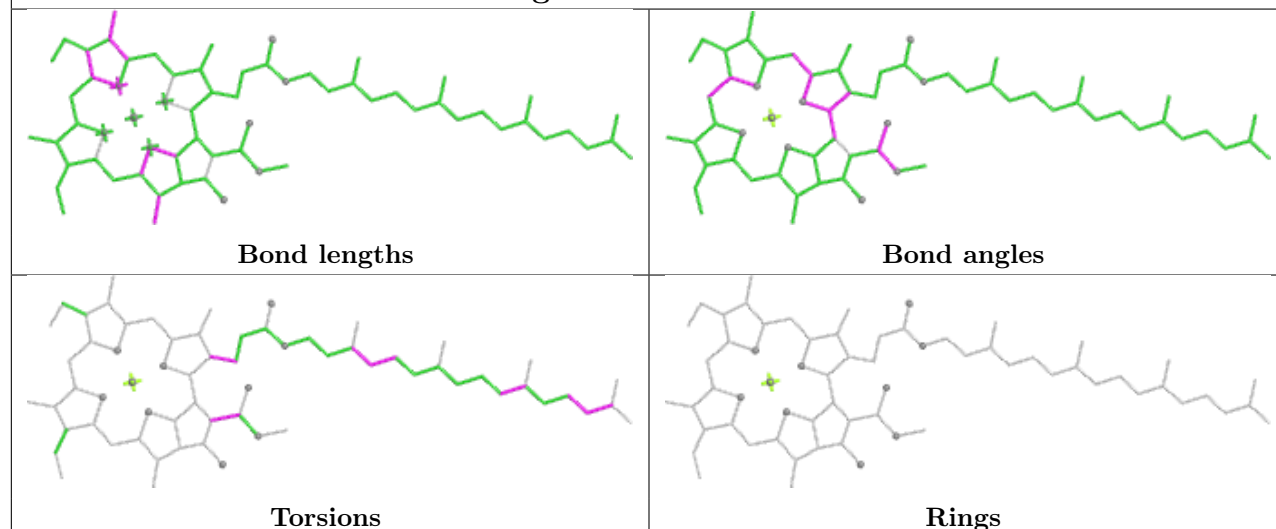
Ligand CLA R 203

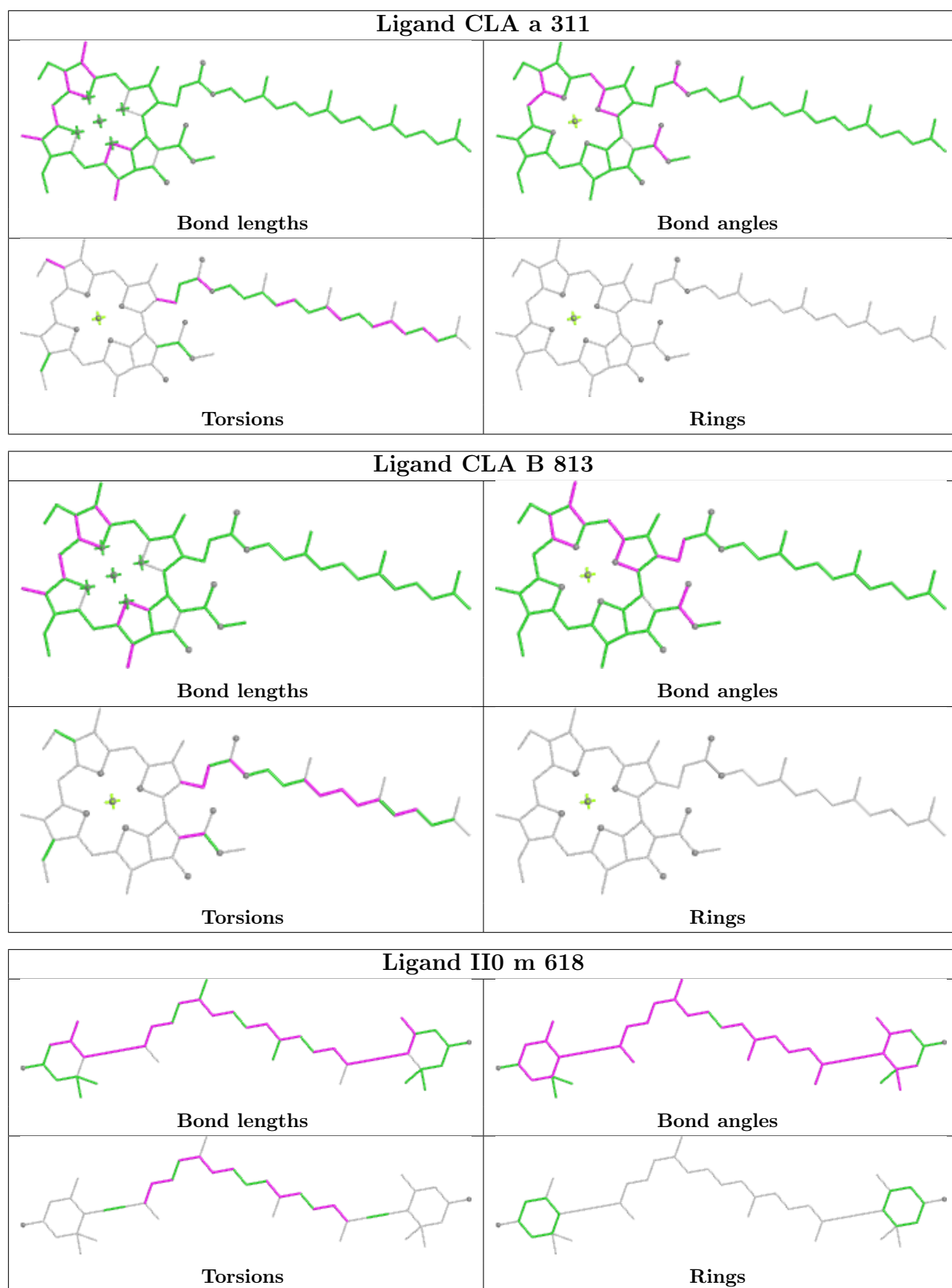


Ligand IHT j 317

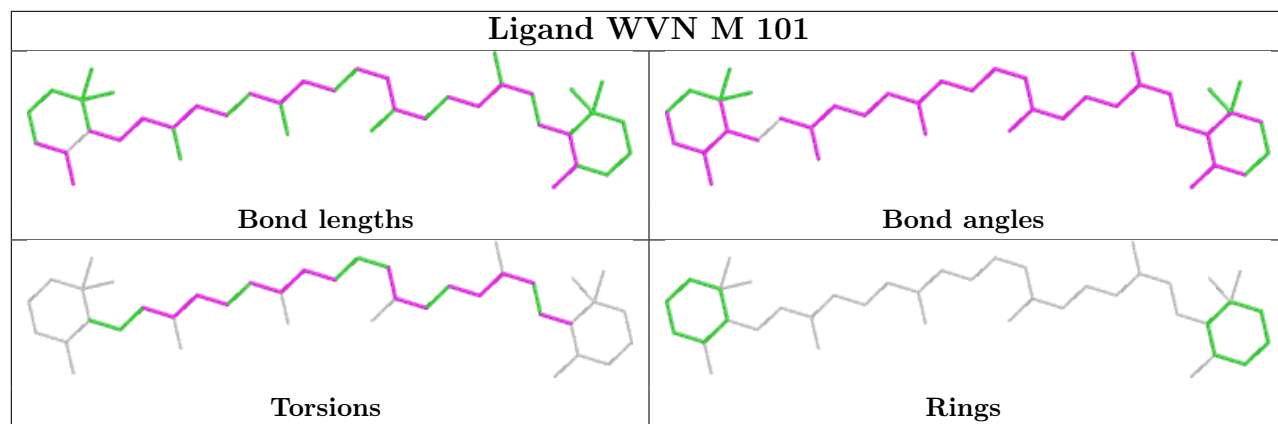


Ligand CLA B 814

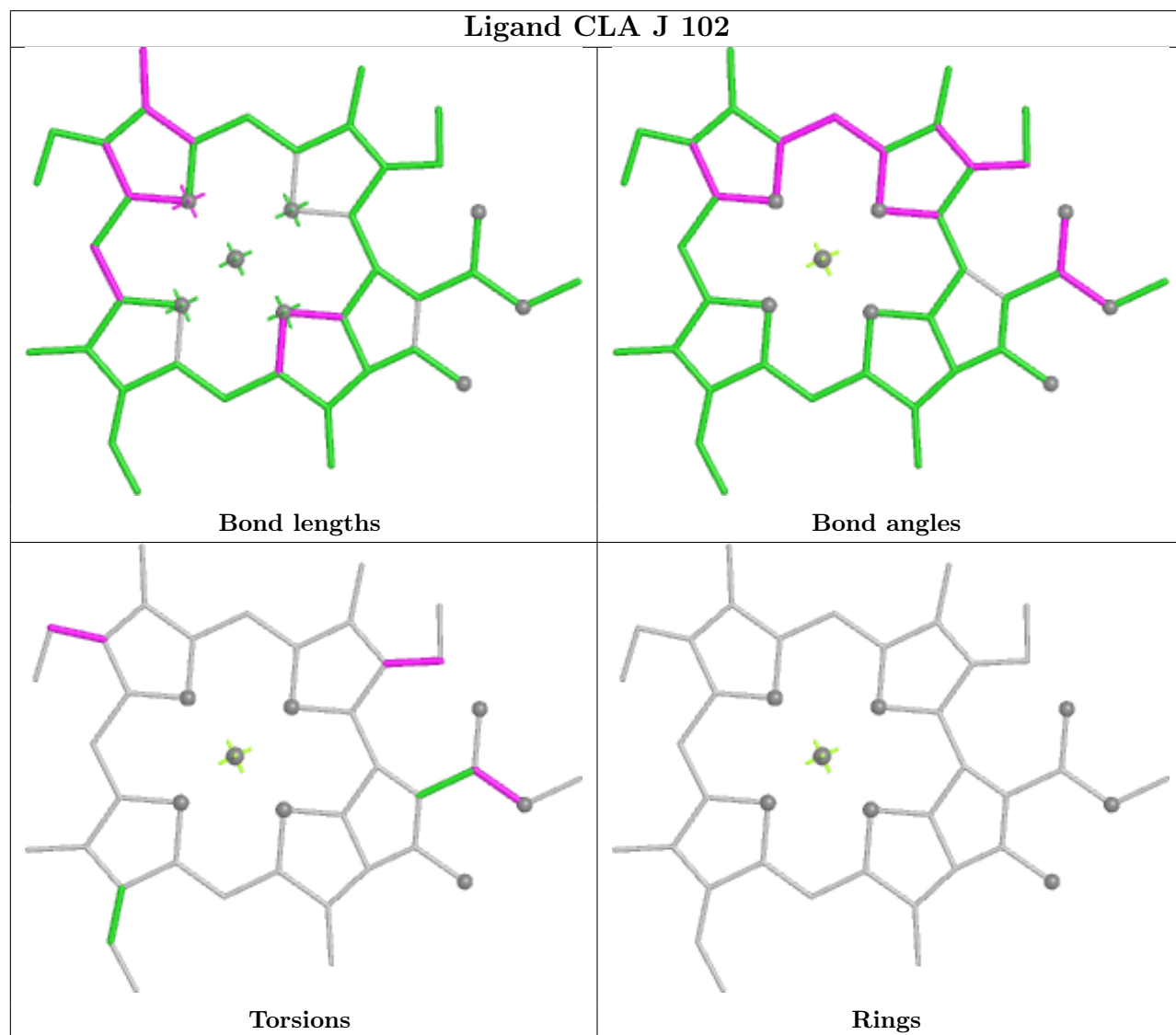


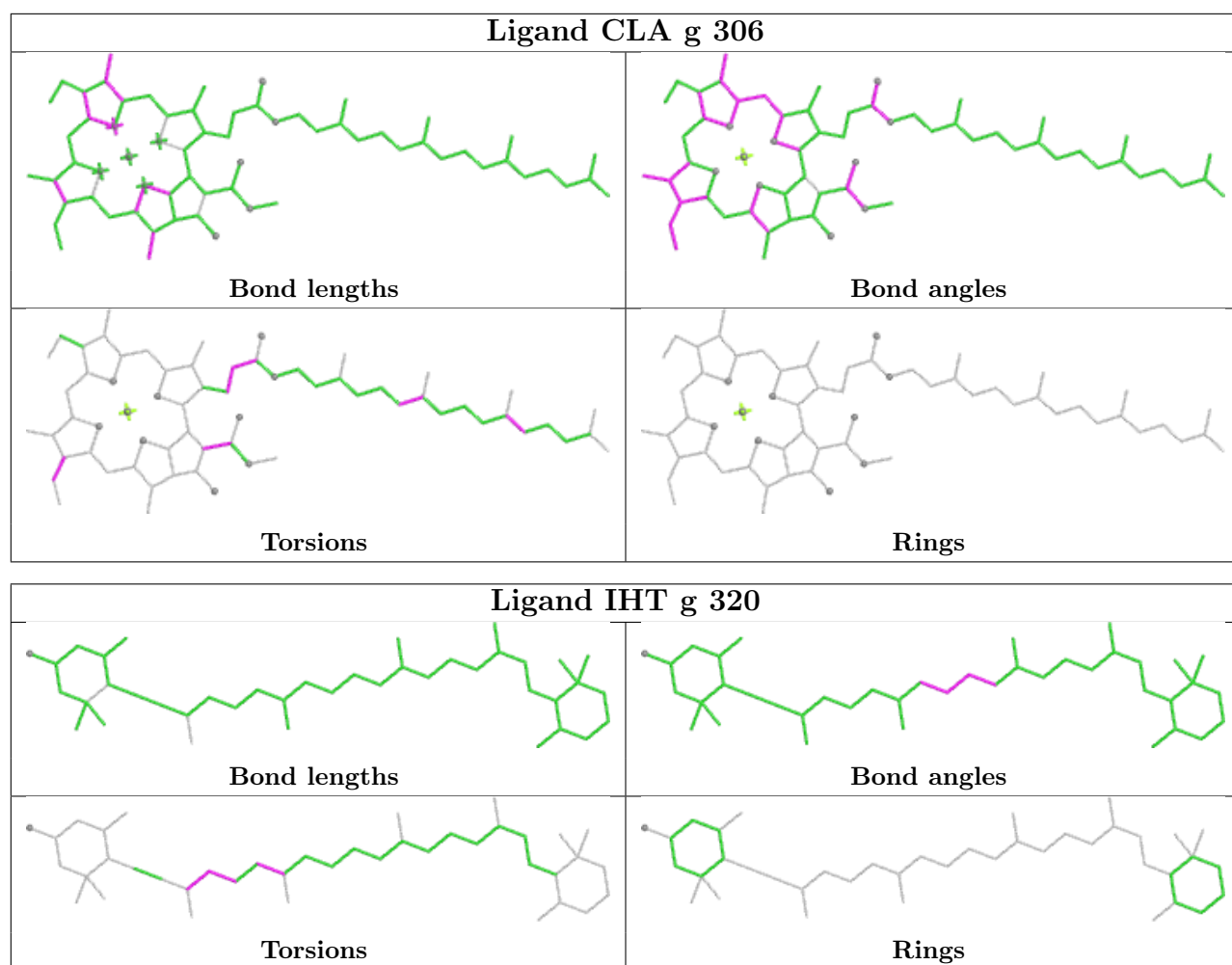


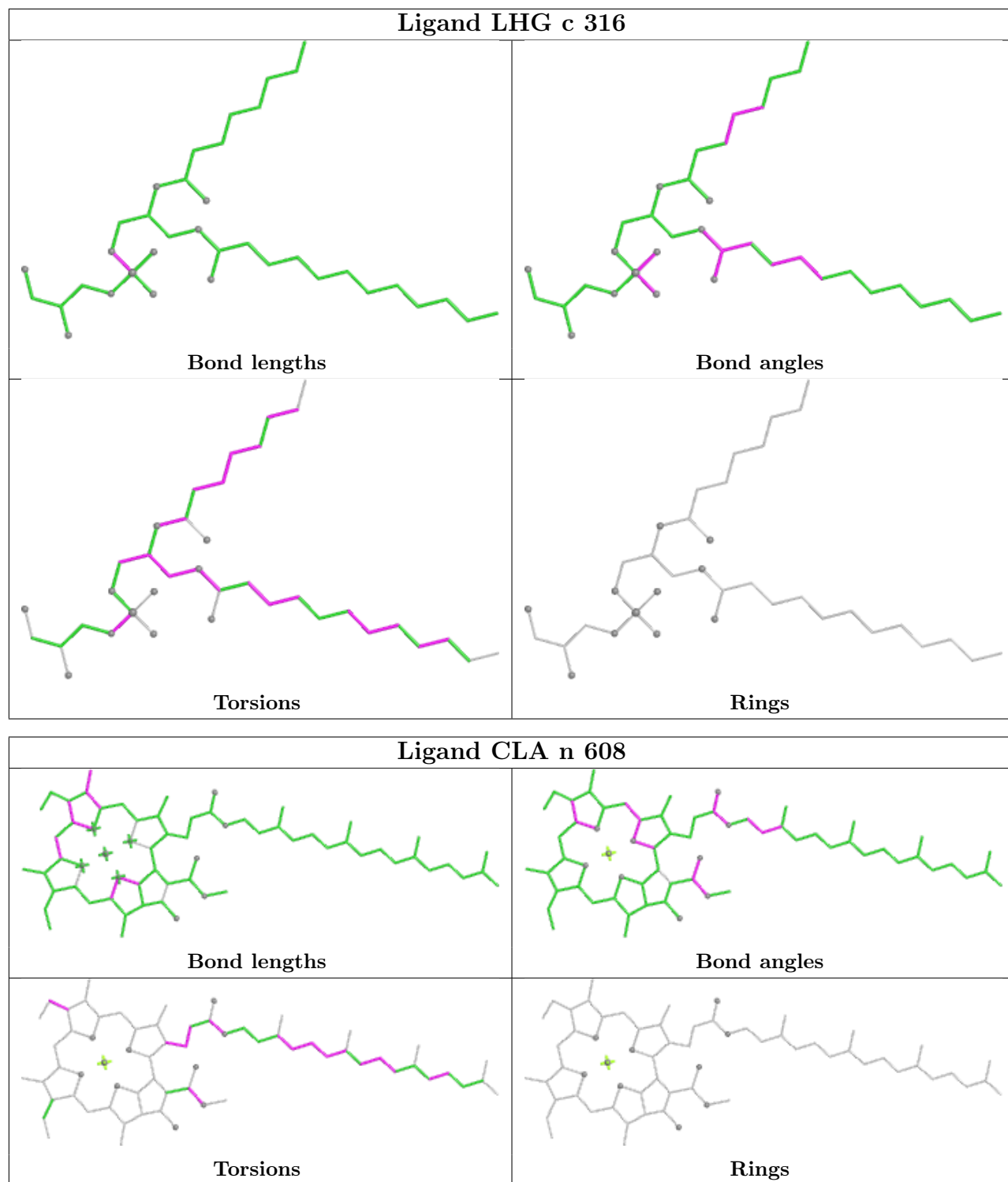
Ligand WVN M 101



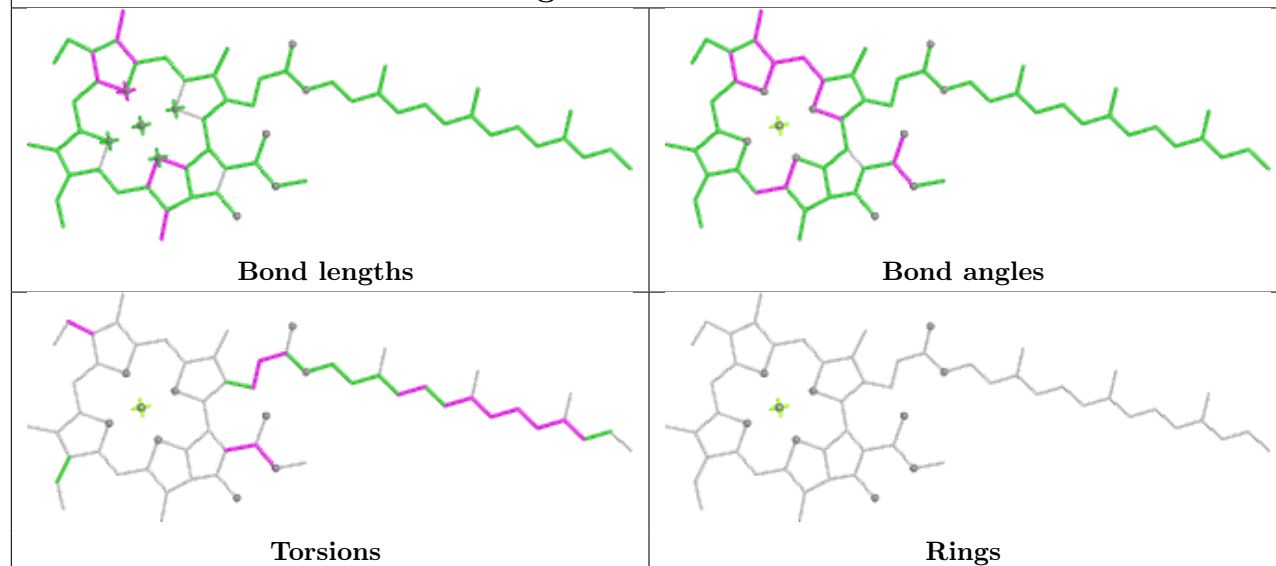
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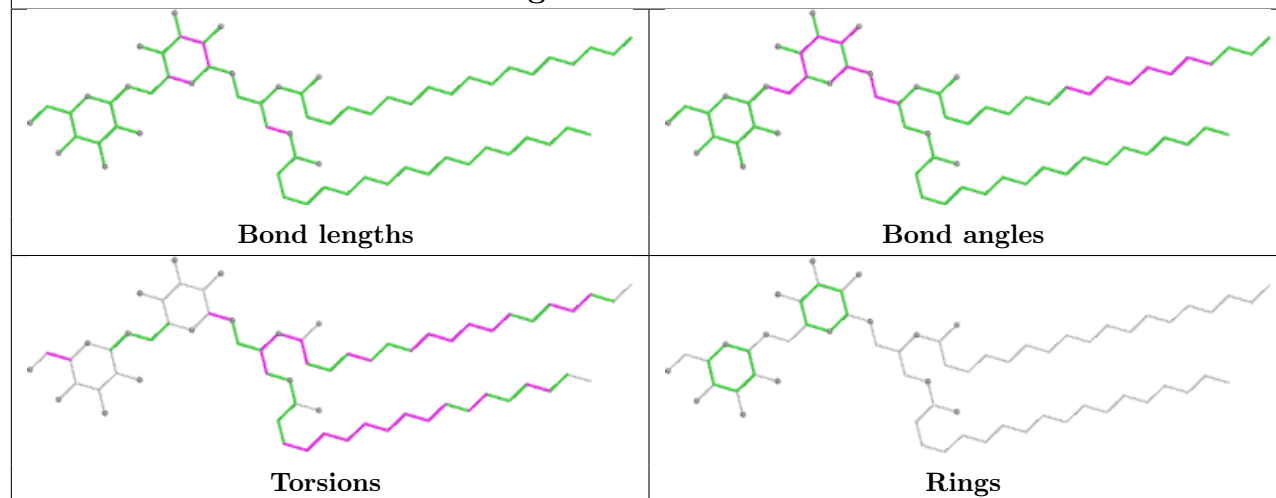




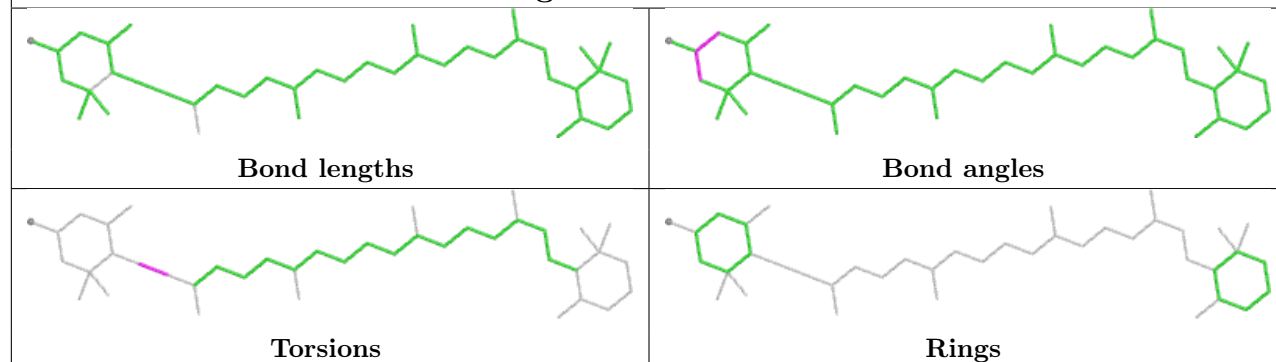
Ligand CLA c 304

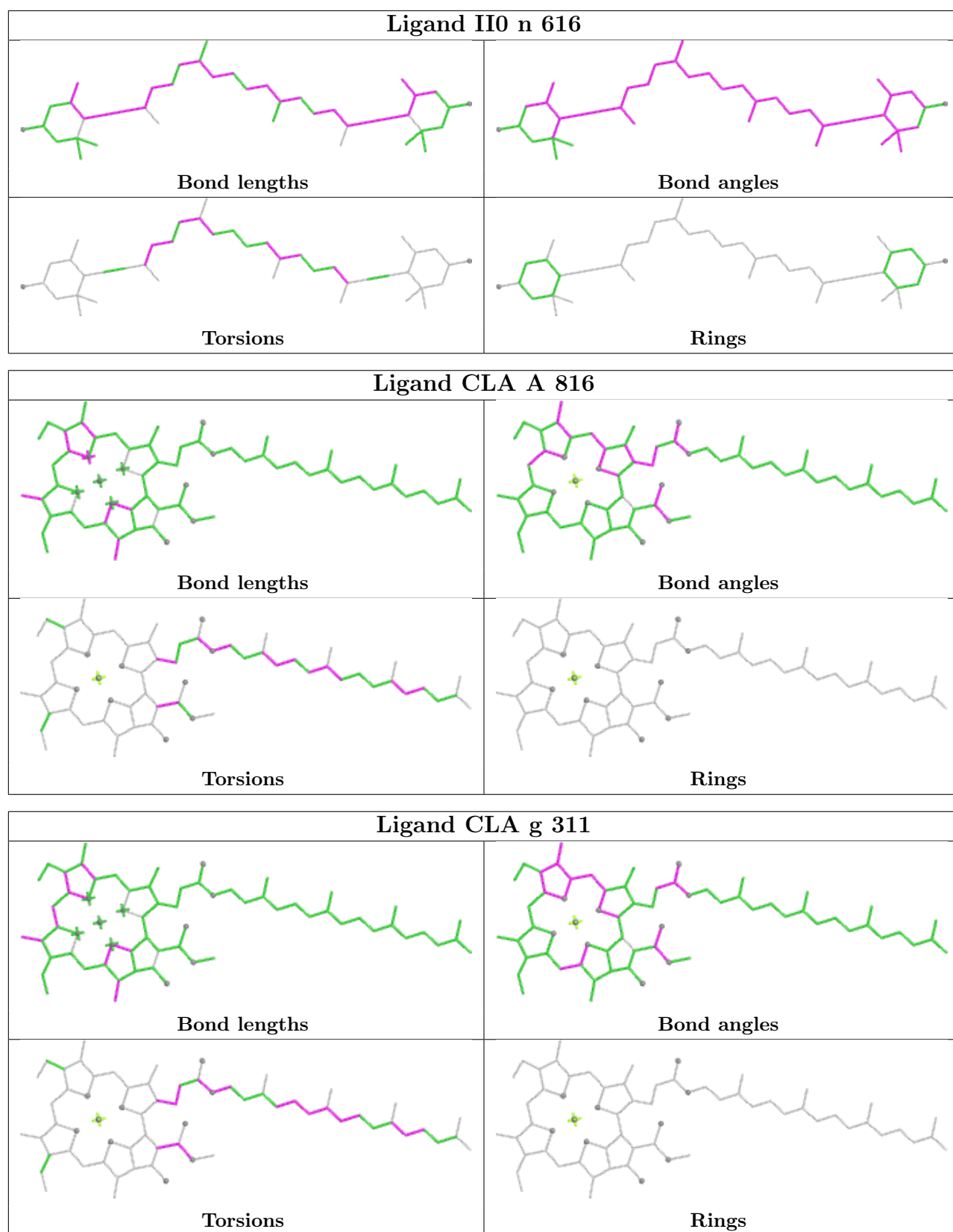


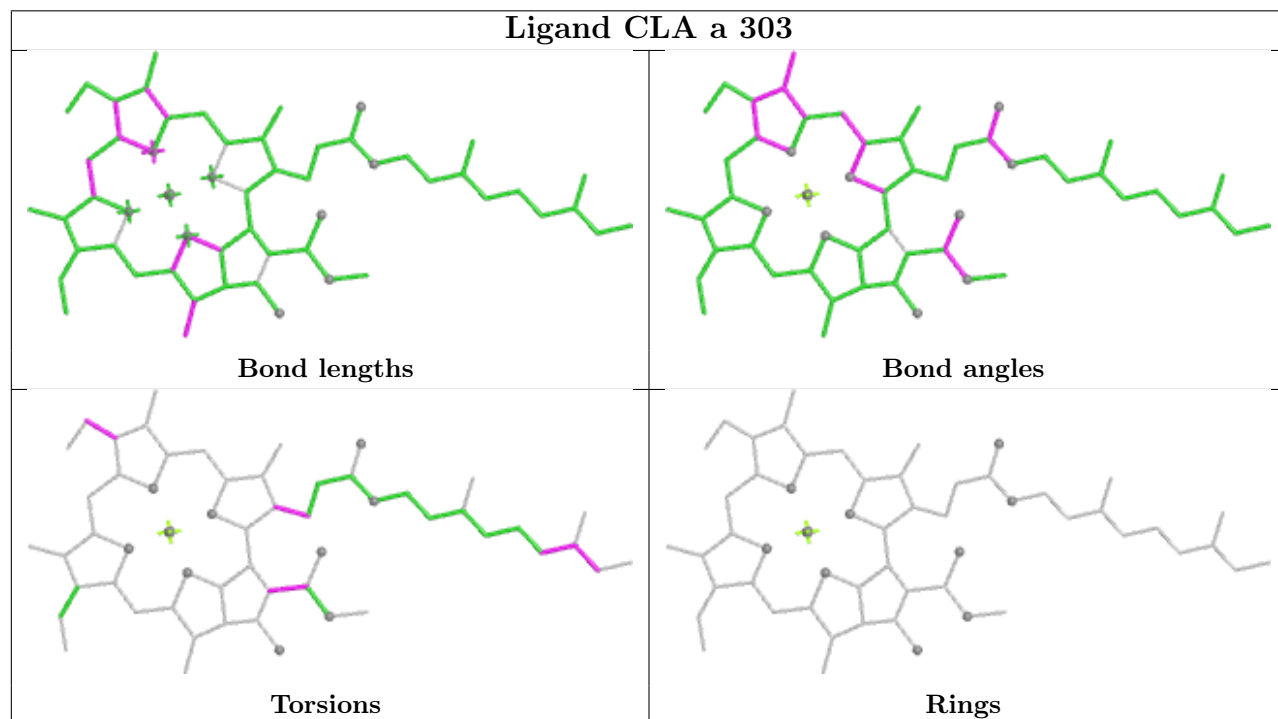
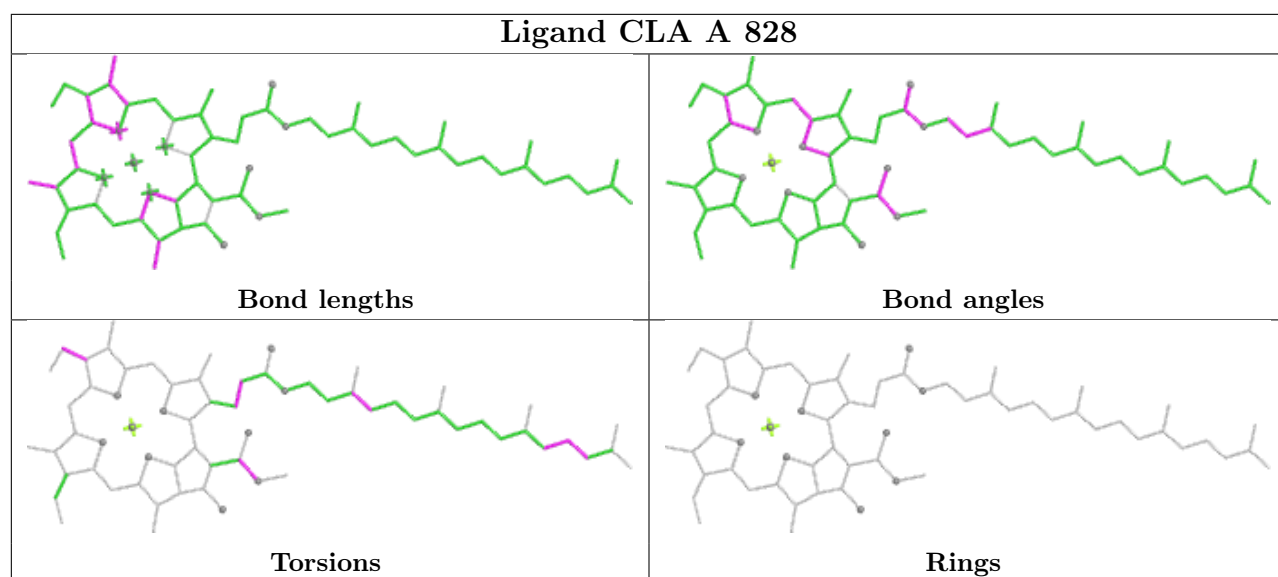
Ligand DGD B 844



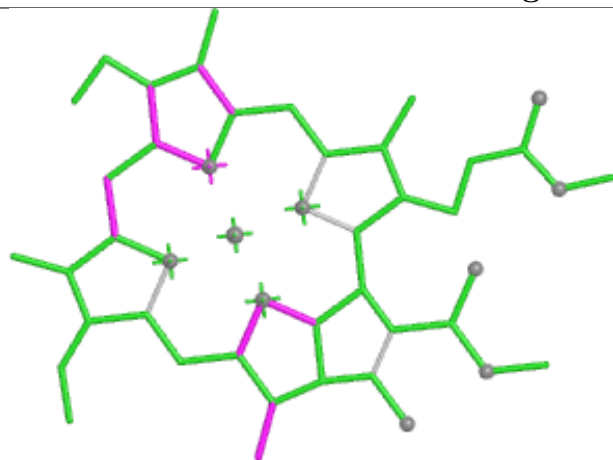
Ligand IHT R 204



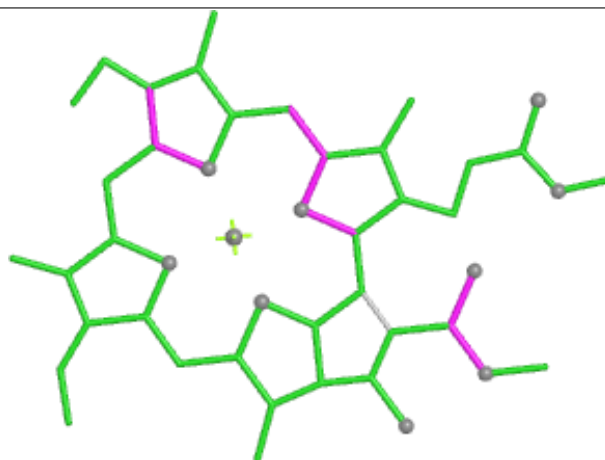




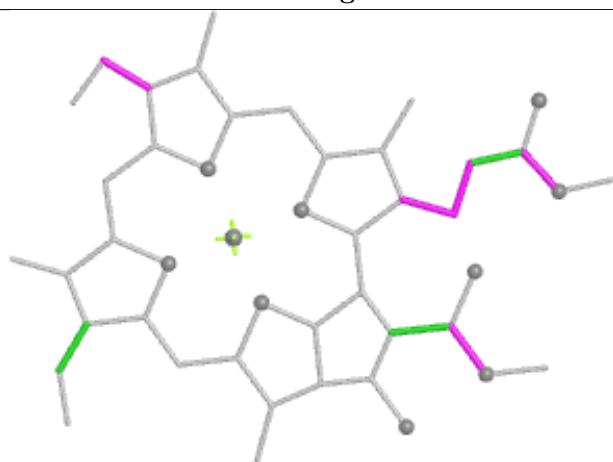
Ligand CLA i 309



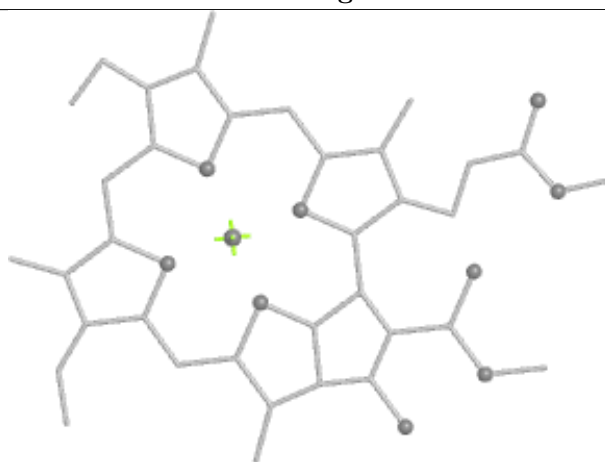
Bond lengths



Bond angles

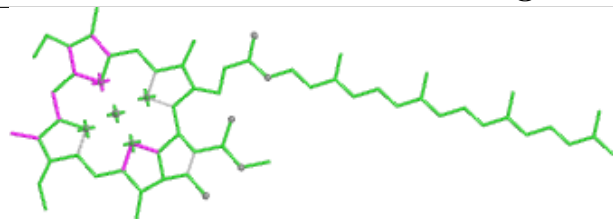


Torsions

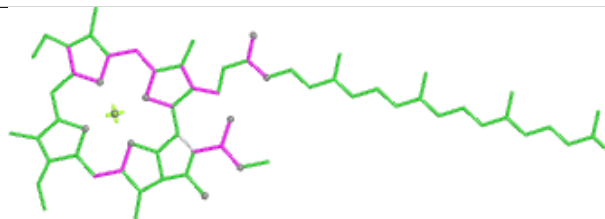


Rings

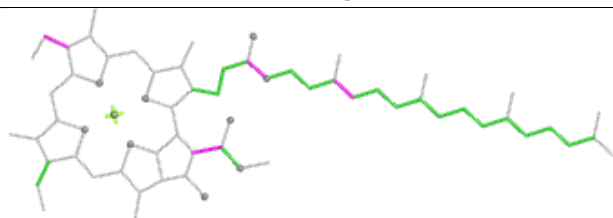
Ligand CLA L 203



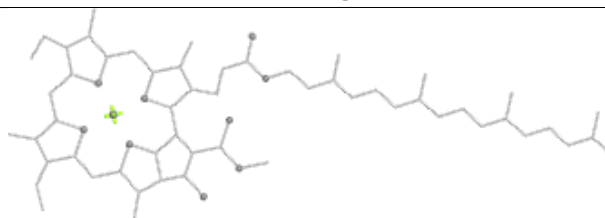
Bond lengths



Bond angles

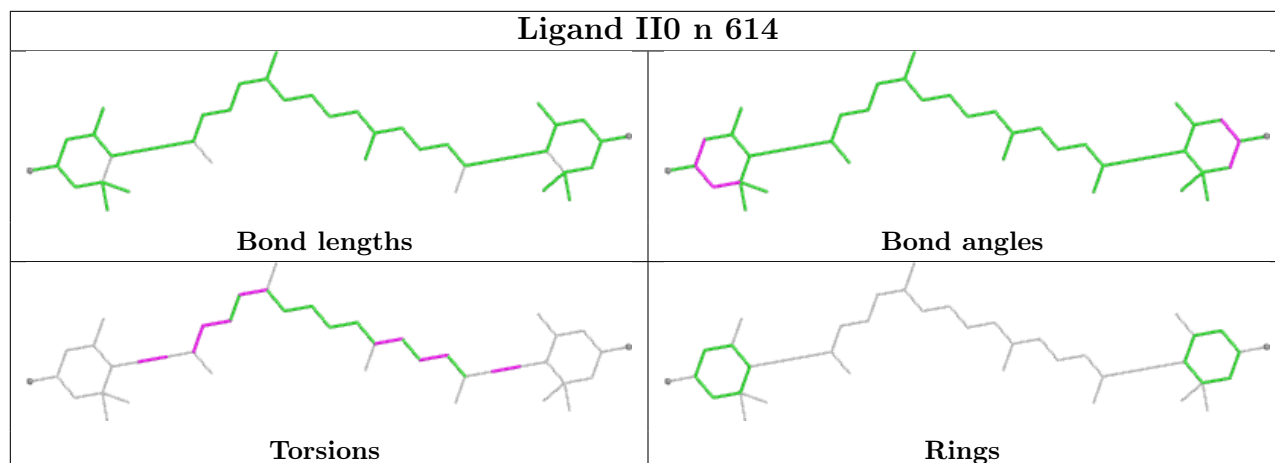


Torsions

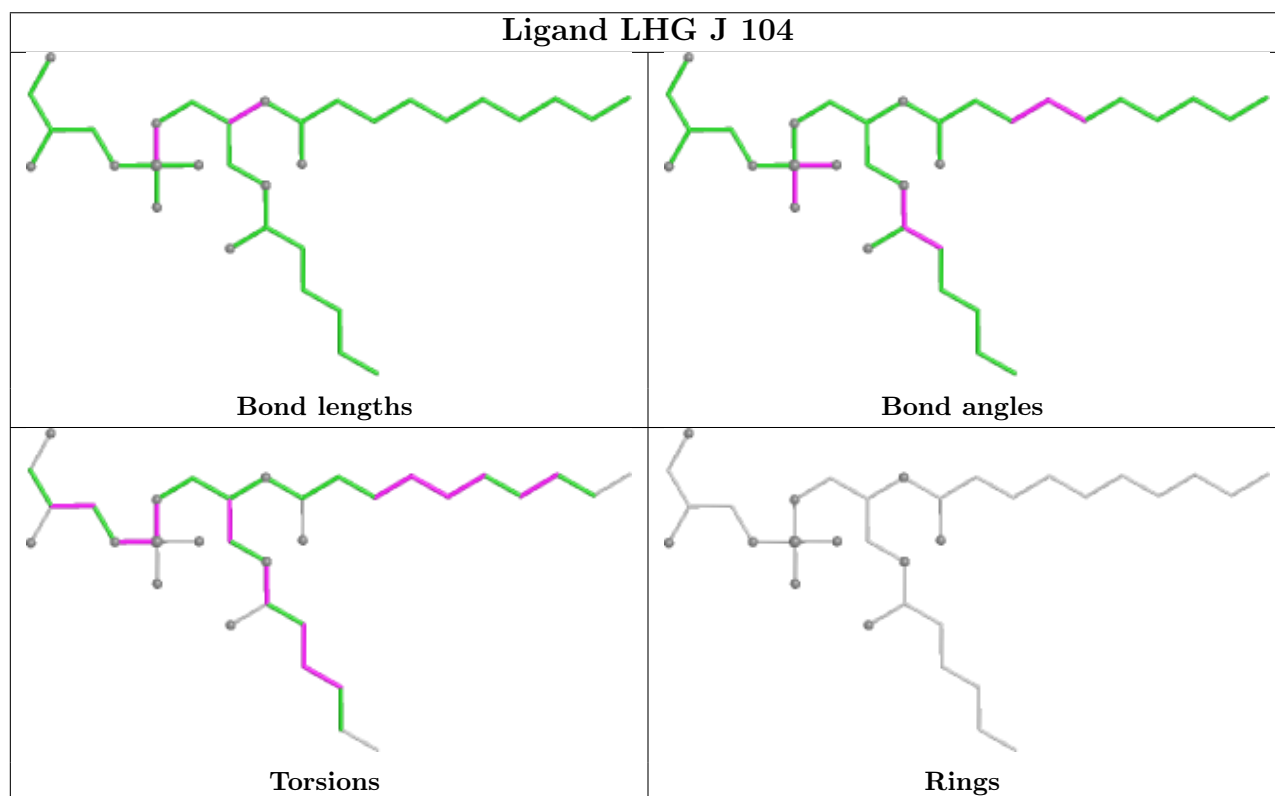


Rings

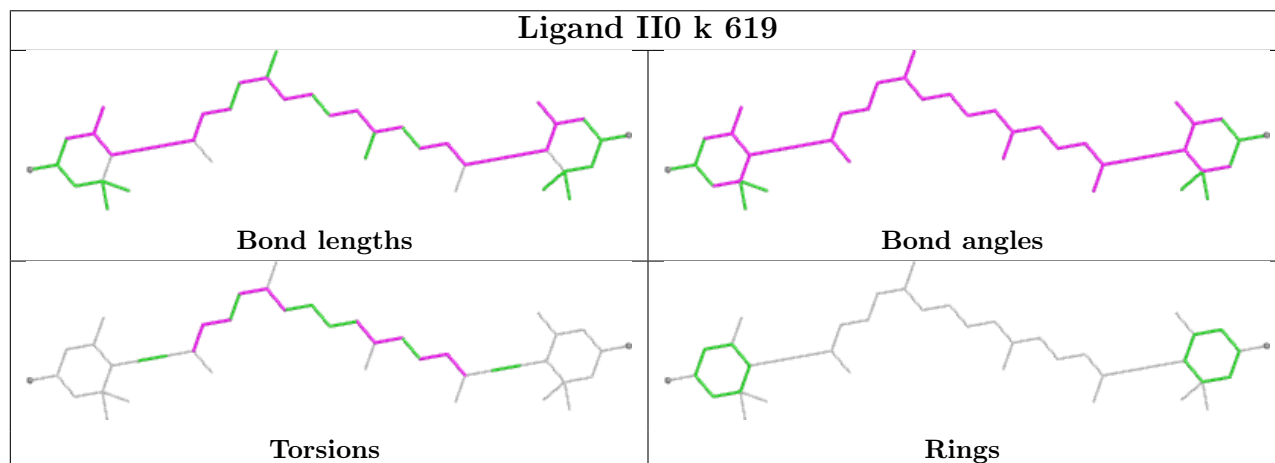
Ligand II0 n 614



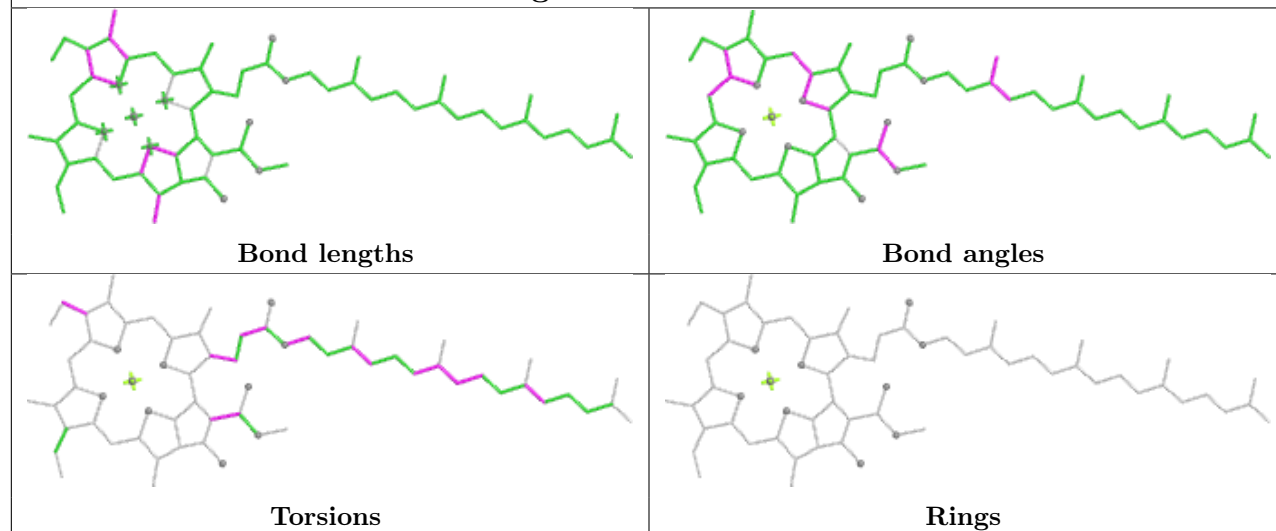
Ligand LHG J 104



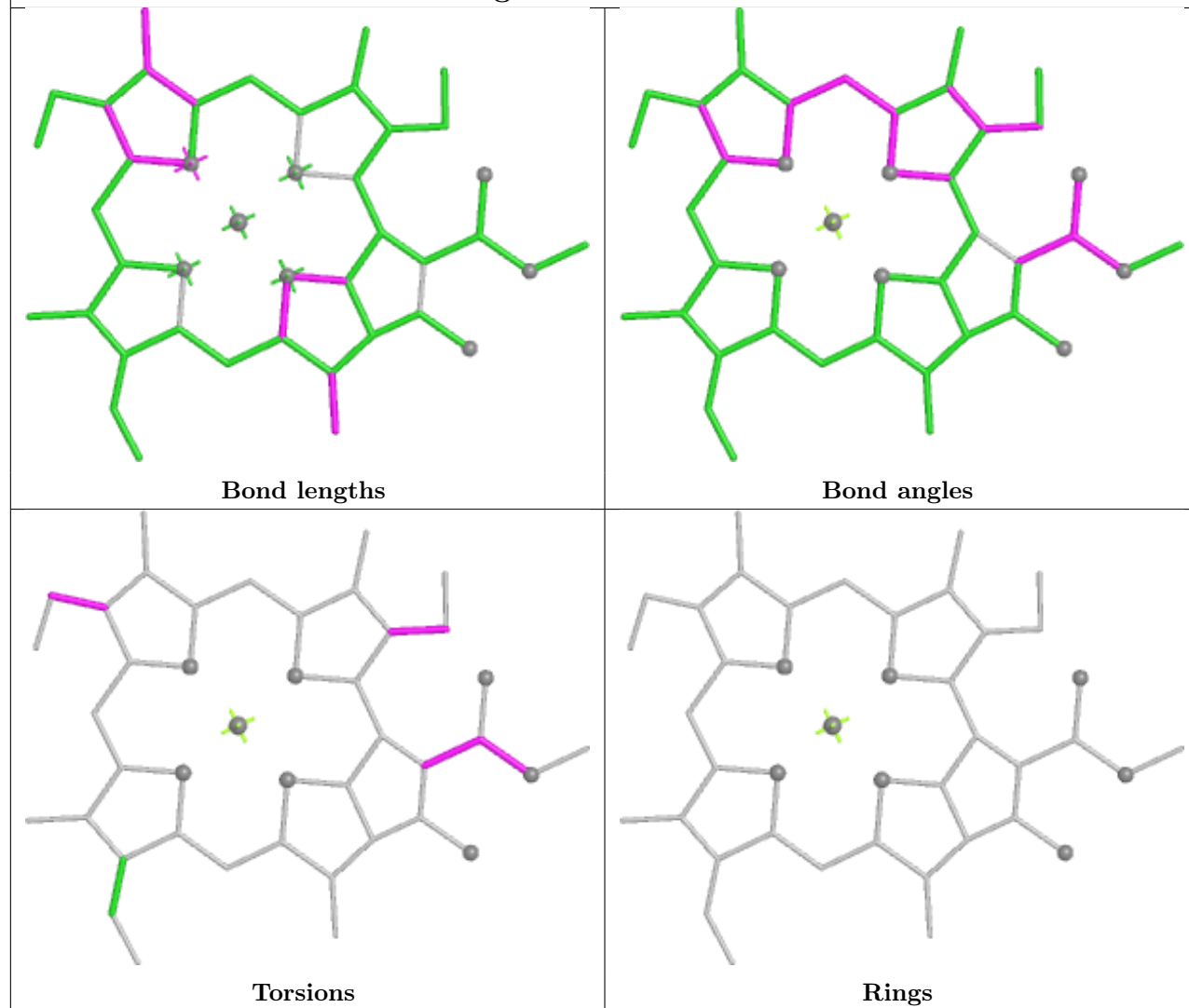
Ligand II0 k 619



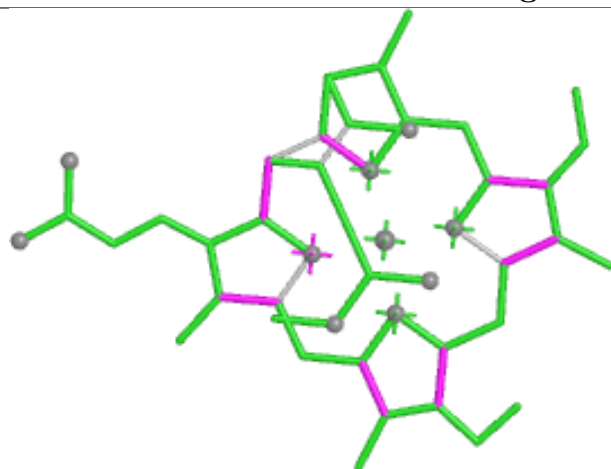
Ligand CLA A 833



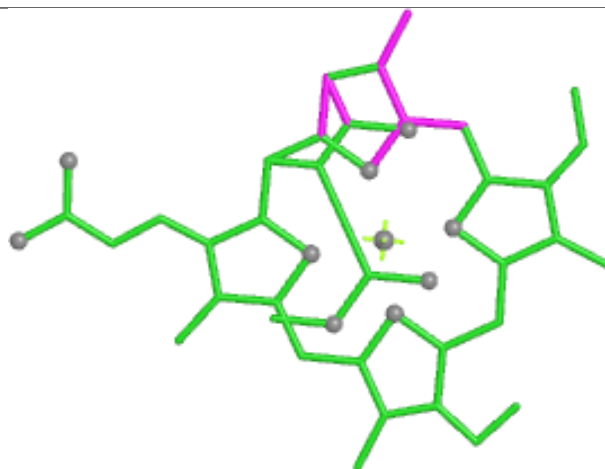
Ligand CLA m 601



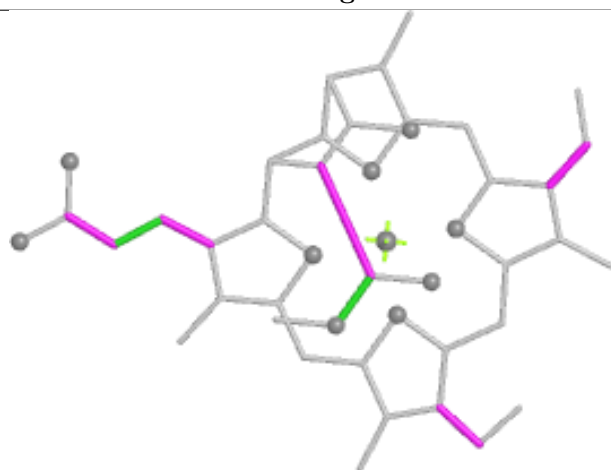
Ligand KC2 k 612



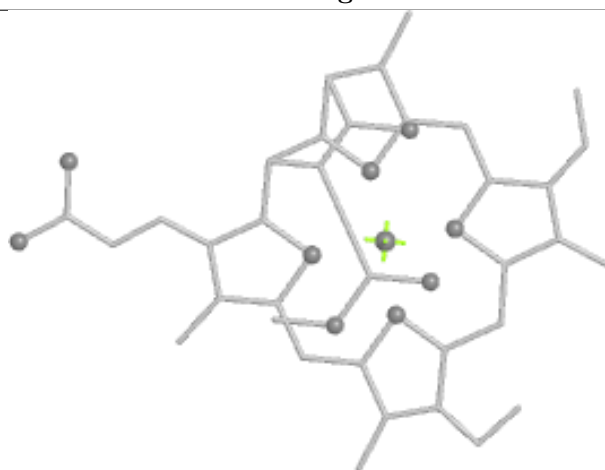
Bond lengths



Bond angles

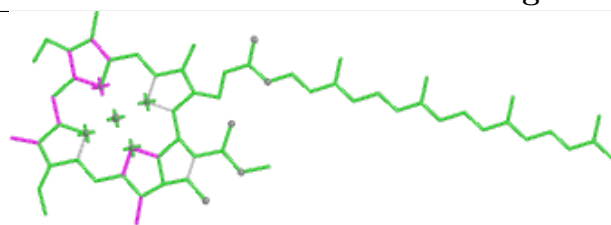


Torsions

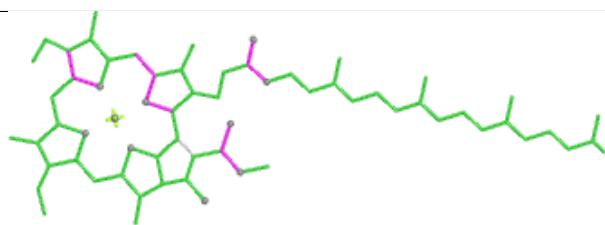


Rings

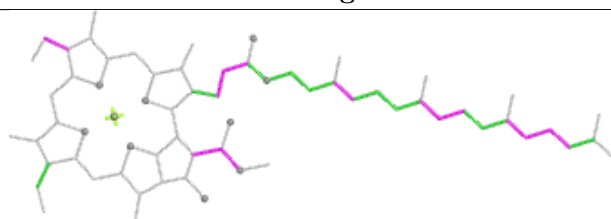
Ligand CLA l 306



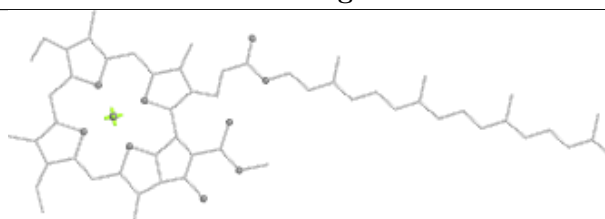
Bond lengths



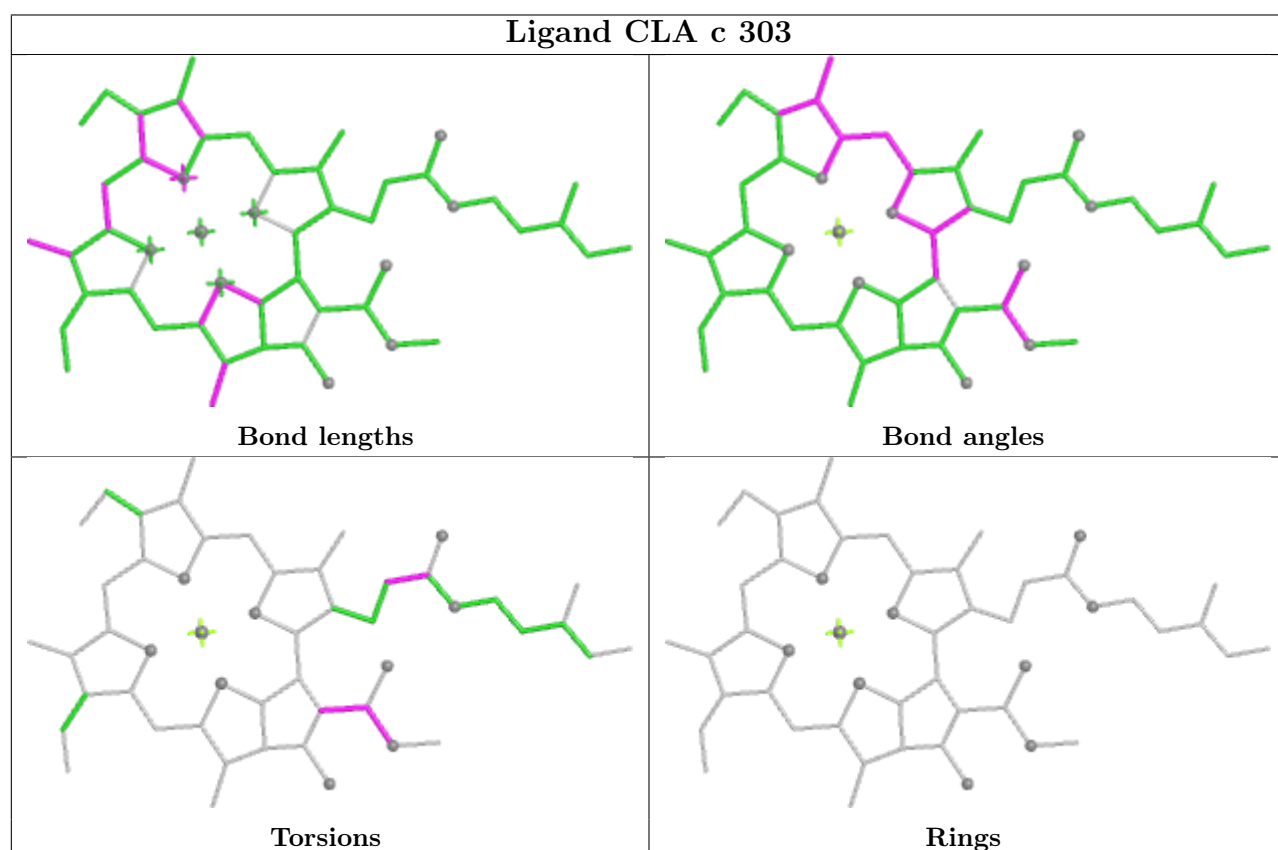
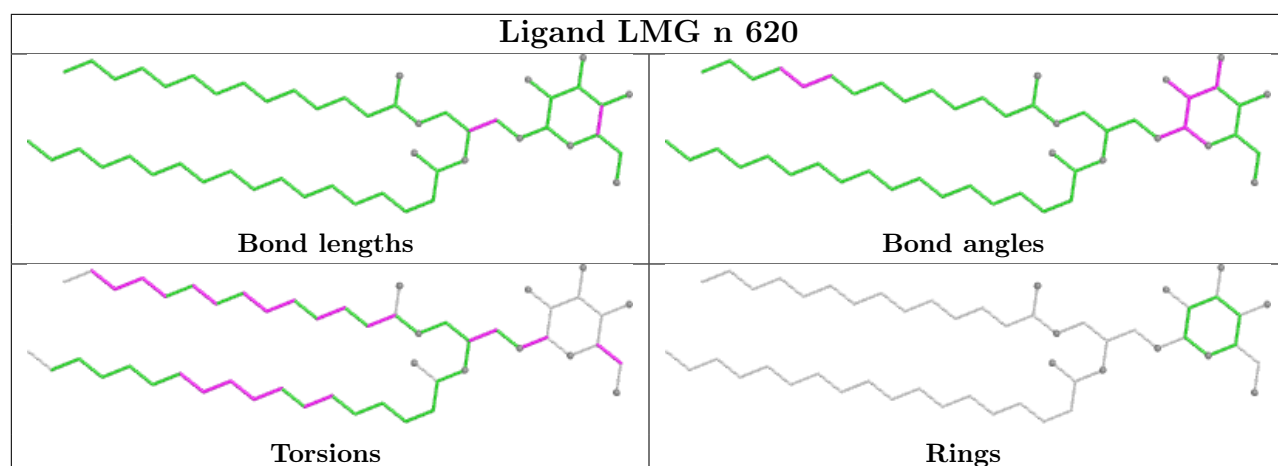
Bond angles



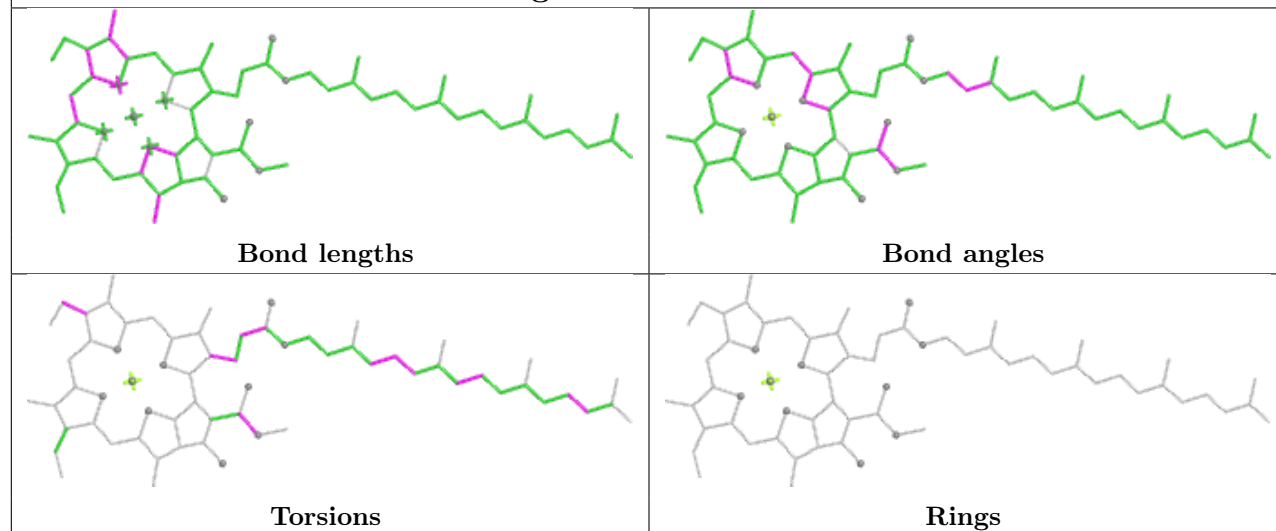
Torsions



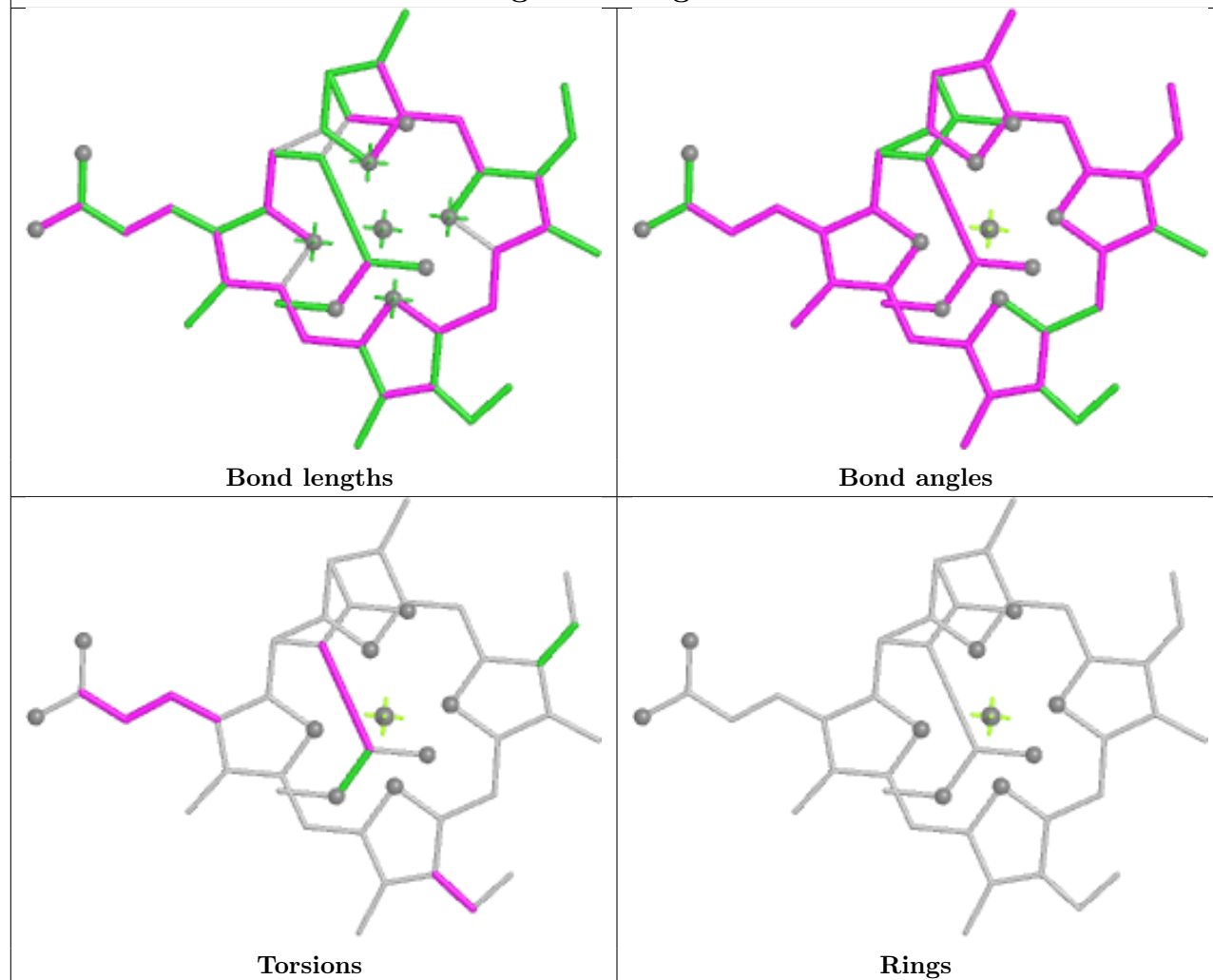
Rings

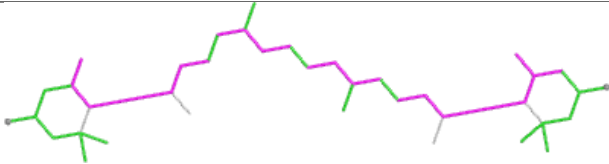
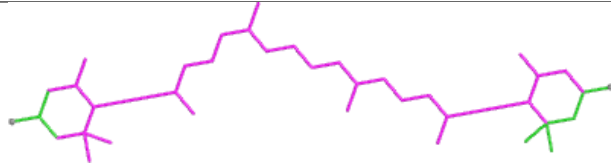
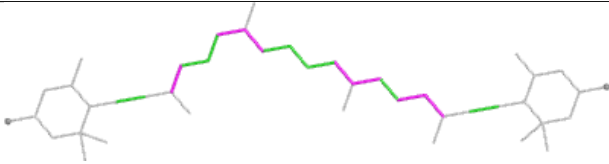
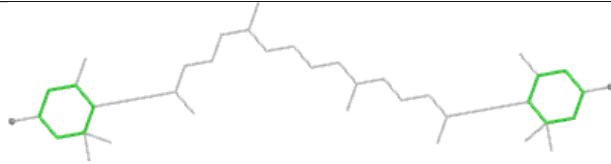


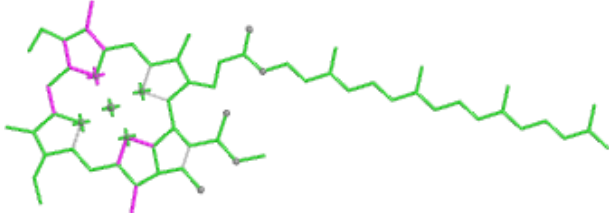
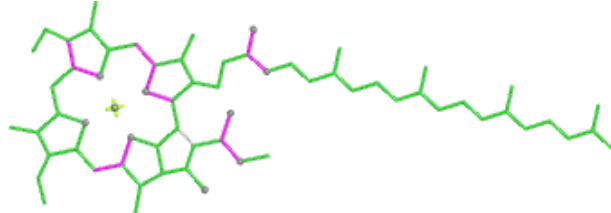
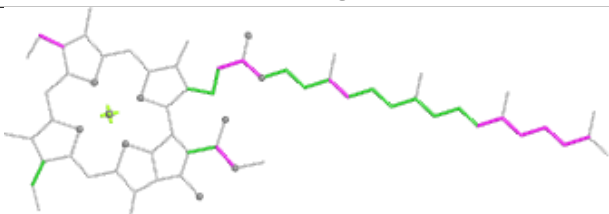
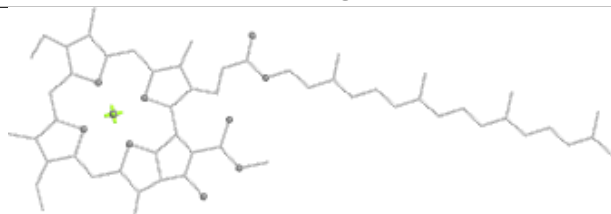
Ligand CLA O 202

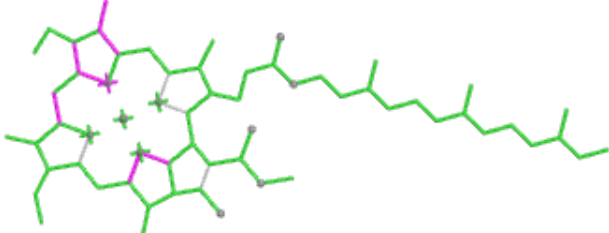
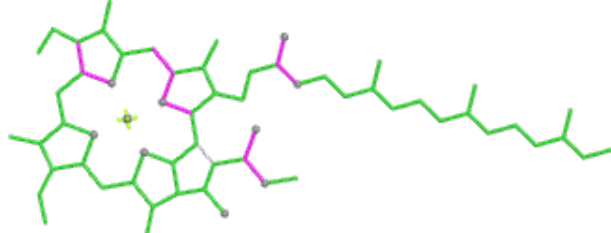
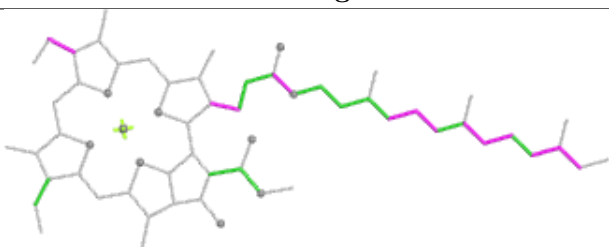
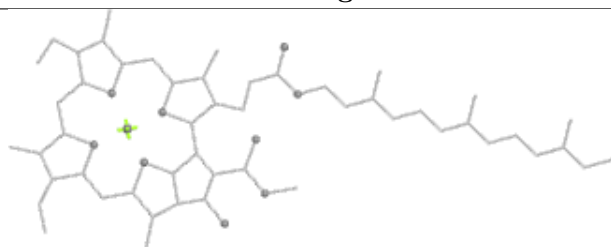


Ligand KC2 g 315

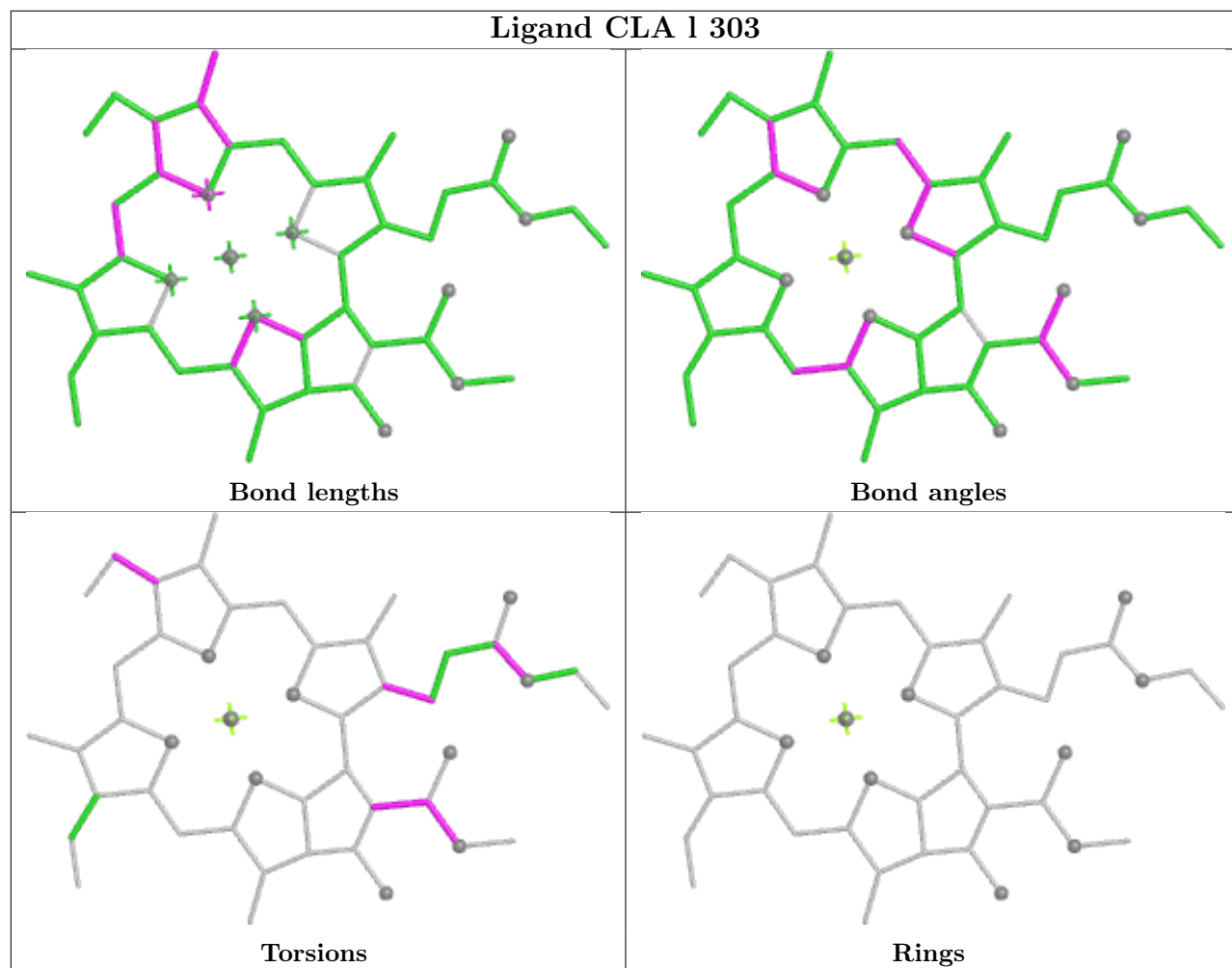


Ligand II0 g 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

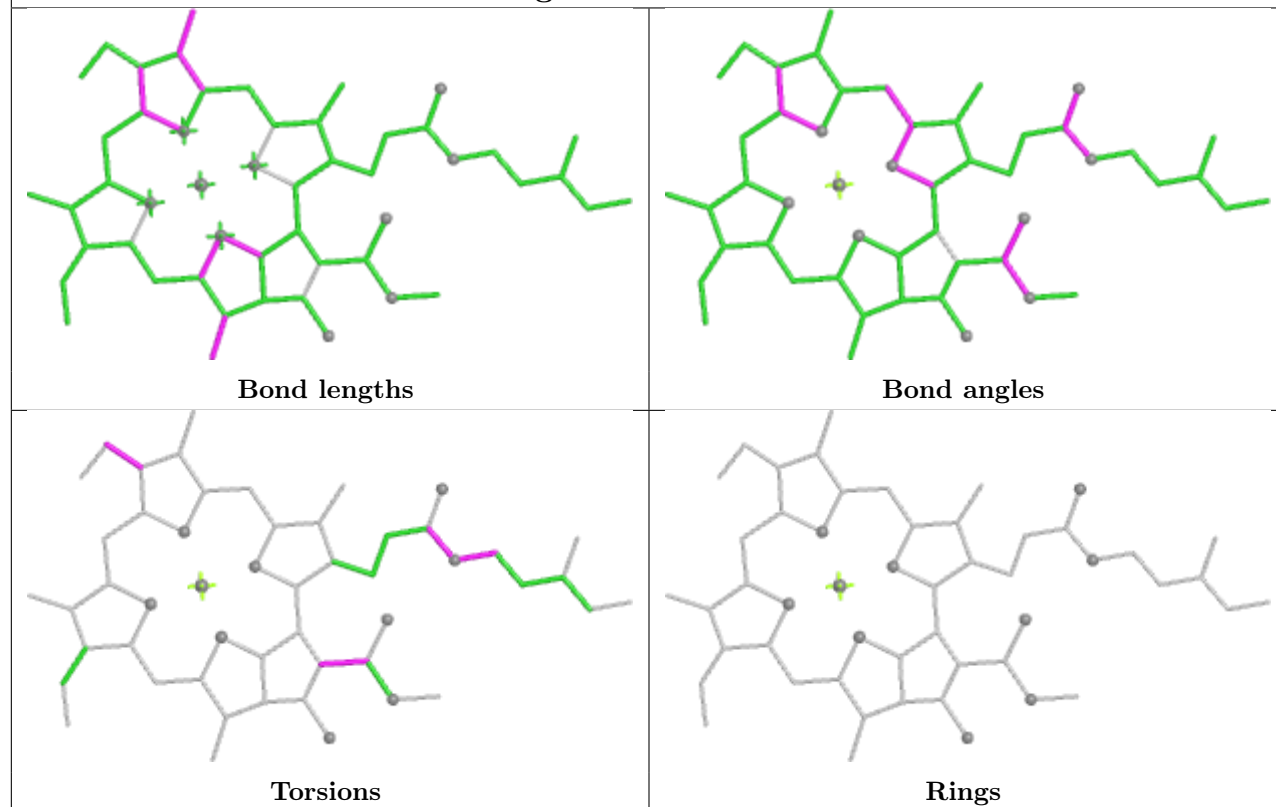
Ligand CLA m 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

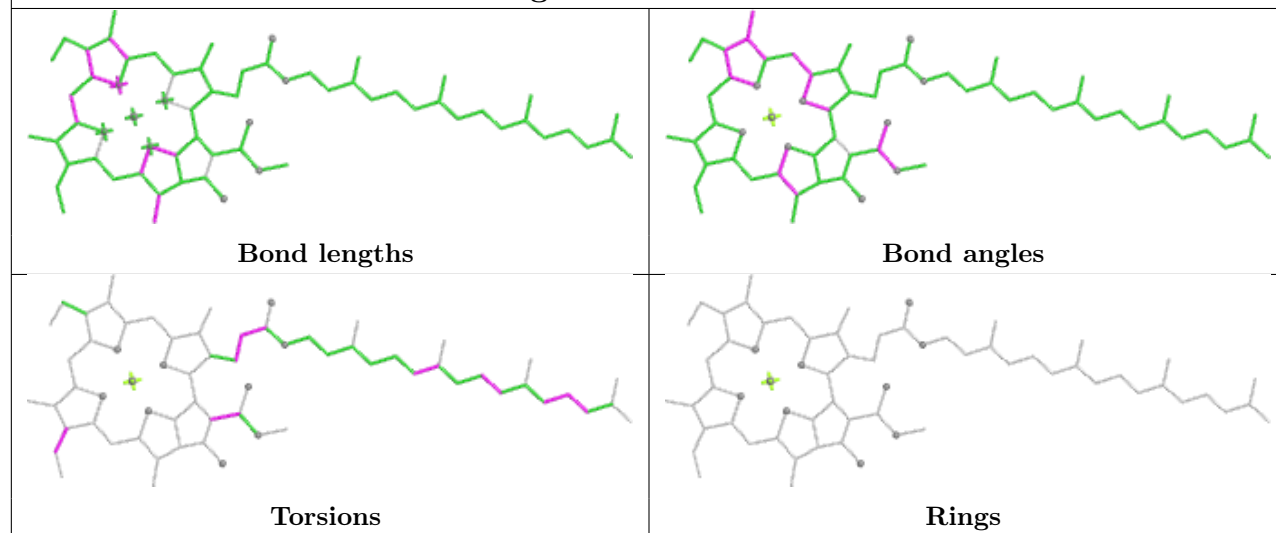
Ligand CLA 1 303



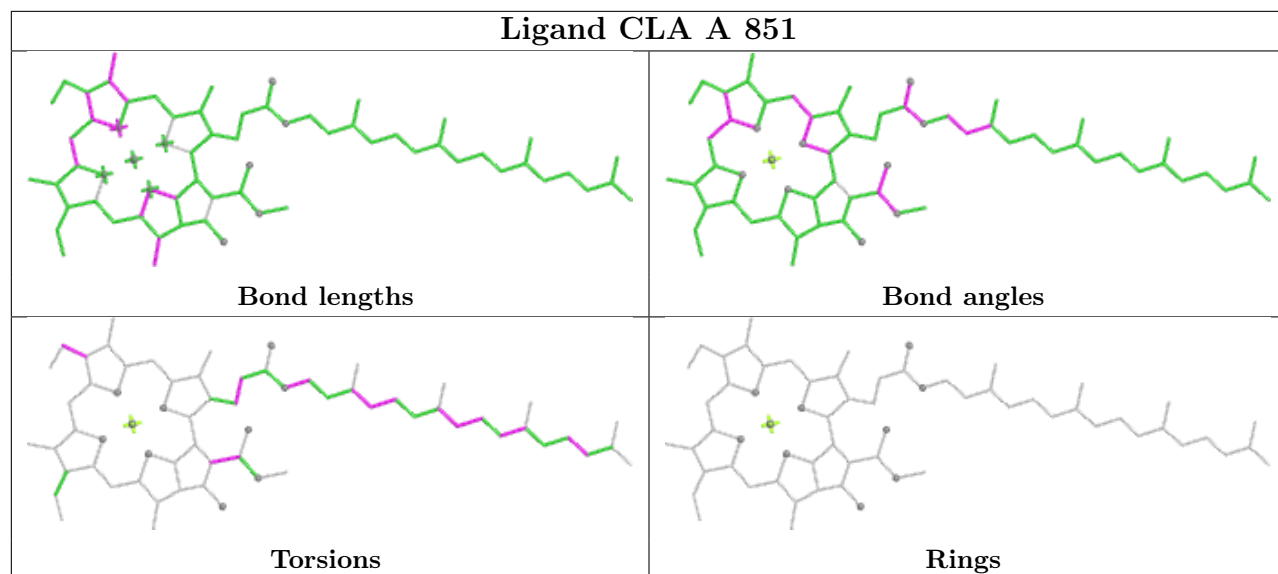
Ligand CLA b 302



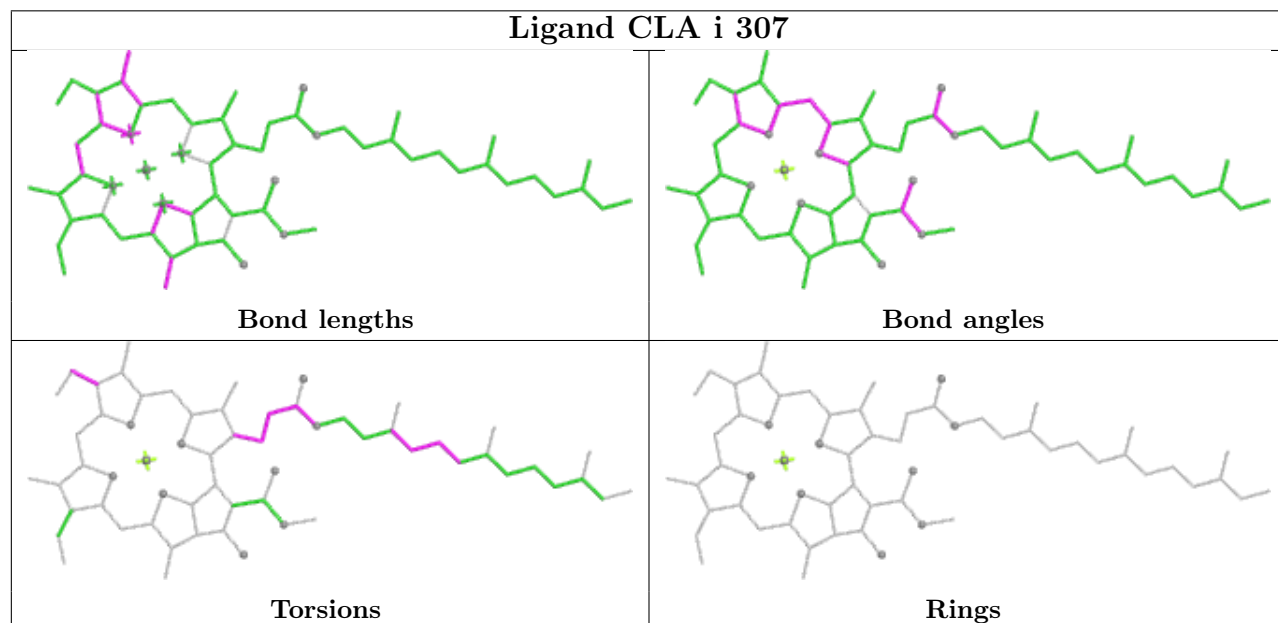
Ligand CLA m 604



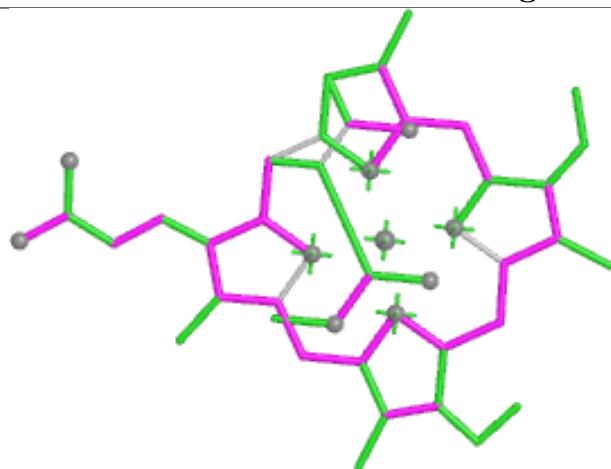
Ligand CLA A 851



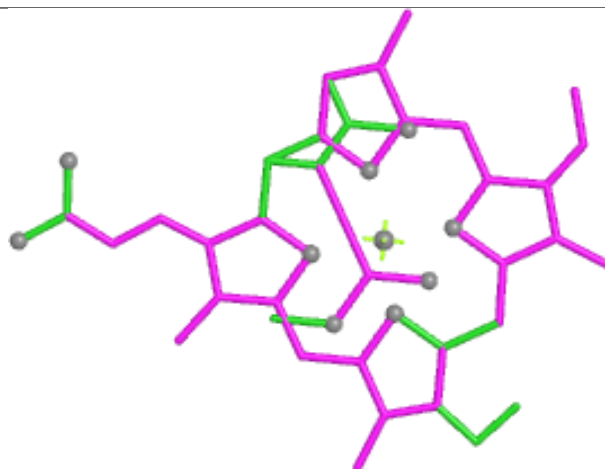
Ligand CLA i 307



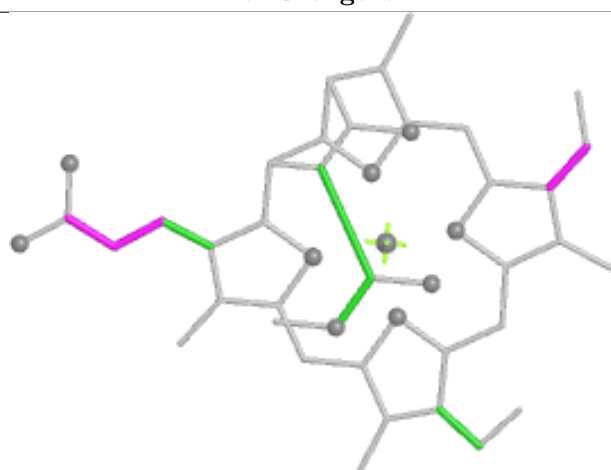
Ligand KC2 n 611



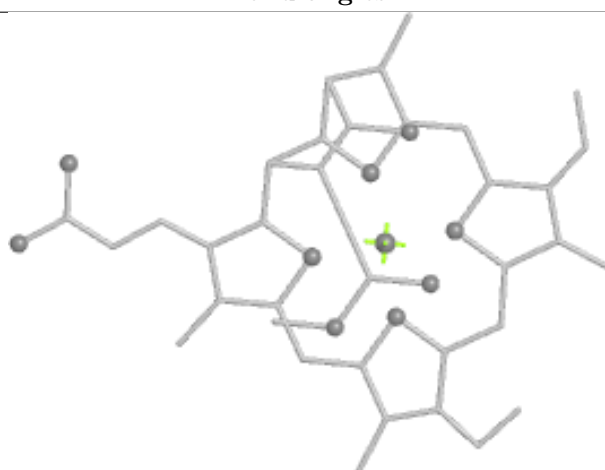
Bond lengths



Bond angles

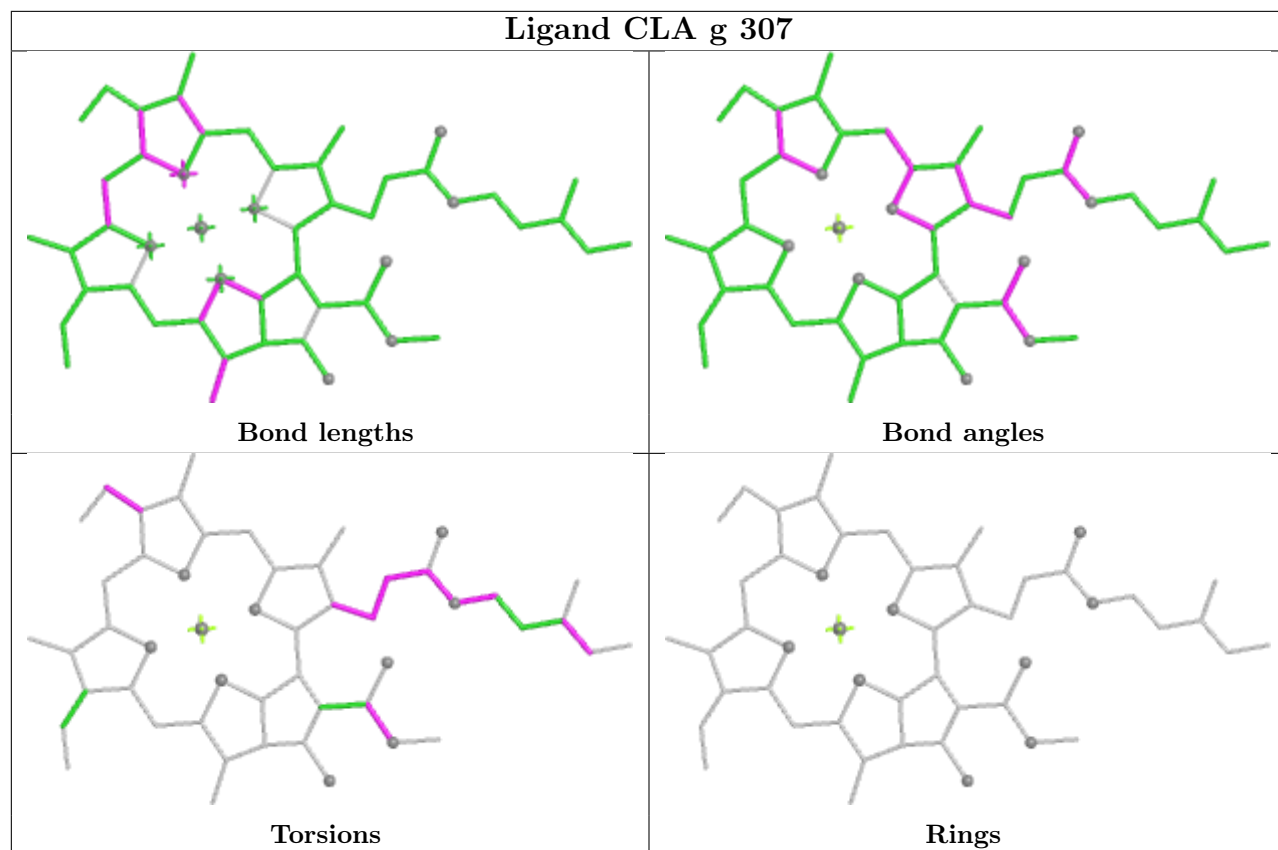


Torsions

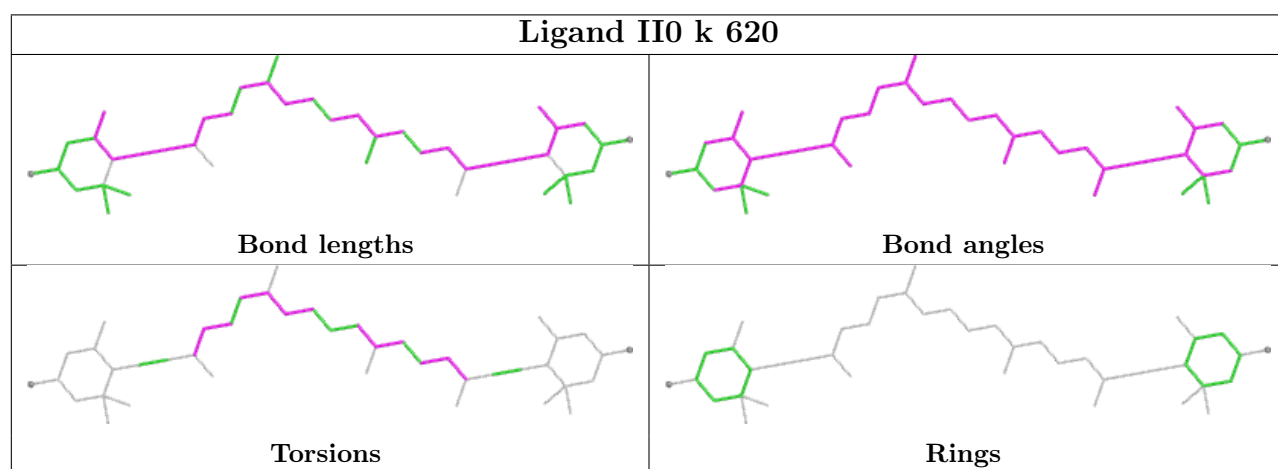


Rings

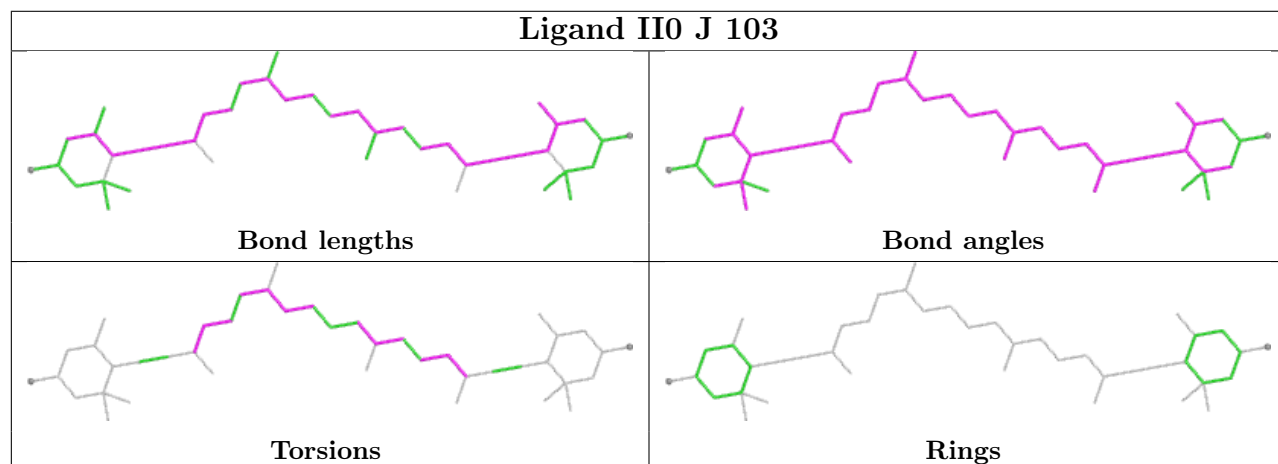
Ligand CLA g 307



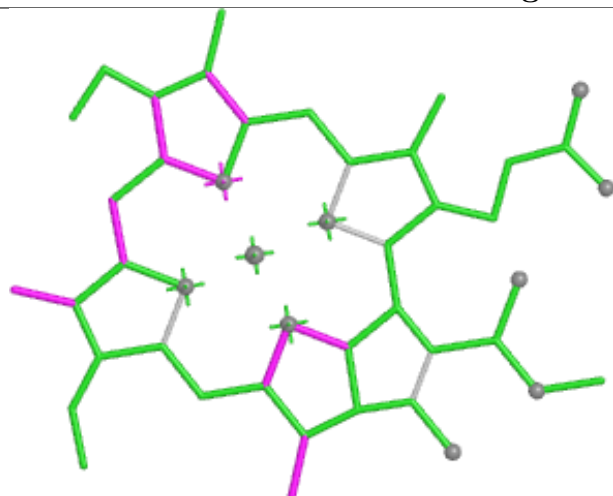
Ligand II0 k 620



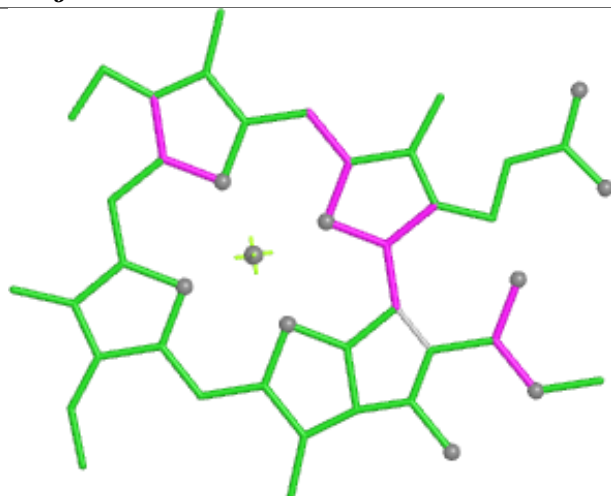
Ligand II0 J 103



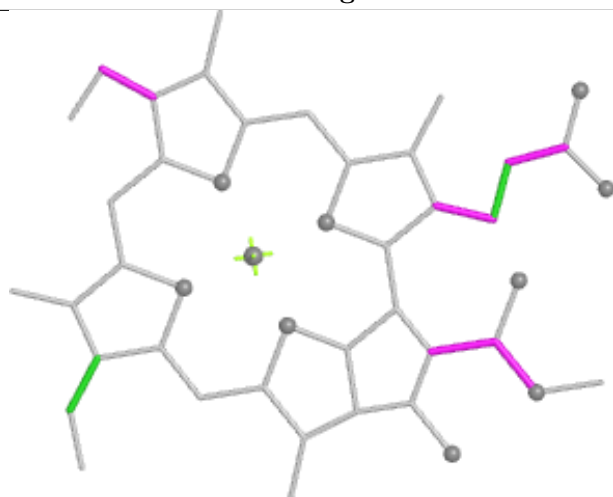
Ligand CLA j 306



Bond lengths



Bond angles

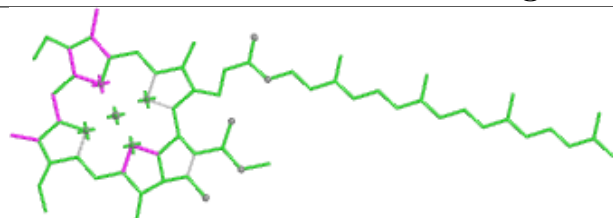


Torsions

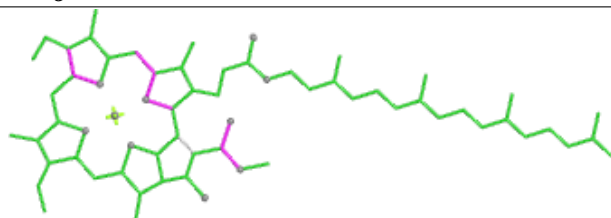


Rings

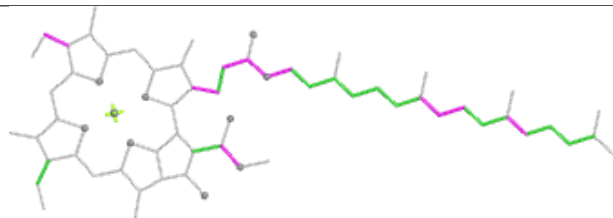
Ligand CLA j 310



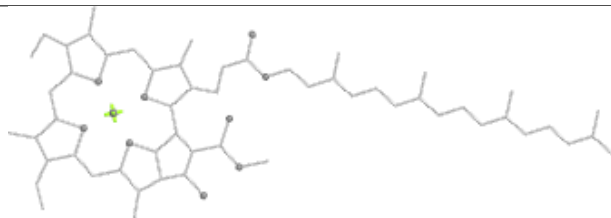
Bond lengths



Bond angles

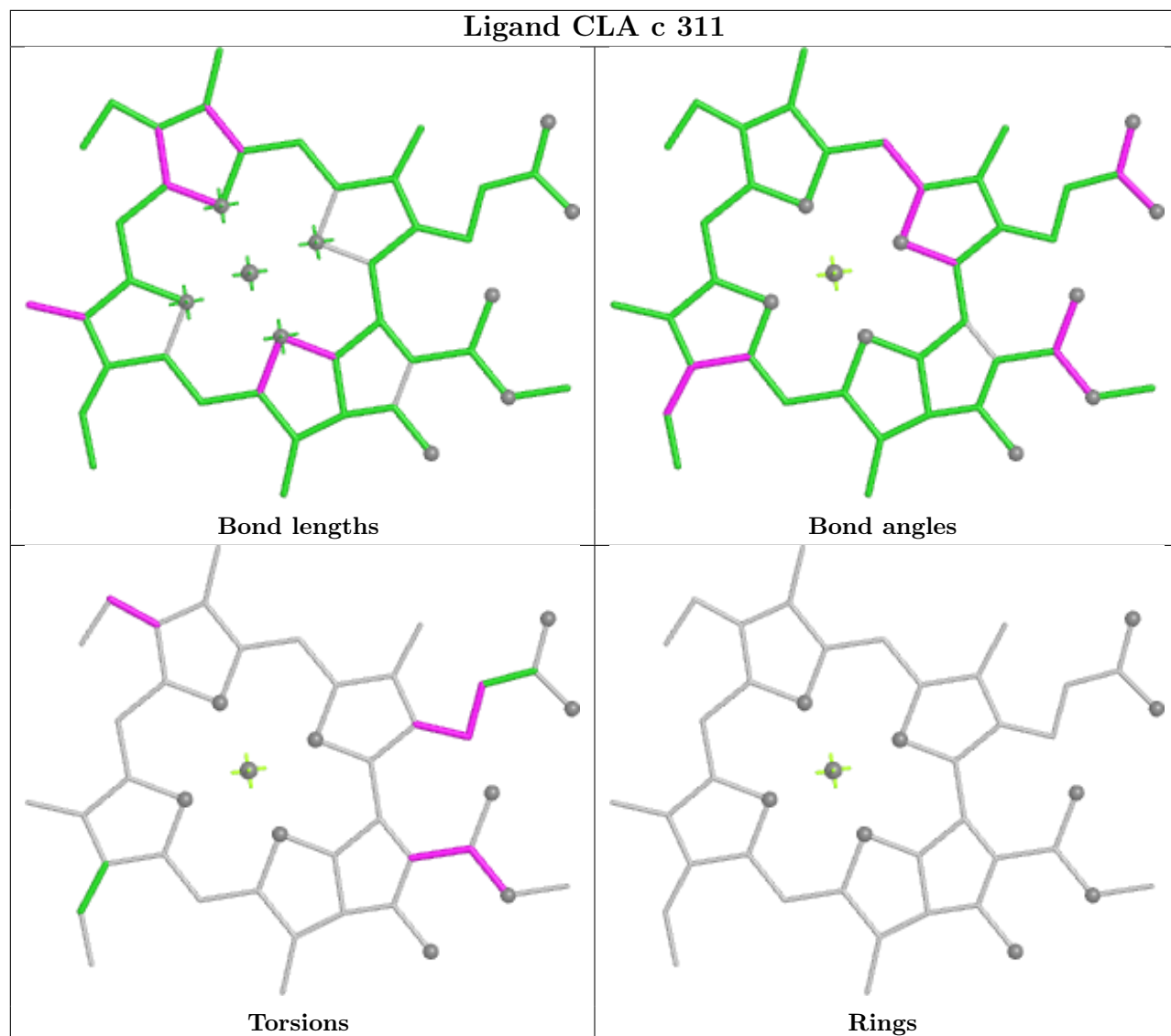


Torsions

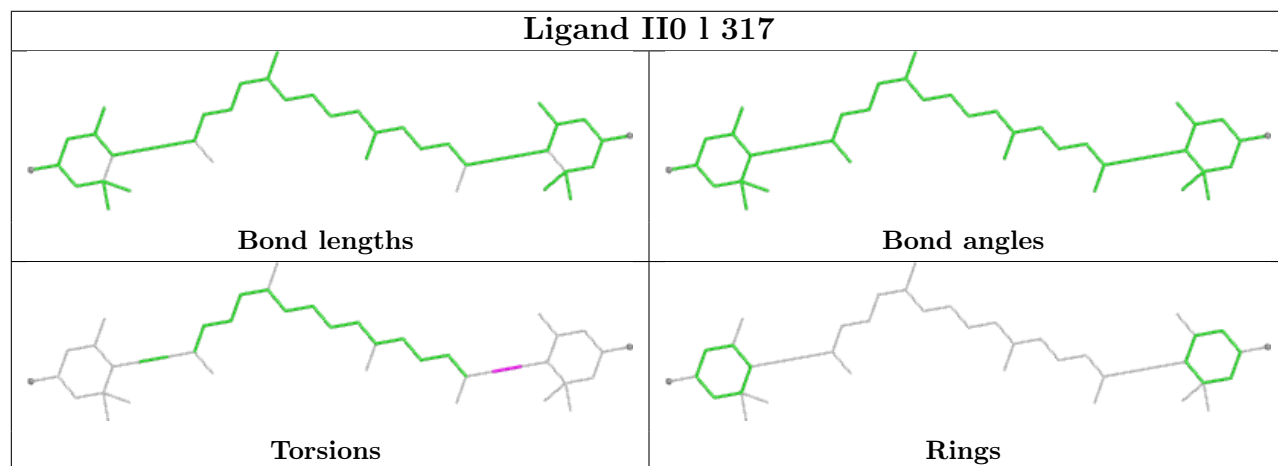


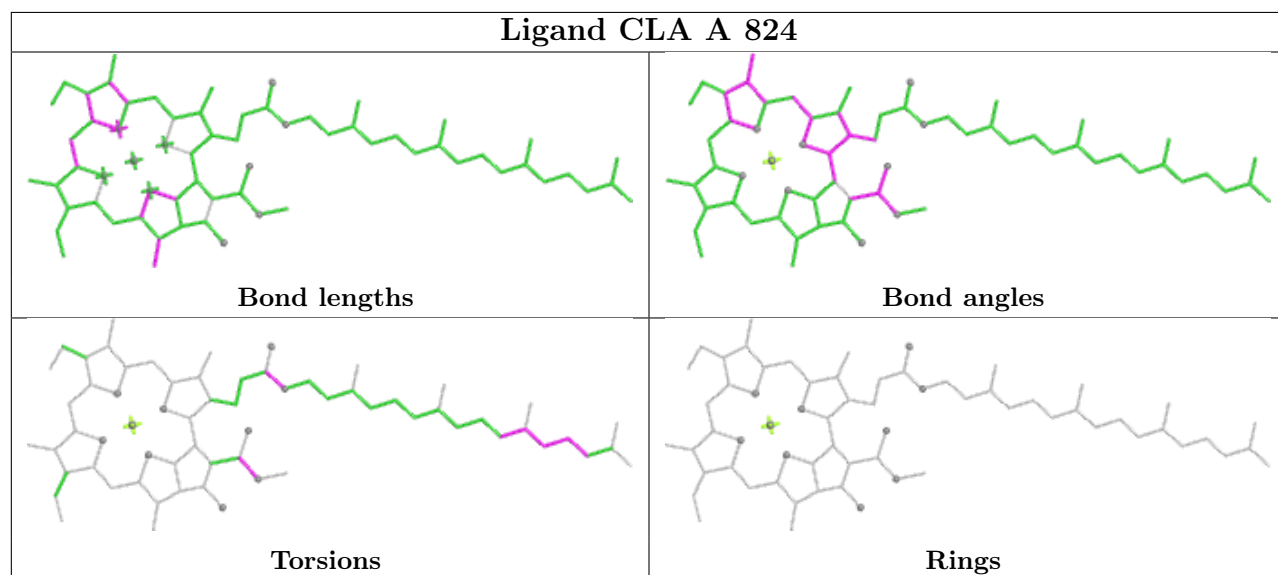
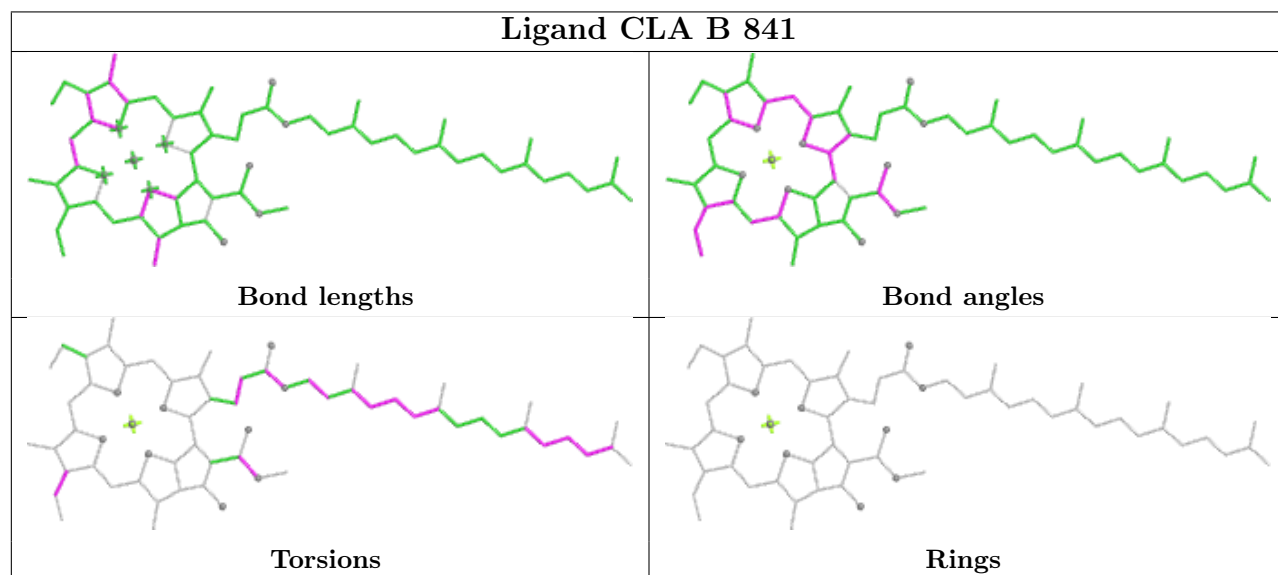
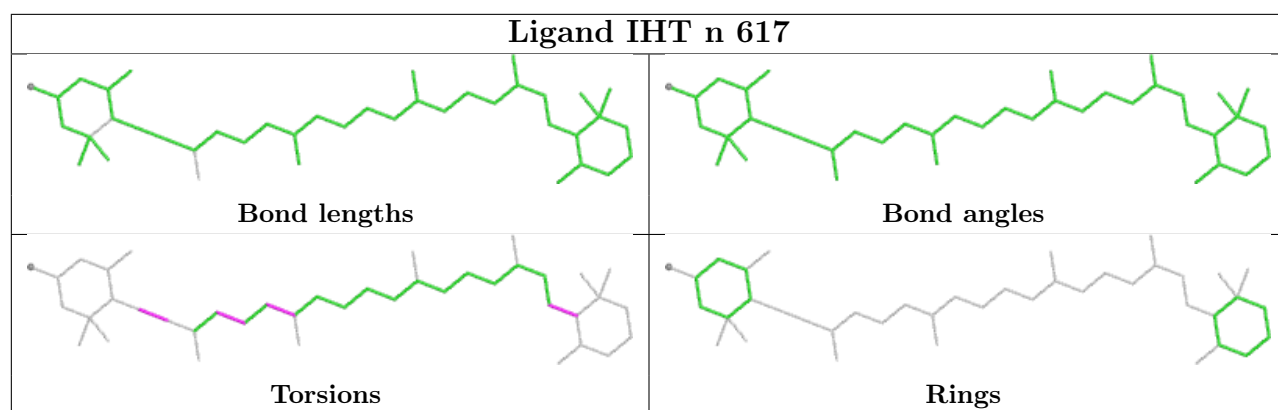
Rings

Ligand CLA c 311

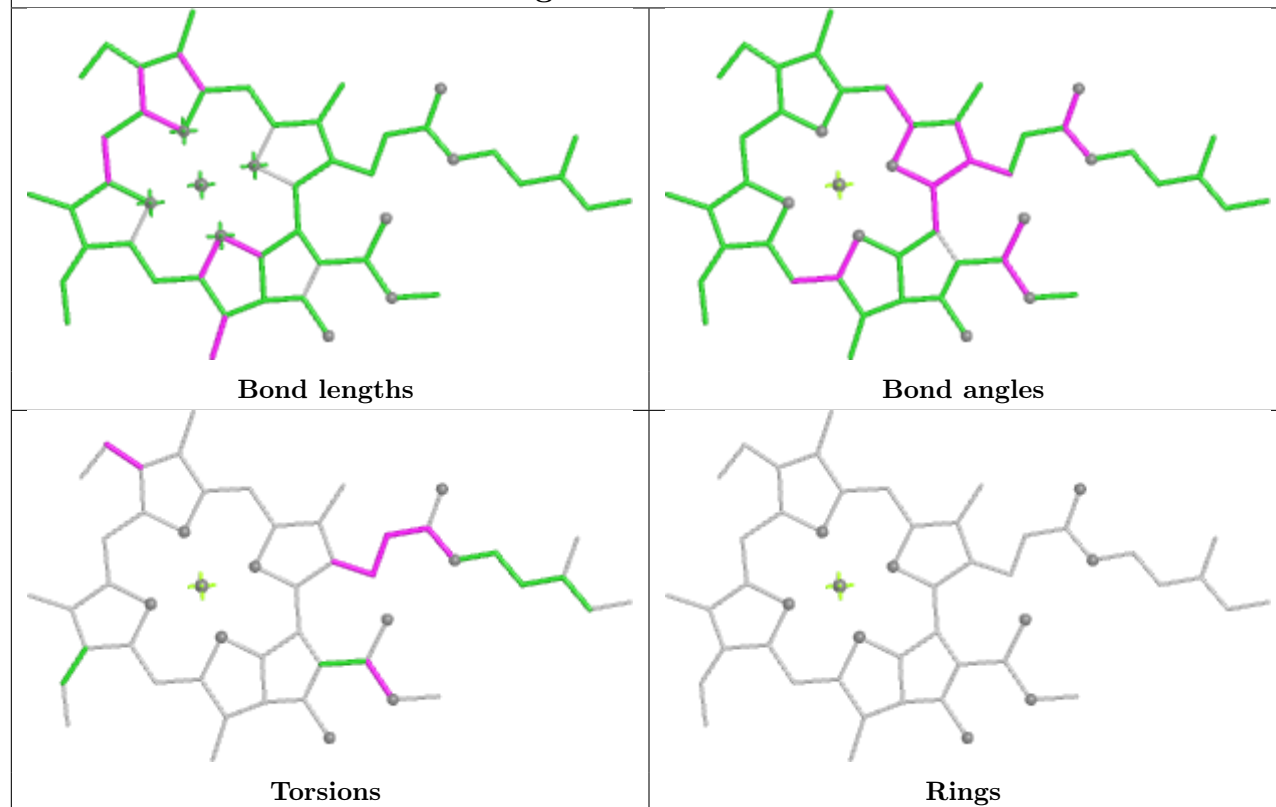


Ligand II0 l 317

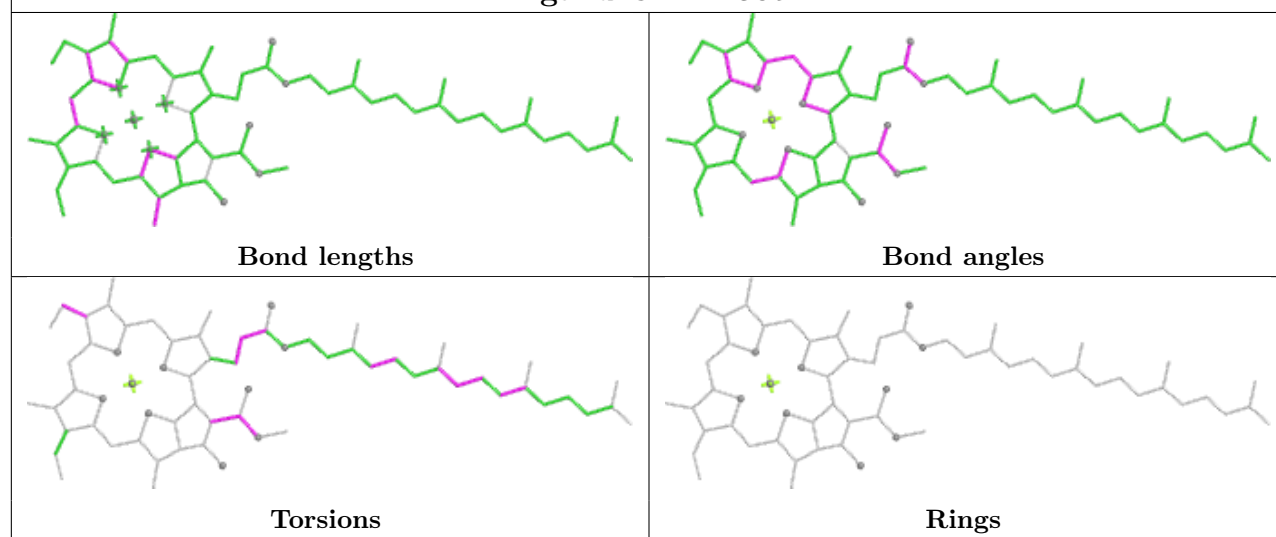




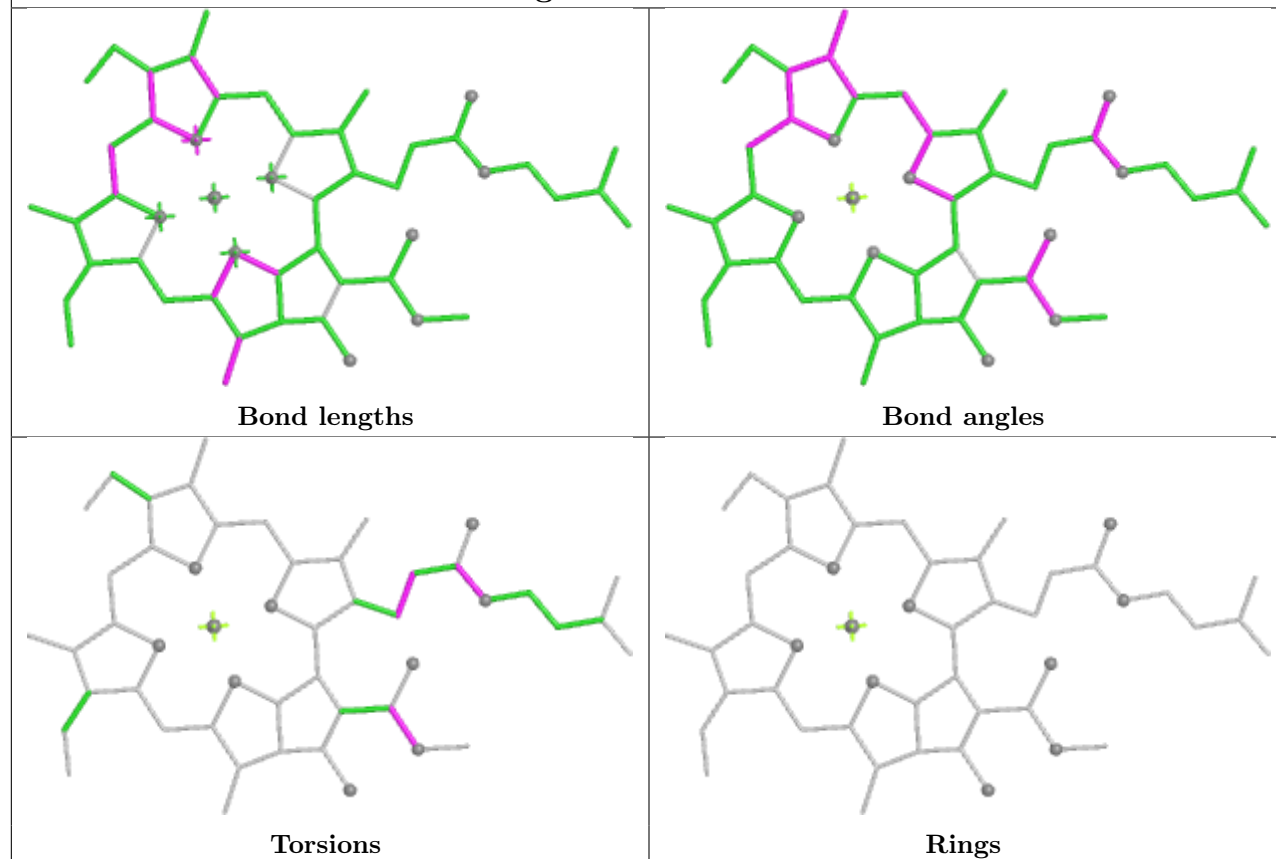
Ligand CLA n 613



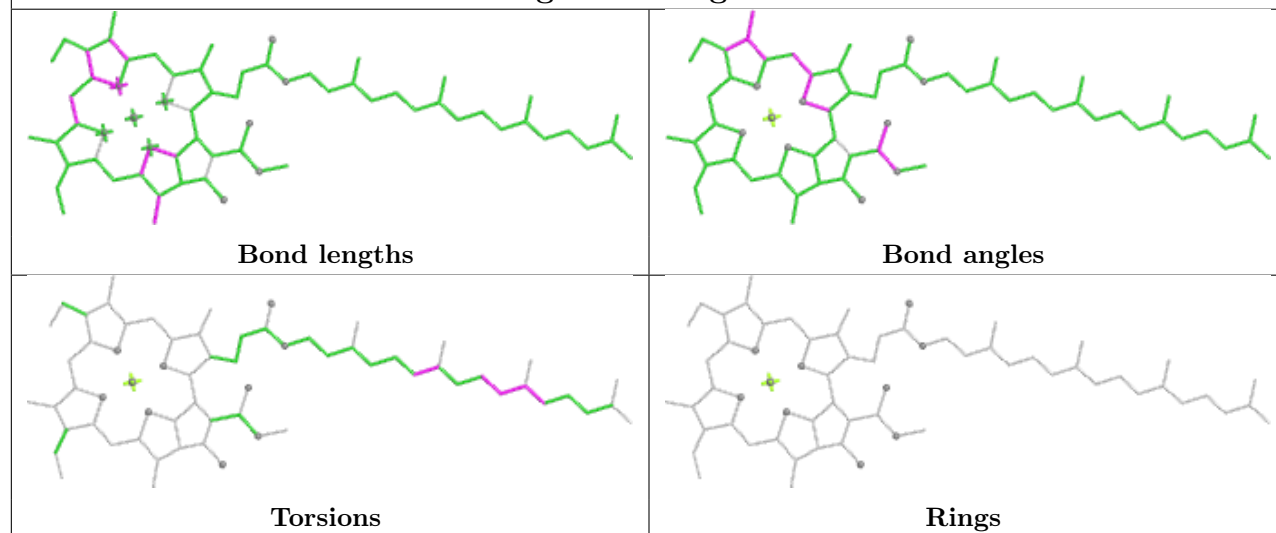
Ligand CLA i 305



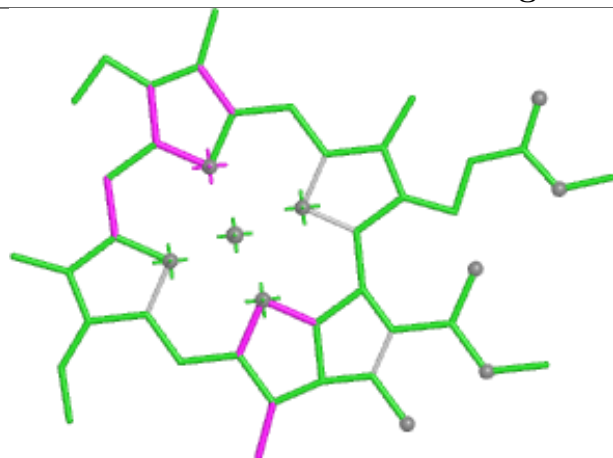
Ligand CLA n 602



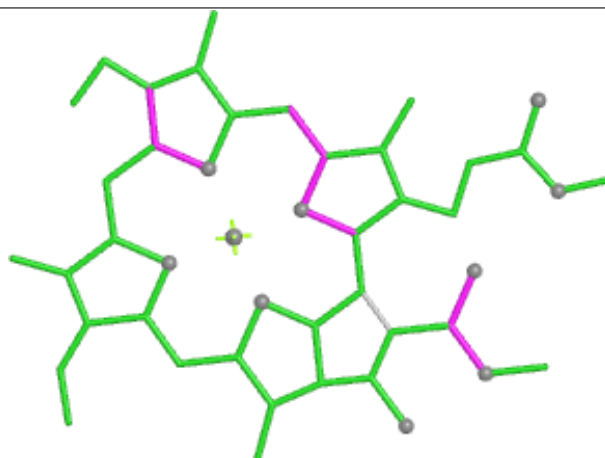
Ligand CLA g 305



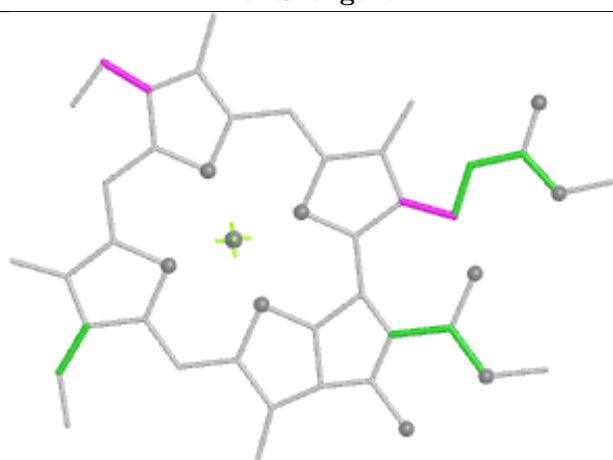
Ligand CLA e 308



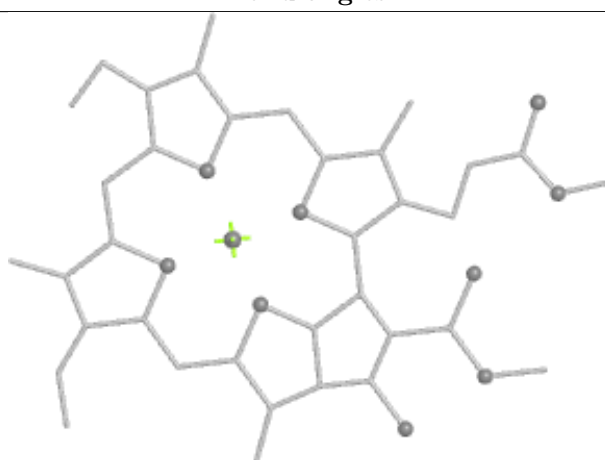
Bond lengths



Bond angles

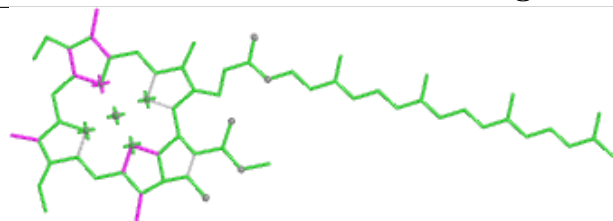


Torsions

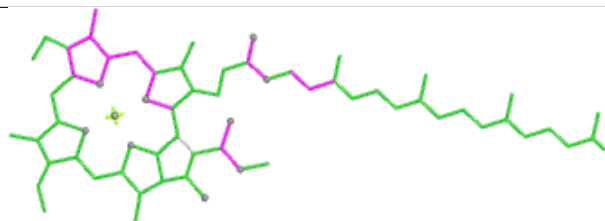


Rings

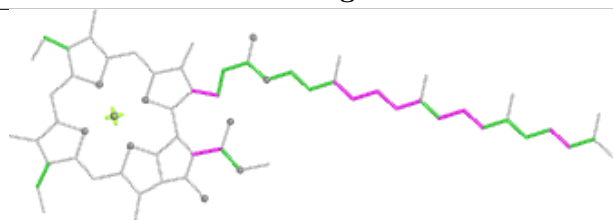
Ligand CLA B 812



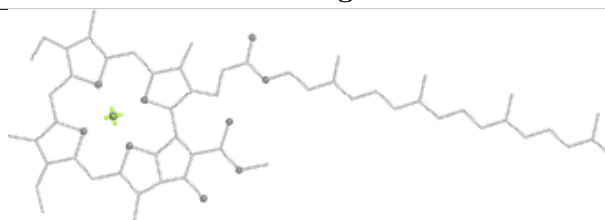
Bond lengths



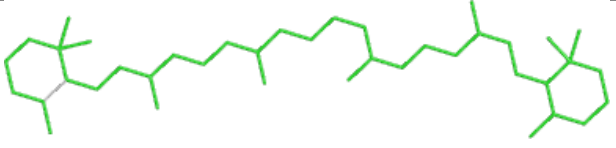
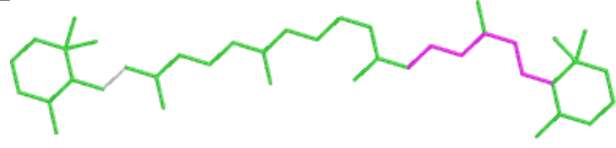
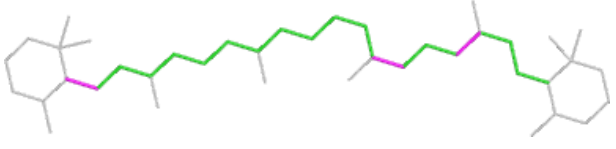
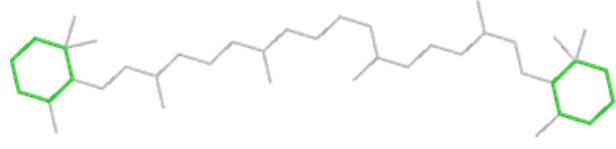
Bond angles

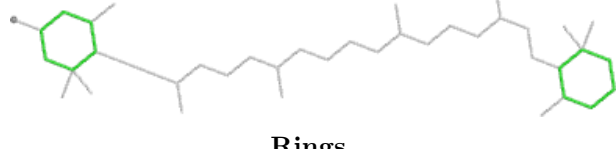


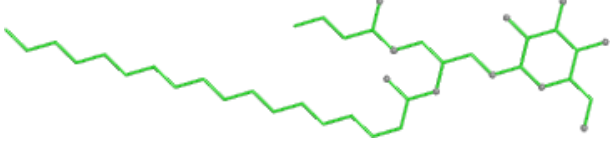
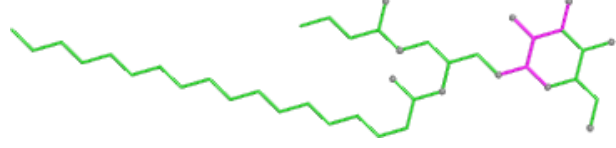
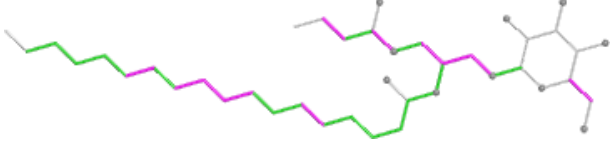
Torsions

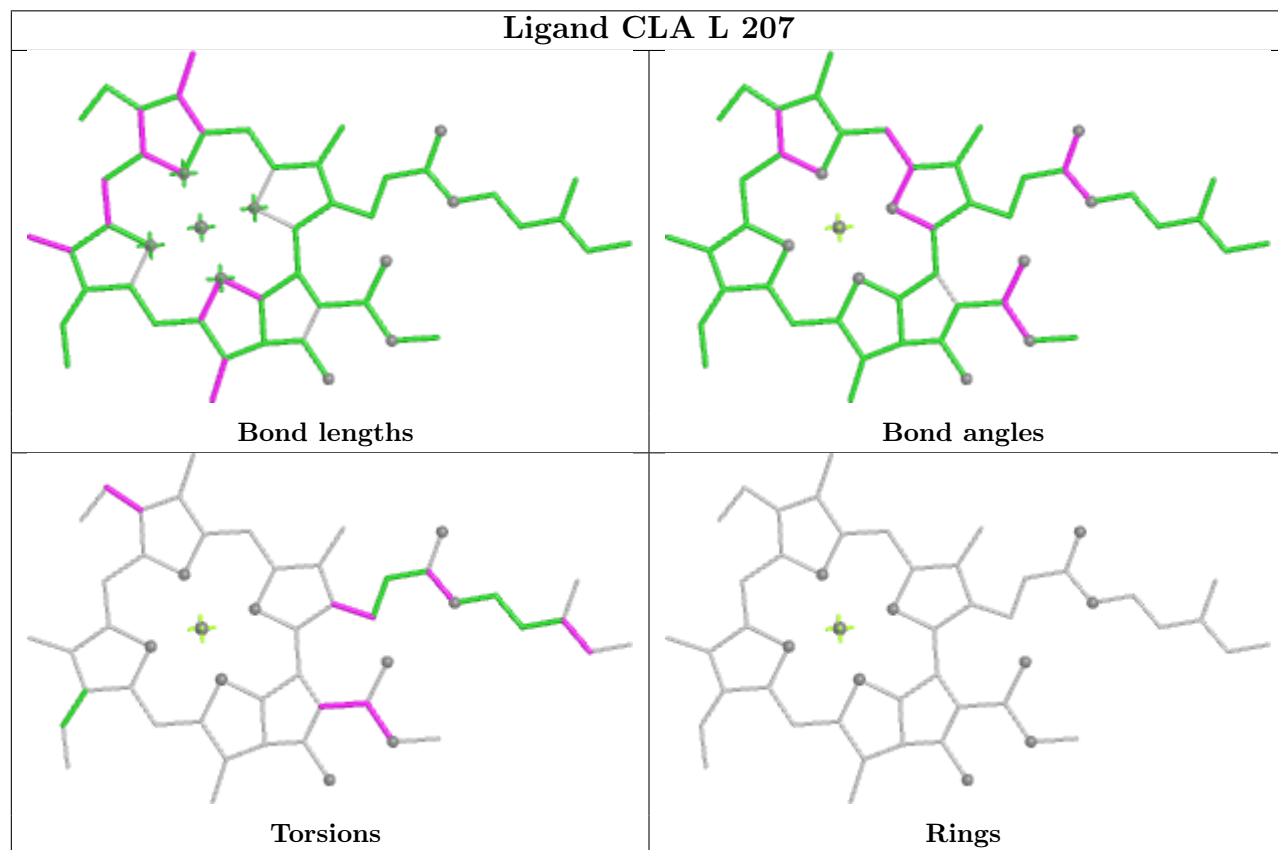
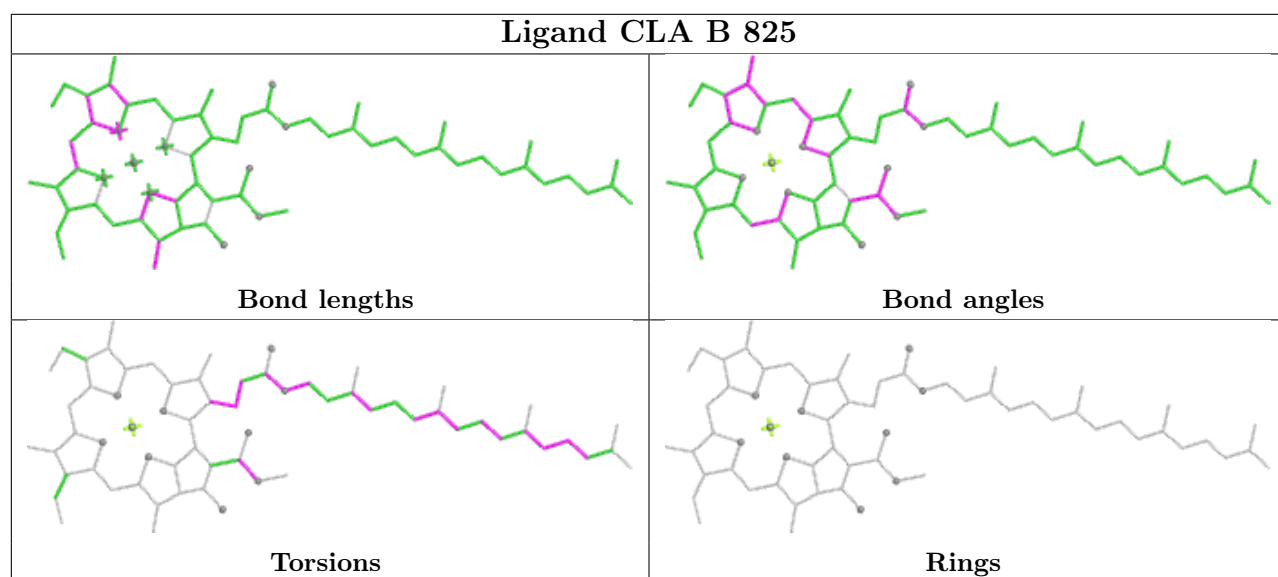


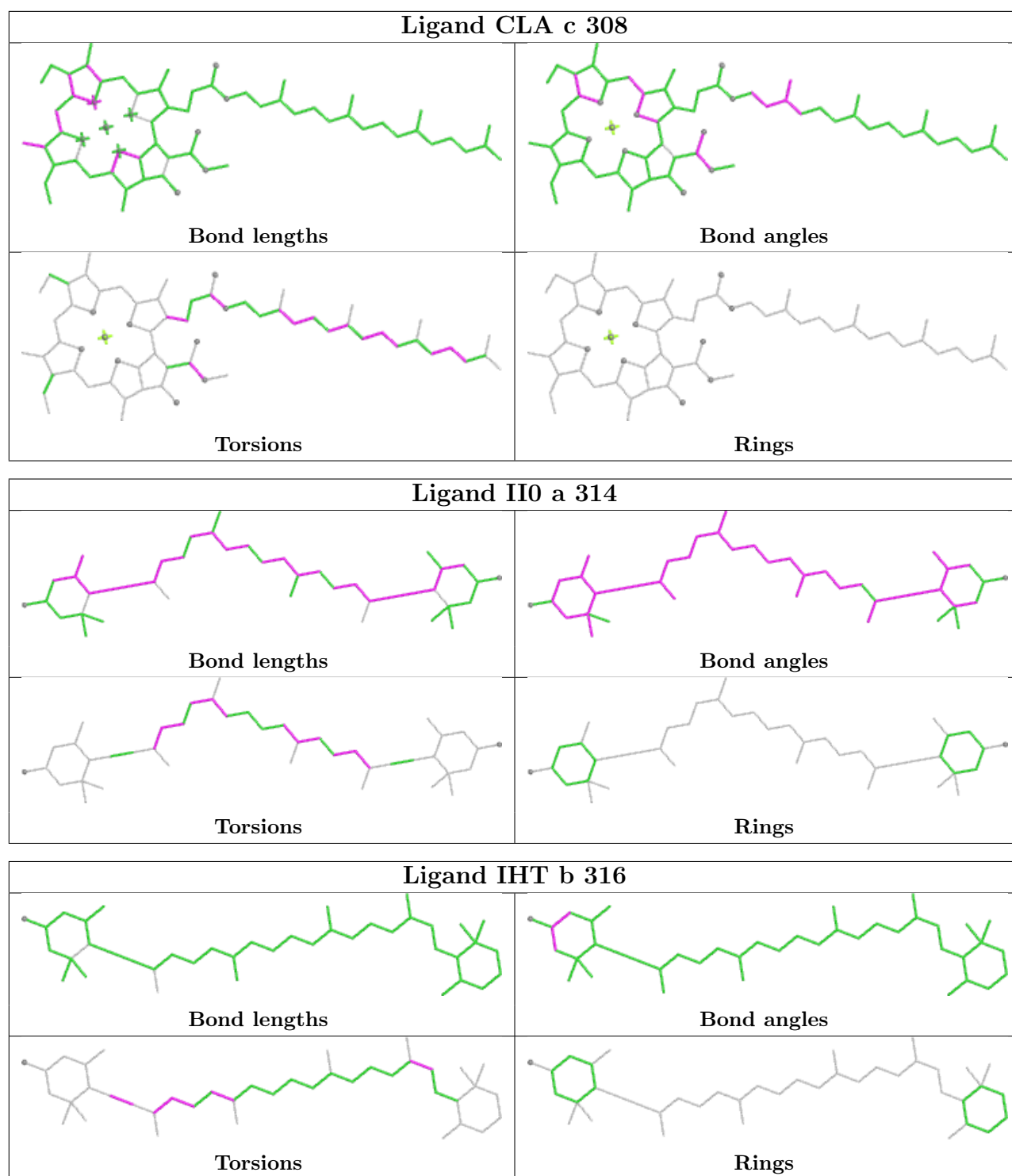
Rings

Ligand WVN B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

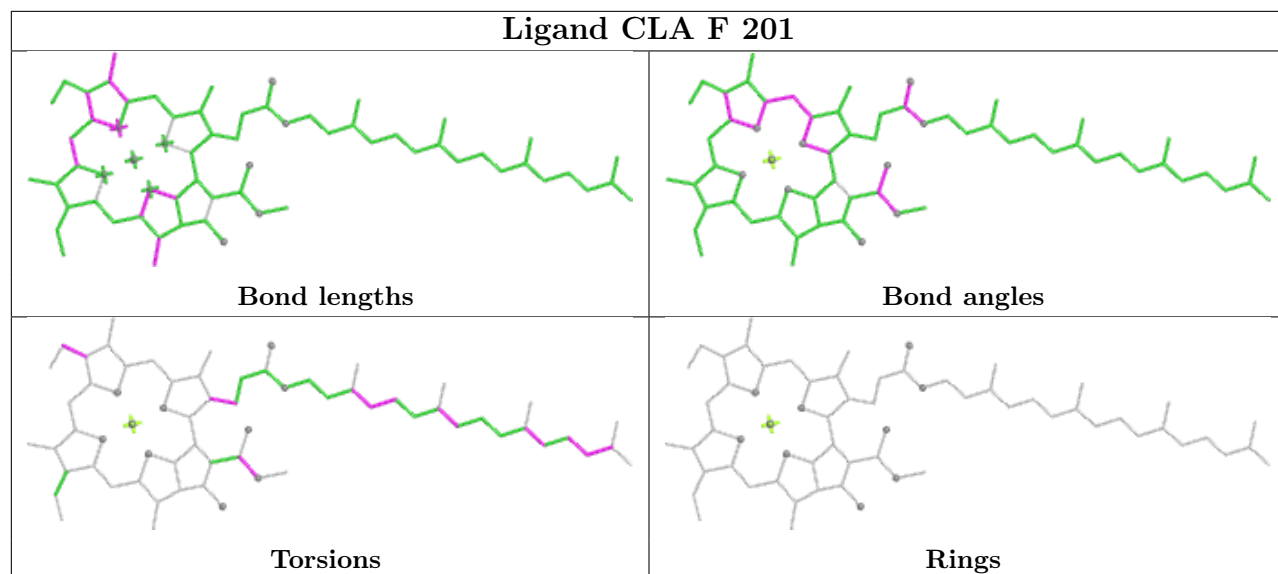
Ligand IHT a 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG F 208	
	
Bond lengths	Bond angles
	
Torsions	Rings

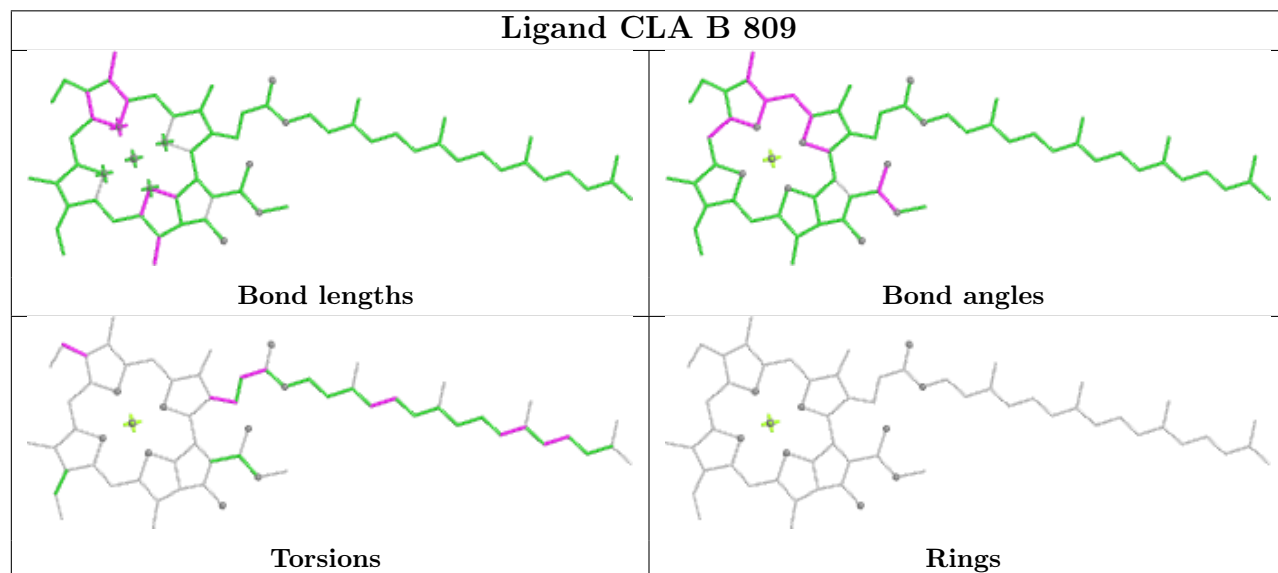




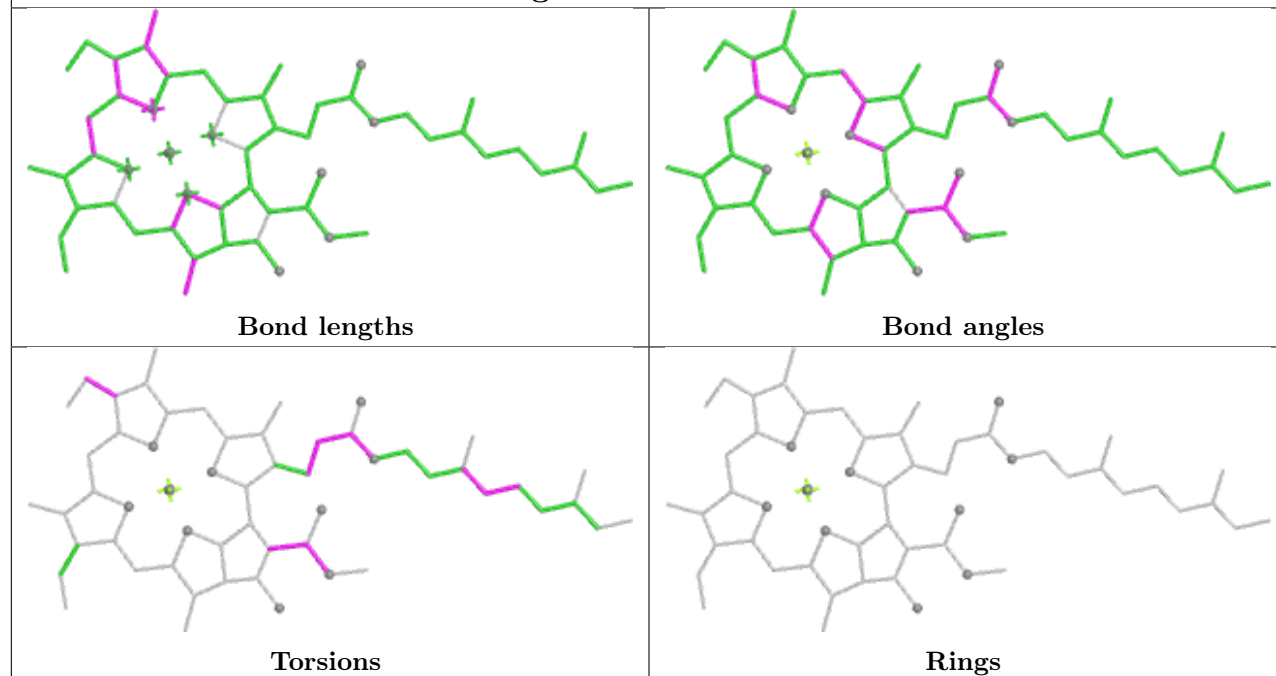
Ligand CLA F 201



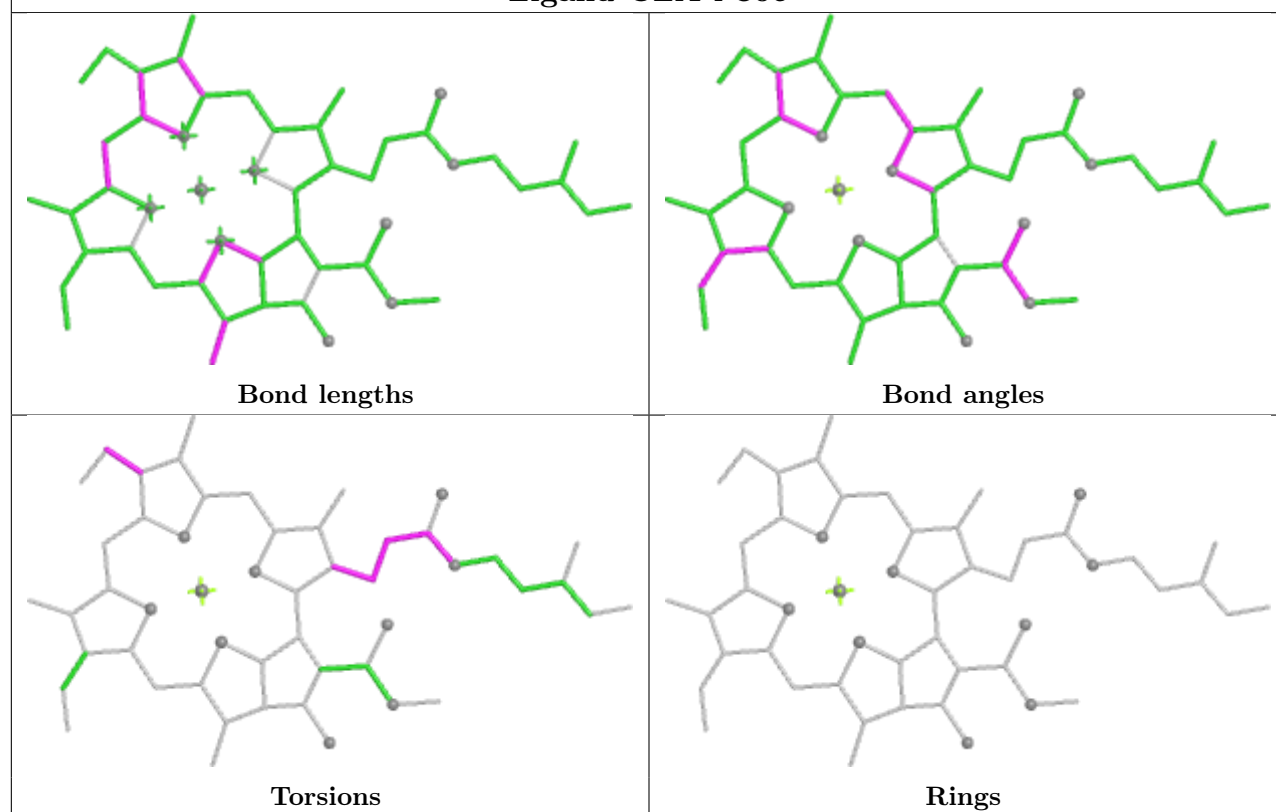
Ligand CLA B 809

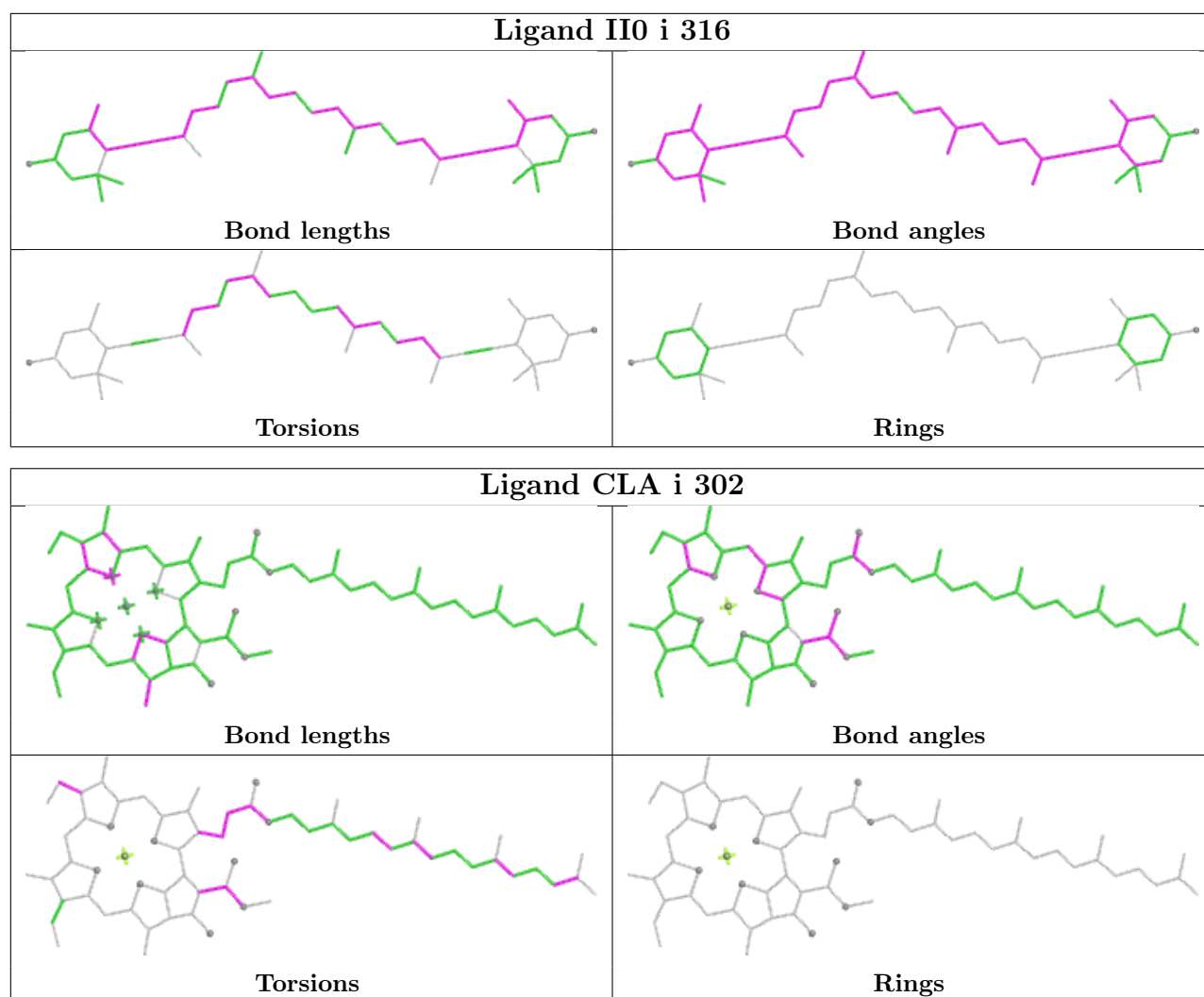


Ligand CLA A 822

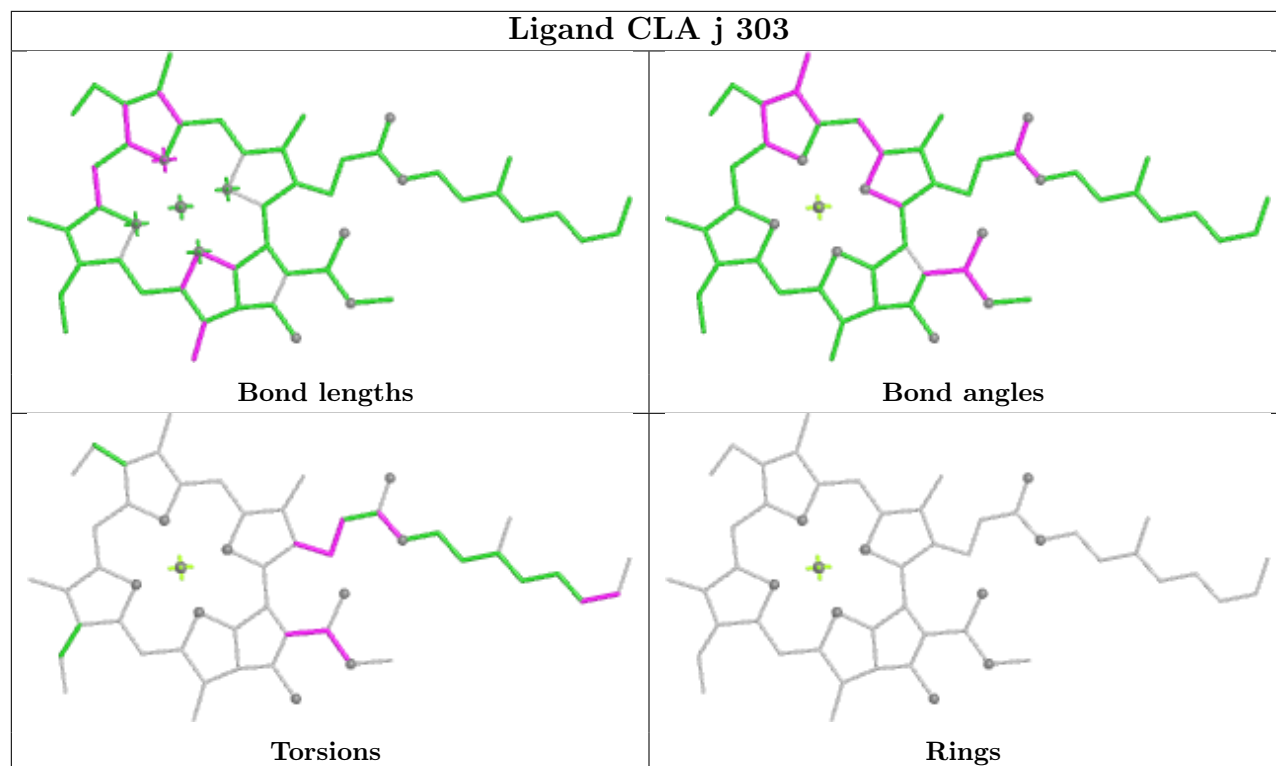


Ligand CLA i 306

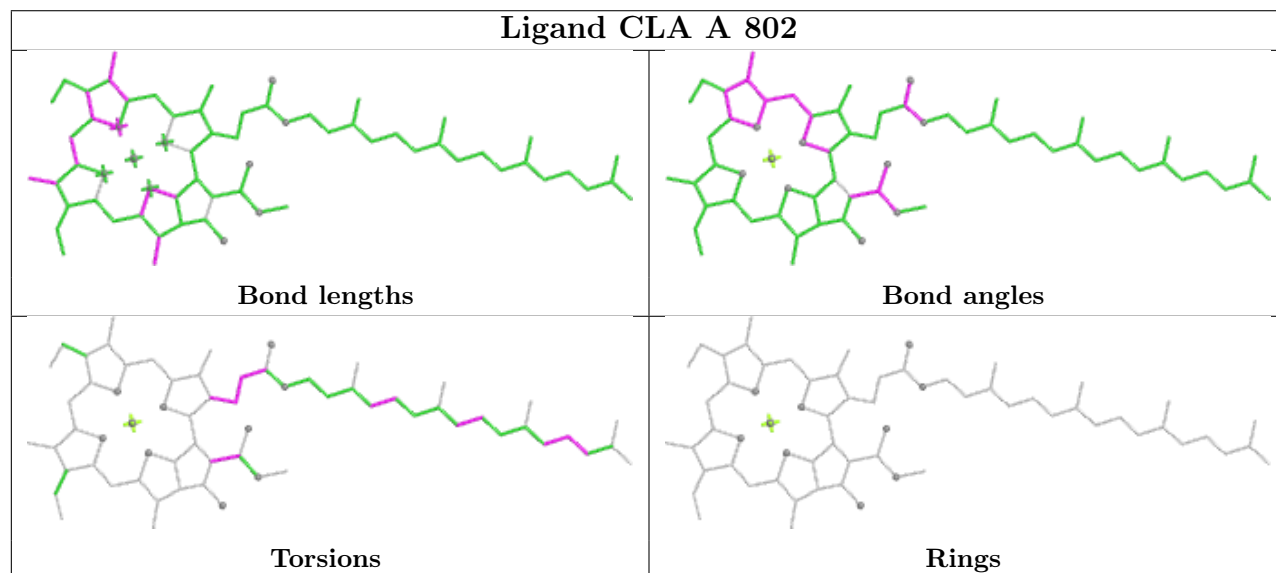


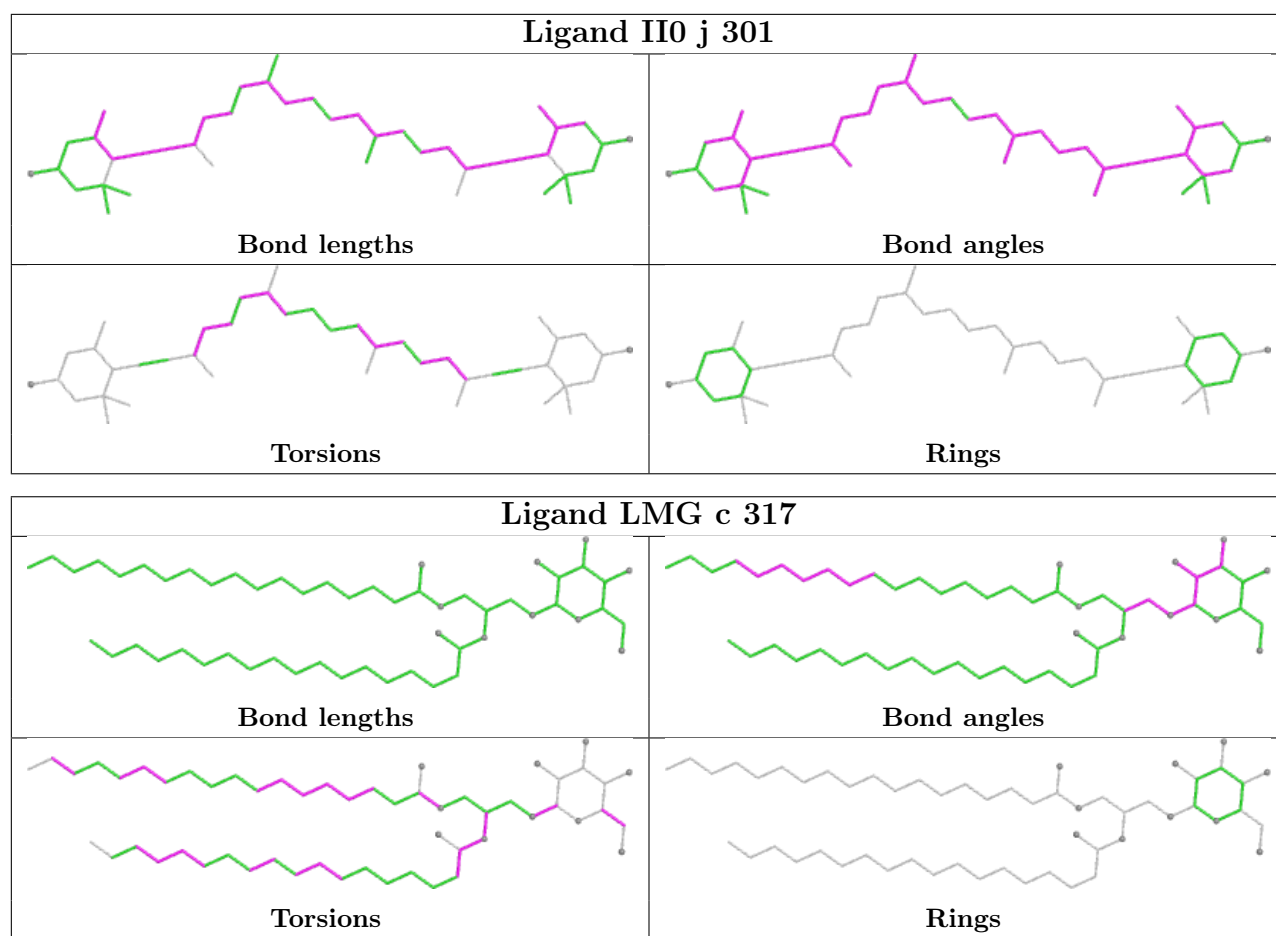


Ligand CLA j 303

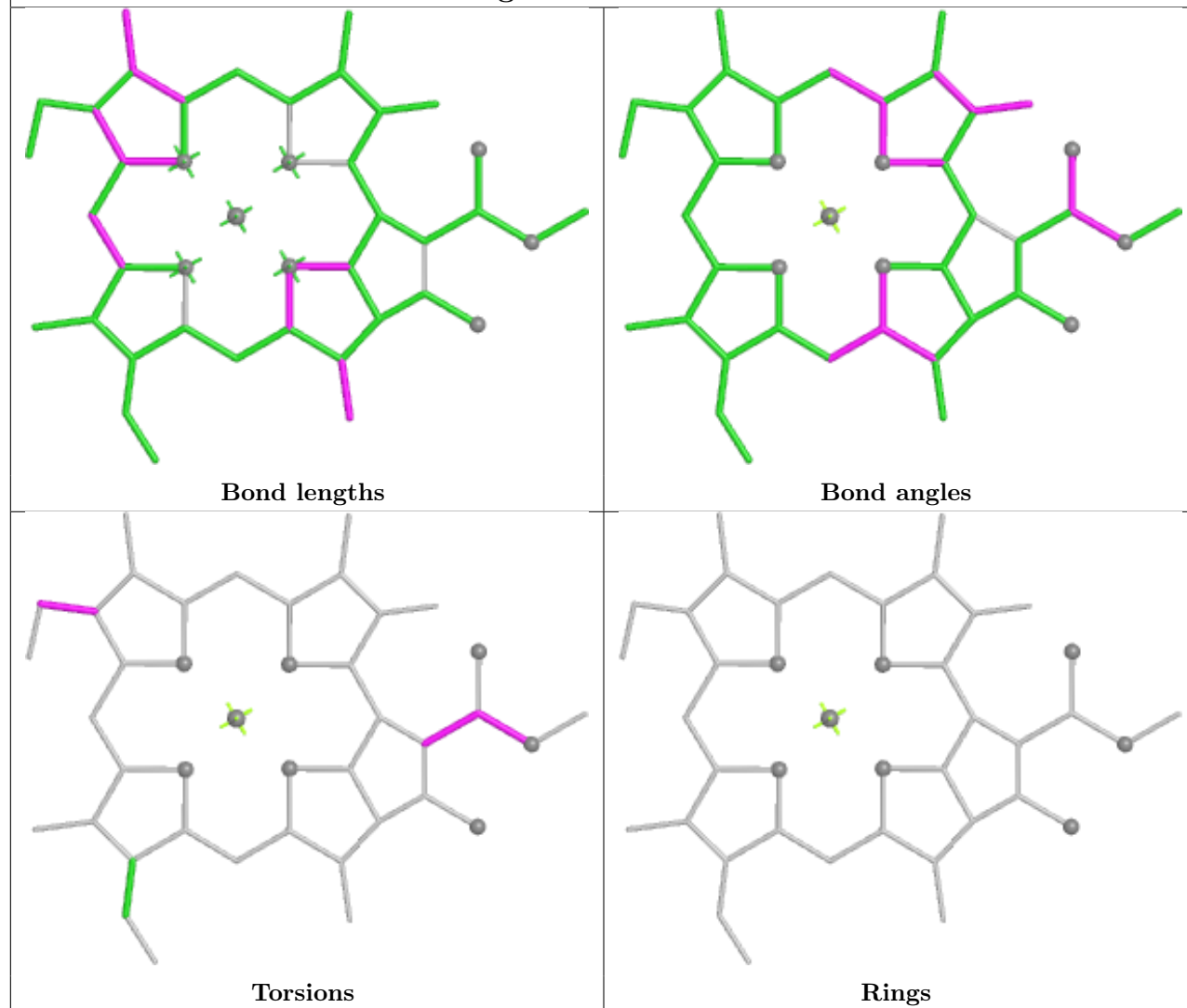


Ligand CLA A 802

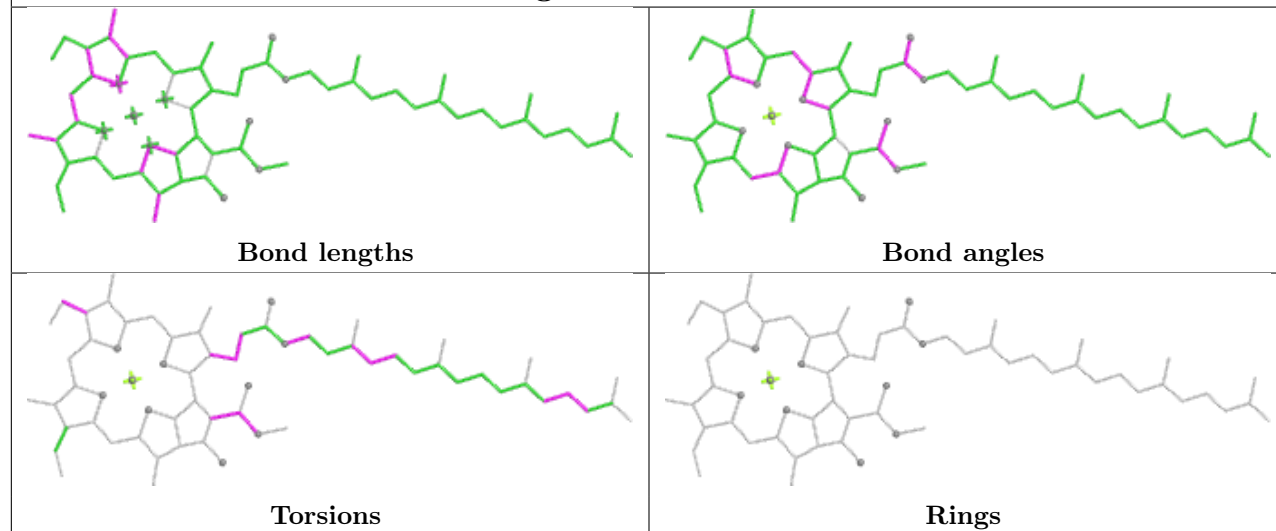


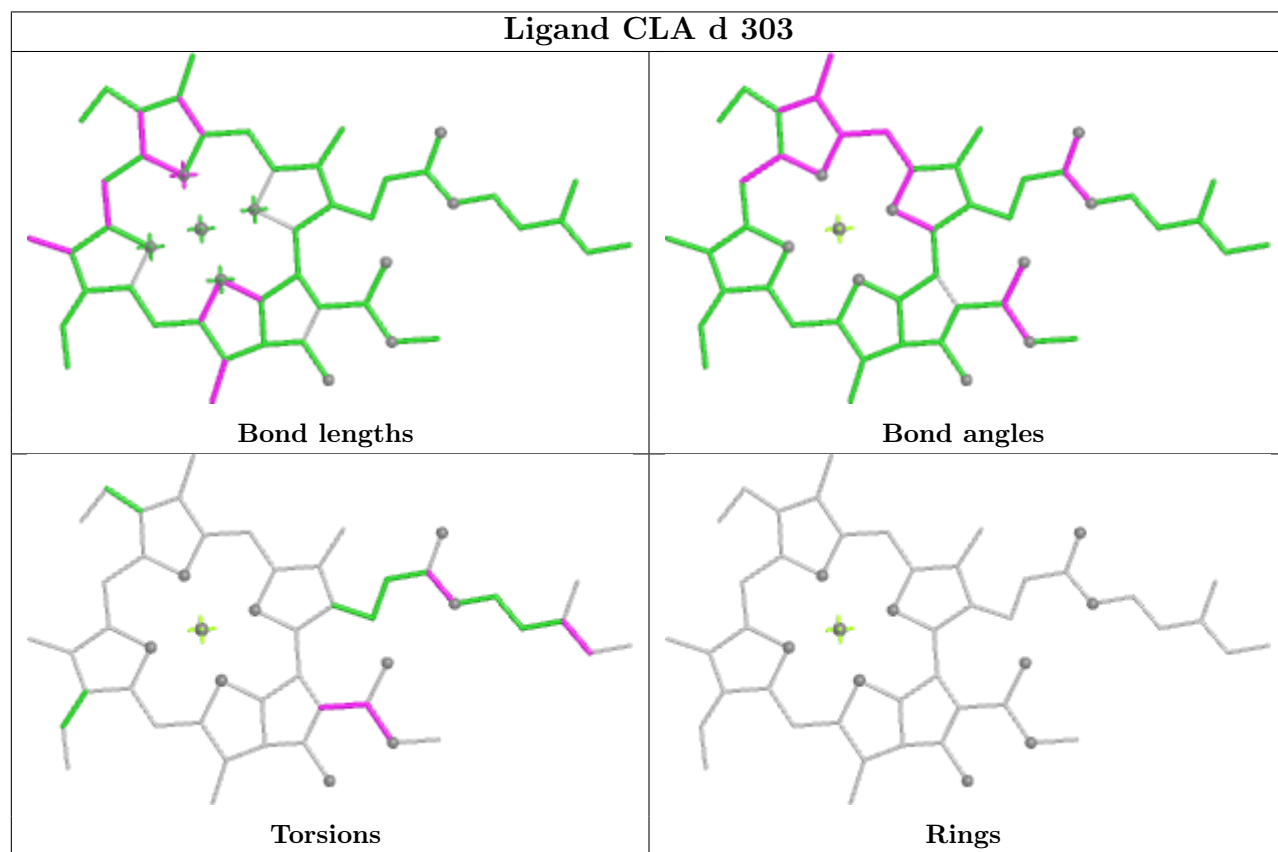
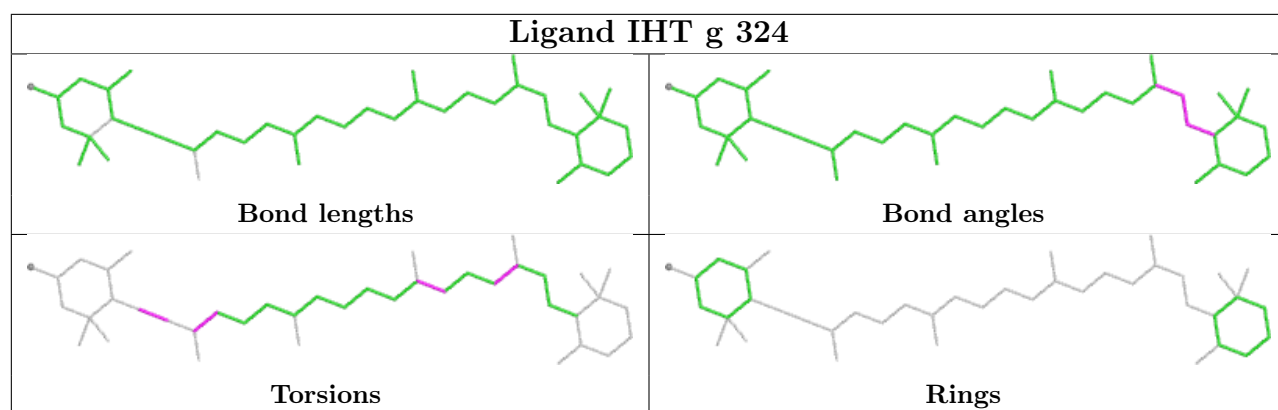


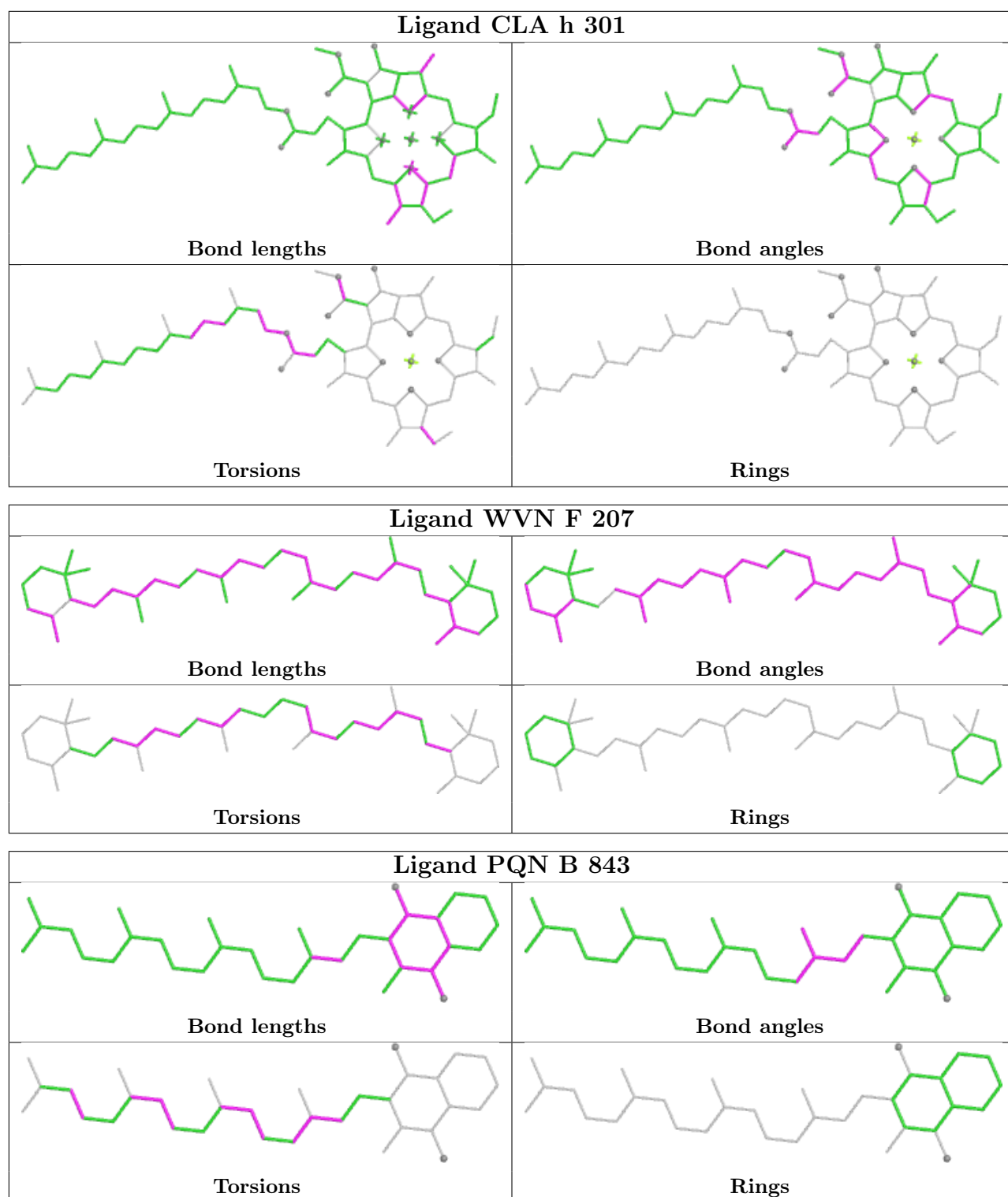
Ligand CLA d 310



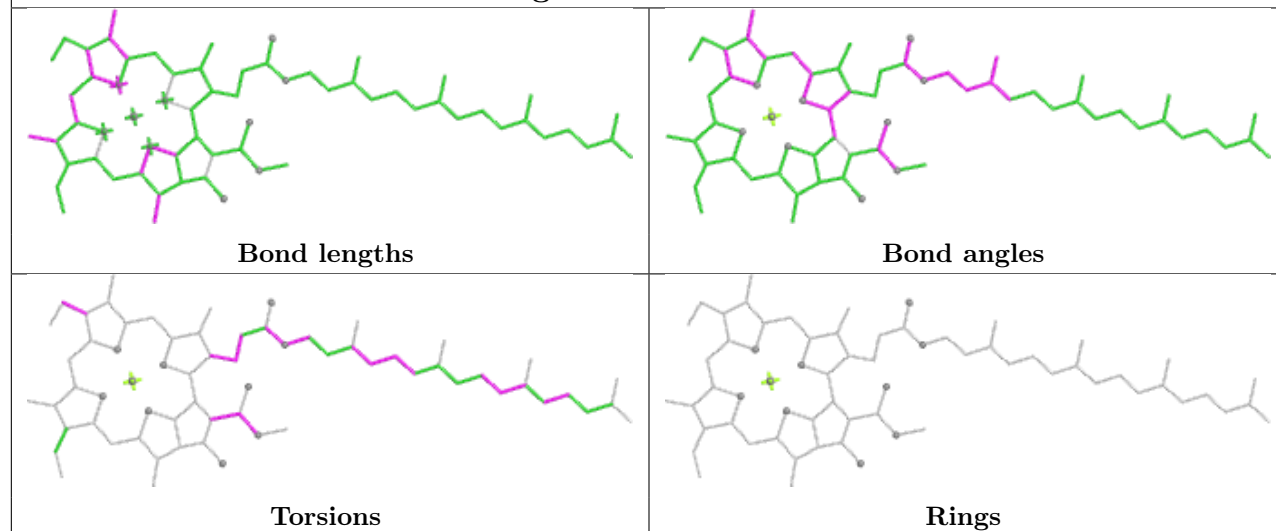
Ligand CLA n 609



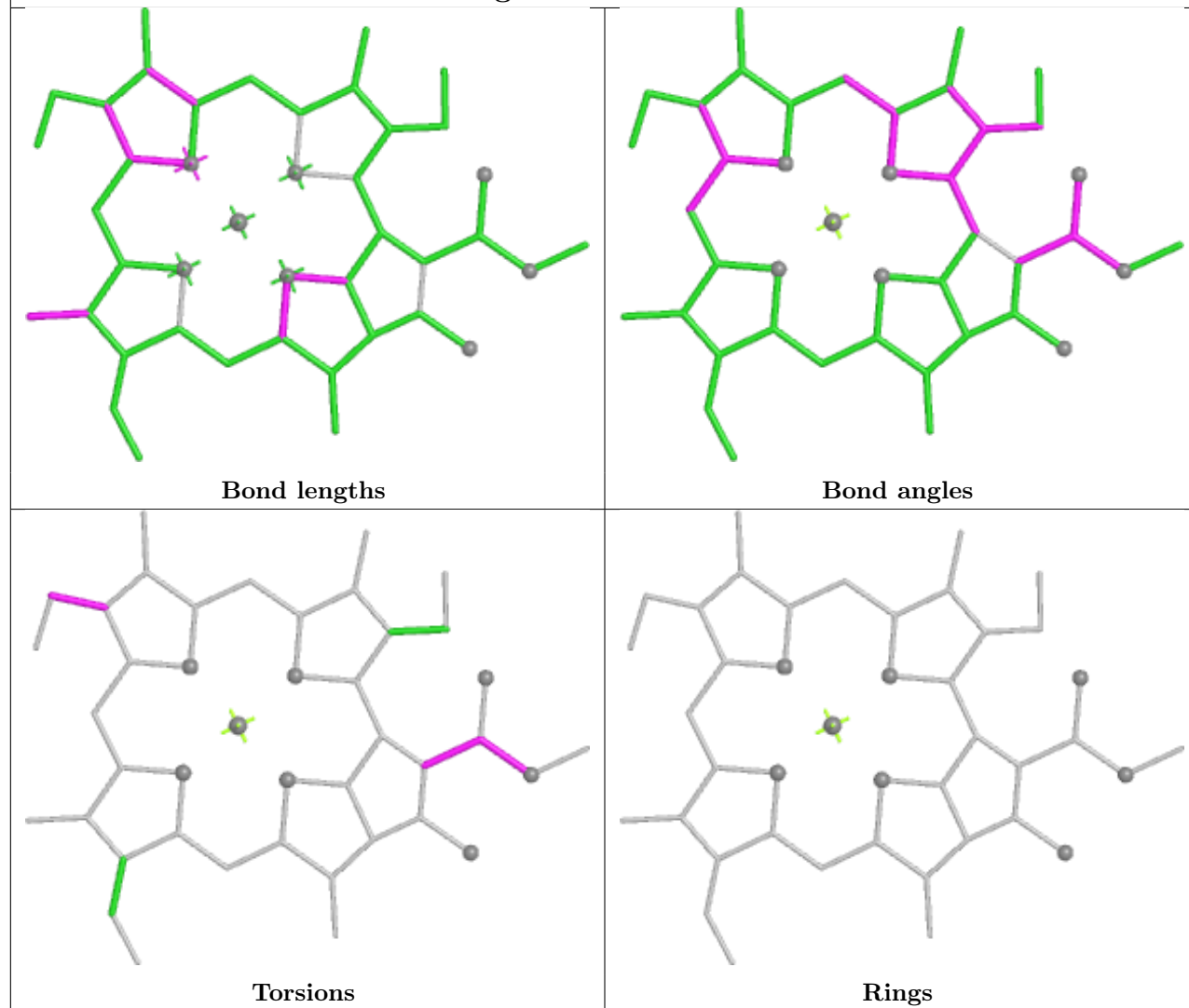


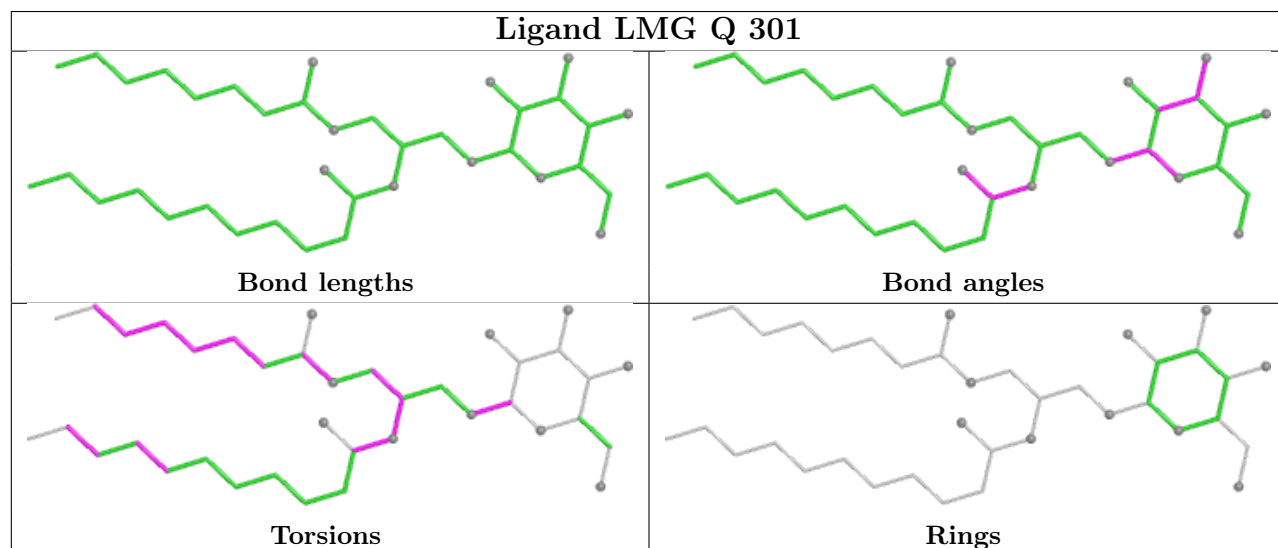
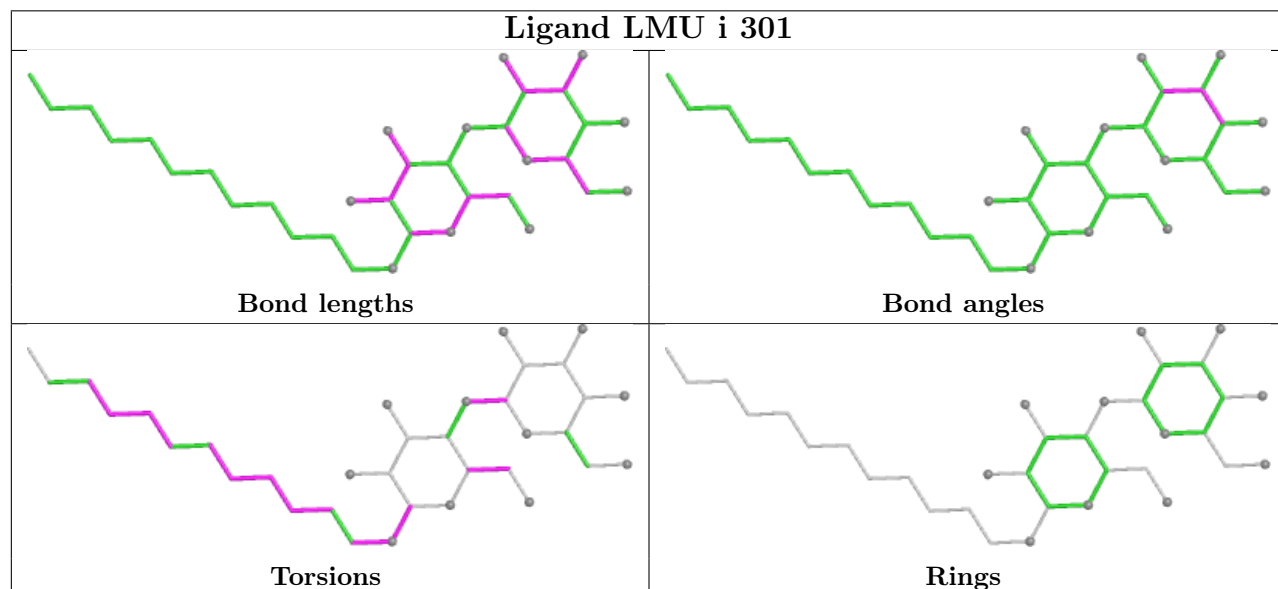
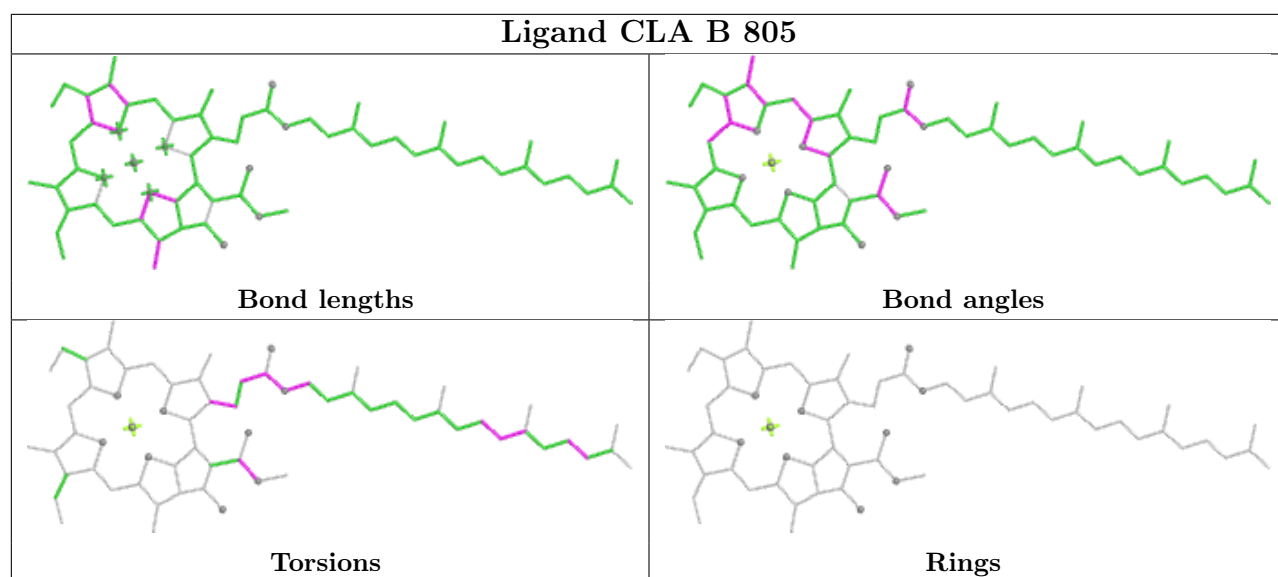


Ligand CLA B 822

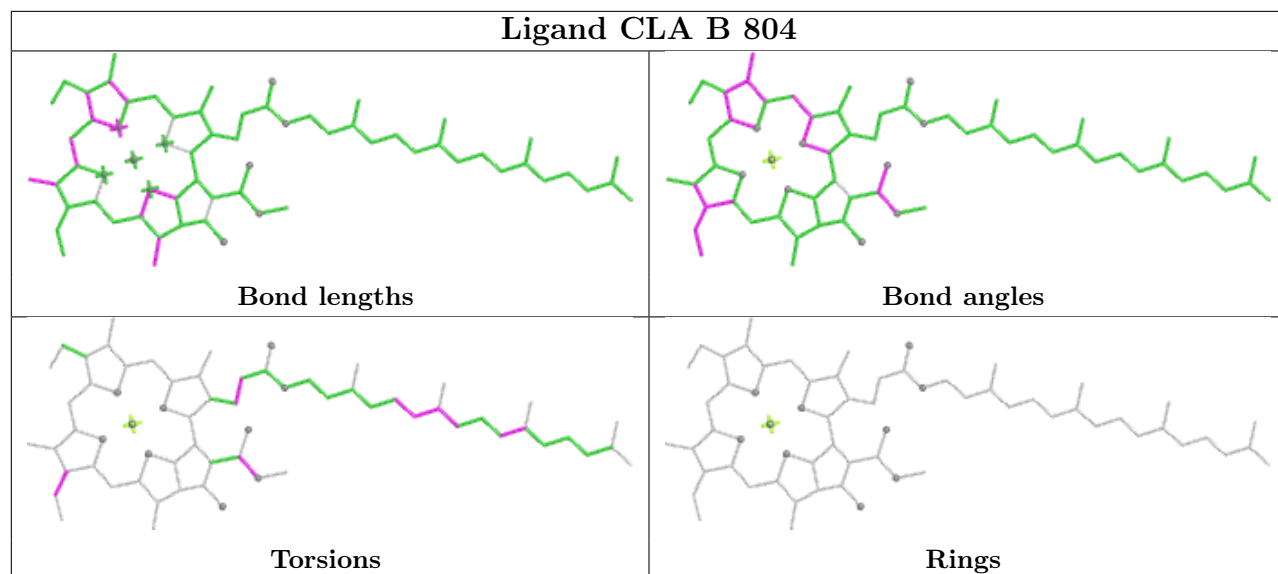


Ligand CLA K 102

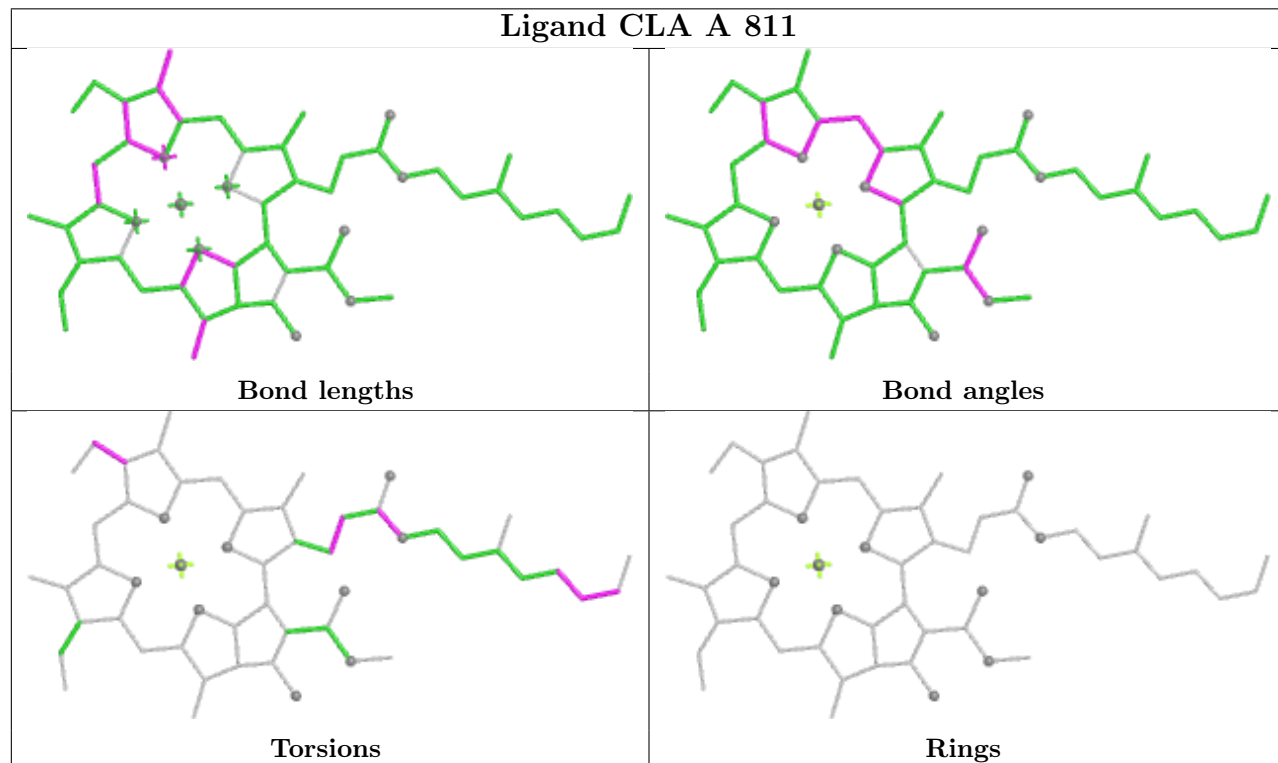




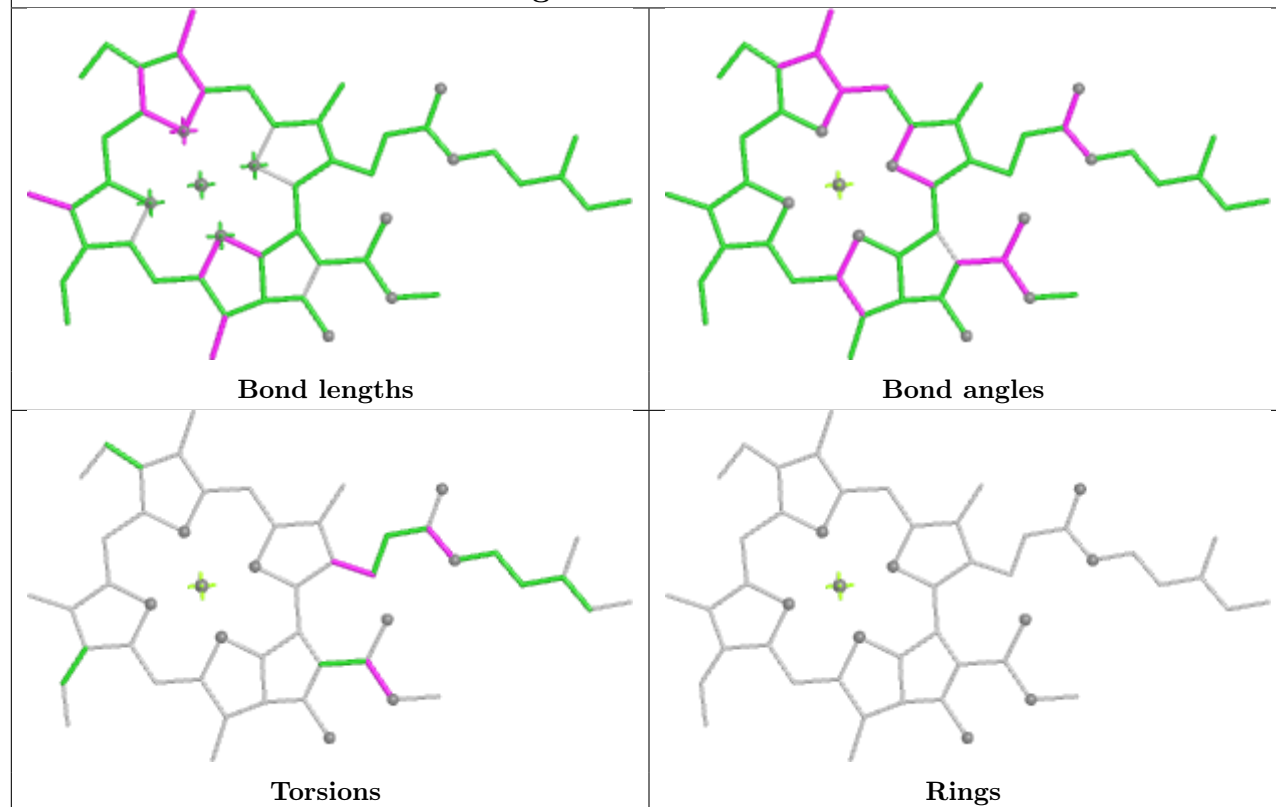
Ligand CLA B 804



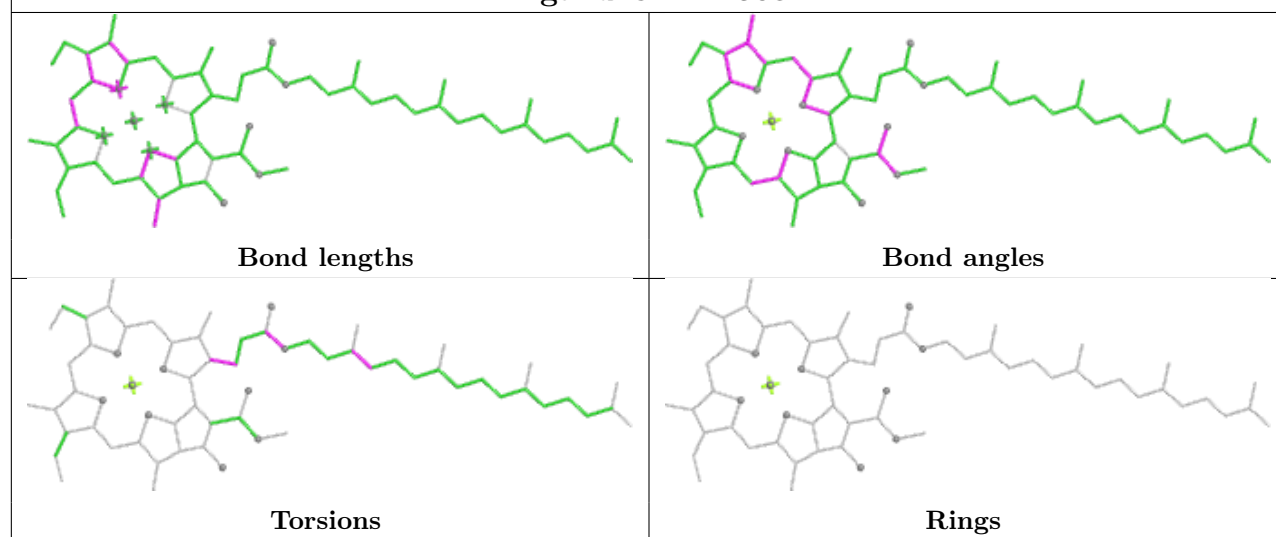
Ligand CLA A 811



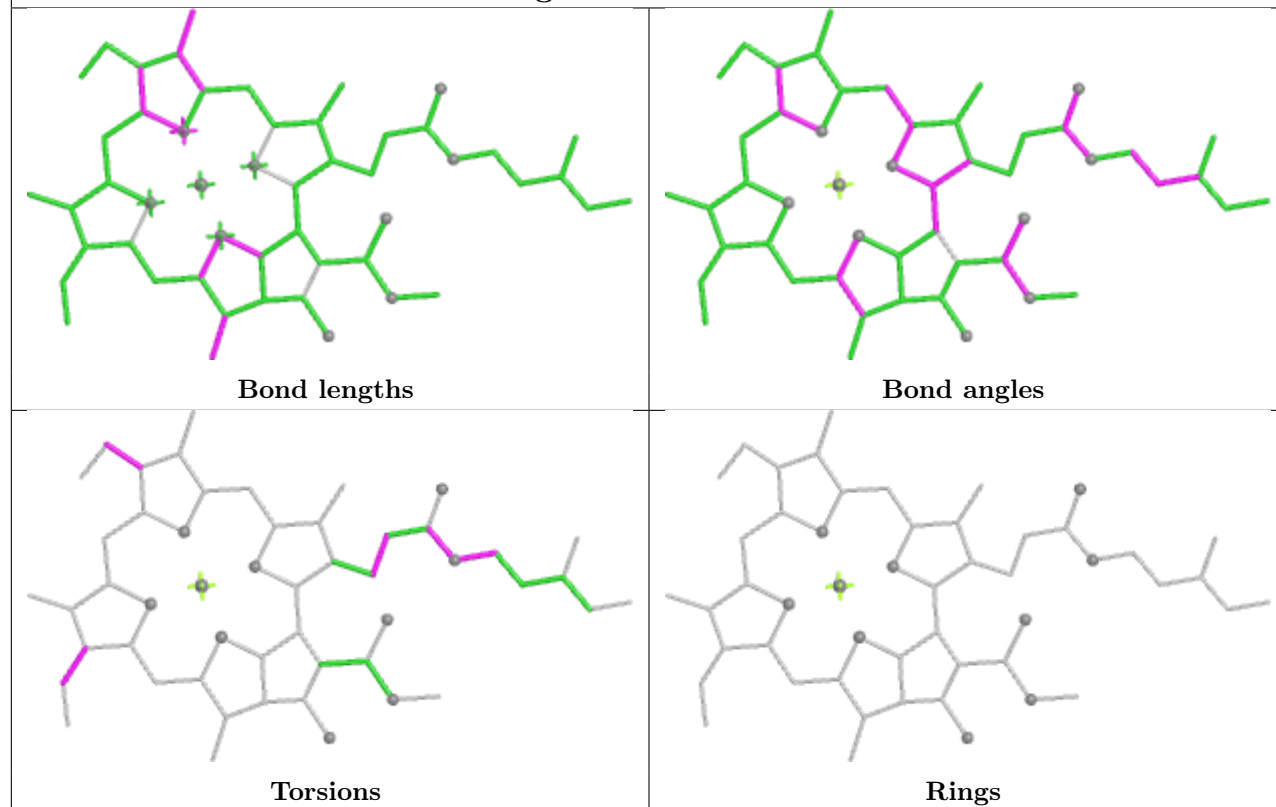
Ligand CLA B 827



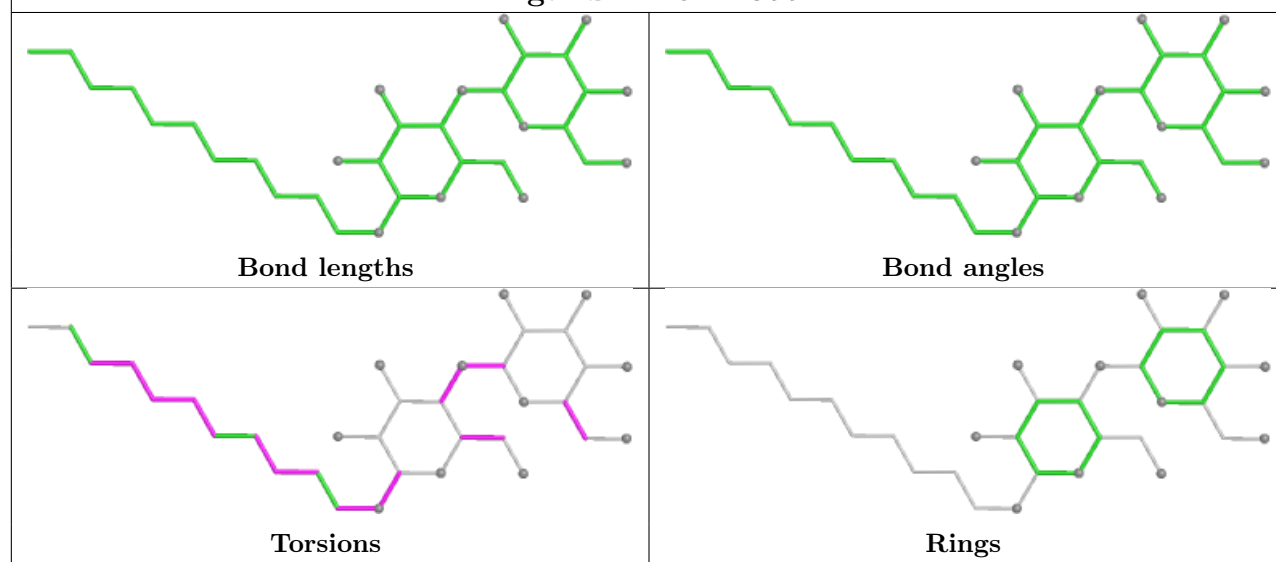
Ligand CLA I 308

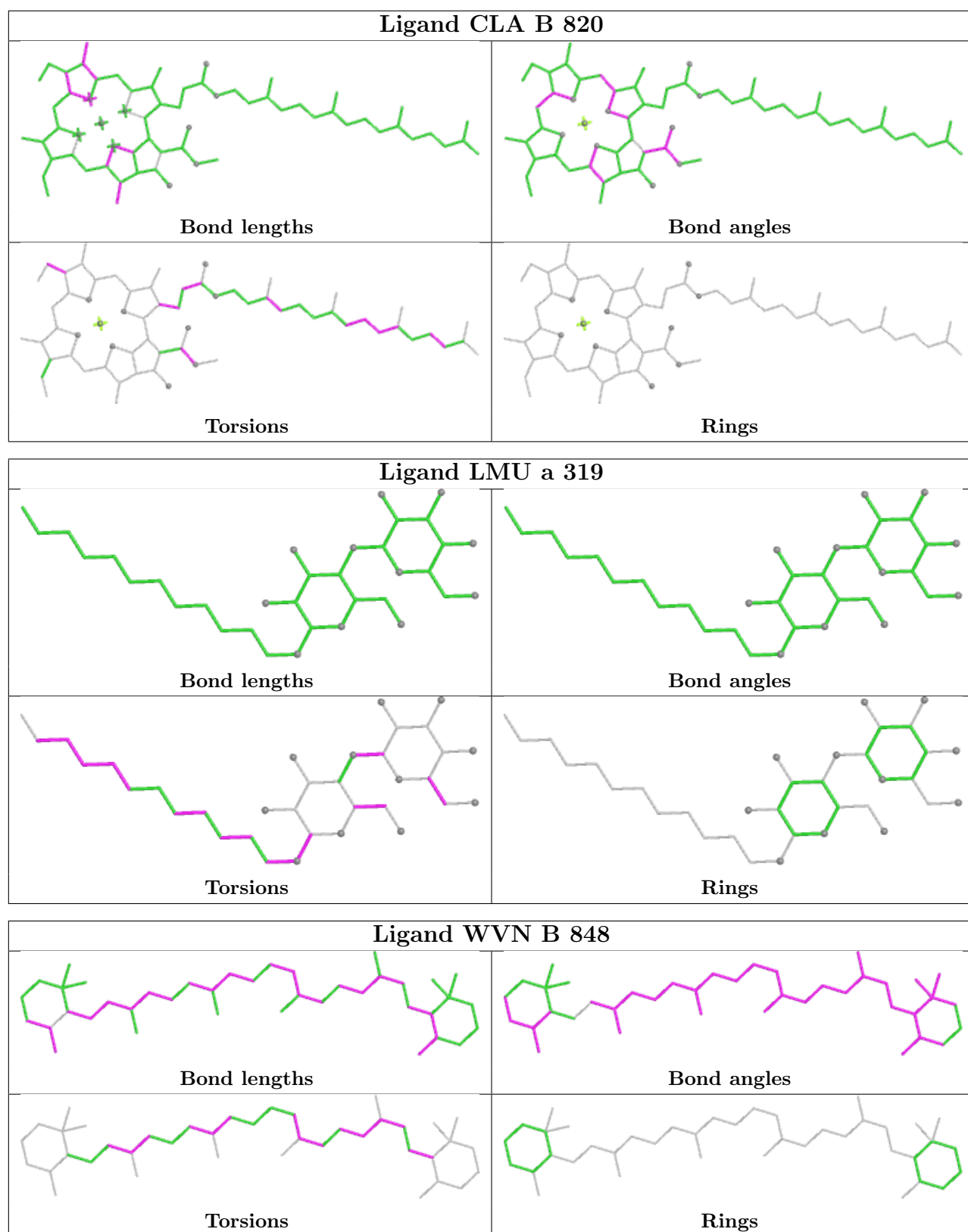


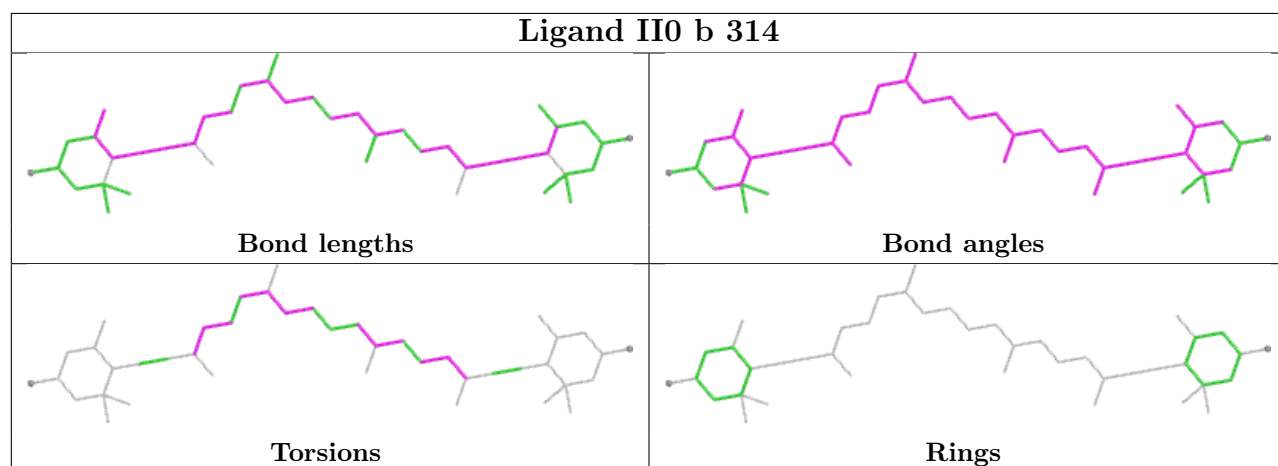
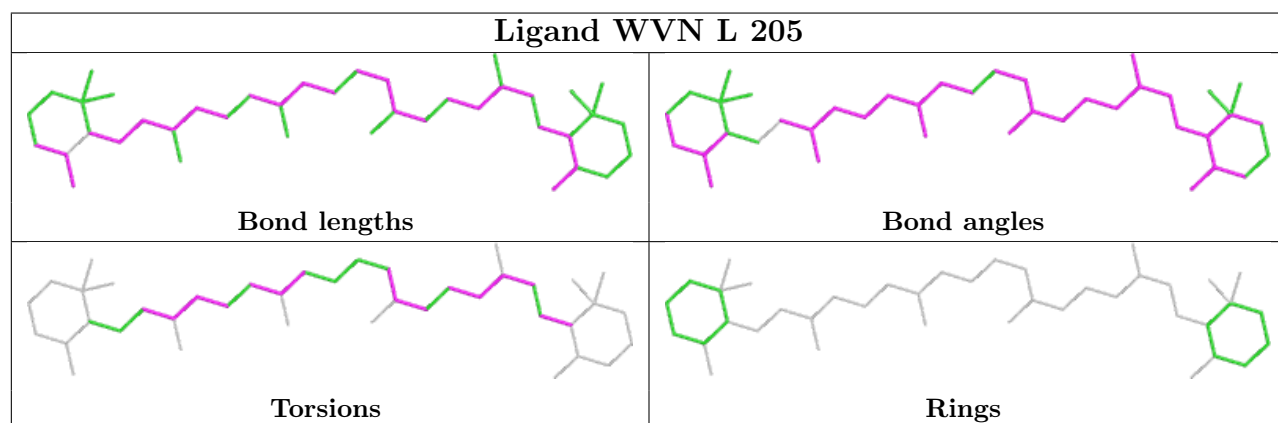
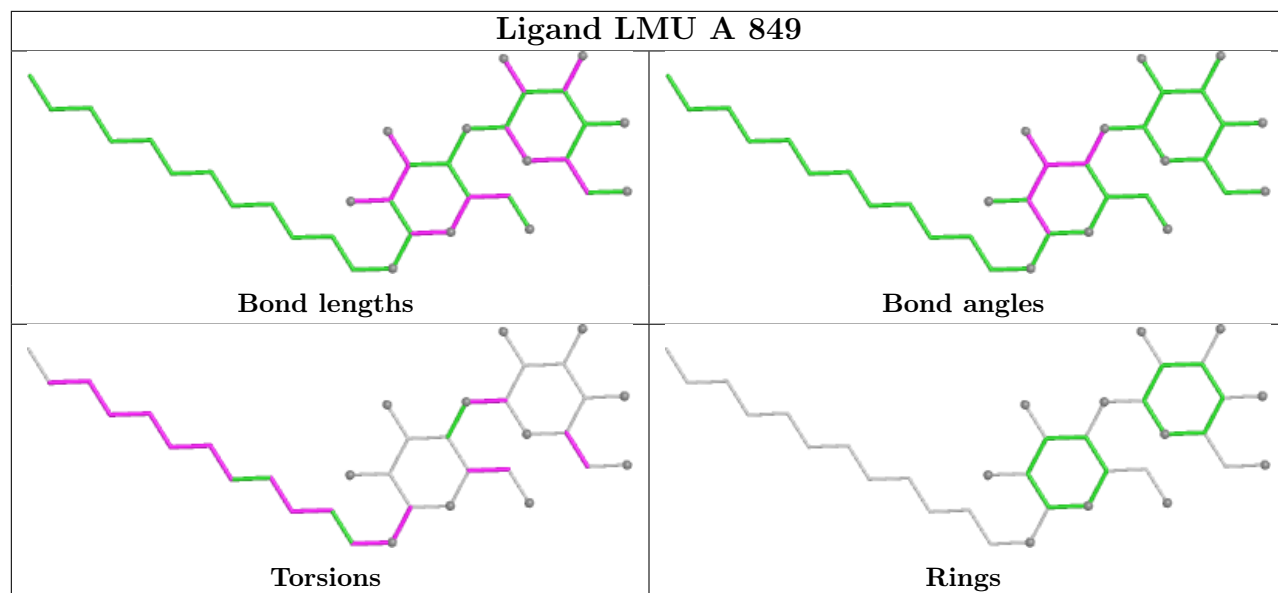
Ligand CLA b 313

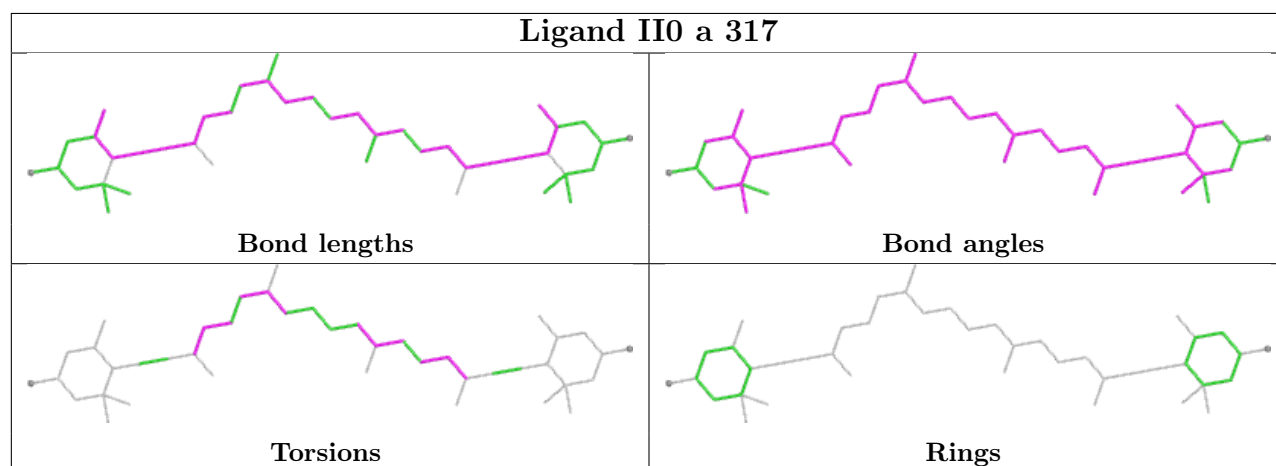
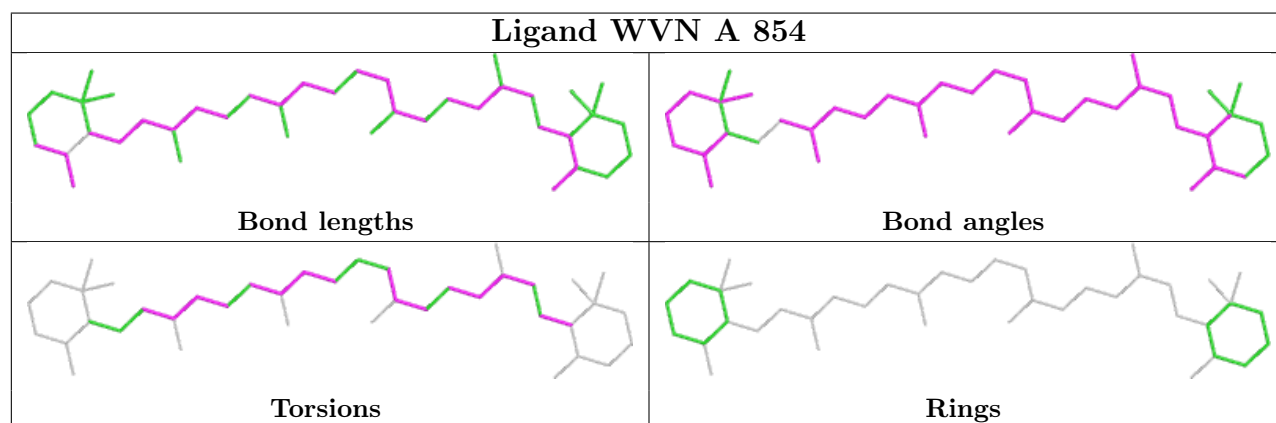
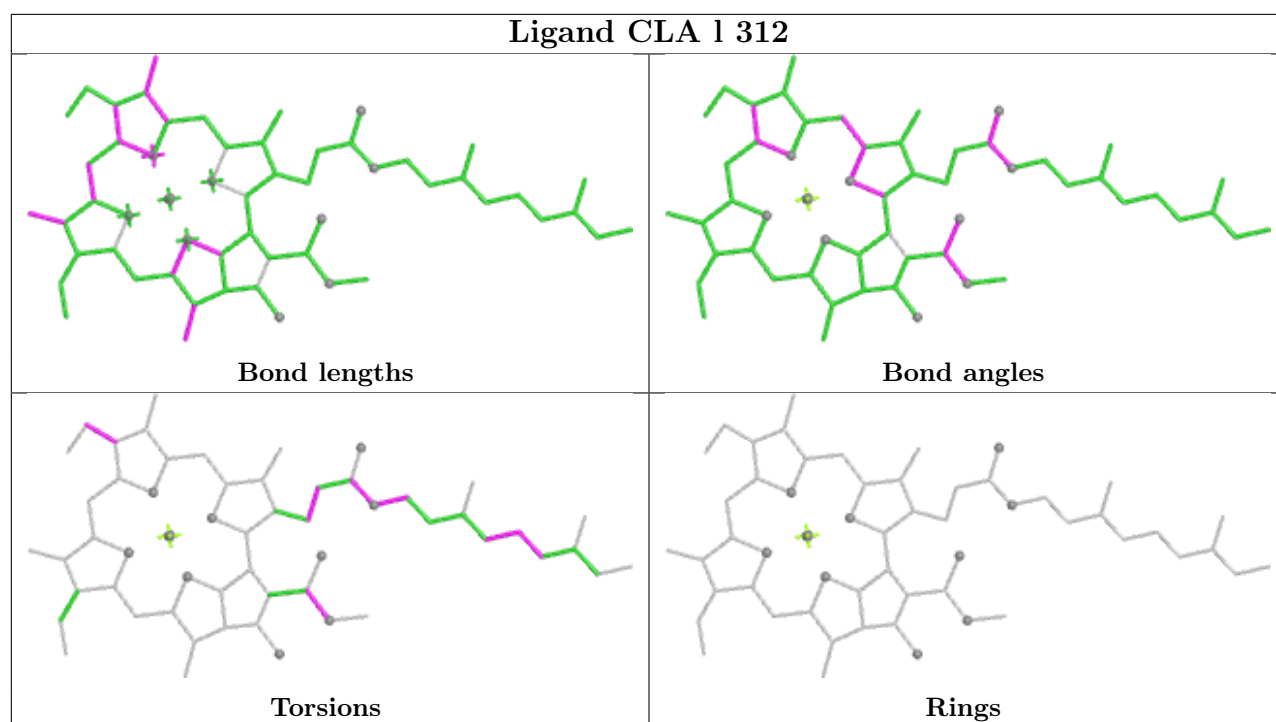


Ligand LMU A 855

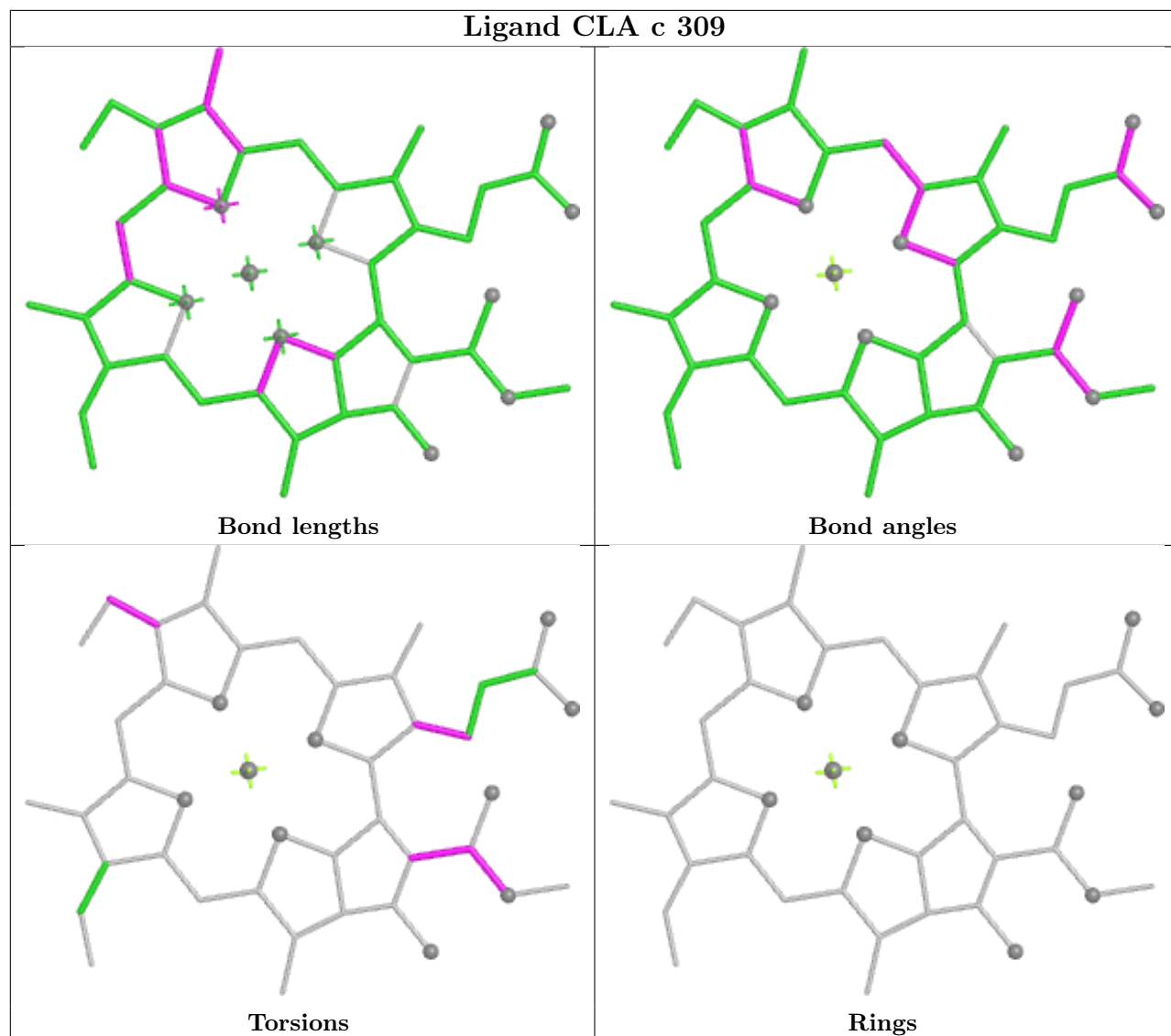




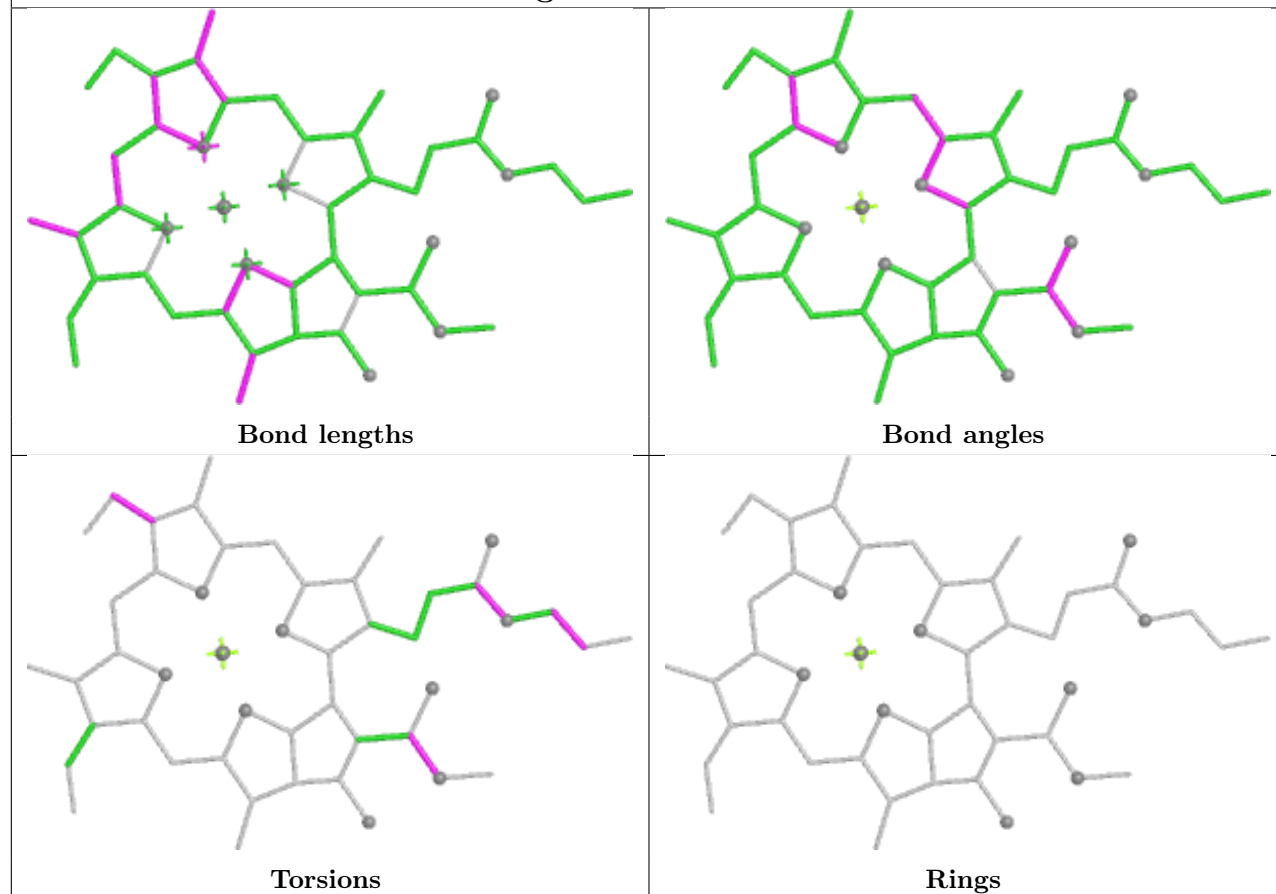




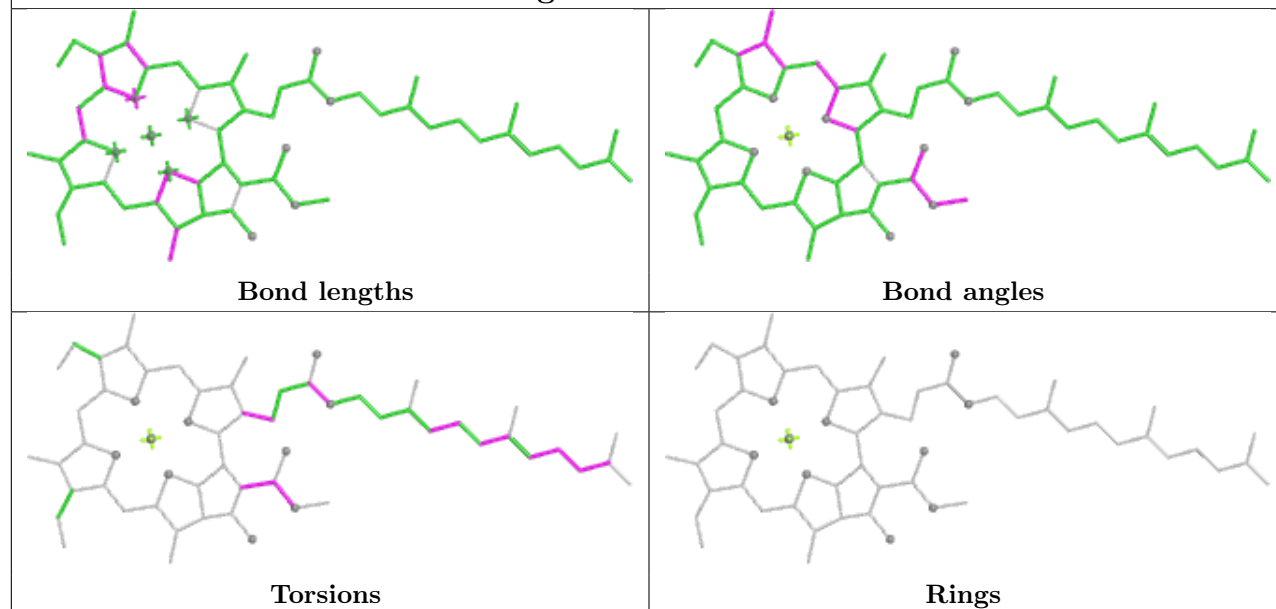
Ligand CLA c 309

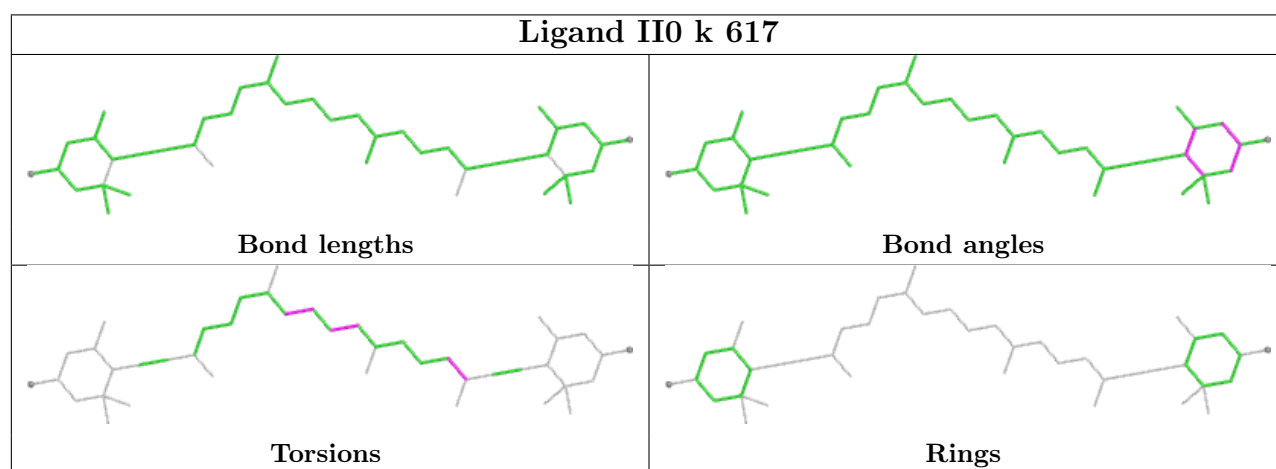
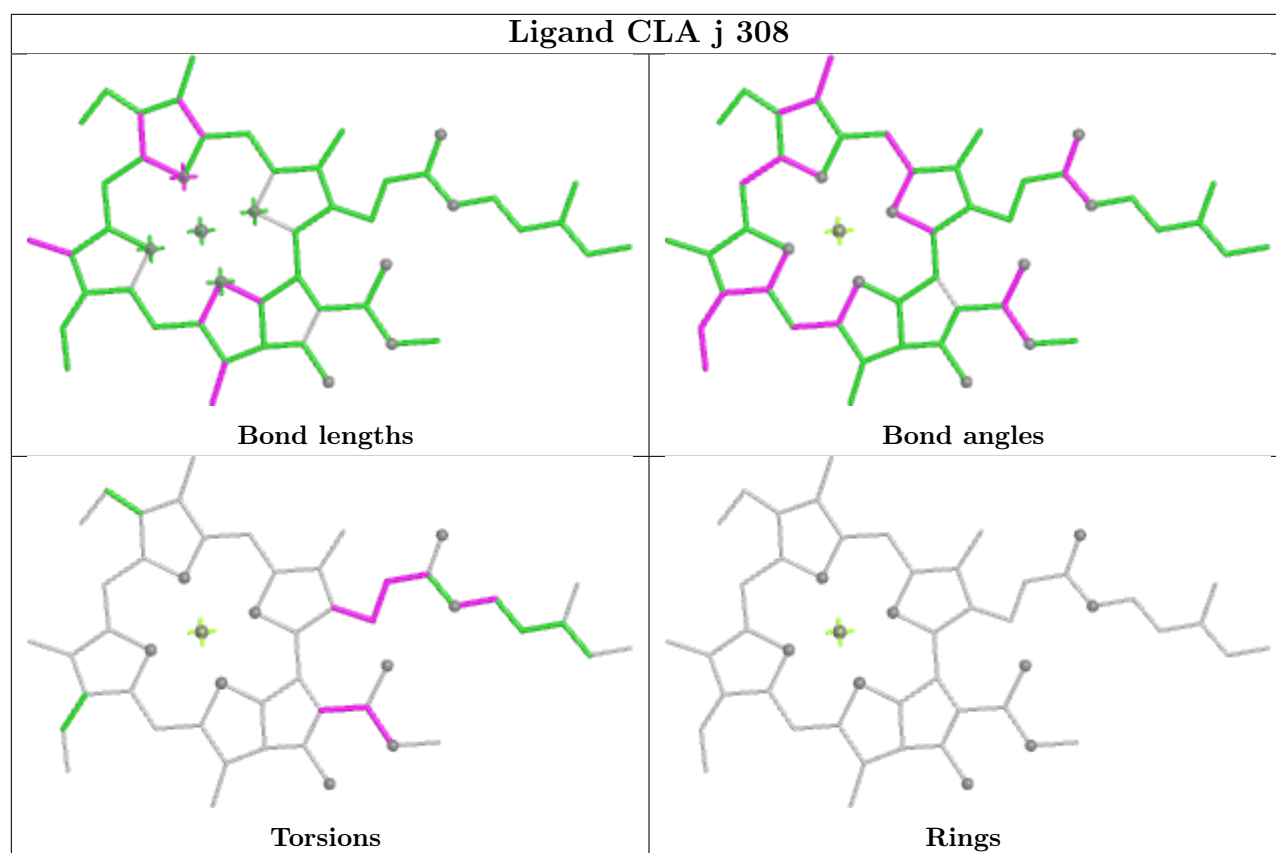


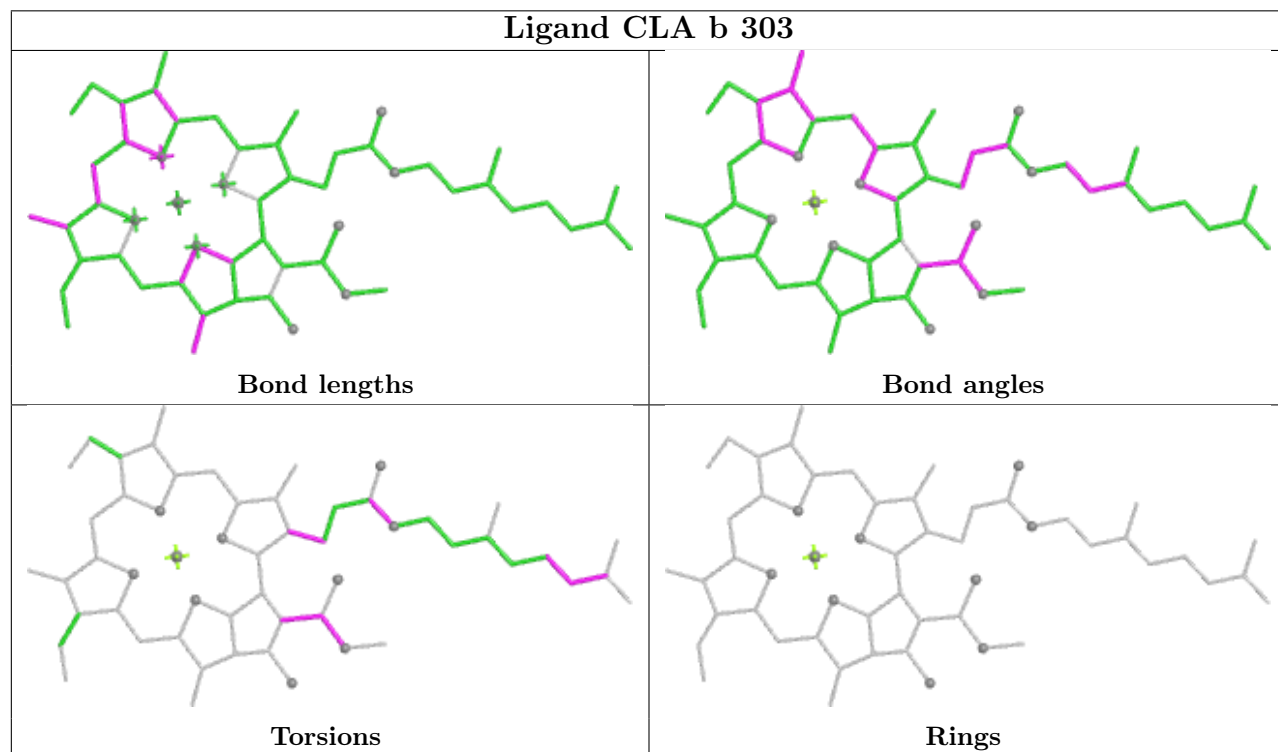
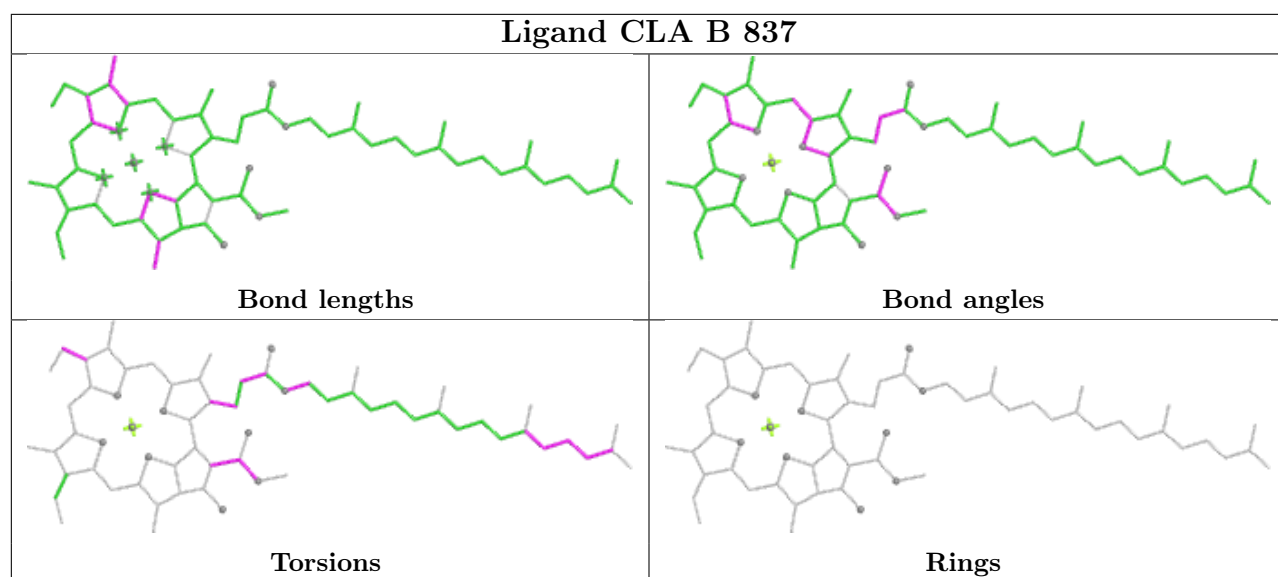
Ligand CLA a 309

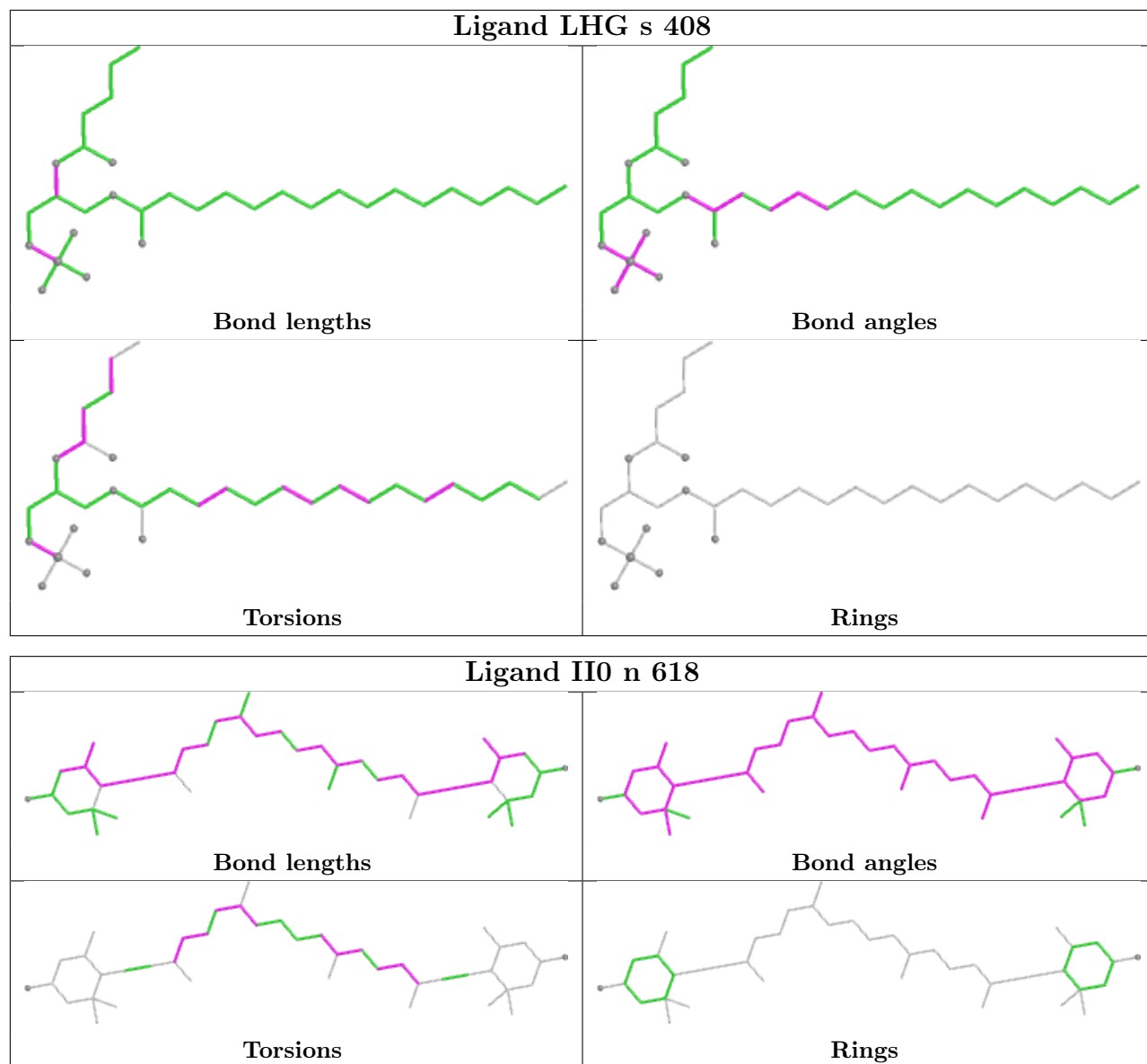


Ligand CLA c 302

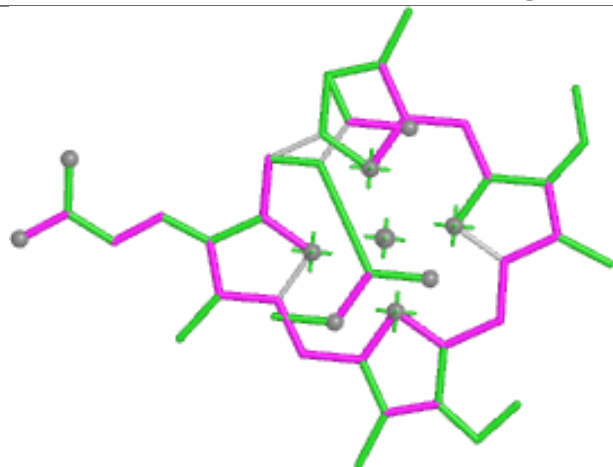




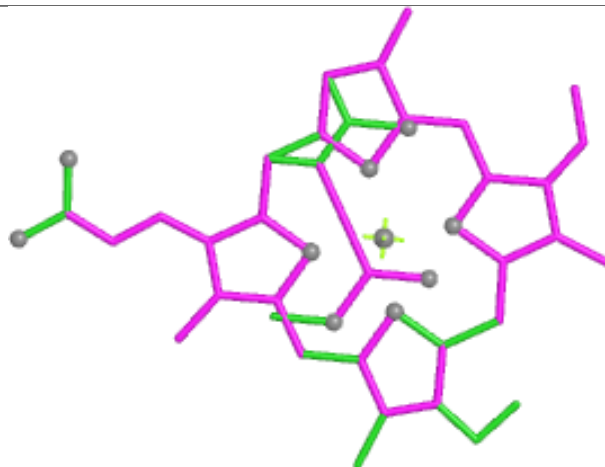




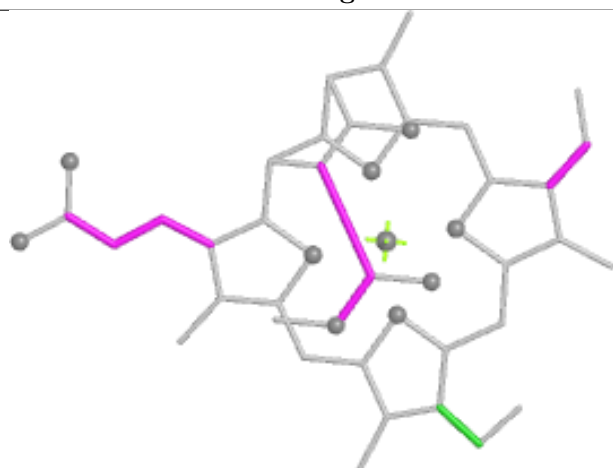
Ligand KC2 c 310



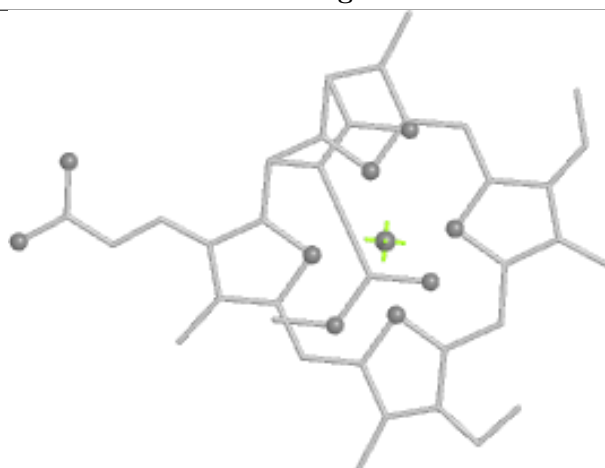
Bond lengths



Bond angles

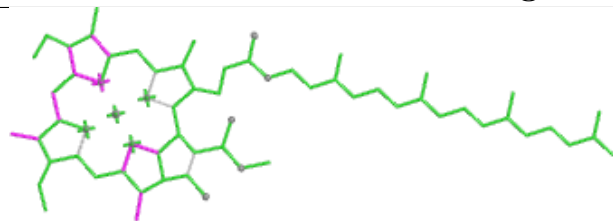


Torsions

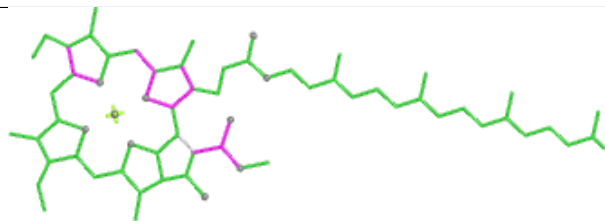


Rings

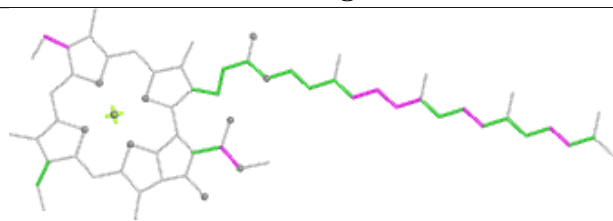
Ligand CLA s 403



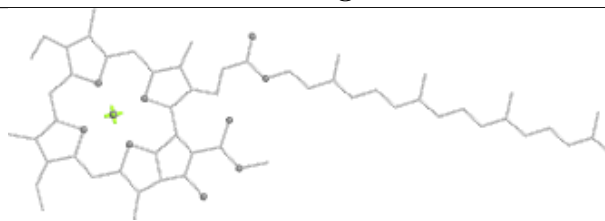
Bond lengths



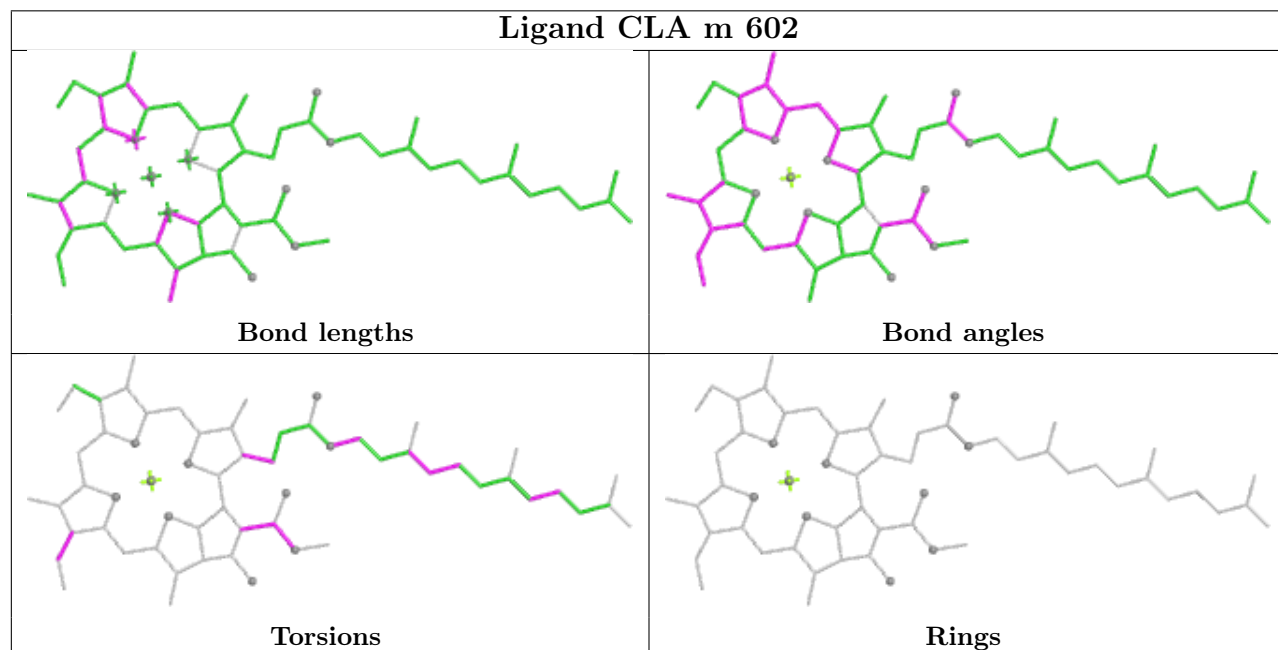
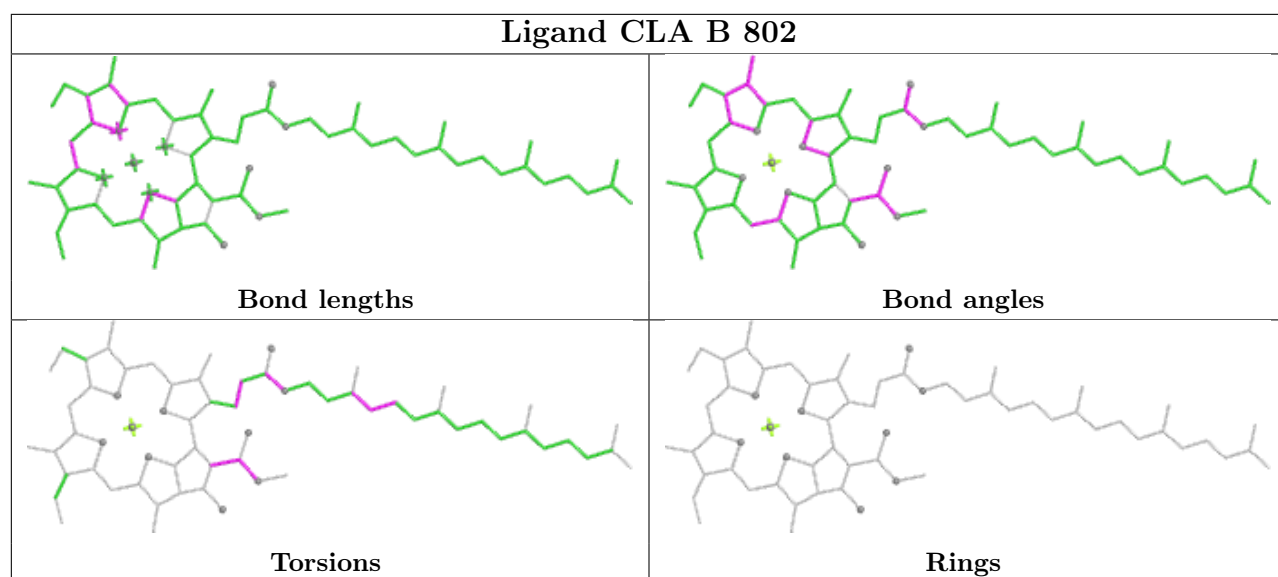
Bond angles

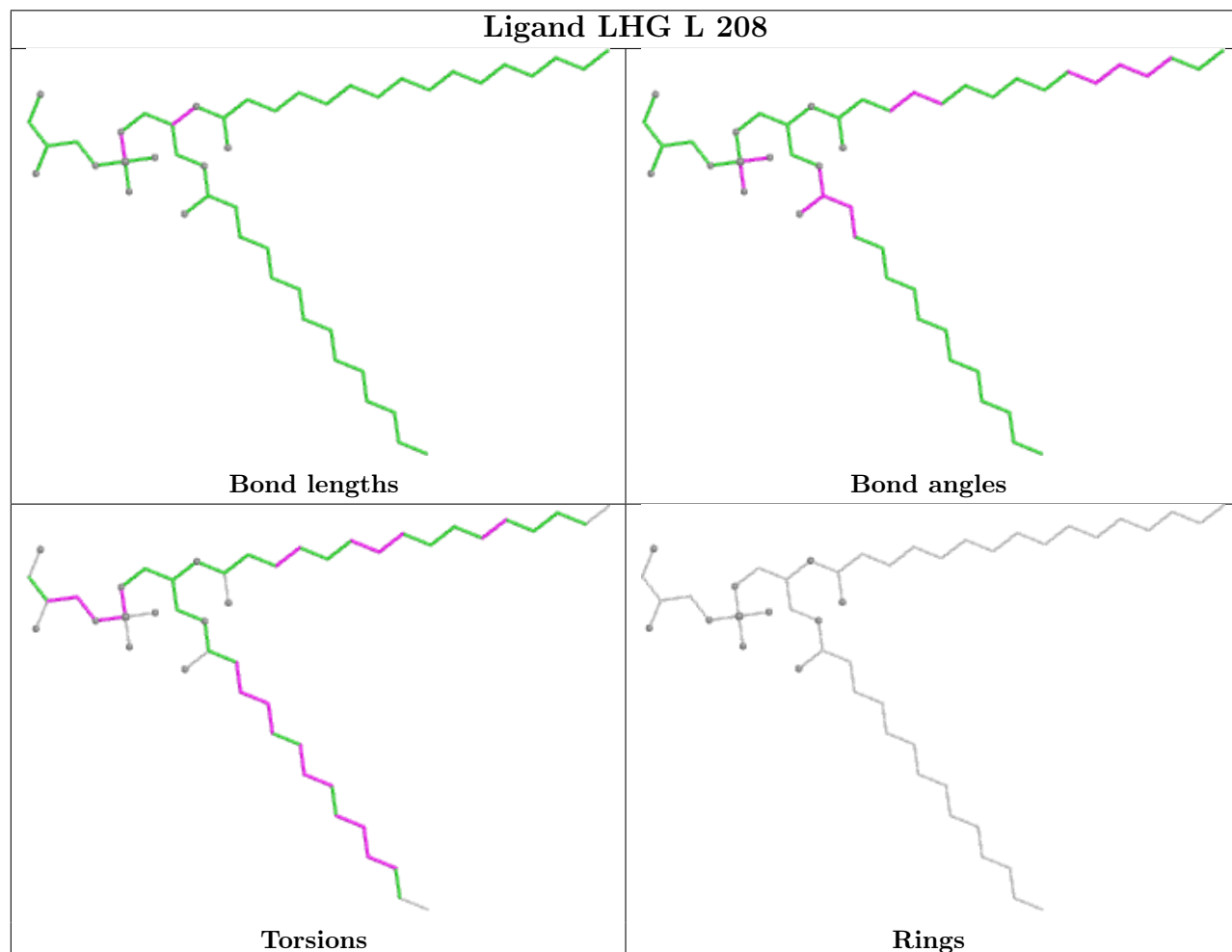
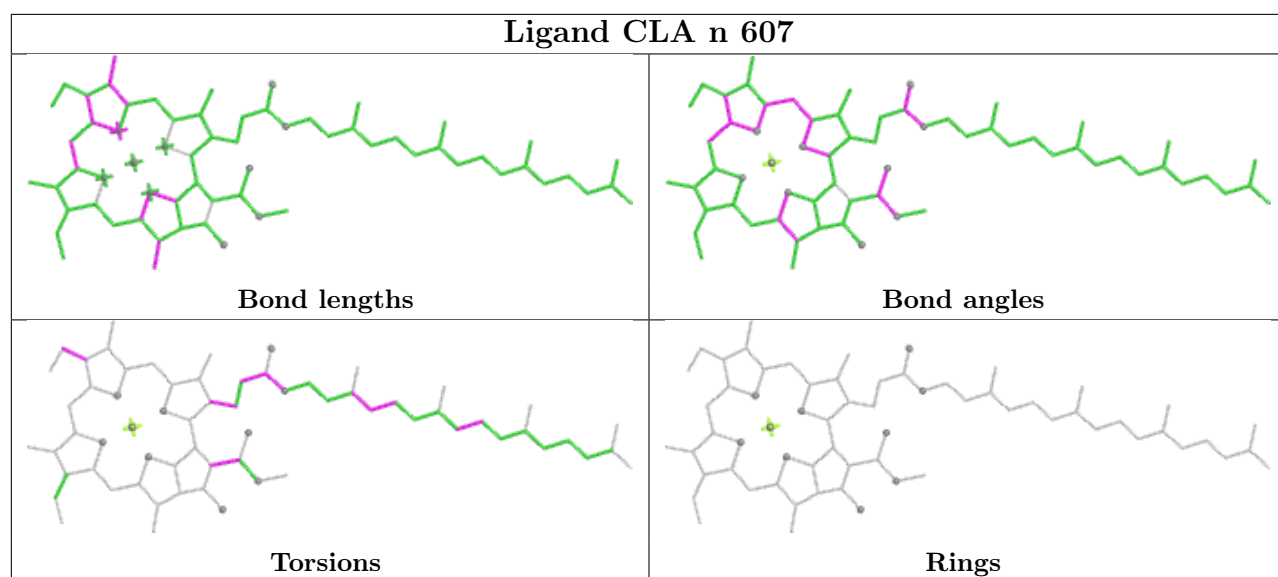


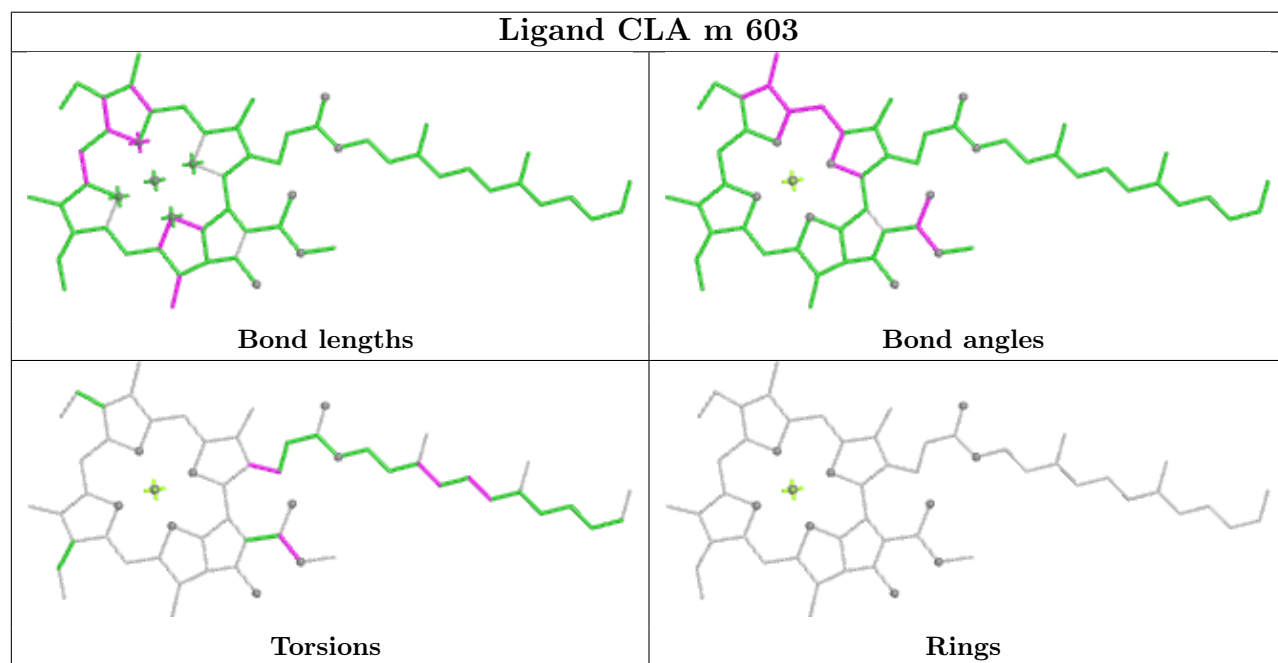
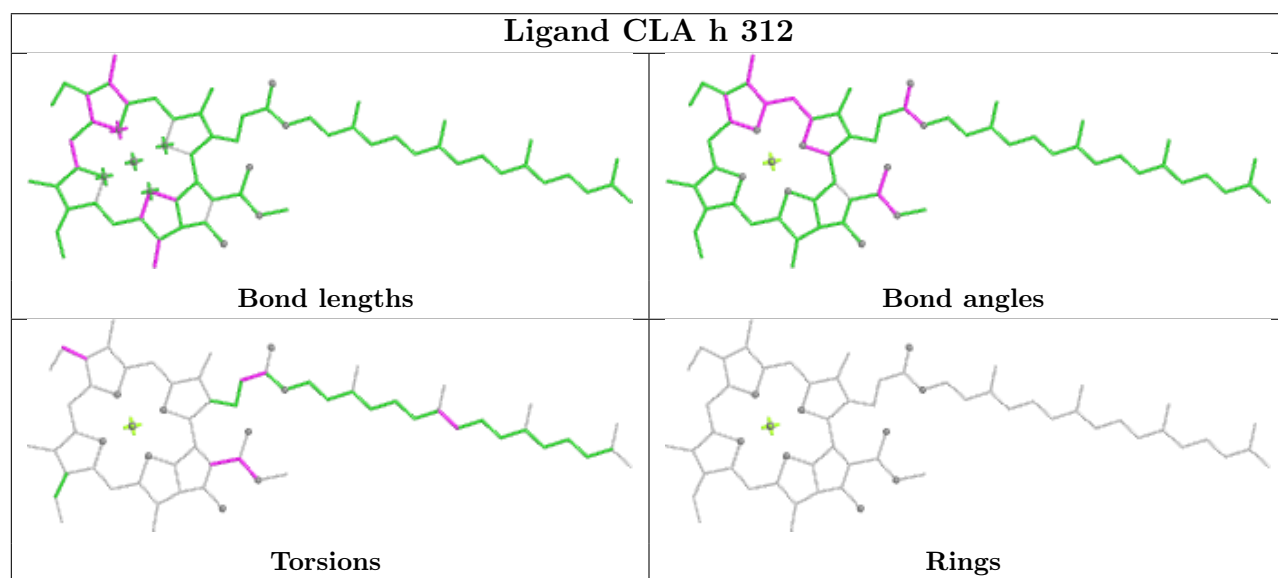
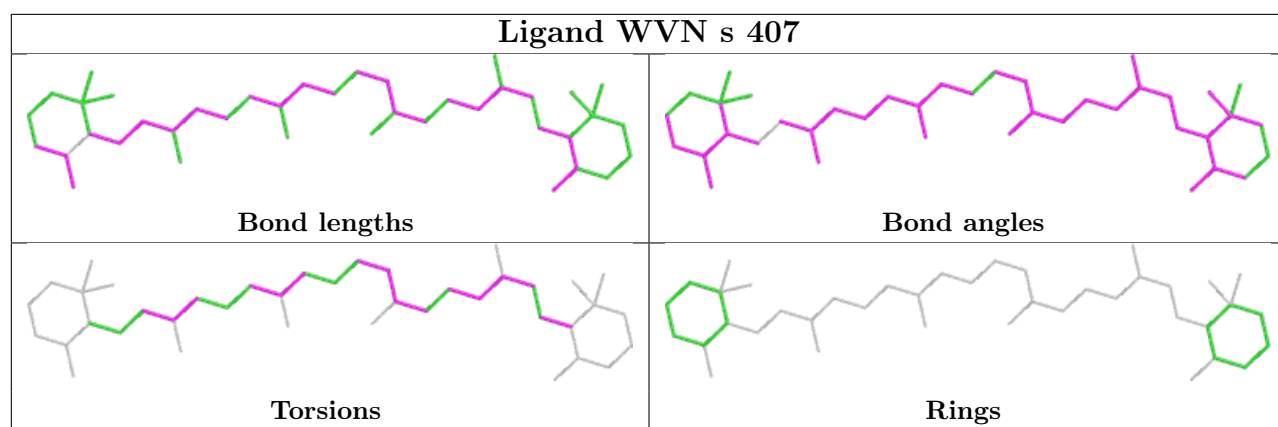
Torsions

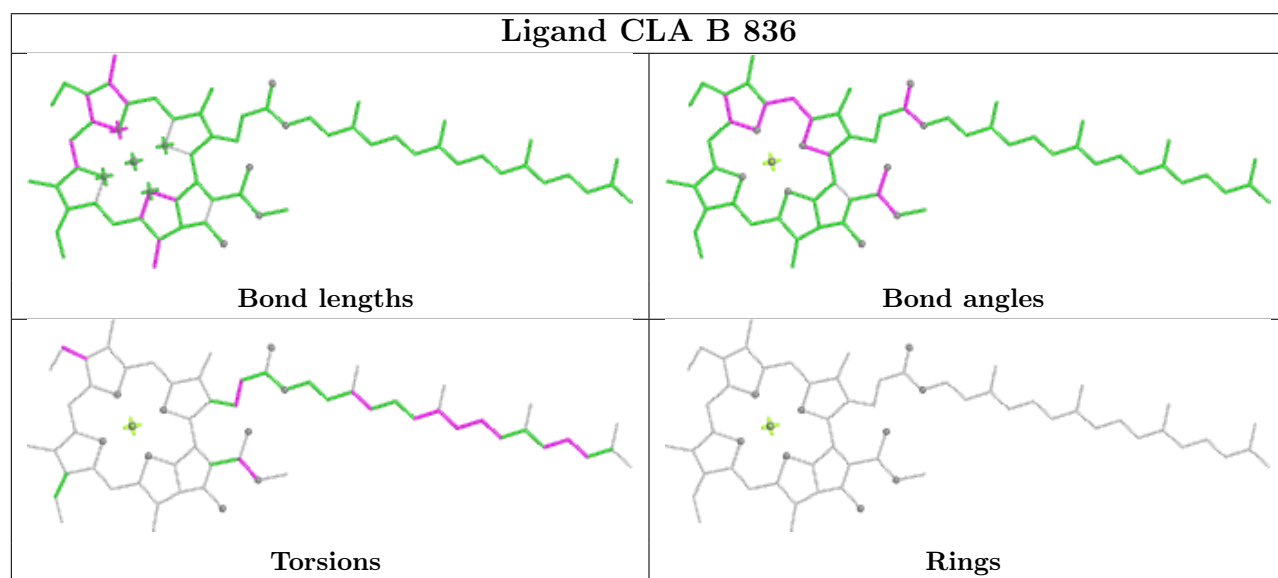
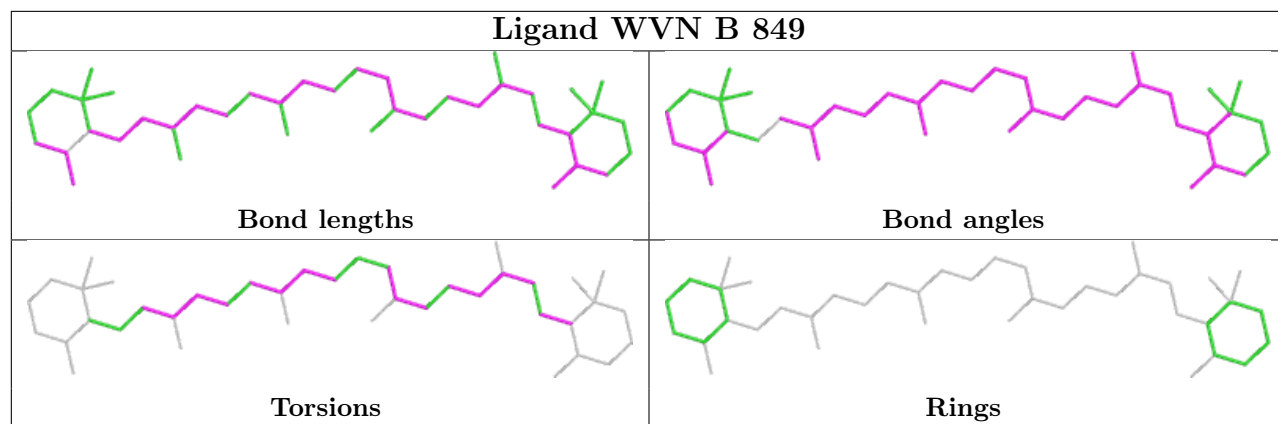


Rings

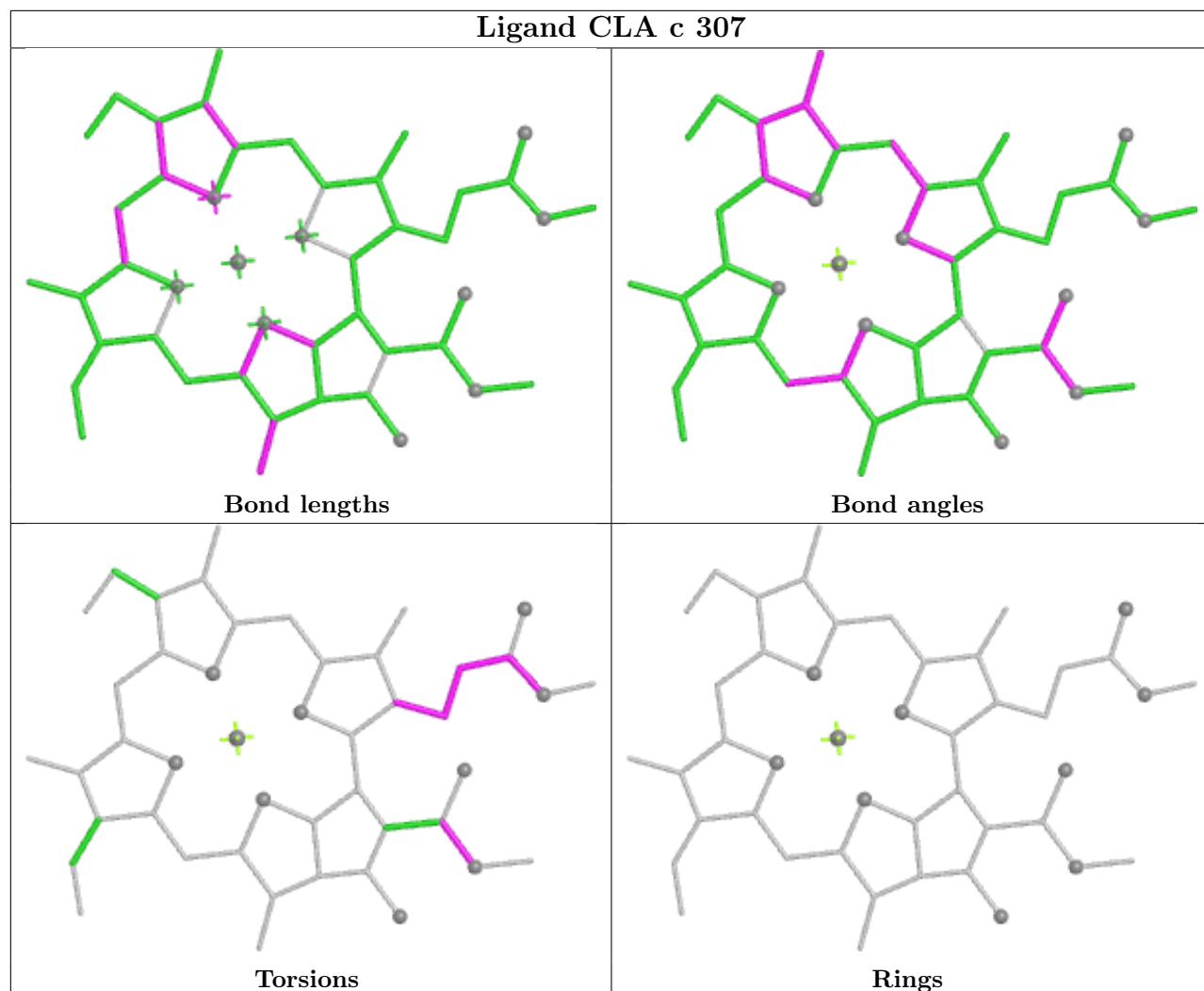




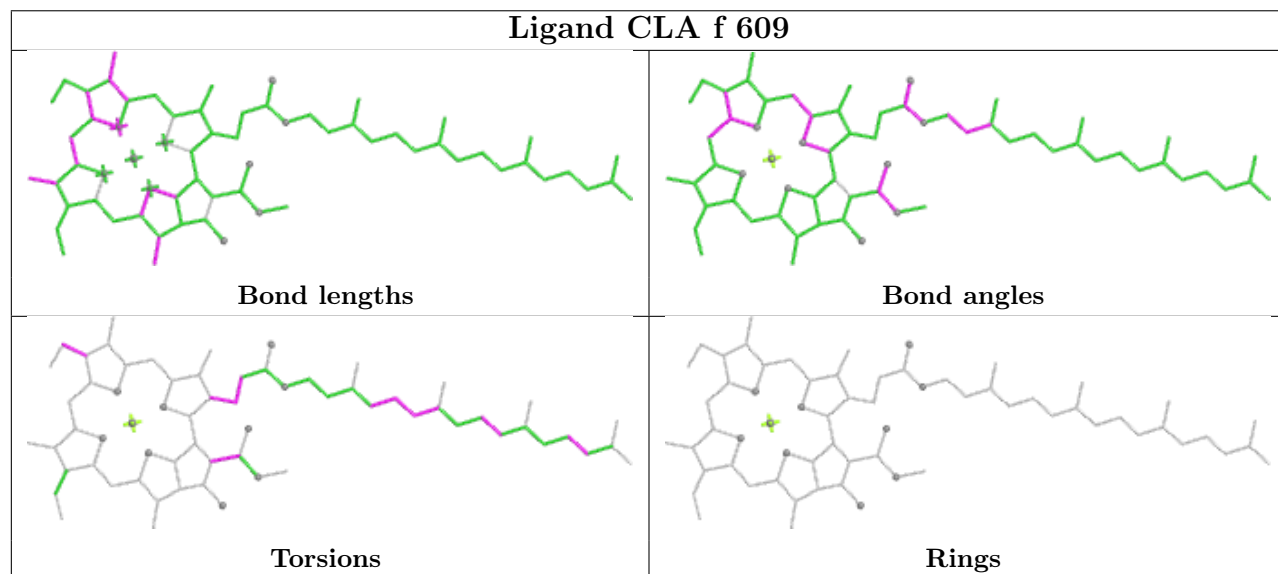




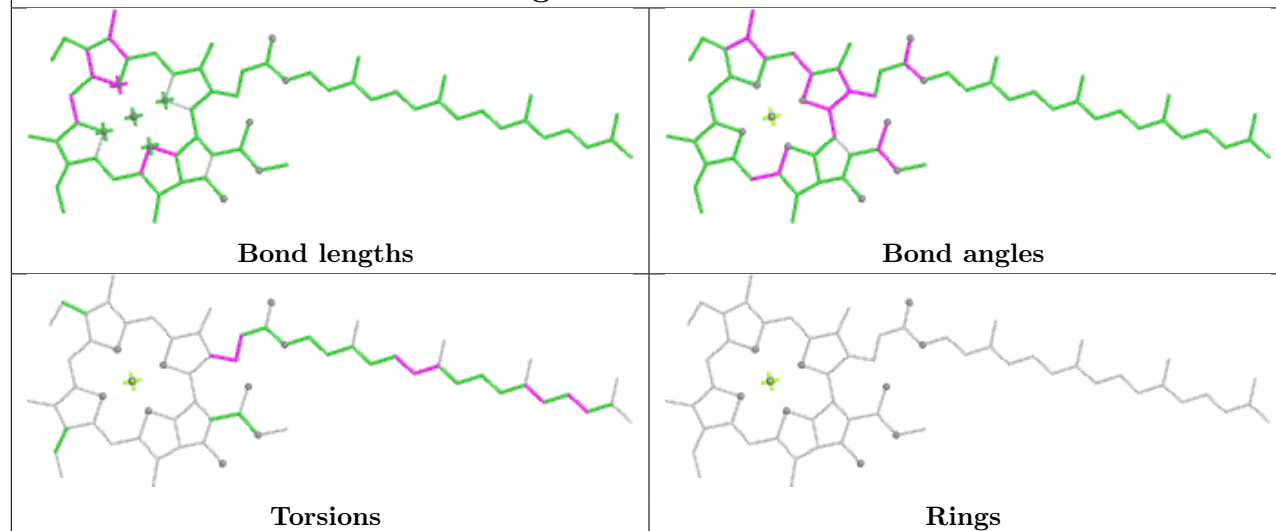
Ligand CLA c 307



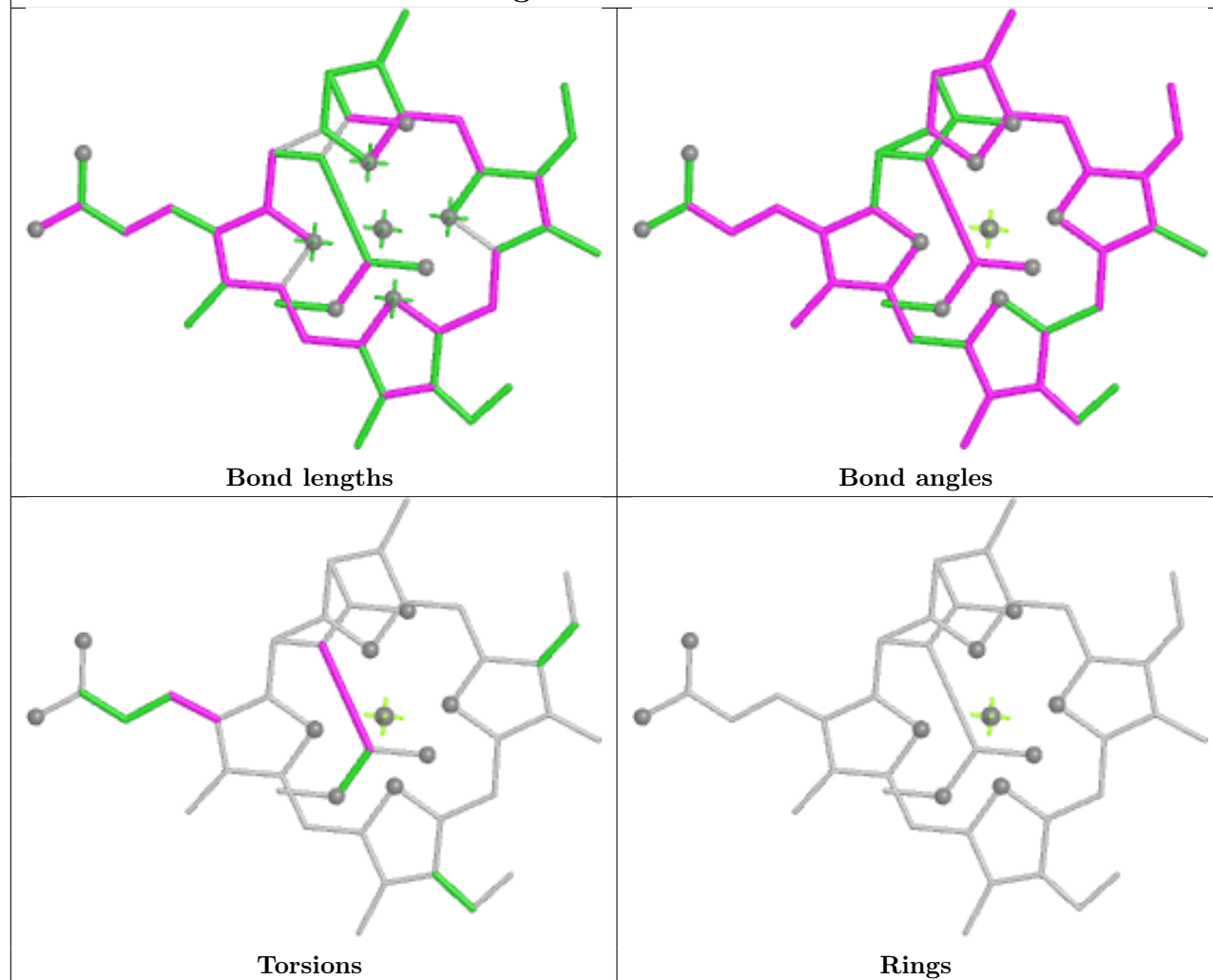
Ligand CLA f 609



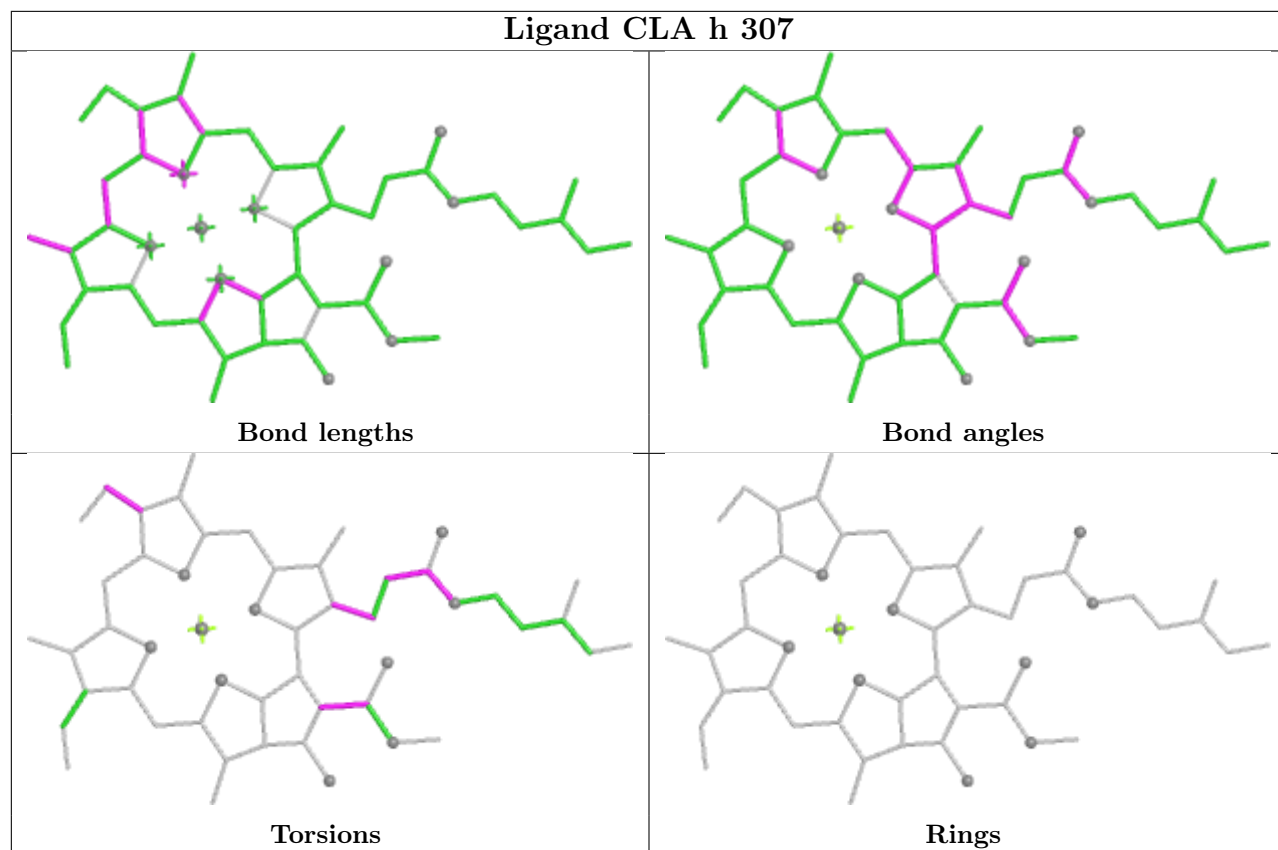
Ligand CLA B 829



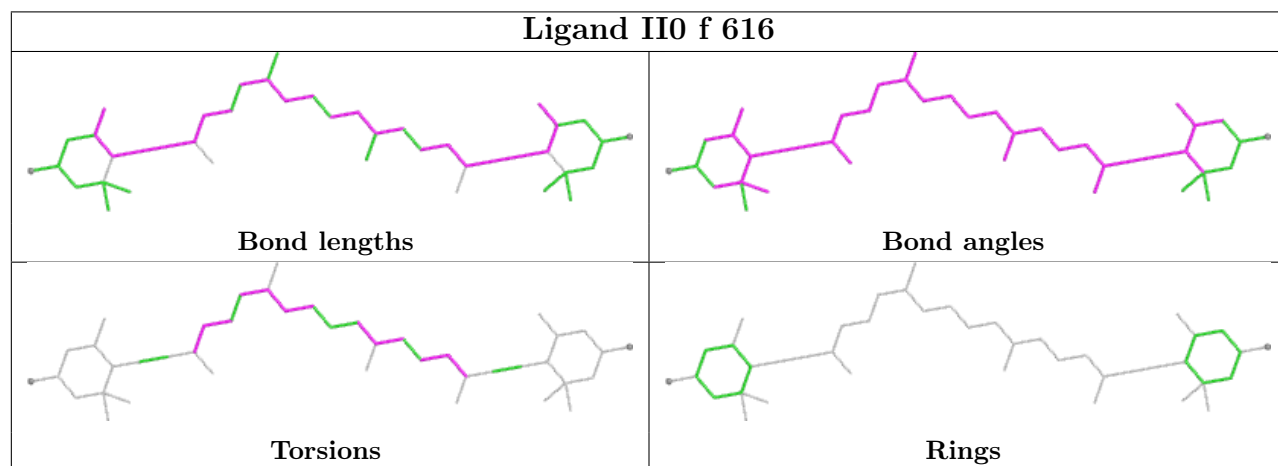
Ligand KC2 s 404



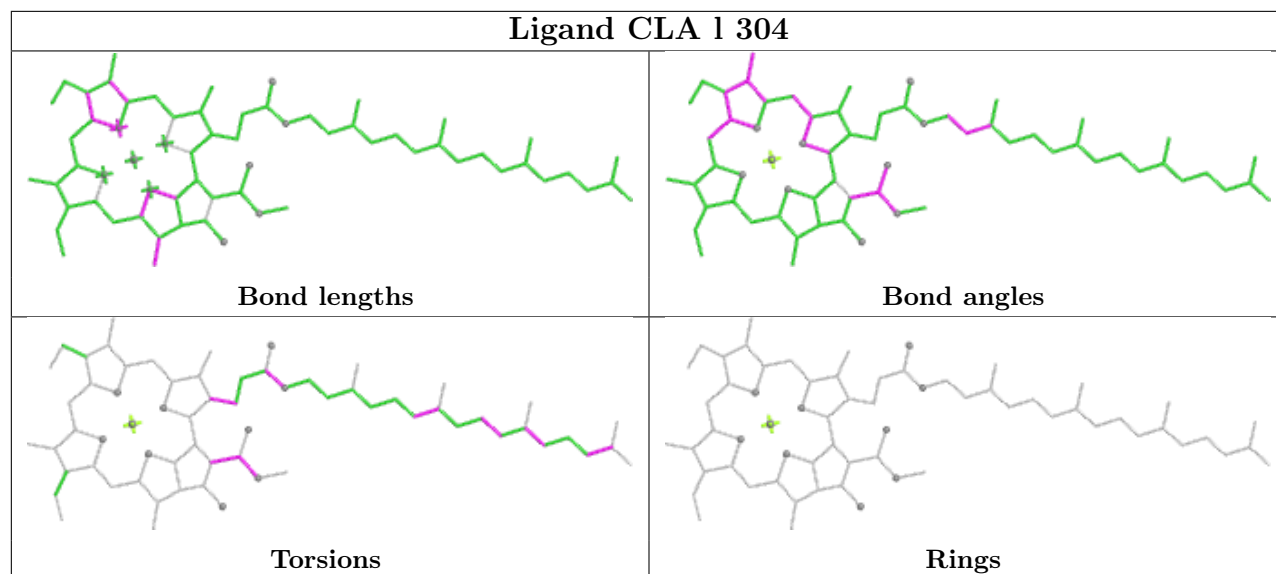
Ligand CLA h 307



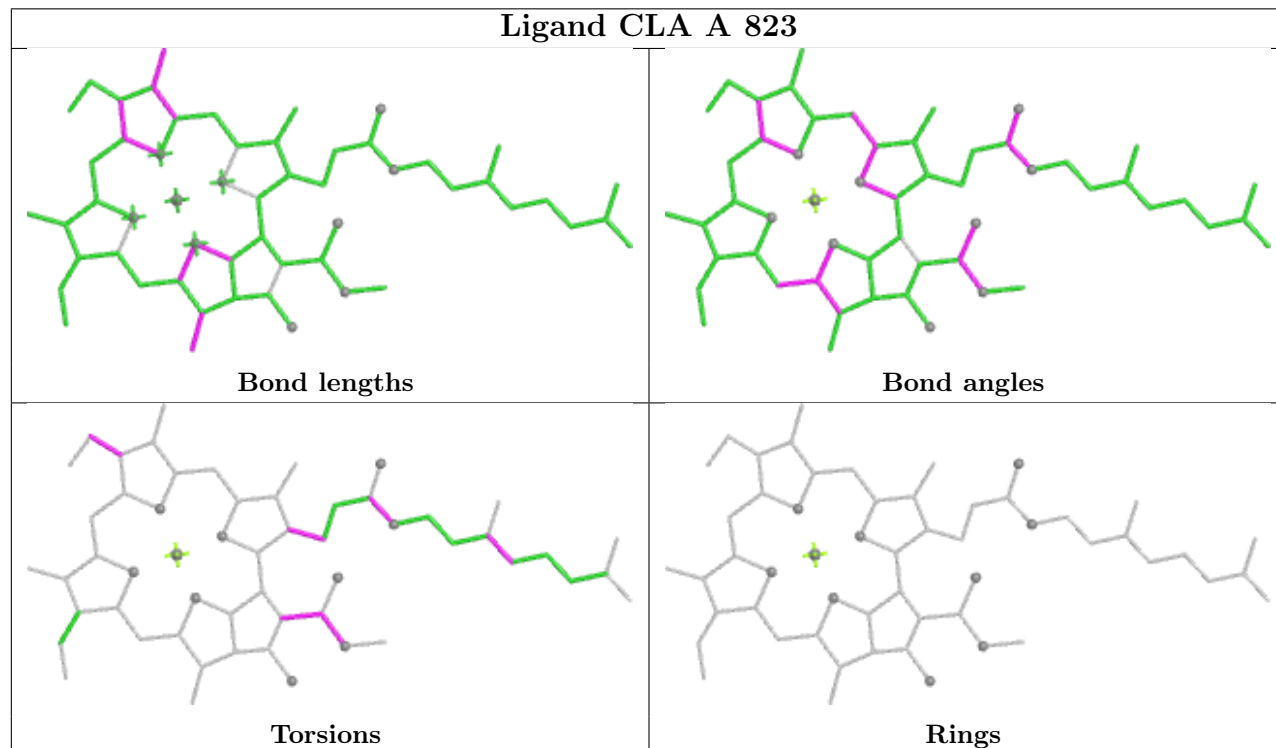
Ligand II0 f 616



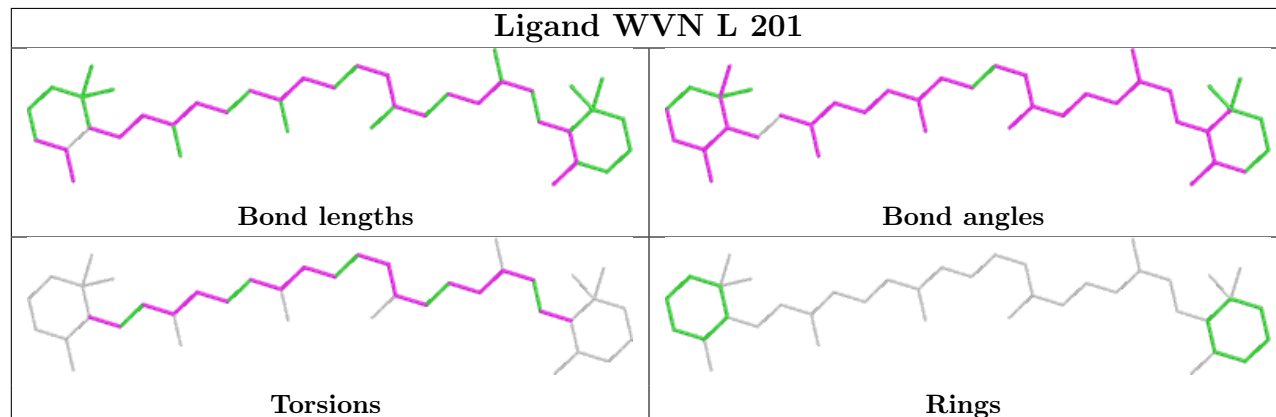
Ligand CLA I 304

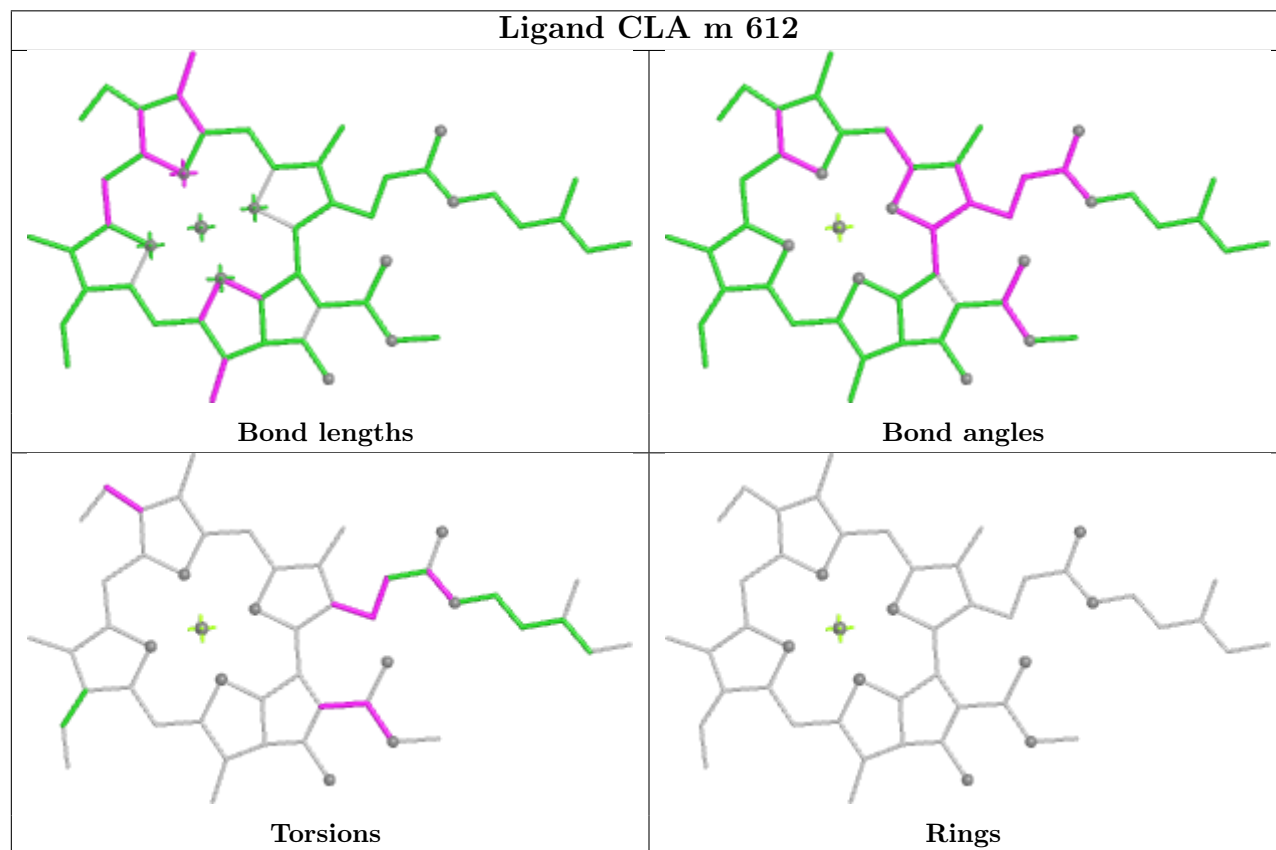
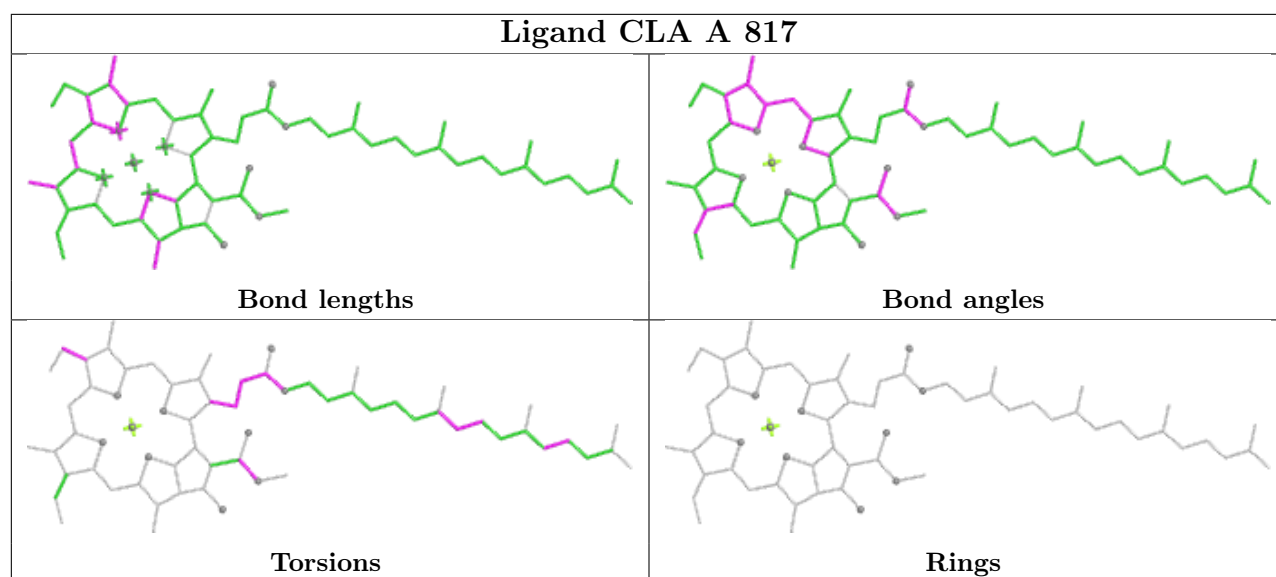


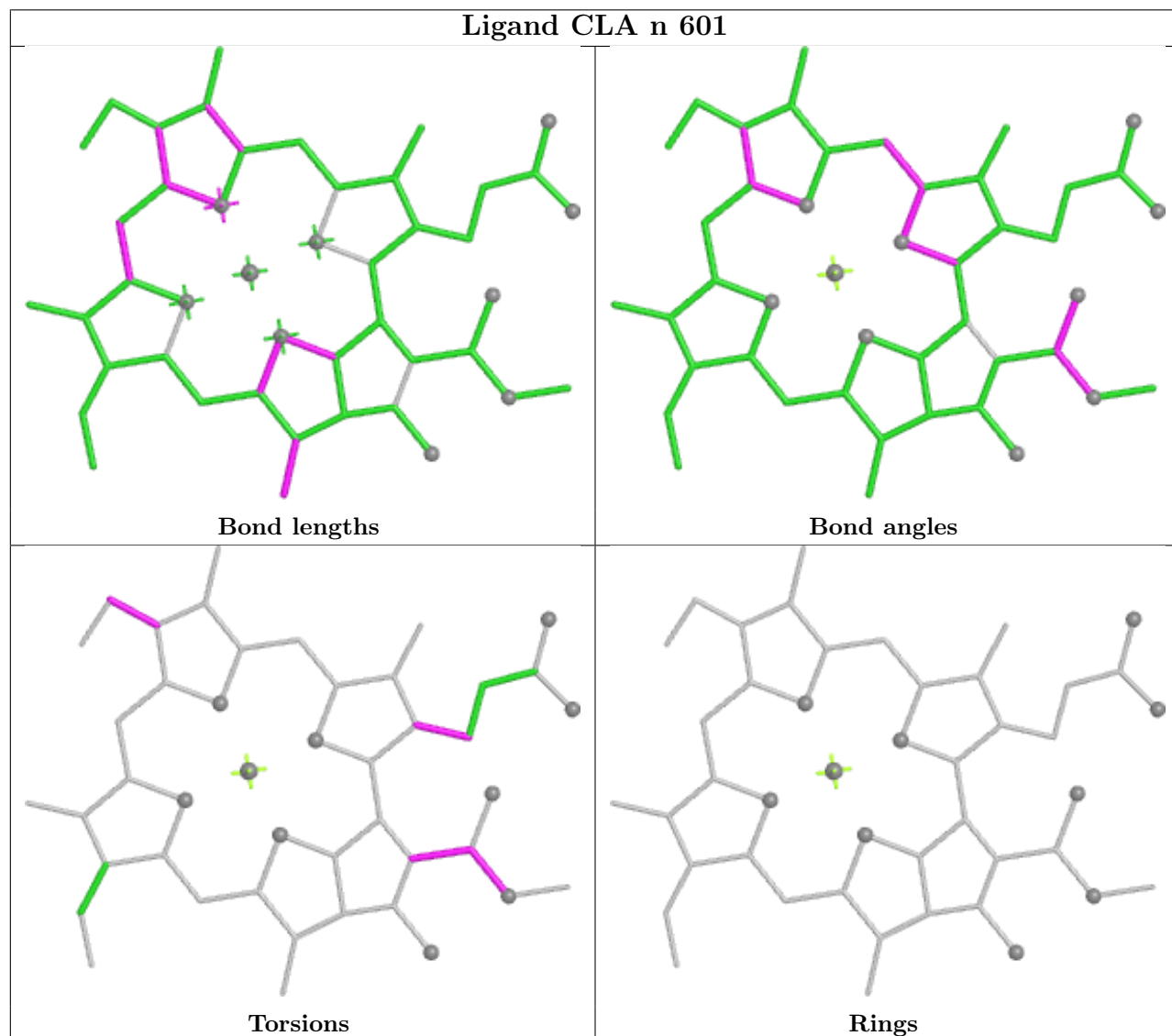
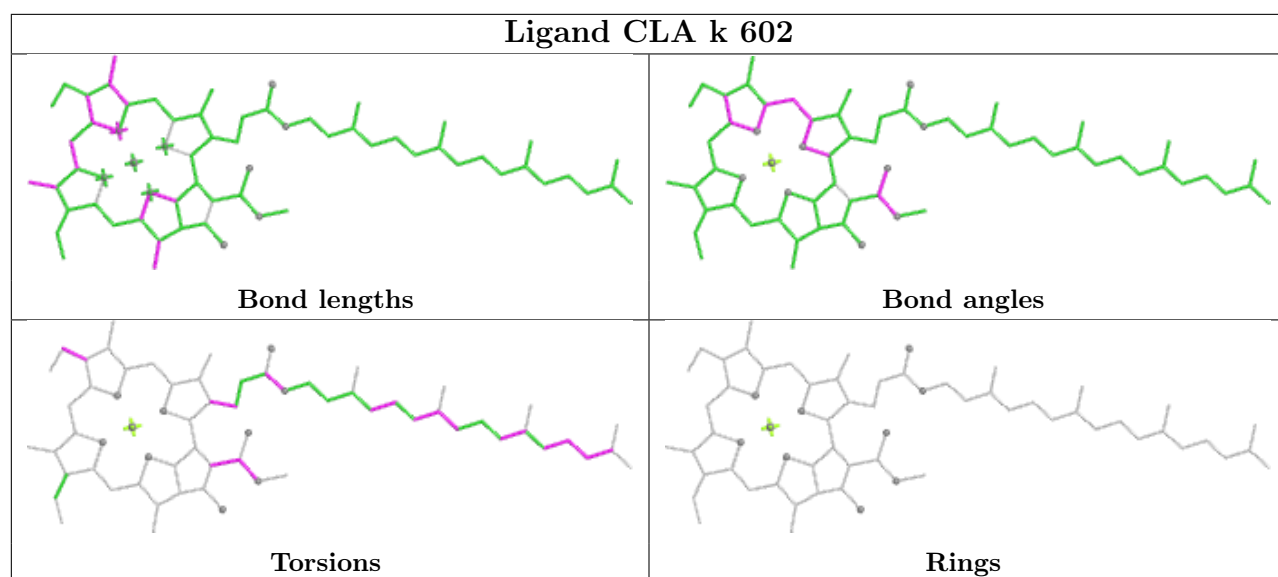
Ligand CLA A 823



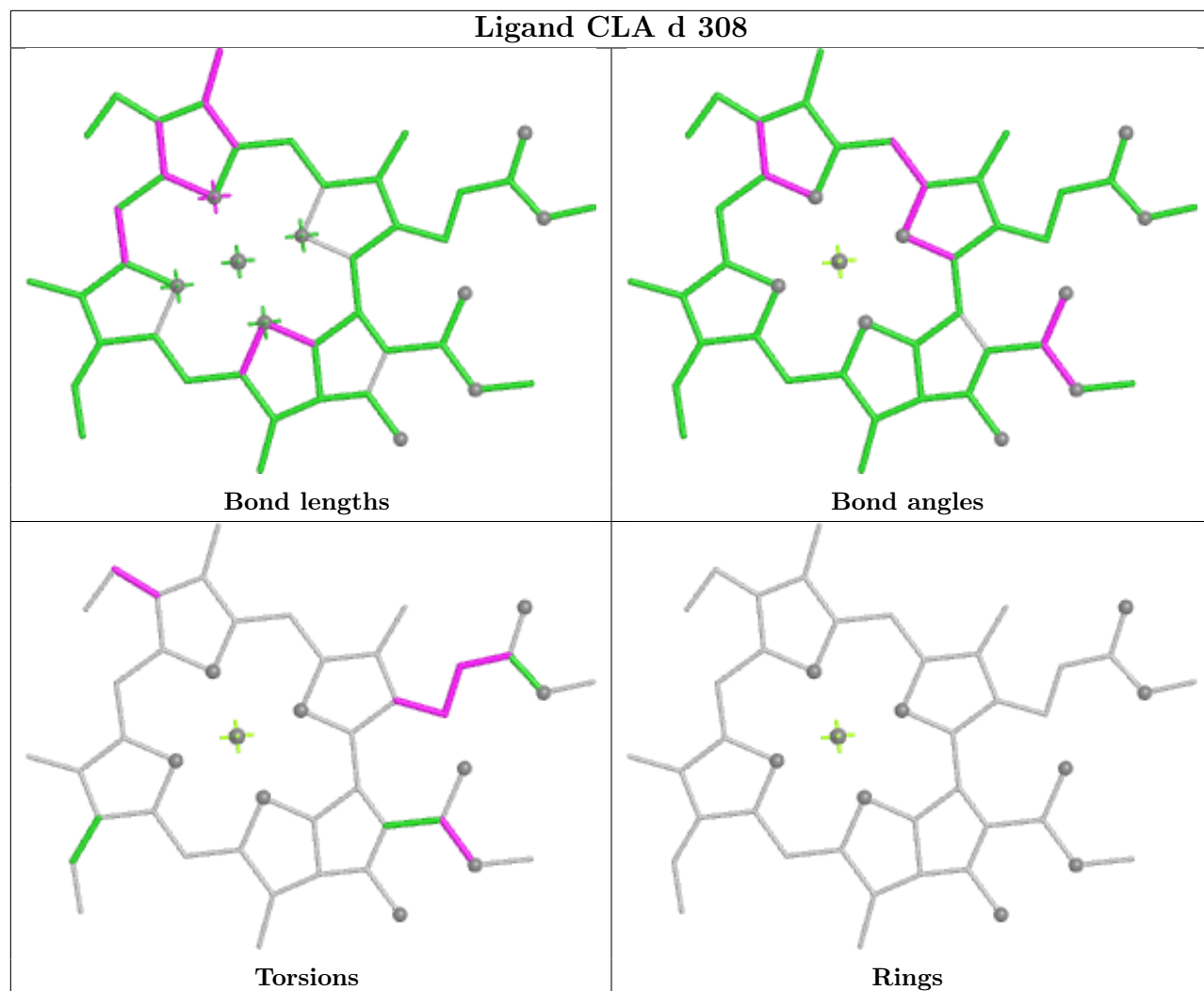
Ligand WVN L 201



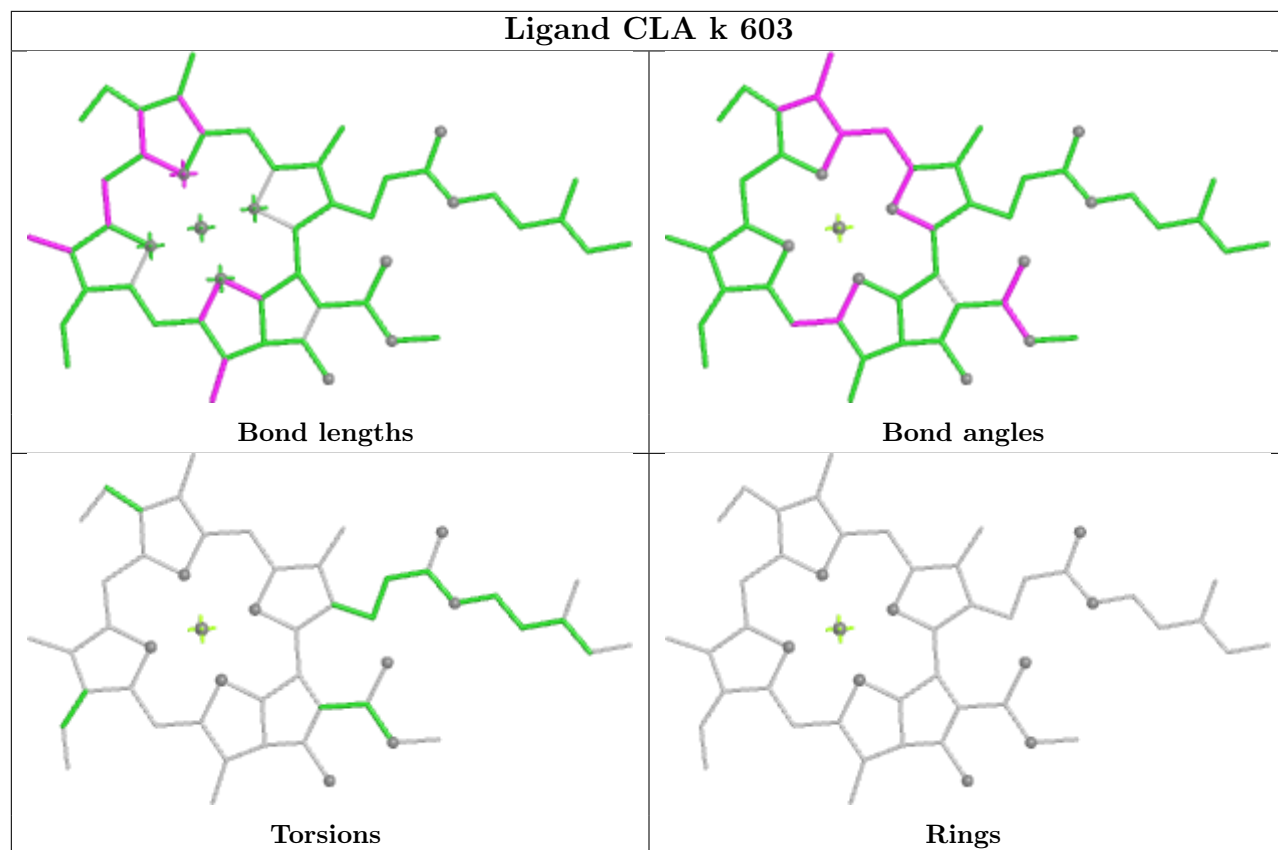




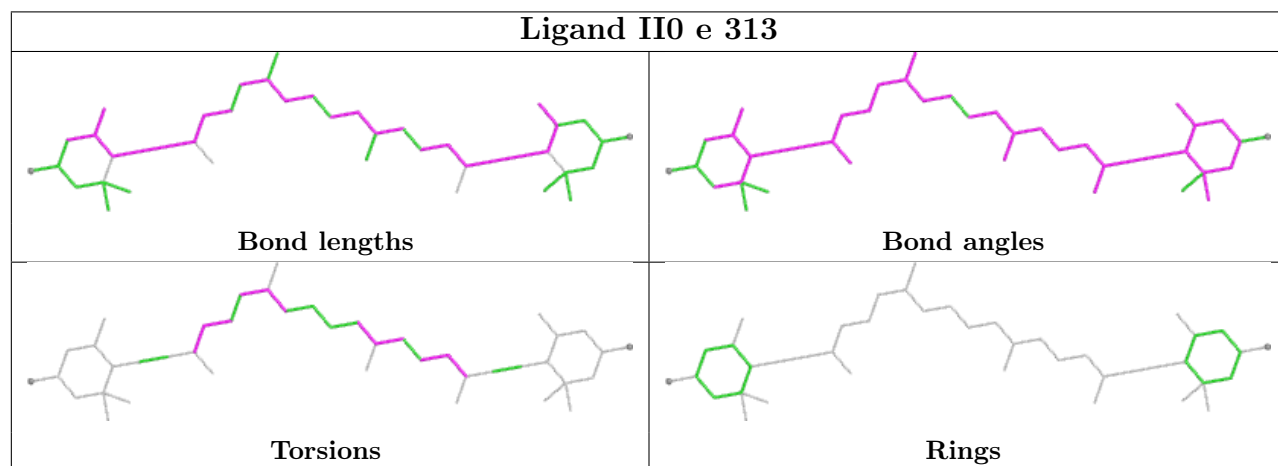
Ligand CLA d 308



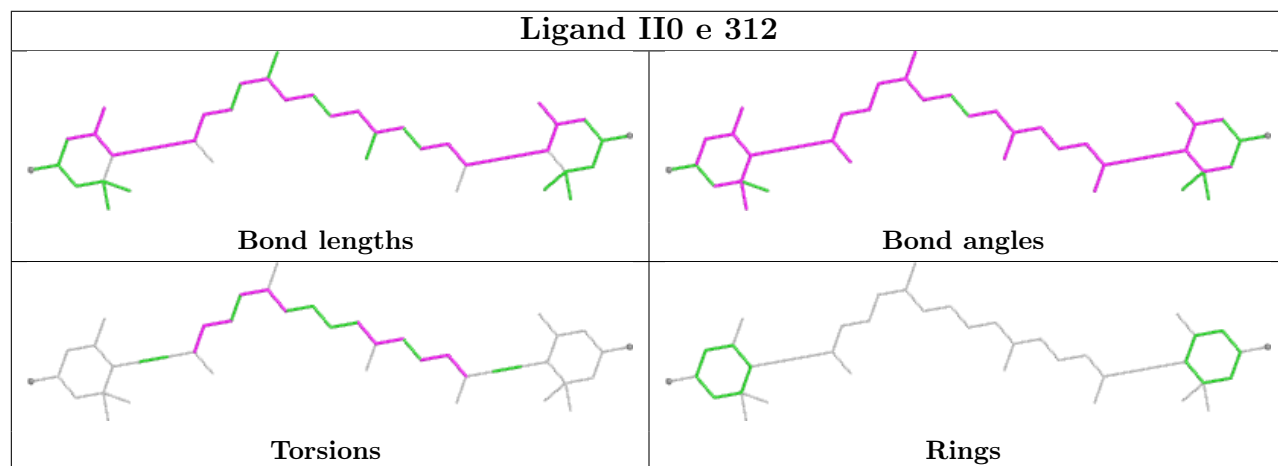
Ligand CLA k 603

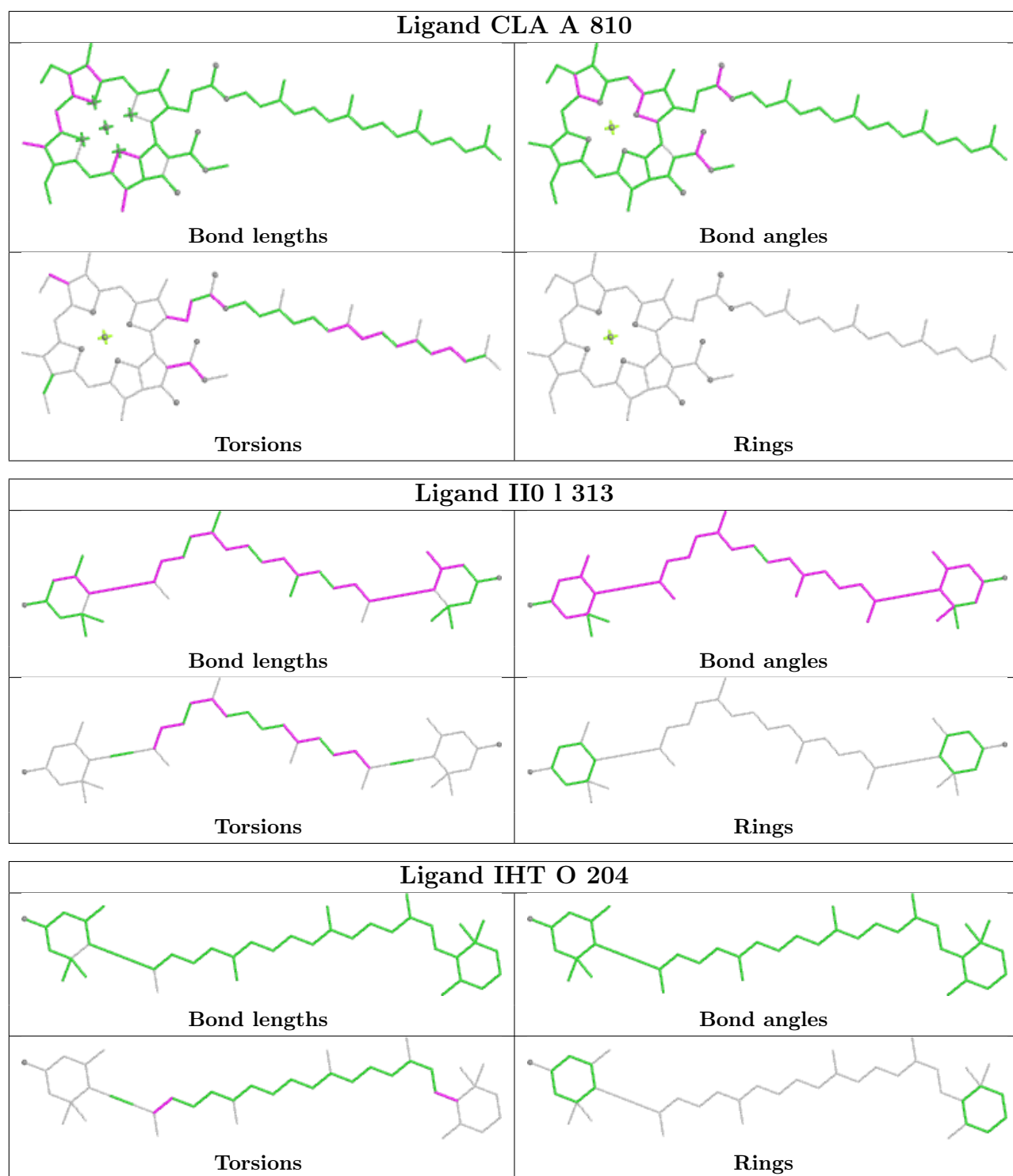


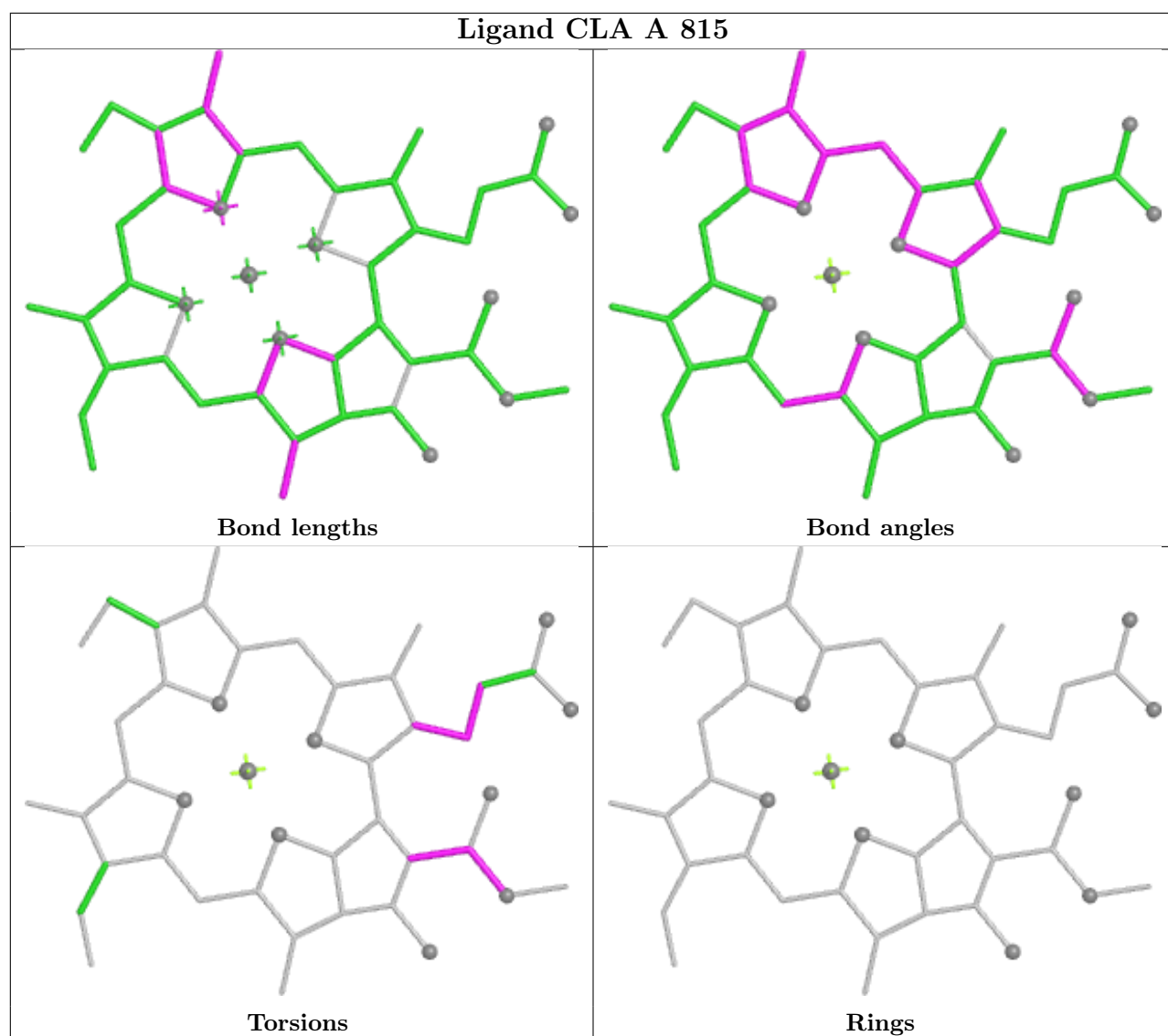
Ligand II0 e 313



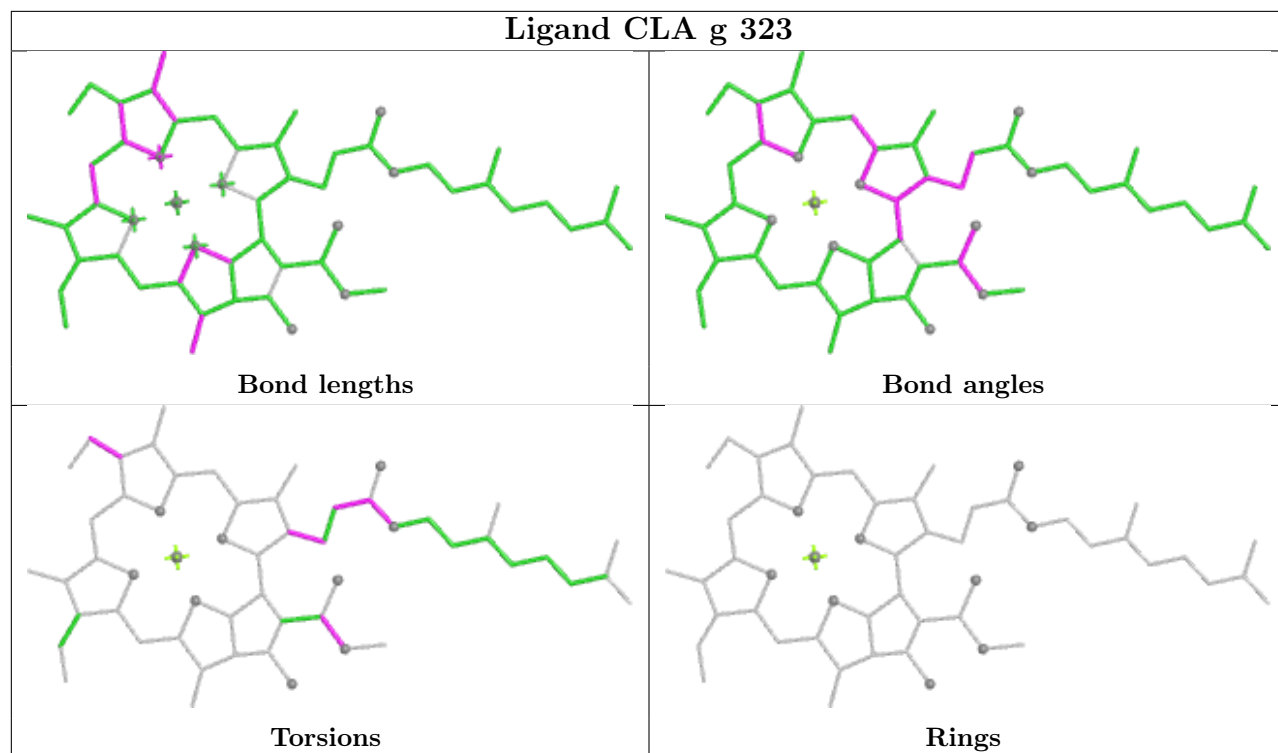
Ligand II0 e 312



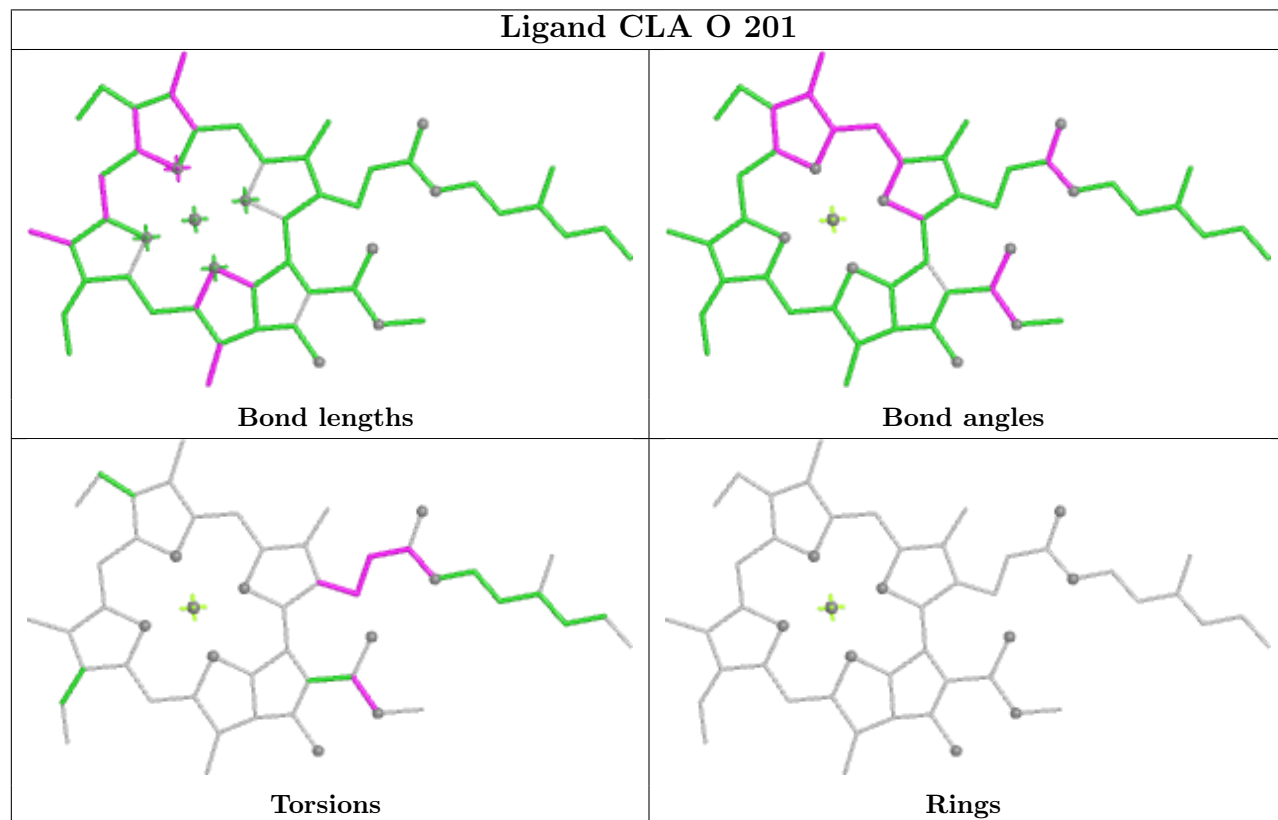


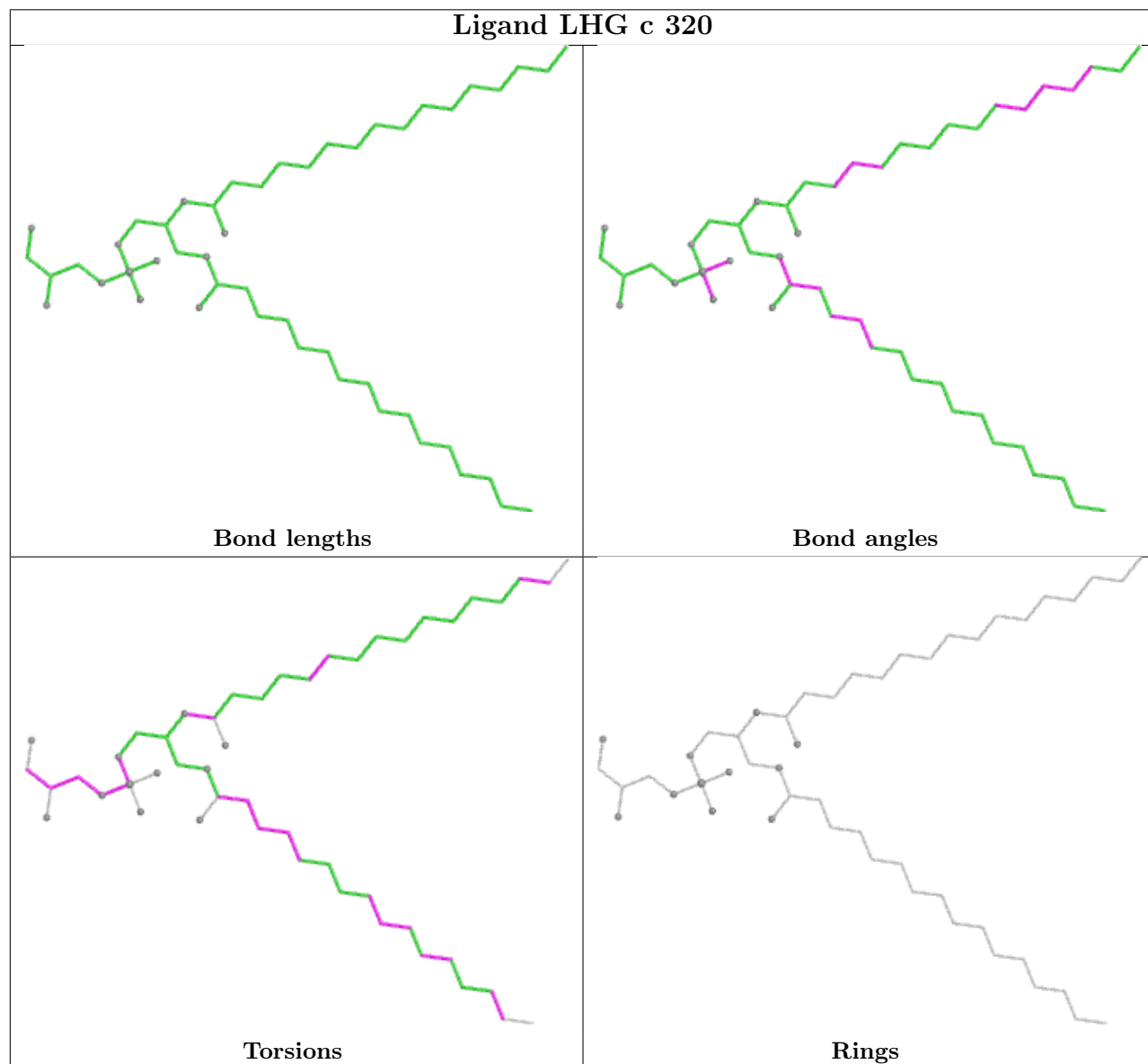
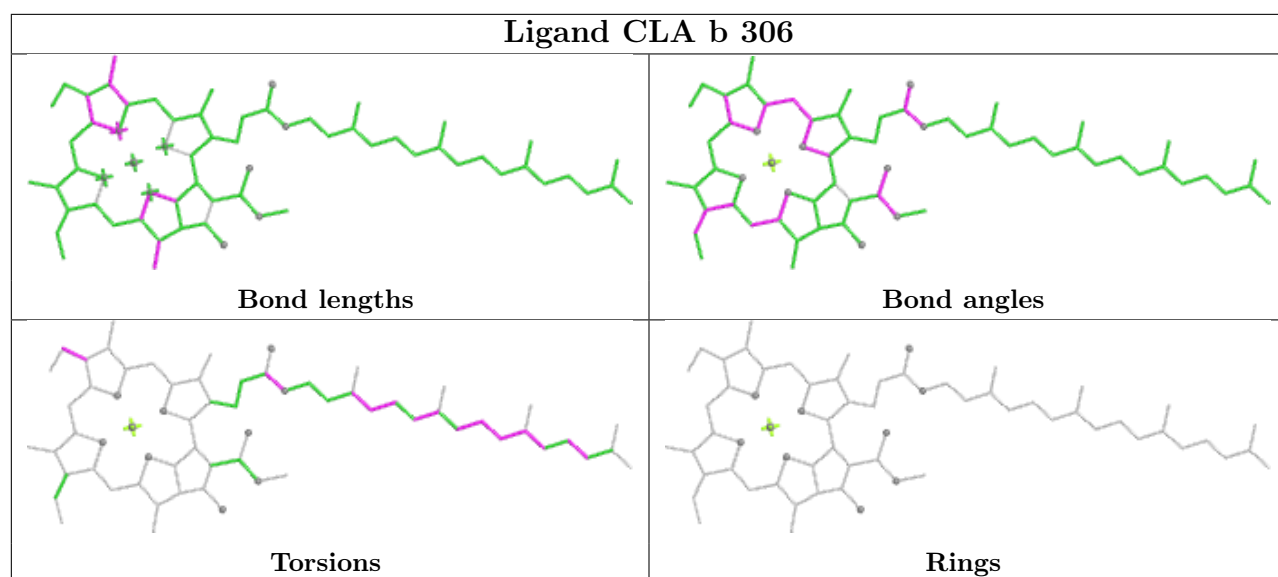


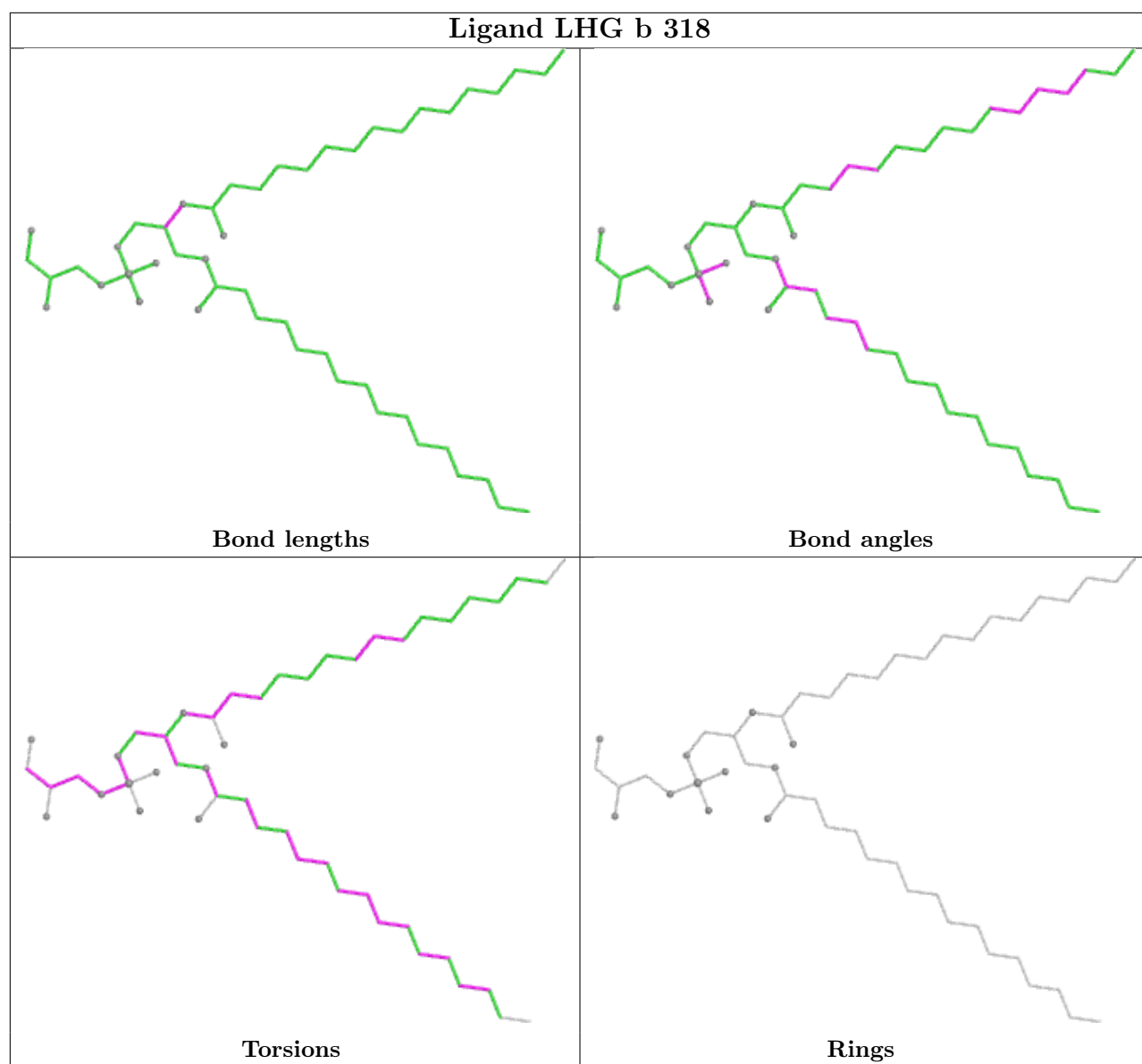
Ligand CLA g 323



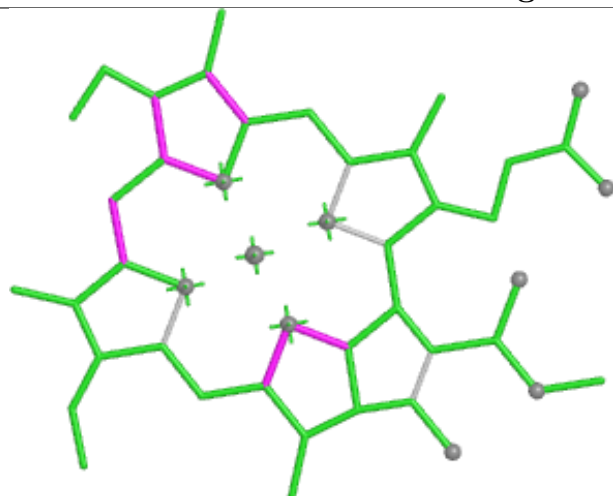
Ligand CLA O 201



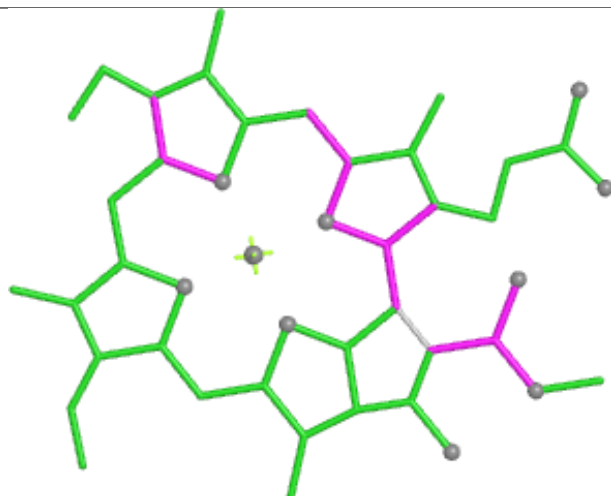




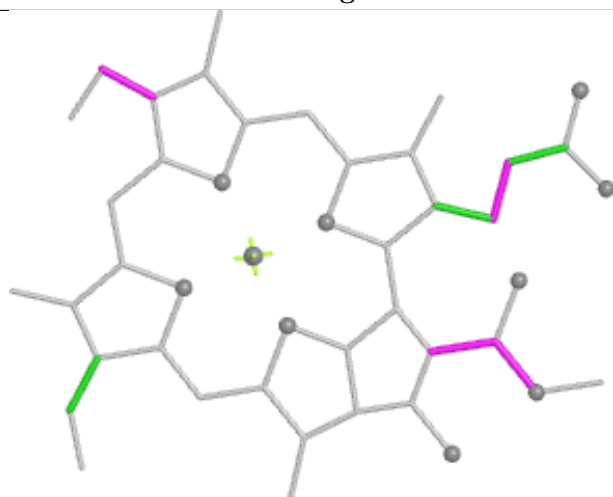
Ligand CLA k 605



Bond lengths



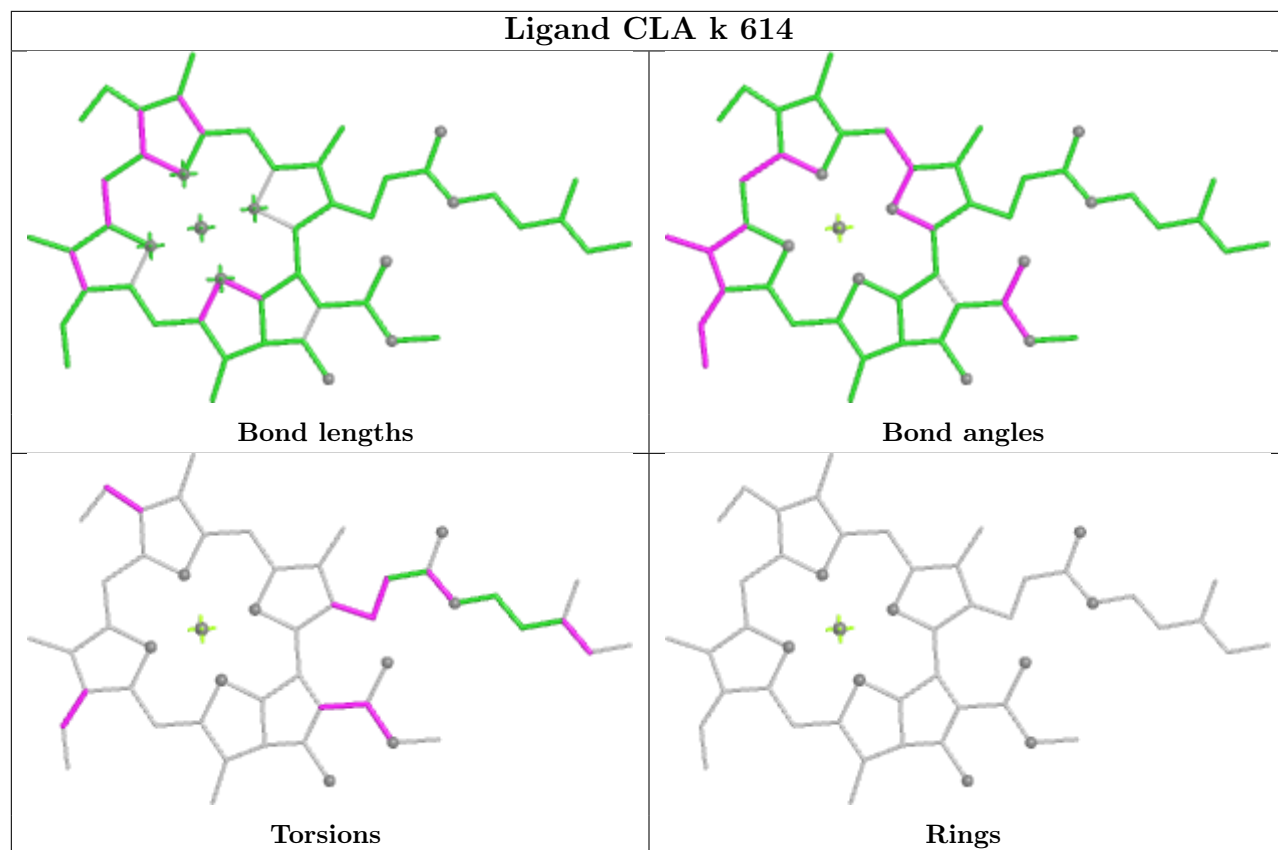
Bond angles



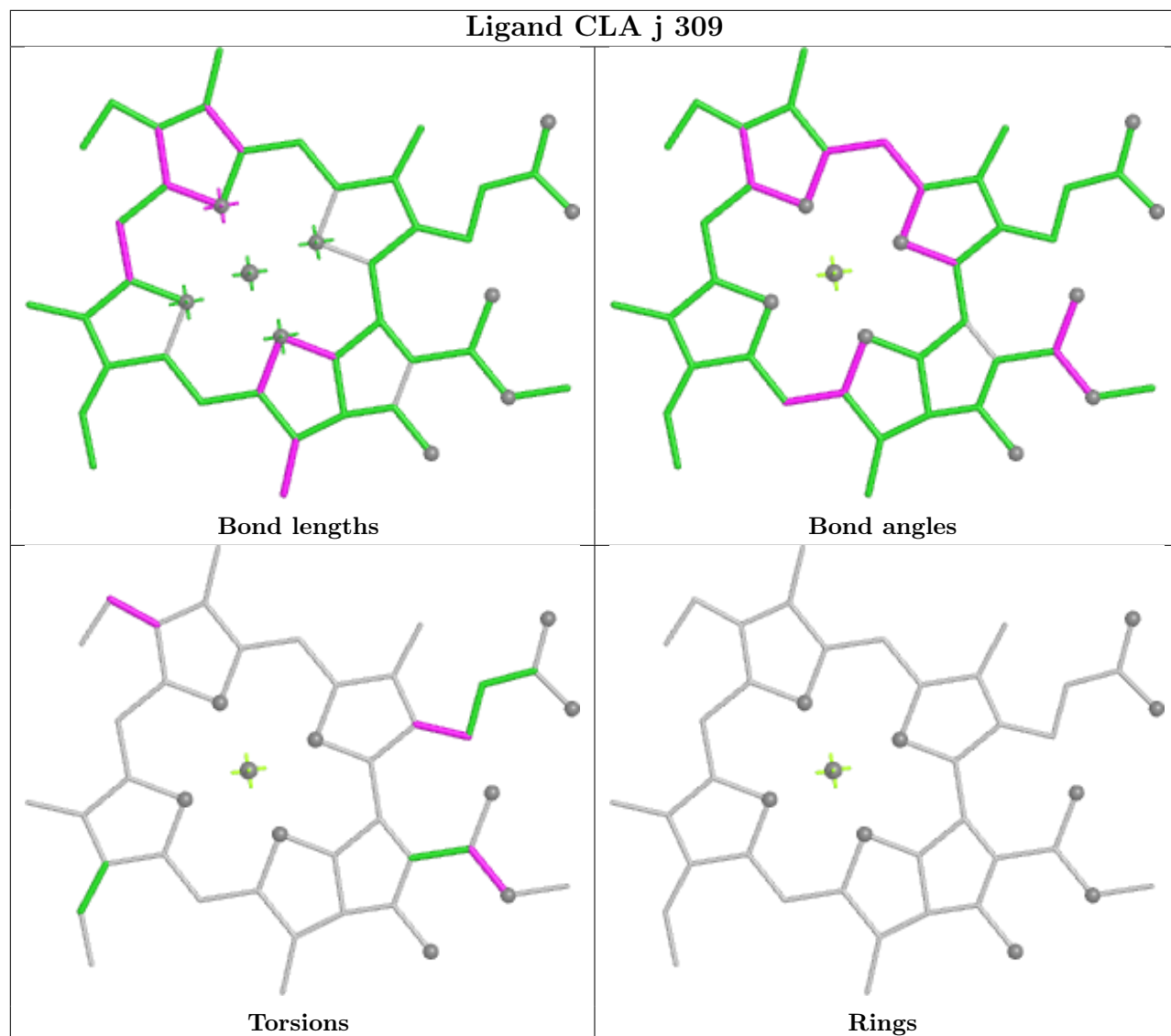
Torsions



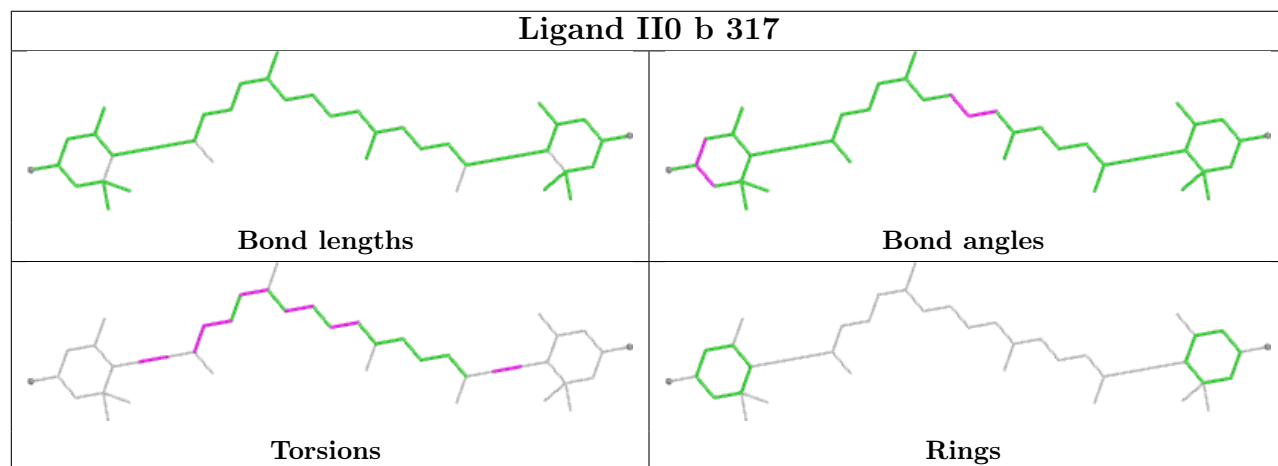
Rings



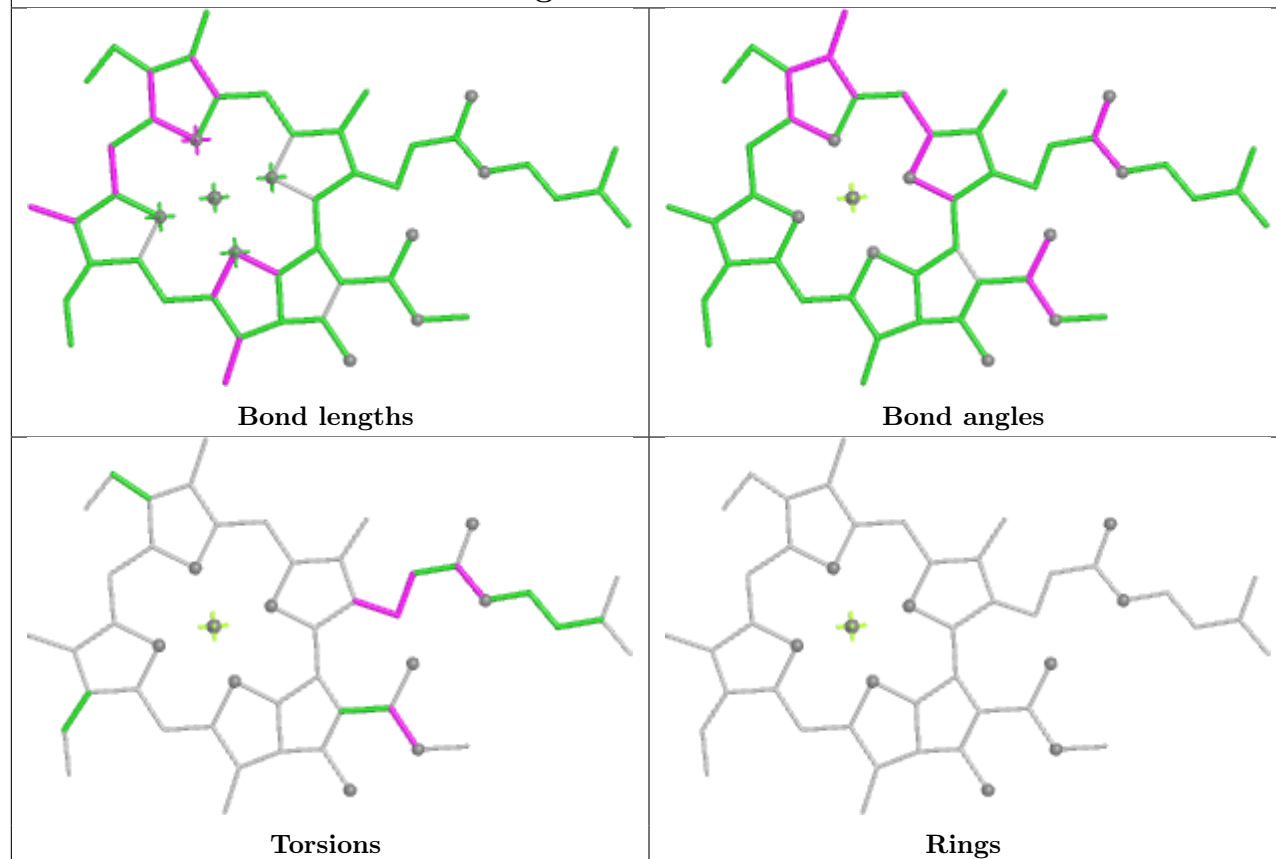
Ligand CLA j 309



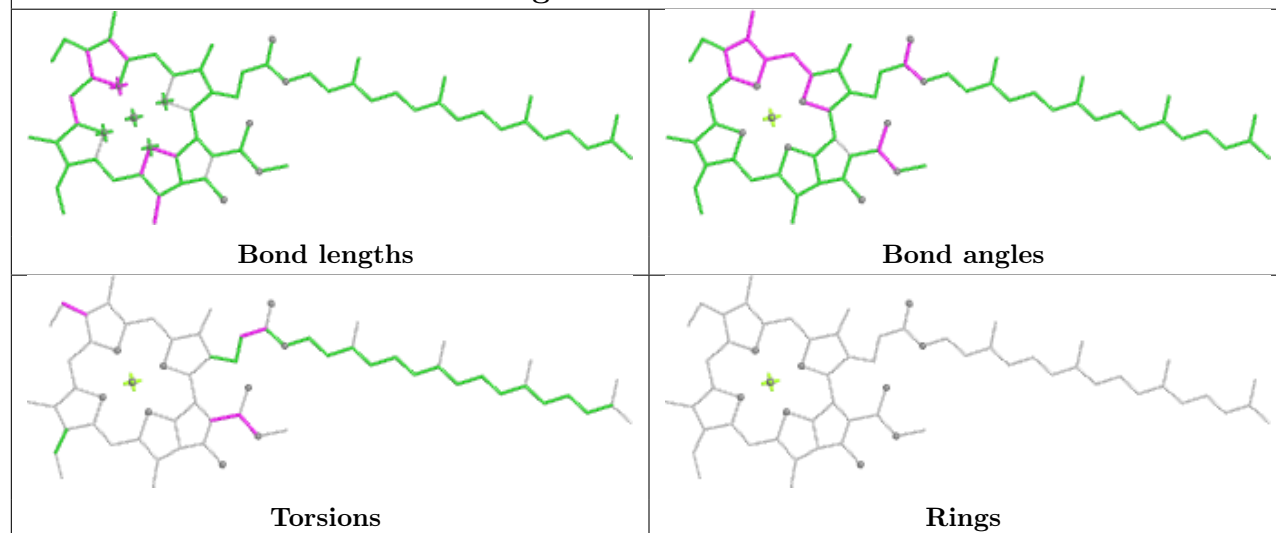
Ligand II0 b 317

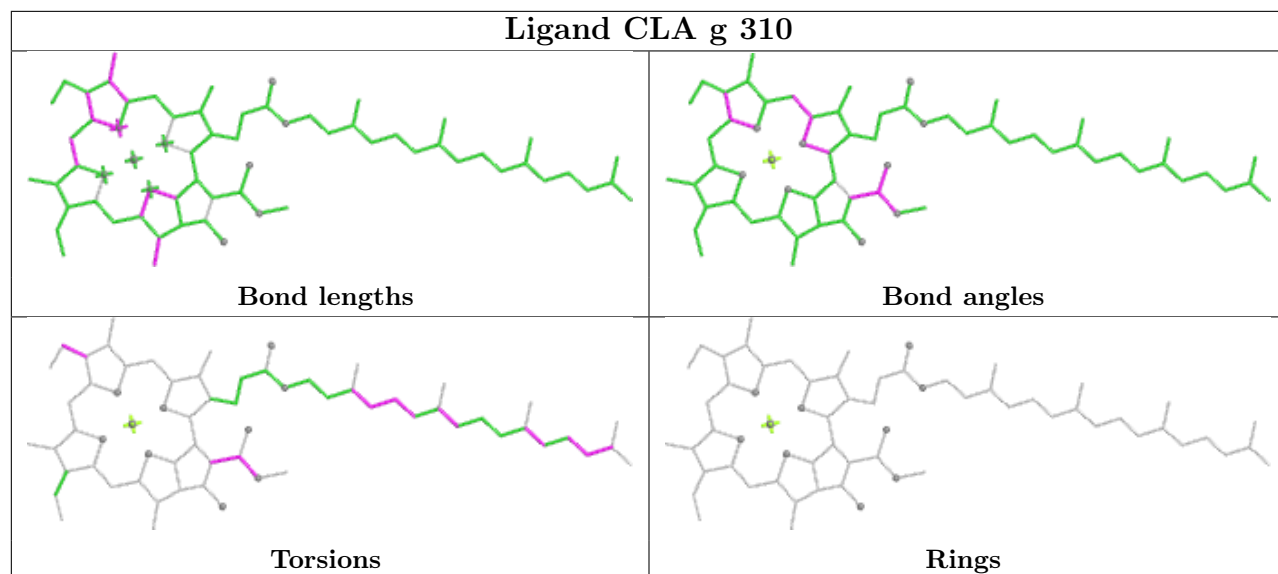
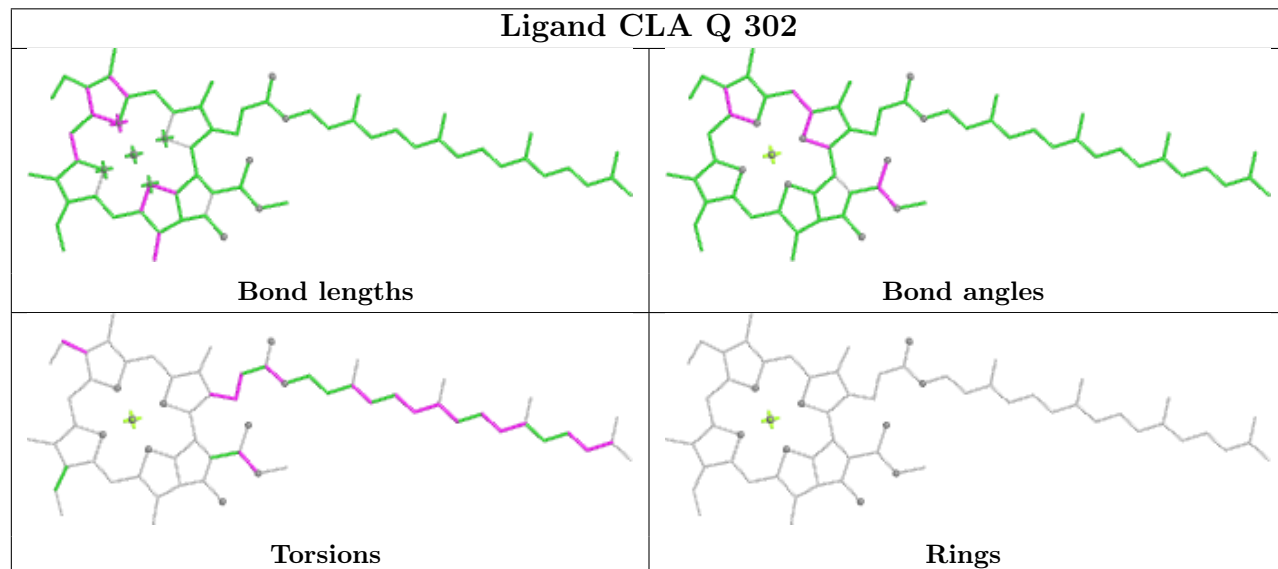


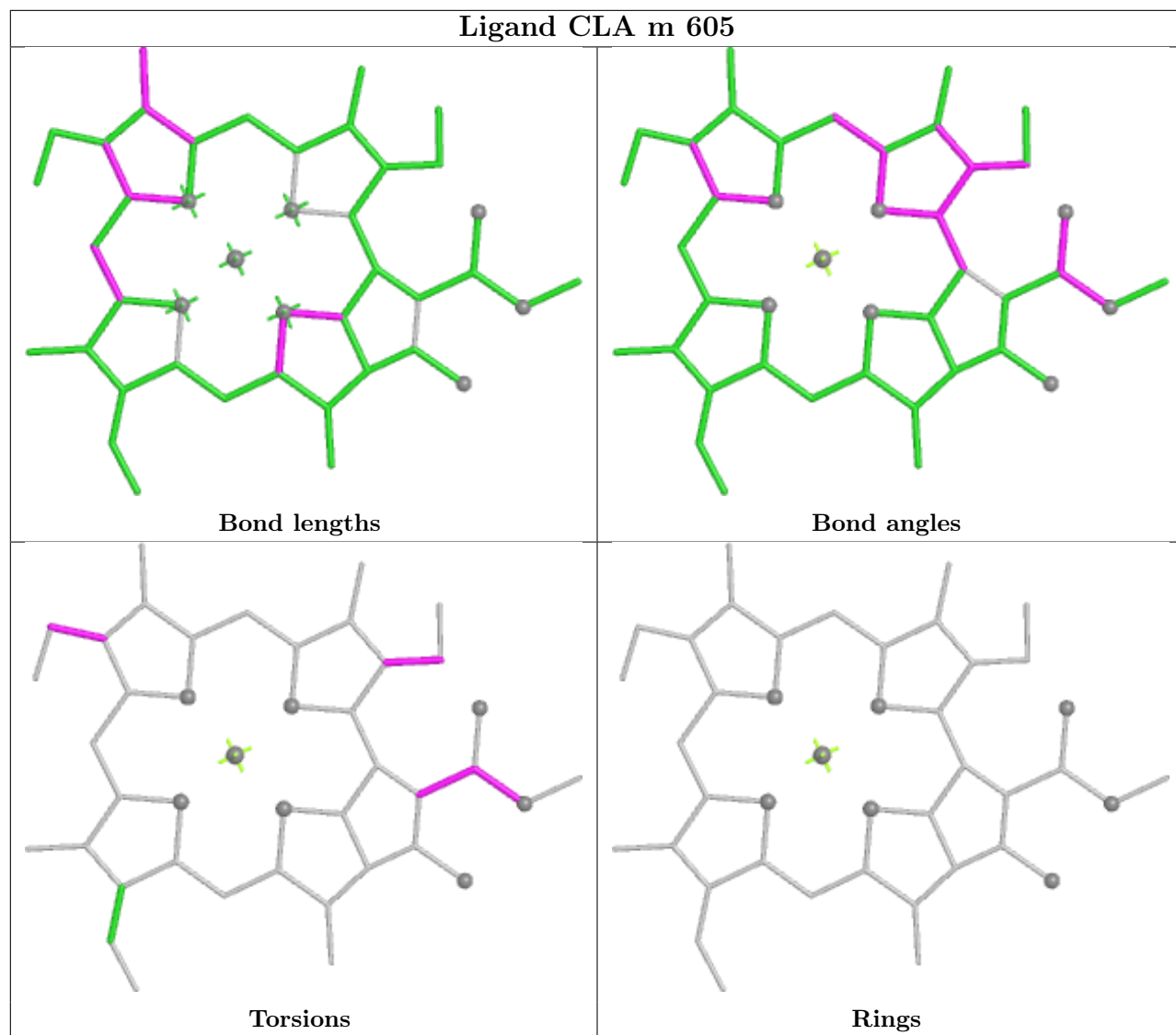
Ligand CLA h 302



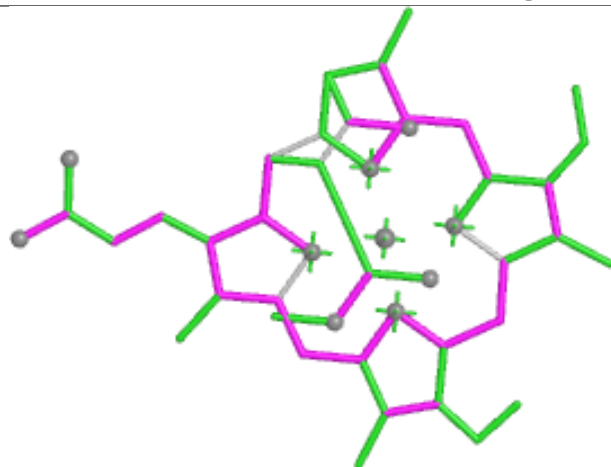
Ligand CLA B 842



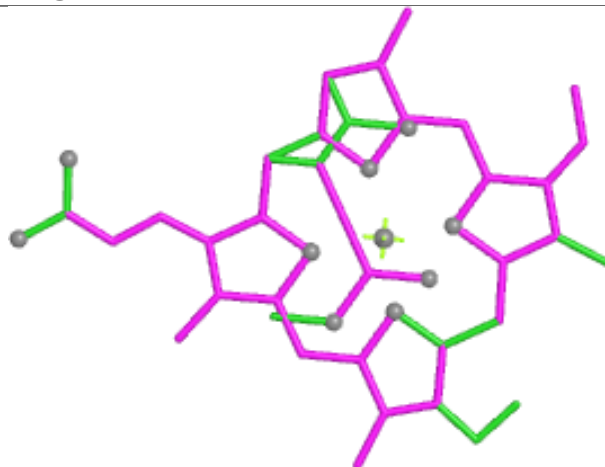
Ligand CLA g 310**Ligand CLA Q 302**



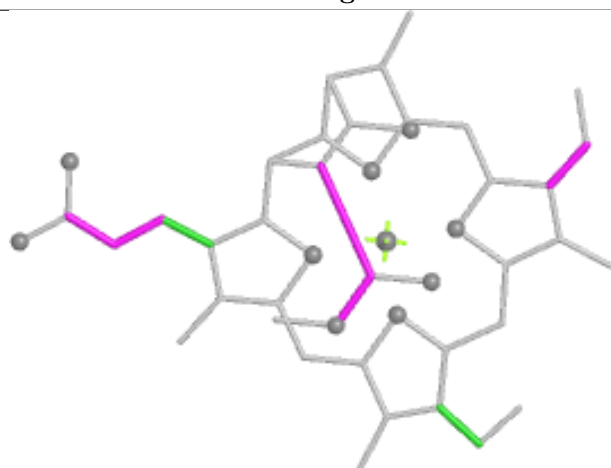
Ligand KC2 g 313



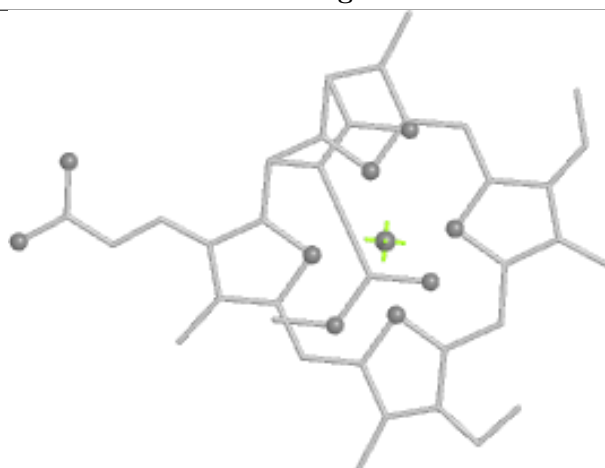
Bond lengths



Bond angles

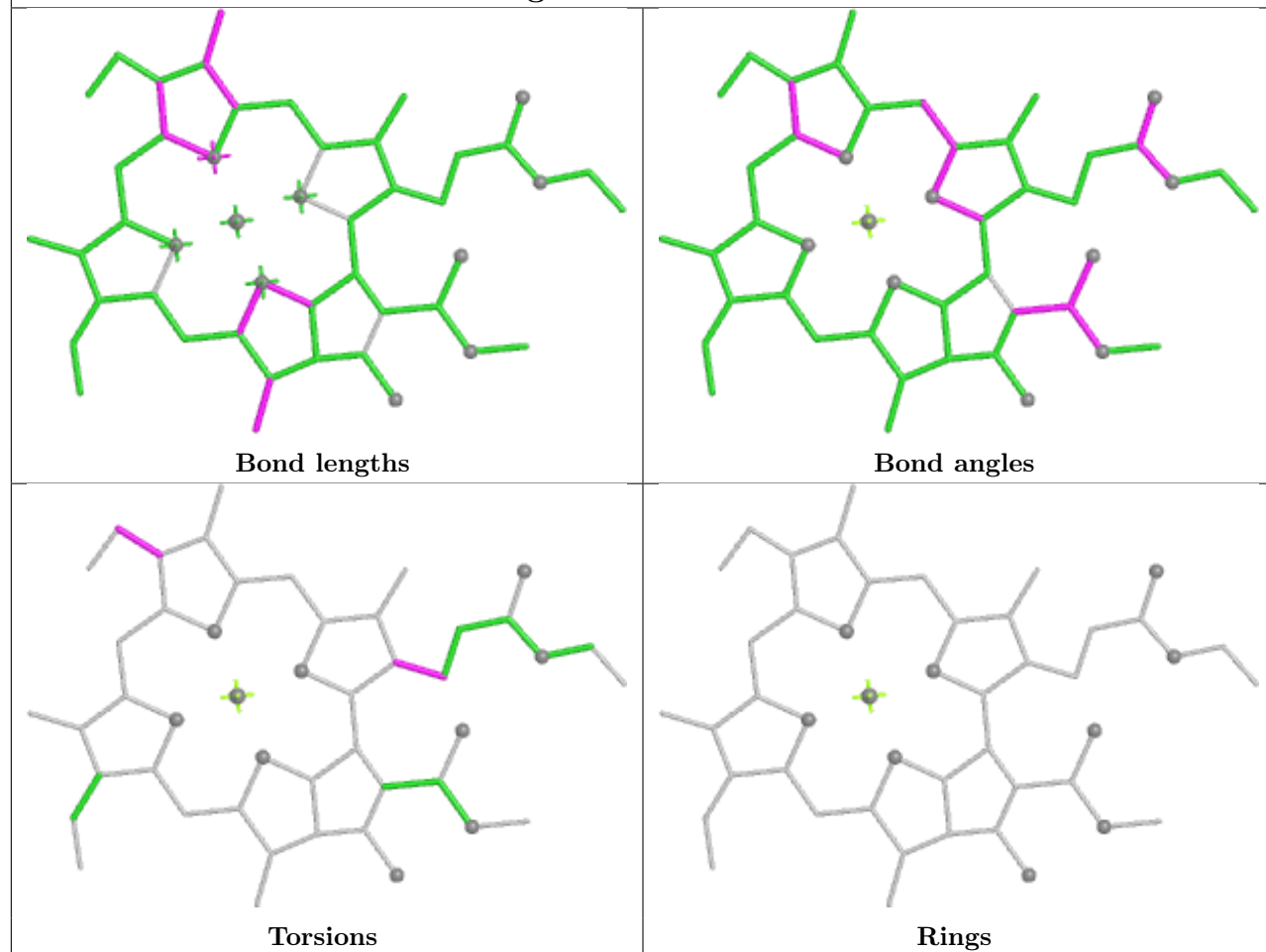


Torsions

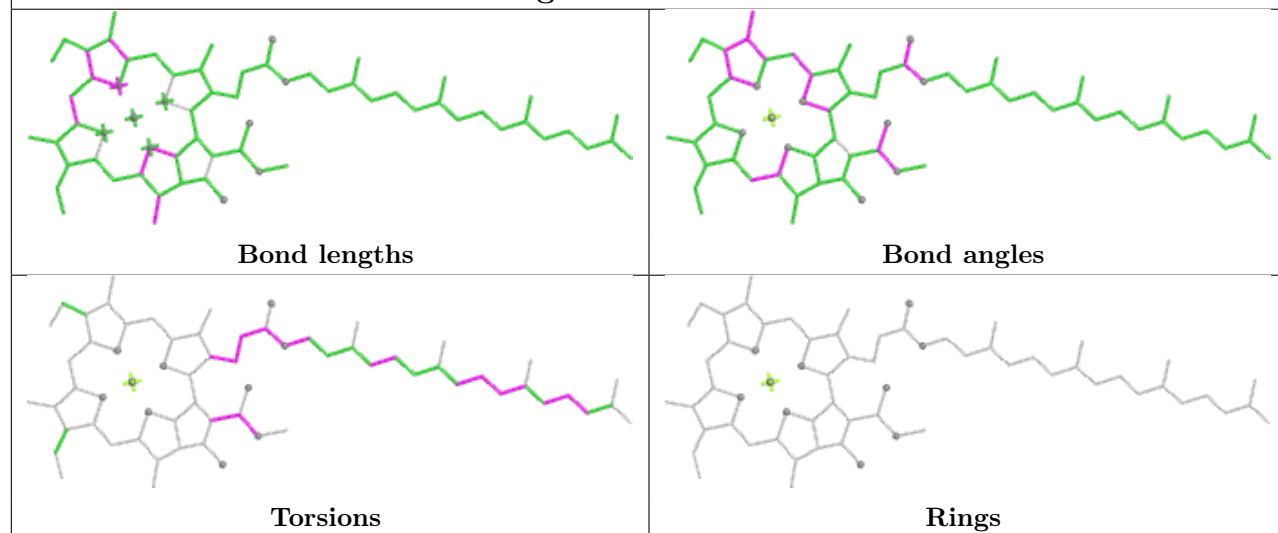


Rings

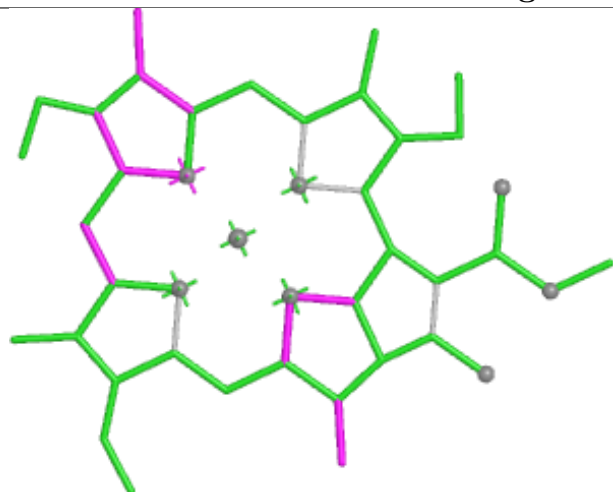
Ligand CLA B 835



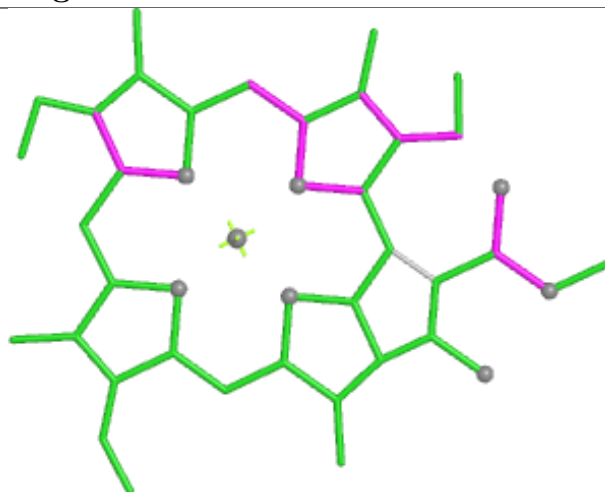
Ligand CLA e 302



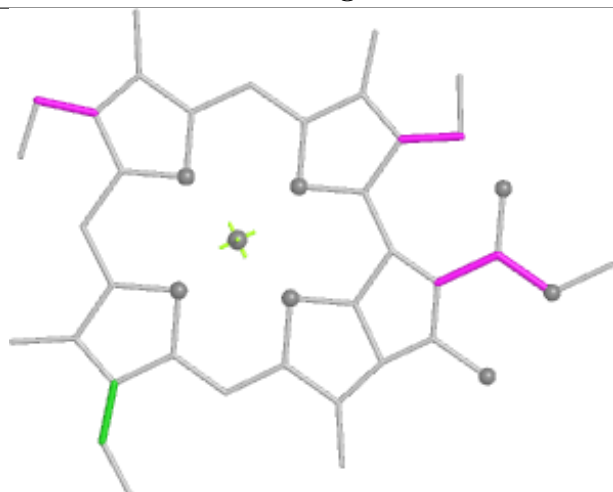
Ligand CLA g 303



Bond lengths



Bond angles

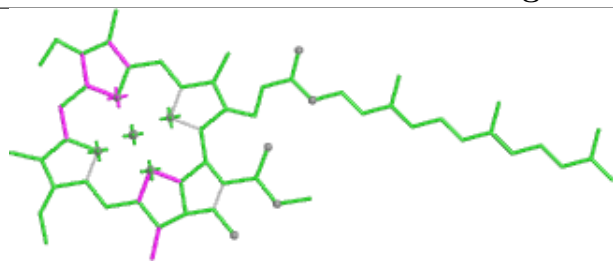


Torsions

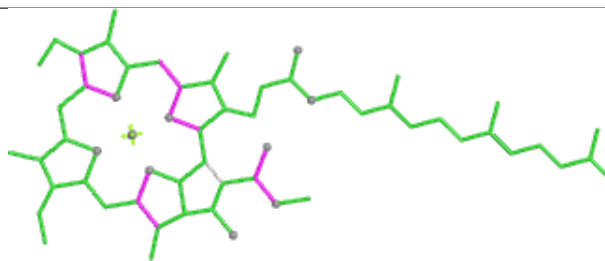


Rings

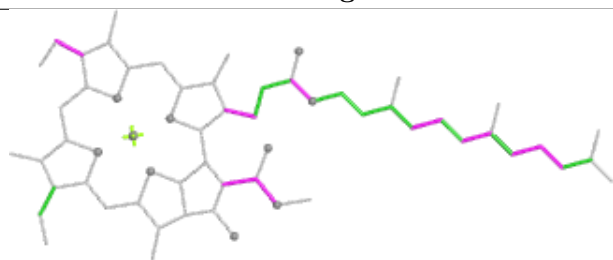
Ligand CLA i 311



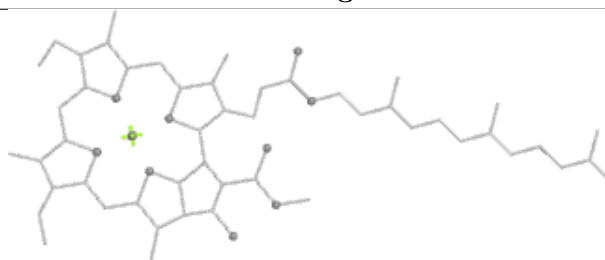
Bond lengths



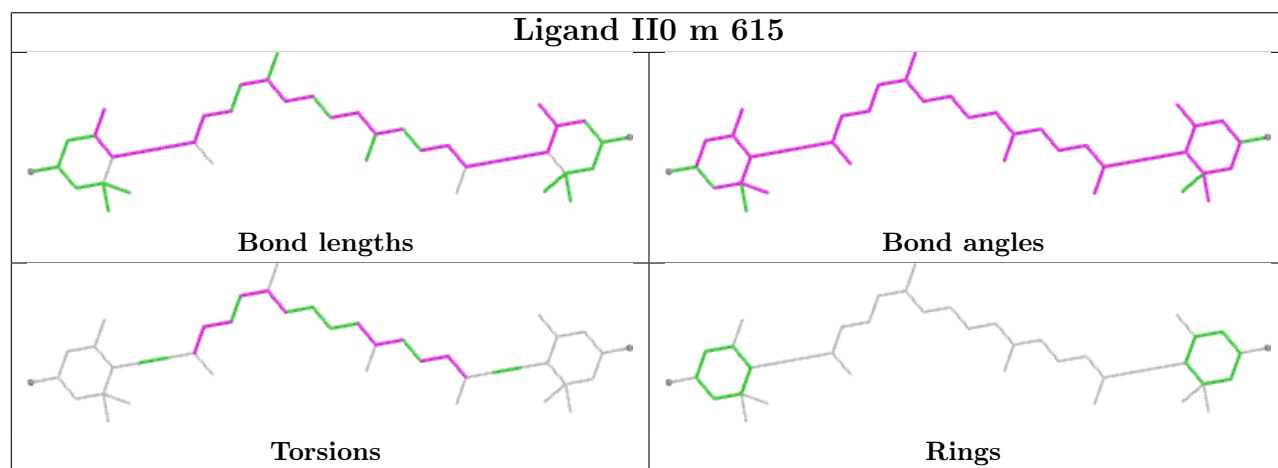
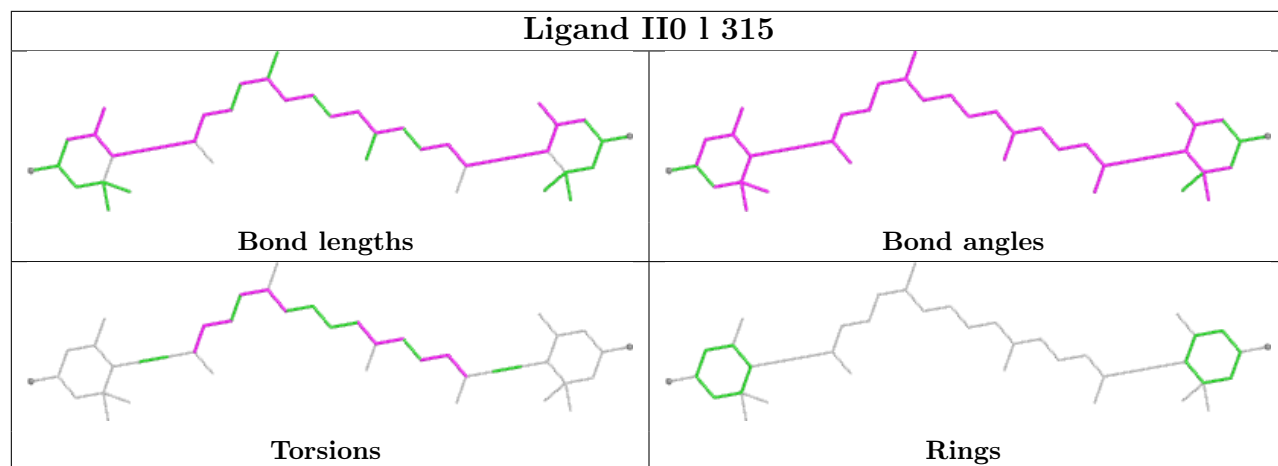
Bond angles

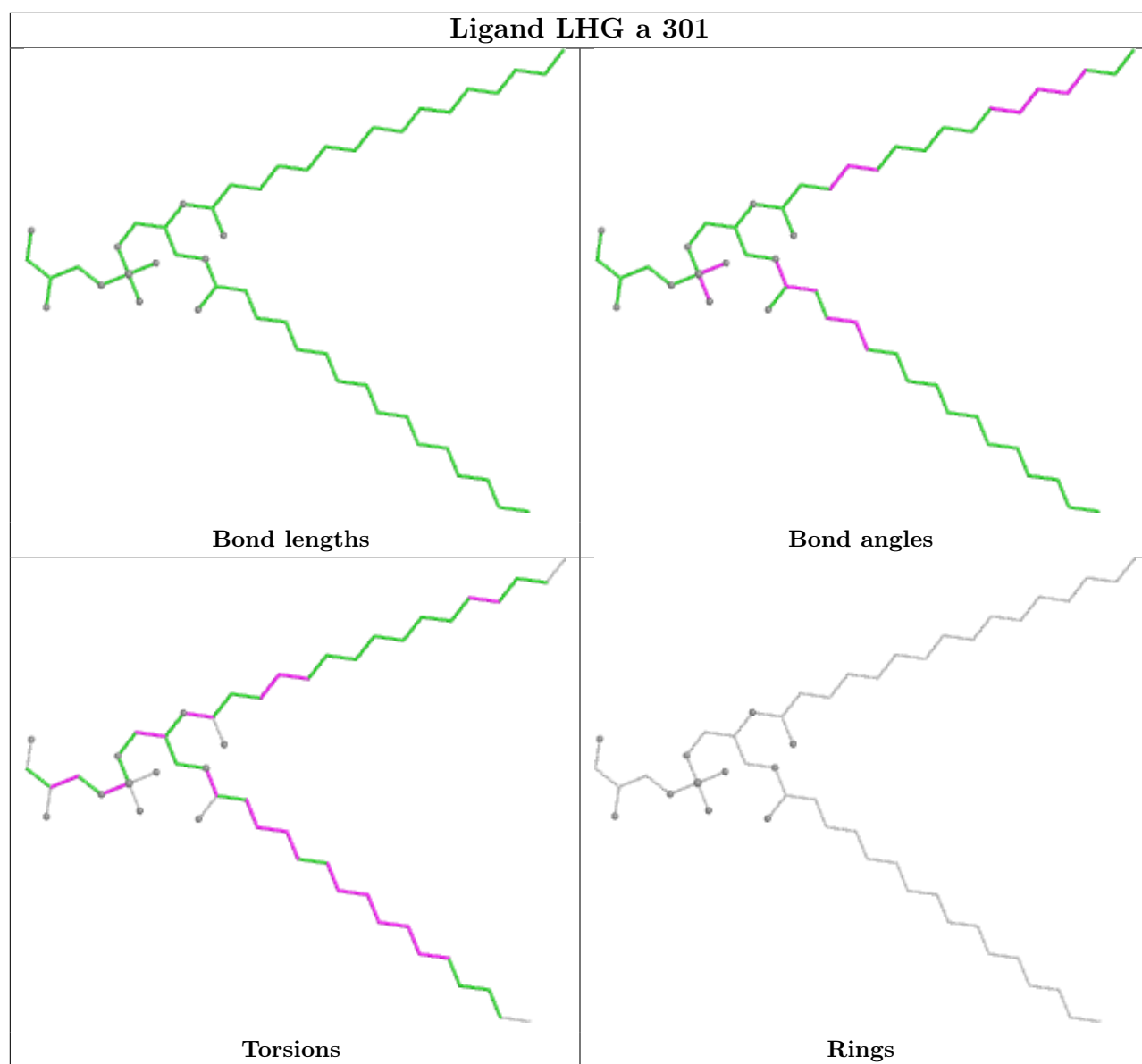


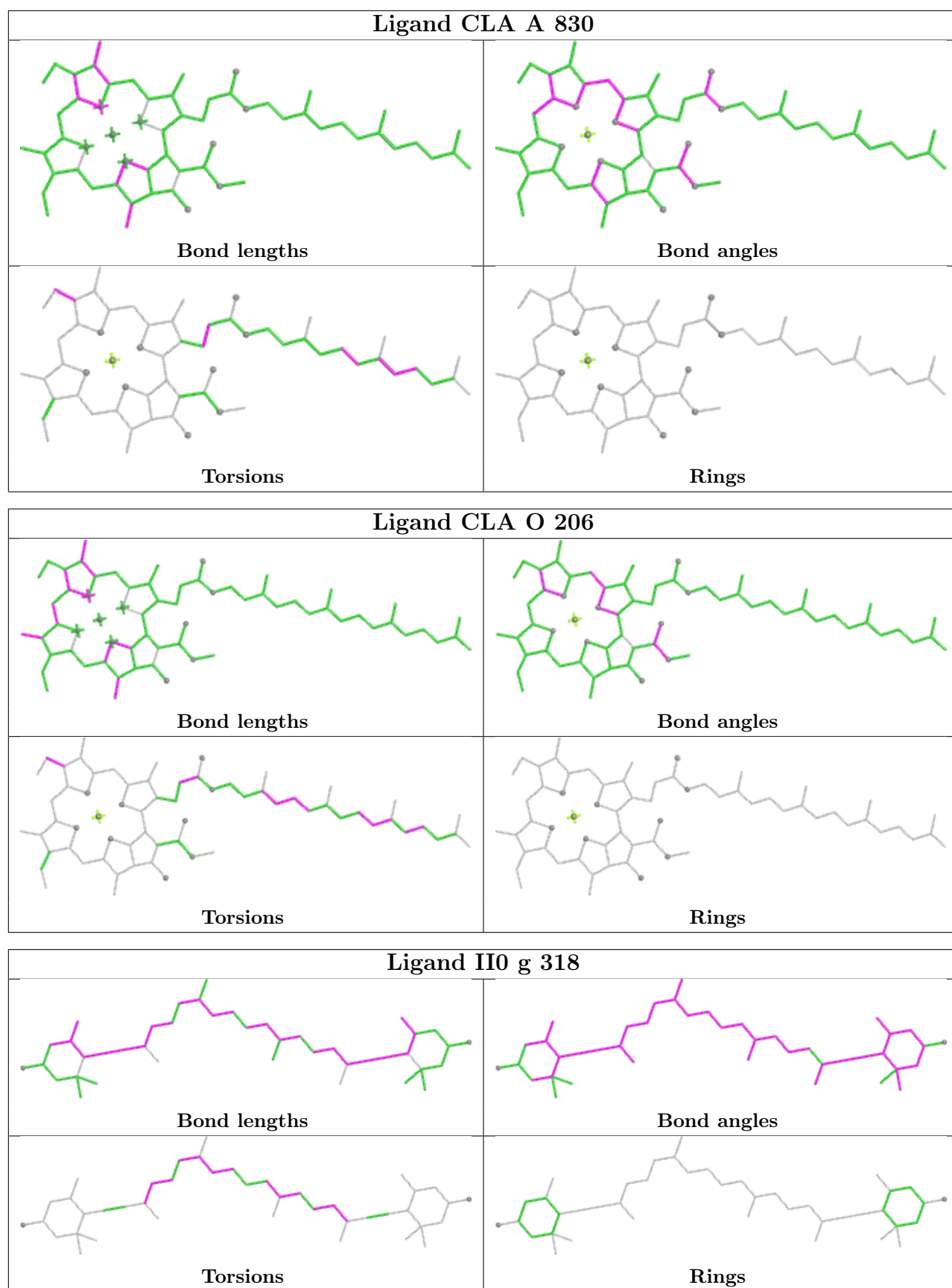
Torsions

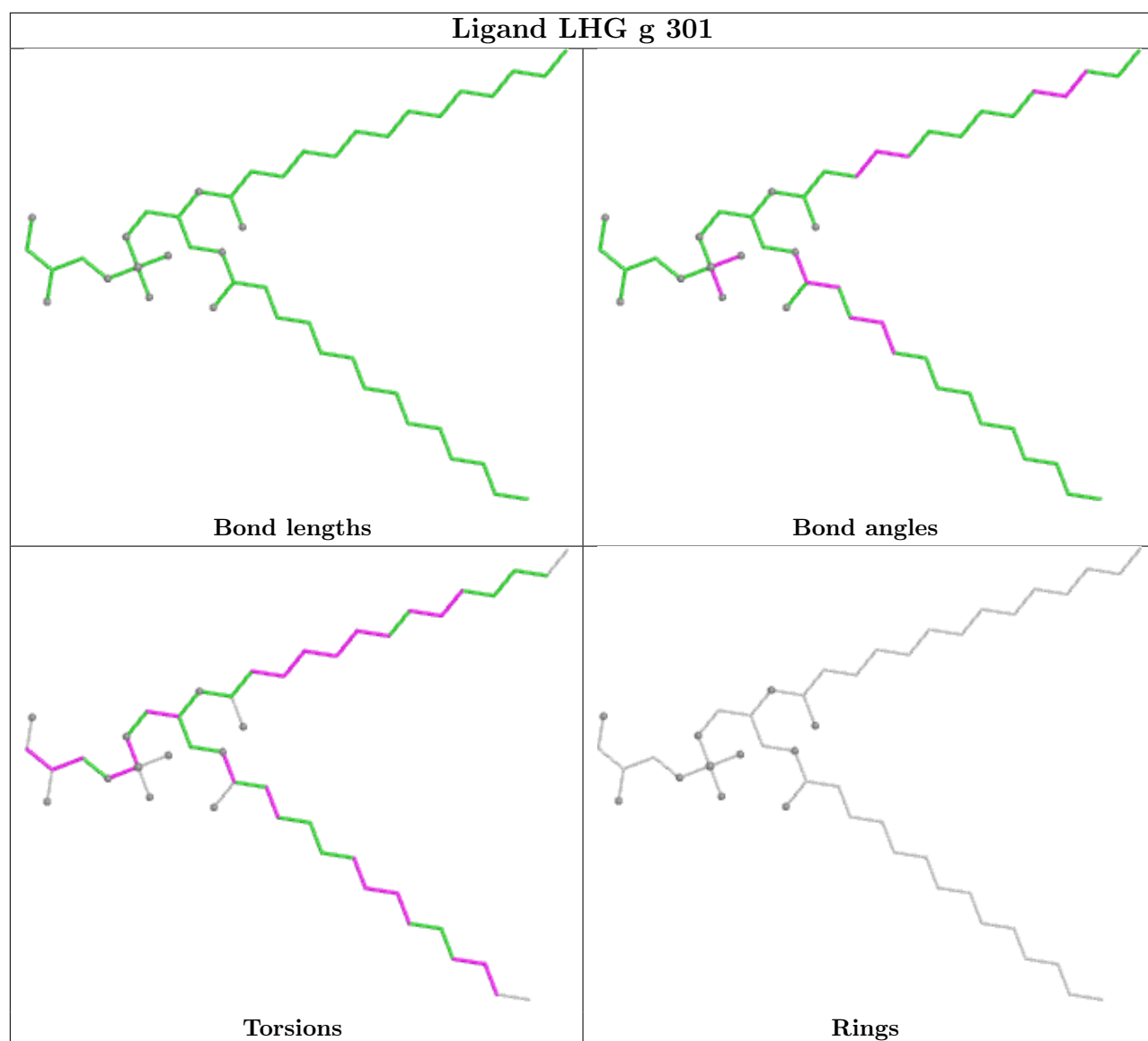


Rings

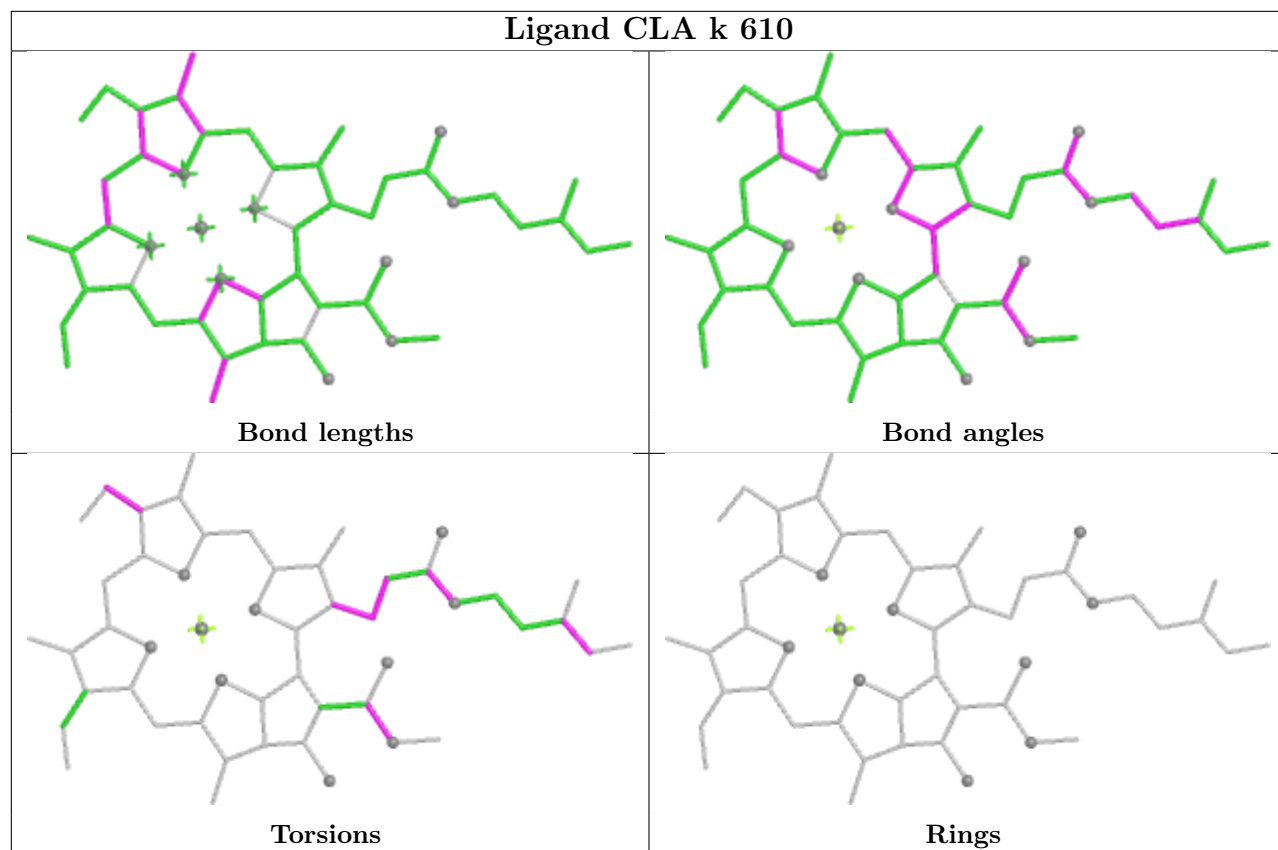




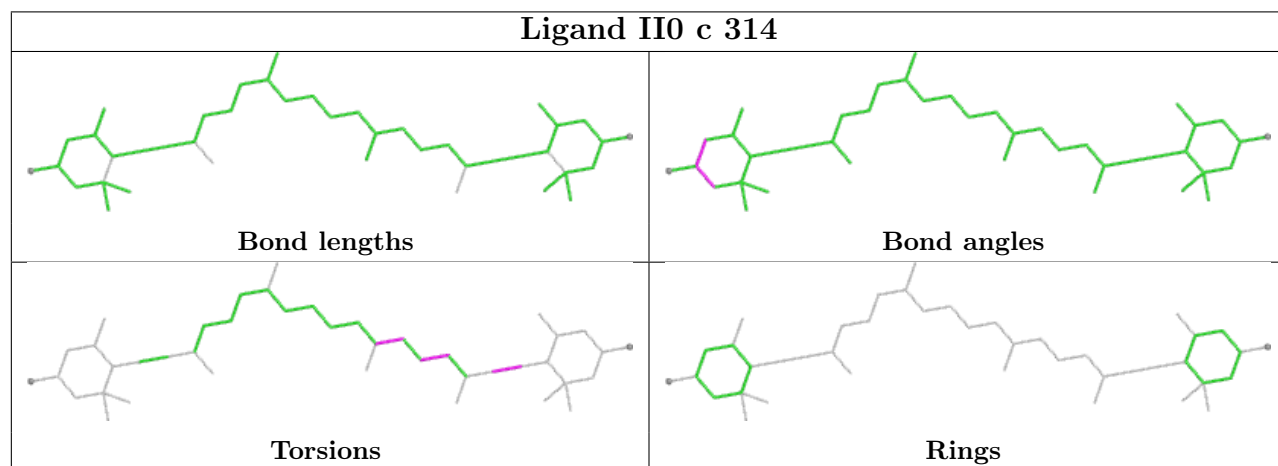




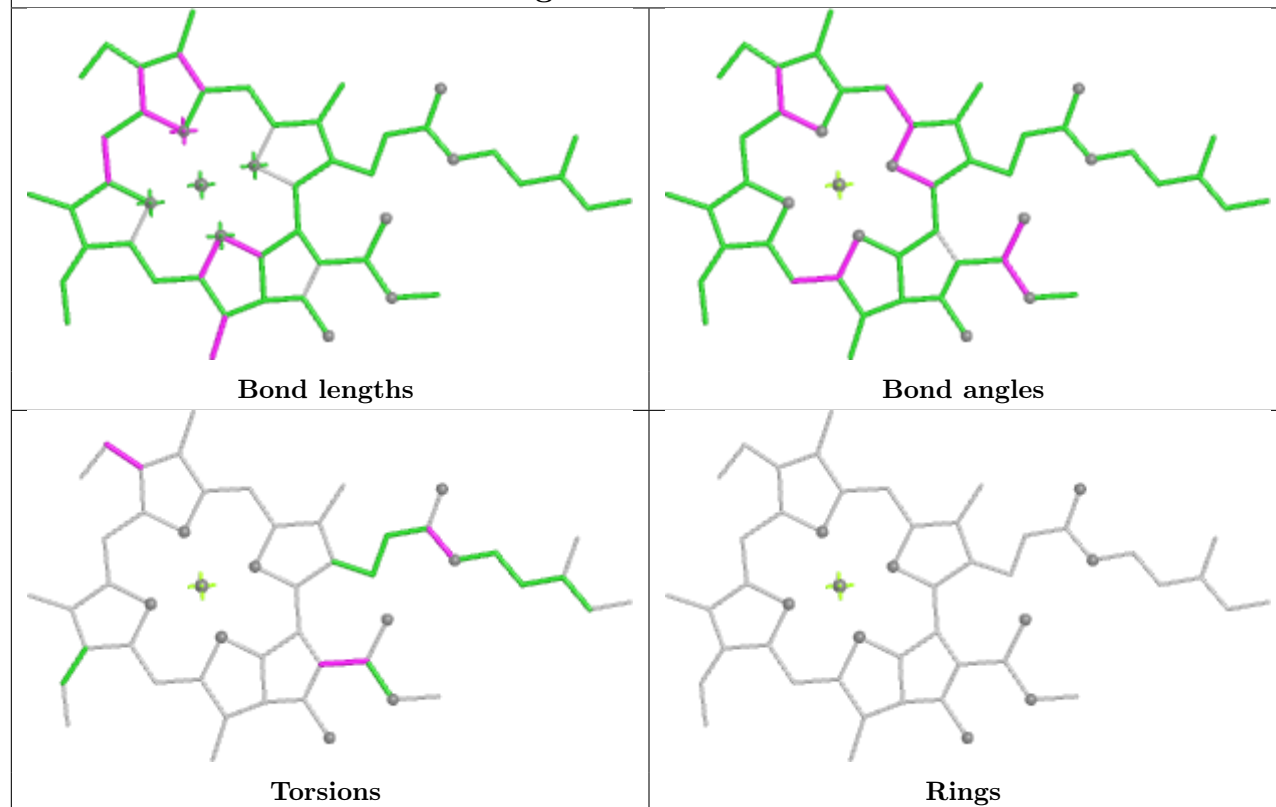
Ligand CLA k 610



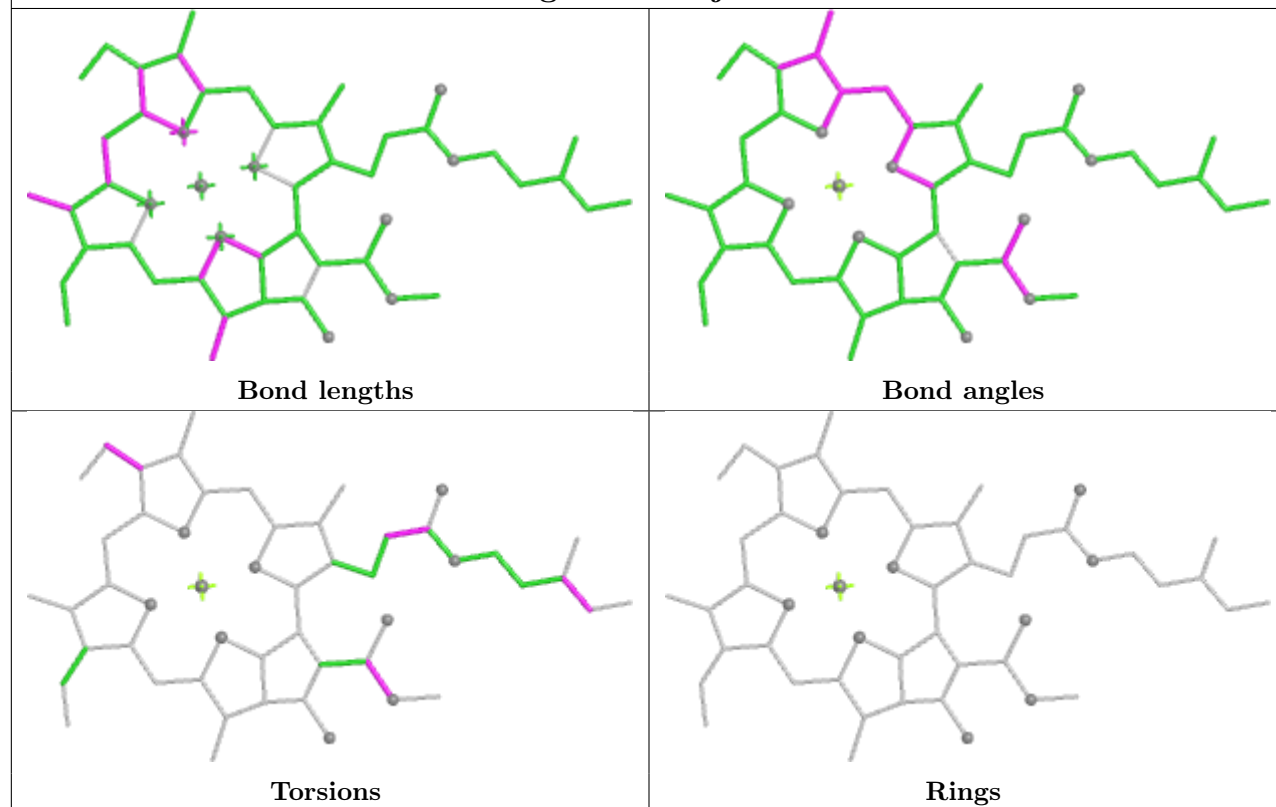
Ligand II0 c 314

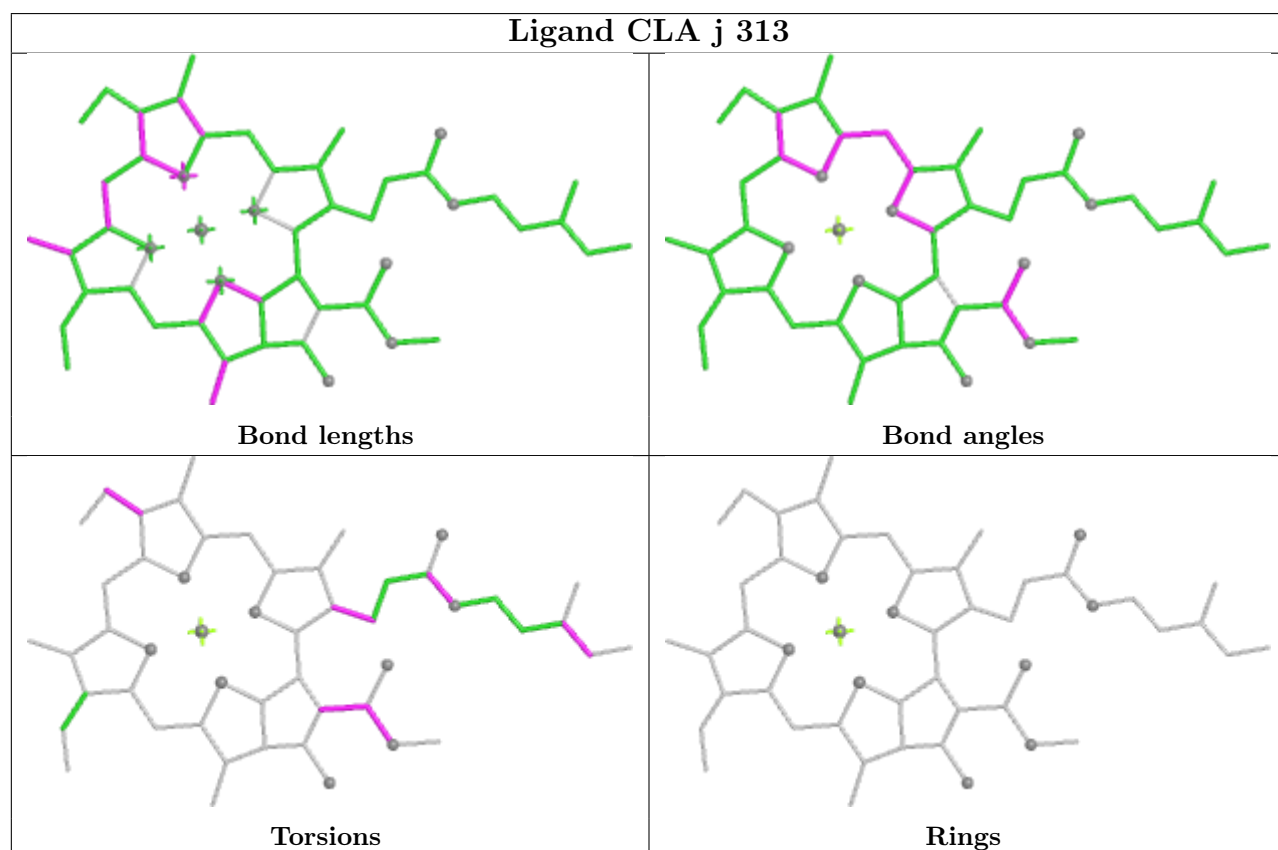
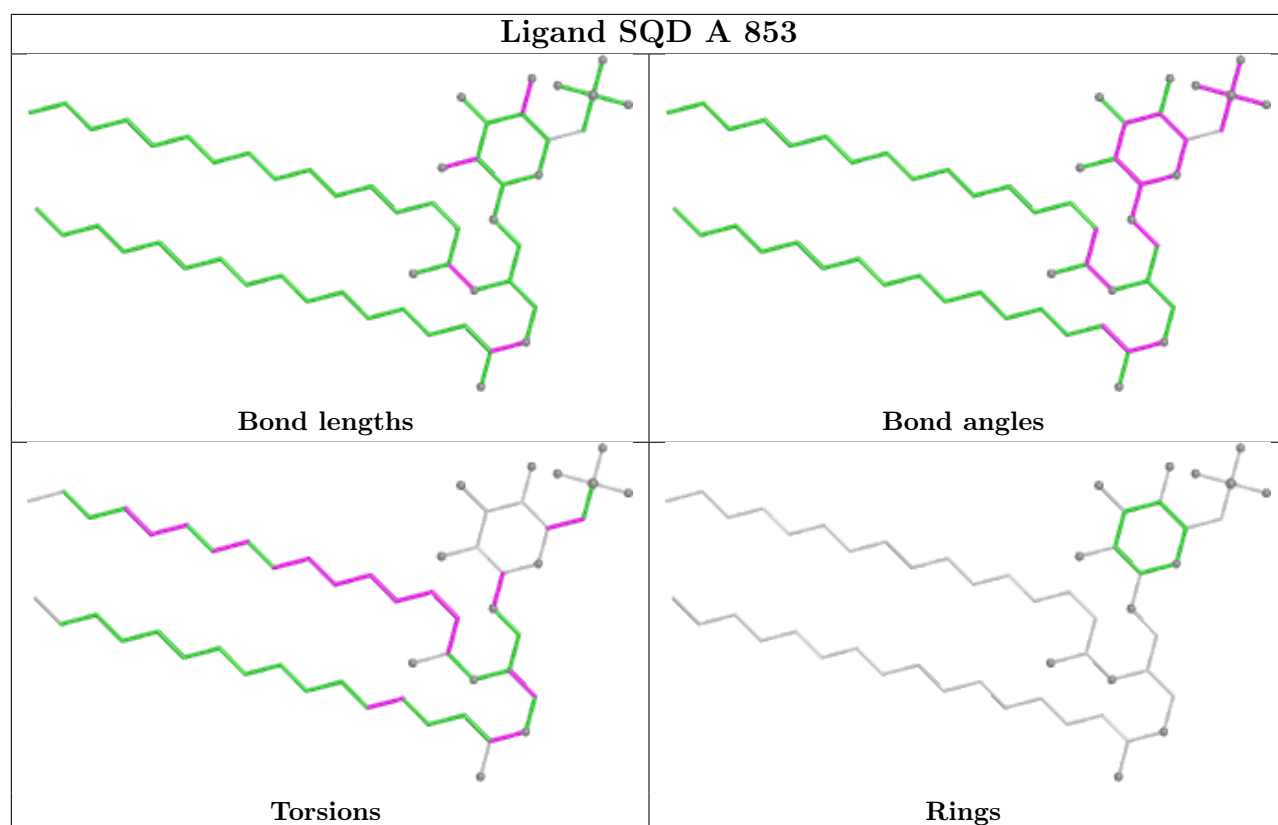


Ligand CLA n 606

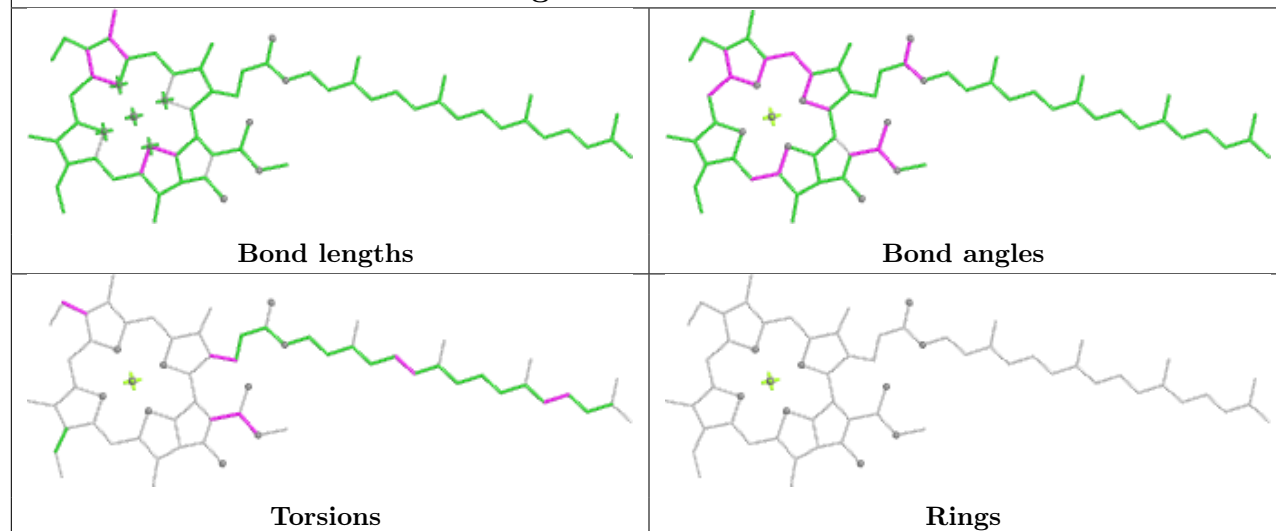


Ligand CLA j 304

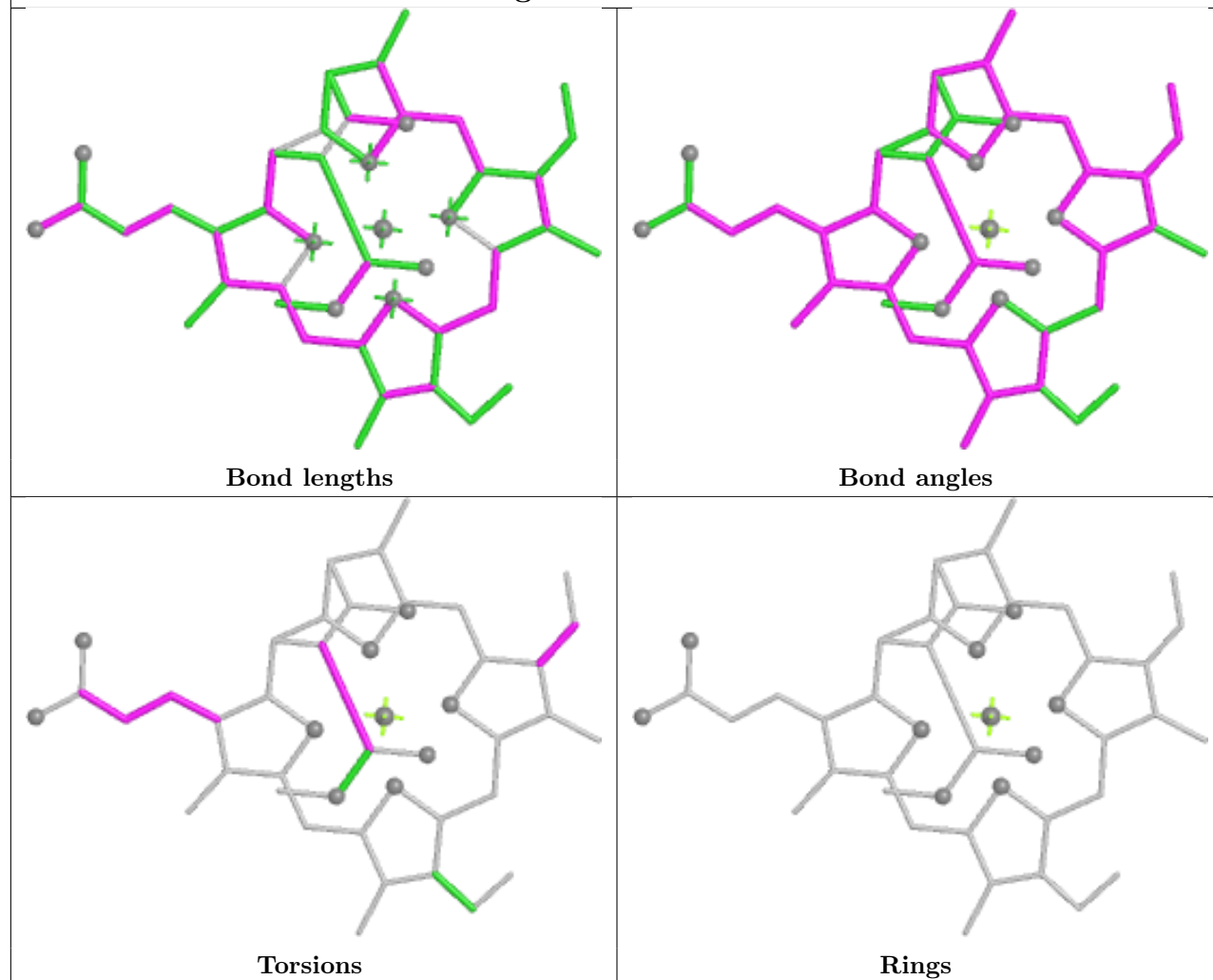


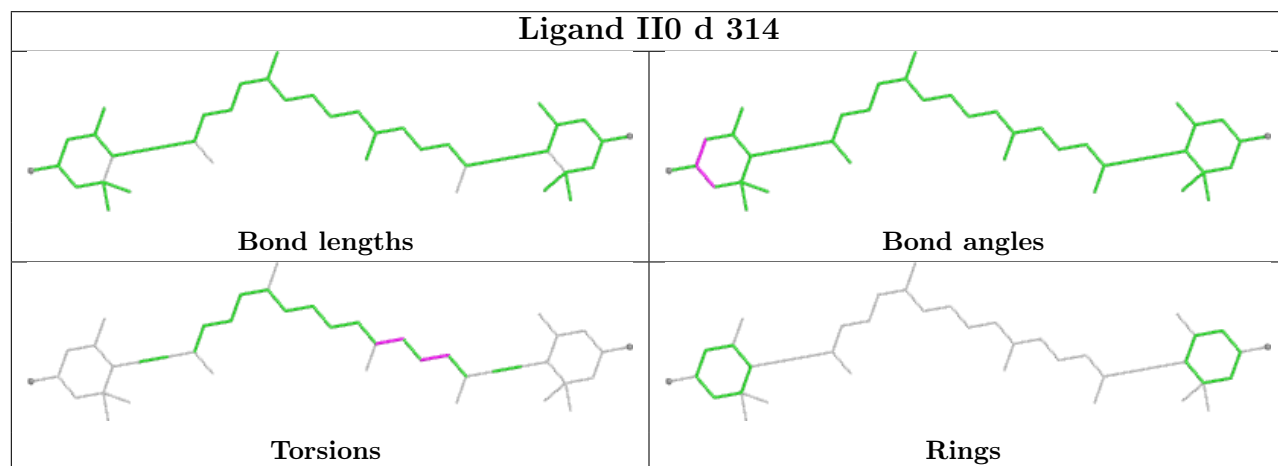
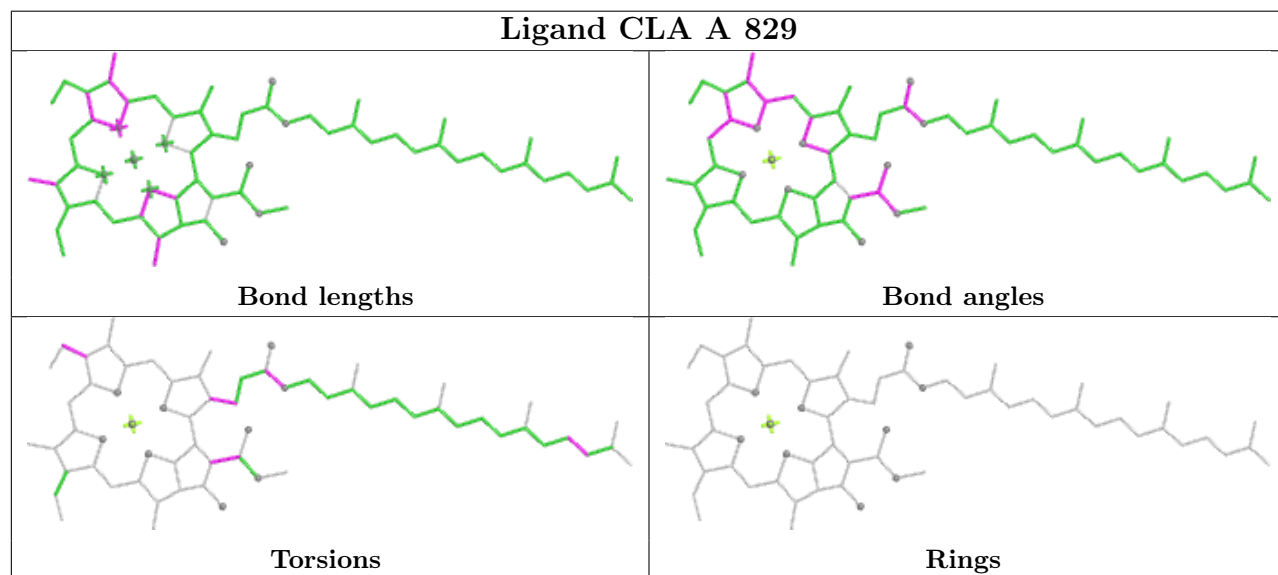
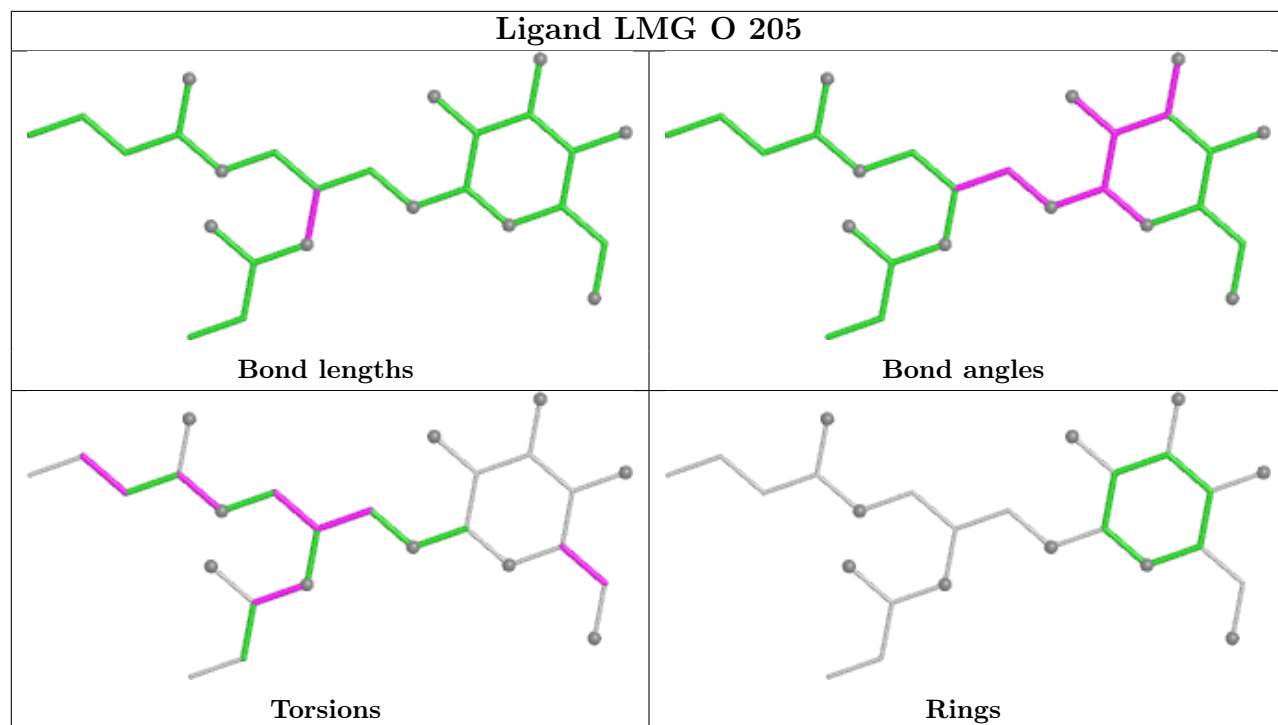


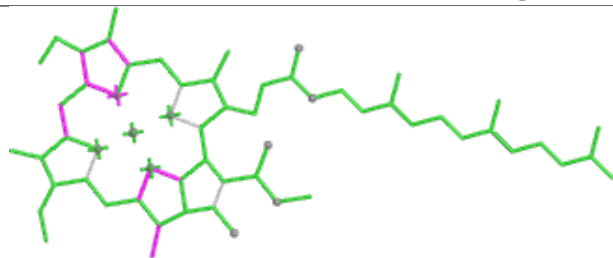
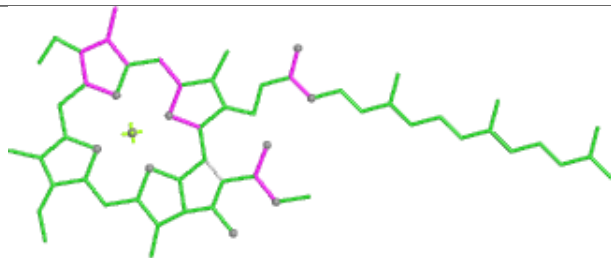
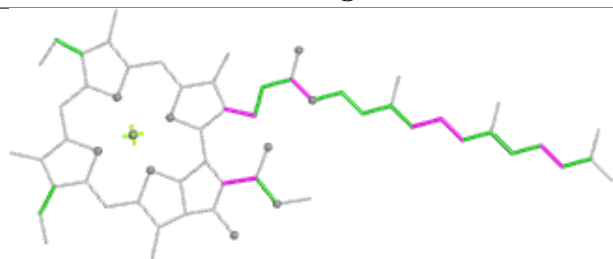
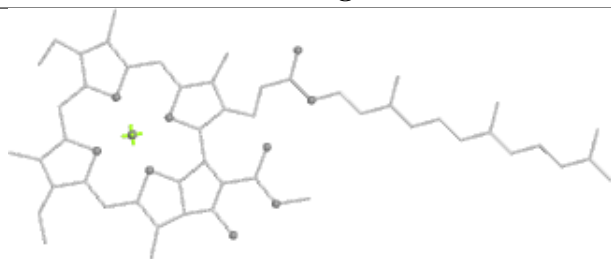
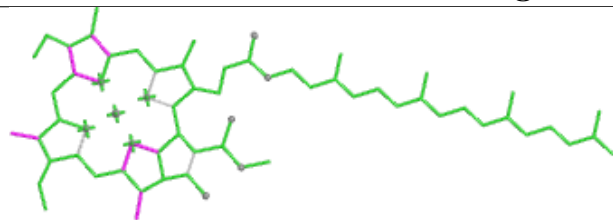
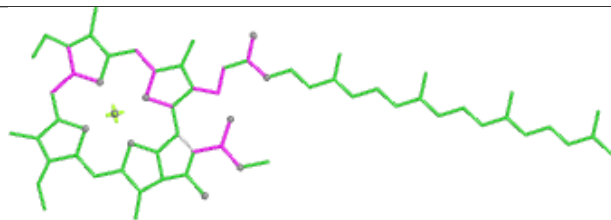
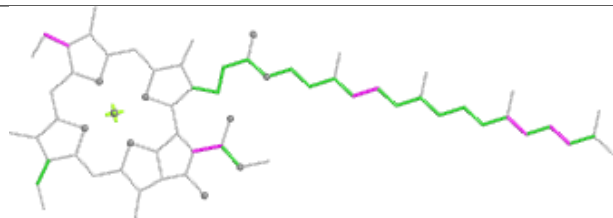
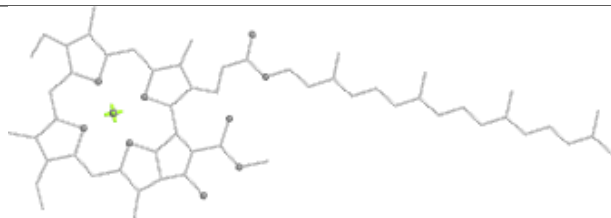
Ligand CLA A 832

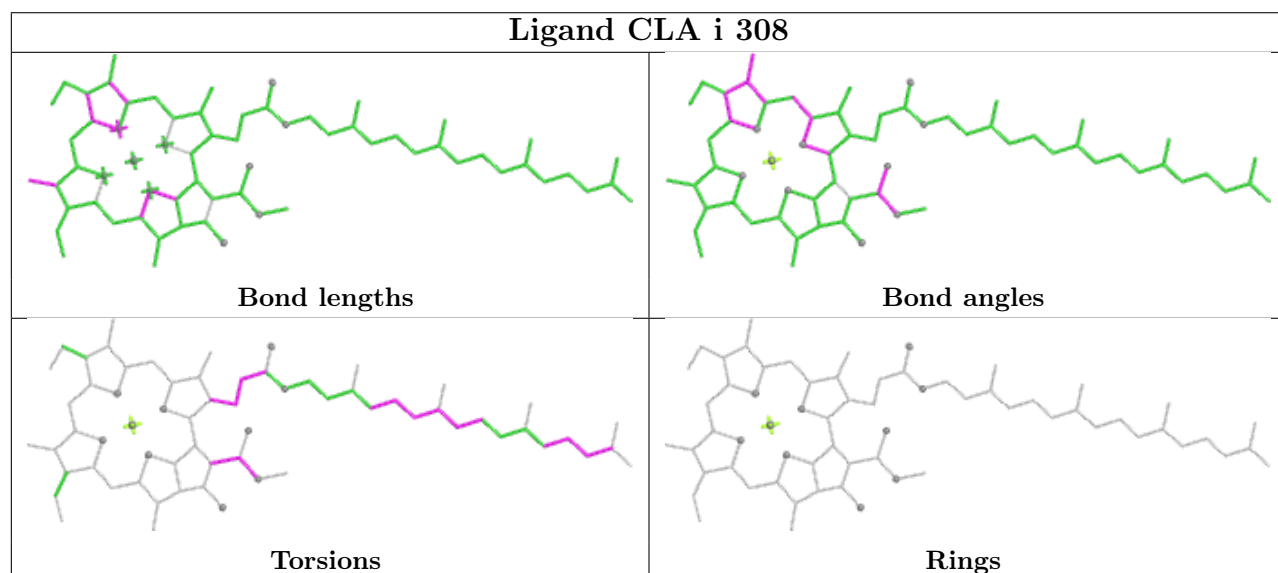
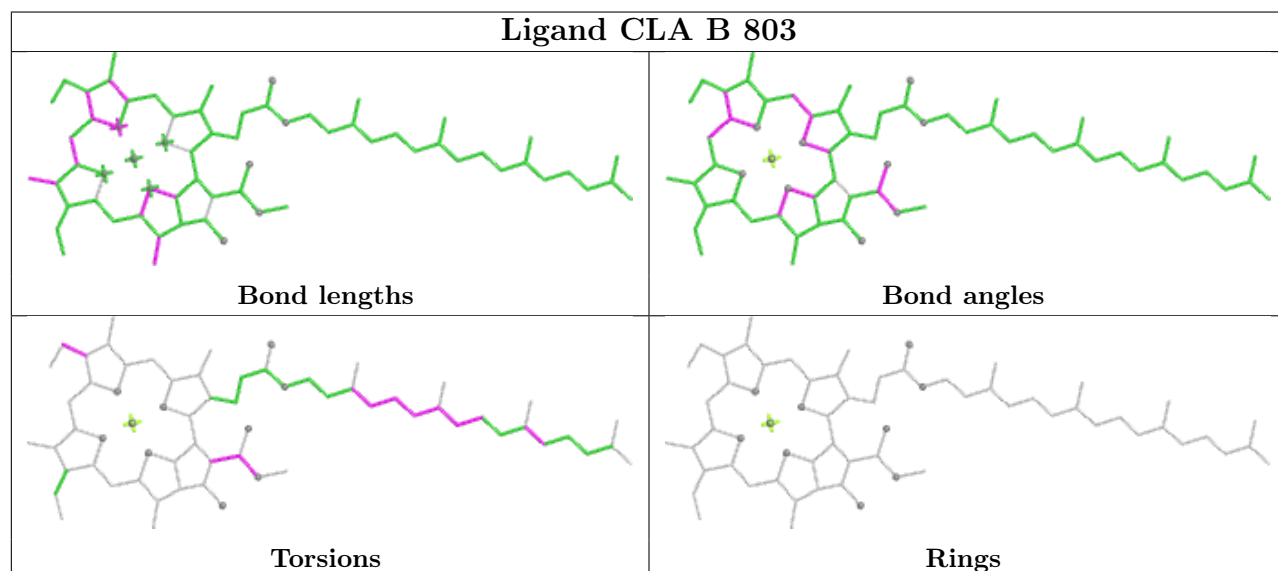
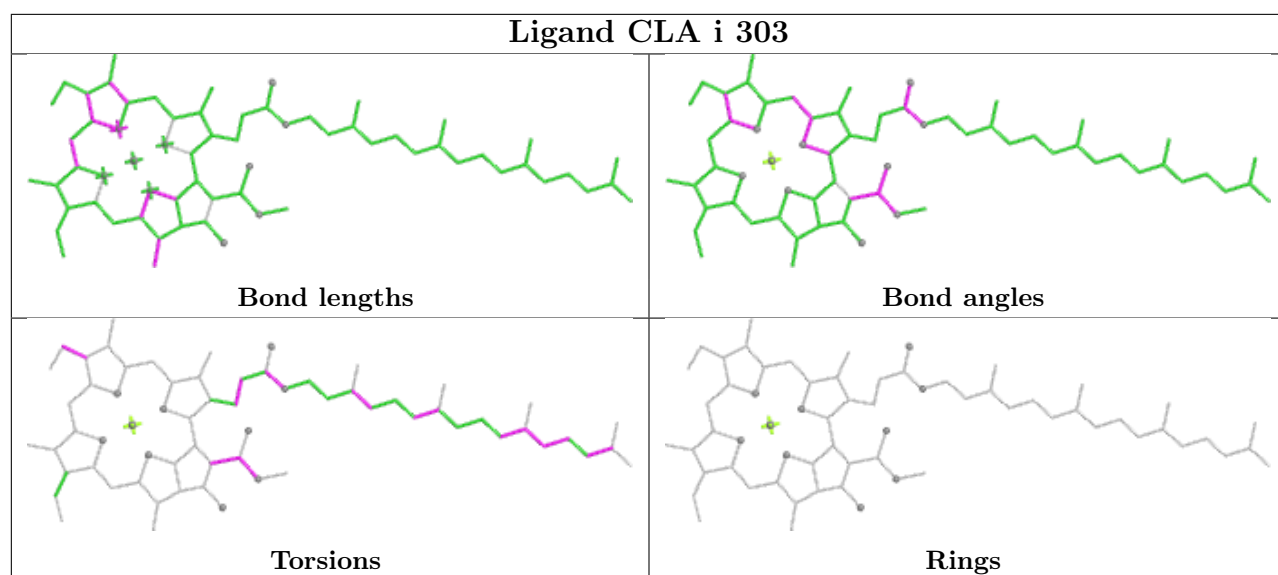


Ligand KC2 f 611

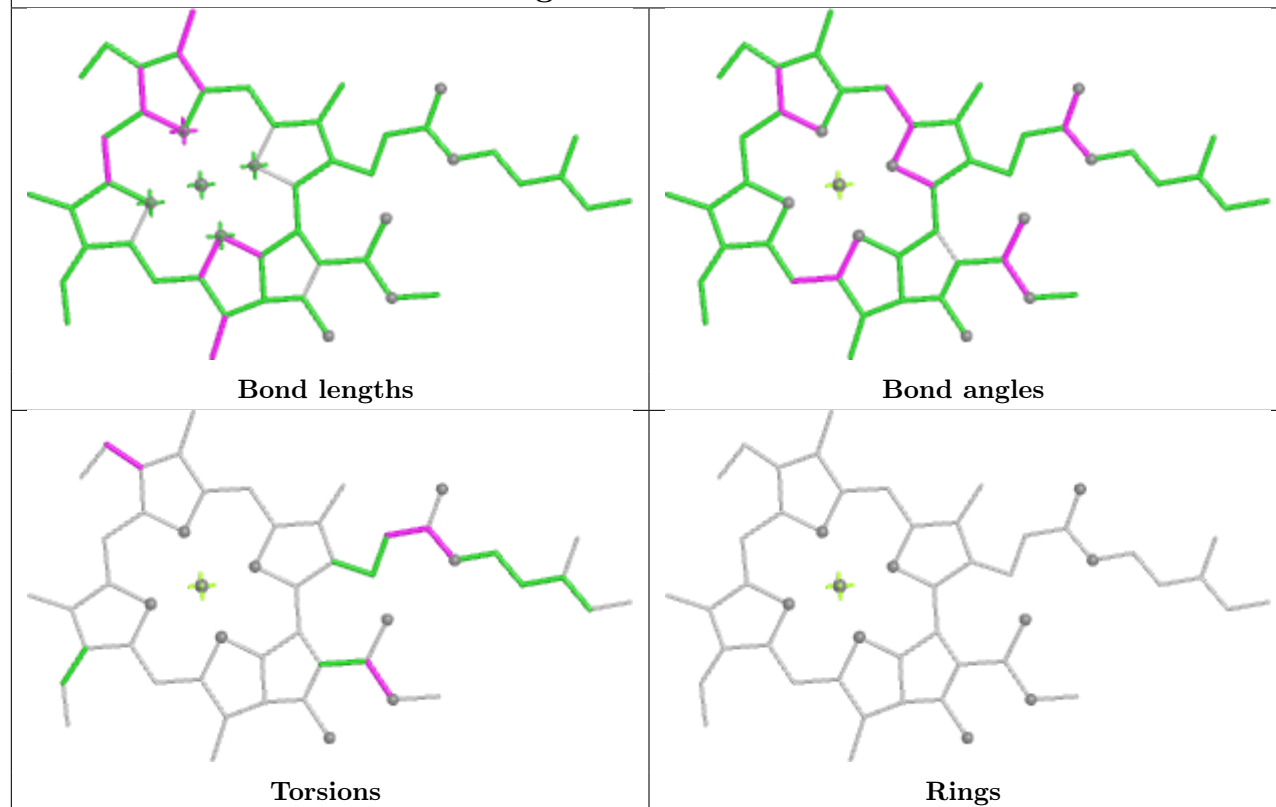




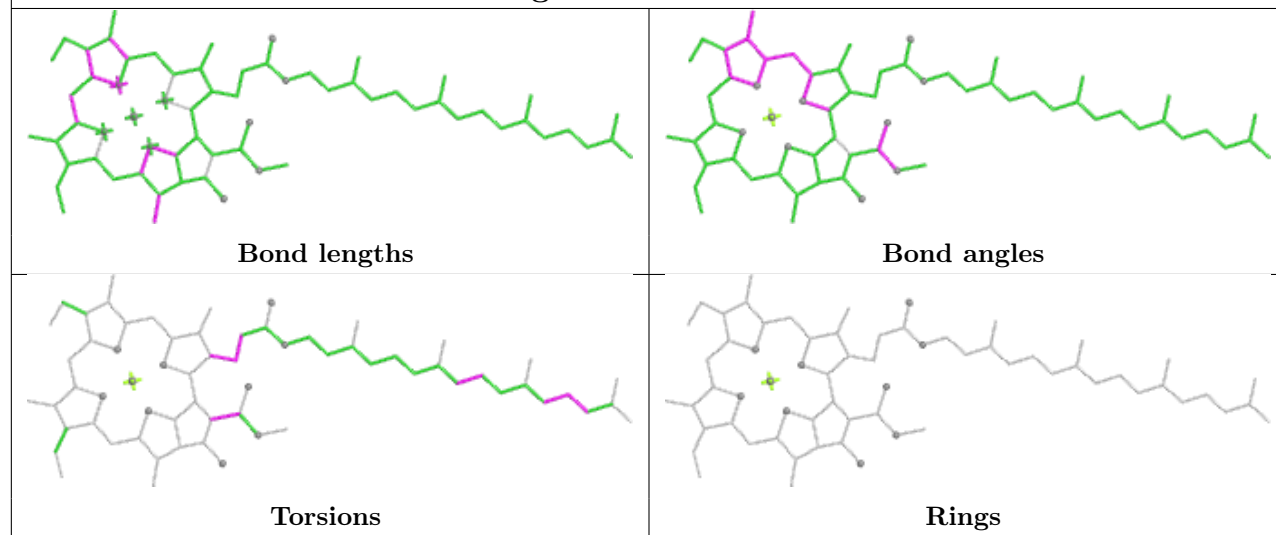
Ligand CLA A 834**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 808****Bond lengths****Bond angles****Torsions****Rings**

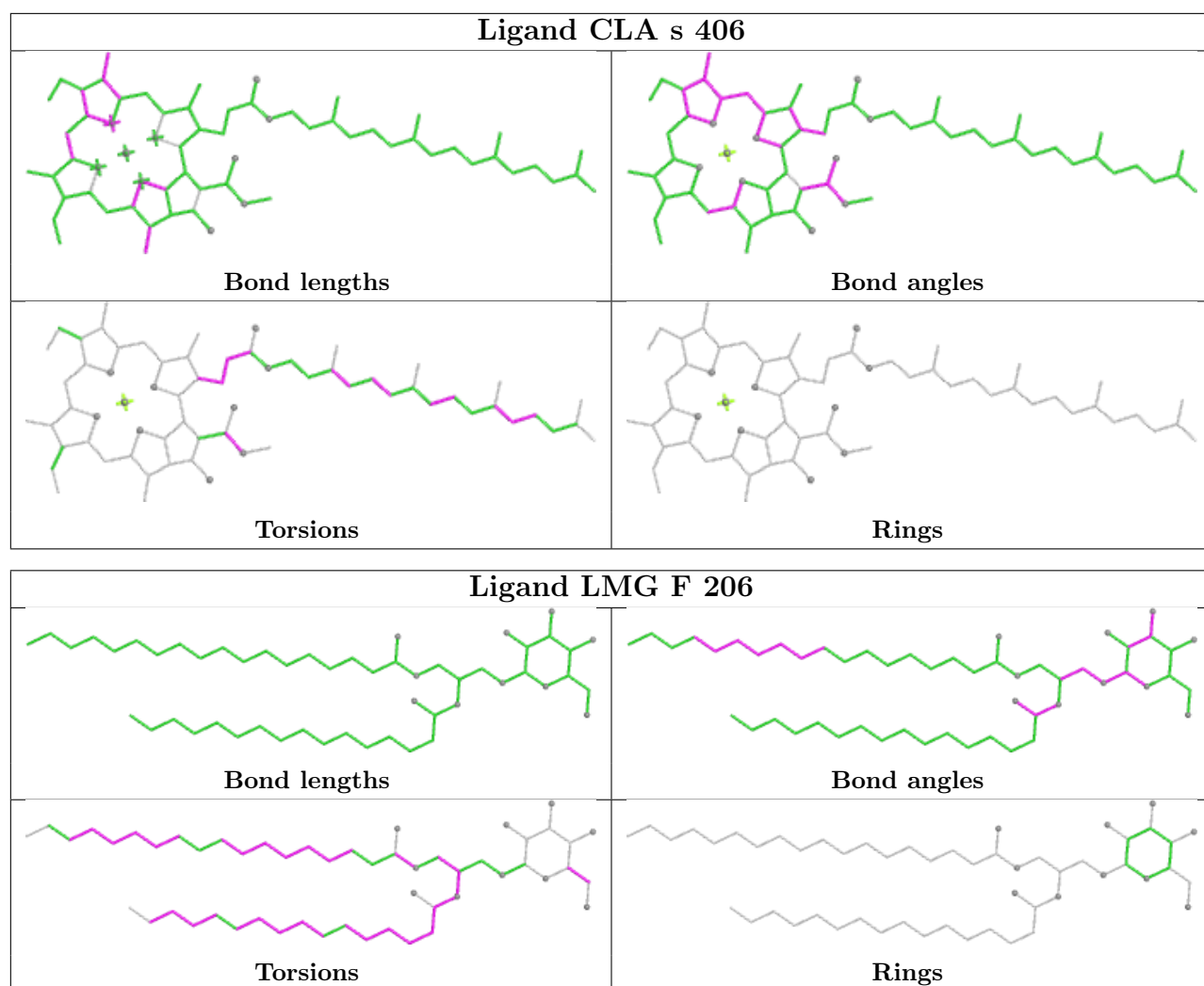


Ligand CLA k 606

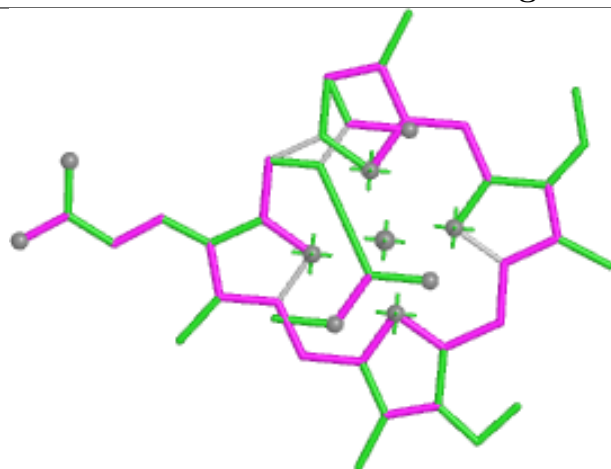


Ligand CLA A 807

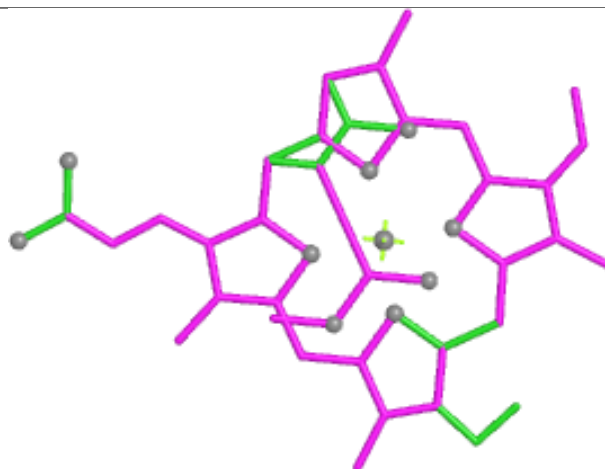




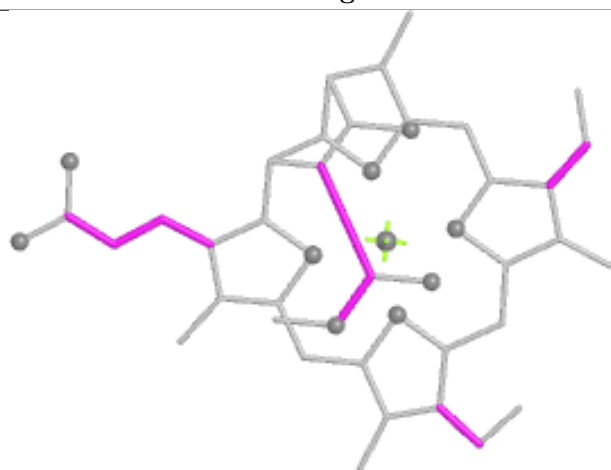
Ligand KC2 d 311



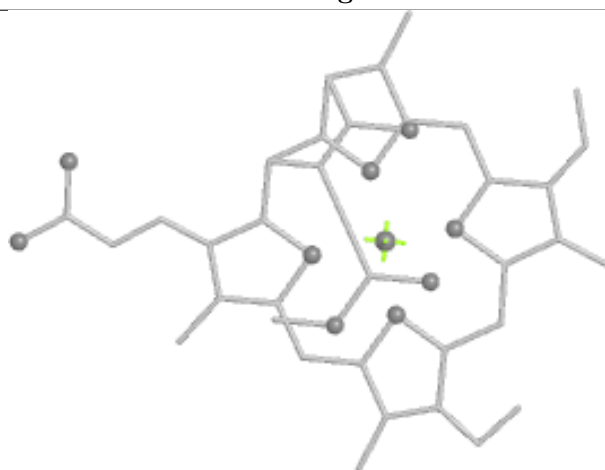
Bond lengths



Bond angles



Torsions

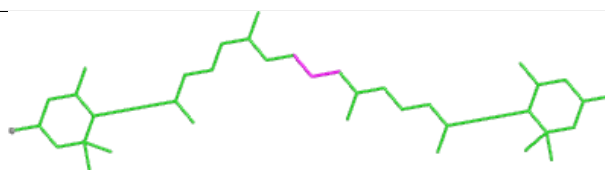


Rings

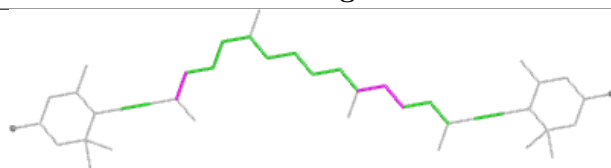
Ligand II0 k 618



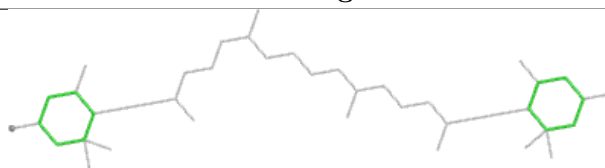
Bond lengths



Bond angles

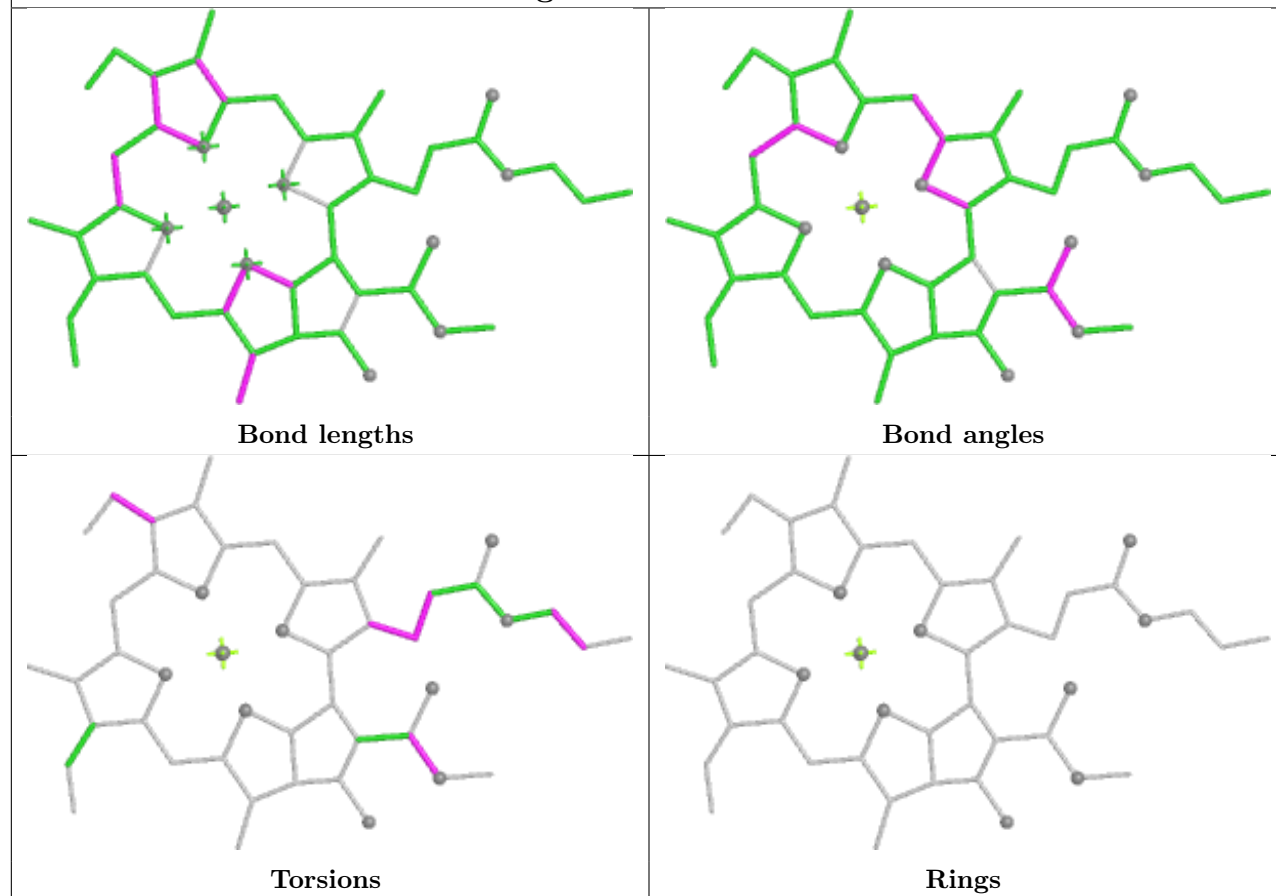


Torsions

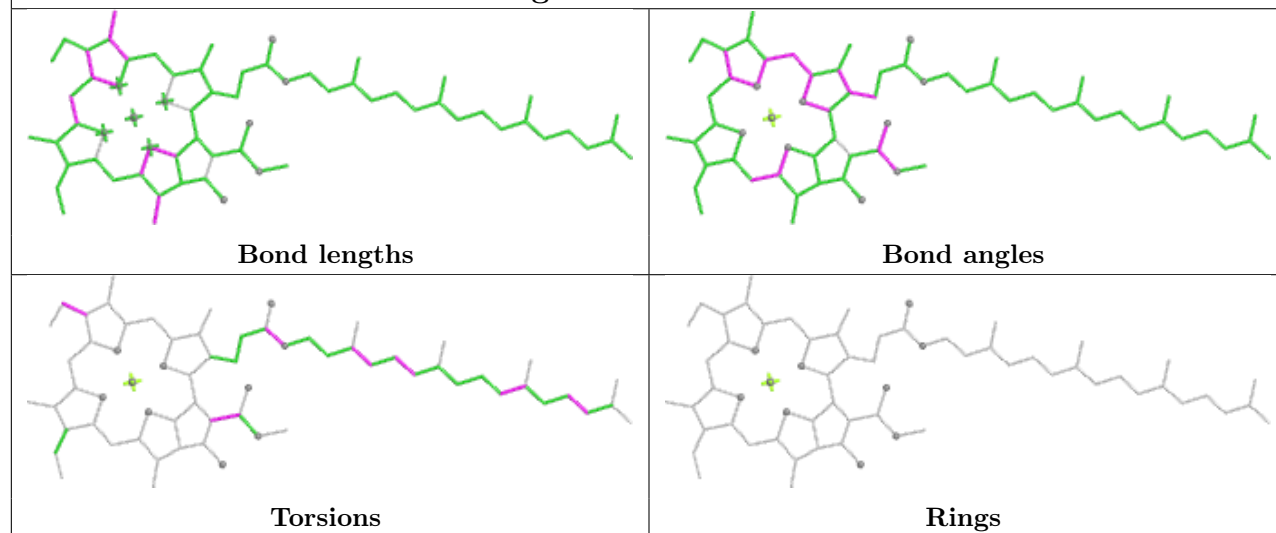


Rings

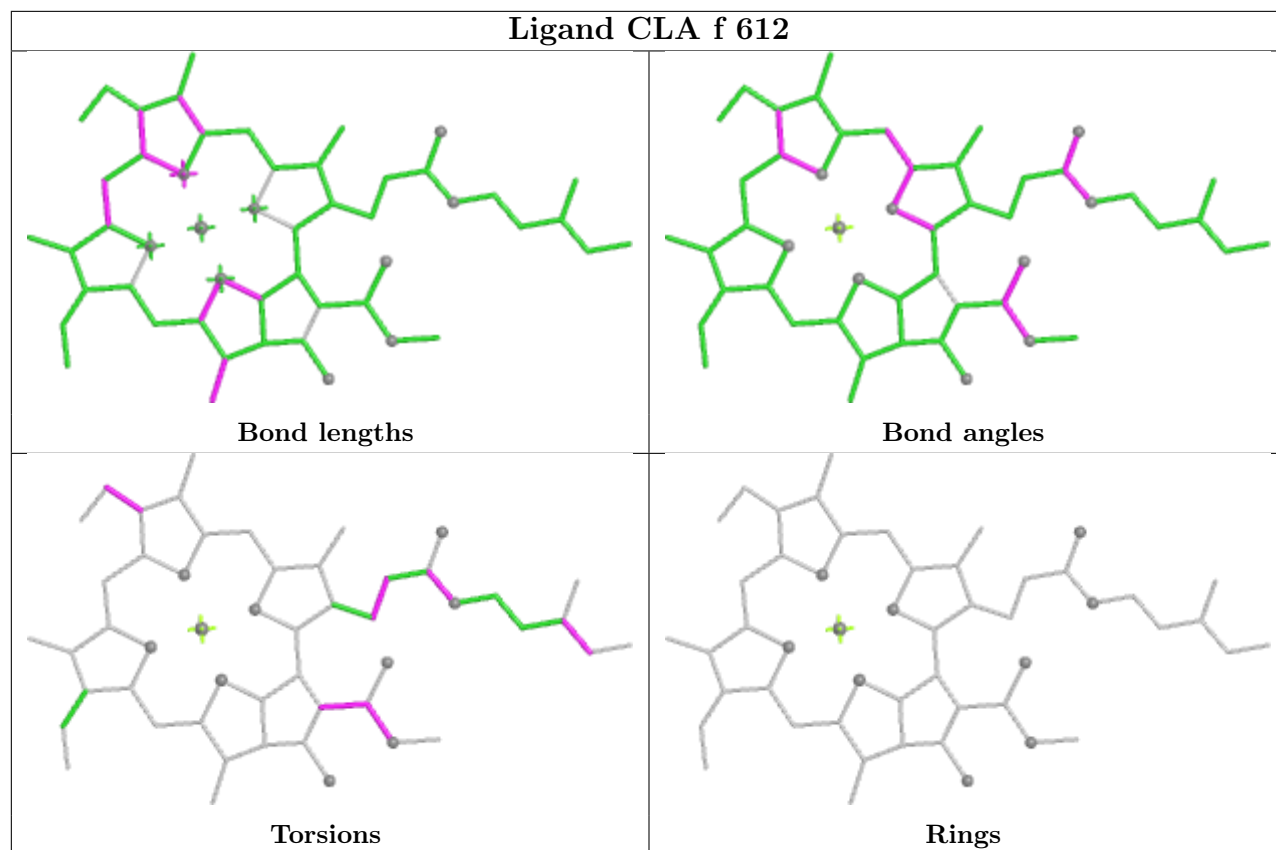
Ligand CLA a 312



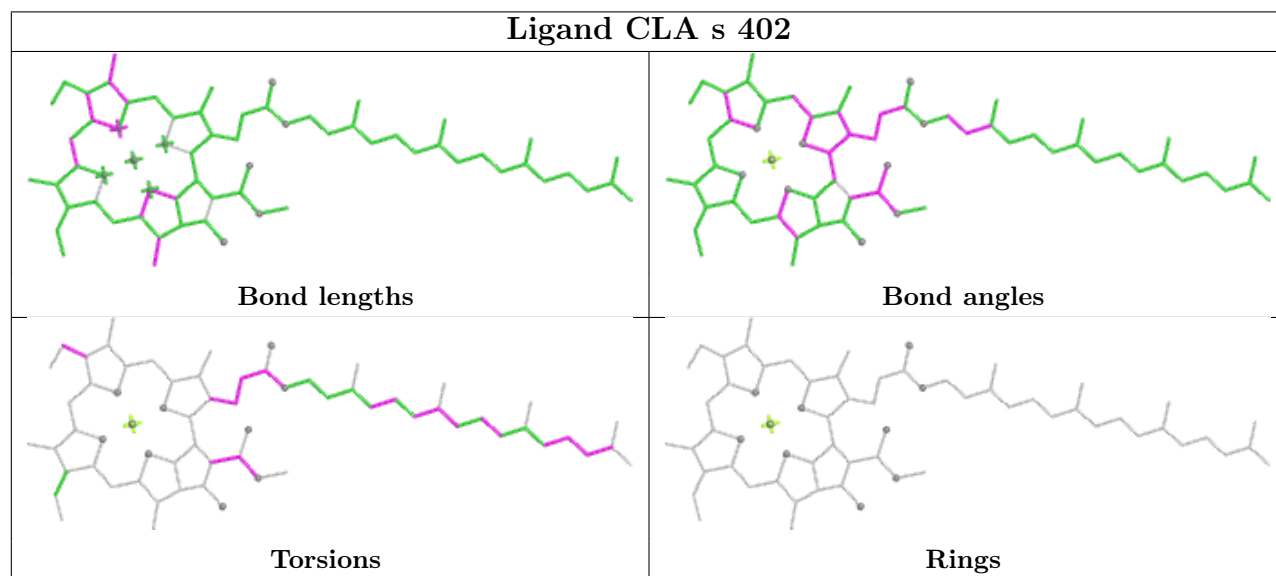
Ligand CLA A 838

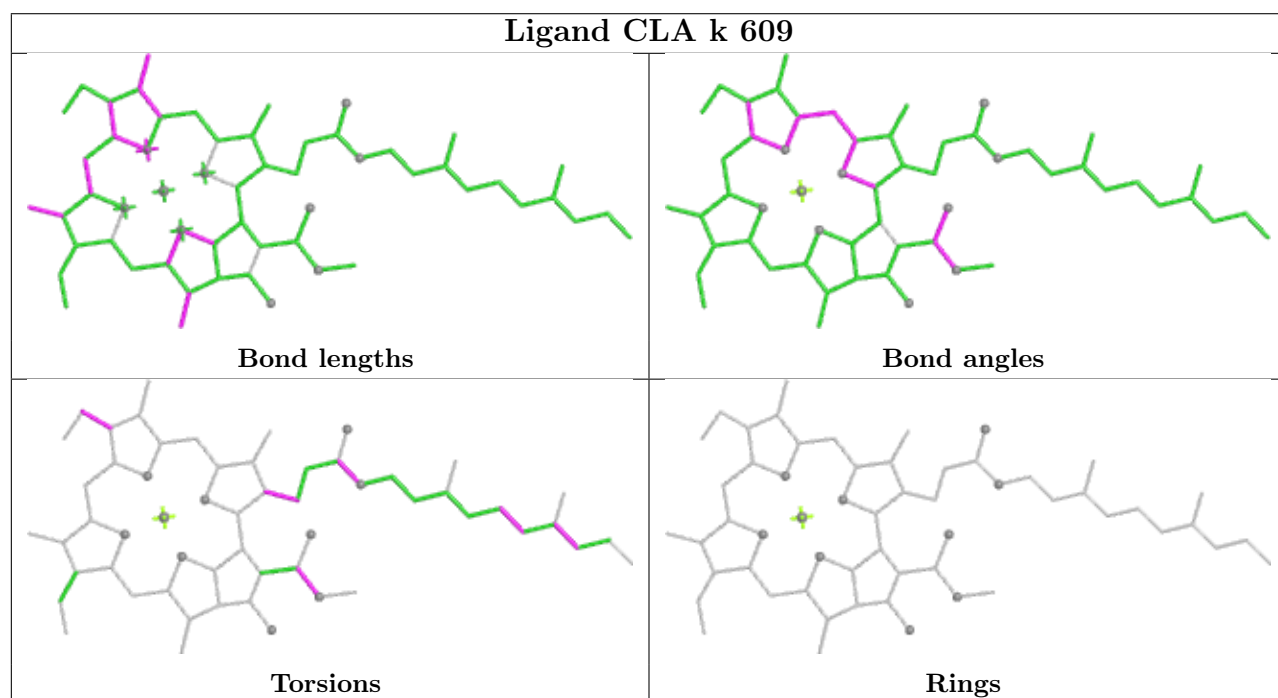
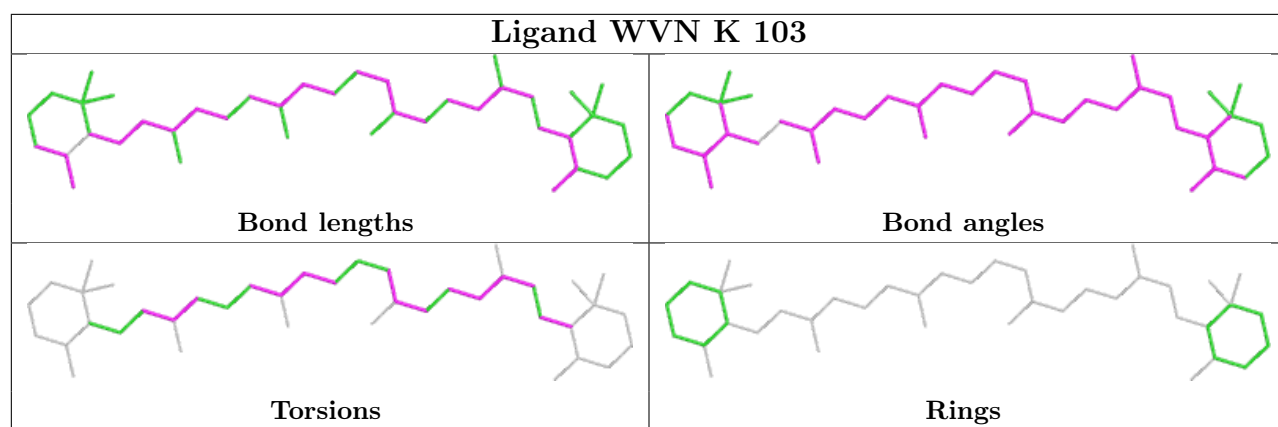


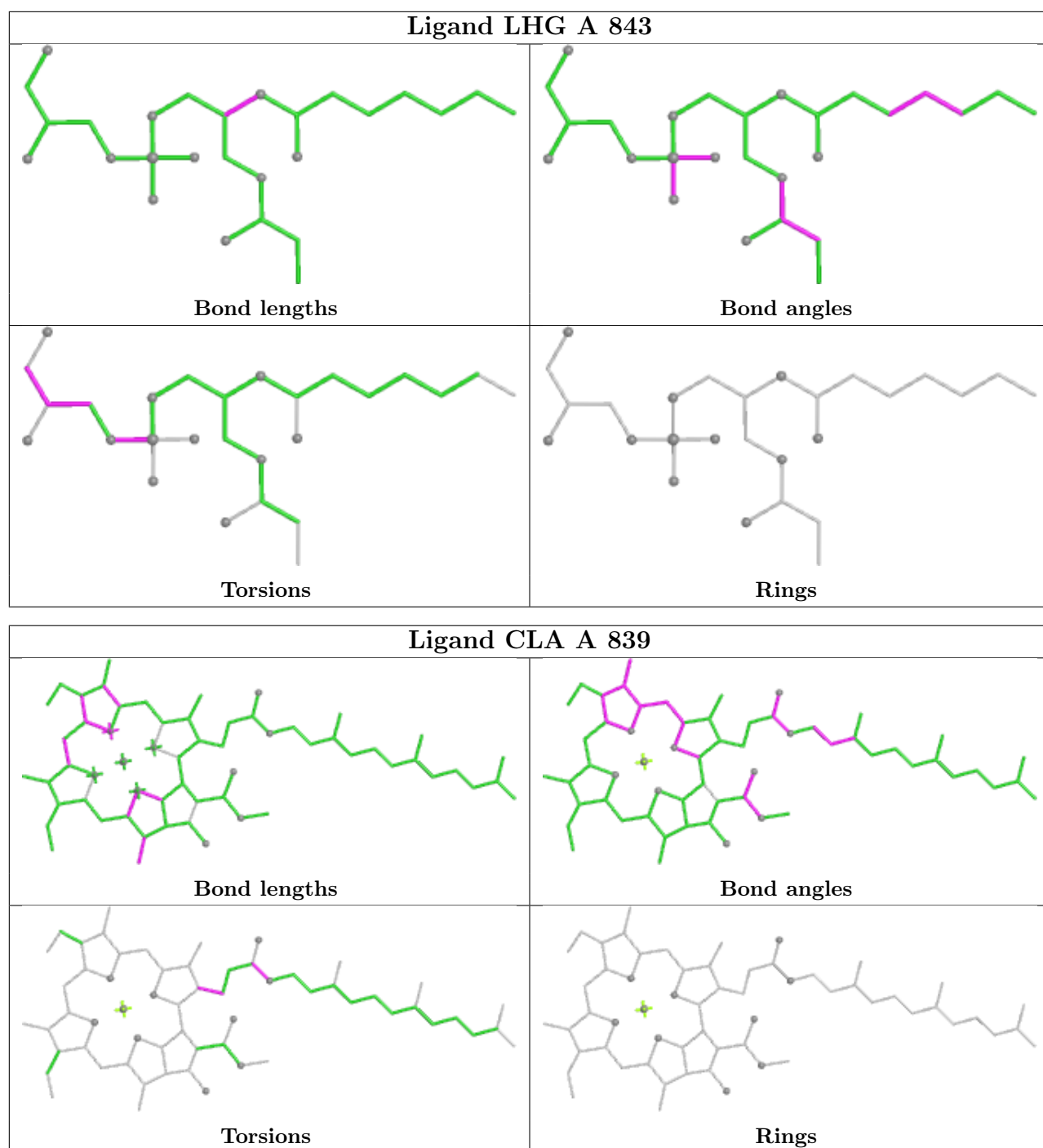
Ligand CLA f 612

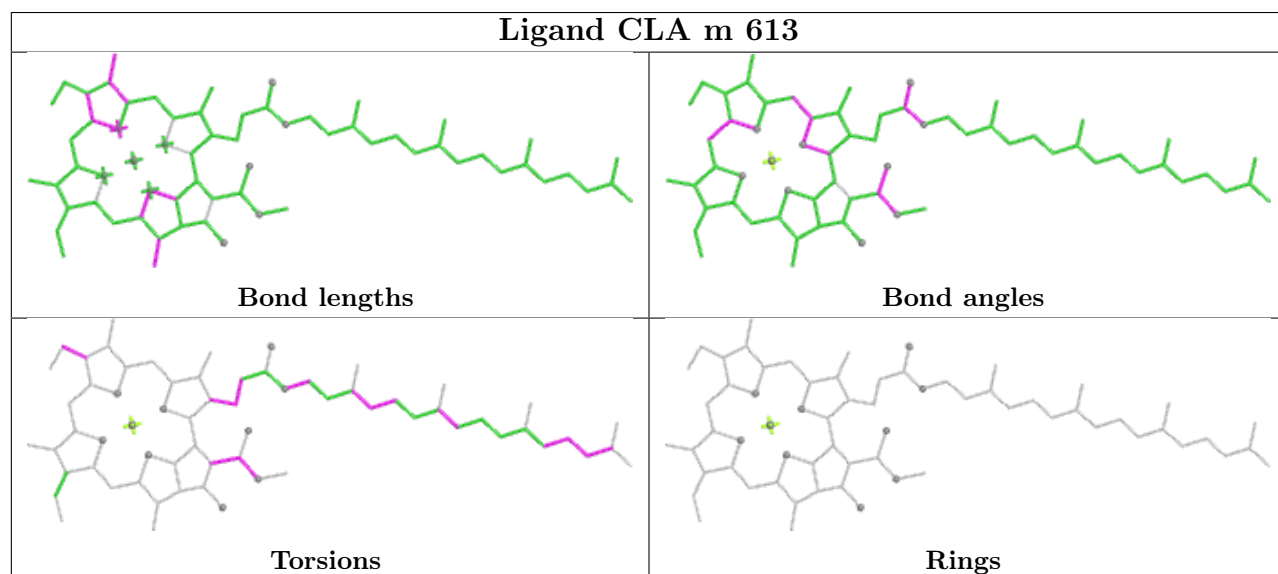
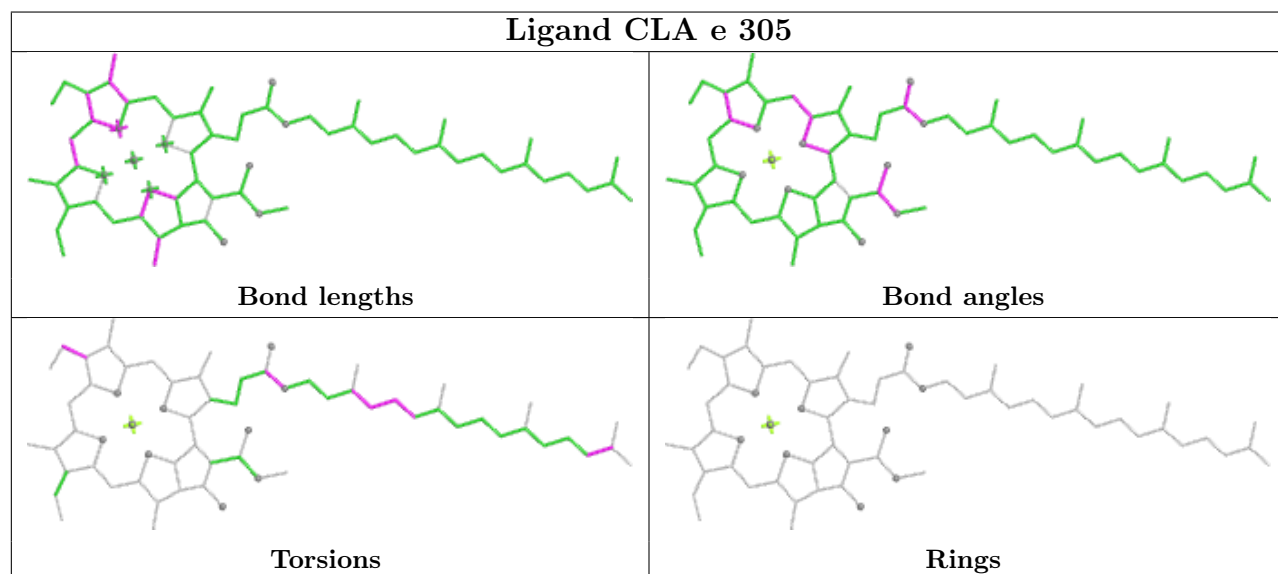
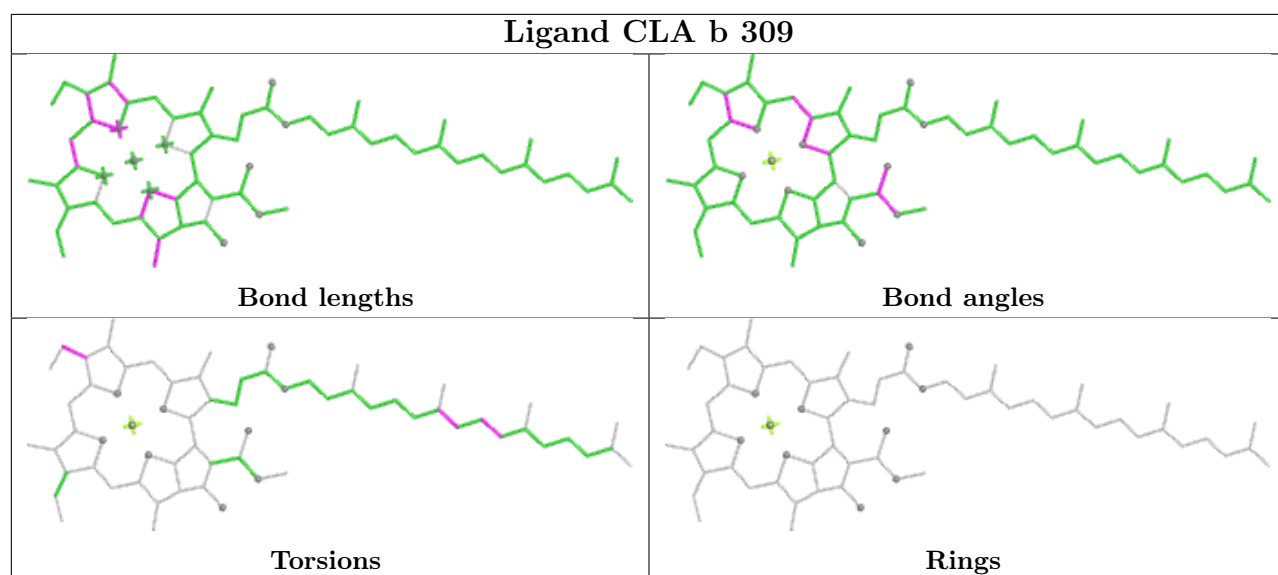


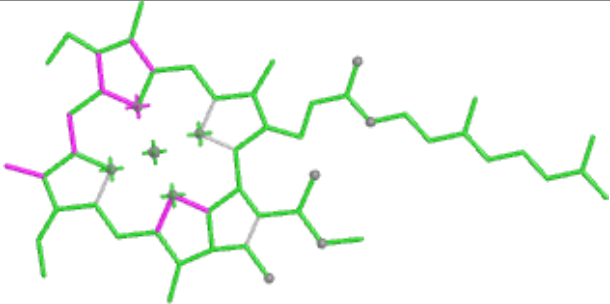
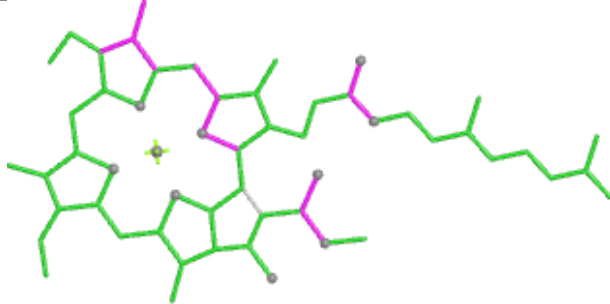
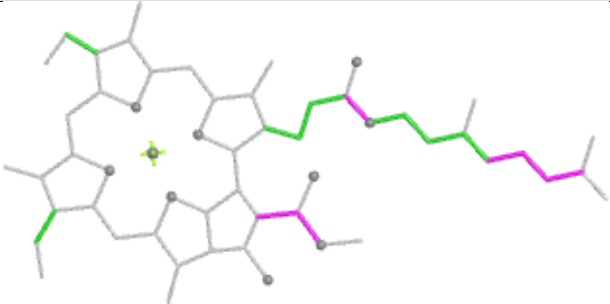
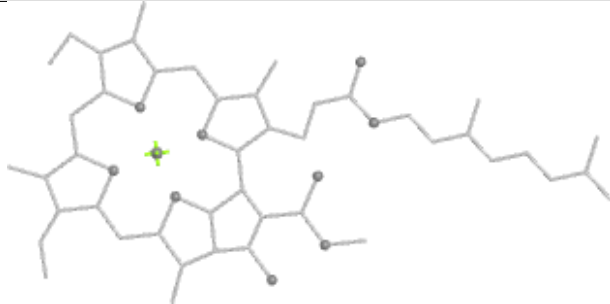
Ligand CLA s 402

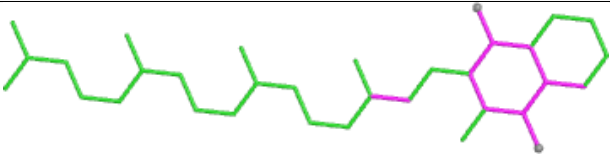
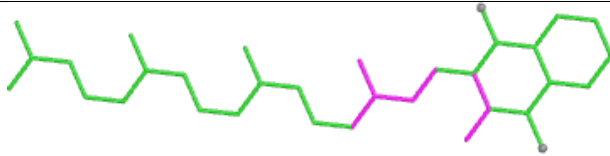
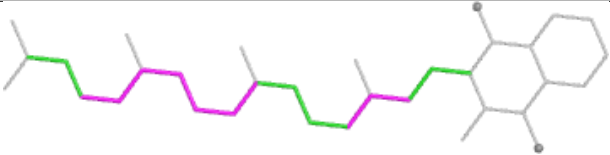
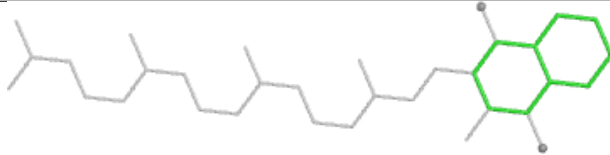


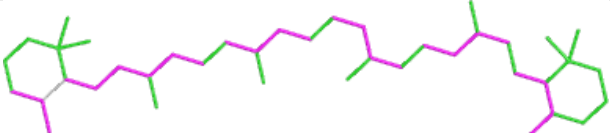
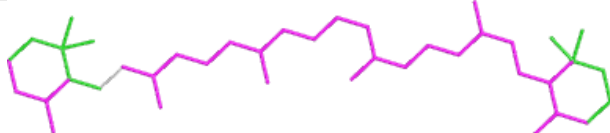
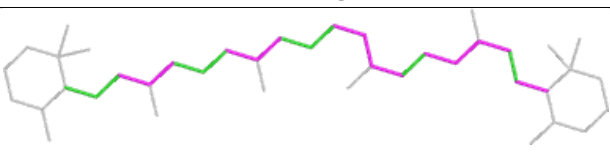
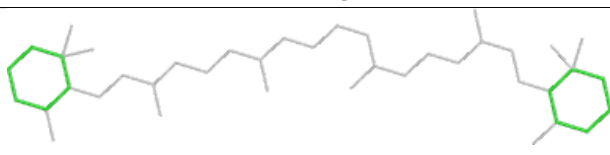




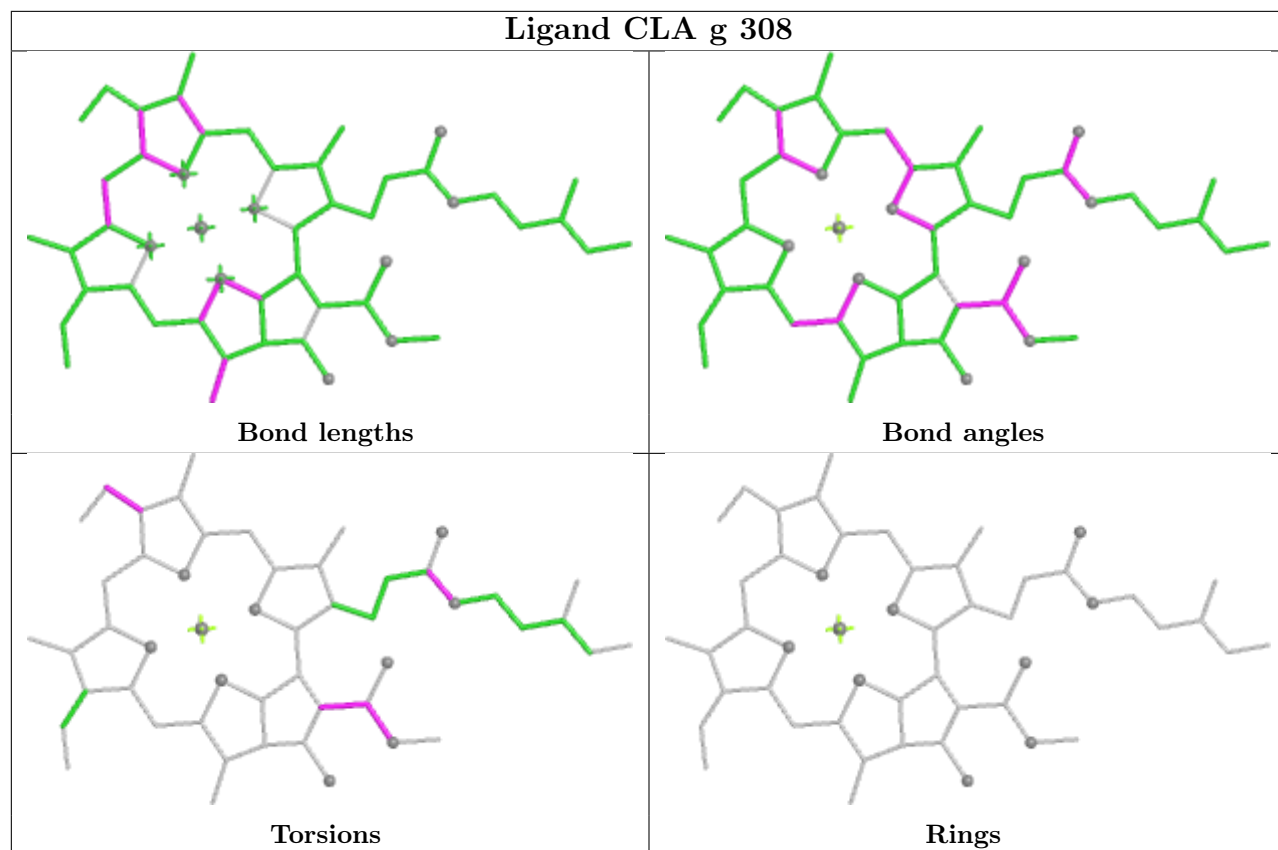


Ligand CLA e 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

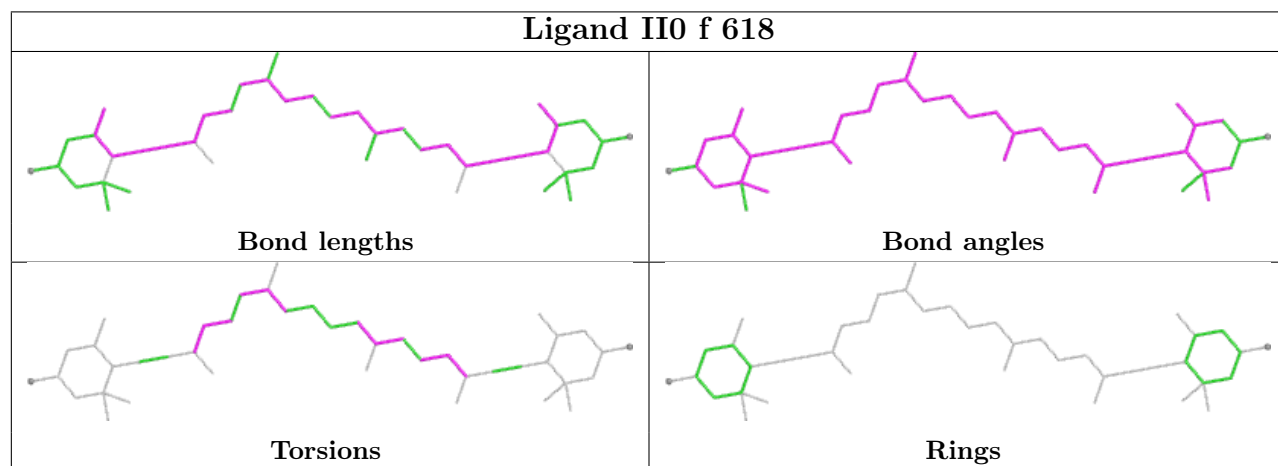
Ligand PQN A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN 1 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

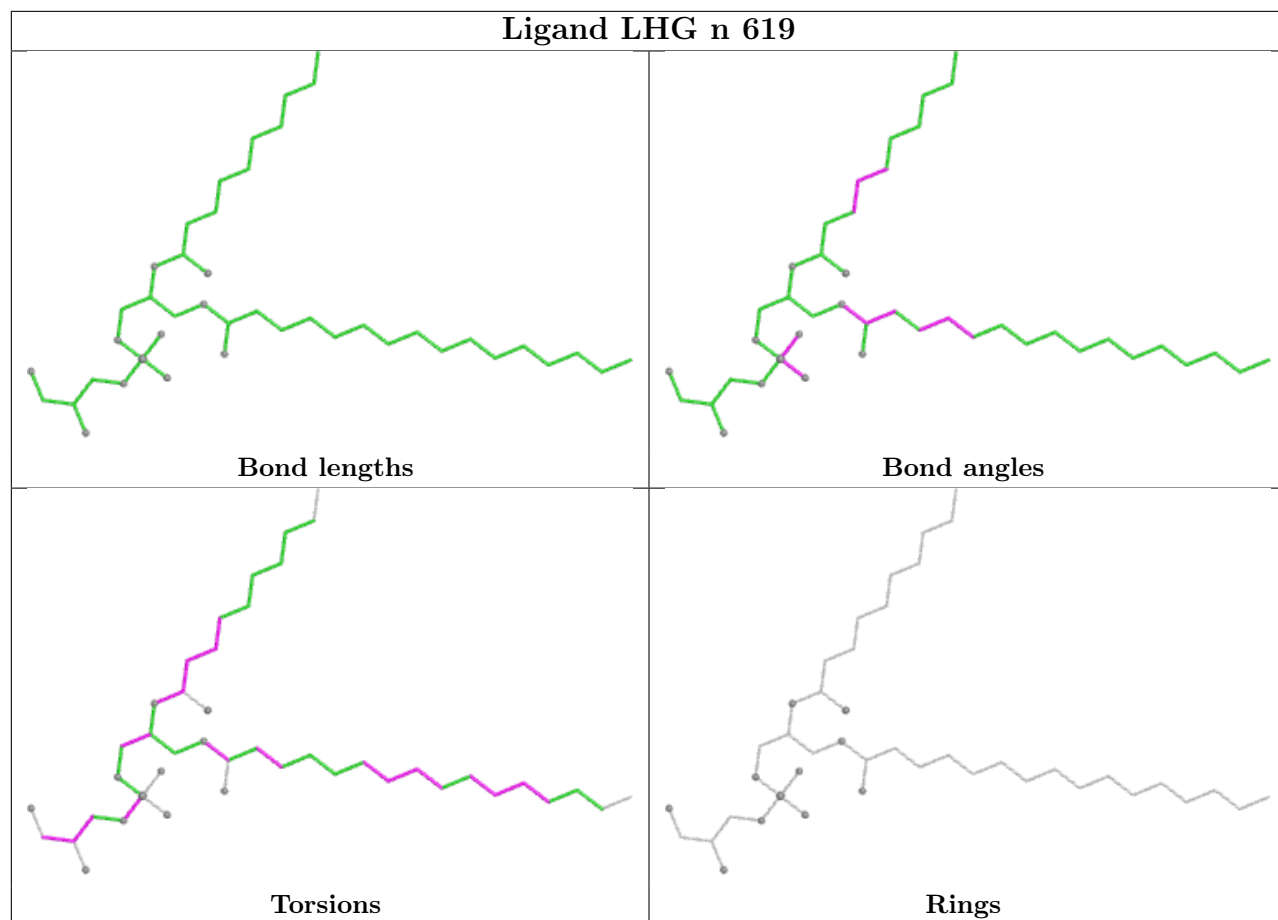
Ligand CLA g 308



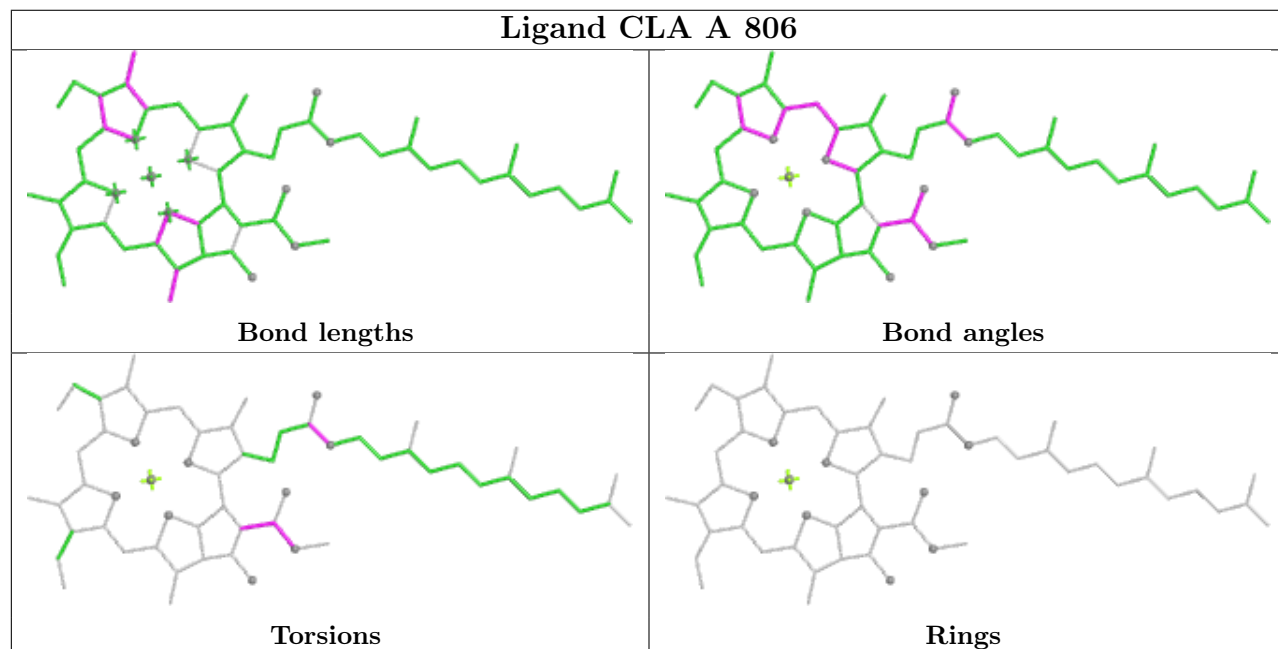
Ligand II0 f 618

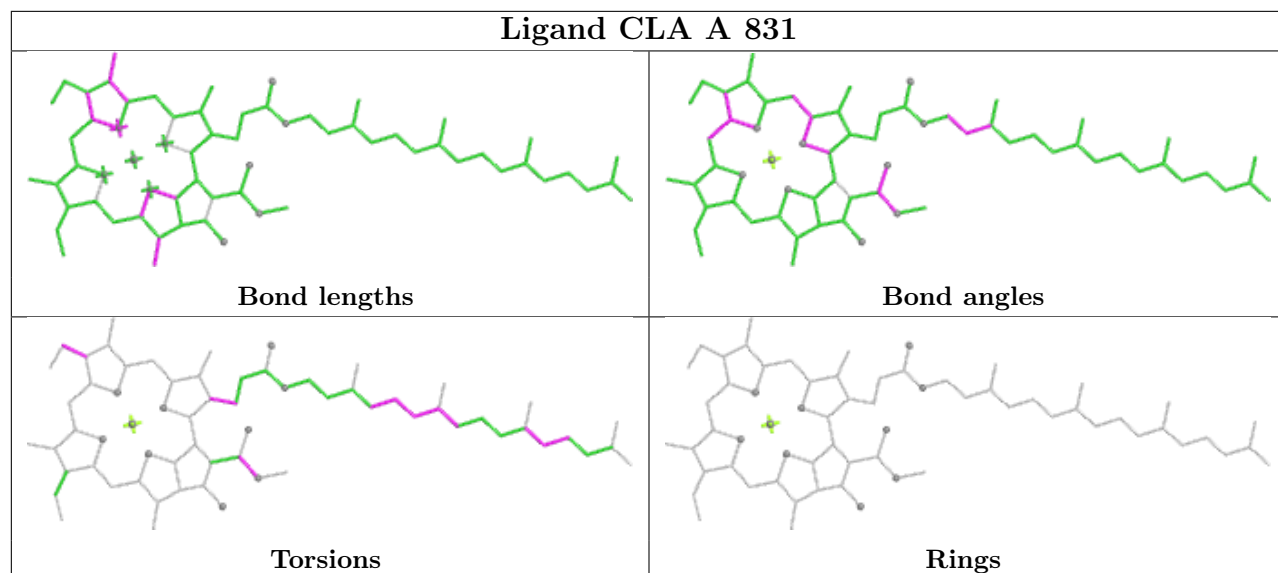
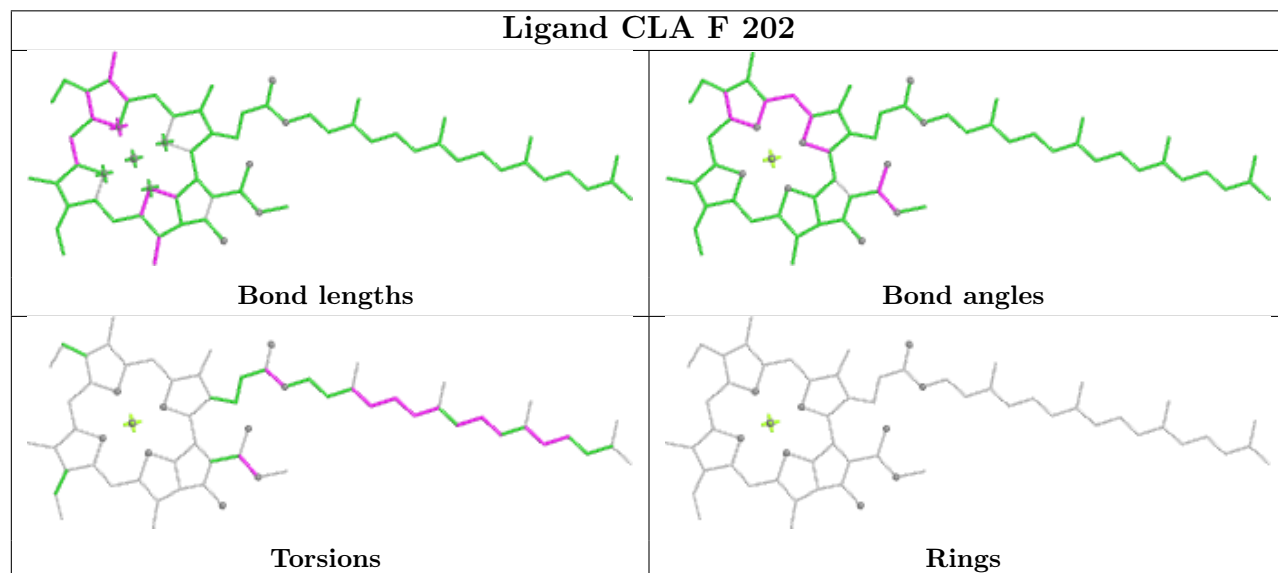
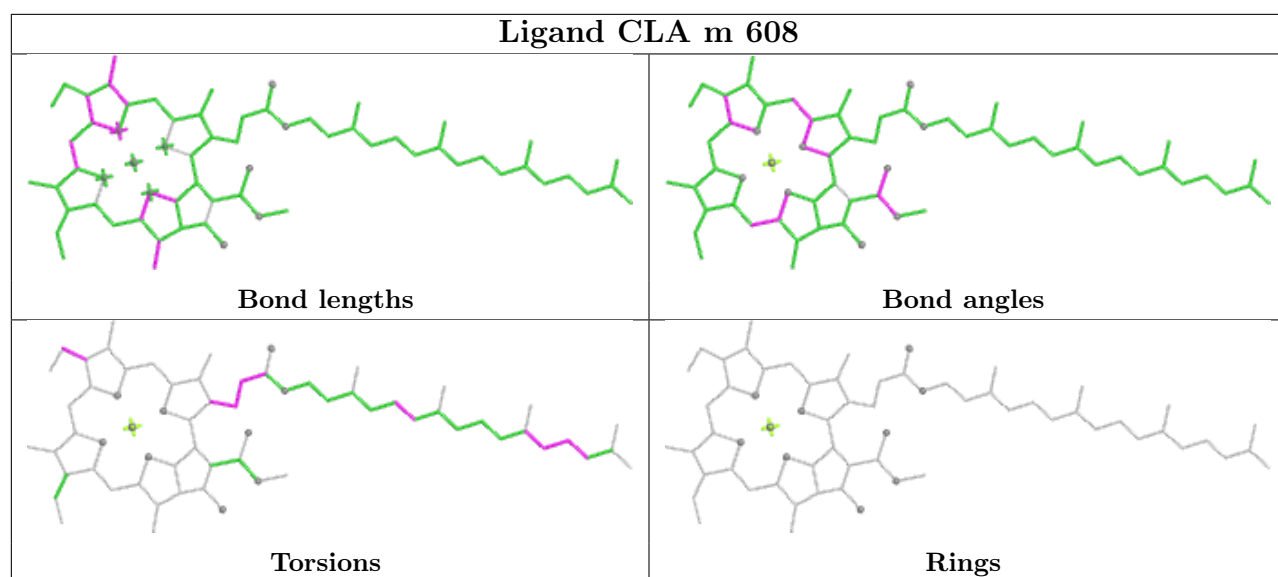


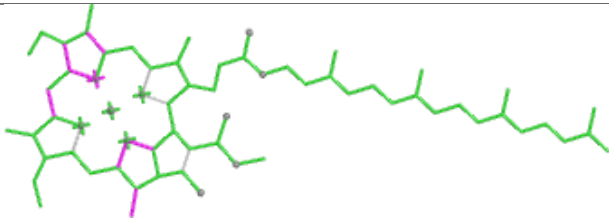
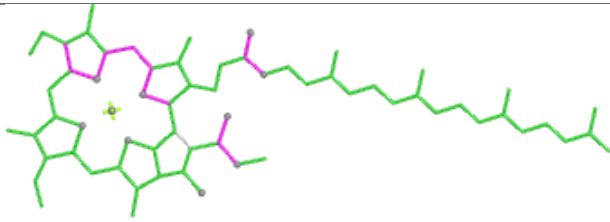
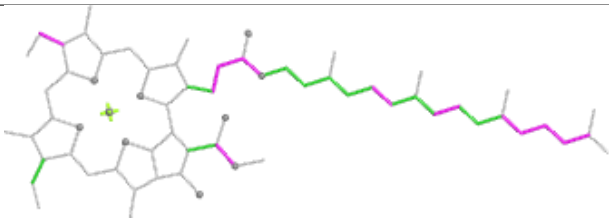
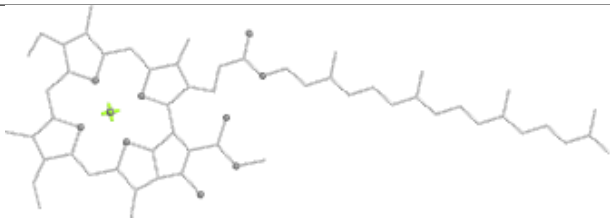
Ligand LHG n 619

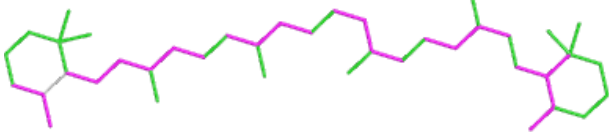
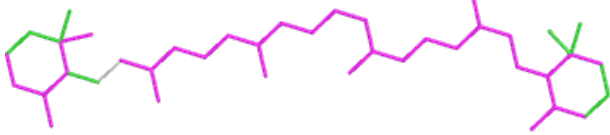
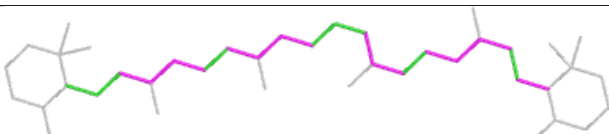
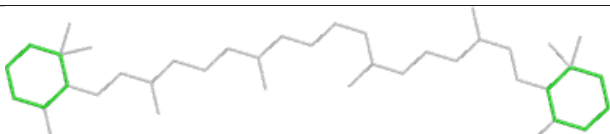


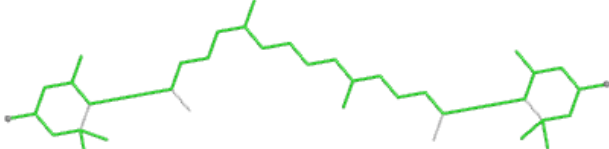
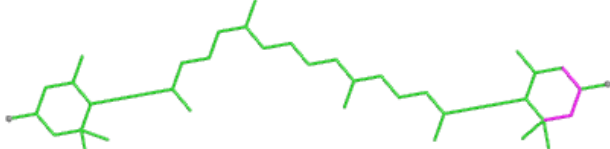
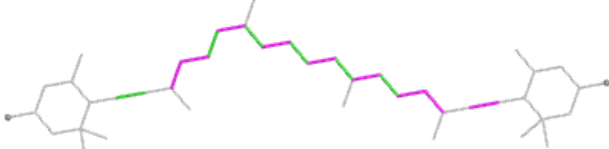
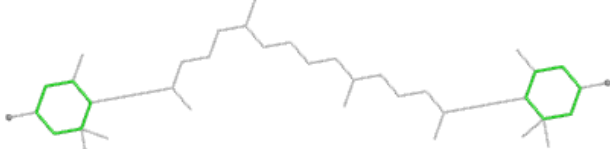
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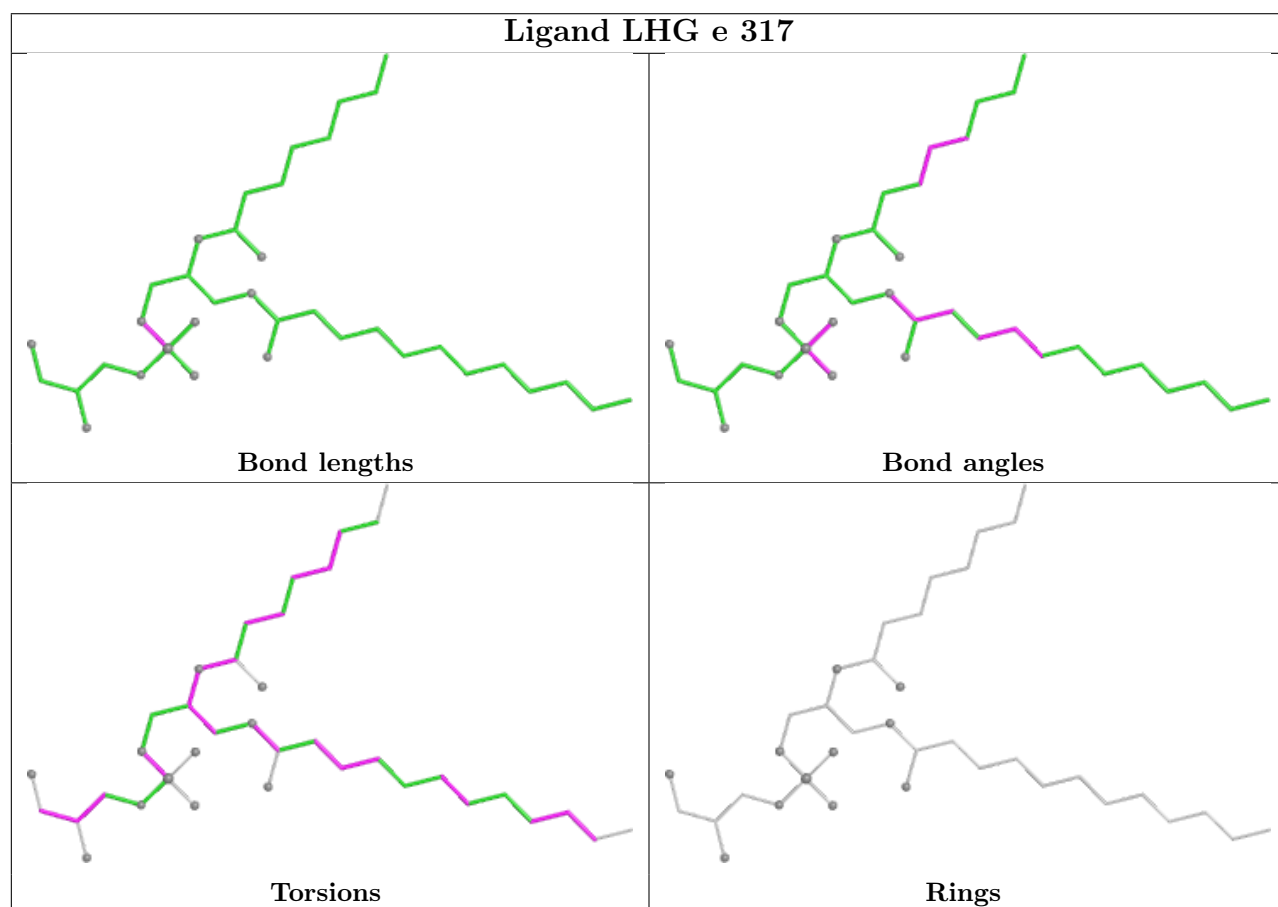
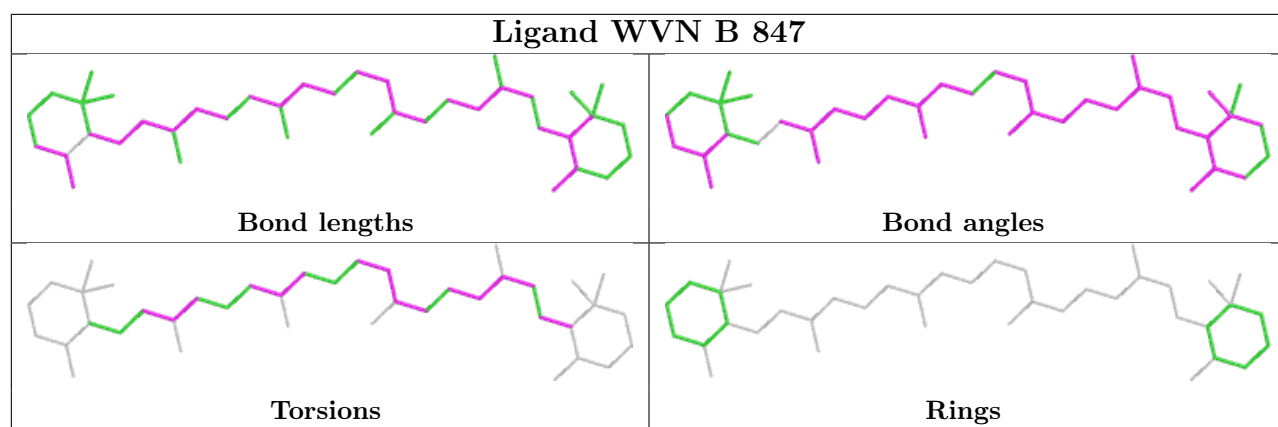




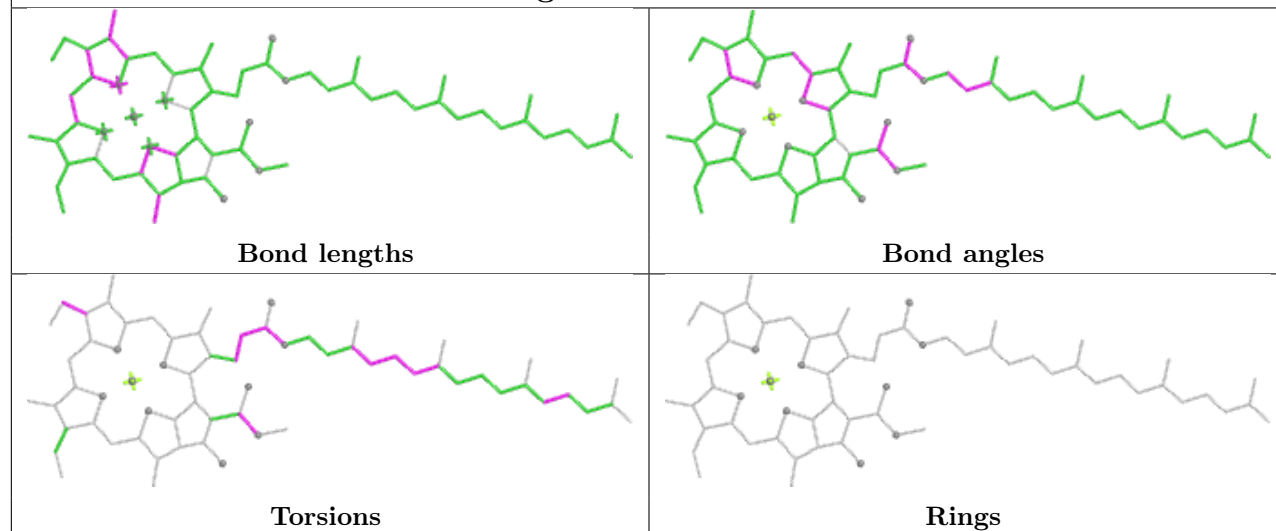
Ligand CLA e 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN h 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

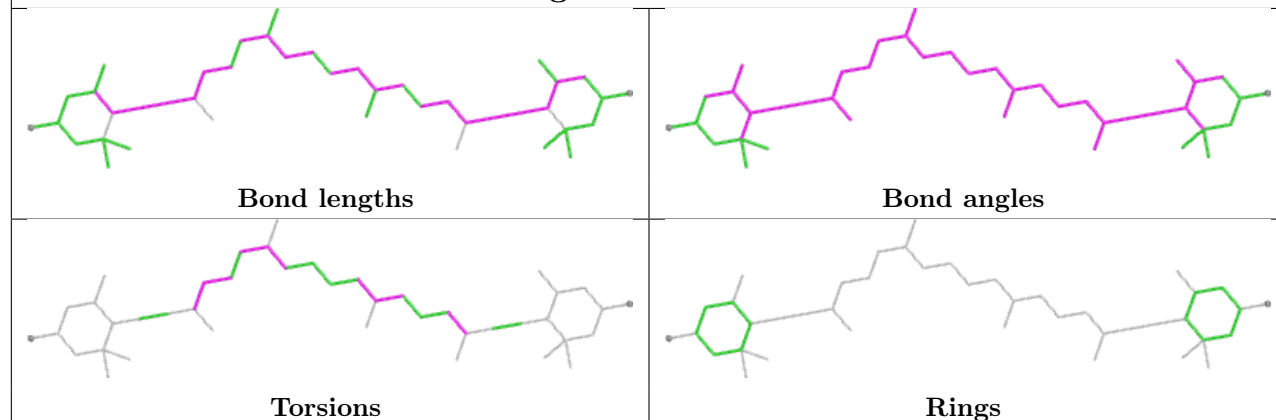
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Bond lengths	Bond angles
	
Torsions	Rings



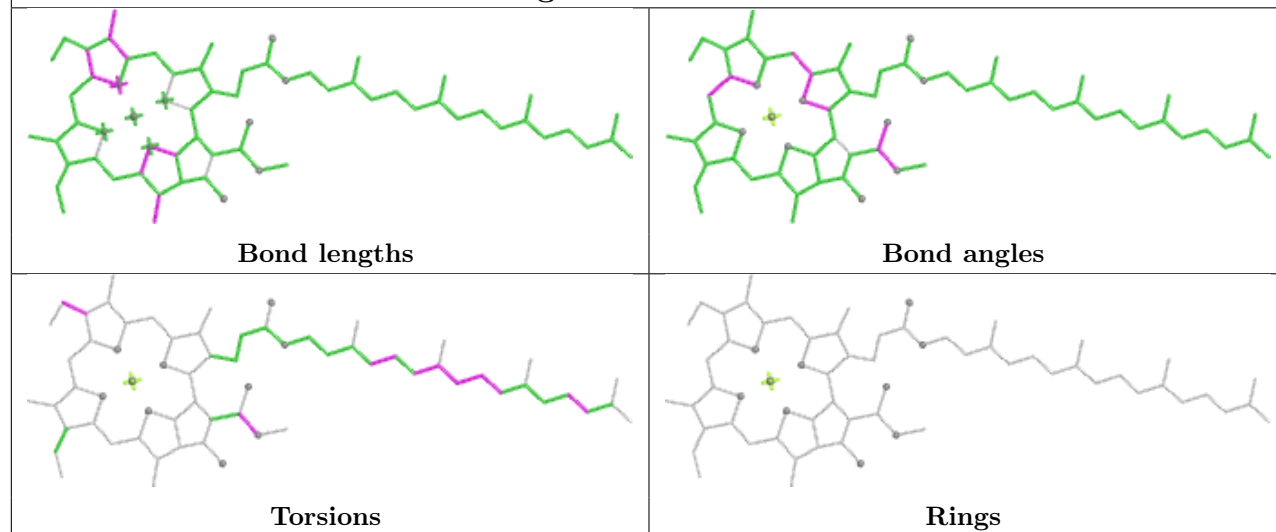
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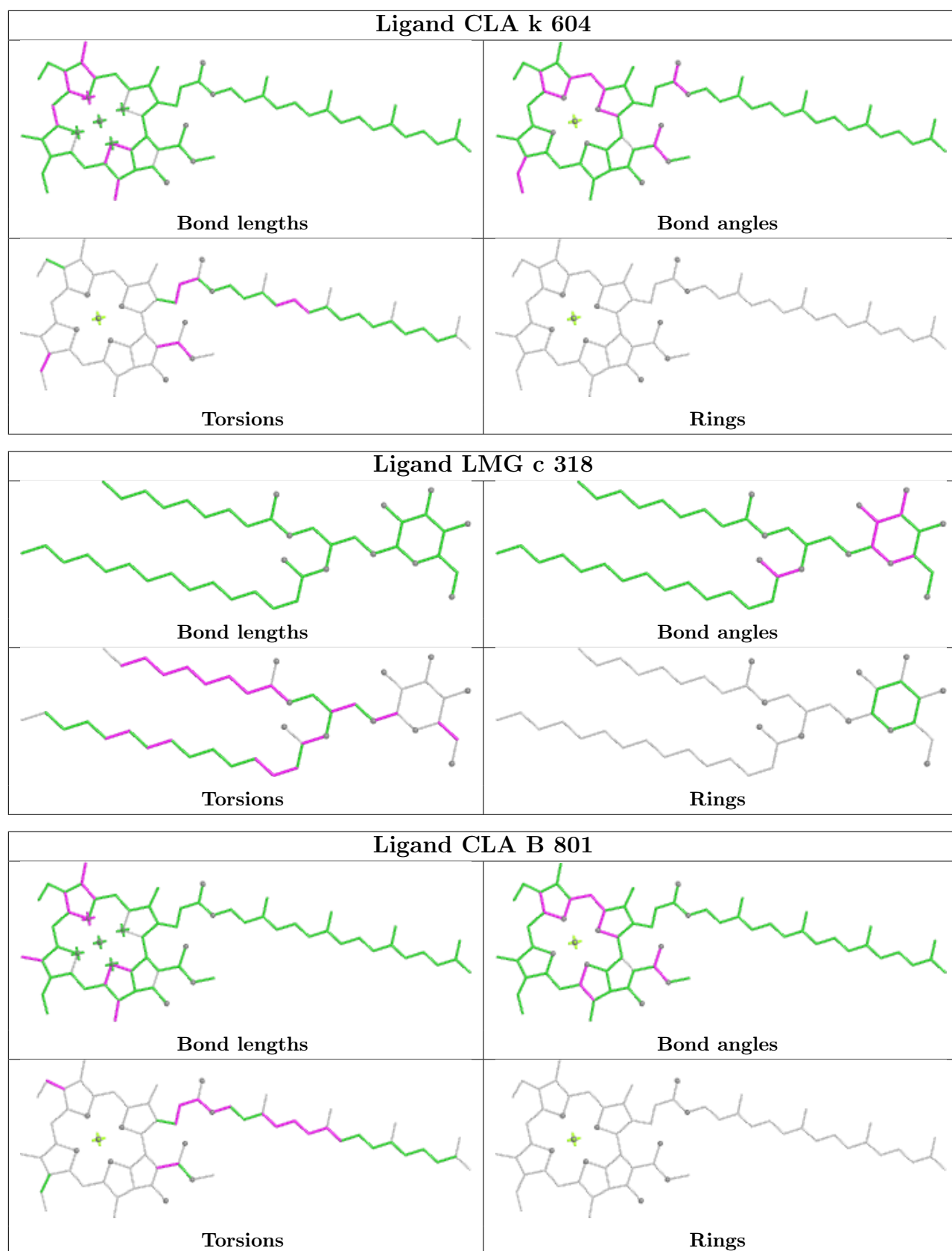


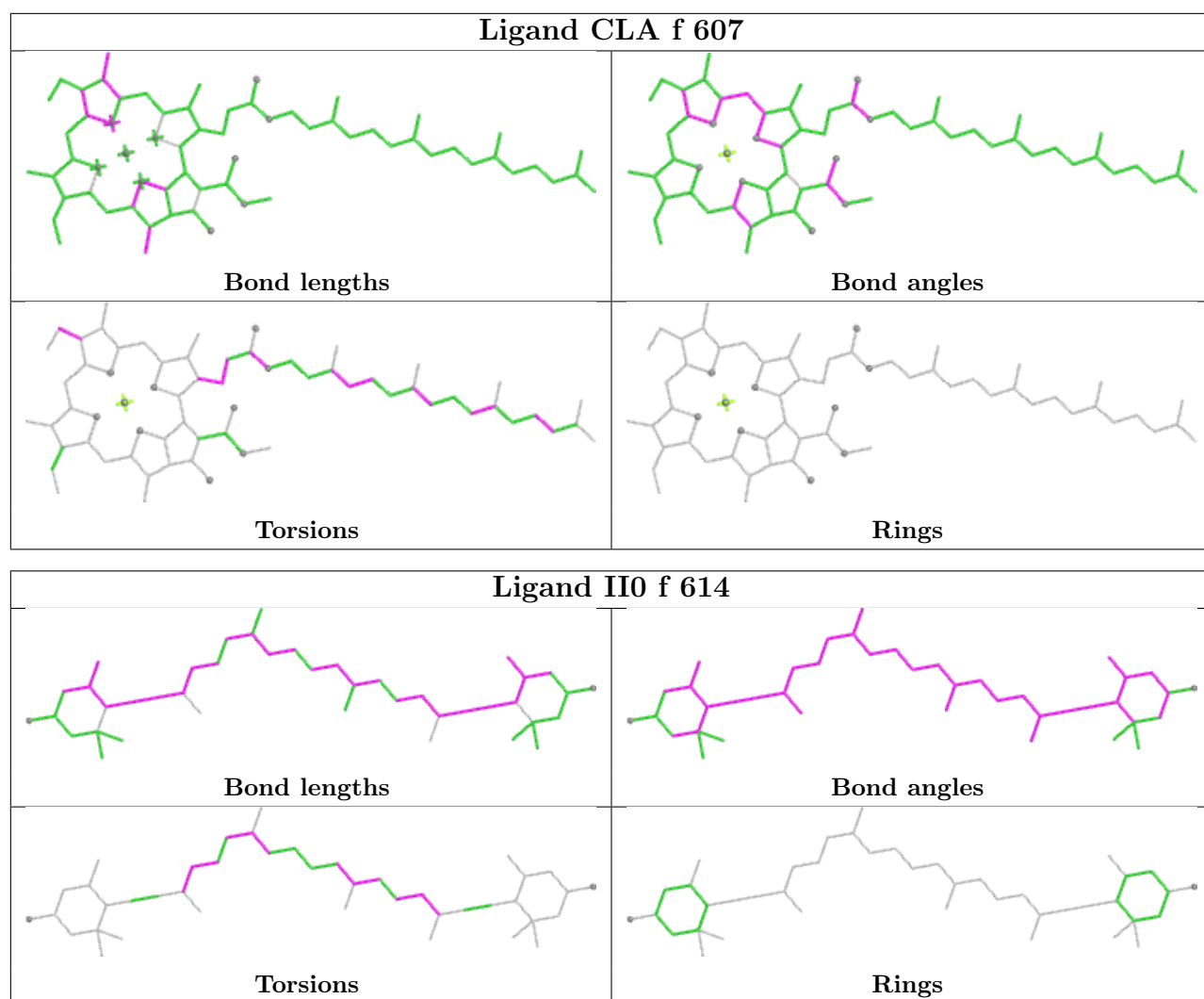
Ligand II0 b 315



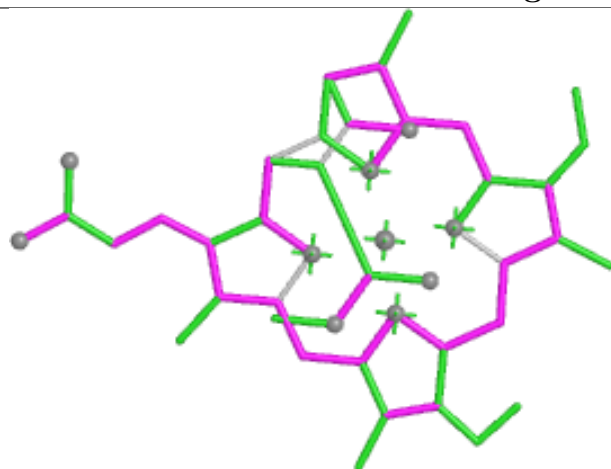
Ligand CLA c 312



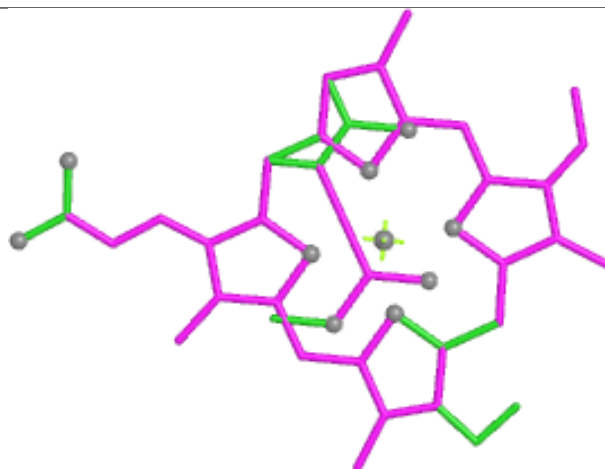




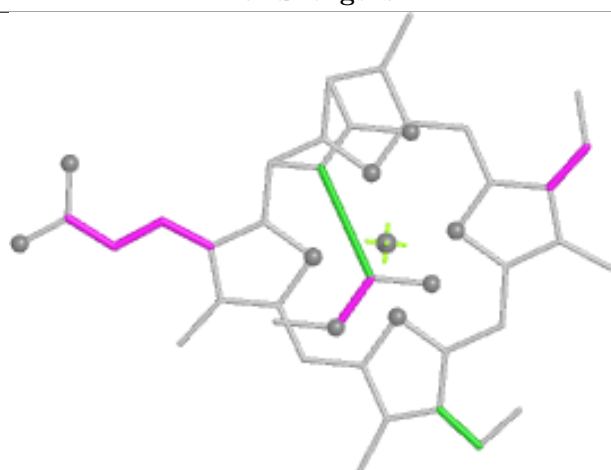
Ligand KC2 i 318



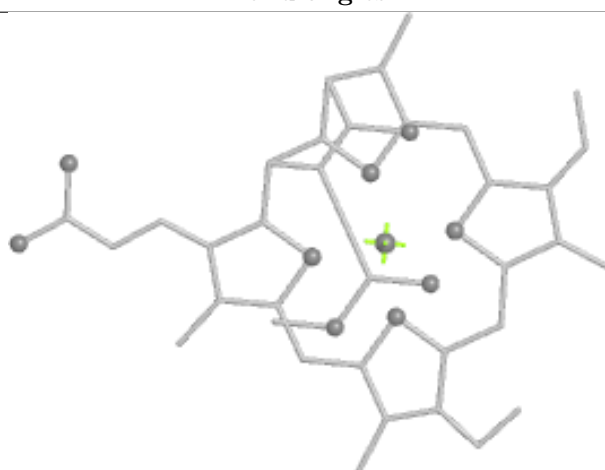
Bond lengths



Bond angles

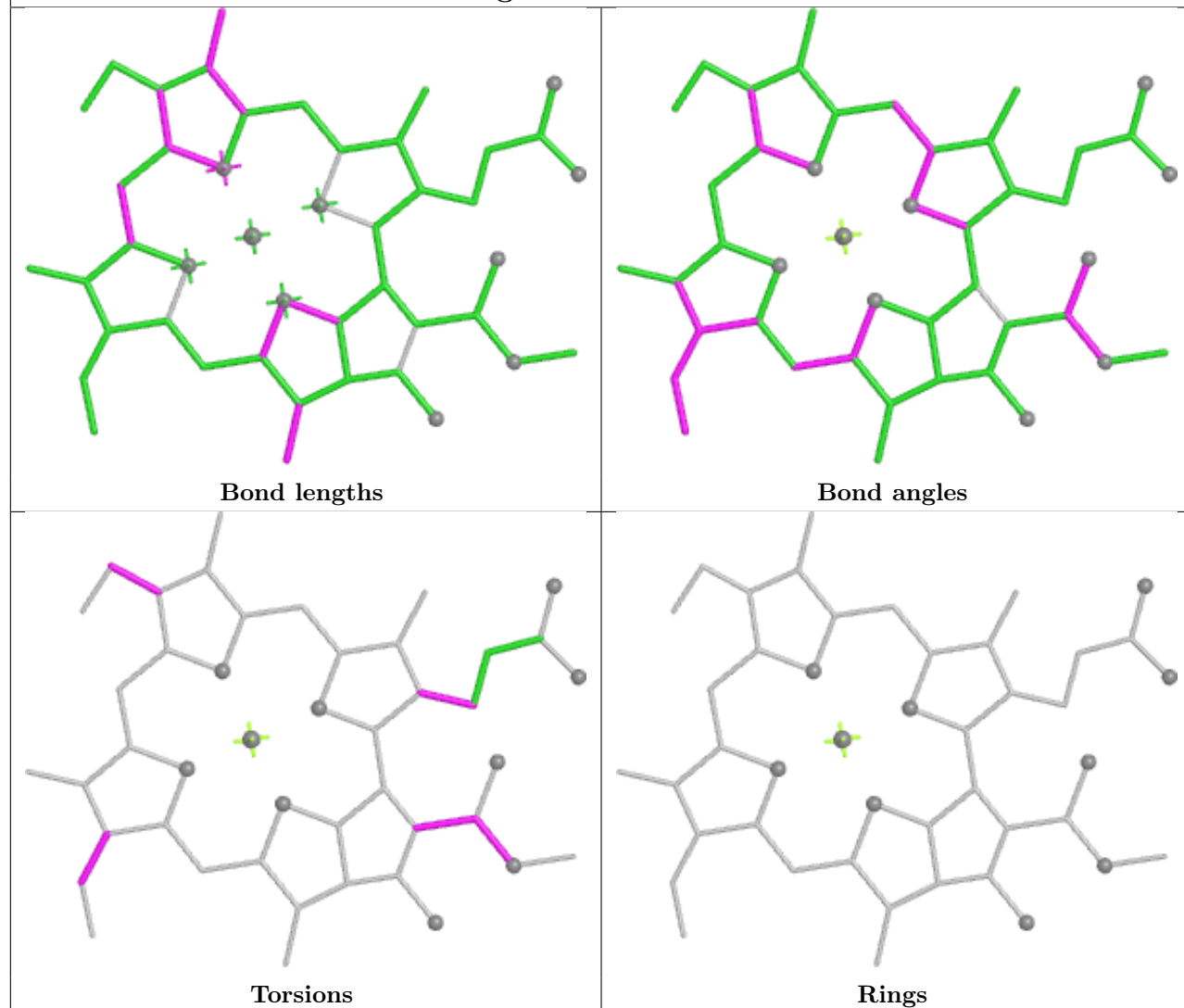


Torsions

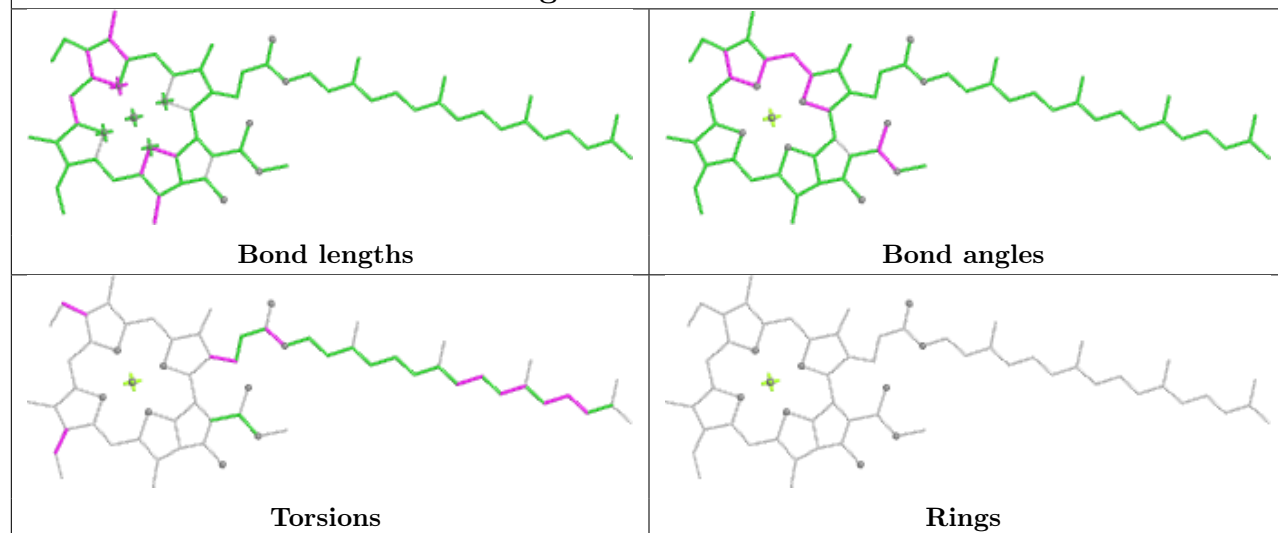


Rings

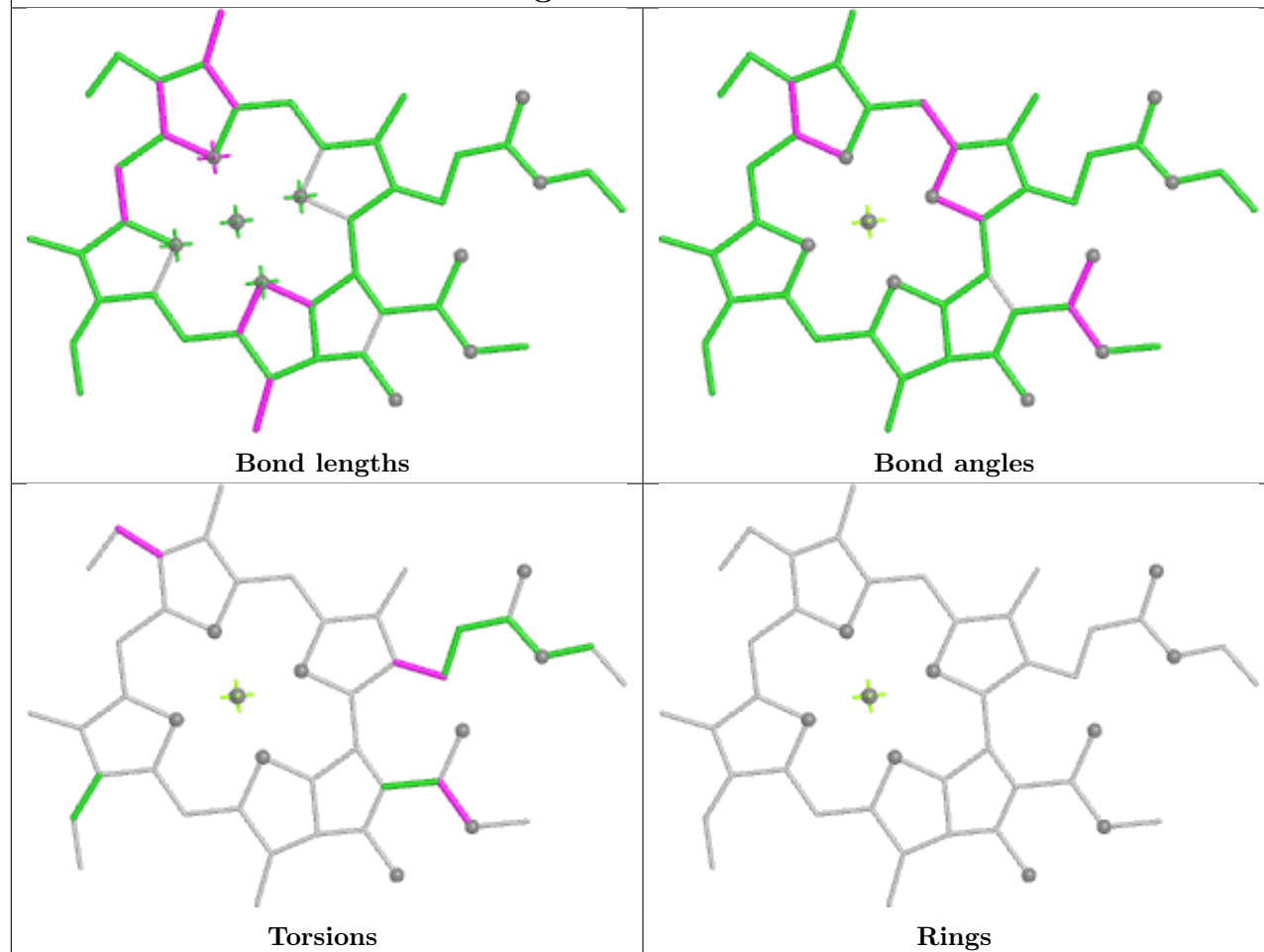
Ligand CLA a 306



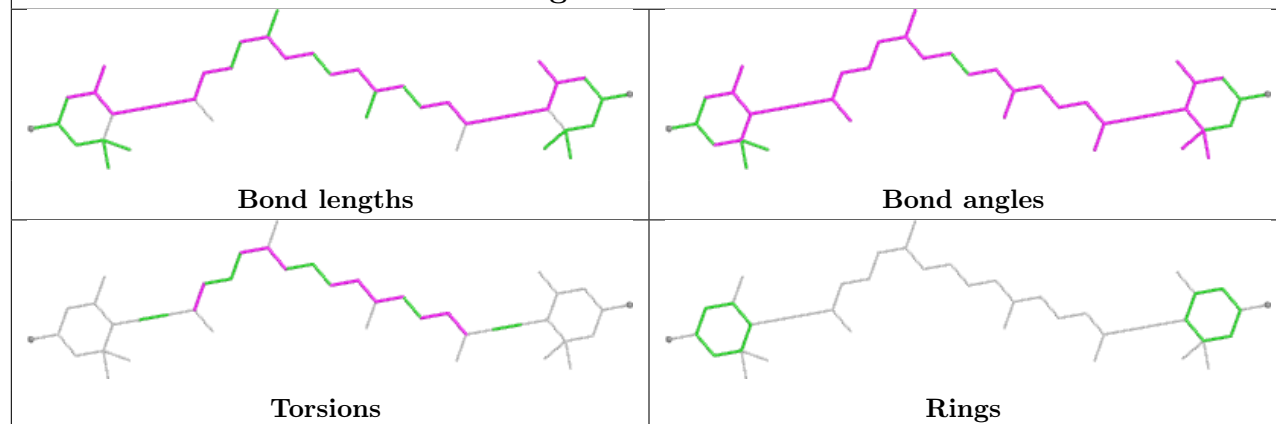
Ligand CLA f 610



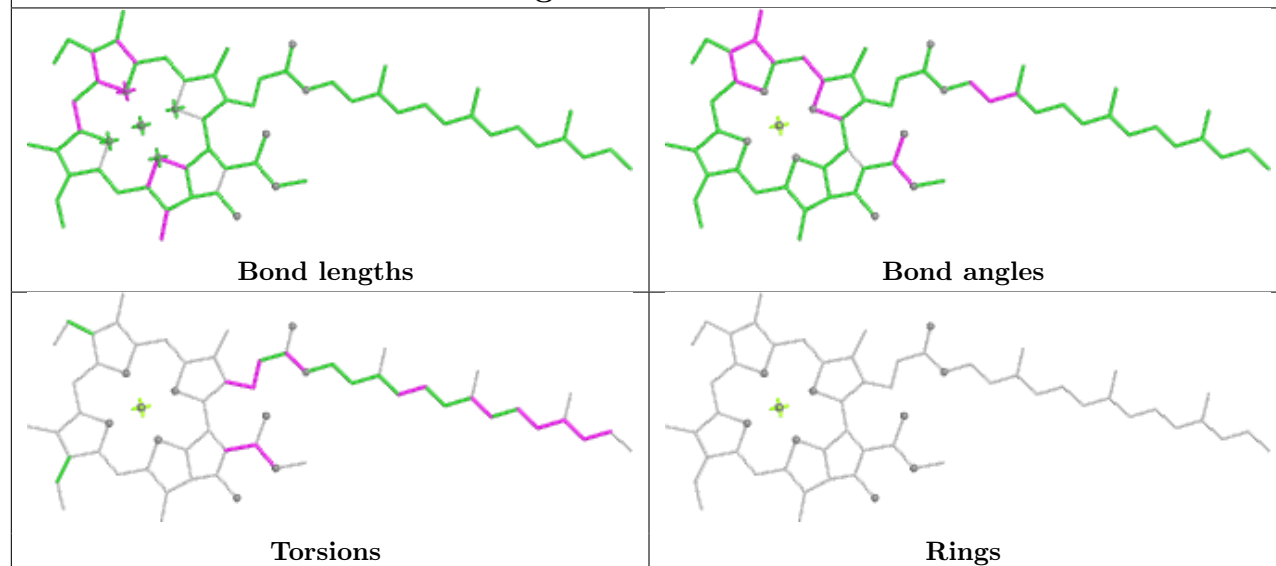
Ligand CLA f 601



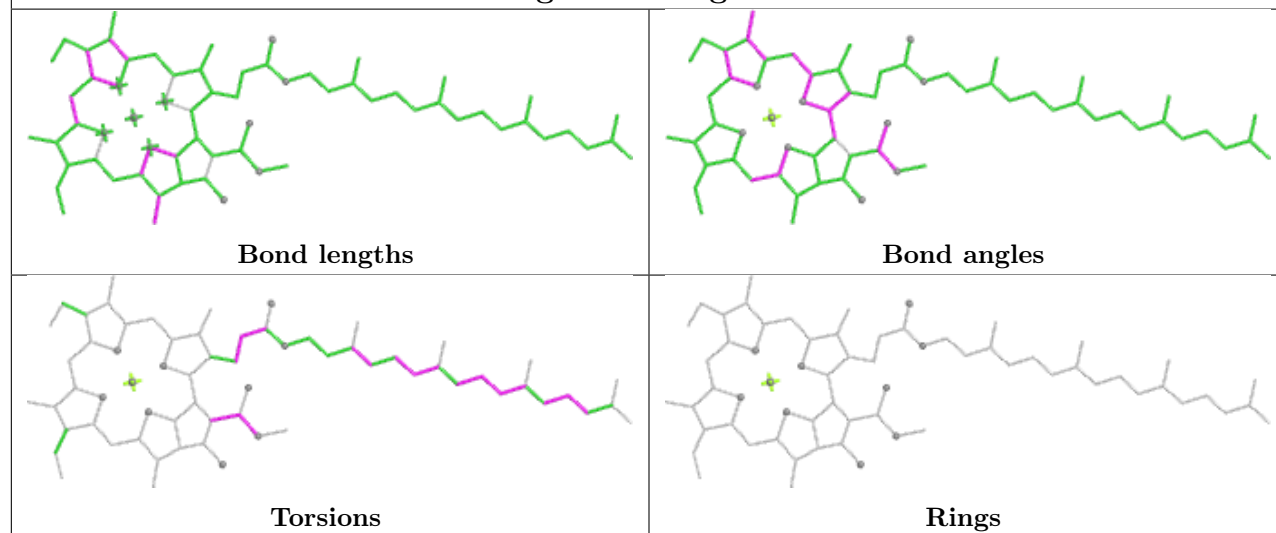
Ligand II0 d 315

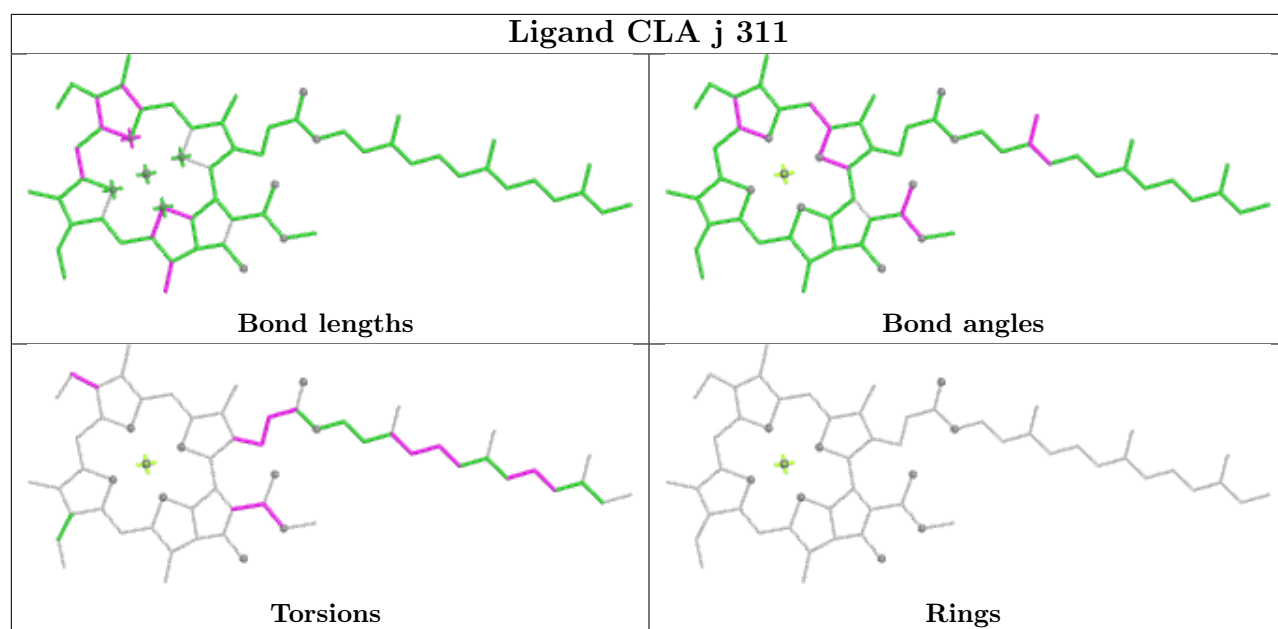


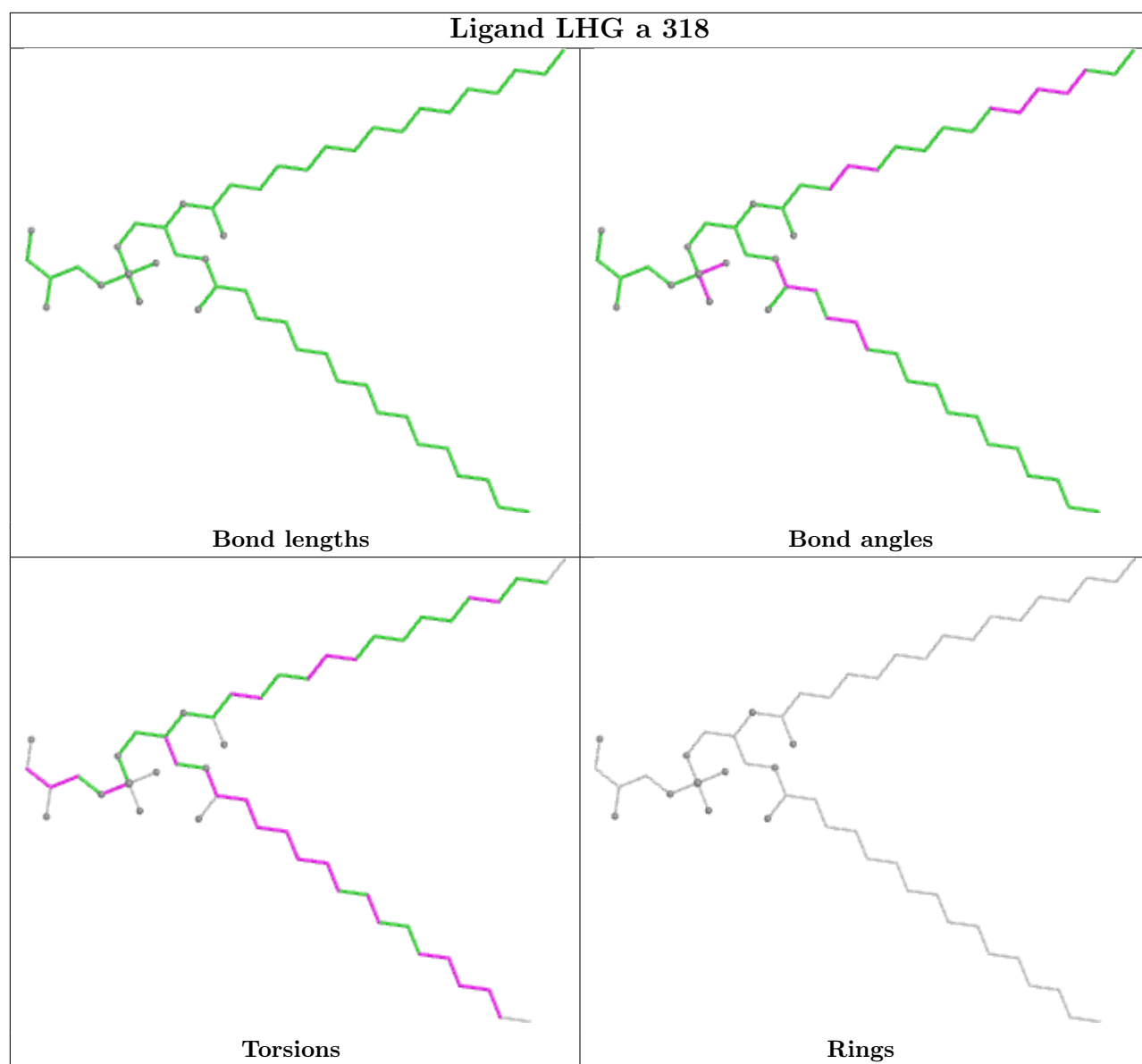
Ligand CLA d 302



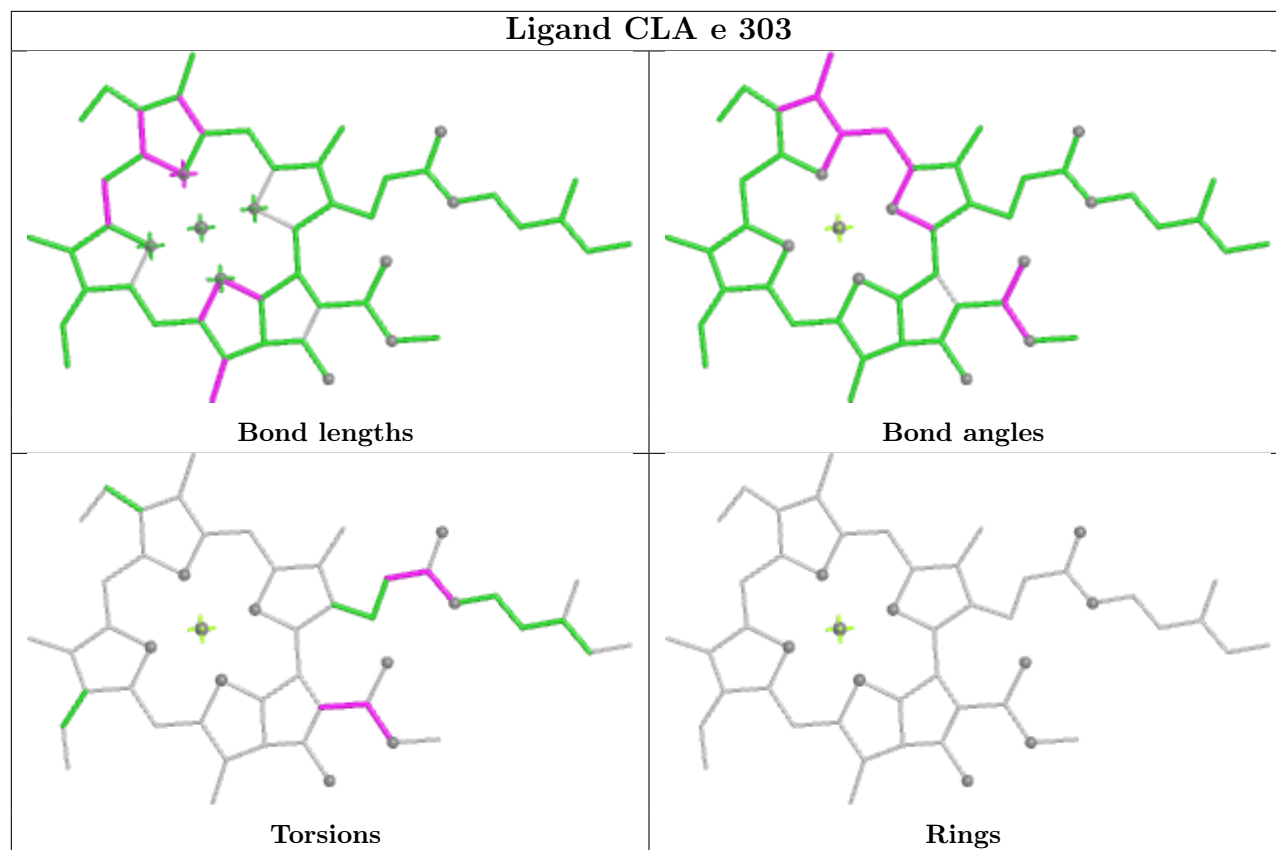
Ligand CLA g 302



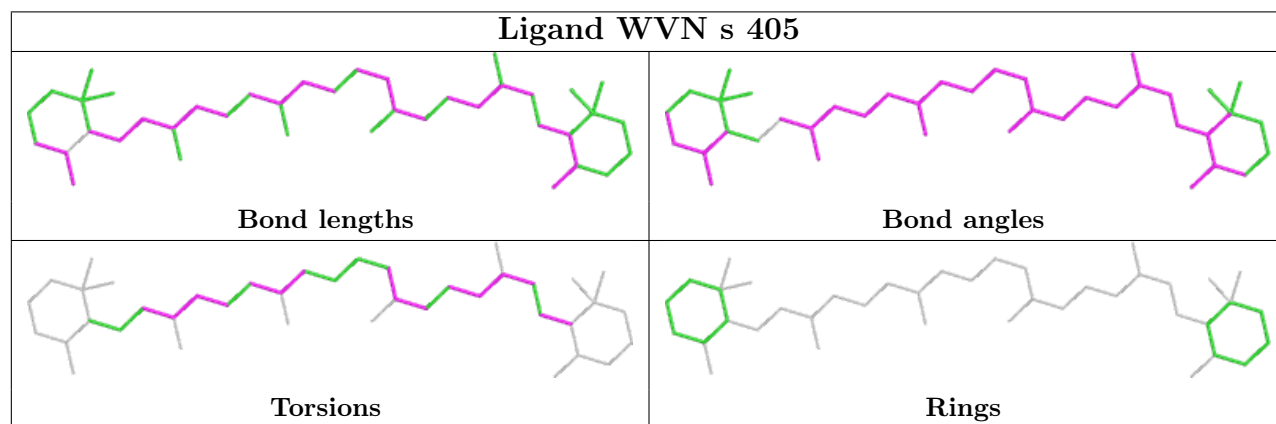




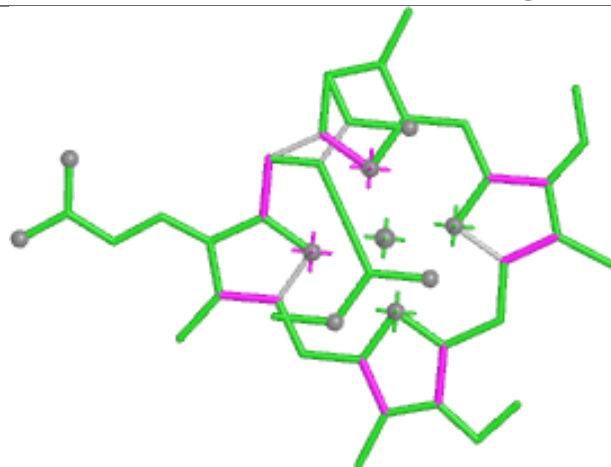
Ligand CLA e 303



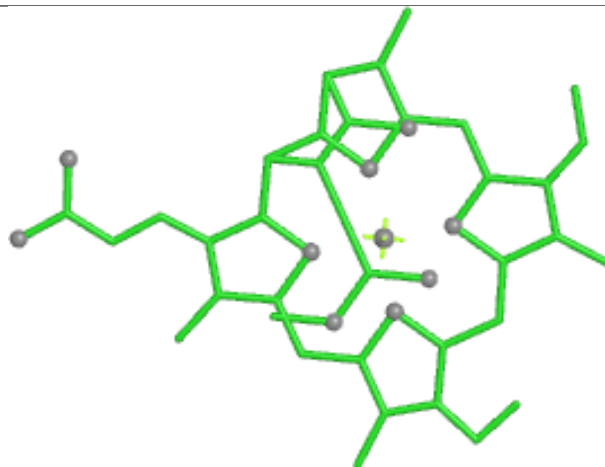
Ligand WVN s 405



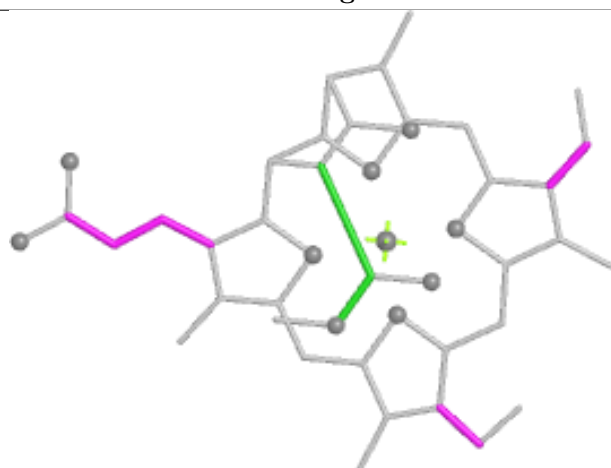
Ligand KC2 k 613



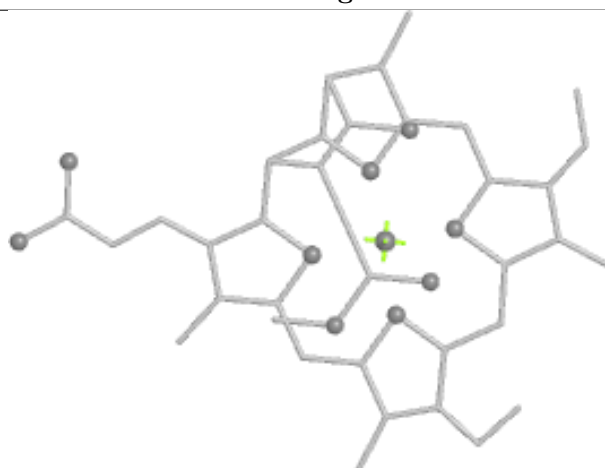
Bond lengths



Bond angles

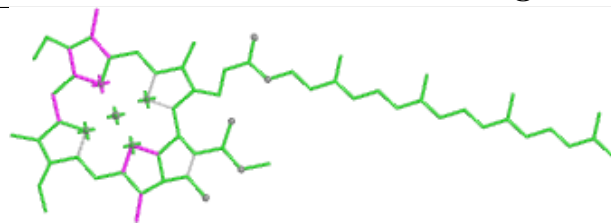


Torsions

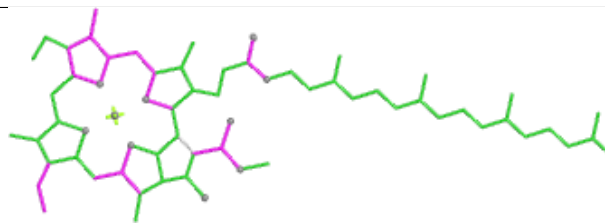


Rings

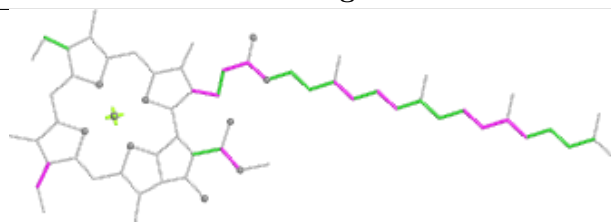
Ligand CLA B 816



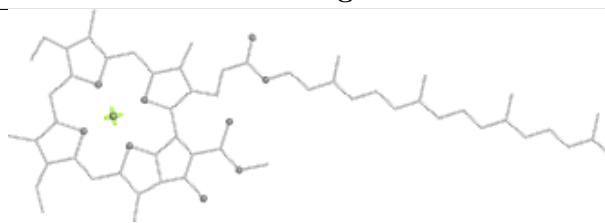
Bond lengths



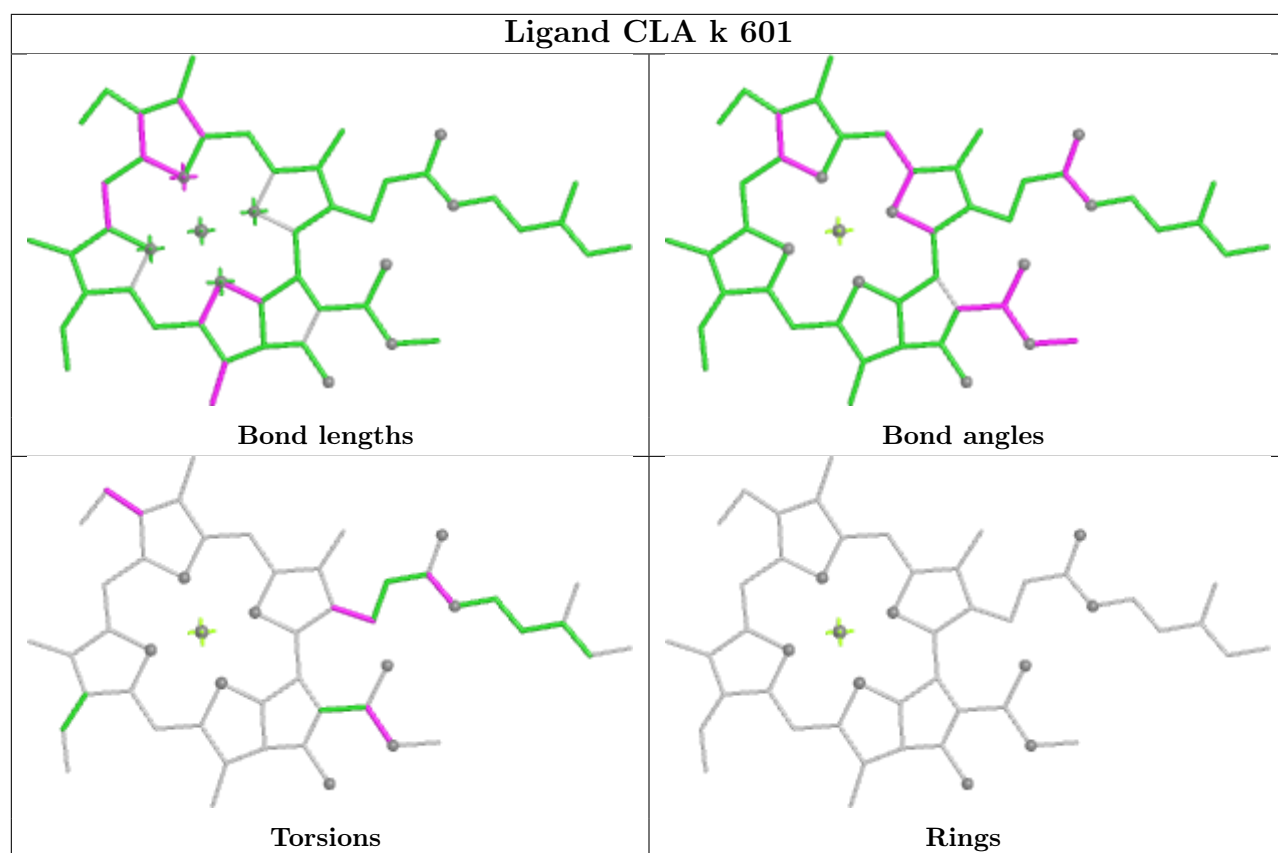
Bond angles

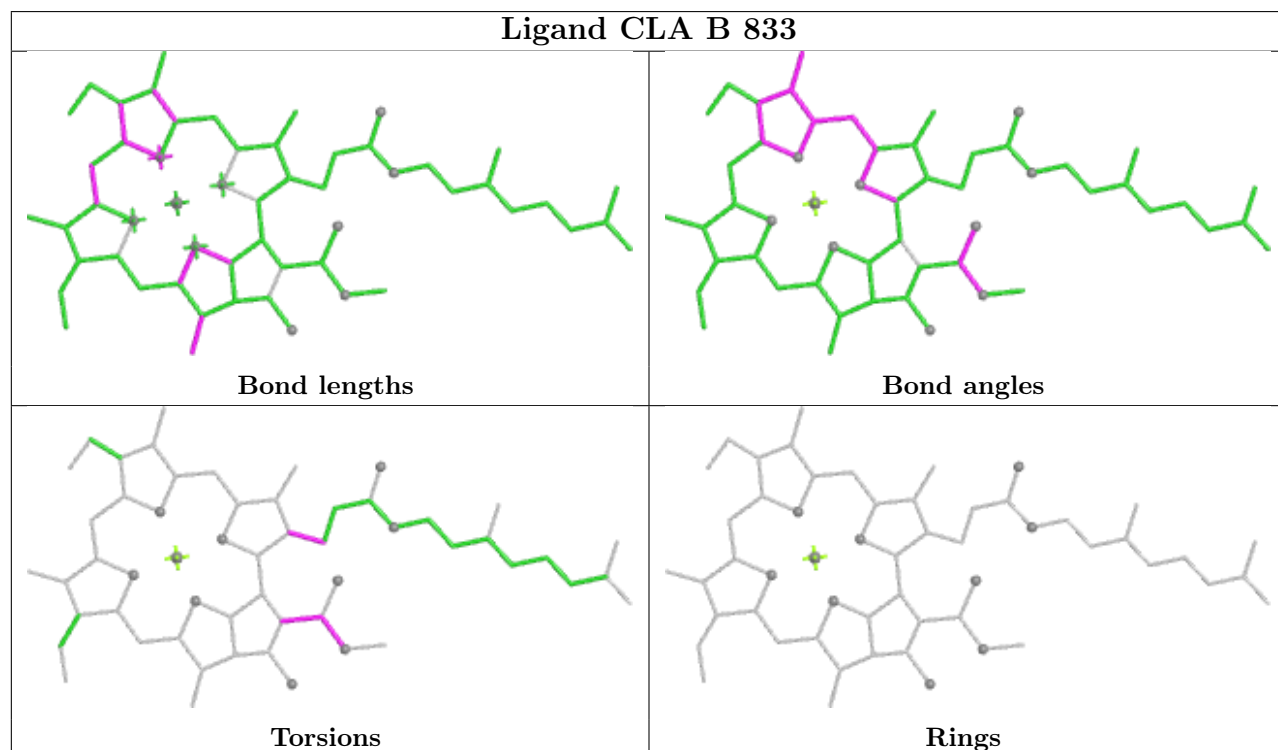
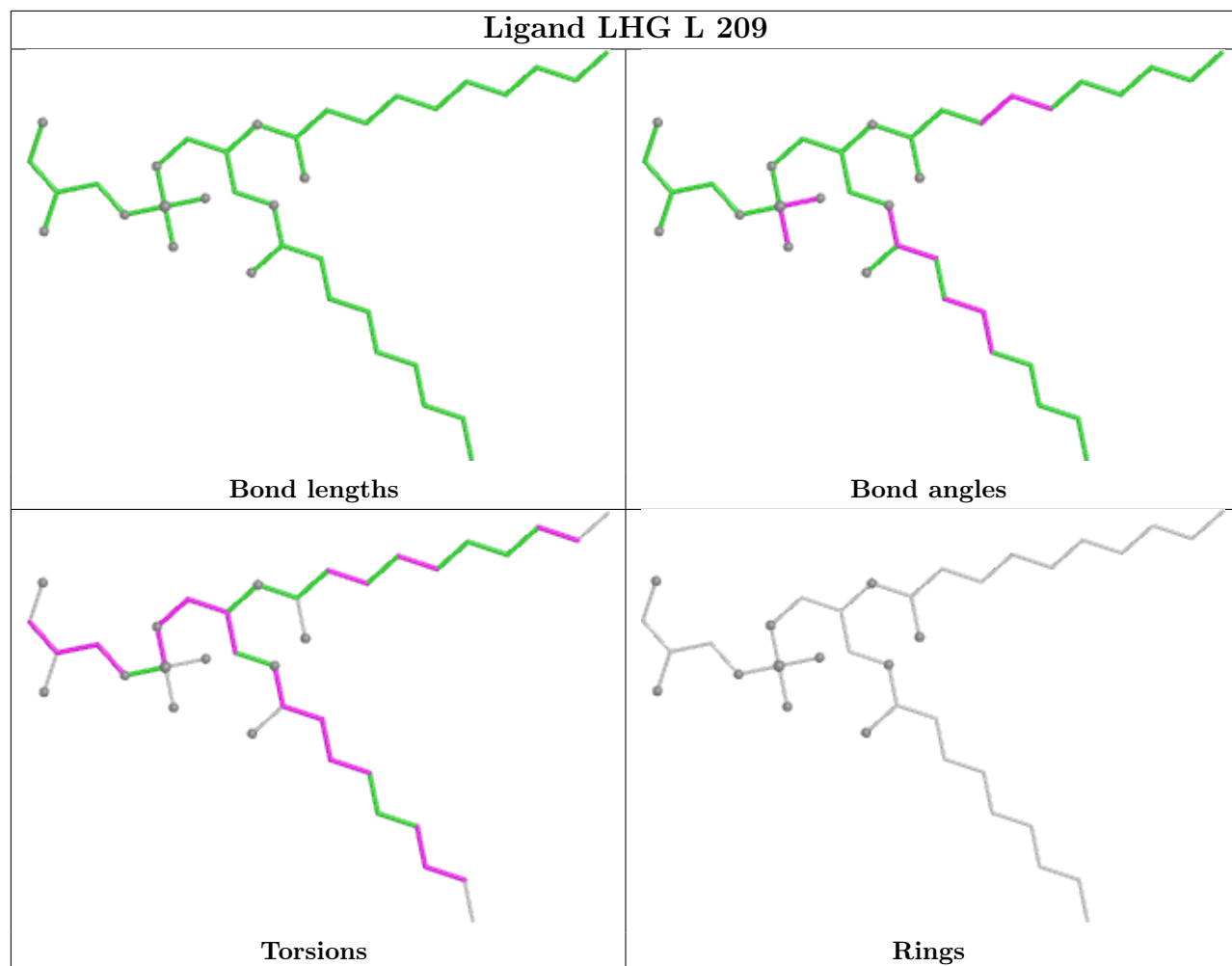


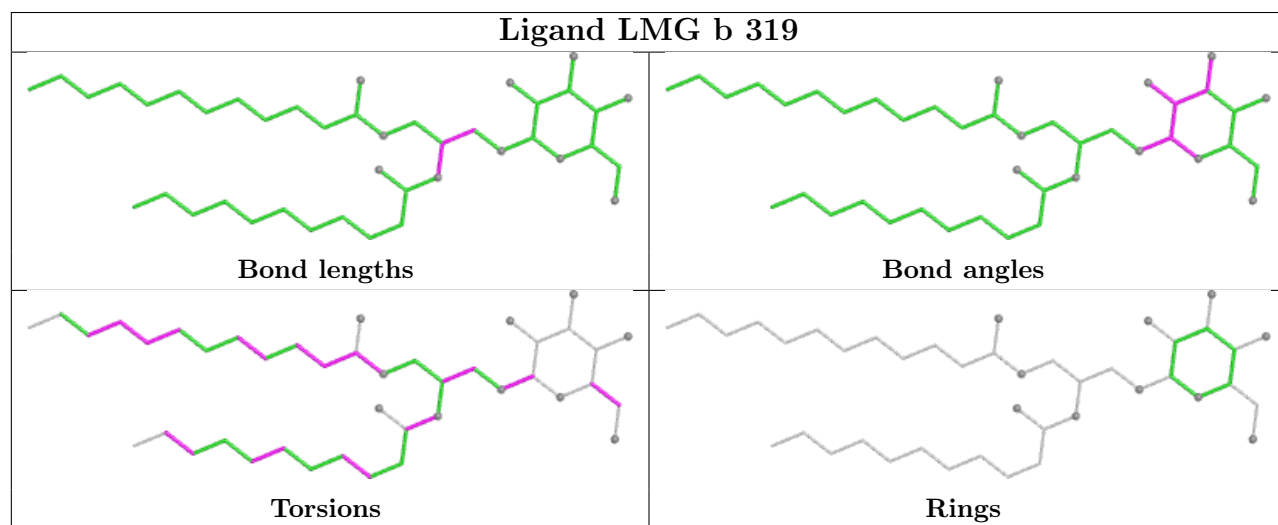
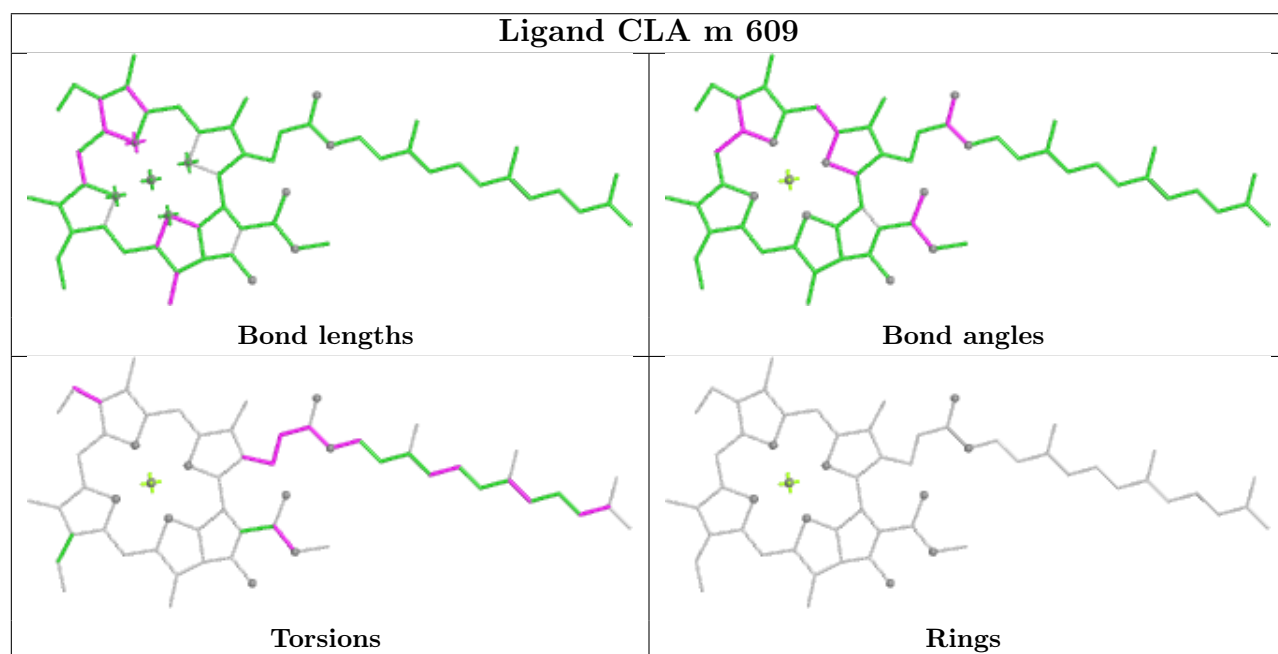
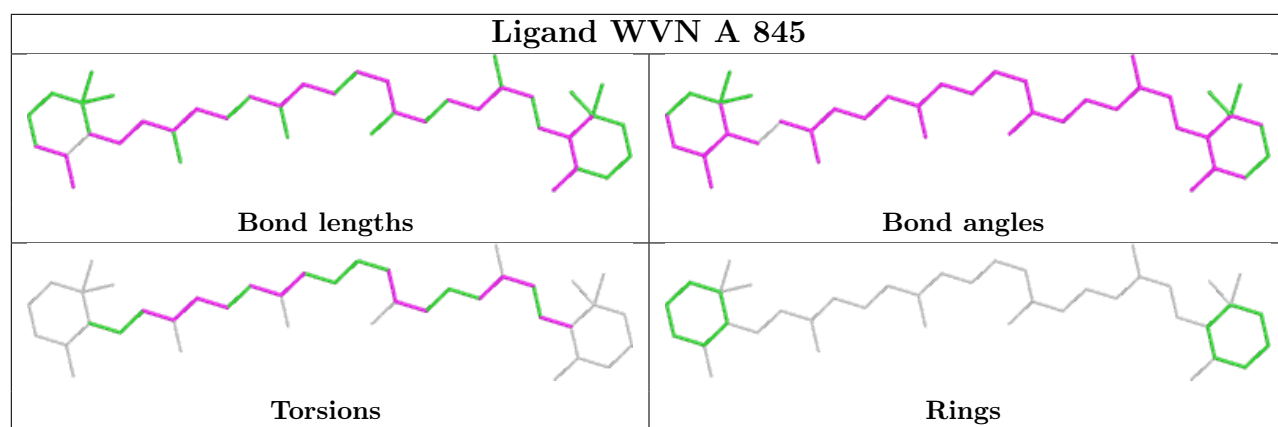
Torsions



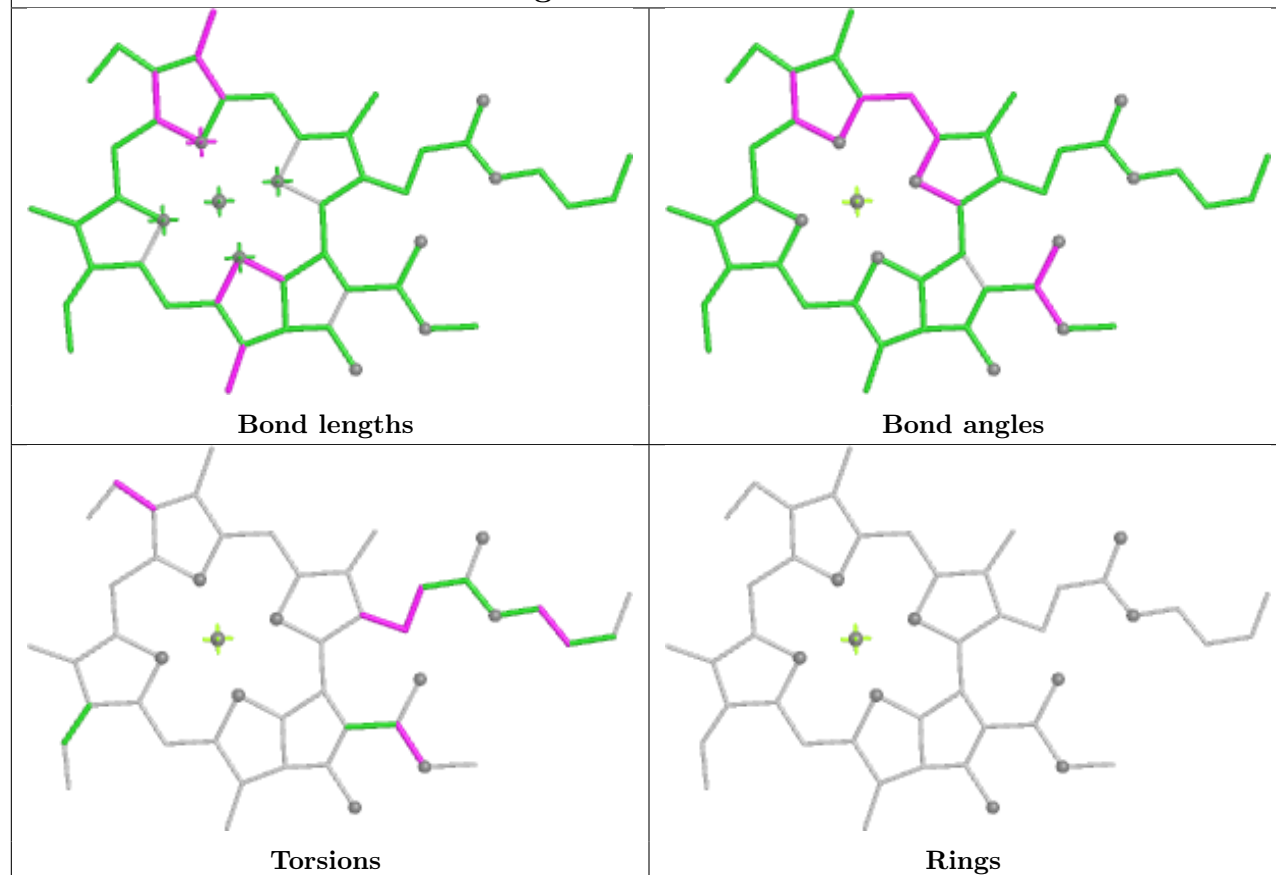
Rings



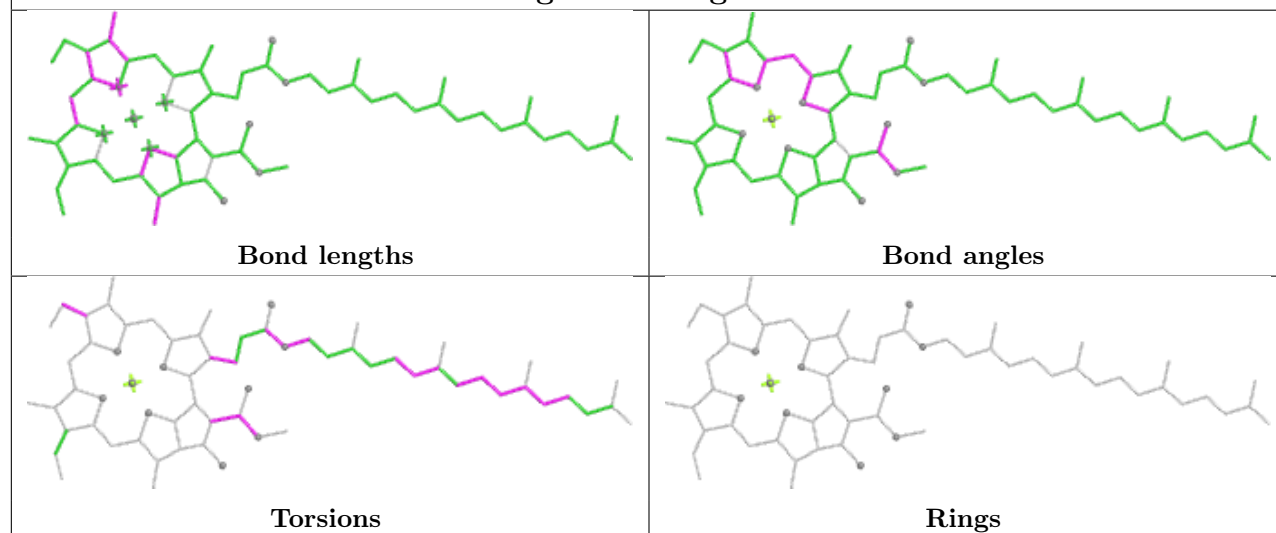




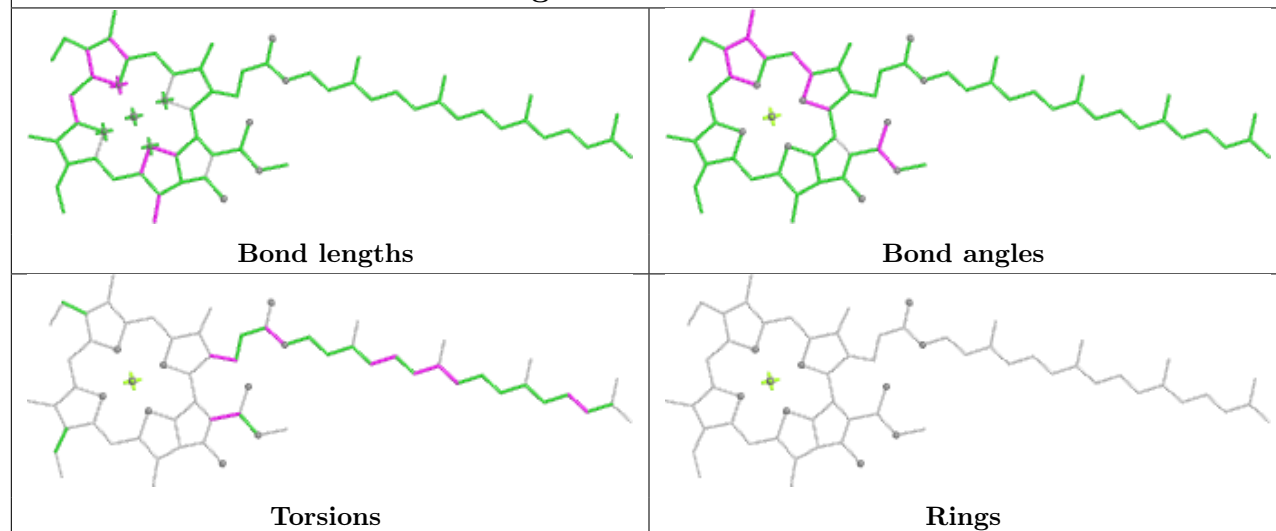
Ligand CLA L 202



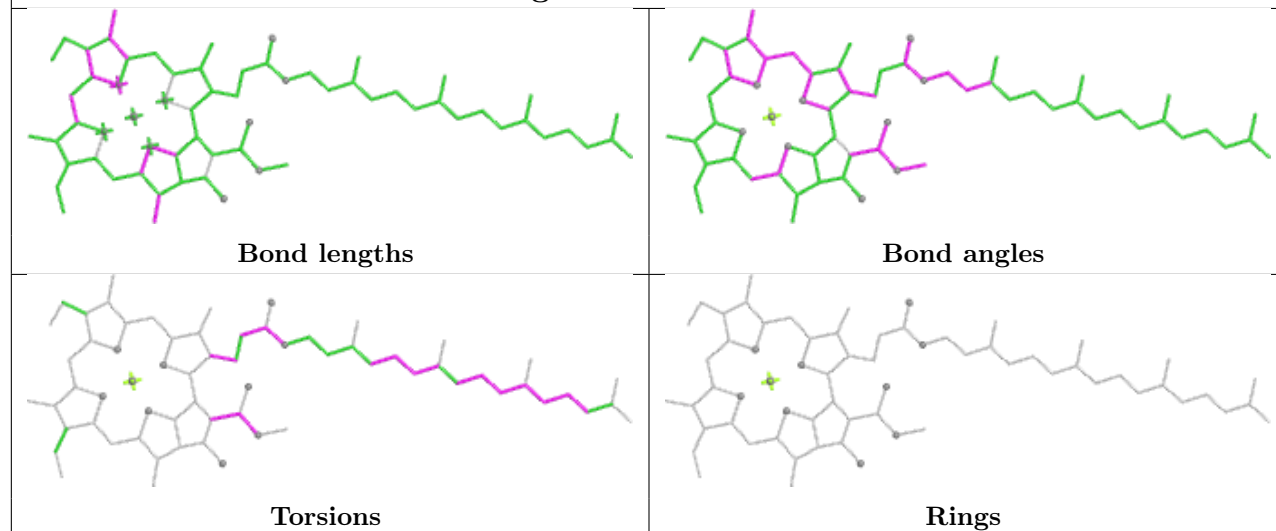
Ligand CLA g 304



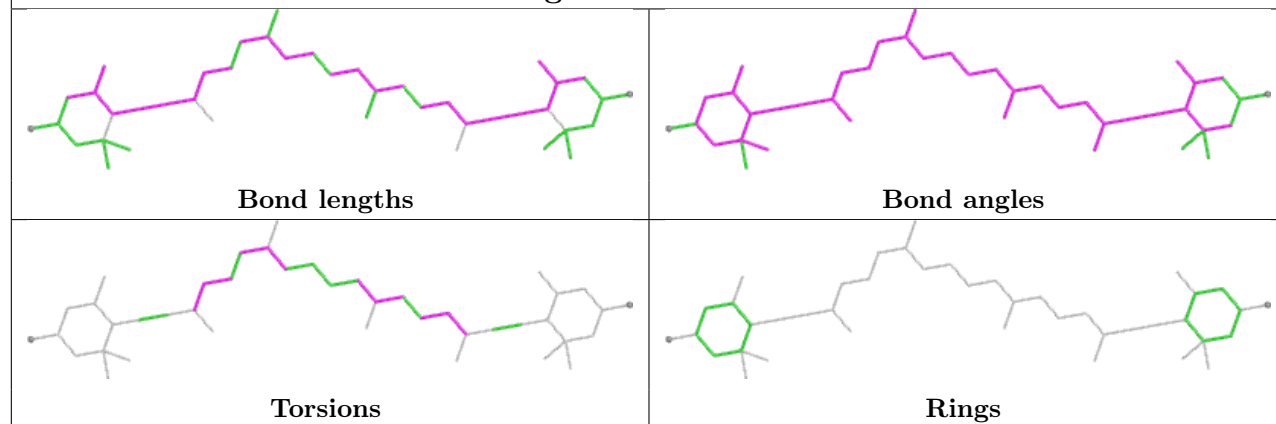
Ligand CLA A 805

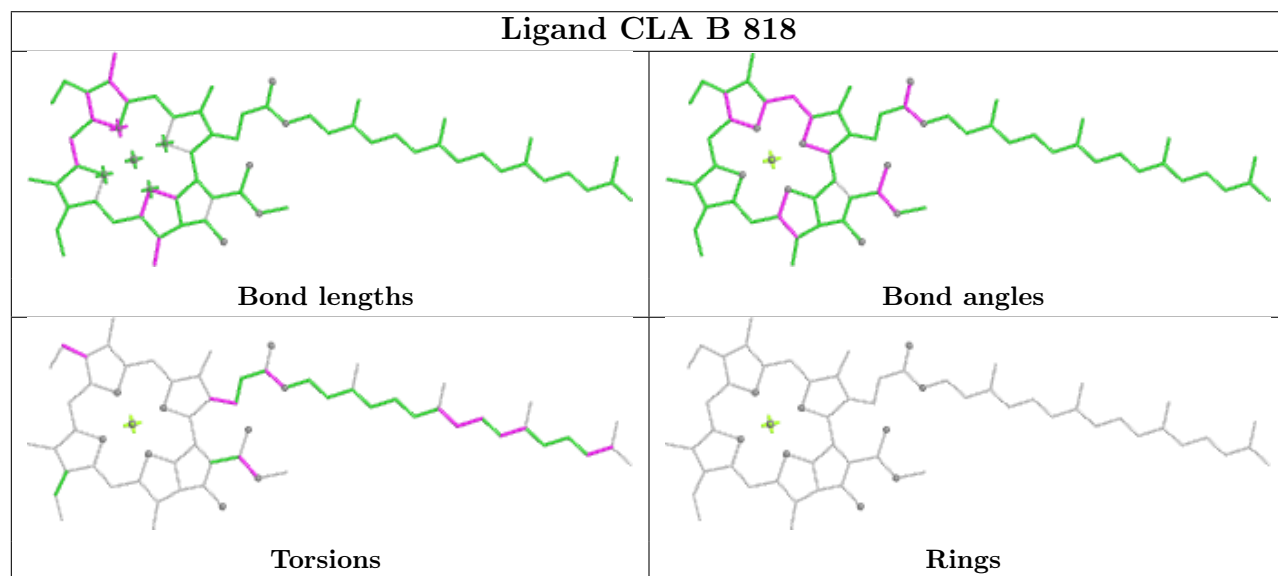
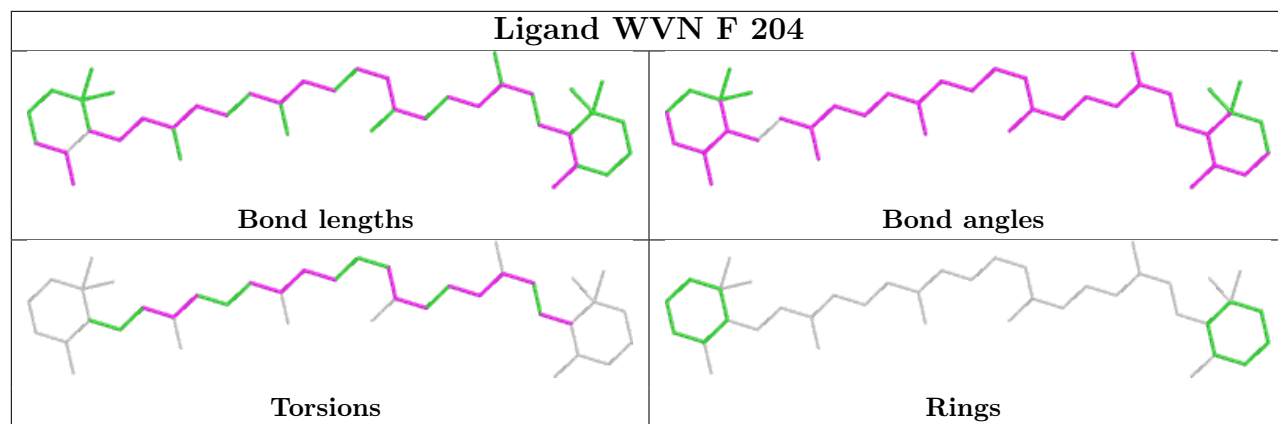


Ligand CLA A 819

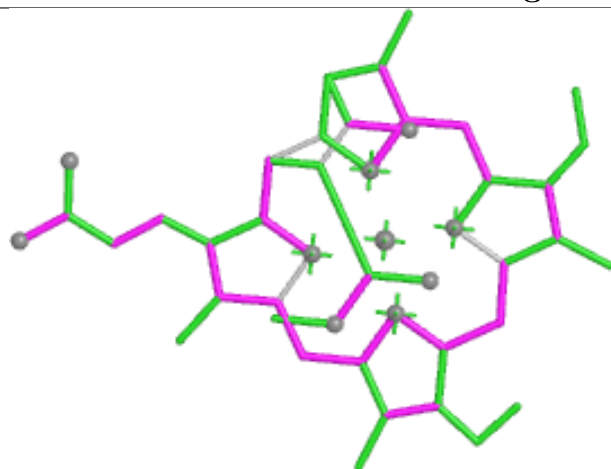


Ligand II0 m 616

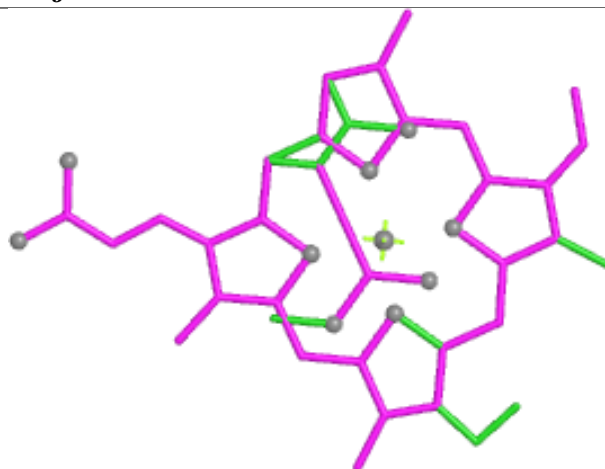




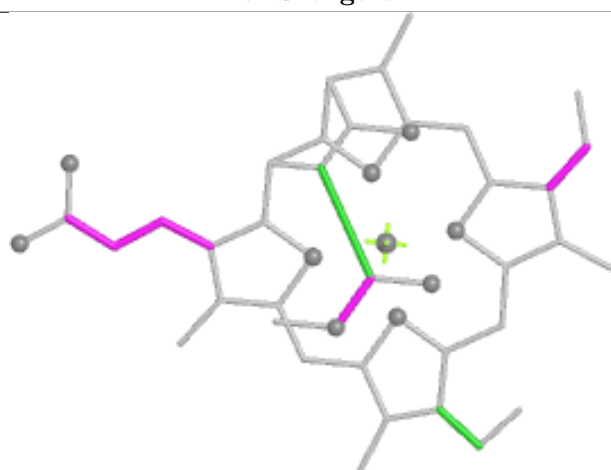
Ligand KC2 j 312



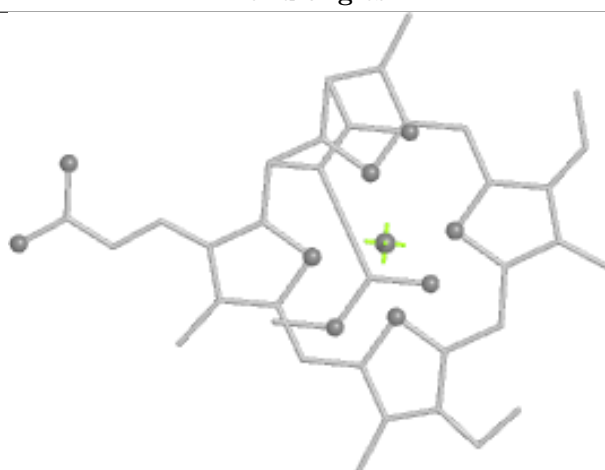
Bond lengths



Bond angles

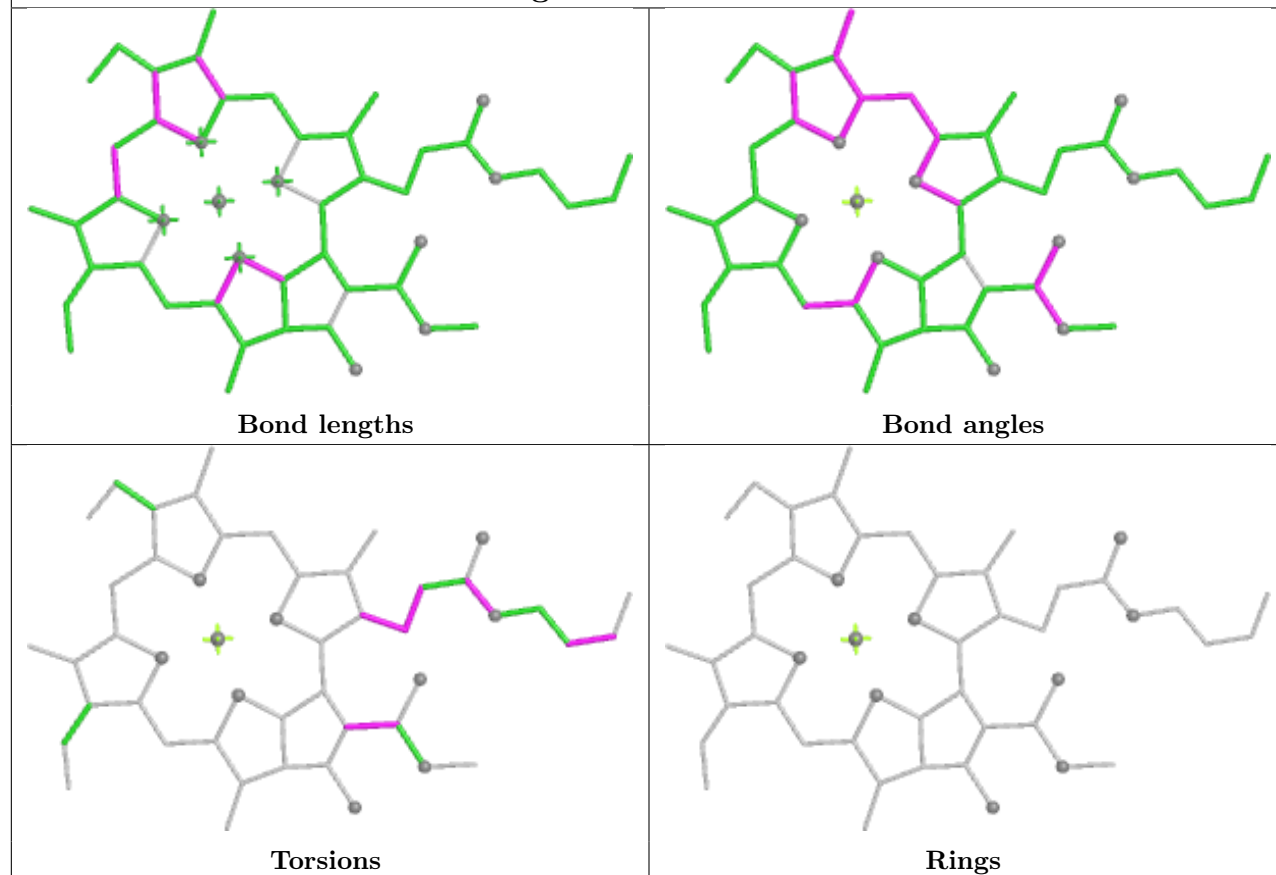


Torsions

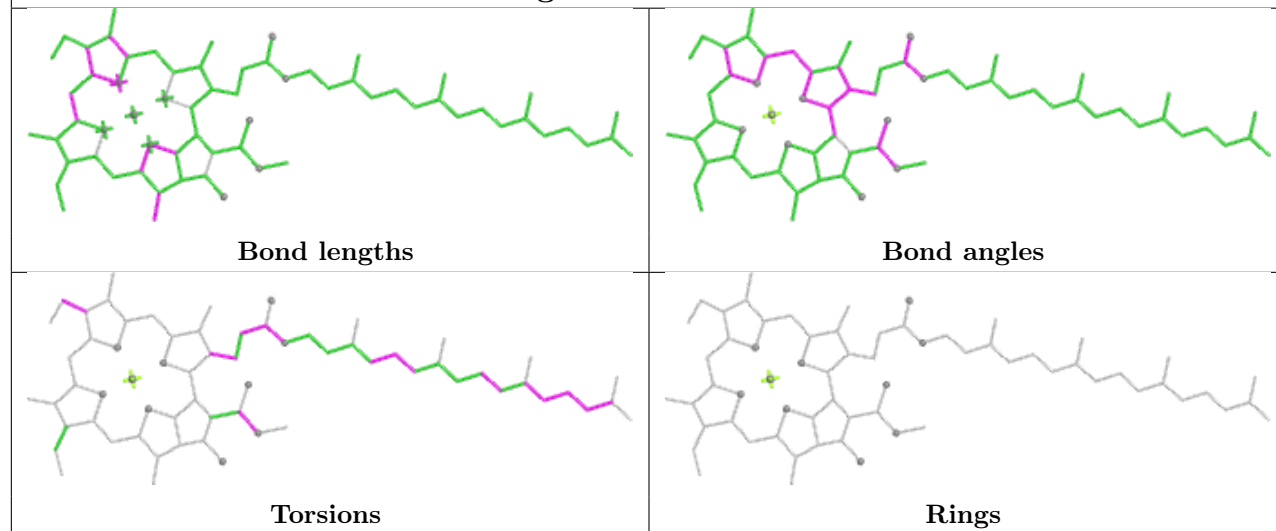


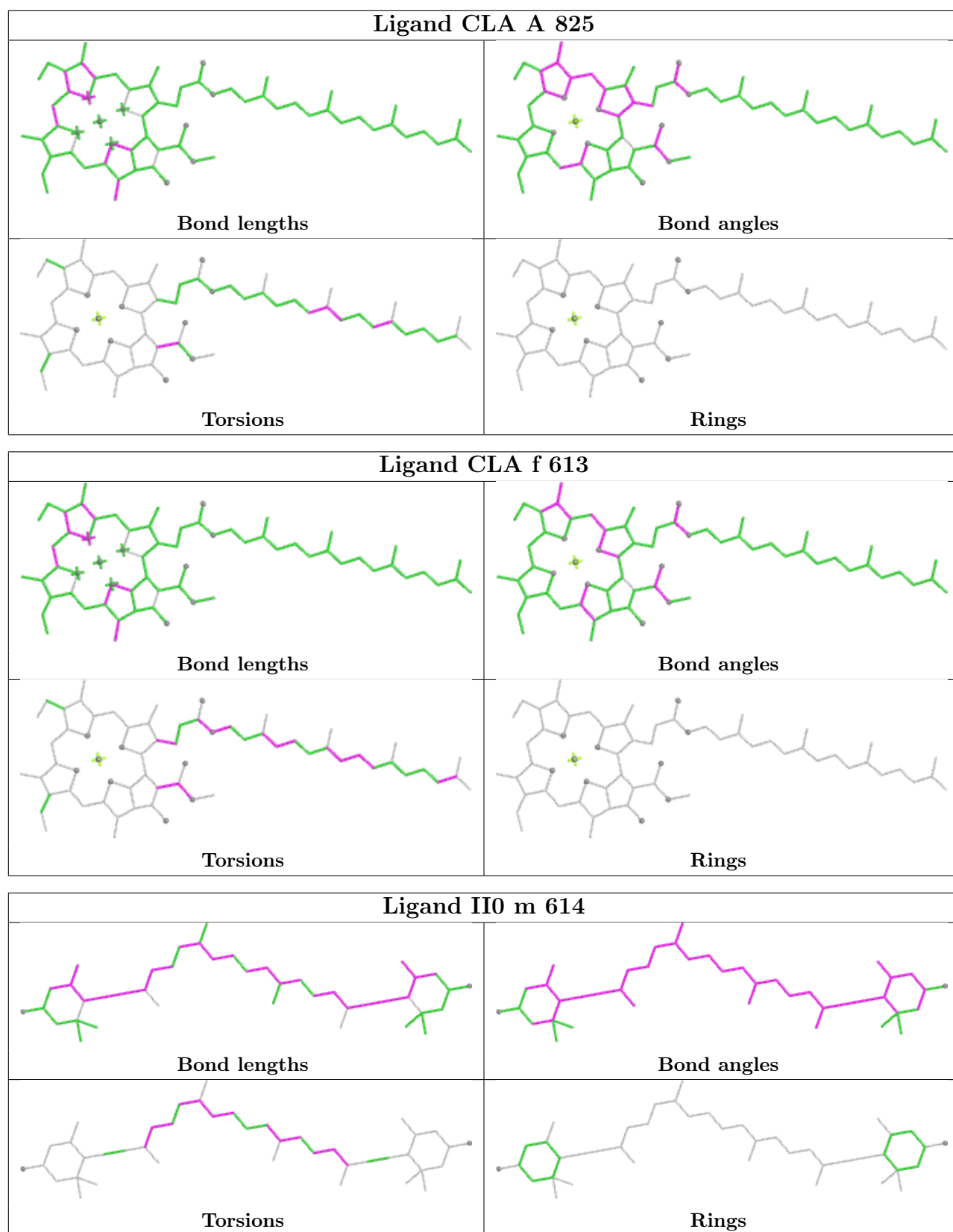
Rings

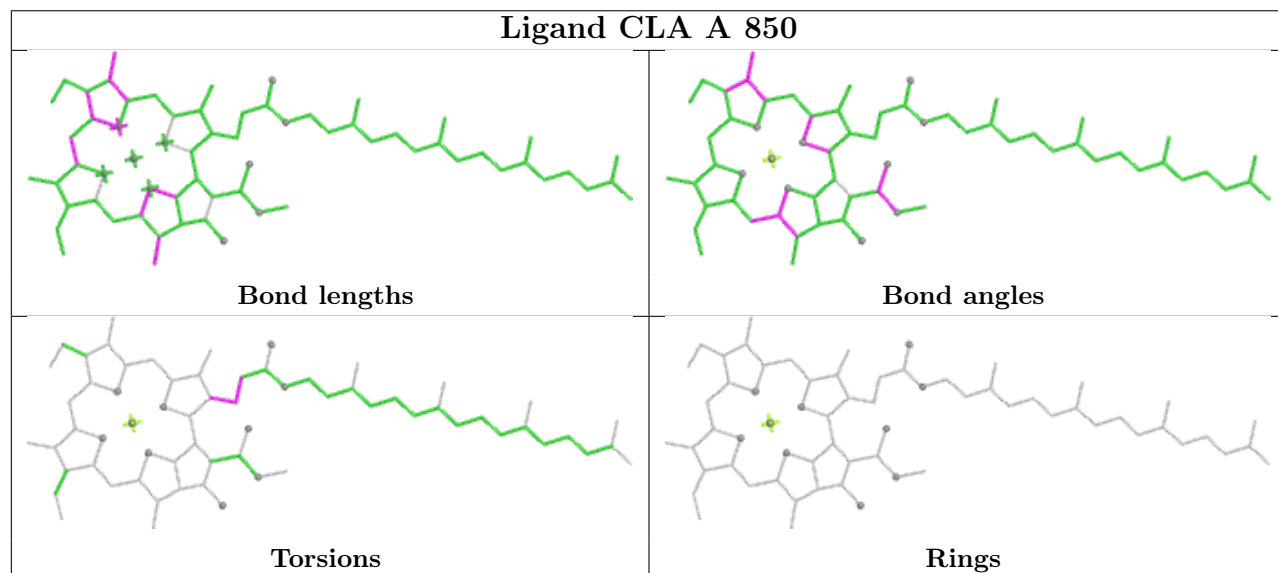
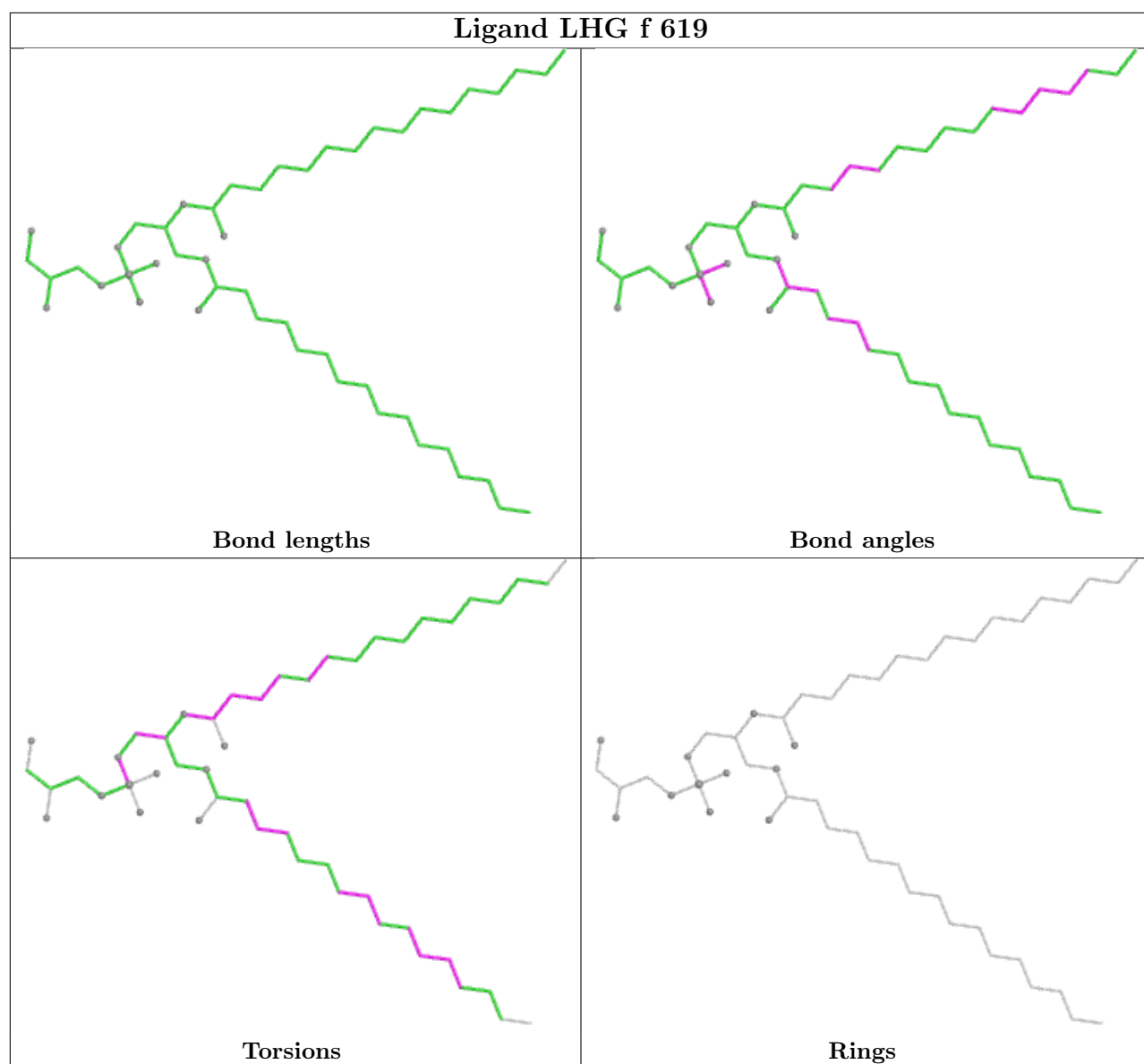
Ligand CLA A 821

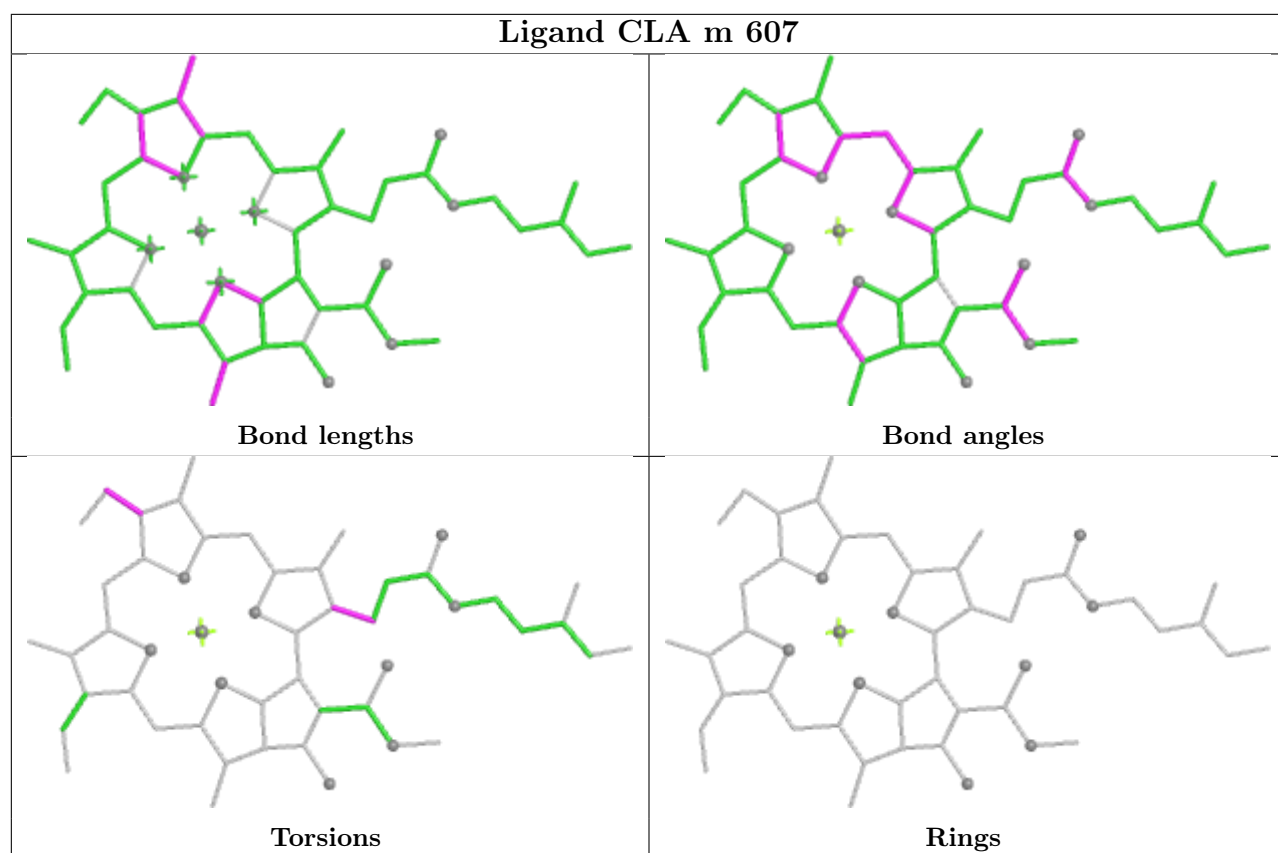


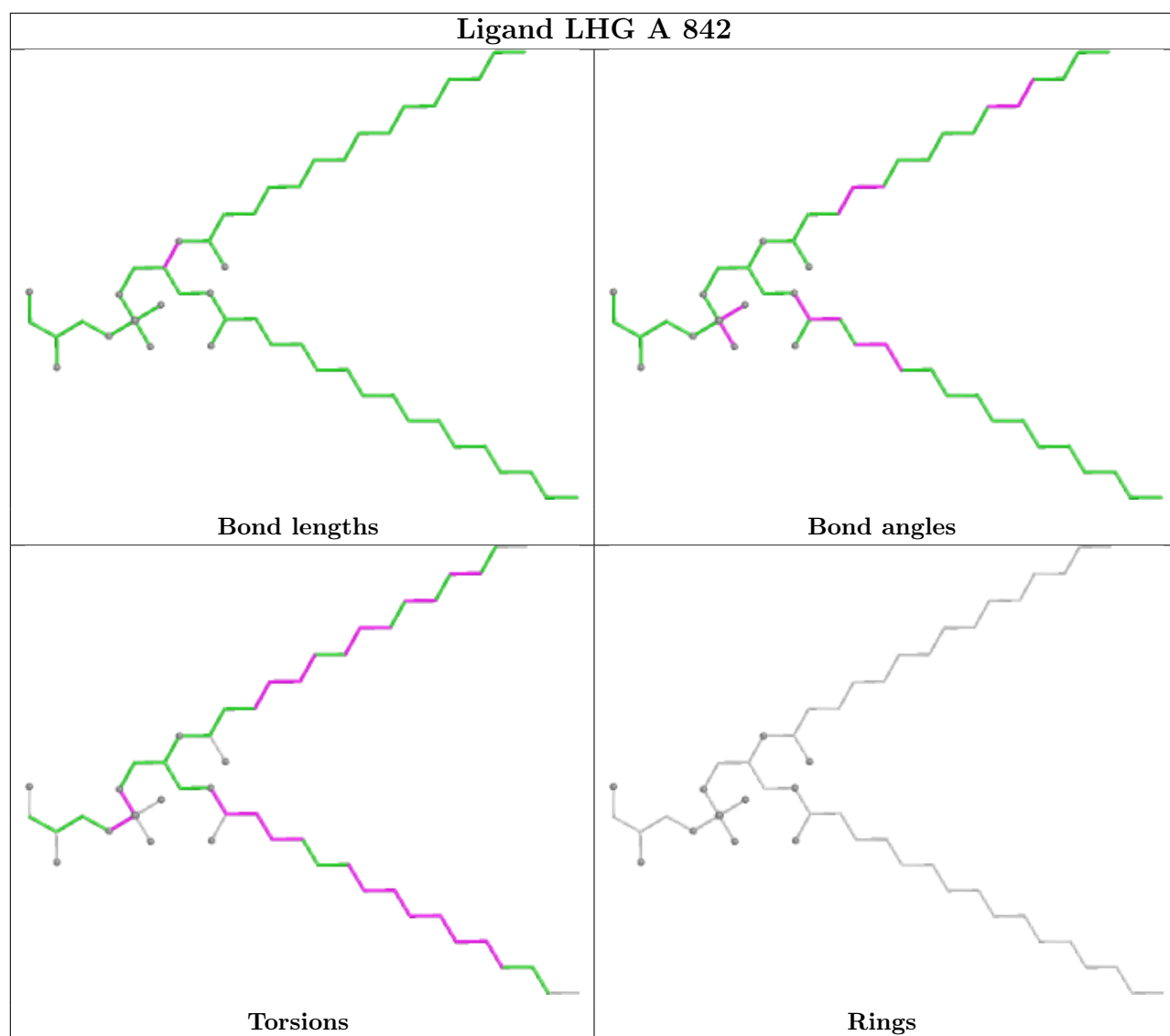
Ligand CLA e 311

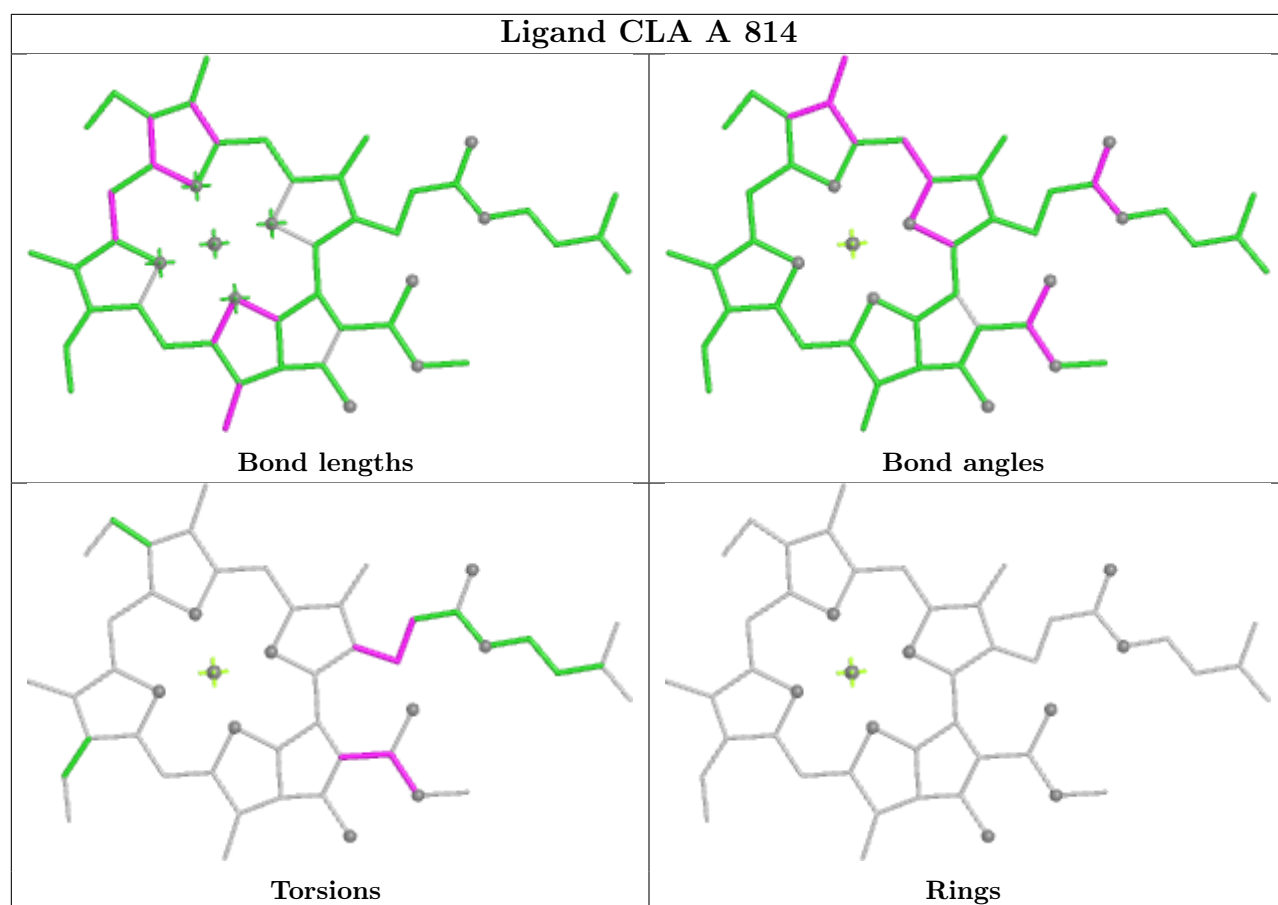




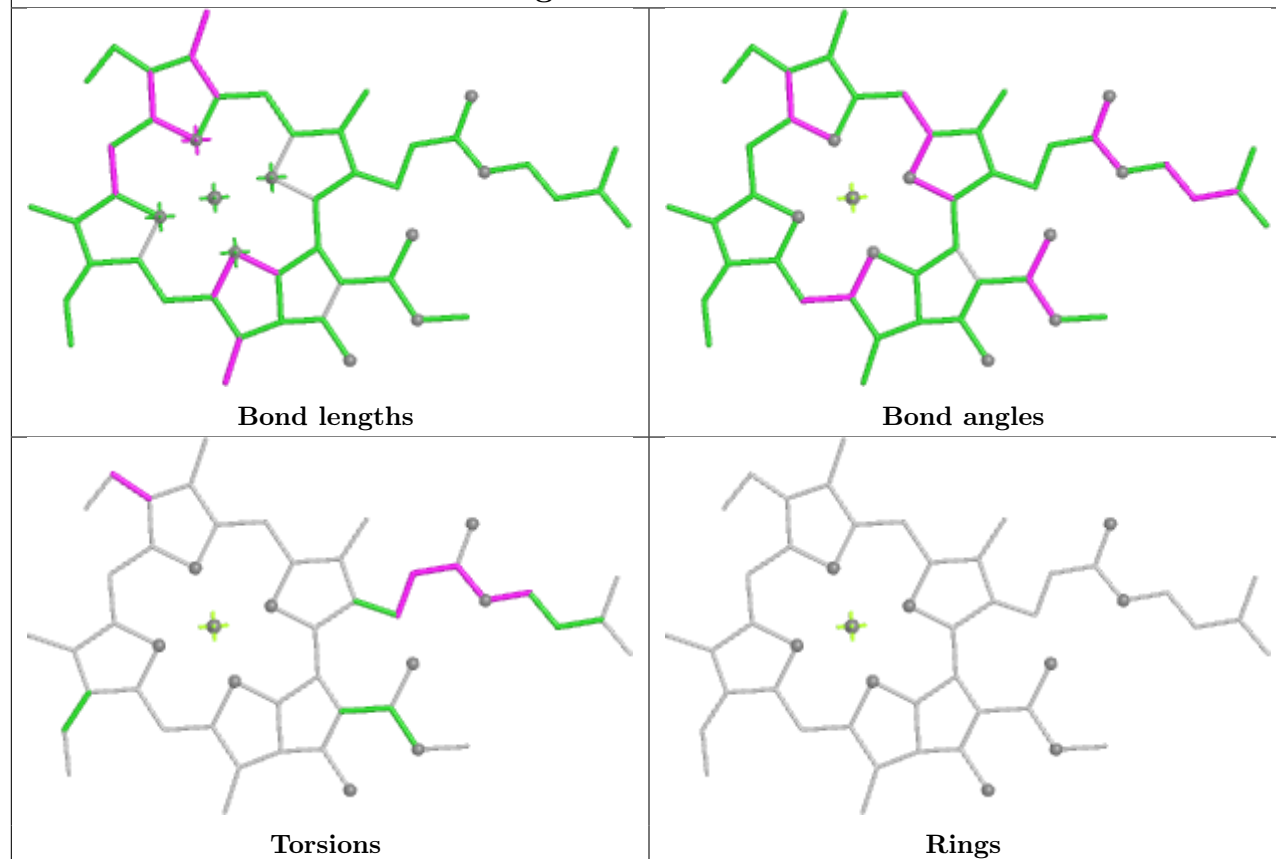




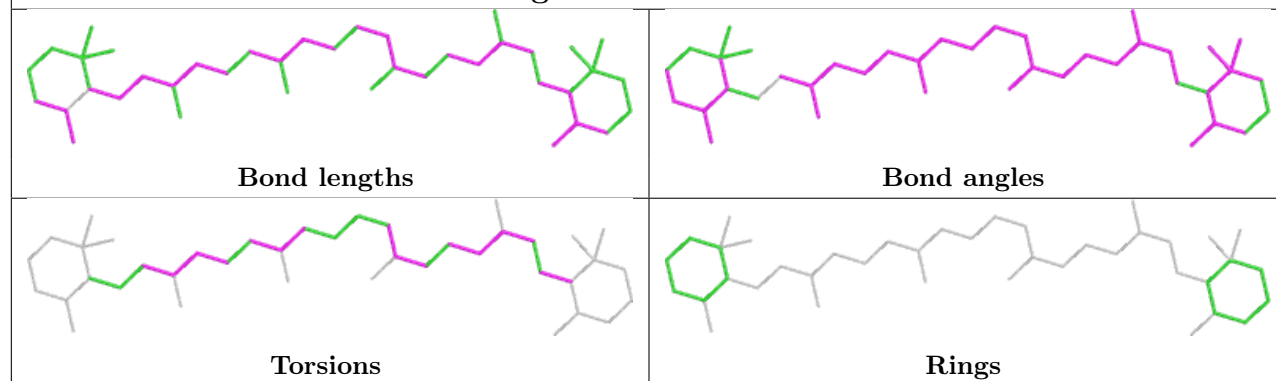




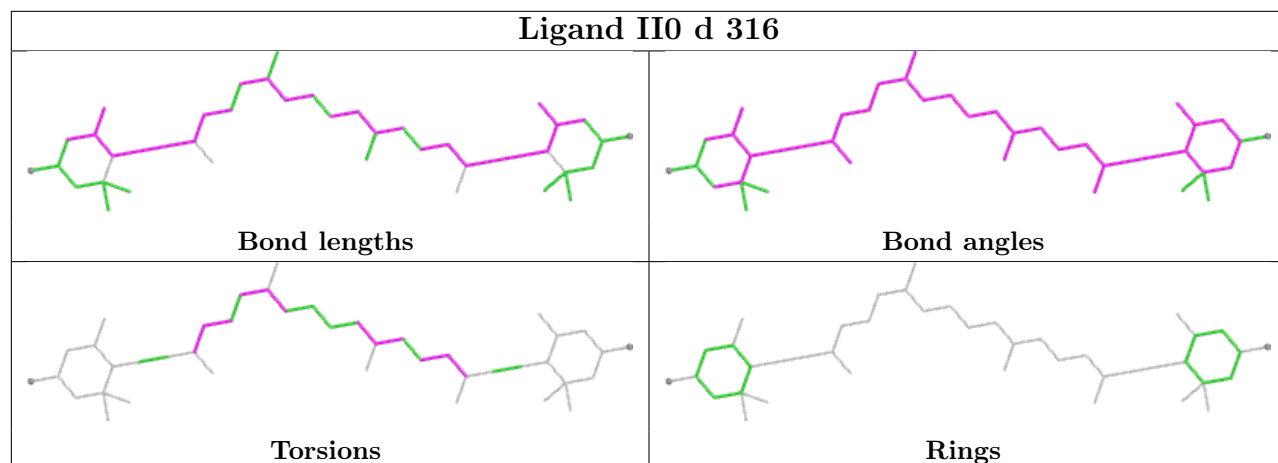
Ligand CLA h 303



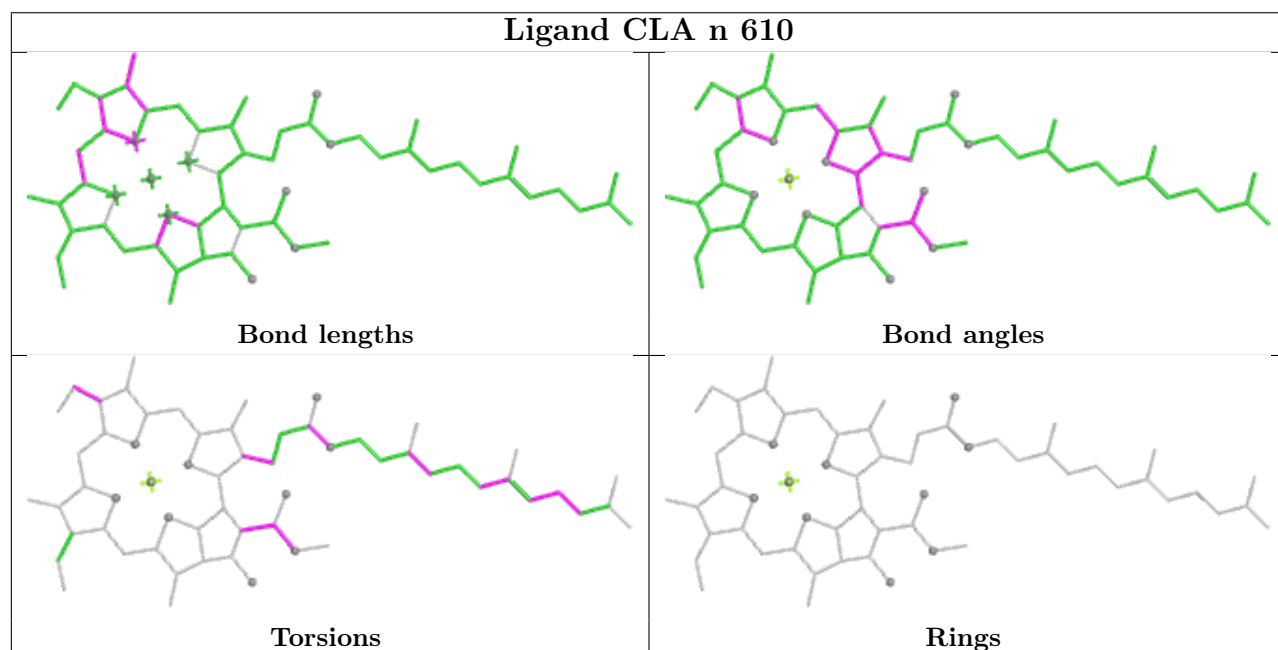
Ligand WVN i 315



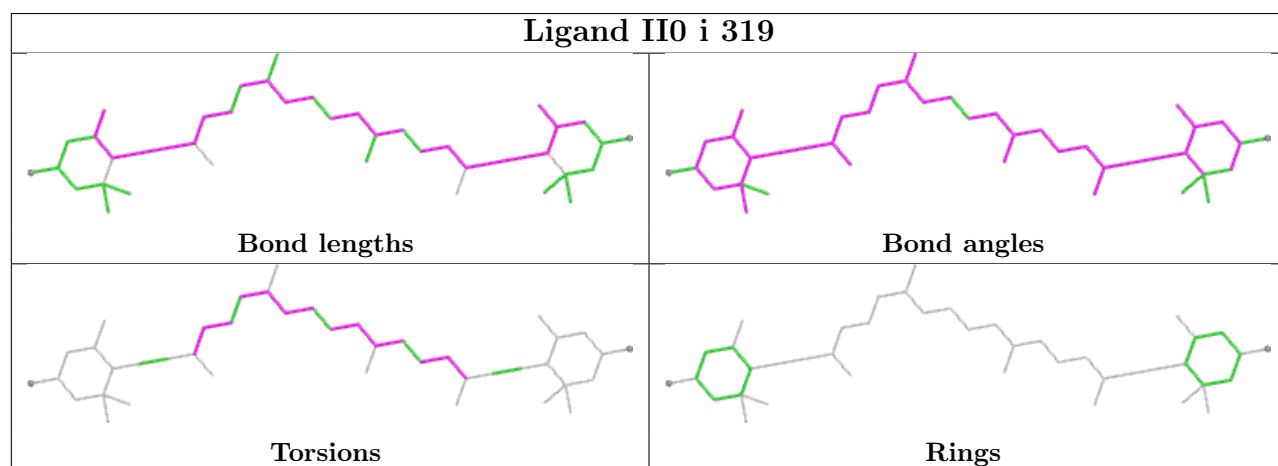
Ligand II0 d 316

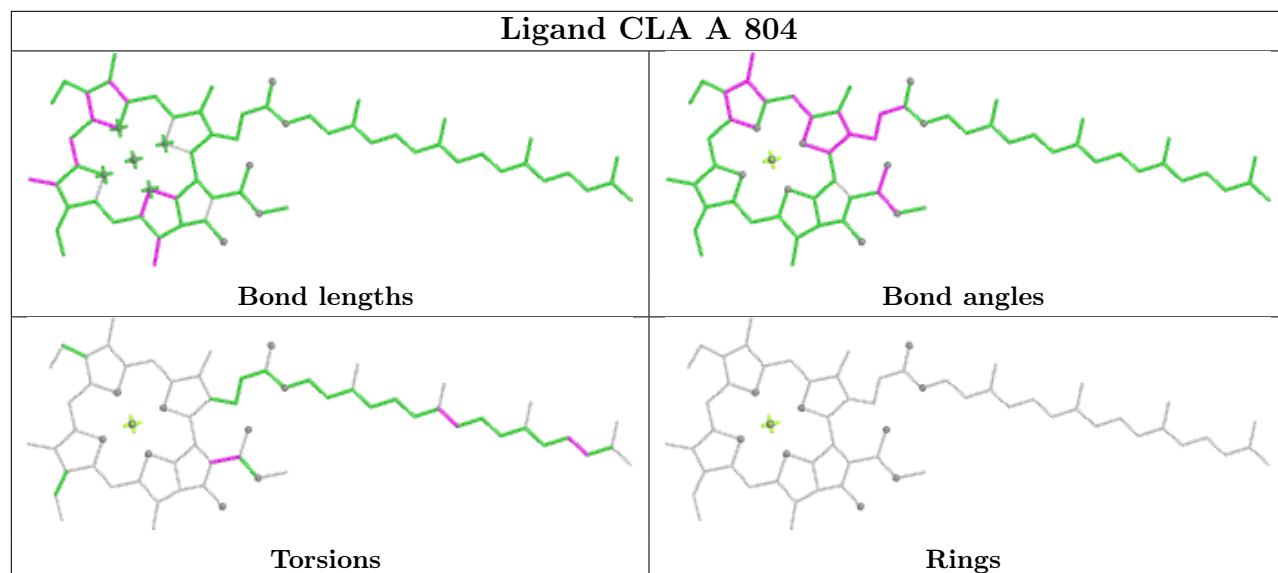
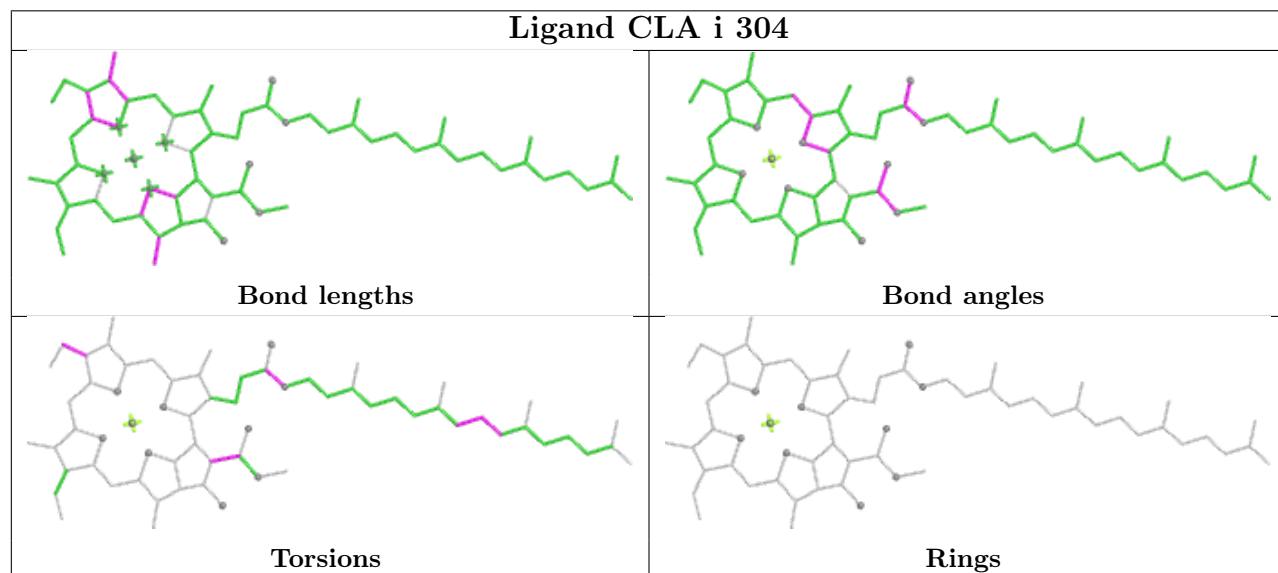
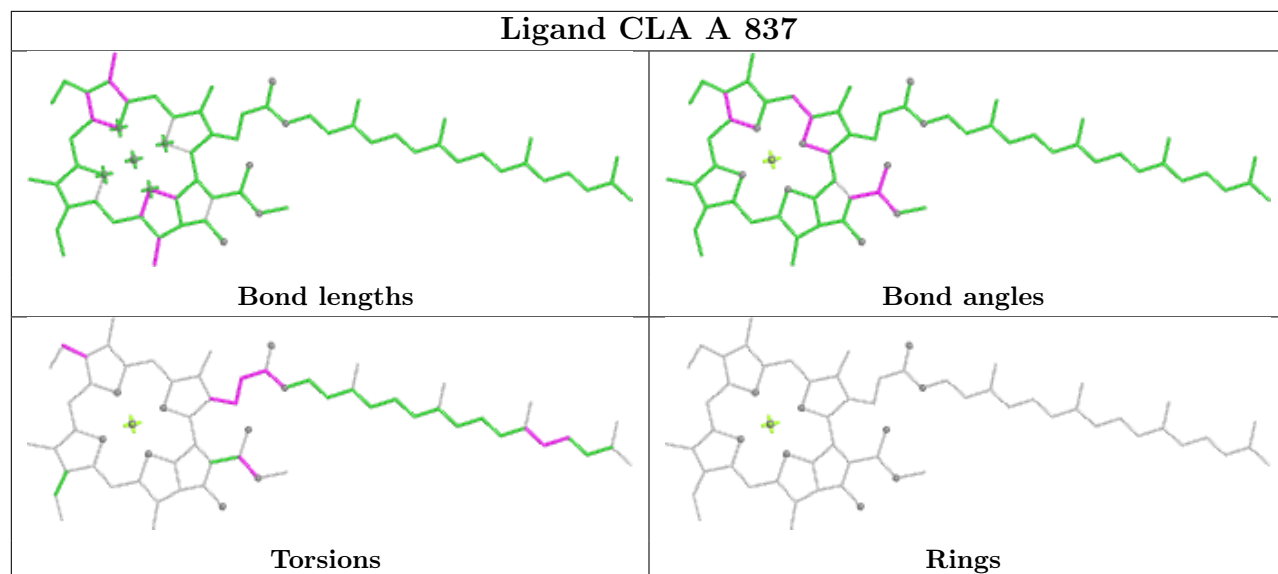


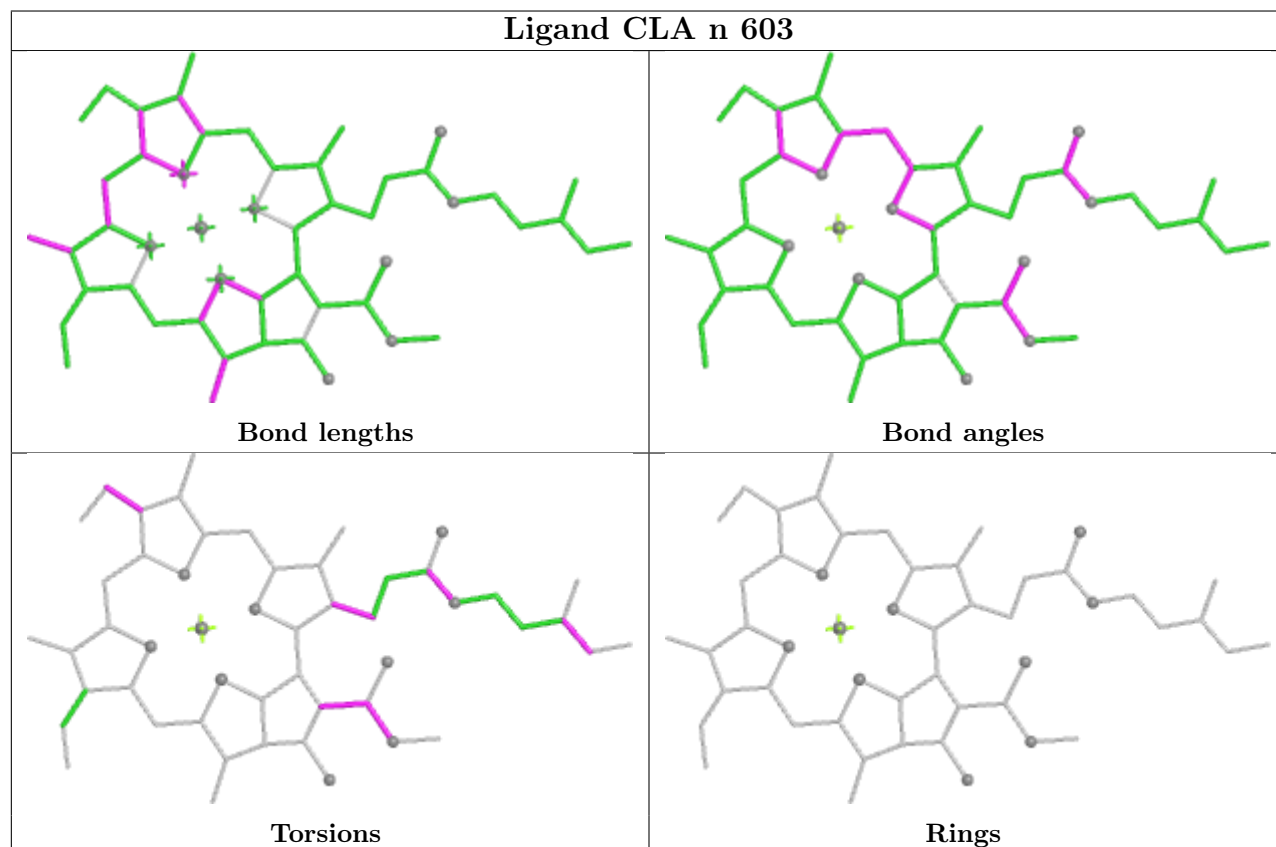
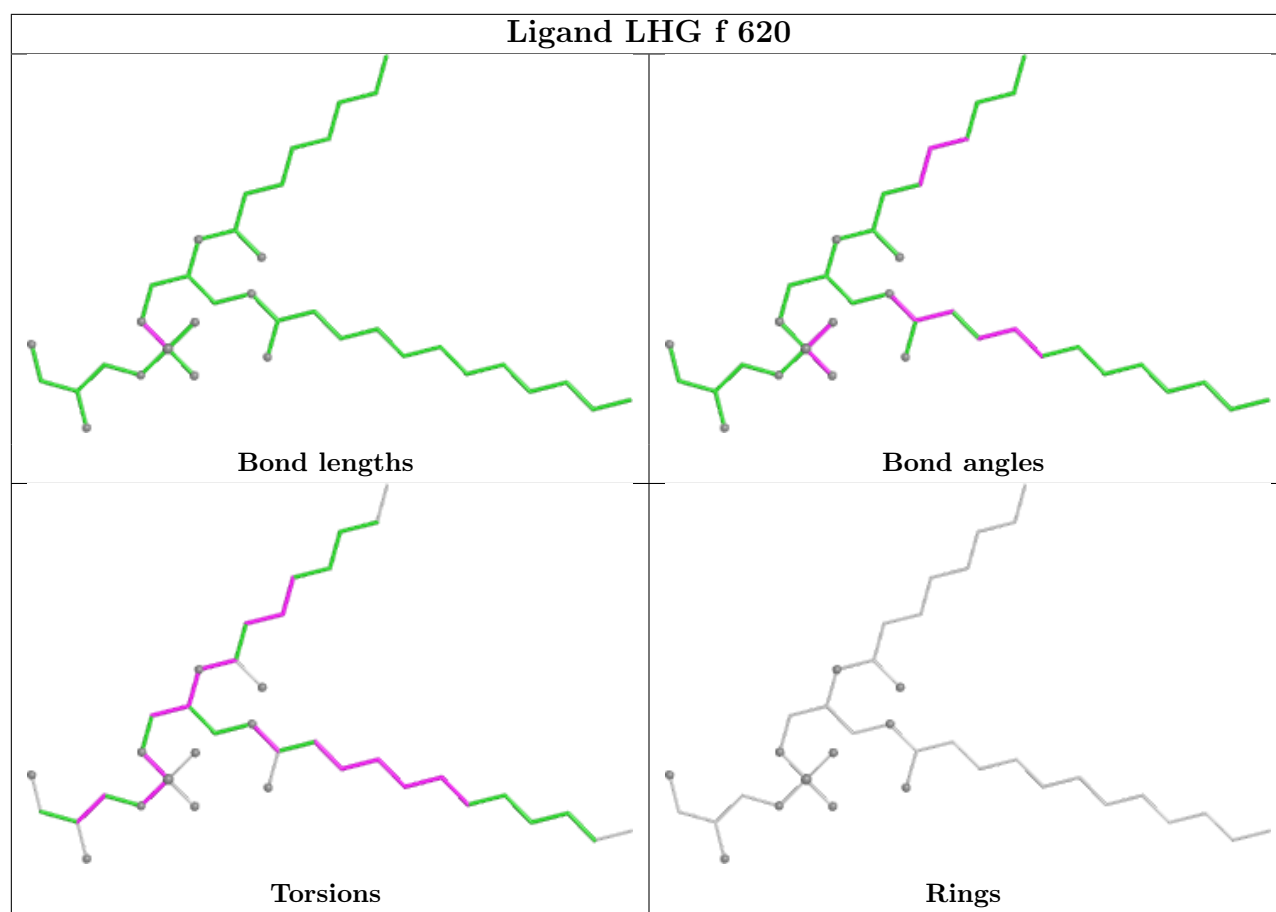
Ligand CLA n 610



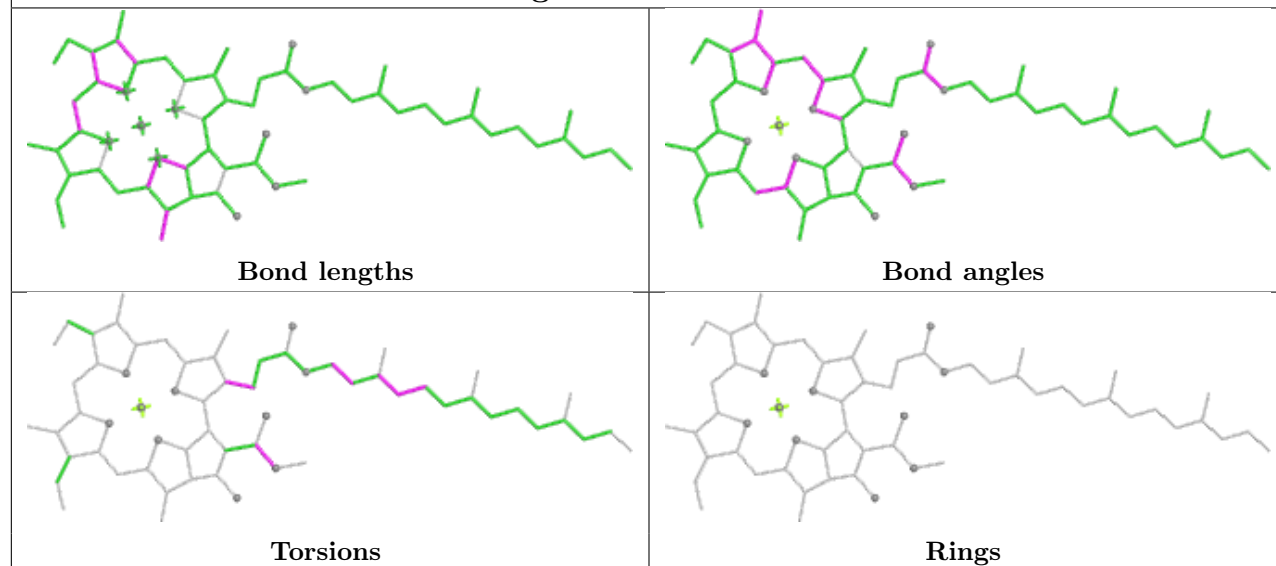
Ligand II0 i 319



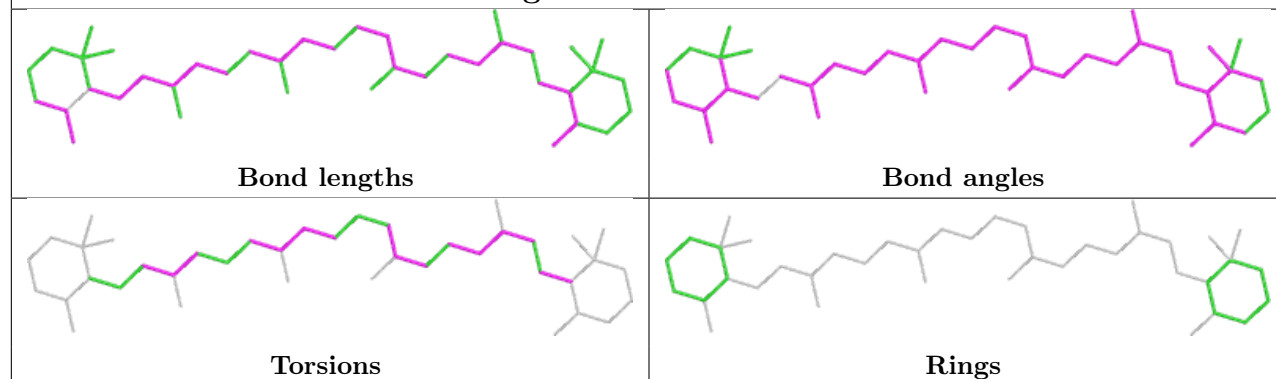




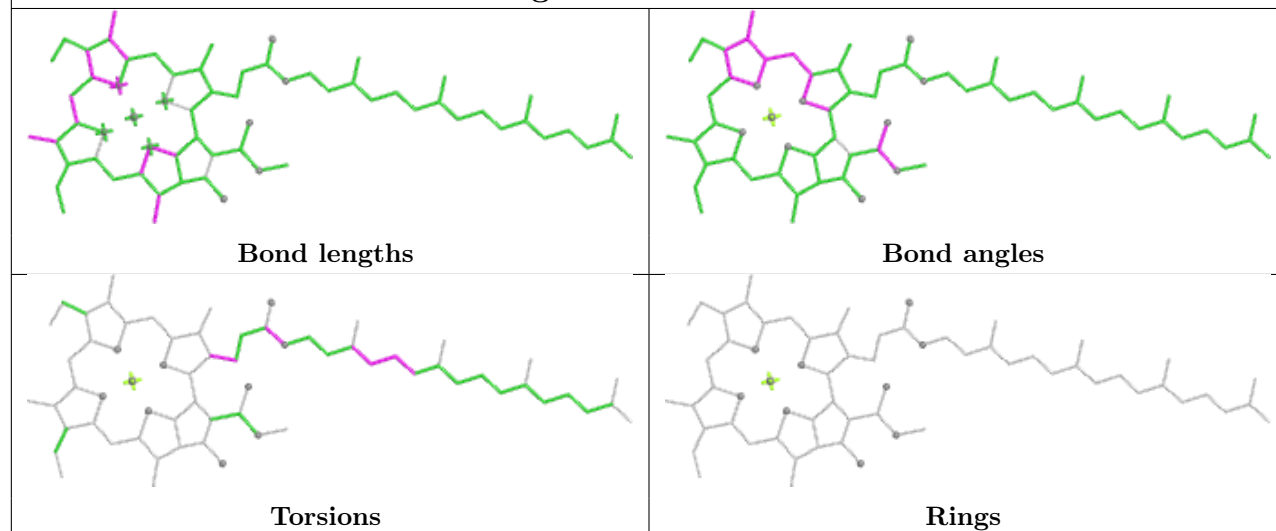
Ligand CLA A 827



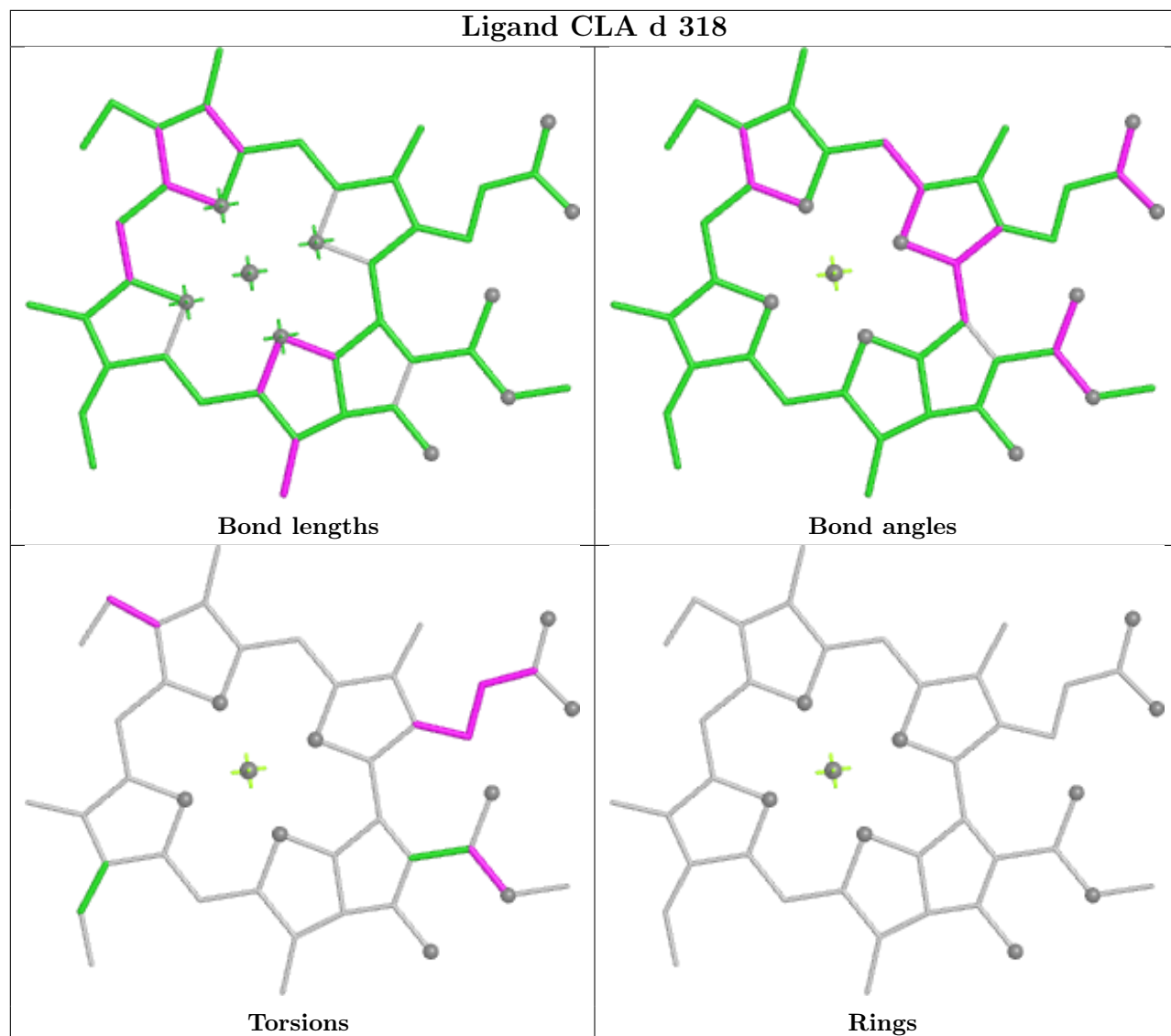
Ligand WVN R 202



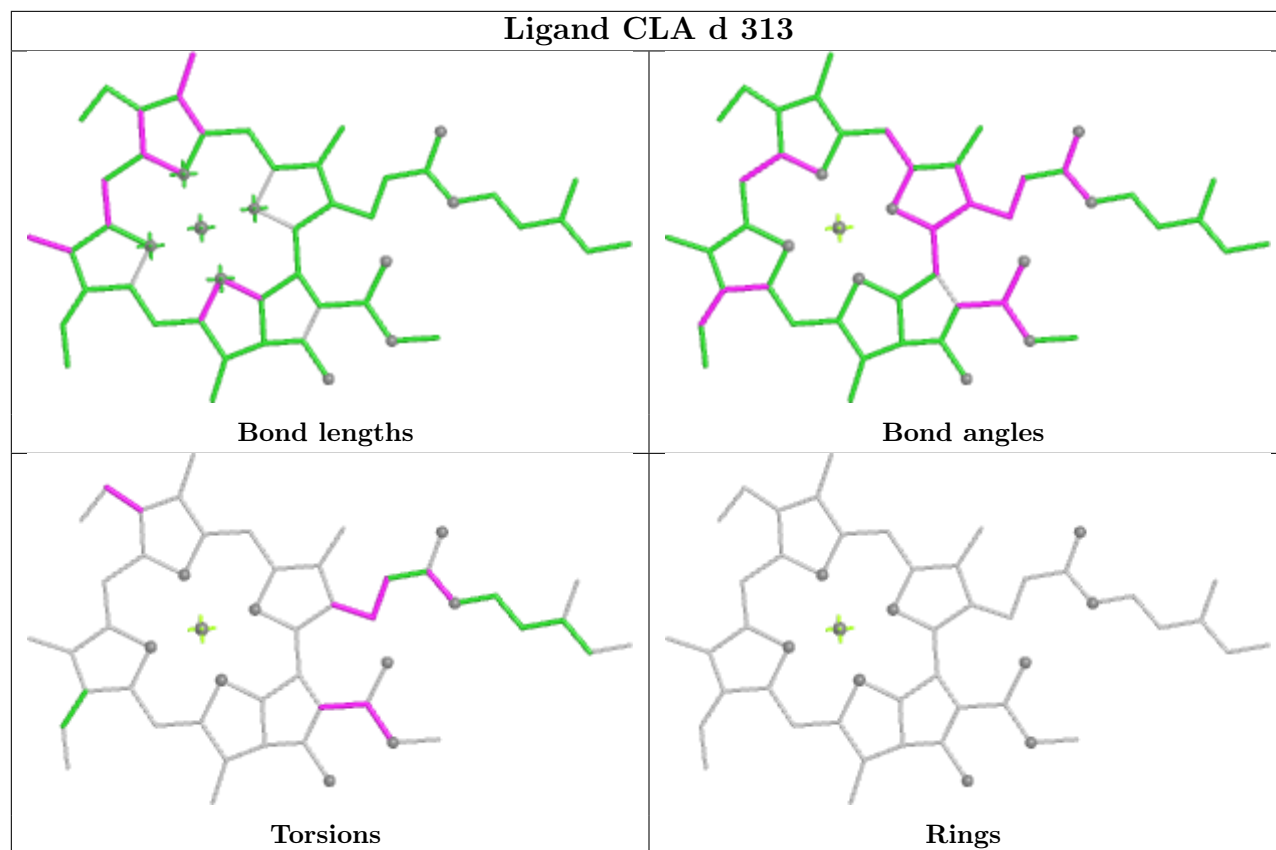
Ligand CLA A 820



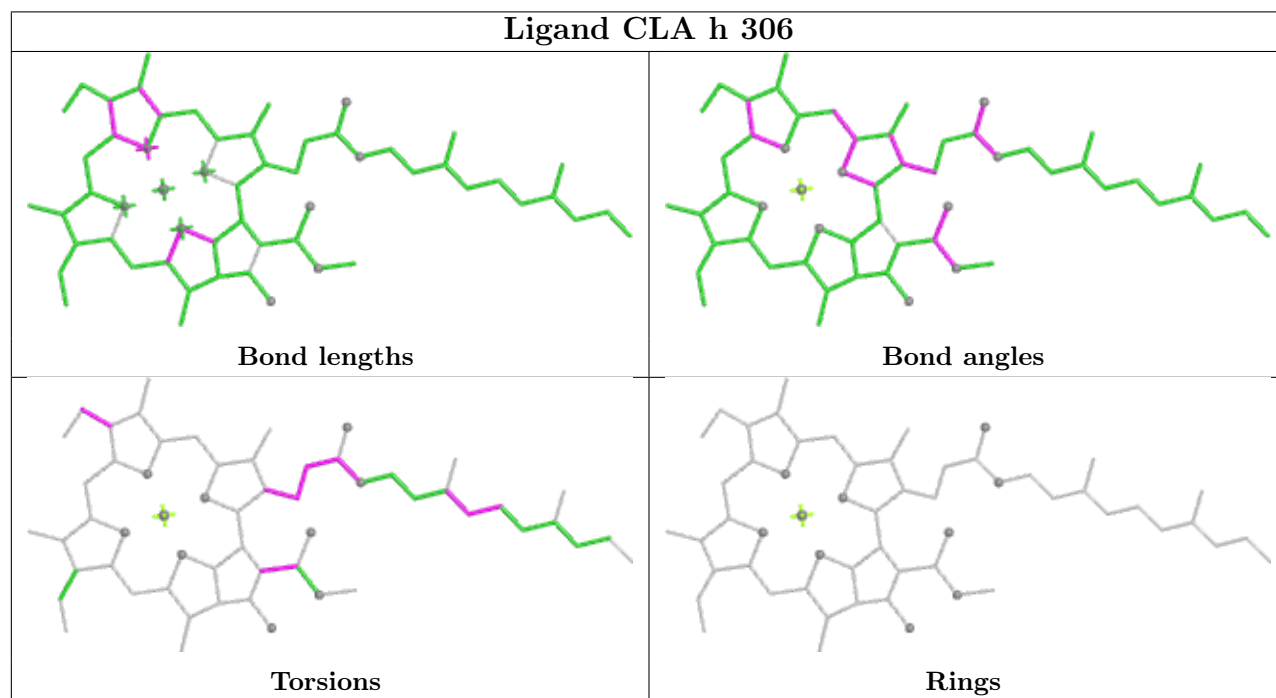
Ligand CLA d 318



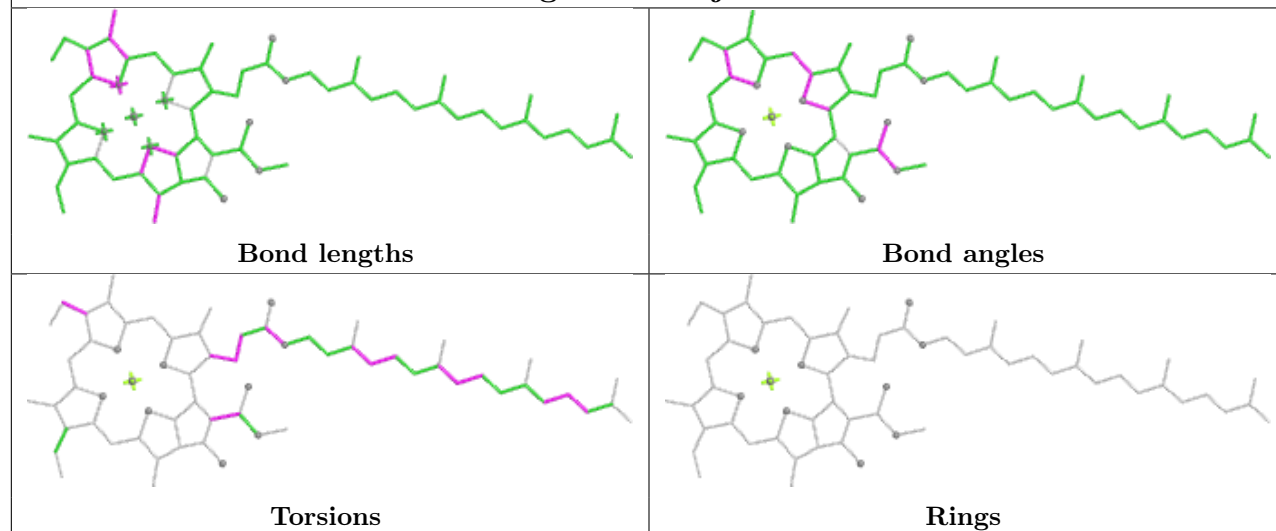
Ligand CLA d 313



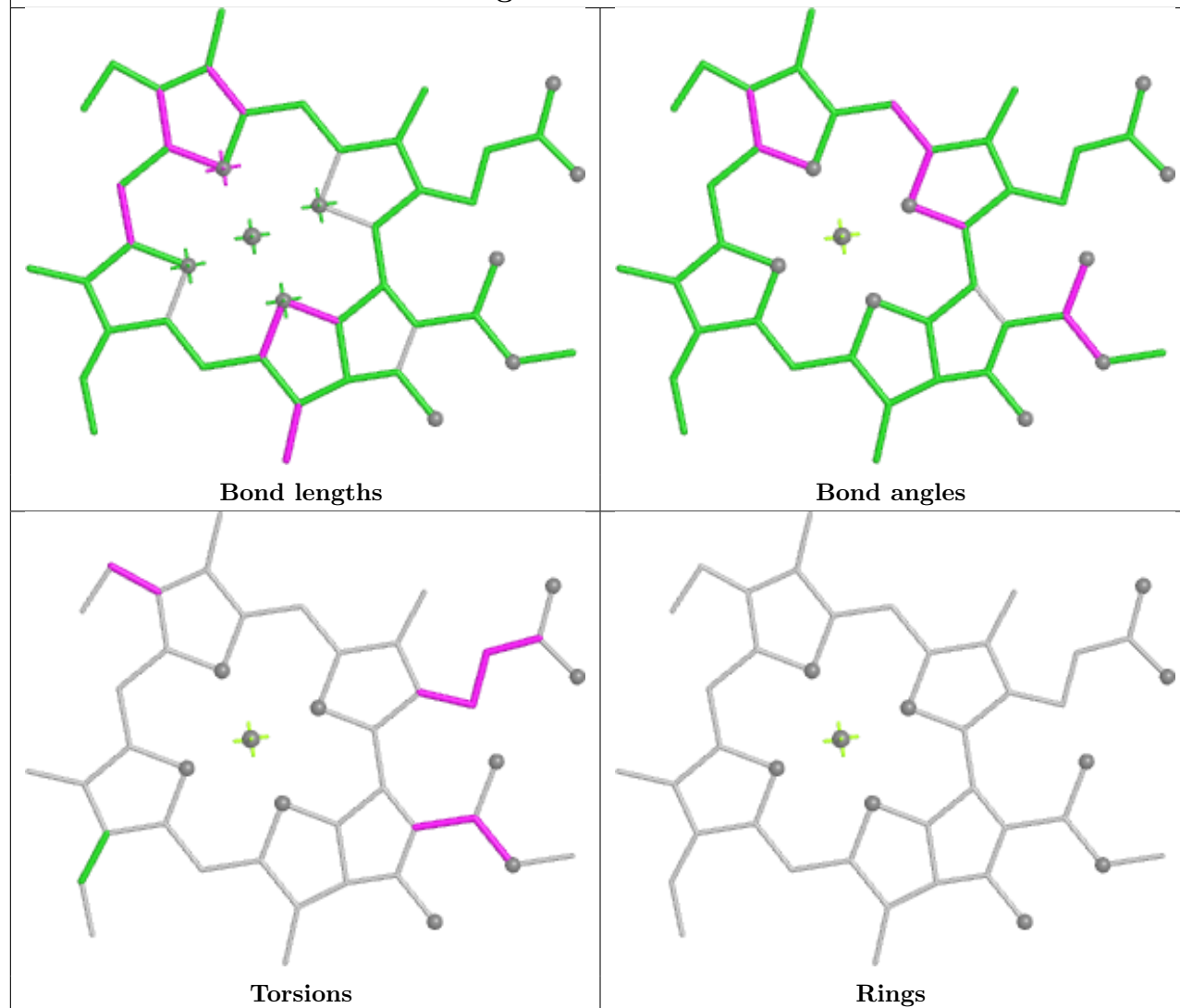
Ligand CLA h 306

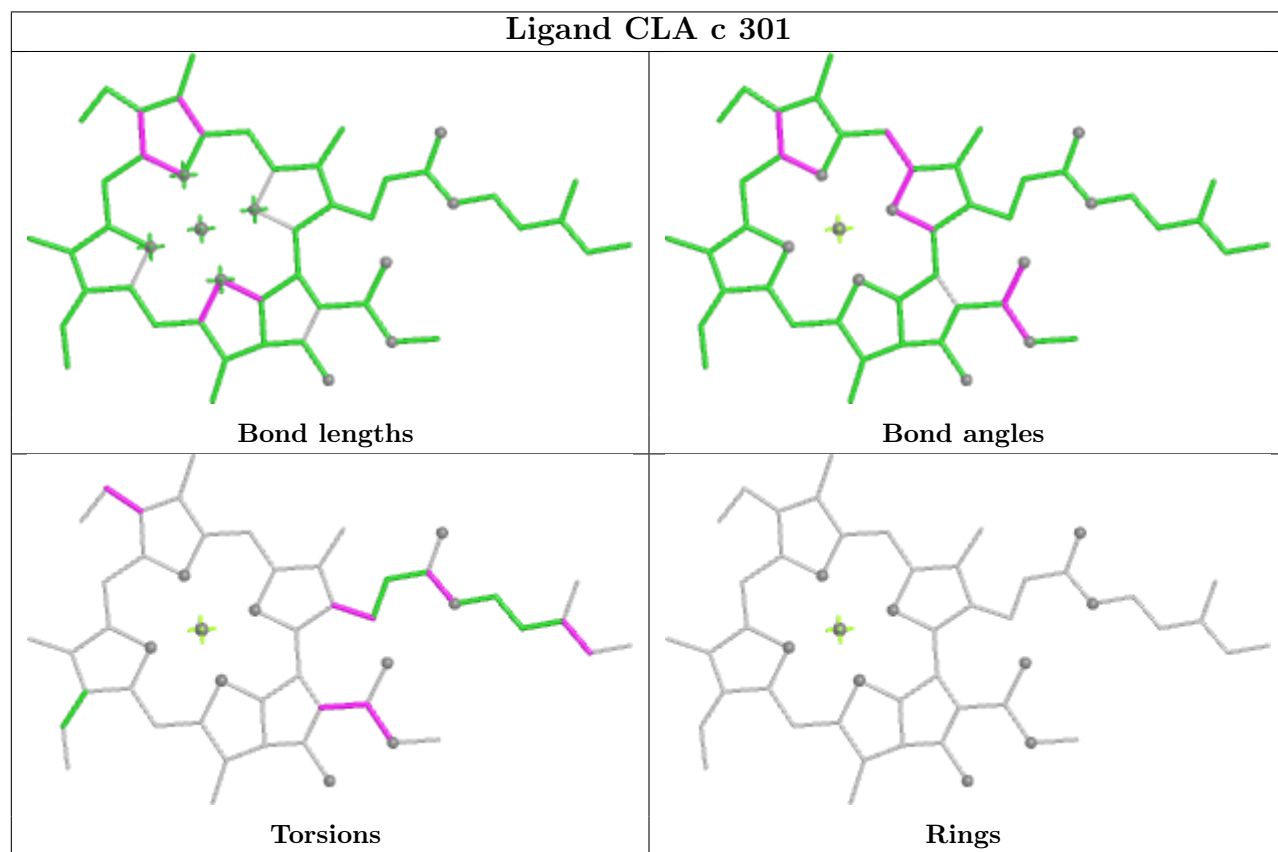
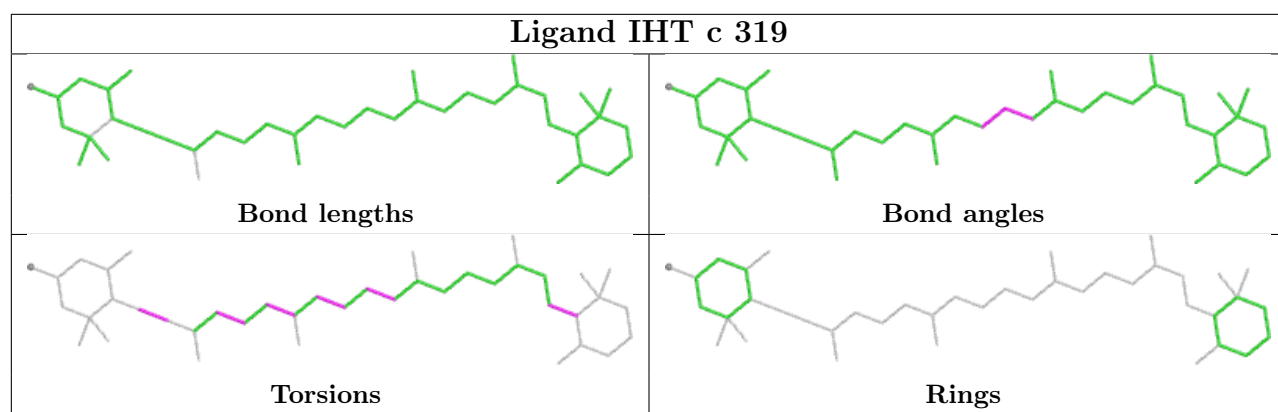


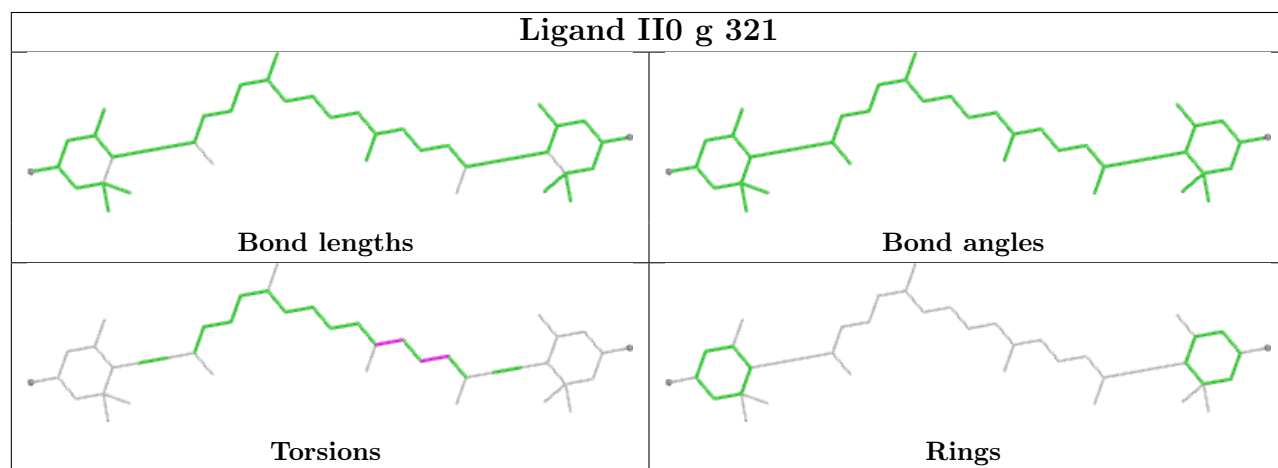
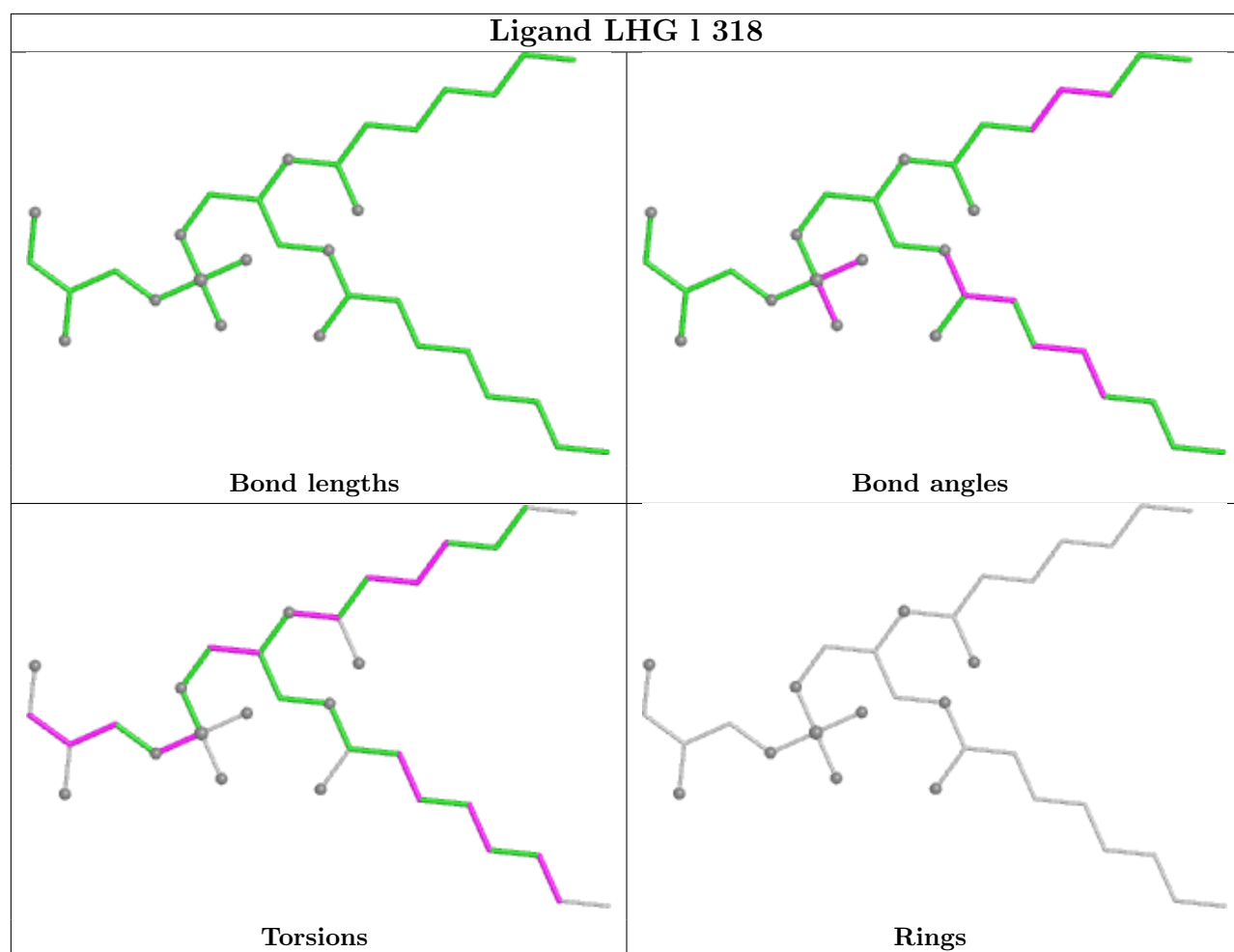
Ligand CLA j 302



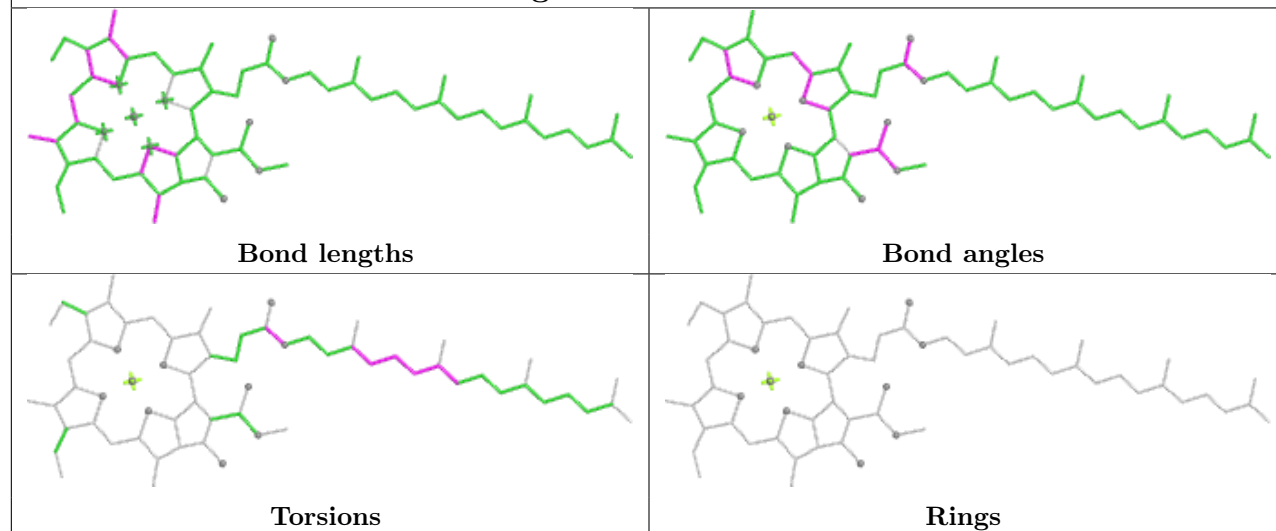
Ligand CLA e 301



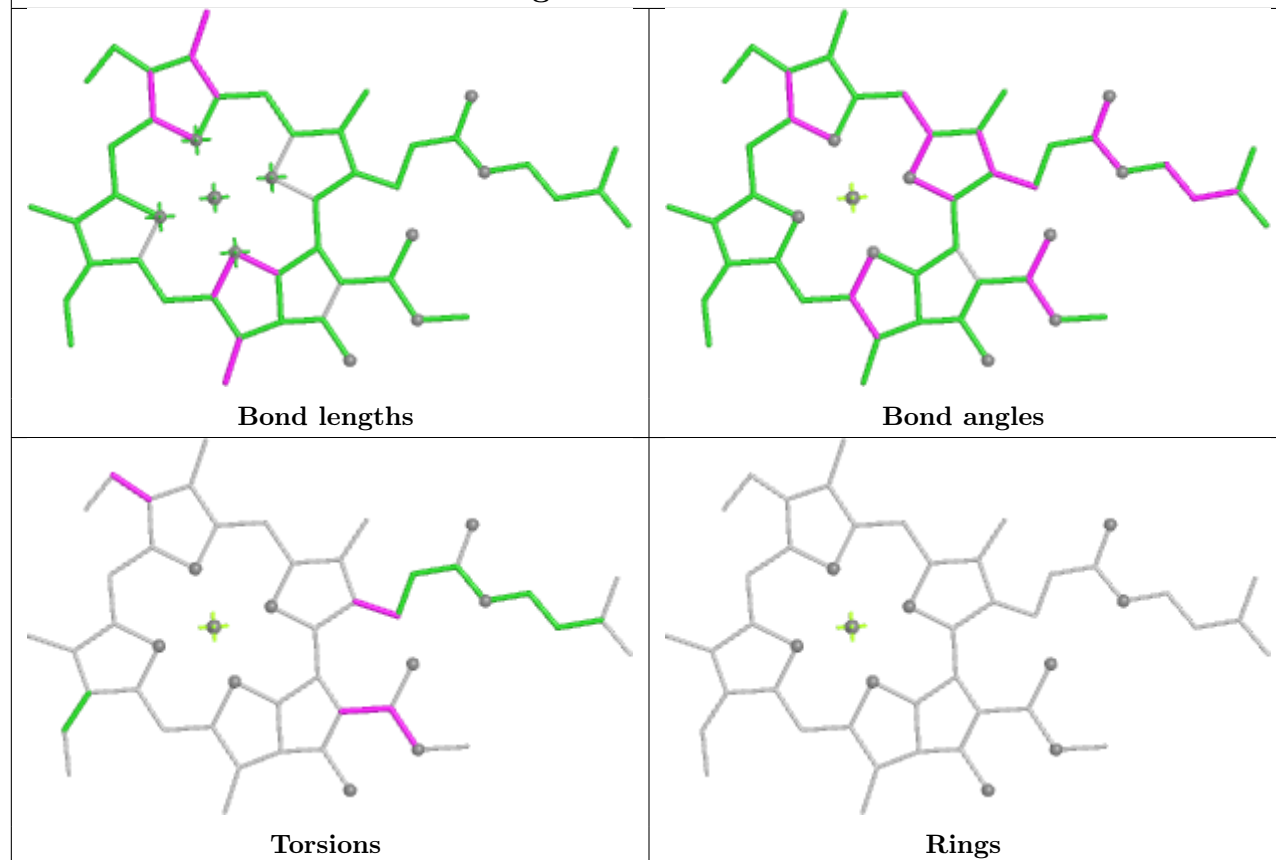


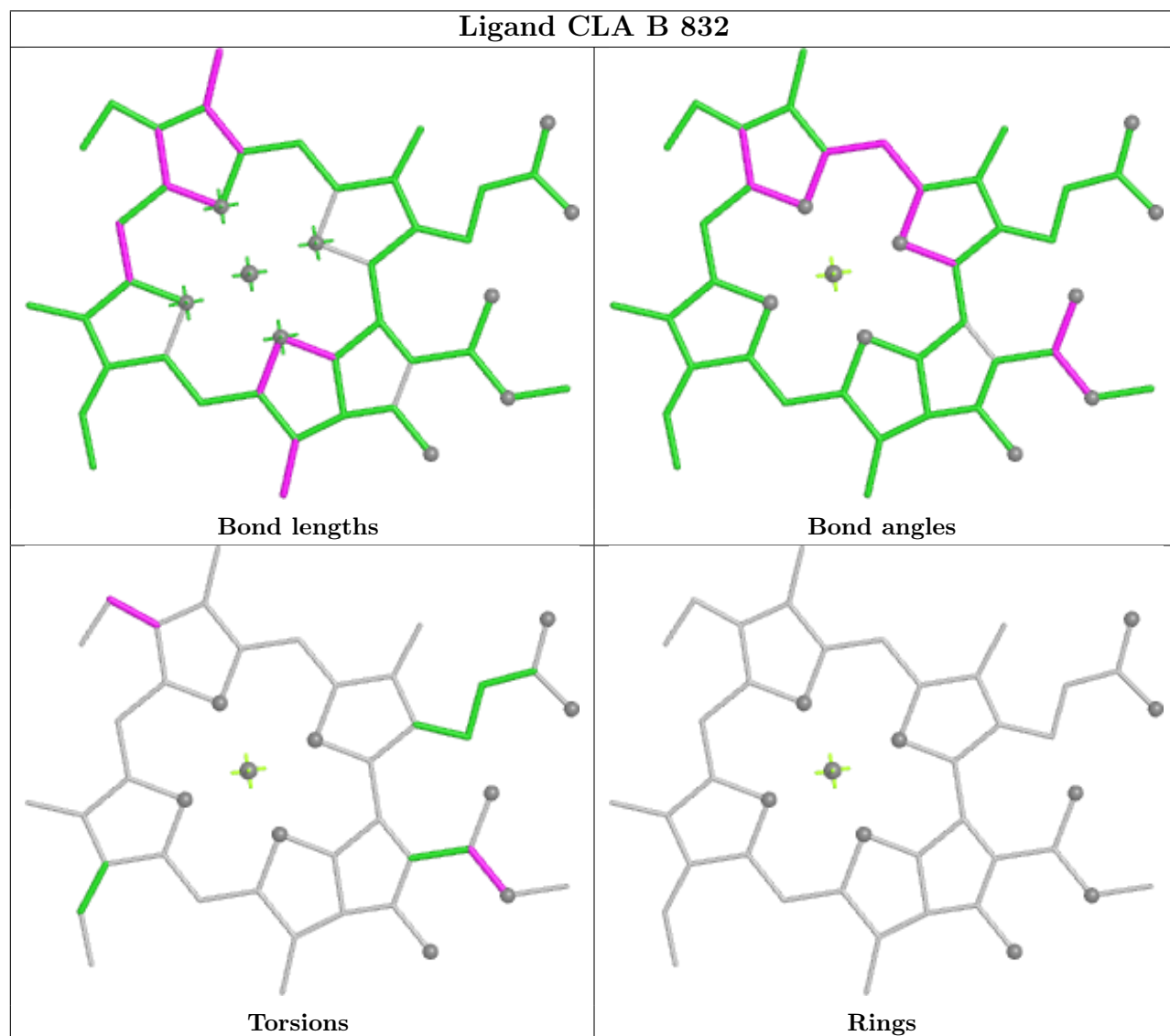
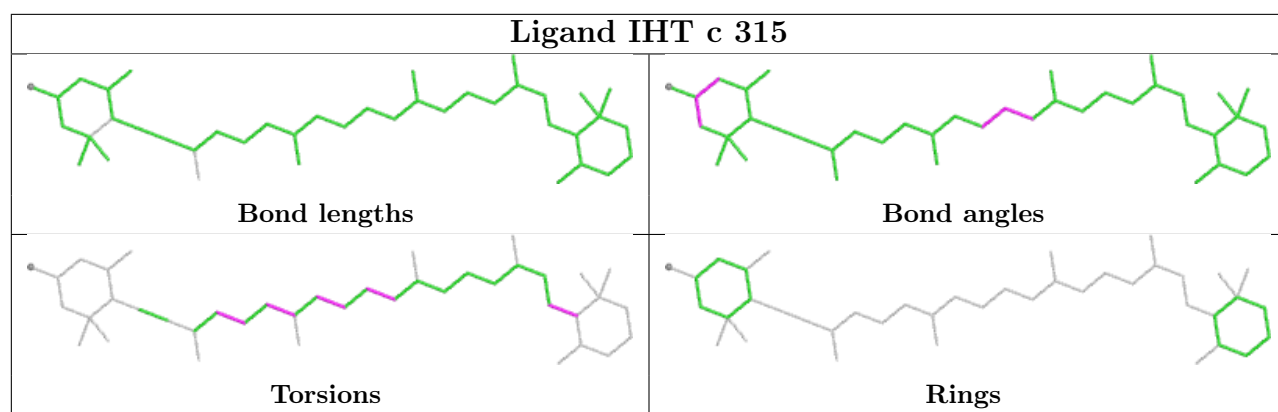


Ligand CLA A 826

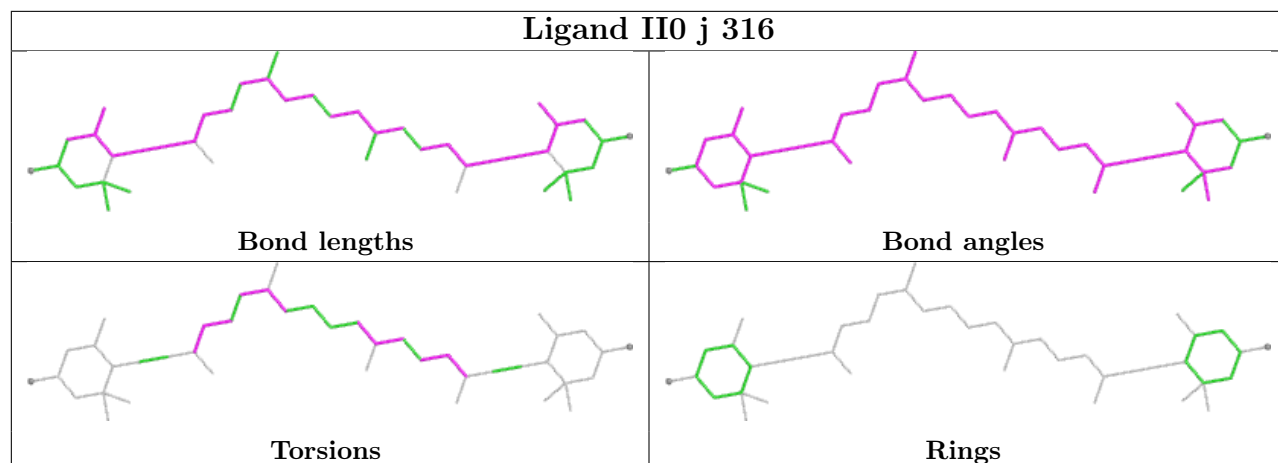


Ligand CLA B 830

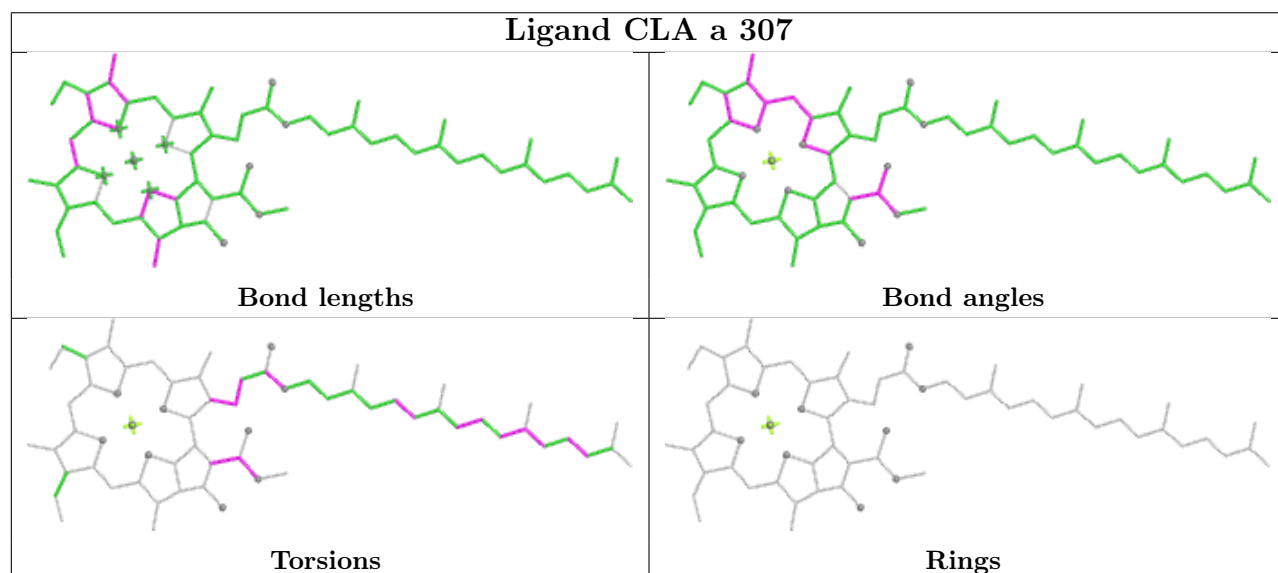




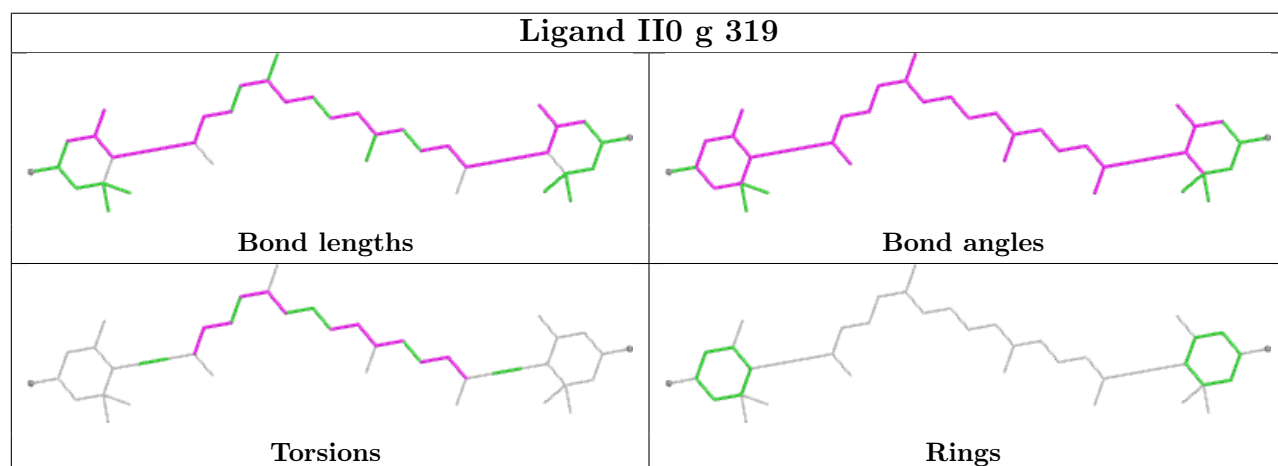
Ligand II0 j 316

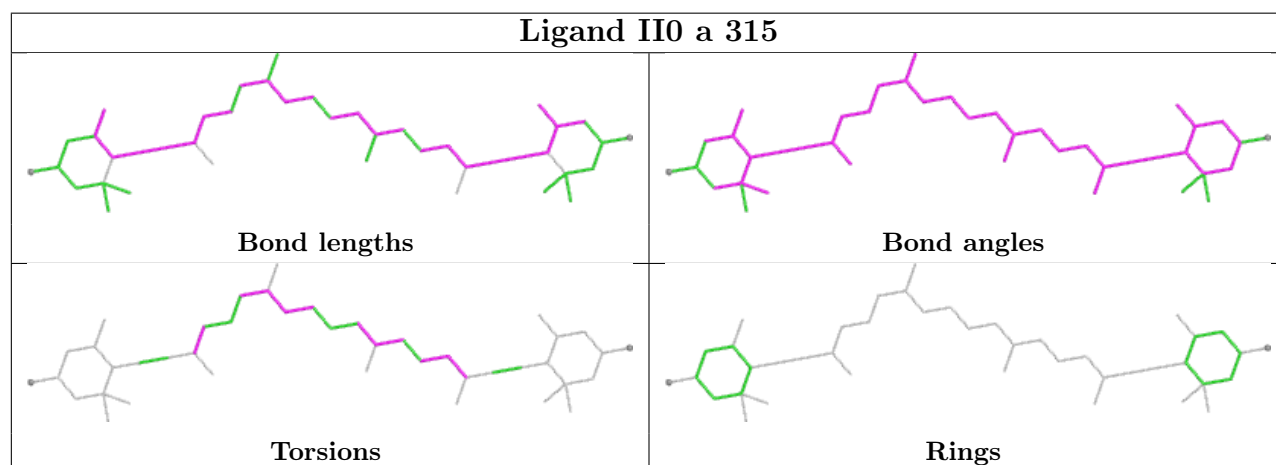
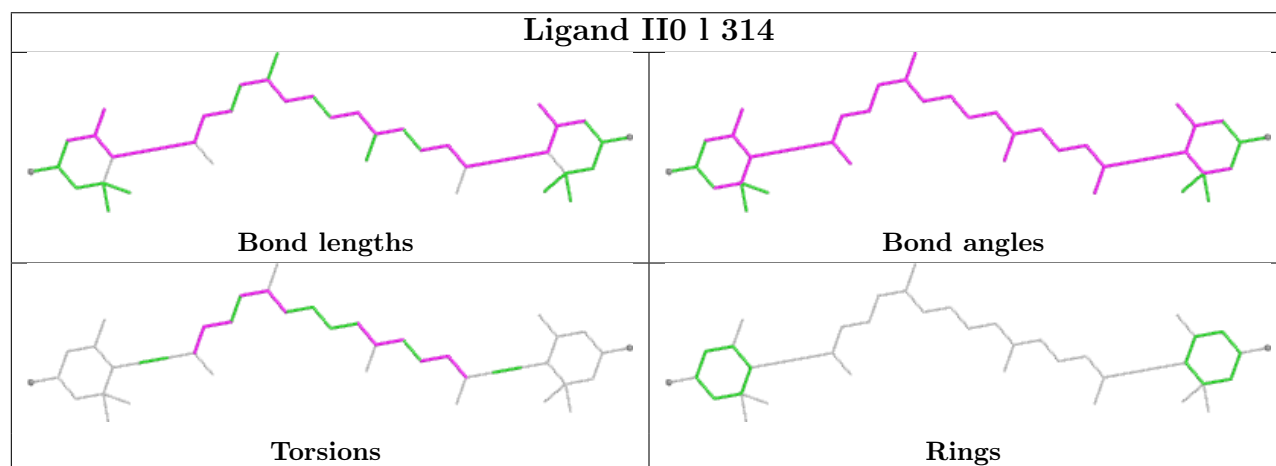
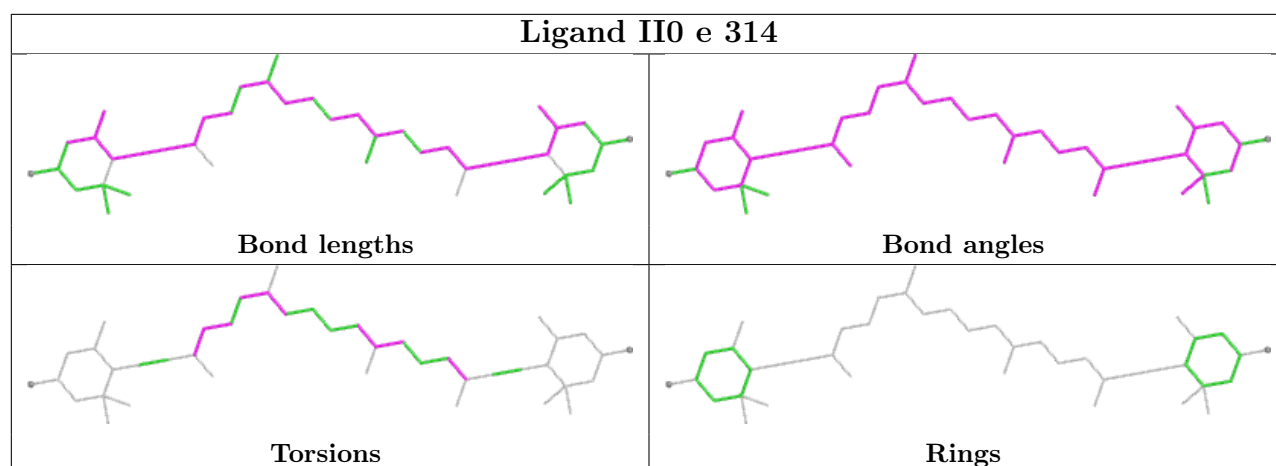


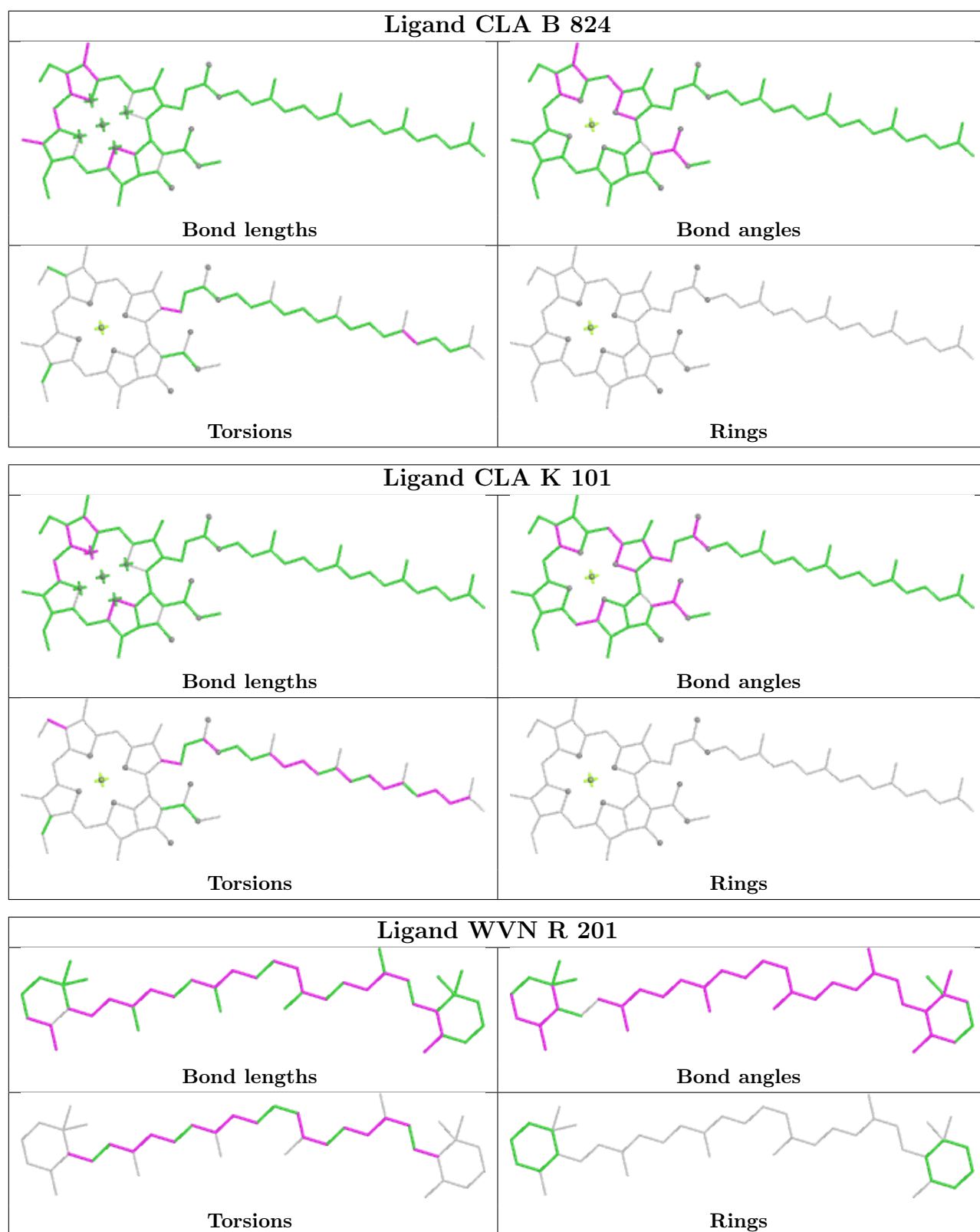
Ligand CLA a 307



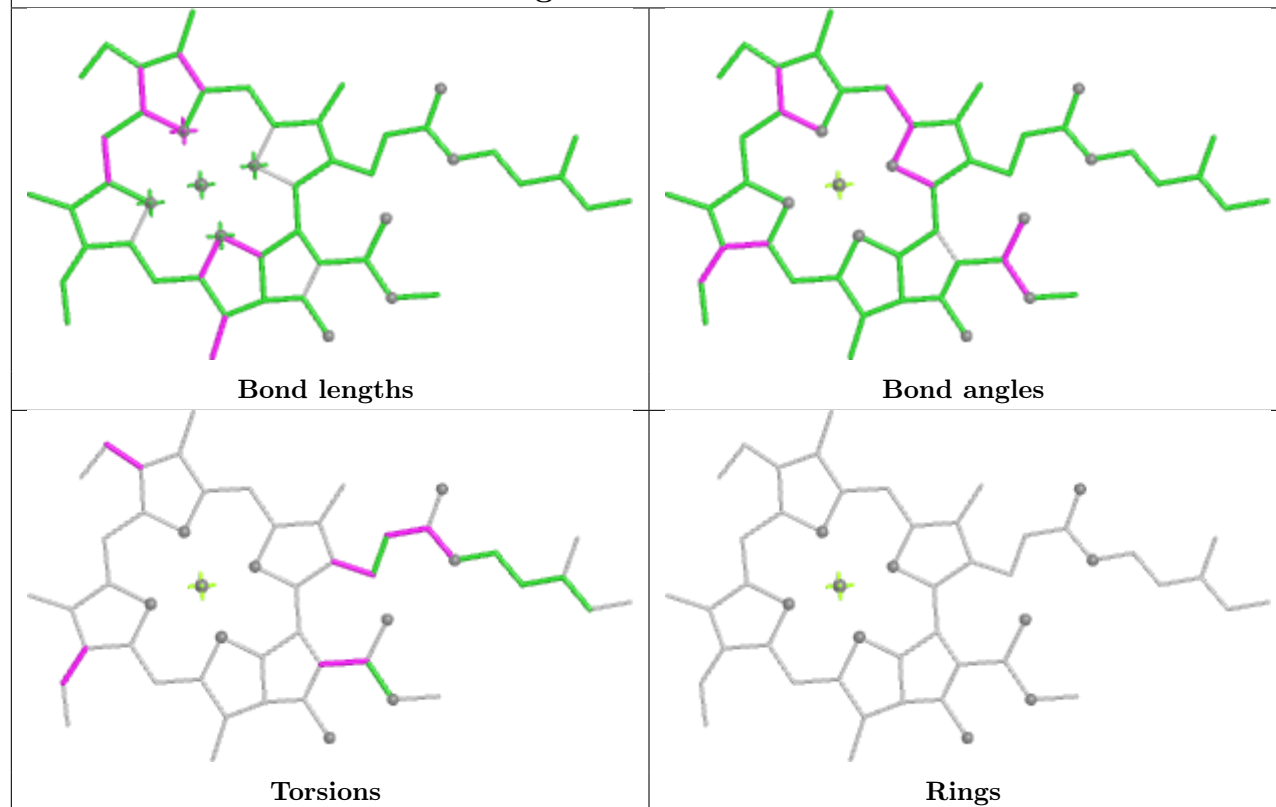
Ligand II0 g 319



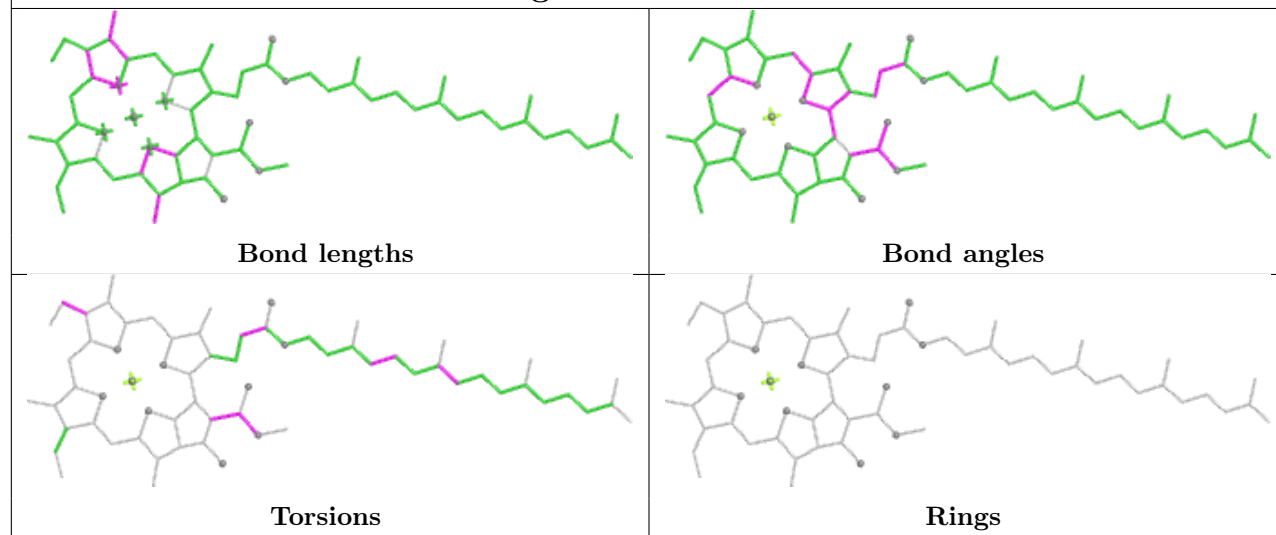




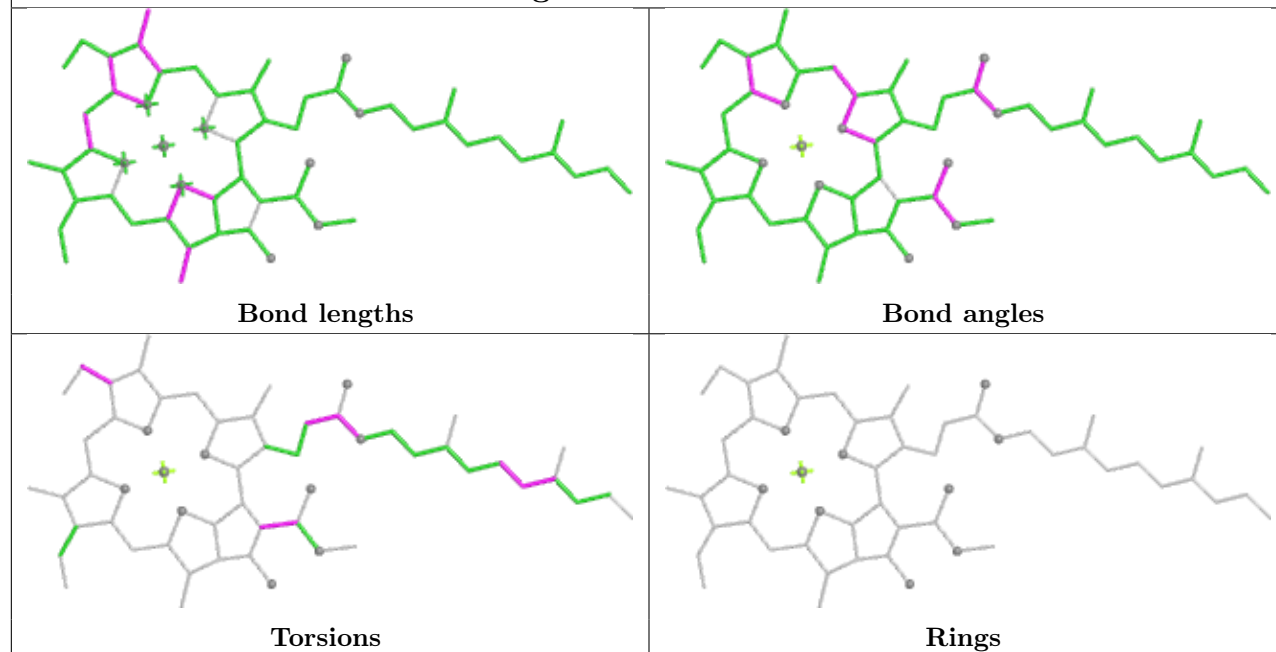
Ligand CLA n 605



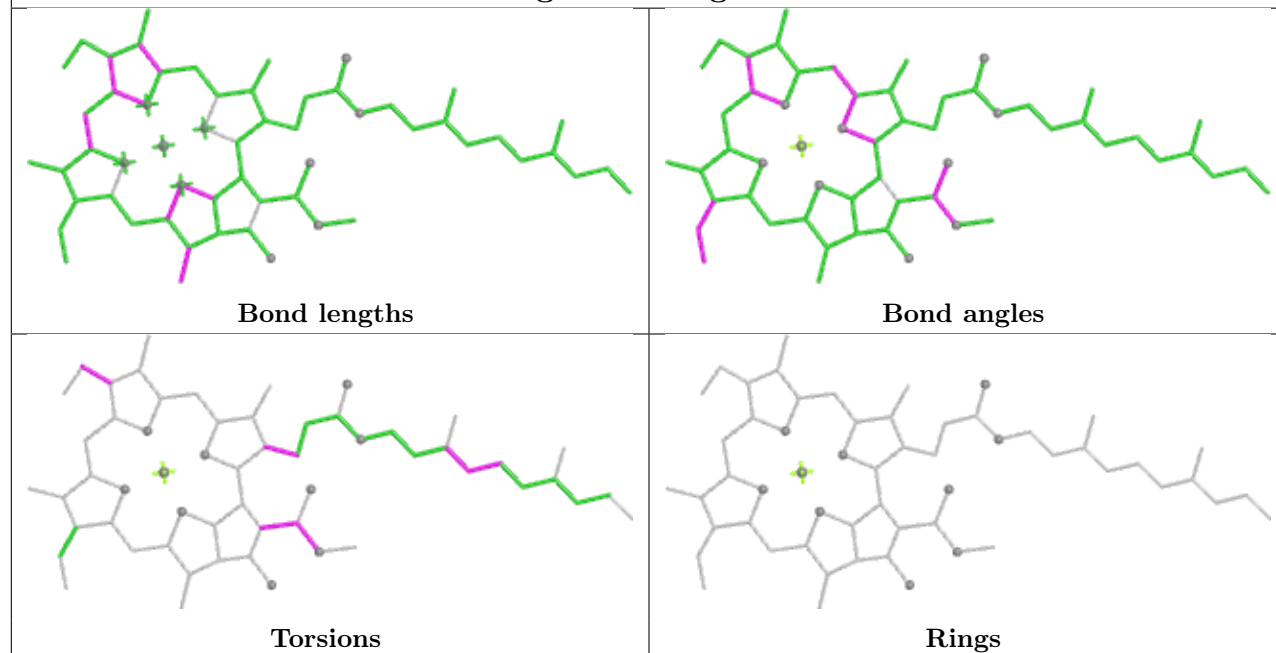
Ligand CLA A 836

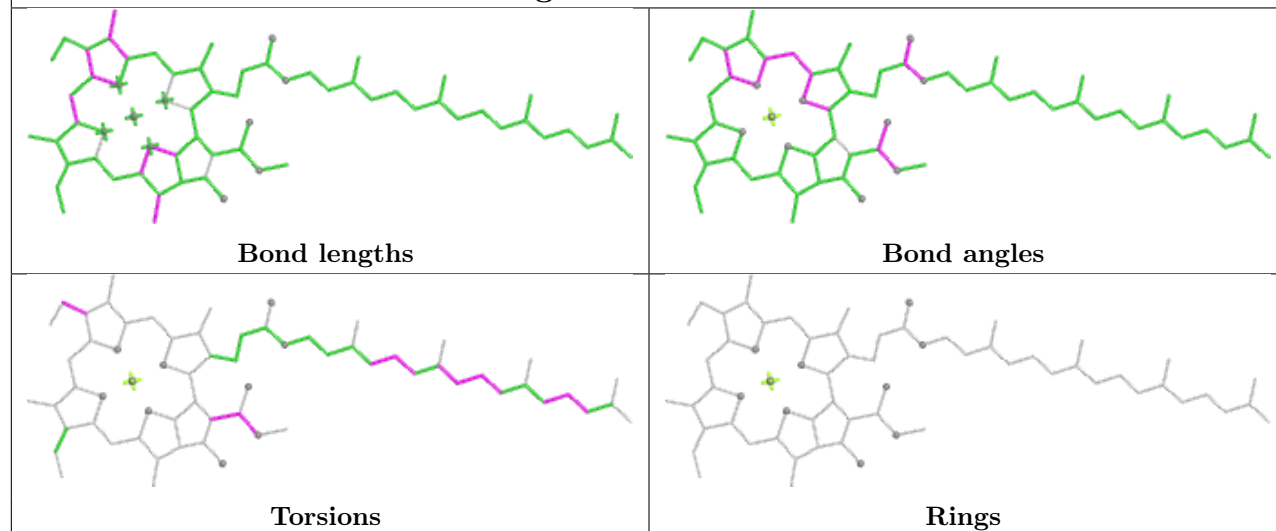
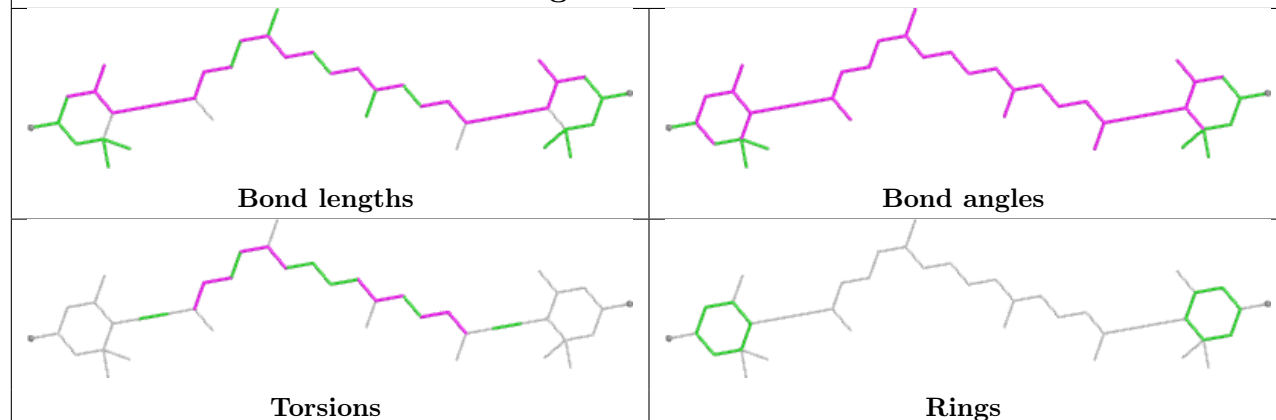
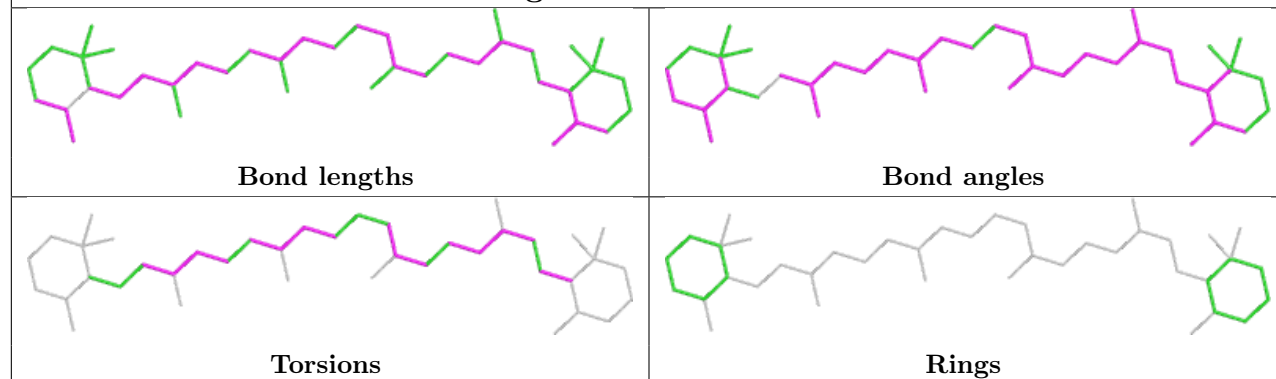


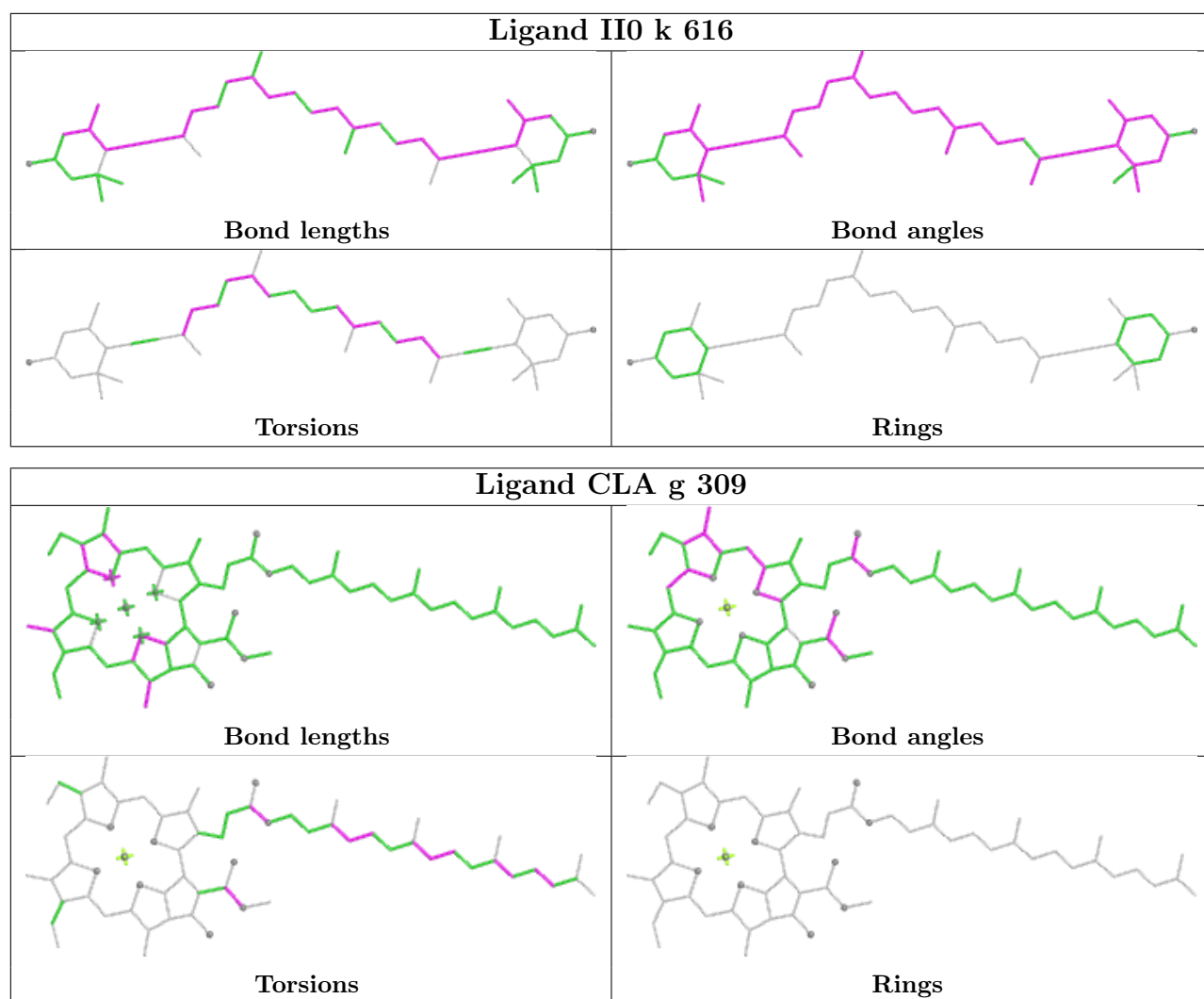
Ligand CLA B 839

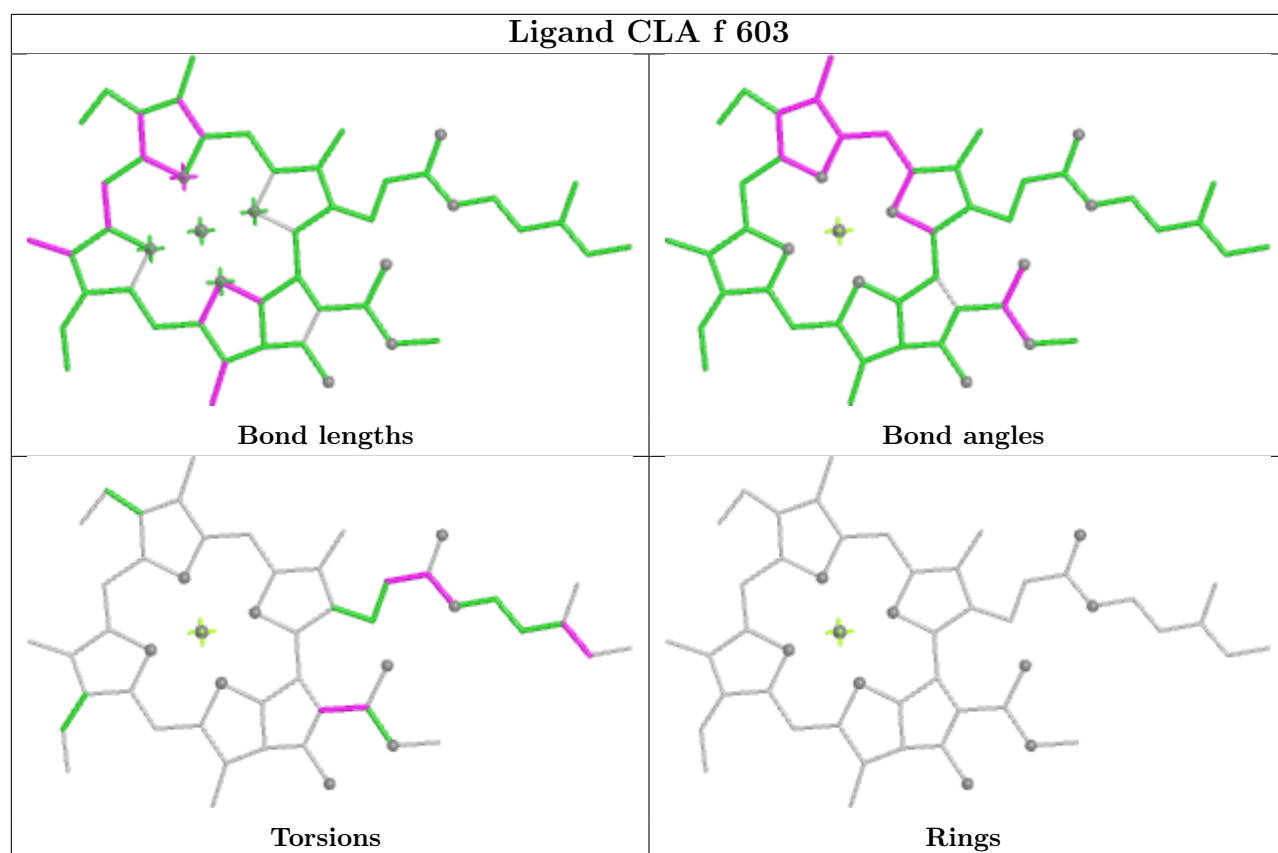


Ligand CLA g 316

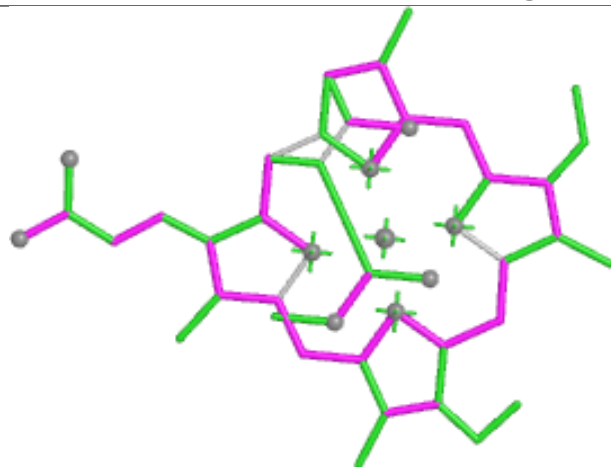


Ligand CLA b 310**Ligand II0 n 615****Ligand WVN L 206**

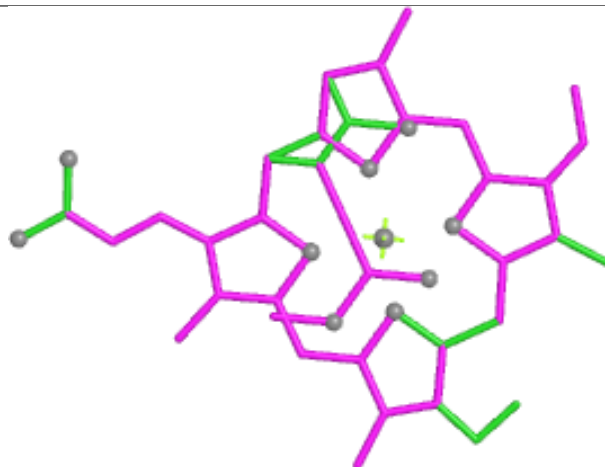




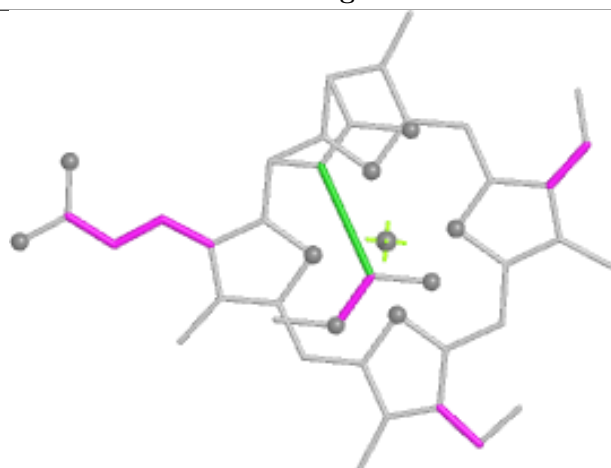
Ligand KC2 e 309



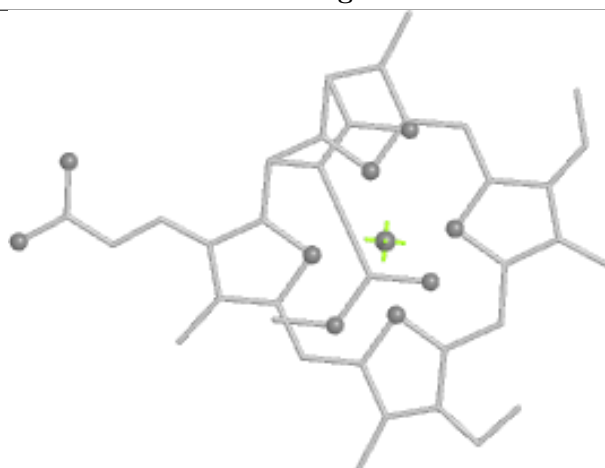
Bond lengths



Bond angles

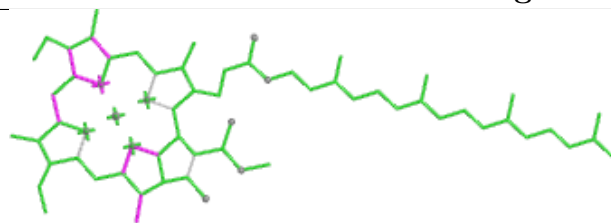


Torsions

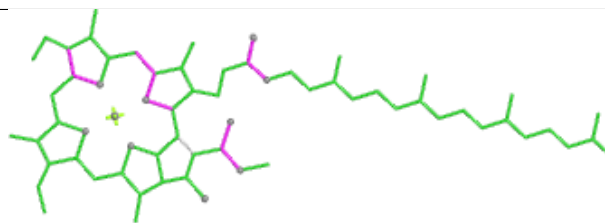


Rings

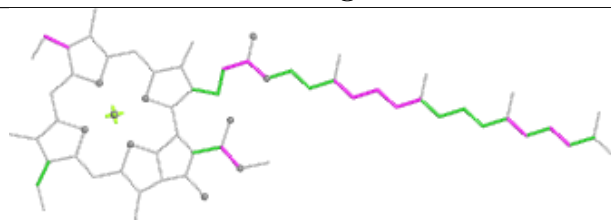
Ligand CLA B 806



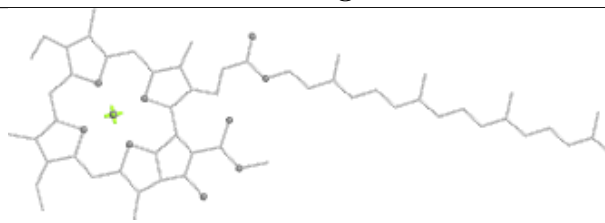
Bond lengths



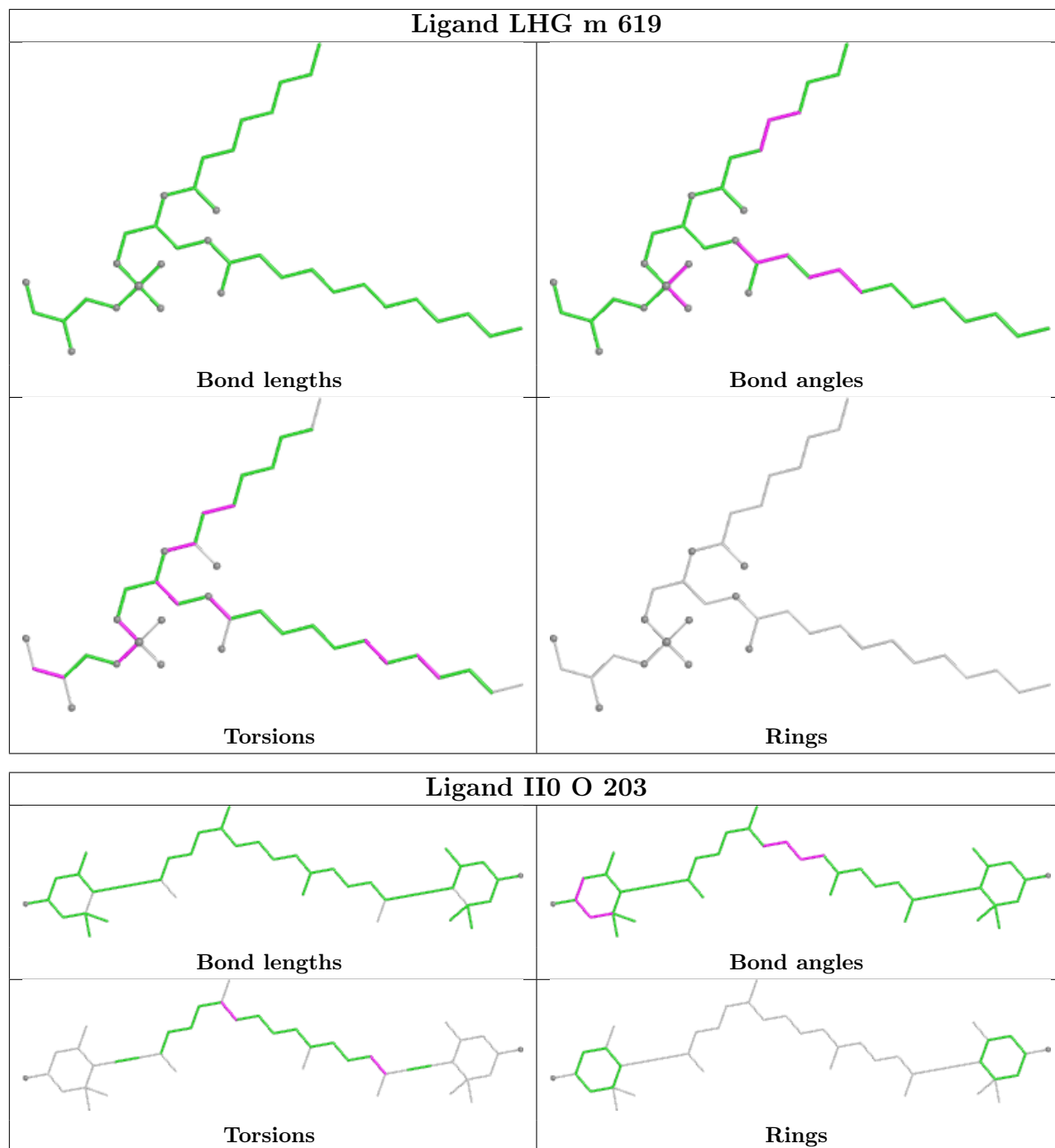
Bond angles

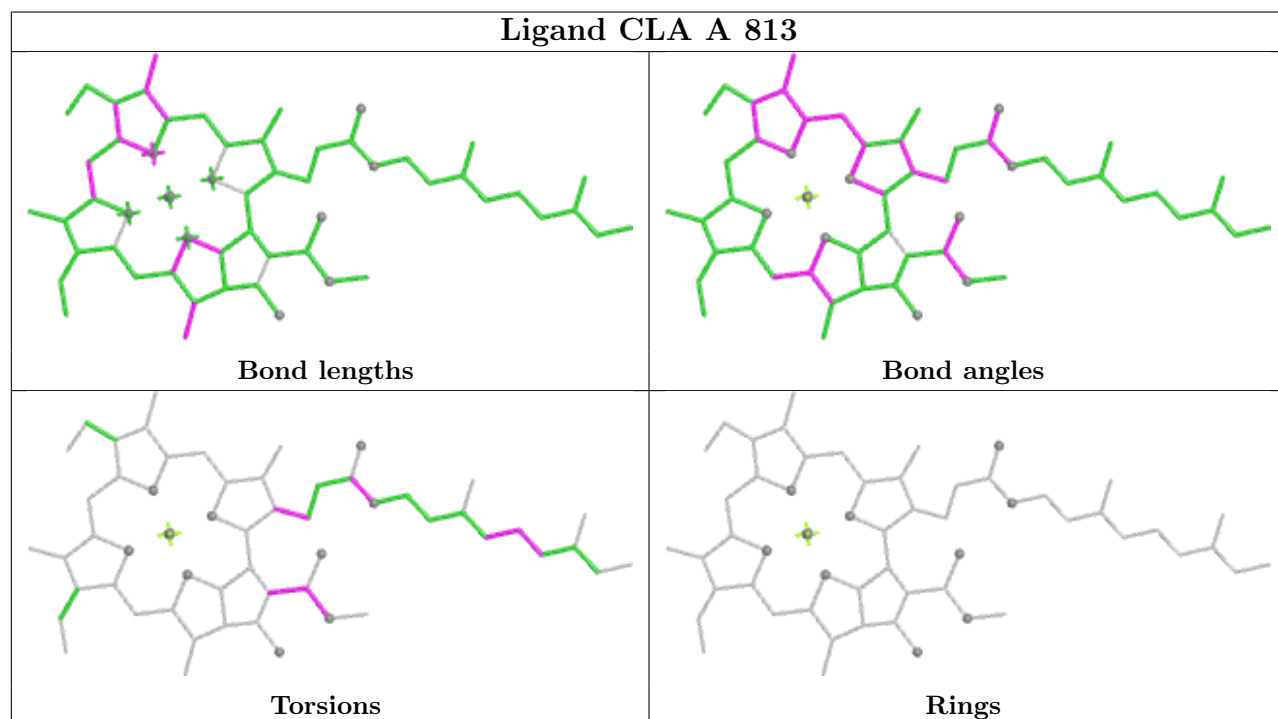
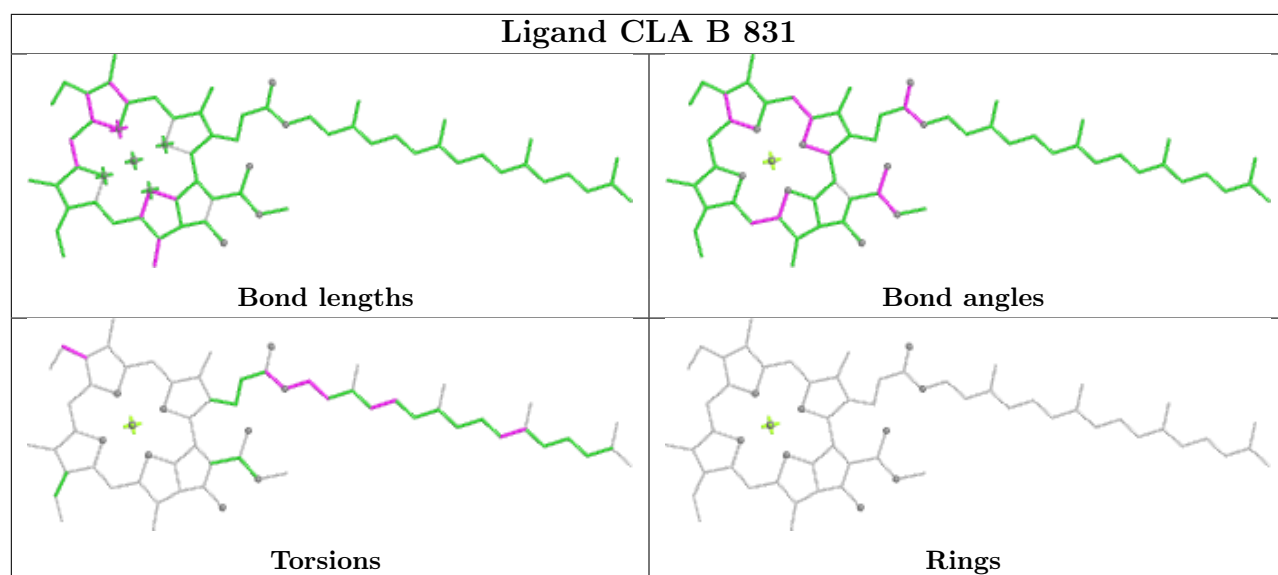


Torsions

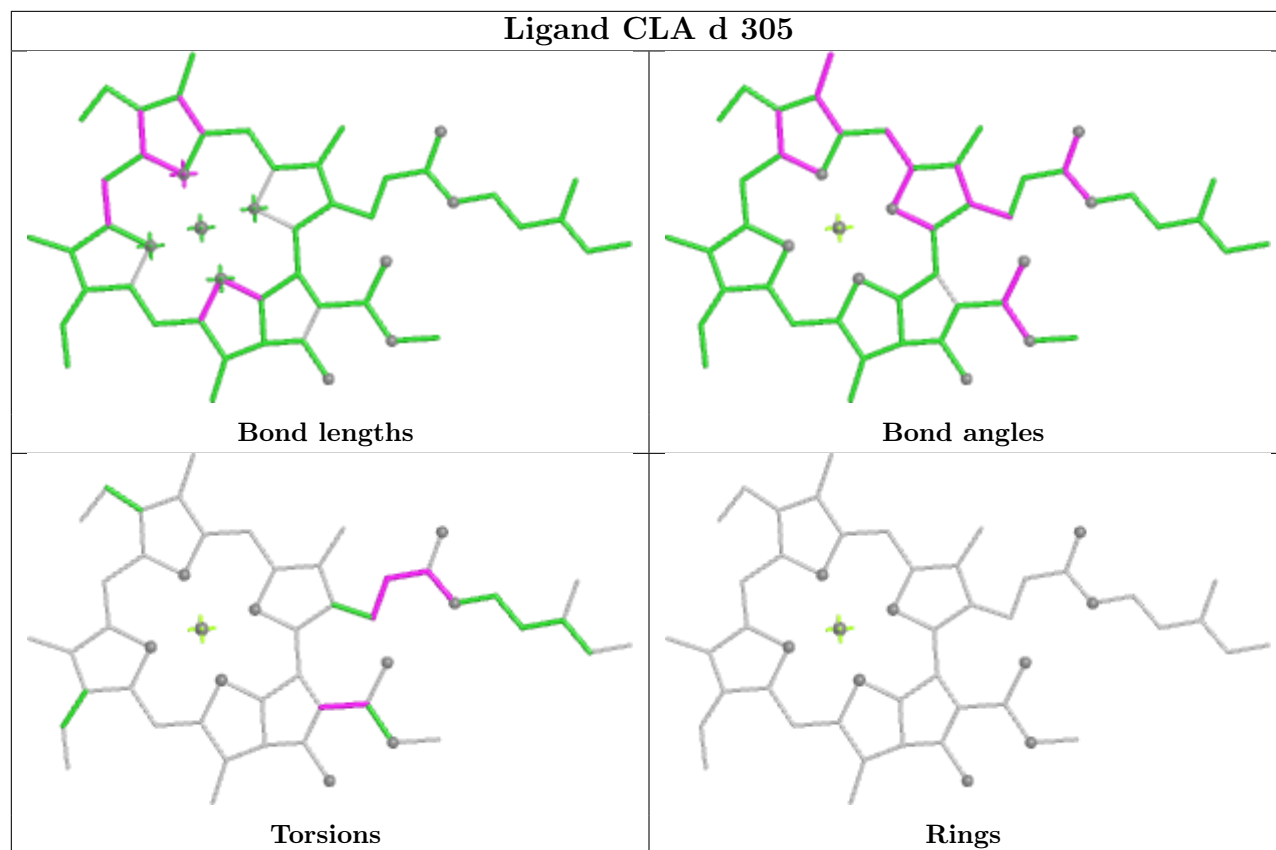


Rings

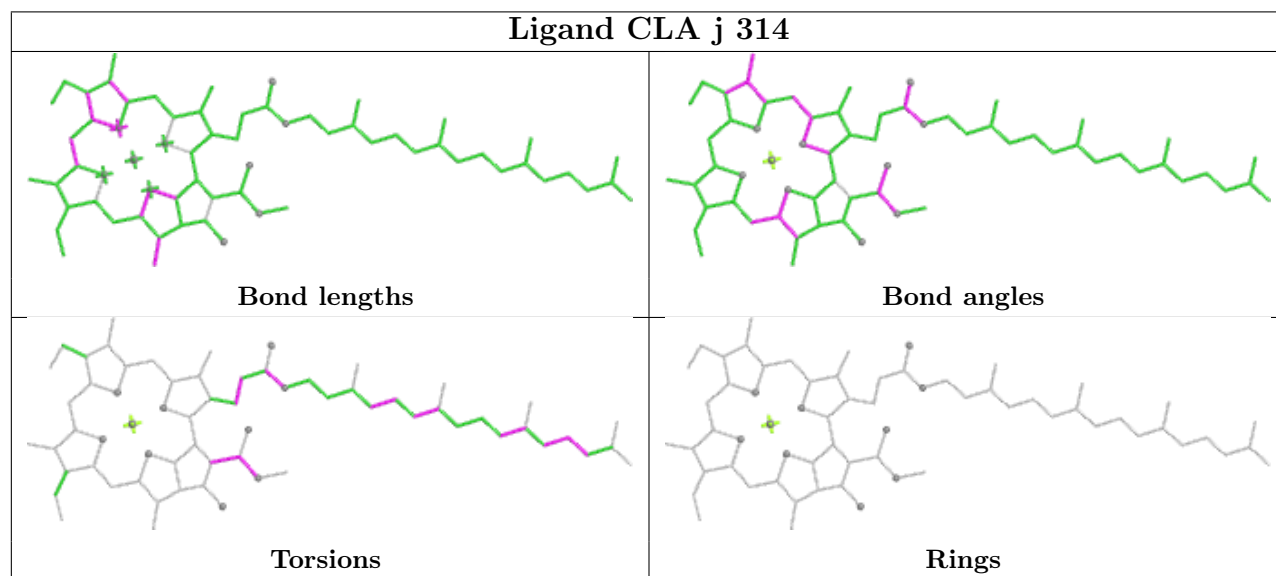


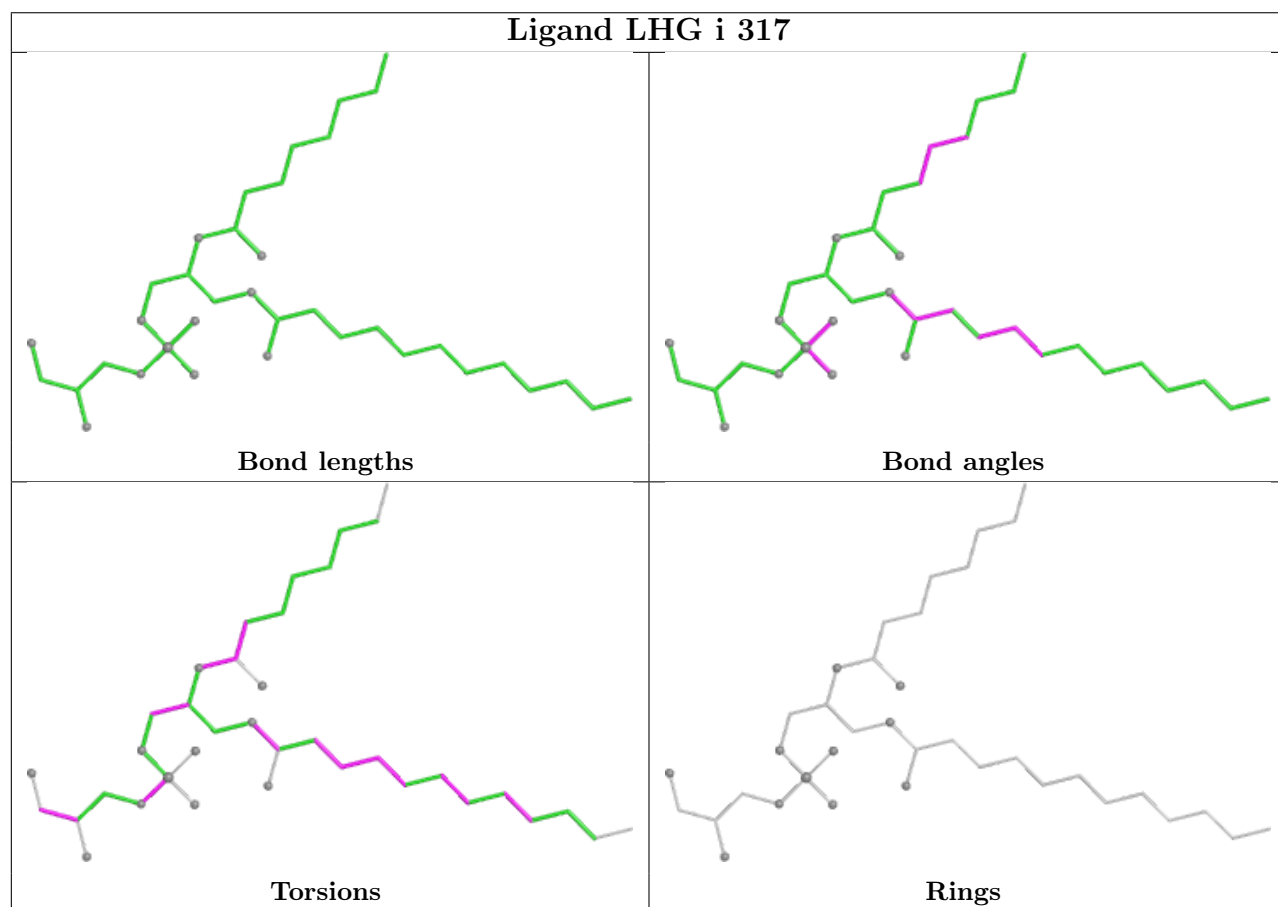
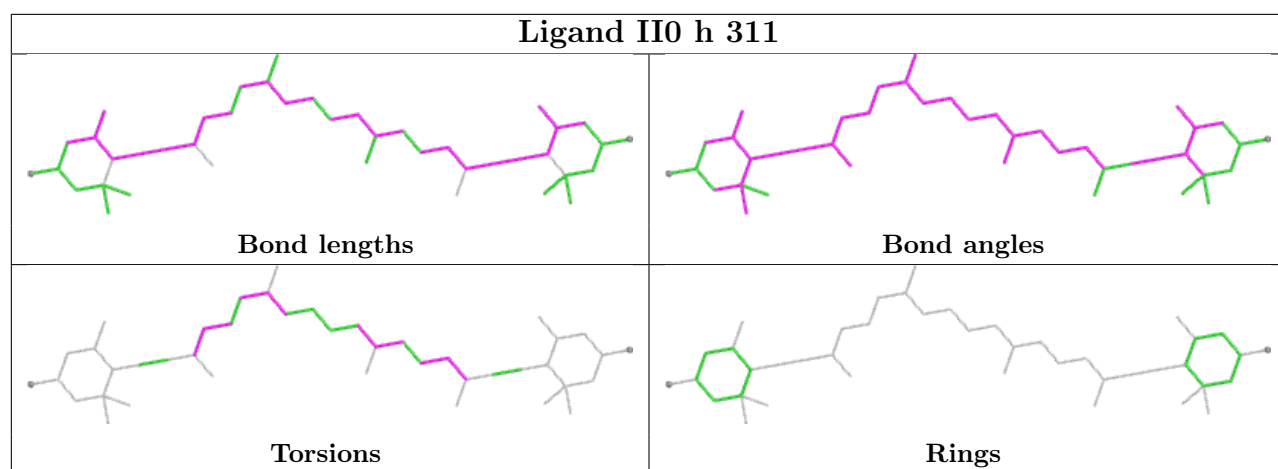


Ligand CLA d 305

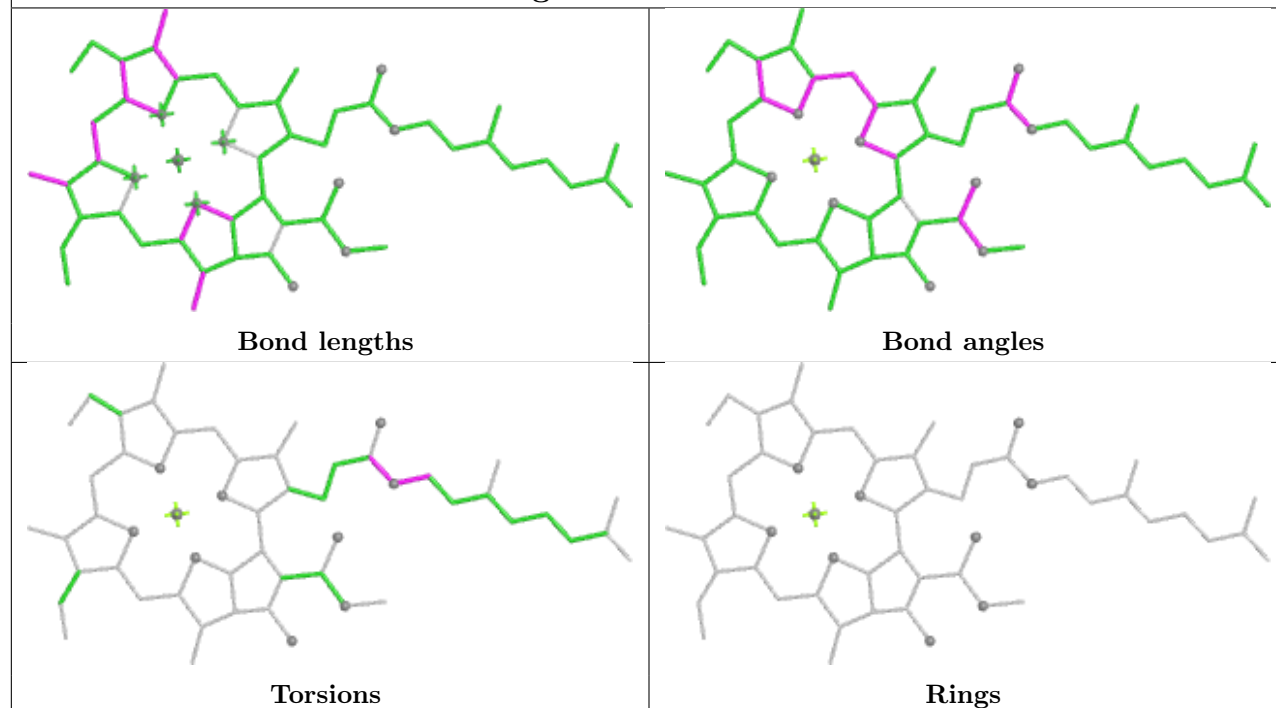


Ligand CLA j 314

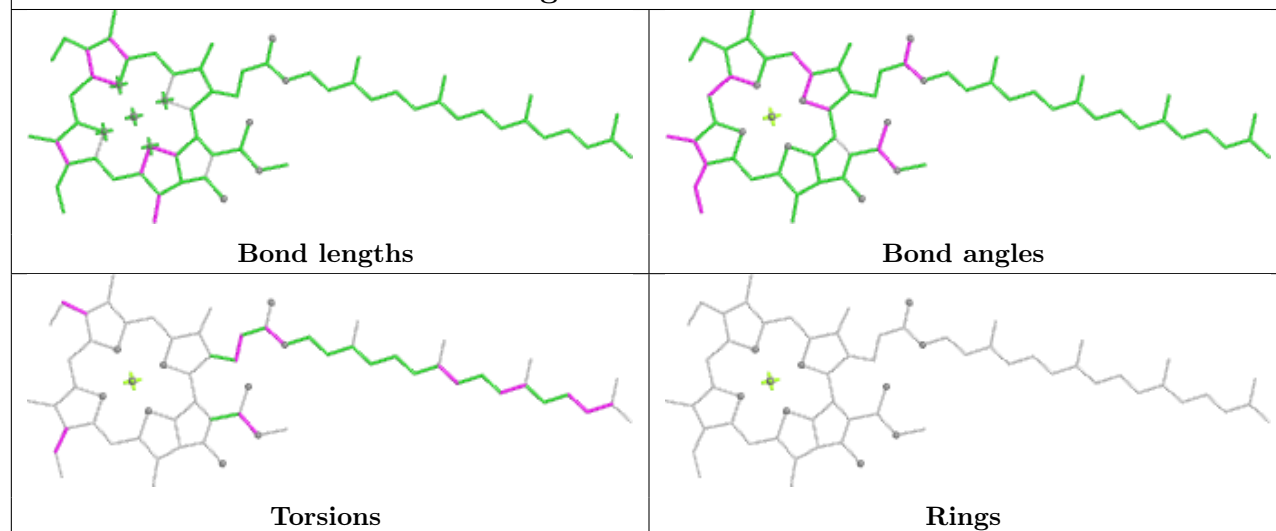




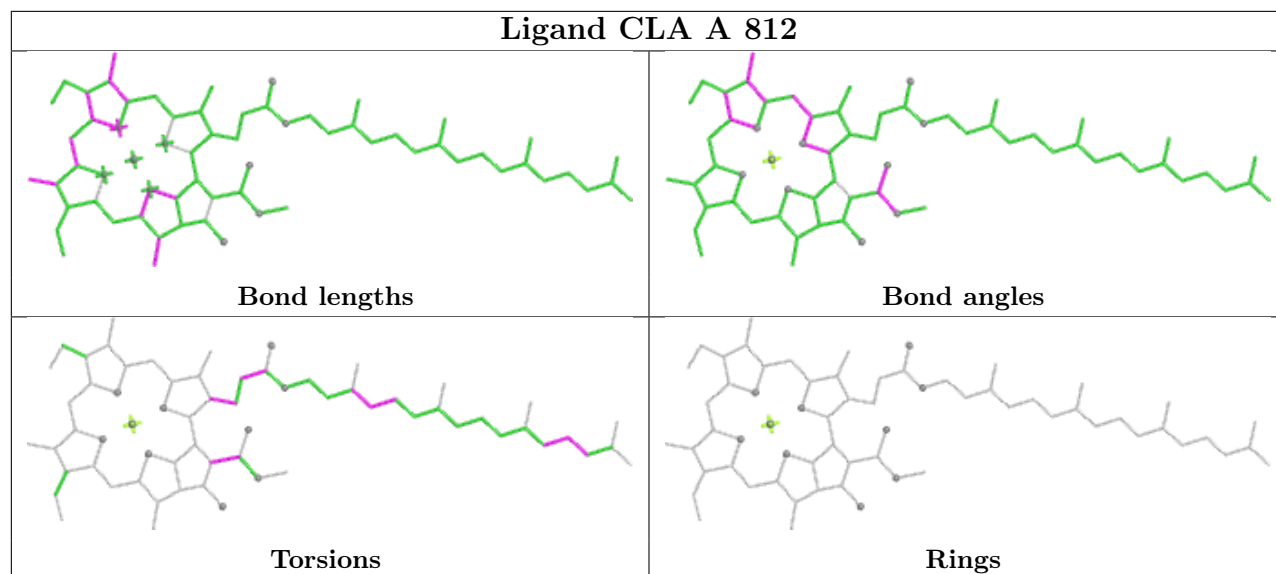
Ligand CLA B 811



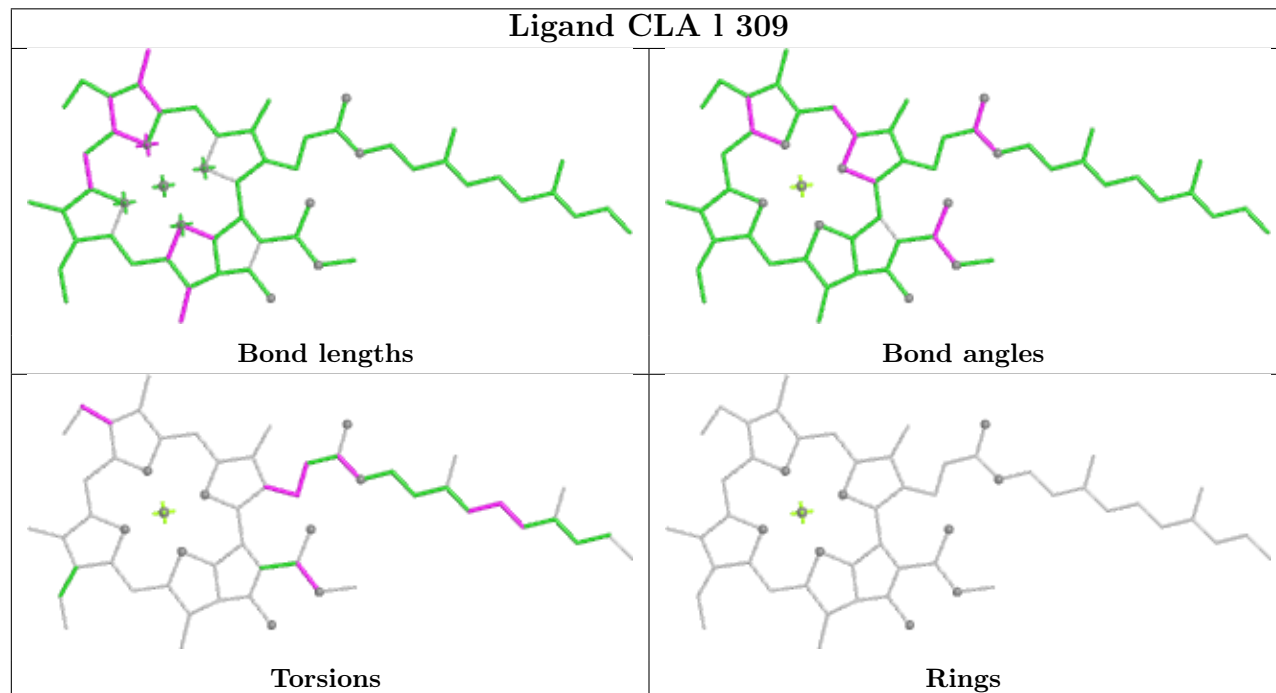
Ligand CLA i 312

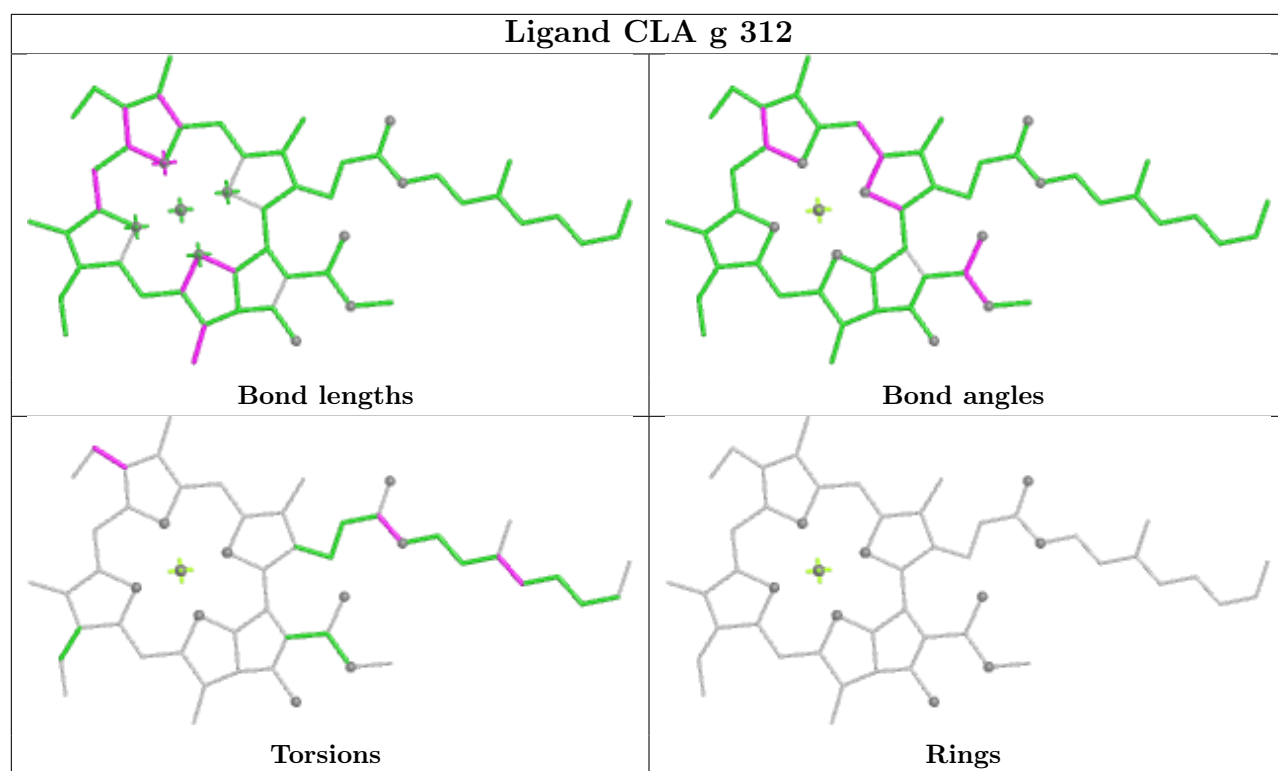


Ligand CLA A 812

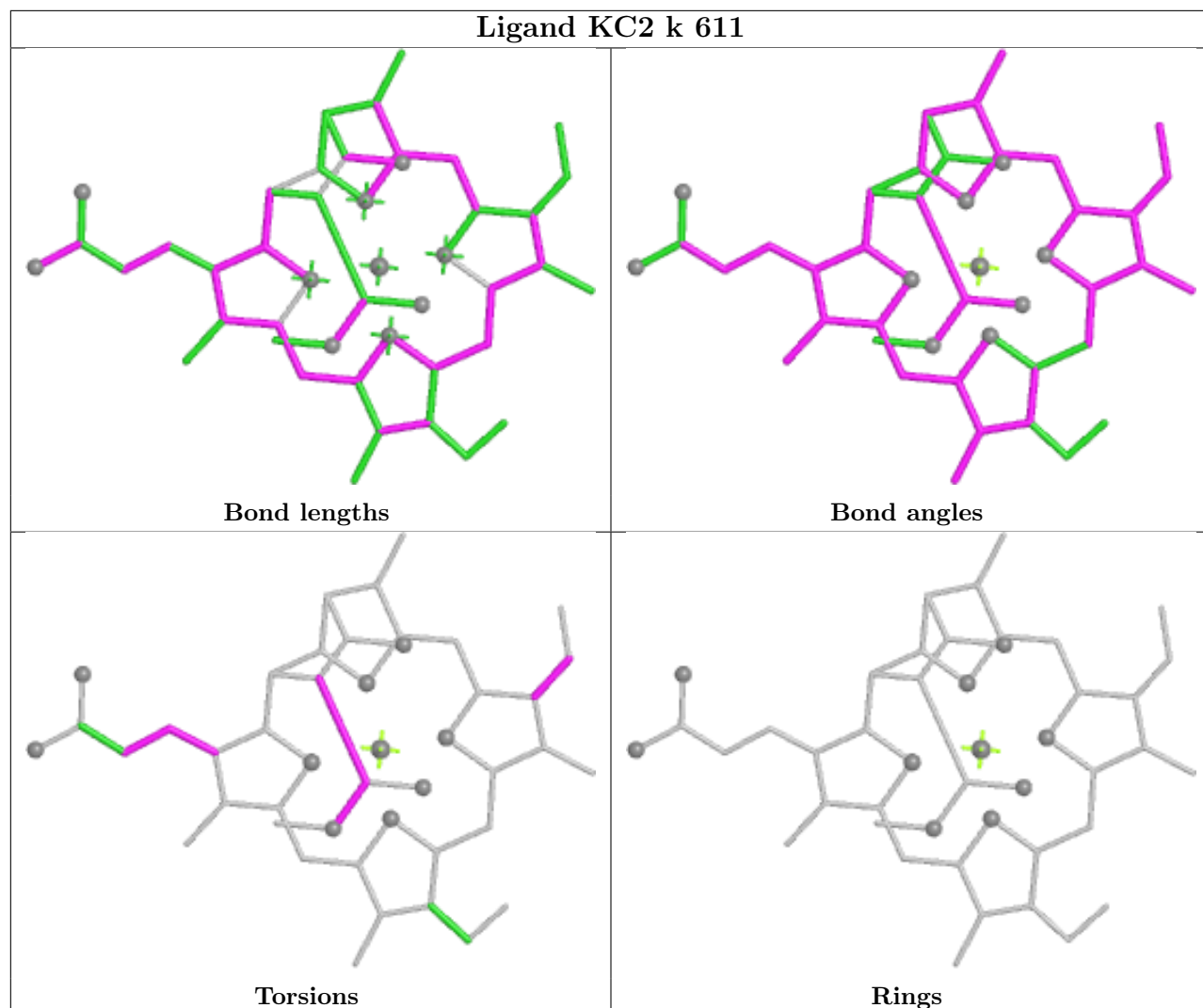


Ligand CLA I 309

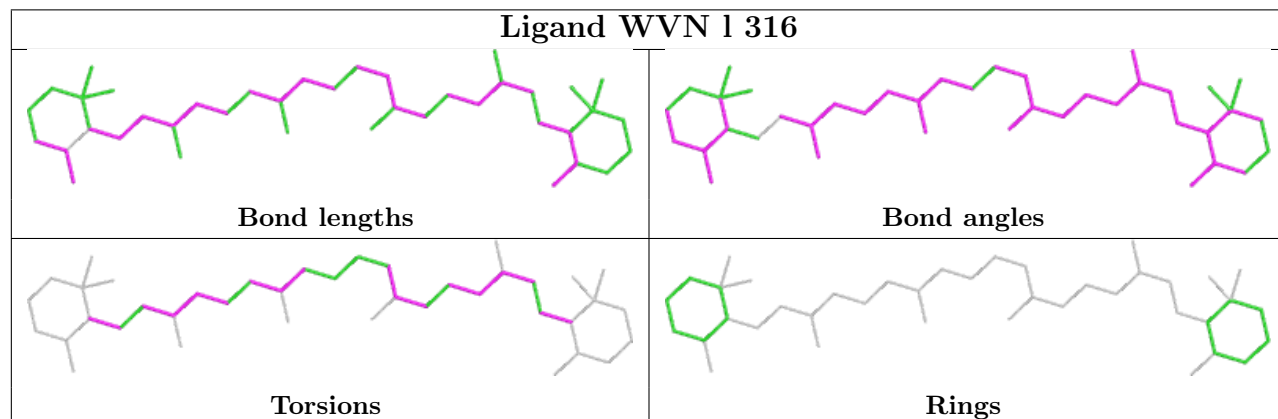




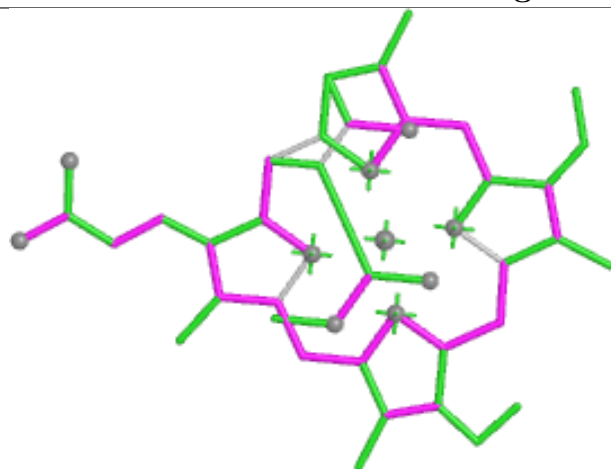
Ligand KC2 k 611



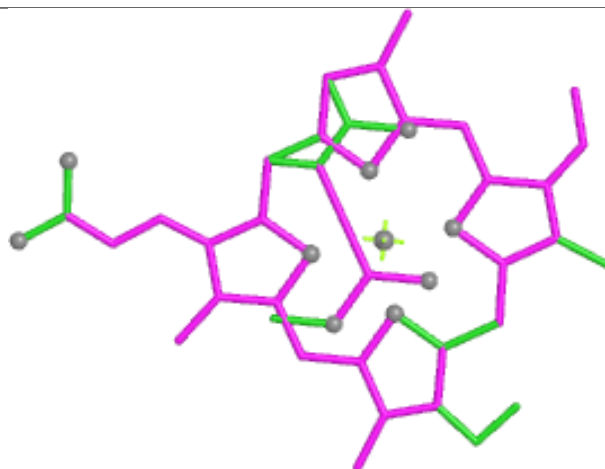
Ligand WVN 1 316



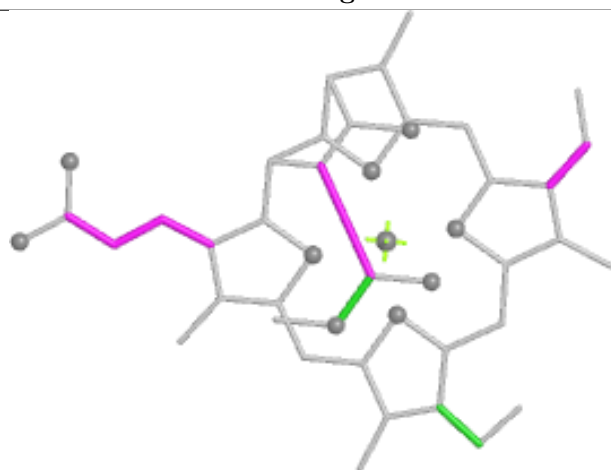
Ligand KC2 m 611



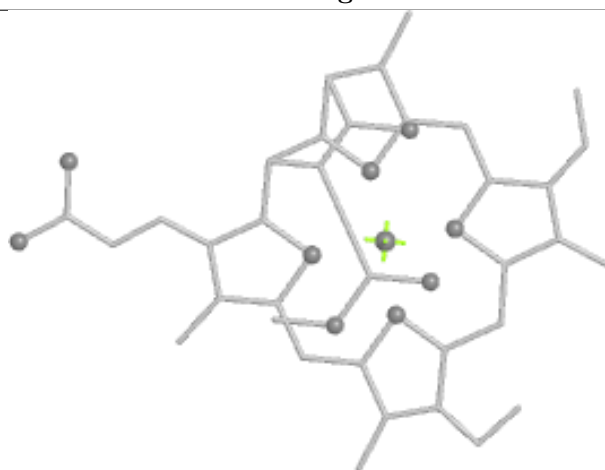
Bond lengths



Bond angles

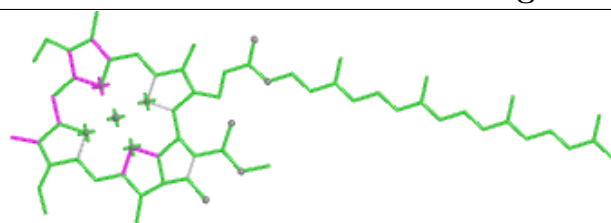


Torsions

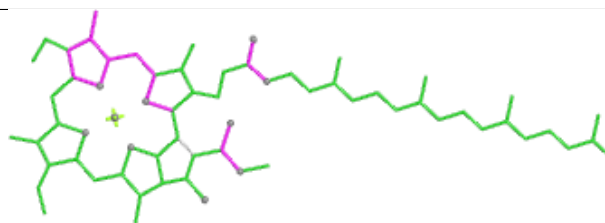


Rings

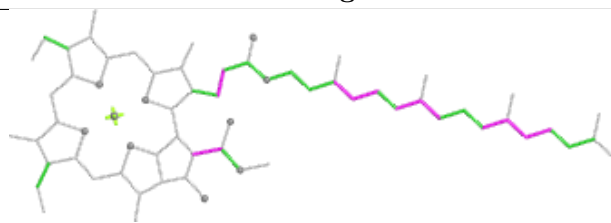
Ligand CLA b 308



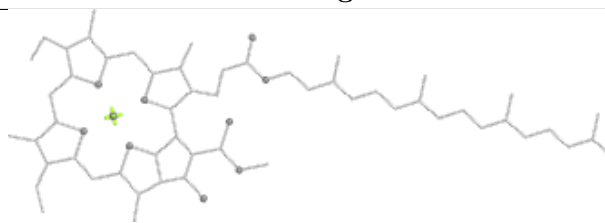
Bond lengths



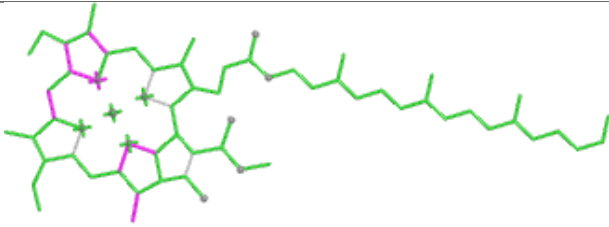
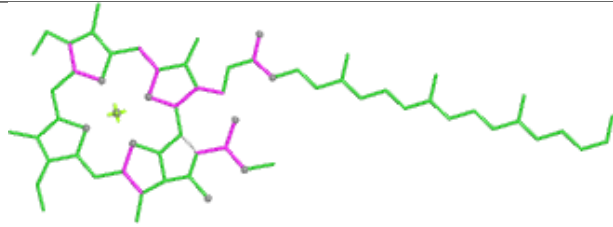
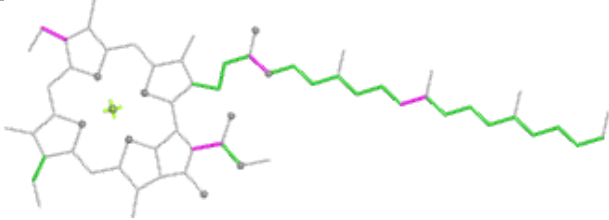
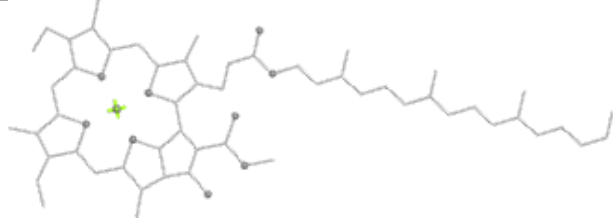
Bond angles

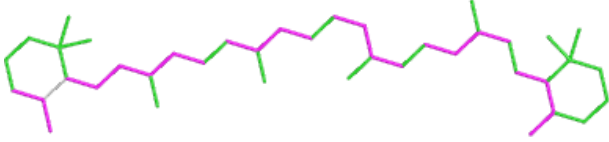
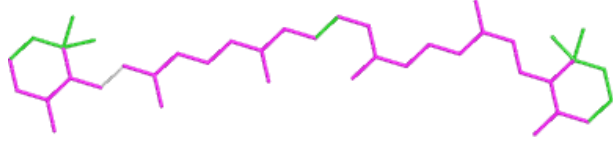
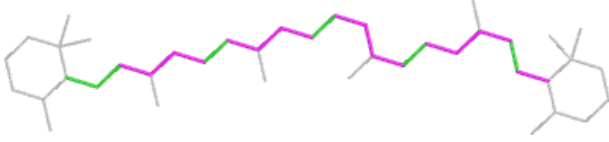
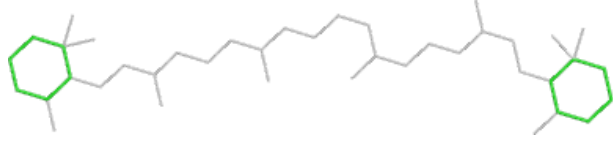


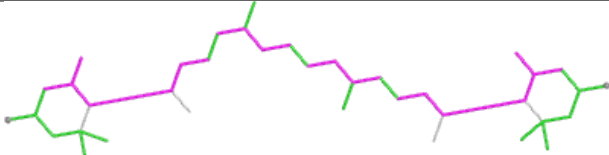
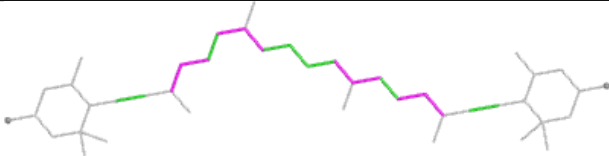
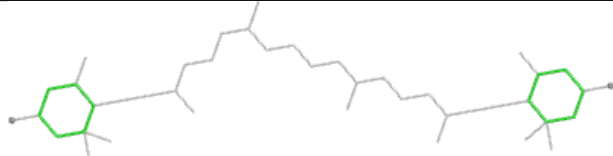
Torsions



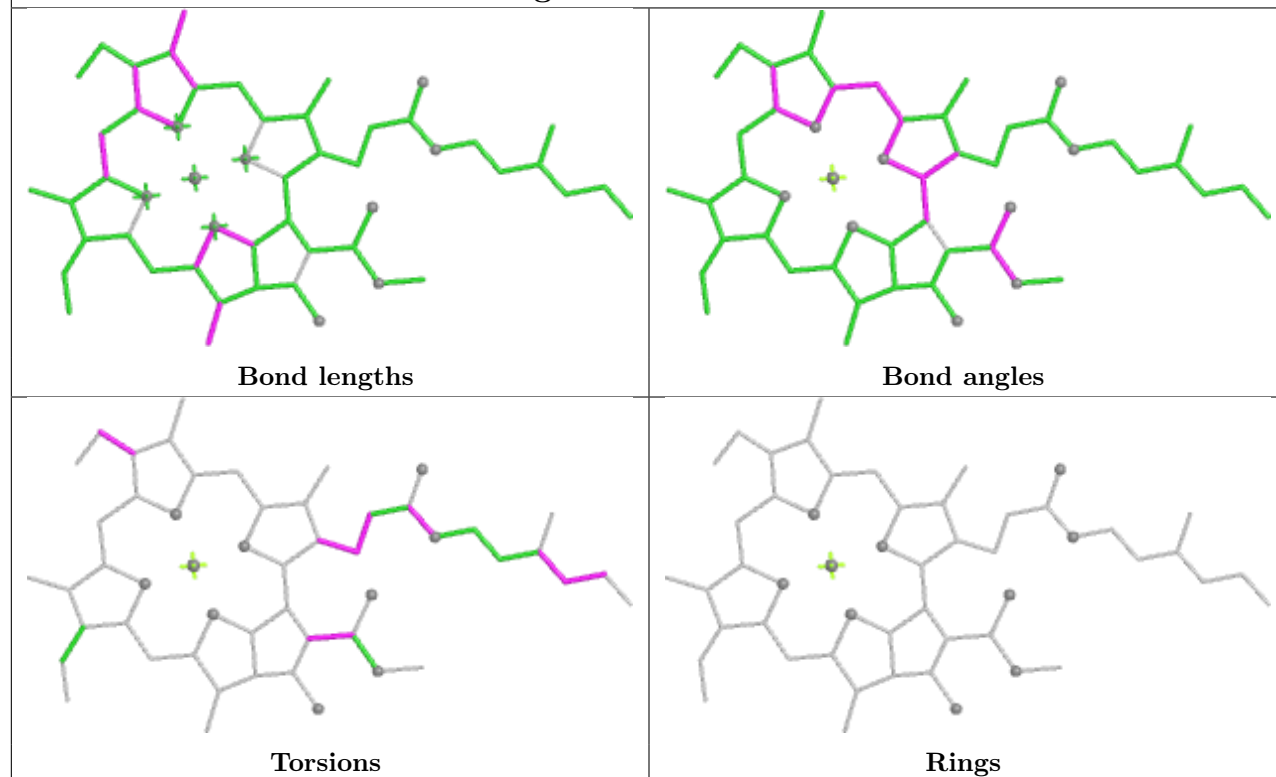
Rings

Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

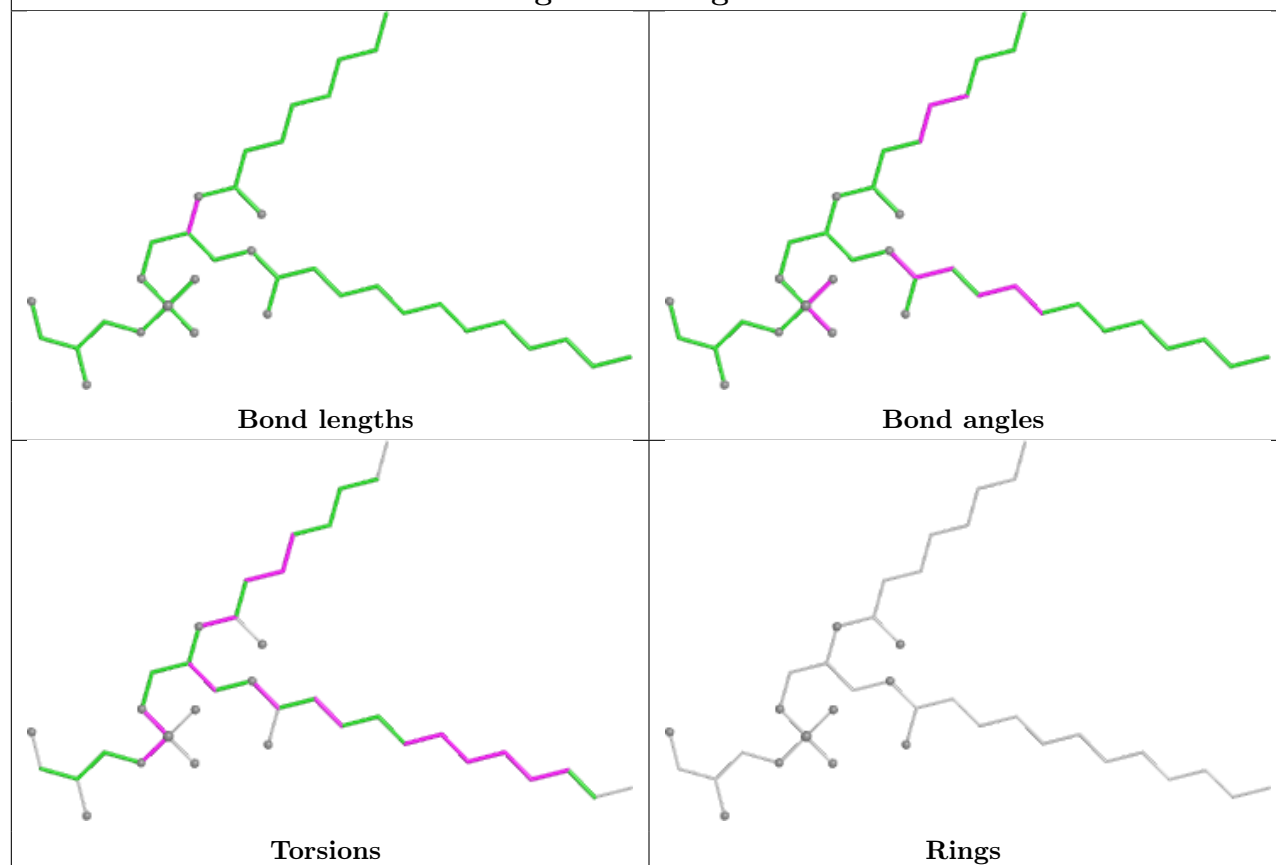
Ligand WVN J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 j 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

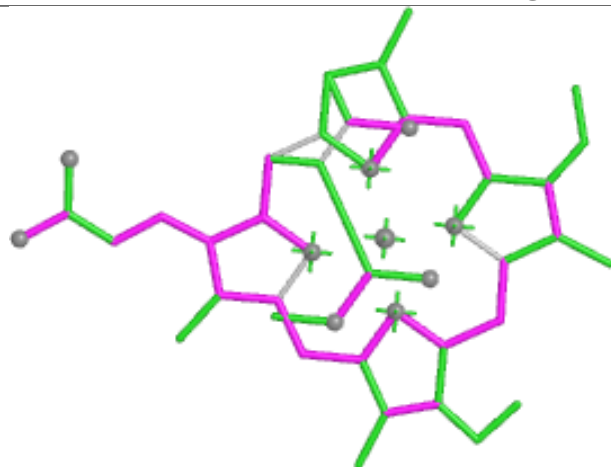
Ligand CLA F 203



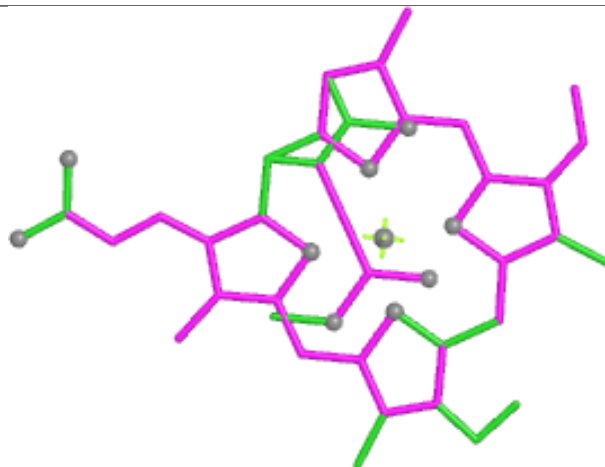
Ligand LHG g 322



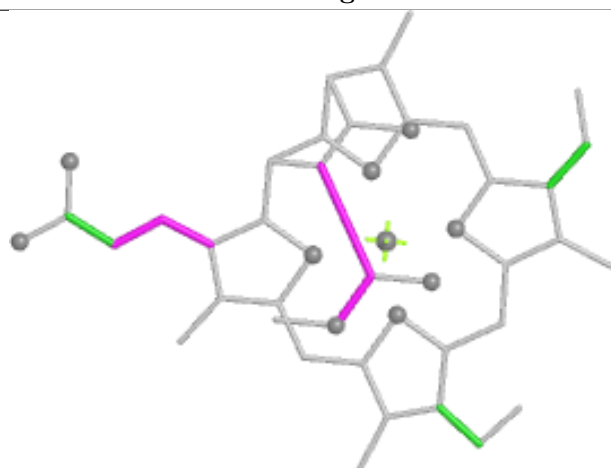
Ligand KC2 l 311



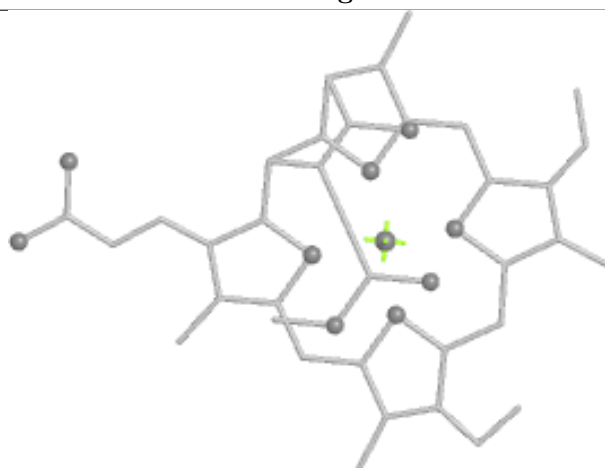
Bond lengths



Bond angles

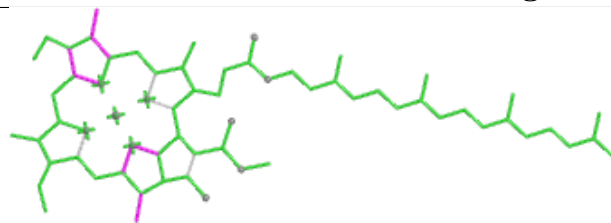


Torsions

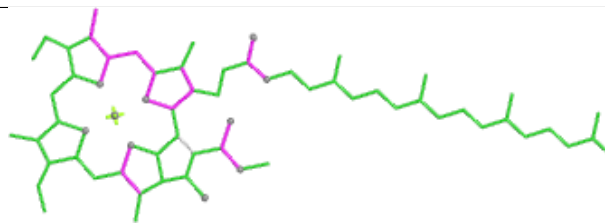


Rings

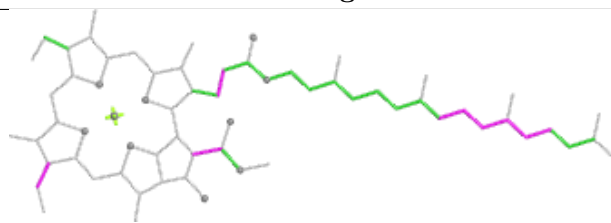
Ligand CLA f 604



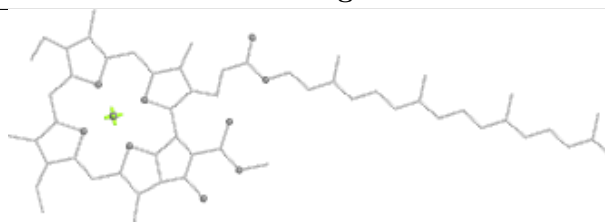
Bond lengths



Bond angles

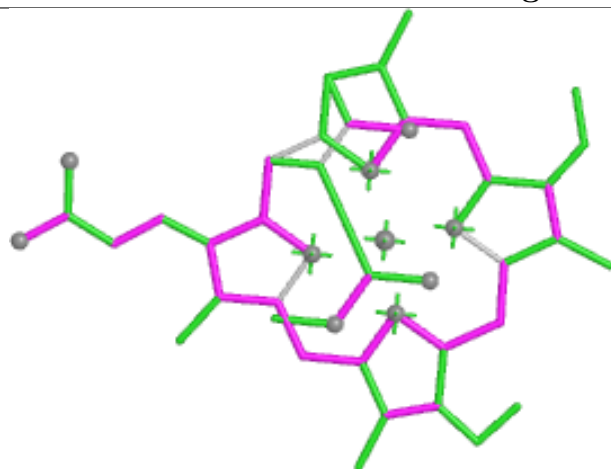


Torsions

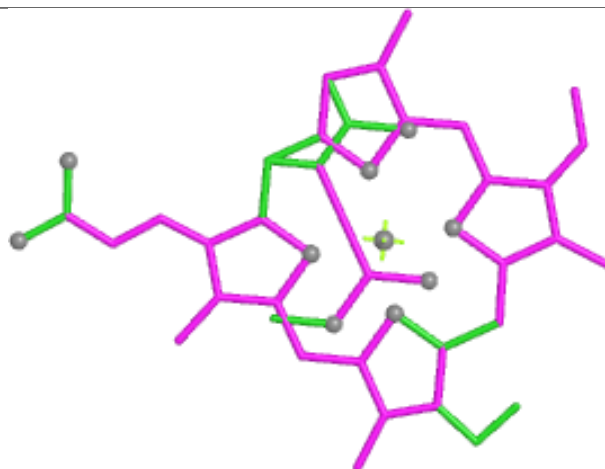


Rings

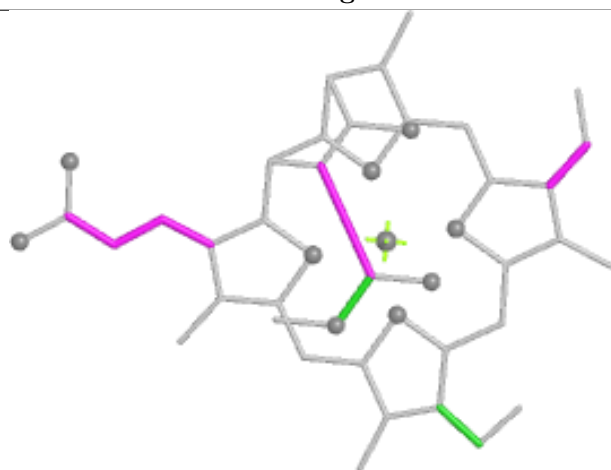
Ligand KC2 s 401



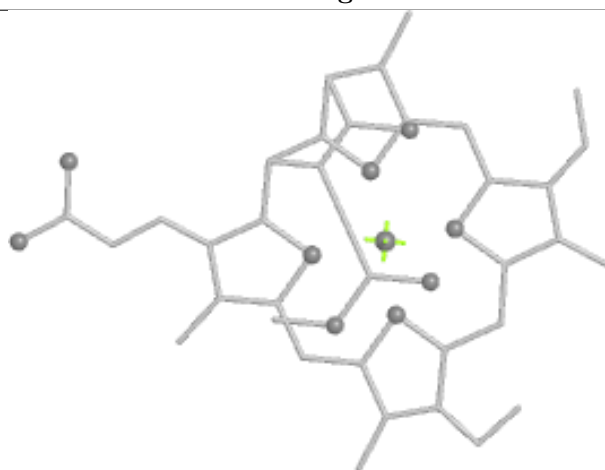
Bond lengths



Bond angles

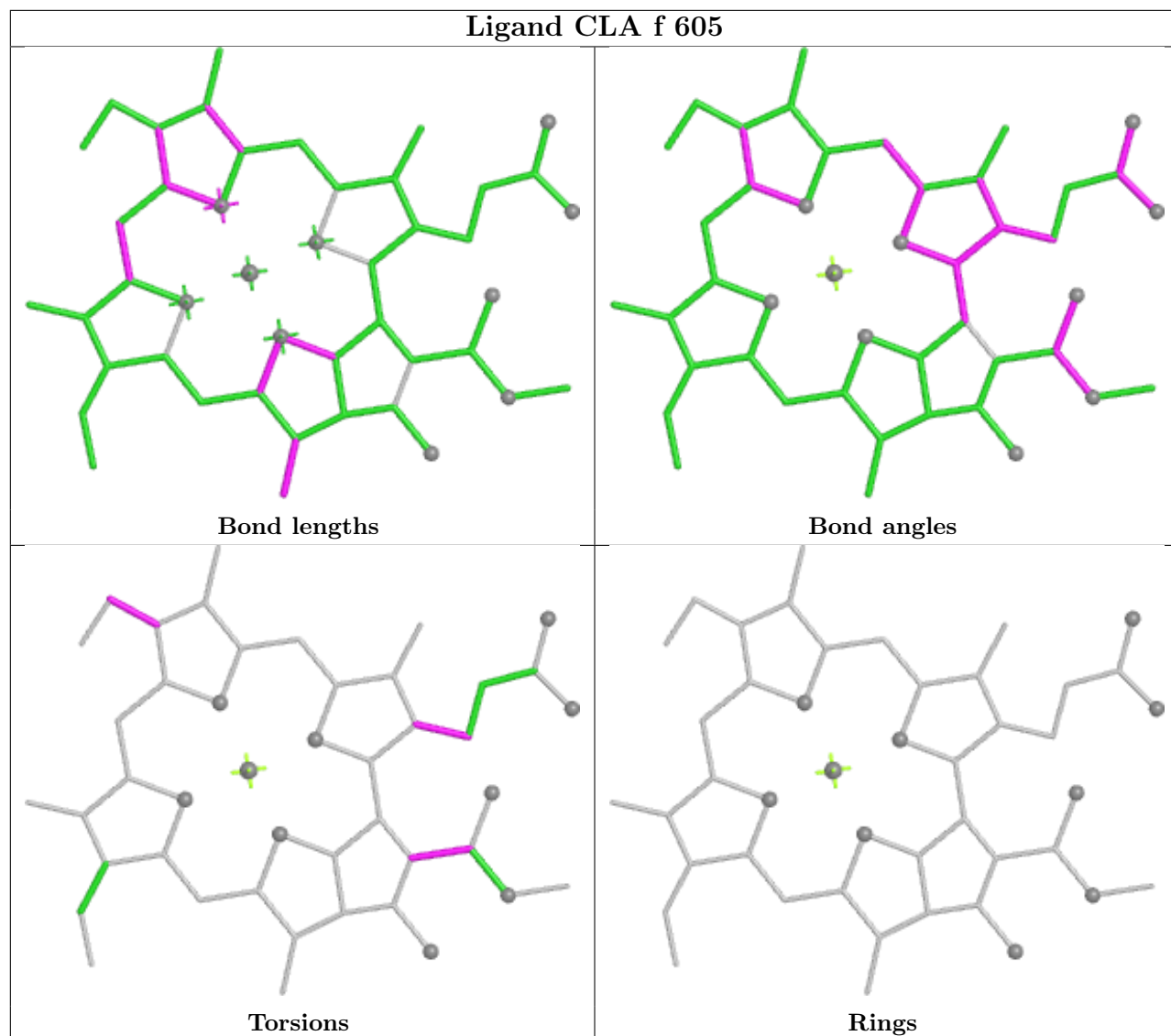


Torsions

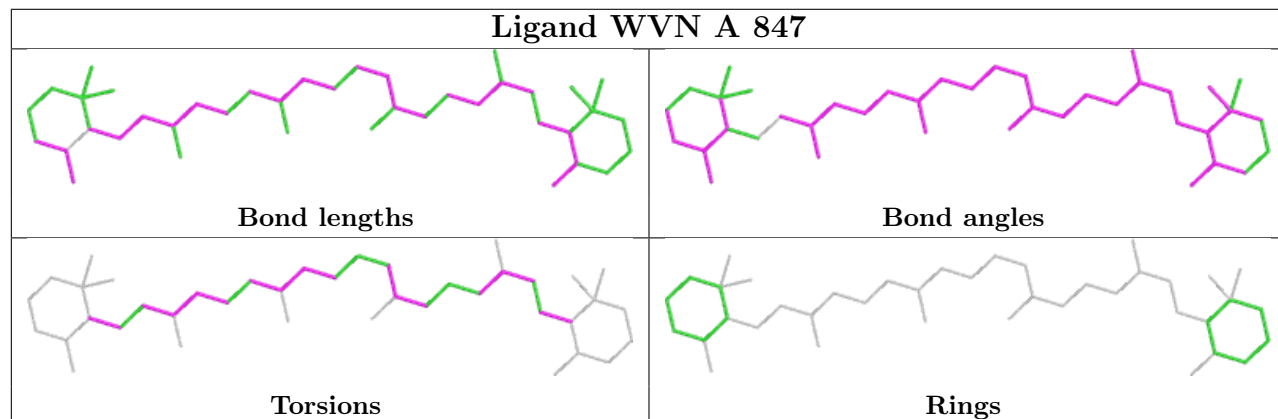


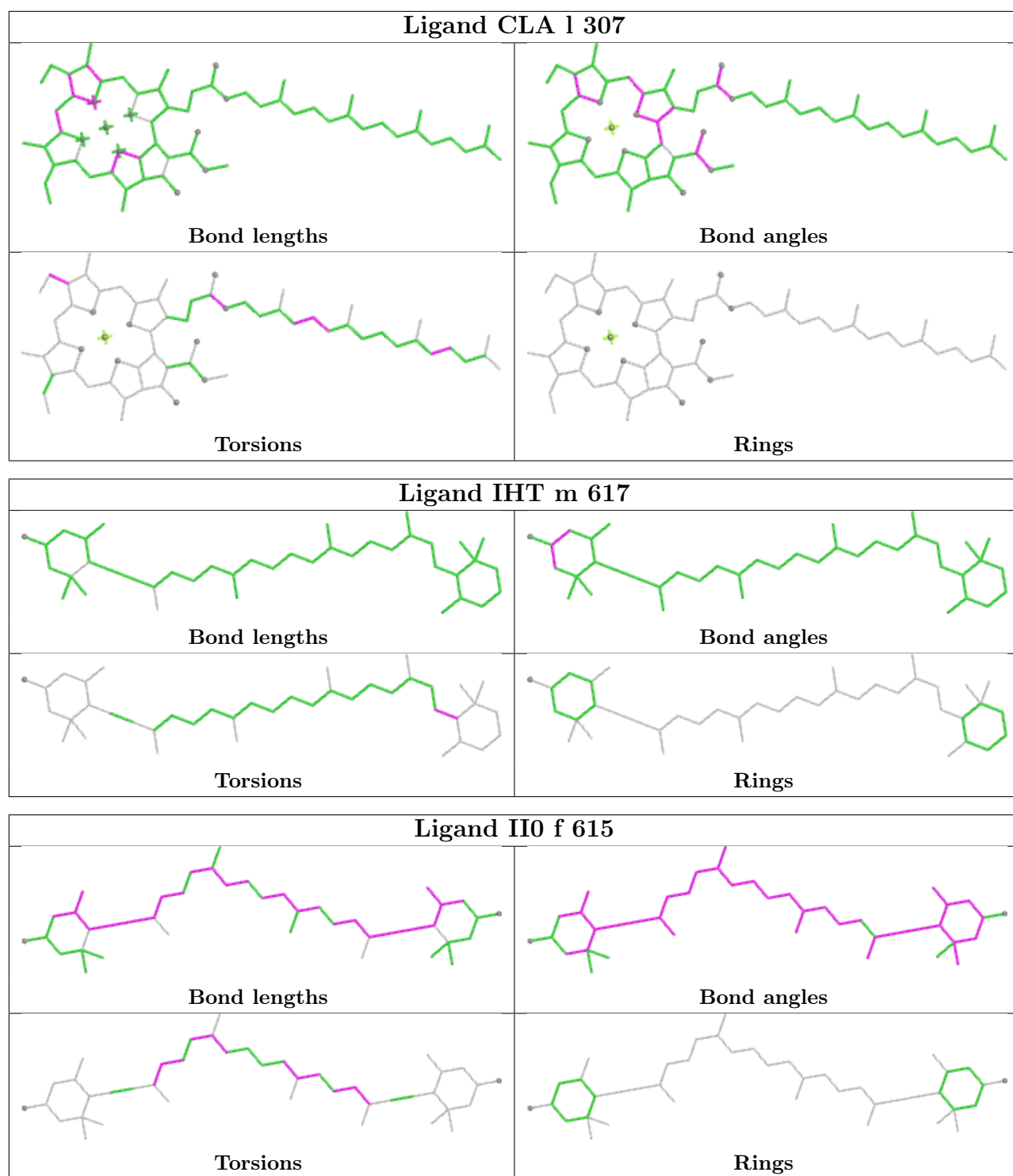
Rings

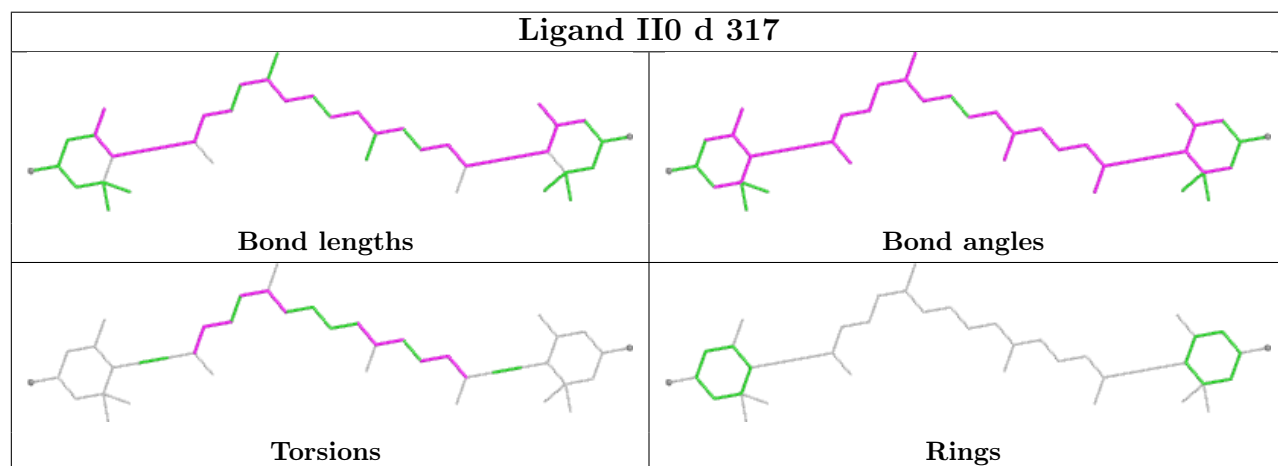
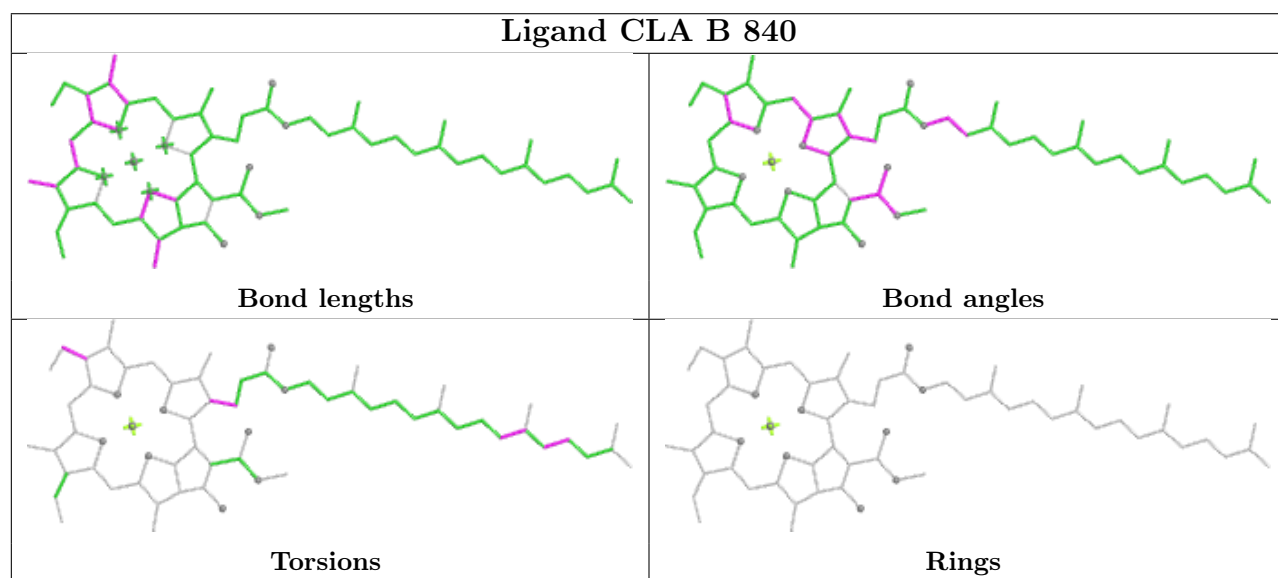
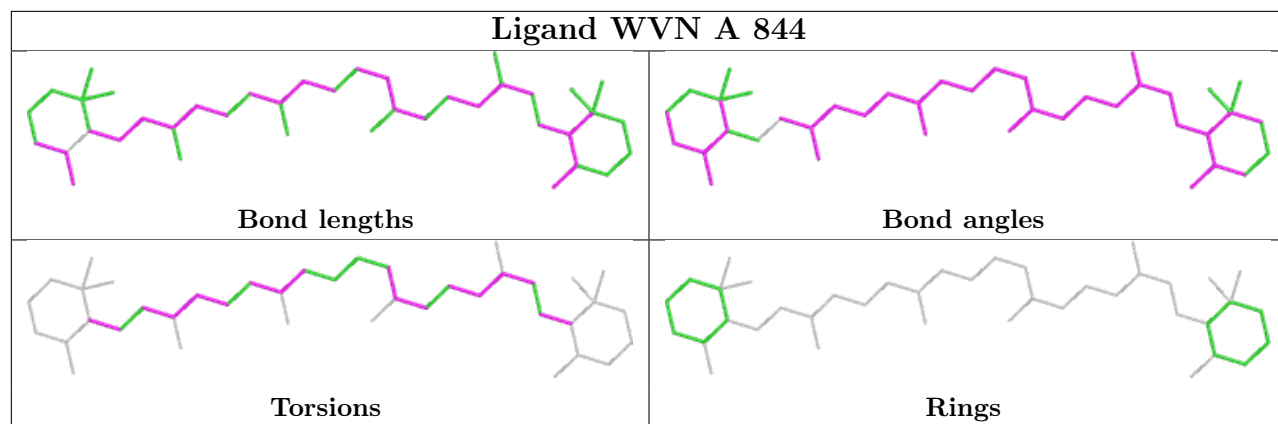
Ligand CLA f 605



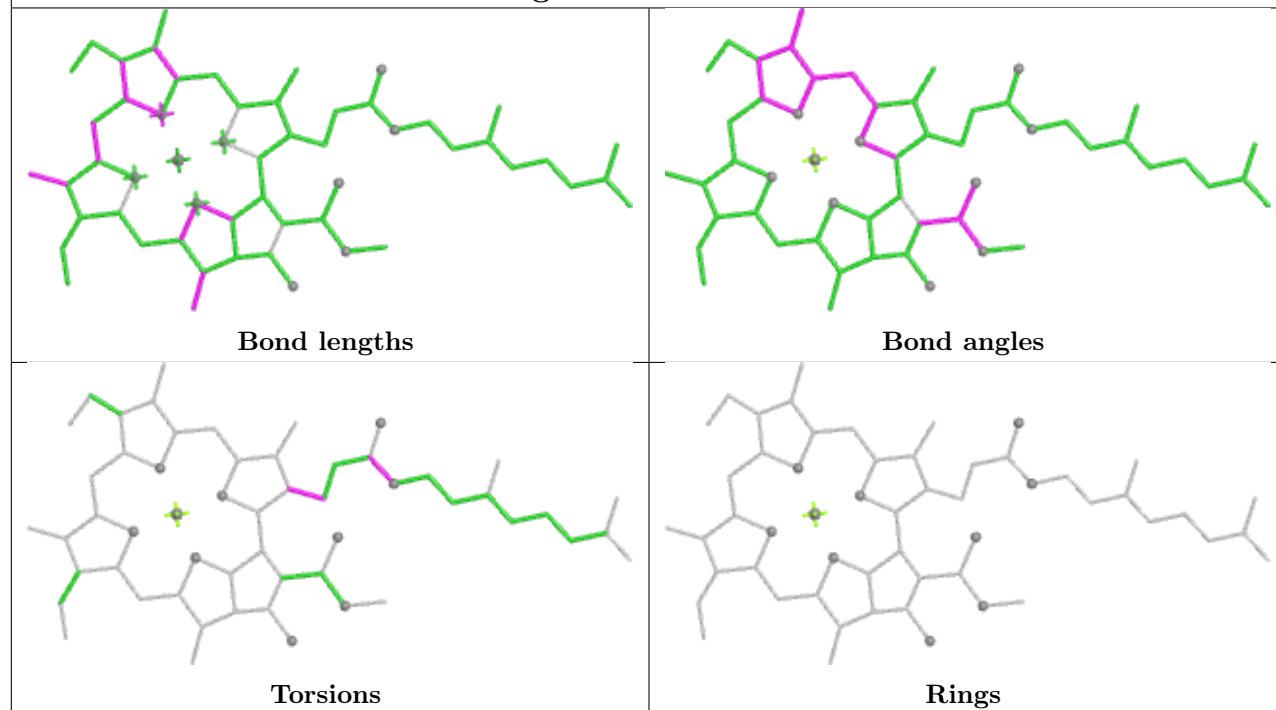
Ligand WVN A 847



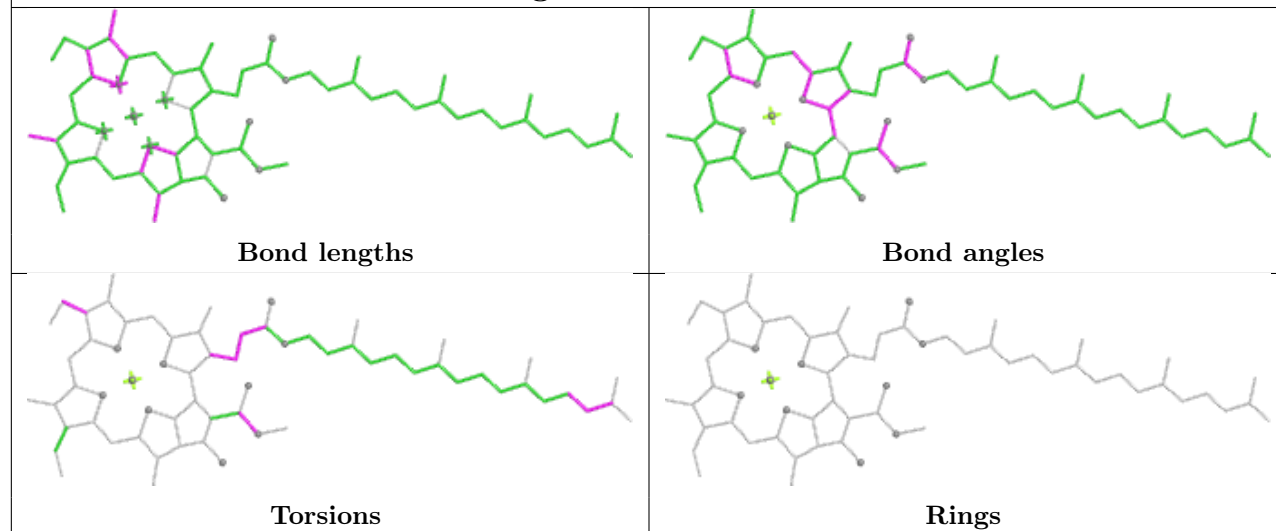


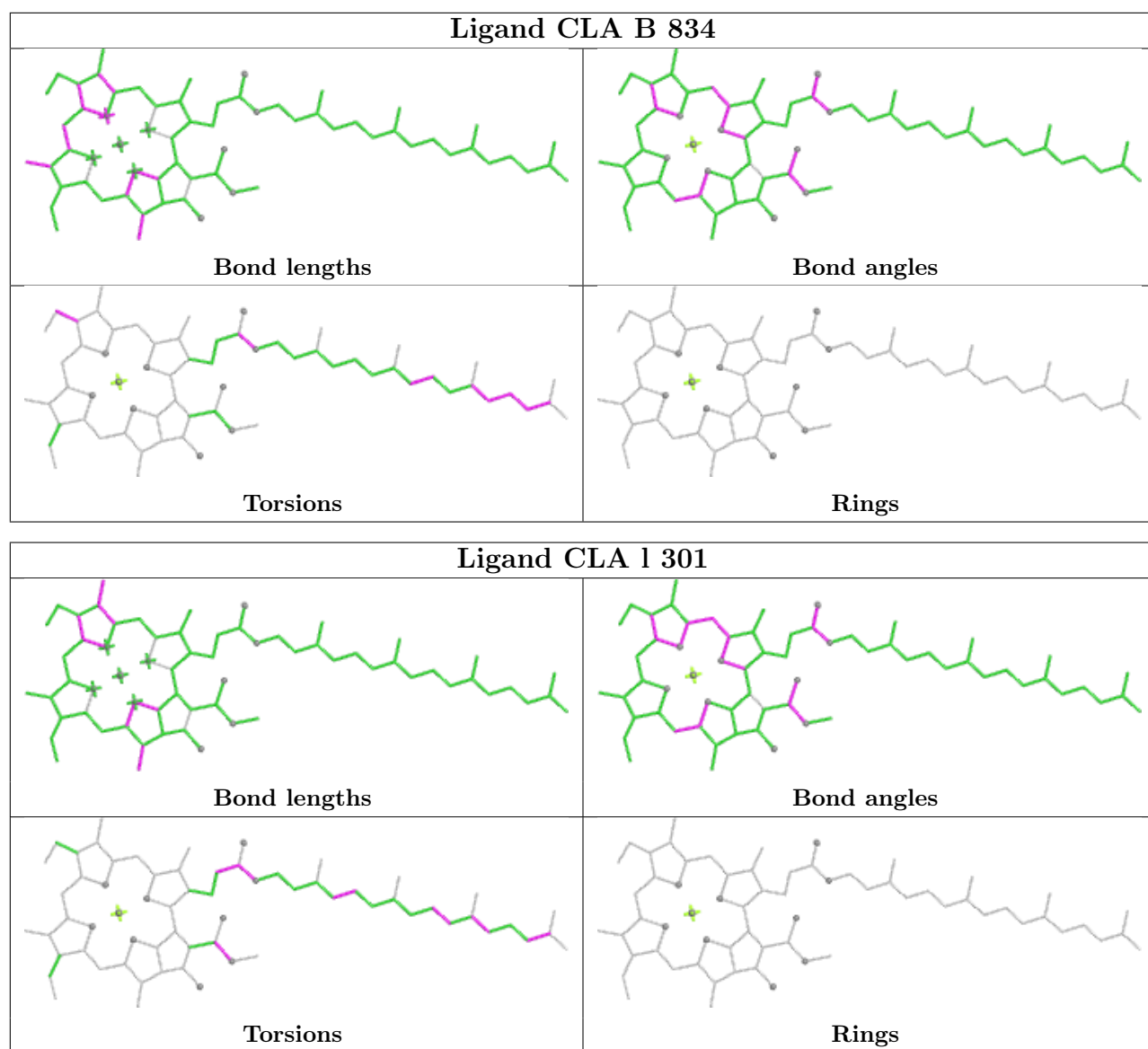


Ligand CLA B 815

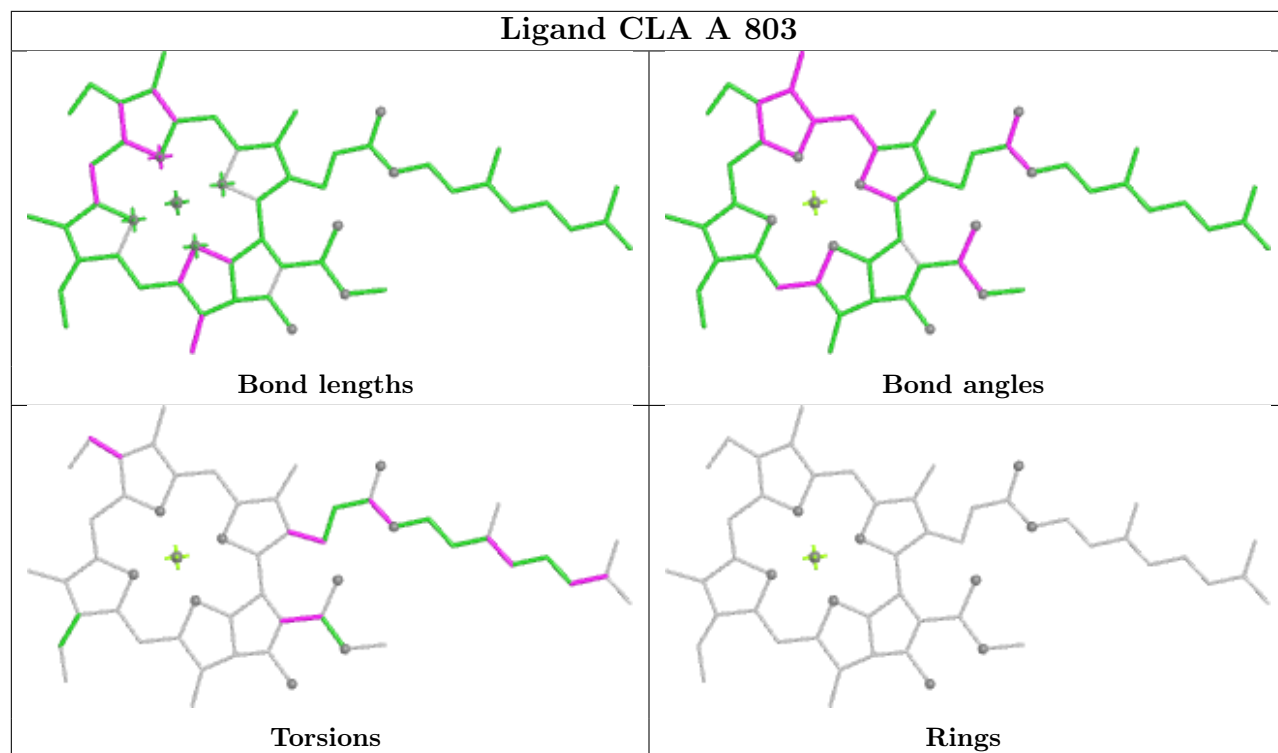


Ligand CLA A 808

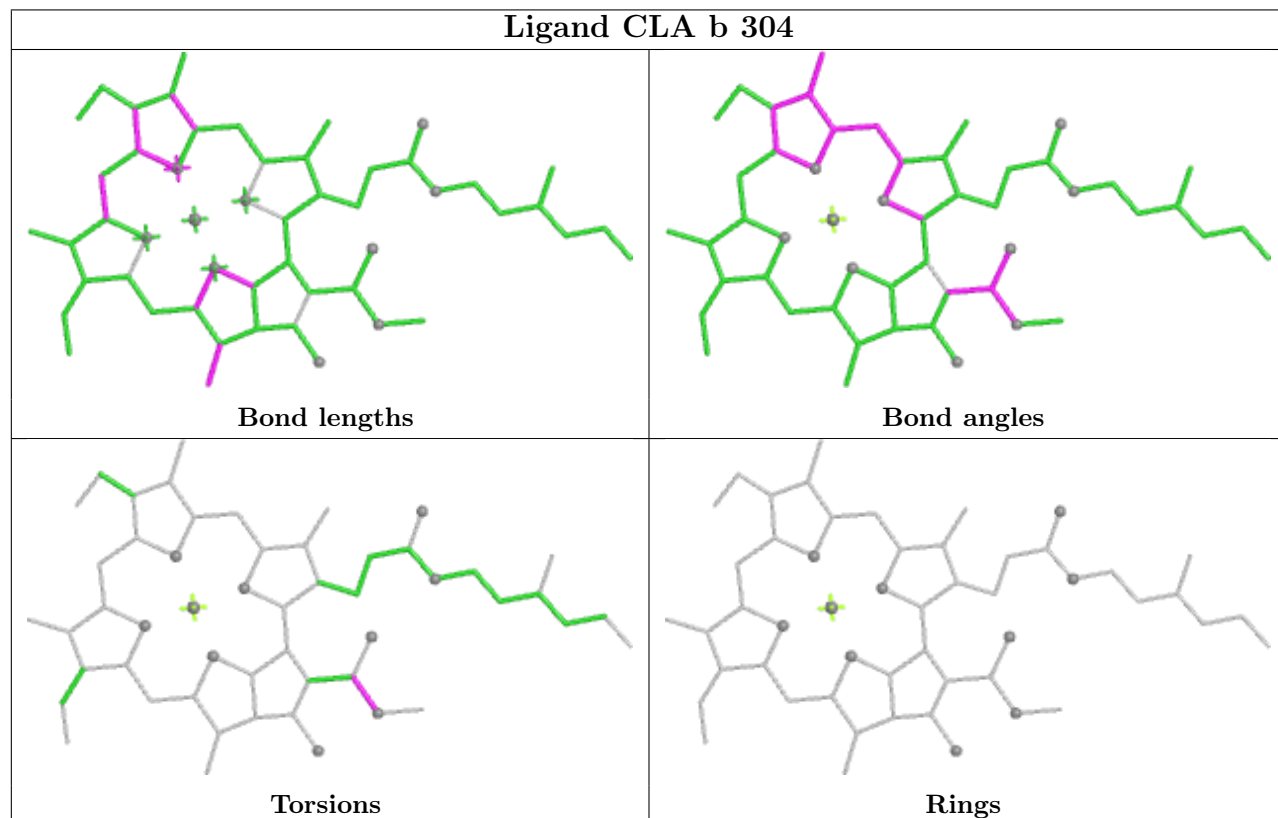




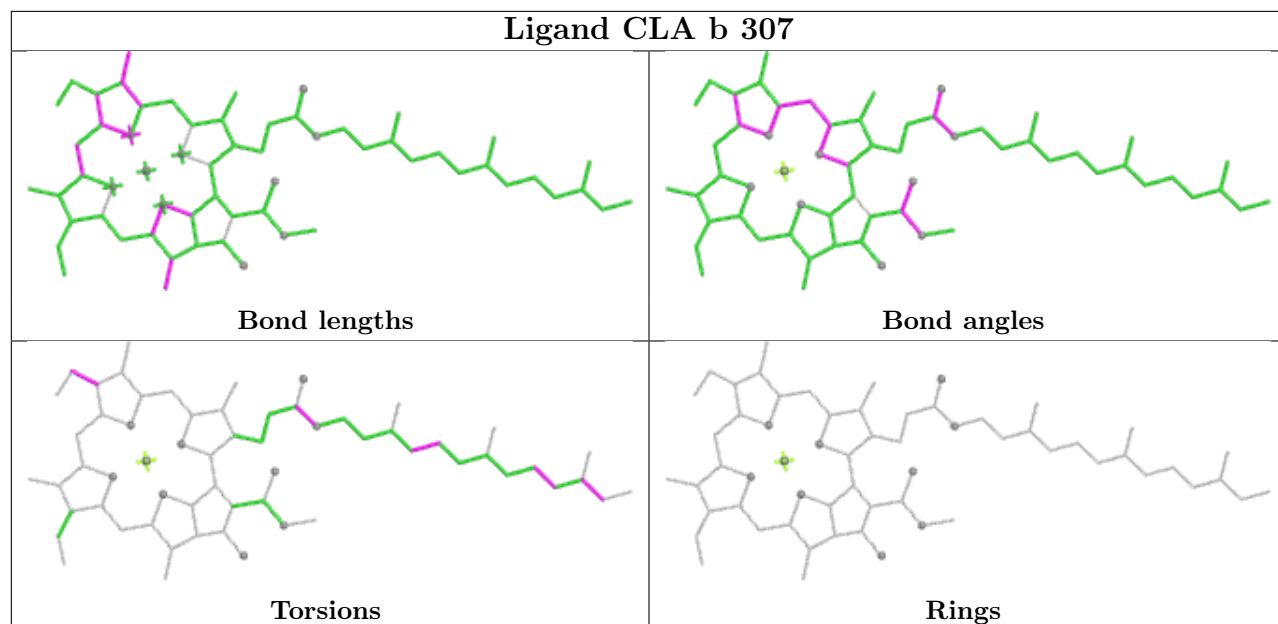
Ligand CLA A 803



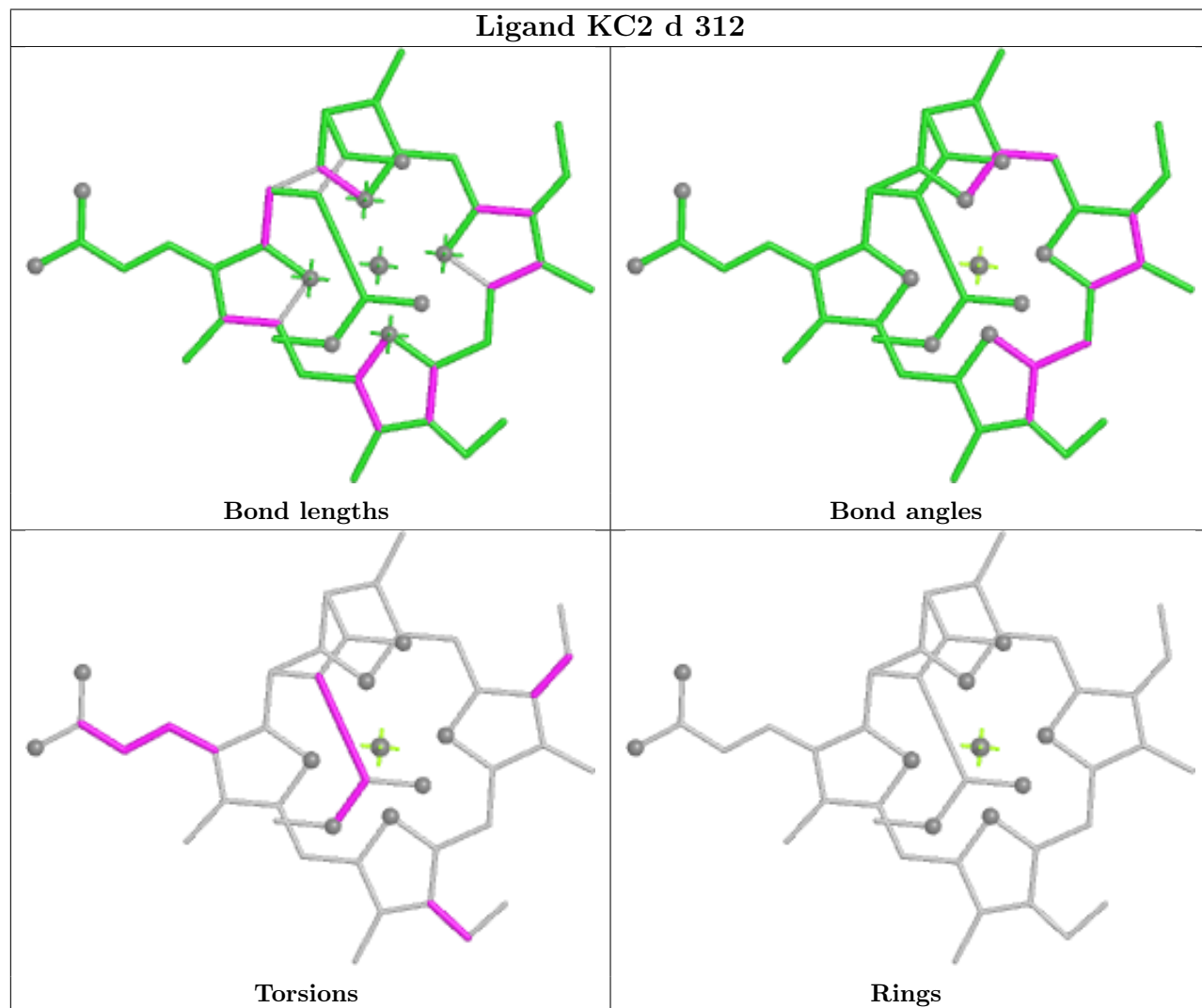
Ligand CLA b 304

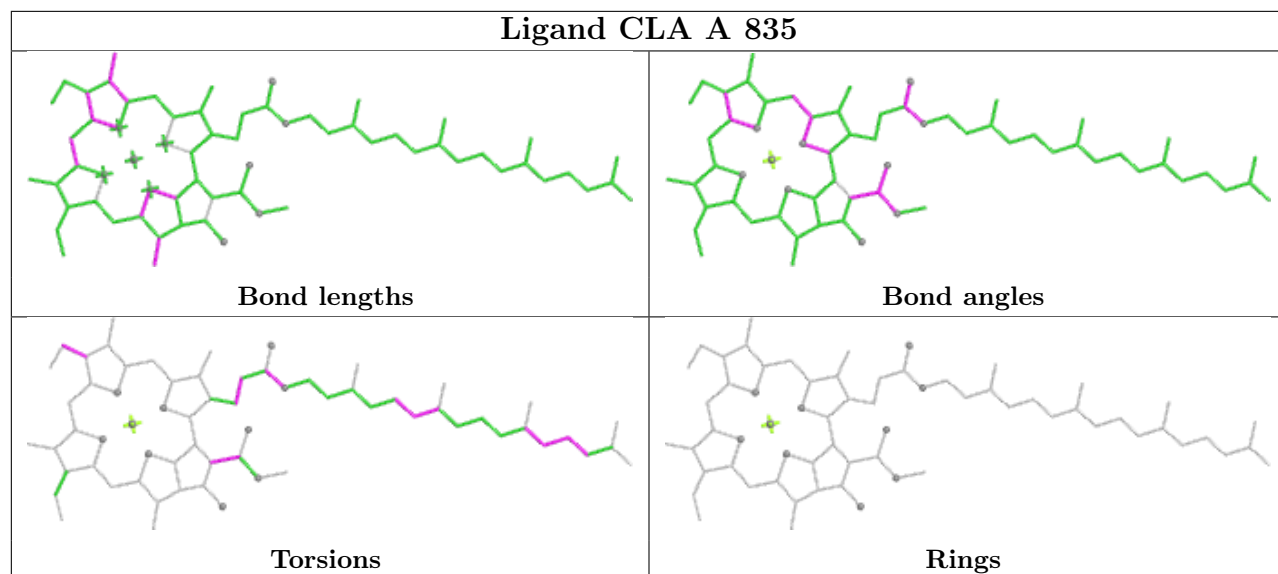
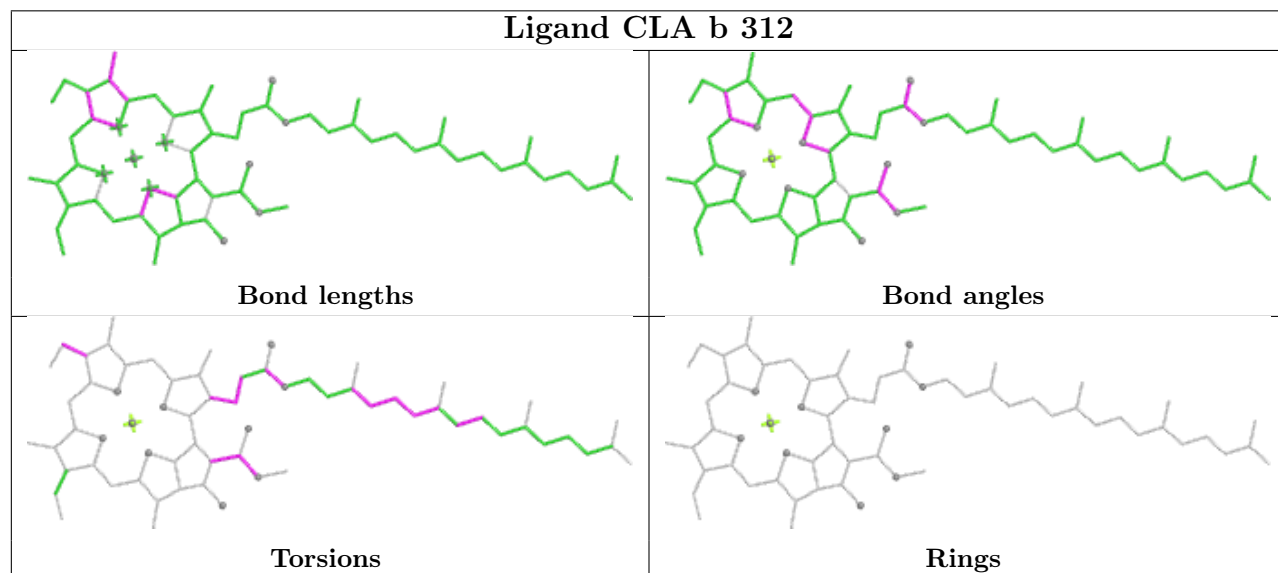


Ligand CLA b 307

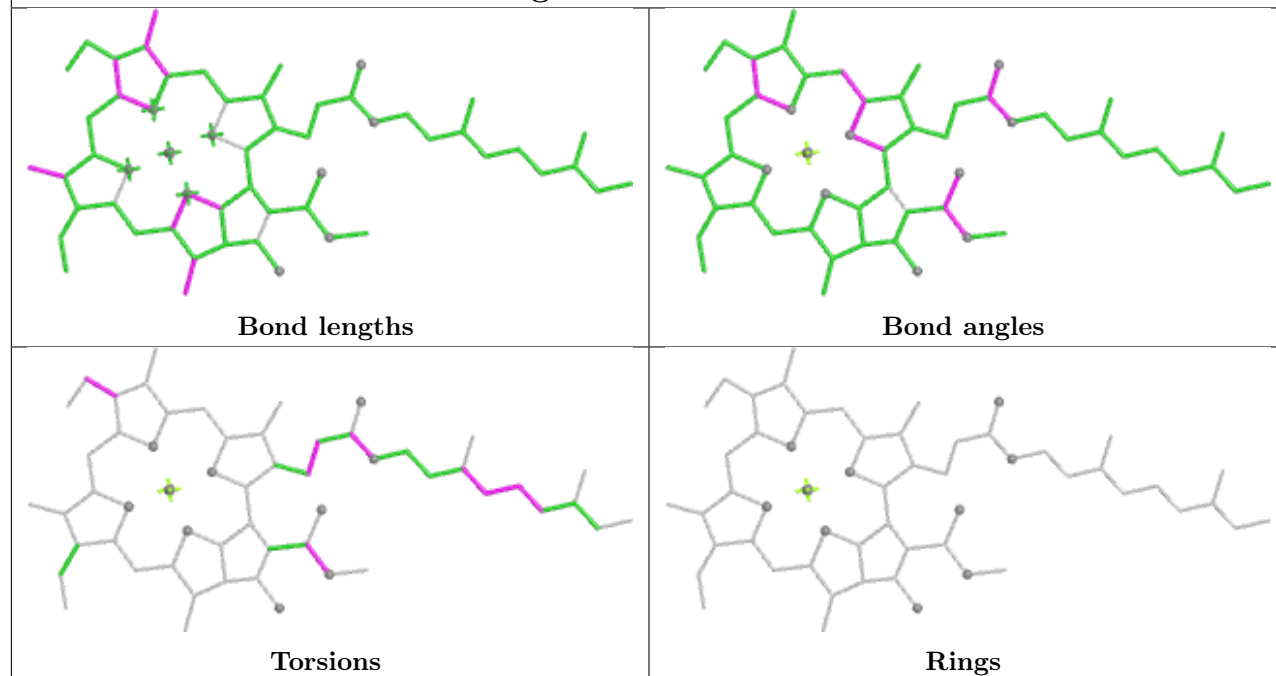


Ligand KC2 d 312

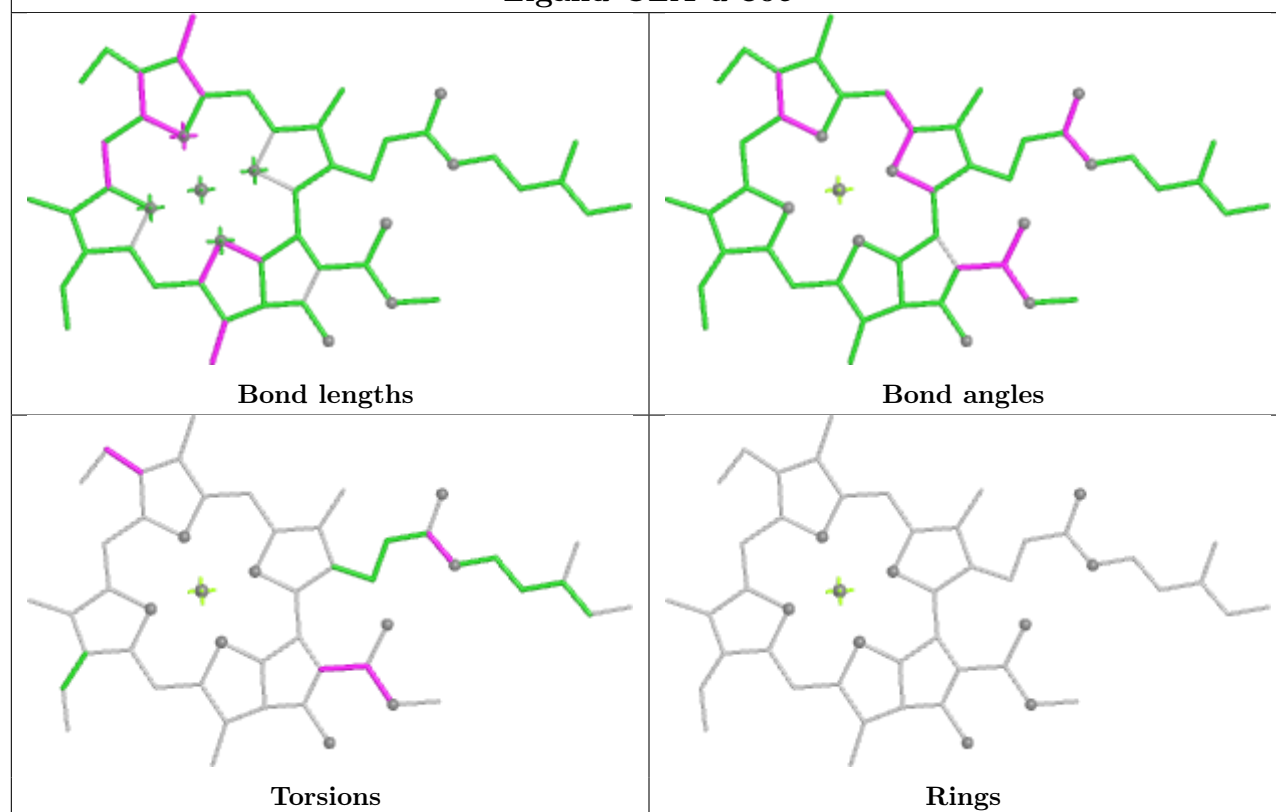


Ligand CLA A 835**Ligand CLA b 312**

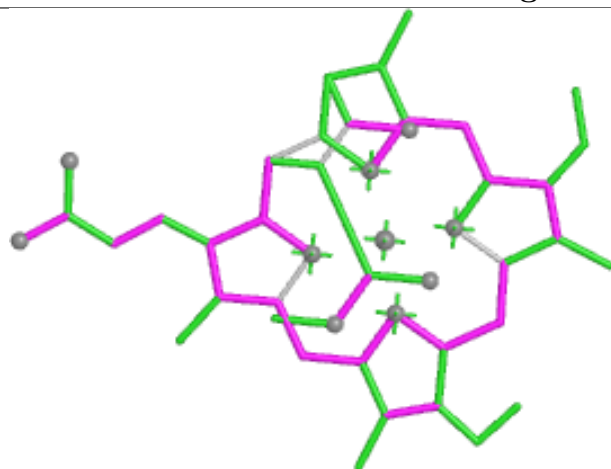
Ligand CLA A 809



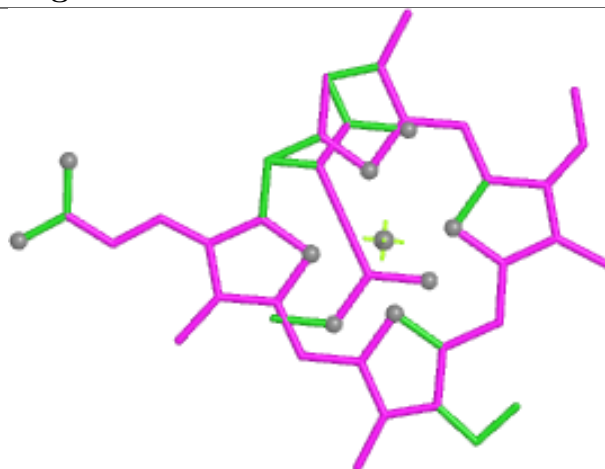
Ligand CLA d 306



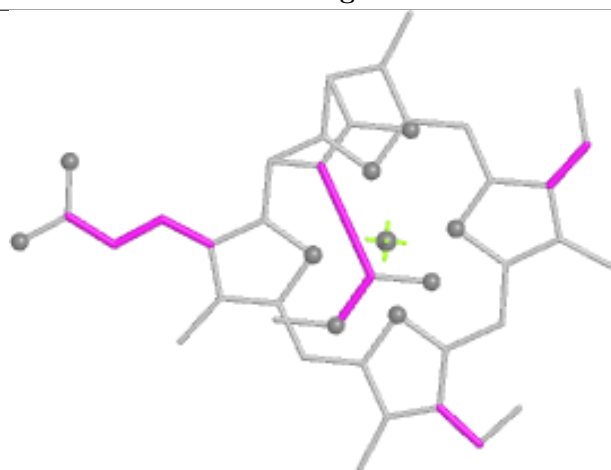
Ligand KC2 g 314



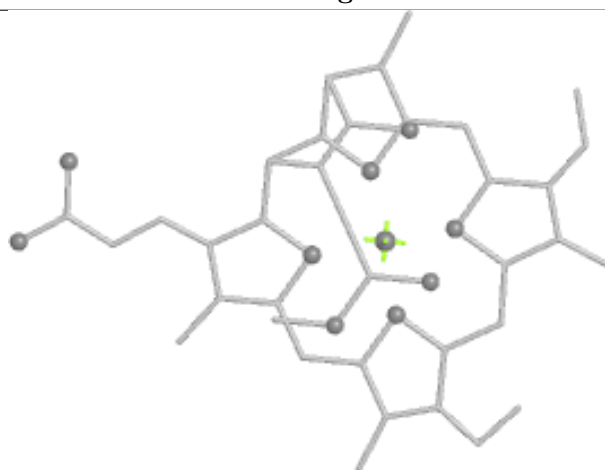
Bond lengths



Bond angles

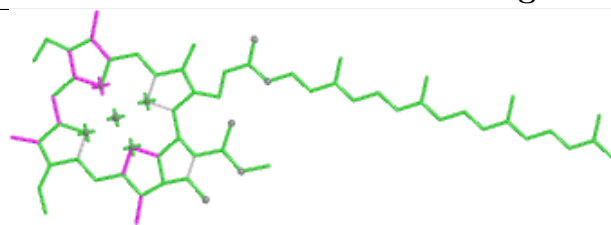


Torsions

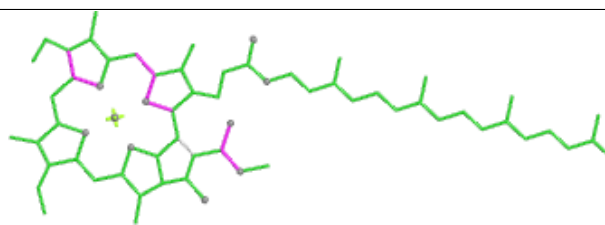


Rings

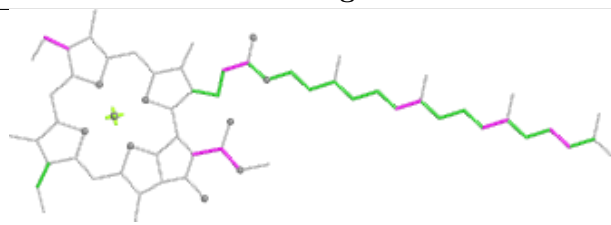
Ligand CLA a 310



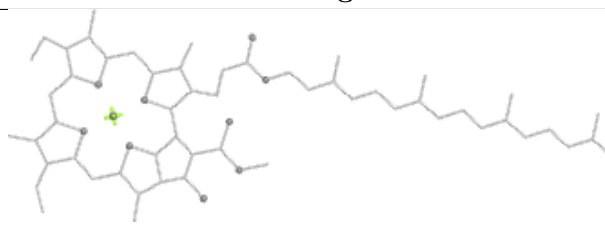
Bond lengths



Bond angles

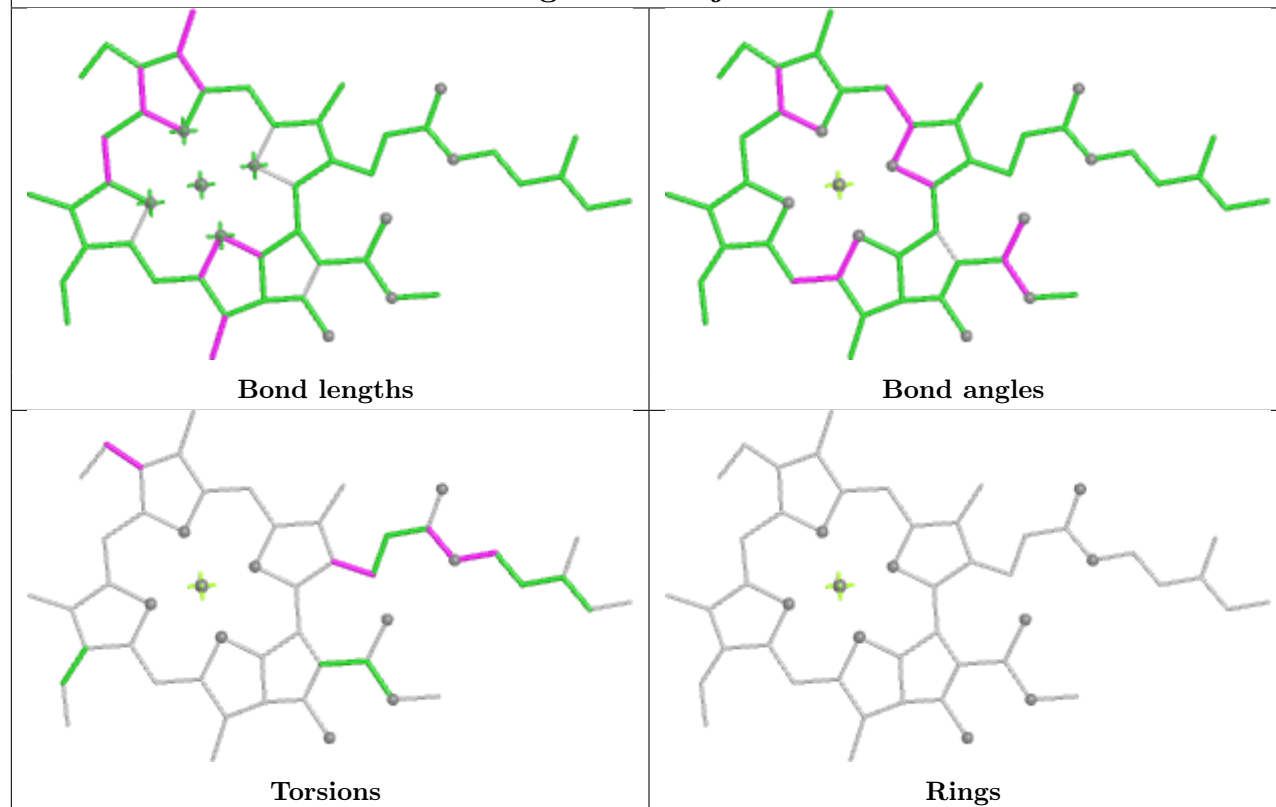


Torsions

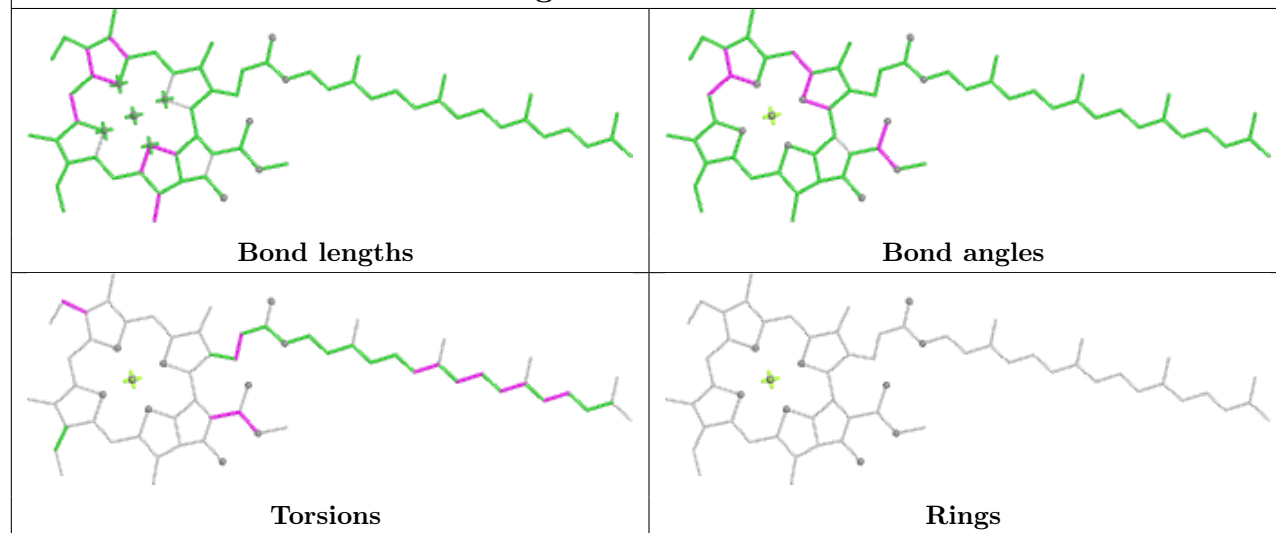


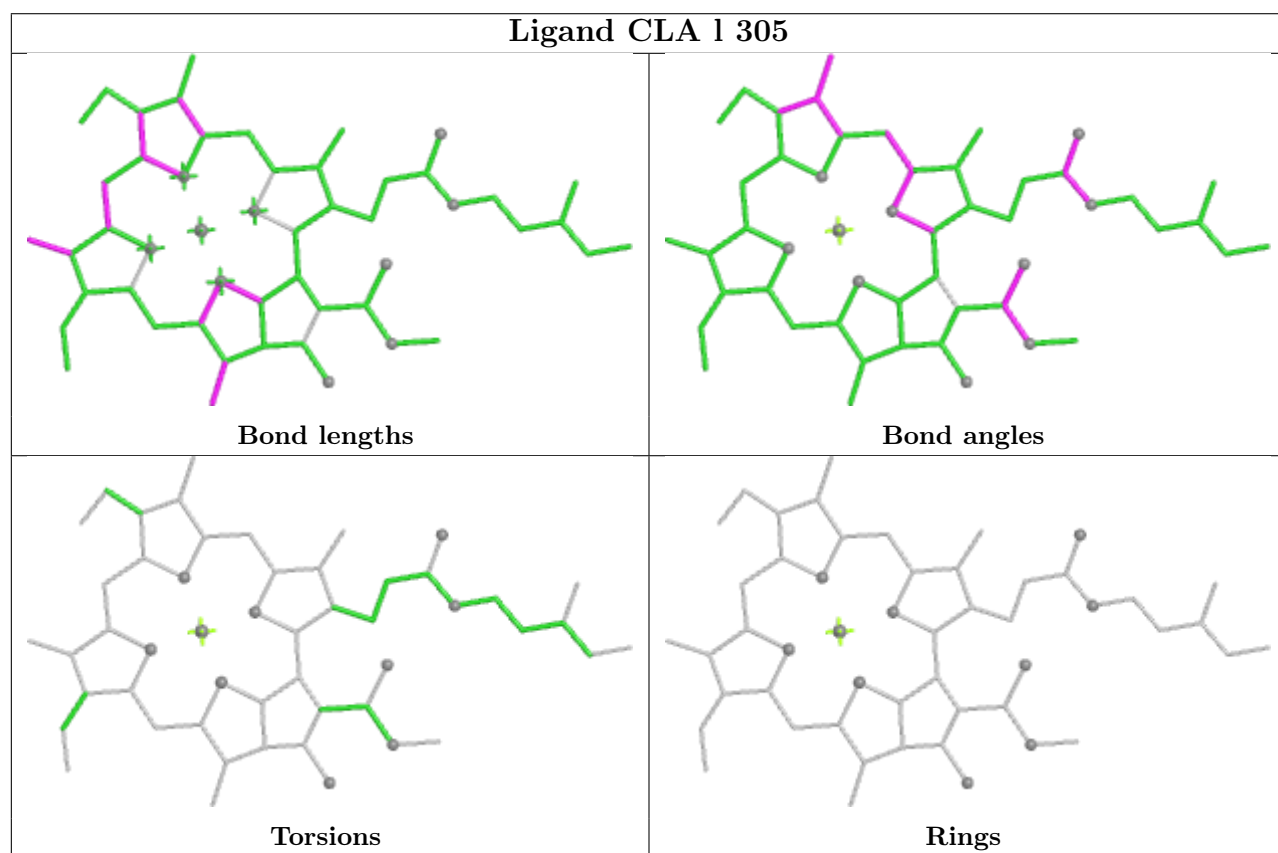
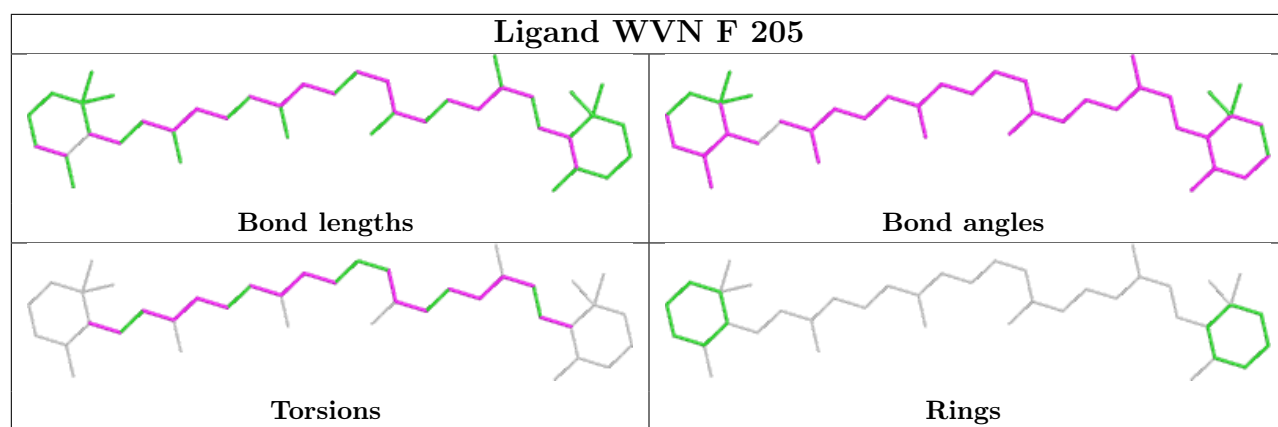
Rings

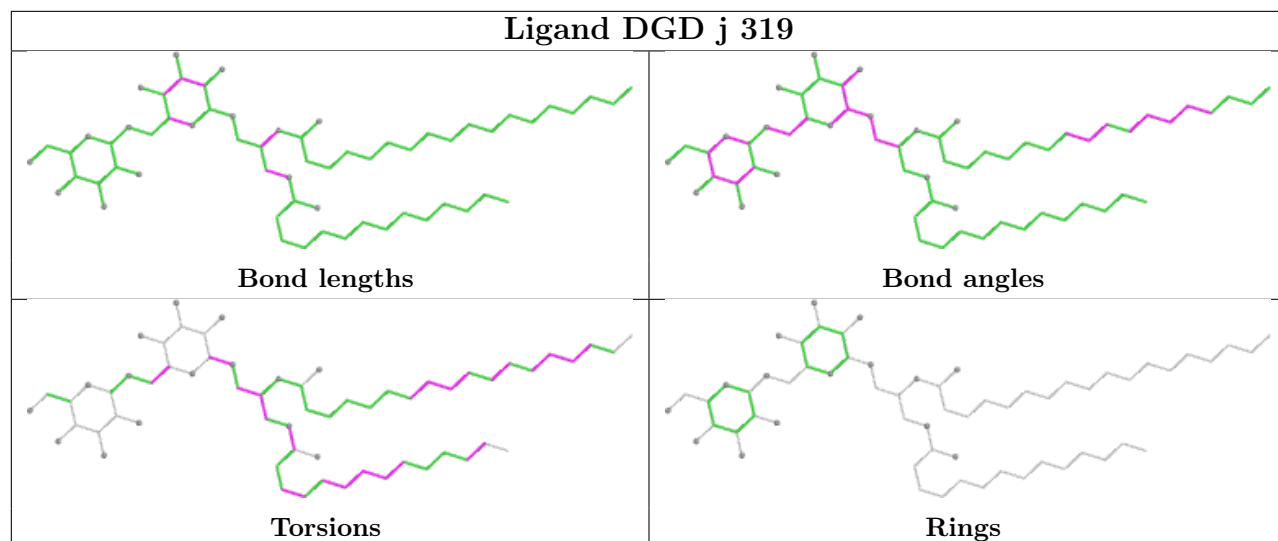
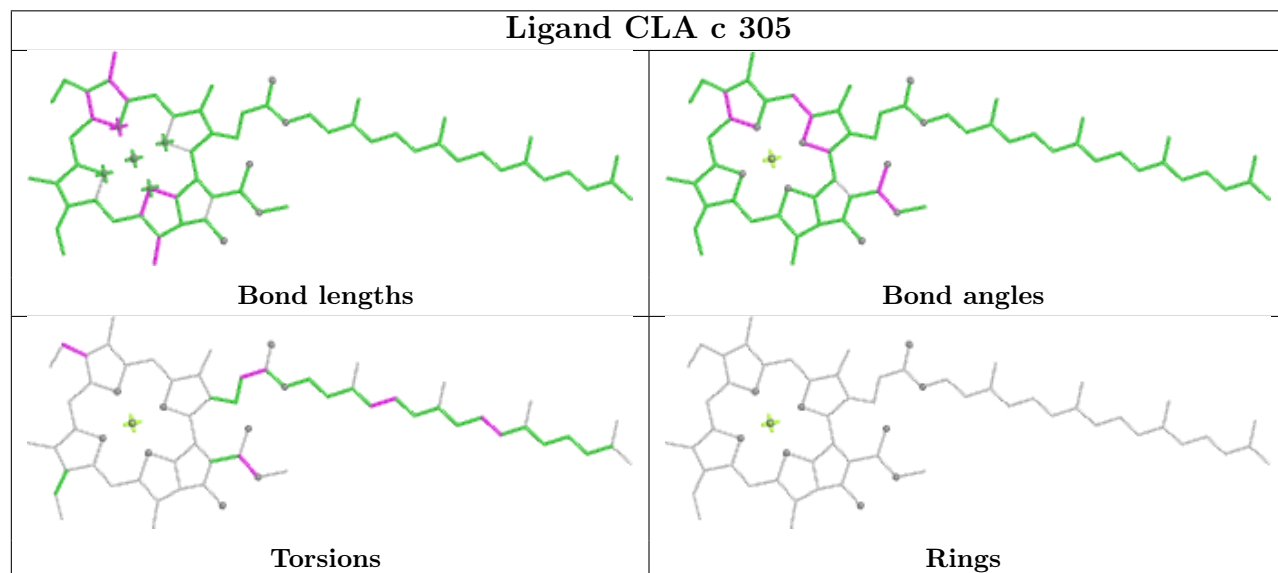
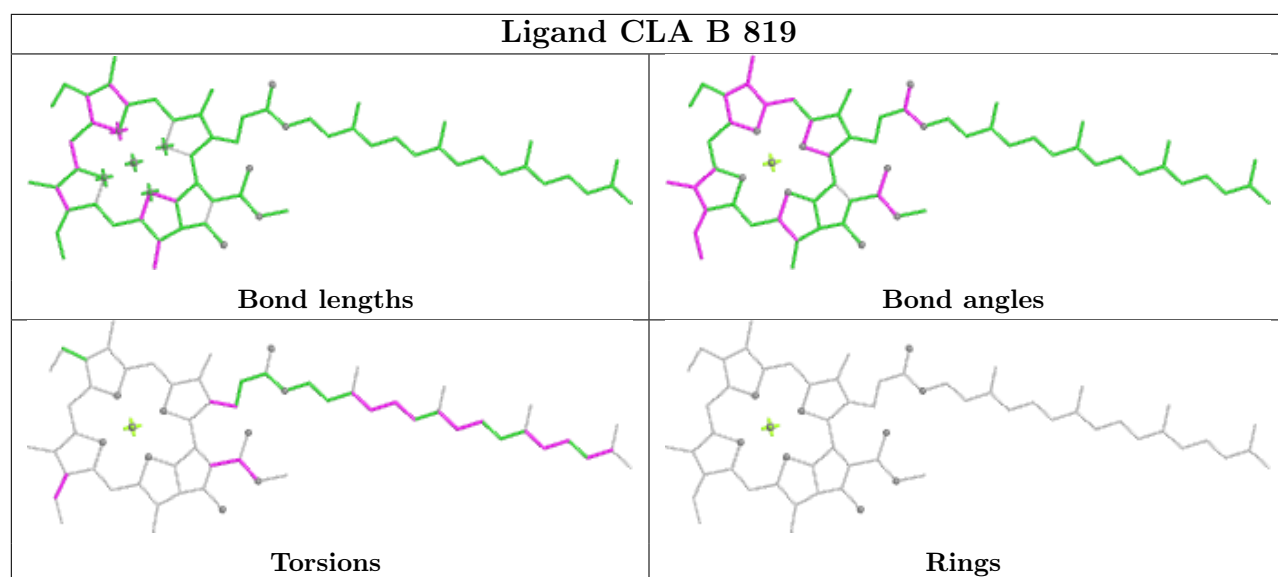
Ligand CLA j 307



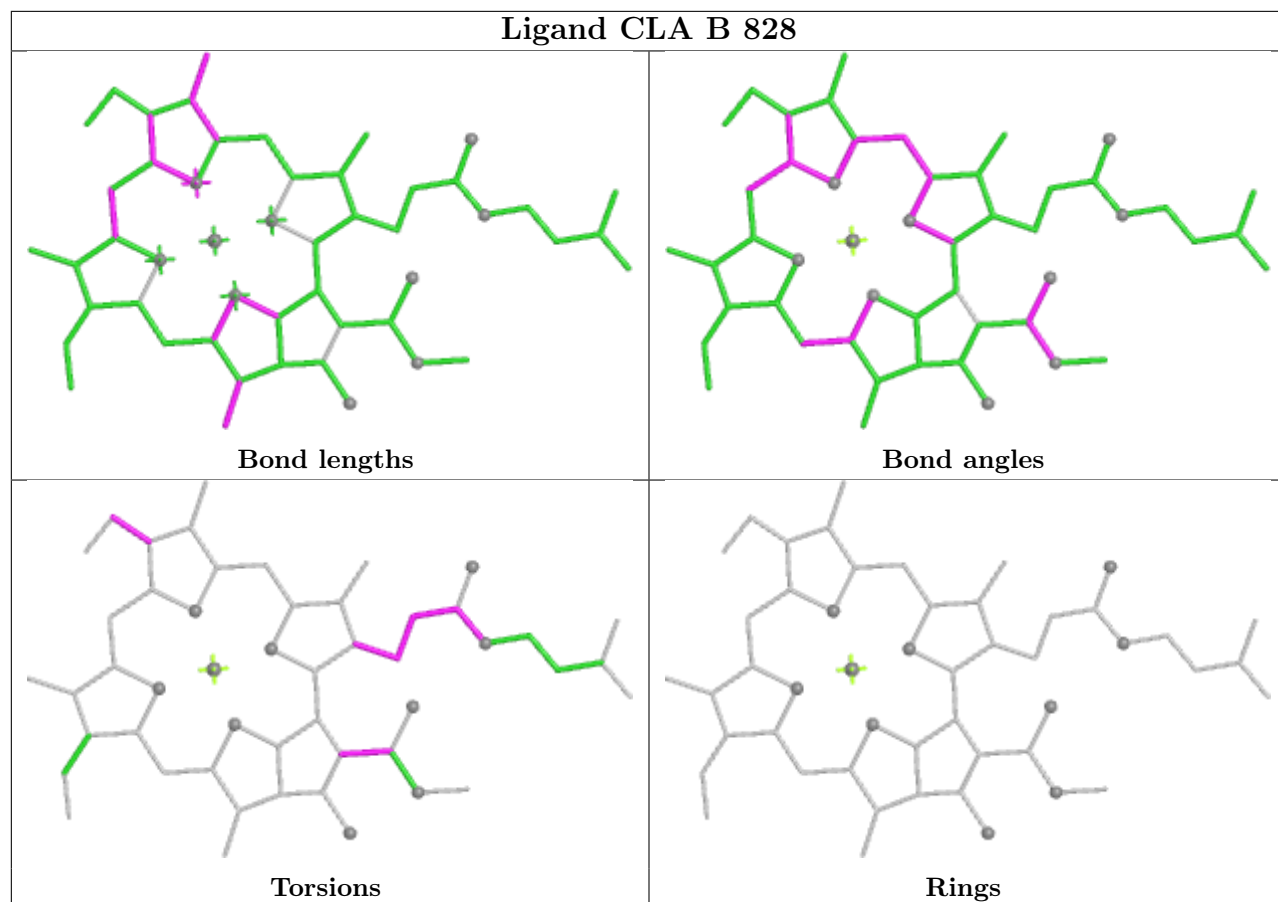
Ligand CLA b 305



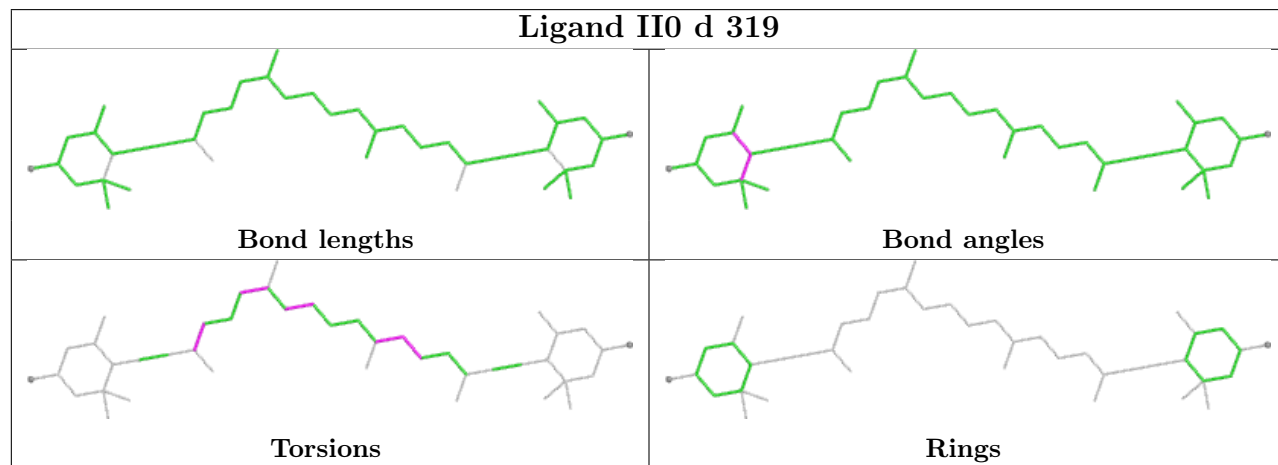




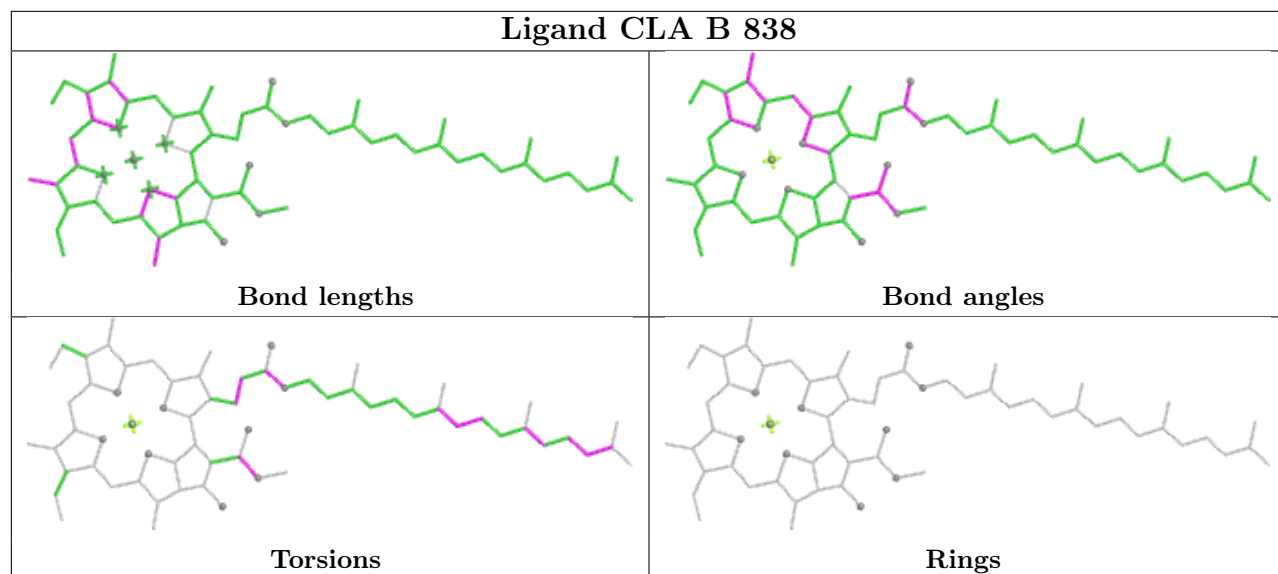
Ligand CLA B 828



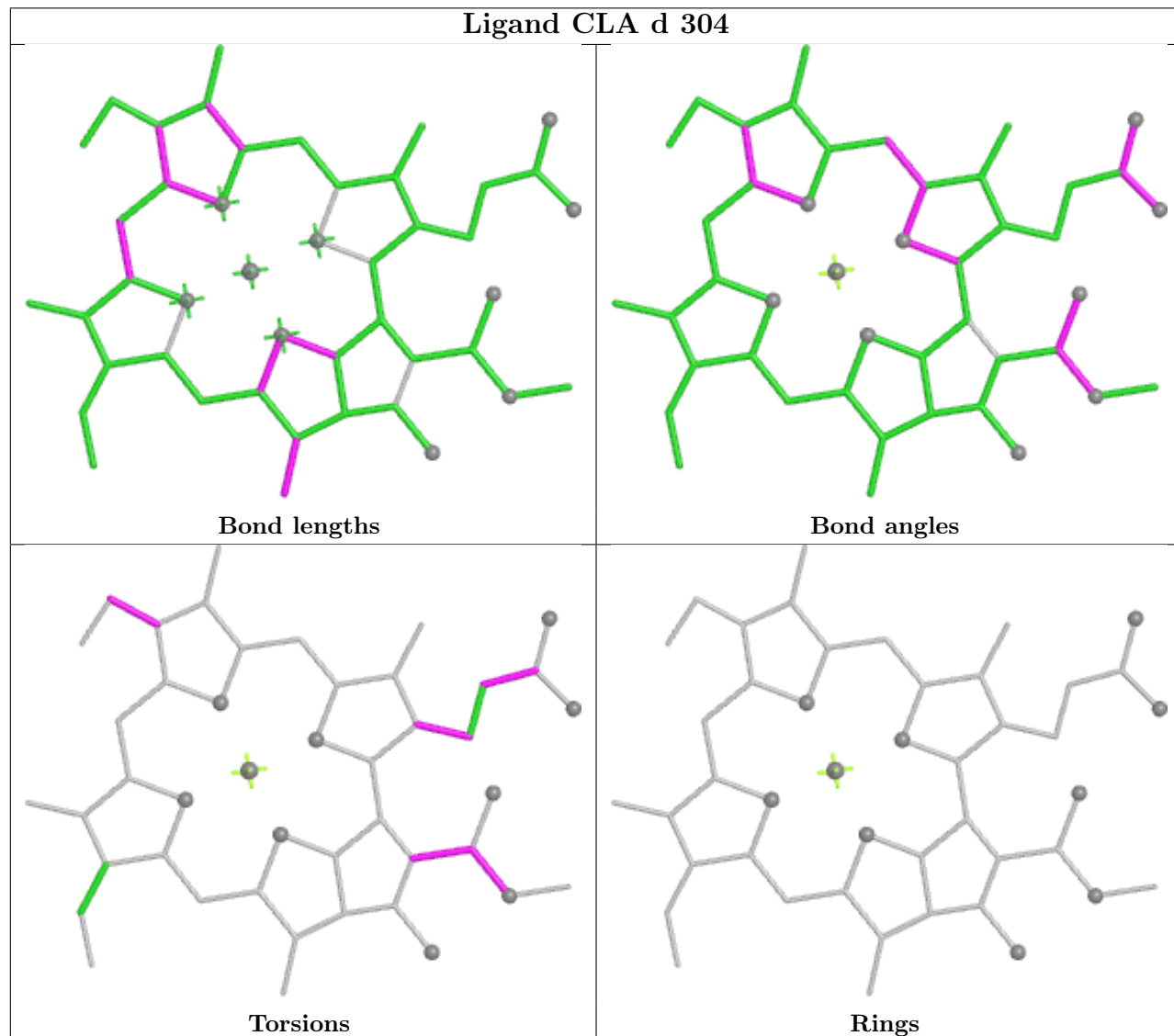
Ligand II0 d 319

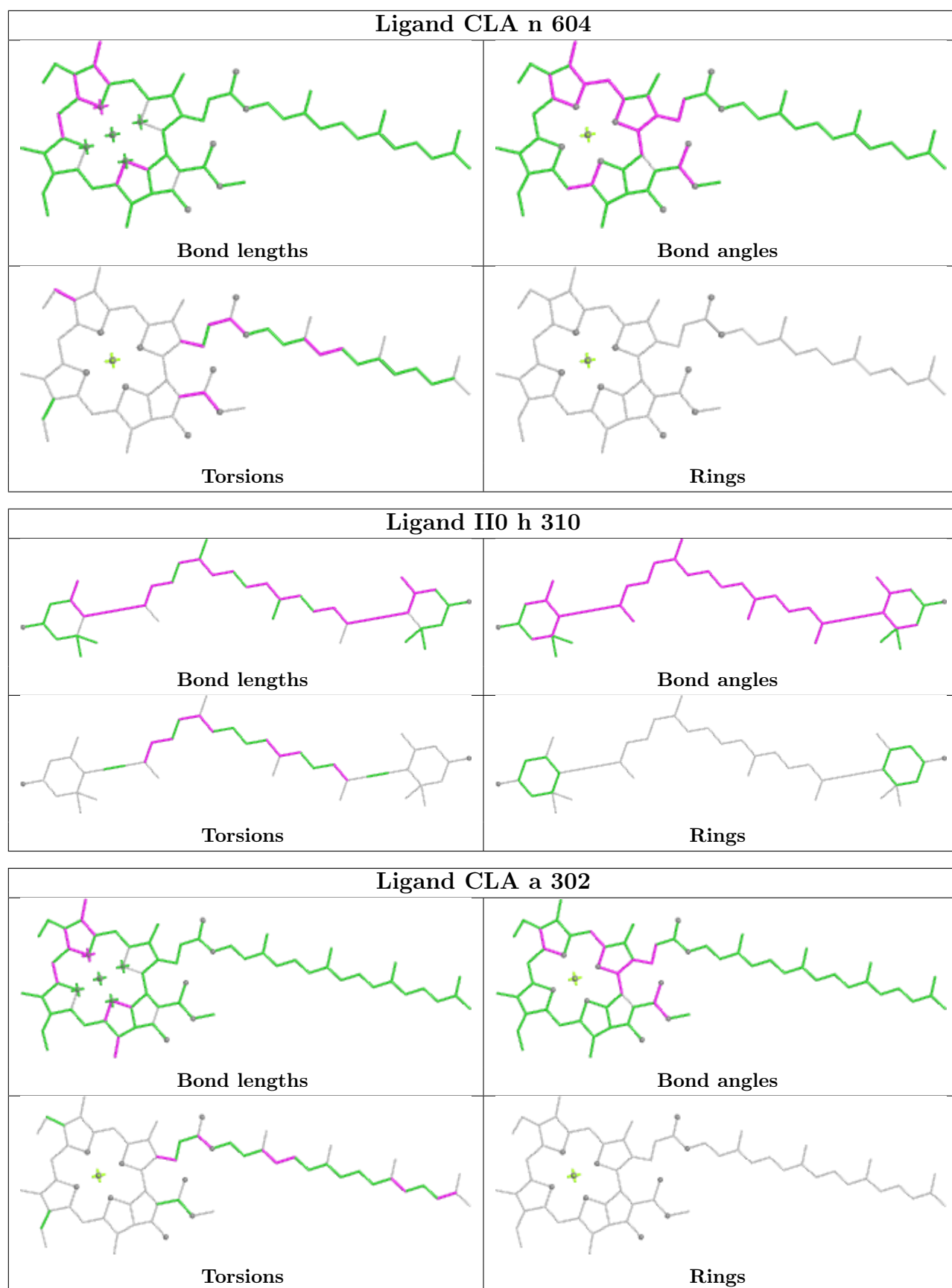


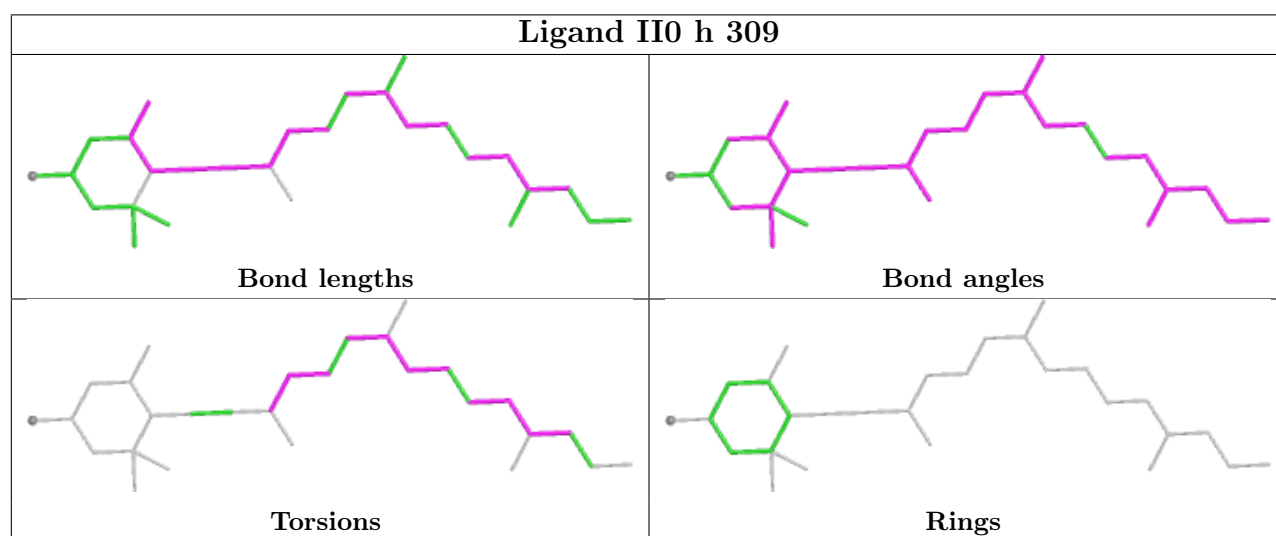
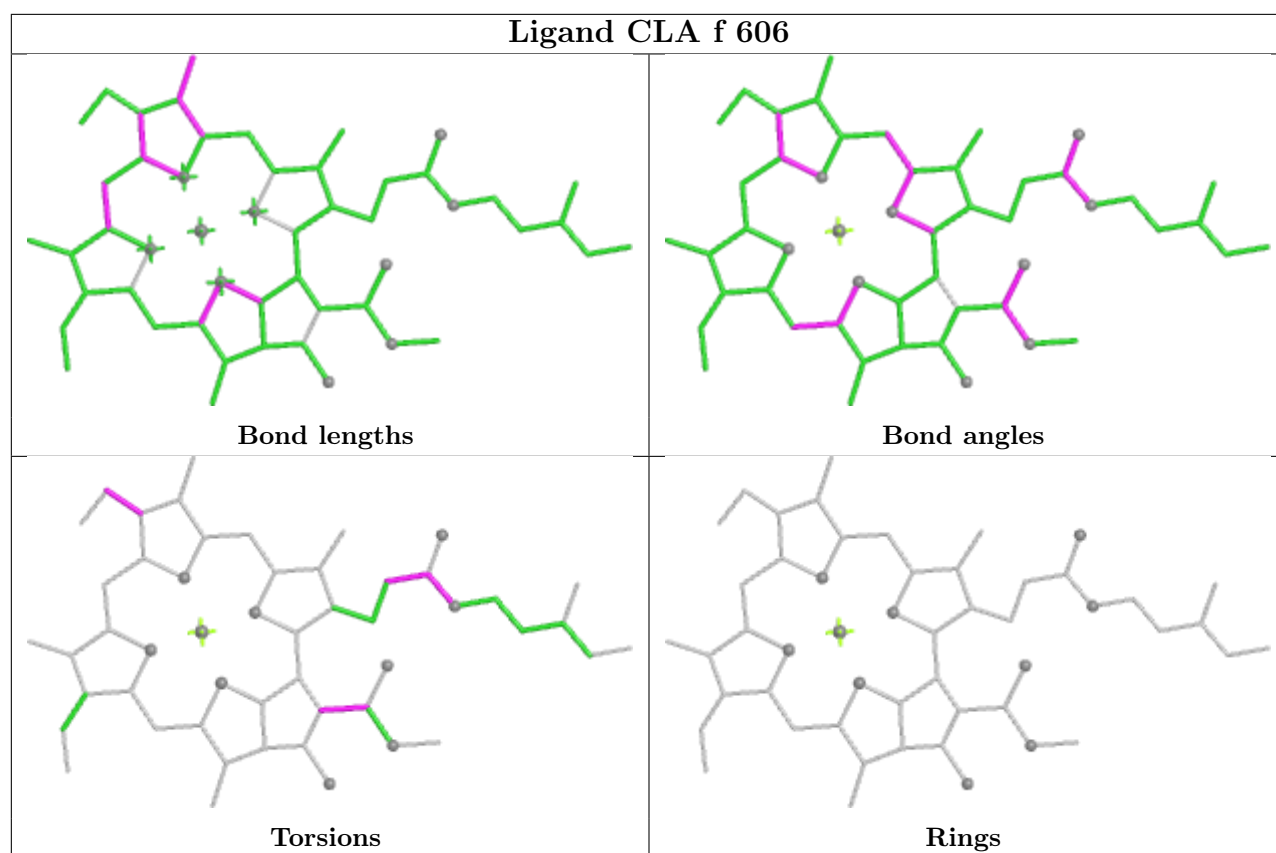
Ligand CLA B 838

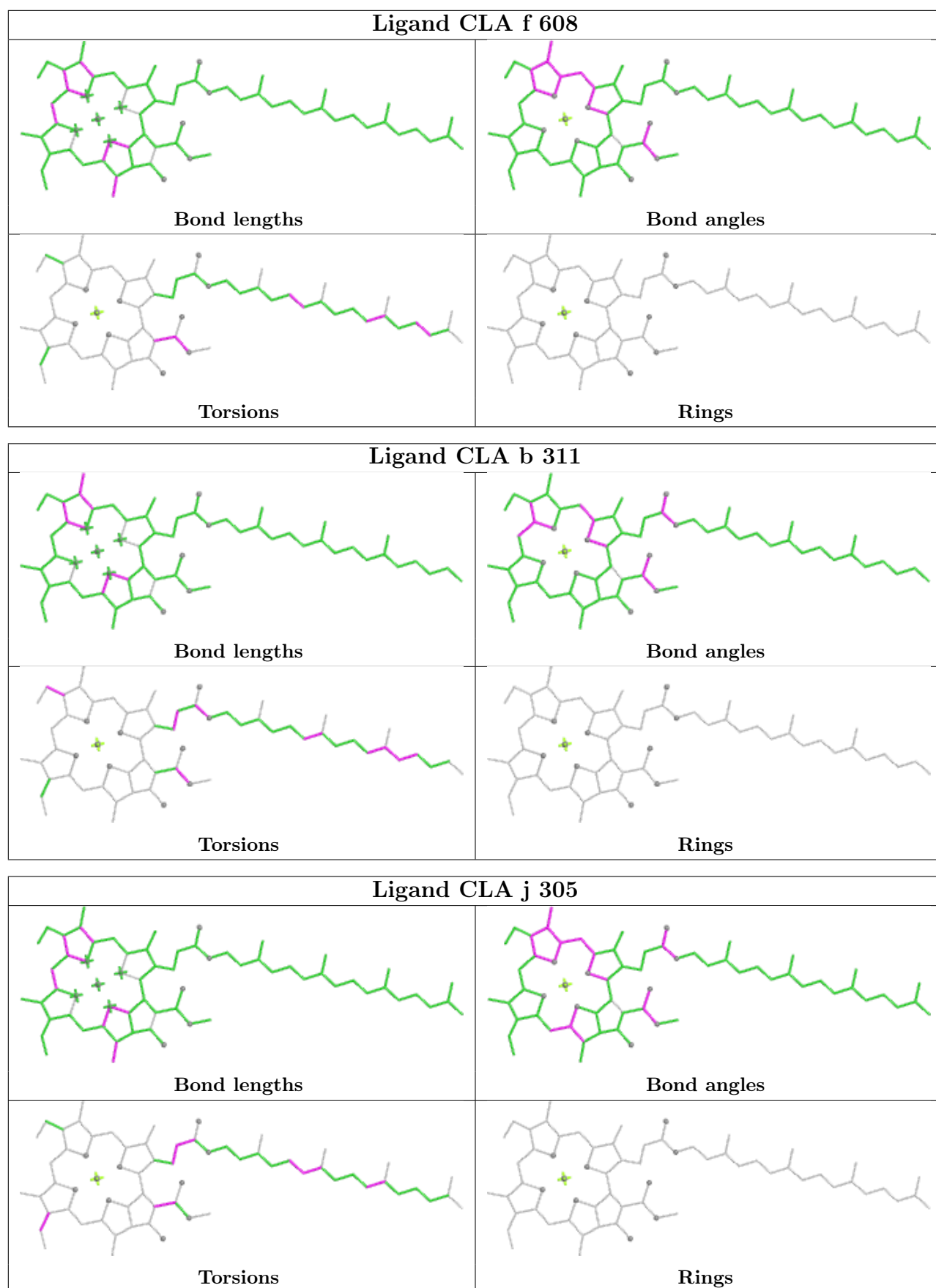


Ligand CLA d 304

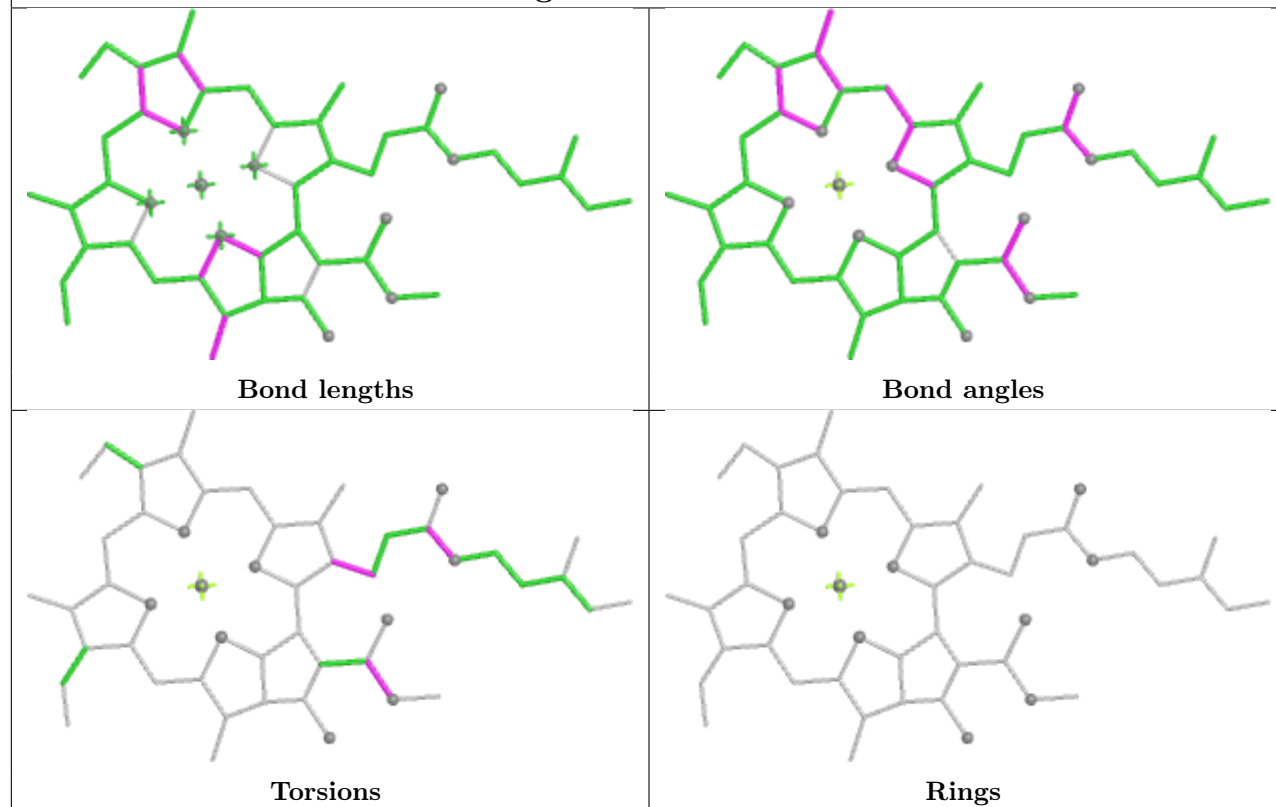




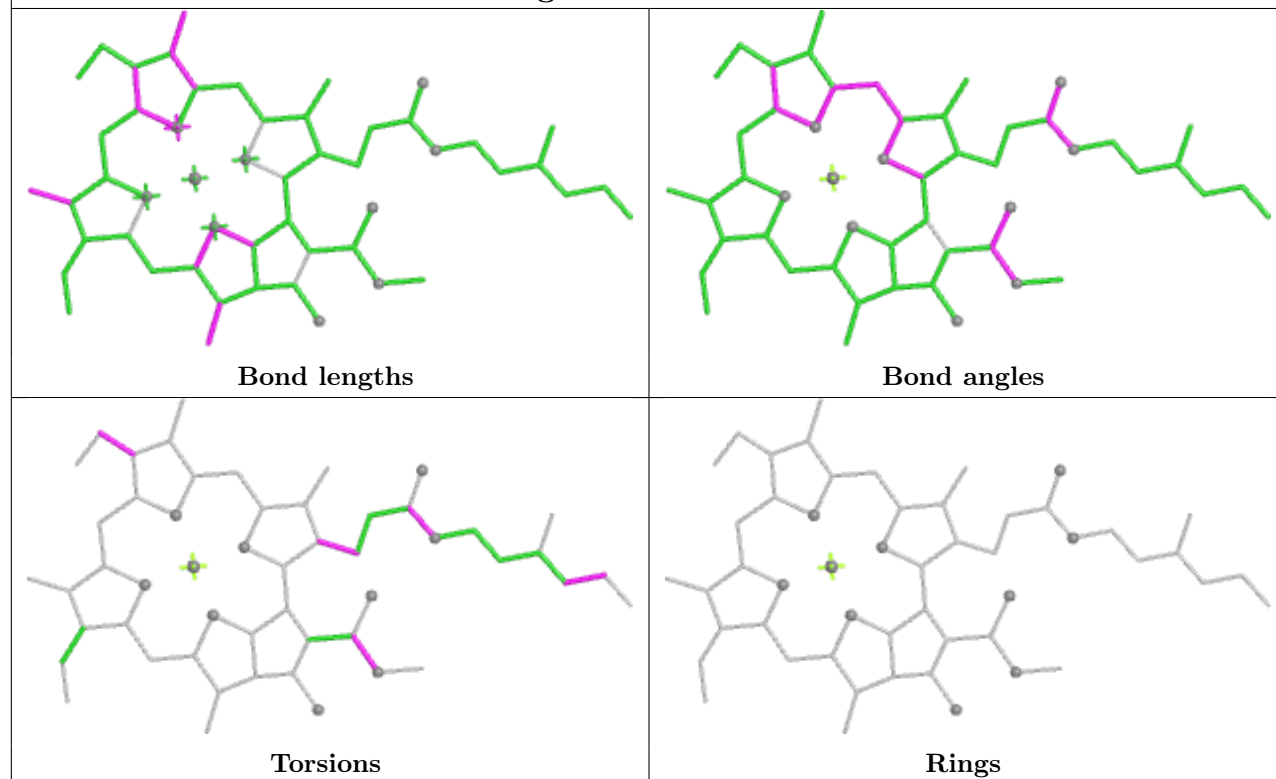




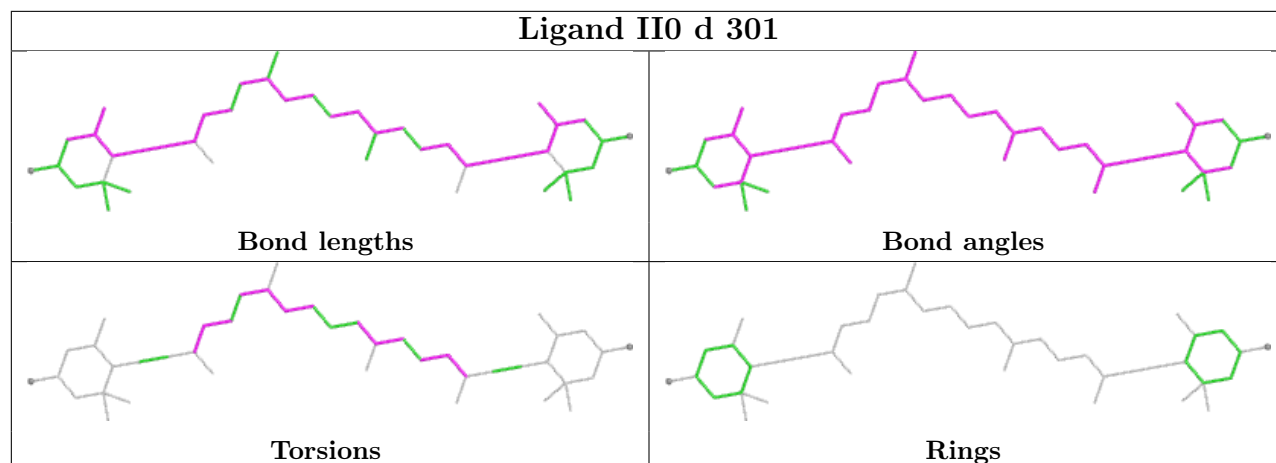
Ligand CLA h 304



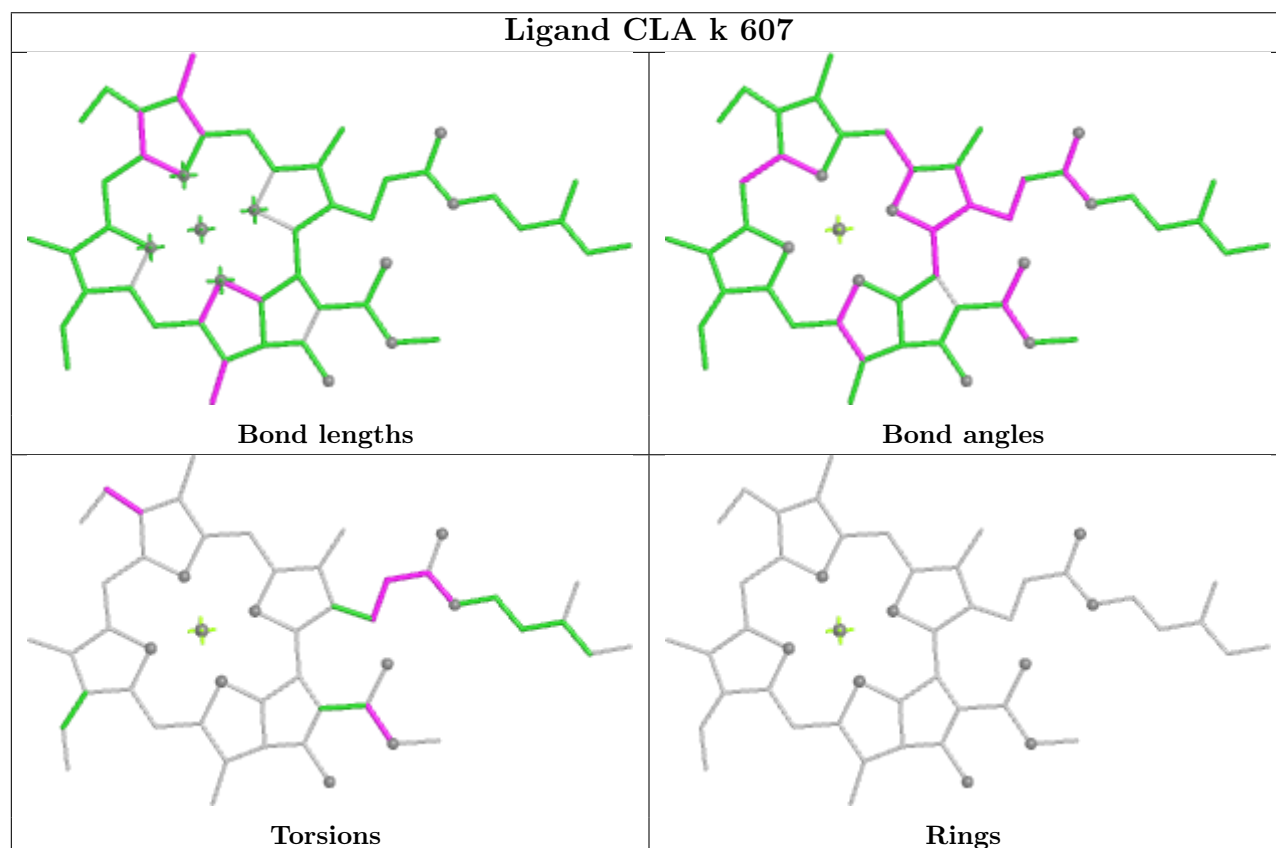
Ligand CLA c 306



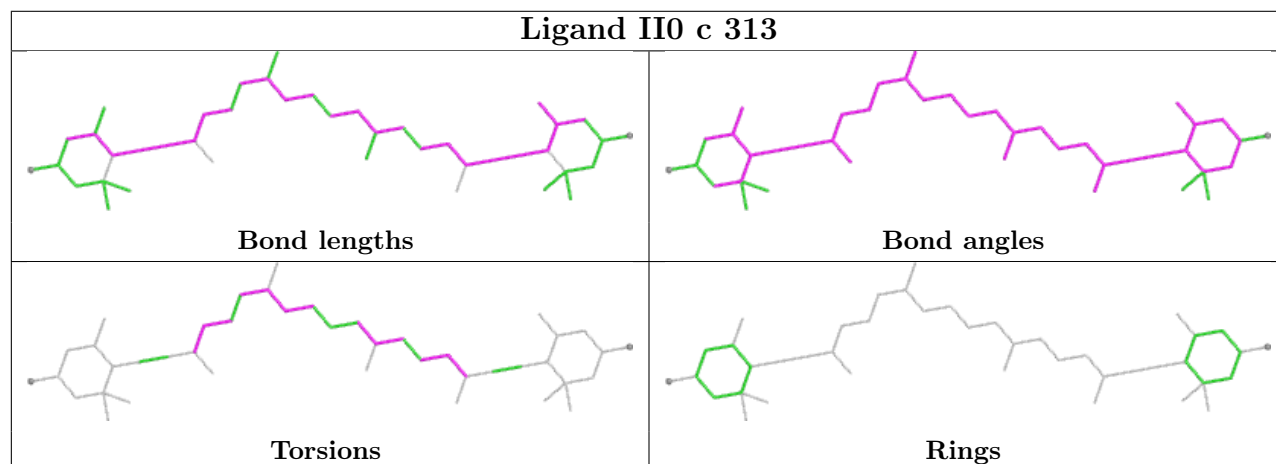
Ligand II0 d 301

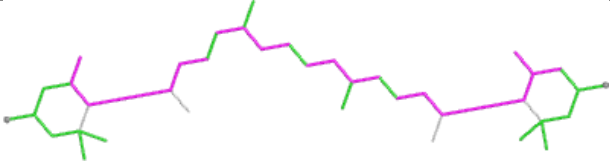
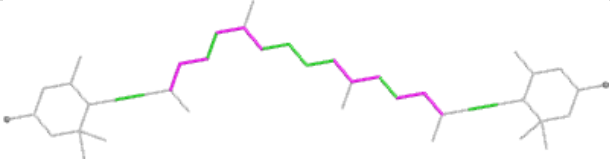
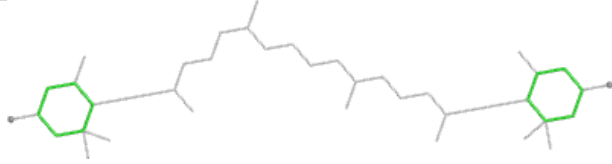
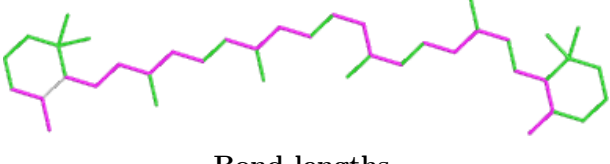
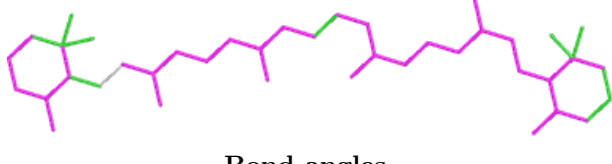
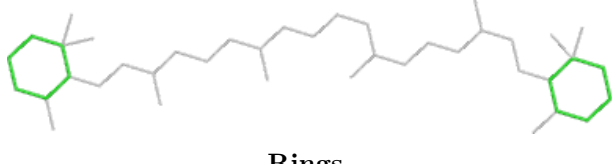
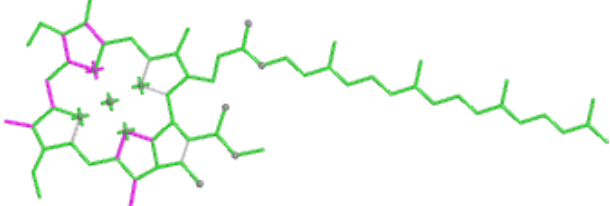
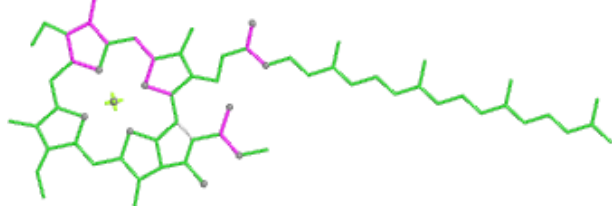
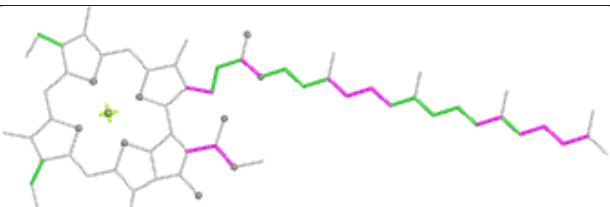
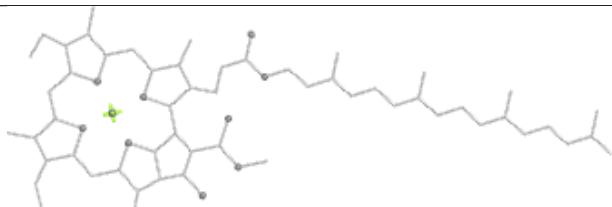


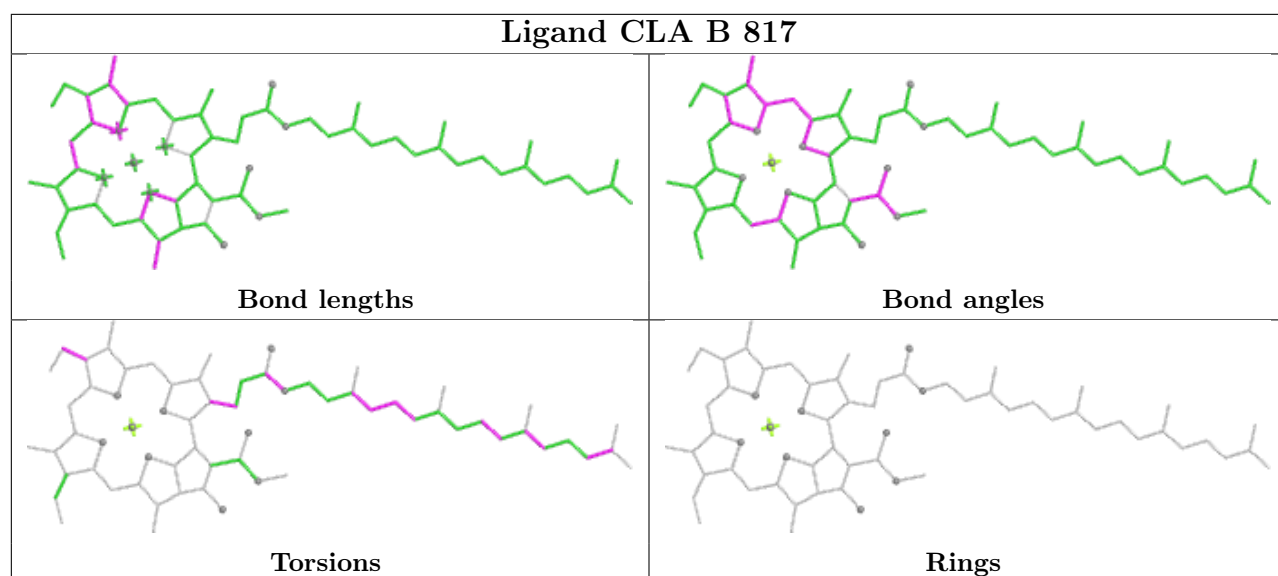
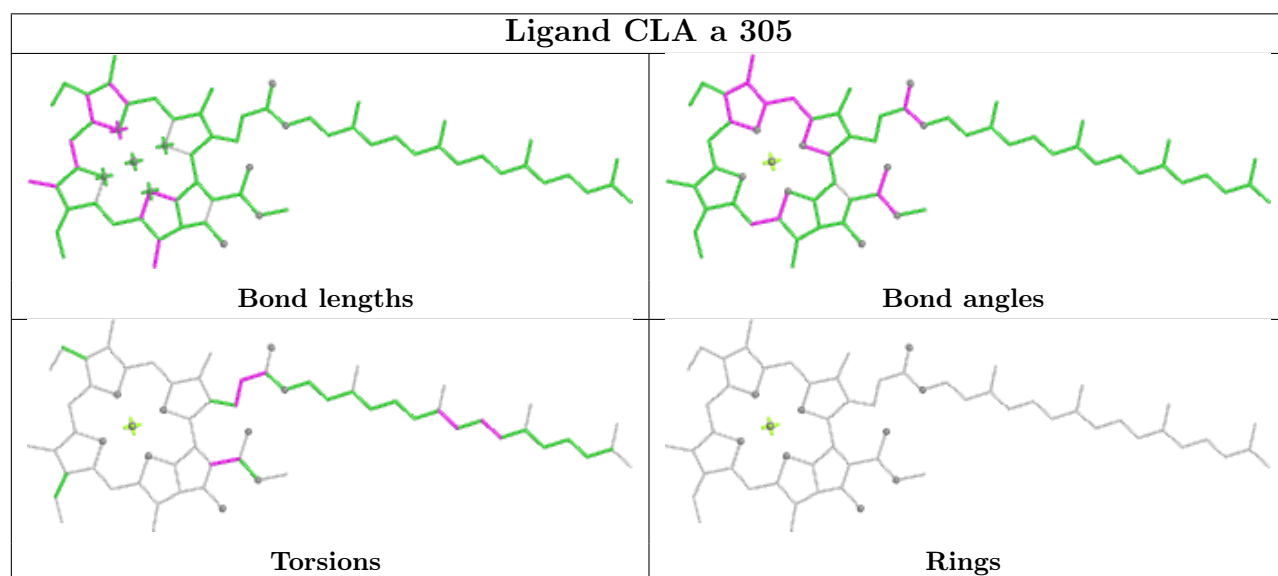
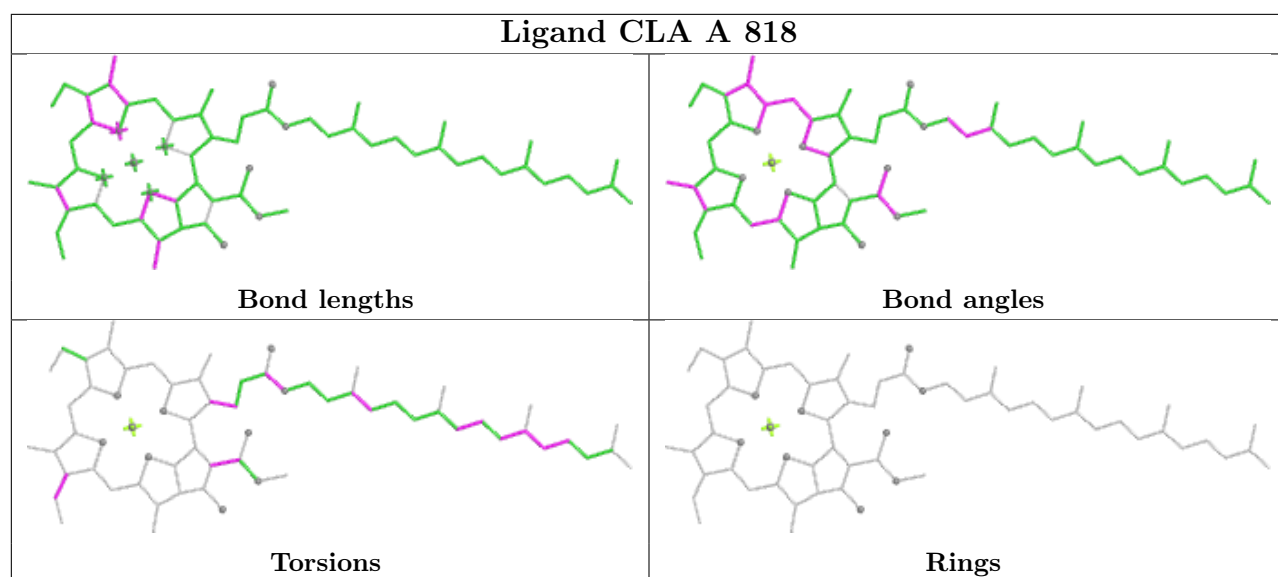
Ligand CLA k 607



Ligand II0 c 313



Ligand II0 a 313	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA f 602	
 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.

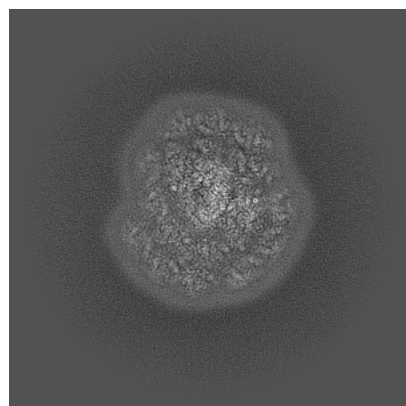
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62656. These allow visual inspection of the internal detail of the map and identification of artifacts.

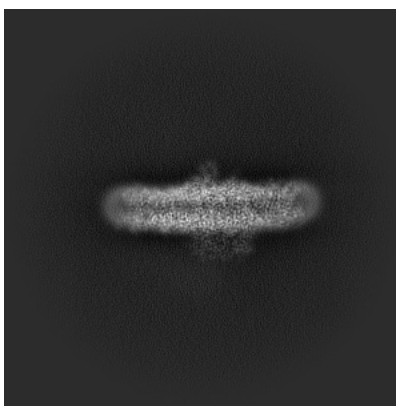
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

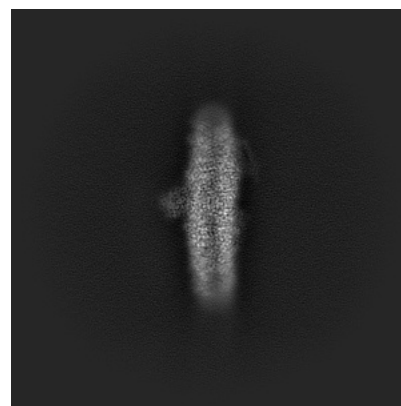
6.1.1 Primary map



X

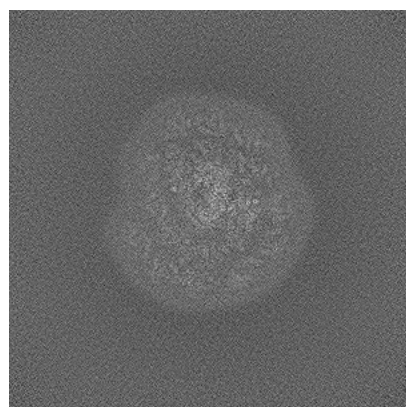


Y

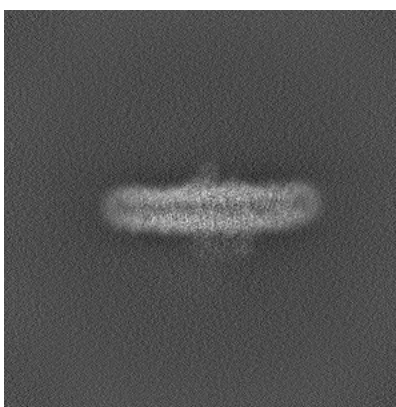


Z

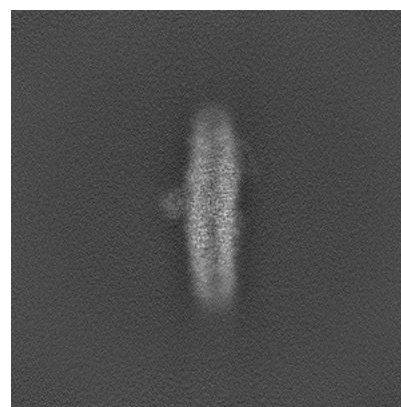
6.1.2 Raw map



X



Y

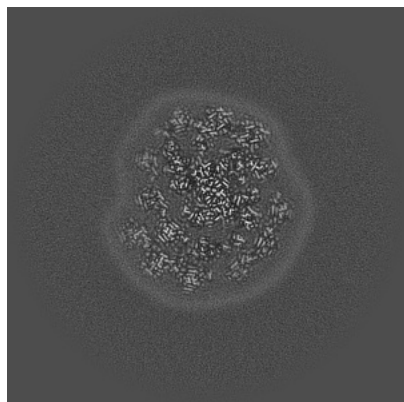


Z

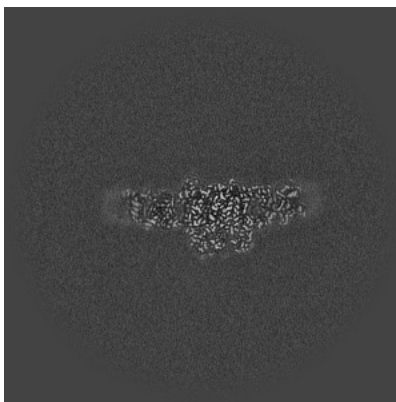
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

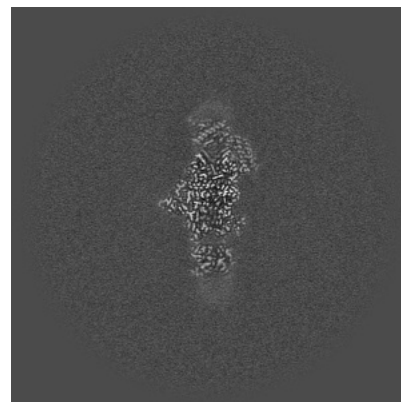
6.2.1 Primary map



X Index: 300

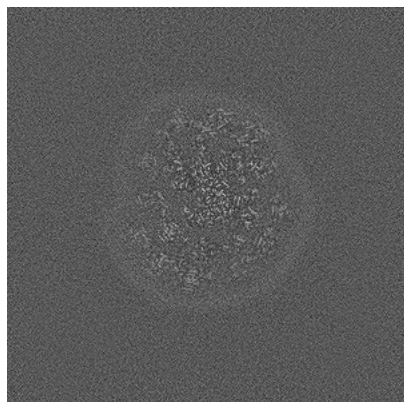


Y Index: 300

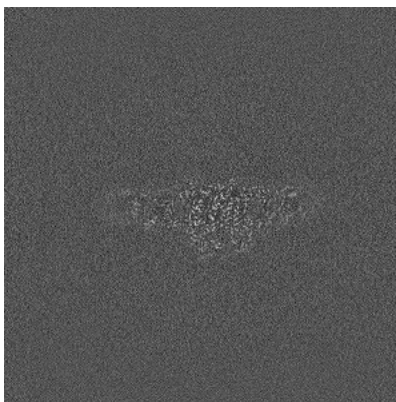


Z Index: 300

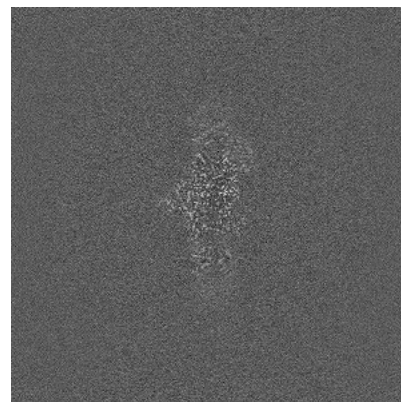
6.2.2 Raw map



X Index: 300



Y Index: 300

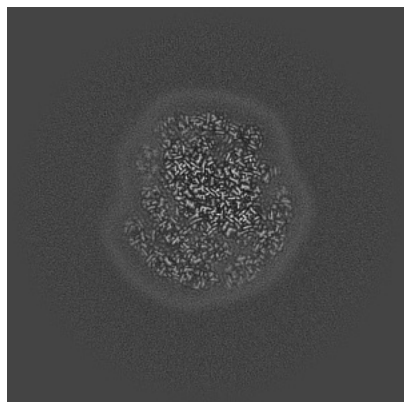


Z Index: 300

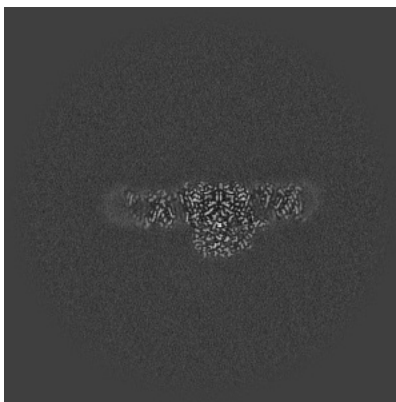
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

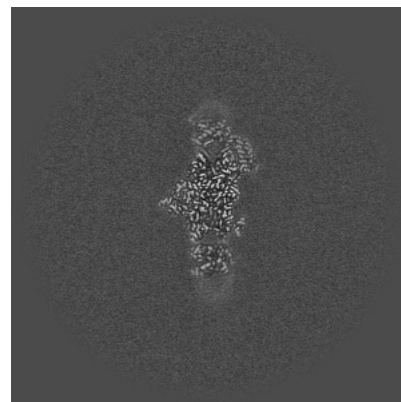
6.3.1 Primary map



X Index: 315

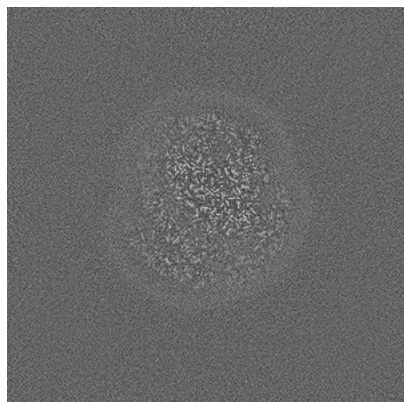


Y Index: 308

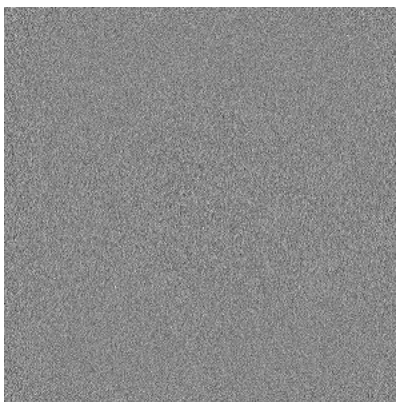


Z Index: 301

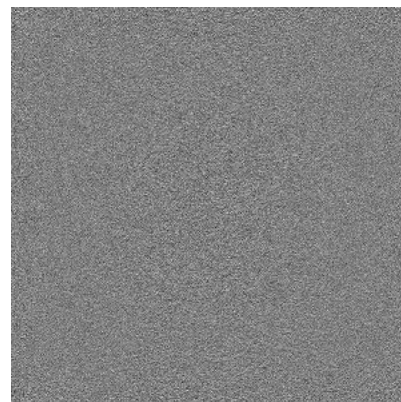
6.3.2 Raw map



X Index: 315



Y Index: 0

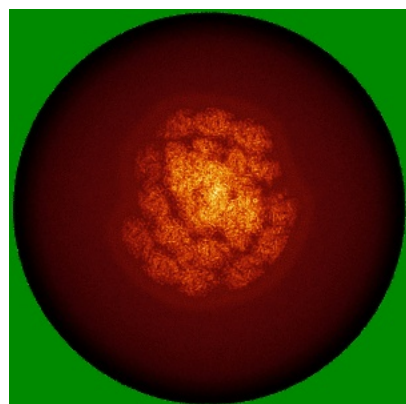


Z Index: 0

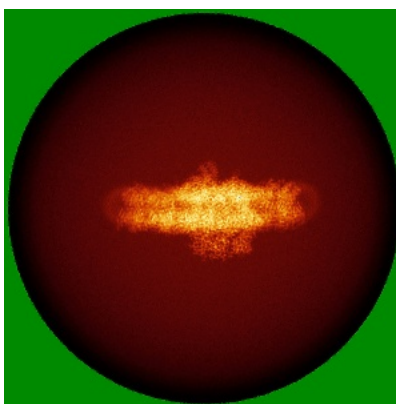
The images above show the largest variance slices of the map in three orthogonal directions.

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

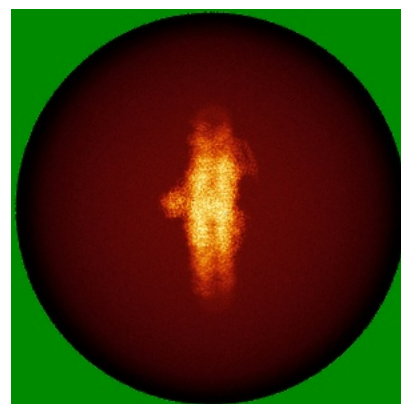
6.4.1 Primary map



X

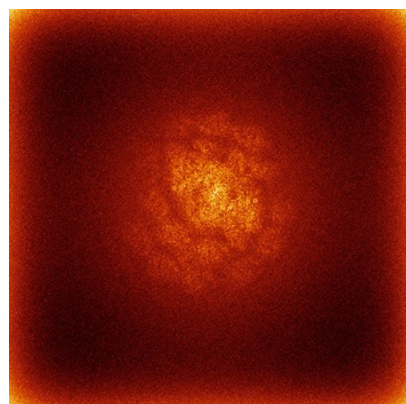


Y

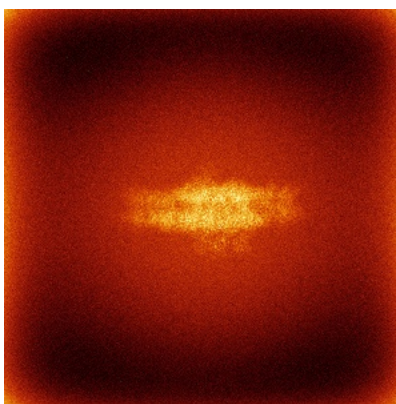


Z

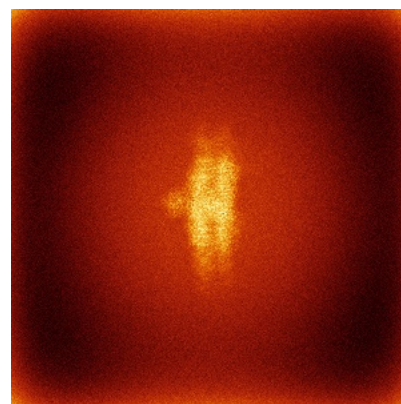
6.4.2 Raw map



X



Y

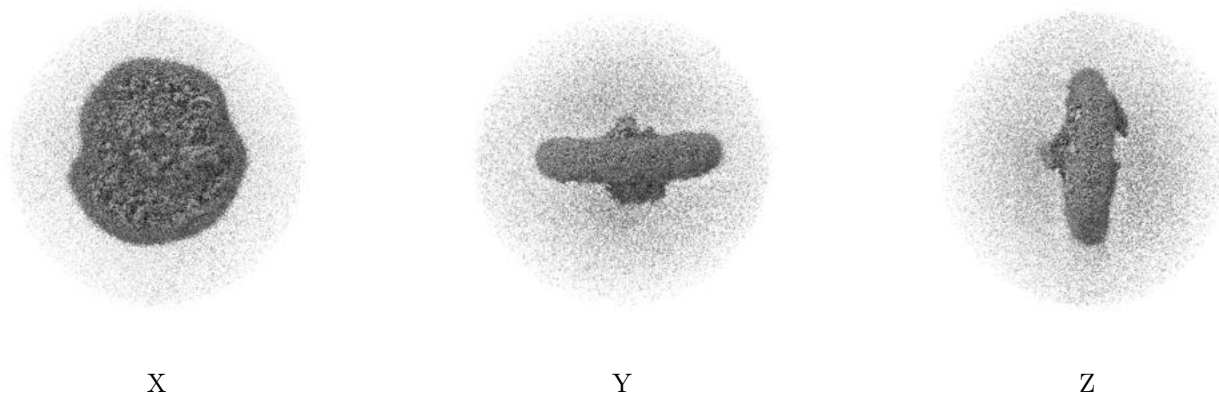


Z

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

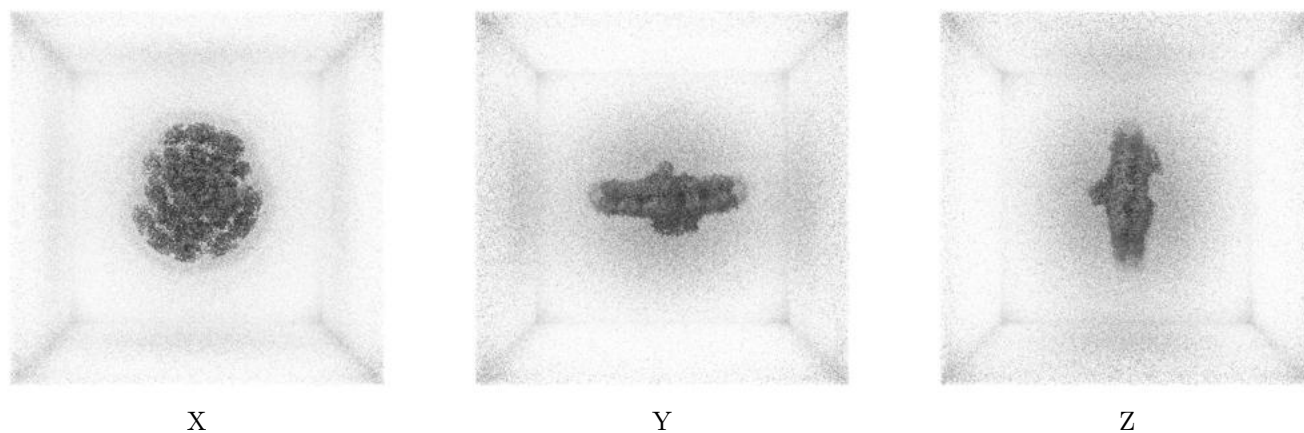
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

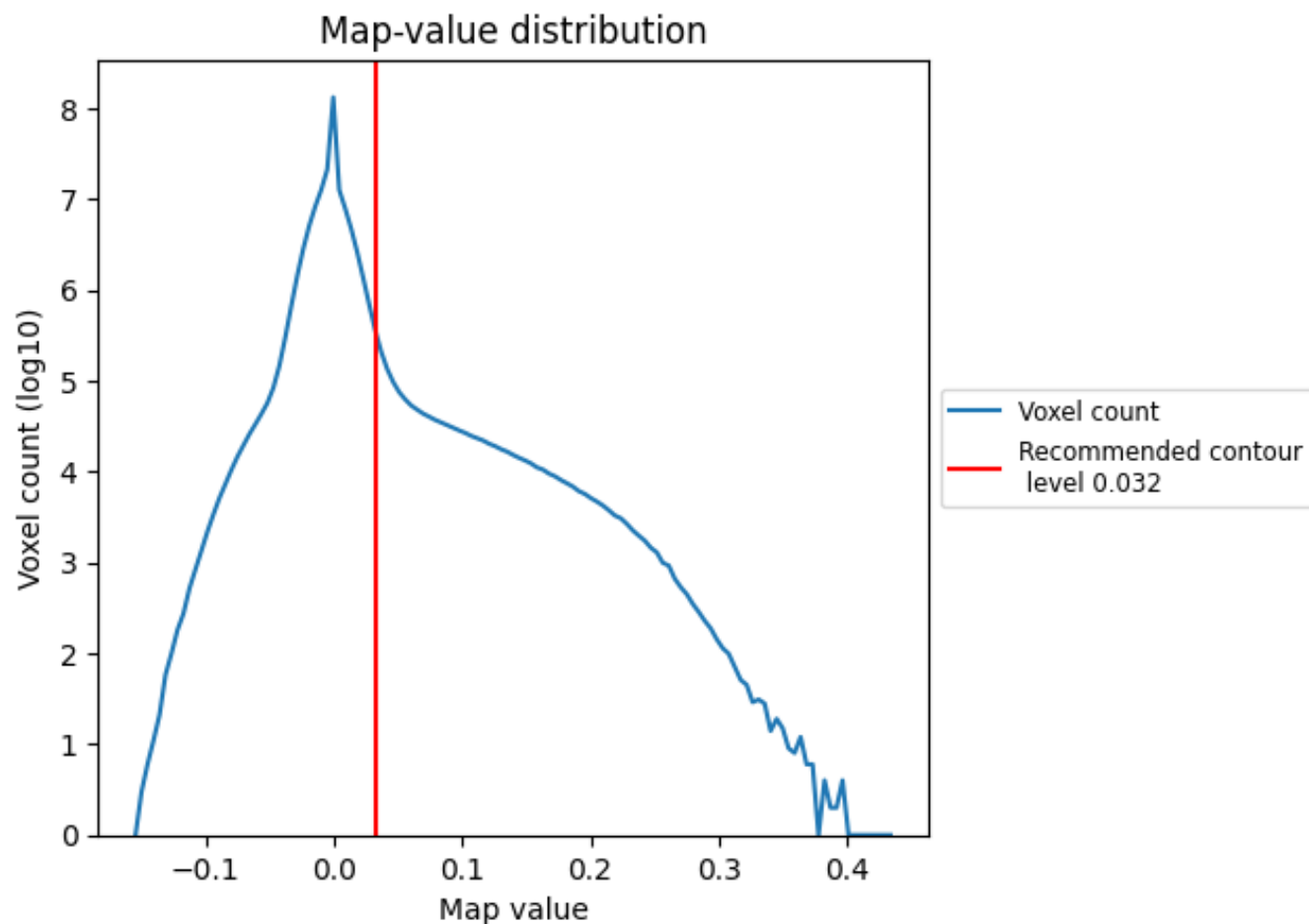
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

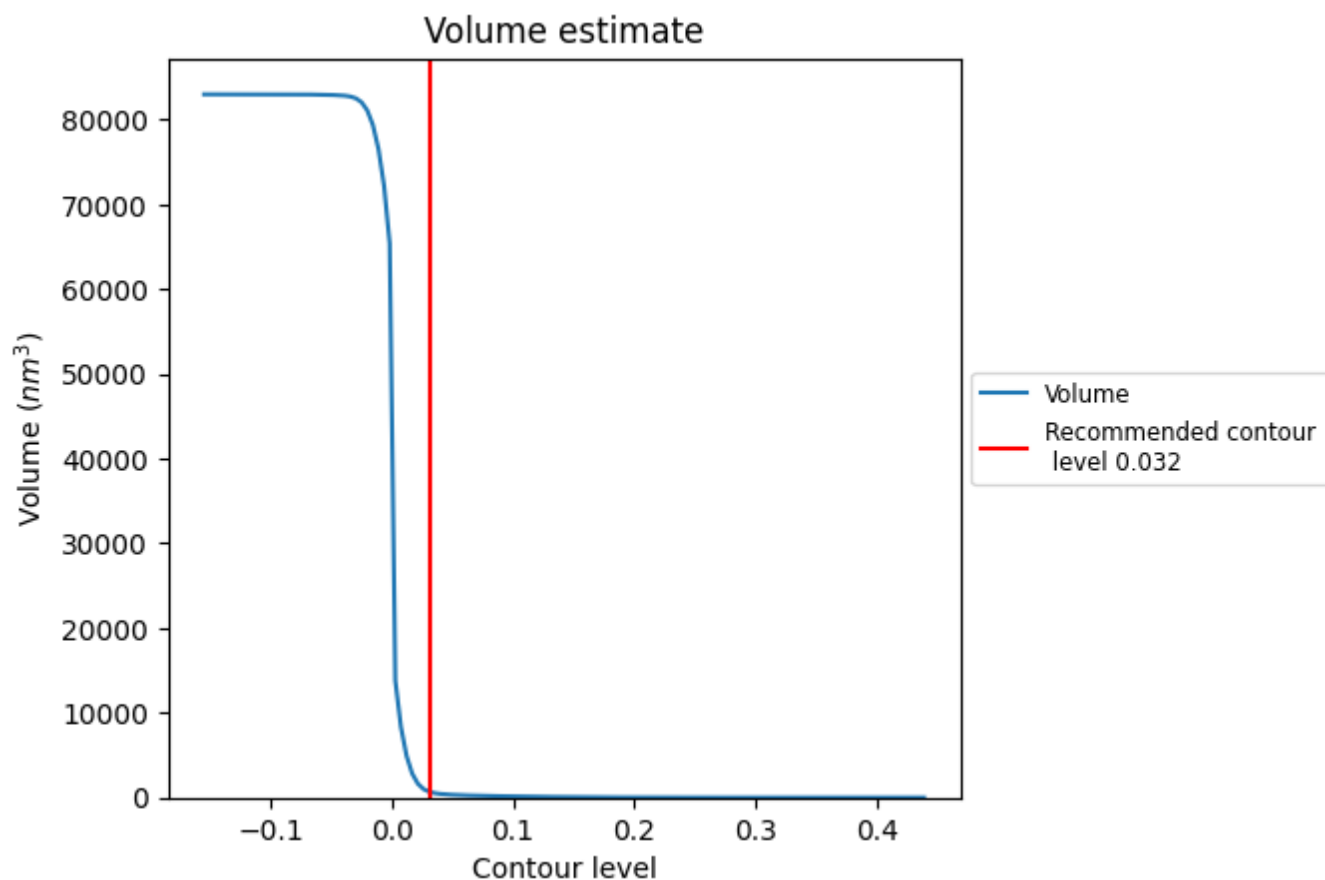
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

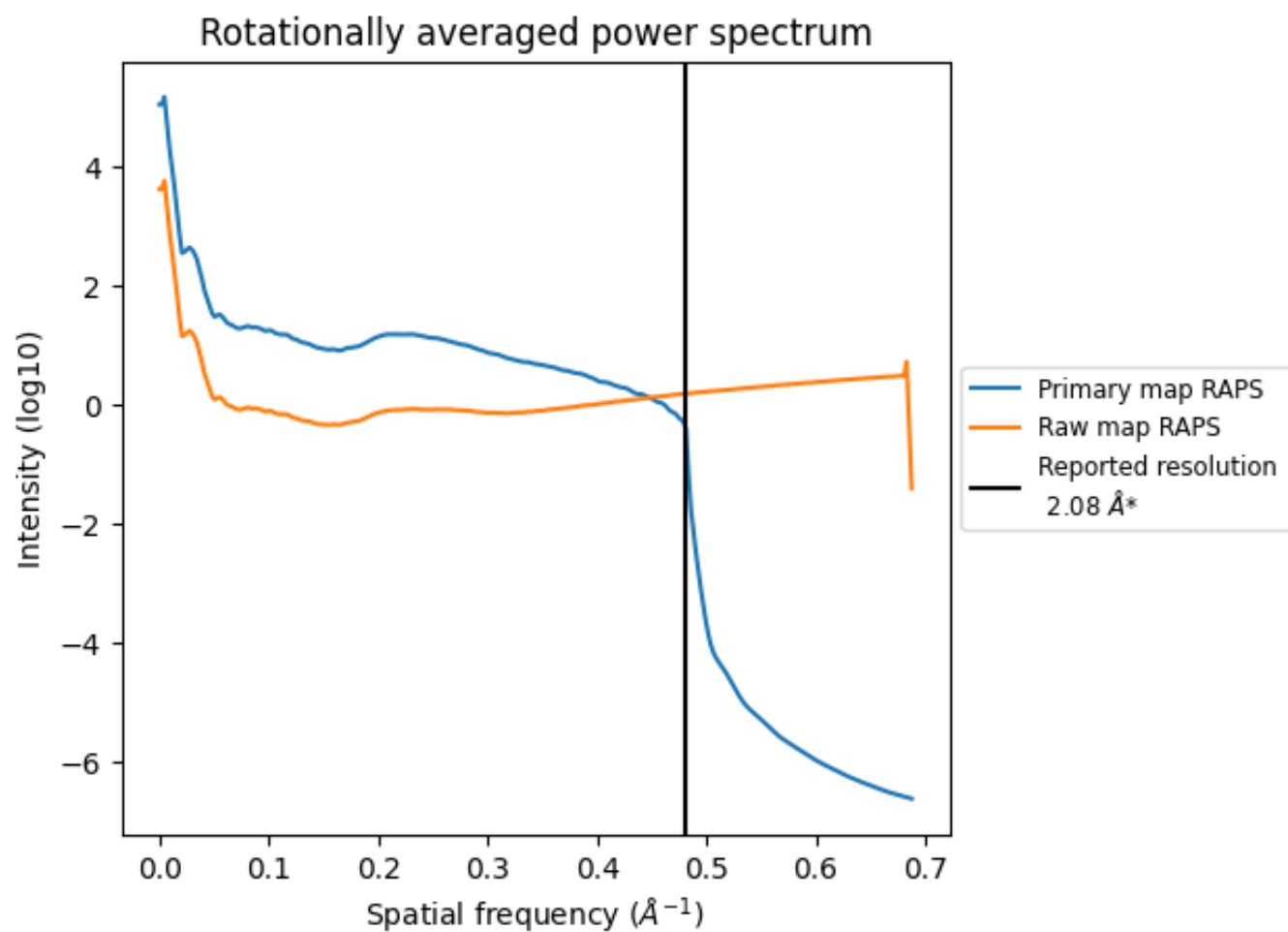
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 646 nm^3 ; this corresponds to an approximate mass of 583 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

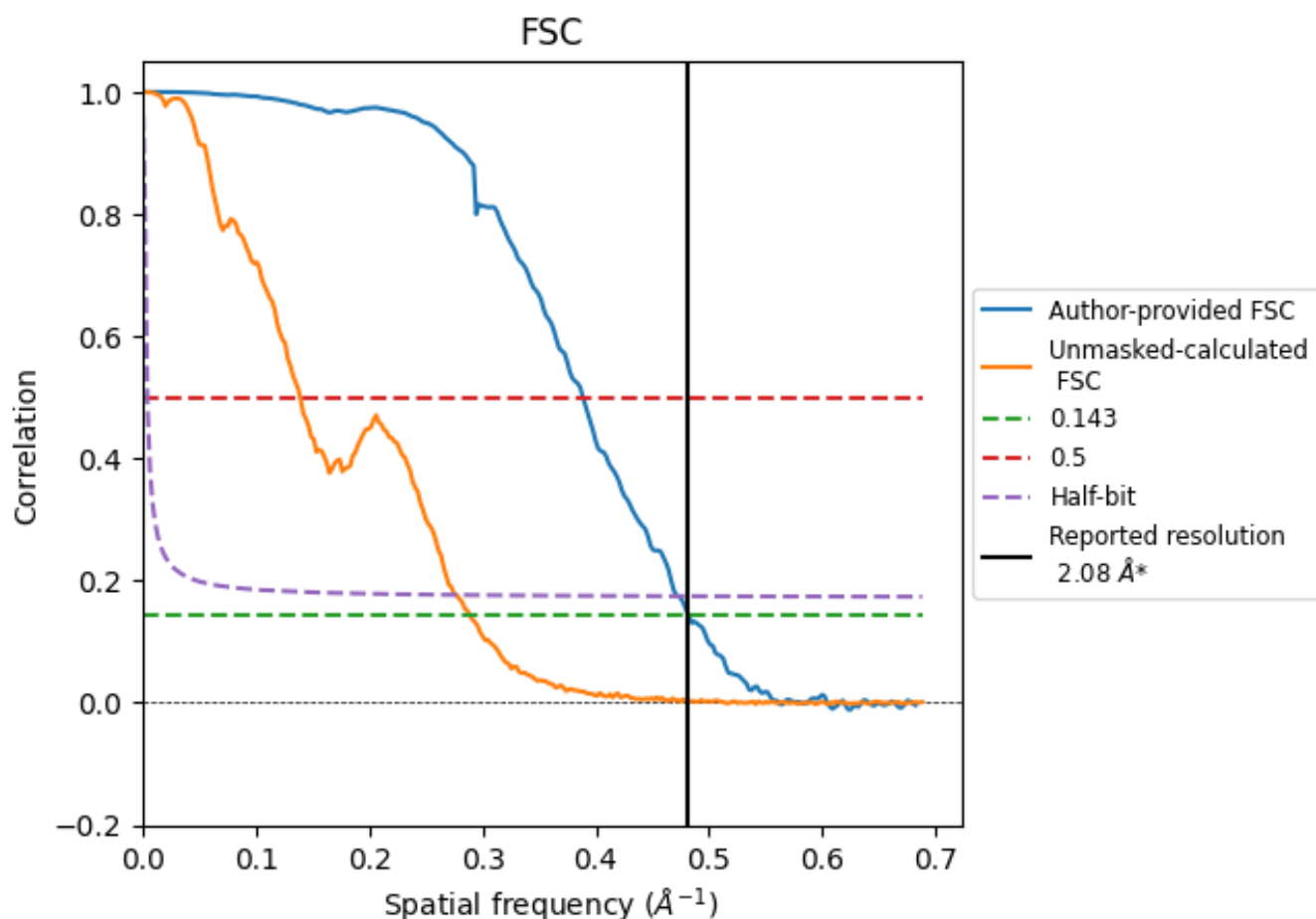


*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

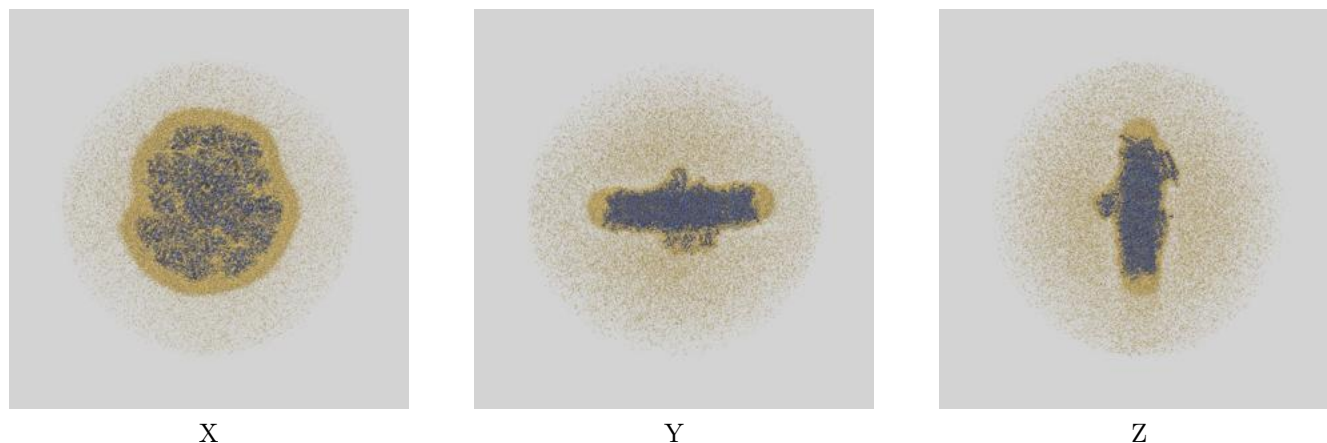
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.57	2.12
Unmasked-calculated*	3.46	7.18	3.61

*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 3.46 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

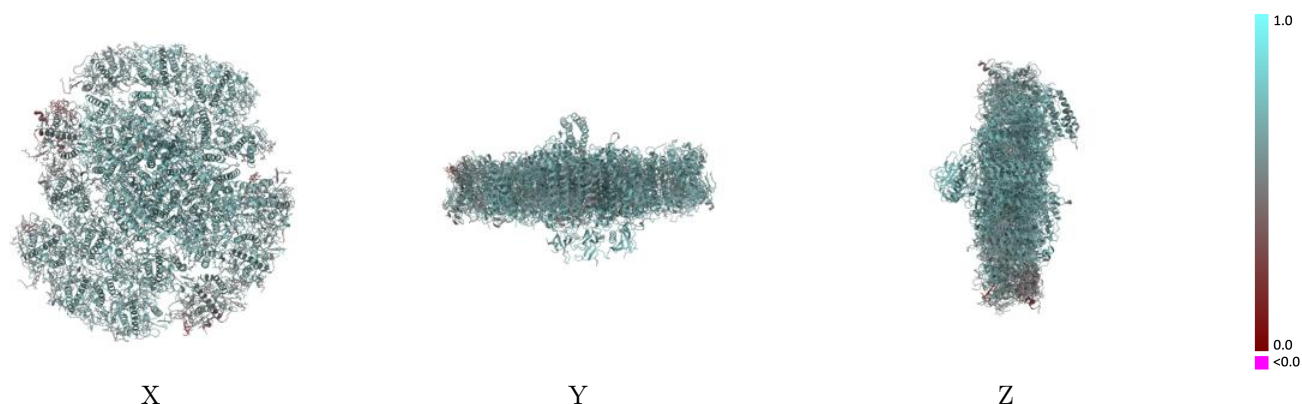
This section contains information regarding the fit between EMDB map EMD-62656 and PDB model 9KZ9. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



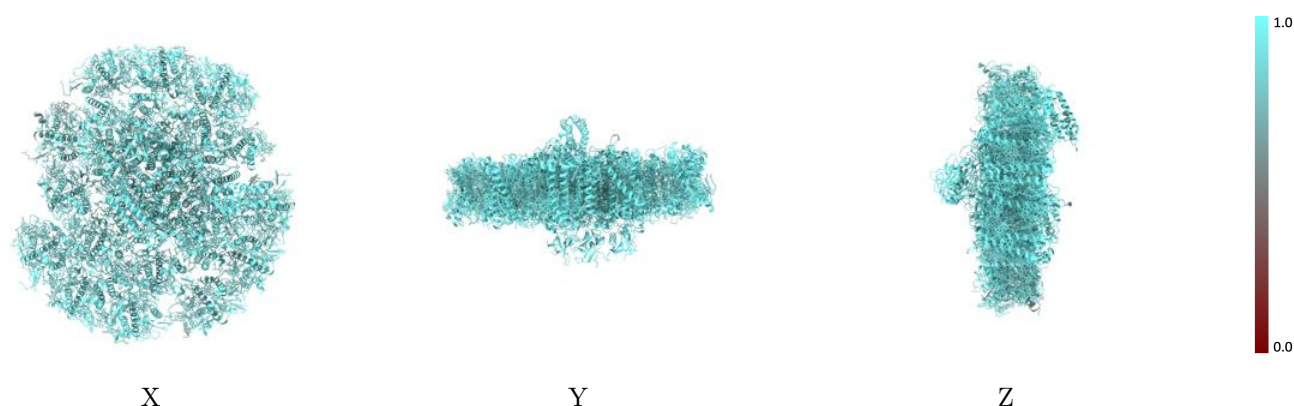
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



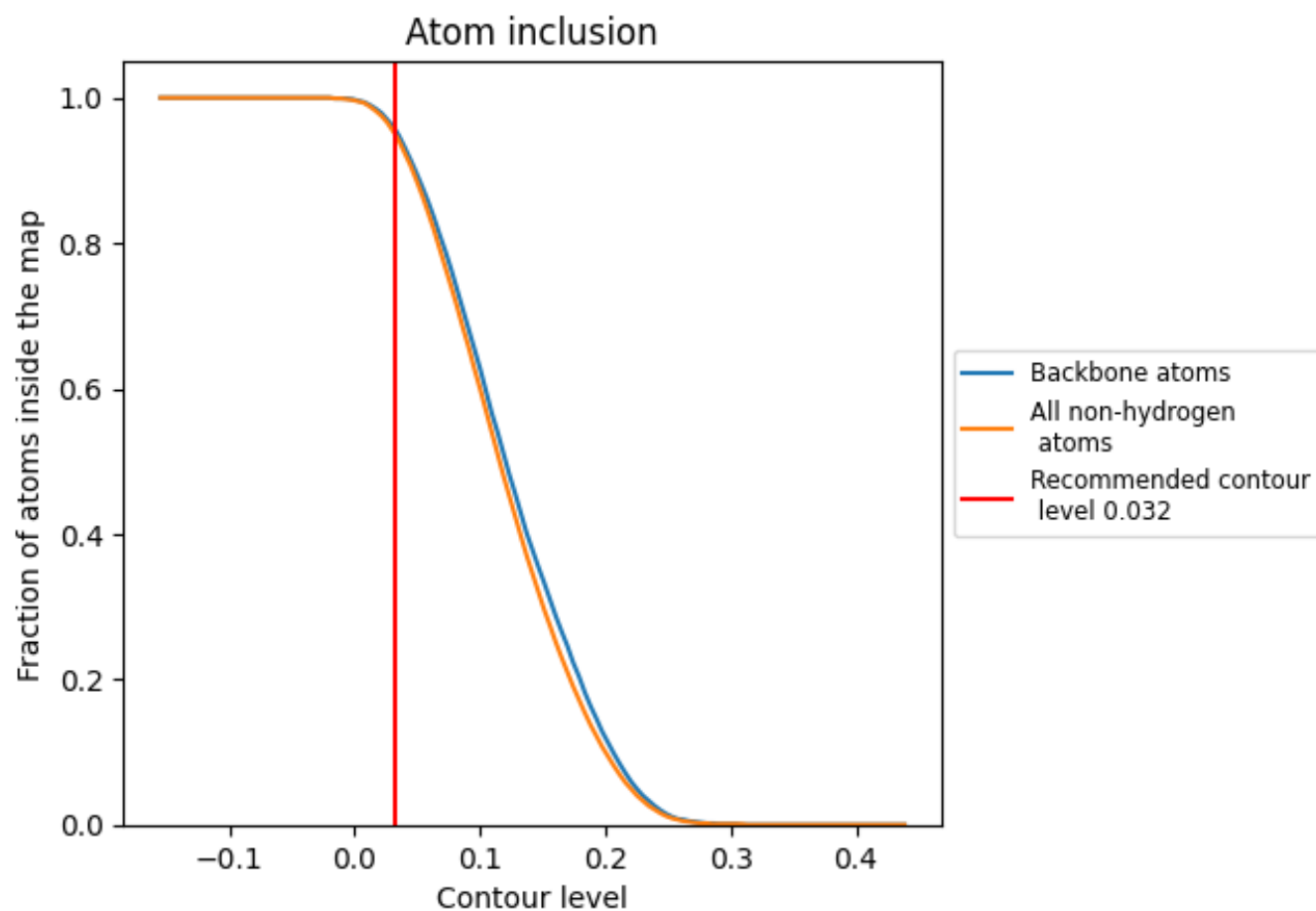
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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	 0.9510	 0.6450
A	 0.9820	 0.6990
B	 0.9830	 0.7020
C	 0.9970	 0.7120
D	 0.9870	 0.6910
E	 0.9680	 0.6680
F	 0.9680	 0.6800
I	 0.9860	 0.6850
J	 0.9720	 0.6720
K	 0.9610	 0.6620
L	 0.9650	 0.6740
M	 0.9550	 0.6570
O	 0.9670	 0.6720
Q	 0.9120	 0.6040
R	 0.9710	 0.6650
a	 0.9690	 0.6670
b	 0.9690	 0.6700
c	 0.9210	 0.6110
d	 0.8310	 0.5040
e	 0.9040	 0.5680
f	 0.9540	 0.6410
g	 0.9500	 0.6330
h	 0.9470	 0.6400
i	 0.9080	 0.5650
j	 0.9220	 0.6080
k	 0.8970	 0.5460
l	 0.9540	 0.6250
m	 0.9390	 0.6290
n	 0.8970	 0.5760
s	 0.9520	 0.6460

