



Full wwPDB EM Validation Report ⓘ

Jun 16, 2025 – 04:11 PM JST

PDB ID : 8XLP / pdb_00008xlp
EMDB ID : EMD-38455
Title : Structure of inactive Photosystem II associated with CAC antenna from Rhodomonas Salina
Authors : Si, L.; Li, M.
Deposited on : 2023-12-26
Resolution : 2.57 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

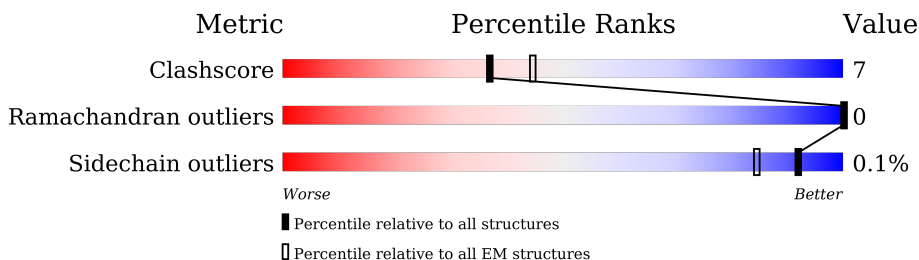
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	
1	a	328	
2	B	509	
2	b	509	
3	C	487	
3	c	487	
4	D	351	
4	d	351	

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Mol	Chain	Length	Quality of chain
5	E	84	
5	e	84	
6	F	42	
6	f	42	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	40	
11	m	40	
12	T	32	
12	t	32	
13	W	74	
13	w	74	
14	X	39	
14	x	39	
15	Y	34	
15	y	34	
16	Z	62	
16	z	62	
17	G	284	

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Mol	Chain	Length	Quality of chain
17	g	284	
18	2	217	
18	O	217	
19	3	221	
19	P	221	
20	4	216	
20	Q	216	
21	5	229	
21	R	229	
22	6	227	
22	S	227	
23	1	233	
23	N	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	601	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	609	X	-	-	-
25	CLA	1	610	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	1	615	X	-	-	-
25	CLA	2	601	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	2	607	X	-	-	-
25	CLA	2	609	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	2	615	X	-	-	-
25	CLA	3	601	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	609	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	615	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	606	X	-	-	-
25	CLA	4	607	X	-	-	-
25	CLA	4	609	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	613	X	-	-	-
25	CLA	4	615	X	-	-	-
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	613	X	-	-	-
25	CLA	5	615	X	-	-	-
25	CLA	6	601	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	609	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	613	X	-	-	-
25	CLA	6	615	X	-	-	-
25	CLA	A	403	X	-	-	-
25	CLA	A	404	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	516	X	-	-	-
25	CLA	C	517	X	-	-	-
25	CLA	C	518	X	-	-	-
25	CLA	C	519	X	-	-	-
25	CLA	C	520	X	-	-	-
25	CLA	C	521	X	-	-	-
25	CLA	C	522	X	-	-	-
25	CLA	C	523	X	-	-	-
25	CLA	C	524	X	-	-	-
25	CLA	C	525	X	-	-	-
25	CLA	C	526	X	-	-	-
25	CLA	C	527	X	-	-	-
25	CLA	C	528	X	-	-	-
25	CLA	D	400	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	G	301	X	-	-	-
25	CLA	G	302	X	-	-	-
25	CLA	N	601	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	N	606	X	-	-	-
25	CLA	N	607	X	-	-	-
25	CLA	N	609	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	N	615	X	-	-	-
25	CLA	O	601	X	-	-	-
25	CLA	O	602	X	-	-	-
25	CLA	O	603	X	-	-	-
25	CLA	O	604	X	-	-	-
25	CLA	O	606	X	-	-	-
25	CLA	O	607	X	-	-	-
25	CLA	O	609	X	-	-	-
25	CLA	O	610	X	-	-	-
25	CLA	O	611	X	-	-	-
25	CLA	O	613	X	-	-	-
25	CLA	O	615	X	-	-	-
25	CLA	P	601	X	-	-	-
25	CLA	P	602	X	-	-	-
25	CLA	P	603	X	-	-	-
25	CLA	P	609	X	-	-	-
25	CLA	P	610	X	-	-	-
25	CLA	P	611	X	-	-	-
25	CLA	P	612	X	-	-	-
25	CLA	P	613	X	-	-	-
25	CLA	P	615	X	-	-	-
25	CLA	Q	602	X	-	-	-
25	CLA	Q	603	X	-	-	-
25	CLA	Q	604	X	-	-	-
25	CLA	Q	606	X	-	-	-
25	CLA	Q	607	X	-	-	-
25	CLA	Q	609	X	-	-	-
25	CLA	Q	610	X	-	-	-
25	CLA	Q	613	X	-	-	-
25	CLA	Q	615	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	606	X	-	-	-
25	CLA	R	607	X	-	-	-
25	CLA	R	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	R	615	X	-	-	-
25	CLA	S	601	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	615	X	-	-	-
25	CLA	a	403	X	-	-	-
25	CLA	a	404	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	516	X	-	-	-
25	CLA	c	517	X	-	-	-
25	CLA	c	518	X	-	-	-
25	CLA	c	519	X	-	-	-
25	CLA	c	520	X	-	-	-
25	CLA	c	521	X	-	-	-
25	CLA	c	522	X	-	-	-
25	CLA	c	523	X	-	-	-
25	CLA	c	524	X	-	-	-
25	CLA	c	525	X	-	-	-
25	CLA	c	526	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	527	X	-	-	-
25	CLA	c	528	X	-	-	-
25	CLA	d	400	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	g	301	X	-	-	-
25	CLA	g	302	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70547 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	327	Total	C	N	O	S	0	0
			2563	1677	420	454	12		
1	A	327	Total	C	N	O	S	0	0
			2563	1677	420	454	12		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	503	Total	C	N	O	S	0	0
			3950	2575	674	689	12		
2	B	503	Total	C	N	O	S	0	0
			3950	2575	674	689	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	434	Total	C	N	O	S	0	0
			3379	2213	569	587	10		
3	C	434	Total	C	N	O	S	0	0
			3379	2213	569	587	10		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	0	0
			2708	1790	443	462	13		
4	D	341	Total	C	N	O	S	0	0
			2708	1790	443	462	13		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	64	Total	C	N	O	0	0
			525	345	85	95		
5	E	64	Total	C	N	O	0	0
			525	345	85	95		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	32	Total	C	N	O	S	0	0
			261	179	43	38	1		
6	F	32	Total	C	N	O	S	0	0
			261	179	43	38	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	65	Total	C	N	O	S	0	0
			508	337	81	88	2		
7	H	65	Total	C	N	O	S	0	0
			508	337	81	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	35	Total	C	N	O	S	0	0
			284	188	46	49	1		
8	I	35	Total	C	N	O	S	0	0
			284	188	46	49	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	k	37	Total	C	N	O	0	0
			296	209	44	43		
9	K	37	Total	C	N	O	0	0
			296	209	44	43		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	37	Total	C	N	O	0	0
			301	204	47	50		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 11 is a protein called Photosystem II protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	38	Total	C	N	O	0	0
			285	189	45	51		
11	M	38	Total	C	N	O	0	0
			285	189	45	51		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			244	169	36	38	1		
12	T	30	Total	C	N	O	S	0	0
			244	169	36	38	1		

- Molecule 13 is a protein called Photosystem II protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	w	45	Total	C	N	O	0	0
			363	235	58	70		
13	W	45	Total	C	N	O	0	0
			363	235	58	70		

- Molecule 14 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	x	36	Total	C	N	O	S	0	0
			268	179	41	47	1		
14	X	36	Total	C	N	O	S	0	0
			268	179	41	47	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	y	32	Total	C	N	O	0	0
			241	159	42	40		
15	Y	32	Total	C	N	O	0	0
			241	159	42	40		

- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		
16	Z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		

- Molecule 17 is a protein called NCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	147	Total	C	N	O	S	0	0
			1163	757	190	215	1		
17	G	147	Total	C	N	O	S	0	0
			1163	757	190	215	1		

- Molecule 18 is a protein called CAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	173	Total	C	N	O	S	0	0
			1380	912	225	240	3		
18	O	173	Total	C	N	O	S	0	0
			1380	912	225	240	3		

- Molecule 19 is a protein called CAC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	180	Total	C	N	O	S	0	0
			1392	902	232	249	9		
19	P	180	Total	C	N	O	S	0	0
			1392	902	232	249	9		

- Molecule 20 is a protein called CAC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	163	Total	C	N	O	S	0	0
			1253	806	216	221	10		
20	Q	163	Total	C	N	O	S	0	0
			1253	806	216	221	10		

- Molecule 21 is a protein called CAC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	183	Total	C	N	O	S	0	0
			1430	936	234	257	3		
21	R	183	Total	C	N	O	S	0	0
			1430	936	234	257	3		

- Molecule 22 is a protein called CAC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	173	Total	C	N	O	S	0	0
			1337	865	228	238	6		
22	S	173	Total	C	N	O	S	0	0
			1337	865	228	238	6		

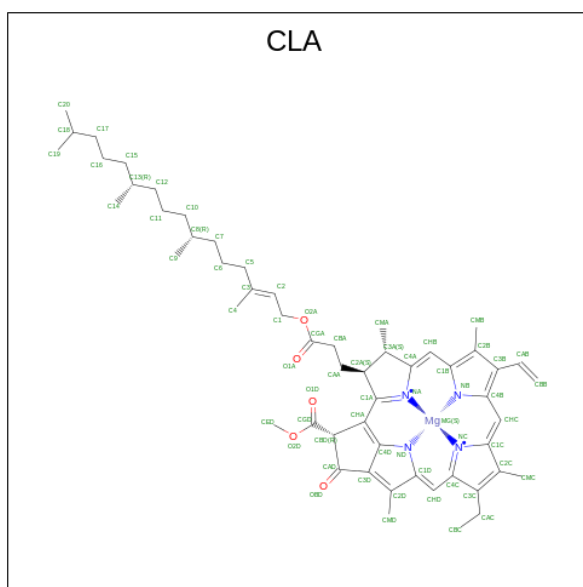
- Molecule 23 is a protein called CAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	190	Total	C	N	O	S	0	0
			1458	933	256	261	8		
23	N	190	Total	C	N	O	S	0	0
			1458	933	256	261	8		

- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
24	a	1	Total	Fe	0
			1	1	
24	A	1	Total	Fe	0
			1	1	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	O	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	O	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	O	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	P	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	P	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	Q	1	Total 56	C 46	Mg 1	N 4	O 5	0

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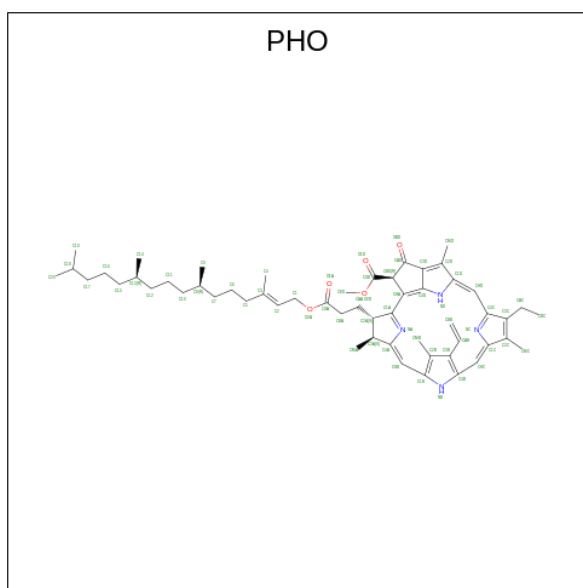
Mol	Chain	Residues	Atoms					AltConf
25	Q	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0

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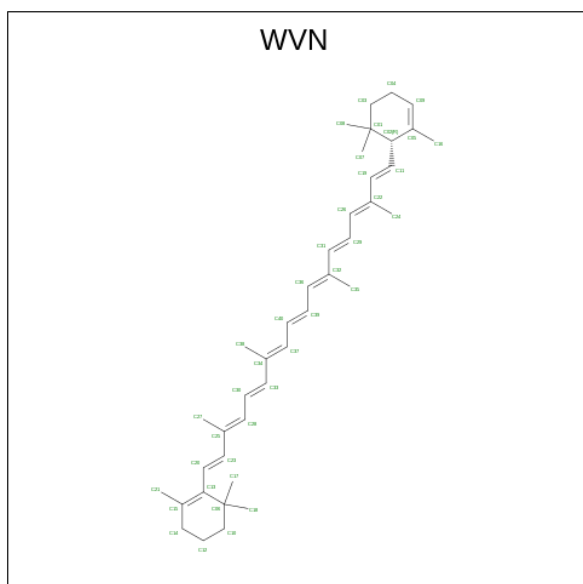
Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	

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



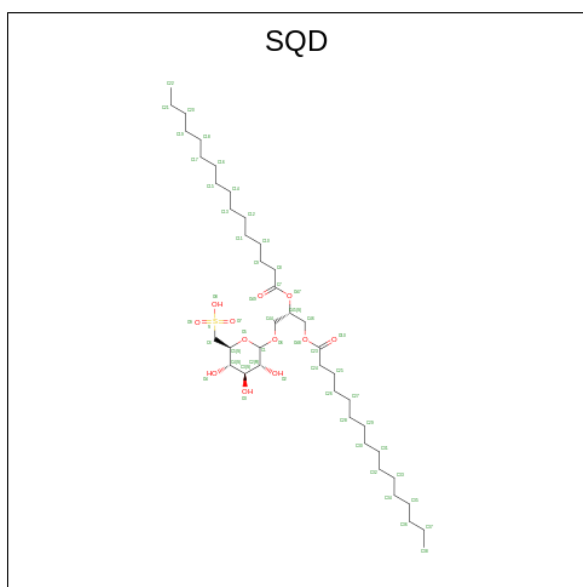
Mol	Chain	Residues	Atoms		AltConf
27	a	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	c	1	Total	C	0
			40	40	
27	c	1	Total	C	0
			40	40	
27	c	1	Total	C	0
			40	40	

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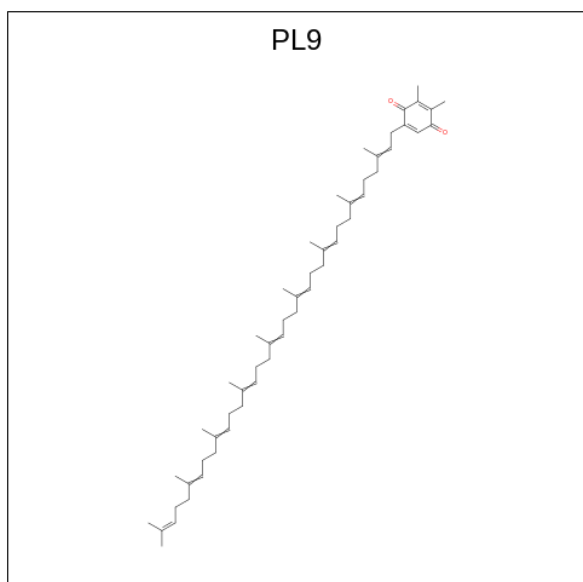
Mol	Chain	Residues	Atoms	AltConf
27	d	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	y	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	Y	1	Total C 40 40	0
27	3	1	Total C 40 40	0
27	6	1	Total C 40 40	0
27	P	1	Total C 40 40	0
27	S	1	Total C 40 40	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



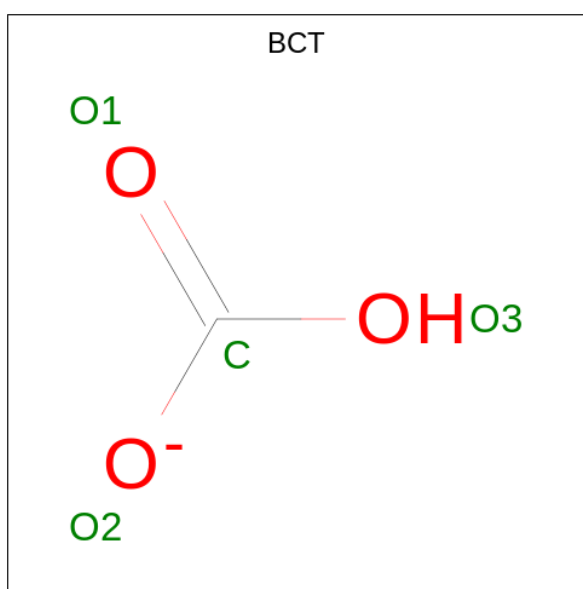
Mol	Chain	Residues	Atoms				AltConf
28	a	1	Total	C	O	S	0
			45	32	12	1	
28	a	1	Total	C	O	S	0
			40	27	12	1	
28	A	1	Total	C	O	S	0
			54	41	12	1	
28	A	1	Total	C	O	S	0
			40	27	12	1	

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



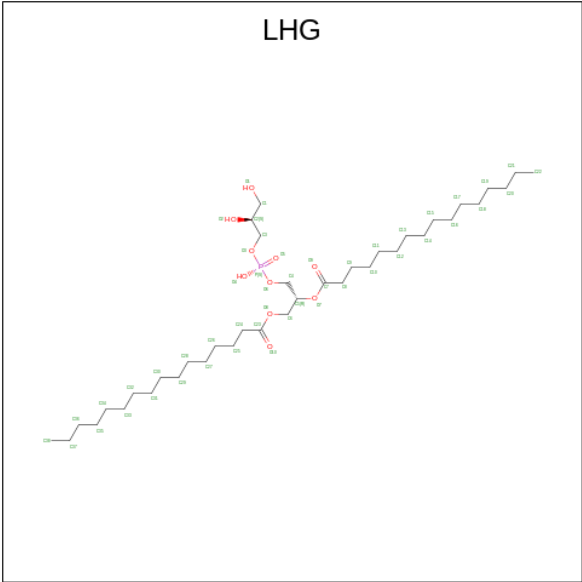
Mol	Chain	Residues	Atoms			AltConf
29	a	1	Total	C	O	0
			33	31	2	
29	d	1	Total	C	O	0
			55	53	2	
29	A	1	Total	C	O	0
			33	31	2	
29	D	1	Total	C	O	0
			55	53	2	

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			4	1	3	
30	A	1	Total	C	O	0
			4	1	3	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	P	0
			42	31	10	1	
31	b	1	Total	C	O	P	0
			43	32	10	1	
31	c	1	Total	C	O	P	0
			40	29	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	z	1	Total	C	O	P	0
			25	14	10	1	
31	A	1	Total	C	O	P	0
			42	31	10	1	
31	B	1	Total	C	O	P	0
			43	32	10	1	
31	C	1	Total	C	O	P	0
			40	29	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	Z	1	Total	C	O	P	0
			25	14	10	1	
31	2	1	Total	C	O	P	0
			46	35	10	1	
31	3	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	5	1	Total	C	O	P	0
			46	35	10	1	
31	6	1	Total	C	O	P	0
			40	29	10	1	
31	O	1	Total	C	O	P	0
			46	35	10	1	
31	P	1	Total	C	O	P	0
			49	38	10	1	
31	R	1	Total	C	O	P	0
			46	35	10	1	
31	S	1	Total	C	O	P	0
			40	29	10	1	

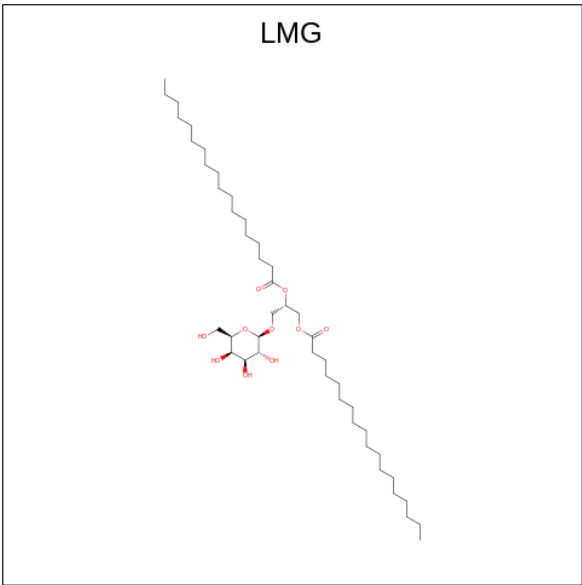
- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Cl	0
			1	1	
32	c	1	Total	Cl	0
			1	1	
32	A	1	Total	Cl	0
			1	1	
32	C	1	Total	Cl	0
			1	1	

- Molecule 33 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
33	a	2	Total	Mn	0
			2	2	
33	A	2	Total	Mn	0
			2	2	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



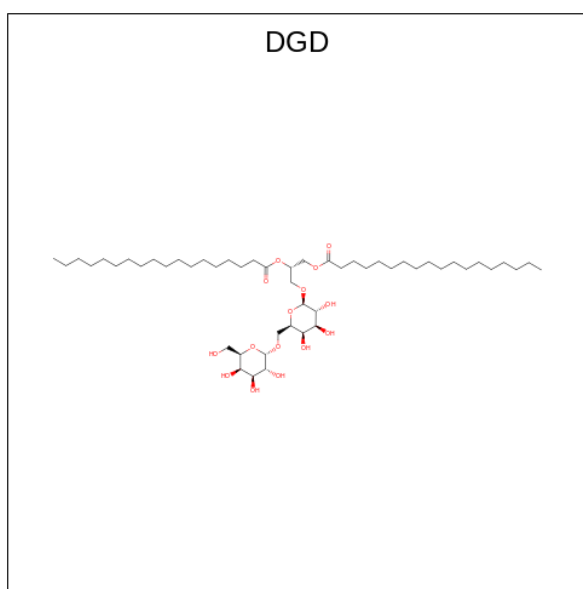
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	
34	d	1	Total	C	O	0
			40	30	10	
34	d	1	Total	C	O	0
			37	27	10	
34	f	1	Total	C	O	0
			46	36	10	
34	m	1	Total	C	O	0
			40	30	10	
34	w	1	Total	C	O	0
			48	38	10	
34	z	1	Total	C	O	0
			31	21	10	
34	g	1	Total	C	O	0
			40	30	10	
34	B	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			47	37	10	
34	D	1	Total	C	O	0
			40	30	10	
34	D	1	Total	C	O	0
			37	27	10	
34	F	1	Total	C	O	0
			46	36	10	

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Mol	Chain	Residues	Atoms			AltConf
34	M	1	Total	C	O	0
			40	30	10	
34	W	1	Total	C	O	0
			48	38	10	
34	Z	1	Total	C	O	0
			31	21	10	
34	2	1	Total	C	O	0
			40	30	10	
34	4	1	Total	C	O	0
			43	33	10	
34	G	1	Total	C	O	0
			40	30	10	
34	O	1	Total	C	O	0
			40	30	10	
34	Q	1	Total	C	O	0
			43	33	10	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



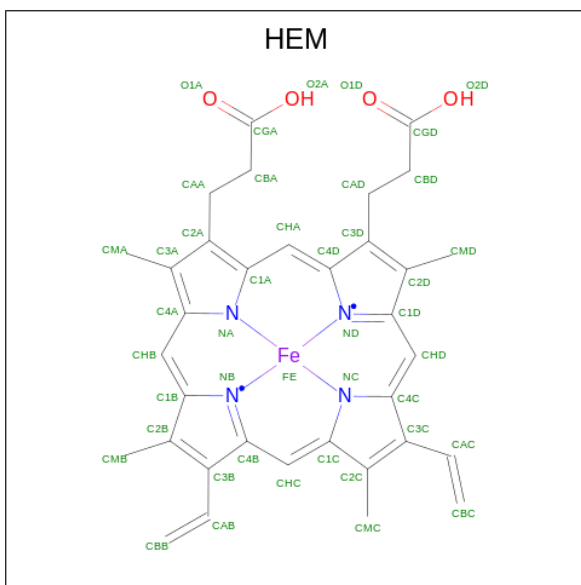
Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			54	39	15	
35	h	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			54	39	15	

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Mol	Chain	Residues	Atoms			AltConf
35	H	1	Total	C	O	0
			62	47	15	

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
36	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
36	E	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 37 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).

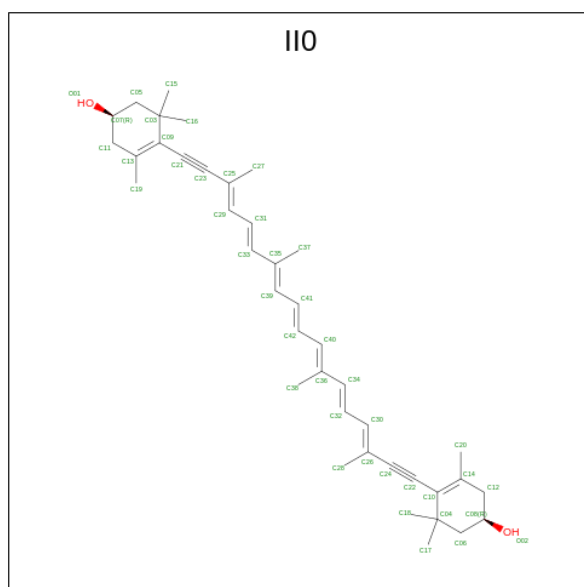


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Mol	Chain	Residues	Atoms					AltConf
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- 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).



Mol	Chain	Residues	Atoms			AltConf
38	2	1	Total	C	O	0
			42	40	2	
38	2	1	Total	C	O	0
			42	40	2	
38	2	1	Total	C	O	0
			42	40	2	
38	2	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	

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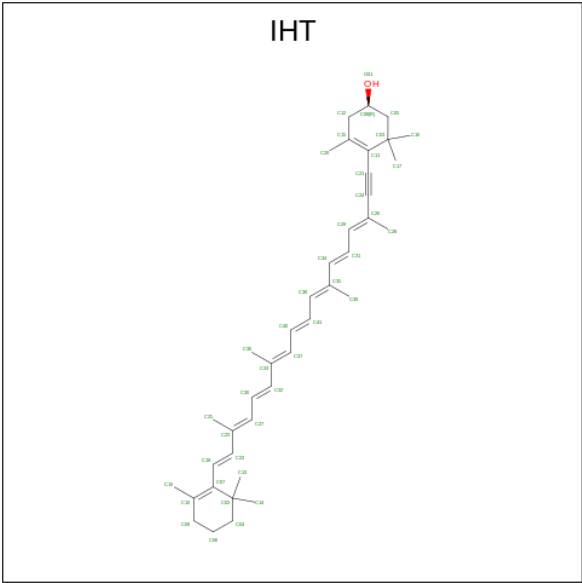
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total 42	C 40	O 2	0
38	1	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	S	1	Total 42	C 40	O 2	0
38	S	1	Total 42	C 40	O 2	0
38	S	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
38	S	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
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).



Mol	Chain	Residues	Atoms			AltConf
39	2	1	Total	C	O	0
			41	40	1	
39	4	1	Total	C	O	0
			41	40	1	
39	5	1	Total	C	O	0
			41	40	1	
39	1	1	Total	C	O	0
			41	40	1	
39	O	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
39	Q	1	Total	C	O	0
			41	40	1	
39	R	1	Total	C	O	0
			41	40	1	
39	N	1	Total	C	O	0
			41	40	1	

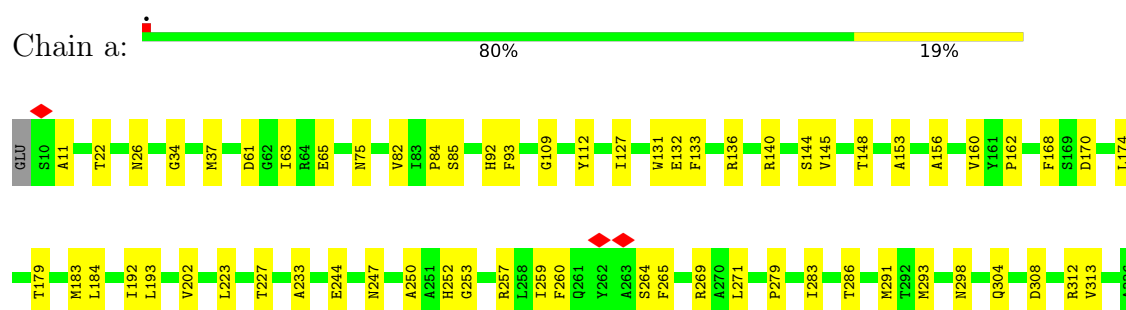
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	c	1	Total	O	0
			1	1	
40	C	1	Total	O	0
			1	1	

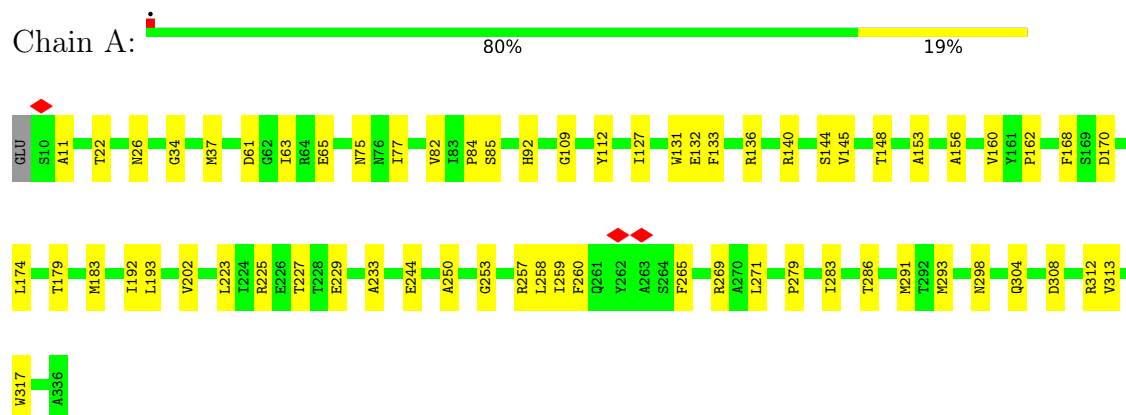
3 Residue-property plots

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.

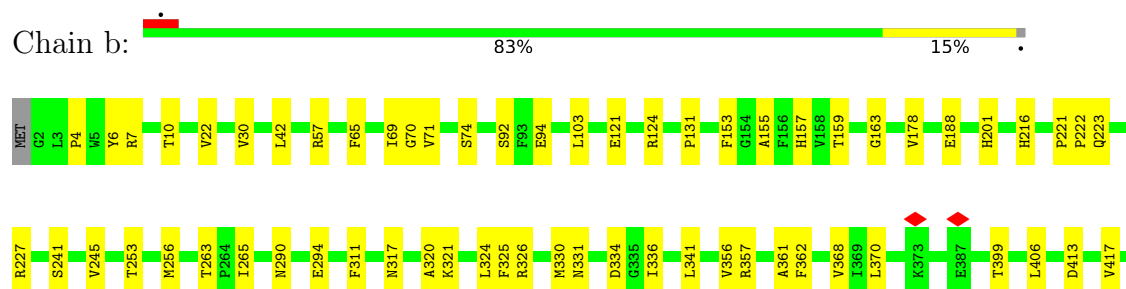
- Molecule 1: Photosystem II protein D1

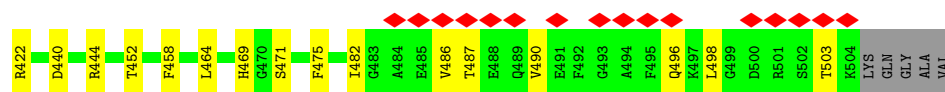


- Molecule 1: Photosystem II protein D1



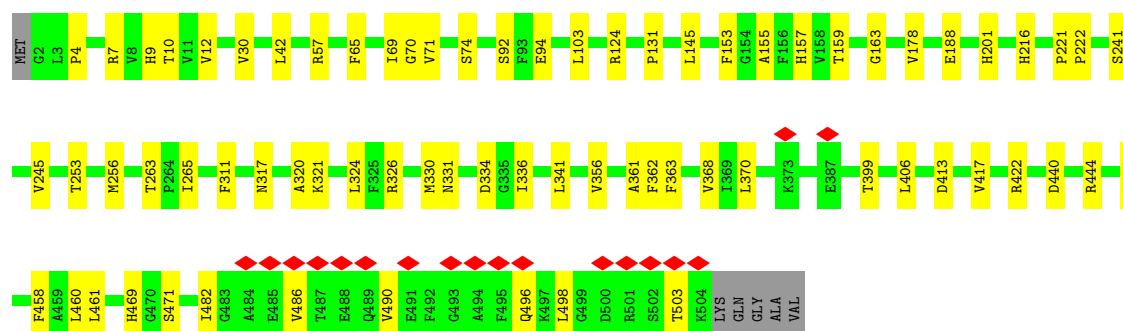
- Molecule 2: Photosystem II CP47 reaction center protein





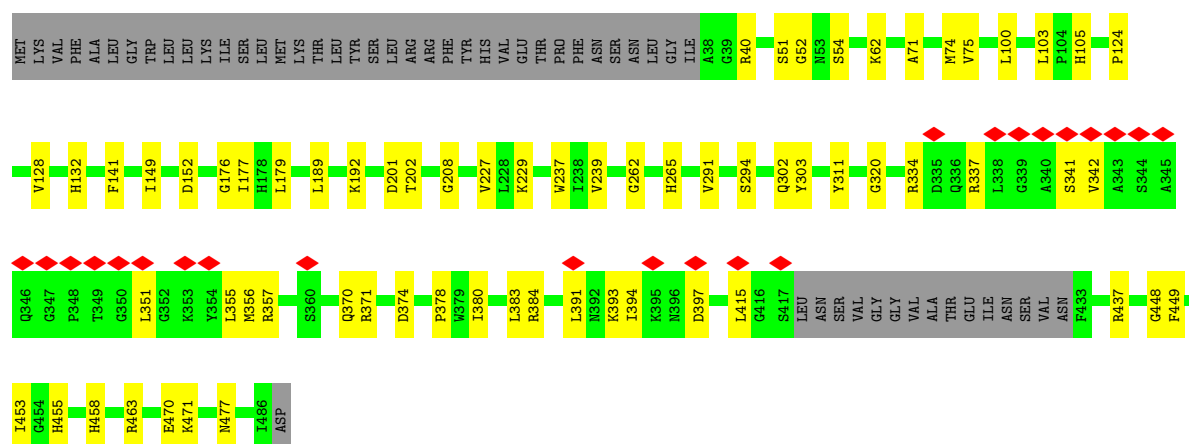
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 85% 14% .



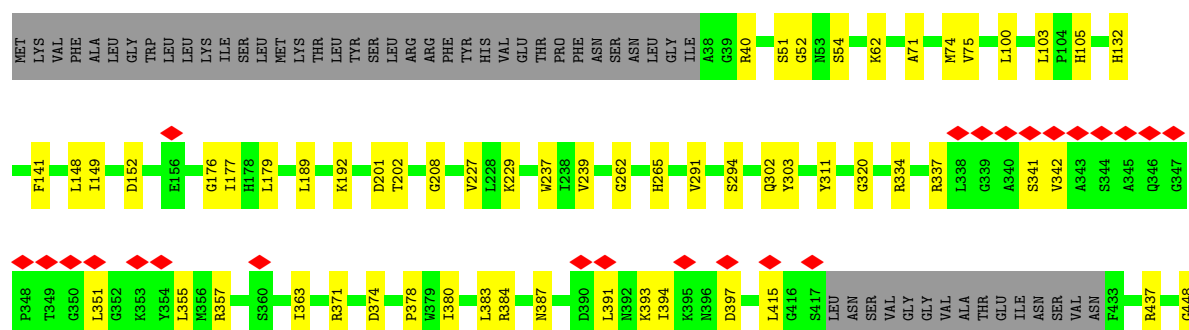
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 5% 75% 14% 11%



• Molecule 3: Photosystem II CP43 reaction center protein

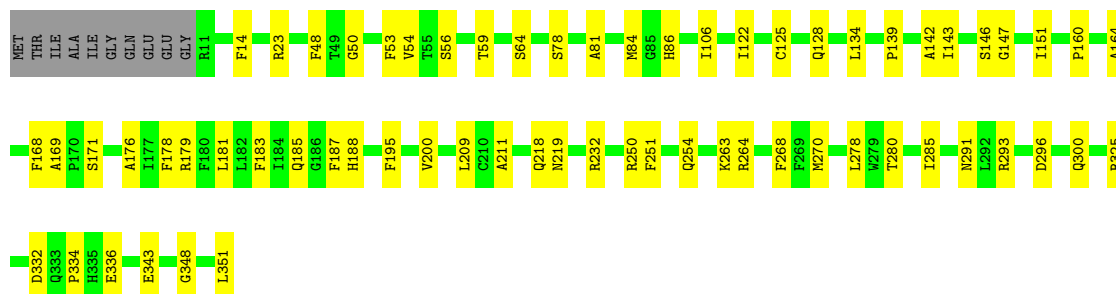
Chain C: 5% 75% 14% 11%





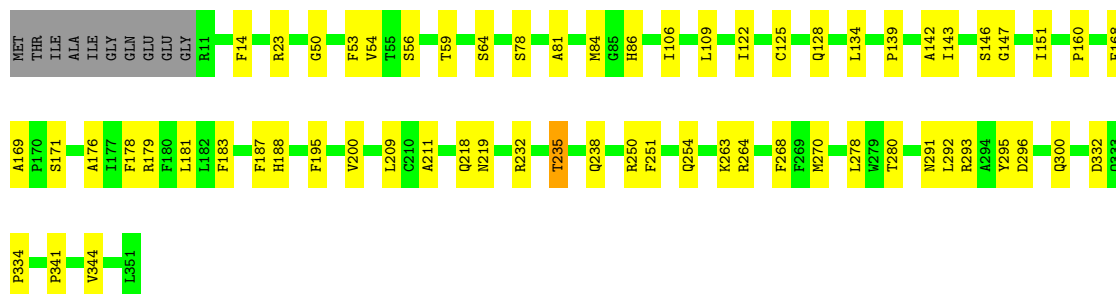
- Molecule 4: Photosystem II D2 protein

Chain d: 79% 19%



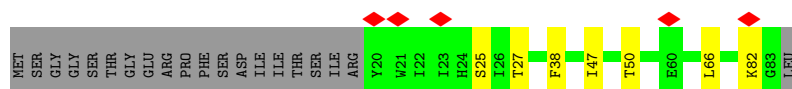
- Molecule 4: Photosystem II D2 protein

Chain D: 79% 18%



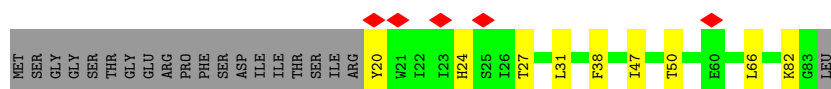
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 6% 68% 8% 24%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 6% 65% 11% 24%

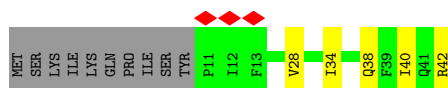


- Molecule 6: Cytochrome b559 subunit beta

Chain f: 7% 62% 14% 24%



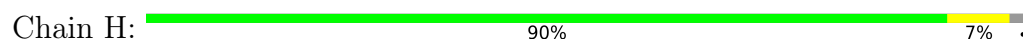
- Molecule 6: Cytochrome b559 subunit beta



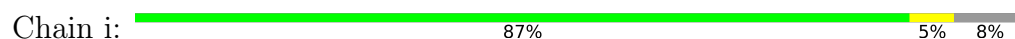
- Molecule 7: Photosystem II reaction center protein H



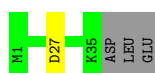
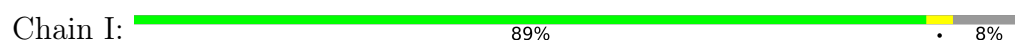
- Molecule 7: Photosystem II reaction center protein H



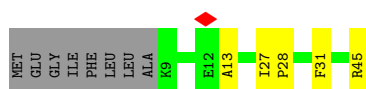
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

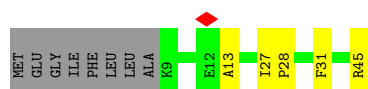


- Molecule 9: Photosystem II reaction center protein K




- Molecule 9: Photosystem II reaction center protein K

Chain K:  71% 11% 18%




- Molecule 10: Photosystem II reaction center protein L

Chain l:  82% 16% .




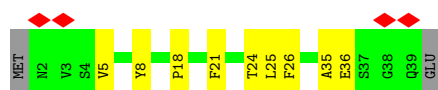
- Molecule 10: Photosystem II reaction center protein L

Chain L:  87% 11% .




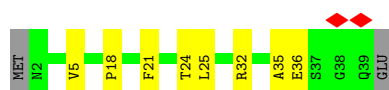
- Molecule 11: Photosystem II protein M

Chain m:  10% 72% 22% 5%



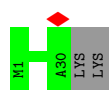
- Molecule 11: Photosystem II protein M

Chain M:  5% 75% 20% 5%




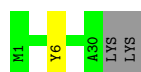
- Molecule 12: Photosystem II reaction center protein T

Chain t:  94% 6%

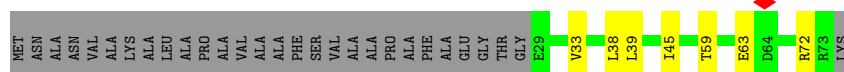


- Molecule 12: Photosystem II reaction center protein T

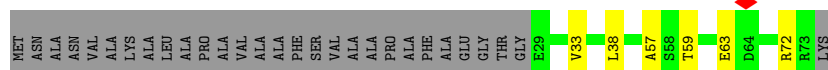
Chain T:  91% . 6%



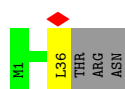
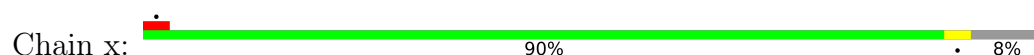
- Molecule 13: Photosystem II protein W



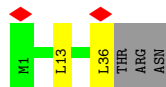
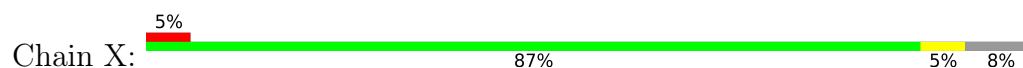
• Molecule 13: Photosystem II protein W



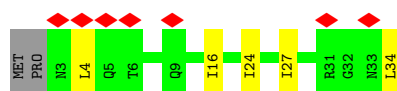
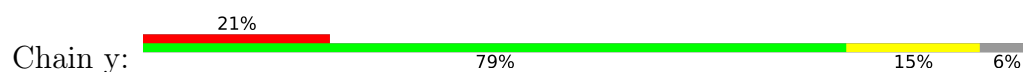
• Molecule 14: Photosystem II reaction center X protein



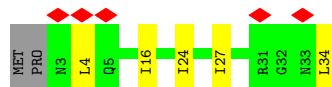
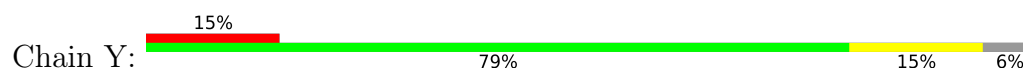
• Molecule 14: Photosystem II reaction center X protein



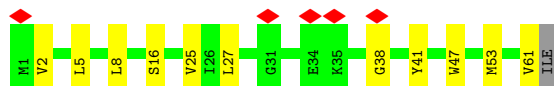
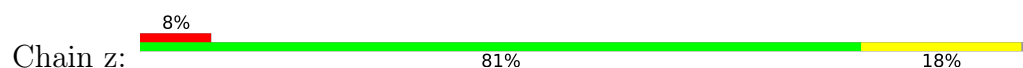
• Molecule 15: Photosystem II reaction center protein Psb30



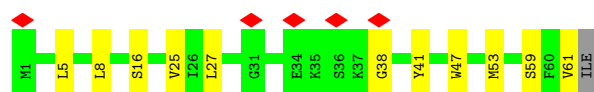
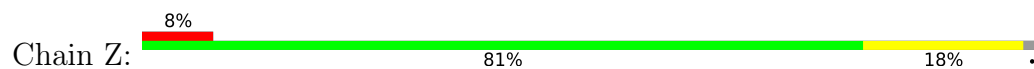
• Molecule 15: Photosystem II reaction center protein Psb30



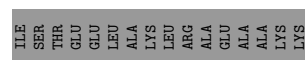
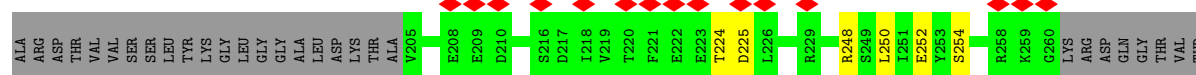
• Molecule 16: Photosystem II reaction center protein Z



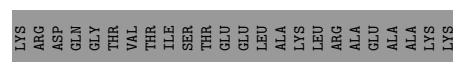
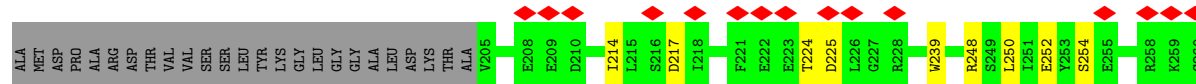
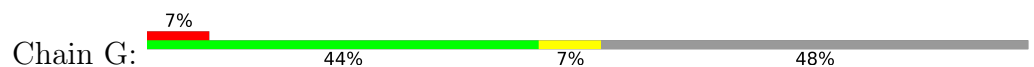
- Molecule 16: Photosystem II reaction center protein Z



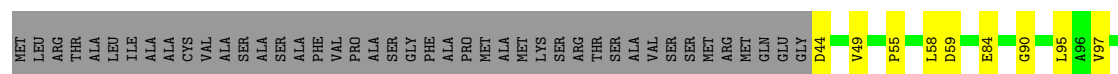
- Molecule 17: NCP



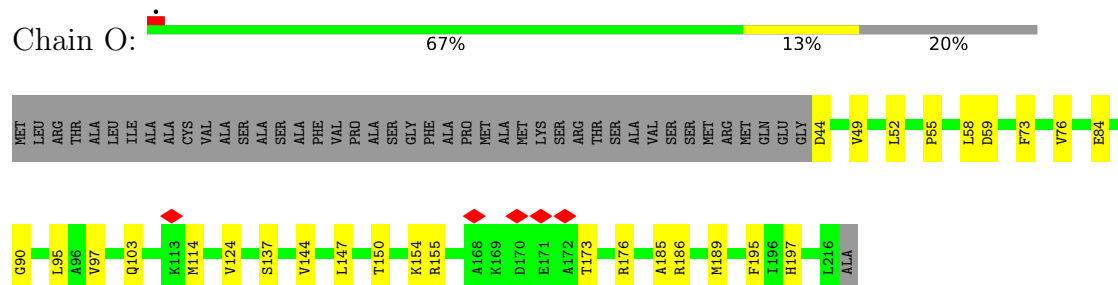
- Molecule 17: NCP



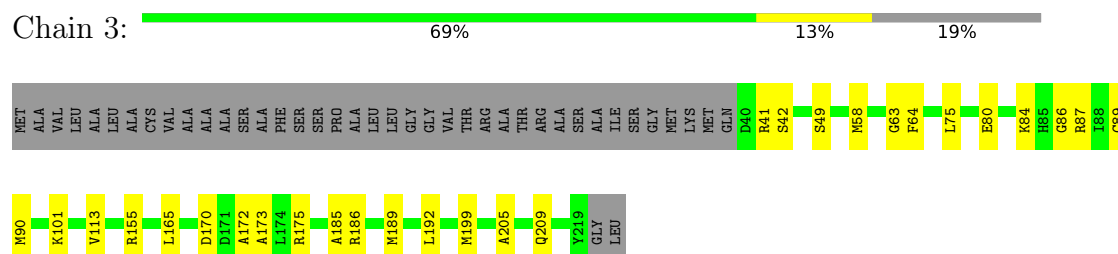
- Molecule 18: CAC2



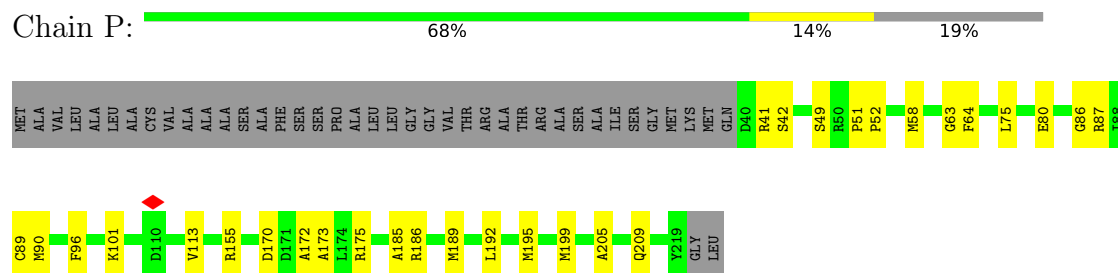
• Molecule 18: CAC2



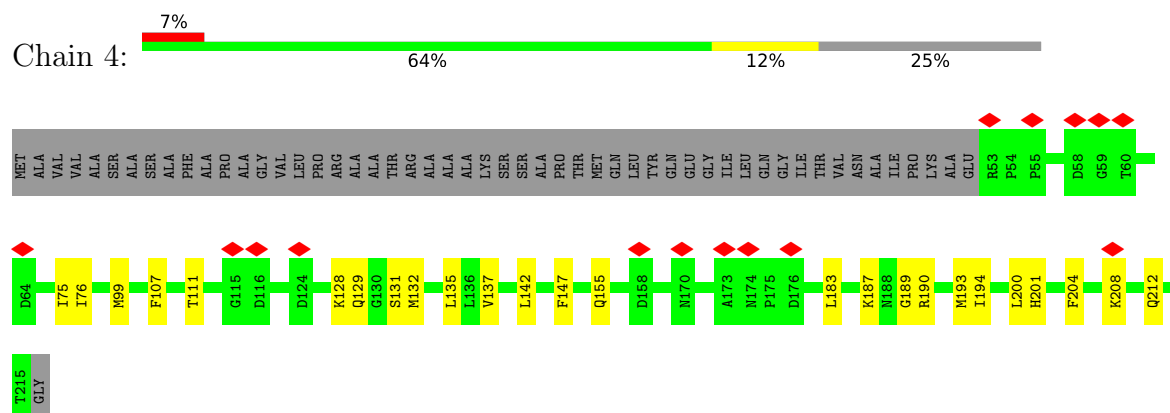
• Molecule 19: CAC3



• Molecule 19: CAC3

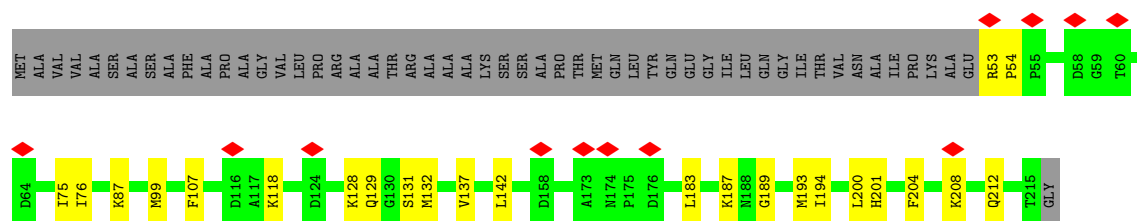


• Molecule 20: CAC4

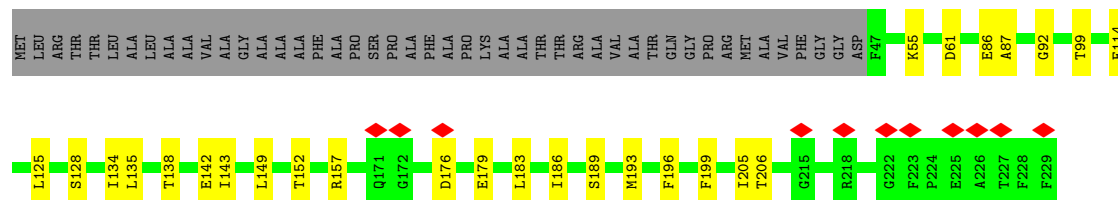


• Molecule 20: CAC4

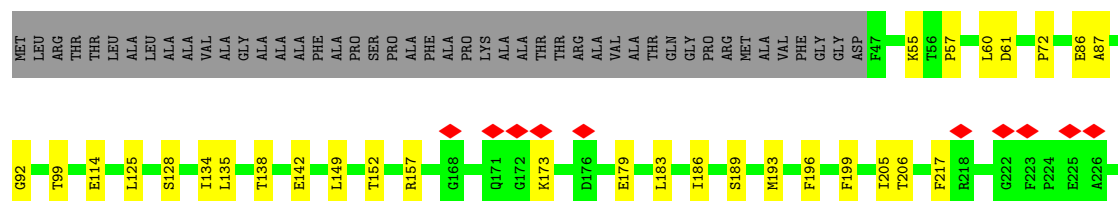




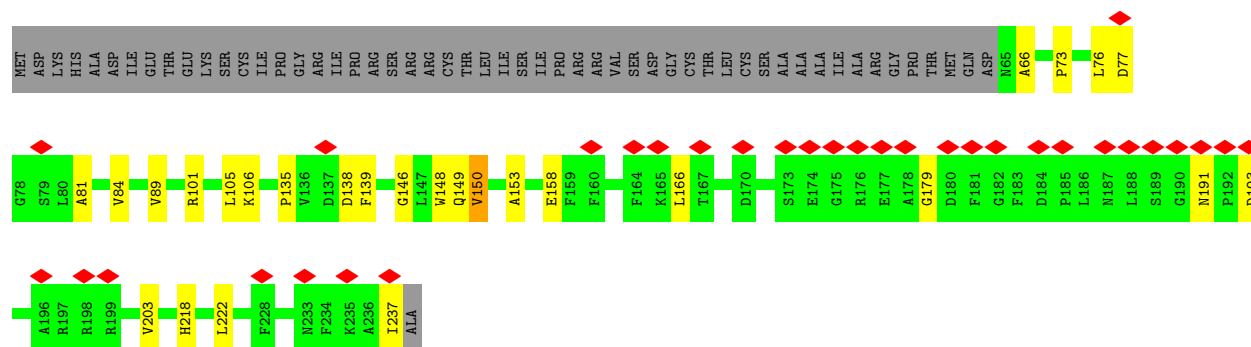
• Molecule 21: CAC5



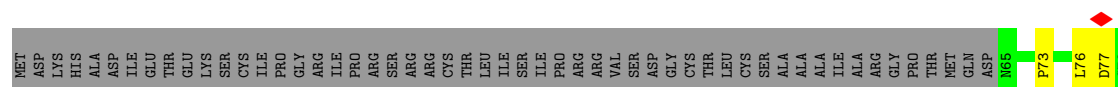
• Molecule 21: CAC5

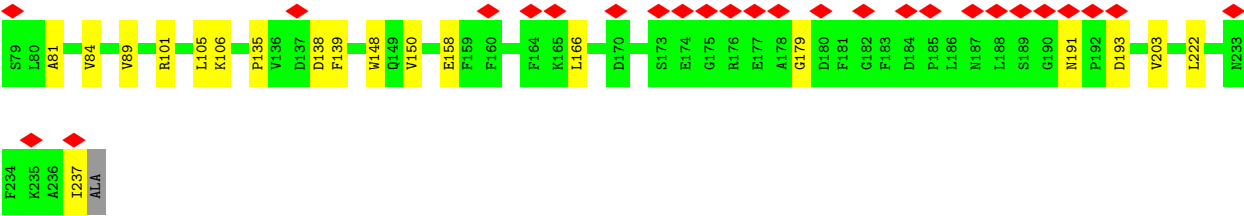


• Molecule 22: CAC6

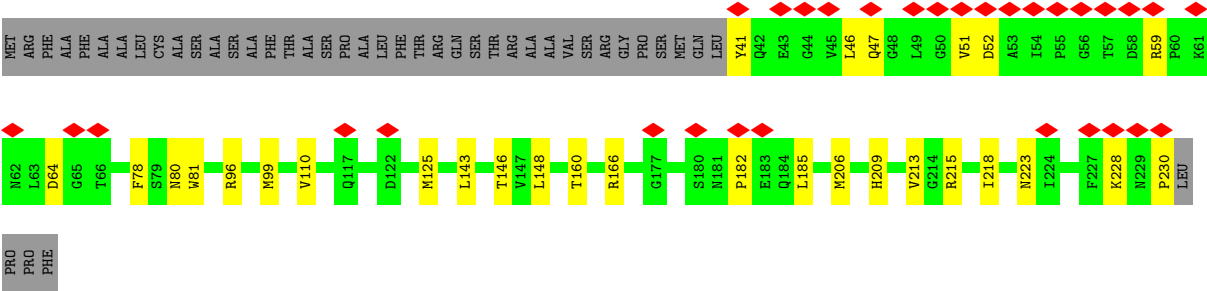


• Molecule 22: CAC6

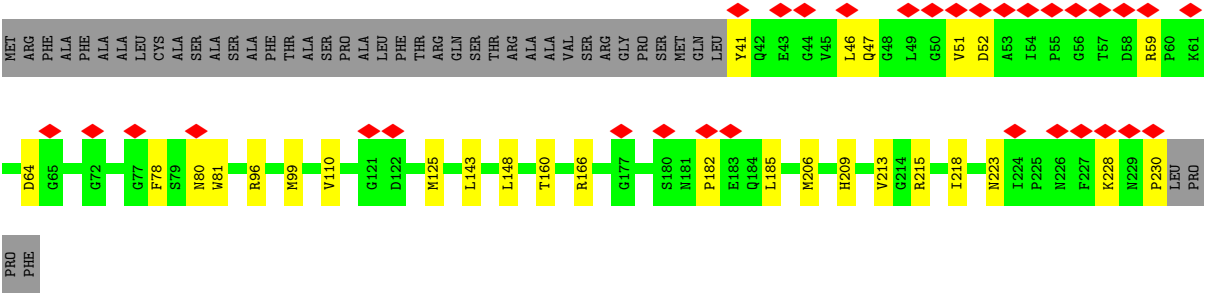




• Molecule 23: CAC1



• Molecule 23: CAC1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112613	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	0.253	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	432.65326, 432.65326, 432.65326	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0400319, 1.0400319, 1.0400319	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, HEM, BCT, IIO, CLA, PHO, WVN, SQD, CL, PL9, IHT, MN, DGD, KC2, FE2, LHG

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	0.19	0/2644	0.33	0/3607
1	a	0.13	0/2644	0.28	0/3607
2	B	0.17	0/4082	0.33	1/5557 (0.0%)
2	b	0.13	0/4082	0.30	0/5557
3	C	0.11	0/3491	0.28	0/4763
3	c	0.15	0/3491	0.32	0/4763
4	D	0.17	0/2801	0.32	0/3815
4	d	0.13	0/2801	0.31	0/3815
5	E	0.10	0/541	0.26	0/738
5	e	0.22	0/541	0.47	1/738 (0.1%)
6	F	0.54	0/270	0.85	0/366
6	f	0.49	0/270	0.62	0/366
7	H	0.19	0/519	0.42	0/707
7	h	0.25	0/519	0.58	1/707 (0.1%)
8	I	0.10	0/290	0.27	0/392
8	i	0.11	0/290	0.26	0/392
9	K	0.18	0/307	0.35	0/421
9	k	0.19	0/307	0.38	0/421
10	L	0.26	0/311	0.42	0/424
10	l	0.26	0/311	0.43	0/424
11	M	0.13	0/289	0.31	0/393
11	m	0.14	0/289	0.28	0/393
12	T	0.09	0/251	0.21	0/341
12	t	0.09	0/251	0.21	0/341
13	W	0.12	0/370	0.30	0/503
13	w	0.13	0/370	0.30	0/503
14	X	0.12	0/272	0.25	0/370
14	x	0.12	0/272	0.25	0/370
15	Y	0.08	0/242	0.23	0/329
15	y	0.09	0/242	0.24	0/329
16	Z	0.26	0/470	0.40	0/641
16	z	0.18	0/470	0.33	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	G	0.16	0/1200	0.35	0/1635
17	g	0.12	0/1200	0.31	0/1635
18	2	0.22	0/1419	0.41	0/1919
18	O	0.16	0/1419	0.35	0/1919
19	3	0.14	0/1428	0.32	0/1930
19	P	0.14	0/1428	0.32	0/1930
20	4	0.23	0/1281	0.43	1/1731 (0.1%)
20	Q	0.22	0/1281	0.41	0/1731
21	5	0.22	0/1469	0.40	0/1988
21	R	0.23	0/1469	0.44	0/1988
22	6	0.22	0/1372	0.61	5/1855 (0.3%)
22	S	0.24	0/1372	0.54	3/1855 (0.2%)
23	1	0.16	0/1490	0.38	0/2017
23	N	0.16	0/1490	0.38	0/2017
All	All	0.18	0/53618	0.36	12/72884 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	89	VAL	CB-CA-C	13.16	132.88	111.29
22	S	150	VAL	N-CA-C	-8.88	101.89	110.42
7	h	48	ILE	N-CA-C	8.25	118.34	110.42
22	6	150	VAL	N-CA-C	-8.22	102.53	110.42
22	S	148	TRP	N-CA-C	7.98	120.06	111.36
5	e	25	SER	N-CA-C	-7.72	103.86	113.28
22	S	150	VAL	N-CA-CB	7.45	119.27	110.55
22	6	148	TRP	N-CA-C	7.18	119.11	111.28
22	6	150	VAL	N-CA-CB	6.77	118.48	110.55
2	B	363	PHE	N-CA-C	6.59	119.27	109.59
22	6	89	VAL	N-CA-C	-6.53	95.77	109.34
20	4	111	THR	N-CA-C	5.46	117.24	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2563	0	2469	52	0
1	a	2563	0	2469	51	0
2	B	3950	0	3830	63	0
2	b	3950	0	3830	73	0
3	C	3379	0	3307	53	0
3	c	3379	0	3307	51	0
4	D	2708	0	2606	54	0
4	d	2708	0	2606	62	0
5	E	525	0	510	8	0
5	e	525	0	510	5	0
6	F	261	0	269	3	0
6	f	261	0	269	3	0
7	H	508	0	529	6	0
7	h	508	0	529	7	0
8	I	284	0	295	1	0
8	i	284	0	295	2	0
9	K	296	0	312	7	0
9	k	296	0	312	5	0
10	L	301	0	301	4	0
10	l	301	0	301	6	0
11	M	285	0	300	12	0
11	m	285	0	300	10	0
12	T	244	0	256	1	0
12	t	244	0	256	0	0
13	W	363	0	350	4	0
13	w	363	0	350	5	0
14	X	268	0	293	2	0
14	x	268	0	293	1	0
15	Y	241	0	275	5	0
15	y	241	0	275	5	0
16	Z	460	0	499	8	0
16	z	460	0	499	8	0
17	G	1163	0	1118	22	0
17	g	1163	0	1118	11	0
18	2	1380	0	1366	21	0
18	O	1380	0	1366	26	0
19	3	1392	0	1377	17	0
19	P	1392	0	1377	19	0
20	4	1253	0	1259	20	0
20	Q	1253	0	1259	19	0
21	5	1430	0	1418	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	R	1430	0	1418	35	0
22	6	1337	0	1307	28	0
22	S	1337	0	1307	19	0
23	1	1458	0	1468	19	0
23	N	1458	0	1468	18	0
24	A	1	0	0	0	0
24	a	1	0	0	0	0
25	1	518	0	444	7	0
25	2	633	0	611	14	0
25	3	570	0	547	10	0
25	4	482	0	445	20	0
25	5	620	0	589	19	0
25	6	525	0	507	14	0
25	A	174	0	170	14	0
25	B	1014	0	1092	42	0
25	C	827	0	894	31	0
25	D	190	0	203	9	0
25	G	110	0	105	3	0
25	N	518	0	444	8	0
25	O	633	0	611	17	0
25	P	570	0	547	11	0
25	Q	482	0	445	17	0
25	R	620	0	589	19	0
25	S	525	0	510	11	0
25	a	174	0	170	15	0
25	b	1014	0	1092	40	0
25	c	828	0	896	26	0
25	d	191	0	205	10	0
25	g	110	0	105	5	0
26	A	64	0	74	2	0
26	D	64	0	74	5	0
26	a	64	0	74	3	0
26	d	64	0	74	5	0
27	3	40	0	0	0	0
27	6	40	0	0	0	0
27	A	40	0	0	0	0
27	B	120	0	0	1	0
27	C	120	0	0	0	0
27	D	40	0	0	0	0
27	H	40	0	0	0	0
27	P	40	0	0	0	0
27	S	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Y	40	0	0	0	0
27	a	40	0	0	0	0
27	b	120	0	0	1	0
27	c	120	0	0	0	0
27	d	40	0	0	0	0
27	h	40	0	0	0	0
27	y	40	0	0	0	0
28	A	94	0	122	2	0
28	a	85	0	101	2	0
29	A	33	0	42	0	0
29	D	55	0	80	3	0
29	a	33	0	42	2	0
29	d	55	0	80	4	0
30	A	4	0	0	0	0
30	a	4	0	0	0	0
31	2	46	0	65	1	0
31	3	49	0	74	2	0
31	5	46	0	65	4	0
31	6	40	0	53	2	0
31	A	42	0	57	0	0
31	B	43	0	59	3	0
31	C	40	0	50	1	0
31	D	49	0	74	4	0
31	L	49	0	74	6	0
31	O	46	0	65	1	0
31	P	49	0	74	3	0
31	R	46	0	65	4	0
31	S	40	0	53	2	0
31	Z	25	0	20	0	0
31	a	42	0	57	0	0
31	b	43	0	59	2	0
31	c	40	0	50	2	0
31	d	49	0	74	4	0
31	l	49	0	74	8	0
31	z	25	0	20	0	0
32	A	1	0	0	0	0
32	C	1	0	0	0	0
32	a	1	0	0	0	0
32	c	1	0	0	0	0
33	A	2	0	0	0	0
33	a	2	0	0	0	0
34	2	40	0	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	4	43	0	56	2	0
34	B	51	0	72	1	0
34	C	47	0	64	0	0
34	D	77	0	94	4	0
34	F	46	0	62	0	0
34	G	40	0	50	5	0
34	M	40	0	50	1	0
34	O	40	0	50	1	0
34	Q	43	0	56	2	0
34	W	48	0	66	2	0
34	Z	31	0	32	2	0
34	b	51	0	72	1	0
34	c	51	0	72	4	0
34	d	77	0	94	3	0
34	f	46	0	62	3	0
34	g	40	0	50	3	0
34	m	40	0	50	1	0
34	w	48	0	66	1	0
34	z	31	0	32	2	0
35	C	54	0	66	1	0
35	H	62	0	82	5	0
35	c	54	0	66	1	0
35	h	62	0	82	4	0
36	E	43	0	30	1	0
36	e	43	0	30	1	0
37	1	180	0	0	1	0
37	2	45	0	0	0	0
37	3	45	0	0	0	0
37	4	135	0	0	0	0
37	5	45	0	0	0	0
37	6	90	0	0	10	0
37	N	180	0	0	2	0
37	O	45	0	0	0	0
37	P	45	0	0	0	0
37	Q	135	0	0	0	0
37	R	45	0	0	0	0
37	S	90	0	0	0	0
38	1	168	0	0	0	0
38	2	168	0	0	1	0
38	3	168	0	0	0	0
38	4	168	0	0	1	0
38	5	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	6	168	0	0	2	0
38	N	168	0	0	0	0
38	O	168	0	0	1	0
38	P	168	0	0	0	0
38	Q	168	0	0	0	0
38	R	168	0	0	0	0
38	S	168	0	0	2	0
39	1	41	0	0	0	0
39	2	41	0	0	0	0
39	4	41	0	0	0	0
39	5	41	0	0	0	0
39	N	41	0	0	0	0
39	O	41	0	0	0	0
39	Q	41	0	0	0	0
39	R	41	0	0	0	0
40	C	1	0	0	0	0
40	c	1	0	0	0	0
All	All	70547	0	66150	1008	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1008) 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)
2:b:362:PHE:HE2	4:d:183:PHE:CZ	1.36	1.43
2:b:362:PHE:CE2	4:d:183:PHE:CZ	2.08	1.41
2:b:362:PHE:CE2	4:d:183:PHE:HZ	1.47	1.22
1:a:257:ARG:HH11	2:b:498:LEU:HD13	1.16	1.10
1:A:257:ARG:HH11	2:B:498:LEU:HD13	1.15	1.09
19:3:58:MET:SD	19:3:75:LEU:HD13	1.91	1.08
2:B:145:LEU:HD11	25:B:615:CLA:HMB2	1.33	1.05
1:a:257:ARG:NH1	2:b:498:LEU:HD13	1.75	1.01
1:A:257:ARG:NH1	2:B:498:LEU:HD13	1.73	1.01
2:b:362:PHE:CZ	4:d:183:PHE:CZ	2.53	0.96
2:B:241:SER:O	2:B:245:VAL:HG23	1.67	0.95
25:a:403:CLA:HAB	25:a:404:CLA:HMD2	1.49	0.94
2:b:362:PHE:HE2	4:d:183:PHE:CE1	1.86	0.94
2:b:241:SER:O	2:b:245:VAL:HG23	1.66	0.94
25:A:403:CLA:HAB	25:A:404:CLA:HMD2	1.49	0.93
1:A:257:ARG:HH11	2:B:498:LEU:CD1	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HD11	25:B:615:CLA:CMB	2.03	0.88
1:a:257:ARG:HH11	2:b:498:LEU:CD1	1.86	0.87
22:6:153:ALA:CB	37:6:606:KC2:CBC	2.54	0.84
3:c:356:MET:SD	3:c:370:GLN:HG3	2.18	0.83
2:b:362:PHE:CZ	4:d:183:PHE:HZ	1.94	0.81
23:1:125:MET:HE1	23:1:206:MET:HB3	1.62	0.81
23:N:125:MET:HE1	23:N:206:MET:HB3	1.62	0.81
1:A:257:ARG:NH1	2:B:498:LEU:CD1	2.45	0.79
22:6:153:ALA:HB3	37:6:606:KC2:CBC	2.14	0.77
17:G:224:THR:HG22	17:G:225:ASP:N	2.00	0.76
1:a:257:ARG:NH1	2:b:498:LEU:CD1	2.46	0.75
22:S:222:LEU:HD21	22:S:237:ILE:CD1	2.16	0.75
21:R:114:GLU:OE2	21:R:114:GLU:HA	1.86	0.75
16:Z:59:SER:HB3	37:6:606:KC2:O2A	1.86	0.74
5:E:27:THR:HB	36:E:102:HEM:HAB	1.69	0.74
1:a:252:HIS:CD2	1:a:264:SER:OG	2.41	0.74
17:G:224:THR:HG22	17:G:225:ASP:H	1.51	0.73
25:g:301:CLA:HBC1	25:5:609:CLA:HBB2	1.70	0.73
21:R:57:PRO:HG2	21:R:60:LEU:CD2	2.20	0.72
19:P:86:GLY:HA3	19:P:185:ALA:HB1	1.71	0.72
21:R:138:THR:HG21	25:R:609:CLA:HBC2	1.72	0.71
22:6:153:ALA:HB2	37:6:606:KC2:CBC	2.21	0.71
19:3:86:GLY:HA3	19:3:185:ALA:HB1	1.71	0.71
2:B:362:PHE:CZ	4:D:183:PHE:CZ	2.80	0.70
18:2:90:GLY:HA3	18:2:185:ALA:HB1	1.73	0.70
21:5:114:GLU:OE2	21:5:114:GLU:HA	1.90	0.70
18:O:173:THR:HG23	18:O:176:ARG:HH21	1.56	0.69
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.74	0.69
21:5:138:THR:HG21	25:5:609:CLA:HBC2	1.75	0.69
5:e:27:THR:HB	36:e:102:HEM:HAB	1.74	0.69
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.75	0.69
18:2:173:THR:HG23	18:2:176:ARG:HH21	1.56	0.68
18:O:90:GLY:HA3	18:O:185:ALA:HB1	1.73	0.68
2:B:362:PHE:CZ	4:D:183:PHE:HZ	2.12	0.67
22:S:84:VAL:HG12	22:S:84:VAL:O	1.94	0.67
22:6:146:GLY:HA3	37:6:606:KC2:OBD	1.95	0.66
28:a:408:SQD:H62	4:d:232:ARG:HD3	1.76	0.66
3:c:341:SER:O	3:c:342:VAL:HG22	1.95	0.66
3:C:334:ARG:HG2	3:C:337:ARG:HH12	1.61	0.66
26:D:401:PHO:H51	25:D:403:CLA:H13	1.78	0.66
28:A:408:SQD:H62	4:D:232:ARG:HD3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:351:LEU:HD11	3:C:357:ARG:HE	1.60	0.65
21:R:57:PRO:CG	21:R:60:LEU:CD2	2.74	0.65
22:S:222:LEU:HD21	22:S:237:ILE:HD13	1.77	0.65
26:d:401:PHO:H51	25:d:403:CLA:H13	1.78	0.65
3:c:52:GLY:HA3	25:c:526:CLA:HMD2	1.78	0.65
4:D:178:PHE:HA	4:D:181:LEU:HD12	1.77	0.65
3:C:341:SER:O	3:C:342:VAL:HG22	1.96	0.65
4:d:178:PHE:HA	4:d:181:LEU:HD12	1.77	0.65
3:c:128:VAL:HG22	34:c:536:LMG:H162	1.79	0.64
3:C:52:GLY:HA3	25:C:526:CLA:HMD2	1.77	0.64
25:G:301:CLA:HBC1	25:R:609:CLA:HBB2	1.80	0.63
3:c:334:ARG:HG2	3:c:337:ARG:HH12	1.61	0.63
21:R:92:GLY:HA3	21:R:189:SER:HB3	1.81	0.63
23:1:41:TYR:O	23:1:47:GLN:NE2	2.32	0.63
25:C:518:CLA:H172	25:C:525:CLA:HBB2	1.80	0.62
22:6:84:VAL:HG12	22:6:84:VAL:O	1.97	0.62
6:F:40:ILE:HD12	6:F:42:ARG:HH21	1.64	0.62
21:5:125:LEU:N	21:5:125:LEU:HD23	2.13	0.62
21:R:57:PRO:CG	21:R:60:LEU:HD23	2.29	0.62
23:N:41:TYR:O	23:N:47:GLN:NE2	2.32	0.62
17:G:224:THR:CG2	17:G:225:ASP:H	2.12	0.62
1:A:269:ARG:O	4:D:218:GLN:NE2	2.33	0.62
22:6:149:GLN:OE1	37:6:606:KC2:C4D	2.48	0.62
2:b:326:ARG:NH2	4:d:296:ASP:OD2	2.32	0.61
25:c:518:CLA:H172	25:c:525:CLA:HBB2	1.81	0.61
3:c:351:LEU:HD11	3:c:357:ARG:HE	1.64	0.61
18:2:55:PRO:HG2	18:2:58:LEU:HD22	1.82	0.61
21:5:87:ALA:HB2	25:5:609:CLA:HED2	1.83	0.61
21:5:92:GLY:HA3	21:5:189:SER:HB3	1.81	0.61
4:d:171:SER:HB2	4:d:176:ALA:HB1	1.83	0.61
18:O:73:PHE:HA	18:O:76:VAL:CG1	2.31	0.61
25:N:603:CLA:HED3	25:N:603:CLA:H2	1.83	0.61
22:6:73:PRO:HG2	22:6:76:LEU:HD22	1.83	0.60
3:c:229:LYS:HB3	3:c:237:TRP:HA	1.83	0.60
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.83	0.60
6:f:40:ILE:HD12	6:f:42:ARG:HH21	1.66	0.60
21:5:152:THR:OG1	21:5:157:ARG:NH1	2.34	0.60
21:R:152:THR:OG1	21:R:157:ARG:NH1	2.34	0.60
9:k:13:ALA:HB2	16:z:61:VAL:HG11	1.84	0.60
18:2:55:PRO:HB2	18:2:58:LEU:HB2	1.84	0.60
18:O:55:PRO:HG2	18:O:58:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:269:ARG:O	4:d:218:GLN:NE2	2.33	0.60
1:A:92:HIS:NE2	3:C:374:ASP:OD2	2.35	0.60
4:D:171:SER:HB2	4:D:176:ALA:HB1	1.83	0.60
2:B:7:ARG:O	2:B:10:THR:OG1	2.18	0.60
22:S:73:PRO:HG2	22:S:76:LEU:HD22	1.83	0.60
25:5:603:CLA:HBC1	25:5:609:CLA:HAC1	1.82	0.59
22:6:106:LYS:NZ	22:6:158:GLU:OE1	2.34	0.59
17:g:105:LEU:O	17:g:109:SER:CB	2.50	0.59
17:G:105:LEU:O	17:G:109:SER:CB	2.51	0.59
25:R:603:CLA:HBC1	25:R:609:CLA:HAC1	1.83	0.59
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.83	0.59
9:K:13:ALA:HB2	16:Z:61:VAL:HG11	1.84	0.59
17:G:96:VAL:HG21	21:R:135:LEU:HD11	1.85	0.59
22:S:73:PRO:HB2	22:S:76:LEU:HB2	1.85	0.59
2:b:265:ILE:HD13	7:h:62:TRP:CH2	2.37	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.85	0.59
22:6:73:PRO:HB2	22:6:76:LEU:HB2	1.85	0.59
18:O:55:PRO:HB2	18:O:58:LEU:HB2	1.84	0.59
11:m:36:GLU:HG3	11:M:35:ALA:HB1	1.84	0.59
3:c:311:TYR:O	3:c:437:ARG:NH2	2.36	0.59
5:E:20:TYR:CE1	5:E:24:HIS:CE1	2.90	0.59
21:R:87:ALA:HB2	25:R:609:CLA:HED2	1.83	0.59
5:E:20:TYR:CE1	5:E:24:HIS:HE1	2.21	0.59
15:Y:4:LEU:HD13	15:Y:4:LEU:O	2.03	0.59
21:5:142:GLU:HG2	25:5:609:CLA:NB	2.17	0.59
3:C:179:LEU:HD21	25:C:521:CLA:HAB	1.85	0.58
2:B:265:ILE:HD13	7:H:62:TRP:CH2	2.38	0.58
25:4:603:CLA:OBD	25:4:609:CLA:HAA1	2.03	0.58
21:5:205:ILE:HG23	21:5:206:THR:HG23	1.85	0.58
2:b:399:THR:HG22	2:b:417:VAL:HG22	1.84	0.58
3:c:179:LEU:HD21	25:c:521:CLA:HAB	1.85	0.58
11:m:21:PHE:HD1	34:m:101:LMG:H141	1.68	0.58
2:B:326:ARG:NH2	4:D:296:ASP:OD2	2.33	0.58
2:B:399:THR:HG22	2:B:417:VAL:HG22	1.84	0.58
21:R:142:GLU:HG2	25:R:609:CLA:NB	2.18	0.58
1:A:227:THR:HG21	1:A:233:ALA:HA	1.86	0.58
3:C:229:LYS:HB3	3:C:237:TRP:HA	1.85	0.58
21:R:125:LEU:CD2	25:R:604:CLA:HAA2	2.34	0.58
2:b:30:VAL:HG12	25:b:605:CLA:HHD	1.86	0.58
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.84	0.58
2:b:121:GLU:HG3	7:h:4:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:405:PL9:H111	31:D:406:LHG:H102	1.86	0.58
1:a:170:ASP:OD2	3:c:371:ARG:NH1	2.31	0.58
2:b:362:PHE:CZ	4:d:183:PHE:CE2	2.90	0.58
17:g:105:LEU:O	17:g:109:SER:HB2	2.03	0.58
1:A:140:ARG:HB2	4:D:219:ASN:HA	1.86	0.58
2:b:155:ALA:O	2:b:159:THR:OG1	2.21	0.58
1:A:145:VAL:O	1:A:148:THR:OG1	2.22	0.58
21:5:125:LEU:HD12	25:5:604:CLA:HAA2	1.86	0.58
17:G:224:THR:CG2	17:G:225:ASP:N	2.66	0.58
1:a:253:GLY:HA3	2:b:490:VAL:HG22	1.86	0.58
34:D:402:LMG:H132	34:D:407:LMG:H312	1.85	0.58
1:a:92:HIS:NE2	3:c:374:ASP:OD2	2.34	0.57
17:g:224:THR:HG22	17:g:225:ASP:H	1.69	0.57
3:C:291:VAL:HB	3:C:455:HIS:CG	2.39	0.57
25:B:605:CLA:HBC3	25:B:612:CLA:H42	1.86	0.57
3:C:148:LEU:HD11	25:C:526:CLA:H92	1.85	0.57
29:d:405:PL9:H111	31:d:406:LHG:H102	1.86	0.57
1:A:253:GLY:HA3	2:B:490:VAL:HG22	1.87	0.57
1:a:145:VAL:O	1:a:148:THR:OG1	2.22	0.57
17:G:105:LEU:O	17:G:109:SER:HB2	2.03	0.57
23:1:52:ASP:OD1	23:1:59:ARG:NH1	2.38	0.57
18:O:150:THR:OG1	18:O:155:ARG:NH1	2.33	0.57
2:B:30:VAL:HG12	25:B:605:CLA:HHD	1.86	0.57
2:B:311:PHE:O	2:B:317:ASN:ND2	2.38	0.57
2:B:155:ALA:O	2:B:159:THR:OG1	2.21	0.57
21:R:205:ILE:HG23	21:R:206:THR:HG23	1.85	0.57
1:A:131:TRP:CH2	25:C:520:CLA:HAA2	2.40	0.57
3:C:227:VAL:O	3:C:237:TRP:NE1	2.36	0.57
19:3:172:ALA:HA	19:3:175:ARG:HH11	1.70	0.57
1:a:227:THR:HG21	1:a:233:ALA:HA	1.86	0.56
25:C:521:CLA:HBB2	25:C:522:CLA:H52	1.87	0.56
3:c:291:VAL:HB	3:c:455:HIS:CG	2.40	0.56
25:b:614:CLA:H2	27:b:617:WVN:C23	2.35	0.56
19:P:172:ALA:HA	19:P:175:ARG:HH11	1.70	0.56
1:a:136:ARG:NH2	8:i:27:ASP:OD1	2.38	0.56
1:a:140:ARG:HB2	4:d:219:ASN:HA	1.87	0.56
25:c:521:CLA:HBB2	25:c:522:CLA:H52	1.87	0.56
20:4:99:MET:HE1	20:4:200:LEU:HG	1.88	0.56
4:d:188:HIS:HA	4:d:293:ARG:HD2	1.87	0.56
25:5:606:CLA:HBB1	25:6:613:CLA:H61	1.88	0.56
22:6:166:LEU:HD22	25:6:609:CLA:HMA1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:605:CLA:HBC3	25:b:612:CLA:H42	1.86	0.56
1:A:244:GLU:OE2	4:D:263:LYS:NZ	2.36	0.56
22:6:101:ARG:HH21	22:6:203:VAL:HG11	1.71	0.56
22:S:106:LYS:NZ	22:S:158:GLU:OE1	2.34	0.56
23:N:52:ASP:OD1	23:N:59:ARG:NH1	2.38	0.56
34:d:402:LMG:H132	34:d:407:LMG:H312	1.86	0.56
1:a:131:TRP:CH2	25:c:520:CLA:HAA2	2.41	0.56
4:D:235:THR:HG23	4:D:238:GLN:HG3	1.88	0.56
1:a:26:ASN:O	4:d:254:GLN:NE2	2.39	0.55
3:C:311:TYR:O	3:C:437:ARG:NH2	2.36	0.55
25:1:603:CLA:OBD	25:1:609:CLA:HAA1	2.07	0.55
2:b:330:MET:HA	2:b:444:ARG:HB2	1.88	0.55
2:b:458:PHE:HB3	25:b:604:CLA:HBC2	1.88	0.55
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.38	0.55
1:a:244:GLU:OE2	4:d:263:LYS:NZ	2.37	0.55
22:S:101:ARG:HH21	22:S:203:VAL:HG11	1.71	0.55
22:S:193:ASP:N	22:S:193:ASP:OD1	2.40	0.55
2:b:256:MET:HA	2:b:263:THR:HG21	1.89	0.55
17:g:96:VAL:HG21	21:5:135:LEU:HD11	1.87	0.55
2:B:256:MET:HA	2:B:263:THR:HG21	1.89	0.55
2:B:71:VAL:HG23	25:B:606:CLA:HMA2	1.89	0.55
21:5:134:ILE:HA	25:5:606:CLA:HBC3	1.89	0.55
2:b:71:VAL:HG23	25:b:606:CLA:HMA2	1.88	0.55
15:y:27:ILE:HD11	16:z:25:VAL:HA	1.88	0.55
9:K:27:ILE:HD11	15:Y:16:ILE:HD13	1.88	0.55
2:b:7:ARG:O	2:b:10:THR:OG1	2.18	0.55
1:A:26:ASN:O	4:D:254:GLN:NE2	2.39	0.55
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.89	0.55
31:R:621:LHG:H282	31:R:621:LHG:H182	1.89	0.55
4:D:188:HIS:HA	4:D:293:ARG:HD2	1.88	0.54
20:Q:99:MET:HE1	20:Q:200:LEU:HG	1.88	0.54
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.89	0.54
1:A:170:ASP:OD2	3:C:371:ARG:NH1	2.35	0.54
2:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.89	0.54
21:R:134:ILE:HA	25:R:606:CLA:HBC3	1.89	0.54
21:R:57:PRO:CG	21:R:60:LEU:HD22	2.37	0.54
17:g:250:LEU:O	17:g:254:SER:OG	2.22	0.54
2:B:461:LEU:HD13	25:B:613:CLA:H111	1.90	0.54
11:m:35:ALA:HB1	11:M:36:GLU:HG3	1.90	0.54
2:b:265:ILE:CD1	7:h:62:TRP:CH2	2.90	0.54
25:R:606:CLA:HBB1	25:S:613:CLA:H61	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:153:PHE:HB2	25:b:606:CLA:HBB1	1.90	0.54
2:B:330:MET:HA	2:B:444:ARG:HB2	1.88	0.54
31:5:621:LHG:H282	31:5:621:LHG:H182	1.89	0.54
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.40	0.53
20:Q:132:MET:CE	25:Q:604:CLA:H3A	2.38	0.53
2:b:362:PHE:HZ	4:d:183:PHE:CE2	2.24	0.53
34:g:303:LMG:HC62	21:5:55:LYS:HZ3	1.73	0.53
3:C:51:SER:OG	25:C:523:CLA:O1D	2.25	0.53
3:C:201:ASP:O	3:C:208:GLY:HA2	2.09	0.53
20:4:132:MET:CE	25:4:604:CLA:H3A	2.38	0.53
25:1:603:CLA:H2	25:1:603:CLA:HED3	1.90	0.53
2:b:223:GLN:NE2	2:b:227:ARG:NH2	2.56	0.53
20:4:132:MET:HE1	25:4:604:CLA:H3A	1.90	0.53
4:d:56:SER:OG	4:d:64:SER:OG	2.26	0.53
9:k:27:ILE:HD11	15:y:16:ILE:HD13	1.90	0.53
23:N:78:PHE:HD1	23:N:81:TRP:HE1	1.57	0.53
4:D:250:ARG:NE	4:D:254:GLN:OE1	2.35	0.53
21:R:57:PRO:HG2	21:R:60:LEU:CB	2.39	0.53
2:b:368:VAL:HG21	2:b:422:ARG:HG2	1.91	0.53
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.91	0.53
4:D:23:ARG:NH1	14:X:36:LEU:O	2.40	0.53
25:G:301:CLA:HBC3	25:G:301:CLA:H71	1.89	0.53
2:b:320:ALA:HB1	4:d:291:ASN:HD22	1.74	0.53
11:m:8:TYR:HB2	11:M:5:VAL:HG21	1.90	0.53
2:B:368:VAL:HG21	2:B:422:ARG:HG2	1.90	0.53
21:R:86:GLU:HG2	21:R:149:LEU:HD13	1.91	0.53
2:B:265:ILE:CD1	7:H:62:TRP:CH2	2.92	0.52
2:B:320:ALA:HB1	4:D:291:ASN:HD22	1.74	0.52
2:B:471:SER:HB2	4:D:139:PRO:HG2	1.91	0.52
21:R:57:PRO:HG2	21:R:60:LEU:HD23	1.90	0.52
1:a:293:MET:HG2	1:a:298:ASN:HA	1.92	0.52
3:c:177:ILE:HD13	25:c:527:CLA:HAB	1.91	0.52
3:c:201:ASP:O	3:c:208:GLY:HA2	2.08	0.52
17:g:125:VAL:HG11	20:4:155:GLN:HG3	1.90	0.52
19:P:186:ARG:HA	19:P:189:MET:HE3	1.91	0.52
20:Q:132:MET:HE1	25:Q:604:CLA:H3A	1.89	0.52
21:R:125:LEU:HD22	25:R:604:CLA:HAA2	1.91	0.52
1:A:317:TRP:CZ3	4:D:179:ARG:HD2	2.44	0.52
25:a:406:CLA:H13	34:w:134:LMG:H142	1.92	0.52
4:D:179:ARG:NE	4:D:332:ASP:OD1	2.41	0.52
2:b:241:SER:O	2:b:245:VAL:CG2	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:33:VAL:HG13	13:W:38:LEU:HB2	1.90	0.52
7:h:61:ASP:OD1	35:h:90:DGD:O4E	2.27	0.52
2:b:471:SER:HB2	4:d:139:PRO:HG2	1.90	0.52
34:c:536:LMG:H321	34:c:536:LMG:H142	1.90	0.52
23:1:46:LEU:H	23:1:51:VAL:HG21	1.75	0.52
25:S:603:CLA:HBB1	25:S:615:CLA:H122	1.92	0.52
9:K:45:ARG:NH2	15:Y:34:LEU:O	2.43	0.52
21:R:57:PRO:HG3	21:R:60:LEU:CD2	2.40	0.52
2:b:311:PHE:O	2:b:317:ASN:ND2	2.43	0.52
25:A:403:CLA:HMC3	25:D:403:CLA:HBC3	1.91	0.52
22:6:150:VAL:HG23	37:6:606:KC2:CMD	2.39	0.52
22:6:222:LEU:HD21	22:6:237:ILE:HD13	1.91	0.52
21:R:57:PRO:HG3	21:R:60:LEU:HD23	1.91	0.52
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.91	0.52
3:c:470:GLU:OE2	3:c:471:LYS:NZ	2.36	0.51
2:B:253:THR:HG23	2:B:452:THR:HG23	1.92	0.51
18:2:124:VAL:HG22	25:2:607:CLA:C2D	2.41	0.51
25:O:602:CLA:H201	23:N:143:LEU:HD11	1.92	0.51
3:C:177:ILE:HD13	25:C:527:CLA:HAB	1.92	0.51
1:a:11:ALA:HB1	13:w:59:THR:HG21	1.92	0.51
20:4:75:ILE:HG13	20:4:76:ILE:HG13	1.92	0.51
23:1:64:ASP:N	23:1:64:ASP:OD1	2.43	0.51
3:C:470:GLU:OE2	3:C:471:LYS:NZ	2.35	0.51
20:Q:75:ILE:HG13	20:Q:76:ILE:HG13	1.93	0.51
22:S:81:ALA:O	22:S:101:ARG:NH2	2.34	0.51
2:b:498:LEU:HG	4:d:134:LEU:HB3	1.92	0.51
2:B:221:PRO:HA	25:B:609:CLA:HED2	1.93	0.51
20:4:129:GLN:OE1	20:4:131:SER:N	2.42	0.51
18:O:124:VAL:HG22	25:O:607:CLA:C2D	2.40	0.51
20:Q:129:GLN:OE1	20:Q:131:SER:N	2.42	0.51
17:g:83:PRO:HB2	17:g:88:SER:HA	1.93	0.51
10:L:24:LEU:HD13	31:L:101:LHG:H151	1.93	0.51
18:2:150:THR:OG1	18:2:155:ARG:NH1	2.33	0.51
19:P:80:GLU:OE1	19:P:155:ARG:NH2	2.44	0.51
23:N:46:LEU:H	23:N:51:VAL:HG21	1.75	0.51
2:B:153:PHE:HB2	25:B:606:CLA:HBB1	1.93	0.51
4:D:143:ILE:O	4:D:146:SER:OG	2.26	0.51
34:D:402:LMG:HC3	34:D:407:LMG:HC3	1.92	0.51
21:5:86:GLU:HG2	21:5:149:LEU:HD13	1.92	0.51
18:O:59:ASP:N	18:O:59:ASP:OD1	2.44	0.51
25:a:403:CLA:HMC3	25:d:403:CLA:HBC3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:525:CLA:H52	25:c:525:CLA:HED2	1.92	0.51
25:g:301:CLA:H121	21:5:143:ILE:HD12	1.93	0.51
31:D:406:LHG:O1	31:L:101:LHG:O4	2.25	0.51
19:3:186:ARG:HA	19:3:189:MET:HE3	1.91	0.51
14:X:13:LEU:HD21	25:N:607:CLA:HAA2	1.91	0.50
2:b:103:LEU:HD22	25:b:606:CLA:H51	1.94	0.50
2:b:253:THR:HG23	2:b:452:THR:HG23	1.93	0.50
4:d:128:GLN:HB2	4:d:142:ALA:HB2	1.91	0.50
1:A:131:TRP:HZ2	3:C:463:ARG:HG3	1.76	0.50
25:C:525:CLA:H52	25:C:525:CLA:HED2	1.92	0.50
4:D:128:GLN:HB2	4:D:142:ALA:HB2	1.92	0.50
34:d:402:LMG:HC3	34:d:407:LMG:HC3	1.93	0.50
31:d:406:LHG:O1	31:l:101:LHG:O4	2.25	0.50
2:B:216:HIS:HE1	25:B:609:CLA:NC	2.09	0.50
22:6:166:LEU:HD13	25:6:609:CLA:HBB	1.93	0.50
2:b:216:HIS:HE1	25:b:609:CLA:NC	2.10	0.50
15:y:4:LEU:HD13	15:y:4:LEU:O	2.12	0.50
25:c:528:CLA:HBC1	34:z:102:LMG:H131	1.94	0.50
21:5:183:LEU:O	21:5:186:ILE:HG13	2.11	0.50
25:c:521:CLA:HMC2	25:c:522:CLA:H101	1.93	0.50
1:a:131:TRP:HZ2	3:c:463:ARG:HG3	1.77	0.50
13:w:33:VAL:HG13	13:w:38:LEU:HB2	1.94	0.50
1:A:250:ALA:HA	2:B:490:VAL:HG21	1.94	0.50
21:R:183:LEU:O	21:R:186:ILE:HG13	2.11	0.50
22:S:77:ASP:OD1	22:S:77:ASP:N	2.43	0.50
22:S:222:LEU:HD21	22:S:237:ILE:HD11	1.91	0.50
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.39	0.50
2:b:221:PRO:HA	25:b:609:CLA:HED2	1.93	0.50
2:B:498:LEU:HG	4:D:134:LEU:HB3	1.92	0.50
25:C:528:CLA:HBC1	34:Z:102:LMG:H131	1.94	0.50
1:a:250:ALA:HA	2:b:490:VAL:HG21	1.94	0.50
34:G:303:LMG:HC62	21:R:55:LYS:HZ3	1.76	0.50
25:b:612:CLA:H13	25:b:613:CLA:HBB2	1.94	0.49
25:B:612:CLA:H13	25:B:613:CLA:HBB2	1.94	0.49
7:H:61:ASP:OD1	35:H:90:DGD:O4E	2.27	0.49
11:M:21:PHE:HD1	34:M:101:LMG:H141	1.76	0.49
20:Q:201:HIS:HA	20:Q:204:PHE:CD2	2.47	0.49
22:S:191:ASN:OD1	22:S:191:ASN:N	2.45	0.49
21:5:99:THR:HG23	21:5:199:PHE:HE2	1.77	0.49
23:1:80:ASN:OD1	23:1:81:TRP:N	2.45	0.49
23:N:64:ASP:N	23:N:64:ASP:OD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:85:SER:HA	1:a:109:GLY:HA3	1.93	0.49
2:b:362:PHE:CD2	4:d:187:PHE:CD2	3.00	0.49
4:d:200:VAL:HG22	25:d:403:CLA:C1B	2.42	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	1.93	0.49
3:c:227:VAL:O	3:c:237:TRP:NE1	2.38	0.49
4:D:334:PRO:HB2	5:E:66:LEU:HD11	1.94	0.49
25:2:602:CLA:H201	23:1:143:LEU:HD11	1.93	0.49
17:G:167:LEU:HD21	25:O:609:CLA:H2	1.95	0.49
3:c:105:HIS:NE2	25:c:517:CLA:O1D	2.46	0.49
4:d:334:PRO:HB2	5:e:66:LEU:HD11	1.94	0.49
2:B:356:VAL:HG22	2:B:370:LEU:HG	1.94	0.49
23:1:78:PHE:HD1	23:1:81:TRP:HE1	1.60	0.49
31:O:621:LHG:H341	23:N:148:LEU:HD11	1.93	0.49
25:P:611:CLA:H12	25:Q:603:CLA:H12	1.95	0.49
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.94	0.49
1:a:286:THR:OG1	25:a:403:CLA:O1D	2.27	0.49
1:A:279:PRO:HG2	4:D:211:ALA:HB2	1.95	0.49
4:D:200:VAL:HG22	25:D:403:CLA:C1B	2.43	0.49
25:3:611:CLA:H41	25:3:611:CLA:H62	1.55	0.49
25:3:611:CLA:H12	25:4:603:CLA:H12	1.95	0.49
22:6:193:ASP:N	22:6:193:ASP:OD1	2.40	0.49
22:S:84:VAL:O	22:S:84:VAL:CG1	2.59	0.49
4:d:56:SER:HG	4:d:64:SER:HG	1.61	0.49
31:2:621:LHG:H341	23:1:148:LEU:HD11	1.94	0.49
21:R:99:THR:HG23	21:R:199:PHE:HE2	1.77	0.49
23:N:80:ASN:OD1	23:N:81:TRP:N	2.46	0.49
1:a:127:ILE:HG23	1:a:144:SER:HB2	1.94	0.49
2:b:74:SER:HA	2:b:92:SER:HB3	1.95	0.49
2:B:321:LYS:HD3	2:B:361:ALA:HA	1.95	0.49
25:C:521:CLA:HMC2	25:C:522:CLA:H101	1.93	0.49
21:R:57:PRO:HG2	21:R:60:LEU:HD22	1.92	0.49
1:a:279:PRO:HG2	4:d:211:ALA:HB2	1.95	0.49
25:B:614:CLA:H2	27:B:617:WVN:C19	2.43	0.49
3:C:40:ARG:HH21	9:K:45:ARG:HH22	1.60	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.48
4:d:23:ARG:NH1	14:x:36:LEU:O	2.40	0.48
1:A:179:THR:O	1:A:183:MET:HG3	2.13	0.48
25:B:613:CLA:H52	31:B:622:LHG:H352	1.94	0.48
3:C:105:HIS:NE2	25:C:517:CLA:O1D	2.46	0.48
19:3:80:GLU:OE1	19:3:155:ARG:NH2	2.44	0.48
4:d:250:ARG:NE	4:d:254:GLN:OE1	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:z:38:GLY:HA2	16:z:41:TYR:HD2	1.78	0.48
21:R:183:LEU:HD23	25:R:611:CLA:HED2	1.95	0.48
4:D:56:SER:OG	4:D:64:SER:OG	2.26	0.48
20:4:201:HIS:HA	20:4:204:PHE:CD2	2.48	0.48
22:6:84:VAL:O	22:6:84:VAL:CG1	2.61	0.48
25:6:611:CLA:H61	25:6:611:CLA:H41	1.55	0.48
3:c:51:SER:OG	25:c:523:CLA:O1D	2.25	0.48
11:m:24:THR:HA	11:M:24:THR:HG23	1.96	0.48
2:B:74:SER:HA	2:B:92:SER:HB3	1.95	0.48
4:D:86:HIS:HB2	35:H:90:DGD:HG11	1.96	0.48
2:b:356:VAL:HG22	2:b:370:LEU:HG	1.94	0.48
3:c:239:VAL:HG13	3:c:303:TYR:HA	1.96	0.48
3:C:483:LEU:O	17:G:239:TRP:NE1	2.43	0.48
11:M:36:GLU:CD	17:G:254:SER:OG	2.57	0.48
22:6:135:PRO:O	38:6:617:II0:O01	2.31	0.48
17:G:141:ALA:HB3	19:P:58:MET:HG2	1.95	0.48
25:P:611:CLA:H43	25:Q:603:CLA:HED3	1.96	0.48
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.94	0.48
3:C:62:LYS:NZ	3:C:152:ASP:OD1	2.46	0.48
19:P:41:ARG:HA	19:P:49:SER:HA	1.96	0.48
1:a:179:THR:O	1:a:183:MET:HG3	2.13	0.48
15:y:24:ILE:HG23	15:y:34:LEU:HD11	1.96	0.48
1:A:127:ILE:HG23	1:A:144:SER:HB2	1.95	0.48
25:3:610:CLA:HBA2	25:3:610:CLA:H3A	1.44	0.48
20:4:147:PHE:HB2	25:4:609:CLA:HMA1	1.96	0.48
25:S:609:CLA:H2	25:S:609:CLA:H61	1.68	0.48
4:d:209:LEU:HB3	4:d:270:MET:HG2	1.96	0.48
25:3:609:CLA:H92	25:3:609:CLA:H61	1.75	0.48
22:S:135:PRO:O	38:S:617:II0:O01	2.31	0.48
1:a:63:ILE:HG13	1:a:65:GLU:HG2	1.96	0.48
25:3:611:CLA:H43	25:4:603:CLA:HED3	1.95	0.48
11:m:24:THR:HG23	11:M:24:THR:HA	1.96	0.47
2:B:241:SER:O	2:B:245:VAL:CG2	2.52	0.47
10:l:21:GLY:HA2	31:l:101:LHG:H262	1.96	0.47
2:B:362:PHE:CE1	4:D:183:PHE:HZ	2.32	0.47
10:L:21:GLY:HA2	31:L:101:LHG:H262	1.97	0.47
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.47
29:D:405:PL9:H221	31:L:101:LHG:H192	1.97	0.47
4:d:187:PHE:O	4:d:293:ARG:NH1	2.47	0.47
19:3:41:ARG:HA	19:3:49:SER:HA	1.96	0.47
21:5:183:LEU:HD23	25:5:611:CLA:HED2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:VAL:HG13	3:C:303:TYR:HA	1.95	0.47
3:C:302:GLN:HG3	35:C:532:DGD:HB42	1.96	0.47
22:6:146:GLY:HA2	37:6:606:KC2:C3D	2.45	0.47
23:1:160:THR:OG1	23:1:166:ARG:NH1	2.45	0.47
25:R:606:CLA:H172	31:S:621:LHG:H282	1.96	0.47
17:g:157:VAL:O	17:g:160:PHE:HB2	2.15	0.47
25:g:301:CLA:H142	25:g:301:CLA:H112	1.76	0.47
2:B:188:GLU:HA	7:H:58:VAL:HG22	1.96	0.47
4:D:187:PHE:O	4:D:293:ARG:NH1	2.48	0.47
4:D:209:LEU:HB3	4:D:270:MET:HG2	1.96	0.47
17:G:157:VAL:O	17:G:160:PHE:HB2	2.15	0.47
18:O:49:VAL:HG13	18:O:52:LEU:HB2	1.96	0.47
4:d:84:MET:HE3	4:d:106:ILE:HB	1.96	0.47
4:d:86:HIS:HB2	35:h:90:DGD:HG11	1.96	0.47
2:B:103:LEU:HD22	25:B:606:CLA:H51	1.97	0.47
25:B:607:CLA:HBA2	34:B:620:LMG:H121	1.96	0.47
18:2:206:VAL:HG13	18:2:207:LEU:N	2.29	0.47
25:2:610:CLA:H3A	25:2:610:CLA:HBA2	1.53	0.47
25:3:611:CLA:H11	25:4:603:CLA:HED3	1.96	0.47
21:5:205:ILE:HB	25:5:615:CLA:HED3	1.96	0.47
22:6:135:PRO:HA	22:6:138:ASP:HB2	1.97	0.47
18:O:150:THR:HG1	18:O:155:ARG:HH11	1.61	0.47
25:P:610:CLA:H3A	25:P:610:CLA:HBA2	1.44	0.47
25:b:607:CLA:H141	25:b:607:CLA:H162	1.74	0.47
3:c:75:VAL:HG13	3:c:132:HIS:CD2	2.49	0.47
25:c:518:CLA:H193	25:c:518:CLA:H161	1.77	0.47
4:d:147:GLY:O	4:d:151:ILE:HG12	2.15	0.47
1:A:63:ILE:HG13	1:A:65:GLU:HG2	1.96	0.47
1:A:156:ALA:HA	1:A:160:VAL:HB	1.96	0.47
3:C:265:HIS:HE1	25:C:521:CLA:NA	2.13	0.47
2:b:331:ASN:HB3	2:b:336:ILE:HG12	1.97	0.47
2:b:482:ILE:HD12	2:b:486:VAL:HG21	1.97	0.47
2:B:201:HIS:HE2	25:B:603:CLA:C2B	2.28	0.47
25:C:527:CLA:H3A	25:C:527:CLA:HBA2	1.66	0.47
25:5:606:CLA:H172	31:6:621:LHG:H282	1.96	0.47
22:6:77:ASP:OD1	22:6:77:ASP:N	2.43	0.47
2:b:188:GLU:HA	7:h:58:VAL:HG22	1.96	0.47
25:B:605:CLA:H92	25:B:605:CLA:H61	1.76	0.47
25:C:520:CLA:H13	25:C:520:CLA:H101	1.74	0.47
25:3:615:CLA:H3A	25:3:615:CLA:HBA2	1.72	0.47
18:O:76:VAL:O	18:O:76:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:603:CLA:H41	25:b:603:CLA:H61	1.72	0.46
1:A:265:PHE:HB3	1:A:271:LEU:HB2	1.97	0.46
3:C:380:ILE:HG23	3:C:384:ARG:HH12	1.80	0.46
4:D:147:GLY:O	4:D:151:ILE:HG12	2.15	0.46
18:2:97:VAL:HG13	18:2:195:PHE:HE2	1.81	0.46
22:6:146:GLY:CA	37:6:606:KC2:CAD	2.93	0.46
2:b:413:ASP:OD1	2:b:413:ASP:N	2.46	0.46
10:l:13:LEU:HB2	11:m:25:LEU:HG	1.96	0.46
17:g:169:ALA:HA	18:2:151:LEU:HD21	1.96	0.46
2:B:482:ILE:HD12	2:B:486:VAL:HG21	1.97	0.46
4:D:84:MET:HE3	4:D:106:ILE:HB	1.96	0.46
4:D:122:ILE:HD11	35:H:90:DGD:HAH2	1.98	0.46
21:R:205:ILE:HB	25:R:615:CLA:HED3	1.96	0.46
22:S:135:PRO:HA	22:S:138:ASP:HB2	1.97	0.46
3:c:149:ILE:HG21	16:z:27:LEU:HB3	1.98	0.46
3:c:302:GLN:HG3	35:c:532:DGD:HB42	1.96	0.46
2:B:331:ASN:HB3	2:B:336:ILE:HG12	1.97	0.46
1:a:156:ALA:HA	1:a:160:VAL:HB	1.97	0.46
1:a:160:VAL:HG11	1:a:291:MET:HG2	1.98	0.46
25:6:604:CLA:H151	25:6:610:CLA:HBC1	1.98	0.46
2:b:201:HIS:HE2	25:b:603:CLA:C2B	2.28	0.46
11:M:32:ARG:HE	17:G:250:LEU:HD21	1.80	0.46
20:4:193:MET:SD	25:4:602:CLA:HAB	2.56	0.46
18:O:73:PHE:HA	18:O:76:VAL:HG12	1.97	0.46
21:R:179:GLU:OE1	21:R:179:GLU:N	2.41	0.46
1:a:283:ILE:HA	1:a:286:THR:HG22	1.96	0.46
3:c:380:ILE:HG23	3:c:384:ARG:HH12	1.80	0.46
1:A:283:ILE:HA	1:A:286:THR:HG22	1.97	0.46
2:B:124:ARG:HA	2:B:131:PRO:HA	1.98	0.46
25:B:604:CLA:C1C	25:B:613:CLA:HBB1	2.46	0.46
22:6:81:ALA:O	22:6:101:ARG:NH2	2.34	0.46
25:b:604:CLA:C1C	25:b:613:CLA:HBB1	2.46	0.46
25:b:613:CLA:H62	25:b:613:CLA:H2	1.59	0.46
3:c:62:LYS:NZ	3:c:152:ASP:OD1	2.46	0.46
4:d:122:ILE:HD11	35:h:90:DGD:HAH2	1.98	0.46
25:g:301:CLA:H2	25:g:301:CLA:H62	1.74	0.46
1:A:229:GLU:HB3	17:G:214:ILE:HG13	1.97	0.46
15:Y:24:ILE:HG23	15:Y:34:LEU:HD11	1.97	0.46
19:3:42:SER:OG	19:3:63:GLY:O	2.33	0.46
25:4:609:CLA:H3A	25:4:609:CLA:HBA2	1.56	0.46
25:P:609:CLA:H92	25:P:609:CLA:H61	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:71:ALA:O	3:c:75:VAL:HG23	2.16	0.46
25:d:403:CLA:HBA1	25:d:403:CLA:H3A	1.62	0.46
3:C:75:VAL:HG13	3:C:132:HIS:CD2	2.50	0.46
25:6:604:CLA:H152	25:6:604:CLA:H112	1.70	0.46
25:6:609:CLA:H2	25:6:609:CLA:H61	1.61	0.46
25:O:610:CLA:HBA2	25:O:610:CLA:H3A	1.53	0.46
20:Q:142:LEU:HD11	31:R:621:LHG:H212	1.98	0.46
23:N:110:VAL:HG23	23:N:218:ILE:HG13	1.98	0.46
25:N:609:CLA:HBA2	25:N:609:CLA:H3A	1.42	0.46
1:A:160:VAL:HG11	1:A:291:MET:HG2	1.98	0.46
2:B:413:ASP:OD1	2:B:413:ASP:N	2.46	0.46
3:C:71:ALA:O	3:C:75:VAL:HG23	2.16	0.46
25:D:404:CLA:H91	7:H:36:LEU:HD11	1.98	0.46
22:6:105:LEU:HD12	22:6:179:GLY:HA3	1.98	0.46
25:a:404:CLA:HMD3	4:d:181:LEU:HD11	1.98	0.45
25:b:613:CLA:H61	25:b:613:CLA:H102	1.64	0.45
3:c:320:GLY:HA3	3:c:415:LEU:HG	1.98	0.45
4:d:50:GLY:HA2	4:d:54:VAL:HB	1.98	0.45
4:d:179:ARG:HD3	4:d:332:ASP:OD1	2.16	0.45
22:6:191:ASN:OD1	22:6:191:ASN:N	2.45	0.45
25:6:602:CLA:H41	25:6:603:CLA:HMA3	1.98	0.45
21:R:196:PHE:O	21:R:199:PHE:HB2	2.16	0.45
23:N:160:THR:OG1	23:N:166:ARG:NH1	2.45	0.45
1:a:304:GLN:HG2	1:a:313:VAL:HG11	1.98	0.45
3:c:40:ARG:HH21	9:k:45:ARG:HH22	1.64	0.45
15:Y:27:ILE:HD11	16:Z:25:VAL:HA	1.97	0.45
25:4:603:CLA:H92	25:4:603:CLA:H62	1.78	0.45
34:G:303:LMG:O3	21:R:72:PRO:O	2.30	0.45
23:1:110:VAL:HG23	23:1:218:ILE:HG13	1.98	0.45
25:P:611:CLA:H11	25:Q:603:CLA:HED3	1.97	0.45
2:b:124:ARG:HA	2:b:131:PRO:HA	1.98	0.45
4:d:187:PHE:HA	4:d:325:ARG:HD3	1.97	0.45
9:k:13:ALA:HB1	16:z:5:LEU:HD12	1.97	0.45
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.97	0.45
20:4:142:LEU:HD11	31:5:621:LHG:H212	1.98	0.45
3:c:265:HIS:HE1	25:c:521:CLA:NA	2.13	0.45
25:A:404:CLA:HMD3	4:D:181:LEU:HD11	1.98	0.45
21:5:196:PHE:O	21:5:199:PHE:HB2	2.16	0.45
20:Q:193:MET:SD	25:Q:602:CLA:HAB	2.56	0.45
25:b:607:CLA:HBA2	34:b:620:LMG:H121	1.99	0.45
3:c:75:VAL:HG13	3:c:132:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:405:PL9:H221	31:l:101:LHG:H192	1.99	0.45
25:A:403:CLA:H151	25:D:400:CLA:H151	1.99	0.45
2:B:496:GLN:HB3	2:B:503:THR:HB	1.98	0.45
3:C:54:SER:OG	25:C:523:CLA:H2A	2.17	0.45
4:D:268:PHE:HE2	31:L:101:LHG:HC82	1.81	0.45
21:5:179:GLU:OE1	21:5:179:GLU:N	2.41	0.45
25:S:611:CLA:H3A	25:S:611:CLA:HBA2	1.65	0.45
2:b:496:GLN:HB3	2:b:503:THR:HB	1.98	0.45
25:b:615:CLA:H152	25:b:615:CLA:H112	1.77	0.45
31:c:535:LHG:H122	31:c:535:LHG:H151	1.79	0.45
5:E:38:PHE:HE1	5:E:47:ILE:HD12	1.82	0.45
18:2:44:ASP:N	18:2:44:ASP:OD1	2.48	0.45
11:m:5:VAL:HG13	11:M:5:VAL:HG23	1.99	0.45
25:A:406:CLA:HBA1	34:W:134:LMG:H132	1.99	0.45
25:B:613:CLA:H61	25:B:613:CLA:H102	1.76	0.45
18:2:59:ASP:OD1	18:2:59:ASP:N	2.44	0.45
25:5:601:CLA:O1A	31:5:621:LHG:O2	2.34	0.45
31:P:621:LHG:O3	31:P:621:LHG:O1	2.26	0.45
25:S:604:CLA:H151	25:S:610:CLA:HBC1	1.98	0.45
9:k:28:PRO:O	9:k:31:PHE:HB2	2.16	0.45
25:C:518:CLA:H193	25:C:518:CLA:H161	1.77	0.45
31:5:621:LHG:H181	31:5:621:LHG:H211	1.79	0.45
22:S:139:PHE:HB2	38:S:617:II0:C05	2.46	0.45
2:b:321:LYS:HD3	2:b:361:ALA:HA	1.99	0.45
25:b:606:CLA:H162	25:b:606:CLA:H122	1.84	0.45
20:4:201:HIS:CD2	25:4:615:CLA:NA	2.85	0.45
22:6:146:GLY:HA3	37:6:606:KC2:CAD	2.45	0.45
23:1:209:HIS:HE1	37:1:613:KC2:NB	2.14	0.45
18:O:97:VAL:HG13	18:O:195:PHE:HE2	1.81	0.45
25:N:604:CLA:H93	25:N:604:CLA:H111	1.80	0.45
25:d:404:CLA:H91	7:h:36:LEU:HD11	1.98	0.45
10:l:24:LEU:HD13	31:l:101:LHG:H151	1.98	0.45
25:B:610:CLA:H193	25:B:612:CLA:HMD2	1.99	0.45
16:Z:16:SER:OG	16:Z:47:TRP:NE1	2.40	0.45
25:2:603:CLA:H3A	25:2:603:CLA:HBA1	1.67	0.45
25:5:606:CLA:H192	31:6:621:LHG:H261	1.99	0.45
34:G:303:LMG:H361	34:G:303:LMG:H121	1.98	0.45
20:Q:189:GLY:O	20:Q:193:MET:HG3	2.17	0.45
25:R:606:CLA:H192	31:S:621:LHG:H261	1.99	0.45
1:a:265:PHE:HB3	1:a:271:LEU:HB2	1.99	0.44
3:c:124:PRO:HB3	34:c:536:LMG:HC71	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:143:ILE:O	4:d:146:SER:OG	2.26	0.44
3:C:202:THR:HB	3:C:378:PRO:HG2	1.99	0.44
3:C:363:ILE:HD12	3:C:387:ASN:ND2	2.32	0.44
16:Z:8:LEU:HD21	16:Z:53:MET:HB3	1.98	0.44
22:6:139:PHE:HB2	38:6:617:II0:C05	2.46	0.44
25:1:609:CLA:H3A	25:1:609:CLA:HBA2	1.64	0.44
20:Q:137:VAL:HG12	34:Q:621:LMG:H142	1.99	0.44
25:S:609:CLA:H3A	25:S:609:CLA:HBA2	1.44	0.44
3:c:192:LYS:HD3	25:c:517:CLA:H192	1.98	0.44
13:w:63:GLU:O	13:w:72:ARG:NH2	2.45	0.44
17:g:248:ARG:NH1	17:g:252:GLU:OE2	2.51	0.44
1:A:22:THR:HB	1:A:136:ARG:HE	1.82	0.44
3:C:192:LYS:HD3	25:C:517:CLA:H192	1.99	0.44
4:D:50:GLY:HA2	4:D:54:VAL:HB	1.98	0.44
4:D:53:PHE:O	5:E:50:THR:OG1	2.30	0.44
18:O:44:ASP:N	18:O:44:ASP:OD1	2.48	0.44
25:S:615:CLA:H101	25:S:615:CLA:H13	1.83	0.44
1:a:22:THR:HB	1:a:136:ARG:HE	1.82	0.44
25:B:608:CLA:HMB3	4:D:125:CYS:HB3	2.00	0.44
3:C:342:VAL:O	3:C:342:VAL:HG23	2.16	0.44
9:K:13:ALA:HB1	16:Z:5:LEU:HD12	2.00	0.44
19:3:87:ARG:HA	19:3:90:MET:HE3	1.99	0.44
17:G:248:ARG:NH1	17:G:252:GLU:OE2	2.51	0.44
25:R:601:CLA:O1A	31:R:621:LHG:O2	2.34	0.44
25:b:605:CLA:H92	25:b:605:CLA:H61	1.76	0.44
1:A:308:ASP:OD1	1:A:312:ARG:N	2.51	0.44
17:G:145:TYR:OH	17:G:148:PRO:O	2.33	0.44
22:S:105:LEU:HD12	22:S:179:GLY:HA3	1.98	0.44
25:a:403:CLA:H151	25:d:400:CLA:H151	1.98	0.44
25:b:610:CLA:H193	25:b:612:CLA:HMD2	1.99	0.44
25:c:520:CLA:H13	25:c:520:CLA:H101	1.78	0.44
4:d:78:SER:HA	4:d:171:SER:HB3	2.00	0.44
34:g:303:LMG:H121	34:g:303:LMG:H361	1.98	0.44
2:B:4:PRO:HB3	31:L:101:LHG:HC12	1.99	0.44
25:B:613:CLA:H111	25:B:613:CLA:H142	1.77	0.44
25:B:615:CLA:H152	25:B:615:CLA:H112	1.77	0.44
16:Z:38:GLY:HA2	16:Z:41:TYR:HD2	1.82	0.44
19:3:89:CYS:HA	19:3:192:LEU:HD13	1.99	0.44
20:4:137:VAL:HG12	34:4:621:LMG:H142	1.99	0.44
25:S:603:CLA:HMD2	25:S:609:CLA:H8	1.99	0.44
25:S:604:CLA:H2	25:S:604:CLA:H62	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:OD1	1:A:61:ASP:N	2.45	0.44
31:R:621:LHG:H211	31:R:621:LHG:H181	1.78	0.44
23:N:209:HIS:HE1	37:N:613:KC2:NB	2.14	0.44
16:z:8:LEU:HD21	16:z:53:MET:HB3	1.99	0.44
19:P:89:CYS:HA	19:P:192:LEU:HD13	1.99	0.44
3:c:54:SER:OG	25:c:523:CLA:H2A	2.17	0.44
3:c:342:VAL:O	3:c:342:VAL:HG23	2.18	0.44
34:f:99:LMG:H231	34:f:99:LMG:H202	1.87	0.44
25:D:403:CLA:HBA1	25:D:403:CLA:H3A	1.62	0.44
25:5:602:CLA:H41	25:5:602:CLA:H62	1.58	0.44
19:P:42:SER:OG	19:P:63:GLY:O	2.33	0.44
19:P:87:ARG:HA	19:P:90:MET:HE3	1.99	0.44
25:Q:606:CLA:H61	21:R:217:PHE:HE2	1.83	0.44
3:c:132:HIS:CE1	34:c:536:LMG:H191	2.53	0.44
4:d:268:PHE:HE2	31:l:101:LHG:HC82	1.82	0.44
25:C:517:CLA:H12	25:C:517:CLA:H51	1.83	0.44
4:D:78:SER:HA	4:D:171:SER:HB3	2.00	0.44
18:2:197:HIS:CD2	25:2:615:CLA:NA	2.86	0.44
25:a:403:CLA:NB	25:d:403:CLA:HBB1	2.33	0.43
1:A:250:ALA:HA	2:B:490:VAL:HG11	2.00	0.43
1:A:304:GLN:HG2	1:A:313:VAL:HG11	1.98	0.43
25:B:606:CLA:H122	25:B:606:CLA:H162	1.84	0.43
3:C:141:PHE:CG	34:Z:102:LMG:H292	2.53	0.43
26:D:401:PHO:H51	25:D:403:CLA:H111	2.00	0.43
22:6:218:HIS:HD2	25:6:615:CLA:NA	2.15	0.43
20:Q:201:HIS:CD2	25:Q:615:CLA:NA	2.85	0.43
25:N:607:CLA:HHC	25:N:607:CLA:HBB1	2.00	0.43
25:A:404:CLA:HBA2	25:A:404:CLA:H3A	1.71	0.43
3:C:149:ILE:HG21	16:Z:27:LEU:HB3	2.01	0.43
13:W:63:GLU:O	13:W:72:ARG:NH2	2.46	0.43
25:2:611:CLA:H41	25:2:611:CLA:H61	1.80	0.43
31:3:621:LHG:H142	31:3:621:LHG:H171	1.85	0.43
31:3:621:LHG:O3	31:3:621:LHG:O1	2.26	0.43
25:6:613:CLA:H61	25:6:613:CLA:H2	1.70	0.43
25:1:607:CLA:HHC	25:1:607:CLA:HBB1	2.00	0.43
20:Q:128:LYS:HE3	20:Q:128:LYS:HB2	1.85	0.43
1:a:308:ASP:OD1	1:a:312:ARG:N	2.51	0.43
25:b:613:CLA:H193	31:l:101:LHG:H383	2.00	0.43
25:C:525:CLA:H41	25:C:525:CLA:H61	1.76	0.43
20:4:189:GLY:O	20:4:193:MET:HG3	2.17	0.43
1:a:250:ALA:HA	2:b:490:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:615:CLA:H11	25:b:616:CLA:HBB2	2.00	0.43
3:c:202:THR:HB	3:c:378:PRO:HG2	2.00	0.43
1:A:293:MET:HG2	1:A:298:ASN:HA	2.00	0.43
25:B:613:CLA:HBA1	25:B:613:CLA:H3A	1.75	0.43
18:2:186:ARG:NH1	38:2:618:II0:O02	2.44	0.43
19:3:113:VAL:HG13	19:3:199:MET:HG2	2.00	0.43
25:1:603:CLA:H2	25:1:603:CLA:H62	1.75	0.43
25:N:602:CLA:H142	25:N:602:CLA:H112	1.86	0.43
2:b:222:PRO:HG3	7:h:26:GLY:HA3	1.99	0.43
25:d:400:CLA:H3A	25:d:400:CLA:HBA2	1.78	0.43
5:e:82:LYS:HE3	5:e:82:LYS:HB2	1.87	0.43
25:A:403:CLA:NB	25:D:403:CLA:HBB1	2.33	0.43
2:B:362:PHE:HE1	4:D:168:PHE:CD1	2.36	0.43
25:B:610:CLA:H43	25:B:612:CLA:H51	2.00	0.43
3:C:458:HIS:HE1	25:C:523:CLA:NA	2.13	0.43
4:D:195:PHE:HB3	4:D:280:THR:O	2.19	0.43
9:K:28:PRO:O	9:K:31:PHE:HB2	2.18	0.43
11:M:36:GLU:CD	17:G:254:SER:HG	2.26	0.43
25:G:301:CLA:H142	25:G:301:CLA:H112	1.70	0.43
2:b:201:HIS:HB2	25:b:602:CLA:CHB	2.49	0.43
25:B:610:CLA:H11	25:B:612:CLA:H191	2.01	0.43
23:1:215:ARG:NH2	23:1:228:LYS:O	2.52	0.43
25:Q:609:CLA:H3A	25:Q:609:CLA:HBA2	1.39	0.43
25:Q:613:CLA:HBA1	25:Q:613:CLA:H3A	1.86	0.43
25:R:613:CLA:H92	25:R:613:CLA:H62	1.72	0.43
25:S:604:CLA:H152	25:S:604:CLA:H112	1.69	0.43
3:C:75:VAL:HG13	3:C:132:HIS:HD2	1.84	0.43
25:C:520:CLA:H122	25:C:520:CLA:H162	1.87	0.43
4:D:341:PRO:HD2	4:D:344:VAL:HG21	1.99	0.43
19:3:205:ALA:O	19:3:209:GLN:N	2.48	0.43
25:4:607:CLA:HHC	25:4:607:CLA:HBB1	2.01	0.43
20:Q:118:LYS:HE2	20:Q:118:LYS:HB2	1.91	0.43
3:c:294:SER:OG	3:c:448:GLY:O	2.33	0.43
1:A:258:LEU:C	1:A:259:ILE:HD13	2.44	0.43
25:B:613:CLA:H62	25:B:613:CLA:H2	1.69	0.43
3:C:100:LEU:HD13	3:C:103:LEU:HD22	2.01	0.43
25:2:603:CLA:H8	25:2:603:CLA:H52	1.85	0.43
25:5:610:CLA:HED2	25:5:610:CLA:HBD	1.83	0.43
23:1:146:THR:HG23	25:1:609:CLA:HAB	1.99	0.43
18:O:186:ARG:NH1	38:O:618:II0:O02	2.44	0.43
21:R:173:LYS:HB3	21:R:173:LYS:HE2	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:357:ARG:NH2	4:d:336:GLU:O	2.32	0.43
25:b:611:CLA:H112	25:b:611:CLA:H72	1.78	0.43
3:c:355:LEU:HD11	3:c:391:LEU:HD13	2.01	0.43
4:d:195:PHE:HB3	4:d:280:THR:O	2.19	0.43
3:C:179:LEU:HG	25:C:522:CLA:HED1	2.01	0.43
25:Q:607:CLA:HHC	25:Q:607:CLA:HBB1	2.01	0.43
25:b:608:CLA:HMB3	4:d:125:CYS:HB3	1.99	0.43
3:c:393:LYS:HG3	3:c:397:ASP:HB2	2.00	0.43
3:c:449:PHE:CZ	3:c:453:ILE:HD11	2.53	0.43
25:c:517:CLA:H41	25:c:517:CLA:H62	1.73	0.43
5:e:38:PHE:HE1	5:e:47:ILE:HD12	1.83	0.43
1:A:259:ILE:HG22	1:A:260:PHE:H	1.84	0.43
26:A:405:PHO:H92	26:A:405:PHO:H62	1.75	0.43
25:C:516:CLA:H92	25:C:516:CLA:H62	1.90	0.43
25:4:609:CLA:H92	25:4:609:CLA:H62	1.79	0.43
18:O:154:LYS:HE3	18:O:154:LYS:HB2	1.93	0.43
25:O:610:CLA:H202	25:O:610:CLA:H162	1.84	0.43
2:b:6:TYR:HB2	31:b:622:LHG:H382	2.00	0.42
3:c:179:LEU:HG	25:c:522:CLA:HED1	2.00	0.42
20:4:208:LYS:HB3	20:4:212:GLN:HB2	2.01	0.42
25:O:607:CLA:H61	25:O:607:CLA:H2	1.77	0.42
1:a:202:VAL:HG22	25:a:403:CLA:C1B	2.49	0.42
2:b:325:PHE:CG	10:l:35:TYR:HB3	2.54	0.42
3:c:189:LEU:HD22	25:c:516:CLA:C1D	2.49	0.42
4:d:48:PHE:HZ	34:f:99:LMG:H341	1.84	0.42
26:d:401:PHO:H3A	25:d:403:CLA:H142	2.00	0.42
2:B:201:HIS:HB2	25:B:602:CLA:CHB	2.50	0.42
3:C:189:LEU:HD22	25:C:516:CLA:C1D	2.49	0.42
3:C:449:PHE:CZ	3:C:453:ILE:HD11	2.53	0.42
10:L:13:LEU:HB2	11:M:25:LEU:HG	2.00	0.42
19:P:101:LYS:HD3	19:P:101:LYS:HA	1.77	0.42
22:S:166:LEU:HD13	25:S:609:CLA:HHB	2.01	0.42
2:b:253:THR:HG22	35:h:90:DGD:HBH1	2.02	0.42
25:b:616:CLA:H143	25:b:616:CLA:H161	1.74	0.42
1:A:202:VAL:HG22	25:A:403:CLA:C1B	2.50	0.42
1:A:225:ARG:HD2	17:G:217:ASP:H	1.85	0.42
3:C:383:LEU:HD22	3:C:394:ILE:HA	2.00	0.42
18:2:107:THR:CG2	18:2:113:LYS:HD3	2.49	0.42
18:2:195:PHE:CE1	18:2:206:VAL:HG21	2.54	0.42
25:2:607:CLA:H61	25:2:607:CLA:H2	1.78	0.42
25:4:609:CLA:C1C	34:4:621:LMG:H372	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:G:303:LMG:H161	34:G:303:LMG:H132	1.85	0.42
22:S:222:LEU:CD2	22:S:237:ILE:HD11	2.48	0.42
1:a:259:ILE:HG22	1:a:260:PHE:H	1.84	0.42
25:b:609:CLA:H43	25:b:610:CLA:HBB2	2.01	0.42
25:b:610:CLA:H11	25:b:612:CLA:H191	2.00	0.42
25:c:518:CLA:H151	25:c:525:CLA:HBB2	2.01	0.42
10:l:25:ILE:HG13	11:m:18:PRO:HB2	2.01	0.42
1:A:223:LEU:HD13	4:D:264:ARG:HD3	2.02	0.42
3:C:40:ARG:HB3	9:K:45:ARG:HH12	1.83	0.42
3:C:320:GLY:HA3	3:C:415:LEU:HD13	2.02	0.42
3:C:355:LEU:HD11	3:C:391:LEU:HD13	2.01	0.42
25:C:521:CLA:H203	34:W:134:LMG:H372	2.02	0.42
4:D:341:PRO:HD2	4:D:344:VAL:CG2	2.49	0.42
26:D:401:PHO:H3A	25:D:403:CLA:H142	2.00	0.42
18:2:124:VAL:HG22	25:2:607:CLA:C3D	2.50	0.42
22:6:66:ALA:HB2	22:6:84:VAL:HG12	2.00	0.42
25:1:602:CLA:H142	25:1:602:CLA:H112	1.87	0.42
19:P:113:VAL:HG13	19:P:199:MET:HG2	2.00	0.42
19:P:170:ASP:HB3	19:P:173:ALA:HB3	2.02	0.42
31:P:621:LHG:H122	31:P:621:LHG:H151	1.95	0.42
1:a:153:ALA:HB1	25:a:403:CLA:HED1	2.01	0.42
1:a:193:LEU:HD11	25:a:403:CLA:HMC2	2.01	0.42
3:c:458:HIS:HE1	25:c:523:CLA:NA	2.13	0.42
25:c:525:CLA:HBA1	25:c:525:CLA:H11	1.71	0.42
26:d:401:PHO:H51	25:d:403:CLA:H111	2.01	0.42
34:f:99:LMG:H191	34:f:99:LMG:H161	1.76	0.42
16:z:16:SER:OG	16:z:47:TRP:NE1	2.40	0.42
34:D:402:LMG:H171	34:D:402:LMG:H142	1.93	0.42
29:D:405:PL9:H122	29:D:405:PL9:H101	1.89	0.42
31:D:406:LHG:H251	31:D:406:LHG:H281	1.87	0.42
5:E:82:LYS:HE3	5:E:82:LYS:HB2	1.86	0.42
25:5:610:CLA:H142	25:5:610:CLA:H111	1.86	0.42
18:O:197:HIS:CD2	25:O:615:CLA:NA	2.87	0.42
31:P:621:LHG:H171	31:P:621:LHG:H142	1.85	0.42
20:Q:208:LYS:HB3	20:Q:212:GLN:HB2	2.01	0.42
25:R:602:CLA:H41	25:R:602:CLA:H62	1.58	0.42
25:a:403:CLA:H122	26:a:405:PHO:H3A	2.01	0.42
1:A:132:GLU:O	1:A:136:ARG:HG2	2.19	0.42
25:B:605:CLA:H101	25:B:605:CLA:H13	1.90	0.42
25:B:611:CLA:H72	25:B:611:CLA:H112	1.77	0.42
25:B:616:CLA:H143	25:B:616:CLA:H161	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:95:LEU:HD13	25:2:604:CLA:H91	2.01	0.42
19:3:170:ASP:HB3	19:3:173:ALA:HB3	2.02	0.42
34:O:622:LMG:H161	34:O:622:LMG:H131	1.86	0.42
4:d:285:ILE:HD13	4:d:285:ILE:HA	1.92	0.42
13:w:33:VAL:HG11	13:w:39:LEU:HG	2.02	0.42
1:A:153:ALA:HB1	25:A:403:CLA:HED1	2.00	0.42
25:A:403:CLA:H112	25:A:403:CLA:H142	1.83	0.42
2:B:65:PHE:HE2	25:B:604:CLA:HED2	1.83	0.42
3:C:393:LYS:HG3	3:C:397:ASP:HB2	2.00	0.42
6:F:34:ILE:O	6:F:38:GLN:HG2	2.19	0.42
23:N:215:ARG:NH2	23:N:228:LYS:O	2.52	0.42
1:a:132:GLU:O	1:a:136:ARG:HG2	2.19	0.42
1:a:133:PHE:CE2	4:d:251:PHE:HA	2.55	0.42
25:b:610:CLA:H43	25:b:612:CLA:H51	2.01	0.42
25:B:611:CLA:H202	25:B:611:CLA:H161	1.87	0.42
31:D:406:LHG:H352	31:D:406:LHG:H322	1.89	0.42
25:2:602:CLA:H192	25:2:602:CLA:H162	1.92	0.42
18:O:124:VAL:HG22	25:O:607:CLA:C3D	2.50	0.42
19:P:64:PHE:CG	25:P:601:CLA:HMD2	2.54	0.42
25:N:603:CLA:HED3	25:N:603:CLA:H62	2.00	0.42
2:b:69:ILE:HB	2:b:157:HIS:CE1	2.55	0.42
3:c:383:LEU:HD22	3:c:394:ILE:HA	2.00	0.42
34:g:303:LMG:H382	19:3:165:LEU:HD11	2.02	0.42
25:B:609:CLA:H43	25:B:610:CLA:HBB2	2.01	0.42
31:B:622:LHG:HC81	31:B:622:LHG:H362	2.02	0.42
25:2:607:CLA:H61	25:2:607:CLA:H92	1.83	0.42
20:Q:53:ARG:HA	20:Q:54:PRO:HD3	1.96	0.42
23:N:96:ARG:HA	23:N:99:MET:HE3	2.01	0.42
1:a:223:LEU:HD13	4:d:264:ARG:HD3	2.02	0.42
2:b:201:HIS:HB2	25:b:602:CLA:C1B	2.50	0.42
25:b:608:CLA:H152	25:b:609:CLA:H172	2.02	0.42
1:A:77:ILE:HD11	12:T:6:TYR:HB3	2.01	0.42
25:B:601:CLA:H3A	25:B:601:CLA:H2	2.02	0.42
25:C:518:CLA:H62	25:C:518:CLA:H41	1.70	0.42
25:O:610:CLA:H91	25:O:610:CLA:H112	1.85	0.42
25:O:611:CLA:H41	25:O:611:CLA:H61	1.80	0.42
20:Q:87:LYS:HE3	20:Q:87:LYS:HB2	1.94	0.42
1:a:93:PHE:HZ	25:a:406:CLA:HAA2	1.85	0.41
26:a:405:PHO:H92	26:a:405:PHO:H62	1.75	0.41
25:b:611:CLA:H61	25:b:611:CLA:H2	1.83	0.41
25:b:612:CLA:H91	25:b:613:CLA:HAB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:535:LHG:H291	31:c:535:LHG:H262	1.72	0.41
4:d:128:GLN:NE2	26:d:401:PHO:OBD	2.53	0.41
3:C:176:GLY:HA2	3:C:262:GLY:HA2	2.02	0.41
3:C:351:LEU:HD21	3:C:357:ARG:HH21	1.85	0.41
3:C:477:ASN:OD1	3:C:477:ASN:N	2.53	0.41
18:2:144:VAL:HG22	25:2:609:CLA:HMA1	2.03	0.41
21:5:61:ASP:OD1	21:5:61:ASP:N	2.51	0.41
21:5:125:LEU:HA	21:5:128:SER:HB3	2.01	0.41
25:P:610:CLA:H41	25:P:610:CLA:H62	1.86	0.41
21:R:61:ASP:OD1	21:R:61:ASP:N	2.51	0.41
1:a:34:GLY:HA2	1:a:37:MET:HB3	2.02	0.41
3:c:100:LEU:HD13	3:c:103:LEU:HD22	2.01	0.41
3:c:477:ASN:OD1	3:c:477:ASN:N	2.53	0.41
4:d:53:PHE:O	5:e:50:THR:OG1	2.30	0.41
10:l:18:LEU:HD22	11:m:26:PHE:CD2	2.55	0.41
31:l:101:LHG:H131	31:l:101:LHG:H162	1.92	0.41
3:C:294:SER:OG	3:C:448:GLY:O	2.33	0.41
25:C:518:CLA:H151	25:C:525:CLA:HBB2	2.00	0.41
35:H:90:DGD:HBN1	35:H:90:DGD:HBW2	1.94	0.41
25:O:607:CLA:H61	25:O:607:CLA:H92	1.84	0.41
19:P:51:PRO:HA	19:P:52:PRO:HD3	1.96	0.41
19:P:205:ALA:O	19:P:209:GLN:N	2.48	0.41
1:a:184:LEU:HD21	4:d:185:GLN:HG2	2.03	0.41
25:g:301:CLA:H161	25:6:602:CLA:H91	2.01	0.41
1:A:131:TRP:CZ2	3:C:463:ARG:HG3	2.56	0.41
20:Q:107:PHE:HE2	25:Q:604:CLA:H11	1.85	0.41
20:Q:183:LEU:O	20:Q:187:LYS:HG3	2.20	0.41
21:R:186:ILE:O	21:R:189:SER:HB2	2.21	0.41
1:a:247:ASN:HD21	2:b:487:THR:HB	1.85	0.41
3:c:74:MET:HE3	25:c:525:CLA:HAB	2.03	0.41
4:d:59:THR:HG22	4:d:81:ALA:HB2	2.02	0.41
25:B:608:CLA:H152	25:B:609:CLA:H172	2.03	0.41
4:D:128:GLN:NE2	26:D:401:PHO:OBD	2.53	0.41
4:D:292:LEU:HD12	4:D:292:LEU:HA	1.93	0.41
19:3:64:PHE:CG	25:3:601:CLA:HMD2	2.55	0.41
18:O:76:VAL:O	18:O:76:VAL:CG2	2.68	0.41
23:N:182:PRO:HA	23:N:185:LEU:HB3	2.03	0.41
3:c:141:PHE:CG	34:z:102:LMG:H292	2.54	0.41
25:c:527:CLA:HBA2	25:c:527:CLA:H3A	1.66	0.41
4:d:160:PRO:HB3	4:d:169:ALA:HB2	2.03	0.41
4:d:348:GLY:HA2	4:d:351:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:11:PRO:HB2	6:f:12:ILE:H	1.67	0.41
16:z:2:VAL:HG22	16:z:61:VAL:HG13	2.02	0.41
1:A:193:LEU:HD11	25:A:403:CLA:HMC2	2.01	0.41
31:B:622:LHG:H292	31:B:622:LHG:H261	1.87	0.41
23:1:213:VAL:HG12	23:1:230:PRO:HD2	2.02	0.41
18:O:84:GLU:HG2	18:O:147:LEU:HD13	2.02	0.41
19:P:58:MET:CE	19:P:75:LEU:HB3	2.51	0.41
23:N:215:ARG:NE	23:N:223:ASN:HD21	2.19	0.41
25:a:403:CLA:H112	25:a:403:CLA:H142	1.83	0.41
25:a:403:CLA:H72	25:a:403:CLA:H111	1.80	0.41
2:b:4:PRO:HB3	31:l:101:LHG:HC12	2.02	0.41
2:b:290:ASN:O	2:b:294:GLU:HG2	2.21	0.41
2:b:324:LEU:HD21	4:d:195:PHE:HE2	1.85	0.41
25:c:518:CLA:H41	25:c:518:CLA:H62	1.70	0.41
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.02	0.41
25:A:406:CLA:HBC1	28:A:411:SQD:H312	2.02	0.41
2:B:201:HIS:HB2	25:B:602:CLA:C1B	2.51	0.41
2:B:341:LEU:HD22	2:B:406:LEU:HD13	2.01	0.41
25:B:612:CLA:H91	25:B:613:CLA:HAB	2.03	0.41
3:C:74:MET:HE3	25:C:525:CLA:HAB	2.02	0.41
3:C:201:ASP:O	3:C:208:GLY:CA	2.69	0.41
3:C:291:VAL:HB	3:C:455:HIS:CD2	2.56	0.41
18:2:84:GLU:HG2	18:2:147:LEU:HD13	2.03	0.41
20:4:107:PHE:HE2	25:4:604:CLA:H11	1.84	0.41
18:O:95:LEU:HD13	25:O:604:CLA:H91	2.01	0.41
19:P:75:LEU:HD23	19:P:75:LEU:HA	1.93	0.41
25:P:611:CLA:H62	25:P:611:CLA:H41	1.55	0.41
25:Q:603:CLA:H92	25:Q:603:CLA:H62	1.78	0.41
25:R:610:CLA:HED2	25:R:610:CLA:HBD	1.83	0.41
2:b:341:LEU:HD22	2:b:406:LEU:HD13	2.01	0.41
4:d:164:ALA:HB3	4:d:168:PHE:HE2	1.86	0.41
29:d:405:PL9:H122	29:d:405:PL9:H101	1.89	0.41
6:f:34:ILE:O	6:f:38:GLN:HG2	2.20	0.41
25:C:525:CLA:H11	25:C:525:CLA:HBA1	1.70	0.41
4:D:59:THR:HG22	4:D:81:ALA:HB2	2.02	0.41
25:P:611:CLA:HBA1	25:Q:603:CLA:H43	2.01	0.41
25:R:611:CLA:H141	25:R:611:CLA:H203	2.03	0.41
29:a:409:PL9:HC8	29:a:409:PL9:HC2	1.92	0.41
25:b:612:CLA:HBA1	25:b:612:CLA:H3A	1.98	0.41
4:d:14:PHE:HE2	34:d:402:LMG:HC72	1.84	0.41
8:i:10:THR:HG23	13:w:45:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LEU:HD21	4:D:195:PHE:HE2	1.85	0.41
23:N:213:VAL:HG12	23:N:230:PRO:HD2	2.02	0.41
1:a:75:ASN:HA	4:d:300:GLN:HE22	1.86	0.41
25:a:406:CLA:HBC1	28:a:411:SQD:H312	2.03	0.41
2:b:65:PHE:HE2	25:b:604:CLA:HED2	1.85	0.41
2:b:464:LEU:HD21	31:b:622:LHG:H261	2.02	0.41
29:d:405:PL9:H401	31:d:406:LHG:H202	2.03	0.41
31:d:406:LHG:H352	31:d:406:LHG:H322	1.89	0.41
17:g:117:CYS:HB3	17:g:122:TRP:CD1	2.56	0.41
1:A:11:ALA:HB1	13:W:59:THR:HG21	2.03	0.41
1:A:75:ASN:HA	4:D:300:GLN:HE22	1.85	0.41
25:A:403:CLA:H111	25:A:403:CLA:H72	1.80	0.41
25:A:403:CLA:H122	26:A:405:PHO:H3A	2.01	0.41
2:B:69:ILE:HB	2:B:157:HIS:CE1	2.55	0.41
2:B:469:HIS:HE1	25:B:611:CLA:NA	2.19	0.41
31:C:535:LHG:HC41	13:W:57:ALA:HB1	2.02	0.41
4:D:14:PHE:HE2	34:D:402:LMG:HC72	1.85	0.41
19:3:75:LEU:HD23	19:3:75:LEU:HA	1.93	0.41
19:3:84:LYS:HE3	19:3:84:LYS:HB2	1.90	0.41
25:3:604:CLA:H92	25:3:604:CLA:H62	1.88	0.41
25:3:611:CLA:HBA1	25:4:603:CLA:H43	2.02	0.41
25:6:603:CLA:H92	25:6:603:CLA:H61	1.84	0.41
25:6:611:CLA:H3A	25:6:611:CLA:HBA2	1.65	0.41
17:G:137:LEU:HD23	17:G:137:LEU:HA	1.92	0.41
18:O:103:GLN:HG2	25:O:604:CLA:C4D	2.51	0.41
18:O:144:VAL:HG22	25:O:609:CLA:HMA1	2.03	0.41
19:P:96:PHE:HD2	19:P:195:MET:HE3	1.86	0.41
25:P:615:CLA:H3A	25:P:615:CLA:HBA2	1.72	0.41
20:Q:194:ILE:HG22	25:Q:613:CLA:HAB	2.02	0.41
21:R:125:LEU:HA	21:R:128:SER:HB3	2.01	0.41
23:N:209:HIS:HE1	37:N:613:KC2:C1B	2.34	0.41
25:N:603:CLA:H2	25:N:603:CLA:H62	1.79	0.41
29:a:409:PL9:HC8	29:a:409:PL9:H121	1.83	0.41
2:b:475:PHE:CD1	4:d:139:PRO:HG3	2.56	0.41
3:c:176:GLY:HA2	3:c:262:GLY:HA2	2.02	0.41
4:d:278:LEU:HD12	26:d:401:PHO:HBC3	2.02	0.41
1:A:133:PHE:CE2	4:D:251:PHE:HA	2.55	0.41
4:D:293:ARG:HG3	4:D:295:TYR:HB2	2.03	0.41
18:2:189:MET:SD	25:2:602:CLA:HAB	2.61	0.41
20:4:183:LEU:O	20:4:187:LYS:HG3	2.21	0.41
17:G:105:LEU:O	17:G:109:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:137:SER:CB	25:O:609:CLA:HAB	2.51	0.41
18:O:189:MET:SD	25:O:602:CLA:HAB	2.61	0.41
26:a:405:PHO:H2	26:a:405:PHO:H61	1.84	0.40
15:y:4:LEU:HD13	15:y:4:LEU:C	2.46	0.40
20:4:194:ILE:HG22	25:4:613:CLA:HAB	2.02	0.40
25:4:606:CLA:HMB1	25:5:613:CLA:HBA2	2.02	0.40
21:5:193:MET:SD	25:5:602:CLA:HAB	2.61	0.40
25:5:611:CLA:H203	25:5:611:CLA:H141	2.03	0.40
34:G:303:LMG:H121	34:G:303:LMG:H331	2.02	0.40
23:1:215:ARG:NE	23:1:223:ASN:HD21	2.19	0.40
25:b:616:CLA:H111	25:b:616:CLA:H72	1.83	0.40
3:c:201:ASP:O	3:c:208:GLY:CA	2.69	0.40
25:c:516:CLA:H93	25:c:516:CLA:HBB1	2.03	0.40
25:B:605:CLA:HMA1	25:B:606:CLA:H3A	2.04	0.40
4:D:160:PRO:HB3	4:D:169:ALA:HB2	2.03	0.40
21:5:186:ILE:O	21:5:189:SER:HB2	2.20	0.40
25:Q:609:CLA:C1C	34:Q:621:LMG:H372	2.52	0.40
25:b:605:CLA:H142	25:b:610:CLA:H2	2.02	0.40
4:d:343:GLU:H	4:d:343:GLU:HG2	1.72	0.40
4:D:278:LEU:HD12	26:D:401:PHO:HBC3	2.02	0.40
5:E:31:LEU:HD23	6:F:28:VAL:HB	2.03	0.40
10:L:25:ILE:HG13	11:M:18:PRO:HB2	2.02	0.40
18:2:186:ARG:HA	18:2:189:MET:HE3	2.03	0.40
20:4:128:LYS:HE3	20:4:128:LYS:HB2	1.84	0.40
23:1:223:ASN:ND2	23:1:223:ASN:O	2.55	0.40
25:O:603:CLA:H3A	25:O:603:CLA:HBA1	1.68	0.40
1:a:61:ASP:N	1:a:61:ASP:OD1	2.45	0.40
2:b:22:VAL:HG11	25:b:614:CLA:HMA1	2.03	0.40
2:B:253:THR:HG22	35:H:90:DGD:HBH1	2.04	0.40
25:C:517:CLA:H62	25:C:517:CLA:H41	1.73	0.40
4:D:109:LEU:HD12	4:D:109:LEU:HA	1.92	0.40
20:4:135:LEU:HB2	25:4:607:CLA:HBC1	2.04	0.40
25:4:603:CLA:H2	25:4:603:CLA:HMA1	2.04	0.40
21:5:176:ASP:OD1	21:5:176:ASP:N	2.54	0.40
17:G:154:LEU:HD22	25:P:603:CLA:H61	2.04	0.40
23:1:96:ARG:HA	23:1:99:MET:HE3	2.02	0.40
18:O:114:MET:HE3	18:O:114:MET:HB2	1.88	0.40
21:R:193:MET:SD	25:R:602:CLA:HAB	2.61	0.40
2:b:469:HIS:HE1	25:b:611:CLA:NA	2.20	0.40
3:c:291:VAL:HB	3:c:455:HIS:CD2	2.56	0.40
2:B:9:HIS:O	2:B:12:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:LEU:HD12	2:B:460:LEU:HA	1.95	0.40
25:B:605:CLA:H142	25:B:610:CLA:H2	2.02	0.40
19:3:101:LYS:HA	19:3:101:LYS:HD3	1.77	0.40
20:4:190:ARG:NH1	38:4:618:II0:O01	2.54	0.40
25:6:609:CLA:H3A	25:6:609:CLA:HBA2	1.59	0.40
17:G:139:ALA:HB2	19:P:175:ARG:HG3	2.03	0.40
23:1:182:PRO:HA	23:1:185:LEU:HB3	2.03	0.40
25:Q:603:CLA:HMC1	25:Q:607:CLA:HAB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/328 (99%)	320 (98%)	5 (2%)	0	100	100
1	a	325/328 (99%)	319 (98%)	6 (2%)	0	100	100
2	B	501/509 (98%)	495 (99%)	6 (1%)	0	100	100
2	b	501/509 (98%)	495 (99%)	6 (1%)	0	100	100
3	C	430/487 (88%)	421 (98%)	9 (2%)	0	100	100
3	c	430/487 (88%)	420 (98%)	10 (2%)	0	100	100
4	D	339/351 (97%)	329 (97%)	10 (3%)	0	100	100
4	d	339/351 (97%)	330 (97%)	9 (3%)	0	100	100
5	E	62/84 (74%)	62 (100%)	0	0	100	100
5	e	62/84 (74%)	62 (100%)	0	0	100	100
6	F	30/42 (71%)	30 (100%)	0	0	100	100
6	f	30/42 (71%)	30 (100%)	0	0	100	100
7	H	63/67 (94%)	56 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	63/67 (94%)	55 (87%)	8 (13%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	K	35/45 (78%)	35 (100%)	0	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	35/38 (92%)	35 (100%)	0	0	100	100
10	l	35/38 (92%)	35 (100%)	0	0	100	100
11	M	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
11	m	36/40 (90%)	36 (100%)	0	0	100	100
12	T	28/32 (88%)	28 (100%)	0	0	100	100
12	t	28/32 (88%)	28 (100%)	0	0	100	100
13	W	43/74 (58%)	40 (93%)	3 (7%)	0	100	100
13	w	43/74 (58%)	40 (93%)	3 (7%)	0	100	100
14	X	34/39 (87%)	34 (100%)	0	0	100	100
14	x	34/39 (87%)	34 (100%)	0	0	100	100
15	Y	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
15	y	30/34 (88%)	30 (100%)	0	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	G	143/284 (50%)	137 (96%)	6 (4%)	0	100	100
17	g	143/284 (50%)	137 (96%)	6 (4%)	0	100	100
18	2	171/217 (79%)	164 (96%)	7 (4%)	0	100	100
18	O	171/217 (79%)	162 (95%)	9 (5%)	0	100	100
19	3	178/221 (80%)	168 (94%)	10 (6%)	0	100	100
19	P	178/221 (80%)	168 (94%)	10 (6%)	0	100	100
20	4	161/216 (74%)	153 (95%)	8 (5%)	0	100	100
20	Q	161/216 (74%)	153 (95%)	8 (5%)	0	100	100
21	5	181/229 (79%)	172 (95%)	9 (5%)	0	100	100
21	R	181/229 (79%)	171 (94%)	10 (6%)	0	100	100
22	6	171/227 (75%)	163 (95%)	8 (5%)	0	100	100
22	S	171/227 (75%)	165 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	1	188/233 (81%)	174 (93%)	14 (7%)	0	100	100
23	N	188/233 (81%)	174 (93%)	14 (7%)	0	100	100
All	All	6552/7794 (84%)	6341 (97%)	211 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/266 (100%)	265 (100%)	0	100	100
1	a	265/266 (100%)	265 (100%)	0	100	100
2	B	400/404 (99%)	399 (100%)	1 (0%)	91	97
2	b	400/404 (99%)	399 (100%)	1 (0%)	91	97
3	C	342/389 (88%)	342 (100%)	0	100	100
3	c	342/389 (88%)	342 (100%)	0	100	100
4	D	274/281 (98%)	273 (100%)	1 (0%)	89	96
4	d	274/281 (98%)	274 (100%)	0	100	100
5	E	56/73 (77%)	56 (100%)	0	100	100
5	e	56/73 (77%)	56 (100%)	0	100	100
6	F	27/37 (73%)	27 (100%)	0	100	100
6	f	27/37 (73%)	27 (100%)	0	100	100
7	H	55/57 (96%)	55 (100%)	0	100	100
7	h	55/57 (96%)	55 (100%)	0	100	100
8	I	33/36 (92%)	33 (100%)	0	100	100
8	i	33/36 (92%)	33 (100%)	0	100	100
9	K	30/36 (83%)	30 (100%)	0	100	100
9	k	30/36 (83%)	30 (100%)	0	100	100
10	L	34/35 (97%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	l	34/35 (97%)	34 (100%)	0	100	100
11	M	30/32 (94%)	30 (100%)	0	100	100
11	m	30/32 (94%)	30 (100%)	0	100	100
12	T	26/28 (93%)	26 (100%)	0	100	100
12	t	26/28 (93%)	26 (100%)	0	100	100
13	W	40/56 (71%)	40 (100%)	0	100	100
13	w	40/56 (71%)	40 (100%)	0	100	100
14	X	31/34 (91%)	31 (100%)	0	100	100
14	x	31/34 (91%)	31 (100%)	0	100	100
15	Y	27/29 (93%)	27 (100%)	0	100	100
15	y	27/29 (93%)	27 (100%)	0	100	100
16	Z	51/52 (98%)	51 (100%)	0	100	100
16	z	51/52 (98%)	51 (100%)	0	100	100
17	G	120/227 (53%)	120 (100%)	0	100	100
17	g	120/227 (53%)	120 (100%)	0	100	100
18	2	141/172 (82%)	140 (99%)	1 (1%)	81	92
18	O	141/172 (82%)	141 (100%)	0	100	100
19	3	142/168 (84%)	142 (100%)	0	100	100
19	P	142/168 (84%)	142 (100%)	0	100	100
20	4	131/166 (79%)	131 (100%)	0	100	100
20	Q	131/166 (79%)	131 (100%)	0	100	100
21	5	151/179 (84%)	151 (100%)	0	100	100
21	R	151/179 (84%)	151 (100%)	0	100	100
22	6	138/183 (75%)	138 (100%)	0	100	100
22	S	138/183 (75%)	137 (99%)	1 (1%)	81	92
23	1	152/184 (83%)	152 (100%)	0	100	100
23	N	152/184 (83%)	152 (100%)	0	100	100
All	All	5392/6248 (86%)	5387 (100%)	5 (0%)	92	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	440	ASP

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Mol	Chain	Res	Type
2	B	440	ASP
4	D	235	THR
18	2	49	VAL
22	S	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	26	ASN
1	a	247	ASN
1	a	252	HIS
1	a	310	GLN
2	b	87	ASN
2	b	114	HIS
2	b	130	ASN
2	b	223	GLN
2	b	290	ASN
2	b	457	ASN
2	b	489	GLN
3	c	302	GLN
3	c	325	GLN
4	d	196	HIS
4	d	238	GLN
4	d	335	HIS
9	k	39	GLN
11	m	2	ASN
16	z	58	ASN
17	g	243	ASN
1	A	26	ASN
1	A	310	GLN
2	B	87	ASN
2	B	114	HIS
2	B	130	ASN
2	B	290	ASN
2	B	457	ASN
2	B	489	GLN
3	C	325	GLN
4	D	238	GLN
4	D	335	HIS
4	D	349	ASN
5	E	24	HIS
10	L	7	ASN

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Mol	Chain	Res	Type
10	L	14	ASN
18	2	212	ASN
19	3	141	ASN
19	3	204	GLN
19	3	212	ASN
20	4	182	GLN
21	5	202	GLN
17	G	243	ASN
23	1	117	GLN
23	1	223	ASN
23	1	226	ASN
18	O	212	ASN
19	P	141	ASN
19	P	204	GLN
19	P	212	ASN
20	Q	182	GLN
23	N	117	GLN
23	N	130	ASN
23	N	223	ASN
23	N	226	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 370 ligands modelled in this entry, 10 are monoatomic - leaving 360 for Mogul analysis.

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
25	CLA	b	610	-	65,73,73	1.55	5 (7%)	76,113,113	1.25	8 (10%)
38	II0	Q	618	-	39,43,43	2.56	11 (28%)	50,60,60	3.36	19 (38%)
25	CLA	a	403	-	65,73,73	1.54	8 (12%)	76,113,113	1.20	7 (9%)
34	LMG	G	303	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	3 (6%)
27	WVN	c	530	-	40,41,41	1.85	14 (35%)	50,56,56	1.86	13 (26%)
25	CLA	b	605	-	65,73,73	1.54	6 (9%)	76,113,113	1.29	8 (10%)
27	WVN	B	618	-	40,41,41	1.88	14 (35%)	50,56,56	2.41	13 (26%)
25	CLA	B	610	-	65,73,73	1.54	5 (7%)	76,113,113	1.25	8 (10%)
26	PHO	A	405	-	51,69,69	0.99	3 (5%)	47,99,99	1.13	5 (10%)
31	LHG	5	621	25	45,45,48	0.97	2 (4%)	48,51,54	1.10	4 (8%)
25	CLA	A	403	-	65,73,73	1.54	8 (12%)	76,113,113	1.20	7 (9%)
38	II0	5	616	-	39,43,43	2.51	11 (28%)	50,60,60	3.34	17 (34%)
25	CLA	3	604	-	63,71,73	1.49	6 (9%)	73,110,113	1.40	6 (8%)
38	II0	2	617	-	39,43,43	2.50	11 (28%)	50,60,60	3.31	16 (32%)
25	CLA	4	604	20	61,69,73	1.56	5 (8%)	71,108,113	1.33	7 (9%)
27	WVN	B	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.36	15 (30%)
37	KC2	4	612	-	48,53,53	3.20	22 (45%)	54,89,89	4.54	31 (57%)
25	CLA	C	518	-	65,73,73	1.55	6 (9%)	76,113,113	1.23	6 (7%)
25	CLA	D	404	-	60,68,73	1.58	5 (8%)	70,107,113	1.35	7 (10%)
25	CLA	g	301	-	65,73,73	1.54	5 (7%)	76,113,113	1.28	9 (11%)
25	CLA	S	615	-	65,73,73	1.49	6 (9%)	76,113,113	1.31	7 (9%)
37	KC2	4	611	-	48,53,53	3.18	21 (43%)	54,89,89	4.54	31 (57%)
38	II0	R	617	-	39,43,43	2.53	11 (28%)	50,60,60	3.31	18 (36%)
25	CLA	R	601	21	55,63,73	1.68	5 (9%)	64,101,113	1.38	8 (12%)
25	CLA	c	519	-	60,68,73	1.57	5 (8%)	70,107,113	1.36	8 (11%)
25	CLA	4	609	-	56,64,73	1.62	6 (10%)	65,102,113	1.45	6 (9%)
25	CLA	3	613	19	55,63,73	1.63	6 (10%)	64,101,113	1.43	7 (10%)
25	CLA	Q	602	20	65,73,73	1.50	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	3	612	-	53,61,73	1.69	6 (11%)	61,98,113	1.44	8 (13%)
25	CLA	B	616	-	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
31	LHG	C	535	-	39,39,48	1.02	2 (5%)	42,45,54	1.10	3 (7%)
25	CLA	1	615	-	47,55,73	1.78	5 (10%)	54,91,113	1.47	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	O	609	18	48,56,73	1.78	5 (10%)	55,92,113	1.35	7 (12%)
25	CLA	O	602	18	65,73,73	1.52	5 (7%)	76,113,113	1.33	9 (11%)
37	KC2	O	612	-	48,53,53	3.16	21 (43%)	54,89,89	4.48	30 (55%)
25	CLA	Q	607	-	43,51,73	1.88	6 (13%)	49,86,113	1.37	6 (12%)
37	KC2	1	605	-	48,53,53	3.15	21 (43%)	54,89,89	4.51	31 (57%)
38	II0	6	617	-	39,43,43	2.53	12 (30%)	50,60,60	3.32	16 (32%)
27	WVN	b	619	-	40,41,41	1.87	14 (35%)	50,56,56	2.32	16 (32%)
25	CLA	O	615	-	45,53,73	1.80	6 (13%)	52,89,113	1.48	7 (13%)
27	WVN	b	618	-	40,41,41	1.88	14 (35%)	50,56,56	2.53	17 (34%)
28	SQD	A	411	-	39,40,54	1.37	4 (10%)	48,51,65	1.12	6 (12%)
38	II0	1	616	-	39,43,43	2.54	11 (28%)	50,60,60	3.37	16 (32%)
31	LHG	3	621	25	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
27	WVN	y	89	-	40,41,41	1.87	14 (35%)	50,56,56	2.49	16 (32%)
25	CLA	C	516	-	65,73,73	1.53	6 (9%)	76,113,113	1.29	7 (9%)
25	CLA	4	610	20	51,59,73	1.71	5 (9%)	59,96,113	1.44	8 (13%)
25	CLA	4	613	-	43,51,73	1.78	6 (13%)	49,86,113	1.52	8 (16%)
25	CLA	S	601	22	55,63,73	1.68	5 (9%)	64,101,113	1.32	7 (10%)
25	CLA	C	525	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
38	II0	O	616	-	39,43,43	2.53	11 (28%)	50,60,60	3.33	16 (32%)
31	LHG	a	413	-	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
25	CLA	4	606	20	55,63,73	1.64	7 (12%)	64,101,113	1.40	9 (14%)
25	CLA	N	603	-	60,68,73	1.58	5 (8%)	70,107,113	1.32	6 (8%)
25	CLA	B	607	-	65,73,73	1.52	5 (7%)	76,113,113	1.26	7 (9%)
25	CLA	O	610	18	65,73,73	1.52	5 (7%)	76,113,113	1.30	7 (9%)
27	WVN	D	408	-	40,41,41	1.88	14 (35%)	50,56,56	2.13	15 (30%)
37	KC2	N	613	-	48,53,53	3.26	21 (43%)	54,89,89	4.50	31 (57%)
31	LHG	b	622	-	42,42,48	1.00	2 (4%)	45,48,54	1.09	3 (6%)
31	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
25	CLA	6	610	22	57,65,73	1.60	5 (8%)	66,103,113	1.43	8 (12%)
38	II0	2	616	-	39,43,43	2.53	11 (28%)	50,60,60	3.34	16 (32%)
37	KC2	N	605	-	48,53,53	3.15	21 (43%)	54,89,89	4.50	31 (57%)
25	CLA	3	615	-	45,53,73	1.78	6 (13%)	52,89,113	1.52	7 (13%)
25	CLA	Q	609	20	56,64,73	1.60	6 (10%)	65,102,113	1.43	7 (10%)
27	WVN	H	89	-	40,41,41	1.87	14 (35%)	50,56,56	2.53	13 (26%)
27	WVN	C	529	-	40,41,41	1.92	14 (35%)	50,56,56	2.26	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	521	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
25	CLA	P	604	-	63,71,73	1.50	6 (9%)	73,110,113	1.40	6 (8%)
25	CLA	b	604	-	59,67,73	1.59	6 (10%)	68,105,113	1.43	9 (13%)
25	CLA	2	610	18	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	b	616	-	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	1	610	23	60,68,73	1.59	5 (8%)	70,107,113	1.34	7 (10%)
29	PL9	A	409	-	33,33,55	1.22	3 (9%)	41,42,69	1.59	9 (21%)
35	DGD	c	532	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)
25	CLA	5	613	21	55,63,73	1.63	6 (10%)	64,101,113	1.51	8 (12%)
25	CLA	1	609	23	46,54,73	1.77	6 (13%)	53,90,113	1.43	6 (11%)
34	LMG	D	402	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	2 (4%)
25	CLA	R	606	21	65,73,73	1.54	5 (7%)	76,113,113	1.27	7 (9%)
25	CLA	4	602	20	65,73,73	1.50	5 (7%)	76,113,113	1.31	7 (9%)
25	CLA	C	523	-	65,73,73	1.51	5 (7%)	76,113,113	1.33	8 (10%)
27	WVN	P	620	-	40,41,41	1.86	14 (35%)	50,56,56	2.35	19 (38%)
31	LHG	d	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	b	601	-	50,58,73	1.75	5 (10%)	58,95,113	1.46	9 (15%)
25	CLA	4	615	-	43,51,73	1.83	6 (13%)	49,86,113	1.41	6 (12%)
25	CLA	N	601	23	45,53,73	1.85	5 (11%)	52,89,113	1.50	6 (11%)
36	HEM	E	102	5,6	41,50,50	1.34	5 (12%)	45,82,82	1.74	9 (20%)
25	CLA	Q	613	-	43,51,73	1.78	6 (13%)	49,86,113	1.51	7 (14%)
25	CLA	2	606	18	51,59,73	1.73	5 (9%)	59,96,113	1.36	8 (13%)
25	CLA	2	601	18	49,57,73	1.73	5 (10%)	55,93,113	1.51	9 (16%)
25	CLA	4	603	-	65,73,73	1.55	5 (7%)	76,113,113	1.28	9 (11%)
25	CLA	P	609	19	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
25	CLA	N	610	23	60,68,73	1.59	5 (8%)	70,107,113	1.34	7 (10%)
25	CLA	P	612	-	53,61,73	1.68	5 (9%)	61,98,113	1.44	8 (13%)
25	CLA	Q	615	-	43,51,73	1.83	6 (13%)	49,86,113	1.41	6 (12%)
25	CLA	P	611	31	52,60,73	1.71	5 (9%)	60,97,113	1.34	8 (13%)
34	LMG	O	622	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
27	WVN	C	531	-	40,41,41	1.87	14 (35%)	50,56,56	2.30	15 (30%)
37	KC2	1	612	23	48,53,53	3.15	21 (43%)	54,89,89	4.58	31 (57%)
25	CLA	B	611	-	65,73,73	1.52	5 (7%)	76,113,113	1.30	9 (11%)
25	CLA	1	601	23	45,53,73	1.84	5 (11%)	52,89,113	1.50	6 (11%)
30	BCT	a	412	24	2,3,3	1.21	0	2,3,3	4.19	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	520	-	65,73,73	1.51	6 (9%)	76,113,113	1.28	8 (10%)
38	II0	R	616	-	39,43,43	2.52	11 (28%)	50,60,60	3.34	17 (34%)
25	CLA	6	609	22	55,63,73	1.60	6 (10%)	64,101,113	1.44	8 (12%)
37	KC2	P	606	19	48,53,53	3.16	21 (43%)	54,89,89	4.46	32 (59%)
26	PHO	d	401	-	51,69,69	1.00	3 (5%)	47,99,99	1.15	5 (10%)
25	CLA	2	611	-	60,68,73	1.59	5 (8%)	70,107,113	1.33	8 (11%)
25	CLA	B	606	-	65,73,73	1.54	6 (9%)	76,113,113	1.28	9 (11%)
25	CLA	6	611	31	55,63,73	1.65	5 (9%)	64,101,113	1.32	8 (12%)
39	IHT	2	620	-	40,42,42	2.14	11 (27%)	53,58,58	2.71	22 (41%)
25	CLA	c	524	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	6 (7%)
25	CLA	2	607	-	60,68,73	1.62	6 (10%)	70,107,113	1.17	7 (10%)
25	CLA	1	614	-	48,56,73	1.73	5 (10%)	55,92,113	1.50	8 (14%)
38	II0	N	618	-	39,43,43	2.56	10 (25%)	50,60,60	3.33	19 (38%)
31	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
25	CLA	c	516	-	65,73,73	1.53	6 (9%)	76,113,113	1.30	7 (9%)
38	II0	5	617	-	39,43,43	2.52	11 (28%)	50,60,60	3.31	17 (34%)
37	KC2	1	613	-	48,53,53	3.26	21 (43%)	54,89,89	4.51	31 (57%)
25	CLA	R	603	-	52,60,73	1.71	6 (11%)	60,97,113	1.50	8 (13%)
31	LHG	6	621	25	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)
38	II0	4	617	-	39,43,43	2.54	11 (28%)	50,60,60	3.32	17 (34%)
25	CLA	c	525	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	8 (10%)
38	II0	5	619	-	39,43,43	2.55	11 (28%)	50,60,60	3.30	15 (30%)
34	LMG	f	99	-	46,46,55	0.99	2 (4%)	54,54,63	1.03	3 (5%)
38	II0	6	616	-	39,43,43	2.51	11 (28%)	50,60,60	3.37	14 (28%)
27	WVN	c	531	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
38	II0	S	616	-	39,43,43	2.52	11 (28%)	50,60,60	3.37	14 (28%)
25	CLA	b	613	-	65,73,73	1.54	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	O	606	18	51,59,73	1.72	6 (11%)	59,96,113	1.35	8 (13%)
38	II0	4	618	-	39,43,43	2.57	11 (28%)	50,60,60	3.36	18 (36%)
25	CLA	2	604	18	65,73,73	1.53	5 (7%)	76,113,113	1.29	7 (9%)
25	CLA	3	601	19	45,53,73	1.86	6 (13%)	52,89,113	1.41	7 (13%)
25	CLA	B	613	-	65,73,73	1.53	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	S	609	22	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
38	II0	4	616	-	39,43,43	2.54	11 (28%)	50,60,60	3.27	16 (32%)
27	WVN	6	620	-	40,41,41	1.90	14 (35%)	50,56,56	1.90	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	KC2	Q	612	-	48,53,53	3.20	22 (45%)	54,89,89	4.54	31 (57%)
25	CLA	B	605	-	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	R	611	31	65,73,73	1.52	6 (9%)	76,113,113	1.25	6 (7%)
38	II0	2	619	-	39,43,43	2.60	11 (28%)	50,60,60	3.28	19 (38%)
25	CLA	C	527	-	65,73,73	1.53	6 (9%)	76,113,113	1.30	7 (9%)
25	CLA	R	604	21	60,68,73	1.59	6 (10%)	70,107,113	1.32	8 (11%)
25	CLA	S	603	-	55,63,73	1.62	6 (10%)	64,101,113	1.48	8 (12%)
25	CLA	6	604	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
34	LMG	W	134	-	48,48,55	0.96	2 (4%)	56,56,63	1.09	4 (7%)
27	WVN	S	620	-	40,41,41	1.89	14 (35%)	50,56,56	1.88	12 (24%)
25	CLA	N	615	-	47,55,73	1.78	5 (10%)	54,91,113	1.48	8 (14%)
27	WVN	b	617	-	40,41,41	1.85	14 (35%)	50,56,56	2.57	15 (30%)
34	LMG	Q	621	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
25	CLA	A	404	-	49,57,73	1.76	6 (12%)	55,93,113	1.43	8 (14%)
38	II0	1	619	-	39,43,43	2.57	10 (25%)	50,60,60	3.42	18 (36%)
31	LHG	D	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
25	CLA	C	521	-	65,73,73	1.51	5 (7%)	76,113,113	1.33	8 (10%)
35	DGD	h	90	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	3 (3%)
28	SQD	a	408	-	44,45,54	1.29	4 (9%)	53,56,65	1.21	6 (11%)
25	CLA	B	603	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	6 (7%)
27	WVN	B	617	-	40,41,41	1.84	14 (35%)	50,56,56	2.50	16 (32%)
25	CLA	d	403	-	65,73,73	1.55	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	B	602	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	9 (11%)
38	II0	S	617	-	39,43,43	2.51	12 (30%)	50,60,60	3.32	16 (32%)
37	KC2	2	612	-	48,53,53	3.17	21 (43%)	54,89,89	4.49	30 (55%)
25	CLA	2	609	18	48,56,73	1.78	5 (10%)	55,92,113	1.35	7 (12%)
27	WVN	c	529	-	40,41,41	1.88	14 (35%)	50,56,56	2.15	15 (30%)
25	CLA	B	615	-	65,73,73	1.52	5 (7%)	76,113,113	1.38	6 (7%)
25	CLA	g	302	17	45,53,73	1.77	6 (13%)	52,89,113	1.68	9 (17%)
25	CLA	N	614	-	48,56,73	1.74	5 (10%)	55,92,113	1.51	8 (14%)
25	CLA	S	604	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
34	LMG	m	101	-	40,40,55	1.03	2 (5%)	48,48,63	1.08	4 (8%)
38	II0	Q	616	-	39,43,43	2.54	11 (28%)	50,60,60	3.27	16 (32%)
25	CLA	P	610	19	65,73,73	1.53	5 (7%)	76,113,113	1.29	7 (9%)
38	II0	N	617	-	39,43,43	2.51	11 (28%)	50,60,60	3.32	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PHO	D	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	5 (10%)
25	CLA	N	602	23	60,68,73	1.58	6 (10%)	70,107,113	1.34	8 (11%)
27	WVN	A	407	-	40,41,41	1.88	14 (35%)	50,56,56	2.33	15 (30%)
25	CLA	C	526	-	65,73,73	1.54	5 (7%)	76,113,113	1.35	8 (10%)
25	CLA	C	528	-	52,60,73	1.70	6 (11%)	60,97,113	1.38	9 (15%)
38	II0	3	616	-	39,43,43	2.53	11 (28%)	50,60,60	3.34	15 (30%)
34	LMG	F	99	-	46,46,55	0.98	2 (4%)	54,54,63	1.02	3 (5%)
25	CLA	3	609	19	65,73,73	1.49	5 (7%)	76,113,113	1.35	8 (10%)
30	BCT	A	412	24	2,3,3	1.22	0	2,3,3	4.19	1 (50%)
31	LHG	2	621	-	45,45,48	0.97	2 (4%)	48,51,54	0.99	3 (6%)
29	PL9	a	409	-	33,33,55	1.22	3 (9%)	41,42,69	1.58	9 (21%)
25	CLA	O	613	18	60,68,73	1.57	6 (10%)	70,107,113	1.35	7 (10%)
39	IHT	4	620	-	40,42,42	2.10	11 (27%)	53,58,58	2.77	23 (43%)
31	LHG	R	621	25	45,45,48	0.97	2 (4%)	48,51,54	1.10	4 (8%)
38	II0	P	618	-	39,43,43	2.52	10 (25%)	50,60,60	3.35	19 (38%)
25	CLA	P	603	-	65,73,73	1.52	6 (9%)	76,113,113	1.29	9 (11%)
25	CLA	c	527	-	65,73,73	1.53	6 (9%)	76,113,113	1.29	7 (9%)
25	CLA	B	601	-	50,58,73	1.75	6 (12%)	58,95,113	1.49	9 (15%)
25	CLA	3	603	-	65,73,73	1.52	6 (9%)	76,113,113	1.29	9 (11%)
34	LMG	Z	102	-	31,31,55	1.20	2 (6%)	39,39,63	1.08	3 (7%)
25	CLA	S	610	22	57,65,73	1.60	5 (8%)	66,103,113	1.43	7 (10%)
25	CLA	C	519	-	60,68,73	1.57	5 (8%)	70,107,113	1.35	8 (11%)
25	CLA	C	522	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
34	LMG	d	407	-	37,37,55	1.09	2 (5%)	45,45,63	1.03	3 (6%)
38	II0	1	617	-	39,43,43	2.51	11 (28%)	50,60,60	3.33	16 (32%)
25	CLA	2	603	-	65,73,73	1.54	5 (7%)	76,113,113	1.27	6 (7%)
25	CLA	Q	610	20	51,59,73	1.71	5 (9%)	59,96,113	1.45	8 (13%)
25	CLA	5	603	-	52,60,73	1.71	6 (11%)	60,97,113	1.50	8 (13%)
35	DGD	H	90	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	3 (3%)
34	LMG	z	102	-	31,31,55	1.20	2 (6%)	39,39,63	1.08	3 (7%)
38	II0	N	616	-	39,43,43	2.54	11 (28%)	50,60,60	3.37	16 (32%)
27	WVN	Y	89	-	40,41,41	1.90	14 (35%)	50,56,56	2.25	12 (24%)
37	KC2	Q	605	-	48,53,53	3.19	21 (43%)	54,89,89	4.45	31 (57%)
29	PL9	D	405	-	55,55,55	1.05	4 (7%)	68,69,69	1.50	11 (16%)
25	CLA	b	606	-	65,73,73	1.53	5 (7%)	76,113,113	1.28	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	B	622	-	42,42,48	1.00	2 (4%)	45,48,54	1.07	3 (6%)
34	LMG	M	101	-	40,40,55	1.04	2 (5%)	48,48,63	1.08	4 (8%)
25	CLA	a	404	-	49,57,73	1.76	6 (12%)	55,93,113	1.44	8 (14%)
25	CLA	c	528	-	53,61,73	1.69	5 (9%)	61,98,113	1.38	9 (14%)
25	CLA	6	603	-	55,63,73	1.65	5 (9%)	64,101,113	1.37	8 (12%)
34	LMG	c	536	-	51,51,55	0.91	2 (3%)	59,59,63	0.98	3 (5%)
38	II0	P	619	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	16 (32%)
25	CLA	b	614	-	60,68,73	1.58	5 (8%)	70,107,113	1.26	7 (10%)
31	LHG	O	621	-	45,45,48	0.97	2 (4%)	48,51,54	0.99	3 (6%)
38	II0	R	618	-	39,43,43	2.55	10 (25%)	50,60,60	3.35	17 (34%)
38	II0	6	618	-	39,43,43	2.65	10 (25%)	50,60,60	3.41	22 (44%)
31	LHG	P	621	25	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
28	SQD	A	408	-	53,54,54	1.18	4 (7%)	62,65,65	1.15	6 (9%)
25	CLA	C	524	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
25	CLA	5	607	-	43,51,73	1.80	6 (13%)	49,86,113	1.54	8 (16%)
25	CLA	b	608	-	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	B	608	-	65,73,73	1.51	5 (7%)	76,113,113	1.30	7 (9%)
38	II0	R	619	-	39,43,43	2.54	11 (28%)	50,60,60	3.30	15 (30%)
37	KC2	S	606	22	48,53,53	3.18	22 (45%)	54,89,89	4.42	31 (57%)
25	CLA	b	607	-	65,73,73	1.51	5 (7%)	76,113,113	1.28	8 (10%)
27	WVN	d	408	-	40,41,41	1.88	14 (35%)	50,56,56	2.21	16 (32%)
39	IHT	1	620	-	40,42,42	2.08	11 (27%)	53,58,58	2.84	22 (41%)
34	LMG	d	402	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	3 (6%)
31	LHG	z	103	-	24,24,48	1.33	2 (8%)	27,30,54	1.14	2 (7%)
25	CLA	N	606	23	50,58,73	1.74	5 (10%)	58,95,113	1.37	9 (15%)
25	CLA	D	403	-	65,73,73	1.55	6 (9%)	76,113,113	1.27	7 (9%)
37	KC2	3	606	19	48,53,53	3.17	21 (43%)	54,89,89	4.46	32 (59%)
25	CLA	C	520	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	9 (11%)
25	CLA	P	601	19	45,53,73	1.87	6 (13%)	52,89,113	1.42	7 (13%)
25	CLA	O	603	-	65,73,73	1.55	6 (9%)	76,113,113	1.27	6 (7%)
25	CLA	c	526	-	65,73,73	1.54	5 (7%)	76,113,113	1.34	8 (10%)
31	LHG	c	535	-	39,39,48	1.04	2 (5%)	42,45,54	1.12	2 (4%)
25	CLA	P	615	-	45,53,73	1.78	6 (13%)	52,89,113	1.52	8 (15%)
25	CLA	b	615	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	7 (9%)
25	CLA	c	517	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	h	89	-	40,41,41	1.87	14 (35%)	50,56,56	2.46	13 (26%)
38	II0	S	618	-	39,43,43	2.65	10 (25%)	50,60,60	3.41	22 (44%)
38	II0	S	619	-	39,43,43	2.53	11 (28%)	50,60,60	3.32	16 (32%)
25	CLA	Q	603	-	65,73,73	1.55	6 (9%)	76,113,113	1.29	9 (11%)
25	CLA	d	400	-	65,73,73	1.54	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	3	610	19	65,73,73	1.53	5 (7%)	76,113,113	1.28	7 (9%)
25	CLA	A	406	-	60,68,73	1.58	5 (8%)	70,107,113	1.30	7 (10%)
25	CLA	5	601	21	55,63,73	1.67	5 (9%)	64,101,113	1.37	8 (12%)
25	CLA	Q	604	20	61,69,73	1.55	5 (8%)	71,108,113	1.32	7 (9%)
29	PL9	d	405	-	55,55,55	1.05	3 (5%)	68,69,69	1.51	11 (16%)
39	IHT	N	620	-	40,42,42	2.08	10 (25%)	53,58,58	2.84	22 (41%)
25	CLA	B	609	-	65,73,73	1.53	5 (7%)	76,113,113	1.26	8 (10%)
35	DGD	C	532	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
25	CLA	b	603	-	65,73,73	1.54	6 (9%)	76,113,113	1.22	6 (7%)
38	II0	3	617	-	39,43,43	2.53	12 (30%)	50,60,60	3.34	17 (34%)
25	CLA	N	607	-	43,51,73	1.90	7 (16%)	49,86,113	1.34	6 (12%)
27	WVN	C	530	-	40,41,41	1.85	14 (35%)	50,56,56	1.95	13 (26%)
38	II0	O	618	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)
39	IHT	R	620	-	40,42,42	2.00	10 (25%)	53,58,58	2.96	25 (47%)
34	LMG	D	407	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
25	CLA	6	601	22	55,63,73	1.68	5 (9%)	64,101,113	1.32	7 (10%)
25	CLA	S	611	31	55,63,73	1.65	5 (9%)	64,101,113	1.32	8 (12%)
25	CLA	c	522	-	65,73,73	1.49	5 (7%)	76,113,113	1.33	6 (7%)
37	KC2	R	612	-	48,53,53	3.17	21 (43%)	54,89,89	4.49	33 (61%)
25	CLA	Q	606	20	55,63,73	1.67	5 (9%)	64,101,113	1.31	8 (12%)
37	KC2	6	612	22	48,53,53	3.14	21 (43%)	54,89,89	4.61	31 (57%)
38	II0	O	617	-	39,43,43	2.50	10 (25%)	50,60,60	3.32	17 (34%)
25	CLA	5	604	21	60,68,73	1.58	6 (10%)	70,107,113	1.33	8 (11%)
34	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	3 (5%)
25	CLA	S	602	22	65,73,73	1.51	5 (7%)	76,113,113	1.30	7 (9%)
26	PHO	a	405	-	51,69,69	0.99	4 (7%)	47,99,99	1.14	5 (10%)
37	KC2	5	612	-	48,53,53	3.17	21 (43%)	54,89,89	4.48	32 (59%)
38	II0	6	619	-	39,43,43	2.50	12 (30%)	50,60,60	3.31	17 (34%)
25	CLA	b	609	-	65,73,73	1.53	5 (7%)	76,113,113	1.26	8 (10%)
25	CLA	d	404	-	61,69,73	1.56	5 (8%)	71,108,113	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	612	-	65,73,73	1.48	7 (10%)	76,113,113	1.48	10 (13%)
25	CLA	O	607	-	60,68,73	1.62	7 (11%)	70,107,113	1.16	7 (10%)
38	II0	2	618	-	39,43,43	2.51	11 (28%)	50,60,60	3.29	18 (36%)
25	CLA	b	611	-	65,73,73	1.52	5 (7%)	76,113,113	1.30	9 (11%)
25	CLA	5	610	21	59,67,73	1.61	5 (8%)	68,105,113	1.33	7 (10%)
25	CLA	G	301	-	65,73,73	1.49	6 (9%)	76,113,113	1.25	8 (10%)
36	HEM	e	102	5,6	41,50,50	1.34	6 (14%)	45,82,82	1.75	8 (17%)
31	LHG	A	413	-	41,41,48	1.01	2 (4%)	44,47,54	0.98	2 (4%)
34	LMG	w	134	-	48,48,55	0.97	2 (4%)	56,56,63	1.12	4 (7%)
25	CLA	P	613	19	55,63,73	1.64	6 (10%)	64,101,113	1.42	7 (10%)
38	II0	1	618	-	39,43,43	2.57	11 (28%)	50,60,60	3.33	19 (38%)
25	CLA	b	602	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	9 (11%)
37	KC2	Q	611	-	48,53,53	3.17	21 (43%)	54,89,89	4.54	31 (57%)
37	KC2	S	612	22	48,53,53	3.15	21 (43%)	54,89,89	4.60	31 (57%)
25	CLA	R	610	21	59,67,73	1.62	5 (8%)	68,105,113	1.34	7 (10%)
25	CLA	R	607	-	43,51,73	1.80	6 (13%)	49,86,113	1.53	8 (16%)
25	CLA	R	613	21	55,63,73	1.64	6 (10%)	64,101,113	1.52	8 (12%)
25	CLA	2	613	18	60,68,73	1.57	6 (10%)	70,107,113	1.35	8 (11%)
39	IHT	5	620	-	40,42,42	2.05	11 (27%)	53,58,58	2.83	20 (37%)
25	CLA	1	607	-	43,51,73	1.90	7 (16%)	49,86,113	1.34	6 (12%)
25	CLA	O	604	18	65,73,73	1.53	5 (7%)	76,113,113	1.29	7 (9%)
31	LHG	Z	103	-	24,24,48	1.34	2 (8%)	27,30,54	1.14	2 (7%)
34	LMG	2	622	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
39	IHT	Q	620	-	40,42,42	2.14	11 (27%)	53,58,58	2.80	23 (43%)
37	KC2	1	611	-	48,53,53	3.20	21 (43%)	54,89,89	4.46	31 (57%)
25	CLA	N	604	23	59,67,73	1.60	5 (8%)	68,105,113	1.35	7 (10%)
28	SQD	a	411	-	39,40,54	1.37	4 (10%)	48,51,65	1.12	6 (12%)
39	IHT	O	620	-	40,42,42	2.13	10 (25%)	53,58,58	2.70	20 (37%)
25	CLA	c	518	-	65,73,73	1.55	5 (7%)	76,113,113	1.23	6 (7%)
38	II0	3	618	-	39,43,43	2.54	11 (28%)	50,60,60	3.29	17 (34%)
38	II0	5	618	-	39,43,43	2.54	11 (28%)	50,60,60	3.35	17 (34%)
25	CLA	5	606	21	65,73,73	1.54	5 (7%)	76,113,113	1.26	7 (9%)
37	KC2	N	612	23	48,53,53	3.15	21 (43%)	54,89,89	4.58	31 (57%)
37	KC2	N	611	-	48,53,53	3.20	21 (43%)	54,89,89	4.46	31 (57%)
25	CLA	1	602	23	60,68,73	1.58	6 (10%)	70,107,113	1.33	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	G	302	17	45,53,73	1.82	6 (13%)	52,89,113	1.44	7 (13%)
38	II0	N	619	-	39,43,43	2.58	12 (30%)	50,60,60	3.43	18 (36%)
25	CLA	1	604	23	59,67,73	1.60	5 (8%)	68,105,113	1.35	7 (10%)
25	CLA	O	601	18	49,57,73	1.74	6 (12%)	55,93,113	1.52	8 (14%)
25	CLA	6	613	-	53,61,73	1.63	6 (11%)	61,98,113	1.43	8 (13%)
25	CLA	3	602	19	62,70,73	1.52	5 (8%)	72,109,113	1.39	7 (9%)
25	CLA	C	517	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)
38	II0	O	619	-	39,43,43	2.60	11 (28%)	50,60,60	3.27	19 (38%)
25	CLA	S	613	-	53,61,73	1.63	6 (11%)	61,98,113	1.43	8 (13%)
38	II0	P	616	-	39,43,43	2.53	11 (28%)	50,60,60	3.34	15 (30%)
27	WVN	3	620	-	40,41,41	1.86	14 (35%)	50,56,56	2.36	19 (38%)
25	CLA	5	615	-	46,54,73	1.78	6 (13%)	53,90,113	1.39	7 (13%)
25	CLA	5	611	31	65,73,73	1.52	6 (9%)	76,113,113	1.24	6 (7%)
27	WVN	a	407	-	40,41,41	1.95	14 (35%)	50,56,56	2.30	19 (38%)
34	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.01	3 (5%)
38	II0	Q	617	-	39,43,43	2.55	11 (28%)	50,60,60	3.32	17 (34%)
25	CLA	B	604	-	59,67,73	1.58	6 (10%)	68,105,113	1.42	8 (11%)
25	CLA	4	607	-	43,51,73	1.88	6 (13%)	49,86,113	1.37	6 (12%)
38	II0	Q	619	-	39,43,43	2.57	12 (30%)	50,60,60	3.32	20 (40%)
25	CLA	D	400	-	65,73,73	1.54	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	3	611	31	52,60,73	1.70	5 (9%)	60,97,113	1.34	8 (13%)
31	LHG	S	621	25	39,39,48	1.04	2 (5%)	42,45,54	1.04	2 (4%)
25	CLA	O	611	-	60,68,73	1.60	5 (8%)	70,107,113	1.34	8 (11%)
25	CLA	B	614	-	60,68,73	1.58	5 (8%)	70,107,113	1.26	8 (11%)
38	II0	P	617	-	39,43,43	2.50	11 (28%)	50,60,60	3.35	18 (36%)
38	II0	4	619	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	19 (38%)
25	CLA	P	602	19	62,70,73	1.53	5 (8%)	72,109,113	1.39	7 (9%)
25	CLA	B	612	-	65,73,73	1.47	7 (10%)	76,113,113	1.48	10 (13%)
25	CLA	N	609	23	46,54,73	1.74	6 (13%)	53,90,113	1.50	8 (15%)
25	CLA	a	406	-	60,68,73	1.58	6 (10%)	70,107,113	1.30	7 (10%)
25	CLA	2	615	-	45,53,73	1.78	6 (13%)	52,89,113	1.48	7 (13%)
34	LMG	4	621	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
34	LMG	C	536	-	47,47,55	0.97	2 (4%)	55,55,63	1.18	4 (7%)
37	KC2	4	605	-	48,53,53	3.19	21 (43%)	54,89,89	4.45	31 (57%)
38	II0	3	619	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	523	-	65,73,73	1.51	5 (7%)	76,113,113	1.32	8 (10%)
25	CLA	R	609	21	65,73,73	1.53	9 (13%)	76,113,113	1.34	9 (11%)
25	CLA	R	602	21	55,63,73	1.65	5 (9%)	64,101,113	1.37	8 (12%)
25	CLA	2	602	18	65,73,73	1.52	5 (7%)	76,113,113	1.32	9 (11%)
25	CLA	6	602	22	65,73,73	1.51	5 (7%)	76,113,113	1.30	8 (10%)
37	KC2	6	606	-	48,53,53	3.17	22 (45%)	54,89,89	4.43	32 (59%)
25	CLA	5	609	21	65,73,73	1.54	9 (13%)	76,113,113	1.34	9 (11%)
25	CLA	5	602	21	55,63,73	1.66	5 (9%)	64,101,113	1.36	8 (12%)
25	CLA	R	615	-	46,54,73	1.79	6 (13%)	53,90,113	1.38	7 (13%)
25	CLA	1	606	23	50,58,73	1.73	5 (10%)	58,95,113	1.37	9 (15%)
25	CLA	6	615	-	65,73,73	1.49	6 (9%)	76,113,113	1.31	7 (9%)
34	LMG	g	303	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	3 (6%)
25	CLA	1	603	-	60,68,73	1.59	5 (8%)	70,107,113	1.32	7 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	610	-	1/1/15/20	9/37/115/115	-
38	II0	Q	618	-	-	2/21/67/67	0/2/2/2
25	CLA	a	403	-	1/1/15/20	8/37/115/115	-
34	LMG	G	303	-	-	8/35/55/70	0/1/1/1
27	WVN	c	530	-	-	10/29/63/63	0/2/2/2
25	CLA	b	605	-	1/1/15/20	9/37/115/115	-
27	WVN	B	618	-	-	11/29/63/63	0/2/2/2
25	CLA	B	610	-	1/1/15/20	9/37/115/115	-
26	PHO	A	405	-	-	14/37/103/103	0/5/6/6
31	LHG	5	621	25	-	15/50/50/53	-
25	CLA	A	403	-	1/1/15/20	8/37/115/115	-
38	II0	5	616	-	-	0/21/67/67	0/2/2/2
25	CLA	3	604	-	-	8/35/113/115	-
38	II0	2	617	-	-	0/21/67/67	0/2/2/2
25	CLA	4	604	20	1/1/14/20	16/33/111/115	-
27	WVN	B	619	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC2	4	612	-	-	3/15/71/71	-
25	CLA	C	518	-	1/1/15/20	9/37/115/115	-
25	CLA	g	301	-	1/1/15/20	9/37/115/115	-
25	CLA	D	404	-	1/1/14/20	13/31/109/115	-
25	CLA	S	615	-	1/1/15/20	10/37/115/115	-
37	KC2	4	611	-	-	8/15/71/71	-
38	II0	R	617	-	-	1/21/67/67	0/2/2/2
25	CLA	R	601	21	1/1/13/20	6/25/103/115	-
25	CLA	c	519	-	1/1/14/20	12/31/109/115	-
25	CLA	4	609	-	1/1/13/20	11/27/105/115	-
25	CLA	3	613	19	1/1/13/20	11/25/103/115	-
25	CLA	Q	602	20	1/1/15/20	8/37/115/115	-
25	CLA	3	612	-	1/1/12/20	5/23/101/115	-
25	CLA	B	616	-	1/1/15/20	15/37/115/115	-
31	LHG	C	535	-	-	16/44/44/53	-
25	CLA	1	615	-	1/1/11/20	10/16/94/115	-
25	CLA	O	609	18	1/1/11/20	2/17/95/115	-
25	CLA	O	602	18	1/1/15/20	16/37/115/115	-
37	KC2	O	612	-	-	7/15/71/71	-
25	CLA	Q	607	-	1/1/10/20	3/11/89/115	-
37	KC2	1	605	-	-	12/15/71/71	-
38	II0	6	617	-	-	1/21/67/67	0/2/2/2
27	WVN	b	619	-	-	10/29/63/63	0/2/2/2
25	CLA	O	615	-	1/1/11/20	8/13/91/115	-
27	WVN	b	618	-	-	10/29/63/63	0/2/2/2
28	SQD	A	411	-	-	3/35/55/69	0/1/1/1
38	II0	1	616	-	-	4/21/67/67	0/2/2/2
31	LHG	3	621	25	-	19/53/53/53	-
27	WVN	y	89	-	-	8/29/63/63	0/2/2/2
25	CLA	C	516	-	1/1/15/20	7/37/115/115	-
25	CLA	4	610	20	1/1/12/20	4/21/99/115	-
25	CLA	4	613	-	1/1/10/20	8/11/89/115	-
25	CLA	S	601	22	1/1/13/20	8/25/103/115	-
25	CLA	C	525	-	1/1/15/20	11/37/115/115	-
38	II0	O	616	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	a	413	-	-	28/46/46/53	-
25	CLA	4	606	20	1/1/13/20	11/25/103/115	-
25	CLA	N	603	-	1/1/14/20	7/31/109/115	-
25	CLA	B	607	-	1/1/15/20	13/37/115/115	-
25	CLA	O	610	18	1/1/15/20	10/37/115/115	-
27	WVN	D	408	-	-	9/29/63/63	0/2/2/2
37	KC2	N	613	-	-	10/15/71/71	-
31	LHG	b	622	-	-	20/47/47/53	-
31	LHG	l	101	-	-	6/53/53/53	-
25	CLA	6	610	22	1/1/13/20	11/28/106/115	-
38	II0	2	616	-	-	1/21/67/67	0/2/2/2
37	KC2	N	605	-	-	12/15/71/71	-
25	CLA	3	615	-	1/1/11/20	8/13/91/115	-
25	CLA	Q	609	20	1/1/13/20	9/27/105/115	-
27	WVN	H	89	-	-	9/29/63/63	0/2/2/2
27	WVN	C	529	-	-	10/29/63/63	0/2/2/2
25	CLA	c	521	-	1/1/15/20	7/37/115/115	-
25	CLA	P	604	-	-	8/35/113/115	-
25	CLA	b	604	-	1/1/13/20	12/30/108/115	-
25	CLA	2	610	18	1/1/15/20	10/37/115/115	-
25	CLA	b	616	-	1/1/15/20	15/37/115/115	-
25	CLA	1	610	23	1/1/14/20	6/31/109/115	-
29	PL9	A	409	-	-	10/27/47/73	0/1/1/1
35	DGD	c	532	-	-	8/43/83/95	0/2/2/2
25	CLA	5	613	21	1/1/13/20	13/25/103/115	-
25	CLA	1	609	23	1/1/11/20	5/15/93/115	-
34	LMG	D	402	-	-	9/35/55/70	0/1/1/1
25	CLA	R	606	21	1/1/15/20	14/37/115/115	-
25	CLA	4	602	20	1/1/15/20	8/37/115/115	-
25	CLA	C	523	-	1/1/15/20	12/37/115/115	-
27	WVN	P	620	-	-	8/29/63/63	0/2/2/2
31	LHG	d	406	-	-	13/53/53/53	-
25	CLA	b	601	-	1/1/12/20	9/19/97/115	-
25	CLA	4	615	-	1/1/10/20	2/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	N	601	23	1/1/11/20	7/13/91/115	-
36	HEM	E	102	5,6	-	6/12/54/54	-
25	CLA	Q	613	-	1/1/10/20	8/11/89/115	-
25	CLA	2	606	18	1/1/12/20	6/21/99/115	-
25	CLA	2	601	18	1/1/11/20	7/18/96/115	-
25	CLA	4	603	-	1/1/15/20	14/37/115/115	-
25	CLA	P	609	19	1/1/15/20	9/37/115/115	-
25	CLA	N	610	23	1/1/14/20	6/31/109/115	-
25	CLA	P	612	-	1/1/12/20	5/23/101/115	-
25	CLA	Q	615	-	1/1/10/20	2/11/89/115	-
25	CLA	P	611	31	1/1/12/20	6/22/100/115	-
34	LMG	O	622	-	-	2/35/55/70	0/1/1/1
27	WVN	C	531	-	-	10/29/63/63	0/2/2/2
37	KC2	1	612	23	-	3/15/71/71	-
25	CLA	B	611	-	1/1/15/20	10/37/115/115	-
25	CLA	1	601	23	1/1/11/20	7/13/91/115	-
25	CLA	c	520	-	1/1/15/20	8/37/115/115	-
38	II0	R	616	-	-	0/21/67/67	0/2/2/2
25	CLA	6	609	22	1/1/13/20	8/25/103/115	-
37	KC2	P	606	19	-	9/15/71/71	-
26	PHO	d	401	-	-	12/37/103/103	0/5/6/6
25	CLA	2	611	-	1/1/14/20	15/31/109/115	-
25	CLA	B	606	-	1/1/15/20	12/37/115/115	-
25	CLA	6	611	31	1/1/13/20	11/25/103/115	-
39	IHT	2	620	-	-	5/25/65/65	0/2/2/2
25	CLA	c	524	-	1/1/15/20	13/37/115/115	-
25	CLA	2	607	-	1/1/14/20	14/31/109/115	-
25	CLA	1	614	-	1/1/11/20	6/17/95/115	-
38	II0	N	618	-	-	3/21/67/67	0/2/2/2
31	LHG	L	101	-	-	6/53/53/53	-
25	CLA	c	516	-	1/1/15/20	8/37/115/115	-
38	II0	5	617	-	-	1/21/67/67	0/2/2/2
37	KC2	1	613	-	-	10/15/71/71	-
25	CLA	R	603	-	1/1/12/20	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	6	621	25	-	12/44/44/53	-
38	II0	4	617	-	-	1/21/67/67	0/2/2/2
25	CLA	c	525	-	1/1/15/20	11/37/115/115	-
38	II0	5	619	-	-	3/21/67/67	0/2/2/2
34	LMG	f	99	-	-	3/41/61/70	0/1/1/1
38	II0	6	616	-	-	5/21/67/67	0/2/2/2
27	WVN	c	531	-	-	11/29/63/63	0/2/2/2
38	II0	S	616	-	-	6/21/67/67	0/2/2/2
25	CLA	b	613	-	1/1/15/20	16/37/115/115	-
25	CLA	O	606	18	1/1/12/20	6/21/99/115	-
38	II0	4	618	-	-	2/21/67/67	0/2/2/2
25	CLA	2	604	18	1/1/15/20	12/37/115/115	-
25	CLA	3	601	19	1/1/11/20	0/13/91/115	-
25	CLA	B	613	-	1/1/15/20	15/37/115/115	-
25	CLA	S	609	22	1/1/13/20	14/25/103/115	-
38	II0	4	616	-	-	2/21/67/67	0/2/2/2
27	WVN	6	620	-	-	7/29/63/63	0/2/2/2
37	KC2	Q	612	-	-	3/15/71/71	-
25	CLA	B	605	-	1/1/15/20	9/37/115/115	-
25	CLA	R	611	31	1/1/15/20	17/37/115/115	-
38	II0	2	619	-	-	5/21/67/67	0/2/2/2
25	CLA	C	527	-	1/1/15/20	11/37/115/115	-
25	CLA	R	604	21	1/1/14/20	11/31/109/115	-
25	CLA	S	603	-	1/1/13/20	9/25/103/115	-
25	CLA	6	604	-	1/1/15/20	18/37/115/115	-
34	LMG	W	134	-	-	9/43/63/70	0/1/1/1
27	WVN	S	620	-	-	9/29/63/63	0/2/2/2
25	CLA	N	615	-	1/1/11/20	10/16/94/115	-
27	WVN	b	617	-	-	13/29/63/63	0/2/2/2
34	LMG	Q	621	-	-	4/38/58/70	0/1/1/1
25	CLA	A	404	-	1/1/11/20	10/18/96/115	-
38	II0	1	619	-	-	3/21/67/67	0/2/2/2
31	LHG	D	406	-	-	13/53/53/53	-
25	CLA	C	521	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	h	90	-	-	14/51/91/95	0/2/2/2
28	SQD	a	408	-	-	6/40/60/69	0/1/1/1
25	CLA	B	603	-	1/1/15/20	9/37/115/115	-
27	WVN	B	617	-	-	11/29/63/63	0/2/2/2
25	CLA	d	403	-	1/1/15/20	5/37/115/115	-
25	CLA	B	602	-	-	6/37/115/115	-
38	II0	S	617	-	-	1/21/67/67	0/2/2/2
37	KC2	2	612	-	-	7/15/71/71	-
25	CLA	2	609	18	1/1/11/20	2/17/95/115	-
27	WVN	c	529	-	-	10/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	10/37/115/115	-
25	CLA	g	302	17	1/1/11/20	6/13/91/115	-
25	CLA	N	614	-	1/1/11/20	6/17/95/115	-
25	CLA	S	604	-	1/1/15/20	18/37/115/115	-
34	LMG	m	101	-	-	7/35/55/70	0/1/1/1
38	II0	Q	616	-	-	2/21/67/67	0/2/2/2
25	CLA	P	610	19	1/1/15/20	14/37/115/115	-
38	II0	N	617	-	-	1/21/67/67	0/2/2/2
26	PHO	D	401	-	-	11/37/103/103	0/5/6/6
25	CLA	N	602	23	1/1/14/20	7/31/109/115	-
27	WVN	A	407	-	-	2/29/63/63	0/2/2/2
25	CLA	C	526	-	1/1/15/20	13/37/115/115	-
25	CLA	C	528	-	1/1/12/20	9/22/100/115	-
38	II0	3	616	-	-	2/21/67/67	0/2/2/2
34	LMG	F	99	-	-	3/41/61/70	0/1/1/1
25	CLA	3	609	19	1/1/15/20	9/37/115/115	-
31	LHG	2	621	-	-	9/50/50/53	-
29	PL9	a	409	-	-	10/27/47/73	0/1/1/1
25	CLA	O	613	18	1/1/14/20	10/31/109/115	-
39	IHT	4	620	-	-	9/25/65/65	0/2/2/2
31	LHG	R	621	25	-	15/50/50/53	-
38	II0	P	618	-	-	2/21/67/67	0/2/2/2
25	CLA	P	603	-	1/1/15/20	15/37/115/115	-
25	CLA	c	527	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	601	-	1/1/12/20	9/19/97/115	-
25	CLA	3	603	-	1/1/15/20	15/37/115/115	-
34	LMG	Z	102	-	-	5/26/46/70	0/1/1/1
25	CLA	S	610	22	1/1/13/20	11/28/106/115	-
25	CLA	C	519	-	1/1/14/20	12/31/109/115	-
25	CLA	C	522	-	1/1/15/20	9/37/115/115	-
34	LMG	d	407	-	-	2/32/52/70	0/1/1/1
38	II0	1	617	-	-	1/21/67/67	0/2/2/2
25	CLA	2	603	-	1/1/15/20	8/37/115/115	-
25	CLA	Q	610	20	1/1/12/20	4/21/99/115	-
25	CLA	5	603	-	1/1/12/20	9/22/100/115	-
35	DGD	H	90	-	-	14/51/91/95	0/2/2/2
34	LMG	z	102	-	-	5/26/46/70	0/1/1/1
38	II0	N	616	-	-	4/21/67/67	0/2/2/2
27	WVN	Y	89	-	-	9/29/63/63	0/2/2/2
37	KC2	Q	605	-	-	7/15/71/71	-
29	PL9	D	405	-	-	7/53/73/73	0/1/1/1
25	CLA	b	606	-	1/1/15/20	10/37/115/115	-
31	LHG	B	622	-	-	12/47/47/53	-
34	LMG	M	101	-	-	6/35/55/70	0/1/1/1
25	CLA	a	404	-	1/1/11/20	10/18/96/115	-
25	CLA	c	528	-	1/1/12/20	9/23/101/115	-
25	CLA	6	603	-	1/1/13/20	7/25/103/115	-
34	LMG	c	536	-	-	19/46/66/70	0/1/1/1
38	II0	P	619	-	-	6/21/67/67	0/2/2/2
25	CLA	b	614	-	1/1/14/20	12/31/109/115	-
31	LHG	O	621	-	-	9/50/50/53	-
38	II0	R	618	-	-	0/21/67/67	0/2/2/2
38	II0	6	618	-	-	4/21/67/67	0/2/2/2
31	LHG	P	621	25	-	19/53/53/53	-
28	SQD	A	408	-	-	7/49/69/69	0/1/1/1
25	CLA	C	524	-	1/1/15/20	13/37/115/115	-
25	CLA	5	607	-	1/1/10/20	5/11/89/115	-
25	CLA	b	608	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	608	-	1/1/15/20	4/37/115/115	-
38	II0	R	619	-	-	3/21/67/67	0/2/2/2
37	KC2	S	606	22	-	8/15/71/71	-
25	CLA	b	607	-	1/1/15/20	12/37/115/115	-
27	WVN	d	408	-	-	12/29/63/63	0/2/2/2
39	IHT	1	620	-	-	8/25/65/65	0/2/2/2
34	LMG	d	402	-	-	9/35/55/70	0/1/1/1
31	LHG	z	103	-	-	8/29/29/53	-
25	CLA	N	606	23	1/1/12/20	6/19/97/115	-
25	CLA	D	403	-	1/1/15/20	5/37/115/115	-
37	KC2	3	606	19	-	9/15/71/71	-
25	CLA	C	520	-	1/1/15/20	11/37/115/115	-
25	CLA	P	601	19	1/1/11/20	2/13/91/115	-
25	CLA	O	603	-	1/1/15/20	8/37/115/115	-
25	CLA	c	526	-	1/1/15/20	12/37/115/115	-
31	LHG	c	535	-	-	13/44/44/53	-
25	CLA	P	615	-	1/1/11/20	8/13/91/115	-
25	CLA	b	615	-	1/1/15/20	9/37/115/115	-
25	CLA	c	517	-	1/1/15/20	16/37/115/115	-
27	WVN	h	89	-	-	11/29/63/63	0/2/2/2
38	II0	S	618	-	-	4/21/67/67	0/2/2/2
38	II0	S	619	-	-	4/21/67/67	0/2/2/2
25	CLA	Q	603	-	1/1/15/20	14/37/115/115	-
25	CLA	d	400	-	1/1/15/20	10/37/115/115	-
25	CLA	3	610	19	1/1/15/20	14/37/115/115	-
25	CLA	A	406	-	1/1/14/20	10/31/109/115	-
25	CLA	5	601	21	1/1/13/20	6/25/103/115	-
25	CLA	Q	604	20	1/1/14/20	17/33/111/115	-
29	PL9	d	405	-	-	8/53/73/73	0/1/1/1
39	IHT	N	620	-	-	7/25/65/65	0/2/2/2
25	CLA	B	609	-	1/1/15/20	9/37/115/115	-
35	DGD	C	532	-	-	8/43/83/95	0/2/2/2
25	CLA	b	603	-	1/1/15/20	9/37/115/115	-
38	II0	3	617	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	N	607	-	1/1/10/20	5/11/89/115	-
27	WVN	C	530	-	-	10/29/63/63	0/2/2/2
38	II0	O	618	-	-	3/21/67/67	0/2/2/2
39	IHT	R	620	-	-	11/25/65/65	0/2/2/2
34	LMG	D	407	-	-	2/32/52/70	0/1/1/1
25	CLA	6	601	22	1/1/13/20	8/25/103/115	-
25	CLA	S	611	31	1/1/13/20	11/25/103/115	-
25	CLA	c	522	-	1/1/15/20	9/37/115/115	-
37	KC2	R	612	-	-	8/15/71/71	-
25	CLA	Q	606	20	1/1/13/20	9/25/103/115	-
37	KC2	6	612	22	-	5/15/71/71	-
38	II0	O	617	-	-	1/21/67/67	0/2/2/2
25	CLA	5	604	21	1/1/14/20	11/31/109/115	-
34	LMG	B	620	-	-	7/46/66/70	0/1/1/1
25	CLA	S	602	22	1/1/15/20	17/37/115/115	-
26	PHO	a	405	-	-	14/37/103/103	0/5/6/6
37	KC2	5	612	-	-	8/15/71/71	-
38	II0	6	619	-	-	3/21/67/67	0/2/2/2
25	CLA	b	609	-	1/1/15/20	8/37/115/115	-
25	CLA	d	404	-	1/1/14/20	16/33/111/115	-
25	CLA	b	612	-	1/1/15/20	12/37/115/115	-
25	CLA	O	607	-	1/1/14/20	14/31/109/115	-
38	II0	2	618	-	-	1/21/67/67	0/2/2/2
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
25	CLA	5	610	21	1/1/13/20	10/30/108/115	-
25	CLA	G	301	-	1/1/15/20	19/37/115/115	-
36	HEM	e	102	5,6	-	6/12/54/54	-
31	LHG	A	413	-	-	29/46/46/53	-
34	LMG	w	134	-	-	8/43/63/70	0/1/1/1
25	CLA	P	613	19	1/1/13/20	11/25/103/115	-
38	II0	1	618	-	-	3/21/67/67	0/2/2/2
25	CLA	b	602	-	-	6/37/115/115	-
37	KC2	Q	611	-	-	8/15/71/71	-
37	KC2	S	612	22	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	610	21	1/1/13/20	10/30/108/115	-
25	CLA	R	607	-	1/1/10/20	4/11/89/115	-
25	CLA	R	613	21	1/1/13/20	14/25/103/115	-
25	CLA	2	613	18	1/1/14/20	10/31/109/115	-
39	IHT	5	620	-	-	7/25/65/65	0/2/2/2
25	CLA	1	607	-	1/1/10/20	5/11/89/115	-
25	CLA	O	604	18	1/1/15/20	12/37/115/115	-
31	LHG	Z	103	-	-	8/29/29/53	-
34	LMG	2	622	-	-	2/35/55/70	0/1/1/1
39	IHT	Q	620	-	-	10/25/65/65	0/2/2/2
37	KC2	1	611	-	-	4/15/71/71	-
25	CLA	N	604	23	1/1/13/20	8/30/108/115	-
28	SQD	a	411	-	-	4/35/55/69	0/1/1/1
39	IHT	O	620	-	-	6/25/65/65	0/2/2/2
25	CLA	c	518	-	1/1/15/20	9/37/115/115	-
38	II0	3	618	-	-	2/21/67/67	0/2/2/2
38	II0	5	618	-	-	0/21/67/67	0/2/2/2
25	CLA	5	606	21	1/1/15/20	14/37/115/115	-
37	KC2	N	612	23	-	4/15/71/71	-
37	KC2	N	611	-	-	4/15/71/71	-
25	CLA	1	602	23	1/1/14/20	7/31/109/115	-
25	CLA	G	302	17	1/1/11/20	4/13/91/115	-
38	II0	N	619	-	-	4/21/67/67	0/2/2/2
25	CLA	1	604	23	1/1/13/20	8/30/108/115	-
25	CLA	O	601	18	1/1/11/20	7/18/96/115	-
25	CLA	6	613	-	1/1/12/20	5/23/101/115	-
25	CLA	3	602	19	1/1/14/20	15/34/112/115	-
25	CLA	C	517	-	1/1/15/20	16/37/115/115	-
38	II0	O	619	-	-	5/21/67/67	0/2/2/2
25	CLA	S	613	-	1/1/12/20	5/23/101/115	-
38	II0	P	616	-	-	2/21/67/67	0/2/2/2
27	WVN	3	620	-	-	8/29/63/63	0/2/2/2
25	CLA	5	615	-	1/1/11/20	5/15/93/115	-
25	CLA	5	611	31	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	WVN	a	407	-	-	9/29/63/63	0/2/2/2
34	LMG	b	620	-	-	6/46/66/70	0/1/1/1
38	II0	Q	617	-	-	1/21/67/67	0/2/2/2
25	CLA	B	604	-	1/1/13/20	11/30/108/115	-
25	CLA	4	607	-	1/1/10/20	3/11/89/115	-
38	II0	Q	619	-	-	5/21/67/67	0/2/2/2
25	CLA	D	400	-	1/1/15/20	10/37/115/115	-
25	CLA	3	611	31	1/1/12/20	6/22/100/115	-
31	LHG	S	621	25	-	12/44/44/53	-
25	CLA	O	611	-	1/1/14/20	15/31/109/115	-
25	CLA	B	614	-	1/1/14/20	11/31/109/115	-
38	II0	P	617	-	-	0/21/67/67	0/2/2/2
38	II0	4	619	-	-	4/21/67/67	0/2/2/2
25	CLA	P	602	19	1/1/14/20	15/34/112/115	-
25	CLA	B	612	-	1/1/15/20	12/37/115/115	-
25	CLA	N	609	23	1/1/11/20	7/15/93/115	-
25	CLA	a	406	-	1/1/14/20	11/31/109/115	-
25	CLA	2	615	-	1/1/11/20	8/13/91/115	-
34	LMG	4	621	-	-	4/38/58/70	0/1/1/1
34	LMG	C	536	-	-	20/42/62/70	0/1/1/1
37	KC2	4	605	-	-	7/15/71/71	-
38	II0	3	619	-	-	6/21/67/67	0/2/2/2
25	CLA	c	523	-	1/1/15/20	12/37/115/115	-
25	CLA	R	609	21	1/1/15/20	10/37/115/115	-
25	CLA	R	602	21	1/1/13/20	12/25/103/115	-
25	CLA	2	602	18	1/1/15/20	16/37/115/115	-
25	CLA	6	602	22	1/1/15/20	17/37/115/115	-
37	KC2	6	606	-	-	8/15/71/71	-
25	CLA	5	609	21	1/1/15/20	10/37/115/115	-
25	CLA	5	602	21	1/1/13/20	12/25/103/115	-
25	CLA	R	615	-	1/1/11/20	5/15/93/115	-
25	CLA	1	606	23	1/1/12/20	6/19/97/115	-
25	CLA	6	615	-	1/1/15/20	10/37/115/115	-
34	LMG	g	303	-	-	8/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	1	603	-	1/1/14/20	9/31/109/115	-

All (2689) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	S	618	II0	C13-C09	-10.77	1.22	1.34
38	6	618	II0	C13-C09	-10.73	1.23	1.34
38	2	619	II0	C13-C09	-10.34	1.23	1.34
38	4	619	II0	C13-C09	-10.32	1.23	1.34
38	O	619	II0	C13-C09	-10.31	1.23	1.34
38	N	619	II0	C13-C09	-10.04	1.23	1.34
38	Q	618	II0	C13-C09	-10.03	1.23	1.34
38	N	618	II0	C13-C09	-10.01	1.23	1.34
38	1	618	II0	C13-C09	-10.01	1.23	1.34
38	R	618	II0	C13-C09	-10.00	1.23	1.34
38	O	618	II0	C13-C09	-10.00	1.23	1.34
38	5	618	II0	C13-C09	-9.99	1.23	1.34
38	4	618	II0	C13-C09	-9.99	1.23	1.34
38	1	616	II0	C13-C09	-9.92	1.23	1.34
38	N	616	II0	C13-C09	-9.89	1.23	1.34
38	Q	617	II0	C13-C09	-9.88	1.23	1.34
38	Q	619	II0	C13-C09	-9.86	1.23	1.34
38	R	617	II0	C13-C09	-9.85	1.23	1.34
38	3	616	II0	C13-C09	-9.84	1.24	1.34
38	4	617	II0	C13-C09	-9.84	1.24	1.34
38	1	619	II0	C13-C09	-9.83	1.24	1.34
38	P	616	II0	C13-C09	-9.82	1.24	1.34
38	5	619	II0	C13-C09	-9.82	1.24	1.34
38	P	619	II0	C13-C09	-9.81	1.24	1.34
38	3	619	II0	C13-C09	-9.80	1.24	1.34
38	4	616	II0	C13-C09	-9.80	1.24	1.34
38	Q	616	II0	C13-C09	-9.79	1.24	1.34
38	5	617	II0	C13-C09	-9.77	1.24	1.34
38	3	618	II0	C13-C09	-9.75	1.24	1.34
38	R	619	II0	C13-C09	-9.74	1.24	1.34
38	2	616	II0	C13-C09	-9.73	1.24	1.34
38	O	616	II0	C13-C09	-9.73	1.24	1.34
38	6	617	II0	C13-C09	-9.71	1.24	1.34
38	O	617	II0	C13-C09	-9.69	1.24	1.34
38	R	616	II0	C13-C09	-9.62	1.24	1.34
38	3	617	II0	C13-C09	-9.60	1.24	1.34
38	S	617	II0	C13-C09	-9.59	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	616	II0	C13-C09	-9.58	1.24	1.34
38	N	617	II0	C13-C09	-9.57	1.24	1.34
38	2	617	II0	C13-C09	-9.55	1.24	1.34
38	P	618	II0	C13-C09	-9.54	1.24	1.34
38	S	619	II0	C13-C09	-9.54	1.24	1.34
38	1	617	II0	C13-C09	-9.54	1.24	1.34
38	S	616	II0	C13-C09	-9.51	1.24	1.34
38	6	616	II0	C13-C09	-9.49	1.24	1.34
38	2	618	II0	C13-C09	-9.48	1.24	1.34
38	P	617	II0	C13-C09	-9.45	1.24	1.34
38	6	619	II0	C13-C09	-9.06	1.24	1.34
37	Q	612	KC2	C4D-ND	8.43	1.42	1.35
37	4	612	KC2	C4D-ND	8.43	1.42	1.35
37	N	613	KC2	C4D-ND	8.23	1.42	1.35
37	1	613	KC2	C4D-ND	8.22	1.42	1.35
37	N	611	KC2	C4D-ND	8.21	1.42	1.35
25	1	607	CLA	C4B-NB	8.17	1.42	1.35
25	N	607	CLA	C4B-NB	8.16	1.42	1.35
37	1	611	KC2	C4D-ND	8.15	1.42	1.35
37	N	613	KC2	C4C-NC	8.10	1.49	1.37
25	D	403	CLA	C4B-NB	8.09	1.42	1.35
25	d	403	CLA	C4B-NB	8.08	1.42	1.35
37	4	605	KC2	C4D-ND	8.08	1.42	1.35
37	Q	605	KC2	C4D-ND	8.07	1.42	1.35
25	b	610	CLA	C4B-NB	8.07	1.42	1.35
25	P	601	CLA	C4B-NB	8.06	1.42	1.35
37	1	613	KC2	C4C-NC	8.05	1.49	1.37
37	2	612	KC2	C4D-ND	8.05	1.42	1.35
25	3	601	CLA	C4B-NB	8.03	1.42	1.35
37	R	612	KC2	C4D-ND	8.03	1.42	1.35
37	O	612	KC2	C4D-ND	8.03	1.42	1.35
25	2	607	CLA	C4B-NB	8.02	1.42	1.35
37	6	612	KC2	C4D-ND	8.01	1.42	1.35
37	S	612	KC2	C4D-ND	8.01	1.42	1.35
37	N	612	KC2	C4D-ND	8.00	1.42	1.35
37	1	612	KC2	C4D-ND	8.00	1.42	1.35
25	d	400	CLA	C4B-NB	7.99	1.42	1.35
25	D	400	CLA	C4B-NB	7.99	1.42	1.35
25	B	610	CLA	C4B-NB	7.98	1.42	1.35
25	c	518	CLA	C4B-NB	7.98	1.42	1.35
25	O	607	CLA	C4B-NB	7.97	1.42	1.35
25	b	613	CLA	C4B-NB	7.96	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	C4B-NB	7.95	1.42	1.35
25	P	610	CLA	C4B-NB	7.95	1.42	1.35
25	b	608	CLA	C4B-NB	7.92	1.42	1.35
25	C	518	CLA	C4B-NB	7.92	1.42	1.35
25	2	610	CLA	C4B-NB	7.92	1.42	1.35
25	B	611	CLA	C4B-NB	7.92	1.42	1.35
25	C	527	CLA	C4B-NB	7.91	1.42	1.35
25	C	526	CLA	C4B-NB	7.91	1.42	1.35
25	R	610	CLA	C4B-NB	7.91	1.42	1.35
25	C	516	CLA	C4B-NB	7.91	1.42	1.35
25	g	301	CLA	C4B-NB	7.91	1.42	1.35
25	S	601	CLA	C4B-NB	7.90	1.42	1.35
25	R	601	CLA	C4B-NB	7.90	1.42	1.35
25	R	606	CLA	C4B-NB	7.90	1.42	1.35
25	c	526	CLA	C4B-NB	7.90	1.42	1.35
25	A	404	CLA	C4B-NB	7.90	1.42	1.35
37	1	611	KC2	C4C-NC	7.90	1.49	1.37
25	O	603	CLA	C4B-NB	7.89	1.42	1.35
37	5	612	KC2	C4D-ND	7.89	1.42	1.35
25	O	604	CLA	C4B-NB	7.89	1.42	1.35
25	5	606	CLA	C4B-NB	7.89	1.42	1.35
37	4	611	KC2	C4D-ND	7.89	1.42	1.35
25	c	516	CLA	C4B-NB	7.88	1.42	1.35
25	b	603	CLA	C4B-NB	7.88	1.42	1.35
25	B	607	CLA	C4B-NB	7.88	1.42	1.35
25	Q	607	CLA	C4B-NB	7.88	1.42	1.35
25	a	404	CLA	C4B-NB	7.88	1.42	1.35
25	B	606	CLA	C4B-NB	7.88	1.42	1.35
25	O	611	CLA	C4B-NB	7.88	1.42	1.35
37	3	606	KC2	C4D-ND	7.88	1.42	1.35
25	b	601	CLA	C4B-NB	7.88	1.42	1.35
25	R	604	CLA	C4B-NB	7.87	1.42	1.35
37	Q	612	KC2	C4C-NC	7.87	1.49	1.37
25	b	611	CLA	C4B-NB	7.86	1.42	1.35
37	Q	605	KC2	C4C-NC	7.86	1.49	1.37
25	b	606	CLA	C4B-NB	7.86	1.42	1.35
25	c	527	CLA	C4B-NB	7.86	1.42	1.35
25	5	610	CLA	C4B-NB	7.85	1.42	1.35
25	6	601	CLA	C4B-NB	7.85	1.42	1.35
25	6	603	CLA	C4B-NB	7.85	1.42	1.35
37	N	611	KC2	C4C-NC	7.85	1.49	1.37
25	N	601	CLA	C4B-NB	7.85	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	612	KC2	C4C-NC	7.85	1.49	1.37
25	5	601	CLA	C4B-NB	7.85	1.42	1.35
25	B	613	CLA	C4B-NB	7.84	1.42	1.35
37	Q	611	KC2	C4D-ND	7.84	1.42	1.35
25	5	611	CLA	C4B-NB	7.84	1.42	1.35
37	4	605	KC2	C4C-NC	7.84	1.49	1.37
25	O	609	CLA	C4B-NB	7.83	1.42	1.35
37	4	612	KC2	C4C-NC	7.83	1.49	1.37
25	C	528	CLA	C4B-NB	7.83	1.42	1.35
25	P	611	CLA	C4B-NB	7.83	1.42	1.35
37	P	606	KC2	C4C-NC	7.83	1.49	1.37
25	R	611	CLA	C4B-NB	7.83	1.42	1.35
25	1	601	CLA	C4B-NB	7.82	1.42	1.35
25	1	610	CLA	C4B-NB	7.82	1.42	1.35
25	N	604	CLA	C4B-NB	7.82	1.42	1.35
25	2	604	CLA	C4B-NB	7.82	1.42	1.35
25	3	610	CLA	C4B-NB	7.81	1.42	1.35
25	3	612	CLA	C4B-NB	7.81	1.42	1.35
25	5	604	CLA	C4B-NB	7.81	1.42	1.35
25	5	609	CLA	C4B-NB	7.81	1.42	1.35
25	O	610	CLA	C4B-NB	7.81	1.42	1.35
37	6	606	KC2	C4C-NC	7.81	1.49	1.37
25	d	404	CLA	C4B-NB	7.81	1.42	1.35
25	C	525	CLA	C4B-NB	7.81	1.42	1.35
25	2	609	CLA	C4B-NB	7.81	1.42	1.35
25	B	609	CLA	C4B-NB	7.81	1.42	1.35
25	4	607	CLA	C4B-NB	7.81	1.42	1.35
25	5	602	CLA	C4B-NB	7.81	1.42	1.35
25	2	603	CLA	C4B-NB	7.80	1.42	1.35
25	N	610	CLA	C4B-NB	7.80	1.42	1.35
37	3	606	KC2	C4C-NC	7.80	1.49	1.37
37	O	612	KC2	C4C-NC	7.80	1.49	1.37
25	R	609	CLA	C4B-NB	7.79	1.42	1.35
25	b	605	CLA	C4B-NB	7.79	1.42	1.35
25	D	404	CLA	C4B-NB	7.79	1.42	1.35
25	c	525	CLA	C4B-NB	7.79	1.42	1.35
25	O	602	CLA	C4B-NB	7.78	1.42	1.35
25	O	613	CLA	C4B-NB	7.78	1.42	1.35
25	2	611	CLA	C4B-NB	7.78	1.42	1.35
37	N	605	KC2	C4D-ND	7.78	1.42	1.35
37	1	605	KC2	C4C-NC	7.78	1.49	1.37
37	N	605	KC2	C4C-NC	7.78	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	612	KC2	C4C-NC	7.77	1.49	1.37
37	4	611	KC2	C4C-NC	7.77	1.49	1.37
25	c	519	CLA	C4B-NB	7.77	1.42	1.35
25	b	614	CLA	C4B-NB	7.77	1.42	1.35
25	1	604	CLA	C4B-NB	7.77	1.42	1.35
25	N	606	CLA	C4B-NB	7.77	1.42	1.35
25	Q	606	CLA	C4B-NB	7.77	1.42	1.35
37	Q	611	KC2	C4C-NC	7.76	1.49	1.37
25	S	611	CLA	C4B-NB	7.76	1.42	1.35
37	P	606	KC2	C4D-ND	7.76	1.42	1.35
25	B	615	CLA	C4B-NB	7.76	1.42	1.35
25	b	609	CLA	C4B-NB	7.76	1.42	1.35
25	c	528	CLA	C4B-NB	7.76	1.42	1.35
25	B	608	CLA	C4B-NB	7.76	1.42	1.35
25	P	613	CLA	C4B-NB	7.76	1.42	1.35
25	2	602	CLA	C4B-NB	7.76	1.42	1.35
25	N	614	CLA	C4B-NB	7.76	1.42	1.35
37	5	612	KC2	C4C-NC	7.76	1.49	1.37
25	b	616	CLA	C4B-NB	7.75	1.42	1.35
25	B	603	CLA	C4B-NB	7.75	1.42	1.35
25	C	523	CLA	C4B-NB	7.75	1.42	1.35
25	a	406	CLA	C4B-NB	7.74	1.42	1.35
25	3	611	CLA	C4B-NB	7.74	1.42	1.35
25	6	611	CLA	C4B-NB	7.74	1.42	1.35
25	1	603	CLA	C4B-NB	7.74	1.42	1.35
37	1	605	KC2	C4D-ND	7.73	1.42	1.35
25	R	602	CLA	C4B-NB	7.73	1.42	1.35
25	A	406	CLA	C4B-NB	7.73	1.42	1.35
25	P	612	CLA	C4B-NB	7.73	1.42	1.35
25	c	523	CLA	C4B-NB	7.73	1.42	1.35
37	S	606	KC2	C4C-NC	7.73	1.49	1.37
25	5	603	CLA	C4B-NB	7.72	1.42	1.35
25	Q	615	CLA	C4B-NB	7.72	1.42	1.35
25	R	613	CLA	C4B-NB	7.72	1.42	1.35
25	4	610	CLA	C4B-NB	7.72	1.42	1.35
37	S	612	KC2	C4C-NC	7.72	1.49	1.37
25	3	613	CLA	C4B-NB	7.72	1.42	1.35
25	2	613	CLA	C4B-NB	7.72	1.42	1.35
25	c	521	CLA	C4B-NB	7.72	1.42	1.35
25	B	614	CLA	C4B-NB	7.72	1.42	1.35
25	1	614	CLA	C4B-NB	7.72	1.42	1.35
25	c	520	CLA	C4B-NB	7.72	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	610	CLA	C4B-NB	7.72	1.42	1.35
25	b	615	CLA	C4B-NB	7.71	1.42	1.35
37	1	612	KC2	C4C-NC	7.71	1.49	1.37
25	C	519	CLA	C4B-NB	7.71	1.42	1.35
25	1	602	CLA	C4B-NB	7.71	1.42	1.35
25	P	603	CLA	C4B-NB	7.71	1.42	1.35
25	5	613	CLA	C4B-NB	7.70	1.42	1.35
25	B	605	CLA	C4B-NB	7.70	1.42	1.35
25	C	521	CLA	C4B-NB	7.70	1.42	1.35
25	4	615	CLA	C4B-NB	7.70	1.42	1.35
25	b	607	CLA	C4B-NB	7.70	1.42	1.35
25	N	602	CLA	C4B-NB	7.70	1.42	1.35
37	N	612	KC2	C4C-NC	7.69	1.49	1.37
25	b	602	CLA	C4B-NB	7.69	1.42	1.35
25	O	601	CLA	C4B-NB	7.69	1.42	1.35
25	1	615	CLA	C4B-NB	7.69	1.42	1.35
25	b	604	CLA	C4B-NB	7.69	1.42	1.35
25	R	615	CLA	C4B-NB	7.68	1.42	1.35
25	R	603	CLA	C4B-NB	7.68	1.42	1.35
25	S	602	CLA	C4B-NB	7.68	1.42	1.35
25	c	524	CLA	C4B-NB	7.68	1.42	1.35
25	Q	604	CLA	C4B-NB	7.68	1.42	1.35
25	N	615	CLA	C4B-NB	7.68	1.42	1.35
25	a	403	CLA	C4B-NB	7.67	1.42	1.35
25	A	403	CLA	C4B-NB	7.67	1.42	1.35
25	2	606	CLA	C4B-NB	7.67	1.42	1.35
25	B	616	CLA	C4B-NB	7.67	1.42	1.35
25	1	606	CLA	C4B-NB	7.66	1.42	1.35
25	C	524	CLA	C4B-NB	7.66	1.42	1.35
37	6	612	KC2	C4C-NC	7.65	1.49	1.37
25	3	603	CLA	C4B-NB	7.65	1.42	1.35
25	B	604	CLA	C4B-NB	7.65	1.42	1.35
25	6	610	CLA	C4B-NB	7.65	1.42	1.35
25	6	602	CLA	C4B-NB	7.64	1.42	1.35
25	C	520	CLA	C4B-NB	7.64	1.42	1.35
37	6	606	KC2	C4D-ND	7.64	1.42	1.35
25	C	517	CLA	C4B-NB	7.63	1.42	1.35
25	4	604	CLA	C4B-NB	7.63	1.42	1.35
25	c	517	CLA	C4B-NB	7.62	1.42	1.35
25	B	602	CLA	C4B-NB	7.62	1.42	1.35
25	2	601	CLA	C4B-NB	7.61	1.42	1.35
25	6	615	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	606	CLA	C4B-NB	7.61	1.42	1.35
25	C	522	CLA	C4B-NB	7.60	1.42	1.35
25	Q	603	CLA	C4B-NB	7.60	1.42	1.35
25	5	615	CLA	C4B-NB	7.60	1.42	1.35
37	S	606	KC2	C4D-ND	7.60	1.42	1.35
25	S	610	CLA	C4B-NB	7.59	1.42	1.35
25	S	615	CLA	C4B-NB	7.59	1.42	1.35
25	4	606	CLA	C4B-NB	7.59	1.42	1.35
25	N	603	CLA	C4B-NB	7.59	1.42	1.35
25	G	302	CLA	C4B-NB	7.59	1.42	1.35
25	P	602	CLA	C4B-NB	7.59	1.42	1.35
25	G	301	CLA	C4B-NB	7.56	1.41	1.35
39	5	620	IHT	C38-C35	7.55	1.45	1.35
25	Q	602	CLA	C4B-NB	7.53	1.41	1.35
25	4	603	CLA	C4B-NB	7.53	1.41	1.35
25	O	615	CLA	C4B-NB	7.53	1.41	1.35
25	3	615	CLA	C4B-NB	7.53	1.41	1.35
25	P	609	CLA	C4B-NB	7.53	1.41	1.35
25	3	602	CLA	C4B-NB	7.52	1.41	1.35
25	P	615	CLA	C4B-NB	7.50	1.41	1.35
25	3	609	CLA	C4B-NB	7.48	1.41	1.35
25	4	609	CLA	C4B-NB	7.48	1.41	1.35
25	2	615	CLA	C4B-NB	7.46	1.41	1.35
25	4	602	CLA	C4B-NB	7.46	1.41	1.35
39	O	620	IHT	C38-C35	7.45	1.45	1.35
39	Q	620	IHT	C38-C35	7.45	1.45	1.35
25	S	603	CLA	C4B-NB	7.45	1.41	1.35
25	S	609	CLA	C4B-NB	7.45	1.41	1.35
39	2	620	IHT	C38-C35	7.44	1.45	1.35
25	6	609	CLA	C4B-NB	7.44	1.41	1.35
25	c	522	CLA	C4B-NB	7.44	1.41	1.35
25	Q	609	CLA	C4B-NB	7.41	1.41	1.35
39	4	620	IHT	C38-C35	7.41	1.45	1.35
25	b	612	CLA	C4B-NB	7.41	1.41	1.35
25	P	604	CLA	C4B-NB	7.38	1.41	1.35
25	6	604	CLA	C4B-NB	7.36	1.41	1.35
25	5	607	CLA	C4B-NB	7.36	1.41	1.35
25	S	613	CLA	C4B-NB	7.36	1.41	1.35
25	1	609	CLA	C4B-NB	7.34	1.41	1.35
25	6	613	CLA	C4B-NB	7.32	1.41	1.35
25	3	604	CLA	C4B-NB	7.32	1.41	1.35
25	S	604	CLA	C4B-NB	7.31	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	620	IHT	C38-C35	7.31	1.45	1.35
25	B	612	CLA	C4B-NB	7.31	1.41	1.35
25	R	607	CLA	C4B-NB	7.31	1.41	1.35
25	4	613	CLA	C4B-NB	7.29	1.41	1.35
25	N	609	CLA	C4B-NB	7.29	1.41	1.35
25	g	302	CLA	C4B-NB	7.25	1.41	1.35
25	Q	613	CLA	C4B-NB	7.23	1.41	1.35
39	1	620	IHT	C38-C35	7.21	1.45	1.35
39	N	620	IHT	C38-C35	7.14	1.45	1.35
37	4	605	KC2	C2A-C3A	5.97	1.49	1.37
37	Q	605	KC2	C2A-C3A	5.97	1.49	1.37
37	S	606	KC2	C2A-C3A	5.95	1.49	1.37
37	6	606	KC2	C2A-C3A	5.88	1.49	1.37
37	1	611	KC2	C2A-C3A	5.87	1.49	1.37
37	4	611	KC2	C2A-C3A	5.87	1.49	1.37
37	Q	611	KC2	C2A-C3A	5.84	1.49	1.37
37	N	611	KC2	C2A-C3A	5.84	1.49	1.37
37	1	613	KC2	C2A-C3A	5.77	1.49	1.37
37	N	613	KC2	C2A-C3A	5.76	1.49	1.37
37	1	613	KC2	OBD-CAD	5.71	1.30	1.22
37	N	605	KC2	C2A-C3A	5.70	1.48	1.37
37	N	613	KC2	OBD-CAD	5.70	1.30	1.22
37	1	605	KC2	C2A-C3A	5.69	1.48	1.37
37	3	606	KC2	CHD-C4C	5.67	1.49	1.35
37	1	613	KC2	CHD-C4C	5.67	1.49	1.35
37	3	606	KC2	C2A-C3A	5.64	1.48	1.37
37	N	613	KC2	CHD-C4C	5.64	1.49	1.35
37	P	606	KC2	CHD-C4C	5.63	1.49	1.35
37	P	606	KC2	C2A-C3A	5.63	1.48	1.37
37	6	606	KC2	CHD-C4C	5.62	1.49	1.35
37	N	605	KC2	CHD-C4C	5.61	1.49	1.35
37	1	605	KC2	CHD-C4C	5.61	1.49	1.35
37	5	612	KC2	C2A-C3A	5.59	1.48	1.37
37	6	612	KC2	C2A-C3A	5.59	1.48	1.37
37	S	612	KC2	C2A-C3A	5.57	1.48	1.37
37	O	612	KC2	CHD-C4C	5.57	1.49	1.35
37	R	612	KC2	C2A-C3A	5.57	1.48	1.37
37	2	612	KC2	CHD-C4C	5.57	1.49	1.35
37	Q	611	KC2	CHD-C4C	5.56	1.49	1.35
37	S	606	KC2	CHD-C4C	5.56	1.49	1.35
37	4	611	KC2	CHD-C4C	5.55	1.49	1.35
37	Q	612	KC2	C2A-C3A	5.54	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	620	IHT	C24-C26	5.54	1.53	1.42
37	5	612	KC2	CHD-C4C	5.53	1.49	1.35
37	Q	605	KC2	CHD-C4C	5.53	1.49	1.35
37	1	611	KC2	CHD-C4C	5.53	1.49	1.35
37	N	611	KC2	CHD-C4C	5.53	1.49	1.35
37	1	612	KC2	C2A-C3A	5.52	1.48	1.37
37	4	605	KC2	CHD-C4C	5.52	1.49	1.35
37	4	612	KC2	C2A-C3A	5.51	1.48	1.37
37	R	612	KC2	CHD-C4C	5.51	1.49	1.35
37	N	612	KC2	C2A-C3A	5.50	1.48	1.37
37	4	612	KC2	CHD-C4C	5.49	1.49	1.35
37	Q	612	KC2	CHD-C4C	5.48	1.49	1.35
37	Q	612	KC2	C1A-NA	5.47	1.48	1.38
37	4	612	KC2	C1A-NA	5.46	1.48	1.38
37	N	612	KC2	CHD-C4C	5.44	1.48	1.35
37	N	613	KC2	C3D-C2D	5.43	1.49	1.39
37	1	612	KC2	CHD-C4C	5.43	1.48	1.35
37	S	612	KC2	OBD-CAD	5.39	1.29	1.22
37	6	612	KC2	CHD-C4C	5.38	1.48	1.35
37	6	606	KC2	OBD-CAD	5.38	1.29	1.22
38	2	619	II0	C24-C26	5.37	1.52	1.42
37	6	612	KC2	OBD-CAD	5.37	1.29	1.22
37	N	605	KC2	OBD-CAD	5.37	1.29	1.22
38	O	619	II0	C24-C26	5.36	1.52	1.42
37	S	612	KC2	CHD-C4C	5.36	1.48	1.35
37	Q	605	KC2	OBD-CAD	5.35	1.29	1.22
37	1	613	KC2	C3D-C2D	5.35	1.49	1.39
37	4	611	KC2	OBD-CAD	5.35	1.29	1.22
37	1	611	KC2	OBD-CAD	5.35	1.29	1.22
37	2	612	KC2	C2A-C3A	5.35	1.48	1.37
37	O	612	KC2	C2A-C3A	5.34	1.48	1.37
37	3	606	KC2	OBD-CAD	5.34	1.29	1.22
37	Q	611	KC2	OBD-CAD	5.33	1.29	1.22
39	1	620	IHT	C24-C26	5.33	1.52	1.42
37	P	606	KC2	OBD-CAD	5.33	1.29	1.22
37	N	612	KC2	OBD-CAD	5.32	1.29	1.22
37	4	605	KC2	OBD-CAD	5.31	1.29	1.22
37	1	612	KC2	OBD-CAD	5.31	1.29	1.22
37	1	605	KC2	OBD-CAD	5.30	1.29	1.22
37	S	606	KC2	OBD-CAD	5.30	1.29	1.22
37	6	612	KC2	C1A-NA	5.29	1.48	1.38
37	1	612	KC2	C1A-NA	5.29	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	611	KC2	OBD-CAD	5.29	1.29	1.22
37	2	612	KC2	OBD-CAD	5.29	1.29	1.22
37	S	612	KC2	C1A-NA	5.29	1.48	1.38
37	5	612	KC2	OBD-CAD	5.27	1.29	1.22
37	1	613	KC2	C3C-C2C	5.27	1.48	1.37
37	N	612	KC2	C1A-NA	5.27	1.48	1.38
38	6	619	II0	C24-C26	5.26	1.52	1.42
38	R	619	II0	C24-C26	5.26	1.52	1.42
38	Q	618	II0	C24-C26	5.25	1.52	1.42
38	4	618	II0	C24-C26	5.25	1.52	1.42
37	6	606	KC2	C1A-NA	5.24	1.48	1.38
38	1	619	II0	C24-C26	5.24	1.52	1.42
37	O	612	KC2	OBD-CAD	5.24	1.29	1.22
38	4	619	II0	C24-C26	5.23	1.52	1.42
37	R	612	KC2	OBD-CAD	5.22	1.29	1.22
38	O	618	II0	C24-C26	5.22	1.52	1.42
38	2	618	II0	C24-C26	5.22	1.52	1.42
37	N	613	KC2	C3C-C2C	5.22	1.47	1.37
38	6	618	II0	C24-C26	5.22	1.52	1.42
38	N	619	II0	C24-C26	5.22	1.52	1.42
37	5	612	KC2	C1A-NA	5.22	1.48	1.38
38	S	616	II0	C24-C26	5.21	1.52	1.42
37	R	612	KC2	C1A-NA	5.21	1.48	1.38
38	5	619	II0	C24-C26	5.21	1.52	1.42
38	S	619	II0	C24-C26	5.21	1.52	1.42
37	O	612	KC2	C1A-NA	5.21	1.48	1.38
37	Q	611	KC2	C1A-NA	5.21	1.48	1.38
38	6	616	II0	C24-C26	5.20	1.52	1.42
38	Q	619	II0	C24-C26	5.20	1.52	1.42
38	N	617	II0	C24-C26	5.20	1.52	1.42
37	Q	612	KC2	OBD-CAD	5.20	1.29	1.22
38	1	618	II0	C24-C26	5.19	1.52	1.42
38	R	616	II0	C24-C26	5.19	1.52	1.42
38	S	618	II0	C24-C26	5.19	1.52	1.42
37	2	612	KC2	C1A-NA	5.19	1.48	1.38
38	N	618	II0	C24-C26	5.18	1.52	1.42
38	2	616	II0	C24-C26	5.18	1.52	1.42
37	4	611	KC2	C1A-NA	5.18	1.48	1.38
37	1	611	KC2	C1A-NA	5.18	1.48	1.38
37	N	605	KC2	C1A-NA	5.18	1.48	1.38
37	N	611	KC2	C1A-NA	5.18	1.48	1.38
37	N	611	KC2	C3C-C2C	5.16	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	3	606	KC2	C1A-NA	5.16	1.48	1.38
37	4	612	KC2	OBD-CAD	5.16	1.29	1.22
38	O	616	II0	C24-C26	5.16	1.52	1.42
38	5	616	II0	C24-C26	5.16	1.52	1.42
37	1	611	KC2	C3C-C2C	5.15	1.47	1.37
38	3	616	II0	C24-C26	5.15	1.52	1.42
37	4	611	KC2	C3C-C2C	5.15	1.47	1.37
38	P	616	II0	C24-C26	5.15	1.52	1.42
37	1	605	KC2	C1A-NA	5.15	1.48	1.38
37	5	612	KC2	C3C-C2C	5.15	1.47	1.37
37	3	606	KC2	C3C-C2C	5.15	1.47	1.37
37	S	606	KC2	C3D-C2D	5.15	1.48	1.39
38	1	617	II0	C24-C26	5.13	1.52	1.42
37	P	606	KC2	C3C-C2C	5.13	1.47	1.37
38	S	617	II0	C24-C26	5.13	1.52	1.42
38	3	618	II0	C24-C26	5.13	1.52	1.42
38	3	619	II0	C24-C26	5.13	1.52	1.42
37	N	612	KC2	C3C-C2C	5.13	1.47	1.37
38	R	618	II0	C24-C26	5.12	1.52	1.42
38	6	617	II0	C24-C26	5.12	1.52	1.42
38	Q	616	II0	C24-C26	5.12	1.52	1.42
39	2	620	IHT	C24-C26	5.12	1.52	1.42
38	4	616	II0	C24-C26	5.12	1.52	1.42
37	P	606	KC2	C1A-NA	5.12	1.48	1.38
38	3	617	II0	C24-C26	5.12	1.52	1.42
38	4	617	II0	C24-C26	5.12	1.52	1.42
37	Q	611	KC2	C3C-C2C	5.12	1.47	1.37
37	S	612	KC2	C3C-C2C	5.12	1.47	1.37
37	R	612	KC2	C3C-C2C	5.11	1.47	1.37
37	2	612	KC2	C3C-C2C	5.11	1.47	1.37
37	S	606	KC2	C1A-NA	5.11	1.48	1.38
37	6	612	KC2	C3C-C2C	5.11	1.47	1.37
37	1	612	KC2	C3C-C2C	5.11	1.47	1.37
38	N	616	II0	C24-C26	5.11	1.52	1.42
38	P	619	II0	C24-C26	5.11	1.52	1.42
38	P	618	II0	C24-C26	5.10	1.52	1.42
38	Q	617	II0	C24-C26	5.10	1.52	1.42
38	5	617	II0	C24-C26	5.10	1.52	1.42
38	5	618	II0	C24-C26	5.10	1.52	1.42
38	R	617	II0	C24-C26	5.09	1.52	1.42
37	2	612	KC2	C3B-C2B	5.08	1.47	1.37
37	S	606	KC2	C3C-C2C	5.08	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	P	617	II0	C24-C26	5.08	1.52	1.42
37	O	612	KC2	C3C-C2C	5.07	1.47	1.37
38	1	616	II0	C24-C26	5.06	1.52	1.42
39	Q	620	IHT	C24-C26	5.06	1.52	1.42
37	1	613	KC2	C3B-C2B	5.06	1.47	1.37
37	N	612	KC2	C3B-C2B	5.06	1.47	1.37
37	O	612	KC2	C3B-C2B	5.05	1.47	1.37
37	Q	612	KC2	C3C-C2C	5.05	1.47	1.37
37	N	613	KC2	C3B-C2B	5.05	1.47	1.37
37	3	606	KC2	C3D-C2D	5.05	1.48	1.39
37	4	605	KC2	C1A-NA	5.05	1.47	1.38
37	Q	605	KC2	C1A-NA	5.05	1.47	1.38
37	4	612	KC2	C3C-C2C	5.04	1.47	1.37
39	O	620	IHT	C24-C26	5.04	1.52	1.42
39	4	620	IHT	C24-C26	5.03	1.52	1.42
37	R	612	KC2	C3B-C2B	5.03	1.47	1.37
37	Q	605	KC2	C3D-C2D	5.03	1.48	1.39
37	6	606	KC2	C3D-C2D	5.03	1.48	1.39
39	2	620	IHT	C21-C11	5.03	1.53	1.42
38	1	619	II0	C21-C09	5.03	1.53	1.42
37	6	606	KC2	C3C-C2C	5.03	1.47	1.37
38	O	617	II0	C21-C09	5.03	1.53	1.42
38	2	617	II0	C21-C09	5.02	1.53	1.42
37	1	612	KC2	C3B-C2B	5.02	1.47	1.37
37	4	605	KC2	C3C-C2C	5.02	1.47	1.37
37	P	606	KC2	C3D-C2D	5.02	1.48	1.39
38	O	617	II0	C24-C26	5.01	1.52	1.42
37	4	605	KC2	C3D-C2D	5.01	1.48	1.39
37	1	611	KC2	C3D-C2D	5.01	1.48	1.39
38	N	619	II0	C21-C09	5.00	1.52	1.42
37	4	611	KC2	C3D-C2D	5.00	1.48	1.39
37	Q	605	KC2	C3C-C2C	4.99	1.47	1.37
39	N	620	IHT	C21-C11	4.99	1.52	1.42
38	4	619	II0	C21-C09	4.99	1.52	1.42
39	Q	620	IHT	C21-C11	4.99	1.52	1.42
38	S	619	II0	C21-C09	4.98	1.52	1.42
38	S	616	II0	C21-C09	4.98	1.52	1.42
37	N	605	KC2	C3C-C2C	4.98	1.47	1.37
37	N	611	KC2	C3D-C2D	4.98	1.48	1.39
37	1	605	KC2	C3C-C2C	4.97	1.47	1.37
38	O	619	II0	C21-C09	4.97	1.52	1.42
37	Q	611	KC2	C3D-C2D	4.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	2	617	II0	C24-C26	4.97	1.52	1.42
38	P	618	II0	C21-C09	4.97	1.52	1.42
38	3	619	II0	C21-C09	4.97	1.52	1.42
38	O	618	II0	C21-C09	4.96	1.52	1.42
37	5	612	KC2	C3B-C2B	4.96	1.47	1.37
38	2	619	II0	C21-C09	4.95	1.52	1.42
37	Q	605	KC2	C3B-C2B	4.95	1.47	1.37
38	P	619	II0	C21-C09	4.95	1.52	1.42
37	S	612	KC2	C3B-C2B	4.94	1.47	1.37
37	6	612	KC2	C3B-C2B	4.94	1.47	1.37
38	3	617	II0	C21-C09	4.94	1.52	1.42
37	5	612	KC2	C3D-C2D	4.94	1.48	1.39
37	N	613	KC2	C1A-NA	4.94	1.47	1.38
38	R	619	II0	C21-C09	4.93	1.52	1.42
38	3	618	II0	C21-C09	4.93	1.52	1.42
37	1	613	KC2	C1A-NA	4.92	1.47	1.38
38	5	616	II0	C21-C09	4.92	1.52	1.42
38	5	619	II0	C21-C09	4.92	1.52	1.42
39	1	620	IHT	C21-C11	4.92	1.52	1.42
37	4	612	KC2	C3D-C2D	4.92	1.48	1.39
37	R	612	KC2	C3D-C2D	4.91	1.48	1.39
38	6	616	II0	C21-C09	4.91	1.52	1.42
38	1	618	II0	C21-C09	4.91	1.52	1.42
38	4	618	II0	C21-C09	4.90	1.52	1.42
37	4	605	KC2	C3B-C2B	4.90	1.47	1.37
38	5	618	II0	C21-C09	4.89	1.52	1.42
38	R	616	II0	C21-C09	4.89	1.52	1.42
39	O	620	IHT	C21-C11	4.89	1.52	1.42
38	6	619	II0	C21-C09	4.89	1.52	1.42
38	Q	619	II0	C21-C09	4.88	1.52	1.42
38	4	616	II0	C21-C09	4.88	1.52	1.42
38	2	616	II0	C21-C09	4.88	1.52	1.42
38	S	618	II0	C21-C09	4.88	1.52	1.42
38	P	617	II0	C21-C09	4.88	1.52	1.42
38	N	618	II0	C21-C09	4.88	1.52	1.42
38	6	618	II0	C21-C09	4.87	1.52	1.42
37	4	611	KC2	C3B-C2B	4.87	1.47	1.37
37	Q	611	KC2	C3B-C2B	4.87	1.47	1.37
37	Q	612	KC2	C3D-C2D	4.87	1.48	1.39
38	N	616	II0	C21-C09	4.87	1.52	1.42
37	4	612	KC2	C3B-C2B	4.86	1.47	1.37
38	2	618	II0	C21-C09	4.86	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	605	KC2	C3D-C2D	4.86	1.48	1.39
38	Q	618	II0	C21-C09	4.86	1.52	1.42
38	6	617	II0	C21-C09	4.86	1.52	1.42
39	5	620	IHT	C24-C26	4.86	1.51	1.42
37	S	606	KC2	C3B-C2B	4.85	1.47	1.37
38	1	616	II0	C21-C09	4.85	1.52	1.42
37	2	612	KC2	C3D-C2D	4.85	1.48	1.39
37	1	612	KC2	C3D-C2D	4.85	1.48	1.39
37	N	605	KC2	C3D-C2D	4.85	1.48	1.39
38	N	617	II0	C21-C09	4.85	1.52	1.42
38	R	618	II0	C21-C09	4.85	1.52	1.42
38	Q	616	II0	C21-C09	4.84	1.52	1.42
38	S	617	II0	C21-C09	4.84	1.52	1.42
37	Q	612	KC2	C3B-C2B	4.84	1.47	1.37
38	O	616	II0	C21-C09	4.84	1.52	1.42
38	1	617	II0	C21-C09	4.82	1.52	1.42
37	N	612	KC2	C3D-C2D	4.82	1.48	1.39
37	6	606	KC2	C3B-C2B	4.82	1.47	1.37
37	P	606	KC2	C3B-C2B	4.82	1.47	1.37
37	1	611	KC2	C3B-C2B	4.82	1.47	1.37
37	O	612	KC2	C3D-C2D	4.81	1.48	1.39
38	4	617	II0	C21-C09	4.81	1.52	1.42
37	1	605	KC2	O2D-CGD	4.80	1.44	1.33
38	P	616	II0	C21-C09	4.80	1.52	1.42
38	R	617	II0	C21-C09	4.79	1.52	1.42
39	4	620	IHT	C21-C11	4.79	1.52	1.42
37	3	606	KC2	C3B-C2B	4.78	1.47	1.37
38	Q	617	II0	C21-C09	4.78	1.52	1.42
37	N	611	KC2	C3B-C2B	4.78	1.47	1.37
37	S	612	KC2	C3D-C2D	4.78	1.48	1.39
38	3	616	II0	C21-C09	4.78	1.52	1.42
38	5	617	II0	C21-C09	4.77	1.52	1.42
37	1	613	KC2	O2D-CGD	4.76	1.44	1.33
37	6	612	KC2	C3D-C2D	4.75	1.48	1.39
37	N	613	KC2	O2D-CGD	4.75	1.44	1.33
39	5	620	IHT	C21-C11	4.75	1.52	1.42
38	4	619	II0	C20-C14	-4.74	1.43	1.50
38	Q	619	II0	C20-C14	-4.74	1.43	1.50
37	N	605	KC2	O2D-CGD	4.74	1.44	1.33
38	R	619	II0	C20-C14	-4.74	1.43	1.50
39	R	620	IHT	C24-C26	4.73	1.51	1.42
37	6	606	KC2	CHB-C1B	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	606	KC2	CHB-C1B	4.71	1.47	1.38
38	Q	616	II0	C20-C14	-4.70	1.43	1.50
38	4	616	II0	C20-C14	-4.70	1.43	1.50
38	S	619	II0	C20-C14	-4.68	1.43	1.50
37	4	612	KC2	O2D-CGD	4.68	1.44	1.33
37	R	612	KC2	O2D-CGD	4.67	1.44	1.33
37	Q	612	KC2	O2D-CGD	4.67	1.44	1.33
38	5	619	II0	C20-C14	-4.67	1.43	1.50
37	3	606	KC2	O2D-CGD	4.67	1.44	1.33
37	N	611	KC2	O2D-CGD	4.67	1.44	1.33
38	3	619	II0	C20-C14	-4.66	1.43	1.50
38	6	619	II0	C20-C14	-4.66	1.43	1.50
38	N	619	II0	C20-C14	-4.65	1.43	1.50
38	1	618	II0	C20-C14	-4.65	1.43	1.50
37	1	611	KC2	O2D-CGD	4.65	1.44	1.33
38	P	619	II0	C20-C14	-4.64	1.43	1.50
37	S	612	KC2	O2D-CGD	4.64	1.44	1.33
37	4	605	KC2	O2D-CGD	4.64	1.44	1.33
37	S	606	KC2	O2D-CGD	4.64	1.44	1.33
37	1	612	KC2	O2D-CGD	4.63	1.44	1.33
37	Q	611	KC2	O2D-CGD	4.63	1.44	1.33
38	1	619	II0	C20-C14	-4.63	1.43	1.50
39	R	620	IHT	C21-C11	4.63	1.52	1.42
37	N	612	KC2	O2D-CGD	4.63	1.44	1.33
37	N	605	KC2	C3B-C2B	4.63	1.46	1.37
37	P	606	KC2	O2D-CGD	4.63	1.44	1.33
28	a	408	SQD	O8-S	4.63	1.64	1.47
28	A	408	SQD	O8-S	4.63	1.64	1.47
37	6	612	KC2	O2D-CGD	4.63	1.44	1.33
37	Q	605	KC2	O2D-CGD	4.63	1.44	1.33
38	P	617	II0	C20-C14	-4.62	1.43	1.50
28	a	411	SQD	O8-S	4.62	1.63	1.47
37	5	612	KC2	O2D-CGD	4.62	1.44	1.33
38	2	619	II0	C20-C14	-4.62	1.43	1.50
37	6	606	KC2	O2D-CGD	4.62	1.44	1.33
28	A	411	SQD	O8-S	4.62	1.63	1.47
38	3	618	II0	C20-C14	-4.61	1.43	1.50
38	Q	617	II0	C20-C14	-4.61	1.43	1.50
38	6	616	II0	C20-C14	-4.61	1.43	1.50
37	2	612	KC2	O2D-CGD	4.61	1.44	1.33
38	1	617	II0	C20-C14	-4.61	1.43	1.50
38	2	618	II0	C20-C14	-4.61	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	616	II0	C20-C14	-4.61	1.43	1.50
38	S	616	II0	C20-C14	-4.61	1.43	1.50
37	4	611	KC2	O2D-CGD	4.61	1.44	1.33
38	3	617	II0	C20-C14	-4.61	1.43	1.50
38	O	619	II0	C20-C14	-4.61	1.43	1.50
38	N	618	II0	C20-C14	-4.60	1.43	1.50
37	1	605	KC2	C3B-C2B	4.60	1.46	1.37
38	4	617	II0	C20-C14	-4.60	1.43	1.50
38	2	616	II0	C20-C14	-4.60	1.43	1.50
37	1	613	KC2	CHB-C1B	4.60	1.47	1.38
38	N	617	II0	C20-C14	-4.59	1.43	1.50
38	5	617	II0	C20-C14	-4.59	1.43	1.50
38	O	616	II0	C20-C14	-4.59	1.43	1.50
38	R	616	II0	C20-C14	-4.59	1.43	1.50
38	Q	618	II0	C20-C14	-4.59	1.43	1.50
38	O	618	II0	C20-C14	-4.59	1.43	1.50
37	N	613	KC2	CHB-C1B	4.58	1.47	1.38
38	P	616	II0	C20-C14	-4.58	1.43	1.50
37	O	612	KC2	O2D-CGD	4.58	1.44	1.33
38	O	617	II0	C20-C14	-4.58	1.43	1.50
38	3	616	II0	C20-C14	-4.57	1.43	1.50
38	4	618	II0	C20-C14	-4.57	1.43	1.50
38	5	618	II0	C20-C14	-4.57	1.43	1.50
38	S	618	II0	C20-C14	-4.57	1.43	1.50
38	P	618	II0	C20-C14	-4.57	1.43	1.50
38	6	617	II0	C20-C14	-4.56	1.43	1.50
38	2	617	II0	C20-C14	-4.56	1.43	1.50
38	6	618	II0	C20-C14	-4.56	1.43	1.50
38	N	616	II0	C20-C14	-4.56	1.43	1.50
38	S	617	II0	C20-C14	-4.56	1.43	1.50
38	R	618	II0	C20-C14	-4.55	1.43	1.50
38	5	616	II0	C20-C14	-4.55	1.43	1.50
38	R	617	II0	C20-C14	-4.53	1.43	1.50
34	Q	621	LMG	O7-C10	4.49	1.47	1.34
34	4	621	LMG	O7-C10	4.47	1.46	1.34
31	Z	103	LHG	O7-C7	4.42	1.46	1.34
31	z	103	LHG	O7-C7	4.40	1.46	1.34
37	4	605	KC2	CHB-C1B	4.37	1.46	1.38
37	Q	605	KC2	CHB-C1B	4.36	1.46	1.38
37	N	605	KC2	CHB-C1B	4.32	1.46	1.38
37	1	605	KC2	CHB-C1B	4.32	1.46	1.38
34	Z	102	LMG	O8-C28	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	99	LMG	O8-C28	4.31	1.45	1.33
34	Q	621	LMG	O8-C28	4.30	1.45	1.33
34	O	622	LMG	O8-C28	4.30	1.45	1.33
34	2	622	LMG	O8-C28	4.29	1.45	1.33
34	4	621	LMG	O8-C28	4.29	1.45	1.33
34	z	102	LMG	O8-C28	4.29	1.45	1.33
31	P	621	LHG	O8-C23	4.28	1.45	1.33
34	F	99	LMG	O8-C28	4.28	1.45	1.33
34	B	620	LMG	O8-C28	4.27	1.45	1.33
31	3	621	LHG	O8-C23	4.27	1.45	1.33
34	D	402	LMG	O8-C28	4.27	1.45	1.33
34	b	620	LMG	O8-C28	4.26	1.45	1.33
34	g	303	LMG	O8-C28	4.26	1.45	1.33
31	2	621	LHG	O8-C23	4.26	1.45	1.33
35	H	90	DGD	O1G-C1A	4.26	1.45	1.33
34	D	407	LMG	O8-C28	4.26	1.45	1.33
37	1	605	KC2	CHC-C4B	4.25	1.46	1.38
34	d	402	LMG	O8-C28	4.25	1.45	1.33
31	O	621	LHG	O8-C23	4.25	1.45	1.33
37	R	612	KC2	CHB-C1B	4.25	1.46	1.38
31	R	621	LHG	O8-C23	4.25	1.45	1.33
31	S	621	LHG	O8-C23	4.25	1.45	1.33
28	A	411	SQD	O48-C23	4.25	1.45	1.33
37	5	612	KC2	CHB-C1B	4.24	1.46	1.38
31	5	621	LHG	O8-C23	4.24	1.45	1.33
31	c	535	LHG	O8-C23	4.24	1.45	1.33
31	6	621	LHG	O8-C23	4.24	1.45	1.33
31	l	101	LHG	O8-C23	4.24	1.45	1.33
37	3	606	KC2	CHB-C1B	4.24	1.46	1.38
34	G	303	LMG	O8-C28	4.24	1.45	1.33
35	h	90	DGD	O1G-C1A	4.23	1.45	1.33
31	L	101	LHG	O8-C23	4.23	1.45	1.33
31	B	622	LHG	O8-C23	4.23	1.45	1.33
37	N	611	KC2	CHB-C1B	4.23	1.46	1.38
37	1	611	KC2	CHB-C1B	4.23	1.46	1.38
34	d	407	LMG	O8-C28	4.22	1.45	1.33
34	M	101	LMG	O8-C28	4.22	1.45	1.33
31	A	413	LHG	O8-C23	4.22	1.45	1.33
37	Q	612	KC2	CHC-C4B	4.22	1.46	1.38
31	b	622	LHG	O7-C7	4.22	1.46	1.34
28	a	411	SQD	O48-C23	4.21	1.45	1.33
37	2	612	KC2	CHB-C1B	4.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	605	KC2	CHC-C4B	4.21	1.46	1.38
31	a	413	LHG	O8-C23	4.21	1.45	1.33
35	c	532	DGD	O1G-C1A	4.20	1.45	1.33
31	d	406	LHG	O8-C23	4.20	1.45	1.33
28	a	408	SQD	O48-C23	4.20	1.45	1.33
34	m	101	LMG	O8-C28	4.20	1.45	1.33
37	4	612	KC2	CHC-C4B	4.19	1.46	1.38
31	Z	103	LHG	O8-C23	4.19	1.45	1.33
37	O	612	KC2	CHB-C1B	4.19	1.46	1.38
37	4	611	KC2	CHB-C1B	4.19	1.46	1.38
37	P	606	KC2	CHB-C1B	4.18	1.46	1.38
34	W	134	LMG	O8-C28	4.18	1.45	1.33
28	A	408	SQD	O48-C23	4.18	1.45	1.33
31	D	406	LHG	O8-C23	4.18	1.45	1.33
31	z	103	LHG	O8-C23	4.17	1.45	1.33
34	C	536	LMG	O8-C28	4.17	1.45	1.33
31	c	535	LHG	O7-C7	4.17	1.46	1.34
34	w	134	LMG	O7-C10	4.17	1.46	1.34
34	z	102	LMG	O7-C10	4.17	1.46	1.34
37	Q	611	KC2	CHB-C1B	4.17	1.46	1.38
37	4	612	KC2	CBC-CAC	4.17	1.50	1.30
34	O	622	LMG	O7-C10	4.17	1.46	1.34
37	1	613	KC2	CBC-CAC	4.17	1.50	1.30
35	c	532	DGD	O2G-C1B	4.16	1.46	1.34
25	4	603	CLA	C1D-ND	4.16	1.42	1.37
37	N	611	KC2	CBC-CAC	4.16	1.50	1.30
31	2	621	LHG	O7-C7	4.16	1.46	1.34
37	Q	605	KC2	CBC-CAC	4.16	1.50	1.30
37	N	613	KC2	CBC-CAC	4.16	1.50	1.30
37	N	605	KC2	CBC-CAC	4.16	1.50	1.30
37	1	611	KC2	CBC-CAC	4.16	1.50	1.30
37	2	612	KC2	CHC-C4B	4.16	1.46	1.38
37	3	606	KC2	CBC-CAC	4.16	1.50	1.30
37	4	605	KC2	CBC-CAC	4.16	1.50	1.30
34	Z	102	LMG	O7-C10	4.15	1.46	1.34
35	C	532	DGD	O1G-C1A	4.15	1.45	1.33
31	a	413	LHG	O7-C7	4.15	1.46	1.34
37	Q	612	KC2	CBC-CAC	4.15	1.50	1.30
34	2	622	LMG	O7-C10	4.15	1.46	1.34
37	Q	611	KC2	CBC-CAC	4.15	1.50	1.30
37	P	606	KC2	CBC-CAC	4.15	1.50	1.30
34	w	134	LMG	O8-C28	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	603	CLA	C1D-ND	4.15	1.42	1.37
37	5	612	KC2	CBC-CAC	4.14	1.50	1.30
29	A	409	PL9	C7-C3	-4.14	1.47	1.51
37	1	605	KC2	CBC-CAC	4.14	1.50	1.30
37	R	612	KC2	CBC-CAC	4.14	1.50	1.30
34	F	99	LMG	O7-C10	4.14	1.46	1.34
31	O	621	LHG	O7-C7	4.14	1.46	1.34
37	S	612	KC2	CBC-CAC	4.14	1.50	1.30
34	f	99	LMG	O7-C10	4.13	1.46	1.34
25	Q	603	CLA	C1D-ND	4.13	1.42	1.37
31	L	101	LHG	O7-C7	4.13	1.46	1.34
31	A	413	LHG	O7-C7	4.13	1.46	1.34
37	4	611	KC2	CBC-CAC	4.13	1.50	1.30
34	c	536	LMG	O8-C28	4.13	1.45	1.33
37	N	612	KC2	CBC-CAC	4.13	1.50	1.30
37	O	612	KC2	CBC-CAC	4.13	1.50	1.30
34	W	134	LMG	O7-C10	4.13	1.45	1.34
25	4	607	CLA	C1D-ND	4.12	1.42	1.37
37	O	612	KC2	CHC-C4B	4.12	1.46	1.38
37	S	612	KC2	CHB-C1B	4.12	1.46	1.38
29	a	409	PL9	C7-C3	-4.12	1.47	1.51
37	6	612	KC2	CBC-CAC	4.12	1.50	1.30
34	d	402	LMG	O7-C10	4.12	1.45	1.34
37	2	612	KC2	CBC-CAC	4.12	1.50	1.30
31	C	535	LHG	O7-C7	4.11	1.45	1.34
37	1	612	KC2	CBC-CAC	4.11	1.50	1.30
37	P	606	KC2	CHC-C4B	4.11	1.46	1.38
28	A	408	SQD	O47-C7	4.11	1.45	1.34
31	S	621	LHG	O7-C7	4.11	1.45	1.34
34	C	536	LMG	O7-C10	4.11	1.45	1.34
35	h	90	DGD	O2G-C1B	4.11	1.45	1.34
37	6	612	KC2	CHB-C1B	4.10	1.46	1.38
31	5	621	LHG	O7-C7	4.10	1.45	1.34
37	3	606	KC2	CHC-C4B	4.10	1.46	1.38
28	a	408	SQD	O47-C7	4.10	1.45	1.34
31	l	101	LHG	O7-C7	4.10	1.45	1.34
34	B	620	LMG	O7-C10	4.10	1.45	1.34
35	C	532	DGD	O2G-C1B	4.10	1.45	1.34
31	C	535	LHG	O8-C23	4.09	1.45	1.33
37	4	611	KC2	CHC-C4B	4.09	1.46	1.38
31	6	621	LHG	O7-C7	4.09	1.45	1.34
34	d	407	LMG	O7-C10	4.09	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	6	606	KC2	CHC-C4B	4.09	1.46	1.38
34	D	402	LMG	O7-C10	4.09	1.45	1.34
34	c	536	LMG	O7-C10	4.09	1.45	1.34
34	D	407	LMG	O7-C10	4.09	1.45	1.34
34	b	620	LMG	O7-C10	4.09	1.45	1.34
31	B	622	LHG	O7-C7	4.09	1.45	1.34
25	C	526	CLA	C1D-ND	4.09	1.42	1.37
31	R	621	LHG	O7-C7	4.09	1.45	1.34
25	Q	607	CLA	C1D-ND	4.08	1.42	1.37
25	c	526	CLA	C1D-ND	4.08	1.42	1.37
25	R	601	CLA	C1D-ND	4.08	1.42	1.37
37	N	612	KC2	CHB-C1B	4.08	1.46	1.38
28	a	411	SQD	O47-C7	4.08	1.45	1.34
35	H	90	DGD	O2G-C1B	4.08	1.45	1.34
37	6	606	KC2	CBC-CAC	4.07	1.50	1.30
37	1	612	KC2	CHB-C1B	4.07	1.46	1.38
37	R	612	KC2	CHC-C4B	4.06	1.46	1.38
28	A	411	SQD	O47-C7	4.06	1.45	1.34
25	2	603	CLA	C1D-ND	4.06	1.42	1.37
31	b	622	LHG	O8-C23	4.06	1.45	1.33
25	b	605	CLA	C1D-ND	4.06	1.42	1.37
34	G	303	LMG	O7-C10	4.06	1.45	1.34
37	Q	611	KC2	CHC-C4B	4.06	1.46	1.38
37	S	612	KC2	CHC-C4B	4.06	1.46	1.38
25	N	601	CLA	C1D-ND	4.06	1.42	1.37
37	1	612	KC2	CHC-C4B	4.06	1.46	1.38
37	5	612	KC2	CHC-C4B	4.06	1.46	1.38
31	3	621	LHG	O7-C7	4.05	1.45	1.34
31	D	406	LHG	O7-C7	4.05	1.45	1.34
25	O	607	CLA	C1D-ND	4.05	1.42	1.37
31	d	406	LHG	O7-C7	4.05	1.45	1.34
25	A	404	CLA	C1D-ND	4.04	1.42	1.37
37	6	612	KC2	CHC-C4B	4.04	1.46	1.38
37	S	606	KC2	CBC-CAC	4.04	1.50	1.30
25	b	610	CLA	C1D-ND	4.04	1.42	1.37
34	g	303	LMG	O7-C10	4.04	1.45	1.34
25	R	606	CLA	C1D-ND	4.04	1.42	1.37
25	1	603	CLA	C1D-ND	4.04	1.42	1.37
34	m	101	LMG	O7-C10	4.04	1.45	1.34
25	c	518	CLA	C1D-ND	4.04	1.42	1.37
25	B	615	CLA	C1D-ND	4.04	1.42	1.37
34	M	101	LMG	O7-C10	4.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	606	CLA	C1D-ND	4.03	1.42	1.37
25	2	611	CLA	C1D-ND	4.03	1.42	1.37
25	1	604	CLA	C1D-ND	4.03	1.42	1.37
31	P	621	LHG	O7-C7	4.03	1.45	1.34
25	P	609	CLA	C1D-ND	4.02	1.42	1.37
37	N	612	KC2	CHC-C4B	4.02	1.46	1.38
37	1	613	KC2	CHC-C4B	4.02	1.46	1.38
25	N	615	CLA	C1D-ND	4.02	1.42	1.37
25	R	604	CLA	C1D-ND	4.02	1.42	1.37
37	4	605	KC2	CHC-C4B	4.02	1.46	1.38
25	D	404	CLA	C1D-ND	4.02	1.42	1.37
25	c	516	CLA	C1D-ND	4.01	1.42	1.37
25	5	601	CLA	C1D-ND	4.01	1.42	1.37
25	O	604	CLA	C1D-ND	4.01	1.42	1.37
25	N	604	CLA	C1D-ND	4.01	1.42	1.37
37	N	613	KC2	CHC-C4B	4.01	1.46	1.38
25	b	615	CLA	C1D-ND	4.01	1.42	1.37
37	S	606	KC2	CHC-C4B	4.00	1.46	1.38
25	P	603	CLA	C1D-ND	4.00	1.42	1.37
25	2	606	CLA	C1D-ND	4.00	1.42	1.37
25	O	601	CLA	C1D-ND	4.00	1.42	1.37
25	B	614	CLA	C1D-ND	4.00	1.42	1.37
25	2	604	CLA	C1D-ND	4.00	1.42	1.37
25	6	611	CLA	C1D-ND	4.00	1.42	1.37
25	B	604	CLA	C1D-ND	4.00	1.42	1.37
25	B	608	CLA	C1D-ND	3.99	1.42	1.37
25	2	601	CLA	C1D-ND	3.99	1.42	1.37
25	2	609	CLA	C1D-ND	3.99	1.42	1.37
37	N	611	KC2	CHC-C4B	3.99	1.46	1.38
25	C	516	CLA	C1D-ND	3.99	1.42	1.37
25	3	603	CLA	C1D-ND	3.99	1.42	1.37
25	O	611	CLA	C1D-ND	3.99	1.42	1.37
25	P	601	CLA	C1D-ND	3.99	1.42	1.37
25	c	524	CLA	C1D-ND	3.99	1.42	1.37
25	1	601	CLA	C1D-ND	3.99	1.42	1.37
25	B	606	CLA	C1D-ND	3.99	1.42	1.37
25	2	607	CLA	C1D-ND	3.99	1.42	1.37
25	6	601	CLA	C1D-ND	3.98	1.42	1.37
25	d	400	CLA	C1D-ND	3.98	1.42	1.37
25	5	606	CLA	C1D-ND	3.98	1.42	1.37
25	B	605	CLA	C1D-ND	3.98	1.42	1.37
25	B	601	CLA	C1D-ND	3.98	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	C1D-ND	3.98	1.42	1.37
25	R	603	CLA	C1D-ND	3.98	1.42	1.37
25	a	404	CLA	C1D-ND	3.98	1.42	1.37
25	5	604	CLA	C1D-ND	3.98	1.42	1.37
25	B	616	CLA	C1D-ND	3.97	1.42	1.37
25	D	400	CLA	C1D-ND	3.97	1.42	1.37
25	3	609	CLA	C1D-ND	3.97	1.42	1.37
25	B	602	CLA	C1D-ND	3.97	1.42	1.37
25	N	610	CLA	C1D-ND	3.97	1.42	1.37
37	Q	605	KC2	CHC-C4B	3.97	1.46	1.38
25	b	602	CLA	C1D-ND	3.97	1.42	1.37
25	N	603	CLA	C1D-ND	3.97	1.42	1.37
25	C	518	CLA	C1D-ND	3.97	1.42	1.37
25	b	608	CLA	C1D-ND	3.96	1.42	1.37
25	2	610	CLA	C1D-ND	3.96	1.42	1.37
25	c	528	CLA	C1D-ND	3.96	1.42	1.37
25	5	603	CLA	C1D-ND	3.96	1.42	1.37
25	C	522	CLA	C1D-ND	3.96	1.42	1.37
25	4	604	CLA	C1D-ND	3.96	1.42	1.37
25	3	610	CLA	C1D-ND	3.95	1.42	1.37
25	b	613	CLA	C1D-ND	3.95	1.42	1.37
25	b	601	CLA	C1D-ND	3.95	1.42	1.37
25	P	604	CLA	C1D-ND	3.95	1.42	1.37
25	R	610	CLA	C1D-ND	3.95	1.42	1.37
25	c	519	CLA	C1D-ND	3.95	1.42	1.37
25	O	609	CLA	C1D-ND	3.95	1.42	1.37
25	O	606	CLA	C1D-ND	3.95	1.42	1.37
25	N	606	CLA	C1D-ND	3.94	1.42	1.37
25	4	602	CLA	C1D-ND	3.94	1.42	1.37
37	4	612	KC2	CHB-C1B	3.94	1.46	1.38
25	C	524	CLA	C1D-ND	3.94	1.42	1.37
37	Q	612	KC2	CHB-C1B	3.94	1.46	1.38
25	S	611	CLA	C1D-ND	3.94	1.42	1.37
25	1	606	CLA	C1D-ND	3.94	1.42	1.37
25	Q	606	CLA	C1D-ND	3.94	1.42	1.37
25	c	527	CLA	C1D-ND	3.94	1.42	1.37
25	3	612	CLA	C1D-ND	3.94	1.42	1.37
25	O	610	CLA	C1D-ND	3.94	1.42	1.37
25	Q	604	CLA	C1D-ND	3.94	1.42	1.37
25	c	522	CLA	C1D-ND	3.93	1.42	1.37
25	5	610	CLA	C1D-ND	3.93	1.42	1.37
25	Q	613	CLA	C1D-ND	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	519	CLA	C1D-ND	3.93	1.42	1.37
25	Q	610	CLA	C1D-ND	3.93	1.42	1.37
25	6	602	CLA	C1D-ND	3.93	1.42	1.37
25	1	615	CLA	C1D-ND	3.93	1.42	1.37
25	P	610	CLA	C1D-ND	3.93	1.42	1.37
37	1	611	KC2	CHC-C4B	3.93	1.46	1.38
25	S	610	CLA	C1D-ND	3.93	1.42	1.37
25	g	301	CLA	C1D-ND	3.93	1.42	1.37
25	O	602	CLA	C1D-ND	3.93	1.42	1.37
25	1	610	CLA	C1D-ND	3.93	1.42	1.37
25	3	604	CLA	C1D-ND	3.93	1.42	1.37
25	b	609	CLA	C1D-ND	3.92	1.42	1.37
25	b	616	CLA	C1D-ND	3.92	1.42	1.37
25	4	613	CLA	C1D-ND	3.92	1.42	1.37
25	P	611	CLA	C1D-ND	3.92	1.42	1.37
25	B	609	CLA	C1D-ND	3.92	1.42	1.37
25	b	607	CLA	C1D-ND	3.92	1.42	1.37
25	C	523	CLA	C1D-ND	3.92	1.42	1.37
25	B	613	CLA	C1D-ND	3.92	1.42	1.37
25	d	404	CLA	C1D-ND	3.91	1.42	1.37
25	b	614	CLA	C1D-ND	3.91	1.42	1.37
25	B	610	CLA	C1D-ND	3.91	1.42	1.37
25	P	612	CLA	C1D-ND	3.91	1.42	1.37
25	Q	602	CLA	C1D-ND	3.91	1.42	1.37
25	a	406	CLA	C1D-ND	3.91	1.42	1.37
25	S	601	CLA	C1D-ND	3.91	1.42	1.37
25	1	607	CLA	C1D-ND	3.91	1.42	1.37
25	N	614	CLA	C1D-ND	3.91	1.42	1.37
25	5	607	CLA	C1D-ND	3.90	1.42	1.37
25	b	603	CLA	C1D-ND	3.90	1.42	1.37
25	6	610	CLA	C1D-ND	3.90	1.42	1.37
38	S	618	II0	C06-C08	-3.90	1.46	1.52
25	6	603	CLA	C1D-ND	3.90	1.42	1.37
25	3	601	CLA	C1D-ND	3.90	1.42	1.37
25	C	528	CLA	C1D-ND	3.89	1.42	1.37
25	P	615	CLA	C1D-ND	3.89	1.42	1.37
25	3	611	CLA	C1D-ND	3.88	1.42	1.37
25	1	609	CLA	C1D-ND	3.88	1.42	1.37
25	R	607	CLA	C1D-ND	3.88	1.42	1.37
25	C	527	CLA	C1D-ND	3.88	1.42	1.37
25	R	602	CLA	C1D-ND	3.88	1.42	1.37
25	4	610	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	602	CLA	C1D-ND	3.88	1.42	1.37
25	A	406	CLA	C1D-ND	3.87	1.42	1.37
38	6	618	II0	C06-C08	-3.87	1.46	1.52
25	C	521	CLA	C1D-ND	3.87	1.42	1.37
25	b	611	CLA	C1D-ND	3.87	1.42	1.37
25	N	607	CLA	C1D-ND	3.87	1.42	1.37
25	R	613	CLA	C1D-ND	3.86	1.42	1.37
25	B	607	CLA	C1D-ND	3.86	1.42	1.37
25	B	611	CLA	C1D-ND	3.86	1.42	1.37
25	6	604	CLA	C1D-ND	3.86	1.42	1.37
25	c	525	CLA	C1D-ND	3.86	1.42	1.37
25	5	602	CLA	C1D-ND	3.86	1.42	1.37
25	2	602	CLA	C1D-ND	3.85	1.42	1.37
25	c	523	CLA	C1D-ND	3.85	1.42	1.37
38	Q	617	II0	C06-C08	-3.85	1.46	1.52
25	Q	615	CLA	C1D-ND	3.85	1.42	1.37
25	P	602	CLA	C1D-ND	3.85	1.42	1.37
25	1	602	CLA	C1D-ND	3.84	1.42	1.37
25	c	517	CLA	C1D-ND	3.84	1.42	1.37
25	c	521	CLA	C1D-ND	3.84	1.42	1.37
25	3	602	CLA	C1D-ND	3.84	1.42	1.37
25	C	517	CLA	C1D-ND	3.84	1.42	1.37
25	5	609	CLA	C1D-ND	3.84	1.42	1.37
25	B	603	CLA	C1D-ND	3.83	1.42	1.37
25	C	525	CLA	C1D-ND	3.83	1.42	1.37
25	R	615	CLA	C1D-ND	3.83	1.42	1.37
38	3	619	II0	C06-C08	-3.83	1.46	1.52
25	S	602	CLA	C1D-ND	3.83	1.42	1.37
38	N	619	II0	C06-C08	-3.82	1.46	1.52
25	4	615	CLA	C1D-ND	3.82	1.42	1.37
27	a	407	WVN	C02-C11	3.82	1.55	1.50
38	3	618	II0	C06-C08	-3.82	1.46	1.52
25	3	615	CLA	C1D-ND	3.82	1.42	1.37
25	R	609	CLA	C1D-ND	3.82	1.42	1.37
25	6	613	CLA	C1D-ND	3.82	1.42	1.37
38	4	617	II0	C06-C08	-3.82	1.46	1.52
25	5	615	CLA	C1D-ND	3.81	1.42	1.37
25	A	403	CLA	C1D-ND	3.81	1.42	1.37
38	P	619	II0	C06-C08	-3.81	1.46	1.52
25	1	614	CLA	C1D-ND	3.81	1.42	1.37
25	S	609	CLA	C1D-ND	3.80	1.42	1.37
25	N	609	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	403	CLA	C1D-ND	3.80	1.42	1.37
25	2	613	CLA	C1D-ND	3.80	1.42	1.37
25	O	615	CLA	C1D-ND	3.80	1.42	1.37
25	5	611	CLA	C1D-ND	3.79	1.42	1.37
25	G	302	CLA	C1D-ND	3.79	1.42	1.37
38	P	618	II0	C06-C08	-3.79	1.46	1.52
25	S	604	CLA	C1D-ND	3.79	1.42	1.37
38	6	617	II0	C06-C08	-3.79	1.46	1.52
25	R	611	CLA	C1D-ND	3.78	1.42	1.37
25	5	613	CLA	C1D-ND	3.78	1.42	1.37
38	N	617	II0	C06-C08	-3.76	1.46	1.52
29	d	405	PL9	C7-C3	-3.76	1.47	1.51
38	1	617	II0	C06-C08	-3.76	1.46	1.52
38	S	617	II0	C06-C08	-3.76	1.46	1.52
38	P	617	II0	C06-C08	-3.76	1.46	1.52
29	D	405	PL9	C7-C3	-3.76	1.47	1.51
25	O	613	CLA	C1D-ND	3.76	1.42	1.37
38	2	618	II0	C06-C08	-3.76	1.46	1.52
38	1	619	II0	C06-C08	-3.76	1.46	1.52
25	S	603	CLA	C1D-ND	3.75	1.42	1.37
37	6	606	KC2	CHB-C4A	3.75	1.47	1.39
25	S	613	CLA	C1D-ND	3.74	1.42	1.37
38	4	616	II0	C06-C08	-3.74	1.46	1.52
25	C	520	CLA	C1D-ND	3.74	1.42	1.37
25	4	606	CLA	C1D-ND	3.74	1.42	1.37
25	P	613	CLA	C1D-ND	3.73	1.42	1.37
38	Q	618	II0	C06-C08	-3.73	1.47	1.52
37	S	606	KC2	CHB-C4A	3.72	1.47	1.39
38	O	618	II0	C06-C08	-3.72	1.47	1.52
25	6	609	CLA	C1D-ND	3.72	1.42	1.37
25	4	609	CLA	C1D-ND	3.71	1.42	1.37
25	2	615	CLA	C1D-ND	3.71	1.42	1.37
38	N	618	II0	C06-C08	-3.71	1.47	1.52
25	d	403	CLA	C1D-ND	3.71	1.42	1.37
25	3	613	CLA	C1D-ND	3.71	1.42	1.37
38	O	619	II0	C22-C10	3.70	1.50	1.42
38	Q	616	II0	C06-C08	-3.69	1.47	1.52
27	C	529	WVN	C02-C11	3.69	1.55	1.50
38	5	616	II0	C06-C08	-3.68	1.47	1.52
38	5	619	II0	C06-C08	-3.68	1.47	1.52
38	3	617	II0	C06-C08	-3.68	1.47	1.52
38	1	618	II0	C06-C08	-3.68	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	302	CLA	C1D-ND	3.67	1.42	1.37
38	6	616	II0	C06-C08	-3.67	1.47	1.52
38	S	616	II0	C06-C08	-3.66	1.47	1.52
38	R	618	II0	C06-C08	-3.66	1.47	1.52
38	2	619	II0	C22-C10	3.66	1.50	1.42
25	B	612	CLA	C1D-ND	3.66	1.42	1.37
38	4	618	II0	C06-C08	-3.64	1.47	1.52
38	6	619	II0	C06-C08	-3.64	1.47	1.52
25	b	612	CLA	C1D-ND	3.64	1.42	1.37
38	R	616	II0	C06-C08	-3.63	1.47	1.52
38	P	618	II0	C22-C10	3.63	1.50	1.42
38	O	616	II0	C06-C08	-3.63	1.47	1.52
38	R	617	II0	C06-C08	-3.63	1.47	1.52
25	S	615	CLA	C1D-ND	3.63	1.42	1.37
25	Q	609	CLA	C1D-ND	3.63	1.42	1.37
25	c	520	CLA	C1D-ND	3.63	1.42	1.37
25	D	403	CLA	C1D-ND	3.62	1.42	1.37
38	2	616	II0	C06-C08	-3.62	1.47	1.52
25	6	615	CLA	C1D-ND	3.62	1.42	1.37
38	5	617	II0	C06-C08	-3.62	1.47	1.52
38	3	618	II0	C22-C10	3.62	1.50	1.42
38	6	616	II0	C22-C10	3.62	1.50	1.42
38	S	619	II0	C06-C08	-3.61	1.47	1.52
38	4	618	II0	C22-C10	3.61	1.50	1.42
25	G	301	CLA	C1D-ND	3.60	1.42	1.37
27	b	617	WVN	C28-C25	-3.60	1.31	1.35
38	Q	618	II0	C22-C10	3.60	1.50	1.42
38	R	619	II0	C06-C08	-3.59	1.47	1.52
38	P	616	II0	C06-C08	-3.59	1.47	1.52
38	5	618	II0	C06-C08	-3.58	1.47	1.52
38	3	616	II0	C06-C08	-3.58	1.47	1.52
38	6	617	II0	C22-C10	3.58	1.50	1.42
38	6	619	II0	C22-C10	3.58	1.50	1.42
39	R	620	IHT	C37-C33	-3.58	1.31	1.35
38	2	618	II0	C22-C10	3.56	1.49	1.42
38	O	616	II0	C22-C10	3.56	1.49	1.42
38	5	616	II0	C22-C10	3.56	1.49	1.42
38	S	616	II0	C22-C10	3.55	1.49	1.42
38	4	619	II0	C22-C10	3.55	1.49	1.42
38	N	616	II0	C06-C08	-3.55	1.47	1.52
38	O	618	II0	C22-C10	3.55	1.49	1.42
38	6	618	II0	C22-C10	3.54	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	S	617	II0	C22-C10	3.54	1.49	1.42
38	S	619	II0	C22-C10	3.54	1.49	1.42
38	1	616	II0	C06-C08	-3.53	1.47	1.52
38	Q	619	II0	C22-C10	3.53	1.49	1.42
38	3	617	II0	C22-C10	3.53	1.49	1.42
38	O	619	II0	C06-C08	-3.53	1.47	1.52
38	S	618	II0	C22-C10	3.53	1.49	1.42
38	N	619	II0	C22-C10	3.53	1.49	1.42
38	2	616	II0	C22-C10	3.53	1.49	1.42
38	P	617	II0	C22-C10	3.53	1.49	1.42
38	2	619	II0	C06-C08	-3.52	1.47	1.52
38	R	616	II0	C22-C10	3.52	1.49	1.42
39	4	620	IHT	C37-C33	-3.52	1.31	1.35
38	5	617	II0	C22-C10	3.52	1.49	1.42
38	R	619	II0	C22-C10	3.51	1.49	1.42
38	N	618	II0	C22-C10	3.51	1.49	1.42
38	1	619	II0	C22-C10	3.50	1.49	1.42
38	4	619	II0	C06-C08	-3.50	1.47	1.52
38	R	617	II0	C22-C10	3.50	1.49	1.42
36	e	102	HEM	C1B-NB	-3.49	1.34	1.40
38	3	619	II0	C22-C10	3.49	1.49	1.42
38	O	617	II0	C06-C08	-3.48	1.47	1.52
38	5	619	II0	C22-C10	3.48	1.49	1.42
38	1	618	II0	C22-C10	3.48	1.49	1.42
38	R	618	II0	C22-C10	3.48	1.49	1.42
36	e	102	HEM	C4D-ND	-3.47	1.34	1.40
38	4	616	II0	C22-C10	3.47	1.49	1.42
38	N	617	II0	C22-C10	3.47	1.49	1.42
38	5	618	II0	C22-C10	3.46	1.49	1.42
36	E	102	HEM	C1B-NB	-3.46	1.34	1.40
38	Q	616	II0	C22-C10	3.46	1.49	1.42
38	Q	619	II0	C06-C08	-3.45	1.47	1.52
38	2	617	II0	C06-C08	-3.45	1.47	1.52
36	E	102	HEM	C4D-ND	-3.45	1.34	1.40
38	3	616	II0	C22-C10	3.45	1.49	1.42
38	Q	617	II0	C22-C10	3.45	1.49	1.42
38	4	617	II0	C22-C10	3.45	1.49	1.42
39	Q	620	IHT	C37-C33	-3.44	1.31	1.35
38	P	616	II0	C22-C10	3.44	1.49	1.42
37	1	611	KC2	C4D-CHA	3.44	1.49	1.45
38	P	619	II0	C22-C10	3.43	1.49	1.42
37	1	613	KC2	C4D-CHA	3.43	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	617	II0	C22-C10	3.43	1.49	1.42
38	N	616	II0	C22-C10	3.42	1.49	1.42
37	Q	605	KC2	CHB-C4A	3.42	1.47	1.39
38	1	616	II0	C22-C10	3.40	1.49	1.42
37	N	611	KC2	C4D-CHA	3.40	1.49	1.45
37	4	605	KC2	CHB-C4A	3.40	1.47	1.39
27	6	620	WVN	C02-C11	3.40	1.55	1.50
37	5	612	KC2	CHB-C4A	3.39	1.47	1.39
37	1	613	KC2	CHB-C4A	3.39	1.47	1.39
37	R	612	KC2	CHB-C4A	3.38	1.47	1.39
27	A	407	WVN	C36-C32	-3.38	1.31	1.35
27	A	407	WVN	C37-C34	-3.38	1.31	1.35
37	N	605	KC2	CHB-C4A	3.38	1.46	1.39
37	1	611	KC2	CHB-C4A	3.37	1.46	1.39
37	N	605	KC2	CHC-C1C	3.36	1.46	1.39
37	N	611	KC2	CHB-C4A	3.36	1.46	1.39
37	1	605	KC2	CHB-C4A	3.36	1.46	1.39
27	D	408	WVN	C33-C34	3.36	1.53	1.45
37	Q	612	KC2	CHC-C1C	3.35	1.46	1.39
37	N	613	KC2	CHB-C4A	3.35	1.46	1.39
37	N	613	KC2	C4D-CHA	3.35	1.49	1.45
39	O	620	IHT	C32-C33	3.35	1.53	1.45
37	1	605	KC2	CHC-C1C	3.34	1.46	1.39
38	2	617	II0	C22-C10	3.34	1.49	1.42
27	B	619	WVN	C26-C22	-3.34	1.31	1.35
37	P	606	KC2	CHB-C4A	3.34	1.46	1.39
27	3	620	WVN	C28-C25	-3.34	1.31	1.35
37	3	606	KC2	CHB-C4A	3.33	1.46	1.39
38	O	617	II0	C22-C10	3.33	1.49	1.42
27	Y	89	WVN	C19-C22	3.33	1.53	1.45
27	6	620	WVN	C31-C32	3.33	1.53	1.45
27	d	408	WVN	C33-C34	3.33	1.53	1.45
37	4	612	KC2	CHC-C1C	3.33	1.46	1.39
39	O	620	IHT	C37-C33	-3.33	1.31	1.35
39	2	620	IHT	C32-C33	3.33	1.53	1.45
39	5	620	IHT	C37-C33	-3.32	1.31	1.35
27	c	530	WVN	C26-C22	-3.32	1.31	1.35
37	Q	611	KC2	CHB-C4A	3.32	1.46	1.39
37	4	611	KC2	CHB-C4A	3.31	1.46	1.39
27	B	617	WVN	C26-C22	-3.30	1.31	1.35
27	P	620	WVN	C28-C25	-3.30	1.31	1.35
37	O	612	KC2	CHB-C4A	3.30	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	612	KC2	CHC-C1C	3.29	1.46	1.39
37	2	612	KC2	CHB-C4A	3.29	1.46	1.39
37	O	612	KC2	CHC-C1C	3.29	1.46	1.39
27	S	620	WVN	C23-C25	3.29	1.53	1.45
37	6	612	KC2	CHB-C4A	3.28	1.46	1.39
37	S	612	KC2	CHB-C4A	3.28	1.46	1.39
27	S	620	WVN	C31-C32	3.28	1.53	1.45
37	N	612	KC2	CHB-C4A	3.28	1.46	1.39
37	1	612	KC2	CHB-C4A	3.27	1.46	1.39
27	Y	89	WVN	C23-C25	3.27	1.53	1.45
27	a	407	WVN	C33-C34	3.27	1.53	1.45
37	R	612	KC2	CHC-C1C	3.27	1.46	1.39
27	S	620	WVN	C29-C26	3.27	1.53	1.43
27	C	531	WVN	C33-C34	3.27	1.53	1.45
27	b	619	WVN	C33-C34	3.27	1.53	1.45
27	D	408	WVN	C23-C25	3.27	1.53	1.45
27	C	530	WVN	C26-C22	-3.26	1.31	1.35
27	b	618	WVN	C33-C34	3.26	1.52	1.45
37	5	612	KC2	CHC-C1C	3.24	1.46	1.39
25	G	302	CLA	C4D-ND	-3.24	1.33	1.37
27	6	620	WVN	C23-C25	3.24	1.52	1.45
27	6	620	WVN	C29-C26	3.24	1.53	1.43
37	Q	605	KC2	CHC-C1C	3.24	1.46	1.39
37	4	612	KC2	CHB-C4A	3.24	1.46	1.39
37	6	612	KC2	CHC-C1C	3.23	1.46	1.39
27	b	617	WVN	C37-C34	-3.23	1.31	1.35
37	Q	611	KC2	CHC-C1C	3.23	1.46	1.39
37	4	611	KC2	CHC-C1C	3.23	1.46	1.39
27	A	407	WVN	C28-C25	-3.22	1.31	1.35
27	H	89	WVN	C33-C34	3.22	1.52	1.45
37	Q	612	KC2	CHB-C4A	3.22	1.46	1.39
27	H	89	WVN	C23-C25	3.22	1.52	1.45
37	3	606	KC2	CHC-C1C	3.21	1.46	1.39
37	Q	612	KC2	C4D-CHA	3.21	1.49	1.45
27	C	531	WVN	C23-C25	3.21	1.52	1.45
37	4	605	KC2	CHC-C1C	3.21	1.46	1.39
27	6	620	WVN	C39-C36	3.20	1.53	1.43
27	b	619	WVN	C23-C25	3.20	1.52	1.45
37	P	606	KC2	CHC-C1C	3.20	1.46	1.39
27	d	408	WVN	C23-C25	3.20	1.52	1.45
27	a	407	WVN	C30-C28	3.20	1.53	1.43
37	S	612	KC2	CHC-C1C	3.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	529	WVN	C23-C25	3.20	1.52	1.45
27	B	617	WVN	C23-C25	3.20	1.52	1.45
27	C	529	WVN	C31-C32	3.20	1.52	1.45
27	S	620	WVN	C33-C34	3.19	1.52	1.45
27	c	530	WVN	C33-C34	3.19	1.52	1.45
27	Y	89	WVN	C30-C28	3.19	1.53	1.43
27	h	89	WVN	C23-C25	3.19	1.52	1.45
27	B	618	WVN	C33-C34	3.19	1.52	1.45
27	6	620	WVN	C33-C34	3.18	1.52	1.45
37	Q	605	KC2	C4D-CHA	3.18	1.49	1.45
27	a	407	WVN	C31-C32	3.18	1.52	1.45
39	2	620	IHT	C37-C33	-3.18	1.31	1.35
37	1	612	KC2	CHC-C1C	3.18	1.46	1.39
27	P	620	WVN	C37-C34	-3.18	1.31	1.35
27	c	529	WVN	C31-C32	3.18	1.52	1.45
27	C	531	WVN	C31-C32	3.18	1.52	1.45
27	b	619	WVN	C30-C28	3.18	1.53	1.43
27	B	617	WVN	C33-C34	3.18	1.52	1.45
27	D	408	WVN	C30-C28	3.17	1.53	1.43
37	N	612	KC2	CHC-C1C	3.17	1.46	1.39
27	h	89	WVN	C33-C34	3.17	1.52	1.45
27	B	618	WVN	C31-C32	3.17	1.52	1.45
27	3	620	WVN	C37-C34	-3.16	1.31	1.35
27	A	407	WVN	C26-C22	-3.16	1.31	1.35
39	5	620	IHT	C32-C33	3.16	1.52	1.45
27	H	89	WVN	C30-C28	3.16	1.53	1.43
37	1	613	KC2	CHC-C1C	3.16	1.46	1.39
27	S	620	WVN	C39-C36	3.16	1.53	1.43
37	6	606	KC2	CHC-C1C	3.16	1.46	1.39
27	c	529	WVN	C33-C34	3.16	1.52	1.45
27	Y	89	WVN	C29-C26	3.16	1.53	1.43
27	b	617	WVN	C19-C22	3.16	1.52	1.45
27	d	408	WVN	C30-C28	3.16	1.53	1.43
27	h	89	WVN	C31-C32	3.15	1.52	1.45
37	1	611	KC2	CHC-C1C	3.15	1.46	1.39
27	h	89	WVN	C30-C28	3.15	1.53	1.43
37	N	611	KC2	CHC-C1C	3.15	1.46	1.39
27	y	89	WVN	C19-C22	3.15	1.52	1.45
27	Y	89	WVN	C33-C34	3.15	1.52	1.45
27	6	620	WVN	C40-C37	3.15	1.53	1.43
27	6	620	WVN	C19-C22	3.15	1.52	1.45
37	4	605	KC2	C4D-CHA	3.15	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	611	KC2	C4D-CHA	3.15	1.49	1.45
27	D	408	WVN	C19-C22	3.14	1.52	1.45
39	4	620	IHT	C32-C33	3.14	1.52	1.45
39	1	620	IHT	C32-C33	3.14	1.52	1.45
27	H	89	WVN	C31-C32	3.14	1.52	1.45
37	4	612	KC2	C4D-CHA	3.14	1.48	1.45
27	a	407	WVN	C23-C25	3.14	1.52	1.45
39	N	620	IHT	C32-C33	3.14	1.52	1.45
27	B	617	WVN	C36-C32	-3.14	1.31	1.35
37	N	613	KC2	CHC-C1C	3.13	1.46	1.39
27	c	531	WVN	C19-C22	3.13	1.52	1.45
25	1	615	CLA	CHC-C1C	3.13	1.43	1.35
39	1	620	IHT	C37-C33	-3.13	1.31	1.35
27	b	618	WVN	C23-C25	3.13	1.52	1.45
39	N	620	IHT	C37-C33	-3.13	1.31	1.35
27	C	529	WVN	C33-C34	3.13	1.52	1.45
27	D	408	WVN	C31-C32	3.13	1.52	1.45
27	b	619	WVN	C26-C22	-3.13	1.31	1.35
25	2	610	CLA	CHC-C1C	3.12	1.43	1.35
37	S	606	KC2	CHC-C1C	3.12	1.46	1.39
27	C	529	WVN	C29-C26	3.12	1.53	1.43
25	P	609	CLA	CHC-C1C	3.12	1.43	1.35
39	Q	620	IHT	C32-C33	3.12	1.52	1.45
27	S	620	WVN	C40-C37	3.12	1.53	1.43
27	d	408	WVN	C19-C22	3.12	1.52	1.45
25	3	603	CLA	CHC-C1C	3.11	1.42	1.35
27	c	529	WVN	C39-C36	3.11	1.53	1.43
25	Q	603	CLA	CHC-C1C	3.11	1.42	1.35
37	O	612	KC2	C4D-CHA	3.11	1.48	1.45
27	b	618	WVN	C31-C32	3.11	1.52	1.45
27	6	620	WVN	C28-C25	-3.11	1.31	1.35
25	N	615	CLA	CHC-C1C	3.11	1.42	1.35
37	2	612	KC2	C4D-CHA	3.11	1.48	1.45
27	h	89	WVN	C29-C26	3.11	1.53	1.43
25	4	603	CLA	CHC-C1C	3.11	1.42	1.35
27	B	618	WVN	C23-C25	3.10	1.52	1.45
27	H	89	WVN	C29-C26	3.10	1.53	1.43
27	C	530	WVN	C28-C25	-3.10	1.31	1.35
25	B	614	CLA	CHC-C1C	3.10	1.42	1.35
25	R	602	CLA	CHC-C1C	3.10	1.42	1.35
37	5	612	KC2	C4D-CHA	3.10	1.48	1.45
27	C	529	WVN	C19-C22	3.10	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	610	CLA	CHC-C1C	3.10	1.42	1.35
27	c	529	WVN	C29-C26	3.10	1.53	1.43
27	S	620	WVN	C30-C28	3.10	1.53	1.43
27	C	531	WVN	C30-C28	3.09	1.53	1.43
25	O	610	CLA	CHC-C1C	3.09	1.42	1.35
25	3	609	CLA	CHC-C1C	3.09	1.42	1.35
27	b	619	WVN	C19-C22	3.09	1.52	1.45
27	6	620	WVN	C30-C28	3.09	1.53	1.43
25	Q	606	CLA	CHC-C1C	3.09	1.42	1.35
27	P	620	WVN	C26-C22	-3.09	1.31	1.35
38	Q	619	II0	C42-C40	3.09	1.53	1.43
27	H	89	WVN	C39-C36	3.09	1.53	1.43
25	5	602	CLA	CHC-C1C	3.08	1.42	1.35
37	P	606	KC2	C4D-CHA	3.08	1.48	1.45
27	d	408	WVN	C31-C32	3.08	1.52	1.45
25	b	613	CLA	CHC-C1C	3.08	1.42	1.35
27	c	529	WVN	C40-C37	3.08	1.53	1.43
25	O	602	CLA	CHC-C1C	3.08	1.42	1.35
27	h	89	WVN	C39-C36	3.08	1.53	1.43
27	B	618	WVN	C29-C26	3.08	1.53	1.43
27	c	529	WVN	C19-C22	3.08	1.52	1.45
27	S	620	WVN	C02-C11	3.08	1.54	1.50
27	3	620	WVN	C26-C22	-3.08	1.31	1.35
27	b	617	WVN	C29-C26	3.08	1.53	1.43
25	B	607	CLA	CHC-C1C	3.07	1.42	1.35
27	P	620	WVN	C19-C22	3.07	1.52	1.45
25	P	610	CLA	CHC-C1C	3.07	1.42	1.35
25	B	606	CLA	CHC-C1C	3.07	1.42	1.35
25	2	602	CLA	CHC-C1C	3.07	1.42	1.35
27	B	619	WVN	C33-C34	3.07	1.52	1.45
25	c	520	CLA	CHC-C1C	3.07	1.42	1.35
25	2	613	CLA	CHC-C1C	3.07	1.42	1.35
38	O	619	II0	C42-C40	3.07	1.53	1.43
25	d	403	CLA	CHC-C1C	3.07	1.42	1.35
25	P	613	CLA	CHC-C1C	3.07	1.42	1.35
27	B	618	WVN	C39-C36	3.07	1.53	1.43
38	4	619	II0	C42-C40	3.07	1.53	1.43
27	y	89	WVN	C37-C34	-3.07	1.31	1.35
38	2	619	II0	C42-C40	3.07	1.52	1.43
25	P	603	CLA	CHC-C1C	3.07	1.42	1.35
27	C	529	WVN	C23-C25	3.07	1.52	1.45
25	P	604	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	529	WVN	C28-C25	-3.06	1.31	1.35
27	C	530	WVN	C33-C34	3.06	1.52	1.45
27	c	531	WVN	C33-C34	3.06	1.52	1.45
27	c	531	WVN	C37-C34	-3.06	1.31	1.35
25	c	525	CLA	CHC-C1C	3.06	1.42	1.35
27	b	619	WVN	C31-C32	3.06	1.52	1.45
27	S	620	WVN	C28-C25	-3.06	1.31	1.35
25	S	604	CLA	CHC-C1C	3.06	1.42	1.35
27	y	89	WVN	C23-C25	3.06	1.52	1.45
27	S	620	WVN	C19-C22	3.06	1.52	1.45
25	C	525	CLA	CHC-C1C	3.06	1.42	1.35
25	D	403	CLA	CHC-C1C	3.06	1.42	1.35
25	2	615	CLA	CHC-C1C	3.06	1.42	1.35
25	b	614	CLA	CHC-C1C	3.06	1.42	1.35
25	b	601	CLA	CHC-C1C	3.06	1.42	1.35
27	B	619	WVN	C19-C22	3.06	1.52	1.45
37	S	606	KC2	C4A-C3A	3.06	1.50	1.44
27	b	619	WVN	C39-C36	3.06	1.52	1.43
27	D	408	WVN	C29-C26	3.06	1.52	1.43
27	d	408	WVN	C37-C34	-3.06	1.31	1.35
27	C	530	WVN	C37-C34	-3.06	1.31	1.35
25	1	606	CLA	CHC-C1C	3.06	1.42	1.35
25	S	610	CLA	CHC-C1C	3.06	1.42	1.35
25	5	606	CLA	CHC-C1C	3.06	1.42	1.35
27	C	529	WVN	C40-C37	3.06	1.52	1.43
25	c	523	CLA	CHC-C1C	3.06	1.42	1.35
25	4	609	CLA	CHC-C1C	3.06	1.42	1.35
25	S	615	CLA	CHC-C1C	3.06	1.42	1.35
38	1	619	II0	C41-C39	3.05	1.52	1.43
25	R	603	CLA	CHC-C1C	3.05	1.42	1.35
25	3	613	CLA	CHC-C1C	3.05	1.42	1.35
27	B	619	WVN	C36-C32	-3.05	1.31	1.35
27	c	530	WVN	C30-C28	3.05	1.52	1.43
25	C	523	CLA	CHC-C1C	3.05	1.42	1.35
27	C	531	WVN	C29-C26	3.05	1.52	1.43
27	b	618	WVN	C37-C34	-3.05	1.31	1.35
25	B	605	CLA	CHC-C1C	3.05	1.42	1.35
25	3	604	CLA	CHC-C1C	3.05	1.42	1.35
25	1	602	CLA	CHC-C1C	3.05	1.42	1.35
38	4	618	II0	C42-C40	3.05	1.52	1.43
25	5	603	CLA	CHC-C1C	3.05	1.42	1.35
37	Q	611	KC2	C4D-CHA	3.05	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	601	CLA	CHC-C1C	3.05	1.42	1.35
25	5	604	CLA	CHC-C1C	3.05	1.42	1.35
25	N	602	CLA	CHC-C1C	3.05	1.42	1.35
25	b	616	CLA	CHC-C1C	3.05	1.42	1.35
27	b	619	WVN	C40-C37	3.05	1.52	1.43
27	C	529	WVN	C39-C36	3.05	1.52	1.43
25	N	606	CLA	CHC-C1C	3.04	1.42	1.35
38	3	619	II0	C42-C40	3.04	1.52	1.43
27	b	618	WVN	C39-C36	3.04	1.52	1.43
25	O	609	CLA	CHC-C1C	3.04	1.42	1.35
27	c	530	WVN	C19-C22	3.04	1.52	1.45
27	C	531	WVN	C39-C36	3.04	1.52	1.43
25	g	301	CLA	CHC-C1C	3.04	1.42	1.35
25	B	602	CLA	CHC-C1C	3.04	1.42	1.35
25	6	603	CLA	CHC-C1C	3.04	1.42	1.35
25	6	604	CLA	CHC-C1C	3.04	1.42	1.35
25	2	606	CLA	CHC-C1C	3.04	1.42	1.35
38	3	618	II0	C42-C40	3.04	1.52	1.43
38	S	619	II0	C42-C40	3.04	1.52	1.43
25	6	610	CLA	CHC-C1C	3.04	1.42	1.35
25	S	602	CLA	CHC-C1C	3.04	1.42	1.35
25	B	613	CLA	CHC-C1C	3.04	1.42	1.35
27	b	618	WVN	C30-C28	3.04	1.52	1.43
27	b	618	WVN	C19-C22	3.04	1.52	1.45
27	B	618	WVN	C19-C22	3.04	1.52	1.45
25	R	610	CLA	CHC-C1C	3.04	1.42	1.35
27	A	407	WVN	C31-C32	3.04	1.52	1.45
25	O	611	CLA	CHC-C1C	3.04	1.42	1.35
25	O	606	CLA	CHC-C1C	3.04	1.42	1.35
25	3	612	CLA	CHC-C1C	3.04	1.42	1.35
27	a	407	WVN	C36-C32	-3.04	1.31	1.35
25	Q	615	CLA	CHC-C1C	3.04	1.42	1.35
27	3	620	WVN	C19-C22	3.04	1.52	1.45
38	P	619	II0	C42-C40	3.04	1.52	1.43
25	R	604	CLA	CHC-C1C	3.03	1.42	1.35
25	O	615	CLA	CHC-C1C	3.03	1.42	1.35
25	6	615	CLA	CHC-C1C	3.03	1.42	1.35
27	b	618	WVN	C29-C26	3.03	1.52	1.43
25	b	606	CLA	CHC-C1C	3.03	1.42	1.35
25	1	601	CLA	CHC-C1C	3.03	1.42	1.35
25	2	611	CLA	CHC-C1C	3.03	1.42	1.35
25	2	609	CLA	CHC-C1C	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	606	CLA	CHC-C1C	3.03	1.42	1.35
27	b	618	WVN	C40-C37	3.03	1.52	1.43
25	5	610	CLA	CHC-C1C	3.03	1.42	1.35
27	D	408	WVN	C39-C36	3.03	1.52	1.43
38	6	619	II0	C42-C40	3.03	1.52	1.43
25	B	601	CLA	CHC-C1C	3.03	1.42	1.35
25	O	613	CLA	CHC-C1C	3.02	1.42	1.35
25	P	612	CLA	CHC-C1C	3.02	1.42	1.35
25	3	615	CLA	CHC-C1C	3.02	1.42	1.35
38	5	619	II0	C42-C40	3.02	1.52	1.43
27	d	408	WVN	C29-C26	3.02	1.52	1.43
38	Q	618	II0	C42-C40	3.02	1.52	1.43
25	C	520	CLA	CHC-C1C	3.02	1.42	1.35
25	1	610	CLA	CHC-C1C	3.02	1.42	1.35
27	a	407	WVN	C29-C26	3.02	1.52	1.43
25	6	602	CLA	CHC-C1C	3.02	1.42	1.35
38	N	618	II0	C42-C40	3.02	1.52	1.43
27	c	531	WVN	C31-C32	3.02	1.52	1.45
25	4	604	CLA	CHC-C1C	3.02	1.42	1.35
38	1	618	II0	C42-C40	3.02	1.52	1.43
25	c	521	CLA	CHC-C1C	3.02	1.42	1.35
37	R	612	KC2	C4D-CHA	3.02	1.48	1.45
25	O	603	CLA	CHC-C1C	3.02	1.42	1.35
25	B	610	CLA	CHC-C1C	3.02	1.42	1.35
27	B	618	WVN	C30-C28	3.02	1.52	1.43
25	2	603	CLA	CHC-C1C	3.02	1.42	1.35
25	N	609	CLA	CHC-C1C	3.02	1.42	1.35
27	y	89	WVN	C29-C26	3.02	1.52	1.43
25	b	610	CLA	CHC-C1C	3.02	1.42	1.35
25	b	602	CLA	CHC-C1C	3.02	1.42	1.35
27	C	531	WVN	C40-C37	3.02	1.52	1.43
25	S	609	CLA	CHC-C1C	3.02	1.42	1.35
27	c	531	WVN	C26-C22	-3.02	1.31	1.35
38	O	616	II0	C42-C40	3.02	1.52	1.43
27	B	619	WVN	C37-C34	-3.02	1.31	1.35
25	C	519	CLA	CHC-C1C	3.01	1.42	1.35
25	N	603	CLA	CHC-C1C	3.01	1.42	1.35
38	6	616	II0	C42-C40	3.01	1.52	1.43
25	3	602	CLA	CHC-C1C	3.01	1.42	1.35
25	C	521	CLA	CHC-C1C	3.01	1.42	1.35
38	2	616	II0	C42-C40	3.01	1.52	1.43
25	c	528	CLA	CHC-C1C	3.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	602	CLA	CHC-C1C	3.01	1.42	1.35
25	Q	610	CLA	CHC-C1C	3.01	1.42	1.35
27	B	617	WVN	C30-C28	3.01	1.52	1.43
25	N	604	CLA	CHC-C1C	3.01	1.42	1.35
27	c	529	WVN	C30-C28	3.01	1.52	1.43
25	c	517	CLA	C4D-ND	-3.01	1.33	1.37
25	c	523	CLA	C4D-ND	-3.01	1.33	1.37
27	a	407	WVN	C37-C34	-3.01	1.31	1.35
27	H	89	WVN	C36-C32	-3.01	1.31	1.35
27	H	89	WVN	C40-C37	3.01	1.52	1.43
27	b	617	WVN	C31-C32	3.01	1.52	1.45
25	6	601	CLA	CHC-C1C	3.01	1.42	1.35
25	Q	604	CLA	CHC-C1C	3.01	1.42	1.35
38	1	617	II0	C42-C40	3.01	1.52	1.43
25	B	616	CLA	CHC-C1C	3.01	1.42	1.35
38	N	619	II0	C41-C39	3.01	1.52	1.43
25	b	603	CLA	CHC-C1C	3.01	1.42	1.35
25	4	615	CLA	CHC-C1C	3.01	1.42	1.35
38	4	617	II0	C42-C40	3.01	1.52	1.43
38	N	619	II0	C42-C40	3.01	1.52	1.43
38	P	618	II0	C41-C39	3.01	1.52	1.43
25	b	611	CLA	CHC-C1C	3.01	1.42	1.35
27	B	618	WVN	C40-C37	3.01	1.52	1.43
25	c	519	CLA	CHC-C1C	3.01	1.42	1.35
25	C	527	CLA	CHC-C1C	3.01	1.42	1.35
25	d	404	CLA	CHC-C1C	3.00	1.42	1.35
25	5	611	CLA	CHC-C1C	3.00	1.42	1.35
25	R	611	CLA	CHC-C1C	3.00	1.42	1.35
25	1	603	CLA	CHC-C1C	3.00	1.42	1.35
38	R	619	II0	C42-C40	3.00	1.52	1.43
25	b	607	CLA	CHC-C1C	3.00	1.42	1.35
25	Q	609	CLA	CHC-C1C	3.00	1.42	1.35
25	P	601	CLA	C4D-ND	-3.00	1.33	1.37
27	a	407	WVN	C19-C22	3.00	1.52	1.45
25	b	605	CLA	CHC-C1C	3.00	1.42	1.35
25	D	404	CLA	CHC-C1C	3.00	1.42	1.35
25	b	608	CLA	CHC-C1C	3.00	1.42	1.35
38	2	618	II0	C42-C40	3.00	1.52	1.43
27	y	89	WVN	C33-C34	3.00	1.52	1.45
38	P	618	II0	C42-C40	3.00	1.52	1.43
25	B	611	CLA	CHC-C1C	3.00	1.42	1.35
39	R	620	IHT	C32-C33	3.00	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	524	CLA	CHC-C1C	3.00	1.42	1.35
27	B	619	WVN	C40-C37	3.00	1.52	1.43
25	1	604	CLA	CHC-C1C	3.00	1.42	1.35
27	c	531	WVN	C30-C28	3.00	1.52	1.43
38	O	618	II0	C42-C40	3.00	1.52	1.43
25	B	611	CLA	C4D-ND	-3.00	1.33	1.37
25	4	610	CLA	CHC-C1C	3.00	1.42	1.35
27	Y	89	WVN	C39-C36	3.00	1.52	1.43
38	Q	617	II0	C42-C40	3.00	1.52	1.43
25	c	516	CLA	CHC-C1C	2.99	1.42	1.35
25	P	602	CLA	CHC-C1C	2.99	1.42	1.35
38	N	616	II0	C42-C40	2.99	1.52	1.43
37	N	612	KC2	C4D-CHA	2.99	1.48	1.45
25	a	404	CLA	CHC-C1C	2.99	1.42	1.35
25	A	404	CLA	CHC-C1C	2.99	1.42	1.35
27	H	89	WVN	C37-C34	-2.99	1.31	1.35
27	c	530	WVN	C40-C37	2.99	1.52	1.43
38	S	616	II0	C42-C40	2.99	1.52	1.43
27	h	89	WVN	C26-C22	-2.99	1.31	1.35
27	y	89	WVN	C28-C25	-2.99	1.31	1.35
27	3	620	WVN	C36-C32	-2.99	1.31	1.35
27	h	89	WVN	C40-C37	2.99	1.52	1.43
37	1	612	KC2	C4D-CHA	2.99	1.48	1.45
25	A	406	CLA	CHC-C1C	2.99	1.42	1.35
25	C	524	CLA	CHC-C1C	2.99	1.42	1.35
25	P	615	CLA	CHC-C1C	2.99	1.42	1.35
25	4	613	CLA	CHC-C1C	2.99	1.42	1.35
25	4	606	CLA	CHC-C1C	2.99	1.42	1.35
25	N	601	CLA	CHC-C1C	2.99	1.42	1.35
38	1	616	II0	C42-C40	2.99	1.52	1.43
25	C	516	CLA	CHC-C1C	2.99	1.42	1.35
25	N	610	CLA	CHC-C1C	2.99	1.42	1.35
25	b	612	CLA	CHC-C1C	2.99	1.42	1.35
25	b	611	CLA	C4D-ND	-2.99	1.33	1.37
27	H	89	WVN	C26-C22	-2.99	1.31	1.35
25	A	403	CLA	CHC-C1C	2.99	1.42	1.35
27	c	531	WVN	C40-C37	2.99	1.52	1.43
38	3	618	II0	C41-C39	2.99	1.52	1.43
38	P	617	II0	C42-C40	2.99	1.52	1.43
38	2	619	II0	C41-C39	2.99	1.52	1.43
25	C	528	CLA	CHC-C1C	2.99	1.42	1.35
38	1	619	II0	C42-C40	2.99	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	602	CLA	CHC-C1C	2.99	1.42	1.35
27	y	89	WVN	C26-C22	-2.99	1.31	1.35
25	B	608	CLA	CHC-C1C	2.98	1.42	1.35
25	c	526	CLA	CHC-C1C	2.98	1.42	1.35
27	c	531	WVN	C39-C36	2.98	1.52	1.43
27	d	408	WVN	C39-C36	2.98	1.52	1.43
27	C	529	WVN	C30-C28	2.98	1.52	1.43
27	P	620	WVN	C40-C37	2.98	1.52	1.43
38	Q	619	II0	C41-C39	2.98	1.52	1.43
27	C	530	WVN	C31-C32	2.98	1.52	1.45
27	y	89	WVN	C39-C36	2.98	1.52	1.43
25	C	518	CLA	CHC-C1C	2.98	1.42	1.35
25	6	611	CLA	CHC-C1C	2.98	1.42	1.35
27	B	619	WVN	C30-C28	2.98	1.52	1.43
38	5	617	II0	C42-C40	2.98	1.52	1.43
38	Q	616	II0	C42-C40	2.98	1.52	1.43
38	5	618	II0	C42-C40	2.98	1.52	1.43
27	3	620	WVN	C40-C37	2.98	1.52	1.43
27	P	620	WVN	C36-C32	-2.98	1.31	1.35
37	3	606	KC2	C4D-CHA	2.98	1.48	1.45
27	c	531	WVN	C29-C26	2.98	1.52	1.43
27	D	408	WVN	C40-C37	2.98	1.52	1.43
27	y	89	WVN	C36-C32	-2.98	1.31	1.35
27	B	618	WVN	C37-C34	-2.98	1.31	1.35
25	G	301	CLA	C4D-ND	-2.98	1.33	1.37
25	O	604	CLA	CHC-C1C	2.98	1.42	1.35
38	4	619	II0	C41-C39	2.98	1.52	1.43
25	P	611	CLA	CHC-C1C	2.98	1.42	1.35
27	d	408	WVN	C26-C22	-2.98	1.31	1.35
38	5	616	II0	C42-C40	2.97	1.52	1.43
25	3	601	CLA	CHC-C1C	2.97	1.42	1.35
25	a	406	CLA	CHC-C1C	2.97	1.42	1.35
38	R	616	II0	C42-C40	2.97	1.52	1.43
25	3	601	CLA	C4D-ND	-2.97	1.33	1.37
27	a	407	WVN	C40-C37	2.97	1.52	1.43
27	y	89	WVN	C30-C28	2.97	1.52	1.43
27	h	89	WVN	C36-C32	-2.97	1.31	1.35
38	3	619	II0	C41-C39	2.97	1.52	1.43
38	O	619	II0	C41-C39	2.97	1.52	1.43
25	B	603	CLA	CHC-C1C	2.97	1.42	1.35
25	C	526	CLA	CHC-C1C	2.97	1.42	1.35
27	B	617	WVN	C40-C37	2.97	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	620	IHT	C34-C35	2.97	1.52	1.45
38	S	618	II0	C42-C40	2.97	1.52	1.43
25	B	615	CLA	CHC-C1C	2.97	1.42	1.35
27	c	529	WVN	C28-C25	-2.97	1.31	1.35
25	4	604	CLA	C4D-ND	-2.97	1.33	1.37
27	c	531	WVN	C36-C32	-2.97	1.31	1.35
25	b	609	CLA	C4D-ND	-2.97	1.33	1.37
27	C	531	WVN	C19-C22	2.97	1.52	1.45
38	R	618	II0	C42-C40	2.97	1.52	1.43
25	c	527	CLA	CHC-C1C	2.97	1.42	1.35
27	3	620	WVN	C31-C32	2.97	1.52	1.45
27	y	89	WVN	C31-C32	2.97	1.52	1.45
25	C	522	CLA	CHC-C1C	2.96	1.42	1.35
38	6	617	II0	C42-C40	2.96	1.52	1.43
27	Y	89	WVN	C31-C32	2.96	1.52	1.45
27	a	407	WVN	C39-C36	2.96	1.52	1.43
38	P	619	II0	C41-C39	2.96	1.52	1.43
27	C	530	WVN	C19-C22	2.96	1.52	1.45
25	2	603	CLA	C4D-ND	-2.96	1.33	1.37
27	C	530	WVN	C29-C26	2.96	1.52	1.43
27	B	617	WVN	C31-C32	2.96	1.52	1.45
25	B	609	CLA	CHC-C1C	2.96	1.42	1.35
38	N	617	II0	C42-C40	2.96	1.52	1.43
25	5	602	CLA	C4D-ND	-2.96	1.33	1.37
27	d	408	WVN	C40-C37	2.96	1.52	1.43
27	c	530	WVN	C37-C34	-2.96	1.31	1.35
25	c	518	CLA	CHC-C1C	2.96	1.42	1.35
25	a	403	CLA	CHC-C1C	2.96	1.42	1.35
25	Q	613	CLA	CHC-C1C	2.96	1.42	1.35
27	3	620	WVN	C39-C36	2.96	1.52	1.43
25	S	611	CLA	CHC-C1C	2.96	1.42	1.35
25	c	521	CLA	C4D-ND	-2.96	1.33	1.37
25	5	615	CLA	CHC-C1C	2.96	1.42	1.35
27	h	89	WVN	C37-C34	-2.96	1.31	1.35
38	6	618	II0	C42-C40	2.96	1.52	1.43
27	c	530	WVN	C29-C26	2.96	1.52	1.43
25	b	605	CLA	C4D-ND	-2.96	1.33	1.37
25	5	601	CLA	C4D-ND	-2.96	1.33	1.37
38	R	617	II0	C42-C40	2.96	1.52	1.43
38	N	618	II0	C41-C39	2.96	1.52	1.43
25	C	521	CLA	C4D-ND	-2.96	1.33	1.37
27	P	620	WVN	C33-C34	2.96	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	407	WVN	C29-C26	2.96	1.52	1.43
38	1	618	II0	C41-C39	2.96	1.52	1.43
25	R	609	CLA	CHC-C1C	2.96	1.42	1.35
25	4	610	CLA	C4D-ND	-2.96	1.33	1.37
27	c	531	WVN	C28-C25	-2.96	1.31	1.35
27	3	620	WVN	C33-C34	2.95	1.52	1.45
25	R	615	CLA	CHC-C1C	2.95	1.42	1.35
25	6	609	CLA	CHC-C1C	2.95	1.42	1.35
25	b	615	CLA	CHC-C1C	2.95	1.42	1.35
25	O	603	CLA	C4D-ND	-2.95	1.33	1.37
38	O	618	II0	C41-C39	2.95	1.52	1.43
27	A	407	WVN	C33-C34	2.95	1.52	1.45
25	S	603	CLA	C4D-ND	-2.95	1.33	1.37
27	Y	89	WVN	C37-C34	-2.95	1.31	1.35
27	Y	89	WVN	C40-C37	2.95	1.52	1.43
38	3	616	II0	C42-C40	2.95	1.52	1.43
27	y	89	WVN	C40-C37	2.95	1.52	1.43
38	P	616	II0	C42-C40	2.95	1.52	1.43
27	P	620	WVN	C39-C36	2.95	1.52	1.43
25	2	604	CLA	CHC-C1C	2.95	1.42	1.35
38	Q	618	II0	C41-C39	2.95	1.52	1.43
25	b	609	CLA	CHC-C1C	2.95	1.42	1.35
27	b	619	WVN	C29-C26	2.95	1.52	1.43
25	2	602	CLA	C4D-ND	-2.95	1.33	1.37
38	Q	616	II0	C41-C39	2.94	1.52	1.43
25	N	602	CLA	C4D-ND	-2.94	1.33	1.37
25	d	400	CLA	C4D-ND	-2.94	1.33	1.37
38	2	617	II0	C42-C40	2.94	1.52	1.43
27	B	619	WVN	C39-C36	2.94	1.52	1.43
27	b	617	WVN	C36-C32	-2.94	1.31	1.35
27	B	617	WVN	C39-C36	2.94	1.52	1.43
38	4	616	II0	C42-C40	2.94	1.52	1.43
25	6	602	CLA	C4D-ND	-2.94	1.33	1.37
25	3	602	CLA	C4D-ND	-2.94	1.33	1.37
25	1	614	CLA	CHC-C1C	2.94	1.42	1.35
25	C	517	CLA	C4D-ND	-2.94	1.33	1.37
25	D	400	CLA	C4D-ND	-2.94	1.33	1.37
25	R	607	CLA	CHC-C1C	2.94	1.42	1.35
25	P	611	CLA	C4D-ND	-2.94	1.33	1.37
25	B	612	CLA	CHC-C1C	2.94	1.42	1.35
27	Y	89	WVN	C36-C32	-2.94	1.31	1.35
25	3	611	CLA	CHC-C1C	2.94	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	602	CLA	C4D-ND	-2.94	1.33	1.37
25	P	602	CLA	C4D-ND	-2.94	1.33	1.37
25	R	601	CLA	C4D-ND	-2.94	1.33	1.37
25	A	406	CLA	C4D-ND	-2.94	1.33	1.37
25	B	616	CLA	C4D-ND	-2.94	1.33	1.37
28	A	408	SQD	C6-S	-2.94	1.66	1.77
38	2	616	II0	C41-C39	2.93	1.52	1.43
27	P	620	WVN	C31-C32	2.93	1.52	1.45
27	C	530	WVN	C40-C37	2.93	1.52	1.43
25	c	520	CLA	C4D-ND	-2.93	1.33	1.37
25	2	601	CLA	CHC-C1C	2.93	1.42	1.35
25	5	609	CLA	C4D-ND	-2.93	1.33	1.37
25	R	609	CLA	C4D-ND	-2.93	1.33	1.37
27	A	407	WVN	C19-C22	2.93	1.52	1.45
25	C	519	CLA	C4D-ND	-2.93	1.33	1.37
27	D	408	WVN	C37-C34	-2.93	1.31	1.35
38	4	616	II0	C41-C39	2.93	1.52	1.43
25	C	518	CLA	C4D-ND	-2.93	1.33	1.37
25	C	523	CLA	C4D-ND	-2.93	1.33	1.37
25	N	607	CLA	CHC-C1C	2.93	1.42	1.35
27	B	619	WVN	C29-C26	2.93	1.52	1.43
27	b	617	WVN	C39-C36	2.93	1.52	1.43
38	1	617	II0	C41-C39	2.93	1.52	1.43
38	R	618	II0	C41-C39	2.93	1.52	1.43
28	a	408	SQD	C6-S	-2.93	1.66	1.77
25	B	609	CLA	C4D-ND	-2.93	1.33	1.37
25	5	607	CLA	CHC-C1C	2.93	1.42	1.35
25	a	403	CLA	C4D-ND	-2.92	1.33	1.37
38	6	618	II0	C41-C39	2.92	1.52	1.43
25	D	400	CLA	CHC-C1C	2.92	1.42	1.35
25	P	601	CLA	CHC-C1C	2.92	1.42	1.35
38	S	617	II0	C42-C40	2.92	1.52	1.43
25	N	610	CLA	C4D-ND	-2.92	1.33	1.37
25	G	302	CLA	CHC-C1C	2.92	1.42	1.35
25	5	609	CLA	CHC-C1C	2.92	1.42	1.35
25	S	613	CLA	CHC-C1C	2.92	1.42	1.35
25	R	610	CLA	C4D-ND	-2.92	1.33	1.37
25	C	516	CLA	C4D-ND	-2.92	1.33	1.37
25	C	520	CLA	C4D-ND	-2.92	1.33	1.37
36	E	102	HEM	FE-NB	2.92	2.11	1.96
25	S	609	CLA	C4D-ND	-2.92	1.33	1.37
25	1	609	CLA	CHC-C1C	2.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	S	618	II0	C41-C39	2.92	1.52	1.43
25	5	604	CLA	C4D-ND	-2.92	1.33	1.37
25	O	602	CLA	C4D-ND	-2.92	1.33	1.37
27	c	530	WVN	C31-C32	2.92	1.52	1.45
38	O	617	II0	C42-C40	2.92	1.52	1.43
38	S	619	II0	C41-C39	2.92	1.52	1.43
25	S	610	CLA	C4D-ND	-2.91	1.33	1.37
27	d	408	WVN	C36-C32	-2.91	1.31	1.35
38	4	618	II0	C41-C39	2.91	1.52	1.43
38	S	616	II0	C41-C39	2.91	1.52	1.43
27	C	530	WVN	C36-C32	-2.91	1.31	1.35
25	2	607	CLA	CHC-C1C	2.91	1.42	1.35
27	C	530	WVN	C30-C28	2.91	1.52	1.43
25	Q	604	CLA	C4D-ND	-2.91	1.33	1.37
38	R	619	II0	C41-C39	2.91	1.52	1.43
25	S	603	CLA	CHC-C1C	2.91	1.42	1.35
27	B	619	WVN	C31-C32	2.91	1.52	1.45
25	c	516	CLA	C4D-ND	-2.91	1.33	1.37
25	Q	607	CLA	C4D-ND	-2.91	1.33	1.37
25	g	302	CLA	CHC-C1C	2.91	1.42	1.35
25	6	613	CLA	CHC-C1C	2.91	1.42	1.35
25	O	601	CLA	CHC-C1C	2.91	1.42	1.35
38	O	617	II0	C41-C39	2.91	1.52	1.43
25	O	607	CLA	CHC-C1C	2.90	1.42	1.35
25	S	602	CLA	C4D-ND	-2.90	1.33	1.37
38	5	618	II0	C41-C39	2.90	1.52	1.43
38	N	617	II0	C41-C39	2.90	1.52	1.43
38	6	616	II0	C41-C39	2.90	1.52	1.43
27	B	617	WVN	C29-C26	2.90	1.52	1.43
27	c	530	WVN	C23-C25	2.90	1.52	1.45
25	1	609	CLA	C4D-ND	-2.90	1.33	1.37
27	3	620	WVN	C29-C26	2.90	1.52	1.43
25	N	614	CLA	CHC-C1C	2.90	1.42	1.35
25	a	406	CLA	C4D-ND	-2.90	1.33	1.37
27	c	529	WVN	C26-C22	-2.90	1.31	1.35
38	R	616	II0	C41-C39	2.90	1.52	1.43
38	5	616	II0	C41-C39	2.90	1.52	1.43
38	P	616	II0	C41-C39	2.90	1.52	1.43
39	O	620	IHT	C34-C35	2.90	1.52	1.45
25	1	610	CLA	C4D-ND	-2.90	1.33	1.37
28	a	411	SQD	C6-S	-2.90	1.66	1.77
27	H	89	WVN	C28-C25	-2.90	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	400	CLA	CHC-C1C	2.90	1.42	1.35
25	N	604	CLA	C4D-ND	-2.90	1.33	1.37
25	c	522	CLA	CHC-C1C	2.90	1.42	1.35
38	5	619	II0	C41-C39	2.90	1.52	1.43
25	C	525	CLA	C4D-ND	-2.90	1.33	1.37
25	P	613	CLA	C4D-ND	-2.90	1.33	1.37
25	b	616	CLA	C4D-ND	-2.89	1.33	1.37
27	b	619	WVN	C37-C34	-2.89	1.31	1.35
38	Q	617	II0	C41-C39	2.89	1.52	1.43
37	N	605	KC2	C4A-C3A	2.89	1.50	1.44
25	P	610	CLA	C4D-ND	-2.89	1.33	1.37
38	O	616	II0	C41-C39	2.89	1.52	1.43
37	6	606	KC2	C4A-C3A	2.89	1.50	1.44
25	A	403	CLA	C4D-ND	-2.89	1.33	1.37
25	3	610	CLA	C4D-ND	-2.89	1.33	1.37
27	b	618	WVN	C28-C25	-2.89	1.31	1.35
38	3	617	II0	C42-C40	2.89	1.52	1.43
25	B	605	CLA	C4D-ND	-2.89	1.33	1.37
25	1	602	CLA	C4D-ND	-2.89	1.33	1.37
38	2	618	II0	C41-C39	2.89	1.52	1.43
38	4	617	II0	C41-C39	2.89	1.52	1.43
28	A	411	SQD	C6-S	-2.89	1.66	1.77
25	O	610	CLA	C4D-ND	-2.89	1.33	1.37
25	1	607	CLA	CHC-C1C	2.89	1.42	1.35
25	B	607	CLA	C4D-ND	-2.89	1.33	1.37
25	6	610	CLA	C4D-ND	-2.89	1.33	1.37
38	3	616	II0	C41-C39	2.89	1.52	1.43
25	b	603	CLA	C4D-ND	-2.89	1.33	1.37
25	B	602	CLA	C4D-ND	-2.89	1.33	1.37
25	B	603	CLA	C4D-ND	-2.89	1.33	1.37
27	P	620	WVN	C29-C26	2.89	1.52	1.43
25	4	607	CLA	C4D-ND	-2.89	1.33	1.37
27	y	89	WVN	C02-C11	2.89	1.54	1.50
25	5	610	CLA	C4D-ND	-2.88	1.33	1.37
27	c	530	WVN	C39-C36	2.88	1.52	1.43
29	d	405	PL9	C3-C4	-2.88	1.44	1.49
27	B	618	WVN	C26-C22	-2.88	1.32	1.35
25	d	403	CLA	C4D-ND	-2.88	1.33	1.37
25	R	602	CLA	C4D-ND	-2.88	1.33	1.37
38	N	616	II0	C41-C39	2.88	1.52	1.43
25	b	608	CLA	C4D-ND	-2.88	1.33	1.37
25	Q	610	CLA	C4D-ND	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	617	WVN	C26-C22	-2.88	1.32	1.35
38	1	616	II0	C41-C39	2.88	1.52	1.43
29	D	405	PL9	C3-C4	-2.88	1.44	1.49
38	2	617	II0	C41-C39	2.88	1.52	1.43
37	1	605	KC2	C4D-CHA	2.88	1.48	1.45
25	b	614	CLA	C4D-ND	-2.88	1.33	1.37
25	g	302	CLA	C4D-ND	-2.88	1.33	1.37
25	C	517	CLA	CHC-C1C	2.88	1.42	1.35
27	B	618	WVN	C28-C25	-2.88	1.32	1.35
25	b	610	CLA	C4D-ND	-2.88	1.33	1.37
25	5	607	CLA	C4D-ND	-2.88	1.33	1.37
25	6	601	CLA	C4D-ND	-2.88	1.33	1.37
27	C	529	WVN	C26-C22	-2.88	1.32	1.35
36	e	102	HEM	FE-NB	2.87	2.11	1.96
25	c	519	CLA	C4D-ND	-2.87	1.33	1.37
25	R	607	CLA	C4D-ND	-2.87	1.33	1.37
37	N	605	KC2	C4D-CHA	2.87	1.48	1.45
37	1	605	KC2	C4A-C3A	2.87	1.50	1.44
38	R	617	II0	C41-C39	2.87	1.52	1.43
25	3	611	CLA	C4D-ND	-2.87	1.33	1.37
27	A	407	WVN	C39-C36	2.87	1.52	1.43
25	2	606	CLA	C4D-ND	-2.87	1.33	1.37
25	1	606	CLA	C4D-ND	-2.87	1.33	1.37
25	R	604	CLA	C4D-ND	-2.87	1.33	1.37
25	6	609	CLA	C4D-ND	-2.87	1.33	1.37
25	c	518	CLA	C4D-ND	-2.87	1.33	1.37
25	N	606	CLA	C4D-ND	-2.87	1.33	1.37
25	1	607	CLA	C4D-ND	-2.87	1.33	1.37
38	3	617	II0	C41-C39	2.87	1.52	1.43
25	Q	602	CLA	C4D-ND	-2.87	1.33	1.37
25	O	606	CLA	C4D-ND	-2.86	1.33	1.37
38	5	617	II0	C41-C39	2.86	1.52	1.43
25	G	301	CLA	CHC-C1C	2.86	1.42	1.35
25	D	404	CLA	C4D-ND	-2.86	1.33	1.37
27	b	618	WVN	C26-C22	-2.86	1.32	1.35
25	B	614	CLA	C4D-ND	-2.86	1.33	1.37
39	Q	620	IHT	C34-C35	2.86	1.52	1.45
25	4	606	CLA	C4D-ND	-2.86	1.33	1.37
25	S	601	CLA	C4D-ND	-2.86	1.33	1.37
27	h	89	WVN	C28-C25	-2.86	1.32	1.35
27	D	408	WVN	C26-C22	-2.86	1.32	1.35
25	5	611	CLA	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	517	CLA	CHC-C1C	2.86	1.42	1.35
25	B	608	CLA	C4D-ND	-2.86	1.33	1.37
25	C	528	CLA	C4D-ND	-2.86	1.33	1.37
25	3	613	CLA	C4D-ND	-2.86	1.33	1.37
27	C	530	WVN	C39-C36	2.86	1.52	1.43
27	P	620	WVN	C23-C25	2.85	1.52	1.45
27	C	531	WVN	C28-C25	-2.85	1.32	1.35
25	N	607	CLA	C4D-ND	-2.85	1.33	1.37
27	3	620	WVN	C23-C25	2.85	1.52	1.45
27	Y	89	WVN	C28-C25	-2.85	1.32	1.35
27	B	619	WVN	C28-C25	-2.85	1.32	1.35
27	B	619	WVN	C23-C25	2.85	1.52	1.45
25	B	610	CLA	C4D-ND	-2.85	1.33	1.37
25	b	607	CLA	C4D-ND	-2.85	1.33	1.37
25	O	604	CLA	C4D-ND	-2.85	1.33	1.37
25	b	602	CLA	C4D-ND	-2.85	1.33	1.37
27	C	529	WVN	C36-C32	-2.84	1.32	1.35
25	4	609	CLA	C4D-ND	-2.84	1.33	1.37
25	O	615	CLA	C4D-ND	-2.84	1.33	1.37
25	Q	603	CLA	C4D-ND	-2.84	1.33	1.37
37	S	612	KC2	C4D-CHA	2.84	1.48	1.45
25	C	526	CLA	C4D-ND	-2.84	1.33	1.37
38	6	619	II0	C41-C39	2.84	1.52	1.43
25	c	525	CLA	C4D-ND	-2.84	1.33	1.37
25	b	604	CLA	CHC-C1C	2.84	1.42	1.35
25	1	604	CLA	C4D-ND	-2.84	1.33	1.37
25	6	611	CLA	C4D-ND	-2.84	1.33	1.37
38	P	617	II0	C41-C39	2.84	1.52	1.43
27	B	617	WVN	C37-C34	-2.84	1.32	1.35
25	2	609	CLA	C4D-ND	-2.83	1.33	1.37
25	4	603	CLA	C4D-ND	-2.83	1.33	1.37
25	4	607	CLA	CHC-C1C	2.83	1.42	1.35
25	d	404	CLA	C4D-ND	-2.83	1.33	1.37
27	c	531	WVN	C23-C25	2.83	1.52	1.45
25	g	301	CLA	C4D-ND	-2.83	1.33	1.37
25	5	613	CLA	CHC-C1C	2.83	1.42	1.35
25	C	522	CLA	C4D-ND	-2.83	1.33	1.37
27	B	617	WVN	C28-C25	-2.83	1.32	1.35
25	O	609	CLA	C4D-ND	-2.83	1.33	1.37
25	R	606	CLA	C4D-ND	-2.82	1.33	1.37
25	Q	606	CLA	C4D-ND	-2.82	1.33	1.37
25	D	403	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	619	WVN	C36-C32	-2.82	1.32	1.35
25	R	613	CLA	C4D-ND	-2.82	1.33	1.37
27	b	617	WVN	C33-C34	2.82	1.52	1.45
27	P	620	WVN	C30-C28	2.82	1.52	1.43
25	R	611	CLA	C4D-ND	-2.82	1.33	1.37
37	S	606	KC2	C4D-CHA	2.82	1.48	1.45
25	B	604	CLA	CHC-C1C	2.82	1.42	1.35
25	5	615	CLA	C4D-ND	-2.82	1.33	1.37
25	Q	613	CLA	C4D-ND	-2.82	1.33	1.37
25	4	613	CLA	C4D-ND	-2.82	1.33	1.37
27	c	530	WVN	C28-C25	-2.82	1.32	1.35
38	6	617	II0	C41-C39	2.82	1.52	1.43
25	2	610	CLA	C4D-ND	-2.82	1.33	1.37
27	C	530	WVN	C23-C25	2.82	1.52	1.45
25	c	522	CLA	C4D-ND	-2.82	1.33	1.37
27	3	620	WVN	C30-C28	2.81	1.52	1.43
25	Q	607	CLA	CHC-C1C	2.81	1.42	1.35
25	c	527	CLA	C4D-ND	-2.81	1.33	1.37
25	2	615	CLA	C4D-ND	-2.81	1.33	1.37
25	R	613	CLA	CHC-C1C	2.81	1.42	1.35
25	c	524	CLA	C4D-ND	-2.80	1.33	1.37
27	b	617	WVN	C40-C37	2.80	1.52	1.43
27	Y	89	WVN	C26-C22	-2.80	1.32	1.35
25	A	404	CLA	C4D-ND	-2.80	1.33	1.37
38	S	617	II0	C41-C39	2.80	1.52	1.43
38	Q	616	II0	C40-C36	-2.80	1.32	1.35
25	C	524	CLA	C4D-ND	-2.80	1.33	1.37
25	C	527	CLA	C4D-ND	-2.80	1.33	1.37
25	O	607	CLA	C4D-ND	-2.79	1.33	1.37
25	b	613	CLA	C4D-ND	-2.79	1.33	1.37
25	5	603	CLA	C4D-ND	-2.79	1.33	1.37
25	2	604	CLA	C4D-ND	-2.79	1.33	1.37
25	S	611	CLA	C4D-ND	-2.79	1.33	1.37
25	3	612	CLA	C4D-ND	-2.79	1.33	1.37
25	N	601	CLA	C4D-ND	-2.79	1.33	1.37
27	a	407	WVN	C26-C22	-2.78	1.32	1.35
27	C	531	WVN	C36-C32	-2.78	1.32	1.35
27	B	618	WVN	C36-C32	-2.78	1.32	1.35
25	O	613	CLA	C4D-ND	-2.78	1.33	1.37
25	P	603	CLA	C4D-ND	-2.78	1.33	1.37
27	D	408	WVN	C36-C32	-2.78	1.32	1.35
37	3	606	KC2	C1D-CHD	2.78	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	P	606	KC2	C1D-CHD	2.78	1.48	1.41
25	2	613	CLA	C4D-ND	-2.78	1.33	1.37
27	b	618	WVN	C36-C32	-2.78	1.32	1.35
25	S	613	CLA	C4D-ND	-2.78	1.33	1.37
25	5	606	CLA	C4D-ND	-2.78	1.33	1.37
25	b	601	CLA	C4D-ND	-2.78	1.33	1.37
27	A	407	WVN	C23-C25	2.78	1.51	1.45
25	c	526	CLA	C4D-ND	-2.78	1.33	1.37
25	5	613	CLA	C4D-ND	-2.78	1.33	1.37
37	6	612	KC2	C4D-CHA	2.77	1.48	1.45
25	R	615	CLA	C4D-ND	-2.77	1.33	1.37
37	1	612	KC2	C1B-NB	-2.77	1.34	1.37
38	4	616	II0	C40-C36	-2.77	1.32	1.35
27	A	407	WVN	C40-C37	2.77	1.52	1.43
39	1	620	IHT	C34-C35	2.77	1.51	1.45
27	C	531	WVN	C26-C22	-2.77	1.32	1.35
25	B	613	CLA	C4D-ND	-2.77	1.33	1.37
25	B	615	CLA	C4D-ND	-2.77	1.33	1.37
25	a	404	CLA	C4D-ND	-2.77	1.33	1.37
25	c	528	CLA	C4D-ND	-2.77	1.33	1.37
27	a	407	WVN	C28-C25	-2.76	1.32	1.35
27	c	529	WVN	C37-C34	-2.76	1.32	1.35
27	b	617	WVN	C30-C28	2.76	1.52	1.43
25	N	614	CLA	C4D-ND	-2.76	1.33	1.37
25	R	603	CLA	C4D-ND	-2.76	1.33	1.37
25	B	604	CLA	C4D-ND	-2.76	1.33	1.37
25	Q	615	CLA	C4D-ND	-2.76	1.33	1.37
27	A	407	WVN	C30-C28	2.76	1.52	1.43
25	R	601	CLA	CHC-C1C	2.76	1.42	1.35
37	Q	611	KC2	C1B-NB	-2.76	1.34	1.37
37	N	612	KC2	C1B-NB	-2.76	1.34	1.37
25	6	615	CLA	C4D-ND	-2.76	1.33	1.37
25	P	609	CLA	C4D-ND	-2.76	1.33	1.37
37	4	605	KC2	C4A-C3A	2.76	1.49	1.44
25	b	612	CLA	C4D-ND	-2.76	1.33	1.37
25	N	615	CLA	C4D-ND	-2.76	1.33	1.37
25	B	601	CLA	C4D-ND	-2.75	1.33	1.37
25	N	603	CLA	C4D-ND	-2.75	1.33	1.37
37	N	613	KC2	C1D-CHD	2.75	1.48	1.41
27	b	619	WVN	C28-C25	-2.75	1.32	1.35
25	b	606	CLA	C4D-ND	-2.75	1.33	1.37
25	3	603	CLA	C4D-ND	-2.75	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	613	CLA	C4D-ND	-2.75	1.33	1.37
25	1	603	CLA	C4D-ND	-2.75	1.33	1.37
27	h	89	WVN	C19-C22	2.75	1.51	1.45
25	b	604	CLA	C4D-ND	-2.75	1.33	1.37
25	1	601	CLA	C4D-ND	-2.75	1.33	1.37
27	H	89	WVN	C19-C22	2.75	1.51	1.45
25	5	601	CLA	CHC-C1C	2.74	1.42	1.35
37	6	612	KC2	C1B-NB	-2.74	1.34	1.37
25	O	611	CLA	C4D-ND	-2.74	1.33	1.37
37	S	612	KC2	C1B-NB	-2.74	1.34	1.37
37	Q	605	KC2	C4A-C3A	2.74	1.49	1.44
25	2	611	CLA	C4D-ND	-2.74	1.33	1.37
37	4	611	KC2	C1B-NB	-2.74	1.34	1.37
29	A	409	PL9	C3-C4	-2.74	1.45	1.49
25	b	615	CLA	C4D-ND	-2.74	1.33	1.37
37	N	613	KC2	C4A-C3A	2.73	1.49	1.44
38	O	618	II0	C40-C36	-2.73	1.32	1.35
29	a	409	PL9	C3-C4	-2.73	1.45	1.49
25	4	615	CLA	C4D-ND	-2.73	1.33	1.37
37	R	612	KC2	C1B-NB	-2.73	1.34	1.37
37	5	612	KC2	C4A-C3A	2.73	1.49	1.44
25	S	615	CLA	C4D-ND	-2.72	1.33	1.37
37	S	606	KC2	C1D-CHD	2.72	1.48	1.41
37	1	613	KC2	C1D-CHD	2.72	1.48	1.41
25	1	614	CLA	C4D-ND	-2.72	1.33	1.37
39	4	620	IHT	C34-C35	2.72	1.51	1.45
25	3	609	CLA	C4D-ND	-2.72	1.33	1.37
25	2	607	CLA	C4D-ND	-2.72	1.34	1.37
37	6	606	KC2	C1D-CHD	2.72	1.48	1.41
27	c	530	WVN	C36-C32	-2.72	1.32	1.35
25	3	615	CLA	C4D-ND	-2.72	1.34	1.37
25	1	615	CLA	C4D-ND	-2.71	1.34	1.37
25	P	612	CLA	C4D-ND	-2.71	1.34	1.37
37	2	612	KC2	C1B-NB	-2.71	1.34	1.37
25	O	601	CLA	C4D-ND	-2.71	1.34	1.37
37	P	606	KC2	C4A-C3A	2.71	1.49	1.44
38	3	616	II0	C40-C36	-2.71	1.32	1.35
27	C	531	WVN	C37-C34	-2.70	1.32	1.35
37	3	606	KC2	C4A-C3A	2.70	1.49	1.44
25	B	606	CLA	C4D-ND	-2.70	1.34	1.37
25	S	604	CLA	C4D-ND	-2.70	1.34	1.37
37	4	611	KC2	C1D-CHD	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	612	KC2	C1B-NB	-2.70	1.34	1.37
25	N	609	CLA	C4D-ND	-2.69	1.34	1.37
37	R	612	KC2	C4A-C3A	2.69	1.49	1.44
27	Y	89	WVN	C02-C11	2.69	1.54	1.50
38	2	618	II0	C40-C36	-2.69	1.32	1.35
38	6	618	II0	C40-C36	-2.69	1.32	1.35
37	1	613	KC2	C4A-C3A	2.69	1.49	1.44
25	P	615	CLA	C4D-ND	-2.69	1.34	1.37
25	Q	609	CLA	C4D-ND	-2.69	1.34	1.37
37	Q	611	KC2	C1D-CHD	2.69	1.48	1.41
37	N	613	KC2	C3C-C4C	2.68	1.50	1.44
25	2	601	CLA	C4D-ND	-2.68	1.34	1.37
38	O	617	II0	C40-C36	-2.68	1.32	1.35
25	B	612	CLA	C4D-ND	-2.68	1.34	1.37
38	6	617	II0	C40-C36	-2.68	1.32	1.35
27	c	529	WVN	C36-C32	-2.67	1.32	1.35
38	5	617	II0	C40-C36	-2.67	1.32	1.35
38	S	618	II0	C40-C36	-2.67	1.32	1.35
37	3	606	KC2	C1B-NB	-2.67	1.34	1.37
38	P	616	II0	C40-C36	-2.67	1.32	1.35
38	R	617	II0	C40-C36	-2.67	1.32	1.35
37	S	612	KC2	C4A-C3A	2.67	1.49	1.44
37	R	612	KC2	C1D-CHD	2.67	1.48	1.41
38	Q	617	II0	C40-C36	-2.66	1.32	1.35
37	Q	612	KC2	C1D-CHD	2.66	1.48	1.41
39	O	620	IHT	C22-C23	2.66	1.51	1.45
38	R	618	II0	C40-C36	-2.66	1.32	1.35
27	D	408	WVN	C02-C11	2.66	1.54	1.50
38	5	618	II0	C40-C36	-2.66	1.32	1.35
38	1	618	II0	C40-C36	-2.66	1.32	1.35
38	N	619	II0	C40-C36	-2.66	1.32	1.35
37	1	611	KC2	C1D-CHD	2.66	1.48	1.41
37	N	605	KC2	C1D-CHD	2.66	1.48	1.41
37	4	612	KC2	C1D-CHD	2.66	1.48	1.41
38	R	616	II0	C40-C36	-2.66	1.32	1.35
37	1	605	KC2	C1D-CHD	2.65	1.48	1.41
37	1	613	KC2	C3C-C4C	2.65	1.50	1.44
38	P	617	II0	C40-C36	-2.65	1.32	1.35
38	4	617	II0	C40-C36	-2.65	1.32	1.35
25	6	603	CLA	C4D-ND	-2.65	1.34	1.37
39	2	620	IHT	C22-C23	2.65	1.51	1.45
25	3	604	CLA	C4D-ND	-2.65	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	619	II0	C40-C36	-2.65	1.32	1.35
37	5	612	KC2	C1D-CHD	2.64	1.48	1.41
27	C	531	WVN	C02-C11	2.64	1.54	1.50
38	2	617	II0	C40-C36	-2.63	1.32	1.35
38	3	618	II0	C40-C36	-2.63	1.32	1.35
37	N	611	KC2	C1D-CHD	2.63	1.48	1.41
38	S	617	II0	C40-C36	-2.63	1.32	1.35
38	N	618	II0	C40-C36	-2.63	1.32	1.35
37	6	612	KC2	C4A-C3A	2.63	1.49	1.44
27	c	529	WVN	C02-C11	2.62	1.54	1.50
38	1	616	II0	C40-C36	-2.62	1.32	1.35
37	Q	611	KC2	C4A-C3A	2.61	1.49	1.44
38	5	616	II0	C40-C36	-2.61	1.32	1.35
25	2	607	CLA	CMB-C2B	-2.61	1.46	1.51
38	6	619	II0	C40-C36	-2.61	1.32	1.35
38	2	616	II0	C40-C36	-2.61	1.32	1.35
25	P	604	CLA	C4D-ND	-2.61	1.34	1.37
25	6	604	CLA	C4D-ND	-2.61	1.34	1.37
37	N	605	KC2	C1B-NB	-2.60	1.34	1.37
37	4	605	KC2	C1D-CHD	2.60	1.48	1.41
37	P	606	KC2	C1B-NB	-2.60	1.34	1.37
38	3	619	II0	C40-C36	-2.60	1.32	1.35
38	6	616	II0	C40-C36	-2.60	1.32	1.35
37	Q	605	KC2	C1D-CHD	2.60	1.48	1.41
37	Q	612	KC2	C3C-C4C	2.60	1.50	1.44
38	4	618	II0	C40-C36	-2.60	1.32	1.35
37	N	611	KC2	C1B-NB	-2.60	1.34	1.37
37	S	606	KC2	C3C-C4C	2.60	1.50	1.44
37	N	611	KC2	C4A-C3A	2.60	1.49	1.44
37	O	612	KC2	C1B-NB	-2.60	1.34	1.37
38	S	616	II0	C40-C36	-2.60	1.32	1.35
37	4	605	KC2	C1B-NB	-2.59	1.34	1.37
37	N	612	KC2	C4A-C3A	2.59	1.49	1.44
37	4	612	KC2	C3C-C4C	2.59	1.50	1.44
37	4	611	KC2	C4A-C3A	2.59	1.49	1.44
38	N	616	II0	C40-C36	-2.59	1.32	1.35
37	N	611	KC2	C3C-C4C	2.58	1.50	1.44
38	R	619	II0	C40-C36	-2.58	1.32	1.35
38	3	617	II0	C40-C36	-2.58	1.32	1.35
27	b	619	WVN	C20-C13	2.58	1.54	1.45
25	O	607	CLA	CMB-C2B	-2.58	1.46	1.51
27	C	529	WVN	C37-C34	-2.58	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	611	KC2	C3C-C4C	2.58	1.50	1.44
37	1	611	KC2	C4A-C3A	2.58	1.49	1.44
38	1	617	II0	C40-C36	-2.58	1.32	1.35
37	S	606	KC2	C1B-NB	-2.58	1.34	1.37
37	2	612	KC2	C1D-CHD	2.57	1.48	1.41
37	N	613	KC2	C1A-CHA	2.57	1.47	1.40
38	Q	618	II0	C40-C36	-2.57	1.32	1.35
26	A	405	PHO	CAC-C3C	-2.57	1.47	1.52
27	S	620	WVN	C37-C34	-2.57	1.32	1.35
38	P	619	II0	C40-C36	-2.57	1.32	1.35
38	O	616	II0	C40-C36	-2.56	1.32	1.35
27	B	617	WVN	C19-C22	2.56	1.51	1.45
38	5	619	II0	C40-C36	-2.56	1.32	1.35
39	1	620	IHT	C22-C23	2.56	1.51	1.45
37	6	606	KC2	C4D-CHA	2.56	1.48	1.45
37	N	612	KC2	C1D-CHD	2.56	1.48	1.41
37	1	613	KC2	C1A-CHA	2.56	1.47	1.40
37	1	611	KC2	C1B-NB	-2.56	1.34	1.37
37	1	612	KC2	C4A-C3A	2.56	1.49	1.44
25	b	604	CLA	CMB-C2B	-2.56	1.46	1.51
37	1	612	KC2	C1D-CHD	2.56	1.48	1.41
37	S	612	KC2	C1D-CHD	2.56	1.48	1.41
37	4	612	KC2	C1B-NB	-2.55	1.34	1.37
37	O	612	KC2	C1D-CHD	2.55	1.48	1.41
25	N	607	CLA	CMB-C2B	-2.55	1.46	1.51
37	Q	612	KC2	C1B-NB	-2.55	1.34	1.37
37	Q	605	KC2	C1B-NB	-2.54	1.34	1.37
25	5	609	CLA	CMB-C2B	-2.54	1.46	1.51
37	3	606	KC2	C3C-C4C	2.54	1.50	1.44
27	d	408	WVN	C02-C11	2.54	1.54	1.50
25	1	607	CLA	CMB-C2B	-2.54	1.46	1.51
26	a	405	PHO	CAC-C3C	-2.54	1.47	1.52
38	S	619	II0	C40-C36	-2.54	1.32	1.35
38	P	618	II0	C40-C36	-2.54	1.32	1.35
37	6	606	KC2	C3C-C4C	2.54	1.49	1.44
39	5	620	IHT	C22-C23	2.54	1.51	1.45
27	6	620	WVN	C26-C22	-2.53	1.32	1.35
39	Q	620	IHT	C22-C23	2.53	1.51	1.45
27	S	620	WVN	C36-C32	-2.53	1.32	1.35
25	O	604	CLA	CMB-C2B	-2.53	1.46	1.51
27	c	530	WVN	C02-C11	2.53	1.54	1.50
25	B	604	CLA	CMB-C2B	-2.53	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	603	CLA	CMB-C2B	-2.53	1.46	1.51
27	C	529	WVN	C20-C13	2.52	1.54	1.45
39	4	620	IHT	C22-C23	2.52	1.51	1.45
25	4	607	CLA	CMB-C2B	-2.52	1.46	1.51
27	S	620	WVN	C26-C22	-2.52	1.32	1.35
27	C	531	WVN	C20-C13	2.52	1.54	1.45
26	D	401	PHO	CAC-C3C	-2.52	1.47	1.52
25	R	609	CLA	CMB-C2B	-2.52	1.46	1.51
39	N	620	IHT	C34-C35	2.51	1.51	1.45
25	c	521	CLA	CMB-C2B	-2.51	1.46	1.51
25	Q	607	CLA	CMB-C2B	-2.51	1.46	1.51
27	c	529	WVN	C20-C13	2.51	1.54	1.45
26	d	401	PHO	CAC-C3C	-2.51	1.47	1.52
25	2	604	CLA	CMB-C2B	-2.51	1.46	1.51
25	C	517	CLA	CMB-C2B	-2.51	1.46	1.51
37	6	612	KC2	C1D-CHD	2.51	1.48	1.41
37	1	605	KC2	C1B-NB	-2.50	1.34	1.37
27	d	408	WVN	C28-C25	-2.50	1.32	1.35
37	P	606	KC2	C3C-C4C	2.50	1.49	1.44
25	R	613	CLA	CMB-C2B	-2.50	1.46	1.51
27	b	617	WVN	C23-C25	2.49	1.51	1.45
25	B	608	CLA	CMB-C2B	-2.49	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.49	1.46	1.51
25	4	606	CLA	CMB-C2B	-2.49	1.46	1.51
38	N	617	II0	C40-C36	-2.49	1.32	1.35
39	N	620	IHT	C22-C23	2.49	1.51	1.45
37	Q	611	KC2	C3C-C4C	2.49	1.49	1.44
37	N	613	KC2	C1B-NB	-2.49	1.34	1.37
27	H	89	WVN	C20-C13	2.49	1.53	1.45
25	6	601	CLA	CMB-C2B	-2.48	1.46	1.51
27	c	531	WVN	C02-C11	2.48	1.53	1.50
27	B	619	WVN	C20-C13	2.48	1.53	1.45
27	Y	89	WVN	C20-C13	2.48	1.53	1.45
37	2	612	KC2	C4A-C3A	2.48	1.49	1.44
27	D	408	WVN	C20-C13	2.48	1.53	1.45
27	h	89	WVN	C20-C13	2.48	1.53	1.45
25	c	517	CLA	CMB-C2B	-2.48	1.46	1.51
27	a	407	WVN	C20-C13	2.47	1.53	1.45
25	S	601	CLA	CMB-C2B	-2.47	1.46	1.51
25	1	609	CLA	CMB-C2B	-2.47	1.46	1.51
37	O	612	KC2	C4A-C3A	2.47	1.49	1.44
25	5	613	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	613	KC2	C1B-NB	-2.47	1.34	1.37
25	B	609	CLA	CMB-C2B	-2.47	1.46	1.51
25	1	610	CLA	CMB-C2B	-2.47	1.46	1.51
37	1	612	KC2	C3C-C4C	2.47	1.49	1.44
38	2	619	II0	C40-C36	-2.47	1.32	1.35
25	5	603	CLA	CMB-C2B	-2.46	1.46	1.51
25	C	521	CLA	CMB-C2B	-2.46	1.46	1.51
25	R	603	CLA	CMB-C2B	-2.46	1.46	1.51
37	Q	612	KC2	C4A-C3A	2.46	1.49	1.44
27	6	620	WVN	C37-C34	-2.46	1.32	1.35
38	4	619	II0	C40-C36	-2.46	1.32	1.35
25	g	302	CLA	CMB-C2B	-2.46	1.46	1.51
27	d	408	WVN	C20-C13	2.46	1.53	1.45
37	4	612	KC2	C4A-C3A	2.46	1.49	1.44
27	6	620	WVN	C36-C32	-2.46	1.32	1.35
25	g	301	CLA	CMB-C2B	-2.45	1.46	1.51
25	1	601	CLA	CMB-C2B	-2.45	1.46	1.51
25	Q	603	CLA	CMB-C2B	-2.45	1.46	1.51
37	2	612	KC2	C3C-C4C	2.45	1.49	1.44
25	N	609	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.45	1.46	1.51
25	4	609	CLA	CMB-C2B	-2.45	1.46	1.51
27	y	89	WVN	C20-C13	2.45	1.53	1.45
27	S	620	WVN	C20-C13	2.45	1.53	1.45
27	D	408	WVN	C28-C25	-2.45	1.32	1.35
25	4	603	CLA	CMB-C2B	-2.45	1.46	1.51
27	6	620	WVN	C20-C13	2.45	1.53	1.45
25	b	603	CLA	CMB-C2B	-2.45	1.46	1.51
37	N	612	KC2	C3C-C4C	2.45	1.49	1.44
25	G	302	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.45	1.46	1.51
25	A	403	CLA	CMB-C2B	-2.45	1.46	1.51
25	Q	609	CLA	CMB-C2B	-2.44	1.46	1.51
37	4	611	KC2	C3C-C4C	2.44	1.49	1.44
25	a	403	CLA	CMB-C2B	-2.44	1.46	1.51
38	3	617	II0	C29-C25	-2.44	1.31	1.37
38	Q	619	II0	C40-C36	-2.44	1.32	1.35
37	O	612	KC2	C3C-C4C	2.44	1.49	1.44
25	N	610	CLA	CMB-C2B	-2.44	1.46	1.51
27	C	530	WVN	C20-C13	2.44	1.53	1.45
25	C	523	CLA	CMB-C2B	-2.44	1.46	1.51
25	4	610	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	610	CLA	CMB-C2B	-2.43	1.46	1.51
25	P	612	CLA	CMB-C2B	-2.43	1.46	1.51
25	R	615	CLA	CMB-C2B	-2.43	1.46	1.51
37	S	612	KC2	C3C-C4C	2.43	1.49	1.44
25	3	612	CLA	CMB-C2B	-2.43	1.46	1.51
27	h	89	WVN	C02-C11	2.43	1.53	1.50
25	b	601	CLA	CMB-C2B	-2.43	1.46	1.51
27	B	619	WVN	C02-C11	2.43	1.53	1.50
39	5	620	IHT	C34-C35	2.43	1.51	1.45
25	1	615	CLA	CMB-C2B	-2.43	1.46	1.51
25	G	301	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.42	1.46	1.51
27	B	618	WVN	C02-C11	2.42	1.53	1.50
25	B	613	CLA	CMB-C2B	-2.42	1.46	1.51
25	d	400	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.42	1.46	1.51
39	N	620	IHT	C22-C18	2.42	1.40	1.33
37	R	612	KC2	C3C-C4C	2.42	1.49	1.44
25	2	606	CLA	CMB-C2B	-2.42	1.46	1.51
37	1	611	KC2	C1A-CHA	2.42	1.47	1.40
27	B	617	WVN	C20-C13	2.42	1.53	1.45
27	c	530	WVN	C20-C13	2.42	1.53	1.45
25	C	520	CLA	CMB-C2B	-2.42	1.46	1.51
25	3	611	CLA	CMB-C2B	-2.42	1.46	1.51
37	N	611	KC2	C1A-CHA	2.41	1.47	1.40
25	R	601	CLA	CMB-C2B	-2.41	1.46	1.51
25	5	615	CLA	CMB-C2B	-2.41	1.46	1.51
37	6	606	KC2	C1B-NB	-2.41	1.34	1.37
25	2	601	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	526	CLA	CMB-C2B	-2.41	1.46	1.51
39	1	620	IHT	C22-C18	2.41	1.40	1.33
25	C	527	CLA	CMB-C2B	-2.41	1.46	1.51
38	O	619	II0	C40-C36	-2.41	1.32	1.35
25	N	601	CLA	CMB-C2B	-2.41	1.46	1.51
25	P	603	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.40	1.46	1.51
25	2	609	CLA	CMB-C2B	-2.40	1.46	1.51
27	H	89	WVN	C02-C11	2.40	1.53	1.50
25	5	606	CLA	CMB-C2B	-2.40	1.46	1.51
25	D	400	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	523	CLA	CMB-C2B	-2.40	1.46	1.51
37	5	612	KC2	C3C-C4C	2.40	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	CMB-C2B	-2.40	1.46	1.51
25	O	609	CLA	CMB-C2B	-2.40	1.46	1.51
27	B	618	WVN	C20-C13	2.40	1.53	1.45
25	6	611	CLA	CMB-C2B	-2.40	1.46	1.51
25	5	607	CLA	CMB-C2B	-2.40	1.46	1.51
25	Q	606	CLA	CMB-C2B	-2.40	1.46	1.51
25	O	606	CLA	CMB-C2B	-2.40	1.46	1.51
25	5	601	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	526	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	520	CLA	CMB-C2B	-2.39	1.46	1.51
37	4	605	KC2	C3C-C4C	2.39	1.49	1.44
25	N	603	CLA	CMB-C2B	-2.39	1.46	1.51
39	R	620	IHT	C22-C23	2.39	1.51	1.45
25	O	603	CLA	CMB-C2B	-2.39	1.46	1.51
39	R	620	IHT	C34-C35	2.39	1.51	1.45
25	d	403	CLA	CMB-C2B	-2.39	1.46	1.51
25	P	601	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	601	CLA	CMB-C2B	-2.39	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.39	1.46	1.51
25	2	603	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.39	1.46	1.51
25	3	601	CLA	CMB-C2B	-2.39	1.46	1.51
37	1	605	KC2	C3C-C4C	2.39	1.49	1.44
37	N	605	KC2	C3C-C4C	2.38	1.49	1.44
37	6	612	KC2	C3C-C4C	2.38	1.49	1.44
25	c	527	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.38	1.46	1.51
25	O	611	CLA	CMB-C2B	-2.38	1.46	1.51
39	R	620	IHT	C22-C18	2.38	1.40	1.33
25	S	611	CLA	CMB-C2B	-2.38	1.46	1.51
25	a	406	CLA	CMB-C2B	-2.38	1.46	1.51
37	Q	605	KC2	C3C-C4C	2.38	1.49	1.44
25	b	613	CLA	CMB-C2B	-2.37	1.46	1.51
25	O	601	CLA	CMB-C2B	-2.37	1.46	1.51
37	4	605	KC2	C1A-CHA	2.37	1.46	1.40
25	b	606	CLA	CMB-C2B	-2.37	1.46	1.51
25	3	603	CLA	CMB-C2B	-2.37	1.46	1.51
25	N	615	CLA	CMB-C2B	-2.37	1.46	1.51
25	S	602	CLA	CMB-C2B	-2.37	1.46	1.51
25	O	607	CLA	C3B-C2B	-2.37	1.37	1.40
25	5	610	CLA	CMB-C2B	-2.37	1.46	1.51
25	P	611	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Q	605	KC2	C1A-CHA	2.37	1.46	1.40
25	c	516	CLA	CMB-C2B	-2.37	1.46	1.51
25	C	516	CLA	CMB-C2B	-2.37	1.46	1.51
27	A	407	WVN	C20-C13	2.37	1.53	1.45
25	b	605	CLA	CMB-C2B	-2.37	1.46	1.51
25	2	611	CLA	CMB-C2B	-2.37	1.46	1.51
25	1	603	CLA	CMB-C2B	-2.36	1.46	1.51
25	S	609	CLA	CMB-C2B	-2.36	1.46	1.51
25	5	611	CLA	CMB-C2B	-2.36	1.46	1.51
25	R	610	CLA	CMB-C2B	-2.36	1.46	1.51
25	R	607	CLA	CMB-C2B	-2.36	1.46	1.51
25	b	602	CLA	CMB-C2B	-2.36	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	518	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	522	CLA	CMB-C2B	-2.36	1.46	1.51
25	6	609	CLA	CMB-C2B	-2.36	1.46	1.51
39	Q	620	IHT	C22-C18	2.36	1.40	1.33
25	2	613	CLA	CMB-C2B	-2.36	1.46	1.51
25	R	604	CLA	CMB-C2B	-2.36	1.46	1.51
25	1	606	CLA	CMB-C2B	-2.36	1.46	1.51
25	R	606	CLA	CMB-C2B	-2.36	1.46	1.51
25	B	611	CLA	CMB-C2B	-2.35	1.46	1.51
39	O	620	IHT	C22-C18	2.35	1.40	1.33
25	5	602	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	522	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	528	CLA	CMB-C2B	-2.35	1.46	1.51
25	A	404	CLA	CMB-C2B	-2.35	1.46	1.51
25	2	602	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	524	CLA	CMB-C2B	-2.35	1.46	1.51
39	2	620	IHT	C22-C18	2.35	1.40	1.33
25	c	518	CLA	CMB-C2B	-2.35	1.46	1.51
25	A	406	CLA	CMB-C2B	-2.35	1.46	1.51
25	2	607	CLA	C3B-C2B	-2.35	1.37	1.40
27	b	618	WVN	C20-C13	2.34	1.53	1.45
25	5	604	CLA	CMB-C2B	-2.34	1.46	1.51
25	P	613	CLA	CMB-C2B	-2.34	1.46	1.51
39	4	620	IHT	C22-C18	2.34	1.40	1.33
25	1	602	CLA	CMB-C2B	-2.34	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.34	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.34	1.46	1.51
25	d	404	CLA	CMB-C2B	-2.34	1.46	1.51
25	6	602	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	604	CLA	CMB-C2B	-2.34	1.46	1.51
37	4	611	KC2	C1A-CHA	2.34	1.46	1.40
25	R	611	CLA	CMB-C2B	-2.34	1.46	1.51
37	Q	611	KC2	C1A-CHA	2.34	1.46	1.40
25	N	606	CLA	CMB-C2B	-2.34	1.46	1.51
37	R	612	KC2	C1A-CHA	2.34	1.46	1.40
38	N	616	II0	C39-C35	-2.34	1.32	1.35
25	N	604	CLA	CMB-C2B	-2.34	1.46	1.51
25	d	403	CLA	CMD-C2D	-2.33	1.45	1.50
25	D	403	CLA	CMD-C2D	-2.33	1.45	1.50
25	1	604	CLA	CMB-C2B	-2.33	1.46	1.51
38	1	617	II0	C39-C35	-2.33	1.32	1.35
38	5	617	II0	C39-C35	-2.33	1.32	1.35
38	P	617	II0	C39-C35	-2.33	1.32	1.35
25	O	610	CLA	CMB-C2B	-2.33	1.46	1.51
25	1	614	CLA	CMB-C2B	-2.33	1.46	1.51
25	3	610	CLA	CMB-C2B	-2.33	1.46	1.51
38	6	617	II0	C39-C35	-2.33	1.32	1.35
25	b	614	CLA	CMB-C2B	-2.33	1.46	1.51
25	N	602	CLA	CMB-C2B	-2.33	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.33	1.46	1.51
25	O	602	CLA	CMB-C2B	-2.33	1.46	1.51
27	c	531	WVN	C20-C13	2.32	1.53	1.45
25	C	528	CLA	CMB-C2B	-2.32	1.46	1.51
25	R	602	CLA	CMB-C2B	-2.32	1.46	1.51
37	5	612	KC2	C1A-CHA	2.32	1.46	1.40
25	b	616	CLA	CMB-C2B	-2.32	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.32	1.46	1.51
25	2	610	CLA	CMB-C2B	-2.32	1.46	1.51
25	3	609	CLA	CMB-C2B	-2.32	1.46	1.51
25	N	614	CLA	CMB-C2B	-2.32	1.46	1.51
27	b	618	WVN	C02-C11	2.32	1.53	1.50
25	O	613	CLA	CMB-C2B	-2.31	1.46	1.51
25	P	609	CLA	CMB-C2B	-2.31	1.46	1.51
25	a	404	CLA	CMB-C2B	-2.31	1.46	1.51
25	4	615	CLA	CMB-C2B	-2.31	1.46	1.51
25	Q	602	CLA	CMB-C2B	-2.31	1.46	1.51
25	Q	615	CLA	CMB-C2B	-2.31	1.46	1.51
37	P	606	KC2	C1A-CHA	2.31	1.46	1.40
38	S	619	II0	C39-C35	-2.31	1.32	1.35
25	3	613	CLA	CMB-C2B	-2.31	1.46	1.51
39	5	620	IHT	C22-C18	2.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	524	CLA	CMB-C2B	-2.31	1.46	1.51
25	D	404	CLA	CMB-C2B	-2.31	1.46	1.51
38	S	618	II0	C39-C35	-2.31	1.32	1.35
25	B	612	CLA	CMB-C2B	-2.31	1.46	1.51
25	B	605	CLA	CMB-C2B	-2.30	1.46	1.51
25	6	603	CLA	CMB-C2B	-2.30	1.46	1.51
25	P	610	CLA	CMB-C2B	-2.30	1.46	1.51
38	S	617	II0	C39-C35	-2.30	1.32	1.35
25	P	602	CLA	CMB-C2B	-2.30	1.46	1.51
25	4	604	CLA	CMB-C2B	-2.30	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.30	1.46	1.51
25	O	615	CLA	CMB-C2B	-2.30	1.46	1.51
38	O	617	II0	C39-C35	-2.30	1.32	1.35
25	C	519	CLA	CMB-C2B	-2.29	1.46	1.51
25	6	610	CLA	CMB-C2B	-2.29	1.46	1.51
38	2	617	II0	C39-C35	-2.29	1.32	1.35
38	6	619	II0	C39-C35	-2.29	1.32	1.35
25	c	525	CLA	CMB-C2B	-2.29	1.46	1.51
39	1	620	IHT	C36-C33	2.29	1.55	1.50
25	c	519	CLA	CMB-C2B	-2.29	1.46	1.51
25	C	525	CLA	CMB-C2B	-2.29	1.46	1.51
38	1	616	II0	C39-C35	-2.29	1.32	1.35
25	4	602	CLA	CMB-C2B	-2.28	1.46	1.51
25	4	613	CLA	CMB-C2B	-2.28	1.46	1.51
37	Q	612	KC2	C1A-CHA	2.28	1.46	1.40
37	3	606	KC2	C1A-CHA	2.28	1.46	1.40
25	6	613	CLA	CMB-C2B	-2.28	1.46	1.51
25	S	610	CLA	CMB-C2B	-2.28	1.46	1.51
37	4	612	KC2	C1A-CHA	2.28	1.46	1.40
38	3	616	II0	C39-C35	-2.27	1.32	1.35
27	3	620	WVN	C20-C13	2.27	1.53	1.45
38	3	617	II0	C39-C35	-2.27	1.32	1.35
27	A	407	WVN	C02-C11	2.26	1.53	1.50
37	S	606	KC2	C1B-C2B	2.26	1.49	1.45
27	b	619	WVN	C02-C11	2.26	1.53	1.50
38	R	618	II0	C39-C35	-2.26	1.32	1.35
38	O	616	II0	C39-C35	-2.26	1.32	1.35
25	S	613	CLA	CMB-C2B	-2.26	1.46	1.51
27	b	617	WVN	C02-C11	2.26	1.53	1.50
38	4	619	II0	C14-C10	-2.26	1.32	1.34
37	2	612	KC2	C1A-CHA	2.26	1.46	1.40
37	S	606	KC2	C1A-CHA	2.26	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	R	617	II0	C39-C35	-2.26	1.32	1.35
38	S	616	II0	C39-C35	-2.26	1.32	1.35
25	3	602	CLA	CMB-C2B	-2.26	1.46	1.51
38	6	618	II0	C39-C35	-2.26	1.32	1.35
38	P	616	II0	C39-C35	-2.26	1.32	1.35
38	R	619	II0	C39-C35	-2.25	1.32	1.35
25	2	615	CLA	CMB-C2B	-2.24	1.47	1.51
39	N	620	IHT	C36-C33	2.24	1.55	1.50
25	Q	613	CLA	CMB-C2B	-2.24	1.47	1.51
38	2	616	II0	C39-C35	-2.24	1.32	1.35
38	5	619	II0	C39-C35	-2.24	1.32	1.35
37	6	612	KC2	C1A-CHA	2.24	1.46	1.40
37	O	612	KC2	C1A-CHA	2.24	1.46	1.40
37	S	612	KC2	C1A-CHA	2.23	1.46	1.40
27	P	620	WVN	C20-C13	2.23	1.53	1.45
25	Q	607	CLA	C3B-C2B	-2.23	1.37	1.40
37	1	612	KC2	C1A-CHA	2.22	1.46	1.40
39	O	620	IHT	C36-C33	2.22	1.55	1.50
25	a	404	CLA	CMD-C2D	-2.22	1.46	1.50
25	c	520	CLA	CMD-C2D	-2.22	1.46	1.50
38	5	618	II0	C39-C35	-2.22	1.32	1.35
38	N	617	II0	C39-C35	-2.22	1.32	1.35
39	2	620	IHT	C36-C33	2.22	1.55	1.50
25	S	615	CLA	CMD-C2D	-2.22	1.46	1.50
25	C	520	CLA	CMD-C2D	-2.21	1.46	1.50
25	S	615	CLA	CMB-C2B	-2.21	1.47	1.51
38	4	617	II0	C39-C35	-2.21	1.32	1.35
27	3	620	WVN	C02-C11	2.21	1.53	1.50
37	1	605	KC2	C1A-CHA	2.21	1.46	1.40
38	Q	617	II0	C39-C35	-2.21	1.32	1.35
27	P	620	WVN	C02-C11	2.20	1.53	1.50
25	3	615	CLA	CMB-C2B	-2.20	1.47	1.51
38	4	618	II0	C39-C35	-2.20	1.32	1.35
25	P	604	CLA	CMB-C2B	-2.20	1.47	1.51
38	Q	619	II0	C29-C25	-2.20	1.32	1.37
27	C	530	WVN	C02-C11	2.20	1.53	1.50
25	N	607	CLA	C3B-C2B	-2.20	1.37	1.40
38	O	619	II0	C30-C26	2.20	1.41	1.37
25	6	615	CLA	CMD-C2D	-2.20	1.46	1.50
37	N	612	KC2	C1A-CHA	2.20	1.46	1.40
25	3	604	CLA	CMB-C2B	-2.20	1.47	1.51
38	O	618	II0	C39-C35	-2.20	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	609	CLA	C3B-C2B	-2.20	1.37	1.40
38	6	619	II0	C30-C26	2.19	1.41	1.37
25	A	404	CLA	CMD-C2D	-2.19	1.46	1.50
25	6	615	CLA	CMB-C2B	-2.19	1.47	1.51
38	2	619	II0	C30-C26	2.19	1.41	1.37
38	S	619	II0	C30-C26	2.19	1.41	1.37
38	Q	619	II0	C14-C10	-2.19	1.32	1.34
38	4	618	II0	C30-C26	2.19	1.41	1.37
38	6	619	II0	C29-C25	-2.19	1.32	1.37
38	R	616	II0	C39-C35	-2.19	1.32	1.35
39	R	620	IHT	C05-C08	2.18	1.55	1.52
25	B	612	CLA	CMD-C2D	-2.18	1.46	1.50
29	A	409	PL9	C53-C6	-2.18	1.46	1.50
37	N	605	KC2	C1A-CHA	2.18	1.46	1.40
25	4	607	CLA	C3B-C2B	-2.18	1.37	1.40
39	2	620	IHT	C30-C27	2.17	1.50	1.43
38	6	616	II0	C39-C35	-2.17	1.32	1.35
39	O	620	IHT	C30-C27	2.17	1.50	1.43
38	5	619	II0	C30-C26	2.17	1.41	1.37
25	5	609	CLA	C3B-CAB	-2.17	1.43	1.47
37	6	606	KC2	C1A-CHA	2.16	1.46	1.40
38	1	619	II0	C30-C26	2.16	1.41	1.37
25	6	604	CLA	CMB-C2B	-2.16	1.47	1.51
38	O	619	II0	C39-C35	-2.16	1.32	1.35
38	Q	616	II0	C39-C35	-2.16	1.32	1.35
25	1	607	CLA	C3B-C2B	-2.16	1.37	1.40
25	5	609	CLA	C3B-C2B	-2.15	1.37	1.40
25	S	604	CLA	CMB-C2B	-2.15	1.47	1.51
38	R	619	II0	C30-C26	2.15	1.41	1.37
27	b	617	WVN	C20-C13	2.14	1.52	1.45
25	P	615	CLA	CMB-C2B	-2.14	1.47	1.51
38	Q	618	II0	C30-C26	2.14	1.41	1.37
38	N	619	II0	C30-C26	2.14	1.41	1.37
38	5	616	II0	C39-C35	-2.14	1.32	1.35
25	4	606	CLA	CMD-C2D	-2.14	1.46	1.50
38	4	619	II0	C30-C26	2.13	1.41	1.37
38	Q	618	II0	C39-C35	-2.13	1.33	1.35
39	4	620	IHT	C05-C08	2.13	1.55	1.52
25	b	612	CLA	CMD-C2D	-2.13	1.46	1.50
25	1	607	CLA	CMD-C2D	-2.13	1.46	1.50
26	d	401	PHO	CMD-C2D	-2.13	1.46	1.51
25	A	403	CLA	C3B-C2B	-2.13	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	P	619	II0	C39-C35	-2.13	1.33	1.35
26	D	401	PHO	CMD-C2D	-2.13	1.46	1.51
29	a	409	PL9	C53-C6	-2.13	1.46	1.50
29	d	405	PL9	C6-C1	-2.13	1.44	1.48
38	O	618	II0	C30-C26	2.13	1.41	1.37
25	a	403	CLA	CMD-C2D	-2.13	1.46	1.50
39	Q	620	IHT	C05-C08	2.12	1.55	1.52
25	A	403	CLA	CMD-C2D	-2.12	1.46	1.50
38	N	618	II0	C30-C26	2.12	1.41	1.37
36	e	102	HEM	C1D-ND	-2.12	1.34	1.38
25	P	615	CLA	CMD-C2D	-2.12	1.46	1.50
38	Q	617	II0	C30-C26	2.12	1.41	1.37
25	N	607	CLA	CMD-C2D	-2.12	1.46	1.50
39	4	620	IHT	C36-C33	2.12	1.55	1.50
37	6	606	KC2	C1B-C2B	2.12	1.49	1.45
38	P	619	II0	C30-C26	2.11	1.41	1.37
38	Q	619	II0	C30-C26	2.11	1.41	1.37
25	a	403	CLA	C3B-C2B	-2.11	1.37	1.40
25	B	603	CLA	CMD-C2D	-2.11	1.46	1.50
25	3	615	CLA	CMD-C2D	-2.11	1.46	1.50
25	Q	609	CLA	CMD-C2D	-2.11	1.46	1.50
38	3	619	II0	C30-C26	2.11	1.41	1.37
38	1	618	II0	C30-C26	2.11	1.41	1.37
25	b	616	CLA	CMC-C2C	-2.11	1.46	1.50
39	5	620	IHT	C36-C33	2.11	1.55	1.50
38	4	616	II0	C30-C26	2.11	1.41	1.37
29	D	405	PL9	C6-C1	-2.11	1.44	1.48
38	O	616	II0	C30-C26	2.10	1.41	1.37
25	4	609	CLA	CMD-C2D	-2.10	1.46	1.50
38	2	619	II0	C39-C35	-2.10	1.33	1.35
38	Q	616	II0	C30-C26	2.10	1.41	1.37
38	2	616	II0	C30-C26	2.10	1.41	1.37
38	3	617	II0	C30-C26	2.10	1.41	1.37
25	b	604	CLA	CMD-C2D	-2.10	1.46	1.50
25	S	604	CLA	CMD-C2D	-2.10	1.46	1.50
25	6	613	CLA	CMD-C2D	-2.10	1.46	1.50
25	R	615	CLA	CMD-C2D	-2.09	1.46	1.50
25	Q	615	CLA	CMD-C2D	-2.09	1.46	1.50
39	Q	620	IHT	C36-C33	2.09	1.55	1.50
25	S	609	CLA	CMD-C2D	-2.09	1.46	1.50
25	B	616	CLA	CMC-C2C	-2.09	1.46	1.50
38	2	618	II0	C30-C26	2.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	517	CLA	CMC-C2C	-2.09	1.46	1.50
38	4	616	II0	C39-C35	-2.09	1.33	1.35
36	E	102	HEM	C1D-ND	-2.09	1.34	1.38
25	G	301	CLA	CMD-C2D	-2.09	1.46	1.50
26	A	405	PHO	CMC-C2C	-2.09	1.46	1.51
38	6	617	II0	C29-C25	-2.09	1.32	1.37
25	C	525	CLA	CMD-C2D	-2.08	1.46	1.50
25	S	613	CLA	CMD-C2D	-2.08	1.46	1.50
25	O	613	CLA	CMD-C2D	-2.08	1.46	1.50
39	5	620	IHT	C05-C08	2.08	1.55	1.52
39	1	620	IHT	C30-C27	2.08	1.49	1.43
25	B	604	CLA	CMD-C2D	-2.08	1.46	1.50
25	P	601	CLA	CMD-C2D	-2.08	1.46	1.50
38	4	617	II0	C30-C26	2.08	1.41	1.37
38	R	616	II0	C30-C26	2.08	1.41	1.37
38	N	617	II0	C30-C26	2.08	1.41	1.37
36	E	102	HEM	C4B-NB	-2.08	1.34	1.38
25	C	517	CLA	CMD-C2D	-2.08	1.46	1.50
39	2	620	IHT	C05-C08	2.08	1.55	1.52
26	a	405	PHO	CMC-C2C	-2.08	1.46	1.51
26	d	401	PHO	CMC-C2C	-2.08	1.46	1.51
25	2	615	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	603	CLA	CMD-C2D	-2.08	1.46	1.50
25	5	609	CLA	CMC-C2C	-2.08	1.46	1.50
25	5	609	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	613	CLA	C3B-C2B	-2.08	1.37	1.40
25	5	603	CLA	CMD-C2D	-2.07	1.46	1.50
38	2	618	II0	C39-C35	-2.07	1.33	1.35
38	5	617	II0	C30-C26	2.07	1.41	1.37
38	S	616	II0	C30-C26	2.07	1.41	1.37
39	4	620	IHT	C30-C27	2.07	1.49	1.43
25	R	603	CLA	CMD-C2D	-2.07	1.46	1.50
38	3	618	II0	C39-C35	-2.07	1.33	1.35
25	3	601	CLA	CMD-C2D	-2.07	1.46	1.50
39	N	620	IHT	C30-C27	2.07	1.49	1.43
39	1	620	IHT	C05-C08	2.07	1.55	1.52
38	1	617	II0	C30-C26	2.07	1.41	1.37
39	Q	620	IHT	C30-C27	2.06	1.49	1.43
25	c	524	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	612	CLA	C3D-C4D	2.06	1.48	1.44
38	6	616	II0	C30-C26	2.06	1.41	1.37
25	c	517	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	607	CLA	CMD-C2D	-2.06	1.46	1.50
25	S	603	CLA	CMD-C2D	-2.06	1.46	1.50
38	N	619	II0	C39-C35	-2.06	1.33	1.35
25	6	609	CLA	CMD-C2D	-2.06	1.46	1.50
25	c	517	CLA	CMD-C2D	-2.06	1.46	1.50
25	3	613	CLA	CMD-C2D	-2.06	1.46	1.50
38	5	616	II0	C30-C26	2.06	1.41	1.37
38	R	617	II0	C30-C26	2.06	1.41	1.37
27	B	617	WVN	C02-C11	2.06	1.53	1.50
25	6	604	CLA	CMD-C2D	-2.06	1.46	1.50
36	e	102	HEM	C4B-NB	-2.06	1.34	1.38
38	3	619	II0	C39-C35	-2.05	1.33	1.35
38	P	616	II0	C30-C26	2.05	1.41	1.37
25	2	613	CLA	CMD-C2D	-2.05	1.46	1.50
25	4	615	CLA	CMD-C2D	-2.05	1.46	1.50
39	5	620	IHT	C30-C27	2.05	1.49	1.43
38	5	618	II0	C30-C26	2.05	1.41	1.37
25	P	604	CLA	CMD-C2D	-2.05	1.46	1.50
25	Q	613	CLA	CMD-C2D	-2.05	1.46	1.50
38	P	617	II0	C30-C26	2.05	1.41	1.37
25	O	615	CLA	CMD-C2D	-2.05	1.46	1.50
25	N	602	CLA	CMD-C2D	-2.05	1.46	1.50
38	P	618	II0	C30-C26	2.05	1.41	1.37
25	R	609	CLA	CMC-C2C	-2.05	1.46	1.50
38	3	616	II0	C30-C26	2.05	1.41	1.37
25	B	612	CLA	C3D-C4D	2.05	1.48	1.44
38	3	618	II0	C30-C26	2.05	1.41	1.37
25	1	602	CLA	CMD-C2D	-2.05	1.46	1.50
25	P	613	CLA	CMD-C2D	-2.05	1.46	1.50
25	N	609	CLA	CMD-C2D	-2.05	1.46	1.50
26	D	401	PHO	CMC-C2C	-2.05	1.46	1.51
25	5	607	CLA	CMD-C2D	-2.05	1.46	1.50
25	3	604	CLA	CMD-C2D	-2.05	1.46	1.50
38	N	619	II0	C29-C25	-2.04	1.32	1.37
25	R	609	CLA	C3B-CAB	-2.04	1.43	1.47
37	Q	612	KC2	C1D-ND	2.04	1.37	1.35
25	c	525	CLA	CMD-C2D	-2.04	1.46	1.50
38	S	617	II0	C29-C25	-2.04	1.32	1.37
25	R	609	CLA	CMD-C2D	-2.04	1.46	1.50
25	5	615	CLA	CMD-C2D	-2.04	1.46	1.50
25	R	613	CLA	CMD-C2D	-2.04	1.46	1.50
38	S	617	II0	C30-C26	2.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	611	CLA	CMD-C2D	-2.03	1.46	1.50
38	2	617	II0	C29-C25	-2.03	1.32	1.37
25	O	603	CLA	CMC-C2C	-2.03	1.46	1.50
25	C	524	CLA	CMD-C2D	-2.03	1.46	1.50
38	1	618	II0	C39-C35	-2.03	1.33	1.35
25	B	605	CLA	CMD-C2D	-2.03	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.03	1.46	1.50
25	R	604	CLA	CMD-C2D	-2.03	1.46	1.50
25	5	613	CLA	CMD-C2D	-2.02	1.46	1.50
38	1	616	II0	C30-C26	2.02	1.41	1.37
25	g	302	CLA	CMD-C2D	-2.02	1.46	1.50
38	N	616	II0	C30-C26	2.02	1.41	1.37
25	3	603	CLA	CMD-C2D	-2.02	1.46	1.50
25	4	606	CLA	CMC-C2C	-2.02	1.46	1.50
36	e	102	HEM	CHB-C1B	2.02	1.40	1.35
38	6	617	II0	C30-C26	2.02	1.41	1.37
25	Q	603	CLA	C3B-C2B	-2.02	1.37	1.40
25	A	403	CLA	C3B-CAB	-2.02	1.43	1.47
26	A	405	PHO	CMD-C2D	-2.02	1.46	1.51
25	b	613	CLA	C3B-C2B	-2.02	1.37	1.40
25	a	403	CLA	C3B-CAB	-2.02	1.43	1.47
25	4	613	CLA	CMD-C2D	-2.02	1.46	1.50
25	a	406	CLA	CMD-C2D	-2.02	1.46	1.50
25	5	611	CLA	CMD-C2D	-2.01	1.46	1.50
25	O	607	CLA	CMD-C2D	-2.01	1.46	1.50
25	O	606	CLA	CMD-C2D	-2.01	1.46	1.50
26	a	405	PHO	CMB-C2B	-2.01	1.46	1.51
25	B	601	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	606	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	528	CLA	CMD-C2D	-2.01	1.46	1.50
29	D	405	PL9	C53-C6	-2.01	1.46	1.50
37	4	612	KC2	C1D-ND	2.01	1.37	1.35
25	P	603	CLA	CMD-C2D	-2.01	1.46	1.50
38	4	619	II0	C39-C35	-2.01	1.33	1.35
25	B	602	CLA	CMD-C2D	-2.01	1.46	1.50
39	R	620	IHT	C36-C33	2.01	1.55	1.50
25	1	609	CLA	CMD-C2D	-2.01	1.46	1.50
26	a	405	PHO	CMD-C2D	-2.01	1.46	1.51
25	C	527	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	527	CLA	CMD-C2D	-2.01	1.46	1.50
38	O	618	II0	C29-C25	-2.01	1.32	1.37
25	3	612	CLA	C3D-C4D	2.00	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	516	CLA	CMD-C2D	-2.00	1.46	1.50
25	G	302	CLA	CMD-C2D	-2.00	1.46	1.50
25	C	516	CLA	CMD-C2D	-2.00	1.46	1.50
25	5	604	CLA	CMD-C2D	-2.00	1.46	1.50
25	O	601	CLA	CMD-C2D	-2.00	1.46	1.50
25	C	518	CLA	CMD-C2D	-2.00	1.46	1.50

All (3804) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	6	612	KC2	C1A-NA-C4A	-12.47	101.10	106.71
37	4	612	KC2	C1A-NA-C4A	-12.46	101.11	106.71
37	Q	612	KC2	C1A-NA-C4A	-12.45	101.11	106.71
37	S	612	KC2	C1A-NA-C4A	-12.45	101.11	106.71
37	O	612	KC2	C1A-NA-C4A	-12.39	101.14	106.71
37	2	612	KC2	C1A-NA-C4A	-12.35	101.16	106.71
37	N	612	KC2	C1A-NA-C4A	-12.31	101.17	106.71
37	1	612	KC2	C1A-NA-C4A	-12.24	101.20	106.71
37	1	605	KC2	C1A-NA-C4A	-12.13	101.25	106.71
37	N	605	KC2	C1A-NA-C4A	-12.05	101.29	106.71
37	Q	611	KC2	C1A-NA-C4A	-11.78	101.41	106.71
37	4	611	KC2	C1A-NA-C4A	-11.78	101.41	106.71
38	S	619	II0	C06-C08-C12	11.44	125.97	110.30
38	6	619	II0	C06-C08-C12	11.42	125.94	110.30
38	2	617	II0	C06-C08-C12	11.40	125.92	110.30
38	O	617	II0	C06-C08-C12	11.40	125.91	110.30
38	Q	618	II0	C06-C08-C12	11.38	125.88	110.30
38	N	618	II0	C06-C08-C12	11.36	125.86	110.30
38	1	618	II0	C06-C08-C12	11.35	125.84	110.30
37	R	612	KC2	C1A-NA-C4A	-11.34	101.61	106.71
38	4	618	II0	C06-C08-C12	11.34	125.82	110.30
38	N	616	II0	C06-C08-C12	11.25	125.70	110.30
37	5	612	KC2	C1A-NA-C4A	-11.24	101.65	106.71
38	1	616	II0	C06-C08-C12	11.20	125.64	110.30
38	R	617	II0	C06-C08-C12	11.18	125.61	110.30
38	5	617	II0	C06-C08-C12	11.17	125.59	110.30
38	N	617	II0	C06-C08-C12	11.16	125.58	110.30
38	5	616	II0	C06-C08-C12	11.14	125.55	110.30
38	1	617	II0	C06-C08-C12	11.13	125.54	110.30
38	R	616	II0	C06-C08-C12	11.12	125.53	110.30
38	6	616	II0	C06-C08-C12	11.09	125.49	110.30
38	S	616	II0	C06-C08-C12	11.07	125.45	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	P	606	KC2	C1A-NA-C4A	-11.07	101.73	106.71
38	2	619	II0	C06-C08-C12	11.06	125.45	110.30
38	3	617	II0	C06-C08-C12	11.06	125.44	110.30
38	P	617	II0	C06-C08-C12	11.05	125.44	110.30
38	O	619	II0	C06-C08-C12	11.05	125.43	110.30
38	5	618	II0	C06-C08-C12	11.04	125.42	110.30
38	Q	619	II0	C06-C08-C12	11.04	125.42	110.30
37	6	606	KC2	CHC-C4B-NB	11.04	134.60	124.45
38	R	618	II0	C06-C08-C12	11.03	125.41	110.30
37	3	606	KC2	C1A-NA-C4A	-11.03	101.75	106.71
38	4	619	II0	C06-C08-C12	11.03	125.40	110.30
37	S	606	KC2	CHC-C4B-NB	11.01	134.58	124.45
38	5	619	II0	C06-C08-C12	10.98	125.33	110.30
38	Q	616	II0	C06-C08-C12	10.97	125.32	110.30
38	4	616	II0	C06-C08-C12	10.96	125.30	110.30
38	O	618	II0	C06-C08-C12	10.95	125.30	110.30
38	2	618	II0	C06-C08-C12	10.95	125.29	110.30
38	R	619	II0	C06-C08-C12	10.94	125.28	110.30
38	2	616	II0	C06-C08-C12	10.94	125.28	110.30
38	O	616	II0	C06-C08-C12	10.93	125.26	110.30
38	Q	617	II0	C06-C08-C12	10.86	125.16	110.30
38	4	617	II0	C06-C08-C12	10.83	125.13	110.30
38	P	619	II0	C06-C08-C12	10.82	125.12	110.30
38	3	619	II0	C06-C08-C12	10.82	125.12	110.30
38	P	616	II0	C06-C08-C12	10.74	125.01	110.30
38	S	617	II0	C06-C08-C12	10.74	125.01	110.30
38	3	616	II0	C06-C08-C12	10.73	124.99	110.30
38	6	617	II0	C06-C08-C12	10.71	124.97	110.30
38	6	618	II0	C06-C08-C12	10.69	124.94	110.30
38	S	618	II0	C06-C08-C12	10.67	124.90	110.30
37	1	611	KC2	C1A-NA-C4A	-10.65	101.92	106.71
38	N	619	II0	C06-C08-C12	10.64	124.87	110.30
38	1	619	II0	C06-C08-C12	10.64	124.86	110.30
37	N	611	KC2	C1A-NA-C4A	-10.62	101.93	106.71
37	S	606	KC2	C1A-NA-C4A	-10.58	101.95	106.71
38	Q	616	II0	C41-C39-C35	-10.44	112.41	127.31
38	4	616	II0	C41-C39-C35	-10.42	112.44	127.31
37	4	605	KC2	C1A-NA-C4A	-10.38	102.04	106.71
38	1	619	II0	C41-C39-C35	-10.34	112.55	127.31
37	Q	611	KC2	CHC-C4B-NB	10.32	133.94	124.45
38	N	619	II0	C41-C39-C35	-10.32	112.58	127.31
37	Q	605	KC2	C1A-NA-C4A	-10.32	102.07	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	1	613	KC2	CHC-C4B-NB	10.29	133.91	124.45
38	P	618	II0	C06-C08-C12	10.29	124.39	110.30
38	3	618	II0	C06-C08-C12	10.27	124.36	110.30
37	4	611	KC2	CHC-C4B-NB	10.27	133.89	124.45
38	P	618	II0	C41-C39-C35	-10.25	112.69	127.31
37	N	613	KC2	CHC-C4B-NB	10.25	133.87	124.45
37	P	606	KC2	CHC-C4B-NB	10.22	133.84	124.45
37	3	606	KC2	CHC-C4B-NB	10.21	133.84	124.45
37	6	612	KC2	CHC-C4B-NB	10.21	133.83	124.45
37	S	612	KC2	CHC-C4B-NB	10.16	133.79	124.45
38	6	616	II0	C42-C40-C36	-10.16	112.81	127.31
38	S	616	II0	C42-C40-C36	-10.15	112.82	127.31
37	R	612	KC2	CHC-C4B-NB	10.15	133.78	124.45
37	5	612	KC2	CHC-C4B-NB	10.12	133.76	124.45
37	N	612	KC2	CHC-C4B-NB	10.10	133.74	124.45
38	N	618	II0	C41-C39-C35	-10.09	112.91	127.31
37	6	606	KC2	C1A-NA-C4A	-10.08	102.17	106.71
37	1	612	KC2	CHC-C4B-NB	10.08	133.72	124.45
37	Q	605	KC2	CHC-C4B-NB	10.07	133.71	124.45
38	1	618	II0	C41-C39-C35	-10.06	112.96	127.31
37	N	611	KC2	CHC-C4B-NB	10.04	133.68	124.45
37	4	605	KC2	CHC-C4B-NB	10.03	133.67	124.45
38	1	616	II0	C42-C40-C36	-10.02	113.00	127.31
38	R	616	II0	C41-C39-C35	-10.01	113.03	127.31
38	N	616	II0	C42-C40-C36	-10.00	113.04	127.31
37	N	613	KC2	C1A-NA-C4A	-9.99	102.21	106.71
38	5	616	II0	C41-C39-C35	-9.99	113.05	127.31
37	1	613	KC2	C1A-NA-C4A	-9.99	102.22	106.71
38	3	618	II0	C41-C39-C35	-9.98	113.06	127.31
37	1	611	KC2	CHC-C4B-NB	9.95	133.59	124.45
37	1	605	KC2	CHC-C4B-NB	9.90	133.55	124.45
37	N	605	KC2	CHC-C4B-NB	9.90	133.55	124.45
38	R	618	II0	C41-C39-C35	-9.89	113.20	127.31
38	Q	618	II0	C41-C39-C35	-9.88	113.20	127.31
38	5	618	II0	C41-C39-C35	-9.86	113.23	127.31
38	4	618	II0	C41-C39-C35	-9.85	113.26	127.31
38	3	617	II0	C42-C40-C36	-9.84	113.26	127.31
38	P	617	II0	C42-C40-C36	-9.83	113.28	127.31
38	P	616	II0	C41-C39-C35	-9.82	113.29	127.31
38	3	616	II0	C41-C39-C35	-9.82	113.30	127.31
38	Q	619	II0	C41-C39-C35	-9.80	113.33	127.31
37	2	612	KC2	CHC-C4B-NB	9.79	133.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Q	612	KC2	CHC-C4B-NB	9.78	133.44	124.45
38	4	618	II0	C42-C40-C36	-9.77	113.36	127.31
38	S	618	II0	C41-C39-C35	-9.76	113.39	127.31
38	Q	618	II0	C42-C40-C36	-9.75	113.40	127.31
37	4	612	KC2	CHC-C4B-NB	9.74	133.41	124.45
37	O	612	KC2	CHC-C4B-NB	9.74	133.40	124.45
38	6	618	II0	C41-C39-C35	-9.73	113.42	127.31
38	4	617	II0	C41-C39-C35	-9.73	113.43	127.31
38	4	619	II0	C41-C39-C35	-9.72	113.43	127.31
38	4	617	II0	C42-C40-C36	-9.72	113.43	127.31
38	S	618	II0	C42-C40-C36	-9.71	113.45	127.31
37	1	613	KC2	OBD-CAD-CBD	9.71	139.77	125.89
38	Q	617	II0	C42-C40-C36	-9.71	113.46	127.31
38	Q	617	II0	C41-C39-C35	-9.71	113.46	127.31
37	N	613	KC2	OBD-CAD-CBD	9.70	139.75	125.89
38	2	616	II0	C42-C40-C36	-9.69	113.47	127.31
38	O	616	II0	C42-C40-C36	-9.68	113.49	127.31
37	6	606	KC2	OBD-CAD-CBD	9.66	139.70	125.89
38	S	616	II0	C41-C39-C35	-9.65	113.54	127.31
38	6	616	II0	C41-C39-C35	-9.64	113.55	127.31
38	1	619	II0	C42-C40-C36	-9.64	113.55	127.31
38	6	618	II0	C42-C40-C36	-9.62	113.58	127.31
38	2	618	II0	C41-C39-C35	-9.61	113.59	127.31
38	6	617	II0	C42-C40-C36	-9.56	113.66	127.31
38	R	617	II0	C41-C39-C35	-9.56	113.67	127.31
38	S	617	II0	C42-C40-C36	-9.55	113.68	127.31
38	5	617	II0	C41-C39-C35	-9.54	113.69	127.31
38	O	618	II0	C41-C39-C35	-9.54	113.70	127.31
38	N	619	II0	C42-C40-C36	-9.53	113.71	127.31
38	2	617	II0	C42-C40-C36	-9.51	113.73	127.31
38	2	616	II0	C41-C39-C35	-9.50	113.76	127.31
38	R	617	II0	C42-C40-C36	-9.49	113.77	127.31
38	O	617	II0	C42-C40-C36	-9.49	113.77	127.31
37	1	612	KC2	OBD-CAD-CBD	9.48	139.44	125.89
38	O	616	II0	C41-C39-C35	-9.47	113.79	127.31
38	5	617	II0	C42-C40-C36	-9.47	113.80	127.31
37	N	612	KC2	OBD-CAD-CBD	9.43	139.37	125.89
37	4	611	KC2	OBD-CAD-CBD	9.36	139.27	125.89
38	2	617	II0	C41-C39-C35	-9.36	113.95	127.31
38	2	619	II0	C41-C39-C35	-9.36	113.95	127.31
38	1	617	II0	C42-C40-C36	-9.35	113.96	127.31
37	Q	611	KC2	OBD-CAD-CBD	9.34	139.24	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	O	619	II0	C41-C39-C35	-9.33	113.99	127.31
38	N	617	II0	C42-C40-C36	-9.33	114.00	127.31
38	5	618	II0	C42-C40-C36	-9.32	114.01	127.31
38	O	617	II0	C41-C39-C35	-9.31	114.02	127.31
38	R	618	II0	C42-C40-C36	-9.30	114.04	127.31
37	1	611	KC2	OBD-CAD-CBD	9.29	139.17	125.89
37	N	611	KC2	OBD-CAD-CBD	9.29	139.17	125.89
38	6	617	II0	C41-C39-C35	-9.26	114.10	127.31
38	3	619	II0	C41-C39-C35	-9.25	114.11	127.31
38	S	617	II0	C41-C39-C35	-9.24	114.12	127.31
38	1	616	II0	C41-C39-C35	-9.24	114.13	127.31
38	5	619	II0	C42-C40-C36	-9.23	114.14	127.31
37	S	606	KC2	OBD-CAD-CBD	9.22	139.07	125.89
38	P	619	II0	C41-C39-C35	-9.21	114.16	127.31
37	R	612	KC2	OBD-CAD-CBD	9.20	139.04	125.89
38	R	619	II0	C42-C40-C36	-9.20	114.18	127.31
38	N	616	II0	C41-C39-C35	-9.20	114.18	127.31
38	R	616	II0	C42-C40-C36	-9.18	114.21	127.31
37	1	605	KC2	OBD-CAD-CBD	9.18	139.01	125.89
37	4	612	KC2	OBD-CAD-CBD	9.18	139.01	125.89
38	5	616	II0	C42-C40-C36	-9.17	114.22	127.31
37	Q	612	KC2	OBD-CAD-CBD	9.15	138.97	125.89
37	5	612	KC2	OBD-CAD-CBD	9.15	138.97	125.89
37	N	605	KC2	OBD-CAD-CBD	9.14	138.95	125.89
38	P	616	II0	C42-C40-C36	-9.11	114.31	127.31
38	3	616	II0	C42-C40-C36	-9.10	114.32	127.31
38	3	618	II0	C42-C40-C36	-9.10	114.32	127.31
37	Q	605	KC2	CHD-C4C-NC	9.07	137.97	124.20
37	4	605	KC2	CHD-C4C-NC	9.06	137.95	124.20
38	6	619	II0	C42-C40-C36	-9.04	114.41	127.31
37	O	612	KC2	CHD-C4C-NC	9.04	137.91	124.20
38	S	619	II0	C42-C40-C36	-9.03	114.43	127.31
37	N	613	KC2	CHD-C4C-NC	9.02	137.89	124.20
37	2	612	KC2	CHD-C4C-NC	9.02	137.88	124.20
37	1	613	KC2	CHD-C4C-NC	9.00	137.85	124.20
38	N	617	II0	C41-C39-C35	-8.96	114.53	127.31
37	R	612	KC2	CHD-C4C-NC	8.95	137.78	124.20
38	1	617	II0	C41-C39-C35	-8.94	114.55	127.31
27	b	618	WVN	C04-C09-C05	-8.93	116.28	124.85
38	P	618	II0	C42-C40-C36	-8.93	114.57	127.31
38	5	619	II0	C41-C39-C35	-8.93	114.57	127.31
38	2	618	II0	C42-C40-C36	-8.92	114.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	612	KC2	CHD-C4C-NC	8.92	137.73	124.20
37	3	606	KC2	OBD-CAD-CBD	8.92	138.63	125.89
37	3	606	KC2	CHD-C4C-NC	8.91	137.73	124.20
38	O	618	II0	C42-C40-C36	-8.91	114.59	127.31
38	R	619	II0	C41-C39-C35	-8.91	114.59	127.31
37	P	606	KC2	OBD-CAD-CBD	8.89	138.60	125.89
37	Q	605	KC2	OBD-CAD-CBD	8.89	138.60	125.89
37	S	612	KC2	OBD-CAD-CBD	8.88	138.59	125.89
37	P	606	KC2	CHD-C4C-NC	8.88	137.68	124.20
37	4	605	KC2	OBD-CAD-CBD	8.87	138.57	125.89
37	6	612	KC2	OBD-CAD-CBD	8.87	138.57	125.89
38	6	619	II0	C41-C39-C35	-8.82	114.73	127.31
38	N	618	II0	C42-C40-C36	-8.80	114.74	127.31
37	1	611	KC2	CHD-C4C-NC	8.79	137.53	124.20
37	N	605	KC2	CHD-C4C-NC	8.79	137.53	124.20
37	1	605	KC2	CHD-C4C-NC	8.78	137.53	124.20
37	Q	611	KC2	CHD-C4C-NC	8.78	137.52	124.20
37	S	612	KC2	CHD-C4C-NC	8.78	137.52	124.20
37	N	611	KC2	CHD-C4C-NC	8.78	137.52	124.20
38	S	619	II0	C41-C39-C35	-8.78	114.78	127.31
37	O	612	KC2	OBD-CAD-CBD	8.76	138.41	125.89
37	1	613	KC2	CHB-C1B-NB	8.76	132.50	124.45
37	2	612	KC2	OBD-CAD-CBD	8.76	138.40	125.89
37	4	611	KC2	CHD-C4C-NC	8.76	137.49	124.20
38	1	618	II0	C42-C40-C36	-8.75	114.82	127.31
37	6	612	KC2	CHD-C4C-NC	8.74	137.46	124.20
37	N	612	KC2	CHD-C4C-NC	8.74	137.46	124.20
38	Q	619	II0	C42-C40-C36	-8.73	114.84	127.31
38	3	617	II0	C41-C39-C35	-8.72	114.87	127.31
37	1	612	KC2	CHD-C4C-NC	8.71	137.42	124.20
38	P	617	II0	C41-C39-C35	-8.68	114.92	127.31
38	4	619	II0	C42-C40-C36	-8.68	114.92	127.31
37	N	613	KC2	CHB-C1B-NB	8.68	132.43	124.45
37	P	606	KC2	CHB-C1B-NB	8.57	132.33	124.45
38	Q	616	II0	C42-C40-C36	-8.56	115.09	127.31
38	4	616	II0	C42-C40-C36	-8.54	115.11	127.31
37	4	605	KC2	CHB-C1B-NB	8.54	132.31	124.45
37	3	606	KC2	CHB-C1B-NB	8.53	132.29	124.45
27	A	407	WVN	C04-C09-C05	-8.51	116.69	124.85
37	1	611	KC2	CHB-C1B-NB	8.51	132.28	124.45
38	O	619	II0	C42-C40-C36	-8.51	115.16	127.31
37	N	605	KC2	CHB-C1B-NB	8.51	132.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	619	II0	C42-C40-C36	-8.51	115.17	127.31
37	Q	605	KC2	CHB-C1B-NB	8.50	132.27	124.45
38	P	619	II0	C42-C40-C36	-8.48	115.21	127.31
38	3	619	II0	C42-C40-C36	-8.48	115.21	127.31
37	S	606	KC2	CHD-C4C-NC	8.47	137.06	124.20
37	1	605	KC2	CHB-C1B-NB	8.47	132.24	124.45
37	4	612	KC2	CHD-C4C-NC	8.45	137.03	124.20
37	Q	612	KC2	CHD-C4C-NC	8.44	137.01	124.20
37	N	611	KC2	CHB-C1B-NB	8.44	132.21	124.45
27	B	618	WVN	C04-C09-C05	-8.38	116.81	124.85
37	6	606	KC2	CHD-C4C-NC	8.37	136.91	124.20
37	R	612	KC2	CHB-C1B-NB	8.28	132.07	124.45
37	5	612	KC2	CHB-C1B-NB	8.28	132.06	124.45
37	Q	611	KC2	CHB-C1B-NB	8.19	131.98	124.45
37	1	612	KC2	CHB-C1B-NB	8.14	131.94	124.45
37	4	611	KC2	CHB-C1B-NB	8.13	131.92	124.45
37	N	612	KC2	CHB-C1B-NB	8.11	131.91	124.45
37	N	605	KC2	OBD-CAD-C3D	-8.09	114.55	127.98
37	1	605	KC2	OBD-CAD-C3D	-8.09	114.55	127.98
37	6	612	KC2	CHB-C1B-NB	8.08	131.88	124.45
37	S	612	KC2	CHB-C1B-NB	8.05	131.85	124.45
37	Q	605	KC2	OBD-CAD-C3D	-8.04	114.63	127.98
37	4	605	KC2	OBD-CAD-C3D	-8.03	114.65	127.98
37	2	612	KC2	CHB-C1B-NB	8.03	131.83	124.45
37	3	606	KC2	OBD-CAD-C3D	-8.03	114.66	127.98
37	P	606	KC2	OBD-CAD-C3D	-8.01	114.69	127.98
37	O	612	KC2	CHB-C1B-NB	7.99	131.80	124.45
39	5	620	IHT	C05-C03-C11	7.99	125.82	109.62
37	1	613	KC2	CMD-C2D-C1D	-7.99	116.19	128.46
39	R	620	IHT	C05-C03-C11	7.95	125.73	109.62
37	N	613	KC2	CMD-C2D-C1D	-7.93	116.28	128.46
37	6	612	KC2	OBD-CAD-C3D	-7.92	114.84	127.98
37	S	612	KC2	OBD-CAD-C3D	-7.91	114.85	127.98
37	6	606	KC2	OBD-CAD-C3D	-7.91	114.85	127.98
37	Q	612	KC2	CHB-C1B-NB	7.81	131.63	124.45
27	y	89	WVN	C04-C09-C05	-7.78	117.39	124.85
37	4	612	KC2	CHB-C1B-NB	7.77	131.60	124.45
27	b	617	WVN	C04-C09-C05	-7.76	117.41	124.85
39	5	620	IHT	C09-C10-C07	-7.72	111.52	122.73
37	S	606	KC2	OBD-CAD-C3D	-7.72	115.16	127.98
37	6	606	KC2	C1A-C2A-C3A	-7.71	101.00	107.11
27	B	619	WVN	C04-C09-C05	-7.70	117.47	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	613	KC2	OBD-CAD-C3D	-7.68	115.22	127.98
37	1	613	KC2	OBD-CAD-C3D	-7.68	115.24	127.98
37	1	611	KC2	OBD-CAD-C3D	-7.64	115.30	127.98
37	N	611	KC2	OBD-CAD-C3D	-7.64	115.30	127.98
37	R	612	KC2	OBD-CAD-C3D	-7.61	115.34	127.98
37	5	612	KC2	OBD-CAD-C3D	-7.60	115.36	127.98
37	Q	612	KC2	OBD-CAD-C3D	-7.60	115.37	127.98
37	4	612	KC2	OBD-CAD-C3D	-7.59	115.37	127.98
39	1	620	IHT	C09-C10-C07	-7.58	111.72	122.73
27	H	89	WVN	C04-C09-C05	-7.58	117.58	124.85
37	6	606	KC2	CHB-C1B-NB	7.57	131.41	124.45
37	4	611	KC2	OBD-CAD-C3D	-7.57	115.41	127.98
37	Q	611	KC2	OBD-CAD-C3D	-7.57	115.41	127.98
27	3	620	WVN	C04-C09-C05	-7.57	117.59	124.85
27	h	89	WVN	C04-C09-C05	-7.55	117.61	124.85
27	b	619	WVN	C30-C28-C25	-7.55	116.54	127.31
39	N	620	IHT	C09-C10-C07	-7.53	111.80	122.73
27	P	620	WVN	C04-C09-C05	-7.51	117.65	124.85
37	1	611	KC2	C2C-C1C-NC	7.44	118.69	110.57
37	1	612	KC2	OBD-CAD-C3D	-7.44	115.64	127.98
37	N	612	KC2	OBD-CAD-C3D	-7.43	115.64	127.98
37	O	612	KC2	OBD-CAD-C3D	-7.38	115.73	127.98
37	N	611	KC2	C2C-C1C-NC	7.38	118.62	110.57
37	2	612	KC2	OBD-CAD-C3D	-7.37	115.74	127.98
37	N	613	KC2	C2C-C1C-NC	7.32	118.57	110.57
37	1	613	KC2	C2C-C1C-NC	7.31	118.56	110.57
39	R	620	IHT	C09-C10-C07	-7.31	112.12	122.73
37	S	606	KC2	CHC-C4B-C3B	-7.29	112.80	125.26
39	4	620	IHT	C05-C03-C11	7.27	124.36	109.62
37	1	612	KC2	C2C-C1C-NC	7.26	118.50	110.57
37	N	612	KC2	C2C-C1C-NC	7.24	118.48	110.57
37	S	606	KC2	CHB-C1B-NB	7.21	131.08	124.45
37	S	612	KC2	C2C-C1C-NC	7.20	118.44	110.57
37	6	612	KC2	C2C-C1C-NC	7.19	118.42	110.57
37	S	606	KC2	C1A-C2A-C3A	-7.18	101.42	107.11
27	C	529	WVN	C02-C05-C09	-7.17	112.65	121.47
37	Q	612	KC2	C4C-C3C-C2C	-7.11	101.47	107.11
37	4	612	KC2	C4C-C3C-C2C	-7.10	101.48	107.11
37	Q	605	KC2	C2C-C1C-NC	7.09	118.31	110.57
37	4	605	KC2	C2C-C1C-NC	7.09	118.31	110.57
37	Q	612	KC2	C2C-C1C-NC	7.08	118.30	110.57
37	4	611	KC2	C2C-C1C-NC	7.06	118.28	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	620	IHT	C05-C03-C11	7.05	123.91	109.62
38	3	618	II0	C17-C04-C10	7.05	121.66	110.47
37	4	612	KC2	C2C-C1C-NC	7.04	118.26	110.57
37	6	606	KC2	CMD-C2D-C1D	-7.04	117.64	128.46
37	3	606	KC2	C2C-C1C-NC	7.04	118.25	110.57
38	P	618	II0	C17-C04-C10	7.03	121.63	110.47
37	S	606	KC2	C2C-C1C-NC	7.02	118.24	110.57
37	R	612	KC2	C2C-C1C-NC	7.02	118.23	110.57
37	6	606	KC2	CHC-C4B-C3B	-7.00	113.29	125.26
37	Q	611	KC2	C2C-C1C-NC	6.99	118.21	110.57
37	P	606	KC2	C2C-C1C-NC	6.99	118.20	110.57
37	5	612	KC2	C2C-C1C-NC	6.98	118.19	110.57
37	6	612	KC2	CMD-C2D-C1D	-6.98	117.74	128.46
37	4	611	KC2	C1A-C2A-C3A	-6.97	101.58	107.11
37	1	613	KC2	C4C-C3C-C2C	-6.97	101.58	107.11
37	S	612	KC2	CMD-C2D-C1D	-6.97	117.75	128.46
38	1	619	II0	C28-C26-C24	-6.97	103.04	116.84
38	N	619	II0	C28-C26-C24	-6.96	103.06	116.84
37	4	605	KC2	C1A-C2A-C3A	-6.94	101.60	107.11
37	Q	605	KC2	C1A-C2A-C3A	-6.94	101.60	107.11
37	1	613	KC2	CMD-C2D-C3D	6.93	137.65	124.68
37	6	606	KC2	C2C-C1C-NC	6.92	118.13	110.57
37	Q	611	KC2	C1A-C2A-C3A	-6.91	101.62	107.11
37	N	613	KC2	CMD-C2D-C3D	6.91	137.61	124.68
37	2	612	KC2	C2C-C1C-NC	6.91	118.12	110.57
27	Y	89	WVN	C21-C15-C13	-6.90	116.78	124.53
37	N	613	KC2	C4C-C3C-C2C	-6.89	101.64	107.11
37	1	612	KC2	CHC-C4B-C3B	-6.89	113.47	125.26
37	N	612	KC2	CHC-C4B-C3B	-6.87	113.50	125.26
37	6	612	KC2	CHC-C4B-C3B	-6.86	113.52	125.26
37	O	612	KC2	C2C-C1C-NC	6.86	118.06	110.57
37	1	613	KC2	CHC-C4B-C3B	-6.84	113.55	125.26
38	3	619	II0	C28-C26-C24	-6.84	103.29	116.84
37	S	612	KC2	CHC-C4B-C3B	-6.84	113.56	125.26
38	R	618	II0	C17-C04-C10	6.84	121.33	110.47
38	3	617	II0	C42-C41-C39	-6.83	109.48	123.47
38	6	619	II0	C42-C41-C39	-6.83	109.49	123.47
38	P	619	II0	C28-C26-C24	-6.82	103.34	116.84
37	N	613	KC2	CHC-C4B-C3B	-6.80	113.62	125.26
37	Q	612	KC2	C1A-C2A-C3A	-6.80	101.71	107.11
38	5	618	II0	C17-C04-C10	6.80	121.28	110.47
38	1	619	II0	C17-C04-C10	6.80	121.28	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	619	II0	C17-C04-C10	6.80	121.27	110.47
38	P	617	II0	C42-C41-C39	-6.80	109.54	123.47
37	4	612	KC2	CHB-C4A-C3A	-6.80	114.36	124.98
38	Q	618	II0	C28-C26-C24	-6.80	103.37	116.84
37	N	611	KC2	C1A-C2A-C3A	-6.79	101.72	107.11
39	O	620	IHT	C05-C03-C11	6.79	123.39	109.62
38	4	618	II0	C28-C26-C24	-6.79	103.39	116.84
37	S	612	KC2	C4C-C3C-C2C	-6.79	101.72	107.11
37	N	611	KC2	CMD-C2D-C1D	-6.79	118.03	128.46
39	2	620	IHT	C05-C03-C11	6.79	123.38	109.62
38	2	619	II0	C17-C04-C10	6.78	121.25	110.47
37	1	612	KC2	C1A-C2A-C3A	-6.78	101.73	107.11
37	R	612	KC2	CHC-C4B-C3B	-6.78	113.66	125.26
37	5	612	KC2	CHC-C4B-C3B	-6.78	113.67	125.26
37	1	611	KC2	C1A-C2A-C3A	-6.77	101.74	107.11
37	4	611	KC2	CHC-C4B-C3B	-6.77	113.67	125.26
37	Q	611	KC2	CHC-C4B-C3B	-6.77	113.67	125.26
37	4	605	KC2	CMD-C2D-C1D	-6.77	118.06	128.46
37	1	611	KC2	CMD-C2D-C1D	-6.77	118.06	128.46
38	O	619	II0	C17-C04-C10	6.77	121.22	110.47
37	4	612	KC2	C1A-C2A-C3A	-6.77	101.74	107.11
38	4	619	II0	C28-C26-C24	-6.76	103.44	116.84
37	Q	612	KC2	CHB-C4A-C3A	-6.76	114.41	124.98
37	6	612	KC2	C4C-C3C-C2C	-6.76	101.75	107.11
38	S	619	II0	C42-C41-C39	-6.76	109.63	123.47
38	3	616	II0	C17-C04-C10	6.76	121.21	110.47
38	R	619	II0	C28-C26-C24	-6.76	103.46	116.84
38	O	616	II0	C28-C26-C24	-6.76	103.46	116.84
37	Q	605	KC2	CMD-C2D-C1D	-6.75	118.09	128.46
37	S	606	KC2	CMD-C2D-C1D	-6.75	118.09	128.46
38	2	616	II0	C28-C26-C24	-6.75	103.47	116.84
37	O	612	KC2	CHB-C4A-C3A	-6.75	114.44	124.98
38	P	616	II0	C17-C04-C10	6.75	121.19	110.47
37	N	612	KC2	CMD-C2D-C1D	-6.74	118.10	128.46
38	Q	619	II0	C28-C26-C24	-6.74	103.49	116.84
37	2	612	KC2	CHB-C4A-C3A	-6.74	114.45	124.98
37	N	605	KC2	C1A-C2A-C3A	-6.74	101.77	107.11
37	Q	611	KC2	CMD-C2D-C1D	-6.74	118.11	128.46
38	5	619	II0	C28-C26-C24	-6.73	103.50	116.84
38	S	616	II0	C28-C26-C24	-6.73	103.50	116.84
37	1	612	KC2	CMD-C2D-C1D	-6.73	118.11	128.46
37	1	605	KC2	C1A-C2A-C3A	-6.73	101.77	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	616	II0	C28-C26-C24	-6.73	103.51	116.84
37	2	612	KC2	C1A-C2A-C3A	-6.73	101.78	107.11
37	4	611	KC2	CMD-C2D-C1D	-6.72	118.13	128.46
38	P	616	II0	C28-C26-C24	-6.72	103.53	116.84
38	5	619	II0	C17-C04-C10	6.72	121.14	110.47
37	N	612	KC2	C1A-C2A-C3A	-6.71	101.78	107.11
38	3	616	II0	C28-C26-C24	-6.71	103.55	116.84
37	R	612	KC2	CMD-C2D-C1D	-6.70	118.17	128.46
38	R	619	II0	C17-C04-C10	6.70	121.11	110.47
37	5	612	KC2	CMD-C2D-C1D	-6.70	118.17	128.46
37	1	605	KC2	CMD-C2D-C1D	-6.69	118.17	128.46
39	N	620	IHT	C05-C03-C11	6.69	123.19	109.62
38	1	618	II0	C28-C26-C24	-6.69	103.59	116.84
37	N	605	KC2	CMD-C2D-C1D	-6.69	118.18	128.46
38	6	619	II0	C28-C26-C24	-6.68	103.62	116.84
37	S	612	KC2	C1A-C2A-C3A	-6.67	101.82	107.11
37	O	612	KC2	C1A-C2A-C3A	-6.67	101.82	107.11
38	N	618	II0	C28-C26-C24	-6.67	103.63	116.84
37	N	605	KC2	C2C-C1C-NC	6.67	117.85	110.57
38	1	617	II0	C28-C26-C24	-6.67	103.63	116.84
37	1	605	KC2	C2C-C1C-NC	6.67	117.85	110.57
39	Q	620	IHT	C05-C03-C11	6.67	123.13	109.62
37	2	612	KC2	CHC-C4B-C3B	-6.67	113.86	125.26
37	S	606	KC2	C4C-C3C-C2C	-6.67	101.82	107.11
37	P	606	KC2	CHC-C4B-C3B	-6.66	113.86	125.26
37	6	612	KC2	C1A-C2A-C3A	-6.66	101.83	107.11
37	5	612	KC2	C1A-C2A-C3A	-6.66	101.83	107.11
37	O	612	KC2	CHC-C4B-C3B	-6.66	113.87	125.26
38	5	616	II0	C28-C26-C24	-6.66	103.65	116.84
37	P	606	KC2	CMD-C2D-C1D	-6.66	118.23	128.46
37	R	612	KC2	C1A-C2A-C3A	-6.66	101.83	107.11
37	3	606	KC2	CMD-C2D-C1D	-6.65	118.24	128.46
37	3	606	KC2	CHC-C4B-C3B	-6.65	113.88	125.26
38	R	616	II0	C28-C26-C24	-6.65	103.67	116.84
38	N	617	II0	C28-C26-C24	-6.65	103.67	116.84
38	6	617	II0	C17-C04-C10	6.65	121.03	110.47
37	Q	605	KC2	CHC-C4B-C3B	-6.65	113.89	125.26
37	P	606	KC2	C1A-C2A-C3A	-6.65	101.84	107.11
38	S	617	II0	C17-C04-C10	6.64	121.02	110.47
37	3	606	KC2	C1A-C2A-C3A	-6.64	101.84	107.11
37	N	611	KC2	CHC-C4B-C3B	-6.64	113.90	125.26
38	4	617	II0	C28-C26-C24	-6.63	103.71	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	605	KC2	CHC-C4B-C3B	-6.63	113.92	125.26
38	2	616	II0	C17-C04-C10	6.62	120.99	110.47
37	N	611	KC2	C4C-C3C-C2C	-6.62	101.86	107.11
38	O	616	II0	C17-C04-C10	6.62	120.98	110.47
38	1	616	II0	C28-C26-C24	-6.62	103.73	116.84
38	N	616	II0	C28-C26-C24	-6.62	103.73	116.84
38	Q	617	II0	C28-C26-C24	-6.61	103.74	116.84
38	4	616	II0	C28-C26-C24	-6.61	103.75	116.84
37	1	611	KC2	CHC-C4B-C3B	-6.61	113.96	125.26
38	S	619	II0	C28-C26-C24	-6.61	103.76	116.84
38	Q	616	II0	C28-C26-C24	-6.60	103.76	116.84
37	4	605	KC2	C4C-C3C-C2C	-6.60	101.87	107.11
27	C	530	WVN	C04-C09-C05	-6.59	118.53	124.85
37	1	611	KC2	C4C-C3C-C2C	-6.59	101.88	107.11
38	S	618	II0	C28-C26-C24	-6.59	103.79	116.84
38	6	618	II0	C28-C26-C24	-6.58	103.80	116.84
37	N	612	KC2	C4C-C3C-C2C	-6.57	101.90	107.11
38	S	616	II0	C17-C04-C10	6.56	120.90	110.47
38	3	619	II0	C42-C41-C39	-6.56	110.03	123.47
37	1	612	KC2	C4C-C3C-C2C	-6.56	101.90	107.11
38	6	616	II0	C17-C04-C10	6.56	120.89	110.47
37	5	612	KC2	C4C-C3C-C2C	-6.55	101.91	107.11
37	Q	605	KC2	C4C-C3C-C2C	-6.55	101.91	107.11
38	5	617	II0	C28-C26-C24	-6.55	103.87	116.84
38	P	619	II0	C42-C41-C39	-6.55	110.06	123.47
37	Q	612	KC2	CHC-C4B-C3B	-6.55	114.06	125.26
37	4	612	KC2	CHC-C4B-C3B	-6.53	114.09	125.26
37	N	612	KC2	CHB-C4A-C3A	-6.53	114.78	124.98
38	R	617	II0	C17-C04-C10	6.52	120.83	110.47
38	R	617	II0	C28-C26-C24	-6.52	103.92	116.84
38	R	616	II0	C17-C04-C10	6.52	120.83	110.47
38	5	616	II0	C17-C04-C10	6.51	120.82	110.47
37	1	612	KC2	CHB-C4A-C3A	-6.51	114.81	124.98
38	1	616	II0	C42-C41-C39	-6.50	110.16	123.47
38	O	619	II0	C28-C26-C24	-6.50	103.96	116.84
38	N	616	II0	C42-C41-C39	-6.50	110.16	123.47
38	2	618	II0	C28-C26-C24	-6.49	103.98	116.84
38	S	619	II0	C17-C04-C10	6.49	120.78	110.47
38	O	618	II0	C28-C26-C24	-6.49	103.98	116.84
37	6	606	KC2	C4C-C3C-C2C	-6.49	101.96	107.11
37	S	612	KC2	CHB-C4A-C3A	-6.49	114.84	124.98
38	6	619	II0	C17-C04-C10	6.49	120.78	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	619	II0	C28-C26-C24	-6.49	103.99	116.84
38	5	617	II0	C17-C04-C10	6.49	120.77	110.47
37	R	612	KC2	C4C-C3C-C2C	-6.48	101.97	107.11
38	3	618	II0	C28-C26-C24	-6.48	104.01	116.84
39	N	620	IHT	C16-C03-C11	-6.47	100.18	110.47
38	P	618	II0	C28-C26-C24	-6.47	104.03	116.84
38	2	618	II0	C17-C04-C10	6.47	120.74	110.47
37	6	612	KC2	CHB-C4A-C3A	-6.46	114.88	124.98
37	Q	611	KC2	CHB-C4A-C3A	-6.45	114.90	124.98
37	4	611	KC2	CHB-C4A-C3A	-6.45	114.91	124.98
27	B	617	WVN	C21-C15-C13	-6.44	117.30	124.53
38	O	618	II0	C17-C04-C10	6.44	120.70	110.47
37	Q	611	KC2	C4C-C3C-C2C	-6.44	102.00	107.11
38	P	617	II0	C28-C26-C24	-6.44	104.09	116.84
27	C	531	WVN	C04-C09-C05	-6.43	118.69	124.85
38	6	617	II0	C42-C41-C39	-6.42	110.31	123.47
38	3	617	II0	C28-C26-C24	-6.42	104.12	116.84
37	4	611	KC2	C4C-C3C-C2C	-6.41	102.02	107.11
38	6	616	II0	C42-C41-C39	-6.41	110.34	123.47
37	Q	612	KC2	CMD-C2D-C1D	-6.41	118.61	128.46
37	4	612	KC2	CMD-C2D-C1D	-6.41	118.62	128.46
38	S	617	II0	C42-C41-C39	-6.40	110.36	123.47
38	S	616	II0	C42-C41-C39	-6.40	110.36	123.47
38	P	617	II0	C17-C04-C10	6.40	120.64	110.47
37	O	612	KC2	CMD-C2D-C1D	-6.39	118.64	128.46
39	Q	620	IHT	C16-C03-C11	-6.38	100.33	110.47
37	1	613	KC2	C1A-C2A-C3A	-6.38	102.05	107.11
37	6	612	KC2	CMD-C2D-C3D	6.38	136.62	124.68
25	4	609	CLA	C4A-NA-C1A	6.38	109.57	106.71
37	N	613	KC2	C1A-C2A-C3A	-6.38	102.05	107.11
38	3	617	II0	C17-C04-C10	6.37	120.60	110.47
38	O	617	II0	C28-C26-C24	-6.37	104.22	116.84
27	B	617	WVN	C04-C09-C05	-6.37	118.74	124.85
37	2	612	KC2	CMD-C2D-C1D	-6.37	118.67	128.46
37	S	612	KC2	CMD-C2D-C3D	6.37	136.59	124.68
25	Q	609	CLA	C4A-NA-C1A	6.37	109.57	106.71
38	4	619	II0	C17-C04-C10	6.36	120.58	110.47
25	S	603	CLA	C4A-NA-C1A	6.36	109.56	106.71
38	6	617	II0	C28-C26-C24	-6.35	104.27	116.84
27	c	531	WVN	C04-C09-C05	-6.35	118.76	124.85
38	2	617	II0	C28-C26-C24	-6.34	104.28	116.84
38	Q	619	II0	C17-C04-C10	6.34	120.54	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	529	WVN	C04-C09-C05	-6.34	118.77	124.85
38	N	616	II0	C17-C04-C10	6.34	120.54	110.47
38	S	617	II0	C28-C26-C24	-6.34	104.29	116.84
38	1	616	II0	C17-C04-C10	6.33	120.53	110.47
37	1	612	KC2	CMD-C2D-C3D	6.29	136.45	124.68
37	N	612	KC2	CMD-C2D-C3D	6.29	136.44	124.68
37	1	605	KC2	CHC-C4B-C3B	-6.28	114.51	125.26
37	6	606	KC2	CMD-C2D-C3D	6.28	136.43	124.68
38	2	617	II0	C42-C41-C39	-6.28	110.61	123.47
37	3	606	KC2	C4C-C3C-C2C	-6.28	102.13	107.11
27	3	620	WVN	C39-C36-C32	-6.27	118.36	127.31
37	N	605	KC2	CHC-C4B-C3B	-6.27	114.53	125.26
37	O	612	KC2	CMD-C2D-C3D	6.27	136.41	124.68
37	2	612	KC2	CMD-C2D-C3D	6.27	136.41	124.68
38	2	616	II0	C42-C41-C39	-6.25	110.67	123.47
38	O	617	II0	C42-C41-C39	-6.24	110.69	123.47
37	N	611	KC2	CHB-C4A-C3A	-6.24	115.24	124.98
37	1	605	KC2	CMD-C2D-C3D	6.24	136.34	124.68
38	O	616	II0	C42-C41-C39	-6.23	110.71	123.47
27	Y	89	WVN	C04-C09-C05	-6.23	118.88	124.85
27	P	620	WVN	C39-C36-C32	-6.23	118.42	127.31
38	1	617	II0	C42-C41-C39	-6.23	110.72	123.47
37	1	611	KC2	CHB-C4A-C3A	-6.22	115.26	124.98
37	N	605	KC2	CMD-C2D-C3D	6.22	136.32	124.68
37	Q	611	KC2	CMD-C2D-C3D	6.22	136.31	124.68
38	N	617	II0	C42-C41-C39	-6.21	110.75	123.47
37	P	606	KC2	C4C-C3C-C2C	-6.21	102.18	107.11
37	4	605	KC2	CMD-C2D-C3D	6.21	136.30	124.68
37	4	611	KC2	CMD-C2D-C3D	6.21	136.29	124.68
37	S	606	KC2	CMD-C2D-C3D	6.20	136.28	124.68
37	1	611	KC2	CMD-C2D-C3D	6.20	136.28	124.68
37	N	611	KC2	CMD-C2D-C3D	6.20	136.28	124.68
37	N	605	KC2	C4C-C3C-C2C	-6.20	102.19	107.11
37	5	612	KC2	CMD-C2D-C3D	6.20	136.27	124.68
37	R	612	KC2	CMD-C2D-C3D	6.20	136.27	124.68
37	Q	605	KC2	CMD-C2D-C3D	6.20	136.27	124.68
38	5	619	II0	C42-C41-C39	-6.19	110.78	123.47
37	R	612	KC2	CHB-C4A-C3A	-6.19	115.31	124.98
37	5	612	KC2	CHB-C4A-C3A	-6.19	115.31	124.98
38	R	619	II0	C42-C41-C39	-6.18	110.81	123.47
37	1	605	KC2	C4C-C3C-C2C	-6.17	102.22	107.11
27	Y	89	WVN	C20-C23-C25	-6.13	116.97	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	89	WVN	C20-C23-C25	-6.13	116.97	126.23
38	N	617	II0	C17-C04-C10	6.11	120.18	110.47
37	P	606	KC2	CHB-C4A-C3A	-6.11	115.43	124.98
37	3	606	KC2	CHB-C4A-C3A	-6.11	115.44	124.98
38	1	617	II0	C17-C04-C10	6.11	120.17	110.47
38	5	618	II0	C28-C26-C24	-6.10	104.75	116.84
38	R	618	II0	C28-C26-C24	-6.10	104.75	116.84
38	S	618	II0	C42-C41-C39	-6.09	111.00	123.47
27	a	407	WVN	C29-C26-C22	-6.09	118.62	127.31
38	1	618	II0	C17-C04-C10	6.09	120.14	110.47
38	6	618	II0	C42-C41-C39	-6.08	111.02	123.47
38	N	618	II0	C17-C04-C10	6.06	120.09	110.47
25	R	613	CLA	C4A-NA-C1A	6.06	109.43	106.71
38	5	617	II0	C42-C41-C39	-6.05	111.08	123.47
27	H	89	WVN	C20-C13-C15	-6.04	106.83	121.46
38	R	617	II0	C42-C41-C39	-6.04	111.11	123.47
38	P	616	II0	C42-C41-C39	-6.03	111.12	123.47
38	3	616	II0	C42-C41-C39	-6.03	111.13	123.47
27	b	619	WVN	C21-C15-C13	-6.02	117.77	124.53
38	4	618	II0	C17-C04-C10	6.01	120.01	110.47
37	3	606	KC2	CMD-C2D-C3D	5.99	135.89	124.68
38	Q	618	II0	C17-C04-C10	5.98	119.97	110.47
37	P	606	KC2	CMD-C2D-C3D	5.98	135.86	124.68
37	1	605	KC2	CHB-C4A-C3A	-5.97	115.66	124.98
38	Q	618	II0	C42-C41-C39	-5.96	111.26	123.47
37	N	605	KC2	CHB-C4A-C3A	-5.96	115.67	124.98
37	2	612	KC2	C4C-C3C-C2C	-5.95	102.39	107.11
25	5	613	CLA	C4A-NA-C1A	5.95	109.38	106.71
38	4	618	II0	C42-C41-C39	-5.94	111.30	123.47
25	S	609	CLA	C4A-NA-C1A	5.94	109.38	106.71
38	4	617	II0	C42-C41-C39	-5.93	111.32	123.47
38	2	617	II0	C17-C04-C10	5.93	119.89	110.47
37	4	612	KC2	CMD-C2D-C3D	5.93	135.77	124.68
25	O	601	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	2	601	CLA	C4A-NA-C1A	5.93	109.37	106.71
39	R	620	IHT	C17-C03-C11	-5.92	101.07	110.47
37	Q	612	KC2	CMD-C2D-C3D	5.91	135.74	124.68
38	Q	617	II0	C42-C41-C39	-5.91	111.37	123.47
38	O	617	II0	C17-C04-C10	5.91	119.85	110.47
39	5	620	IHT	C17-C03-C11	-5.90	101.09	110.47
37	O	612	KC2	C4C-C3C-C2C	-5.90	102.43	107.11
38	3	619	II0	C17-C04-C10	5.89	119.83	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	P	619	II0	C17-C04-C10	5.89	119.83	110.47
38	R	616	II0	C42-C41-C39	-5.89	111.41	123.47
39	4	620	IHT	C03-C11-C15	-5.89	114.32	122.63
39	2	620	IHT	C16-C03-C11	-5.89	101.11	110.47
39	O	620	IHT	C09-C10-C07	-5.88	114.19	122.73
38	5	616	II0	C42-C41-C39	-5.88	111.44	123.47
39	2	620	IHT	C09-C10-C07	-5.87	114.22	122.73
37	4	605	KC2	CHB-C4A-C3A	-5.84	115.85	124.98
39	O	620	IHT	C16-C03-C11	-5.84	101.19	110.47
37	Q	605	KC2	CHB-C4A-C3A	-5.83	115.86	124.98
27	B	618	WVN	C21-C15-C13	-5.82	117.99	124.53
27	B	619	WVN	C30-C28-C25	-5.81	119.01	127.31
25	N	614	CLA	C4A-NA-C1A	5.81	109.32	106.71
38	5	618	II0	C42-C41-C39	-5.80	111.59	123.47
38	R	618	II0	C42-C41-C39	-5.79	111.60	123.47
27	a	407	WVN	C06-C13-C15	-5.78	114.47	122.61
39	O	620	IHT	C41-C38-C35	-5.77	119.08	127.31
39	2	620	IHT	C25-C23-C27	-5.76	114.86	122.92
27	c	530	WVN	C04-C09-C05	-5.76	119.33	124.85
38	Q	617	II0	C17-C04-C10	5.75	119.61	110.47
25	P	604	CLA	C4A-NA-C1A	5.74	109.29	106.71
25	g	302	CLA	C4A-NA-C1A	5.74	109.29	106.71
25	1	614	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	3	604	CLA	C4A-NA-C1A	5.72	109.28	106.71
38	4	617	II0	C17-C04-C10	5.72	119.56	110.47
25	N	609	CLA	C4A-NA-C1A	5.69	109.27	106.71
39	1	620	IHT	C16-C03-C11	-5.68	101.44	110.47
27	c	529	WVN	C29-C26-C22	-5.68	119.21	127.31
38	2	618	II0	C42-C41-C39	-5.67	111.86	123.47
39	O	620	IHT	C25-C23-C27	-5.67	114.98	122.92
39	1	620	IHT	C25-C23-C27	-5.66	115.00	122.92
39	N	620	IHT	C25-C23-C27	-5.66	115.00	122.92
39	Q	620	IHT	C25-C23-C27	-5.65	115.01	122.92
27	h	89	WVN	C20-C23-C25	-5.64	117.71	126.23
38	S	618	II0	C17-C04-C10	5.64	119.43	110.47
38	P	618	II0	C19-C13-C09	-5.64	116.69	124.35
25	3	609	CLA	C4A-NA-C1A	5.64	109.24	106.71
39	R	620	IHT	C16-C03-C11	-5.63	101.52	110.47
38	6	618	II0	C17-C04-C10	5.63	119.41	110.47
39	5	620	IHT	C16-C03-C11	-5.62	101.53	110.47
39	4	620	IHT	C16-C03-C11	-5.62	101.53	110.47
25	P	609	CLA	C4A-NA-C1A	5.62	109.23	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	412	BCT	O2-C-O1	5.62	134.12	119.55
30	a	412	BCT	O2-C-O1	5.61	134.11	119.55
39	4	620	IHT	C25-C23-C27	-5.61	115.06	122.92
27	h	89	WVN	C20-C13-C15	-5.61	107.88	121.46
38	O	618	II0	C42-C41-C39	-5.60	111.99	123.47
27	c	531	WVN	C30-C28-C25	-5.60	119.32	127.31
38	4	619	II0	C42-C41-C39	-5.59	112.02	123.47
37	1	613	KC2	CHB-C4A-C3A	-5.58	116.26	124.98
38	N	619	II0	C42-C41-C39	-5.56	112.08	123.47
37	N	613	KC2	CHB-C4A-C3A	-5.56	116.29	124.98
25	B	612	CLA	CMB-C2B-C1B	-5.55	119.93	128.46
25	c	522	CLA	C4A-NA-C1A	5.55	109.20	106.71
27	b	618	WVN	C39-C36-C32	-5.54	119.41	127.31
25	b	604	CLA	C4A-NA-C1A	5.53	109.19	106.71
38	1	619	II0	C42-C41-C39	-5.53	112.14	123.47
25	b	612	CLA	CMB-C2B-C1B	-5.52	119.98	128.46
27	d	408	WVN	C20-C13-C15	-5.52	108.09	121.46
38	Q	619	II0	C42-C41-C39	-5.52	112.17	123.47
38	2	619	II0	C42-C41-C39	-5.50	112.21	123.47
38	4	616	II0	C17-C04-C10	5.50	119.20	110.47
25	b	601	CLA	C4A-NA-C1A	5.49	109.17	106.71
25	B	604	CLA	C4A-NA-C1A	5.49	109.17	106.71
38	O	619	II0	C42-C41-C39	-5.49	112.24	123.47
38	Q	616	II0	C17-C04-C10	5.48	119.18	110.47
39	Q	620	IHT	C09-C10-C07	-5.47	114.79	122.73
25	C	522	CLA	C4A-NA-C1A	5.47	109.16	106.71
39	4	620	IHT	C09-C10-C07	-5.46	114.80	122.73
27	y	89	WVN	C40-C37-C34	-5.46	119.51	127.31
25	O	611	CLA	C4A-NA-C1A	5.46	109.16	106.71
27	B	619	WVN	C21-C15-C13	-5.46	118.40	124.53
39	R	620	IHT	C25-C23-C27	-5.45	115.29	122.92
39	Q	620	IHT	C40-C37-C33	-5.44	119.55	127.31
25	c	524	CLA	C4A-NA-C1A	5.43	109.14	106.71
39	2	620	IHT	C41-C38-C35	-5.42	119.57	127.31
25	C	517	CLA	C4A-NA-C1A	5.42	109.14	106.71
27	c	529	WVN	C39-C36-C32	-5.42	119.57	127.31
27	b	618	WVN	C40-C37-C34	-5.41	119.59	127.31
25	B	601	CLA	C4A-NA-C1A	5.40	109.13	106.71
39	Q	620	IHT	C17-C03-C11	-5.40	101.89	110.47
25	c	525	CLA	C4A-NA-C1A	5.39	109.13	106.71
38	P	618	II0	C42-C41-C39	-5.39	112.43	123.47
38	3	617	II0	C19-C13-C09	-5.38	117.04	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	601	CLA	C4A-NA-C1A	5.38	109.12	106.71
25	2	611	CLA	C4A-NA-C1A	5.38	109.12	106.71
27	y	89	WVN	C20-C13-C15	-5.36	108.47	121.46
25	S	604	CLA	C4A-NA-C1A	5.36	109.12	106.71
25	C	525	CLA	C4A-NA-C1A	5.36	109.11	106.71
25	6	604	CLA	C4A-NA-C1A	5.36	109.11	106.71
25	6	609	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	N	601	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	O	613	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	c	517	CLA	C4A-NA-C1A	5.34	109.11	106.71
25	C	524	CLA	C4A-NA-C1A	5.34	109.11	106.71
27	b	617	WVN	C20-C13-C15	-5.32	108.57	121.46
25	B	616	CLA	C4A-NA-C1A	5.29	109.09	106.71
38	N	618	II0	C42-C41-C39	-5.29	112.63	123.47
25	4	606	CLA	C4A-NA-C1A	5.29	109.08	106.71
29	A	409	PL9	C7-C3-C4	5.28	121.17	116.88
25	3	613	CLA	C4A-NA-C1A	5.28	109.08	106.71
38	3	618	II0	C42-C41-C39	-5.28	112.66	123.47
27	d	408	WVN	C21-C15-C13	-5.27	118.61	124.53
38	1	618	II0	C42-C41-C39	-5.27	112.68	123.47
25	D	403	CLA	C4A-NA-C1A	5.27	109.07	106.71
25	2	613	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	6	615	CLA	C4A-NA-C1A	5.24	109.06	106.71
25	2	610	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	5	603	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	S	615	CLA	C4A-NA-C1A	5.23	109.06	106.71
37	S	606	KC2	CHB-C4A-C3A	-5.22	116.82	124.98
39	5	620	IHT	C25-C23-C27	-5.22	115.61	122.92
37	6	612	KC2	C3A-C4A-NA	5.22	116.27	110.57
25	b	616	CLA	C4A-NA-C1A	5.22	109.05	106.71
25	R	606	CLA	C4A-NA-C1A	5.22	109.05	106.71
29	a	409	PL9	C7-C3-C4	5.21	121.11	116.88
25	B	615	CLA	C4A-NA-C1A	5.21	109.05	106.71
25	R	603	CLA	C4A-NA-C1A	5.20	109.05	106.71
25	b	612	CLA	C4A-NA-C1A	5.20	109.04	106.71
37	S	612	KC2	C3A-C4A-NA	5.20	116.25	110.57
25	P	613	CLA	C4A-NA-C1A	5.19	109.04	106.71
27	B	618	WVN	C40-C37-C34	-5.19	119.90	127.31
39	N	620	IHT	C17-C03-C11	-5.19	102.22	110.47
27	B	617	WVN	C29-C26-C22	-5.19	119.90	127.31
25	d	403	CLA	C4A-NA-C1A	5.19	109.04	106.71
25	5	606	CLA	C4A-NA-C1A	5.19	109.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	C4A-NA-C1A	5.18	109.03	106.71
25	3	602	CLA	C4A-NA-C1A	5.18	109.03	106.71
27	B	618	WVN	C39-C36-C32	-5.18	119.92	127.31
25	b	613	CLA	C4A-NA-C1A	5.18	109.03	106.71
37	4	612	KC2	C3A-C4A-NA	5.18	116.22	110.57
25	B	612	CLA	C4A-NA-C1A	5.17	109.03	106.71
38	P	617	II0	C19-C13-C09	-5.17	117.33	124.35
27	C	529	WVN	C40-C37-C34	-5.17	119.93	127.31
27	D	408	WVN	C21-C15-C13	-5.17	118.72	124.53
25	P	602	CLA	C4A-NA-C1A	5.16	109.03	106.71
27	a	407	WVN	C08-C01-C02	5.16	117.36	109.55
37	4	611	KC2	C3A-C4A-NA	5.16	116.21	110.57
37	Q	612	KC2	C3A-C4A-NA	5.16	116.20	110.57
25	O	610	CLA	C4A-NA-C1A	5.16	109.03	106.71
37	O	612	KC2	C3A-C4A-NA	5.15	116.20	110.57
37	N	612	KC2	C3A-C4A-NA	5.15	116.19	110.57
27	D	408	WVN	C20-C13-C15	-5.15	108.99	121.46
37	Q	611	KC2	C3A-C4A-NA	5.14	116.19	110.57
29	d	405	PL9	C7-C3-C4	5.13	121.05	116.88
27	3	620	WVN	C14-C15-C13	-5.12	115.30	122.73
37	2	612	KC2	C3A-C4A-NA	5.12	116.16	110.57
25	C	527	CLA	C4A-NA-C1A	5.11	109.00	106.71
27	P	620	WVN	C14-C15-C13	-5.11	115.31	122.73
27	C	529	WVN	C04-C09-C05	-5.11	119.95	124.85
27	b	617	WVN	C29-C26-C22	-5.11	120.01	127.31
37	1	612	KC2	C3A-C4A-NA	5.11	116.15	110.57
37	S	606	KC2	CHC-C1C-NC	-5.11	116.16	124.20
25	S	610	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	1	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
27	H	89	WVN	C30-C28-C25	-5.10	120.03	127.31
25	N	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
27	y	89	WVN	C20-C23-C25	-5.07	118.57	126.23
25	B	613	CLA	C4A-NA-C1A	5.07	108.98	106.71
25	C	520	CLA	C4A-NA-C1A	5.06	108.98	106.71
37	Q	612	KC2	CHC-C1C-NC	-5.06	116.23	124.20
25	O	602	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	2	604	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	N	615	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	5	609	CLA	C4A-NA-C1A	5.06	108.98	106.71
39	4	620	IHT	C17-C03-C11	-5.05	102.44	110.47
27	b	617	WVN	C40-C37-C34	-5.05	120.10	127.31
37	S	612	KC2	CHC-C1C-NC	-5.05	116.25	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	620	IHT	C40-C37-C33	-5.05	120.10	127.31
27	B	617	WVN	C39-C36-C32	-5.05	120.11	127.31
37	5	612	KC2	CHC-C1C-NC	-5.04	116.26	124.20
37	6	612	KC2	CHC-C1C-NC	-5.04	116.27	124.20
25	4	602	CLA	C4A-NA-C1A	5.04	108.97	106.71
37	R	612	KC2	CHC-C1C-NC	-5.04	116.27	124.20
37	4	612	KC2	CHC-C1C-NC	-5.04	116.27	124.20
27	b	619	WVN	C04-C09-C05	-5.03	120.03	124.85
38	S	617	II0	C19-C13-C09	-5.03	117.51	124.35
25	c	520	CLA	C4A-NA-C1A	5.03	108.97	106.71
37	1	612	KC2	CHC-C1C-NC	-5.03	116.29	124.20
38	6	617	II0	C19-C13-C09	-5.03	117.52	124.35
37	N	612	KC2	CHC-C1C-NC	-5.02	116.30	124.20
25	6	610	CLA	C4A-NA-C1A	5.02	108.96	106.71
25	2	602	CLA	C4A-NA-C1A	5.02	108.96	106.71
37	4	605	KC2	CHD-C4C-C3C	-5.01	107.95	126.11
29	D	405	PL9	C7-C3-C4	5.01	120.95	116.88
25	S	602	CLA	C4A-NA-C1A	5.00	108.96	106.71
37	Q	605	KC2	CHD-C4C-C3C	-5.00	107.98	126.11
25	R	609	CLA	C4A-NA-C1A	5.00	108.95	106.71
37	N	605	KC2	CHC-C1C-NC	-5.00	116.33	124.20
27	b	617	WVN	C21-C15-C13	-5.00	118.91	124.53
25	C	526	CLA	C4A-NA-C1A	5.00	108.95	106.71
25	N	604	CLA	C4A-NA-C1A	5.00	108.95	106.71
25	O	604	CLA	C4A-NA-C1A	4.99	108.95	106.71
27	D	408	WVN	C39-C36-C32	-4.99	120.19	127.31
25	B	602	CLA	C4A-NA-C1A	4.99	108.95	106.71
25	b	602	CLA	C4A-NA-C1A	4.99	108.95	106.71
25	1	615	CLA	C4A-NA-C1A	4.99	108.95	106.71
37	1	605	KC2	CHC-C1C-NC	-4.99	116.35	124.20
37	1	613	KC2	CHD-C4C-C3C	-4.98	108.04	126.11
25	P	610	CLA	C4A-NA-C1A	4.98	108.95	106.71
36	e	102	HEM	CHC-C4B-NB	4.98	129.84	124.43
27	h	89	WVN	C39-C36-C32	-4.98	120.21	127.31
37	N	613	KC2	CHD-C4C-C3C	-4.98	108.08	126.11
27	y	89	WVN	C21-C15-C13	-4.97	118.94	124.53
39	R	620	IHT	C41-C38-C35	-4.97	120.21	127.31
25	Q	602	CLA	C4A-NA-C1A	4.97	108.94	106.71
39	O	620	IHT	C17-C03-C11	-4.97	102.57	110.47
25	c	519	CLA	C4A-NA-C1A	4.97	108.94	106.71
25	c	527	CLA	C4A-NA-C1A	4.96	108.94	106.71
27	h	89	WVN	C29-C26-C22	-4.96	120.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	620	IHT	C17-C03-C11	-4.96	102.59	110.47
37	1	605	KC2	C3A-C4A-NA	4.96	115.98	110.57
37	6	606	KC2	CHB-C4A-C3A	-4.95	117.25	124.98
25	1	604	CLA	C4A-NA-C1A	4.95	108.93	106.71
36	E	102	HEM	CHC-C4B-NB	4.95	129.81	124.43
37	N	605	KC2	C3A-C4A-NA	4.94	115.97	110.57
37	3	606	KC2	CHC-C1C-NC	-4.94	116.43	124.20
25	6	602	CLA	C4A-NA-C1A	4.94	108.92	106.71
25	g	301	CLA	C4A-NA-C1A	4.93	108.92	106.71
27	b	619	WVN	C40-C37-C34	-4.93	120.27	127.31
25	B	610	CLA	C4A-NA-C1A	4.93	108.92	106.71
37	4	611	KC2	CHC-C1C-NC	-4.93	116.44	124.20
27	C	531	WVN	C29-C26-C22	-4.93	120.28	127.31
37	S	612	KC2	CHD-C4C-C3C	-4.92	108.26	126.11
37	6	612	KC2	CHD-C4C-C3C	-4.92	108.26	126.11
37	6	606	KC2	CHC-C1C-NC	-4.92	116.45	124.20
27	c	531	WVN	C40-C37-C34	-4.91	120.30	127.31
37	Q	611	KC2	CHC-C1C-NC	-4.91	116.47	124.20
39	N	620	IHT	C40-C37-C33	-4.91	120.31	127.31
25	1	609	CLA	C4A-NA-C1A	4.90	108.91	106.71
37	P	606	KC2	CHC-C1C-NC	-4.89	116.50	124.20
37	5	612	KC2	CHD-C4C-C3C	-4.88	108.42	126.11
37	R	612	KC2	CHD-C4C-C3C	-4.88	108.42	126.11
25	3	610	CLA	C4A-NA-C1A	4.88	108.90	106.71
37	2	612	KC2	C4B-CHC-C1C	-4.88	115.53	126.06
25	b	608	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
25	b	610	CLA	C4A-NA-C1A	4.88	108.90	106.71
37	2	612	KC2	CHC-C1C-NC	-4.87	116.53	124.20
37	O	612	KC2	CHC-C1C-NC	-4.87	116.53	124.20
39	Q	620	IHT	C03-C11-C15	-4.87	115.75	122.63
37	O	612	KC2	C4B-CHC-C1C	-4.87	115.56	126.06
27	b	617	WVN	C39-C36-C32	-4.86	120.37	127.31
37	1	611	KC2	CHD-C4C-C3C	-4.86	108.49	126.11
25	R	602	CLA	C4A-NA-C1A	4.86	108.89	106.71
37	N	611	KC2	CHD-C4C-C3C	-4.86	108.50	126.11
27	C	531	WVN	C20-C23-C25	-4.86	118.89	126.23
37	N	611	KC2	C3A-C4A-NA	4.86	115.87	110.57
25	c	526	CLA	C4A-NA-C1A	4.86	108.89	106.71
25	B	608	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
27	C	531	WVN	C02-C05-C09	-4.85	115.50	121.47
37	N	612	KC2	CHD-C4C-C3C	-4.85	108.53	126.11
37	1	613	KC2	C4B-CHC-C1C	-4.85	115.59	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	620	IHT	C08-C12-C15	4.85	121.52	111.85
37	1	611	KC2	C3A-C4A-NA	4.85	115.87	110.57
25	C	519	CLA	C4A-NA-C1A	4.85	108.89	106.71
27	h	89	WVN	C30-C28-C25	-4.84	120.40	127.31
37	1	612	KC2	CHD-C4C-C3C	-4.84	108.57	126.11
27	C	531	WVN	C39-C36-C32	-4.83	120.41	127.31
37	N	613	KC2	C4B-CHC-C1C	-4.83	115.63	126.06
37	N	611	KC2	C4B-CHC-C1C	-4.82	115.67	126.06
25	D	404	CLA	C4A-NA-C1A	4.82	108.87	106.71
38	Q	616	II0	C42-C41-C39	-4.81	113.61	123.47
27	H	89	WVN	C29-C26-C22	-4.81	120.44	127.31
37	4	612	KC2	CHD-C4C-C3C	-4.81	108.66	126.11
37	Q	612	KC2	CHD-C4C-C3C	-4.81	108.67	126.11
25	2	606	CLA	C4A-NA-C1A	4.81	108.87	106.71
37	Q	605	KC2	C4B-CHC-C1C	-4.81	115.69	126.06
37	4	605	KC2	C4B-CHC-C1C	-4.80	115.69	126.06
25	1	610	CLA	C4A-NA-C1A	4.80	108.86	106.71
27	b	618	WVN	C30-C28-C25	-4.80	120.47	127.31
39	1	620	IHT	C40-C37-C33	-4.80	120.47	127.31
37	1	611	KC2	C4B-CHC-C1C	-4.79	115.72	126.06
37	6	612	KC2	C4B-CHC-C1C	-4.79	115.72	126.06
37	N	612	KC2	C4B-CHC-C1C	-4.79	115.73	126.06
37	4	611	KC2	CHD-C4C-C3C	-4.79	108.76	126.11
37	1	612	KC2	C4B-CHC-C1C	-4.79	115.73	126.06
37	Q	605	KC2	CHC-C1C-NC	-4.78	116.67	124.20
25	Q	610	CLA	C4A-NA-C1A	4.78	108.86	106.71
37	Q	611	KC2	CHD-C4C-C3C	-4.78	108.78	126.11
25	C	523	CLA	CMB-C2B-C1B	-4.78	121.11	128.46
25	c	523	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
37	1	611	KC2	CHC-C1C-NC	-4.78	116.68	124.20
38	4	616	II0	C42-C41-C39	-4.78	113.69	123.47
25	N	610	CLA	C4A-NA-C1A	4.78	108.85	106.71
37	S	612	KC2	C4B-CHC-C1C	-4.77	115.76	126.06
37	4	605	KC2	CHC-C1C-NC	-4.77	116.69	124.20
37	R	612	KC2	C3A-C4A-NA	4.77	115.78	110.57
37	3	606	KC2	CHD-C4C-C3C	-4.77	108.83	126.11
25	d	400	CLA	C4A-NA-C1A	4.77	108.85	106.71
39	2	620	IHT	C08-C12-C15	4.77	121.35	111.85
27	B	619	WVN	C40-C37-C34	-4.77	120.51	127.31
25	5	602	CLA	C4A-NA-C1A	4.76	108.85	106.71
27	S	620	WVN	C04-C09-C05	-4.76	120.28	124.85
38	O	617	II0	C19-C13-C09	-4.76	117.88	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	521	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
27	6	620	WVN	C04-C09-C05	-4.76	120.29	124.85
25	P	612	CLA	C4A-NA-C1A	4.75	108.84	106.71
37	N	611	KC2	CHC-C1C-NC	-4.75	116.72	124.20
37	5	612	KC2	C3A-C4A-NA	4.75	115.76	110.57
37	6	606	KC2	C4B-CHC-C1C	-4.75	115.81	126.06
37	P	606	KC2	CHD-C4C-C3C	-4.75	108.89	126.11
25	c	521	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
25	3	612	CLA	C4A-NA-C1A	4.75	108.84	106.71
37	2	612	KC2	CHD-C4C-C3C	-4.75	108.90	126.11
37	O	612	KC2	CHD-C4C-C3C	-4.75	108.90	126.11
25	R	611	CLA	C4A-NA-C1A	4.74	108.84	106.71
27	H	89	WVN	C39-C36-C32	-4.74	120.54	127.31
39	2	620	IHT	C17-C03-C11	-4.74	102.93	110.47
37	3	606	KC2	C3A-C4A-NA	4.74	115.75	110.57
37	P	606	KC2	C3A-C4A-NA	4.73	115.74	110.57
37	N	605	KC2	CHD-C4C-C3C	-4.72	109.00	126.11
25	5	604	CLA	C4A-NA-C1A	4.72	108.83	106.71
25	P	601	CLA	C4A-NA-C1A	4.72	108.83	106.71
37	R	612	KC2	C4B-CHC-C1C	-4.72	115.88	126.06
37	1	613	KC2	C3A-C4A-NA	4.72	115.72	110.57
37	1	605	KC2	CHD-C4C-C3C	-4.72	109.02	126.11
27	A	407	WVN	C30-C28-C25	-4.71	120.58	127.31
25	O	606	CLA	C4A-NA-C1A	4.71	108.82	106.71
25	B	612	CLA	CMB-C2B-C3B	4.71	133.49	124.68
27	B	617	WVN	C40-C37-C34	-4.71	120.59	127.31
25	R	610	CLA	C4A-NA-C1A	4.71	108.82	106.71
37	N	613	KC2	C3A-C4A-NA	4.71	115.71	110.57
37	5	612	KC2	C4B-CHC-C1C	-4.70	115.92	126.06
37	N	613	KC2	CHC-C1C-NC	-4.70	116.81	124.20
25	d	404	CLA	C4A-NA-C1A	4.70	108.82	106.71
37	1	613	KC2	CHC-C1C-NC	-4.69	116.81	124.20
39	O	620	IHT	C03-C11-C15	-4.69	116.01	122.63
25	4	610	CLA	C4A-NA-C1A	4.68	108.81	106.71
39	N	620	IHT	C08-C12-C15	4.68	121.17	111.85
37	4	605	KC2	C3A-C4A-NA	4.68	115.68	110.57
27	B	618	WVN	C20-C13-C15	-4.67	110.14	121.46
25	P	615	CLA	C4A-NA-C1A	4.67	108.81	106.71
25	b	612	CLA	CMB-C2B-C3B	4.67	133.42	124.68
37	Q	605	KC2	C3A-C4A-NA	4.67	115.67	110.57
25	G	302	CLA	C4A-NA-C1A	4.65	108.80	106.71
37	4	612	KC2	CHB-C1B-C2B	-4.65	115.73	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	606	KC2	CHD-C4C-C3C	-4.65	109.26	126.11
38	P	619	II0	C19-C13-C09	-4.65	118.03	124.35
37	Q	612	KC2	CHB-C1B-C2B	-4.65	115.73	125.48
25	b	605	CLA	C4A-NA-C1A	4.65	108.80	106.71
25	G	301	CLA	C4A-NA-C1A	4.64	108.79	106.71
38	3	619	II0	C19-C13-C09	-4.64	118.04	124.35
37	Q	611	KC2	C4B-CHC-C1C	-4.64	116.04	126.06
37	4	612	KC2	C1B-CHB-C4A	-4.64	116.05	126.06
25	R	604	CLA	C4A-NA-C1A	4.64	108.79	106.71
37	4	611	KC2	C4B-CHC-C1C	-4.63	116.06	126.06
25	5	610	CLA	C4A-NA-C1A	4.63	108.79	106.71
37	Q	612	KC2	C1B-CHB-C4A	-4.63	116.07	126.06
37	S	606	KC2	C4B-CHC-C1C	-4.63	116.08	126.06
27	Y	89	WVN	C39-C36-C32	-4.62	120.71	127.31
25	B	605	CLA	C4A-NA-C1A	4.62	108.78	106.71
37	P	606	KC2	C4B-CHC-C1C	-4.61	116.11	126.06
39	N	620	IHT	C30-C27-C23	-4.61	120.73	127.31
25	A	406	CLA	C4A-NA-C1A	4.61	108.78	106.71
25	D	400	CLA	C4A-NA-C1A	4.61	108.78	106.71
38	1	617	II0	C19-C13-C09	-4.61	118.09	124.35
37	1	611	KC2	CHB-C1B-C2B	-4.61	115.82	125.48
37	N	605	KC2	C1B-CHB-C4A	-4.60	116.13	126.06
25	3	615	CLA	C4A-NA-C1A	4.60	108.78	106.71
39	O	620	IHT	C08-C12-C15	4.60	121.02	111.85
37	S	612	KC2	C1B-CHB-C4A	-4.60	116.14	126.06
39	1	620	IHT	C30-C27-C23	-4.60	120.75	127.31
37	Q	612	KC2	C4B-CHC-C1C	-4.59	116.15	126.06
25	4	604	CLA	C4A-NA-C1A	4.59	108.77	106.71
37	1	605	KC2	C1B-CHB-C4A	-4.59	116.16	126.06
25	6	601	CLA	C4A-NA-C1A	4.59	108.77	106.71
37	3	606	KC2	CHB-C1B-C2B	-4.59	115.86	125.48
25	5	611	CLA	C4A-NA-C1A	4.59	108.77	106.71
37	6	612	KC2	C1B-CHB-C4A	-4.59	116.16	126.06
37	3	606	KC2	C4B-CHC-C1C	-4.59	116.17	126.06
38	N	617	II0	C19-C13-C09	-4.58	118.12	124.35
37	4	612	KC2	C4B-CHC-C1C	-4.58	116.18	126.06
37	P	606	KC2	CHB-C1B-C2B	-4.58	115.88	125.48
37	1	612	KC2	CHB-C1B-C2B	-4.57	115.89	125.48
37	N	612	KC2	CHB-C1B-C2B	-4.57	115.89	125.48
25	R	601	CLA	C4A-NA-C1A	4.57	108.76	106.71
37	1	613	KC2	C4B-C3B-C2B	-4.57	103.00	106.75
37	6	606	KC2	CHD-C4C-C3C	-4.57	109.56	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	611	KC2	CHB-C1B-C2B	-4.57	115.91	125.48
37	4	605	KC2	CHB-C1B-C2B	-4.56	115.91	125.48
25	a	406	CLA	C4A-NA-C1A	4.56	108.76	106.71
25	b	609	CLA	C4A-NA-C1A	4.56	108.75	106.71
37	N	613	KC2	C4B-C3B-C2B	-4.56	103.01	106.75
25	S	613	CLA	C4A-NA-C1A	4.55	108.75	106.71
38	2	617	II0	C19-C13-C09	-4.55	118.17	124.35
37	Q	605	KC2	CHB-C1B-C2B	-4.55	115.95	125.48
27	B	617	WVN	C20-C13-C15	-4.54	110.46	121.46
25	3	601	CLA	C4A-NA-C1A	4.54	108.75	106.71
37	2	612	KC2	C4B-C3B-C2B	-4.54	103.02	106.75
25	B	609	CLA	C4A-NA-C1A	4.54	108.75	106.71
37	O	612	KC2	C4B-C3B-C2B	-4.54	103.02	106.75
27	d	408	WVN	C39-C36-C32	-4.53	120.84	127.31
25	S	601	CLA	C4A-NA-C1A	4.53	108.74	106.71
25	c	521	CLA	C4A-NA-C1A	4.53	108.74	106.71
25	5	601	CLA	C4A-NA-C1A	4.53	108.74	106.71
37	6	612	KC2	CHB-C1B-C2B	-4.52	115.99	125.48
27	b	617	WVN	C30-C28-C25	-4.52	120.86	127.31
25	b	611	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
25	c	528	CLA	C4A-NA-C1A	4.52	108.74	106.71
39	5	620	IHT	C41-C38-C35	-4.52	120.86	127.31
37	S	612	KC2	CHB-C1B-C2B	-4.51	116.02	125.48
37	1	612	KC2	C1B-CHB-C4A	-4.51	116.33	126.06
27	c	529	WVN	C20-C13-C15	-4.50	110.56	121.46
27	c	531	WVN	C14-C15-C13	-4.50	116.20	122.73
37	N	612	KC2	C1B-CHB-C4A	-4.49	116.37	126.06
39	Q	620	IHT	C41-C38-C35	-4.49	120.90	127.31
37	R	612	KC2	CHB-C1B-C2B	-4.49	116.07	125.48
27	b	618	WVN	C29-C26-C22	-4.49	120.91	127.31
27	S	620	WVN	C39-C36-C32	-4.49	120.91	127.31
39	R	620	IHT	C41-C40-C37	-4.49	114.29	123.47
34	w	134	LMG	O7-C10-C11	4.48	121.17	111.50
37	Q	611	KC2	CHB-C1B-C2B	-4.48	116.08	125.48
25	B	611	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
25	4	613	CLA	C4A-NA-C1A	4.48	108.72	106.71
38	S	618	II0	C06-C04-C10	4.48	118.70	109.62
27	A	407	WVN	C20-C13-C15	-4.48	110.61	121.46
37	5	612	KC2	CHB-C1B-C2B	-4.48	116.09	125.48
37	N	605	KC2	CHB-C1B-C2B	-4.47	116.10	125.48
25	6	610	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
25	S	610	CLA	CMB-C2B-C1B	-4.47	121.59	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	611	KC2	CHB-C1B-C2B	-4.47	116.11	125.48
38	5	616	II0	C19-C13-C09	-4.47	118.28	124.35
25	O	615	CLA	C4A-NA-C1A	4.46	108.71	106.71
37	1	605	KC2	C4B-CHC-C1C	-4.46	116.43	126.06
27	B	619	WVN	C39-C40-C37	-4.46	114.34	123.47
25	2	615	CLA	C4A-NA-C1A	4.46	108.71	106.71
25	Q	604	CLA	C4A-NA-C1A	4.46	108.71	106.71
25	C	521	CLA	C4A-NA-C1A	4.45	108.71	106.71
27	S	620	WVN	C20-C13-C15	-4.45	110.68	121.46
25	P	609	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
37	N	605	KC2	C4B-CHC-C1C	-4.45	116.47	126.06
38	6	618	II0	C06-C04-C10	4.45	118.63	109.62
27	B	619	WVN	C20-C13-C15	-4.44	110.70	121.46
38	Q	619	II0	C19-C13-C09	-4.44	118.31	124.35
37	1	605	KC2	CHB-C1B-C2B	-4.44	116.17	125.48
38	S	619	II0	C19-C13-C09	-4.44	118.32	124.35
25	R	607	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
38	R	616	II0	C19-C13-C09	-4.43	118.33	124.35
25	3	602	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
25	N	606	CLA	C4A-NA-C1A	4.43	108.70	106.71
38	3	616	II0	C19-C13-C09	-4.42	118.34	124.35
25	6	613	CLA	C4A-NA-C1A	4.42	108.69	106.71
25	5	607	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
25	Q	613	CLA	C4A-NA-C1A	4.41	108.69	106.71
39	5	620	IHT	C03-C11-C15	-4.41	116.40	122.63
25	P	611	CLA	C4A-NA-C1A	4.41	108.69	106.71
38	3	618	II0	C19-C13-C09	-4.41	118.36	124.35
37	Q	611	KC2	C1B-CHB-C4A	-4.40	116.57	126.06
39	4	620	IHT	C30-C27-C23	-4.39	121.04	127.31
25	a	404	CLA	C4A-NA-C1A	4.39	108.68	106.71
25	c	516	CLA	C4A-NA-C1A	4.39	108.68	106.71
25	3	611	CLA	C4A-NA-C1A	4.39	108.68	106.71
27	c	531	WVN	C20-C23-C25	-4.39	119.60	126.23
25	b	606	CLA	C4A-NA-C1A	4.39	108.68	106.71
38	P	616	II0	C19-C13-C09	-4.38	118.39	124.35
25	B	606	CLA	C4A-NA-C1A	4.38	108.67	106.71
25	O	609	CLA	C4A-NA-C1A	4.38	108.67	106.71
37	4	611	KC2	C1B-CHB-C4A	-4.37	116.62	126.06
25	1	606	CLA	C4A-NA-C1A	4.37	108.67	106.71
25	P	602	CLA	CMB-C2B-C1B	-4.36	121.75	128.46
39	R	620	IHT	C03-C11-C15	-4.36	116.48	122.63
25	6	604	CLA	CMB-C2B-C1B	-4.36	121.76	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	609	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
27	b	617	WVN	C40-C39-C36	-4.36	114.55	123.47
25	b	607	CLA	C4A-NA-C1A	4.35	108.66	106.71
25	c	519	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
37	1	612	KC2	C4B-C3B-C2B	-4.34	103.19	106.75
37	S	606	KC2	C3A-C4A-NA	4.34	115.31	110.57
25	S	604	CLA	CMB-C2B-C1B	-4.33	121.80	128.46
25	S	611	CLA	C4A-NA-C1A	4.33	108.65	106.71
37	1	613	KC2	CHB-C1B-C2B	-4.33	116.39	125.48
37	6	606	KC2	C1B-CHB-C4A	-4.33	116.72	126.06
39	4	620	IHT	C41-C38-C35	-4.33	121.13	127.31
25	B	607	CLA	C4A-NA-C1A	4.32	108.65	106.71
38	4	619	II0	C19-C13-C09	-4.32	118.48	124.35
25	C	519	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
37	S	606	KC2	C4B-C3B-C2B	-4.31	103.21	106.75
27	H	89	WVN	C21-C15-C13	-4.31	119.69	124.53
37	N	613	KC2	CHB-C1B-C2B	-4.31	116.45	125.48
39	Q	620	IHT	C30-C27-C23	-4.29	121.18	127.31
37	N	612	KC2	C4B-C3B-C2B	-4.29	103.22	106.75
38	2	616	II0	C19-C13-C09	-4.29	118.52	124.35
25	6	611	CLA	C4A-NA-C1A	4.29	108.64	106.71
25	A	404	CLA	C4A-NA-C1A	4.29	108.63	106.71
27	y	89	WVN	C39-C36-C32	-4.29	121.19	127.31
39	2	620	IHT	C03-C11-C15	-4.29	116.58	122.63
39	N	620	IHT	C03-C11-C15	-4.28	116.58	122.63
34	W	134	LMG	O7-C10-C11	4.28	120.73	111.50
25	2	603	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
38	N	619	II0	C19-C13-C09	-4.28	118.54	124.35
25	C	516	CLA	C4A-NA-C1A	4.28	108.63	106.71
25	C	524	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
25	Q	606	CLA	C4A-NA-C1A	4.27	108.63	106.71
37	2	612	KC2	C1B-CHB-C4A	-4.27	116.85	126.06
27	6	620	WVN	C20-C13-C15	-4.27	111.13	121.46
38	O	616	II0	C19-C13-C09	-4.27	118.55	124.35
25	3	604	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
25	O	603	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
37	O	612	KC2	C1B-CHB-C4A	-4.26	116.86	126.06
25	B	611	CLA	C4A-NA-C1A	4.26	108.62	106.71
25	3	612	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
25	2	609	CLA	C4A-NA-C1A	4.26	108.62	106.71
27	B	618	WVN	C29-C26-C22	-4.25	121.24	127.31
25	P	604	CLA	CMB-C2B-C1B	-4.25	121.93	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	606	KC2	C1B-CHB-C4A	-4.25	116.90	126.06
37	R	612	KC2	C4B-C3B-C2B	-4.24	103.27	106.75
27	c	530	WVN	C20-C13-C15	-4.24	111.18	121.46
37	P	606	KC2	C1B-CHB-C4A	-4.24	116.91	126.06
35	c	532	DGD	O2G-C1B-C2B	4.24	120.64	111.50
37	5	612	KC2	C1B-CHB-C4A	-4.24	116.92	126.06
25	P	612	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
37	R	612	KC2	C1B-CHB-C4A	-4.24	116.92	126.06
38	4	617	II0	C19-C13-C09	-4.23	118.59	124.35
25	C	528	CLA	C4A-NA-C1A	4.23	108.61	106.71
37	5	612	KC2	C4B-C3B-C2B	-4.23	103.28	106.75
39	1	620	IHT	C41-C38-C35	-4.23	121.28	127.31
36	e	102	HEM	C1B-NB-C4B	4.22	109.44	105.07
27	6	620	WVN	C39-C36-C32	-4.22	121.28	127.31
25	c	524	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
31	L	101	LHG	O7-C7-C8	4.22	120.59	111.50
35	C	532	DGD	O2G-C1B-C2B	4.22	120.59	111.50
38	Q	617	II0	C19-C13-C09	-4.21	118.62	124.35
37	S	606	KC2	C1B-CHB-C4A	-4.21	116.97	126.06
25	6	609	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
37	2	612	KC2	CHB-C1B-C2B	-4.21	116.66	125.48
27	6	620	WVN	C29-C26-C22	-4.21	121.31	127.31
25	5	615	CLA	C4A-NA-C1A	4.20	108.60	106.71
31	l	101	LHG	O7-C7-C8	4.20	120.55	111.50
25	P	613	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
25	B	607	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
25	3	613	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
25	Q	613	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
25	Q	615	CLA	C4A-NA-C1A	4.18	108.59	106.71
38	6	616	II0	C19-C13-C09	-4.18	118.66	124.35
25	c	516	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
37	O	612	KC2	CHB-C1B-C2B	-4.18	116.71	125.48
27	C	529	WVN	C29-C26-C22	-4.18	121.34	127.31
36	E	102	HEM	CHD-C1D-ND	4.18	128.97	124.43
27	C	531	WVN	C20-C13-C15	-4.18	111.34	121.46
25	4	613	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
25	b	611	CLA	C4A-NA-C1A	4.16	108.58	106.71
25	4	615	CLA	C4A-NA-C1A	4.15	108.57	106.71
39	5	620	IHT	C18-C22-C23	-4.15	119.96	126.23
25	R	615	CLA	C4A-NA-C1A	4.15	108.57	106.71
37	S	612	KC2	C4B-C3B-C2B	-4.14	103.35	106.75
38	S	616	II0	C19-C13-C09	-4.14	118.73	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	603	CLA	C4A-NA-C1A	4.13	108.56	106.71
34	f	99	LMG	O7-C10-C11	4.13	120.41	111.50
25	S	609	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
37	1	611	KC2	C1B-CHB-C4A	-4.13	117.14	126.06
25	C	516	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
25	6	613	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
37	6	612	KC2	C4B-C3B-C2B	-4.13	103.36	106.75
34	C	536	LMG	O7-C10-C11	4.12	120.37	111.50
37	N	611	KC2	C1B-CHB-C4A	-4.11	117.18	126.06
25	S	613	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
25	4	610	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
25	3	603	CLA	C4A-NA-C1A	4.11	108.55	106.71
25	Q	610	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
39	R	620	IHT	C19-C10-C07	-4.11	119.92	124.53
31	b	622	LHG	O7-C7-C8	4.10	120.35	111.50
34	F	99	LMG	O7-C10-C11	4.10	120.35	111.50
38	P	618	II0	C20-C14-C10	-4.10	118.78	124.35
27	a	407	WVN	C20-C23-C25	-4.10	120.05	126.23
27	A	407	WVN	C02-C05-C09	-4.10	116.43	121.47
25	b	607	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
34	B	620	LMG	O7-C10-C11	4.09	120.32	111.50
31	c	535	LHG	O7-C7-C8	4.09	120.31	111.50
28	A	408	SQD	O47-C7-C8	4.08	120.30	111.50
25	D	404	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
37	Q	605	KC2	C4B-C3B-C2B	-4.08	103.40	106.75
39	1	620	IHT	C03-C11-C15	-4.08	116.88	122.63
38	3	619	II0	C06-C04-C10	4.08	117.88	109.62
25	d	404	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
28	a	408	SQD	O47-C7-C8	4.07	120.28	111.50
38	5	617	II0	C19-C13-C09	-4.07	118.82	124.35
25	c	525	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
34	b	620	LMG	O7-C10-C11	4.07	120.27	111.50
36	e	102	HEM	CHD-C1D-ND	4.06	128.84	124.43
38	3	618	II0	C20-C14-C10	-4.06	118.83	124.35
25	6	603	CLA	C4A-NA-C1A	4.06	108.53	106.71
25	6	604	CLA	CMB-C2B-C3B	4.06	132.27	124.68
31	d	406	LHG	O7-C7-C8	4.06	120.25	111.50
31	D	406	LHG	O7-C7-C8	4.05	120.24	111.50
25	C	525	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
34	z	102	LMG	O7-C10-C11	4.05	120.23	111.50
38	P	619	II0	C06-C04-C10	4.05	117.83	109.62
27	b	617	WVN	C23-C20-C13	-4.05	115.84	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	603	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
25	Q	604	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
25	5	604	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
38	R	617	II0	C19-C13-C09	-4.04	118.86	124.35
37	4	605	KC2	C1B-CHB-C4A	-4.04	117.35	126.06
34	D	402	LMG	O7-C10-C11	4.03	120.19	111.50
38	1	617	II0	C06-C04-C10	4.03	117.79	109.62
27	Y	89	WVN	C40-C37-C34	-4.03	121.56	127.31
25	4	604	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
25	S	604	CLA	CMB-C2B-C3B	4.02	132.21	124.68
38	4	616	II0	C19-C13-C09	-4.02	118.88	124.35
37	4	605	KC2	C4B-C3B-C2B	-4.02	103.45	106.75
34	Z	102	LMG	O7-C10-C11	4.02	120.17	111.50
38	Q	616	II0	C19-C13-C09	-4.02	118.89	124.35
27	h	89	WVN	C40-C37-C34	-4.02	121.58	127.31
37	Q	605	KC2	C1B-CHB-C4A	-4.02	117.39	126.06
38	N	617	II0	C06-C04-C10	4.02	117.76	109.62
27	c	531	WVN	C39-C36-C32	-4.02	121.58	127.31
34	d	402	LMG	O7-C10-C11	4.01	120.15	111.50
25	R	604	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
25	B	614	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
25	b	608	CLA	CMB-C2B-C3B	4.00	132.17	124.68
25	C	523	CLA	CMB-C2B-C3B	4.00	132.16	124.68
25	B	608	CLA	CMB-C2B-C3B	3.99	132.15	124.68
27	B	617	WVN	C12-C14-C15	-3.99	106.95	114.08
27	Y	89	WVN	C29-C26-C22	-3.99	121.62	127.31
38	2	616	II0	C20-C14-C10	-3.99	118.93	124.35
25	B	603	CLA	C4A-NA-C1A	3.98	108.50	106.71
25	N	603	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
25	O	613	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
25	1	603	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
25	1	603	CLA	C4A-NA-C1A	3.98	108.50	106.71
39	N	620	IHT	C41-C38-C35	-3.98	121.63	127.31
38	O	616	II0	C20-C14-C10	-3.97	118.95	124.35
25	2	613	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	c	523	CLA	CMB-C2B-C3B	3.97	132.10	124.68
25	b	615	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
37	N	611	KC2	C4B-C3B-C2B	-3.96	103.50	106.75
38	1	619	II0	C20-C14-C10	-3.96	118.97	124.35
37	4	611	KC2	C4B-C3B-C2B	-3.96	103.50	106.75
25	N	603	CLA	C4A-NA-C1A	3.96	108.49	106.71
38	N	616	II0	C19-C13-C09	-3.96	118.97	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	P	616	II0	C20-C14-C10	-3.96	118.97	124.35
25	3	603	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
38	N	619	II0	C20-C14-C10	-3.95	118.98	124.35
25	O	615	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
38	3	616	II0	C20-C14-C10	-3.95	118.98	124.35
39	5	620	IHT	C41-C40-C37	-3.95	115.38	123.47
37	1	611	KC2	C4B-C3B-C2B	-3.94	103.51	106.75
25	1	610	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
38	1	616	II0	C19-C13-C09	-3.94	119.00	124.35
25	b	614	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
25	1	604	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
25	B	615	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
27	a	407	WVN	C04-C09-C05	-3.94	121.08	124.85
25	2	615	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
27	d	408	WVN	C30-C28-C25	-3.93	121.70	127.31
25	P	603	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
34	c	536	LMG	O7-C10-C11	3.93	119.97	111.50
34	m	101	LMG	O7-C10-C11	3.93	119.97	111.50
25	N	610	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
25	3	604	CLA	CMB-C2B-C3B	3.93	132.03	124.68
25	B	605	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
37	Q	611	KC2	C4B-C3B-C2B	-3.93	103.53	106.75
38	4	617	II0	C20-C14-C10	-3.92	119.02	124.35
37	S	612	KC2	O2D-CGD-CBD	3.92	118.24	111.27
37	1	613	KC2	C1B-CHB-C4A	-3.92	117.61	126.06
25	5	607	CLA	CMB-C2B-C3B	3.91	132.00	124.68
25	P	615	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	R	611	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	3	615	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	P	604	CLA	CMB-C2B-C3B	3.91	131.99	124.68
38	Q	617	II0	C20-C14-C10	-3.91	119.04	124.35
38	2	619	II0	C03-C09-C13	-3.91	117.11	122.63
37	6	612	KC2	O2D-CGD-CBD	3.91	118.21	111.27
38	R	618	II0	C03-C09-C13	-3.91	117.12	122.63
27	H	89	WVN	C40-C37-C34	-3.90	121.74	127.31
25	C	521	CLA	CMB-C2B-C3B	3.90	131.98	124.68
25	P	609	CLA	CMB-C2B-C3B	3.90	131.98	124.68
25	C	523	CLA	C4A-NA-C1A	3.90	108.46	106.71
25	c	521	CLA	CMB-C2B-C3B	3.90	131.97	124.68
27	C	529	WVN	C14-C15-C13	-3.89	117.08	122.73
38	O	619	II0	C03-C09-C13	-3.89	117.14	122.63
25	N	604	CLA	CMB-C2B-C1B	-3.89	122.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	613	KC2	C1B-CHB-C4A	-3.89	117.66	126.06
38	5	618	II0	C03-C09-C13	-3.89	117.14	122.63
25	R	607	CLA	CMB-C2B-C3B	3.89	131.95	124.68
25	5	611	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
37	N	605	KC2	O2D-CGD-CBD	3.88	118.16	111.27
25	4	603	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
25	Q	603	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
34	2	622	LMG	O7-C10-C11	3.87	119.85	111.50
34	g	303	LMG	O7-C10-C11	3.87	119.85	111.50
25	1	614	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
27	d	408	WVN	C20-C23-C25	-3.87	120.39	126.23
25	C	518	CLA	C4A-NA-C1A	3.87	108.44	106.71
25	B	616	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
27	d	408	WVN	C40-C37-C34	-3.87	121.79	127.31
25	2	604	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
34	G	303	LMG	O7-C10-C11	3.86	119.83	111.50
37	P	606	KC2	C4B-C3B-C2B	-3.86	103.58	106.75
25	b	602	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
27	C	530	WVN	C23-C20-C13	-3.86	116.37	127.20
25	6	610	CLA	CMB-C2B-C3B	3.85	131.89	124.68
25	a	403	CLA	C4A-NA-C1A	3.85	108.44	106.71
25	b	603	CLA	C4A-NA-C1A	3.85	108.44	106.71
34	O	622	LMG	O7-C10-C11	3.85	119.80	111.50
34	d	407	LMG	O7-C10-C11	3.85	119.80	111.50
25	b	616	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
25	N	614	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
37	3	606	KC2	C4B-C3B-C2B	-3.85	103.59	106.75
34	D	407	LMG	O7-C10-C11	3.84	119.79	111.50
25	b	611	CLA	CMB-C2B-C3B	3.84	131.87	124.68
25	S	610	CLA	CMB-C2B-C3B	3.84	131.87	124.68
37	1	605	KC2	O2D-CGD-CBD	3.84	118.09	111.27
38	P	617	II0	C20-C14-C10	-3.84	119.13	124.35
25	O	604	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
35	H	90	DGD	O2G-C1B-C2B	3.84	119.77	111.50
38	Q	619	II0	C20-C14-C10	-3.84	119.14	124.35
38	4	616	II0	C20-C14-C10	-3.83	119.14	124.35
31	C	535	LHG	O7-C7-C8	3.83	119.76	111.50
25	c	523	CLA	C4A-NA-C1A	3.83	108.43	106.71
34	M	101	LMG	O7-C10-C11	3.82	119.74	111.50
35	h	90	DGD	O2G-C1B-C2B	3.82	119.74	111.50
31	5	621	LHG	O7-C7-C8	3.82	119.74	111.50
38	Q	616	II0	C41-C42-C40	-3.82	115.64	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	407	WVN	C39-C36-C32	-3.82	121.86	127.31
25	b	605	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
25	B	602	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
25	2	602	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
25	3	609	CLA	CMB-C2B-C3B	3.82	131.82	124.68
38	3	617	II0	C20-C14-C10	-3.82	119.16	124.35
31	R	621	LHG	O7-C7-C8	3.82	119.73	111.50
25	A	403	CLA	C4A-NA-C1A	3.81	108.42	106.71
31	3	621	LHG	O7-C7-C8	3.81	119.71	111.50
38	1	617	II0	C20-C14-C10	-3.81	119.18	124.35
25	a	404	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
38	6	617	II0	C20-C14-C10	-3.81	119.18	124.35
38	S	617	II0	C20-C14-C10	-3.81	119.18	124.35
39	O	620	IHT	C19-C10-C07	-3.81	120.25	124.53
31	P	621	LHG	O7-C7-C8	3.80	119.70	111.50
36	E	102	HEM	C1B-NB-C4B	3.80	109.00	105.07
25	O	602	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
38	4	619	II0	C20-C14-C10	-3.80	119.19	124.35
27	D	408	WVN	C30-C28-C25	-3.80	121.89	127.31
25	6	613	CLA	CMB-C2B-C3B	3.80	131.78	124.68
25	B	611	CLA	CMB-C2B-C3B	3.79	131.78	124.68
38	Q	617	II0	C06-C04-C10	3.79	117.31	109.62
31	B	622	LHG	O7-C7-C8	3.79	119.67	111.50
38	4	616	II0	C41-C42-C40	-3.79	115.71	123.47
37	6	606	KC2	C2A-C1A-NA	3.79	115.48	109.40
25	O	610	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
38	Q	616	II0	C20-C14-C10	-3.79	119.20	124.35
27	A	407	WVN	C14-C15-C13	-3.79	117.23	122.73
39	2	620	IHT	C19-C10-C07	-3.79	120.28	124.53
31	O	621	LHG	O7-C7-C8	3.79	119.66	111.50
25	5	615	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
25	2	603	CLA	C4A-NA-C1A	3.78	108.41	106.71
31	2	621	LHG	O7-C7-C8	3.78	119.65	111.50
38	4	617	II0	C06-C04-C10	3.78	117.29	109.62
25	B	603	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
25	A	404	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
25	c	518	CLA	C4A-NA-C1A	3.78	108.41	106.71
27	b	618	WVN	C21-C15-C13	-3.78	120.29	124.53
25	R	615	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
25	C	517	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
38	4	618	II0	C03-C09-C13	-3.77	117.31	122.63
25	3	602	CLA	CMB-C2B-C3B	3.77	131.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	618	II0	C06-C04-C10	3.76	117.25	109.62
25	S	613	CLA	CMB-C2B-C3B	3.76	131.71	124.68
37	1	605	KC2	C2A-C1A-NA	3.76	115.43	109.40
38	1	618	II0	C06-C04-C10	3.76	117.23	109.62
38	N	617	II0	C20-C14-C10	-3.76	119.25	124.35
25	c	519	CLA	CMB-C2B-C3B	3.76	131.71	124.68
25	D	400	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
38	P	619	II0	C20-C14-C10	-3.76	119.25	124.35
25	P	602	CLA	CMB-C2B-C3B	3.75	131.70	124.68
25	d	400	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
38	O	618	II0	C19-C13-C09	-3.75	119.25	124.35
27	C	530	WVN	C14-C15-C13	-3.75	117.29	122.73
25	P	610	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
38	R	617	II0	C20-C14-C10	-3.74	119.26	124.35
37	N	605	KC2	C2A-C1A-NA	3.74	115.40	109.40
25	2	610	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
25	c	517	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
25	5	613	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
25	6	602	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
25	3	610	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
27	c	529	WVN	C40-C37-C34	-3.72	122.00	127.31
25	C	519	CLA	CMB-C2B-C3B	3.72	131.64	124.68
25	Q	613	CLA	CMB-C2B-C3B	3.72	131.64	124.68
38	1	616	II0	C20-C14-C10	-3.72	119.29	124.35
25	C	522	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
25	c	524	CLA	CMB-C2B-C3B	3.72	131.64	124.68
25	C	524	CLA	CMB-C2B-C3B	3.72	131.63	124.68
25	b	603	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
38	3	619	II0	C20-C14-C10	-3.71	119.30	124.35
25	B	614	CLA	C4A-NA-C1A	3.71	108.38	106.71
25	4	613	CLA	CMB-C2B-C3B	3.71	131.62	124.68
31	S	621	LHG	O7-C7-C8	3.71	119.50	111.50
38	5	619	II0	C20-C14-C10	-3.71	119.31	124.35
37	6	606	KC2	C3A-C4A-NA	3.71	114.62	110.57
37	4	612	KC2	C4B-C3B-C2B	-3.71	103.71	106.75
38	5	616	II0	C20-C14-C10	-3.71	119.31	124.35
38	5	617	II0	C20-C14-C10	-3.71	119.31	124.35
38	N	616	II0	C20-C14-C10	-3.71	119.31	124.35
39	Q	620	IHT	C08-C12-C15	3.70	119.23	111.85
25	c	526	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
38	R	619	II0	C19-C13-C09	-3.70	119.32	124.35
25	a	406	CLA	CMB-C2B-C1B	-3.70	122.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	602	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	b	604	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	S	615	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
38	R	616	II0	C20-C14-C10	-3.69	119.33	124.35
37	S	606	KC2	C2A-C1A-NA	3.69	115.32	109.40
25	C	526	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
39	1	620	IHT	C04-C06-C09	3.69	119.62	111.38
25	A	406	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
31	6	621	LHG	O7-C7-C8	3.69	119.45	111.50
38	5	619	II0	C19-C13-C09	-3.69	119.34	124.35
38	R	619	II0	C20-C14-C10	-3.68	119.34	124.35
37	6	606	KC2	CHB-C1B-C2B	-3.68	117.75	125.48
25	6	615	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
25	Q	602	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
39	N	620	IHT	C04-C06-C09	3.68	119.60	111.38
25	S	603	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
37	Q	605	KC2	O2D-CGD-CBD	3.67	117.80	111.27
25	S	602	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	b	614	CLA	C4A-NA-C1A	3.67	108.36	106.71
39	R	620	IHT	C02-C07-C10	-3.67	117.45	122.61
37	Q	612	KC2	C4B-C3B-C2B	-3.66	103.74	106.75
27	B	617	WVN	C08-C01-C02	3.66	115.09	109.55
37	N	605	KC2	C4B-C3B-C2B	-3.66	103.75	106.75
29	A	409	PL9	C7-C3-C2	-3.66	118.49	123.30
25	3	615	CLA	CMB-C2B-C3B	3.66	131.52	124.68
38	1	619	II0	C19-C13-C09	-3.66	119.38	124.35
38	Q	618	II0	C03-C09-C13	-3.66	117.47	122.63
25	R	613	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
25	B	604	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
37	N	605	KC2	CBC-CAC-C3C	-3.65	109.46	127.62
25	P	615	CLA	CMB-C2B-C3B	3.65	131.50	124.68
37	N	612	KC2	O2D-CGD-CBD	3.65	117.75	111.27
27	a	407	WVN	C39-C36-C32	-3.64	122.11	127.31
37	1	605	KC2	CBC-CAC-C3C	-3.64	109.51	127.62
37	4	605	KC2	O2D-CGD-CBD	3.64	117.73	111.27
25	C	527	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
37	P	606	KC2	CBC-CAC-C3C	-3.63	109.56	127.62
37	1	605	KC2	C4B-C3B-C2B	-3.63	103.77	106.75
37	S	612	KC2	C2A-C1A-NA	3.63	115.22	109.40
37	3	606	KC2	CBC-CAC-C3C	-3.63	109.57	127.62
37	6	612	KC2	C2A-C1A-NA	3.63	115.22	109.40
25	P	613	CLA	CMB-C2B-C3B	3.62	131.46	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	618	WVN	C21-C15-C14	3.62	120.58	113.62
25	N	602	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
25	R	602	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
27	C	529	WVN	C08-C01-C02	3.62	115.02	109.55
25	c	520	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
25	c	525	CLA	CMB-C2B-C3B	3.62	131.44	124.68
25	C	526	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
25	b	609	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
25	c	516	CLA	CMB-C2B-C3B	3.61	131.44	124.68
29	a	409	PL9	C7-C3-C2	-3.61	118.55	123.30
25	C	528	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
25	5	602	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
25	B	609	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
27	3	620	WVN	C23-C20-C13	-3.61	117.07	127.20
25	C	525	CLA	CMB-C2B-C3B	3.61	131.43	124.68
25	R	610	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
25	B	606	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
39	2	620	IHT	C28-C26-C24	3.60	123.98	116.84
25	3	613	CLA	CMB-C2B-C3B	3.60	131.42	124.68
25	3	612	CLA	CMB-C2B-C3B	3.60	131.41	124.68
25	1	602	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
25	4	615	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
25	c	527	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
25	5	610	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
37	1	612	KC2	O2D-CGD-CBD	3.59	117.66	111.27
38	6	616	II0	C20-C14-C10	-3.59	119.47	124.35
25	C	520	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
27	P	620	WVN	C23-C20-C13	-3.59	117.11	127.20
38	S	616	II0	C20-C14-C10	-3.59	119.47	124.35
37	4	611	KC2	C2A-C1A-NA	3.59	115.15	109.40
25	c	526	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
25	c	518	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
38	2	618	II0	C03-C09-C13	-3.58	117.58	122.63
39	5	620	IHT	C04-C06-C09	3.58	119.38	111.38
25	R	613	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
37	6	606	KC2	C4B-C3B-C2B	-3.58	103.81	106.75
31	A	413	LHG	O7-C7-C8	3.58	119.21	111.50
25	S	609	CLA	CMB-C2B-C3B	3.58	131.37	124.68
37	Q	611	KC2	C2A-C1A-NA	3.58	115.14	109.40
25	g	302	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
25	b	606	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
28	a	411	SQD	O47-C7-C8	3.56	119.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	CLA	CMB-C2B-C3B	3.56	131.35	124.68
25	Q	615	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
37	N	612	KC2	C2A-C1A-NA	3.56	115.12	109.40
25	P	612	CLA	CMB-C2B-C3B	3.56	131.34	124.68
37	2	612	KC2	C2A-C1A-NA	3.56	115.11	109.40
38	Q	618	II0	C20-C14-C10	-3.56	119.51	124.35
25	6	609	CLA	CMB-C2B-C3B	3.56	131.34	124.68
37	1	612	KC2	C2A-C1A-NA	3.56	115.11	109.40
27	y	89	WVN	C26-C29-C31	-3.56	112.12	123.22
25	c	528	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
27	B	618	WVN	C30-C28-C25	-3.56	122.24	127.31
25	S	609	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
25	O	603	CLA	C4A-NA-C1A	3.55	108.30	106.71
27	b	618	WVN	C06-C13-C15	-3.55	117.61	122.61
25	B	608	CLA	C4A-NA-C1A	3.55	108.30	106.71
28	A	411	SQD	O47-C7-C8	3.55	119.15	111.50
37	Q	612	KC2	C3B-C2B-C1B	-3.55	103.69	107.08
37	O	612	KC2	C2A-C1A-NA	3.55	115.09	109.40
39	Q	620	IHT	C28-C26-C24	3.55	123.87	116.84
38	1	619	II0	C18-C04-C10	-3.55	104.83	110.47
25	Q	604	CLA	CMB-C2B-C3B	3.55	131.31	124.68
27	c	531	WVN	C01-C02-C11	-3.54	108.22	112.70
37	Q	612	KC2	C2A-C1A-NA	3.54	115.09	109.40
25	2	615	CLA	CMB-C2B-C3B	3.54	131.31	124.68
25	O	603	CLA	CMB-C2B-C3B	3.54	131.31	124.68
25	O	615	CLA	CMB-C2B-C3B	3.54	131.30	124.68
25	Q	603	CLA	C4A-NA-C1A	3.54	108.30	106.71
25	b	608	CLA	C4A-NA-C1A	3.53	108.30	106.71
25	5	607	CLA	C4A-NA-C1A	3.53	108.30	106.71
38	4	618	II0	C20-C14-C10	-3.53	119.55	124.35
25	C	518	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
31	a	413	LHG	O7-C7-C8	3.53	119.10	111.50
25	R	603	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
25	5	603	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
37	4	612	KC2	C2A-C1A-NA	3.52	115.05	109.40
25	5	613	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
38	N	619	II0	C18-C04-C10	-3.52	104.88	110.47
25	B	607	CLA	CMB-C2B-C3B	3.52	131.25	124.68
27	c	531	WVN	C26-C29-C31	-3.51	112.25	123.22
37	4	612	KC2	C3B-C2B-C1B	-3.51	103.72	107.08
25	2	603	CLA	CMB-C2B-C3B	3.51	131.25	124.68
25	R	607	CLA	C4A-NA-C1A	3.51	108.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	604	CLA	CMB-C2B-C3B	3.51	131.24	124.68
25	g	301	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
36	e	102	HEM	CHA-C4D-ND	3.50	128.71	124.38
38	Q	618	II0	C19-C13-C09	-3.50	119.59	124.35
25	4	603	CLA	C4A-NA-C1A	3.50	108.28	106.71
27	c	531	WVN	C02-C05-C09	-3.50	117.16	121.47
37	R	612	KC2	CBC-CAC-C3C	-3.50	110.22	127.62
25	d	404	CLA	CMB-C2B-C3B	3.49	131.22	124.68
27	S	620	WVN	C29-C26-C22	-3.49	122.33	127.31
37	5	612	KC2	CBC-CAC-C3C	-3.49	110.26	127.62
27	b	617	WVN	C12-C14-C15	-3.49	107.85	114.08
37	Q	611	KC2	CBC-CAC-C3C	-3.49	110.27	127.62
38	S	618	II0	C20-C14-C10	-3.49	119.61	124.35
37	4	611	KC2	CBC-CAC-C3C	-3.49	110.28	127.62
37	O	612	KC2	O2D-CGD-CBD	3.48	117.46	111.27
27	d	408	WVN	C29-C26-C22	-3.48	122.34	127.31
25	G	301	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	Q	607	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
37	4	612	KC2	C2B-C1B-NB	3.48	112.67	110.10
37	N	612	KC2	CBC-CAC-C3C	-3.48	110.31	127.62
25	c	522	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
37	Q	605	KC2	CBC-CAC-C3C	-3.47	110.34	127.62
37	1	612	KC2	CBC-CAC-C3C	-3.47	110.35	127.62
25	D	404	CLA	CMB-C2B-C3B	3.47	131.17	124.68
37	4	605	KC2	CBC-CAC-C3C	-3.47	110.35	127.62
27	b	619	WVN	C20-C13-C15	-3.47	113.05	121.46
29	d	405	PL9	C7-C3-C2	-3.47	118.74	123.30
27	y	89	WVN	C30-C28-C25	-3.47	122.36	127.31
25	5	604	CLA	CMB-C2B-C3B	3.47	131.17	124.68
27	B	617	WVN	C20-C23-C25	-3.47	121.00	126.23
38	6	618	II0	C20-C14-C10	-3.47	119.64	124.35
37	O	612	KC2	CBC-CAC-C3C	-3.46	110.39	127.62
25	6	603	CLA	CMB-C2B-C3B	3.46	131.15	124.68
37	2	612	KC2	CBC-CAC-C3C	-3.46	110.41	127.62
37	2	612	KC2	O2D-CGD-CBD	3.46	117.42	111.27
25	b	607	CLA	CMB-C2B-C3B	3.46	131.15	124.68
39	4	620	IHT	C08-C12-C15	3.46	118.74	111.85
37	P	606	KC2	C2A-C1A-NA	3.46	114.95	109.40
37	R	612	KC2	C2A-C1A-NA	3.46	114.95	109.40
27	H	89	WVN	C02-C05-C09	-3.46	117.21	121.47
38	N	619	II0	C03-C09-C13	-3.46	117.75	122.63
27	D	408	WVN	C29-C26-C22	-3.46	122.38	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	612	KC2	O2D-CGD-CBD	3.45	117.41	111.27
36	E	102	HEM	CHB-C1B-NB	3.45	128.65	124.38
37	Q	612	KC2	O2D-CGD-CBD	3.45	117.39	111.27
37	5	612	KC2	C2A-C1A-NA	3.45	114.93	109.40
36	E	102	HEM	CHA-C4D-ND	3.44	128.63	124.38
37	4	605	KC2	C2A-C1A-NA	3.44	114.92	109.40
25	R	604	CLA	CMB-C2B-C3B	3.44	131.12	124.68
39	R	620	IHT	C04-C06-C09	3.44	119.06	111.38
29	D	405	PL9	C7-C3-C2	-3.44	118.78	123.30
37	Q	612	KC2	C2B-C1B-NB	3.43	112.64	110.10
38	5	618	II0	C20-C14-C10	-3.43	119.68	124.35
37	3	606	KC2	C2A-C1A-NA	3.43	114.91	109.40
31	z	103	LHG	O7-C7-C8	3.43	118.90	111.50
37	S	606	KC2	CHB-C1B-C2B	-3.43	118.28	125.48
27	c	531	WVN	C20-C13-C15	-3.43	113.15	121.46
25	C	528	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
39	R	620	IHT	C18-C22-C23	-3.43	121.05	126.23
25	N	609	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
27	c	531	WVN	C39-C40-C37	-3.43	116.45	123.47
31	Z	103	LHG	O7-C7-C8	3.42	118.88	111.50
25	b	615	CLA	CMB-C2B-C3B	3.42	131.08	124.68
25	4	607	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
37	Q	605	KC2	C2A-C1A-NA	3.42	114.89	109.40
27	y	89	WVN	C03-C04-C09	-3.42	106.32	112.00
25	N	607	CLA	C4A-NA-C1A	3.42	108.24	106.71
39	R	620	IHT	C31-C34-C35	-3.42	116.82	126.42
27	h	89	WVN	C02-C05-C09	-3.42	117.27	121.47
37	4	612	KC2	CBC-CAC-C3C	-3.41	110.64	127.62
25	1	604	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	Q	606	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	B	615	CLA	CMB-C2B-C3B	3.41	131.06	124.68
37	Q	612	KC2	CBC-CAC-C3C	-3.41	110.66	127.62
25	B	614	CLA	CMB-C2B-C3B	3.41	131.06	124.68
38	6	619	II0	C31-C33-C35	-3.41	116.85	126.42
27	3	620	WVN	C20-C13-C15	-3.40	113.22	121.46
25	B	601	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	R	606	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
38	6	619	II0	C19-C13-C09	-3.39	119.74	124.35
27	P	620	WVN	C20-C13-C15	-3.39	113.25	121.46
27	S	620	WVN	C20-C23-C25	-3.39	121.11	126.23
38	4	618	II0	C19-C13-C09	-3.39	119.74	124.35
25	1	603	CLA	CMB-C2B-C3B	3.39	131.02	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	528	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
25	6	609	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
25	S	601	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
25	Q	610	CLA	CMB-C2B-C3B	3.38	131.01	124.68
25	b	610	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
25	B	610	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
25	4	610	CLA	CMB-C2B-C3B	3.38	131.01	124.68
25	2	611	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
25	N	604	CLA	CMB-C2B-C3B	3.38	131.00	124.68
25	6	601	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
37	3	606	KC2	O2D-CGD-CBD	3.38	117.27	111.27
38	2	619	II0	C19-C13-C09	-3.38	119.76	124.35
25	S	611	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
25	5	606	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
25	6	611	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
25	S	615	CLA	CMB-C2B-C3B	3.37	130.99	124.68
37	P	606	KC2	O2D-CGD-CBD	3.37	117.26	111.27
25	N	603	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	O	611	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
38	R	618	II0	C20-C14-C10	-3.36	119.78	124.35
27	D	408	WVN	C20-C23-C25	-3.36	121.16	126.23
25	G	302	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
27	b	619	WVN	C29-C26-C22	-3.36	122.52	127.31
38	6	618	II0	C19-C13-C09	-3.36	119.79	124.35
25	P	601	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
39	4	620	IHT	C30-C32-C33	-3.36	116.98	126.42
25	1	601	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
38	5	618	II0	C18-C04-C10	-3.36	105.13	110.47
25	b	614	CLA	CMB-C2B-C3B	3.35	130.95	124.68
25	P	603	CLA	CMB-C2B-C3B	3.35	130.95	124.68
25	R	613	CLA	O2D-CGD-CBD	3.35	117.22	111.27
27	c	530	WVN	C23-C20-C13	-3.35	117.79	127.20
25	6	615	CLA	CMB-C2B-C3B	3.35	130.95	124.68
25	N	601	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
38	1	619	II0	C03-C09-C13	-3.35	117.91	122.63
27	A	407	WVN	C23-C20-C13	-3.35	117.80	127.20
25	3	603	CLA	CMB-C2B-C3B	3.34	130.94	124.68
39	O	620	IHT	C30-C27-C23	-3.34	122.54	127.31
38	S	618	II0	C18-C04-C10	-3.34	105.15	110.47
38	2	618	II0	C20-C14-C10	-3.34	119.81	124.35
25	1	607	CLA	C4A-NA-C1A	3.34	108.21	106.71
25	N	606	CLA	CMB-C2B-C1B	-3.34	123.33	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	620	WVN	C30-C28-C25	-3.34	122.54	127.31
38	R	618	II0	C18-C04-C10	-3.34	105.16	110.47
25	5	611	CLA	CMB-C2B-C3B	3.34	130.93	124.68
39	Q	620	IHT	C18-C22-C23	-3.34	121.19	126.23
39	Q	620	IHT	C30-C32-C33	-3.34	117.03	126.42
25	P	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	2	613	CLA	CMB-C2B-C3B	3.34	130.92	124.68
25	b	616	CLA	CMB-C2B-C3B	3.34	130.92	124.68
38	O	617	II0	C20-C14-C10	-3.34	119.82	124.35
37	6	606	KC2	O2D-CGD-CBD	3.33	117.19	111.27
25	1	606	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
38	1	617	II0	C18-C04-C10	-3.33	105.17	110.47
27	3	620	WVN	C30-C33-C34	-3.33	117.05	126.42
27	d	408	WVN	C29-C31-C32	-3.33	117.06	126.42
27	P	620	WVN	C30-C33-C34	-3.33	117.06	126.42
27	a	407	WVN	C21-C15-C14	3.33	120.01	113.62
25	N	615	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
38	O	619	II0	C19-C13-C09	-3.33	119.83	124.35
25	O	613	CLA	CMB-C2B-C3B	3.33	130.90	124.68
27	D	408	WVN	C39-C40-C37	-3.33	116.66	123.47
25	3	611	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
38	O	618	II0	C03-C09-C13	-3.33	117.94	122.63
25	1	615	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	d	403	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
39	2	620	IHT	C40-C37-C33	-3.32	122.57	127.31
25	D	403	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
25	4	609	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
38	6	618	II0	C18-C04-C10	-3.32	105.19	110.47
25	b	601	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
38	S	618	II0	C19-C13-C09	-3.32	119.84	124.35
25	B	616	CLA	CMB-C2B-C3B	3.32	130.89	124.68
38	1	618	II0	C20-C14-C10	-3.32	119.84	124.35
38	O	618	II0	C20-C14-C10	-3.32	119.84	124.35
38	N	617	II0	C18-C04-C10	-3.32	105.19	110.47
39	2	620	IHT	C25-C23-C22	3.32	123.30	118.08
25	B	605	CLA	CMB-C2B-C3B	3.32	130.88	124.68
25	R	611	CLA	CMB-C2B-C3B	3.32	130.88	124.68
37	1	611	KC2	C2A-C1A-NA	3.32	114.72	109.40
27	3	620	WVN	C30-C28-C25	-3.31	122.58	127.31
25	3	601	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
37	4	612	KC2	CHB-C4A-NA	3.31	129.42	124.20
37	S	612	KC2	CBC-CAC-C3C	-3.31	111.14	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	606	KC2	CBC-CAC-C3C	-3.31	111.16	127.62
39	4	620	IHT	C04-C06-C09	3.31	118.77	111.38
39	Q	620	IHT	C04-C06-C09	3.31	118.77	111.38
27	b	618	WVN	C12-C14-C15	-3.31	108.17	114.08
25	6	615	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
37	S	606	KC2	O2D-CGD-CBD	3.30	117.14	111.27
37	N	611	KC2	C2A-C1A-NA	3.30	114.70	109.40
37	6	612	KC2	CBC-CAC-C3C	-3.30	111.20	127.62
38	N	618	II0	C20-C14-C10	-3.30	119.86	124.35
25	2	607	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	S	615	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
39	4	620	IHT	C18-C22-C23	-3.30	121.25	126.23
38	2	617	II0	C20-C14-C10	-3.29	119.87	124.35
25	1	610	CLA	CMB-C2B-C3B	3.29	130.84	124.68
25	a	404	CLA	CMB-C2B-C3B	3.29	130.84	124.68
27	3	620	WVN	C40-C37-C34	-3.29	122.61	127.31
25	A	404	CLA	CMB-C2B-C3B	3.29	130.84	124.68
27	C	530	WVN	C39-C36-C32	-3.29	122.61	127.31
37	2	612	KC2	CHB-C4A-NA	3.29	129.38	124.20
39	R	620	IHT	C30-C27-C23	-3.29	122.62	127.31
38	S	619	II0	C31-C33-C35	-3.29	117.18	126.42
37	Q	612	KC2	CHB-C4A-NA	3.29	129.38	124.20
38	1	618	II0	C19-C13-C09	-3.29	119.88	124.35
25	4	602	CLA	CMB-C2B-C3B	3.29	130.83	124.68
25	Q	602	CLA	CMB-C2B-C3B	3.29	130.83	124.68
38	P	616	II0	O02-C08-C12	3.29	116.72	109.68
37	N	611	KC2	O2D-CGD-CBD	3.28	117.10	111.27
38	N	618	II0	C19-C13-C09	-3.28	119.89	124.35
38	3	616	II0	O02-C08-C12	3.28	116.71	109.68
25	R	601	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
27	P	620	WVN	C12-C14-C15	-3.28	108.22	114.08
25	O	601	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
39	2	620	IHT	C30-C27-C23	-3.28	122.63	127.31
37	1	611	KC2	O2D-CGD-CBD	3.27	117.08	111.27
37	O	612	KC2	CHB-C4A-NA	3.27	129.36	124.20
25	N	610	CLA	CMB-C2B-C3B	3.27	130.80	124.68
27	3	620	WVN	C39-C40-C37	-3.27	116.77	123.47
25	Q	603	CLA	CMB-C2B-C3B	3.27	130.80	124.68
25	1	607	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	R	609	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	D	400	CLA	CMB-C2B-C3B	3.26	130.79	124.68
25	2	602	CLA	CMB-C2B-C3B	3.26	130.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	620	WVN	C12-C14-C15	-3.26	108.25	114.08
25	O	607	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	O	610	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	2	607	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
25	C	522	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	4	603	CLA	CMB-C2B-C3B	3.26	130.78	124.68
27	P	620	WVN	C40-C37-C34	-3.26	122.66	127.31
36	e	102	HEM	CHB-C1B-NB	3.26	128.41	124.38
25	d	400	CLA	CMB-C2B-C3B	3.26	130.77	124.68
27	6	620	WVN	C20-C23-C25	-3.26	121.31	126.23
25	1	614	CLA	CMB-C2B-C3B	3.25	130.77	124.68
25	N	607	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
25	P	610	CLA	CMB-C2B-C3B	3.25	130.76	124.68
38	R	619	II0	C03-C09-C13	-3.25	118.04	122.63
25	5	601	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
39	O	620	IHT	C25-C23-C22	3.25	123.20	118.08
25	5	607	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	P	604	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	Q	613	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
38	4	618	II0	C06-C04-C10	3.25	116.20	109.62
25	3	604	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
25	4	613	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
25	5	613	CLA	O2D-CGD-CBD	3.24	117.03	111.27
38	5	619	II0	C03-C09-C13	-3.24	118.05	122.63
38	1	618	II0	C18-C04-C10	-3.24	105.31	110.47
39	N	620	IHT	C28-C26-C24	3.24	123.26	116.84
25	b	605	CLA	CMB-C2B-C3B	3.24	130.75	124.68
38	N	618	II0	C18-C04-C10	-3.24	105.31	110.47
26	d	401	PHO	CMB-C2B-C3B	3.24	130.74	124.68
37	N	611	KC2	CBC-CAC-C3C	-3.24	111.49	127.62
27	C	531	WVN	C30-C28-C25	-3.24	122.68	127.31
25	2	601	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
37	1	611	KC2	CBC-CAC-C3C	-3.24	111.50	127.62
38	O	618	II0	C06-C04-C10	3.24	116.19	109.62
27	b	618	WVN	C02-C05-C09	-3.24	117.48	121.47
25	Q	609	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	3	610	CLA	CMB-C2B-C3B	3.24	130.74	124.68
25	b	602	CLA	CMB-C2B-C3B	3.24	130.73	124.68
27	a	407	WVN	C30-C28-C25	-3.24	122.69	127.31
27	C	529	WVN	C39-C36-C32	-3.23	122.69	127.31
27	a	407	WVN	C40-C37-C34	-3.23	122.69	127.31
39	O	620	IHT	C40-C37-C33	-3.23	122.69	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	620	IHT	C28-C26-C24	3.23	123.24	116.84
25	O	607	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
25	d	404	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
25	2	609	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	4	606	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
38	Q	618	II0	C06-C04-C10	3.22	116.16	109.62
25	R	607	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
34	4	621	LMG	O7-C10-C11	3.22	118.45	111.50
25	N	614	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	O	606	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
25	O	602	CLA	CMB-C2B-C3B	3.22	130.71	124.68
26	D	401	PHO	CMB-C2B-C3B	3.22	130.70	124.68
25	6	602	CLA	CMB-C2B-C3B	3.22	130.70	124.68
27	B	617	WVN	C30-C28-C25	-3.22	122.72	127.31
27	P	620	WVN	C39-C40-C37	-3.22	116.88	123.47
25	D	404	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	2	610	CLA	CMB-C2B-C3B	3.21	130.69	124.68
27	D	408	WVN	C40-C37-C34	-3.21	122.72	127.31
39	5	620	IHT	C08-C12-C15	3.21	118.25	111.85
25	4	607	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
38	2	618	II0	C06-C04-C10	3.21	116.13	109.62
34	Q	621	LMG	O7-C10-C11	3.21	118.42	111.50
25	B	602	CLA	CMB-C2B-C3B	3.21	130.68	124.68
37	4	611	KC2	O2D-CGD-CBD	3.21	116.97	111.27
27	d	408	WVN	C12-C14-C15	-3.21	108.35	114.08
25	Q	607	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
25	a	406	CLA	CMB-C2B-C3B	3.21	130.68	124.68
25	2	606	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
27	C	530	WVN	C20-C13-C15	-3.20	113.70	121.46
37	N	613	KC2	C2A-C1A-NA	3.20	114.54	109.40
38	S	619	II0	C06-C04-C10	3.20	116.11	109.62
37	1	613	KC2	C2A-C1A-NA	3.20	114.54	109.40
25	N	606	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
27	b	619	WVN	C23-C25-C28	3.20	123.85	118.94
25	S	602	CLA	CMB-C2B-C3B	3.19	130.66	124.68
27	A	407	WVN	C29-C26-C22	-3.19	122.75	127.31
38	6	619	II0	C06-C04-C10	3.19	116.09	109.62
38	N	618	II0	C03-C09-C13	-3.19	118.12	122.63
27	S	620	WVN	C08-C01-C02	3.19	114.38	109.55
27	b	619	WVN	C30-C33-C34	-3.19	117.45	126.42
38	2	616	II0	O02-C08-C12	3.19	116.51	109.68
25	b	606	CLA	O2D-CGD-O1D	-3.19	117.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	618	II0	C03-C09-C13	-3.19	118.13	122.63
27	C	529	WVN	C20-C13-C15	-3.19	113.74	121.46
39	O	620	IHT	C28-C26-C24	3.18	123.14	116.84
25	5	609	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
25	g	302	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	B	602	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
38	O	616	II0	O02-C08-C12	3.18	116.49	109.68
25	S	604	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
25	g	302	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
25	O	609	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
37	1	605	KC2	C3D-CAD-CBD	-3.17	103.42	107.61
25	Q	603	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
27	C	531	WVN	C26-C29-C31	-3.17	113.31	123.22
25	6	604	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
38	3	616	II0	C18-C04-C10	-3.17	105.43	110.47
38	P	618	II0	C03-C09-C13	-3.17	118.16	122.63
38	P	616	II0	C18-C04-C10	-3.17	105.43	110.47
39	R	620	IHT	C08-C12-C15	3.17	118.17	111.85
37	6	606	KC2	CBC-CAC-C3C	-3.17	111.86	127.62
25	G	301	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
37	Q	611	KC2	O2D-CGD-CBD	3.17	116.90	111.27
25	4	603	CLA	C1B-CHB-C4A	-3.17	123.85	130.12
27	c	531	WVN	C28-C30-C33	-3.16	113.34	123.22
25	1	602	CLA	CMB-C2B-C3B	3.16	130.60	124.68
25	5	603	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
25	B	606	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
25	4	606	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
25	1	609	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
25	2	604	CLA	CMB-C2B-C3B	3.16	130.58	124.68
25	A	406	CLA	CMB-C2B-C3B	3.15	130.58	124.68
25	N	602	CLA	CMB-C2B-C3B	3.15	130.58	124.68
37	N	605	KC2	C3D-CAD-CBD	-3.15	103.45	107.61
38	1	619	II0	C32-C30-C26	-3.15	117.43	126.58
25	R	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
25	1	606	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
38	N	619	II0	C32-C30-C26	-3.15	117.43	126.58
38	4	616	II0	C06-C04-C10	3.15	116.01	109.62
25	R	602	CLA	CMB-C2B-C3B	3.15	130.57	124.68
38	2	619	II0	C32-C34-C36	-3.15	117.57	126.42
38	O	619	II0	C32-C34-C36	-3.15	117.57	126.42
27	Y	89	WVN	C20-C13-C15	-3.15	113.84	121.46
25	6	613	CLA	O2D-CGD-O1D	-3.15	117.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	607	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
25	b	602	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
27	6	620	WVN	C14-C15-C13	-3.14	118.17	122.73
25	Q	606	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
38	S	618	II0	C03-C09-C13	-3.14	118.19	122.63
25	c	526	CLA	CMB-C2B-C3B	3.14	130.55	124.68
27	h	89	WVN	C21-C15-C13	-3.14	121.00	124.53
38	6	619	II0	C18-C04-C10	-3.14	105.48	110.47
25	B	614	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
38	S	619	II0	C18-C04-C10	-3.14	105.48	110.47
27	d	408	WVN	C04-C09-C05	-3.14	121.84	124.85
25	4	607	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
25	Q	607	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
27	b	617	WVN	C14-C15-C13	-3.13	118.18	122.73
37	S	606	KC2	CMB-C2B-C1B	3.13	130.23	124.71
25	b	613	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
25	5	602	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	a	403	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
27	B	617	WVN	C07-C01-C02	-3.13	104.81	109.55
25	O	604	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	C	526	CLA	CMB-C2B-C3B	3.13	130.53	124.68
38	Q	616	II0	C06-C04-C10	3.13	115.95	109.62
27	c	529	WVN	C02-C05-C09	-3.12	117.62	121.47
25	b	614	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
25	D	400	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
38	4	617	II0	O02-C08-C12	3.12	116.37	109.68
38	6	618	II0	C03-C09-C13	-3.12	118.23	122.63
31	P	621	LHG	C5-O7-C7	-3.12	110.11	117.79
38	R	618	II0	C19-C13-C09	-3.12	120.11	124.35
38	2	618	II0	C19-C13-C09	-3.12	120.11	124.35
25	c	518	CLA	CMB-C2B-C3B	3.12	130.51	124.68
25	c	522	CLA	CMB-C2B-C3B	3.12	130.51	124.68
25	4	615	CLA	CMB-C2B-C3B	3.12	130.51	124.68
25	1	615	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
31	3	621	LHG	C5-O7-C7	-3.11	110.13	117.79
25	B	608	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
38	Q	617	II0	O02-C08-C12	3.11	116.34	109.68
38	3	618	II0	O02-C08-C12	3.11	116.33	109.68
25	d	400	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
25	N	615	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
25	B	607	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
25	B	603	CLA	CMB-C2B-C3B	3.10	130.49	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	618	II0	O02-C08-C12	3.10	116.33	109.68
27	S	620	WVN	C14-C15-C13	-3.10	118.23	122.73
25	1	607	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	S	613	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	5	610	CLA	CMB-C2B-C3B	3.10	130.48	124.68
25	4	604	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
25	R	609	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
38	P	619	II0	C18-C04-C10	-3.10	105.54	110.47
38	4	619	II0	O02-C08-C12	3.10	116.31	109.68
25	A	403	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
25	N	615	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
25	A	403	CLA	CMB-C2B-C1B	-3.10	123.71	128.46
38	5	618	II0	C19-C13-C09	-3.09	120.15	124.35
25	N	607	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
38	N	616	II0	C06-C04-C10	3.09	115.89	109.62
25	C	527	CLA	CMB-C2B-C3B	3.09	130.46	124.68
25	a	403	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
38	P	618	II0	O02-C08-C12	3.09	116.30	109.68
38	O	619	II0	C20-C14-C10	-3.09	120.15	124.35
25	C	523	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
38	S	618	II0	O02-C08-C12	3.09	116.30	109.68
25	R	610	CLA	CMB-C2B-C3B	3.09	130.46	124.68
25	Q	604	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	O	615	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
25	Q	615	CLA	CMB-C2B-C3B	3.09	130.45	124.68
38	N	619	II0	O02-C08-C12	3.08	116.29	109.68
25	B	613	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
25	b	608	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
25	5	604	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
37	N	613	KC2	O2D-CGD-O1D	-3.08	117.81	123.84
25	O	601	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
25	P	611	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
38	3	619	II0	C18-C04-C10	-3.08	105.57	110.47
25	1	607	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
37	1	613	KC2	O2D-CGD-O1D	-3.08	117.81	123.84
37	6	612	KC2	C3B-C2B-C1B	-3.08	104.13	107.08
38	1	616	II0	C06-C04-C10	3.08	115.86	109.62
25	5	613	CLA	CMB-C2B-C3B	3.08	130.44	124.68
25	2	615	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
39	5	620	IHT	C25-C23-C22	3.08	122.93	118.08
25	D	400	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
34	C	536	LMG	C8-O7-C10	-3.08	110.21	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	612	KC2	C3B-C2B-C1B	-3.08	104.14	107.08
25	C	518	CLA	CMB-C2B-C3B	3.08	130.43	124.68
25	R	615	CLA	CMB-C2B-C3B	3.08	130.43	124.68
38	O	619	II0	O02-C08-C12	3.08	116.27	109.68
38	1	619	II0	O02-C08-C12	3.07	116.27	109.68
25	R	604	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	c	523	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	3	615	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	C	528	CLA	CMB-C2B-C3B	3.07	130.42	124.68
25	S	603	CLA	CMB-C2B-C3B	3.07	130.42	124.68
27	A	407	WVN	C40-C37-C34	-3.07	122.93	127.31
27	B	618	WVN	C23-C20-C13	-3.07	118.58	127.20
37	1	612	KC2	CHB-C4A-NA	3.07	129.04	124.20
38	2	619	II0	C20-C14-C10	-3.07	120.18	124.35
37	6	606	KC2	CMB-C2B-C1B	3.07	130.12	124.71
25	O	609	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
38	P	619	II0	O02-C08-C12	3.07	116.25	109.68
25	O	606	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
27	D	408	WVN	C04-C09-C05	-3.07	121.91	124.85
25	5	615	CLA	CMB-C2B-C3B	3.07	130.41	124.68
25	1	615	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
25	d	400	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
25	P	609	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
38	2	619	II0	O02-C08-C12	3.06	116.24	109.68
25	C	520	CLA	CMB-C2B-C3B	3.06	130.41	124.68
25	N	607	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
25	b	603	CLA	CMB-C2B-C3B	3.06	130.41	124.68
25	c	520	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	C	520	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
37	N	612	KC2	CHB-C4A-NA	3.06	129.02	124.20
38	Q	619	II0	O02-C08-C12	3.06	116.23	109.68
25	A	406	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	5	602	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
25	C	517	CLA	CMB-C2B-C3B	3.06	130.40	124.68
25	R	602	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
38	3	619	II0	O02-C08-C12	3.05	116.22	109.68
25	2	601	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	5	609	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
38	1	616	II0	C18-C04-C10	-3.05	105.61	110.47
25	3	611	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
25	a	406	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	P	615	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	602	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
25	c	527	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	b	604	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
39	1	620	IHT	C18-C22-C23	-3.05	121.63	126.23
25	b	603	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
37	5	612	KC2	O2D-CGD-CBD	3.05	116.68	111.27
27	b	619	WVN	C39-C36-C32	-3.04	122.97	127.31
25	C	523	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	B	603	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
25	c	520	CLA	CMB-C2B-C3B	3.04	130.37	124.68
25	3	609	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
26	A	405	PHO	CMB-C2B-C3B	3.04	130.37	124.68
25	B	604	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
37	S	612	KC2	C3B-C2B-C1B	-3.04	104.17	107.08
39	R	620	IHT	C28-C26-C24	3.04	122.86	116.84
25	2	606	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
27	C	531	WVN	C40-C37-C34	-3.04	122.97	127.31
38	6	618	II0	C03-C05-C07	3.04	120.51	113.64
38	P	617	II0	O02-C08-C12	3.04	116.19	109.68
25	Q	607	CLA	C4A-NA-C1A	3.04	108.07	106.71
25	a	406	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
25	R	613	CLA	CMB-C2B-C3B	3.04	130.36	124.68
37	1	612	KC2	C3B-C2B-C1B	-3.03	104.18	107.08
25	G	301	CLA	CMB-C2B-C3B	3.03	130.35	124.68
25	g	302	CLA	O2D-CGD-CBD	3.03	116.66	111.27
37	R	612	KC2	O2D-CGD-CBD	3.03	116.66	111.27
26	a	405	PHO	CMB-C2B-C3B	3.03	130.35	124.68
25	c	522	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
25	c	517	CLA	CMB-C2B-C3B	3.03	130.35	124.68
38	N	616	II0	C18-C04-C10	-3.03	105.65	110.47
37	4	611	KC2	C3B-C2B-C1B	-3.03	104.18	107.08
37	Q	611	KC2	C3B-C2B-C1B	-3.03	104.18	107.08
38	3	617	II0	O02-C08-C12	3.03	116.17	109.68
38	5	618	II0	C30-C32-C34	-3.03	113.77	123.22
38	R	618	II0	C30-C32-C34	-3.03	113.77	123.22
38	R	619	II0	C18-C04-C10	-3.03	105.66	110.47
38	S	618	II0	C03-C05-C07	3.03	120.48	113.64
25	C	522	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	G	302	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
38	O	618	II0	O02-C08-C12	3.02	116.16	109.68
25	A	406	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
38	2	618	II0	O02-C08-C12	3.02	116.16	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	530	WVN	C39-C36-C32	-3.02	123.00	127.31
25	5	602	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	c	523	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	1	609	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
38	5	619	II0	C18-C04-C10	-3.02	105.67	110.47
25	b	609	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
25	B	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
39	1	620	IHT	C06-C09-C10	-3.02	108.69	114.08
25	g	301	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	2	609	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
25	P	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
27	C	530	WVN	C40-C37-C34	-3.01	123.01	127.31
25	b	602	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
25	c	528	CLA	CMB-C2B-C3B	3.01	130.31	124.68
25	1	615	CLA	CMB-C2B-C3B	3.01	130.31	124.68
27	c	530	WVN	C39-C40-C37	-3.01	117.31	123.47
25	G	302	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
27	3	620	WVN	C21-C15-C14	3.01	119.39	113.62
27	c	530	WVN	C14-C15-C13	-3.01	118.37	122.73
25	B	609	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
25	C	521	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
25	6	601	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
39	N	620	IHT	C06-C09-C10	-3.00	108.72	114.08
27	P	620	WVN	C21-C15-C14	3.00	119.38	113.62
25	3	602	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
27	c	529	WVN	C21-C15-C13	-3.00	121.16	124.53
25	b	611	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
38	N	617	II0	O02-C08-C12	3.00	116.10	109.68
38	6	617	II0	O02-C08-C12	3.00	116.10	109.68
37	5	612	KC2	CHB-C4A-NA	3.00	128.92	124.20
25	N	615	CLA	CMB-C2B-C3B	3.00	130.28	124.68
25	6	611	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
38	5	619	II0	O02-C08-C12	2.99	116.09	109.68
25	b	611	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
38	1	616	II0	O02-C08-C12	2.99	116.09	109.68
38	S	617	II0	O02-C08-C12	2.99	116.09	109.68
38	N	616	II0	O02-C08-C12	2.99	116.09	109.68
37	R	612	KC2	CHB-C4A-NA	2.99	128.91	124.20
37	S	612	KC2	CHB-C4A-NA	2.99	128.91	124.20
38	R	619	II0	O02-C08-C12	2.99	116.08	109.68
27	6	620	WVN	C08-C01-C02	2.99	114.07	109.55
25	B	606	CLA	CMB-C2B-C3B	2.99	130.27	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	620	IHT	C25-C23-C22	2.99	122.79	118.08
37	Q	611	KC2	CHB-C4A-NA	2.99	128.91	124.20
34	w	134	LMG	C8-O7-C10	-2.99	110.44	117.79
38	R	616	II0	O02-C08-C12	2.99	116.08	109.68
25	S	611	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	B	619	WVN	C39-C36-C32	-2.99	123.05	127.31
38	2	619	II0	C31-C33-C35	-2.99	118.03	126.42
38	O	618	II0	C18-C04-C10	-2.99	105.72	110.47
25	B	611	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
38	1	617	II0	O02-C08-C12	2.98	116.07	109.68
25	C	528	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	4	607	CLA	C4A-NA-C1A	2.98	108.05	106.71
25	G	302	CLA	CMB-C2B-C3B	2.98	130.26	124.68
25	3	601	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
38	O	619	II0	C31-C33-C35	-2.98	118.04	126.42
38	2	617	II0	O02-C08-C12	2.98	116.06	109.68
25	S	601	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
38	5	616	II0	O02-C08-C12	2.98	116.05	109.68
37	4	611	KC2	CHB-C4A-NA	2.97	128.89	124.20
38	2	618	II0	C18-C04-C10	-2.97	105.74	110.47
25	S	611	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
37	N	611	KC2	CHB-C4A-NA	2.97	128.89	124.20
25	b	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	c	521	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
25	Q	606	CLA	CMB-C2B-C3B	2.97	130.24	124.68
25	4	602	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	2	604	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
27	b	617	WVN	C01-C02-C11	-2.97	108.95	112.70
25	B	601	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	B	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	B	609	CLA	CMB-C2B-C3B	2.97	130.23	124.68
37	1	611	KC2	CHB-C4A-NA	2.96	128.88	124.20
25	B	611	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
31	D	406	LHG	C5-O7-C7	-2.96	110.49	117.79
38	O	617	II0	O02-C08-C12	2.96	116.03	109.68
25	b	604	CLA	CMB-C2B-C3B	2.96	130.22	124.68
39	N	620	IHT	C18-C22-C23	-2.96	121.76	126.23
25	c	518	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	B	606	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
37	1	611	KC2	C3B-C2B-C1B	-2.96	104.25	107.08
25	5	601	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
38	N	618	II0	C41-C42-C40	-2.96	117.42	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	B	604	CLA	CMB-C2B-C3B	2.96	130.21	124.68
34	W	134	LMG	C8-O7-C10	-2.96	110.51	117.79
25	R	601	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	b	606	CLA	CMB-C2B-C3B	2.95	130.20	124.68
37	3	606	KC2	C3B-C2B-C1B	-2.95	104.26	107.08
25	b	606	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	P	601	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	O	604	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	a	407	WVN	C14-C15-C13	-2.95	118.45	122.73
29	D	405	PL9	C40-C39-C41	2.95	120.23	115.27
25	C	518	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
37	6	612	KC2	CHB-C4A-NA	2.95	128.85	124.20
25	5	609	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	c	528	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
38	6	616	II0	O02-C08-C12	2.95	115.99	109.68
25	N	609	CLA	CMB-C2B-C3B	2.95	130.19	124.68
38	S	616	II0	O02-C08-C12	2.94	115.99	109.68
25	1	610	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
38	1	618	II0	C41-C42-C40	-2.94	117.45	123.47
34	m	101	LMG	O8-C28-C29	2.94	121.14	111.91
27	C	531	WVN	C40-C39-C36	-2.94	117.45	123.47
25	c	520	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	B	601	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	b	605	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	N	610	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	6	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
38	R	617	II0	O02-C08-C12	2.94	115.97	109.68
25	P	602	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	N	604	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
37	P	606	KC2	CHB-C4A-NA	2.94	128.83	124.20
34	M	101	LMG	O8-C28-C29	2.94	121.12	111.91
25	Q	602	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	R	615	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
27	b	618	WVN	C30-C33-C34	-2.93	118.17	126.42
25	b	610	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
25	b	601	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
37	N	611	KC2	C3B-C2B-C1B	-2.93	104.28	107.08
25	C	520	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
25	g	301	CLA	CMB-C2B-C3B	2.93	130.16	124.68
29	d	405	PL9	C40-C39-C41	2.93	120.20	115.27
25	A	404	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	606	KC2	CHB-C4A-NA	2.93	128.82	124.20
25	6	611	CLA	CMB-C2B-C3B	2.93	130.15	124.68
25	B	605	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
38	5	617	II0	O02-C08-C12	2.93	115.95	109.68
25	3	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
39	Q	620	IHT	C25-C23-C22	2.92	122.68	118.08
37	P	606	KC2	C3B-C2B-C1B	-2.92	104.28	107.08
25	S	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
39	4	620	IHT	C25-C23-C22	2.92	122.68	118.08
38	Q	616	II0	O02-C08-C12	2.92	115.94	109.68
25	6	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
39	5	620	IHT	C28-C26-C24	2.92	122.62	116.84
25	R	606	CLA	CMB-C2B-C3B	2.92	130.14	124.68
25	2	607	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	c	519	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	1	604	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	O	604	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
38	3	618	II0	C03-C09-C13	-2.92	118.51	122.63
25	5	606	CLA	CMB-C2B-C3B	2.92	130.13	124.68
38	5	618	II0	O02-C08-C12	2.91	115.92	109.68
25	S	611	CLA	CMB-C2B-C3B	2.91	130.13	124.68
25	2	607	CLA	C4A-NA-C1A	2.91	108.02	106.71
25	B	610	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	1	606	CLA	CMB-C2B-C3B	2.91	130.12	124.68
25	O	607	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
38	R	618	II0	O02-C08-C12	2.91	115.91	109.68
25	a	404	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	c	516	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	A	404	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	6	613	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	a	404	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	d	404	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	S	613	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
37	4	605	KC2	C3B-C2B-C1B	-2.91	104.30	107.08
25	O	602	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
38	4	616	II0	O02-C08-C12	2.91	115.90	109.68
25	R	609	CLA	CHB-C4A-NA	2.90	128.53	124.51
25	5	615	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
25	2	611	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	2	611	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	D	404	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	O	611	CLA	O2D-CGD-O1D	-2.90	118.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	610	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
38	Q	619	II0	C32-C30-C26	-2.90	118.16	126.58
31	d	406	LHG	C5-O7-C7	-2.90	110.65	117.79
25	R	610	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	b	601	CLA	CMB-C2B-C3B	2.90	130.10	124.68
38	S	619	II0	O02-C08-C12	2.90	115.89	109.68
39	O	620	IHT	C41-C40-C37	-2.90	117.54	123.47
37	1	612	KC2	C3D-CAD-CBD	-2.90	103.79	107.61
25	c	521	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	N	606	CLA	CMB-C2B-C3B	2.89	130.09	124.68
39	R	620	IHT	C20-C15-C11	-2.89	120.42	124.35
25	O	602	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	C	519	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
26	a	405	PHO	O1D-CGD-CBD	2.89	129.55	124.74
38	6	619	II0	O02-C08-C12	2.89	115.87	109.68
25	2	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	Q	615	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	1	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	C	531	WVN	C28-C30-C33	-2.89	114.21	123.22
25	O	611	CLA	CMB-C2B-C3B	2.89	130.08	124.68
25	6	601	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
25	6	610	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
38	1	616	II0	C03-C09-C13	-2.89	118.56	122.63
25	4	610	CLA	C1B-CHB-C4A	-2.88	124.40	130.12
38	N	616	II0	C03-C09-C13	-2.88	118.56	122.63
26	A	405	PHO	O1D-CGD-CBD	2.88	129.54	124.74
25	S	601	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
37	N	613	KC2	CBC-CAC-C3C	-2.88	113.28	127.62
25	g	302	CLA	CHB-C4A-NA	2.88	128.50	124.51
25	R	603	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	Q	610	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	S	610	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	C	516	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	3	611	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	2	604	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	2	602	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	2	615	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	O	607	CLA	C4A-NA-C1A	2.88	108.00	106.71
37	N	612	KC2	C3D-CAD-CBD	-2.87	103.82	107.61
34	w	134	LMG	O8-C28-C29	2.87	120.93	111.91
25	B	603	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	O	601	CLA	CMB-C2B-C3B	2.87	130.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	WVN	C14-C15-C13	-2.87	118.56	122.73
25	Q	602	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
25	P	611	CLA	CMB-C2B-C3B	2.87	130.06	124.68
38	P	619	II0	C30-C32-C34	-2.87	114.25	123.22
25	1	603	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
27	h	89	WVN	C01-C02-C11	-2.87	109.07	112.70
38	3	619	II0	C30-C32-C34	-2.87	114.25	123.22
25	N	602	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	R	611	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	g	301	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	N	602	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	C	521	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	b	619	WVN	C40-C39-C36	-2.87	117.59	123.47
29	a	409	PL9	C7-C8-C9	-2.87	122.01	126.79
37	R	612	KC2	C3B-C2B-C1B	-2.87	104.33	107.08
25	S	602	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
37	Q	605	KC2	C3B-C2B-C1B	-2.87	104.34	107.08
25	S	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	4	602	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
25	D	403	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	R	609	CLA	CMB-C2B-C3B	2.87	130.04	124.68
39	2	620	IHT	C41-C40-C37	-2.87	117.60	123.47
25	2	601	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	3	613	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
25	1	601	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	b	610	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	6	610	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	2	609	CLA	CMB-C2B-C3B	2.86	130.03	124.68
38	4	618	II0	O02-C08-C12	2.86	115.81	109.68
25	5	611	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	O	615	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
37	1	613	KC2	CBC-CAC-C3C	-2.86	113.38	127.62
31	5	621	LHG	O8-C23-C24	2.86	120.88	111.91
25	5	603	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
25	6	601	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	3	610	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	4	615	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	S	601	CLA	CMB-C2B-C3B	2.86	130.02	124.68
27	d	408	WVN	C39-C40-C37	-2.86	117.62	123.47
38	4	619	II0	C32-C30-C26	-2.86	118.29	126.58
38	N	616	II0	C32-C30-C26	-2.86	118.29	126.58
25	3	613	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	N	601	CLA	CMB-C2B-C3B	2.86	130.02	124.68
27	D	408	WVN	C29-C31-C32	-2.85	118.40	126.42
25	b	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
31	R	621	LHG	O8-C23-C24	2.85	120.86	111.91
25	1	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
25	C	517	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	5	611	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
25	O	610	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	d	403	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	N	601	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	3	601	CLA	CMB-C2B-C3B	2.85	130.00	124.68
37	5	612	KC2	C3B-C2B-C1B	-2.85	104.36	107.08
25	b	607	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	2	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	5	620	IHT	C31-C34-C35	-2.85	118.42	126.42
25	c	517	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	A	409	PL9	C7-C8-C9	-2.85	122.05	126.79
25	N	609	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	P	610	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	B	610	CLA	CMB-C2B-C3B	2.85	130.00	124.68
25	b	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	c	516	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	1	601	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	R	611	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	3	615	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	N	603	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	B	615	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
37	N	612	KC2	C2B-C1B-NB	2.84	112.20	110.10
25	5	607	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	R	610	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	B	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
38	1	618	II0	O02-C08-C12	2.84	115.76	109.68
25	O	603	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
38	1	616	II0	C32-C30-C26	-2.84	118.34	126.58
38	N	618	II0	O02-C08-C12	2.84	115.76	109.68
25	P	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
38	3	618	II0	C41-C42-C40	-2.84	117.66	123.47
38	Q	618	II0	O02-C08-C12	2.84	115.75	109.68
25	P	601	CLA	CMB-C2B-C3B	2.84	129.98	124.68
27	A	407	WVN	C39-C40-C37	-2.83	117.67	123.47
25	b	608	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	6	609	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
25	R	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	O	613	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	R	606	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	C	524	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	P	613	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
25	5	603	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	Q	606	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	c	524	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
25	c	525	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
25	c	524	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	5	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	5	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	N	609	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	O	609	CLA	CMB-C2B-C3B	2.82	129.95	124.68
25	C	516	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	b	616	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
25	c	522	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
25	B	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	P	615	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
25	B	615	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	C	525	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
25	5	606	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
38	3	617	II0	C06-C04-C10	2.82	115.33	109.62
25	B	615	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
38	2	617	II0	C30-C32-C34	-2.81	114.44	123.22
25	R	609	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	R	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
38	N	618	II0	C32-C30-C26	-2.81	118.42	126.58
25	Q	609	CLA	CHB-C4A-NA	2.81	128.40	124.51
38	1	618	II0	C32-C30-C26	-2.81	118.42	126.58
25	4	610	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	C	524	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
38	3	619	II0	C31-C33-C35	-2.81	118.53	126.42
27	H	89	WVN	C39-C40-C37	-2.81	117.72	123.47
25	B	607	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	Q	609	CLA	CMB-C2B-C3B	2.81	129.93	124.68
27	B	617	WVN	C39-C40-C37	-2.81	117.72	123.47
25	B	613	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
25	C	517	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
37	1	612	KC2	C2B-C1B-NB	2.80	112.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	O	617	II0	C30-C32-C34	-2.80	114.46	123.22
25	1	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	c	517	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
25	4	606	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	C	522	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
25	b	615	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
38	O	618	II0	C30-C32-C34	-2.80	114.48	123.22
34	2	622	LMG	O8-C28-C29	2.80	120.69	111.91
25	4	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
25	3	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	5	609	CLA	CMB-C2B-C3B	2.79	129.91	124.68
25	Q	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	c	519	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	c	527	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	4	609	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	b	613	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
38	2	618	II0	C30-C32-C34	-2.79	114.52	123.22
25	R	613	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	C	527	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
38	S	618	II0	C32-C30-C26	-2.79	118.49	126.58
25	1	604	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
39	1	620	IHT	C03-C05-C08	-2.79	107.35	113.64
25	2	603	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
38	P	617	II0	C06-C04-C10	2.79	115.27	109.62
38	6	618	II0	C32-C30-C26	-2.78	118.49	126.58
25	C	525	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
34	O	622	LMG	O8-C28-C29	2.78	120.65	111.91
25	b	615	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
25	a	403	CLA	CMB-C2B-C3B	2.78	129.89	124.68
38	2	618	II0	C41-C42-C40	-2.78	117.77	123.47
25	O	606	CLA	CMB-C2B-C3B	2.78	129.88	124.68
38	O	618	II0	C41-C42-C40	-2.78	117.78	123.47
25	R	606	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	R	607	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	5	609	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	P	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	2	620	IHT	C03-C05-C08	-2.78	107.37	113.64
25	2	613	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	N	610	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
38	P	619	II0	C31-C33-C35	-2.78	118.61	126.42
25	2	606	CLA	CMB-C2B-C3B	2.78	129.87	124.68
25	C	519	CLA	O2D-CGD-O1D	-2.77	118.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	610	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
38	3	616	II0	C06-C04-C10	2.77	115.24	109.62
25	2	610	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
25	B	616	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	b	615	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	P	603	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
27	3	620	WVN	C20-C23-C25	-2.77	122.05	126.23
25	5	606	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
38	3	618	II0	C30-C32-C34	-2.77	114.58	123.22
27	D	408	WVN	C12-C14-C15	-2.77	109.14	114.08
38	6	618	II0	C05-C07-C11	2.77	114.09	110.30
25	B	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
38	P	618	II0	C30-C32-C34	-2.77	114.59	123.22
25	B	610	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	b	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	D	403	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
38	P	618	II0	C41-C42-C40	-2.76	117.81	123.47
25	c	522	CLA	CHB-C4A-NA	2.76	128.33	124.51
38	P	616	II0	C06-C04-C10	2.76	115.22	109.62
38	S	618	II0	C05-C07-C11	2.76	114.09	110.30
25	3	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	O	613	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	5	613	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	2	603	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	d	401	PHO	O2D-CGD-O1D	-2.76	118.44	123.84
25	4	609	CLA	CHB-C4A-NA	2.76	128.33	124.51
38	N	619	II0	C31-C33-C35	-2.76	118.67	126.42
31	3	621	LHG	O8-C23-C24	2.76	120.56	111.91
25	N	604	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	G	301	CLA	CHB-C4A-NA	2.76	128.32	124.51
37	6	612	KC2	C2B-C1B-NB	2.76	112.14	110.10
25	d	403	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	4	606	CLA	CMB-C2B-C3B	2.76	129.83	124.68
25	B	616	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
26	D	401	PHO	O2D-CGD-O1D	-2.75	118.45	123.84
25	2	601	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
25	c	525	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	C	518	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
37	S	612	KC2	C2B-C1B-NB	2.75	112.13	110.10
25	b	610	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
38	1	619	II0	C06-C04-C10	2.75	115.19	109.62
27	S	620	WVN	C39-C40-C37	-2.75	117.84	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	619	II0	C18-C04-C10	-2.75	106.10	110.47
38	Q	619	II0	C06-C04-C10	2.75	115.19	109.62
25	C	526	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
38	1	618	II0	C30-C32-C34	-2.75	114.65	123.22
25	A	403	CLA	CMB-C2B-C3B	2.75	129.82	124.68
38	4	619	II0	C06-C04-C10	2.75	115.18	109.62
38	6	619	II0	C20-C14-C10	-2.74	120.62	124.35
25	O	603	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
31	P	621	LHG	O8-C23-C24	2.74	120.52	111.91
27	C	529	WVN	C28-C30-C33	-2.74	114.66	123.22
39	5	620	IHT	C20-C15-C11	-2.74	120.62	124.35
34	C	536	LMG	O8-C28-C29	2.74	120.51	111.91
25	5	615	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
37	N	605	KC2	C3B-C2B-C1B	-2.74	104.46	107.08
38	S	619	II0	C20-C14-C10	-2.74	120.63	124.35
25	1	601	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	c	524	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	3	612	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
37	1	605	KC2	C3B-C2B-C1B	-2.74	104.46	107.08
38	R	616	II0	C41-C42-C40	-2.74	117.87	123.47
25	2	611	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
25	Q	609	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
38	O	619	II0	C18-C04-C10	-2.74	106.12	110.47
26	D	401	PHO	O1D-CGD-CBD	2.73	129.29	124.74
38	N	618	II0	C30-C32-C34	-2.73	114.69	123.22
27	a	407	WVN	C21-C15-C13	-2.73	121.46	124.53
27	P	620	WVN	C20-C23-C25	-2.73	122.11	126.23
27	C	530	WVN	C39-C40-C37	-2.73	117.88	123.47
37	6	606	KC2	C3B-C2B-C1B	-2.73	104.47	107.08
25	O	601	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
38	Q	619	II0	C18-C04-C10	-2.73	106.13	110.47
25	P	601	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
38	5	616	II0	C41-C42-C40	-2.73	117.89	123.47
38	N	619	II0	C06-C04-C10	2.73	115.15	109.62
25	b	616	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
38	2	616	II0	C06-C04-C10	2.73	115.15	109.62
25	C	522	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	R	613	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
25	N	601	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
25	6	609	CLA	CHB-C4A-NA	2.73	128.28	124.51
38	P	619	II0	C05-C03-C09	2.73	115.14	109.62
25	R	601	CLA	CMB-C2B-C3B	2.73	129.78	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	524	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	g	302	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
25	O	611	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
25	1	609	CLA	CMB-C2B-C3B	2.72	129.77	124.68
39	5	620	IHT	C02-C07-C10	-2.72	118.78	122.61
26	d	401	PHO	O1D-CGD-CBD	2.72	129.27	124.74
38	O	616	II0	C06-C04-C10	2.72	115.14	109.62
39	N	620	IHT	C25-C23-C22	2.72	122.37	118.08
25	R	615	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	O	609	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	N	603	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	R	620	IHT	C40-C37-C33	-2.72	123.43	127.31
38	2	619	II0	C18-C04-C10	-2.72	106.15	110.47
38	6	617	II0	C30-C32-C34	-2.72	114.73	123.22
25	P	612	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	2	609	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
38	S	617	II0	C30-C32-C34	-2.72	114.74	123.22
25	4	606	CLA	CHD-C1D-ND	-2.72	121.96	124.45
38	5	616	II0	C06-C04-C10	2.72	115.12	109.62
25	c	526	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
25	4	615	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
25	c	518	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
25	3	610	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
27	b	618	WVN	C20-C23-C25	-2.71	122.14	126.23
27	H	89	WVN	C01-C02-C11	-2.71	109.27	112.70
38	3	619	II0	C05-C03-C09	2.71	115.12	109.62
35	c	532	DGD	C2G-O2G-C1B	-2.71	111.11	117.79
25	A	403	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
35	C	532	DGD	C2G-O2G-C1B	-2.71	111.12	117.79
38	N	619	II0	C41-C42-C40	-2.71	117.92	123.47
34	d	402	LMG	O8-C28-C29	2.71	120.41	111.91
38	Q	619	II0	C30-C32-C34	-2.71	114.76	123.22
34	D	402	LMG	O8-C28-C29	2.71	120.41	111.91
25	4	609	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
31	c	535	LHG	O8-C23-C24	2.71	120.41	111.91
37	4	605	KC2	CHB-C4A-NA	2.71	128.47	124.20
37	Q	605	KC2	CHB-C4A-NA	2.71	128.47	124.20
25	R	604	CLA	CHD-C1D-ND	-2.71	121.97	124.45
38	S	617	II0	C29-C31-C33	-2.71	114.77	123.22
34	W	134	LMG	O8-C28-C29	2.71	120.40	111.91
25	5	603	CLA	CMB-C2B-C3B	2.71	129.74	124.68
37	6	606	KC2	CBD-CHA-C1A	2.70	133.93	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	615	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
25	5	601	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
25	a	403	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
29	D	405	PL9	C7-C8-C9	-2.70	122.29	126.79
25	6	604	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
38	Q	619	II0	C31-C33-C35	-2.70	118.83	126.42
38	R	616	II0	C06-C04-C10	2.70	115.09	109.62
25	S	604	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
38	R	619	II0	C32-C30-C26	-2.70	118.74	126.58
38	R	618	II0	C41-C42-C40	-2.70	117.94	123.47
25	R	603	CLA	CMB-C2B-C3B	2.70	129.73	124.68
25	3	604	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
38	4	616	II0	C03-C09-C13	-2.70	118.83	122.63
38	1	619	II0	C41-C42-C40	-2.70	117.95	123.47
25	O	606	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
25	5	601	CLA	CMB-C2B-C3B	2.70	129.72	124.68
25	b	601	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
25	C	527	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	5	613	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
38	5	619	II0	C32-C30-C26	-2.69	118.76	126.58
25	C	525	CLA	C1-C2-C3	-2.69	121.38	126.04
38	5	618	II0	C41-C42-C40	-2.69	117.96	123.47
25	Q	615	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
25	Q	604	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
38	Q	616	II0	C03-C09-C13	-2.69	118.84	122.63
27	a	407	WVN	C20-C13-C15	-2.69	114.95	121.46
25	1	603	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	1	609	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	B	601	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
25	6	603	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
27	b	619	WVN	C23-C20-C13	-2.69	119.66	127.20
25	3	601	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
25	c	525	CLA	C1-C2-C3	-2.68	121.40	126.04
25	4	604	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	d	405	PL9	C7-C8-C9	-2.68	122.33	126.79
25	S	609	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	R	620	IHT	C02-C07-C18	2.68	123.36	115.78
38	S	616	II0	C32-C30-C26	-2.68	118.80	126.58
25	2	606	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
38	6	617	II0	C29-C31-C33	-2.68	114.85	123.22
27	c	530	WVN	C40-C37-C34	-2.68	123.48	127.31
25	R	601	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	527	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
27	6	620	WVN	C40-C37-C34	-2.68	123.49	127.31
25	N	614	CLA	CHB-C4A-NA	2.68	128.22	124.51
27	c	531	WVN	C29-C26-C22	-2.68	123.49	127.31
38	O	617	II0	C18-C04-C10	-2.68	106.21	110.47
37	4	611	KC2	O2D-CGD-O1D	-2.68	118.61	123.84
27	y	89	WVN	C12-C14-C15	-2.68	109.30	114.08
38	5	618	II0	C06-C04-C10	2.67	115.04	109.62
25	b	605	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	b	612	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	1	614	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	N	609	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	P	610	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	Q	609	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	B	605	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
37	Q	611	KC2	O2D-CGD-O1D	-2.67	118.62	123.84
25	P	604	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
38	6	616	II0	C32-C30-C26	-2.67	118.83	126.58
25	6	604	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	S	604	CLA	CHB-C4A-NA	2.66	128.20	124.51
25	4	604	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	5	604	CLA	CHD-C1D-ND	-2.66	122.01	124.45
38	1	619	II0	C31-C29-C25	-2.66	118.85	126.58
38	4	619	II0	C30-C32-C34	-2.66	114.91	123.22
31	B	622	LHG	O8-C23-C24	2.66	120.26	111.91
25	S	603	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
25	4	604	CLA	CHB-C4A-NA	2.66	128.19	124.51
27	B	619	WVN	C23-C20-C13	-2.66	119.74	127.20
38	2	617	II0	C18-C04-C10	-2.66	106.25	110.47
25	6	615	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
39	O	620	IHT	C03-C05-C08	-2.66	107.64	113.64
31	B	622	LHG	C5-O7-C7	-2.66	111.25	117.79
25	Q	604	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	b	612	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	O	602	CLA	CHD-C1D-ND	-2.65	122.02	124.45
38	Q	619	II0	C20-C14-C12	2.65	119.27	114.36
28	A	408	SQD	O48-C23-C24	2.65	120.23	111.91
37	S	606	KC2	CBD-CHA-C1A	2.65	133.83	128.88
39	1	620	IHT	C41-C40-C37	-2.65	118.04	123.47
25	Q	613	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
25	B	612	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
28	a	408	SQD	O48-C23-C24	2.65	120.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	621	LHG	O8-C23-C24	2.65	120.22	111.91
25	b	613	CLA	CMB-C2B-C3B	2.65	129.63	124.68
39	4	620	IHT	C03-C05-C08	-2.65	107.67	113.64
39	Q	620	IHT	C03-C05-C08	-2.65	107.67	113.64
25	b	604	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
38	3	617	II0	C30-C32-C34	-2.65	114.96	123.22
25	4	606	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
39	1	620	IHT	C25-C23-C22	2.64	122.24	118.08
31	S	621	LHG	O8-C23-C24	2.64	120.20	111.91
25	4	613	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
27	C	529	WVN	C23-C20-C13	-2.64	119.78	127.20
27	6	620	WVN	C39-C40-C37	-2.64	118.06	123.47
37	N	605	KC2	CHB-C4A-NA	2.64	128.37	124.20
25	S	609	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
25	Q	604	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	P	612	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
38	5	617	II0	C41-C42-C40	-2.64	118.07	123.47
29	D	405	PL9	C22-C23-C24	-2.64	121.31	127.66
25	3	612	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
38	2	616	II0	C32-C30-C26	-2.64	118.93	126.58
37	1	605	KC2	CHB-C4A-NA	2.64	128.36	124.20
38	R	618	II0	C06-C04-C10	2.64	114.96	109.62
27	B	617	WVN	C17-C06-C13	-2.63	106.03	110.30
25	1	614	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
37	N	612	KC2	CAB-C3B-C2B	2.63	137.28	128.60
25	N	614	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
37	1	612	KC2	CAB-C3B-C2B	2.63	137.28	128.60
34	f	99	LMG	O8-C28-C29	2.63	120.16	111.91
38	O	616	II0	C32-C30-C26	-2.63	118.95	126.58
29	d	405	PL9	C22-C23-C24	-2.63	121.33	127.66
27	c	531	WVN	C23-C20-C13	-2.63	119.82	127.20
39	2	620	IHT	C31-C34-C35	-2.63	119.04	126.42
25	c	528	CLA	O2D-CGD-CBD	2.63	115.93	111.27
25	B	604	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
38	R	617	II0	C41-C42-C40	-2.62	118.10	123.47
27	h	89	WVN	C39-C40-C37	-2.62	118.10	123.47
38	O	619	II0	C41-C42-C40	-2.62	118.10	123.47
36	E	102	HEM	CHD-C1D-C2D	-2.62	120.88	124.98
38	2	619	II0	C41-C42-C40	-2.62	118.11	123.47
25	B	613	CLA	CMB-C2B-C3B	2.62	129.58	124.68
27	d	408	WVN	C01-C02-C11	-2.62	109.39	112.70
25	d	403	CLA	C1B-CHB-C4A	-2.62	124.93	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	527	CLA	CHB-C4A-NA	2.62	128.13	124.51
39	N	620	IHT	C41-C40-C37	-2.62	118.11	123.47
38	P	617	II0	C30-C32-C34	-2.62	115.05	123.22
25	S	613	CLA	CHB-C4A-NA	2.62	128.13	124.51
38	Q	617	II0	C18-C04-C10	-2.62	106.31	110.47
25	3	612	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	B	612	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
38	4	619	II0	C20-C14-C12	2.62	119.20	114.36
25	6	613	CLA	CHB-C4A-NA	2.61	128.13	124.51
27	S	620	WVN	C40-C37-C34	-2.61	123.58	127.31
38	R	619	II0	C06-C04-C10	2.61	114.91	109.62
25	6	610	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	R	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
38	4	617	II0	C18-C04-C10	-2.61	106.32	110.47
31	A	413	LHG	O8-C23-C24	2.61	120.09	111.91
38	4	616	II0	C30-C32-C34	-2.61	115.09	123.22
38	4	617	II0	C32-C30-C26	-2.61	119.02	126.58
38	5	619	II0	C06-C04-C10	2.60	114.90	109.62
27	y	89	WVN	C24-C22-C19	2.60	122.18	118.08
27	C	530	WVN	C02-C05-C09	-2.60	118.27	121.47
25	1	606	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
38	2	619	II0	C19-C13-C11	2.60	119.17	114.36
38	Q	617	II0	C32-C30-C26	-2.60	119.03	126.58
38	O	619	II0	C19-C13-C11	2.60	119.17	114.36
25	D	403	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
38	Q	616	II0	C30-C32-C34	-2.60	115.11	123.22
39	1	620	IHT	C39-C35-C34	2.59	122.16	118.08
39	1	620	IHT	C20-C15-C11	-2.59	120.83	124.35
31	a	413	LHG	O8-C23-C24	2.59	120.04	111.91
25	S	603	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	5	603	CLA	CHB-C4A-NA	2.59	128.09	124.51
38	2	617	II0	C06-C04-C10	2.59	114.87	109.62
25	C	528	CLA	O2D-CGD-CBD	2.59	115.87	111.27
34	F	99	LMG	O8-C28-C29	2.59	120.03	111.91
38	O	617	II0	C06-C04-C10	2.59	114.86	109.62
38	4	619	II0	C41-C42-C40	-2.58	118.18	123.47
38	P	616	II0	C41-C42-C40	-2.58	118.18	123.47
34	M	101	LMG	C8-O7-C10	-2.58	111.43	117.79
25	S	610	CLA	CHB-C4A-NA	2.58	128.09	124.51
25	2	602	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	3	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
25	Q	607	CLA	CMB-C2B-C3B	2.58	129.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	605	KC2	CMB-C2B-C1B	2.58	129.26	124.71
25	P	612	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	N	606	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
25	5	609	CLA	C1-C2-C3	-2.58	121.58	126.04
27	C	529	WVN	C01-C02-C11	-2.58	109.44	112.70
39	5	620	IHT	C19-C10-C07	-2.58	121.63	124.53
38	6	618	II0	C19-C13-C11	2.58	119.13	114.36
25	R	609	CLA	C1-C2-C3	-2.58	121.58	126.04
34	F	99	LMG	C8-O7-C10	-2.58	111.45	117.79
38	3	616	II0	C41-C42-C40	-2.58	118.20	123.47
29	a	409	PL9	C22-C23-C24	-2.57	121.46	127.66
25	3	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
38	4	619	II0	C31-C33-C35	-2.57	119.19	126.42
37	1	605	KC2	CMB-C2B-C1B	2.57	129.24	124.71
29	A	409	PL9	C22-C23-C24	-2.57	121.47	127.66
38	5	617	II0	C06-C04-C10	2.57	114.83	109.62
27	y	89	WVN	C19-C22-C26	-2.57	115.00	118.94
38	4	618	II0	C32-C30-C26	-2.57	119.13	126.58
25	c	527	CLA	CHB-C4A-NA	2.57	128.06	124.51
38	4	616	II0	C31-C33-C35	-2.56	119.22	126.42
27	B	618	WVN	C30-C33-C34	-2.56	119.22	126.42
38	Q	616	II0	C31-C33-C35	-2.56	119.23	126.42
25	P	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	2	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
38	4	617	II0	C41-C42-C40	-2.56	118.23	123.47
27	b	618	WVN	C23-C20-C13	-2.56	120.02	127.20
34	f	99	LMG	C8-O7-C10	-2.56	111.50	117.79
39	2	620	IHT	C22-C18-C07	-2.56	120.02	127.20
38	1	617	II0	C32-C30-C26	-2.56	119.16	126.58
38	N	617	II0	C32-C30-C26	-2.56	119.16	126.58
38	5	617	II0	C30-C32-C34	-2.56	115.24	123.22
31	C	535	LHG	O8-C23-C24	2.56	119.93	111.91
25	4	607	CLA	CMB-C2B-C3B	2.55	129.46	124.68
27	6	620	WVN	C23-C20-C13	-2.55	120.03	127.20
27	D	408	WVN	C07-C01-C02	2.55	113.41	109.55
37	4	612	KC2	C3D-CAD-CBD	-2.55	104.24	107.61
37	4	605	KC2	CBD-CHA-C1A	2.55	133.64	128.88
34	D	407	LMG	O8-C28-C29	2.55	119.91	111.91
25	O	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	Q	620	IHT	C36-C33-C37	-2.55	119.35	122.92
25	b	601	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	2	611	CLA	CHB-C4A-NA	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	618	II0	C19-C13-C11	2.55	119.08	114.36
25	O	601	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	A	407	WVN	C20-C23-C25	-2.55	122.39	126.23
34	d	407	LMG	O8-C28-C29	2.55	119.90	111.91
35	H	90	DGD	O1G-C1A-C2A	2.55	119.90	111.91
38	R	617	II0	C06-C04-C10	2.55	114.78	109.62
27	y	89	WVN	C40-C39-C36	-2.55	118.26	123.47
37	R	612	KC2	O2D-CGD-O1D	-2.55	118.86	123.84
27	d	408	WVN	C14-C15-C13	-2.54	119.04	122.73
37	Q	605	KC2	CBD-CHA-C1A	2.54	133.62	128.88
38	6	618	II0	C41-C42-C40	-2.54	118.27	123.47
25	g	302	CLA	C3A-C2A-C1A	2.54	105.14	101.34
38	3	619	II0	C32-C30-C26	-2.54	119.20	126.58
38	P	619	II0	C32-C30-C26	-2.54	119.21	126.58
25	P	603	CLA	CHB-C4A-NA	2.54	128.02	124.51
31	l	101	LHG	O8-C23-C24	2.54	119.87	111.91
38	5	617	II0	C03-C09-C13	-2.54	119.05	122.63
38	S	618	II0	C41-C42-C40	-2.54	118.28	123.47
37	5	612	KC2	O2D-CGD-O1D	-2.54	118.88	123.84
37	4	611	KC2	C2B-C1B-NB	2.54	111.97	110.10
38	Q	617	II0	C41-C42-C40	-2.54	118.28	123.47
38	Q	618	II0	C32-C30-C26	-2.54	119.22	126.58
38	3	616	II0	C03-C09-C13	-2.54	119.05	122.63
38	2	616	II0	C18-C04-C10	-2.53	106.44	110.47
39	O	620	IHT	C22-C18-C07	-2.53	120.09	127.20
31	L	101	LHG	O8-C23-C24	2.53	119.86	111.91
34	B	620	LMG	C8-O7-C10	-2.53	111.56	117.79
34	C	536	LMG	C7-O1-C1	-2.53	108.79	113.74
25	P	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	1	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	B	618	WVN	C02-C05-C09	-2.53	118.35	121.47
25	4	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	Y	89	WVN	C28-C30-C33	-2.53	115.32	123.22
25	S	603	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
26	a	405	PHO	O2D-CGD-O1D	-2.53	118.89	123.84
35	h	90	DGD	O1G-C1A-C2A	2.53	119.84	111.91
27	D	408	WVN	C23-C20-C13	-2.53	120.11	127.20
25	N	604	CLA	CHB-C4A-NA	2.53	128.00	124.51
25	C	526	CLA	O2D-CGD-CBD	2.53	115.75	111.27
37	6	612	KC2	CAA-CBA-CGA	-2.52	114.29	127.26
38	R	617	II0	C30-C32-C34	-2.52	115.34	123.22
25	3	603	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	601	CLA	CHB-C4A-NA	2.52	128.00	124.51
25	3	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
37	Q	612	KC2	C3D-CAD-CBD	-2.52	104.29	107.61
27	S	620	WVN	C23-C20-C13	-2.52	120.13	127.20
38	P	616	II0	C03-C09-C13	-2.52	119.08	122.63
37	3	606	KC2	O2D-CGD-O1D	-2.52	118.92	123.84
25	O	609	CLA	CHB-C4A-NA	2.51	127.99	124.51
37	2	612	KC2	C3B-C2B-C1B	-2.51	104.67	107.08
26	A	405	PHO	O2D-CGD-O1D	-2.51	118.92	123.84
37	S	612	KC2	CAA-CBA-CGA	-2.51	114.34	127.26
25	1	610	CLA	CHD-C1D-ND	-2.51	122.14	124.45
25	Q	603	CLA	CHB-C4A-NA	2.51	127.99	124.51
25	C	526	CLA	CHB-C4A-NA	2.51	127.98	124.51
34	m	101	LMG	C8-O7-C10	-2.51	111.61	117.79
25	N	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
37	6	606	KC2	CAB-C3B-C2B	2.51	136.87	128.60
27	b	617	WVN	C02-C05-C09	-2.51	118.38	121.47
37	N	613	KC2	O2D-CGD-CBD	2.51	115.72	111.27
31	D	406	LHG	O8-C23-C24	2.51	119.77	111.91
25	P	609	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
31	b	622	LHG	C5-O7-C7	-2.50	111.62	117.79
38	S	618	II0	C30-C32-C34	-2.50	115.40	123.22
37	O	612	KC2	CAB-C3B-C2B	2.50	136.85	128.60
25	4	603	CLA	CHB-C4A-NA	2.50	127.97	124.51
34	g	303	LMG	O8-C28-C29	2.50	119.76	111.91
25	D	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	1	614	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
31	d	406	LHG	O8-C23-C24	2.50	119.76	111.91
25	c	526	CLA	O2D-CGD-CBD	2.50	115.71	111.27
27	B	619	WVN	C26-C29-C31	-2.50	115.41	123.22
25	c	528	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	b	619	WVN	C08-C01-C02	2.50	113.33	109.55
38	6	617	II0	C41-C42-C40	-2.50	118.35	123.47
37	2	612	KC2	CAB-C3B-C2B	2.50	136.84	128.60
38	3	616	II0	C30-C32-C34	-2.50	115.42	123.22
25	G	301	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
25	6	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	B	601	CLA	CHB-C4A-NA	2.50	127.97	124.51
38	P	616	II0	C30-C32-C34	-2.50	115.43	123.22
27	C	531	WVN	C14-C15-C13	-2.50	119.11	122.73
25	N	610	CLA	CHD-C1D-ND	-2.50	122.16	124.45
37	6	606	KC2	CHB-C4A-NA	2.49	128.13	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Q	611	KC2	C2B-C1B-NB	2.49	111.94	110.10
38	6	618	II0	C30-C32-C34	-2.49	115.44	123.22
27	b	618	WVN	C14-C15-C13	-2.49	119.11	122.73
38	O	616	II0	C18-C04-C10	-2.49	106.51	110.47
38	R	618	II0	C19-C13-C11	2.49	118.97	114.36
37	P	606	KC2	O2D-CGD-O1D	-2.49	118.97	123.84
37	1	613	KC2	O2D-CGD-CBD	2.49	115.69	111.27
25	6	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
34	G	303	LMG	O8-C28-C29	2.49	119.72	111.91
38	1	616	II0	C31-C33-C35	-2.49	119.42	126.42
38	N	616	II0	C31-C33-C35	-2.49	119.43	126.42
38	S	617	II0	C41-C42-C40	-2.49	118.38	123.47
38	3	616	II0	C32-C30-C26	-2.49	119.36	126.58
27	B	617	WVN	C29-C31-C32	-2.49	119.43	126.42
39	1	620	IHT	C22-C23-C27	2.49	122.76	118.94
29	A	409	PL9	C20-C19-C21	2.49	119.45	115.27
25	Q	603	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
38	O	618	II0	C31-C33-C35	-2.49	119.43	126.42
31	L	101	LHG	C5-O7-C7	-2.48	111.68	117.79
25	1	604	CLA	CHD-C1D-ND	-2.48	122.17	124.45
38	P	616	II0	C32-C30-C26	-2.48	119.37	126.58
25	P	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	P	615	CLA	CHB-C4A-NA	2.48	127.94	124.51
38	5	618	II0	C19-C13-C11	2.48	118.95	114.36
25	6	603	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	N	614	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
27	P	620	WVN	C07-C01-C02	2.48	113.30	109.55
37	N	611	KC2	O2D-CGD-O1D	-2.48	118.99	123.84
25	1	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	R	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
38	R	617	II0	C03-C09-C13	-2.48	119.13	122.63
38	Q	619	II0	C41-C42-C40	-2.48	118.40	123.47
25	Q	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	S	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	Z	102	LMG	O8-C28-C29	2.48	119.68	111.91
27	a	407	WVN	C16-C05-C09	-2.48	113.52	122.33
31	l	101	LHG	C5-O7-C7	-2.48	111.69	117.79
37	S	612	KC2	C3D-CAD-CBD	-2.48	104.34	107.61
27	3	620	WVN	C07-C01-C02	2.48	113.30	109.55
25	N	610	CLA	CHB-C4A-NA	2.48	127.94	124.51
38	S	619	II0	C30-C32-C34	-2.47	115.49	123.22
27	b	617	WVN	C28-C30-C33	-2.47	115.50	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	603	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
38	O	617	II0	C41-C42-C40	-2.47	118.41	123.47
25	R	602	CLA	CHD-C1D-ND	-2.47	122.18	124.45
28	a	411	SQD	O9-S-C6	2.47	109.88	106.94
39	R	620	IHT	C12-C15-C11	-2.47	114.96	120.57
25	S	610	CLA	CHD-C1D-ND	-2.47	122.18	124.45
27	C	530	WVN	C23-C25-C28	-2.47	115.15	118.94
25	5	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	d	404	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	a	407	WVN	C40-C39-C36	-2.47	118.41	123.47
25	1	609	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
25	N	604	CLA	CHD-C1D-ND	-2.47	122.19	124.45
37	5	612	KC2	CAB-C3B-C2B	2.47	136.74	128.60
25	P	610	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	2	609	CLA	CHB-C4A-NA	2.47	127.92	124.51
34	z	102	LMG	O8-C28-C29	2.46	119.64	111.91
38	Q	616	II0	C17-C04-C06	-2.46	97.99	109.05
25	b	605	CLA	CHD-C1D-ND	-2.46	122.19	124.45
25	6	610	CLA	CHD-C1D-ND	-2.46	122.19	124.45
37	4	611	KC2	CBD-CHA-C1A	2.46	133.47	128.88
25	N	601	CLA	CHB-C4A-NA	2.46	127.92	124.51
37	R	612	KC2	CAB-C3B-C2B	2.46	136.72	128.60
29	a	409	PL9	C20-C19-C21	2.46	119.41	115.27
39	4	620	IHT	C36-C33-C37	-2.46	119.47	122.92
27	Y	89	WVN	C30-C28-C25	-2.46	123.80	127.31
37	6	612	KC2	C3D-CAD-CBD	-2.46	104.36	107.61
37	O	612	KC2	C3B-C2B-C1B	-2.46	104.73	107.08
25	3	611	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	4	603	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
37	6	612	KC2	O2D-CGD-O1D	-2.46	119.03	123.84
37	N	613	KC2	CAB-C3B-C2B	2.46	136.71	128.60
34	b	620	LMG	C8-O7-C10	-2.46	111.74	117.79
25	R	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
38	4	616	II0	C17-C04-C06	-2.46	98.02	109.05
25	B	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
37	3	606	KC2	CMB-C2B-C1B	2.46	129.04	124.71
34	c	536	LMG	O8-C28-C29	2.46	119.61	111.91
25	B	612	CLA	CHD-C1D-ND	-2.45	122.20	124.45
38	2	617	II0	C41-C42-C40	-2.45	118.45	123.47
25	3	615	CLA	CHB-C4A-NA	2.45	127.90	124.51
37	P	606	KC2	CMB-C2B-C1B	2.45	129.03	124.71
38	1	619	II0	C31-C33-C35	-2.45	119.53	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	604	CLA	CHD-C1D-ND	-2.45	122.20	124.45
36	e	102	HEM	CHD-C1D-C2D	-2.45	121.15	124.98
37	1	611	KC2	CMB-C2B-C1B	2.45	129.03	124.71
25	1	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
38	6	616	II0	C06-C04-C10	2.45	114.58	109.62
37	1	605	KC2	O2D-CGD-O1D	-2.45	119.05	123.84
25	B	606	CLA	CHB-C4A-NA	2.45	127.90	124.51
37	1	613	KC2	CAB-C3B-C2B	2.45	136.67	128.60
38	S	616	II0	C06-C04-C10	2.45	114.58	109.62
25	5	602	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	3	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
27	B	618	WVN	C29-C31-C32	-2.45	119.54	126.42
25	N	602	CLA	CHB-C4A-NA	2.45	127.89	124.51
37	1	613	KC2	C3D-CAD-CBD	-2.45	104.38	107.61
25	A	406	CLA	CHB-C4A-NA	2.45	127.89	124.51
25	C	517	CLA	CHB-C4A-NA	2.45	127.89	124.51
27	H	89	WVN	C12-C14-C15	-2.45	109.71	114.08
38	1	617	II0	C41-C42-C40	-2.44	118.47	123.47
25	b	612	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	b	613	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	c	526	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	c	529	WVN	C14-C15-C13	-2.44	119.19	122.73
25	b	607	CLA	CHB-C4A-NA	2.44	127.89	124.51
37	1	611	KC2	O2D-CGD-O1D	-2.44	119.06	123.84
38	N	617	II0	C41-C42-C40	-2.44	118.47	123.47
31	b	622	LHG	O8-C23-C24	2.44	119.57	111.91
37	S	612	KC2	O2D-CGD-O1D	-2.44	119.07	123.84
25	6	602	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	b	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
37	1	611	KC2	C2B-C1B-NB	2.44	111.90	110.10
25	b	602	CLA	CHB-C4A-NA	2.44	127.88	124.51
38	5	617	II0	C32-C30-C26	-2.44	119.50	126.58
39	4	620	IHT	C28-C26-C24	2.44	121.67	116.84
25	2	604	CLA	CHD-C1D-ND	-2.44	122.22	124.45
25	2	610	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	B	602	CLA	CHB-C4A-NA	2.44	127.88	124.51
37	6	606	KC2	O2D-CGD-O1D	-2.44	119.08	123.84
25	a	406	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	D	403	CLA	CHB-C4A-NA	2.43	127.88	124.51
37	R	612	KC2	CAA-CBA-CGA	-2.43	114.76	127.26
25	B	605	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	O	602	CLA	CHB-C4A-NA	2.43	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	d	403	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	Q	606	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	3	602	CLA	CHD-C1D-ND	-2.43	122.22	124.45
39	Q	620	IHT	C22-C18-C07	-2.43	120.38	127.20
37	N	605	KC2	O2D-CGD-O1D	-2.43	119.09	123.84
25	B	612	CLA	CHB-C4A-NA	2.43	127.87	124.51
37	Q	611	KC2	CBD-CHA-C1A	2.43	133.41	128.88
25	4	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
38	6	616	II0	C03-C09-C13	-2.43	119.21	122.63
27	B	618	WVN	C20-C23-C25	-2.43	122.57	126.23
25	P	610	CLA	CHD-C1D-ND	-2.43	122.22	124.45
38	6	619	II0	C30-C32-C34	-2.43	115.65	123.22
37	N	613	KC2	C3D-CAD-CBD	-2.43	104.41	107.61
25	C	528	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	3	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
38	S	617	II0	C06-C04-C10	2.42	114.53	109.62
37	5	612	KC2	CAA-CBA-CGA	-2.42	114.81	127.26
25	5	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	Q	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
37	N	611	KC2	CMB-C2B-C1B	2.42	128.98	124.71
34	d	407	LMG	C8-O7-C10	-2.42	111.84	117.79
27	B	619	WVN	C24-C22-C19	2.42	121.89	118.08
38	P	618	II0	C06-C04-C10	2.42	114.52	109.62
37	N	611	KC2	C2B-C1B-NB	2.42	111.89	110.10
37	1	613	KC2	CHB-C4A-NA	2.42	128.01	124.20
38	6	617	II0	C06-C04-C10	2.42	114.52	109.62
25	1	602	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	B	607	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	5	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	2	613	CLA	CHB-C4A-NA	2.41	127.85	124.51
38	R	617	II0	C32-C30-C26	-2.41	119.57	126.58
25	S	602	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	S	609	CLA	O1D-CGD-CBD	2.41	129.42	124.48
25	2	607	CLA	CMB-C2B-C3B	2.41	129.19	124.68
25	3	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	5	601	CLA	CHB-C4A-NA	2.41	127.84	124.51
38	5	616	II0	C30-C32-C34	-2.41	115.70	123.22
25	O	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
34	D	407	LMG	C8-O7-C10	-2.41	111.86	117.79
25	R	601	CLA	CHB-C4A-NA	2.41	127.84	124.51
29	D	405	PL9	C27-C28-C29	-2.41	121.86	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	3	618	II0	C06-C04-C10	2.41	114.50	109.62
37	4	611	KC2	CMB-C2B-C1B	2.41	128.96	124.71
38	5	616	II0	C32-C30-C26	-2.41	119.59	126.58
25	S	602	CLA	CHD-C1D-ND	-2.41	122.24	124.45
39	N	620	IHT	C22-C23-C27	2.41	122.63	118.94
37	N	613	KC2	CHB-C4A-NA	2.40	127.99	124.20
25	b	612	CLA	CHB-C4A-NA	2.40	127.84	124.51
28	A	411	SQD	O48-C23-C24	2.40	119.45	111.91
28	A	411	SQD	O9-S-C6	2.40	109.80	106.94
27	c	529	WVN	C28-C30-C33	-2.40	115.72	123.22
27	h	89	WVN	C12-C14-C15	-2.40	109.79	114.08
38	5	618	II0	C31-C33-C35	-2.40	119.67	126.42
27	C	529	WVN	C27-C25-C23	2.40	121.86	118.08
37	S	612	KC2	CAB-C3B-C2B	2.40	136.51	128.60
25	6	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
37	6	612	KC2	CAB-C3B-C2B	2.40	136.51	128.60
25	2	610	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	3	610	CLA	CHD-C1D-ND	-2.40	122.25	124.45
38	R	618	II0	C31-C33-C35	-2.40	119.68	126.42
27	B	617	WVN	C23-C20-C13	-2.40	120.47	127.20
27	b	619	WVN	C27-C25-C28	-2.40	119.56	122.92
25	O	607	CLA	CMB-C2B-C3B	2.40	129.16	124.68
39	4	620	IHT	C22-C18-C07	-2.40	120.47	127.20
37	Q	611	KC2	CMB-C2B-C1B	2.40	128.93	124.71
25	G	302	CLA	O2D-CGD-CBD	2.39	115.52	111.27
36	e	102	HEM	C4D-ND-C1D	2.39	107.54	105.07
25	c	518	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	B	619	WVN	C02-C05-C09	-2.39	118.53	121.47
37	R	612	KC2	C2B-C1B-NB	2.39	111.86	110.10
27	C	529	WVN	C12-C14-C15	-2.39	109.81	114.08
34	Q	621	LMG	O8-C28-C29	2.39	119.40	111.91
39	Q	620	IHT	C41-C40-C37	-2.39	118.58	123.47
34	c	536	LMG	C8-O7-C10	-2.39	111.91	117.79
25	c	517	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	C	520	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	O	610	CLA	CHB-C4A-NA	2.39	127.81	124.51
37	Q	612	KC2	CMB-C2B-C1B	2.39	128.92	124.71
25	c	520	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	c	519	CLA	CHB-C4A-NA	2.39	127.81	124.51
38	R	616	II0	C32-C30-C26	-2.38	119.66	126.58
39	N	620	IHT	C03-C05-C08	-2.38	108.26	113.64
25	N	606	CLA	CHB-C4A-NA	2.38	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	5	620	IHT	C12-C15-C11	-2.38	115.16	120.57
37	N	612	KC2	O2D-CGD-O1D	-2.38	119.18	123.84
25	b	604	CLA	CHB-C4A-NA	2.38	127.81	124.51
25	R	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
27	d	408	WVN	C07-C01-C02	2.38	113.15	109.55
25	3	603	CLA	C1-C2-C3	-2.38	121.92	126.04
25	O	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
29	d	405	PL9	C27-C28-C29	-2.38	121.93	127.66
34	4	621	LMG	O8-C28-C29	2.38	119.38	111.91
38	S	619	II0	C20-C14-C12	2.38	118.76	114.36
37	1	612	KC2	O2D-CGD-O1D	-2.38	119.19	123.84
39	O	620	IHT	C31-C34-C35	-2.38	119.73	126.42
38	R	616	II0	C30-C32-C34	-2.38	115.79	123.22
25	C	518	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	2	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	2	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
37	S	606	KC2	CAB-C3B-C2B	2.38	136.44	128.60
35	c	532	DGD	O1G-C1A-C2A	2.38	119.37	111.91
37	4	605	KC2	O2D-CGD-O1D	-2.38	119.19	123.84
38	S	616	II0	C03-C09-C13	-2.38	119.28	122.63
25	P	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
37	Q	605	KC2	O2D-CGD-O1D	-2.38	119.19	123.84
38	P	618	II0	C04-C06-C08	-2.37	108.28	113.64
37	N	611	KC2	CBD-CHA-C1A	2.37	133.31	128.88
37	4	612	KC2	CMB-C2B-C1B	2.37	128.90	124.71
37	1	611	KC2	CBD-CHA-C1A	2.37	133.31	128.88
38	R	616	II0	C18-C04-C10	-2.37	106.70	110.47
25	B	614	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	d	400	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	B	604	CLA	CHB-C4A-NA	2.37	127.79	124.51
35	C	532	DGD	O1G-C1A-C2A	2.37	119.34	111.91
37	O	612	KC2	C3D-CAD-CBD	-2.37	104.49	107.61
25	O	604	CLA	CHB-C4A-NA	2.37	127.78	124.51
25	4	615	CLA	CHB-C4A-NA	2.37	127.78	124.51
37	5	612	KC2	C2B-C1B-NB	2.36	111.85	110.10
37	3	606	KC2	C2B-C1B-NB	2.36	111.84	110.10
38	3	618	II0	C04-C06-C08	-2.36	108.31	113.64
28	a	411	SQD	O48-C23-C24	2.36	119.32	111.91
25	g	301	CLA	CHD-C1D-ND	-2.36	122.28	124.45
38	5	616	II0	C18-C04-C10	-2.36	106.72	110.47
25	5	611	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	A	407	WVN	C30-C33-C34	-2.36	119.79	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	620	WVN	C29-C31-C32	-2.36	119.79	126.42
25	b	616	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	R	606	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	O	615	CLA	CHB-C4A-NA	2.36	127.77	124.51
37	2	612	KC2	C3D-CAD-CBD	-2.36	104.50	107.61
27	Y	89	WVN	C39-C40-C37	-2.35	118.65	123.47
39	2	620	IHT	C18-C22-C23	-2.35	122.68	126.23
25	Q	615	CLA	CHB-C4A-NA	2.35	127.77	124.51
38	6	619	II0	C20-C14-C12	2.35	118.71	114.36
25	P	603	CLA	C1-C2-C3	-2.35	121.97	126.04
25	a	404	CLA	CHB-C4A-NA	2.35	127.76	124.51
27	S	620	WVN	C28-C30-C33	-2.35	115.88	123.22
25	R	601	CLA	CHD-C1D-ND	-2.35	122.29	124.45
25	2	615	CLA	CHB-C4A-NA	2.35	127.76	124.51
38	N	618	II0	C31-C33-C35	-2.35	119.81	126.42
25	Q	610	CLA	CHD-C1D-ND	-2.35	122.30	124.45
38	4	617	II0	C17-C04-C06	-2.35	98.50	109.05
25	R	604	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	5	601	CLA	CHD-C1D-ND	-2.35	122.30	124.45
25	B	610	CLA	CHB-C4A-NA	2.35	127.76	124.51
38	Q	617	II0	C17-C04-C06	-2.35	98.51	109.05
25	B	604	CLA	O2D-CGD-CBD	2.35	115.44	111.27
25	Q	610	CLA	CHB-C4A-NA	2.35	127.75	124.51
25	Q	610	CLA	C1-C2-C3	-2.35	121.99	126.04
25	b	607	CLA	CHD-C1D-ND	-2.34	122.30	124.45
38	O	616	II0	C03-C09-C13	-2.34	119.32	122.63
27	C	530	WVN	C28-C30-C33	-2.34	115.90	123.22
27	c	530	WVN	C26-C29-C31	-2.34	115.90	123.22
38	2	618	II0	C31-C33-C35	-2.34	119.83	126.42
39	O	620	IHT	C30-C32-C33	-2.34	119.83	126.42
38	Q	617	II0	C03-C09-C13	-2.34	119.33	122.63
38	4	618	II0	C41-C42-C40	-2.34	118.67	123.47
25	A	404	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	D	405	PL9	C20-C19-C21	2.34	119.21	115.27
38	2	616	II0	C03-C09-C13	-2.34	119.33	122.63
27	B	619	WVN	C28-C30-C33	-2.34	115.91	123.22
38	1	618	II0	C31-C33-C35	-2.34	119.84	126.42
37	1	613	KC2	CBD-CHA-C1A	2.34	133.25	128.88
25	b	605	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	b	610	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	G	302	CLA	CHB-C4A-NA	2.34	127.75	124.51
38	1	617	II0	C30-C32-C34	-2.34	115.92	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	519	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	2	604	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	1	607	CLA	CMB-C2B-C3B	2.34	129.05	124.68
25	6	601	CLA	CHB-C4A-NA	2.34	127.74	124.51
38	R	619	II0	C41-C42-C40	-2.34	118.69	123.47
25	P	602	CLA	CHD-C1D-ND	-2.34	122.31	124.45
25	R	610	CLA	CHD-C1D-ND	-2.34	122.31	124.45
25	B	605	CLA	CHB-C4A-NA	2.34	127.74	124.51
27	P	620	WVN	C29-C31-C32	-2.33	119.86	126.42
27	C	530	WVN	C27-C25-C23	2.33	121.75	118.08
38	5	619	II0	C41-C42-C40	-2.33	118.69	123.47
25	b	614	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	c	525	CLA	CHB-C4A-NA	2.33	127.74	124.51
38	1	618	II0	C17-C04-C06	-2.33	98.57	109.05
27	D	408	WVN	C01-C02-C11	-2.33	109.75	112.70
25	C	521	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	Q	602	CLA	CHD-C1D-ND	-2.33	122.31	124.45
39	R	620	IHT	C06-C09-C10	-2.33	109.92	114.08
37	S	606	KC2	CHB-C4A-NA	2.33	127.87	124.20
37	P	606	KC2	CBD-CHA-C1A	2.33	133.22	128.88
25	D	400	CLA	CHB-C4A-NA	2.33	127.73	124.51
27	C	529	WVN	C16-C05-C09	-2.33	114.05	122.33
25	5	610	CLA	CHD-C1D-ND	-2.33	122.32	124.45
25	1	606	CLA	CHB-C4A-NA	2.32	127.73	124.51
38	R	619	II0	C30-C32-C34	-2.32	115.96	123.22
37	3	606	KC2	CBD-CHA-C1A	2.32	133.22	128.88
25	4	610	CLA	CHD-C1D-ND	-2.32	122.32	124.45
27	d	408	WVN	C23-C20-C13	-2.32	120.67	127.20
25	B	616	CLA	CHB-C4A-NA	2.32	127.72	124.51
38	N	618	II0	C17-C04-C06	-2.32	98.62	109.05
38	P	618	II0	C32-C30-C26	-2.32	119.83	126.58
25	O	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
27	b	618	WVN	C29-C31-C32	-2.32	119.90	126.42
27	B	619	WVN	C18-C06-C13	2.32	114.06	110.30
25	5	606	CLA	CHB-C4A-NA	2.32	127.72	124.51
38	5	619	II0	C30-C32-C34	-2.32	115.98	123.22
25	4	610	CLA	C1-C2-C3	-2.32	122.03	126.04
38	N	617	II0	C30-C32-C34	-2.32	115.99	123.22
25	C	521	CLA	CHB-C4A-NA	2.32	127.72	124.51
39	4	620	IHT	C39-C35-C34	2.32	121.73	118.08
25	g	301	CLA	CHB-C4A-NA	2.32	127.72	124.51
25	N	607	CLA	CMB-C2B-C3B	2.32	129.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	620	IHT	C20-C15-C11	-2.31	121.20	124.35
29	d	405	PL9	C20-C19-C21	2.31	119.16	115.27
25	P	601	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	d	400	CLA	O2D-CGD-CBD	2.31	115.38	111.27
25	c	521	CLA	CHD-C1D-ND	-2.31	122.33	124.45
37	S	606	KC2	C3B-C2B-C1B	-2.31	104.87	107.08
25	S	601	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	4	610	CLA	CHB-C4A-NA	2.31	127.71	124.51
39	Q	620	IHT	C17-C03-C05	2.31	119.42	109.05
38	Q	618	II0	C41-C42-C40	-2.31	118.74	123.47
25	c	521	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	C	523	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	3	601	CLA	CHB-C4A-NA	2.31	127.70	124.51
39	R	620	IHT	C14-C02-C07	-2.31	106.55	110.30
38	O	619	II0	C20-C14-C12	2.31	118.63	114.36
27	6	620	WVN	C28-C30-C33	-2.31	116.01	123.22
37	6	606	KC2	CAB-C3B-C4B	-2.31	119.32	124.90
25	O	610	CLA	CHD-C1D-ND	-2.31	122.33	124.45
38	4	618	II0	C17-C04-C06	-2.31	98.70	109.05
27	c	530	WVN	C02-C05-C09	-2.31	118.63	121.47
38	4	617	II0	C03-C09-C13	-2.31	119.38	122.63
39	2	620	IHT	C30-C32-C33	-2.30	119.94	126.42
25	A	403	CLA	CHD-C1D-ND	-2.30	122.34	124.45
27	b	617	WVN	C18-C06-C13	-2.30	106.56	110.30
25	C	525	CLA	CHB-C4A-NA	2.30	127.70	124.51
39	4	620	IHT	C31-C34-C35	-2.30	119.95	126.42
38	Q	618	II0	C17-C04-C06	-2.30	98.72	109.05
38	N	619	II0	C31-C29-C25	-2.30	119.90	126.58
39	O	620	IHT	C18-C22-C23	-2.30	122.76	126.23
39	5	620	IHT	C40-C37-C33	-2.30	124.03	127.31
25	b	604	CLA	O2D-CGD-CBD	2.30	115.35	111.27
25	2	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
38	3	619	II0	C17-C04-C06	-2.30	98.74	109.05
37	S	606	KC2	O2D-CGD-O1D	-2.29	119.35	123.84
25	1	607	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	S	615	CLA	CHB-C4A-NA	2.29	127.68	124.51
38	2	619	II0	C20-C14-C12	2.29	118.60	114.36
37	N	613	KC2	CBD-CHA-C1A	2.29	133.15	128.88
25	P	609	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	1	615	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
25	Q	606	CLA	CHD-C1D-ND	-2.29	122.35	124.45
38	P	619	II0	C17-C04-C06	-2.29	98.77	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	400	CLA	O2D-CGD-CBD	2.29	115.33	111.27
37	P	606	KC2	C2B-C1B-NB	2.29	111.79	110.10
27	P	620	WVN	C29-C26-C22	-2.29	124.05	127.31
38	S	618	II0	C17-C04-C06	-2.29	98.78	109.05
25	3	609	CLA	CHB-C4A-NA	2.29	127.67	124.51
25	N	606	CLA	CHD-C1D-ND	-2.29	122.35	124.45
27	A	407	WVN	C40-C39-C36	-2.28	118.80	123.47
27	c	529	WVN	C12-C14-C15	-2.28	110.00	114.08
37	Q	605	KC2	C2B-C1B-NB	2.28	111.78	110.10
25	4	602	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	c	530	WVN	C30-C28-C25	-2.28	124.06	127.31
25	4	606	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
37	4	605	KC2	C2B-C1B-NB	2.28	111.78	110.10
25	B	602	CLA	CHD-C1D-ND	-2.28	122.36	124.45
38	3	618	II0	C17-C04-C06	-2.28	98.82	109.05
25	N	615	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
37	4	612	KC2	CAA-CBA-CGA	-2.28	115.57	127.26
38	P	618	II0	C17-C04-C06	-2.27	98.84	109.05
37	Q	612	KC2	CAA-CBA-CGA	-2.27	115.58	127.26
25	C	519	CLA	CHD-C1D-ND	-2.27	122.37	124.45
38	6	618	II0	C17-C04-C06	-2.27	98.85	109.05
28	A	408	SQD	O7-S-C6	2.27	109.64	106.94
39	N	620	IHT	C39-C35-C34	2.27	121.65	118.08
25	b	610	CLA	CHD-C1D-ND	-2.27	122.37	124.45
27	C	531	WVN	C06-C13-C20	-2.27	109.36	115.78
38	O	617	II0	C20-C14-C12	2.27	118.56	114.36
38	N	618	II0	C19-C13-C11	2.27	118.56	114.36
38	3	618	II0	C32-C30-C26	-2.27	120.00	126.58
27	3	620	WVN	C29-C26-C22	-2.27	124.08	127.31
38	3	618	II0	C31-C33-C35	-2.27	120.05	126.42
25	c	523	CLA	CHB-C4A-NA	2.27	127.64	124.51
25	3	611	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	1	602	CLA	CHD-C1D-ND	-2.26	122.37	124.45
36	E	102	HEM	CHA-C4D-C3D	-2.26	121.08	125.33
34	G	303	LMG	C8-O7-C10	-2.26	112.22	117.79
28	A	411	SQD	O8-S-C6	2.26	109.35	105.74
25	1	606	CLA	CHD-C1D-ND	-2.26	122.37	124.45
38	2	617	II0	C20-C14-C12	2.26	118.55	114.36
25	c	516	CLA	CHB-C4A-NA	2.26	127.64	124.51
31	2	621	LHG	O8-C23-C24	2.26	119.00	111.91
38	O	617	II0	C27-C25-C23	2.26	121.31	116.84
28	a	411	SQD	O8-S-C6	2.26	109.34	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	608	CLA	CHB-C4A-NA	2.26	127.63	124.51
37	O	612	KC2	CAA-CBA-CGA	-2.26	115.67	127.26
27	C	531	WVN	C03-C04-C09	-2.26	108.25	112.00
38	1	618	II0	C19-C13-C11	2.25	118.53	114.36
31	Z	103	LHG	O8-C23-C24	2.25	118.98	111.91
37	4	605	KC2	CAB-C3B-C2B	2.25	136.03	128.60
25	b	602	CLA	CHD-C1D-ND	-2.25	122.38	124.45
38	R	617	II0	C18-C04-C10	-2.25	106.89	110.47
37	Q	605	KC2	CAB-C3B-C2B	2.25	136.02	128.60
25	a	403	CLA	CHB-C4A-NA	2.25	127.63	124.51
38	S	617	II0	C27-C25-C23	2.25	121.30	116.84
25	P	611	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	a	403	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	c	519	CLA	CHD-C1D-ND	-2.25	122.39	124.45
31	2	621	LHG	C5-O7-C7	-2.25	112.25	117.79
31	O	621	LHG	O8-C23-C24	2.25	118.96	111.91
38	O	619	II0	C06-C04-C10	2.25	114.17	109.62
34	w	134	LMG	O8-C28-O10	-2.25	117.92	123.59
37	2	612	KC2	CAA-CBA-CGA	-2.25	115.72	127.26
38	5	617	II0	C18-C04-C10	-2.25	106.90	110.47
25	N	609	CLA	CHD-C1D-ND	-2.24	122.39	124.45
37	1	605	KC2	CBD-CHA-C1A	2.24	133.06	128.88
25	1	606	CLA	C1-C2-C3	-2.24	123.12	126.75
25	S	603	CLA	C1-C2-C3	-2.24	122.16	126.04
38	6	617	II0	C27-C25-C23	2.24	121.28	116.84
27	y	89	WVN	C30-C33-C34	-2.24	120.12	126.42
31	z	103	LHG	O8-C23-C24	2.24	118.94	111.91
27	A	407	WVN	C26-C29-C31	-2.24	116.22	123.22
38	P	618	II0	C31-C33-C35	-2.24	120.12	126.42
34	z	102	LMG	C8-O7-C10	-2.24	112.28	117.79
38	6	618	II0	C31-C33-C35	-2.24	120.12	126.42
38	4	619	II0	C31-C29-C25	-2.24	120.08	126.58
37	N	612	KC2	CAB-C3B-C4B	-2.24	119.49	124.90
25	A	403	CLA	CHB-C4A-NA	2.24	127.61	124.51
31	C	535	LHG	C6-C5-C4	-2.24	106.50	111.79
25	D	404	CLA	CHD-C1D-ND	-2.24	122.40	124.45
38	P	618	II0	C19-C13-C11	2.24	118.50	114.36
37	1	613	KC2	C3B-C2B-C1B	-2.24	104.94	107.08
25	R	615	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	B	610	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	g	301	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
25	6	615	CLA	CHB-C4A-NA	2.23	127.60	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	g	303	LMG	C8-O7-C10	-2.23	112.29	117.79
38	3	617	II0	C05-C07-C11	-2.23	107.25	110.30
27	Y	89	WVN	C14-C15-C13	-2.23	119.49	122.73
27	a	407	WVN	C38-C34-C33	2.23	121.59	118.08
31	O	621	LHG	C5-O7-C7	-2.23	112.29	117.79
27	C	531	WVN	C06-C13-C15	-2.23	119.47	122.61
31	R	621	LHG	C5-O7-C7	-2.23	112.30	117.79
25	N	606	CLA	C1-C2-C3	-2.23	123.14	126.75
37	N	605	KC2	CBD-CHA-C1A	2.23	133.04	128.88
25	B	603	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	5	615	CLA	CHD-C1D-ND	-2.23	122.40	124.45
38	2	619	II0	C06-C04-C10	2.23	114.14	109.62
27	c	529	WVN	C20-C23-C25	-2.23	122.86	126.23
38	3	617	II0	C18-C04-C10	-2.23	106.93	110.47
29	A	409	PL9	O2-C1-C6	2.23	124.45	120.59
36	e	102	HEM	CHA-C4D-C3D	-2.23	121.15	125.33
25	N	607	CLA	CHB-C4A-NA	2.23	127.59	124.51
28	a	408	SQD	O7-S-C6	2.23	109.58	106.94
25	5	615	CLA	CHB-C4A-NA	2.23	127.59	124.51
37	4	611	KC2	CAA-CBA-CGA	-2.22	115.83	127.26
25	2	615	CLA	CHD-C1D-ND	-2.22	122.41	124.45
27	c	529	WVN	C23-C20-C13	-2.22	120.96	127.20
38	S	618	II0	C31-C33-C35	-2.22	120.17	126.42
25	b	608	CLA	CHB-C4A-NA	2.22	127.58	124.51
37	1	612	KC2	CAB-C3B-C4B	-2.22	119.53	124.90
37	P	606	KC2	CAA-CBA-CGA	-2.22	115.85	127.26
31	5	621	LHG	C5-O7-C7	-2.22	112.32	117.79
25	S	611	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	b	606	CLA	CHD-C1D-ND	-2.22	122.42	124.45
25	N	602	CLA	CHD-C1D-ND	-2.22	122.42	124.45
25	6	611	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	B	609	CLA	CHD-C1D-ND	-2.22	122.42	124.45
39	N	620	IHT	C22-C18-C07	-2.22	120.97	127.20
37	Q	611	KC2	CAA-CBA-CGA	-2.22	115.87	127.26
37	N	613	KC2	C3B-C2B-C1B	-2.22	104.96	107.08
29	a	409	PL9	O2-C1-C6	2.22	124.43	120.59
25	O	615	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	5	606	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
37	3	606	KC2	CAA-CBA-CGA	-2.21	115.88	127.26
25	B	613	CLA	CHD-C1D-ND	-2.21	122.42	124.45
38	2	616	II0	C41-C42-C40	-2.21	118.94	123.47
38	N	617	II0	C17-C04-C06	-2.21	99.11	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	620	WVN	C24-C22-C19	2.21	121.56	118.08
25	A	406	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	R	615	CLA	CHB-C4A-NA	2.21	127.57	124.51
28	a	408	SQD	O8-S-C6	2.21	109.27	105.74
38	1	618	II0	C20-C14-C12	2.21	118.45	114.36
34	b	620	LMG	O8-C28-C29	2.21	118.85	111.91
25	d	404	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	R	606	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
27	D	408	WVN	C14-C15-C13	-2.21	119.52	122.73
25	6	603	CLA	CHD-C1D-ND	-2.21	122.42	124.45
38	O	617	II0	C03-C09-C13	-2.21	119.52	122.63
38	R	616	II0	C31-C33-C35	-2.21	120.21	126.42
38	1	617	II0	C17-C04-C06	-2.21	99.14	109.05
38	O	616	II0	C41-C42-C40	-2.21	118.95	123.47
38	4	618	II0	C31-C33-C35	-2.21	120.22	126.42
25	B	607	CLA	CHD-C1D-ND	-2.21	122.43	124.45
37	4	612	KC2	CAB-C3B-C2B	2.21	135.87	128.60
34	B	620	LMG	O8-C28-C29	2.21	118.83	111.91
25	a	406	CLA	CHD-C1D-ND	-2.20	122.43	124.45
25	B	606	CLA	CHD-C1D-ND	-2.20	122.43	124.45
38	P	617	II0	C18-C04-C10	-2.20	106.96	110.47
25	b	603	CLA	CHB-C4A-NA	2.20	127.56	124.51
29	d	405	PL9	O1-C4-C3	-2.20	118.29	120.72
25	B	611	CLA	CHB-C4A-NA	2.20	127.56	124.51
28	A	408	SQD	O8-S-C6	2.20	109.25	105.74
38	N	618	II0	C20-C14-C12	2.20	118.43	114.36
27	S	620	WVN	C21-C15-C14	2.20	117.84	113.62
25	B	601	CLA	CHD-C1D-ND	-2.20	122.43	124.45
25	R	609	CLA	CHD-C1D-ND	-2.20	122.43	124.45
38	Q	617	II0	C30-C32-C34	-2.20	116.35	123.22
37	Q	612	KC2	CAB-C3B-C2B	2.20	135.85	128.60
25	B	602	CLA	O2D-CGD-CBD	2.20	115.18	111.27
38	4	617	II0	C30-C32-C34	-2.20	116.35	123.22
25	b	602	CLA	O2D-CGD-CBD	2.20	115.17	111.27
39	1	620	IHT	C22-C18-C07	-2.20	121.03	127.20
25	B	611	CLA	C1-C2-C3	-2.20	122.24	126.04
38	5	616	II0	C31-C33-C35	-2.20	120.25	126.42
25	b	611	CLA	CHB-C4A-NA	2.19	127.55	124.51
37	1	605	KC2	CAA-CBA-CGA	-2.19	115.98	127.26
37	Q	611	KC2	CAB-C3B-C2B	2.19	135.83	128.60
25	O	602	CLA	C1-C2-C3	-2.19	122.25	126.04
37	4	611	KC2	CAB-C3B-C2B	2.19	135.83	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	601	CLA	O2D-CGD-CBD	2.19	115.17	111.27
25	B	605	CLA	C1-C2-C3	-2.19	122.25	126.04
25	R	602	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
39	Q	620	IHT	C22-C23-C27	2.19	122.30	118.94
25	5	609	CLA	CHD-C1D-ND	-2.19	122.44	124.45
28	A	411	SQD	O7-S-C6	2.19	109.54	106.94
38	P	617	II0	C27-C25-C23	2.19	121.18	116.84
25	C	516	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	B	614	CLA	CHD-C1D-ND	-2.19	122.44	124.45
28	A	411	SQD	C45-O47-C7	-2.19	112.40	117.79
37	6	606	KC2	CAA-CBA-CGA	-2.19	116.03	127.26
38	Q	618	II0	C18-C04-C10	-2.19	106.99	110.47
25	N	615	CLA	CHB-C4A-NA	2.19	127.53	124.51
27	C	530	WVN	C12-C14-C15	-2.18	110.18	114.08
25	b	609	CLA	CHB-C4A-NA	2.18	127.53	124.51
37	N	605	KC2	CAA-CBA-CGA	-2.18	116.04	127.26
27	P	620	WVN	C24-C22-C19	2.18	121.52	118.08
25	P	615	CLA	CHD-C1D-ND	-2.18	122.45	124.45
38	Q	618	II0	C31-C33-C35	-2.18	120.28	126.42
25	5	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
34	Z	102	LMG	C8-O7-C10	-2.18	112.42	117.79
37	1	612	KC2	CAA-CBA-CGA	-2.18	116.06	127.26
38	N	619	II0	C30-C32-C34	-2.18	116.41	123.22
25	g	302	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
25	C	520	CLA	O2D-CGD-CBD	2.18	115.14	111.27
38	1	619	II0	C30-C32-C34	-2.18	116.42	123.22
25	B	612	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
37	1	613	KC2	CAA-CBA-CGA	-2.18	116.08	127.26
38	O	618	II0	C32-C30-C26	-2.17	120.27	126.58
25	b	613	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	b	611	CLA	C1-C2-C3	-2.17	122.28	126.04
25	5	607	CLA	CHB-C4A-NA	2.17	127.52	124.51
37	Q	605	KC2	CMB-C2B-C1B	2.17	128.54	124.71
25	O	607	CLA	CHD-C1D-ND	-2.17	122.46	124.45
39	2	620	IHT	C39-C35-C38	-2.17	119.88	122.92
25	6	609	CLA	O1D-CGD-CBD	2.17	128.93	124.48
39	N	620	IHT	C20-C15-C11	-2.17	121.40	124.35
38	2	618	II0	C32-C30-C26	-2.17	120.28	126.58
37	N	612	KC2	CAA-CBA-CGA	-2.17	116.10	127.26
25	P	603	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
38	O	616	II0	C30-C32-C34	-2.17	116.44	123.22
27	d	408	WVN	C10-C06-C13	2.17	113.82	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	407	WVN	C30-C33-C34	-2.17	120.32	126.42
38	4	618	II0	C18-C04-C10	-2.17	107.02	110.47
27	y	89	WVN	C14-C15-C13	-2.17	119.58	122.73
26	a	405	PHO	CMC-C2C-C3C	2.17	129.03	124.94
25	3	603	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
38	P	617	II0	C05-C07-C11	-2.17	107.34	110.30
25	B	609	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
37	4	605	KC2	CMB-C2B-C1B	2.17	128.53	124.71
27	C	529	WVN	C40-C39-C36	-2.17	119.03	123.47
25	b	616	CLA	CHD-C1D-ND	-2.17	122.46	124.45
38	4	616	II0	C38-C36-C34	2.17	121.49	118.08
25	b	609	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	b	612	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	B	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
27	b	618	WVN	C38-C34-C37	-2.17	119.89	122.92
38	S	619	II0	C32-C30-C26	-2.17	120.29	126.58
28	A	408	SQD	O9-S-C6	2.16	109.51	106.94
39	Q	620	IHT	C31-C34-C35	-2.16	120.33	126.42
25	B	609	CLA	CHB-C4A-NA	2.16	127.50	124.51
25	c	526	CLA	CHD-C1D-ND	-2.16	122.47	124.45
38	S	616	II0	C18-C04-C10	-2.16	107.03	110.47
36	E	102	HEM	C4D-ND-C1D	2.16	107.31	105.07
25	2	607	CLA	CHB-C4A-NA	2.16	127.50	124.51
37	N	613	KC2	CAA-CBA-CGA	-2.16	116.14	127.26
28	a	411	SQD	C45-O47-C7	-2.16	112.47	117.79
28	a	408	SQD	O9-S-C6	2.16	109.51	106.94
38	2	617	II0	C32-C30-C26	-2.16	120.31	126.58
25	G	301	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	d	401	PHO	CMC-C2C-C3C	2.16	129.01	124.94
25	b	614	CLA	CHD-C1D-ND	-2.16	122.47	124.45
38	2	616	II0	C30-C32-C34	-2.16	116.48	123.22
27	c	529	WVN	C29-C31-C32	-2.16	120.36	126.42
39	4	620	IHT	C22-C23-C27	2.16	122.25	118.94
25	b	609	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	a	411	SQD	O7-S-C6	2.16	109.50	106.94
37	6	612	KC2	CMB-C2B-C1B	2.16	128.51	124.71
28	A	408	SQD	C45-O47-C7	-2.16	112.48	117.79
25	2	602	CLA	C1-C2-C3	-2.15	122.32	126.04
26	D	401	PHO	CMC-C2C-C3C	2.15	129.00	124.94
25	2	601	CLA	O2D-CGD-CBD	2.15	115.09	111.27
25	b	611	CLA	CHD-C1D-ND	-2.15	122.48	124.45
38	6	616	II0	C18-C04-C10	-2.15	107.05	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	6	606	KC2	CAC-C3C-C4C	2.15	134.48	124.47
27	3	620	WVN	C03-C04-C09	-2.15	108.43	112.00
27	6	620	WVN	C21-C15-C14	2.15	117.74	113.62
38	Q	616	II0	C38-C36-C34	2.15	121.46	118.08
39	N	620	IHT	C17-C03-C05	2.15	118.69	109.05
26	D	401	PHO	O2A-CGA-O1A	-2.15	118.17	123.59
38	O	617	II0	C32-C30-C26	-2.15	120.35	126.58
28	a	408	SQD	C45-O47-C7	-2.14	112.51	117.79
37	O	612	KC2	O2D-CGD-O1D	-2.14	119.65	123.84
25	b	601	CLA	C1-C2-C3	-2.14	123.28	126.75
25	2	607	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	C	520	CLA	CHD-C1D-ND	-2.14	122.48	124.45
27	A	407	WVN	C35-C32-C31	2.14	121.45	118.08
25	g	301	CLA	C1-C2-C3	-2.14	122.34	126.04
38	3	617	II0	C41-C42-C40	-2.14	119.09	123.47
38	P	617	II0	C29-C31-C33	-2.14	116.54	123.22
27	B	619	WVN	C21-C15-C14	2.14	117.72	113.62
25	A	404	CLA	C2D-C1D-ND	-2.14	108.53	110.10
27	c	530	WVN	C28-C30-C33	-2.14	116.55	123.22
37	S	612	KC2	CMB-C2B-C1B	2.14	128.48	124.71
38	O	619	II0	C31-C29-C25	-2.14	120.38	126.58
38	O	619	II0	C04-C10-C14	-2.14	119.62	122.63
29	A	409	PL9	O2-C1-C2	-2.14	116.89	121.78
31	5	621	LHG	C6-C5-C4	-2.14	106.74	111.79
25	1	615	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	C	520	CLA	C1-C2-C3	-2.14	122.35	126.04
37	2	612	KC2	CMB-C2B-C1B	2.14	128.48	124.71
38	P	617	II0	C41-C42-C40	-2.13	119.10	123.47
25	B	616	CLA	CHD-C1D-ND	-2.13	122.49	124.45
26	A	405	PHO	CMC-C2C-C3C	2.13	128.96	124.94
27	P	620	WVN	C03-C04-C09	-2.13	108.46	112.00
38	2	619	II0	C31-C29-C25	-2.13	120.39	126.58
25	P	613	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	4	603	CLA	C1-C2-C3	-2.13	122.36	126.04
27	b	618	WVN	C39-C40-C37	-2.13	119.11	123.47
25	C	528	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	4	620	IHT	C41-C40-C37	-2.13	119.11	123.47
25	B	601	CLA	C1-C2-C3	-2.13	123.31	126.75
38	3	617	II0	C29-C31-C33	-2.13	116.58	123.22
37	2	612	KC2	O2D-CGD-O1D	-2.13	119.68	123.84
25	N	606	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	6	615	CLA	CHD-C1D-ND	-2.13	122.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	520	CLA	O2D-CGD-CBD	2.12	115.04	111.27
38	6	619	II0	C32-C30-C26	-2.12	120.41	126.58
38	4	618	II0	C30-C32-C34	-2.12	116.59	123.22
25	Q	603	CLA	C1-C2-C3	-2.12	122.37	126.04
37	1	613	KC2	CMB-C2B-C1B	2.12	128.45	124.71
31	R	621	LHG	C6-C5-C4	-2.12	106.77	111.79
25	b	605	CLA	C1-C2-C3	-2.12	122.38	126.04
26	d	401	PHO	O2A-CGA-O1A	-2.12	118.24	123.59
37	N	611	KC2	CAA-CBA-CGA	-2.12	116.37	127.26
37	O	612	KC2	CMB-C2B-C1B	2.12	128.44	124.71
25	1	615	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	6	613	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
37	5	612	KC2	CBD-CHA-C1A	2.12	132.83	128.88
25	N	615	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	N	609	CLA	O1D-CGD-CBD	2.11	128.81	124.48
25	5	607	CLA	C2D-C1D-ND	-2.11	108.55	110.10
38	2	619	II0	C04-C10-C14	-2.11	119.65	122.63
25	b	611	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	5	613	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
25	S	615	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	B	611	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
37	1	611	KC2	CAA-CBA-CGA	-2.11	116.41	127.26
25	1	606	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
39	R	620	IHT	C27-C30-C32	-2.11	116.63	123.22
27	a	407	WVN	C12-C14-C15	-2.11	110.31	114.08
37	N	613	KC2	CMB-C2B-C1B	2.11	128.43	124.71
35	h	90	DGD	C2G-O2G-C1B	-2.11	112.60	117.79
38	2	617	II0	C03-C09-C13	-2.11	119.66	122.63
25	2	606	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
29	D	405	PL9	O1-C4-C3	-2.11	118.40	120.72
38	1	617	II0	C05-C07-C11	-2.11	107.42	110.30
25	4	603	CLA	CAC-C3C-C4C	2.11	127.55	124.81
29	d	405	PL9	O2-C1-C6	2.11	124.24	120.59
25	Q	607	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	S	613	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
38	4	617	II0	C27-C25-C23	2.11	121.01	116.84
38	6	619	II0	C27-C25-C23	2.11	121.01	116.84
29	D	405	PL9	O2-C1-C6	2.10	124.23	120.59
38	N	617	II0	C05-C07-C11	-2.10	107.42	110.30
25	R	613	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
25	O	607	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	6	613	CLA	O1D-CGD-CBD	2.10	128.79	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	607	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	b	616	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
38	Q	618	II0	C30-C32-C34	-2.10	116.66	123.22
25	3	615	CLA	CHD-C1D-ND	-2.10	122.52	124.45
25	O	606	CLA	CHD-C1D-ND	-2.10	122.52	124.45
25	3	613	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	C	528	CLA	CHD-C1D-ND	-2.10	122.53	124.45
25	1	614	CLA	CHD-C1D-ND	-2.10	122.53	124.45
38	Q	619	II0	C19-C13-C11	2.10	118.24	114.36
27	c	530	WVN	C12-C14-C15	-2.10	110.33	114.08
25	2	606	CLA	CHD-C1D-ND	-2.10	122.53	124.45
39	5	620	IHT	C04-C02-C07	-2.10	107.25	110.48
35	H	90	DGD	C2G-O2G-C1B	-2.10	112.63	117.79
25	4	607	CLA	CHB-C4A-NA	2.10	127.41	124.51
27	h	89	WVN	C19-C22-C26	2.10	122.16	118.94
29	a	409	PL9	O2-C1-C2	-2.10	116.98	121.78
25	c	525	CLA	CHD-C1D-ND	-2.09	122.53	124.45
37	R	612	KC2	CBD-CHA-C1A	2.09	132.78	128.88
27	C	530	WVN	C26-C29-C31	-2.09	116.69	123.22
25	Q	603	CLA	CAC-C3C-C4C	2.09	127.53	124.81
27	3	620	WVN	C26-C29-C31	-2.09	116.69	123.22
34	m	101	LMG	O8-C28-O10	-2.09	118.31	123.59
34	W	134	LMG	O8-C28-O10	-2.09	118.32	123.59
25	5	609	CLA	O1D-CGD-CBD	2.09	128.76	124.48
25	S	613	CLA	O1D-CGD-CBD	2.09	128.75	124.48
25	B	604	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
25	C	526	CLA	CHD-C1D-ND	-2.09	122.54	124.45
25	B	616	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	D	403	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	a	405	PHO	O2A-CGA-O1A	-2.08	118.33	123.59
38	P	618	II0	C27-C25-C23	2.08	120.97	116.84
25	O	606	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	b	604	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
25	O	613	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	5	603	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
27	P	620	WVN	C27-C25-C23	2.08	121.36	118.08
38	R	616	II0	C03-C09-C13	-2.08	119.70	122.63
25	c	527	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	R	603	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
38	4	619	II0	C17-C04-C06	-2.08	99.72	109.05
25	c	516	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	c	528	CLA	CHD-C1D-ND	-2.08	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Q	619	II0	C31-C29-C25	-2.08	120.55	126.58
25	C	527	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	C	529	WVN	C23-C25-C28	-2.08	115.75	118.94
25	6	601	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	S	601	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	S	611	CLA	CHD-C1D-ND	-2.08	122.55	124.45
38	5	616	II0	C03-C09-C13	-2.08	119.70	122.63
37	S	606	KC2	CAA-CBA-CGA	-2.08	116.59	127.26
26	A	405	PHO	O2A-CGA-O1A	-2.08	118.35	123.59
38	Q	617	II0	C27-C25-C23	2.07	120.95	116.84
37	4	605	KC2	CAA-CBA-CGA	-2.07	116.60	127.26
38	R	617	II0	C29-C31-C33	-2.07	116.74	123.22
25	a	404	CLA	C2D-C1D-ND	-2.07	108.58	110.10
37	Q	612	KC2	O2D-CGD-O1D	-2.07	119.78	123.84
39	R	620	IHT	C39-C35-C34	2.07	121.34	118.08
25	b	602	CLA	C1-C2-C3	-2.07	122.46	126.04
38	6	616	II0	C17-C04-C06	-2.07	99.74	109.05
38	6	617	II0	C32-C30-C26	-2.07	120.57	126.58
38	5	617	II0	C29-C31-C33	-2.07	116.75	123.22
25	S	603	CLA	C3A-C2A-C1A	2.07	104.44	101.34
38	S	616	II0	C17-C04-C06	-2.07	99.75	109.05
38	2	618	II0	C31-C29-C25	-2.07	120.57	126.58
37	N	605	KC2	C2B-C1B-NB	2.07	111.63	110.10
38	5	618	II0	C04-C10-C14	-2.07	119.71	122.63
27	P	620	WVN	C26-C29-C31	-2.07	116.76	123.22
38	Q	619	II0	C17-C04-C06	-2.07	99.75	109.05
25	c	528	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	d	403	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
37	Q	605	KC2	CAA-CBA-CGA	-2.07	116.63	127.26
38	Q	619	II0	C04-C10-C14	-2.07	119.71	122.63
38	Q	618	II0	C20-C14-C12	2.07	118.19	114.36
25	B	601	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	N	614	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	2	609	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
38	N	616	II0	C17-C04-C06	-2.06	99.78	109.05
25	2	613	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
34	d	402	LMG	C8-O7-C10	-2.06	112.71	117.79
27	a	407	WVN	C06-C13-C20	2.06	121.61	115.78
38	N	616	II0	C30-C32-C34	-2.06	116.78	123.22
38	S	617	II0	C32-C30-C26	-2.06	120.59	126.58
25	c	520	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	B	602	CLA	C1-C2-C3	-2.06	122.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	619	II0	C04-C06-C08	-2.06	108.99	113.64
27	c	529	WVN	C39-C40-C37	-2.06	119.25	123.47
25	c	523	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	a	409	PL9	O1-C4-C3	-2.06	118.45	120.72
27	3	620	WVN	C27-C25-C23	2.06	121.32	118.08
37	S	606	KC2	CAC-C3C-C4C	2.06	134.06	124.47
29	A	409	PL9	O1-C4-C3	-2.06	118.45	120.72
38	1	616	II0	C17-C04-C06	-2.06	99.81	109.05
25	P	612	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
38	N	619	II0	C04-C06-C08	-2.06	109.00	113.64
25	4	606	CLA	C1-C2-C3	-2.06	122.48	126.04
37	4	612	KC2	O2D-CGD-O1D	-2.06	119.82	123.84
25	B	612	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
25	Q	603	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
25	6	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	B	606	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
27	a	407	WVN	C29-C31-C32	-2.06	120.64	126.42
38	6	617	II0	C17-C04-C06	-2.05	99.83	109.05
25	c	519	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	B	610	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
39	2	620	IHT	C39-C35-C34	2.05	121.31	118.08
39	Q	620	IHT	C39-C35-C34	2.05	121.31	118.08
38	S	617	II0	C17-C04-C06	-2.05	99.83	109.05
25	1	603	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	5	604	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
36	E	102	HEM	CHB-C1B-C2B	-2.05	121.04	126.72
25	2	601	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	C	523	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	6	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	S	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
37	N	611	KC2	CAB-C3B-C2B	2.05	135.36	128.60
25	R	609	CLA	O1D-CGD-CBD	2.05	128.68	124.48
29	D	405	PL9	O2-C1-C2	-2.05	117.08	121.78
29	D	405	PL9	C36-C34-C33	-2.05	116.97	121.12
25	b	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
38	6	619	II0	C17-C04-C06	-2.05	99.85	109.05
37	1	611	KC2	CAB-C3B-C2B	2.05	135.35	128.60
38	S	618	II0	C31-C29-C25	-2.05	120.63	126.58
25	3	612	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
38	S	619	II0	C17-C04-C06	-2.05	99.86	109.05
38	4	619	II0	C04-C10-C14	-2.05	119.74	122.63
34	M	101	LMG	O8-C28-O10	-2.05	118.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	601	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
37	3	606	KC2	C3D-CAD-CBD	-2.05	104.91	107.61
38	6	618	II0	C31-C29-C25	-2.05	120.64	126.58
25	3	603	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
27	6	620	WVN	C07-C01-C02	-2.05	106.45	109.55
25	C	522	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	R	607	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	4	613	CLA	O1D-CGD-CBD	2.05	128.67	124.48
25	C	519	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
38	R	617	II0	C17-C04-C06	-2.04	99.87	109.05
29	d	405	PL9	O2-C1-C2	-2.04	117.10	121.78
29	d	405	PL9	C36-C34-C33	-2.04	116.98	121.12
25	C	521	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	P	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	4	603	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
37	P	606	KC2	C3D-CAD-CBD	-2.04	104.92	107.61
27	b	619	WVN	C06-C13-C20	-2.04	110.00	115.78
25	4	613	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	b	601	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	P	603	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
37	R	612	KC2	CMB-C2B-C1B	2.04	128.31	124.71
25	b	606	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
27	Y	89	WVN	C40-C39-C36	-2.04	119.30	123.47
38	6	618	II0	C20-C14-C12	2.04	118.13	114.36
38	5	617	II0	C17-C04-C06	-2.04	99.90	109.05
25	R	604	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	3	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	c	521	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
27	B	618	WVN	C21-C15-C14	2.04	117.53	113.62
38	1	616	II0	C30-C32-C34	-2.04	116.86	123.22
25	Q	606	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	1	614	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
38	P	617	II0	C17-C04-C06	-2.03	99.91	109.05
38	O	618	II0	C19-C13-C11	2.03	118.12	114.36
38	3	617	II0	C17-C04-C06	-2.03	99.92	109.05
27	c	529	WVN	C27-C25-C23	2.03	121.28	118.08
37	5	612	KC2	CAB-C3B-C4B	-2.03	119.98	124.90
25	b	601	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	D	400	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
38	Q	618	II0	C31-C29-C25	-2.03	120.68	126.58
38	4	618	II0	C20-C14-C12	2.03	118.12	114.36
27	y	89	WVN	C23-C20-C13	-2.03	121.50	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	609	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	B	606	CLA	C1-C2-C3	-2.03	122.53	126.04
25	R	607	CLA	C2D-C1D-ND	-2.03	108.61	110.10
39	2	620	IHT	C17-C03-C05	2.03	118.16	109.05
29	a	409	PL9	C12-C13-C14	-2.03	122.78	127.66
39	O	620	IHT	C17-C03-C05	2.03	118.15	109.05
25	O	609	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
37	3	606	KC2	CAB-C3B-C2B	2.03	135.28	128.60
38	O	616	II0	C17-C04-C06	-2.03	99.95	109.05
37	1	605	KC2	C2B-C1B-NB	2.03	111.60	110.10
39	1	620	IHT	C30-C32-C33	-2.03	120.72	126.42
38	S	618	II0	C20-C14-C12	2.03	118.11	114.36
37	P	606	KC2	CAB-C3B-C2B	2.03	135.28	128.60
25	B	612	CLA	C3A-C2A-C1A	2.02	104.37	101.34
25	3	611	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	3	612	CLA	C1-C2-C3	-2.02	122.55	126.04
38	R	618	II0	C04-C10-C14	-2.02	119.78	122.63
25	3	609	CLA	O1D-CGD-CBD	2.02	128.62	124.48
25	C	523	CLA	CHD-C1D-ND	-2.02	122.60	124.45
27	H	89	WVN	C19-C22-C26	2.02	122.04	118.94
38	5	616	II0	C17-C04-C06	-2.02	99.97	109.05
25	N	614	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	5	607	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	b	607	CLA	C1-C2-C3	-2.02	122.55	126.04
25	P	612	CLA	C1-C2-C3	-2.02	122.55	126.04
25	C	517	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
37	R	612	KC2	CAB-C3B-C4B	-2.02	120.02	124.90
25	C	516	CLA	CHD-C1D-ND	-2.02	122.60	124.45
38	3	617	II0	C32-C30-C26	-2.02	120.72	126.58
25	Q	613	CLA	O1D-CGD-CBD	2.02	128.61	124.48
25	2	611	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	1	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	5	601	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
27	b	619	WVN	C03-C04-C09	-2.02	108.65	112.00
25	B	614	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	2	613	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	P	609	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	A	409	PL9	C12-C13-C14	-2.02	122.81	127.66
25	C	524	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
25	b	604	CLA	C1-C2-C3	-2.02	122.56	126.04
25	c	523	CLA	CHD-C1D-ND	-2.01	122.60	124.45
25	O	611	CLA	O2A-CGA-O1A	-2.01	118.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	615	CLA	O1A-CGA-CBA	2.01	129.55	123.08
38	2	616	II0	C17-C04-C06	-2.01	100.01	109.05
25	2	611	CLA	CHD-C1D-ND	-2.01	122.60	124.45
38	R	616	II0	C17-C04-C06	-2.01	100.01	109.05
25	b	608	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	b	615	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	2	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	P	611	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
38	2	618	II0	C17-C04-C06	-2.01	100.02	109.05
27	B	619	WVN	C19-C22-C26	-2.01	115.86	118.94
25	B	608	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	O	602	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	G	301	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	A	404	CLA	O2D-CGD-CBD	2.01	114.84	111.27
25	d	400	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
25	O	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
38	P	617	II0	C32-C30-C26	-2.01	120.75	126.58
37	R	612	KC2	C3D-CAD-CBD	-2.01	104.96	107.61
25	b	612	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
27	c	530	WVN	C03-C04-C09	-2.01	108.67	112.00
38	O	618	II0	C17-C04-C06	-2.01	100.05	109.05
25	Q	609	CLA	O1D-CGD-CBD	2.00	128.59	124.48
25	3	609	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	a	404	CLA	O2D-CGD-CBD	2.00	114.83	111.27
38	R	617	II0	C27-C25-C23	2.00	120.81	116.84
25	c	517	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	N	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	R	601	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	6	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
27	b	619	WVN	C26-C29-C31	-2.00	116.97	123.22
25	2	601	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	6	610	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	b	612	CLA	C3A-C2A-C1A	2.00	104.33	101.34
37	5	612	KC2	CMB-C2B-C1B	2.00	128.24	124.71

All (190) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	a	403	CLA	ND
25	a	404	CLA	ND
25	a	406	CLA	ND
25	b	601	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	516	CLA	ND
25	c	517	CLA	ND
25	c	518	CLA	ND
25	c	519	CLA	ND
25	c	520	CLA	ND
25	c	521	CLA	ND
25	c	522	CLA	ND
25	c	523	CLA	ND
25	c	524	CLA	ND
25	c	525	CLA	ND
25	c	526	CLA	ND
25	c	527	CLA	ND
25	c	528	CLA	ND
25	d	400	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND
25	g	301	CLA	ND
25	g	302	CLA	ND
25	A	403	CLA	ND
25	A	404	CLA	ND
25	A	406	CLA	ND
25	B	601	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	516	CLA	ND
25	C	517	CLA	ND
25	C	518	CLA	ND
25	C	519	CLA	ND
25	C	520	CLA	ND
25	C	521	CLA	ND
25	C	522	CLA	ND
25	C	523	CLA	ND
25	C	524	CLA	ND
25	C	525	CLA	ND
25	C	526	CLA	ND
25	C	527	CLA	ND
25	C	528	CLA	ND
25	D	400	CLA	ND
25	D	403	CLA	ND
25	D	404	CLA	ND
25	2	601	CLA	ND
25	2	602	CLA	ND
25	2	603	CLA	ND
25	2	604	CLA	ND
25	2	606	CLA	ND
25	2	607	CLA	ND
25	2	609	CLA	ND
25	2	610	CLA	ND
25	2	611	CLA	ND
25	2	613	CLA	ND
25	2	615	CLA	ND
25	3	601	CLA	ND
25	3	602	CLA	ND
25	3	603	CLA	ND
25	3	609	CLA	ND
25	3	610	CLA	ND
25	3	611	CLA	ND
25	3	612	CLA	ND

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Mol	Chain	Res	Type	Atom
25	3	613	CLA	ND
25	3	615	CLA	ND
25	4	602	CLA	ND
25	4	603	CLA	ND
25	4	604	CLA	ND
25	4	606	CLA	ND
25	4	607	CLA	ND
25	4	609	CLA	ND
25	4	610	CLA	ND
25	4	613	CLA	ND
25	4	615	CLA	ND
25	5	601	CLA	ND
25	5	602	CLA	ND
25	5	603	CLA	ND
25	5	604	CLA	ND
25	5	606	CLA	ND
25	5	607	CLA	ND
25	5	609	CLA	ND
25	5	610	CLA	ND
25	5	611	CLA	ND
25	5	613	CLA	ND
25	5	615	CLA	ND
25	6	601	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND
25	6	604	CLA	ND
25	6	609	CLA	ND
25	6	610	CLA	ND
25	6	611	CLA	ND
25	6	613	CLA	ND
25	6	615	CLA	ND
25	G	301	CLA	ND
25	G	302	CLA	ND
25	1	601	CLA	ND
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	604	CLA	ND
25	1	606	CLA	ND
25	1	607	CLA	ND
25	1	609	CLA	ND
25	1	610	CLA	ND
25	1	614	CLA	ND

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Mol	Chain	Res	Type	Atom
25	1	615	CLA	ND
25	O	601	CLA	ND
25	O	602	CLA	ND
25	O	603	CLA	ND
25	O	604	CLA	ND
25	O	606	CLA	ND
25	O	607	CLA	ND
25	O	609	CLA	ND
25	O	610	CLA	ND
25	O	611	CLA	ND
25	O	613	CLA	ND
25	O	615	CLA	ND
25	P	601	CLA	ND
25	P	602	CLA	ND
25	P	603	CLA	ND
25	P	609	CLA	ND
25	P	610	CLA	ND
25	P	611	CLA	ND
25	P	612	CLA	ND
25	P	613	CLA	ND
25	P	615	CLA	ND
25	Q	602	CLA	ND
25	Q	603	CLA	ND
25	Q	604	CLA	ND
25	Q	606	CLA	ND
25	Q	607	CLA	ND
25	Q	609	CLA	ND
25	Q	610	CLA	ND
25	Q	613	CLA	ND
25	Q	615	CLA	ND
25	R	601	CLA	ND
25	R	602	CLA	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	606	CLA	ND
25	R	607	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	613	CLA	ND
25	R	615	CLA	ND
25	S	601	CLA	ND

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Mol	Chain	Res	Type	Atom
25	S	602	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	609	CLA	ND
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	613	CLA	ND
25	S	615	CLA	ND
25	N	601	CLA	ND
25	N	602	CLA	ND
25	N	603	CLA	ND
25	N	604	CLA	ND
25	N	606	CLA	ND
25	N	607	CLA	ND
25	N	609	CLA	ND
25	N	610	CLA	ND
25	N	614	CLA	ND
25	N	615	CLA	ND

All (3039) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	a	404	CLA	C1A-C2A-CAA-CBA
25	a	404	CLA	C3A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C3A-C2A-CAA-CBA
25	a	406	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CHA-CBD-CGD-O1D
25	b	601	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	602	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CAD-CBD-CGD-O1D
25	b	606	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
25	b	611	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C1A-C2A-CAA-CBA
25	c	516	CLA	C1A-C2A-CAA-CBA
25	c	516	CLA	CBD-CGD-O2D-CED
25	c	517	CLA	CHA-CBD-CGD-O1D
25	c	517	CLA	CHA-CBD-CGD-O2D
25	c	517	CLA	CAD-CBD-CGD-O1D
25	c	517	CLA	CBD-CGD-O2D-CED
25	c	525	CLA	O1A-CGA-O2A-C1
25	c	526	CLA	CHA-CBD-CGD-O1D
25	c	526	CLA	CAD-CBD-CGD-O1D
25	c	526	CLA	CAD-CBD-CGD-O2D
25	c	528	CLA	CHA-CBD-CGD-O2D
25	d	400	CLA	C1A-C2A-CAA-CBA
25	d	400	CLA	C3A-C2A-CAA-CBA
25	d	404	CLA	CHA-CBD-CGD-O1D
25	d	404	CLA	CAD-CBD-CGD-O1D
25	d	404	CLA	CAD-CBD-CGD-O2D
25	A	404	CLA	C1A-C2A-CAA-CBA
25	A	404	CLA	C3A-C2A-CAA-CBA
25	A	406	CLA	C1A-C2A-CAA-CBA
25	A	406	CLA	C3A-C2A-CAA-CBA
25	A	406	CLA	CBD-CGD-O2D-CED
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	B	611	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	615	CLA	C1A-C2A-CAA-CBA
25	B	615	CLA	C3A-C2A-CAA-CBA
25	C	516	CLA	C1A-C2A-CAA-CBA
25	C	516	CLA	CBD-CGD-O2D-CED
25	C	517	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	517	CLA	CHA-CBD-CGD-O2D
25	C	517	CLA	CAD-CBD-CGD-O1D
25	C	517	CLA	CBD-CGD-O2D-CED
25	C	526	CLA	CHA-CBD-CGD-O1D
25	C	526	CLA	CAD-CBD-CGD-O1D
25	C	526	CLA	CAD-CBD-CGD-O2D
25	C	528	CLA	CHA-CBD-CGD-O1D
25	C	528	CLA	CHA-CBD-CGD-O2D
25	C	528	CLA	C3-C5-C6-C7
25	D	400	CLA	C1A-C2A-CAA-CBA
25	D	400	CLA	C3A-C2A-CAA-CBA
25	D	404	CLA	CHA-CBD-CGD-O1D
25	D	404	CLA	CAD-CBD-CGD-O1D
25	D	404	CLA	CAD-CBD-CGD-O2D
25	2	602	CLA	CHA-CBD-CGD-O1D
25	2	602	CLA	CHA-CBD-CGD-O2D
25	2	606	CLA	C1A-C2A-CAA-CBA
25	2	606	CLA	C3A-C2A-CAA-CBA
25	2	610	CLA	C1A-C2A-CAA-CBA
25	2	610	CLA	C3A-C2A-CAA-CBA
25	2	610	CLA	CHA-CBD-CGD-O1D
25	2	610	CLA	CHA-CBD-CGD-O2D
25	2	611	CLA	C1A-C2A-CAA-CBA
25	2	611	CLA	CBD-CGD-O2D-CED
25	2	615	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C3A-C2A-CAA-CBA
25	3	611	CLA	C4-C3-C5-C6
25	3	613	CLA	C1A-C2A-CAA-CBA
25	3	613	CLA	C2-C3-C5-C6
25	3	613	CLA	C4-C3-C5-C6
25	3	615	CLA	C1A-C2A-CAA-CBA
25	3	615	CLA	C3A-C2A-CAA-CBA
25	4	606	CLA	C1A-C2A-CAA-CBA
25	4	606	CLA	C3A-C2A-CAA-CBA
25	4	609	CLA	C1A-C2A-CAA-CBA
25	4	609	CLA	C3A-C2A-CAA-CBA
25	4	613	CLA	C1A-C2A-CAA-CBA
25	4	613	CLA	C3A-C2A-CAA-CBA
25	4	613	CLA	CHA-CBD-CGD-O1D
25	4	613	CLA	CHA-CBD-CGD-O2D
25	4	613	CLA	CAD-CBD-CGD-O1D
25	4	613	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	4	615	CLA	CBD-CGD-O2D-CED
25	5	602	CLA	CHA-CBD-CGD-O1D
25	5	602	CLA	CHA-CBD-CGD-O2D
25	5	602	CLA	C2-C3-C5-C6
25	5	602	CLA	C4-C3-C5-C6
25	5	606	CLA	C1A-C2A-CAA-CBA
25	5	606	CLA	C3A-C2A-CAA-CBA
25	5	607	CLA	C1A-C2A-CAA-CBA
25	5	609	CLA	CHA-CBD-CGD-O1D
25	5	609	CLA	CHA-CBD-CGD-O2D
25	5	610	CLA	CHA-CBD-CGD-O1D
25	5	610	CLA	CBD-CGD-O2D-CED
25	5	613	CLA	C1A-C2A-CAA-CBA
25	5	613	CLA	CHA-CBD-CGD-O1D
25	5	613	CLA	CHA-CBD-CGD-O2D
25	6	602	CLA	CHA-CBD-CGD-O1D
25	6	602	CLA	CHA-CBD-CGD-O2D
25	6	603	CLA	C3A-C2A-CAA-CBA
25	6	604	CLA	CHA-CBD-CGD-O1D
25	6	604	CLA	CAD-CBD-CGD-O1D
25	6	604	CLA	CAD-CBD-CGD-O2D
25	6	609	CLA	C3A-C2A-CAA-CBA
25	6	610	CLA	CHA-CBD-CGD-O1D
25	6	610	CLA	CHA-CBD-CGD-O2D
25	6	611	CLA	C1A-C2A-CAA-CBA
25	6	611	CLA	C3A-C2A-CAA-CBA
25	6	611	CLA	CHA-CBD-CGD-O1D
25	6	611	CLA	CHA-CBD-CGD-O2D
25	6	611	CLA	C4-C3-C5-C6
25	6	613	CLA	CBD-CGD-O2D-CED
25	6	615	CLA	CBD-CGD-O2D-CED
25	1	602	CLA	CHA-CBD-CGD-O1D
25	1	602	CLA	CHA-CBD-CGD-O2D
25	1	604	CLA	CHA-CBD-CGD-O1D
25	1	604	CLA	CHA-CBD-CGD-O2D
25	1	604	CLA	CAD-CBD-CGD-O1D
25	1	607	CLA	CBD-CGD-O2D-CED
25	1	609	CLA	C1A-C2A-CAA-CBA
25	1	609	CLA	C3A-C2A-CAA-CBA
25	1	614	CLA	CBD-CGD-O2D-CED
25	1	615	CLA	C1A-C2A-CAA-CBA
25	1	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	O	602	CLA	CHA-CBD-CGD-O1D
25	O	602	CLA	CHA-CBD-CGD-O2D
25	O	606	CLA	C1A-C2A-CAA-CBA
25	O	606	CLA	C3A-C2A-CAA-CBA
25	O	610	CLA	C1A-C2A-CAA-CBA
25	O	610	CLA	C3A-C2A-CAA-CBA
25	O	610	CLA	CHA-CBD-CGD-O1D
25	O	610	CLA	CHA-CBD-CGD-O2D
25	O	611	CLA	C1A-C2A-CAA-CBA
25	O	611	CLA	CBD-CGD-O2D-CED
25	O	615	CLA	C1A-C2A-CAA-CBA
25	P	610	CLA	C3A-C2A-CAA-CBA
25	P	611	CLA	C4-C3-C5-C6
25	P	613	CLA	C1A-C2A-CAA-CBA
25	P	613	CLA	C2-C3-C5-C6
25	P	613	CLA	C4-C3-C5-C6
25	P	615	CLA	C1A-C2A-CAA-CBA
25	P	615	CLA	C3A-C2A-CAA-CBA
25	Q	606	CLA	CHA-CBD-CGD-O1D
25	Q	606	CLA	CHA-CBD-CGD-O2D
25	Q	609	CLA	C1A-C2A-CAA-CBA
25	Q	609	CLA	C3A-C2A-CAA-CBA
25	Q	613	CLA	C1A-C2A-CAA-CBA
25	Q	613	CLA	C3A-C2A-CAA-CBA
25	Q	613	CLA	CHA-CBD-CGD-O1D
25	Q	613	CLA	CHA-CBD-CGD-O2D
25	Q	613	CLA	CAD-CBD-CGD-O1D
25	Q	613	CLA	CAD-CBD-CGD-O2D
25	Q	615	CLA	CBD-CGD-O2D-CED
25	R	602	CLA	CHA-CBD-CGD-O1D
25	R	602	CLA	CHA-CBD-CGD-O2D
25	R	602	CLA	C2-C3-C5-C6
25	R	602	CLA	C4-C3-C5-C6
25	R	606	CLA	C1A-C2A-CAA-CBA
25	R	606	CLA	C3A-C2A-CAA-CBA
25	R	607	CLA	C1A-C2A-CAA-CBA
25	R	609	CLA	CHA-CBD-CGD-O1D
25	R	609	CLA	CHA-CBD-CGD-O2D
25	R	610	CLA	CHA-CBD-CGD-O1D
25	R	610	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	C1A-C2A-CAA-CBA
25	R	613	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	R	613	CLA	CHA-CBD-CGD-O2D
25	R	613	CLA	CAD-CBD-CGD-O1D
25	S	602	CLA	CHA-CBD-CGD-O1D
25	S	602	CLA	CHA-CBD-CGD-O2D
25	S	603	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	CHA-CBD-CGD-O1D
25	S	604	CLA	CAD-CBD-CGD-O1D
25	S	604	CLA	CAD-CBD-CGD-O2D
25	S	609	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C3A-C2A-CAA-CBA
25	S	609	CLA	C2A-CAA-CBA-CGA
25	S	610	CLA	CHA-CBD-CGD-O1D
25	S	610	CLA	CHA-CBD-CGD-O2D
25	S	611	CLA	C1A-C2A-CAA-CBA
25	S	611	CLA	C3A-C2A-CAA-CBA
25	S	611	CLA	CHA-CBD-CGD-O1D
25	S	611	CLA	CHA-CBD-CGD-O2D
25	S	611	CLA	C4-C3-C5-C6
25	S	613	CLA	CBD-CGD-O2D-CED
25	S	615	CLA	CBD-CGD-O2D-CED
25	N	602	CLA	CHA-CBD-CGD-O1D
25	N	602	CLA	CHA-CBD-CGD-O2D
25	N	604	CLA	CHA-CBD-CGD-O1D
25	N	604	CLA	CHA-CBD-CGD-O2D
25	N	604	CLA	CAD-CBD-CGD-O1D
25	N	607	CLA	CBD-CGD-O2D-CED
25	N	609	CLA	C1A-C2A-CAA-CBA
25	N	609	CLA	C3A-C2A-CAA-CBA
25	N	614	CLA	CBD-CGD-O2D-CED
25	N	615	CLA	C1A-C2A-CAA-CBA
25	N	615	CLA	CBD-CGD-O2D-CED
26	d	401	PHO	C2-C1-O2A-CGA
26	D	401	PHO	C2-C1-O2A-CGA
27	a	407	WVN	C11-C19-C22-C24
27	a	407	WVN	C11-C19-C22-C26
27	a	407	WVN	C30-C33-C34-C37
27	a	407	WVN	C30-C33-C34-C38
27	b	617	WVN	C11-C19-C22-C24
27	b	617	WVN	C11-C19-C22-C26
27	b	617	WVN	C20-C23-C25-C27
27	b	617	WVN	C20-C23-C25-C28
27	b	617	WVN	C22-C26-C29-C31

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Mol	Chain	Res	Type	Atoms
27	b	617	WVN	C29-C31-C32-C35
27	b	617	WVN	C29-C31-C32-C36
27	b	617	WVN	C30-C33-C34-C38
27	b	617	WVN	C32-C36-C39-C40
27	b	618	WVN	C11-C19-C22-C24
27	b	618	WVN	C11-C19-C22-C26
27	b	618	WVN	C22-C26-C29-C31
27	b	618	WVN	C29-C31-C32-C35
27	b	618	WVN	C29-C31-C32-C36
27	b	619	WVN	C15-C13-C20-C23
27	b	619	WVN	C29-C31-C32-C35
27	b	619	WVN	C30-C33-C34-C37
27	b	619	WVN	C30-C33-C34-C38
27	c	529	WVN	C15-C13-C20-C23
27	c	529	WVN	C29-C31-C32-C35
27	c	529	WVN	C29-C31-C32-C36
27	c	530	WVN	C01-C02-C11-C19
27	c	530	WVN	C15-C13-C20-C23
27	c	530	WVN	C22-C26-C29-C31
27	c	530	WVN	C29-C31-C32-C35
27	c	530	WVN	C29-C31-C32-C36
27	c	530	WVN	C30-C33-C34-C37
27	c	530	WVN	C30-C33-C34-C38
27	c	531	WVN	C15-C13-C20-C23
27	c	531	WVN	C11-C19-C22-C24
27	c	531	WVN	C11-C19-C22-C26
27	c	531	WVN	C22-C26-C29-C31
27	c	531	WVN	C30-C33-C34-C37
27	c	531	WVN	C30-C33-C34-C38
27	d	408	WVN	C15-C13-C20-C23
27	d	408	WVN	C20-C23-C25-C27
27	d	408	WVN	C20-C23-C25-C28
27	d	408	WVN	C29-C31-C32-C35
27	d	408	WVN	C29-C31-C32-C36
27	d	408	WVN	C30-C33-C34-C37
27	d	408	WVN	C30-C33-C34-C38
27	h	89	WVN	C15-C13-C20-C23
27	h	89	WVN	C29-C31-C32-C35
27	h	89	WVN	C29-C31-C32-C36
27	h	89	WVN	C30-C33-C34-C37
27	h	89	WVN	C30-C33-C34-C38
27	y	89	WVN	C15-C13-C20-C23

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Mol	Chain	Res	Type	Atoms
27	A	407	WVN	C06-C13-C20-C23
27	A	407	WVN	C15-C13-C20-C23
27	B	617	WVN	C06-C13-C20-C23
27	B	617	WVN	C15-C13-C20-C23
27	B	617	WVN	C20-C23-C25-C27
27	B	617	WVN	C20-C23-C25-C28
27	B	617	WVN	C29-C31-C32-C35
27	B	617	WVN	C29-C31-C32-C36
27	B	618	WVN	C15-C13-C20-C23
27	B	618	WVN	C11-C19-C22-C24
27	B	618	WVN	C11-C19-C22-C26
27	B	618	WVN	C22-C26-C29-C31
27	B	618	WVN	C29-C31-C32-C35
27	B	618	WVN	C29-C31-C32-C36
27	B	618	WVN	C30-C33-C34-C38
27	B	619	WVN	C11-C19-C22-C24
27	B	619	WVN	C11-C19-C22-C26
27	C	529	WVN	C15-C13-C20-C23
27	C	529	WVN	C11-C19-C22-C24
27	C	529	WVN	C11-C19-C22-C26
27	C	529	WVN	C30-C33-C34-C38
27	C	529	WVN	C34-C37-C40-C39
27	C	530	WVN	C01-C02-C11-C19
27	C	530	WVN	C15-C13-C20-C23
27	C	530	WVN	C22-C26-C29-C31
27	C	530	WVN	C29-C31-C32-C35
27	C	530	WVN	C29-C31-C32-C36
27	C	530	WVN	C30-C33-C34-C37
27	C	530	WVN	C30-C33-C34-C38
27	C	531	WVN	C15-C13-C20-C23
27	C	531	WVN	C20-C23-C25-C27
27	C	531	WVN	C20-C23-C25-C28
27	C	531	WVN	C22-C26-C29-C31
27	C	531	WVN	C29-C31-C32-C35
27	C	531	WVN	C29-C31-C32-C36
27	C	531	WVN	C30-C33-C34-C37
27	C	531	WVN	C30-C33-C34-C38
27	D	408	WVN	C15-C13-C20-C23
27	D	408	WVN	C11-C19-C22-C26
27	D	408	WVN	C20-C23-C25-C27
27	D	408	WVN	C20-C23-C25-C28
27	D	408	WVN	C30-C33-C34-C37

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Mol	Chain	Res	Type	Atoms
27	D	408	WVN	C30-C33-C34-C38
27	H	89	WVN	C15-C13-C20-C23
27	H	89	WVN	C29-C31-C32-C35
27	H	89	WVN	C29-C31-C32-C36
27	Y	89	WVN	C01-C02-C11-C19
27	Y	89	WVN	C05-C02-C11-C19
27	Y	89	WVN	C20-C23-C25-C27
27	Y	89	WVN	C20-C23-C25-C28
27	Y	89	WVN	C29-C31-C32-C35
27	Y	89	WVN	C29-C31-C32-C36
27	3	620	WVN	C30-C33-C34-C37
27	3	620	WVN	C30-C33-C34-C38
27	6	620	WVN	C15-C13-C20-C23
27	P	620	WVN	C30-C33-C34-C37
27	P	620	WVN	C30-C33-C34-C38
27	S	620	WVN	C15-C13-C20-C23
27	S	620	WVN	C29-C31-C32-C35
27	S	620	WVN	C29-C31-C32-C36
29	a	409	PL9	C7-C8-C9-C11
29	a	409	PL9	C19-C21-C22-C23
29	a	409	PL9	C22-C23-C24-C26
29	A	409	PL9	C7-C8-C9-C11
29	A	409	PL9	C19-C21-C22-C23
29	A	409	PL9	C22-C23-C24-C26
31	a	413	LHG	C3-O3-P-O4
31	a	413	LHG	C4-O6-P-O5
31	b	622	LHG	C3-O3-P-O4
31	b	622	LHG	C3-O3-P-O5
31	b	622	LHG	C4-O6-P-O5
31	c	535	LHG	O1-C1-C2-C3
31	c	535	LHG	C3-O3-P-O5
31	z	103	LHG	C4-O6-P-O5
31	A	413	LHG	C3-O3-P-O4
31	A	413	LHG	C4-O6-P-O5
31	C	535	LHG	C4-O6-P-O3
31	C	535	LHG	C4-O6-P-O4
31	C	535	LHG	C4-O6-P-O5
31	Z	103	LHG	C4-O6-P-O5
31	2	621	LHG	C3-O3-P-O5
31	3	621	LHG	C3-O3-P-O5
31	5	621	LHG	C3-O3-P-O6
31	O	621	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
31	P	621	LHG	C3-O3-P-O5
31	R	621	LHG	C3-O3-P-O6
34	c	536	LMG	C2-C1-O1-C7
34	c	536	LMG	O6-C1-O1-C7
34	w	134	LMG	O6-C1-O1-C7
34	w	134	LMG	O7-C8-C9-O8
34	W	134	LMG	O6-C1-O1-C7
34	W	134	LMG	O7-C8-C9-O8
36	e	102	HEM	C2B-C3B-CAB-CBB
36	e	102	HEM	C4B-C3B-CAB-CBB
36	E	102	HEM	C2B-C3B-CAB-CBB
37	2	612	KC2	C1A-C2A-CAA-CBA
37	2	612	KC2	C3A-C2A-CAA-CBA
37	2	612	KC2	C2C-C3C-CAC-CBC
37	2	612	KC2	C4C-C3C-CAC-CBC
37	2	612	KC2	C2A-CAA-CBA-CGA
37	3	606	KC2	C1A-C2A-CAA-CBA
37	3	606	KC2	C2B-C3B-CAB-CBB
37	3	606	KC2	C4B-C3B-CAB-CBB
37	3	606	KC2	C2C-C3C-CAC-CBC
37	3	606	KC2	C4C-C3C-CAC-CBC
37	3	606	KC2	C2A-CAA-CBA-CGA
37	4	605	KC2	C2C-C3C-CAC-CBC
37	4	605	KC2	C4C-C3C-CAC-CBC
37	4	605	KC2	C2A-CAA-CBA-CGA
37	4	611	KC2	C2C-C3C-CAC-CBC
37	4	611	KC2	C4C-C3C-CAC-CBC
37	4	611	KC2	CBD-CGD-O2D-CED
37	4	611	KC2	O1D-CGD-O2D-CED
37	4	612	KC2	C2C-C3C-CAC-CBC
37	4	612	KC2	C4C-C3C-CAC-CBC
37	5	612	KC2	C1A-C2A-CAA-CBA
37	5	612	KC2	C2C-C3C-CAC-CBC
37	5	612	KC2	C4C-C3C-CAC-CBC
37	5	612	KC2	C2A-CAA-CBA-CGA
37	5	612	KC2	CAA-CBA-CGA-O2A
37	6	606	KC2	C2C-C3C-CAC-CBC
37	6	606	KC2	C4C-C3C-CAC-CBC
37	6	606	KC2	C2A-CAA-CBA-CGA
37	6	606	KC2	CBD-CGD-O2D-CED
37	6	606	KC2	O1D-CGD-O2D-CED
37	6	612	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
37	6	612	KC2	C4C-C3C-CAC-CBC
37	1	605	KC2	C2B-C3B-CAB-CBB
37	1	605	KC2	C4B-C3B-CAB-CBB
37	1	605	KC2	C2C-C3C-CAC-CBC
37	1	605	KC2	C4C-C3C-CAC-CBC
37	1	605	KC2	C2A-CAA-CBA-CGA
37	1	611	KC2	C2B-C3B-CAB-CBB
37	1	611	KC2	C4B-C3B-CAB-CBB
37	1	611	KC2	C2C-C3C-CAC-CBC
37	1	612	KC2	C2C-C3C-CAC-CBC
37	1	612	KC2	C4C-C3C-CAC-CBC
37	1	613	KC2	C2B-C3B-CAB-CBB
37	1	613	KC2	C4B-C3B-CAB-CBB
37	1	613	KC2	CBD-CGD-O2D-CED
37	O	612	KC2	C1A-C2A-CAA-CBA
37	O	612	KC2	C3A-C2A-CAA-CBA
37	O	612	KC2	C2C-C3C-CAC-CBC
37	O	612	KC2	C4C-C3C-CAC-CBC
37	O	612	KC2	C2A-CAA-CBA-CGA
37	P	606	KC2	C1A-C2A-CAA-CBA
37	P	606	KC2	C2B-C3B-CAB-CBB
37	P	606	KC2	C4B-C3B-CAB-CBB
37	P	606	KC2	C2C-C3C-CAC-CBC
37	P	606	KC2	C4C-C3C-CAC-CBC
37	P	606	KC2	C2A-CAA-CBA-CGA
37	Q	605	KC2	C2C-C3C-CAC-CBC
37	Q	605	KC2	C4C-C3C-CAC-CBC
37	Q	605	KC2	C2A-CAA-CBA-CGA
37	Q	611	KC2	C2C-C3C-CAC-CBC
37	Q	611	KC2	C4C-C3C-CAC-CBC
37	Q	611	KC2	CBD-CGD-O2D-CED
37	Q	611	KC2	O1D-CGD-O2D-CED
37	Q	612	KC2	C2C-C3C-CAC-CBC
37	Q	612	KC2	C4C-C3C-CAC-CBC
37	R	612	KC2	C1A-C2A-CAA-CBA
37	R	612	KC2	C2C-C3C-CAC-CBC
37	R	612	KC2	C4C-C3C-CAC-CBC
37	R	612	KC2	C2A-CAA-CBA-CGA
37	R	612	KC2	CAA-CBA-CGA-O2A
37	S	606	KC2	C1A-C2A-CAA-CBA
37	S	606	KC2	C2C-C3C-CAC-CBC
37	S	606	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
37	S	606	KC2	CAA-CBA-CGA-O2A
37	S	606	KC2	CBD-CGD-O2D-CED
37	S	606	KC2	O1D-CGD-O2D-CED
37	S	612	KC2	C2C-C3C-CAC-CBC
37	S	612	KC2	C4C-C3C-CAC-CBC
37	N	605	KC2	C2B-C3B-CAB-CBB
37	N	605	KC2	C4B-C3B-CAB-CBB
37	N	605	KC2	C2C-C3C-CAC-CBC
37	N	605	KC2	C4C-C3C-CAC-CBC
37	N	605	KC2	C2A-CAA-CBA-CGA
37	N	611	KC2	C2B-C3B-CAB-CBB
37	N	611	KC2	C4B-C3B-CAB-CBB
37	N	611	KC2	C2C-C3C-CAC-CBC
37	N	612	KC2	C2C-C3C-CAC-CBC
37	N	612	KC2	C4C-C3C-CAC-CBC
37	N	613	KC2	C2B-C3B-CAB-CBB
37	N	613	KC2	C4B-C3B-CAB-CBB
37	N	613	KC2	CBD-CGD-O2D-CED
38	2	619	II0	C31-C33-C35-C37
38	2	619	II0	C31-C33-C35-C39
38	3	619	II0	C31-C33-C35-C37
38	3	619	II0	C31-C33-C35-C39
38	4	616	II0	C32-C34-C36-C38
38	4	616	II0	C32-C34-C36-C40
38	4	619	II0	C31-C33-C35-C37
38	4	619	II0	C31-C33-C35-C39
38	6	616	II0	C31-C33-C35-C37
38	6	616	II0	C31-C33-C35-C39
38	6	618	II0	C10-C22-C24-C26
38	1	618	II0	C10-C22-C24-C26
38	1	619	II0	C31-C33-C35-C37
38	1	619	II0	C31-C33-C35-C39
38	O	619	II0	C31-C33-C35-C37
38	O	619	II0	C31-C33-C35-C39
38	P	619	II0	C31-C33-C35-C37
38	P	619	II0	C31-C33-C35-C39
38	Q	616	II0	C32-C34-C36-C38
38	Q	616	II0	C32-C34-C36-C40
38	Q	619	II0	C09-C21-C23-C25
38	Q	619	II0	C31-C33-C35-C37
38	Q	619	II0	C31-C33-C35-C39
38	S	616	II0	C31-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
38	S	616	II0	C31-C33-C35-C39
38	S	618	II0	C10-C22-C24-C26
38	N	616	II0	C09-C21-C23-C25
38	N	618	II0	C10-C22-C24-C26
39	4	620	IHT	C30-C32-C33-C36
39	4	620	IHT	C30-C32-C33-C37
39	5	620	IHT	C18-C22-C23-C25
39	5	620	IHT	C18-C22-C23-C27
39	5	620	IHT	C31-C34-C35-C38
39	1	620	IHT	C18-C22-C23-C25
39	1	620	IHT	C18-C22-C23-C27
39	1	620	IHT	C30-C32-C33-C36
39	1	620	IHT	C30-C32-C33-C37
39	1	620	IHT	C35-C38-C41-C40
39	Q	620	IHT	C30-C32-C33-C36
39	Q	620	IHT	C30-C32-C33-C37
39	R	620	IHT	C30-C32-C33-C36
39	R	620	IHT	C30-C32-C33-C37
39	R	620	IHT	C31-C34-C35-C38
39	R	620	IHT	C31-C34-C35-C39
39	N	620	IHT	C18-C22-C23-C25
39	N	620	IHT	C18-C22-C23-C27
39	N	620	IHT	C30-C32-C33-C36
39	N	620	IHT	C30-C32-C33-C37
39	N	620	IHT	C35-C38-C41-C40
25	a	403	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	A	403	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	2	611	CLA	O1D-CGD-O2D-CED
25	5	606	CLA	O1D-CGD-O2D-CED
25	5	610	CLA	O1D-CGD-O2D-CED
25	O	611	CLA	O1D-CGD-O2D-CED
25	R	606	CLA	O1D-CGD-O2D-CED
25	R	610	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
25	c	528	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
25	4	615	CLA	O1D-CGD-O2D-CED
25	1	607	CLA	O1D-CGD-O2D-CED
25	Q	615	CLA	O1D-CGD-O2D-CED
25	N	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	a	403	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	607	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	c	521	CLA	CBD-CGD-O2D-CED
25	c	523	CLA	CBD-CGD-O2D-CED
25	c	528	CLA	CBD-CGD-O2D-CED
25	A	403	CLA	CBD-CGD-O2D-CED
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	521	CLA	CBD-CGD-O2D-CED
25	C	523	CLA	CBD-CGD-O2D-CED
25	C	528	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	CBD-CGD-O2D-CED
25	3	613	CLA	CBD-CGD-O2D-CED
25	3	615	CLA	CBD-CGD-O2D-CED
25	4	603	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	CBD-CGD-O2D-CED
25	4	606	CLA	CBD-CGD-O2D-CED
25	4	613	CLA	CBD-CGD-O2D-CED
25	5	606	CLA	CBD-CGD-O2D-CED
25	5	609	CLA	CBD-CGD-O2D-CED
25	5	613	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	609	CLA	CBD-CGD-O2D-CED
25	1	606	CLA	CBD-CGD-O2D-CED
25	O	604	CLA	CBD-CGD-O2D-CED
25	P	613	CLA	CBD-CGD-O2D-CED
25	P	615	CLA	CBD-CGD-O2D-CED
25	Q	603	CLA	CBD-CGD-O2D-CED
25	Q	604	CLA	CBD-CGD-O2D-CED
25	Q	613	CLA	CBD-CGD-O2D-CED
25	R	606	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	CBD-CGD-O2D-CED
25	S	604	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	N	606	CLA	CBD-CGD-O2D-CED
37	1	605	KC2	CBD-CGD-O2D-CED
37	N	605	KC2	CBD-CGD-O2D-CED
25	b	615	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
25	B	615	CLA	O1A-CGA-O2A-C1
25	C	525	CLA	O1A-CGA-O2A-C1
25	2	607	CLA	O1A-CGA-O2A-C1
25	O	607	CLA	O1A-CGA-O2A-C1
25	Q	606	CLA	O1A-CGA-O2A-C1
26	a	405	PHO	O1A-CGA-O2A-C1
26	A	405	PHO	O1A-CGA-O2A-C1
25	c	521	CLA	O1D-CGD-O2D-CED
25	C	521	CLA	O1D-CGD-O2D-CED
25	C	528	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	O1D-CGD-O2D-CED
25	4	606	CLA	O1D-CGD-O2D-CED
25	6	609	CLA	O1D-CGD-O2D-CED
25	Q	603	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
25	c	516	CLA	O1D-CGD-O2D-CED
25	B	611	CLA	O1D-CGD-O2D-CED
25	C	516	CLA	O1D-CGD-O2D-CED
25	3	615	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	O1D-CGD-O2D-CED
25	6	615	CLA	O1D-CGD-O2D-CED
25	P	615	CLA	O1D-CGD-O2D-CED
25	S	609	CLA	O1D-CGD-O2D-CED
25	S	613	CLA	O1D-CGD-O2D-CED
25	S	615	CLA	O1D-CGD-O2D-CED
25	N	614	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	CBA-CGA-O2A-C1
25	B	616	CLA	CBA-CGA-O2A-C1
25	Q	606	CLA	CBA-CGA-O2A-C1
26	a	405	PHO	CBA-CGA-O2A-C1
26	A	405	PHO	CBA-CGA-O2A-C1
25	b	603	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	602	CLA	CBD-CGD-O2D-CED
25	2	613	CLA	CBD-CGD-O2D-CED
25	4	609	CLA	CBD-CGD-O2D-CED
25	5	611	CLA	CBD-CGD-O2D-CED
25	G	301	CLA	CBD-CGD-O2D-CED
25	O	602	CLA	CBD-CGD-O2D-CED
25	O	613	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	CBD-CGD-O2D-CED
26	d	401	PHO	CBD-CGD-O2D-CED
26	D	401	PHO	CBD-CGD-O2D-CED
25	a	404	CLA	O1A-CGA-O2A-C1
25	a	406	CLA	O1A-CGA-O2A-C1
25	c	519	CLA	O1A-CGA-O2A-C1
25	g	301	CLA	O1A-CGA-O2A-C1
25	A	404	CLA	O1A-CGA-O2A-C1
25	A	406	CLA	O1A-CGA-O2A-C1
25	B	616	CLA	O1A-CGA-O2A-C1
25	C	519	CLA	O1A-CGA-O2A-C1
25	2	606	CLA	O1A-CGA-O2A-C1
25	5	601	CLA	O1A-CGA-O2A-C1
25	5	606	CLA	O1A-CGA-O2A-C1
25	6	611	CLA	O1A-CGA-O2A-C1
25	1	603	CLA	O1A-CGA-O2A-C1
25	1	614	CLA	O1A-CGA-O2A-C1
25	O	606	CLA	O1A-CGA-O2A-C1
25	R	601	CLA	O1A-CGA-O2A-C1
25	R	606	CLA	O1A-CGA-O2A-C1
25	S	603	CLA	O1A-CGA-O2A-C1
25	S	611	CLA	O1A-CGA-O2A-C1
25	N	603	CLA	O1A-CGA-O2A-C1
25	N	614	CLA	O1A-CGA-O2A-C1
26	d	401	PHO	O1A-CGA-O2A-C1
26	D	401	PHO	O1A-CGA-O2A-C1
25	a	406	CLA	O1D-CGD-O2D-CED
25	A	406	CLA	O1D-CGD-O2D-CED
25	1	614	CLA	O1D-CGD-O2D-CED
25	1	615	CLA	O1D-CGD-O2D-CED
25	N	615	CLA	O1D-CGD-O2D-CED
25	c	517	CLA	O1D-CGD-O2D-CED
25	C	517	CLA	O1D-CGD-O2D-CED
25	4	604	CLA	O1D-CGD-O2D-CED
25	Q	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	609	CLA	CBA-CGA-O2A-C1
25	N	609	CLA	CBA-CGA-O2A-C1
25	a	406	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	b	616	CLA	C3-C5-C6-C7
25	c	519	CLA	C3-C5-C6-C7
25	A	406	CLA	C3-C5-C6-C7
25	B	604	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	C	519	CLA	C3-C5-C6-C7
25	3	602	CLA	C3-C5-C6-C7
25	3	613	CLA	C3-C5-C6-C7
25	4	606	CLA	C3-C5-C6-C7
25	5	601	CLA	C3-C5-C6-C7
25	5	602	CLA	C3-C5-C6-C7
25	5	610	CLA	C3-C5-C6-C7
25	5	611	CLA	C3-C5-C6-C7
25	6	601	CLA	C3-C5-C6-C7
25	6	609	CLA	C3-C5-C6-C7
25	6	610	CLA	C3-C5-C6-C7
25	6	613	CLA	C3-C5-C6-C7
25	P	602	CLA	C3-C5-C6-C7
25	P	613	CLA	C3-C5-C6-C7
25	Q	609	CLA	C3-C5-C6-C7
25	R	601	CLA	C3-C5-C6-C7
25	R	602	CLA	C3-C5-C6-C7
25	R	610	CLA	C3-C5-C6-C7
25	R	611	CLA	C3-C5-C6-C7
25	S	601	CLA	C3-C5-C6-C7
25	S	609	CLA	C3-C5-C6-C7
25	S	610	CLA	C3-C5-C6-C7
25	S	613	CLA	C3-C5-C6-C7
26	d	401	PHO	C3-C5-C6-C7
26	D	401	PHO	C3-C5-C6-C7
25	a	403	CLA	CBA-CGA-O2A-C1
25	a	404	CLA	CBA-CGA-O2A-C1
25	b	615	CLA	CBA-CGA-O2A-C1
25	c	525	CLA	CBA-CGA-O2A-C1
25	g	301	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	403	CLA	CBA-CGA-O2A-C1
25	A	404	CLA	CBA-CGA-O2A-C1
25	B	615	CLA	CBA-CGA-O2A-C1
25	C	525	CLA	CBA-CGA-O2A-C1
25	2	606	CLA	CBA-CGA-O2A-C1
25	2	607	CLA	CBA-CGA-O2A-C1
25	5	606	CLA	CBA-CGA-O2A-C1
25	6	611	CLA	CBA-CGA-O2A-C1
25	1	603	CLA	CBA-CGA-O2A-C1
25	1	614	CLA	CBA-CGA-O2A-C1
25	1	615	CLA	CBA-CGA-O2A-C1
25	O	606	CLA	CBA-CGA-O2A-C1
25	O	607	CLA	CBA-CGA-O2A-C1
25	R	606	CLA	CBA-CGA-O2A-C1
25	S	603	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
25	N	603	CLA	CBA-CGA-O2A-C1
25	N	614	CLA	CBA-CGA-O2A-C1
25	N	615	CLA	CBA-CGA-O2A-C1
25	2	604	CLA	O1D-CGD-O2D-CED
25	O	604	CLA	O1D-CGD-O2D-CED
25	R	609	CLA	O1D-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	CBD-CGD-O2D-CED
25	1	609	CLA	O1A-CGA-O2A-C1
25	N	609	CLA	O1A-CGA-O2A-C1
37	4	605	KC2	CAA-CBA-CGA-O2A
37	1	605	KC2	CAA-CBA-CGA-O1A
37	Q	605	KC2	CAA-CBA-CGA-O2A
37	N	605	KC2	CAA-CBA-CGA-O1A
25	3	611	CLA	C3-C5-C6-C7
25	P	611	CLA	C3-C5-C6-C7
25	c	518	CLA	C4-C3-C5-C6
25	C	518	CLA	C4-C3-C5-C6
25	3	611	CLA	C2-C3-C5-C6
25	6	611	CLA	C2-C3-C5-C6
25	P	611	CLA	C2-C3-C5-C6
25	S	611	CLA	C2-C3-C5-C6
25	S	603	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C2A-CAA-CBA-CGA
25	c	517	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	c	524	CLA	C2A-CAA-CBA-CGA
25	c	525	CLA	C2A-CAA-CBA-CGA
25	d	400	CLA	C2A-CAA-CBA-CGA
25	g	301	CLA	C2A-CAA-CBA-CGA
25	B	606	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C2A-CAA-CBA-CGA
25	C	517	CLA	C2A-CAA-CBA-CGA
25	C	524	CLA	C2A-CAA-CBA-CGA
25	C	525	CLA	C2A-CAA-CBA-CGA
25	D	400	CLA	C2A-CAA-CBA-CGA
25	3	612	CLA	C2A-CAA-CBA-CGA
25	4	602	CLA	C2A-CAA-CBA-CGA
25	4	609	CLA	C2A-CAA-CBA-CGA
25	5	613	CLA	C2A-CAA-CBA-CGA
25	6	611	CLA	C2A-CAA-CBA-CGA
25	P	612	CLA	C2A-CAA-CBA-CGA
25	Q	602	CLA	C2A-CAA-CBA-CGA
25	R	613	CLA	C2A-CAA-CBA-CGA
25	S	611	CLA	C2A-CAA-CBA-CGA
25	N	609	CLA	C2A-CAA-CBA-CGA
25	c	522	CLA	C3-C5-C6-C7
25	C	522	CLA	C3-C5-C6-C7
25	a	406	CLA	CBA-CGA-O2A-C1
25	c	519	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	CBA-CGA-O2A-C1
25	B	612	CLA	CBA-CGA-O2A-C1
25	C	519	CLA	CBA-CGA-O2A-C1
25	3	610	CLA	CBA-CGA-O2A-C1
25	5	601	CLA	CBA-CGA-O2A-C1
25	P	610	CLA	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
26	d	401	PHO	CBA-CGA-O2A-C1
26	D	401	PHO	CBA-CGA-O2A-C1
29	a	409	PL9	C17-C18-C19-C20
29	A	409	PL9	C17-C18-C19-C20
34	c	536	LMG	C13-C14-C15-C16
25	b	607	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	O1D-CGD-O2D-CED
25	3	613	CLA	O1D-CGD-O2D-CED
25	4	613	CLA	O1D-CGD-O2D-CED
25	P	613	CLA	O1D-CGD-O2D-CED
25	Q	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	R	613	CLA	O1D-CGD-O2D-CED
25	a	403	CLA	O1A-CGA-O2A-C1
25	A	403	CLA	O1A-CGA-O2A-C1
25	2	609	CLA	O1A-CGA-O2A-C1
25	3	610	CLA	O1A-CGA-O2A-C1
25	4	602	CLA	O1A-CGA-O2A-C1
25	1	615	CLA	O1A-CGA-O2A-C1
25	O	609	CLA	O1A-CGA-O2A-C1
25	P	610	CLA	O1A-CGA-O2A-C1
25	Q	602	CLA	O1A-CGA-O2A-C1
25	N	615	CLA	O1A-CGA-O2A-C1
25	5	613	CLA	O1D-CGD-O2D-CED
27	a	407	WVN	C25-C28-C30-C33
27	b	617	WVN	C25-C28-C30-C33
27	c	529	WVN	C34-C37-C40-C39
27	c	531	WVN	C25-C28-C30-C33
27	B	619	WVN	C25-C28-C30-C33
27	B	619	WVN	C34-C37-C40-C39
27	C	529	WVN	C22-C26-C29-C31
38	1	616	II0	C25-C29-C31-C33
38	N	616	II0	C25-C29-C31-C33
25	b	604	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	CBD-CGD-O2D-CED
25	1	601	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	S	602	CLA	CBD-CGD-O2D-CED
25	N	601	CLA	CBD-CGD-O2D-CED
37	5	612	KC2	CBD-CGD-O2D-CED
37	R	612	KC2	CBD-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
25	5	609	CLA	O1D-CGD-O2D-CED
25	1	606	CLA	O1D-CGD-O2D-CED
25	N	606	CLA	O1D-CGD-O2D-CED
31	a	413	LHG	O2-C2-C3-O3
31	A	413	LHG	O2-C2-C3-O3
25	B	613	CLA	C3-C5-C6-C7
25	2	613	CLA	C3-C5-C6-C7
25	4	609	CLA	C3-C5-C6-C7
25	6	604	CLA	C3-C5-C6-C7
25	1	604	CLA	C3-C5-C6-C7
25	O	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	S	603	CLA	C3-C5-C6-C7
25	S	604	CLA	C3-C5-C6-C7
25	N	604	CLA	C3-C5-C6-C7
25	b	612	CLA	CBA-CGA-O2A-C1
25	C	528	CLA	CBA-CGA-O2A-C1
25	4	606	CLA	CBA-CGA-O2A-C1
25	5	603	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
31	C	535	LHG	C24-C23-O8-C6
25	b	616	CLA	O1D-CGD-O2D-CED
25	C	523	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	S	604	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	Q	609	CLA	CBD-CGD-O2D-CED
25	c	523	CLA	O1D-CGD-O2D-CED
25	C	528	CLA	O1A-CGA-O2A-C1
25	2	609	CLA	CBA-CGA-O2A-C1
25	4	602	CLA	CBA-CGA-O2A-C1
25	O	609	CLA	CBA-CGA-O2A-C1
25	Q	602	CLA	CBA-CGA-O2A-C1
37	2	612	KC2	CAA-CBA-CGA-O1A
37	4	611	KC2	CAA-CBA-CGA-O2A
37	6	606	KC2	CAA-CBA-CGA-O1A
37	O	612	KC2	CAA-CBA-CGA-O1A
37	Q	611	KC2	CAA-CBA-CGA-O2A
25	b	612	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	O1A-CGA-O2A-C1
25	R	603	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	C2A-CAA-CBA-CGA
25	B	610	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	O1D-CGD-O2D-CED
25	4	606	CLA	O1A-CGA-O2A-C1
25	5	603	CLA	O1A-CGA-O2A-C1
25	6	603	CLA	CBA-CGA-O2A-C1
25	1	602	CLA	CBA-CGA-O2A-C1
25	b	602	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	6	601	CLA	CBD-CGD-O2D-CED
25	S	601	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	O1D-CGD-O2D-CED
25	b	603	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	O1D-CGD-O2D-CED
25	5	611	CLA	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
37	1	605	KC2	CAA-CBA-CGA-O2A
37	N	605	KC2	CAA-CBA-CGA-O2A
31	a	413	LHG	C1-C2-C3-O3
31	A	413	LHG	C1-C2-C3-O3
29	a	409	PL9	C17-C18-C19-C21
29	A	409	PL9	C17-C18-C19-C21
25	6	603	CLA	O1A-CGA-O2A-C1
25	6	602	CLA	C3-C5-C6-C7
25	S	602	CLA	C3-C5-C6-C7
25	2	613	CLA	O1D-CGD-O2D-CED
25	O	613	CLA	O1D-CGD-O2D-CED
25	b	604	CLA	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
25	c	520	CLA	CBA-CGA-O2A-C1
25	c	524	CLA	CBA-CGA-O2A-C1
25	d	400	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	B	604	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	CBA-CGA-O2A-C1
25	C	520	CLA	CBA-CGA-O2A-C1
25	C	524	CLA	CBA-CGA-O2A-C1
25	D	400	CLA	CBA-CGA-O2A-C1
25	D	403	CLA	CBA-CGA-O2A-C1
25	2	601	CLA	CBA-CGA-O2A-C1
25	3	612	CLA	CBA-CGA-O2A-C1
25	5	602	CLA	CBA-CGA-O2A-C1
25	5	613	CLA	CBA-CGA-O2A-C1
25	6	609	CLA	CBA-CGA-O2A-C1
25	O	601	CLA	CBA-CGA-O2A-C1
25	P	612	CLA	CBA-CGA-O2A-C1
25	R	602	CLA	CBA-CGA-O2A-C1
25	R	613	CLA	CBA-CGA-O2A-C1
25	N	602	CLA	CBA-CGA-O2A-C1
31	b	622	LHG	C24-C23-O8-C6
25	B	602	CLA	CBD-CGD-O2D-CED
25	3	602	CLA	CBD-CGD-O2D-CED
25	P	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	h	89	WVN	C32-C36-C39-C40
27	B	617	WVN	C22-C26-C29-C31
27	B	619	WVN	C32-C36-C39-C40
27	H	89	WVN	C32-C36-C39-C40
38	1	618	II0	C26-C30-C32-C34
38	N	618	II0	C26-C30-C32-C34
39	4	620	IHT	C23-C27-C30-C32
39	5	620	IHT	C26-C29-C31-C34
39	Q	620	IHT	C23-C27-C30-C32
34	g	303	LMG	C28-C29-C30-C31
34	G	303	LMG	C28-C29-C30-C31
37	3	606	KC2	CAA-CBA-CGA-O2A
37	5	612	KC2	CAA-CBA-CGA-O1A
37	P	606	KC2	CAA-CBA-CGA-O2A
37	R	612	KC2	CAA-CBA-CGA-O1A
37	S	606	KC2	CAA-CBA-CGA-O1A
25	P	601	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	C10-C11-C12-C13
31	2	621	LHG	O2-C2-C3-O3
31	O	621	LHG	O2-C2-C3-O3
25	6	610	CLA	CBA-CGA-O2A-C1
25	S	610	CLA	CBA-CGA-O2A-C1
25	5	602	CLA	O1A-CGA-O2A-C1
25	R	602	CLA	O1A-CGA-O2A-C1
31	C	535	LHG	O10-C23-O8-C6
25	b	603	CLA	C4-C3-C5-C6
25	B	603	CLA	C4-C3-C5-C6
25	c	518	CLA	C2-C3-C5-C6
25	C	518	CLA	C2-C3-C5-C6
25	2	607	CLA	C6-C7-C8-C9
25	2	607	CLA	C11-C10-C8-C9
25	3	609	CLA	C6-C7-C8-C9
25	G	301	CLA	C14-C13-C15-C16
25	O	607	CLA	C6-C7-C8-C9
25	O	607	CLA	C11-C10-C8-C9
25	P	609	CLA	C6-C7-C8-C9
25	G	301	CLA	O1D-CGD-O2D-CED
37	1	605	KC2	O1D-CGD-O2D-CED
37	N	605	KC2	O1D-CGD-O2D-CED
25	6	604	CLA	C5-C6-C7-C8
25	S	604	CLA	C5-C6-C7-C8
25	a	404	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	A	404	CLA	C2A-CAA-CBA-CGA
27	c	529	WVN	C30-C33-C34-C38
27	c	531	WVN	C29-C31-C32-C35
27	d	408	WVN	C11-C19-C22-C24
27	y	89	WVN	C29-C31-C32-C35
27	B	617	WVN	C11-C19-C22-C24
27	B	619	WVN	C20-C23-C25-C27
27	D	408	WVN	C11-C19-C22-C24
27	Y	89	WVN	C11-C19-C22-C24
27	3	620	WVN	C11-C19-C22-C24
27	6	620	WVN	C11-C19-C22-C24
27	P	620	WVN	C11-C19-C22-C24
27	S	620	WVN	C11-C19-C22-C24
38	2	619	II0	C32-C34-C36-C38
38	5	619	II0	C31-C33-C35-C37
38	6	618	II0	C31-C33-C35-C37
38	O	619	II0	C32-C34-C36-C38
38	R	619	II0	C31-C33-C35-C37
38	S	618	II0	C31-C33-C35-C37
38	N	619	II0	C31-C33-C35-C37
39	4	620	IHT	C18-C22-C23-C25
39	5	620	IHT	C31-C34-C35-C39
39	O	620	IHT	C30-C32-C33-C36
39	Q	620	IHT	C18-C22-C23-C25
39	R	620	IHT	C18-C22-C23-C25
27	c	529	WVN	C30-C33-C34-C37
27	c	531	WVN	C29-C31-C32-C36
27	d	408	WVN	C11-C19-C22-C26
27	B	617	WVN	C11-C19-C22-C26
27	B	619	WVN	C20-C23-C25-C28
27	C	529	WVN	C30-C33-C34-C37
27	Y	89	WVN	C11-C19-C22-C26
27	3	620	WVN	C11-C19-C22-C26
27	P	620	WVN	C11-C19-C22-C26
27	S	620	WVN	C11-C19-C22-C26
38	2	619	II0	C32-C34-C36-C40
38	6	619	II0	C31-C33-C35-C39
38	1	616	II0	C31-C33-C35-C39
38	O	619	II0	C32-C34-C36-C40
38	S	619	II0	C31-C33-C35-C39
38	N	616	II0	C31-C33-C35-C39
39	4	620	IHT	C18-C22-C23-C27

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Mol	Chain	Res	Type	Atoms
39	Q	620	IHT	C18-C22-C23-C27
31	b	622	LHG	C8-C7-O7-C5
25	b	604	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
25	c	524	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	O1A-CGA-O2A-C1
25	B	614	CLA	O1A-CGA-O2A-C1
25	C	524	CLA	O1A-CGA-O2A-C1
25	2	601	CLA	O1A-CGA-O2A-C1
25	3	612	CLA	O1A-CGA-O2A-C1
25	6	609	CLA	O1A-CGA-O2A-C1
25	O	601	CLA	O1A-CGA-O2A-C1
25	P	612	CLA	O1A-CGA-O2A-C1
37	2	612	KC2	CAA-CBA-CGA-O2A
37	O	612	KC2	CAA-CBA-CGA-O2A
25	b	614	CLA	O1D-CGD-O2D-CED
25	3	611	CLA	CBA-CGA-O2A-C1
25	P	609	CLA	CBA-CGA-O2A-C1
25	P	611	CLA	CBA-CGA-O2A-C1
25	S	609	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	C5-C6-C7-C8
25	6	602	CLA	C10-C11-C12-C13
25	1	604	CLA	C5-C6-C7-C8
25	O	607	CLA	C5-C6-C7-C8
25	S	602	CLA	C10-C11-C12-C13
25	N	604	CLA	C5-C6-C7-C8
31	a	413	LHG	C7-C8-C9-C10
34	m	101	LMG	C10-C11-C12-C13
25	b	613	CLA	C5-C6-C7-C8
25	2	607	CLA	C5-C6-C7-C8
25	3	609	CLA	C5-C6-C7-C8
25	3	609	CLA	C13-C15-C16-C17
25	3	610	CLA	C10-C11-C12-C13
25	6	604	CLA	C13-C15-C16-C17
25	P	609	CLA	C5-C6-C7-C8
25	P	609	CLA	C13-C15-C16-C17
25	P	610	CLA	C10-C11-C12-C13
25	S	604	CLA	C13-C15-C16-C17
25	C	520	CLA	O1A-CGA-O2A-C1
31	b	622	LHG	C23-C24-C25-C26
31	A	413	LHG	C7-C8-C9-C10
34	M	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	h	90	DGD	C1A-C2A-C3A-C4A
35	H	90	DGD	C1A-C2A-C3A-C4A
25	5	602	CLA	CBD-CGD-O2D-CED
25	R	602	CLA	CBD-CGD-O2D-CED
25	N	609	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	C13-C15-C16-C17
25	c	523	CLA	C13-C15-C16-C17
25	C	523	CLA	C13-C15-C16-C17
25	6	601	CLA	C5-C6-C7-C8
25	S	601	CLA	C5-C6-C7-C8
26	A	405	PHO	C3-C5-C6-C7
25	c	528	CLA	CBA-CGA-O2A-C1
25	3	609	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	O1D-CGD-O2D-CED
25	2	602	CLA	O1D-CGD-O2D-CED
25	O	602	CLA	O1D-CGD-O2D-CED
37	6	606	KC2	CAA-CBA-CGA-O2A
25	c	524	CLA	C2-C1-O2A-CGA
25	C	524	CLA	C2-C1-O2A-CGA
25	5	606	CLA	C2-C1-O2A-CGA
25	R	606	CLA	C2-C1-O2A-CGA
25	2	603	CLA	C10-C11-C12-C13
25	6	603	CLA	CBD-CGD-O2D-CED
25	3	602	CLA	C13-C15-C16-C17
25	P	602	CLA	C13-C15-C16-C17
25	O	603	CLA	C10-C11-C12-C13
25	b	612	CLA	C6-C7-C8-C10
25	c	522	CLA	C12-C13-C15-C16
25	B	612	CLA	C6-C7-C8-C10
25	C	522	CLA	C12-C13-C15-C16
25	6	602	CLA	C11-C12-C13-C15
25	G	301	CLA	C11-C10-C8-C7
25	1	610	CLA	C11-C10-C8-C7
25	S	602	CLA	C11-C12-C13-C15
25	N	610	CLA	C11-C10-C8-C7
25	2	602	CLA	C3-C5-C6-C7
25	3	609	CLA	C3-C5-C6-C7
25	O	602	CLA	C3-C5-C6-C7
25	P	609	CLA	C3-C5-C6-C7
26	a	405	PHO	C3-C5-C6-C7
25	c	520	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	D	403	CLA	O1A-CGA-O2A-C1
25	5	613	CLA	O1A-CGA-O2A-C1
25	R	613	CLA	O1A-CGA-O2A-C1
27	h	89	WVN	C25-C28-C30-C33
27	B	617	WVN	C25-C28-C30-C33
38	2	619	II0	C26-C30-C32-C34
38	O	619	II0	C26-C30-C32-C34
39	4	620	IHT	C35-C38-C41-C40
39	1	620	IHT	C33-C37-C40-C41
39	O	620	IHT	C26-C29-C31-C34
39	R	620	IHT	C26-C29-C31-C34
39	N	620	IHT	C33-C37-C40-C41
25	4	606	CLA	C2A-CAA-CBA-CGA
25	B	606	CLA	O1D-CGD-O2D-CED
25	4	609	CLA	O1D-CGD-O2D-CED
26	d	401	PHO	O1D-CGD-O2D-CED
26	D	401	PHO	O1D-CGD-O2D-CED
25	b	611	CLA	C15-C16-C17-C18
25	b	613	CLA	C10-C11-C12-C13
25	c	518	CLA	C15-C16-C17-C18
25	g	301	CLA	C10-C11-C12-C13
25	B	611	CLA	C15-C16-C17-C18
25	C	518	CLA	C15-C16-C17-C18
25	3	610	CLA	C13-C15-C16-C17
25	P	610	CLA	C13-C15-C16-C17
25	6	610	CLA	O1A-CGA-O2A-C1
31	b	622	LHG	O10-C23-O8-C6
25	2	610	CLA	CBD-CGD-O2D-CED
25	1	610	CLA	C5-C6-C7-C8
25	N	610	CLA	C5-C6-C7-C8
34	d	402	LMG	C10-C11-C12-C13
34	D	402	LMG	C10-C11-C12-C13
37	1	613	KC2	O1D-CGD-O2D-CED
37	N	613	KC2	O1D-CGD-O2D-CED
31	b	622	LHG	O9-C7-O7-C5
25	c	522	CLA	C15-C16-C17-C18
25	C	522	CLA	C15-C16-C17-C18
25	6	615	CLA	C13-C15-C16-C17
25	S	615	CLA	C13-C15-C16-C17
25	d	400	CLA	O1A-CGA-O2A-C1
25	D	400	CLA	O1A-CGA-O2A-C1
25	1	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	S	610	CLA	O1A-CGA-O2A-C1
25	N	602	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	C15-C16-C17-C18
25	O	610	CLA	CBD-CGD-O2D-CED
25	c	528	CLA	O1A-CGA-O2A-C1
25	3	611	CLA	O1A-CGA-O2A-C1
25	P	611	CLA	O1A-CGA-O2A-C1
28	a	411	SQD	C8-C7-O47-C45
28	A	411	SQD	C8-C7-O47-C45
34	C	536	LMG	C11-C10-O7-C8
25	g	301	CLA	C8-C10-C11-C12
25	B	615	CLA	C5-C6-C7-C8
25	3	602	CLA	C10-C11-C12-C13
25	5	604	CLA	C5-C6-C7-C8
25	5	604	CLA	C10-C11-C12-C13
25	5	611	CLA	C10-C11-C12-C13
25	P	602	CLA	C10-C11-C12-C13
25	R	604	CLA	C5-C6-C7-C8
25	R	604	CLA	C10-C11-C12-C13
25	R	611	CLA	C10-C11-C12-C13
31	a	413	LHG	C3-O3-P-O6
31	a	413	LHG	C4-O6-P-O3
31	b	622	LHG	C3-O3-P-O6
31	A	413	LHG	C3-O3-P-O6
31	A	413	LHG	C4-O6-P-O3
31	B	622	LHG	C3-O3-P-O6
25	b	613	CLA	CBA-CGA-O2A-C1
25	c	521	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	C	521	CLA	CBA-CGA-O2A-C1
25	3	609	CLA	O1A-CGA-O2A-C1
25	P	609	CLA	O1A-CGA-O2A-C1
25	1	614	CLA	O2A-C1-C2-C3
25	N	614	CLA	O2A-C1-C2-C3
34	c	536	LMG	C10-C11-C12-C13
25	d	404	CLA	O1D-CGD-O2D-CED
25	D	404	CLA	O1D-CGD-O2D-CED
25	S	603	CLA	O1D-CGD-O2D-CED
31	C	535	LHG	C1-C2-C3-O3
25	c	517	CLA	C5-C6-C7-C8
25	C	517	CLA	C5-C6-C7-C8
25	3	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	P	602	CLA	C8-C10-C11-C12
25	6	615	CLA	C2A-CAA-CBA-CGA
25	1	609	CLA	C2A-CAA-CBA-CGA
25	S	615	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	C16-C17-C18-C20
25	C	524	CLA	C16-C17-C18-C20
37	3	606	KC2	CAA-CBA-CGA-O1A
37	6	612	KC2	CAA-CBA-CGA-O2A
37	P	606	KC2	CAA-CBA-CGA-O1A
37	S	612	KC2	CAA-CBA-CGA-O2A
25	4	610	CLA	CBA-CGA-O2A-C1
25	Q	610	CLA	CBA-CGA-O2A-C1
25	S	615	CLA	CBA-CGA-O2A-C1
27	d	408	WVN	C25-C28-C30-C33
27	D	408	WVN	C25-C28-C30-C33
38	6	619	II0	C36-C40-C42-C41
38	S	619	II0	C36-C40-C42-C41
39	2	620	IHT	C23-C27-C30-C32
39	2	620	IHT	C26-C29-C31-C34
39	1	620	IHT	C23-C27-C30-C32
39	O	620	IHT	C23-C27-C30-C32
39	Q	620	IHT	C35-C38-C41-C40
39	N	620	IHT	C23-C27-C30-C32
31	a	413	LHG	C8-C7-O7-C5
31	A	413	LHG	C8-C7-O7-C5
34	z	102	LMG	C11-C10-O7-C8
34	Z	102	LMG	C11-C10-O7-C8
31	d	406	LHG	C31-C32-C33-C34
31	D	406	LHG	C31-C32-C33-C34
37	4	611	KC2	C2A-CAA-CBA-CGA
37	Q	611	KC2	C2A-CAA-CBA-CGA
25	b	607	CLA	C16-C17-C18-C20
25	c	524	CLA	C16-C17-C18-C20
28	a	411	SQD	O49-C7-O47-C45
28	A	411	SQD	O49-C7-O47-C45
31	a	413	LHG	O9-C7-O7-C5
31	A	413	LHG	O9-C7-O7-C5
34	z	102	LMG	O9-C10-O7-C8
34	C	536	LMG	O9-C10-O7-C8
34	Z	102	LMG	O9-C10-O7-C8
35	c	532	DGD	C1B-C2B-C3B-C4B
35	C	532	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
25	P	604	CLA	CBD-CGD-O2D-CED
25	N	602	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	O1A-CGA-O2A-C1
31	C	535	LHG	O2-C2-C3-O3
31	D	406	LHG	C7-C8-C9-C10
34	C	536	LMG	O1-C7-C8-O7
25	5	611	CLA	CBA-CGA-O2A-C1
25	R	611	CLA	CBA-CGA-O2A-C1
31	b	622	LHG	C26-C27-C28-C29
31	5	621	LHG	C10-C11-C12-C13
25	B	607	CLA	C16-C17-C18-C19
25	B	613	CLA	C16-C17-C18-C19
25	B	616	CLA	C16-C17-C18-C19
25	G	301	CLA	C16-C17-C18-C19
31	R	621	LHG	C10-C11-C12-C13
35	h	90	DGD	C2B-C3B-C4B-C5B
35	H	90	DGD	C2B-C3B-C4B-C5B
25	b	602	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	c	517	CLA	C11-C12-C13-C14
25	B	602	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C12-C13-C14
25	C	517	CLA	C11-C12-C13-C14
31	c	535	LHG	C24-C25-C26-C27
31	A	413	LHG	C32-C33-C34-C35
31	5	621	LHG	C17-C18-C19-C20
37	4	611	KC2	CAA-CBA-CGA-O1A
37	Q	611	KC2	CAA-CBA-CGA-O1A
25	S	603	CLA	C2A-CAA-CBA-CGA
25	c	521	CLA	O1A-CGA-O2A-C1
25	C	521	CLA	O1A-CGA-O2A-C1
27	B	618	WVN	C20-C23-C25-C27
27	B	619	WVN	C30-C33-C34-C38
38	6	619	II0	C31-C33-C35-C37
38	1	616	II0	C31-C33-C35-C37
38	S	619	II0	C31-C33-C35-C37
38	N	616	II0	C31-C33-C35-C37
39	2	620	IHT	C30-C32-C33-C36
31	a	413	LHG	C32-C33-C34-C35
31	R	621	LHG	C17-C18-C19-C20
34	b	620	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	b	622	LHG	O1-C1-C2-C3
27	b	619	WVN	C29-C31-C32-C36
27	B	618	WVN	C30-C33-C34-C37
27	B	619	WVN	C30-C33-C34-C37
27	6	620	WVN	C11-C19-C22-C26
39	2	620	IHT	C30-C32-C33-C37
39	O	620	IHT	C30-C32-C33-C37
25	4	603	CLA	C3-C5-C6-C7
25	Q	603	CLA	C3-C5-C6-C7
25	6	602	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	C13-C15-C16-C17
25	1	602	CLA	CBD-CGD-O2D-CED
25	S	602	CLA	O1D-CGD-O2D-CED
29	d	405	PL9	C47-C48-C49-C51
29	D	405	PL9	C47-C48-C49-C51
31	d	406	LHG	C26-C27-C28-C29
31	5	621	LHG	C28-C29-C30-C31
31	R	621	LHG	C28-C29-C30-C31
34	d	402	LMG	C31-C32-C33-C34
34	C	536	LMG	C34-C35-C36-C37
34	D	402	LMG	C31-C32-C33-C34
35	h	90	DGD	C7B-C8B-C9B-CAB
35	H	90	DGD	C7B-C8B-C9B-CAB
25	b	607	CLA	C16-C17-C18-C19
25	5	611	CLA	C16-C17-C18-C20
25	6	604	CLA	C16-C17-C18-C19
25	6	604	CLA	C16-C17-C18-C20
25	R	611	CLA	C16-C17-C18-C20
25	S	604	CLA	C16-C17-C18-C20
25	B	616	CLA	C15-C16-C17-C18
25	G	301	CLA	C5-C6-C7-C8
31	D	406	LHG	C26-C27-C28-C29
31	3	621	LHG	C31-C32-C33-C34
31	P	621	LHG	C31-C32-C33-C34
34	C	536	LMG	C33-C34-C35-C36
25	3	604	CLA	CBD-CGD-O2D-CED
31	a	413	LHG	C28-C29-C30-C31
31	3	621	LHG	C27-C28-C29-C30
31	P	621	LHG	C27-C28-C29-C30
25	b	605	CLA	C5-C6-C7-C8
25	B	605	CLA	C5-C6-C7-C8
37	1	613	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
37	N	613	KC2	CAA-CBA-CGA-O1A
25	b	613	CLA	O1A-CGA-O2A-C1
25	N	607	CLA	C2C-C3C-CAC-CBC
31	a	413	LHG	C24-C25-C26-C27
31	A	413	LHG	C24-C25-C26-C27
31	A	413	LHG	C28-C29-C30-C31
25	6	615	CLA	CBA-CGA-O2A-C1
25	b	615	CLA	C3A-C2A-CAA-CBA
25	c	516	CLA	C3A-C2A-CAA-CBA
25	c	524	CLA	C3A-C2A-CAA-CBA
25	C	516	CLA	C3A-C2A-CAA-CBA
25	C	524	CLA	C3A-C2A-CAA-CBA
25	2	615	CLA	C3A-C2A-CAA-CBA
25	3	603	CLA	C3A-C2A-CAA-CBA
25	4	607	CLA	C3A-C2A-CAA-CBA
25	5	603	CLA	C3A-C2A-CAA-CBA
25	5	607	CLA	C3A-C2A-CAA-CBA
25	5	613	CLA	C3A-C2A-CAA-CBA
25	1	601	CLA	C3A-C2A-CAA-CBA
25	1	615	CLA	C3A-C2A-CAA-CBA
25	O	615	CLA	C3A-C2A-CAA-CBA
25	P	603	CLA	C3A-C2A-CAA-CBA
25	P	613	CLA	C3A-C2A-CAA-CBA
25	Q	606	CLA	C3A-C2A-CAA-CBA
25	Q	607	CLA	C3A-C2A-CAA-CBA
25	R	603	CLA	C3A-C2A-CAA-CBA
25	R	607	CLA	C3A-C2A-CAA-CBA
25	S	603	CLA	C3A-C2A-CAA-CBA
25	N	601	CLA	C3A-C2A-CAA-CBA
25	N	615	CLA	C3A-C2A-CAA-CBA
34	c	536	LMG	O6-C5-C6-O5
34	B	620	LMG	C17-C18-C19-C20
25	5	611	CLA	C16-C17-C18-C19
25	R	611	CLA	C16-C17-C18-C19
25	S	604	CLA	C16-C17-C18-C19
25	1	607	CLA	C2C-C3C-CAC-CBC
34	c	536	LMG	C30-C31-C32-C33
34	C	536	LMG	C16-C17-C18-C19
25	5	603	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	N	601	CLA	O1D-CGD-O2D-CED
25	a	403	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	A	403	CLA	O2A-C1-C2-C3
25	2	607	CLA	C4-C3-C5-C6
25	3	612	CLA	C4-C3-C5-C6
25	O	607	CLA	C4-C3-C5-C6
25	S	609	CLA	C4-C3-C5-C6
25	2	607	CLA	C2-C3-C5-C6
25	O	607	CLA	C2-C3-C5-C6
25	S	609	CLA	C2-C3-C5-C6
29	a	409	PL9	C23-C24-C26-C27
29	A	409	PL9	C23-C24-C26-C27
25	1	601	CLA	O1D-CGD-O2D-CED
31	c	535	LHG	O1-C1-C2-O2
31	b	622	LHG	C29-C30-C31-C32
25	B	613	CLA	O1A-CGA-O2A-C1
25	4	610	CLA	O1A-CGA-O2A-C1
25	Q	610	CLA	O1A-CGA-O2A-C1
25	S	615	CLA	O1A-CGA-O2A-C1
31	d	406	LHG	C7-C8-C9-C10
25	6	602	CLA	C8-C10-C11-C12
25	S	602	CLA	C8-C10-C11-C12
31	z	103	LHG	O9-C7-O7-C5
31	Z	103	LHG	O9-C7-O7-C5
25	a	404	CLA	C2-C1-O2A-CGA
25	A	404	CLA	C2-C1-O2A-CGA
25	5	611	CLA	C2-C1-O2A-CGA
25	R	611	CLA	C2-C1-O2A-CGA
31	D	406	LHG	C9-C10-C11-C12
34	c	536	LMG	C17-C18-C19-C20
34	g	303	LMG	C32-C33-C34-C35
34	G	303	LMG	C32-C33-C34-C35
25	c	518	CLA	C8-C10-C11-C12
25	C	518	CLA	C8-C10-C11-C12
25	5	611	CLA	O1A-CGA-O2A-C1
25	6	615	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
27	a	407	WVN	C15-C13-C20-C23
27	b	617	WVN	C15-C13-C20-C23
27	b	618	WVN	C06-C13-C20-C23
27	3	620	WVN	C15-C13-C20-C23
27	P	620	WVN	C15-C13-C20-C23
39	5	620	IHT	C02-C07-C18-C22
39	5	620	IHT	C10-C07-C18-C22

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Mol	Chain	Res	Type	Atoms
39	R	620	IHT	C02-C07-C18-C22
39	R	620	IHT	C10-C07-C18-C22
31	b	622	LHG	C25-C26-C27-C28
25	c	519	CLA	C5-C6-C7-C8
25	B	616	CLA	C13-C15-C16-C17
25	C	519	CLA	C5-C6-C7-C8
25	4	603	CLA	C13-C15-C16-C17
25	5	613	CLA	C5-C6-C7-C8
25	G	301	CLA	C13-C15-C16-C17
25	Q	603	CLA	C13-C15-C16-C17
34	F	99	LMG	C15-C16-C17-C18
34	O	622	LMG	C12-C13-C14-C15
25	d	404	CLA	C14-C13-C15-C16
25	4	604	CLA	C14-C13-C15-C16
25	Q	604	CLA	C14-C13-C15-C16
34	2	622	LMG	C12-C13-C14-C15
25	3	603	CLA	C13-C15-C16-C17
25	P	603	CLA	C13-C15-C16-C17
37	1	613	KC2	CAA-CBA-CGA-O2A
37	N	613	KC2	CAA-CBA-CGA-O2A
31	3	621	LHG	C9-C10-C11-C12
25	b	604	CLA	C4-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	C	520	CLA	C4-C3-C5-C6
25	R	609	CLA	C4-C3-C5-C6
25	N	603	CLA	C4-C3-C5-C6
25	b	604	CLA	O1D-CGD-O2D-CED
25	Q	609	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	C6-C7-C8-C10
25	b	603	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C12-C13-C15
25	b	607	CLA	C11-C10-C8-C7
25	c	517	CLA	C11-C12-C13-C15
25	B	602	CLA	C6-C7-C8-C10
25	B	603	CLA	C6-C7-C8-C10
25	B	605	CLA	C11-C12-C13-C15
25	B	607	CLA	C11-C10-C8-C7
25	C	517	CLA	C11-C12-C13-C15
25	2	604	CLA	C11-C10-C8-C7
25	3	612	CLA	C2-C3-C5-C6
25	5	609	CLA	C2-C3-C5-C6
25	5	609	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	6	602	CLA	C6-C7-C8-C10
25	O	604	CLA	C11-C10-C8-C7
25	P	612	CLA	C2-C3-C5-C6
25	R	609	CLA	C11-C12-C13-C15
25	S	602	CLA	C6-C7-C8-C10
25	N	603	CLA	C2-C3-C5-C6
26	a	405	PHO	C11-C10-C8-C7
26	A	405	PHO	C11-C10-C8-C7
29	d	405	PL9	C43-C44-C46-C47
29	D	405	PL9	C43-C44-C46-C47
25	d	404	CLA	C3-C5-C6-C7
25	D	404	CLA	C3-C5-C6-C7
31	P	621	LHG	C9-C10-C11-C12
27	d	408	WVN	C22-C26-C29-C31
38	6	618	II0	C26-C30-C32-C34
38	S	618	II0	C26-C30-C32-C34
25	B	616	CLA	C16-C17-C18-C20
25	O	611	CLA	C11-C12-C13-C14
25	b	610	CLA	O1D-CGD-O2D-CED
34	m	101	LMG	O9-C10-O7-C8
34	M	101	LMG	O9-C10-O7-C8
34	g	303	LMG	C10-C11-C12-C13
34	G	303	LMG	C10-C11-C12-C13
25	b	607	CLA	CBA-CGA-O2A-C1
25	B	607	CLA	CBA-CGA-O2A-C1
25	c	519	CLA	C2A-CAA-CBA-CGA
25	c	520	CLA	C2A-CAA-CBA-CGA
25	C	519	CLA	C2A-CAA-CBA-CGA
25	C	520	CLA	C2A-CAA-CBA-CGA
25	1	602	CLA	C2A-CAA-CBA-CGA
25	P	615	CLA	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA
31	l	101	LHG	C33-C34-C35-C36
31	L	101	LHG	C33-C34-C35-C36
31	d	406	LHG	C9-C10-C11-C12
34	f	99	LMG	C15-C16-C17-C18
26	a	405	PHO	C13-C15-C16-C17
26	A	405	PHO	C13-C15-C16-C17
31	a	413	LHG	C25-C26-C27-C28
31	a	413	LHG	C26-C27-C28-C29
26	a	405	PHO	CBD-CGD-O2D-CED
26	A	405	PHO	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	611	CLA	C11-C12-C13-C14
25	G	301	CLA	C16-C17-C18-C20
31	A	413	LHG	C26-C27-C28-C29
31	z	103	LHG	C8-C7-O7-C5
31	Z	103	LHG	C8-C7-O7-C5
31	3	621	LHG	C8-C7-O7-C5
31	5	621	LHG	C8-C7-O7-C5
31	P	621	LHG	C8-C7-O7-C5
31	R	621	LHG	C8-C7-O7-C5
34	m	101	LMG	C11-C10-O7-C8
34	M	101	LMG	C11-C10-O7-C8
36	E	102	HEM	C4B-C3B-CAB-CBB
37	1	611	KC2	C4C-C3C-CAC-CBC
37	N	611	KC2	C4C-C3C-CAC-CBC
25	c	523	CLA	C15-C16-C17-C18
25	B	616	CLA	C5-C6-C7-C8
25	C	525	CLA	CBD-CGD-O2D-CED
37	P	606	KC2	CBD-CGD-O2D-CED
31	P	621	LHG	O9-C7-O7-C5
34	M	101	LMG	C28-C29-C30-C31
31	A	413	LHG	C25-C26-C27-C28
35	c	532	DGD	C3A-C4A-C5A-C6A
25	S	601	CLA	O1D-CGD-O2D-CED
34	z	102	LMG	O7-C8-C9-O8
34	Z	102	LMG	O7-C8-C9-O8
25	6	601	CLA	O1D-CGD-O2D-CED
25	c	524	CLA	C16-C17-C18-C19
31	L	101	LHG	C32-C33-C34-C35
31	5	621	LHG	C29-C30-C31-C32
31	R	621	LHG	C29-C30-C31-C32
25	b	616	CLA	C5-C6-C7-C8
25	C	523	CLA	C15-C16-C17-C18
25	B	610	CLA	O1D-CGD-O2D-CED
25	g	301	CLA	C4-C3-C5-C6
25	P	612	CLA	C4-C3-C5-C6
29	a	409	PL9	C12-C11-C9-C10
29	A	409	PL9	C12-C11-C9-C10
25	b	603	CLA	C2-C3-C5-C6
25	B	603	CLA	C2-C3-C5-C6
25	R	609	CLA	C2-C3-C5-C6
29	d	405	PL9	C4-C3-C7-C8
29	D	405	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
38	2	616	II0	C09-C21-C23-C25
38	3	618	II0	C10-C22-C24-C26
38	6	617	II0	C09-C21-C23-C25
38	1	616	II0	C09-C21-C23-C25
38	O	616	II0	C09-C21-C23-C25
38	O	617	II0	C09-C21-C23-C25
38	P	618	II0	C10-C22-C24-C26
38	P	619	II0	C09-C21-C23-C25
38	Q	619	II0	C10-C22-C24-C26
38	S	619	II0	C09-C21-C23-C25
38	N	619	II0	C09-C21-C23-C25
25	b	603	CLA	C6-C7-C8-C9
25	b	612	CLA	C6-C7-C8-C9
25	c	522	CLA	C14-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C9
25	B	608	CLA	C14-C13-C15-C16
25	B	612	CLA	C6-C7-C8-C9
25	C	522	CLA	C14-C13-C15-C16
25	2	604	CLA	C11-C10-C8-C9
25	3	604	CLA	C11-C10-C8-C9
25	5	606	CLA	C11-C10-C8-C9
25	6	602	CLA	C6-C7-C8-C9
25	6	602	CLA	C11-C12-C13-C14
25	G	301	CLA	C11-C10-C8-C9
25	1	610	CLA	C11-C10-C8-C9
25	O	604	CLA	C11-C10-C8-C9
25	P	604	CLA	C11-C10-C8-C9
25	R	606	CLA	C11-C10-C8-C9
25	S	602	CLA	C6-C7-C8-C9
25	S	602	CLA	C11-C12-C13-C14
25	N	610	CLA	C11-C10-C8-C9
26	a	405	PHO	C11-C10-C8-C9
26	A	405	PHO	C11-C10-C8-C9
34	w	134	LMG	O6-C5-C6-O5
35	h	90	DGD	O6E-C5E-C6E-O5E
35	H	90	DGD	O6E-C5E-C6E-O5E
25	3	615	CLA	C2A-CAA-CBA-CGA
25	4	604	CLA	C2A-CAA-CBA-CGA
25	6	610	CLA	C2A-CAA-CBA-CGA
25	1	604	CLA	C2A-CAA-CBA-CGA
25	1	615	CLA	C2A-CAA-CBA-CGA
25	Q	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	Q	609	CLA	C2A-CAA-CBA-CGA
25	S	610	CLA	C2A-CAA-CBA-CGA
25	N	604	CLA	C2A-CAA-CBA-CGA
25	N	615	CLA	C2A-CAA-CBA-CGA
31	l	101	LHG	C32-C33-C34-C35
31	6	621	LHG	C11-C10-C9-C8
34	W	134	LMG	O6-C5-C6-O5
27	b	618	WVN	C20-C23-C25-C27
25	3	603	CLA	C5-C6-C7-C8
25	O	603	CLA	C8-C10-C11-C12
25	O	607	CLA	C10-C11-C12-C13
31	B	622	LHG	C25-C26-C27-C28
27	b	617	WVN	C30-C33-C34-C37
27	b	618	WVN	C20-C23-C25-C28
38	N	619	II0	C31-C33-C35-C39
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C1A-C2A-CAA-CBA
25	c	518	CLA	C1A-C2A-CAA-CBA
25	c	524	CLA	C1A-C2A-CAA-CBA
25	c	526	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C1A-C2A-CAA-CBA
25	C	518	CLA	C1A-C2A-CAA-CBA
25	C	524	CLA	C1A-C2A-CAA-CBA
25	C	526	CLA	C1A-C2A-CAA-CBA
25	3	603	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C1A-C2A-CAA-CBA
25	4	607	CLA	C1A-C2A-CAA-CBA
25	5	603	CLA	C1A-C2A-CAA-CBA
25	5	615	CLA	C1A-C2A-CAA-CBA
25	6	603	CLA	C1A-C2A-CAA-CBA
25	6	609	CLA	C1A-C2A-CAA-CBA
25	1	601	CLA	C1A-C2A-CAA-CBA
25	1	607	CLA	C1A-C2A-CAA-CBA
25	P	603	CLA	C1A-C2A-CAA-CBA
25	P	610	CLA	C1A-C2A-CAA-CBA
25	Q	606	CLA	C1A-C2A-CAA-CBA
25	Q	607	CLA	C1A-C2A-CAA-CBA
25	R	603	CLA	C1A-C2A-CAA-CBA
25	R	615	CLA	C1A-C2A-CAA-CBA
25	N	601	CLA	C1A-C2A-CAA-CBA
31	3	621	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
31	S	621	LHG	C11-C10-C9-C8
27	b	617	WVN	C34-C37-C40-C39
39	4	620	IHT	C33-C37-C40-C41
25	2	603	CLA	C8-C10-C11-C12
25	2	607	CLA	C10-C11-C12-C13
25	2	610	CLA	C13-C15-C16-C17
25	O	610	CLA	C13-C15-C16-C17
31	b	622	LHG	C4-O6-P-O3
37	3	606	KC2	CBD-CGD-O2D-CED
25	b	602	CLA	O1D-CGD-O2D-CED
25	c	522	CLA	C13-C15-C16-C17
25	C	522	CLA	C13-C15-C16-C17
25	R	613	CLA	C5-C6-C7-C8
31	b	622	LHG	O6-C4-C5-C6
31	5	621	LHG	O6-C4-C5-C6
31	6	621	LHG	O6-C4-C5-C6
31	R	621	LHG	O6-C4-C5-C6
31	S	621	LHG	O6-C4-C5-C6
34	c	536	LMG	C15-C16-C17-C18
35	C	532	DGD	C3A-C4A-C5A-C6A
25	b	616	CLA	C16-C17-C18-C19
25	C	524	CLA	C16-C17-C18-C19
25	2	613	CLA	C11-C12-C13-C15
25	1	610	CLA	C11-C12-C13-C15
25	O	613	CLA	C11-C12-C13-C15
25	N	610	CLA	C11-C12-C13-C15
25	c	525	CLA	CBD-CGD-O2D-CED
25	c	516	CLA	CBA-CGA-O2A-C1
25	C	516	CLA	CBA-CGA-O2A-C1
31	5	621	LHG	O9-C7-O7-C5
31	R	621	LHG	O9-C7-O7-C5
25	5	609	CLA	C4-C3-C5-C6
25	1	603	CLA	C4-C3-C5-C6
25	b	611	CLA	C13-C15-C16-C17
25	c	519	CLA	CBD-CGD-O2D-CED
25	b	607	CLA	O1A-CGA-O2A-C1
25	3	610	CLA	C2A-CAA-CBA-CGA
25	1	603	CLA	C2A-CAA-CBA-CGA
25	P	610	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C16-C17-C18-C20
25	B	602	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	P	601	CLA	O1D-CGD-O2D-CED
34	w	134	LMG	C7-C8-C9-O8
34	C	536	LMG	O1-C7-C8-C9
34	W	134	LMG	C7-C8-C9-O8
34	4	621	LMG	C7-C8-C9-O8
34	Q	621	LMG	C7-C8-C9-O8
25	B	611	CLA	C13-C15-C16-C17
34	C	536	LMG	C22-C23-C24-C25
34	C	536	LMG	C32-C33-C34-C35
25	3	602	CLA	O1D-CGD-O2D-CED
35	h	90	DGD	O2G-C1B-C2B-C3B
35	H	90	DGD	O2G-C1B-C2B-C3B
25	c	527	CLA	C3-C5-C6-C7
25	C	527	CLA	C3-C5-C6-C7
25	C	519	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	O1A-CGA-O2A-C1
35	c	532	DGD	O6E-C5E-C6E-O5E
35	C	532	DGD	O6E-C5E-C6E-O5E
35	h	90	DGD	C4B-C5B-C6B-C7B
25	P	602	CLA	O1D-CGD-O2D-CED
25	P	603	CLA	C5-C6-C7-C8
34	f	99	LMG	O6-C5-C6-O5
29	d	405	PL9	C15-C14-C16-C17
29	D	405	PL9	C15-C14-C16-C17
25	C	520	CLA	C2-C3-C5-C6
25	2	611	CLA	C11-C12-C13-C15
25	O	611	CLA	C11-C12-C13-C15
25	4	603	CLA	CBA-CGA-O2A-C1
25	Q	603	CLA	CBA-CGA-O2A-C1
31	A	413	LHG	C35-C36-C37-C38
25	b	615	CLA	C5-C6-C7-C8
31	z	103	LHG	C4-C5-O7-C7
31	Z	103	LHG	C4-C5-O7-C7
34	F	99	LMG	O6-C5-C6-O5
25	N	603	CLA	C2A-CAA-CBA-CGA
35	H	90	DGD	C4B-C5B-C6B-C7B
25	5	602	CLA	O1D-CGD-O2D-CED
31	c	535	LHG	C14-C15-C16-C17
25	6	603	CLA	O1D-CGD-O2D-CED
25	R	602	CLA	O1D-CGD-O2D-CED
25	Q	602	CLA	C13-C15-C16-C17
31	a	413	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	a	413	LHG	C24-C23-O8-C6
25	b	616	CLA	C16-C17-C18-C20
25	4	602	CLA	C13-C15-C16-C17
34	M	101	LMG	C29-C30-C31-C32
25	b	612	CLA	C15-C16-C17-C18
25	B	612	CLA	C15-C16-C17-C18
25	G	301	CLA	C10-C11-C12-C13
25	N	609	CLA	O1D-CGD-O2D-CED
25	c	516	CLA	O1A-CGA-O2A-C1
25	C	516	CLA	O1A-CGA-O2A-C1
25	c	523	CLA	C12-C13-C15-C16
25	c	524	CLA	C6-C7-C8-C10
25	C	523	CLA	C12-C13-C15-C16
25	C	524	CLA	C6-C7-C8-C10
25	2	602	CLA	C6-C7-C8-C10
25	2	607	CLA	C6-C7-C8-C10
25	3	602	CLA	C6-C7-C8-C10
25	3	604	CLA	C11-C10-C8-C7
25	5	606	CLA	C11-C10-C8-C7
25	5	610	CLA	C6-C7-C8-C10
25	O	602	CLA	C6-C7-C8-C10
25	O	607	CLA	C6-C7-C8-C10
25	P	602	CLA	C6-C7-C8-C10
25	P	604	CLA	C11-C10-C8-C7
25	R	606	CLA	C11-C10-C8-C7
25	R	610	CLA	C6-C7-C8-C10
25	S	602	CLA	C11-C10-C8-C7
29	a	409	PL9	C12-C11-C9-C8
29	A	409	PL9	C12-C11-C9-C8
25	b	613	CLA	C11-C12-C13-C14
25	c	517	CLA	C6-C7-C8-C9
25	C	517	CLA	C6-C7-C8-C9
25	2	602	CLA	C6-C7-C8-C9
25	2	602	CLA	C11-C10-C8-C9
25	2	602	CLA	C11-C12-C13-C14
25	2	611	CLA	C6-C7-C8-C9
25	3	602	CLA	C6-C7-C8-C9
25	4	603	CLA	C11-C12-C13-C14
25	5	610	CLA	C6-C7-C8-C9
25	5	611	CLA	C6-C7-C8-C9
25	O	602	CLA	C6-C7-C8-C9
25	O	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	O	602	CLA	C11-C12-C13-C14
25	O	602	CLA	C14-C13-C15-C16
25	O	611	CLA	C6-C7-C8-C9
25	P	602	CLA	C6-C7-C8-C9
25	R	610	CLA	C6-C7-C8-C9
25	R	611	CLA	C6-C7-C8-C9
25	2	610	CLA	CBA-CGA-O2A-C1
25	3	613	CLA	CBA-CGA-O2A-C1
25	O	610	CLA	CBA-CGA-O2A-C1
25	P	613	CLA	CBA-CGA-O2A-C1
31	A	413	LHG	C24-C23-O8-C6
25	2	610	CLA	O1D-CGD-O2D-CED
27	h	89	WVN	C11-C19-C22-C24
27	y	89	WVN	C20-C23-C25-C27
25	2	613	CLA	C11-C12-C13-C14
25	1	610	CLA	C11-C12-C13-C14
25	O	613	CLA	C11-C12-C13-C14
25	N	610	CLA	C11-C12-C13-C14
31	C	535	LHG	C12-C13-C14-C15
31	C	535	LHG	C24-C25-C26-C27
31	O	621	LHG	C7-C8-C9-C10
27	y	89	WVN	C20-C23-C25-C28
25	O	610	CLA	O1D-CGD-O2D-CED
25	C	526	CLA	CBA-CGA-O2A-C1
34	D	402	LMG	C29-C28-O8-C9
25	b	609	CLA	C15-C16-C17-C18
31	l	101	LHG	O6-C4-C5-C6
31	B	622	LHG	O6-C4-C5-C6
31	L	101	LHG	O6-C4-C5-C6
31	2	621	LHG	C7-C8-C9-C10
25	c	526	CLA	CBA-CGA-O2A-C1
34	d	402	LMG	C29-C28-O8-C9
25	c	527	CLA	C5-C6-C7-C8
25	B	609	CLA	C15-C16-C17-C18
25	C	527	CLA	C5-C6-C7-C8
25	4	604	CLA	C10-C11-C12-C13
25	Q	604	CLA	C10-C11-C12-C13
35	c	532	DGD	C6B-C7B-C8B-C9B
35	C	532	DGD	C6B-C7B-C8B-C9B
25	C	528	CLA	C4-C3-C5-C6
25	g	301	CLA	C2-C3-C5-C6
25	P	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	m	101	LMG	C29-C30-C31-C32
25	B	611	CLA	C8-C10-C11-C12
25	c	527	CLA	CBA-CGA-O2A-C1
25	C	527	CLA	CBA-CGA-O2A-C1
34	W	134	LMG	C29-C28-O8-C9
25	3	604	CLA	O1D-CGD-O2D-CED
25	b	612	CLA	C3A-C2A-CAA-CBA
25	c	527	CLA	C3A-C2A-CAA-CBA
25	B	612	CLA	C3A-C2A-CAA-CBA
25	C	527	CLA	C3A-C2A-CAA-CBA
25	2	603	CLA	C3A-C2A-CAA-CBA
25	2	611	CLA	C3A-C2A-CAA-CBA
25	3	613	CLA	C3A-C2A-CAA-CBA
25	O	603	CLA	C3A-C2A-CAA-CBA
25	O	611	CLA	C3A-C2A-CAA-CBA
27	c	529	WVN	C25-C28-C30-C33
27	c	530	WVN	C34-C37-C40-C39
27	y	89	WVN	C22-C26-C29-C31
27	3	620	WVN	C25-C28-C30-C33
27	P	620	WVN	C25-C28-C30-C33
39	Q	620	IHT	C33-C37-C40-C41
39	R	620	IHT	C23-C27-C30-C32
25	b	611	CLA	C8-C10-C11-C12
31	3	621	LHG	C13-C14-C15-C16
25	2	613	CLA	C5-C6-C7-C8
25	O	613	CLA	C5-C6-C7-C8
31	C	535	LHG	C4-C5-C6-O8
34	b	620	LMG	C7-C8-C9-O8
34	c	536	LMG	C7-C8-C9-O8
34	z	102	LMG	C7-C8-C9-O8
34	B	620	LMG	C7-C8-C9-O8
34	Z	102	LMG	C7-C8-C9-O8
31	P	621	LHG	C13-C14-C15-C16
35	H	90	DGD	C6A-C7A-C8A-C9A
35	h	90	DGD	C6A-C7A-C8A-C9A
25	N	602	CLA	O1D-CGD-O2D-CED
34	G	303	LMG	C29-C30-C31-C32
25	c	517	CLA	C4-C3-C5-C6
25	C	517	CLA	C4-C3-C5-C6
25	1	603	CLA	C2-C3-C5-C6
35	h	90	DGD	C8A-C9A-CAA-CBA
25	1	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	4	603	CLA	O1A-CGA-O2A-C1
25	Q	603	CLA	O1A-CGA-O2A-C1
31	b	622	LHG	O1-C1-C2-O2
31	b	622	LHG	C28-C29-C30-C31
31	b	622	LHG	O6-C4-C5-O7
31	6	621	LHG	O6-C4-C5-O7
31	S	621	LHG	O6-C4-C5-O7
37	4	612	KC2	C3A-C2A-CAA-CBA
37	1	612	KC2	C3A-C2A-CAA-CBA
37	Q	612	KC2	C3A-C2A-CAA-CBA
37	N	612	KC2	C3A-C2A-CAA-CBA
25	5	613	CLA	C6-C7-C8-C9
25	b	606	CLA	C8-C10-C11-C12
31	a	413	LHG	O10-C23-O8-C6
35	H	90	DGD	C8A-C9A-CAA-CBA
34	g	303	LMG	C29-C30-C31-C32
28	a	408	SQD	O47-C45-C46-O48
28	A	408	SQD	O47-C45-C46-O48
34	b	620	LMG	O7-C8-C9-O8
34	d	402	LMG	O7-C8-C9-O8
34	B	620	LMG	O7-C8-C9-O8
34	D	402	LMG	O7-C8-C9-O8
34	w	134	LMG	C29-C28-O8-C9
25	c	527	CLA	C16-C17-C18-C20
25	C	527	CLA	C16-C17-C18-C20
29	D	405	PL9	C45-C44-C46-C47
25	3	603	CLA	C2-C1-O2A-CGA
25	P	603	CLA	C2-C1-O2A-CGA
25	P	613	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	C11-C12-C13-C14
25	c	525	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C10-C8-C9
25	B	616	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C10-C8-C9
25	2	602	CLA	C14-C13-C15-C16
25	3	603	CLA	C6-C7-C8-C9
25	3	610	CLA	C6-C7-C8-C9
25	5	611	CLA	C14-C13-C15-C16
25	6	602	CLA	C11-C10-C8-C9
25	6	610	CLA	C6-C7-C8-C9
25	P	603	CLA	C6-C7-C8-C9
25	P	610	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	Q	603	CLA	C11-C12-C13-C14
25	R	611	CLA	C14-C13-C15-C16
25	S	602	CLA	C11-C10-C8-C9
25	S	610	CLA	C6-C7-C8-C9
25	S	615	CLA	C11-C12-C13-C14
26	d	401	PHO	C6-C7-C8-C9
26	D	401	PHO	C6-C7-C8-C9
31	C	535	LHG	C11-C10-C9-C8
25	2	604	CLA	C8-C10-C11-C12
25	O	604	CLA	C8-C10-C11-C12
25	3	613	CLA	O1A-CGA-O2A-C1
25	3	604	CLA	C2A-CAA-CBA-CGA
25	6	604	CLA	C2A-CAA-CBA-CGA
25	P	604	CLA	C2A-CAA-CBA-CGA
25	S	604	CLA	C2A-CAA-CBA-CGA
27	c	530	WVN	C06-C13-C20-C23
28	a	408	SQD	C11-C10-C9-C8
26	A	405	PHO	O1D-CGD-O2D-CED
38	5	619	II0	C31-C33-C35-C39
38	6	618	II0	C31-C33-C35-C39
38	R	619	II0	C31-C33-C35-C39
38	S	618	II0	C31-C33-C35-C39
25	C	526	CLA	C8-C10-C11-C12
28	A	408	SQD	C11-C10-C9-C8
26	a	405	PHO	O1D-CGD-O2D-CED
34	2	622	LMG	C10-C11-C12-C13
34	O	622	LMG	C10-C11-C12-C13
31	A	413	LHG	C12-C13-C14-C15
25	2	610	CLA	O1A-CGA-O2A-C1
25	O	610	CLA	O1A-CGA-O2A-C1
31	A	413	LHG	O10-C23-O8-C6
37	Q	605	KC2	CAA-CBA-CGA-O1A
25	c	517	CLA	C6-C7-C8-C10
25	c	519	CLA	C6-C7-C8-C10
25	d	400	CLA	C11-C10-C8-C7
25	d	404	CLA	C11-C10-C8-C7
25	B	606	CLA	C6-C7-C8-C10
25	B	607	CLA	C6-C7-C8-C10
25	C	517	CLA	C6-C7-C8-C10
25	C	519	CLA	C6-C7-C8-C10
25	D	400	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	2	602	CLA	C11-C10-C8-C7
25	2	602	CLA	C11-C12-C13-C15
25	2	602	CLA	C12-C13-C15-C16
25	2	604	CLA	C11-C12-C13-C15
25	3	603	CLA	C6-C7-C8-C10
25	3	603	CLA	C11-C10-C8-C7
25	3	609	CLA	C12-C13-C15-C16
25	3	610	CLA	C6-C7-C8-C10
25	4	603	CLA	C11-C10-C8-C7
25	4	603	CLA	C11-C12-C13-C15
25	5	604	CLA	C6-C7-C8-C10
25	5	611	CLA	C6-C7-C8-C10
25	5	611	CLA	C12-C13-C15-C16
25	6	602	CLA	C11-C10-C8-C7
25	6	604	CLA	C12-C13-C15-C16
25	O	602	CLA	C11-C10-C8-C7
25	O	602	CLA	C11-C12-C13-C15
25	O	602	CLA	C12-C13-C15-C16
25	P	603	CLA	C6-C7-C8-C10
25	P	603	CLA	C11-C10-C8-C7
25	P	609	CLA	C12-C13-C15-C16
25	P	610	CLA	C6-C7-C8-C10
25	Q	603	CLA	C11-C10-C8-C7
25	Q	603	CLA	C11-C12-C13-C15
25	R	604	CLA	C6-C7-C8-C10
25	R	611	CLA	C6-C7-C8-C10
25	R	611	CLA	C12-C13-C15-C16
25	S	604	CLA	C12-C13-C15-C16
26	d	401	PHO	C6-C7-C8-C10
26	D	401	PHO	C6-C7-C8-C10
25	C	525	CLA	O1D-CGD-O2D-CED
31	3	621	LHG	C32-C33-C34-C35
27	b	619	WVN	C32-C36-C39-C40
27	h	89	WVN	C22-C26-C29-C31
27	y	89	WVN	C34-C37-C40-C39
27	C	530	WVN	C34-C37-C40-C39
27	C	531	WVN	C25-C28-C30-C33
27	H	89	WVN	C22-C26-C29-C31
38	5	619	II0	C26-C30-C32-C34
38	6	616	II0	C25-C29-C31-C33
38	R	619	II0	C26-C30-C32-C34
38	S	616	II0	C25-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
25	R	613	CLA	C6-C7-C8-C9
25	g	302	CLA	C4C-C3C-CAC-CBC
31	P	621	LHG	C32-C33-C34-C35
37	4	605	KC2	CAA-CBA-CGA-O1A
37	1	613	KC2	C2A-CAA-CBA-CGA
37	N	613	KC2	C2A-CAA-CBA-CGA
25	c	527	CLA	C16-C17-C18-C19
25	C	527	CLA	C16-C17-C18-C19
25	2	603	CLA	C15-C16-C17-C18
25	4	604	CLA	C12-C13-C15-C16
25	Q	604	CLA	C12-C13-C15-C16
34	g	303	LMG	C12-C13-C14-C15
25	O	603	CLA	C15-C16-C17-C18
25	b	608	CLA	CAD-CBD-CGD-O2D
25	c	517	CLA	CAD-CBD-CGD-O2D
25	c	518	CLA	CAD-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	C	517	CLA	CAD-CBD-CGD-O2D
25	3	610	CLA	CAD-CBD-CGD-O2D
25	5	601	CLA	CAD-CBD-CGD-O2D
25	1	601	CLA	CAD-CBD-CGD-O2D
25	1	614	CLA	CAD-CBD-CGD-O2D
25	P	610	CLA	CAD-CBD-CGD-O2D
25	R	601	CLA	CAD-CBD-CGD-O2D
25	N	601	CLA	CAD-CBD-CGD-O2D
25	N	614	CLA	CAD-CBD-CGD-O2D
37	4	605	KC2	CAD-CBD-CGD-O2D
37	1	613	KC2	C2C-C3C-CAC-CBC
37	1	613	KC2	CAD-CBD-CGD-O2D
37	Q	605	KC2	CAD-CBD-CGD-O2D
37	S	606	KC2	CAD-CBD-CGD-O2D
37	N	613	KC2	C2C-C3C-CAC-CBC
37	N	613	KC2	CAD-CBD-CGD-O2D
34	G	303	LMG	C12-C13-C14-C15
25	C	525	CLA	C8-C10-C11-C12
25	4	603	CLA	C5-C6-C7-C8
25	Q	603	CLA	C5-C6-C7-C8
34	c	536	LMG	C18-C19-C20-C21
25	2	613	CLA	CBA-CGA-O2A-C1
25	4	604	CLA	CBA-CGA-O2A-C1
25	G	301	CLA	CBA-CGA-O2A-C1
25	O	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	Q	604	CLA	CBA-CGA-O2A-C1
25	c	524	CLA	C4-C3-C5-C6
25	C	524	CLA	C4-C3-C5-C6
26	A	405	PHO	C4-C3-C5-C6
29	d	405	PL9	C45-C44-C46-C47
25	c	520	CLA	C5-C6-C7-C8
25	2	604	CLA	C15-C16-C17-C18
25	O	604	CLA	C15-C16-C17-C18
34	C	536	LMG	C7-C8-C9-O8
34	D	407	LMG	C11-C10-O7-C8
25	B	609	CLA	C13-C15-C16-C17
25	3	603	CLA	C16-C17-C18-C19
25	3	603	CLA	C16-C17-C18-C20
25	4	606	CLA	C6-C7-C8-C10
25	P	603	CLA	C16-C17-C18-C19
25	P	603	CLA	C16-C17-C18-C20
25	c	525	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	b	611	CLA	CHA-CBD-CGD-O1D
25	b	611	CLA	CHA-CBD-CGD-O2D
25	c	520	CLA	CHA-CBD-CGD-O1D
25	c	520	CLA	CHA-CBD-CGD-O2D
25	c	528	CLA	CHA-CBD-CGD-O1D
25	d	404	CLA	CHA-CBD-CGD-O2D
25	g	302	CLA	CHA-CBD-CGD-O1D
25	g	302	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	609	CLA	CHA-CBD-CGD-O1D
25	B	611	CLA	CHA-CBD-CGD-O1D
25	B	611	CLA	CHA-CBD-CGD-O2D
25	C	520	CLA	CHA-CBD-CGD-O1D
25	C	520	CLA	CHA-CBD-CGD-O2D
25	C	526	CLA	CHA-CBD-CGD-O2D
25	D	404	CLA	CHA-CBD-CGD-O2D
25	3	603	CLA	CHA-CBD-CGD-O1D
25	3	610	CLA	CHA-CBD-CGD-O1D
25	4	604	CLA	CHA-CBD-CGD-O1D
25	4	604	CLA	CHA-CBD-CGD-O2D
25	5	604	CLA	CHA-CBD-CGD-O1D
25	5	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	6	601	CLA	CHA-CBD-CGD-O1D
25	6	604	CLA	CHA-CBD-CGD-O2D
25	G	302	CLA	CHA-CBD-CGD-O1D
25	P	603	CLA	CHA-CBD-CGD-O1D
25	P	610	CLA	CHA-CBD-CGD-O1D
25	Q	604	CLA	CHA-CBD-CGD-O1D
25	Q	604	CLA	CHA-CBD-CGD-O2D
25	Q	609	CLA	CHA-CBD-CGD-O1D
25	R	604	CLA	CHA-CBD-CGD-O1D
25	R	610	CLA	CHA-CBD-CGD-O2D
25	S	601	CLA	CHA-CBD-CGD-O1D
25	S	604	CLA	CHA-CBD-CGD-O2D
37	1	605	KC2	CHA-CBD-CGD-O1D
37	1	605	KC2	CHA-CBD-CGD-O2D
37	N	605	KC2	CHA-CBD-CGD-O1D
37	N	605	KC2	CHA-CBD-CGD-O2D
25	c	526	CLA	O1A-CGA-O2A-C1
25	C	526	CLA	O1A-CGA-O2A-C1
34	d	402	LMG	O10-C28-O8-C9
34	D	402	LMG	O10-C28-O8-C9
34	W	134	LMG	O10-C28-O8-C9
25	b	609	CLA	C13-C15-C16-C17
31	C	535	LHG	O7-C5-C6-O8
34	C	536	LMG	O7-C8-C9-O8
34	4	621	LMG	O7-C8-C9-O8
34	Q	621	LMG	O7-C8-C9-O8
25	c	525	CLA	C8-C10-C11-C12
25	c	527	CLA	O1A-CGA-O2A-C1
25	C	527	CLA	O1A-CGA-O2A-C1
31	6	621	LHG	C15-C16-C17-C18
31	S	621	LHG	C15-C16-C17-C18
25	5	613	CLA	C6-C7-C8-C10
25	c	519	CLA	O1D-CGD-O2D-CED
25	c	528	CLA	C3-C5-C6-C7
34	d	407	LMG	C11-C10-O7-C8
26	a	405	PHO	C4-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
38	2	618	II0	C10-C22-C24-C26
38	3	616	II0	C10-C22-C24-C26
38	3	619	II0	C09-C21-C23-C25
38	3	619	II0	C10-C22-C24-C26
38	4	618	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
38	4	618	II0	C10-C22-C24-C26
38	4	619	II0	C10-C22-C24-C26
38	5	617	II0	C10-C22-C24-C26
38	6	616	II0	C10-C22-C24-C26
38	O	618	II0	C09-C21-C23-C25
38	O	618	II0	C10-C22-C24-C26
38	P	616	II0	C10-C22-C24-C26
38	P	619	II0	C10-C22-C24-C26
38	Q	618	II0	C10-C22-C24-C26
38	R	617	II0	C10-C22-C24-C26
38	S	616	II0	C10-C22-C24-C26
38	S	617	II0	C09-C21-C23-C25
39	2	620	IHT	C11-C21-C24-C26
39	Q	620	IHT	C11-C21-C24-C26
34	d	407	LMG	O9-C10-O7-C8
34	D	407	LMG	O9-C10-O7-C8
25	C	525	CLA	C6-C7-C8-C9
25	2	604	CLA	C11-C12-C13-C14
25	3	609	CLA	C14-C13-C15-C16
25	5	606	CLA	C14-C13-C15-C16
25	6	604	CLA	C14-C13-C15-C16
25	6	615	CLA	C11-C12-C13-C14
25	O	604	CLA	C11-C12-C13-C14
25	P	609	CLA	C14-C13-C15-C16
25	R	606	CLA	C14-C13-C15-C16
25	S	604	CLA	C14-C13-C15-C16
31	6	621	LHG	C14-C15-C16-C17
34	C	536	LMG	C12-C13-C14-C15
25	C	519	CLA	O1D-CGD-O2D-CED
34	c	536	LMG	C29-C30-C31-C32
25	A	403	CLA	C2A-CAA-CBA-CGA
27	b	618	WVN	C30-C33-C34-C38
27	b	619	WVN	C20-C23-C25-C27
27	c	529	WVN	C11-C19-C22-C24
27	H	89	WVN	C11-C19-C22-C24
31	S	621	LHG	C14-C15-C16-C17
27	b	618	WVN	C30-C33-C34-C37
27	b	619	WVN	C20-C23-C25-C28
27	c	529	WVN	C11-C19-C22-C26
27	h	89	WVN	C11-C19-C22-C26
27	B	618	WVN	C20-C23-C25-C28
27	H	89	WVN	C11-C19-C22-C26

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Mol	Chain	Res	Type	Atoms
39	R	620	IHT	C18-C22-C23-C27
31	A	413	LHG	C30-C31-C32-C33
25	b	611	CLA	C1A-C2A-CAA-CBA
25	c	527	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
25	B	611	CLA	C1A-C2A-CAA-CBA
25	B	612	CLA	C1A-C2A-CAA-CBA
25	C	527	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	603	CLA	C1A-C2A-CAA-CBA
25	3	602	CLA	C1A-C2A-CAA-CBA
25	6	613	CLA	C1A-C2A-CAA-CBA
25	O	602	CLA	C1A-C2A-CAA-CBA
25	P	602	CLA	C1A-C2A-CAA-CBA
25	S	613	CLA	C1A-C2A-CAA-CBA
25	2	603	CLA	C16-C17-C18-C19
25	3	613	CLA	C6-C7-C8-C10
25	O	603	CLA	C16-C17-C18-C19
25	P	613	CLA	C6-C7-C8-C10
27	c	531	WVN	C34-C37-C40-C39
31	c	535	LHG	C3-O3-P-O6
31	d	406	LHG	C4-O6-P-O3
31	6	621	LHG	C4-O6-P-O3
31	S	621	LHG	C4-O6-P-O3
31	a	413	LHG	C30-C31-C32-C33
25	2	611	CLA	C4-C3-C5-C6
25	O	611	CLA	C4-C3-C5-C6
31	a	413	LHG	C5-C4-O6-P
31	A	413	LHG	C5-C4-O6-P
25	B	604	CLA	C2-C3-C5-C6
31	a	413	LHG	C31-C32-C33-C34
31	c	535	LHG	C10-C11-C12-C13
34	w	134	LMG	O10-C28-O8-C9
31	a	413	LHG	C4-O6-P-O4
31	A	413	LHG	C4-O6-P-O4
31	B	622	LHG	C3-O3-P-O5
31	5	621	LHG	C3-O3-P-O4
31	R	621	LHG	C3-O3-P-O4
25	a	404	CLA	O2A-C1-C2-C3
25	A	404	CLA	O2A-C1-C2-C3
25	6	604	CLA	CBA-CGA-O2A-C1
25	S	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	A	413	LHG	C31-C32-C33-C34
25	a	403	CLA	C2A-CAA-CBA-CGA
25	2	613	CLA	O1A-CGA-O2A-C1
25	4	604	CLA	O1A-CGA-O2A-C1
25	O	613	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	611	CLA	CAD-CBD-CGD-O1D
25	c	520	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	611	CLA	CAD-CBD-CGD-O1D
25	C	520	CLA	CAD-CBD-CGD-O1D
25	4	604	CLA	CAD-CBD-CGD-O1D
25	5	613	CLA	CAD-CBD-CGD-O1D
25	Q	604	CLA	CAD-CBD-CGD-O1D
37	1	605	KC2	CAD-CBD-CGD-O1D
37	N	605	KC2	CAD-CBD-CGD-O1D
25	Q	603	CLA	C8-C10-C11-C12
25	Q	604	CLA	O1A-CGA-O2A-C1
25	g	302	CLA	C2C-C3C-CAC-CBC
34	m	101	LMG	C28-C29-C30-C31
31	5	621	LHG	C9-C10-C11-C12
25	4	603	CLA	C8-C10-C11-C12
31	R	621	LHG	C9-C10-C11-C12
25	A	406	CLA	C11-C12-C13-C15
25	b	606	CLA	C6-C7-C8-C10
25	b	607	CLA	C6-C7-C8-C10
25	c	518	CLA	C11-C10-C8-C7
25	C	518	CLA	C11-C10-C8-C7
25	3	602	CLA	C11-C12-C13-C15
25	4	604	CLA	C11-C12-C13-C15
25	5	604	CLA	C11-C10-C8-C7
25	6	602	CLA	C12-C13-C15-C16
25	6	610	CLA	C6-C7-C8-C10
25	G	301	CLA	C12-C13-C15-C16
25	O	604	CLA	C11-C12-C13-C15
25	P	602	CLA	C11-C12-C13-C15
25	Q	604	CLA	C11-C12-C13-C15
25	R	604	CLA	C11-C10-C8-C7
25	S	602	CLA	C12-C13-C15-C16
25	S	610	CLA	C6-C7-C8-C10
27	c	530	WVN	C05-C02-C11-C19
27	C	530	WVN	C05-C02-C11-C19

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Mol	Chain	Res	Type	Atoms
27	6	620	WVN	C05-C02-C11-C19
27	S	620	WVN	C05-C02-C11-C19
31	l	101	LHG	O6-C4-C5-O7
31	D	406	LHG	O6-C4-C5-O7
31	L	101	LHG	O6-C4-C5-O7
31	5	621	LHG	O6-C4-C5-O7
31	P	621	LHG	C7-C8-C9-C10
31	R	621	LHG	O6-C4-C5-O7
34	d	402	LMG	C13-C14-C15-C16
34	C	536	LMG	C17-C18-C19-C20
25	B	606	CLA	C8-C10-C11-C12
25	2	601	CLA	C2A-CAA-CBA-CGA
25	O	601	CLA	C2A-CAA-CBA-CGA
31	3	621	LHG	C7-C8-C9-C10
34	B	620	LMG	C14-C15-C16-C17
34	c	536	LMG	C32-C33-C34-C35
25	C	522	CLA	C16-C17-C18-C20
25	5	615	CLA	CBA-CGA-O2A-C1
31	A	413	LHG	C2-C3-O3-P
25	6	604	CLA	O1A-CGA-O2A-C1
25	S	604	CLA	O1A-CGA-O2A-C1
25	b	607	CLA	C8-C10-C11-C12
31	R	621	LHG	C18-C19-C20-C21
34	D	402	LMG	C13-C14-C15-C16
26	a	405	PHO	C2-C3-C5-C6
26	A	405	PHO	C2-C3-C5-C6
25	5	610	CLA	C8-C10-C11-C12
25	R	610	CLA	C8-C10-C11-C12
25	b	610	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C10-C8-C9
25	c	519	CLA	C6-C7-C8-C9
25	d	400	CLA	C11-C10-C8-C9
25	B	606	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C10-C8-C9
25	C	519	CLA	C6-C7-C8-C9
25	D	400	CLA	C11-C10-C8-C9
25	4	603	CLA	C11-C10-C8-C9
25	Q	603	CLA	C11-C10-C8-C9
25	c	522	CLA	C16-C17-C18-C20
31	5	621	LHG	C18-C19-C20-C21
25	G	301	CLA	O1A-CGA-O2A-C1
27	y	89	WVN	C29-C31-C32-C36

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Mol	Chain	Res	Type	Atoms
25	C	520	CLA	C5-C6-C7-C8
25	R	615	CLA	CBA-CGA-O2A-C1
25	c	526	CLA	C8-C10-C11-C12
31	P	621	LHG	C35-C36-C37-C38
34	c	536	LMG	C12-C13-C14-C15
25	b	615	CLA	C15-C16-C17-C18
25	a	404	CLA	C1-C2-C3-C4
25	A	404	CLA	C1-C2-C3-C4
31	a	413	LHG	C9-C10-C11-C12
25	4	610	CLA	C2A-CAA-CBA-CGA
25	5	604	CLA	C2A-CAA-CBA-CGA
25	Q	610	CLA	C2A-CAA-CBA-CGA
25	R	604	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	O1A-CGA-O2A-C1
25	B	610	CLA	O1A-CGA-O2A-C1
25	D	404	CLA	CBA-CGA-O2A-C1
25	3	610	CLA	C2-C1-O2A-CGA
25	S	603	CLA	C2-C1-O2A-CGA
34	g	303	LMG	C4-C5-C6-O5
34	G	303	LMG	C4-C5-C6-O5
25	5	611	CLA	C13-C15-C16-C17
25	R	611	CLA	C13-C15-C16-C17
25	D	404	CLA	O1A-CGA-O2A-C1
31	3	621	LHG	C35-C36-C37-C38
31	a	413	LHG	C2-C3-O3-P
31	a	413	LHG	C10-C11-C12-C13
25	b	610	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
25	B	610	CLA	CBA-CGA-O2A-C1
27	S	620	WVN	C22-C26-C29-C31
25	d	404	CLA	O1A-CGA-O2A-C1
31	B	622	LHG	O6-C4-C5-O7
25	B	615	CLA	C15-C16-C17-C18
27	d	408	WVN	C06-C13-C20-C23
27	h	89	WVN	C06-C13-C20-C23
27	B	619	WVN	C06-C13-C20-C23
25	c	524	CLA	C2-C3-C5-C6
34	g	303	LMG	C34-C35-C36-C37
34	G	303	LMG	C34-C35-C36-C37
25	N	607	CLA	C4C-C3C-CAC-CBC
25	S	609	CLA	C6-C7-C8-C9
25	B	607	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	1	607	CLA	C4C-C3C-CAC-CBC
34	g	303	LMG	O1-C7-C8-O7
31	d	406	LHG	C3-O3-P-O6
31	l	101	LHG	C3-O3-P-O6
31	z	103	LHG	C3-O3-P-O6
31	z	103	LHG	C4-O6-P-O3
31	B	622	LHG	C4-O6-P-O3
31	D	406	LHG	C3-O3-P-O6
31	D	406	LHG	C4-O6-P-O3
31	L	101	LHG	C3-O3-P-O6
31	Z	103	LHG	C3-O3-P-O6
31	Z	103	LHG	C4-O6-P-O3
31	2	621	LHG	C3-O3-P-O6
31	2	621	LHG	C4-O6-P-O3
31	3	621	LHG	C3-O3-P-O6
31	3	621	LHG	C4-O6-P-O3
31	6	621	LHG	C3-O3-P-O6
31	O	621	LHG	C3-O3-P-O6
31	O	621	LHG	C4-O6-P-O3
31	P	621	LHG	C3-O3-P-O6
31	P	621	LHG	C4-O6-P-O3
31	S	621	LHG	C3-O3-P-O6
34	d	402	LMG	C28-C29-C30-C31
34	D	402	LMG	C28-C29-C30-C31
26	d	401	PHO	CHA-CBD-CGD-O2D
26	D	401	PHO	CHA-CBD-CGD-O2D
34	b	620	LMG	C14-C15-C16-C17
25	c	523	CLA	C11-C10-C8-C7
25	C	524	CLA	C2-C3-C5-C6
25	G	301	CLA	C6-C7-C8-C10
25	S	615	CLA	C11-C12-C13-C15
25	b	606	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C10-C8-C9
25	c	518	CLA	C11-C10-C8-C9
25	c	523	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C10-C8-C9
25	B	610	CLA	C11-C12-C13-C14
25	C	518	CLA	C11-C10-C8-C9
25	C	523	CLA	C14-C13-C15-C16
25	2	610	CLA	C14-C13-C15-C16
25	3	603	CLA	C11-C10-C8-C9
25	4	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	5	604	CLA	C11-C10-C8-C9
25	6	602	CLA	C14-C13-C15-C16
25	O	610	CLA	C14-C13-C15-C16
25	P	603	CLA	C11-C10-C8-C9
25	Q	604	CLA	C11-C12-C13-C14
25	R	604	CLA	C11-C10-C8-C9
25	S	602	CLA	C14-C13-C15-C16
31	C	535	LHG	C26-C27-C28-C29
34	c	536	LMG	C31-C32-C33-C34
34	4	621	LMG	C33-C34-C35-C36
25	1	603	CLA	C3-C5-C6-C7
34	Q	621	LMG	C33-C34-C35-C36
31	A	413	LHG	O1-C1-C2-C3
31	3	621	LHG	C11-C10-C9-C8
25	Q	603	CLA	C15-C16-C17-C18
25	d	404	CLA	C12-C13-C15-C16
31	2	621	LHG	C1-C2-C3-O3
31	O	621	LHG	C1-C2-C3-O3
25	4	603	CLA	C15-C16-C17-C18
25	6	603	CLA	C5-C6-C7-C8
29	d	405	PL9	C13-C14-C16-C17
29	D	405	PL9	C13-C14-C16-C17
25	b	604	CLA	C11-C12-C13-C14
25	a	406	CLA	C11-C12-C13-C15
25	c	523	CLA	C16-C17-C18-C20
25	3	613	CLA	C6-C7-C8-C9
25	P	613	CLA	C6-C7-C8-C9
25	C	523	CLA	CBA-CGA-O2A-C1
31	P	621	LHG	C11-C10-C9-C8
31	A	413	LHG	C9-C10-C11-C12
25	C	524	CLA	C13-C15-C16-C17
25	6	604	CLA	C15-C16-C17-C18
25	S	604	CLA	C15-C16-C17-C18
25	C	523	CLA	O1A-CGA-O2A-C1
25	S	601	CLA	CBA-CGA-O2A-C1
27	a	407	WVN	C22-C26-C29-C31
27	b	619	WVN	C34-C37-C40-C39
27	3	620	WVN	C32-C36-C39-C40
27	3	620	WVN	C34-C37-C40-C39
27	P	620	WVN	C32-C36-C39-C40
27	P	620	WVN	C34-C37-C40-C39
38	3	618	II0	C26-C30-C32-C34

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Mol	Chain	Res	Type	Atoms
38	3	619	II0	C36-C40-C42-C41
38	4	619	II0	C26-C30-C32-C34
38	P	618	II0	C26-C30-C32-C34
38	P	619	II0	C36-C40-C42-C41
38	Q	619	II0	C26-C30-C32-C34
25	c	527	CLA	C15-C16-C17-C18
25	C	527	CLA	C15-C16-C17-C18
31	d	406	LHG	O6-C4-C5-O7
25	6	615	CLA	C16-C17-C18-C20
25	1	606	CLA	CAA-CBA-CGA-O2A
25	N	606	CLA	CAA-CBA-CGA-O2A
37	1	613	KC2	C4C-C3C-CAC-CBC
37	N	613	KC2	C4C-C3C-CAC-CBC
28	a	411	SQD	C11-C10-C9-C8
28	A	411	SQD	C11-C10-C9-C8
36	E	102	HEM	CAD-CBD-CGD-O2D
25	4	606	CLA	C5-C6-C7-C8
31	2	621	LHG	C11-C10-C9-C8
25	b	601	CLA	CBD-CGD-O2D-CED
25	2	603	CLA	CAA-CBA-CGA-O2A
25	O	603	CLA	CAA-CBA-CGA-O2A
25	d	404	CLA	C2-C1-O2A-CGA
25	D	404	CLA	C2-C1-O2A-CGA
25	6	610	CLA	C2-C1-O2A-CGA
25	P	610	CLA	C2-C1-O2A-CGA
25	S	610	CLA	C2-C1-O2A-CGA
25	C	522	CLA	C16-C17-C18-C19
25	C	523	CLA	C16-C17-C18-C20
25	S	615	CLA	C16-C17-C18-C20
25	B	604	CLA	C11-C12-C13-C14
25	b	603	CLA	C2A-CAA-CBA-CGA
25	B	603	CLA	C2A-CAA-CBA-CGA
25	B	616	CLA	C2A-CAA-CBA-CGA
25	2	604	CLA	C2A-CAA-CBA-CGA
25	5	602	CLA	C2A-CAA-CBA-CGA
25	1	610	CLA	C2A-CAA-CBA-CGA
25	O	604	CLA	C2A-CAA-CBA-CGA
25	R	602	CLA	C2A-CAA-CBA-CGA
25	N	610	CLA	C2A-CAA-CBA-CGA
25	6	601	CLA	CBA-CGA-O2A-C1
34	C	536	LMG	C28-C29-C30-C31
25	c	524	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
35	H	90	DGD	O1B-C1B-C2B-C3B
31	A	413	LHG	C10-C11-C12-C13
25	d	403	CLA	C3A-C2A-CAA-CBA
25	D	403	CLA	C3A-C2A-CAA-CBA
25	R	613	CLA	C3A-C2A-CAA-CBA
25	2	604	CLA	C16-C17-C18-C19
25	O	604	CLA	C16-C17-C18-C19
35	h	90	DGD	O1B-C1B-C2B-C3B
27	C	529	WVN	C32-C36-C39-C40
27	S	620	WVN	C25-C28-C30-C33
38	P	616	II0	C26-C30-C32-C34
39	R	620	IHT	C33-C37-C40-C41
31	O	621	LHG	C11-C10-C9-C8
36	e	102	HEM	CAA-CBA-CGA-O1A
28	A	408	SQD	C33-C34-C35-C36
34	c	536	LMG	C19-C20-C21-C22
35	h	90	DGD	CBB-CCB-CDB-CEB
35	H	90	DGD	C3B-C4B-C5B-C6B
29	a	409	PL9	C4-C3-C7-C8
29	A	409	PL9	C4-C3-C7-C8
38	3	617	II0	C09-C21-C23-C25
38	4	617	II0	C09-C21-C23-C25
38	1	617	II0	C10-C22-C24-C26
38	Q	617	II0	C09-C21-C23-C25
38	N	617	II0	C10-C22-C24-C26
39	O	620	IHT	C11-C21-C24-C26
25	2	615	CLA	O1D-CGD-O2D-CED
25	b	603	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14
25	B	616	CLA	C14-C13-C15-C16
25	2	611	CLA	C11-C10-C8-C9
25	G	301	CLA	C11-C12-C13-C14
25	O	611	CLA	C11-C10-C8-C9
26	a	405	PHO	C6-C7-C8-C9
26	A	405	PHO	C6-C7-C8-C9
25	c	522	CLA	C16-C17-C18-C19
34	M	101	LMG	C34-C35-C36-C37
25	B	612	CLA	C2A-CAA-CBA-CGA
25	O	615	CLA	O1D-CGD-O2D-CED
35	H	90	DGD	CBB-CCB-CDB-CEB
25	A	406	CLA	C11-C12-C13-C14
25	S	609	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	5	603	CLA	O2A-C1-C2-C3
25	R	603	CLA	O2A-C1-C2-C3
25	G	302	CLA	CAA-CBA-CGA-O1A
36	e	102	HEM	CAD-CBD-CGD-O2D
34	m	101	LMG	C34-C35-C36-C37
34	W	134	LMG	C34-C35-C36-C37
31	O	621	LHG	C24-C25-C26-C27
25	b	604	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	b	614	CLA	C1A-C2A-CAA-CBA
25	c	521	CLA	C1A-C2A-CAA-CBA
25	B	604	CLA	C1A-C2A-CAA-CBA
25	C	521	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C1A-C2A-CAA-CBA
25	4	610	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	O	603	CLA	C1A-C2A-CAA-CBA
25	Q	610	CLA	C1A-C2A-CAA-CBA
25	S	602	CLA	C1A-C2A-CAA-CBA
25	N	607	CLA	C1A-C2A-CAA-CBA
31	B	622	LHG	O9-C7-O7-C5
25	b	612	CLA	C11-C10-C8-C7
25	B	612	CLA	C11-C10-C8-C7
25	C	523	CLA	C11-C10-C8-C7
25	4	604	CLA	C6-C7-C8-C10
25	6	604	CLA	C11-C12-C13-C15
25	6	615	CLA	C11-C12-C13-C15
25	Q	604	CLA	C6-C7-C8-C10
25	R	609	CLA	C12-C13-C15-C16
25	S	604	CLA	C11-C12-C13-C15
31	2	621	LHG	C24-C25-C26-C27
25	2	611	CLA	C8-C10-C11-C12
25	O	611	CLA	C8-C10-C11-C12
31	A	413	LHG	C23-C24-C25-C26
25	S	601	CLA	O1A-CGA-O2A-C1
25	G	302	CLA	CAA-CBA-CGA-O2A
27	6	620	WVN	C25-C28-C30-C33
38	3	616	II0	C26-C30-C32-C34
25	6	601	CLA	O1A-CGA-O2A-C1
36	e	102	HEM	CAA-CBA-CGA-O2A
25	R	613	CLA	C6-C7-C8-C10
25	b	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	3	602	CLA	C2A-CAA-CBA-CGA
25	P	602	CLA	C2A-CAA-CBA-CGA
25	Q	606	CLA	C2A-CAA-CBA-CGA
25	3	604	CLA	C10-C11-C12-C13
25	P	604	CLA	C10-C11-C12-C13
35	h	90	DGD	C3B-C4B-C5B-C6B
31	3	621	LHG	O6-C4-C5-O7
31	P	621	LHG	O6-C4-C5-O7
25	b	605	CLA	C15-C16-C17-C18
37	4	605	KC2	C3A-C2A-CAA-CBA
37	5	612	KC2	C3A-C2A-CAA-CBA
37	Q	605	KC2	C3A-C2A-CAA-CBA
37	R	612	KC2	C3A-C2A-CAA-CBA
29	d	405	PL9	C47-C48-C49-C50
25	C	521	CLA	C16-C17-C18-C20
31	5	621	LHG	C12-C13-C14-C15
34	C	536	LMG	C29-C30-C31-C32
25	G	301	CLA	C4-C3-C5-C6
31	a	413	LHG	C23-C24-C25-C26
34	z	102	LMG	C10-C11-C12-C13
25	C	528	CLA	C2-C3-C5-C6
35	h	90	DGD	C5B-C6B-C7B-C8B
31	R	621	LHG	C12-C13-C14-C15
25	B	605	CLA	C15-C16-C17-C18
29	D	405	PL9	C47-C48-C49-C50
25	b	601	CLA	O1D-CGD-O2D-CED
25	5	607	CLA	O1D-CGD-O2D-CED
25	5	602	CLA	C6-C7-C8-C10
34	W	134	LMG	C11-C12-C13-C14
35	H	90	DGD	C5B-C6B-C7B-C8B
34	c	536	LMG	O7-C8-C9-O8
34	G	303	LMG	O1-C7-C8-O7
31	b	622	LHG	C27-C28-C29-C30
27	a	407	WVN	C32-C36-C39-C40
27	B	617	WVN	C34-C37-C40-C39
27	Y	89	WVN	C25-C28-C30-C33
38	1	619	II0	C26-C30-C32-C34
38	N	618	II0	C36-C40-C42-C41
38	N	619	II0	C26-C30-C32-C34
36	E	102	HEM	CAD-CBD-CGD-O1D
25	b	613	CLA	C16-C17-C18-C19
25	R	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	4	602	CLA	C10-C11-C12-C13
31	l	101	LHG	C1-C2-C3-O3
31	L	101	LHG	C1-C2-C3-O3
25	G	301	CLA	C2C-C3C-CAC-CBC
25	a	406	CLA	C2-C1-O2A-CGA
25	6	611	CLA	C2-C1-O2A-CGA
25	1	603	CLA	C2-C1-O2A-CGA
25	S	611	CLA	C2-C1-O2A-CGA
25	Q	602	CLA	C10-C11-C12-C13
25	1	601	CLA	CAA-CBA-CGA-O2A
25	N	601	CLA	CAA-CBA-CGA-O2A
36	e	102	HEM	CAD-CBD-CGD-O1D
35	H	90	DGD	C5A-C6A-C7A-C8A
25	g	301	CLA	C3-C5-C6-C7
25	1	615	CLA	C2-C1-O2A-CGA
37	S	612	KC2	CAA-CBA-CGA-O1A
25	N	615	CLA	C2-C1-O2A-CGA
35	h	90	DGD	C5A-C6A-C7A-C8A
25	2	602	CLA	C2A-CAA-CBA-CGA
25	6	609	CLA	C2A-CAA-CBA-CGA
25	O	602	CLA	C2A-CAA-CBA-CGA
25	R	606	CLA	C2A-CAA-CBA-CGA
25	5	610	CLA	C10-C11-C12-C13
25	c	523	CLA	O1A-CGA-O2A-C1
27	c	529	WVN	C06-C13-C20-C23
27	y	89	WVN	C06-C13-C20-C23
27	B	618	WVN	C06-C13-C20-C23
27	C	530	WVN	C06-C13-C20-C23
27	H	89	WVN	C06-C13-C20-C23
39	4	620	IHT	C02-C07-C18-C22
39	Q	620	IHT	C02-C07-C18-C22
25	B	601	CLA	CBD-CGD-O2D-CED
25	R	610	CLA	C10-C11-C12-C13
27	C	529	WVN	C25-C28-C30-C33
38	3	619	II0	C26-C30-C32-C34
38	1	618	II0	C36-C40-C42-C41
38	P	619	II0	C26-C30-C32-C34
25	C	525	CLA	C4-C3-C5-C6
25	c	523	CLA	C16-C17-C18-C19
25	b	616	CLA	C10-C11-C12-C13
26	a	405	PHO	C10-C11-C12-C13
25	C	517	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	A	405	PHO	C10-C11-C12-C13
31	a	413	LHG	C12-C13-C14-C15
37	6	612	KC2	CAA-CBA-CGA-O1A
25	B	601	CLA	O1D-CGD-O2D-CED
25	2	611	CLA	C2A-CAA-CBA-CGA
25	5	606	CLA	C2A-CAA-CBA-CGA
25	O	611	CLA	C2A-CAA-CBA-CGA
25	c	526	CLA	CBD-CGD-O2D-CED
25	C	526	CLA	CBD-CGD-O2D-CED
31	S	621	LHG	O9-C7-O7-C5
31	d	406	LHG	O6-C4-C5-C6
31	D	406	LHG	O6-C4-C5-C6
25	c	525	CLA	C4-C3-C5-C6
25	2	613	CLA	C4-C3-C5-C6
25	O	613	CLA	C4-C3-C5-C6
25	Q	606	CLA	C4-C3-C5-C6
25	b	603	CLA	C11-C12-C13-C15
25	c	517	CLA	C2-C3-C5-C6
25	c	520	CLA	C11-C10-C8-C7
25	B	603	CLA	C11-C12-C13-C15
25	B	616	CLA	C11-C10-C8-C7
25	C	520	CLA	C11-C10-C8-C7
25	3	602	CLA	C12-C13-C15-C16
25	P	602	CLA	C12-C13-C15-C16
25	c	523	CLA	CBA-CGA-O2A-C1
38	S	616	II0	C36-C40-C42-C41
25	b	613	CLA	CAA-CBA-CGA-O2A
34	c	536	LMG	C39-C40-C41-C42
31	6	621	LHG	O9-C7-O7-C5
26	d	401	PHO	C8-C10-C11-C12
26	D	401	PHO	C8-C10-C11-C12
25	S	611	CLA	C3-C5-C6-C7
25	2	611	CLA	O1A-CGA-O2A-C1
31	R	621	LHG	C14-C15-C16-C17
25	C	523	CLA	C16-C17-C18-C19
25	2	604	CLA	C16-C17-C18-C20
25	6	615	CLA	C16-C17-C18-C19
25	O	604	CLA	C16-C17-C18-C20
25	S	615	CLA	C16-C17-C18-C19
31	5	621	LHG	C14-C15-C16-C17
25	P	603	CLA	CBA-CGA-O2A-C1
25	a	403	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	A	403	CLA	CAA-CBA-CGA-O2A
25	N	603	CLA	CAA-CBA-CGA-O2A
25	c	526	CLA	C4-C3-C5-C6
25	3	610	CLA	C4-C3-C5-C6
25	P	610	CLA	C4-C3-C5-C6
29	a	409	PL9	C15-C14-C16-C17
29	A	409	PL9	C15-C14-C16-C17
25	B	616	CLA	C10-C11-C12-C13
26	a	405	PHO	C5-C6-C7-C8
25	2	611	CLA	C2-C3-C5-C6
25	O	611	CLA	C2-C3-C5-C6
31	z	103	LHG	C24-C23-O8-C6
31	d	406	LHG	C11-C10-C9-C8
25	b	607	CLA	C6-C7-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	611	CLA	C11-C12-C13-C14
25	b	612	CLA	C11-C10-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	B	609	CLA	C6-C7-C8-C9
25	B	611	CLA	C11-C12-C13-C14
25	B	612	CLA	C11-C10-C8-C9
25	3	610	CLA	C11-C10-C8-C9
25	4	604	CLA	C6-C7-C8-C9
25	G	301	CLA	C6-C7-C8-C9
25	P	610	CLA	C11-C10-C8-C9
25	Q	604	CLA	C6-C7-C8-C9
25	R	609	CLA	C11-C12-C13-C14
25	6	611	CLA	C3-C5-C6-C7
34	C	536	LMG	C19-C20-C21-C22
28	A	408	SQD	C7-C8-C9-C10
25	2	601	CLA	C3A-C2A-CAA-CBA
25	O	601	CLA	C3A-C2A-CAA-CBA
25	O	611	CLA	O1A-CGA-O2A-C1
25	B	613	CLA	CAA-CBA-CGA-O2A
25	1	603	CLA	CAA-CBA-CGA-O2A
31	6	621	LHG	O7-C7-C8-C9
31	S	621	LHG	O7-C7-C8-C9
25	O	615	CLA	CBD-CGD-O2D-CED
25	a	406	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	516	CLA	CAD-CBD-CGD-O2D
25	c	521	CLA	CAD-CBD-CGD-O2D
25	c	522	CLA	CAD-CBD-CGD-O2D
25	A	406	CLA	CAD-CBD-CGD-O2D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	516	CLA	CAD-CBD-CGD-O2D
25	C	518	CLA	CAD-CBD-CGD-O2D
25	C	521	CLA	CAD-CBD-CGD-O2D
25	C	522	CLA	CAD-CBD-CGD-O2D
25	2	611	CLA	CAD-CBD-CGD-O2D
25	3	611	CLA	CAD-CBD-CGD-O2D
25	3	615	CLA	CAD-CBD-CGD-O2D
25	4	607	CLA	CAD-CBD-CGD-O2D
25	6	613	CLA	CAD-CBD-CGD-O2D
25	1	615	CLA	CAD-CBD-CGD-O2D
25	O	611	CLA	CAD-CBD-CGD-O2D
25	P	611	CLA	CAD-CBD-CGD-O2D
25	P	615	CLA	CAD-CBD-CGD-O2D
25	Q	607	CLA	CAD-CBD-CGD-O2D
25	R	613	CLA	CAD-CBD-CGD-O2D
25	S	613	CLA	CAD-CBD-CGD-O2D
25	N	615	CLA	CAD-CBD-CGD-O2D
26	a	405	PHO	CAD-CBD-CGD-O2D
26	A	405	PHO	CAD-CBD-CGD-O2D
37	4	611	KC2	CAD-CBD-CGD-O2D
37	6	606	KC2	CAD-CBD-CGD-O2D
37	6	612	KC2	CAD-CBD-CGD-O2D
37	Q	611	KC2	CAD-CBD-CGD-O2D
37	S	612	KC2	CAD-CBD-CGD-O2D
28	a	408	SQD	C7-C8-C9-C10
25	a	406	CLA	C11-C12-C13-C14
38	6	616	II0	C36-C40-C42-C41
25	b	616	CLA	C2A-CAA-CBA-CGA
25	2	615	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	C2-C1-O2A-CGA
25	g	302	CLA	CAA-CBA-CGA-O2A
25	1	601	CLA	CAA-CBA-CGA-O1A
25	N	601	CLA	CAA-CBA-CGA-O1A
25	B	610	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	Z	103	LHG	C24-C23-O8-C6
31	b	622	LHG	C35-C36-C37-C38
25	5	615	CLA	O1A-CGA-O2A-C1
25	C	526	CLA	C4-C3-C5-C6
25	G	301	CLA	C2-C3-C5-C6
25	b	610	CLA	CAA-CBA-CGA-O2A
25	c	519	CLA	CAA-CBA-CGA-O2A
34	B	620	LMG	C19-C20-C21-C22
27	6	620	WVN	C20-C23-C25-C28
28	a	408	SQD	C44-C45-C46-O48
28	A	408	SQD	C44-C45-C46-O48
34	d	402	LMG	C7-C8-C9-O8
34	D	402	LMG	C7-C8-C9-O8
25	C	520	CLA	C10-C11-C12-C13
25	b	612	CLA	CAA-CBA-CGA-O2A
25	A	404	CLA	CAA-CBA-CGA-O2A
25	B	612	CLA	CAA-CBA-CGA-O2A
25	C	519	CLA	CAA-CBA-CGA-O2A
34	W	134	LMG	C29-C30-C31-C32
25	2	601	CLA	O2A-C1-C2-C3
25	O	601	CLA	O2A-C1-C2-C3
25	b	613	CLA	O2A-C1-C2-C3
25	d	400	CLA	O2A-C1-C2-C3
25	d	403	CLA	O2A-C1-C2-C3
25	d	404	CLA	O2A-C1-C2-C3
25	B	613	CLA	O2A-C1-C2-C3
25	D	400	CLA	O2A-C1-C2-C3
25	D	403	CLA	O2A-C1-C2-C3
25	5	611	CLA	O2A-C1-C2-C3
25	R	611	CLA	O2A-C1-C2-C3
26	d	401	PHO	O2A-C1-C2-C3
31	c	535	LHG	C29-C30-C31-C32
25	2	611	CLA	CBA-CGA-O2A-C1
25	3	603	CLA	CBA-CGA-O2A-C1
31	B	622	LHG	C24-C23-O8-C6
25	O	603	CLA	C2A-CAA-CBA-CGA
25	a	404	CLA	CAA-CBA-CGA-O2A
31	c	535	LHG	O7-C7-C8-C9
31	d	406	LHG	O8-C23-C24-C25
25	P	603	CLA	O1A-CGA-O2A-C1
36	E	102	HEM	CAA-CBA-CGA-O2A
25	b	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C16-C17-C18-C20
25	C	521	CLA	C16-C17-C18-C19
25	R	615	CLA	O1A-CGA-O2A-C1
31	c	535	LHG	C23-C24-C25-C26
25	b	604	CLA	CHA-CBD-CGD-O1D
25	c	525	CLA	CHA-CBD-CGD-O2D
25	c	526	CLA	CHA-CBD-CGD-O2D
25	B	604	CLA	CHA-CBD-CGD-O1D
25	C	525	CLA	CHA-CBD-CGD-O2D
25	2	601	CLA	CHA-CBD-CGD-O2D
25	2	607	CLA	CHA-CBD-CGD-O1D
25	2	615	CLA	CHA-CBD-CGD-O1D
25	2	615	CLA	CHA-CBD-CGD-O2D
25	3	602	CLA	CHA-CBD-CGD-O1D
25	3	602	CLA	CHA-CBD-CGD-O2D
25	3	603	CLA	CHA-CBD-CGD-O2D
25	3	604	CLA	CHA-CBD-CGD-O1D
25	4	602	CLA	CHA-CBD-CGD-O1D
25	4	602	CLA	CHA-CBD-CGD-O2D
25	4	609	CLA	CHA-CBD-CGD-O1D
25	4	609	CLA	CHA-CBD-CGD-O2D
25	5	604	CLA	CHA-CBD-CGD-O2D
25	5	606	CLA	CHA-CBD-CGD-O1D
25	5	606	CLA	CHA-CBD-CGD-O2D
25	5	607	CLA	CHA-CBD-CGD-O1D
25	6	601	CLA	CHA-CBD-CGD-O2D
25	G	302	CLA	CHA-CBD-CGD-O2D
25	1	606	CLA	CHA-CBD-CGD-O1D
25	1	606	CLA	CHA-CBD-CGD-O2D
25	O	601	CLA	CHA-CBD-CGD-O2D
25	O	607	CLA	CHA-CBD-CGD-O1D
25	O	615	CLA	CHA-CBD-CGD-O1D
25	O	615	CLA	CHA-CBD-CGD-O2D
25	P	602	CLA	CHA-CBD-CGD-O1D
25	P	602	CLA	CHA-CBD-CGD-O2D
25	P	603	CLA	CHA-CBD-CGD-O2D
25	P	604	CLA	CHA-CBD-CGD-O1D
25	Q	602	CLA	CHA-CBD-CGD-O1D
25	Q	602	CLA	CHA-CBD-CGD-O2D
25	Q	609	CLA	CHA-CBD-CGD-O2D
25	R	604	CLA	CHA-CBD-CGD-O2D
25	R	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	R	606	CLA	CHA-CBD-CGD-O2D
25	R	607	CLA	CHA-CBD-CGD-O1D
25	S	601	CLA	CHA-CBD-CGD-O2D
25	N	606	CLA	CHA-CBD-CGD-O1D
25	N	606	CLA	CHA-CBD-CGD-O2D
27	C	531	WVN	C32-C36-C39-C40
25	S	609	CLA	CAA-CBA-CGA-O2A
31	C	535	LHG	O8-C23-C24-C25
31	D	406	LHG	O8-C23-C24-C25
34	C	536	LMG	O7-C10-C11-C12
25	c	525	CLA	C3-C5-C6-C7
26	A	405	PHO	C5-C6-C7-C8
31	3	621	LHG	O6-C4-C5-C6
31	P	621	LHG	O6-C4-C5-C6
25	g	302	CLA	CAA-CBA-CGA-O1A
36	E	102	HEM	CAA-CBA-CGA-O1A
25	2	602	CLA	C13-C15-C16-C17
35	c	532	DGD	O2G-C1B-C2B-C3B
31	B	622	LHG	O7-C5-C6-O8
31	3	621	LHG	O7-C5-C6-O8
31	5	621	LHG	O7-C5-C6-O8
31	P	621	LHG	O7-C5-C6-O8
31	R	621	LHG	O7-C5-C6-O8
25	O	602	CLA	C13-C15-C16-C17
25	C	525	CLA	C3-C5-C6-C7
25	b	608	CLA	O1D-CGD-O2D-CED
25	c	521	CLA	C13-C15-C16-C17
25	R	611	CLA	C5-C6-C7-C8
25	c	517	CLA	CAA-CBA-CGA-O2A
25	5	603	CLA	CAA-CBA-CGA-O2A
25	5	615	CLA	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
25	R	615	CLA	CAA-CBA-CGA-O2A
35	C	532	DGD	O2G-C1B-C2B-C3B
25	b	613	CLA	C2A-CAA-CBA-CGA
25	2	603	CLA	C2A-CAA-CBA-CGA
26	d	401	PHO	CHA-CBD-CGD-O1D
26	D	401	PHO	CHA-CBD-CGD-O1D
25	O	611	CLA	CBA-CGA-O2A-C1
25	5	604	CLA	C3-C5-C6-C7
25	R	604	CLA	C3-C5-C6-C7
25	D	404	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	6	621	LHG	C8-C7-O7-C5
25	B	601	CLA	CAA-CBA-CGA-O2A
25	C	517	CLA	CAA-CBA-CGA-O2A
31	c	535	LHG	C26-C27-C28-C29
25	5	611	CLA	C5-C6-C7-C8
34	c	536	LMG	C35-C36-C37-C38
25	c	526	CLA	C2-C3-C5-C6
25	B	613	CLA	C2-C3-C5-C6
25	C	526	CLA	C2-C3-C5-C6
25	5	606	CLA	C12-C13-C15-C16
25	R	606	CLA	C12-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C9
38	Q	618	II0	C09-C21-C23-C25
38	S	616	II0	C09-C21-C23-C25
39	1	620	IHT	C11-C21-C24-C26
25	b	601	CLA	CAA-CBA-CGA-O2A
25	5	611	CLA	CAA-CBA-CGA-O2A
25	R	611	CLA	CAA-CBA-CGA-O2A
25	b	610	CLA	C14-C13-C15-C16
25	c	523	CLA	C11-C10-C8-C9
25	c	527	CLA	C14-C13-C15-C16
25	B	607	CLA	C6-C7-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	C	523	CLA	C11-C10-C8-C9
25	C	527	CLA	C14-C13-C15-C16
25	3	602	CLA	C11-C12-C13-C14
25	5	609	CLA	C11-C12-C13-C14
25	1	604	CLA	C6-C7-C8-C9
25	P	602	CLA	C11-C12-C13-C14
25	R	609	CLA	C14-C13-C15-C16
25	N	604	CLA	C6-C7-C8-C9
25	b	608	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	C8-C10-C11-C12
34	m	101	LMG	C35-C36-C37-C38
25	3	603	CLA	O1A-CGA-O2A-C1
25	2	615	CLA	CAA-CBA-CGA-O2A
31	D	406	LHG	C11-C10-C9-C8
25	2	607	CLA	CAA-CBA-CGA-O2A
25	O	607	CLA	CAA-CBA-CGA-O2A
28	a	408	SQD	C5-C6-S-O8
28	A	408	SQD	C5-C6-S-O8
25	R	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	B	622	LHG	C8-C7-O7-C5
31	S	621	LHG	C8-C7-O7-C5
25	O	615	CLA	CAA-CBA-CGA-O2A
25	B	608	CLA	C2A-CAA-CBA-CGA
27	6	620	WVN	C20-C23-C25-C27
25	b	612	CLA	CAA-CBA-CGA-O1A
25	A	403	CLA	CAA-CBA-CGA-O1A
25	1	603	CLA	CAA-CBA-CGA-O1A
31	6	621	LHG	O9-C7-C8-C9
31	S	621	LHG	O9-C7-C8-C9
25	B	615	CLA	C16-C17-C18-C20
25	Q	606	CLA	C2-C3-C5-C6
34	c	536	LMG	C34-C35-C36-C37
25	a	403	CLA	CAA-CBA-CGA-O1A
25	C	519	CLA	CAA-CBA-CGA-O1A
31	d	406	LHG	O10-C23-C24-C25
25	R	607	CLA	O1D-CGD-O2D-CED
25	N	604	CLA	C8-C10-C11-C12
25	2	601	CLA	C1A-C2A-CAA-CBA
25	2	607	CLA	C1A-C2A-CAA-CBA
25	4	602	CLA	C1A-C2A-CAA-CBA
25	O	601	CLA	C1A-C2A-CAA-CBA
25	O	607	CLA	C1A-C2A-CAA-CBA
25	Q	602	CLA	C1A-C2A-CAA-CBA
28	a	411	SQD	C28-C29-C30-C31
25	4	606	CLA	C6-C7-C8-C9
25	A	404	CLA	CAA-CBA-CGA-O1A
34	w	134	LMG	C11-C12-C13-C14
35	H	90	DGD	CCA-CDA-CEA-CFA
25	a	404	CLA	CAA-CBA-CGA-O1A
25	c	519	CLA	CAA-CBA-CGA-O1A
25	B	612	CLA	CAA-CBA-CGA-O1A
25	N	603	CLA	CAA-CBA-CGA-O1A
31	C	535	LHG	C29-C30-C31-C32
25	6	610	CLA	CAA-CBA-CGA-O2A
25	S	610	CLA	CAA-CBA-CGA-O2A
34	B	620	LMG	O8-C28-C29-C30
25	b	608	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2A-CAA-CBA-CGA
25	6	602	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
35	C	532	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
25	b	610	CLA	CAA-CBA-CGA-O1A
25	b	613	CLA	CAA-CBA-CGA-O1A
25	d	400	CLA	C13-C15-C16-C17
25	D	400	CLA	C13-C15-C16-C17
35	h	90	DGD	CCA-CDA-CEA-CFA
25	O	607	CLA	CAA-CBA-CGA-O1A
34	w	134	LMG	C34-C35-C36-C37
34	C	536	LMG	C2-C1-O1-C7
25	C	527	CLA	C13-C15-C16-C17
25	1	604	CLA	C8-C10-C11-C12
31	d	406	LHG	C3-O3-P-O5
31	B	622	LHG	C4-O6-P-O5
31	D	406	LHG	C3-O3-P-O5
31	2	621	LHG	C4-O6-P-O5
31	3	621	LHG	C4-O6-P-O5
31	O	621	LHG	C4-O6-P-O5
31	P	621	LHG	C4-O6-P-O5
25	2	607	CLA	C11-C12-C13-C15
25	O	607	CLA	C11-C12-C13-C15
25	B	610	CLA	CAA-CBA-CGA-O1A
25	B	613	CLA	CAA-CBA-CGA-O1A
25	2	607	CLA	CAA-CBA-CGA-O1A
25	5	615	CLA	CAA-CBA-CGA-O1A
25	S	609	CLA	CAA-CBA-CGA-O1A
31	D	406	LHG	O10-C23-C24-C25
35	C	532	DGD	O6D-C5D-C6D-O5D
39	4	620	IHT	C10-C07-C18-C22
39	Q	620	IHT	C10-C07-C18-C22
25	c	527	CLA	C13-C15-C16-C17
25	R	615	CLA	CAA-CBA-CGA-O1A
31	z	103	LHG	O10-C23-O8-C6
34	C	536	LMG	O8-C28-C29-C30
25	P	615	CLA	CAA-CBA-CGA-O2A
34	Z	102	LMG	C10-C11-C12-C13
25	3	615	CLA	CAA-CBA-CGA-O2A
34	C	536	LMG	O9-C10-C11-C12
25	B	606	CLA	C4-C3-C5-C6
25	c	519	CLA	CAD-CBD-CGD-O1D
25	c	528	CLA	CAD-CBD-CGD-O1D
25	C	519	CLA	CAD-CBD-CGD-O1D
25	3	604	CLA	CAD-CBD-CGD-O1D
25	4	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	5	604	CLA	CAD-CBD-CGD-O1D
25	1	606	CLA	CAD-CBD-CGD-O1D
25	P	604	CLA	CAD-CBD-CGD-O1D
25	Q	609	CLA	CAD-CBD-CGD-O1D
25	R	604	CLA	CAD-CBD-CGD-O1D
25	N	606	CLA	CAD-CBD-CGD-O1D
28	a	408	SQD	C5-C6-S-O7
28	A	408	SQD	C5-C6-S-O7
34	4	621	LMG	C9-C8-O7-C10
34	Q	621	LMG	C9-C8-O7-C10
37	N	612	KC2	CAD-CBD-CGD-O1D
31	B	622	LHG	O10-C23-O8-C6
31	Z	103	LHG	O10-C23-O8-C6
25	c	517	CLA	CAA-CBA-CGA-O1A
25	C	517	CLA	CAA-CBA-CGA-O1A
25	5	603	CLA	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
31	d	406	LHG	C32-C33-C34-C35
34	b	620	LMG	C31-C32-C33-C34
34	B	620	LMG	C31-C32-C33-C34
25	4	609	CLA	C5-C6-C7-C8
35	c	532	DGD	O6D-C5D-C6D-O5D
25	c	516	CLA	C11-C10-C8-C9
25	c	524	CLA	C6-C7-C8-C9
25	C	524	CLA	C6-C7-C8-C9
25	2	613	CLA	C6-C7-C8-C9
25	5	604	CLA	C6-C7-C8-C9
25	5	609	CLA	C14-C13-C15-C16
25	O	613	CLA	C6-C7-C8-C9
25	R	604	CLA	C6-C7-C8-C9
25	5	607	CLA	CBD-CGD-O2D-CED
34	F	99	LMG	C13-C14-C15-C16
35	C	532	DGD	O1B-C1B-C2B-C3B
25	c	518	CLA	CAA-CBA-CGA-O2A
25	g	301	CLA	CAA-CBA-CGA-O2A
25	B	604	CLA	CAA-CBA-CGA-O2A
31	c	535	LHG	O8-C23-C24-C25
34	d	402	LMG	C34-C35-C36-C37
34	D	402	LMG	C34-C35-C36-C37
25	B	607	CLA	C13-C15-C16-C17
25	2	615	CLA	CAA-CBA-CGA-O1A
31	D	406	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	c	532	DGD	O1B-C1B-C2B-C3B
25	c	522	CLA	C2A-CAA-CBA-CGA
25	C	522	CLA	C2A-CAA-CBA-CGA
25	5	610	CLA	C2A-CAA-CBA-CGA
25	R	610	CLA	C2A-CAA-CBA-CGA
25	b	604	CLA	CAA-CBA-CGA-O2A
25	2	606	CLA	CAA-CBA-CGA-O2A
25	5	601	CLA	CAA-CBA-CGA-O2A
25	Q	603	CLA	CAA-CBA-CGA-O2A
25	R	601	CLA	CAA-CBA-CGA-O2A
31	a	413	LHG	O8-C23-C24-C25
31	A	413	LHG	O8-C23-C24-C25
31	P	621	LHG	O7-C7-C8-C9
34	b	620	LMG	O8-C28-C29-C30
25	B	615	CLA	C10-C11-C12-C13
25	P	615	CLA	CAA-CBA-CGA-O1A
34	f	99	LMG	C13-C14-C15-C16
25	B	613	CLA	C4-C3-C5-C6
29	d	405	PL9	C35-C34-C36-C37
25	b	608	CLA	C11-C10-C8-C7
25	b	613	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C10-C8-C7
25	c	525	CLA	C11-C10-C8-C7
25	c	527	CLA	C12-C13-C15-C16
25	B	608	CLA	C11-C10-C8-C7
25	B	614	CLA	C11-C10-C8-C7
25	C	525	CLA	C11-C10-C8-C7
25	C	526	CLA	C3A-C2A-CAA-CBA
25	3	609	CLA	C6-C7-C8-C10
25	5	609	CLA	C12-C13-C15-C16
25	P	609	CLA	C6-C7-C8-C10
27	a	407	WVN	C05-C02-C11-C19
27	C	529	WVN	C05-C02-C11-C19
25	b	601	CLA	CAA-CBA-CGA-O1A
25	3	615	CLA	CAA-CBA-CGA-O1A
25	O	615	CLA	CAA-CBA-CGA-O1A
25	C	518	CLA	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O2A
25	4	604	CLA	CAA-CBA-CGA-O2A
25	O	606	CLA	CAA-CBA-CGA-O2A
25	Q	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	3	621	LHG	O7-C7-C8-C9
25	B	606	CLA	C10-C11-C12-C13
27	H	89	WVN	C30-C33-C34-C37
27	S	620	WVN	C20-C23-C25-C28
25	R	601	CLA	CAA-CBA-CGA-O1A
31	a	413	LHG	O10-C23-C24-C25
31	3	621	LHG	O9-C7-C8-C9
31	P	621	LHG	O9-C7-C8-C9
27	b	619	WVN	C22-C26-C29-C31
27	c	531	WVN	C32-C36-C39-C40
27	D	408	WVN	C22-C26-C29-C31
38	O	618	II0	C26-C30-C32-C34
39	O	620	IHT	C33-C37-C40-C41
31	6	621	LHG	C16-C17-C18-C19
25	b	615	CLA	C10-C11-C12-C13
25	B	601	CLA	CAA-CBA-CGA-O1A
25	2	606	CLA	CAA-CBA-CGA-O1A
25	5	601	CLA	CAA-CBA-CGA-O1A
25	O	606	CLA	CAA-CBA-CGA-O1A
31	c	535	LHG	O10-C23-C24-C25
31	C	535	LHG	O10-C23-C24-C25
35	c	532	DGD	C4A-C5A-C6A-C7A
25	2	604	CLA	CAA-CBA-CGA-O2A
25	4	609	CLA	CAA-CBA-CGA-O2A
25	1	615	CLA	CAA-CBA-CGA-O2A
25	O	604	CLA	CAA-CBA-CGA-O2A
25	N	615	CLA	CAA-CBA-CGA-O2A
31	S	621	LHG	C16-C17-C18-C19
25	6	610	CLA	CAA-CBA-CGA-O1A
25	S	610	CLA	CAA-CBA-CGA-O1A
31	A	413	LHG	O10-C23-C24-C25
25	c	528	CLA	C2A-CAA-CBA-CGA
25	Q	604	CLA	CAA-CBA-CGA-O1A
25	d	400	CLA	CAA-CBA-CGA-O2A
25	D	400	CLA	CAA-CBA-CGA-O2A
25	c	526	CLA	O1D-CGD-O2D-CED
25	C	526	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

217 monomers are involved in 456 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	610	CLA	5	0
25	a	403	CLA	11	0
34	G	303	LMG	5	0
25	b	605	CLA	4	0
25	B	610	CLA	5	0
26	A	405	PHO	2	0
31	5	621	LHG	4	0
25	A	403	CLA	10	0
25	3	604	CLA	1	0
25	4	604	CLA	3	0
25	C	518	CLA	4	0
25	D	404	CLA	1	0
25	g	301	CLA	5	0
25	S	615	CLA	2	0
25	R	601	CLA	1	0
25	4	609	CLA	5	0
25	Q	602	CLA	1	0
25	B	616	CLA	1	0
31	C	535	LHG	1	0
25	O	609	CLA	3	0
25	O	602	CLA	2	0
25	Q	607	CLA	2	0
38	6	617	II0	2	0
25	O	615	CLA	1	0
28	A	411	SQD	1	0
31	3	621	LHG	2	0
25	C	516	CLA	2	0
25	4	613	CLA	1	0
25	C	525	CLA	6	0
25	4	606	CLA	1	0
25	N	603	CLA	3	0
25	B	607	CLA	1	0
25	O	610	CLA	3	0
37	N	613	KC2	2	0
31	b	622	LHG	2	0
31	l	101	LHG	8	0
25	6	610	CLA	1	0
25	3	615	CLA	1	0
25	Q	609	CLA	2	0
25	c	521	CLA	4	0
25	b	604	CLA	3	0
25	2	610	CLA	1	0
25	b	616	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	c	532	DGD	1	0
25	5	613	CLA	1	0
25	1	609	CLA	3	0
34	D	402	LMG	4	0
25	R	606	CLA	4	0
25	4	602	CLA	1	0
25	C	523	CLA	3	0
31	d	406	LHG	4	0
25	4	615	CLA	1	0
36	E	102	HEM	1	0
25	Q	613	CLA	2	0
25	4	603	CLA	7	0
25	P	609	CLA	1	0
25	Q	615	CLA	1	0
25	P	611	CLA	5	0
34	O	622	LMG	1	0
25	B	611	CLA	3	0
25	c	520	CLA	2	0
25	6	609	CLA	4	0
26	d	401	PHO	5	0
25	2	611	CLA	1	0
25	B	606	CLA	5	0
25	6	611	CLA	2	0
25	2	607	CLA	4	0
31	L	101	LHG	6	0
25	c	516	CLA	2	0
37	1	613	KC2	1	0
25	R	603	CLA	1	0
31	6	621	LHG	2	0
25	c	525	CLA	5	0
34	f	99	LMG	3	0
25	b	613	CLA	6	0
38	4	618	II0	1	0
25	2	604	CLA	1	0
25	3	601	CLA	1	0
25	B	613	CLA	9	0
25	S	609	CLA	4	0
25	B	605	CLA	6	0
25	R	611	CLA	2	0
25	C	527	CLA	2	0
25	R	604	CLA	2	0
25	S	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	604	CLA	2	0
34	W	134	LMG	2	0
27	b	617	WVN	1	0
34	Q	621	LMG	2	0
25	A	404	CLA	3	0
31	D	406	LHG	4	0
25	C	521	CLA	5	0
35	h	90	DGD	4	0
28	a	408	SQD	1	0
25	B	603	CLA	1	0
27	B	617	WVN	1	0
25	d	403	CLA	7	0
25	B	602	CLA	2	0
38	S	617	II0	2	0
25	2	609	CLA	1	0
25	B	615	CLA	3	0
25	S	604	CLA	3	0
34	m	101	LMG	1	0
25	P	610	CLA	2	0
26	D	401	PHO	5	0
25	N	602	CLA	1	0
25	C	526	CLA	2	0
25	C	528	CLA	1	0
25	3	609	CLA	1	0
31	2	621	LHG	1	0
29	a	409	PL9	2	0
31	R	621	LHG	4	0
25	P	603	CLA	1	0
25	c	527	CLA	2	0
25	B	601	CLA	1	0
34	Z	102	LMG	2	0
25	S	610	CLA	1	0
25	C	522	CLA	3	0
34	d	407	LMG	2	0
25	2	603	CLA	2	0
25	5	603	CLA	1	0
35	H	90	DGD	5	0
34	z	102	LMG	2	0
29	D	405	PL9	3	0
25	b	606	CLA	4	0
31	B	622	LHG	3	0
34	M	101	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	404	CLA	2	0
25	c	528	CLA	1	0
25	6	603	CLA	2	0
34	c	536	LMG	4	0
25	b	614	CLA	2	0
31	O	621	LHG	1	0
31	P	621	LHG	3	0
28	A	408	SQD	1	0
25	b	608	CLA	2	0
25	B	608	CLA	2	0
25	b	607	CLA	2	0
34	d	402	LMG	3	0
25	D	403	CLA	7	0
25	C	520	CLA	3	0
25	P	601	CLA	1	0
25	O	603	CLA	1	0
25	c	526	CLA	1	0
31	c	535	LHG	2	0
25	P	615	CLA	1	0
25	b	615	CLA	2	0
25	c	517	CLA	3	0
25	Q	603	CLA	6	0
25	d	400	CLA	2	0
25	3	610	CLA	1	0
25	A	406	CLA	2	0
25	5	601	CLA	1	0
25	Q	604	CLA	3	0
29	d	405	PL9	4	0
25	B	609	CLA	4	0
35	C	532	DGD	1	0
25	b	603	CLA	2	0
25	N	607	CLA	2	0
38	O	618	II0	1	0
34	D	407	LMG	2	0
25	S	611	CLA	1	0
25	c	522	CLA	3	0
25	Q	606	CLA	1	0
25	5	604	CLA	1	0
34	B	620	LMG	1	0
26	a	405	PHO	3	0
25	b	609	CLA	4	0
25	d	404	CLA	1	0

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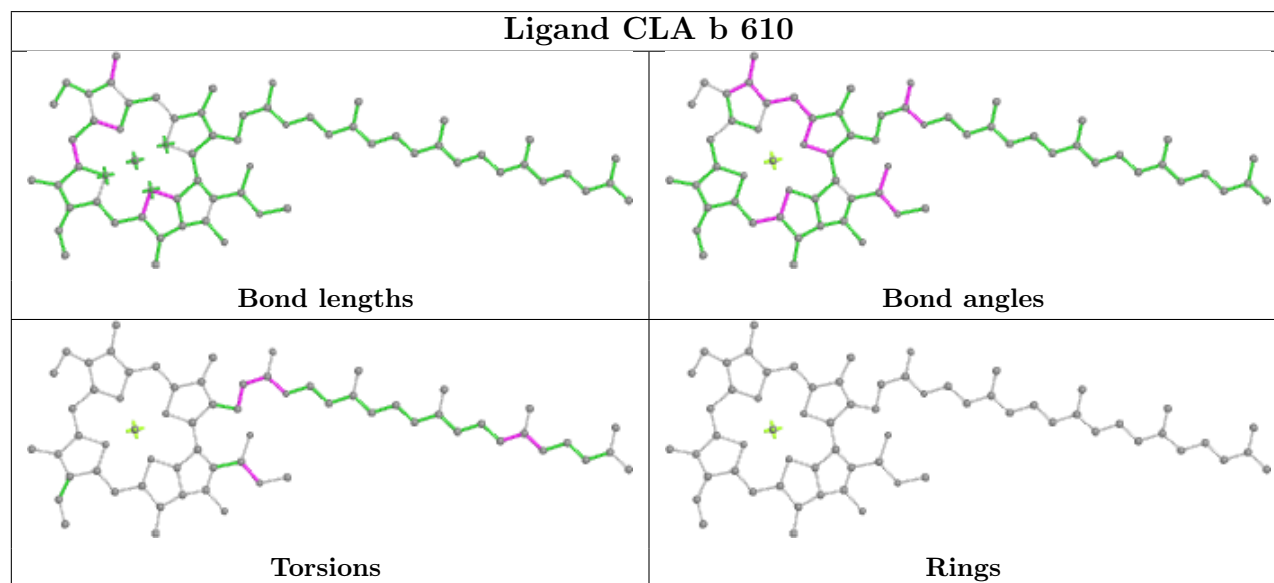
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	612	CLA	7	0
25	O	607	CLA	4	0
38	2	618	II0	1	0
25	b	611	CLA	3	0
25	5	610	CLA	2	0
25	G	301	CLA	3	0
36	e	102	HEM	1	0
34	w	134	LMG	1	0
25	b	602	CLA	2	0
25	R	610	CLA	1	0
25	R	613	CLA	1	0
25	1	607	CLA	1	0
25	O	604	CLA	2	0
25	N	604	CLA	1	0
28	a	411	SQD	1	0
25	c	518	CLA	4	0
25	5	606	CLA	4	0
25	1	602	CLA	1	0
25	6	613	CLA	2	0
25	C	517	CLA	4	0
25	S	613	CLA	1	0
25	5	615	CLA	1	0
25	5	611	CLA	2	0
34	b	620	LMG	1	0
25	B	604	CLA	3	0
25	4	607	CLA	2	0
25	D	400	CLA	1	0
25	3	611	CLA	5	0
31	S	621	LHG	2	0
25	O	611	CLA	1	0
25	B	614	CLA	1	0
25	B	612	CLA	6	0
25	N	609	CLA	1	0
25	a	406	CLA	3	0
25	2	615	CLA	1	0
34	4	621	LMG	2	0
25	c	523	CLA	3	0
25	R	609	CLA	5	0
25	R	602	CLA	2	0
25	2	602	CLA	3	0
25	6	602	CLA	2	0
37	6	606	KC2	10	0

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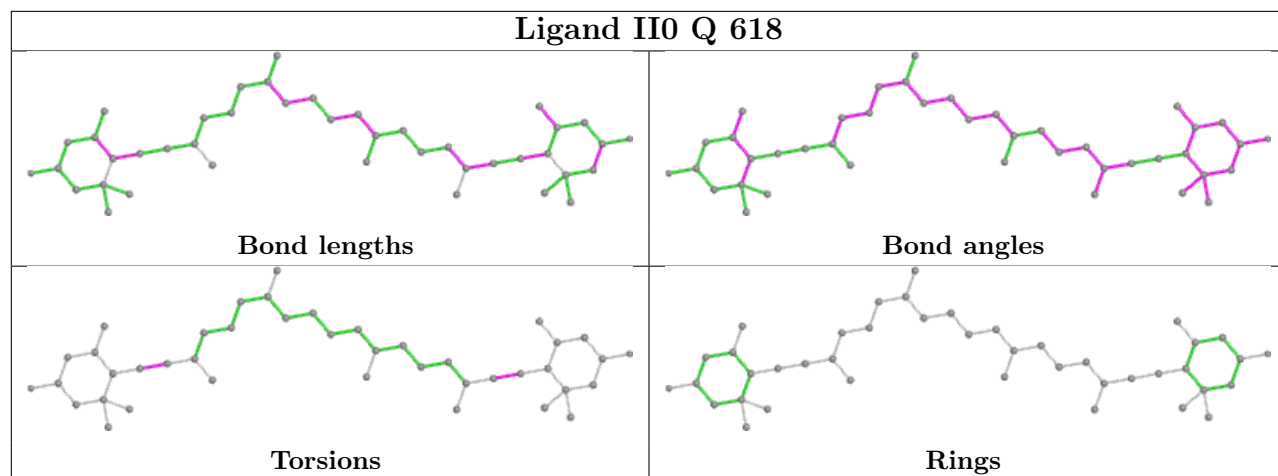
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	609	CLA	5	0
25	5	602	CLA	2	0
25	R	615	CLA	1	0
25	6	615	CLA	1	0
34	g	303	LMG	3	0
25	1	603	CLA	3	0

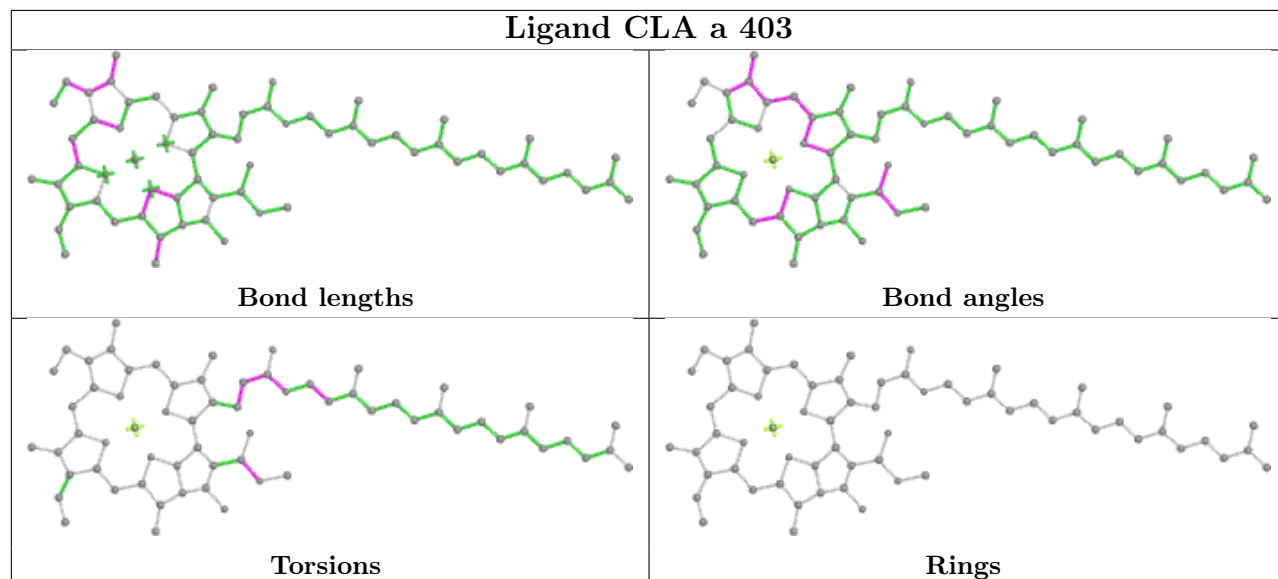
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



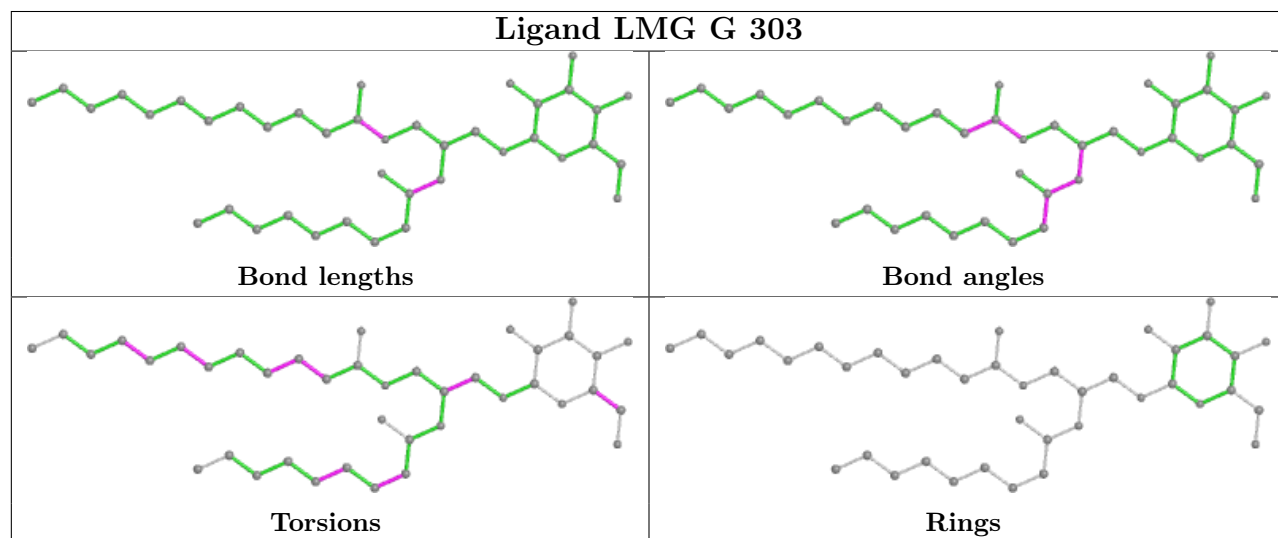
Ligand II0 Q 618

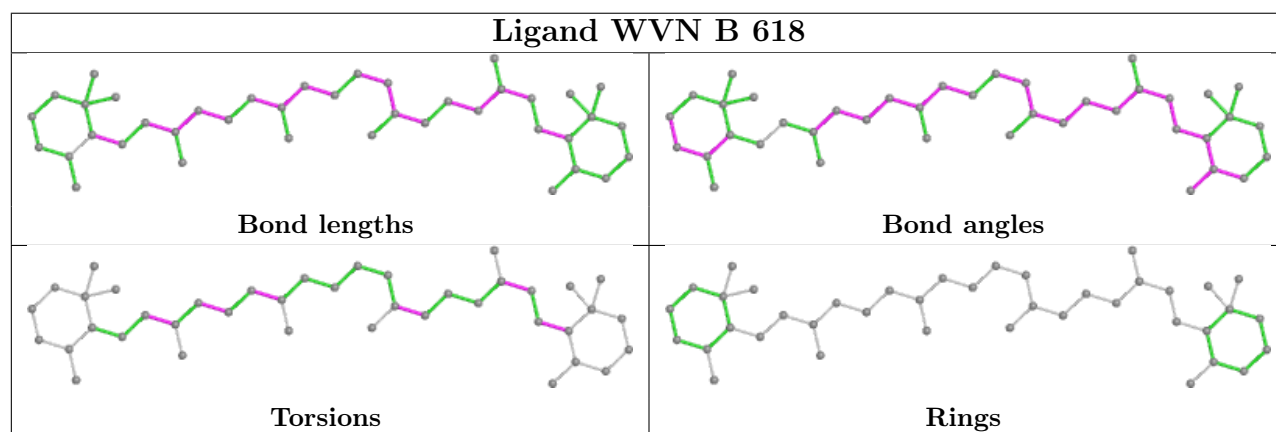
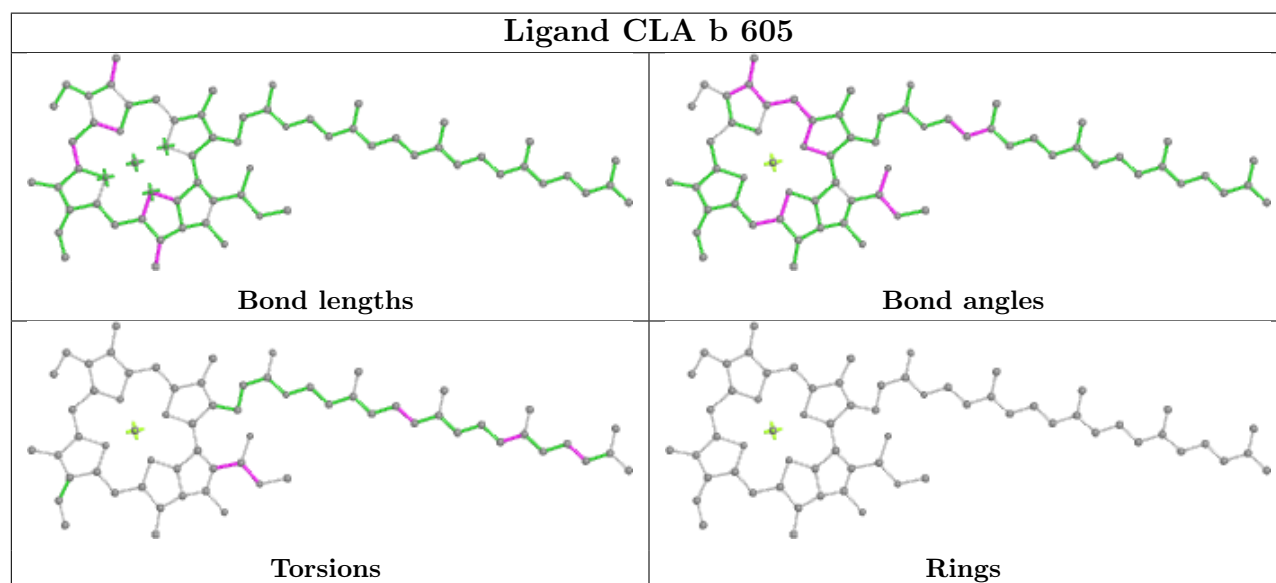
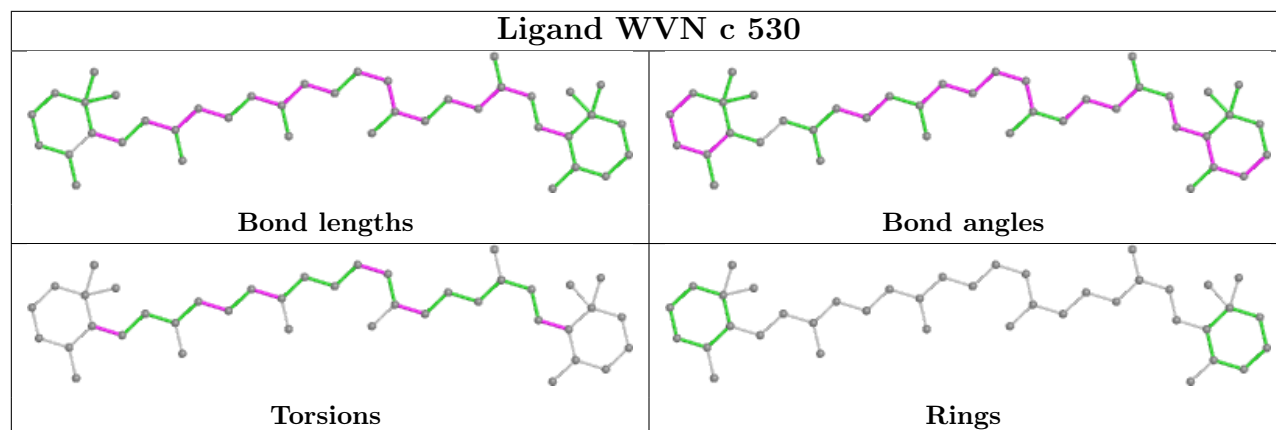


Ligand CLA a 403

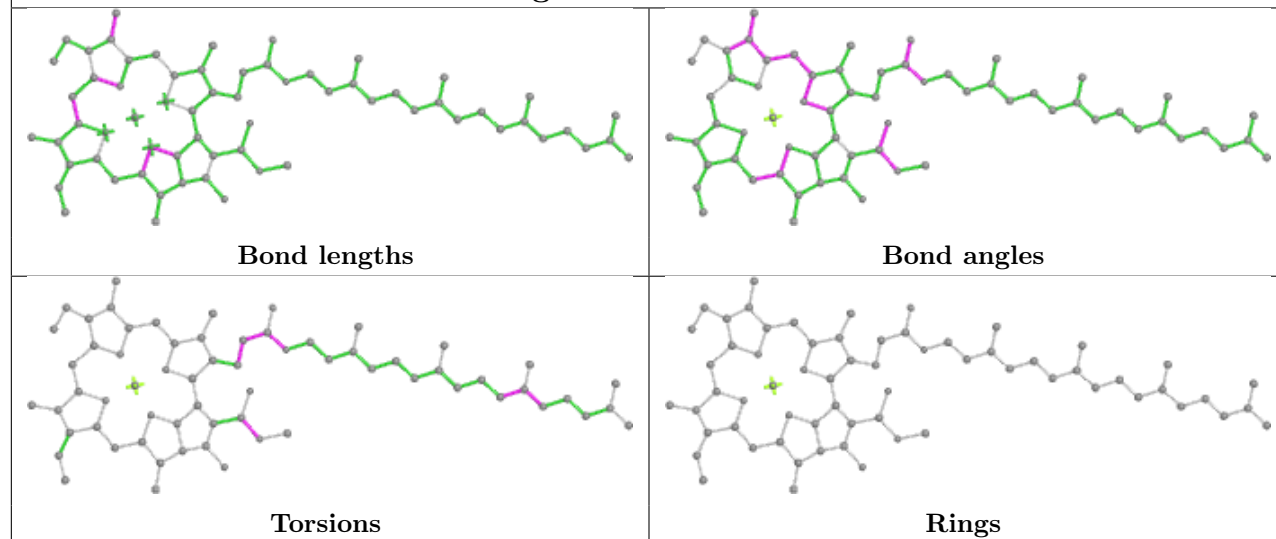


Ligand LMG G 303

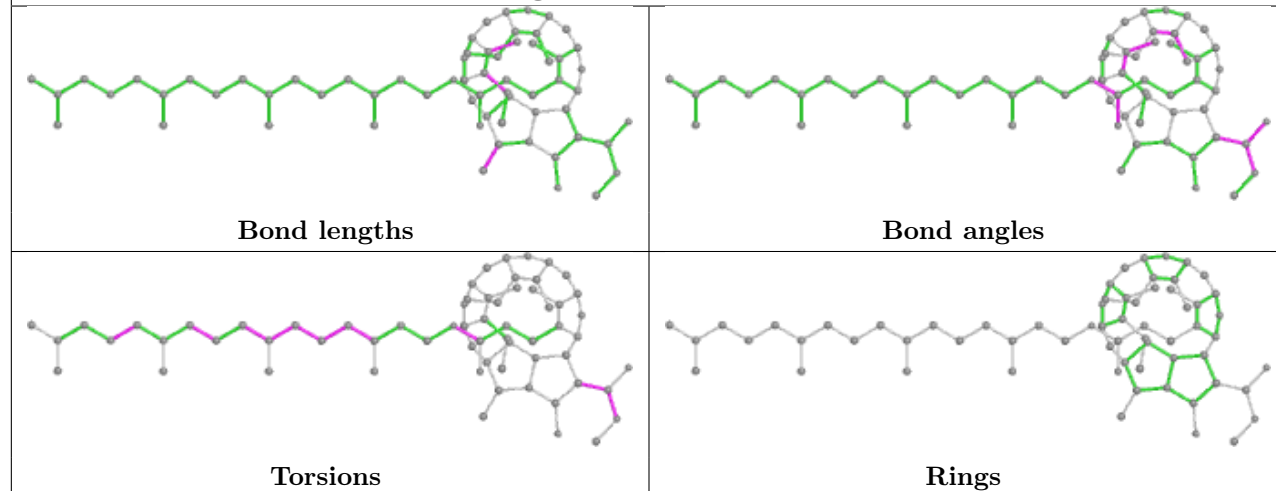




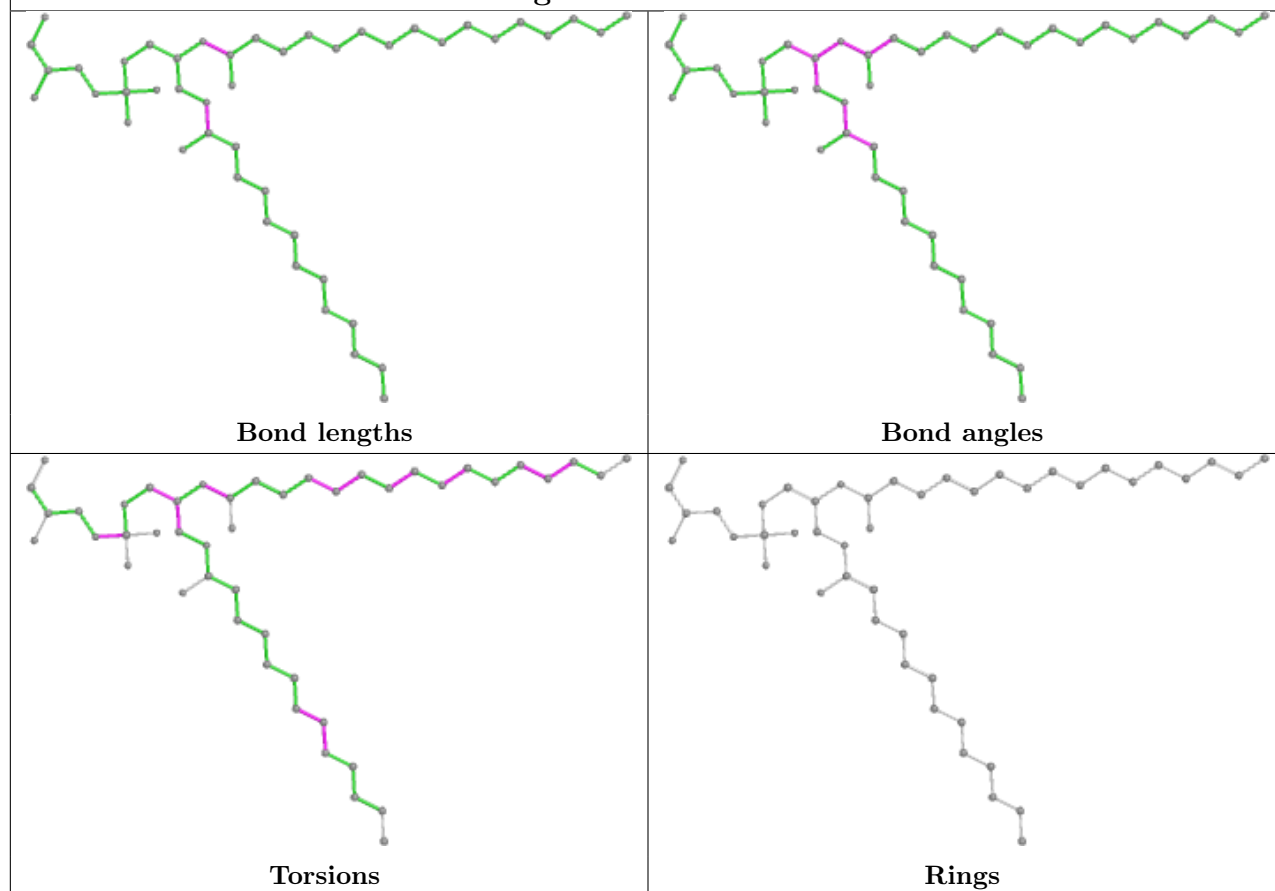
Ligand CLA B 610



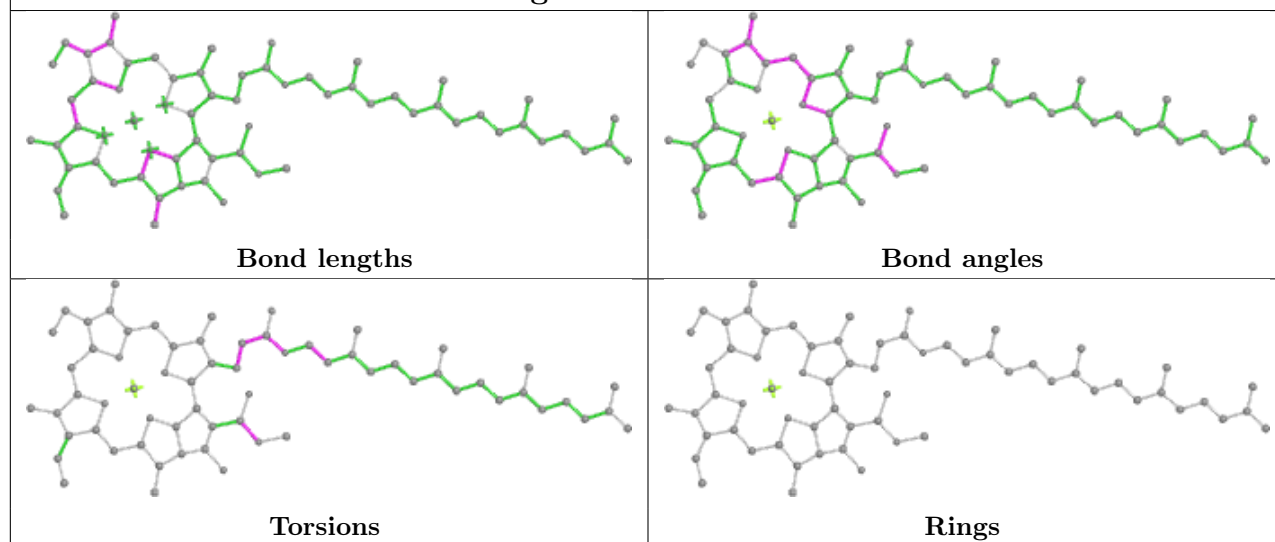
Ligand PHO A 405

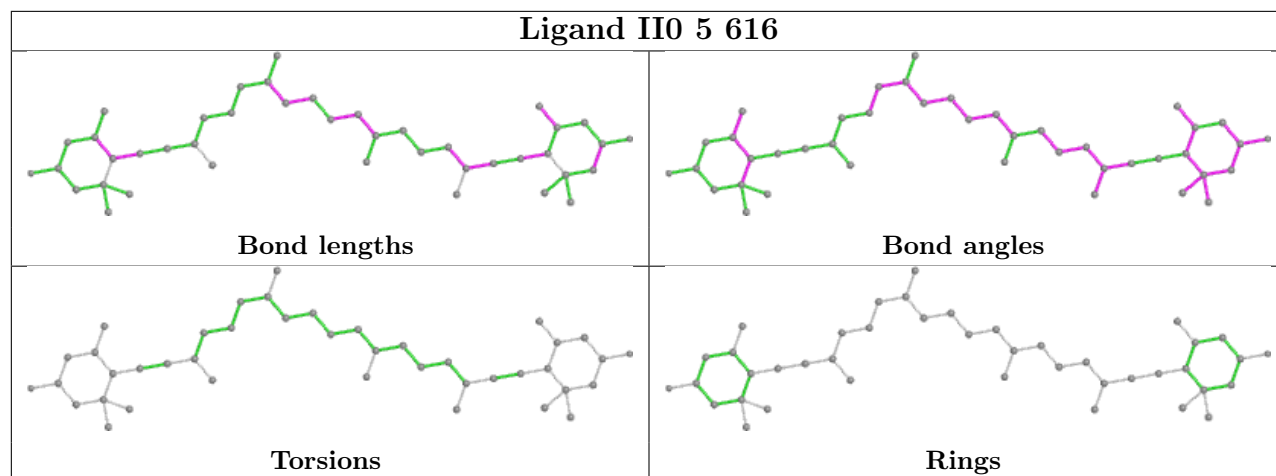
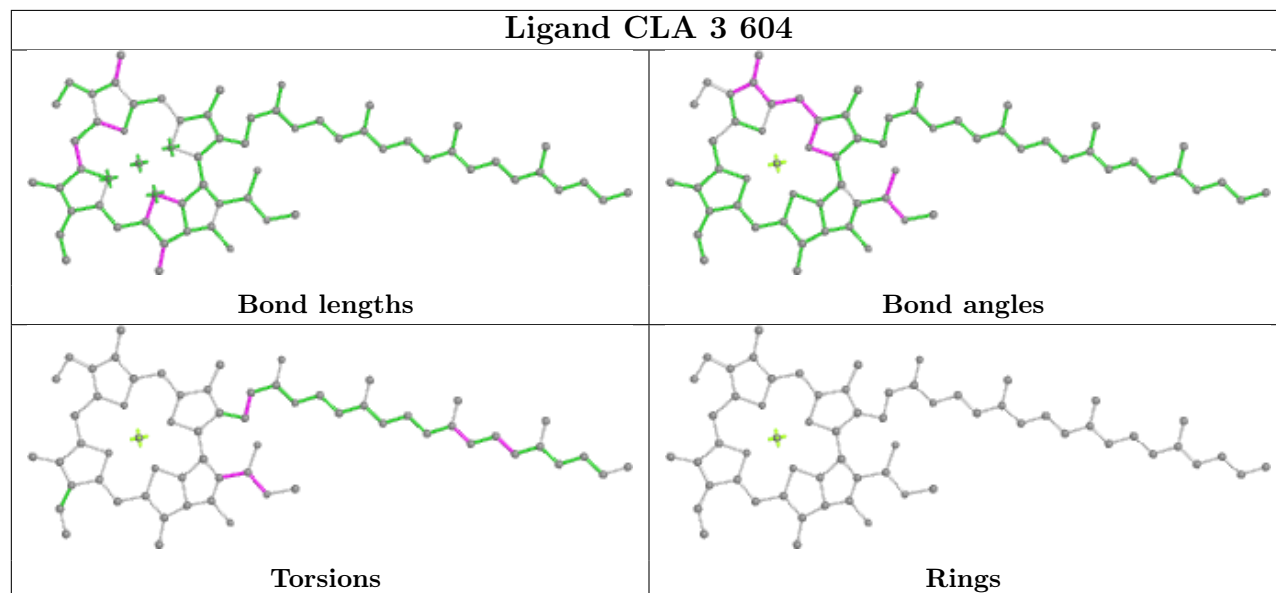
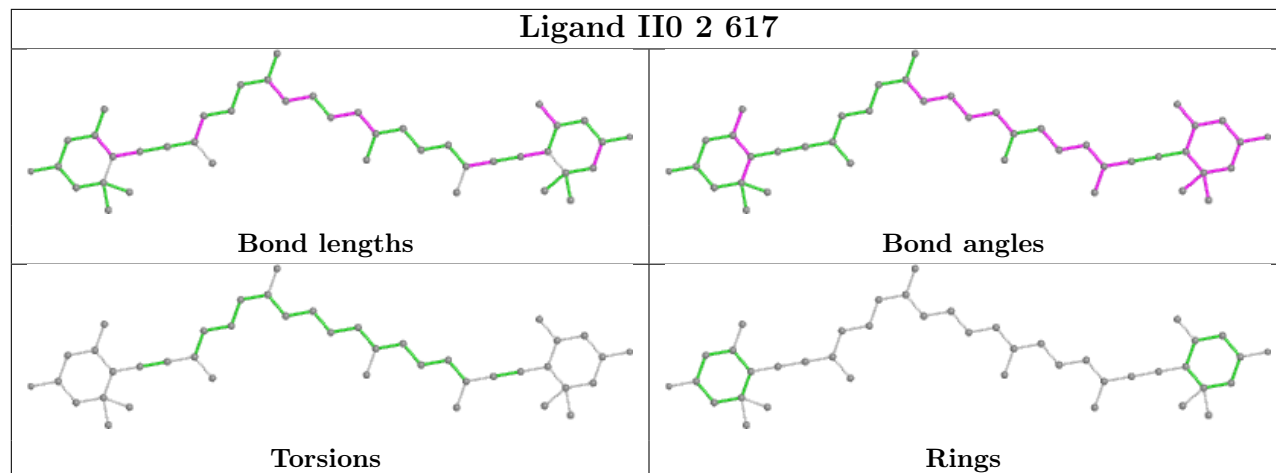


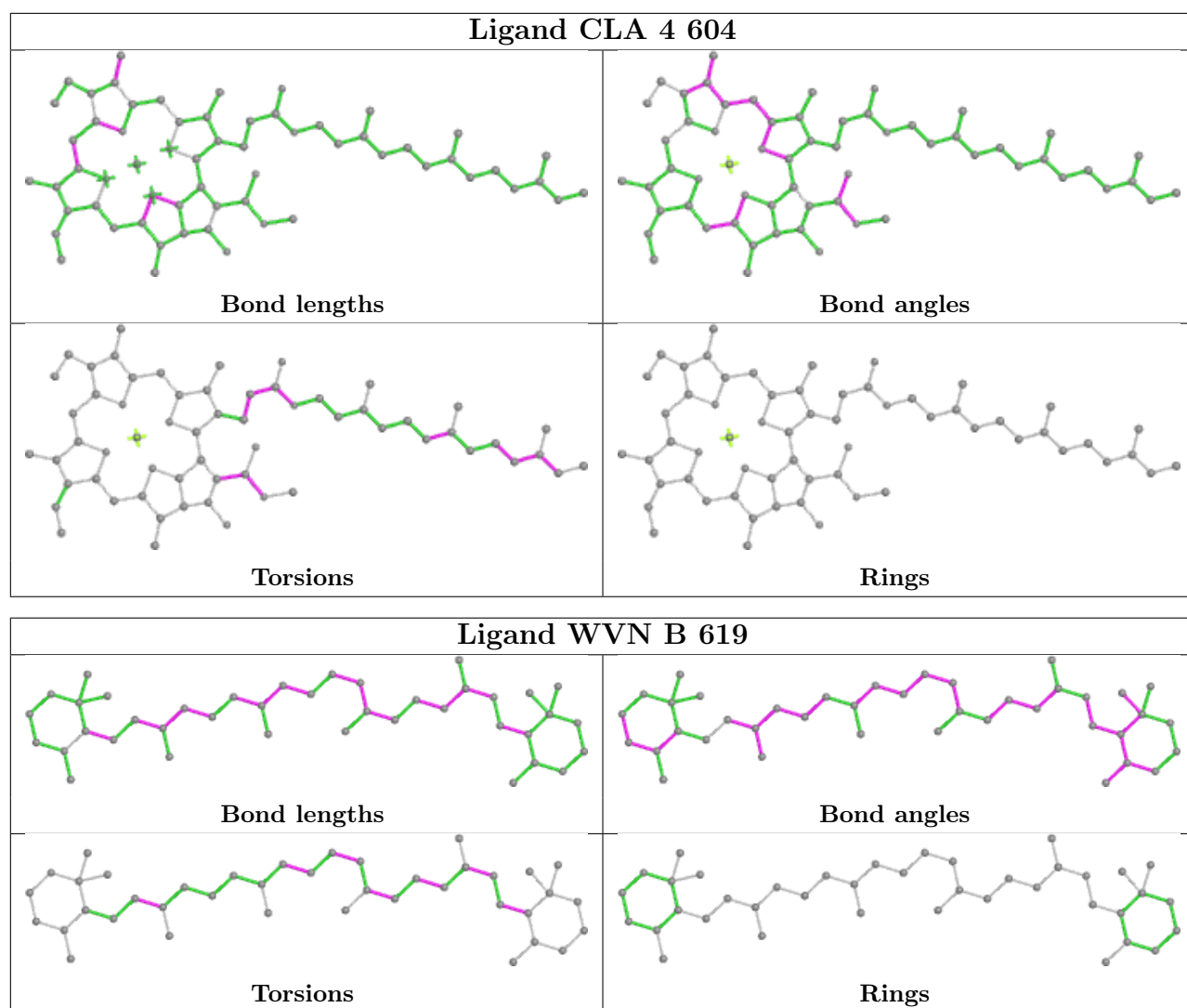
Ligand LHG 5 621



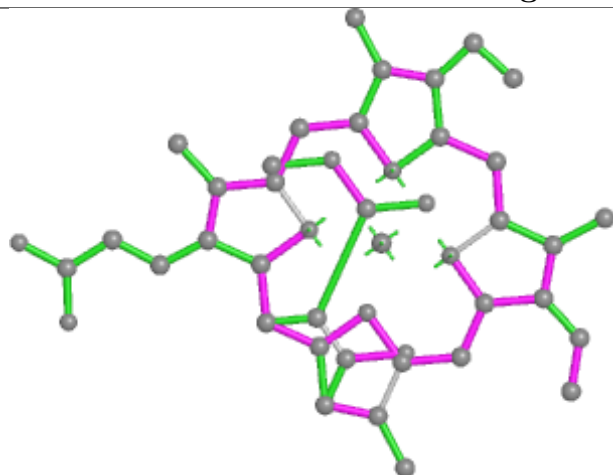
Ligand CLA A 403



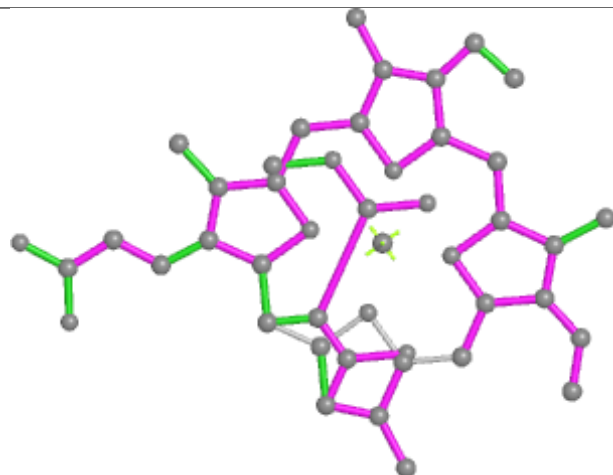
Ligand II0 5 616**Ligand CLA 3 604****Ligand II0 2 617**



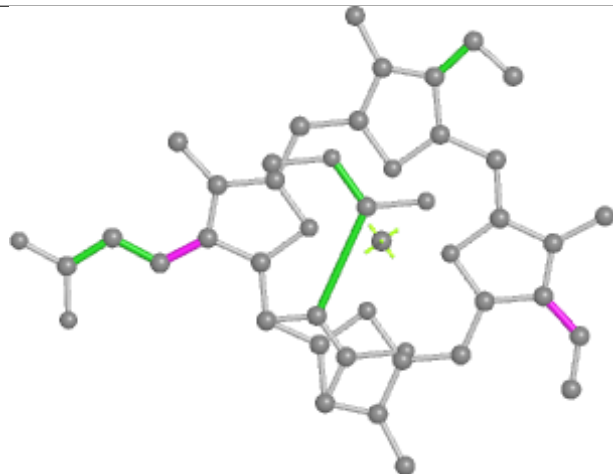
Ligand KC2 4 612



Bond lengths



Bond angles

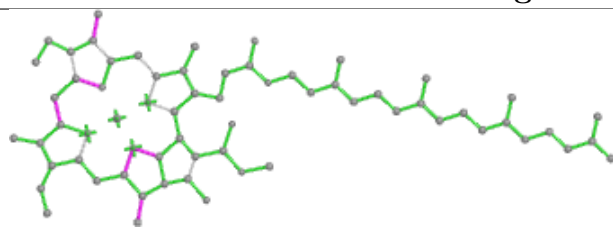


Torsions

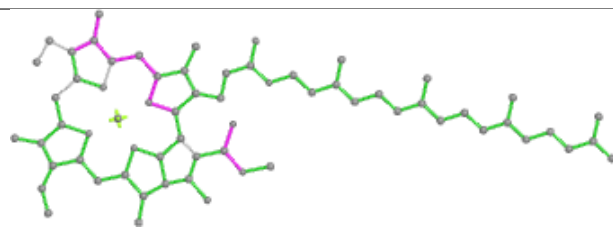


Rings

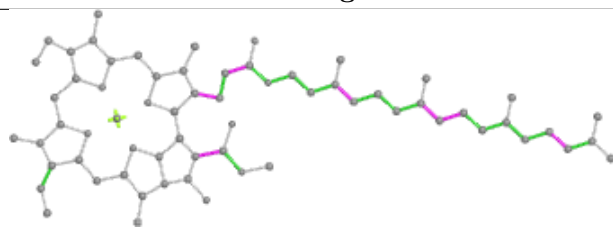
Ligand CLA C 518



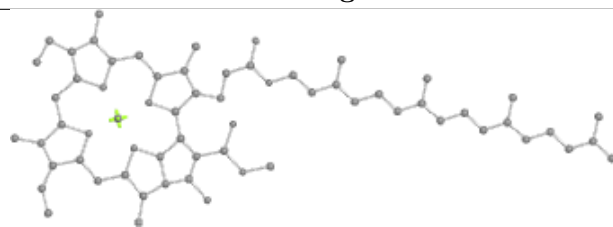
Bond lengths



Bond angles

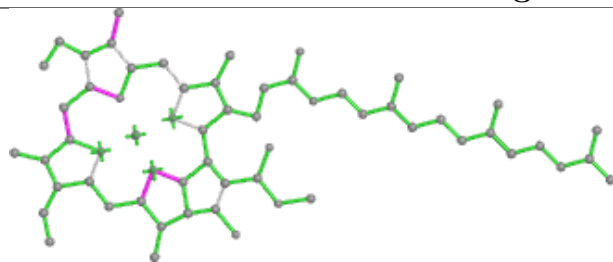


Torsions

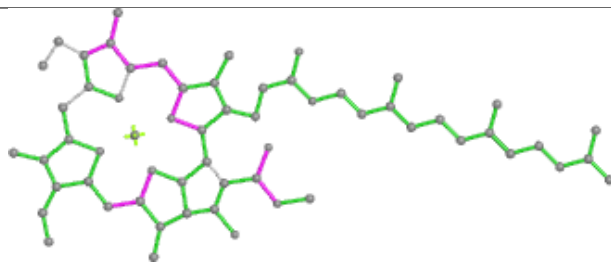


Rings

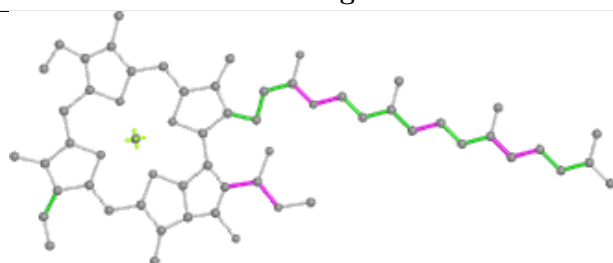
Ligand CLA D 404



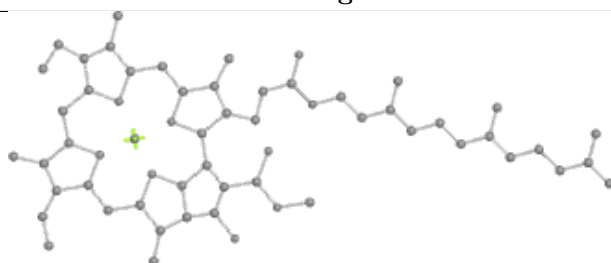
Bond lengths



Bond angles

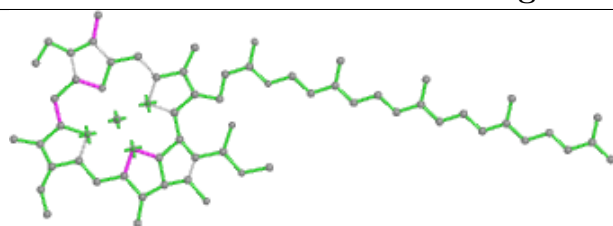


Torsions

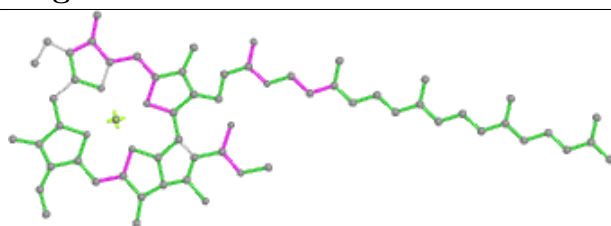


Rings

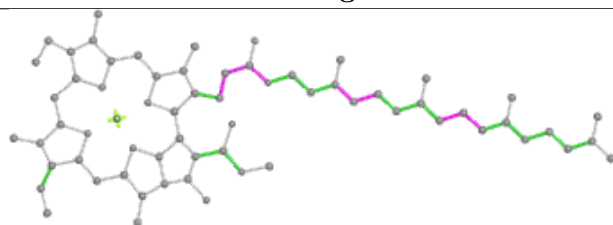
Ligand CLA g 301



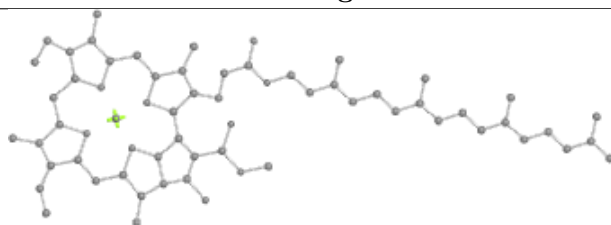
Bond lengths



Bond angles

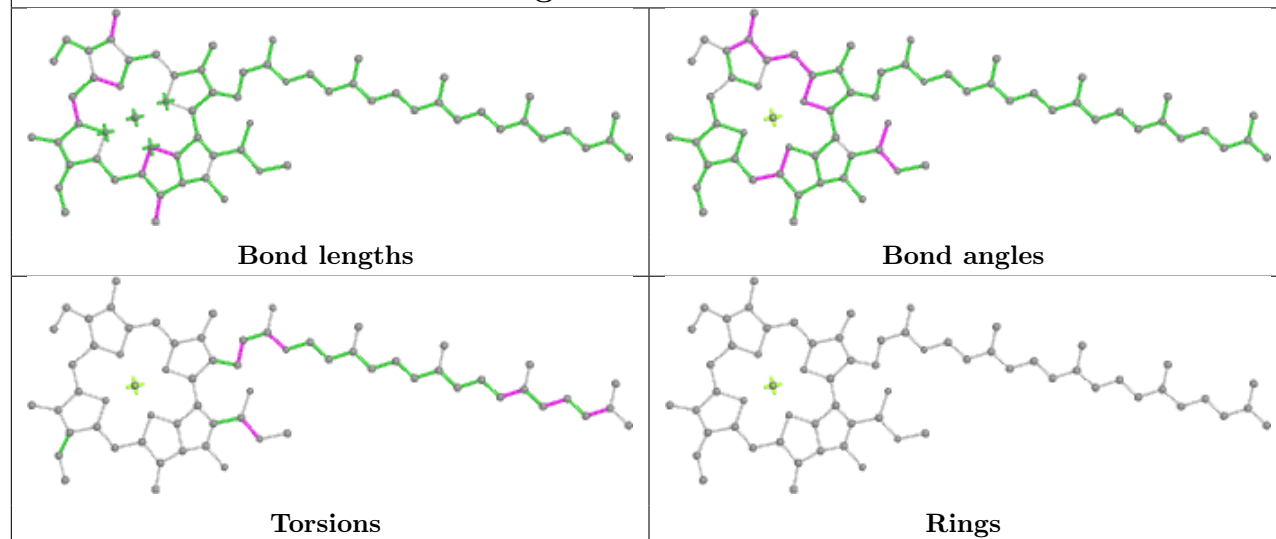


Torsions

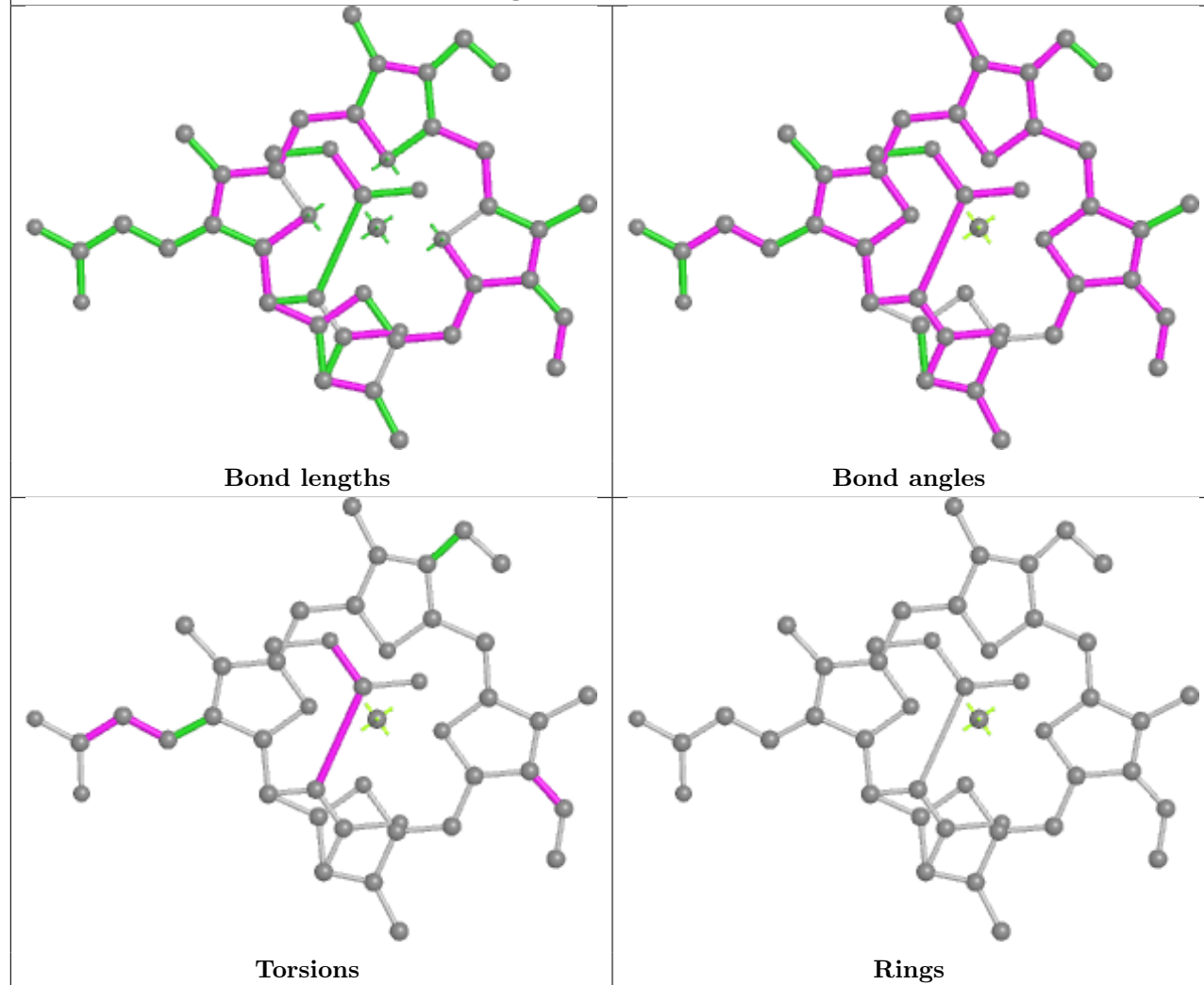


Rings

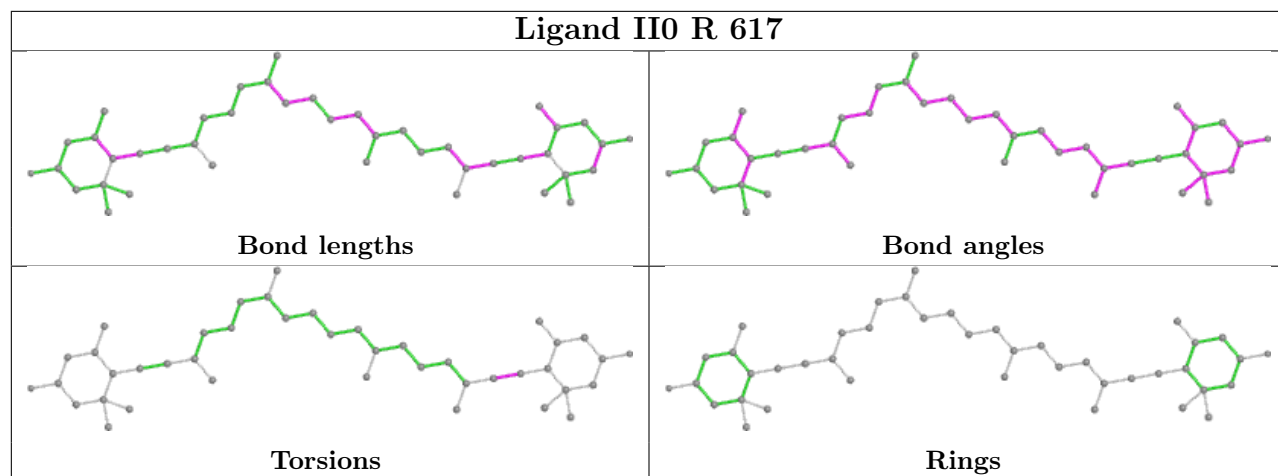
Ligand CLA S 615



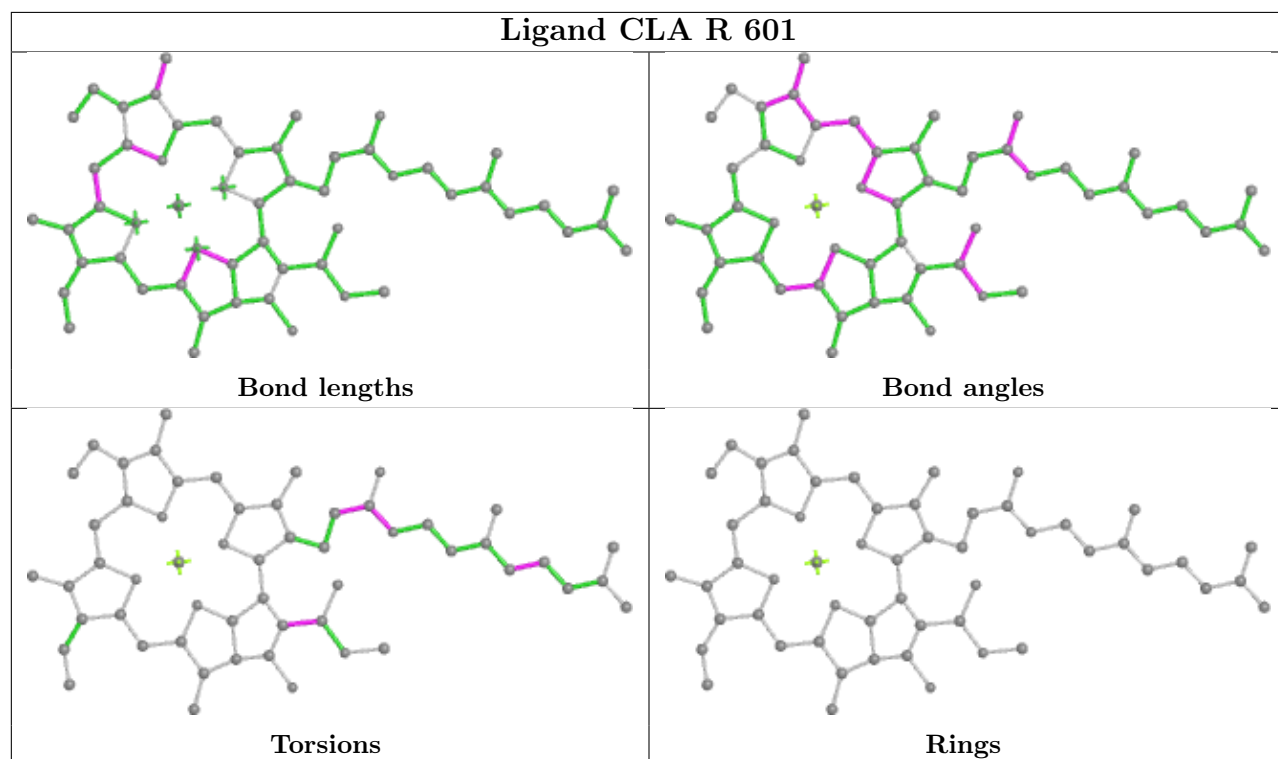
Ligand KC2 4 611



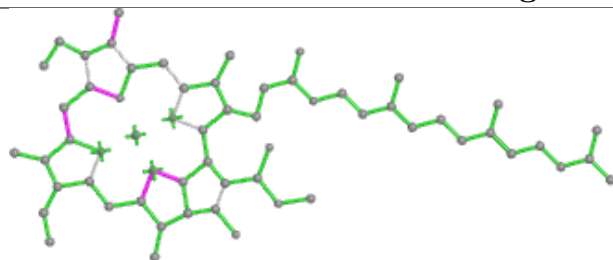
Ligand II0 R 617



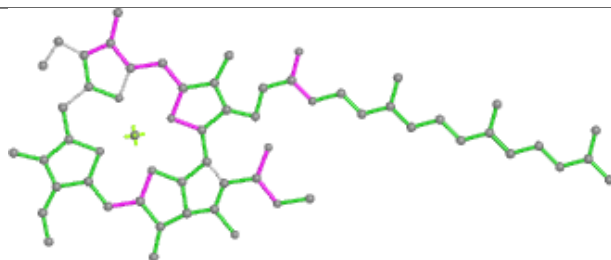
Ligand CLA R 601



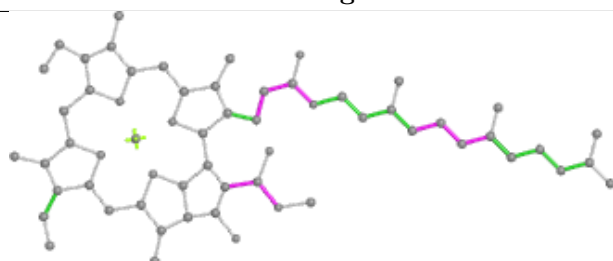
Ligand CLA c 519



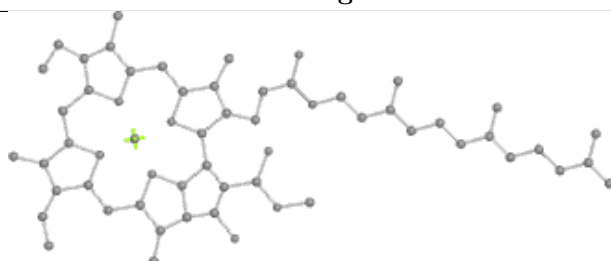
Bond lengths



Bond angles

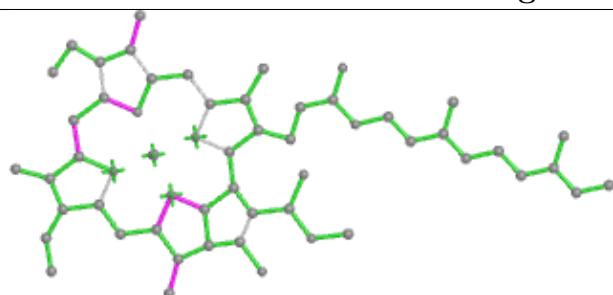


Torsions

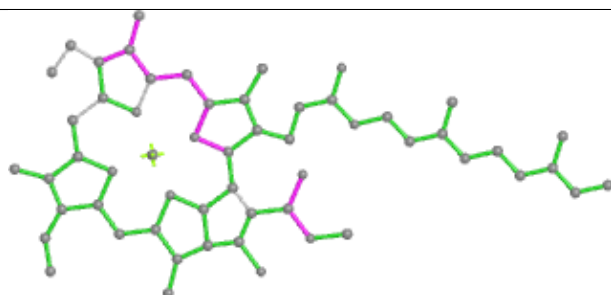


Rings

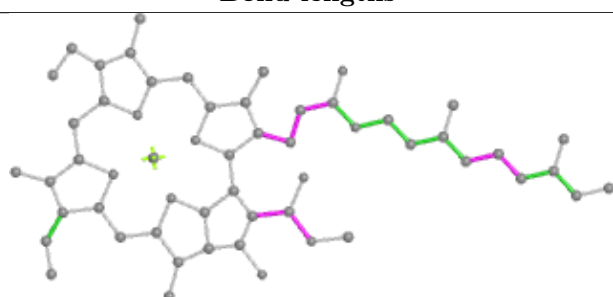
Ligand CLA 4 609



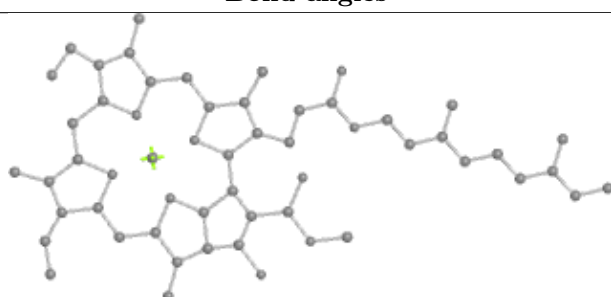
Bond lengths



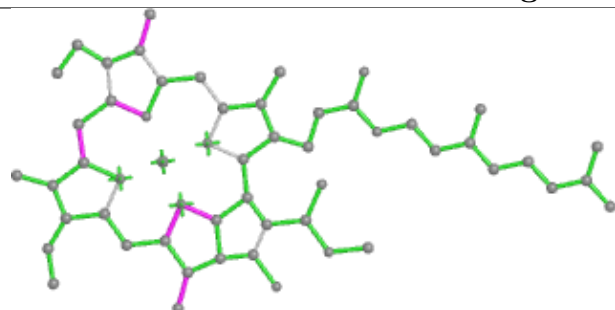
Bond angles



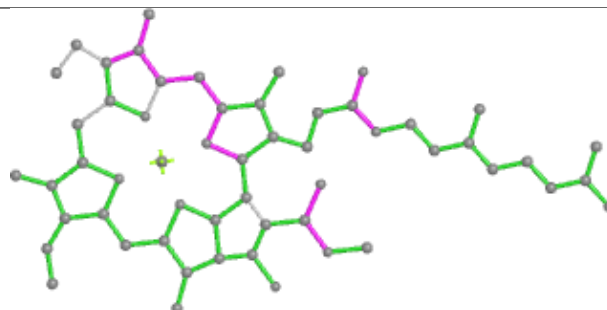
Torsions



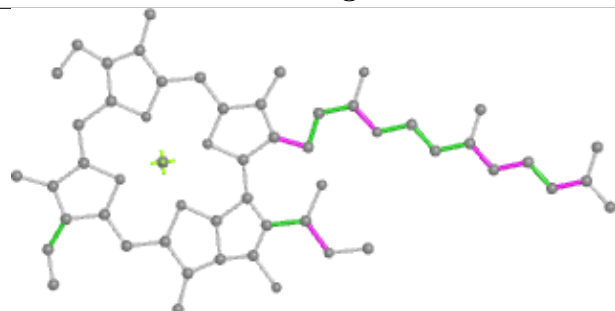
Rings

Ligand CLA 3 613

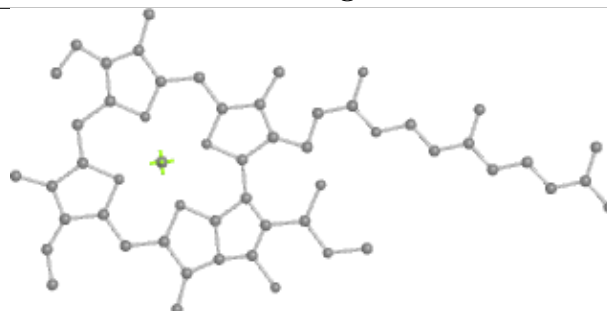
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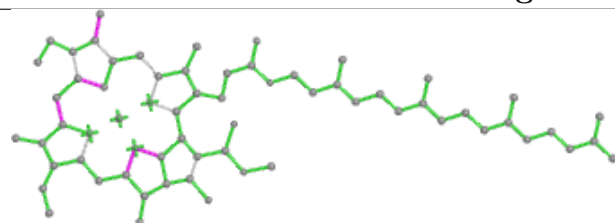
Bond angles



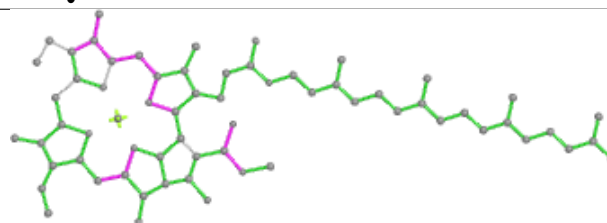
Torsions



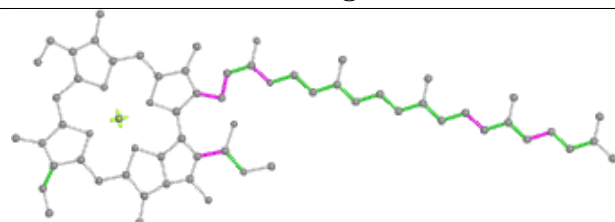
Rings

Ligand CLA Q 602

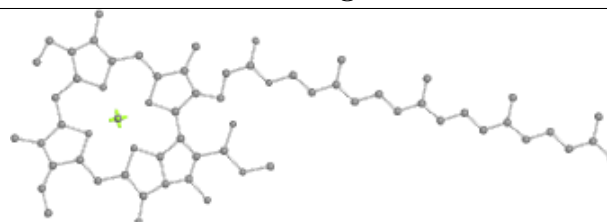
Bond lengths



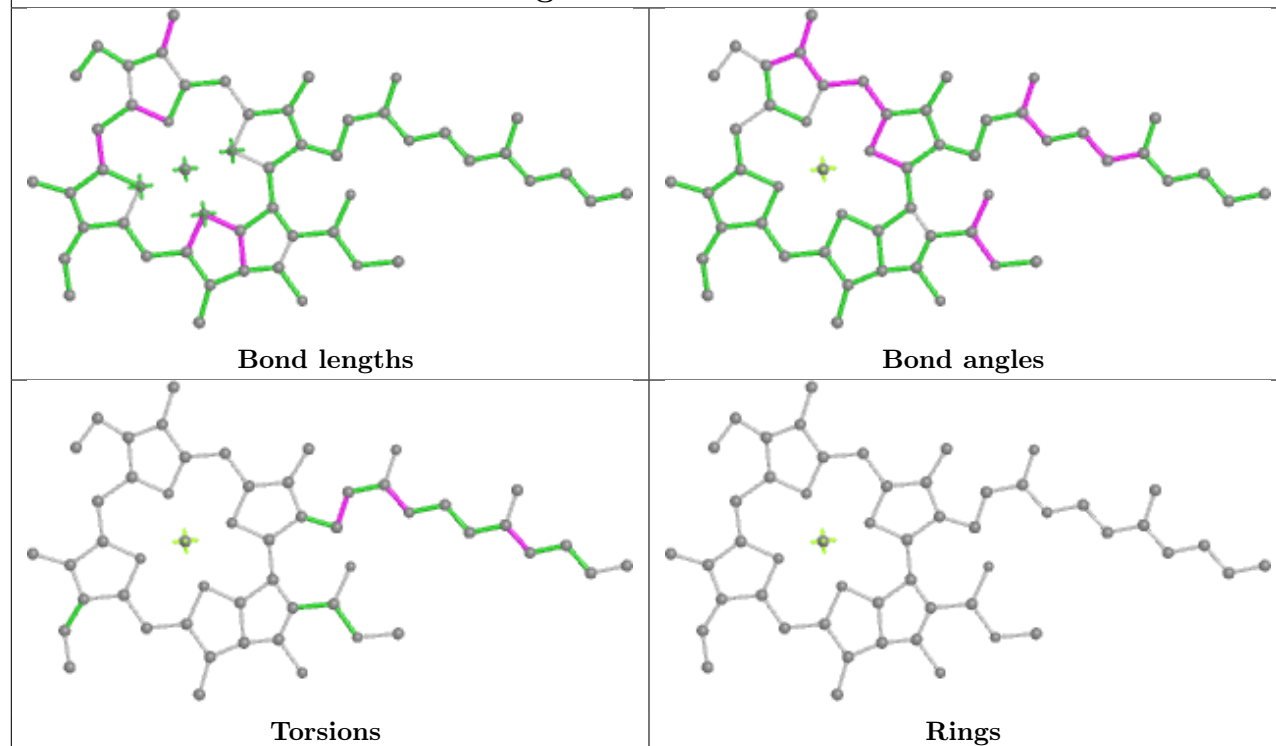
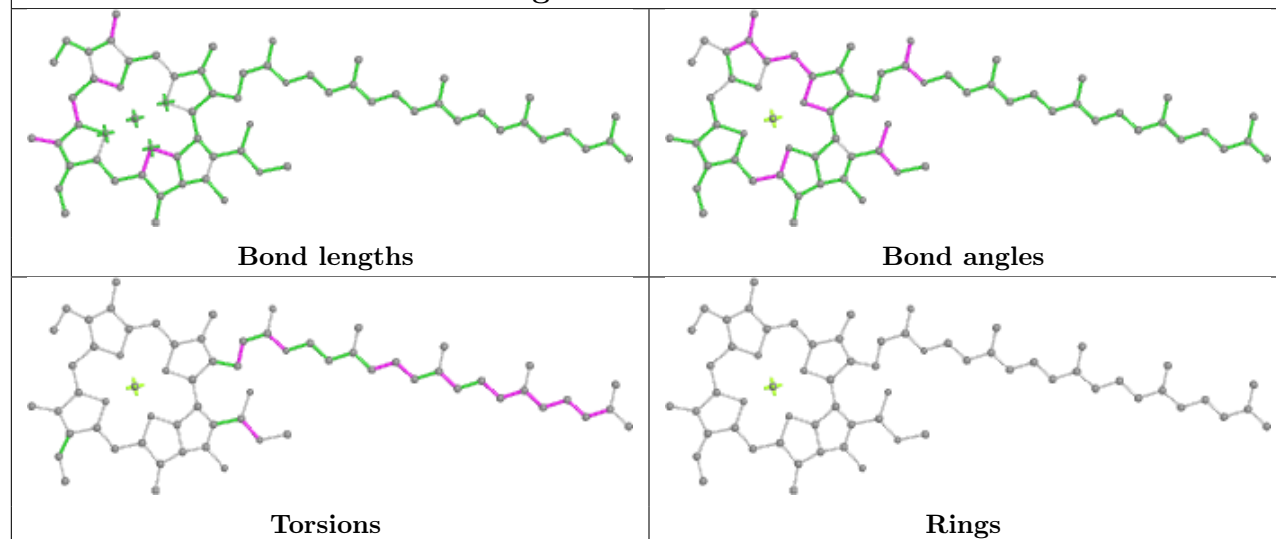
Bond angles

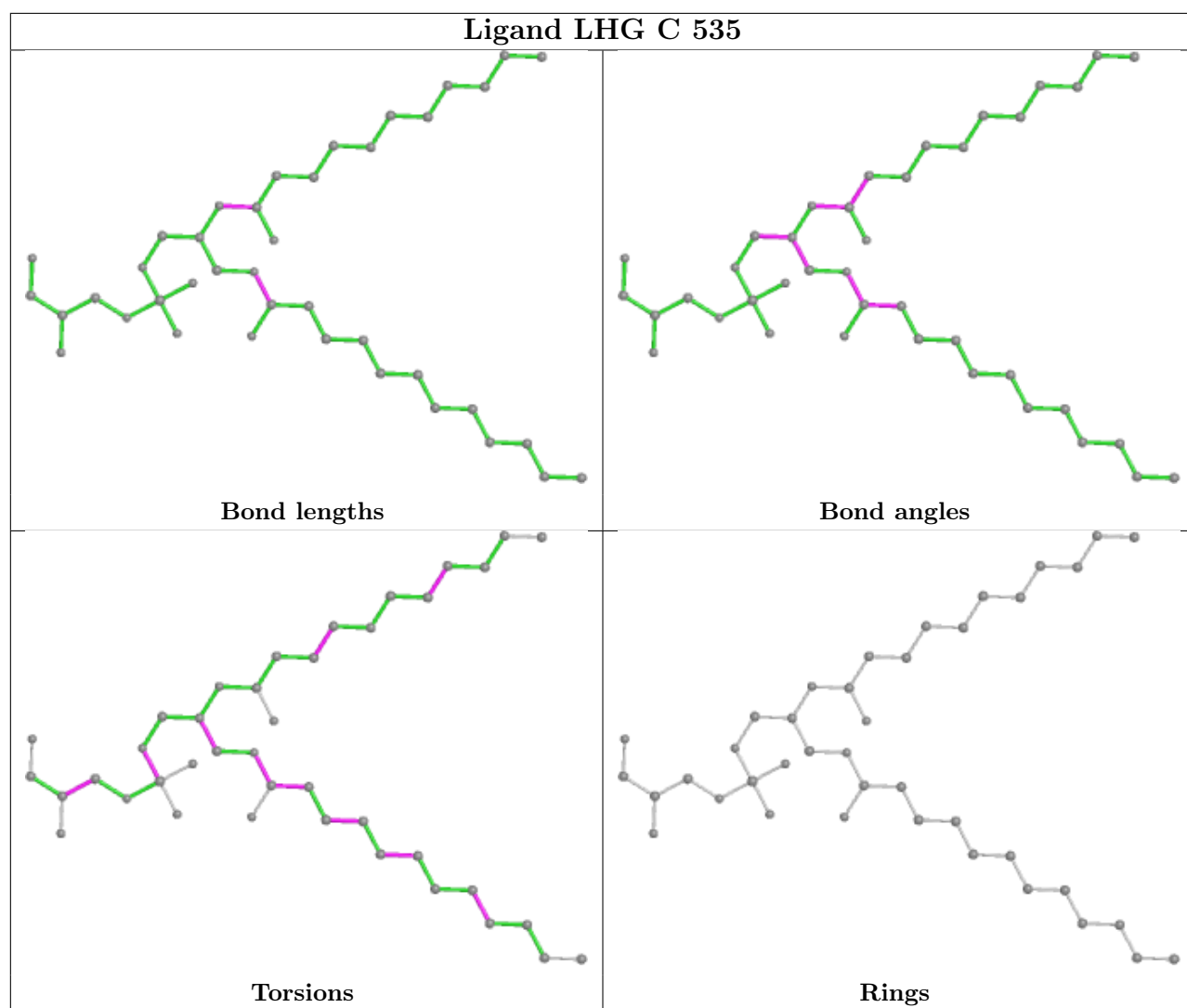


Torsions

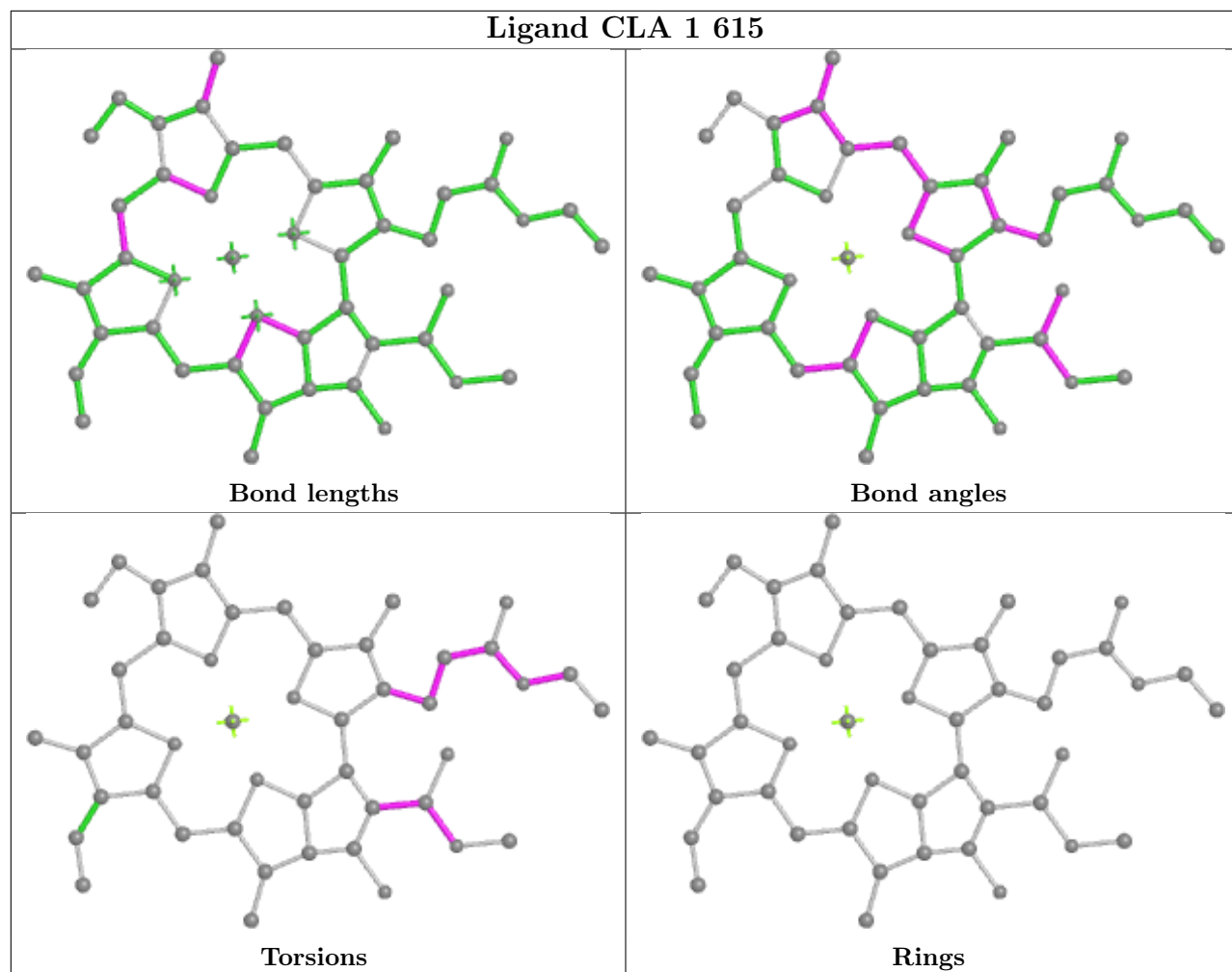


Rings

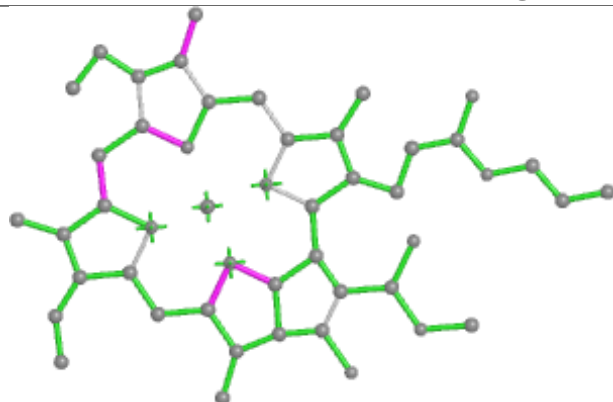
Ligand CLA 3 612**Ligand CLA B 616**



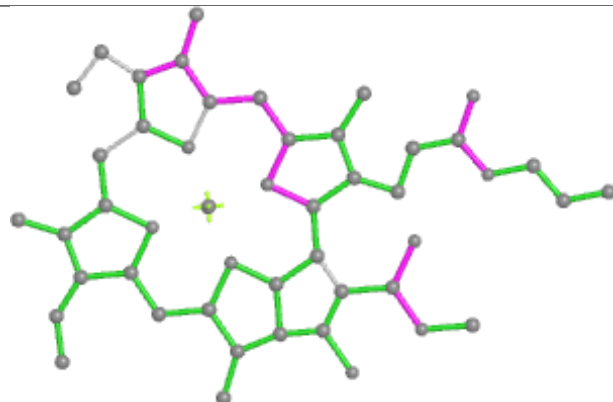
Ligand CLA 1 615



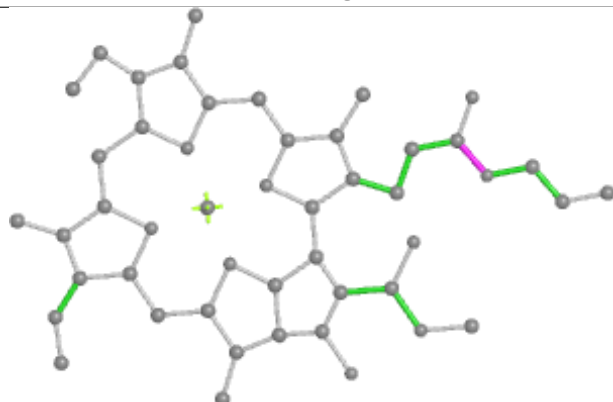
Ligand CLA O 609



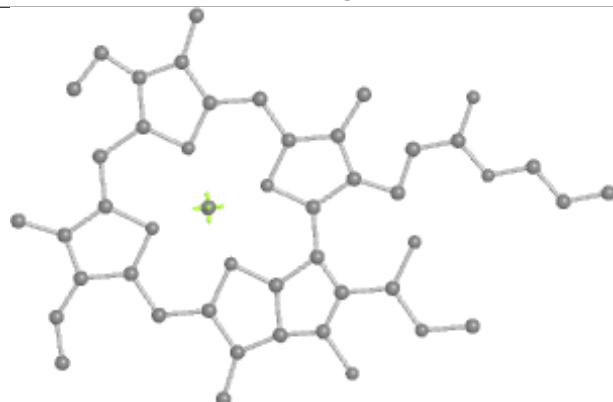
Bond lengths



Bond angles

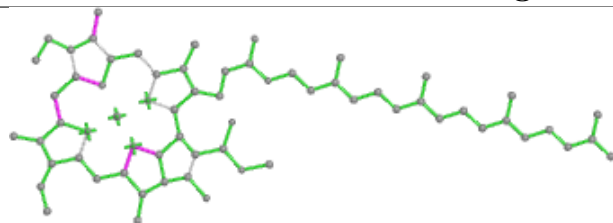


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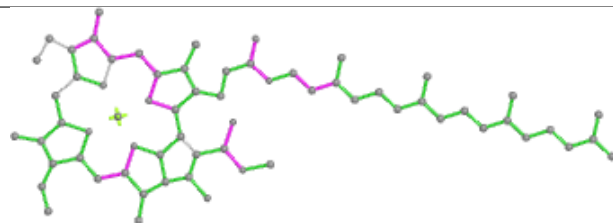


Rings

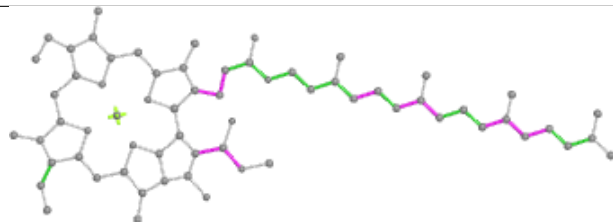
Ligand CLA O 602



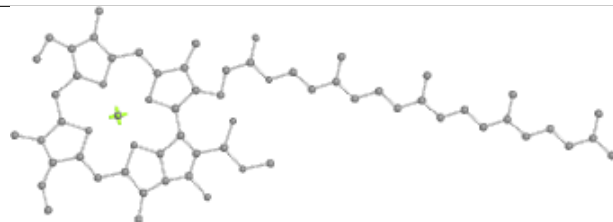
Bond lengths



Bond angles

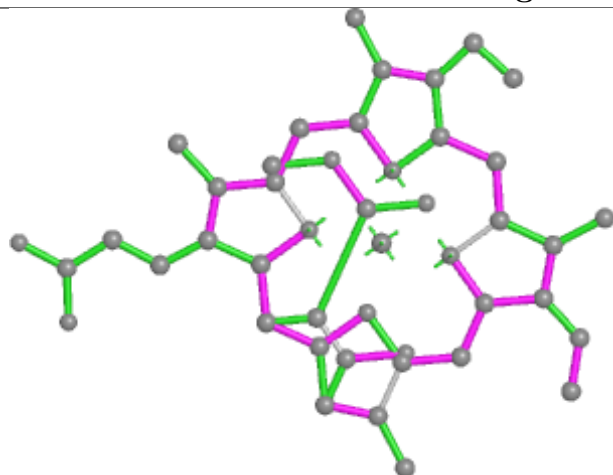


Torsions

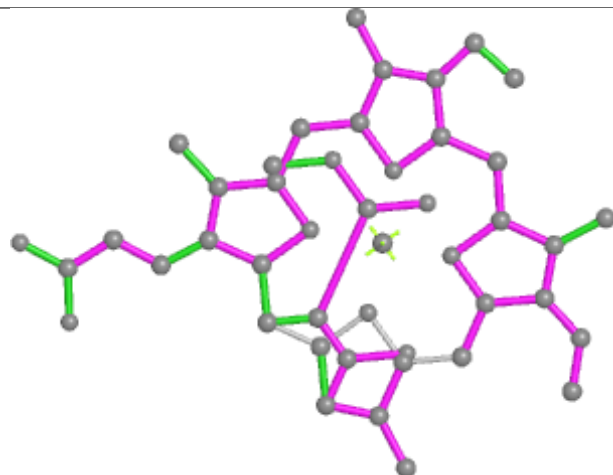


Rings

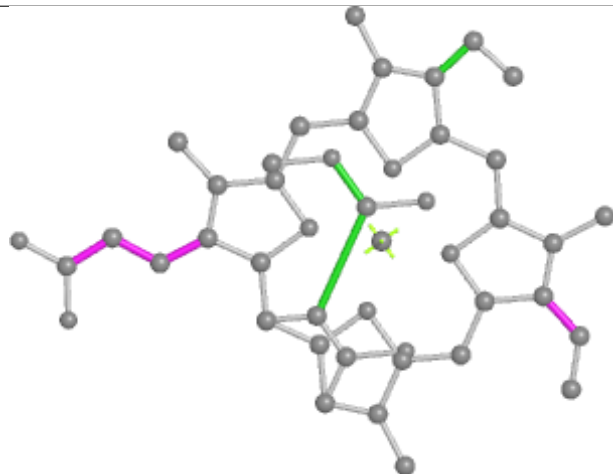
Ligand KC2 O 612



Bond lengths



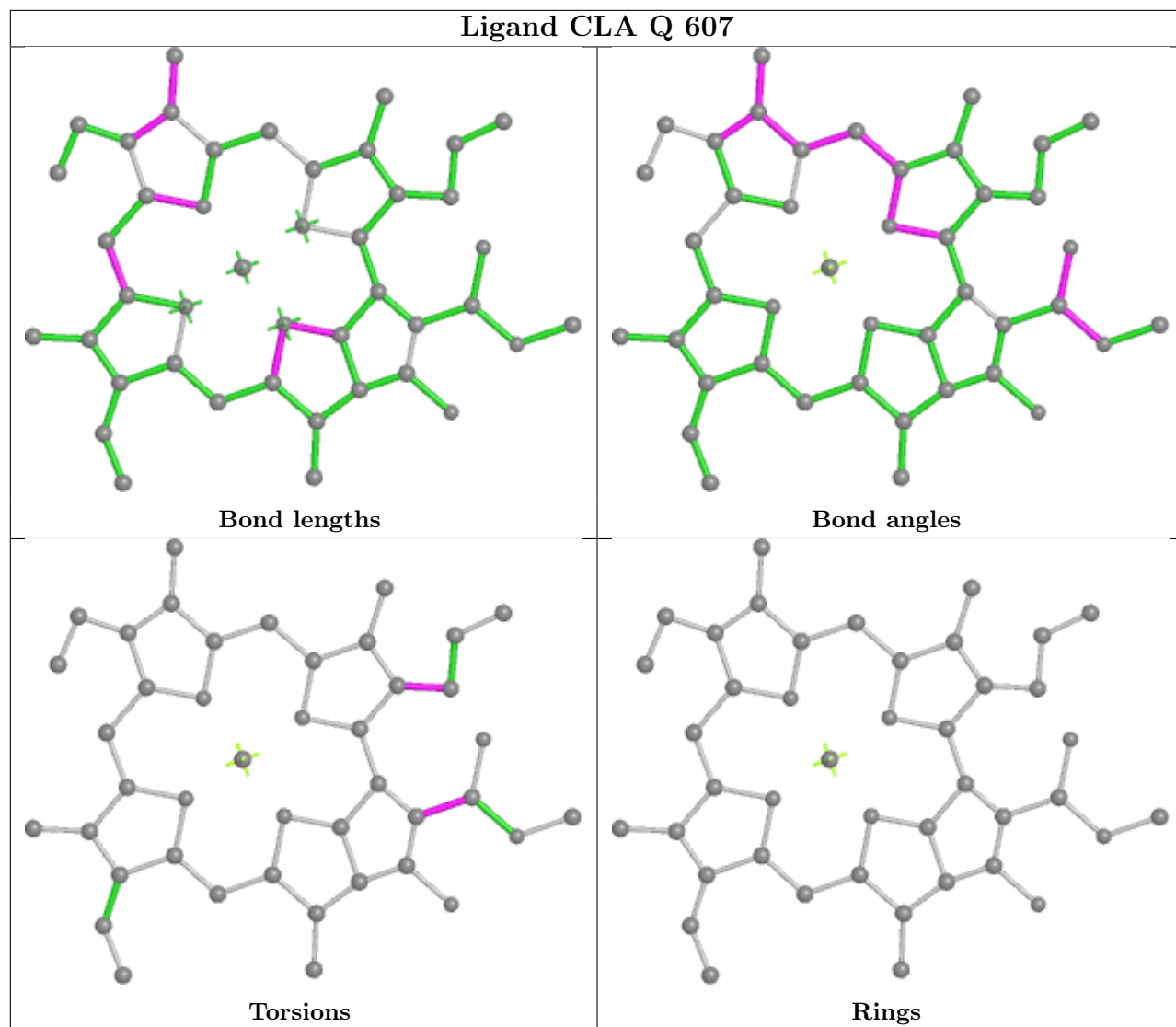
Bond angles



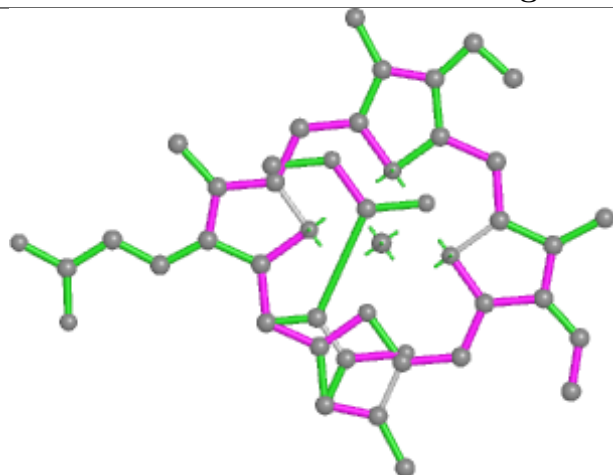
Torsions



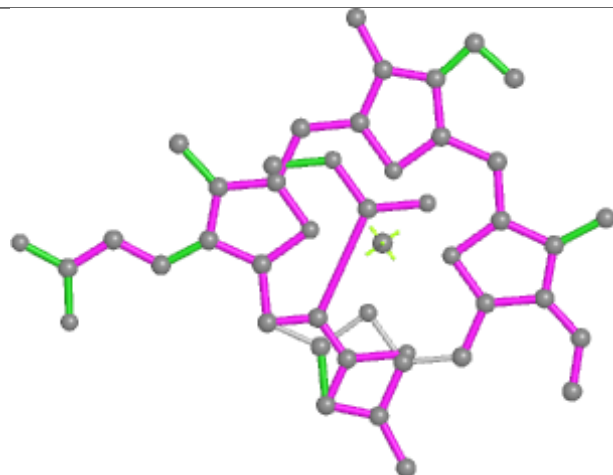
Rings



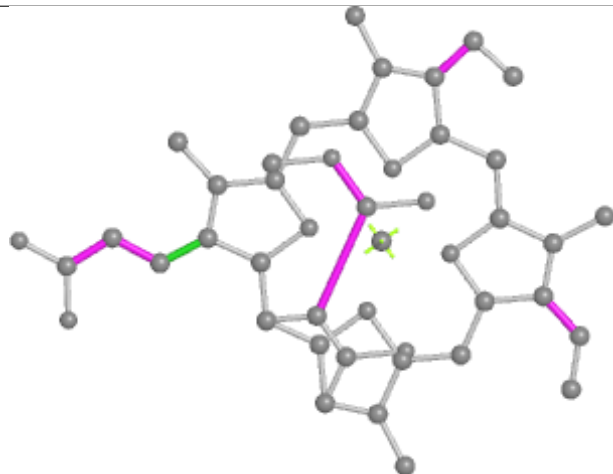
Ligand KC2 1 605



Bond lengths



Bond angles

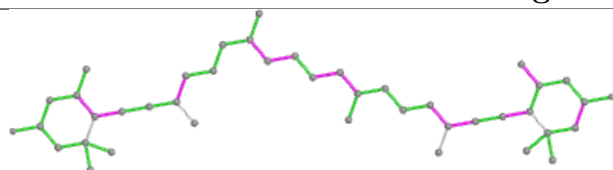


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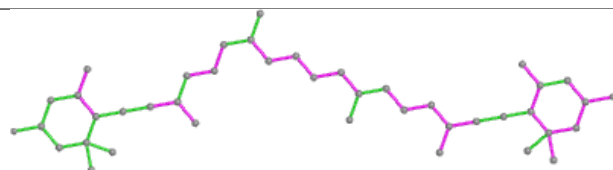


Rings

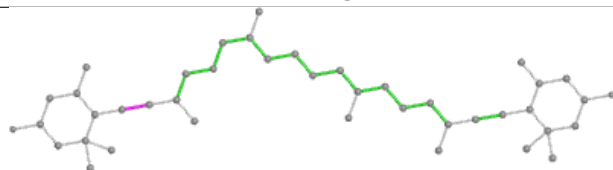
Ligand II0 6 617



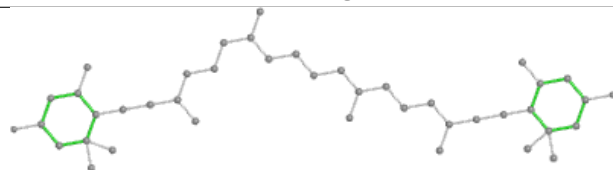
Bond lengths



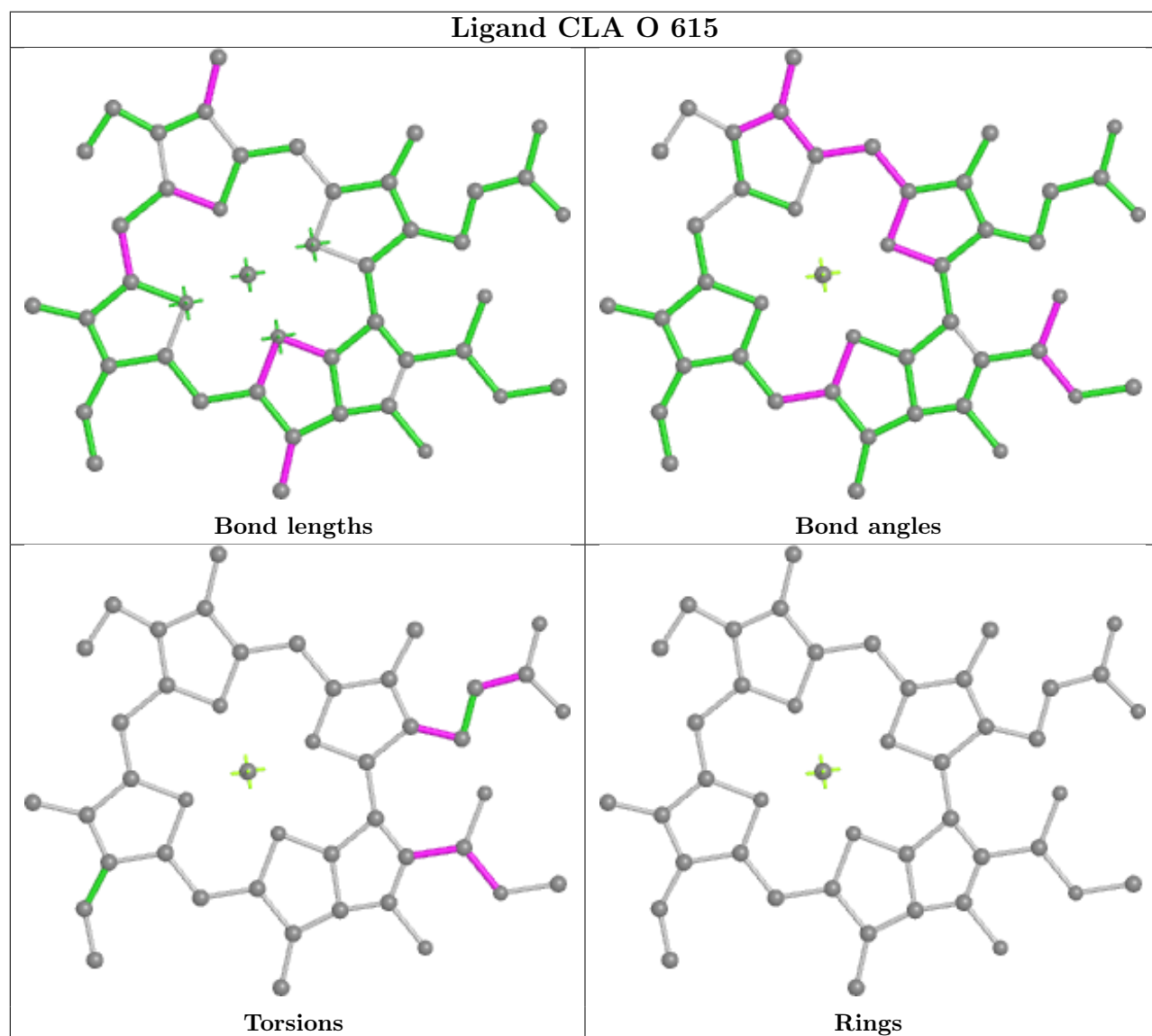
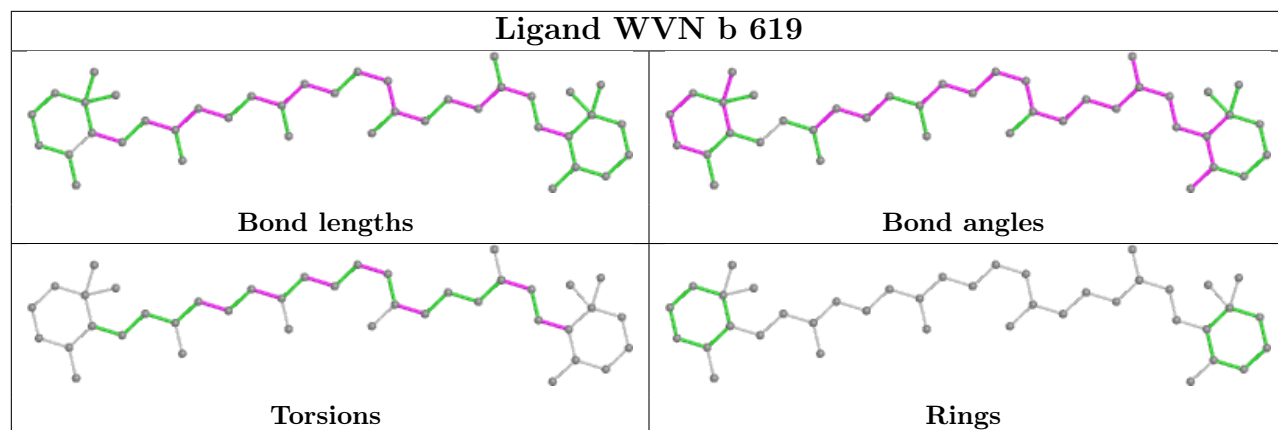
Bond angles

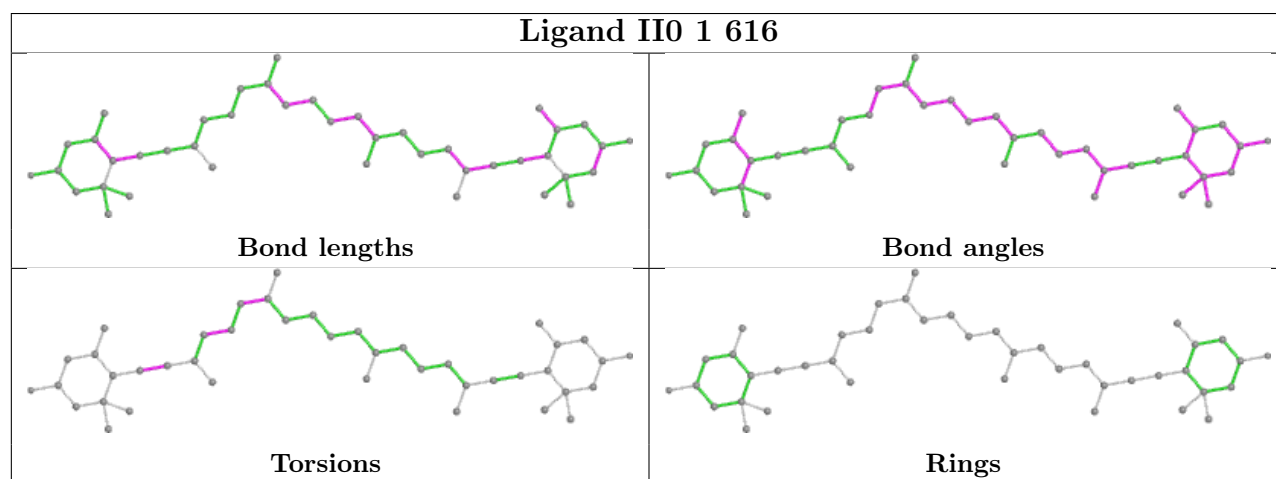
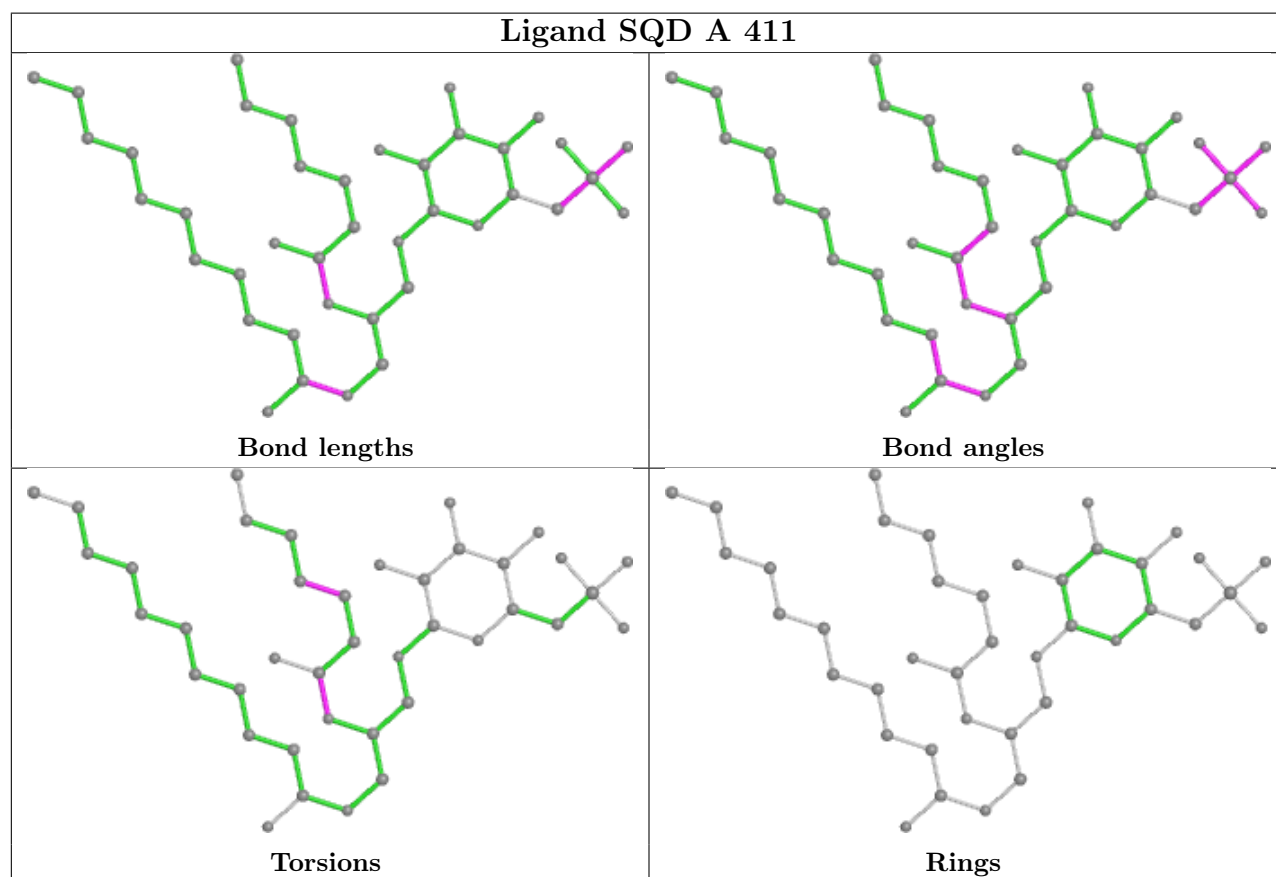
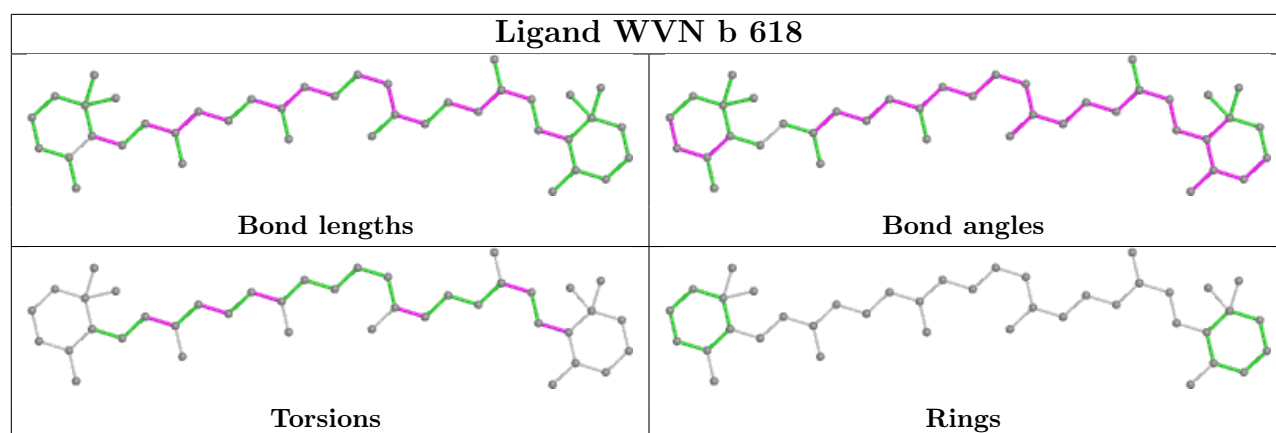


Torsions

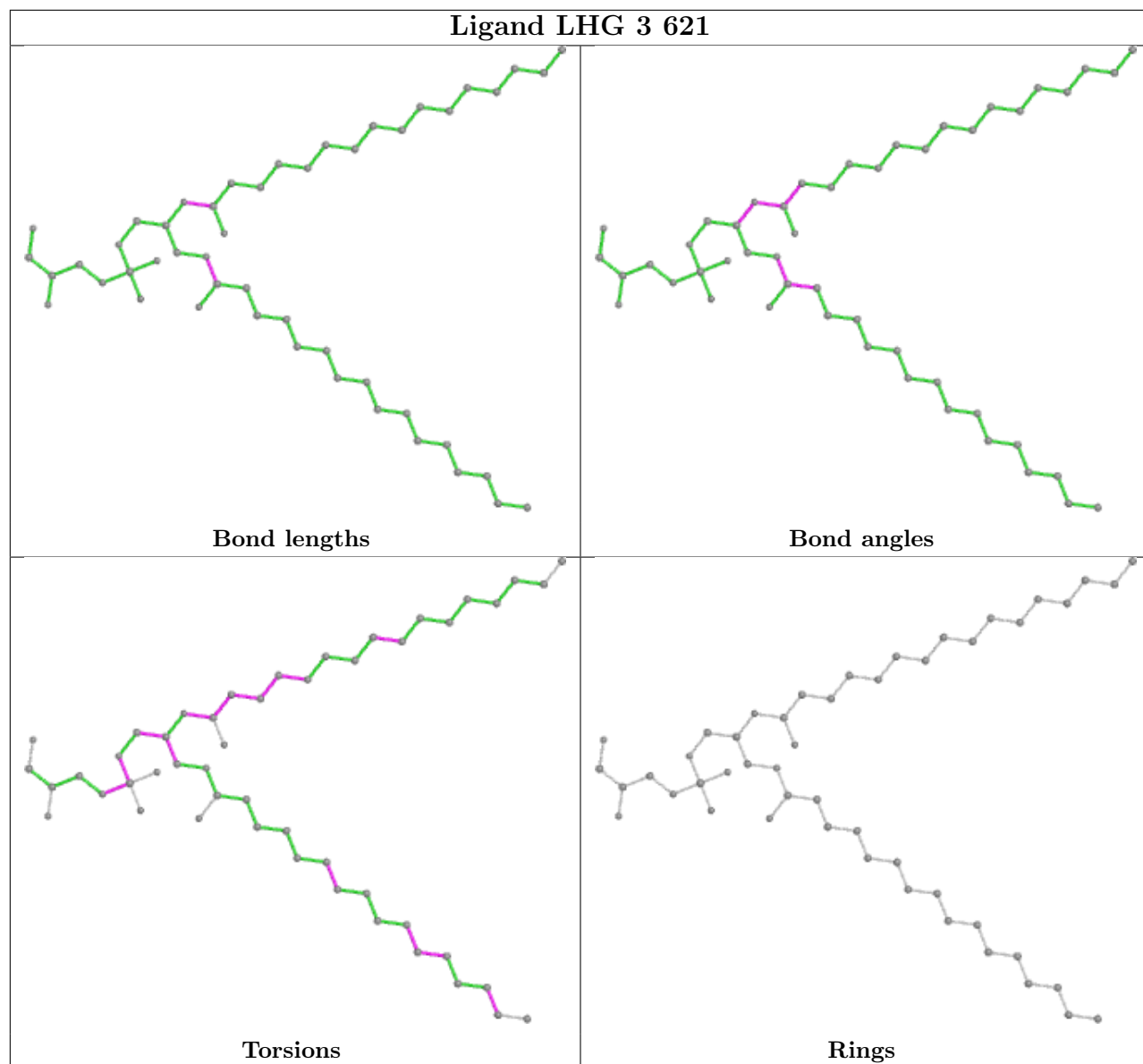


Rings

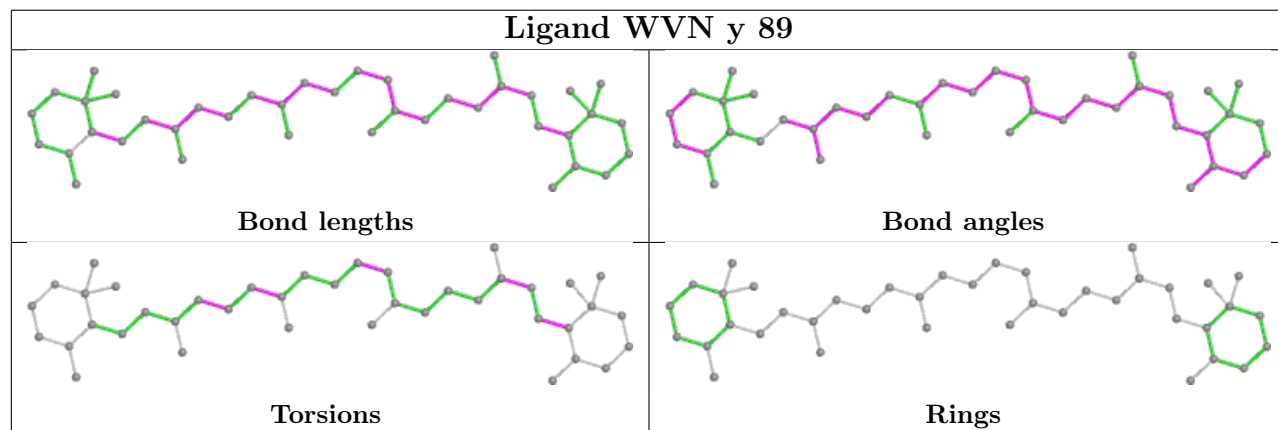




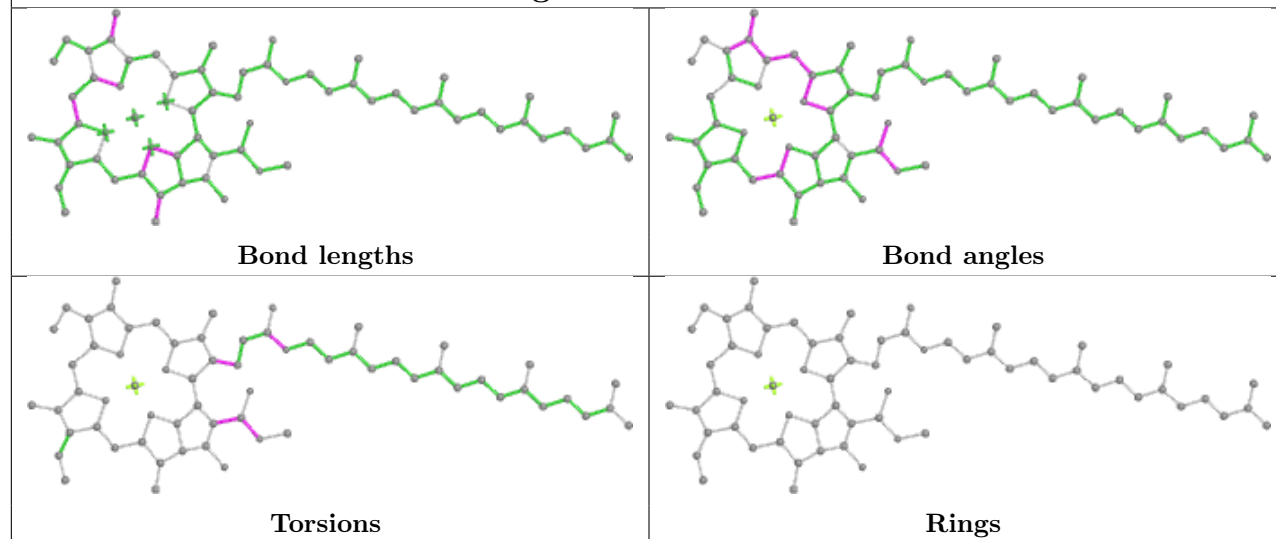
Ligand LHG 3 621



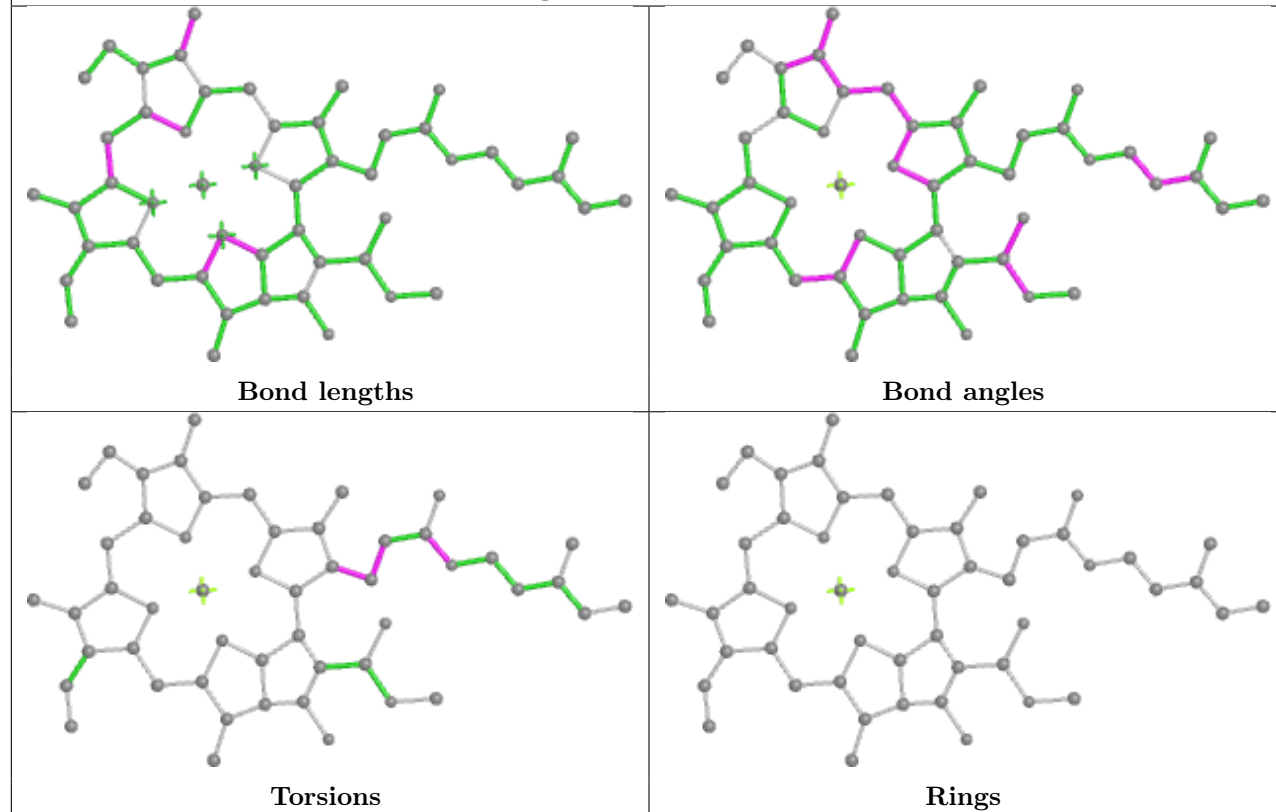
Ligand WVN y 89



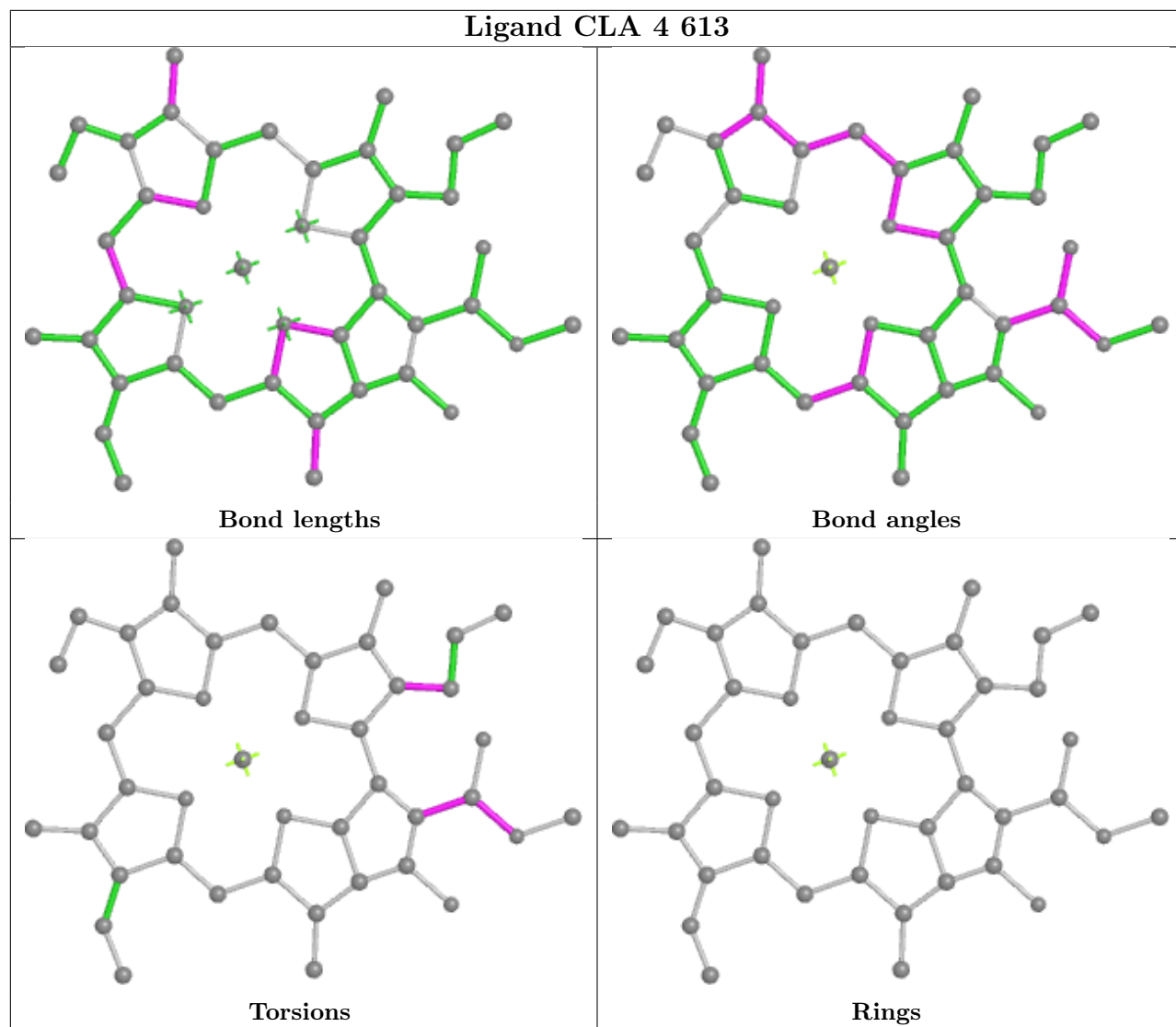
Ligand CLA C 516



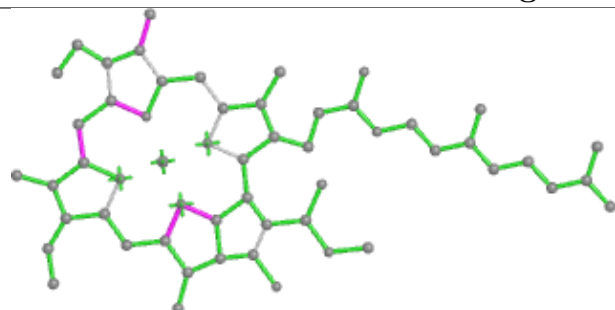
Ligand CLA 4 610



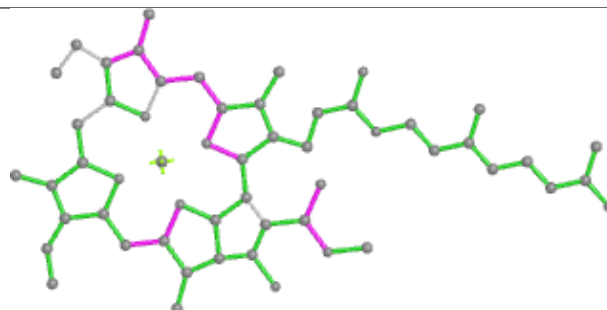
Ligand CLA 4 613



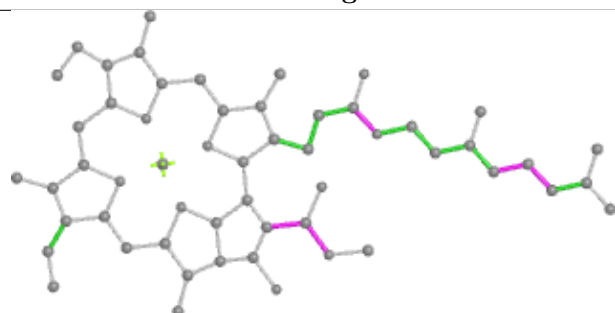
Ligand CLA S 601



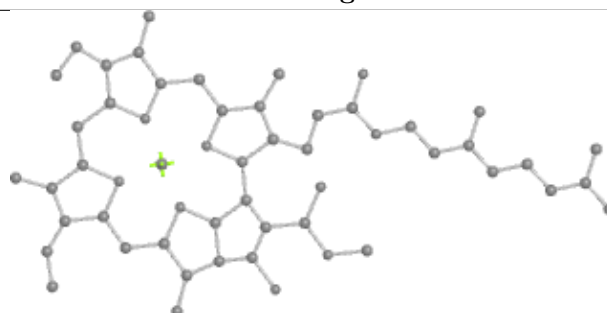
Bond lengths



Bond angles

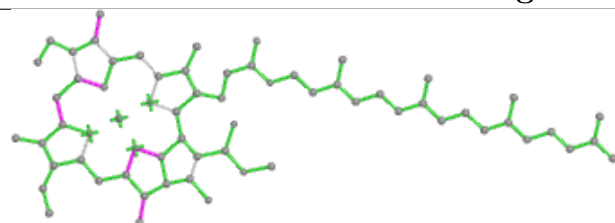


Torsions

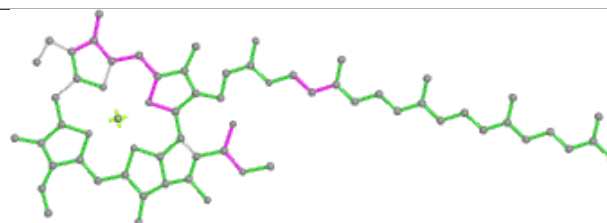


Rings

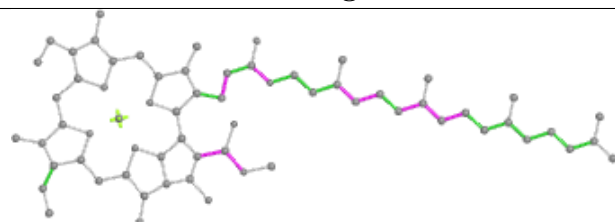
Ligand CLA C 525



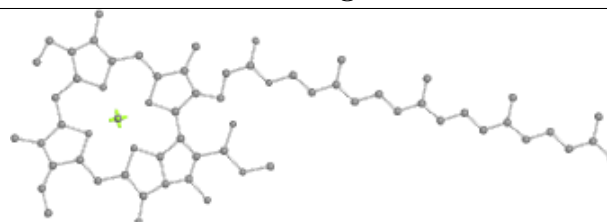
Bond lengths



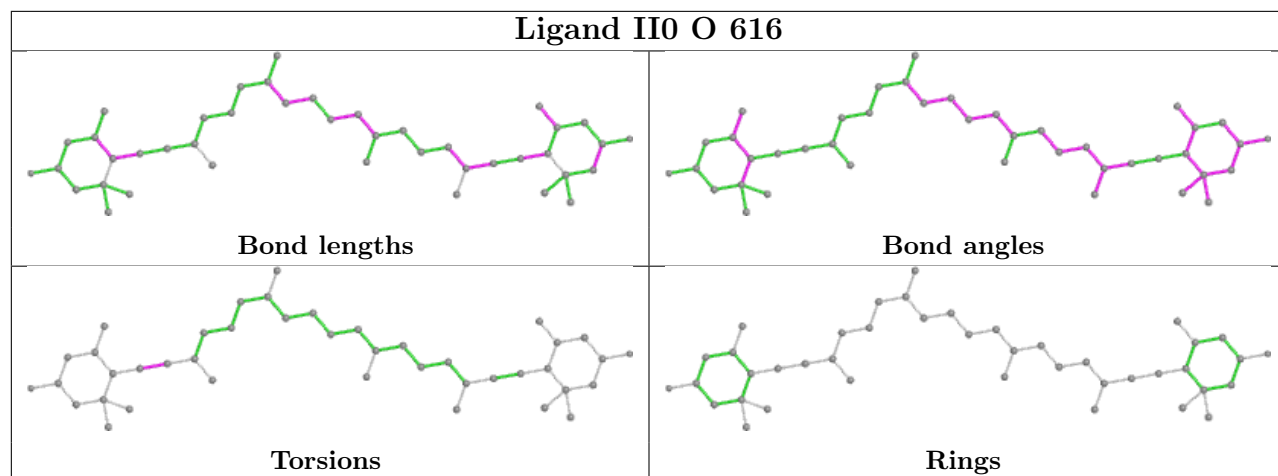
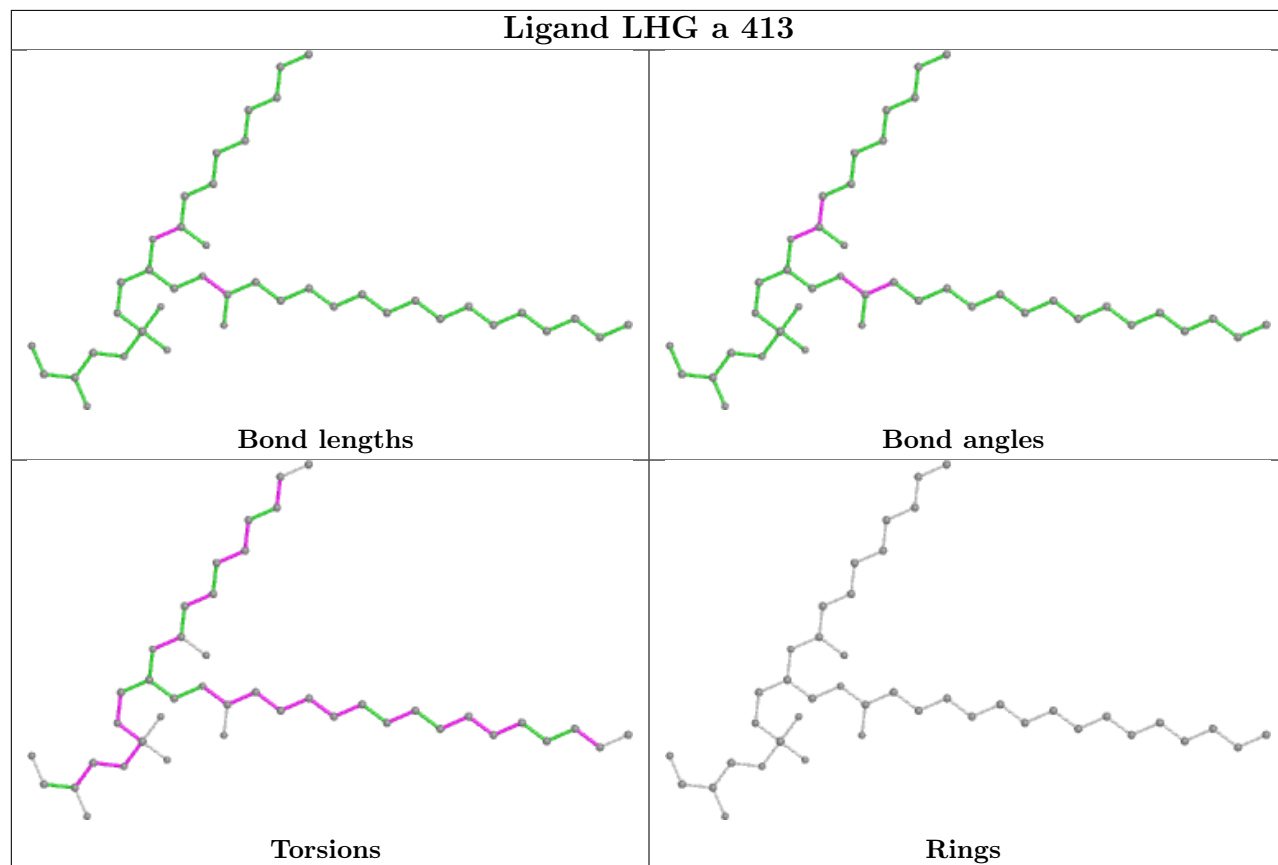
Bond angles



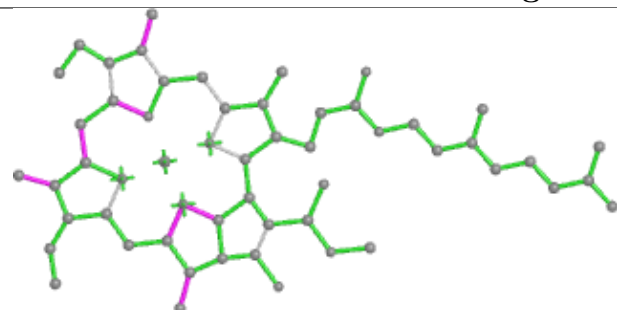
Torsions



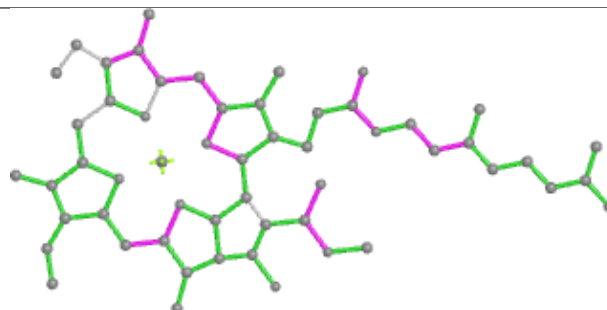
Rings

Ligand II0 O 616**Ligand LHG a 413**

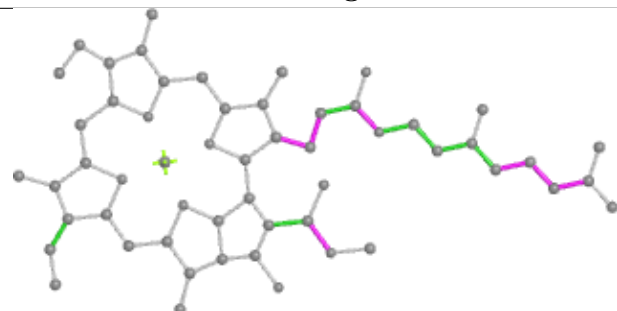
Ligand CLA 4 606



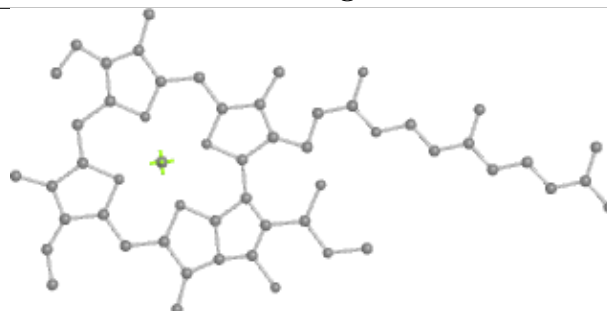
Bond lengths



Bond angles

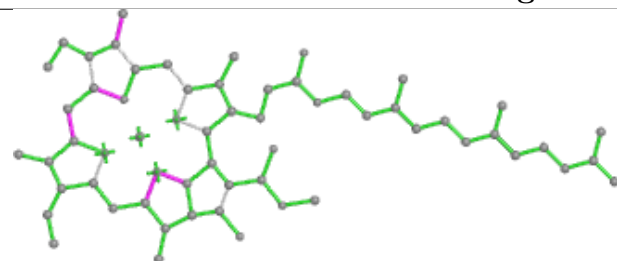


Torsions

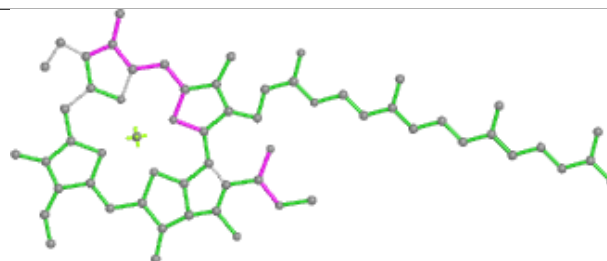


Rings

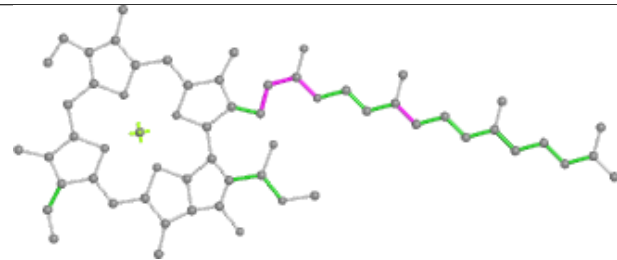
Ligand CLA N 603



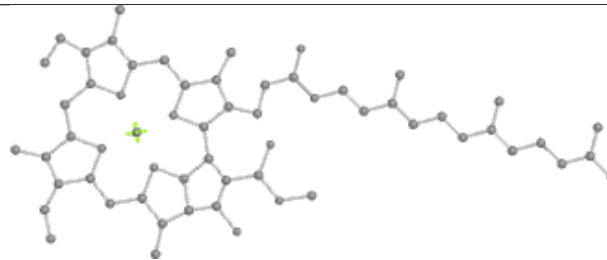
Bond lengths



Bond angles

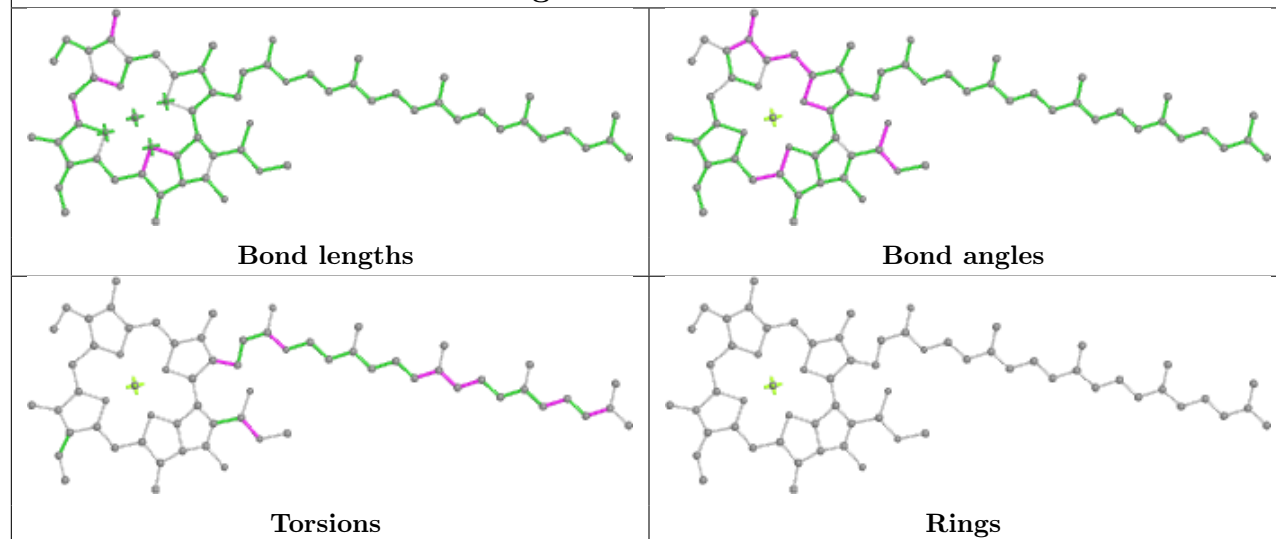


Torsions

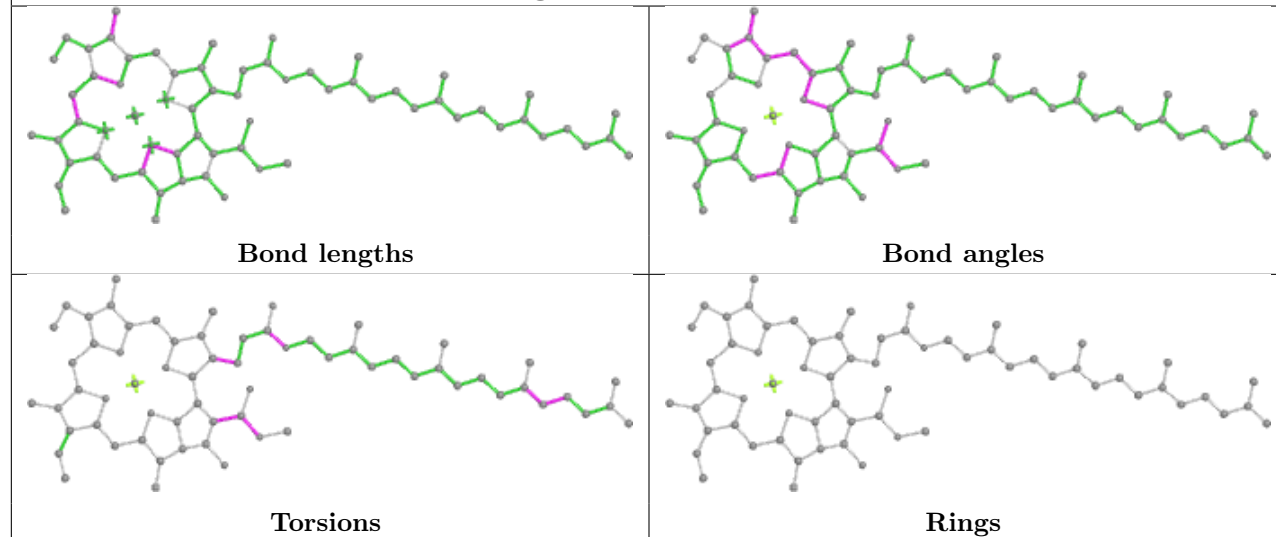


Rings

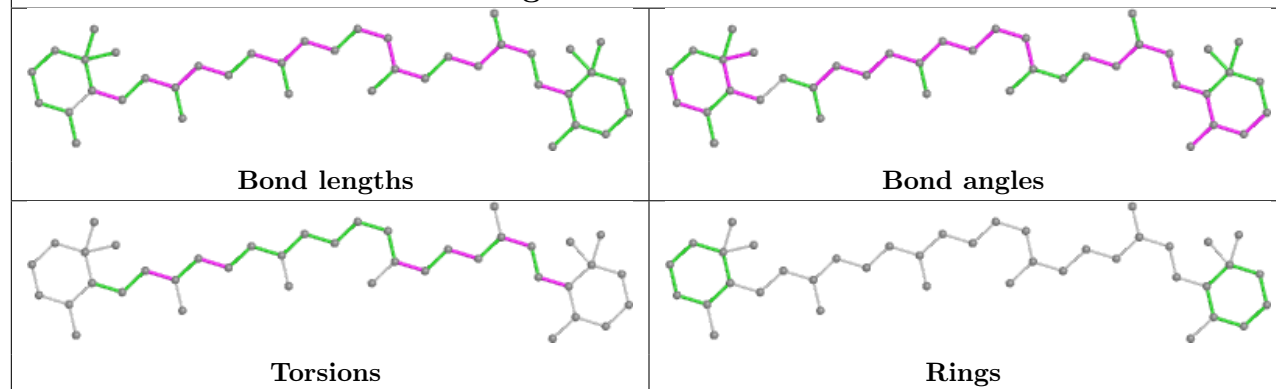
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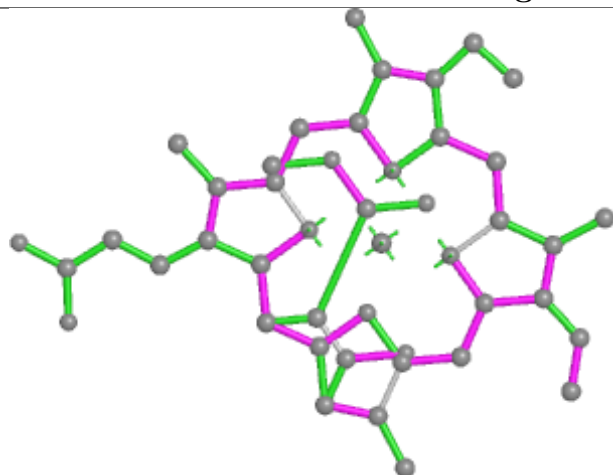
Ligand CLA O 610



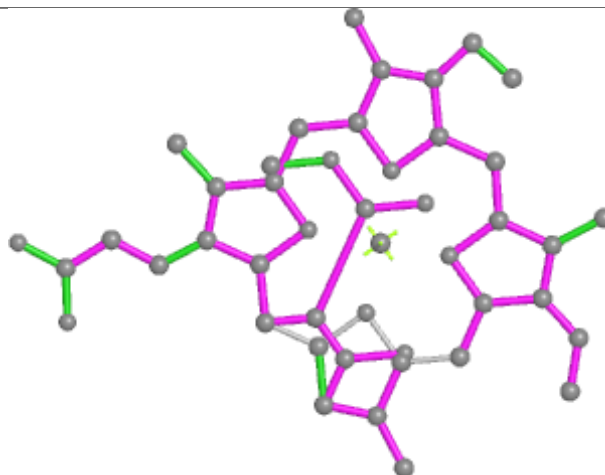
Ligand WVN D 408



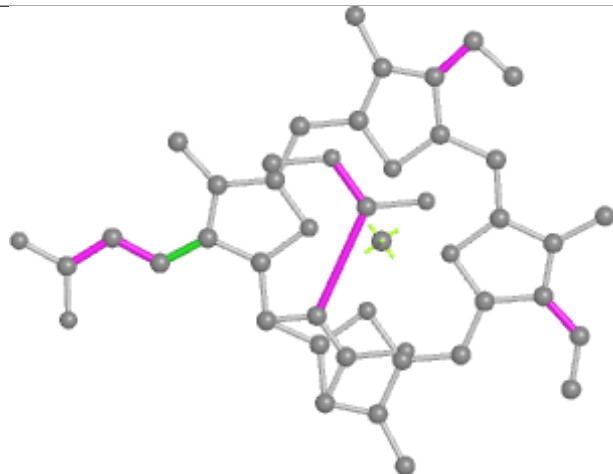
Ligand KC2 N 613



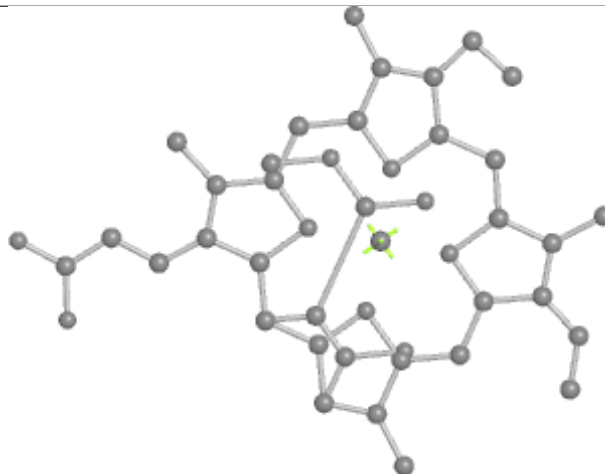
Bond lengths



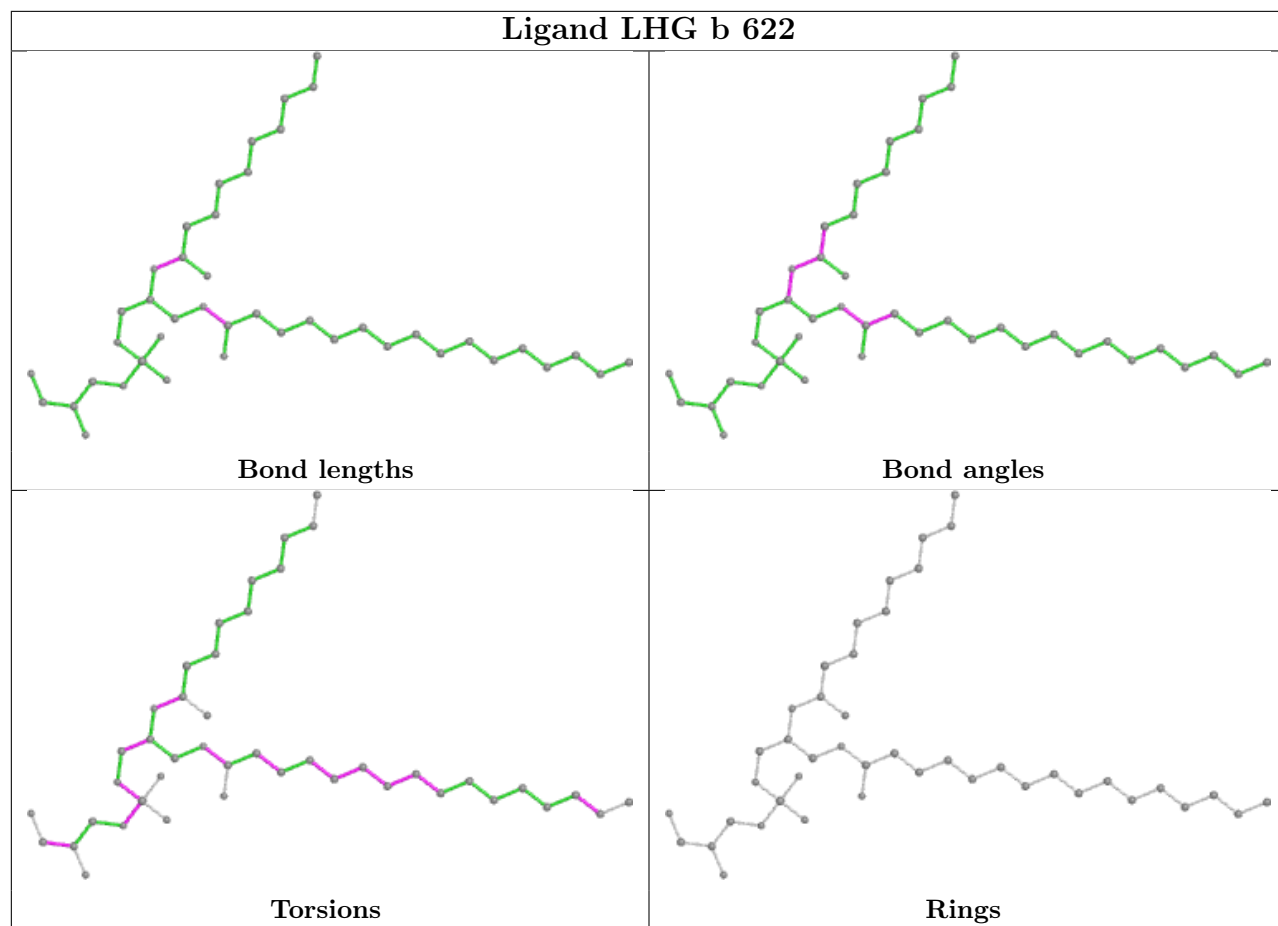
Bond angles

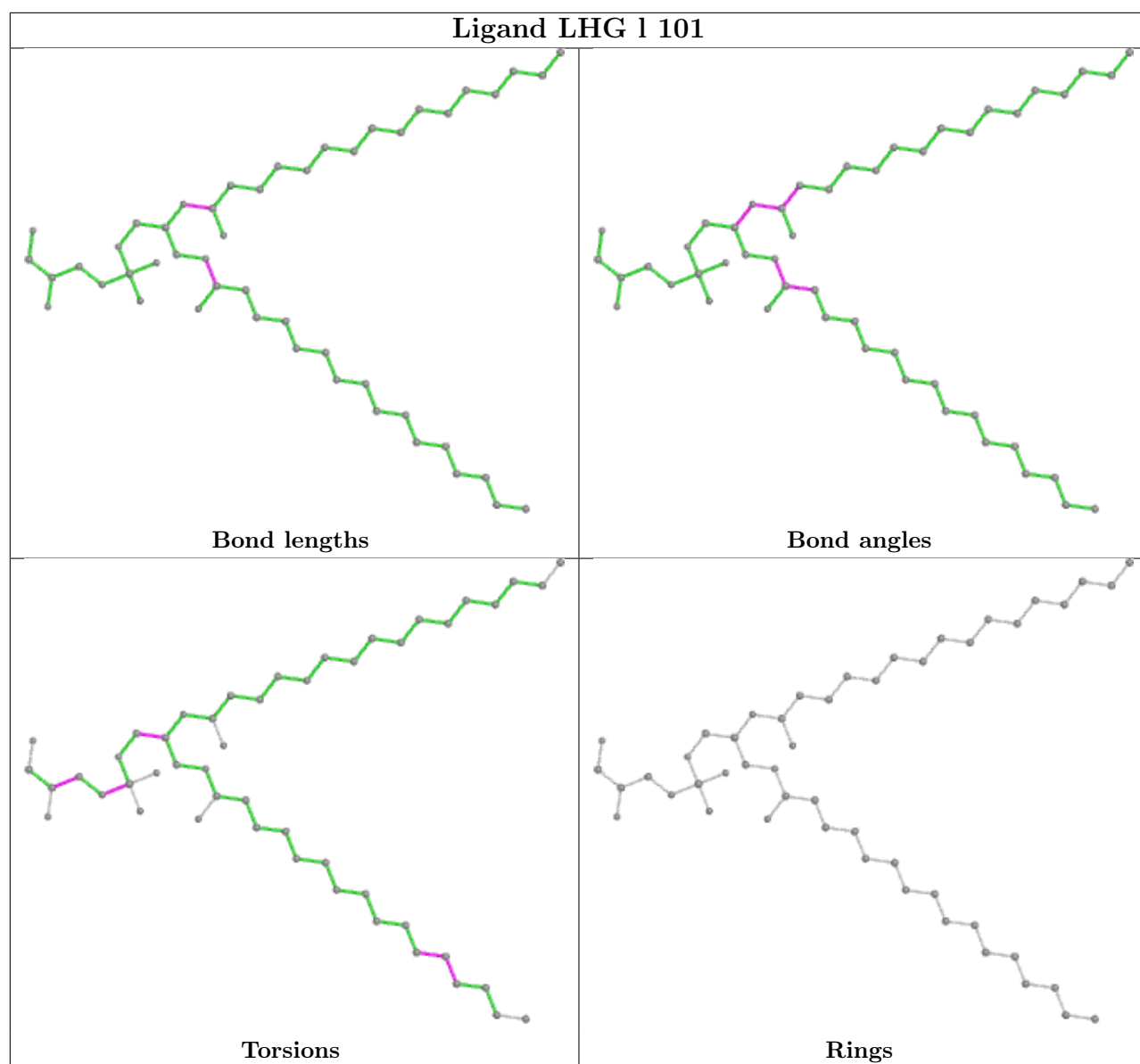


Torsions

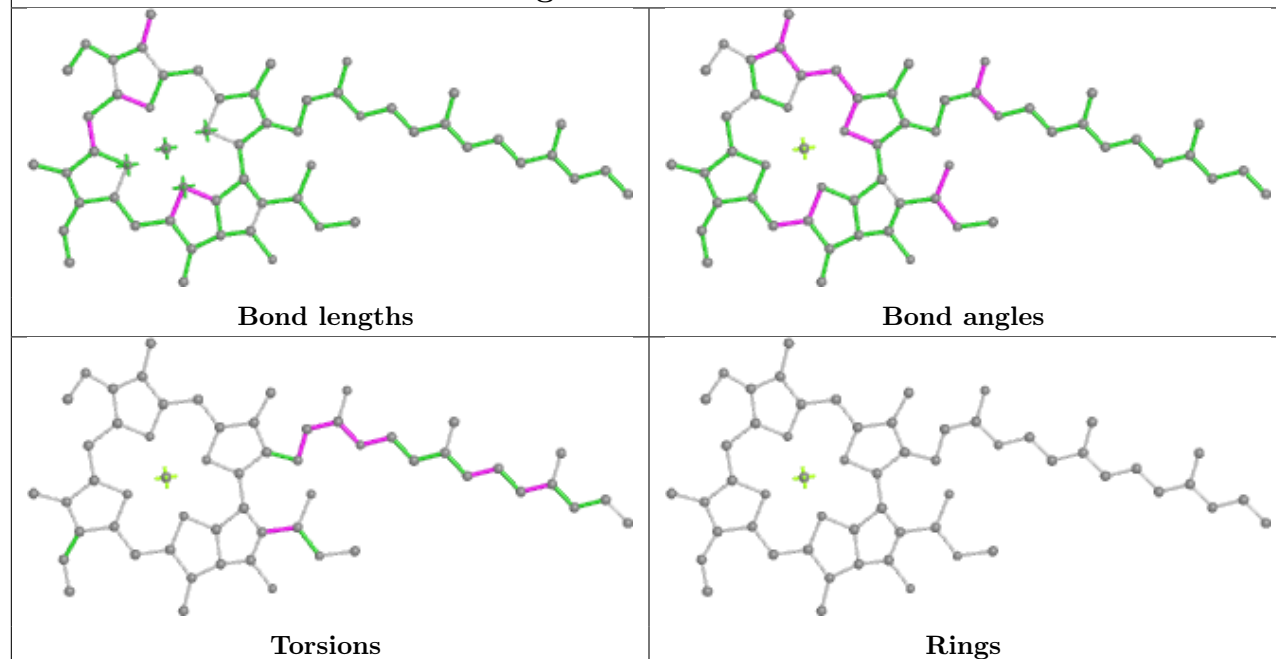


Rings

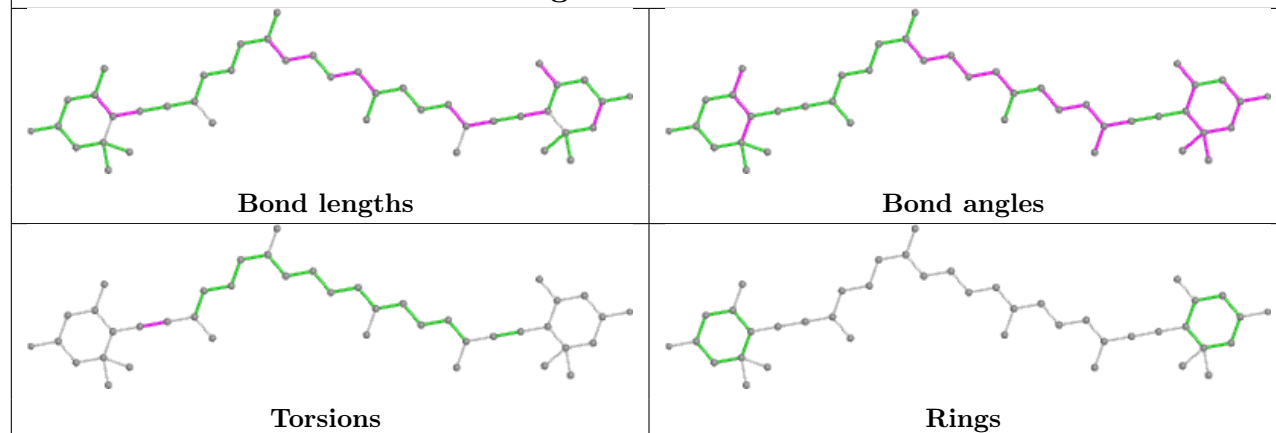




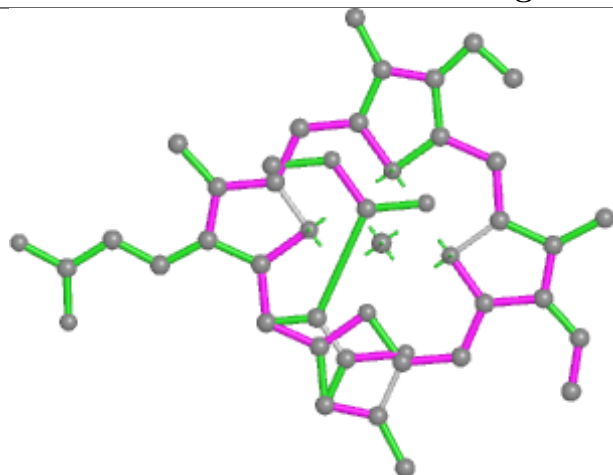
Ligand CLA 6 610



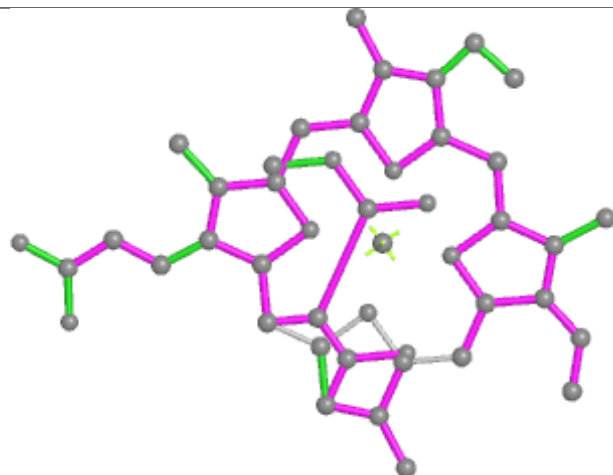
Ligand II0 2 616



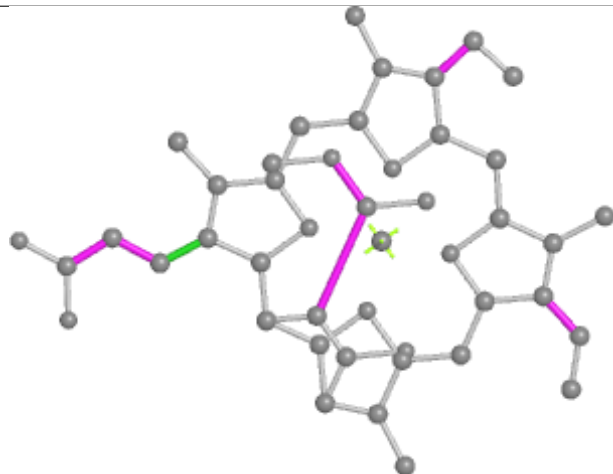
Ligand KC2 N 605



Bond lengths



Bond angles

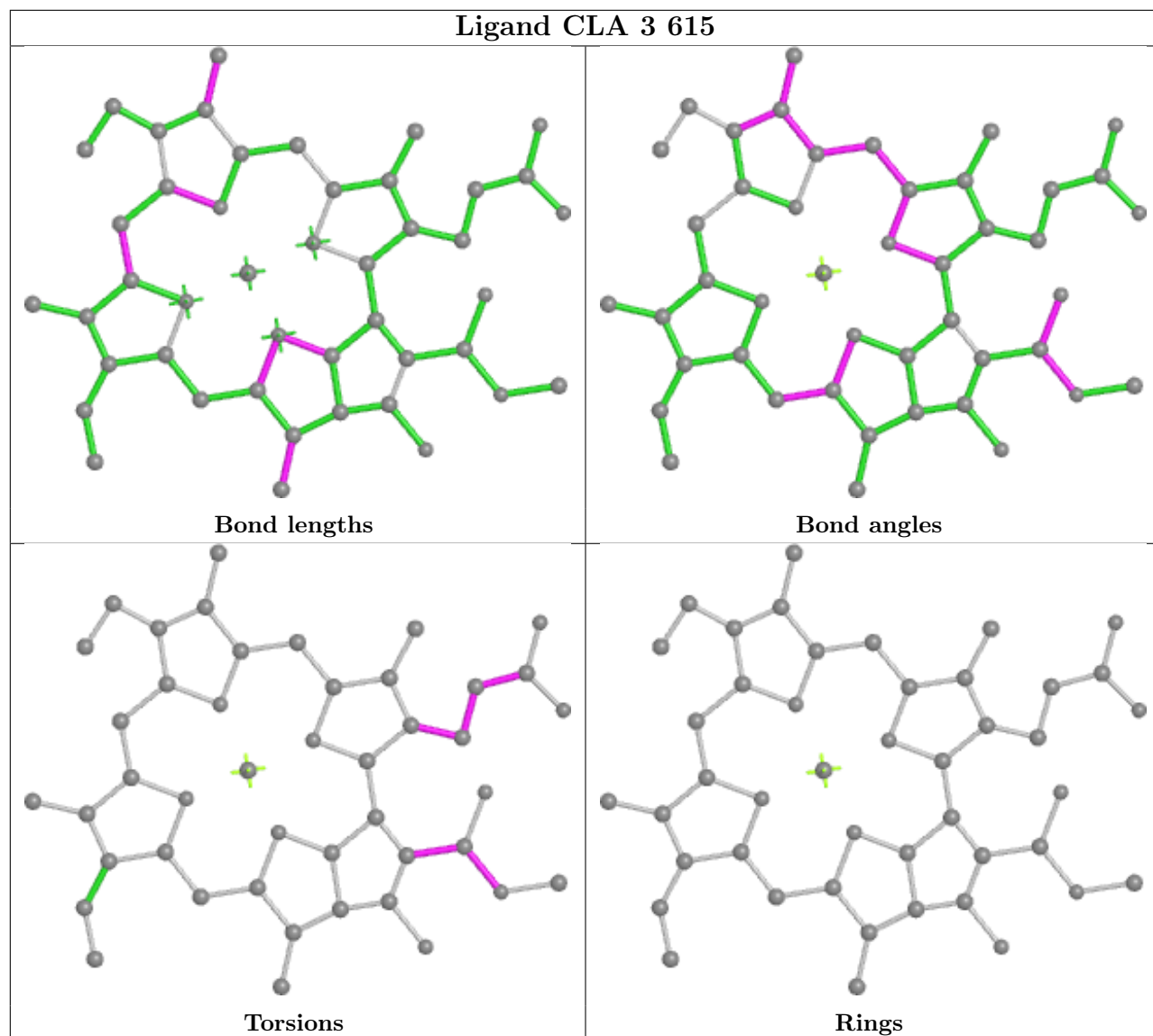


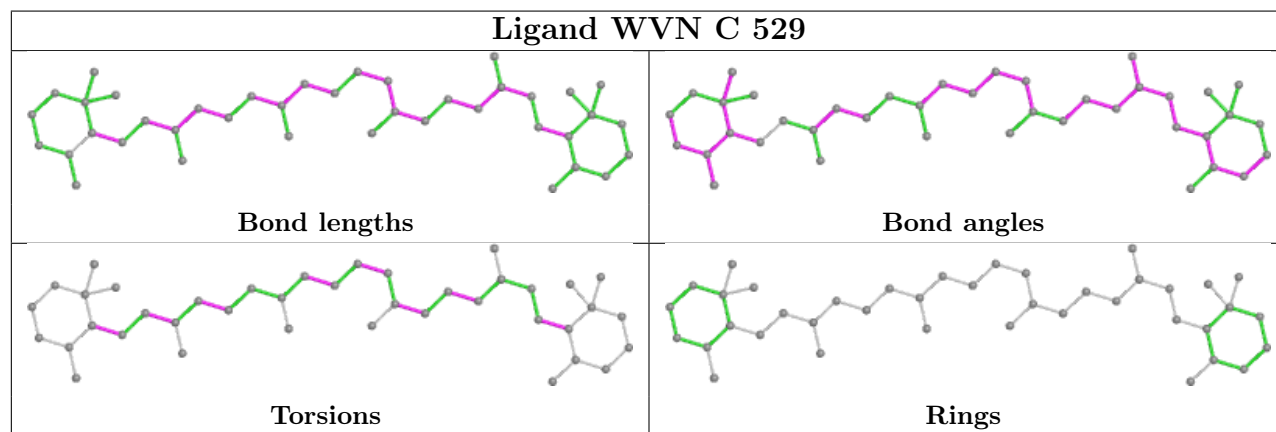
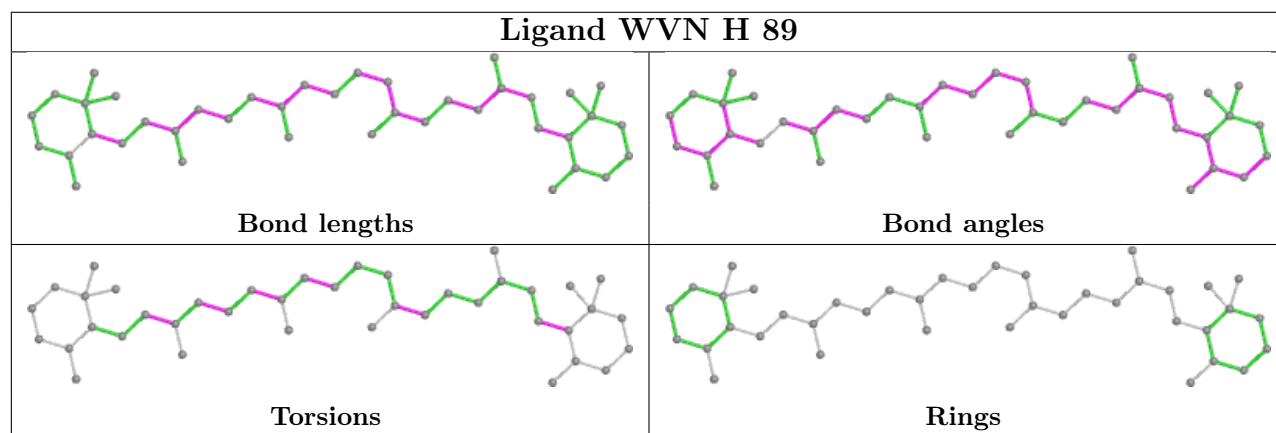
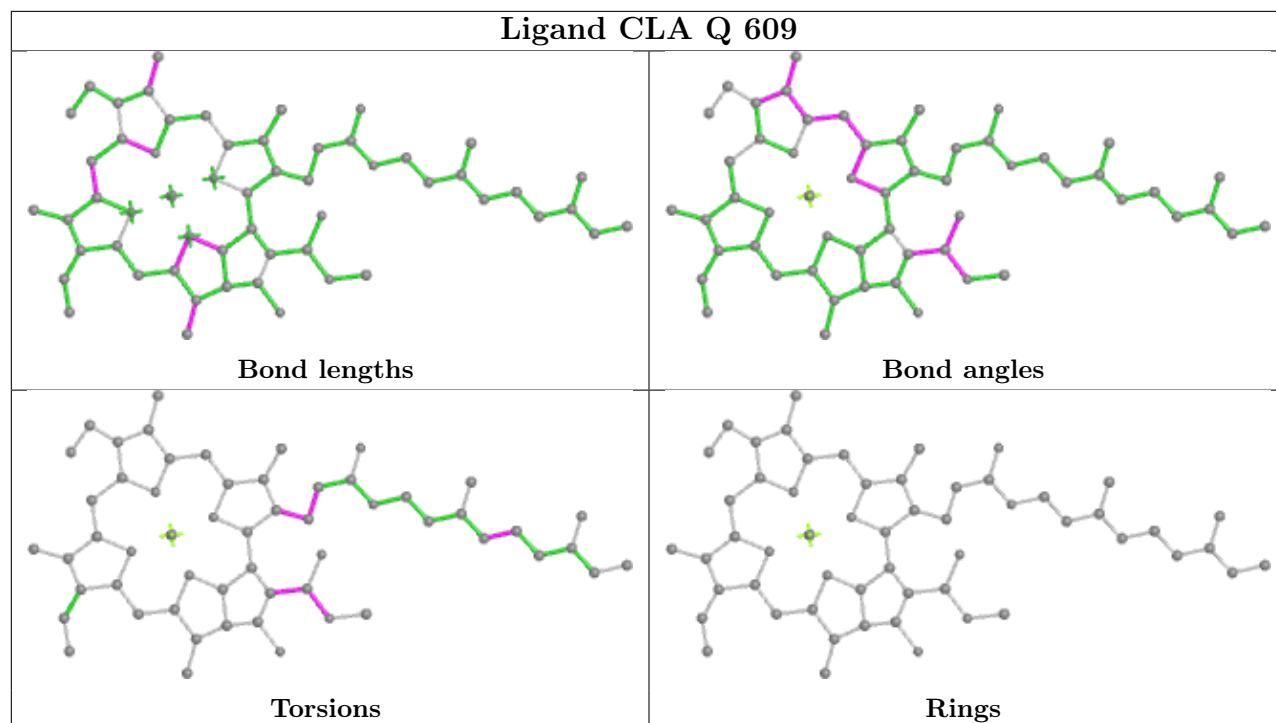
Torsions



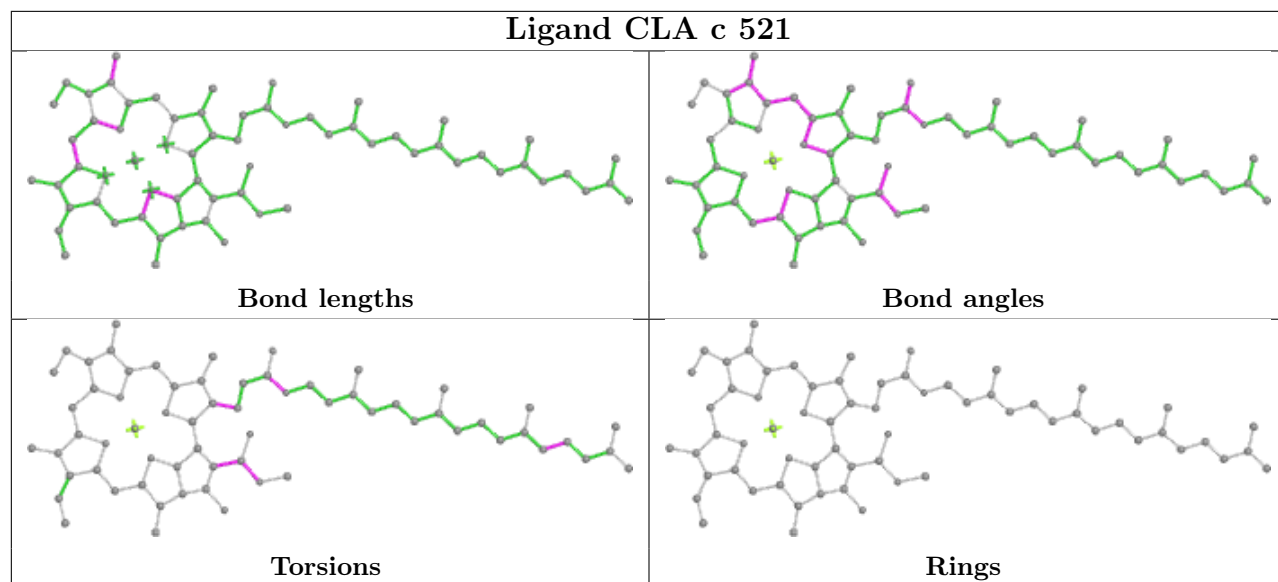
Rings

Ligand CLA 3 615

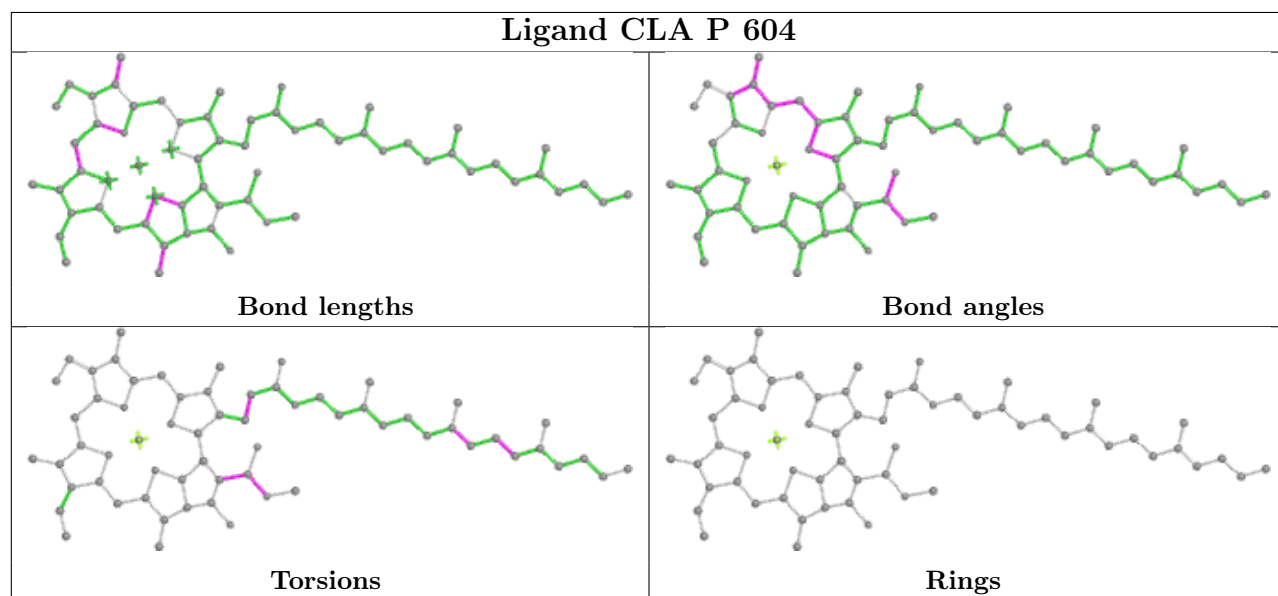




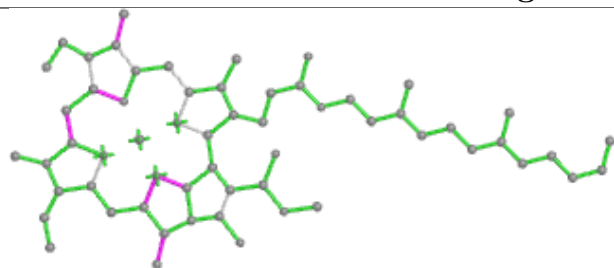
Ligand CLA c 521



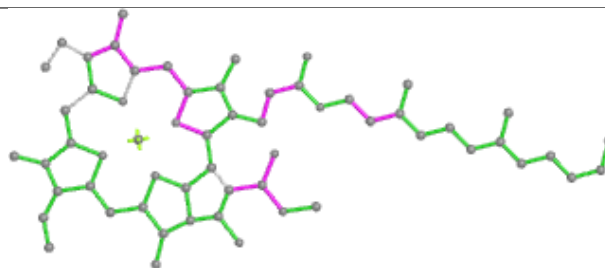
Ligand CLA P 604



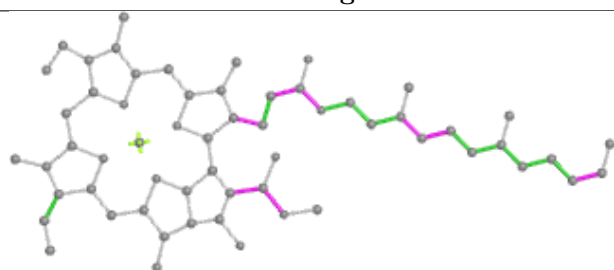
Ligand CLA b 604



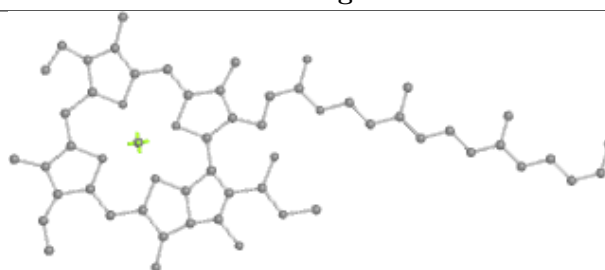
Bond lengths



Bond angles

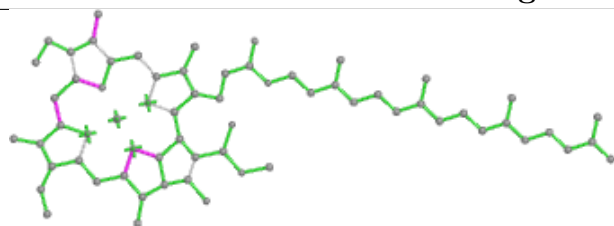


Torsions

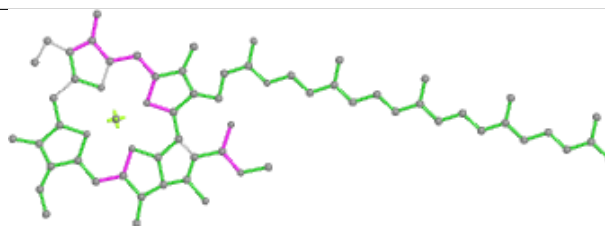


Rings

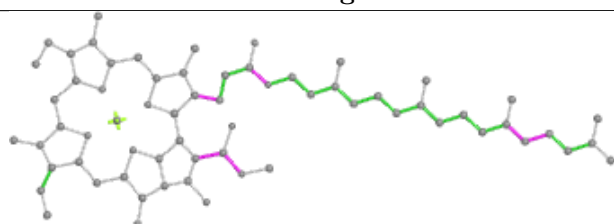
Ligand CLA 2 610



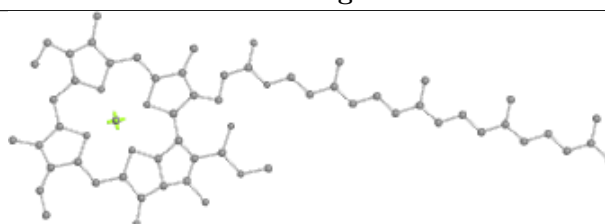
Bond lengths



Bond angles

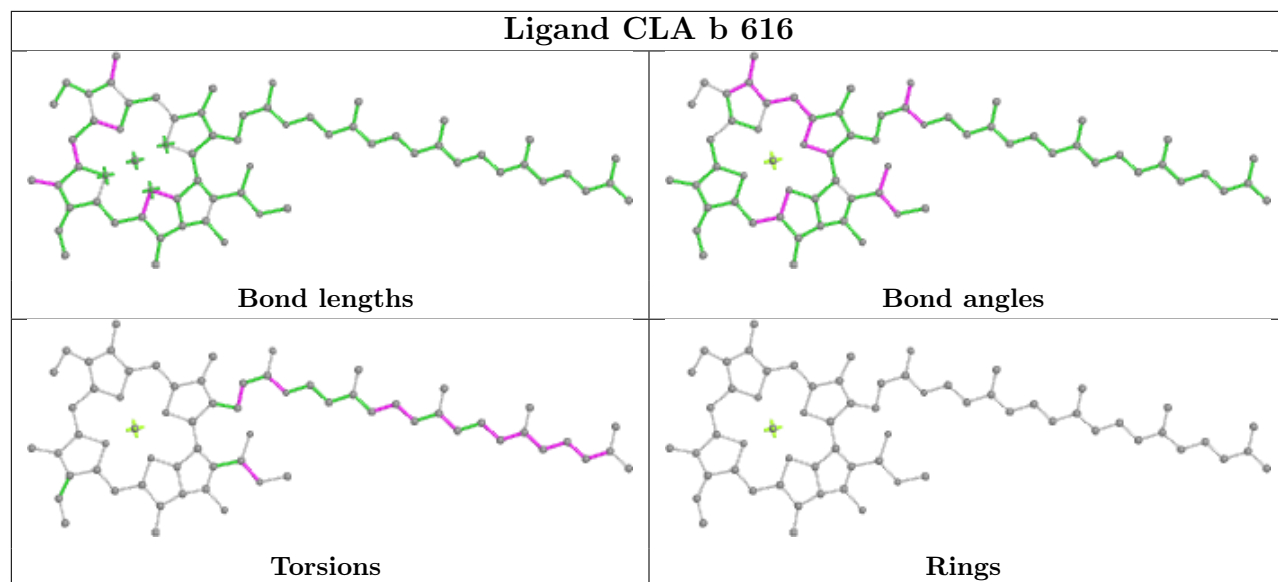


Torsions

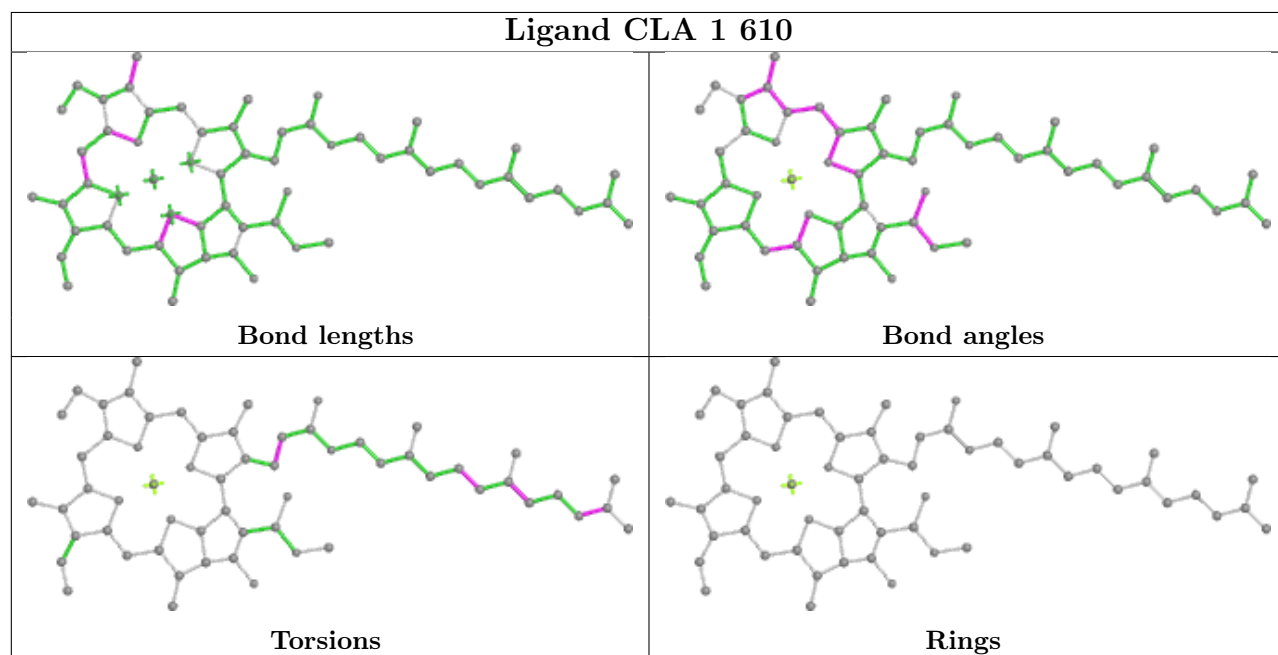


Rings

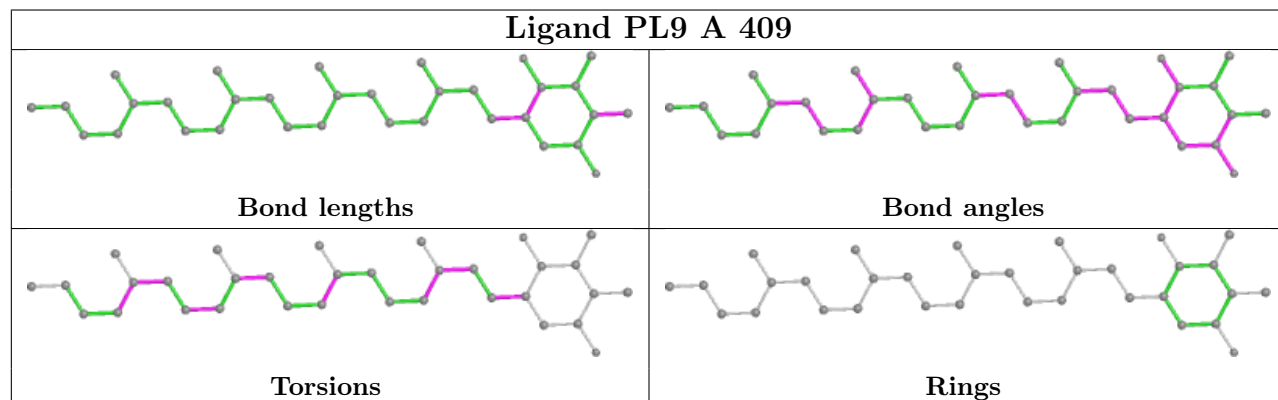
Ligand CLA b 616

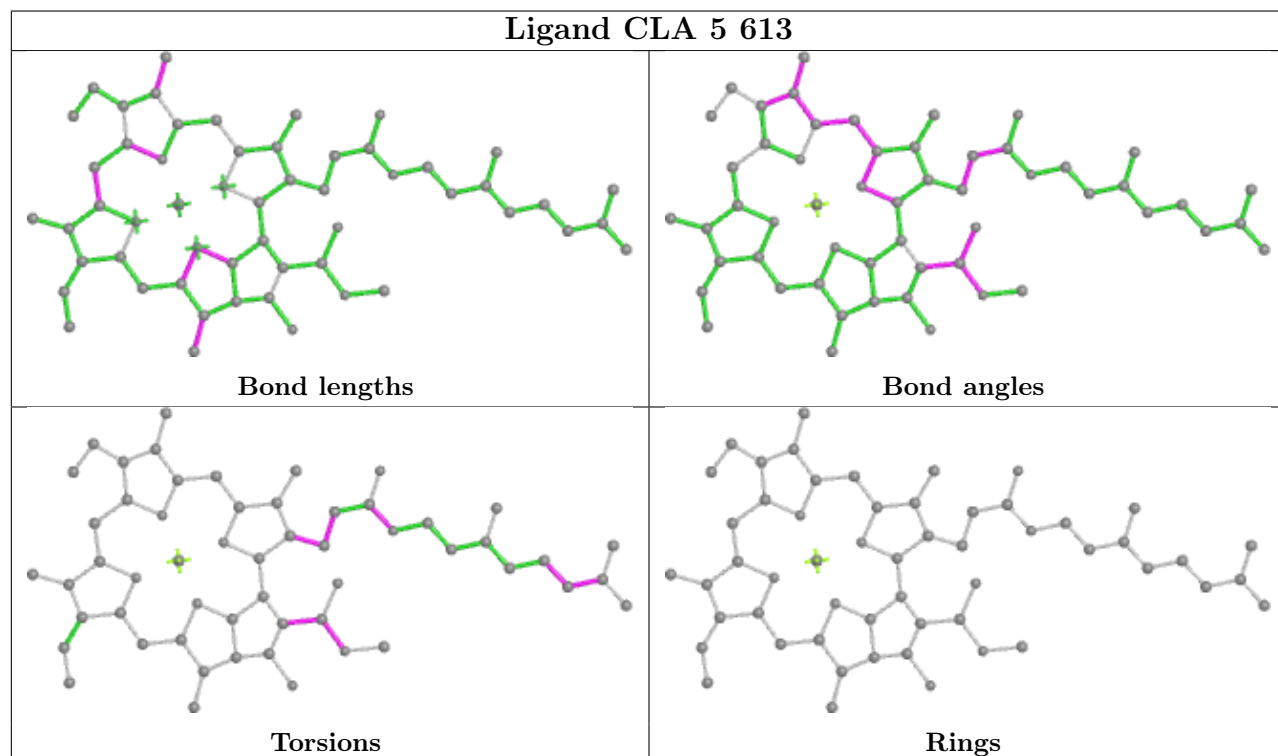
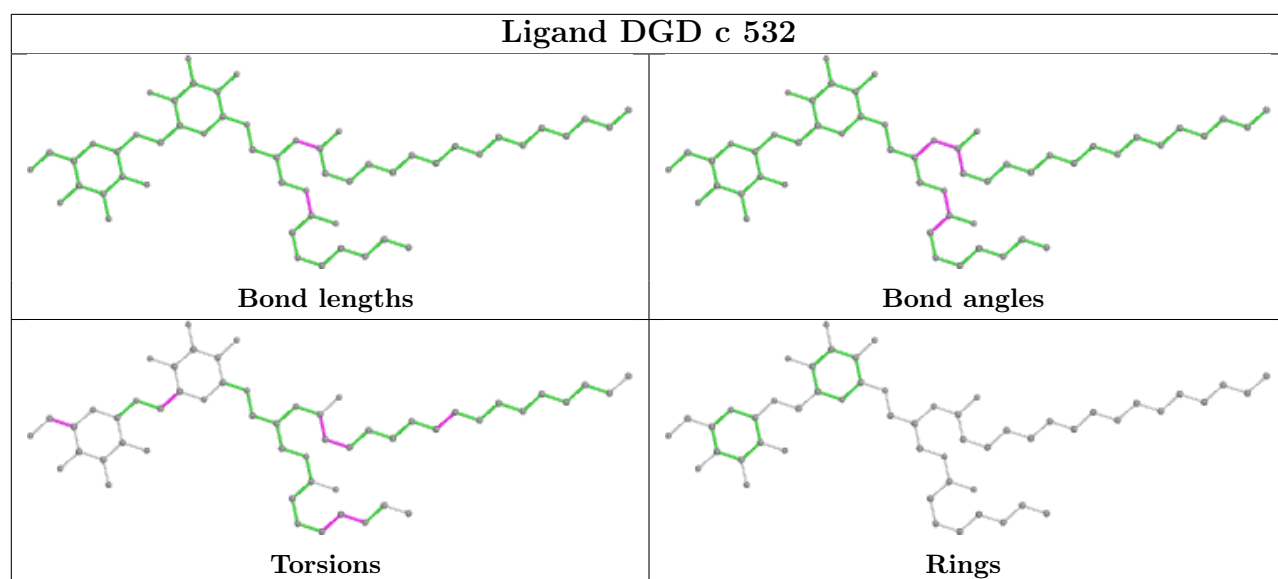


Ligand CLA 1 610

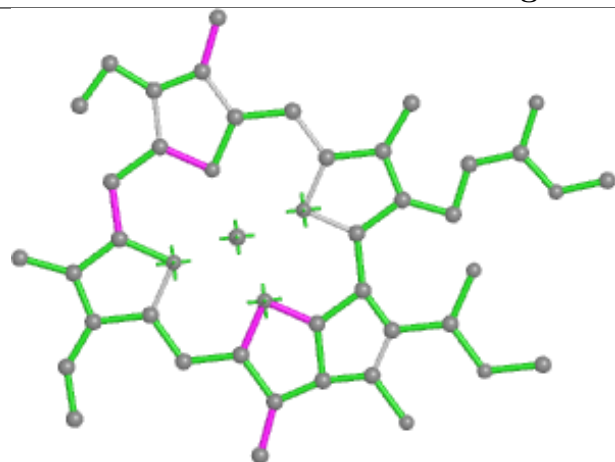


Ligand PL9 A 409

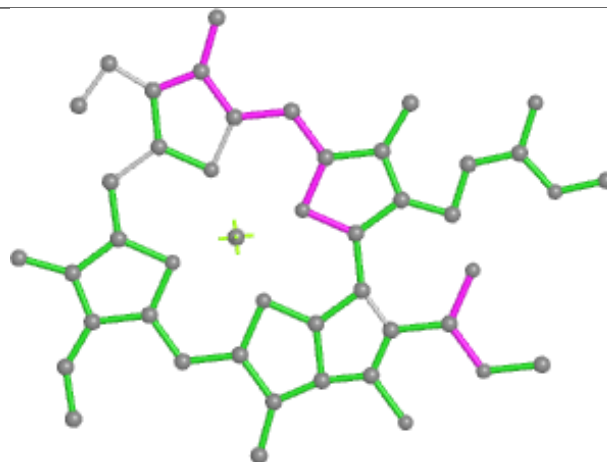




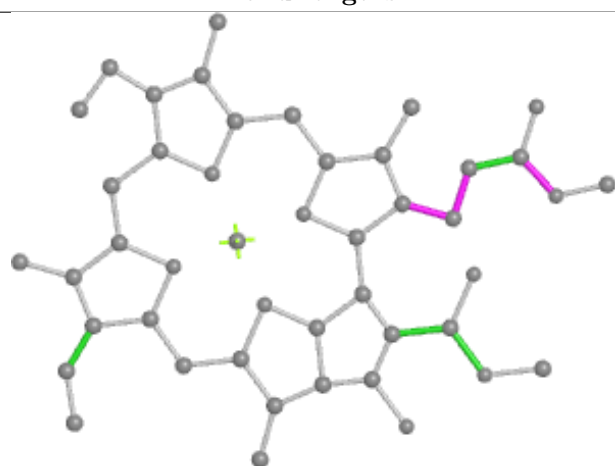
Ligand CLA 1 609



Bond lengths



Bond angles

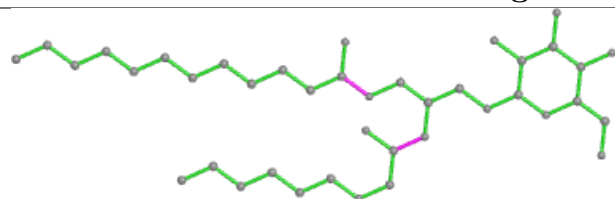


Torsions

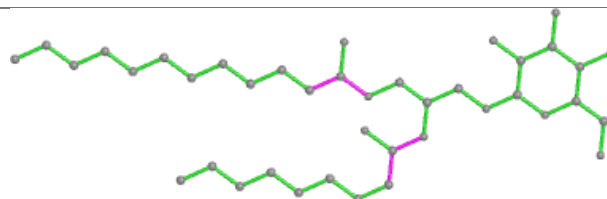


Rings

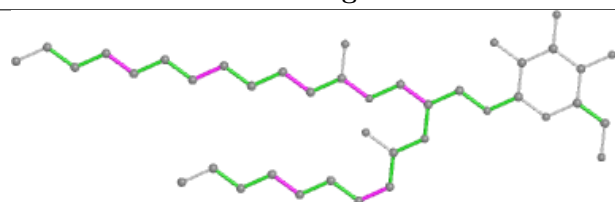
Ligand LMG D 402



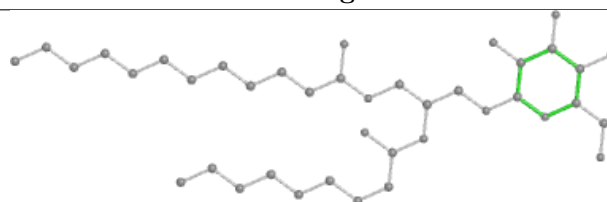
Bond lengths



Bond angles

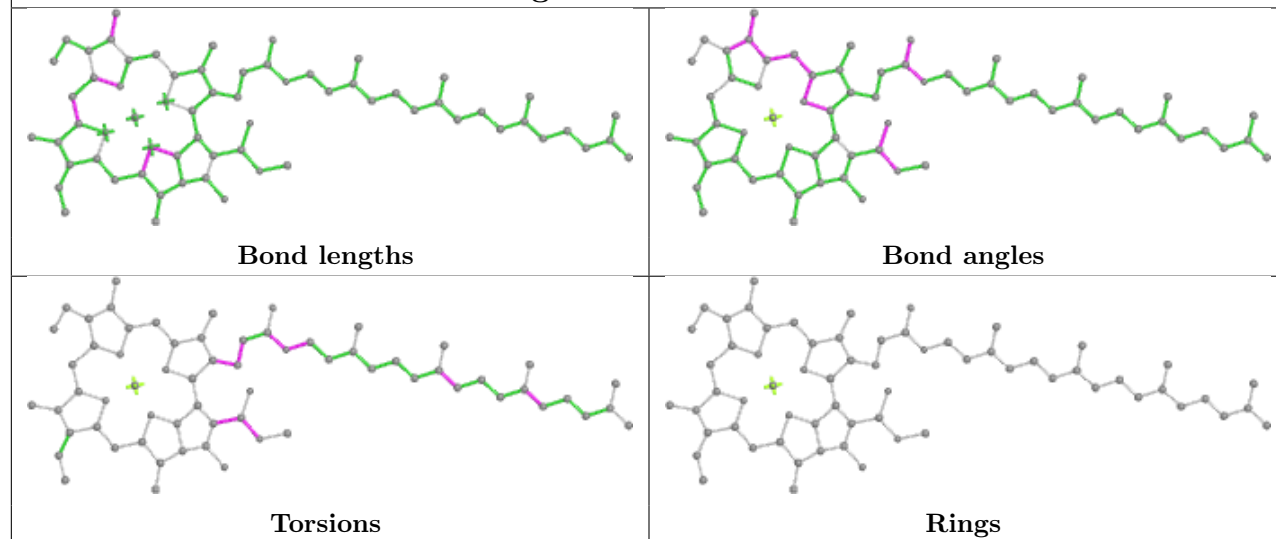


Torsions

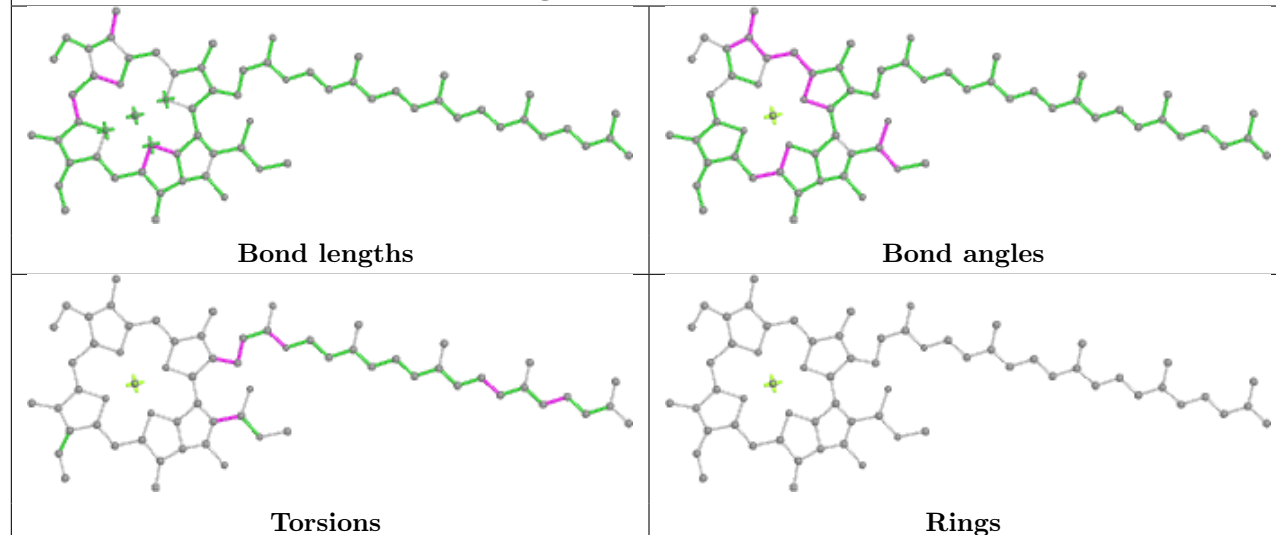


Rings

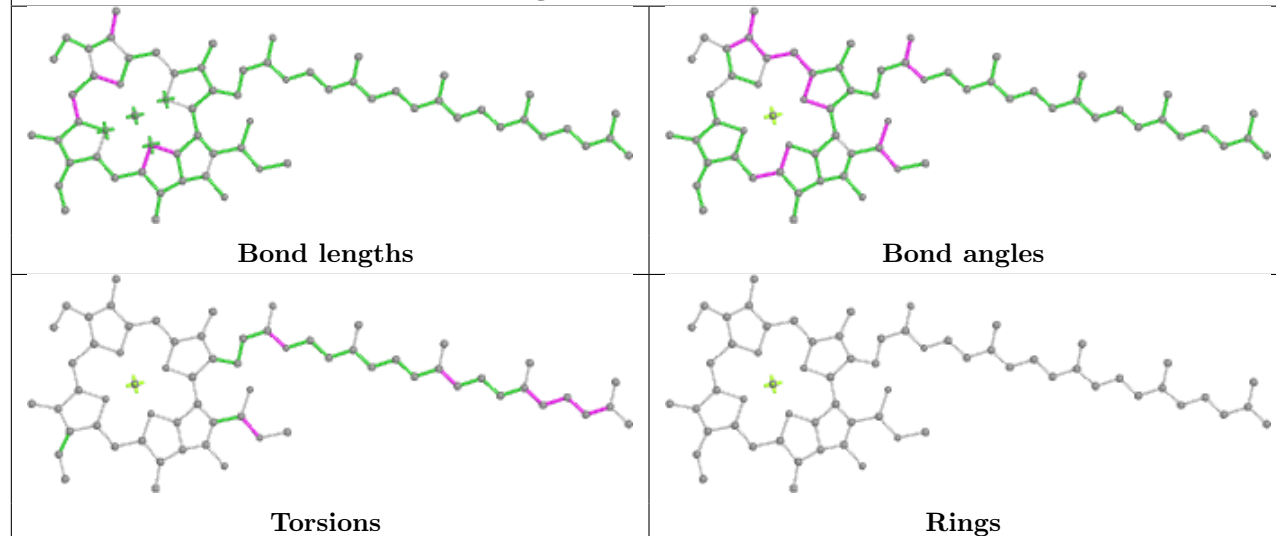
Ligand CLA R 606

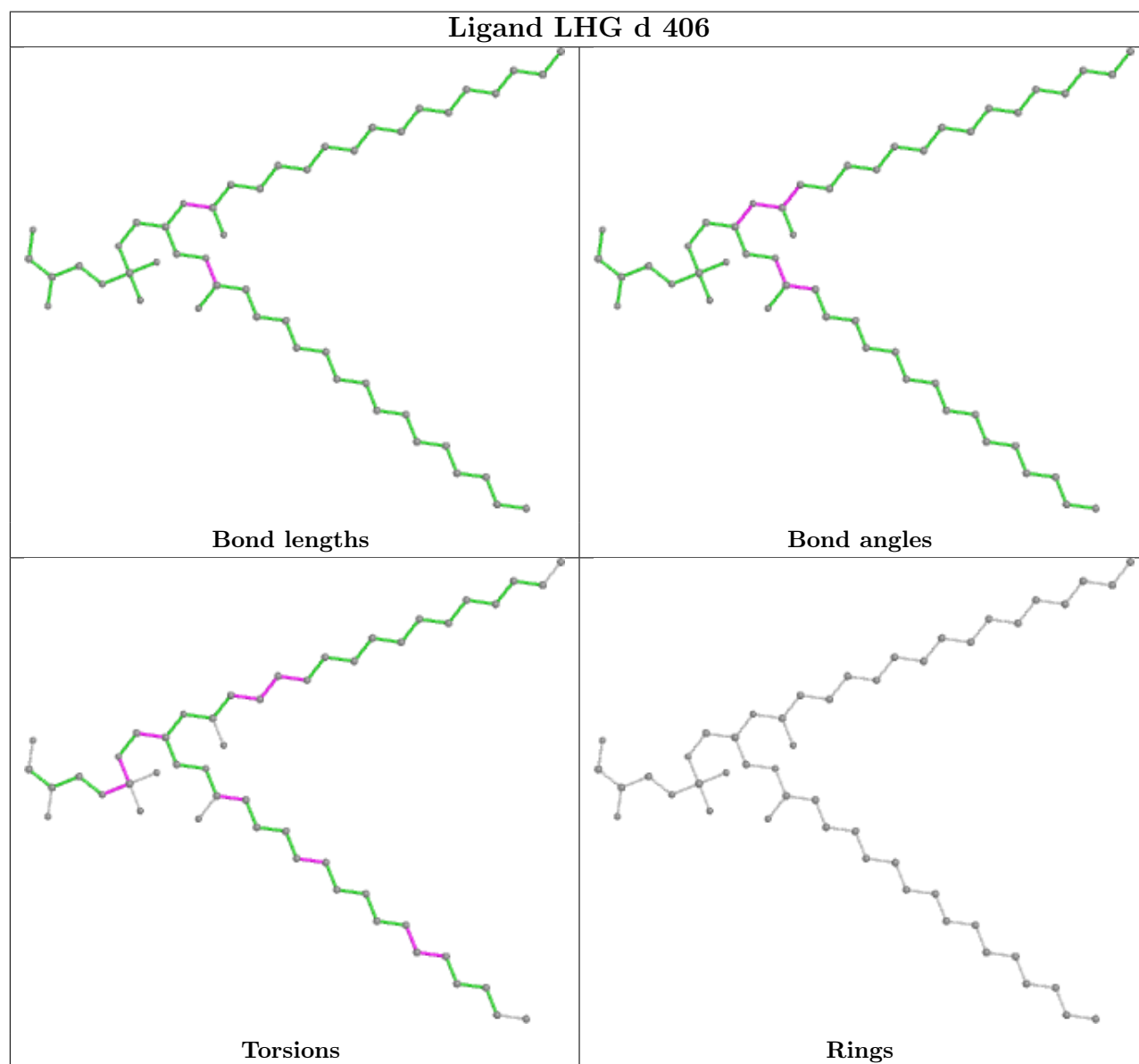
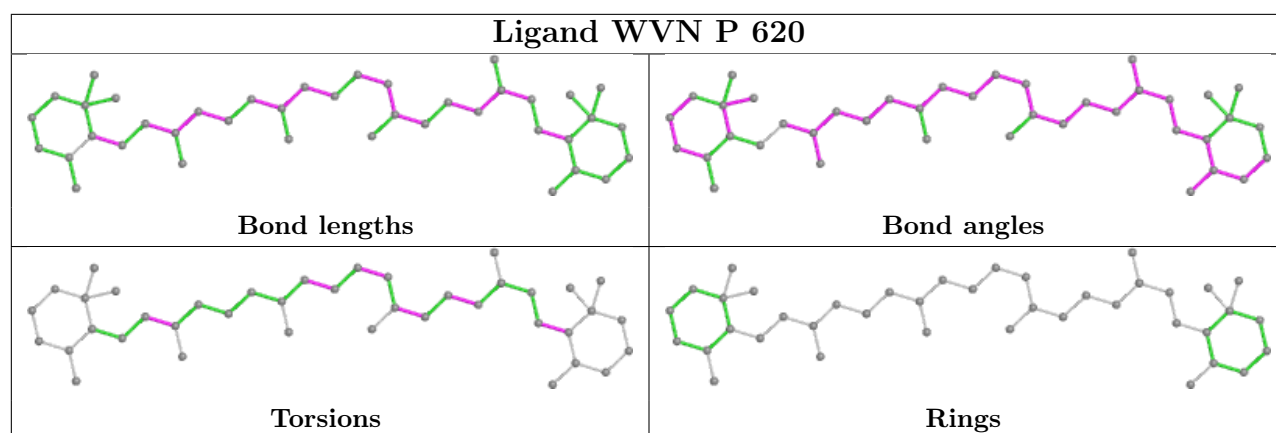


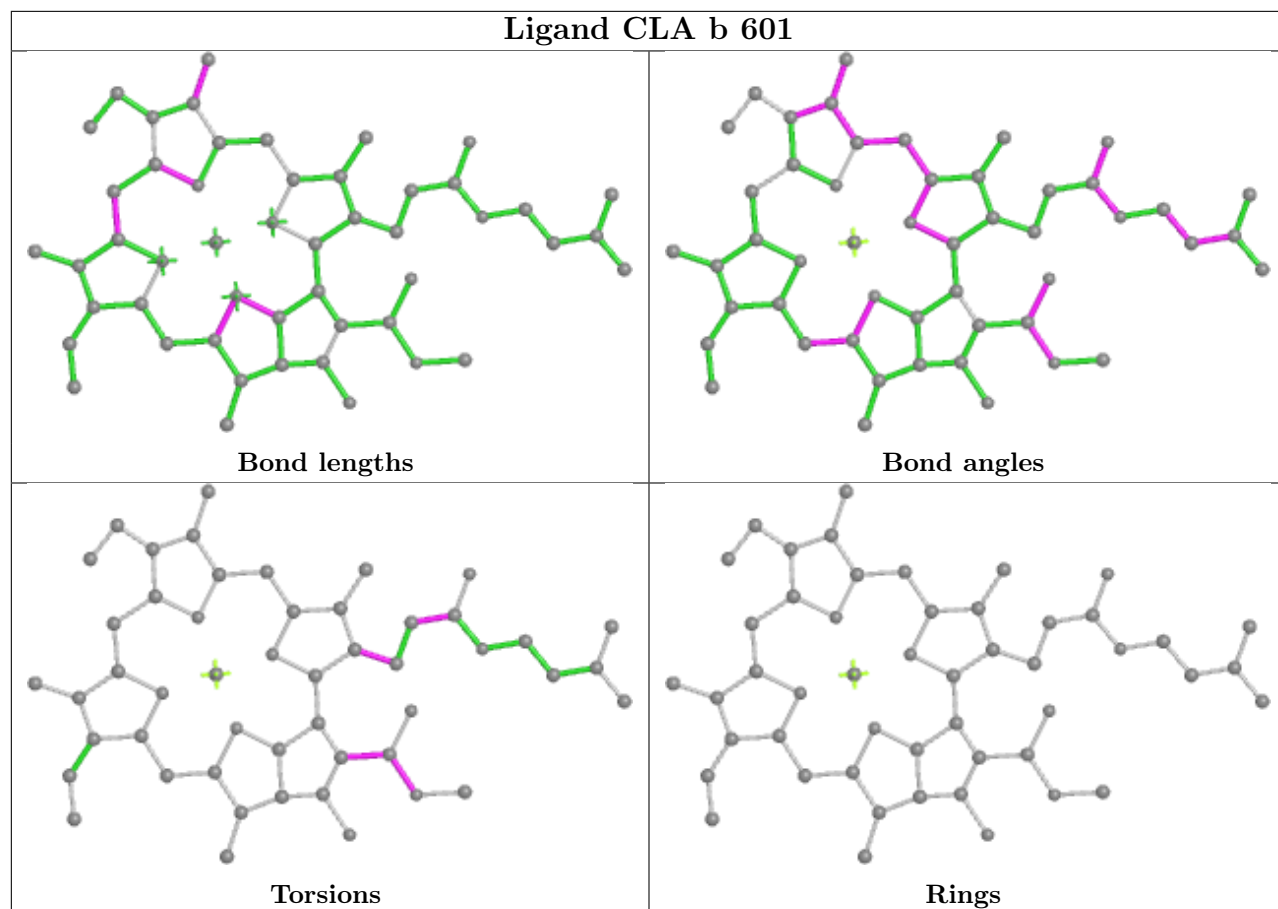
Ligand CLA 4 602



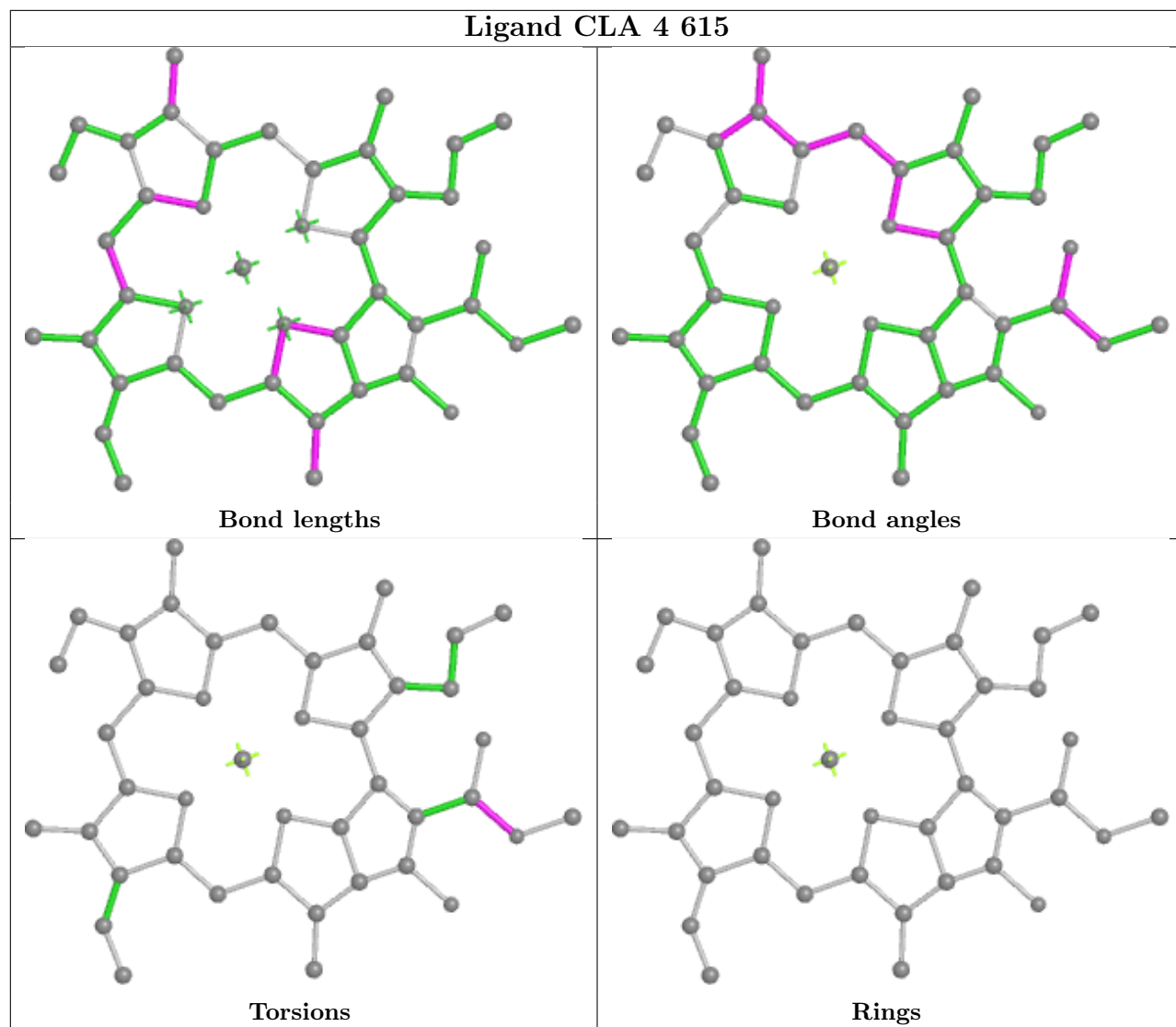
Ligand CLA C 523

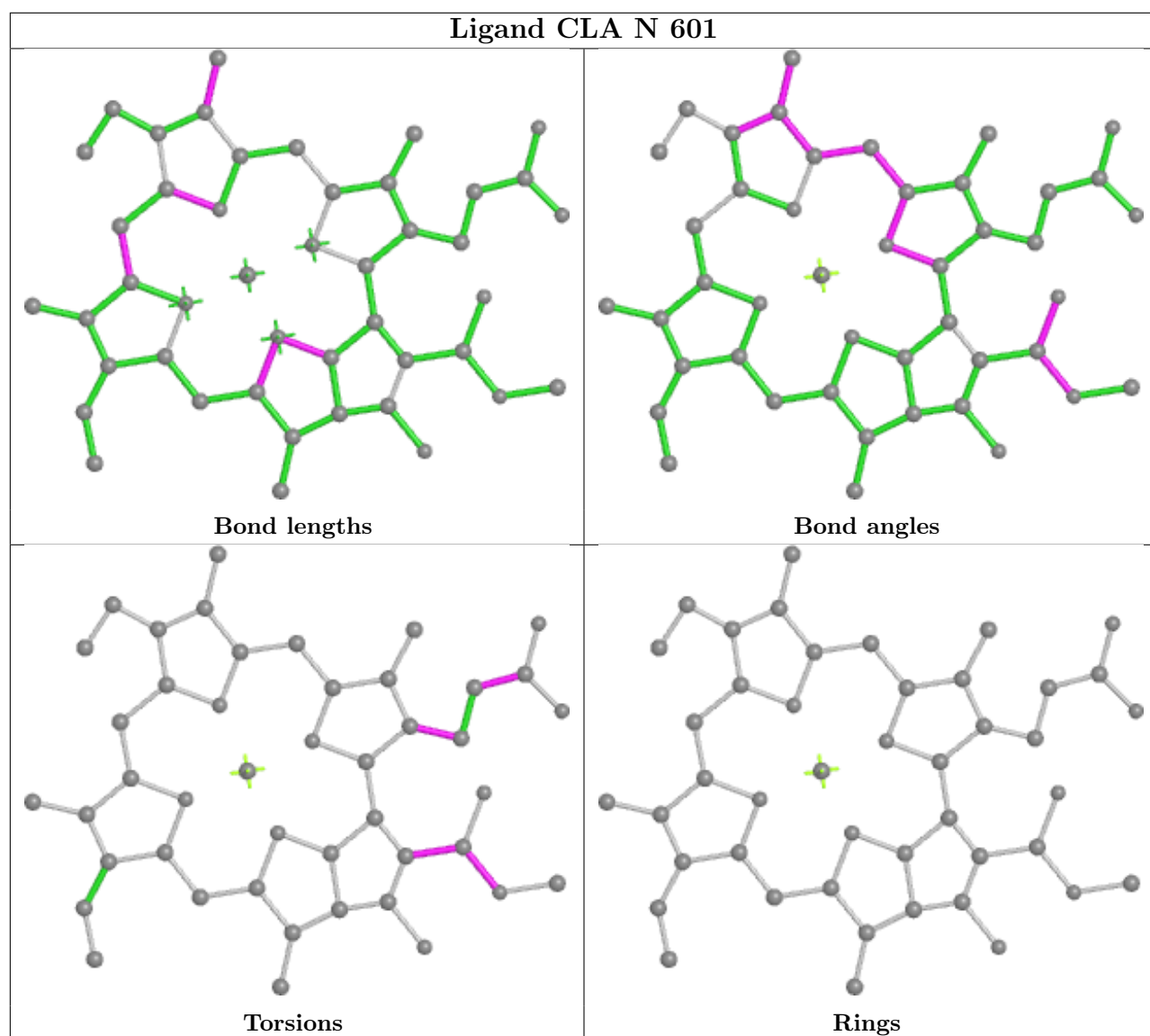


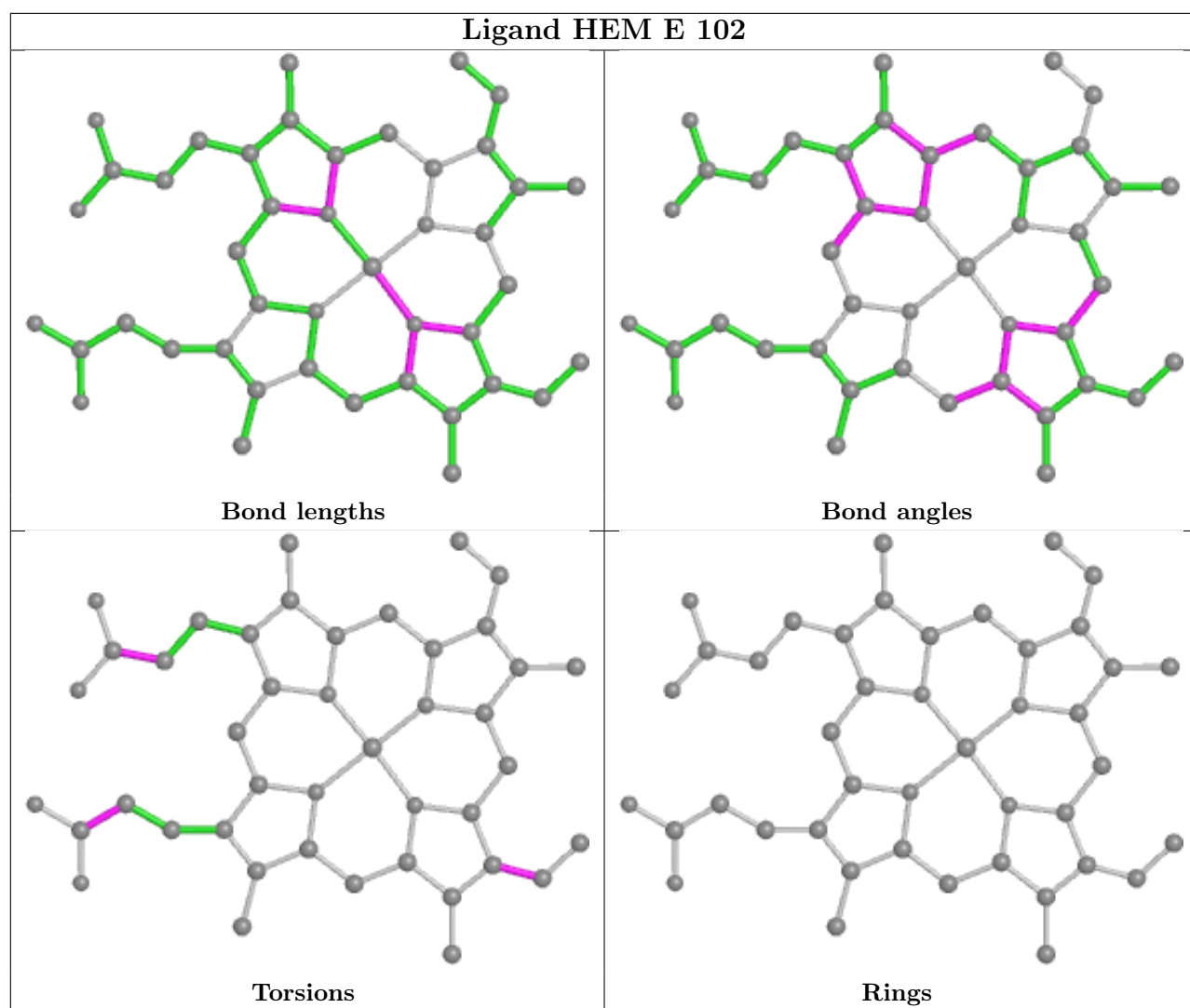


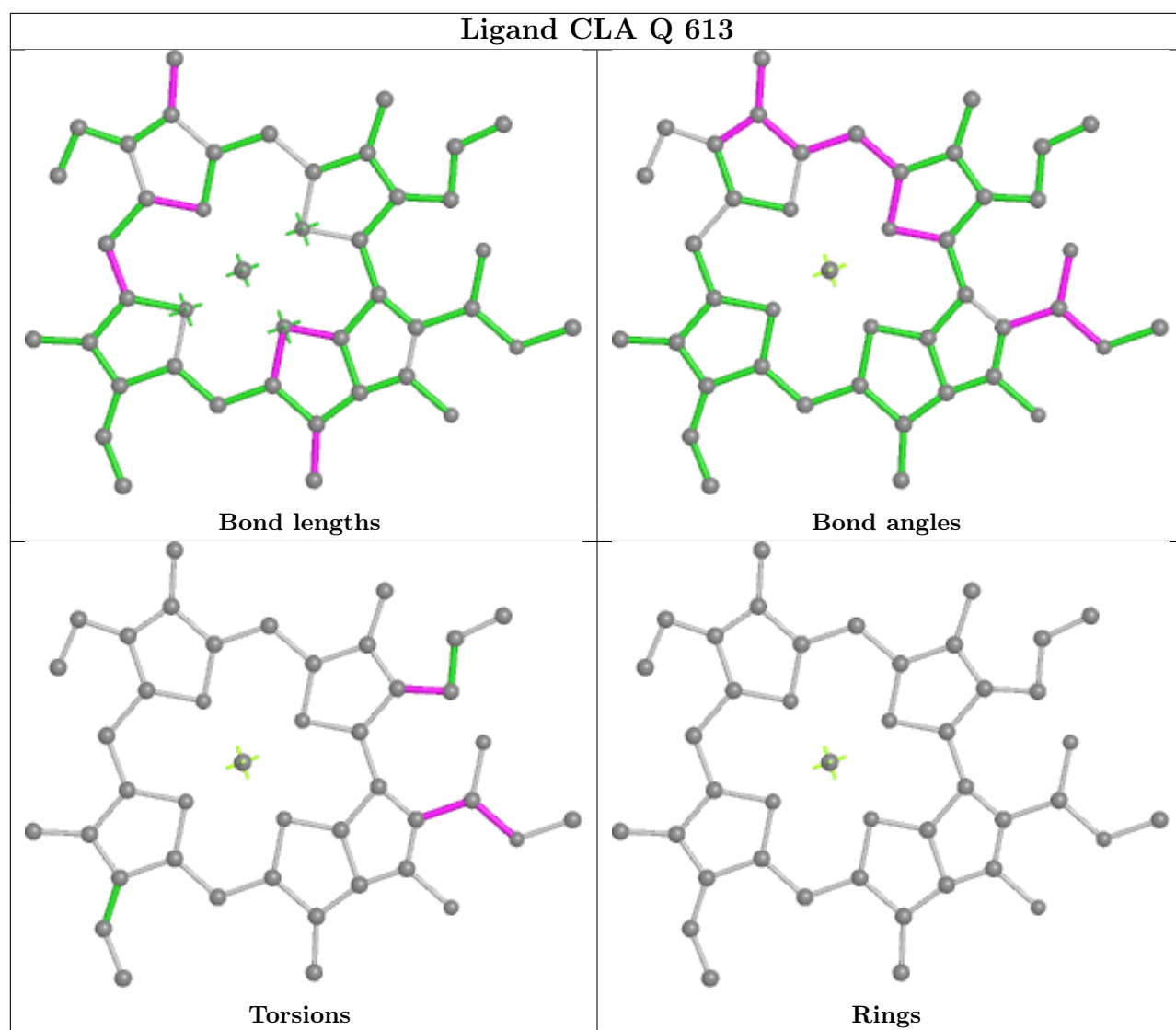


Ligand CLA 4 615

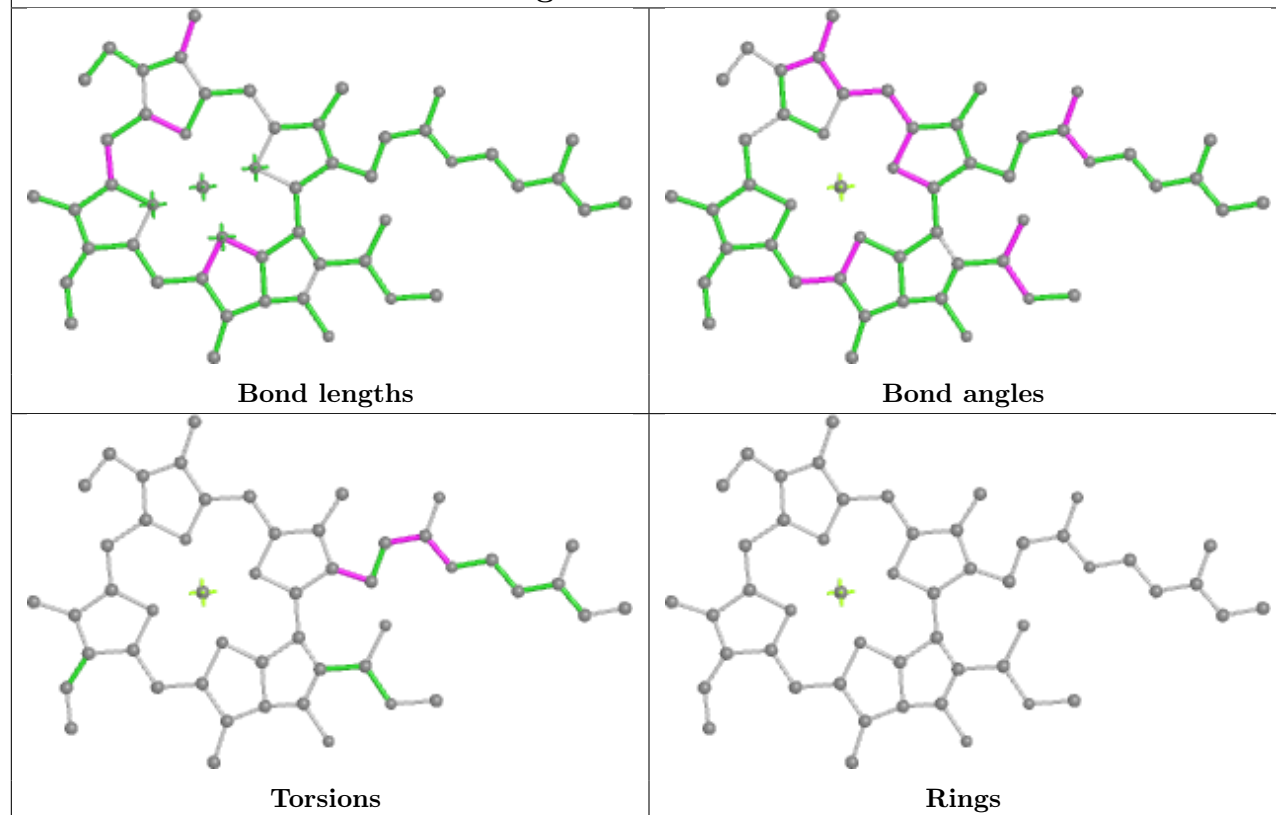




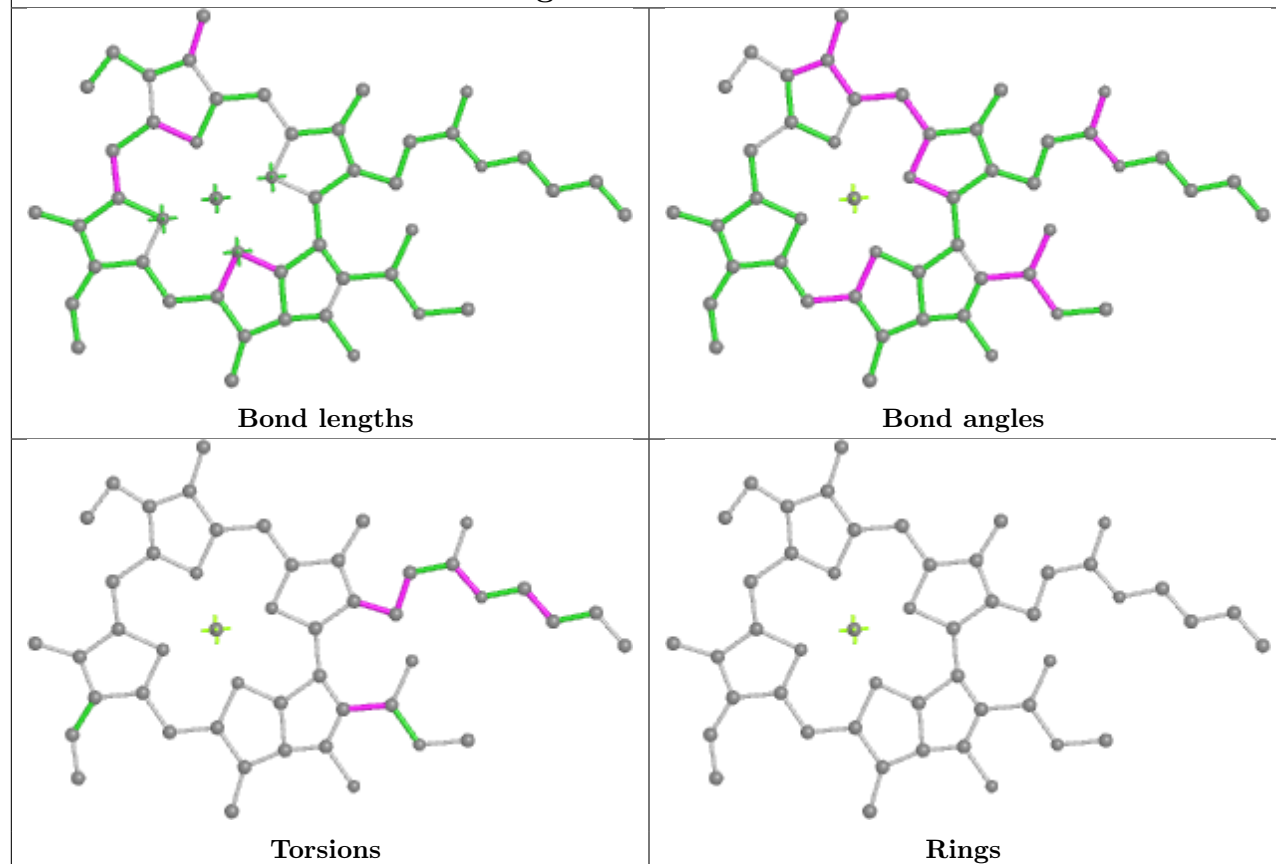


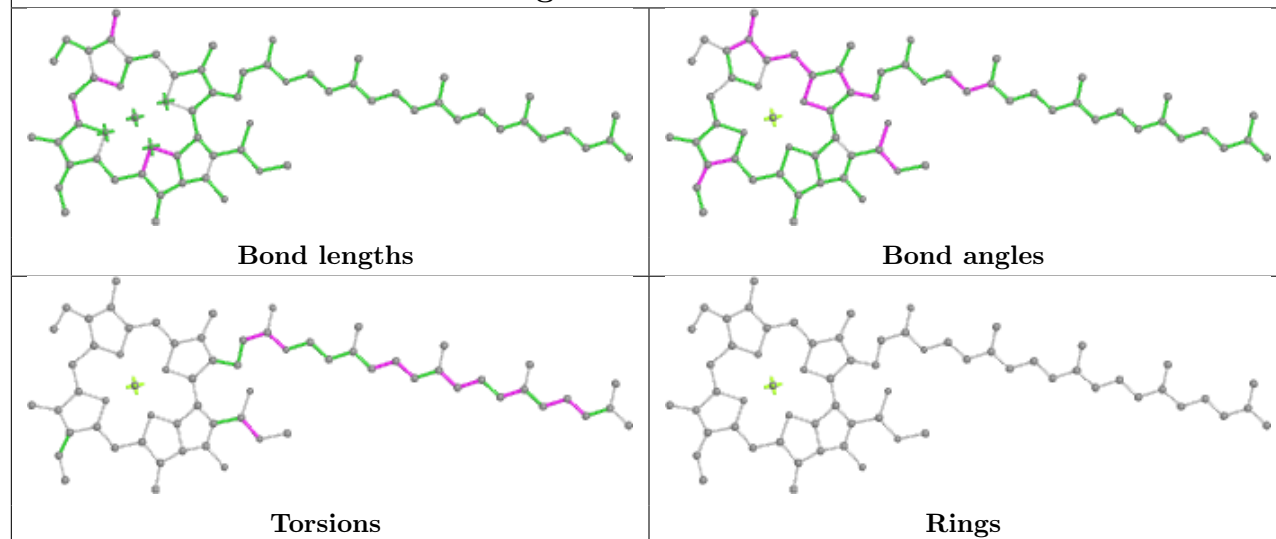
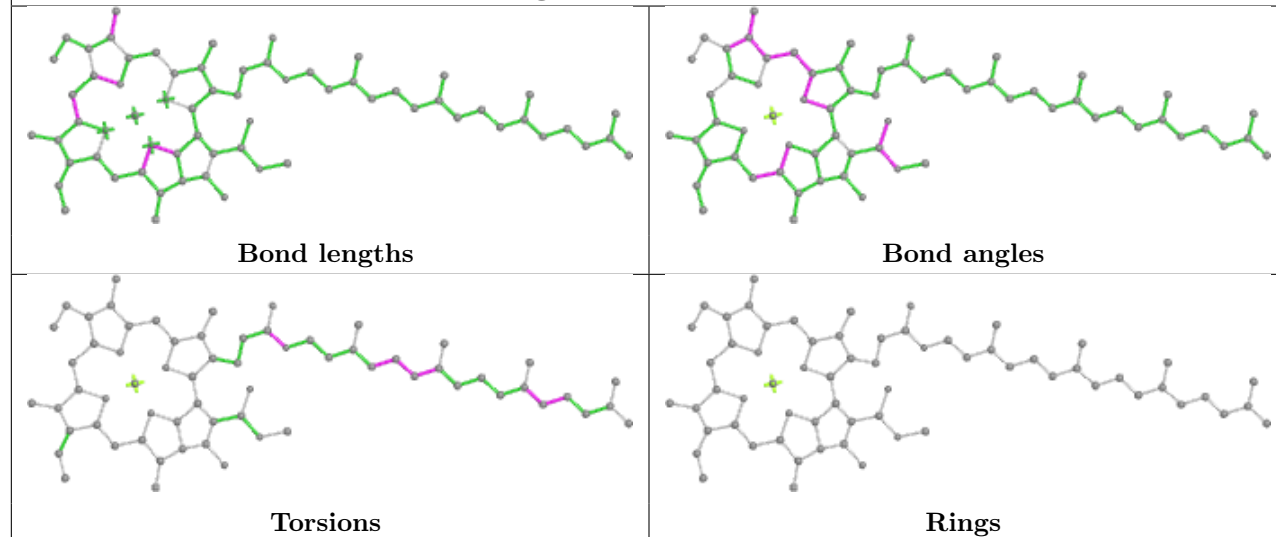


Ligand CLA 2 606

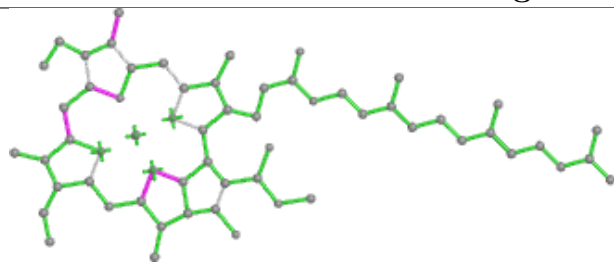


Ligand CLA 2 601

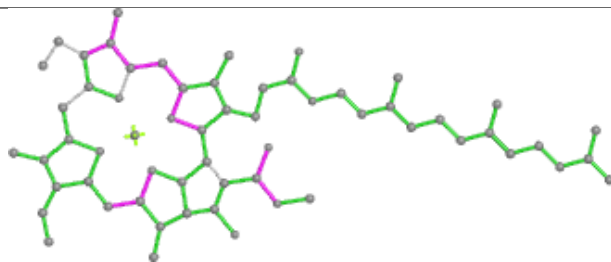


Ligand CLA 4 603**Ligand CLA P 609**

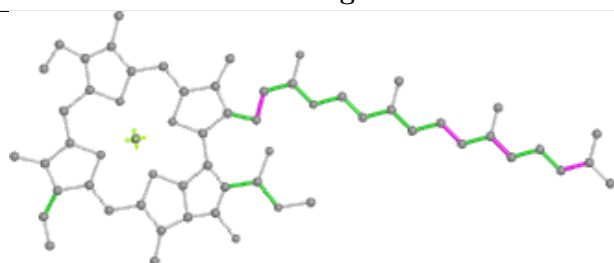
Ligand CLA N 610



Bond lengths



Bond angles

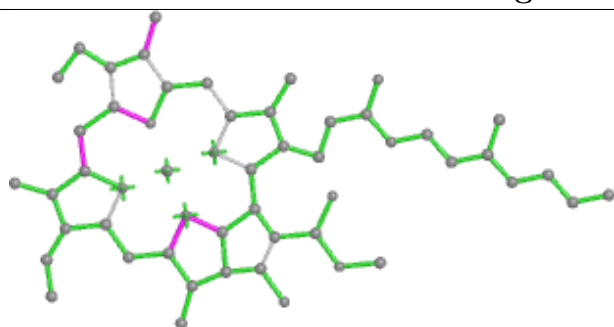


Torsions

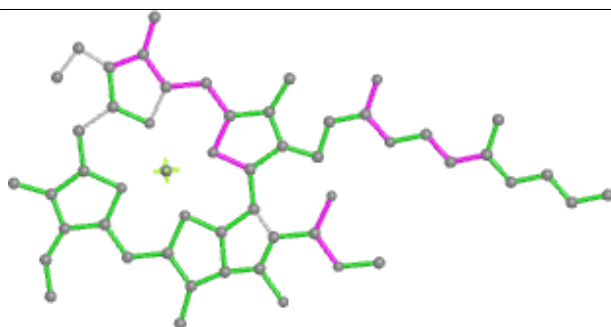


Rings

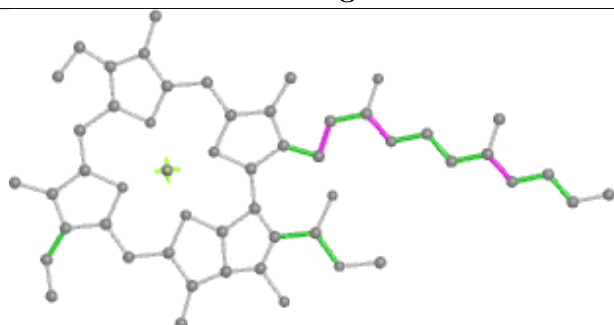
Ligand CLA P 612



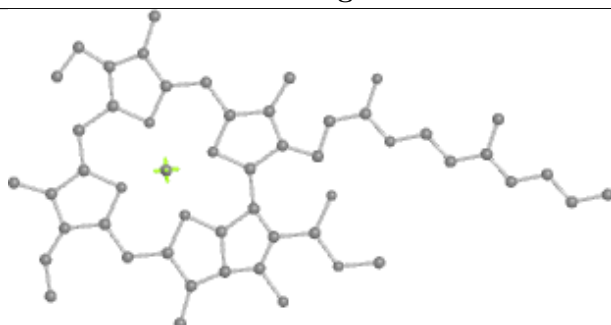
Bond lengths



Bond angles

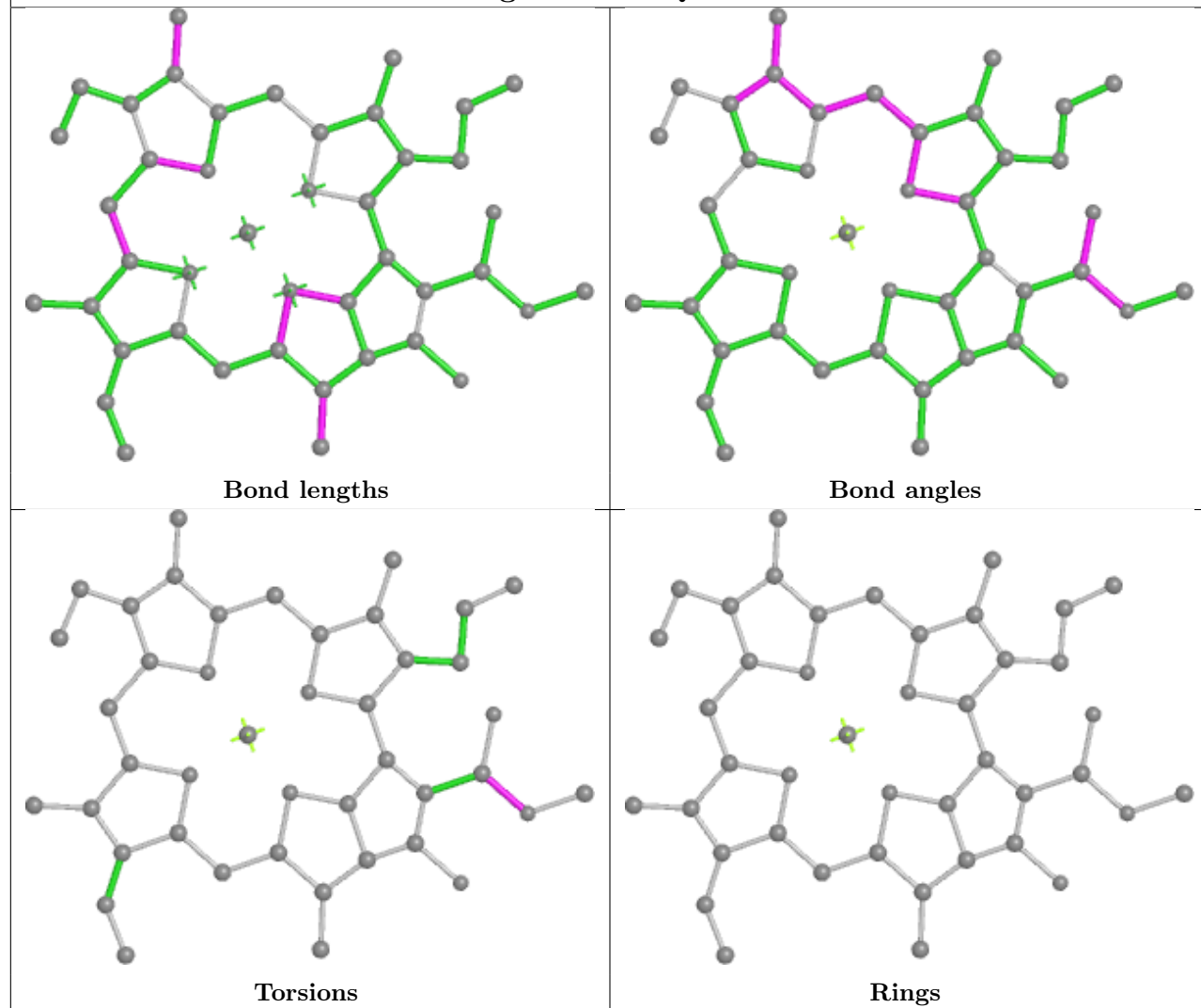


Torsions

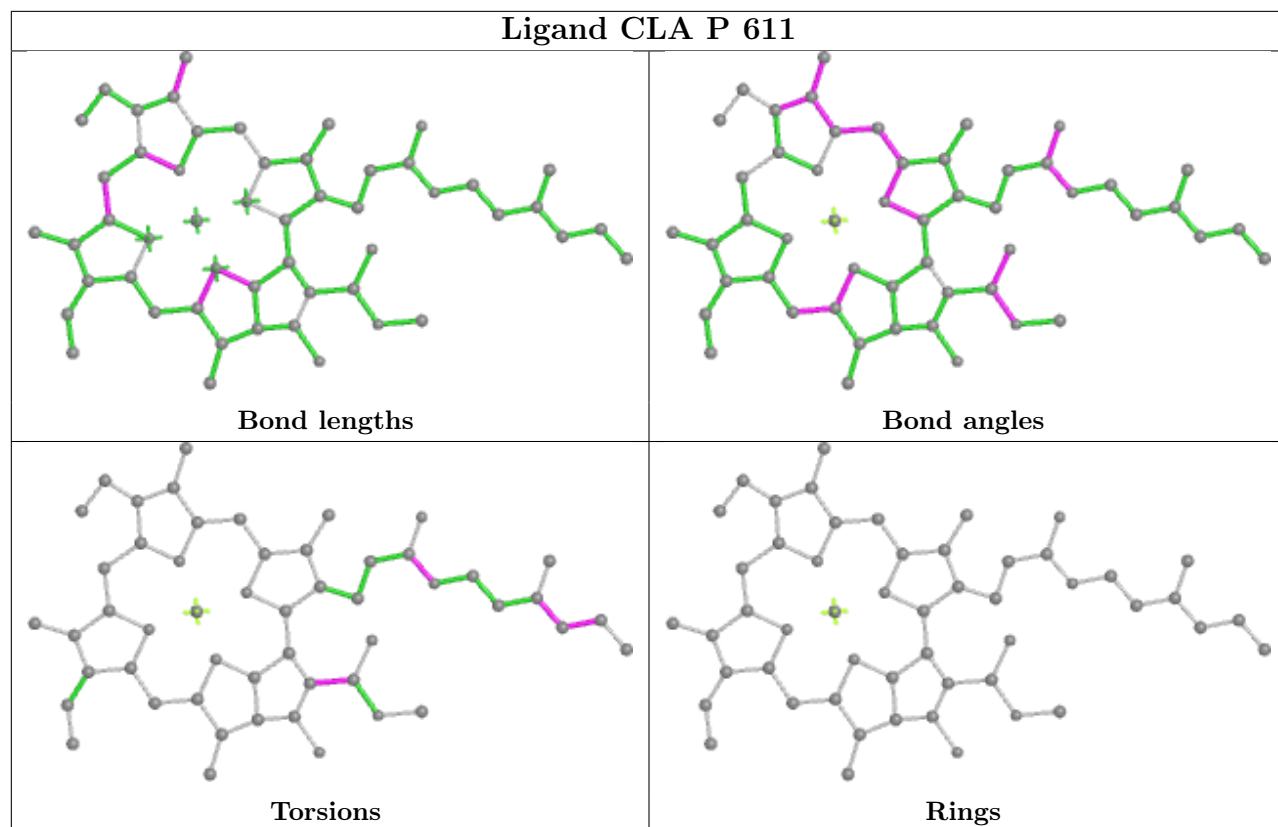


Rings

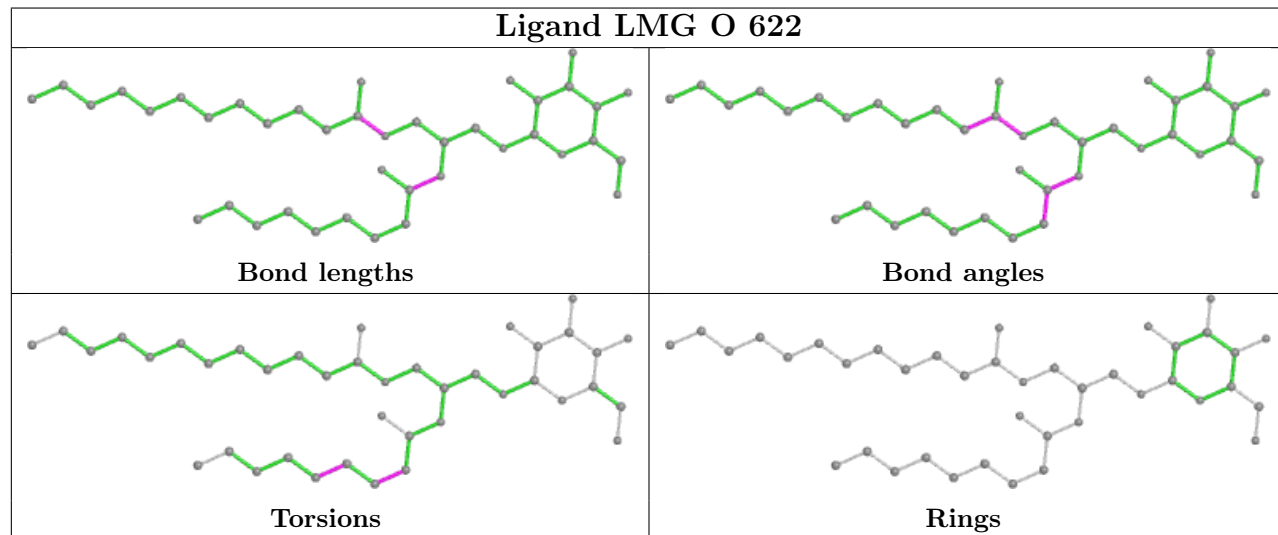
Ligand CLA Q 615

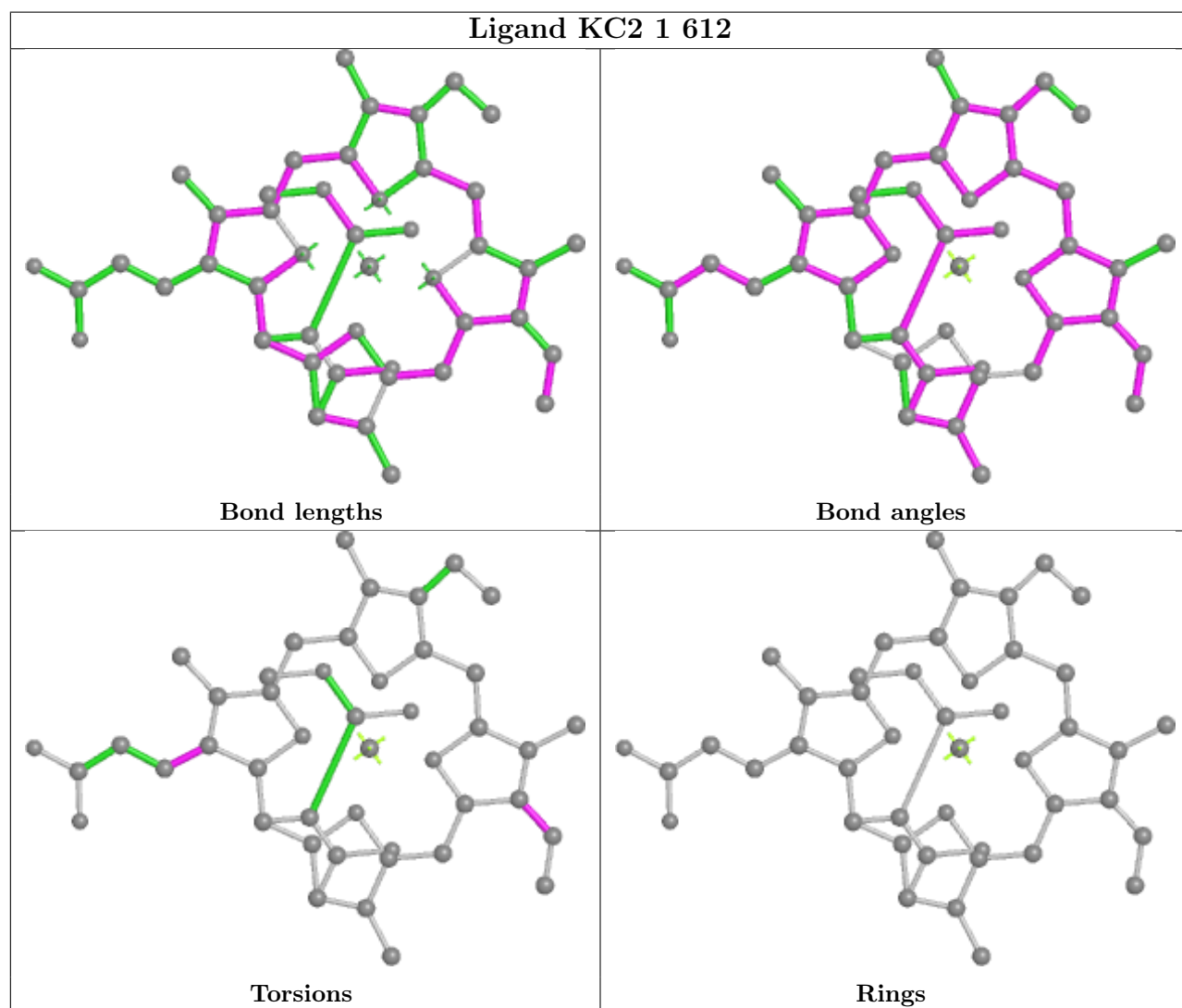
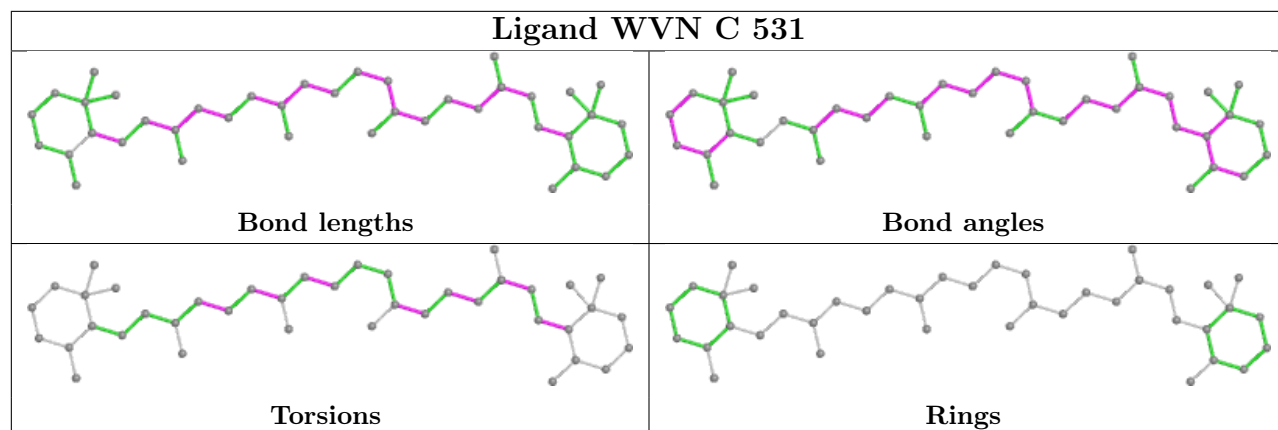


Ligand CLA P 611

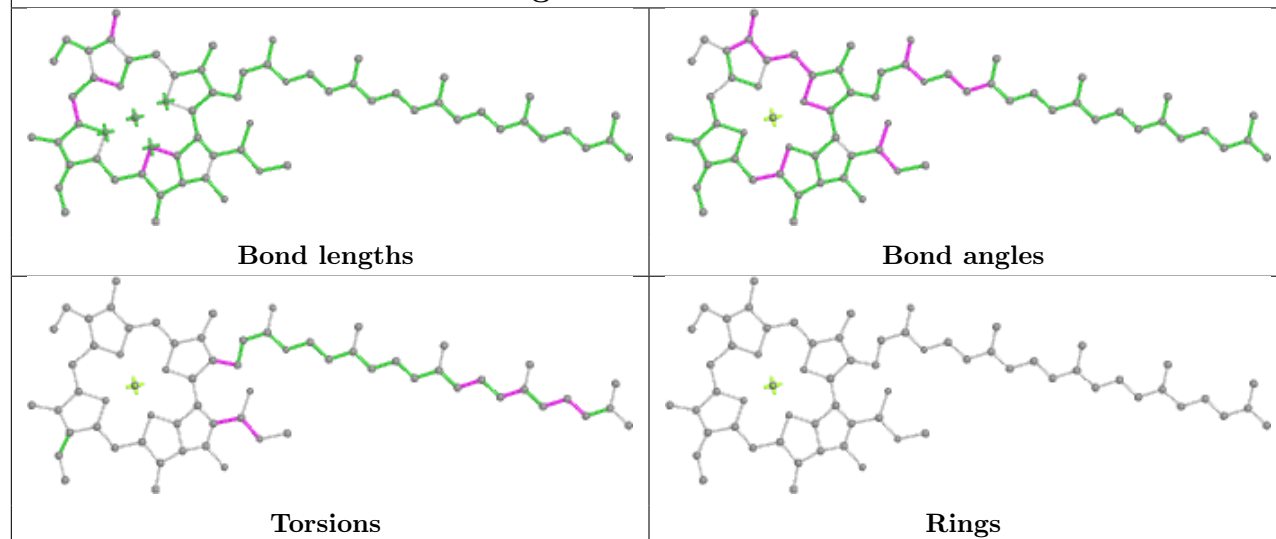


Ligand LMG O 622

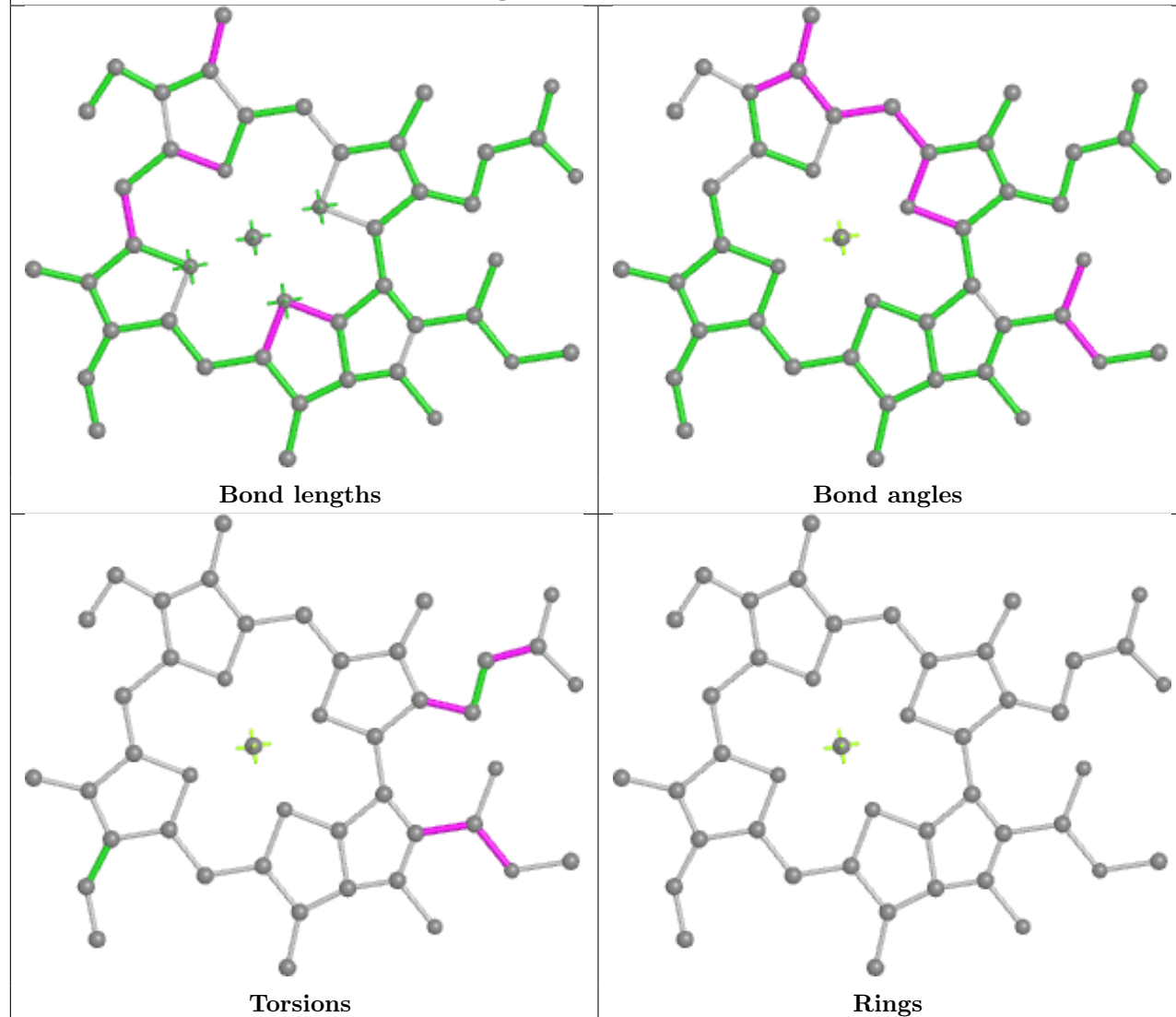


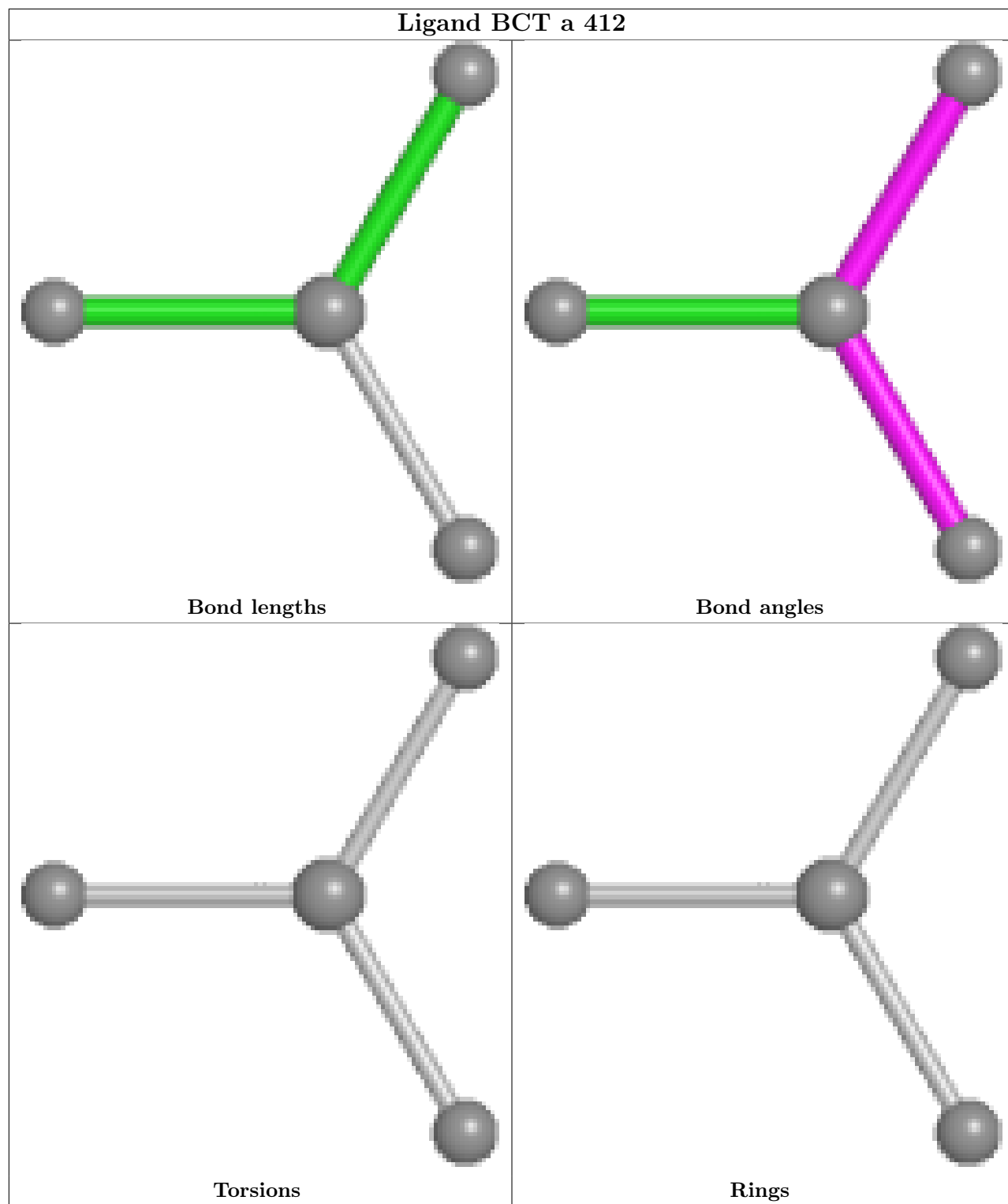


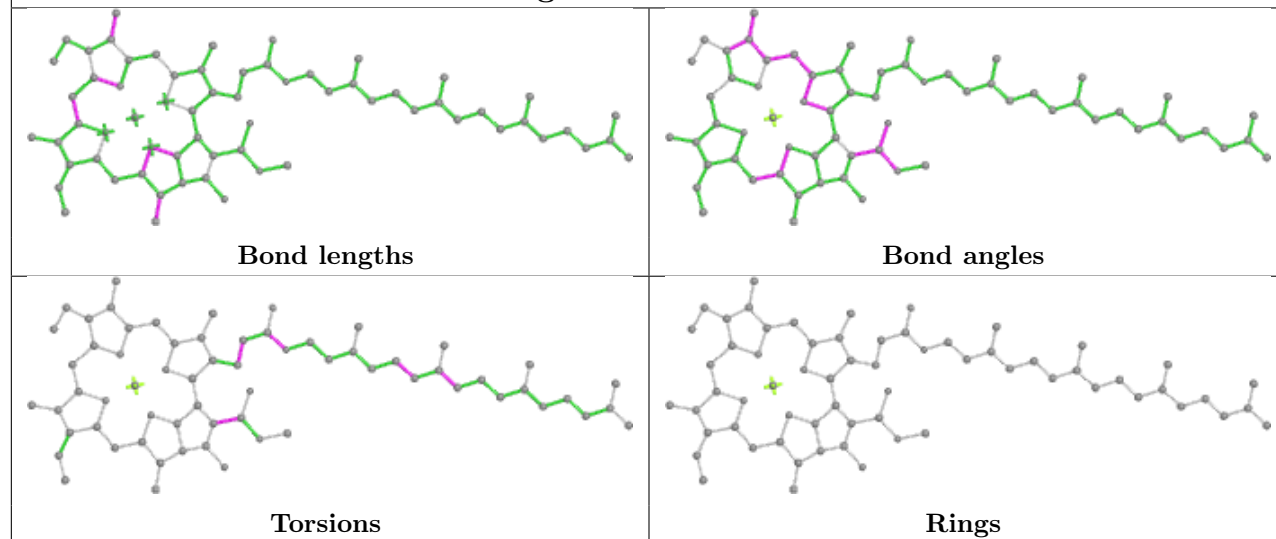
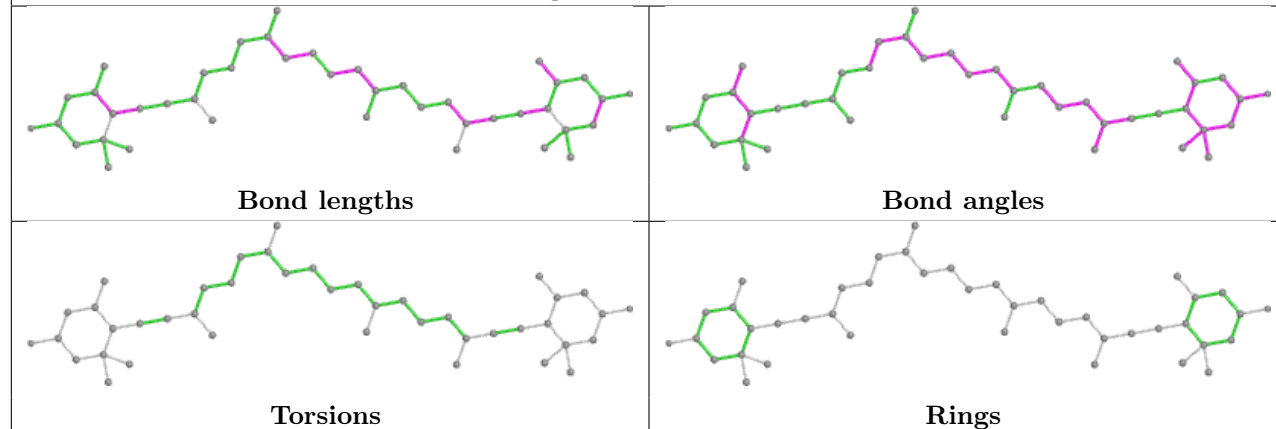
Ligand CLA B 611

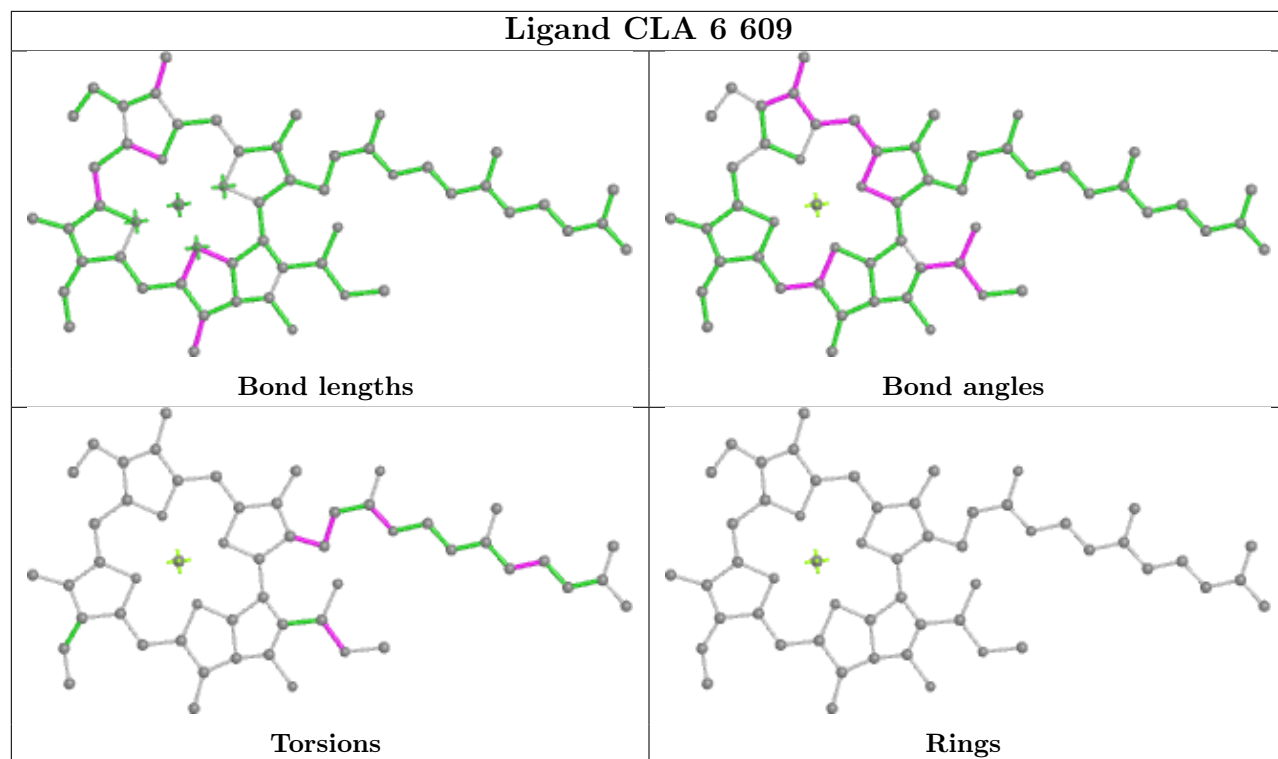


Ligand CLA 1 601

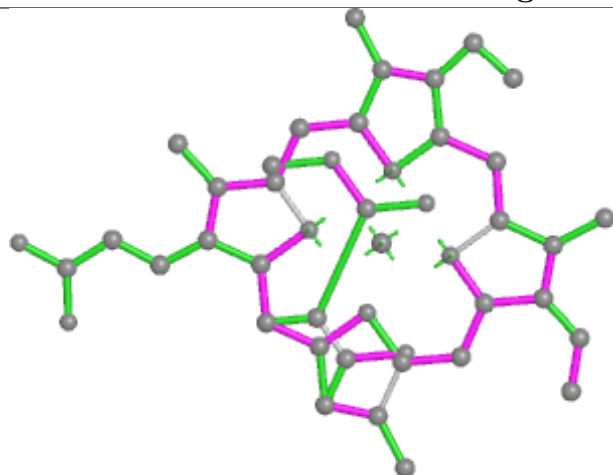




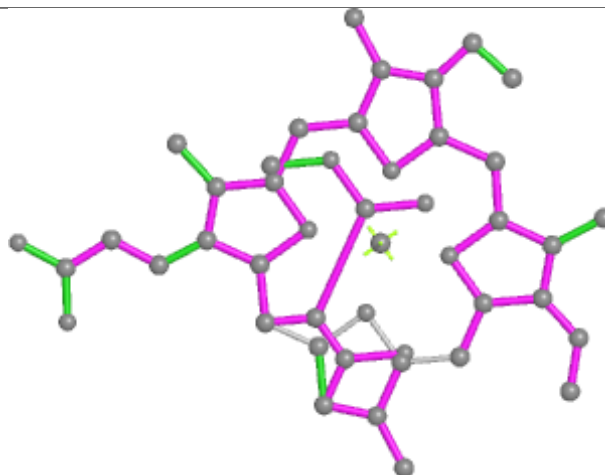
Ligand CLA c 520**Ligand II0 R 616**



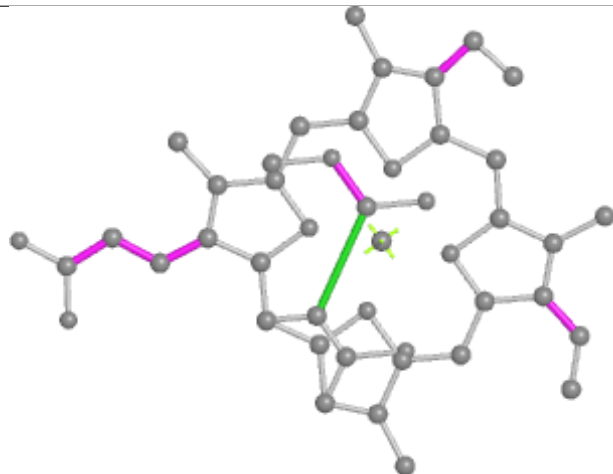
Ligand KC2 P 606



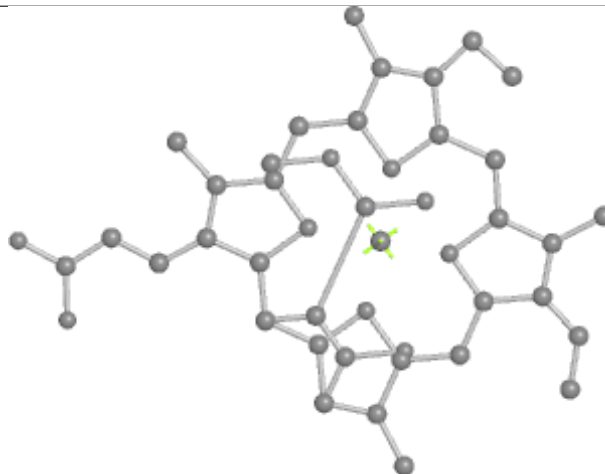
Bond lengths



Bond angles

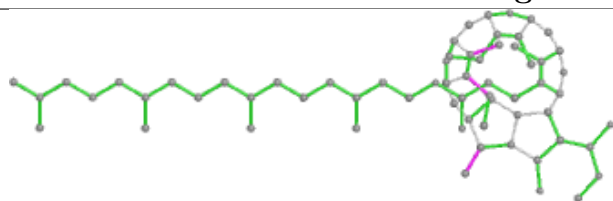


Torsions

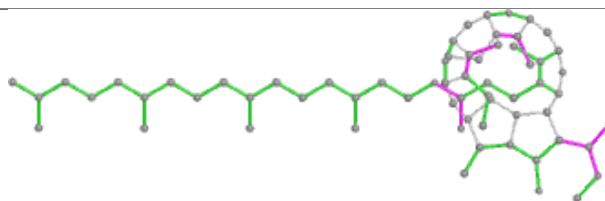


Rings

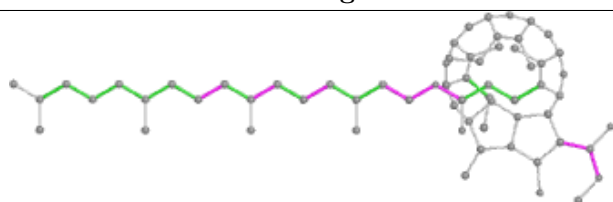
Ligand PHO d 401



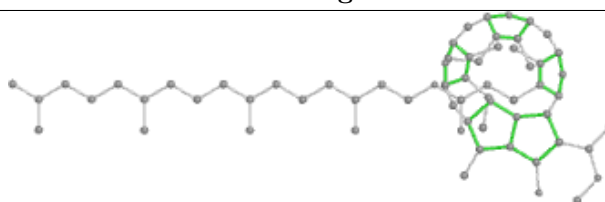
Bond lengths



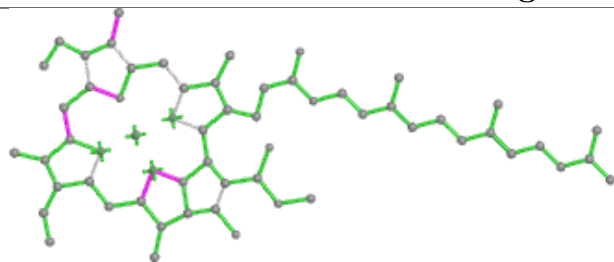
Bond angles



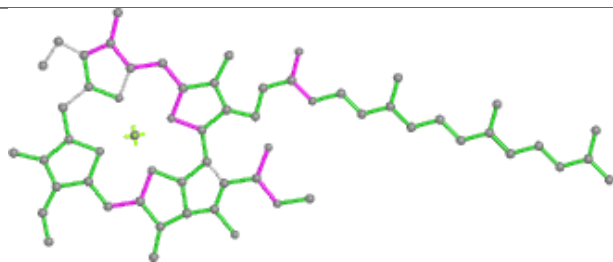
Torsions



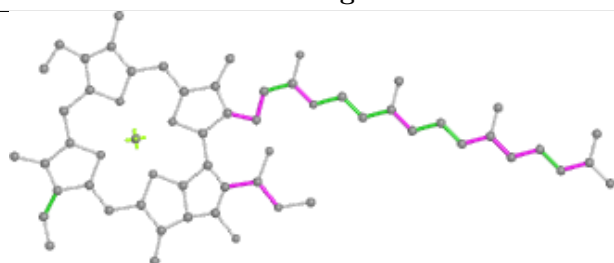
Rings

Ligand CLA 2 611

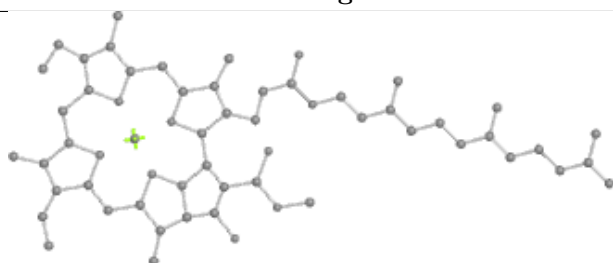
Bond lengths



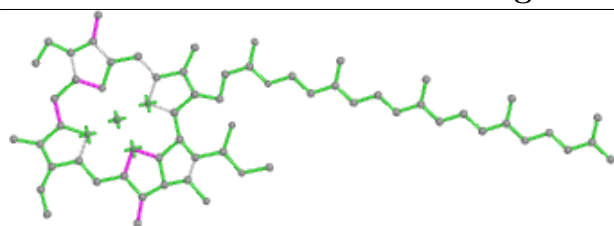
Bond angles



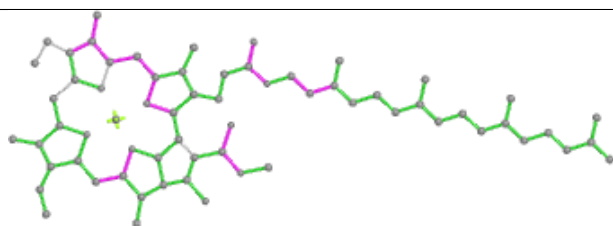
Torsions



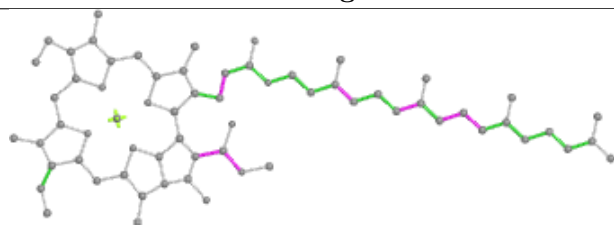
Rings

Ligand CLA B 606

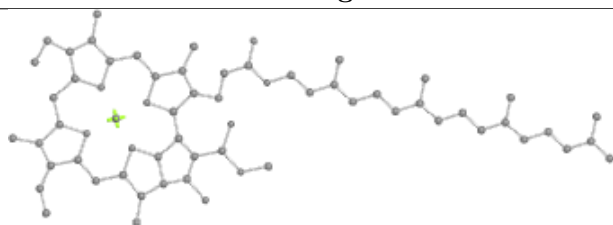
Bond lengths



Bond angles

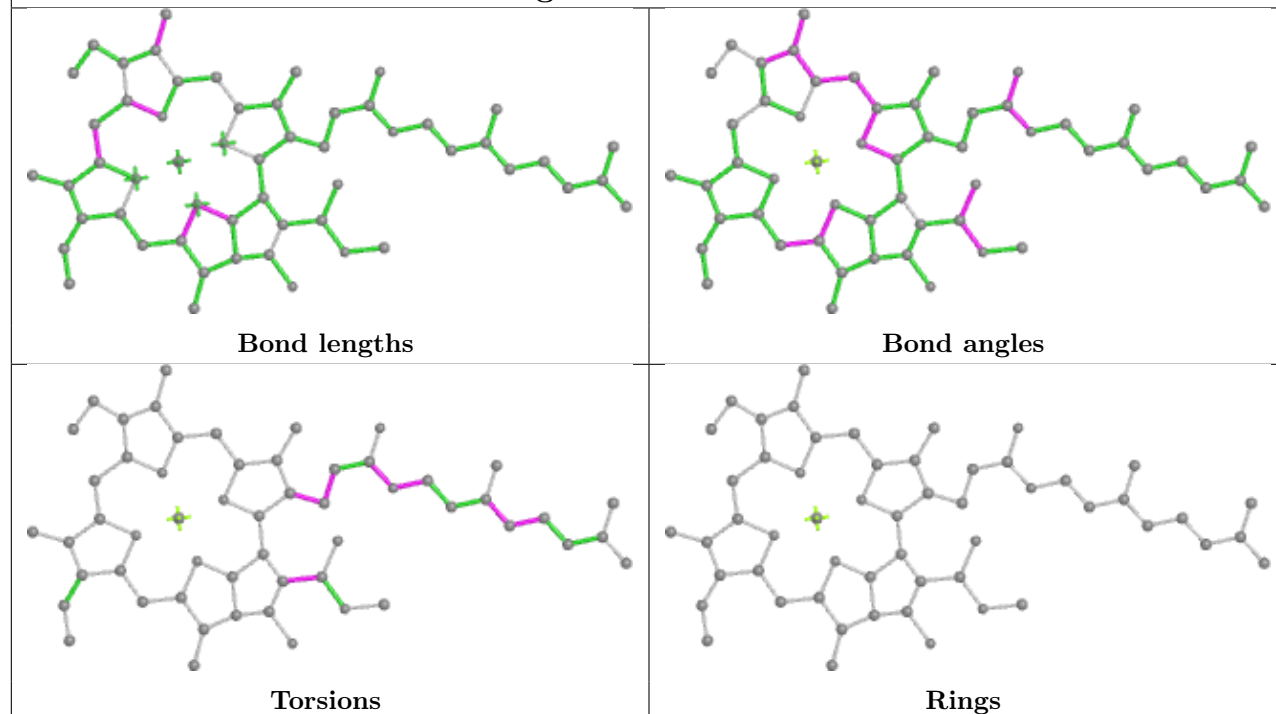


Torsions

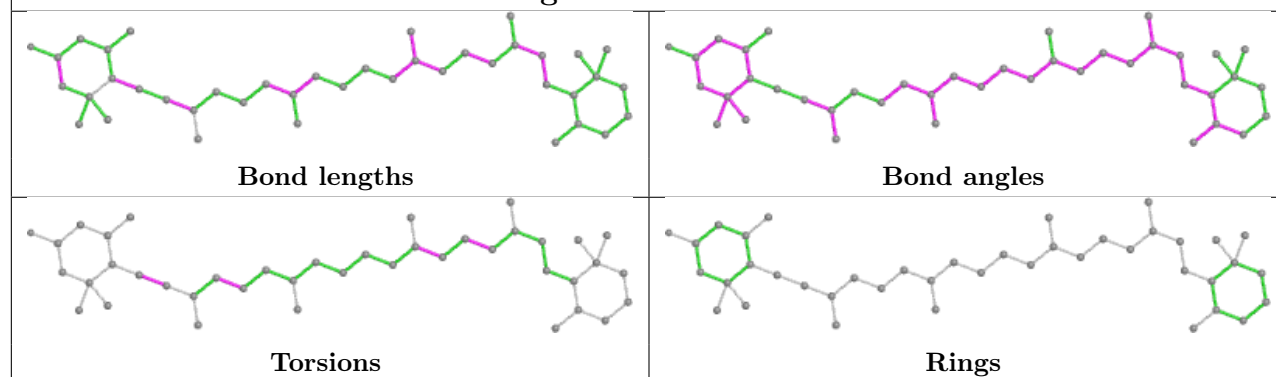


Rings

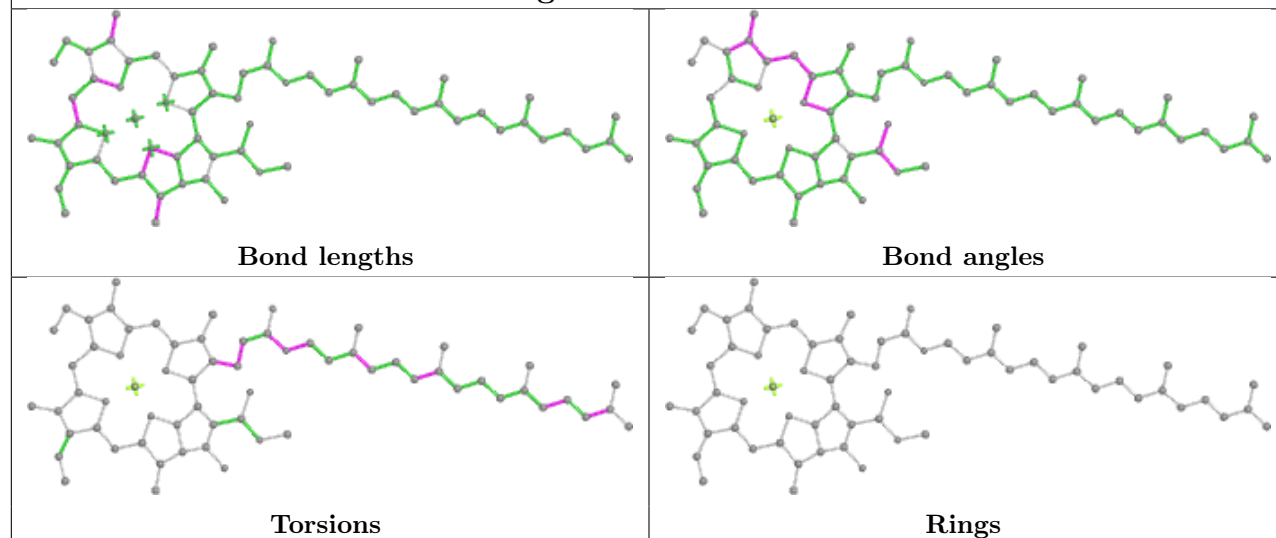
Ligand CLA 6 611



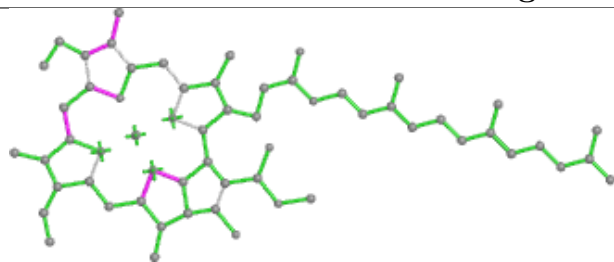
Ligand IHT 2 620



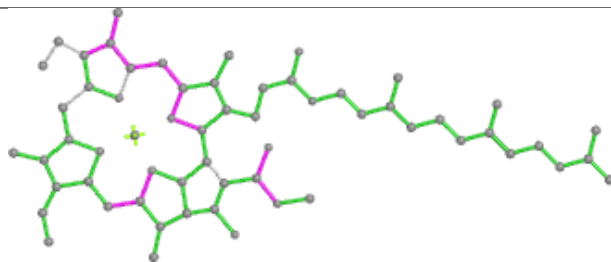
Ligand CLA c 524



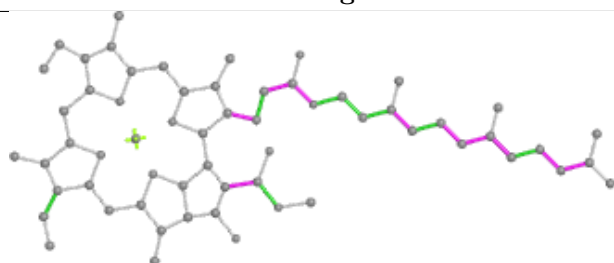
Ligand CLA 2 607



Bond lengths



Bond angles

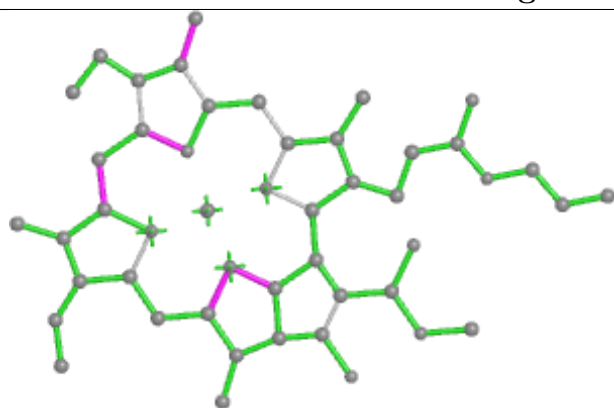


Torsions

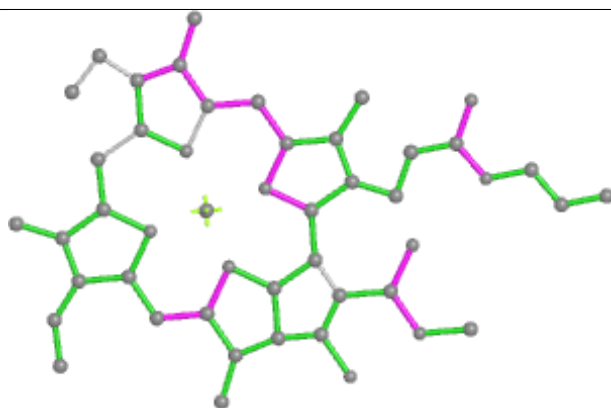


Rings

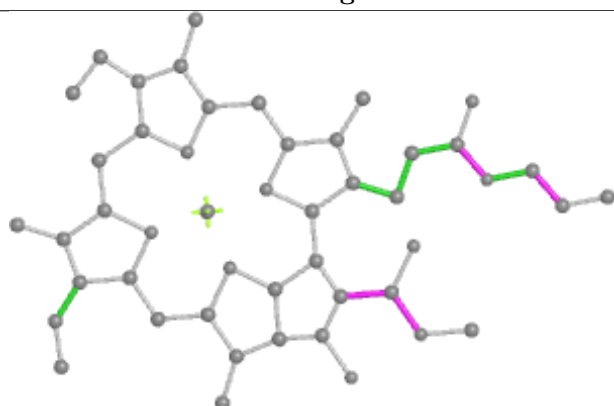
Ligand CLA 1 614



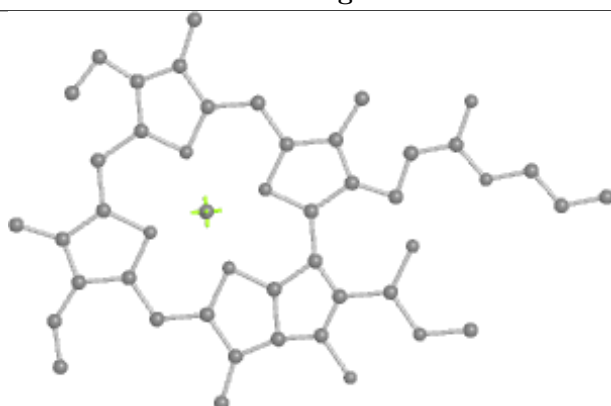
Bond lengths



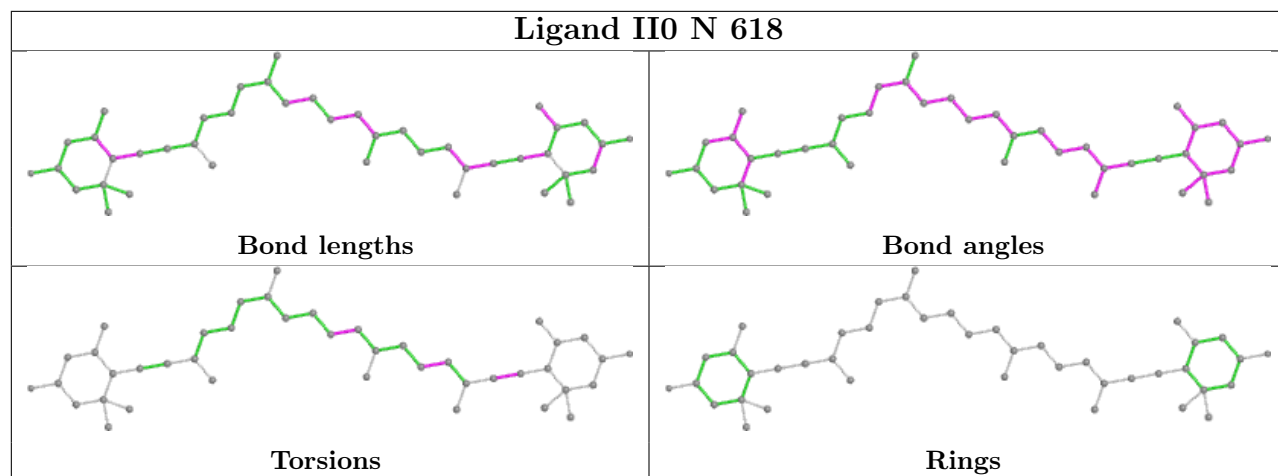
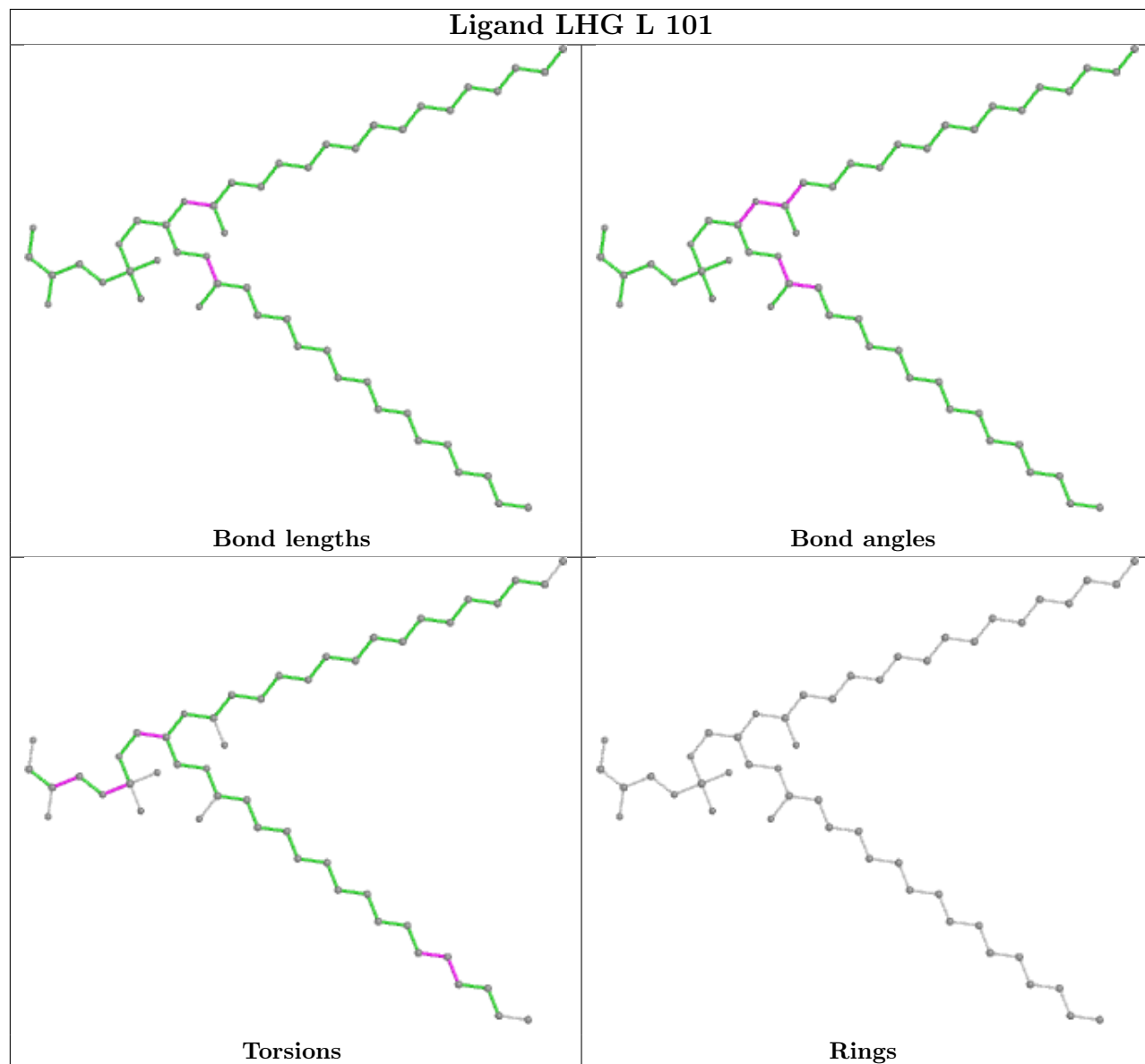
Bond angles

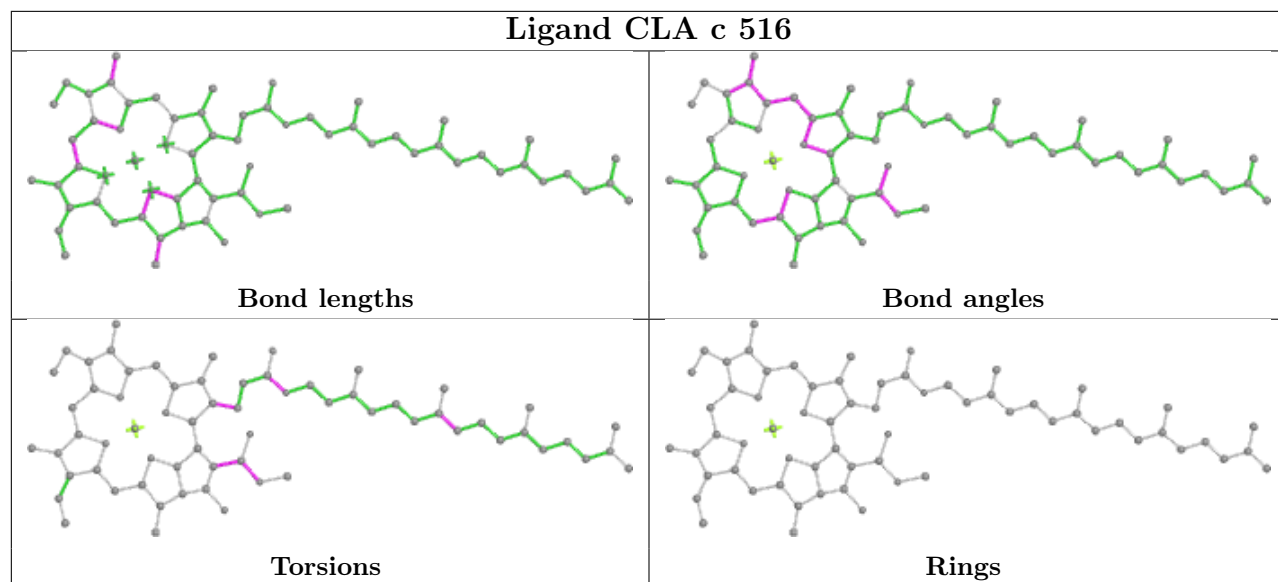
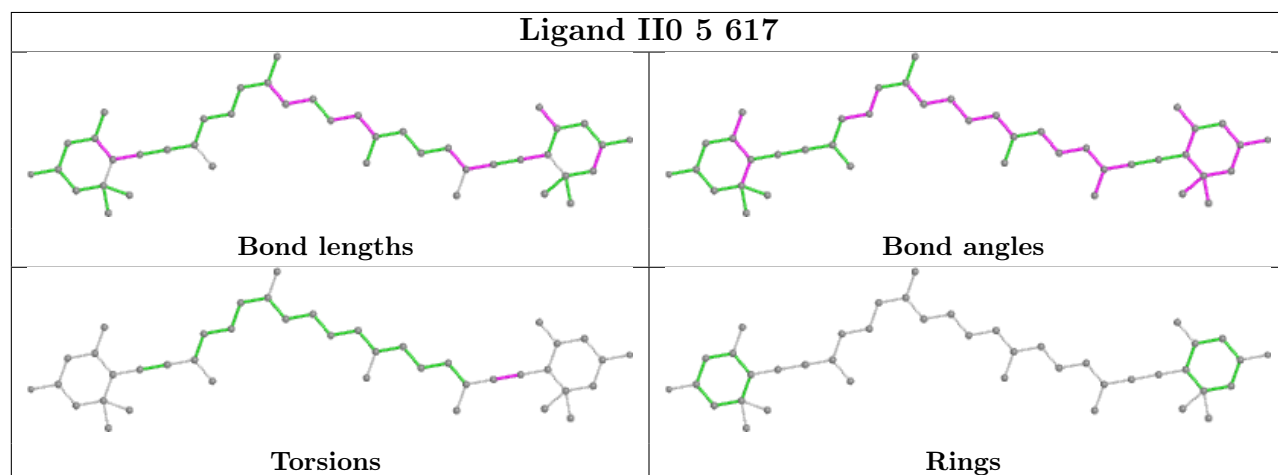


Torsions

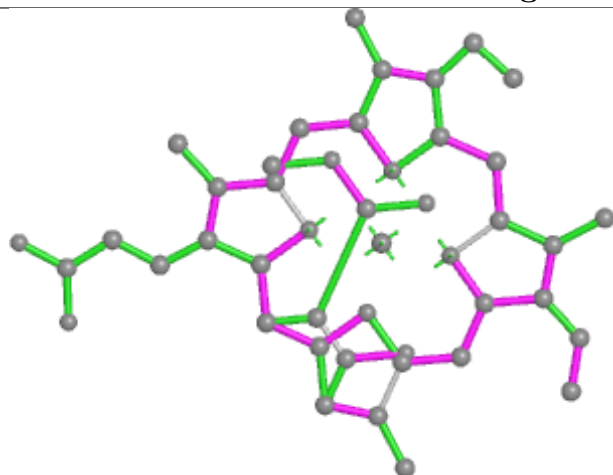


Rings

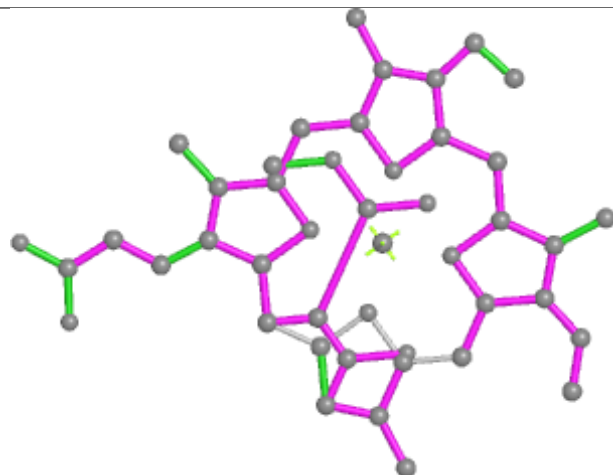
Ligand II0 N 618**Ligand LHG L 101**

Ligand CLA c 516**Ligand II0 5 617**

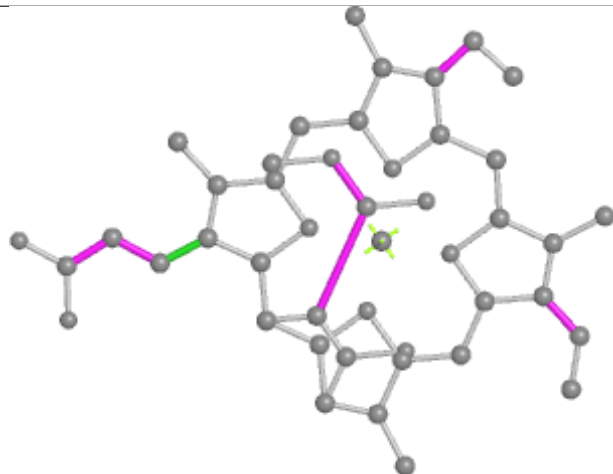
Ligand KC2 1 613



Bond lengths



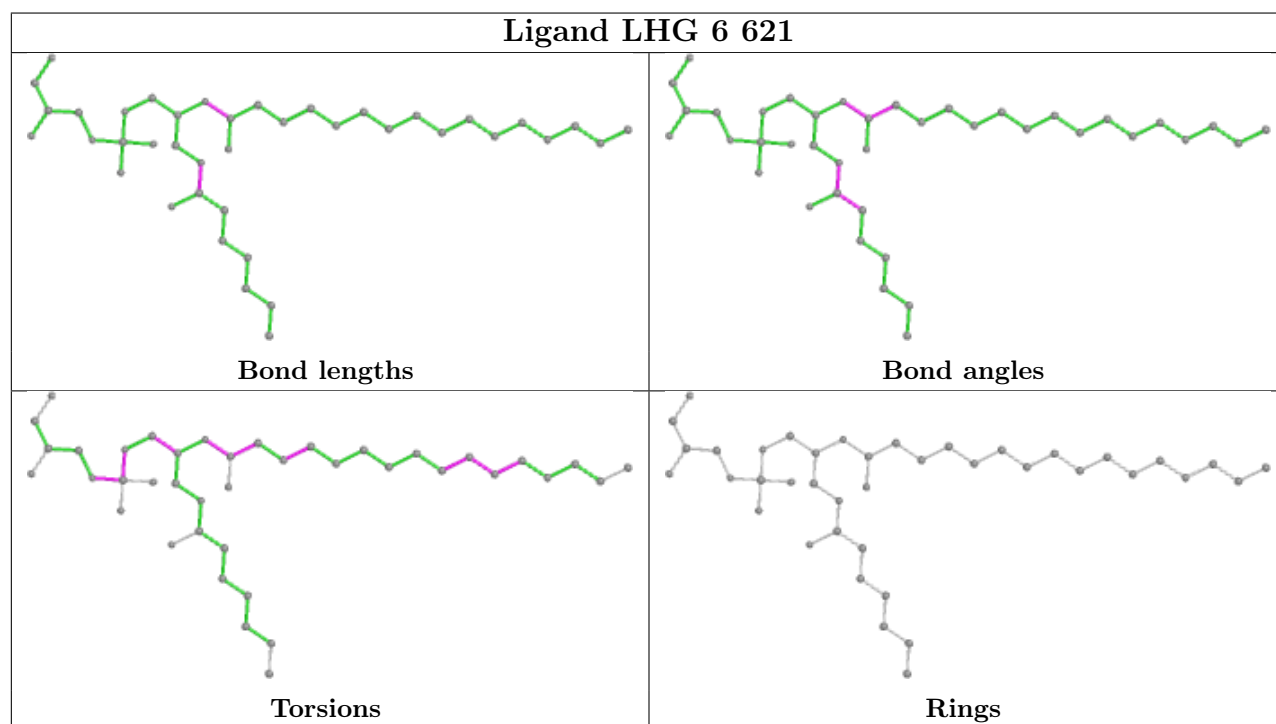
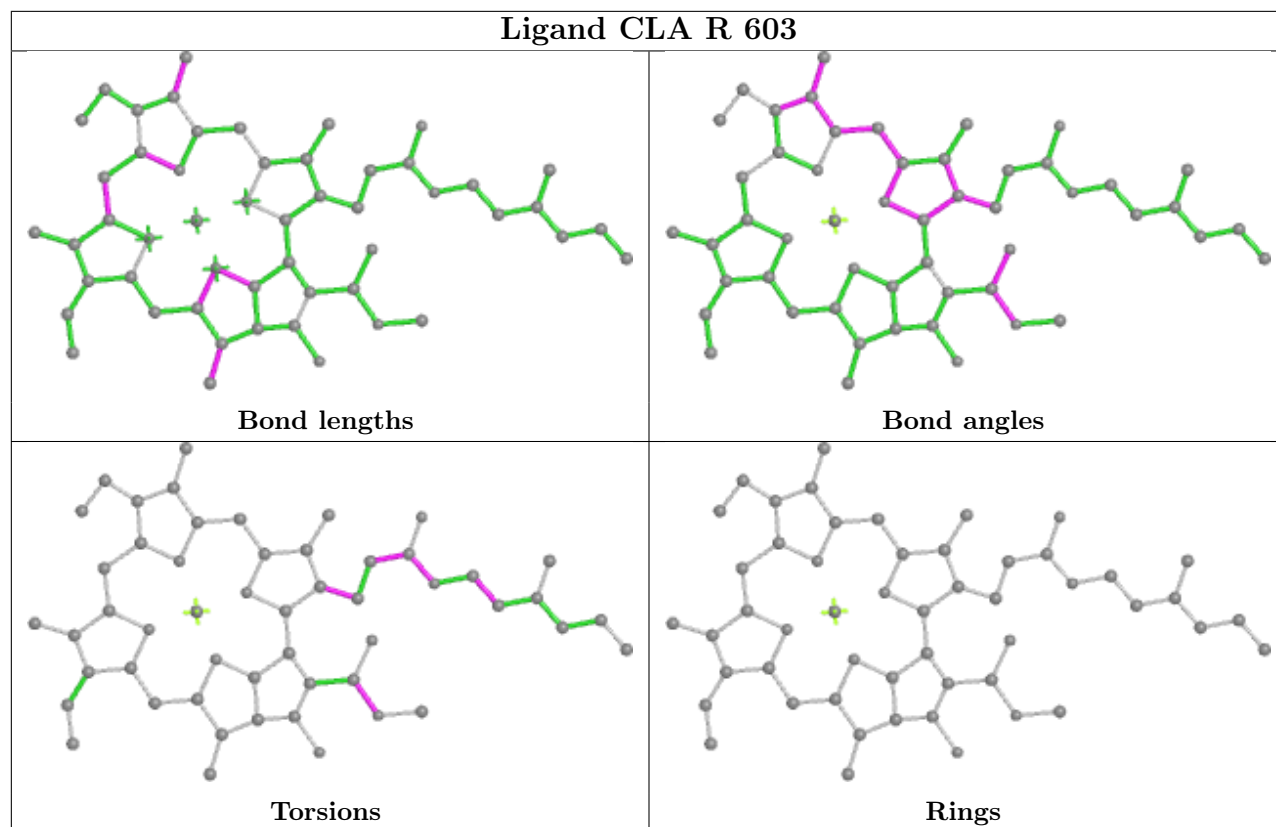
Bond angles

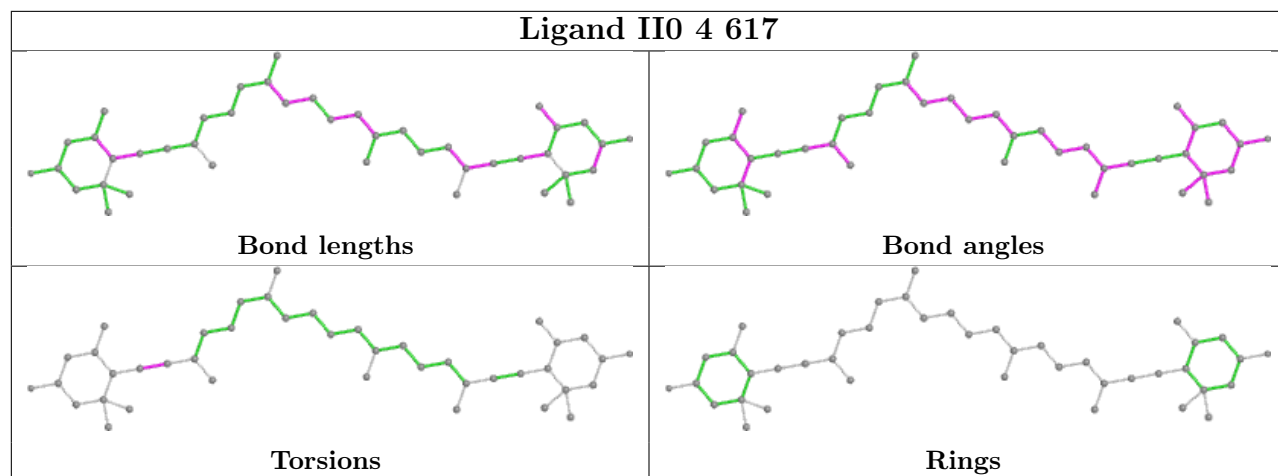
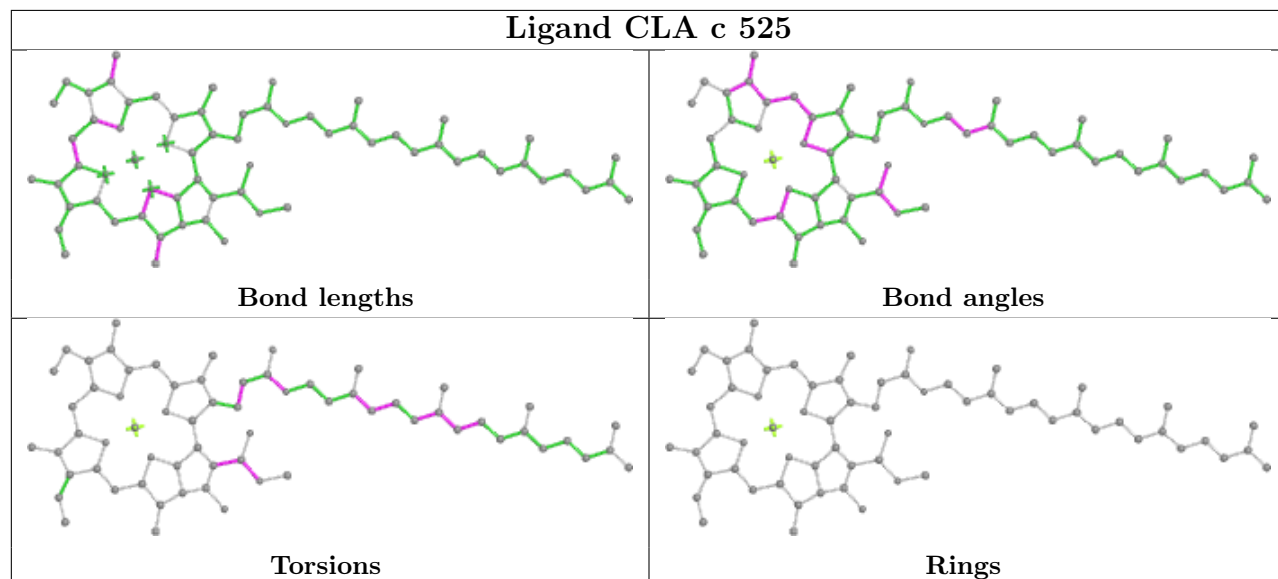
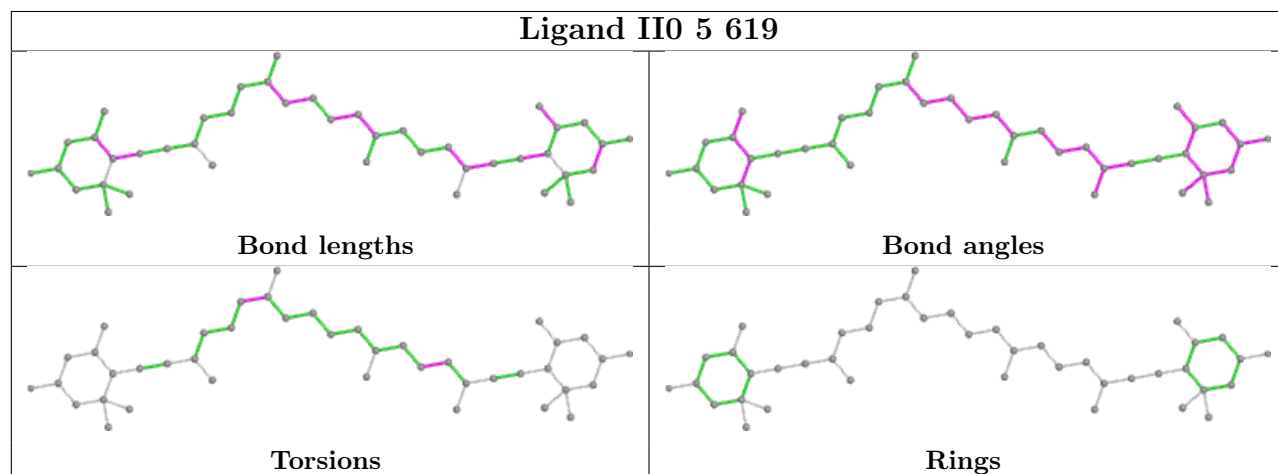


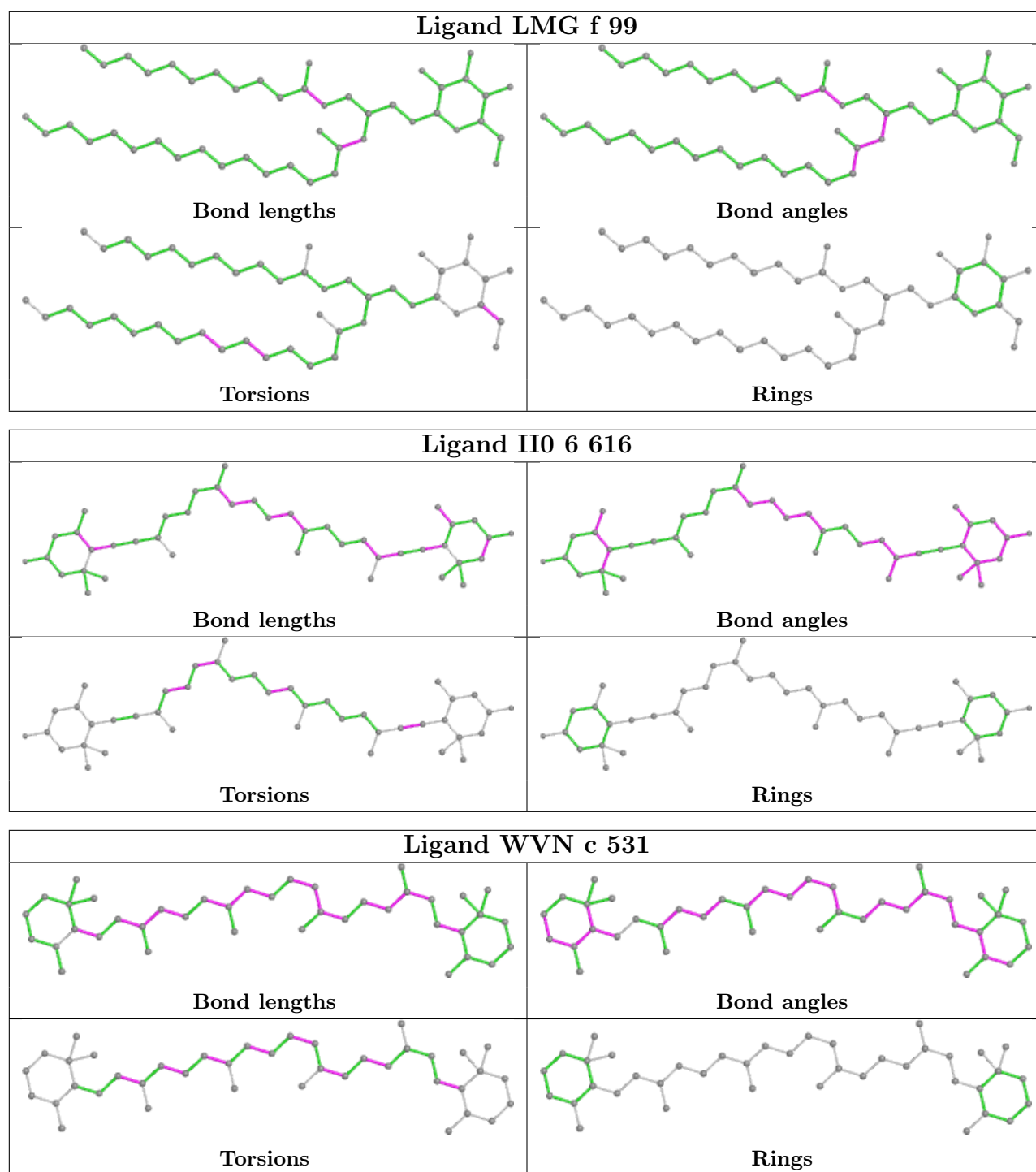
Torsions

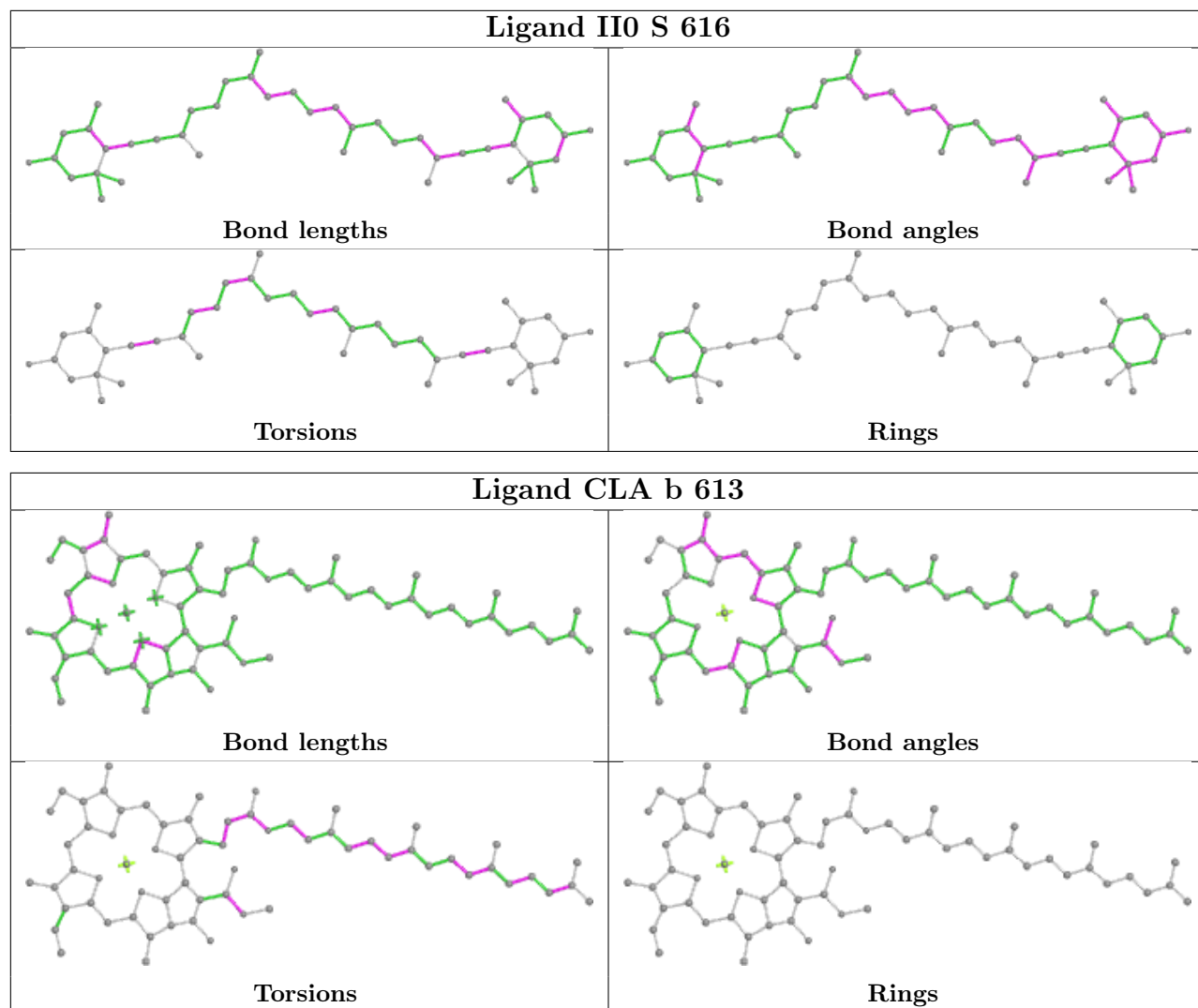


Rings

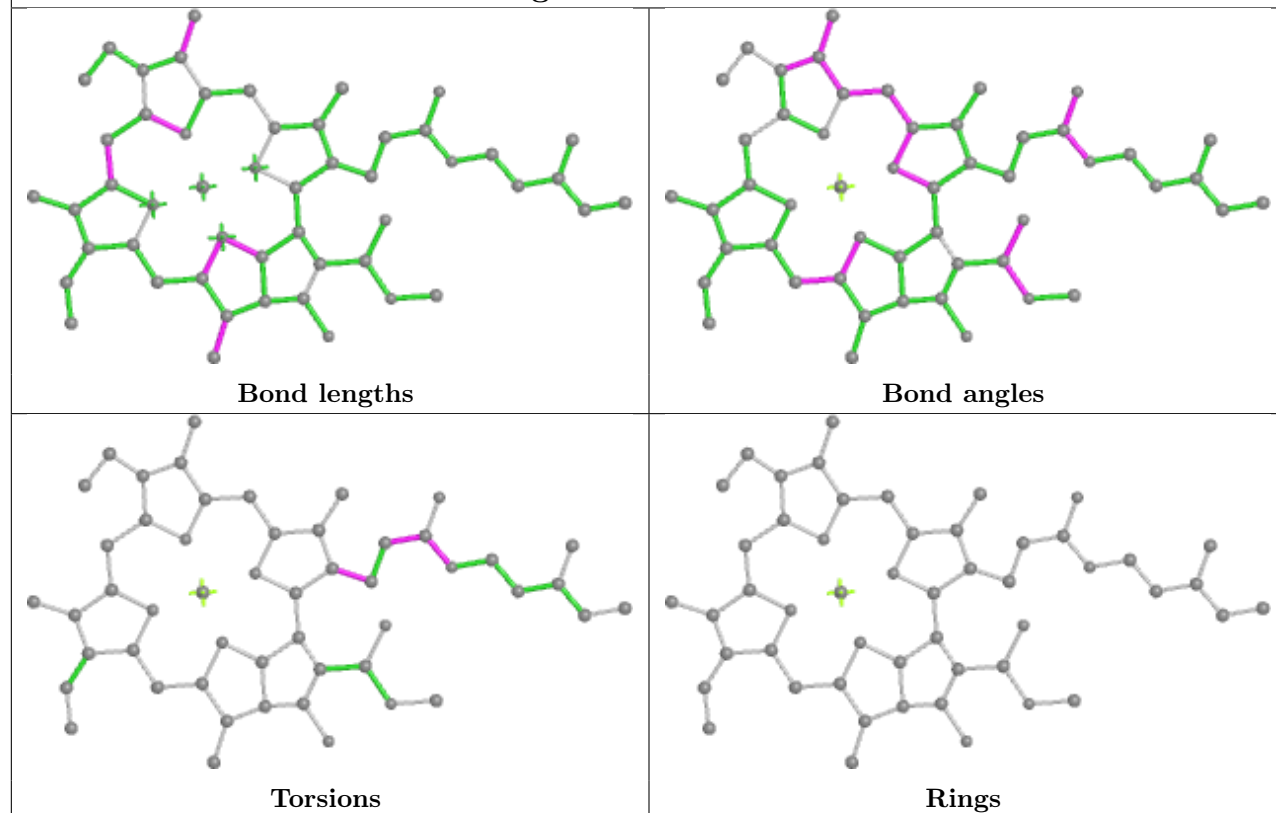


Ligand II0 4 617**Ligand CLA c 525****Ligand II0 5 619**

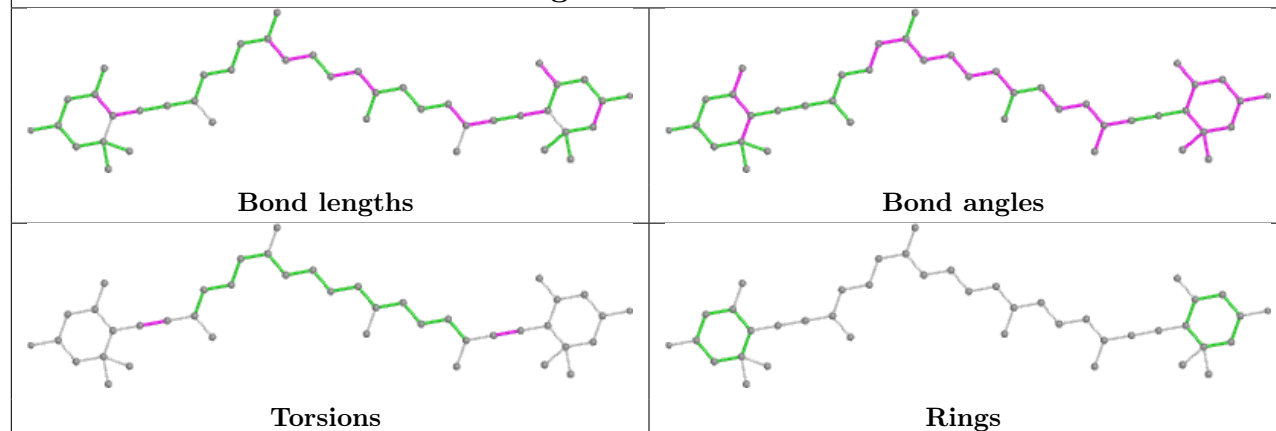




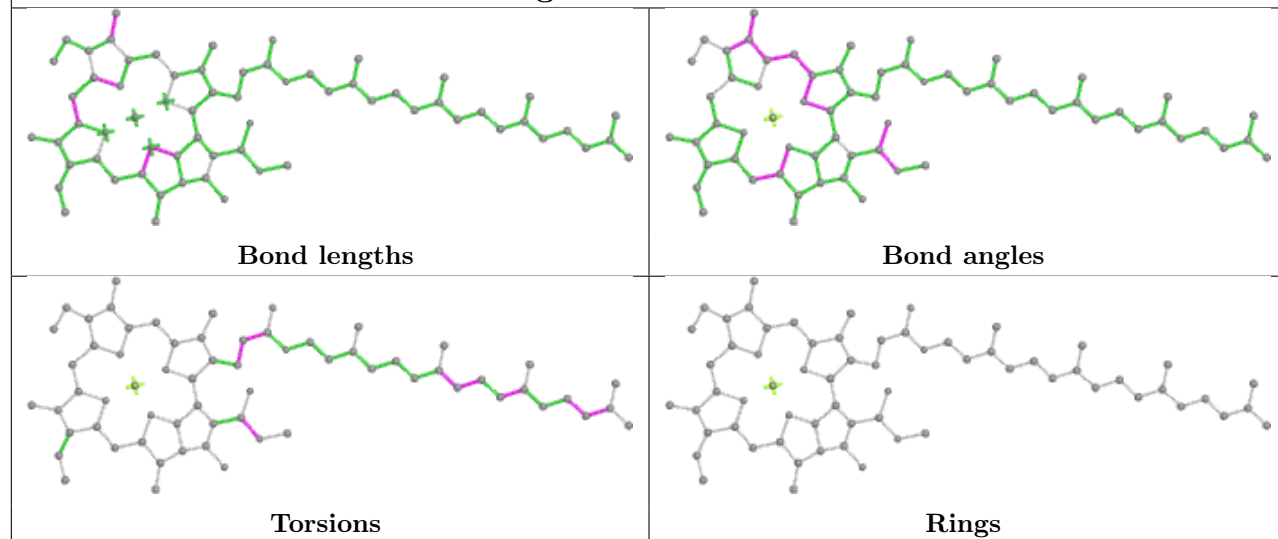
Ligand CLA O 606



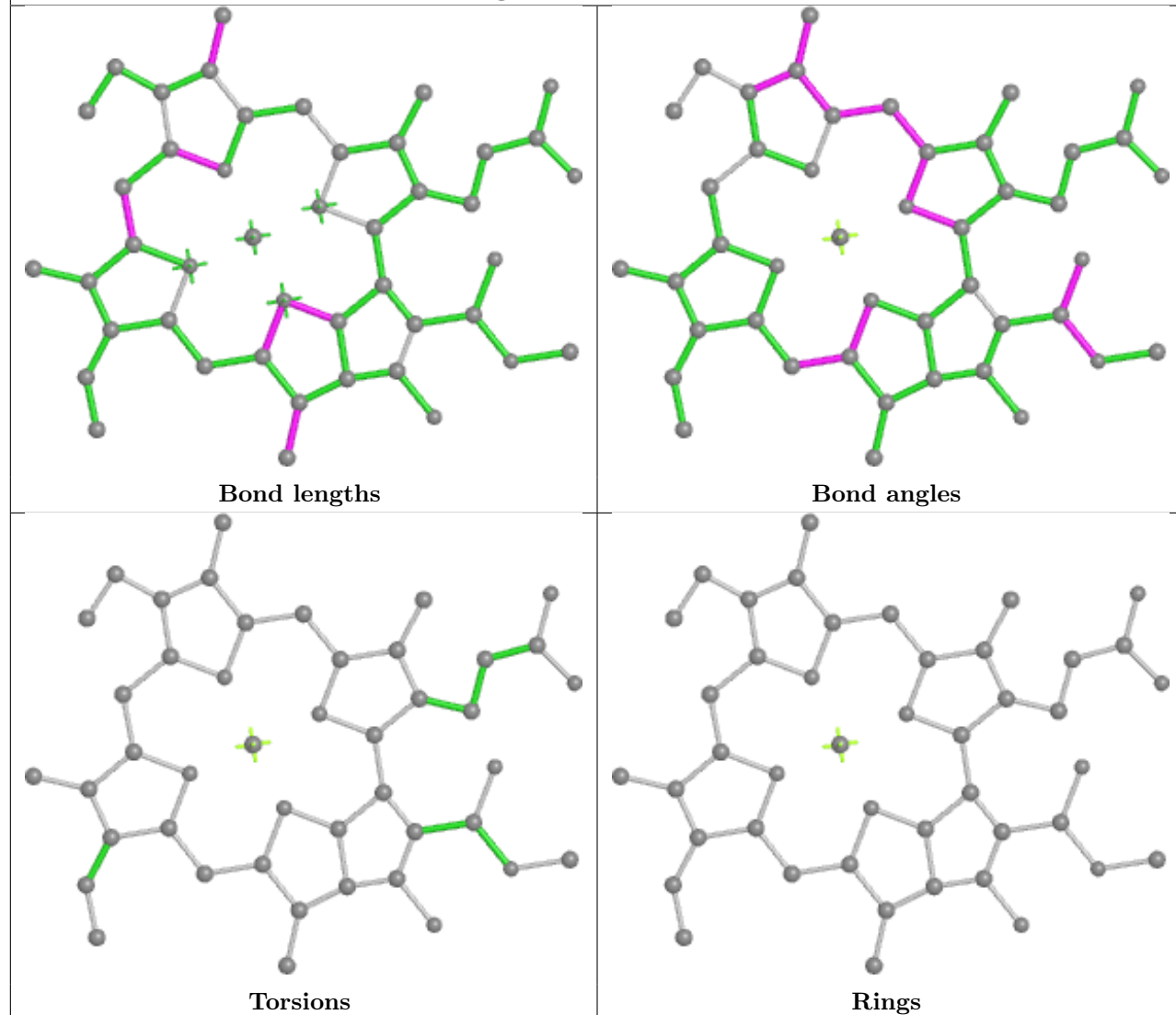
Ligand II0 4 618



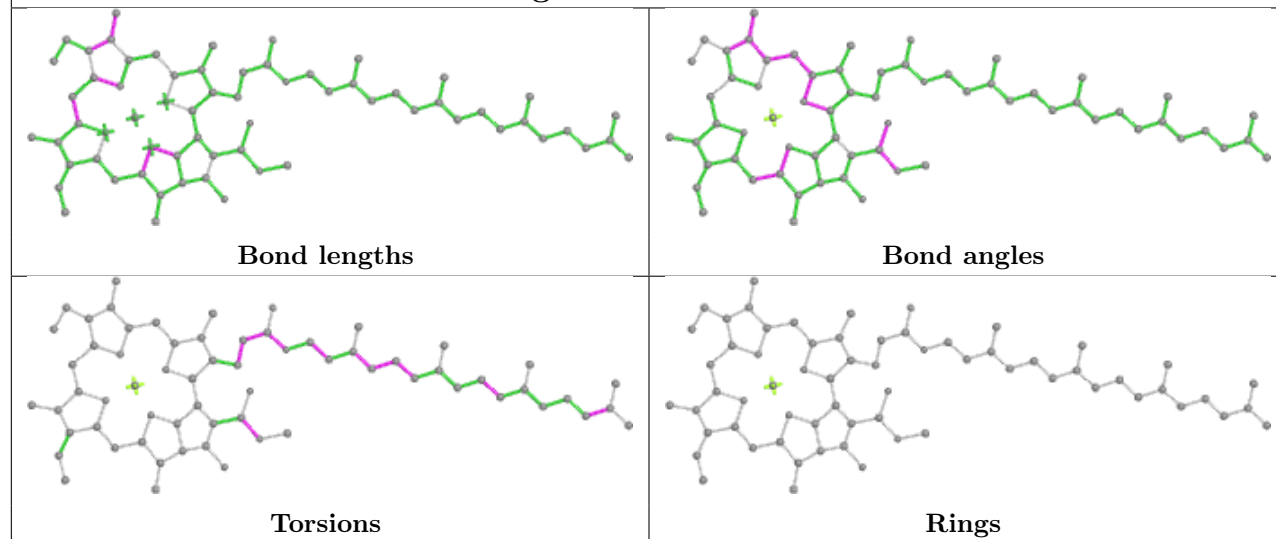
Ligand CLA 2 604



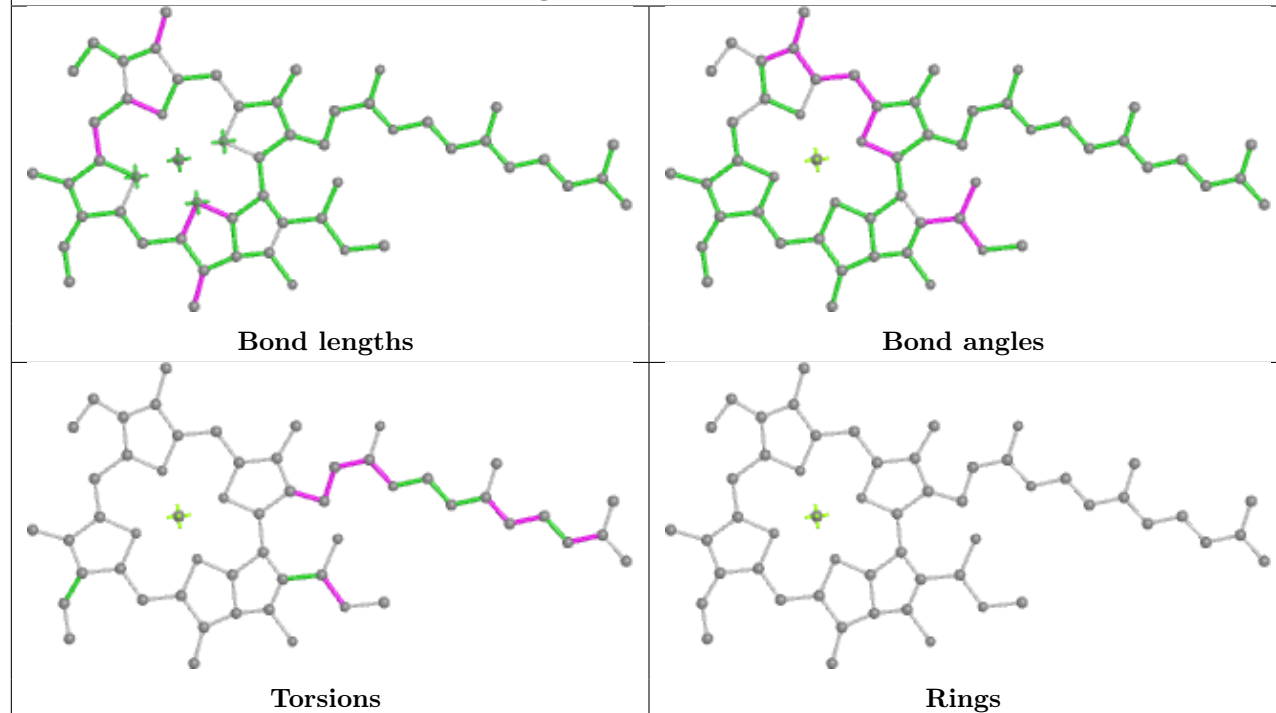
Ligand CLA 3 601

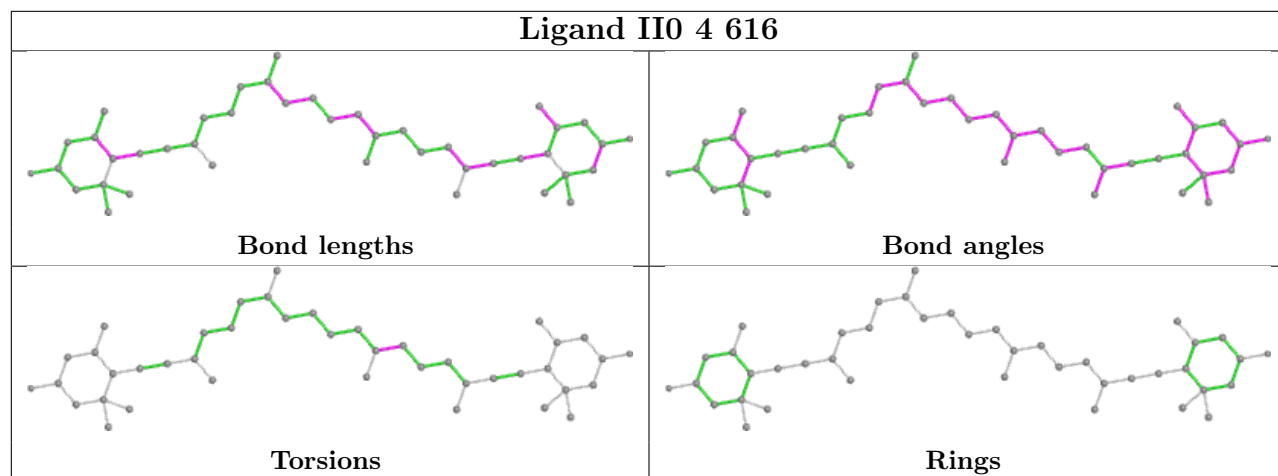
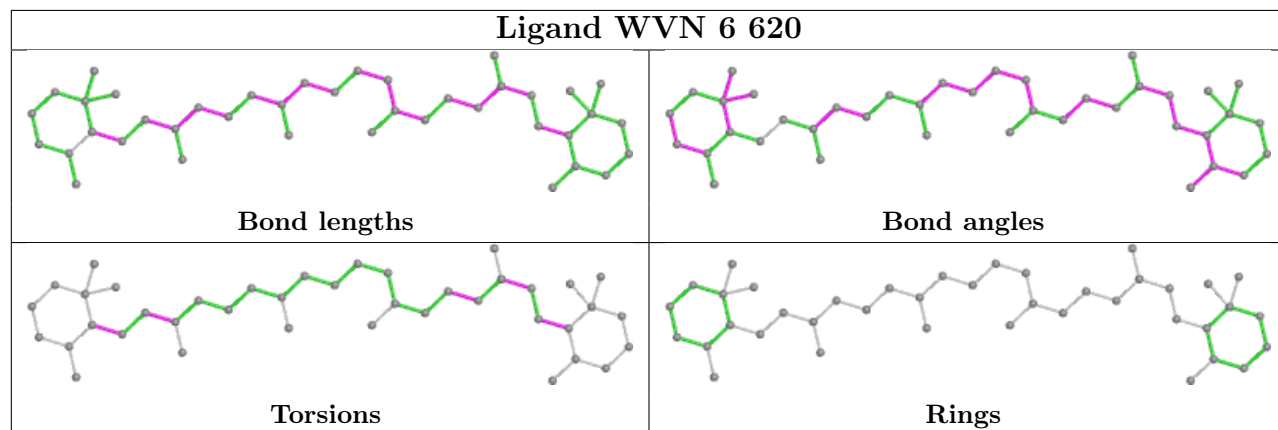


Ligand CLA B 613

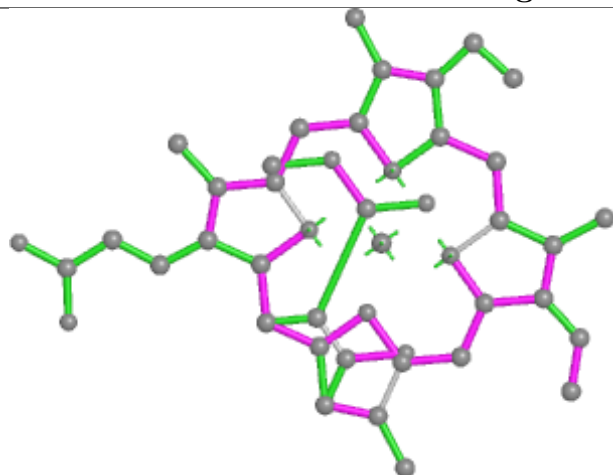


Ligand CLA S 609

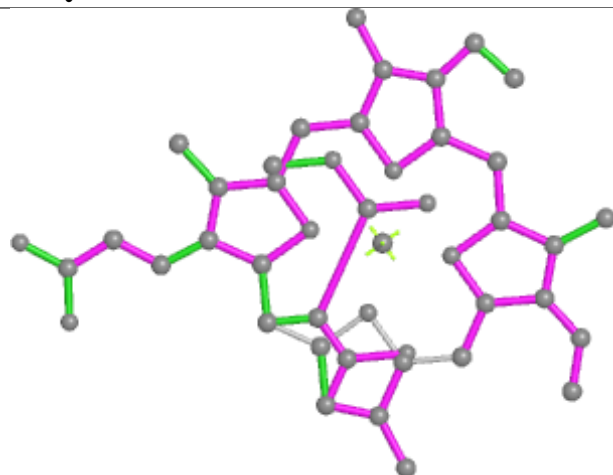


Ligand II0 4 616**Ligand WVN 6 620**

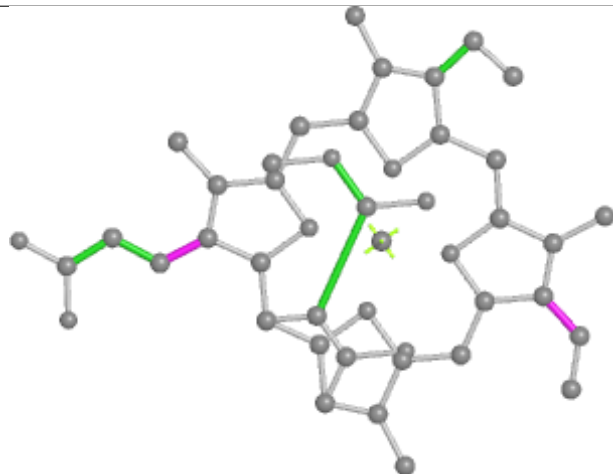
Ligand KC2 Q 612



Bond lengths



Bond angles

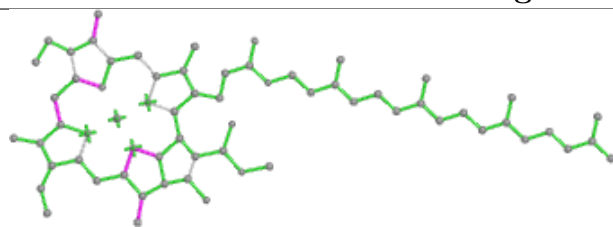


Torsions

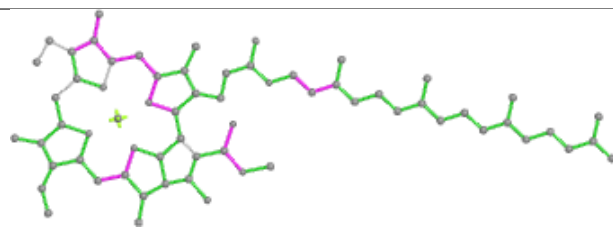


Rings

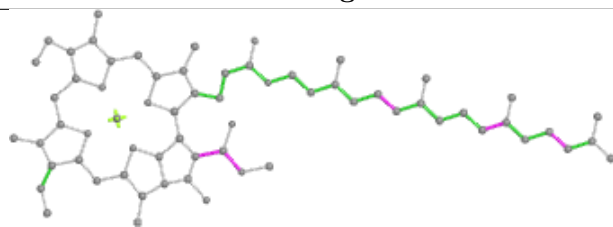
Ligand CLA B 605



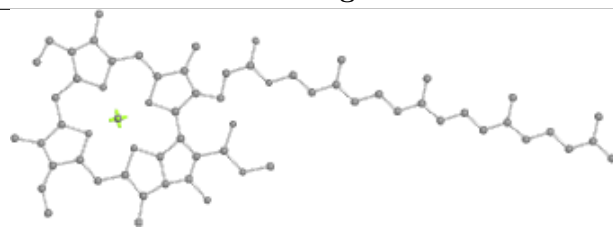
Bond lengths



Bond angles

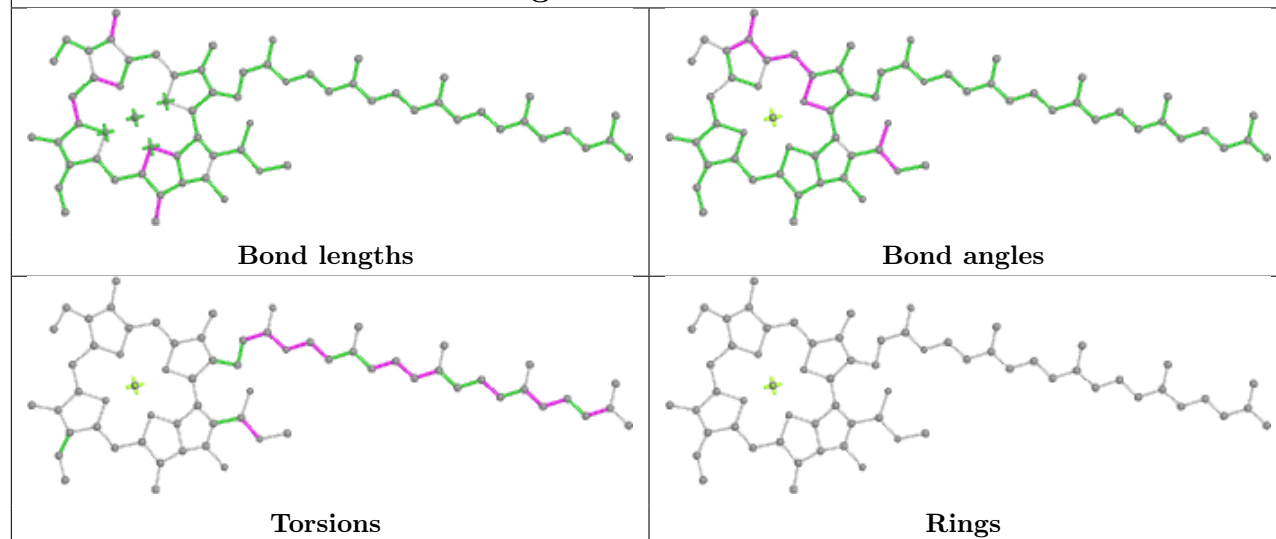


Torsions

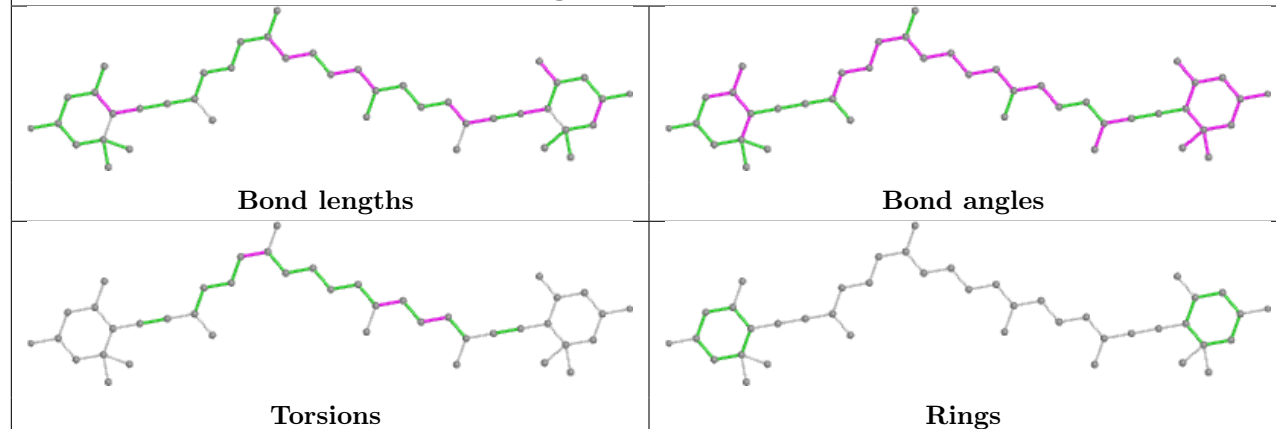


Rings

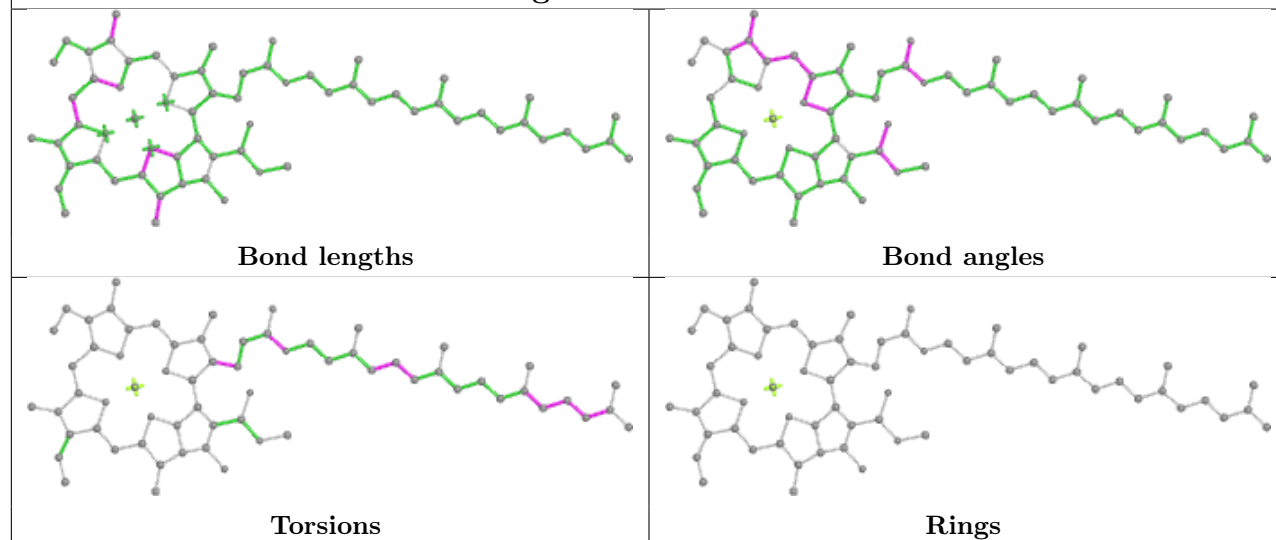
Ligand CLA R 611



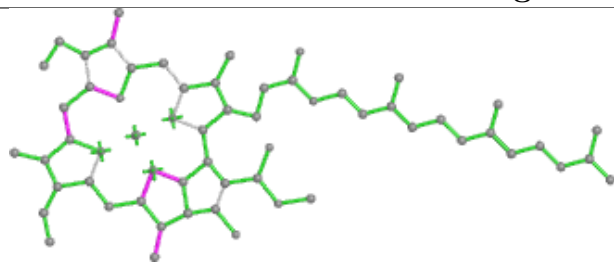
Ligand II0 2 619



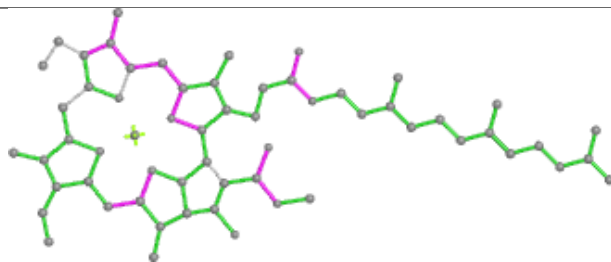
Ligand CLA C 527



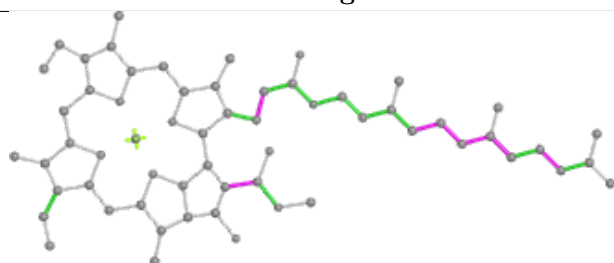
Ligand CLA R 604



Bond lengths



Bond angles

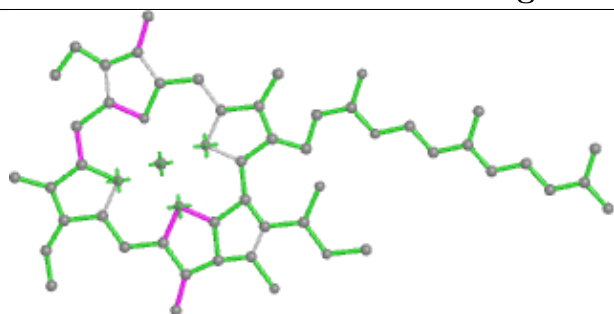


Torsions

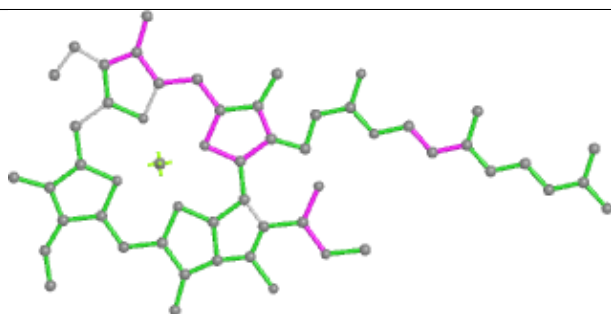


Rings

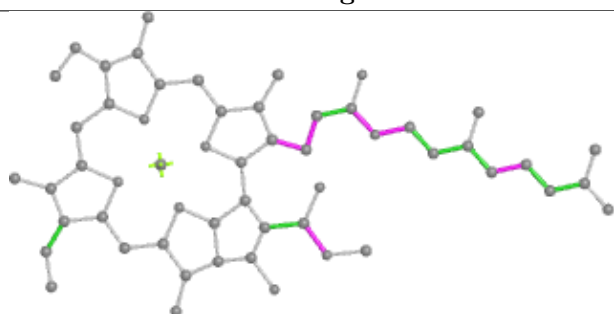
Ligand CLA S 603



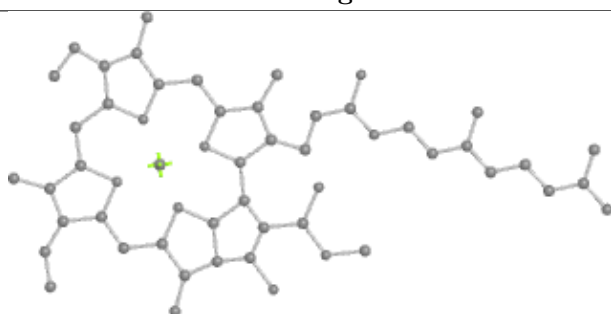
Bond lengths



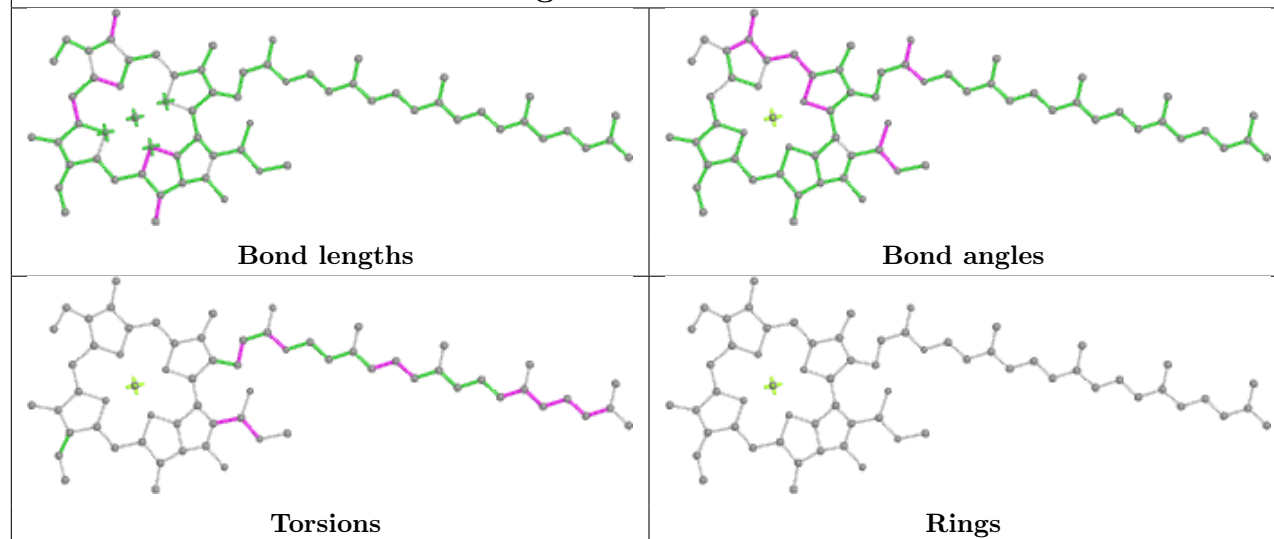
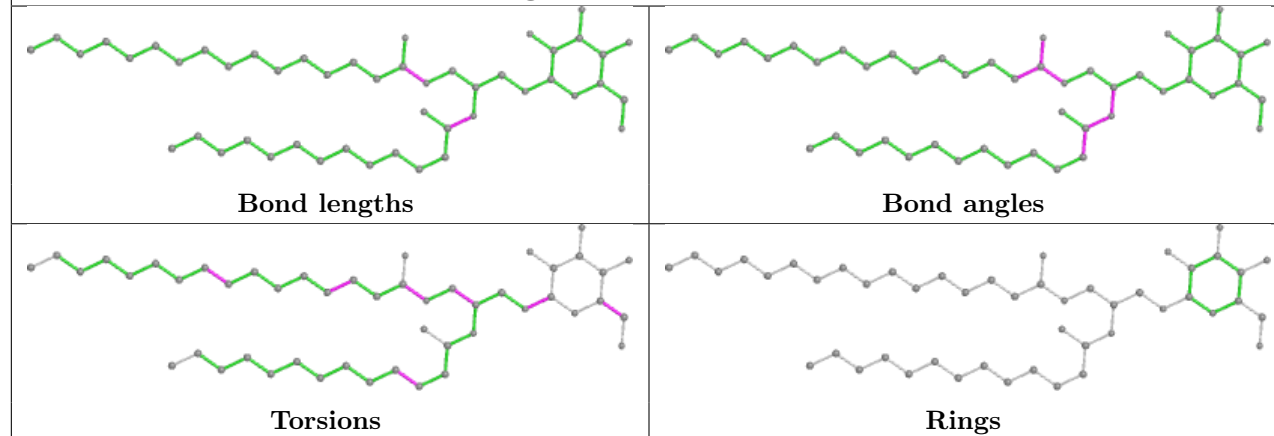
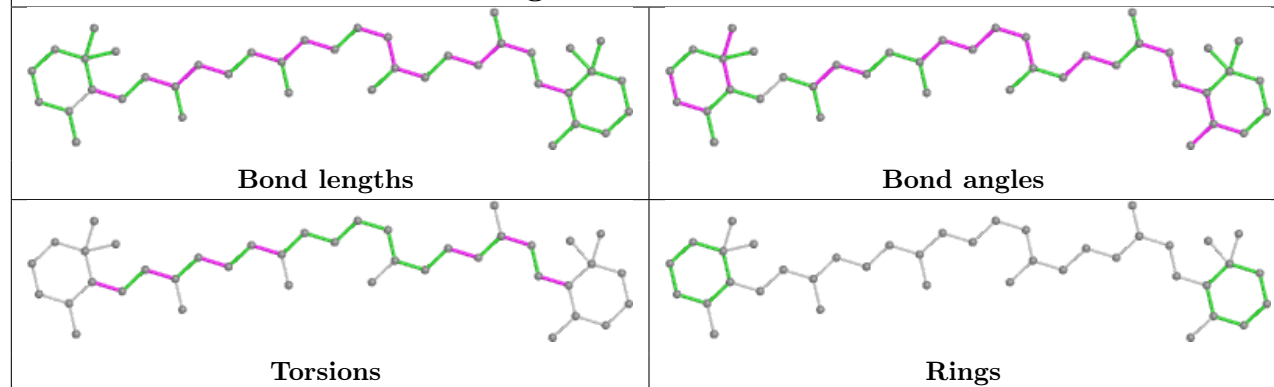
Bond angles



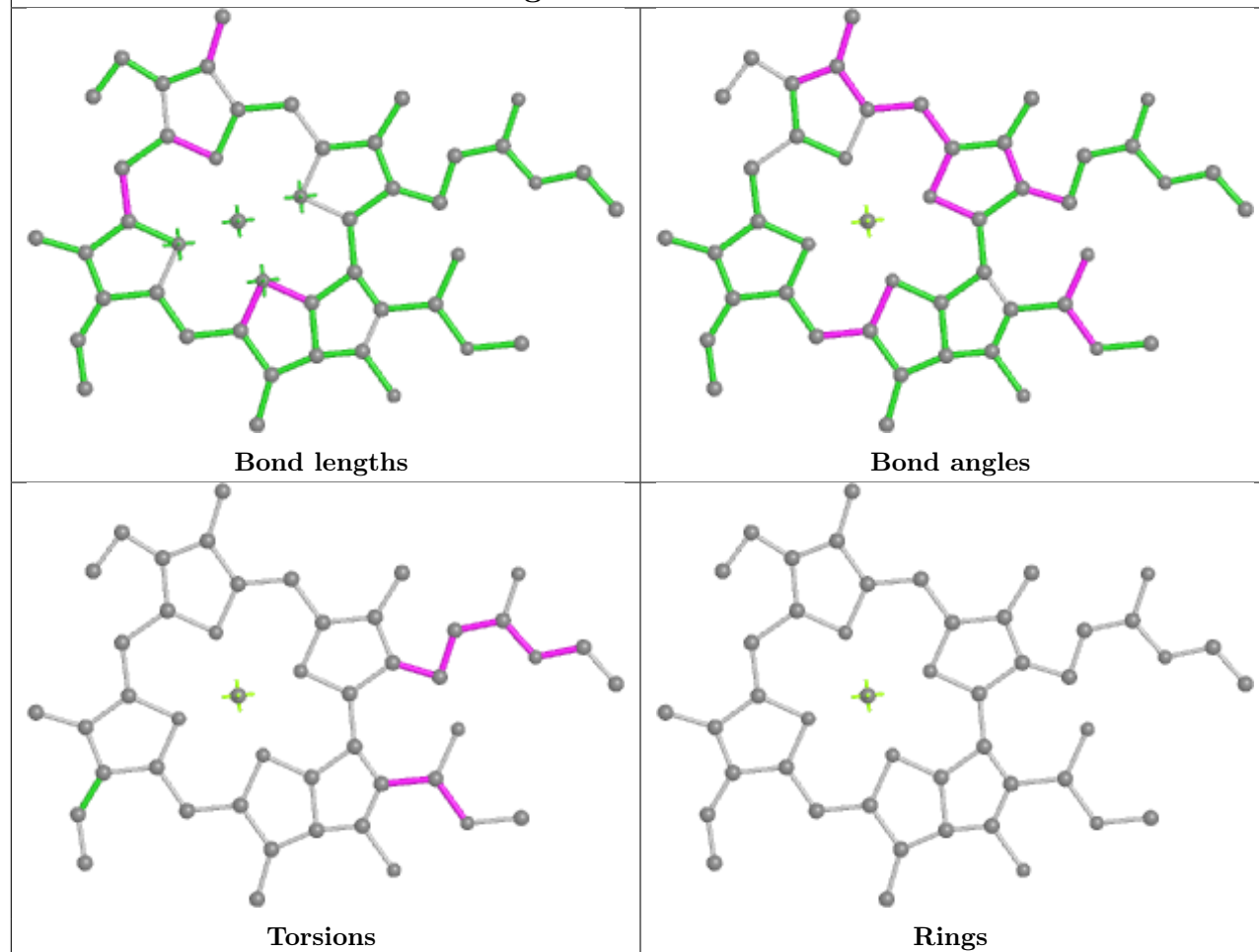
Torsions



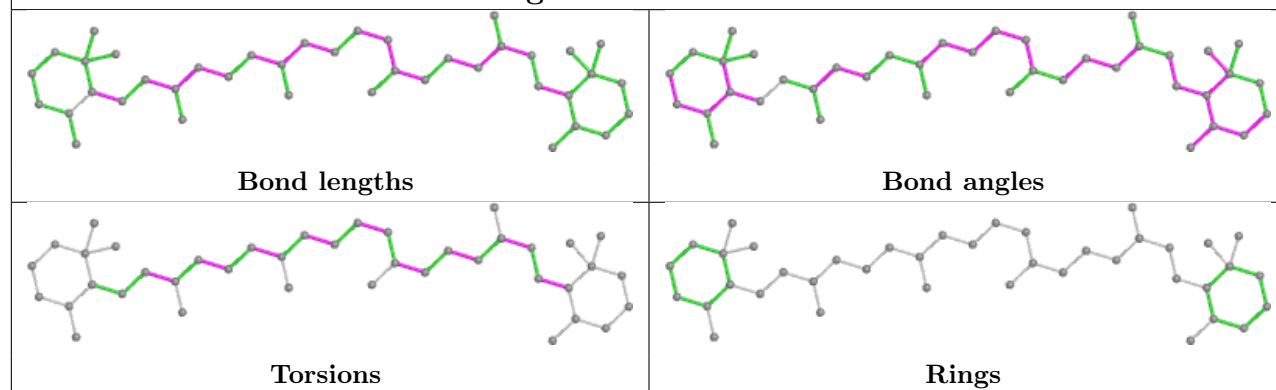
Rings

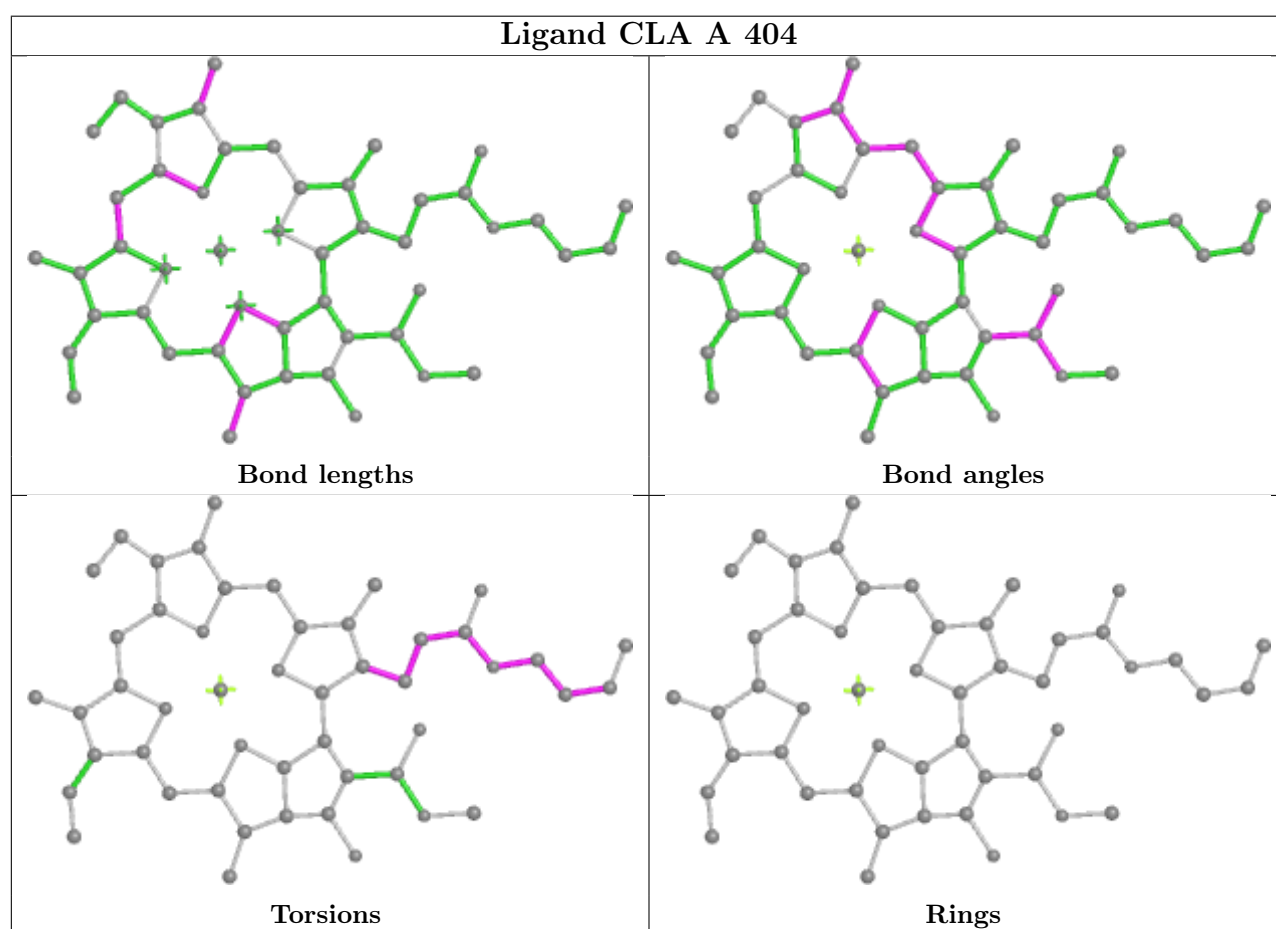
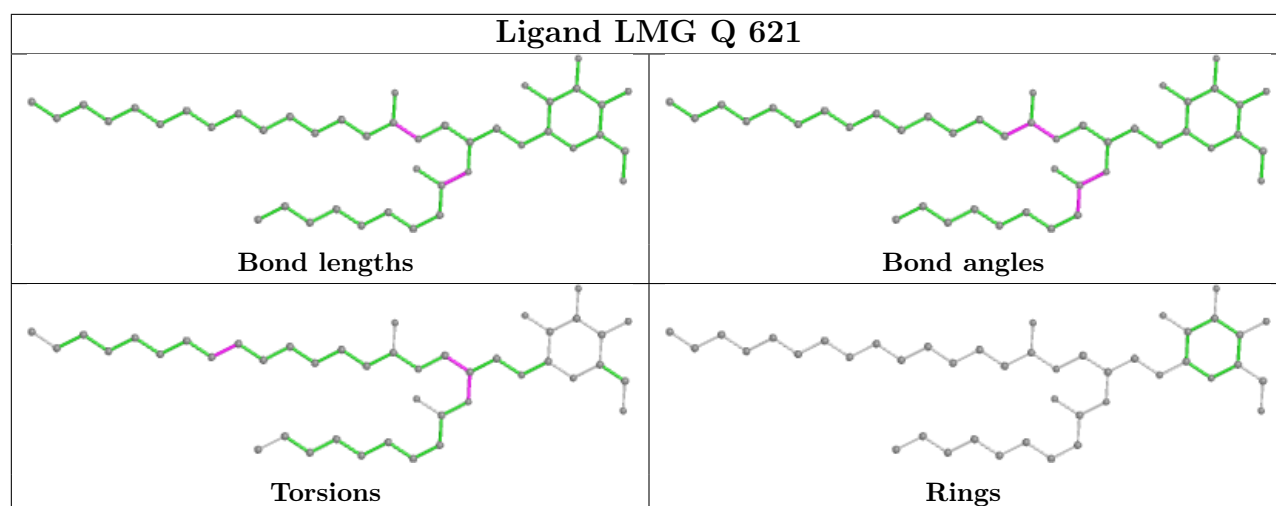
Ligand CLA 6 604**Ligand LMG W 134****Ligand WVN S 620**

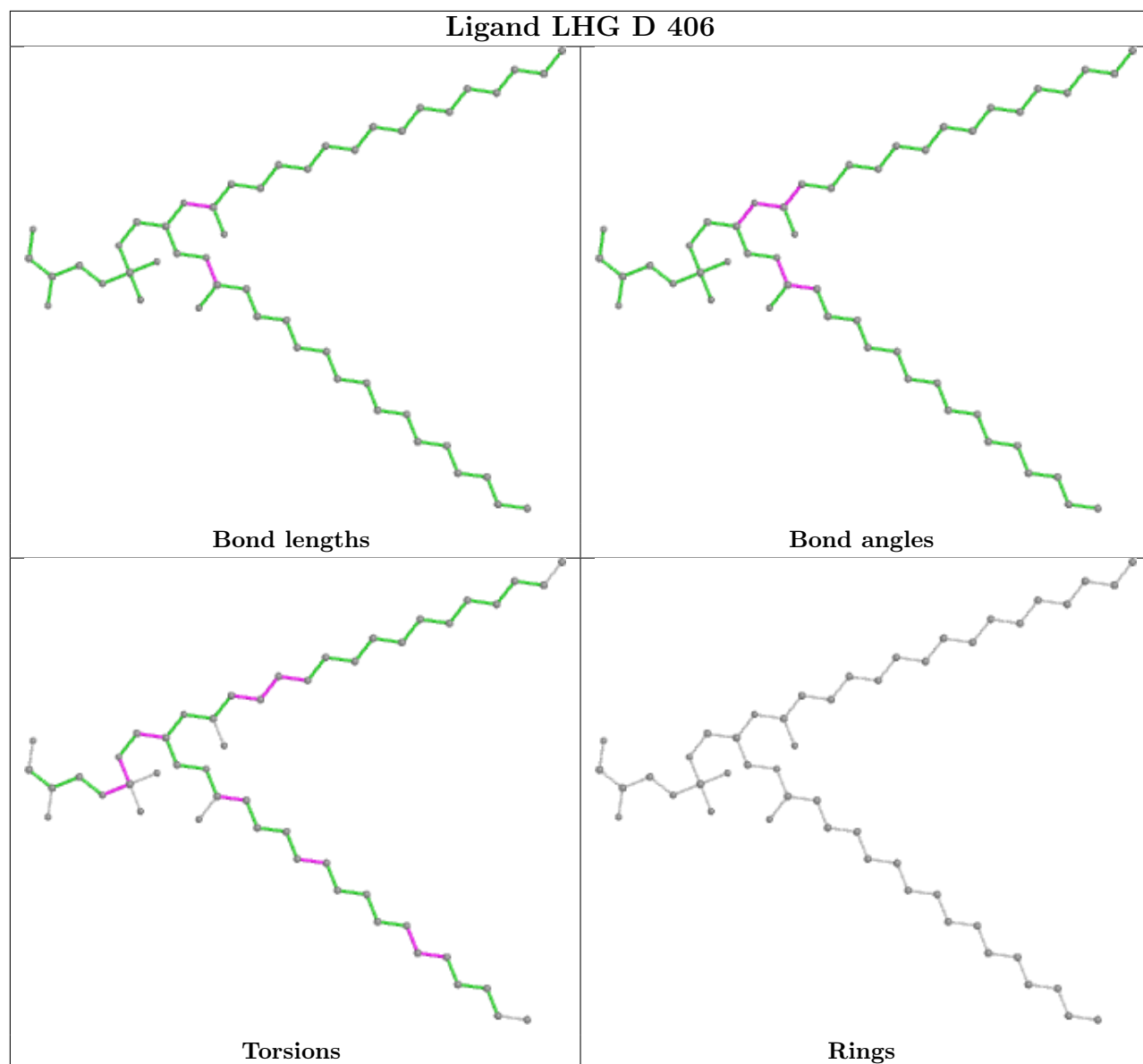
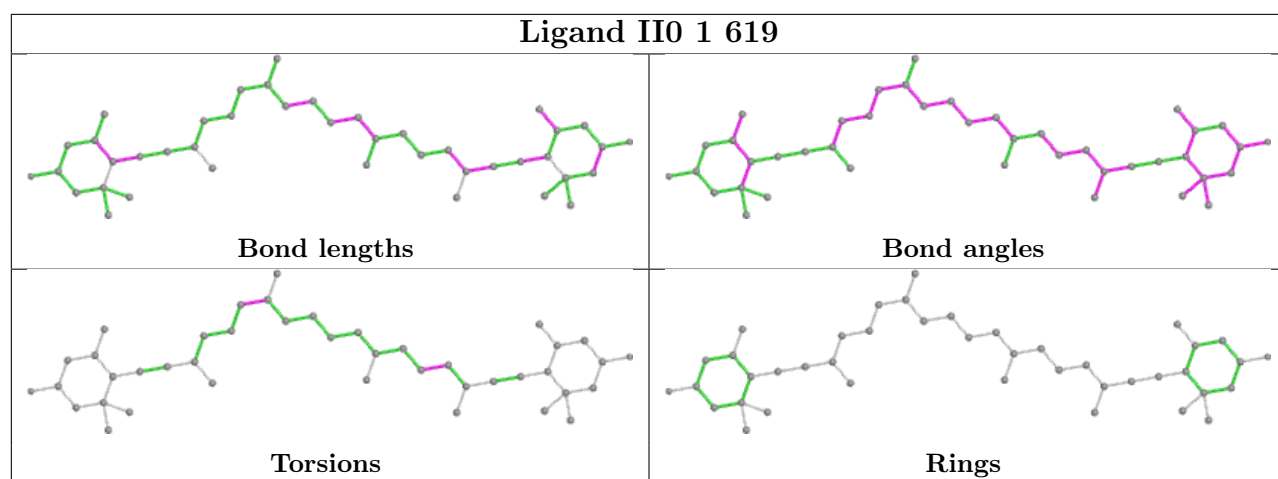
Ligand CLA N 615

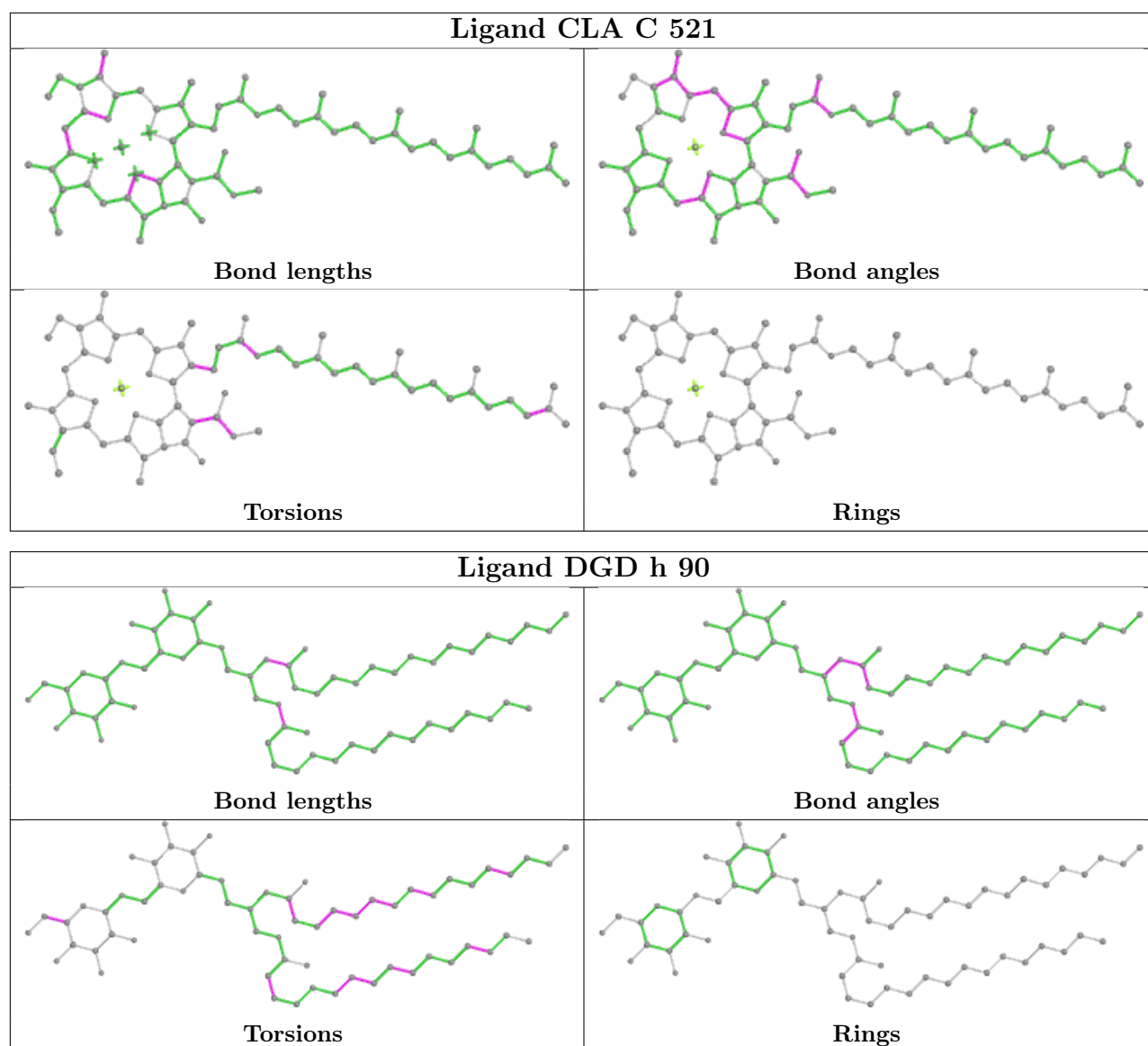


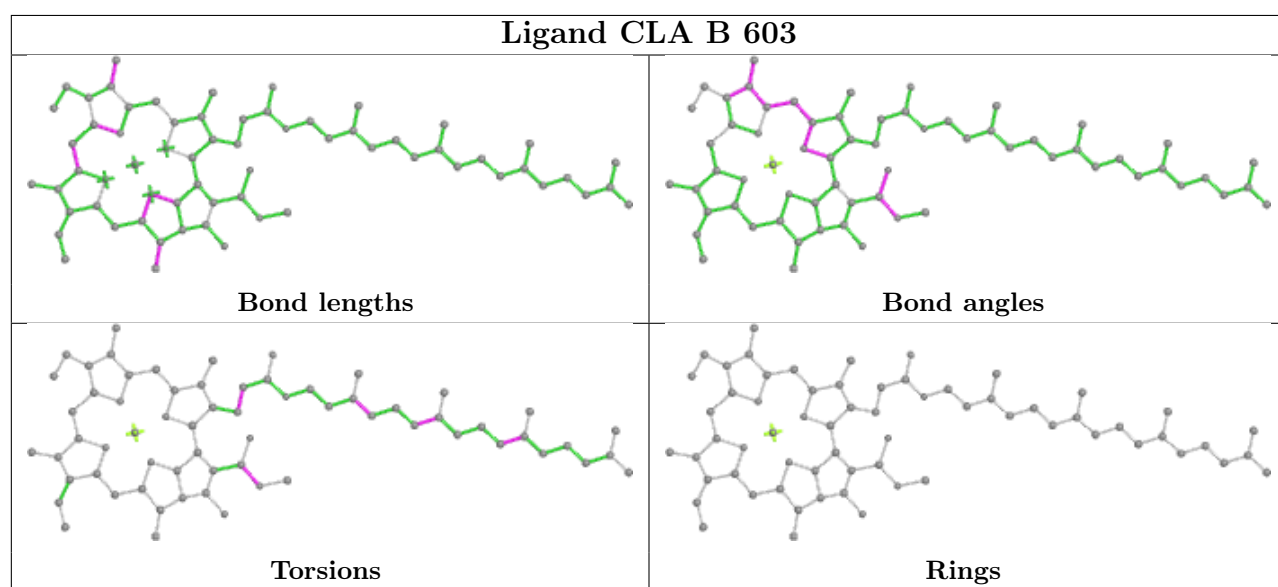
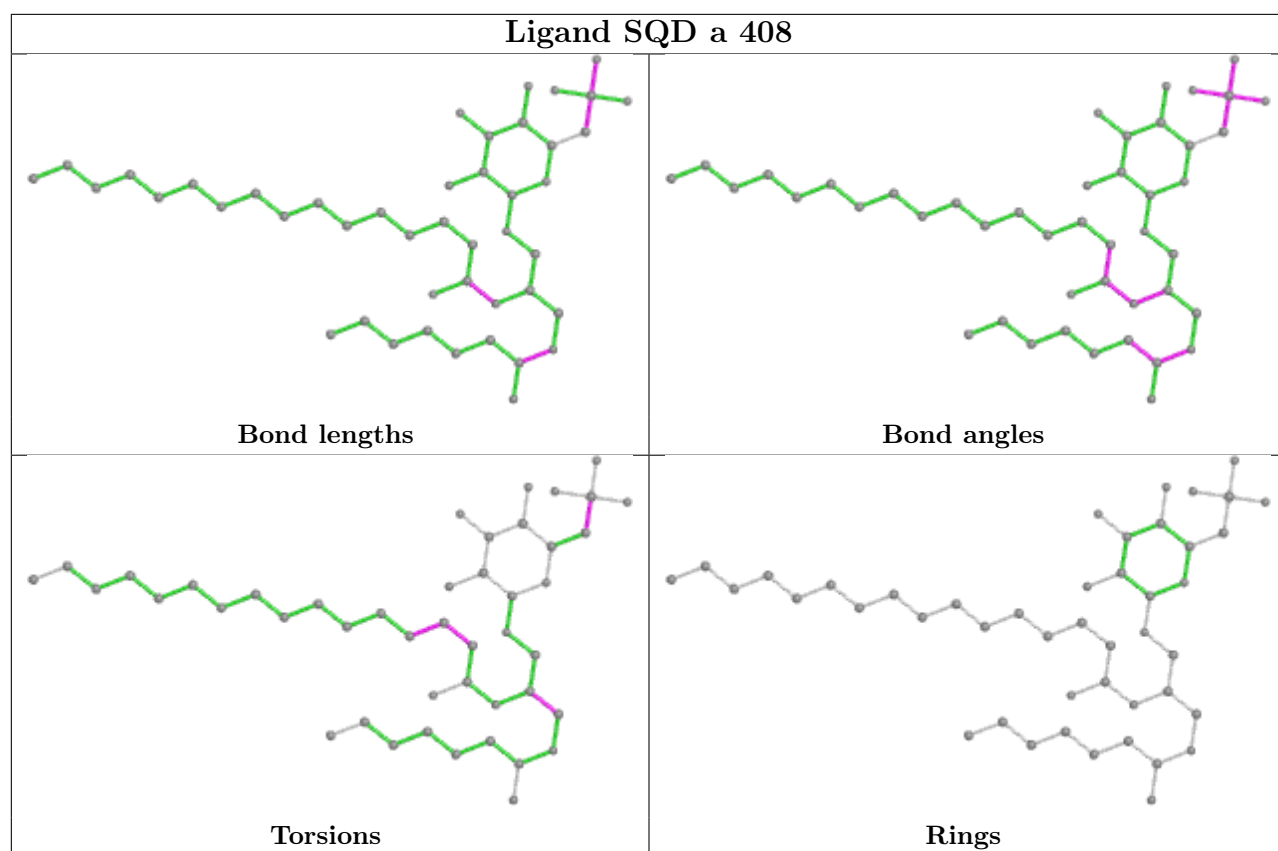
Ligand WVN b 617

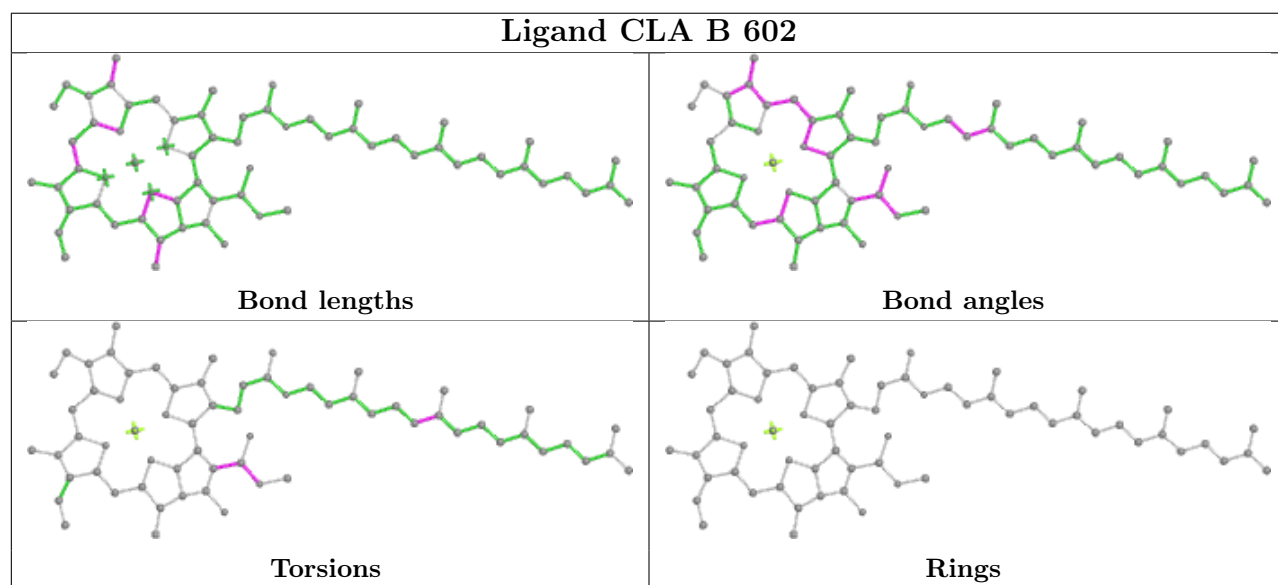
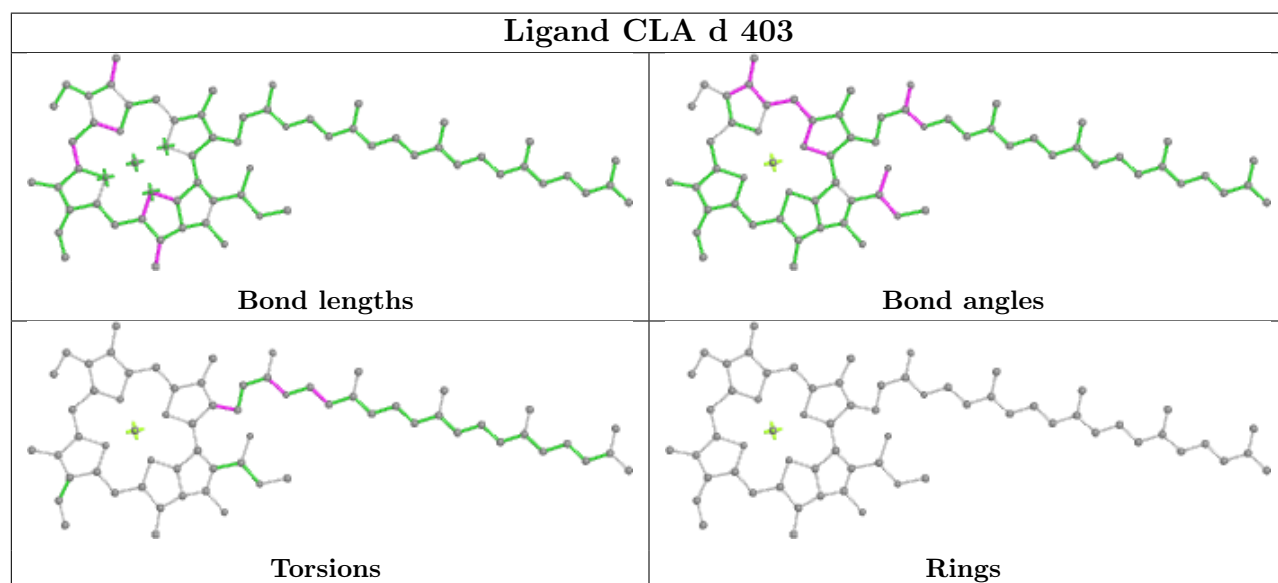
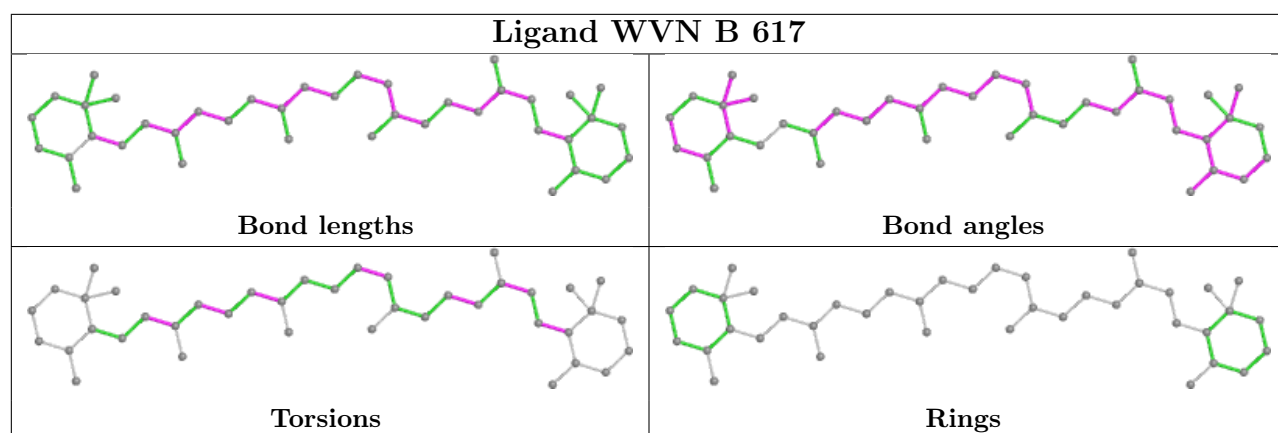




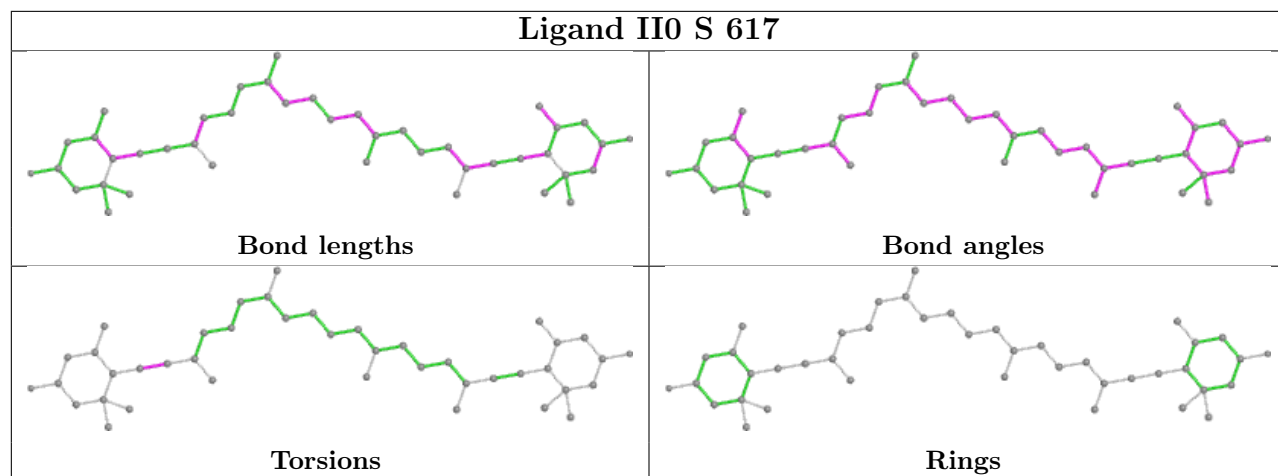




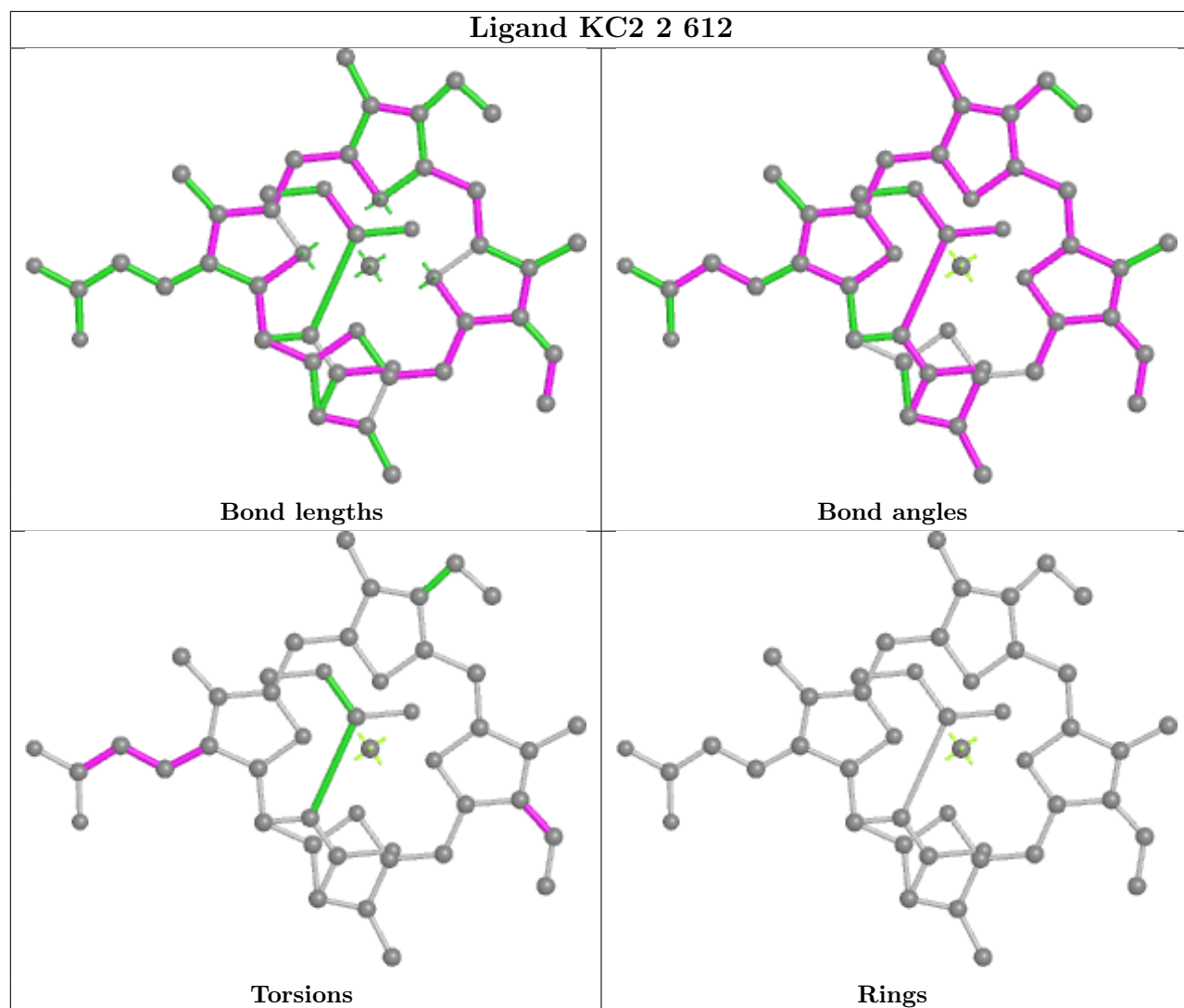




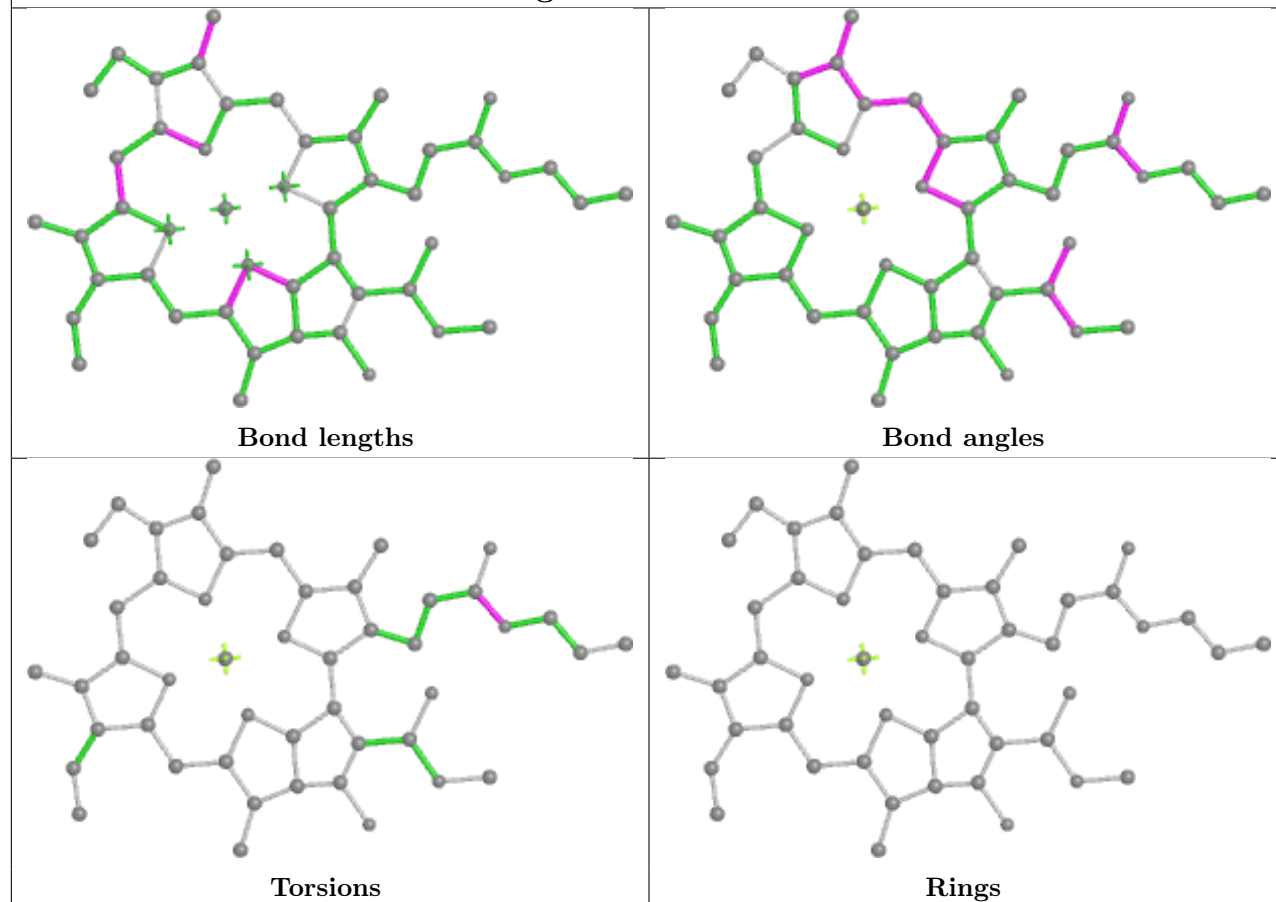
Ligand II0 S 617



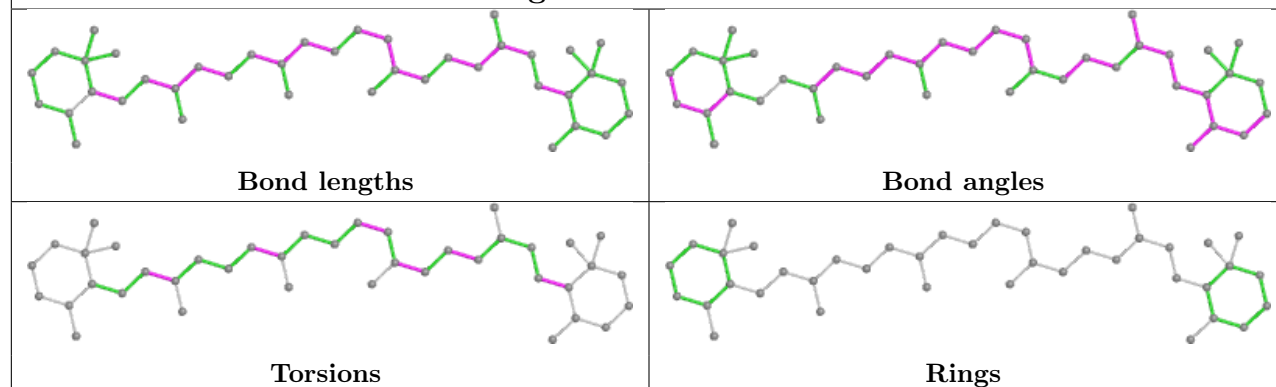
Ligand KC2 2 612



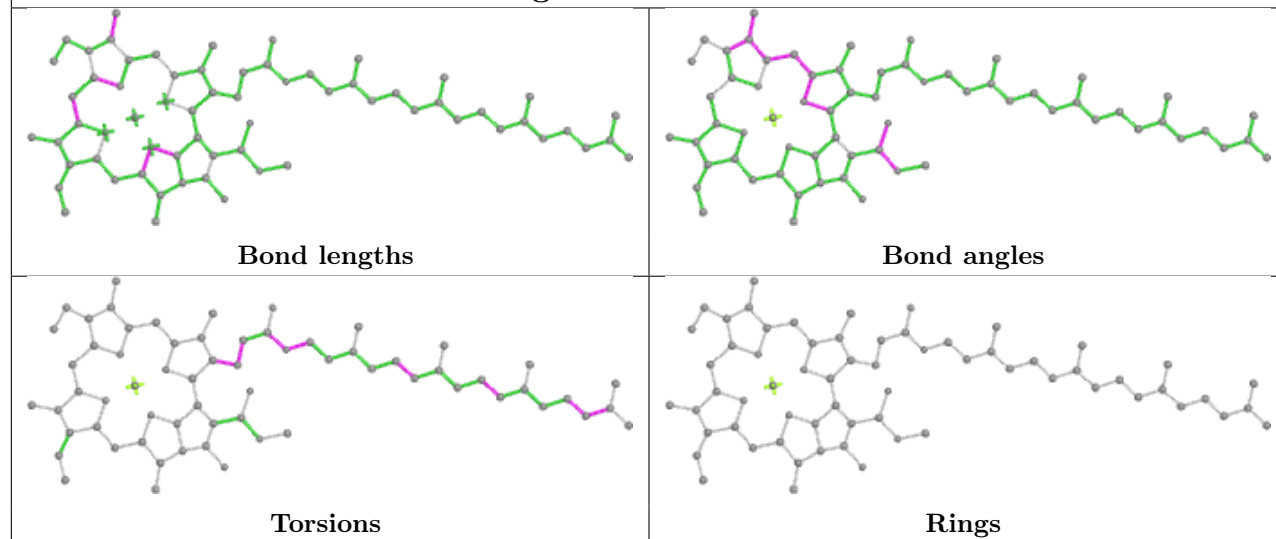
Ligand CLA 2 609



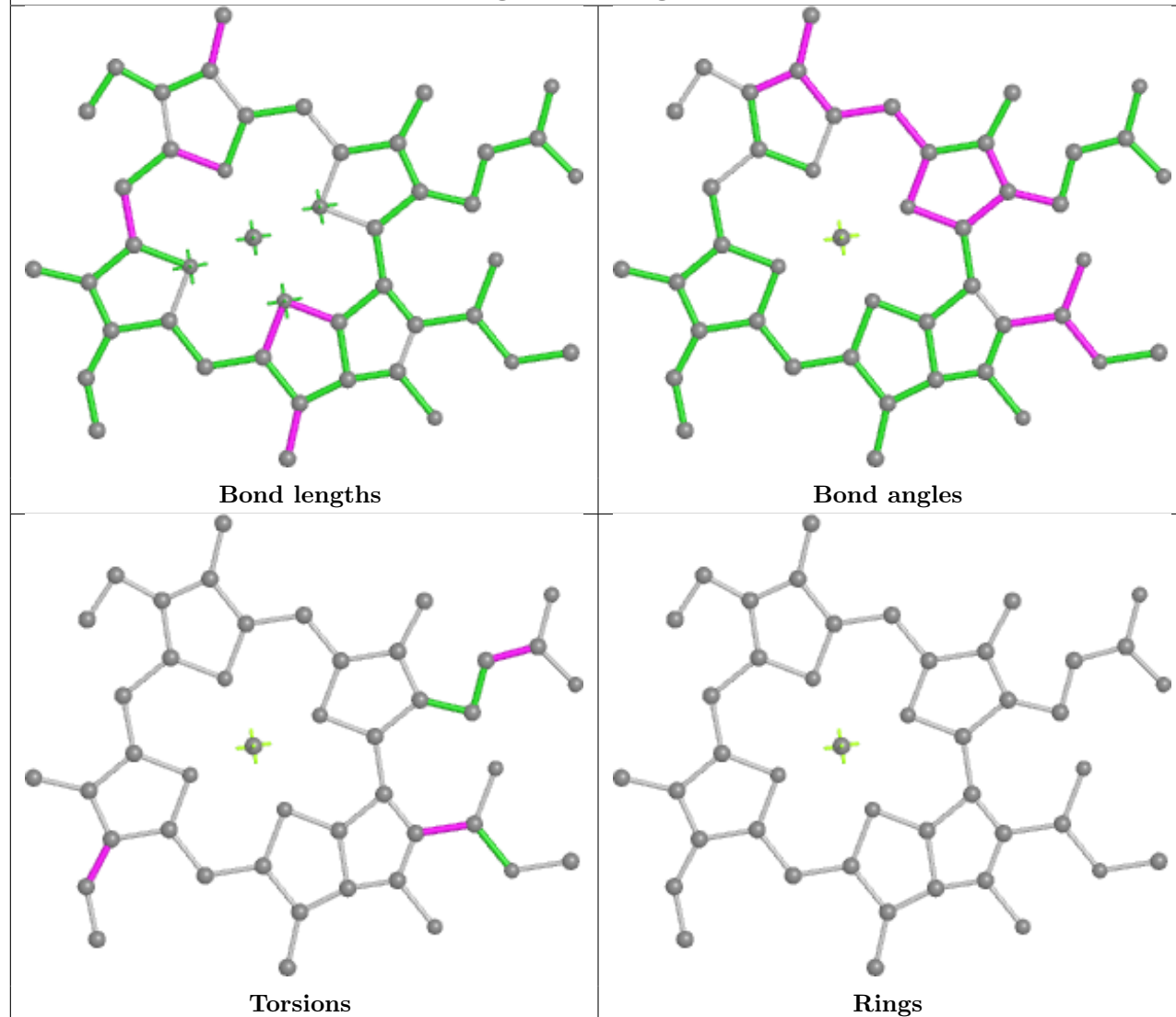
Ligand WVN c 529



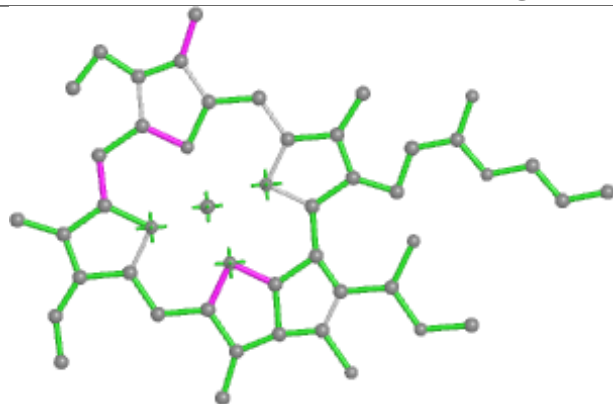
Ligand CLA B 615



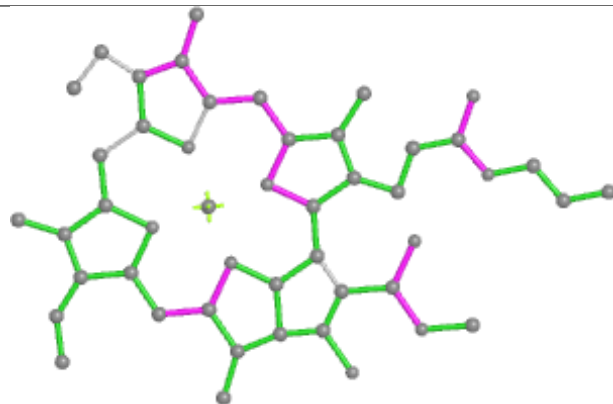
Ligand CLA g 302



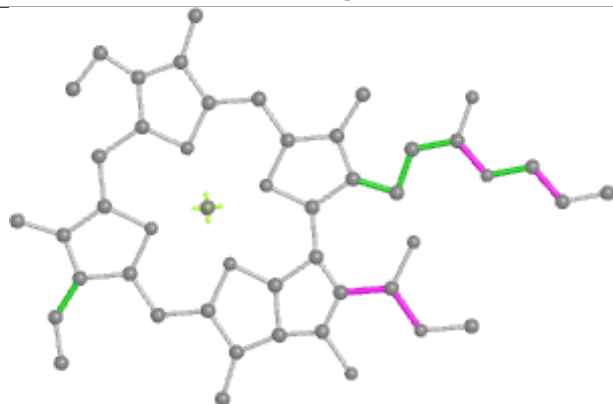
Ligand CLA N 614



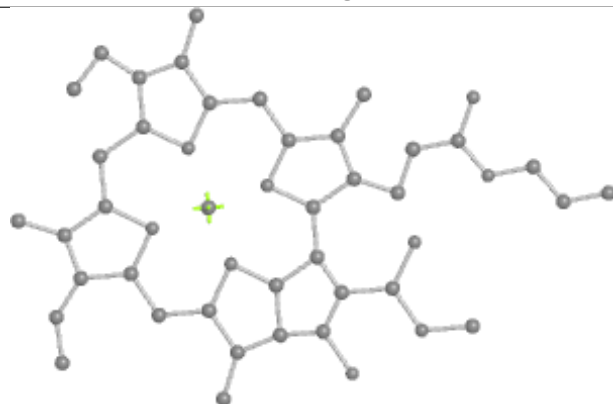
Bond lengths



Bond angles

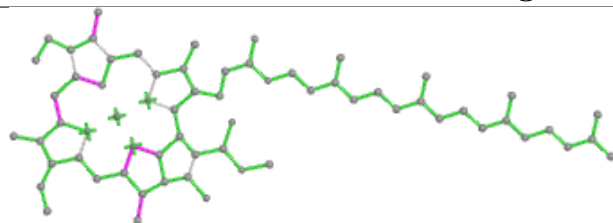


Torsions

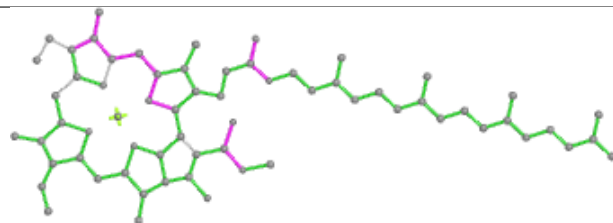


Rings

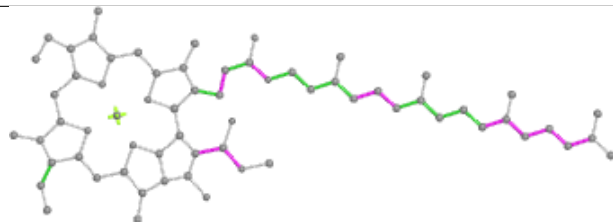
Ligand CLA S 604



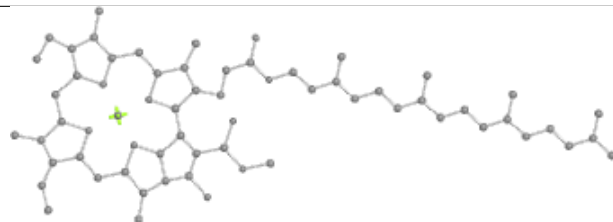
Bond lengths



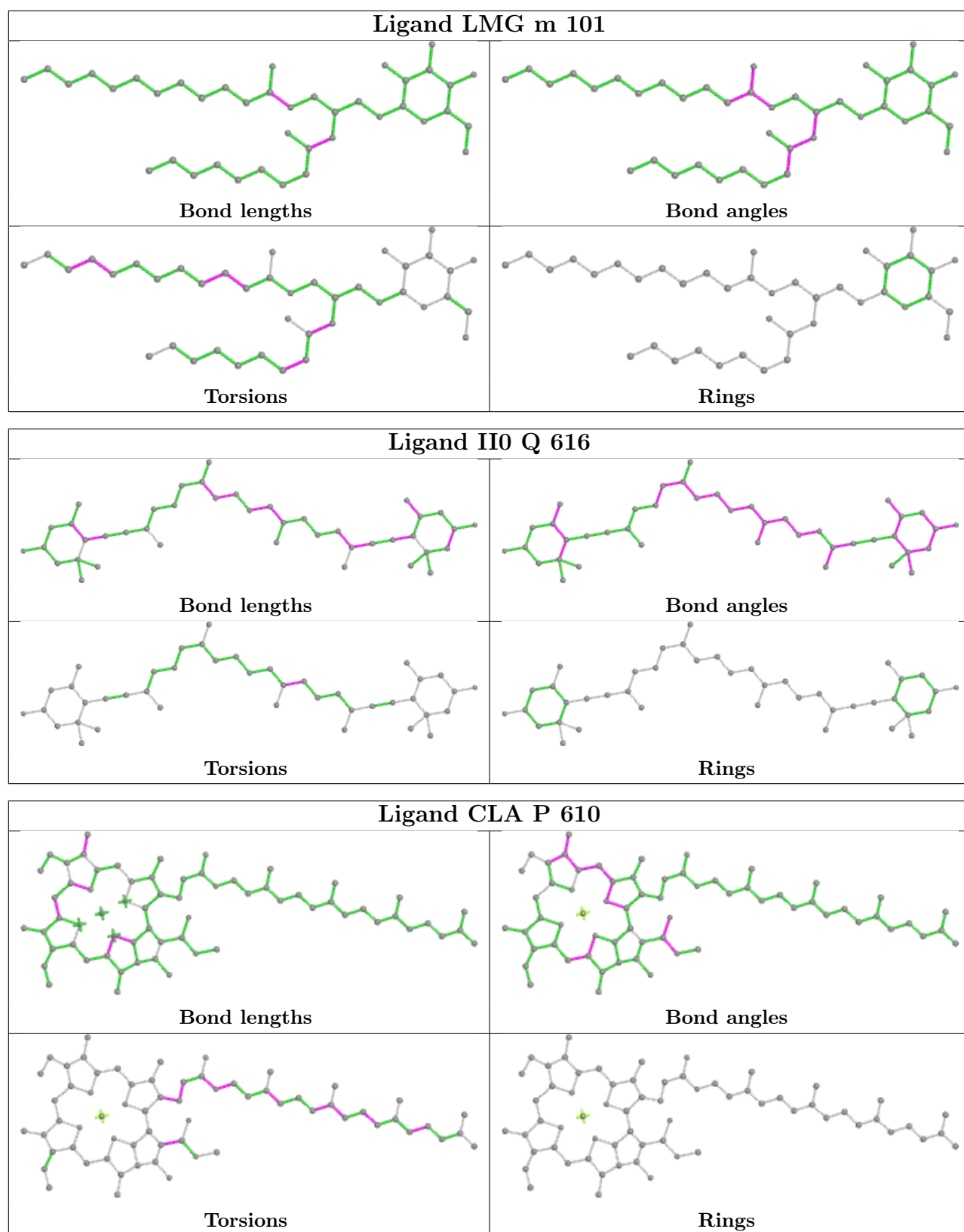
Bond angles



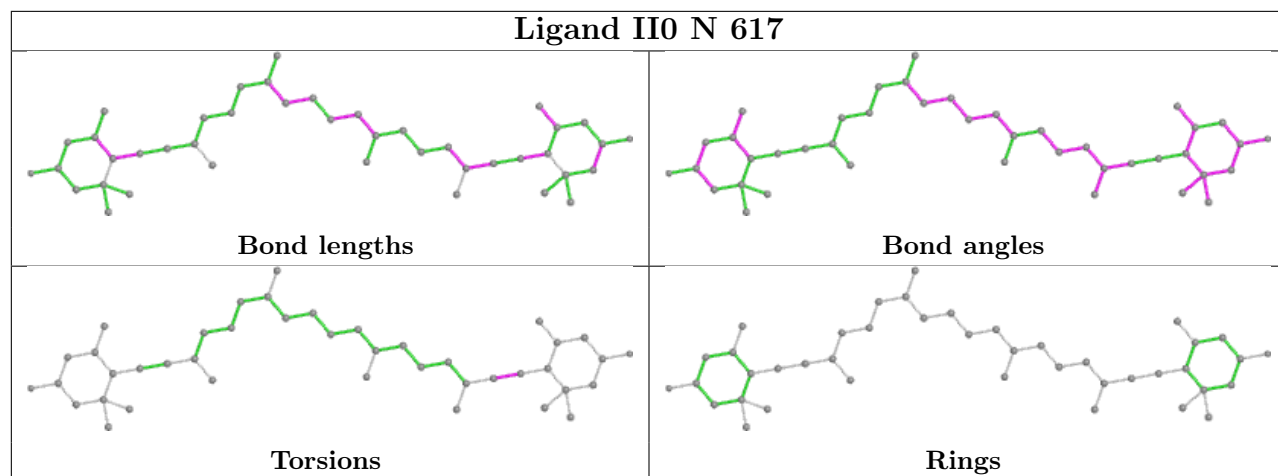
Torsions



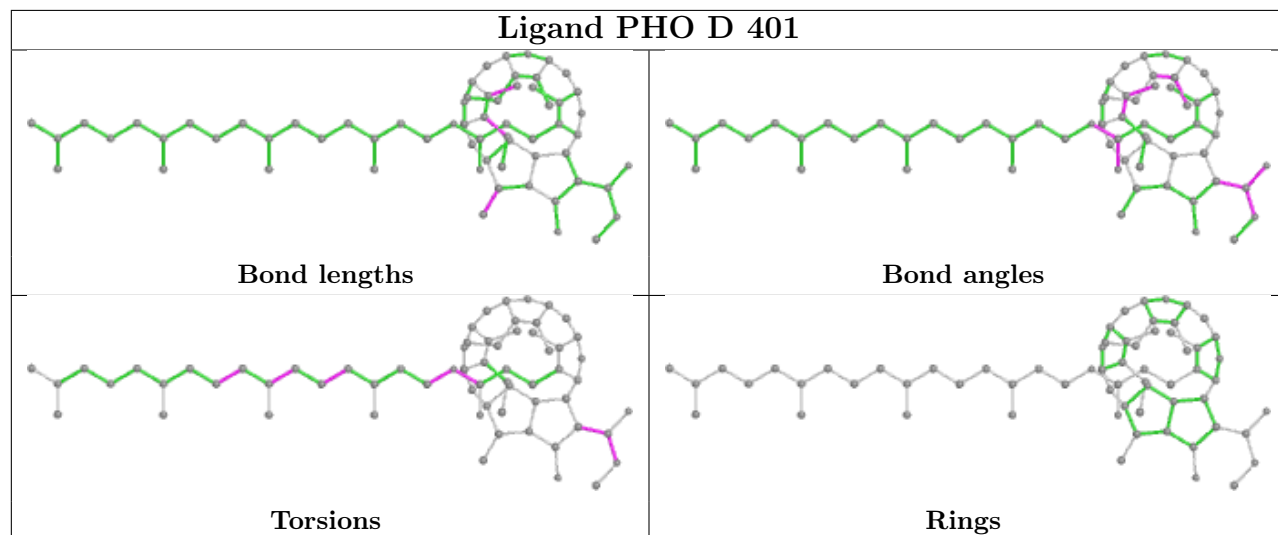
Rings



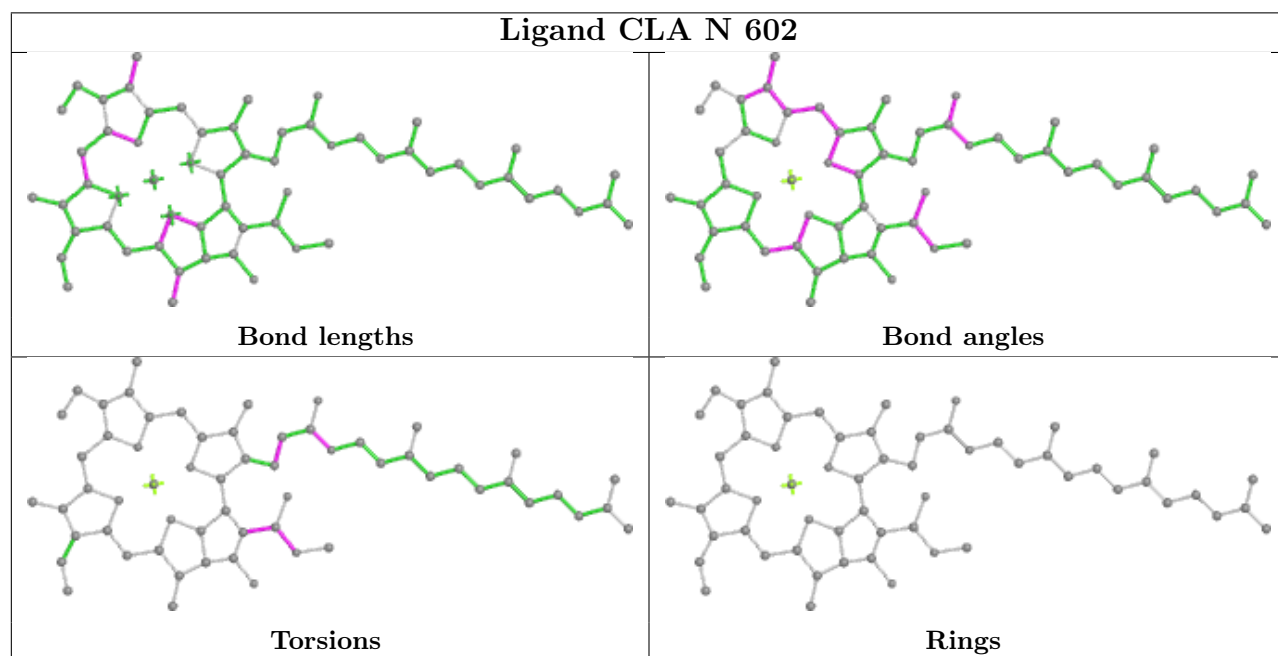
Ligand II0 N 617

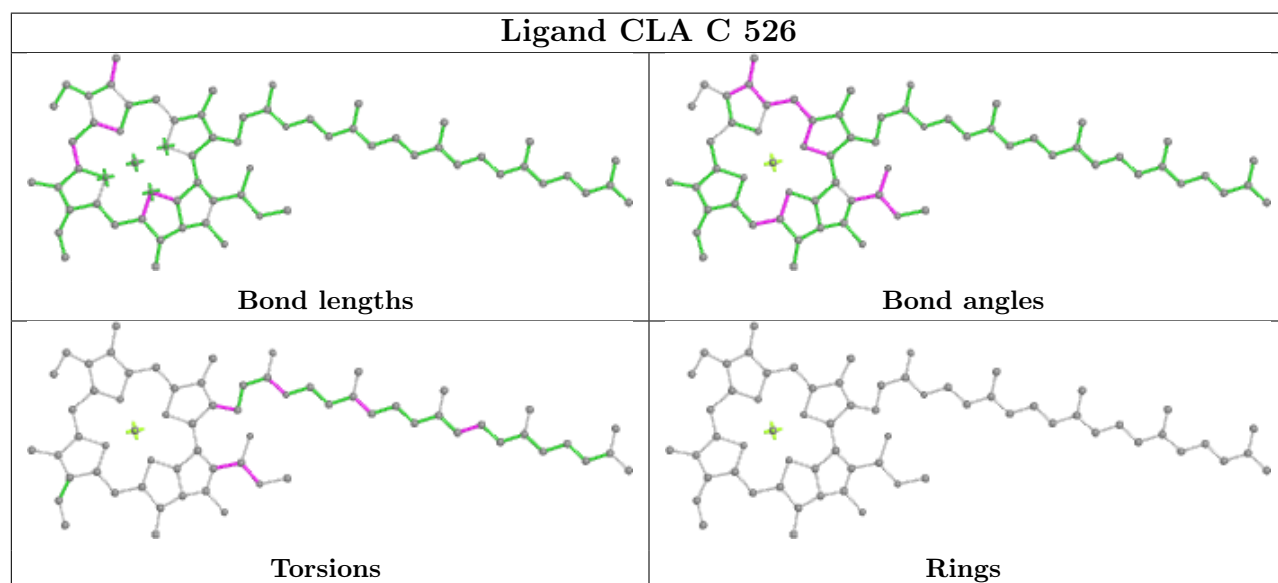
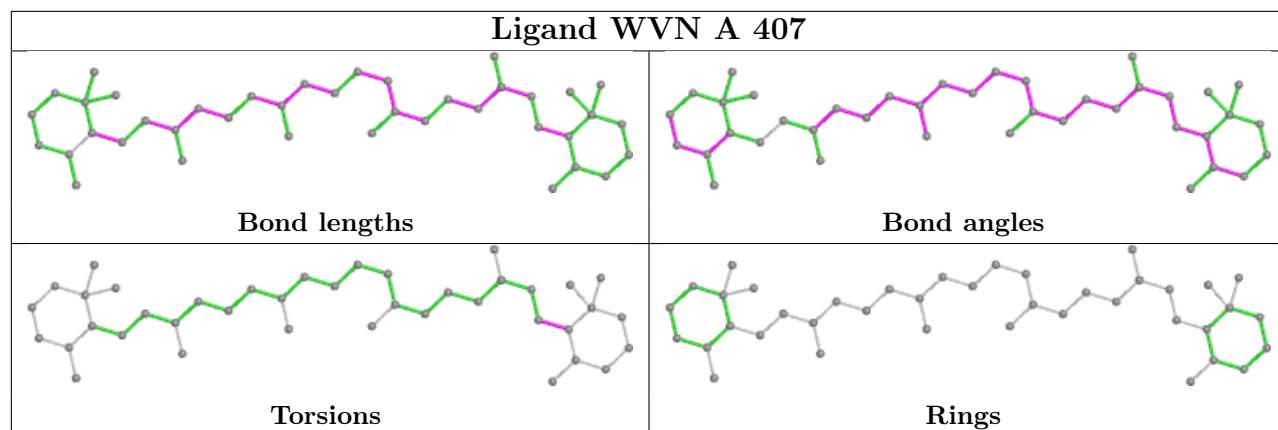


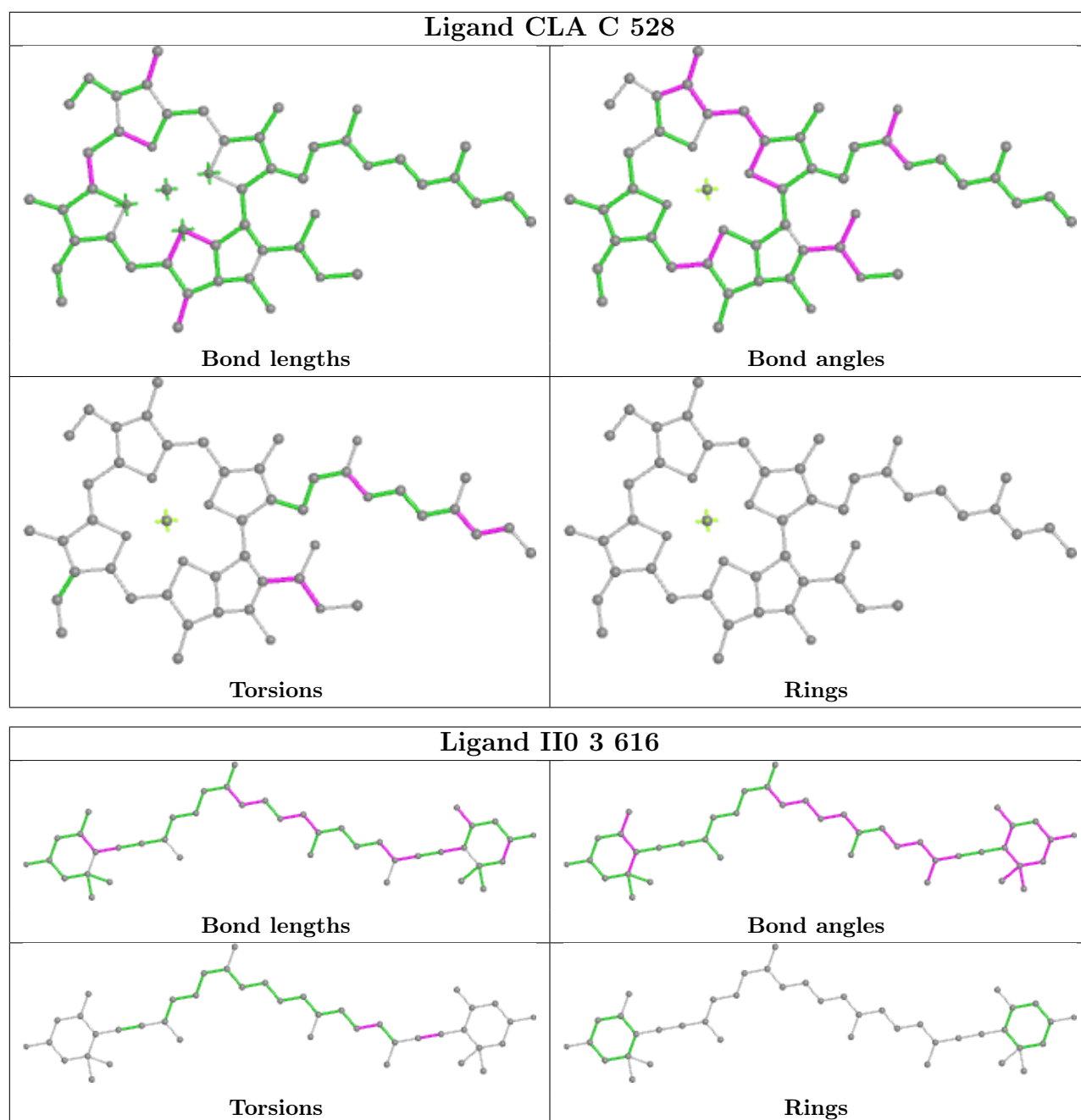
Ligand PHO D 401

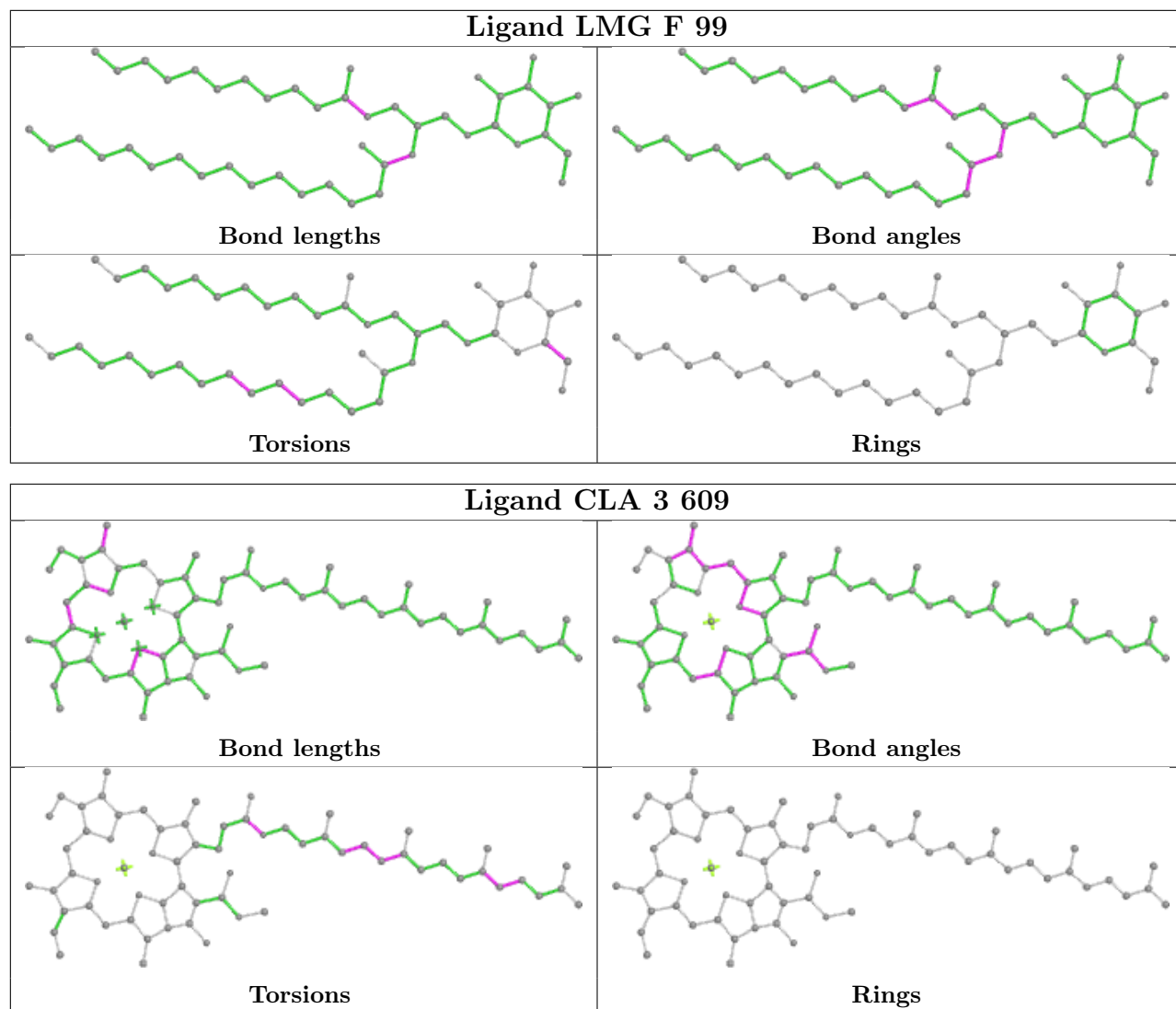


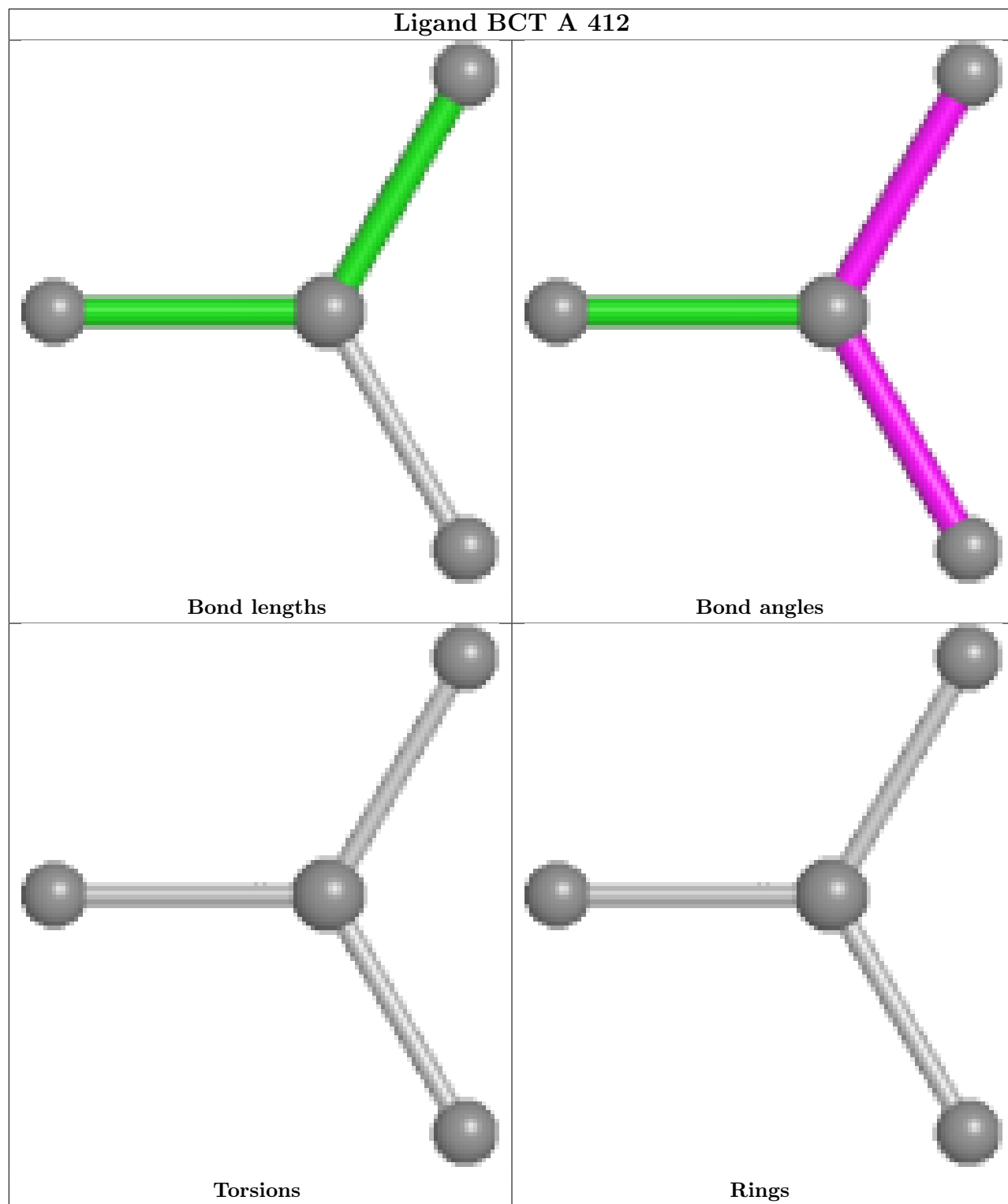
Ligand CLA N 602



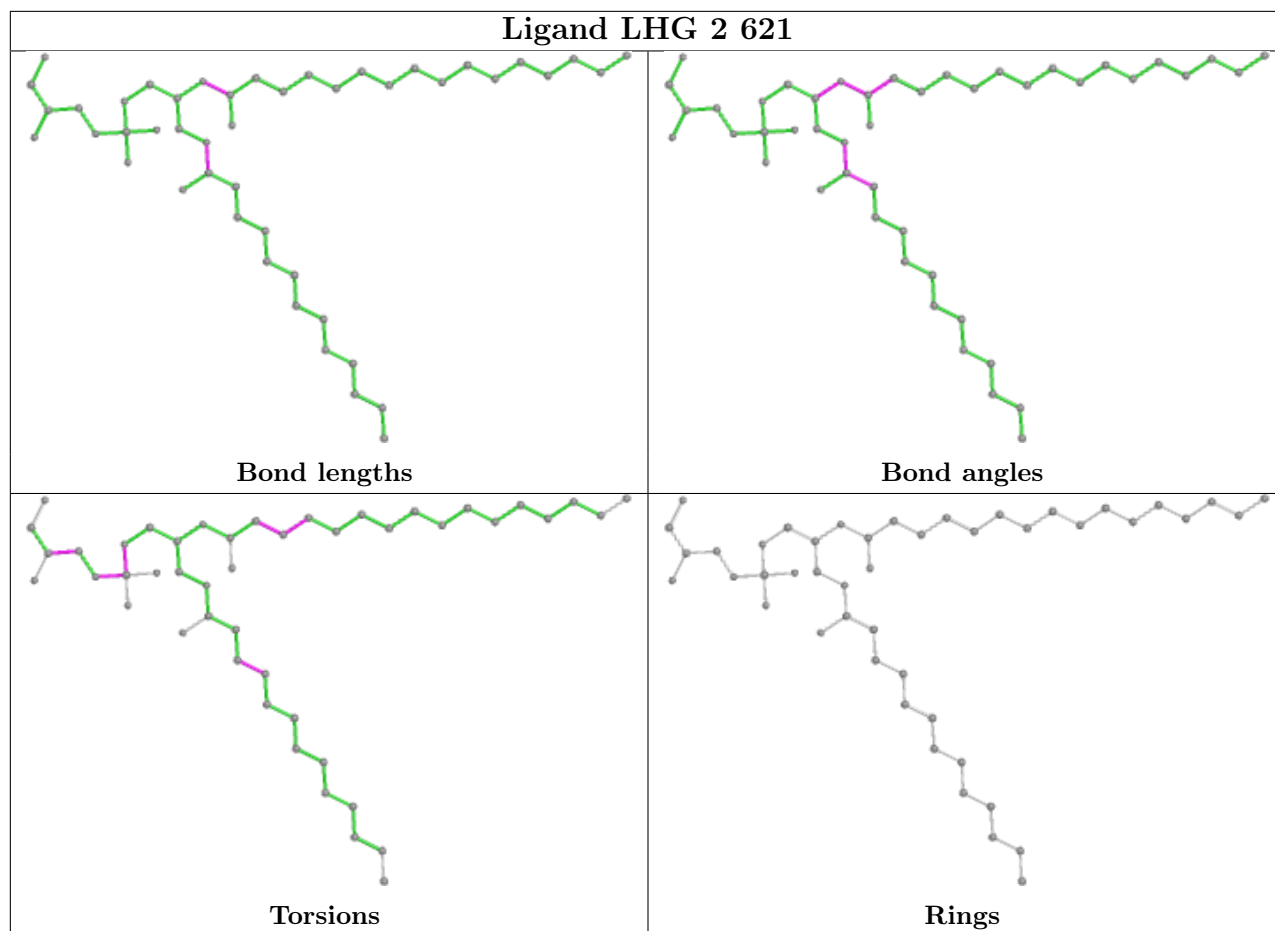




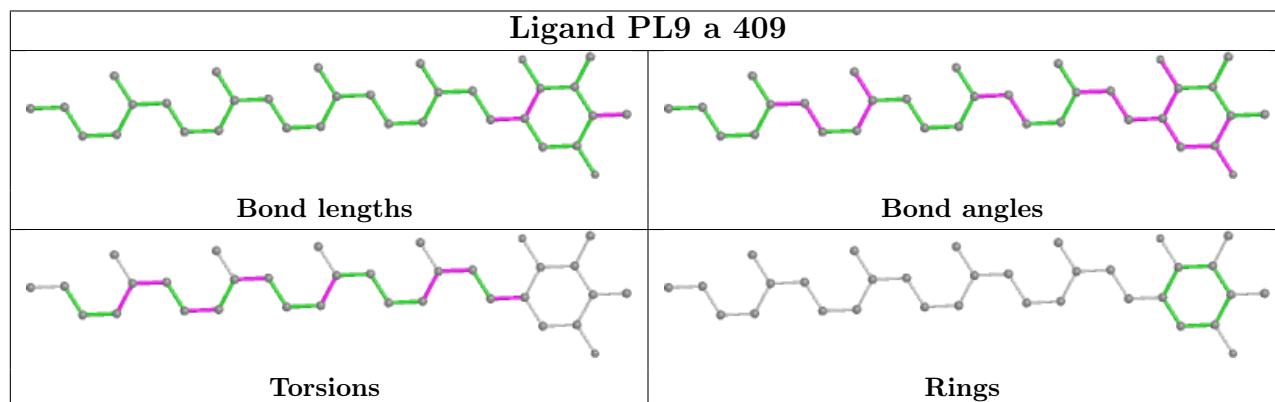


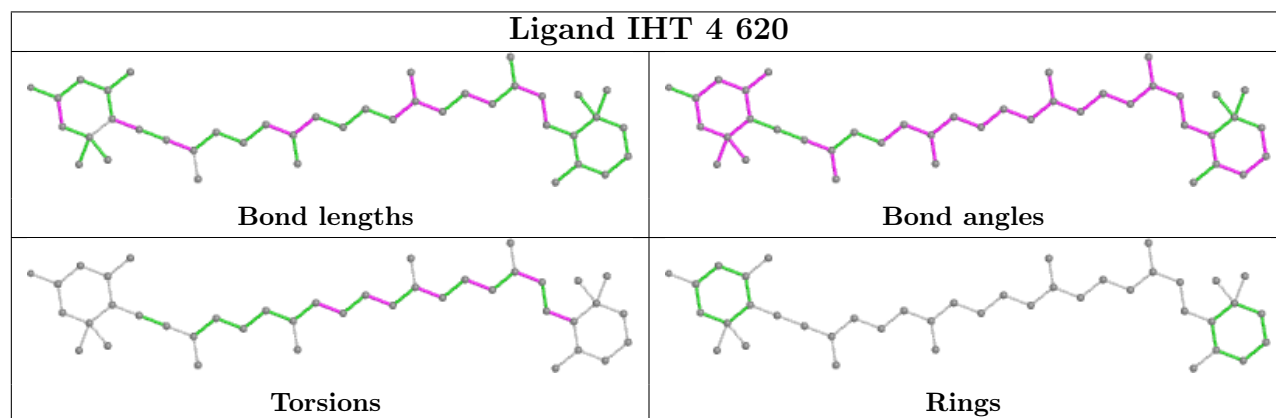
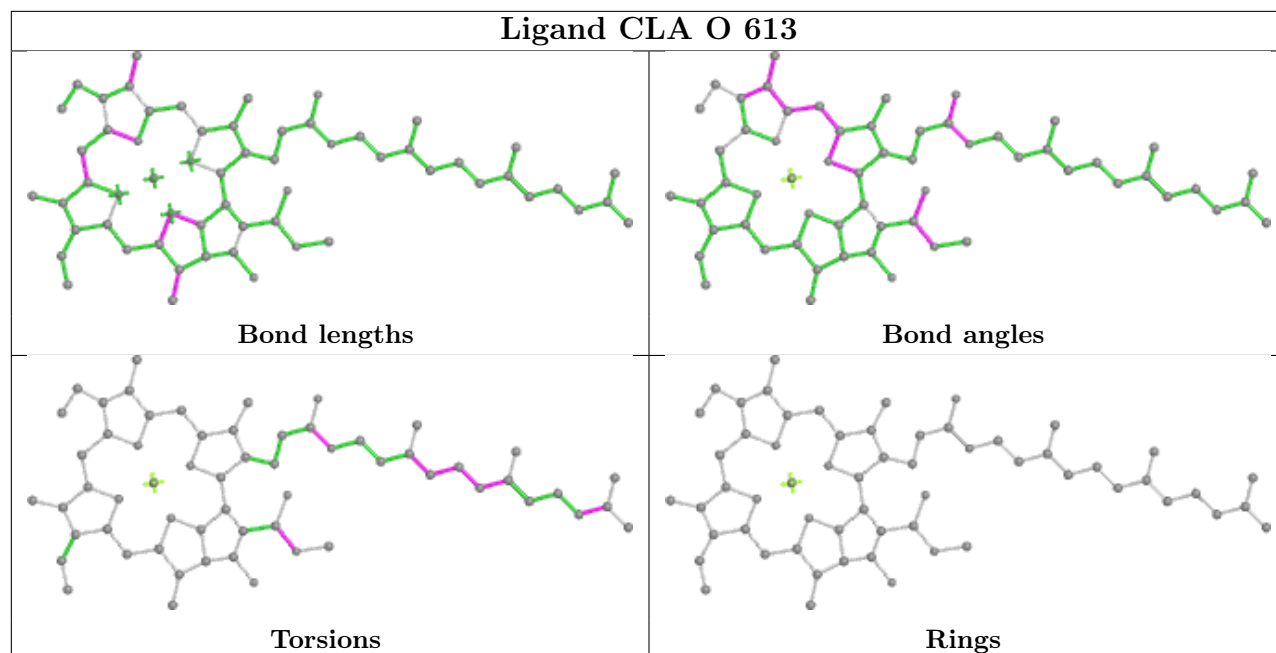


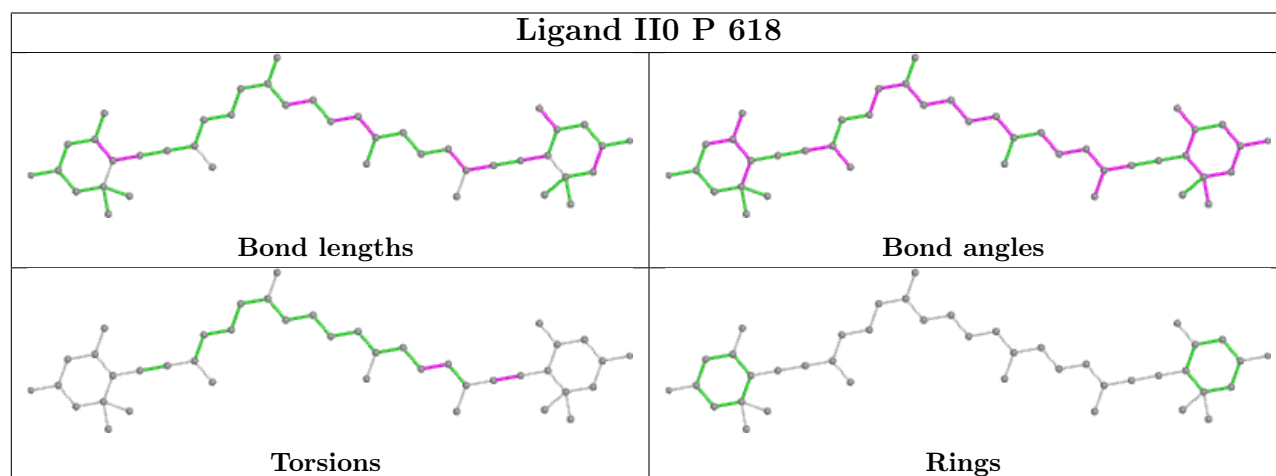
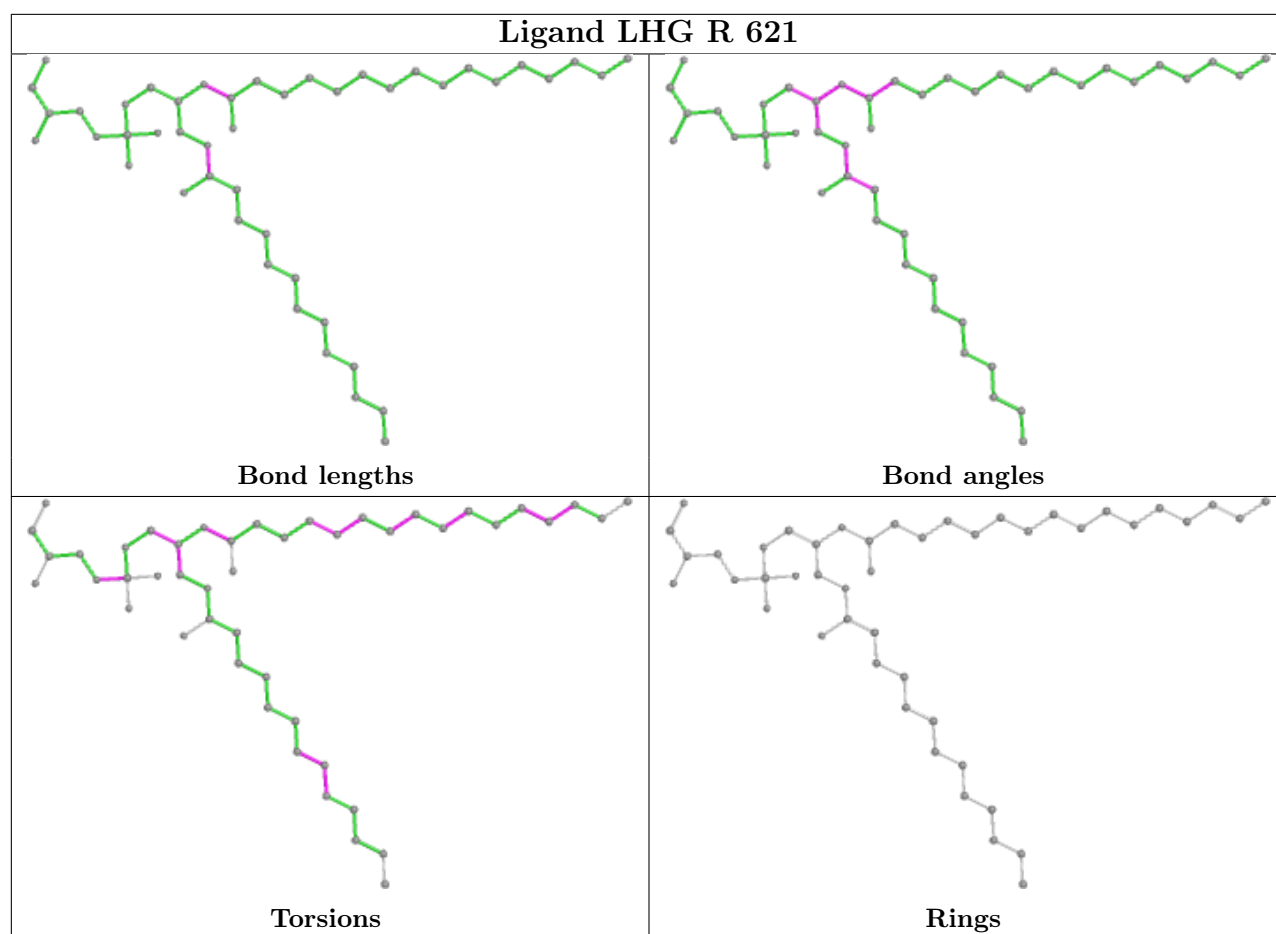
Ligand LHG 2 621

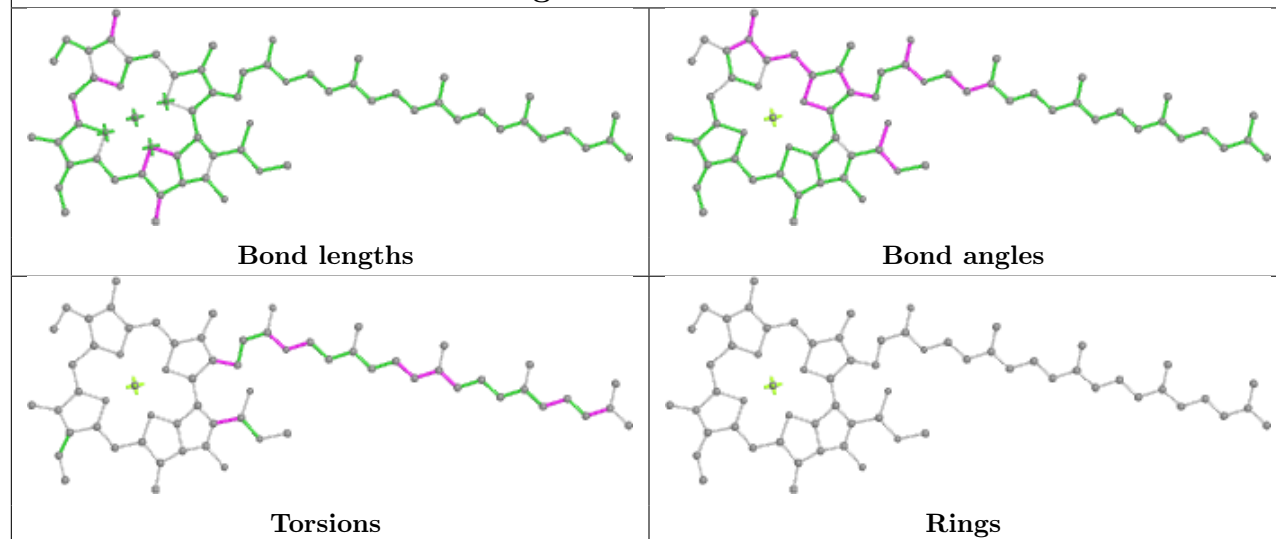
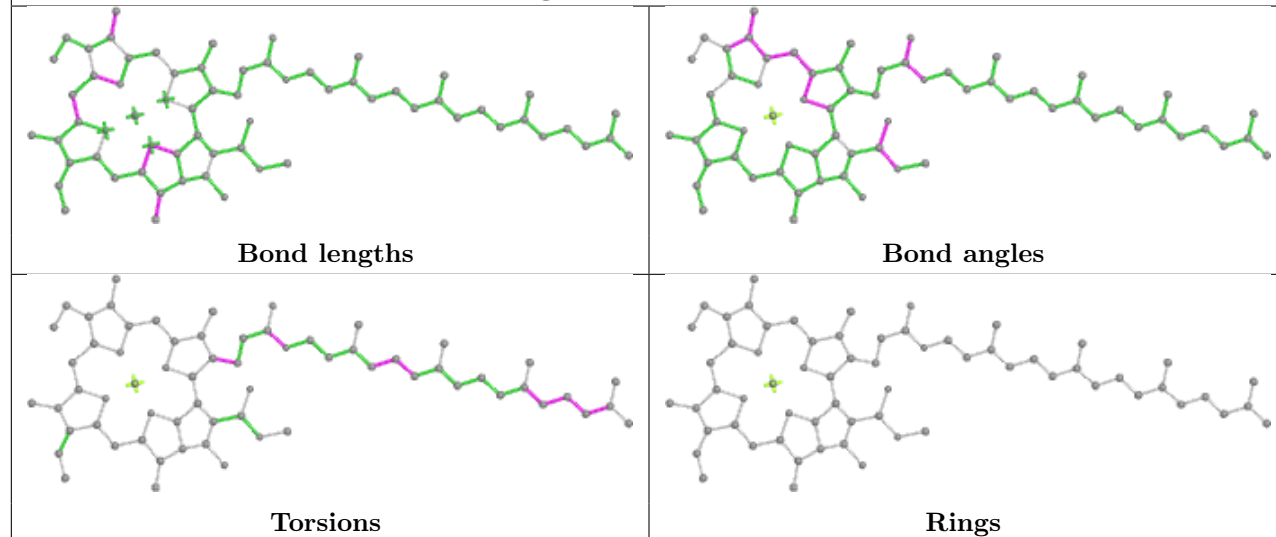


Ligand PL9 a 409

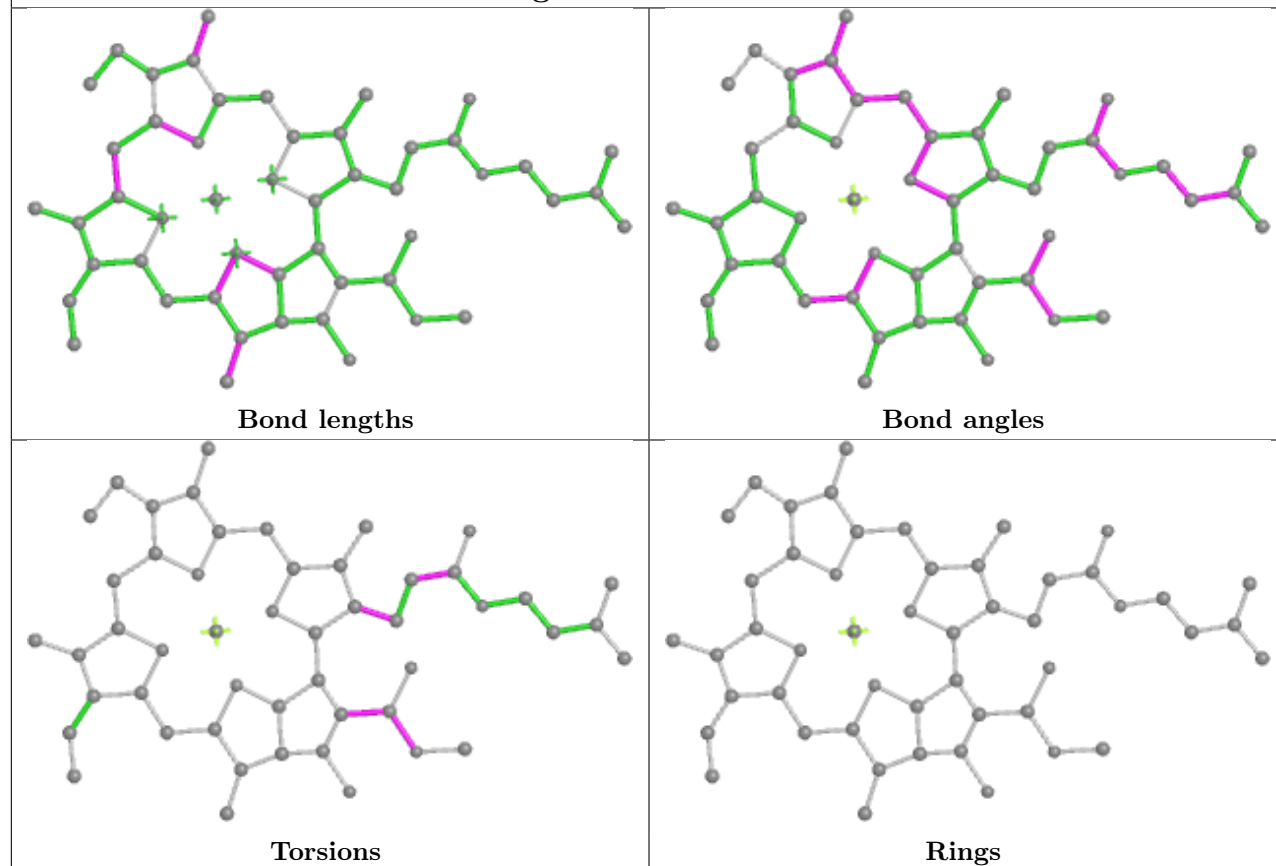




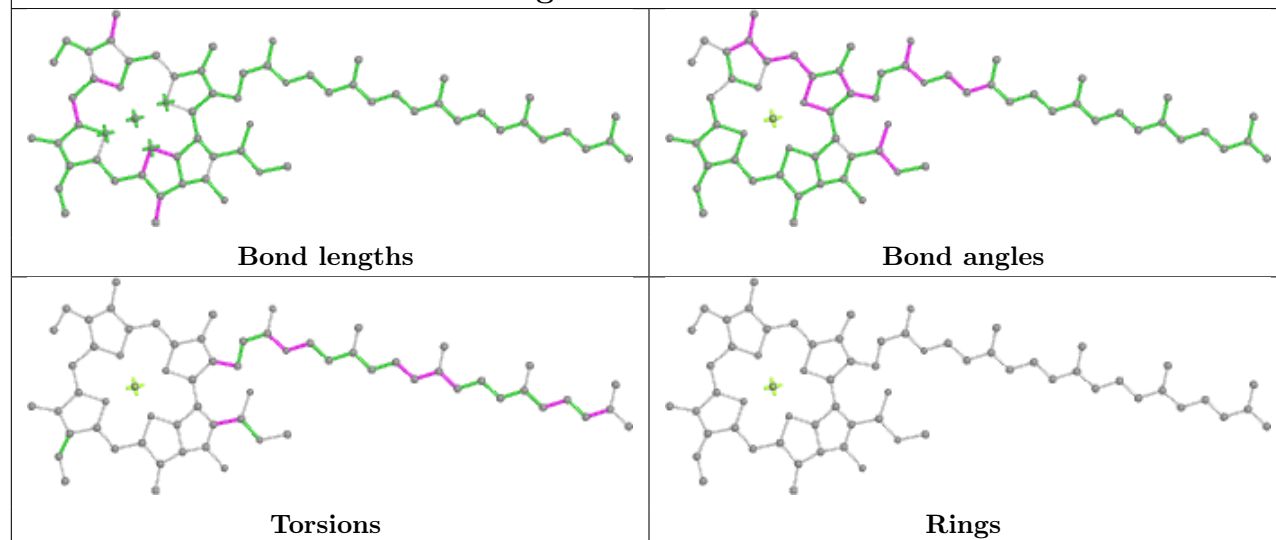


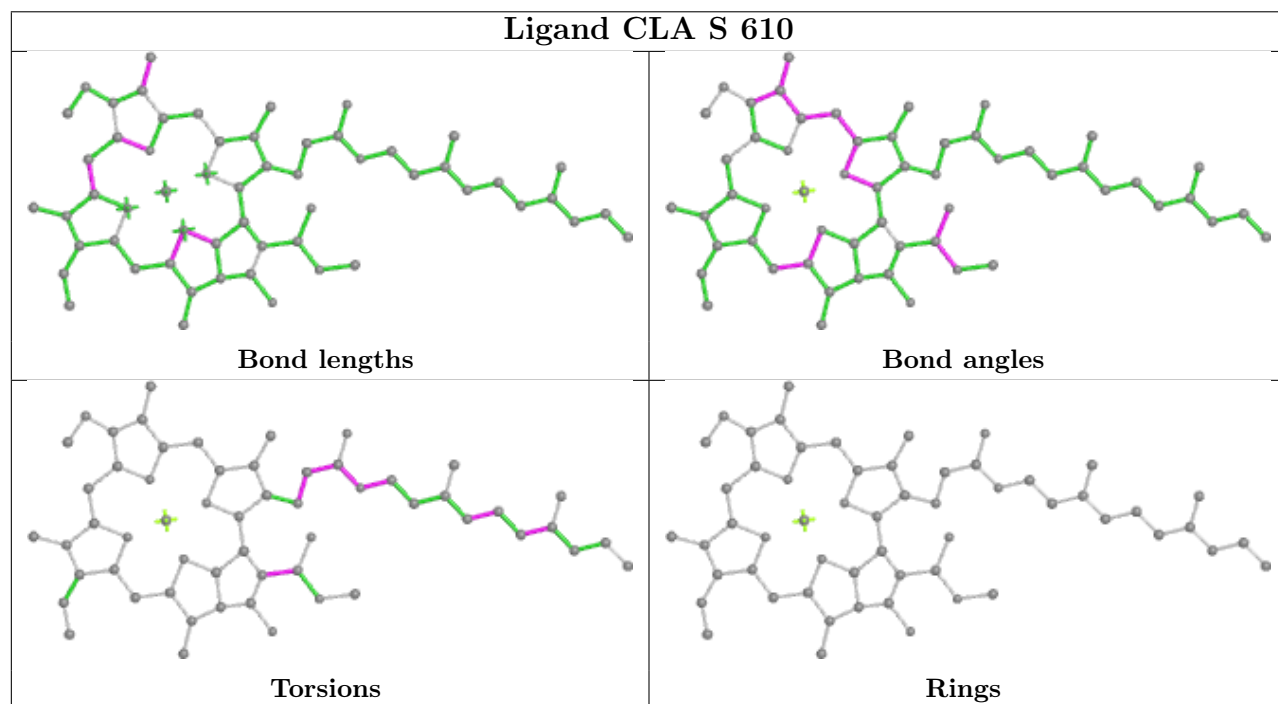
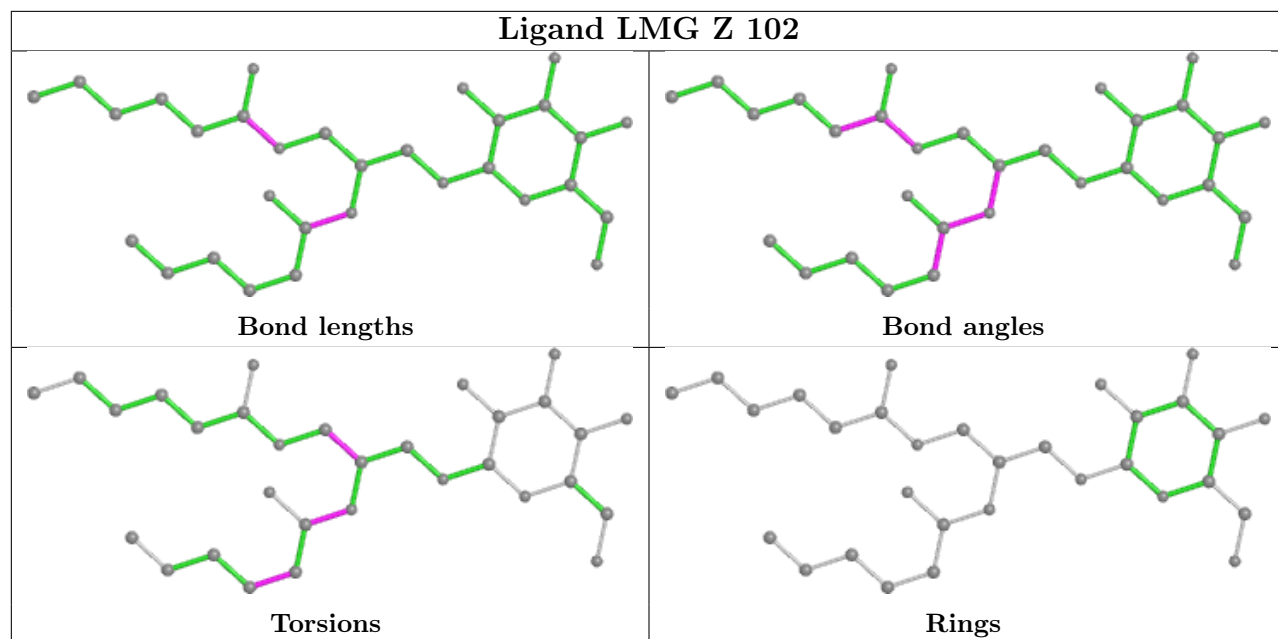
Ligand CLA P 603**Ligand CLA c 527**

Ligand CLA B 601

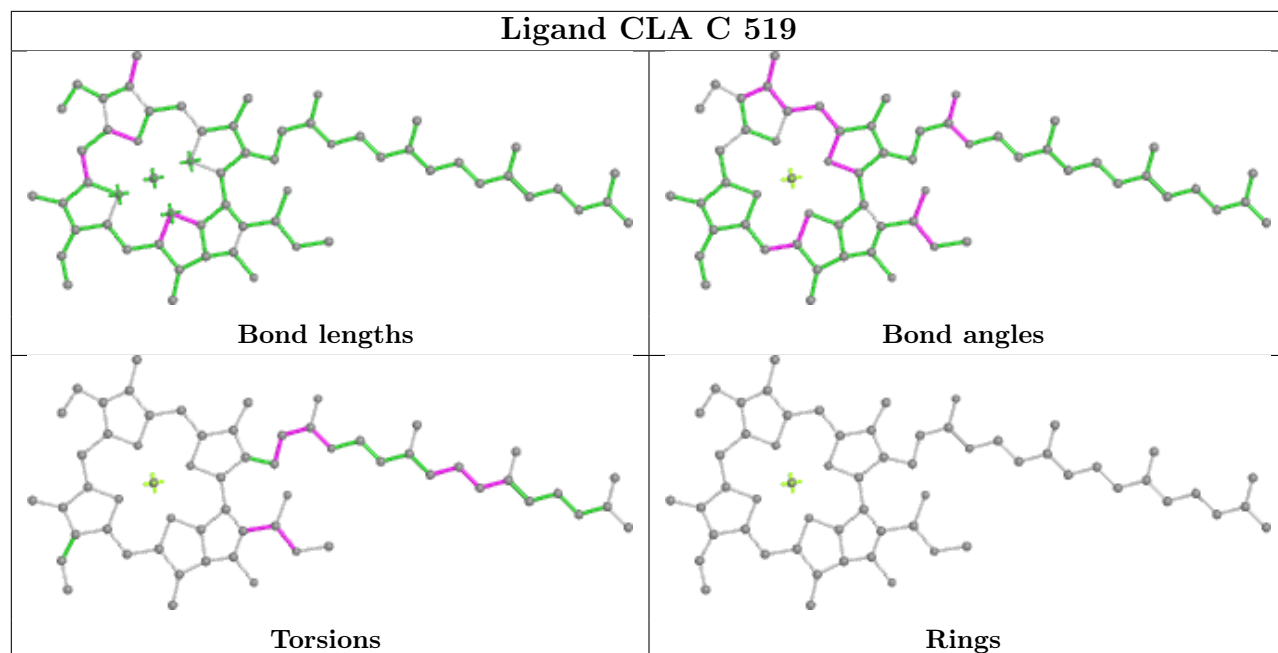


Ligand CLA 3 603

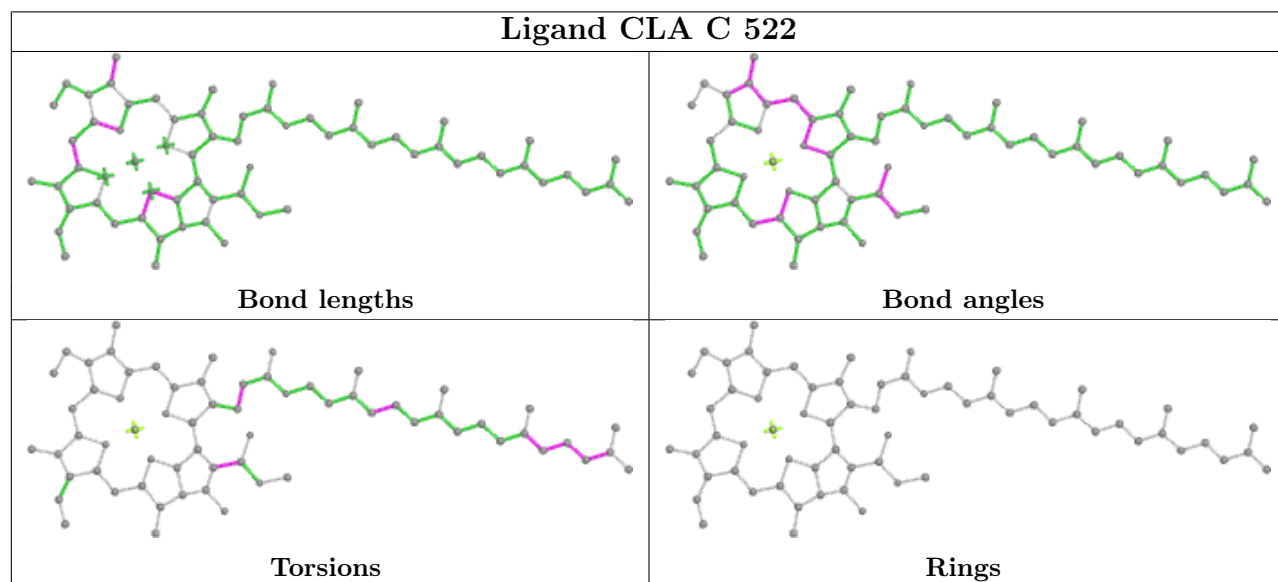


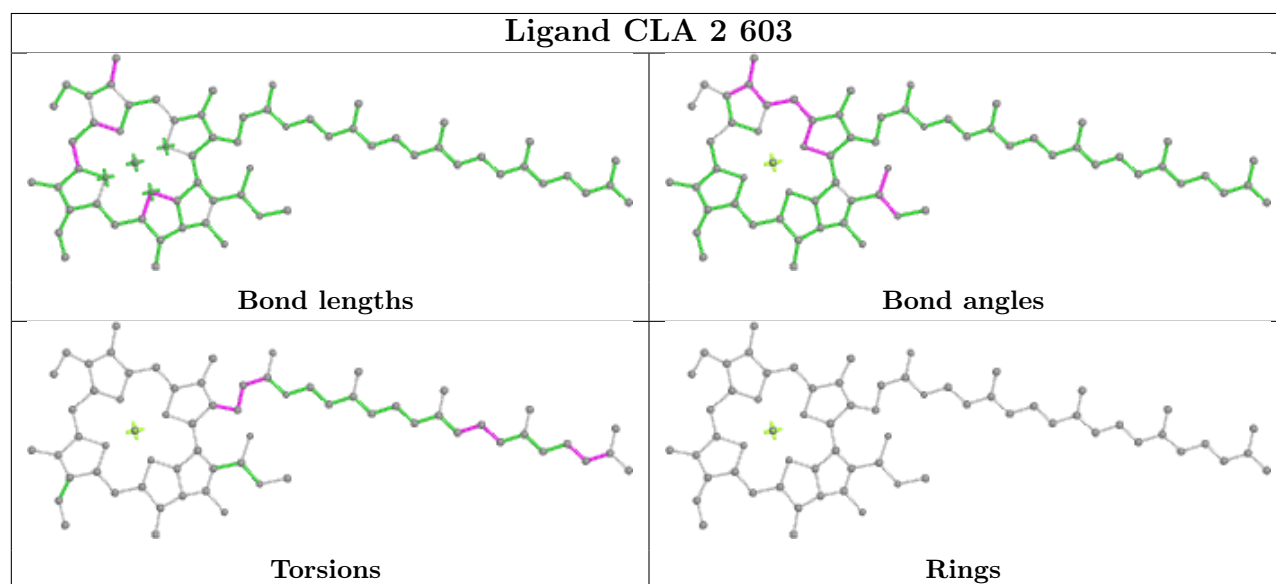
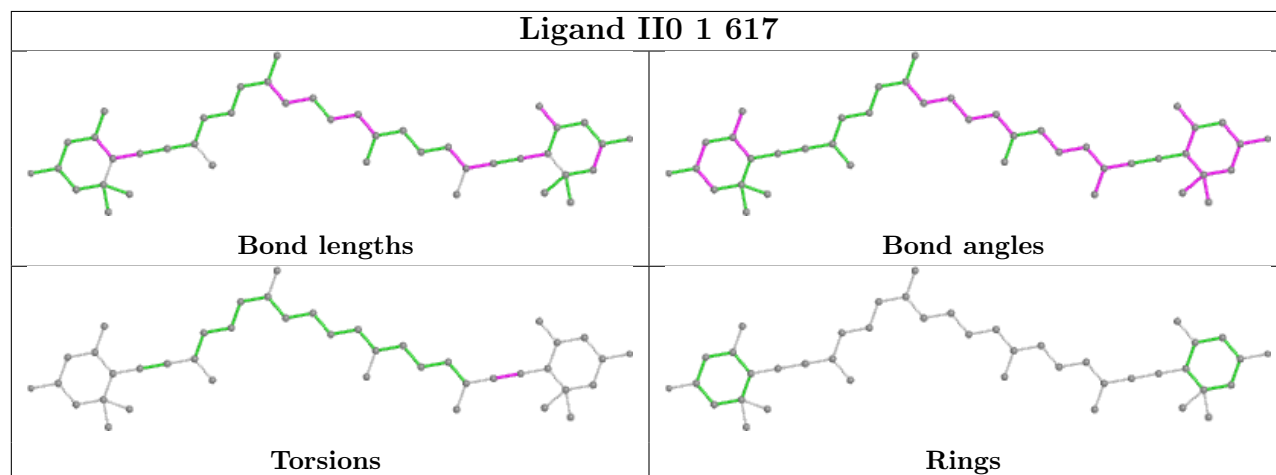
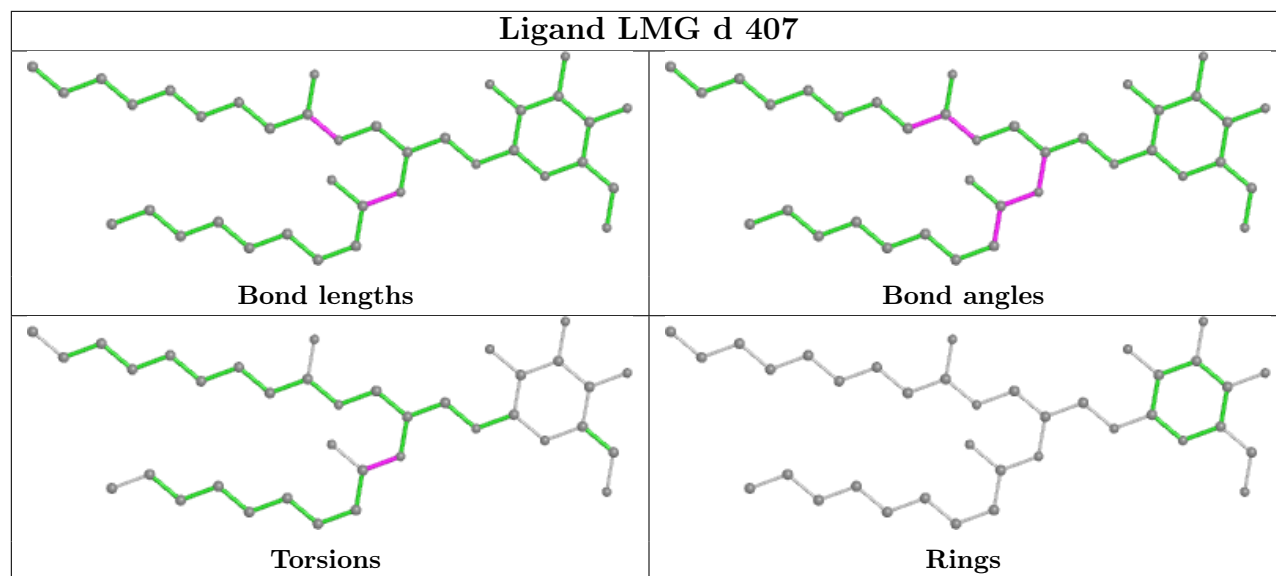


Ligand CLA C 519

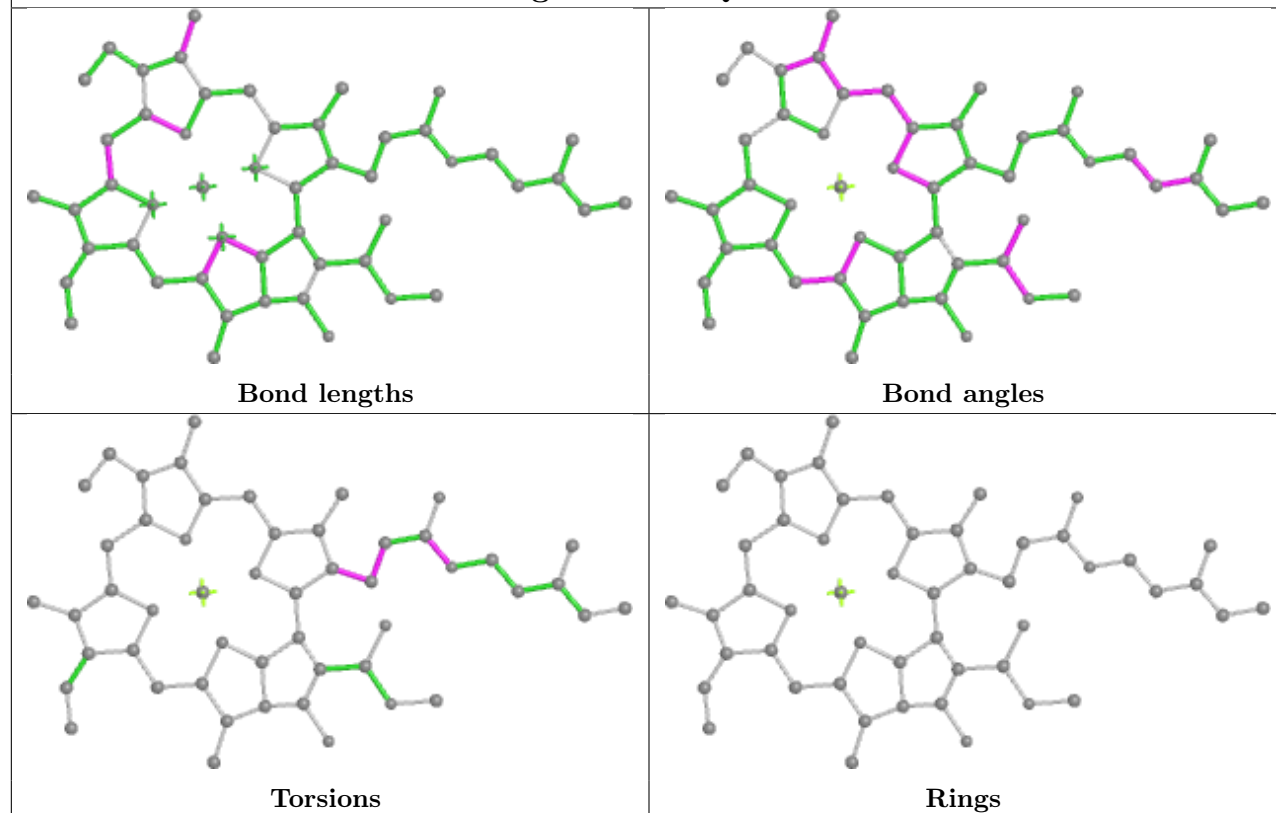


Ligand CLA C 522

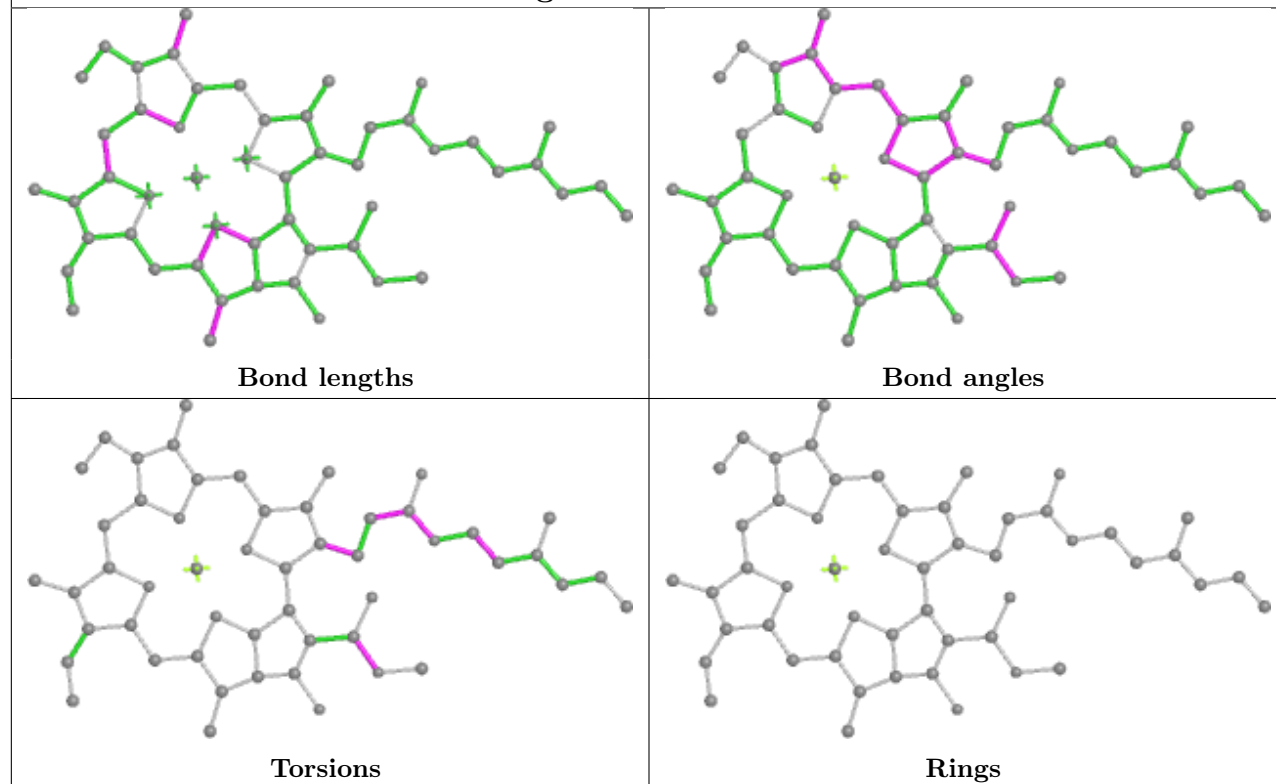


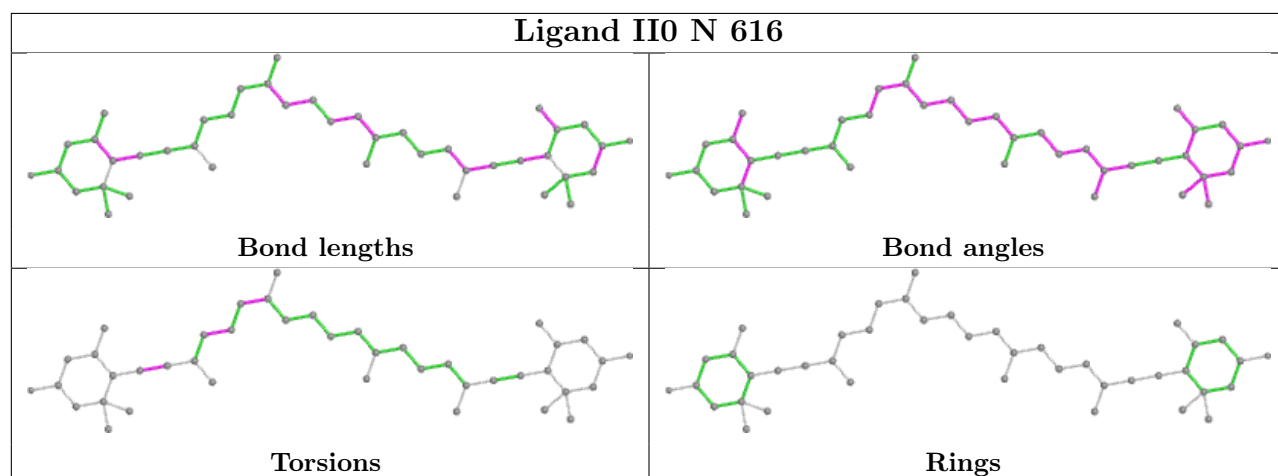
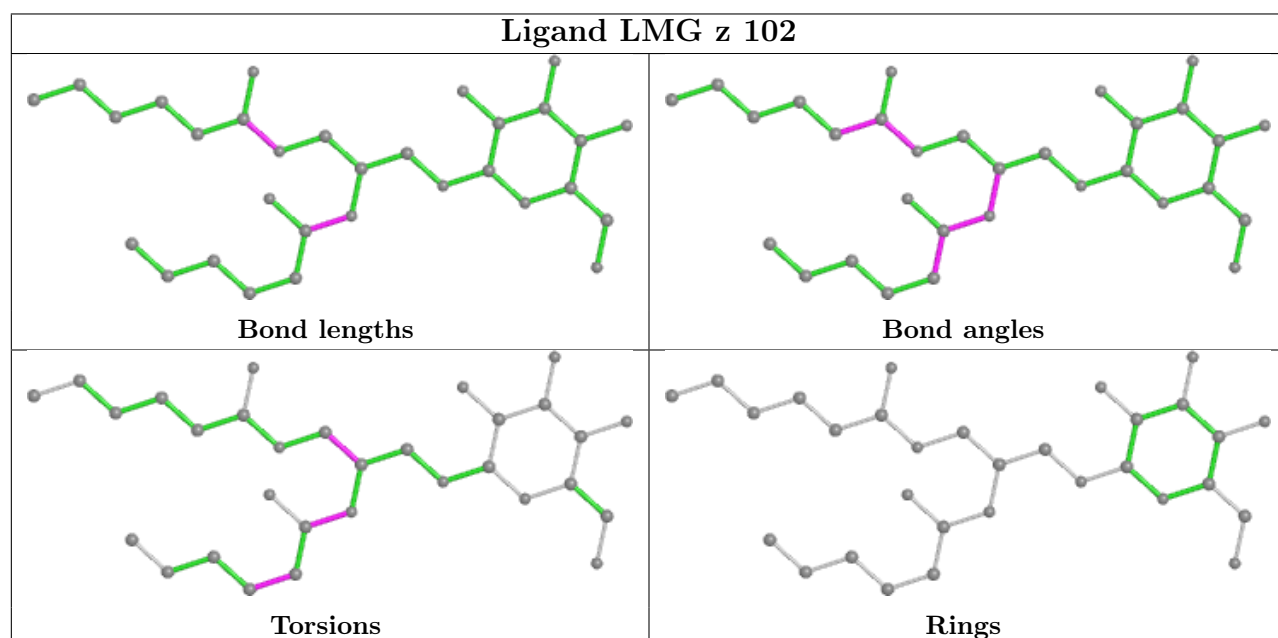
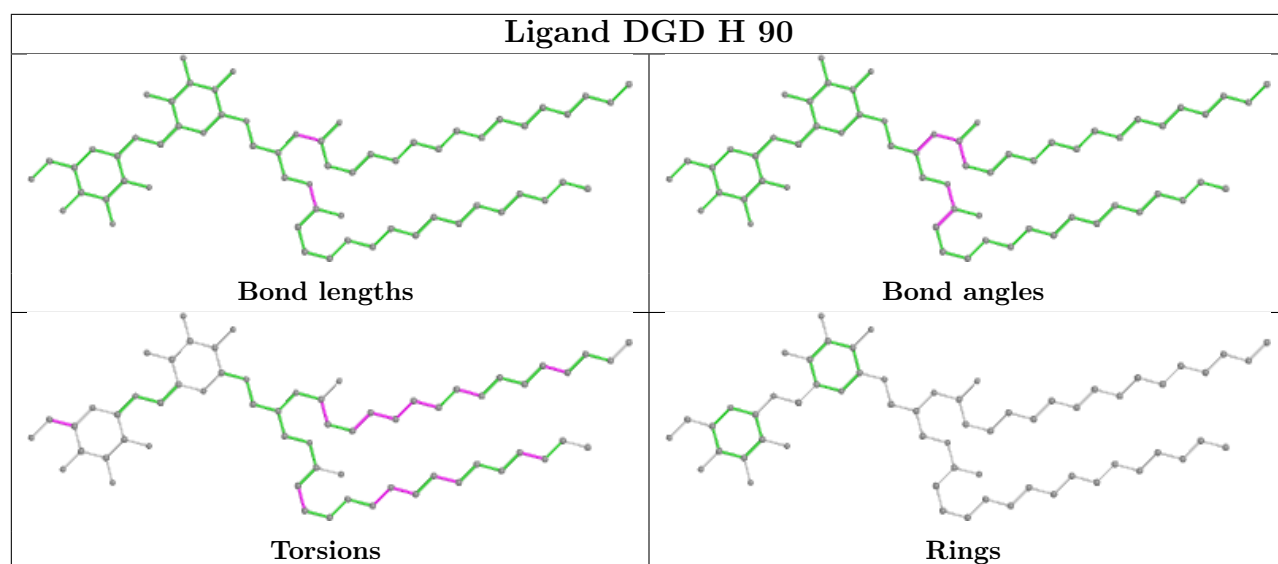


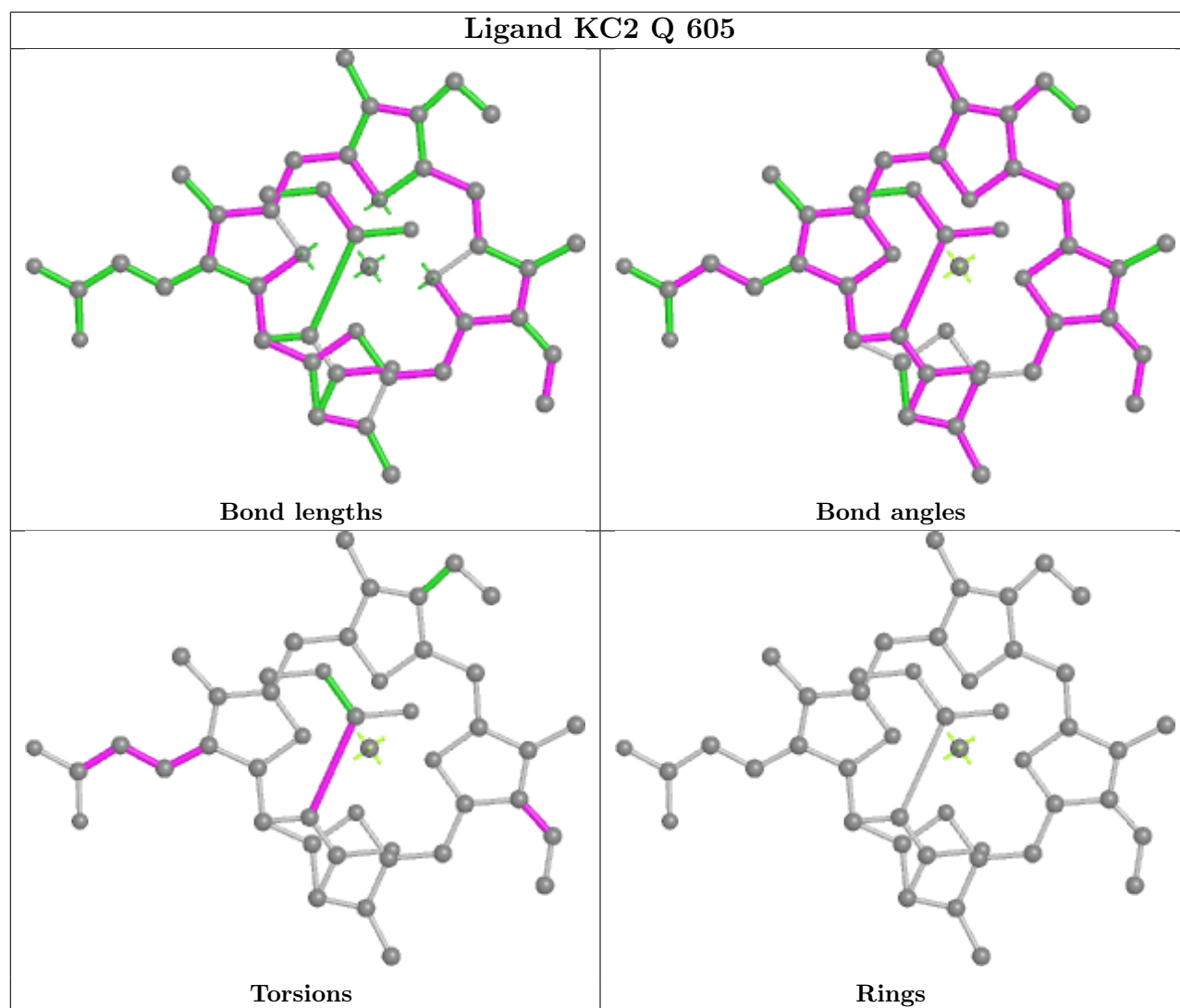
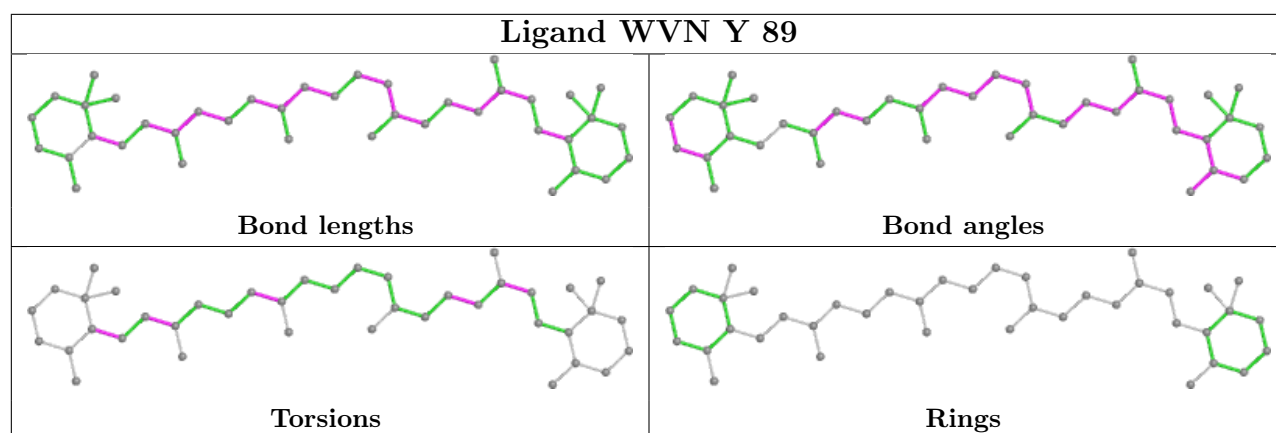
Ligand CLA Q 610

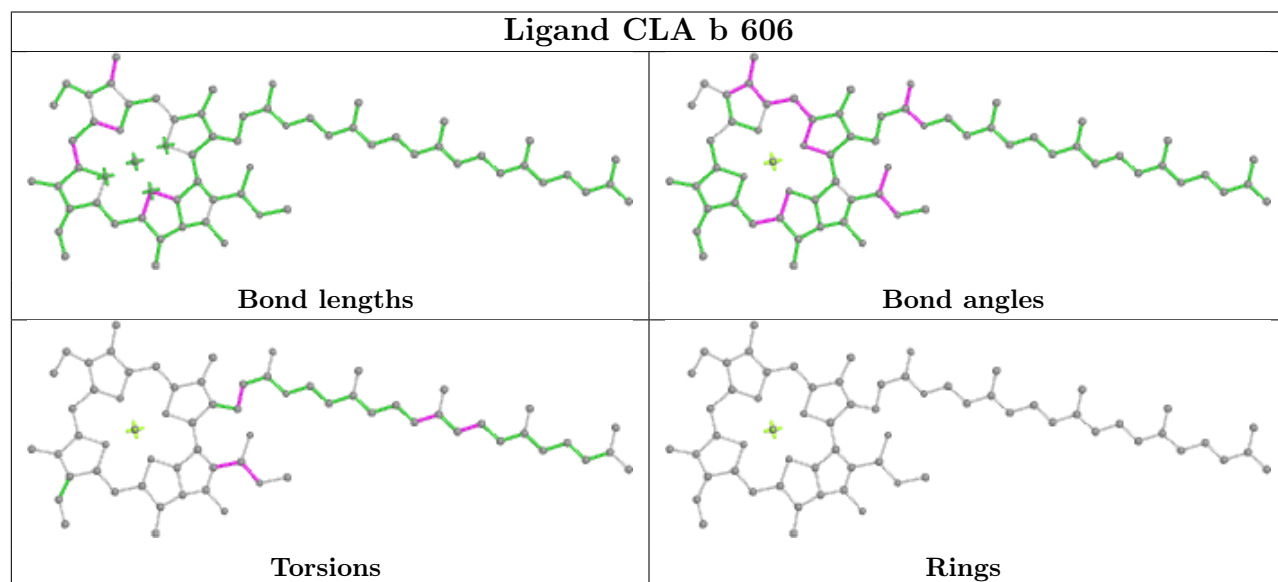
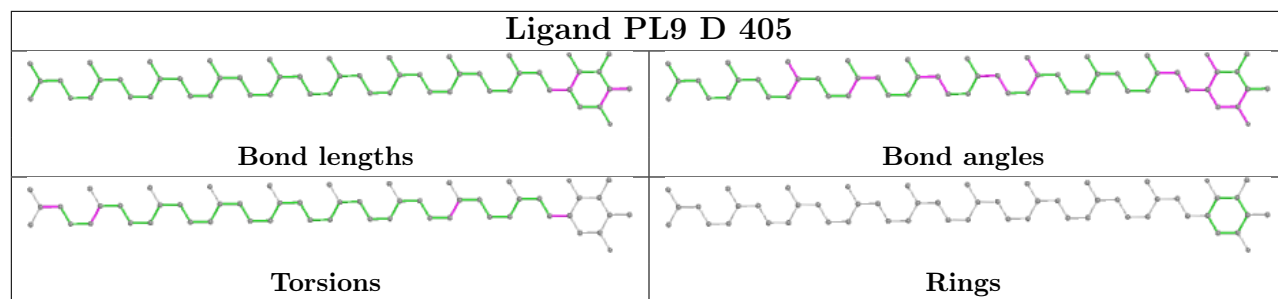


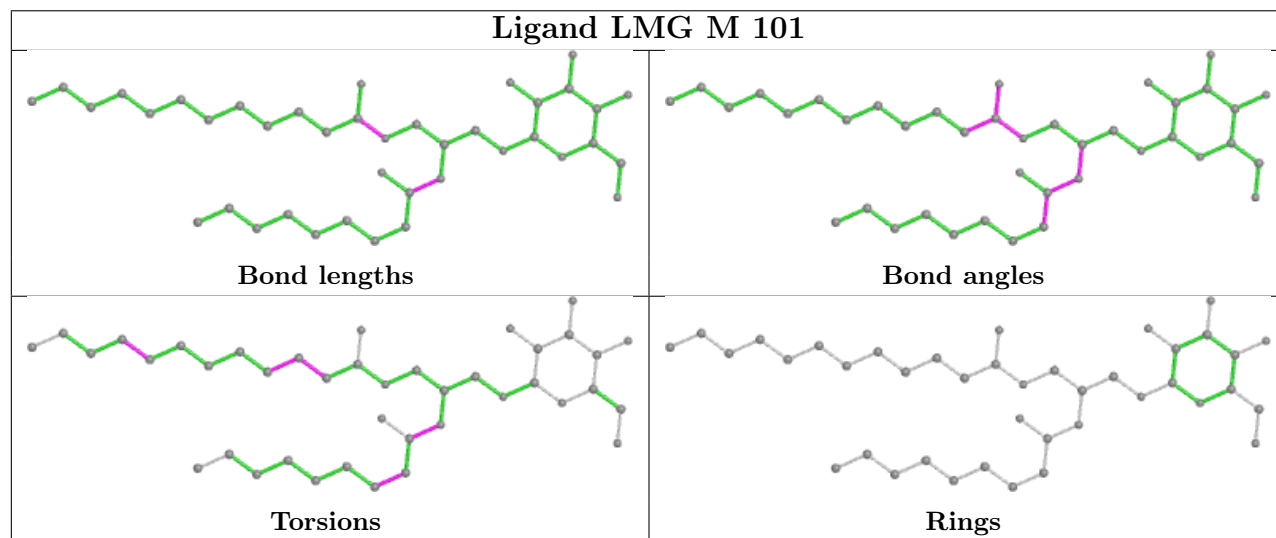
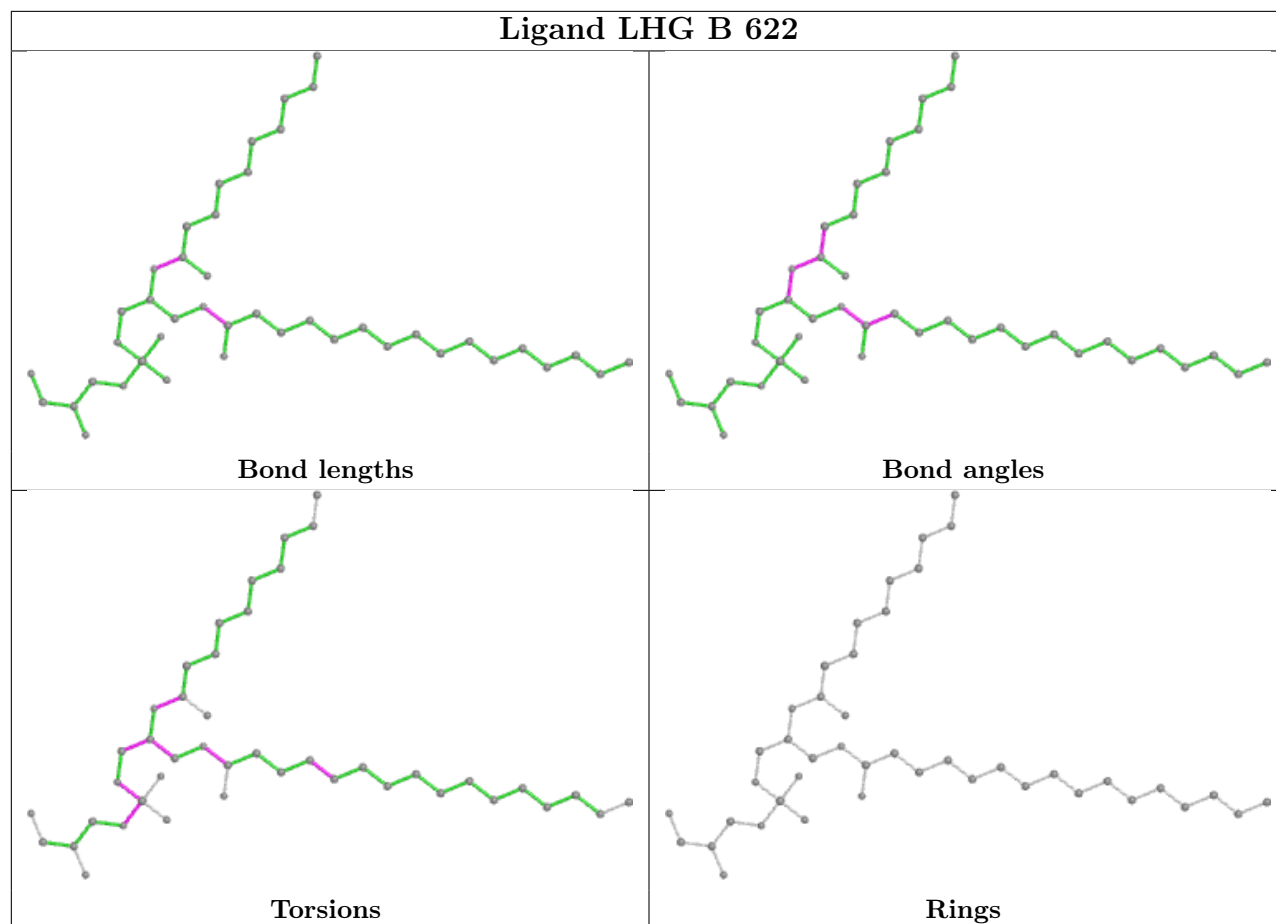
Ligand CLA 5 603



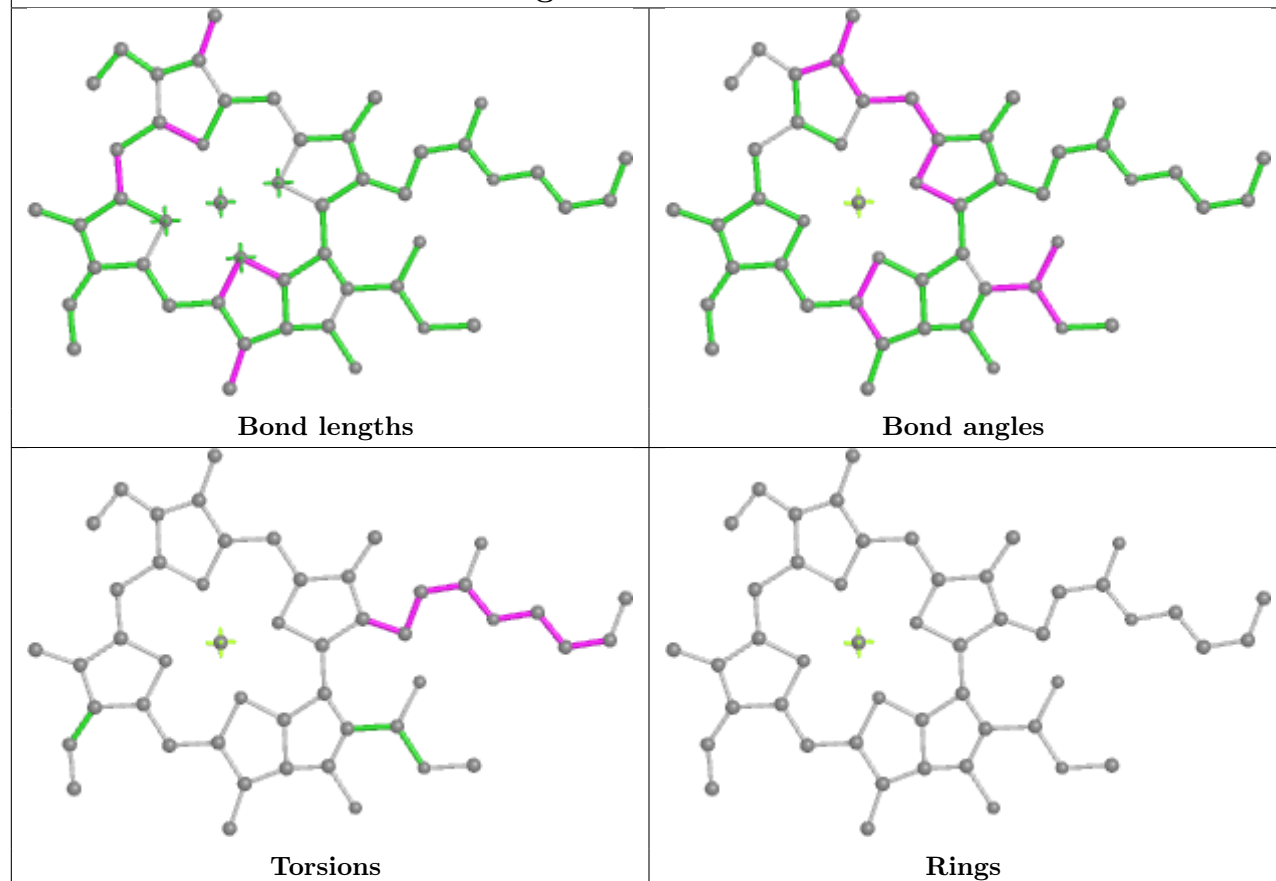




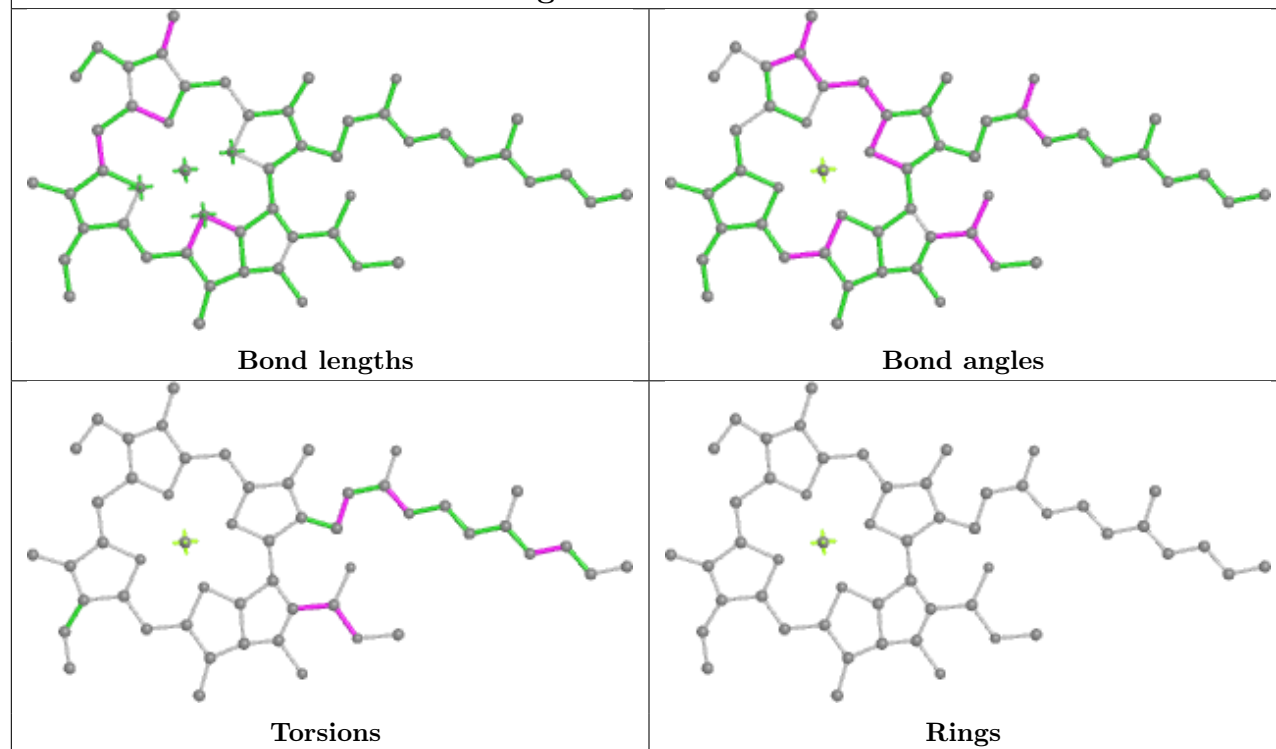




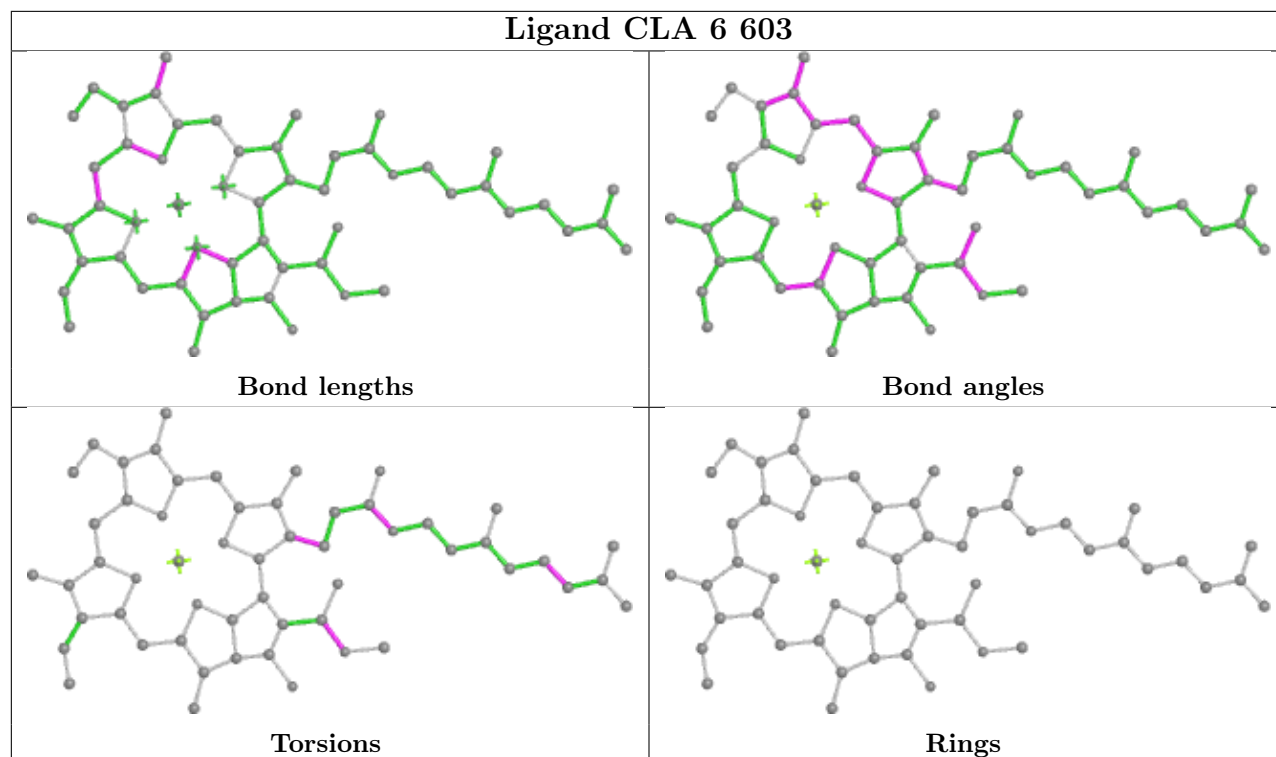
Ligand CLA a 404



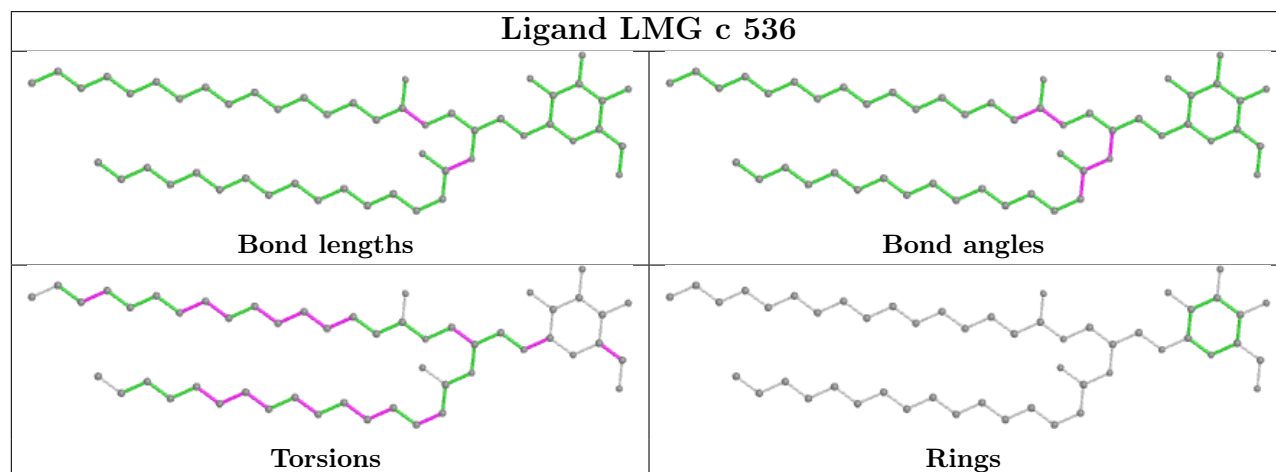
Ligand CLA c 528



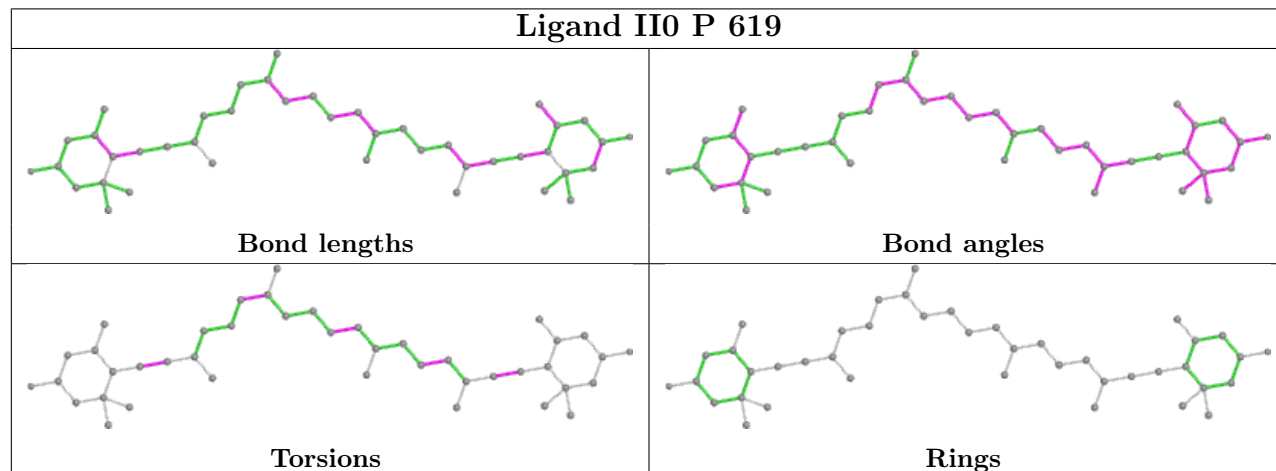
Ligand CLA 6 603

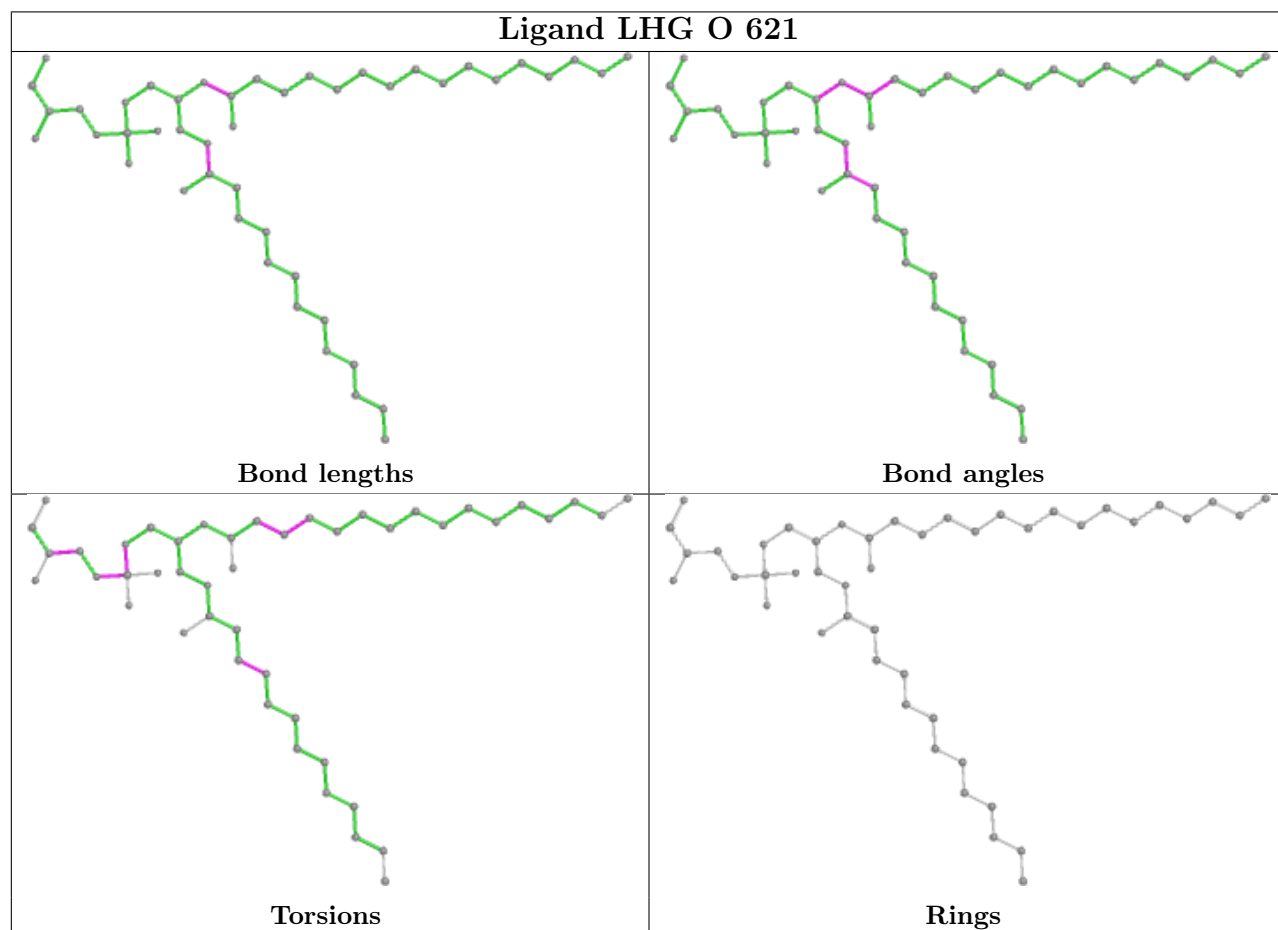
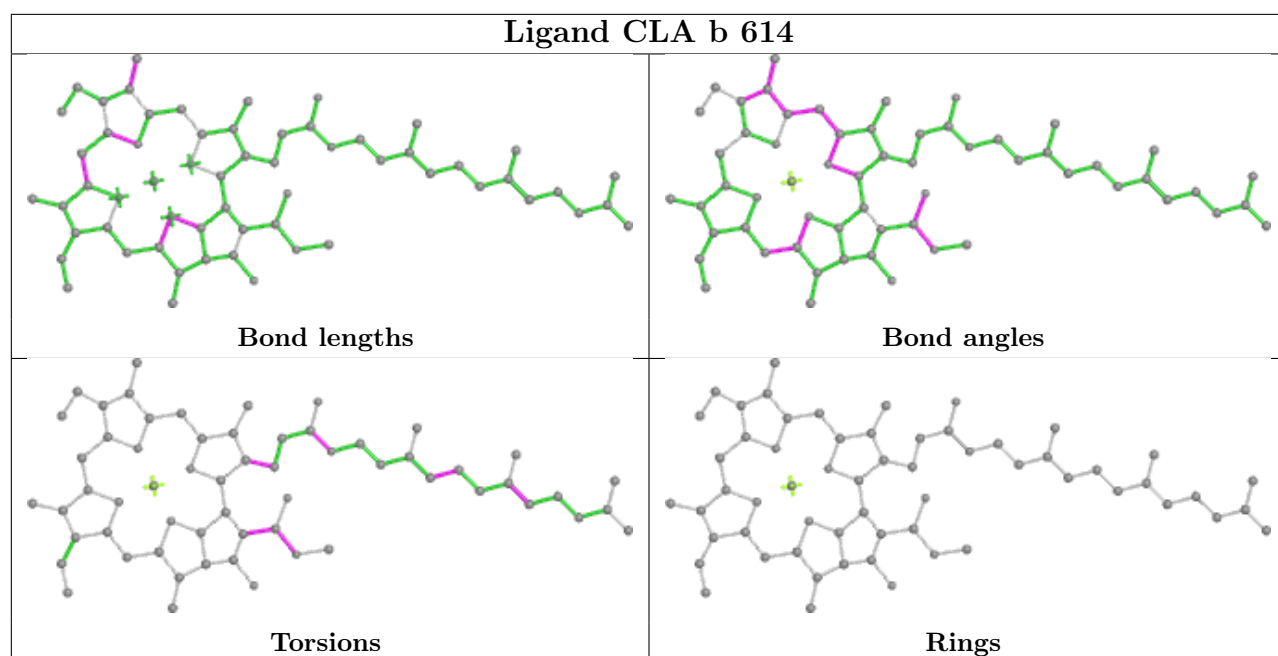


Ligand LMG c 536

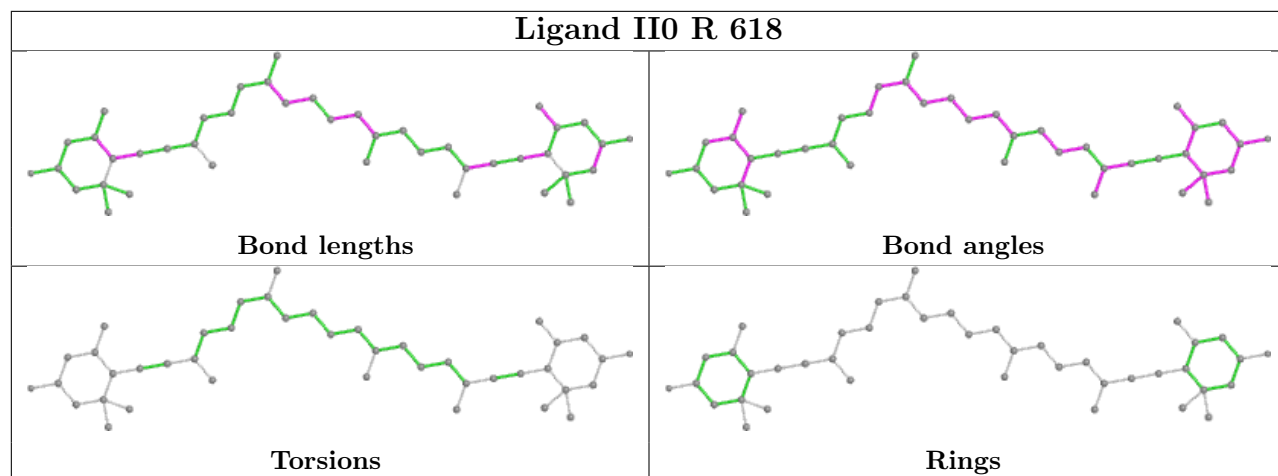


Ligand II0 P 619

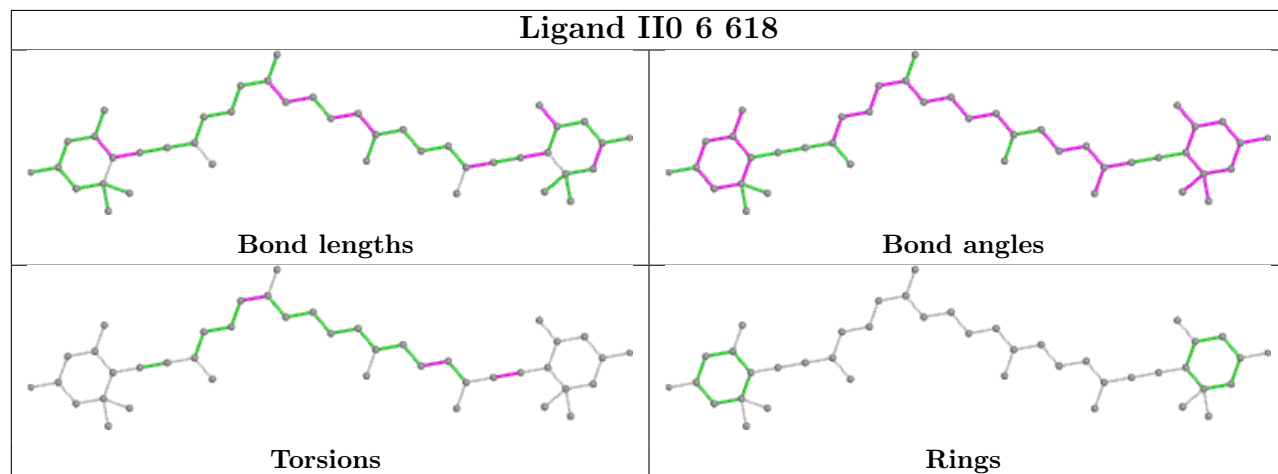


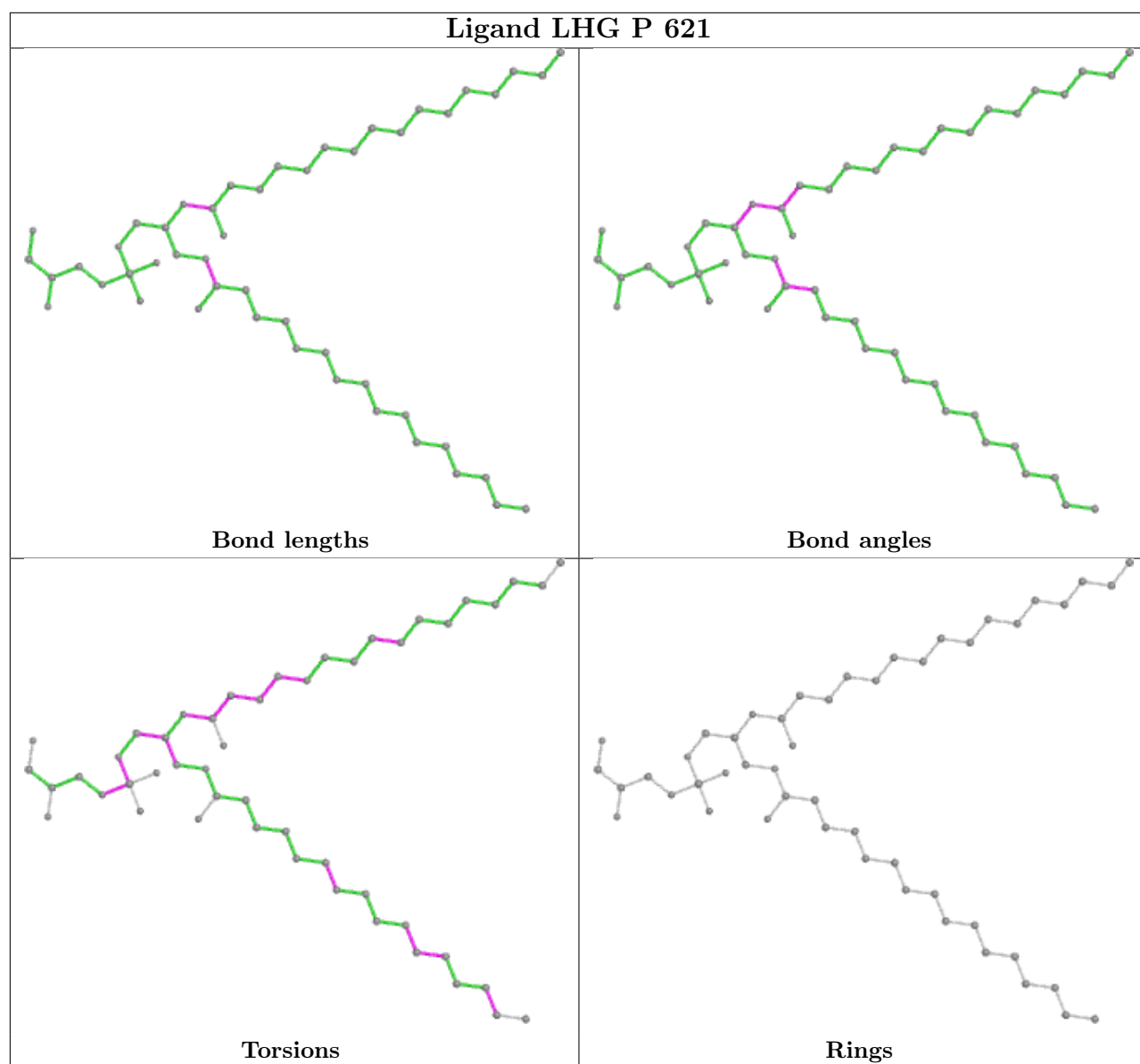


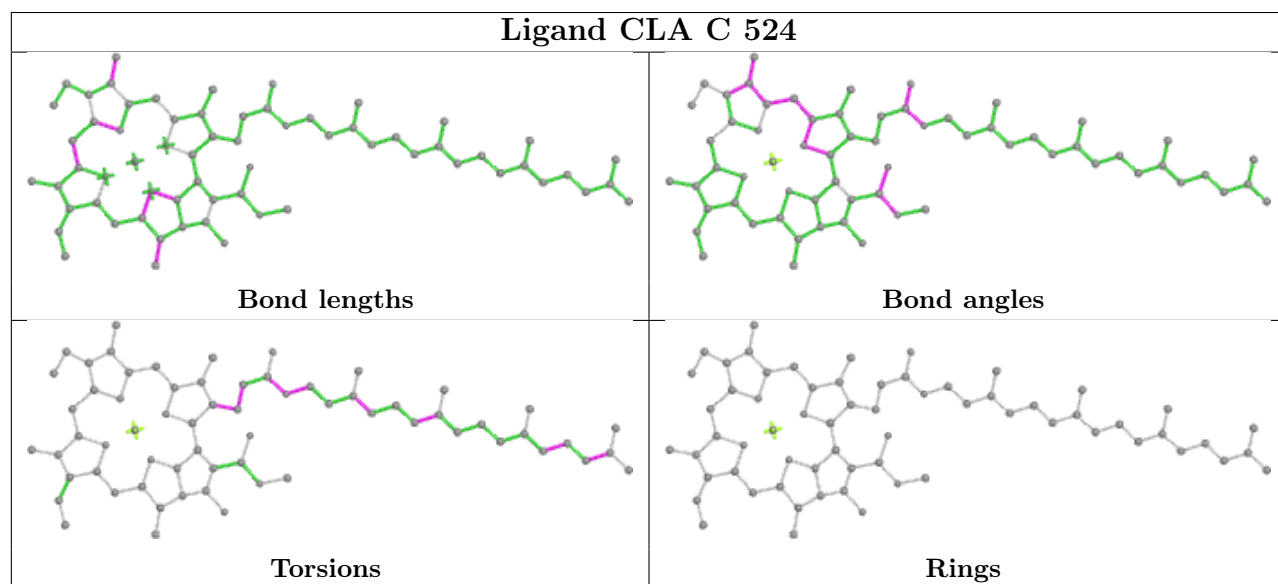
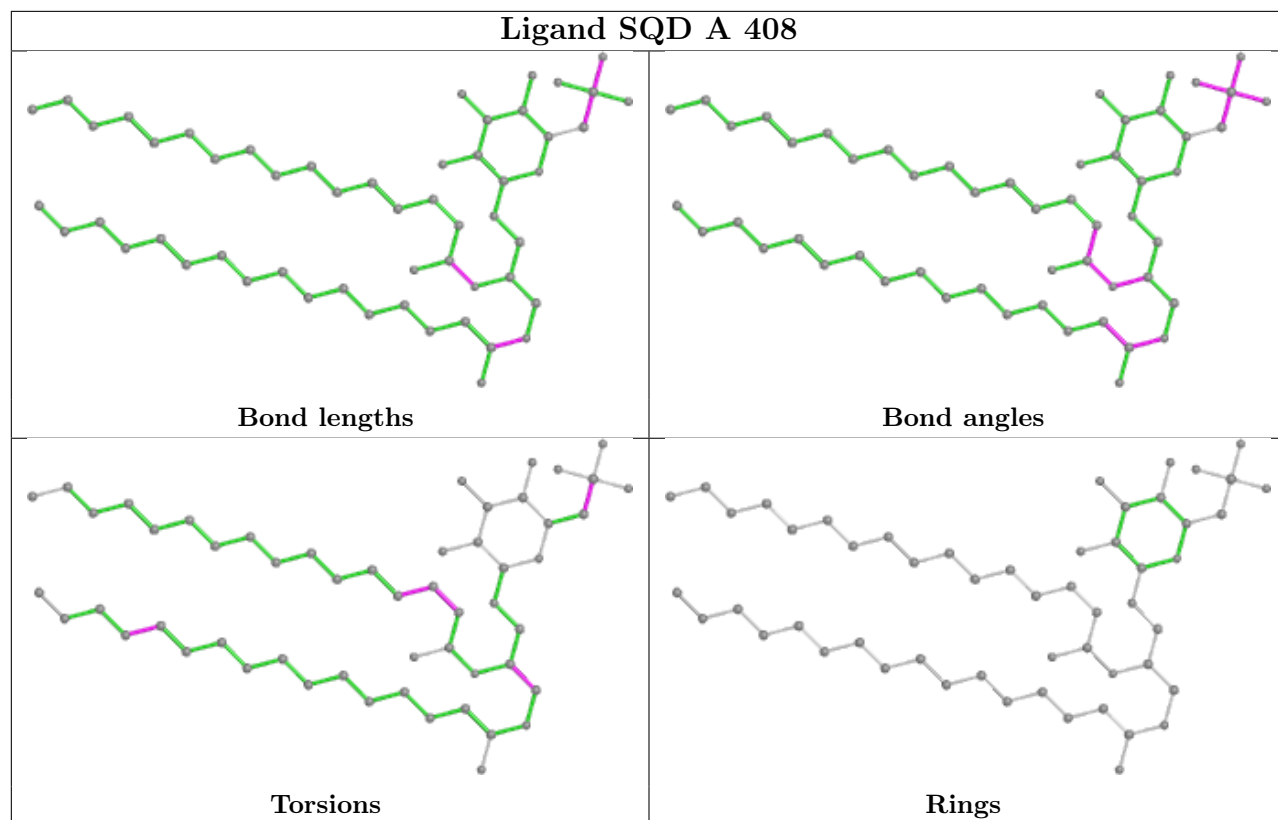
Ligand II0 R 618



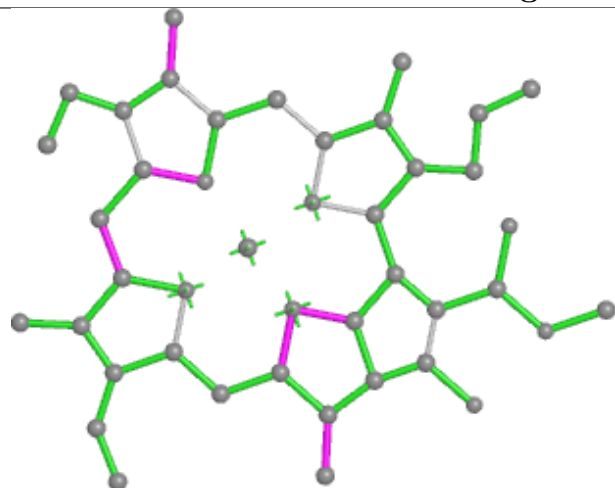
Ligand II0 6 618



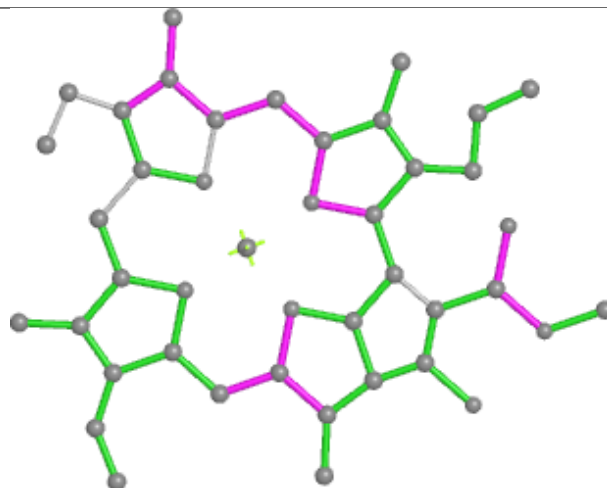




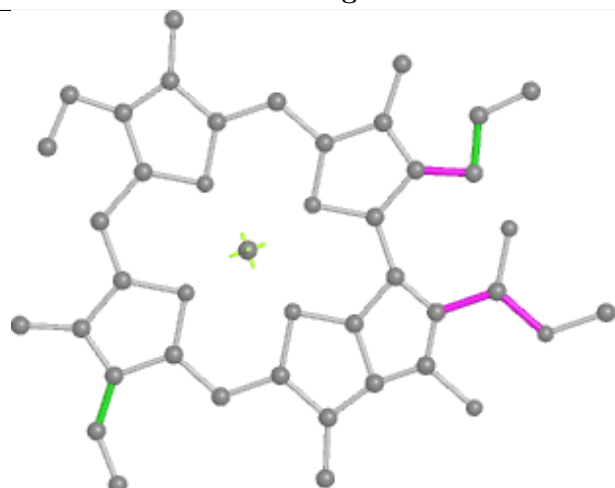
Ligand CLA 5 607



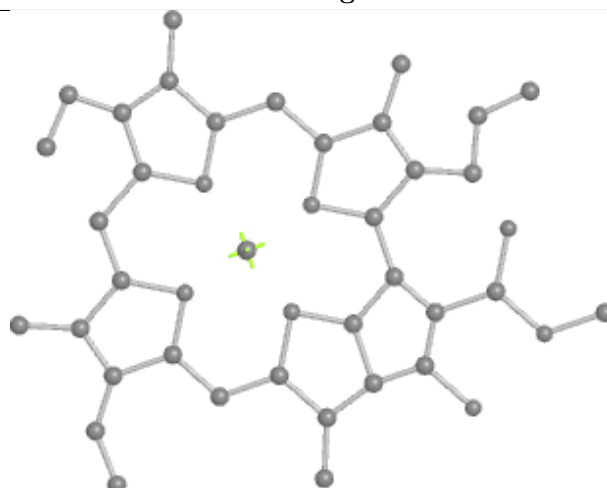
Bond lengths



Bond angles

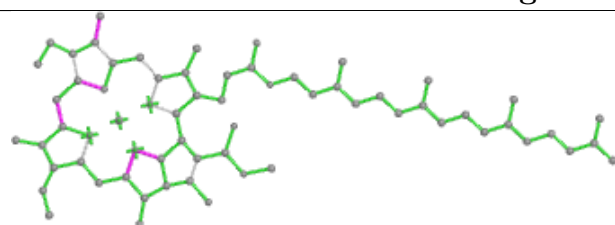


Torsions

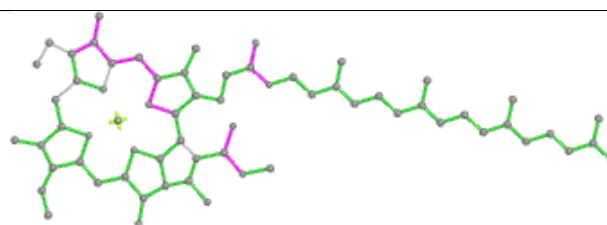


Rings

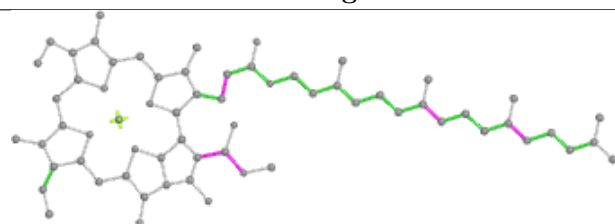
Ligand CLA b 608



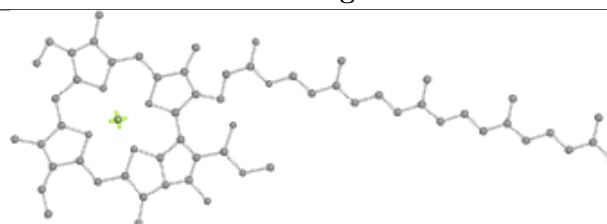
Bond lengths



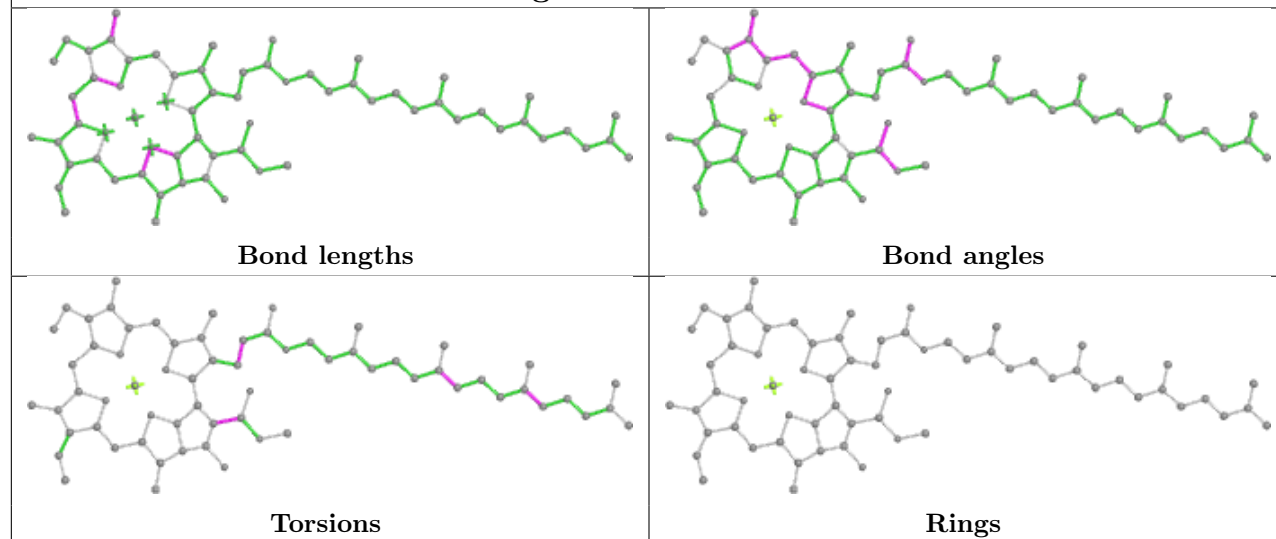
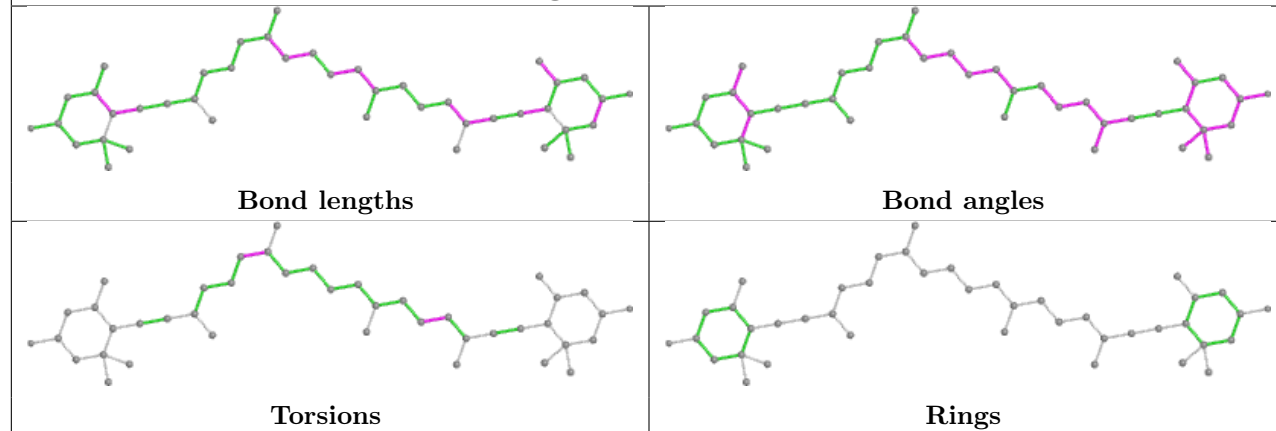
Bond angles



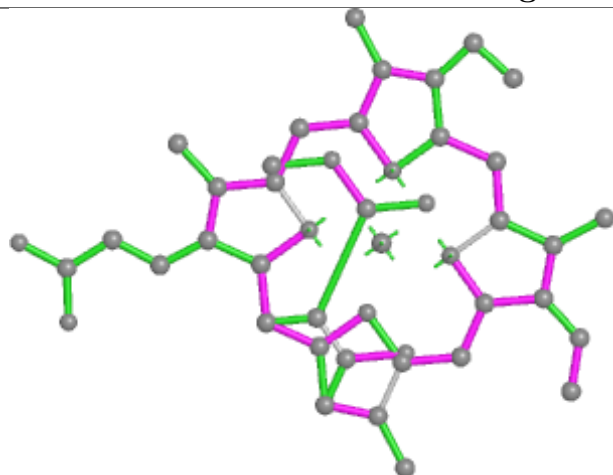
Torsions



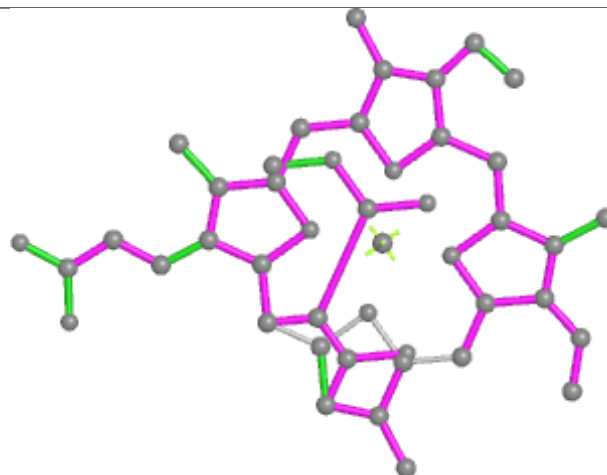
Rings

Ligand CLA B 608**Ligand II0 R 619**

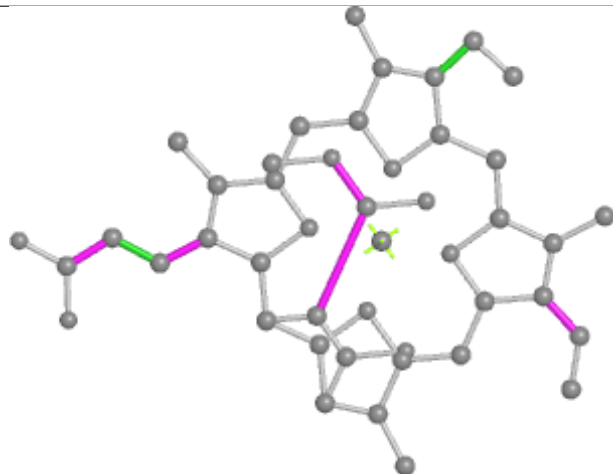
Ligand KC2 S 606



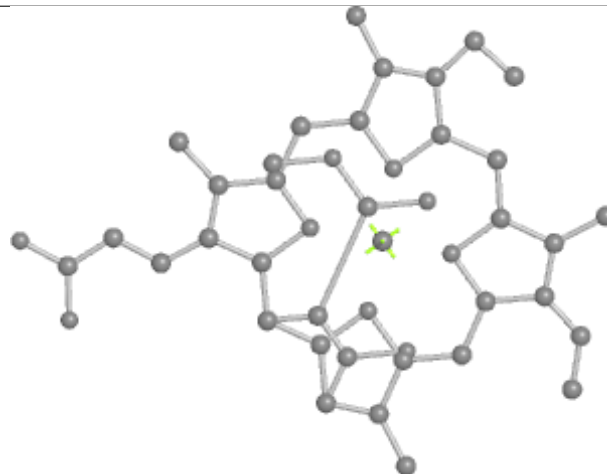
Bond lengths



Bond angles

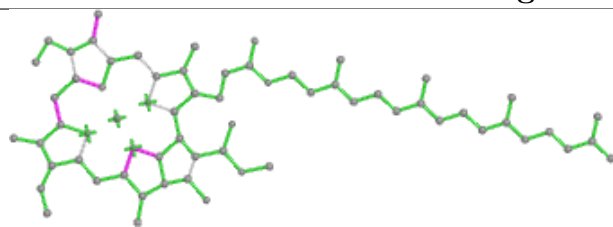


Torsions

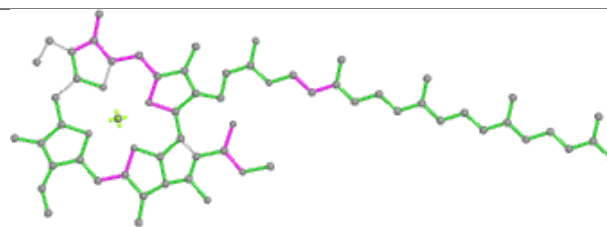


Rings

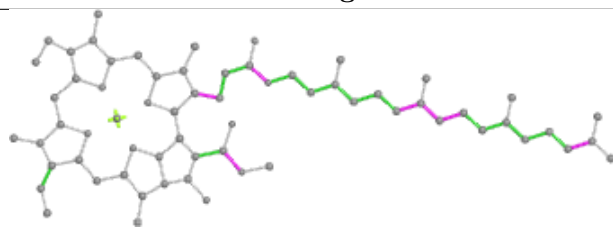
Ligand CLA b 607



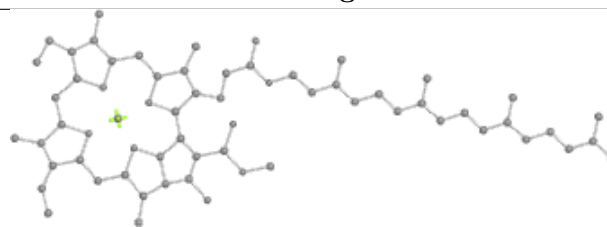
Bond lengths



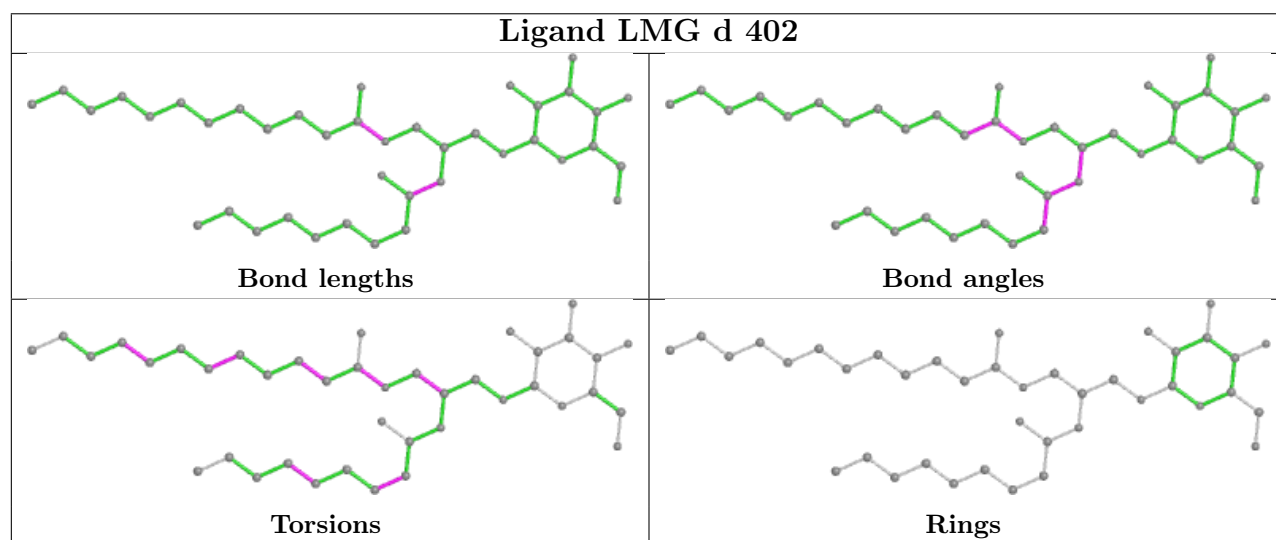
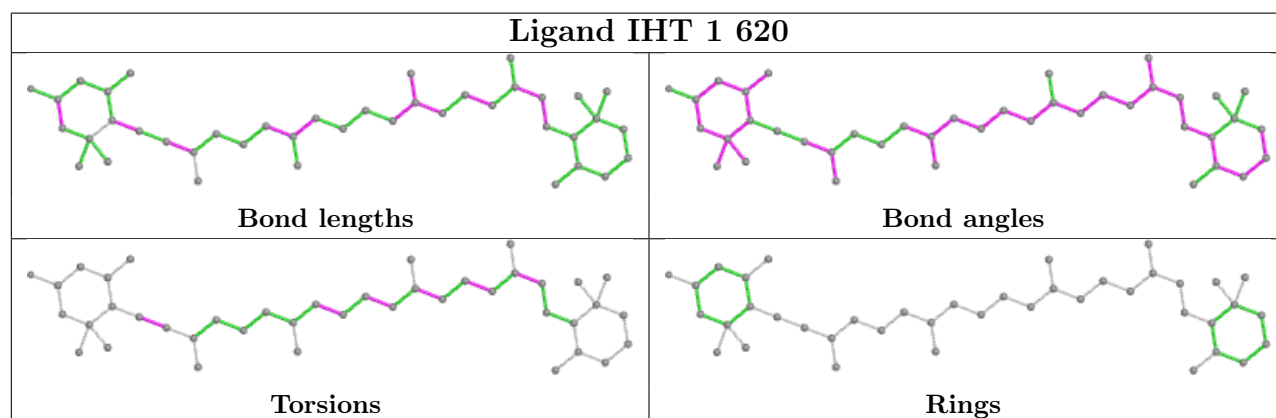
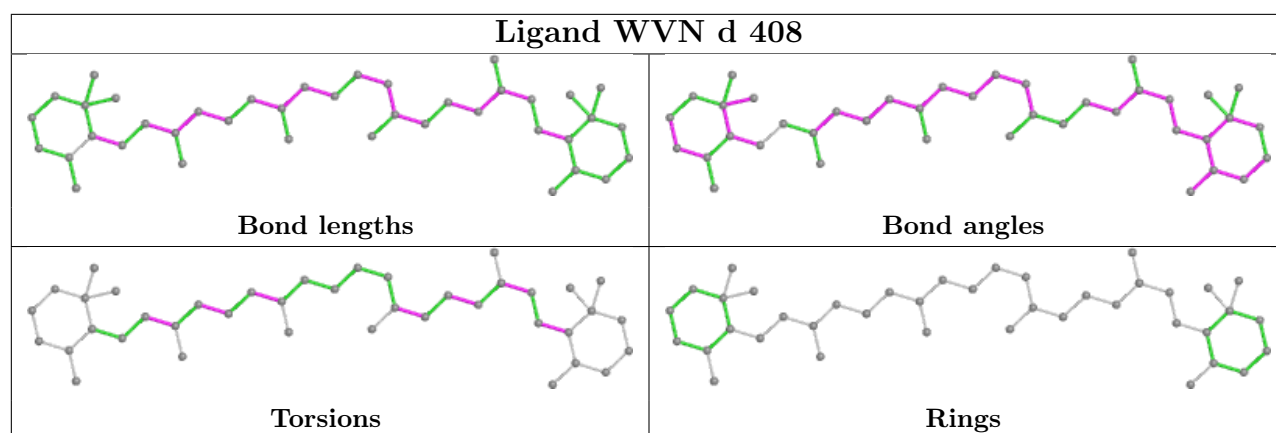
Bond angles



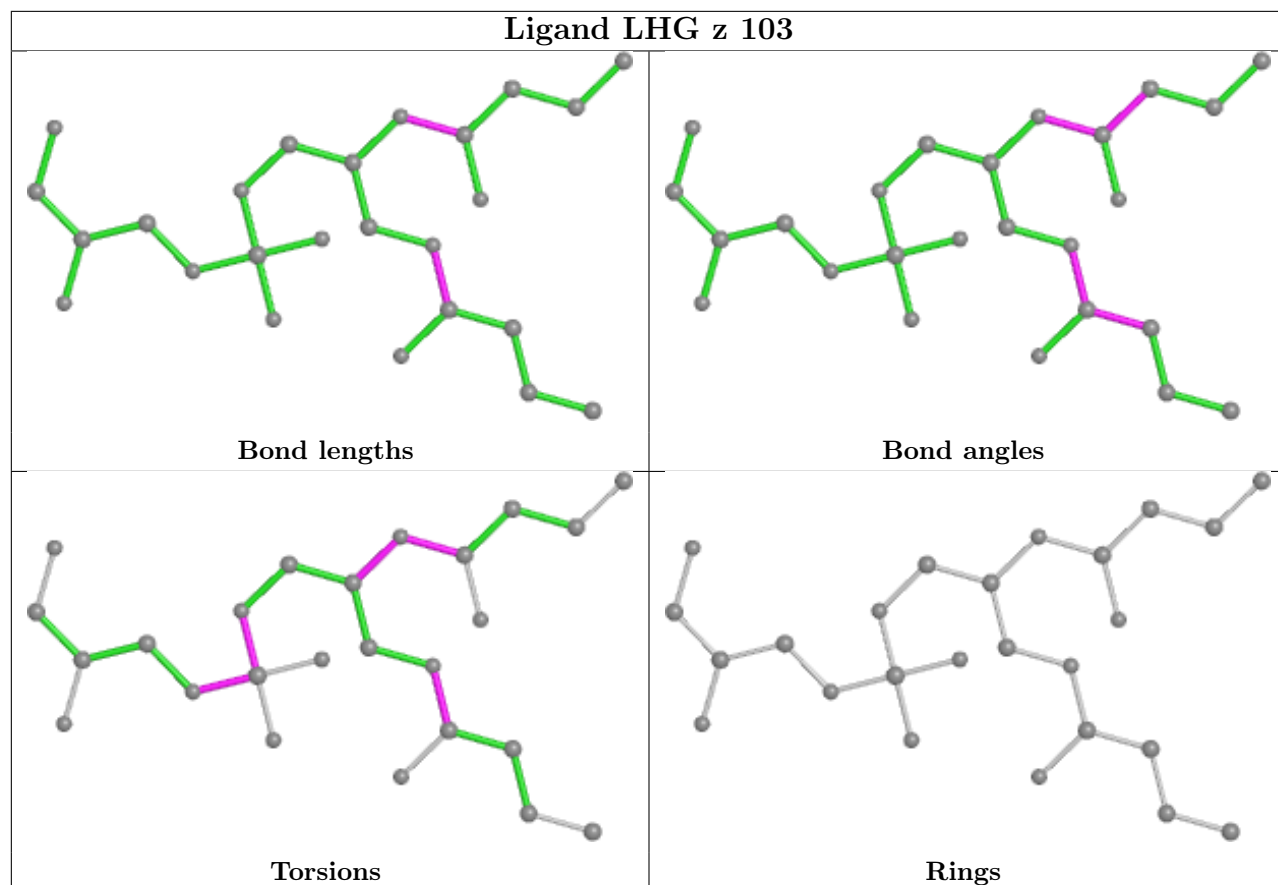
Torsions



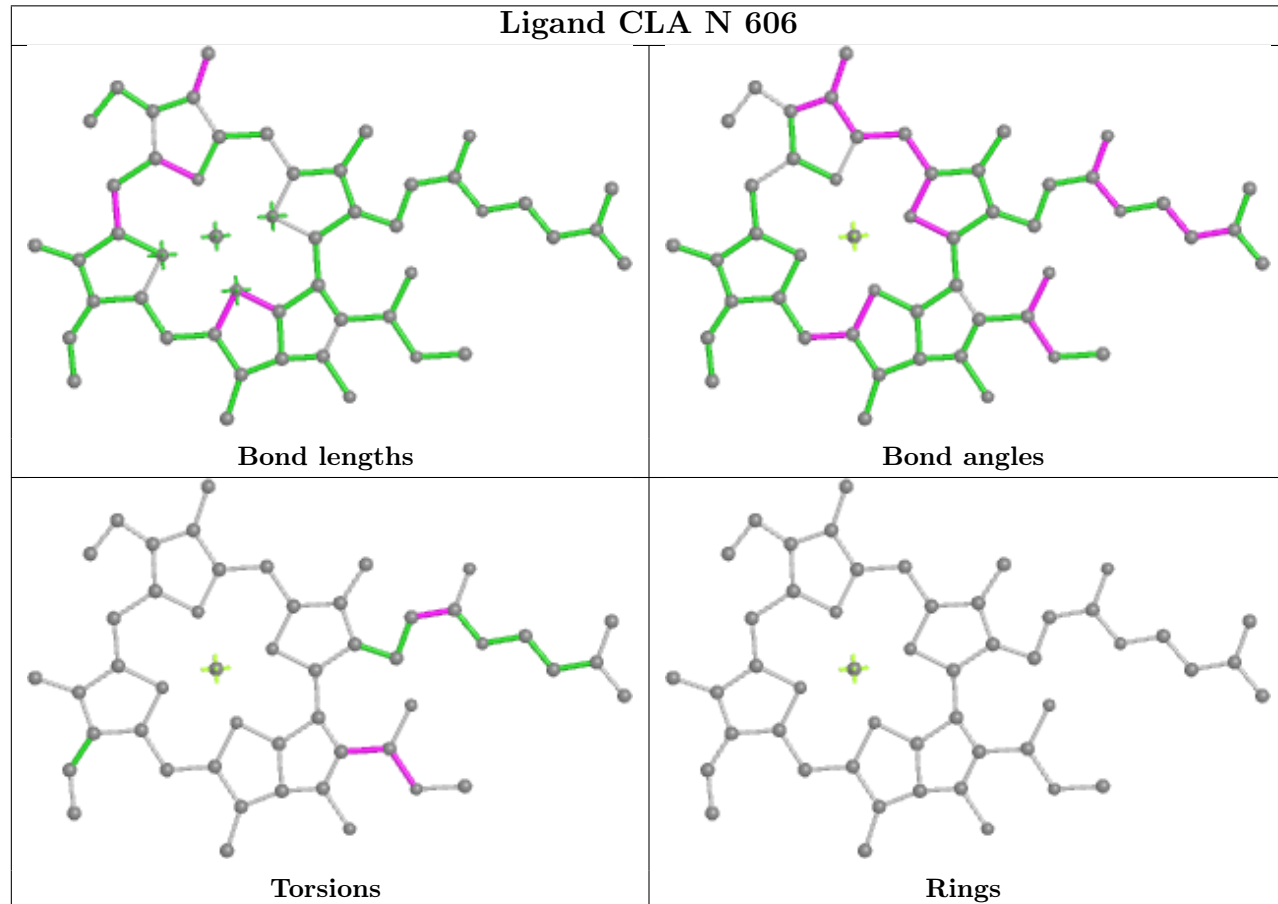
Rings



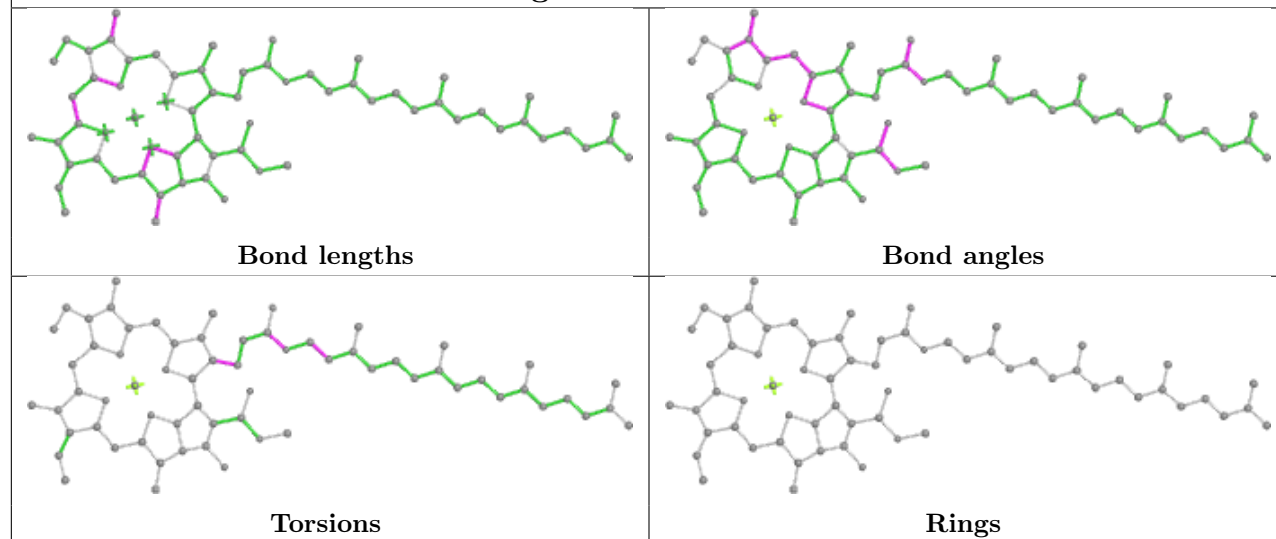
Ligand LHG z 103



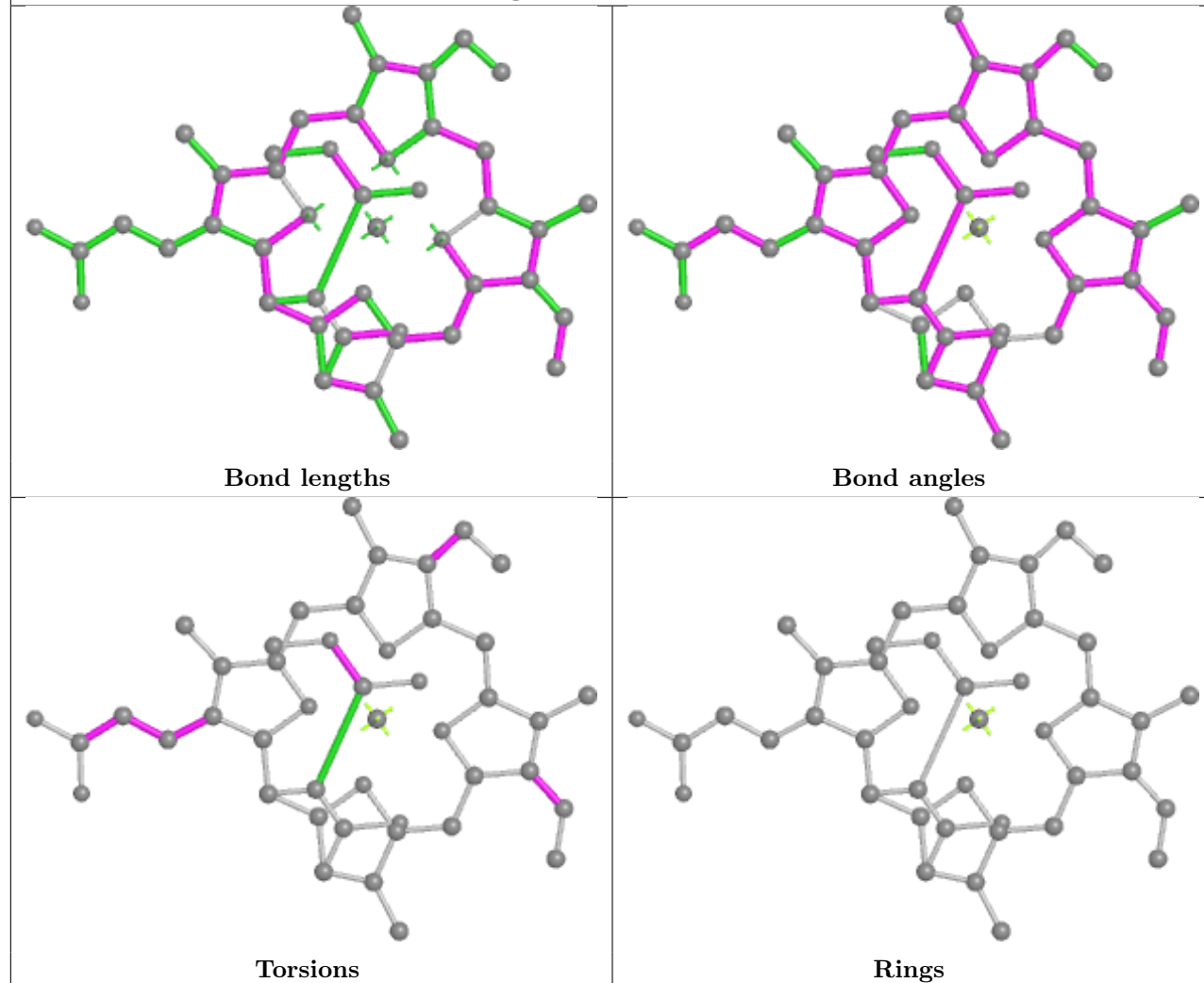
Ligand CLA N 606



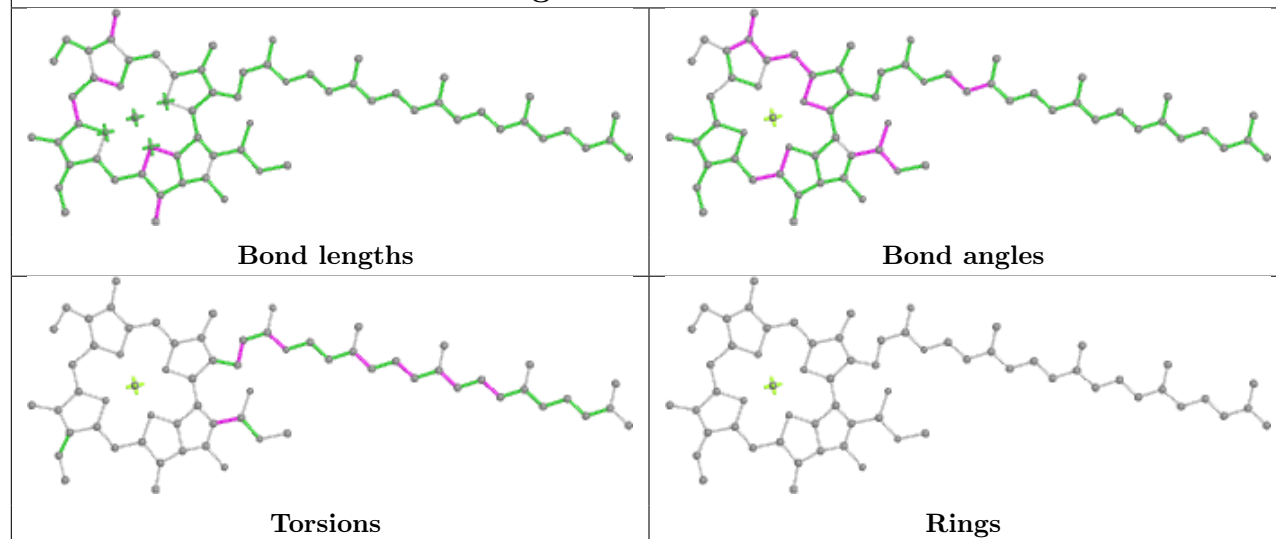
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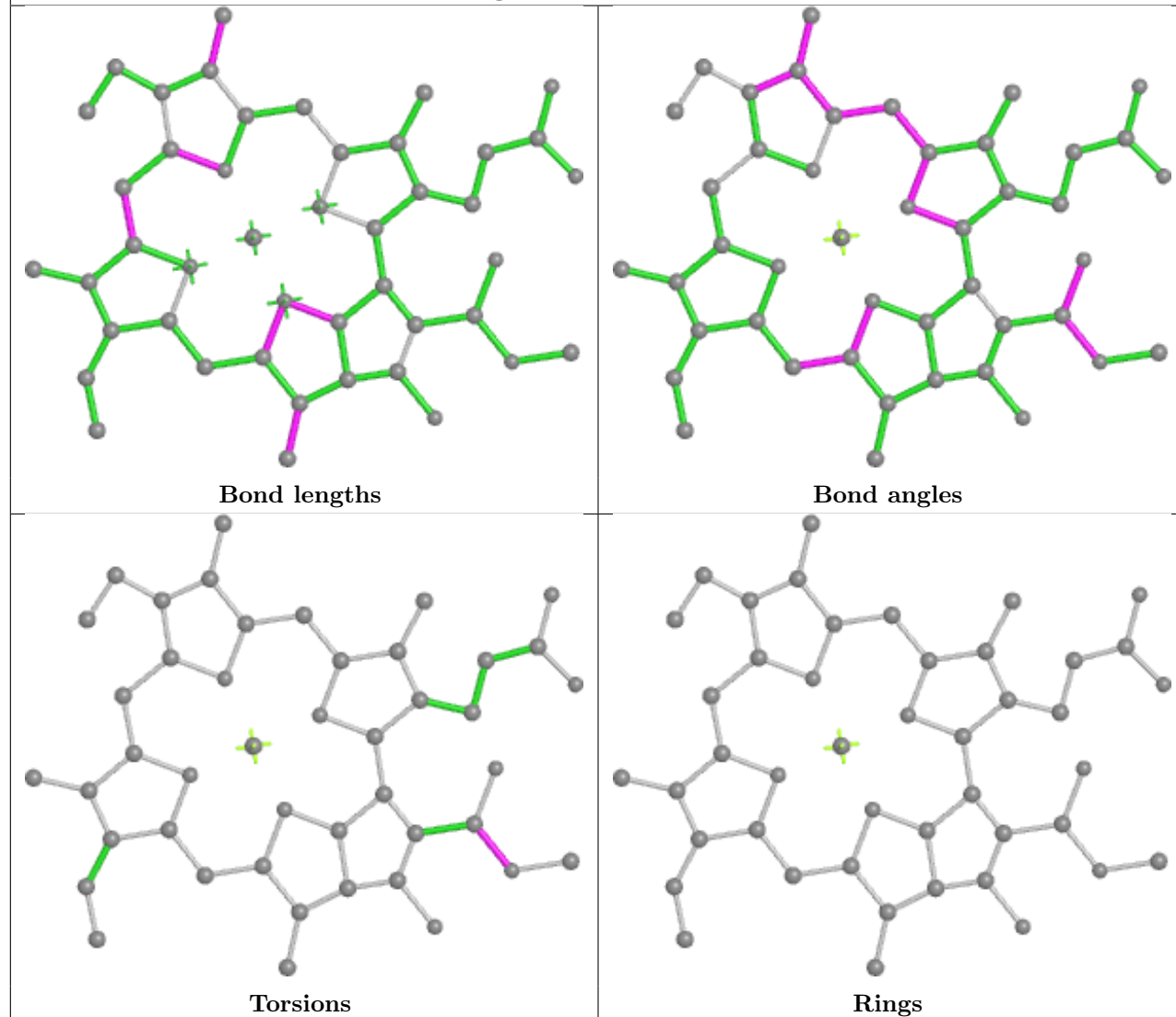
Ligand KC2 3 606



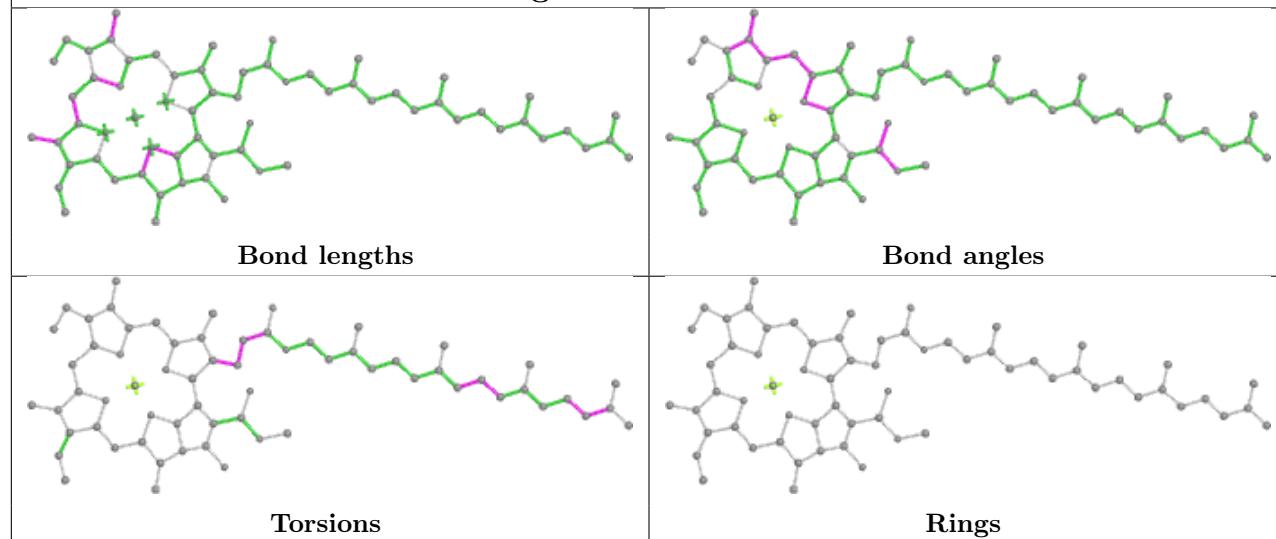
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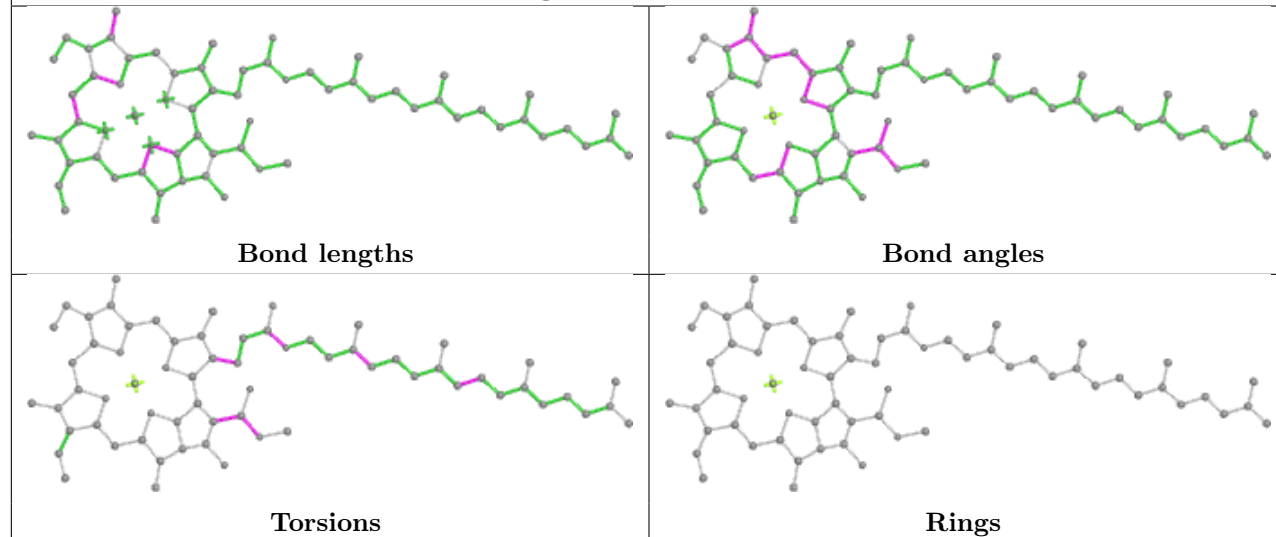
Ligand CLA P 601

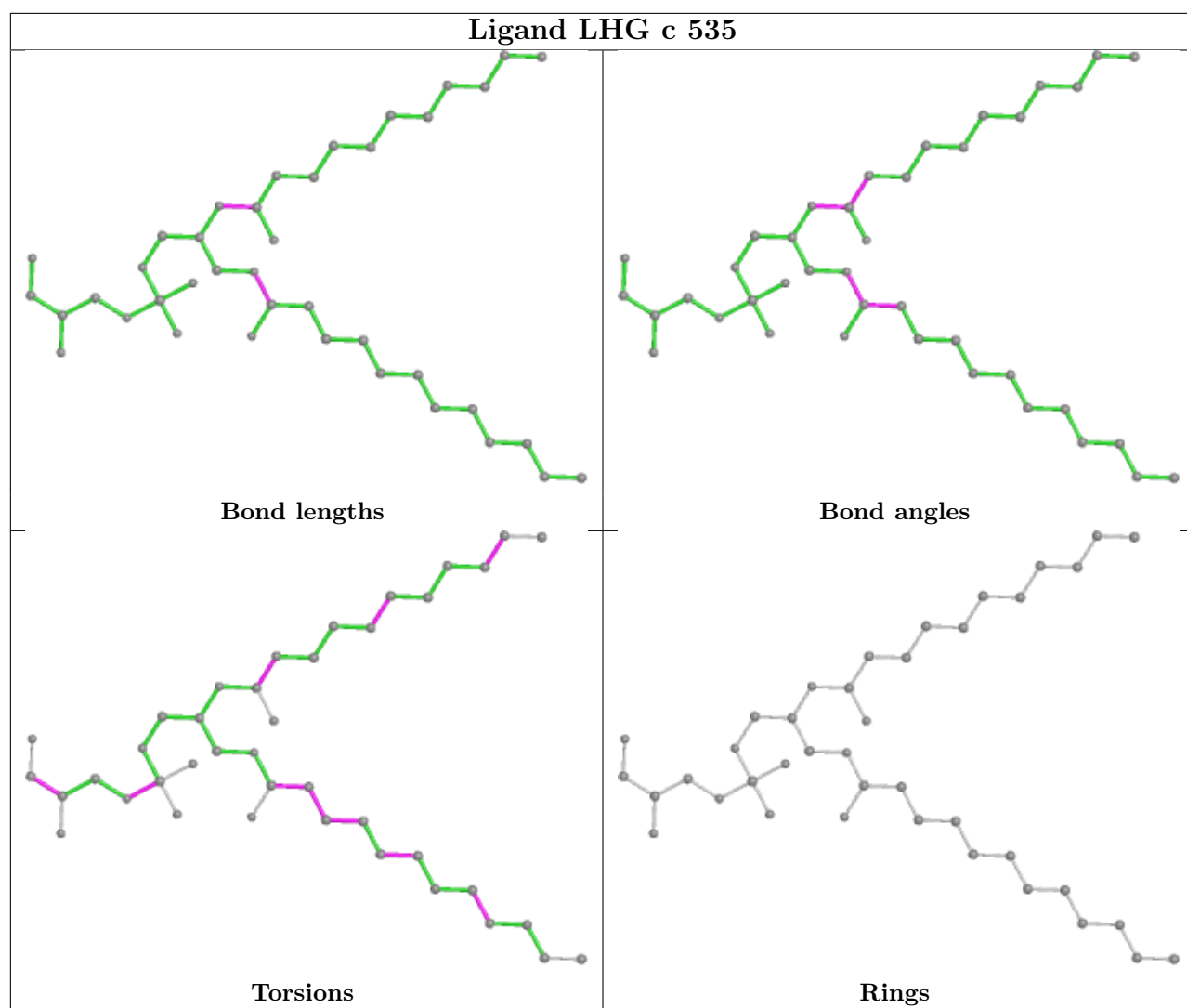


Ligand CLA O 603

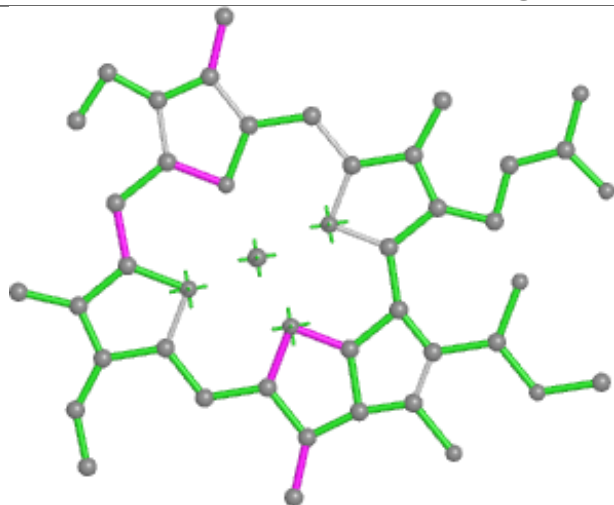


Ligand CLA c 526

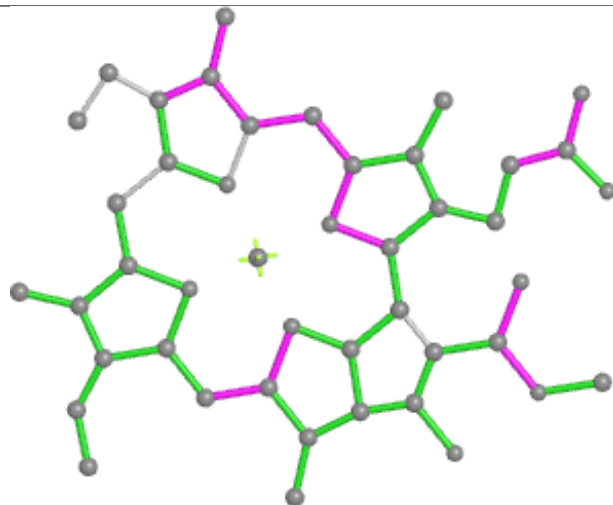




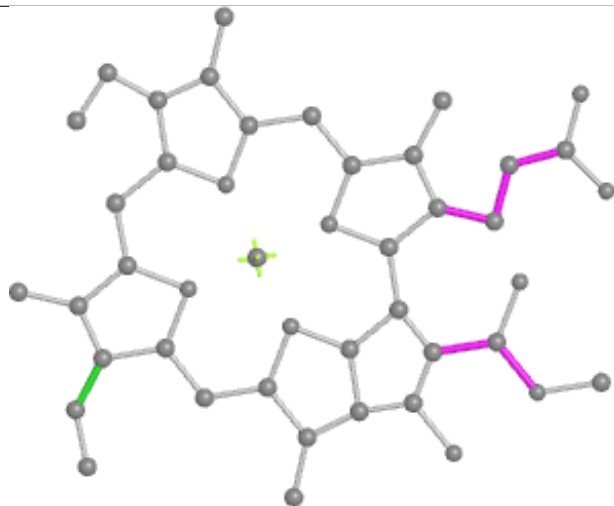
Ligand CLA P 615



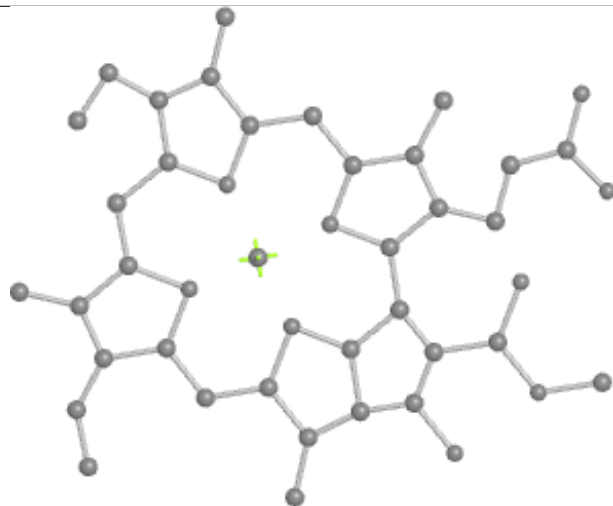
Bond lengths



Bond angles

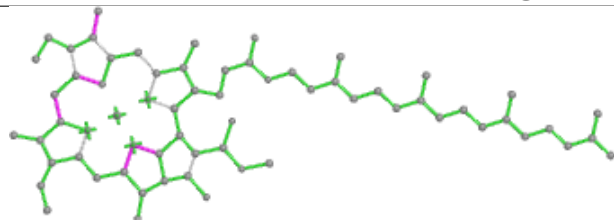


Torsions

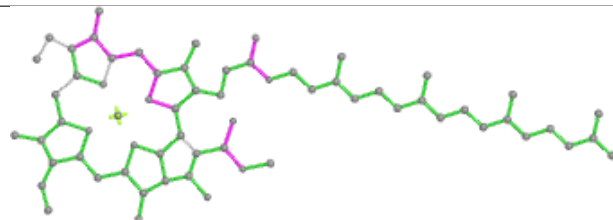


Rings

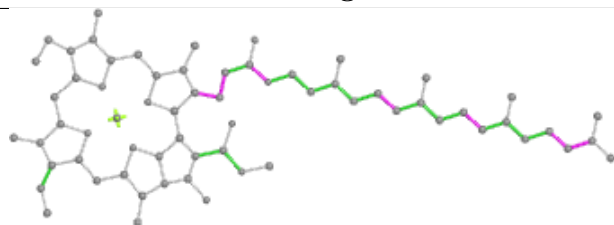
Ligand CLA b 615



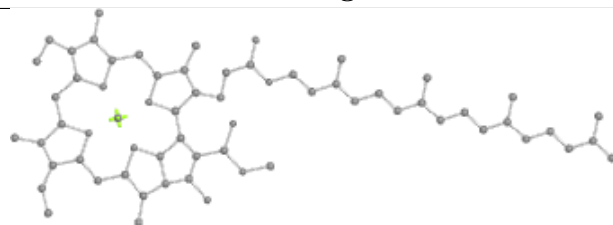
Bond lengths



Bond angles

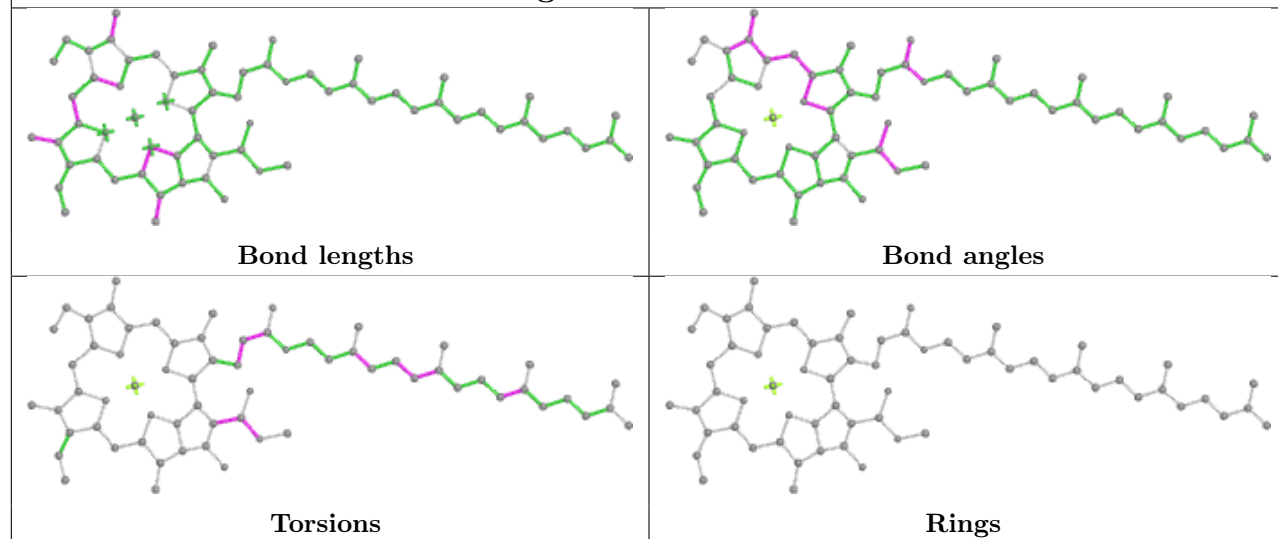


Torsions

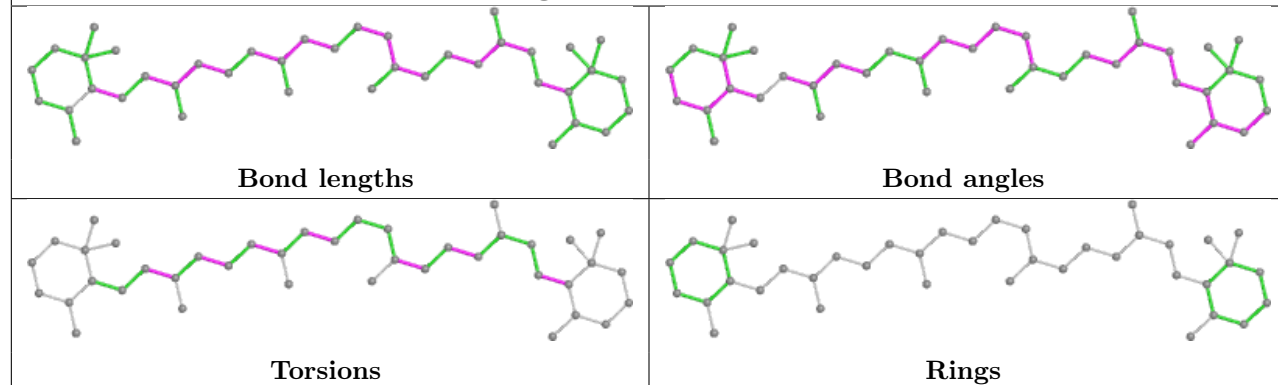


Rings

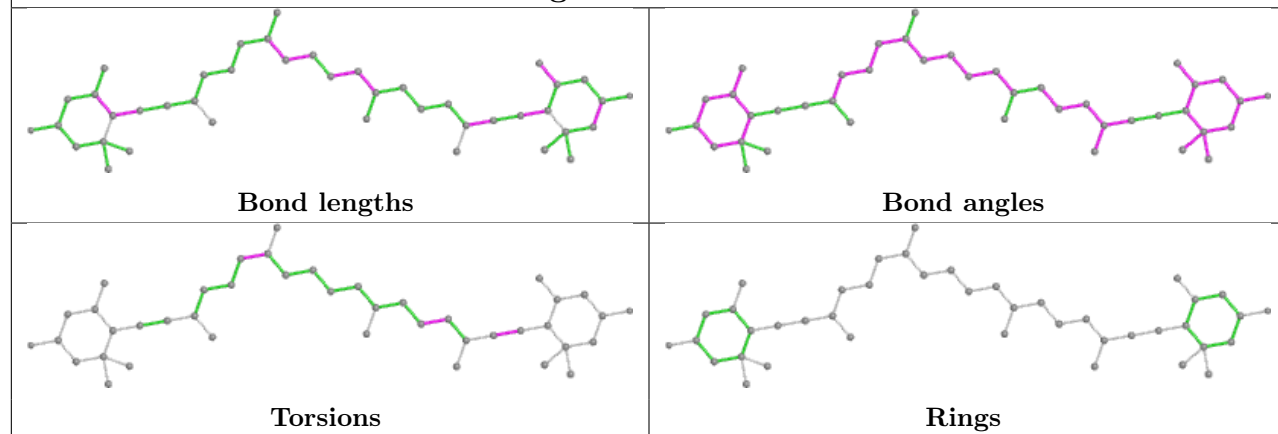
Ligand CLA c 517



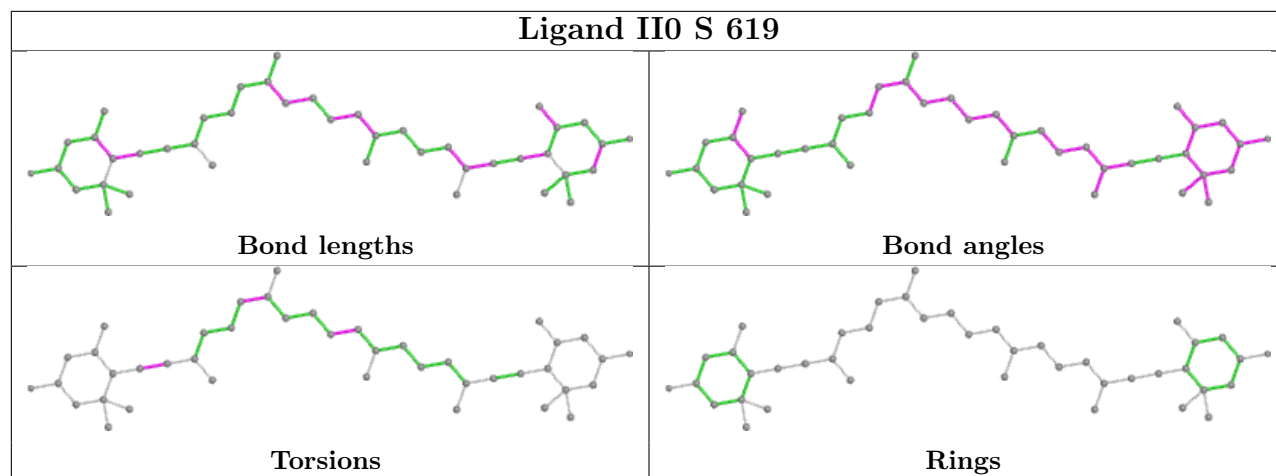
Ligand WVN h 89



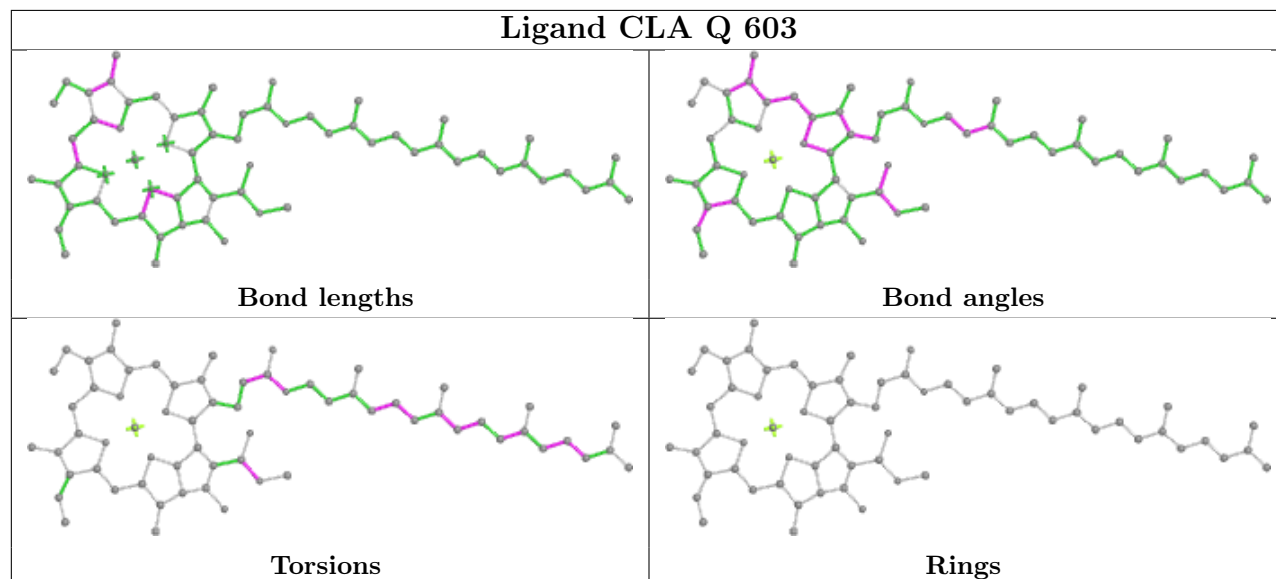
Ligand II0 S 618



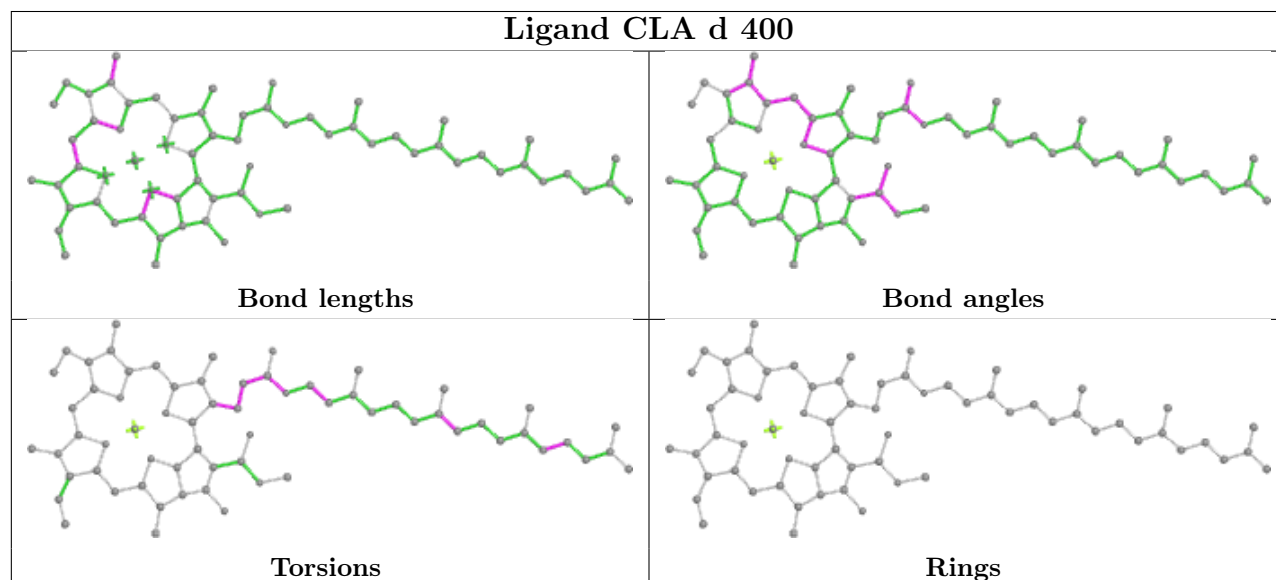
Ligand II0 S 619

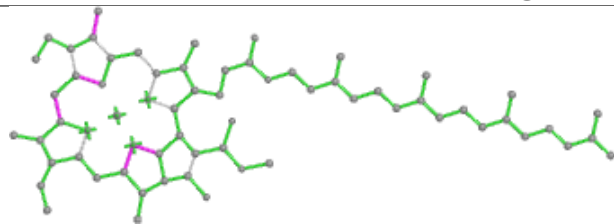
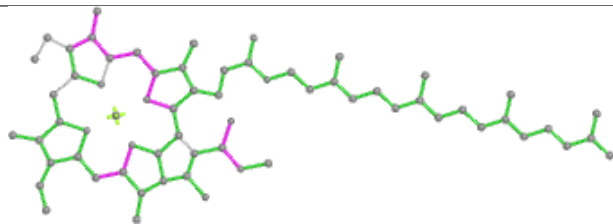
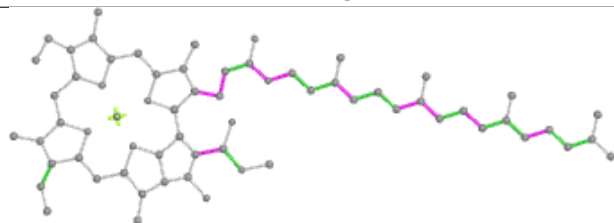
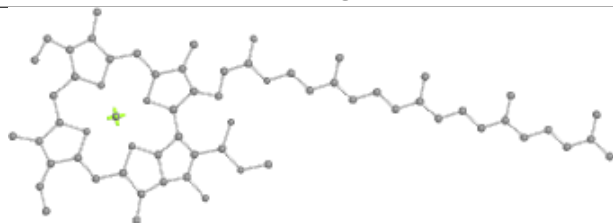
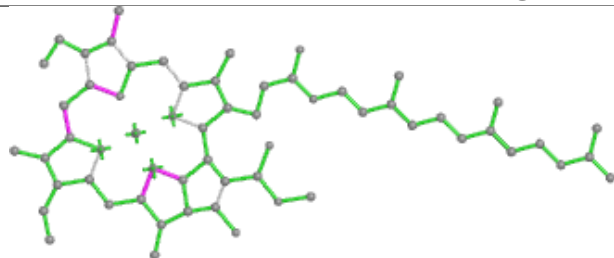
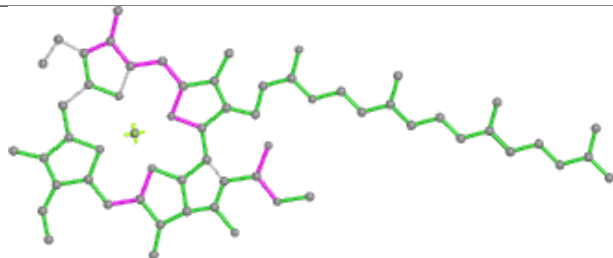
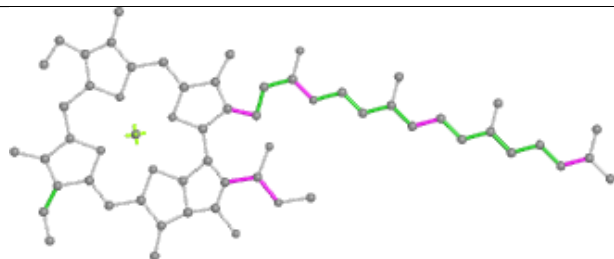
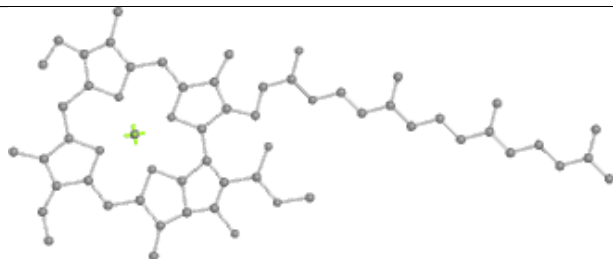


Ligand CLA Q 603

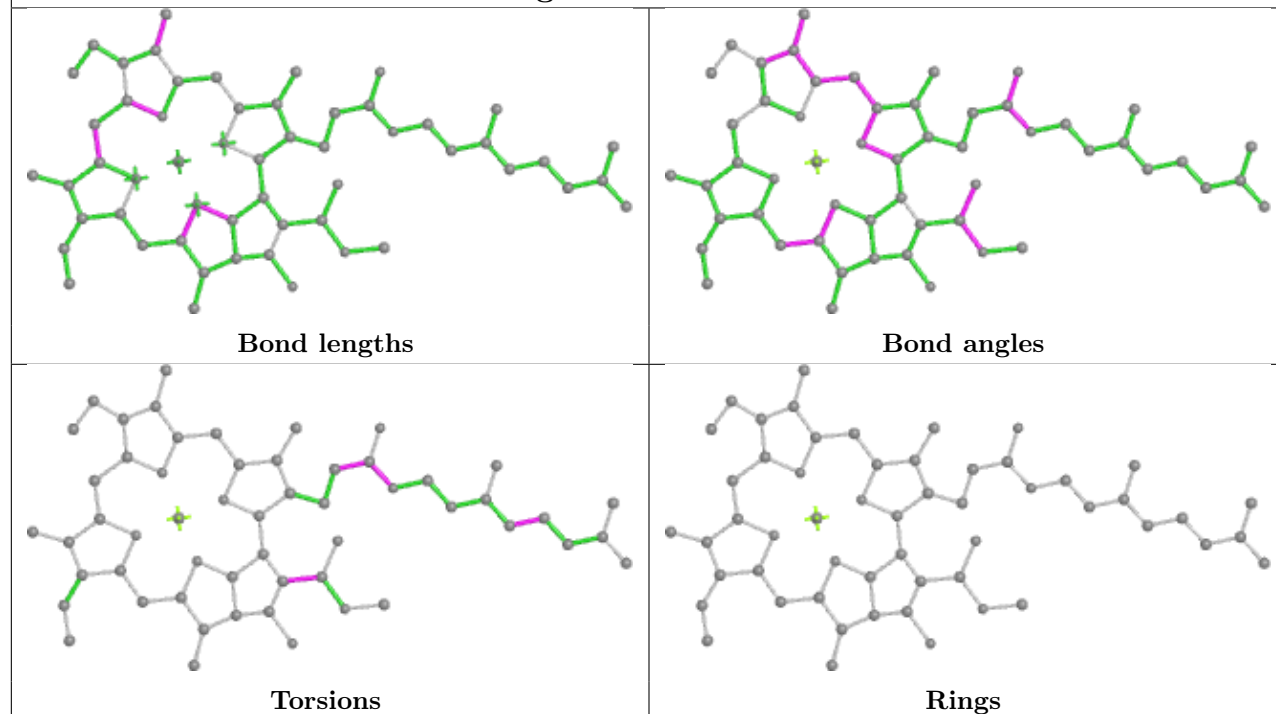


Ligand CLA d 400

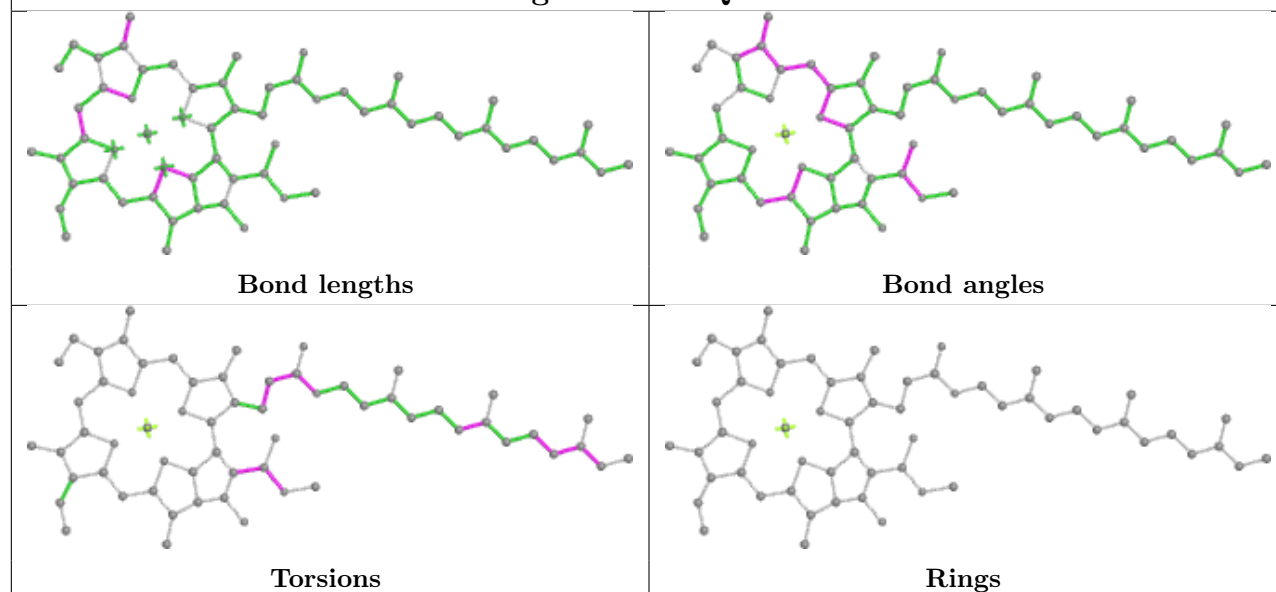


Ligand CLA 3 610**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 406****Bond lengths****Bond angles****Torsions****Rings**

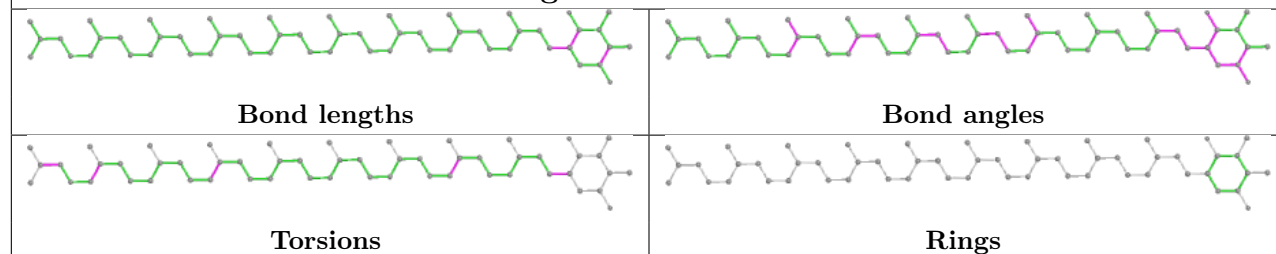
Ligand CLA 5 601

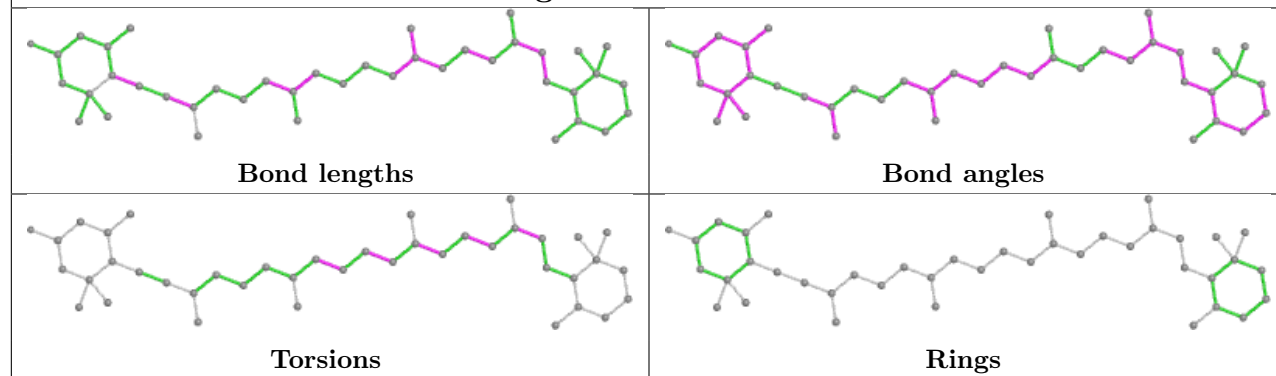
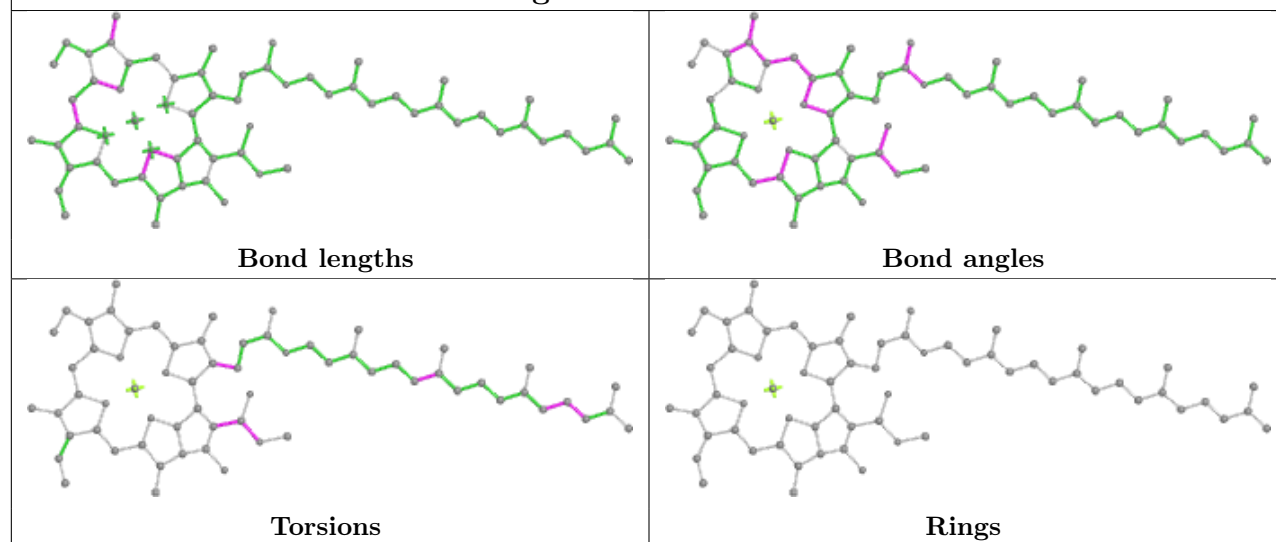
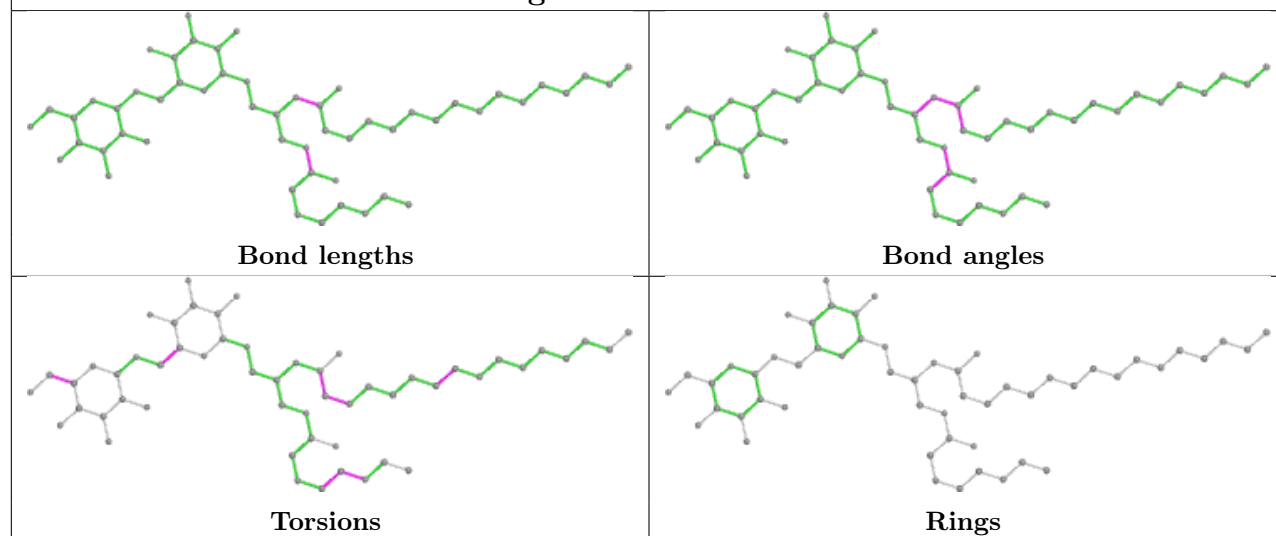


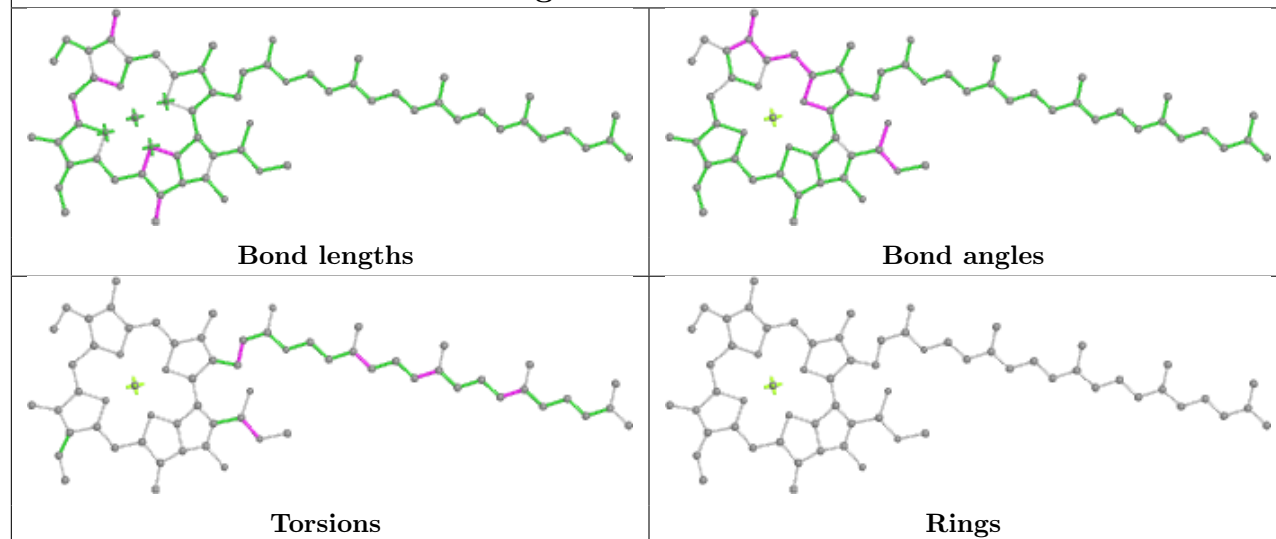
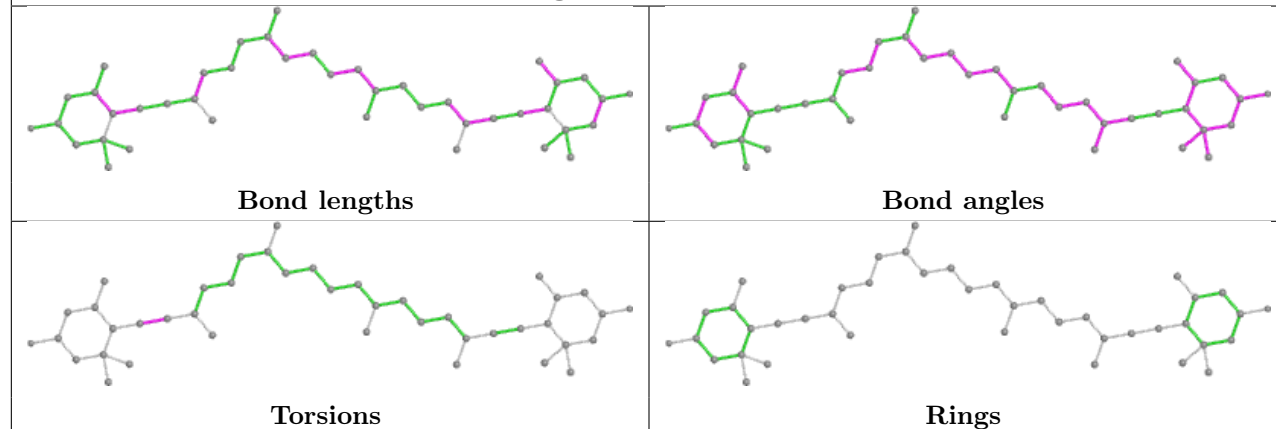
Ligand CLA Q 604



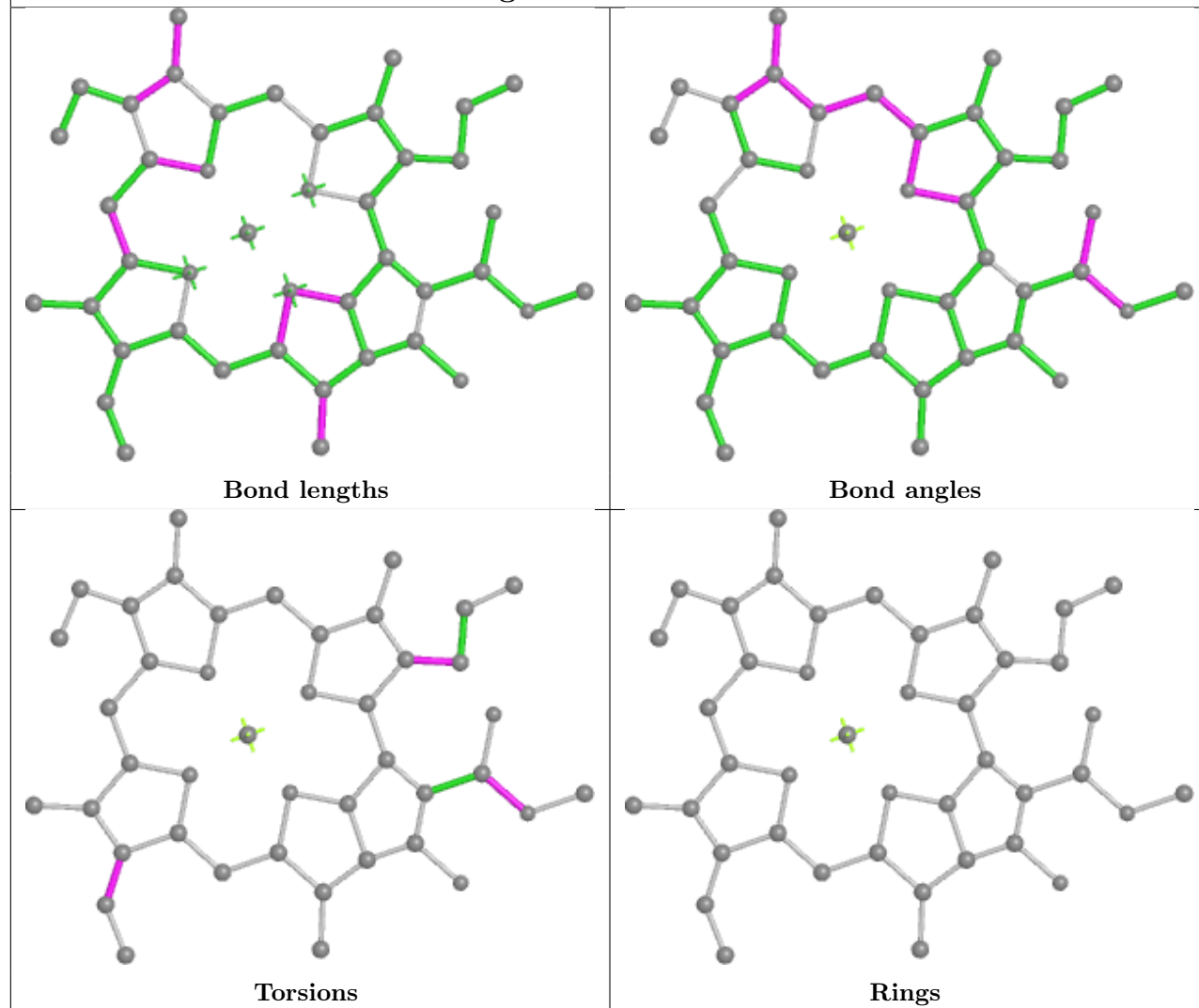
Ligand PL9 d 405



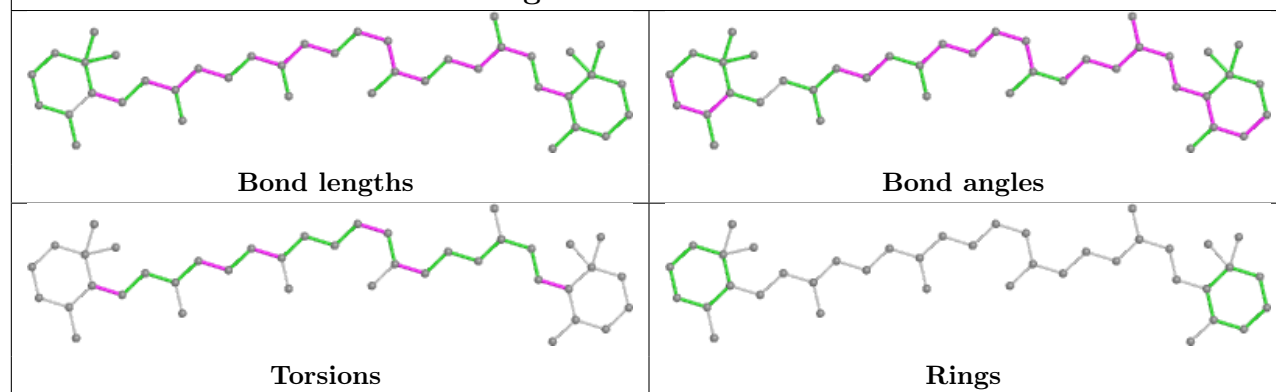
Ligand IHT N 620**Ligand CLA B 609****Ligand DGD C 532**

Ligand CLA b 603**Ligand II0 3 617**

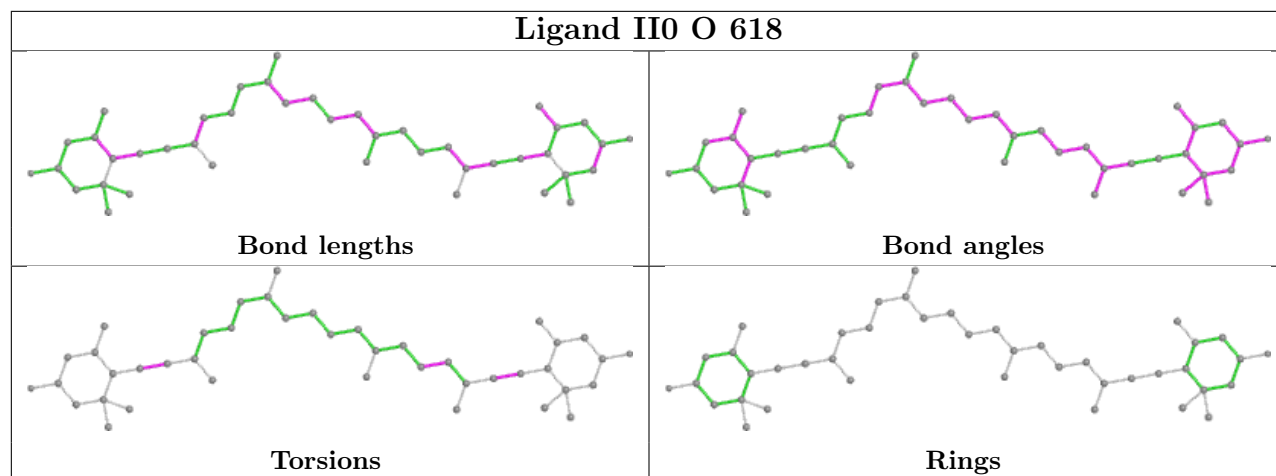
Ligand CLA N 607



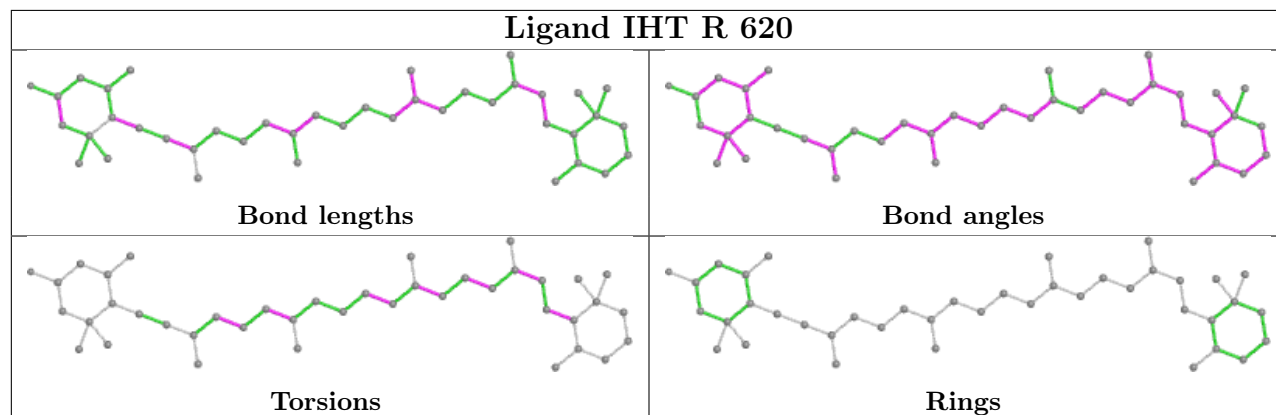
Ligand WVN C 530



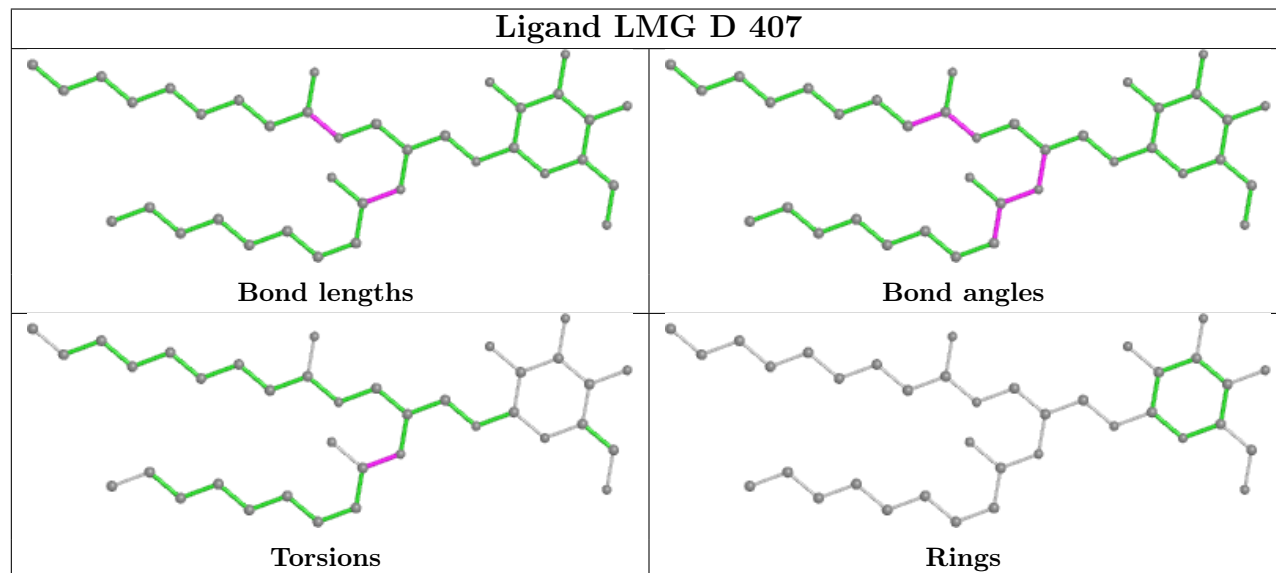
Ligand II0 O 618



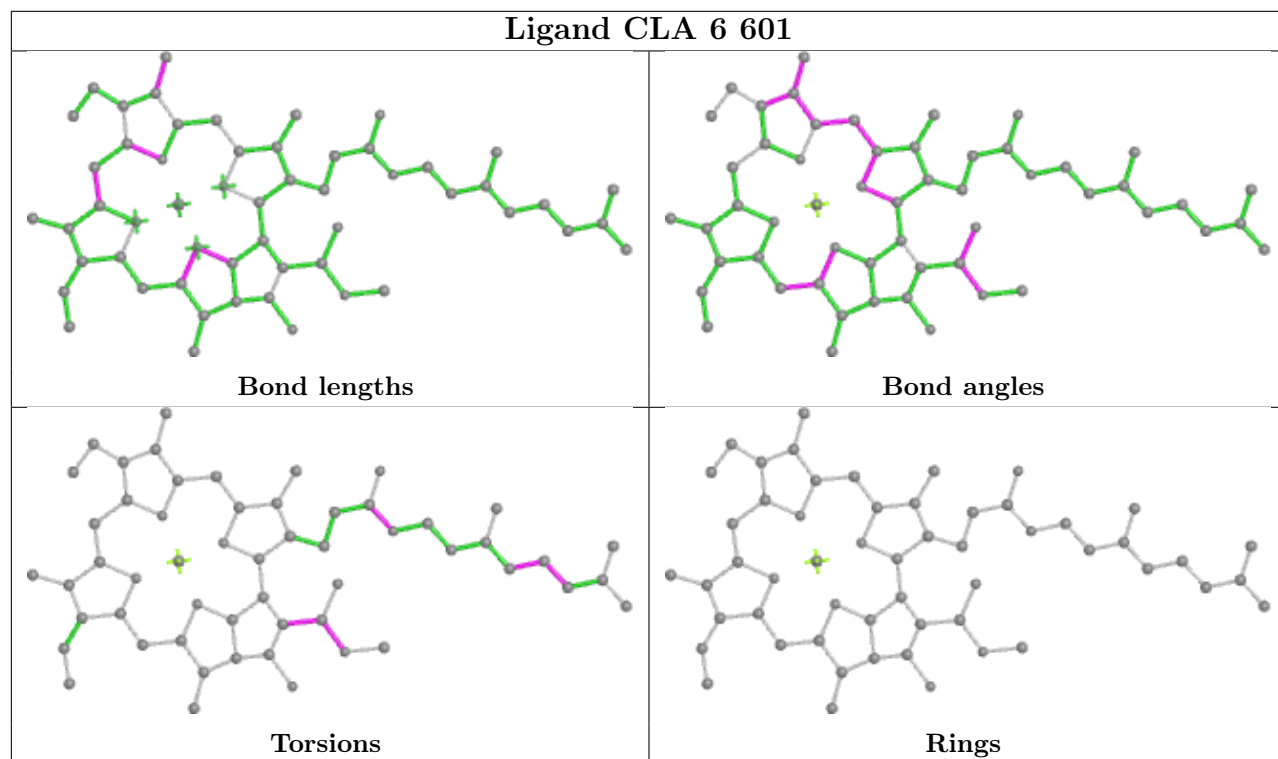
Ligand IHT R 620



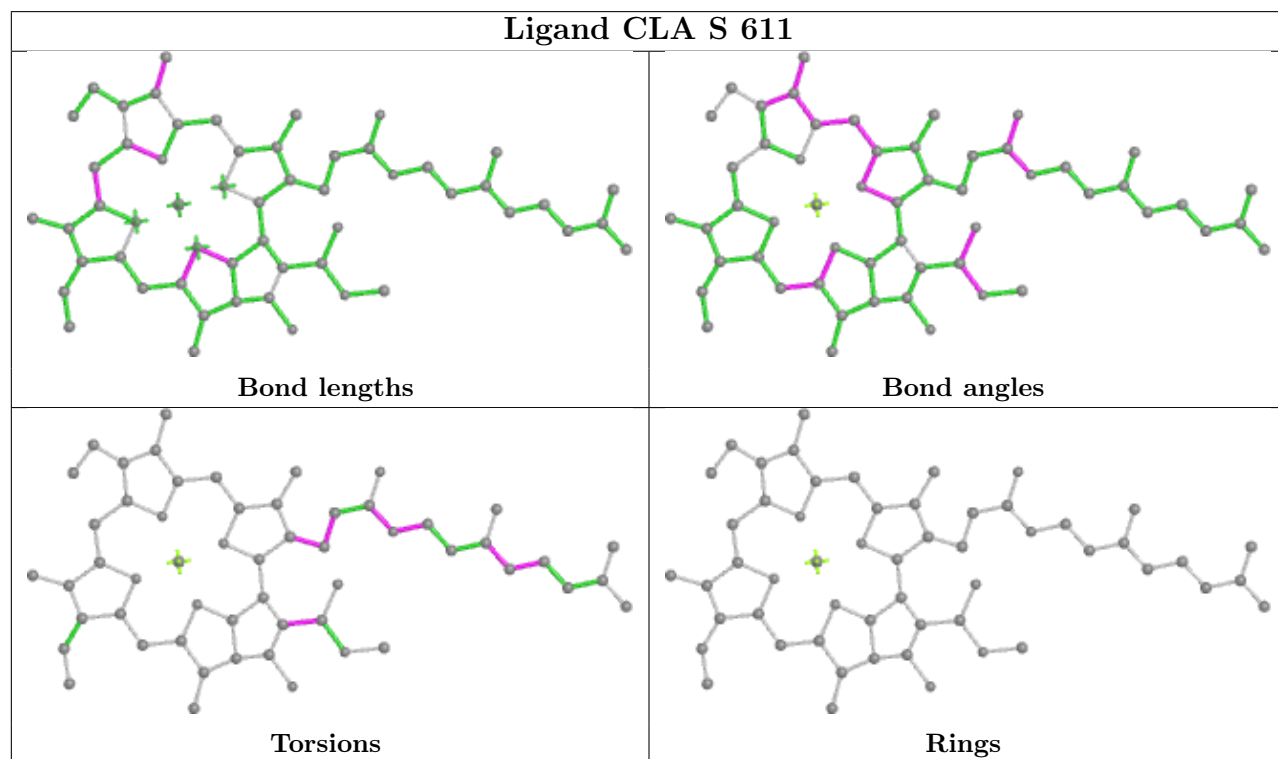
Ligand LMG D 407



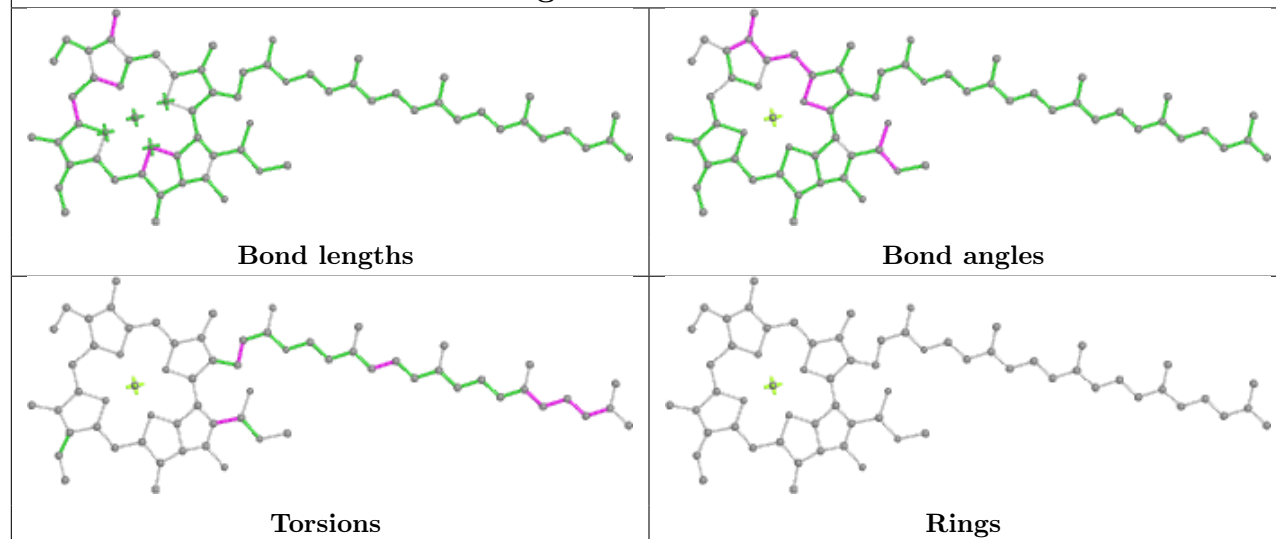
Ligand CLA 6 601



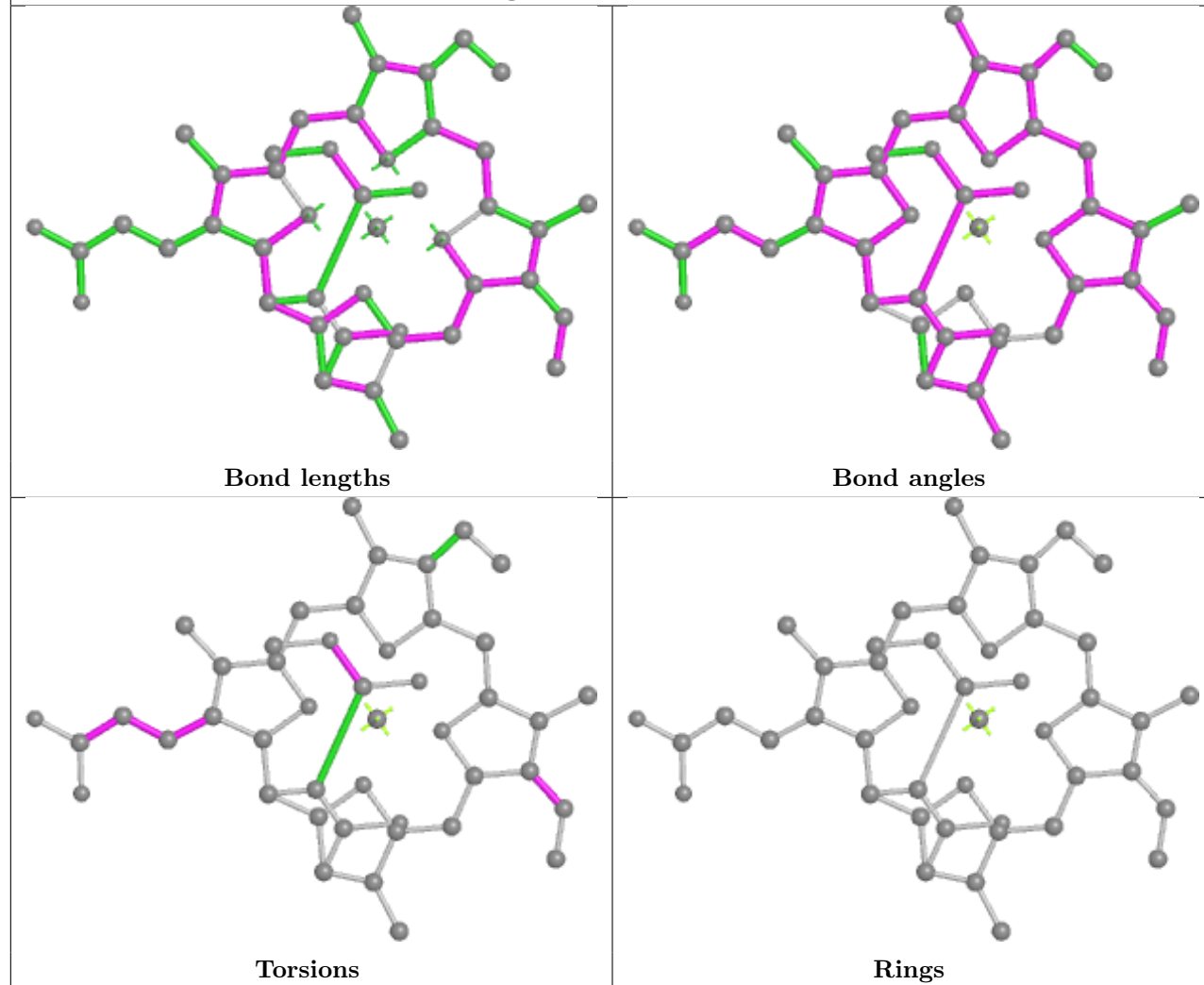
Ligand CLA S 611

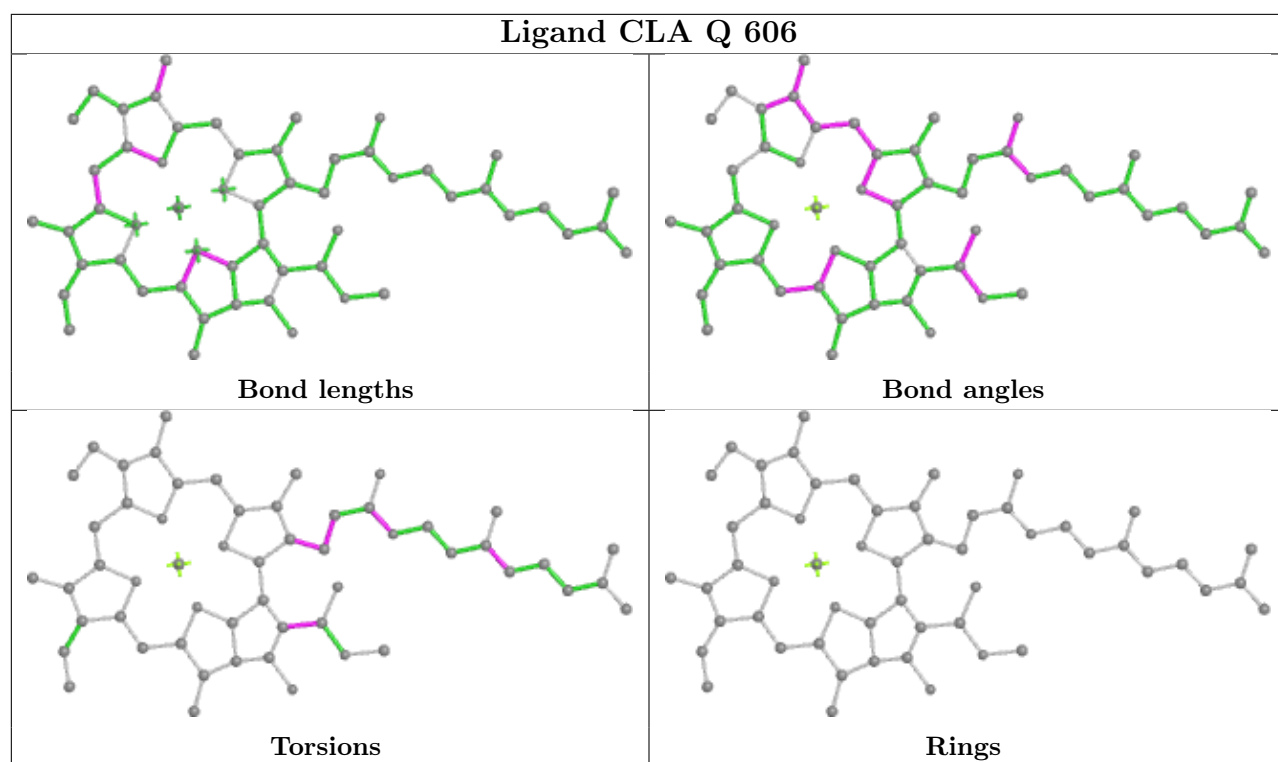


Ligand CLA c 522

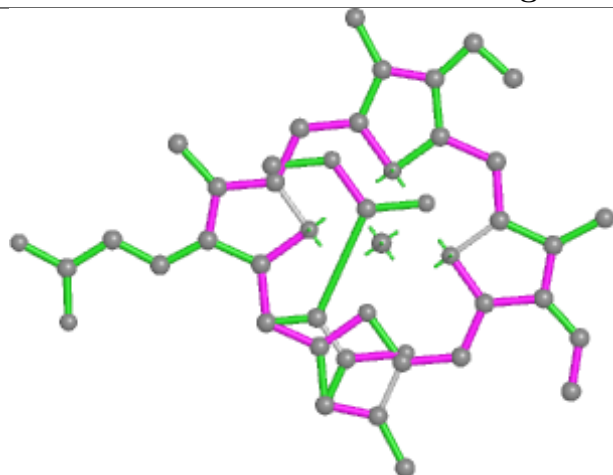


Ligand KC2 R 612

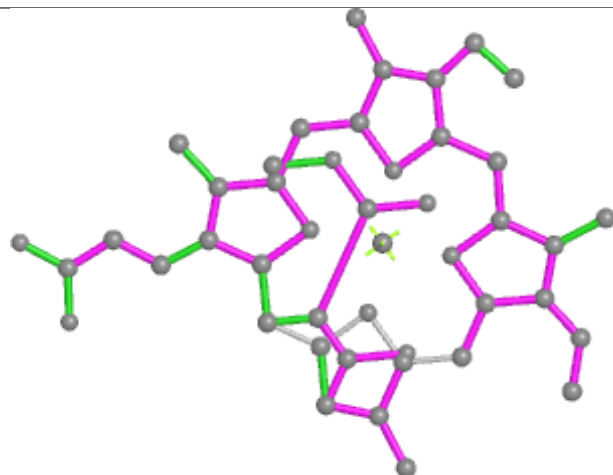




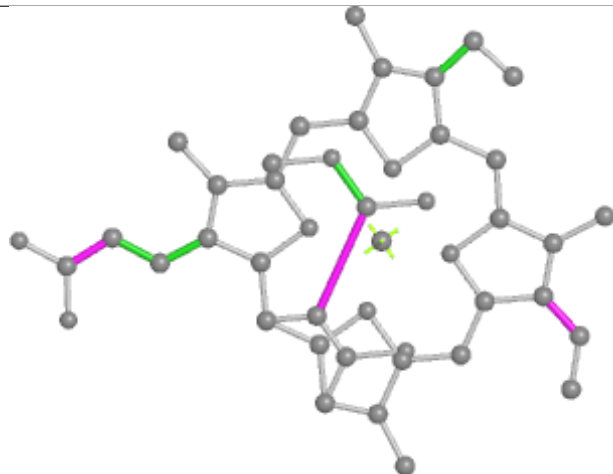
Ligand KC2 6 612



Bond lengths



Bond angles

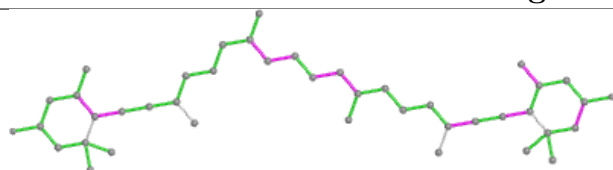


Torsions

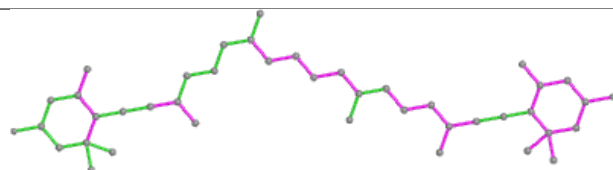


Rings

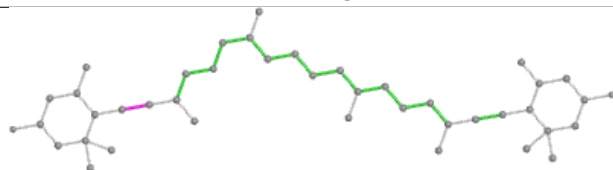
Ligand II0 O 617



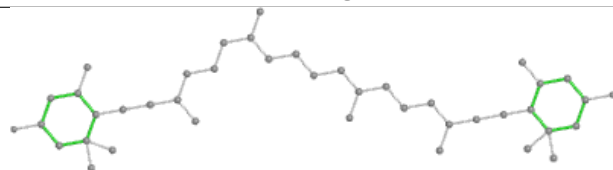
Bond lengths



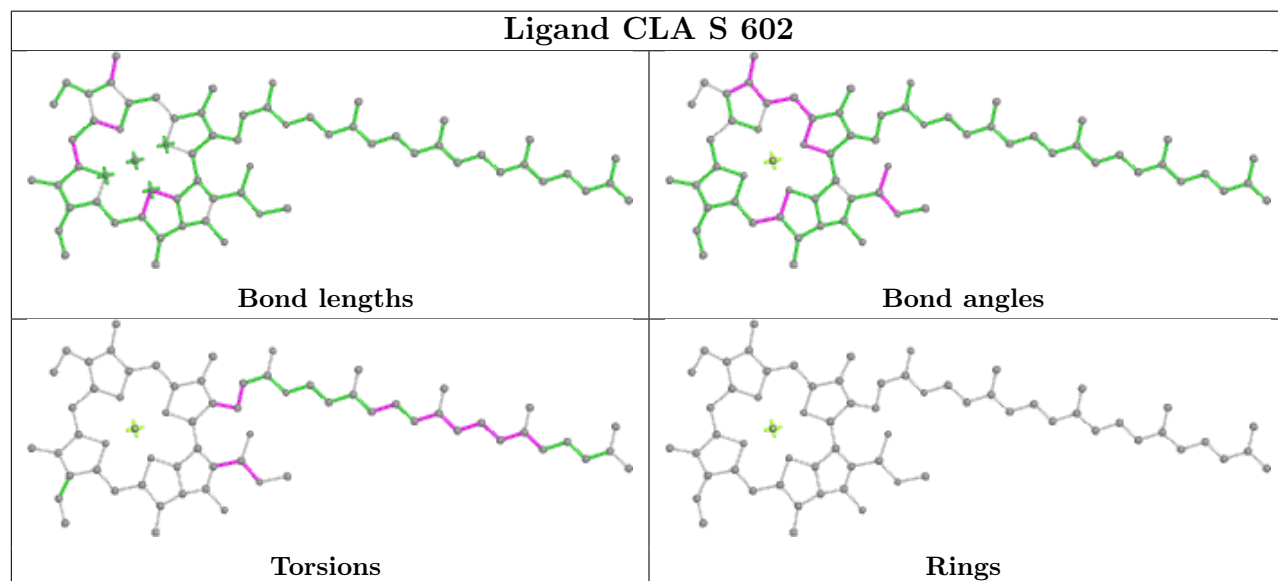
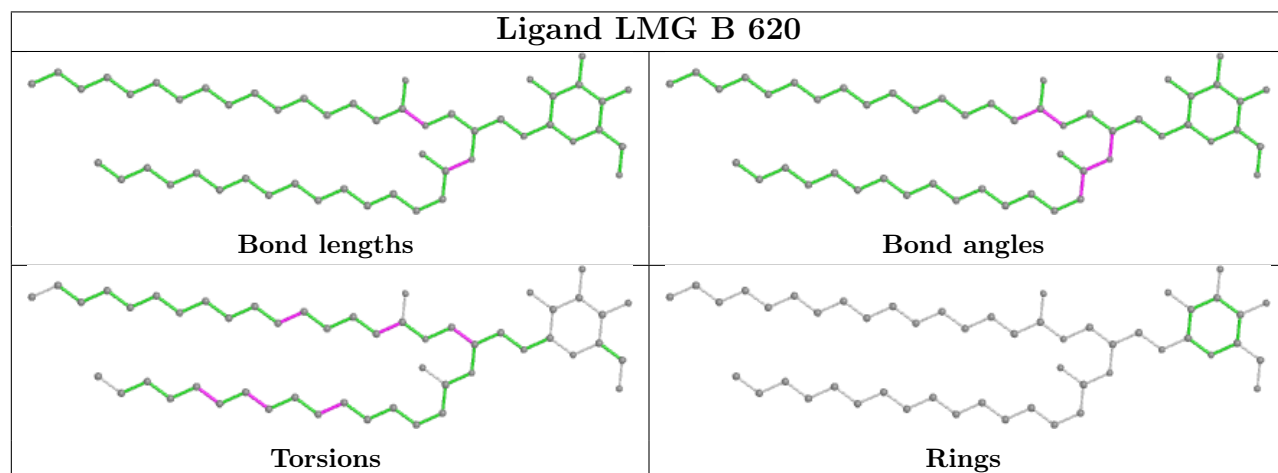
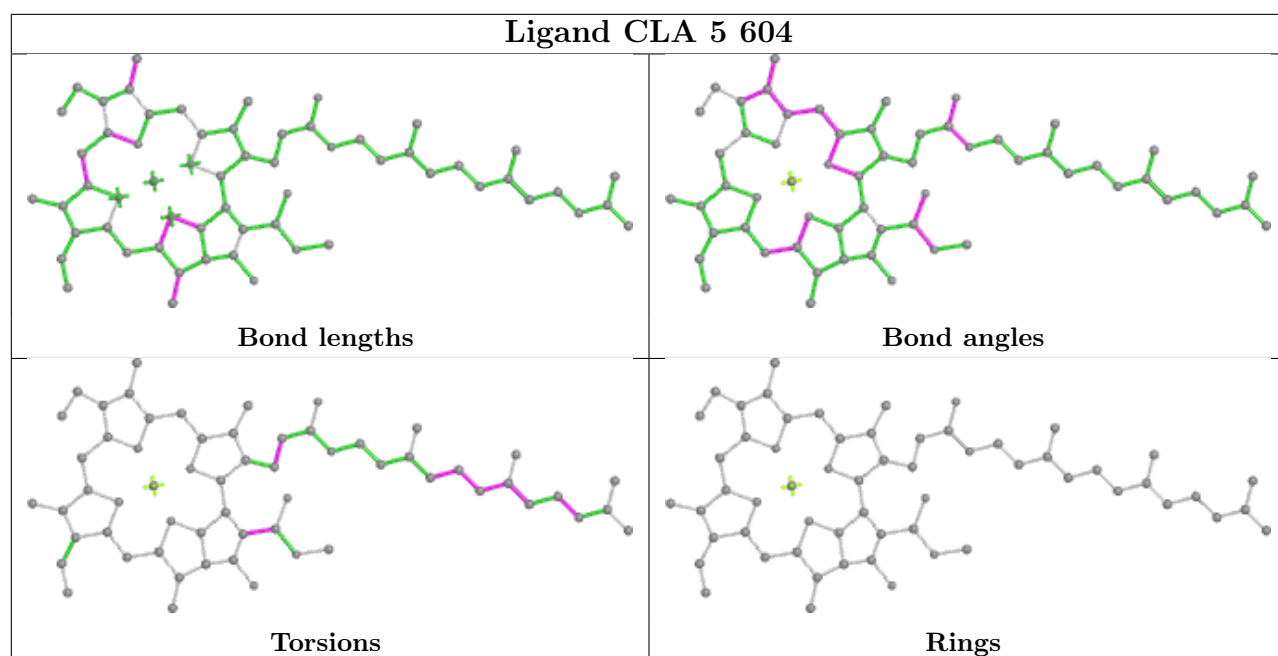
Bond angles

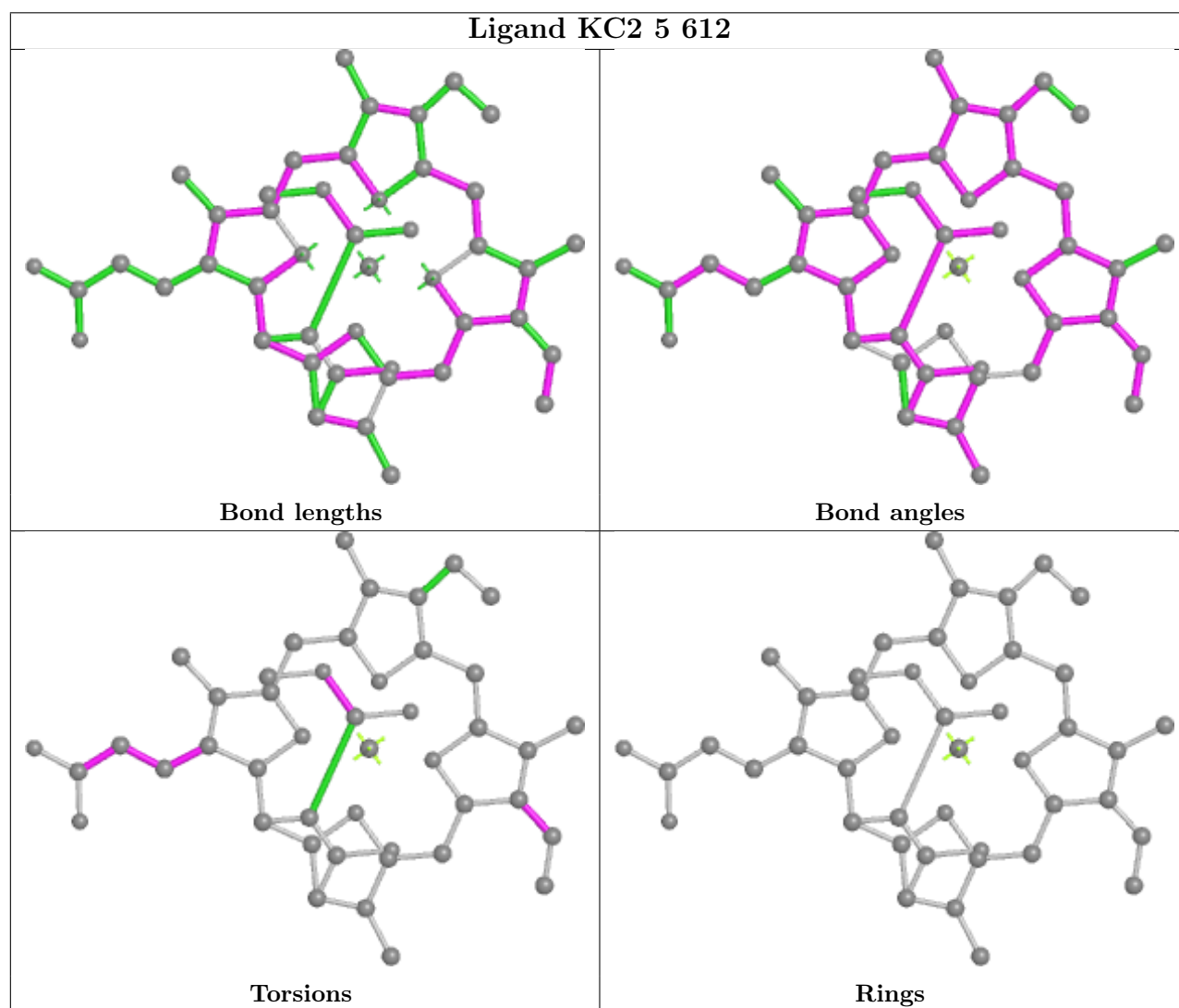
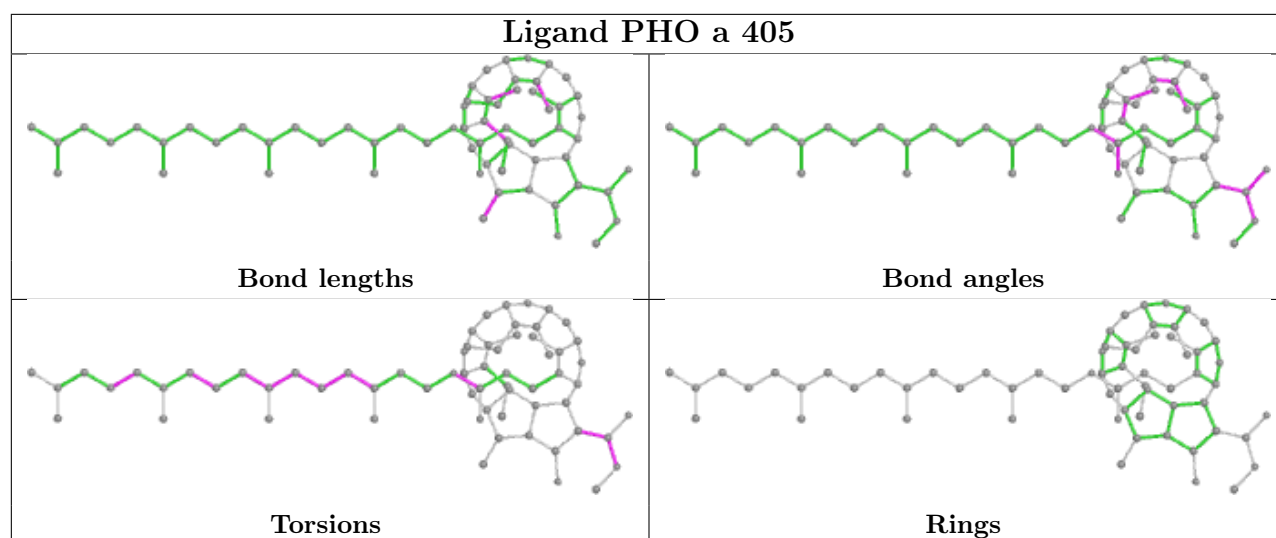


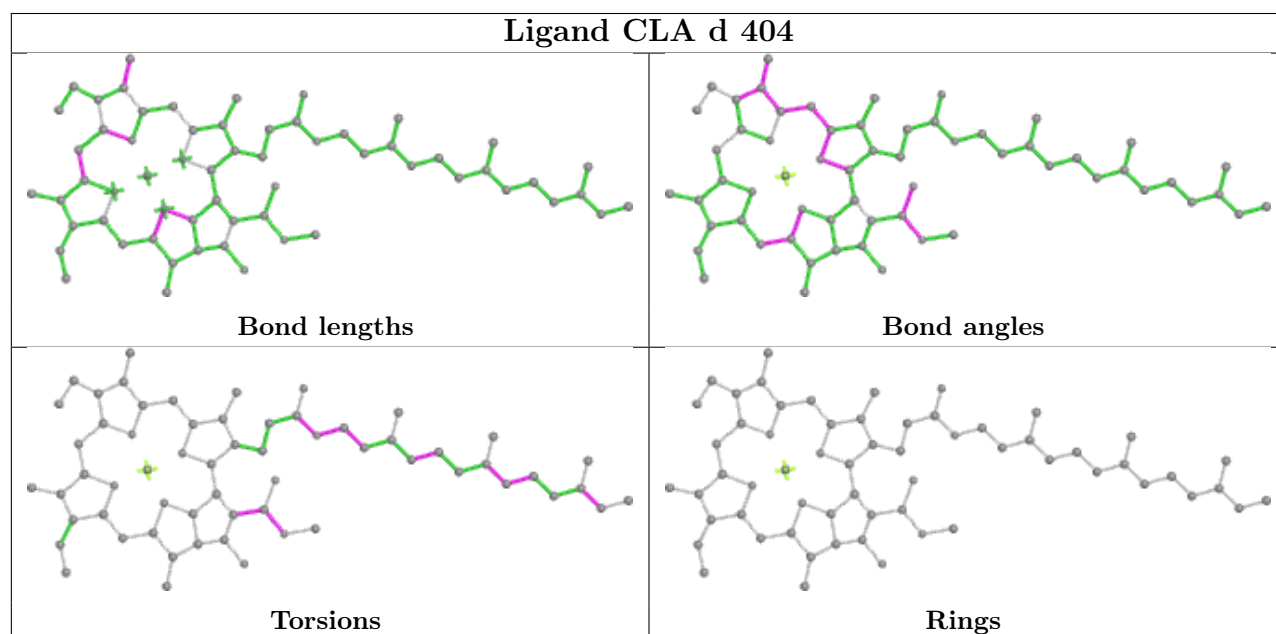
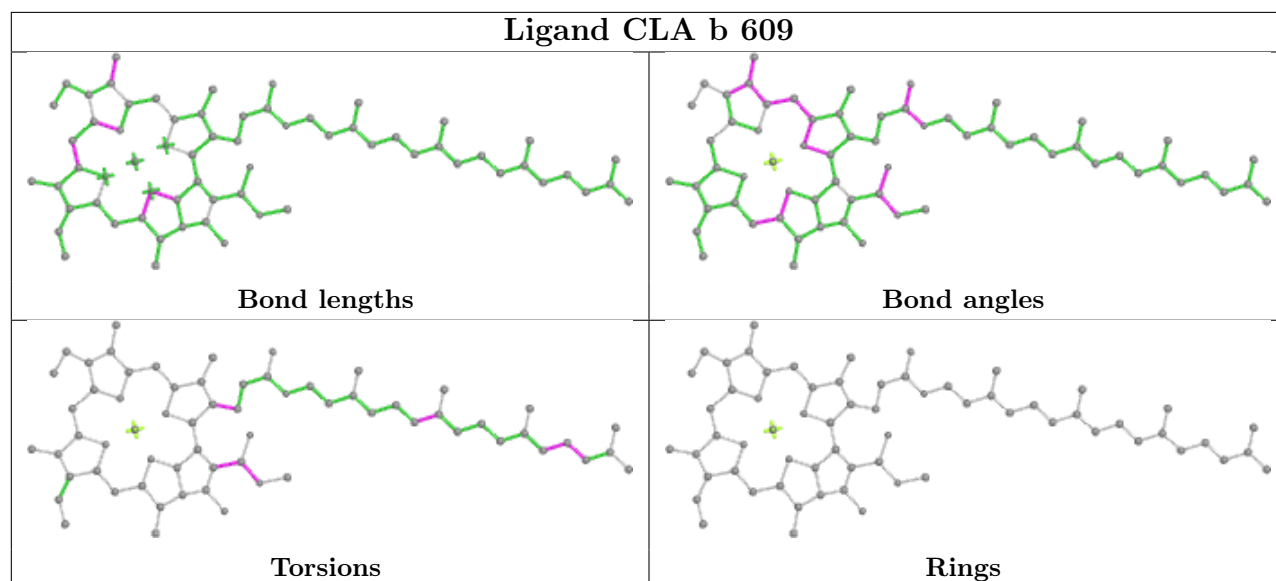
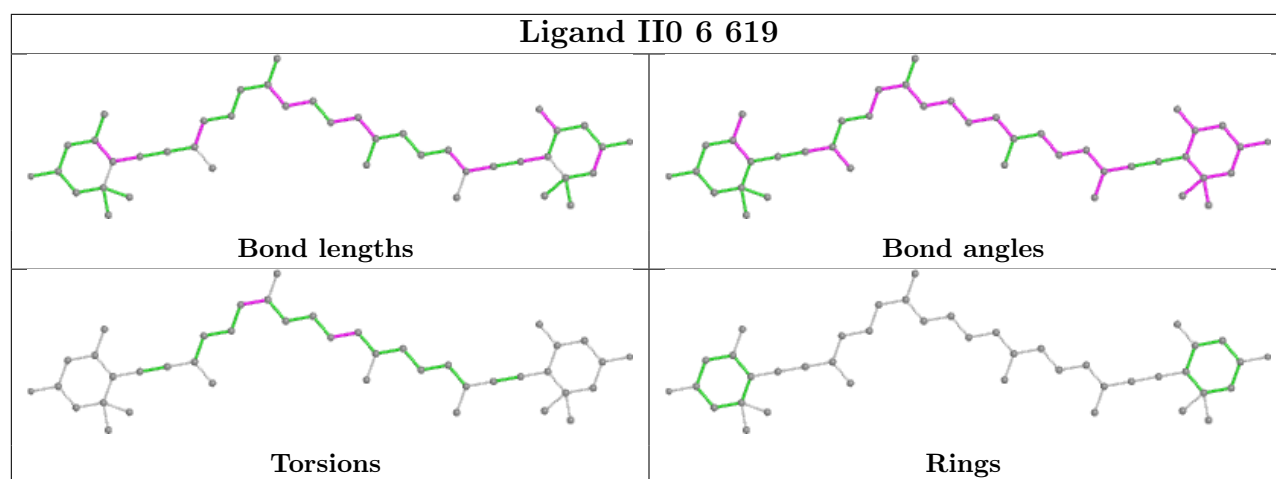
Torsions



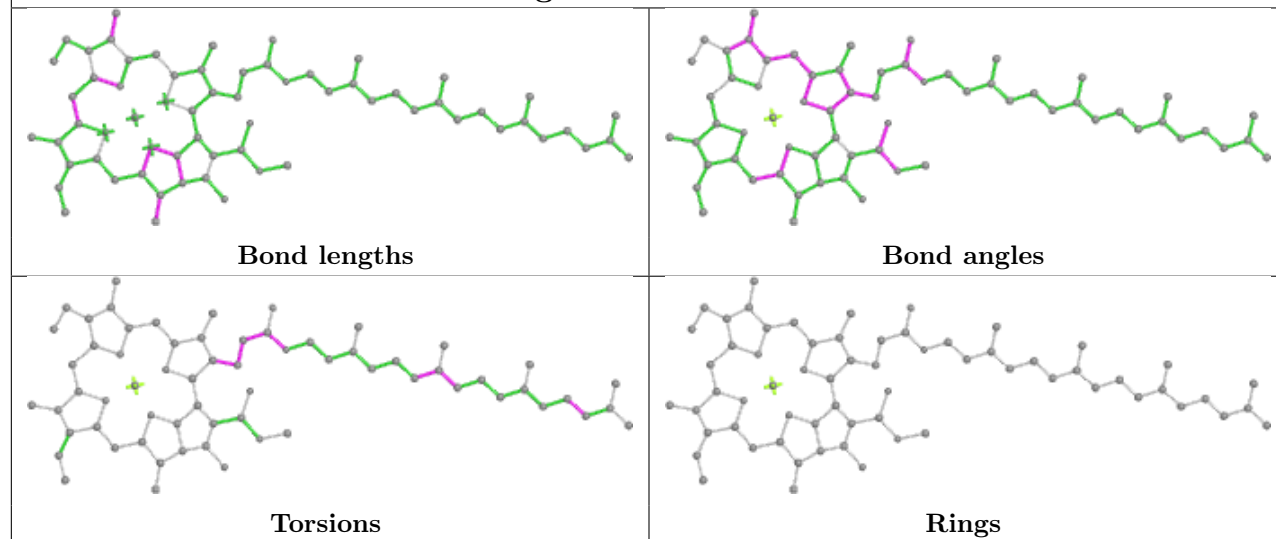
Rings



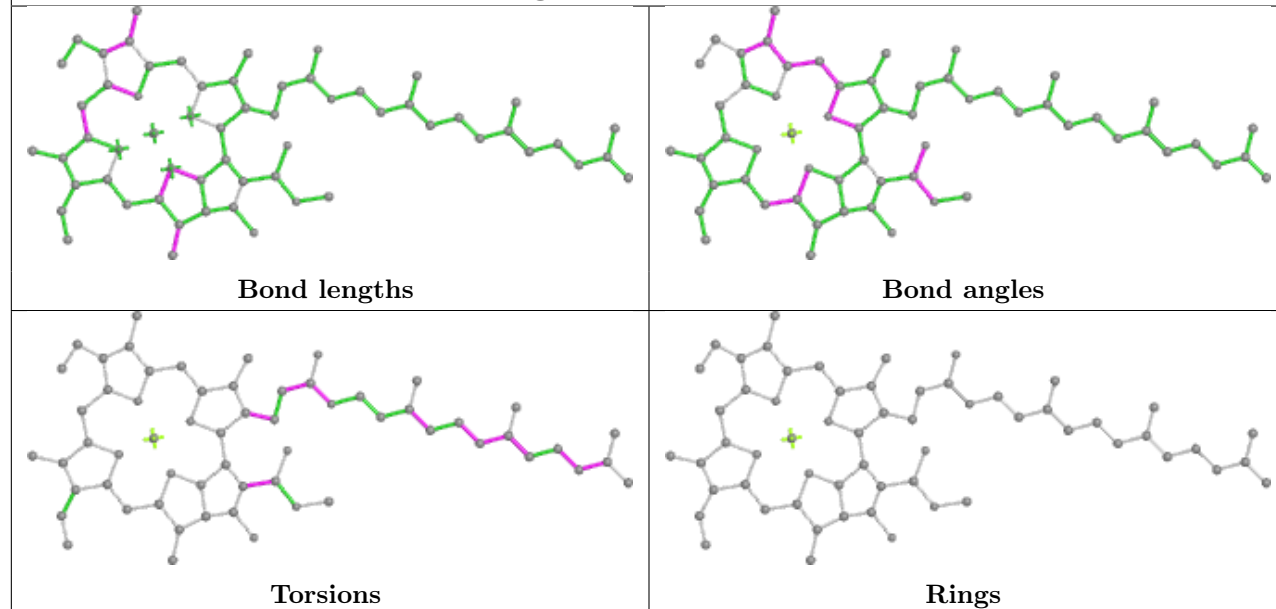




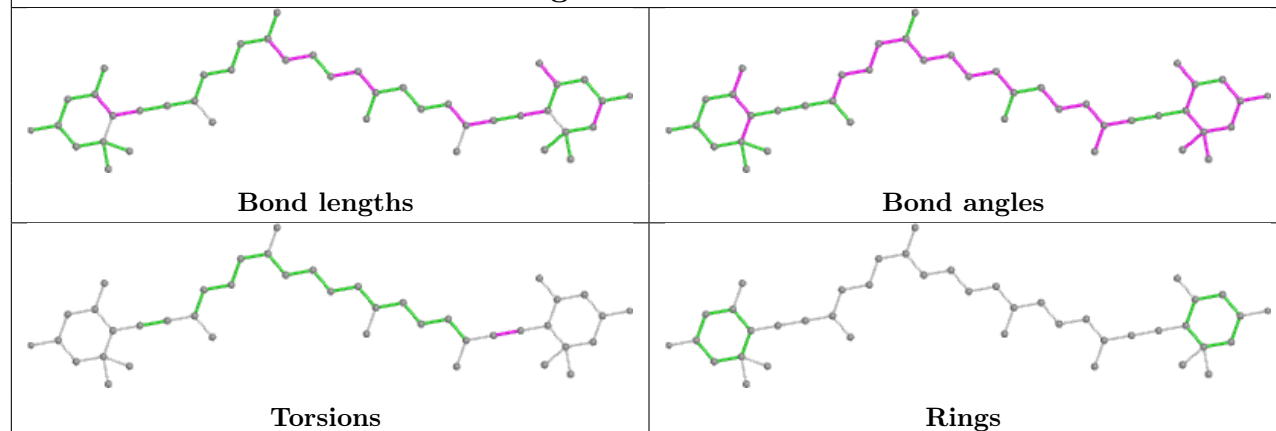
Ligand CLA b 612



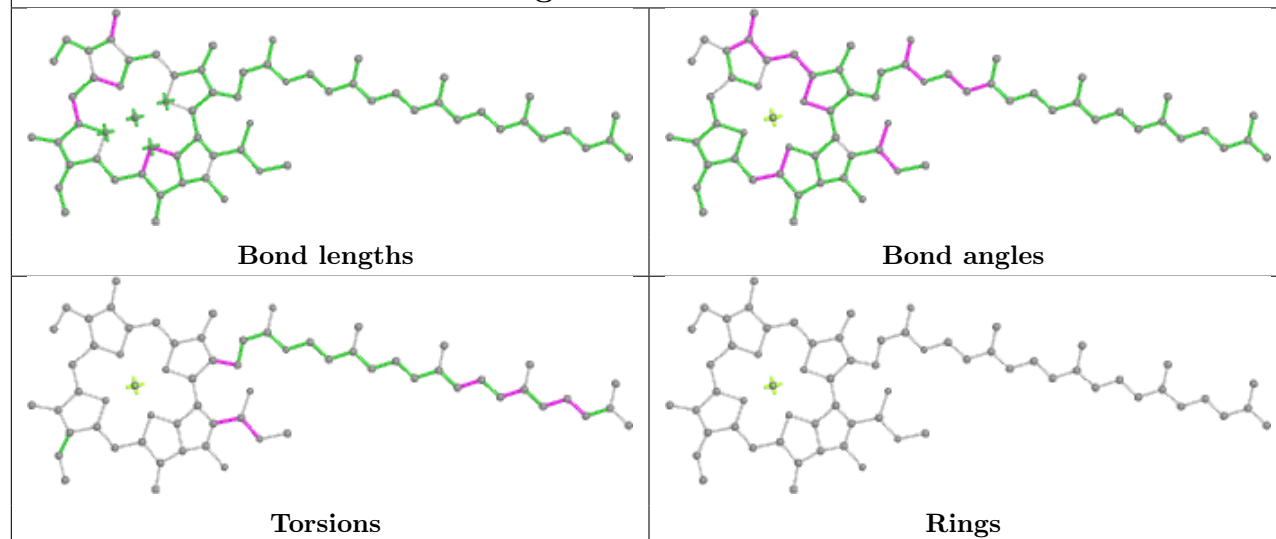
Ligand CLA O 607



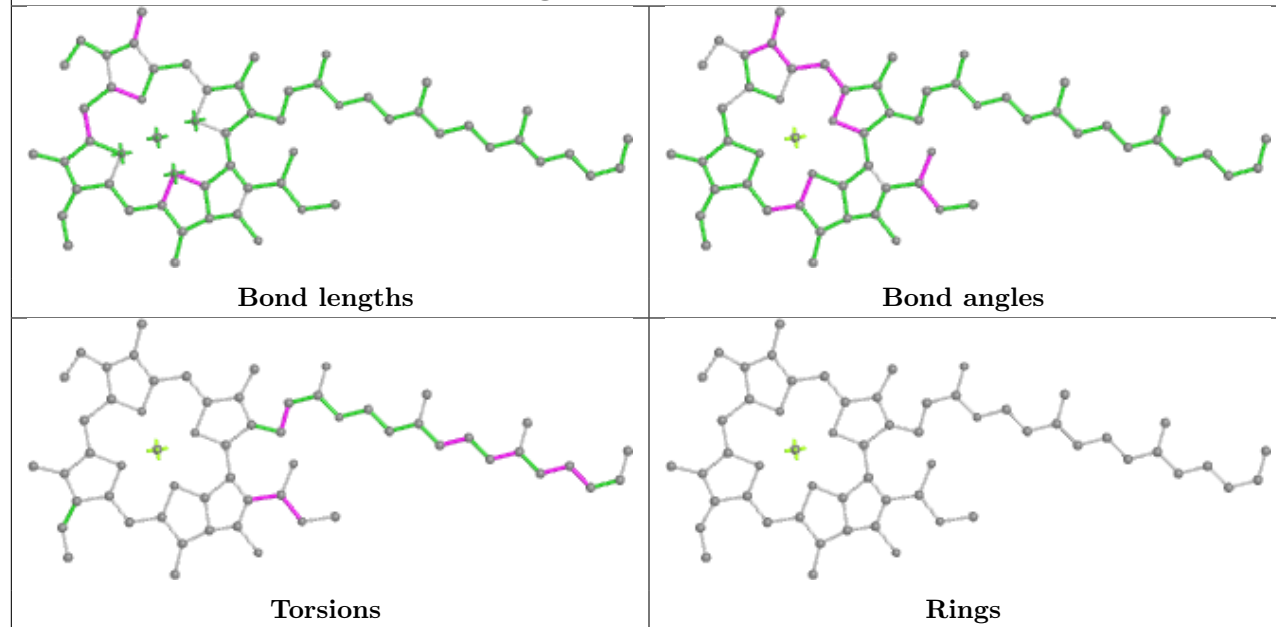
Ligand II0 2 618



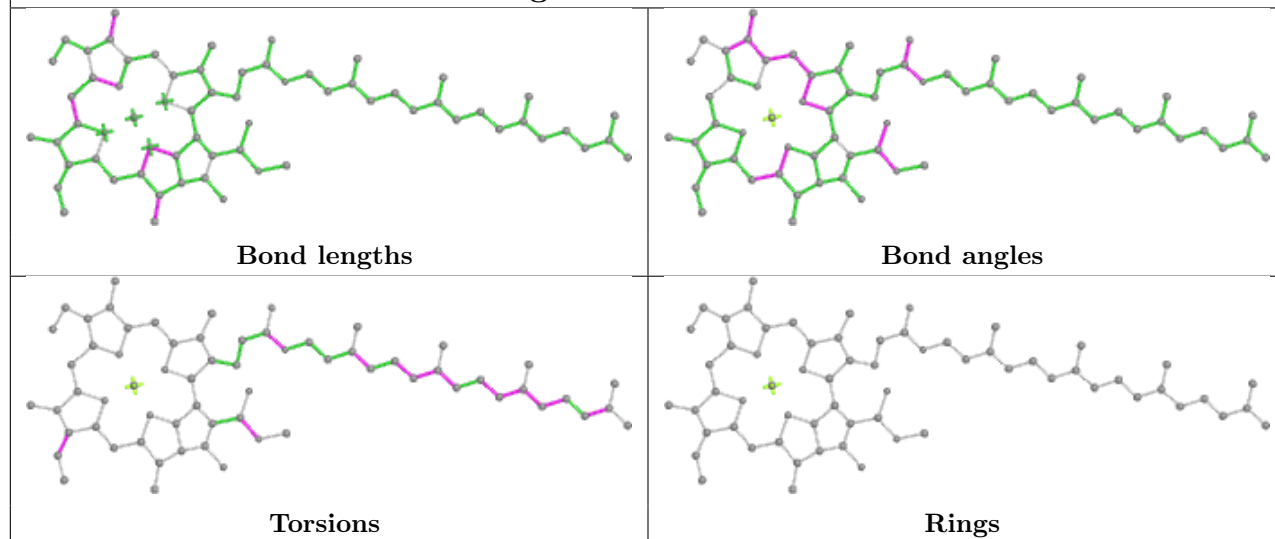
Ligand CLA b 611



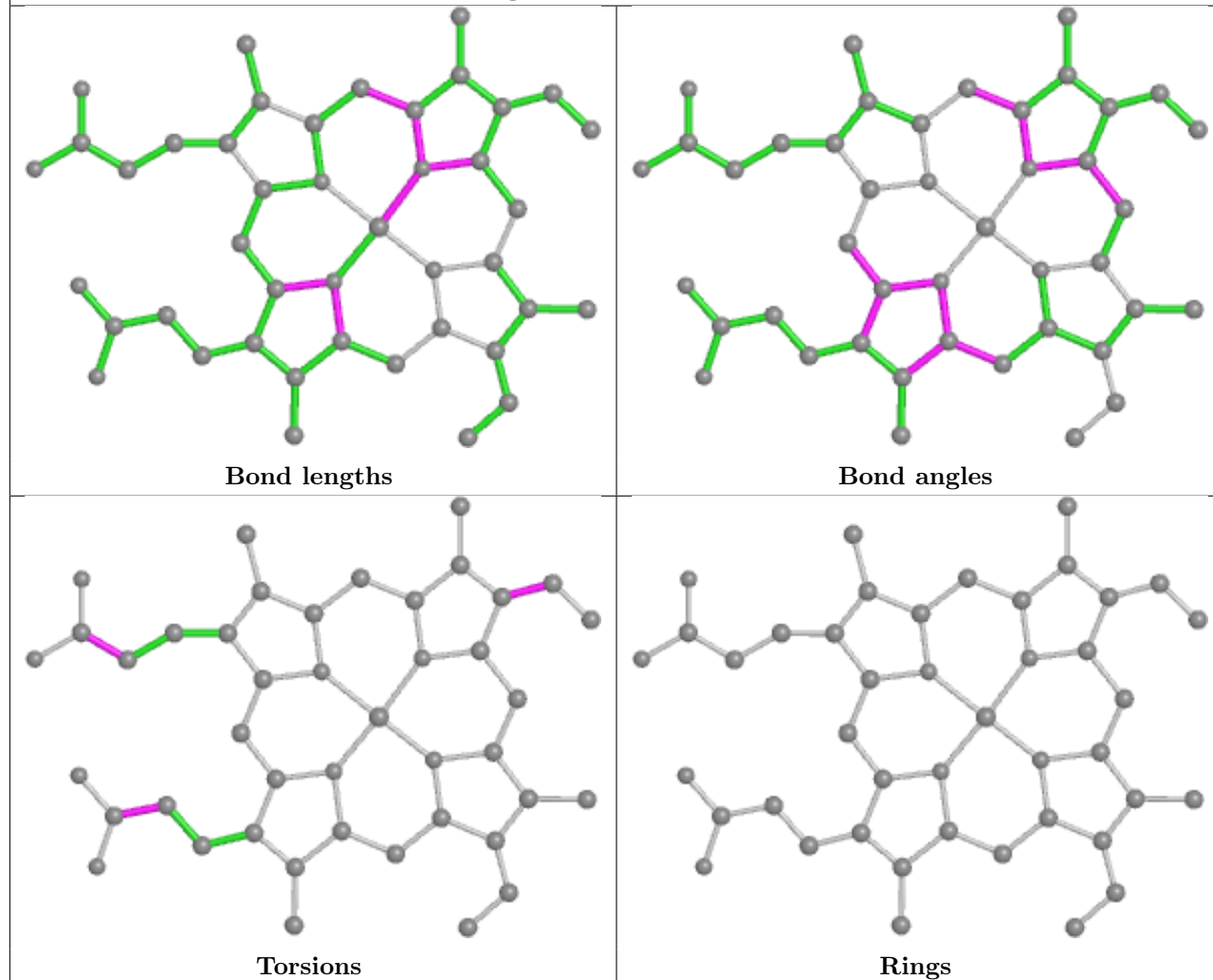
Ligand CLA 5 610

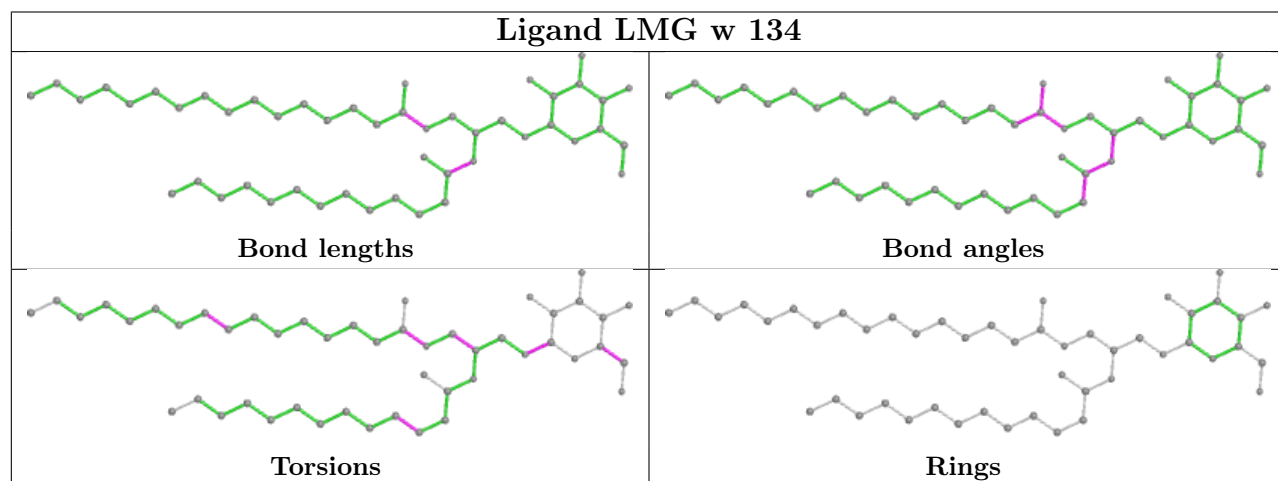
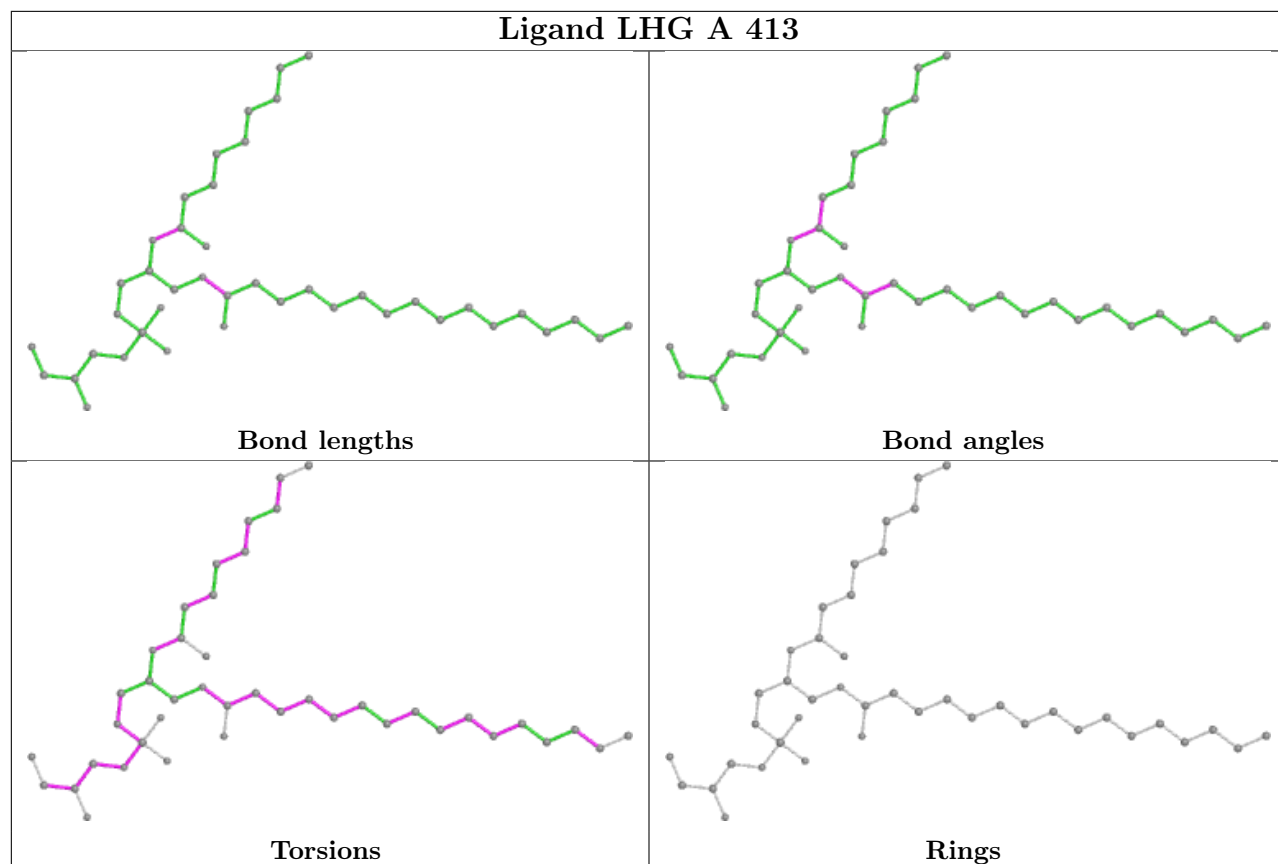


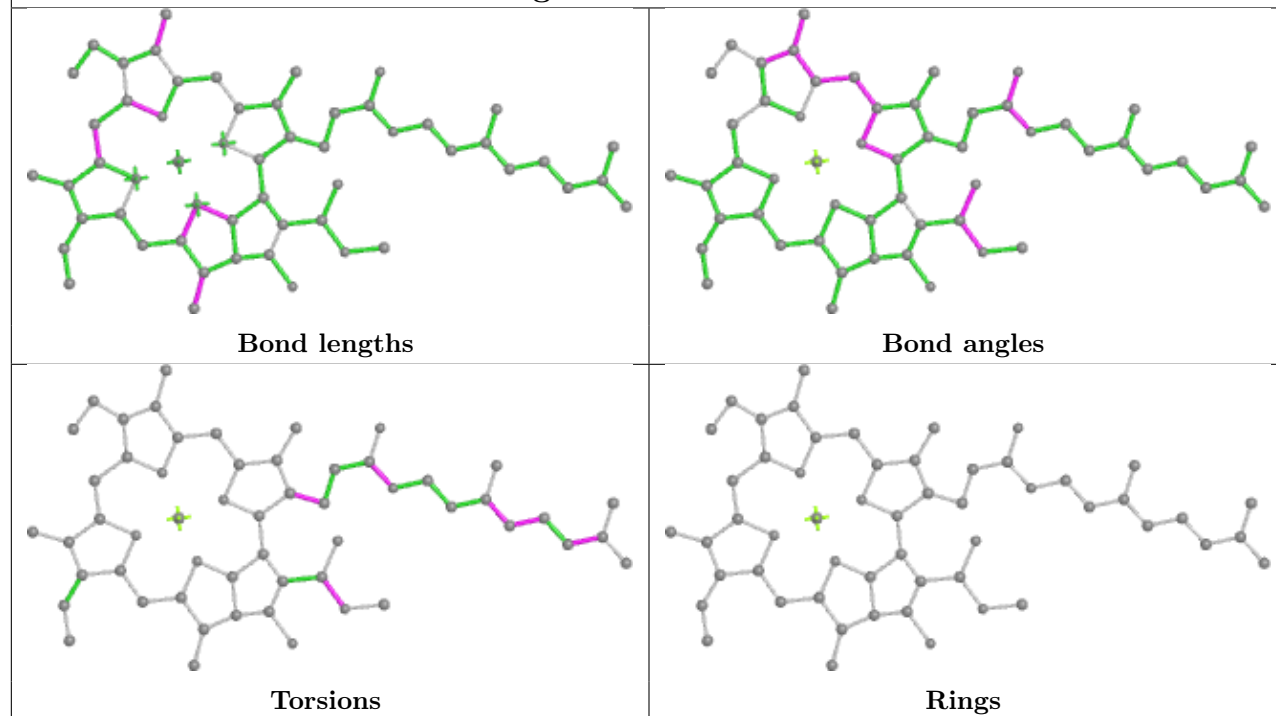
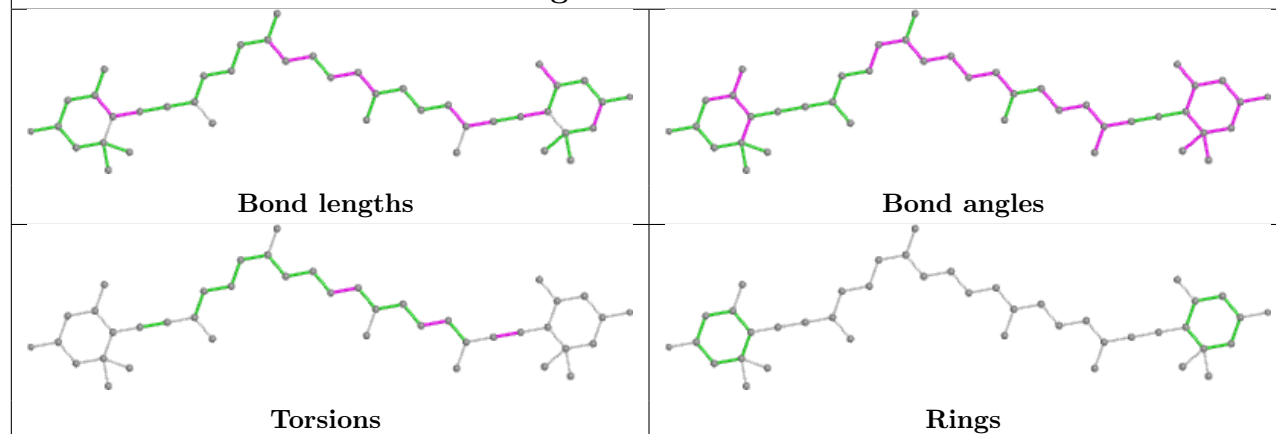
Ligand CLA G 301



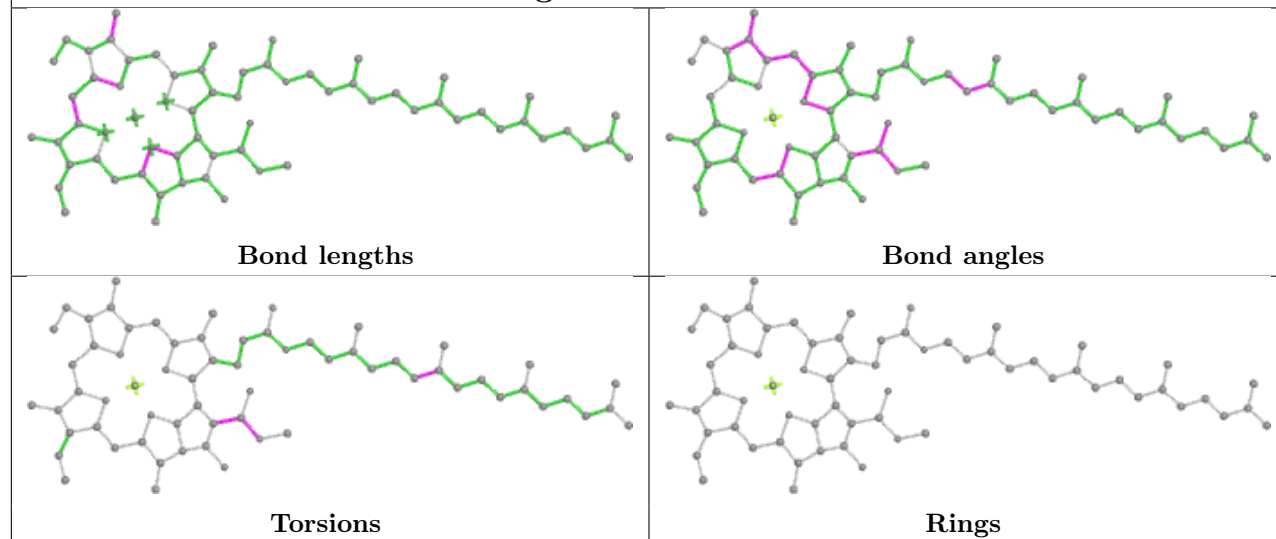
Ligand HEM e 102



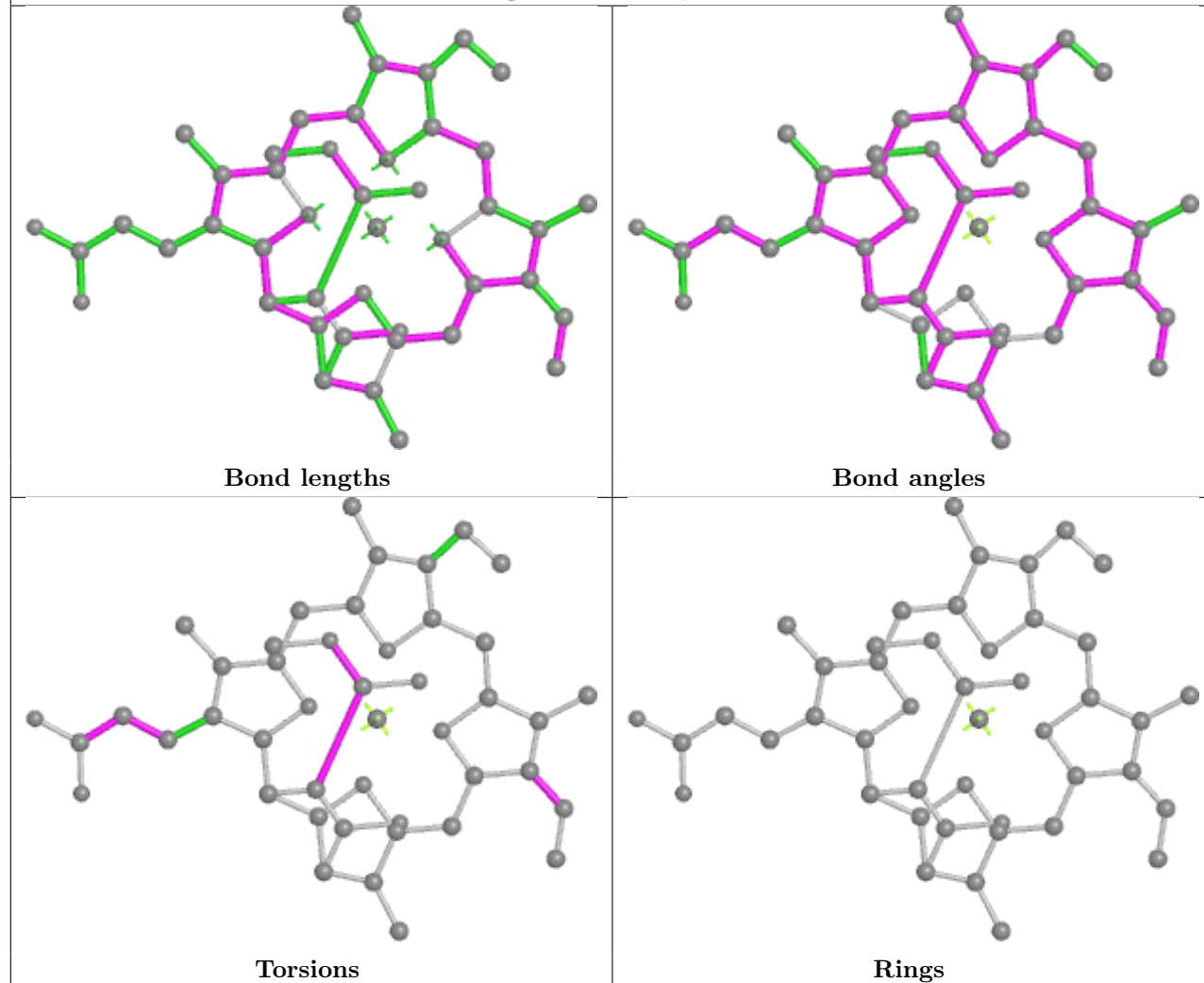


Ligand CLA P 613**Ligand II0 1 618**

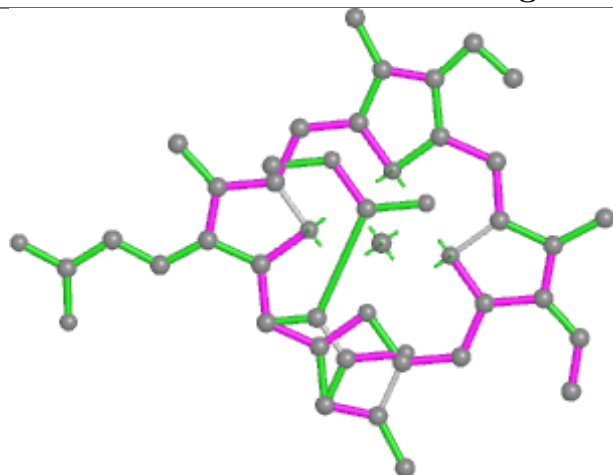
Ligand CLA b 602



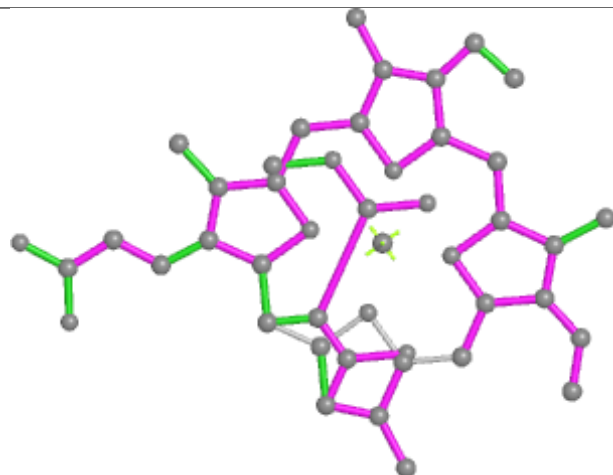
Ligand KC2 Q 611



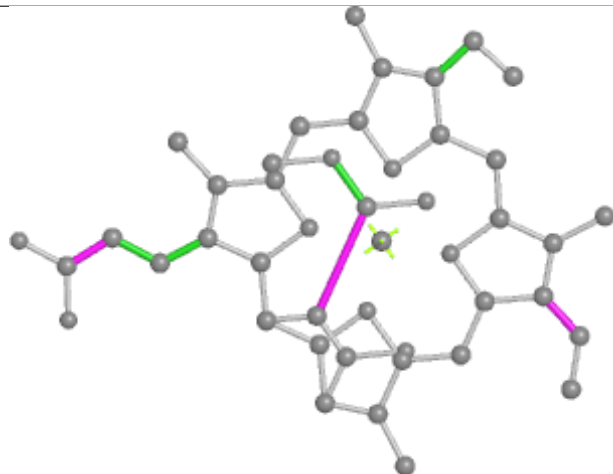
Ligand KC2 S 612



Bond lengths



Bond angles

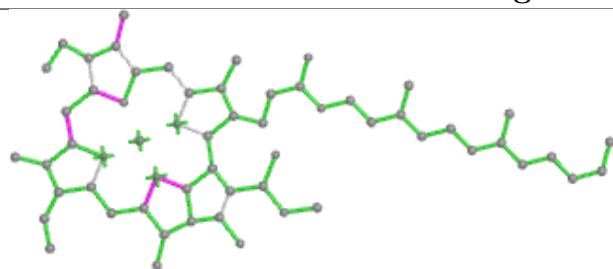


Torsions

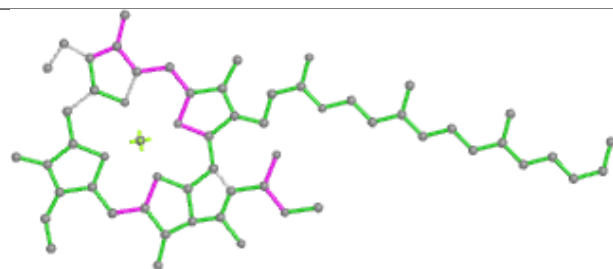


Rings

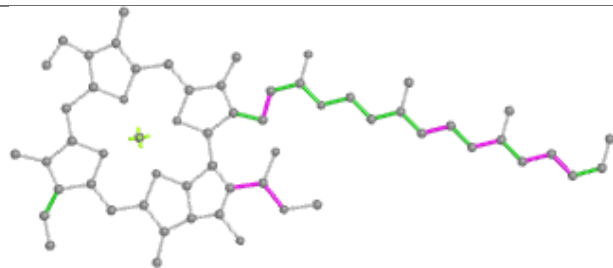
Ligand CLA R 610



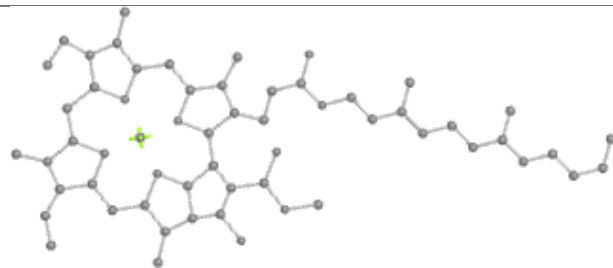
Bond lengths



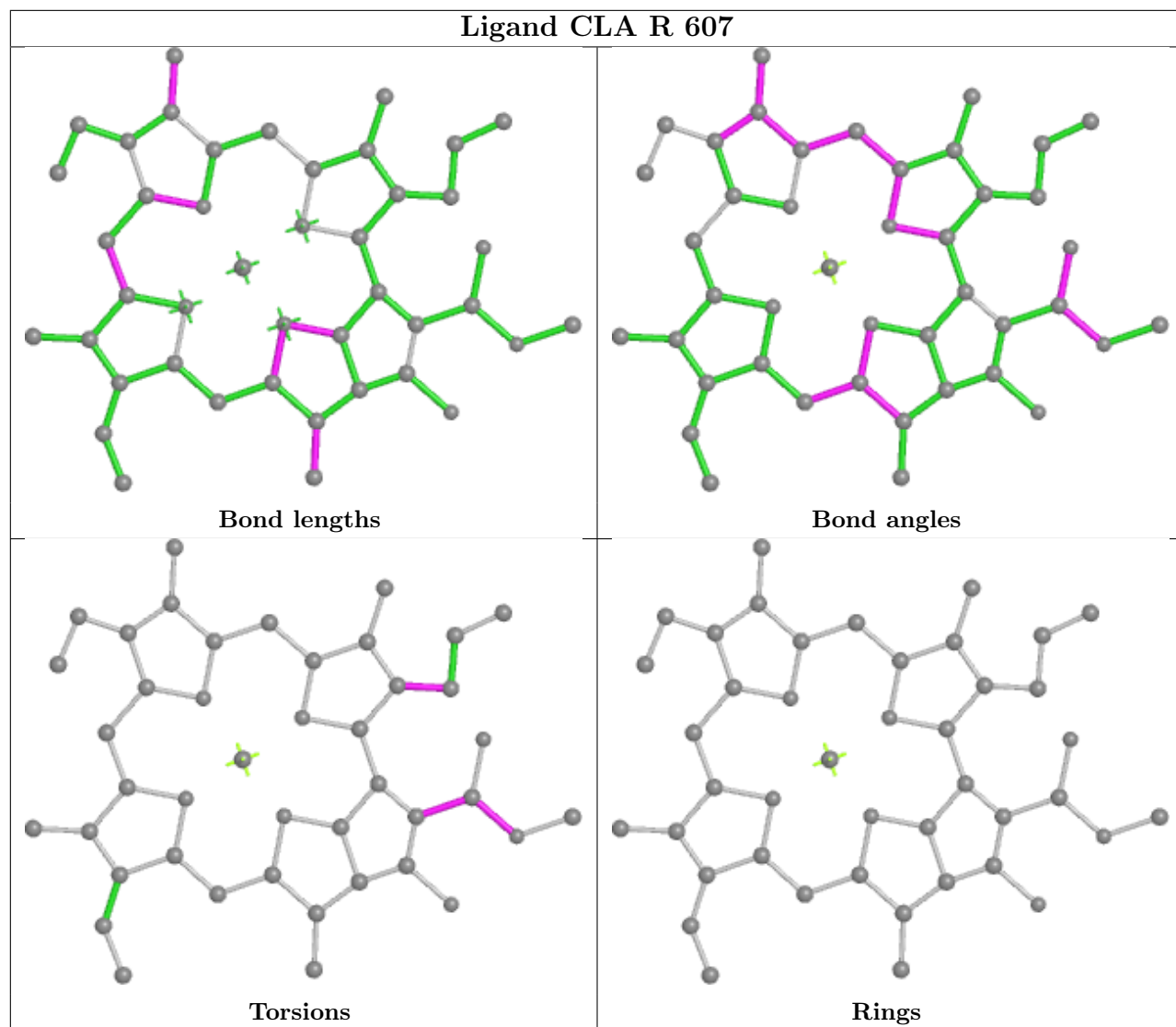
Bond angles



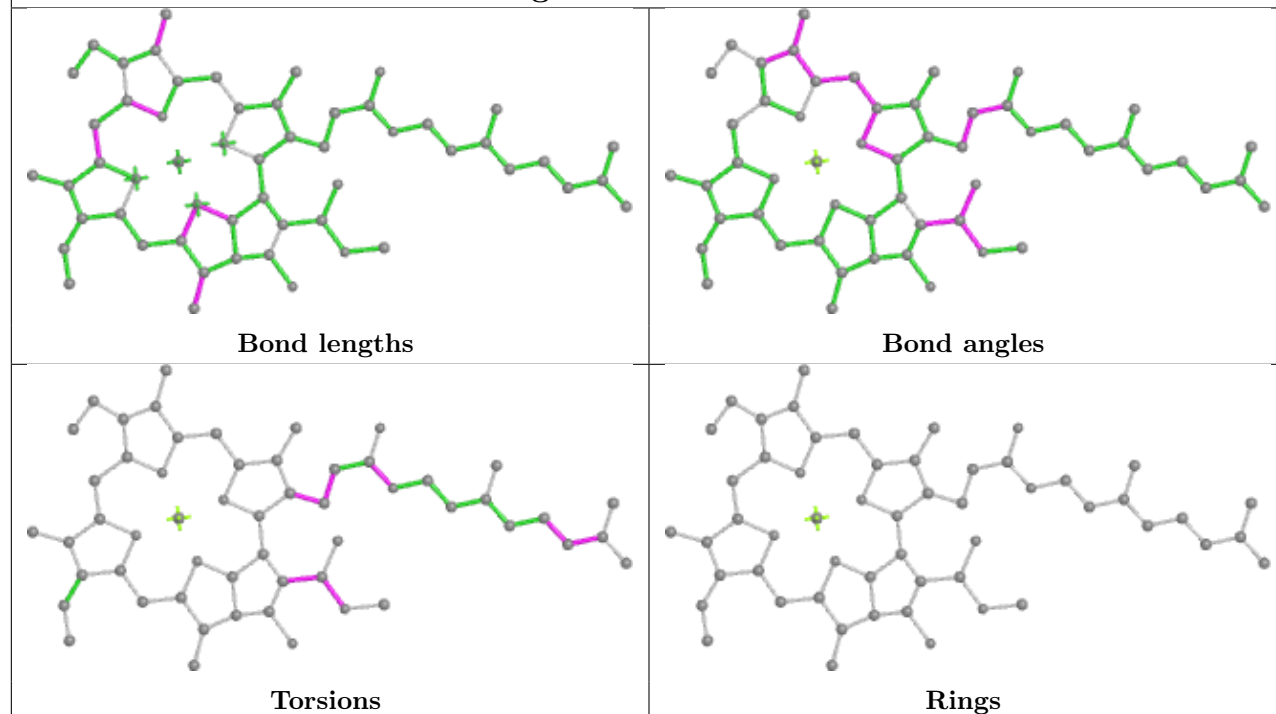
Torsions



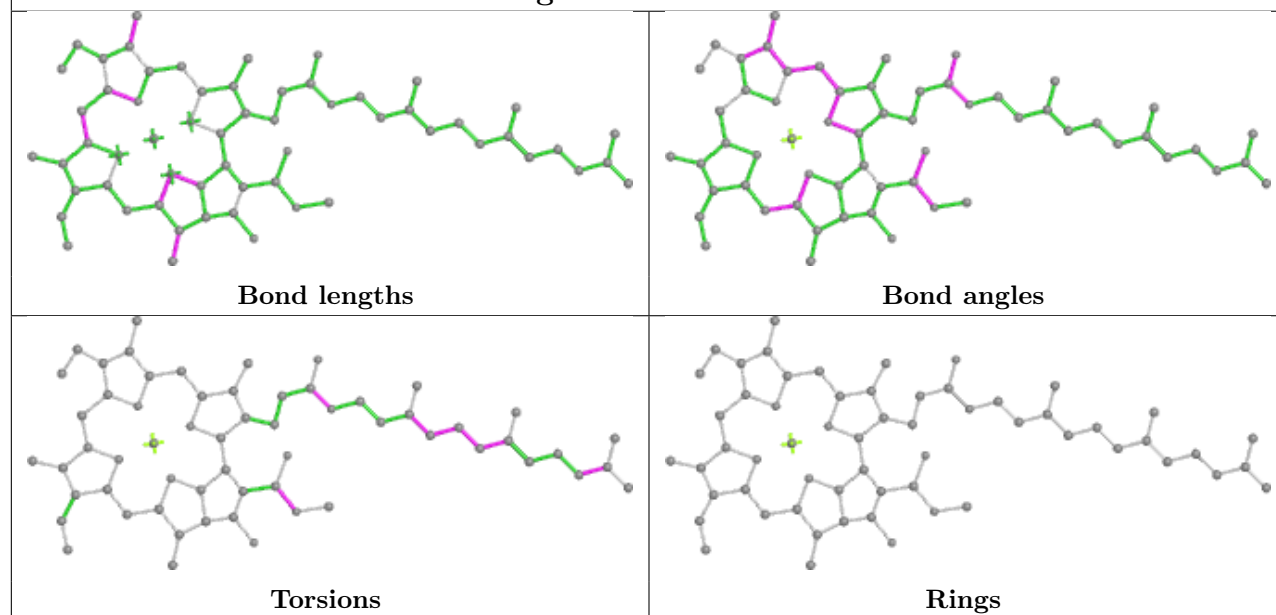
Rings



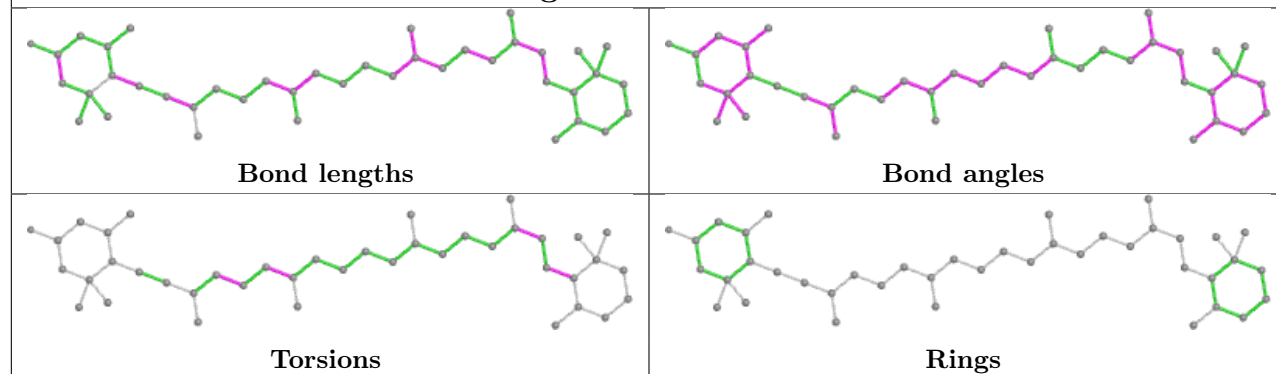
Ligand CLA R 613



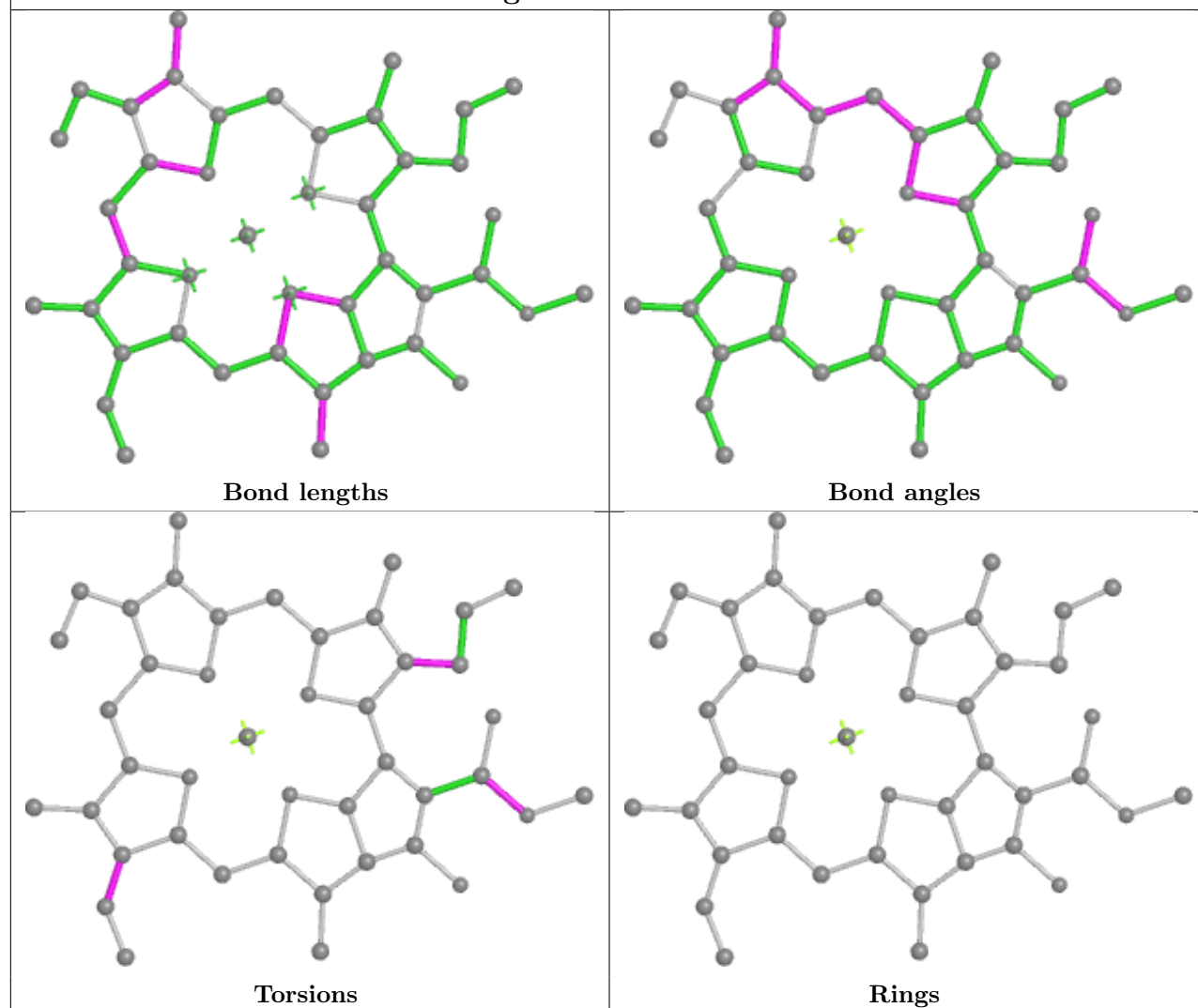
Ligand CLA 2 613

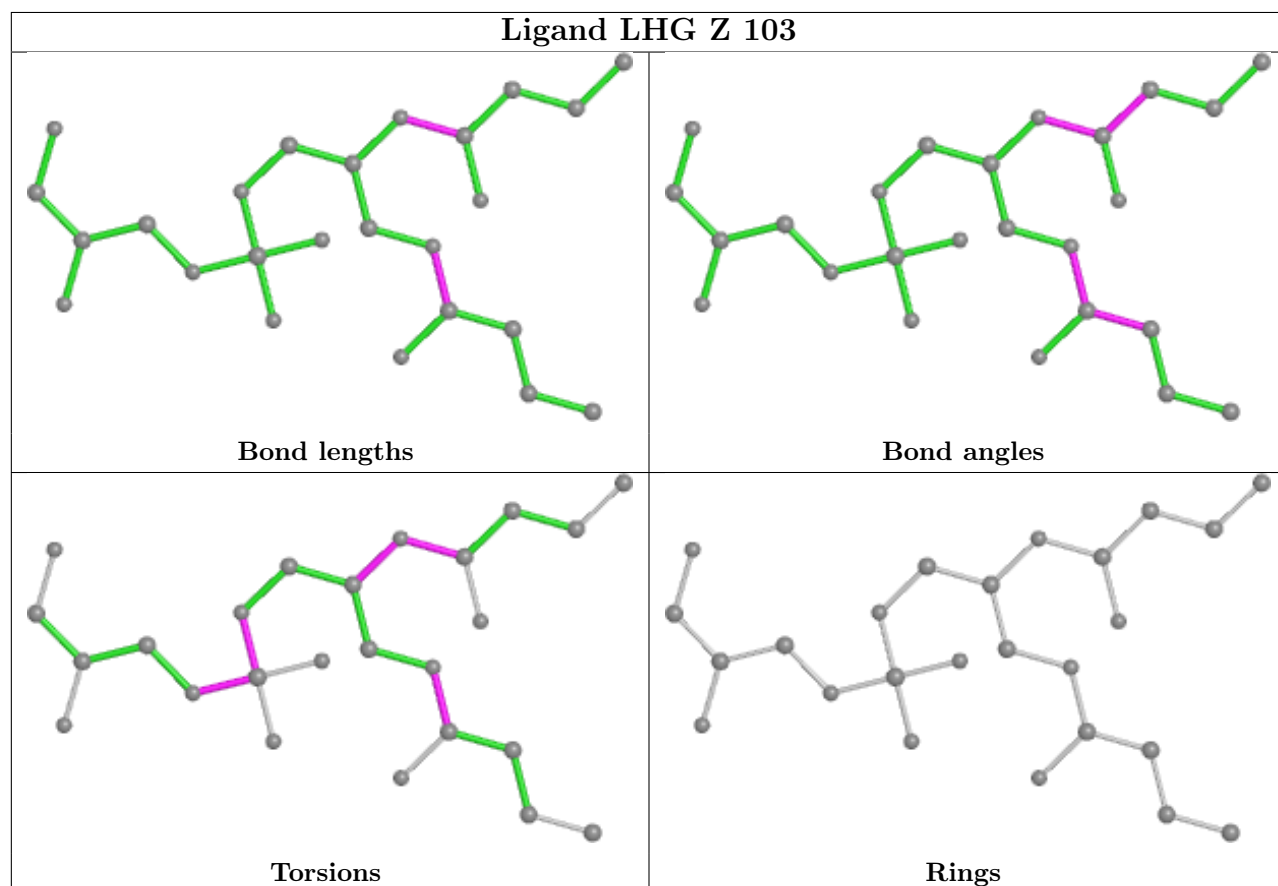
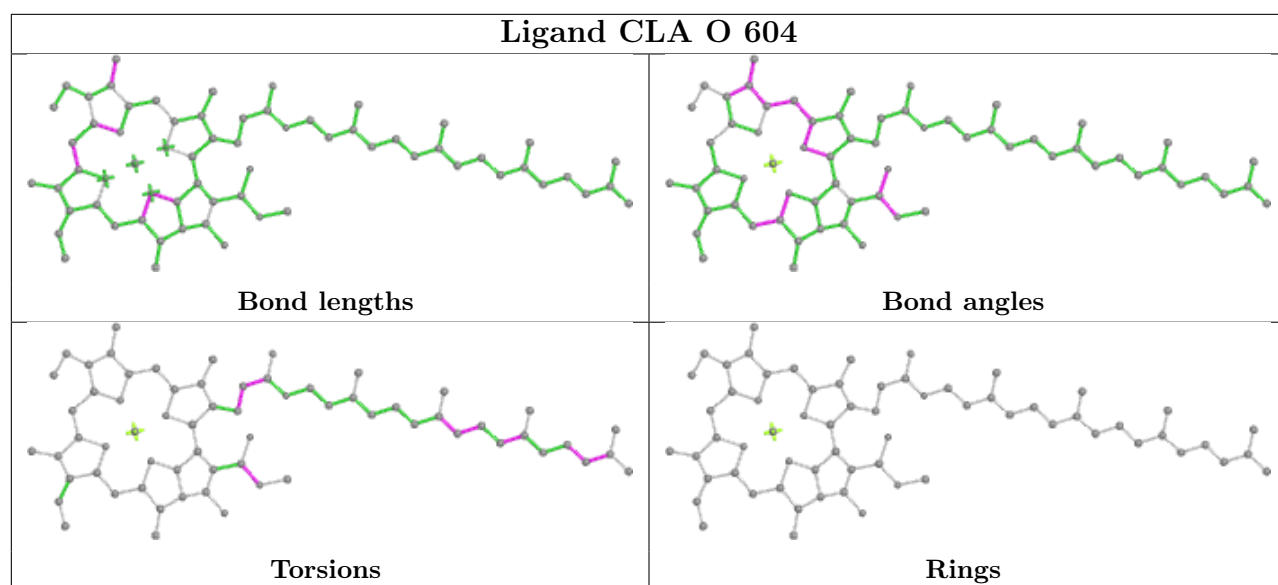


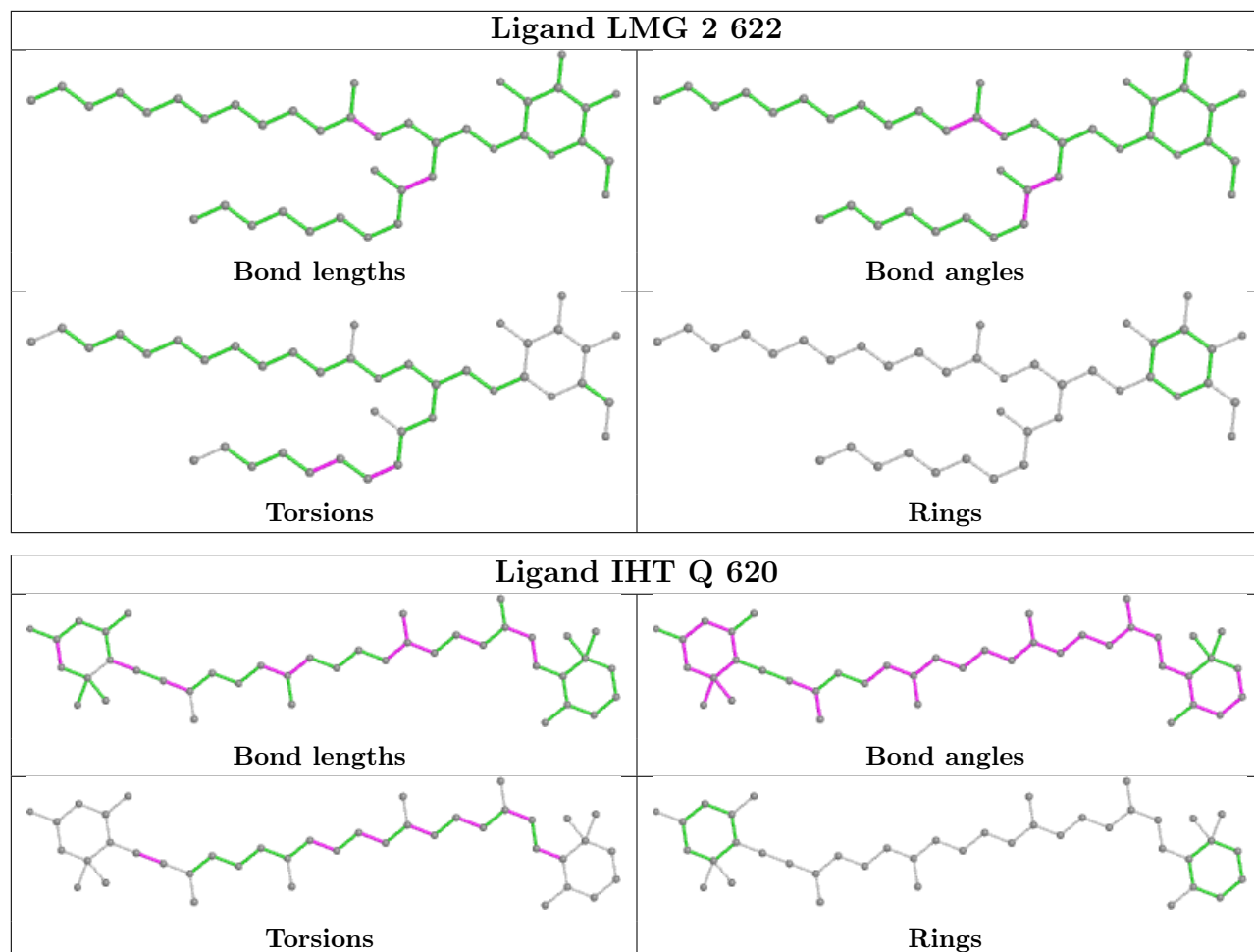
Ligand IHT 5 620



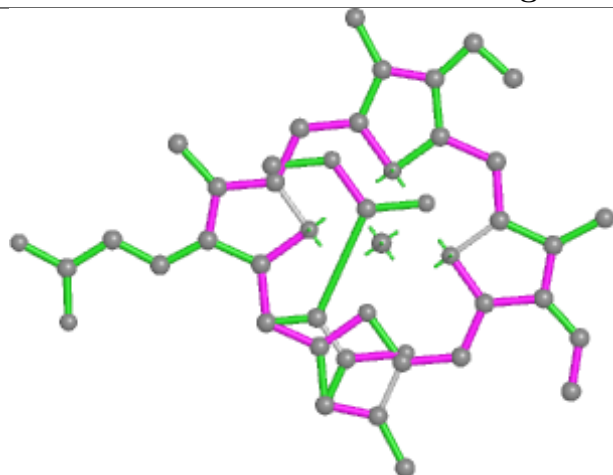
Ligand CLA 1 607



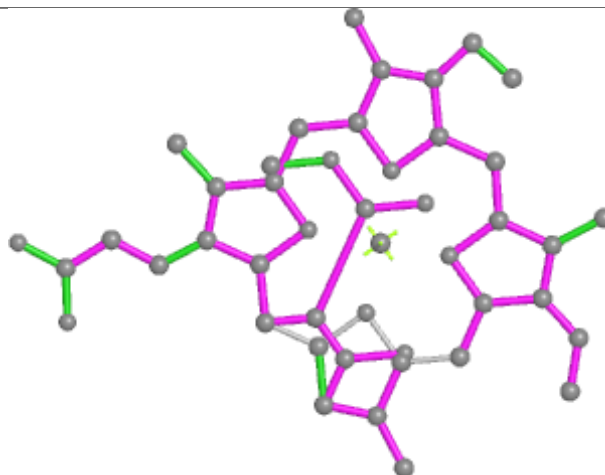




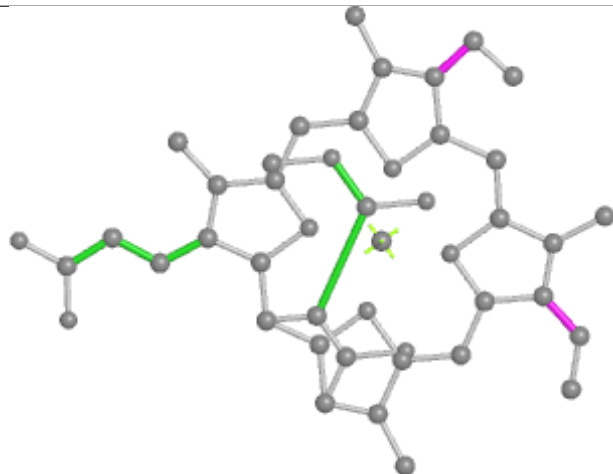
Ligand KC2 1 611



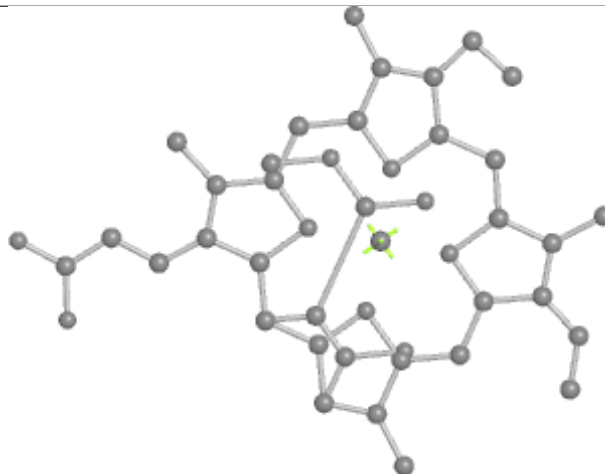
Bond lengths



Bond angles

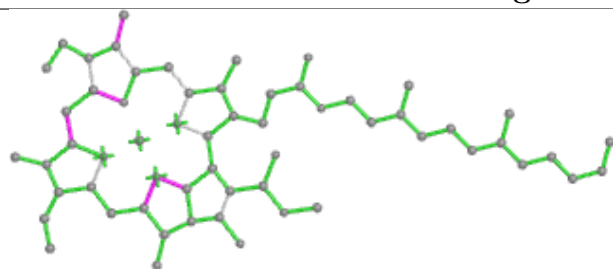


Torsions

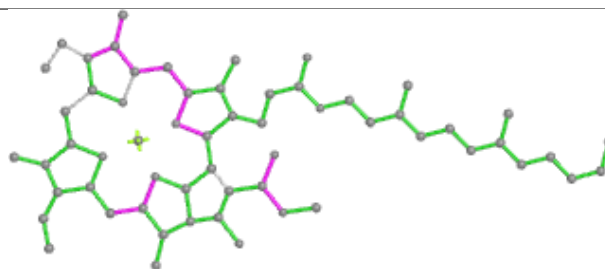


Rings

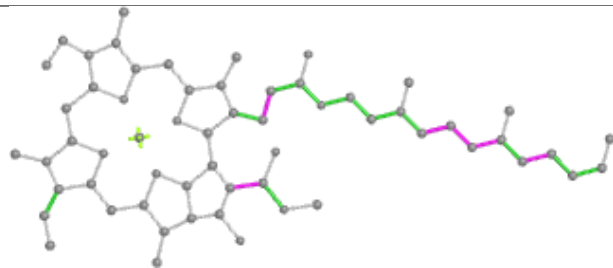
Ligand CLA N 604



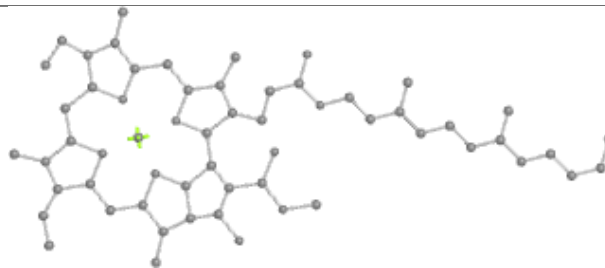
Bond lengths



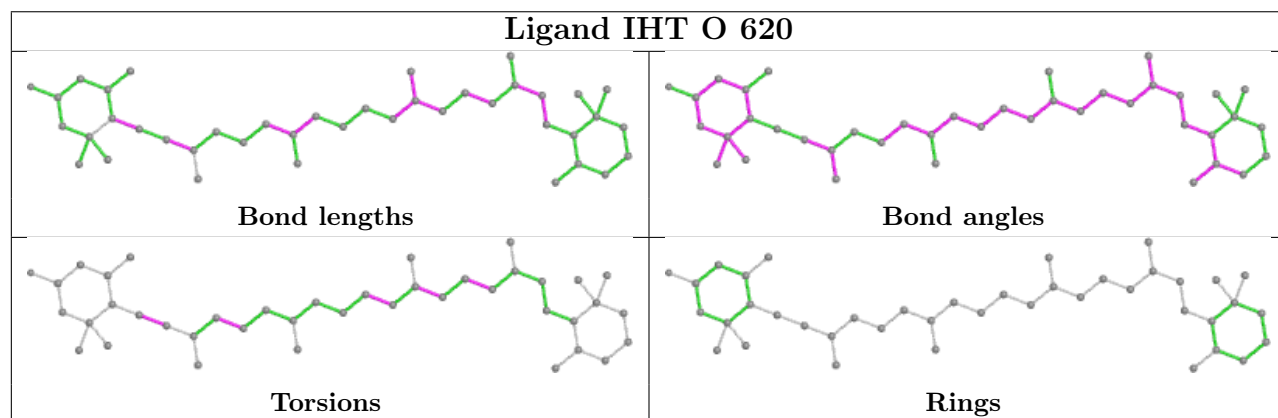
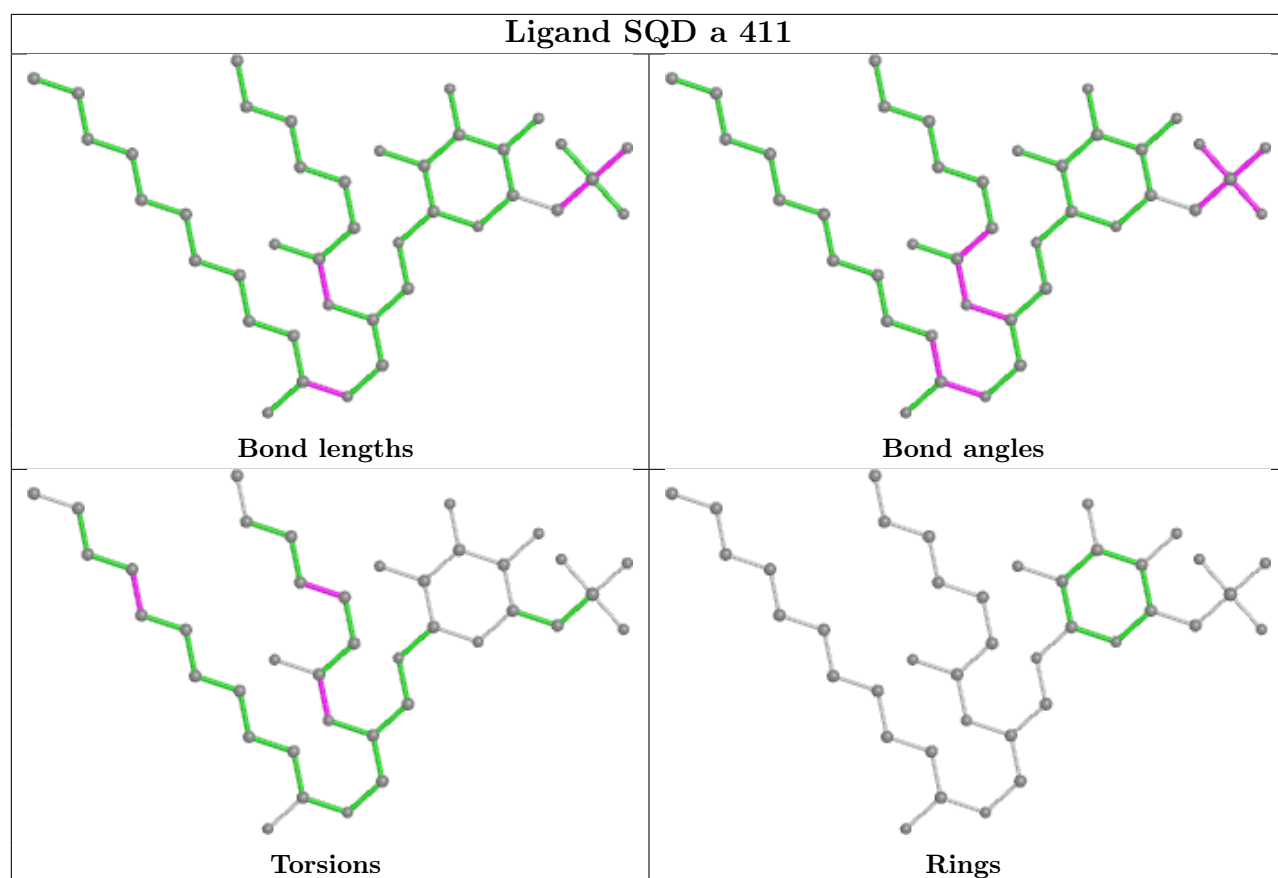
Bond angles



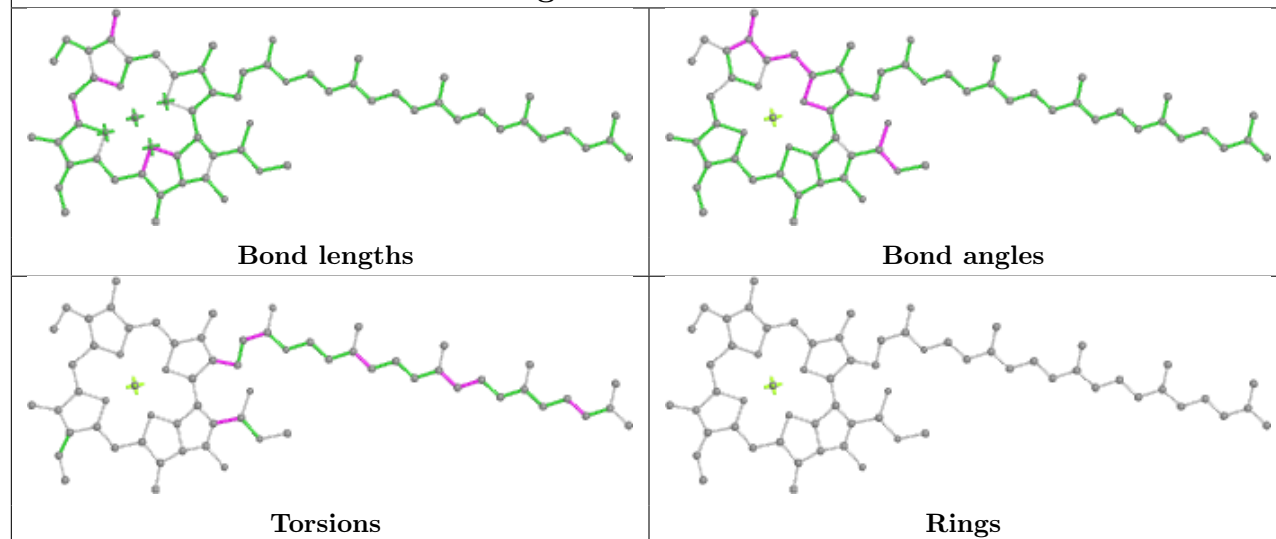
Torsions



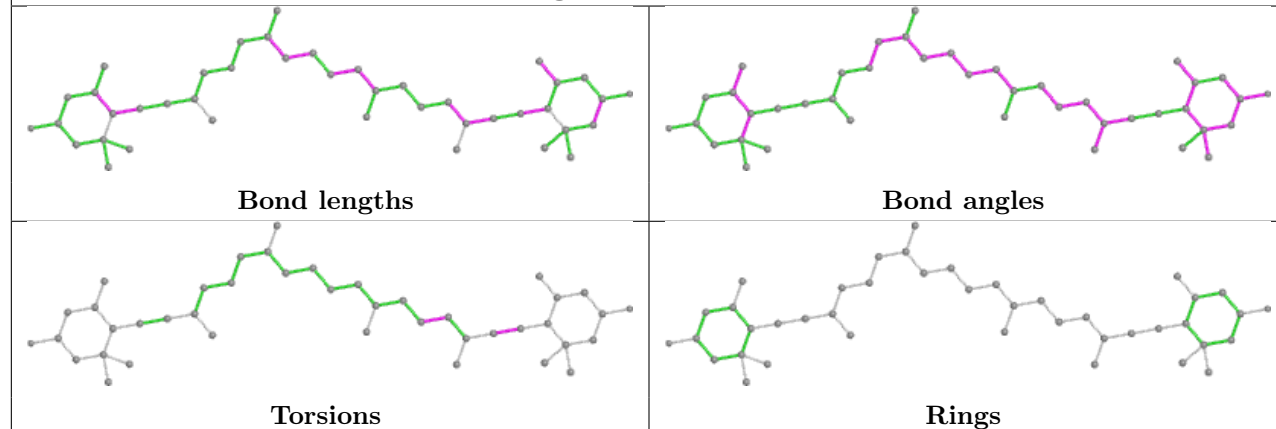
Rings



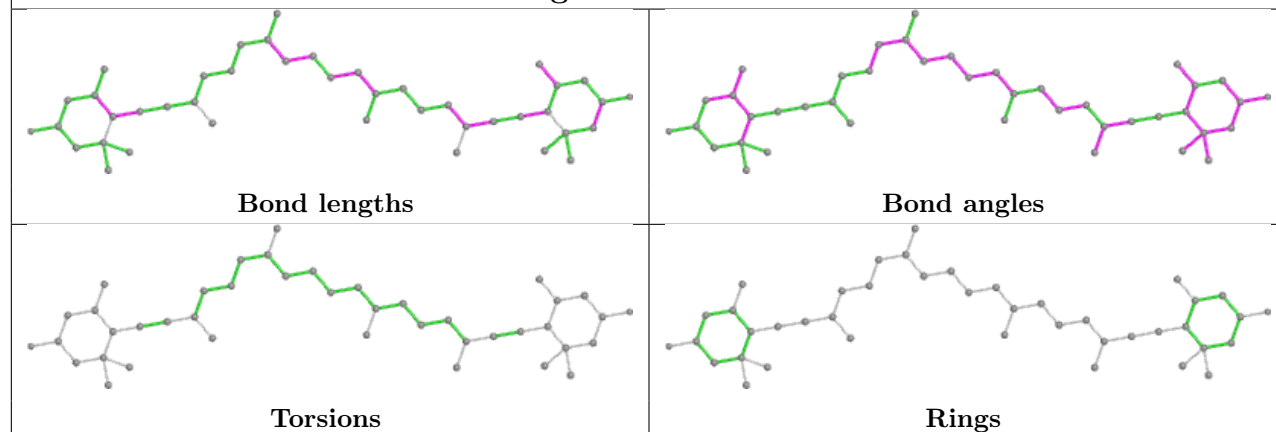
Ligand CLA c 518



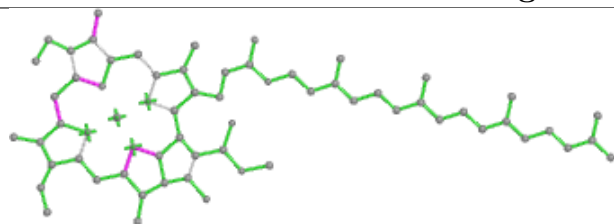
Ligand II0 3 618



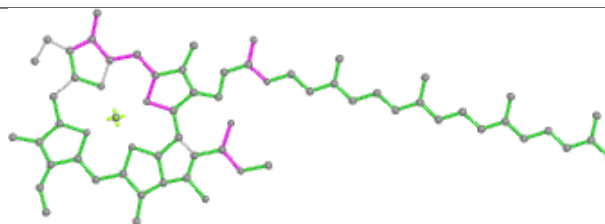
Ligand II0 5 618



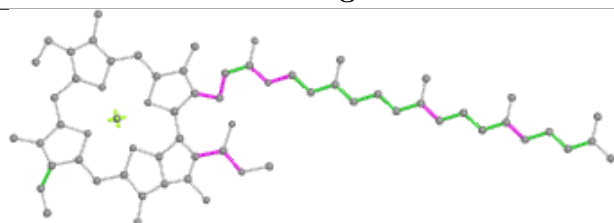
Ligand CLA 5 606



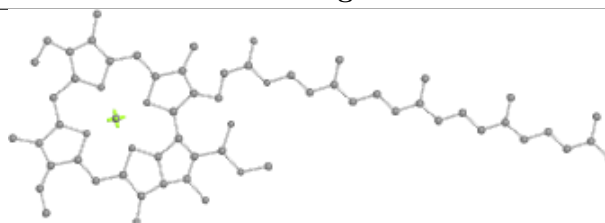
Bond lengths



Bond angles

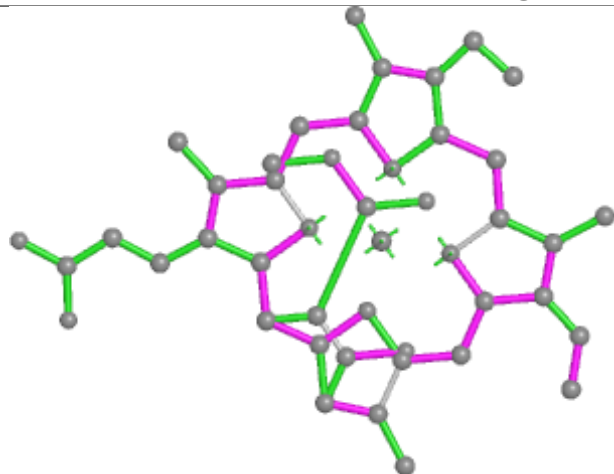


Torsions

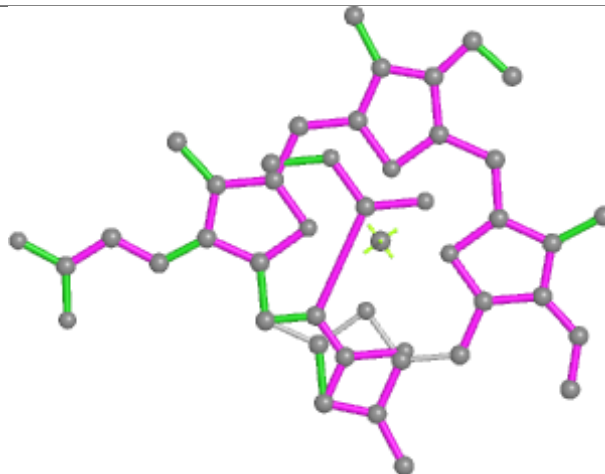


Rings

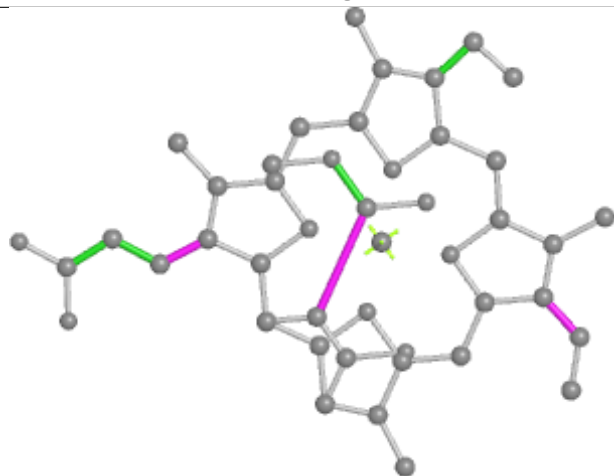
Ligand KC2 N 612



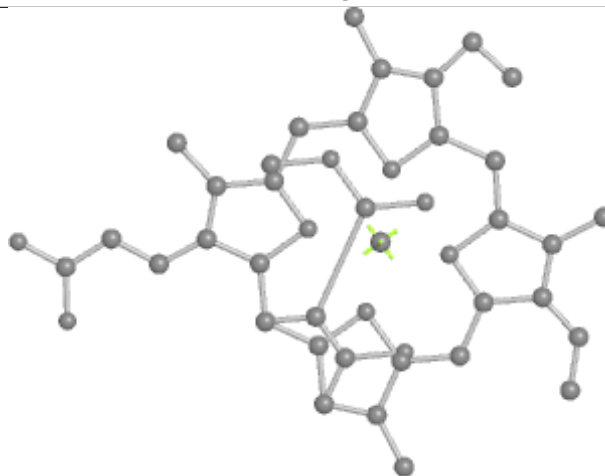
Bond lengths



Bond angles

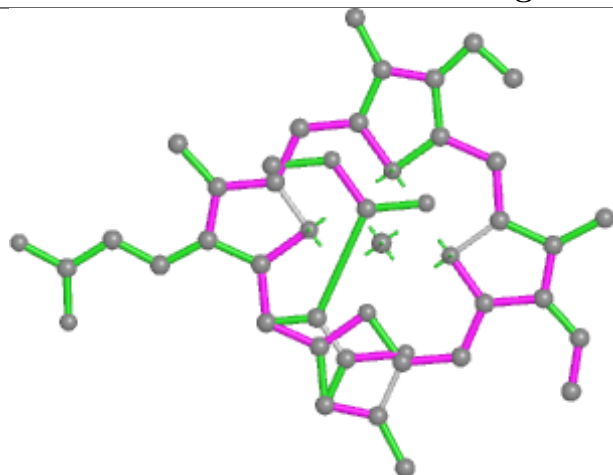


Torsions

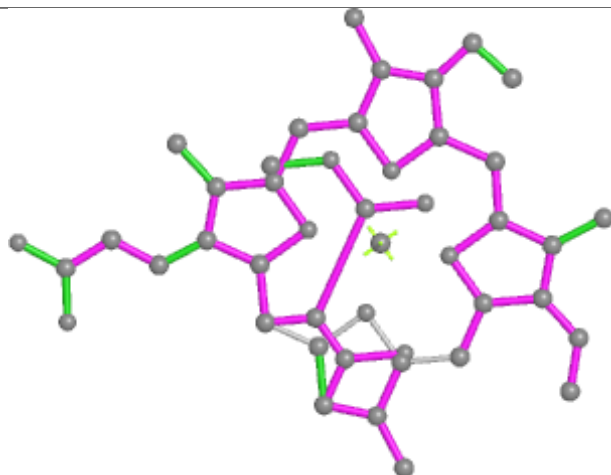


Rings

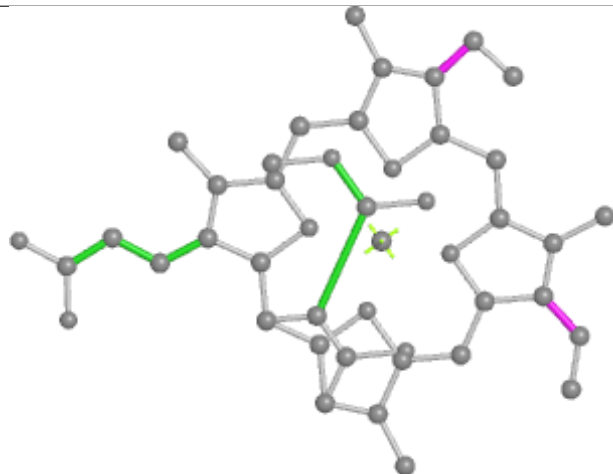
Ligand KC2 N 611



Bond lengths



Bond angles

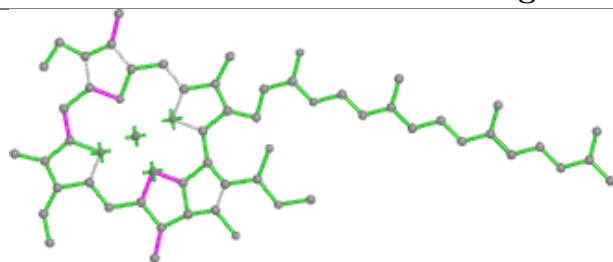


Torsions

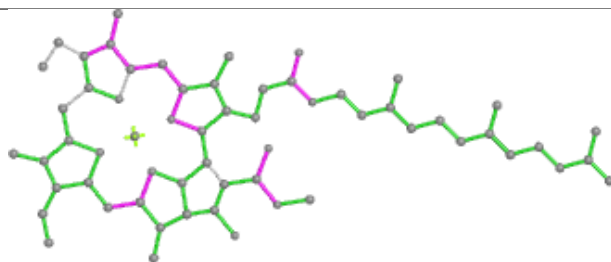


Rings

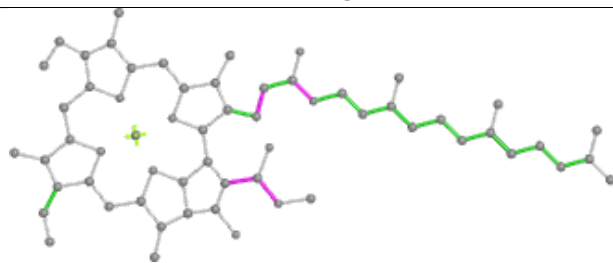
Ligand CLA 1 602



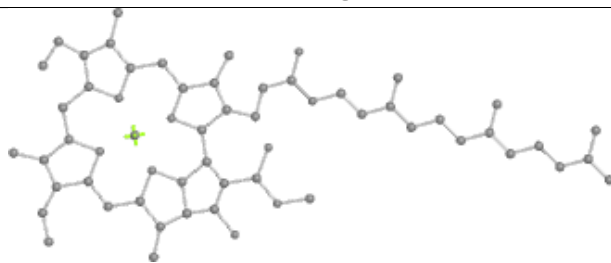
Bond lengths



Bond angles

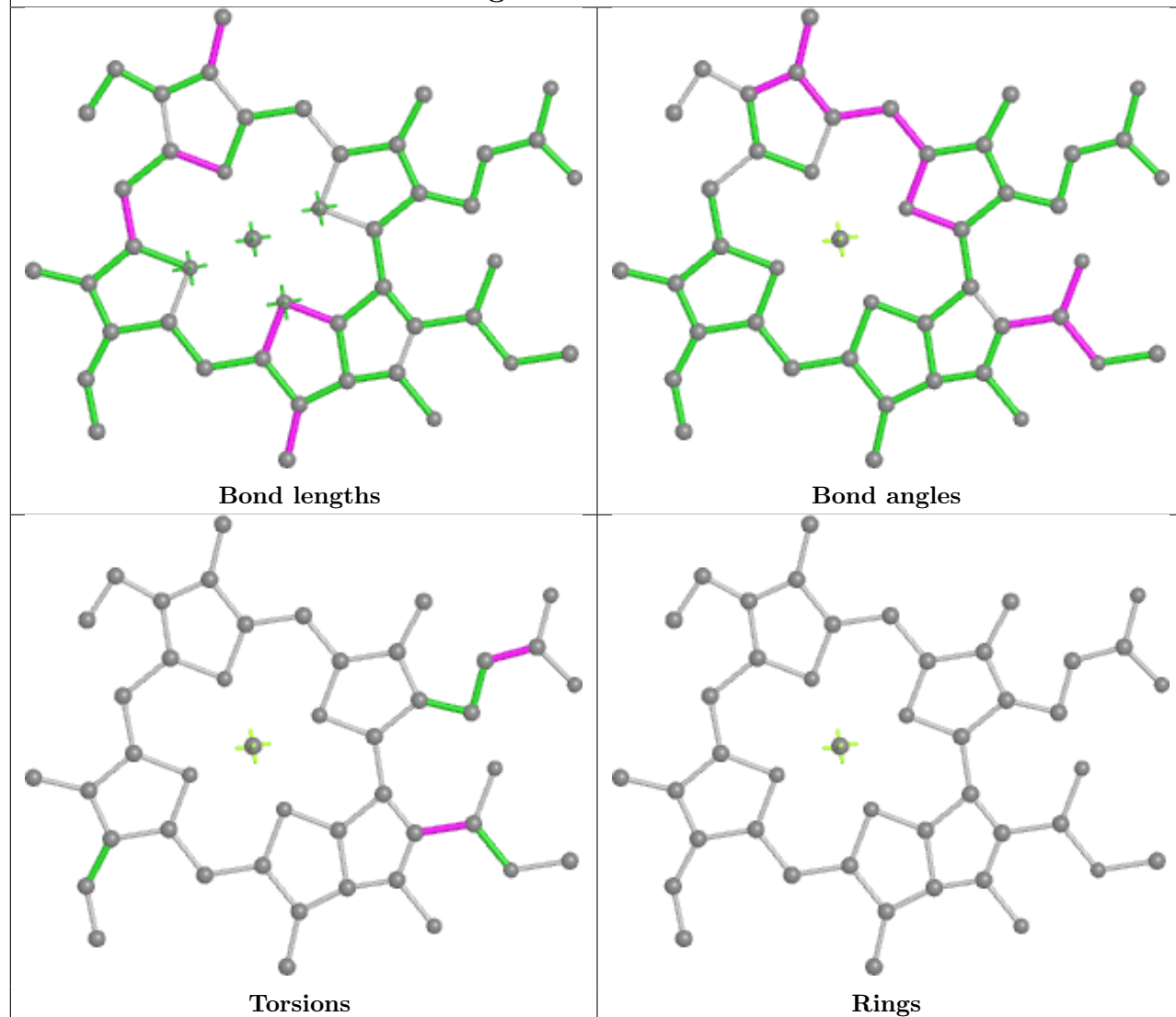


Torsions

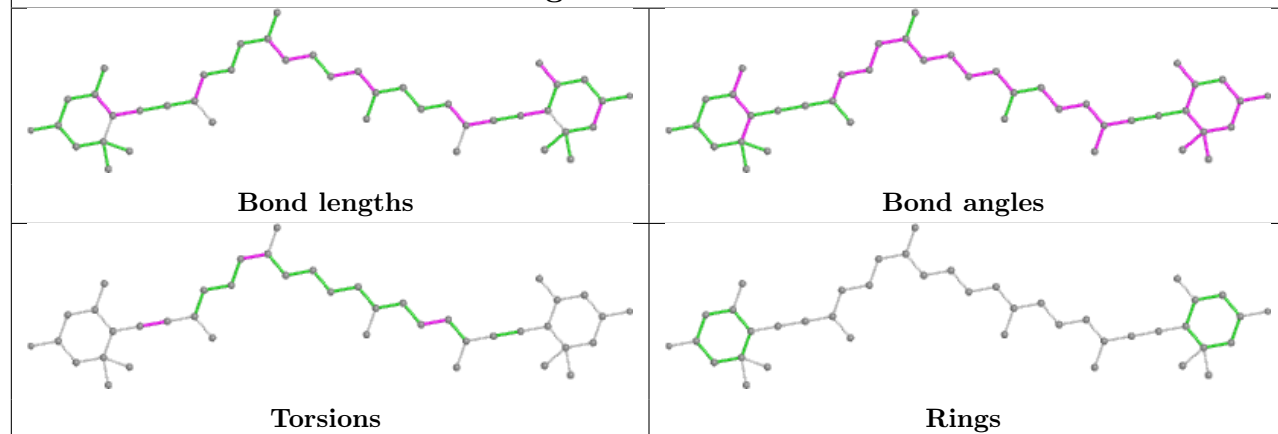


Rings

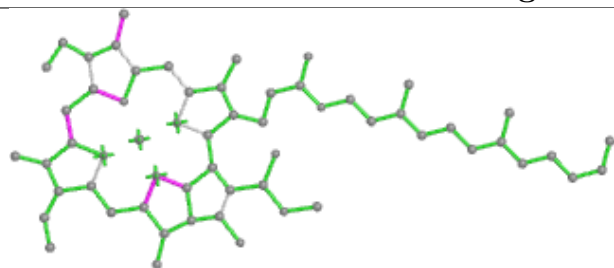
Ligand CLA G 302



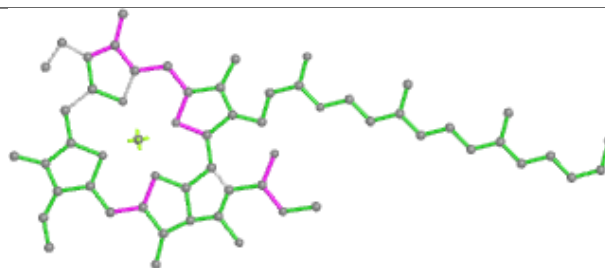
Ligand II0 N 619



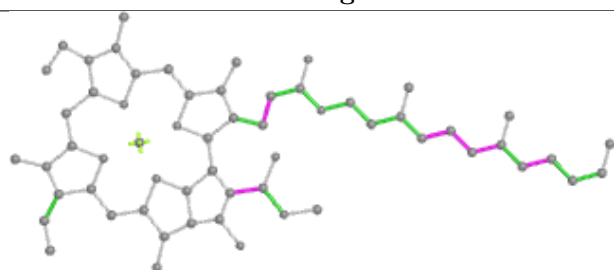
Ligand CLA 1 604



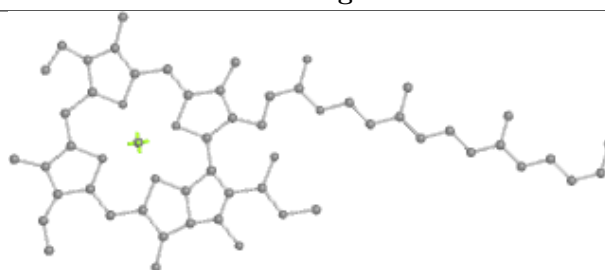
Bond lengths



Bond angles

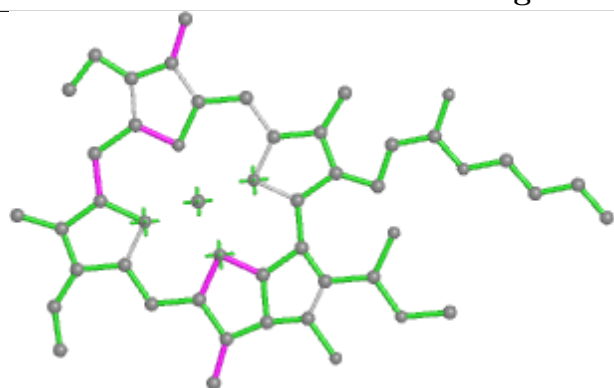


Torsions

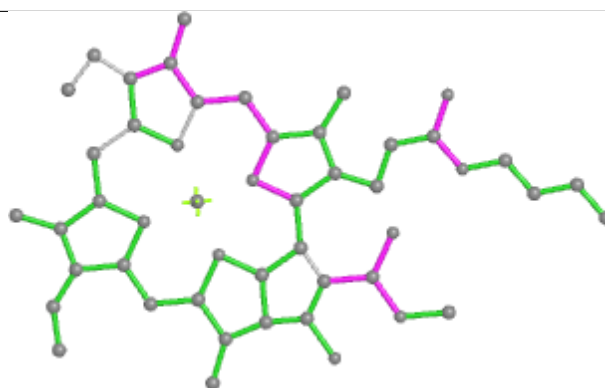


Rings

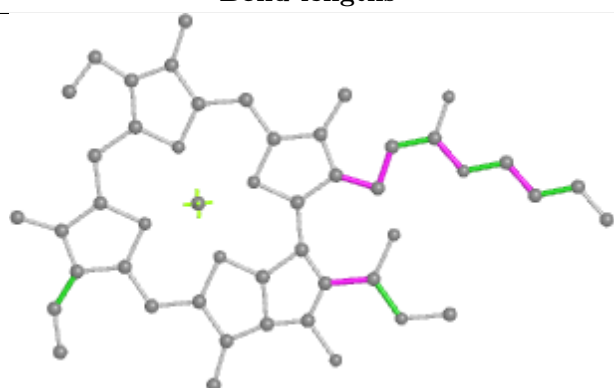
Ligand CLA O 601



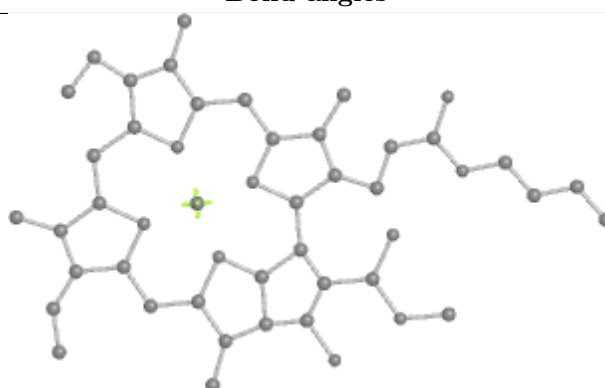
Bond lengths



Bond angles

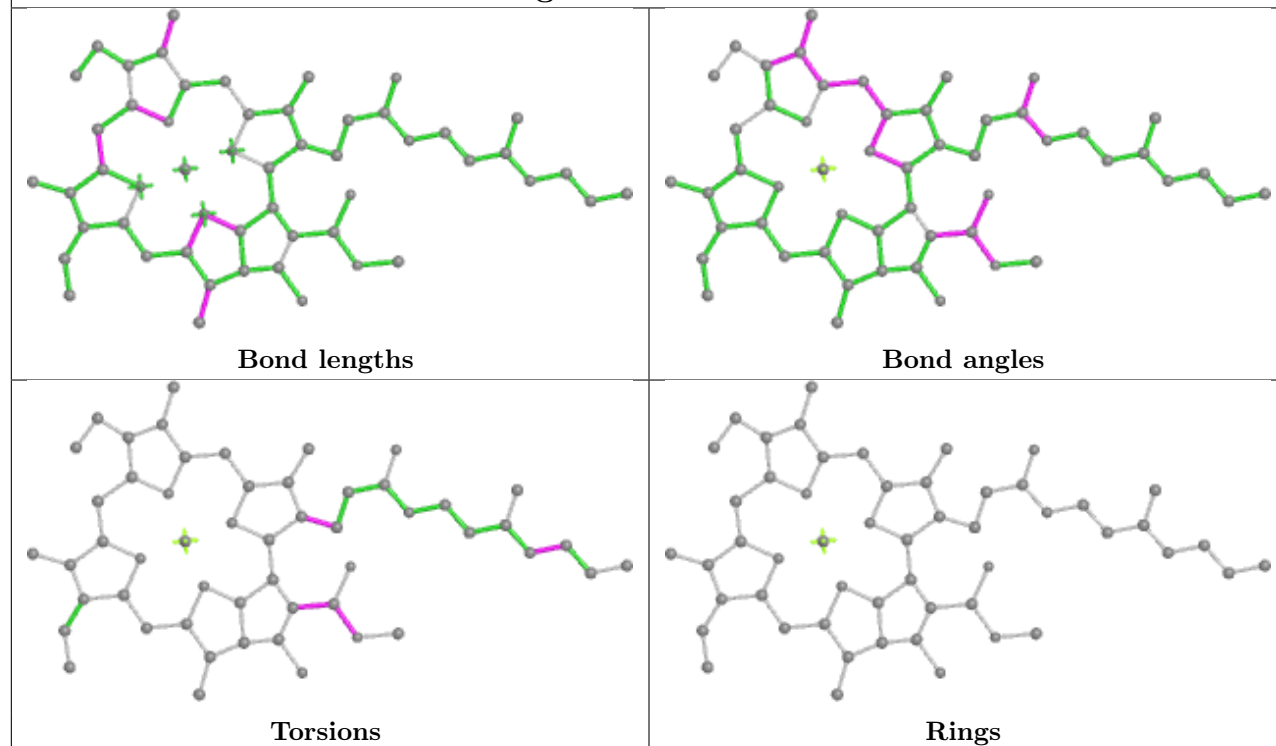


Torsions

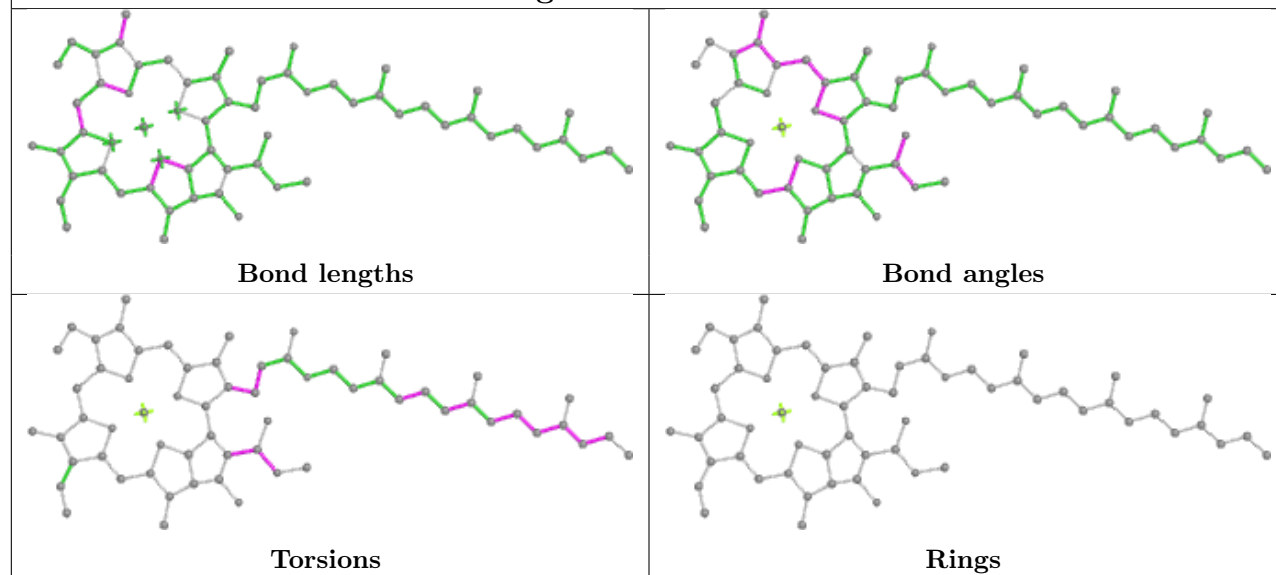


Rings

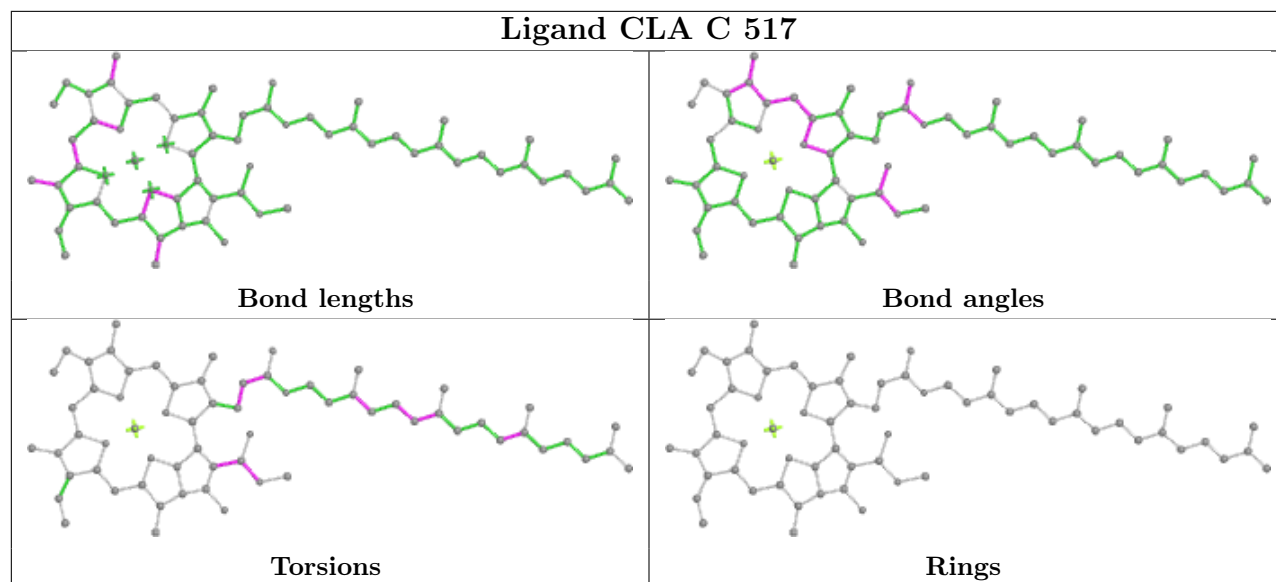
Ligand CLA 6 613



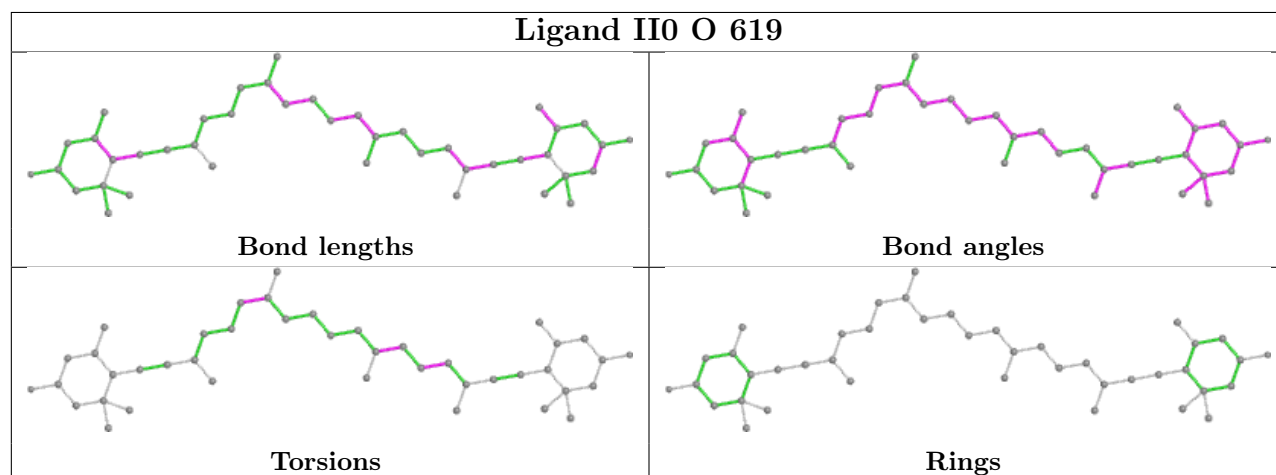
Ligand CLA 3 602



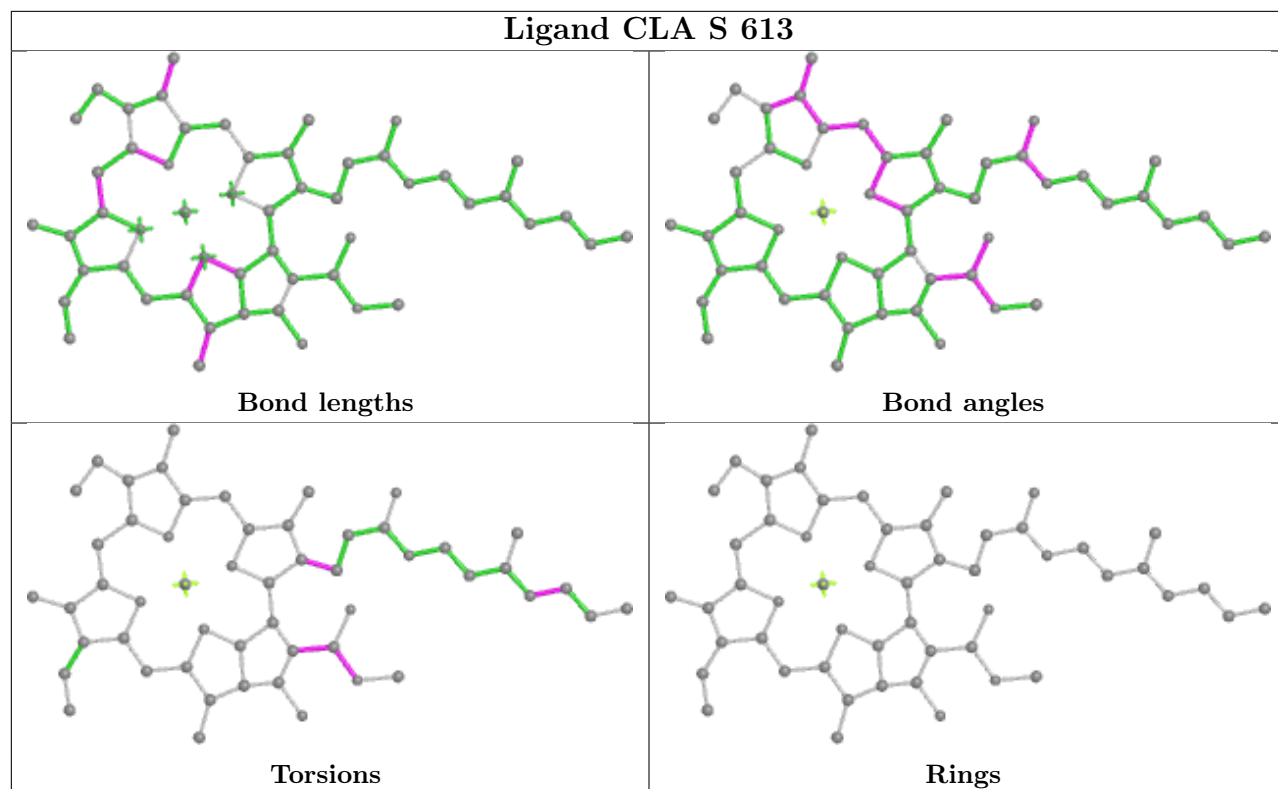
Ligand CLA C 517



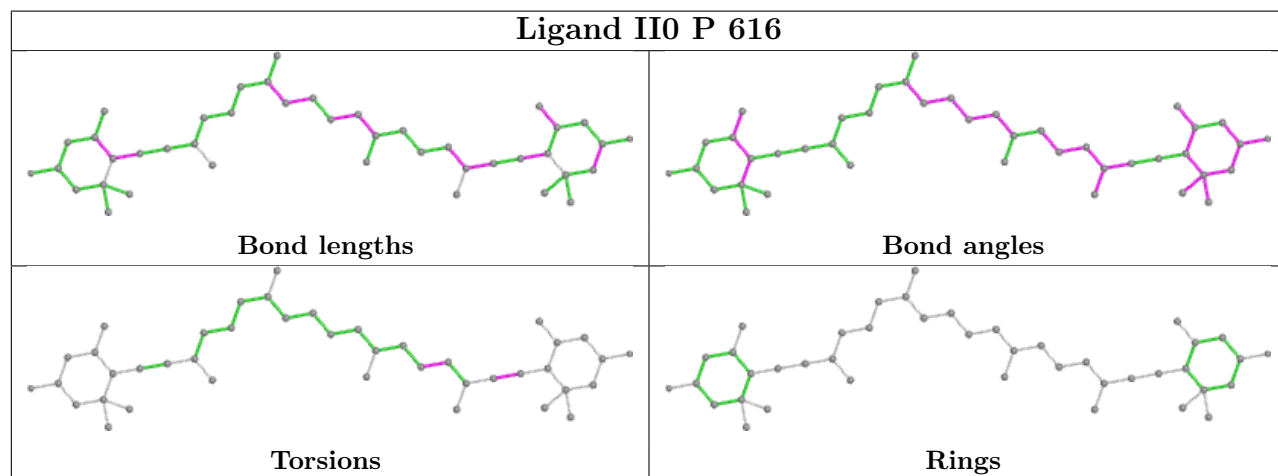
Ligand II0 O 619



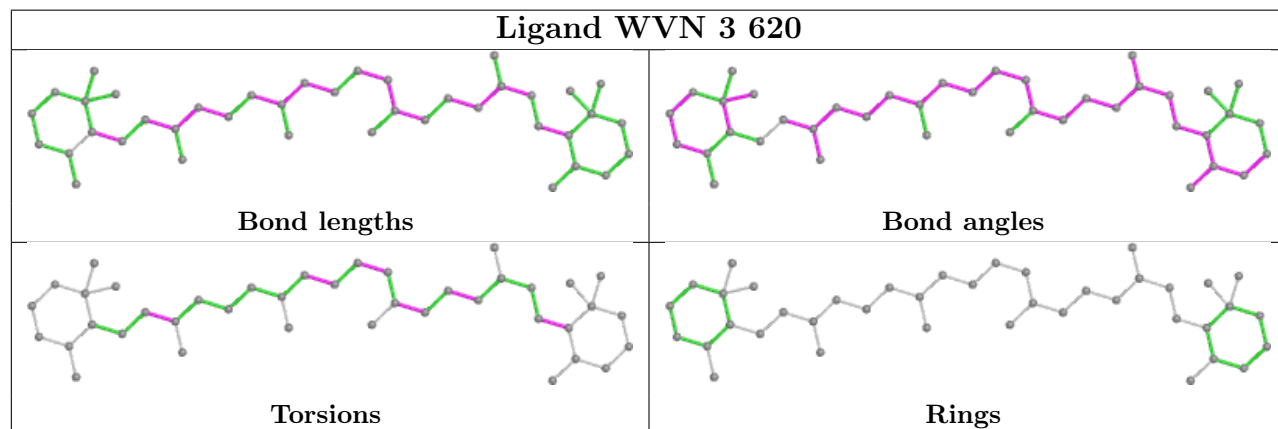
Ligand CLA S 613



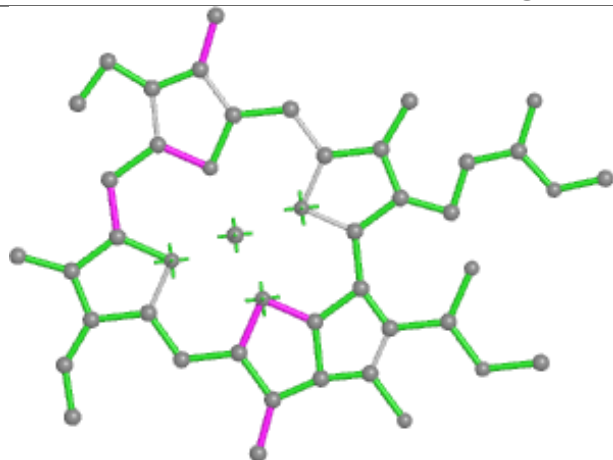
Ligand II0 P 616



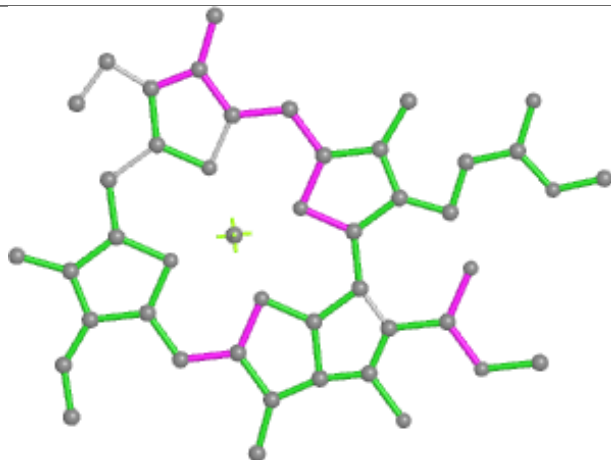
Ligand WVN 3 620



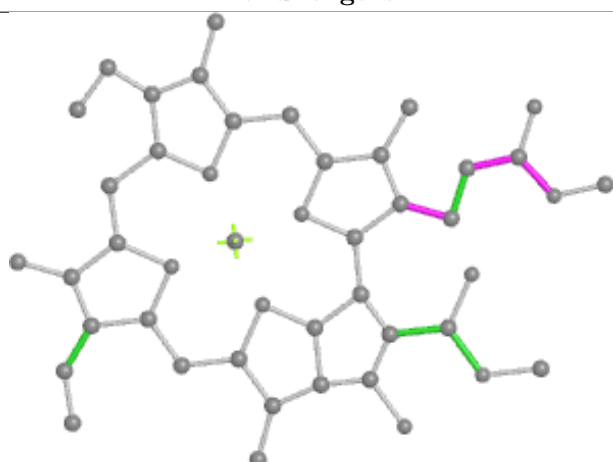
Ligand CLA 5 615



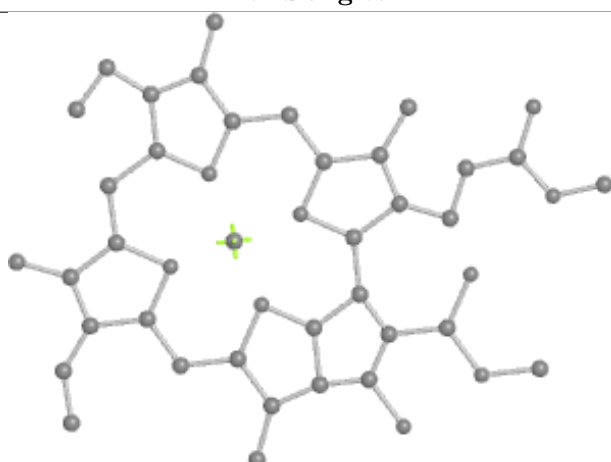
Bond lengths



Bond angles

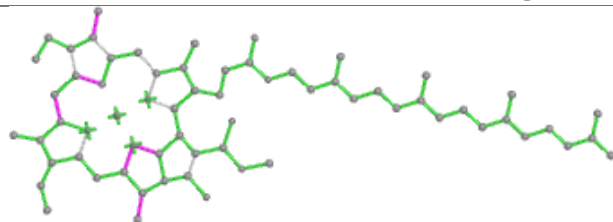


Torsions

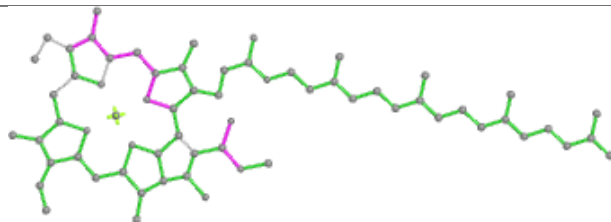


Rings

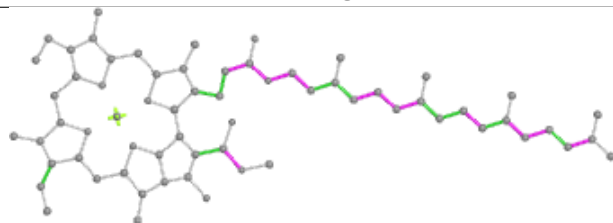
Ligand CLA 5 611



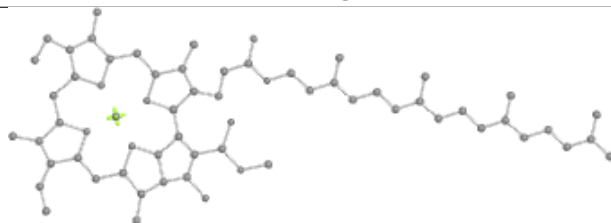
Bond lengths



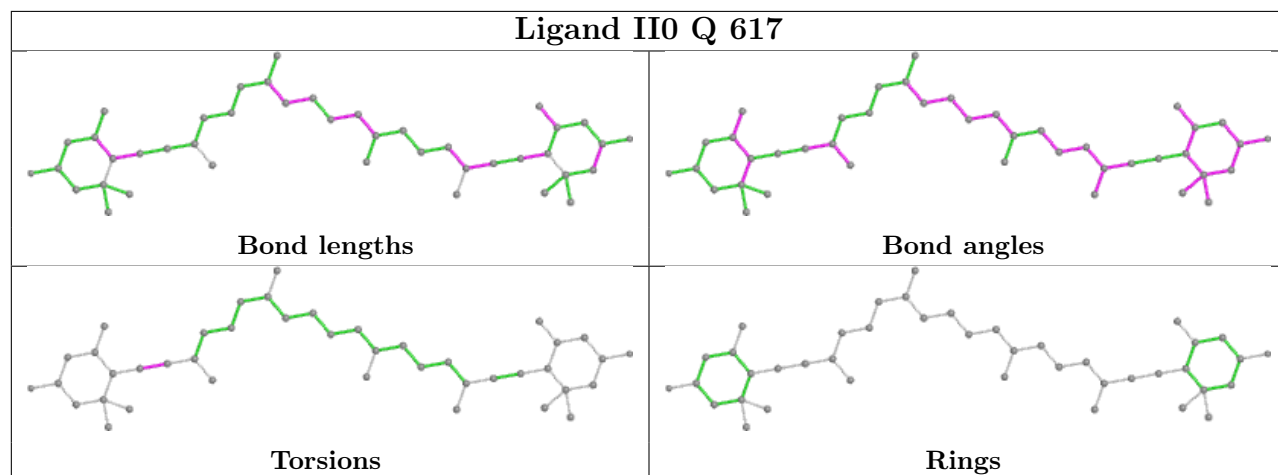
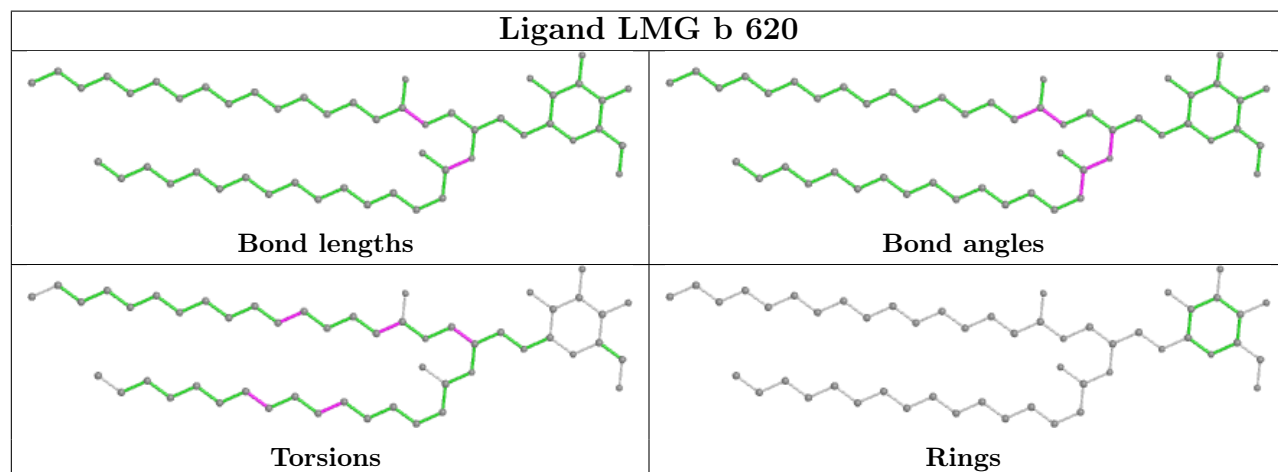
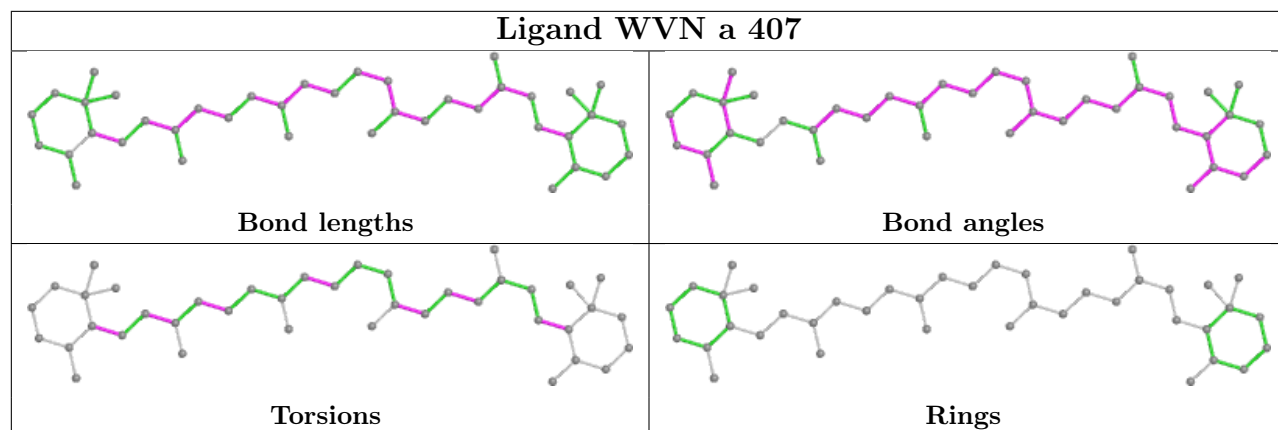
Bond angles



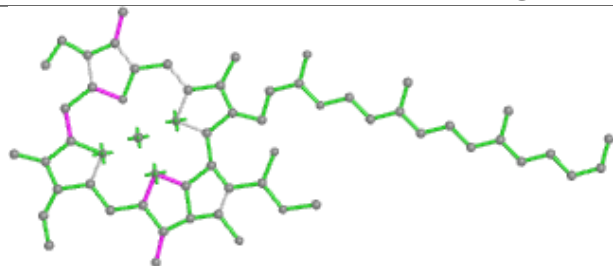
Torsions



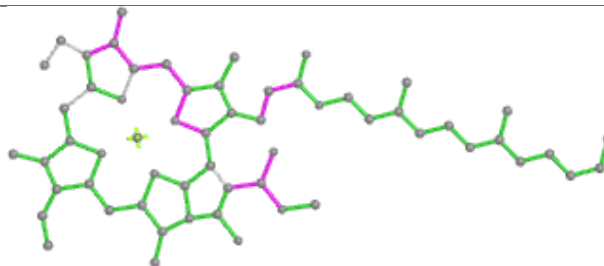
Rings



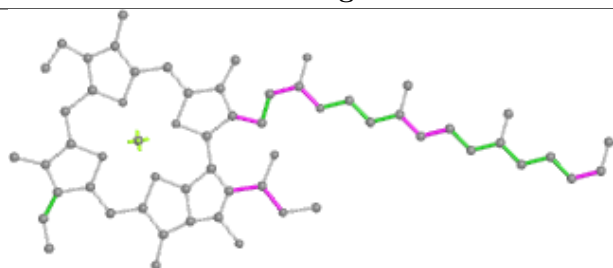
Ligand CLA B 604



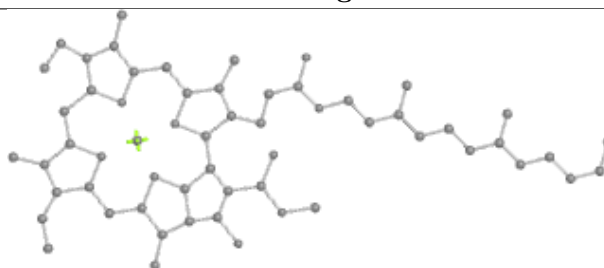
Bond lengths



Bond angles

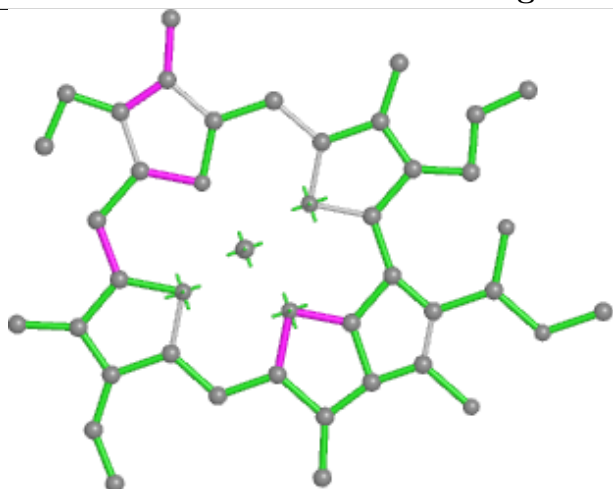


Torsions

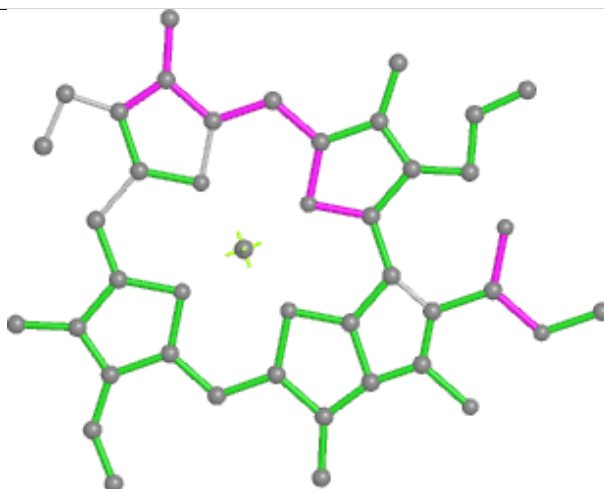


Rings

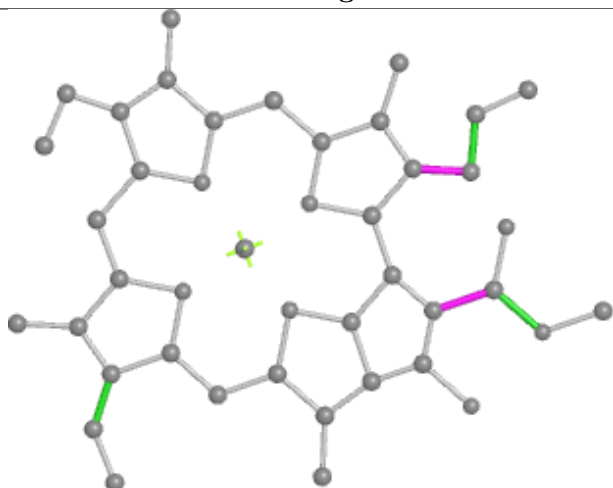
Ligand CLA 4 607



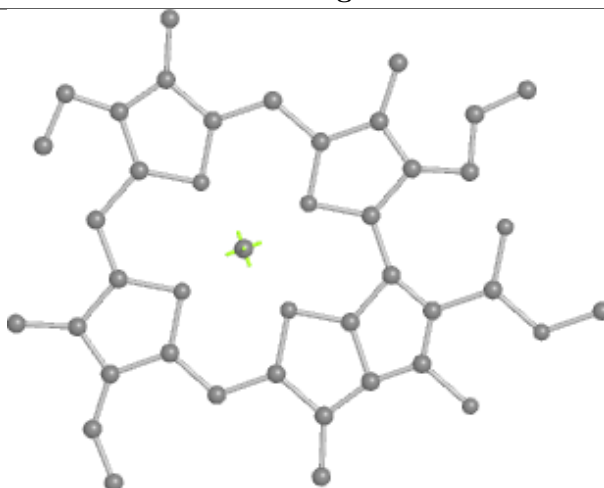
Bond lengths



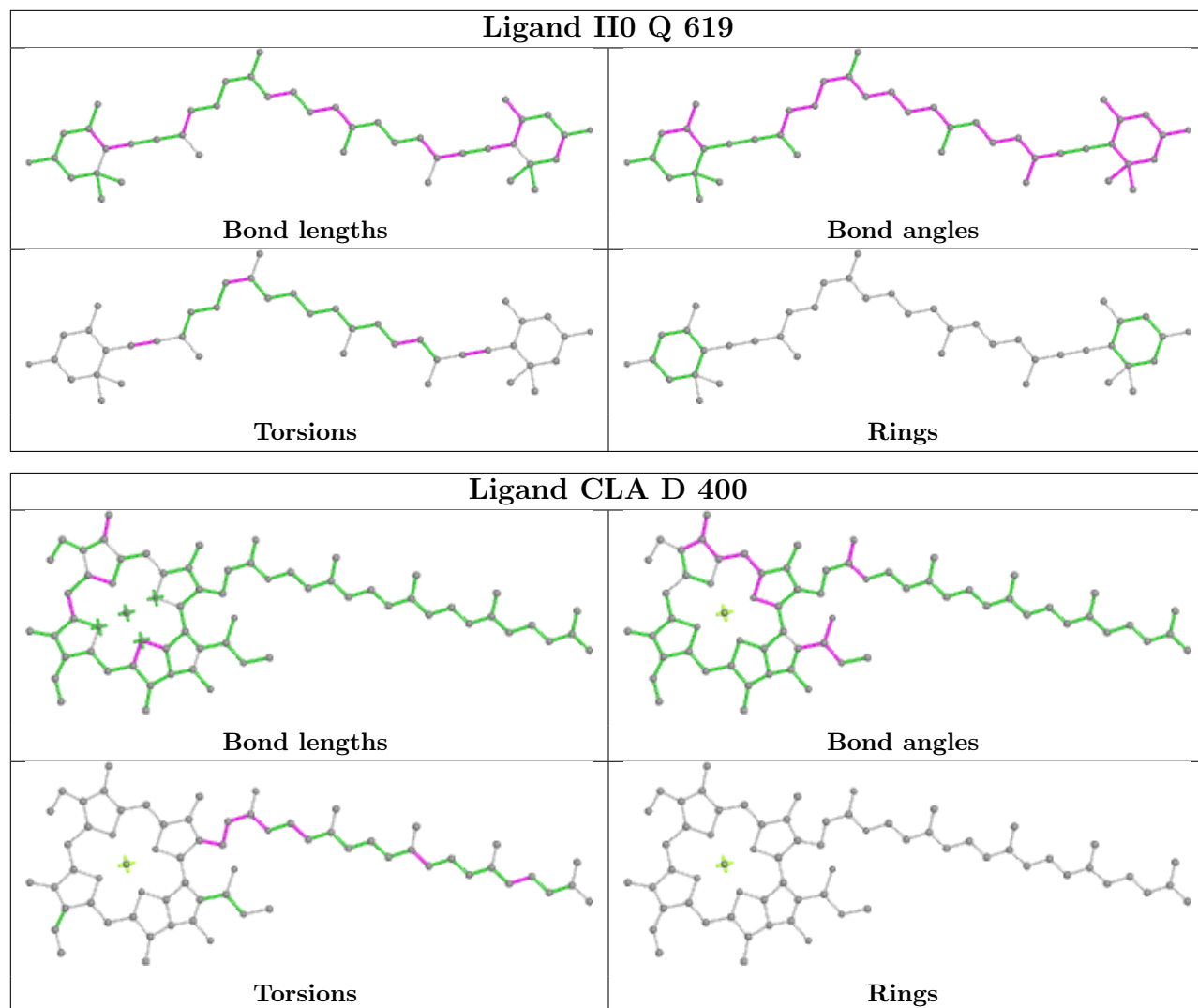
Bond angles



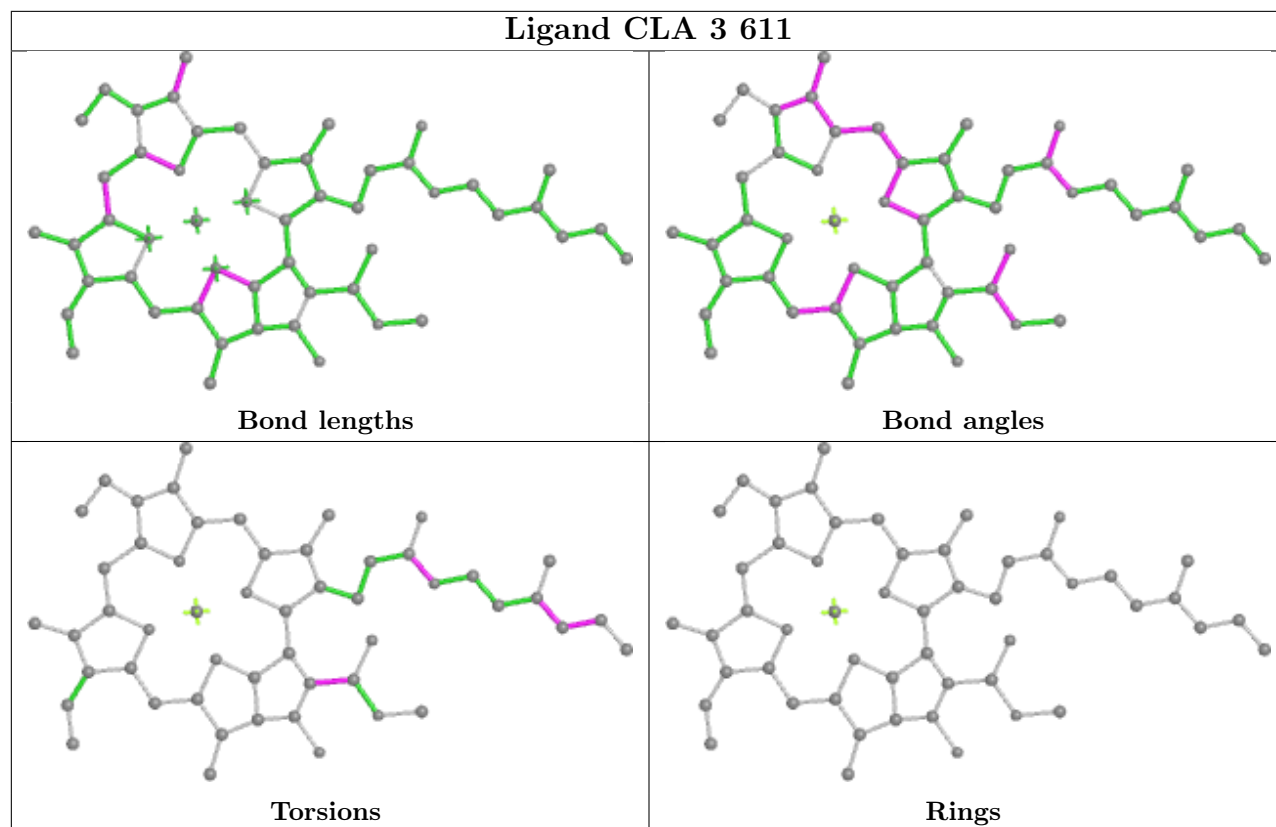
Torsions



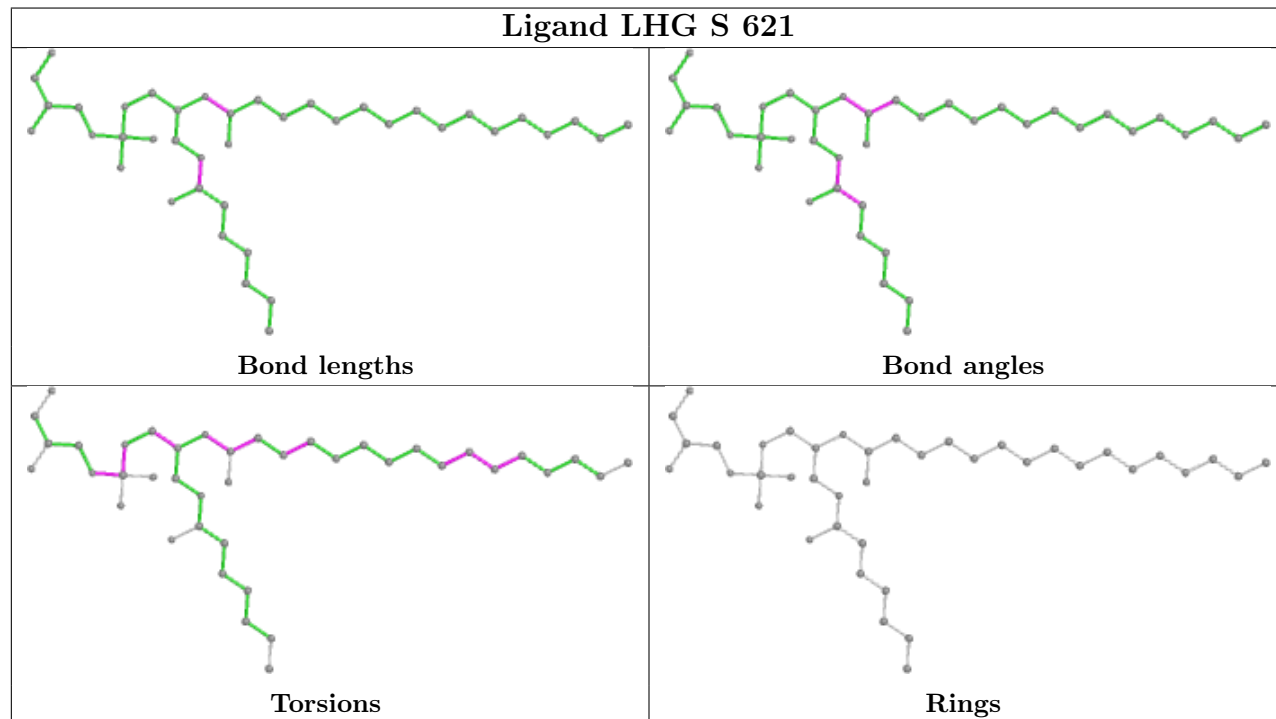
Rings



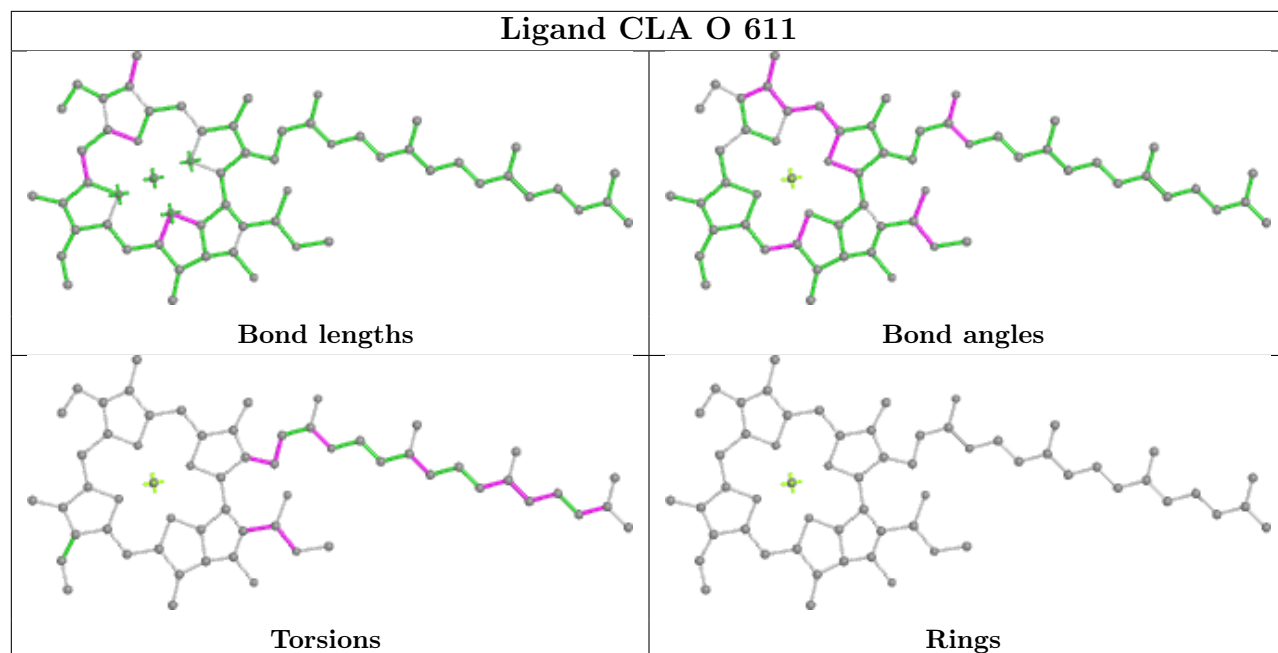
Ligand CLA 3 611



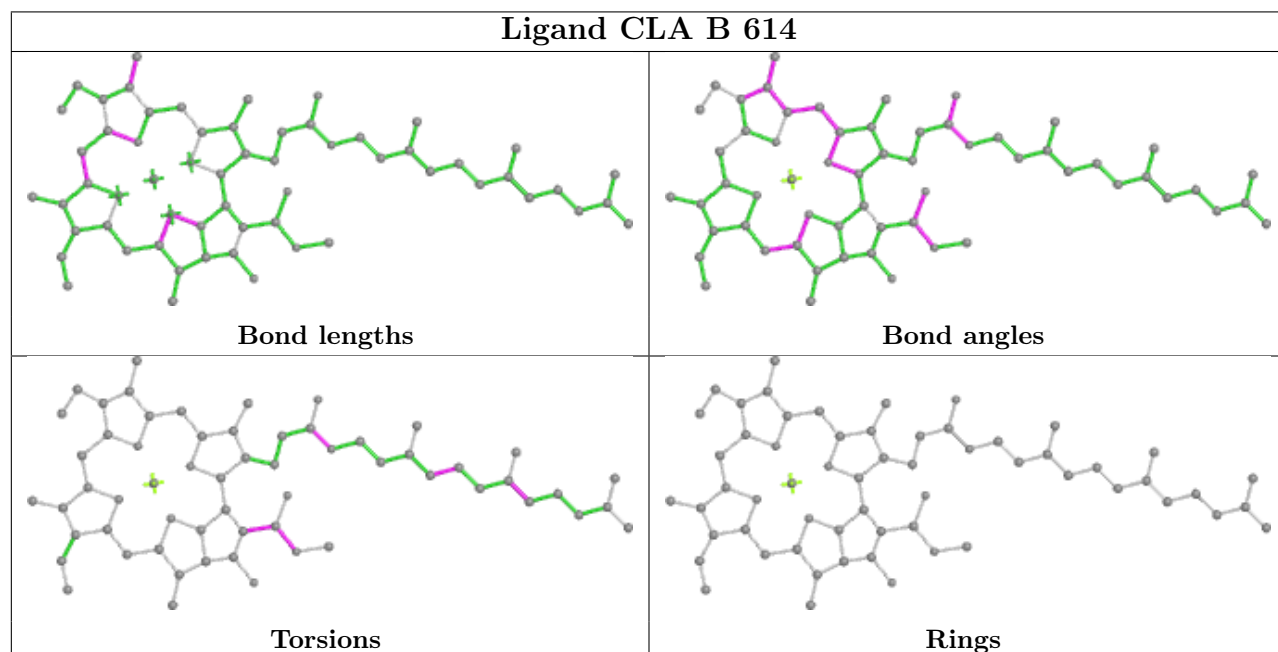
Ligand LHG S 621



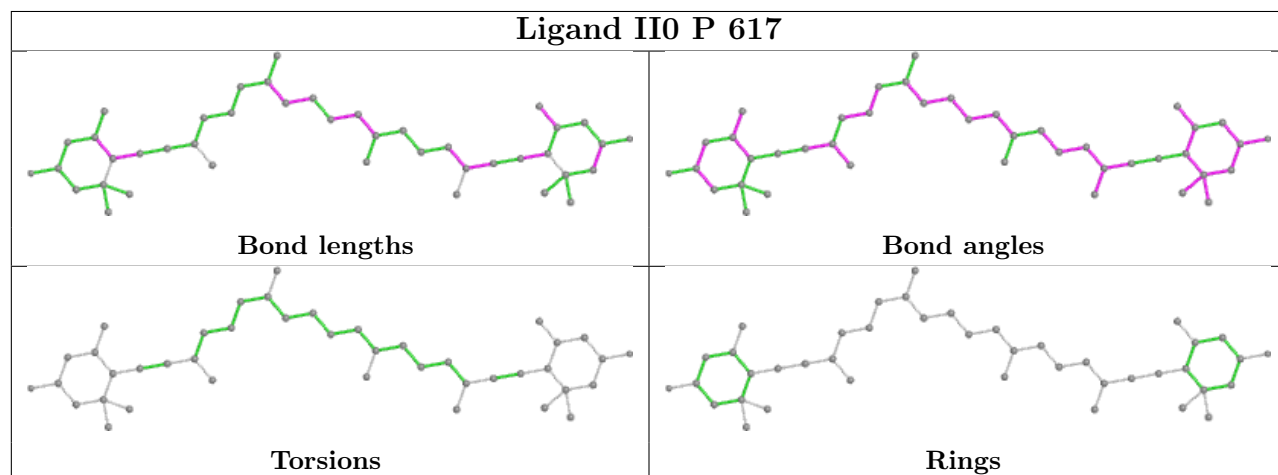
Ligand CLA O 611



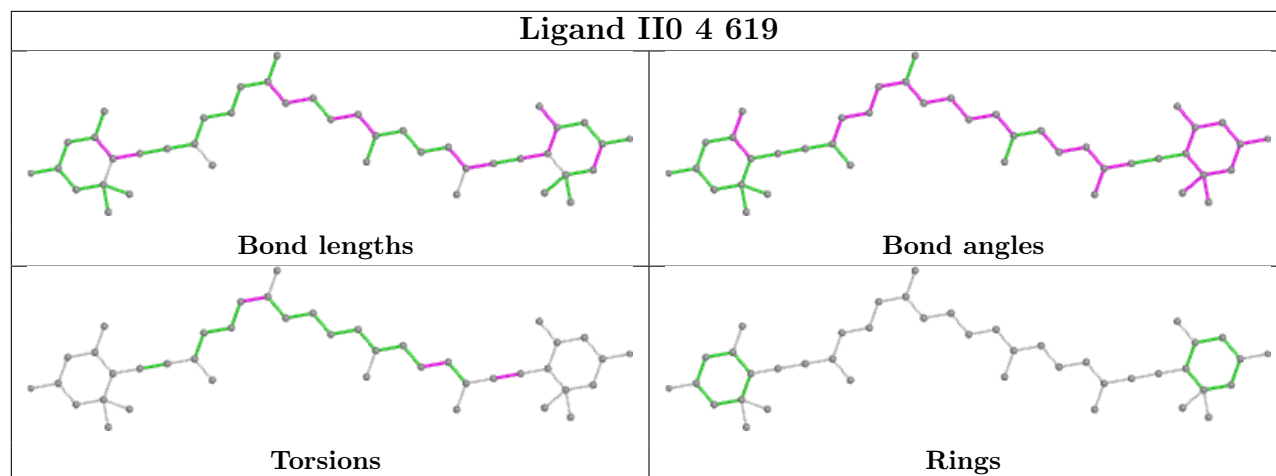
Ligand CLA B 614



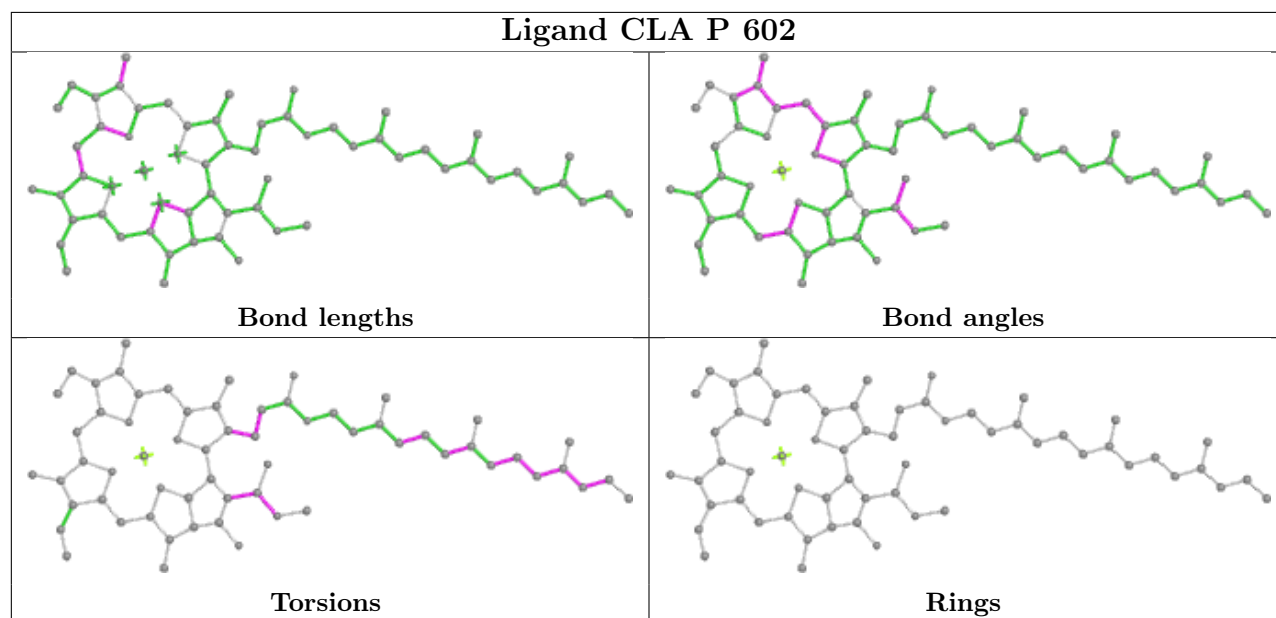
Ligand II0 P 617



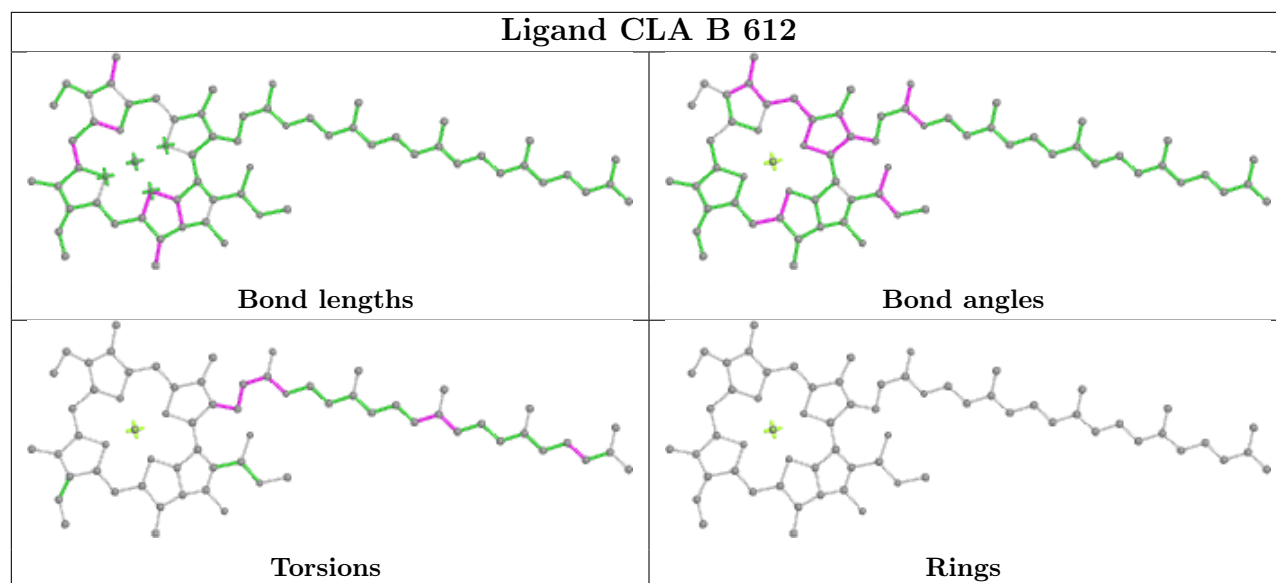
Ligand II0 4 619



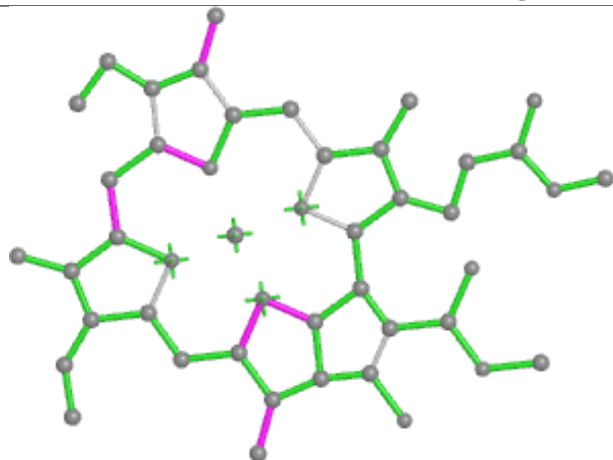
Ligand CLA P 602



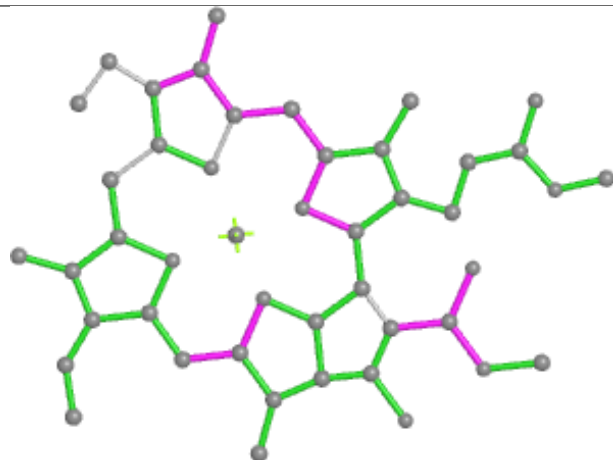
Ligand CLA B 612



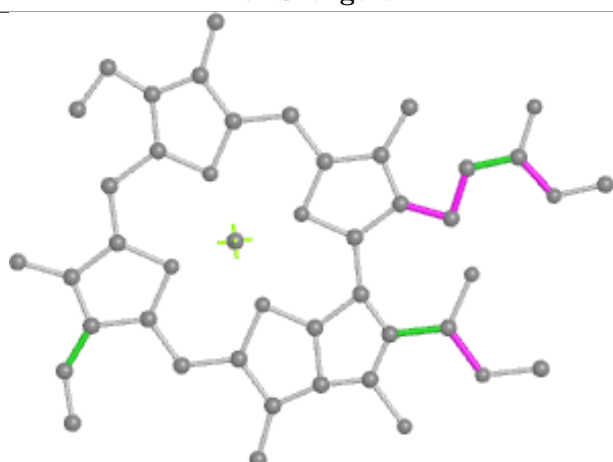
Ligand CLA N 609



Bond lengths



Bond angles

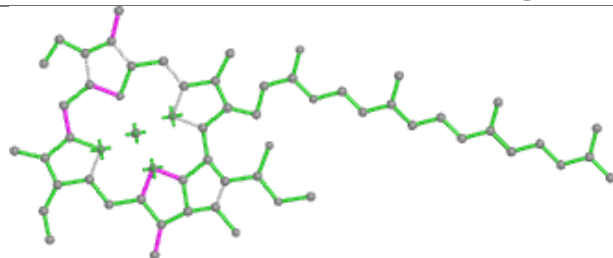


Torsions

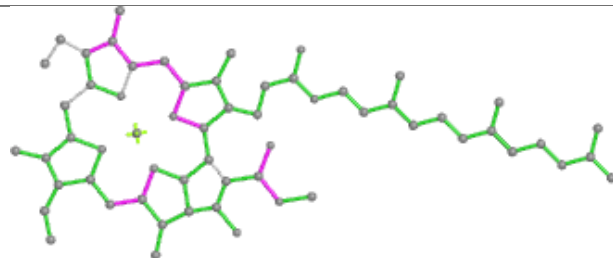


Rings

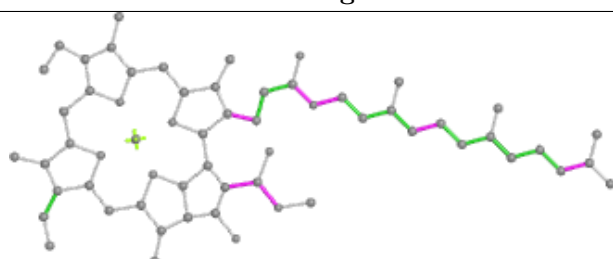
Ligand CLA a 406



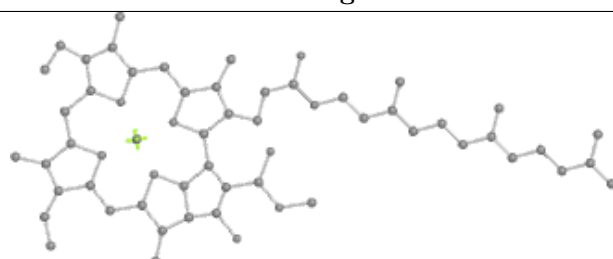
Bond lengths



Bond angles

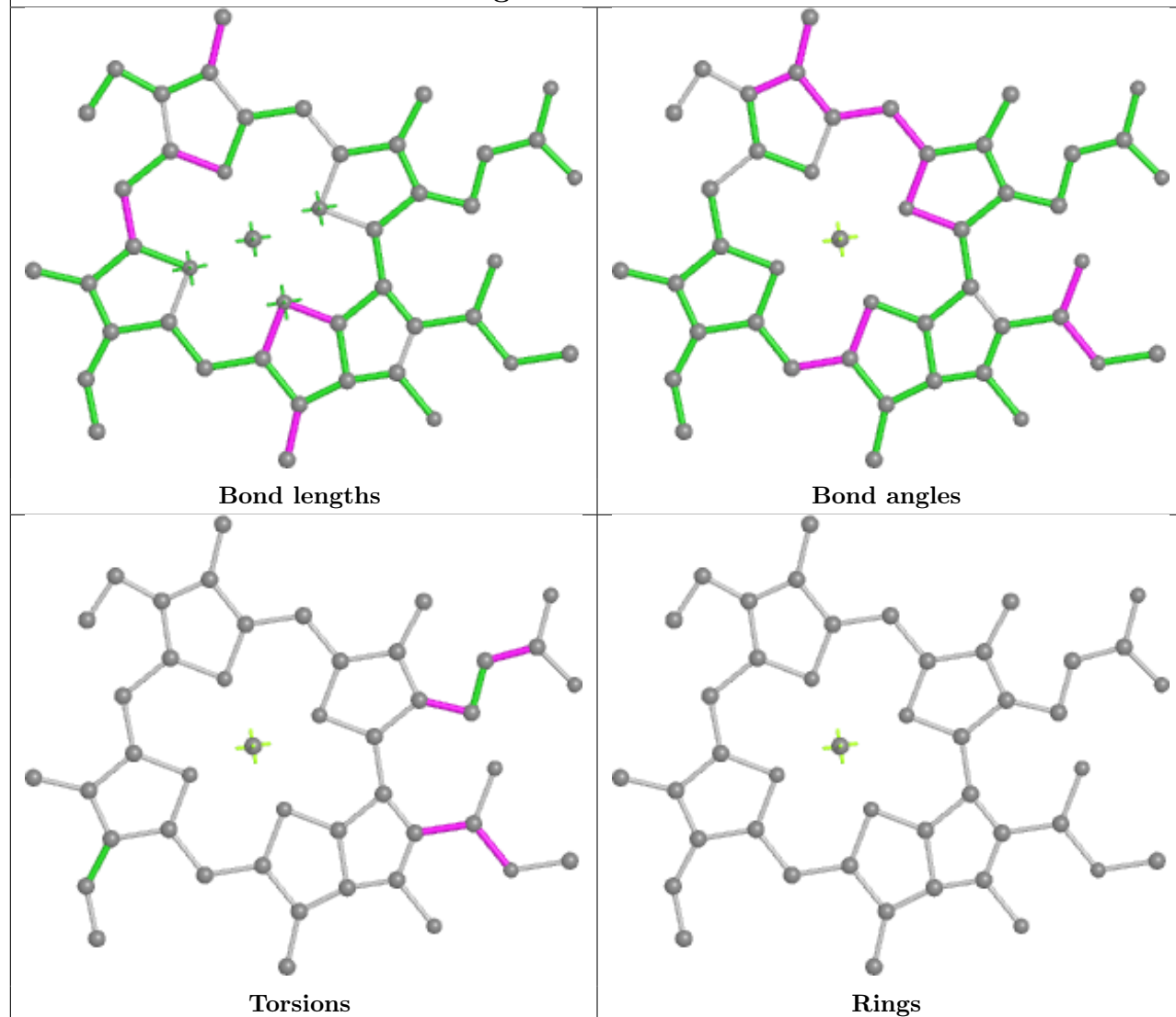


Torsions

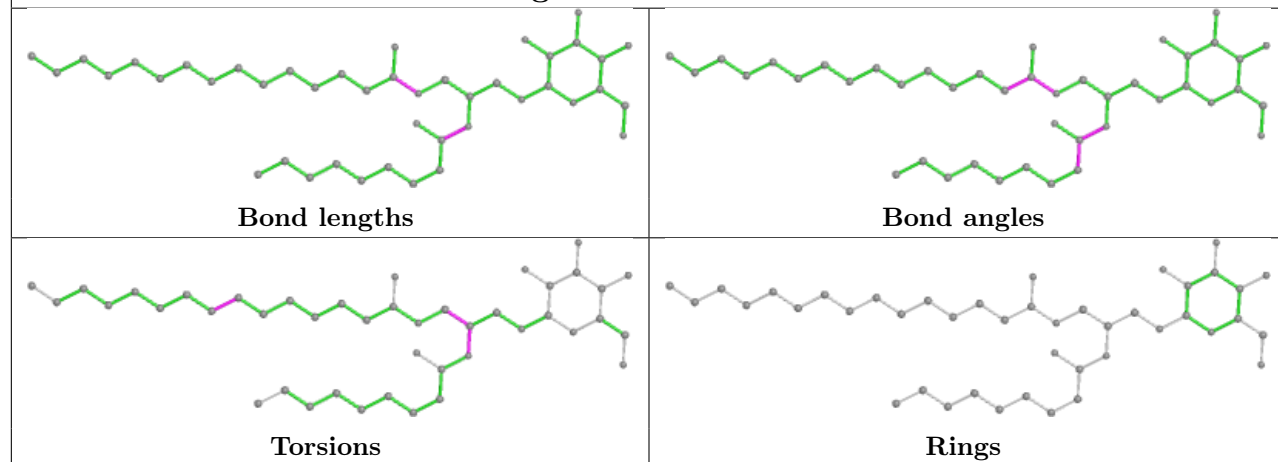


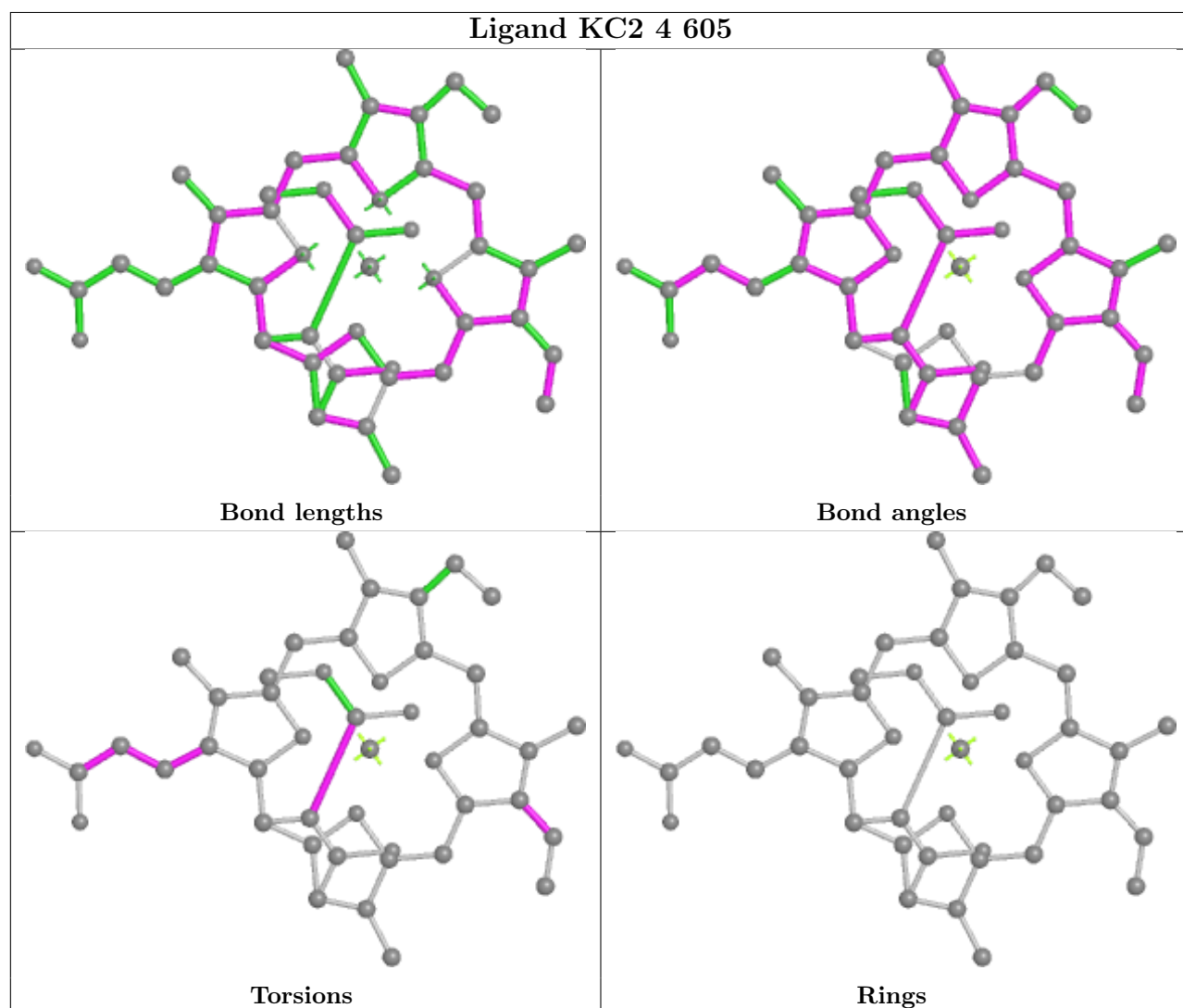
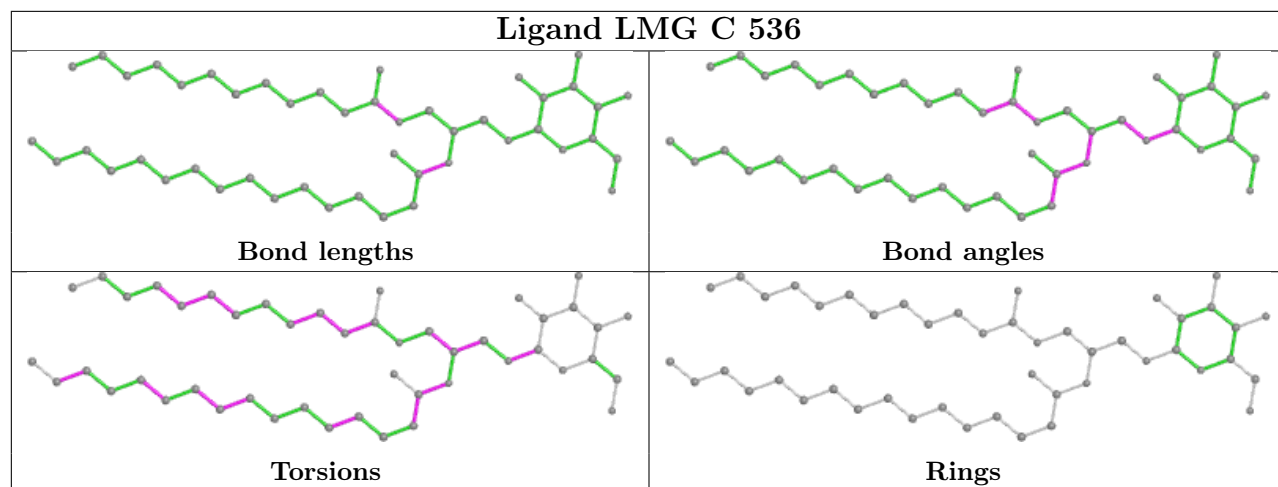
Rings

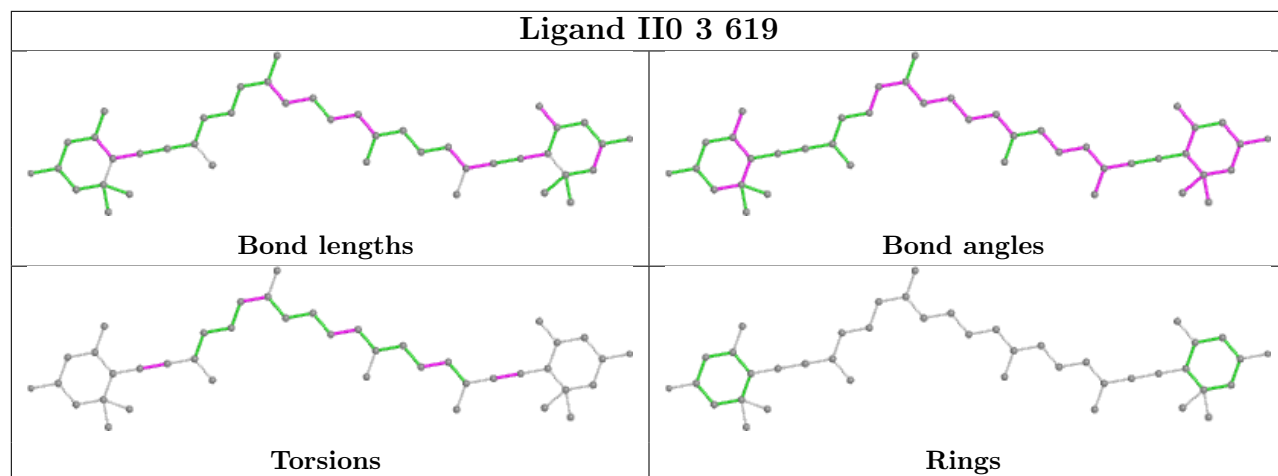
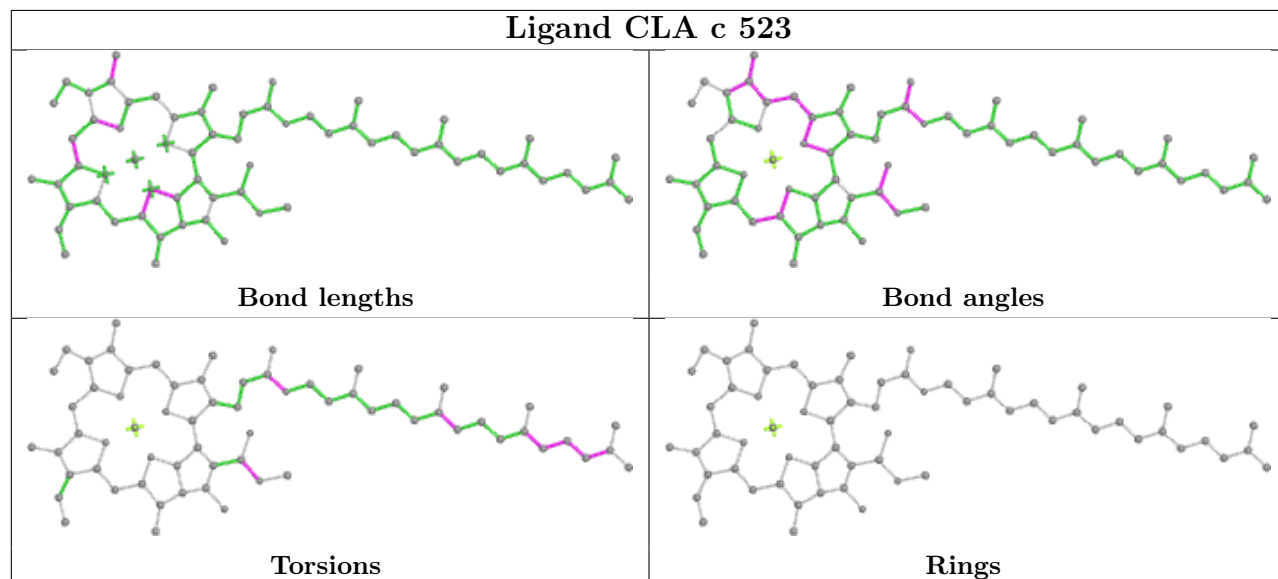
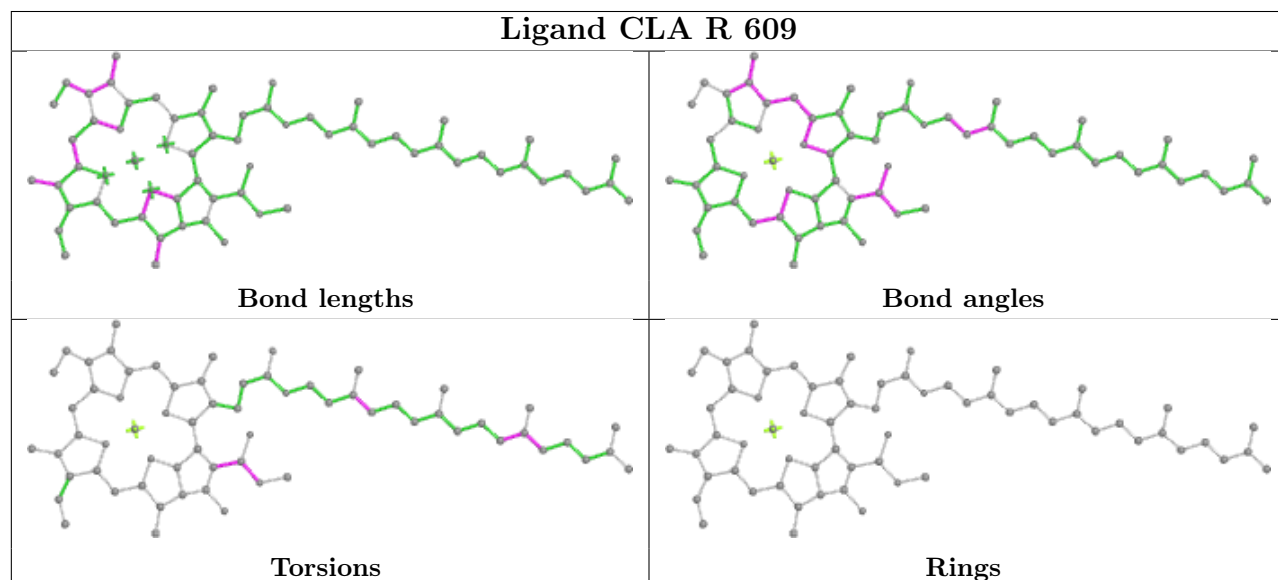
Ligand CLA 2 615



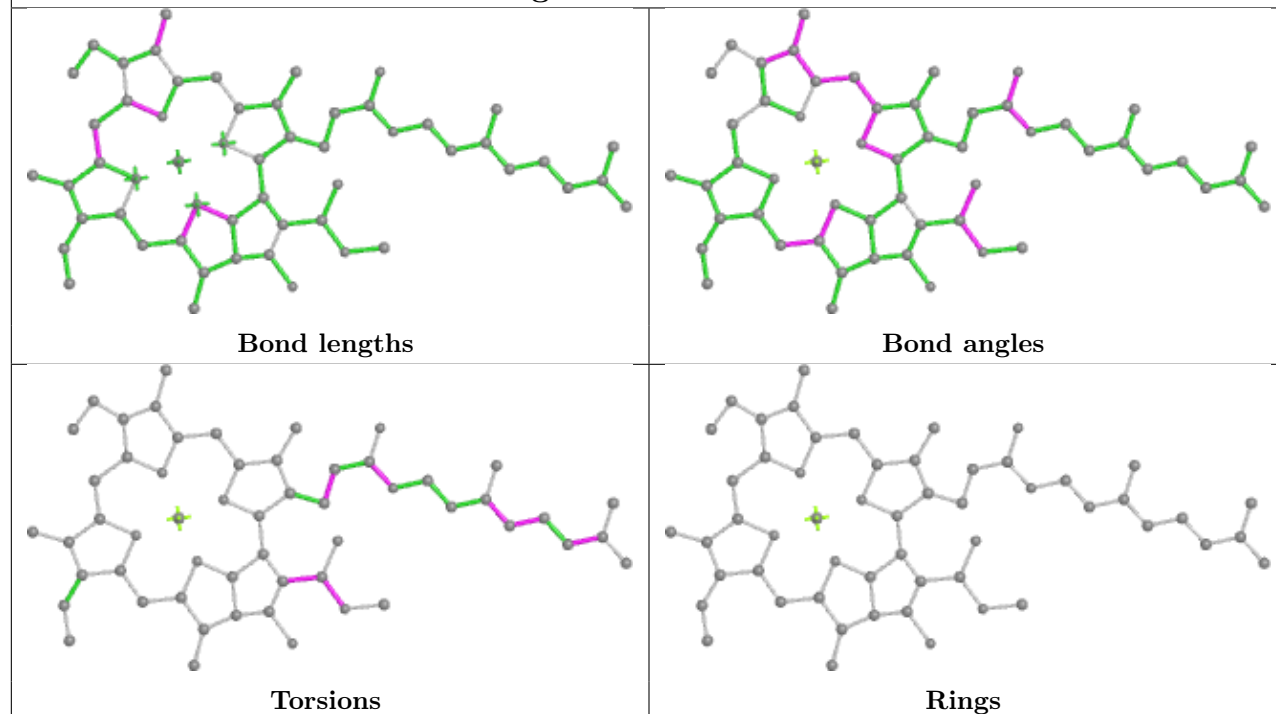
Ligand LMG 4 621



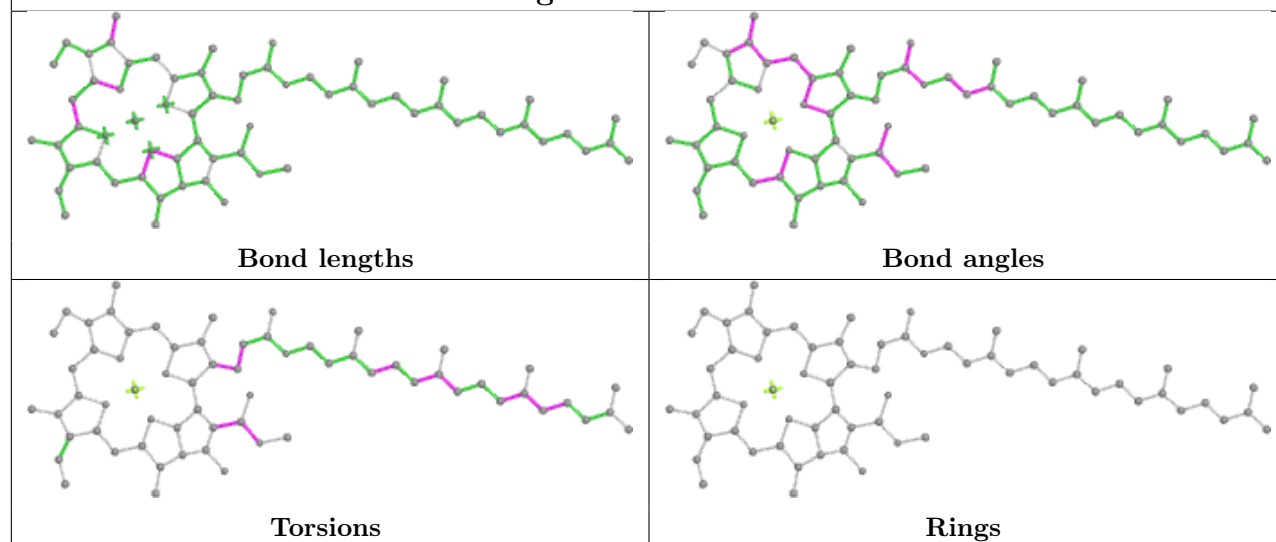


Ligand II0 3 619**Ligand CLA c 523****Ligand CLA R 609**

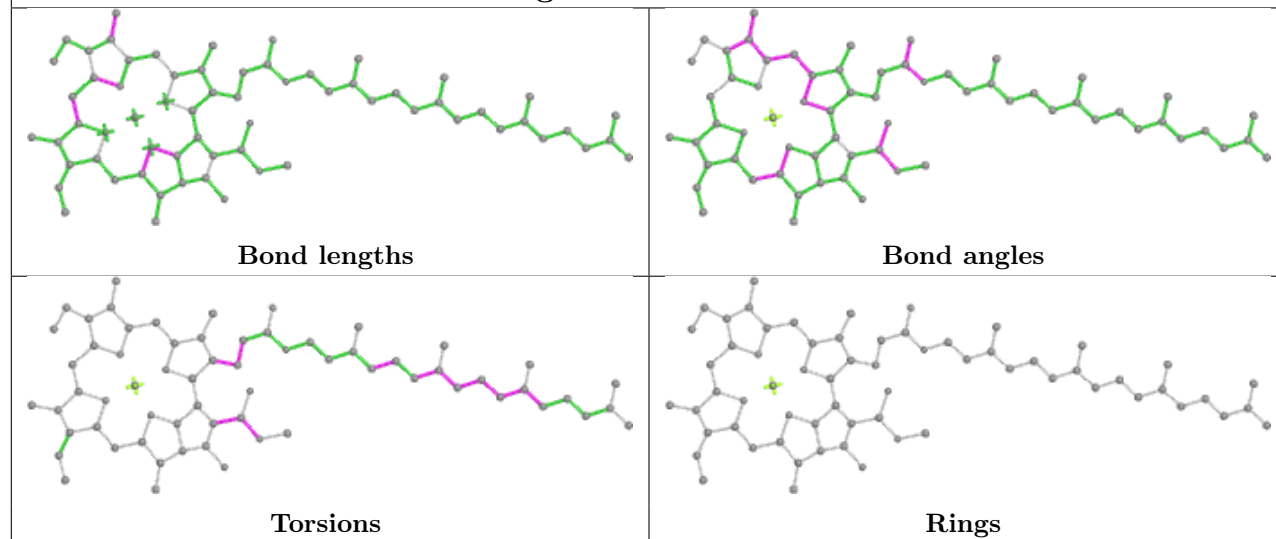
Ligand CLA R 602



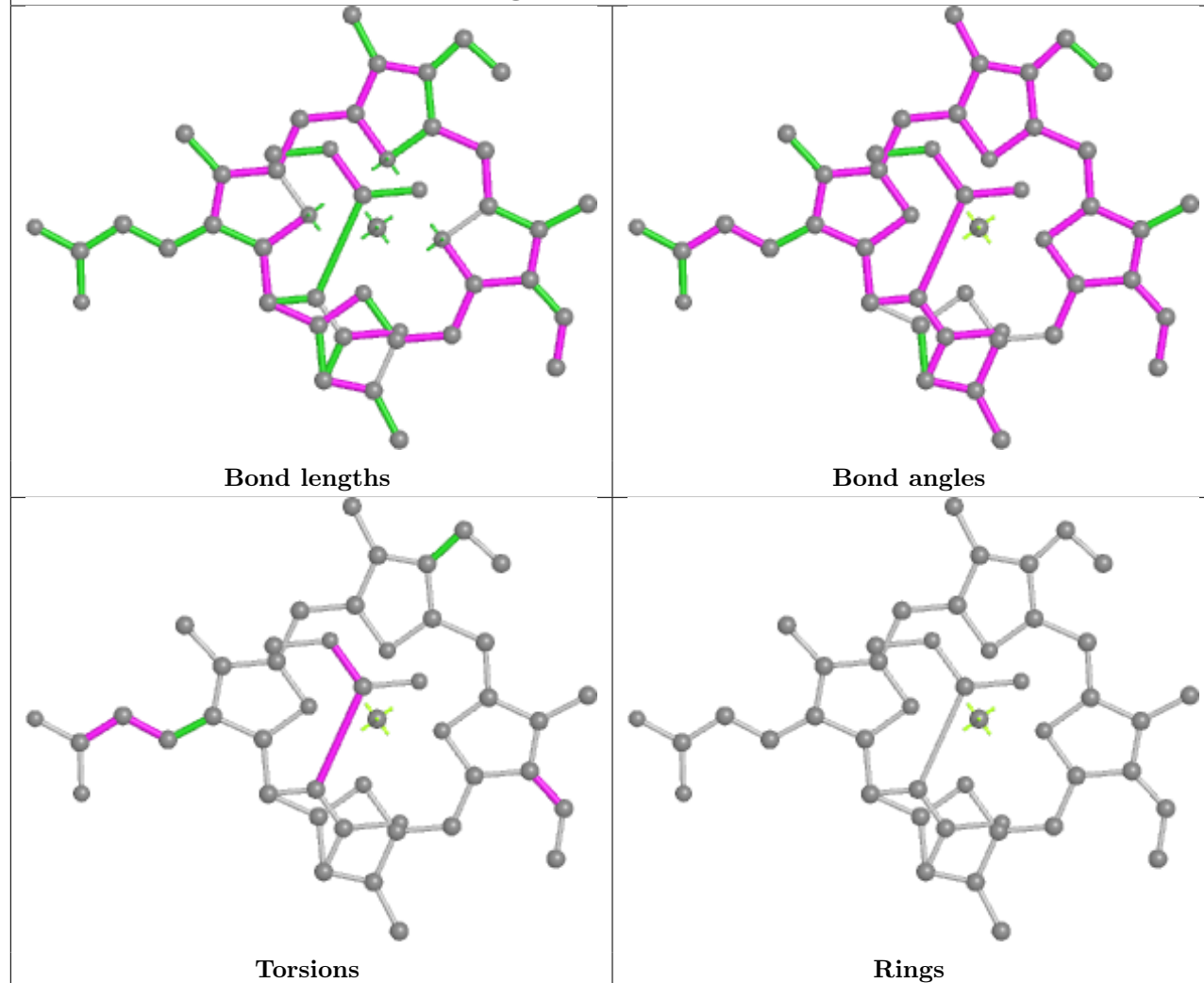
Ligand CLA 2 602



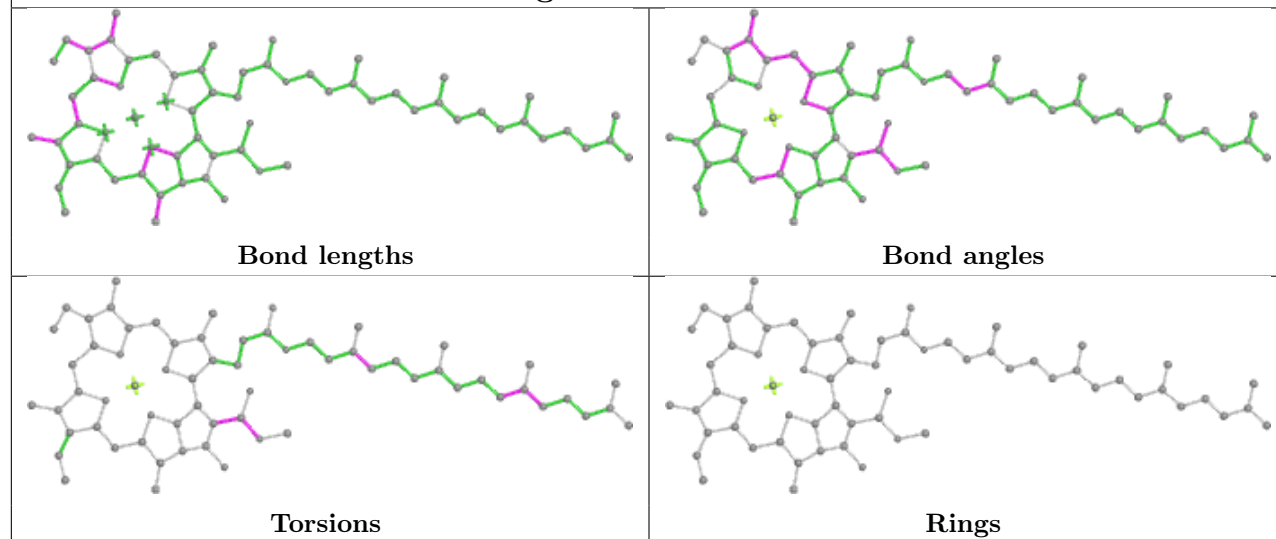
Ligand CLA 6 602



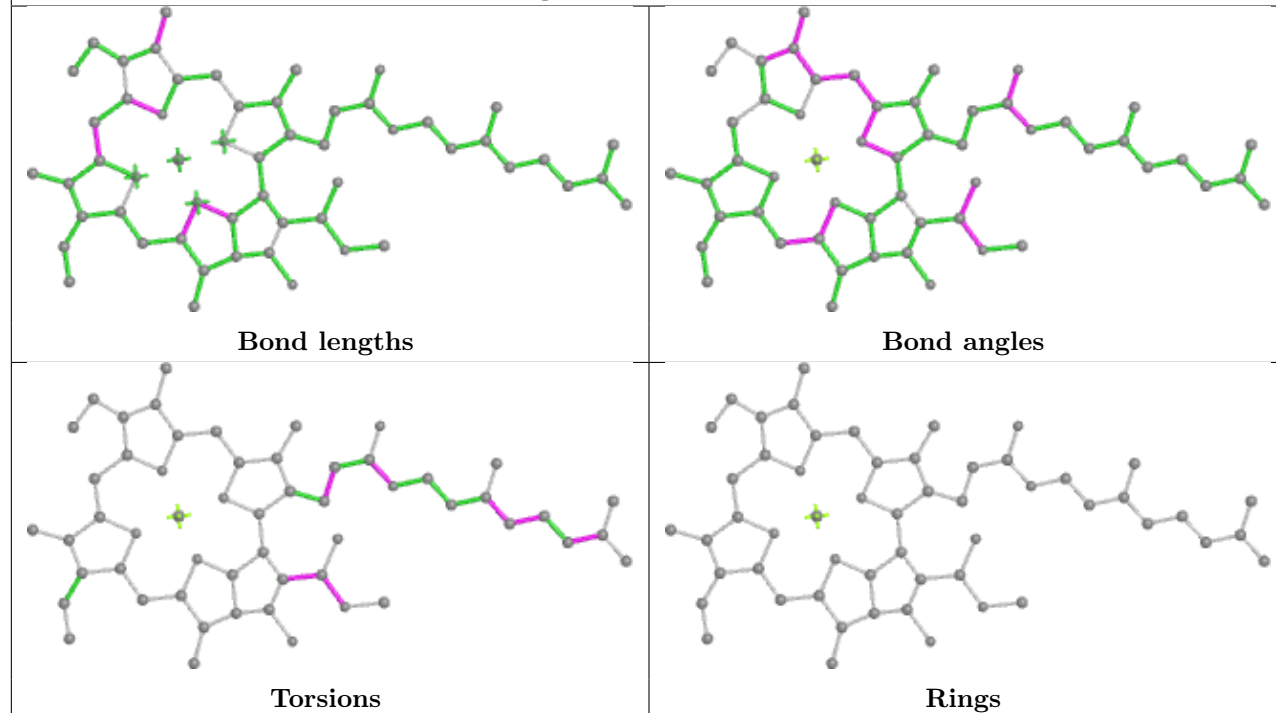
Ligand KC2 6 606



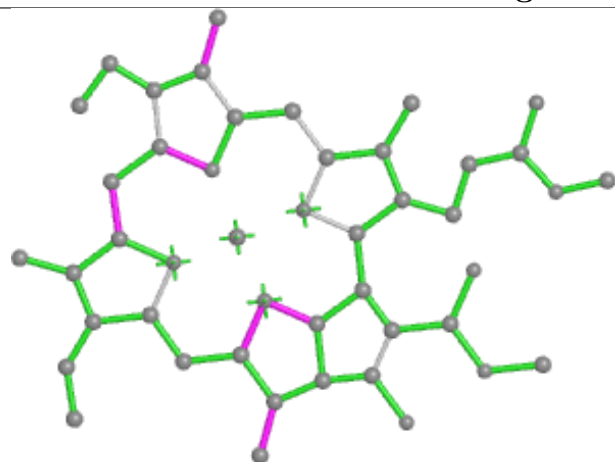
Ligand CLA 5 609



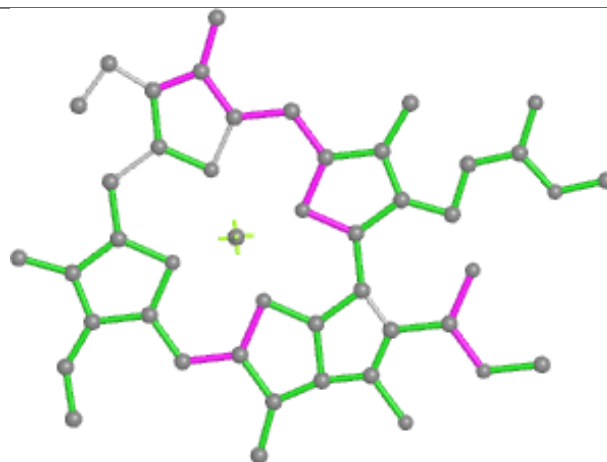
Ligand CLA 5 602



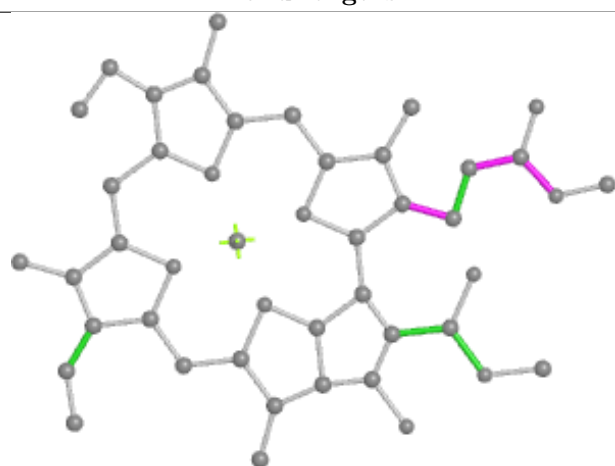
Ligand CLA R 615



Bond lengths



Bond angles

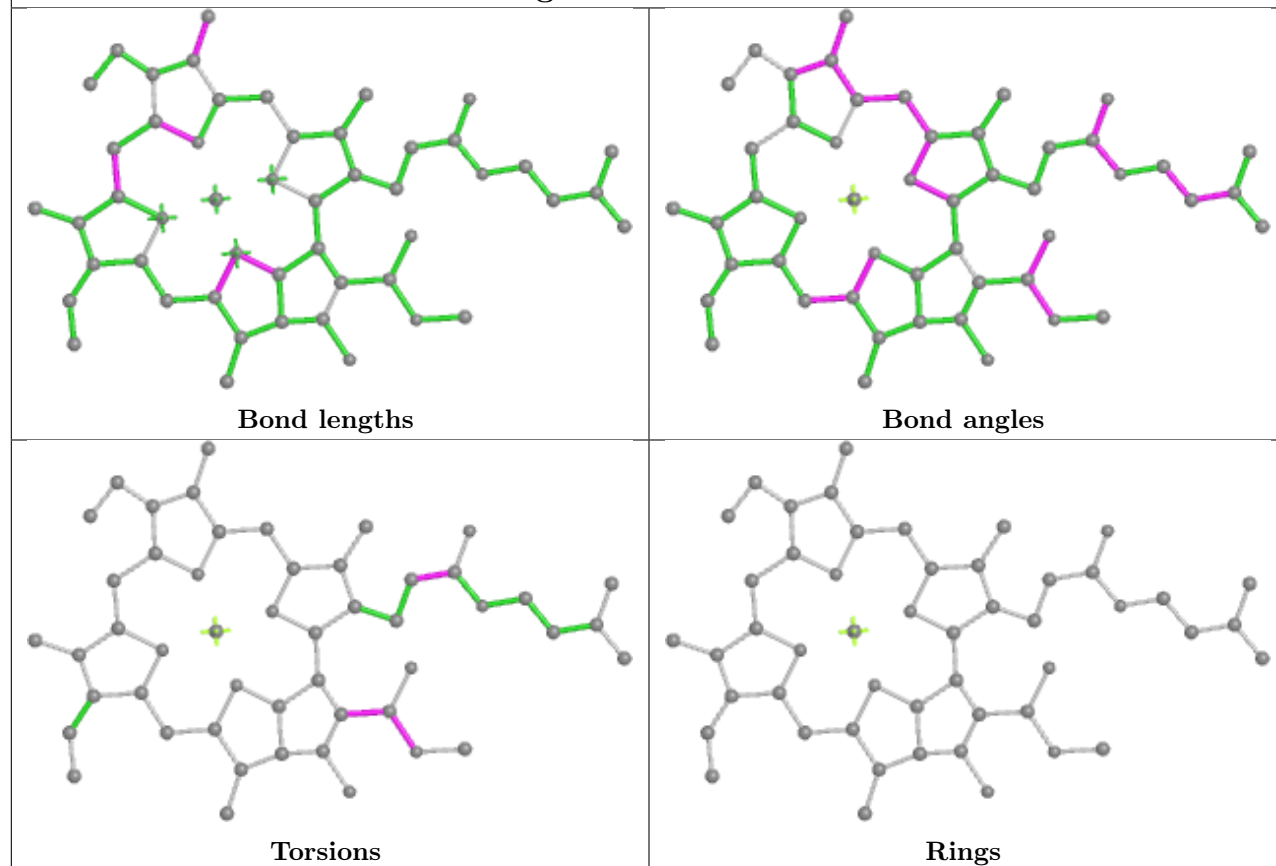


Torsions

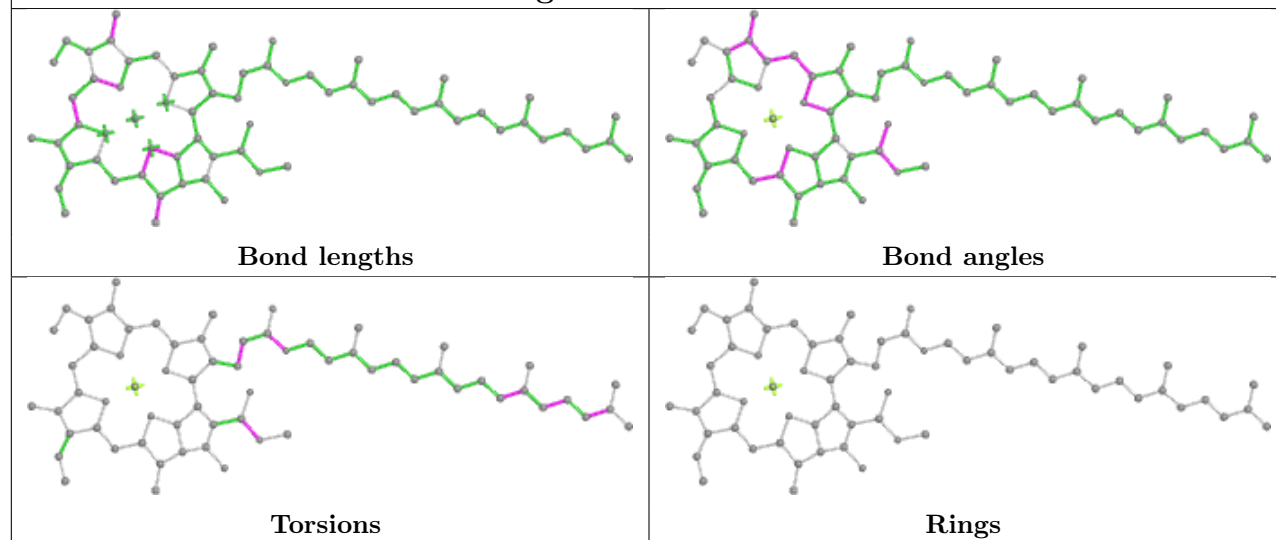


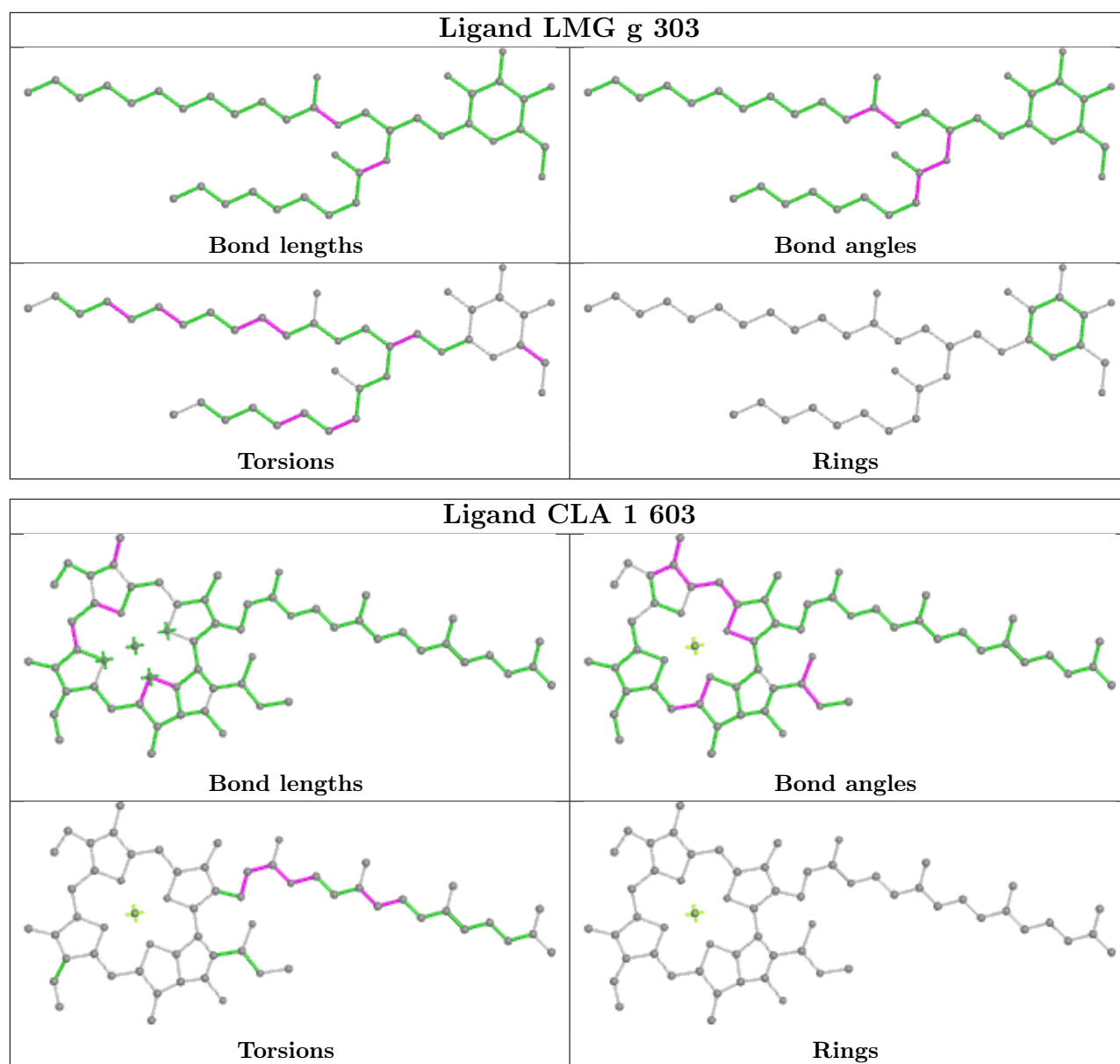
Rings

Ligand CLA 1 606



Ligand CLA 6 615





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.

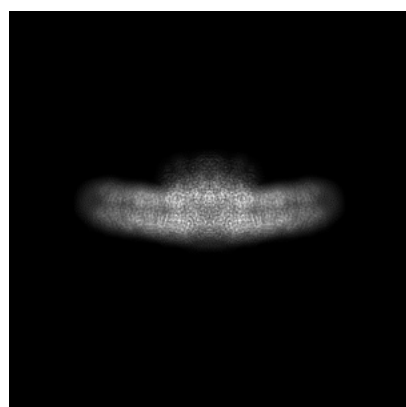
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38455. These allow visual inspection of the internal detail of the map and identification of artifacts.

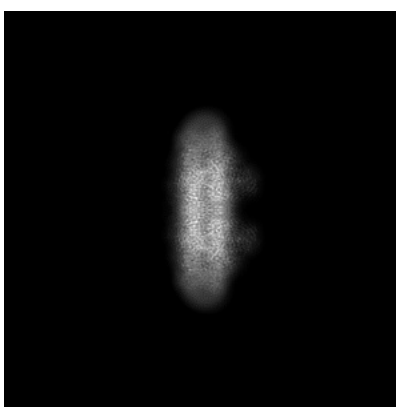
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

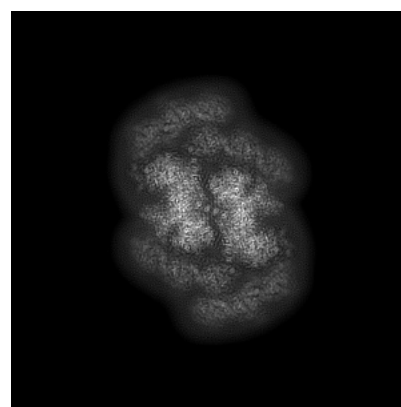
6.1.1 Primary map



X



Y

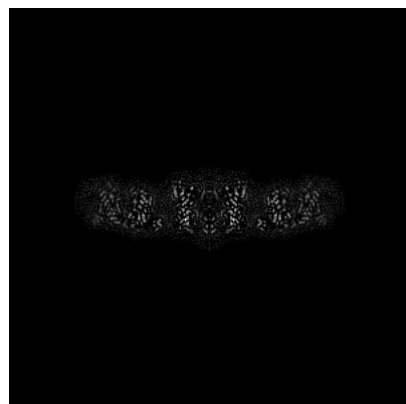


Z

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

6.2 Central slices [i](#)

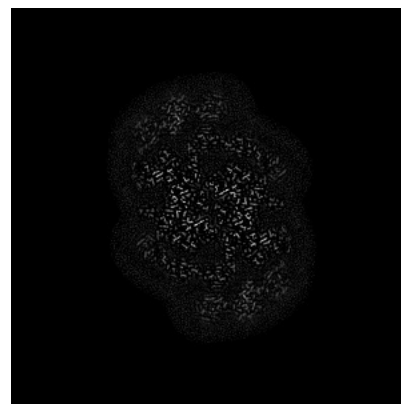
6.2.1 Primary map



X Index: 208



Y Index: 208

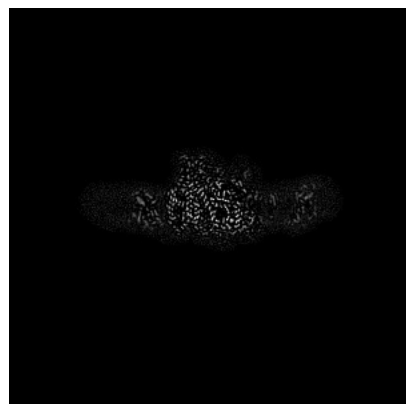


Z Index: 208

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

6.3 Largest variance slices [i](#)

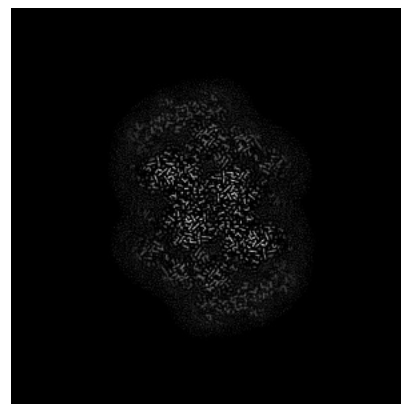
6.3.1 Primary map



X Index: 182



Y Index: 222

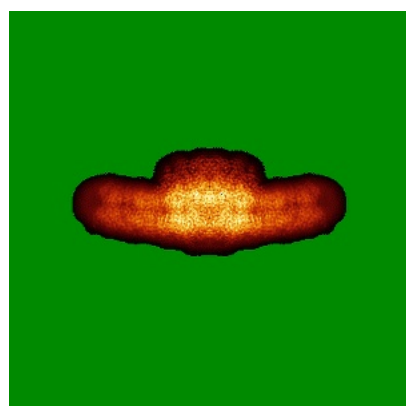


Z Index: 198

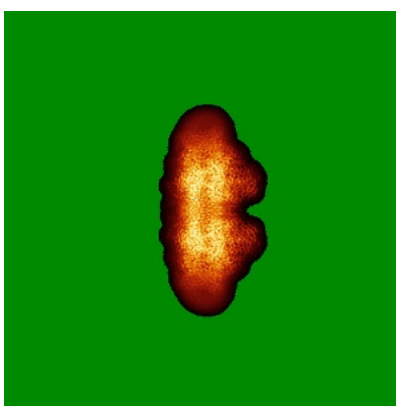
The images above show the largest variance slices of the map in three orthogonal directions.

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

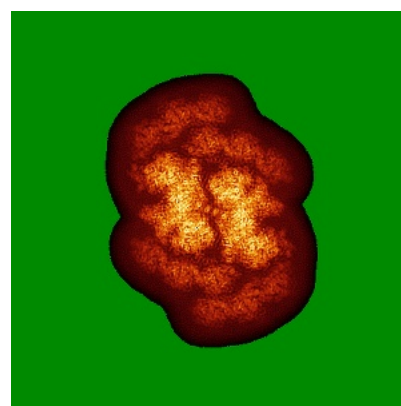
6.4.1 Primary map



X



Y

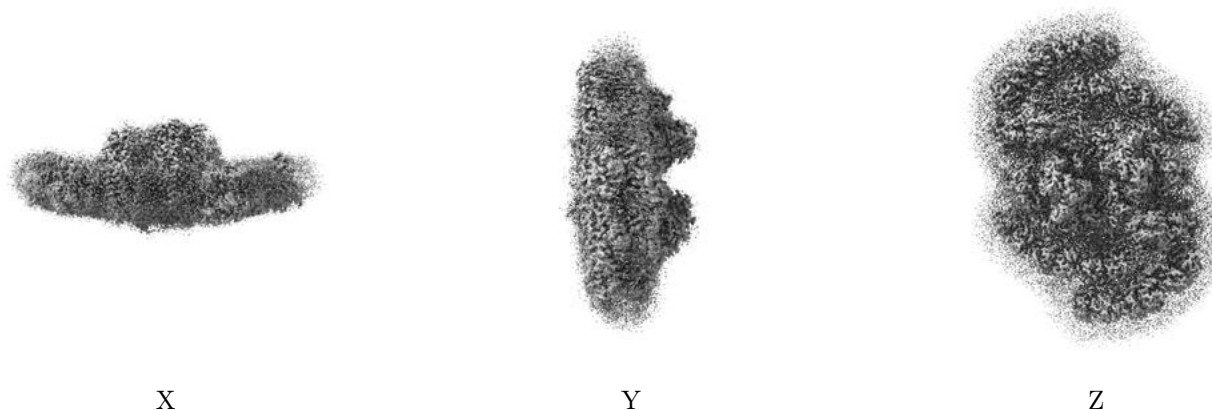


Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

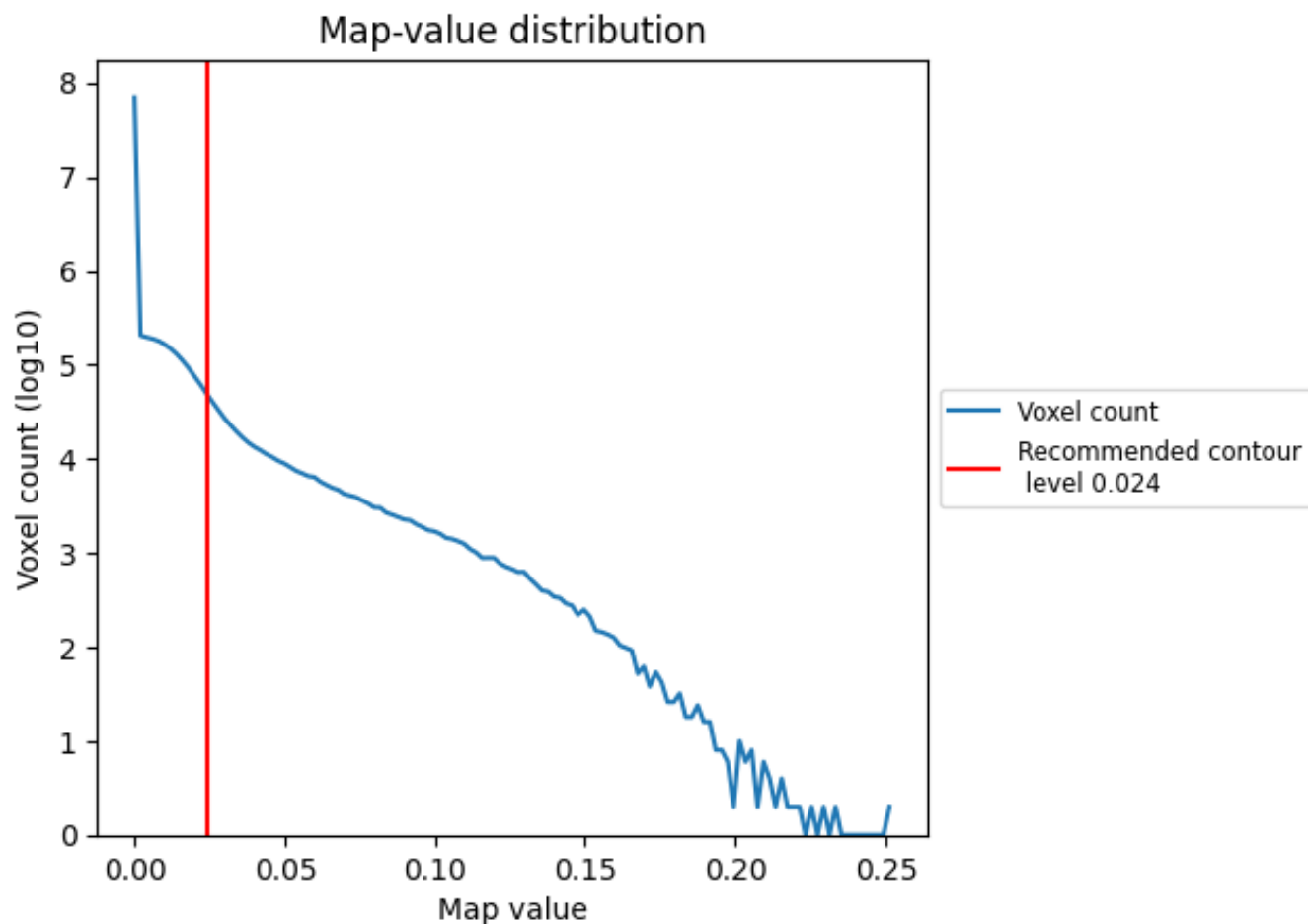
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

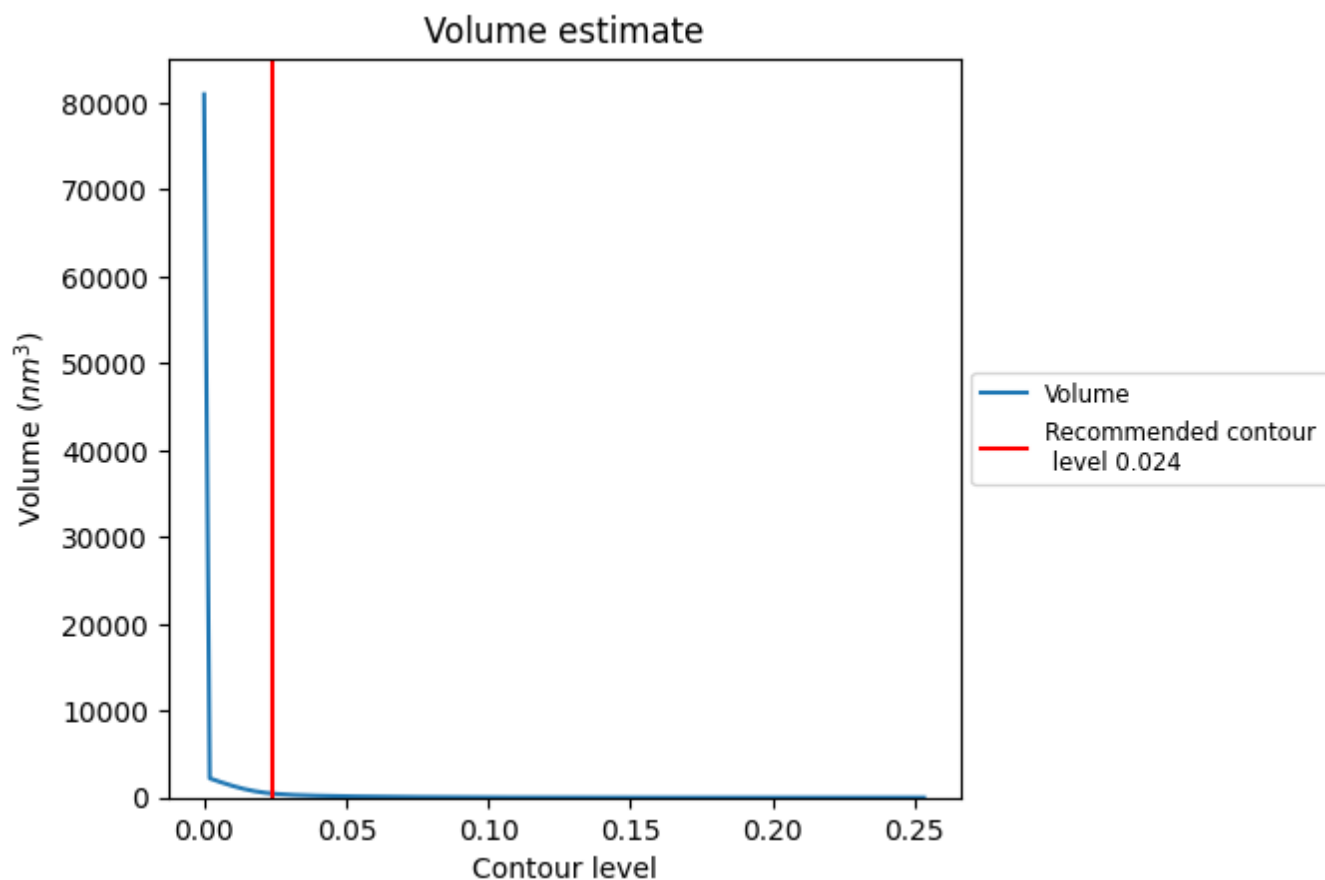
This section contains the results of statistical analysis of the map.

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.

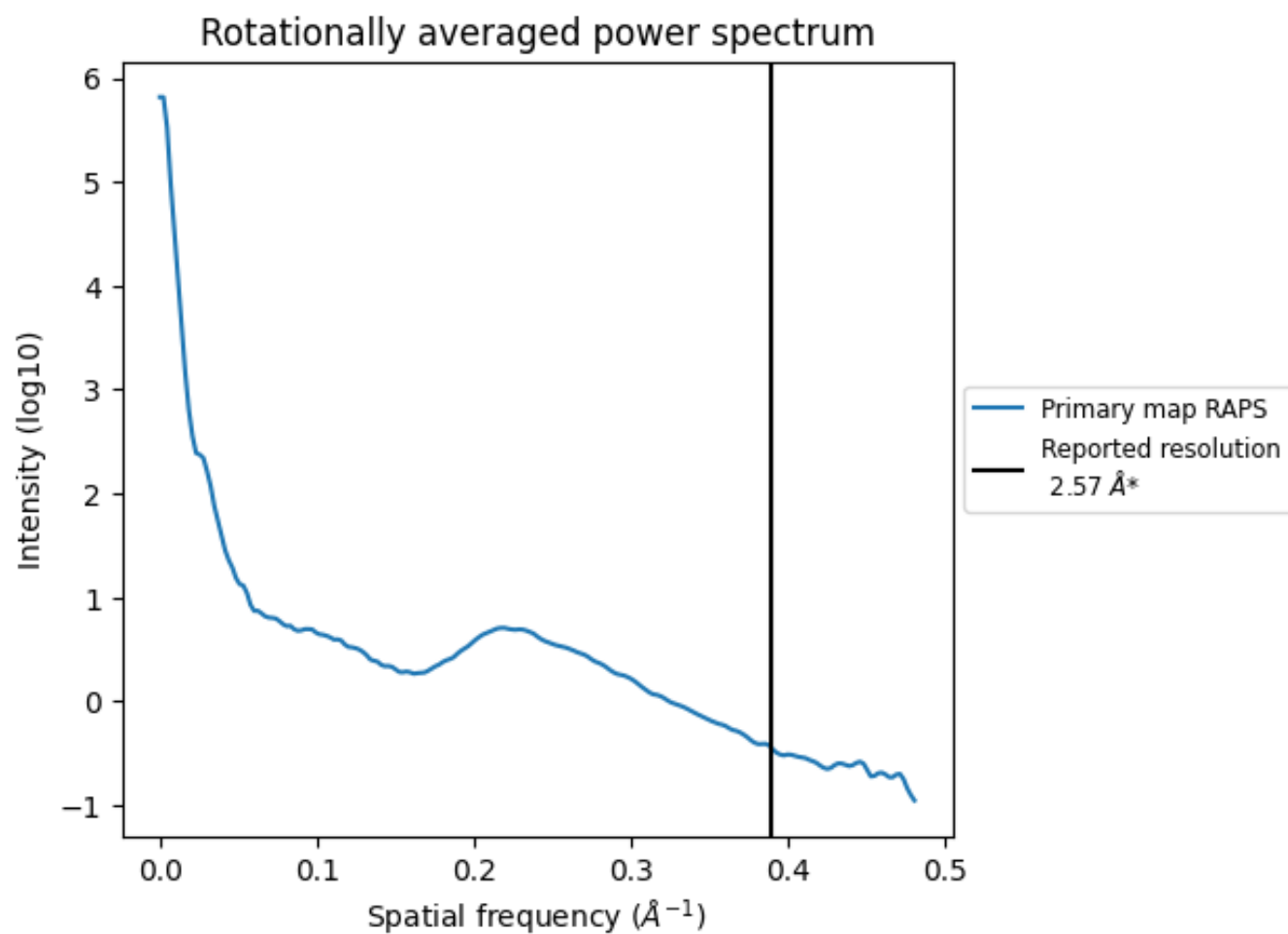
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm³; this corresponds to an approximate mass of 417 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 0.389 Å⁻¹

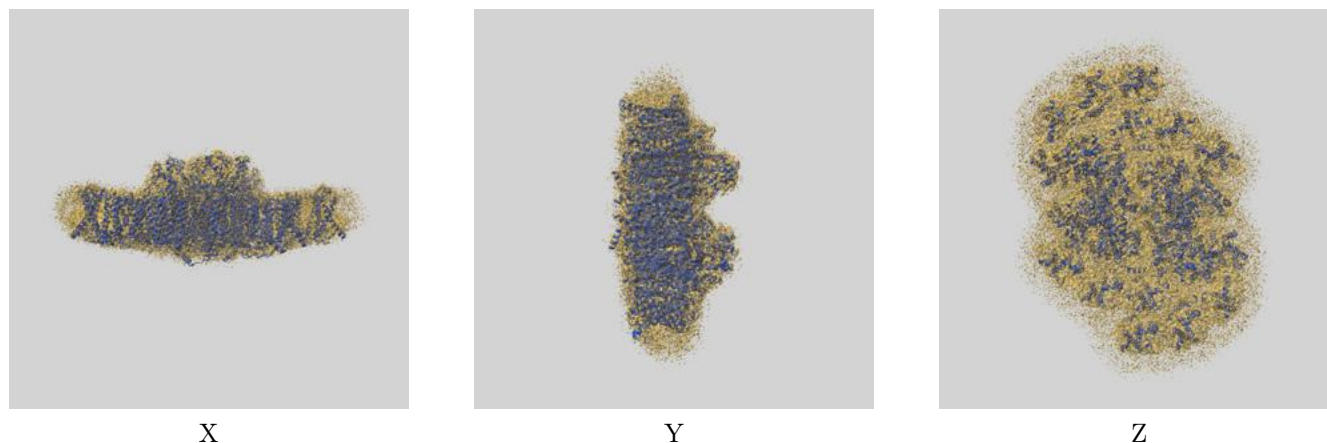
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

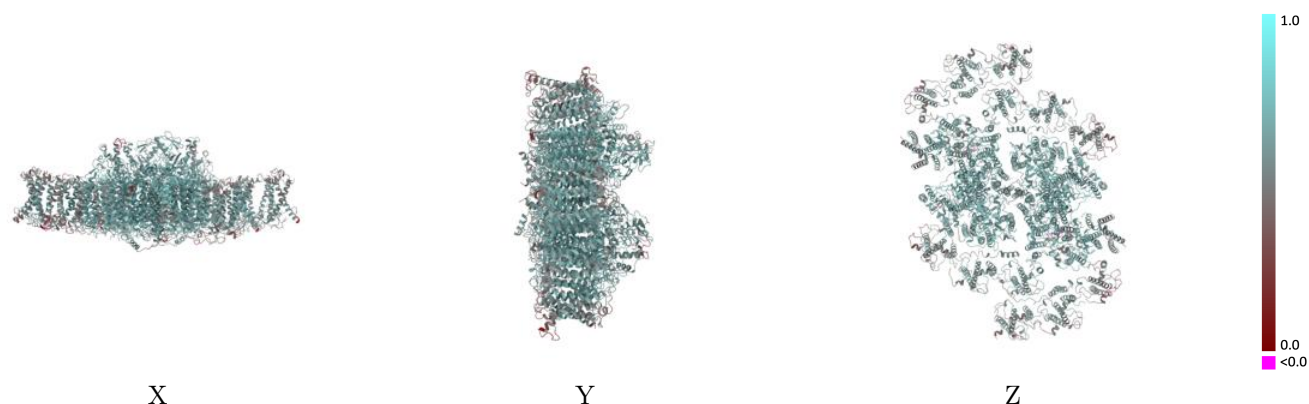
This section contains information regarding the fit between EMDB map EMD-38455 and PDB model 8XLP. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



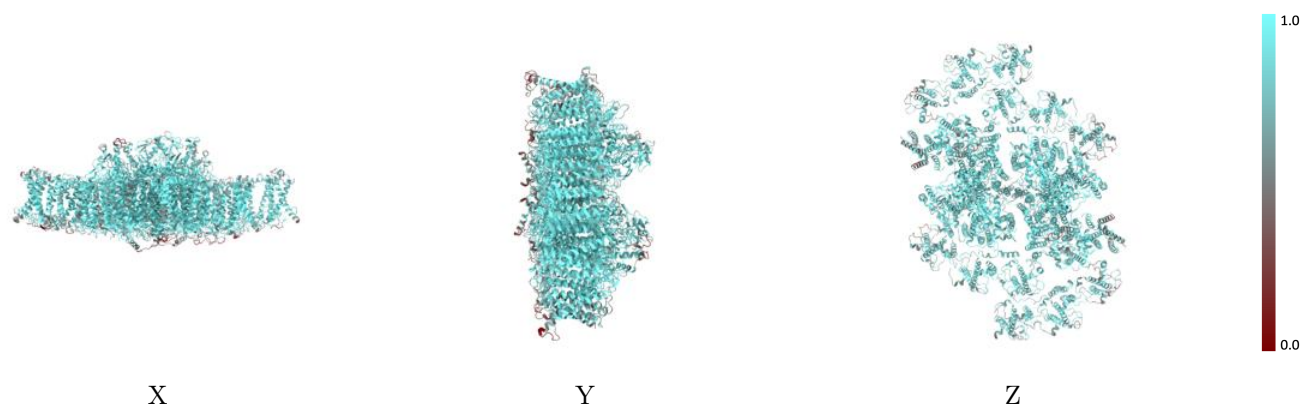
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



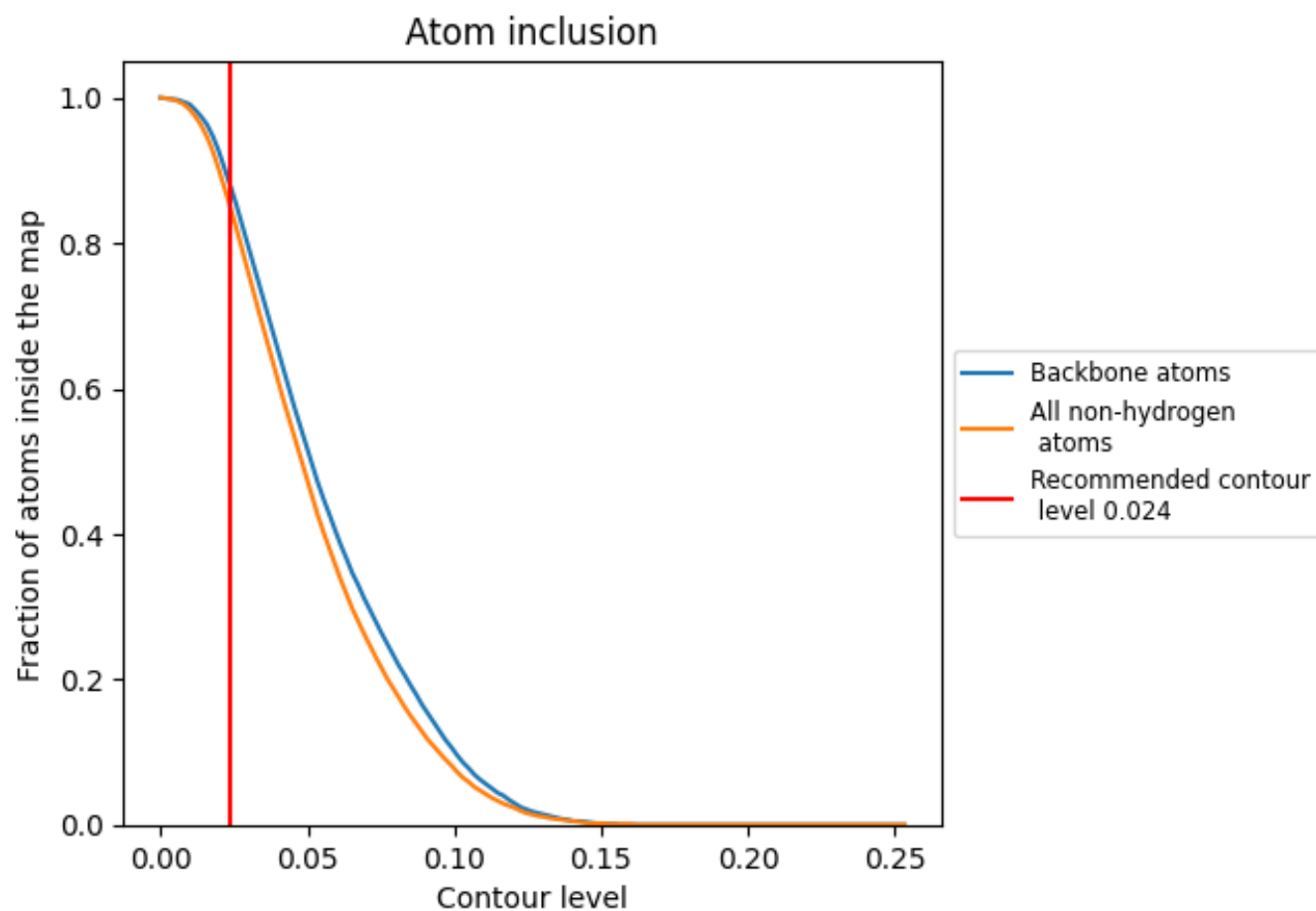
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.5980
1	 0.7140	 0.5020
2	 0.8310	 0.5580
3	 0.8790	 0.5930
4	 0.7750	 0.5350
5	 0.7940	 0.5290
6	 0.6910	 0.4620
A	 0.9410	 0.6790
B	 0.9180	 0.6570
C	 0.8900	 0.6360
D	 0.9550	 0.6820
E	 0.7920	 0.5820
F	 0.7420	 0.5460
G	 0.7280	 0.5440
H	 0.9280	 0.6440
I	 0.9790	 0.6960
K	 0.8700	 0.6110
L	 0.9620	 0.6660
M	 0.8390	 0.5970
N	 0.6900	 0.4630
O	 0.8340	 0.5610
P	 0.8800	 0.5980
Q	 0.7760	 0.5270
R	 0.8050	 0.5410
S	 0.6950	 0.4870
T	 0.9410	 0.6690
W	 0.8860	 0.6330
X	 0.8830	 0.6140
Y	 0.6100	 0.5300
Z	 0.6220	 0.4910
a	 0.9440	 0.6800
b	 0.9160	 0.6570
c	 0.8870	 0.6360
d	 0.9540	 0.6820
e	 0.7830	 0.5780



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Chain	Atom inclusion	Q-score
f	 0.7520	 0.5470
g	 0.7260	 0.5500
h	 0.9230	 0.6430
i	 0.9790	 0.6900
k	 0.8870	 0.6100
l	 0.9650	 0.6690
m	 0.8290	 0.5940
t	 0.9330	 0.6710
w	 0.8590	 0.6060
x	 0.8910	 0.6090
y	 0.5990	 0.5230
z	 0.6160	 0.5020