Full wwPDB EM Validation Report ⓘ

Apr 3, 2024 – 01:04 PM EDT

PDB ID	:	9B4H
EMDB ID	:	EMD-43892
Title	:	Chlamydomonas reinhardtii mastigoneme filament
Authors	:	Dai, J.; Ma, M.; Zhang, R.; Brown, A.
Deposited on	:	2024-03-20
Resolution	:	3.10 Å(reported)
Based on initial model	:	.

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:

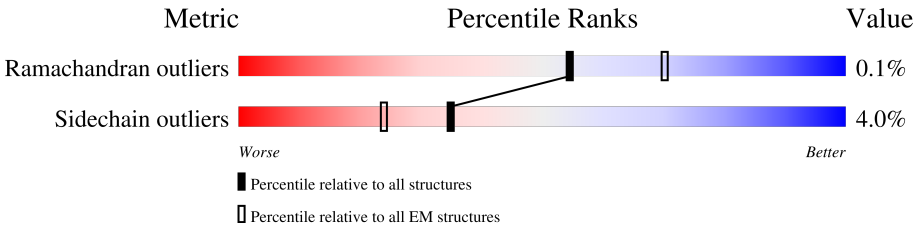
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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.



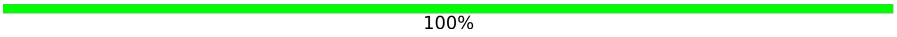
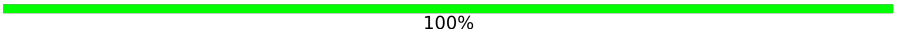
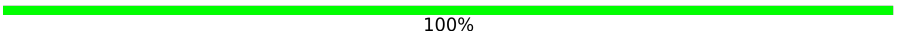
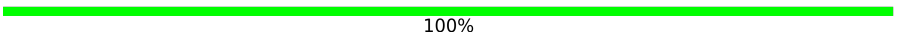
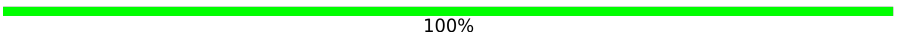
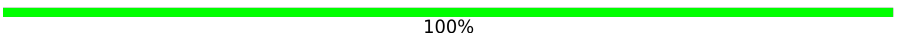
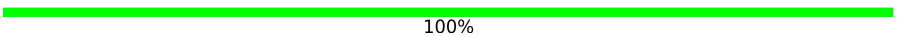
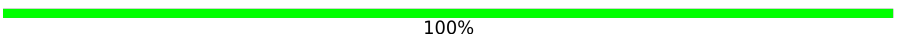
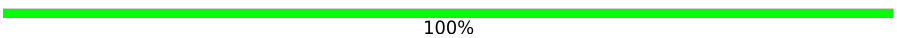
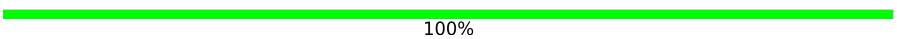
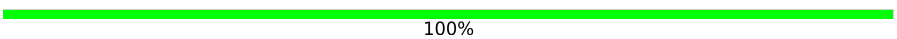
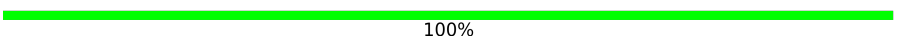
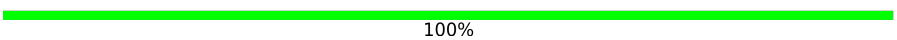
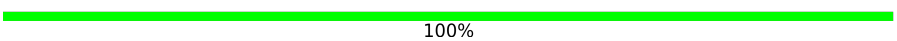
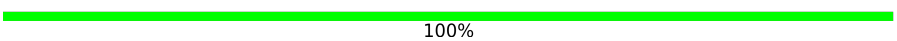
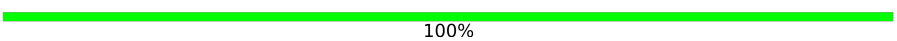
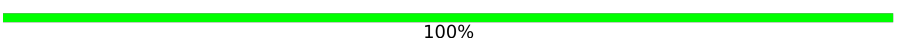
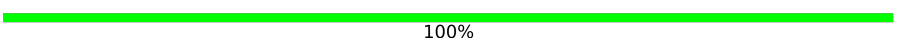
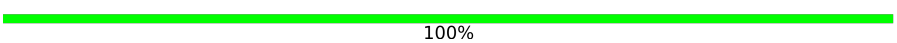
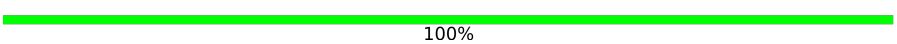
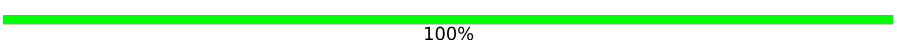
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1987	90% 6% ·
1	B	1987	90% 6% ·
2	X	8572	· 99%
3	A1	2	50% 50%
3	A2	2	50% 50%
3	A3	2	50% 50%
3	a1	2	50% 50%
3	a2	2	50% 50%
3	a3	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A4	2	
4	A5	2	
4	A7	2	
4	B0	2	
4	B1	2	
4	B3	2	
4	B4	2	
4	B5	2	
4	B7	2	
4	B9	2	
4	C0	2	
4	C1	2	
4	C2	2	
4	C3	2	
4	C4	2	
4	C5	2	
4	C6	2	
4	C7	2	
4	C8	2	
4	C9	2	
4	D0	2	
4	D1	2	
4	D2	2	
4	D3	2	
4	D4	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D5	2	100%
4	D6	2	100%
4	D7	2	100%
4	D8	2	100%
4	D9	2	100%
4	E0	2	100%
4	E1	2	100%
4	E2	2	100%
4	E3	2	100%
4	E4	2	100%
4	E5	2	100%
4	E7	2	100%
4	E8	2	100%
4	F0	2	100%
4	F2	2	100%
4	F3	2	100%
4	F5	2	100%
4	F8	2	100%
4	a5	2	50% 50%
4	a7	2	50% 50%
4	b0	2	100%
4	b1	2	100%
4	b3	2	100%
4	b4	2	100%
4	b5	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	b7	2	100%
4	b9	2	100%
4	c0	2	100%
4	c1	2	100%
4	c2	2	100%
4	c3	2	100%
4	c4	2	100%
4	c5	2	100%
4	c6	2	100%
4	c7	2	100%
4	c8	2	100%
4	c9	2	100%
4	d0	2	100%
4	d1	2	50% 50%
4	d2	2	100%
4	d3	2	100%
4	d4	2	100%
4	d5	2	100%
4	d6	2	100%
4	d7	2	100%
4	d8	2	50% 50%
4	d9	2	100%
4	e0	2	100%
4	e1	2	100%
4	e2	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	e3	2	50% 50%
4	e4	2	100%
4	e5	2	100%
4	e6	2	50% 50%
4	e7	2	50% 50%
4	e8	2	100%
4	f0	2	50% 50%
4	f2	2	50% 50%
4	f3	2	100%
4	f5	2	100%
4	f8	2	100%
5	A6	4	100%
5	A9	4	100%
5	B6	4	100%
5	F6	4	100%
5	F7	4	100%
5	a6	4	100%
5	a9	4	25% 75%
5	b6	4	100%
5	f6	4	100%
5	f7	4	100%
6	E6	8	100%
7	a4	2	100%
8	e9	6	100%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	34V	a4	1	X	-	-	-
9	A1AIO	A	2004	X	-	-	-
9	A1AIO	A	2006	X	-	-	-
9	A1AIO	A	2009	X	-	-	-
9	A1AIO	A	2011	X	-	-	-
9	A1AIO	A	2012	X	-	-	-
9	A1AIO	A	2014	X	-	-	-
9	A1AIO	A	2016	X	-	-	-
9	A1AIO	A	2018	X	-	-	-
9	A1AIO	A	2025	X	-	-	-
9	A1AIO	A	2035	X	-	-	-
9	A1AIO	A	2037	X	-	-	-
9	A1AIO	A	2038	X	-	-	-
9	A1AIO	A	2040	X	-	-	-
9	A1AIO	A	2052	X	-	-	-
9	A1AIO	B	2004	X	-	-	-
9	A1AIO	B	2006	X	-	-	-
9	A1AIO	B	2009	X	-	-	-
9	A1AIO	B	2011	X	-	-	-
9	A1AIO	B	2012	X	-	-	-
9	A1AIO	B	2014	X	-	-	-
9	A1AIO	B	2016	X	-	-	-
9	A1AIO	B	2030	X	-	-	-
9	A1AIO	B	2031	X	-	-	-
9	A1AIO	B	2032	X	-	-	-
9	A1AIO	B	2033	X	-	-	-
9	A1AIO	B	2034	X	-	-	-
9	A1AIO	B	2046	X	-	-	-
9	A1AIO	B	2047	X	-	-	-
9	A1AIO	B	2053	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 32328 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 Tyrosine-protein kinase ephrin type A/B receptor-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1908	Total	C	N	O	S	0	0
			13867	8726	2262	2798	81		
1	B	1908	Total	C	N	O	S	0	0
			13867	8726	2262	2798	81		

- Molecule 2 is a protein called C-type lectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	109	Total	C	N	O	S	0	0
			834	509	116	208	1		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A1	2	Total	C	N	O	0	0
			28	16	2	10		
3	A2	2	Total	C	N	O	0	0
			28	16	2	10		
3	A3	2	Total	C	N	O	0	0
			28	16	2	10		
3	a1	2	Total	C	N	O	0	0
			28	16	2	10		
3	a2	2	Total	C	N	O	0	0
			28	16	2	10		
3	a3	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	A4	2	Total C O 18 10 8	0	0
4	A5	2	Total C O 18 10 8	0	0
4	A7	2	Total C O 18 10 8	0	0
4	B0	2	Total C O 18 10 8	0	0
4	B1	2	Total C O 18 10 8	0	0
4	B3	2	Total C O 18 10 8	0	0
4	B4	2	Total C O 18 10 8	0	0
4	B5	2	Total C O 18 10 8	0	0
4	B7	2	Total C O 18 10 8	0	0
4	B9	2	Total C O 18 10 8	0	0
4	C0	2	Total C O 18 10 8	0	0
4	C1	2	Total C O 18 10 8	0	0
4	C2	2	Total C O 18 10 8	0	0
4	C3	2	Total C O 18 10 8	0	0
4	C4	2	Total C O 18 10 8	0	0
4	C5	2	Total C O 18 10 8	0	0
4	C6	2	Total C O 18 10 8	0	0
4	C7	2	Total C O 18 10 8	0	0
4	C8	2	Total C O 18 10 8	0	0
4	C9	2	Total C O 18 10 8	0	0
4	D0	2	Total C O 18 10 8	0	0
4	D1	2	Total C O 18 10 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
4	D2	2	Total C O 18 10 8	0	0
4	D3	2	Total C O 18 10 8	0	0
4	D4	2	Total C O 18 10 8	0	0
4	D5	2	Total C O 18 10 8	0	0
4	D6	2	Total C O 18 10 8	0	0
4	D7	2	Total C O 18 10 8	0	0
4	D8	2	Total C O 18 10 8	0	0
4	D9	2	Total C O 18 10 8	0	0
4	E0	2	Total C O 18 10 8	0	0
4	E1	2	Total C O 18 10 8	0	0
4	E2	2	Total C O 18 10 8	0	0
4	E4	2	Total C O 18 10 8	0	0
4	E5	2	Total C O 18 10 8	0	0
4	E8	2	Total C O 18 10 8	0	0
4	F0	2	Total C O 18 10 8	0	0
4	F3	2	Total C O 18 10 8	0	0
4	F8	2	Total C O 18 10 8	0	0
4	a5	2	Total C O 18 10 8	0	0
4	a7	2	Total C O 18 10 8	0	0
4	b0	2	Total C O 18 10 8	0	0
4	b1	2	Total C O 18 10 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
4	b3	2	Total C O 18 10 8	0	0
4	b4	2	Total C O 18 10 8	0	0
4	b5	2	Total C O 18 10 8	0	0
4	b7	2	Total C O 18 10 8	0	0
4	b9	2	Total C O 18 10 8	0	0
4	c0	2	Total C O 18 10 8	0	0
4	c1	2	Total C O 18 10 8	0	0
4	c2	2	Total C O 18 10 8	0	0
4	c3	2	Total C O 18 10 8	0	0
4	c4	2	Total C O 18 10 8	0	0
4	c5	2	Total C O 18 10 8	0	0
4	c6	2	Total C O 18 10 8	0	0
4	c7	2	Total C O 18 10 8	0	0
4	c8	2	Total C O 18 10 8	0	0
4	c9	2	Total C O 18 10 8	0	0
4	d1	2	Total C O 18 10 8	0	0
4	d2	2	Total C O 18 10 8	0	0
4	d3	2	Total C O 18 10 8	0	0
4	d4	2	Total C O 18 10 8	0	0
4	d5	2	Total C O 18 10 8	0	0
4	e0	2	Total C O 18 10 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
4	e1	2	Total C O 18 10 8	0	0
4	e2	2	Total C O 18 10 8	0	0
4	e4	2	Total C O 18 10 8	0	0
4	e5	2	Total C O 18 10 8	0	0
4	e8	2	Total C O 18 10 8	0	0
4	f0	2	Total C O 18 10 8	0	0
4	f3	2	Total C O 18 10 8	0	0
4	f5	2	Total C O 18 10 8	0	0
4	f8	2	Total C O 18 10 8	0	0
4	E3	2	Total C O 18 10 8	0	0
4	f2	2	Total C O 18 10 8	0	0
4	e7	2	Total C O 18 10 8	0	0
4	e6	2	Total C O 18 10 8	0	0
4	e3	2	Total C O 18 10 8	0	0
4	d9	2	Total C O 18 10 8	0	0
4	d7	2	Total C O 18 10 8	0	0
4	d8	2	Total C O 18 10 8	0	0
4	d6	2	Total C O 18 10 8	0	0
4	d0	2	Total C O 18 10 8	0	0
4	F5	2	Total C O 18 10 8	0	0
4	F2	2	Total C O 18 10 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
4	E7	2	Total 18	C 10	O 8	0	0

- Molecule 5 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
5	A6	4	Total 36	C 20	O 16	0	0
5	A9	4	Total 36	C 20	O 16	0	0
5	B6	4	Total 36	C 20	O 16	0	0
5	F6	4	Total 36	C 20	O 16	0	0
5	F7	4	Total 36	C 20	O 16	0	0
5	a6	4	Total 36	C 20	O 16	0	0
5	a9	4	Total 36	C 20	O 16	0	0
5	b6	4	Total 36	C 20	O 16	0	0
5	f6	4	Total 36	C 20	O 16	0	0
5	f7	4	Total 36	C 20	O 16	0	0

- Molecule 6 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1 -2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	E6	8	Total 72	C 40	O 32	0	0

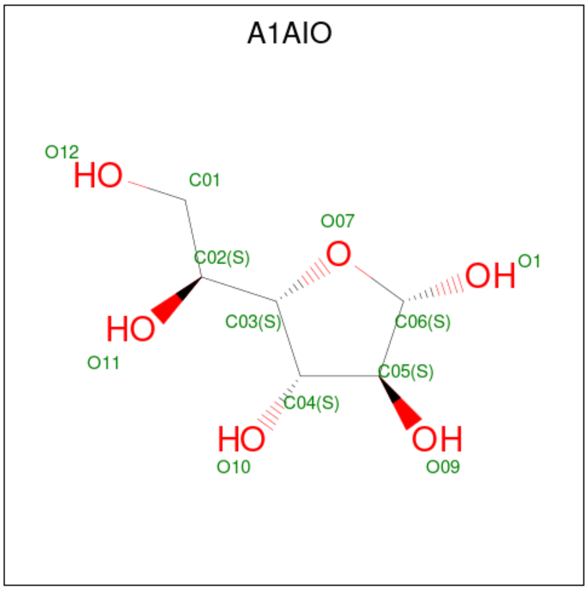
- Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	a4	2	Total 18	C 10	O 8	0	0

- Molecule 8 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose -(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1 -2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	e9	6	Total C O 54 30 24	0	0

- Molecule 9 is beta-L-glucofuranose (three-letter code: A1AIO) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	A	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

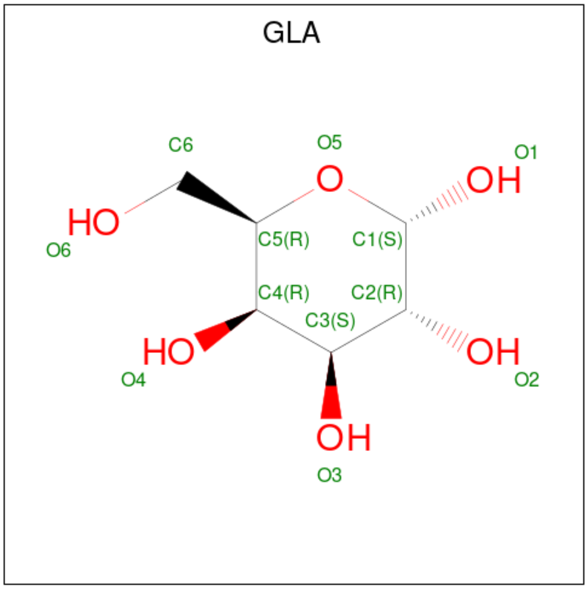
Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0
9	B	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total C O 11 6 5	0

- Molecule 10 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0

Continued on next page...

Continued from previous page...

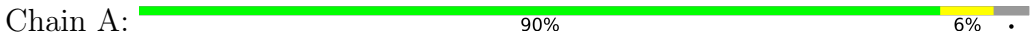
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	A	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0
10	B	1	Total C O 11 6 5	0

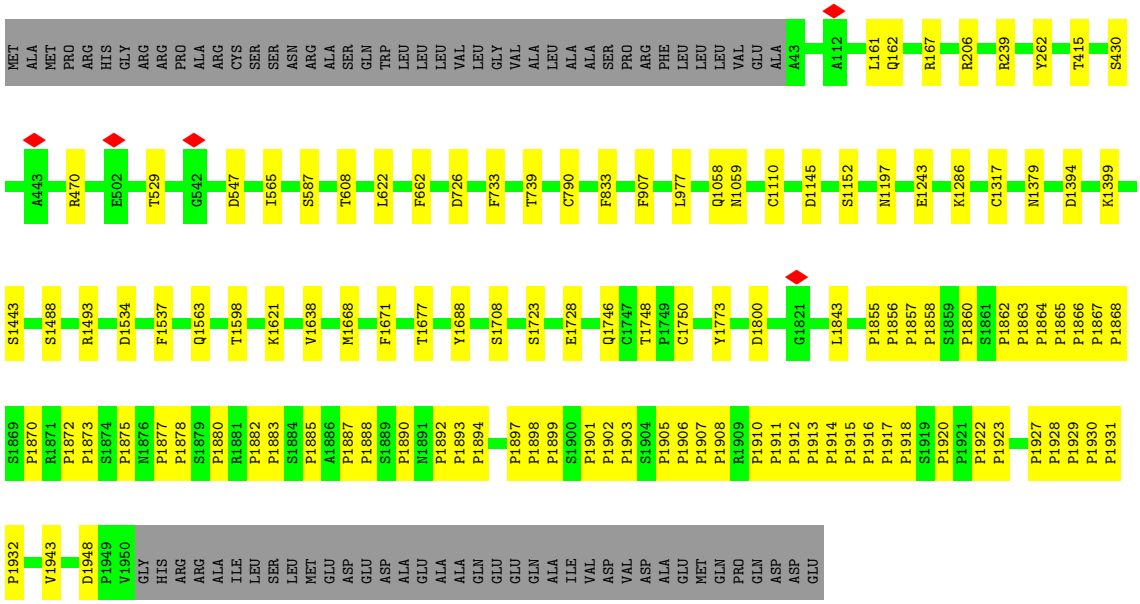
3 Residue-property plots (i)

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: Tyrosine-protein kinase ephrin type A/B receptor-like domain-containing protein

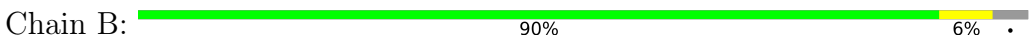
Chain A:

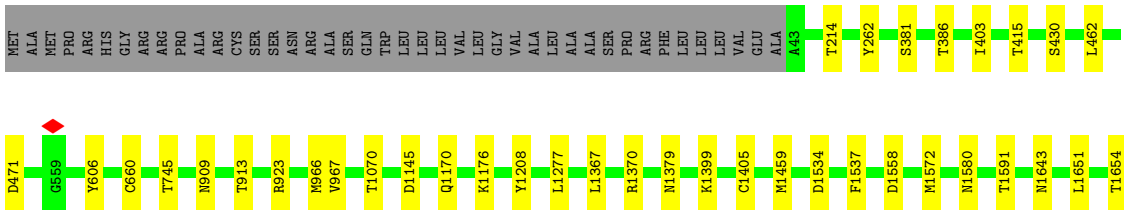


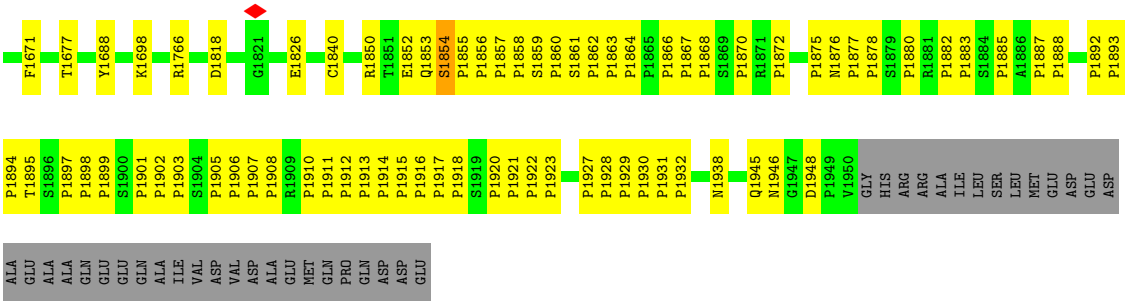


• Molecule 1: Tyrosine-protein kinase ephrin type A/B receptor-like domain-containing protein

Chain B:

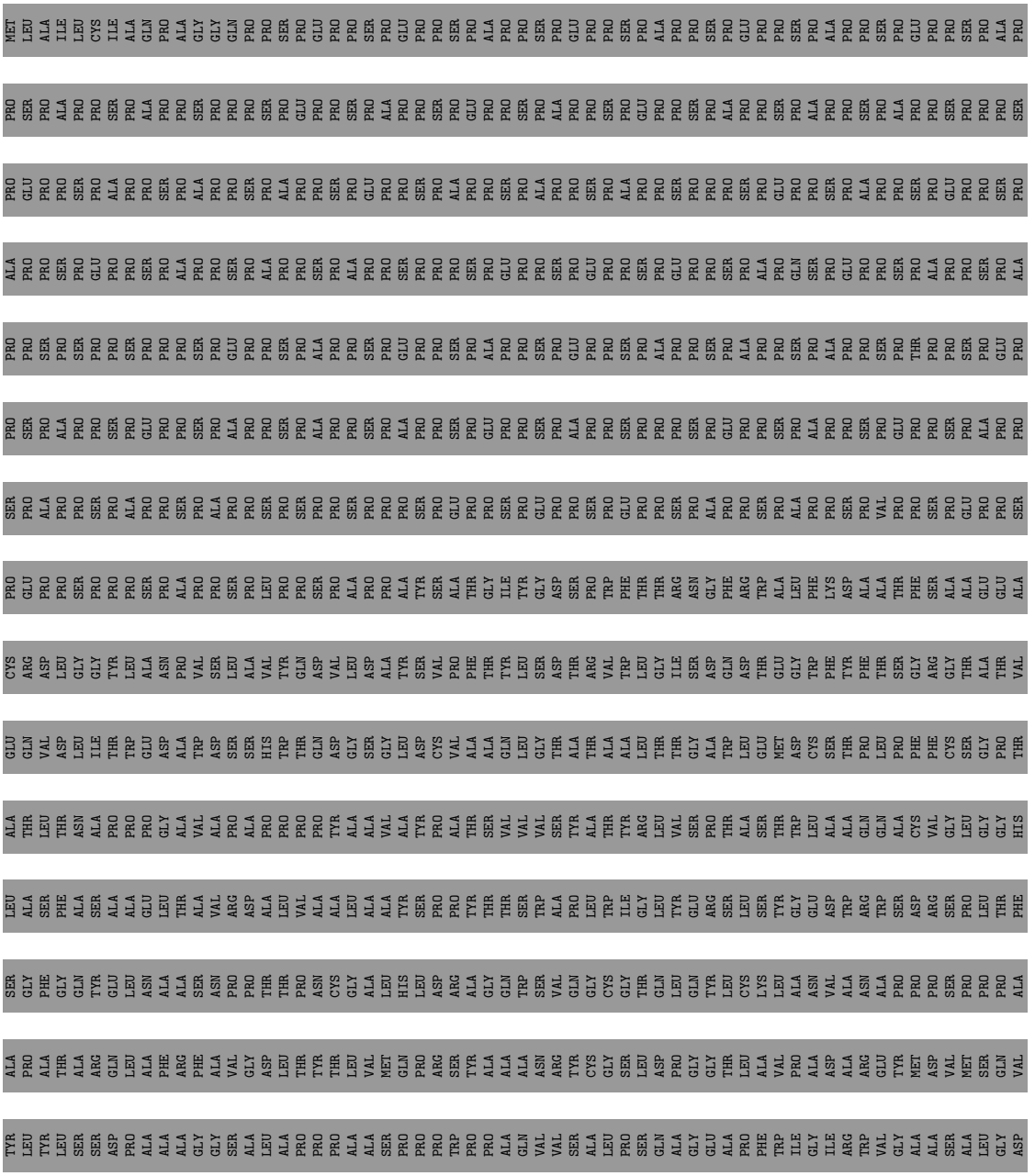


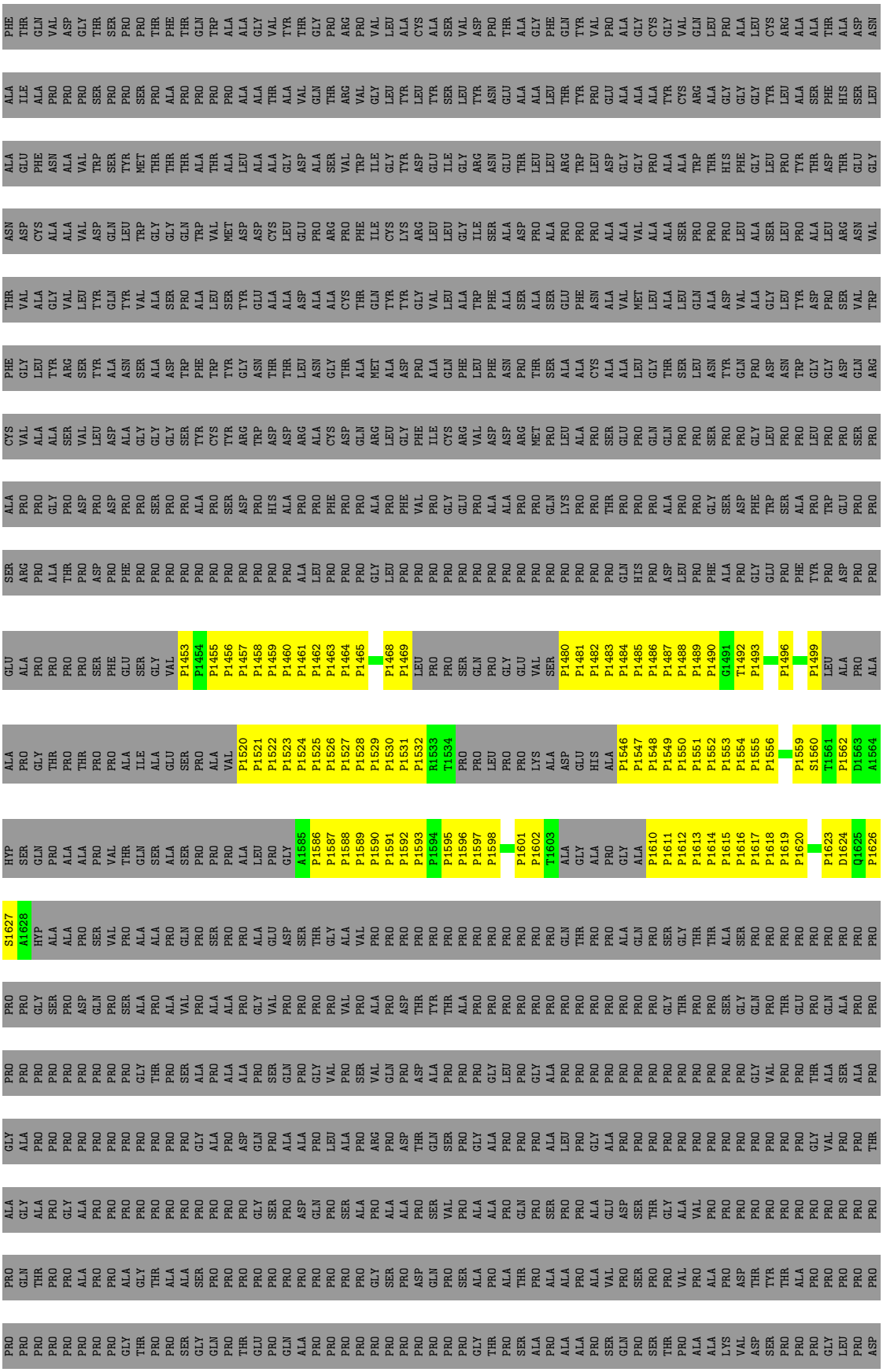




• Molecule 2: C-type lectin domain-containing protein

Chain X: 99%





ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY VAL PRO PRO ALA ALA SER ALA PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY ALA PRO ASP GLN PRO ALA THR PRO LEU ALA PRO ARG PRO ASP THR GLN THR PRO GLY ALA PRO PRO PRO

ALA LEU PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY MET PRO PRO THR ALA GLY ALA PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY SER PRO ASP GLN PRO SER ALA PRO ALA ALA PRO SER VAL PRO ALA ALA PRO GLN PRO

SER PRO PRO ALA GLU ASP SER THR GLY ALA VAL PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLN THR PRO PRO ALA GLN PRO ALA GLY THR ALA ALA SER PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY SER PRO ASP GLN PRO SER ALA PRO ALA THR PRO

ALA ALA PRO ALA VAL PRO SER PRO PRO VAL PRO ALA PRO ASP THR TYR THR ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY THR PRO PRO SER GLY GLN PRO THR GLU PRO GLN ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY THR PRO SER ALA

PRO ALA ALA PRO SER GLN PRO SER THR PRO ALA ALA LYS VAL ASP SER PRO PRO PRO GLY LEU PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY VAL PRO PRO THR ALA THR ALA PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY

ALA PRO ASP GLN PRO ALA ALA PRO ALA ARG PRO GLY PRO ASP ALA PRO ALA ALA PRO PRO PRO ALA GLN PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO SER VAL PRO PRO PRO THR PRO ASP ALA ALA ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO

PRO PRO GLY SER PRO ASP GLN PRO ALA HIS PRO ALA THR PRO SER VAL PRO ALA ALA PRO GLN PRO PRO PRO VAL ASP LYS GLU ASP ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY VAL PRO ASP ALA PRO VAL THR THR GLN ALA PRO ALA ALA PRO PRO

PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY THR PRO THR MET PRO GLY ALA PRO THR LYS PRO GLY ALA PRO LEU ALA PRO GLU GLN PRO ALA GLU HIS ALA PRO PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO ASP ALA PRO LEU PRO PRO PRO ALA ARG

ALA PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY ALA PRO ASP ALA PRO ALA ALA PRO ALA GLN PRO THR ALA SER THR GLN PRO ASP ALA PRO PRO PRO ALA LEU PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO

GLY THR PRO PRO ALA VAL VAL ALA PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY ALA PRO ASP GLN PRO ALA ALA PRO ALA ARG PRO GLY PRO ASP ALA PRO ALA ALA PRO PRO PRO ALA GLN PRO GLY ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO

PRO PRO SER VAL PRO PRO PRO THR PRO ASP ALA ALA ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY SER PRO ASP GLN PRO ALA HIS PRO ALA THR PRO SER VAL PRO ALA ALA PRO GLN PRO PRO PRO VAL ASP LYS VAL ASP ALA ALA PRO PRO PRO PRO PRO PRO

PRO PRO PRO PRO PRO PRO PRO GLY ALA PRO ASP ALA PRO VAL THR THR GLN ALA PRO ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY THR PRO THR MET PRO GLY ALA PRO THR LYS PRO GLY ALA PRO LEU ALA PRO GLU GLN PRO ALA GLU HIS ALA PRO PRO GLY

ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO ASP ALA SER LEU PRO PRO PRO ALA ARG ALA PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY ALA PRO ASP ALA PRO ALA ALA PRO ALA GLN PRO THR ALA SER THR GLN PRO ASP ALA PRO PRO

PRO ALA LEU PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY VAL PRO PRO LYS PRO ALA ALA VAL ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY SER PRO ASP GLN PRO ALA ALA PRO MET SER PRO GLY ALA PRO GLY PRO THR ALA

PRO PRO PRO ALA HIS PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY VAL PRO PRO PRO ALA PRO GLY THR THR PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLN THR PRO ALA MET PRO ASP VAL PRO SER GLU GLY GLN PRO ALA ALA

PRO ILE ALA PRO SER PRO PRO VAL GLN GLU ASP ALA SER ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY THR PRO ALA ALA PRO PRO GLN VAL SER ALA PRO GLN ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY THR PRO ASP ALA PRO ALA MET

PRO ARG LEU PRO ASP ALA PRO LEU THR PRO GLY ALA VAL GLN GLN PRO PRO ALA ALA PRO GLY LEU PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLN ALA PRO PRO VAL PRO GLY SER PRO ASN ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY ALA

PRO ASP GLN PRO ALA ALA PRO ALA ARG PRO GLY PRO ASP ALA PRO SER ALA PRO PRO PRO HIS LEU PRO ASP ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY VAL PRO PRO PRO ILE PRO ASP ALA ALA ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO

PRO GLY SER PRO ASP ARG PRO ALA ALA PRO ALA SER PRO ASP ALA PRO GLY PRO THR ALA PRO PRO PRO ALA HIS PRO ASP THR PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO ASP ALA PRO PRO SER PRO ARG THR HIS PRO GLY LYS LYS GLY ASP ASP ASP ALA PHE

ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO GLY MET PRO ASP MET PRO ALA VAL PRO SER GLN PRO GLY ALA PRO MET PRO PRO ALA ALA GLU GLN VAL PRO ALA SER PRO PRO ARG LEU PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO THR THR PRO PRO PRO

PHE VAL PRO LEU TYR GLY SER TYR LYS GLU LEU GLY ALA ALA TYR ASP LEU LEU ASP GLY THR ILE ASN ASP ASP LEU VAL ILE ILE ASN LEU LYS ARG TRP ASN GLU SER GLU TYR CYS CYS GLU THR THR PHE PRO ILE ASP THR SER GLN VAL THR GLU PRO ASP LYS PRO PHE

ILE VAL THR TYR ASP VAL PHE ASP PHE VAL TRP ASN SER ALA PRO THR VAL GLN ARG LYS VAL HIS VAL TYR ASP PRO CYS ALA GLN ALA SER ASN GLY VAL GLU ARG THR CYS PRO ASP THR ARG LEU CYS SER VAL LEU GLY GLY VAL CYS GLY SER ALA THR LEU PHE SER ASP ILE

ARG ASP LEU ALA THR PRO LEU THR GLU PRO ASP PRO ASN ASN PRO GLY ILE THR LEU GLY ILE HIS THR LEU SER SER ASP PRO VAL TYR ASP THR ILE ILE PRO ASN LEU GLN LEU LEU PRO LEU ASP GLY LEU PHE PHE VAL ILE PRO PRO ASN LEU ASP GLY THR PRO GLY LEU GLN

GLY THR LEU THR TYR LEU THR VAL GLY ASP PRO TRP VAL GLU PRO GLY TYR ILE ALA ASN ASP ASP ARG ASP ASP SER VAL GLN GLN HIS VAL VAL ARG ARG TYR ALA GLU LEU VAL ASP THR THR GLY PRO THR PRO PRO ASN THR PRO PHE ALA ILE THR TYR ASP VAL LYS ASP VAL

SER GLY ASN ALA ALA ILE THR GLN VAL ARG LEU VAL PHE VAL LEU CYS PRO ALA THR LEU PRO VAL LEU CYS PRO PRO ASP GLU ARG VAL LEU ALA ARG PRO VAL TRP TYR CYS ALA ALA GLU VAL CYS GLY VAL PRO ASP PHE PHE THR ASN ALA LEU GLY GLY ALA ALA ALA VAL PRO

ALA VAL THR ARG ASN THR ALA PRO VAL VAL ARG LEU ARG ASP ASN LYS TYR LEU VAL THR ILE PHE ASP ASN ALA THR TYR ALA ARG CYS PRO ASP ARG GLY ASP PRO THR GLY PRO CYS ASP SER GLY VAL THR ALA THR ASP ALA GLU ASP GLY ASP ILE SER TYR LYS VAL HIS ALA

PHE CYS ALA ASP VAL SER THR ALA GLY VAL ASP THR MET TRP GLU ALA VAL GLY LEU ALA ALA CYS GLN PHE GLY ASN VAL LEU LYS ALA GLY ARG ARG VAL ILE THR TYR THR VAL THR ASP THR ALA GLY ALA THR SER GLN ILE SER ARG THR LEU LEU VAL MET GLN ARG CYS GLU

ASP GLY GLU VAL GLN CYS PRO ASP GLY THR CYS THR ASP PHE ASN CYS PHE ASP PRO SER THR VAL ILE THR LEU THR LEU PHE GLY ASN GLY THR ASP ASP THR THR GLY SER GLY LEU ASN VAL THR ASP GLY SER SER PHE VAL ASP SER SER ASN PHE THR THR SER THR VAL ASN

ASP ILE THR GLY GLY GLY SER SER ILE LEU THR ALA PHE ALA SER GLY ALA PRO VAL VAL SER ILE ASN GLU PRO PRO VAL ILE ALA LEU ARG ASN SER THR LEU LEU SER GLN THR VAL GLN VAL PRO GLN ASN PHE VAL TRP ARG ASN CYS ARG ALA SER GLU GLY PRO ASN PRO ALA

THR LEU CYS GLU LEU GLY ALA GLN ALA PHE ASP PRO GLU GLU GLY ASN LEU THR ASN THR ILE TYR VAL CYS PRO PRO VAL ALA CYS LEU ALA THR CYS SER HIS LEU ASN CYS ALA GLY HIS GLU PHE THR SER LYS GLY VAL ARG GLY CYS VAL ASP THR GLY ALA ASP PRO GLY ASN

ILE PHE ASN VAL ILE PHE LEU VAL CYS ASP ASN GLY VAL PRO ARG GLN SER ALA GLN VAL THR ARG THR VAL LEU ILE ALA ARG LYS CYS ALA ALA GLY LEU TYR GLU CYS ASP GLY VAL CYS GLU THR VAL PRO CYS ALA ALA LYS ALA LYS VAL ALA ARG ASP GLN VAL VAL ASN ASN

THR LEU PRO ALA LEU ARG LEU LEU PRO PRO GLY SER SER ALA GLU ASN ALA PRO VAL SER ALA ALA GLY VAL PRO LEU SER LEU THR GLN ILE LEU THR TYR GLY VAL PRO ALA PRO ILE SER PHE SER PRO CYS ALA SER TYR ASP ALA ASN ALA ALA CYS ALA ALA ILE ALA MET ASP

VAL GLU ASP GLY ASP LEU THR SER PHE ILE ASN VAL VAL ASP ALA THR ASP CYS SER GLY LYS THR PRO ASN THR CYS LEU ARG CYS ARG PRO GLU GLN LEU SER LEU GLY LYS CYS LEU PRO GLY THR TYR ARG LEU ARG TYR PHE VAL GLU ASP ASN SER GLY GLY ILE SER GLU ALA

PHE TRP ASN PHE ILE VAL GLU SER VAL ALA ALA VAL ASN ARG VAL TRP PHE LEU MET PRO PRO SER PHE ASN ILE SER ALA PRO ALA SER ASN SER THR ASN ALA THR ARG ARG PHE MET ASP GLN ILE GLN VAL ASN ALA THR ARG SER ARG GLY PHE LEU VAL GLY GLN LEU GLN ARG PHE

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

PHE GLU PRO ASP ASN PHE PRO PRO PRO PRO GLY ARG LEU ARG PRO PRO PRO VAL PRO PRO SER PRO PRO PRO SER PRO ALA PRO ARG PRO PRO SER PRO PRO ALA PRO PRO PRO PRO SER PRO GLY PRO SER PRO PRO PRO ALA PRO PRO ASP PRO PRO SER PRO PRO PRO THR PRO PRO

SER PRO PRO GLN PRO PRO SER PRO PRO PRO PRO PRO SER PRO ALA PRO THR PRO PRO SER PRO PRO ALA PRO PRO PRO VAL PRO PRO SER PRO ALA PRO PRO ARG PRO PRO ALA PRO PRO THR PRO PRO SER PRO PRO ALA PRO PRO SER PRO PRO LEU PRO PRO PRO SER PRO GLY PRO

PRO PRO GLY ASN GLY ASN ALA GLY ARG ARG LEU ILE ASP GLY THR PRO ALA VAL ALA PRO ALA ILE ALA PRO ALA ASN ARG VAL TRP SER TRP GLY ASP ASP TYR GLU MET GLY ALA VAL TRP SER PRO PRO PRO PRO LEU GLN ARG LEU PHE ASN GLN LEU ARG ARG SER MET SER GLU

PRO GLY ALA ALA ALA GLY ALA GLY ALA ASP VAL SER ASP TYR ASP ASP ASP GLY ASP GLY GLU ALA ASP TRP ALA PRO VAL PRO PRO ALA ASP TYR GLU GLU GLU ASP PRO GLU GLN ASP VAL MET VAL VAL SER ALA ALA GLY THR HIS GLY PRO GLY ASP SER ASP ASP ASN PRO LEU

PRO TRP GLY LEU SER ALA ALA ALA TRP GLY GLY PRO ALA VAL ALA GLY VAL ALA ARG LYS ALA SER GLY ALA ALA GLY GLY SER GLY GLY ALA GLN SER ALA PRO ALA PRO ALA PRO SER VAL PRO VAL PRO SER TYR LEU HIS THR ALA LEU MET HIS ALA SER ALA PRO SER GLU

ALA THR GLY PRO ILE ASP PRO LEU LEU SER GLY ALA GLY GLY PRO GLY SER ALA GLY ALA GLY ALA SER ALA ALA GLY ALA PRO LEU ALA ASN THR LEU ALA ALA VAL LEU GLY ALA GLY GLU ILE THR ALA ALA SER SER LEU SER ILE GLY ALA ARG ILE TRP GLN LEU HIS VAL LYS

PRO ALA LEU GLN LYS GLN GLN ALA ALA ALA ALA LEU ALA ALA GLN ALA GLY PRO HIS GLN GLY LEU LEU PRO VAL ALA THR ALA LEU TYR GLU PRO PHE GLY GLY PHE GLY GLY GLY ALA ASP THR GLY ALA SER GLY LEU LEU GLY ALA ALA ALA HIS PRO ALA ALA GLY SER ASN

GLY ALA GLY GLY GLY LEU VAL GLY GLN VAL VAL ARG GLY ASP ALA ALA LYS LEU ARG ALA SER VAL GLY VAL LEU GLY LYS VAL PHE THR ARG GLU GLY GLU GLN TRP ASP LEU PRO GLY SER GLY ALA LEU ARG ARG ALA ALA LEU GLU GLU ALA SER ARG ALA GLU THR ALA ALA ALA

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

LYS GLY GLY PRO VAL GLY GLY LEU ALA ASP ASP PHE ASN LEU HIS GLU LEU MET GLY SER ALA LYS PRO GLN PRO ALA ALA LYS THR ASP ASP ALA ASP ALA GLY ALA ASP GLU PRO SER ARG ARG THR VAL VAL ARG THR LEU LEU SER GLU GLN LEU VAL PRO ALA LEU ALA GLU ILE

SER ARG ARG LEU GLU GLN SER GLN ARG GLU LEU ASP ALA ILE ARG LEU SER PRO THR ALA LEU GLY VAL VAL GLU GLN VAL GLY ARG HIS GLY ARG SER ARG ARG ARG LEU LEU GLN THR THR SER GLY SER VAL ALA ASN GLN THR ALA SER CYS ALA PRO ALA ILE ASN ALA THR ASN

LEU ALA THR ASN CYS THR ALA PRO PRO PRO THR THR THR ASP MET TYR LEU ALA VAL THR LEU SER LEU ILE ALA ASP ILE ASP ASN VAL ASN ARG ALA LEU SER ALA ASN MET THR ASN SER THR ASP THR ILE SER VAL LEU ASP GLU LYS PHE THR ALA THR ASP VAL LYS TYR GLU

SER GLN TYR VAL ALA TYR LYS ASN LEU ALA THR THR TYR LEU SER ALA LEU GLU ASN ARG THR ASN THR VAL ILE LEU ASN LEU ALA ALA LEU ALA ALA ALA ASP ALA THR ASN SER MET LEU LEU SER ALA LEU ALA GLY LEU LEU LYS GLY ALA VAL THR SER ALA ALA GLU GLU ALA

ASP ARG LEU GLY ILE THR THR ALA MET LEU VAL ASP GLY LEU GLY LEU SER GLU GLU ASN TRP PHE PHE GLU SER TYR GLN GLN CYS LEU ILE GLN ARG SER GLY SER GLY THR THR TYR ASN PHE THR ILE ASN ARG GLU GLN GLN ALA ALA LEU ARG TYR ASP LEU GLU THR GLY ARG

VAL ALA ALA PRO PRO PRO PRO PRO ALA ARG ALA GLY PHE THR LEU LEU GLN ALA THR GLN MET GLY ARG GLY ARG SER LEU LEU GLY TRP GLY SER GLU LEU LEU SER ALA ALA ALA ALA GLY ALA GLY LEU GLY TRP ALA GLY LEU GLY PRO ALA ASP PRO GLN ASP ASP SER ALA

ALA SER ALA ALA THR GLY SER GLY TYR HIS ALA VAL ARG ASP ARG ARG LEU GLN THR GLY THR VAL PRO SER THR VAL SER ALA GLU LEU PRO GLN GLY LEU THR PRO ARG LEU GLN TYR GLY GLY TYR GLU LEU GLU VAL ALA ALA GLY ARG PRO PRO ALA GLY LEU THR VAL THR TYR

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

SER THR LYS ASN LEU GLN ASP LEU GLY GLY ILE GLY GLU ASP PRO VAL PHE ASP ARG SER SER SER ILE TYR SER PRO ASP VAL ALA GLY ARG ALA TRP ALA TYR TYR ASN PHE SER GLU GLY ASN SER GLU ILE SER THR LEU LYS LEU PRO PHE GLY PHE THR HIS TYR PRO VAL PRO

GLY LEU PRO ASP GLY TYR PRO VAL PHE PHE ASP THR ARG LEU GLY ALA ASP ARG ALA ARG LYS LEU LEU THR TYR LEU GLU ASP GLY ARG TYR LEU SER PRO ILE PHE SER SER GLU LEU ARG LEU ARG LEU LEU VAL TYR ASN PRO ASP ALA HIS VAL PHE GLY TYR LEU ARG ALA ALA

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

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

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

ASN ASP THR ILE ASP LEU ALA ALA THR ALA ALA ALA MET ALA PRO PRO SER MET PRO PRO ARG GLY GLY ASP TYR ARG TRP LEU LEU PRO ASP ASP VAL SER GLY LEU HIS ALA LEU GLY ASP MET TYR SER TYR LEU ASP ASN MET GLU TYR LEU TRP ASN LEU TYR PHE VAL LEU GLN

SER LEU VAL LEU LEU MET LEU MET VAL ARG LEU MET HIS TYR VAL SER PHE GLN PRO HIS LEU ALA VAL ILE GLY GLY ALA ILE ALA ARG ALA ILE PRO MET LEU LEU TYR TRP ALA VAL ILE ALA GLY MET VAL VAL VAL MET LEU LEU MET LEU ASN ILE ILE ALA PHE GLY ASP ARG

LEU GLU GLN LEU SER THR ILE SER GLY SER ALA TYR ALA VAL ALA ARG TRP LEU LEU ILE LYS HIS SER ASP ARG GLY ASN ARG ALA THR ILE THR GLU MET LEU ASN ASP ASN THR VAL ILE LEU ASN GLY GLY GLU SER LEU VAL ALA ALA LEU VAL ARG GLY LEU GLY ALA ILE PHE

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

TRP VAL THR ARG PRO GLU VAL ARG TYR THR TRP ALA TYR SER VAL LEU TYR SER ALA VAL VAL ARG GLY VAL ALA ALA VAL ALA GLY GLY THR ALA LEU ALA LYS ARG HIS PRO THR GLN HIS GLN ALA VAL THR GLU ARG ALA VAL LEU LEU PRO GLY GLY PRO PRO GLY PHE ASN SER

PRO ASP GLU PRO ASP PRO ARG TYR CYS PRO ARG TYR ASN LEU ARG ALA MET MET MET VAL PHE GLU GLU LEU LEU LEU VAL ASN LYS GLU LEU ARG ARG GLU LEU PHE PHE PHE MET GLN THR ASN ASN GLU ASP GLY ARG THR LYS ARG MET LYS ALA MET GLY ALA PRO ARG ARG ALA

ALA ALA ALA ALA VAL ASN ASP ALA SER ALA ARG ALA MET ALA ASP SER LEU ALA SER LEU LEU LEU GLU ARG PHE GLY LYS ARG VAL PRO ARG ARG ALA ALA ARG SER PHE ASP GLU MET MET HIS GLN LEU ARG LYS ARG LEU GLY THR PRO ALA GLY GLY SER GLY SER ALA ASP

GLY SER GLU PHE SER GLY SER LEU ASP GLY GLY SER ALA ARG GLY GLY ASP SER GLU ASN SER ASP ASP MET LEU PRO THR GLY VAL ARG VAL GLY SER LEU LYS HIS ARG GLY TYR GLY VAL HIS ASN GLN GLN THR VAL HIS ASP LEU GLN LEU GLN ALA ALA VAL GLN THR ALA

MET ARG ASN ILE HIS THR ILE ARG GLU ASN MET GLY ARG GLU LEU GLY ASP ASP PRO GLN LEU LEU ALA THR LEU PHE VAL ALA GLN PHE ALA GLY GLN ILE PRO GLU PRO GLU ARG ARG PRO PRO GLY VAL ARG PRO SER LEU TYR ARG GLN ARG VAL GLN GLN ALA GLY SER GLY ASN

SER LEU VAL ASN VAL GLY ALA GLY SER ALA PRO ALA PRO ALA ALA PRO GLY GLY PRO PRO ARG PRO GLY ARG SER ARG LEU GLY GLY ALA ALA MET MET GLY GLN SER PRO GLN ALA ALA PRO ALA PRO THR GLN GLY PRO VAL ALA ALA VAL LEU ASP THR ASN THR PRO GLU GLY MET

LEU THR LYS ALA LEU GLN ALA MET LEU ALA PRO PRO SER THR THR ALA ASN ALA ALA VAL SER ALA ASP GLY THR VAL PRO ALA GLU ALA GLU ALA SER SER ALA SER VAL THR ASP GLY ALA PRO ARG ALA ARG PRO ARG PRO LYS GLY ALA LYS SER ARG ALA ARG PHE ALA ALA ASP

LEU GLU ILE PRO GLY ASN THR THR SER THR ALA GLY GLU GLU ALA PRO ALA SER PRO GLY VAL ALA SER PRO GLY ALA VAL GLY SER PRO SER GLY ARG HIS ASN SER VAL SER GLY GLN LEU GLY GLY SER ARG THR ALA ARG SER MET LEU PRO ARG HIS LEU GLN PRO GLU PRO ARG

ALA ALA SER PHE ALA HIS PRO ALA PRO ALA THR LEU GLY SER LEU GLY GLN LEU GLY SER PRO SER SER VAL ARG SER SER ARG SER MET VAL MET PRO ALA GLY SER GLY SER ALA TYR PHE THR PRO SER ALA SER MET GLY GLY ALA ALA GLY ALA ALA THR ALA PRO GLY PRO

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

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

ALA VAL VAL GLN ARG LEU THR SER HIS VAL LEU GLN LEU LEU ARG GLU LEU ARG GLY VAL GLN ALA ASP ALA ASP ALA MET LEU ARG SER THR LEU VAL LEU ILE GLU ARG LEU SER ALA GLY SER VAL PRO PHE PRO ARG ARG ALA ALA ARG MET VAL PRO GLY VAL MET GLY SER PRO

ALA SER SER PRO PRO VAL SER PRO GLN ASN GLU LYS PRO PRO GLY TRP GLU ASP ALA ALA VAL ALA ARG VAL ALA ALA ALA ASN ALA ALA ALA ALA GLN ARG ALA ALA VAL GLY THR ALA SER PRO ARG LEU GLY SER SER LEU ARG VAL ARG VAL GLU ASP GLY ALA GLY GLY ALA

ALA HIS GLY HIS GLY ALA ALA GLY ALA ASN VAL ASP ASP GLY GLU ASP MET LEU PRO LEU PRO PRO PRO PRO ALA LEU ARG GLY VAL ASP SER TYR THR ALA SER PRO ARG SER LEU ALA ALA LEU GLN ALA ALA ARG GLY ALA ALA GLY PRO LEU SER GLY LEU LEU THR PRO PRO THR

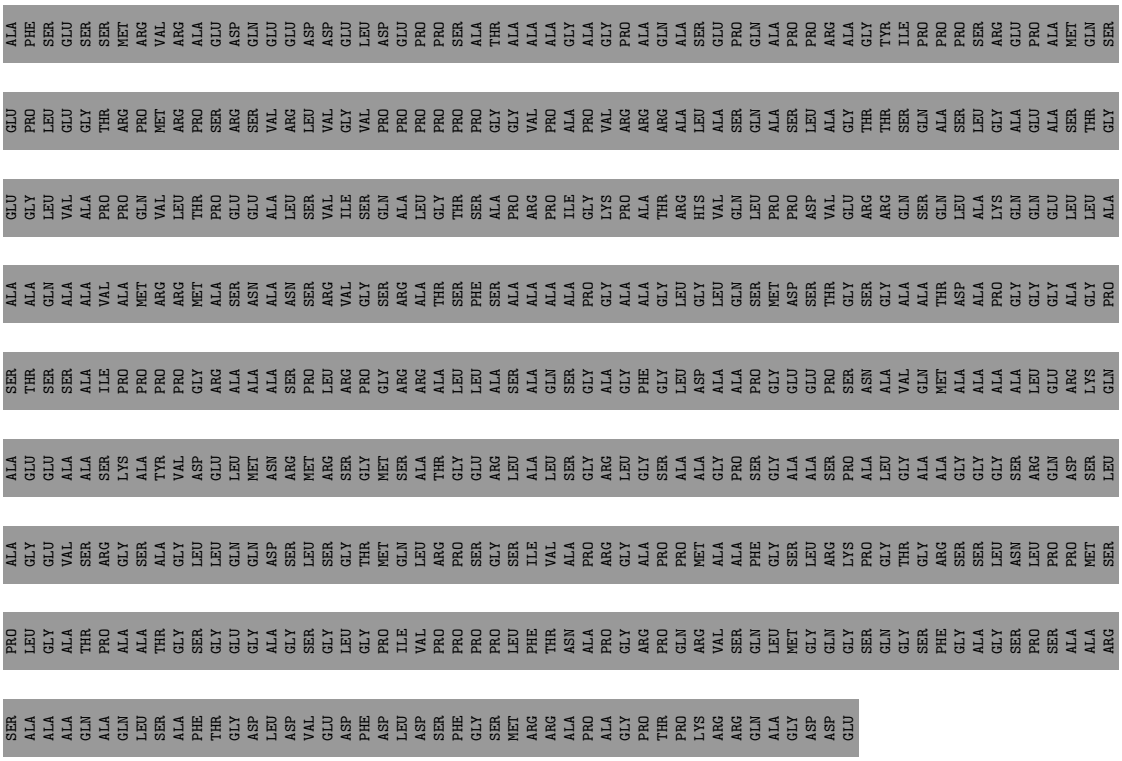
PRO THR PRO GLU ALA SER PRO GLU LYS ALA LEU PRO PRO ALA ALA ALA LYS SER ALA GLU PRO ALA GLN ALA GLU GLU ALA PRO ALA GLY GLU SER ARG VAL VAL SER ARG ALA ALA SER GLN ALA GLY MET LYS PRO VAL ASP GLU MET ARG GLU VAL GLU PRO GLU PRO GLU LEU VAL

THR PHE MET VAL GLN SER GLY MET LYS SER ARG ALA ALA GLY ASP ALA ALA ALA LEU ALA ALA ALA ALA LEU ALA ALA GLU GLU ASP GLU ARG ARG GLU ARG GLU ALA LEU ALA ALA SER GLU GLY LEU ASP SER LEU ALA PRO PRO PRO GLY THR SER SER SER SER GLY GLN VAL HIS

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

ARG VAL GLY SER PRO LEU LEU PRO THR GLU ALA ILE ARG ARG LEU SER PRO GLU THR SER ASN LEU SER ARG PRO GLY SER ALA ALA VAL VAL ASP ALA ALA PRO ALA ARG GLU ALA PRO GLU GLU ALA SER ALA ARG ARG ASN LEU PRO LEU PRO SER PRO GLN GLY GLY SER ARG PRO

ALA SER VAL GLN ARG ASP GLU GLN GLN GLY VAL GLU VAL LEU ALA LEU PRO ASP THR VAL PRO GLU GLY GLN GLU ALA GLU ALA GLY GLY PRO MET ASP GLU PRO VAL GLN GLY GLU GLY GLU GLU GLY GLU HIS GLY ALA LEU GLU ALA SER ARG SER LEU GLY ARG GLN PRO SER ARG ILE



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A1:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A2:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A3:

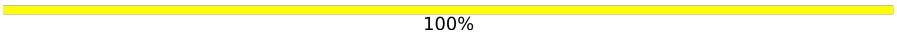
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a1:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a2: 

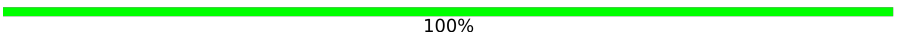
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a3: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A4: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A5: 

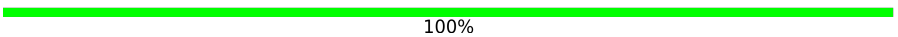
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A7: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B0: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

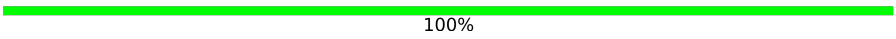
Chain B1: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B3:

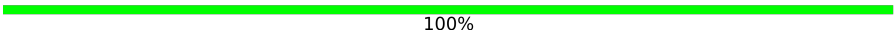
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B4:



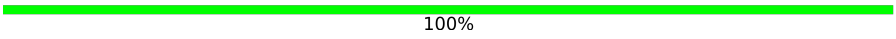
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B5:



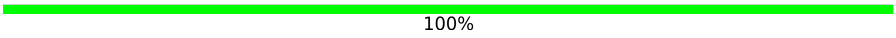
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B7:



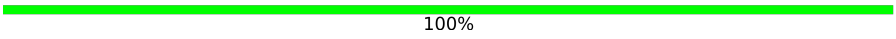
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B9:



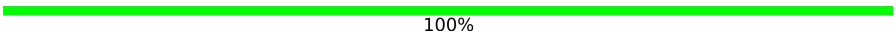
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C0:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C1:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C2: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C3: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C4: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C5: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C6: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C7: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C8: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain C9: 100%

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

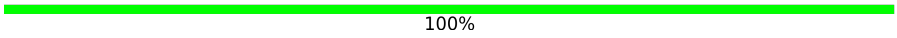
Chain D0:

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D1:

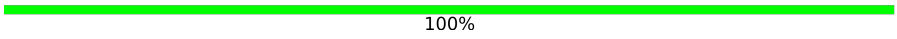
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D2:



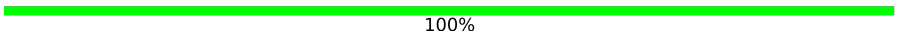
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D3:



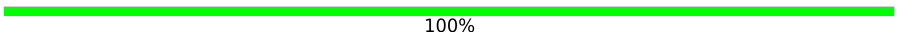
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D4:



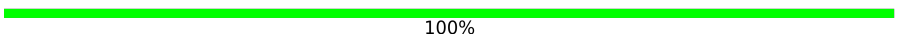
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D5:

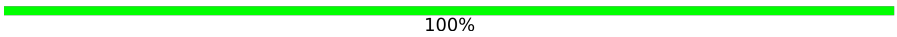


• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

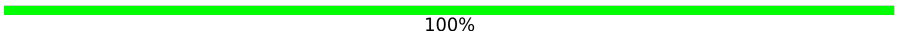
Chain D6:



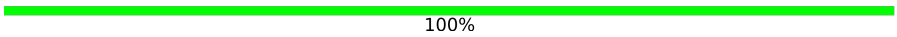
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D7: 

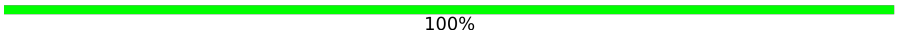
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D8: 

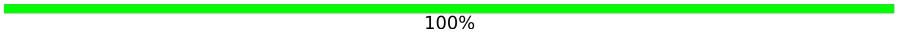
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain D9: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E0: 

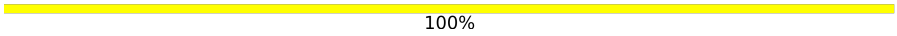
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E1: 

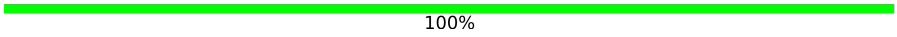
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E2: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

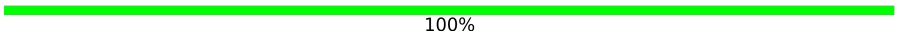
Chain E4: 

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E5: 

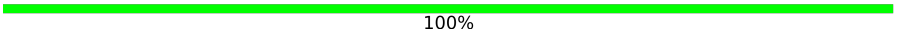
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E8:



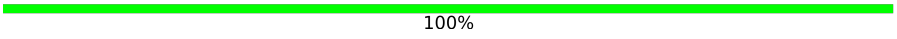
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F0:



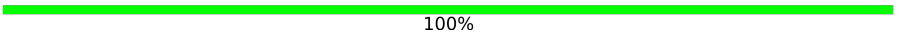
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F3:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F8:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

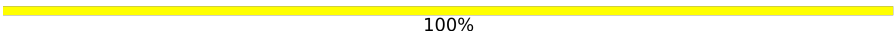
Chain a5:

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain a7:

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b0:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b1: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b3: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b4: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b5: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b7: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b9: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c0: 100%

FUB1 FUB2

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c1: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c2: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c3: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c4: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c5: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c6: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c7: 100%

FUB1
FUB2

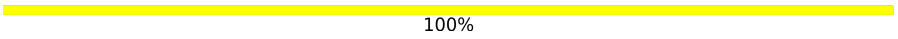
- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c8: 100%

FUB1
FUB2

- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain c9:

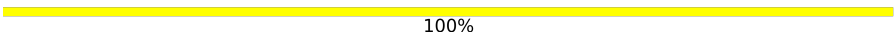


• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d1:

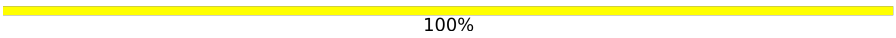
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d2:



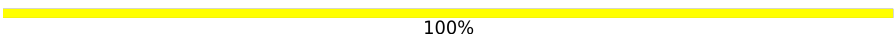
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d3:



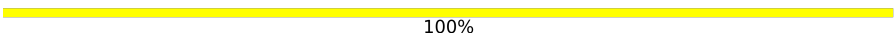
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d4:



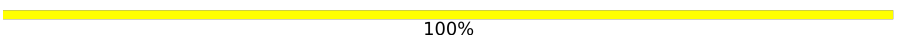
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d5:



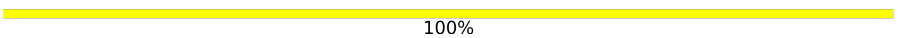
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e0:



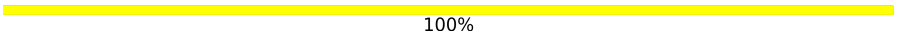
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e1:



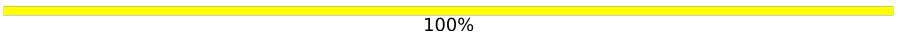
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e2:



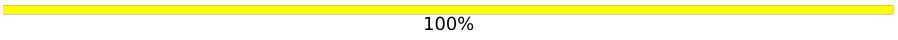
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e4:



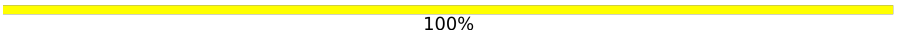
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e5:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e8:

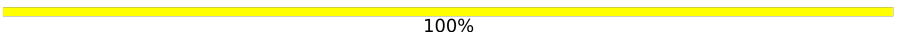


• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f0:

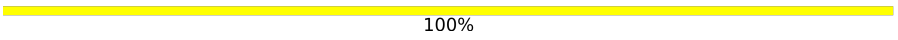
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f3:



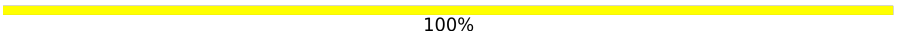
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f5:



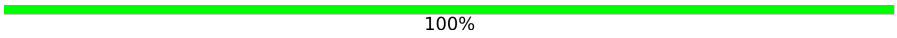
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f8:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E3:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f2:

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e7:

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

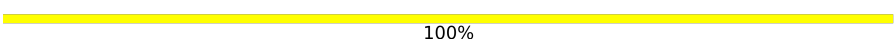
Chain e6:

• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e3:

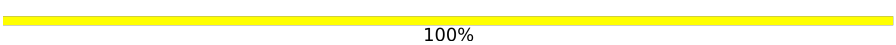
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d9:



• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d7:

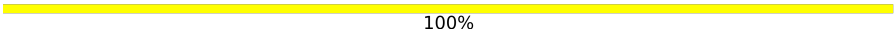


• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d8:

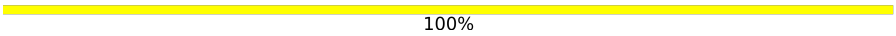
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d6:



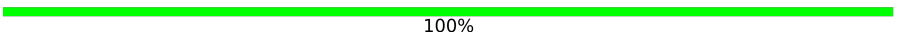
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d0:



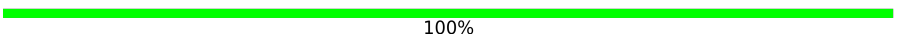
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F5:



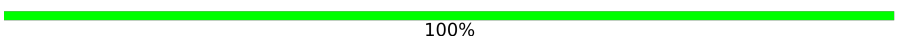
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F2:



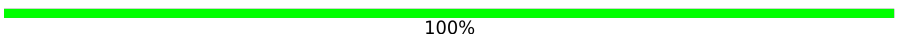
• Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E7:



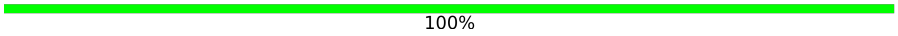
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A6:



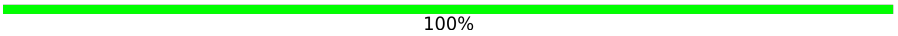
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A9:



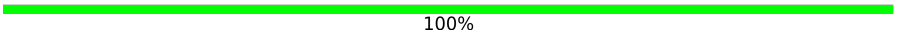
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B6:



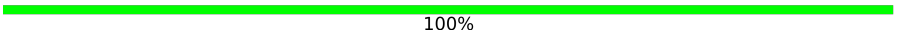
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F6:



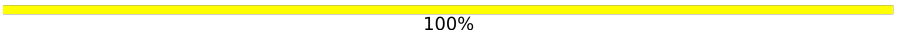
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F7:



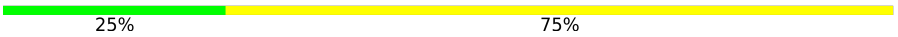
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain a6:



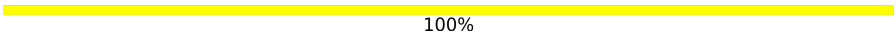
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain a9:



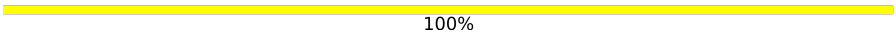
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b6:



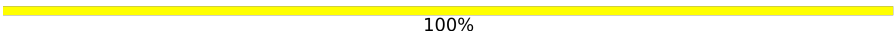
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f6:



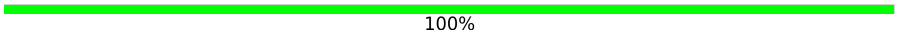
• Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f7:



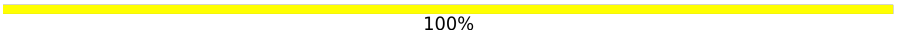
• Molecule 6: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E6:



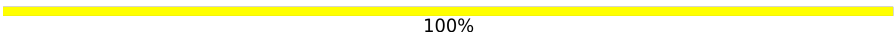
• Molecule 7: beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose

Chain a4:



• Molecule 8: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	687452	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.771	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	711.68, 711.68, 711.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, GLA, FUB, 34V, A1AIO, NAG

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	0.27	0/13729	0.49	0/18855
1	B	0.27	0/13729	0.50	1/18855 (0.0%)
2	X	0.21	0/157	0.51	0/190
All	All	0.27	0/27615	0.49	1/37900 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1643	ASN	CB-CA-C	-5.12	100.17	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1850	ARG	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1849/1987 (93%)	1792 (97%)	57 (3%)	0	100 100
1	B	1849/1987 (93%)	1783 (96%)	65 (4%)	1 (0%)	51 83
2	X	21/8572 (0%)	18 (86%)	1 (5%)	2 (10%)	0 3
All	All	3719/12546 (30%)	3593 (97%)	123 (3%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1854	SER
2	X	1627	SER
2	X	1560	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1451/1514 (96%)	1392 (96%)	59 (4%)	30 64
1	B	1451/1514 (96%)	1395 (96%)	56 (4%)	32 65
2	X	17/6717 (0%)	15 (88%)	2 (12%)	5 21
All	All	2919/9745 (30%)	2802 (96%)	117 (4%)	35 65

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	LEU
1	A	162	GLN
1	A	167	ARG
1	A	206	ARG
1	A	239	ARG
1	A	262	TYR
1	A	415	THR
1	A	430	SER
1	A	470	ARG
1	A	529	THR
1	A	547	ASP
1	A	565	ILE
1	A	587	SER
1	A	608	THR
1	A	622	LEU
1	A	662	PHE
1	A	726	ASP
1	A	733	PHE
1	A	739	THR
1	A	790	CYS
1	A	833	PHE
1	A	907	PHE
1	A	977	LEU
1	A	1058	GLN
1	A	1059	ASN
1	A	1110	CYS
1	A	1145	ASP
1	A	1152	SER
1	A	1197	ASN
1	A	1243	GLU
1	A	1286	LYS
1	A	1317	CYS
1	A	1379	ASN
1	A	1394	ASP
1	A	1399	LYS
1	A	1443	SER
1	A	1488	SER
1	A	1493	ARG
1	A	1534	ASP
1	A	1537	PHE
1	A	1563	GLN
1	A	1598	THR
1	A	1621	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1638	VAL
1	A	1668	MET
1	A	1671	PHE
1	A	1677	THR
1	A	1688	TYR
1	A	1708	SER
1	A	1723	SER
1	A	1728	GLU
1	A	1746	GLN
1	A	1748	THR
1	A	1750	CYS
1	A	1773	TYR
1	A	1800	ASP
1	A	1843	LEU
1	A	1943	VAL
1	A	1948	ASP
2	X	1492	THR
2	X	1624	ASP
1	B	214	THR
1	B	262	TYR
1	B	381	SER
1	B	386	THR
1	B	403	ILE
1	B	415	THR
1	B	430	SER
1	B	462	LEU
1	B	471	ASP
1	B	606	TYR
1	B	660	CYS
1	B	745	THR
1	B	909	ASN
1	B	913	THR
1	B	923	ARG
1	B	966	MET
1	B	967	VAL
1	B	1070	THR
1	B	1145	ASP
1	B	1170	GLN
1	B	1176	LYS
1	B	1208	TYR
1	B	1277	LEU
1	B	1367	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1370	ARG
1	B	1379	ASN
1	B	1399	LYS
1	B	1405	CYS
1	B	1459	MET
1	B	1534	ASP
1	B	1537	PHE
1	B	1558	ASP
1	B	1572	MET
1	B	1580	ASN
1	B	1591	THR
1	B	1651	LEU
1	B	1654	THR
1	B	1671	PHE
1	B	1677	THR
1	B	1688	TYR
1	B	1698	LYS
1	B	1766	ARG
1	B	1818	ASP
1	B	1826	GLU
1	B	1840	CYS
1	B	1852	GLU
1	B	1853	GLN
1	B	1854	SER
1	B	1859	SER
1	B	1861	SER
1	B	1876	ASN
1	B	1895	THR
1	B	1938	ASN
1	B	1945	GLN
1	B	1946	ASN
1	B	1948	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1853	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

197 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	1918	1	6,8,9	0.49	0	5,10,12	2.08	1 (20%)
1	HYP	B	1911	1	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	B	1923	1	6,8,9	0.48	0	5,10,12	1.81	1 (20%)
1	HYP	A	1920	1	6,8,9	0.46	0	5,10,12	2.13	2 (40%)
2	HYP	X	1592	2	6,8,9	0.43	0	5,10,12	1.94	1 (20%)
1	HYP	A	1927	1	6,8,9	0.48	0	5,10,12	1.98	1 (20%)
2	HYP	X	1457	2	6,8,9	0.43	0	5,10,12	1.95	1 (20%)
2	HYP	X	1626	2	6,8,9	0.53	0	5,10,12	1.68	1 (20%)
2	HYP	X	1602	2	6,8,9	0.46	0	5,10,12	1.73	1 (20%)
2	HYP	X	1587	2	6,8,9	0.45	0	5,10,12	1.91	2 (40%)
2	HYP	X	1591	2	6,8,9	0.42	0	5,10,12	1.82	1 (20%)
2	HYP	X	1610	2	6,8,9	0.45	0	5,10,12	1.91	1 (20%)
2	HYP	X	1590	2	6,8,9	0.44	0	5,10,12	2.01	1 (20%)
1	HYP	A	1897	1	6,8,9	0.46	0	5,10,12	2.00	3 (60%)
2	HYP	X	1620	2	6,8,9	0.46	0	5,10,12	1.87	1 (20%)
2	HYP	X	1523	2	6,8,9	0.43	0	5,10,12	1.85	1 (20%)
2	HYP	X	1595	2	6,8,9	0.46	0	5,10,12	1.56	1 (20%)
1	HYP	B	1880	1	6,8,9	0.47	0	5,10,12	1.64	1 (20%)
1	HYP	A	1878	1	6,8,9	0.46	0	5,10,12	1.98	1 (20%)
1	HYP	B	1920	1	6,8,9	0.45	0	5,10,12	1.89	2 (40%)
1	HYP	B	1921	1	6,8,9	0.53	0	5,10,12	1.62	2 (40%)
2	HYP	X	1532	2	6,8,9	0.50	0	5,10,12	1.87	2 (40%)
1	HYP	A	1930	1	6,8,9	0.45	0	5,10,12	1.65	1 (20%)
2	HYP	X	1485	2	6,8,9	0.45	0	5,10,12	1.85	2 (40%)
1	HYP	B	1893	1	6,8,9	0.45	0	5,10,12	1.81	2 (40%)
2	HYP	X	1462	2	6,8,9	0.44	0	5,10,12	1.71	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	A	1928	1	6,8,9	0.48	0	5,10,12	1.96	2 (40%)
1	HYP	A	1922	1	6,8,9	0.48	0	5,10,12	2.04	1 (20%)
1	HYP	B	1890	1	6,8,9	0.49	0	5,10,12	1.27	0
1	HYP	B	1915	1	6,8,9	0.44	0	5,10,12	1.74	1 (20%)
2	HYP	X	1520	2	6,8,9	0.45	0	5,10,12	1.84	1 (20%)
1	HYP	A	1911	1	6,8,9	0.45	0	5,10,12	1.83	3 (60%)
1	HYP	A	1857	1	6,8,9	0.45	0	5,10,12	1.65	2 (40%)
2	HYP	X	1522	2	6,8,9	0.44	0	5,10,12	1.75	1 (20%)
1	HYP	B	1901	1	6,8,9	0.45	0	5,10,12	1.64	2 (40%)
2	HYP	X	1459	2	6,8,9	0.43	0	5,10,12	1.90	2 (40%)
2	HYP	X	1521	2	6,8,9	0.44	0	5,10,12	1.95	2 (40%)
2	HYP	X	1551	2	6,8,9	0.45	0	5,10,12	2.00	1 (20%)
2	HYP	X	1589	2	6,8,9	0.43	0	5,10,12	1.89	1 (20%)
1	HYP	A	1917	1	6,8,9	0.46	0	5,10,12	1.86	3 (60%)
1	HYP	B	1875	1	6,8,9	0.47	0	5,10,12	1.73	1 (20%)
1	HYP	B	1899	1	6,8,9	0.45	0	5,10,12	1.76	1 (20%)
2	HYP	X	1469	2	6,8,9	0.49	0	5,10,12	1.70	1 (20%)
1	HYP	B	1865	1	6,8,9	0.57	0	5,10,12	1.49	0
1	HYP	B	1858	1	6,8,9	0.58	0	5,10,12	1.41	1 (20%)
1	HYP	B	1887	1	6,8,9	0.46	0	5,10,12	1.89	2 (40%)
1	HYP	A	1872	1	6,8,9	0.48	0	5,10,12	1.48	1 (20%)
2	HYP	X	1488	2	6,8,9	0.45	0	5,10,12	1.93	1 (20%)
2	HYP	X	1612	2	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	A	1875	1	6,8,9	0.45	0	5,10,12	1.86	1 (20%)
2	HYP	X	1617	2	6,8,9	0.44	0	5,10,12	1.88	2 (40%)
1	HYP	B	1862	1	6,8,9	0.45	0	5,10,12	1.81	1 (20%)
1	HYP	A	1907	1	6,8,9	0.46	0	5,10,12	1.82	2 (40%)
1	HYP	B	1916	1	6,8,9	0.46	0	5,10,12	1.85	2 (40%)
2	HYP	X	1586	2	6,8,9	0.44	0	5,10,12	1.88	1 (20%)
2	HYP	X	1614	2	6,8,9	0.44	0	5,10,12	1.89	2 (40%)
1	HYP	A	1932	1	6,8,9	0.50	0	5,10,12	1.84	2 (40%)
1	HYP	B	1888	1	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	A	1883	1	6,8,9	0.50	0	5,10,12	1.74	1 (20%)
2	HYP	X	1615	2	6,8,9	0.45	0	5,10,12	1.96	1 (20%)
1	HYP	B	1927	1	6,8,9	0.46	0	5,10,12	1.90	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HYP	X	1468	2	6,8,9	0.44	0	5,10,12	1.95	1 (20%)
2	HYP	X	1496	2	6,8,9	0.49	0	5,10,12	1.74	1 (20%)
2	HYP	X	1546	2	6,8,9	0.46	0	5,10,12	1.93	1 (20%)
1	HYP	A	1890	1	6,8,9	0.47	0	5,10,12	1.79	1 (20%)
1	HYP	A	1902	1	6,8,9	0.45	0	5,10,12	1.84	2 (40%)
1	HYP	A	1860	1	6,8,9	0.47	0	5,10,12	1.85	1 (20%)
1	HYP	A	1898	1	6,8,9	0.45	0	5,10,12	1.89	2 (40%)
2	HYP	X	1550	2	6,8,9	0.44	0	5,10,12	1.96	1 (20%)
1	HYP	B	1897	1	6,8,9	0.46	0	5,10,12	1.79	2 (40%)
2	HYP	X	1465	2	6,8,9	0.46	0	5,10,12	1.75	1 (20%)
1	HYP	B	1878	1	6,8,9	0.47	0	5,10,12	1.70	1 (20%)
1	HYP	B	1872	1	6,8,9	0.45	0	5,10,12	1.94	2 (40%)
2	HYP	X	1529	2	6,8,9	0.44	0	5,10,12	1.95	2 (40%)
2	HYP	X	1601	2	6,8,9	0.44	0	5,10,12	1.98	1 (20%)
1	HYP	A	1863	1	6,8,9	0.50	0	5,10,12	2.32	2 (40%)
1	HYP	B	1906	1	6,8,9	0.45	0	5,10,12	1.91	2 (40%)
1	HYP	A	1931	1	6,8,9	0.44	0	5,10,12	1.84	2 (40%)
2	HYP	X	1524	2	6,8,9	0.43	0	5,10,12	1.95	3 (60%)
1	HYP	A	1894	1	6,8,9	0.54	0	5,10,12	2.25	2 (40%)
1	HYP	A	1892	1	6,8,9	0.50	0	5,10,12	1.54	1 (20%)
1	HYP	A	1865	1	6,8,9	0.48	0	5,10,12	1.89	2 (40%)
1	HYP	A	1908	1	6,8,9	0.46	0	5,10,12	1.86	1 (20%)
2	HYP	X	1453	2	6,8,9	0.47	0	5,10,12	1.77	2 (40%)
1	HYP	A	1913	1	6,8,9	0.45	0	5,10,12	1.85	1 (20%)
2	HYP	X	1526	2	6,8,9	0.43	0	5,10,12	2.03	1 (20%)
2	HYP	X	1531	2	6,8,9	0.43	0	5,10,12	1.99	1 (20%)
1	HYP	A	1916	1	6,8,9	0.46	0	5,10,12	1.68	2 (40%)
1	HYP	A	1888	1	6,8,9	0.45	0	5,10,12	1.86	1 (20%)
1	HYP	B	1929	1	6,8,9	0.46	0	5,10,12	1.83	2 (40%)
1	HYP	A	1864	1	6,8,9	0.52	0	5,10,12	2.35	2 (40%)
2	HYP	X	1464	2	6,8,9	0.44	0	5,10,12	1.82	1 (20%)
1	HYP	A	1877	1	6,8,9	0.51	0	5,10,12	2.12	2 (40%)
1	HYP	B	1913	1	6,8,9	0.48	0	5,10,12	1.80	1 (20%)
2	HYP	X	1554	2	6,8,9	0.44	0	5,10,12	1.89	2 (40%)
1	HYP	B	1932	1	6,8,9	0.47	0	5,10,12	2.07	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	A	1910	1	6,8,9	0.46	0	5,10,12	1.90	1 (20%)
2	HYP	X	1553	2	6,8,9	0.44	0	5,10,12	1.89	2 (40%)
1	HYP	A	1866	1	6,8,9	0.49	0	5,10,12	1.63	1 (20%)
1	HYP	B	1902	1	6,8,9	0.45	0	5,10,12	1.99	2 (40%)
2	HYP	X	1588	2	6,8,9	0.45	0	5,10,12	1.87	1 (20%)
1	HYP	B	1922	1	6,8,9	0.47	0	5,10,12	1.97	2 (40%)
2	HYP	X	1613	2	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
2	HYP	X	1461	2	6,8,9	0.44	0	5,10,12	1.88	1 (20%)
1	HYP	B	1864	1	6,8,9	0.50	0	5,10,12	2.21	3 (60%)
1	HYP	A	1885	1	6,8,9	0.51	0	5,10,12	2.45	2 (40%)
2	HYP	X	1455	2	6,8,9	0.44	0	5,10,12	1.86	1 (20%)
2	HYP	X	1456	2	6,8,9	0.43	0	5,10,12	1.89	2 (40%)
2	HYP	X	1484	2	6,8,9	0.43	0	5,10,12	1.93	2 (40%)
1	HYP	A	1873	1	6,8,9	0.47	0	5,10,12	1.79	1 (20%)
2	HYP	X	1458	2	6,8,9	0.43	0	5,10,12	1.87	1 (20%)
1	HYP	B	1868	1	6,8,9	0.49	0	5,10,12	2.10	1 (20%)
2	HYP	X	1483	2	6,8,9	0.46	0	5,10,12	1.93	1 (20%)
2	HYP	X	1454	2	6,8,9	0.47	0	5,10,12	1.36	0
1	HYP	A	1868	1	6,8,9	0.50	0	5,10,12	1.92	1 (20%)
2	HYP	X	1460	2	6,8,9	0.45	0	5,10,12	1.85	1 (20%)
1	HYP	A	1929	1	6,8,9	0.47	0	5,10,12	1.90	3 (60%)
1	HYP	B	1894	1	6,8,9	0.47	0	5,10,12	1.91	1 (20%)
2	HYP	X	1555	2	6,8,9	0.43	0	5,10,12	1.98	3 (60%)
1	HYP	B	1910	1	6,8,9	0.45	0	5,10,12	2.15	1 (20%)
2	HYP	X	1596	2	6,8,9	0.46	0	5,10,12	1.92	1 (20%)
1	HYP	A	1867	1	6,8,9	0.45	0	5,10,12	1.91	2 (40%)
1	HYP	A	1893	1	6,8,9	0.45	0	5,10,12	1.82	2 (40%)
2	HYP	X	1619	2	6,8,9	0.43	0	5,10,12	1.94	1 (20%)
1	HYP	A	1882	1	6,8,9	0.45	0	5,10,12	1.92	2 (40%)
1	HYP	B	1856	1	6,8,9	0.51	0	5,10,12	2.06	2 (40%)
1	HYP	B	1873	1	6,8,9	0.48	0	5,10,12	1.46	0
2	HYP	X	1559	2	6,8,9	0.47	0	5,10,12	1.86	1 (20%)
1	HYP	A	1905	1	6,8,9	0.44	0	5,10,12	1.63	2 (40%)
1	HYP	B	1857	1	6,8,9	0.47	0	5,10,12	1.61	1 (20%)
2	HYP	X	1481	2	6,8,9	0.44	0	5,10,12	1.90	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HYP	X	1556	2	6,8,9	0.45	0	5,10,12	1.90	1 (20%)
2	HYP	X	1548	2	6,8,9	0.45	0	5,10,12	2.02	1 (20%)
1	HYP	B	1877	1	6,8,9	0.55	0	5,10,12	2.24	2 (40%)
1	HYP	B	1931	1	6,8,9	0.44	0	5,10,12	1.84	2 (40%)
1	HYP	A	1914	1	6,8,9	0.52	0	5,10,12	2.35	2 (40%)
1	HYP	B	1917	1	6,8,9	0.48	0	5,10,12	1.69	2 (40%)
2	HYP	X	1528	2	6,8,9	0.44	0	5,10,12	1.84	1 (20%)
2	HYP	X	1552	2	6,8,9	0.44	0	5,10,12	1.92	2 (40%)
2	HYP	X	1480	2	6,8,9	0.46	0	5,10,12	1.89	1 (20%)
1	HYP	B	1855	1	6,8,9	0.52	0	5,10,12	2.18	3 (60%)
1	HYP	A	1912	1	6,8,9	0.50	0	5,10,12	2.37	1 (20%)
2	HYP	X	1499	2	6,8,9	0.45	0	5,10,12	1.85	2 (40%)
1	HYP	A	1899	1	6,8,9	0.50	0	5,10,12	1.64	1 (20%)
1	HYP	A	1870	1	6,8,9	0.48	0	5,10,12	1.83	1 (20%)
2	HYP	X	1562	2	6,8,9	0.47	0	5,10,12	1.84	1 (20%)
2	HYP	X	1623	2	6,8,9	0.46	0	5,10,12	1.87	1 (20%)
2	HYP	X	1527	2	6,8,9	0.43	0	5,10,12	1.87	1 (20%)
2	HYP	X	1525	2	6,8,9	0.43	0	5,10,12	1.93	2 (40%)
1	HYP	B	1866	1	6,8,9	0.48	0	5,10,12	2.02	2 (40%)
2	HYP	X	1598	2	6,8,9	0.49	0	5,10,12	2.02	2 (40%)
1	HYP	A	1901	1	6,8,9	0.45	0	5,10,12	1.86	2 (40%)
2	HYP	X	1489	2	6,8,9	0.46	0	5,10,12	1.87	2 (40%)
1	HYP	A	1923	1	6,8,9	0.50	0	5,10,12	2.01	1 (20%)
1	HYP	B	1885	1	6,8,9	0.53	0	5,10,12	2.35	2 (40%)
2	HYP	X	1549	2	6,8,9	0.45	0	5,10,12	1.94	1 (20%)
1	HYP	B	1930	1	6,8,9	0.46	0	5,10,12	1.87	2 (40%)
2	HYP	X	1530	2	6,8,9	0.43	0	5,10,12	1.97	1 (20%)
2	HYP	X	1493	2	6,8,9	0.45	0	5,10,12	1.91	1 (20%)
1	HYP	B	1883	1	6,8,9	0.48	0	5,10,12	1.78	1 (20%)
1	HYP	B	1860	1	6,8,9	0.51	0	5,10,12	2.26	1 (20%)
1	HYP	A	1921	1	6,8,9	0.55	0	5,10,12	1.44	0
1	HYP	B	1898	1	6,8,9	0.43	0	5,10,12	1.91	3 (60%)
1	HYP	B	1870	1	6,8,9	0.47	0	5,10,12	1.86	1 (20%)
1	HYP	B	1928	1	6,8,9	0.52	0	5,10,12	1.57	1 (20%)
2	HYP	X	1547	2	6,8,9	0.44	0	5,10,12	1.92	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	A	1858	1	6,8,9	0.52	0	5,10,12	1.63	1 (20%)
1	HYP	A	1903	1	6,8,9	0.47	0	5,10,12	1.89	1 (20%)
1	HYP	A	1862	1	6,8,9	0.46	0	5,10,12	1.84	1 (20%)
1	HYP	A	1855	1	6,8,9	0.44	0	5,10,12	1.84	1 (20%)
1	HYP	B	1882	1	6,8,9	0.46	0	5,10,12	1.81	2 (40%)
2	HYP	X	1593	2	6,8,9	0.44	0	5,10,12	1.93	1 (20%)
1	HYP	B	1908	1	6,8,9	0.48	0	5,10,12	1.93	1 (20%)
2	HYP	X	1618	2	6,8,9	0.43	0	5,10,12	1.94	2 (40%)
1	HYP	A	1915	1	6,8,9	0.45	0	5,10,12	1.81	2 (40%)
1	HYP	A	1906	1	6,8,9	0.44	0	5,10,12	1.77	2 (40%)
1	HYP	B	1905	1	6,8,9	0.49	0	5,10,12	1.62	2 (40%)
2	HYP	X	1463	2	6,8,9	0.43	0	5,10,12	1.89	2 (40%)
1	HYP	B	1892	1	6,8,9	0.50	0	5,10,12	1.41	1 (20%)
1	HYP	B	1914	1	6,8,9	0.54	0	5,10,12	2.36	2 (40%)
2	HYP	X	1487	2	6,8,9	0.44	0	5,10,12	1.86	1 (20%)
1	HYP	A	1856	1	6,8,9	0.49	0	5,10,12	2.01	3 (60%)
2	HYP	X	1597	2	6,8,9	0.45	0	5,10,12	2.07	2 (40%)
2	HYP	X	1594	2	6,8,9	0.49	0	5,10,12	1.41	0
2	HYP	X	1616	2	6,8,9	0.44	0	5,10,12	1.87	2 (40%)
2	HYP	X	1486	2	6,8,9	0.44	0	5,10,12	1.65	1 (20%)
1	HYP	B	1907	1	6,8,9	0.45	0	5,10,12	1.89	2 (40%)
2	HYP	X	1482	2	6,8,9	0.45	0	5,10,12	1.93	2 (40%)
1	HYP	A	1880	1	6,8,9	0.48	0	5,10,12	1.81	1 (20%)
1	HYP	A	1887	1	6,8,9	0.46	0	5,10,12	2.01	3 (60%)
1	HYP	B	1903	1	6,8,9	0.45	0	5,10,12	1.85	1 (20%)
1	HYP	B	1912	1	6,8,9	0.51	0	5,10,12	2.06	2 (40%)
1	HYP	B	1863	1	6,8,9	0.49	0	5,10,12	2.06	1 (20%)
1	HYP	B	1918	1	6,8,9	0.51	0	5,10,12	1.69	1 (20%)
2	HYP	X	1611	2	6,8,9	0.45	0	5,10,12	1.92	1 (20%)
2	HYP	X	1490	2	6,8,9	0.48	0	5,10,12	1.92	1 (20%)
1	HYP	B	1867	1	6,8,9	0.46	0	5,10,12	1.98	2 (40%)

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
1	HYP	A	1918	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1920	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1592	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1457	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1626	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1602	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1587	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1591	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1610	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1590	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1620	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1523	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1595	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1920	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1532	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1485	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1462	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1915	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1520	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1522	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1459	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1521	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1551	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1589	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1469	2	-	0/0/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1488	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1612	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1617	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1586	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1614	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1615	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1468	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1496	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1546	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1550	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1897	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1465	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1529	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1601	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1524	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1453	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1913	1	-	0/0/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	X	1526	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1531	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1464	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1554	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1553	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1588	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1613	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1461	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1455	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1456	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1484	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1458	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1483	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1454	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1460	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1894	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1555	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1596	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1893	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1619	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1856	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1873	1	-	0/0/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	X	1559	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1481	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1556	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1548	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1931	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1917	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1528	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1552	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1480	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1499	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1562	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1623	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1527	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1525	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1598	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1489	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1549	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1530	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1493	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1928	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1547	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1862	1	-	0/0/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1593	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1618	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1463	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1487	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1597	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1594	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1616	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1486	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1907	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1482	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1918	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1611	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1490	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1867	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1912	HYP	CB-CG-CD	-4.36	97.92	103.27
1	B	1914	HYP	CB-CG-CD	-4.24	98.07	103.27
1	B	1860	HYP	CB-CG-CD	-4.18	98.14	103.27
1	A	1914	HYP	CB-CG-CD	-4.08	98.27	103.27
1	A	1885	HYP	CB-CG-CD	-3.92	98.46	103.27
1	B	1877	HYP	CG-CB-CA	-3.89	99.05	103.96
1	A	1863	HYP	CB-CG-CD	-3.82	98.58	103.27
1	B	1868	HYP	CB-CG-CD	-3.79	98.62	103.27
1	A	1923	HYP	CB-CG-CD	-3.78	98.63	103.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1932	HYP	CB-CG-CD	-3.72	98.71	103.27
1	A	1918	HYP	CB-CG-CD	-3.63	98.82	103.27
1	B	1866	HYP	CB-CG-CD	-3.59	98.86	103.27
1	A	1922	HYP	CB-CG-CD	-3.55	98.92	103.27
1	B	1910	HYP	CB-CG-CD	-3.51	98.96	103.27
1	A	1927	HYP	CB-CG-CD	-3.51	98.96	103.27
1	A	1864	HYP	CB-CG-CD	-3.48	99.00	103.27
1	A	1920	HYP	CB-CG-CD	-3.47	99.00	103.27
1	B	1908	HYP	CB-CG-CD	-3.46	99.02	103.27
1	B	1863	HYP	CB-CG-CD	-3.45	99.03	103.27
1	B	1885	HYP	CB-CG-CD	-3.42	99.07	103.27
1	A	1894	HYP	CG-CB-CA	-3.41	99.65	103.96
2	X	1597	HYP	CB-CG-CD	-3.40	99.10	103.27
1	A	1910	HYP	CB-CG-CD	-3.37	99.13	103.27
1	B	1885	HYP	CG-CB-CA	-3.35	99.73	103.96
1	A	1928	HYP	CB-CG-CD	-3.34	99.17	103.27
2	X	1548	HYP	CB-CG-CD	-3.33	99.18	103.27
2	X	1596	HYP	CB-CG-CD	-3.32	99.19	103.27
1	A	1864	HYP	CG-CB-CA	-3.29	99.81	103.96
1	A	1903	HYP	CB-CG-CD	-3.28	99.24	103.27
1	B	1870	HYP	CB-CG-CD	-3.27	99.25	103.27
2	X	1610	HYP	CB-CG-CD	-3.27	99.25	103.27
2	X	1601	HYP	CB-CG-CD	-3.26	99.26	103.27
1	A	1908	HYP	CB-CG-CD	-3.26	99.27	103.27
1	A	1868	HYP	CB-CG-CD	-3.23	99.31	103.27
2	X	1549	HYP	CB-CG-CD	-3.22	99.31	103.27
1	B	1912	HYP	CB-CG-CD	-3.22	99.32	103.27
2	X	1623	HYP	CB-CG-CD	-3.21	99.33	103.27
2	X	1615	HYP	CB-CG-CD	-3.21	99.33	103.27
2	X	1620	HYP	CB-CG-CD	-3.20	99.34	103.27
1	A	1860	HYP	CB-CG-CD	-3.20	99.34	103.27
2	X	1546	HYP	CB-CG-CD	-3.20	99.35	103.27
1	A	1885	HYP	CG-CB-CA	-3.19	99.93	103.96
1	A	1913	HYP	CB-CG-CD	-3.19	99.36	103.27
2	X	1556	HYP	CB-CG-CD	-3.18	99.37	103.27
1	B	1856	HYP	CG-CB-CA	-3.17	99.96	103.96
2	X	1611	HYP	CB-CG-CD	-3.16	99.39	103.27
1	B	1894	HYP	CB-CG-CD	-3.15	99.40	103.27
2	X	1562	HYP	CB-CG-CD	-3.15	99.41	103.27
2	X	1551	HYP	CB-CG-CD	-3.14	99.42	103.27
2	X	1490	HYP	CB-CG-CD	-3.14	99.42	103.27
2	X	1547	HYP	CB-CG-CD	-3.13	99.43	103.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1890	HYP	CB-CG-CD	-3.11	99.45	103.27
1	A	1870	HYP	CB-CG-CD	-3.11	99.45	103.27
1	A	1878	HYP	CB-CG-CD	-3.10	99.46	103.27
2	X	1526	HYP	CB-CG-CD	-3.09	99.47	103.27
1	B	1927	HYP	CB-CG-CD	-3.09	99.48	103.27
2	X	1593	HYP	CB-CG-CD	-3.08	99.49	103.27
2	X	1488	HYP	CB-CG-CD	-3.08	99.49	103.27
2	X	1481	HYP	CB-CG-CD	-3.06	99.51	103.27
2	X	1612	HYP	CB-CG-CD	-3.06	99.51	103.27
1	B	1864	HYP	CB-CG-CD	-3.04	99.54	103.27
1	B	1903	HYP	CB-CG-CD	-3.03	99.55	103.27
1	A	1880	HYP	CB-CG-CD	-3.03	99.55	103.27
1	B	1923	HYP	CB-CG-CD	-3.03	99.56	103.27
2	X	1592	HYP	CB-CG-CD	-3.01	99.57	103.27
2	X	1619	HYP	CB-CG-CD	-3.01	99.58	103.27
2	X	1530	HYP	CB-CG-CD	-3.00	99.59	103.27
2	X	1550	HYP	CB-CG-CD	-3.00	99.59	103.27
2	X	1590	HYP	CB-CG-CD	-2.98	99.61	103.27
1	A	1894	HYP	CB-CG-CD	-2.98	99.61	103.27
1	A	1873	HYP	CB-CG-CD	-2.96	99.63	103.27
2	X	1489	HYP	CB-CG-CD	-2.96	99.63	103.27
2	X	1480	HYP	CB-CG-CD	-2.96	99.63	103.27
2	X	1613	HYP	CB-CG-CD	-2.95	99.64	103.27
2	X	1531	HYP	CB-CG-CD	-2.95	99.65	103.27
2	X	1468	HYP	CB-CG-CD	-2.94	99.67	103.27
1	A	1877	HYP	CB-CG-CD	-2.94	99.67	103.27
1	B	1855	HYP	CG-CB-CA	2.93	107.66	103.96
1	B	1899	HYP	CB-CG-CD	-2.93	99.68	103.27
2	X	1559	HYP	CB-CG-CD	-2.92	99.68	103.27
1	B	1888	HYP	CB-CG-CD	-2.89	99.72	103.27
2	X	1493	HYP	CB-CG-CD	-2.86	99.76	103.27
1	A	1932	HYP	CB-CG-CD	-2.85	99.77	103.27
1	B	1913	HYP	CB-CG-CD	-2.84	99.78	103.27
1	B	1875	HYP	CB-CG-CD	-2.84	99.79	103.27
1	B	1864	HYP	CG-CB-CA	-2.82	100.41	103.96
1	B	1911	HYP	CB-CG-CD	-2.81	99.83	103.27
2	X	1483	HYP	CB-CG-CD	-2.78	99.85	103.27
2	X	1457	HYP	CB-CG-CD	-2.78	99.86	103.27
1	B	1867	HYP	CB-CG-CD	-2.76	99.88	103.27
1	B	1931	HYP	CG-CB-CA	2.76	107.45	103.96
1	B	1922	HYP	CB-CG-CD	-2.76	99.89	103.27
1	B	1882	HYP	CG-CB-CA	2.76	107.44	103.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1453	HYP	CB-CG-CD	-2.75	99.90	103.27
2	X	1521	HYP	CB-CG-CD	-2.75	99.90	103.27
1	A	1897	HYP	CB-CG-CD	-2.74	99.91	103.27
1	B	1887	HYP	CG-CB-CA	2.73	107.41	103.96
2	X	1482	HYP	CB-CG-CD	-2.73	99.92	103.27
1	A	1877	HYP	CG-CB-CA	-2.73	100.52	103.96
1	B	1902	HYP	CB-CG-CD	-2.72	99.94	103.27
1	A	1906	HYP	CG-CB-CA	2.71	107.39	103.96
2	X	1462	HYP	CG-CB-CA	2.70	107.38	103.96
2	X	1522	HYP	CG-CB-CA	2.70	107.37	103.96
1	A	1867	HYP	CB-CG-CD	-2.69	99.96	103.27
1	B	1930	HYP	CG-CB-CA	2.69	107.36	103.96
1	A	1863	HYP	CG-CB-CA	-2.69	100.57	103.96
2	X	1591	HYP	CG-CB-CA	2.68	107.35	103.96
2	X	1598	HYP	CG-CB-CA	-2.68	100.58	103.96
1	A	1898	HYP	CG-CB-CA	2.67	107.34	103.96
1	B	1883	HYP	CB-CG-CD	-2.67	99.99	103.27
1	B	1880	HYP	CB-CG-CD	-2.67	100.00	103.27
2	X	1626	HYP	CG-CB-CA	-2.65	100.62	103.96
1	A	1902	HYP	CG-CB-CA	2.64	107.29	103.96
1	B	1918	HYP	CB-CG-CD	-2.64	100.03	103.27
2	X	1523	HYP	CG-CB-CA	2.63	107.28	103.96
1	A	1907	HYP	CG-CB-CA	2.62	107.27	103.96
2	X	1555	HYP	CB-CG-CD	-2.62	100.06	103.27
1	A	1855	HYP	CG-CB-CA	2.61	107.26	103.96
1	A	1866	HYP	CG-CB-CA	2.61	107.26	103.96
1	B	1878	HYP	CB-CG-CD	-2.60	100.07	103.27
2	X	1589	HYP	CG-CB-CA	2.60	107.24	103.96
1	B	1917	HYP	CB-CG-CD	-2.60	100.08	103.27
1	B	1857	HYP	CG-CB-CA	2.60	107.24	103.96
2	X	1499	HYP	CG-CB-CA	2.59	107.24	103.96
2	X	1528	HYP	CG-CB-CA	2.59	107.24	103.96
2	X	1486	HYP	CG-CB-CA	2.59	107.23	103.96
1	A	1875	HYP	CB-CG-CD	-2.59	100.09	103.27
1	A	1899	HYP	CB-CG-CD	-2.59	100.09	103.27
1	B	1855	HYP	OD1-CG-CD	2.59	116.00	110.35
1	B	1862	HYP	CG-CB-CA	2.58	107.22	103.96
2	X	1465	HYP	CG-CB-CA	2.58	107.22	103.96
1	A	1856	HYP	CG-CB-CA	-2.58	100.71	103.96
1	A	1865	HYP	CB-CG-CD	-2.58	100.11	103.27
1	B	1929	HYP	CG-CB-CA	2.57	107.21	103.96
1	B	1906	HYP	CB-CG-CD	-2.57	100.11	103.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1586	HYP	CB-CG-CD	-2.57	100.11	103.27
2	X	1520	HYP	CB-CG-CD	-2.57	100.11	103.27
2	X	1588	HYP	CG-CB-CA	2.57	107.21	103.96
1	B	1893	HYP	CG-CB-CA	2.56	107.20	103.96
2	X	1553	HYP	CG-CB-CA	2.56	107.19	103.96
2	X	1618	HYP	CB-CG-CD	-2.56	100.13	103.27
2	X	1458	HYP	CG-CB-CA	2.56	107.19	103.96
1	B	1901	HYP	CG-CB-CA	2.56	107.19	103.96
1	A	1916	HYP	CG-CB-CA	2.56	107.19	103.96
1	B	1907	HYP	CG-CB-CA	2.56	107.19	103.96
2	X	1464	HYP	CG-CB-CA	2.56	107.19	103.96
2	X	1455	HYP	CG-CB-CA	2.54	107.17	103.96
2	X	1527	HYP	CG-CB-CA	2.54	107.17	103.96
1	B	1920	HYP	CB-CG-CD	-2.54	100.15	103.27
2	X	1602	HYP	CG-CB-CA	2.54	107.17	103.96
2	X	1461	HYP	CG-CB-CA	2.54	107.17	103.96
1	A	1901	HYP	CG-CB-CA	2.54	107.17	103.96
2	X	1460	HYP	CG-CB-CA	2.54	107.16	103.96
1	A	1888	HYP	CB-CG-CD	-2.53	100.16	103.27
2	X	1598	HYP	CB-CG-CD	-2.53	100.16	103.27
1	A	1929	HYP	CB-CG-CD	-2.53	100.17	103.27
1	A	1857	HYP	CG-CB-CA	2.53	107.15	103.96
2	X	1554	HYP	CG-CB-CA	2.53	107.15	103.96
1	B	1872	HYP	CG-CB-CA	2.51	107.13	103.96
2	X	1532	HYP	CB-CG-CD	-2.49	100.21	103.27
2	X	1456	HYP	CG-CB-CA	2.49	107.11	103.96
1	A	1905	HYP	CG-CB-CA	2.48	107.09	103.96
2	X	1487	HYP	CG-CB-CA	2.48	107.09	103.96
2	X	1587	HYP	CG-CB-CA	2.47	107.08	103.96
1	A	1887	HYP	CB-CG-CD	-2.47	100.24	103.27
2	X	1459	HYP	CG-CB-CA	2.46	107.07	103.96
2	X	1529	HYP	CB-CG-CD	-2.46	100.25	103.27
1	A	1931	HYP	CG-CB-CA	2.46	107.06	103.96
1	A	1882	HYP	CG-CB-CA	2.45	107.05	103.96
1	B	1916	HYP	CB-CG-CD	-2.43	100.28	103.27
2	X	1617	HYP	CG-CB-CA	2.41	107.01	103.96
1	A	1893	HYP	CG-CB-CA	2.40	107.00	103.96
2	X	1595	HYP	CG-CB-CA	2.40	106.99	103.96
2	X	1552	HYP	CG-CB-CA	2.40	106.99	103.96
2	X	1524	HYP	CG-CB-CA	2.39	106.98	103.96
2	X	1616	HYP	CG-CB-CA	2.39	106.98	103.96
2	X	1525	HYP	CG-CB-CA	2.39	106.97	103.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1883	HYP	CB-CG-CD	-2.38	100.34	103.27
2	X	1485	HYP	CG-CB-CA	2.38	106.97	103.96
2	X	1484	HYP	CB-CG-CD	-2.38	100.35	103.27
1	A	1914	HYP	CG-CB-CA	-2.37	100.97	103.96
2	X	1463	HYP	CB-CG-CD	-2.37	100.36	103.27
1	A	1862	HYP	CB-CG-CD	-2.37	100.36	103.27
1	B	1897	HYP	CG-CB-CA	2.36	106.95	103.96
1	A	1887	HYP	CG-CB-CA	2.33	106.91	103.96
2	X	1614	HYP	CB-CG-CD	-2.33	100.41	103.27
1	B	1905	HYP	CB-CG-CD	-2.32	100.42	103.27
1	B	1856	HYP	O-C-CA	-2.32	118.70	124.78
2	X	1552	HYP	CB-CG-CD	-2.30	100.44	103.27
2	X	1529	HYP	CG-CB-CA	2.30	106.87	103.96
2	X	1525	HYP	CB-CG-CD	-2.30	100.45	103.27
1	A	1920	HYP	O-C-CA	-2.30	118.75	124.78
1	B	1898	HYP	CB-CG-CD	-2.29	100.46	103.27
2	X	1484	HYP	CG-CB-CA	2.29	106.85	103.96
1	B	1912	HYP	CG-CB-CA	-2.29	101.07	103.96
2	X	1524	HYP	CB-CG-CD	-2.29	100.46	103.27
1	B	1921	HYP	CG-CB-CA	-2.27	101.09	103.96
1	B	1902	HYP	O-C-CA	-2.27	118.83	124.78
2	X	1614	HYP	CG-CB-CA	2.27	106.83	103.96
2	X	1496	HYP	CB-CG-CD	-2.26	100.49	103.27
2	X	1463	HYP	CG-CB-CA	2.26	106.82	103.96
2	X	1469	HYP	O-C-CA	-2.26	118.85	124.78
1	A	1917	HYP	CB-CG-CD	-2.26	100.50	103.27
1	B	1877	HYP	CB-CG-CD	-2.24	100.52	103.27
1	A	1897	HYP	O-C-CA	-2.24	118.91	124.78
1	A	1898	HYP	O-C-CA	-2.24	118.92	124.78
1	A	1915	HYP	CG-CB-CA	2.23	106.78	103.96
1	A	1872	HYP	O-C-CA	-2.23	118.92	124.78
1	B	1858	HYP	CB-CG-CD	2.23	106.00	103.27
1	B	1867	HYP	O-C-CA	-2.23	118.93	124.78
1	B	1915	HYP	CB-CG-CD	-2.23	100.53	103.27
1	B	1864	HYP	O-C-CA	-2.23	118.93	124.78
1	B	1887	HYP	O-C-CA	-2.23	118.94	124.78
2	X	1499	HYP	O-C-CA	-2.23	118.94	124.78
2	X	1597	HYP	O-C-CA	-2.23	118.94	124.78
1	A	1887	HYP	O-C-CA	-2.21	118.99	124.78
1	B	1914	HYP	CG-CB-CA	-2.21	101.18	103.96
1	A	1911	HYP	CB-CG-CD	-2.20	100.56	103.27
1	A	1902	HYP	O-C-CA	-2.20	119.02	124.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1916	HYP	CG-CB-CA	2.19	106.73	103.96
1	B	1898	HYP	O-C-CA	-2.19	119.04	124.78
1	A	1917	HYP	O-C-CA	-2.19	119.05	124.78
2	X	1485	HYP	CB-CG-CD	-2.19	100.58	103.27
2	X	1618	HYP	CG-CB-CA	2.18	106.72	103.96
1	B	1928	HYP	O-C-CA	-2.18	119.07	124.78
1	A	1893	HYP	O-C-CA	-2.17	119.10	124.78
1	A	1856	HYP	CB-CG-CD	-2.16	100.61	103.27
1	B	1893	HYP	O-C-CA	-2.16	119.11	124.78
2	X	1532	HYP	CG-CB-CA	-2.16	101.23	103.96
1	B	1930	HYP	O-C-CA	-2.16	119.12	124.78
1	A	1901	HYP	O-C-CA	-2.16	119.13	124.78
1	B	1907	HYP	O-C-CA	-2.16	119.13	124.78
1	A	1882	HYP	O-C-CA	-2.15	119.14	124.78
1	B	1921	HYP	O-C-CA	-2.15	119.14	124.78
1	B	1866	HYP	O-C-CA	-2.15	119.14	124.78
1	B	1897	HYP	O-C-CA	-2.15	119.14	124.78
1	A	1907	HYP	O-C-CA	-2.15	119.14	124.78
1	A	1931	HYP	O-C-CA	-2.14	119.16	124.78
2	X	1617	HYP	CB-CG-CD	-2.14	100.64	103.27
1	B	1898	HYP	CG-CB-CA	2.14	106.66	103.96
1	A	1856	HYP	O-C-CA	-2.14	119.18	124.78
1	A	1930	HYP	O-C-CA	-2.13	119.20	124.78
2	X	1453	HYP	O-C-CA	-2.13	119.20	124.78
1	B	1892	HYP	O-C-CA	-2.13	119.20	124.78
1	A	1929	HYP	CG-CB-CA	2.12	106.64	103.96
1	B	1906	HYP	CG-CB-CA	2.12	106.63	103.96
1	B	1920	HYP	CG-CB-CA	2.11	106.63	103.96
1	B	1855	HYP	O-C-CA	-2.11	119.24	124.78
2	X	1587	HYP	CB-CG-CD	-2.11	100.67	103.27
1	B	1882	HYP	O-C-CA	-2.11	119.25	124.78
2	X	1616	HYP	CB-CG-CD	-2.11	100.68	103.27
1	A	1905	HYP	O-C-CA	-2.11	119.26	124.78
2	X	1459	HYP	CB-CG-CD	-2.11	100.68	103.27
1	B	1872	HYP	O-C-CA	-2.10	119.27	124.78
1	A	1865	HYP	CG-CB-CA	2.10	106.61	103.96
2	X	1521	HYP	CG-CB-CA	2.09	106.61	103.96
1	B	1922	HYP	CG-CB-CA	2.09	106.60	103.96
2	X	1489	HYP	O-C-CA	-2.08	119.32	124.78
1	A	1897	HYP	CG-CB-CA	2.08	106.59	103.96
1	B	1931	HYP	O-C-CA	-2.08	119.32	124.78
2	X	1456	HYP	CB-CG-CD	-2.08	100.71	103.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1892	HYP	O-C-CA	-2.07	119.35	124.78
1	B	1932	HYP	O-C-CA	-2.07	119.36	124.78
2	X	1554	HYP	O-C-CA	-2.06	119.38	124.78
2	X	1555	HYP	CG-CB-CA	2.06	106.56	103.96
1	A	1915	HYP	O-C-CA	-2.05	119.40	124.78
1	A	1932	HYP	O-C-CA	-2.04	119.43	124.78
1	A	1867	HYP	O-C-CA	-2.04	119.43	124.78
2	X	1555	HYP	O-C-CA	-2.03	119.45	124.78
1	A	1911	HYP	O-C-CA	-2.03	119.45	124.78
1	B	1901	HYP	O-C-CA	-2.03	119.45	124.78
2	X	1482	HYP	CG-CB-CA	2.03	106.53	103.96
1	A	1911	HYP	CG-CB-CA	2.03	106.53	103.96
1	A	1857	HYP	O-C-CA	-2.03	119.46	124.78
1	B	1905	HYP	O-C-CA	-2.02	119.49	124.78
1	A	1928	HYP	O-C-CA	-2.01	119.50	124.78
1	A	1858	HYP	CB-CG-CD	-2.01	100.80	103.27
1	A	1906	HYP	O-C-CA	-2.01	119.51	124.78
1	B	1917	HYP	O-C-CA	-2.01	119.52	124.78
1	A	1929	HYP	O-C-CA	-2.01	119.52	124.78
2	X	1524	HYP	O-C-CA	-2.01	119.52	124.78
2	X	1553	HYP	O-C-CA	-2.00	119.52	124.78
1	A	1917	HYP	CG-CB-CA	2.00	106.49	103.96
1	B	1929	HYP	O-C-CA	-2.00	119.53	124.78
1	A	1916	HYP	O-C-CA	-2.00	119.53	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

240 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A1	1	1,3	14,14,15	0.77	0	17,19,21	1.02	1 (5%)
3	NAG	A1	2	3	14,14,15	0.72	0	17,19,21	0.87	0
3	NAG	A2	1	1,3	14,14,15	0.72	0	17,19,21	1.23	2 (11%)
3	NAG	A2	2	3	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	A3	1	1,3	14,14,15	0.81	0	17,19,21	0.98	1 (5%)
3	NAG	A3	2	3	14,14,15	0.76	0	17,19,21	0.93	0
4	FUB	A4	1	4	9,9,10	1.08	0	10,12,14	0.79	0
4	FUB	A4	2	9,4	9,9,10	1.03	0	10,12,14	0.82	0
4	FUB	A5	1	4	9,9,10	1.03	0	10,12,14	0.86	0
4	FUB	A5	2	9,4	9,9,10	1.03	0	10,12,14	0.81	0
5	FUB	A6	1	5	9,9,10	1.06	0	10,12,14	0.85	0
5	FUB	A6	2	5,9	9,9,10	1.08	0	10,12,14	0.81	0
5	FUB	A6	3	5	9,9,10	1.04	0	10,12,14	0.88	0
5	FUB	A6	4	5,9	9,9,10	1.05	0	10,12,14	0.84	0
4	FUB	A7	1	4	9,9,10	1.06	0	10,12,14	0.90	0
4	FUB	A7	2	9,4	9,9,10	1.11	0	10,12,14	0.93	1 (10%)
5	FUB	A9	1	5	9,9,10	1.05	0	10,12,14	0.80	0
5	FUB	A9	2	5,9	9,9,10	1.07	0	10,12,14	0.79	0
5	FUB	A9	3	5	9,9,10	1.04	0	10,12,14	0.90	0
5	FUB	A9	4	5,9	9,9,10	1.05	0	10,12,14	0.80	0
4	FUB	B0	1	4	9,9,10	1.10	0	10,12,14	0.99	1 (10%)
4	FUB	B0	2	9,4	9,9,10	1.02	0	10,12,14	0.83	0
4	FUB	B1	1	4	9,9,10	1.05	0	10,12,14	0.85	0
4	FUB	B1	2	9,4	9,9,10	1.05	0	10,12,14	0.78	0
4	FUB	B3	1	4	9,9,10	1.01	0	10,12,14	0.94	0
4	FUB	B3	2	9,4	9,9,10	1.08	0	10,12,14	0.91	0
4	FUB	B4	1	4	9,9,10	1.02	0	10,12,14	0.79	0
4	FUB	B4	2	9,4	9,9,10	1.03	0	10,12,14	0.90	0
4	FUB	B5	1	4	9,9,10	1.04	0	10,12,14	0.79	0
4	FUB	B5	2	9,4	9,9,10	1.05	0	10,12,14	0.79	0
5	FUB	B6	1	5	9,9,10	1.05	0	10,12,14	0.78	0
5	FUB	B6	2	5,9	9,9,10	1.04	0	10,12,14	0.79	0
5	FUB	B6	3	5	9,9,10	1.02	0	10,12,14	0.86	0
5	FUB	B6	4	5,9	9,9,10	1.05	0	10,12,14	0.88	0
4	FUB	B7	1	4	9,9,10	1.05	0	10,12,14	0.77	0
4	FUB	B7	2	9,4	9,9,10	1.05	0	10,12,14	0.88	0
4	FUB	B9	1	4	9,9,10	1.04	0	10,12,14	0.82	0
4	FUB	B9	2	9,4	9,9,10	1.04	0	10,12,14	0.86	0
4	FUB	C0	1	4	9,9,10	1.02	0	10,12,14	0.99	0
4	FUB	C0	2	9,4	9,9,10	1.04	0	10,12,14	0.80	0
4	FUB	C1	1	4	9,9,10	1.03	0	10,12,14	0.83	0
4	FUB	C1	2	9,4	9,9,10	1.02	0	10,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUB	C2	1	4	9,9,10	1.03	0	10,12,14	0.81	0
4	FUB	C2	2	9,4	9,9,10	1.03	0	10,12,14	0.86	0
4	FUB	C3	1	4	9,9,10	1.03	0	10,12,14	0.88	0
4	FUB	C3	2	9,4	9,9,10	1.04	0	10,12,14	0.91	0
4	FUB	C4	1	4	9,9,10	1.04	0	10,12,14	0.81	0
4	FUB	C4	2	9,4	9,9,10	1.02	0	10,12,14	0.89	0
4	FUB	C5	1	4	9,9,10	1.04	0	10,12,14	0.87	0
4	FUB	C5	2	9,4	9,9,10	1.04	0	10,12,14	0.91	0
4	FUB	C6	1	4	9,9,10	1.04	0	10,12,14	0.81	0
4	FUB	C6	2	9,4	9,9,10	1.02	0	10,12,14	0.88	0
4	FUB	C7	1	4	9,9,10	1.03	0	10,12,14	0.80	0
4	FUB	C7	2	9,4	9,9,10	1.03	0	10,12,14	0.92	0
4	FUB	C8	1	4	9,9,10	1.03	0	10,12,14	0.86	0
4	FUB	C8	2	9,4	9,9,10	1.02	0	10,12,14	0.88	0
4	FUB	C9	1	4	9,9,10	1.03	0	10,12,14	0.88	0
4	FUB	C9	2	9,4	9,9,10	1.03	0	10,12,14	0.87	0
4	FUB	D0	1	4	9,9,10	1.04	0	10,12,14	0.92	0
4	FUB	D0	2	9,4	9,9,10	1.03	0	10,12,14	0.90	0
4	FUB	D1	1	4	9,9,10	1.04	0	10,12,14	1.14	1 (10%)
4	FUB	D1	2	9,4	9,9,10	1.04	0	10,12,14	0.85	0
4	FUB	D2	1	4	9,9,10	1.07	0	10,12,14	0.93	0
4	FUB	D2	2	9,4	9,9,10	1.05	0	10,12,14	0.80	0
4	FUB	D3	1	4	9,9,10	1.04	0	10,12,14	0.77	0
4	FUB	D3	2	9,4	9,9,10	1.04	0	10,12,14	0.92	0
4	FUB	D4	1	4	9,9,10	1.05	0	10,12,14	0.74	0
4	FUB	D4	2	9,4	9,9,10	1.05	0	10,12,14	0.89	0
4	FUB	D5	1	4	9,9,10	1.06	0	10,12,14	0.89	0
4	FUB	D5	2	9,4	9,9,10	1.06	0	10,12,14	0.88	0
4	FUB	D6	1	4	9,9,10	1.04	0	10,12,14	0.80	0
4	FUB	D6	2	9,4	9,9,10	1.08	0	10,12,14	1.03	0
4	FUB	D7	1	4	9,9,10	1.06	0	10,12,14	0.97	0
4	FUB	D7	2	9,4	9,9,10	1.07	0	10,12,14	0.88	0
4	FUB	D8	1	4	9,9,10	1.05	0	10,12,14	0.79	0
4	FUB	D8	2	9,4	9,9,10	1.04	0	10,12,14	0.86	0
4	FUB	D9	1	4	9,9,10	1.06	0	10,12,14	0.90	0
4	FUB	D9	2	9,4	9,9,10	1.07	0	10,12,14	0.83	0
4	FUB	E0	1	4	9,9,10	1.05	0	10,12,14	0.80	0
4	FUB	E0	2	9,4	9,9,10	1.05	0	10,12,14	0.76	0
4	FUB	E1	1	4	9,9,10	1.05	0	10,12,14	0.83	0
4	FUB	E1	2	9,4	9,9,10	1.05	0	10,12,14	0.95	0
4	FUB	E2	1	4	9,9,10	1.03	0	10,12,14	0.85	0
4	FUB	E2	2	9,4	9,9,10	1.07	0	10,12,14	0.85	0
4	FUB	E3	1	4	9,9,10	1.06	0	10,12,14	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUB	E3	2	9,4	9,9,10	1.04	0	10,12,14	0.89	0
4	FUB	E4	1	4	9,9,10	1.02	0	10,12,14	1.07	1 (10%)
4	FUB	E4	2	9,4	9,9,10	1.07	0	10,12,14	1.13	1 (10%)
4	FUB	E5	1	4	9,9,10	1.04	0	10,12,14	0.79	0
4	FUB	E5	2	9,4	9,9,10	1.04	0	10,12,14	0.84	0
6	FUB	E6	1	6	9,9,10	1.06	0	10,12,14	0.85	0
6	FUB	E6	2	9,6	9,9,10	1.04	0	10,12,14	0.74	0
6	FUB	E6	3	6	9,9,10	1.03	0	10,12,14	0.84	0
6	FUB	E6	4	9,6	9,9,10	1.06	0	10,12,14	0.75	0
6	FUB	E6	5	6	9,9,10	1.02	0	10,12,14	0.85	0
6	FUB	E6	6	9,6	9,9,10	1.06	0	10,12,14	0.75	0
6	FUB	E6	7	6	9,9,10	1.04	0	10,12,14	0.73	0
6	FUB	E6	8	9,6	9,9,10	1.05	0	10,12,14	0.83	0
4	FUB	E7	1	4	9,9,10	1.07	0	10,12,14	0.78	0
4	FUB	E7	2	9,4	9,9,10	1.07	0	10,12,14	0.90	0
4	FUB	E8	1	4	9,9,10	1.03	0	10,12,14	0.80	0
4	FUB	E8	2	9,4	9,9,10	1.03	0	10,12,14	0.85	0
4	FUB	F0	1	4	9,9,10	1.03	0	10,12,14	0.87	0
4	FUB	F0	2	9,4	9,9,10	1.05	0	10,12,14	0.84	0
4	FUB	F2	1	4	9,9,10	1.04	0	10,12,14	0.78	0
4	FUB	F2	2	9,4	9,9,10	1.08	0	10,12,14	0.90	0
4	FUB	F3	1	4	9,9,10	1.07	0	10,12,14	0.86	0
4	FUB	F3	2	9,4	9,9,10	1.06	0	10,12,14	0.90	0
4	FUB	F5	1	4	9,9,10	1.06	0	10,12,14	0.78	0
4	FUB	F5	2	9,4	9,9,10	1.07	0	10,12,14	0.89	0
5	FUB	F6	1	5	9,9,10	1.06	0	10,12,14	0.78	0
5	FUB	F6	2	5,9	9,9,10	1.07	0	10,12,14	0.84	0
5	FUB	F6	3	5	9,9,10	1.05	0	10,12,14	0.82	0
5	FUB	F6	4	5,9	9,9,10	1.07	0	10,12,14	0.86	0
5	FUB	F7	1	5	9,9,10	1.04	0	10,12,14	0.77	0
5	FUB	F7	2	5,9	9,9,10	1.07	0	10,12,14	0.77	0
5	FUB	F7	3	5	9,9,10	1.02	0	10,12,14	0.80	0
5	FUB	F7	4	5,9	9,9,10	1.04	0	10,12,14	0.81	0
4	FUB	F8	1	4	9,9,10	1.06	0	10,12,14	0.78	0
4	FUB	F8	2	9,4	9,9,10	1.07	0	10,12,14	0.90	0
3	NAG	a1	1	1,3	14,14,15	0.74	0	17,19,21	0.86	1 (5%)
3	NAG	a1	2	3	14,14,15	0.72	0	17,19,21	0.82	0
3	NAG	a2	1	1,3	14,14,15	0.73	0	17,19,21	1.17	1 (5%)
3	NAG	a2	2	3	14,14,15	0.74	0	17,19,21	0.83	0
3	NAG	a3	1	1,3	14,14,15	0.78	0	17,19,21	1.53	2 (11%)
3	NAG	a3	2	3	14,14,15	0.73	0	17,19,21	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	34V	a4	1	7	9,9,10	1.27	0	10,12,15	0.91	1 (10%)
7	FUB	a4	2	7,9	9,9,10	1.33	2 (22%)	10,12,14	1.24	2 (20%)
4	FUB	a5	1	4	9,9,10	1.08	0	10,12,14	0.93	0
4	FUB	a5	2	9,4	9,9,10	1.36	2 (22%)	10,12,14	1.09	1 (10%)
5	FUB	a6	1	5	9,9,10	1.10	1 (11%)	10,12,14	1.08	0
5	FUB	a6	2	5,9	9,9,10	1.33	0	10,12,14	1.26	1 (10%)
5	FUB	a6	3	5	9,9,10	1.17	1 (11%)	10,12,14	1.24	1 (10%)
5	FUB	a6	4	5,9	9,9,10	1.25	1 (11%)	10,12,14	1.12	1 (10%)
4	FUB	a7	1	4	9,9,10	1.13	0	10,12,14	0.98	0
4	FUB	a7	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.99	1 (10%)
5	FUB	a9	1	5	9,9,10	1.32	1 (11%)	10,12,14	1.02	1 (10%)
5	FUB	a9	2	5,9	9,9,10	1.33	1 (11%)	10,12,14	0.91	0
5	FUB	a9	3	5	9,9,10	1.10	0	10,12,14	0.96	0
5	FUB	a9	4	5,9	9,9,10	1.33	1 (11%)	10,12,14	1.06	1 (10%)
4	FUB	b0	1	4	9,9,10	1.45	2 (22%)	10,12,14	1.29	2 (20%)
4	FUB	b0	2	9,4	9,9,10	1.36	1 (11%)	10,12,14	1.00	1 (10%)
4	FUB	b1	1	4	9,9,10	1.41	2 (22%)	10,12,14	1.28	2 (20%)
4	FUB	b1	2	9,4	9,9,10	1.30	0	10,12,14	1.02	1 (10%)
4	FUB	b3	1	4	9,9,10	1.07	0	10,12,14	1.01	1 (10%)
4	FUB	b3	2	9,4	9,9,10	1.36	1 (11%)	10,12,14	1.38	2 (20%)
4	FUB	b4	1	4	9,9,10	1.37	1 (11%)	10,12,14	0.97	1 (10%)
4	FUB	b4	2	9,4	9,9,10	1.43	2 (22%)	10,12,14	1.12	1 (10%)
4	FUB	b5	1	4	9,9,10	1.14	0	10,12,14	1.39	1 (10%)
4	FUB	b5	2	9,4	9,9,10	1.24	0	10,12,14	1.12	1 (10%)
5	FUB	b6	1	5	9,9,10	1.35	2 (22%)	10,12,14	1.08	1 (10%)
5	FUB	b6	2	5,9	9,9,10	1.39	2 (22%)	10,12,14	1.11	1 (10%)
5	FUB	b6	3	5	9,9,10	1.31	1 (11%)	10,12,14	1.04	1 (10%)
5	FUB	b6	4	5,9	9,9,10	1.34	1 (11%)	10,12,14	1.09	1 (10%)
4	FUB	b7	1	4	9,9,10	1.24	0	10,12,14	1.00	1 (10%)
4	FUB	b7	2	9,4	9,9,10	1.39	2 (22%)	10,12,14	1.06	1 (10%)
4	FUB	b9	1	4	9,9,10	1.27	0	10,12,14	0.95	1 (10%)
4	FUB	b9	2	9,4	9,9,10	1.28	0	10,12,14	0.97	1 (10%)
4	FUB	c0	1	4	9,9,10	1.32	1 (11%)	10,12,14	1.23	2 (20%)
4	FUB	c0	2	9,4	9,9,10	1.27	1 (11%)	10,12,14	1.20	2 (20%)
4	FUB	c1	1	4	9,9,10	1.38	2 (22%)	10,12,14	1.04	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FUB	c1	2	9,4	9,9,10	1.24	1 (11%)	10,12,14	1.05	1 (10%)
4	FUB	c2	1	4	9,9,10	1.35	1 (11%)	10,12,14	1.01	1 (10%)
4	FUB	c2	2	9,4	9,9,10	1.26	0	10,12,14	1.02	1 (10%)
4	FUB	c3	1	4	9,9,10	1.30	1 (11%)	10,12,14	1.23	2 (20%)
4	FUB	c3	2	9,4	9,9,10	1.43	2 (22%)	10,12,14	1.01	1 (10%)
4	FUB	c4	1	4	9,9,10	1.31	0	10,12,14	1.01	1 (10%)
4	FUB	c4	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	1.14	1 (10%)
4	FUB	c5	1	4	9,9,10	1.18	0	10,12,14	1.02	1 (10%)
4	FUB	c5	2	9,4	9,9,10	1.27	0	10,12,14	0.93	1 (10%)
4	FUB	c6	1	4	9,9,10	1.40	2 (22%)	10,12,14	1.11	1 (10%)
4	FUB	c6	2	9,4	9,9,10	1.29	1 (11%)	10,12,14	0.98	1 (10%)
4	FUB	c7	1	4	9,9,10	1.42	2 (22%)	10,12,14	1.31	2 (20%)
4	FUB	c7	2	9,4	9,9,10	1.28	0	10,12,14	1.15	1 (10%)
4	FUB	c8	1	4	9,9,10	1.15	0	10,12,14	0.97	1 (10%)
4	FUB	c8	2	9,4	9,9,10	1.44	2 (22%)	10,12,14	1.08	1 (10%)
4	FUB	c9	1	4	9,9,10	1.16	0	10,12,14	1.36	2 (20%)
4	FUB	c9	2	9,4	9,9,10	1.36	2 (22%)	10,12,14	1.35	2 (20%)
4	FUB	d0	1	4	9,9,10	1.16	0	10,12,14	0.97	1 (10%)
4	FUB	d0	2	9,4	9,9,10	1.44	2 (22%)	10,12,14	1.08	1 (10%)
4	FUB	d1	1	4	9,9,10	1.08	0	10,12,14	0.86	0
4	FUB	d1	2	9,4	9,9,10	1.10	0	10,12,14	1.57	4 (40%)
4	FUB	d2	1	4	9,9,10	1.09	0	10,12,14	1.15	1 (10%)
4	FUB	d2	2	9,4	9,9,10	1.29	0	10,12,14	1.00	1 (10%)
4	FUB	d3	1	4	9,9,10	1.27	0	10,12,14	0.96	1 (10%)
4	FUB	d3	2	9,4	9,9,10	1.33	1 (11%)	10,12,14	1.05	1 (10%)
4	FUB	d4	1	4	9,9,10	1.16	0	10,12,14	0.94	1 (10%)
4	FUB	d4	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.96	1 (10%)
4	FUB	d5	1	4	9,9,10	1.23	0	10,12,14	1.03	1 (10%)
4	FUB	d5	2	9,4	9,9,10	1.41	2 (22%)	10,12,14	1.18	1 (10%)
4	FUB	d6	1	4	9,9,10	1.17	0	10,12,14	0.94	1 (10%)
4	FUB	d6	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.96	1 (10%)
4	FUB	d7	1	4	9,9,10	1.46	2 (22%)	10,12,14	1.19	1 (10%)
4	FUB	d7	2	9,4	9,9,10	1.33	1 (11%)	10,12,14	0.99	1 (10%)
4	FUB	d8	1	4	9,9,10	1.09	0	10,12,14	1.00	0
4	FUB	d8	2	9,4	9,9,10	1.38	2 (22%)	10,12,14	1.00	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUB	d9	1	4	9,9,10	1.27	0	10,12,14	0.90	1 (10%)
4	FUB	d9	2	9,4	9,9,10	1.44	2 (22%)	10,12,14	1.03	1 (10%)
4	FUB	e0	1	4	9,9,10	1.27	0	10,12,14	0.99	1 (10%)
4	FUB	e0	2	9,4	9,9,10	1.31	1 (11%)	10,12,14	1.28	2 (20%)
4	FUB	e1	1	4	9,9,10	1.11	0	10,12,14	1.04	1 (10%)
4	FUB	e1	2	9,4	9,9,10	1.40	2 (22%)	10,12,14	1.08	1 (10%)
4	FUB	e2	1	4	9,9,10	1.24	0	10,12,14	1.04	1 (10%)
4	FUB	e2	2	9,4	9,9,10	1.34	1 (11%)	10,12,14	0.98	1 (10%)
4	FUB	e3	1	4	9,9,10	1.10	0	10,12,14	1.00	0
4	FUB	e3	2	9,4	9,9,10	1.39	2 (22%)	10,12,14	1.00	1 (10%)
4	FUB	e4	1	4	9,9,10	1.13	1 (11%)	10,12,14	1.26	1 (10%)
4	FUB	e4	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	1.22	2 (20%)
4	FUB	e5	1	4	9,9,10	1.46	2 (22%)	10,12,14	1.19	1 (10%)
4	FUB	e5	2	9,4	9,9,10	1.32	1 (11%)	10,12,14	0.99	1 (10%)
4	FUB	e6	1	4	9,9,10	1.10	0	10,12,14	1.00	0
4	FUB	e6	2	9,4	9,9,10	1.37	1 (11%)	10,12,14	0.99	1 (10%)
4	FUB	e7	1	4	9,9,10	1.10	0	10,12,14	0.99	0
4	FUB	e7	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.99	1 (10%)
4	FUB	e8	1	4	9,9,10	1.27	0	10,12,14	0.91	1 (10%)
4	FUB	e8	2	9,4	9,9,10	1.42	2 (22%)	10,12,14	1.03	1 (10%)
8	FUB	e9	1	8	9,9,10	1.21	0	10,12,14	1.03	1 (10%)
8	FUB	e9	2	8,9	9,9,10	1.26	0	10,12,14	1.51	1 (10%)
8	FUB	e9	3	8	9,9,10	1.14	0	10,12,14	1.06	1 (10%)
8	FUB	e9	4	8,9	9,9,10	1.23	0	10,12,14	1.42	1 (10%)
8	FUB	e9	5	8	9,9,10	1.25	0	10,12,14	1.02	1 (10%)
8	FUB	e9	6	8,9	9,9,10	1.32	0	10,12,14	1.20	2 (20%)
4	FUB	f0	1	4	9,9,10	1.10	0	10,12,14	0.99	0
4	FUB	f0	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.99	1 (10%)
4	FUB	f2	1	4	9,9,10	1.09	0	10,12,14	1.00	0
4	FUB	f2	2	9,4	9,9,10	1.37	2 (22%)	10,12,14	0.99	1 (10%)
4	FUB	f3	1	4	9,9,10	1.17	0	10,12,14	1.01	1 (10%)
4	FUB	f3	2	9,4	9,9,10	1.46	2 (22%)	10,12,14	1.04	1 (10%)
4	FUB	f5	1	4	9,9,10	1.30	0	10,12,14	1.01	1 (10%)
4	FUB	f5	2	9,4	9,9,10	1.25	1 (11%)	10,12,14	1.40	2 (20%)
5	FUB	f6	1	5	9,9,10	1.16	0	10,12,14	1.06	1 (10%)
5	FUB	f6	2	5,9	9,9,10	1.34	1 (11%)	10,12,14	1.08	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FUB	f6	3	5	9,9,10	1.23	0	10,12,14	1.02	1 (10%)
5	FUB	f6	4	5,9	9,9,10	1.30	1 (11%)	10,12,14	1.49	2 (20%)
5	FUB	f7	1	5	9,9,10	1.36	1 (11%)	10,12,14	1.03	1 (10%)
5	FUB	f7	2	5,9	9,9,10	1.30	0	10,12,14	1.24	1 (10%)
5	FUB	f7	3	5	9,9,10	1.34	2 (22%)	10,12,14	1.03	1 (10%)
5	FUB	f7	4	5,9	9,9,10	1.27	0	10,12,14	1.23	1 (10%)
4	FUB	f8	1	4	9,9,10	1.22	0	10,12,14	1.05	1 (10%)
4	FUB	f8	2	9,4	9,9,10	1.39	2 (22%)	10,12,14	1.31	2 (20%)

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
3	NAG	A1	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A1	2	3	-	1/6/23/26	0/1/1/1
3	NAG	A2	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	A2	2	3	-	0/6/23/26	0/1/1/1
3	NAG	A3	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A3	2	3	-	0/6/23/26	0/1/1/1
4	FUB	A4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	A5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	A6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	A6	2	5,9	-	0/2/15/18	0/1/1/1
5	FUB	A6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	A6	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	A7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A7	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	A9	1	5	-	0/2/15/18	0/1/1/1
5	FUB	A9	2	5,9	-	0/2/15/18	0/1/1/1
5	FUB	A9	3	5	-	0/2/15/18	0/1/1/1
5	FUB	A9	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	B0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B3	2	9,4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	B4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	B6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	B6	2	5,9	-	0/2/15/18	0/1/1/1
5	FUB	B6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	B6	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	B7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	B9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C5	2	9,4	-	1/2/15/18	0/1/1/1
4	FUB	C6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C6	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C8	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	C9	1	4	-	2/2/15/18	0/1/1/1
4	FUB	C9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	D4	2	9,4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	D5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D5	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D6	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	D7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	D8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D8	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	D9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	E0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	E4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E5	2	9,4	-	0/2/15/18	0/1/1/1
6	FUB	E6	1	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	2	9,6	-	0/2/15/18	0/1/1/1
6	FUB	E6	3	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	4	9,6	-	2/2/15/18	0/1/1/1
6	FUB	E6	5	6	-	2/2/15/18	0/1/1/1
6	FUB	E6	6	9,6	-	0/2/15/18	0/1/1/1
6	FUB	E6	7	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	8	9,6	-	2/2/15/18	0/1/1/1
4	FUB	E7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E7	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	E8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E8	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	F5	1	4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	F5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	F6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	F6	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	F6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	F6	4	5,9	-	0/2/15/18	0/1/1/1
5	FUB	F7	1	5	-	0/2/15/18	0/1/1/1
5	FUB	F7	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	F7	3	5	-	0/2/15/18	0/1/1/1
5	FUB	F7	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	F8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F8	2	9,4	-	0/2/15/18	0/1/1/1
3	NAG	a1	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	a1	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a2	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	a2	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a3	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a3	2	3	-	0/6/23/26	0/1/1/1
7	34V	a4	1	7	1/1/3/3	0/2/15/19	0/1/1/1
7	FUB	a4	2	7,9	-	0/2/15/18	0/1/1/1
4	FUB	a5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	a5	2	9,4	-	1/2/15/18	0/1/1/1
5	FUB	a6	1	5	-	1/2/15/18	0/1/1/1
5	FUB	a6	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	a6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	a6	4	5,9	-	0/2/15/18	0/1/1/1
4	FUB	a7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	a7	2	9,4	-	2/2/15/18	0/1/1/1
5	FUB	a9	1	5	-	0/2/15/18	0/1/1/1
5	FUB	a9	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	a9	3	5	-	2/2/15/18	0/1/1/1
5	FUB	a9	4	5,9	-	2/2/15/18	0/1/1/1
4	FUB	b0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	b1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	b1	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	b3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	b3	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	b4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	b4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	b5	1	4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	b5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	b6	1	5	-	2/2/15/18	0/1/1/1
5	FUB	b6	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	b6	3	5	-	2/2/15/18	0/1/1/1
5	FUB	b6	4	5,9	-	2/2/15/18	0/1/1/1
4	FUB	b7	1	4	-	1/2/15/18	0/1/1/1
4	FUB	b7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	b9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b9	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c0	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c1	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c2	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c3	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c3	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c5	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c6	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	c8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c8	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	c9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c9	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	d1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d1	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	d2	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	d3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	d3	2	9,4	-	2/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	d4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d4	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d5	1	4	-	1/2/15/18	0/1/1/1
4	FUB	d5	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d6	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d6	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d8	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	d9	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d9	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	e0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e0	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	e1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e1	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e2	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e3	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e3	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e4	2	9,4	-	0/2/15/18	0/1/1/1
4	FUB	e5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e5	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e6	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e6	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e7	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	e8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e8	2	9,4	-	0/2/15/18	0/1/1/1
8	FUB	e9	1	8	-	1/2/15/18	0/1/1/1
8	FUB	e9	2	8,9	-	1/2/15/18	0/1/1/1
8	FUB	e9	3	8	-	2/2/15/18	0/1/1/1
8	FUB	e9	4	8,9	-	2/2/15/18	0/1/1/1
8	FUB	e9	5	8	-	2/2/15/18	0/1/1/1
8	FUB	e9	6	8,9	-	2/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	f0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f0	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	f2	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f2	2	9,4	-	2/2/15/18	0/1/1/1
4	FUB	f3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	f3	2	9,4	-	1/2/15/18	0/1/1/1
4	FUB	f5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f5	2	9,4	-	0/2/15/18	0/1/1/1
5	FUB	f6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	f6	2	5,9	-	1/2/15/18	0/1/1/1
5	FUB	f6	3	5	-	2/2/15/18	0/1/1/1
5	FUB	f6	4	5,9	-	2/2/15/18	0/1/1/1
5	FUB	f7	1	5	-	0/2/15/18	0/1/1/1
5	FUB	f7	2	5,9	-	2/2/15/18	0/1/1/1
5	FUB	f7	3	5	-	0/2/15/18	0/1/1/1
5	FUB	f7	4	5,9	-	2/2/15/18	0/1/1/1
4	FUB	f8	1	4	-	1/2/15/18	0/1/1/1
4	FUB	f8	2	9,4	-	0/2/15/18	0/1/1/1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f3	2	FUB	C2-C3	-2.49	1.49	1.53
4	c7	1	FUB	O4-C1	-2.48	1.38	1.43
4	d7	1	FUB	C2-C3	-2.46	1.49	1.53
4	e4	2	FUB	O4-C1	-2.45	1.38	1.43
4	e5	1	FUB	C2-C3	-2.44	1.49	1.53
4	d9	2	FUB	C2-C3	-2.43	1.49	1.53
4	c8	2	FUB	C2-C3	-2.43	1.49	1.53
4	b1	1	FUB	O4-C1	-2.42	1.38	1.43
4	e8	2	FUB	C2-C3	-2.42	1.49	1.53
4	b4	2	FUB	C2-C3	-2.42	1.49	1.53
4	d0	2	FUB	C2-C3	-2.41	1.49	1.53
4	c3	2	FUB	C2-C3	-2.41	1.49	1.53
4	b0	1	FUB	C2-C3	-2.40	1.49	1.53
4	b0	1	FUB	O4-C1	-2.39	1.38	1.43
5	a6	3	FUB	O4-C1	-2.37	1.38	1.43
4	c0	1	FUB	O4-C1	-2.36	1.38	1.43
4	c6	1	FUB	C2-C3	-2.35	1.49	1.53
5	b6	2	FUB	C2-C3	-2.35	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c2	1	FUB	C2-C3	-2.32	1.49	1.53
4	c1	1	FUB	C2-C3	-2.31	1.50	1.53
4	b3	2	FUB	O4-C1	-2.31	1.38	1.43
4	e6	2	FUB	C2-C3	-2.30	1.50	1.53
4	b4	1	FUB	C2-C3	-2.29	1.50	1.53
4	e1	2	FUB	C2-C3	-2.29	1.50	1.53
4	d0	2	FUB	C1-C2	2.29	1.55	1.51
4	c3	1	FUB	O4-C1	-2.28	1.38	1.43
4	e3	2	FUB	C2-C3	-2.27	1.50	1.53
4	c8	2	FUB	C1-C2	2.26	1.55	1.51
4	d8	2	FUB	C2-C3	-2.26	1.50	1.53
4	c9	2	FUB	O4-C1	-2.25	1.38	1.43
4	d5	2	FUB	C2-C3	-2.25	1.50	1.53
4	e7	2	FUB	C2-C3	-2.25	1.50	1.53
4	f0	2	FUB	C2-C3	-2.24	1.50	1.53
4	f2	2	FUB	C2-C3	-2.24	1.50	1.53
4	b1	1	FUB	C2-C3	-2.24	1.50	1.53
4	b0	2	FUB	C2-C3	-2.23	1.50	1.53
5	a6	4	FUB	C1-C2	2.22	1.55	1.51
4	e4	2	FUB	C2-C3	-2.20	1.50	1.53
4	e5	1	FUB	O4-C1	-2.20	1.39	1.43
5	f6	4	FUB	O4-C1	-2.20	1.39	1.43
4	a5	2	FUB	C2-C3	-2.20	1.50	1.53
4	d7	1	FUB	O4-C1	-2.19	1.39	1.43
4	c7	1	FUB	C2-C3	-2.19	1.50	1.53
4	b7	2	FUB	C2-C3	-2.18	1.50	1.53
4	e4	1	FUB	O4-C1	-2.18	1.39	1.43
4	c3	2	FUB	C1-C2	2.17	1.55	1.51
4	f8	2	FUB	O4-C1	-2.17	1.39	1.43
7	a4	2	FUB	O4-C1	-2.17	1.39	1.43
4	c0	2	FUB	C1-C2	2.17	1.55	1.51
4	d4	2	FUB	C2-C3	-2.17	1.50	1.53
4	d6	2	FUB	C2-C3	-2.16	1.50	1.53
4	e2	2	FUB	C2-C3	-2.15	1.50	1.53
5	a9	1	FUB	C2-C3	-2.15	1.50	1.53
5	f7	1	FUB	C2-C3	-2.15	1.50	1.53
5	f7	3	FUB	C2-C3	-2.14	1.50	1.53
5	a6	1	FUB	O4-C1	-2.13	1.39	1.43
4	d5	2	FUB	O4-C1	-2.13	1.39	1.43
4	f8	2	FUB	C2-C3	-2.11	1.50	1.53
4	d7	2	FUB	C2-C3	-2.11	1.50	1.53
5	b6	1	FUB	O4-C1	-2.10	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e5	2	FUB	C2-C3	-2.09	1.50	1.53
4	e3	2	FUB	C1-C2	2.09	1.55	1.51
4	e0	2	FUB	O4-C1	-2.09	1.39	1.43
5	a9	2	FUB	C2-C3	-2.08	1.50	1.53
4	c4	2	FUB	C2-C3	-2.08	1.50	1.53
4	c1	2	FUB	C1-C2	2.07	1.55	1.51
4	d8	2	FUB	C1-C2	2.07	1.55	1.51
4	d6	2	FUB	C1-C2	2.06	1.55	1.51
4	b7	2	FUB	C1-C2	2.06	1.55	1.51
5	b6	1	FUB	C2-C3	-2.06	1.50	1.53
5	f6	2	FUB	C2-C3	-2.06	1.50	1.53
4	e1	2	FUB	C1-C2	2.05	1.55	1.51
4	c6	1	FUB	O4-C1	-2.05	1.39	1.43
4	c9	2	FUB	C2-C3	-2.04	1.50	1.53
4	a7	2	FUB	C1-C2	2.04	1.55	1.51
4	c6	2	FUB	C1-C2	2.04	1.55	1.51
5	a9	4	FUB	C2-C3	-2.04	1.50	1.53
4	a5	2	FUB	C1-C2	2.04	1.55	1.51
4	c4	2	FUB	C1-C2	2.04	1.55	1.51
4	f0	2	FUB	C1-C2	2.04	1.55	1.51
4	b4	2	FUB	C1-C2	2.03	1.55	1.51
4	d4	2	FUB	C1-C2	2.03	1.55	1.51
5	b6	4	FUB	C2-C3	-2.03	1.50	1.53
4	f3	2	FUB	C1-C2	2.03	1.55	1.51
4	f2	2	FUB	C1-C2	2.03	1.55	1.51
4	d9	2	FUB	C1-C2	2.02	1.55	1.51
4	c1	1	FUB	O4-C1	-2.02	1.39	1.43
4	d3	2	FUB	C2-C3	-2.02	1.50	1.53
4	e8	2	FUB	C1-C2	2.01	1.55	1.51
7	a4	2	FUB	C2-C3	-2.01	1.50	1.53
5	b6	2	FUB	C1-C2	2.01	1.55	1.51
4	e7	2	FUB	C1-C2	2.01	1.55	1.51
4	f5	2	FUB	O4-C1	-2.01	1.39	1.43
4	a7	2	FUB	C2-C3	-2.00	1.50	1.53
5	f7	3	FUB	O4-C1	-2.00	1.39	1.43
5	b6	3	FUB	C2-C3	-2.00	1.50	1.53

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a3	1	NAG	O5-C1-C2	-4.39	104.35	111.29
8	e9	2	FUB	O4-C4-C3	-4.21	100.98	104.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	e9	4	FUB	O4-C4-C3	-3.96	101.20	104.70
3	a3	2	NAG	C1-O5-C5	3.52	116.96	112.19
5	a6	2	FUB	O4-C4-C3	-3.27	101.81	104.70
5	f7	2	FUB	O4-C4-C3	-3.14	101.93	104.70
5	f7	4	FUB	O4-C4-C3	-3.10	101.96	104.70
5	f6	4	FUB	O4-C4-C3	3.04	107.40	104.70
4	b0	1	FUB	C5-C4-C3	-3.03	107.79	115.09
3	A2	1	NAG	C2-N2-C7	3.00	127.18	122.90
3	a2	1	NAG	C2-N2-C7	2.94	127.09	122.90
4	e5	1	FUB	C5-C4-C3	-2.91	108.07	115.09
4	d7	1	FUB	C5-C4-C3	-2.90	108.08	115.09
4	b3	2	FUB	O4-C4-C3	2.89	107.26	104.70
3	a3	1	NAG	C4-C3-C2	-2.88	106.80	111.02
4	c0	2	FUB	O4-C4-C3	-2.79	102.24	104.70
4	c7	1	FUB	O4-C4-C3	2.76	107.15	104.70
4	b1	1	FUB	C5-C4-C3	-2.74	108.48	115.09
4	d1	2	FUB	C1-C2-C3	2.73	105.79	101.63
4	e1	2	FUB	C5-C4-C3	-2.72	108.52	115.09
4	c6	1	FUB	C5-C4-C3	-2.71	108.56	115.09
4	c9	2	FUB	O4-C4-C3	2.69	107.09	104.70
7	a4	2	FUB	C5-C4-C3	-2.67	108.64	115.09
8	e9	6	FUB	O4-C4-C3	-2.65	102.36	104.70
4	d1	2	FUB	C1-O4-C4	2.63	114.30	108.16
4	e2	1	FUB	C5-C4-C3	-2.63	108.75	115.09
4	f5	2	FUB	O4-C4-C3	2.61	107.02	104.70
4	c4	1	FUB	C5-C4-C3	-2.61	108.80	115.09
4	f8	1	FUB	C5-C4-C3	-2.60	108.81	115.09
4	c9	2	FUB	C5-C4-C3	-2.60	108.83	115.09
4	c3	1	FUB	O4-C4-C3	2.59	106.99	104.70
5	f7	1	FUB	C5-C4-C3	-2.58	108.86	115.09
3	a3	2	NAG	O5-C1-C2	-2.58	107.21	111.29
4	f8	2	FUB	C5-C4-C3	-2.57	108.89	115.09
4	b3	2	FUB	C5-C4-C3	-2.57	108.89	115.09
4	b4	2	FUB	C5-C4-C3	-2.57	108.90	115.09
5	a9	1	FUB	C5-C4-C3	-2.56	108.91	115.09
4	b5	2	FUB	C5-C4-C3	-2.55	108.95	115.09
4	f5	1	FUB	C5-C4-C3	-2.54	108.96	115.09
4	c9	1	FUB	C5-C4-C3	-2.54	108.96	115.09
4	c0	1	FUB	O4-C4-C3	2.54	106.95	104.70
4	f3	2	FUB	C5-C4-C3	-2.53	108.98	115.09
5	f6	4	FUB	C5-C4-C3	-2.52	109.02	115.09
4	c0	1	FUB	C5-C4-C3	-2.51	109.03	115.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b6	3	FUB	C5-C4-C3	-2.51	109.04	115.09
4	d2	2	FUB	C5-C4-C3	-2.51	109.04	115.09
5	a6	4	FUB	O4-C4-C3	-2.51	102.49	104.70
4	b5	1	FUB	C5-C4-C3	-2.50	109.06	115.09
5	b6	4	FUB	C5-C4-C3	-2.50	109.06	115.09
4	e7	2	FUB	C5-C4-C3	-2.49	109.08	115.09
5	f7	3	FUB	C5-C4-C3	-2.49	109.08	115.09
3	A3	1	NAG	O5-C1-C2	-2.49	107.36	111.29
4	e3	2	FUB	C5-C4-C3	-2.49	109.09	115.09
4	d8	2	FUB	C5-C4-C3	-2.49	109.09	115.09
4	f0	2	FUB	C5-C4-C3	-2.49	109.09	115.09
4	f8	2	FUB	O4-C4-C3	2.48	106.90	104.70
4	f5	2	FUB	C5-C4-C3	-2.48	109.11	115.09
4	d0	2	FUB	C5-C4-C3	-2.48	109.11	115.09
4	c8	2	FUB	C5-C4-C3	-2.47	109.12	115.09
4	e6	2	FUB	C5-C4-C3	-2.47	109.12	115.09
4	f2	2	FUB	C5-C4-C3	-2.47	109.13	115.09
4	e8	2	FUB	C5-C4-C3	-2.47	109.14	115.09
4	b0	2	FUB	C5-C4-C3	-2.46	109.14	115.09
4	c1	2	FUB	C5-C4-C3	-2.46	109.16	115.09
4	b7	2	FUB	C5-C4-C3	-2.46	109.16	115.09
4	d9	2	FUB	C5-C4-C3	-2.46	109.16	115.09
4	e0	2	FUB	O4-C4-C3	2.45	106.88	104.70
4	e0	2	FUB	C5-C4-C3	-2.45	109.18	115.09
4	b1	2	FUB	C5-C4-C3	-2.45	109.19	115.09
4	b1	1	FUB	O4-C4-C3	2.44	106.87	104.70
4	b7	1	FUB	C5-C4-C3	-2.44	109.20	115.09
4	c4	2	FUB	C5-C4-C3	-2.44	109.21	115.09
4	d3	1	FUB	C5-C4-C3	-2.43	109.22	115.09
4	c7	2	FUB	C5-C4-C3	-2.43	109.23	115.09
4	a7	2	FUB	C5-C4-C3	-2.43	109.24	115.09
5	f6	2	FUB	C5-C4-C3	-2.42	109.25	115.09
5	f6	1	FUB	C5-C4-C3	-2.41	109.28	115.09
4	c1	1	FUB	C5-C4-C3	-2.39	109.32	115.09
4	d5	2	FUB	C5-C4-C3	-2.38	109.35	115.09
4	c2	2	FUB	C5-C4-C3	-2.37	109.36	115.09
4	c6	2	FUB	C5-C4-C3	-2.37	109.36	115.09
4	c2	1	FUB	C5-C4-C3	-2.37	109.38	115.09
4	c3	1	FUB	C5-C4-C3	-2.36	109.41	115.09
4	e0	1	FUB	C5-C4-C3	-2.35	109.42	115.09
4	d4	2	FUB	C5-C4-C3	-2.34	109.44	115.09
4	d6	2	FUB	C5-C4-C3	-2.34	109.45	115.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b6	1	FUB	C5-C4-C3	-2.33	109.47	115.09
8	e9	5	FUB	C5-C4-C3	-2.33	109.47	115.09
5	a6	3	FUB	O4-C4-C3	2.32	106.76	104.70
4	c7	1	FUB	C5-C4-C3	-2.32	109.49	115.09
4	B0	1	FUB	O4-C4-C3	2.32	106.76	104.70
4	E4	1	FUB	O5-C5-C4	2.32	119.24	111.29
4	b9	1	FUB	C5-C4-C3	-2.31	109.51	115.09
4	c3	2	FUB	C5-C4-C3	-2.31	109.51	115.09
4	D1	1	FUB	O4-C4-C3	2.28	106.73	104.70
4	d2	1	FUB	C5-C4-C3	-2.28	109.58	115.09
4	c5	1	FUB	C5-C4-C3	-2.28	109.59	115.09
4	b3	1	FUB	C5-C4-C3	-2.28	109.60	115.09
4	b9	2	FUB	C5-C4-C3	-2.26	109.64	115.09
4	a5	2	FUB	C5-C4-C3	-2.26	109.65	115.09
8	e9	1	FUB	C5-C4-C3	-2.24	109.70	115.09
4	d3	2	FUB	C5-C4-C3	-2.23	109.70	115.09
4	e8	1	FUB	C5-C4-C3	-2.22	109.73	115.09
3	A1	1	NAG	O5-C1-C2	-2.21	107.79	111.29
4	d9	1	FUB	C5-C4-C3	-2.21	109.77	115.09
4	b0	1	FUB	O4-C4-C3	2.19	106.65	104.70
4	e5	2	FUB	C5-C4-C3	-2.18	109.83	115.09
4	e4	2	FUB	O4-C4-C3	2.17	106.63	104.70
4	d7	2	FUB	C5-C4-C3	-2.17	109.85	115.09
4	d1	2	FUB	C5-C4-C3	-2.17	109.85	115.09
5	a9	4	FUB	C5-C4-C3	-2.17	109.86	115.09
4	e1	1	FUB	C5-C4-C3	-2.16	109.87	115.09
4	f3	1	FUB	C5-C4-C3	-2.16	109.88	115.09
4	c5	2	FUB	C5-C4-C3	-2.15	109.89	115.09
8	e9	3	FUB	C5-C4-C3	-2.14	109.93	115.09
3	A2	1	NAG	O5-C1-C2	-2.13	107.93	111.29
4	d5	1	FUB	C5-C4-C3	-2.12	109.97	115.09
4	c9	1	FUB	O4-C4-C3	2.12	106.58	104.70
4	d0	1	FUB	C5-C4-C3	-2.10	110.02	115.09
4	e2	2	FUB	C5-C4-C3	-2.09	110.04	115.09
4	c8	1	FUB	C5-C4-C3	-2.09	110.05	115.09
4	b4	1	FUB	C5-C4-C3	-2.09	110.06	115.09
5	b6	2	FUB	C5-C4-C3	-2.08	110.06	115.09
7	a4	2	FUB	O4-C4-C3	2.08	106.55	104.70
5	f6	3	FUB	C5-C4-C3	-2.07	110.09	115.09
3	a1	1	NAG	O5-C1-C2	-2.04	108.06	111.29
4	d4	1	FUB	C5-C4-C3	-2.04	110.17	115.09
4	e4	1	FUB	O4-C4-C3	2.04	106.51	104.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c0	2	FUB	C5-C4-C3	-2.04	110.17	115.09
4	d6	1	FUB	C5-C4-C3	-2.03	110.19	115.09
4	E4	2	FUB	C1-C2-C3	2.03	104.72	101.63
7	a4	1	34V	O5-C2-C3	-2.02	102.92	104.70
8	e9	6	FUB	C5-C4-C3	-2.02	110.23	115.09
4	d1	2	FUB	O4-C4-C3	2.01	106.48	104.70
4	e4	2	FUB	O4-C1-C2	-2.01	102.11	105.99
4	A7	2	FUB	O4-C4-C3	2.00	106.48	104.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	a4	1	34V	C3

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	b4	1	FUB	O4-C4-C5-O5
4	b4	1	FUB	C3-C4-C5-O5
4	c3	1	FUB	C3-C4-C5-O5
4	c7	1	FUB	O4-C4-C5-O5
4	c7	1	FUB	C3-C4-C5-O5
4	d1	2	FUB	O4-C4-C5-O5
4	d4	1	FUB	C3-C4-C5-O5
4	d6	1	FUB	C3-C4-C5-O5
5	b6	1	FUB	C3-C4-C5-O5
5	b6	4	FUB	O4-C4-C5-O5
5	f6	4	FUB	O4-C4-C5-O5
4	c3	1	FUB	O4-C4-C5-O5
4	d4	1	FUB	O4-C4-C5-O5
4	d6	1	FUB	O4-C4-C5-O5
5	b6	1	FUB	O4-C4-C5-O5
4	a7	2	FUB	C3-C4-C5-O5
4	c1	1	FUB	C3-C4-C5-O5
4	c7	2	FUB	C3-C4-C5-O5
4	d1	2	FUB	C3-C4-C5-O5
4	e1	1	FUB	C3-C4-C5-O5
5	a9	3	FUB	C3-C4-C5-O5
5	b6	3	FUB	C3-C4-C5-O5
5	f6	3	FUB	C3-C4-C5-O5
8	e9	3	FUB	C3-C4-C5-O5
8	e9	5	FUB	C3-C4-C5-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C9	1	FUB	O4-C4-C5-O5
4	b9	2	FUB	O4-C4-C5-O5
4	c8	1	FUB	O4-C4-C5-O5
4	e1	2	FUB	O4-C4-C5-O5
4	f5	1	FUB	O4-C4-C5-O5
4	d0	1	FUB	O4-C4-C5-O5
5	a9	3	FUB	O4-C4-C5-O5
5	b6	3	FUB	O4-C4-C5-O5
5	f6	3	FUB	O4-C4-C5-O5
5	f7	2	FUB	O4-C4-C5-O5
5	f7	4	FUB	O4-C4-C5-O5
8	e9	3	FUB	O4-C4-C5-O5
4	b9	2	FUB	C3-C4-C5-O5
4	c1	2	FUB	C3-C4-C5-O5
4	e8	1	FUB	C3-C4-C5-O5
4	f5	1	FUB	C3-C4-C5-O5
4	d9	1	FUB	C3-C4-C5-O5
5	a6	2	FUB	C3-C4-C5-O5
5	b6	4	FUB	C3-C4-C5-O5
5	f6	4	FUB	C3-C4-C5-O5
4	d4	2	FUB	O4-C4-C5-O5
4	e8	1	FUB	O4-C4-C5-O5
4	f0	2	FUB	O4-C4-C5-O5
4	f2	2	FUB	O4-C4-C5-O5
4	e7	2	FUB	O4-C4-C5-O5
4	e6	2	FUB	O4-C4-C5-O5
4	e3	2	FUB	O4-C4-C5-O5
4	d9	1	FUB	O4-C4-C5-O5
4	d8	2	FUB	O4-C4-C5-O5
4	d6	2	FUB	O4-C4-C5-O5
4	b7	2	FUB	C3-C4-C5-O5
4	c9	2	FUB	C3-C4-C5-O5
4	d3	2	FUB	C3-C4-C5-O5
4	d4	2	FUB	C3-C4-C5-O5
4	d5	2	FUB	C3-C4-C5-O5
4	f0	2	FUB	C3-C4-C5-O5
4	f2	2	FUB	C3-C4-C5-O5
4	e7	2	FUB	C3-C4-C5-O5
4	e6	2	FUB	C3-C4-C5-O5
4	e3	2	FUB	C3-C4-C5-O5
4	d8	2	FUB	C3-C4-C5-O5
4	d6	2	FUB	C3-C4-C5-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F7	2	FUB	C3-C4-C5-O5
5	f7	2	FUB	C3-C4-C5-O5
5	f7	4	FUB	C3-C4-C5-O5
8	e9	4	FUB	C3-C4-C5-O5
4	a7	2	FUB	O4-C4-C5-O5
4	c1	1	FUB	O4-C4-C5-O5
4	c1	2	FUB	O4-C4-C5-O5
4	c7	2	FUB	O4-C4-C5-O5
4	e1	1	FUB	O4-C4-C5-O5
4	f0	1	FUB	O4-C4-C5-O5
4	f2	1	FUB	O4-C4-C5-O5
4	e7	1	FUB	O4-C4-C5-O5
4	e6	1	FUB	O4-C4-C5-O5
4	e3	1	FUB	O4-C4-C5-O5
4	d8	1	FUB	O4-C4-C5-O5
8	e9	5	FUB	O4-C4-C5-O5
4	C9	1	FUB	C3-C4-C5-O5
4	b1	1	FUB	C3-C4-C5-O5
4	c3	2	FUB	C3-C4-C5-O5
4	e1	2	FUB	C3-C4-C5-O5
6	E6	8	FUB	C3-C4-C5-O5
4	c8	1	FUB	C3-C4-C5-O5
4	e5	1	FUB	C3-C4-C5-O5
4	d7	1	FUB	C3-C4-C5-O5
4	d0	1	FUB	C3-C4-C5-O5
4	a5	1	FUB	O4-C4-C5-O5
4	c2	1	FUB	O4-C4-C5-O5
4	d5	2	FUB	O4-C4-C5-O5
5	F7	2	FUB	O4-C4-C5-O5
5	a6	2	FUB	O4-C4-C5-O5
5	a9	4	FUB	O4-C4-C5-O5
8	e9	6	FUB	O4-C4-C5-O5
4	d1	1	FUB	C3-C4-C5-O5
3	a3	1	NAG	C4-C5-C6-O6
4	E0	1	FUB	O4-C4-C5-O5
4	c9	2	FUB	O4-C4-C5-O5
6	E6	5	FUB	O4-C4-C5-O5
4	D6	2	FUB	O4-C4-C5-O5
4	b7	2	FUB	O4-C4-C5-O5
4	c0	2	FUB	O4-C4-C5-O5
4	d3	2	FUB	O4-C4-C5-O5
4	f3	1	FUB	O4-C4-C5-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	a9	2	FUB	O4-C4-C5-O5
6	E6	8	FUB	O4-C4-C5-O5
8	e9	4	FUB	O4-C4-C5-O5
4	D6	2	FUB	C3-C4-C5-O5
4	a5	1	FUB	C3-C4-C5-O5
4	c5	2	FUB	C3-C4-C5-O5
4	e5	2	FUB	C3-C4-C5-O5
4	f0	1	FUB	C3-C4-C5-O5
4	f2	1	FUB	C3-C4-C5-O5
4	e7	1	FUB	C3-C4-C5-O5
4	e6	1	FUB	C3-C4-C5-O5
4	e3	1	FUB	C3-C4-C5-O5
4	d7	2	FUB	C3-C4-C5-O5
4	d8	1	FUB	C3-C4-C5-O5
5	b6	2	FUB	C3-C4-C5-O5
4	c3	2	FUB	O4-C4-C5-O5
4	E0	1	FUB	C3-C4-C5-O5
6	E6	5	FUB	C3-C4-C5-O5
4	a5	2	FUB	O4-C4-C5-O5
4	b1	1	FUB	O4-C4-C5-O5
4	e2	2	FUB	C3-C4-C5-O5
4	c2	1	FUB	C3-C4-C5-O5
5	a9	4	FUB	C3-C4-C5-O5
4	E4	1	FUB	O4-C4-C5-O5
4	e5	1	FUB	O4-C4-C5-O5
4	d7	1	FUB	O4-C4-C5-O5
4	D4	1	FUB	O4-C4-C5-O5
4	b3	1	FUB	O4-C4-C5-O5
4	D4	1	FUB	C3-C4-C5-O5
8	e9	6	FUB	C3-C4-C5-O5
6	E6	4	FUB	O4-C4-C5-O5
8	e9	2	FUB	O4-C4-C5-O5
4	c5	2	FUB	O4-C4-C5-O5
4	e5	2	FUB	O4-C4-C5-O5
4	d7	2	FUB	O4-C4-C5-O5
4	f3	2	FUB	O4-C4-C5-O5
5	b6	2	FUB	O4-C4-C5-O5
4	d1	1	FUB	O4-C4-C5-O5
6	E6	4	FUB	C3-C4-C5-O5
4	D8	2	FUB	O4-C4-C5-O5
5	F6	2	FUB	O4-C4-C5-O5
3	A1	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

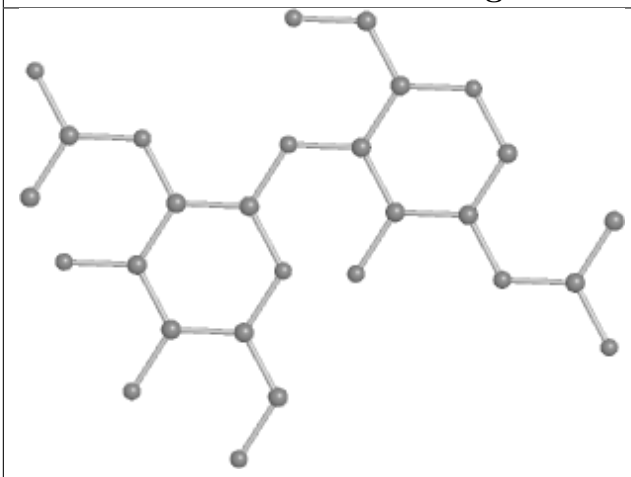
Mol	Chain	Res	Type	Atoms
4	e2	2	FUB	O4-C4-C5-O5
5	f6	2	FUB	O4-C4-C5-O5
4	E4	1	FUB	C3-C4-C5-O5
5	a6	1	FUB	C3-C4-C5-O5
3	a3	1	NAG	O5-C5-C6-O6
4	b7	1	FUB	C3-C4-C5-O5
4	c0	2	FUB	C3-C4-C5-O5
3	a2	1	NAG	C3-C2-N2-C7
5	a9	2	FUB	C3-C4-C5-O5
8	e9	1	FUB	C3-C4-C5-O5
4	C5	2	FUB	O4-C4-C5-O5
4	d3	1	FUB	C3-C4-C5-O5
5	F6	2	FUB	C3-C4-C5-O5
4	D8	2	FUB	C3-C4-C5-O5
4	d5	1	FUB	C3-C4-C5-O5
4	f8	1	FUB	O4-C4-C5-O5
3	A2	1	NAG	C3-C2-N2-C7

There are no ring outliers.

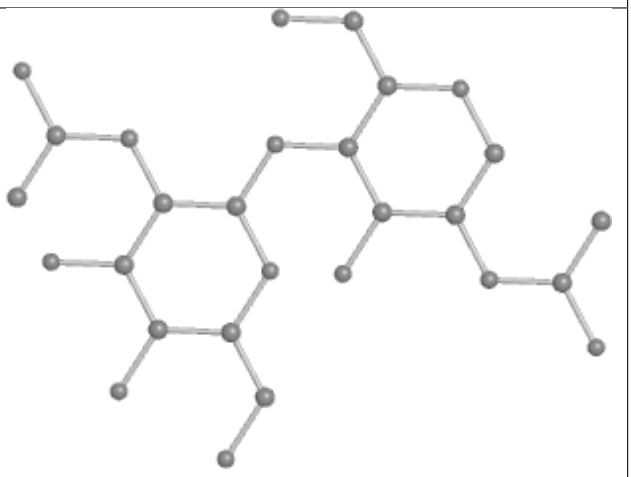
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

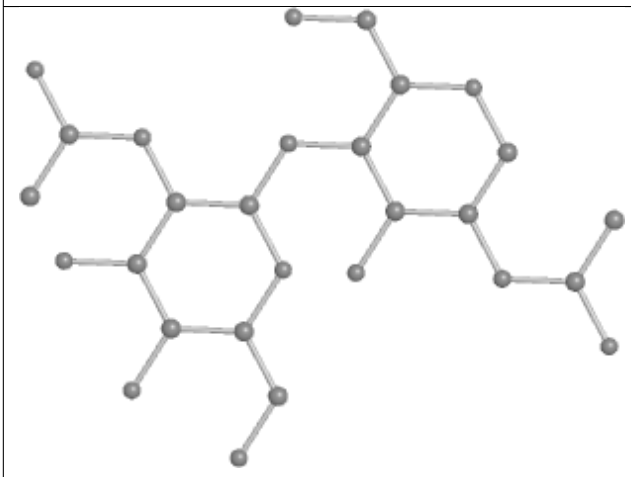
Oligosaccharide Chain A1



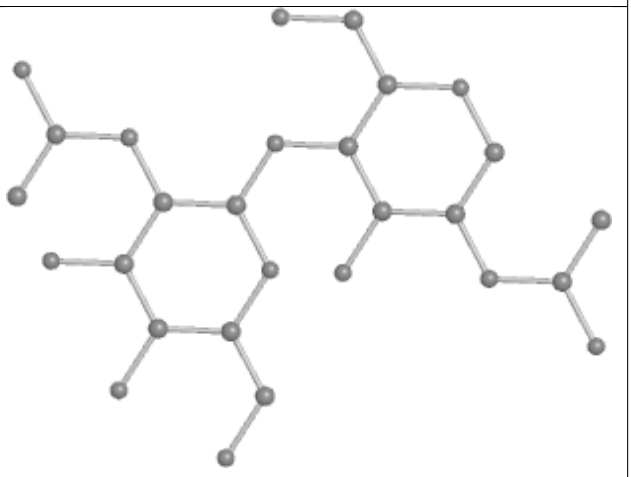
Bond lengths



Bond angles

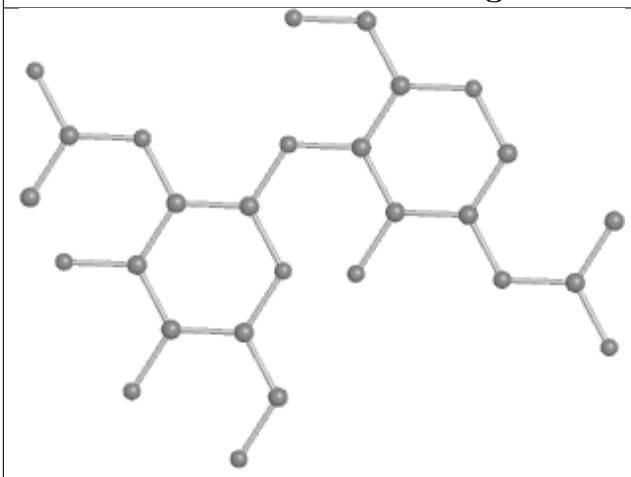


Torsions

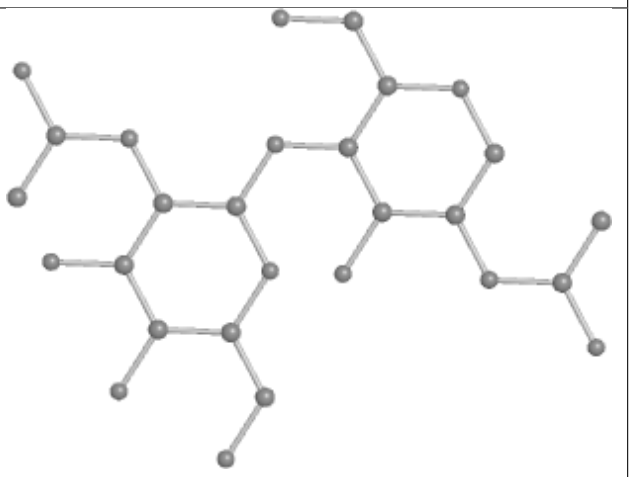


Rings

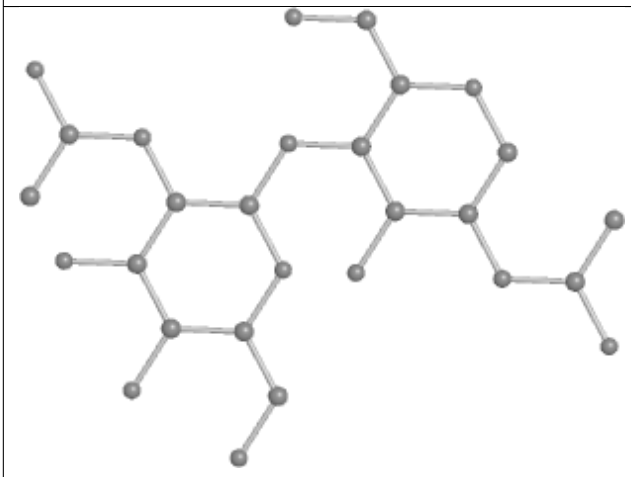
Oligosaccharide Chain A2



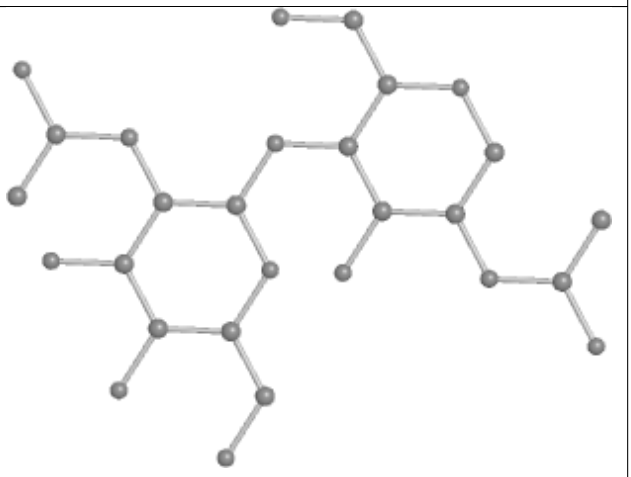
Bond lengths



Bond angles

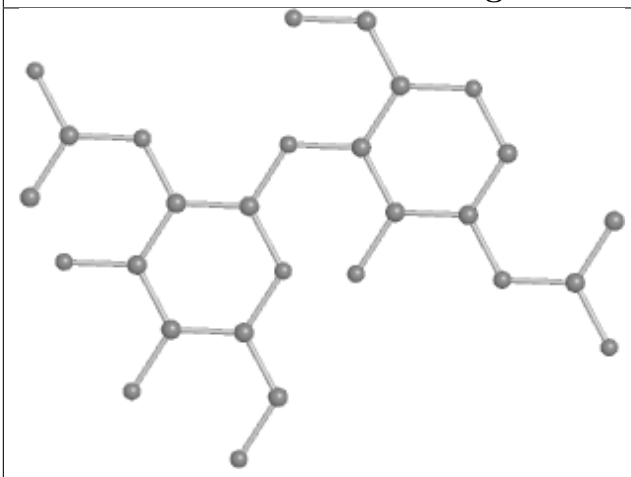


Torsions

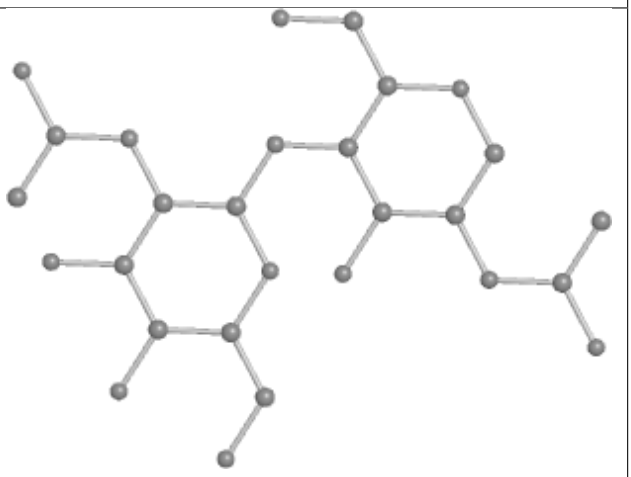


Rings

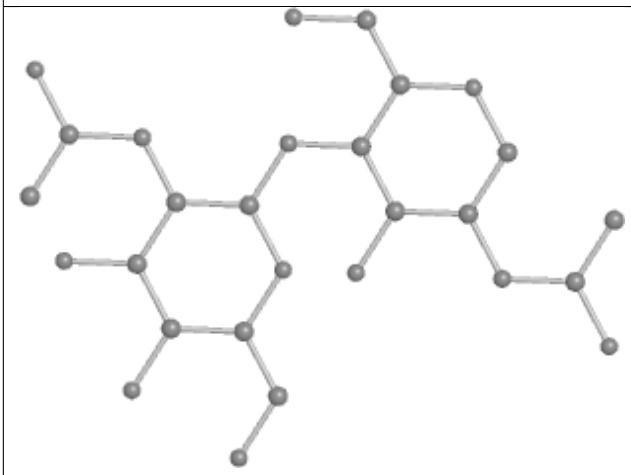
Oligosaccharide Chain A3



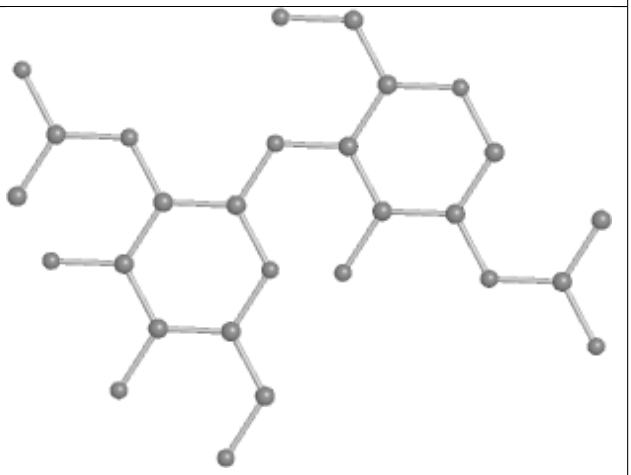
Bond lengths



Bond angles

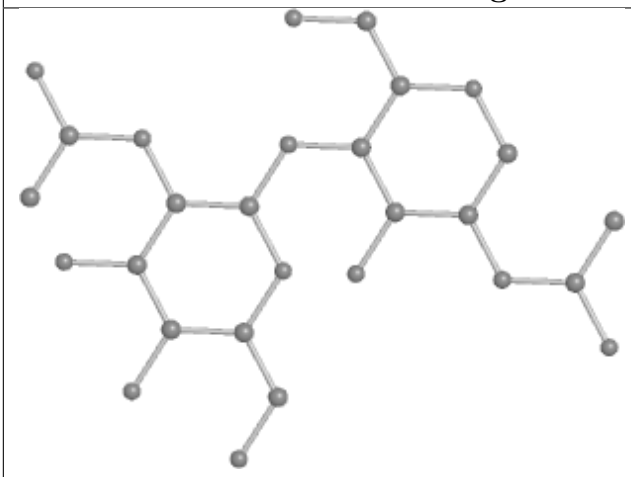


Torsions

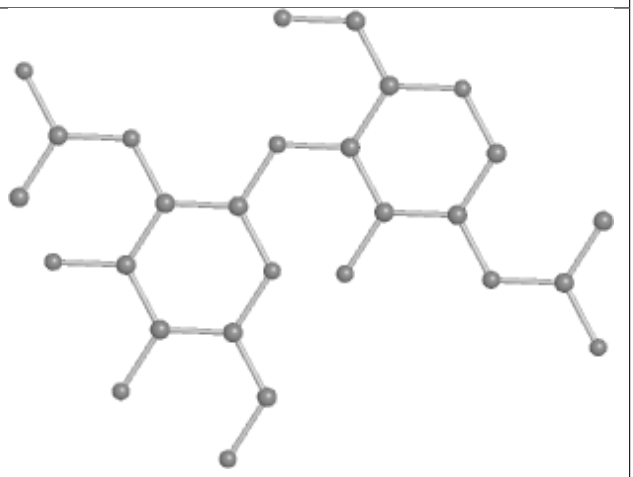


Rings

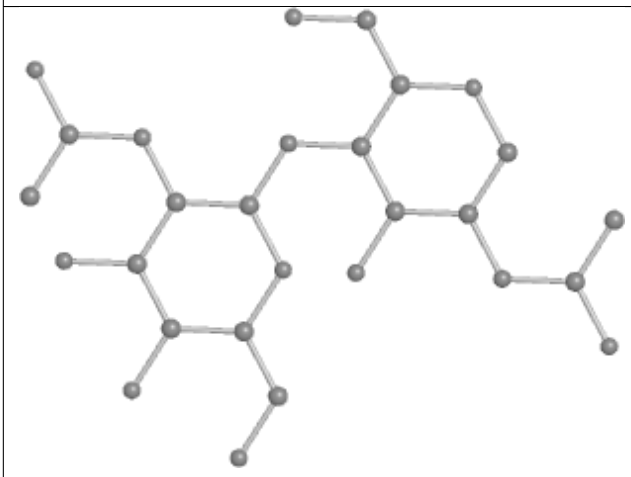
Oligosaccharide Chain a1



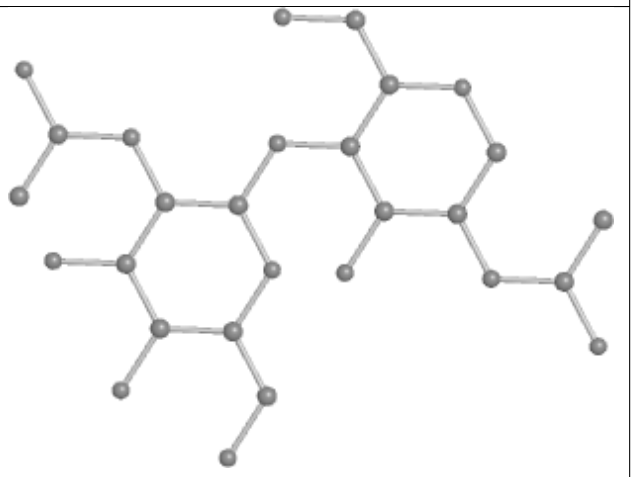
Bond lengths



Bond angles

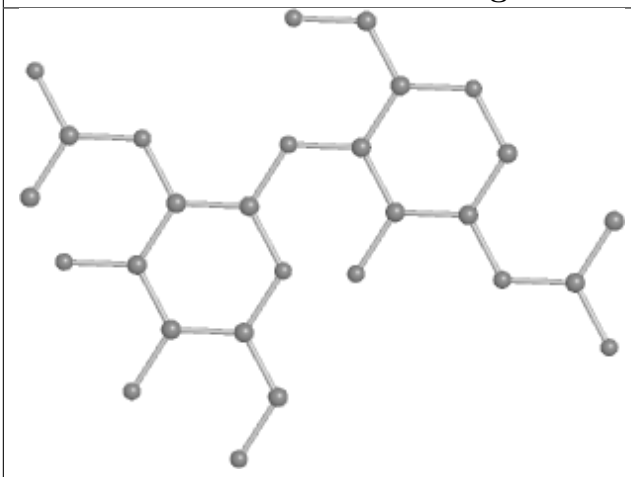


Torsions

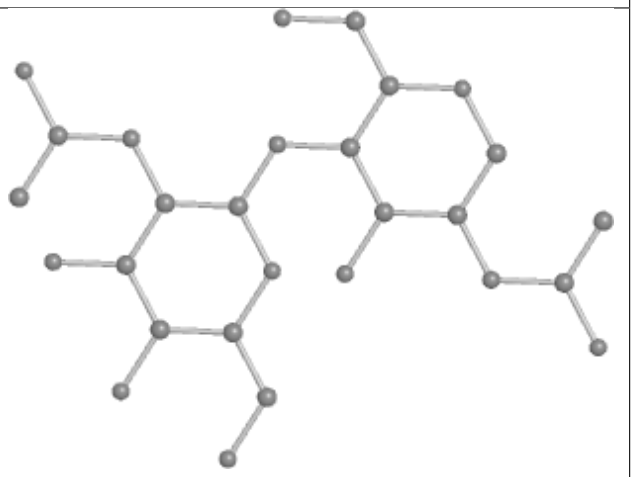


Rings

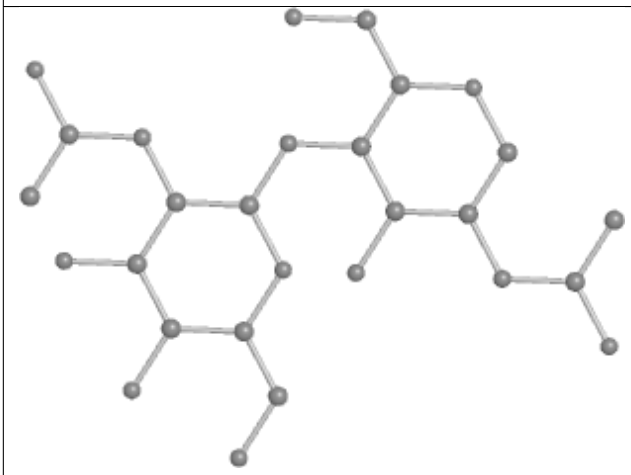
Oligosaccharide Chain a2



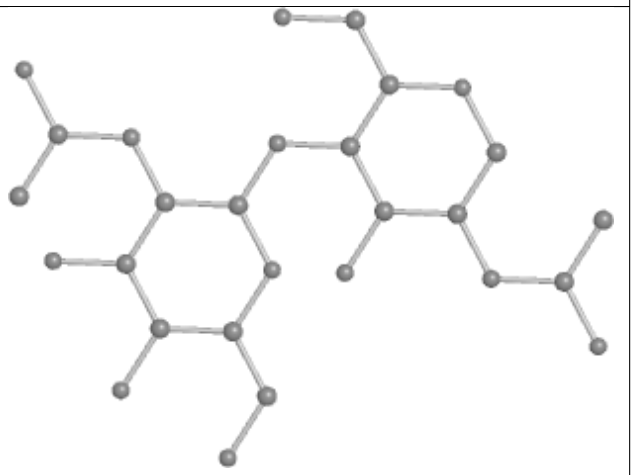
Bond lengths



Bond angles

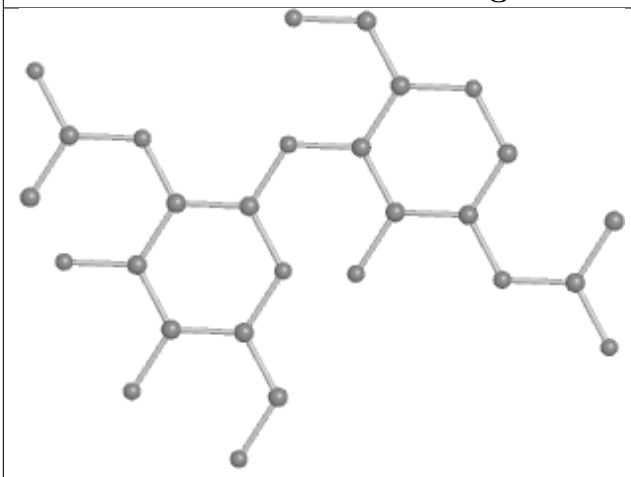


Torsions

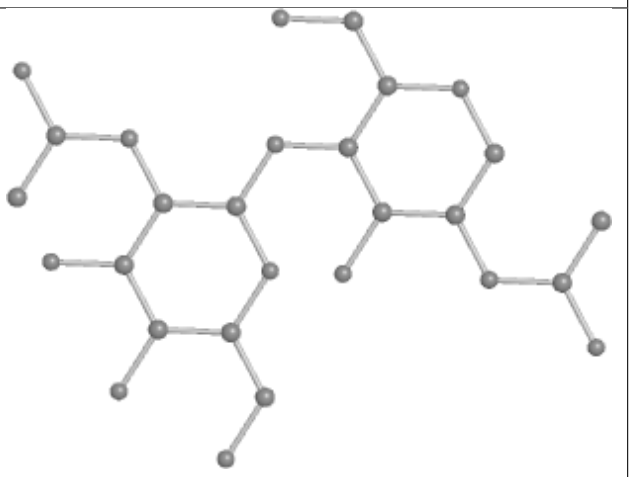


Rings

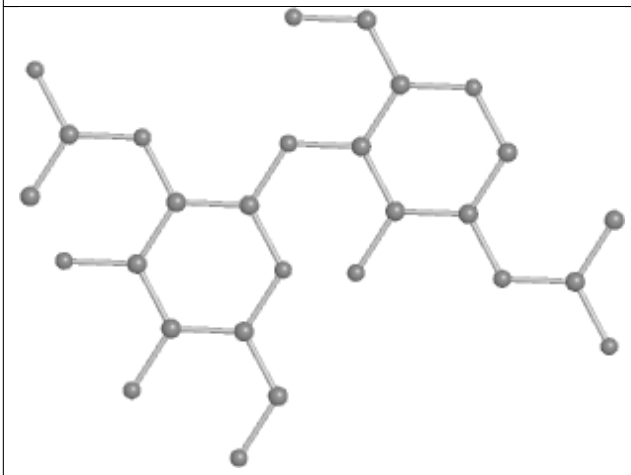
Oligosaccharide Chain a3



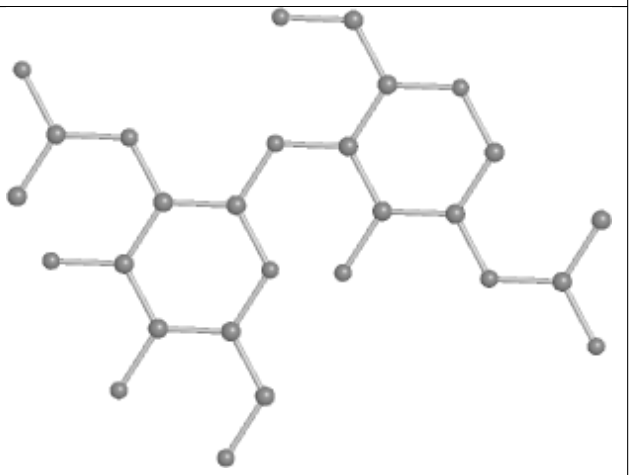
Bond lengths



Bond angles

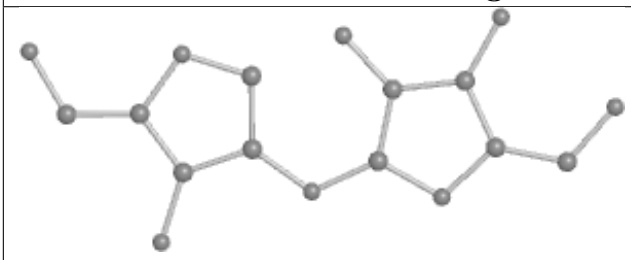


Torsions

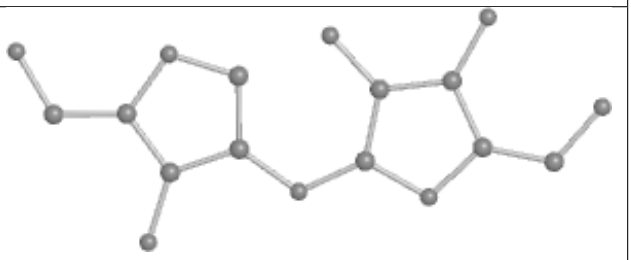


Rings

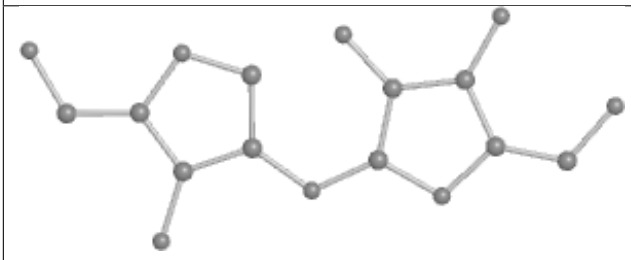
Oligosaccharide Chain A4



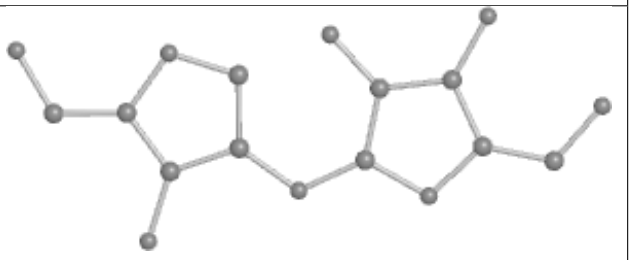
Bond lengths



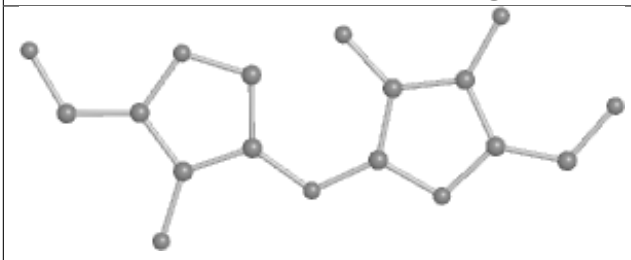
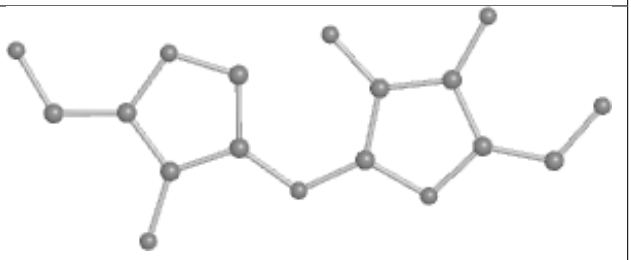
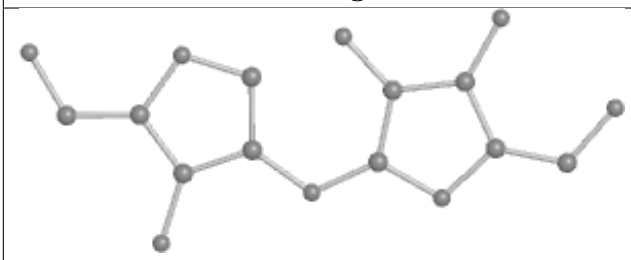
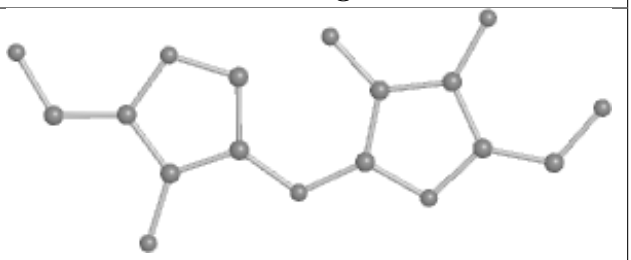
Bond angles

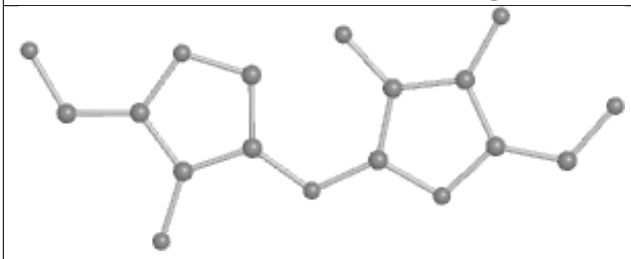
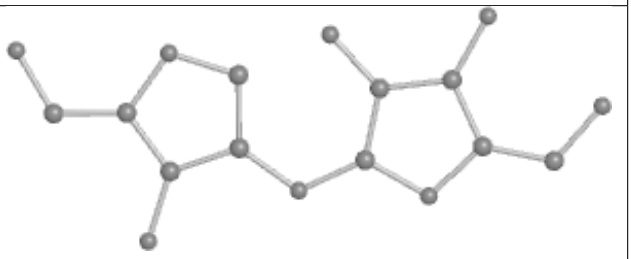
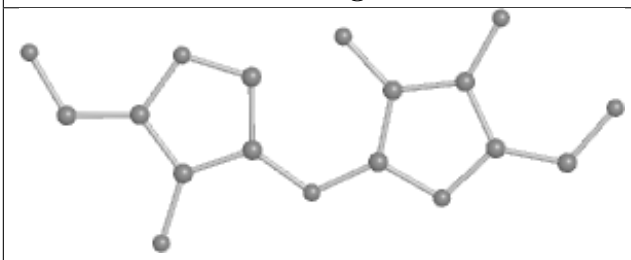
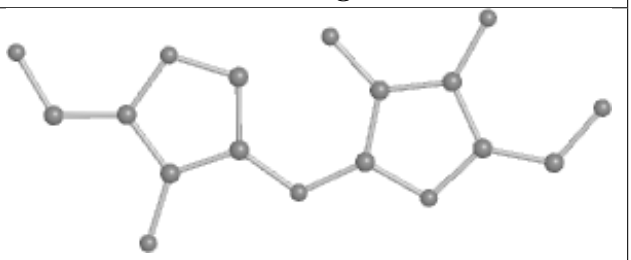


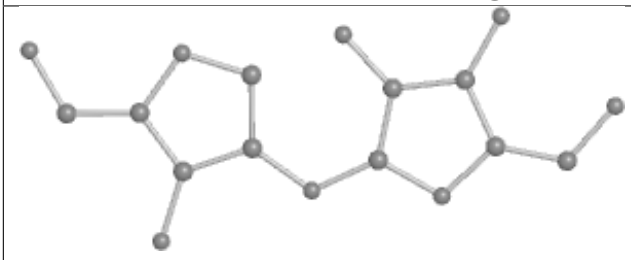
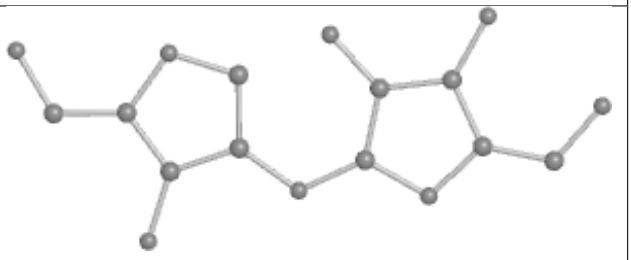
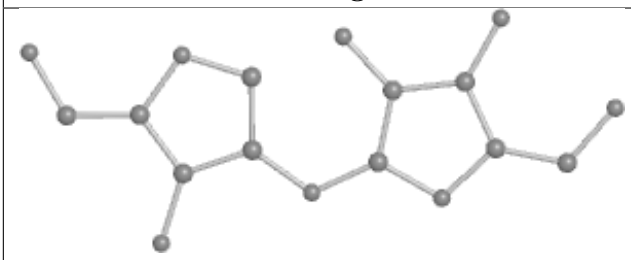
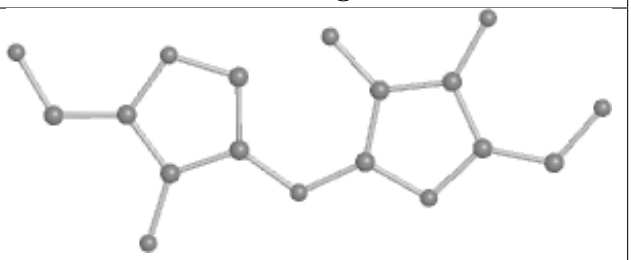
Torsions

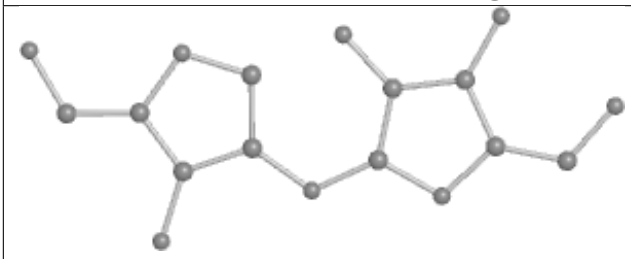
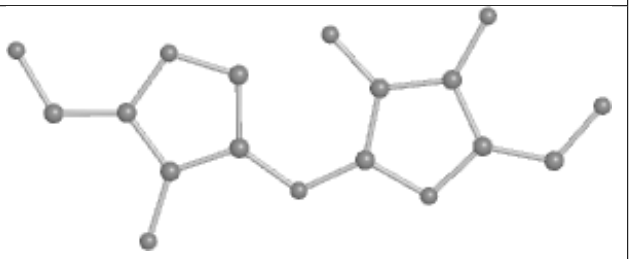
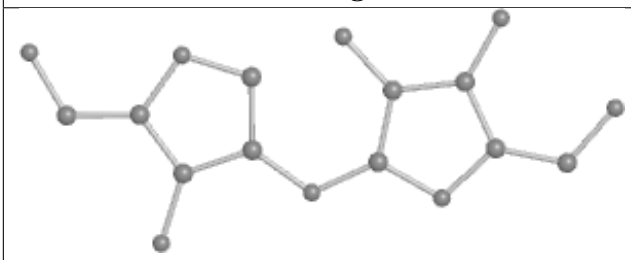
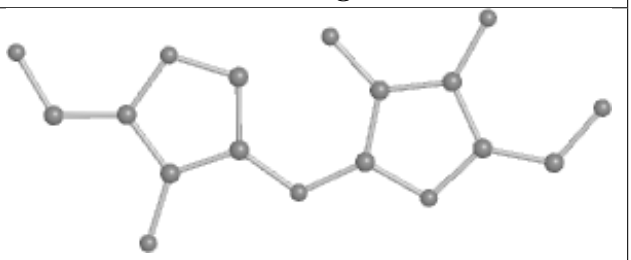


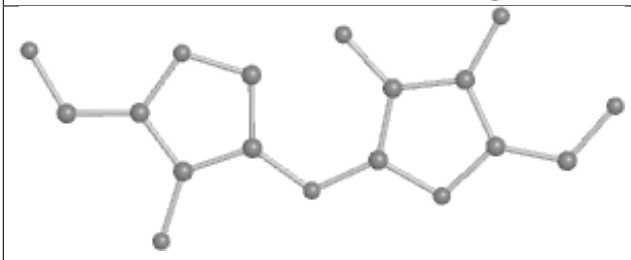
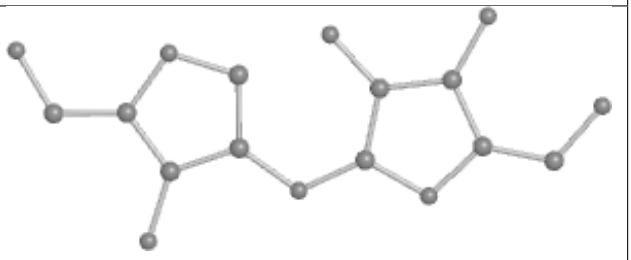
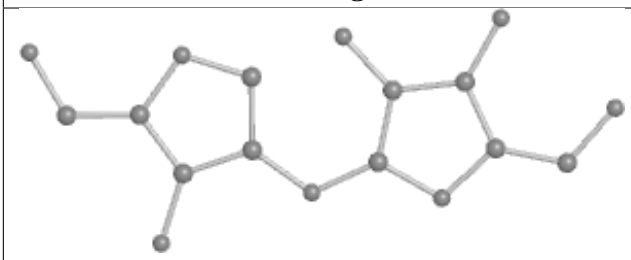
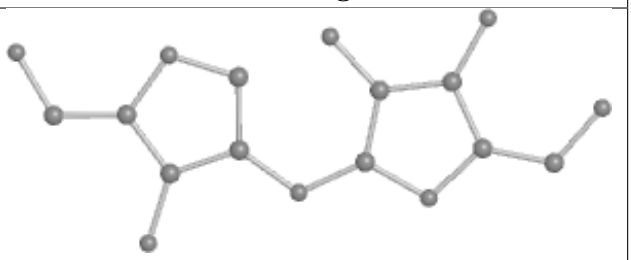
Rings

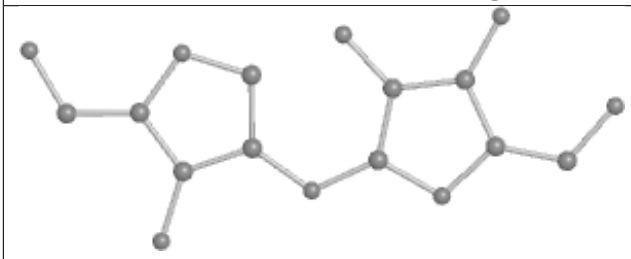
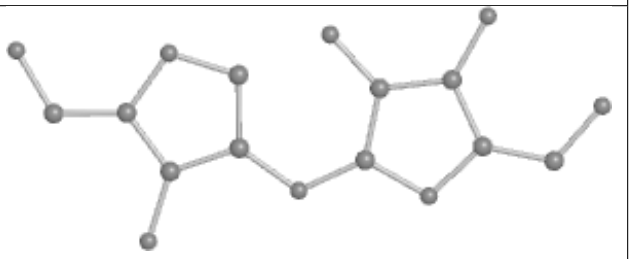
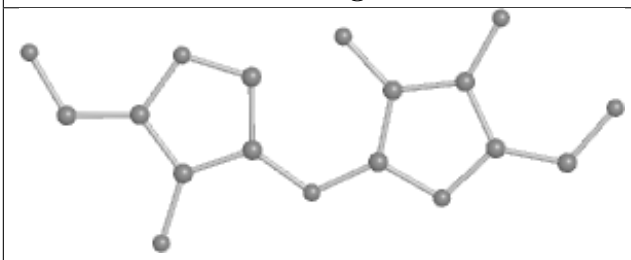
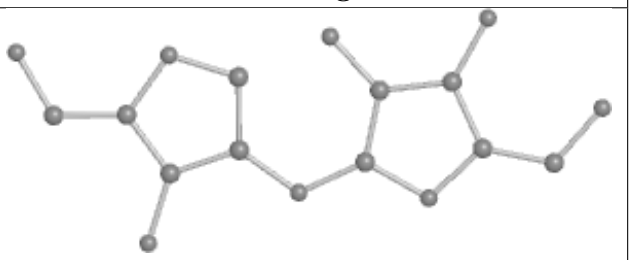
Oligosaccharide Chain A5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

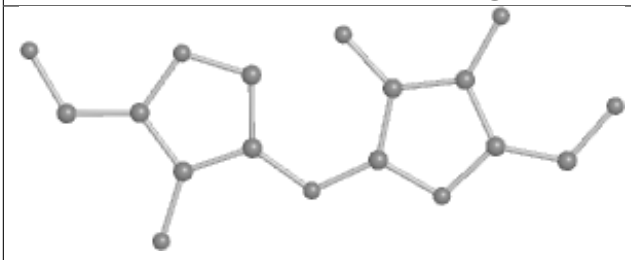
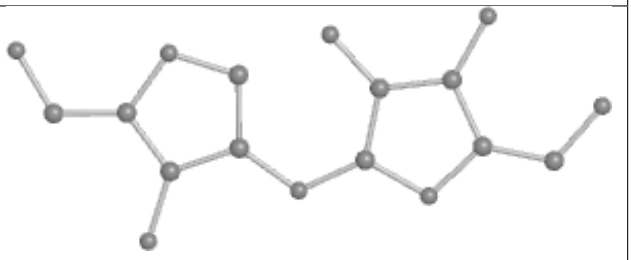
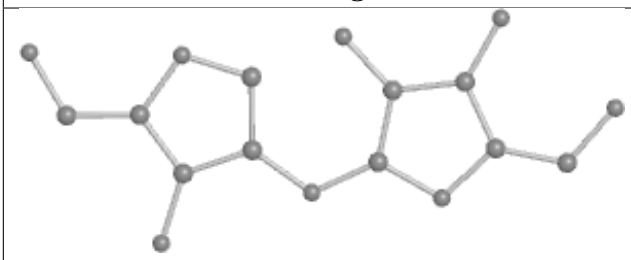
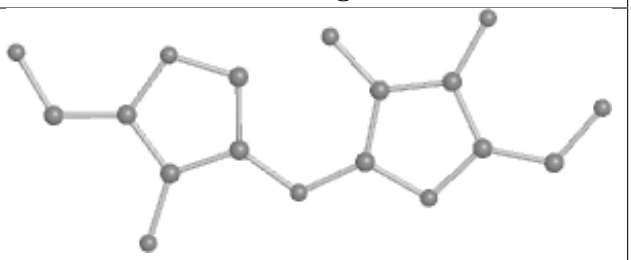
Oligosaccharide Chain A7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

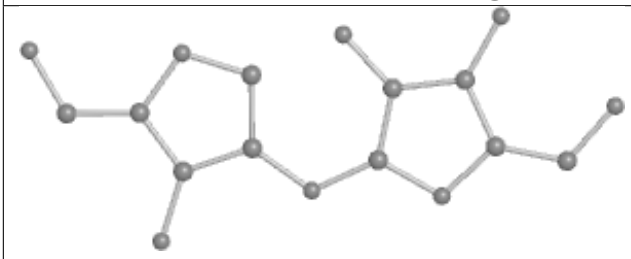
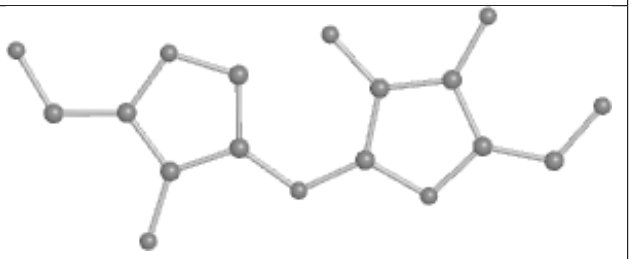
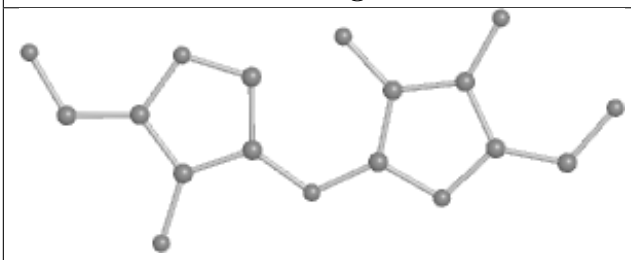
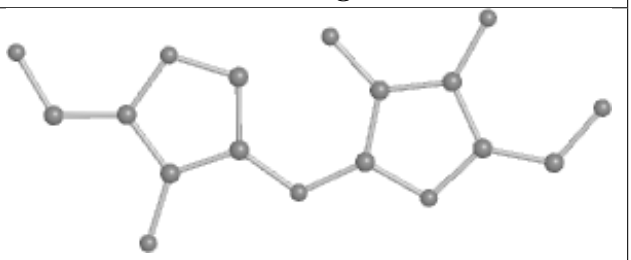
Oligosaccharide Chain B0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

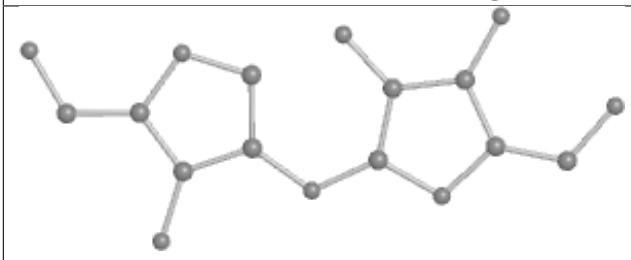
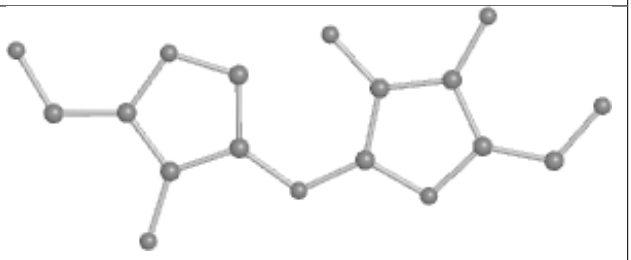
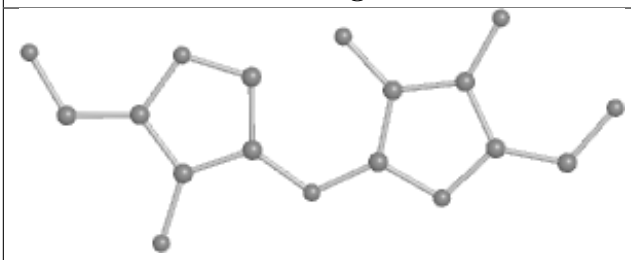
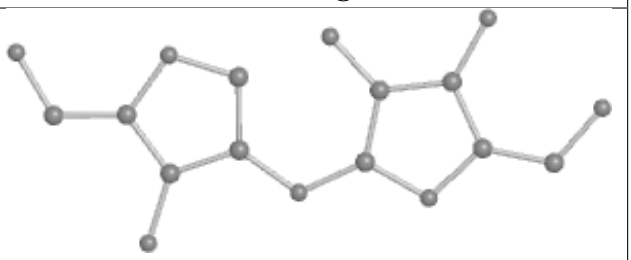
Oligosaccharide Chain B1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

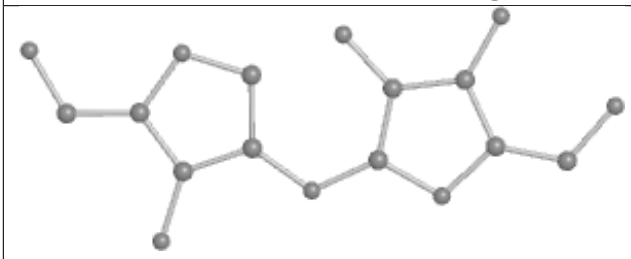
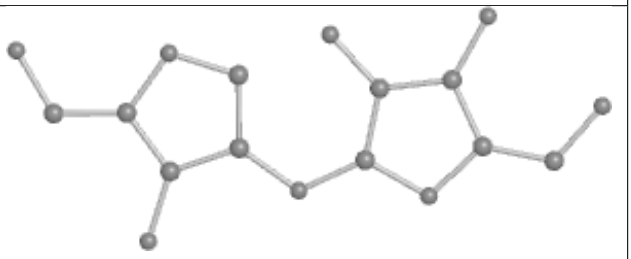
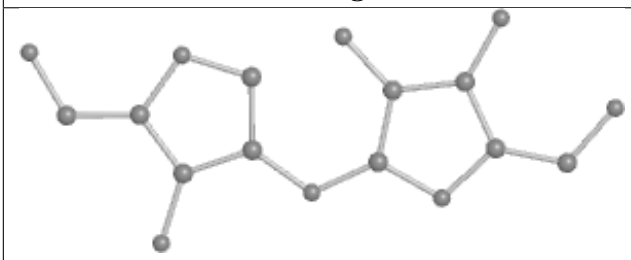
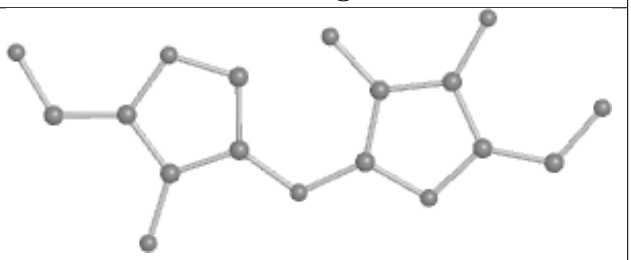
Oligosaccharide Chain B3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

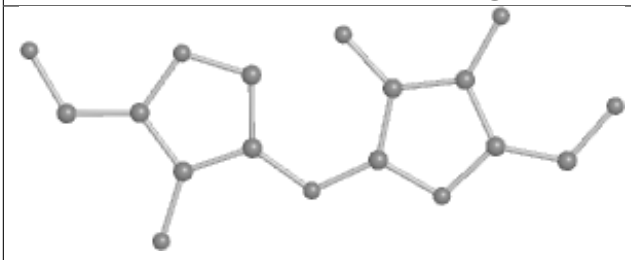
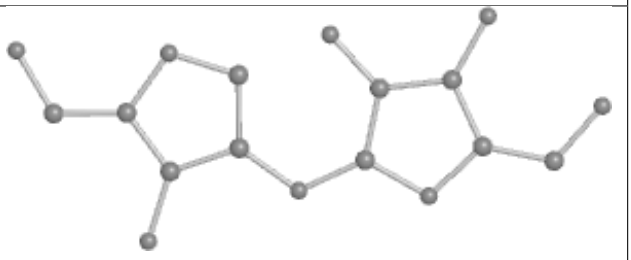
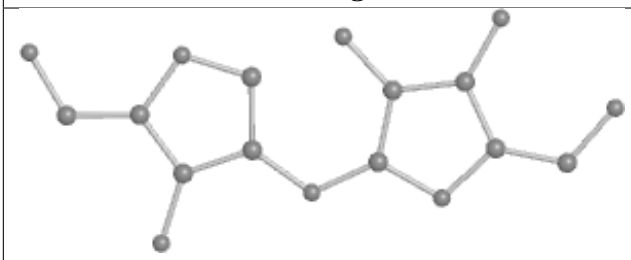
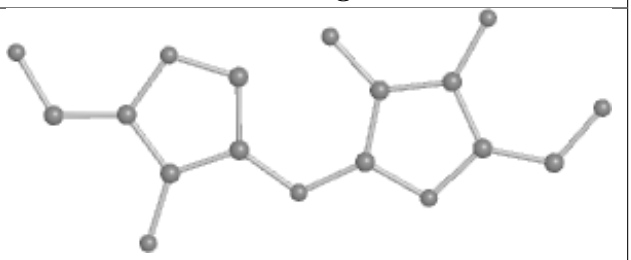
Oligosaccharide Chain B4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

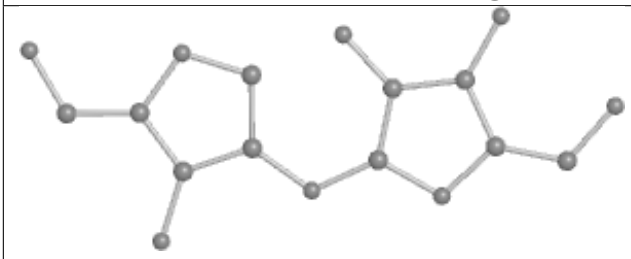
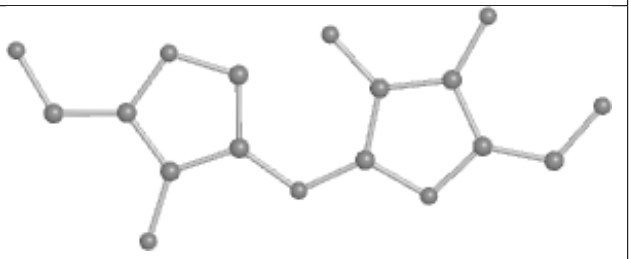
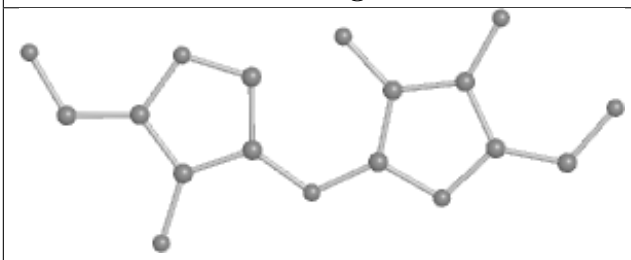
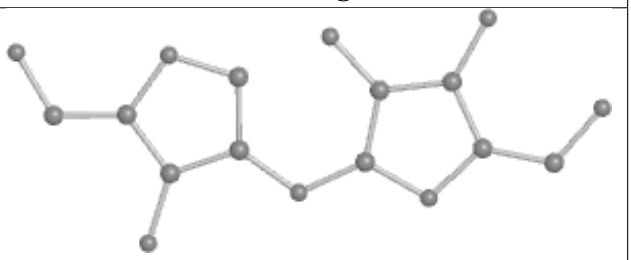
Oligosaccharide Chain B5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

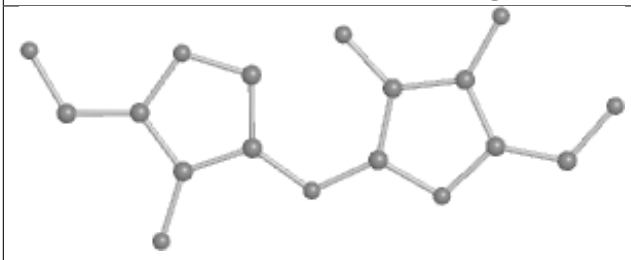
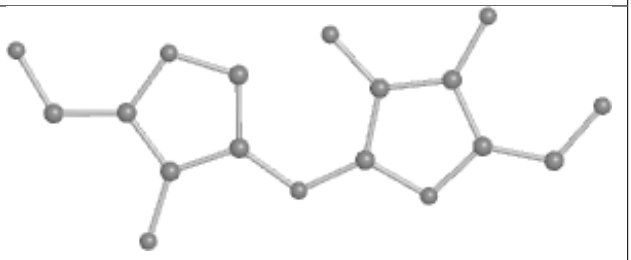
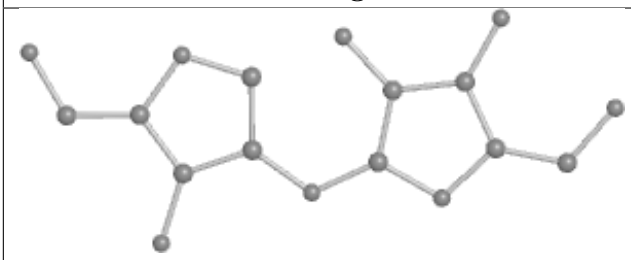
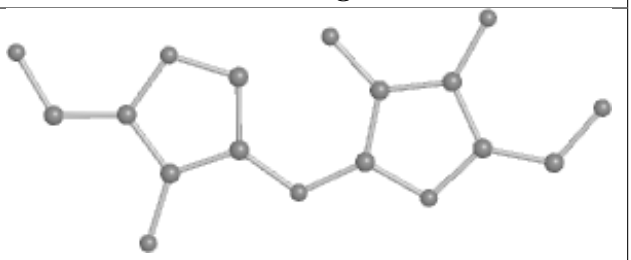
Oligosaccharide Chain B7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

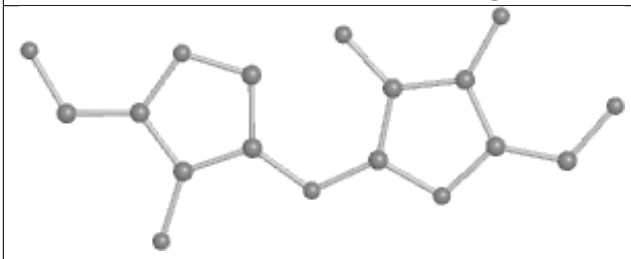
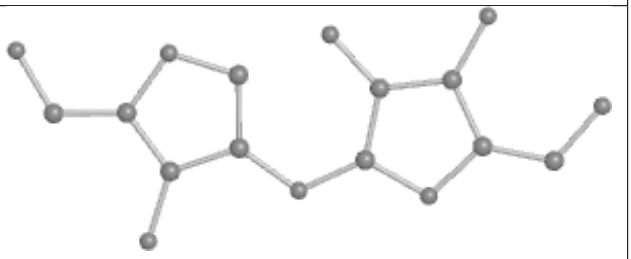
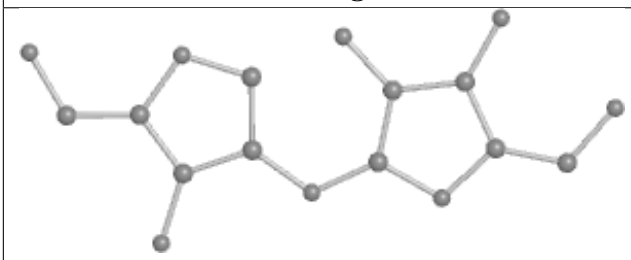
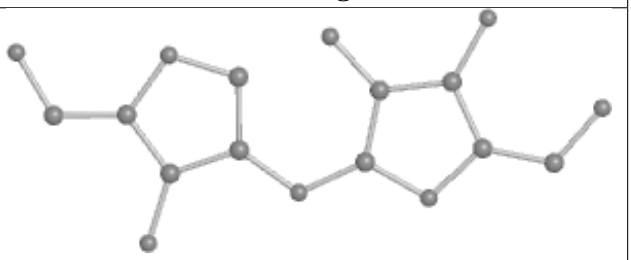
Oligosaccharide Chain B9	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

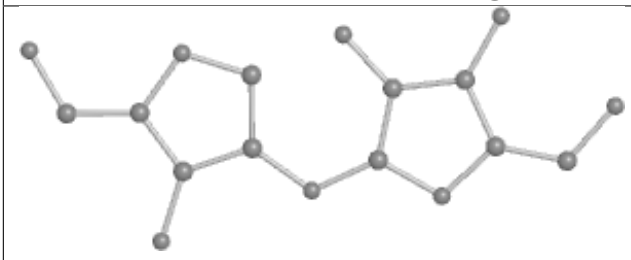
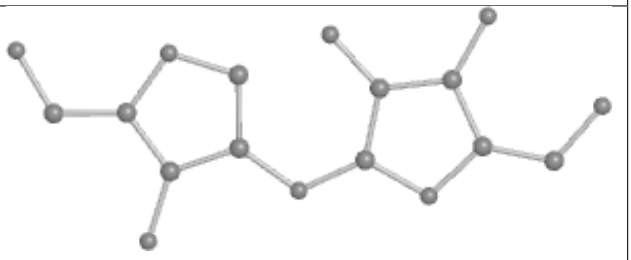
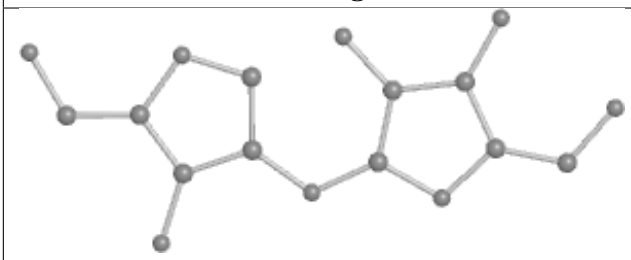
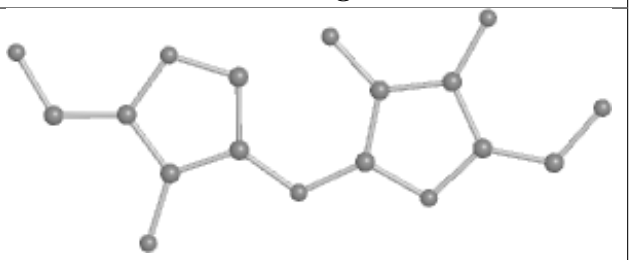
Oligosaccharide Chain C0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

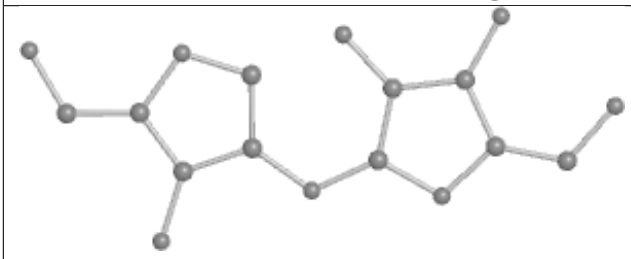
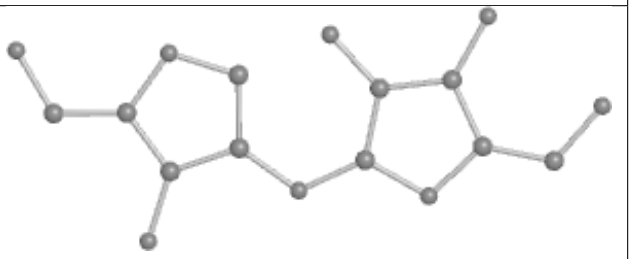
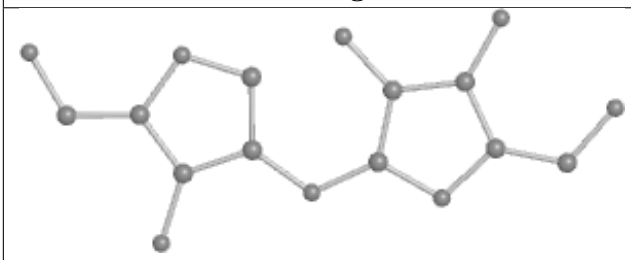
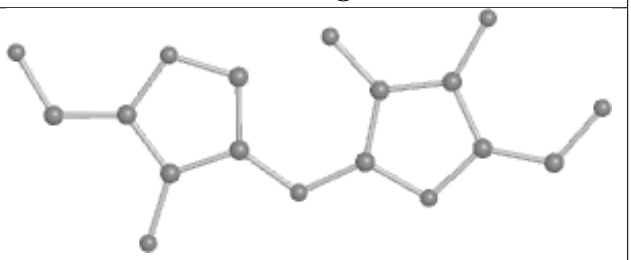
Oligosaccharide Chain C1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

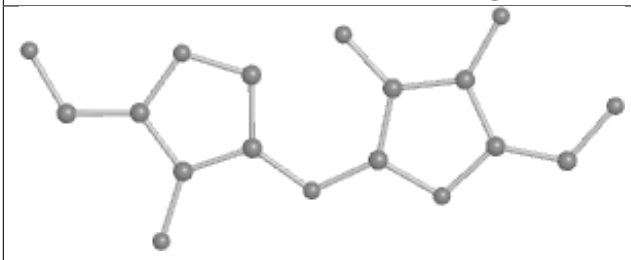
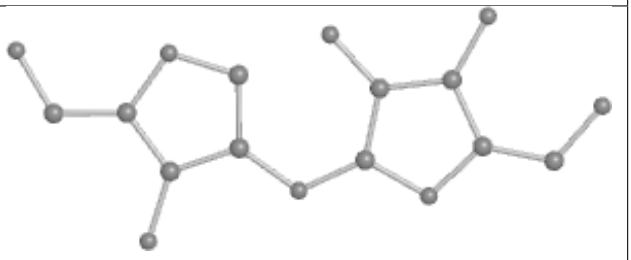
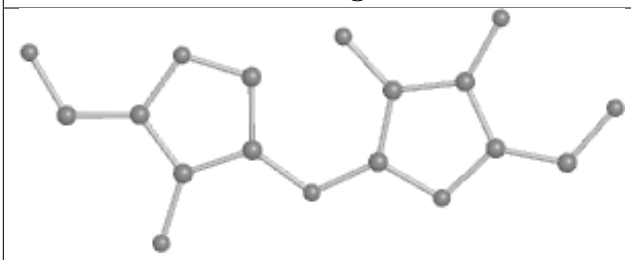
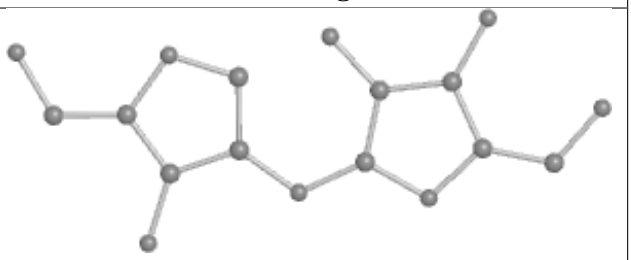
Oligosaccharide Chain C2	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

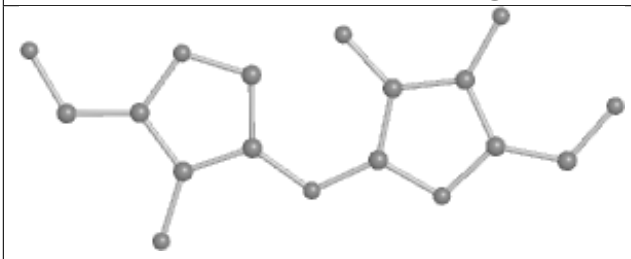
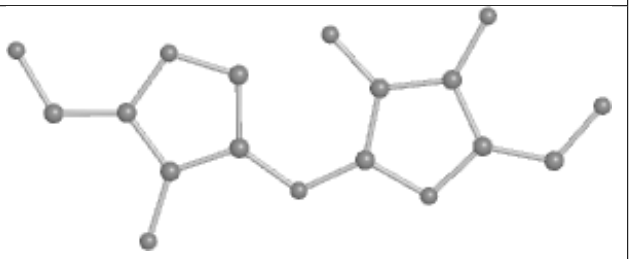
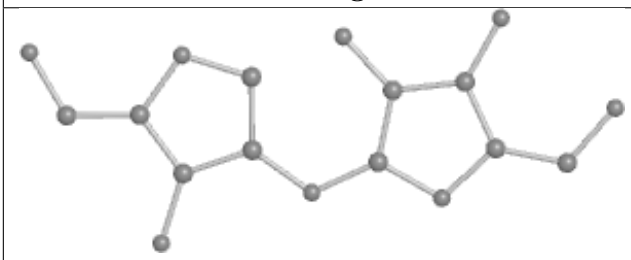
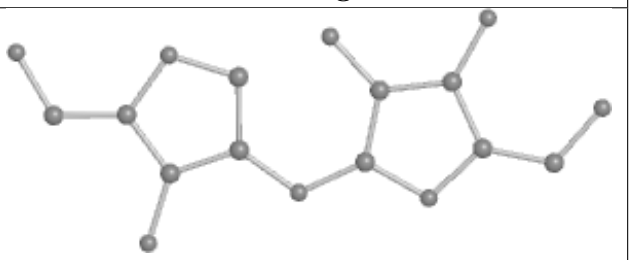
Oligosaccharide Chain C3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

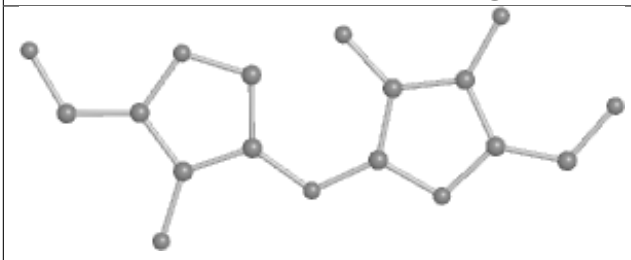
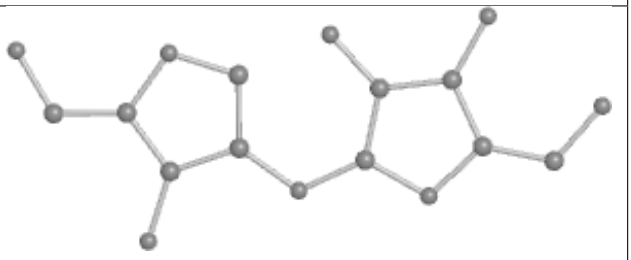
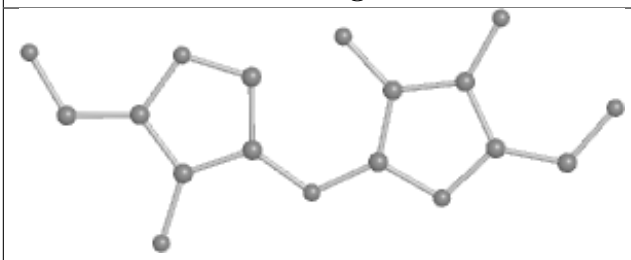
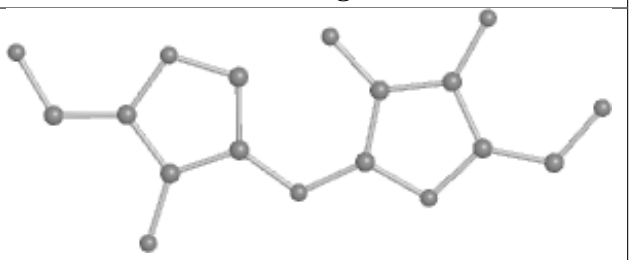
Oligosaccharide Chain C4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

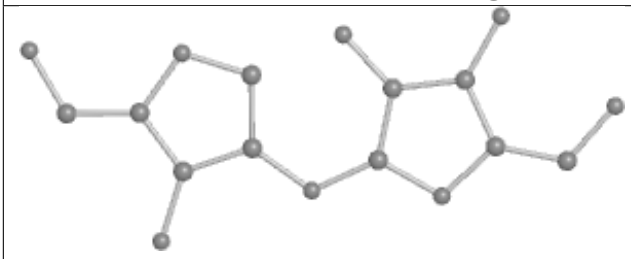
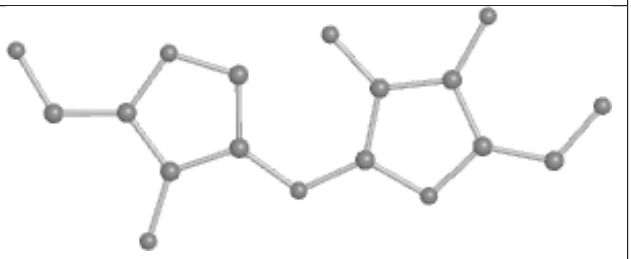
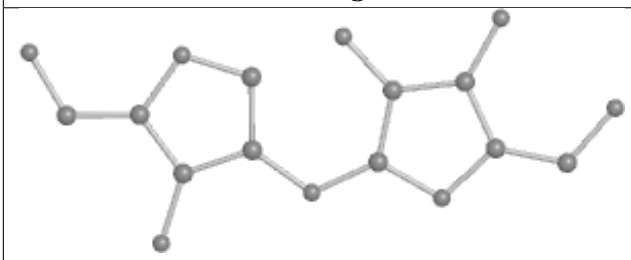
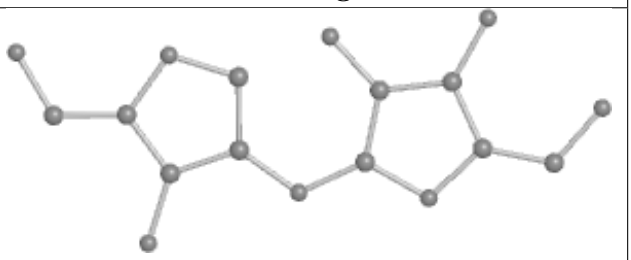
Oligosaccharide Chain C5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain C6	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

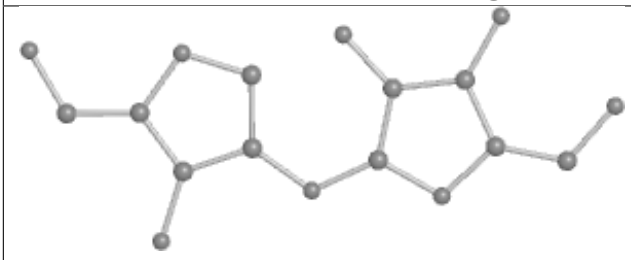
Oligosaccharide Chain C7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain C8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

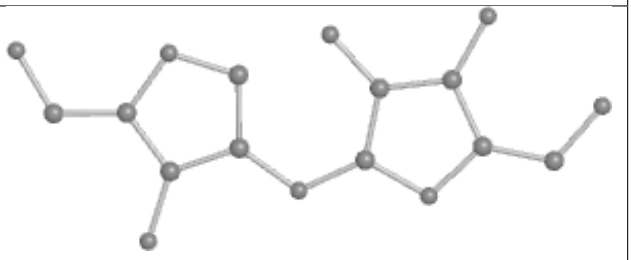
Oligosaccharide Chain C9	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain D0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

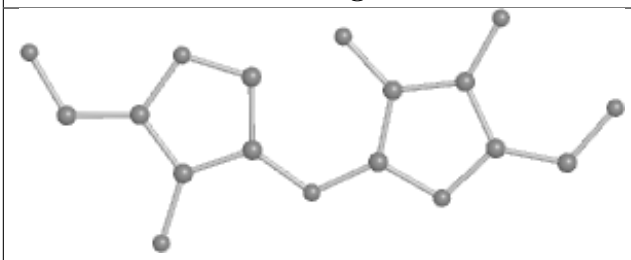
Oligosaccharide Chain D1



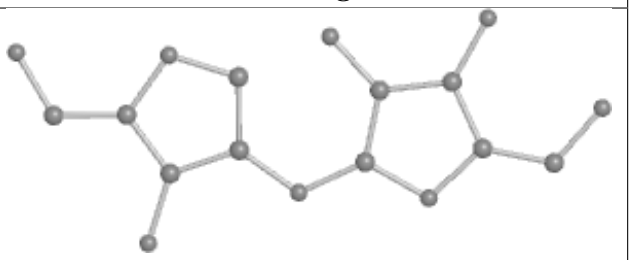
Bond lengths



Bond angles

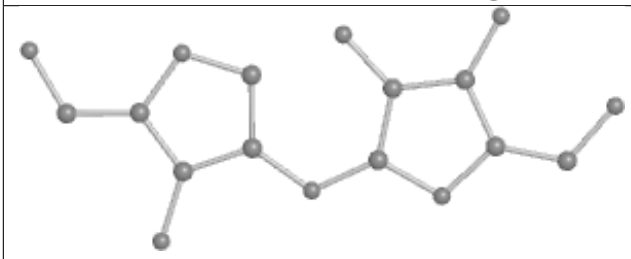


Torsions

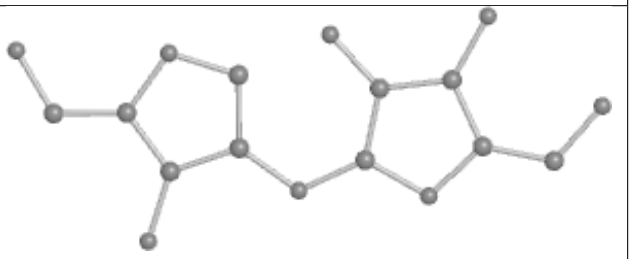


Rings

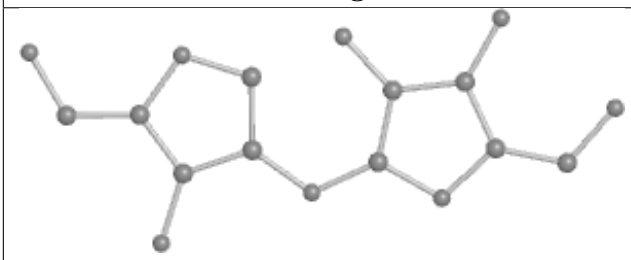
Oligosaccharide Chain D2



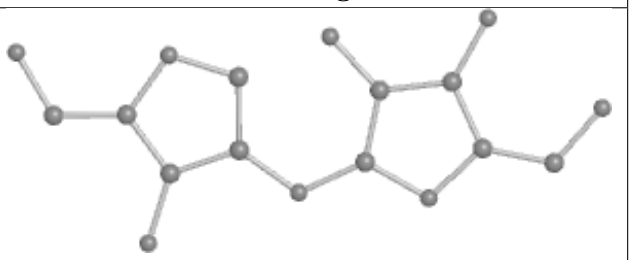
Bond lengths



Bond angles

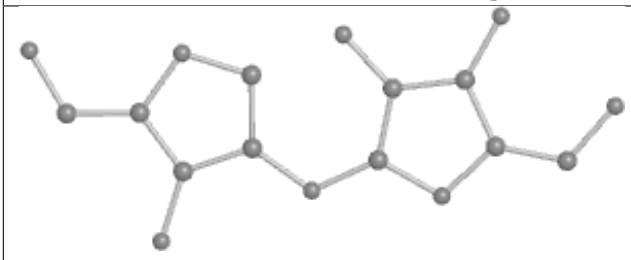


Torsions

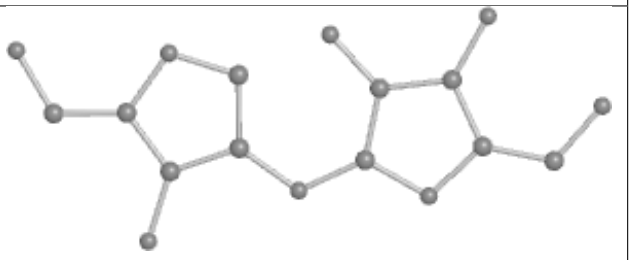


Rings

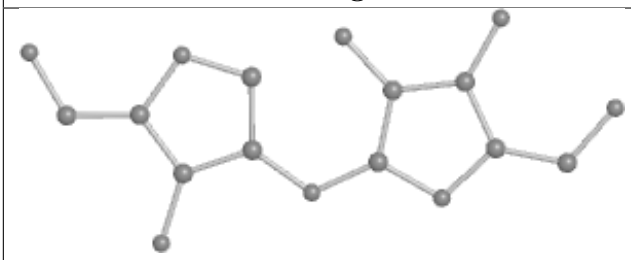
Oligosaccharide Chain D3



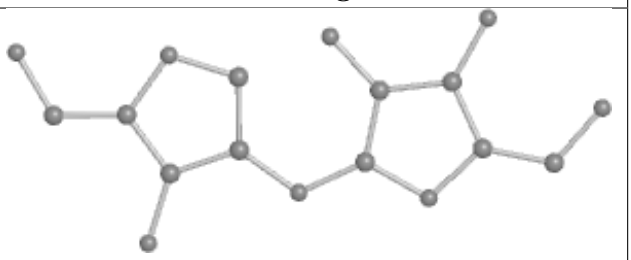
Bond lengths



Bond angles

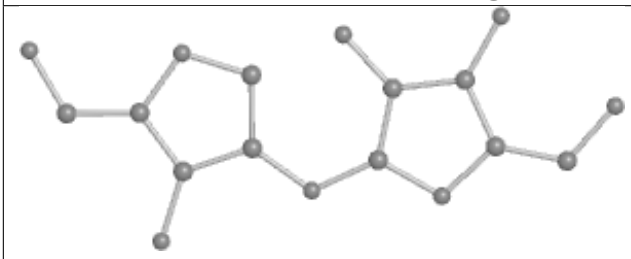


Torsions

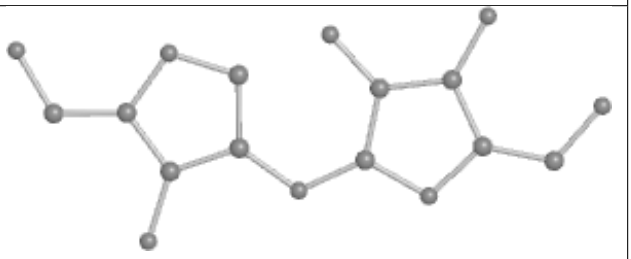


Rings

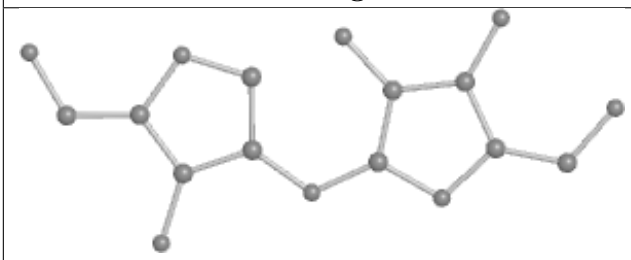
Oligosaccharide Chain D4



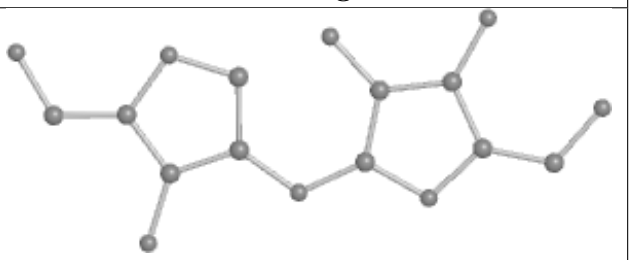
Bond lengths



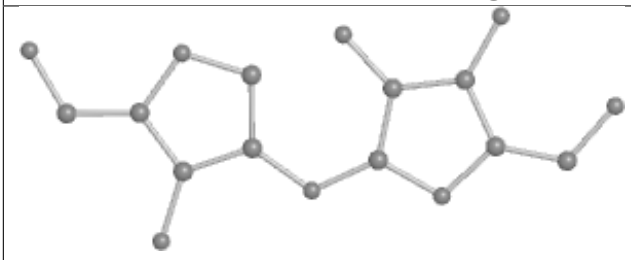
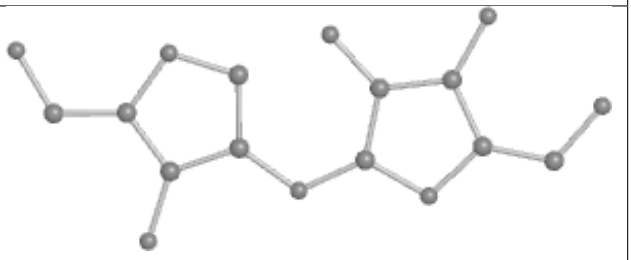
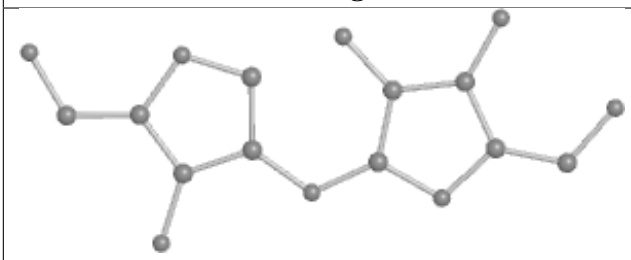
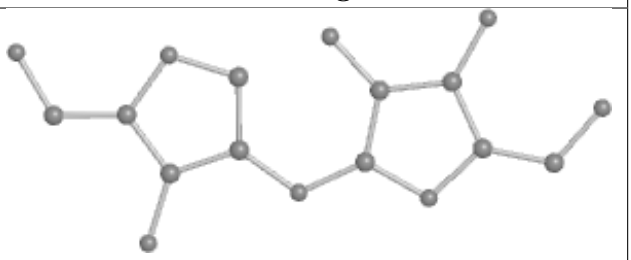
Bond angles

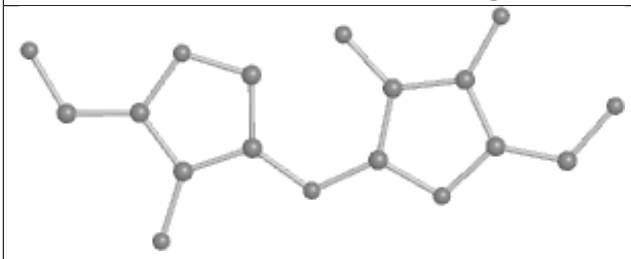
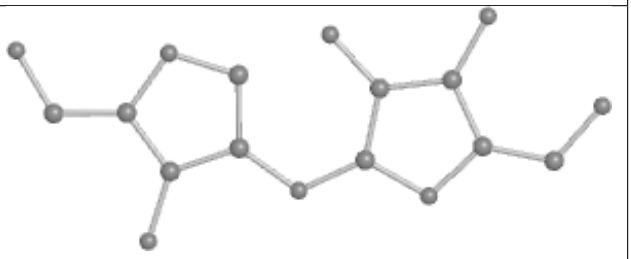
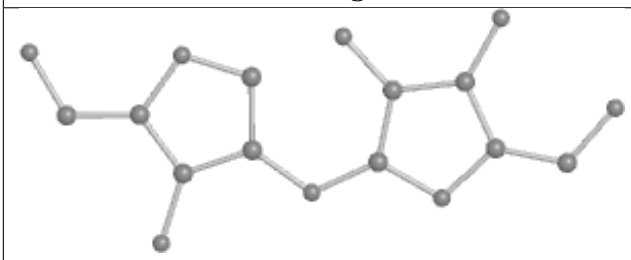
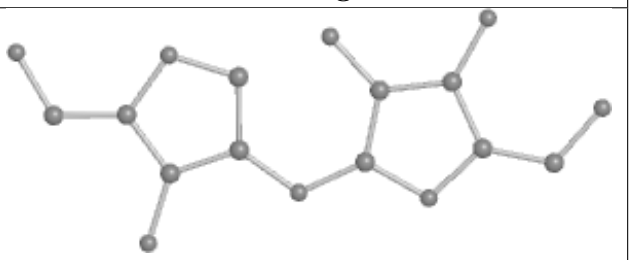


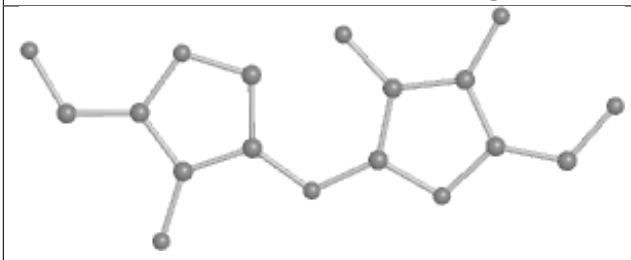
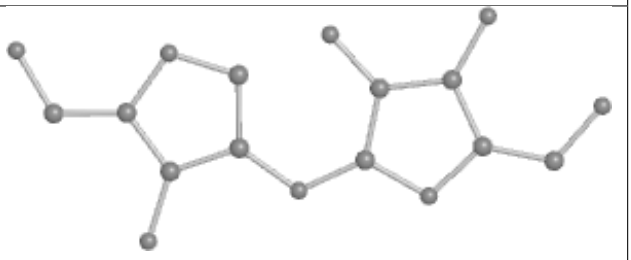
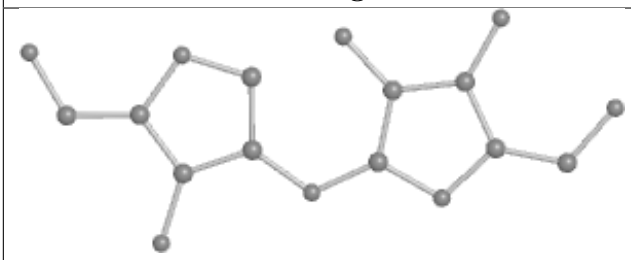
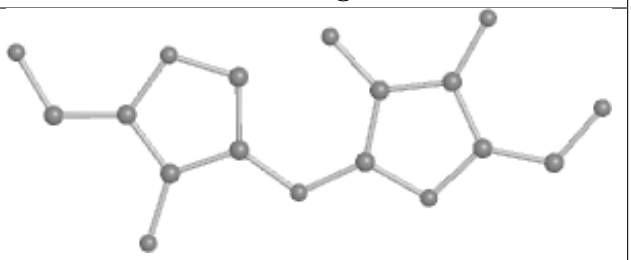
Torsions

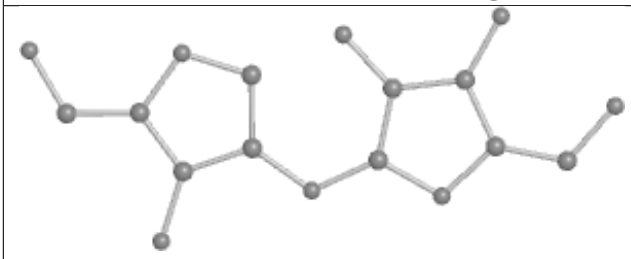
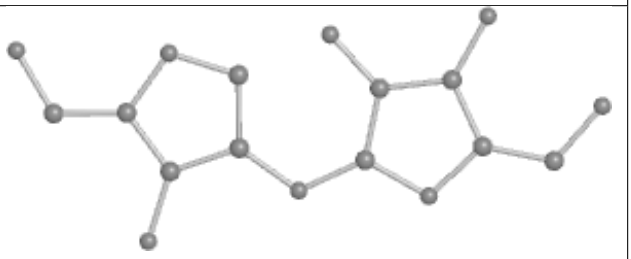
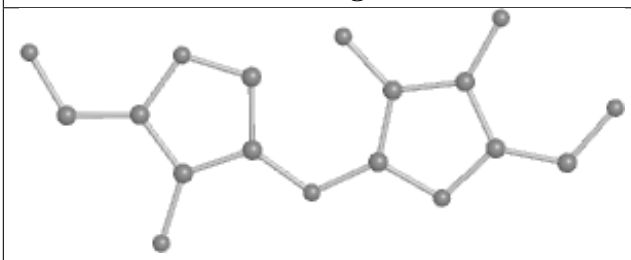
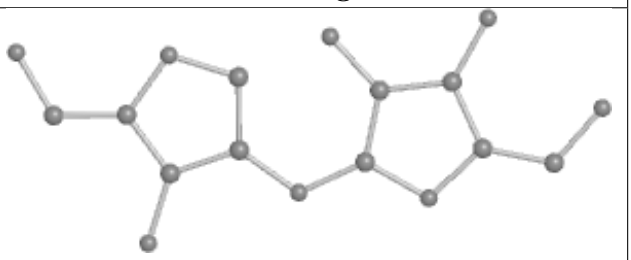


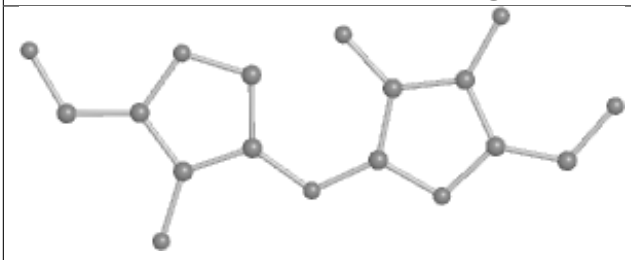
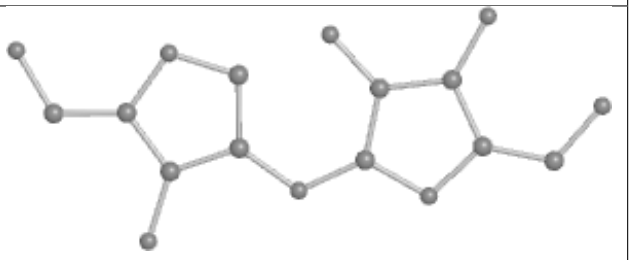
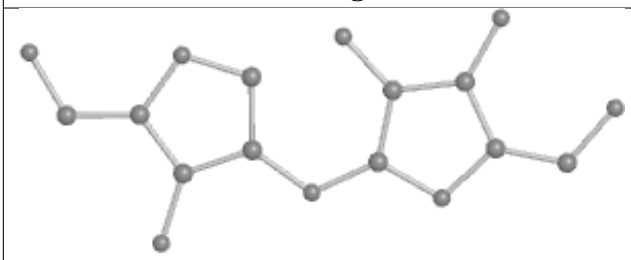
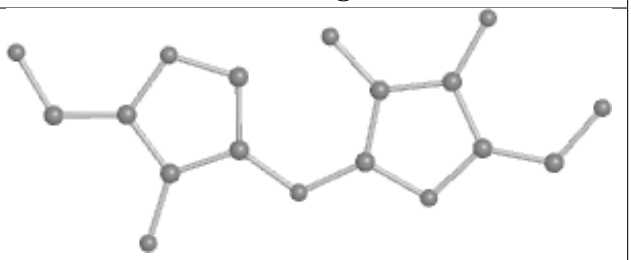
Rings

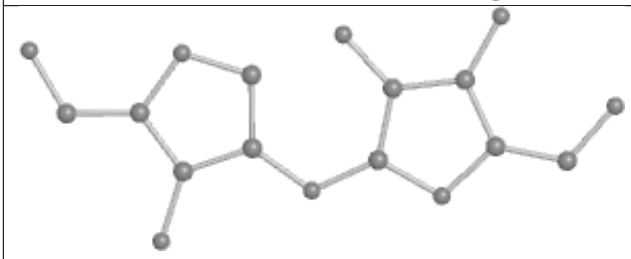
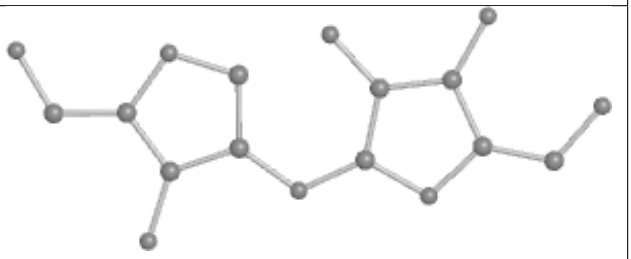
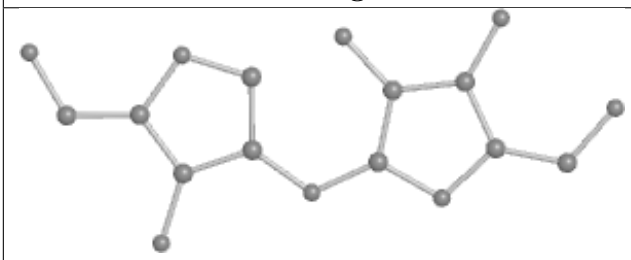
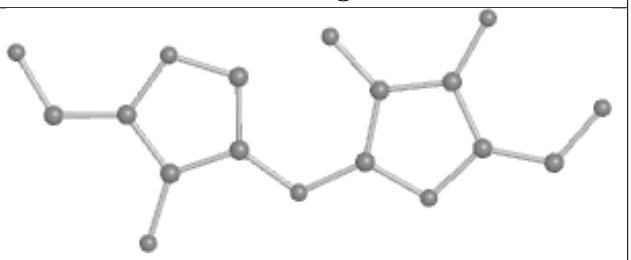
Oligosaccharide Chain D5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain D6	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

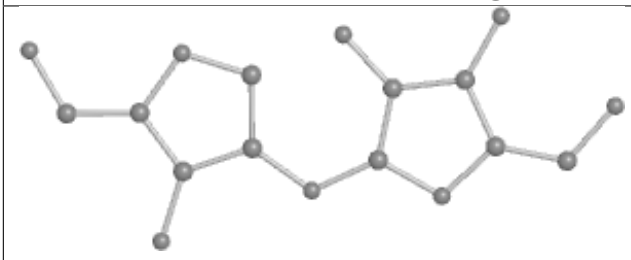
Oligosaccharide Chain D7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain D8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

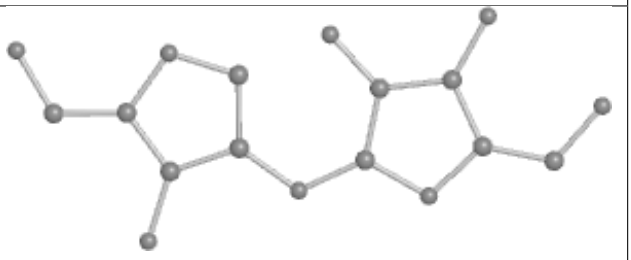
Oligosaccharide Chain D9	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain E0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

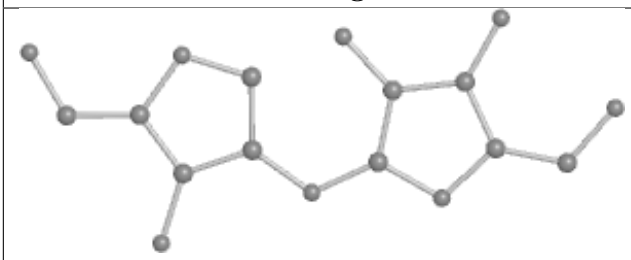
Oligosaccharide Chain E1



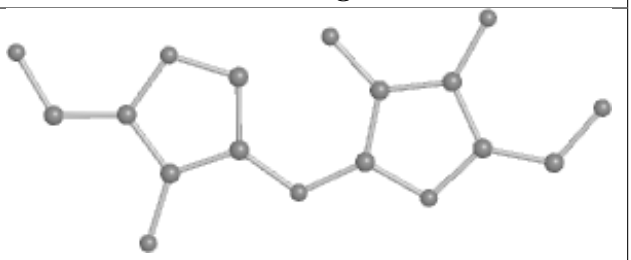
Bond lengths



Bond angles

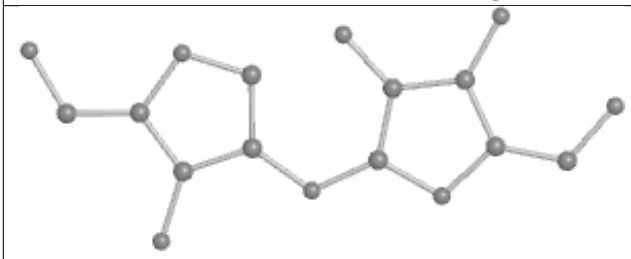


Torsions

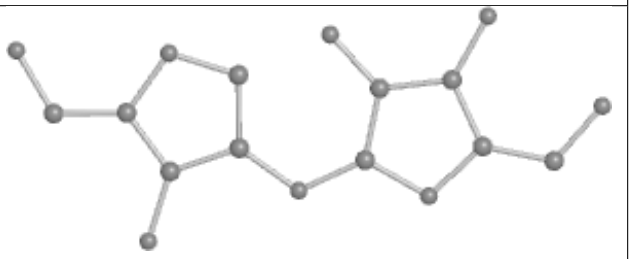


Rings

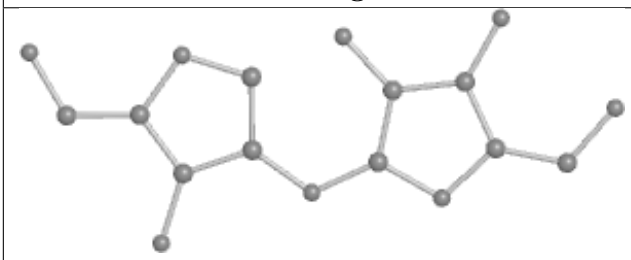
Oligosaccharide Chain E2



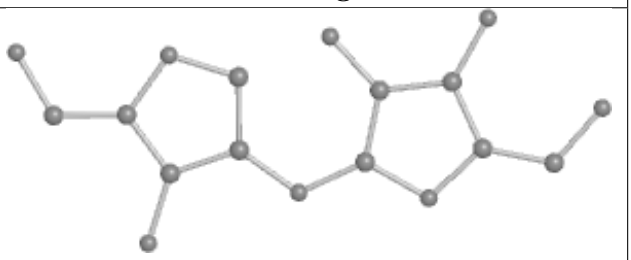
Bond lengths



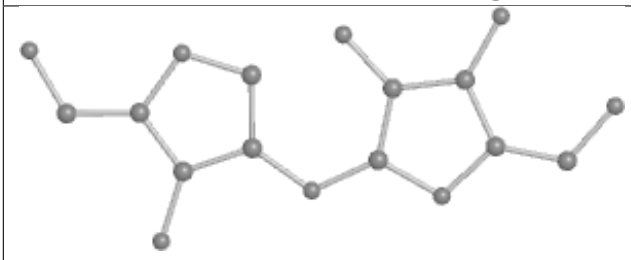
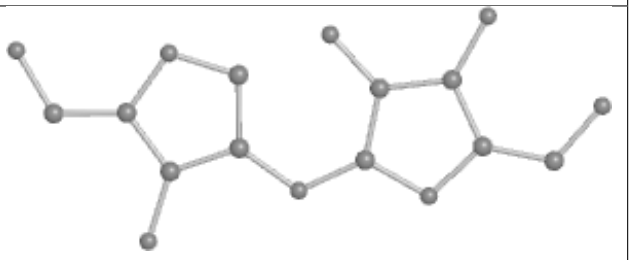
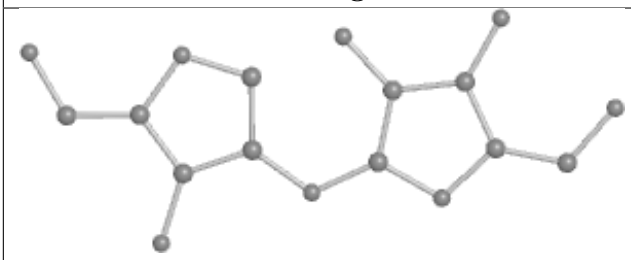
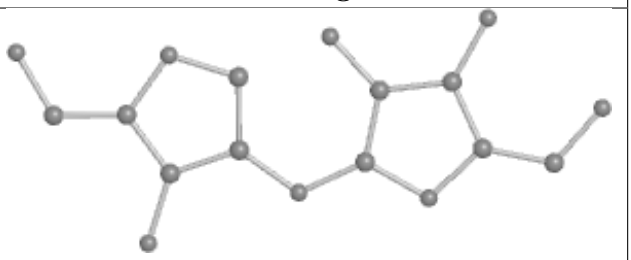
Bond angles

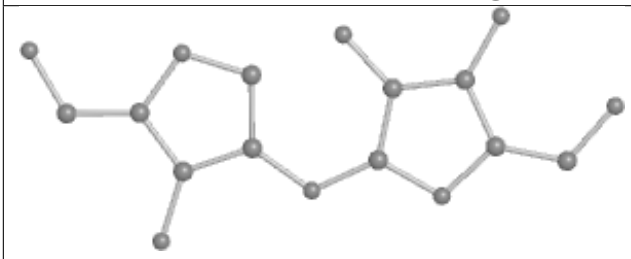
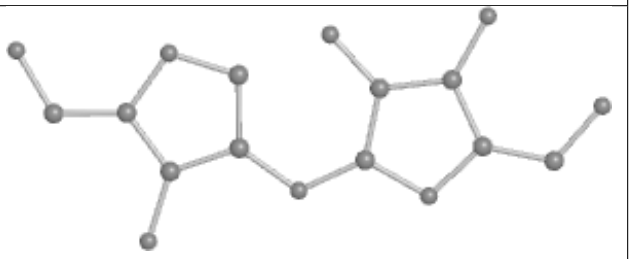
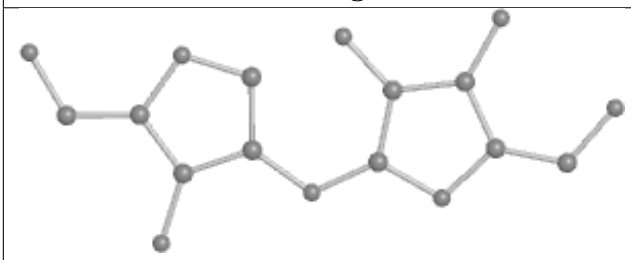
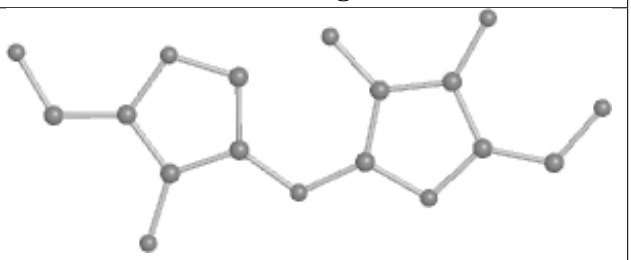


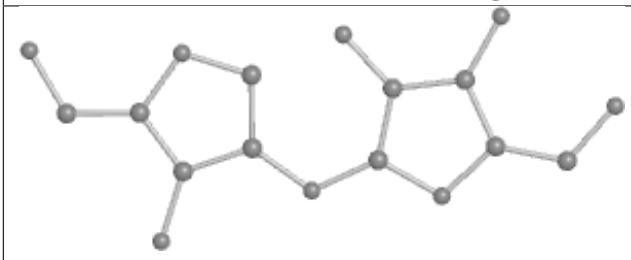
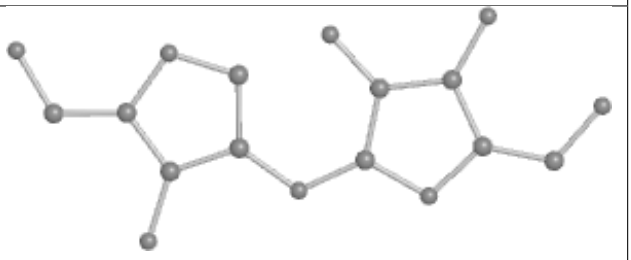
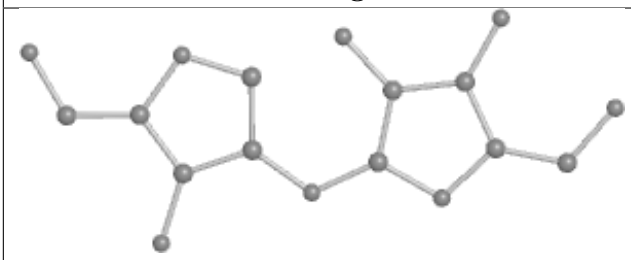
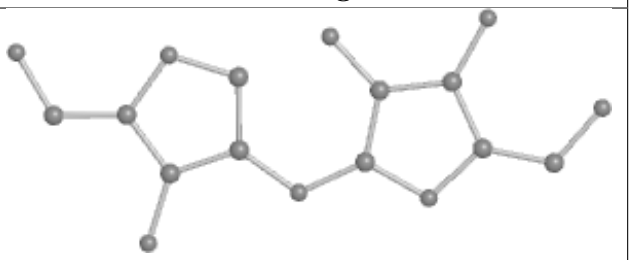
Torsions

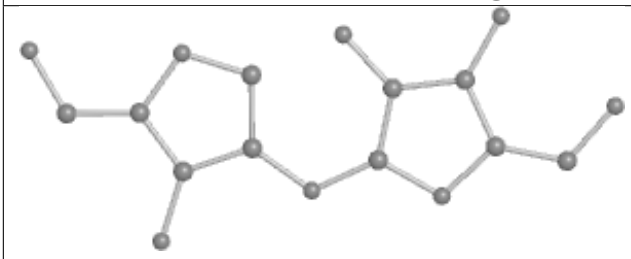
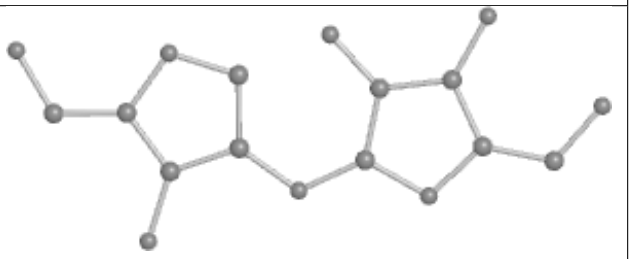
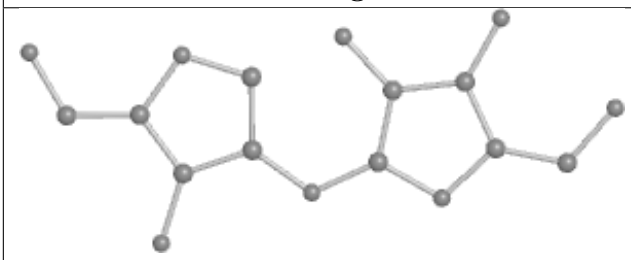
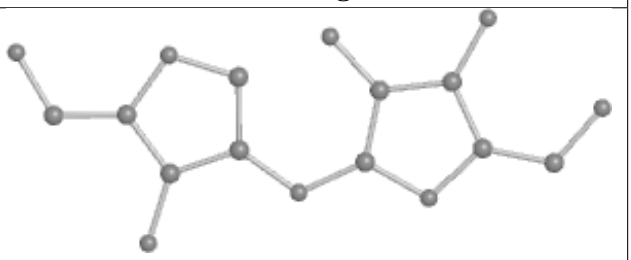


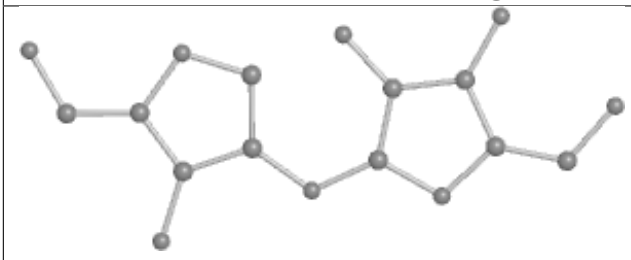
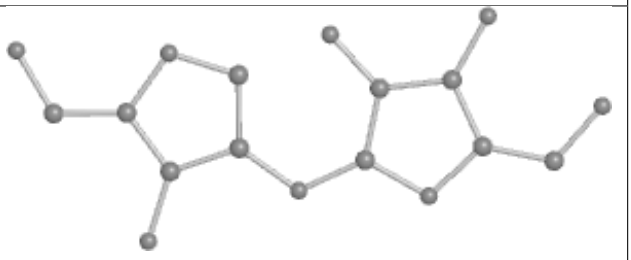
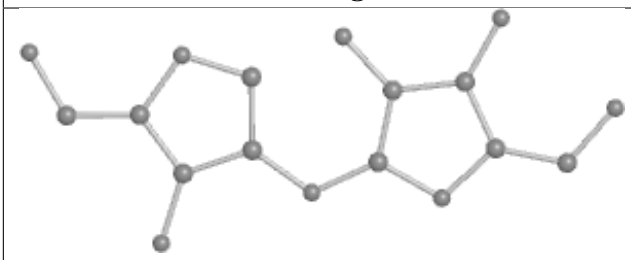
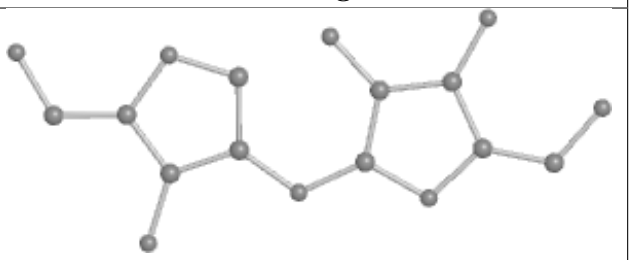
Rings

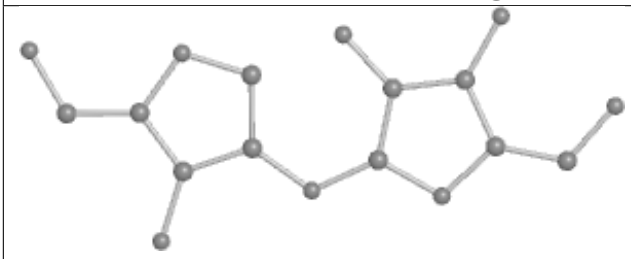
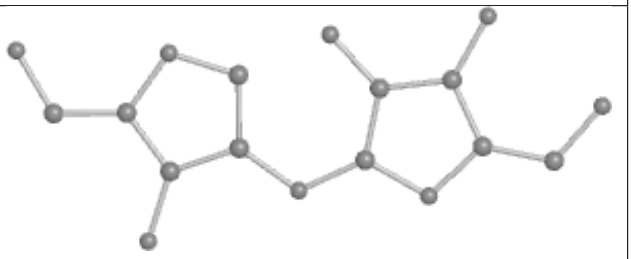
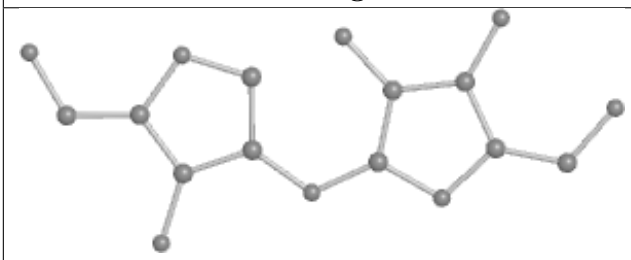
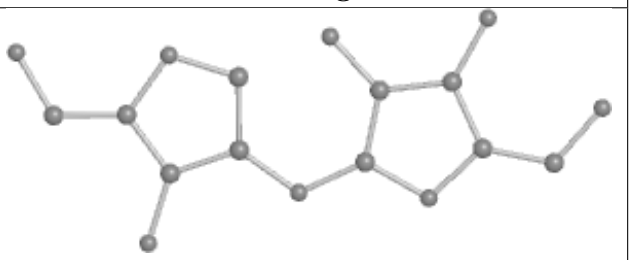
Oligosaccharide Chain E4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

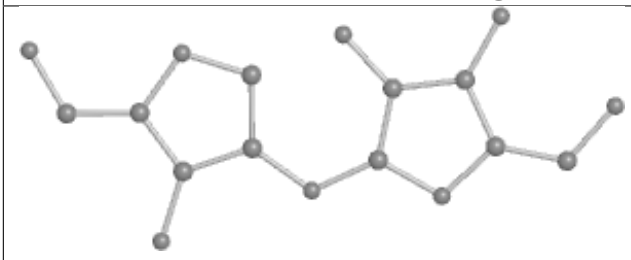
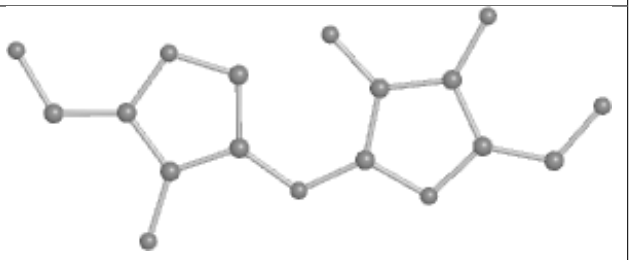
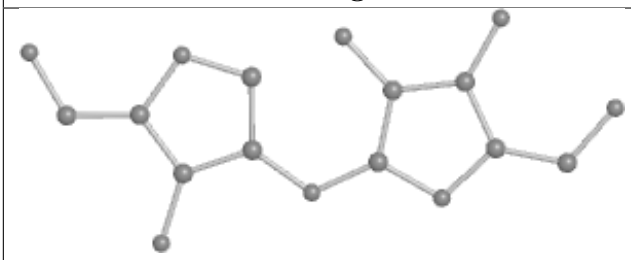
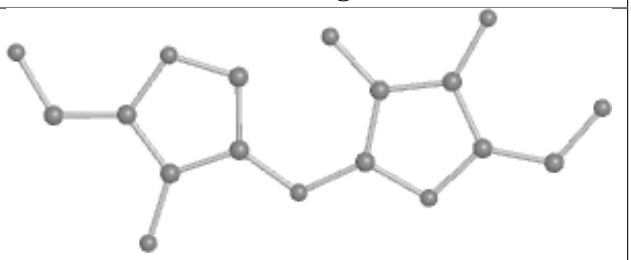
Oligosaccharide Chain E5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

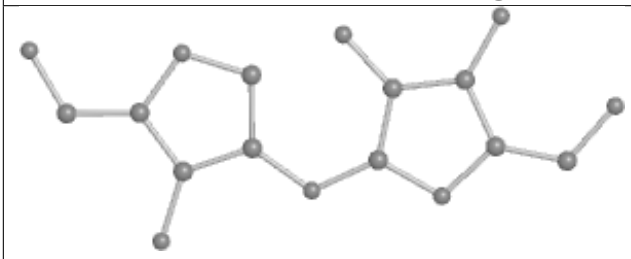
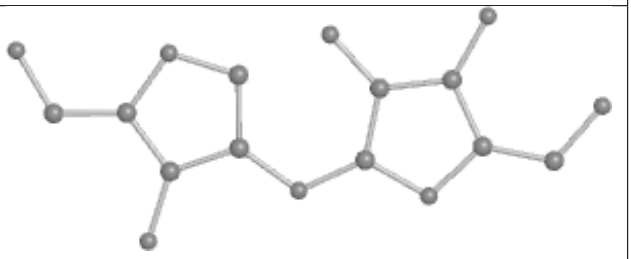
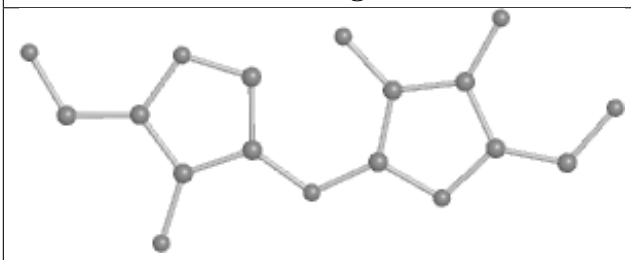
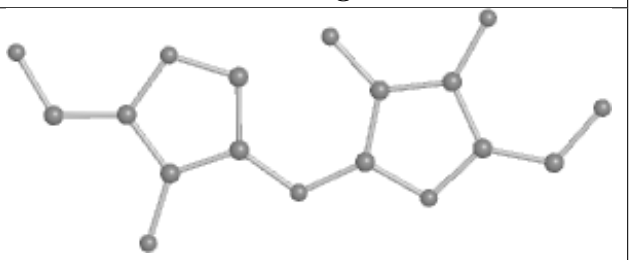
Oligosaccharide Chain E8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

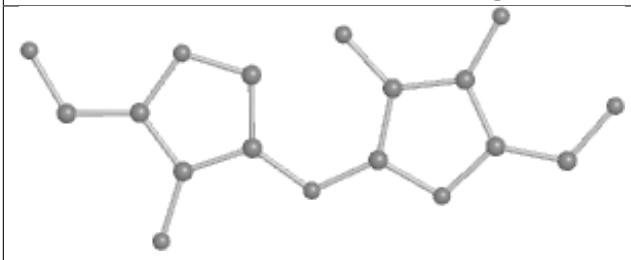
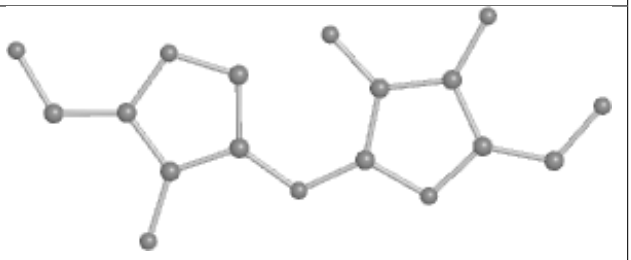
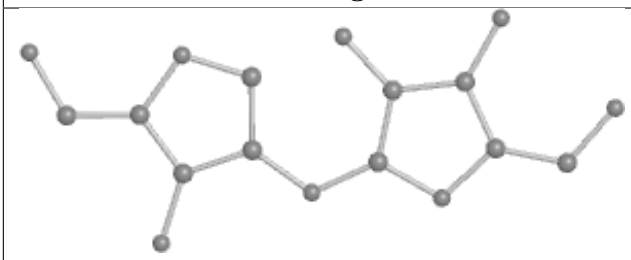
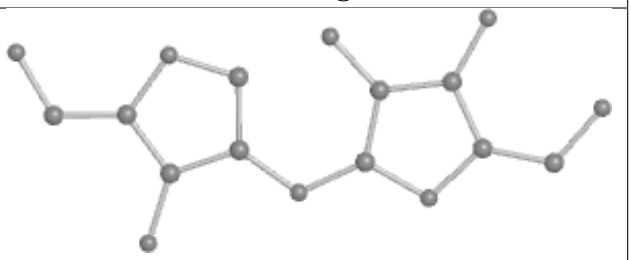
Oligosaccharide Chain F0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

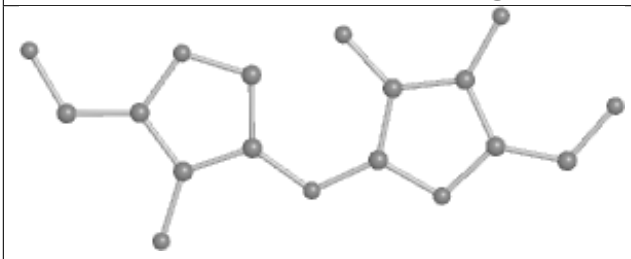
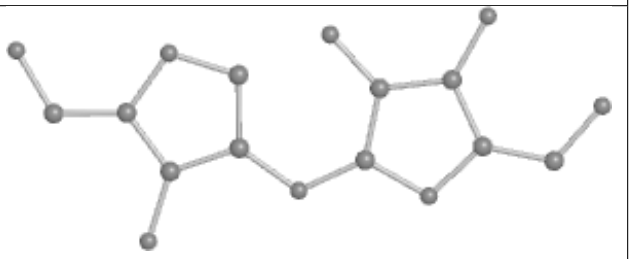
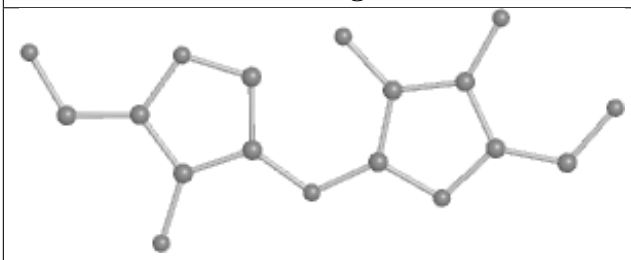
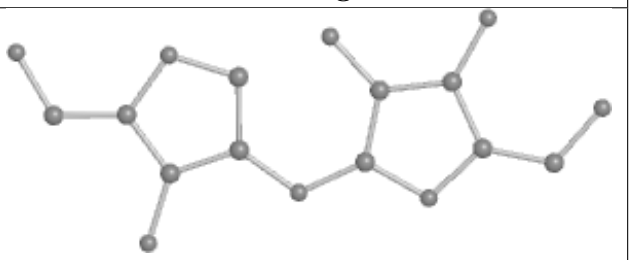
Oligosaccharide Chain F3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

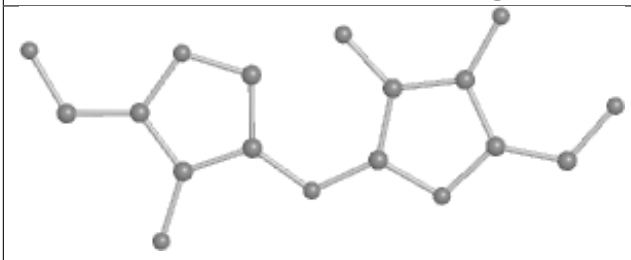
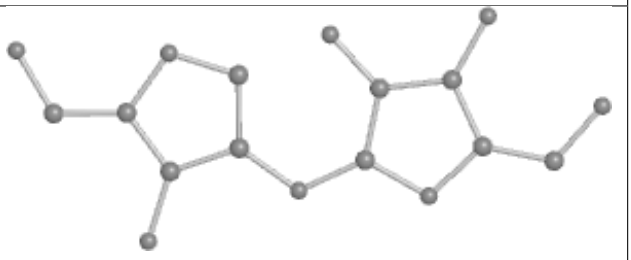
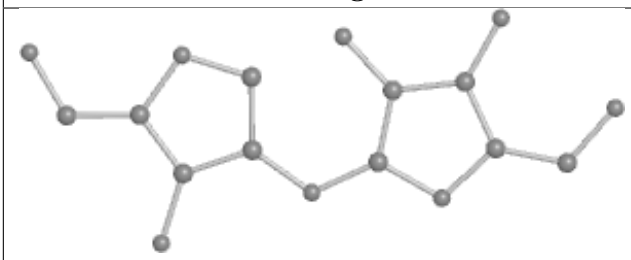
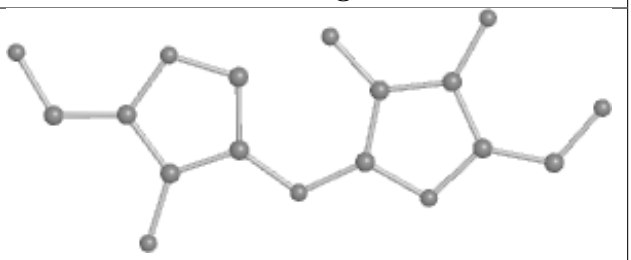
Oligosaccharide Chain F8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

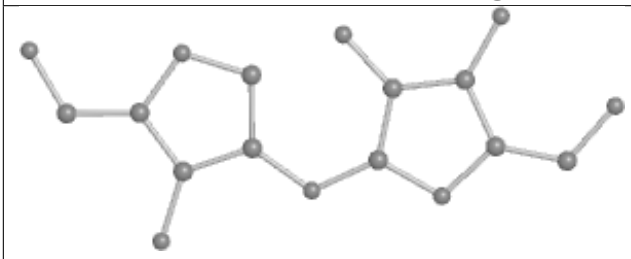
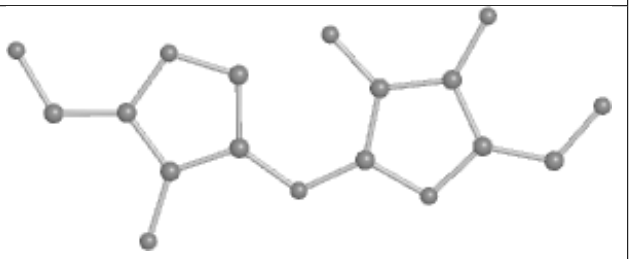
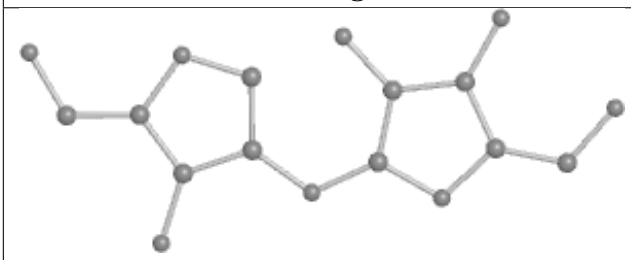
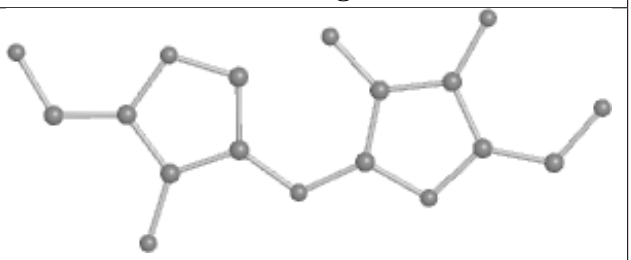
Oligosaccharide Chain a5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

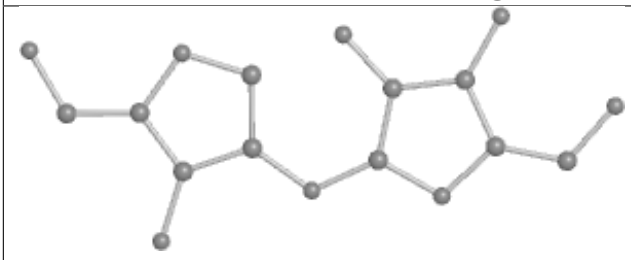
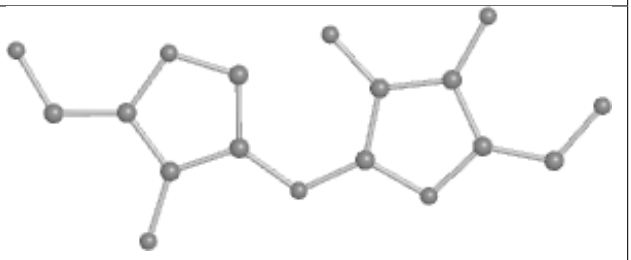
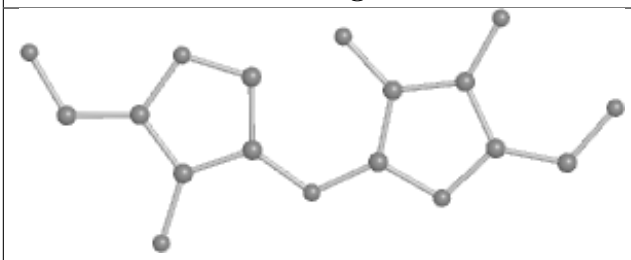
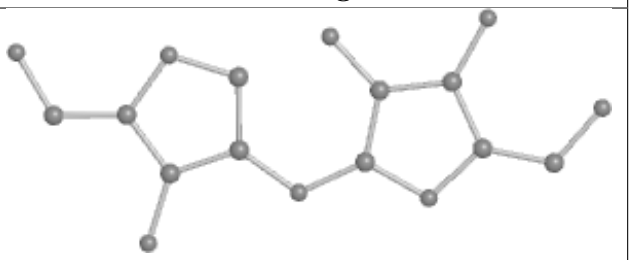
Oligosaccharide Chain a7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

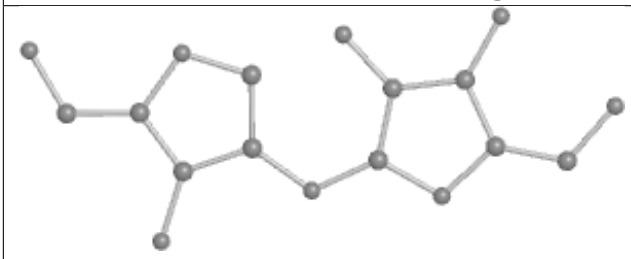
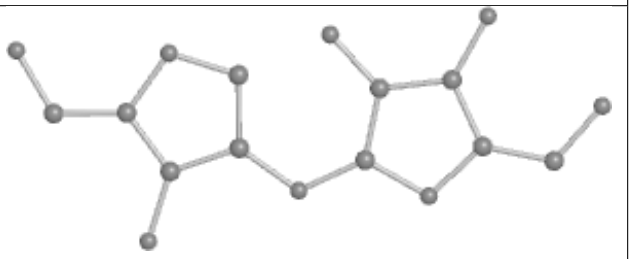
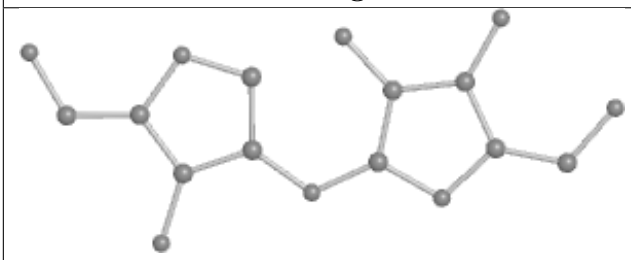
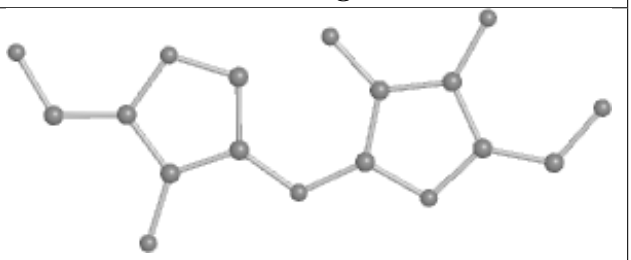
Oligosaccharide Chain b0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

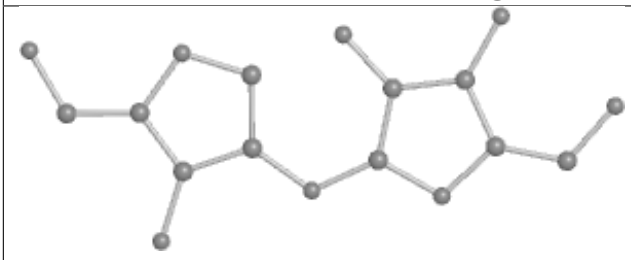
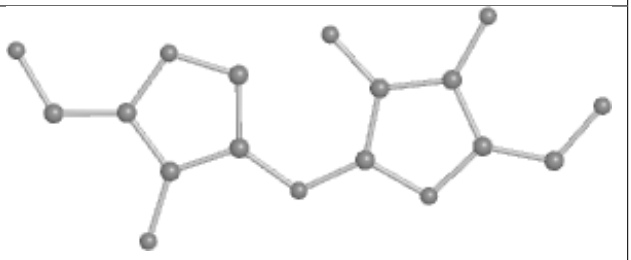
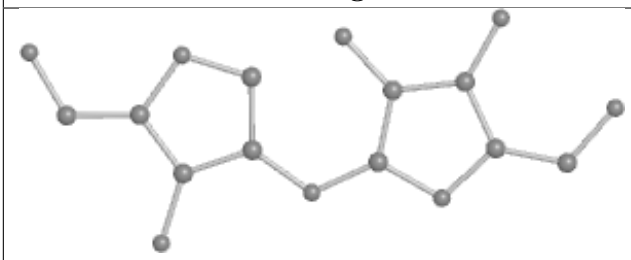
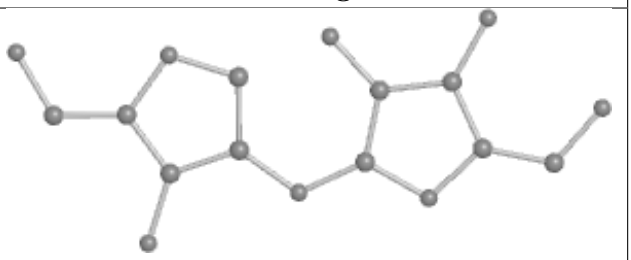
Oligosaccharide Chain b1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

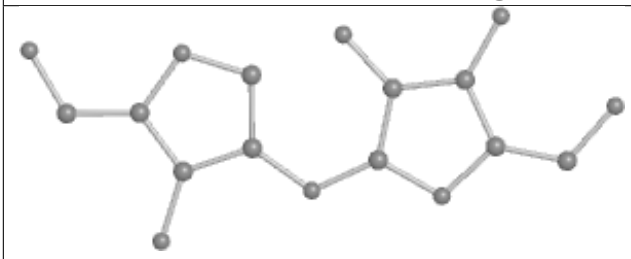
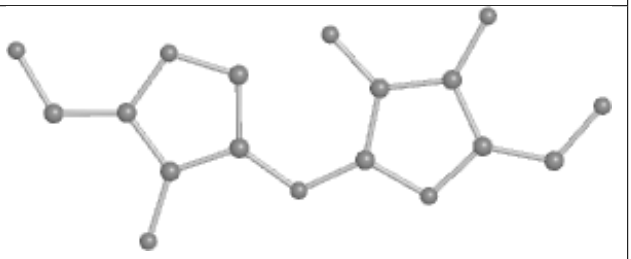
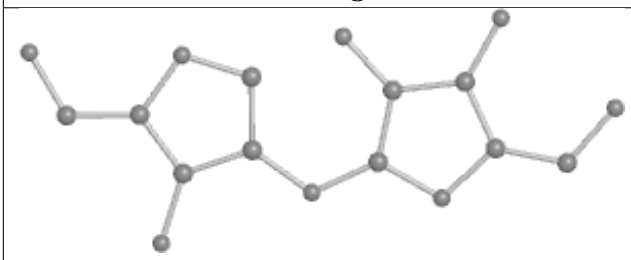
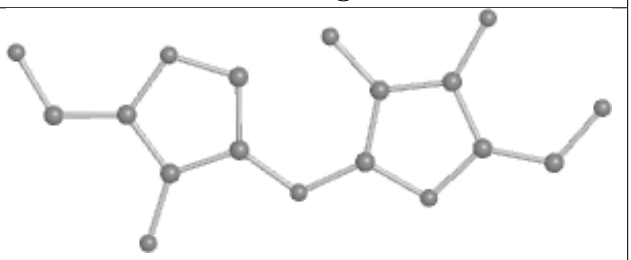
Oligosaccharide Chain b3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

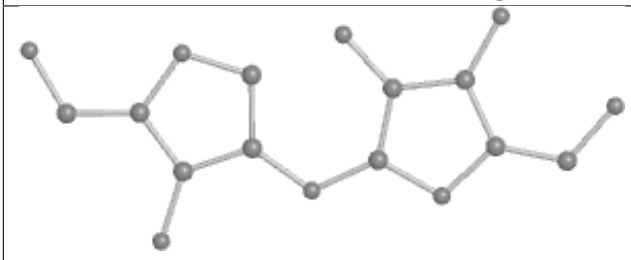
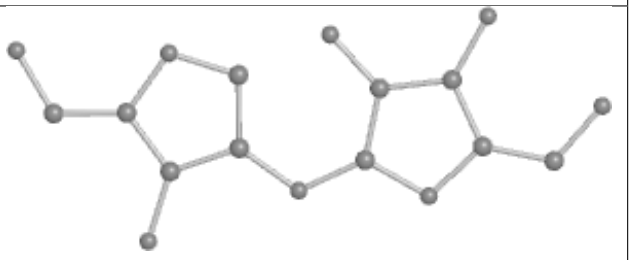
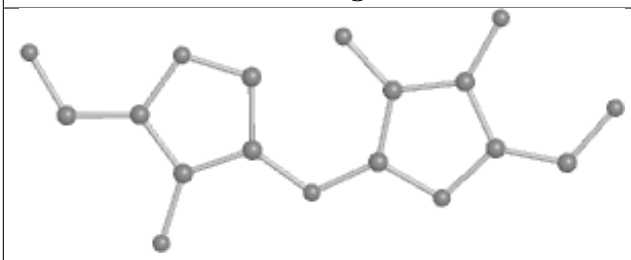
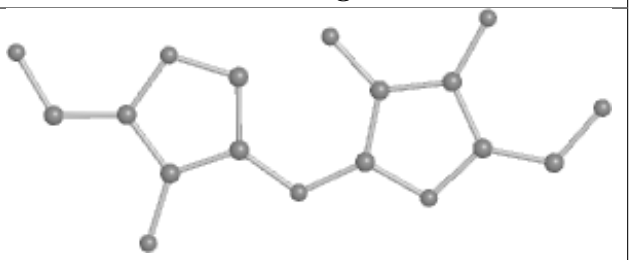
Oligosaccharide Chain b4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

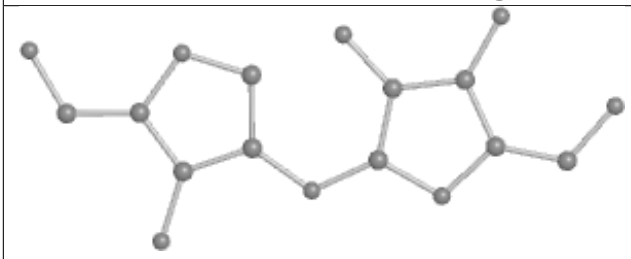
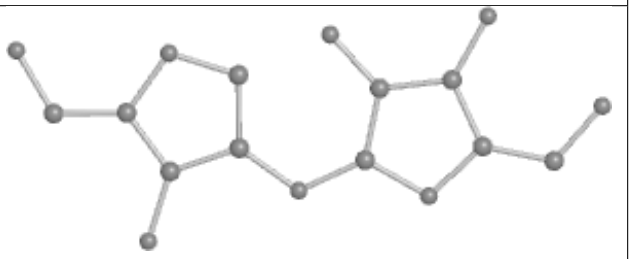
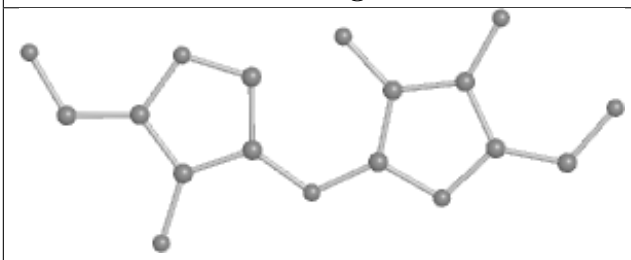
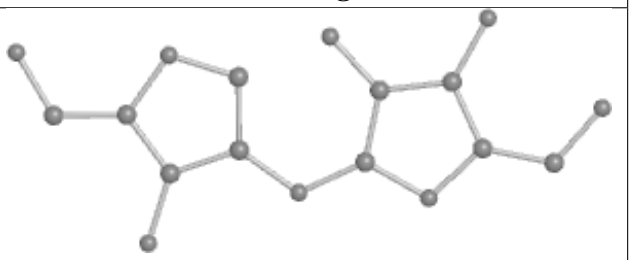
Oligosaccharide Chain b5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

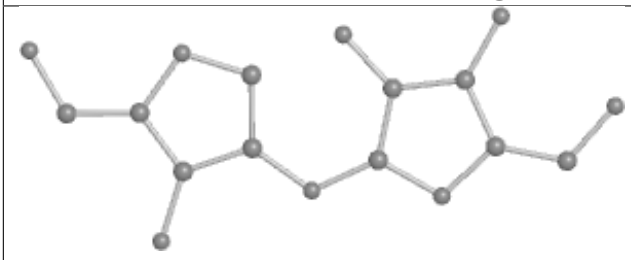
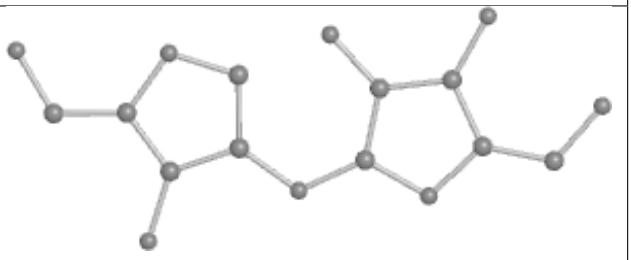
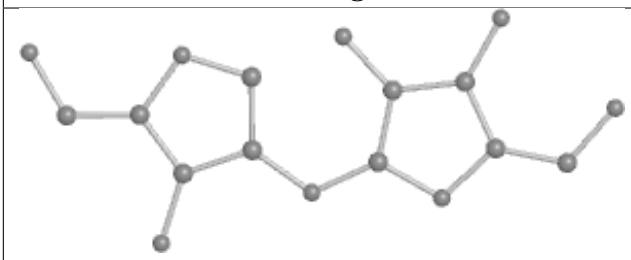
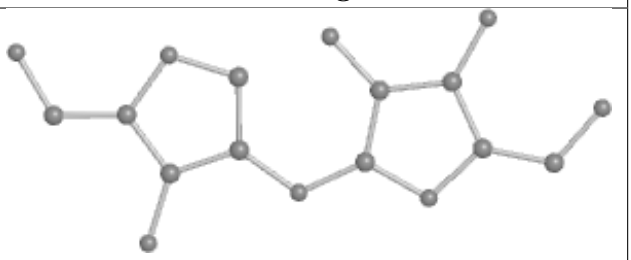
Oligosaccharide Chain b7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

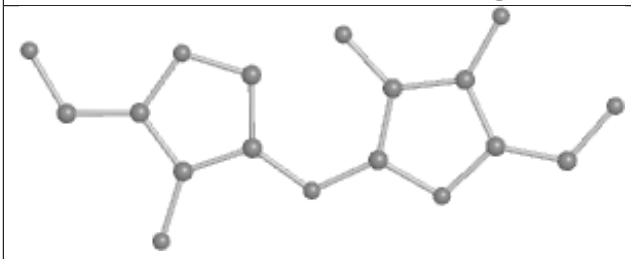
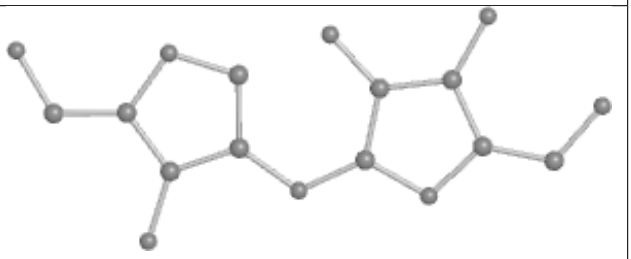
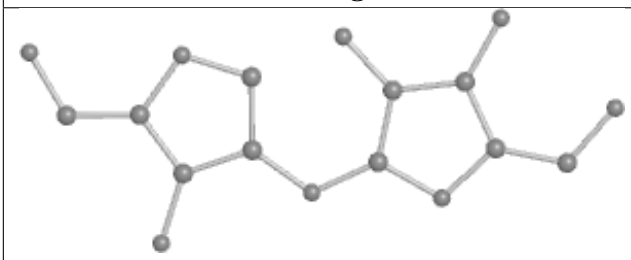
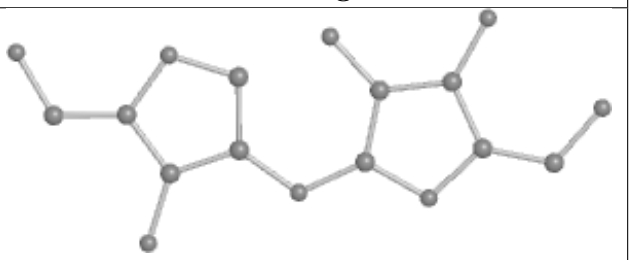
Oligosaccharide Chain b9	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

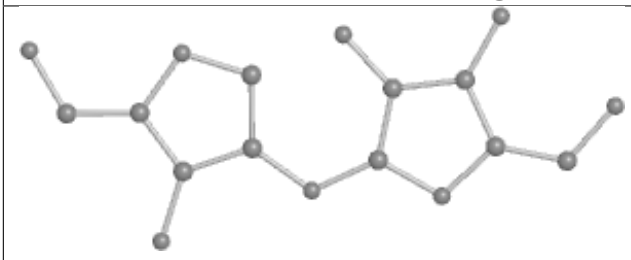
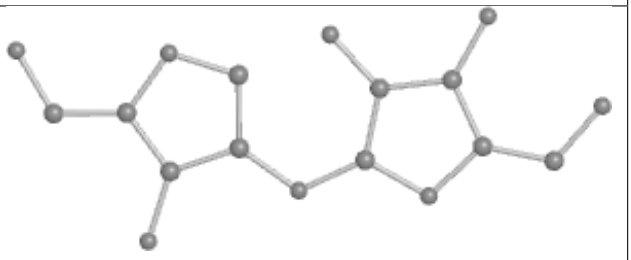
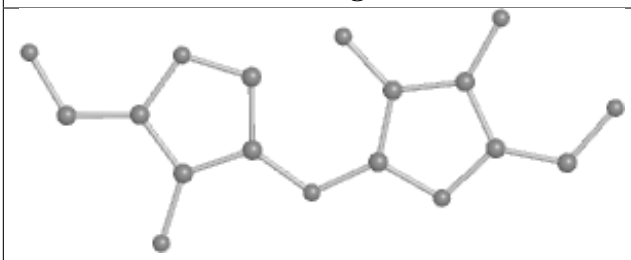
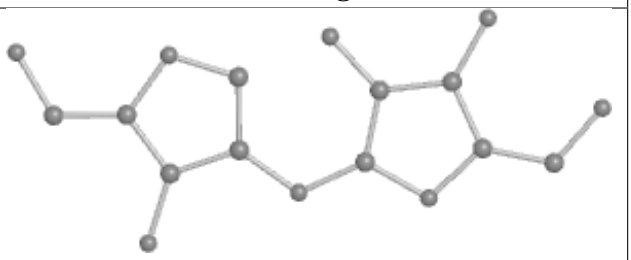
Oligosaccharide Chain c0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

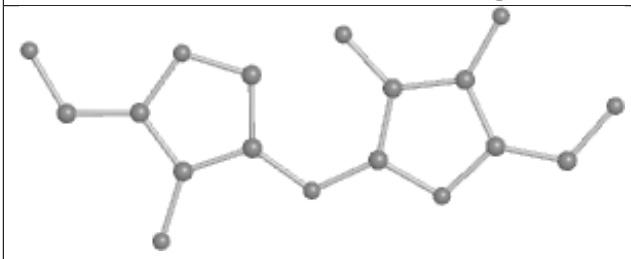
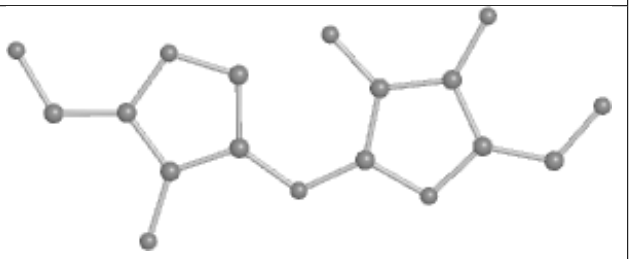
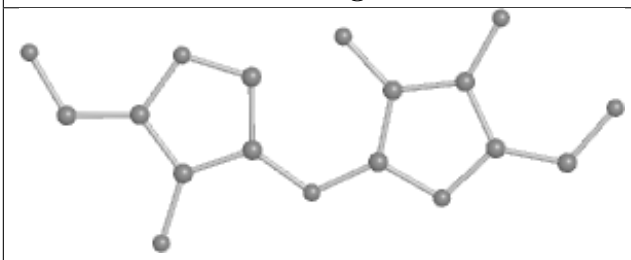
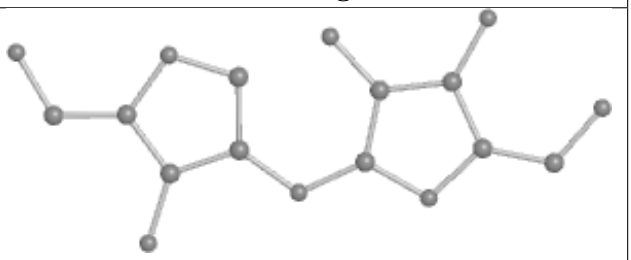
Oligosaccharide Chain c1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

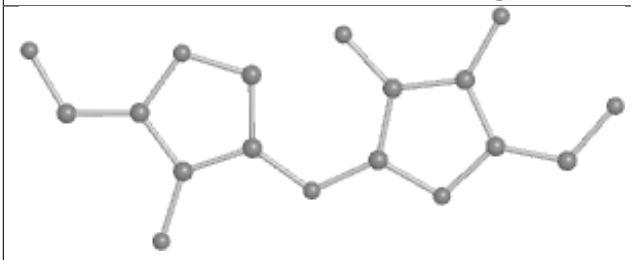
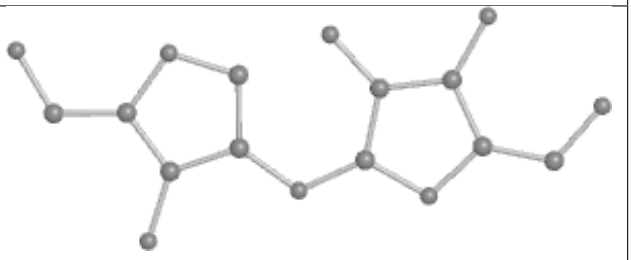
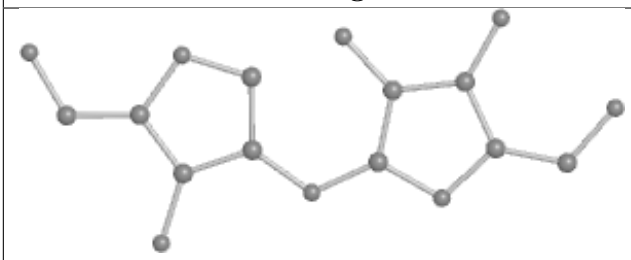
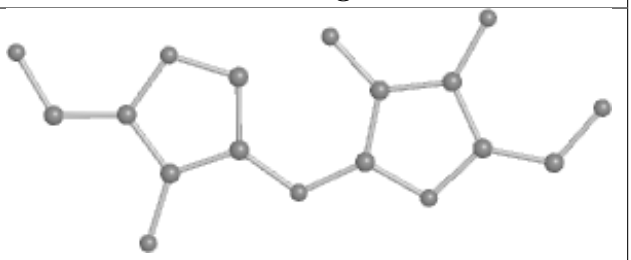
Oligosaccharide Chain c2	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

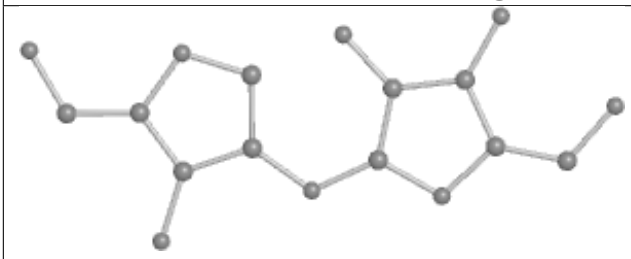
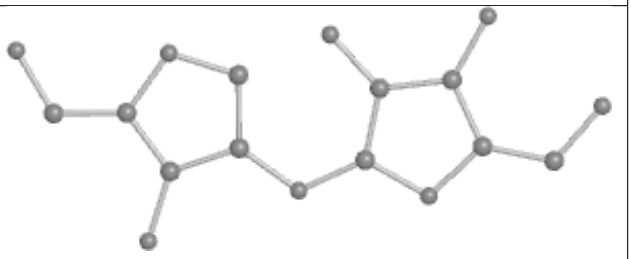
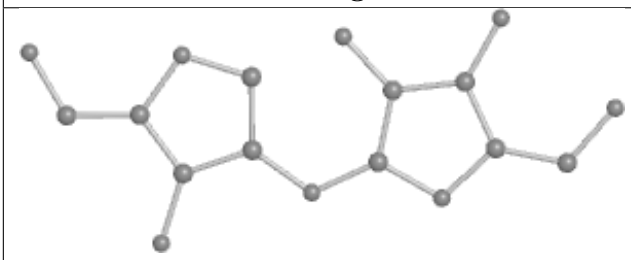
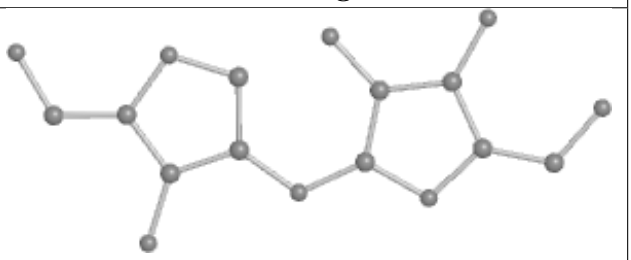
Oligosaccharide Chain c3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

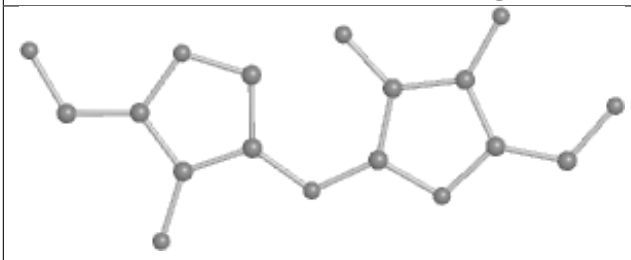
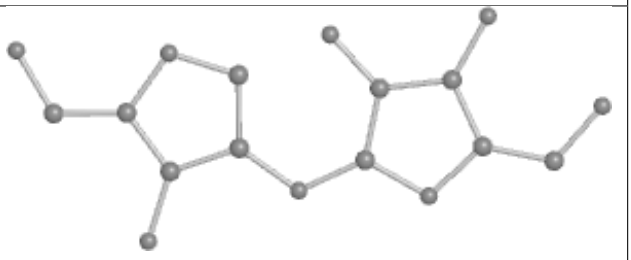
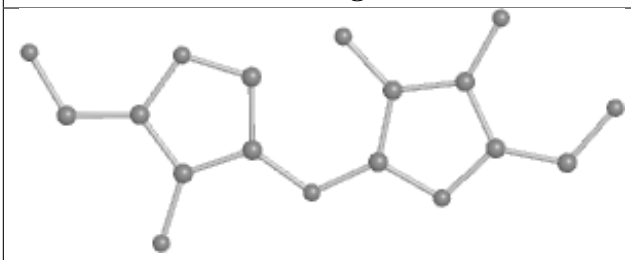
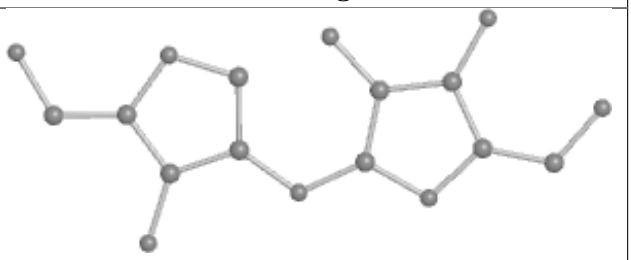
Oligosaccharide Chain c4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

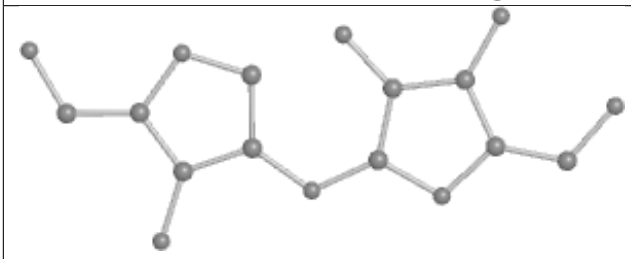
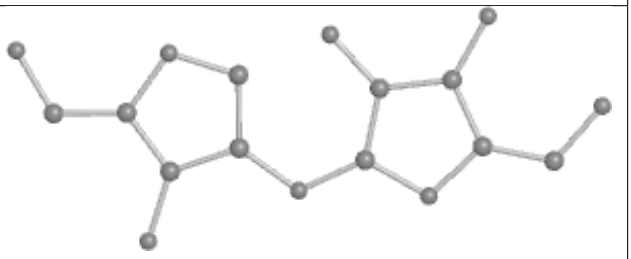
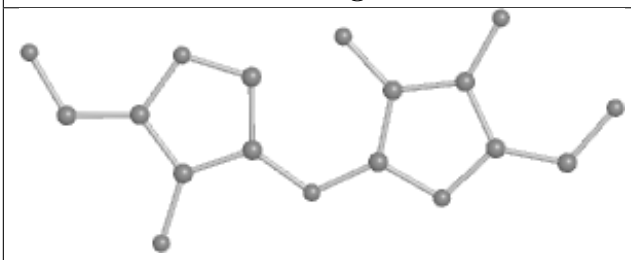
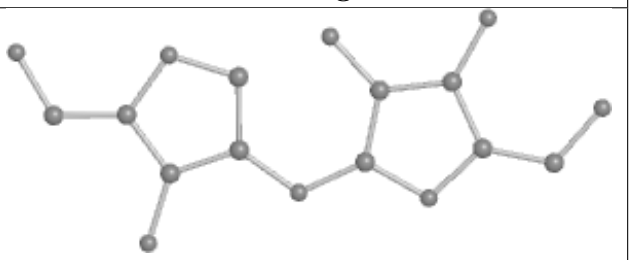
Oligosaccharide Chain c5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

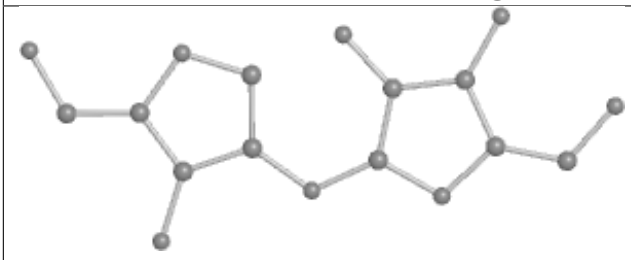
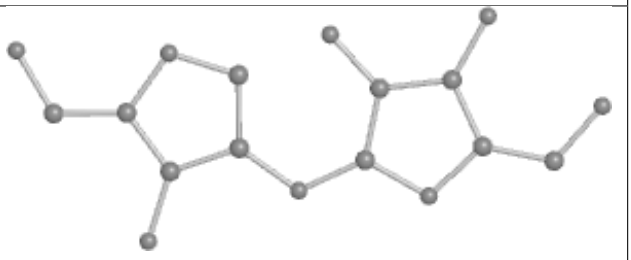
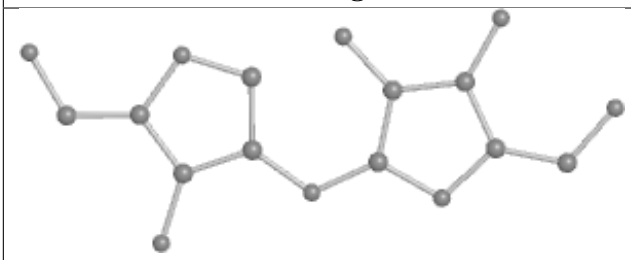
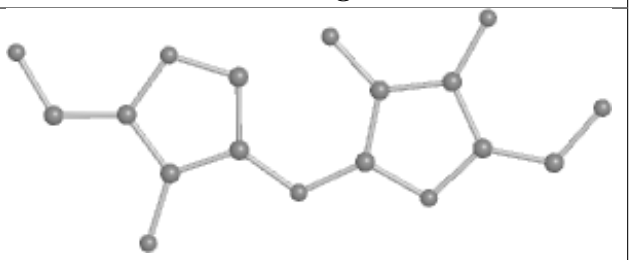
Oligosaccharide Chain c6	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

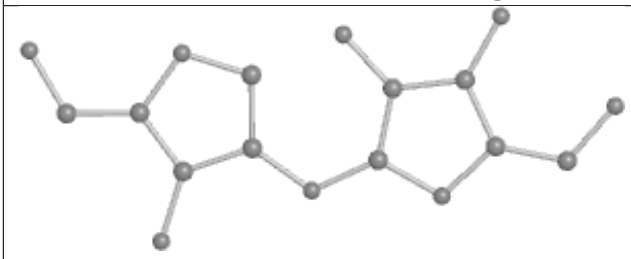
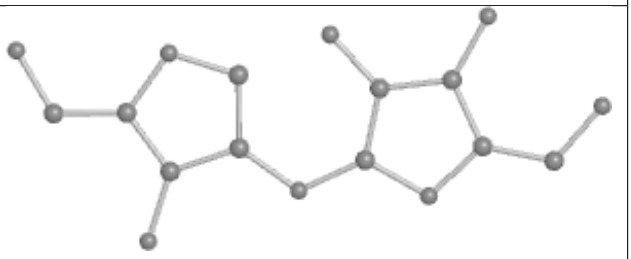
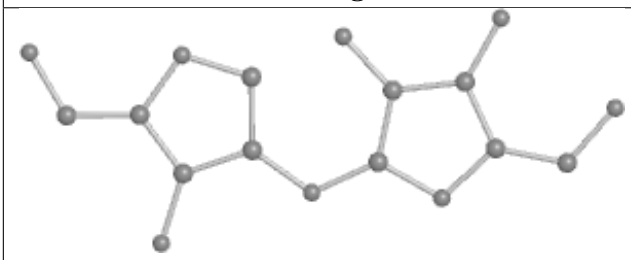
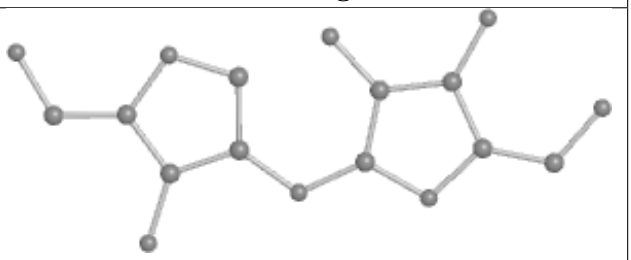
Oligosaccharide Chain c7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

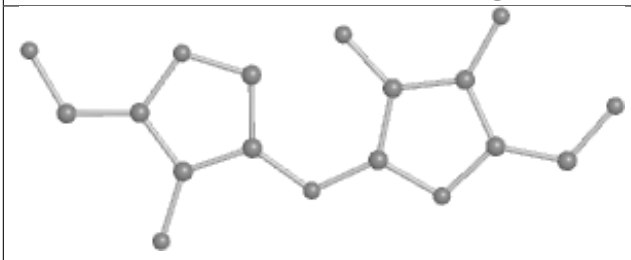
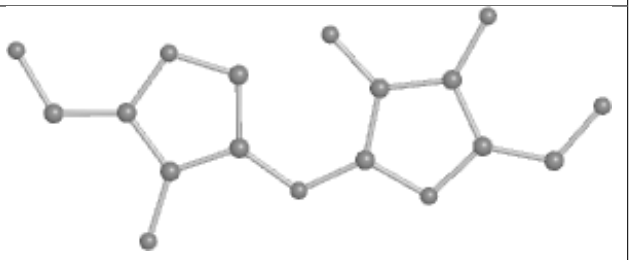
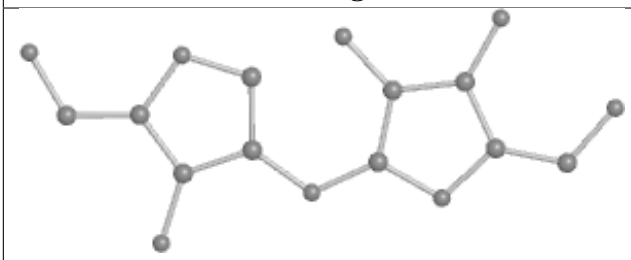
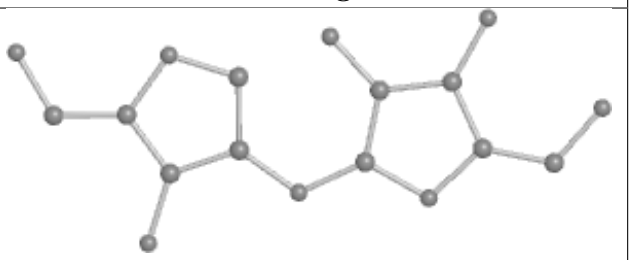
Oligosaccharide Chain c8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

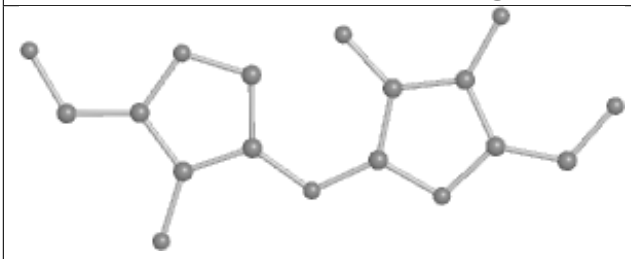
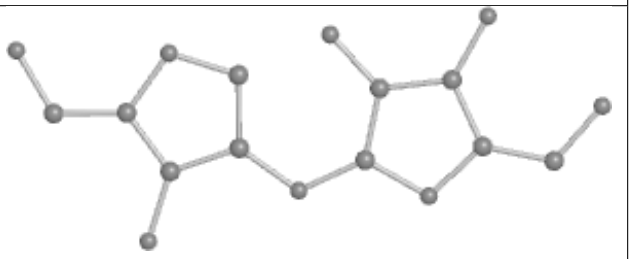
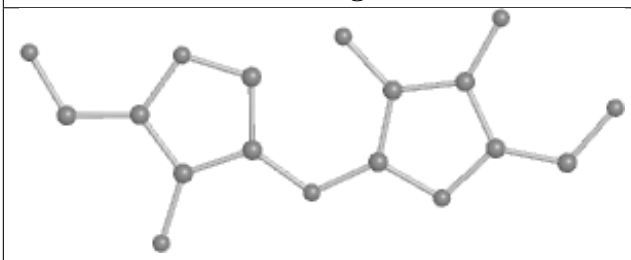
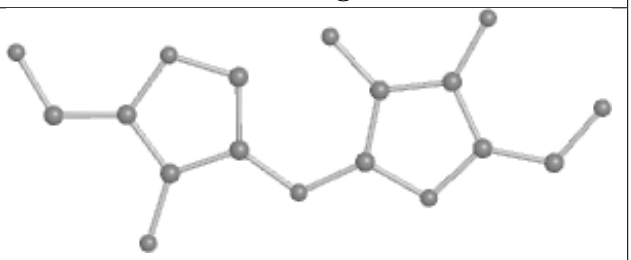
Oligosaccharide Chain c9	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

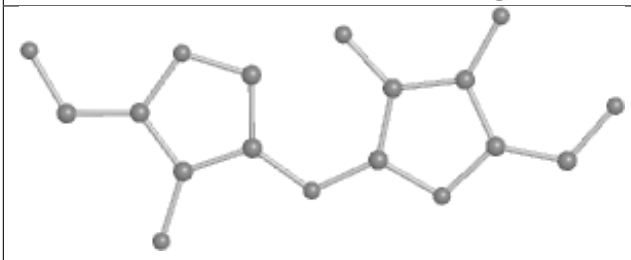
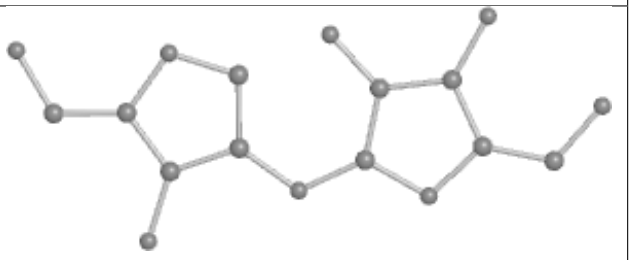
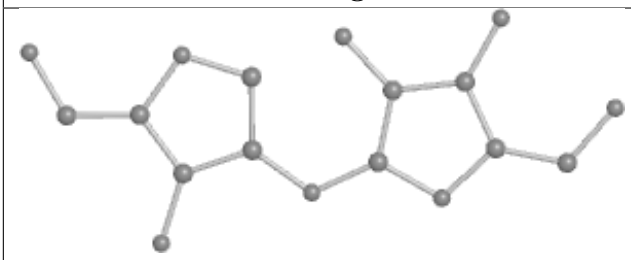
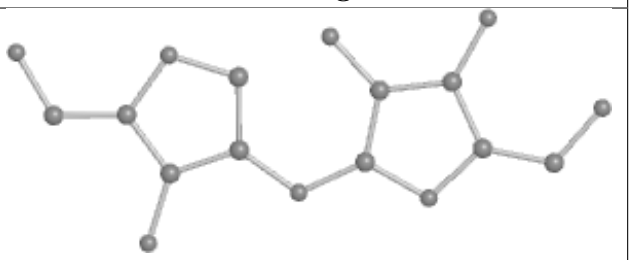
Oligosaccharide Chain d1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

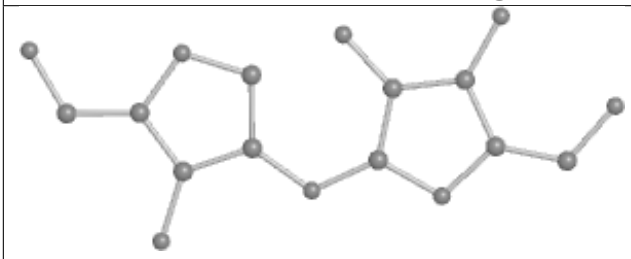
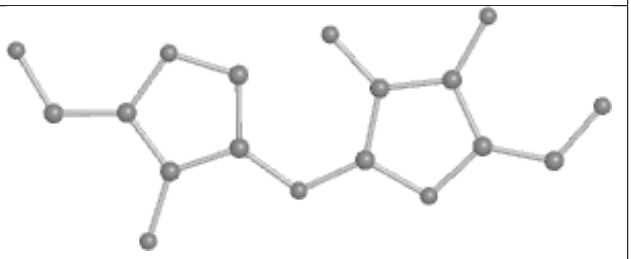
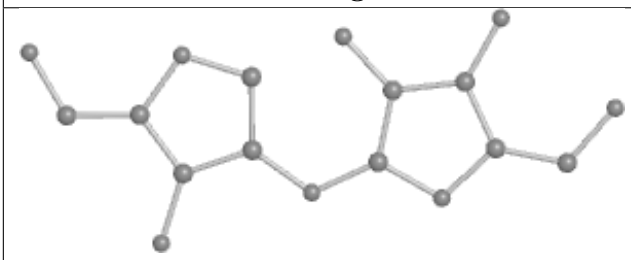
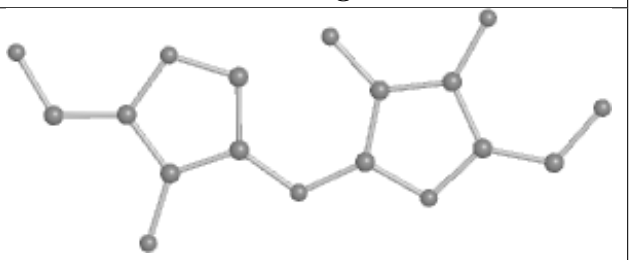
Oligosaccharide Chain d2	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

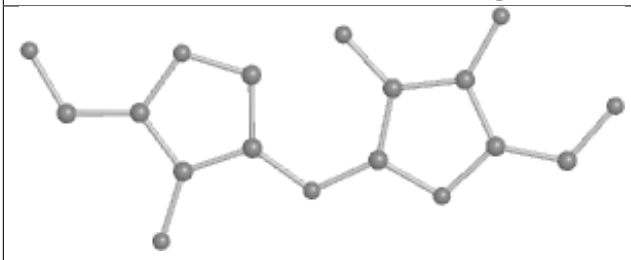
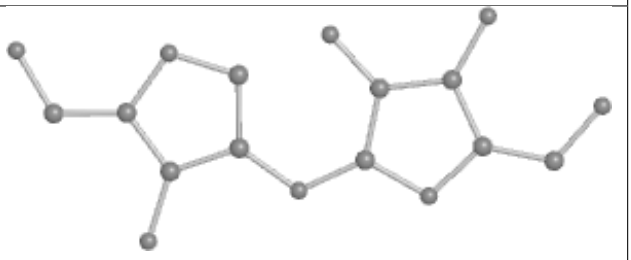
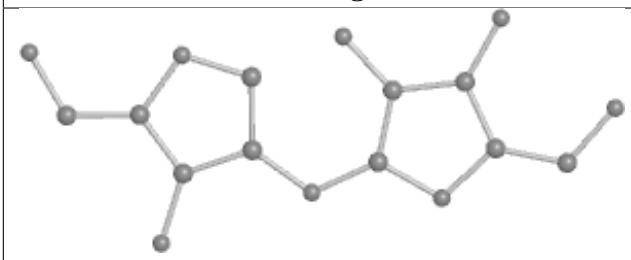
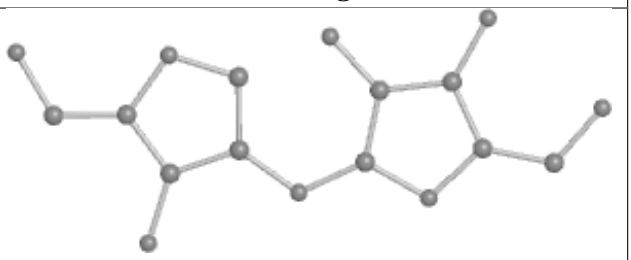
Oligosaccharide Chain d3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

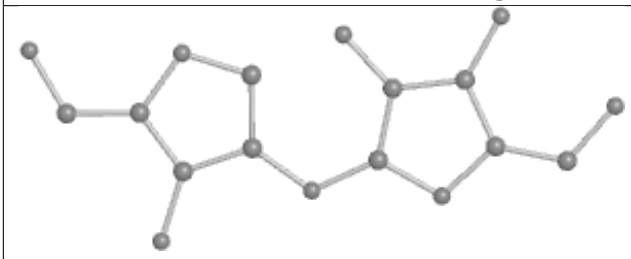
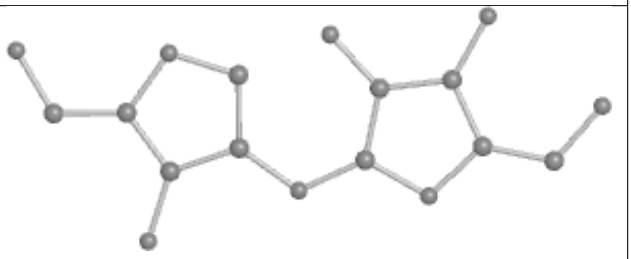
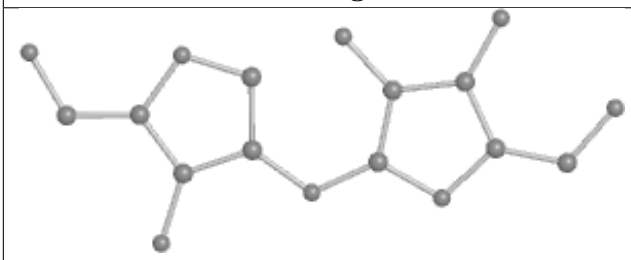
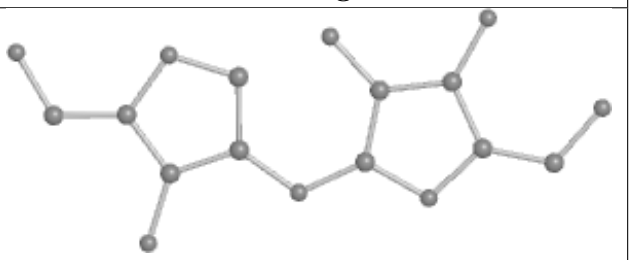
Oligosaccharide Chain d4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

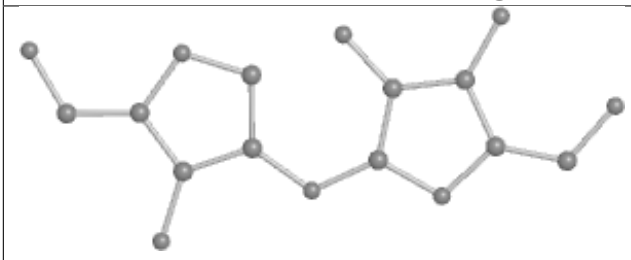
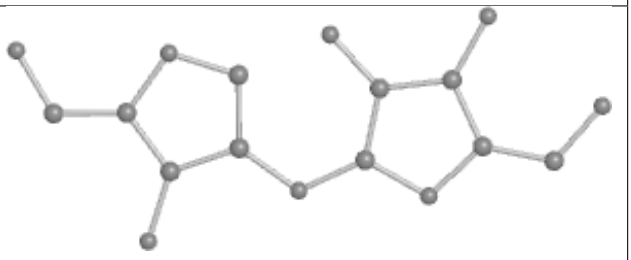
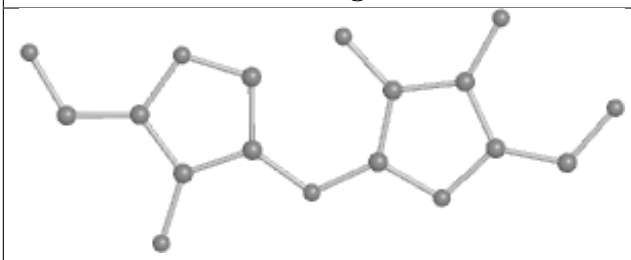
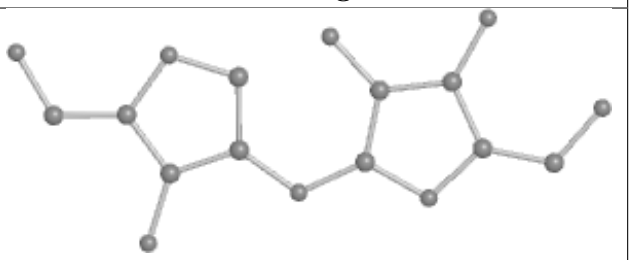
Oligosaccharide Chain d5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

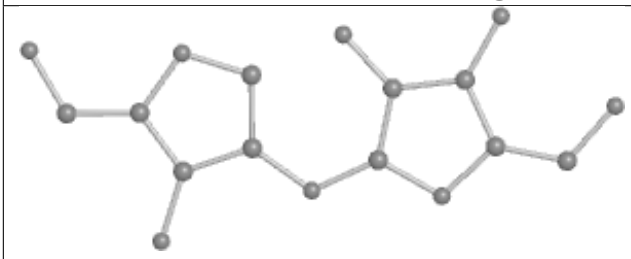
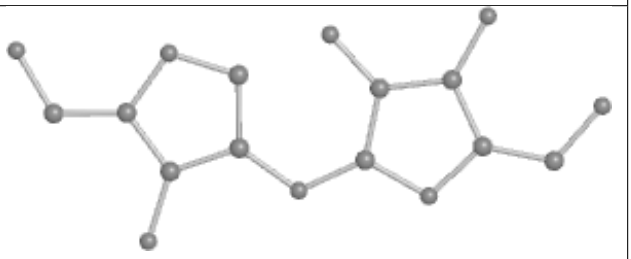
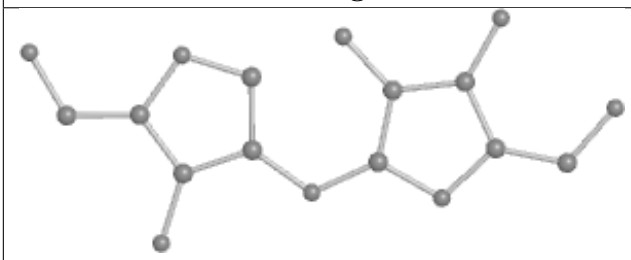
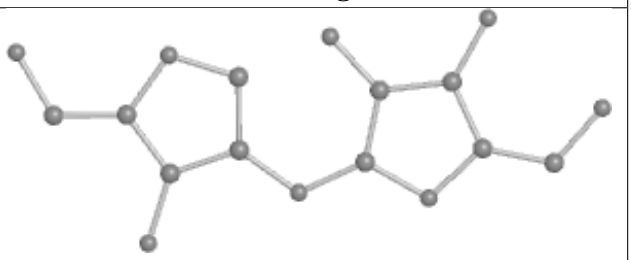
Oligosaccharide Chain e0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

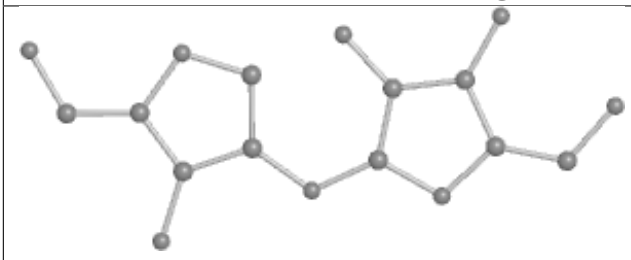
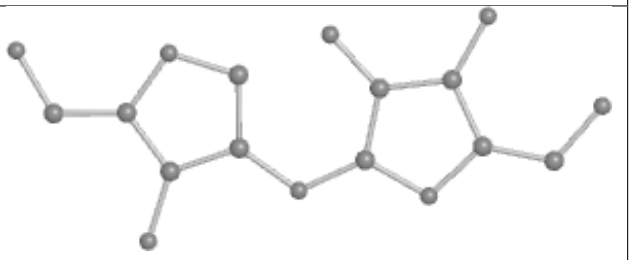
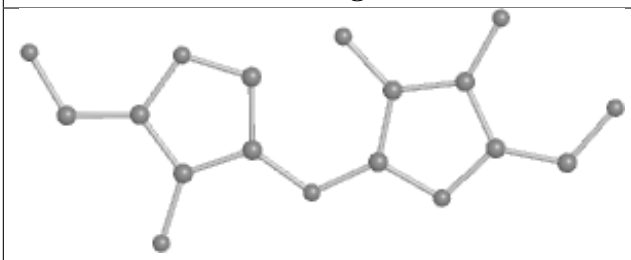
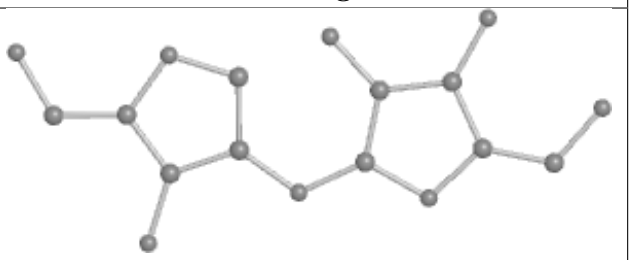
Oligosaccharide Chain e1	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

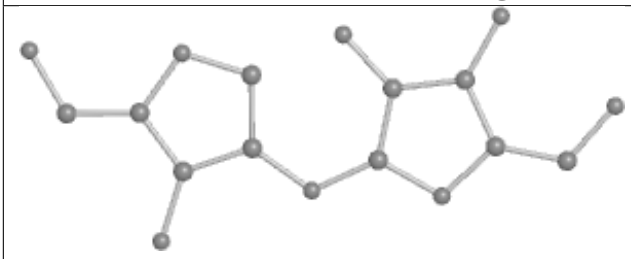
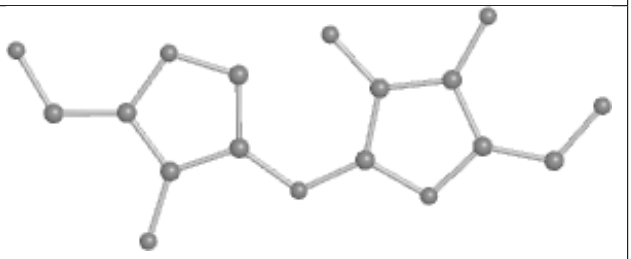
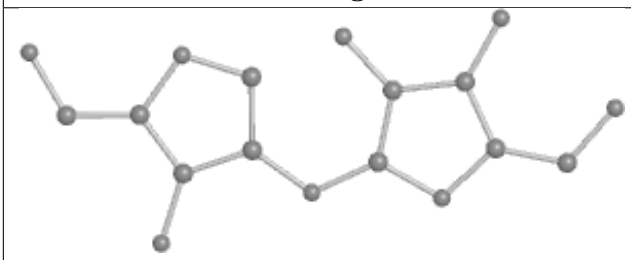
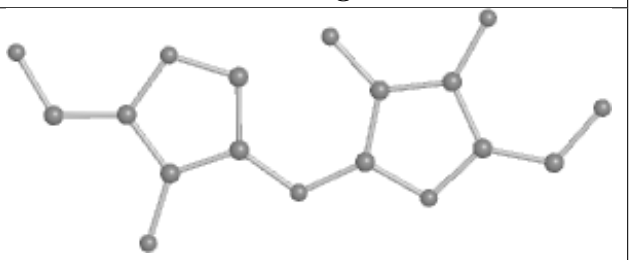
Oligosaccharide Chain e2	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

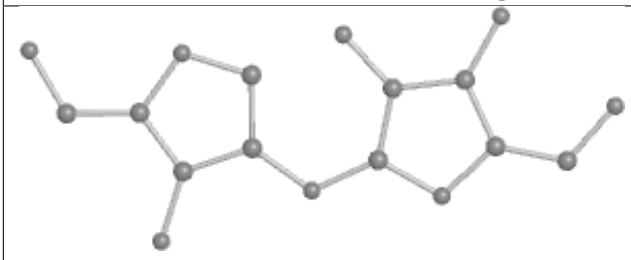
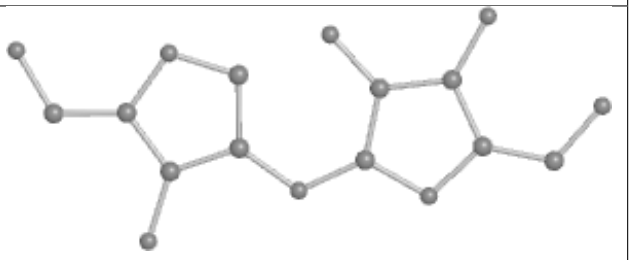
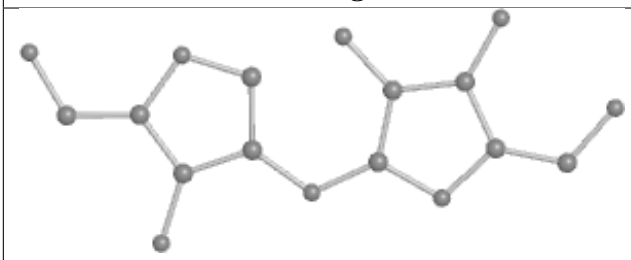
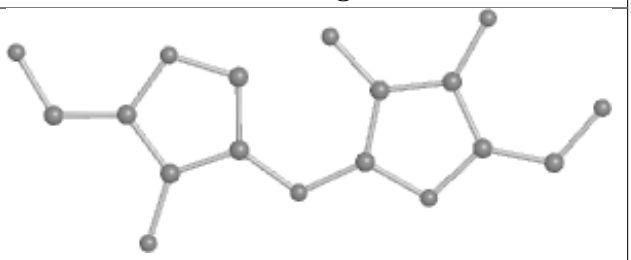
Oligosaccharide Chain e4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

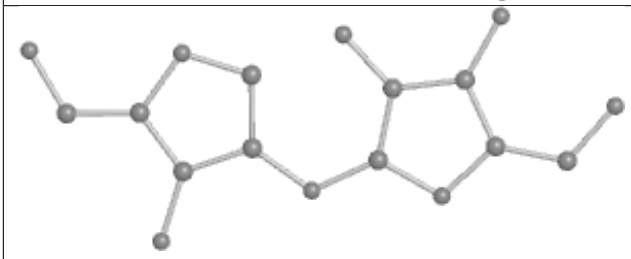
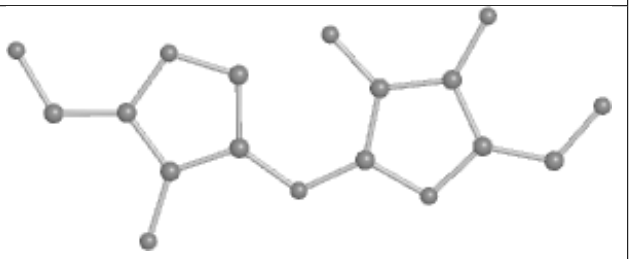
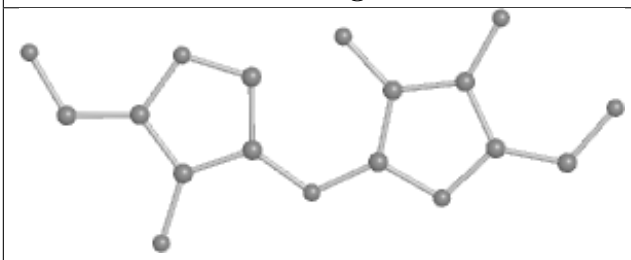
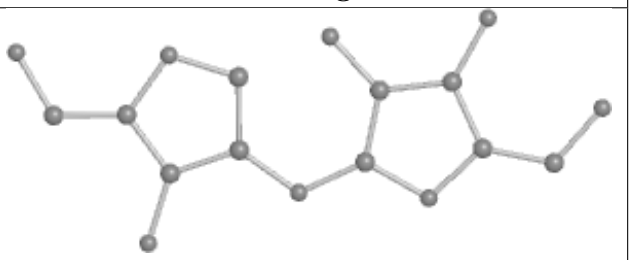
Oligosaccharide Chain e5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

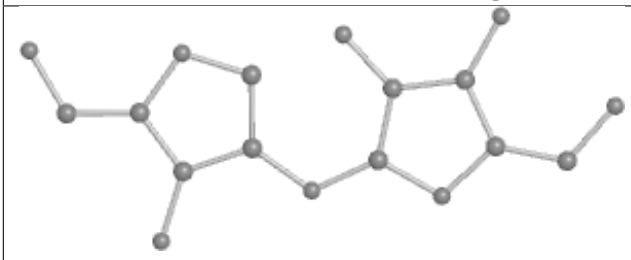
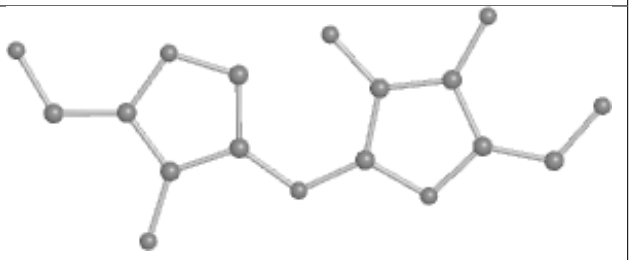
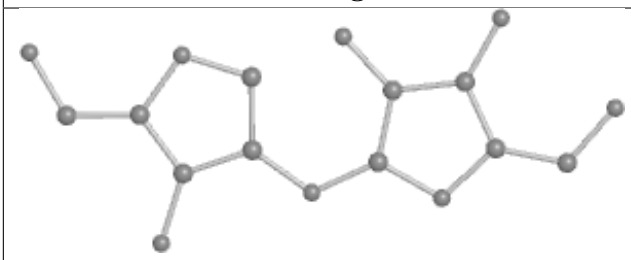
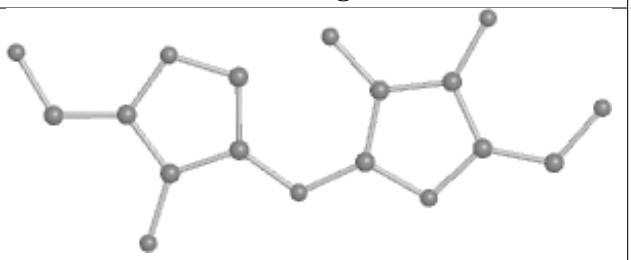
Oligosaccharide Chain e8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

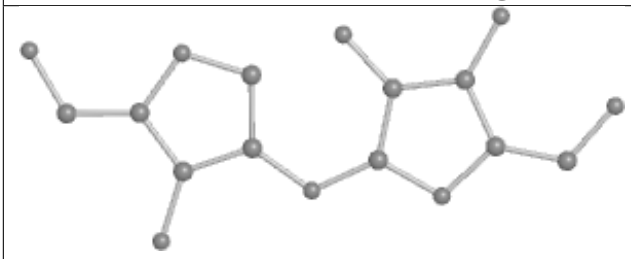
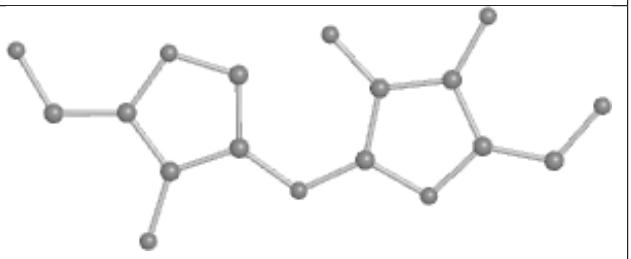
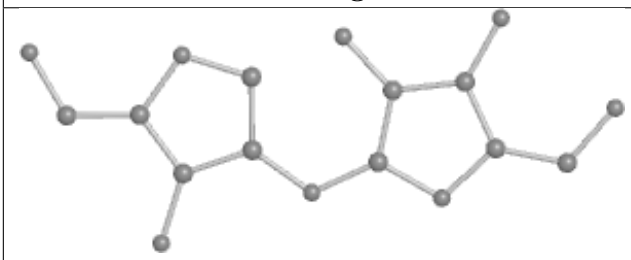
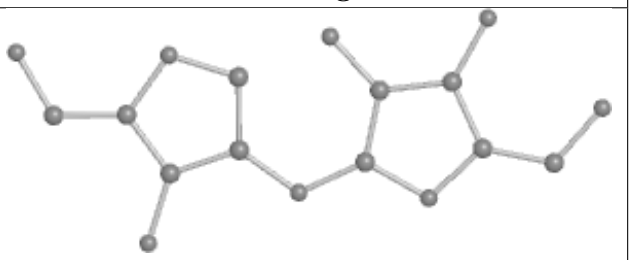
Oligosaccharide Chain f0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

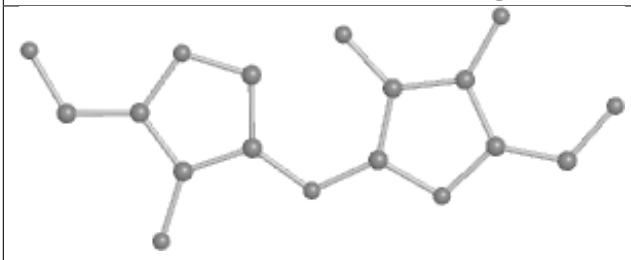
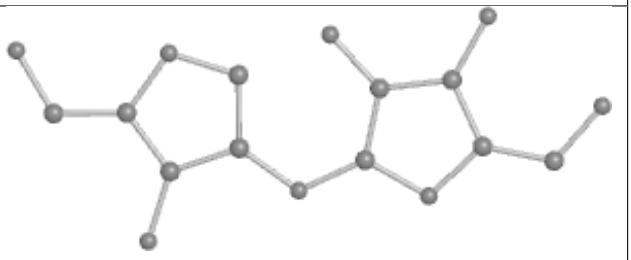
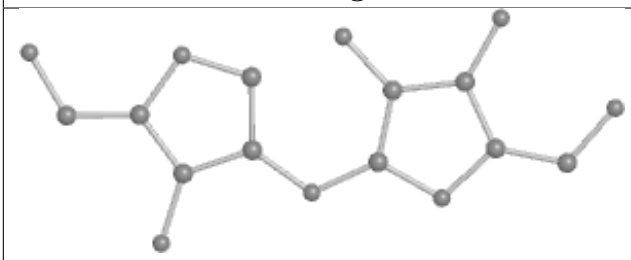
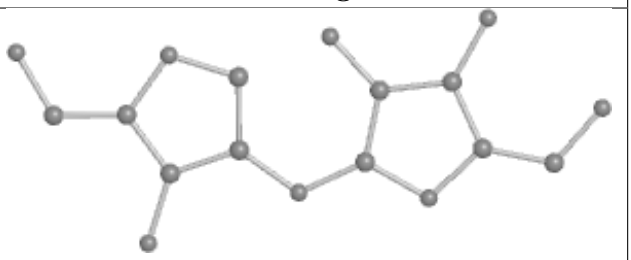
Oligosaccharide Chain f3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

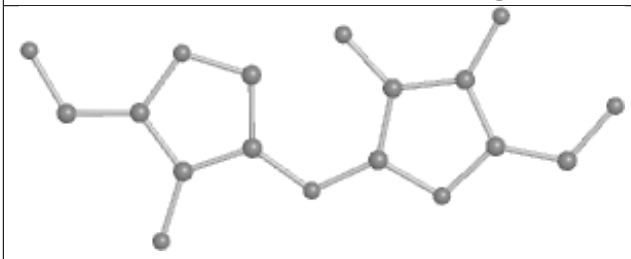
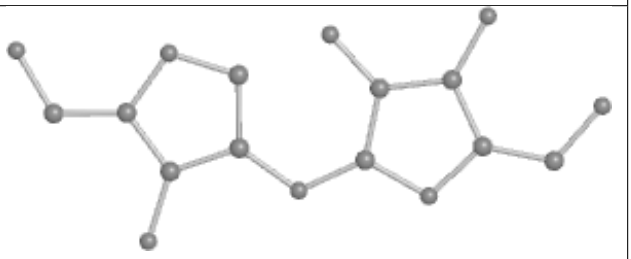
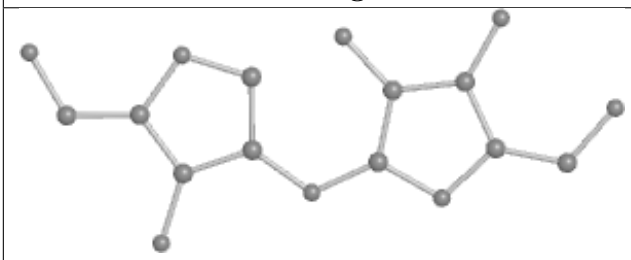
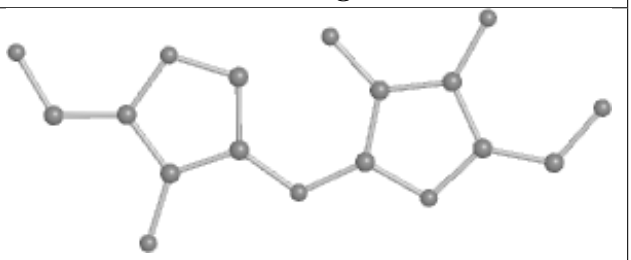
Oligosaccharide Chain f5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

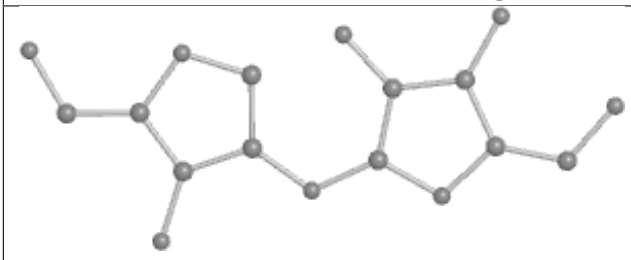
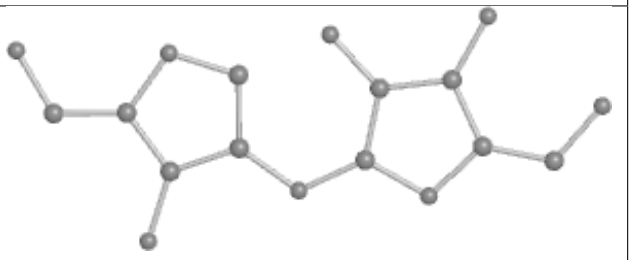
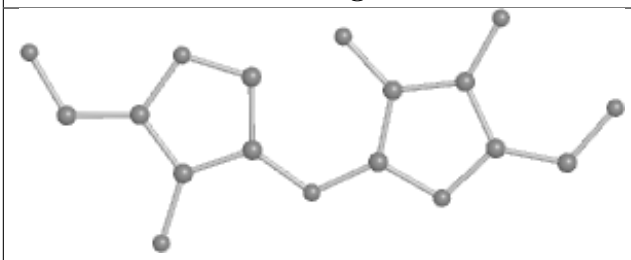
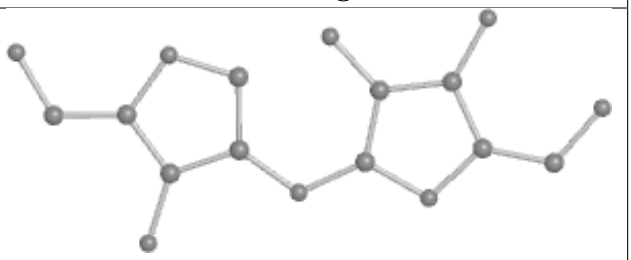
Oligosaccharide Chain f8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

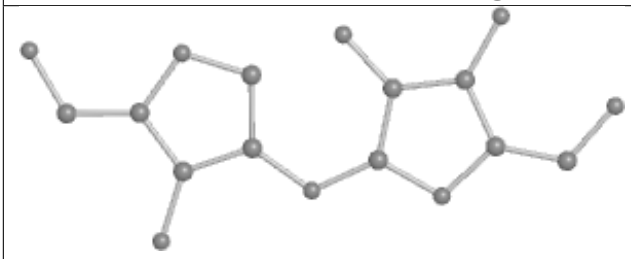
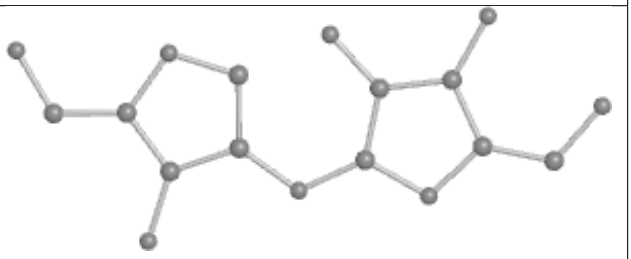
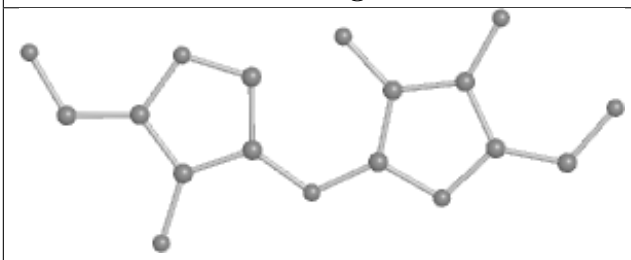
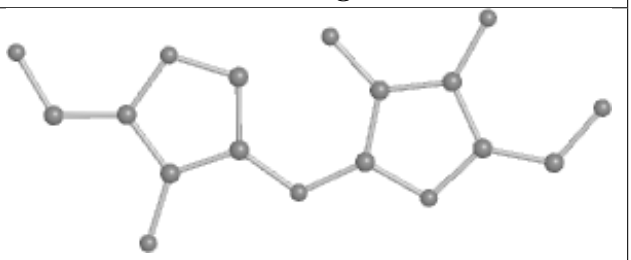
Oligosaccharide Chain E3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

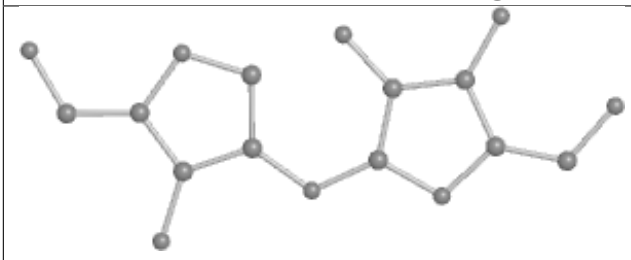
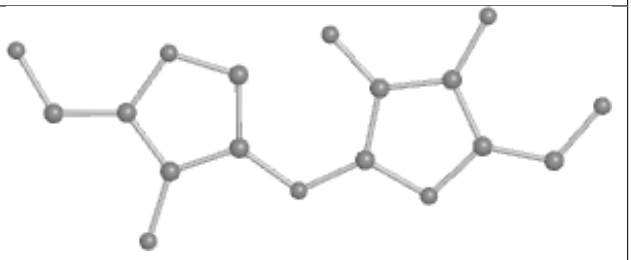
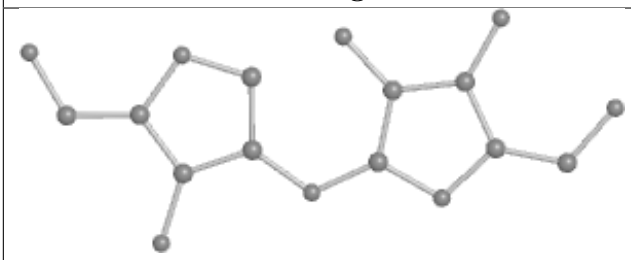
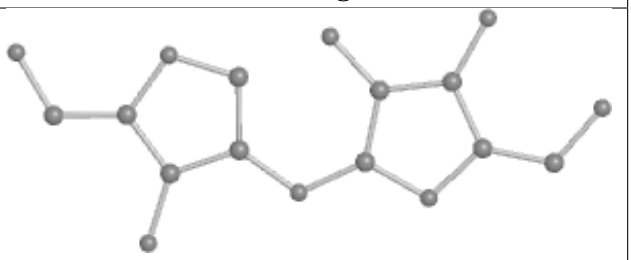
Oligosaccharide Chain f2	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

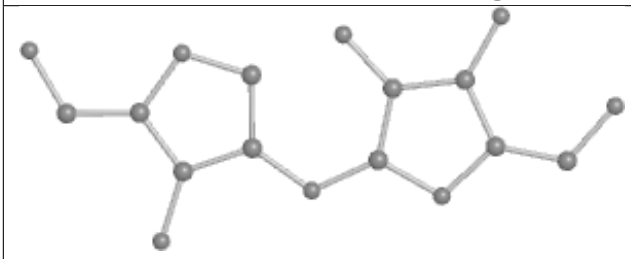
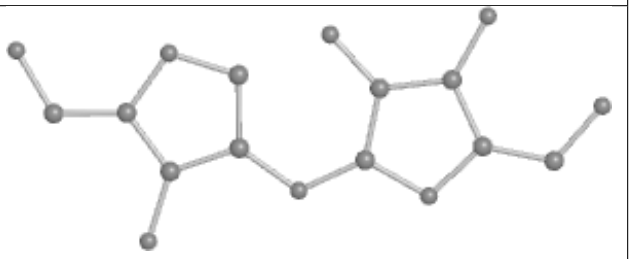
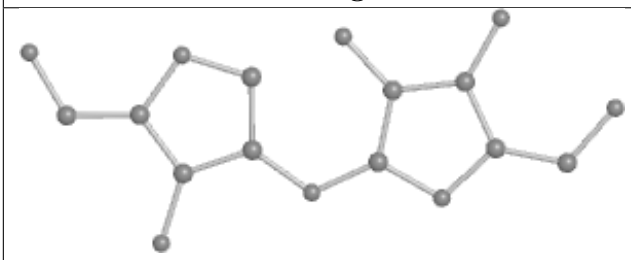
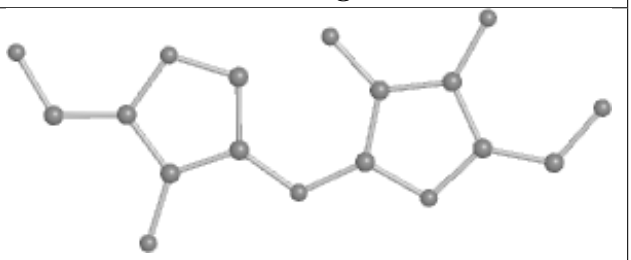
Oligosaccharide Chain e7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

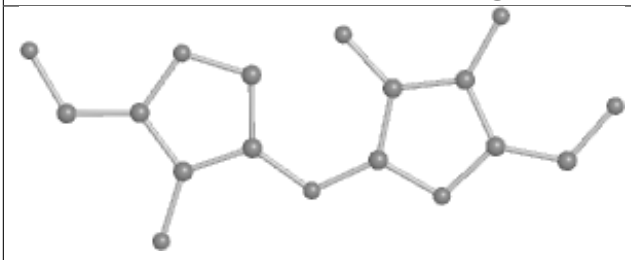
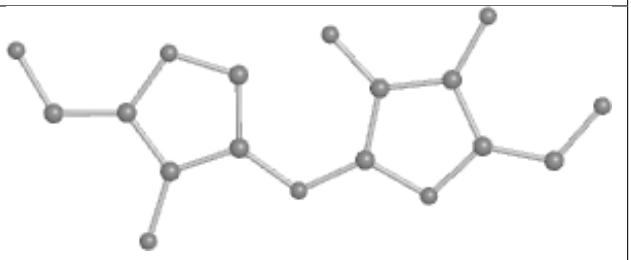
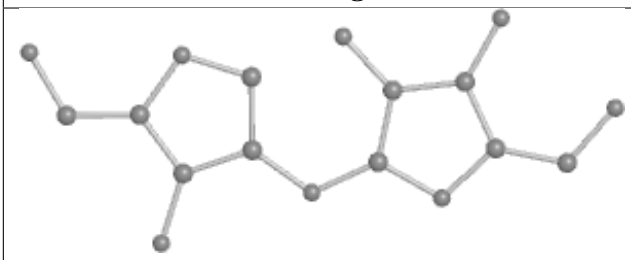
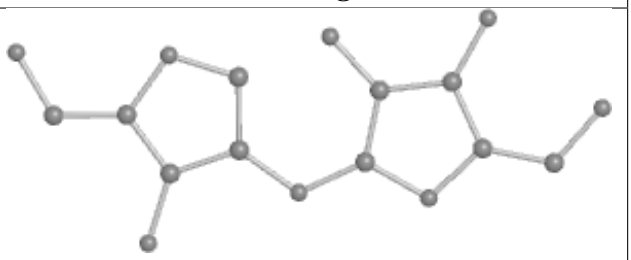
Oligosaccharide Chain e6	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

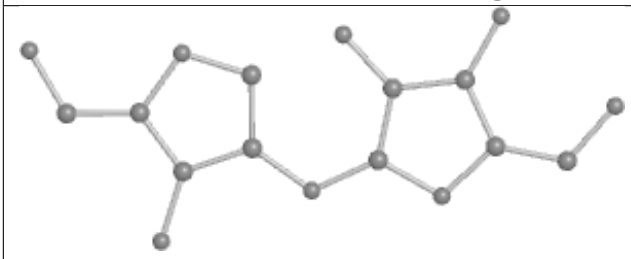
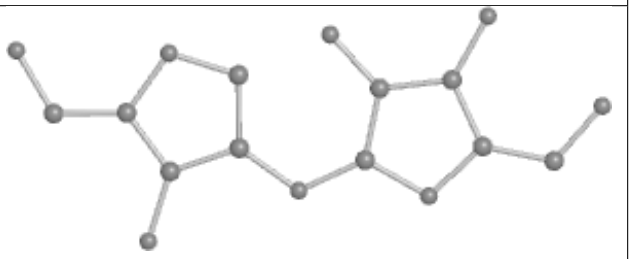
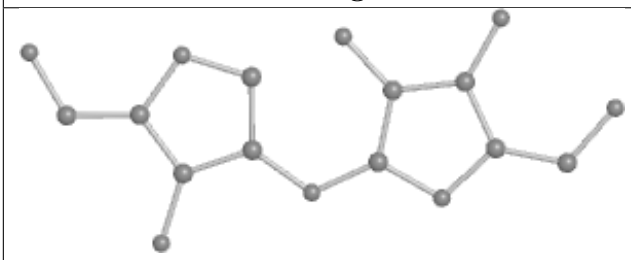
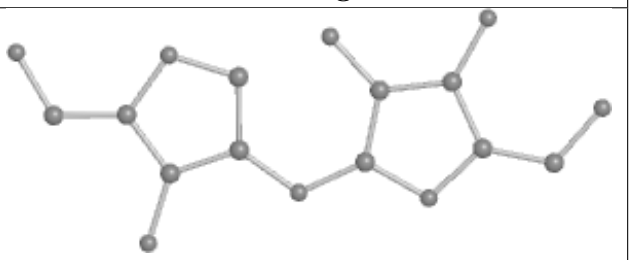
Oligosaccharide Chain e3	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

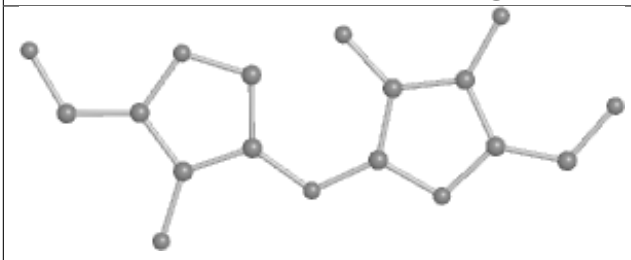
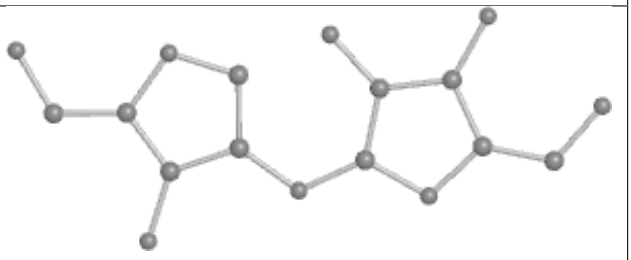
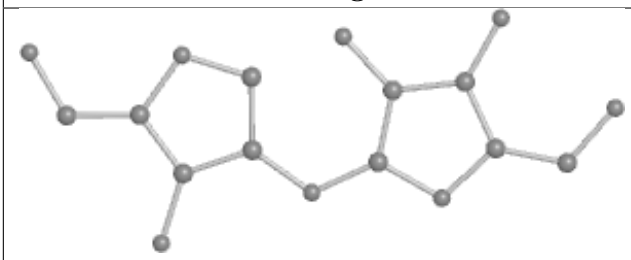
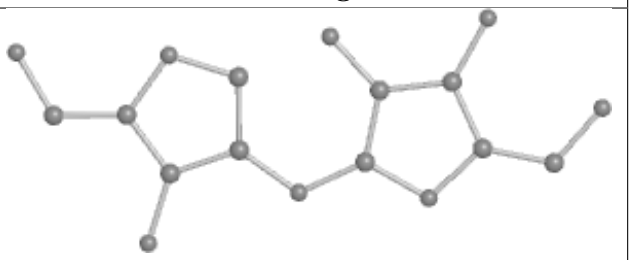
Oligosaccharide Chain d9	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

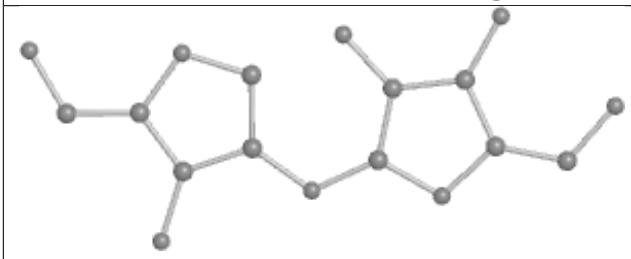
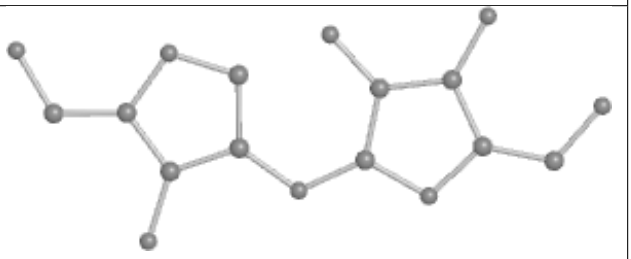
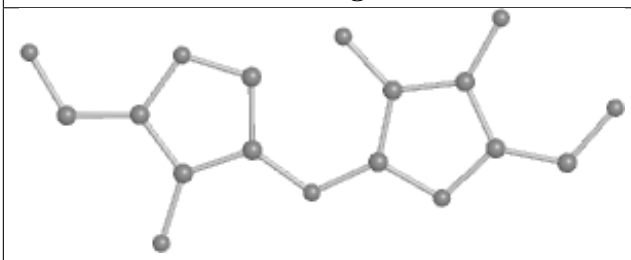
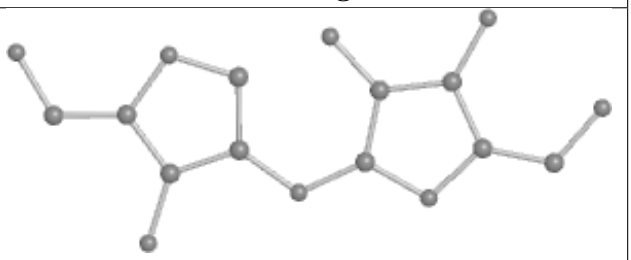
Oligosaccharide Chain d7	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain d8	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

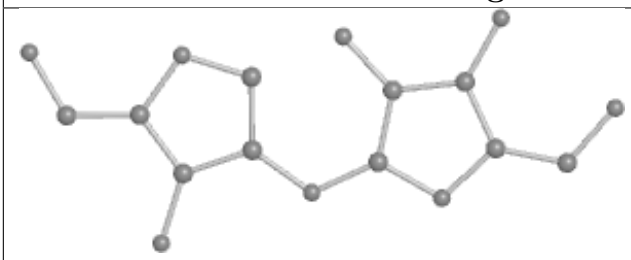
Oligosaccharide Chain d6	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain d0	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

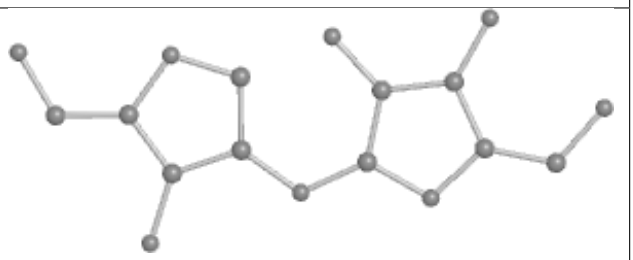
Oligosaccharide Chain F5	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain F2	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

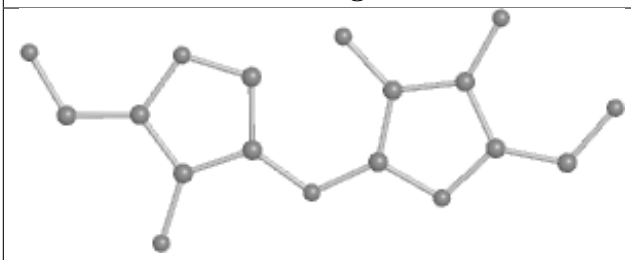
Oligosaccharide Chain E7



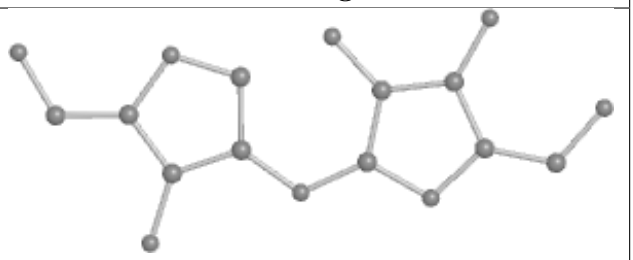
Bond lengths



Bond angles

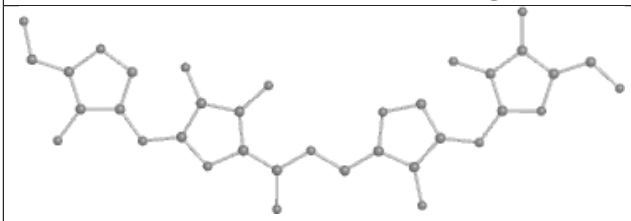


Torsions

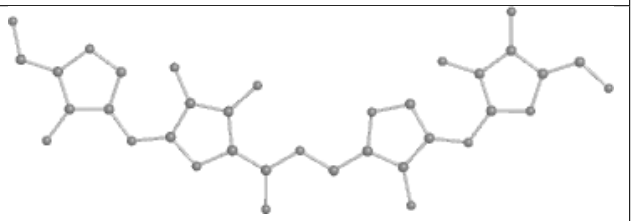


Rings

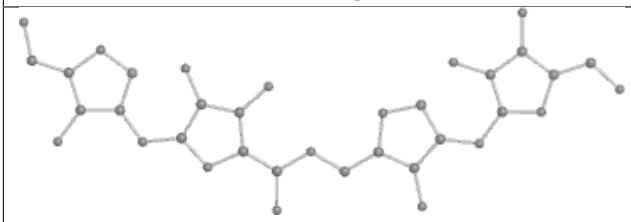
Oligosaccharide Chain A6



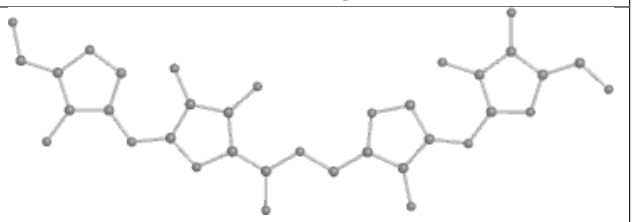
Bond lengths



Bond angles

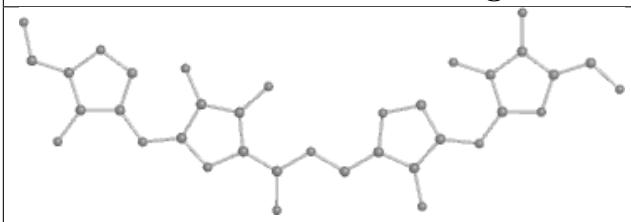


Torsions

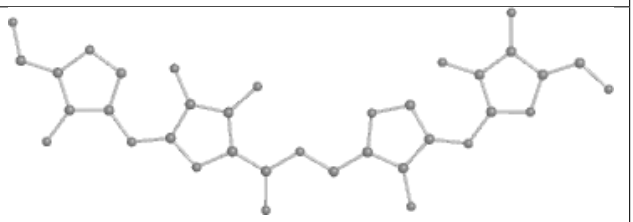


Rings

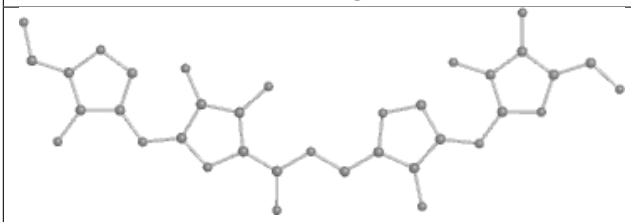
Oligosaccharide Chain A9



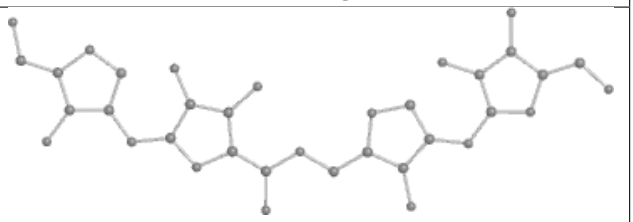
Bond lengths



Bond angles

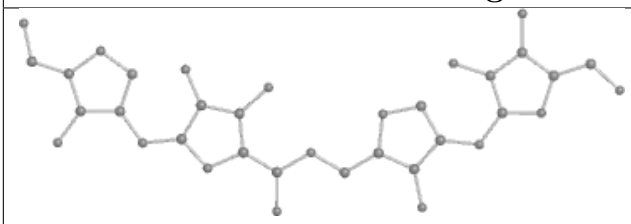


Torsions

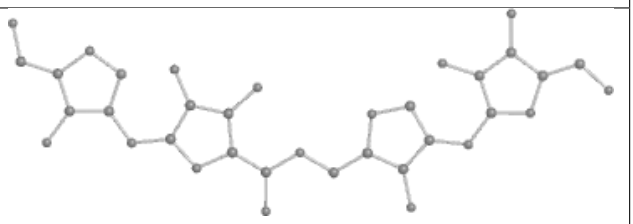


Rings

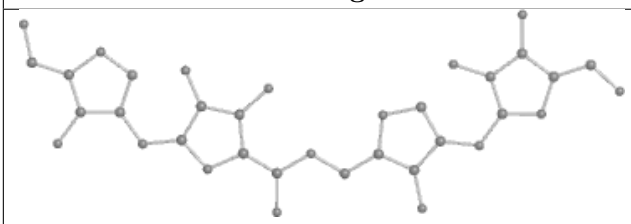
Oligosaccharide Chain B6



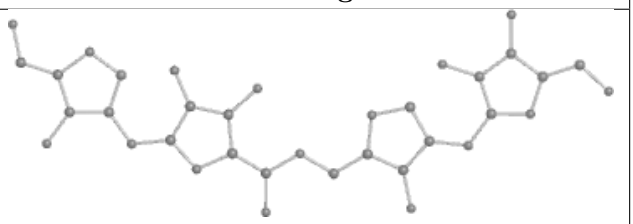
Bond lengths



Bond angles

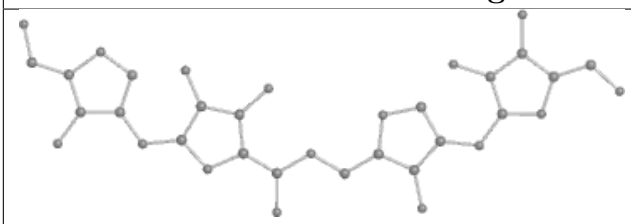


Torsions

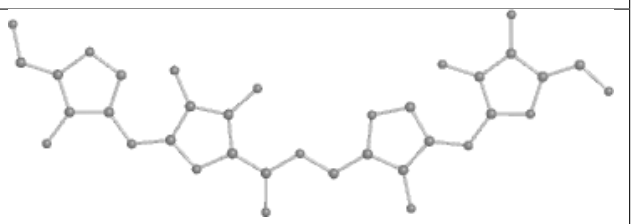


Rings

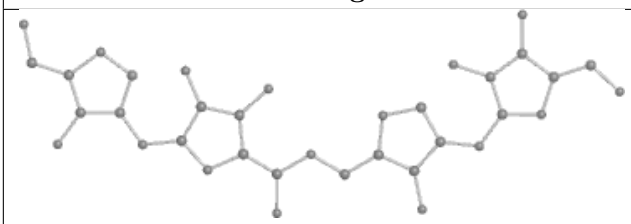
Oligosaccharide Chain F6



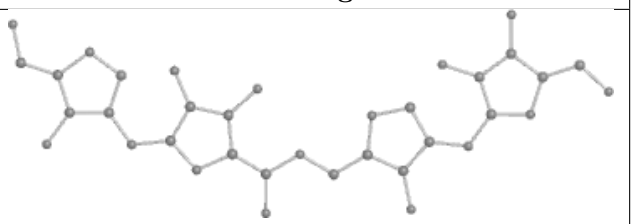
Bond lengths



Bond angles

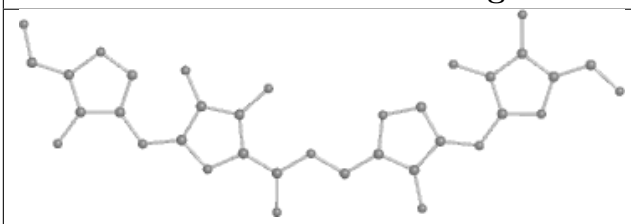


Torsions

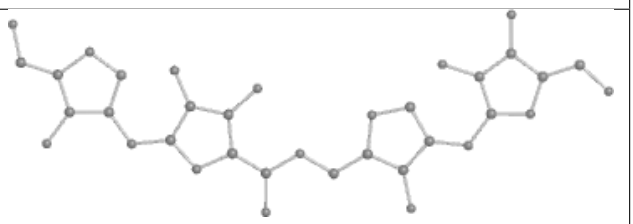


Rings

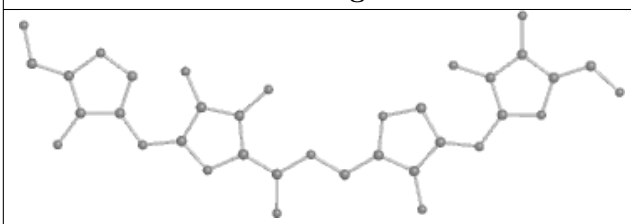
Oligosaccharide Chain F7



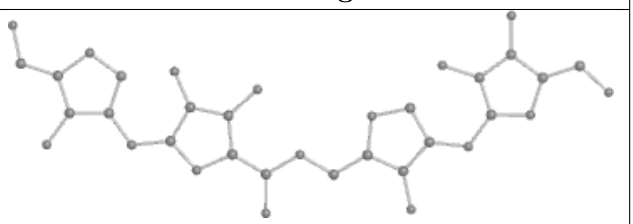
Bond lengths



Bond angles

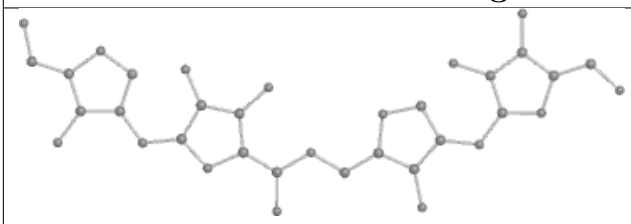


Torsions

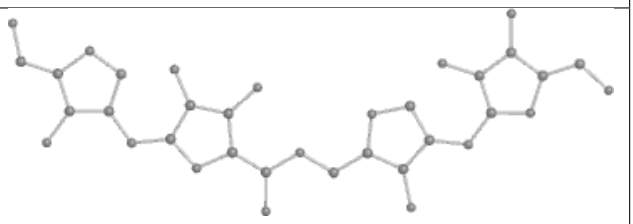


Rings

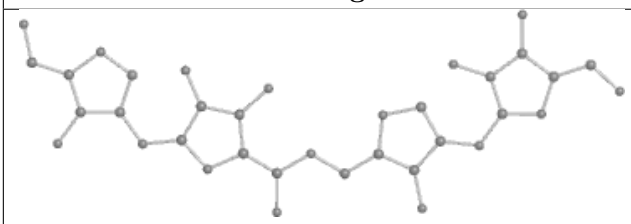
Oligosaccharide Chain a6



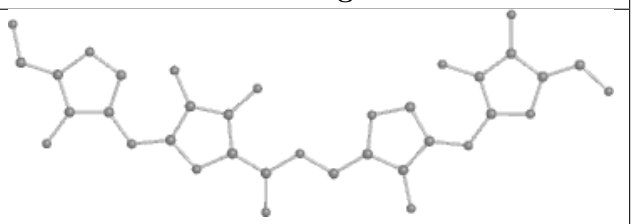
Bond lengths



Bond angles

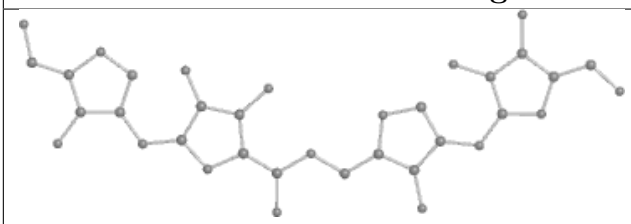


Torsions

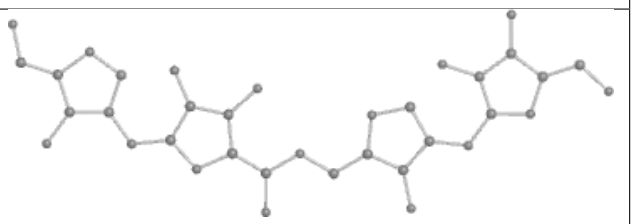


Rings

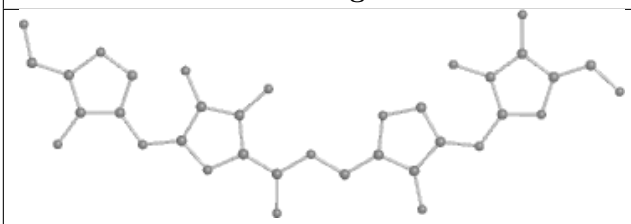
Oligosaccharide Chain a9



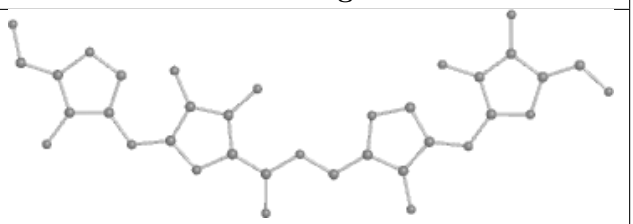
Bond lengths



Bond angles

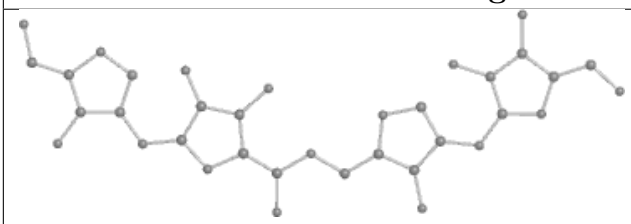


Torsions

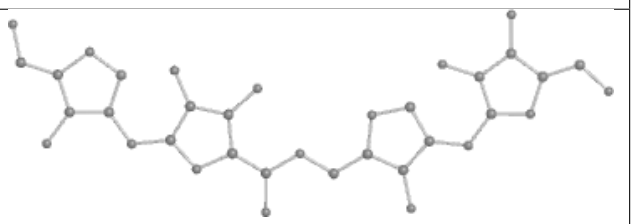


Rings

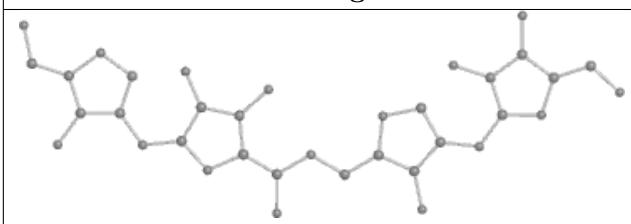
Oligosaccharide Chain b6



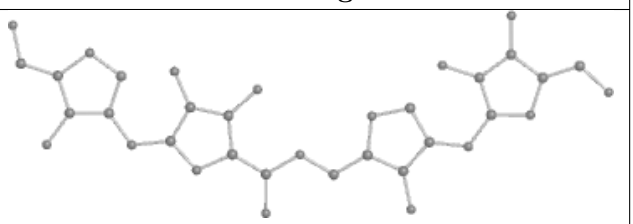
Bond lengths



Bond angles

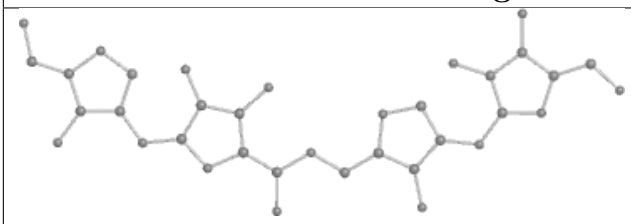


Torsions

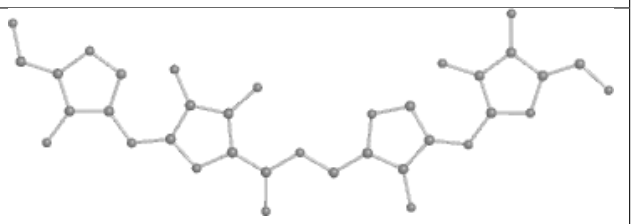


Rings

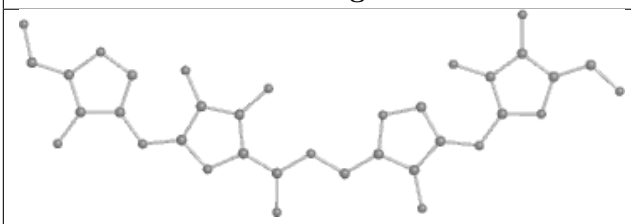
Oligosaccharide Chain f6



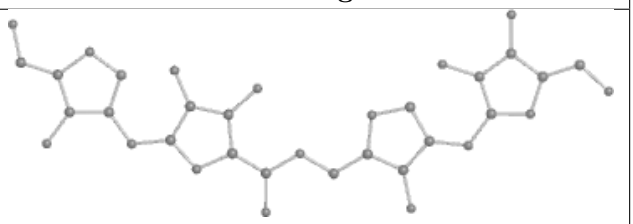
Bond lengths



Bond angles

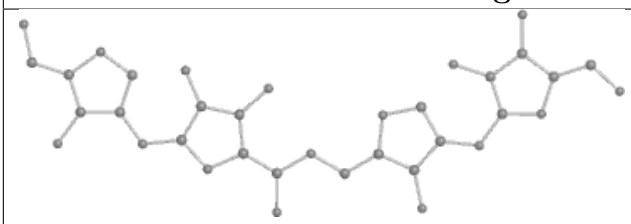


Torsions

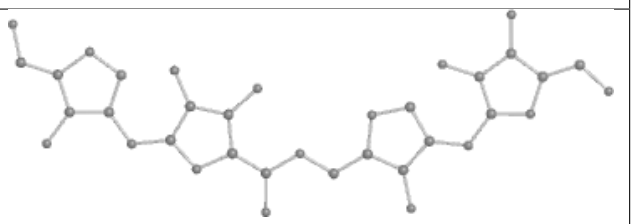


Rings

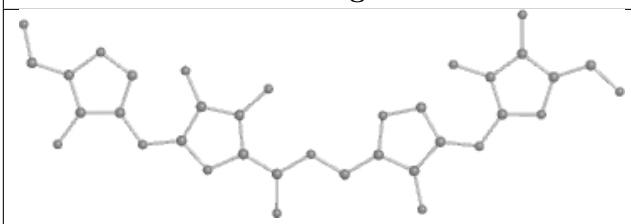
Oligosaccharide Chain f7



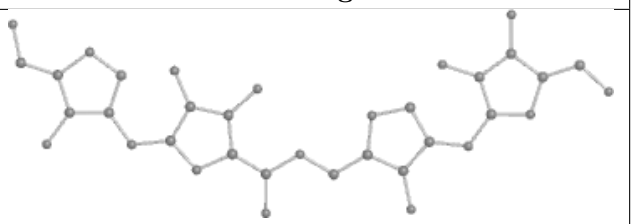
Bond lengths



Bond angles

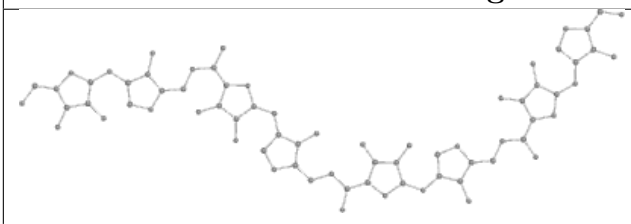


Torsions

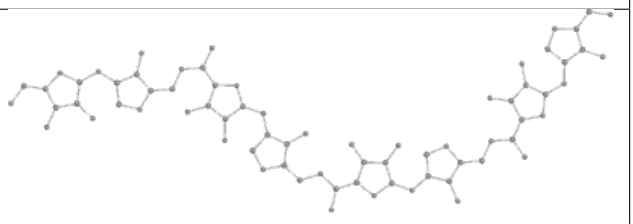


Rings

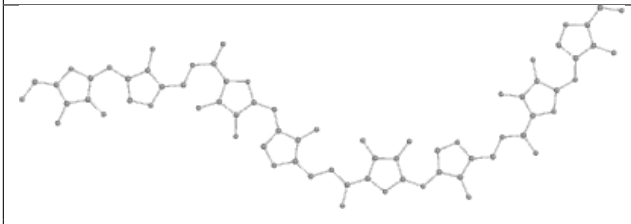
Oligosaccharide Chain E6



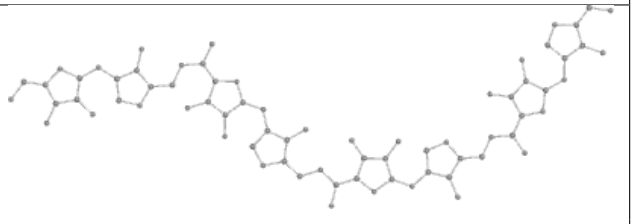
Bond lengths



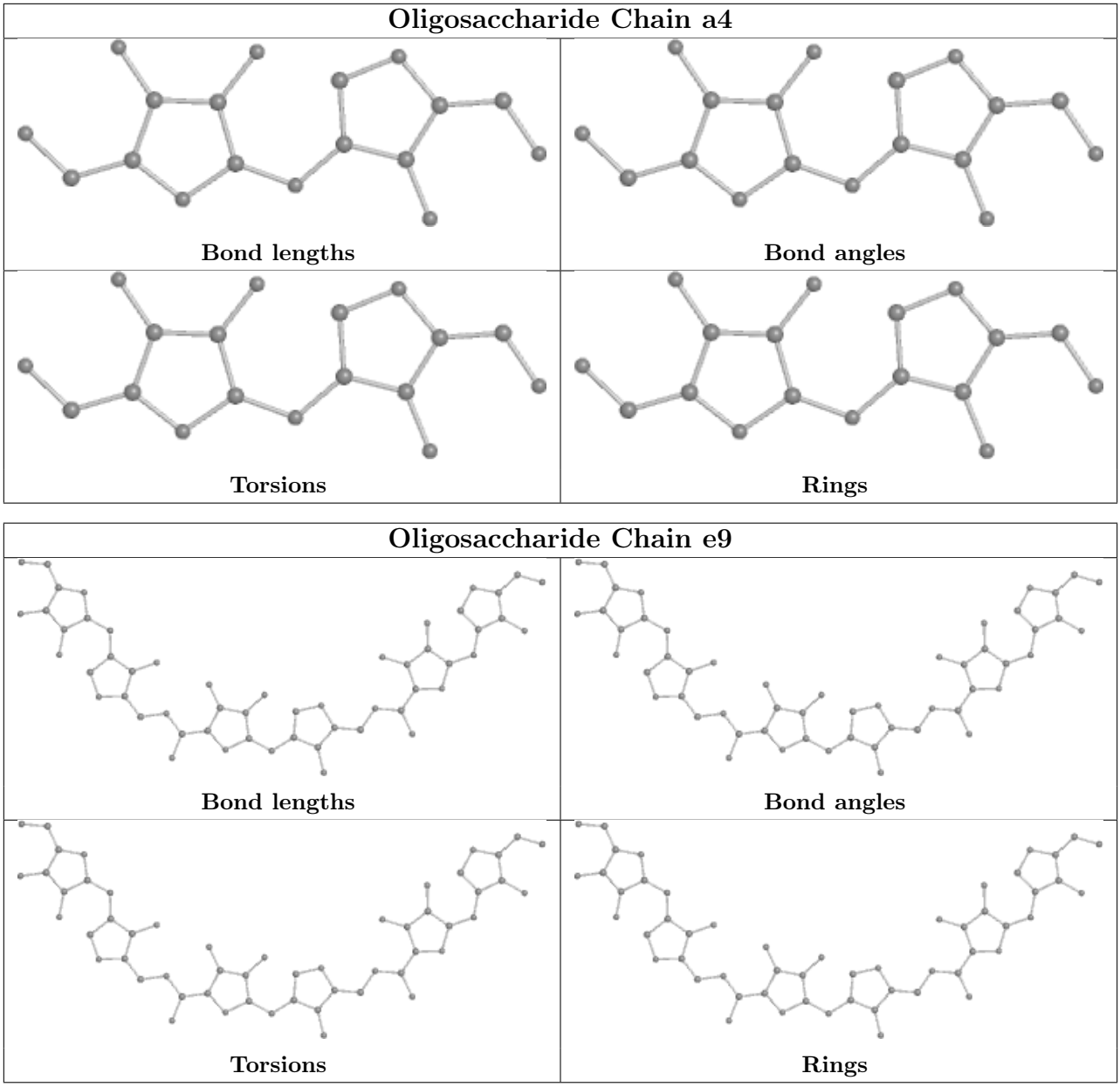
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

140 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	A1AIO	B	2030	4	11,11,12	5.66	6 (54%)	14,15,17	1.55	2 (14%)
10	GLA	A	2063	1	11,11,12	1.74	3 (27%)	15,15,17	1.00	1 (6%)
9	A1AIO	A	2028	4	11,11,12	5.71	6 (54%)	14,15,17	1.46	2 (14%)
10	GLA	A	2058	1	11,11,12	1.71	3 (27%)	15,15,17	0.98	1 (6%)
9	A1AIO	B	2051	5	11,11,12	5.69	6 (54%)	14,15,17	1.43	2 (14%)
9	A1AIO	A	2039	6	11,11,12	5.70	6 (54%)	14,15,17	1.62	3 (21%)
9	A1AIO	A	2040	4	11,11,12	5.66	6 (54%)	14,15,17	1.57	2 (14%)
9	A1AIO	A	2027	4	11,11,12	5.69	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	A	2046	4	11,11,12	5.70	6 (54%)	14,15,17	1.54	2 (14%)
9	A1AIO	B	2003	5	11,11,12	5.70	6 (54%)	14,15,17	1.47	1 (7%)
9	A1AIO	B	2049	4	11,11,12	5.70	6 (54%)	14,15,17	1.51	2 (14%)
10	GLA	A	2069	1	11,11,12	1.73	3 (27%)	15,15,17	0.93	1 (6%)
9	A1AIO	B	2028	4	11,11,12	5.71	6 (54%)	14,15,17	1.35	2 (14%)
9	A1AIO	B	2056	5	11,11,12	5.72	6 (54%)	14,15,17	1.46	2 (14%)
10	GLA	B	2060	-	11,11,12	1.73	3 (27%)	15,15,17	1.02	1 (6%)
10	GLA	A	2059	1	11,11,12	0.40	0	15,15,17	0.77	1 (6%)
9	A1AIO	A	2009	4	11,11,12	5.69	6 (54%)	14,15,17	1.62	2 (14%)
9	A1AIO	B	2021	4	11,11,12	5.71	6 (54%)	14,15,17	1.34	2 (14%)
10	GLA	B	2065	1	11,11,12	1.69	3 (27%)	15,15,17	1.01	1 (6%)
9	A1AIO	B	2016	4	11,11,12	5.64	6 (54%)	14,15,17	1.51	3 (21%)
9	A1AIO	A	2038	4	11,11,12	5.66	6 (54%)	14,15,17	1.56	2 (14%)
9	A1AIO	A	2021	4	11,11,12	5.71	6 (54%)	14,15,17	1.40	2 (14%)
9	A1AIO	B	2020	4	11,11,12	5.67	6 (54%)	14,15,17	1.33	2 (14%)
9	A1AIO	A	2042	4	11,11,12	5.71	6 (54%)	14,15,17	1.52	2 (14%)
9	A1AIO	B	2045	4	11,11,12	5.71	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	B	2050	4	11,11,12	5.67	6 (54%)	14,15,17	1.50	2 (14%)
9	A1AIO	A	2048	4	11,11,12	5.70	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	A	2037	4	11,11,12	5.70	6 (54%)	14,15,17	1.48	2 (14%)
10	GLA	A	2064	1	11,11,12	1.72	3 (27%)	15,15,17	1.02	1 (6%)
9	A1AIO	B	2035	8	11,11,12	5.72	6 (54%)	14,15,17	1.54	2 (14%)
9	A1AIO	A	2054	6	11,11,12	5.73	6 (54%)	14,15,17	1.44	2 (14%)
9	A1AIO	B	2032	4	11,11,12	5.70	6 (54%)	14,15,17	1.62	2 (14%)
9	A1AIO	B	2037	4	11,11,12	5.69	6 (54%)	14,15,17	1.58	2 (14%)
9	A1AIO	B	2054	8	11,11,12	5.69	6 (54%)	14,15,17	1.26	2 (14%)
9	A1AIO	A	2041	4	11,11,12	5.72	6 (54%)	14,15,17	1.35	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	A1AIO	A	2002	4	11,11,12	5.71	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	B	2052	5	11,11,12	5.66	6 (54%)	14,15,17	1.65	3 (21%)
9	A1AIO	A	2049	4	11,11,12	5.68	6 (54%)	14,15,17	1.55	2 (14%)
10	GLA	B	2068	1	11,11,12	1.74	3 (27%)	15,15,17	0.88	0
10	GLA	A	2070	1	11,11,12	1.73	3 (27%)	15,15,17	0.96	1 (6%)
9	A1AIO	B	2008	4	11,11,12	5.70	6 (54%)	14,15,17	1.67	3 (21%)
9	A1AIO	A	2018	4	11,11,12	5.68	6 (54%)	14,15,17	1.53	2 (14%)
9	A1AIO	B	2011	5	11,11,12	5.65	6 (54%)	14,15,17	1.64	2 (14%)
9	A1AIO	B	2048	4	11,11,12	5.70	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	B	2039	5	11,11,12	5.73	6 (54%)	14,15,17	1.48	1 (7%)
9	A1AIO	B	2055	8	11,11,12	5.67	6 (54%)	14,15,17	1.57	2 (14%)
9	A1AIO	B	2040	5	11,11,12	5.67	6 (54%)	14,15,17	1.60	2 (14%)
9	A1AIO	B	2027	4	11,11,12	5.71	6 (54%)	14,15,17	1.51	2 (14%)
10	GLA	B	2069	1	11,11,12	1.72	3 (27%)	15,15,17	0.91	0
9	A1AIO	A	2005	5	11,11,12	5.74	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	B	2023	4	11,11,12	5.66	6 (54%)	14,15,17	1.52	3 (21%)
9	A1AIO	B	2001	7	11,11,12	5.69	6 (54%)	14,15,17	1.65	2 (14%)
9	A1AIO	A	2051	5	11,11,12	5.72	6 (54%)	14,15,17	1.50	2 (14%)
10	GLA	B	2059	1	11,11,12	0.41	0	15,15,17	0.77	1 (6%)
9	A1AIO	B	2009	4	11,11,12	5.65	6 (54%)	14,15,17	1.79	2 (14%)
10	GLA	B	2066	-	11,11,12	1.74	3 (27%)	15,15,17	0.99	1 (6%)
9	A1AIO	B	2038	4	11,11,12	5.72	6 (54%)	14,15,17	1.51	2 (14%)
9	A1AIO	B	2010	4	11,11,12	5.70	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	A	2017	4	11,11,12	5.71	6 (54%)	14,15,17	1.40	1 (7%)
9	A1AIO	B	2053	5	11,11,12	5.68	6 (54%)	14,15,17	1.52	2 (14%)
9	A1AIO	A	2045	4	11,11,12	5.69	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	B	2004	4	11,11,12	5.70	6 (54%)	14,15,17	1.61	2 (14%)
9	A1AIO	B	2006	4	11,11,12	5.72	6 (54%)	14,15,17	1.61	2 (14%)
9	A1AIO	B	2024	4	11,11,12	5.70	6 (54%)	14,15,17	1.42	2 (14%)
9	A1AIO	B	2019	4	11,11,12	5.67	6 (54%)	14,15,17	1.59	2 (14%)
9	A1AIO	A	2053	6	11,11,12	5.70	6 (54%)	14,15,17	1.60	2 (14%)
9	A1AIO	B	2029	4	11,11,12	5.72	6 (54%)	14,15,17	1.47	2 (14%)
10	GLA	A	2068	1	11,11,12	1.74	3 (27%)	15,15,17	0.91	0
9	A1AIO	B	2017	4	11,11,12	5.68	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	A	2022	4	11,11,12	5.70	6 (54%)	14,15,17	1.48	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	A1AIO	A	2006	4	11,11,12	5.67	6 (54%)	14,15,17	1.71	2 (14%)
9	A1AIO	A	2026	4	11,11,12	5.70	6 (54%)	14,15,17	1.53	2 (14%)
9	A1AIO	A	2013	4	11,11,12	5.68	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	B	2033	4	11,11,12	5.66	6 (54%)	14,15,17	1.74	3 (21%)
9	A1AIO	A	2047	4	11,11,12	5.69	6 (54%)	14,15,17	1.55	2 (14%)
9	A1AIO	B	2036	4	11,11,12	5.71	6 (54%)	14,15,17	1.45	2 (14%)
10	GLA	A	2066	1	11,11,12	1.72	3 (27%)	15,15,17	0.92	0
9	A1AIO	A	2012	4	11,11,12	5.67	6 (54%)	14,15,17	1.58	2 (14%)
9	A1AIO	A	2033	4	11,11,12	5.72	6 (54%)	14,15,17	1.39	1 (7%)
9	A1AIO	A	2010	4	11,11,12	5.70	6 (54%)	14,15,17	1.43	2 (14%)
9	A1AIO	A	2031	4	11,11,12	5.70	6 (54%)	14,15,17	1.51	2 (14%)
10	GLA	A	2060	1	11,11,12	0.41	0	15,15,17	0.77	1 (6%)
10	GLA	B	2063	-	11,11,12	1.74	3 (27%)	15,15,17	1.22	1 (6%)
10	GLA	B	2067	1	11,11,12	1.73	3 (27%)	15,15,17	0.95	1 (6%)
9	A1AIO	A	2008	4	11,11,12	5.70	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	B	2046	4	11,11,12	5.64	6 (54%)	14,15,17	1.74	2 (14%)
9	A1AIO	B	2005	5	11,11,12	5.68	6 (54%)	14,15,17	1.46	3 (21%)
9	A1AIO	A	2025	4	11,11,12	5.70	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	A	2057	5	11,11,12	5.71	6 (54%)	14,15,17	1.41	2 (14%)
9	A1AIO	A	2055	6	11,11,12	5.71	6 (54%)	14,15,17	1.39	2 (14%)
9	A1AIO	B	2007	4	11,11,12	5.70	6 (54%)	14,15,17	1.52	2 (14%)
9	A1AIO	A	2023	4	11,11,12	5.70	6 (54%)	14,15,17	1.48	2 (14%)
9	A1AIO	A	2001	4	11,11,12	5.72	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	B	2013	4	11,11,12	5.69	6 (54%)	14,15,17	1.40	2 (14%)
9	A1AIO	B	2014	4	11,11,12	5.67	6 (54%)	14,15,17	1.46	2 (14%)
9	A1AIO	A	2003	5	11,11,12	5.70	6 (54%)	14,15,17	1.50	2 (14%)
9	A1AIO	B	2044	4	11,11,12	5.72	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	B	2026	4	11,11,12	5.69	6 (54%)	14,15,17	1.67	3 (21%)
9	A1AIO	A	2056	5	11,11,12	5.69	6 (54%)	14,15,17	1.59	2 (14%)
9	A1AIO	B	2047	4	11,11,12	5.67	6 (54%)	14,15,17	1.74	3 (21%)
9	A1AIO	A	2011	5	11,11,12	5.68	6 (54%)	14,15,17	1.56	2 (14%)
9	A1AIO	A	2044	5	11,11,12	5.71	6 (54%)	14,15,17	1.74	3 (21%)
10	GLA	A	2065	1	11,11,12	1.74	3 (27%)	15,15,17	0.93	1 (6%)
10	GLA	A	2067	1	11,11,12	1.75	3 (27%)	15,15,17	1.00	1 (6%)
9	A1AIO	A	2024	4	11,11,12	5.71	6 (54%)	14,15,17	1.52	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	A1AIO	B	2034	4	11,11,12	5.63	6 (54%)	14,15,17	1.74	2 (14%)
9	A1AIO	A	2019	4	11,11,12	5.70	6 (54%)	14,15,17	1.41	2 (14%)
9	A1AIO	B	2043	4	11,11,12	5.71	6 (54%)	14,15,17	1.45	2 (14%)
9	A1AIO	A	2007	4	11,11,12	5.71	6 (54%)	14,15,17	1.53	2 (14%)
10	GLA	B	2058	-	11,11,12	1.72	3 (27%)	15,15,17	1.02	1 (6%)
9	A1AIO	B	2041	4	11,11,12	5.68	6 (54%)	14,15,17	1.65	3 (21%)
9	A1AIO	A	2036	4	11,11,12	5.69	6 (54%)	14,15,17	1.47	2 (14%)
10	GLA	A	2061	1	11,11,12	1.75	3 (27%)	15,15,17	0.98	1 (6%)
10	GLA	A	2062	1	11,11,12	1.72	3 (27%)	15,15,17	0.98	1 (6%)
9	A1AIO	A	2020	4	11,11,12	5.70	6 (54%)	14,15,17	1.42	2 (14%)
9	A1AIO	A	2050	5	11,11,12	5.71	6 (54%)	14,15,17	1.31	2 (14%)
9	A1AIO	B	2057	5	11,11,12	5.68	6 (54%)	14,15,17	1.54	2 (14%)
9	A1AIO	A	2035	4	11,11,12	5.72	6 (54%)	14,15,17	1.36	2 (14%)
10	GLA	B	2070	-	11,11,12	1.73	3 (27%)	15,15,17	0.98	1 (6%)
9	A1AIO	B	2042	4	11,11,12	5.72	6 (54%)	14,15,17	1.44	2 (14%)
9	A1AIO	A	2034	4	11,11,12	5.70	6 (54%)	14,15,17	1.59	2 (14%)
9	A1AIO	B	2012	4	11,11,12	5.71	6 (54%)	14,15,17	1.47	2 (14%)
9	A1AIO	B	2015	4	11,11,12	5.68	6 (54%)	14,15,17	1.64	3 (21%)
9	A1AIO	A	2016	4	11,11,12	5.67	6 (54%)	14,15,17	1.59	2 (14%)
9	A1AIO	B	2031	4	11,11,12	5.65	6 (54%)	14,15,17	1.67	3 (21%)
9	A1AIO	A	2029	4	11,11,12	5.72	6 (54%)	14,15,17	1.36	2 (14%)
9	A1AIO	A	2014	4	11,11,12	5.70	6 (54%)	14,15,17	1.49	2 (14%)
10	GLA	B	2064	1	11,11,12	1.72	3 (27%)	15,15,17	0.97	1 (6%)
9	A1AIO	A	2004	4	11,11,12	5.69	6 (54%)	14,15,17	1.52	2 (14%)
9	A1AIO	B	2025	4	11,11,12	5.71	6 (54%)	14,15,17	1.53	2 (14%)
9	A1AIO	B	2022	4	11,11,12	5.66	6 (54%)	14,15,17	1.49	2 (14%)
9	A1AIO	B	2018	4	11,11,12	5.71	6 (54%)	14,15,17	1.37	2 (14%)
9	A1AIO	B	2002	4	11,11,12	5.68	6 (54%)	14,15,17	1.57	2 (14%)
9	A1AIO	A	2032	4	11,11,12	5.67	6 (54%)	14,15,17	1.53	2 (14%)
9	A1AIO	A	2043	5	11,11,12	5.73	6 (54%)	14,15,17	1.52	2 (14%)
9	A1AIO	A	2030	4	11,11,12	5.70	6 (54%)	14,15,17	1.38	2 (14%)
9	A1AIO	A	2052	5	11,11,12	5.69	6 (54%)	14,15,17	1.50	2 (14%)
9	A1AIO	A	2015	4	11,11,12	5.70	6 (54%)	14,15,17	1.39	2 (14%)
10	GLA	B	2061	1	11,11,12	1.74	3 (27%)	15,15,17	0.91	0
10	GLA	B	2062	1	11,11,12	1.73	3 (27%)	15,15,17	0.96	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	B	2030	4	1/1/4/5	4/6/19/22	0/1/1/1
10	GLA	A	2063	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2028	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2058	1	-	1/2/19/22	0/1/1/1
9	A1AIO	B	2051	5	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2039	6	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2040	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	A	2027	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2046	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2003	5	-	3/6/19/22	0/1/1/1
9	A1AIO	B	2049	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2069	1	-	1/2/19/22	0/1/1/1
9	A1AIO	B	2028	4	-	4/6/19/22	0/1/1/1
9	A1AIO	B	2056	5	-	0/6/19/22	0/1/1/1
10	GLA	B	2060	-	-	2/2/19/22	0/1/1/1
10	GLA	A	2059	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2009	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	B	2021	4	-	3/6/19/22	0/1/1/1
10	GLA	B	2065	1	-	2/2/19/22	0/1/1/1
9	A1AIO	B	2016	4	1/1/4/5	6/6/19/22	0/1/1/1
9	A1AIO	A	2038	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	A	2021	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2020	4	-	4/6/19/22	0/1/1/1
9	A1AIO	A	2042	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2045	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2050	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2048	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2037	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	A	2064	1	-	2/2/19/22	0/1/1/1
9	A1AIO	B	2035	8	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2054	6	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2032	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2037	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2054	8	-	6/6/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	A	2041	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2002	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2052	5	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2049	4	-	2/6/19/22	0/1/1/1
10	GLA	B	2068	1	-	2/2/19/22	0/1/1/1
10	GLA	A	2070	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2008	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2018	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	B	2011	5	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2048	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2039	5	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2055	8	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2040	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2027	4	-	0/6/19/22	0/1/1/1
10	GLA	B	2069	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2005	5	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2023	4	-	4/6/19/22	0/1/1/1
9	A1AIO	B	2001	7	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2051	5	-	0/6/19/22	0/1/1/1
10	GLA	B	2059	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2009	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	B	2066	-	-	1/2/19/22	0/1/1/1
9	A1AIO	B	2038	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2010	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2017	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2053	5	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2045	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2004	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2006	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2024	4	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2019	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2053	6	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2029	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2068	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2017	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2022	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2006	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2026	4	-	0/6/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	A	2013	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2033	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2047	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2036	4	-	2/6/19/22	0/1/1/1
10	GLA	A	2066	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2012	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2033	4	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2010	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2031	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2060	1	-	0/2/19/22	0/1/1/1
10	GLA	B	2063	-	-	2/2/19/22	0/1/1/1
10	GLA	B	2067	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2008	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2046	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2005	5	-	6/6/19/22	0/1/1/1
9	A1AIO	A	2025	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2057	5	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2055	6	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2007	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2023	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2001	4	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2013	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2014	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	A	2003	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2044	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2026	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2056	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2047	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2011	5	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2044	5	-	2/6/19/22	0/1/1/1
10	GLA	A	2065	1	-	2/2/19/22	0/1/1/1
10	GLA	A	2067	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2024	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2034	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2019	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2043	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2007	4	-	0/6/19/22	0/1/1/1
10	GLA	B	2058	-	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	B	2041	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2036	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2061	1	-	0/2/19/22	0/1/1/1
10	GLA	A	2062	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2020	4	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2050	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2057	5	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2035	4	1/1/4/5	5/6/19/22	0/1/1/1
10	GLA	B	2070	-	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2042	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2034	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2012	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	B	2015	4	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2016	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	B	2031	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2029	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2014	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	B	2064	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2004	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2025	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2022	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2018	4	-	4/6/19/22	0/1/1/1
9	A1AIO	B	2002	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2032	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2043	5	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2030	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2052	5	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2015	4	-	0/6/19/22	0/1/1/1
10	GLA	B	2061	1	-	2/2/19/22	0/1/1/1
10	GLA	B	2062	1	-	1/2/19/22	0/1/1/1

All (753) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2043	A1AIO	C05-C04	-15.64	1.28	1.53
9	B	2039	A1AIO	C05-C04	-15.61	1.28	1.53
9	A	2005	A1AIO	C05-C04	-15.61	1.28	1.53
9	A	2029	A1AIO	C05-C04	-15.59	1.28	1.53
9	A	2033	A1AIO	C05-C04	-15.58	1.28	1.53
9	B	2035	A1AIO	C05-C04	-15.58	1.28	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2003	A1AIO	C05-C04	-15.57	1.28	1.53
9	A	2044	A1AIO	C05-C04	-15.56	1.28	1.53
9	B	2038	A1AIO	C05-C04	-15.56	1.28	1.53
9	B	2042	A1AIO	C05-C04	-15.54	1.28	1.53
9	B	2056	A1AIO	C05-C04	-15.54	1.28	1.53
9	B	2006	A1AIO	C05-C04	-15.54	1.28	1.53
9	B	2044	A1AIO	C05-C04	-15.53	1.28	1.53
9	A	2054	A1AIO	C05-C04	-15.52	1.28	1.53
9	A	2035	A1AIO	C05-C04	-15.52	1.28	1.53
9	A	2002	A1AIO	C05-C04	-15.52	1.28	1.53
9	A	2041	A1AIO	C05-C04	-15.52	1.28	1.53
9	B	2045	A1AIO	C05-C04	-15.51	1.28	1.53
9	B	2043	A1AIO	C05-C04	-15.51	1.28	1.53
9	A	2050	A1AIO	C05-C04	-15.51	1.28	1.53
9	A	2037	A1AIO	C05-C04	-15.51	1.28	1.53
9	A	2048	A1AIO	C05-C04	-15.51	1.28	1.53
9	A	2004	A1AIO	C05-C04	-15.50	1.28	1.53
9	A	2051	A1AIO	C05-C04	-15.50	1.28	1.53
9	A	2001	A1AIO	C05-C04	-15.50	1.28	1.53
9	A	2027	A1AIO	C05-C04	-15.50	1.28	1.53
9	B	2026	A1AIO	C05-C04	-15.50	1.28	1.53
9	A	2039	A1AIO	C05-C04	-15.50	1.28	1.53
9	B	2029	A1AIO	C05-C04	-15.50	1.28	1.53
9	A	2034	A1AIO	C05-C04	-15.50	1.28	1.53
9	B	2036	A1AIO	C05-C04	-15.50	1.28	1.53
9	B	2028	A1AIO	C05-C04	-15.49	1.28	1.53
9	A	2017	A1AIO	C05-C04	-15.49	1.28	1.53
9	A	2057	A1AIO	C05-C04	-15.49	1.28	1.53
9	B	2025	A1AIO	C05-C04	-15.49	1.28	1.53
9	A	2053	A1AIO	C05-C04	-15.49	1.28	1.53
9	A	2003	A1AIO	C05-C04	-15.49	1.28	1.53
9	A	2030	A1AIO	C05-C04	-15.49	1.28	1.53
9	B	2048	A1AIO	C05-C04	-15.48	1.28	1.53
9	A	2046	A1AIO	C05-C04	-15.48	1.28	1.53
9	A	2047	A1AIO	C05-C04	-15.48	1.28	1.53
9	A	2008	A1AIO	C05-C04	-15.48	1.28	1.53
9	A	2042	A1AIO	C05-C04	-15.48	1.28	1.53
9	A	2045	A1AIO	C05-C04	-15.47	1.28	1.53
9	A	2055	A1AIO	C05-C04	-15.47	1.28	1.53
9	B	2010	A1AIO	C05-C04	-15.47	1.28	1.53
9	A	2026	A1AIO	C05-C04	-15.47	1.28	1.53
9	A	2049	A1AIO	C05-C04	-15.46	1.28	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2021	A1AIO	C05-C04	-15.46	1.28	1.53
9	A	2028	A1AIO	C05-C04	-15.45	1.28	1.53
9	B	2027	A1AIO	C05-C04	-15.45	1.28	1.53
9	A	2021	A1AIO	C05-C04	-15.45	1.28	1.53
9	B	2041	A1AIO	C05-C04	-15.45	1.28	1.53
9	A	2024	A1AIO	C05-C04	-15.45	1.28	1.53
9	A	2031	A1AIO	C05-C04	-15.45	1.28	1.53
9	B	2054	A1AIO	C05-C04	-15.45	1.28	1.53
9	A	2007	A1AIO	C05-C04	-15.45	1.28	1.53
9	B	2008	A1AIO	C05-C04	-15.44	1.28	1.53
9	B	2012	A1AIO	C05-C04	-15.44	1.28	1.53
9	B	2018	A1AIO	C05-C04	-15.44	1.28	1.53
9	B	2024	A1AIO	C05-C04	-15.44	1.28	1.53
9	B	2007	A1AIO	C05-C04	-15.43	1.28	1.53
9	B	2049	A1AIO	C05-C04	-15.43	1.28	1.53
9	B	2004	A1AIO	C05-C04	-15.43	1.28	1.53
9	B	2032	A1AIO	C05-C04	-15.43	1.28	1.53
9	A	2020	A1AIO	C05-C04	-15.42	1.28	1.53
9	A	2014	A1AIO	C05-C04	-15.42	1.28	1.53
9	A	2015	A1AIO	C05-C04	-15.42	1.28	1.53
9	A	2019	A1AIO	C05-C04	-15.41	1.28	1.53
9	A	2056	A1AIO	C05-C04	-15.41	1.28	1.53
9	B	2051	A1AIO	C05-C04	-15.41	1.28	1.53
9	B	2037	A1AIO	C05-C04	-15.40	1.28	1.53
9	A	2010	A1AIO	C05-C04	-15.40	1.28	1.53
9	A	2022	A1AIO	C05-C04	-15.40	1.28	1.53
9	A	2025	A1AIO	C05-C04	-15.40	1.28	1.53
9	B	2001	A1AIO	C05-C04	-15.39	1.28	1.53
9	A	2052	A1AIO	C05-C04	-15.39	1.28	1.53
9	B	2005	A1AIO	C05-C04	-15.39	1.28	1.53
9	B	2047	A1AIO	C05-C04	-15.38	1.28	1.53
9	B	2040	A1AIO	C05-C04	-15.38	1.28	1.53
9	A	2023	A1AIO	C05-C04	-15.37	1.28	1.53
9	B	2002	A1AIO	C05-C04	-15.37	1.28	1.53
9	B	2057	A1AIO	C05-C04	-15.36	1.28	1.53
9	A	2006	A1AIO	C05-C04	-15.36	1.28	1.53
9	A	2036	A1AIO	C05-C04	-15.36	1.28	1.53
9	A	2013	A1AIO	C05-C04	-15.35	1.28	1.53
9	B	2013	A1AIO	C05-C04	-15.35	1.28	1.53
9	A	2009	A1AIO	C05-C04	-15.34	1.28	1.53
9	B	2052	A1AIO	C05-C04	-15.34	1.28	1.53
9	B	2033	A1AIO	C05-C04	-15.34	1.28	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2015	A1AIO	C05-C04	-15.33	1.28	1.53
9	B	2017	A1AIO	C05-C04	-15.33	1.28	1.53
9	A	2011	A1AIO	C05-C04	-15.32	1.29	1.53
9	A	2018	A1AIO	C05-C04	-15.32	1.29	1.53
9	B	2050	A1AIO	C05-C04	-15.31	1.29	1.53
9	A	2032	A1AIO	C05-C04	-15.30	1.29	1.53
9	B	2055	A1AIO	C05-C04	-15.30	1.29	1.53
9	B	2019	A1AIO	C05-C04	-15.29	1.29	1.53
9	B	2020	A1AIO	C05-C04	-15.29	1.29	1.53
9	A	2012	A1AIO	C05-C04	-15.27	1.29	1.53
9	B	2022	A1AIO	C05-C04	-15.27	1.29	1.53
9	B	2023	A1AIO	C05-C04	-15.27	1.29	1.53
9	A	2016	A1AIO	C05-C04	-15.26	1.29	1.53
9	B	2053	A1AIO	C05-C04	-15.26	1.29	1.53
9	B	2014	A1AIO	C05-C04	-15.26	1.29	1.53
9	B	2009	A1AIO	C05-C04	-15.25	1.29	1.53
9	B	2030	A1AIO	C05-C04	-15.24	1.29	1.53
9	A	2040	A1AIO	C05-C04	-15.24	1.29	1.53
9	B	2031	A1AIO	C05-C04	-15.23	1.29	1.53
9	A	2038	A1AIO	C05-C04	-15.23	1.29	1.53
9	B	2011	A1AIO	C05-C04	-15.18	1.29	1.53
9	B	2034	A1AIO	C05-C04	-15.17	1.29	1.53
9	B	2046	A1AIO	C05-C04	-15.17	1.29	1.53
9	B	2016	A1AIO	C05-C04	-15.15	1.29	1.53
9	B	2023	A1AIO	C04-C03	6.19	1.66	1.52
9	B	2016	A1AIO	C04-C03	6.17	1.66	1.52
9	B	2015	A1AIO	C04-C03	6.13	1.66	1.52
9	B	2031	A1AIO	C04-C03	6.08	1.66	1.52
9	B	2005	A1AIO	C04-C03	6.07	1.66	1.52
9	B	2047	A1AIO	C04-C03	6.05	1.66	1.52
9	B	2033	A1AIO	C04-C03	6.02	1.66	1.52
9	B	2011	A1AIO	C04-C03	6.00	1.66	1.52
9	B	2030	A1AIO	C04-C03	6.00	1.66	1.52
9	B	2050	A1AIO	C04-C03	5.99	1.66	1.52
9	B	2017	A1AIO	C04-C03	5.98	1.66	1.52
9	B	2046	A1AIO	C04-C03	5.97	1.66	1.52
9	B	2028	A1AIO	C04-C03	5.96	1.66	1.52
9	B	2022	A1AIO	C04-C03	5.96	1.66	1.52
9	B	2008	A1AIO	C04-C03	5.96	1.66	1.52
9	B	2034	A1AIO	C04-C03	5.95	1.66	1.52
9	B	2051	A1AIO	C04-C03	5.93	1.66	1.52
9	B	2020	A1AIO	C04-C03	5.93	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2013	A1AIO	C04-C03	5.93	1.66	1.52
9	A	2039	A1AIO	C04-C03	5.93	1.66	1.52
9	B	2014	A1AIO	C04-C03	5.92	1.66	1.52
9	B	2054	A1AIO	C04-C03	5.92	1.66	1.52
9	B	2019	A1AIO	C04-C03	5.91	1.66	1.52
9	A	2046	A1AIO	C04-C03	5.90	1.66	1.52
9	B	2021	A1AIO	C04-C03	5.90	1.66	1.52
9	B	2053	A1AIO	C04-C03	5.89	1.66	1.52
9	A	2012	A1AIO	C04-C03	5.89	1.66	1.52
9	B	2041	A1AIO	C04-C03	5.89	1.66	1.52
9	A	2016	A1AIO	C04-C03	5.89	1.66	1.52
9	B	2009	A1AIO	C04-C03	5.88	1.66	1.52
9	A	2038	A1AIO	C04-C03	5.88	1.66	1.52
9	A	2023	A1AIO	C04-C03	5.87	1.66	1.52
9	A	2020	A1AIO	C04-C03	5.87	1.66	1.52
9	A	2019	A1AIO	C04-C03	5.87	1.66	1.52
9	A	2018	A1AIO	C04-C03	5.87	1.66	1.52
9	B	2012	A1AIO	C04-C03	5.87	1.66	1.52
9	A	2025	A1AIO	C04-C03	5.87	1.66	1.52
9	A	2040	A1AIO	C04-C03	5.87	1.66	1.52
9	B	2055	A1AIO	C04-C03	5.87	1.66	1.52
9	A	2032	A1AIO	C04-C03	5.86	1.66	1.52
9	A	2014	A1AIO	C04-C03	5.86	1.66	1.52
9	B	2052	A1AIO	C04-C03	5.86	1.66	1.52
9	A	2056	A1AIO	C04-C03	5.86	1.66	1.52
9	B	2018	A1AIO	C04-C03	5.86	1.66	1.52
9	A	2021	A1AIO	C04-C03	5.85	1.66	1.52
9	A	2026	A1AIO	C04-C03	5.85	1.66	1.52
9	A	2022	A1AIO	C04-C03	5.85	1.66	1.52
9	A	2015	A1AIO	C04-C03	5.85	1.66	1.52
9	A	2029	A1AIO	C04-C03	5.85	1.66	1.52
9	A	2041	A1AIO	C04-C03	5.84	1.66	1.52
9	A	2024	A1AIO	C04-C03	5.84	1.66	1.52
9	A	2054	A1AIO	C04-C03	5.84	1.66	1.52
9	A	2009	A1AIO	C04-C03	5.84	1.66	1.52
9	B	2001	A1AIO	C04-C03	5.83	1.65	1.52
9	B	2032	A1AIO	C04-C03	5.83	1.65	1.52
9	A	2035	A1AIO	C04-C03	5.83	1.65	1.52
9	A	2030	A1AIO	C04-C03	5.83	1.65	1.52
9	A	2044	A1AIO	C04-C03	5.82	1.65	1.52
9	A	2017	A1AIO	C04-C03	5.82	1.65	1.52
9	A	2037	A1AIO	C04-C03	5.82	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2052	A1AIO	C04-C03	5.82	1.65	1.52
9	A	2011	A1AIO	C04-C03	5.81	1.65	1.52
9	A	2008	A1AIO	C04-C03	5.81	1.65	1.52
9	A	2034	A1AIO	C04-C03	5.81	1.65	1.52
9	B	2057	A1AIO	C04-C03	5.81	1.65	1.52
9	A	2050	A1AIO	C04-C03	5.80	1.65	1.52
9	A	2053	A1AIO	C04-C03	5.80	1.65	1.52
9	A	2010	A1AIO	C04-C03	5.80	1.65	1.52
9	A	2055	A1AIO	C04-C03	5.80	1.65	1.52
9	B	2004	A1AIO	C04-C03	5.80	1.65	1.52
9	A	2031	A1AIO	C04-C03	5.80	1.65	1.52
9	B	2024	A1AIO	C04-C03	5.80	1.65	1.52
9	A	2013	A1AIO	C04-C03	5.79	1.65	1.52
9	A	2028	A1AIO	C04-C03	5.79	1.65	1.52
9	B	2035	A1AIO	C04-C03	5.79	1.65	1.52
9	B	2029	A1AIO	C04-C03	5.79	1.65	1.52
9	A	2036	A1AIO	C04-C03	5.79	1.65	1.52
9	B	2002	A1AIO	C04-C03	5.79	1.65	1.52
9	A	2033	A1AIO	C04-C03	5.79	1.65	1.52
9	A	2048	A1AIO	C04-C03	5.79	1.65	1.52
9	A	2001	A1AIO	C04-C03	5.78	1.65	1.52
9	B	2040	A1AIO	C04-C03	5.78	1.65	1.52
9	B	2049	A1AIO	C04-C03	5.77	1.65	1.52
9	A	2007	A1AIO	C04-C03	5.77	1.65	1.52
9	A	2057	A1AIO	C04-C03	5.77	1.65	1.52
9	A	2047	A1AIO	C04-C03	5.77	1.65	1.52
9	A	2045	A1AIO	C04-C03	5.77	1.65	1.52
9	B	2027	A1AIO	C04-C03	5.77	1.65	1.52
9	B	2026	A1AIO	C04-C03	5.77	1.65	1.52
9	A	2051	A1AIO	C04-C03	5.76	1.65	1.52
9	A	2049	A1AIO	C04-C03	5.76	1.65	1.52
9	B	2025	A1AIO	C04-C03	5.76	1.65	1.52
9	B	2010	A1AIO	C04-C03	5.75	1.65	1.52
9	A	2003	A1AIO	C04-C03	5.75	1.65	1.52
9	B	2037	A1AIO	C04-C03	5.75	1.65	1.52
9	B	2044	A1AIO	C04-C03	5.74	1.65	1.52
9	A	2005	A1AIO	C04-C03	5.74	1.65	1.52
9	B	2038	A1AIO	C04-C03	5.74	1.65	1.52
9	A	2027	A1AIO	C04-C03	5.74	1.65	1.52
9	B	2056	A1AIO	C04-C03	5.74	1.65	1.52
9	A	2002	A1AIO	C04-C03	5.73	1.65	1.52
9	A	2006	A1AIO	C04-C03	5.72	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2036	A1AIO	C04-C03	5.72	1.65	1.52
9	B	2042	A1AIO	C04-C03	5.72	1.65	1.52
9	A	2042	A1AIO	C04-C03	5.72	1.65	1.52
9	B	2043	A1AIO	C04-C03	5.72	1.65	1.52
9	B	2048	A1AIO	C04-C03	5.71	1.65	1.52
9	A	2038	A1AIO	O07-C03	-5.71	1.31	1.43
9	B	2037	A1AIO	O07-C03	-5.71	1.31	1.43
9	B	2003	A1AIO	C04-C03	5.71	1.65	1.52
9	A	2009	A1AIO	O07-C03	-5.71	1.31	1.43
9	B	2039	A1AIO	C04-C03	5.70	1.65	1.52
9	B	2045	A1AIO	C04-C03	5.69	1.65	1.52
9	B	2006	A1AIO	O07-C03	-5.69	1.31	1.43
9	A	2004	A1AIO	C04-C03	5.69	1.65	1.52
9	A	2007	A1AIO	O07-C03	-5.69	1.31	1.43
9	B	2007	A1AIO	O07-C03	-5.69	1.31	1.43
9	A	2043	A1AIO	C04-C03	5.69	1.65	1.52
9	B	2055	A1AIO	O07-C03	-5.68	1.31	1.43
9	B	2053	A1AIO	O07-C03	-5.68	1.31	1.43
9	B	2007	A1AIO	C04-C03	5.68	1.65	1.52
9	B	2046	A1AIO	O07-C03	-5.67	1.31	1.43
9	A	2006	A1AIO	O07-C03	-5.67	1.31	1.43
9	A	2042	A1AIO	O07-C03	-5.67	1.31	1.43
9	B	2004	A1AIO	O07-C03	-5.66	1.31	1.43
9	A	2010	A1AIO	O07-C03	-5.66	1.31	1.43
9	A	2011	A1AIO	O07-C03	-5.66	1.31	1.43
9	B	2042	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2040	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2006	A1AIO	C04-C03	5.65	1.65	1.52
9	B	2009	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2034	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2036	A1AIO	O07-C03	-5.65	1.31	1.43
9	A	2001	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2043	A1AIO	O07-C03	-5.64	1.31	1.43
9	B	2045	A1AIO	O07-C03	-5.64	1.31	1.43
9	A	2049	A1AIO	O07-C03	-5.64	1.31	1.43
9	B	2044	A1AIO	O07-C03	-5.64	1.31	1.43
9	B	2049	A1AIO	O07-C03	-5.64	1.31	1.43
9	A	2016	A1AIO	O07-C03	-5.64	1.31	1.43
9	A	2013	A1AIO	O07-C03	-5.64	1.31	1.43
9	A	2048	A1AIO	O07-C03	-5.63	1.31	1.43
9	A	2051	A1AIO	O07-C03	-5.63	1.31	1.43
9	B	2030	A1AIO	O07-C03	-5.63	1.31	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2047	A1AIO	O07-C03	-5.63	1.31	1.43
9	B	2048	A1AIO	O07-C03	-5.63	1.31	1.43
9	A	2050	A1AIO	O07-C03	-5.63	1.31	1.43
9	A	2002	A1AIO	O07-C03	-5.63	1.31	1.43
9	B	2056	A1AIO	O07-C03	-5.63	1.31	1.43
9	A	2045	A1AIO	O07-C03	-5.63	1.31	1.43
9	A	2052	A1AIO	O07-C03	-5.62	1.31	1.43
9	A	2040	A1AIO	O07-C03	-5.62	1.31	1.43
9	B	2029	A1AIO	O07-C03	-5.62	1.31	1.43
9	A	2036	A1AIO	O07-C03	-5.62	1.31	1.43
9	A	2004	A1AIO	O07-C03	-5.62	1.31	1.43
9	A	2057	A1AIO	O07-C03	-5.62	1.31	1.43
9	A	2023	A1AIO	O07-C03	-5.62	1.31	1.43
9	B	2027	A1AIO	O07-C03	-5.61	1.31	1.43
9	A	2028	A1AIO	O07-C03	-5.61	1.31	1.43
9	B	2035	A1AIO	O07-C03	-5.61	1.31	1.43
9	A	2055	A1AIO	O07-C03	-5.61	1.31	1.43
9	B	2002	A1AIO	O07-C03	-5.61	1.31	1.43
9	B	2019	A1AIO	O07-C03	-5.60	1.31	1.43
9	A	2005	A1AIO	O07-C03	-5.60	1.31	1.43
9	A	2054	A1AIO	O07-C03	-5.60	1.31	1.43
9	A	2018	A1AIO	O07-C03	-5.60	1.31	1.43
9	B	2057	A1AIO	O07-C03	-5.60	1.31	1.43
9	A	2012	A1AIO	O07-C03	-5.60	1.31	1.43
9	B	2011	A1AIO	O07-C03	-5.60	1.31	1.43
9	A	2056	A1AIO	O07-C03	-5.59	1.31	1.43
9	A	2032	A1AIO	O07-C03	-5.59	1.31	1.43
9	B	2010	A1AIO	O07-C03	-5.59	1.31	1.43
9	B	2052	A1AIO	O07-C03	-5.59	1.31	1.43
9	A	2031	A1AIO	O07-C03	-5.59	1.31	1.43
9	A	2003	A1AIO	O07-C03	-5.59	1.31	1.43
9	A	2015	A1AIO	O07-C03	-5.59	1.31	1.43
9	B	2038	A1AIO	O07-C03	-5.59	1.31	1.43
9	B	2039	A1AIO	O07-C03	-5.58	1.31	1.43
9	A	2041	A1AIO	O07-C03	-5.58	1.31	1.43
9	B	2001	A1AIO	O07-C03	-5.58	1.31	1.43
9	B	2032	A1AIO	O07-C03	-5.58	1.31	1.43
9	B	2012	A1AIO	O07-C03	-5.57	1.31	1.43
9	A	2024	A1AIO	O07-C03	-5.57	1.31	1.43
9	A	2008	A1AIO	O07-C03	-5.57	1.31	1.43
9	A	2019	A1AIO	O07-C03	-5.57	1.31	1.43
9	B	2014	A1AIO	O07-C03	-5.57	1.31	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2043	A1AIO	O07-C03	-5.56	1.31	1.43
9	A	2022	A1AIO	O07-C03	-5.56	1.31	1.43
9	B	2041	A1AIO	O07-C03	-5.56	1.31	1.43
9	B	2025	A1AIO	O07-C03	-5.55	1.31	1.43
9	A	2035	A1AIO	O07-C03	-5.55	1.31	1.43
9	B	2024	A1AIO	O07-C03	-5.55	1.31	1.43
9	A	2053	A1AIO	O07-C03	-5.55	1.31	1.43
9	A	2025	A1AIO	O07-C03	-5.55	1.31	1.43
9	A	2030	A1AIO	O07-C03	-5.54	1.31	1.43
9	B	2020	A1AIO	O07-C03	-5.54	1.31	1.43
9	B	2033	A1AIO	O07-C03	-5.54	1.31	1.43
9	B	2018	A1AIO	O07-C03	-5.53	1.31	1.43
9	B	2008	A1AIO	O07-C03	-5.53	1.31	1.43
9	B	2013	A1AIO	O07-C03	-5.53	1.31	1.43
9	A	2021	A1AIO	O07-C03	-5.53	1.31	1.43
9	A	2017	A1AIO	O07-C03	-5.53	1.31	1.43
9	A	2026	A1AIO	O07-C03	-5.53	1.31	1.43
9	A	2020	A1AIO	O07-C03	-5.52	1.31	1.43
9	B	2047	A1AIO	O07-C03	-5.52	1.31	1.43
9	A	2027	A1AIO	O07-C03	-5.52	1.31	1.43
9	A	2029	A1AIO	O07-C03	-5.52	1.31	1.43
9	A	2034	A1AIO	O07-C03	-5.52	1.31	1.43
9	B	2026	A1AIO	O07-C03	-5.51	1.31	1.43
9	B	2017	A1AIO	O07-C03	-5.51	1.31	1.43
9	A	2033	A1AIO	O07-C03	-5.51	1.31	1.43
9	B	2021	A1AIO	O07-C03	-5.51	1.31	1.43
9	A	2014	A1AIO	O07-C03	-5.51	1.31	1.43
9	B	2003	A1AIO	O07-C03	-5.50	1.31	1.43
9	B	2054	A1AIO	O07-C03	-5.50	1.31	1.43
9	B	2022	A1AIO	O07-C03	-5.50	1.31	1.43
9	B	2050	A1AIO	O07-C03	-5.49	1.31	1.43
9	B	2031	A1AIO	O07-C03	-5.49	1.31	1.43
9	B	2051	A1AIO	O07-C03	-5.48	1.31	1.43
9	B	2028	A1AIO	O07-C03	-5.48	1.31	1.43
9	A	2046	A1AIO	O07-C03	-5.47	1.31	1.43
9	B	2016	A1AIO	O07-C03	-5.47	1.31	1.43
9	A	2044	A1AIO	O07-C03	-5.45	1.31	1.43
9	A	2037	A1AIO	O07-C03	-5.45	1.31	1.43
9	B	2005	A1AIO	O07-C03	-5.43	1.31	1.43
9	B	2015	A1AIO	O07-C03	-5.43	1.31	1.43
9	B	2023	A1AIO	O07-C03	-5.41	1.31	1.43
9	A	2039	A1AIO	O07-C03	-5.41	1.31	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2020	A1AIO	O07-C06	5.07	1.55	1.43
9	B	2018	A1AIO	O07-C06	5.07	1.55	1.43
9	A	2017	A1AIO	O07-C06	5.06	1.55	1.43
9	B	2024	A1AIO	O07-C06	5.05	1.55	1.43
9	A	2035	A1AIO	O07-C06	5.04	1.55	1.43
9	A	2025	A1AIO	O07-C06	5.04	1.55	1.43
9	A	2021	A1AIO	O07-C06	5.04	1.54	1.43
9	A	2037	A1AIO	O07-C06	5.03	1.54	1.43
9	B	2013	A1AIO	O07-C06	5.03	1.54	1.43
9	A	2024	A1AIO	O07-C06	5.03	1.54	1.43
9	A	2014	A1AIO	O07-C06	5.02	1.54	1.43
9	A	2033	A1AIO	O07-C06	5.02	1.54	1.43
9	A	2036	A1AIO	O07-C06	5.02	1.54	1.43
9	A	2019	A1AIO	O07-C06	5.02	1.54	1.43
9	A	2018	A1AIO	O07-C06	5.01	1.54	1.43
9	B	2012	A1AIO	O07-C06	5.01	1.54	1.43
9	A	2054	A1AIO	O07-C06	5.01	1.54	1.43
9	B	2025	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2022	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2046	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2055	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2041	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2051	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2050	A1AIO	O07-C06	5.00	1.54	1.43
9	B	2021	A1AIO	O07-C06	5.00	1.54	1.43
9	A	2023	A1AIO	O07-C06	4.99	1.54	1.43
9	A	2030	A1AIO	O07-C06	4.99	1.54	1.43
9	B	2004	A1AIO	O07-C06	4.99	1.54	1.43
9	A	2015	A1AIO	O07-C06	4.99	1.54	1.43
9	B	2056	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2020	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2003	A1AIO	O07-C06	4.98	1.54	1.43
9	A	2039	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2049	A1AIO	O07-C06	4.98	1.54	1.43
9	A	2011	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2022	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2044	A1AIO	O07-C06	4.97	1.54	1.43
9	B	2014	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2027	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2032	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2001	A1AIO	O07-C06	4.97	1.54	1.43
9	B	2027	A1AIO	O07-C06	4.97	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2042	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2010	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2026	A1AIO	O07-C06	4.97	1.54	1.43
9	B	2017	A1AIO	O07-C06	4.97	1.54	1.43
9	B	2054	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2052	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2002	A1AIO	O07-C06	4.97	1.54	1.43
9	A	2053	A1AIO	O07-C06	4.96	1.54	1.43
9	A	2028	A1AIO	O07-C06	4.96	1.54	1.43
9	A	2005	A1AIO	O07-C06	4.96	1.54	1.43
9	B	2050	A1AIO	O07-C06	4.96	1.54	1.43
9	B	2006	A1AIO	O07-C06	4.96	1.54	1.43
9	A	2008	A1AIO	O07-C06	4.96	1.54	1.43
9	B	2029	A1AIO	O07-C06	4.96	1.54	1.43
9	B	2026	A1AIO	O07-C06	4.96	1.54	1.43
9	A	2007	A1AIO	O07-C06	4.95	1.54	1.43
9	A	2013	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2019	A1AIO	O07-C06	4.95	1.54	1.43
9	A	2047	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2032	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2039	A1AIO	O07-C06	4.95	1.54	1.43
9	A	2031	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2007	A1AIO	O07-C06	4.95	1.54	1.43
9	A	2043	A1AIO	O07-C06	4.95	1.54	1.43
9	A	2016	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2051	A1AIO	O07-C06	4.94	1.54	1.43
9	B	2010	A1AIO	O07-C06	4.94	1.54	1.43
9	B	2048	A1AIO	O07-C06	4.94	1.54	1.43
9	A	2012	A1AIO	O07-C06	4.94	1.54	1.43
9	A	2034	A1AIO	O07-C06	4.94	1.54	1.43
9	B	2001	A1AIO	O07-C06	4.94	1.54	1.43
9	B	2044	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2036	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2038	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2028	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2052	A1AIO	O07-C06	4.93	1.54	1.43
9	A	2057	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2045	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2043	A1AIO	O07-C06	4.93	1.54	1.43
9	A	2045	A1AIO	O07-C06	4.92	1.54	1.43
9	B	2053	A1AIO	O07-C06	4.92	1.54	1.43
9	A	2003	A1AIO	O07-C06	4.92	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2042	A1AIO	O07-C06	4.92	1.54	1.43
9	B	2002	A1AIO	O07-C06	4.92	1.54	1.43
9	A	2009	A1AIO	O07-C06	4.92	1.54	1.43
9	B	2037	A1AIO	O07-C06	4.92	1.54	1.43
9	B	2035	A1AIO	O07-C06	4.92	1.54	1.43
9	B	2057	A1AIO	O07-C06	4.92	1.54	1.43
9	A	2038	A1AIO	O07-C06	4.91	1.54	1.43
9	A	2049	A1AIO	O07-C06	4.90	1.54	1.43
9	A	2048	A1AIO	O07-C06	4.90	1.54	1.43
9	B	2008	A1AIO	O07-C06	4.89	1.54	1.43
9	B	2011	A1AIO	O07-C06	4.88	1.54	1.43
9	B	2023	A1AIO	O07-C06	4.88	1.54	1.43
9	B	2015	A1AIO	O07-C06	4.88	1.54	1.43
9	B	2016	A1AIO	O07-C06	4.88	1.54	1.43
9	A	2056	A1AIO	O07-C06	4.88	1.54	1.43
9	A	2006	A1AIO	O07-C06	4.88	1.54	1.43
9	A	2040	A1AIO	O07-C06	4.87	1.54	1.43
9	B	2040	A1AIO	O07-C06	4.87	1.54	1.43
9	B	2005	A1AIO	O07-C06	4.87	1.54	1.43
9	A	2029	A1AIO	O07-C06	4.87	1.54	1.43
9	B	2009	A1AIO	O07-C06	4.86	1.54	1.43
9	A	2004	A1AIO	O07-C06	4.86	1.54	1.43
9	B	2046	A1AIO	O07-C06	4.84	1.54	1.43
9	B	2031	A1AIO	O07-C06	4.83	1.54	1.43
9	B	2034	A1AIO	O07-C06	4.83	1.54	1.43
9	B	2047	A1AIO	O07-C06	4.83	1.54	1.43
9	B	2041	A1AIO	O07-C06	4.83	1.54	1.43
9	B	2033	A1AIO	O07-C06	4.82	1.54	1.43
9	B	2030	A1AIO	O07-C06	4.82	1.54	1.43
9	B	2055	A1AIO	O07-C06	4.81	1.54	1.43
9	B	2053	A1AIO	C06-C05	4.30	1.59	1.51
9	B	2007	A1AIO	C06-C05	4.29	1.59	1.51
9	A	2023	A1AIO	C06-C05	4.28	1.59	1.51
9	A	2028	A1AIO	C06-C05	4.28	1.58	1.51
9	B	2021	A1AIO	C06-C05	4.28	1.58	1.51
9	A	2040	A1AIO	C06-C05	4.27	1.58	1.51
9	B	2027	A1AIO	C06-C05	4.26	1.58	1.51
9	B	2002	A1AIO	C06-C05	4.26	1.58	1.51
9	B	2049	A1AIO	C06-C05	4.25	1.58	1.51
9	A	2019	A1AIO	C06-C05	4.25	1.58	1.51
9	A	2036	A1AIO	C06-C05	4.25	1.58	1.51
9	B	2014	A1AIO	C06-C05	4.25	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2010	A1AIO	C06-C05	4.25	1.58	1.51
9	A	2011	A1AIO	C06-C05	4.25	1.58	1.51
9	B	2029	A1AIO	C06-C05	4.24	1.58	1.51
9	A	2012	A1AIO	C06-C05	4.24	1.58	1.51
9	A	2052	A1AIO	C06-C05	4.23	1.58	1.51
9	B	2001	A1AIO	C06-C05	4.23	1.58	1.51
9	B	2006	A1AIO	C06-C05	4.22	1.58	1.51
9	B	2010	A1AIO	C06-C05	4.22	1.58	1.51
9	A	2013	A1AIO	C06-C05	4.22	1.58	1.51
9	B	2037	A1AIO	C06-C05	4.22	1.58	1.51
9	A	2038	A1AIO	C06-C05	4.22	1.58	1.51
9	A	2005	A1AIO	C06-C05	4.22	1.58	1.51
9	A	2016	A1AIO	C06-C05	4.22	1.58	1.51
9	B	2020	A1AIO	C06-C05	4.22	1.58	1.51
9	B	2011	A1AIO	C06-C05	4.22	1.58	1.51
9	A	2018	A1AIO	C06-C05	4.21	1.58	1.51
9	A	2035	A1AIO	C06-C05	4.21	1.58	1.51
9	A	2022	A1AIO	C06-C05	4.21	1.58	1.51
9	A	2001	A1AIO	C06-C05	4.21	1.58	1.51
9	B	2018	A1AIO	C06-C05	4.21	1.58	1.51
9	A	2042	A1AIO	C06-C05	4.20	1.58	1.51
9	A	2009	A1AIO	C06-C05	4.20	1.58	1.51
9	B	2024	A1AIO	C06-C05	4.20	1.58	1.51
9	A	2024	A1AIO	C06-C05	4.20	1.58	1.51
9	B	2042	A1AIO	C06-C05	4.20	1.58	1.51
9	A	2032	A1AIO	C06-C05	4.20	1.58	1.51
9	B	2038	A1AIO	C06-C05	4.20	1.58	1.51
9	A	2007	A1AIO	C06-C05	4.20	1.58	1.51
9	B	2043	A1AIO	C06-C05	4.20	1.58	1.51
9	A	2041	A1AIO	C06-C05	4.19	1.58	1.51
9	A	2020	A1AIO	C06-C05	4.19	1.58	1.51
9	A	2015	A1AIO	C06-C05	4.19	1.58	1.51
9	B	2012	A1AIO	C06-C05	4.19	1.58	1.51
9	B	2030	A1AIO	C06-C05	4.19	1.58	1.51
9	A	2054	A1AIO	C06-C05	4.19	1.58	1.51
9	A	2017	A1AIO	C06-C05	4.19	1.58	1.51
9	B	2032	A1AIO	C06-C05	4.19	1.58	1.51
9	B	2019	A1AIO	C06-C05	4.19	1.58	1.51
9	B	2057	A1AIO	C06-C05	4.18	1.58	1.51
9	A	2014	A1AIO	C06-C05	4.18	1.58	1.51
9	A	2002	A1AIO	C06-C05	4.18	1.58	1.51
9	B	2036	A1AIO	C06-C05	4.18	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2031	A1AIO	C06-C05	4.18	1.58	1.51
9	B	2025	A1AIO	C06-C05	4.18	1.58	1.51
9	A	2055	A1AIO	C06-C05	4.17	1.58	1.51
9	B	2055	A1AIO	C06-C05	4.17	1.58	1.51
9	B	2048	A1AIO	C06-C05	4.17	1.58	1.51
9	A	2051	A1AIO	C06-C05	4.17	1.58	1.51
9	A	2053	A1AIO	C06-C05	4.17	1.58	1.51
9	A	2003	A1AIO	C06-C05	4.17	1.58	1.51
9	A	2021	A1AIO	C06-C05	4.17	1.58	1.51
9	B	2045	A1AIO	C06-C05	4.17	1.58	1.51
9	A	2006	A1AIO	C06-C05	4.16	1.58	1.51
9	A	2008	A1AIO	C06-C05	4.16	1.58	1.51
9	B	2013	A1AIO	C06-C05	4.16	1.58	1.51
9	A	2026	A1AIO	C06-C05	4.15	1.58	1.51
9	B	2022	A1AIO	C06-C05	4.15	1.58	1.51
9	A	2057	A1AIO	C06-C05	4.15	1.58	1.51
9	B	2017	A1AIO	C06-C05	4.15	1.58	1.51
9	B	2044	A1AIO	C06-C05	4.15	1.58	1.51
9	A	2025	A1AIO	C06-C05	4.15	1.58	1.51
9	B	2050	A1AIO	C06-C05	4.15	1.58	1.51
9	A	2056	A1AIO	C06-C05	4.14	1.58	1.51
9	B	2040	A1AIO	C06-C05	4.14	1.58	1.51
9	B	2056	A1AIO	C06-C05	4.14	1.58	1.51
9	A	2043	A1AIO	C06-C05	4.14	1.58	1.51
9	B	2009	A1AIO	C06-C05	4.13	1.58	1.51
9	B	2016	A1AIO	C06-C05	4.13	1.58	1.51
9	A	2034	A1AIO	C06-C05	4.13	1.58	1.51
9	B	2004	A1AIO	C06-C05	4.12	1.58	1.51
9	A	2027	A1AIO	C06-C05	4.11	1.58	1.51
9	A	2033	A1AIO	C06-C05	4.11	1.58	1.51
9	B	2015	A1AIO	C06-C05	4.10	1.58	1.51
9	B	2035	A1AIO	C06-C05	4.10	1.58	1.51
9	A	2050	A1AIO	C06-C05	4.10	1.58	1.51
9	B	2051	A1AIO	C06-C05	4.09	1.58	1.51
9	B	2039	A1AIO	C06-C05	4.09	1.58	1.51
9	A	2030	A1AIO	C06-C05	4.09	1.58	1.51
9	B	2008	A1AIO	C06-C05	4.09	1.58	1.51
9	B	2031	A1AIO	C06-C05	4.08	1.58	1.51
9	A	2037	A1AIO	C06-C05	4.07	1.58	1.51
9	A	2046	A1AIO	C06-C05	4.06	1.58	1.51
9	B	2026	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2004	A1AIO	C06-C05	4.05	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2034	A1AIO	C06-C05	4.05	1.58	1.51
9	A	2049	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2044	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2045	A1AIO	C06-C05	4.04	1.58	1.51
9	B	2023	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2048	A1AIO	C06-C05	4.04	1.58	1.51
9	B	2046	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2054	A1AIO	C06-C05	4.03	1.58	1.51
9	A	2047	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2052	A1AIO	C06-C05	4.03	1.58	1.51
9	A	2039	A1AIO	C06-C05	4.01	1.58	1.51
9	B	2003	A1AIO	C06-C05	4.01	1.58	1.51
9	B	2028	A1AIO	C06-C05	4.01	1.58	1.51
9	A	2029	A1AIO	C06-C05	4.00	1.58	1.51
9	B	2041	A1AIO	C06-C05	4.00	1.58	1.51
9	B	2005	A1AIO	C06-C05	3.97	1.58	1.51
9	B	2033	A1AIO	C06-C05	3.96	1.58	1.51
9	B	2047	A1AIO	C06-C05	3.91	1.58	1.51
10	B	2069	GLA	C2-C3	-3.58	1.47	1.52
10	A	2068	GLA	C2-C3	-3.56	1.47	1.52
10	B	2061	GLA	C2-C3	-3.55	1.47	1.52
10	B	2068	GLA	C2-C3	-3.55	1.47	1.52
10	A	2069	GLA	C2-C3	-3.52	1.47	1.52
10	A	2067	GLA	C2-C3	-3.52	1.47	1.52
10	B	2070	GLA	C2-C3	-3.52	1.47	1.52
10	A	2061	GLA	C2-C3	-3.51	1.47	1.52
10	A	2070	GLA	C2-C3	-3.48	1.47	1.52
10	B	2066	GLA	C2-C3	-3.48	1.47	1.52
10	A	2065	GLA	C2-C3	-3.47	1.47	1.52
10	A	2063	GLA	C2-C3	-3.46	1.47	1.52
10	A	2066	GLA	C2-C3	-3.43	1.47	1.52
10	B	2067	GLA	C2-C3	-3.42	1.47	1.52
10	B	2058	GLA	C2-C3	-3.42	1.47	1.52
10	B	2060	GLA	C2-C3	-3.42	1.47	1.52
10	A	2062	GLA	C2-C3	-3.41	1.47	1.52
10	A	2064	GLA	C2-C3	-3.41	1.47	1.52
10	B	2062	GLA	C2-C3	-3.41	1.47	1.52
10	B	2063	GLA	C2-C3	-3.40	1.47	1.52
10	B	2064	GLA	C2-C3	-3.39	1.47	1.52
10	A	2058	GLA	C2-C3	-3.35	1.47	1.52
10	B	2065	GLA	C2-C3	-3.30	1.47	1.52
10	B	2063	GLA	O5-C1	3.26	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2063	GLA	O5-C1	3.25	1.48	1.43
10	A	2067	GLA	O5-C1	3.24	1.48	1.43
10	B	2062	GLA	O5-C1	3.23	1.48	1.43
10	A	2061	GLA	O5-C1	3.21	1.48	1.43
10	B	2066	GLA	O5-C1	3.21	1.48	1.43
10	A	2058	GLA	O5-C1	3.21	1.48	1.43
10	A	2064	GLA	O5-C1	3.21	1.48	1.43
10	B	2060	GLA	O5-C1	3.20	1.48	1.43
10	A	2062	GLA	O5-C1	3.20	1.48	1.43
10	B	2058	GLA	O5-C1	3.20	1.48	1.43
10	B	2067	GLA	O5-C1	3.19	1.48	1.43
10	B	2068	GLA	O5-C1	3.19	1.48	1.43
10	A	2065	GLA	O5-C1	3.18	1.48	1.43
10	B	2070	GLA	O5-C1	3.18	1.48	1.43
10	B	2064	GLA	O5-C1	3.16	1.48	1.43
10	A	2068	GLA	O5-C1	3.16	1.48	1.43
10	A	2066	GLA	O5-C1	3.15	1.48	1.43
10	B	2065	GLA	O5-C1	3.14	1.48	1.43
10	B	2061	GLA	O5-C1	3.14	1.48	1.43
10	A	2070	GLA	O5-C1	3.12	1.48	1.43
10	A	2069	GLA	O5-C1	3.12	1.48	1.43
10	B	2069	GLA	O5-C1	3.10	1.48	1.43
10	B	2063	GLA	O5-C5	2.43	1.48	1.43
10	A	2065	GLA	O5-C5	2.40	1.48	1.43
10	A	2066	GLA	O5-C5	2.37	1.48	1.43
10	B	2064	GLA	O5-C5	2.34	1.48	1.43
10	A	2061	GLA	O5-C5	2.33	1.48	1.43
10	B	2061	GLA	O5-C5	2.33	1.48	1.43
10	A	2068	GLA	O5-C5	2.33	1.48	1.43
10	A	2070	GLA	O5-C5	2.33	1.48	1.43
10	A	2067	GLA	O5-C5	2.33	1.48	1.43
10	B	2066	GLA	O5-C5	2.33	1.48	1.43
10	A	2058	GLA	O5-C5	2.31	1.48	1.43
10	B	2062	GLA	O5-C5	2.31	1.48	1.43
10	A	2064	GLA	O5-C5	2.31	1.48	1.43
10	B	2067	GLA	O5-C5	2.31	1.48	1.43
10	A	2062	GLA	O5-C5	2.30	1.48	1.43
10	A	2063	GLA	O5-C5	2.29	1.48	1.43
10	B	2058	GLA	O5-C5	2.29	1.48	1.43
10	B	2065	GLA	O5-C5	2.27	1.48	1.43
10	A	2069	GLA	O5-C5	2.27	1.48	1.43
10	B	2060	GLA	O5-C5	2.27	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	2069	GLA	O5-C5	2.27	1.48	1.43
9	B	2039	A1AIO	O11-C02	-2.26	1.38	1.43
10	B	2068	GLA	O5-C5	2.26	1.48	1.43
9	B	2042	A1AIO	O11-C02	-2.25	1.38	1.43
9	A	2029	A1AIO	O11-C02	-2.25	1.38	1.43
10	B	2070	GLA	O5-C5	2.25	1.48	1.43
9	A	2003	A1AIO	O11-C02	-2.25	1.38	1.43
9	A	2056	A1AIO	O11-C02	-2.23	1.38	1.43
9	A	2057	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2028	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2003	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2038	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2044	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2043	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2036	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2045	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2048	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2048	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2055	A1AIO	O11-C02	-2.20	1.38	1.43
9	A	2043	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2051	A1AIO	O11-C02	-2.20	1.38	1.43
9	A	2007	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2035	A1AIO	O11-C02	-2.20	1.38	1.43
9	A	2051	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2055	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2030	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2049	A1AIO	O11-C02	-2.19	1.38	1.43
9	A	2010	A1AIO	O11-C02	-2.19	1.38	1.43
9	A	2050	A1AIO	O11-C02	-2.19	1.38	1.43
9	A	2033	A1AIO	O11-C02	-2.19	1.38	1.43
9	A	2054	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2005	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2027	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2013	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2004	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2057	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2047	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2045	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2008	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2004	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2056	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2052	A1AIO	O11-C02	-2.18	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2010	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2034	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2021	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2049	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2016	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2054	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2005	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2032	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2023	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2006	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2033	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2040	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2008	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2013	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2046	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2032	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2009	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2016	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2028	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2020	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2011	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2041	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2041	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2012	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2050	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2006	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2031	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2011	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2022	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2001	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2015	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2022	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2002	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2024	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2026	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2047	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2040	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2037	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2053	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2012	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2053	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2019	A1AIO	O11-C02	-2.15	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2023	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2036	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2009	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2030	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2046	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2018	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2014	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2029	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2025	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2031	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2021	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2001	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2034	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2037	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2042	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2052	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2039	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2025	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2017	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2015	A1AIO	O11-C02	-2.13	1.38	1.43
9	B	2002	A1AIO	O11-C02	-2.13	1.38	1.43
9	A	2019	A1AIO	O11-C02	-2.13	1.38	1.43
9	B	2007	A1AIO	O11-C02	-2.13	1.38	1.43
9	A	2038	A1AIO	O11-C02	-2.13	1.38	1.43
9	A	2024	A1AIO	O11-C02	-2.13	1.38	1.43
9	B	2018	A1AIO	O11-C02	-2.12	1.38	1.43
9	A	2014	A1AIO	O11-C02	-2.12	1.38	1.43
9	A	2027	A1AIO	O11-C02	-2.12	1.38	1.43
9	B	2020	A1AIO	O11-C02	-2.12	1.38	1.43
9	A	2035	A1AIO	O11-C02	-2.12	1.38	1.43
9	B	2026	A1AIO	O11-C02	-2.11	1.38	1.43
9	B	2017	A1AIO	O11-C02	-2.11	1.38	1.43
9	A	2044	A1AIO	O11-C02	-2.10	1.38	1.43

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	2026	A1AIO	C02-C03-C04	-4.96	109.23	115.86
9	A	2044	A1AIO	C02-C03-C04	-4.83	109.40	115.86
9	B	2033	A1AIO	C02-C03-C04	-4.81	109.42	115.86
9	B	2047	A1AIO	C02-C03-C04	-4.80	109.44	115.86
9	B	2006	A1AIO	C02-C03-C04	-4.73	109.54	115.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2027	A1AIO	C02-C03-C04	-4.70	109.58	115.86
9	B	2009	A1AIO	C02-C03-C04	-4.69	109.58	115.86
9	A	2006	A1AIO	C02-C03-C04	-4.68	109.60	115.86
9	A	2034	A1AIO	C02-C03-C04	-4.68	109.61	115.86
9	A	2053	A1AIO	C02-C03-C04	-4.66	109.63	115.86
9	B	2004	A1AIO	C02-C03-C04	-4.63	109.67	115.86
9	B	2025	A1AIO	C02-C03-C04	-4.62	109.68	115.86
9	A	2043	A1AIO	C02-C03-C04	-4.60	109.72	115.86
9	A	2039	A1AIO	C02-C03-C04	-4.57	109.74	115.86
9	A	2031	A1AIO	C02-C03-C04	-4.55	109.77	115.86
9	B	2037	A1AIO	C02-C03-C04	-4.55	109.78	115.86
9	B	2035	A1AIO	C02-C03-C04	-4.54	109.79	115.86
9	A	2026	A1AIO	C02-C03-C04	-4.52	109.82	115.86
9	A	2042	A1AIO	C02-C03-C04	-4.52	109.82	115.86
9	A	2024	A1AIO	C02-C03-C04	-4.51	109.83	115.86
9	B	2038	A1AIO	C02-C03-C04	-4.51	109.83	115.86
9	B	2008	A1AIO	C02-C03-C04	-4.50	109.84	115.86
9	B	2041	A1AIO	C02-C03-C04	-4.50	109.84	115.86
9	B	2001	A1AIO	C02-C03-C04	-4.50	109.84	115.86
9	A	2003	A1AIO	C02-C03-C04	-4.49	109.86	115.86
9	B	2039	A1AIO	C02-C03-C04	-4.48	109.86	115.86
9	B	2003	A1AIO	C02-C03-C04	-4.48	109.87	115.86
9	B	2032	A1AIO	C02-C03-C04	-4.47	109.88	115.86
9	B	2027	A1AIO	C02-C03-C04	-4.46	109.90	115.86
9	B	2040	A1AIO	C02-C03-C04	-4.46	109.90	115.86
9	B	2049	A1AIO	C02-C03-C04	-4.45	109.90	115.86
9	A	2048	A1AIO	C02-C03-C04	-4.43	109.93	115.86
9	A	2047	A1AIO	C02-C03-C04	-4.43	109.94	115.86
9	A	2049	A1AIO	C02-C03-C04	-4.43	109.94	115.86
9	B	2046	A1AIO	C02-C03-C04	-4.43	109.94	115.86
9	B	2052	A1AIO	C02-C03-C04	-4.43	109.94	115.86
9	A	2045	A1AIO	C02-C03-C04	-4.43	109.94	115.86
9	A	2011	A1AIO	C02-C03-C04	-4.42	109.95	115.86
9	B	2002	A1AIO	C02-C03-C04	-4.42	109.95	115.86
9	B	2034	A1AIO	C02-C03-C04	-4.42	109.95	115.86
9	A	2004	A1AIO	C02-C03-C04	-4.42	109.95	115.86
9	A	2002	A1AIO	C02-C03-C04	-4.41	109.96	115.86
9	A	2046	A1AIO	C02-C03-C04	-4.40	109.98	115.86
9	B	2007	A1AIO	C02-C03-C04	-4.40	109.98	115.86
9	A	2001	A1AIO	C02-C03-C04	-4.40	109.98	115.86
9	A	2051	A1AIO	C02-C03-C04	-4.38	110.00	115.86
9	A	2007	A1AIO	C02-C03-C04	-4.37	110.01	115.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	2048	A1AIO	C02-C03-C04	-4.36	110.03	115.86
9	B	2019	A1AIO	C02-C03-C04	-4.36	110.03	115.86
9	B	2044	A1AIO	C02-C03-C04	-4.36	110.03	115.86
9	A	2036	A1AIO	C02-C03-C04	-4.35	110.05	115.86
9	B	2036	A1AIO	C02-C03-C04	-4.35	110.05	115.86
9	B	2043	A1AIO	C02-C03-C04	-4.35	110.05	115.86
9	A	2028	A1AIO	C02-C03-C04	-4.33	110.07	115.86
9	B	2045	A1AIO	C02-C03-C04	-4.33	110.08	115.86
9	B	2056	A1AIO	C02-C03-C04	-4.32	110.08	115.86
9	A	2025	A1AIO	C02-C03-C04	-4.31	110.09	115.86
9	B	2042	A1AIO	C02-C03-C04	-4.31	110.09	115.86
9	A	2056	A1AIO	C02-C03-C04	-4.31	110.10	115.86
9	A	2009	A1AIO	C02-C03-C04	-4.31	110.10	115.86
9	A	2018	A1AIO	C02-C03-C04	-4.30	110.11	115.86
9	A	2052	A1AIO	C02-C03-C04	-4.27	110.15	115.86
9	B	2012	A1AIO	C02-C03-C04	-4.27	110.15	115.86
9	A	2014	A1AIO	C02-C03-C04	-4.27	110.15	115.86
9	B	2029	A1AIO	C02-C03-C04	-4.27	110.15	115.86
9	B	2010	A1AIO	C02-C03-C04	-4.26	110.16	115.86
9	A	2037	A1AIO	C02-C03-C04	-4.26	110.16	115.86
9	A	2012	A1AIO	C02-C03-C04	-4.26	110.17	115.86
9	A	2017	A1AIO	C02-C03-C04	-4.24	110.19	115.86
9	B	2024	A1AIO	C02-C03-C04	-4.24	110.19	115.86
9	B	2057	A1AIO	C02-C03-C04	-4.23	110.20	115.86
9	A	2008	A1AIO	C02-C03-C04	-4.23	110.20	115.86
9	A	2022	A1AIO	C02-C03-C04	-4.23	110.20	115.86
9	A	2005	A1AIO	C02-C03-C04	-4.23	110.21	115.86
9	A	2033	A1AIO	C02-C03-C04	-4.22	110.21	115.86
9	A	2013	A1AIO	C02-C03-C04	-4.16	110.30	115.86
9	A	2057	A1AIO	C02-C03-C04	-4.15	110.32	115.86
9	A	2016	A1AIO	C02-C03-C04	-4.14	110.32	115.86
9	A	2032	A1AIO	C02-C03-C04	-4.14	110.33	115.86
9	B	2017	A1AIO	C02-C03-C04	-4.11	110.36	115.86
9	A	2040	A1AIO	C02-C03-C04	-4.10	110.38	115.86
9	A	2054	A1AIO	C02-C03-C04	-4.09	110.39	115.86
9	A	2010	A1AIO	C02-C03-C04	-4.07	110.41	115.86
9	A	2023	A1AIO	C02-C03-C04	-4.07	110.41	115.86
9	A	2021	A1AIO	C02-C03-C04	-4.07	110.41	115.86
9	B	2011	A1AIO	C02-C03-C04	-4.06	110.43	115.86
9	B	2055	A1AIO	C02-C03-C04	-4.06	110.43	115.86
9	A	2020	A1AIO	C02-C03-C04	-4.06	110.43	115.86
9	A	2019	A1AIO	C02-C03-C04	-4.05	110.44	115.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	2015	A1AIO	C02-C03-C04	-4.05	110.45	115.86
9	A	2038	A1AIO	C02-C03-C04	-4.02	110.48	115.86
9	B	2031	A1AIO	C02-C03-C04	-4.00	110.51	115.86
9	B	2053	A1AIO	C02-C03-C04	-4.00	110.52	115.86
9	A	2030	A1AIO	C02-C03-C04	-3.97	110.55	115.86
9	B	2013	A1AIO	C02-C03-C04	-3.97	110.55	115.86
9	A	2015	A1AIO	C02-C03-C04	-3.95	110.58	115.86
9	A	2041	A1AIO	C02-C03-C04	-3.93	110.60	115.86
9	B	2018	A1AIO	C02-C03-C04	-3.92	110.62	115.86
9	A	2055	A1AIO	C02-C03-C04	-3.90	110.64	115.86
9	A	2035	A1AIO	C02-C03-C04	-3.90	110.65	115.86
9	B	2050	A1AIO	C02-C03-C04	-3.89	110.65	115.86
9	B	2022	A1AIO	C02-C03-C04	-3.86	110.70	115.86
9	B	2021	A1AIO	C02-C03-C04	-3.84	110.73	115.86
9	A	2050	A1AIO	C02-C03-C04	-3.77	110.82	115.86
9	B	2014	A1AIO	C02-C03-C04	-3.71	110.90	115.86
9	B	2051	A1AIO	C02-C03-C04	-3.69	110.93	115.86
9	A	2029	A1AIO	C02-C03-C04	-3.67	110.95	115.86
9	B	2030	A1AIO	C02-C03-C04	-3.60	111.05	115.86
9	B	2016	A1AIO	C06-C05-C04	3.55	107.04	101.63
9	B	2028	A1AIO	C02-C03-C04	-3.50	111.18	115.86
9	B	2046	A1AIO	C06-C05-C04	3.47	106.91	101.63
9	B	2009	A1AIO	C06-C05-C04	3.47	106.91	101.63
9	B	2023	A1AIO	C02-C03-C04	-3.45	111.24	115.86
9	B	2034	A1AIO	C06-C05-C04	3.43	106.85	101.63
9	B	2031	A1AIO	C06-C05-C04	3.38	106.78	101.63
9	B	2030	A1AIO	C06-C05-C04	3.38	106.77	101.63
9	B	2011	A1AIO	C06-C05-C04	3.37	106.76	101.63
9	B	2020	A1AIO	C02-C03-C04	-3.34	111.39	115.86
9	B	2005	A1AIO	C02-C03-C04	-3.29	111.47	115.86
9	B	2054	A1AIO	C02-C03-C04	-3.28	111.47	115.86
9	B	2055	A1AIO	C06-C05-C04	3.22	106.53	101.63
10	B	2063	GLA	C1-C2-C3	3.17	113.56	109.67
9	A	2016	A1AIO	C06-C05-C04	3.16	106.44	101.63
9	A	2040	A1AIO	C06-C05-C04	3.15	106.43	101.63
9	A	2038	A1AIO	C06-C05-C04	3.13	106.40	101.63
9	A	2009	A1AIO	C06-C05-C04	3.12	106.38	101.63
9	A	2006	A1AIO	C06-C05-C04	3.12	106.38	101.63
9	B	2052	A1AIO	C06-C05-C04	3.07	106.30	101.63
9	B	2001	A1AIO	C06-C05-C04	3.07	106.30	101.63
9	B	2016	A1AIO	C02-C03-C04	-3.06	111.76	115.86
9	B	2014	A1AIO	C06-C05-C04	3.04	106.26	101.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2056	A1AIO	C06-C05-C04	3.04	106.25	101.63
9	B	2050	A1AIO	C06-C05-C04	3.03	106.24	101.63
9	B	2022	A1AIO	C06-C05-C04	3.02	106.23	101.63
9	A	2012	A1AIO	C06-C05-C04	3.02	106.22	101.63
9	B	2017	A1AIO	C06-C05-C04	3.00	106.19	101.63
9	B	2053	A1AIO	C06-C05-C04	2.98	106.17	101.63
9	B	2019	A1AIO	C06-C05-C04	2.97	106.16	101.63
9	A	2032	A1AIO	C06-C05-C04	2.97	106.16	101.63
9	B	2041	A1AIO	C06-C05-C04	2.97	106.15	101.63
9	B	2023	A1AIO	C06-C05-C04	2.93	106.10	101.63
9	B	2015	A1AIO	C06-C05-C04	2.92	106.08	101.63
9	B	2040	A1AIO	C06-C05-C04	2.90	106.05	101.63
9	B	2032	A1AIO	C06-C05-C04	2.90	106.04	101.63
9	B	2008	A1AIO	C06-C05-C04	2.88	106.02	101.63
9	B	2002	A1AIO	C06-C05-C04	2.83	105.95	101.63
9	B	2057	A1AIO	C06-C05-C04	2.83	105.95	101.63
9	B	2005	A1AIO	C06-C05-C04	2.81	105.91	101.63
9	B	2051	A1AIO	C06-C05-C04	2.80	105.90	101.63
9	B	2015	A1AIO	O07-C03-C04	2.79	108.58	103.59
9	B	2020	A1AIO	C06-C05-C04	2.76	105.83	101.63
9	B	2023	A1AIO	O07-C03-C04	2.74	108.48	103.59
9	A	2011	A1AIO	C06-C05-C04	2.70	105.75	101.63
9	A	2023	A1AIO	C06-C05-C04	2.70	105.74	101.63
9	A	2018	A1AIO	C06-C05-C04	2.70	105.73	101.63
9	B	2004	A1AIO	C06-C05-C04	2.69	105.73	101.63
9	A	2044	A1AIO	C06-C05-C04	2.65	105.67	101.63
9	B	2005	A1AIO	O07-C03-C04	2.64	108.31	103.59
9	B	2031	A1AIO	O07-C03-C04	2.64	108.31	103.59
9	A	2048	A1AIO	C06-C05-C04	2.62	105.63	101.63
9	B	2037	A1AIO	C06-C05-C04	2.62	105.62	101.63
9	A	2045	A1AIO	C06-C05-C04	2.60	105.59	101.63
9	A	2047	A1AIO	C06-C05-C04	2.60	105.59	101.63
9	B	2047	A1AIO	C06-C05-C04	2.59	105.57	101.63
9	A	2049	A1AIO	C06-C05-C04	2.57	105.55	101.63
9	B	2033	A1AIO	C06-C05-C04	2.57	105.54	101.63
10	A	2058	GLA	C1-C2-C3	2.55	112.80	109.67
9	A	2052	A1AIO	C06-C05-C04	2.52	105.47	101.63
9	A	2008	A1AIO	C06-C05-C04	2.51	105.45	101.63
9	A	2014	A1AIO	C06-C05-C04	2.51	105.45	101.63
9	A	2022	A1AIO	C06-C05-C04	2.50	105.44	101.63
9	A	2007	A1AIO	C06-C05-C04	2.50	105.43	101.63
9	A	2039	A1AIO	O07-C03-C04	2.47	108.01	103.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2044	A1AIO	O07-C03-C04	2.46	108.00	103.59
10	B	2065	GLA	C1-C2-C3	2.46	112.69	109.67
9	A	2013	A1AIO	C06-C05-C04	2.46	105.38	101.63
9	B	2008	A1AIO	O07-C03-C04	2.44	107.96	103.59
9	A	2053	A1AIO	C06-C05-C04	2.43	105.33	101.63
9	B	2012	A1AIO	C06-C05-C04	2.43	105.33	101.63
9	B	2013	A1AIO	C06-C05-C04	2.43	105.33	101.63
9	B	2006	A1AIO	C06-C05-C04	2.41	105.29	101.63
9	A	2036	A1AIO	C06-C05-C04	2.40	105.29	101.63
9	A	2046	A1AIO	C06-C05-C04	2.40	105.29	101.63
9	B	2054	A1AIO	C06-C05-C04	2.40	105.28	101.63
9	A	2034	A1AIO	C06-C05-C04	2.40	105.28	101.63
10	A	2062	GLA	C1-C2-C3	2.39	112.60	109.67
10	A	2064	GLA	C1-C2-C3	2.39	112.60	109.67
9	B	2028	A1AIO	C06-C05-C04	2.38	105.25	101.63
9	A	2029	A1AIO	C06-C05-C04	2.37	105.24	101.63
10	B	2060	GLA	C1-C2-C3	2.37	112.58	109.67
9	B	2007	A1AIO	C06-C05-C04	2.36	105.22	101.63
9	A	2051	A1AIO	C06-C05-C04	2.35	105.22	101.63
9	A	2010	A1AIO	C06-C05-C04	2.35	105.21	101.63
10	A	2063	GLA	C1-C2-C3	2.35	112.55	109.67
9	B	2033	A1AIO	O07-C03-C04	2.35	107.79	103.59
9	B	2029	A1AIO	C06-C05-C04	2.35	105.20	101.63
9	A	2024	A1AIO	C06-C05-C04	2.34	105.20	101.63
9	A	2015	A1AIO	C06-C05-C04	2.34	105.19	101.63
10	A	2061	GLA	C1-C2-C3	2.34	112.54	109.67
9	A	2020	A1AIO	C06-C05-C04	2.34	105.19	101.63
9	B	2016	A1AIO	O07-C03-C04	2.34	107.77	103.59
9	A	2054	A1AIO	C06-C05-C04	2.33	105.18	101.63
9	B	2047	A1AIO	O07-C03-C04	2.32	107.75	103.59
9	A	2055	A1AIO	C06-C05-C04	2.32	105.17	101.63
10	B	2064	GLA	C1-C2-C3	2.31	112.51	109.67
9	A	2037	A1AIO	C06-C05-C04	2.30	105.14	101.63
9	B	2026	A1AIO	C06-C05-C04	2.30	105.13	101.63
9	B	2027	A1AIO	C06-C05-C04	2.29	105.12	101.63
9	B	2049	A1AIO	C06-C05-C04	2.29	105.12	101.63
9	A	2004	A1AIO	C06-C05-C04	2.29	105.12	101.63
9	B	2035	A1AIO	C06-C05-C04	2.28	105.10	101.63
10	A	2060	GLA	C1-O5-C5	2.27	115.27	112.19
9	A	2002	A1AIO	C06-C05-C04	2.27	105.08	101.63
10	A	2070	GLA	C1-C2-C3	2.26	112.45	109.67
10	A	2059	GLA	C1-O5-C5	2.26	115.25	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	2059	GLA	C1-O5-C5	2.26	115.25	112.19
9	B	2041	A1AIO	O07-C03-C04	2.25	107.62	103.59
9	B	2018	A1AIO	C06-C05-C04	2.24	105.05	101.63
9	B	2056	A1AIO	C06-C05-C04	2.24	105.05	101.63
10	A	2067	GLA	C1-C2-C3	2.24	112.42	109.67
9	A	2042	A1AIO	C06-C05-C04	2.24	105.04	101.63
9	A	2019	A1AIO	C06-C05-C04	2.24	105.04	101.63
9	B	2010	A1AIO	C06-C05-C04	2.23	105.02	101.63
10	B	2062	GLA	C1-C2-C3	2.22	112.40	109.67
9	A	2025	A1AIO	C06-C05-C04	2.22	105.02	101.63
10	B	2070	GLA	C1-C2-C3	2.22	112.39	109.67
9	B	2025	A1AIO	C06-C05-C04	2.21	105.00	101.63
10	B	2066	GLA	C1-C2-C3	2.21	112.38	109.67
9	B	2038	A1AIO	C06-C05-C04	2.20	104.99	101.63
9	B	2044	A1AIO	C06-C05-C04	2.20	104.98	101.63
9	B	2043	A1AIO	C06-C05-C04	2.20	104.97	101.63
9	A	2001	A1AIO	C06-C05-C04	2.19	104.97	101.63
9	A	2003	A1AIO	C06-C05-C04	2.19	104.97	101.63
9	A	2005	A1AIO	C06-C05-C04	2.19	104.96	101.63
9	A	2039	A1AIO	C06-C05-C04	2.18	104.95	101.63
9	B	2045	A1AIO	C06-C05-C04	2.18	104.94	101.63
9	B	2036	A1AIO	C06-C05-C04	2.17	104.94	101.63
9	B	2048	A1AIO	C06-C05-C04	2.17	104.94	101.63
9	B	2042	A1AIO	C06-C05-C04	2.16	104.92	101.63
9	A	2026	A1AIO	C06-C05-C04	2.16	104.92	101.63
9	A	2041	A1AIO	C06-C05-C04	2.16	104.92	101.63
9	A	2050	A1AIO	C06-C05-C04	2.14	104.89	101.63
10	B	2067	GLA	C1-C2-C3	2.14	112.29	109.67
9	A	2028	A1AIO	C06-C05-C04	2.13	104.87	101.63
9	A	2021	A1AIO	C06-C05-C04	2.13	104.87	101.63
9	A	2027	A1AIO	C06-C05-C04	2.11	104.85	101.63
9	A	2031	A1AIO	C06-C05-C04	2.11	104.84	101.63
9	A	2030	A1AIO	C06-C05-C04	2.11	104.84	101.63
9	A	2057	A1AIO	C06-C05-C04	2.10	104.83	101.63
9	B	2052	A1AIO	O07-C03-C04	2.10	107.35	103.59
9	B	2026	A1AIO	O07-C03-C04	2.10	107.34	103.59
9	B	2021	A1AIO	C06-C05-C04	2.10	104.82	101.63
9	A	2035	A1AIO	C06-C05-C04	2.09	104.81	101.63
10	B	2058	GLA	C1-C2-C3	2.06	112.20	109.67
10	A	2065	GLA	C1-C2-C3	2.06	112.19	109.67
10	A	2069	GLA	C1-C2-C3	2.05	112.19	109.67
9	A	2043	A1AIO	C06-C05-C04	2.03	104.73	101.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	2024	A1AIO	C06-C05-C04	2.01	104.69	101.63

All (29) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	2004	A1AIO	C06
9	A	2006	A1AIO	C06
9	A	2009	A1AIO	C06
9	A	2011	A1AIO	C06
9	A	2012	A1AIO	C06
9	A	2014	A1AIO	C06
9	A	2016	A1AIO	C06
9	A	2018	A1AIO	C06
9	A	2025	A1AIO	C06
9	A	2035	A1AIO	C06
9	A	2037	A1AIO	C06
9	A	2038	A1AIO	C06
9	A	2040	A1AIO	C06
9	A	2052	A1AIO	C06
9	B	2004	A1AIO	C06
9	B	2006	A1AIO	C06
9	B	2009	A1AIO	C06
9	B	2011	A1AIO	C06
9	B	2012	A1AIO	C06
9	B	2014	A1AIO	C06
9	B	2016	A1AIO	C06
9	B	2030	A1AIO	C06
9	B	2031	A1AIO	C06
9	B	2032	A1AIO	C06
9	B	2033	A1AIO	C06
9	B	2034	A1AIO	C06
9	B	2046	A1AIO	C06
9	B	2047	A1AIO	C06
9	B	2053	A1AIO	C06

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2002	A1AIO	O12-C01-C02-O11
9	A	2005	A1AIO	O12-C01-C02-O11
9	A	2030	A1AIO	C01-C02-C03-O07
9	A	2033	A1AIO	C01-C02-C03-O07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	2035	A1AIO	O12-C01-C02-C03
9	A	2035	A1AIO	C01-C02-C03-O07
9	A	2038	A1AIO	C01-C02-C03-O07
9	A	2040	A1AIO	C01-C02-C03-O07
9	A	2041	A1AIO	C01-C02-C03-O07
9	A	2054	A1AIO	C01-C02-C03-O07
9	B	2001	A1AIO	O12-C01-C02-C03
9	B	2003	A1AIO	C01-C02-C03-O07
9	B	2005	A1AIO	O12-C01-C02-C03
9	B	2005	A1AIO	O12-C01-C02-O11
9	B	2005	A1AIO	C01-C02-C03-O07
9	B	2013	A1AIO	O12-C01-C02-O11
9	B	2014	A1AIO	C01-C02-C03-O07
9	B	2016	A1AIO	O12-C01-C02-O11
9	B	2016	A1AIO	C01-C02-C03-C04
9	B	2016	A1AIO	C01-C02-C03-O07
9	B	2016	A1AIO	O11-C02-C03-O07
9	B	2018	A1AIO	C01-C02-C03-O07
9	B	2019	A1AIO	O12-C01-C02-O11
9	B	2020	A1AIO	C01-C02-C03-C04
9	B	2020	A1AIO	C01-C02-C03-O07
9	B	2020	A1AIO	O11-C02-C03-C04
9	B	2020	A1AIO	O11-C02-C03-O07
9	B	2021	A1AIO	C01-C02-C03-O07
9	B	2023	A1AIO	C01-C02-C03-C04
9	B	2023	A1AIO	C01-C02-C03-O07
9	B	2023	A1AIO	O11-C02-C03-C04
9	B	2023	A1AIO	O11-C02-C03-O07
9	B	2028	A1AIO	O12-C01-C02-O11
9	B	2028	A1AIO	C01-C02-C03-O07
9	B	2030	A1AIO	C01-C02-C03-O07
9	B	2032	A1AIO	O12-C01-C02-C03
9	B	2032	A1AIO	O12-C01-C02-O11
9	B	2034	A1AIO	O12-C01-C02-O11
9	B	2036	A1AIO	O12-C01-C02-O11
9	B	2037	A1AIO	O12-C01-C02-C03
9	B	2037	A1AIO	O12-C01-C02-O11
9	B	2041	A1AIO	O12-C01-C02-O11
9	B	2042	A1AIO	O12-C01-C02-O11
9	B	2043	A1AIO	O12-C01-C02-O11
9	B	2044	A1AIO	O12-C01-C02-O11
9	B	2045	A1AIO	O12-C01-C02-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	2046	A1AIO	O12-C01-C02-O11
9	B	2048	A1AIO	O12-C01-C02-O11
9	B	2051	A1AIO	C01-C02-C03-O07
9	B	2052	A1AIO	O12-C01-C02-O11
9	B	2053	A1AIO	C01-C02-C03-O07
9	B	2054	A1AIO	O12-C01-C02-C03
9	B	2054	A1AIO	O12-C01-C02-O11
9	B	2054	A1AIO	C01-C02-C03-O07
9	B	2054	A1AIO	O11-C02-C03-O07
10	B	2068	GLA	O5-C5-C6-O6
9	A	2035	A1AIO	O12-C01-C02-O11
9	A	2044	A1AIO	O12-C01-C02-O11
9	B	2001	A1AIO	O12-C01-C02-O11
9	B	2010	A1AIO	O12-C01-C02-O11
9	B	2021	A1AIO	O12-C01-C02-O11
9	B	2025	A1AIO	O12-C01-C02-O11
9	B	2035	A1AIO	O12-C01-C02-O11
9	B	2013	A1AIO	O12-C01-C02-C03
9	B	2016	A1AIO	O12-C01-C02-C03
9	B	2019	A1AIO	O12-C01-C02-C03
9	B	2028	A1AIO	O12-C01-C02-C03
9	B	2034	A1AIO	O12-C01-C02-C03
9	B	2036	A1AIO	O12-C01-C02-C03
9	B	2041	A1AIO	O12-C01-C02-C03
9	B	2042	A1AIO	O12-C01-C02-C03
9	B	2043	A1AIO	O12-C01-C02-C03
9	B	2044	A1AIO	O12-C01-C02-C03
9	B	2045	A1AIO	O12-C01-C02-C03
9	B	2046	A1AIO	O12-C01-C02-C03
9	B	2048	A1AIO	O12-C01-C02-C03
9	B	2052	A1AIO	O12-C01-C02-C03
10	B	2068	GLA	C4-C5-C6-O6
10	A	2063	GLA	O5-C5-C6-O6
10	B	2067	GLA	C4-C5-C6-O6
10	B	2067	GLA	O5-C5-C6-O6
10	B	2058	GLA	O5-C5-C6-O6
10	B	2060	GLA	O5-C5-C6-O6
10	B	2065	GLA	C4-C5-C6-O6
9	A	2004	A1AIO	O12-C01-C02-O11
9	B	2002	A1AIO	O12-C01-C02-O11
10	A	2063	GLA	C4-C5-C6-O6
10	A	2064	GLA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	2002	A1AIO	O12-C01-C02-C03
9	A	2005	A1AIO	O12-C01-C02-C03
9	A	2044	A1AIO	O12-C01-C02-C03
9	B	2021	A1AIO	O12-C01-C02-C03
9	B	2025	A1AIO	O12-C01-C02-C03
10	B	2060	GLA	C4-C5-C6-O6
10	B	2063	GLA	O5-C5-C6-O6
10	B	2063	GLA	C4-C5-C6-O6
10	B	2058	GLA	C4-C5-C6-O6
9	B	2010	A1AIO	O12-C01-C02-C03
9	B	2035	A1AIO	O12-C01-C02-C03
10	B	2065	GLA	O5-C5-C6-O6
10	A	2065	GLA	O5-C5-C6-O6
9	A	2004	A1AIO	O12-C01-C02-C03
9	B	2002	A1AIO	O12-C01-C02-C03
10	A	2064	GLA	C4-C5-C6-O6
10	B	2069	GLA	O5-C5-C6-O6
9	B	2007	A1AIO	O12-C01-C02-O11
9	B	2011	A1AIO	O12-C01-C02-O11
9	A	2038	A1AIO	O11-C02-C03-O07
9	A	2040	A1AIO	O11-C02-C03-O07
9	B	2005	A1AIO	O11-C02-C03-O07
9	B	2014	A1AIO	O11-C02-C03-O07
9	B	2018	A1AIO	O11-C02-C03-O07
9	B	2030	A1AIO	O11-C02-C03-O07
9	B	2005	A1AIO	O11-C02-C03-C04
9	B	2016	A1AIO	O11-C02-C03-C04
9	B	2018	A1AIO	O11-C02-C03-C04
9	B	2030	A1AIO	O11-C02-C03-C04
9	B	2054	A1AIO	O11-C02-C03-C04
10	B	2066	GLA	O5-C5-C6-O6
9	B	2005	A1AIO	C01-C02-C03-C04
9	B	2054	A1AIO	C01-C02-C03-C04
9	A	2020	A1AIO	C01-C02-C03-O07
10	A	2069	GLA	O5-C5-C6-O6
9	B	2006	A1AIO	O12-C01-C02-O11
9	B	2008	A1AIO	O12-C01-C02-O11
10	B	2061	GLA	C4-C5-C6-O6
9	A	2045	A1AIO	O12-C01-C02-O11
9	A	2047	A1AIO	O12-C01-C02-O11
9	A	2048	A1AIO	O12-C01-C02-O11
9	A	2049	A1AIO	O12-C01-C02-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	2038	A1AIO	O11-C02-C03-C04
9	A	2040	A1AIO	O11-C02-C03-C04
9	B	2014	A1AIO	O11-C02-C03-C04
10	A	2058	GLA	C4-C5-C6-O6
9	B	2011	A1AIO	O12-C01-C02-C03
10	B	2061	GLA	O5-C5-C6-O6
9	B	2007	A1AIO	O12-C01-C02-C03
9	A	2052	A1AIO	C01-C02-C03-O07
9	B	2006	A1AIO	O12-C01-C02-C03
9	B	2008	A1AIO	O12-C01-C02-C03
9	A	2001	A1AIO	O12-C01-C02-O11
9	A	2035	A1AIO	O11-C02-C03-O07
9	A	2035	A1AIO	O11-C02-C03-C04
9	B	2028	A1AIO	O11-C02-C03-C04
10	A	2065	GLA	C4-C5-C6-O6
9	A	2016	A1AIO	O12-C01-C02-O11
9	B	2003	A1AIO	O12-C01-C02-O11
9	A	2030	A1AIO	O11-C02-C03-C04
9	B	2004	A1AIO	O12-C01-C02-O11
9	A	2041	A1AIO	O11-C02-C03-C04
9	B	2003	A1AIO	O11-C02-C03-C04
9	B	2053	A1AIO	O11-C02-C03-C04
9	A	2006	A1AIO	O12-C01-C02-O11
9	B	2018	A1AIO	C01-C02-C03-C04
9	B	2030	A1AIO	C01-C02-C03-C04
9	A	2048	A1AIO	O12-C01-C02-C03
9	A	2049	A1AIO	O12-C01-C02-C03
10	B	2069	GLA	C4-C5-C6-O6
9	B	2015	A1AIO	C01-C02-C03-O07
9	B	2024	A1AIO	C01-C02-C03-O07
9	B	2031	A1AIO	C01-C02-C03-O07
9	B	2039	A1AIO	C01-C02-C03-O07
9	A	2045	A1AIO	O12-C01-C02-C03
9	A	2047	A1AIO	O12-C01-C02-C03
9	B	2004	A1AIO	O12-C01-C02-C03
10	B	2062	GLA	C4-C5-C6-O6

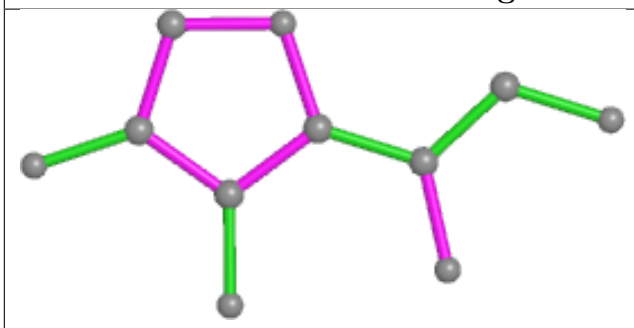
There are no ring outliers.

No monomer is involved in short contacts.

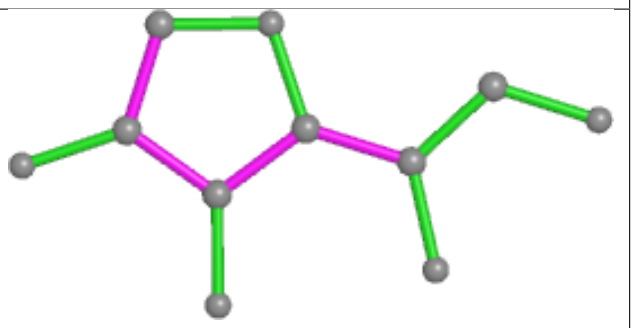
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

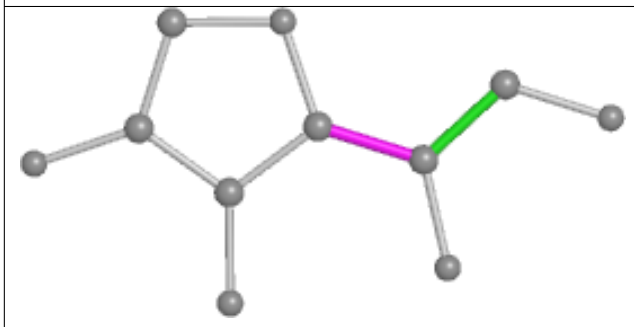
Ligand A1AIO B 2030



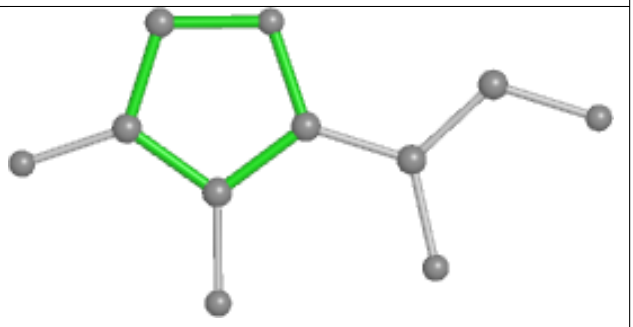
Bond lengths



Bond angles

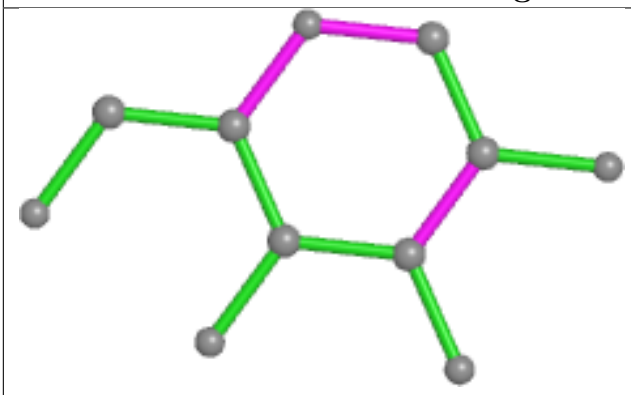


Torsions

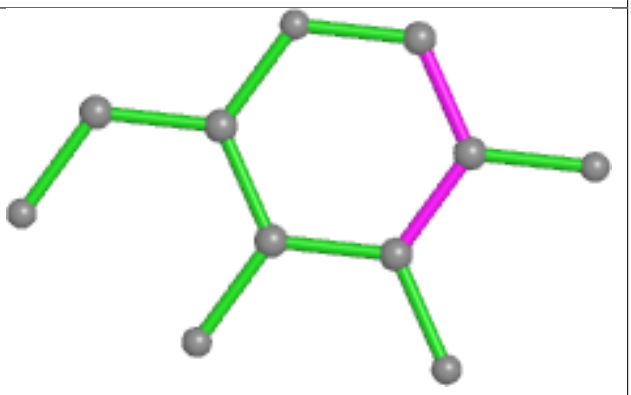


Rings

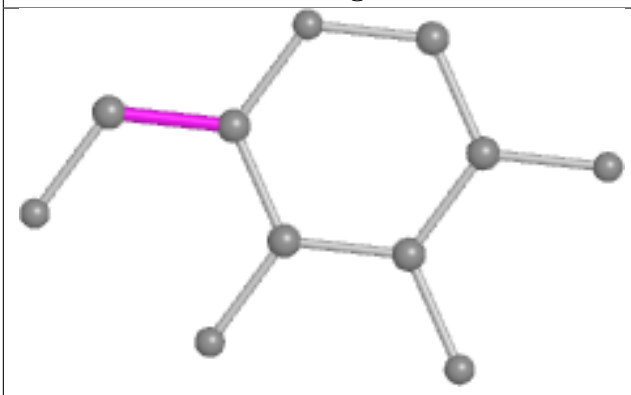
Ligand GLA A 2063



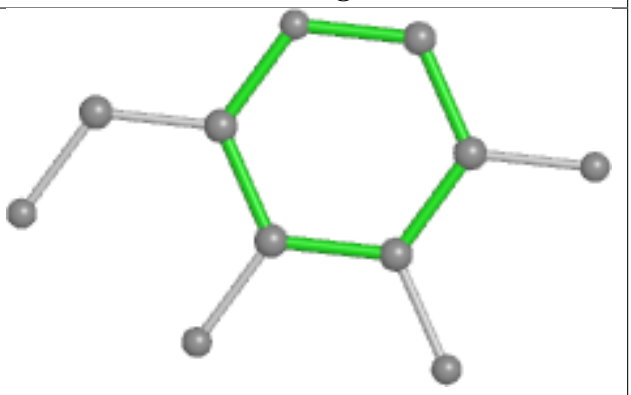
Bond lengths



Bond angles

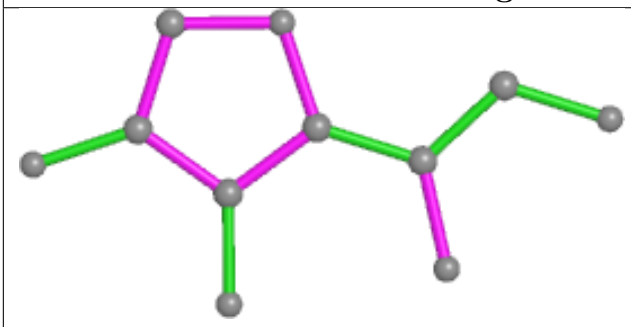


Torsions

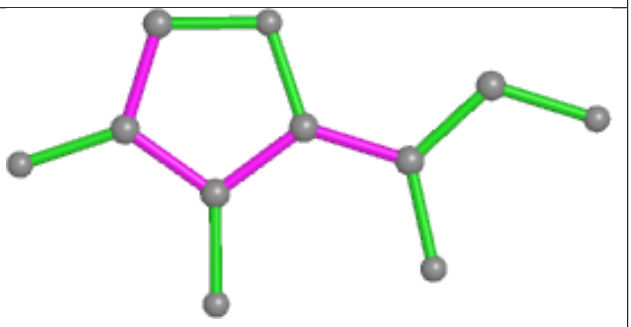


Rings

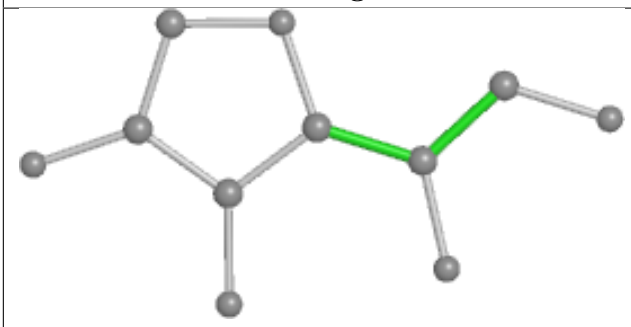
Ligand A1AIO A 2028



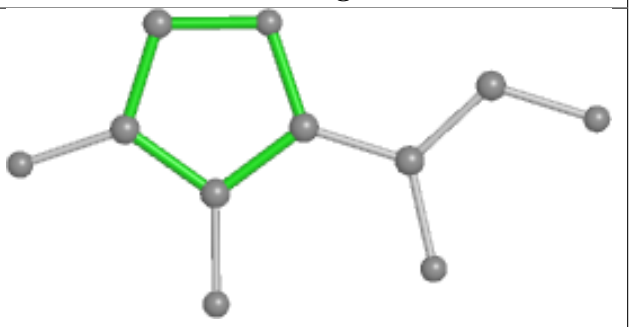
Bond lengths



Bond angles

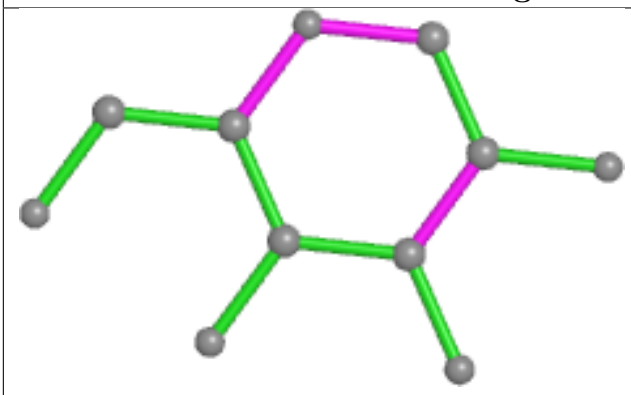


Torsions

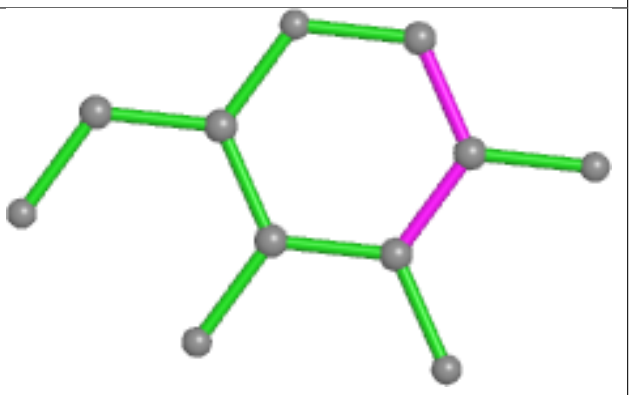


Rings

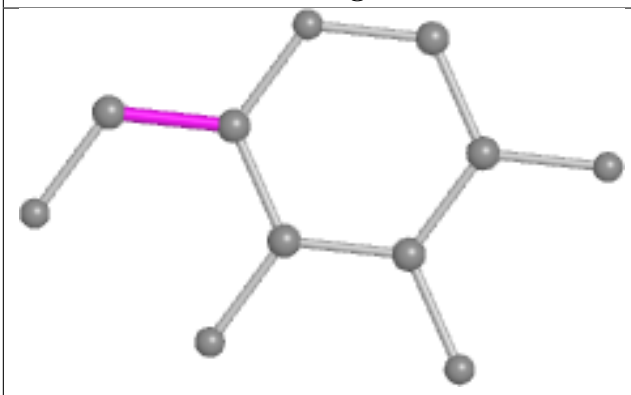
Ligand GLA A 2058



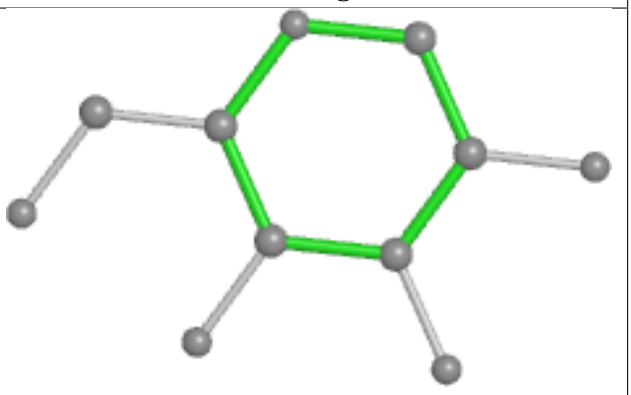
Bond lengths



Bond angles

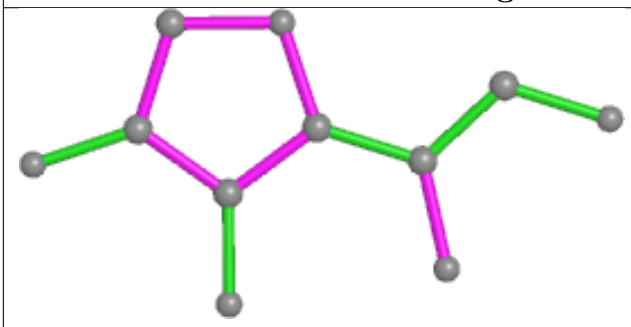


Torsions

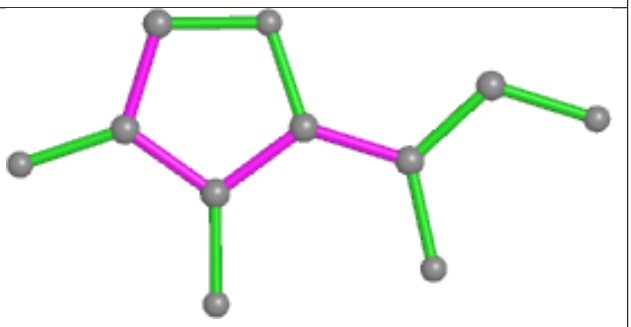


Rings

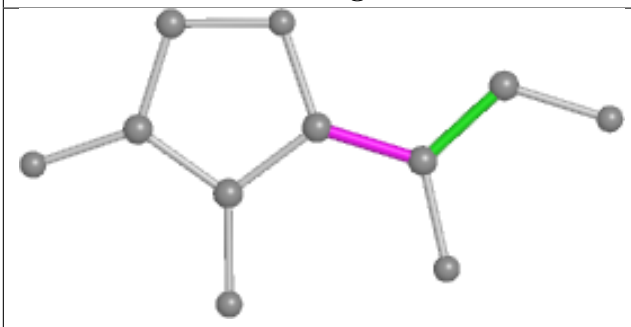
Ligand A1AIO B 2051



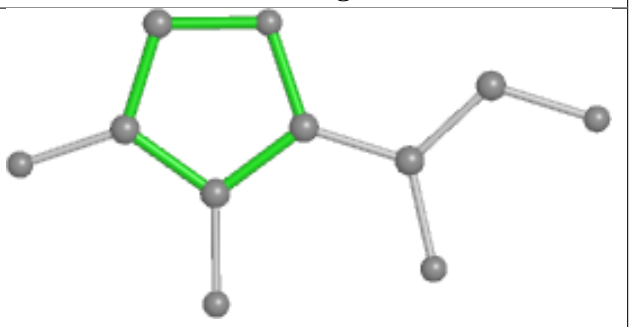
Bond lengths



Bond angles

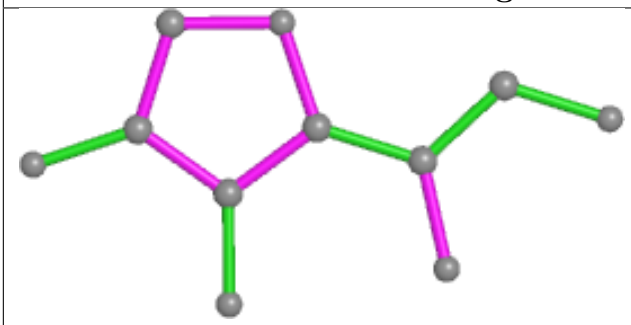


Torsions

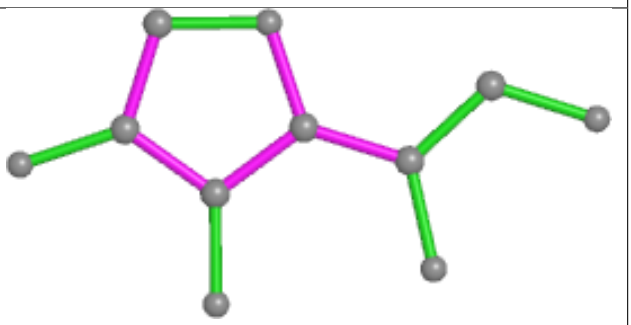


Rings

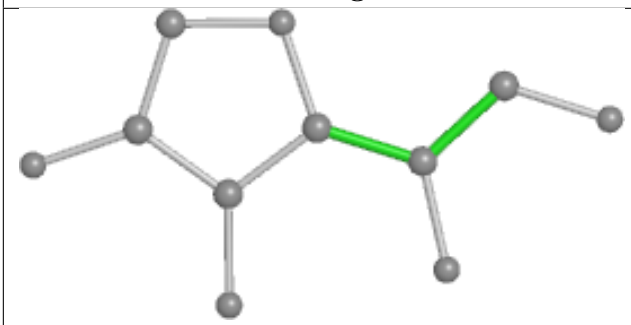
Ligand A1AIO A 2039



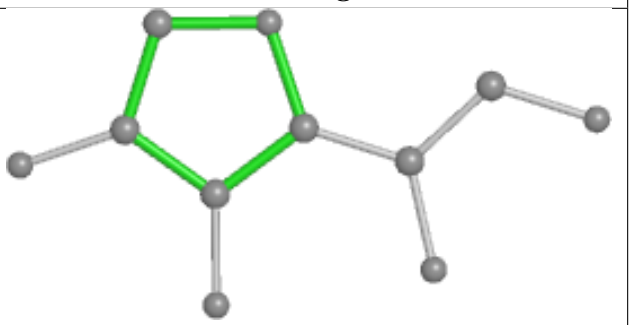
Bond lengths



Bond angles

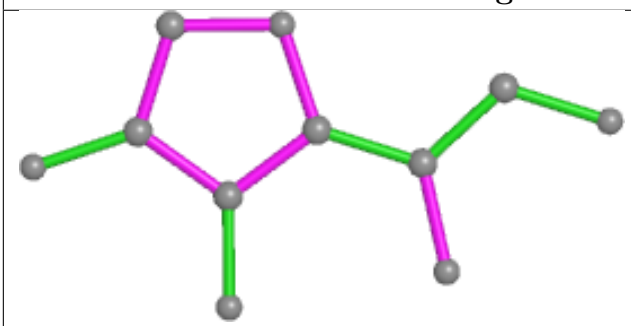


Torsions

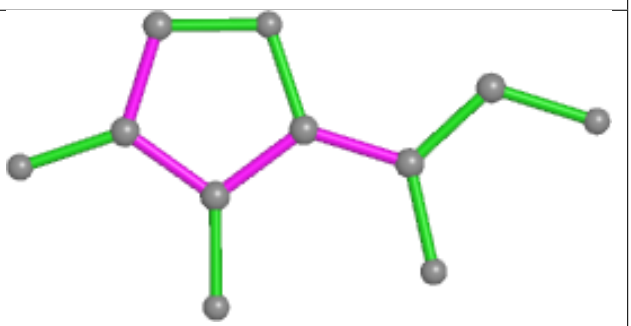


Rings

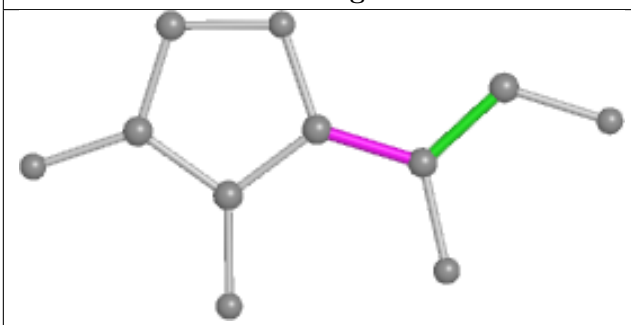
Ligand A1AIO A 2040



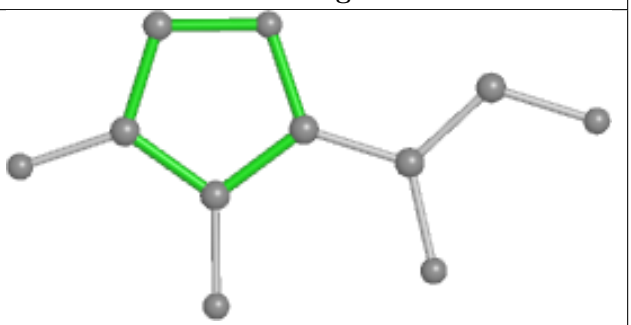
Bond lengths



Bond angles

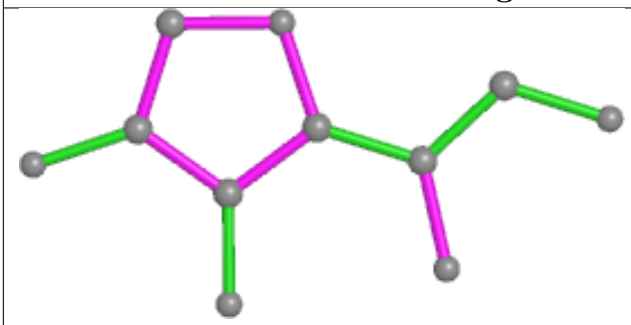


Torsions

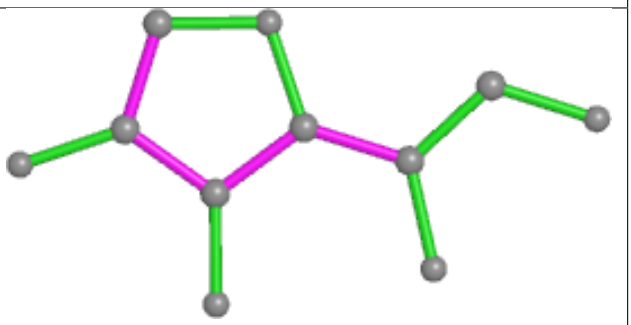


Rings

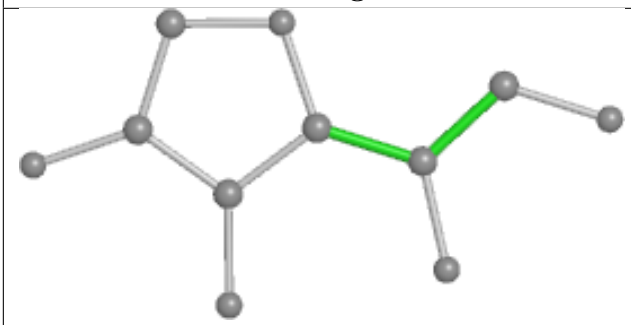
Ligand A1AIO A 2027



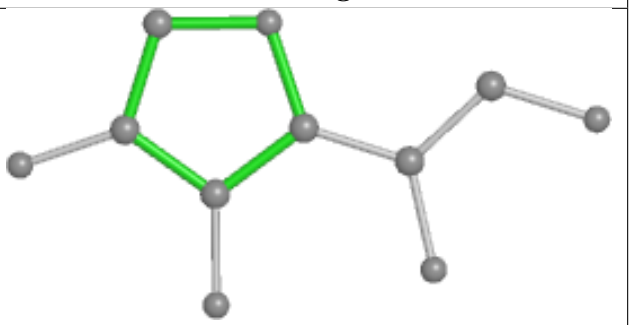
Bond lengths



Bond angles

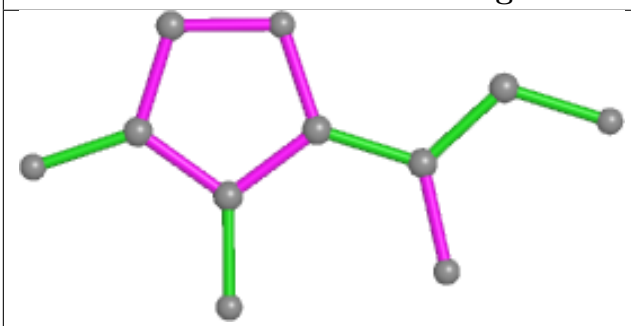


Torsions

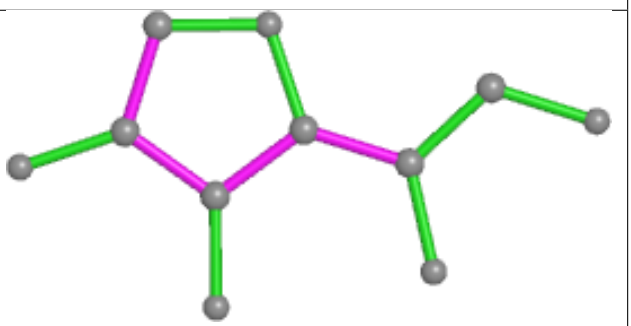


Rings

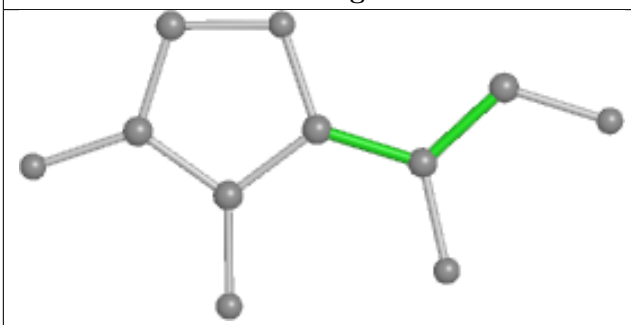
Ligand A1AIO A 2046



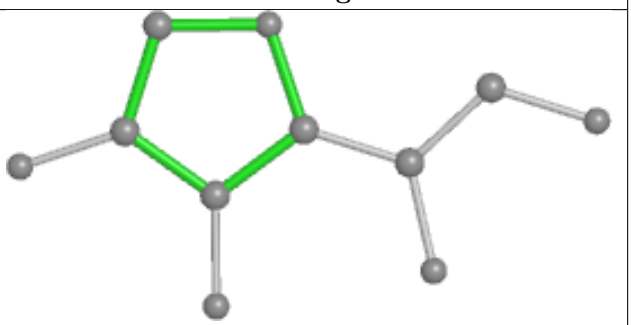
Bond lengths



Bond angles

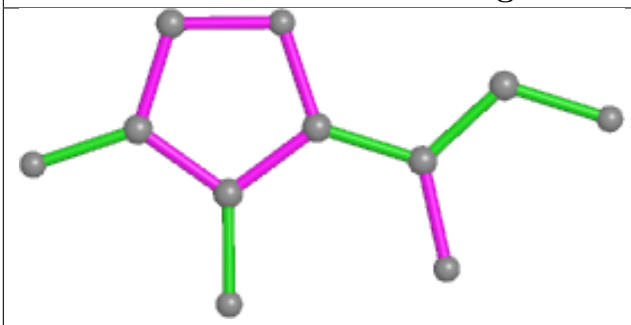


Torsions

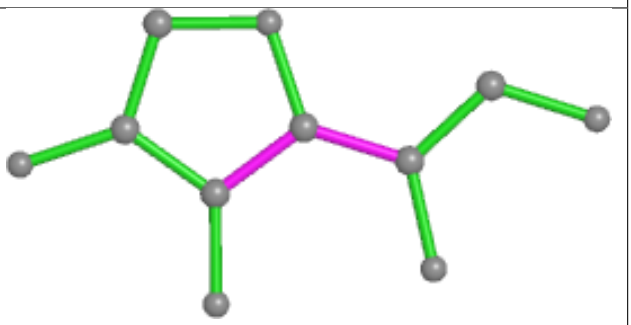


Rings

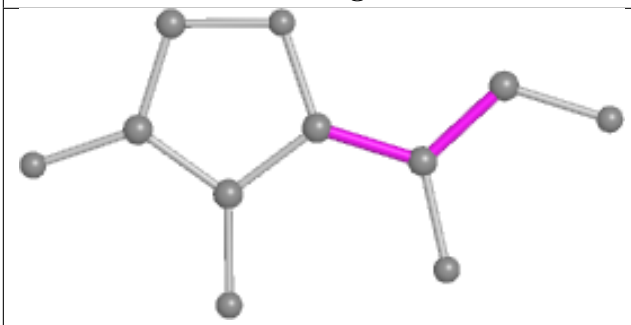
Ligand A1AIO B 2003



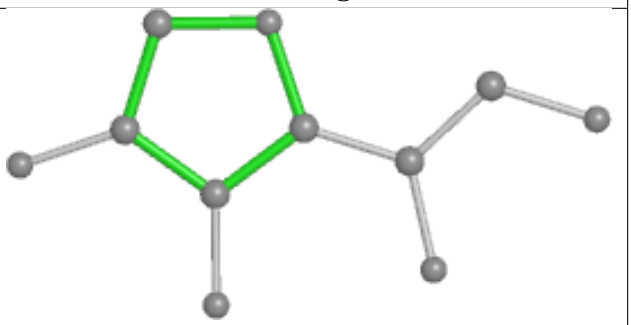
Bond lengths



Bond angles

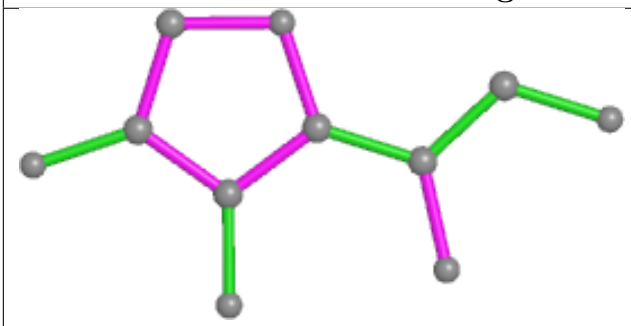


Torsions

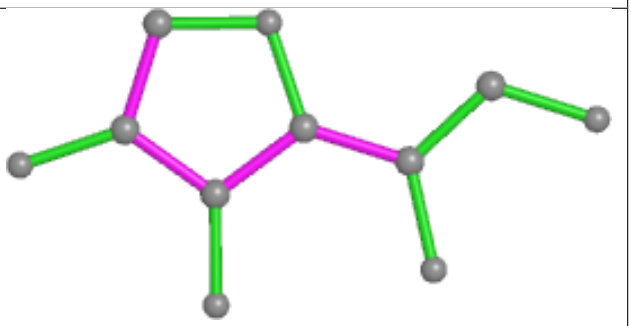


Rings

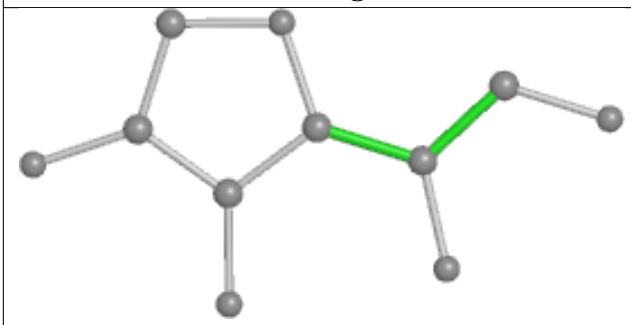
Ligand A1AIO B 2049



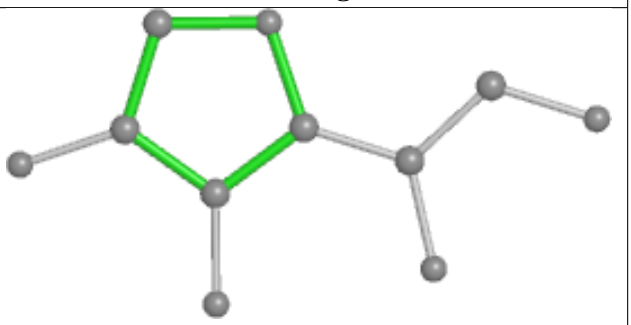
Bond lengths



Bond angles

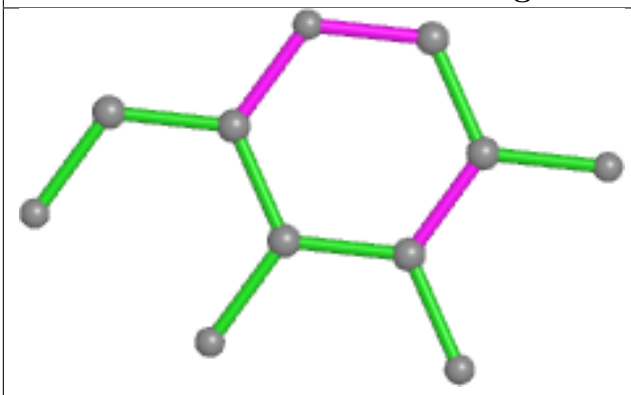


Torsions

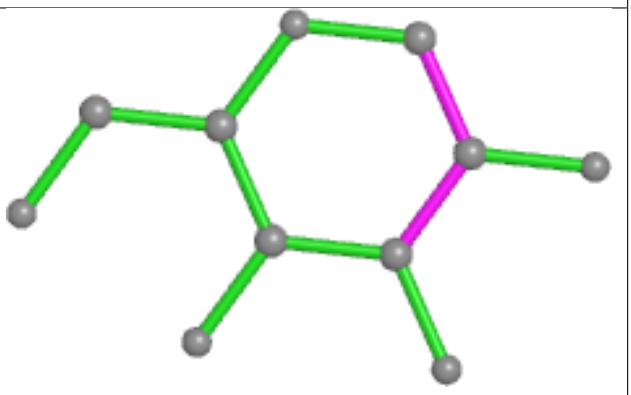


Rings

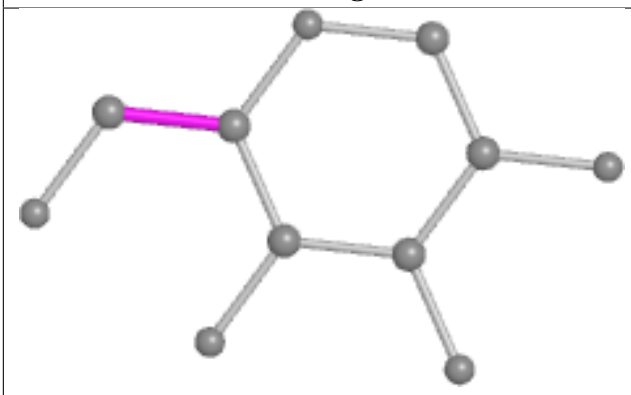
Ligand GLA A 2069



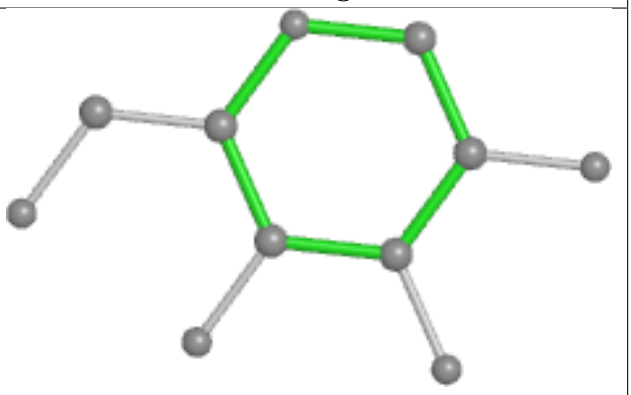
Bond lengths



Bond angles

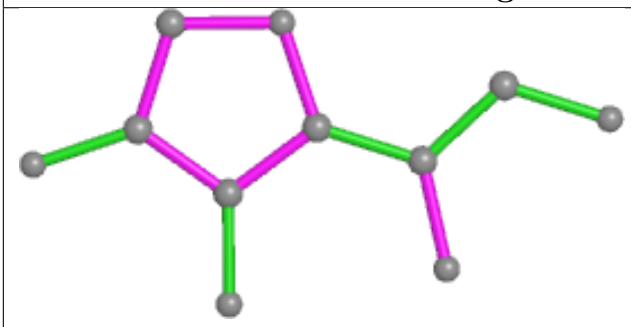


Torsions

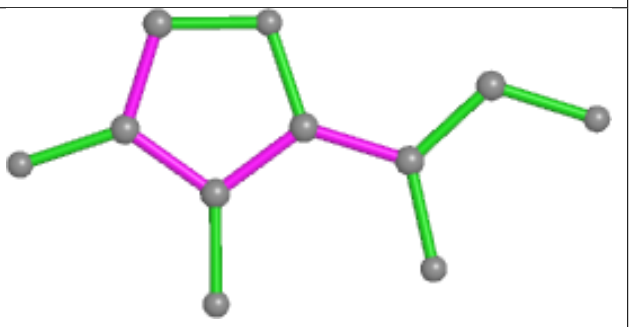


Rings

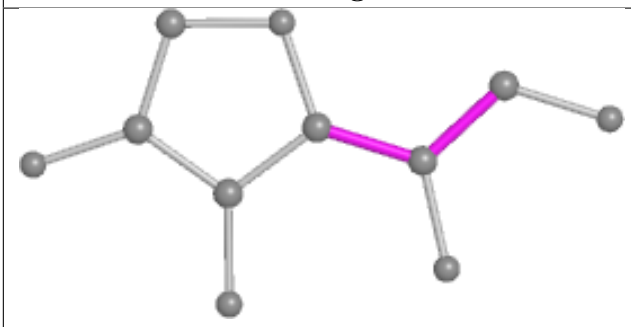
Ligand A1AIO B 2028



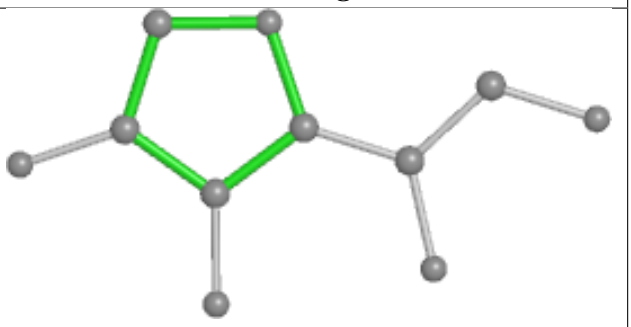
Bond lengths



Bond angles

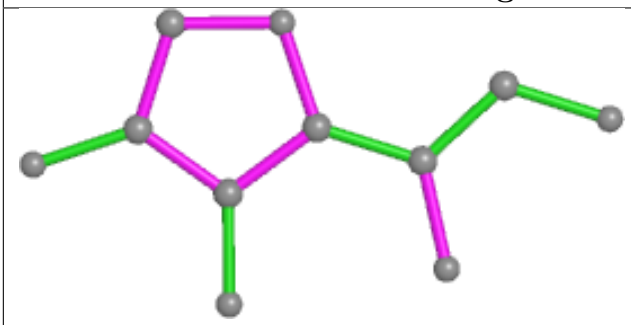


Torsions

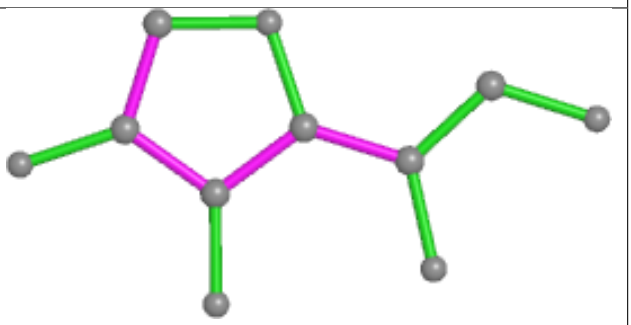


Rings

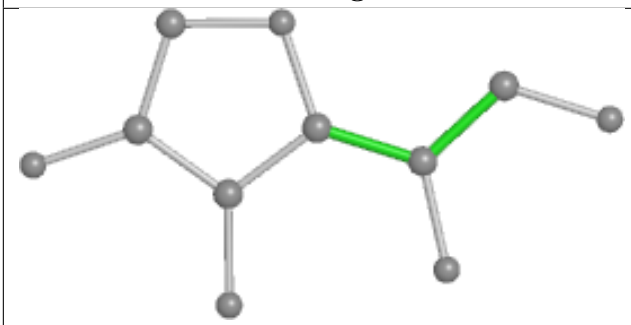
Ligand A1AIO B 2056



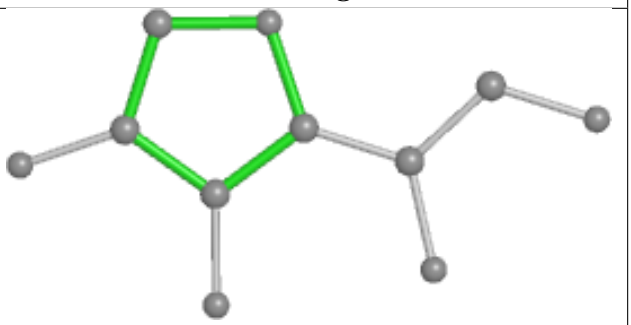
Bond lengths



Bond angles

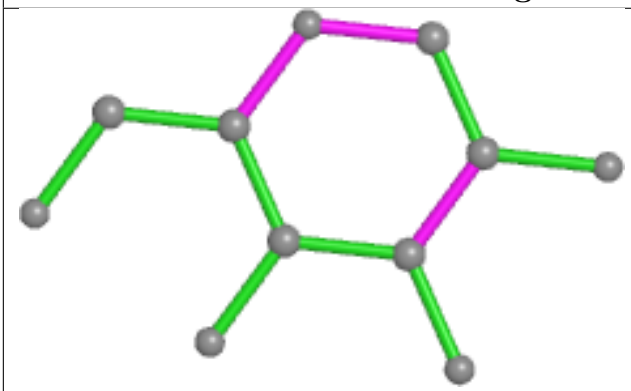


Torsions

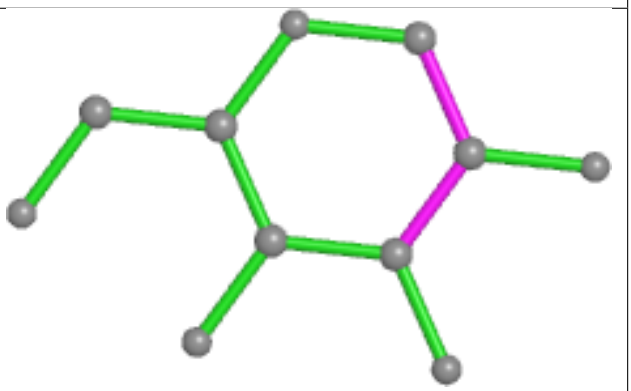


Rings

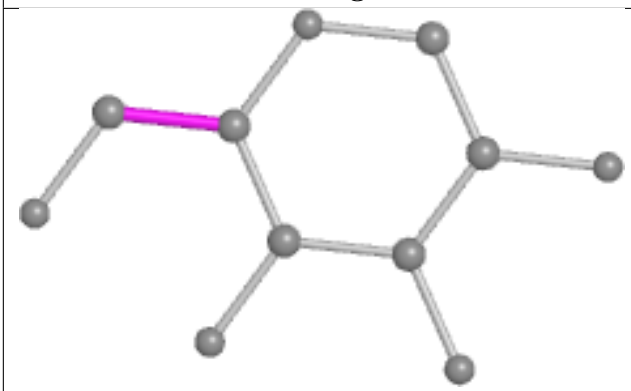
Ligand GLA B 2060



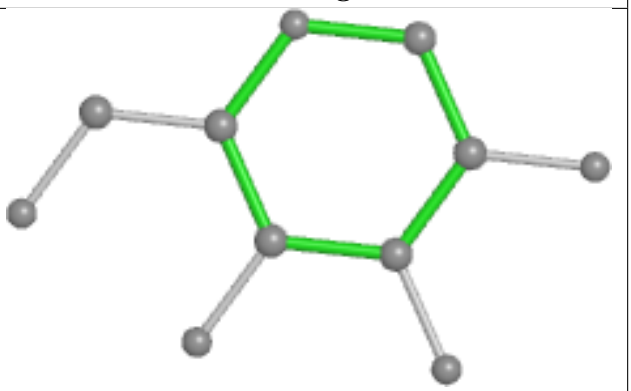
Bond lengths



Bond angles

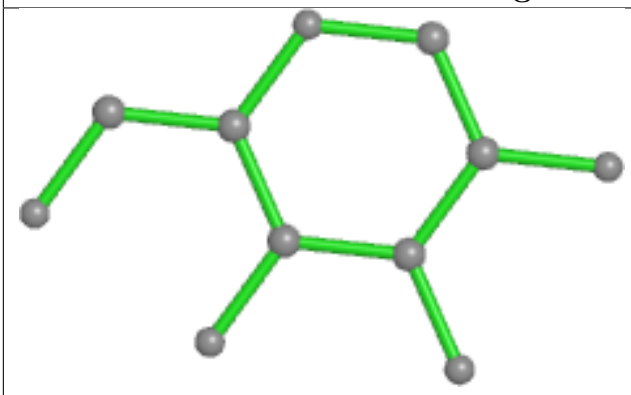


Torsions

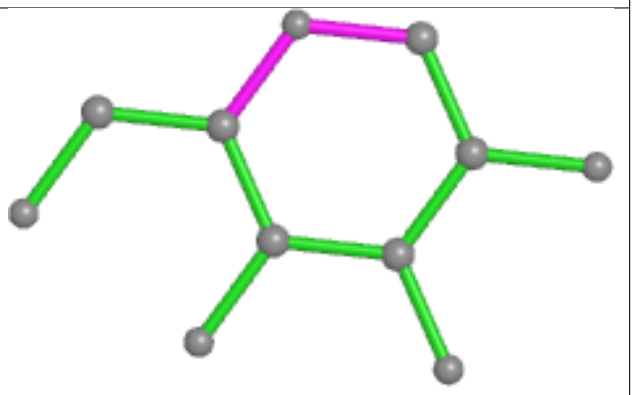


Rings

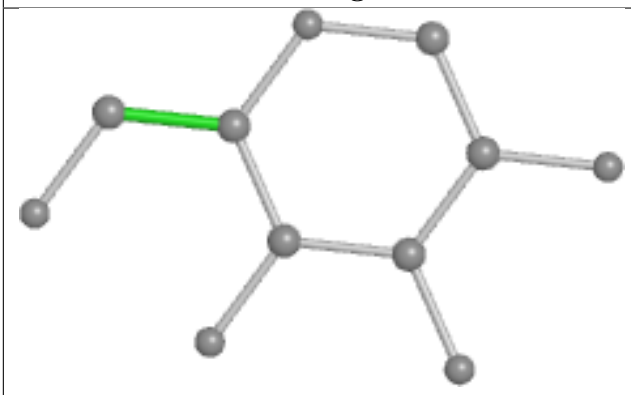
Ligand GLA A 2059



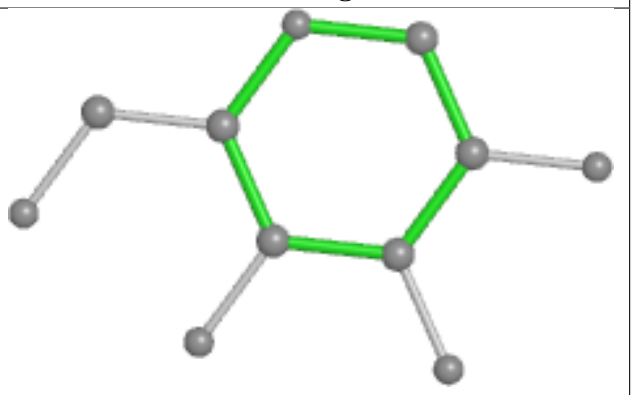
Bond lengths



Bond angles

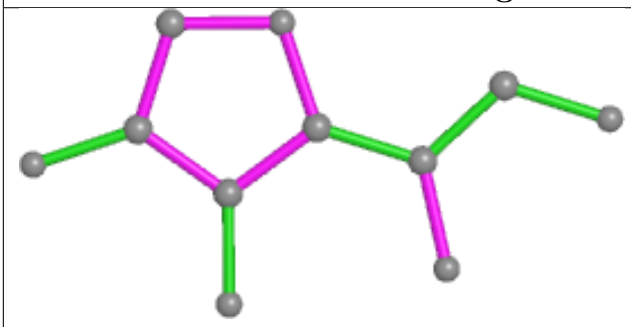


Torsions

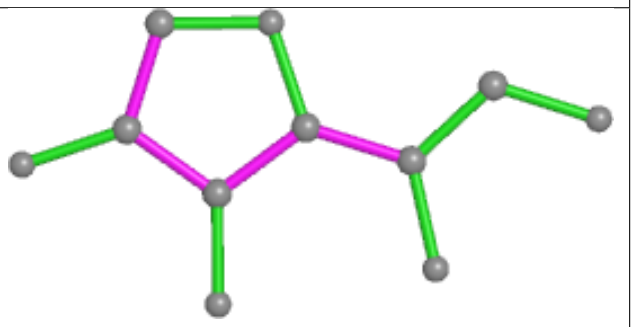


Rings

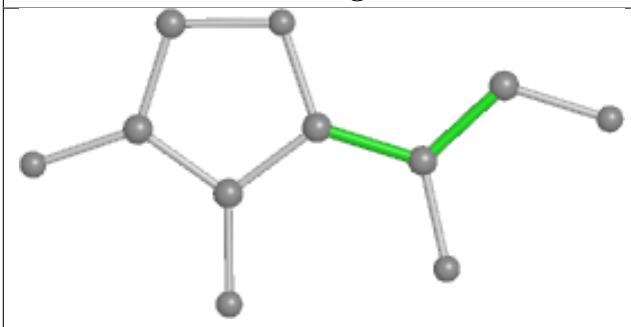
Ligand A1AIO A 2009



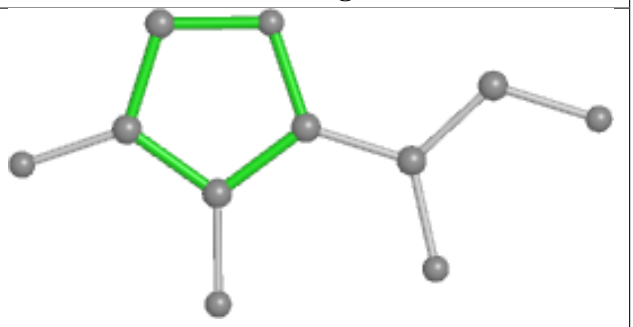
Bond lengths



Bond angles

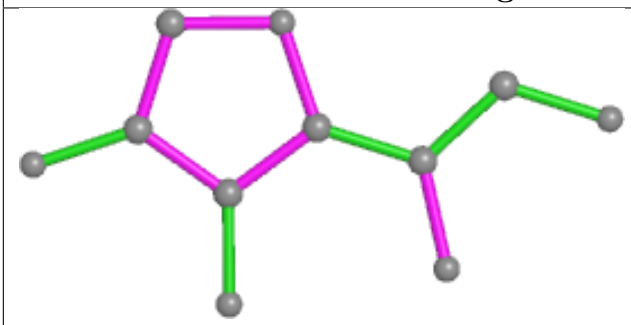


Torsions

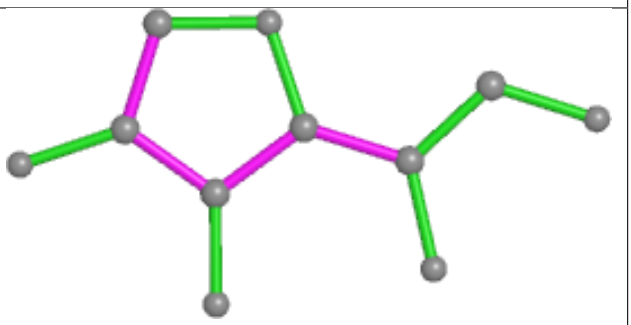


Rings

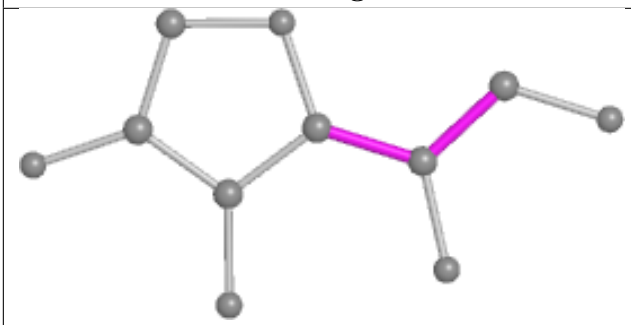
Ligand A1AIO B 2021



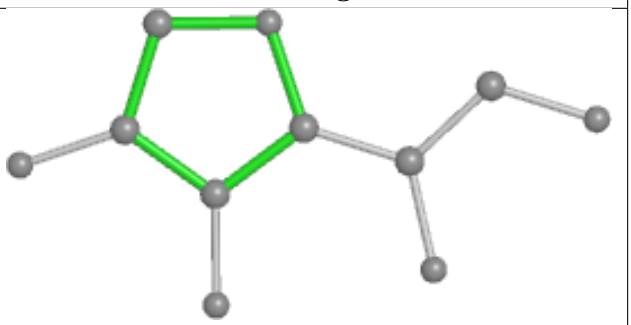
Bond lengths



Bond angles

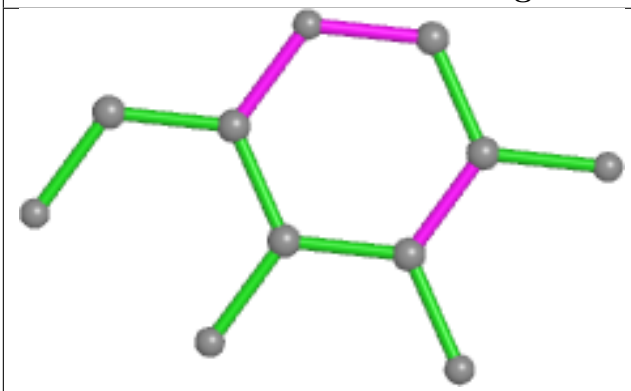


Torsions

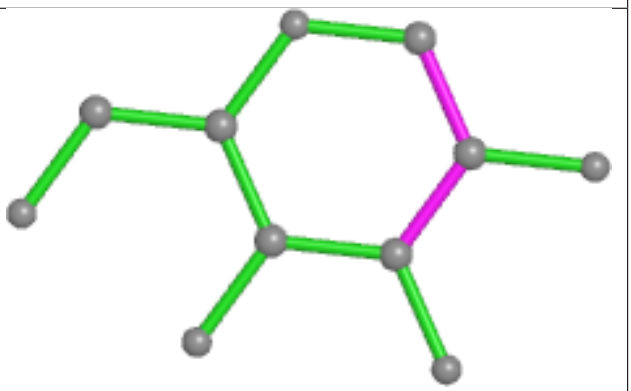


Rings

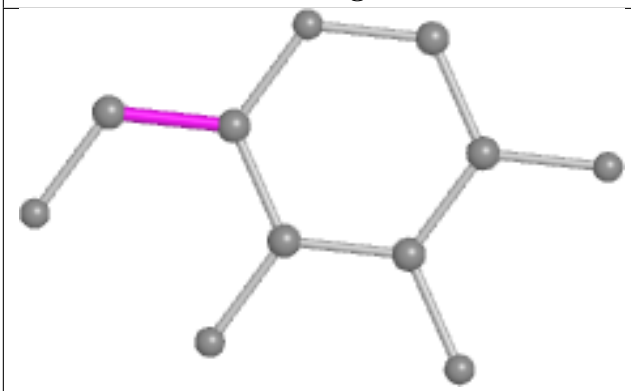
Ligand GLA B 2065



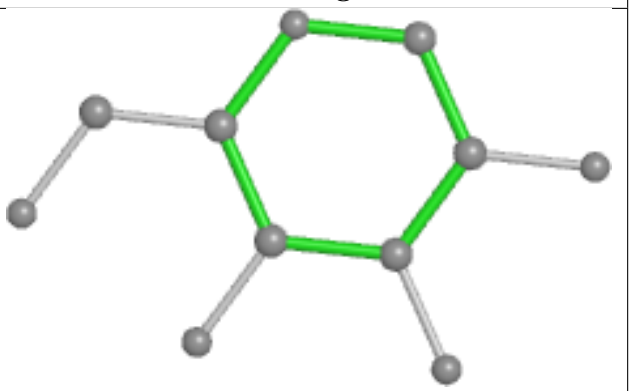
Bond lengths



Bond angles

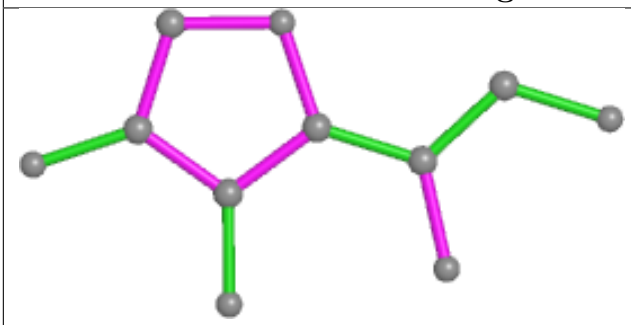


Torsions

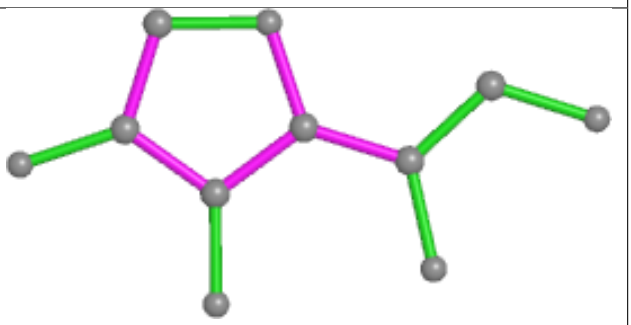


Rings

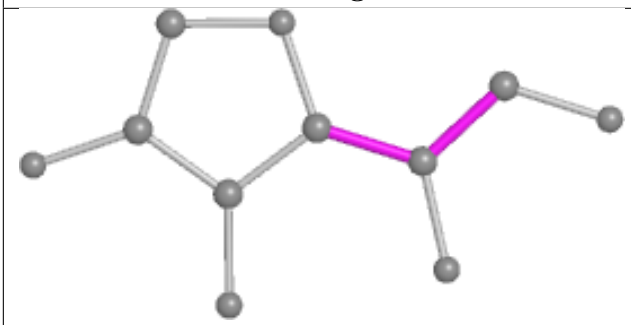
Ligand A1AIO B 2016



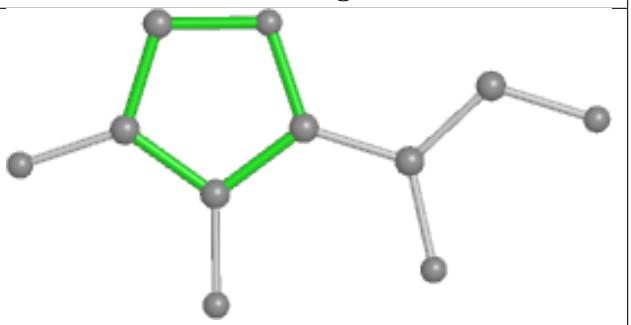
Bond lengths



Bond angles

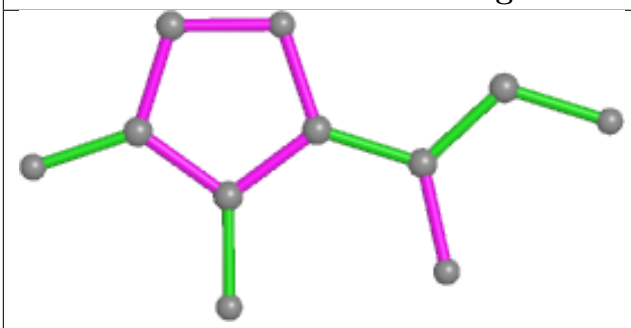


Torsions

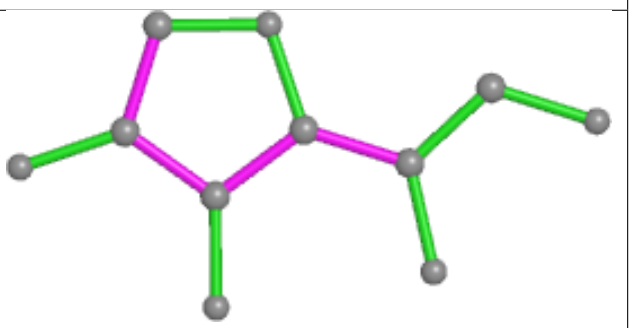


Rings

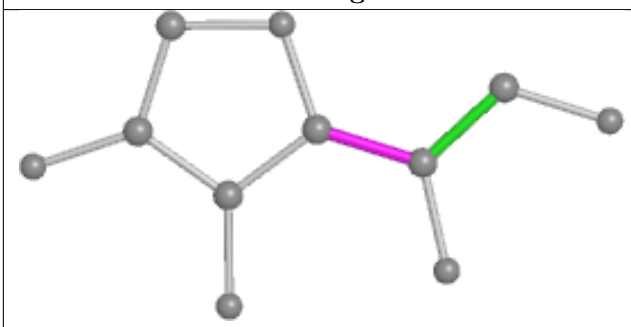
Ligand A1AIO A 2038



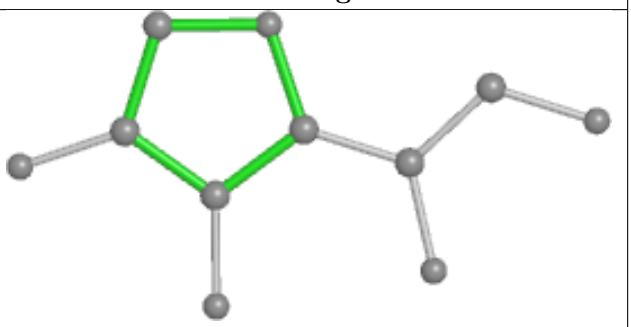
Bond lengths



Bond angles

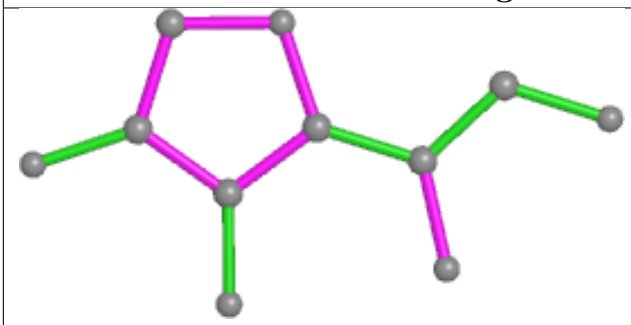


Torsions

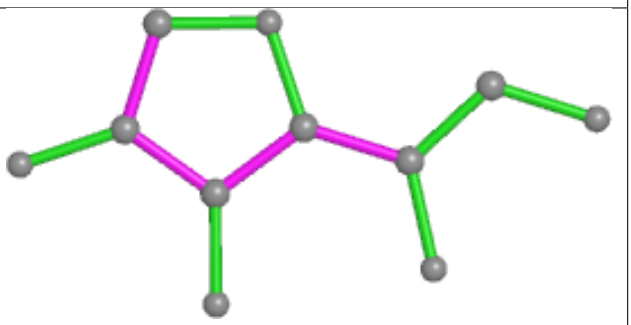


Rings

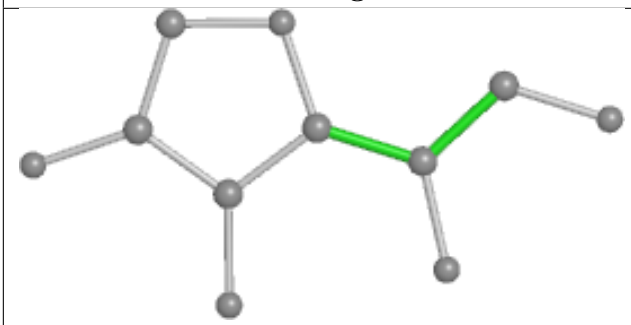
Ligand A1AIO A 2021



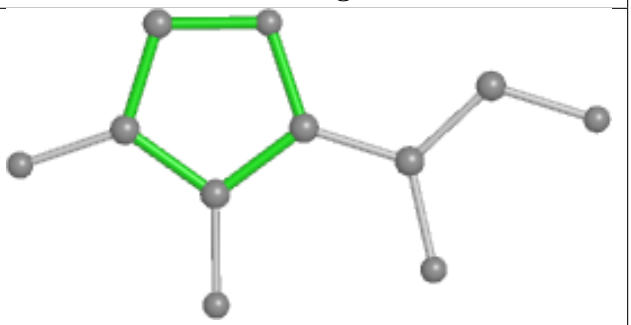
Bond lengths



Bond angles

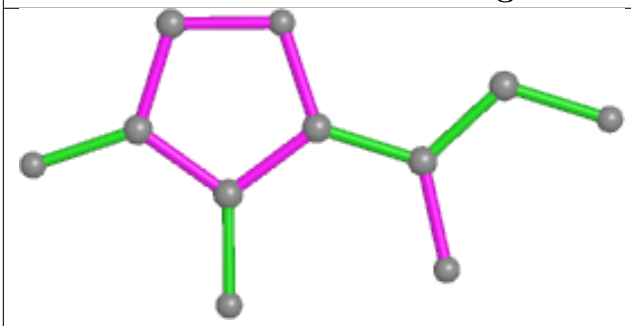


Torsions

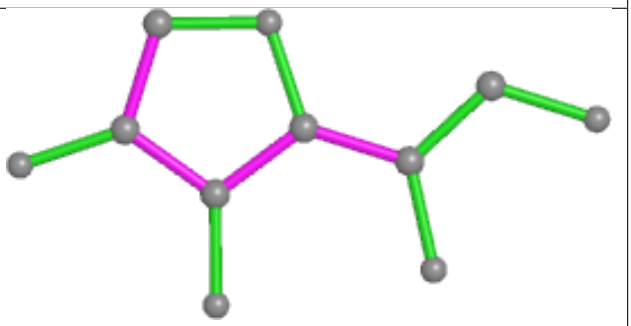


Rings

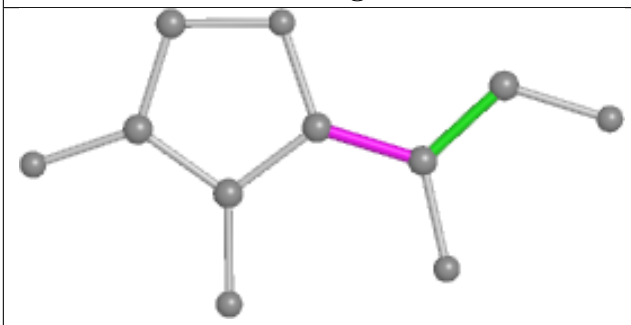
Ligand A1AIO B 2020



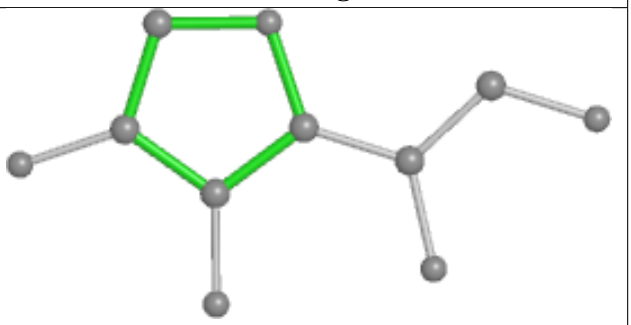
Bond lengths



Bond angles

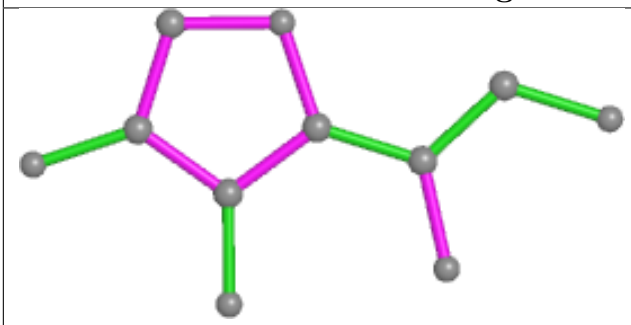


Torsions

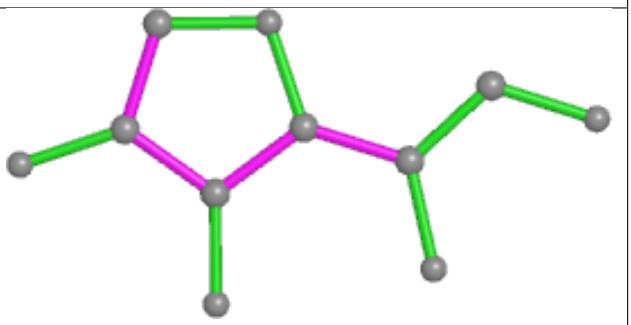


Rings

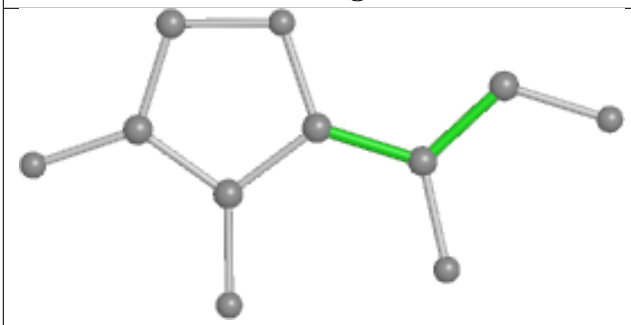
Ligand A1AIO A 2042



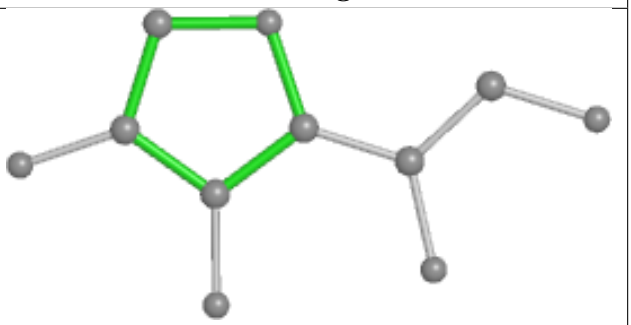
Bond lengths



Bond angles

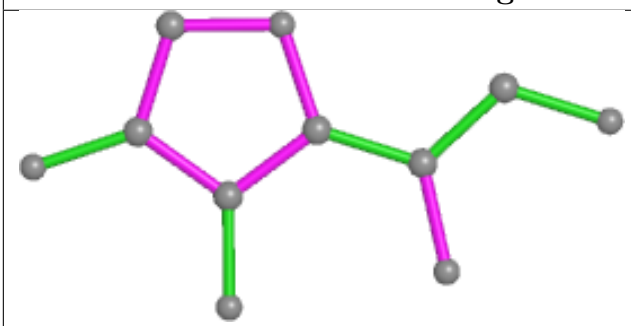


Torsions

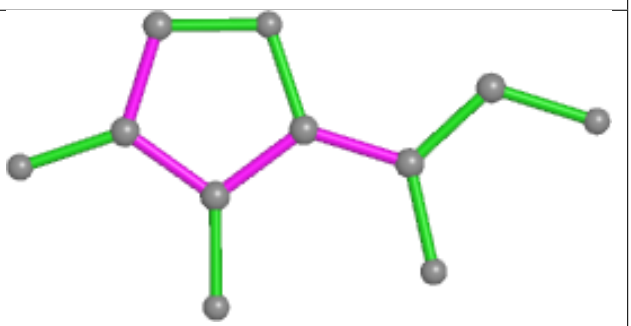


Rings

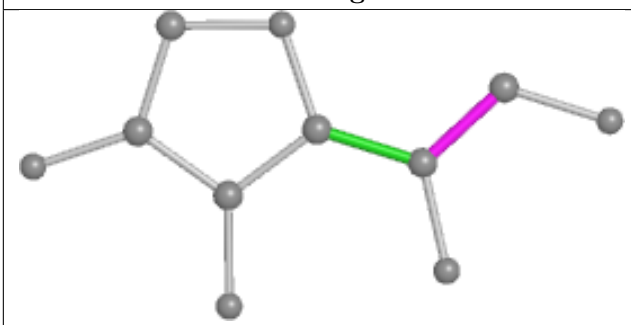
Ligand A1AIO B 2045



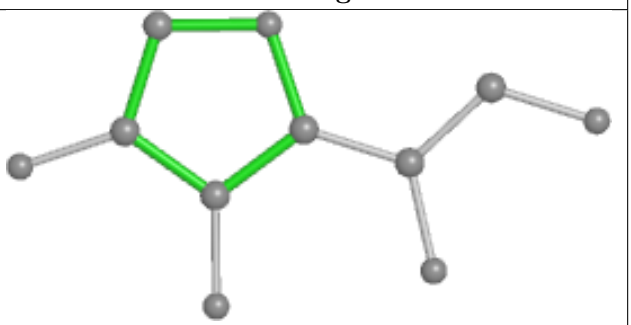
Bond lengths



Bond angles

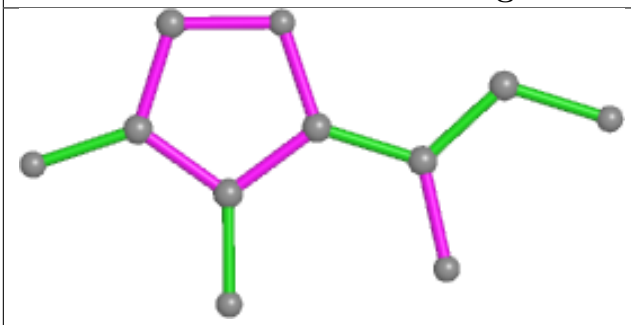


Torsions

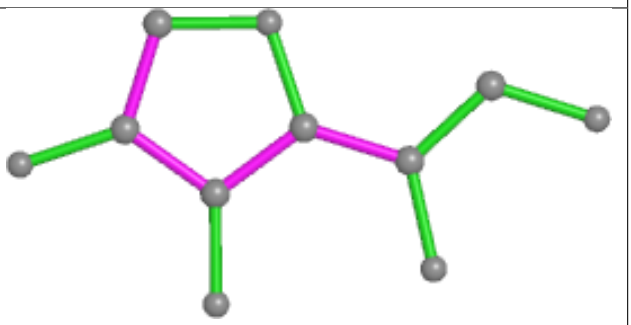


Rings

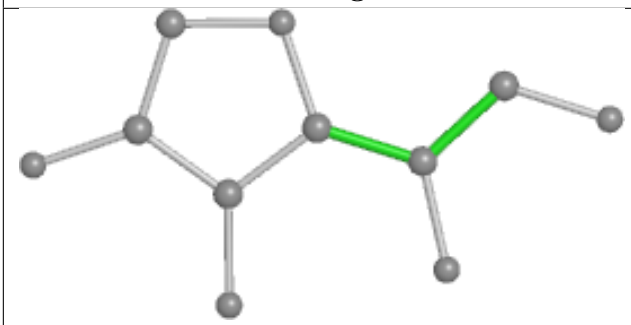
Ligand A1AIO B 2050



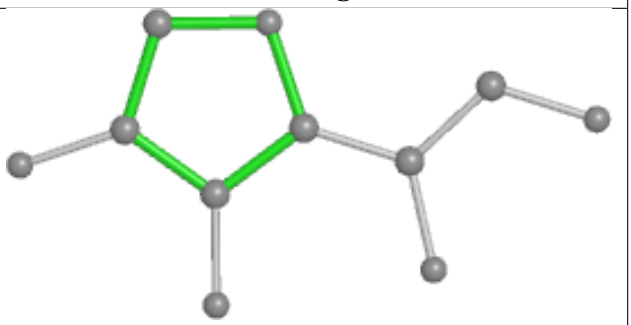
Bond lengths



Bond angles

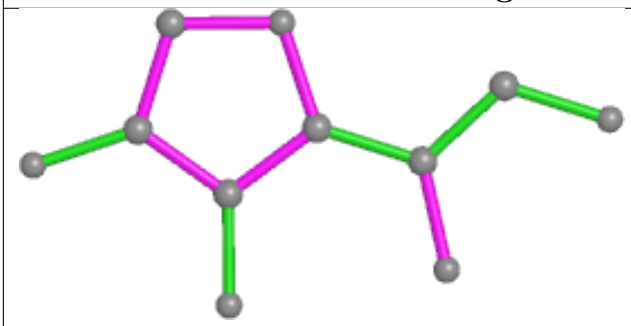


Torsions

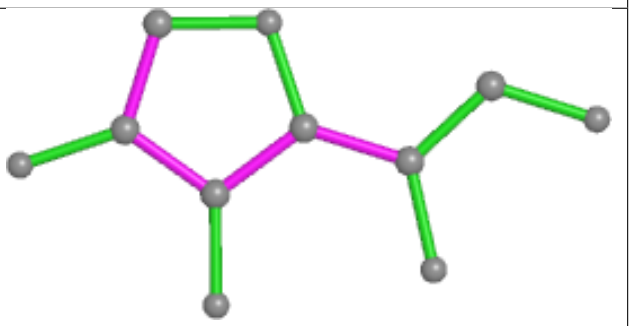


Rings

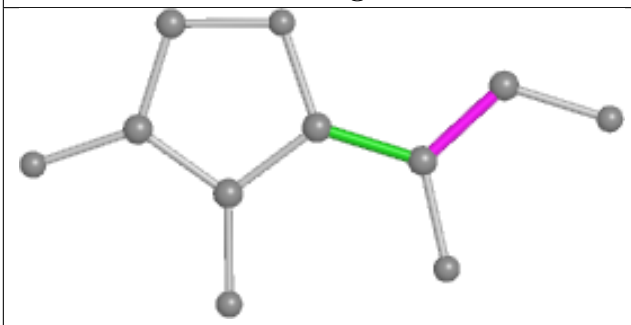
Ligand A1AIO A 2048



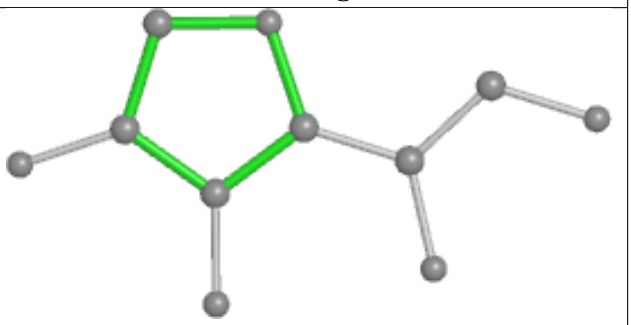
Bond lengths



Bond angles

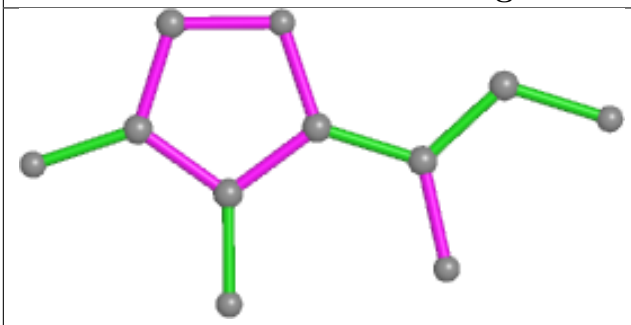


Torsions

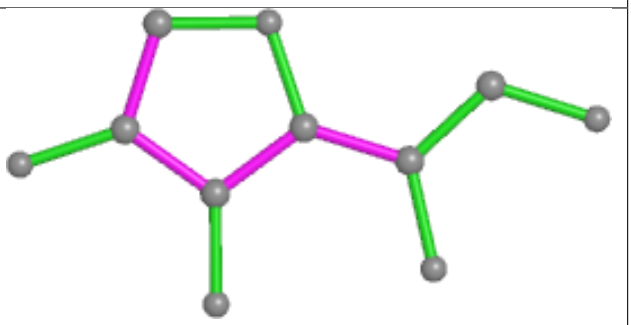


Rings

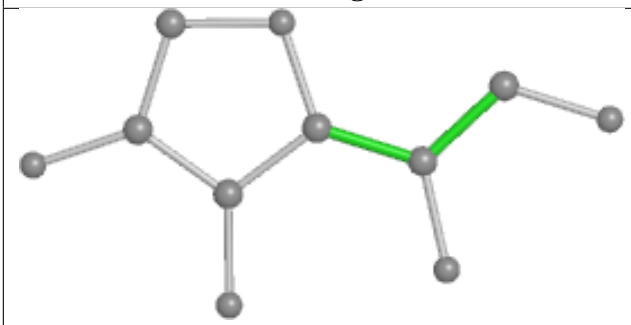
Ligand A1AIO A 2037



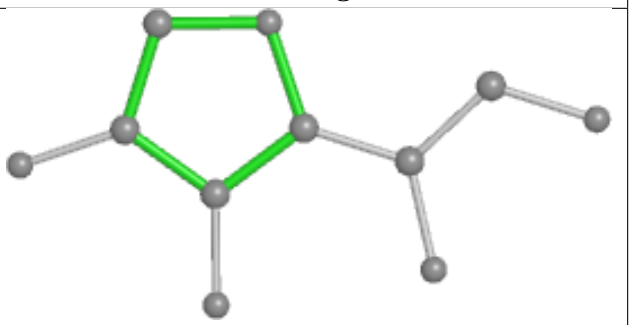
Bond lengths



Bond angles

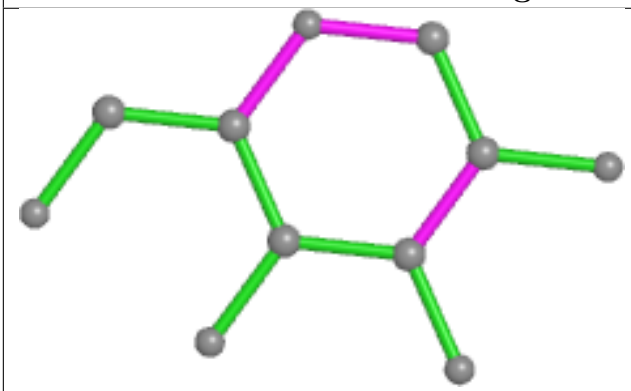


Torsions

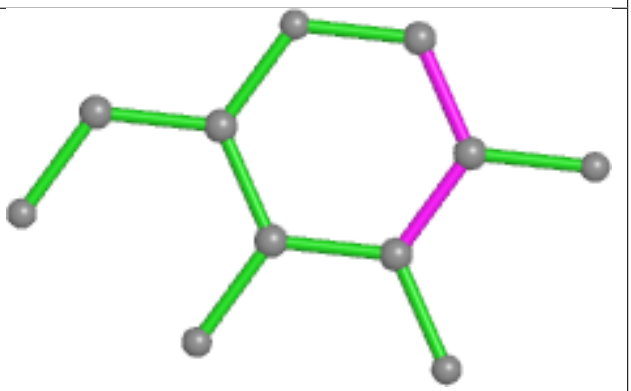


Rings

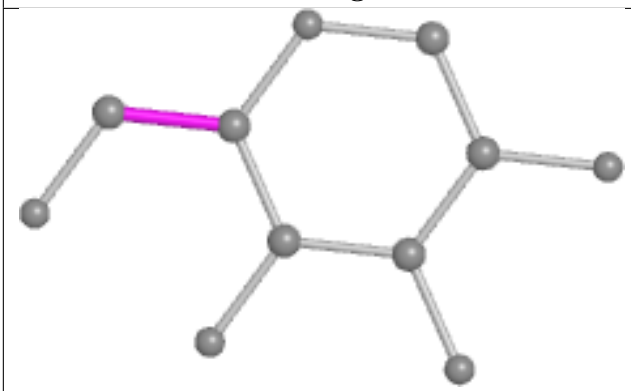
Ligand GLA A 2064



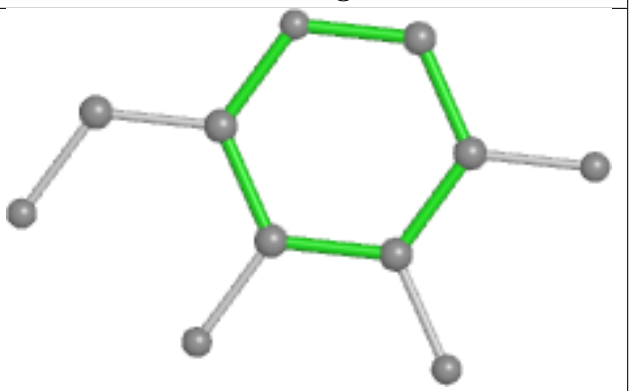
Bond lengths



Bond angles

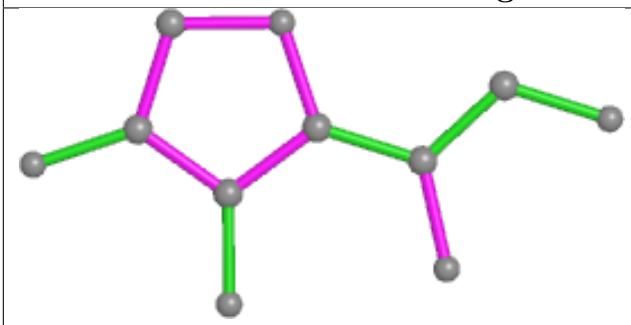


Torsions

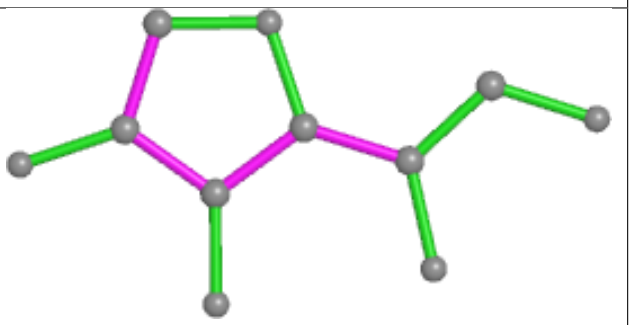


Rings

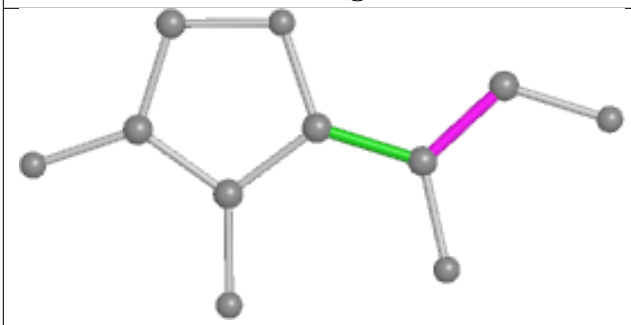
Ligand A1AIO B 2035



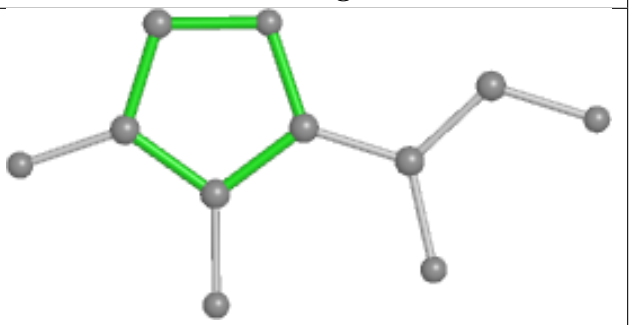
Bond lengths



Bond angles

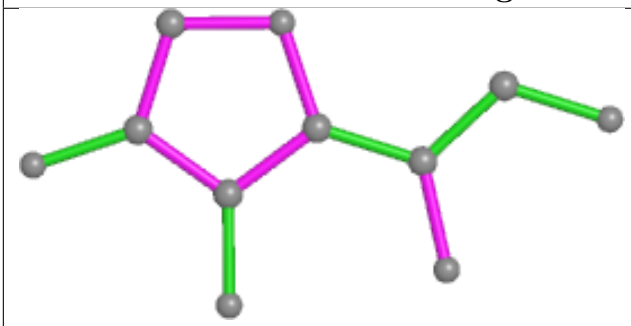


Torsions

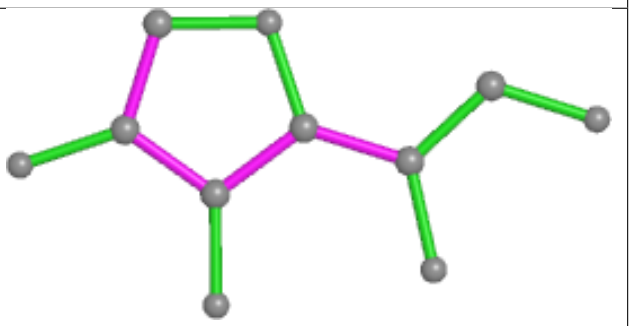


Rings

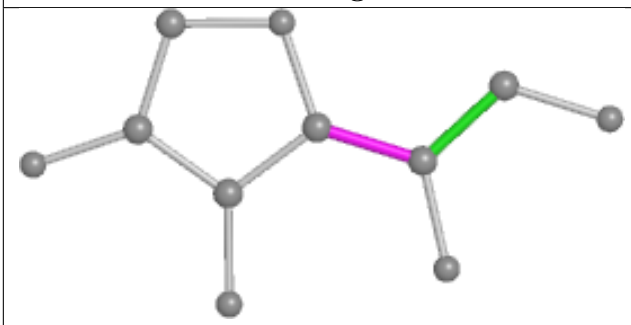
Ligand A1AIO A 2054



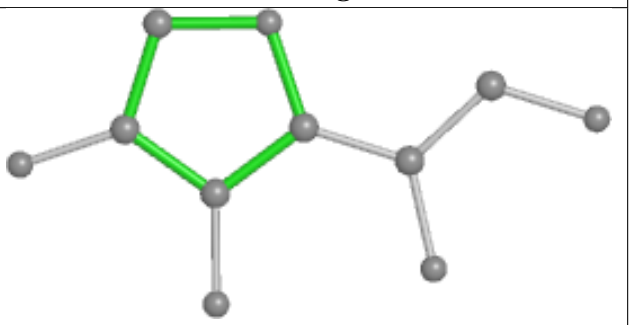
Bond lengths



Bond angles

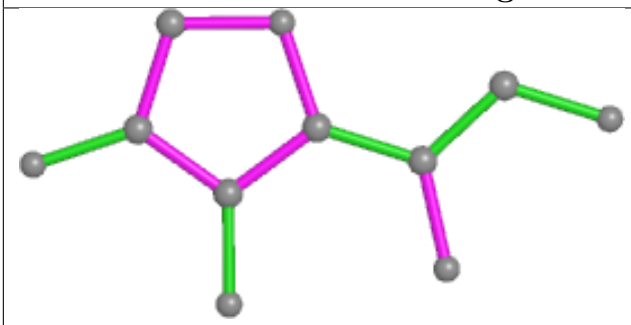


Torsions

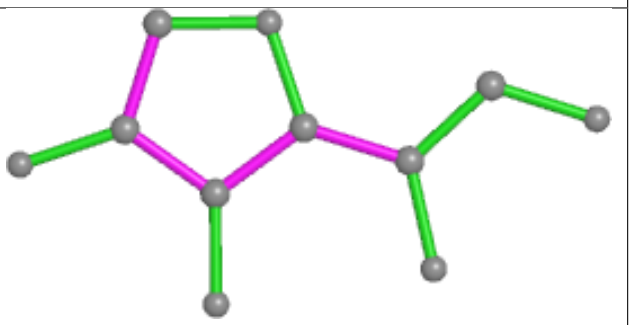


Rings

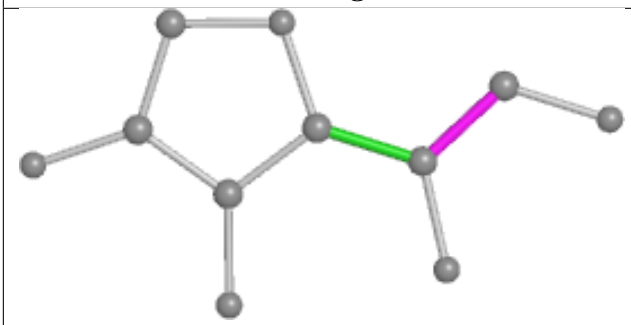
Ligand A1AIO B 2032



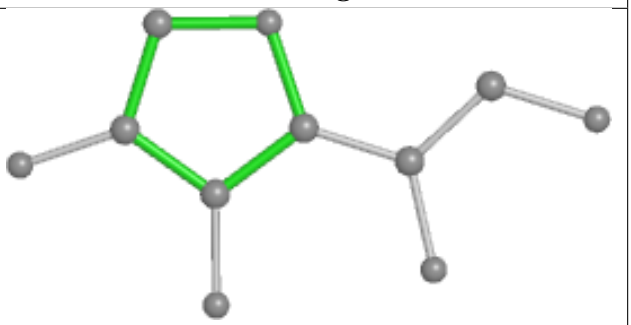
Bond lengths



Bond angles

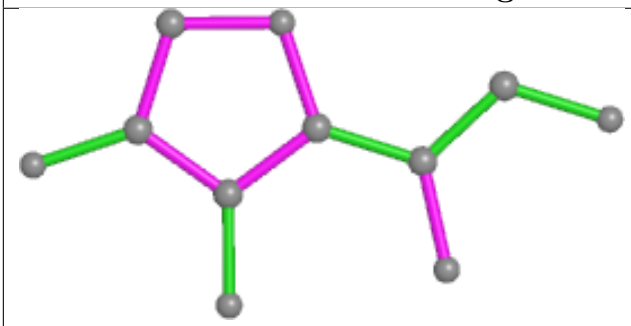


Torsions

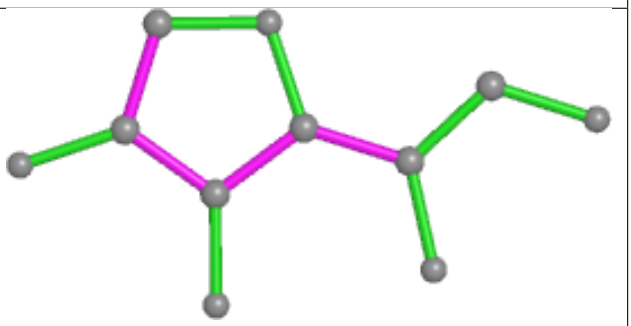


Rings

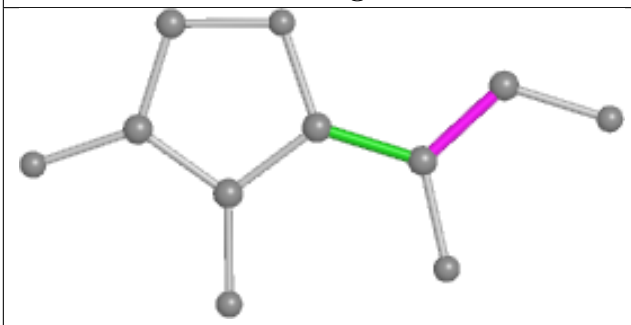
Ligand A1AIO B 2037



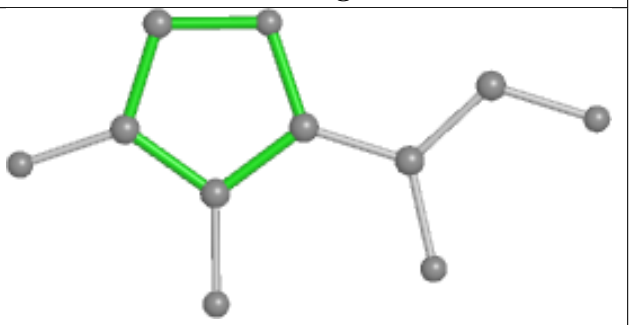
Bond lengths



Bond angles

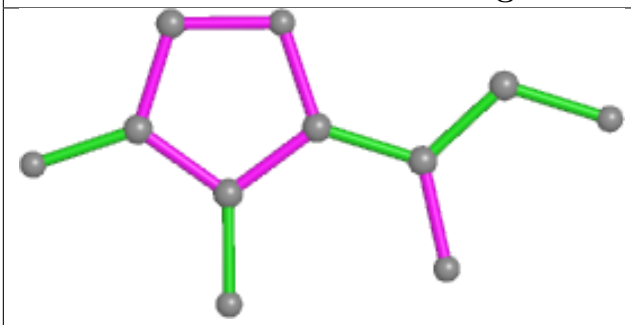


Torsions

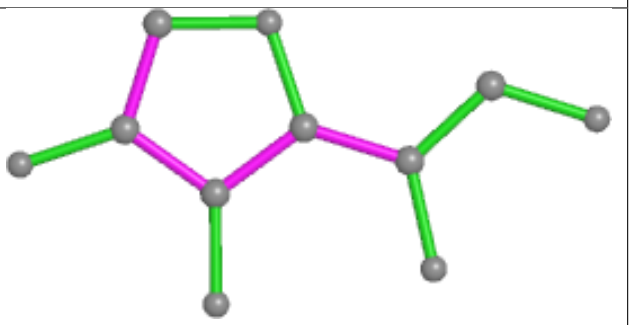


Rings

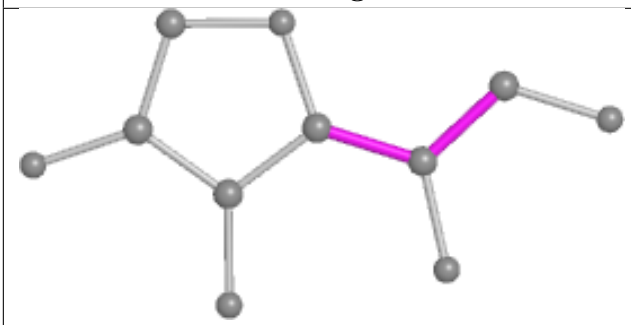
Ligand A1AIO B 2054



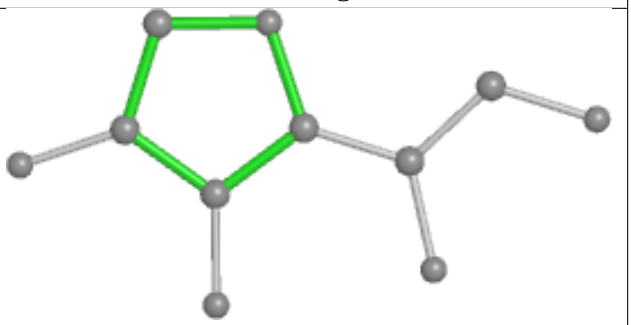
Bond lengths



Bond angles

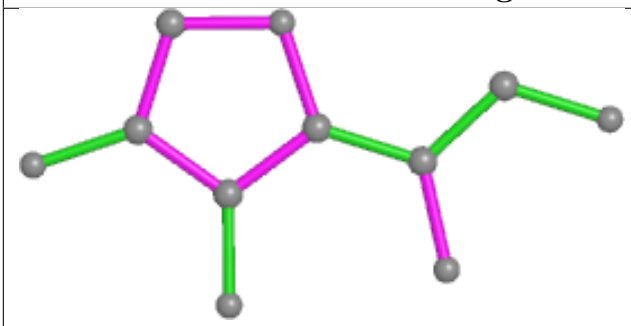


Torsions

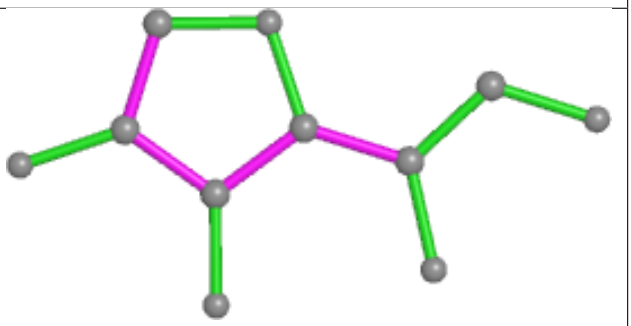


Rings

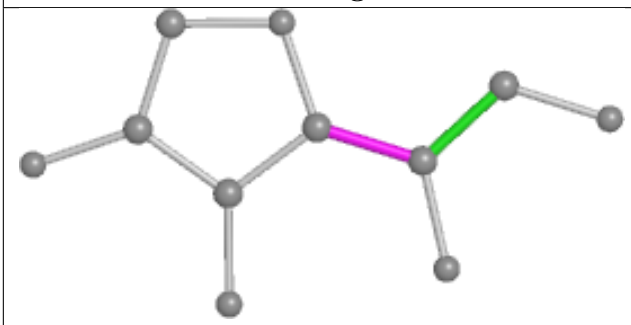
Ligand A1AIO A 2041



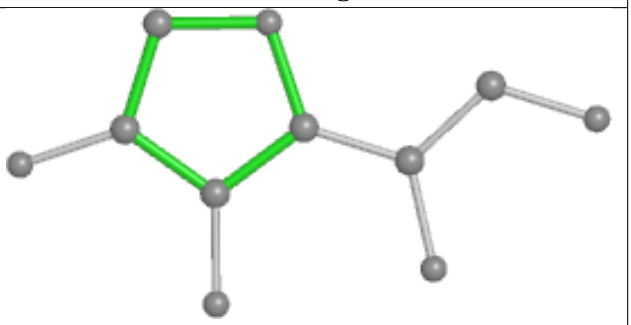
Bond lengths



Bond angles

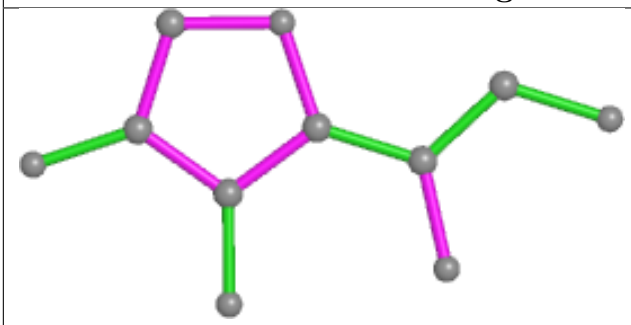


Torsions

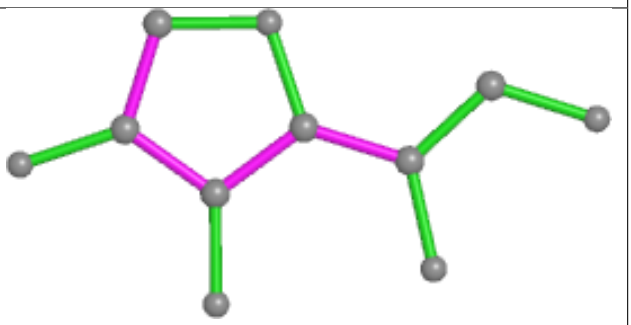


Rings

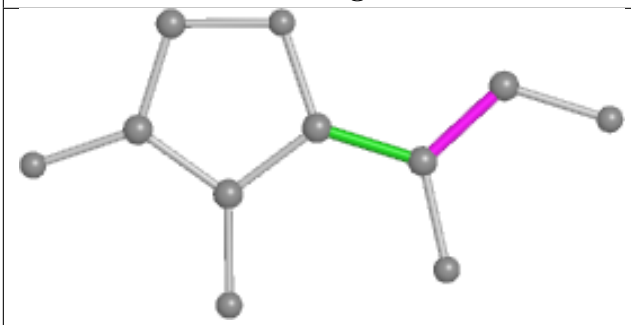
Ligand A1AIO A 2002



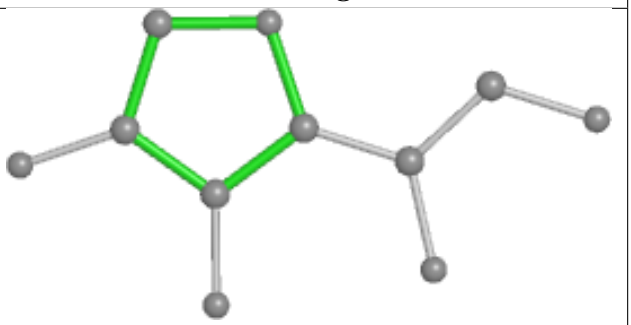
Bond lengths



Bond angles

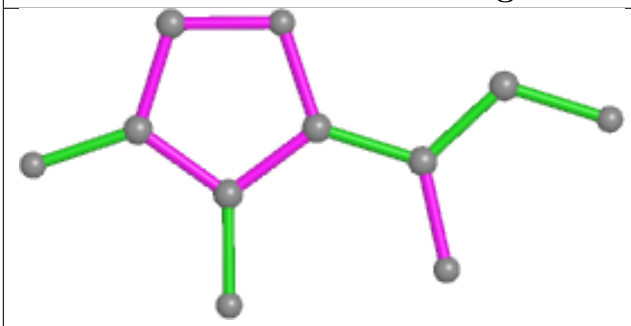


Torsions

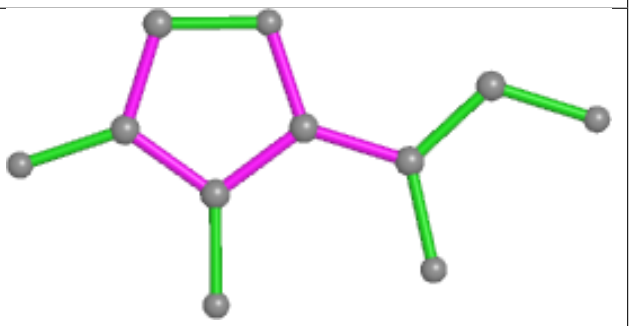


Rings

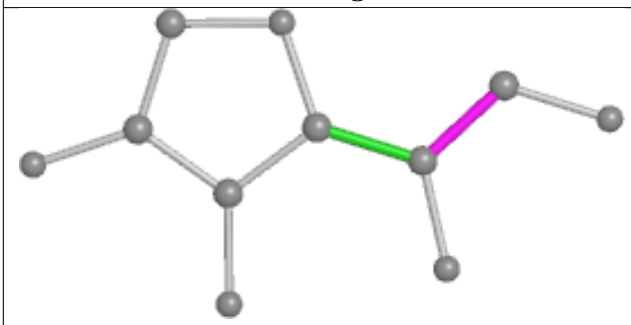
Ligand A1AIO B 2052



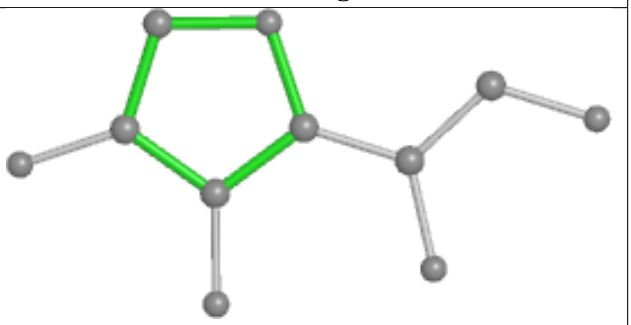
Bond lengths



Bond angles

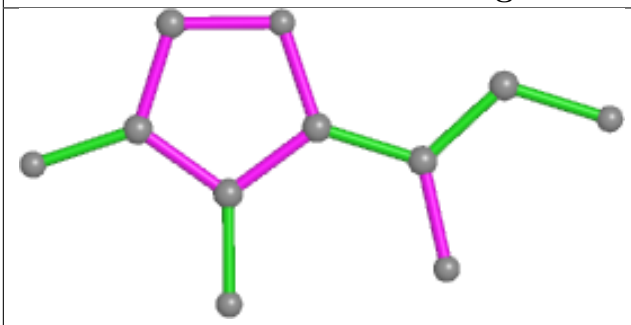


Torsions

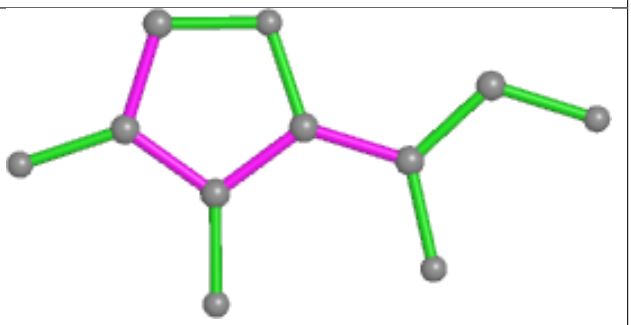


Rings

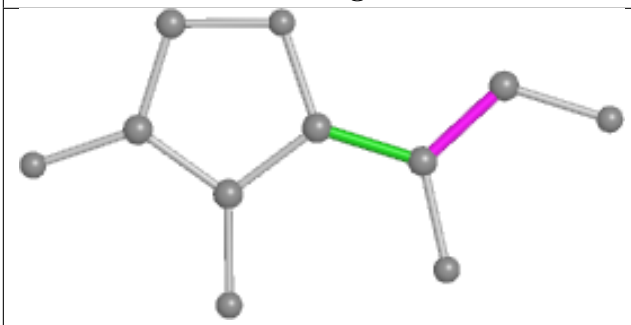
Ligand A1AIO A 2049



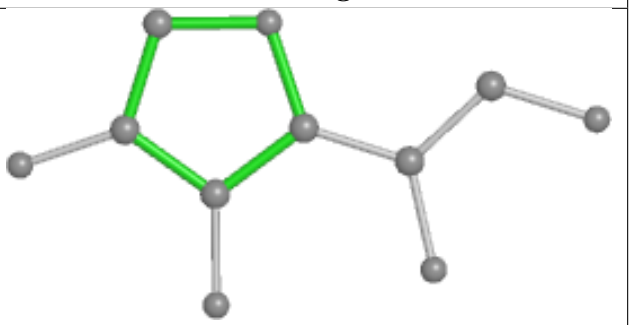
Bond lengths



Bond angles

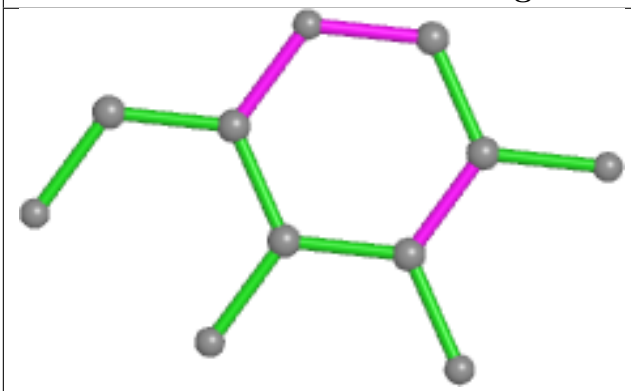


Torsions

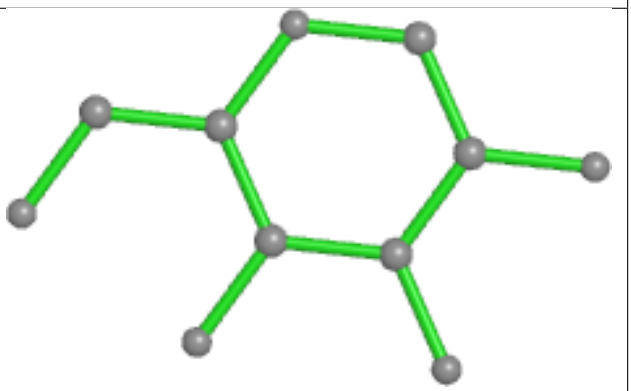


Rings

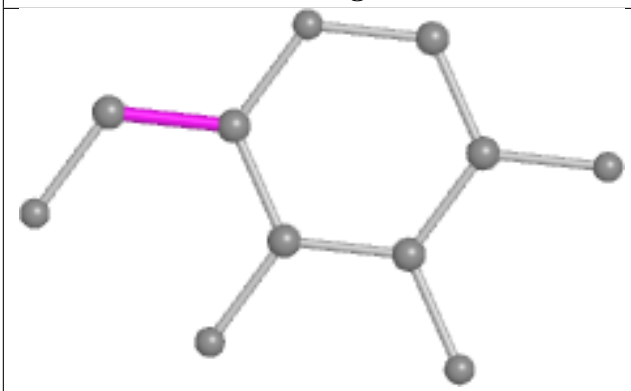
Ligand GLA B 2068



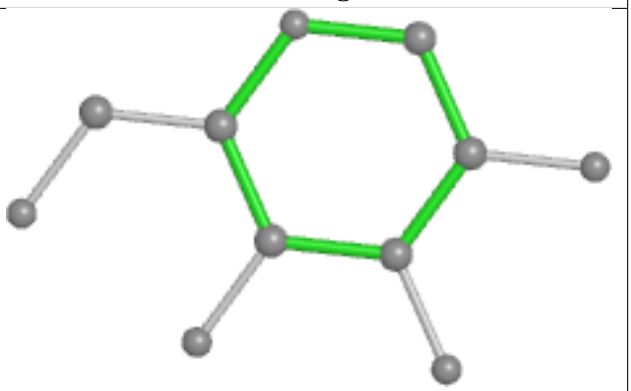
Bond lengths



Bond angles

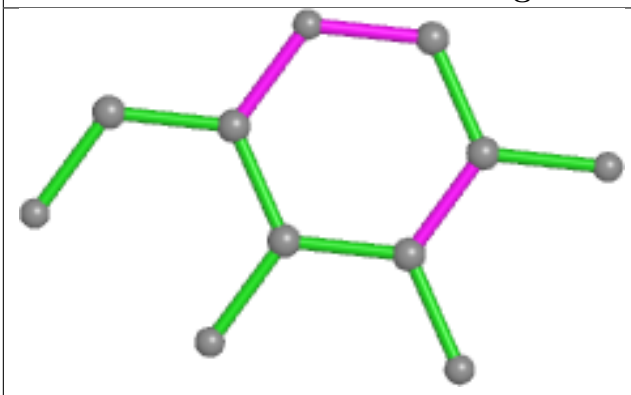


Torsions

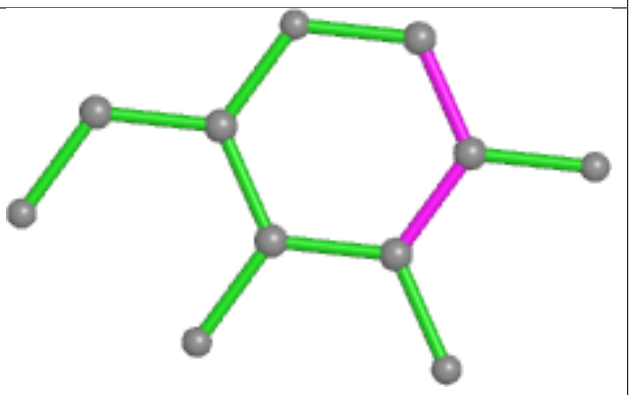


Rings

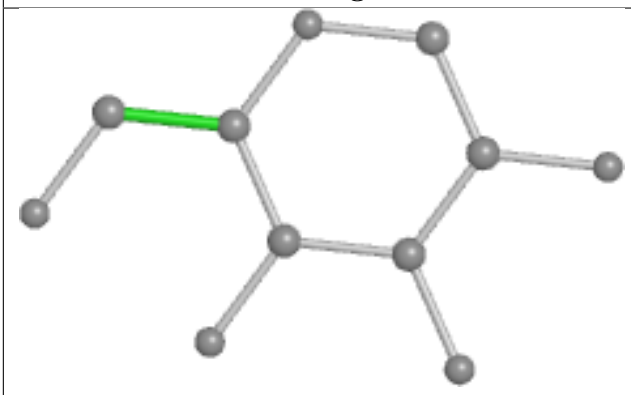
Ligand GLA A 2070



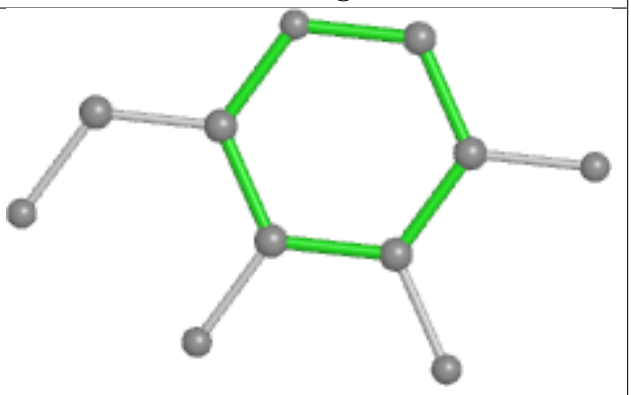
Bond lengths



Bond angles

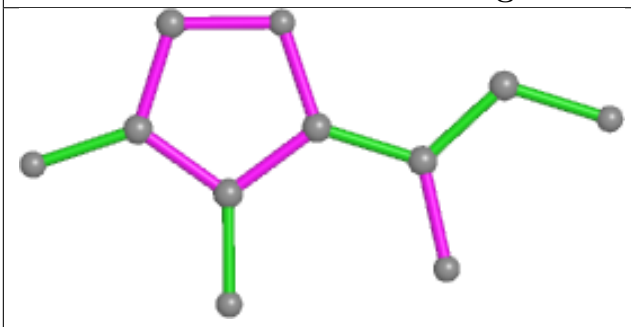


Torsions

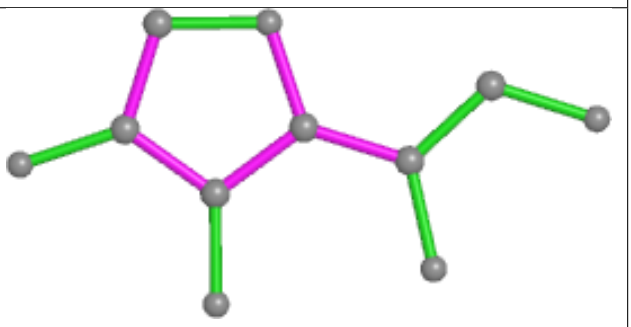


Rings

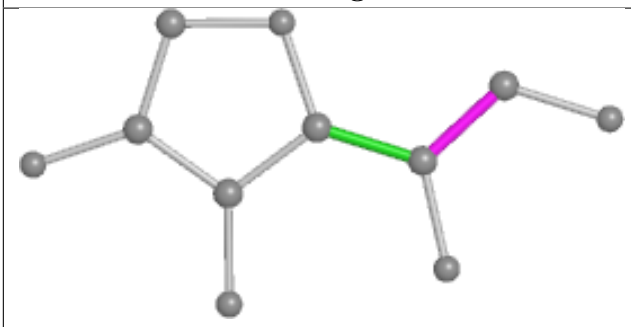
Ligand A1AIO B 2008



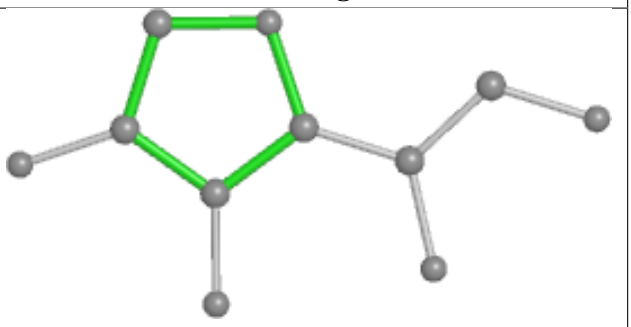
Bond lengths



Bond angles

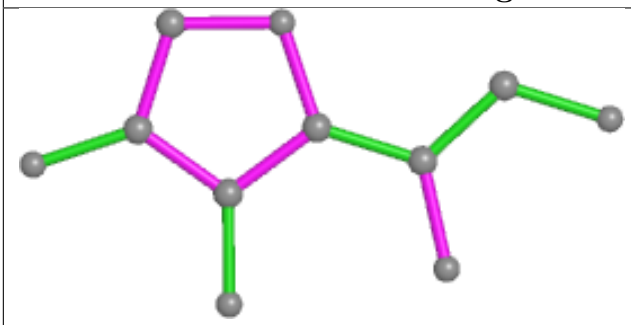


Torsions

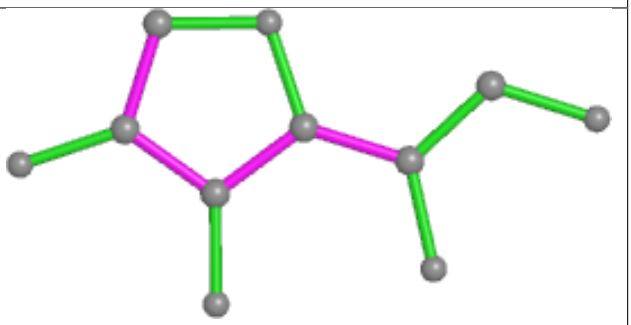


Rings

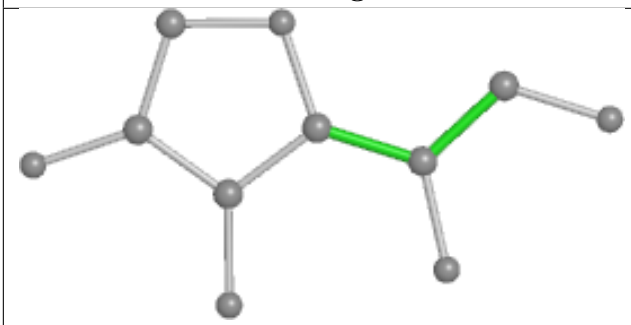
Ligand A1AIO A 2018



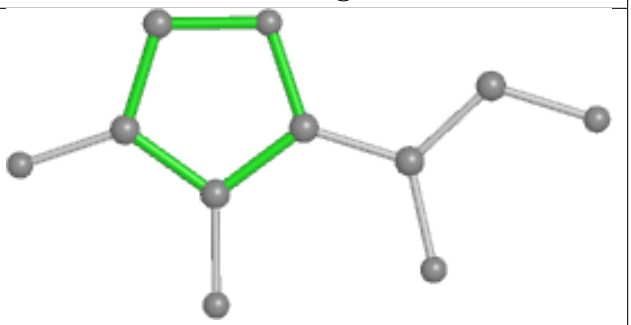
Bond lengths



Bond angles

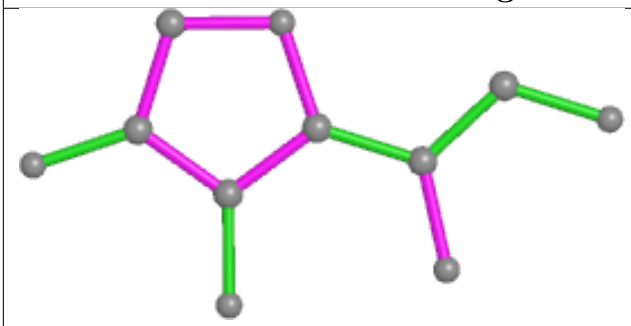


Torsions

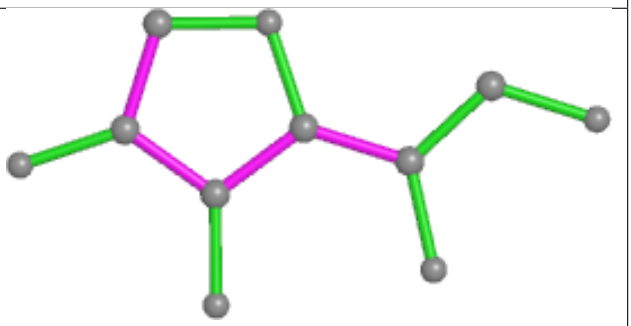


Rings

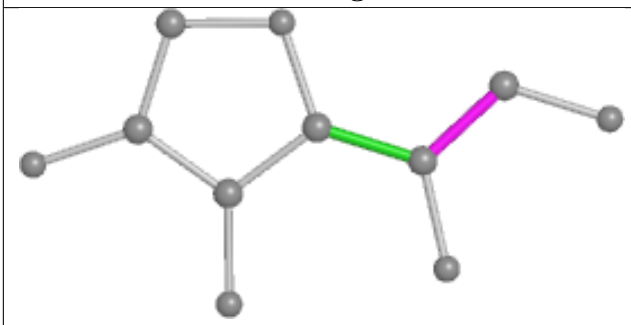
Ligand A1AIO B 2011



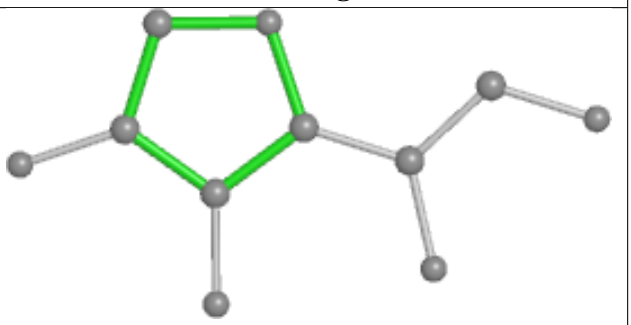
Bond lengths



Bond angles

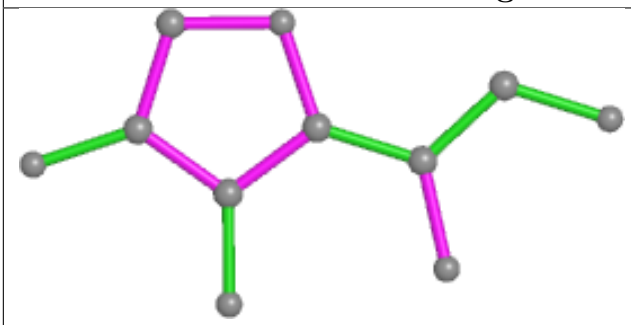


Torsions

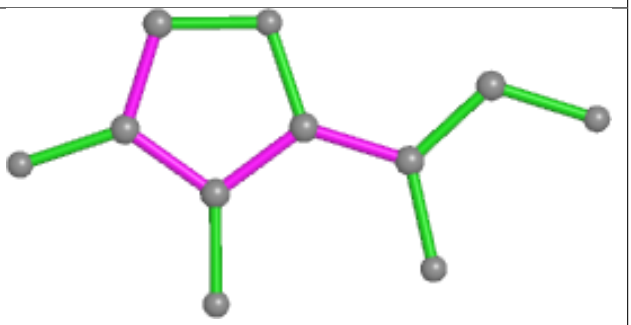


Rings

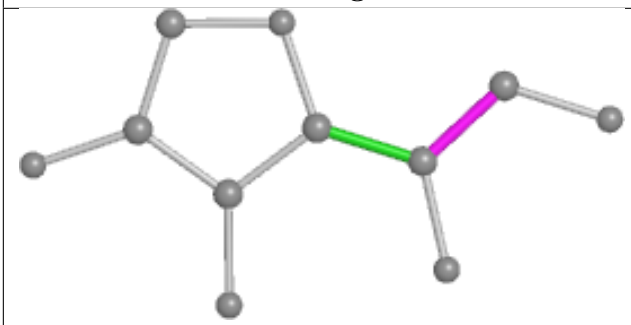
Ligand A1AIO B 2048



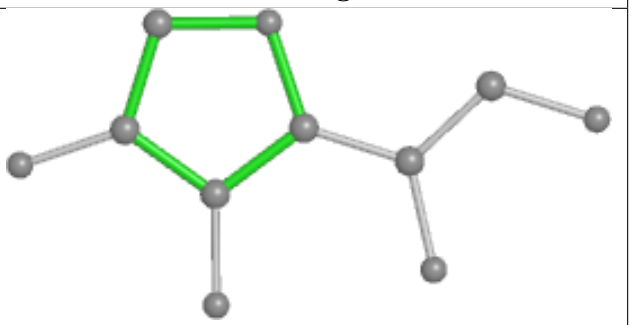
Bond lengths



Bond angles

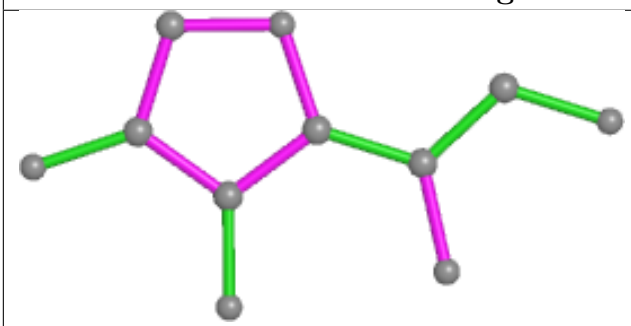


Torsions

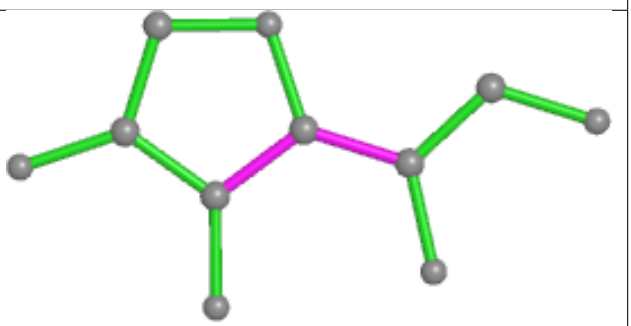


Rings

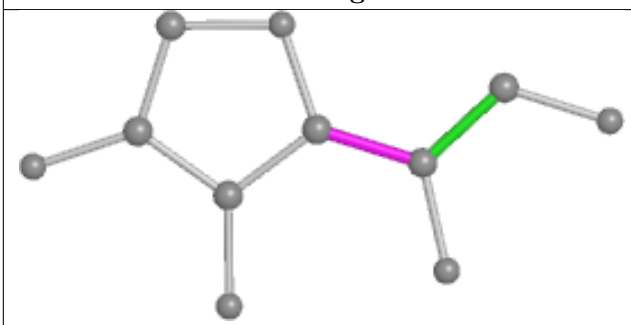
Ligand A1AIO B 2039



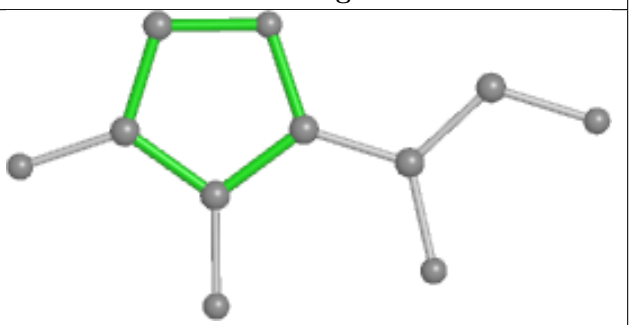
Bond lengths



Bond angles

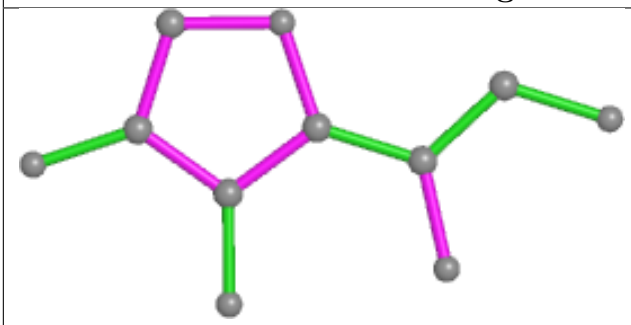


Torsions

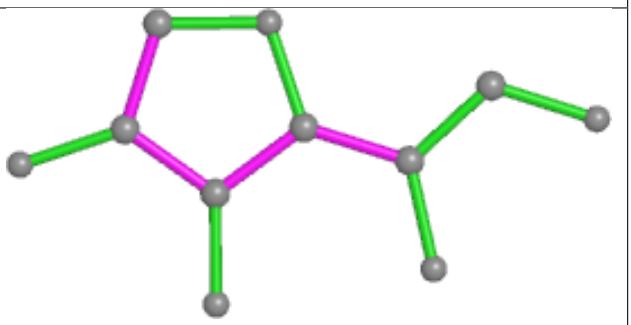


Rings

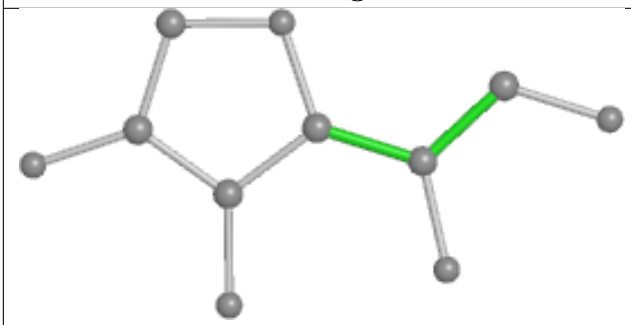
Ligand A1AIO B 2055



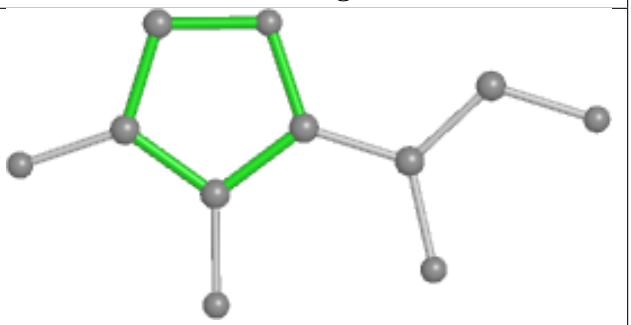
Bond lengths



Bond angles

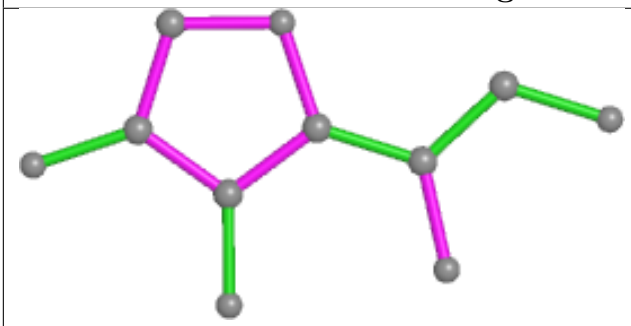


Torsions

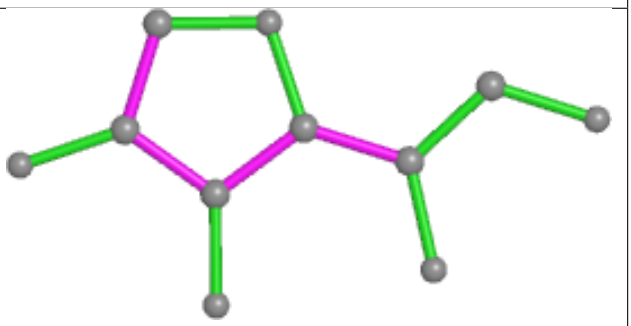


Rings

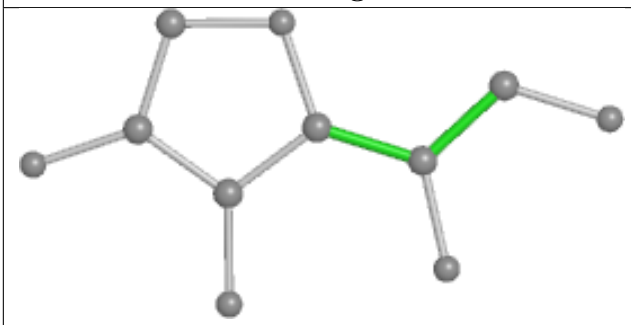
Ligand A1AIO B 2040



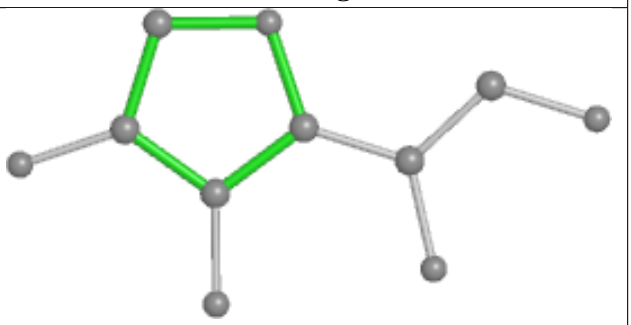
Bond lengths



Bond angles

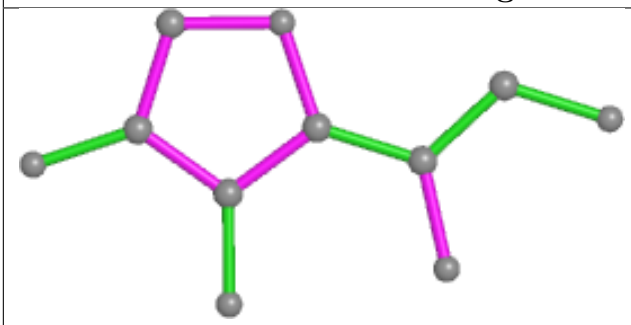


Torsions

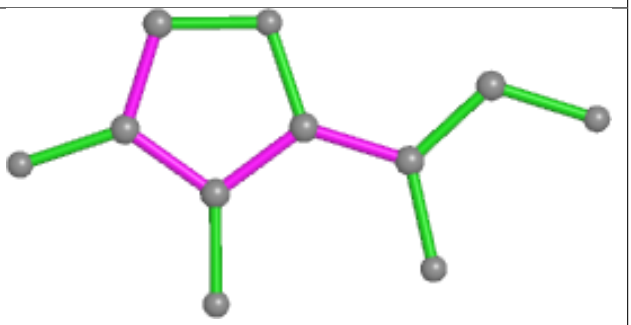


Rings

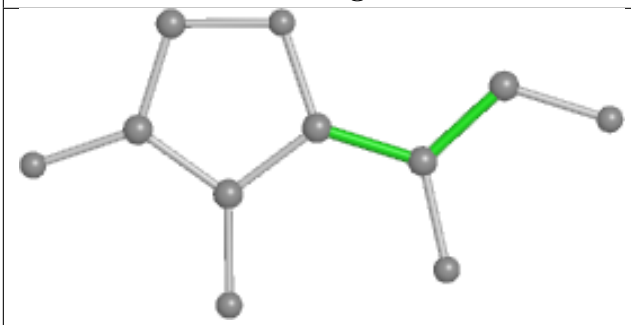
Ligand A1AIO B 2027



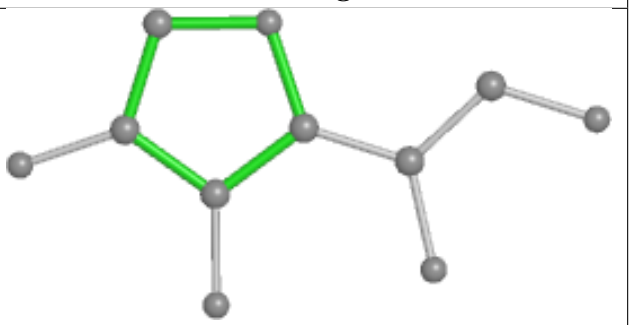
Bond lengths



Bond angles

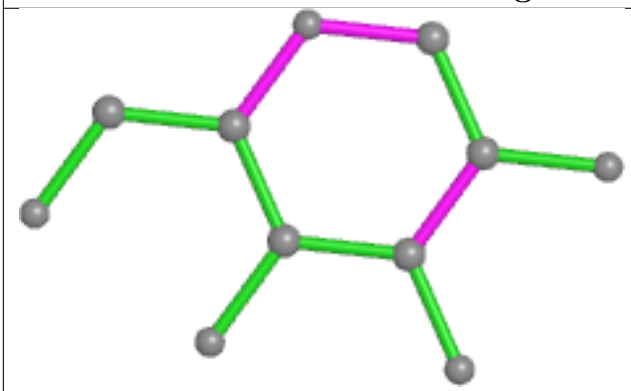


Torsions

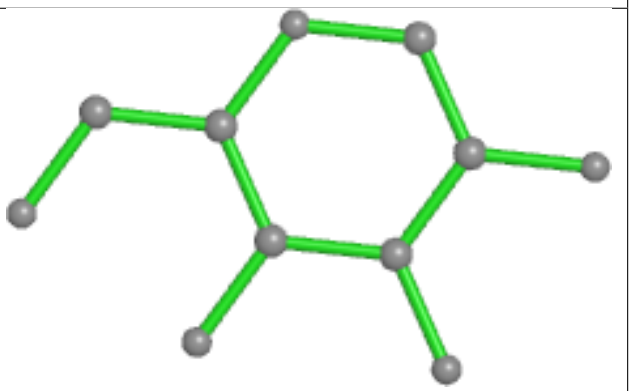


Rings

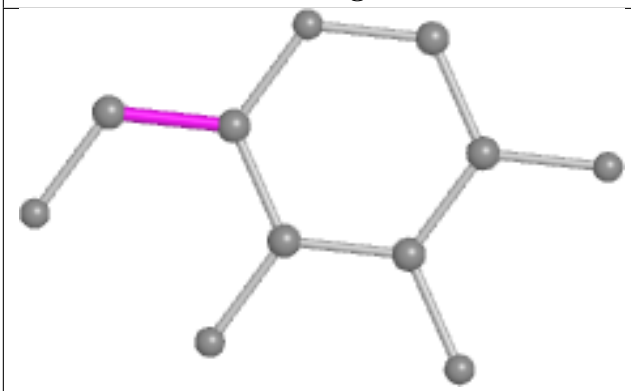
Ligand GLA B 2069



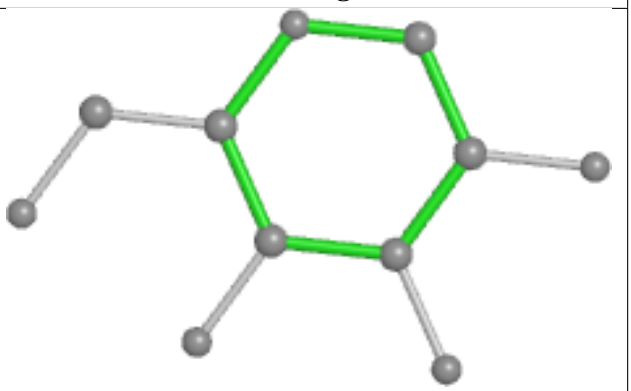
Bond lengths



Bond angles

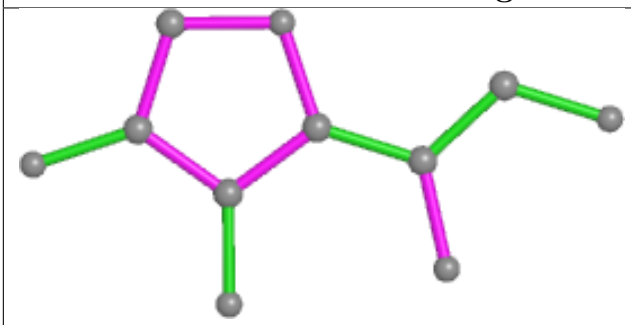


Torsions

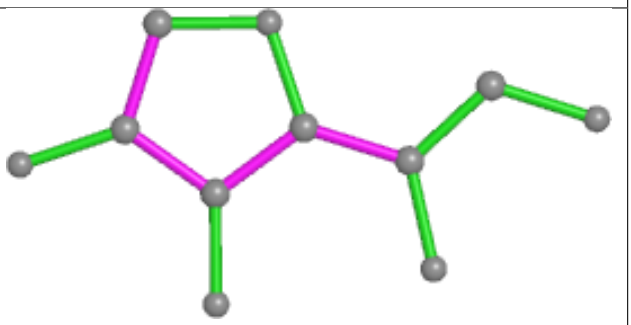


Rings

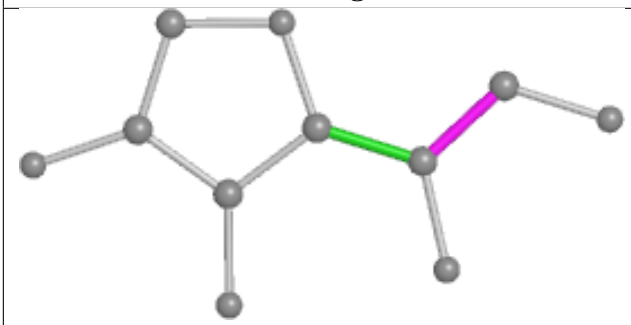
Ligand A1AIO A 2005



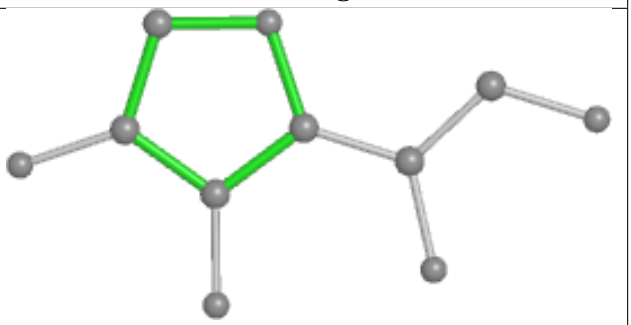
Bond lengths



Bond angles

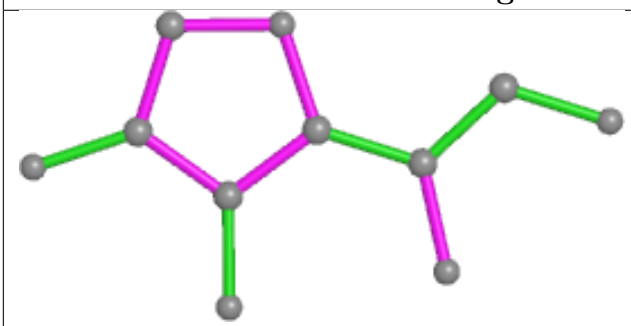


Torsions

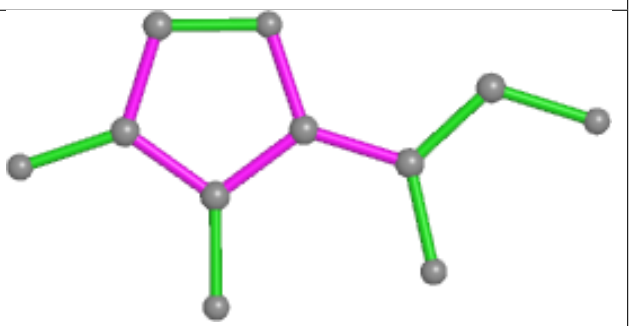


Rings

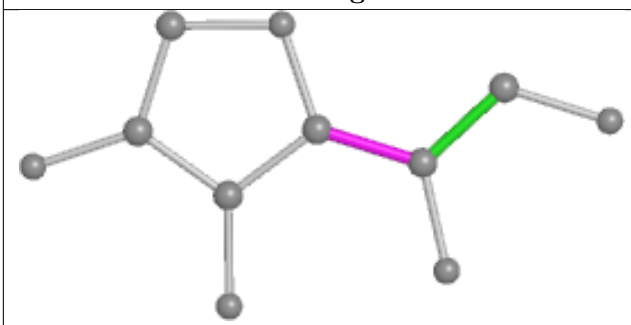
Ligand A1AIO B 2023



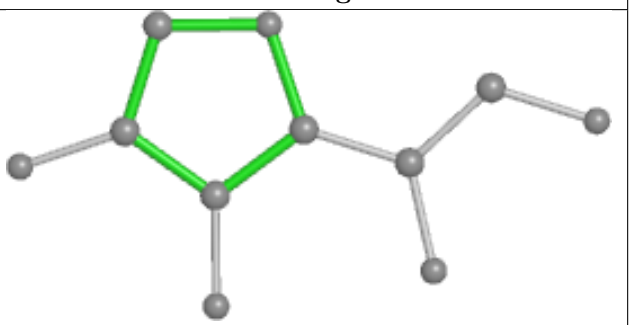
Bond lengths



Bond angles

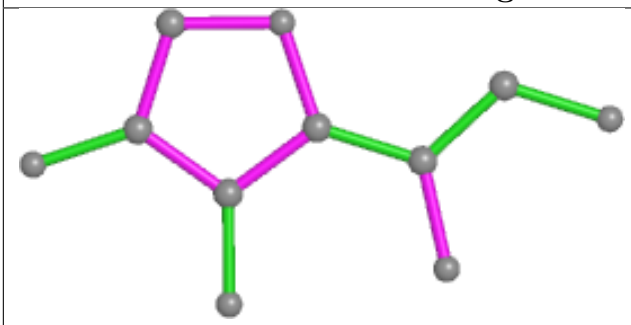


Torsions

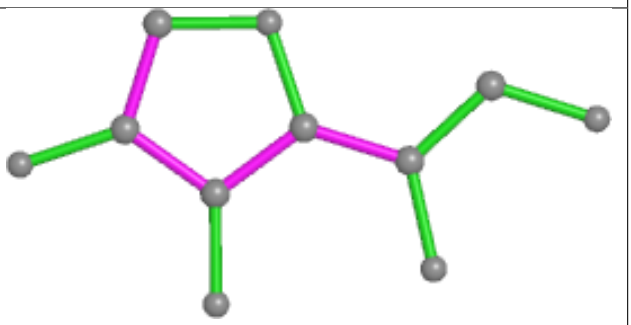


Rings

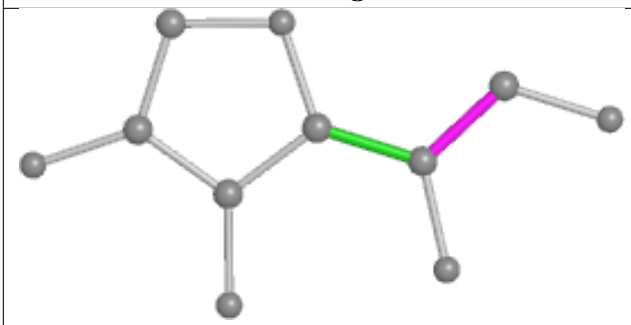
Ligand A1AIO B 2001



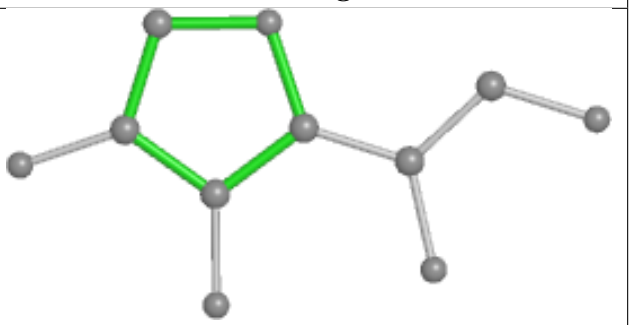
Bond lengths



Bond angles

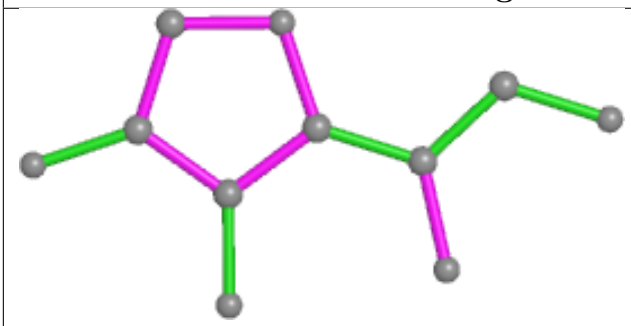


Torsions

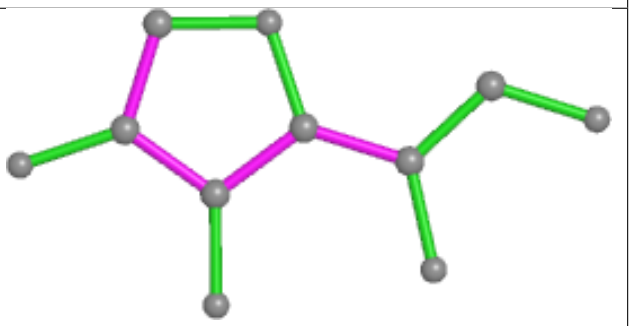


Rings

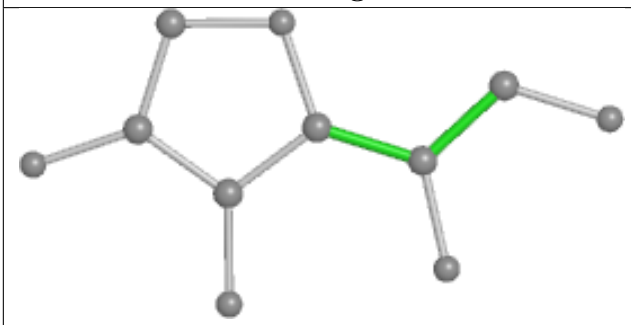
Ligand A1AIO A 2051



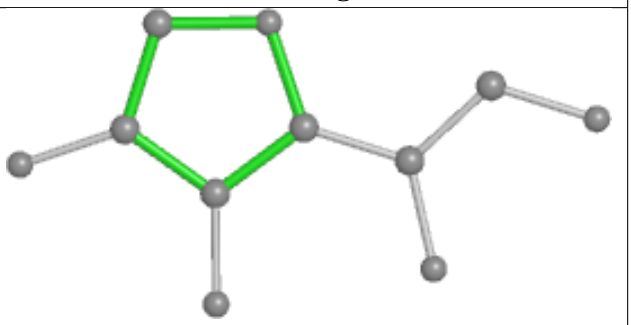
Bond lengths



Bond angles

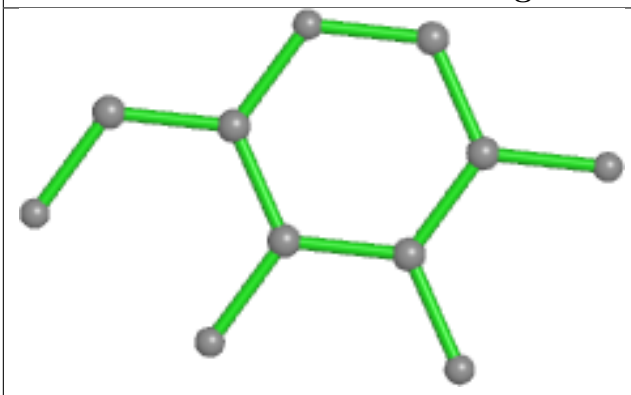


Torsions

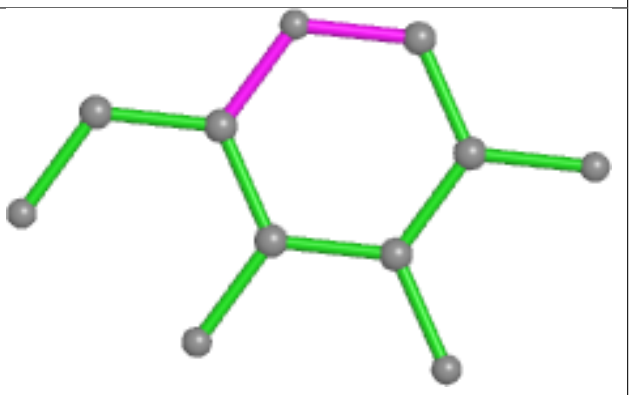


Rings

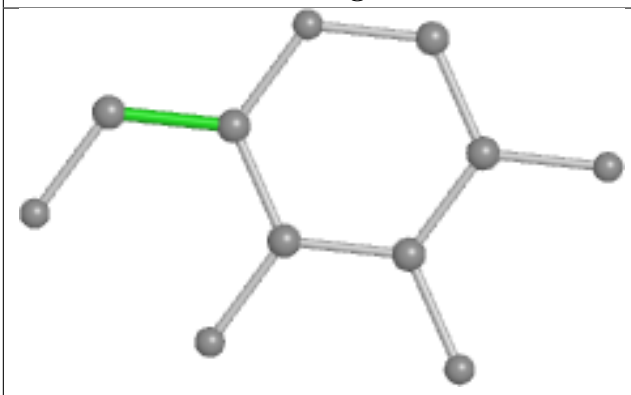
Ligand GLA B 2059



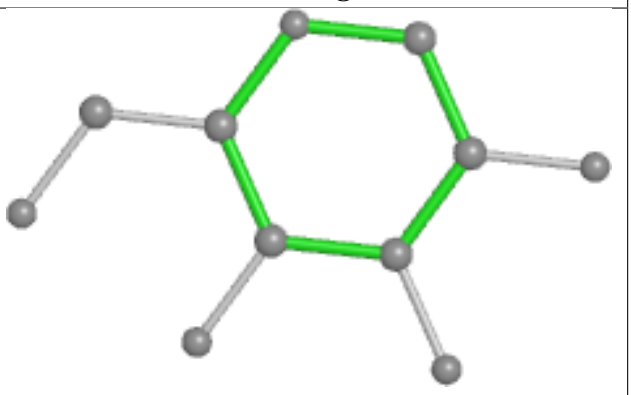
Bond lengths



Bond angles

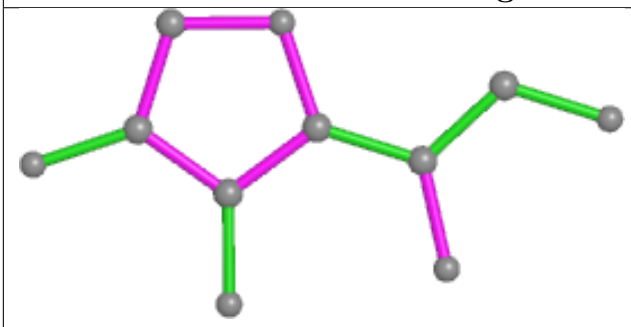


Torsions

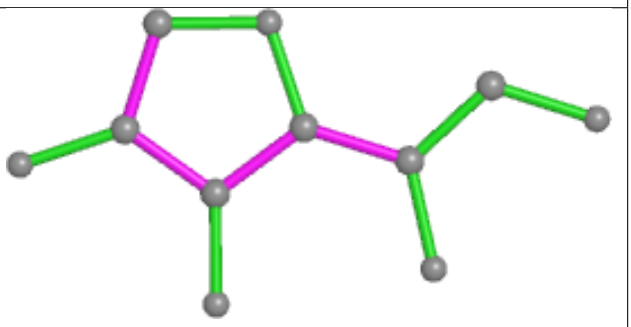


Rings

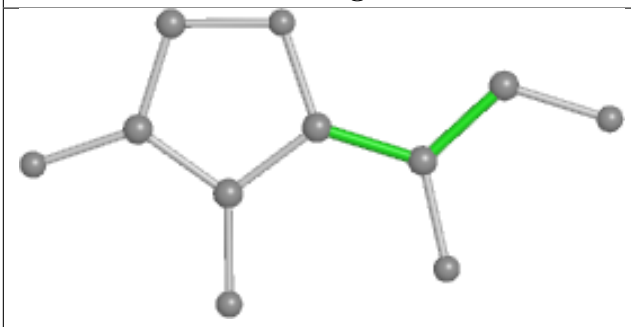
Ligand A1AIO B 2009



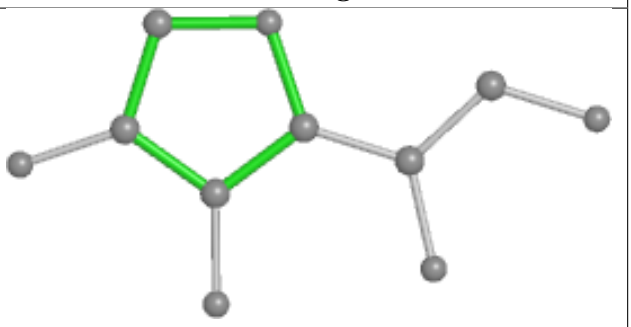
Bond lengths



Bond angles

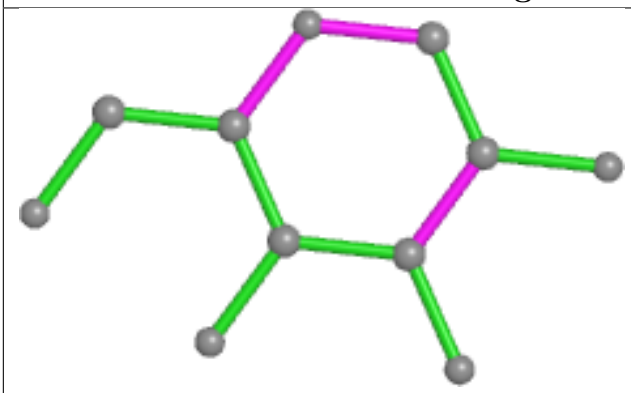


Torsions

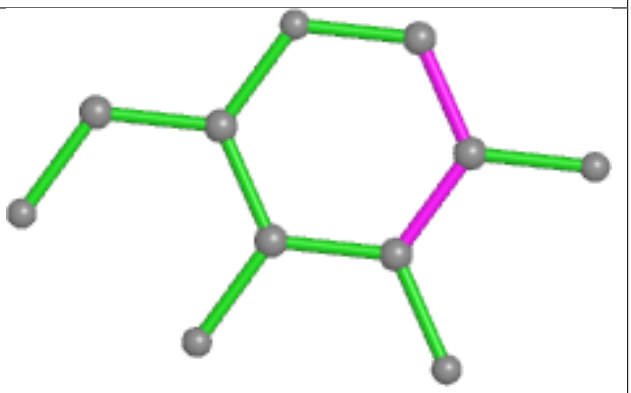


Rings

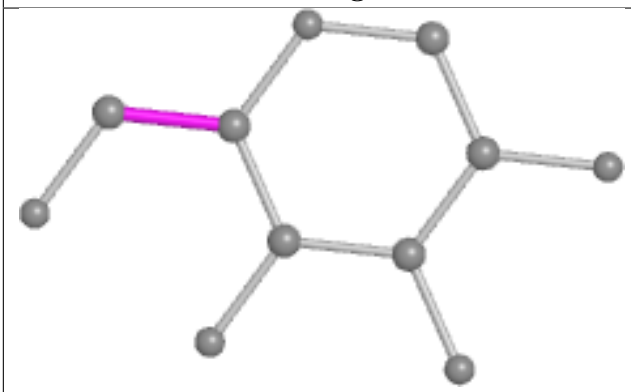
Ligand GLA B 2066



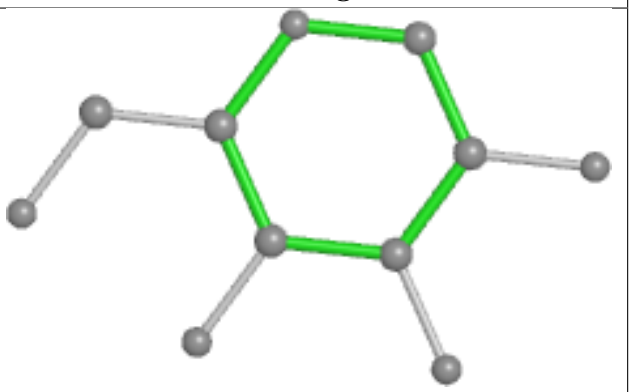
Bond lengths



Bond angles

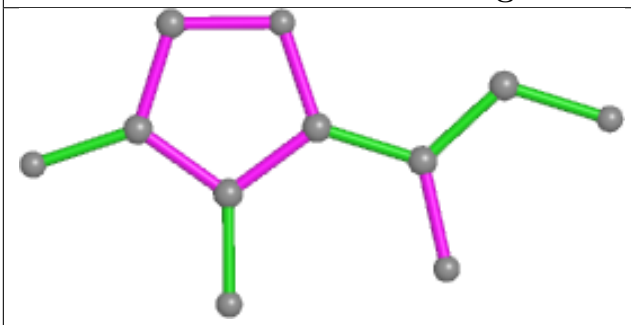


Torsions

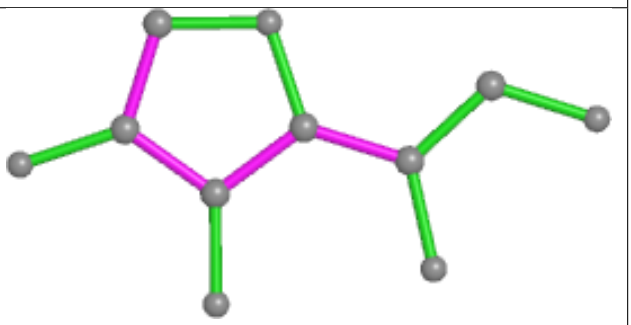


Rings

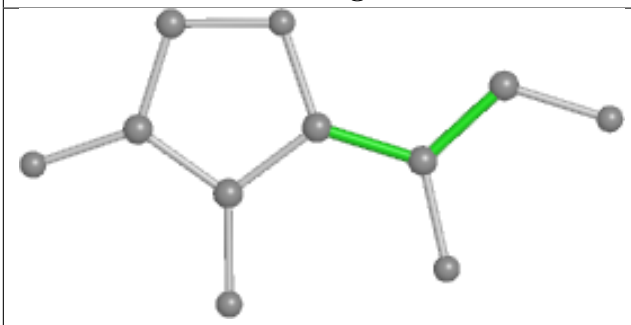
Ligand A1AIO B 2038



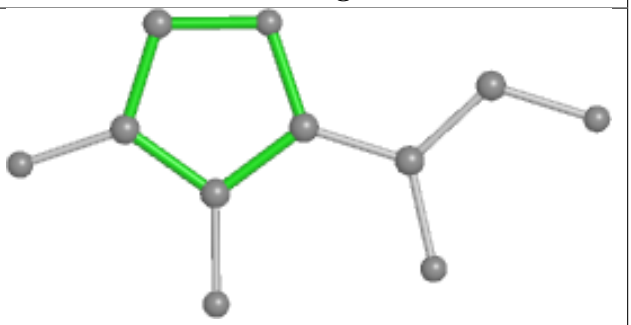
Bond lengths



Bond angles

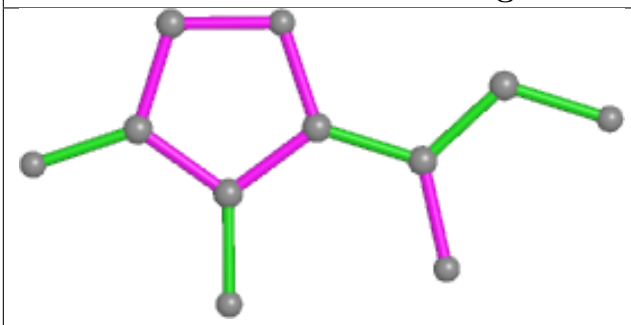


Torsions

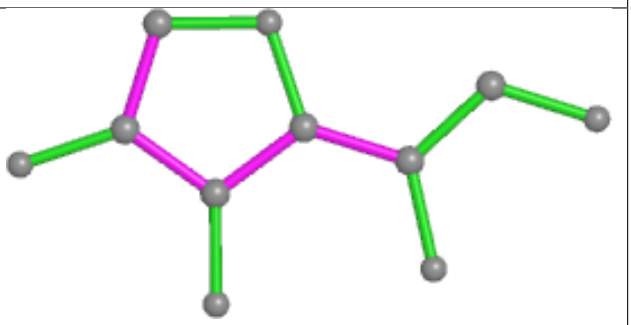


Rings

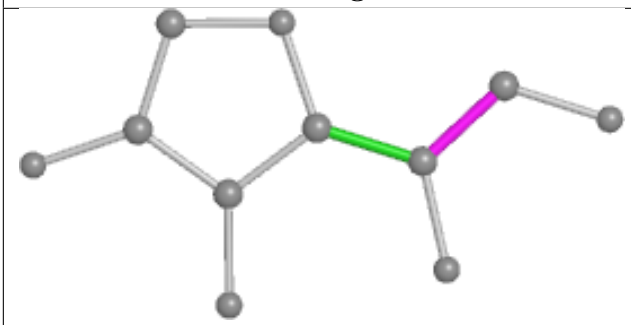
Ligand A1AIO B 2010



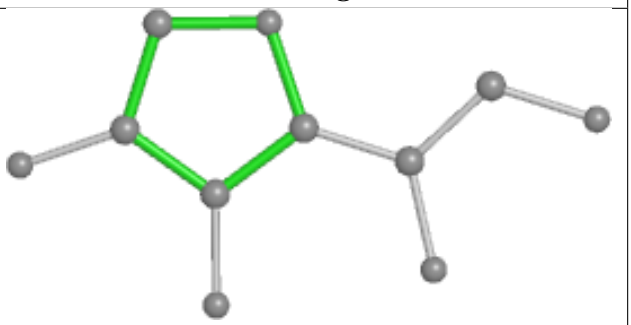
Bond lengths



Bond angles

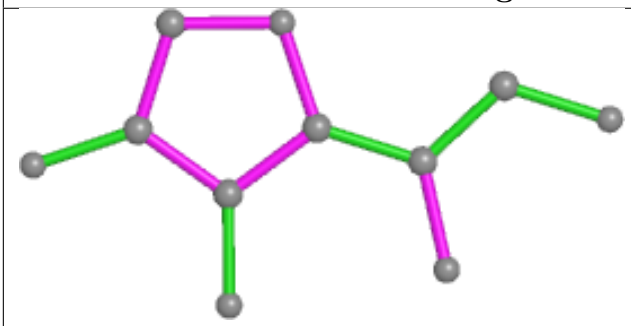


Torsions

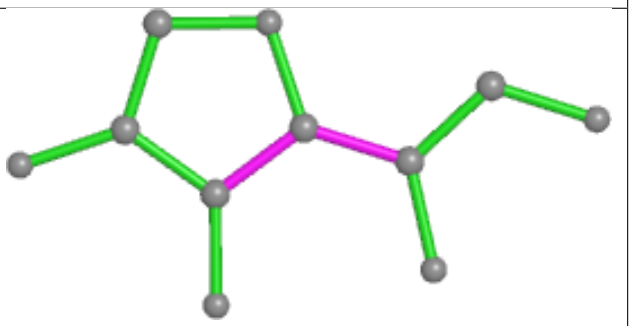


Rings

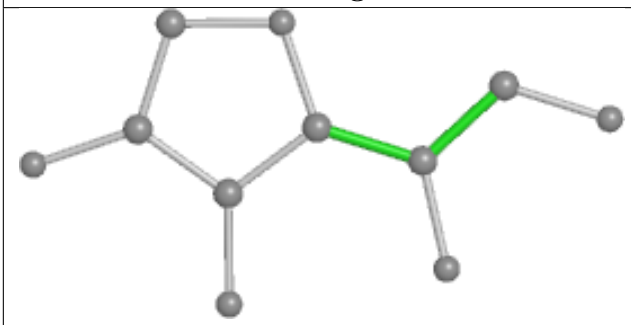
Ligand A1AIO A 2017



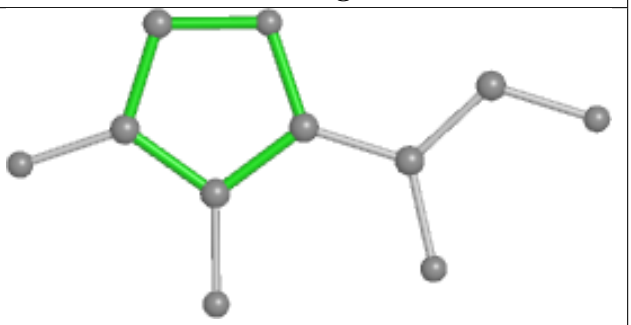
Bond lengths



Bond angles

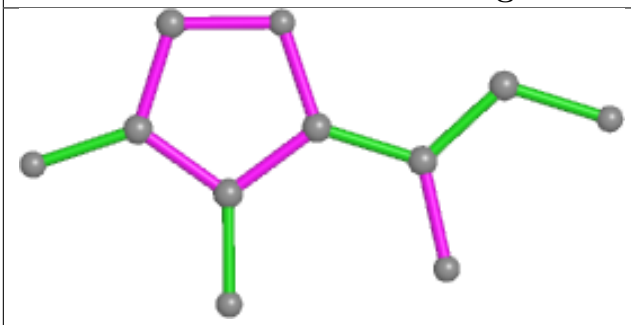


Torsions

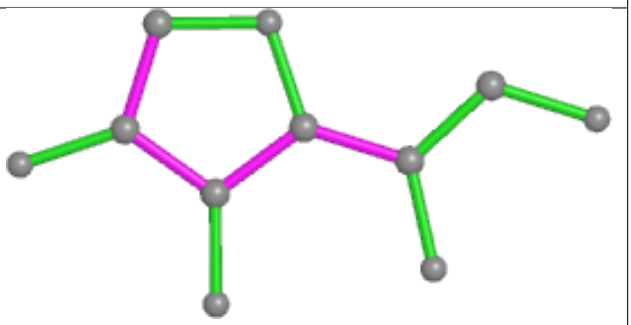


Rings

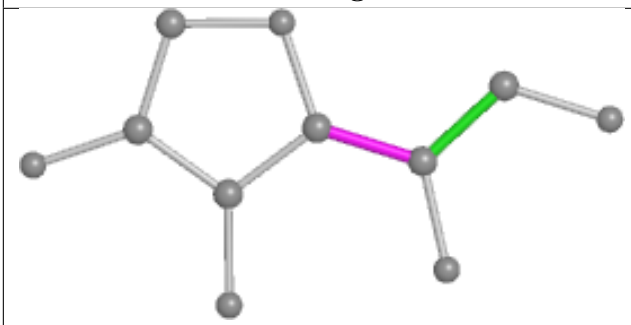
Ligand A1AIO B 2053



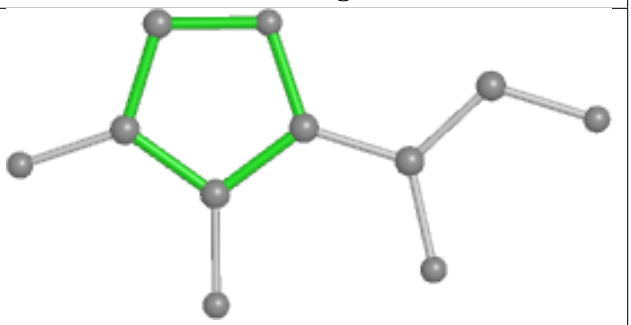
Bond lengths



Bond angles

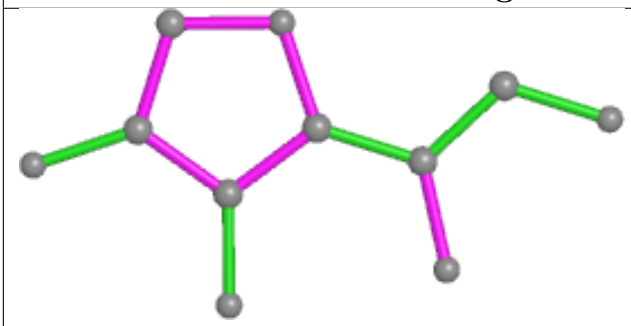


Torsions

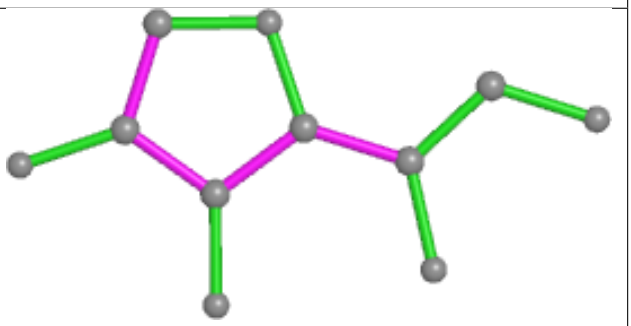


Rings

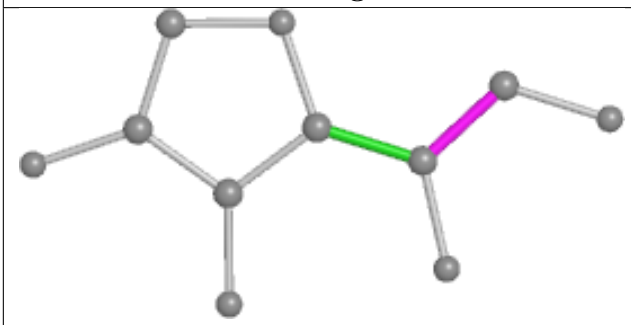
Ligand A1AIO A 2045



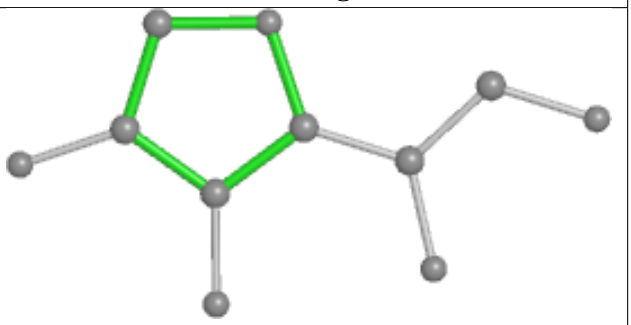
Bond lengths



Bond angles

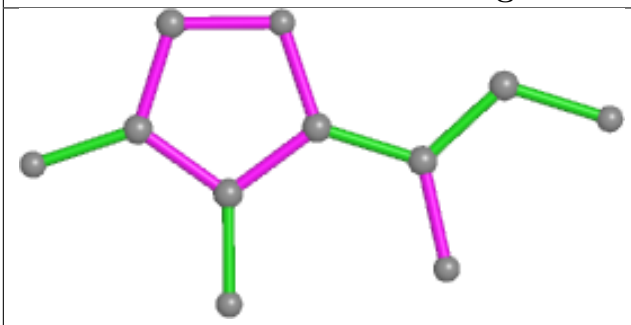


Torsions

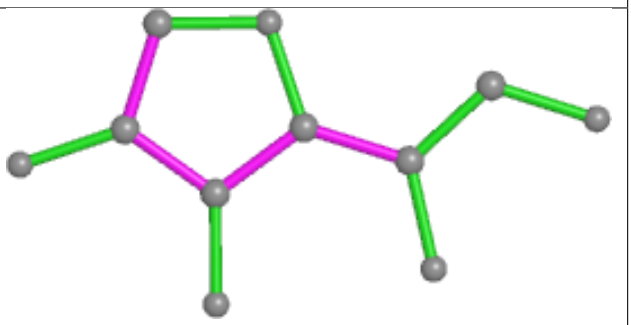


Rings

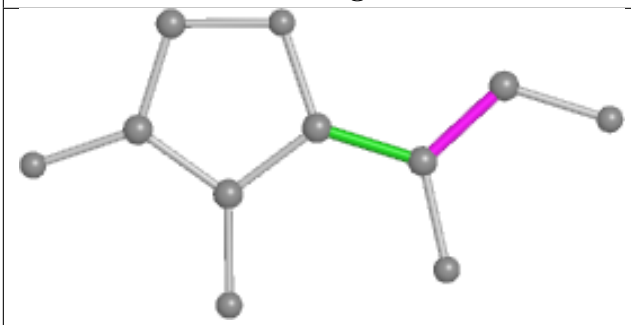
Ligand A1AIO B 2004



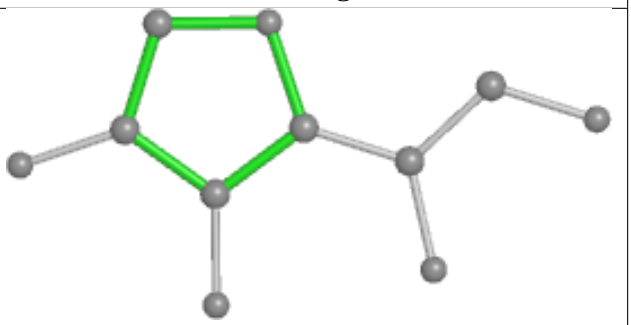
Bond lengths



Bond angles

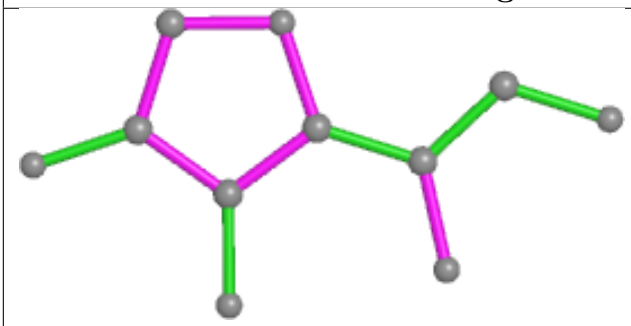


Torsions

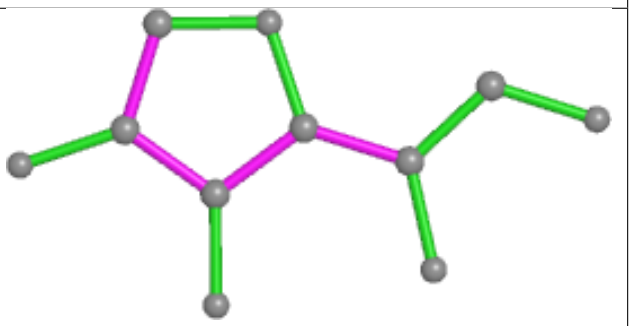


Rings

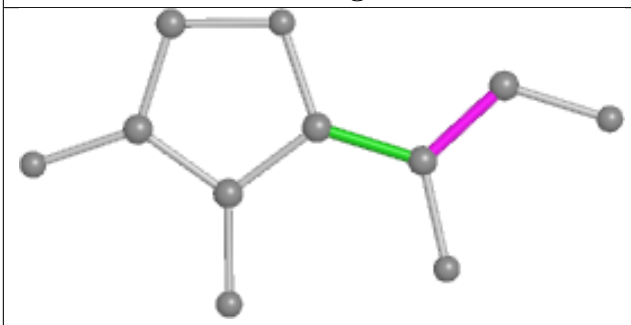
Ligand A1AIO B 2006



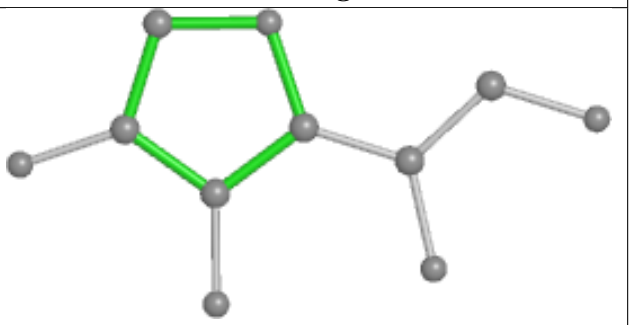
Bond lengths



Bond angles

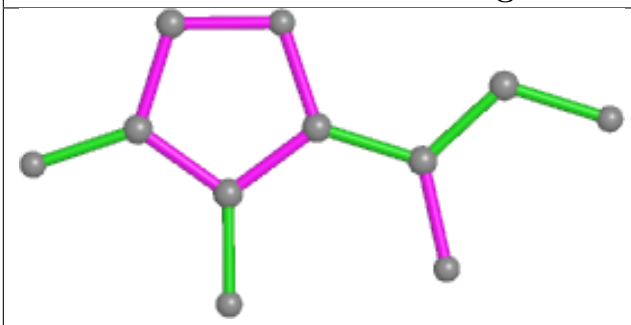


Torsions

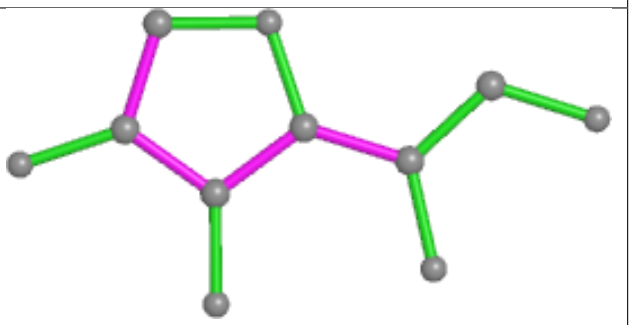


Rings

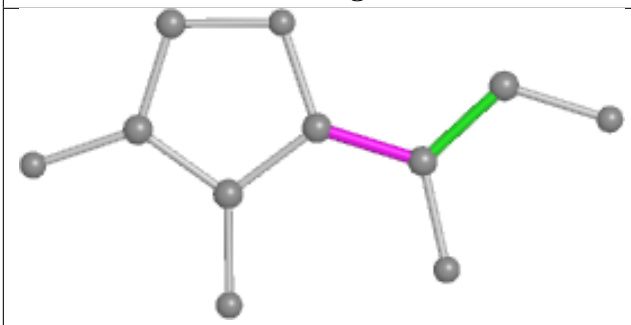
Ligand A1AIO B 2024



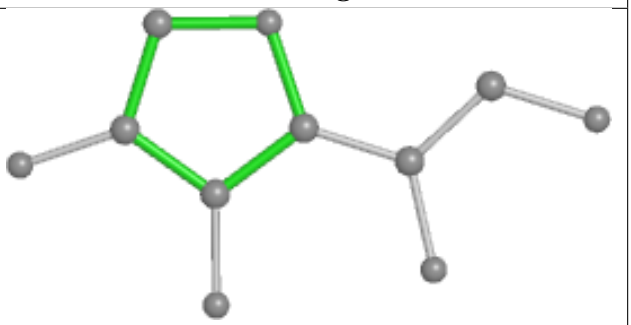
Bond lengths



Bond angles

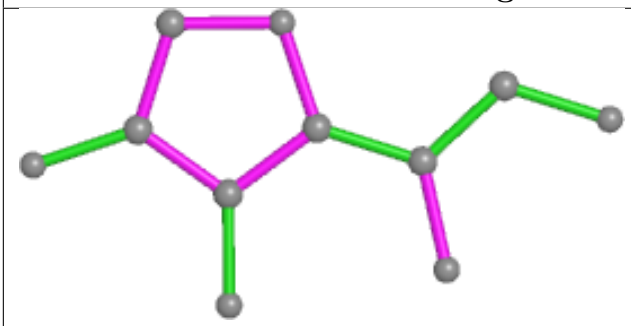


Torsions

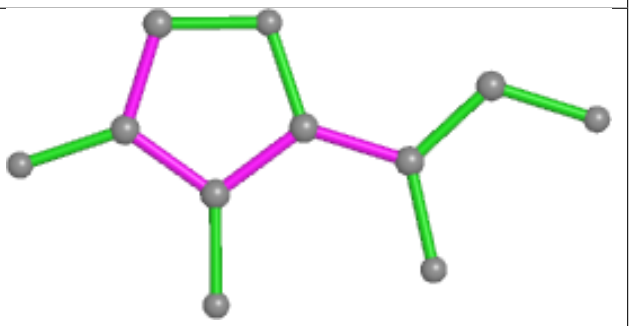


Rings

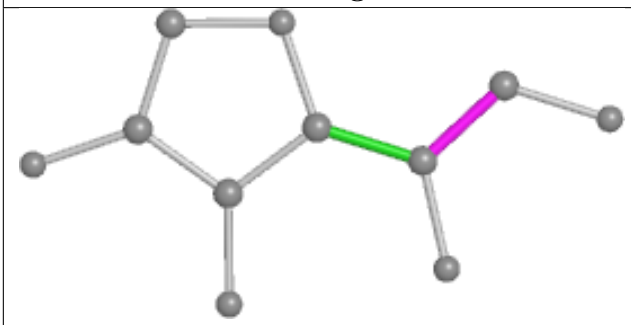
Ligand A1AIO B 2019



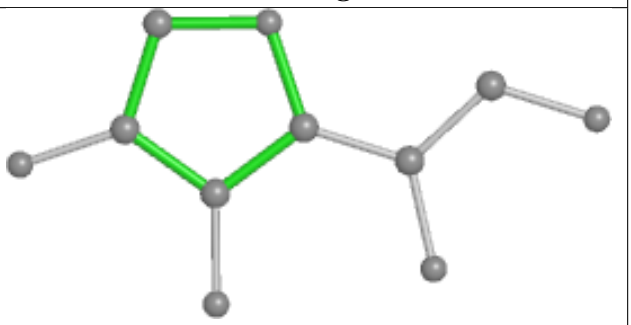
Bond lengths



Bond angles

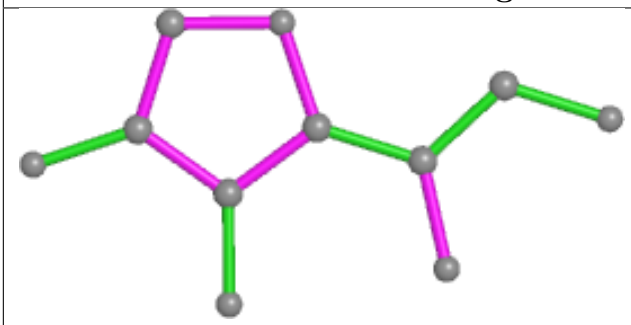


Torsions

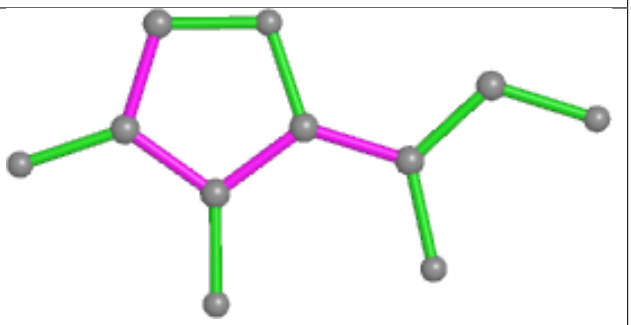


Rings

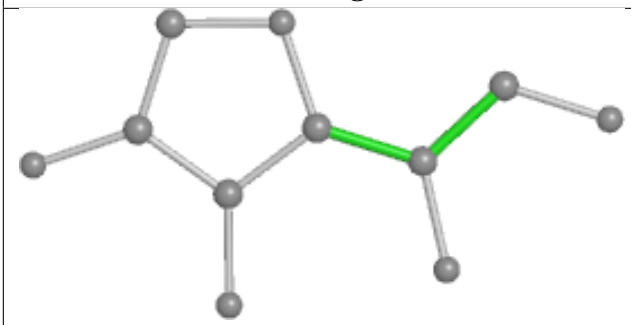
Ligand A1AIO A 2053



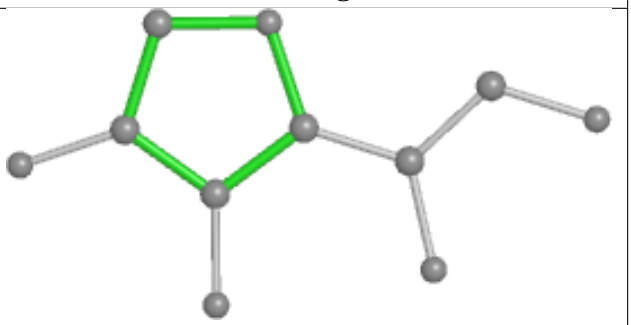
Bond lengths



Bond angles

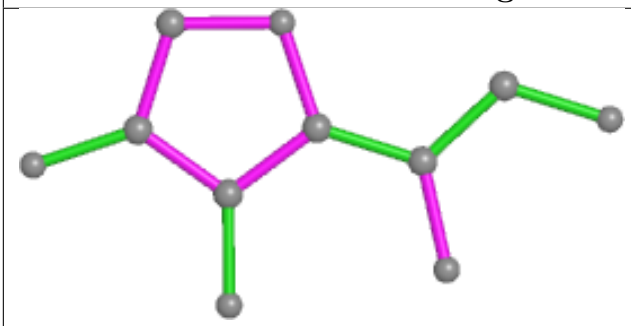


Torsions

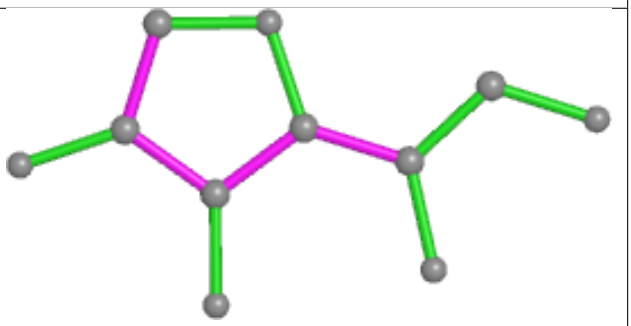


Rings

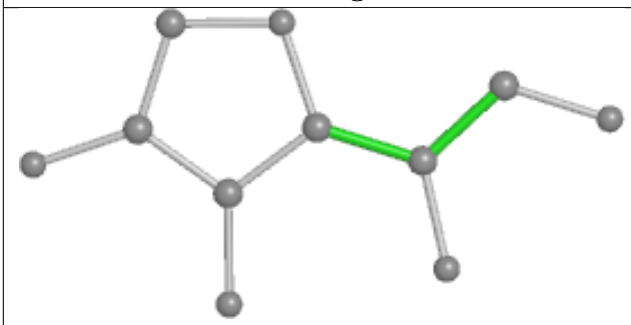
Ligand A1AIO B 2029



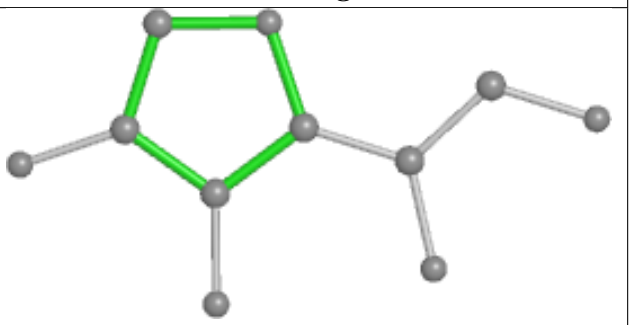
Bond lengths



Bond angles

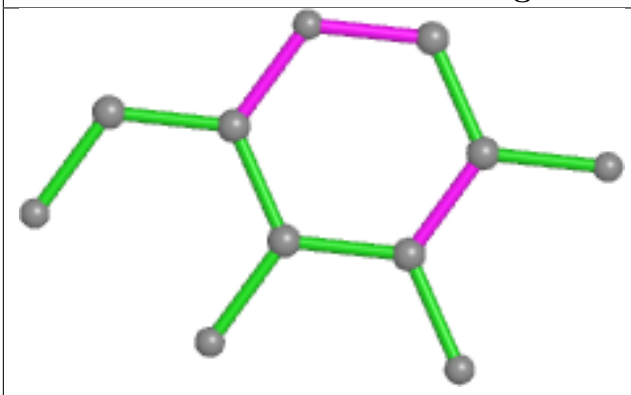


Torsions

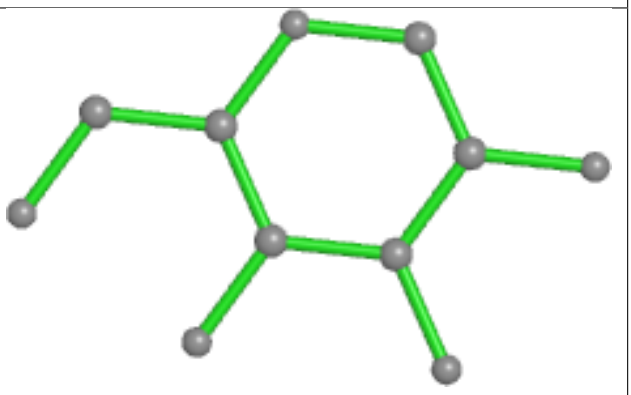


Rings

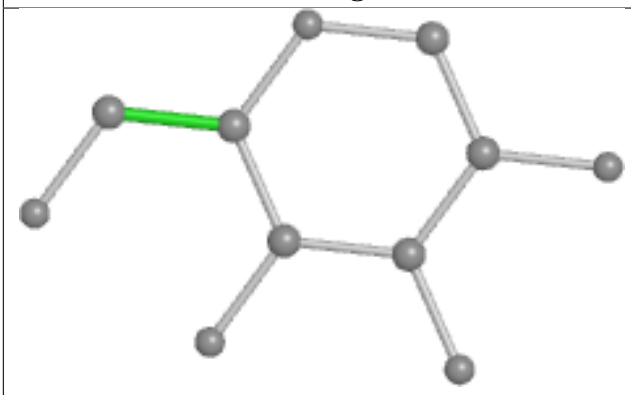
Ligand GLA A 2068



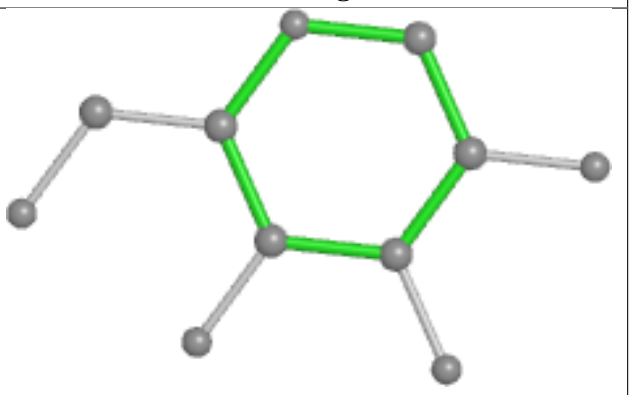
Bond lengths



Bond angles

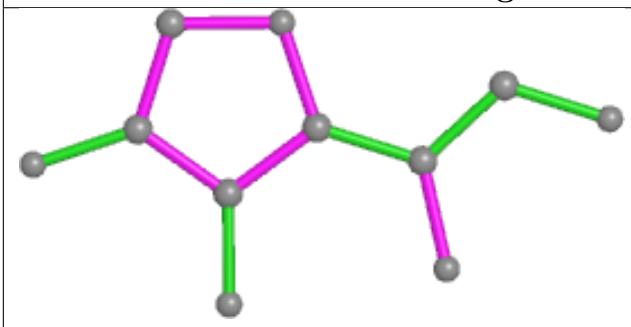


Torsions

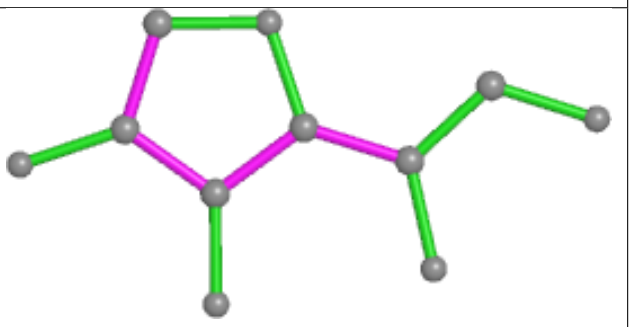


Rings

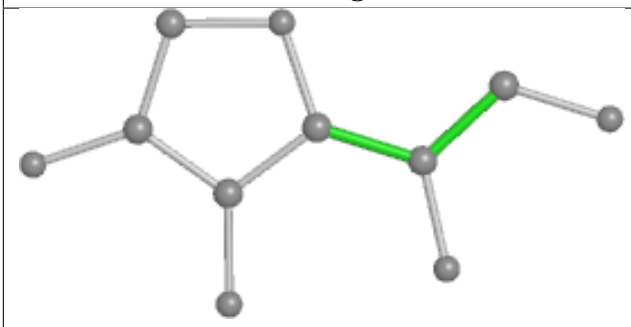
Ligand A1AIO B 2017



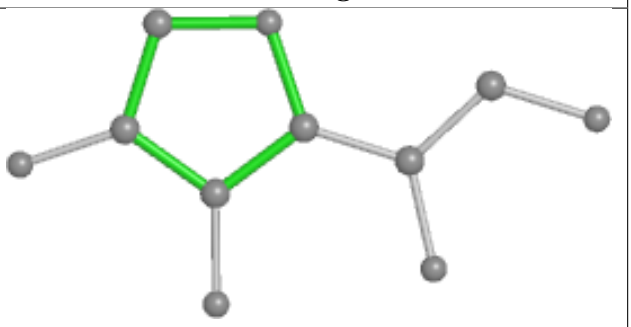
Bond lengths



Bond angles

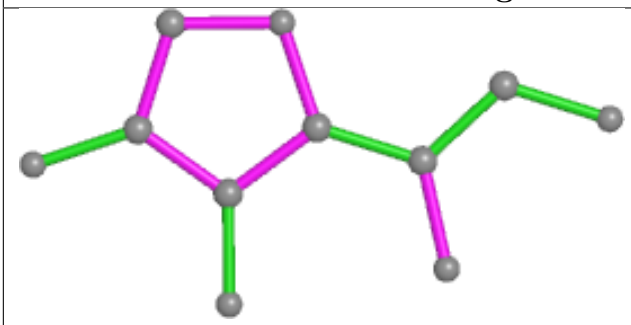


Torsions

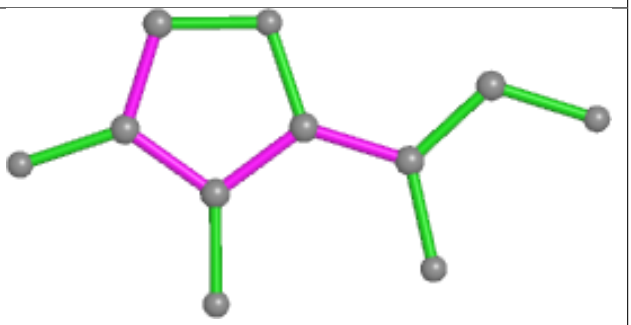


Rings

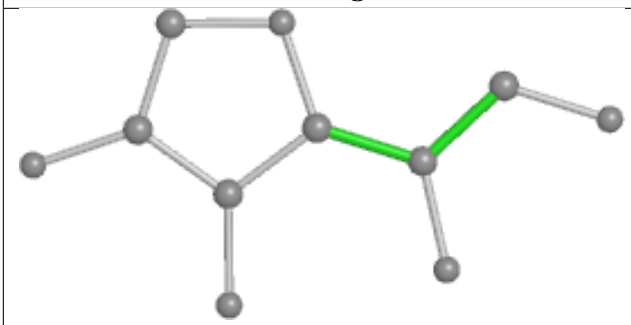
Ligand A1AIO A 2022



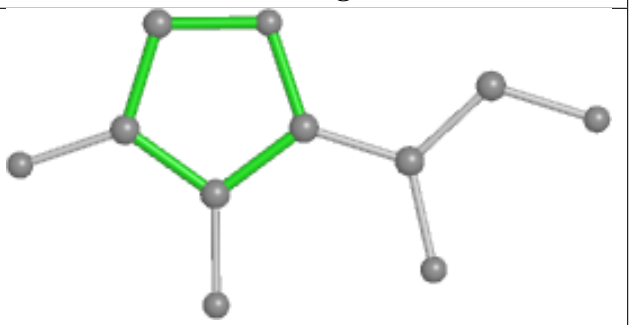
Bond lengths



Bond angles

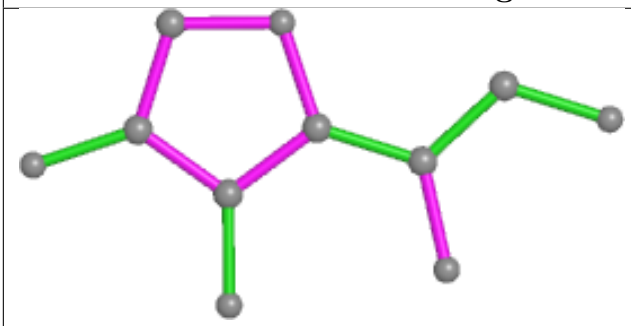


Torsions

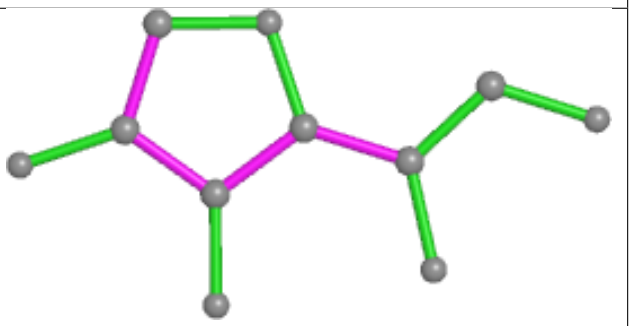


Rings

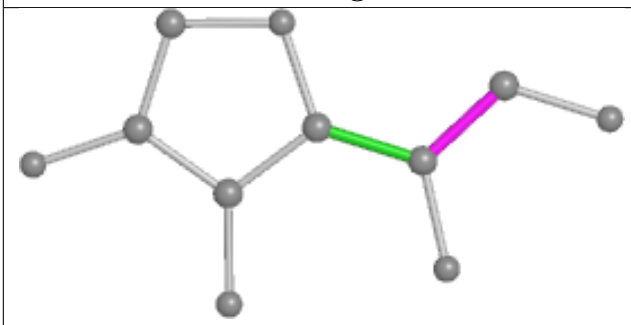
Ligand A1AIO A 2006



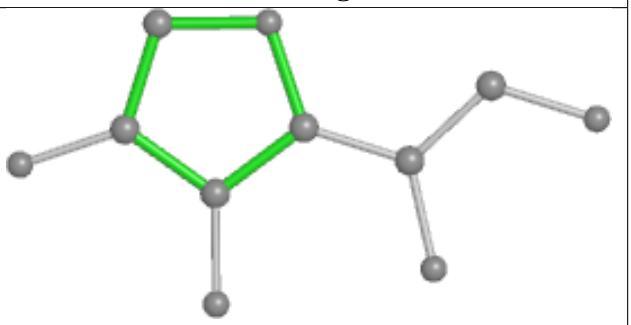
Bond lengths



Bond angles

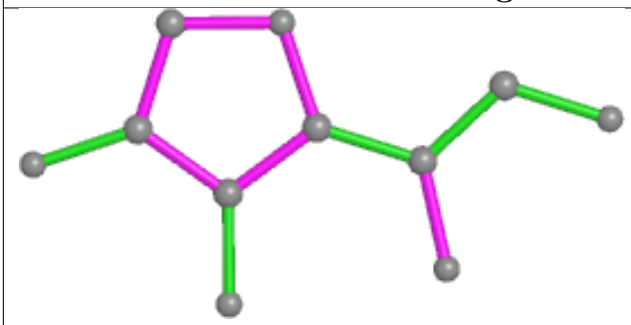


Torsions

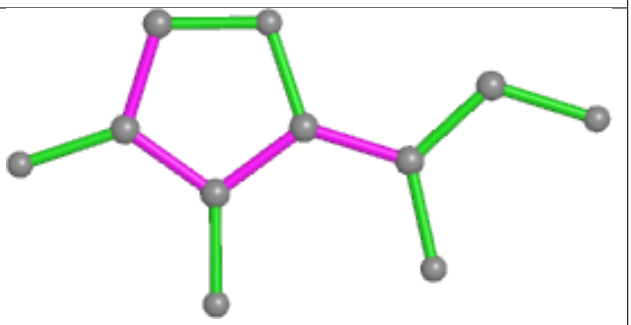


Rings

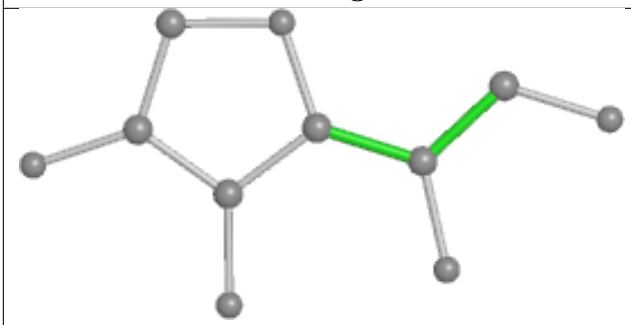
Ligand A1AIO A 2026



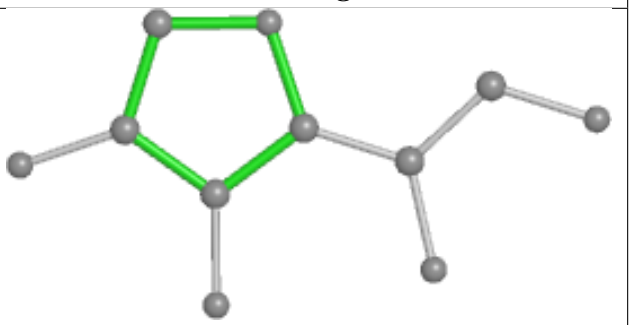
Bond lengths



Bond angles

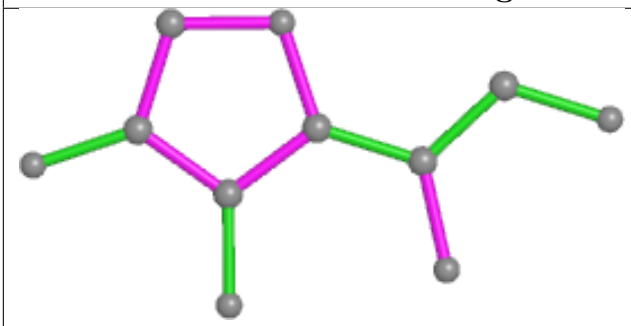


Torsions

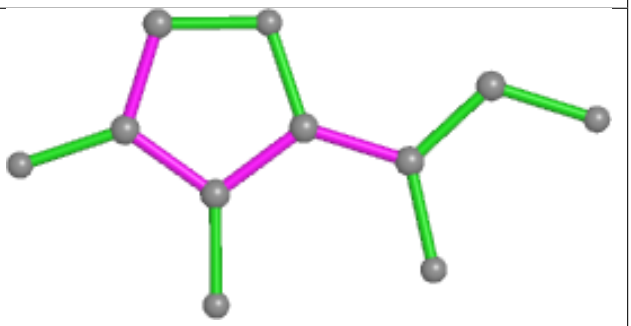


Rings

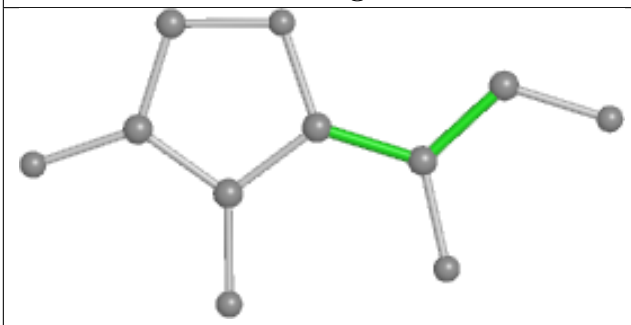
Ligand A1AIO A 2013



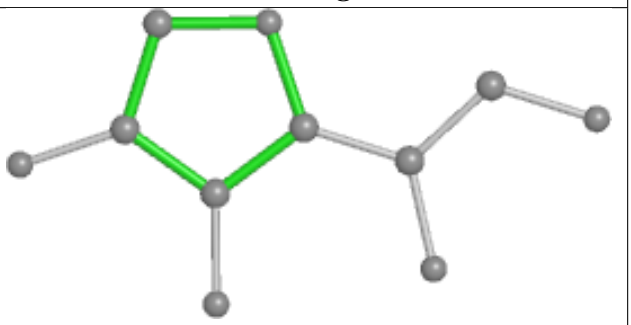
Bond lengths



Bond angles

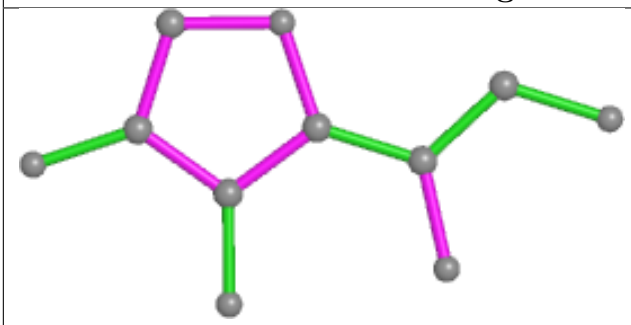


Torsions

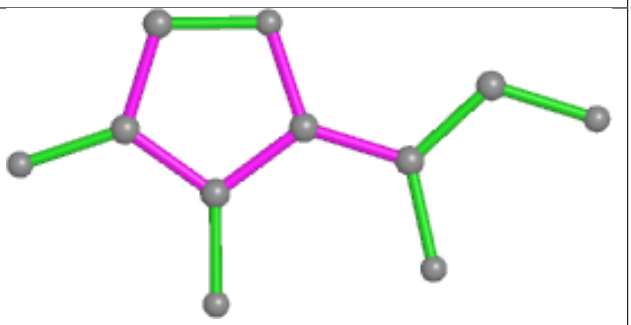


Rings

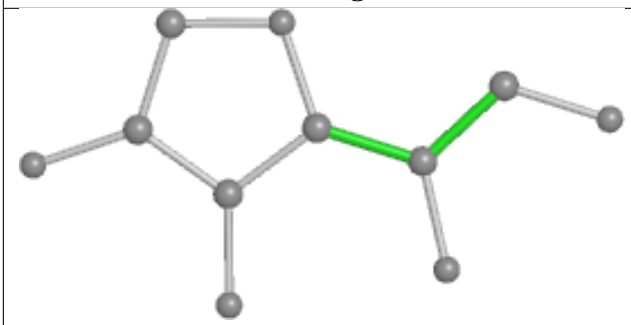
Ligand A1AIO B 2033



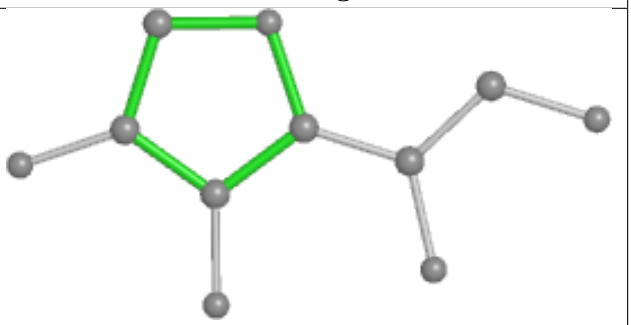
Bond lengths



Bond angles

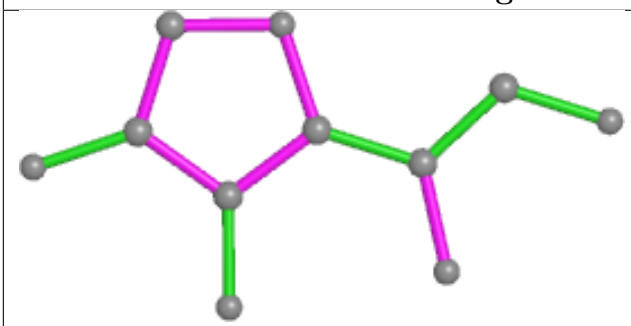


Torsions

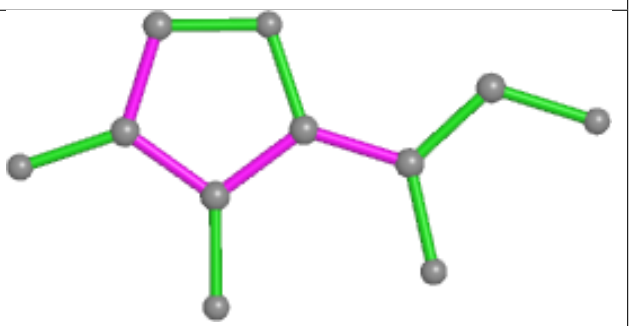


Rings

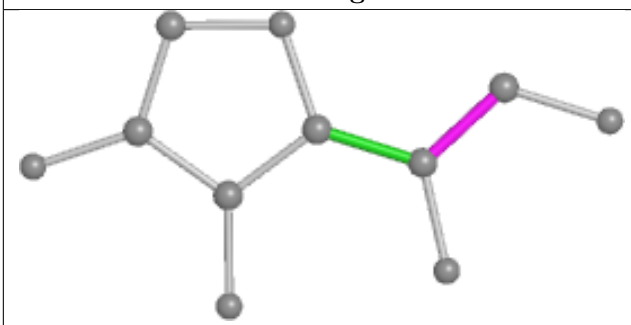
Ligand A1AIO A 2047



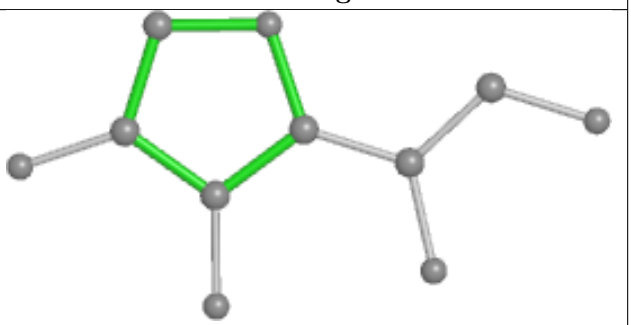
Bond lengths



Bond angles

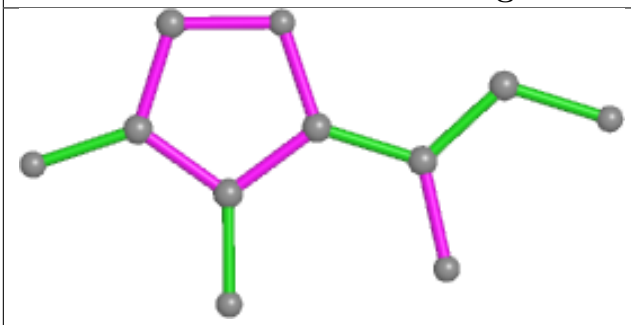


Torsions

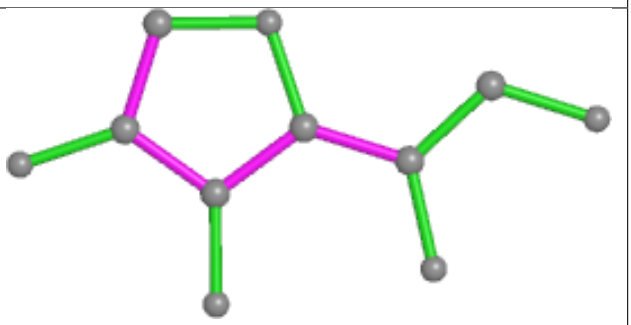


Rings

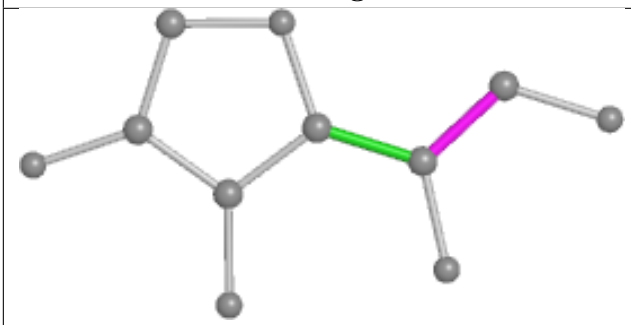
Ligand A1AIO B 2036



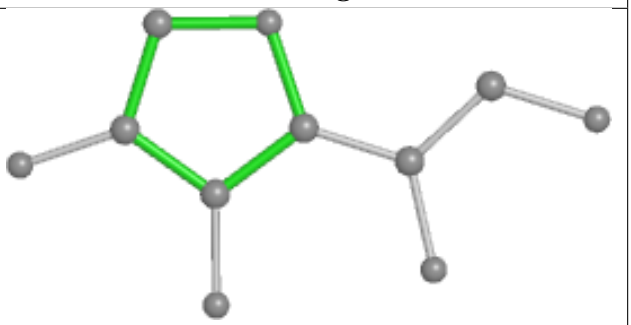
Bond lengths



Bond angles

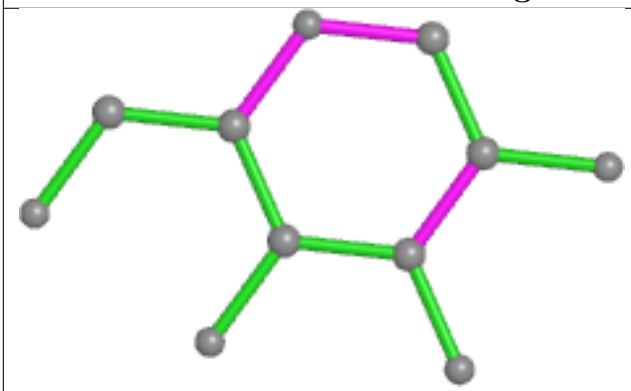


Torsions

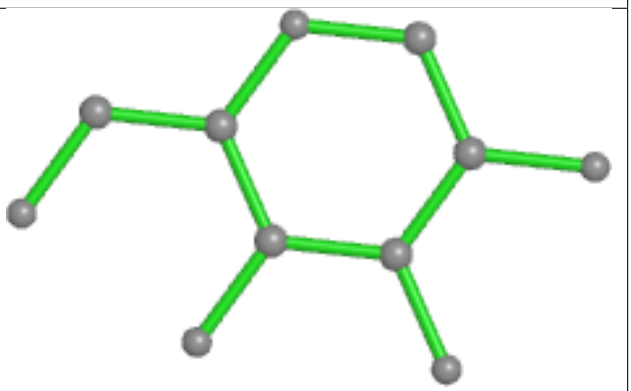


Rings

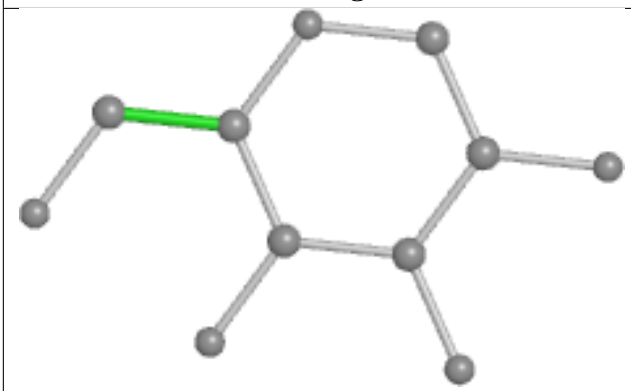
Ligand GLA A 2066



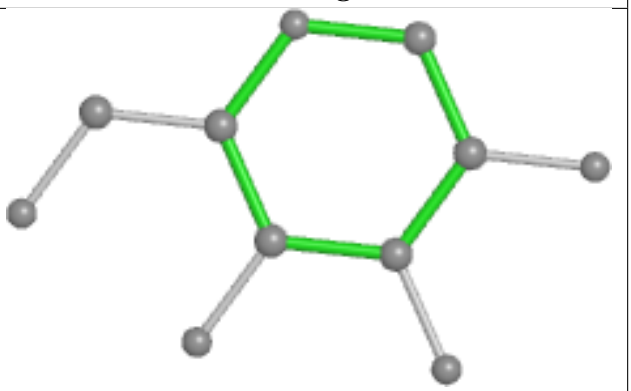
Bond lengths



Bond angles

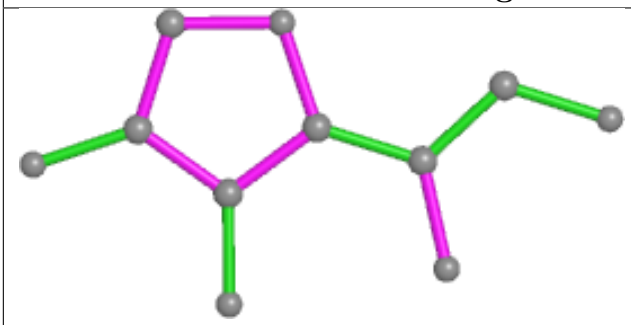


Torsions

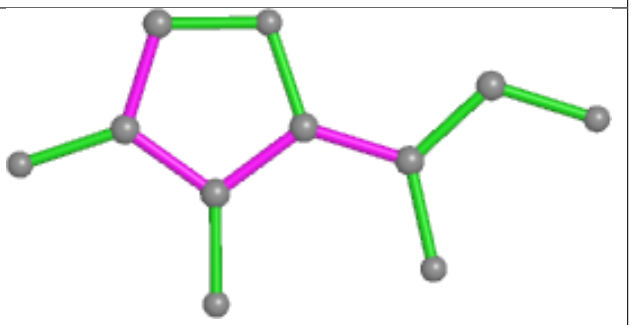


Rings

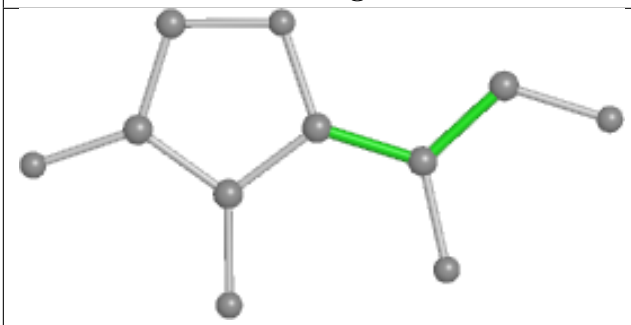
Ligand A1AIO A 2012



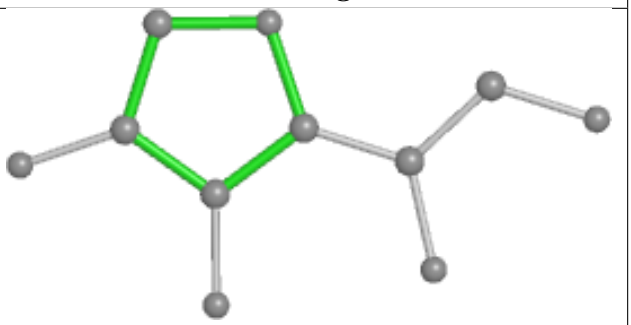
Bond lengths



Bond angles

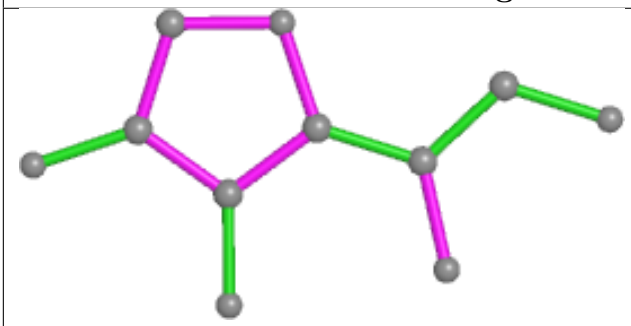


Torsions

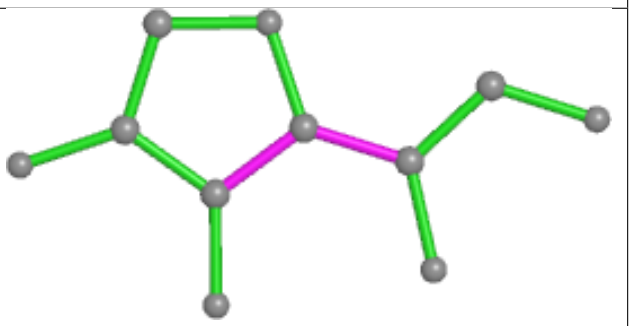


Rings

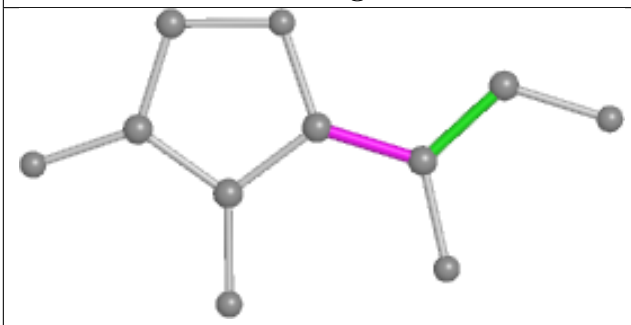
Ligand A1AIO A 2033



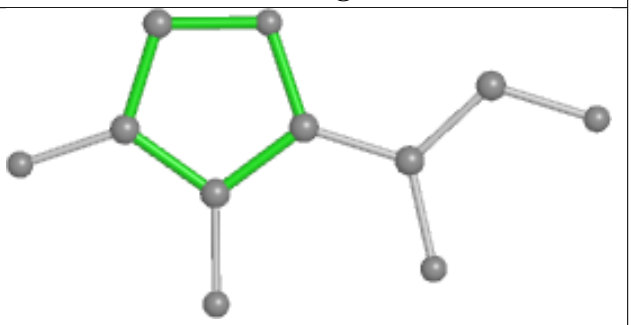
Bond lengths



Bond angles

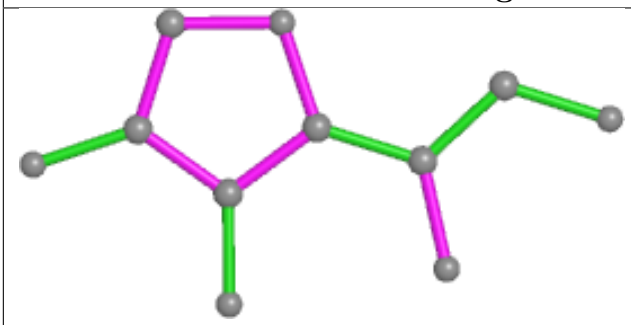


Torsions

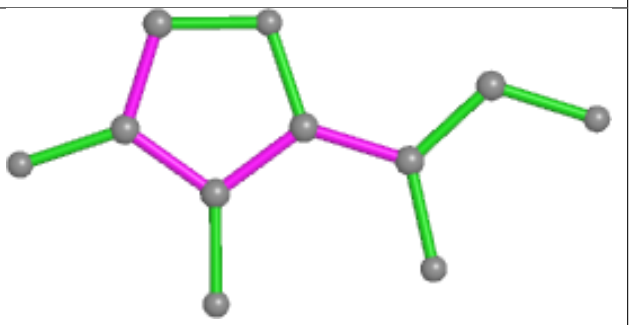


Rings

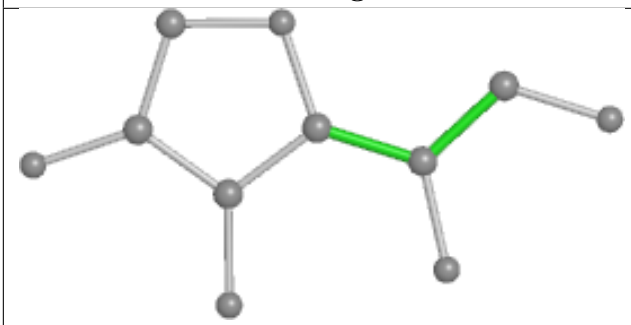
Ligand A1AIO A 2010



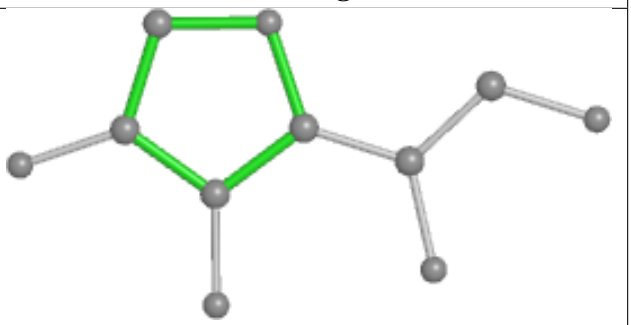
Bond lengths



Bond angles

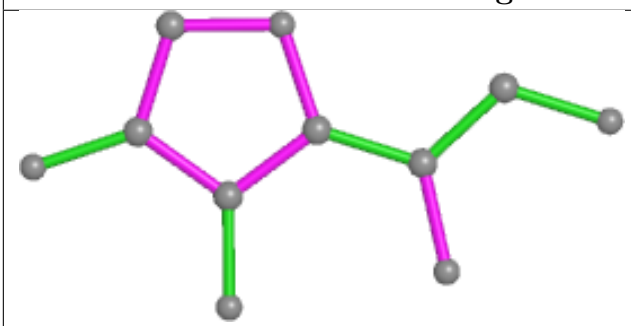


Torsions

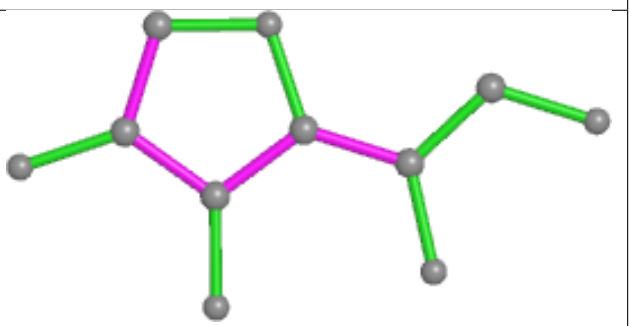


Rings

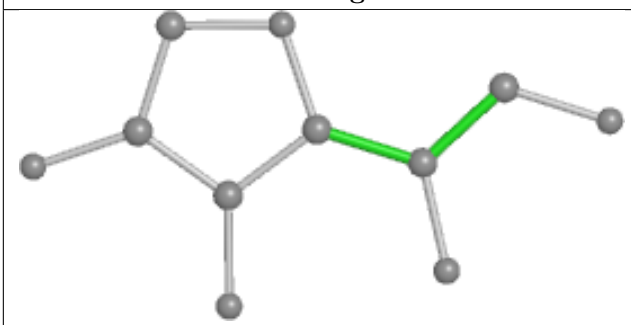
Ligand A1AIO A 2031



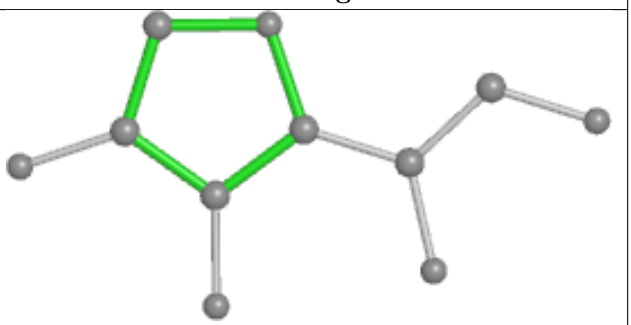
Bond lengths



Bond angles

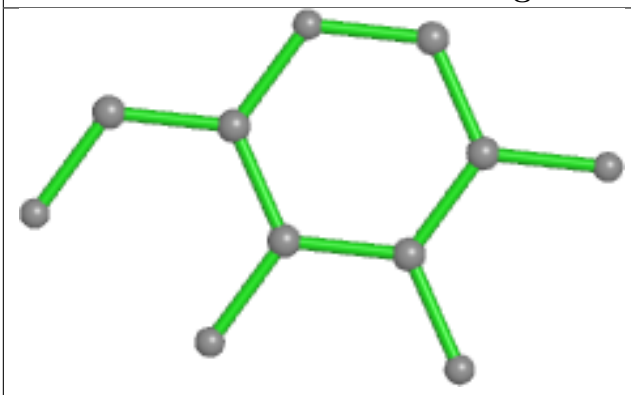


Torsions

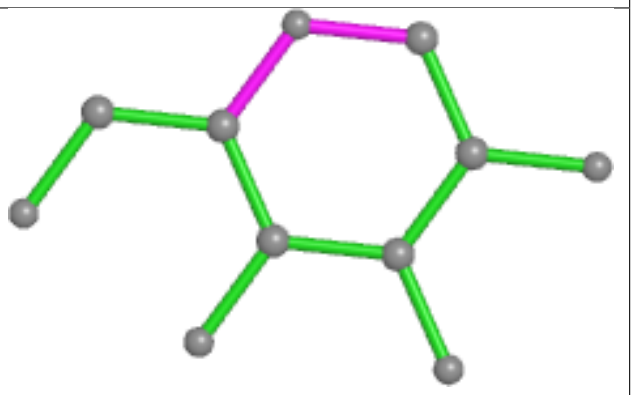


Rings

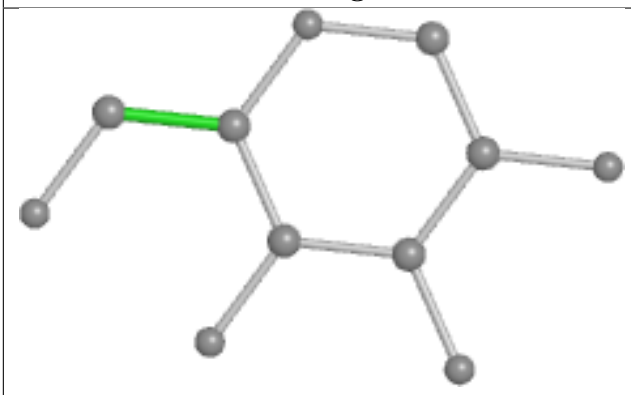
Ligand GLA A 2060



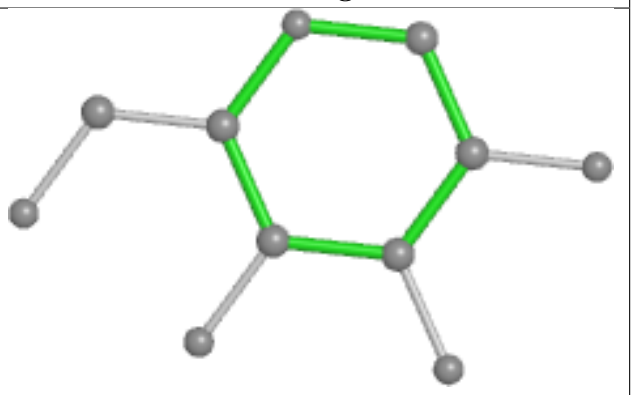
Bond lengths



Bond angles

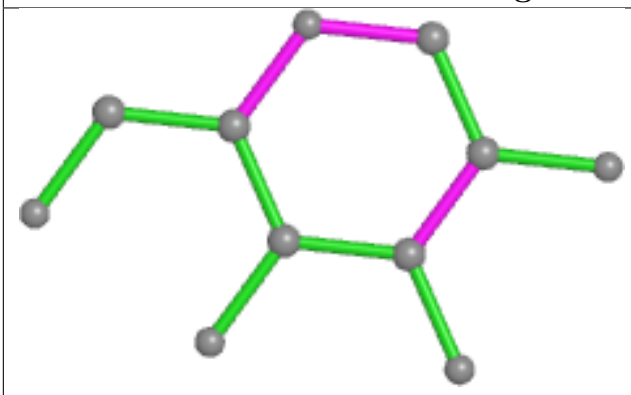


Torsions

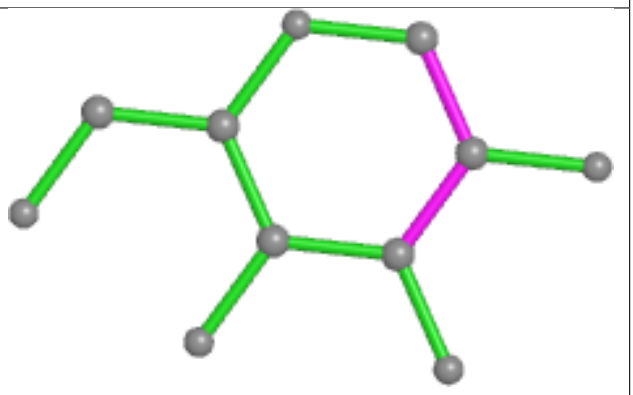


Rings

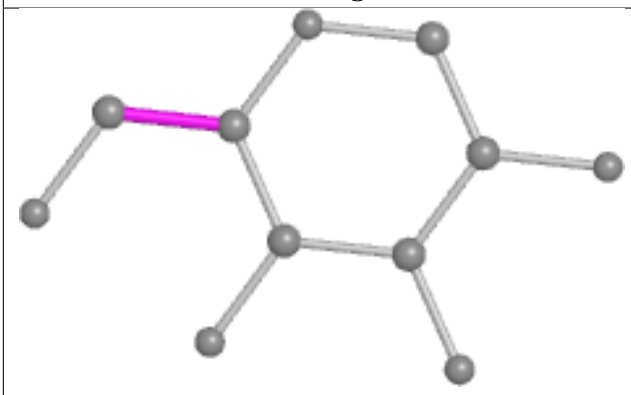
Ligand GLA B 2063



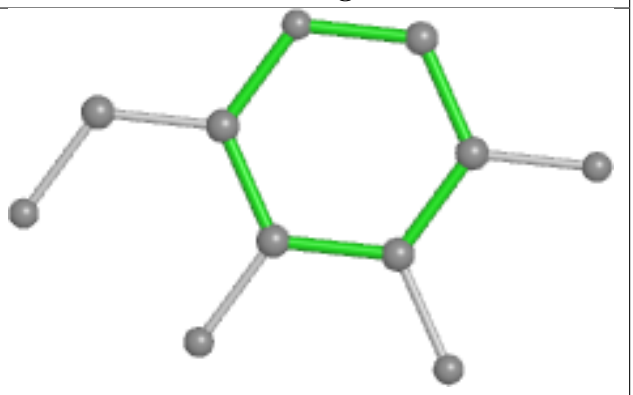
Bond lengths



Bond angles

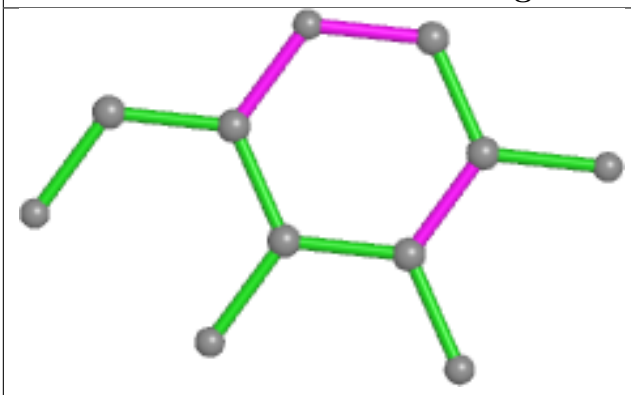


Torsions

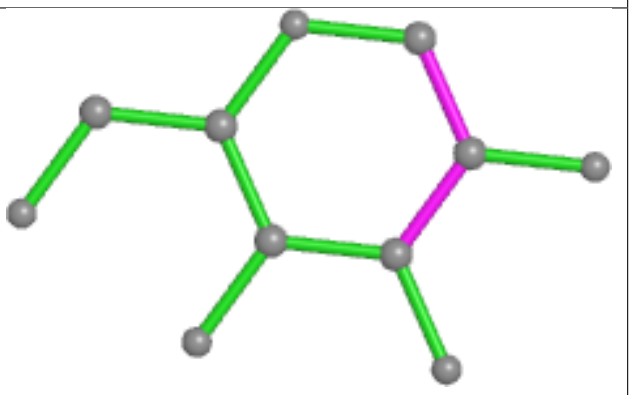


Rings

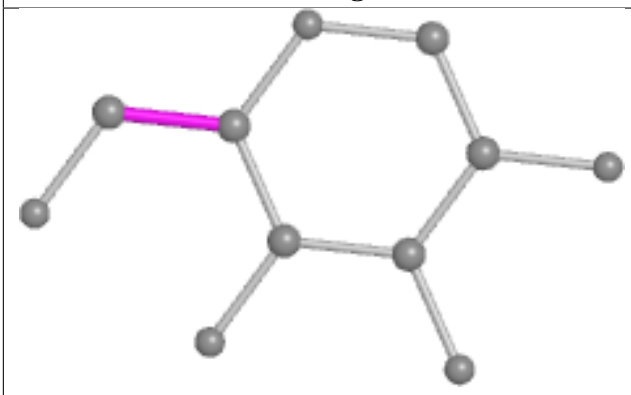
Ligand GLA B 2067



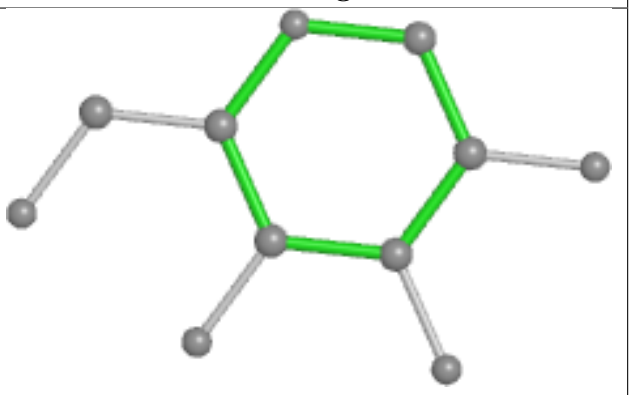
Bond lengths



Bond angles

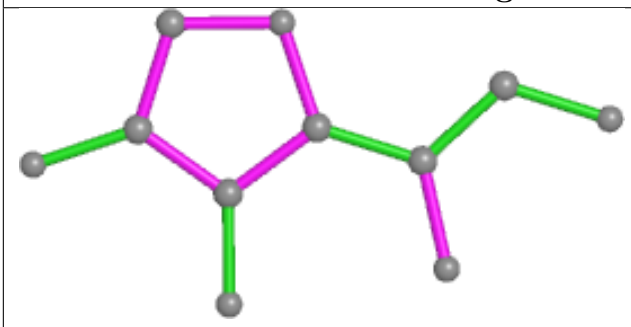


Torsions

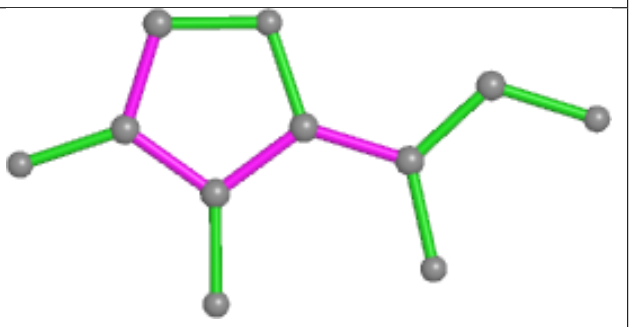


Rings

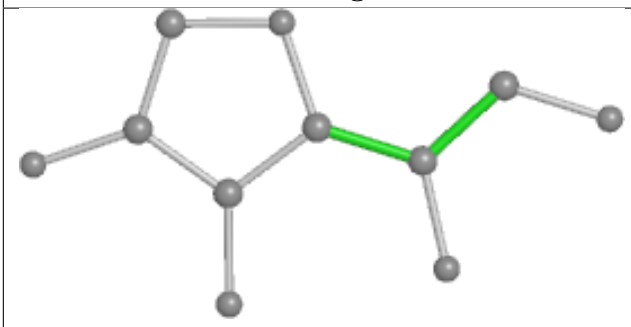
Ligand A1AIO A 2008



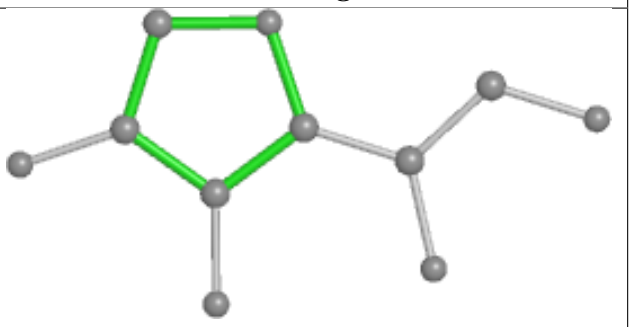
Bond lengths



Bond angles

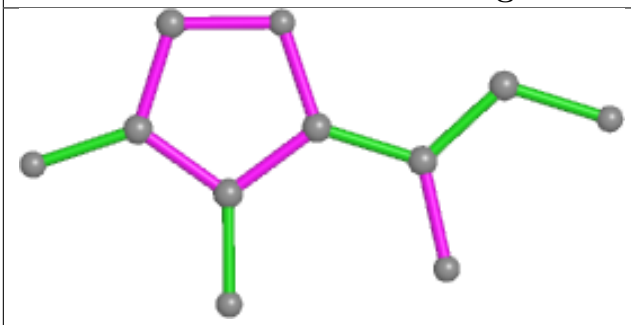


Torsions

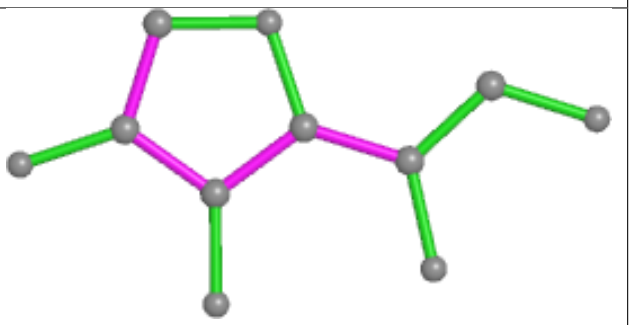


Rings

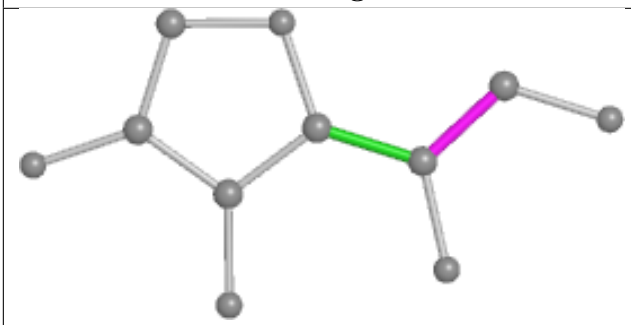
Ligand A1AIO B 2046



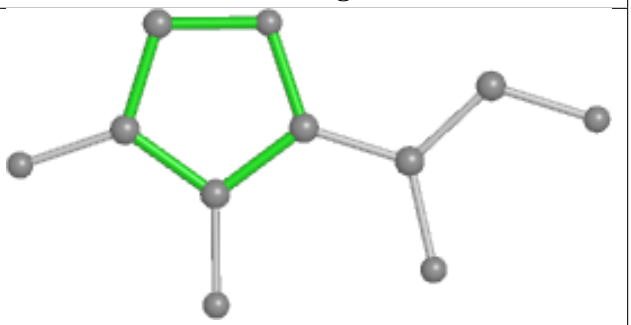
Bond lengths



Bond angles

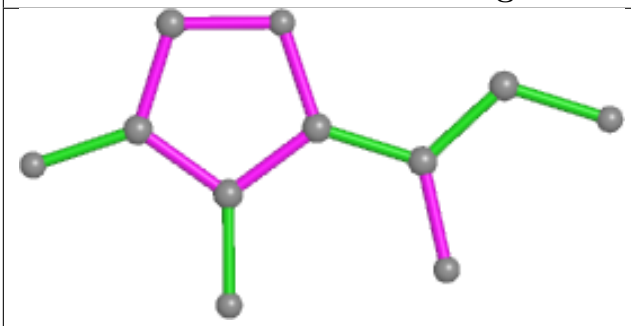


Torsions

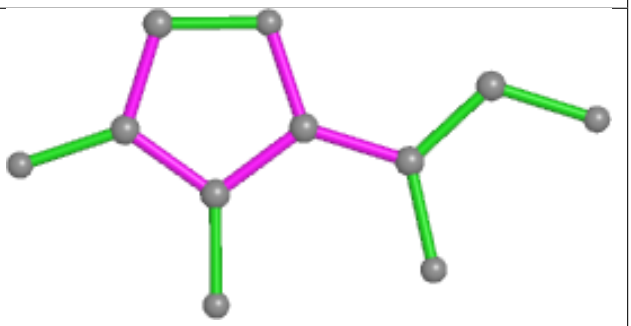


Rings

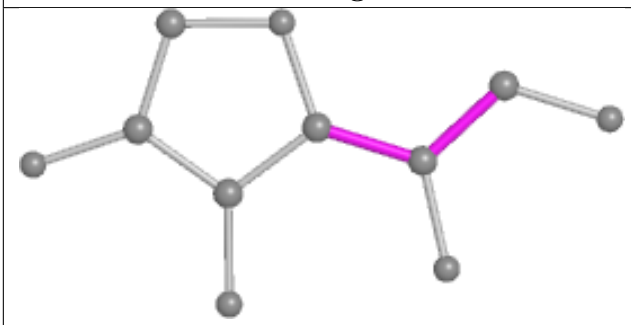
Ligand A1AIO B 2005



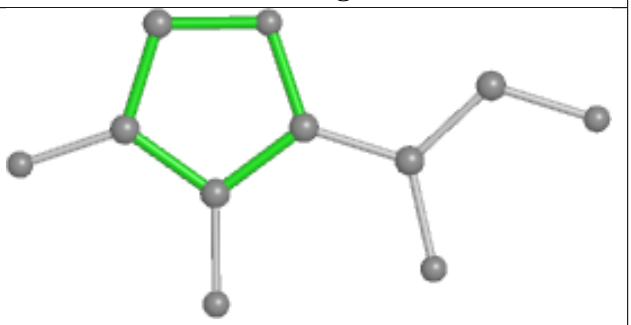
Bond lengths



Bond angles

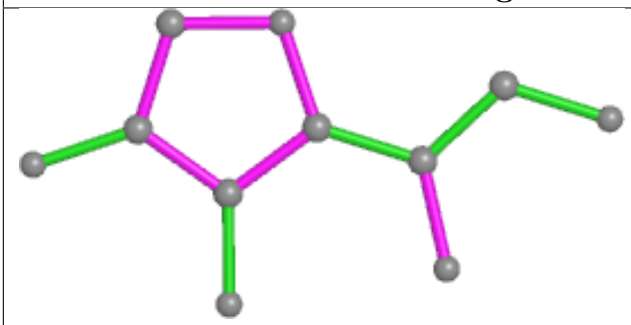


Torsions

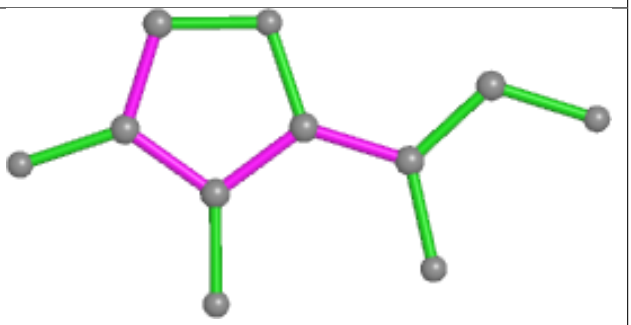


Rings

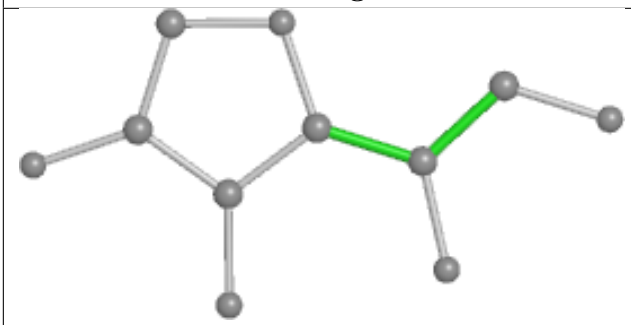
Ligand A1AIO A 2025



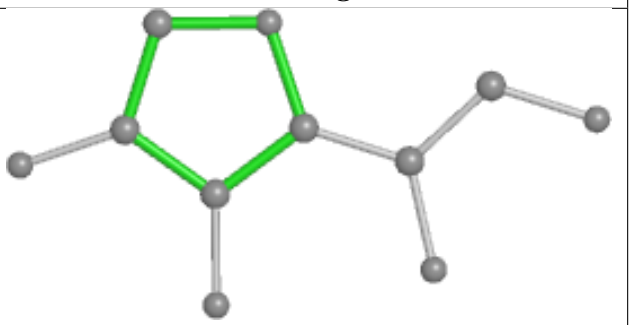
Bond lengths



Bond angles

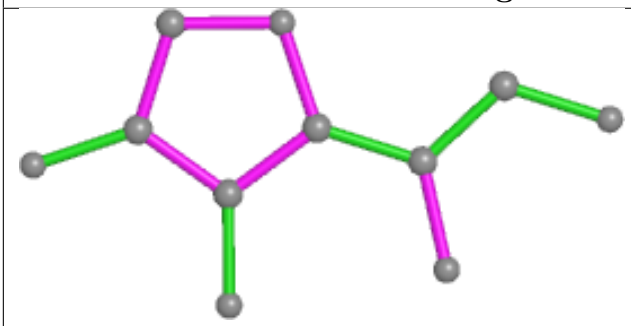


Torsions

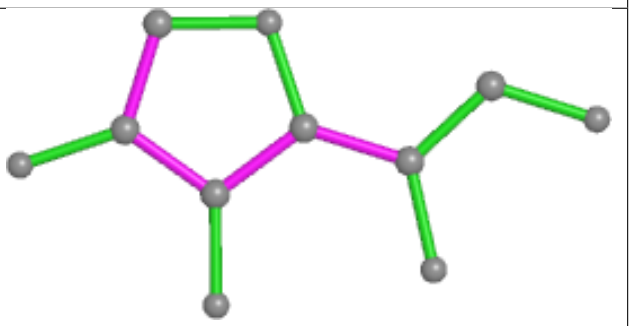


Rings

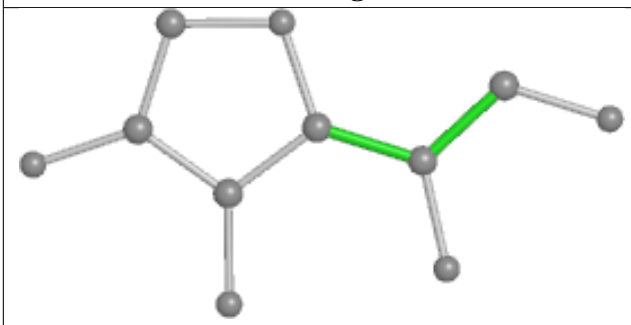
Ligand A1AIO A 2057



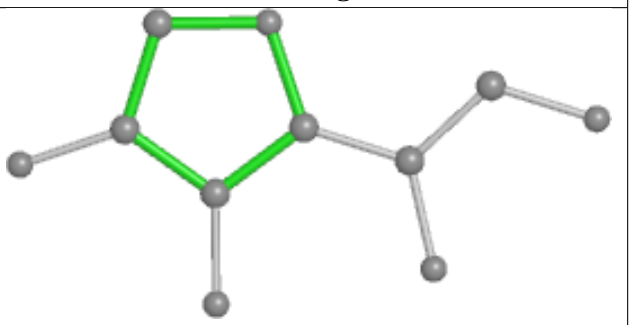
Bond lengths



Bond angles

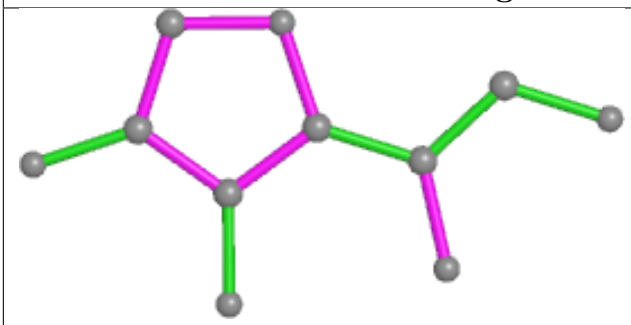


Torsions

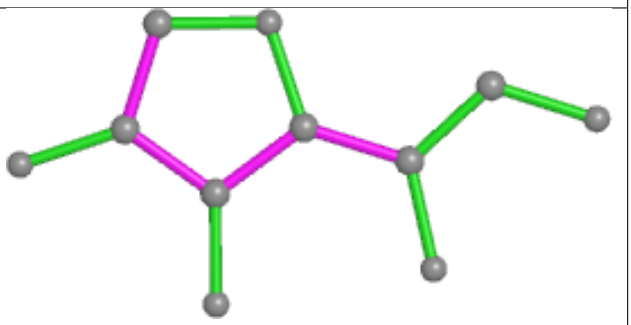


Rings

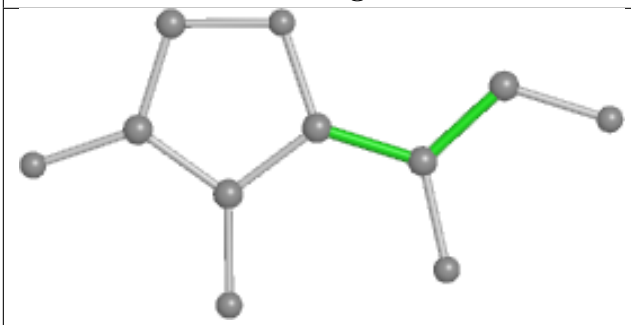
Ligand A1AIO A 2055



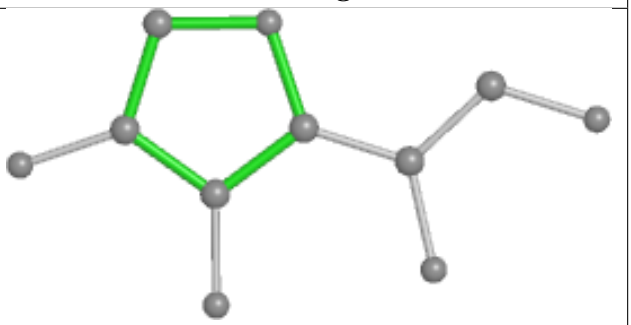
Bond lengths



Bond angles

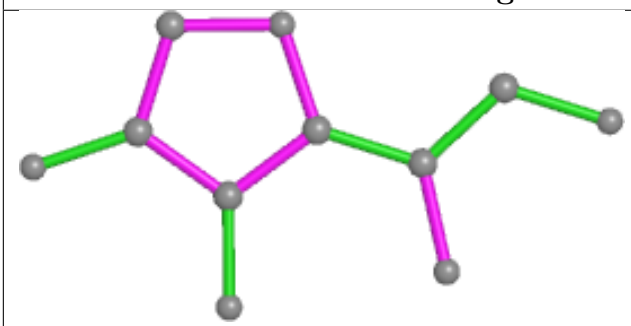


Torsions

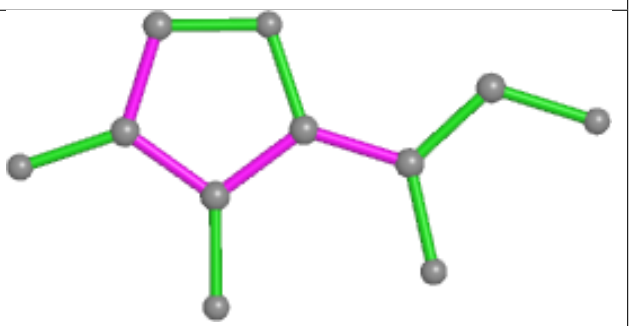


Rings

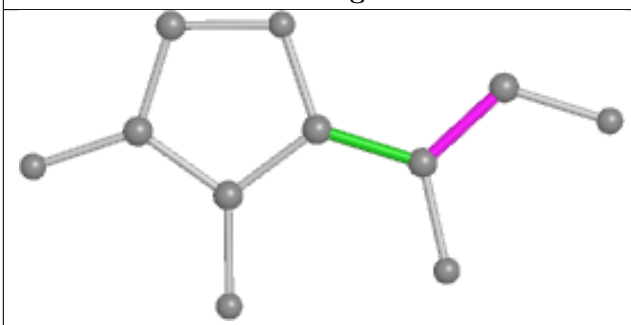
Ligand A1AIO B 2007



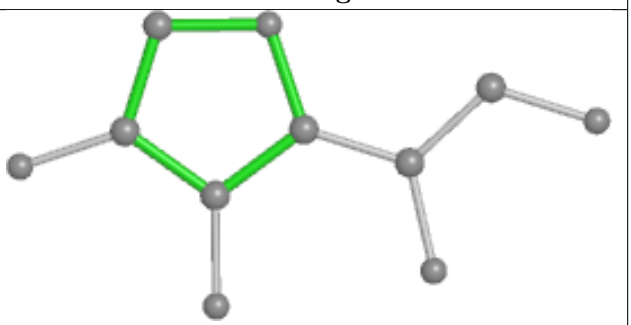
Bond lengths



Bond angles

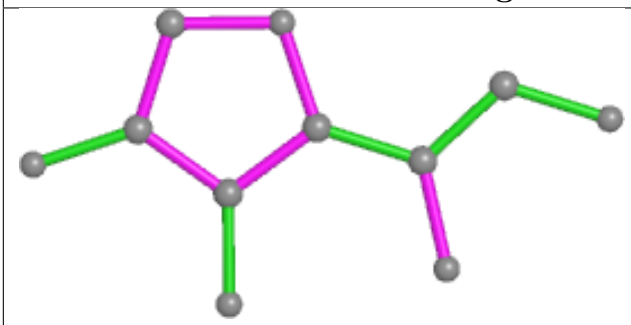


Torsions

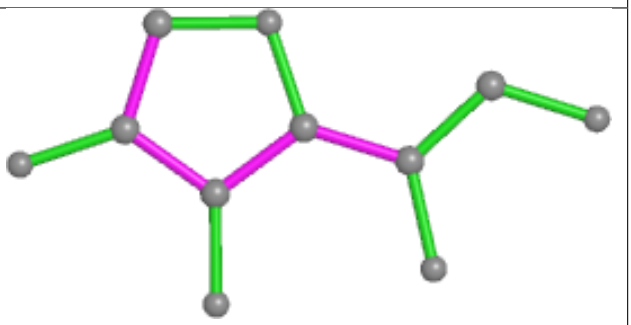


Rings

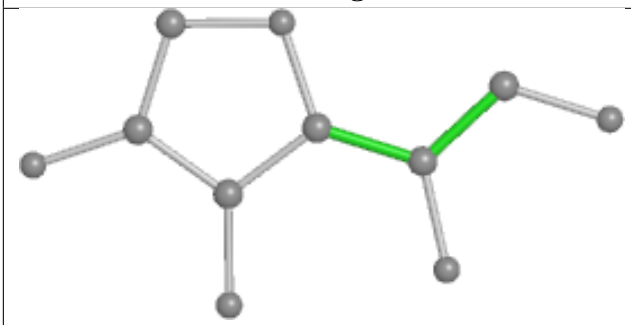
Ligand A1AIO A 2023



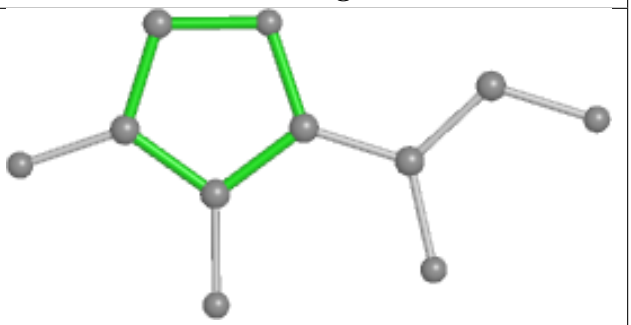
Bond lengths



Bond angles

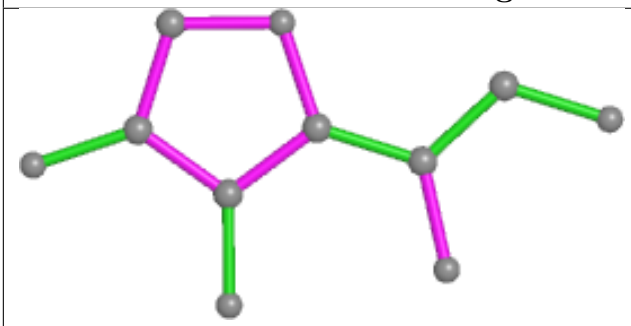


Torsions

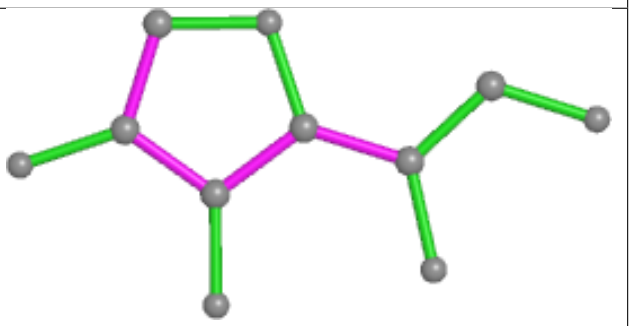


Rings

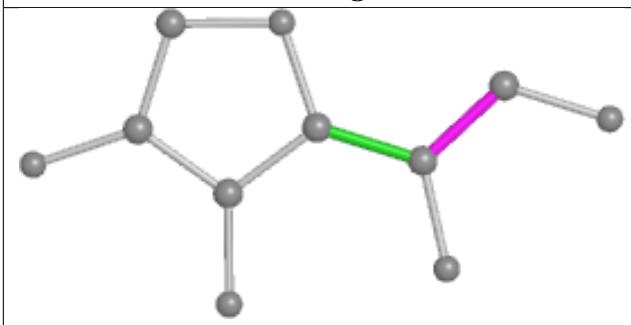
Ligand A1AIO A 2001



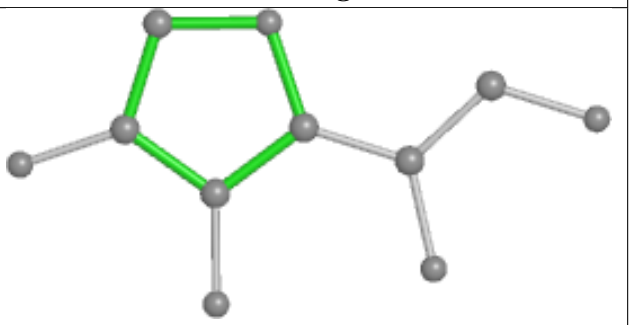
Bond lengths



Bond angles

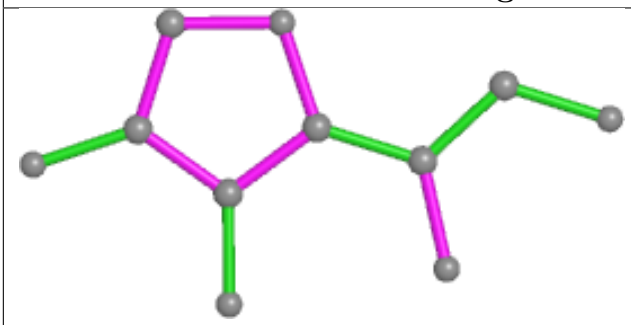


Torsions

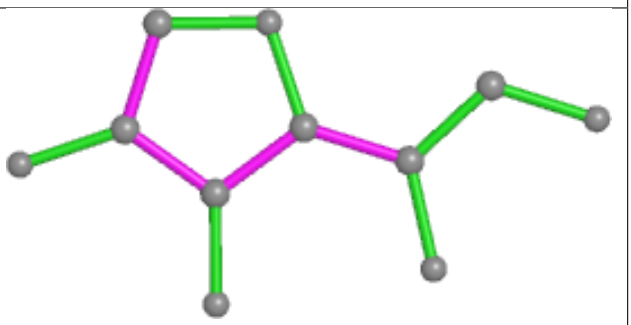


Rings

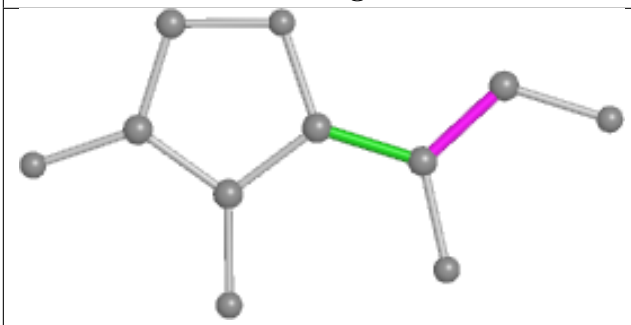
Ligand A1AIO B 2013



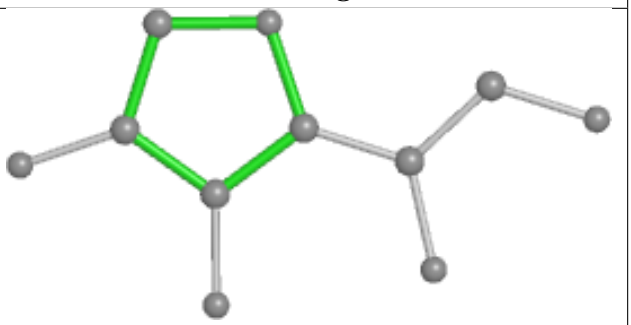
Bond lengths



Bond angles

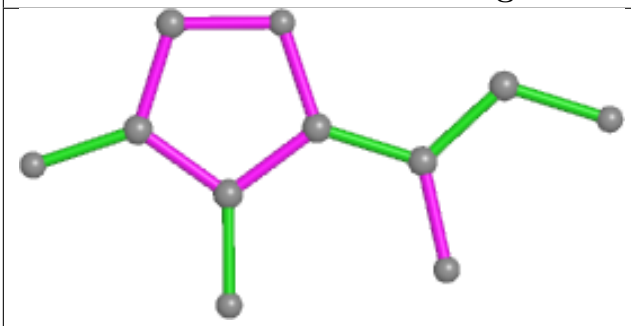


Torsions

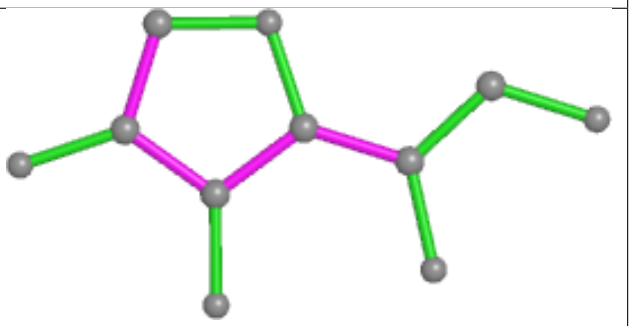


Rings

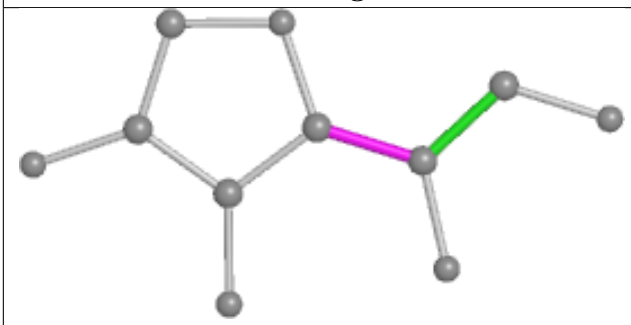
Ligand A1AIO B 2014



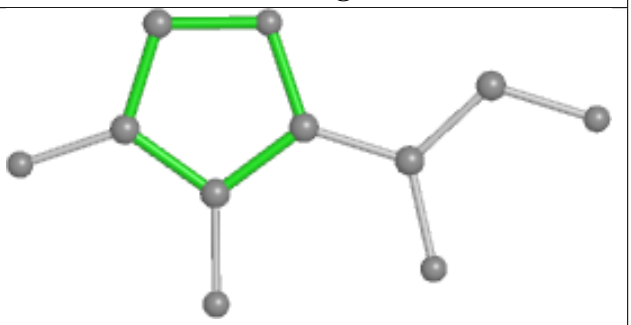
Bond lengths



Bond angles

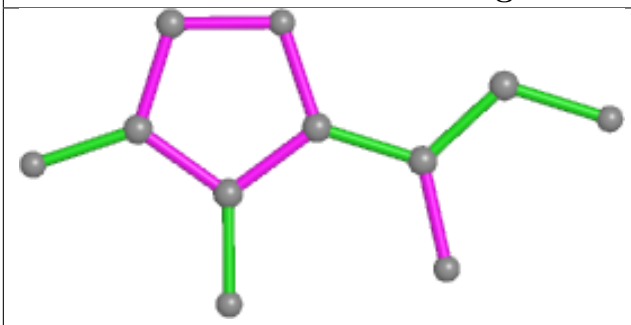


Torsions

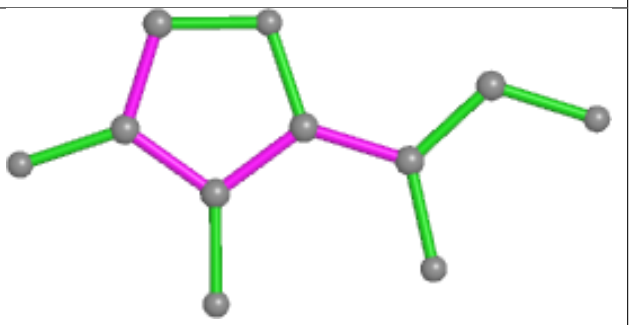


Rings

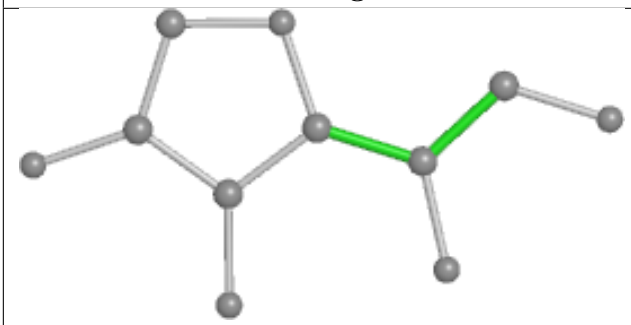
Ligand A1AIO A 2003



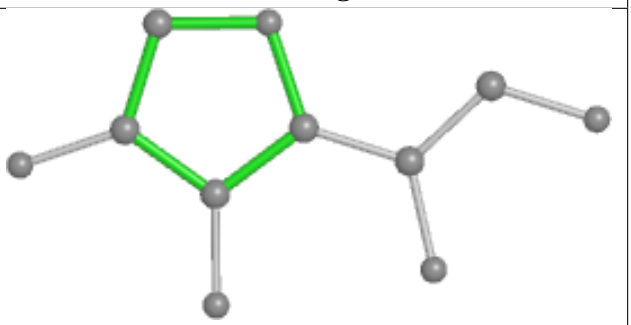
Bond lengths



Bond angles

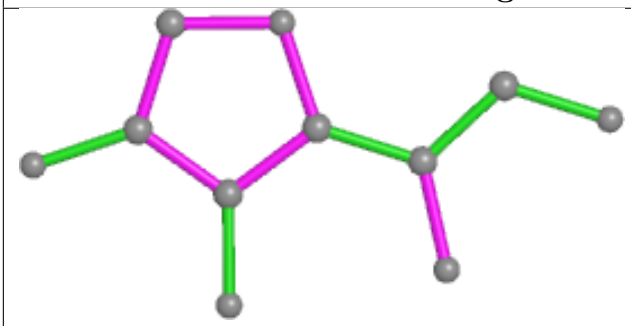


Torsions

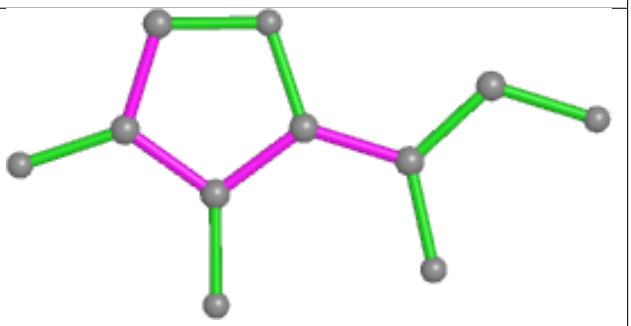


Rings

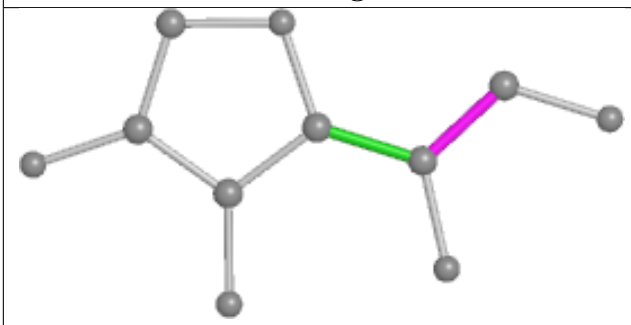
Ligand A1AIO B 2044



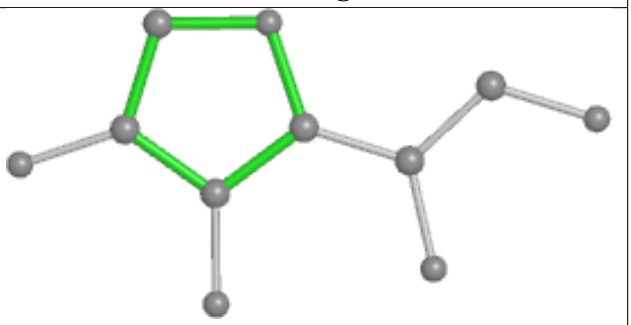
Bond lengths



Bond angles

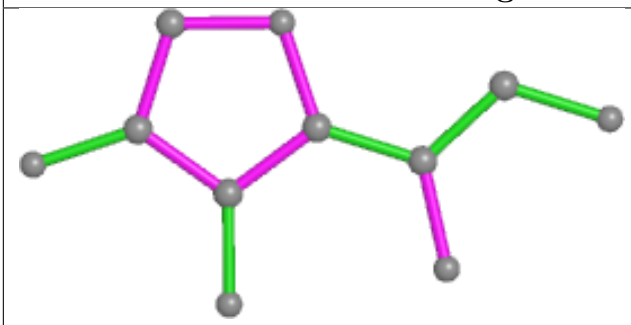


Torsions

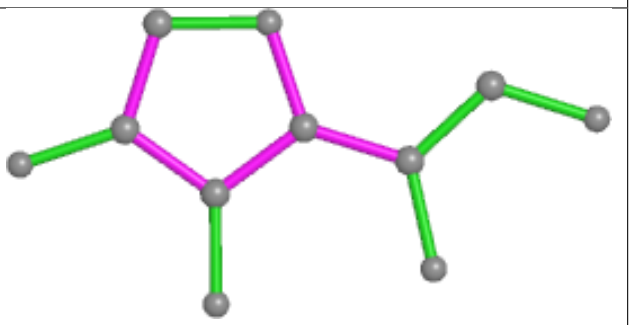


Rings

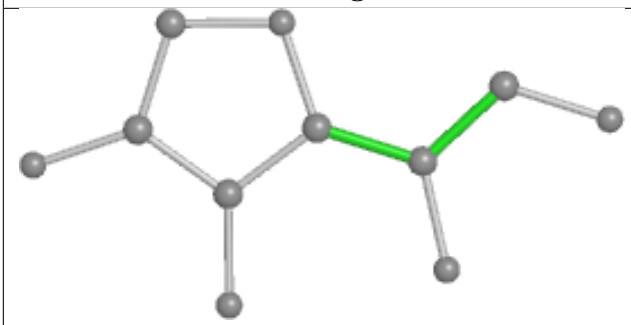
Ligand A1AIO B 2026



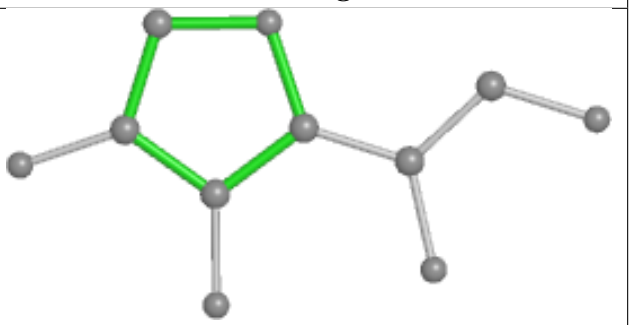
Bond lengths



Bond angles

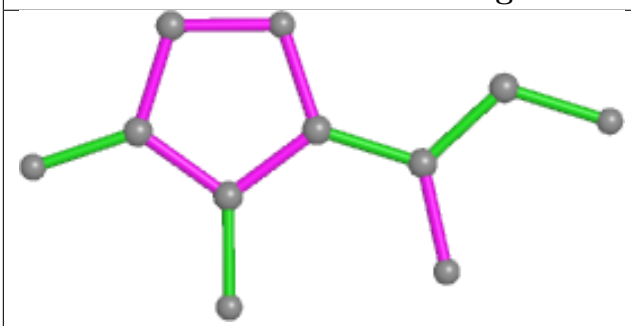


Torsions

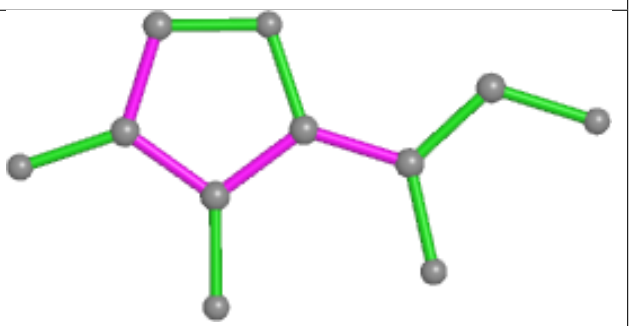


Rings

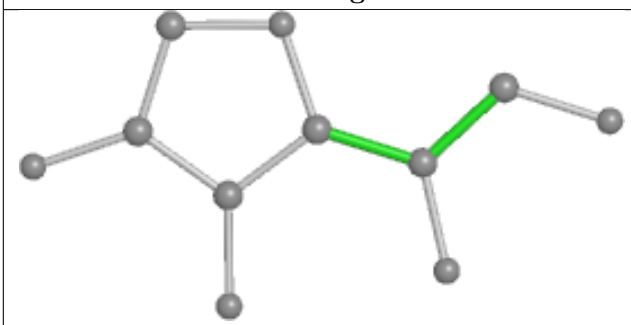
Ligand A1AIO A 2056



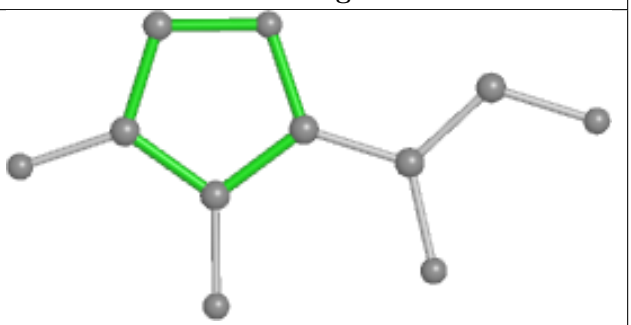
Bond lengths



Bond angles

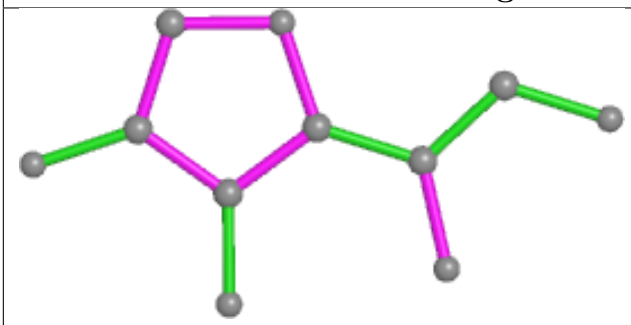


Torsions

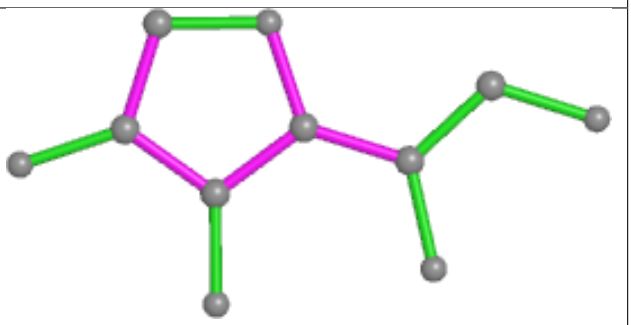


Rings

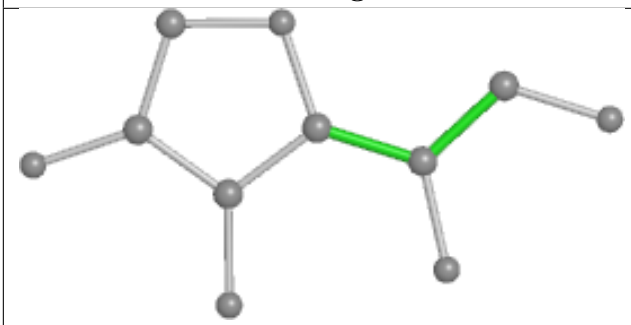
Ligand A1AIO B 2047



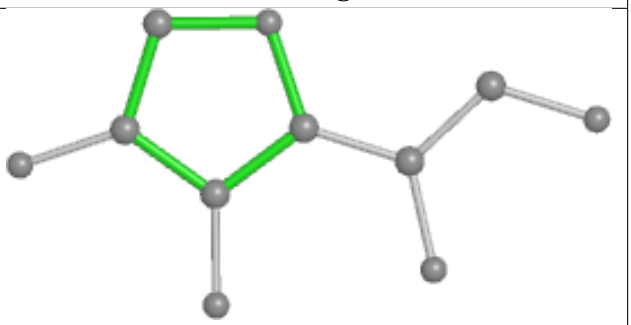
Bond lengths



Bond angles

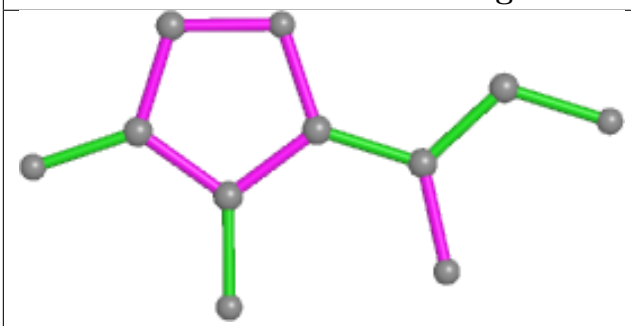


Torsions

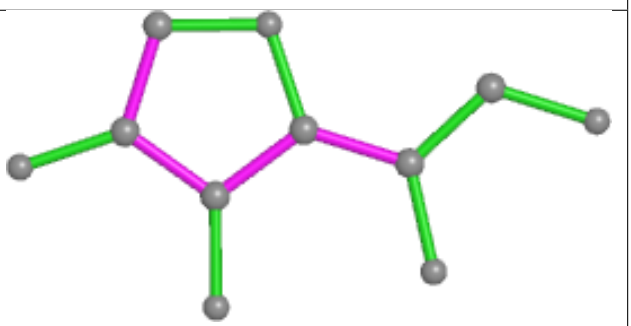


Rings

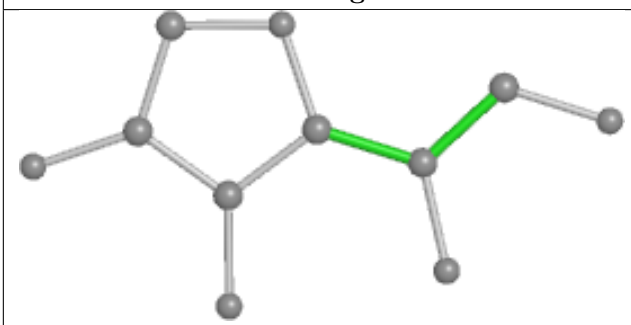
Ligand A1AIO A 2011



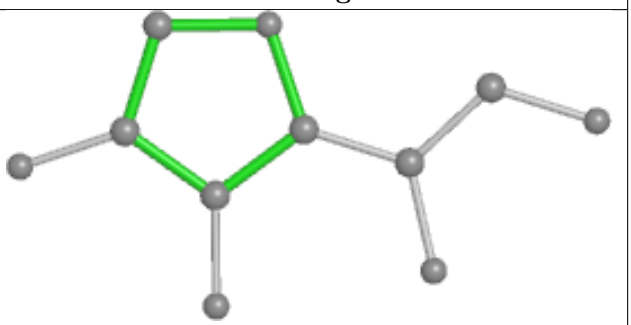
Bond lengths



Bond angles

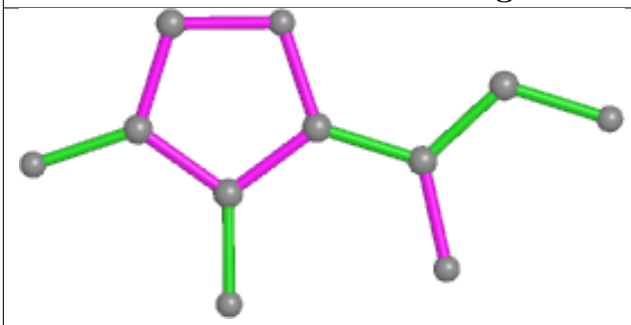


Torsions

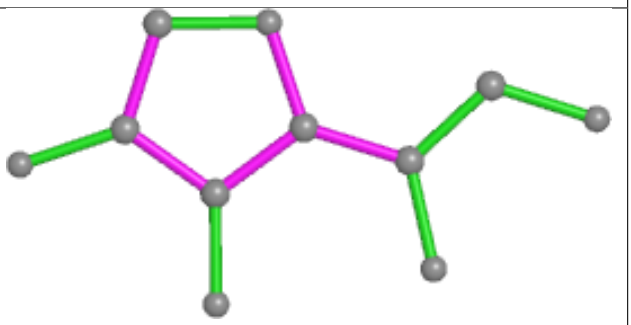


Rings

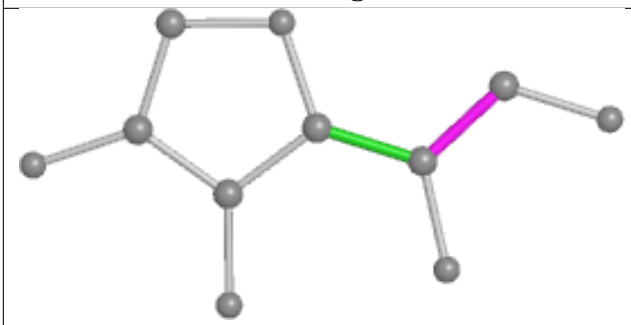
Ligand A1AIO A 2044



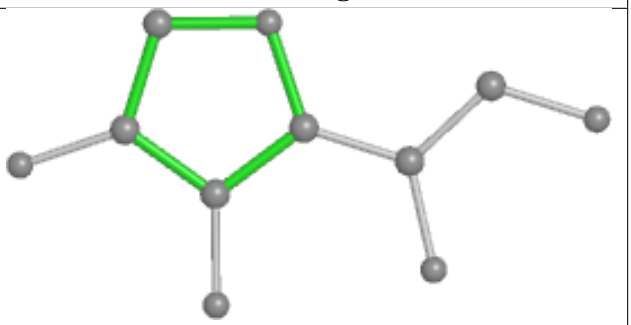
Bond lengths



Bond angles

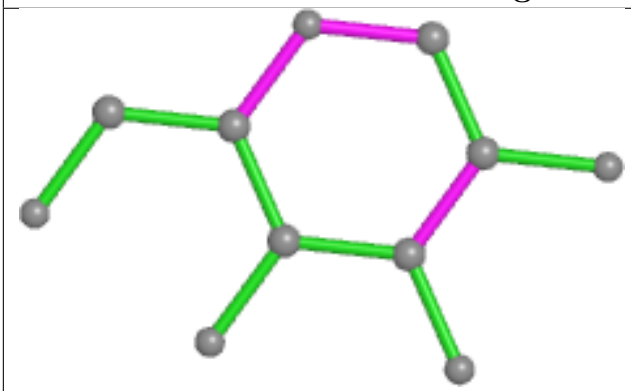


Torsions

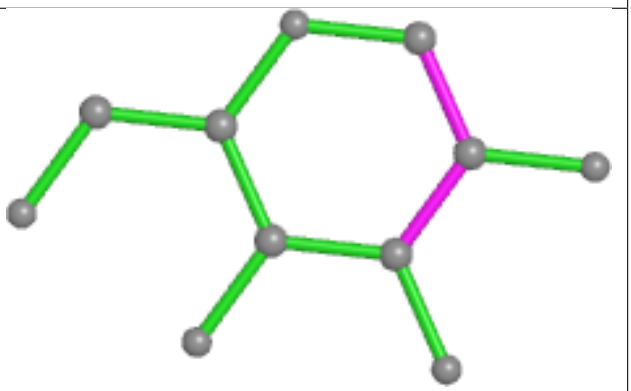


Rings

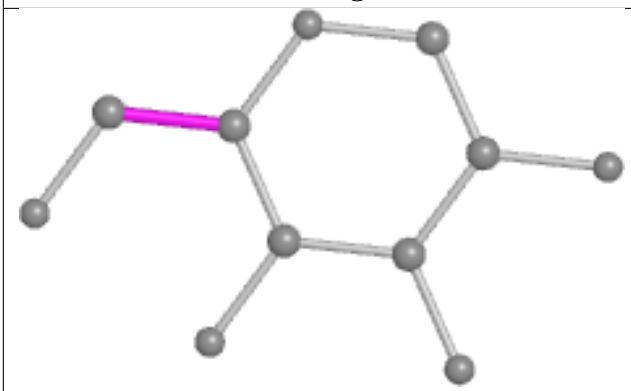
Ligand GLA A 2065



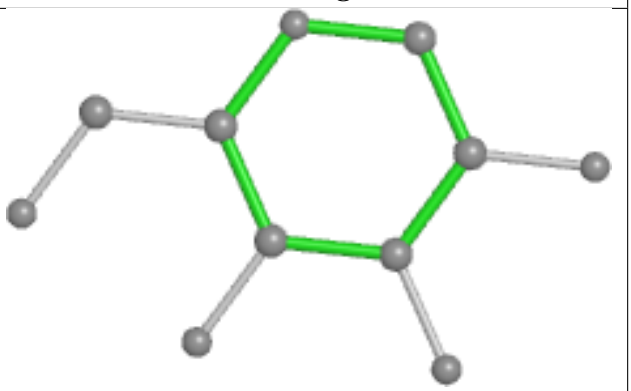
Bond lengths



Bond angles

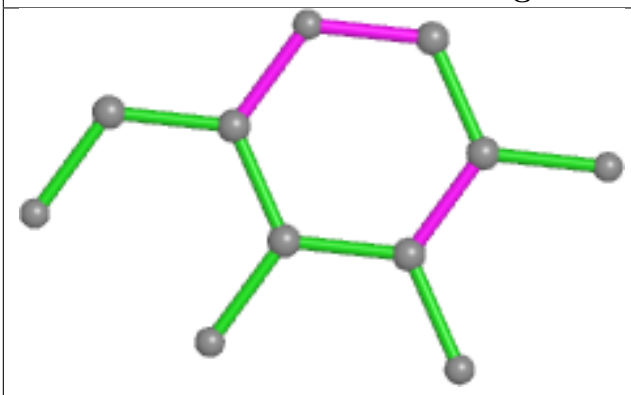


Torsions

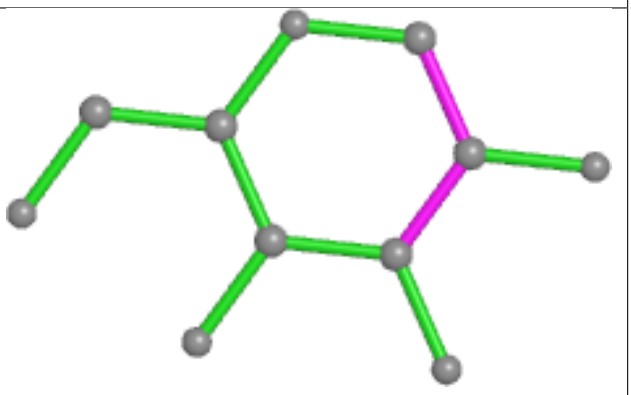


Rings

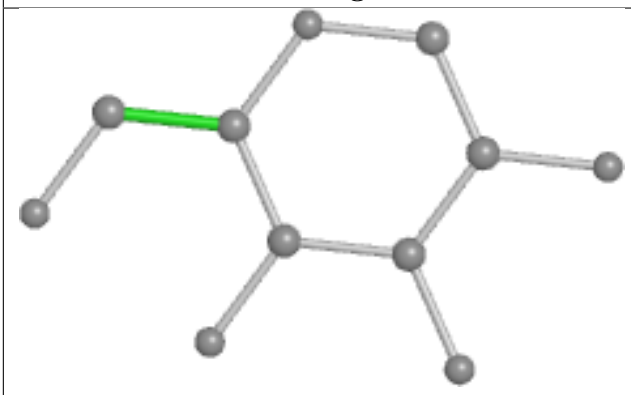
Ligand GLA A 2067



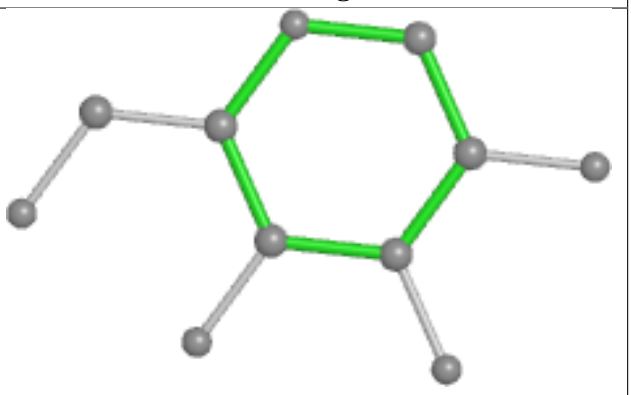
Bond lengths



Bond angles

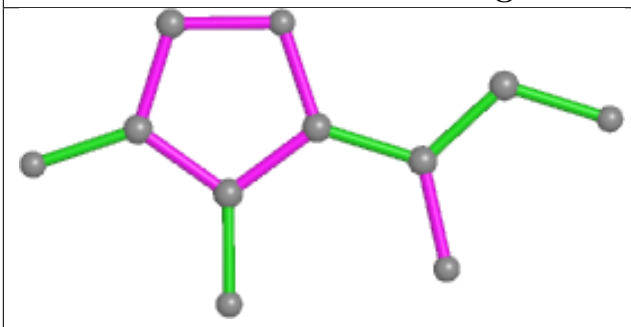


Torsions

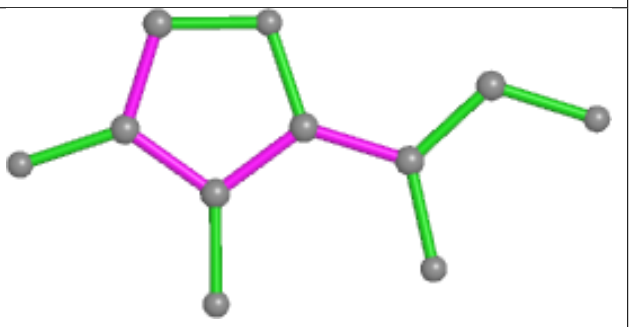


Rings

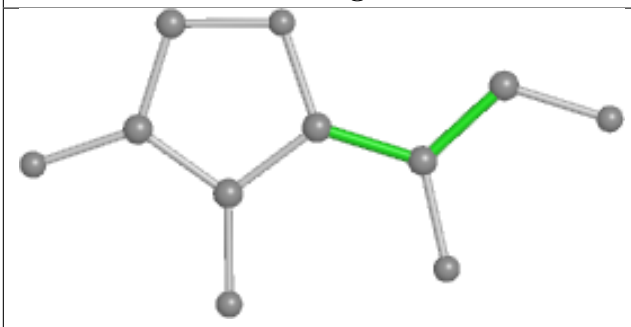
Ligand A1AIO A 2024



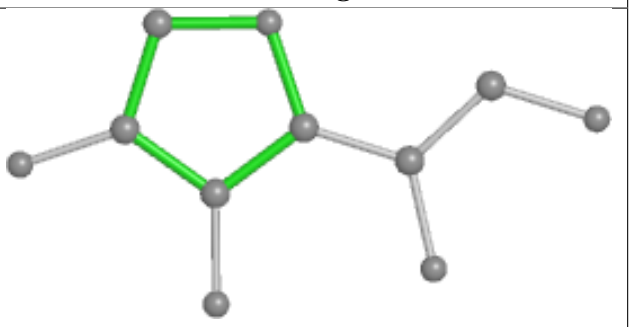
Bond lengths



Bond angles

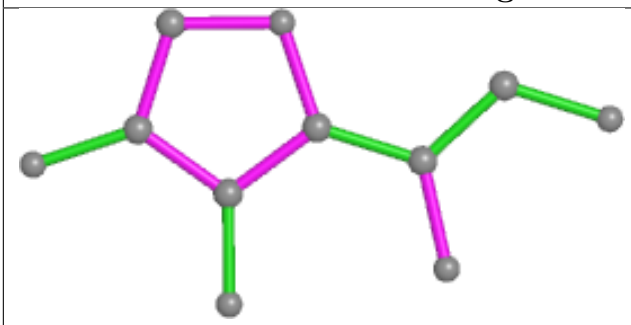


Torsions

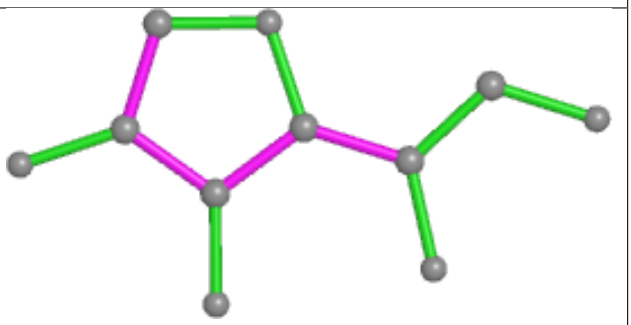


Rings

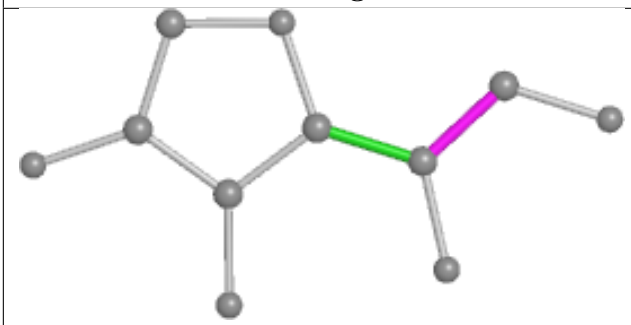
Ligand A1AIO B 2034



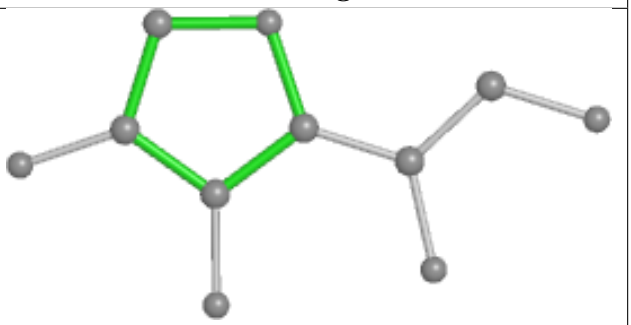
Bond lengths



Bond angles

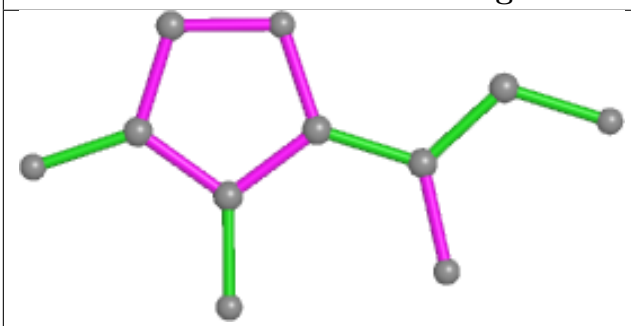


Torsions

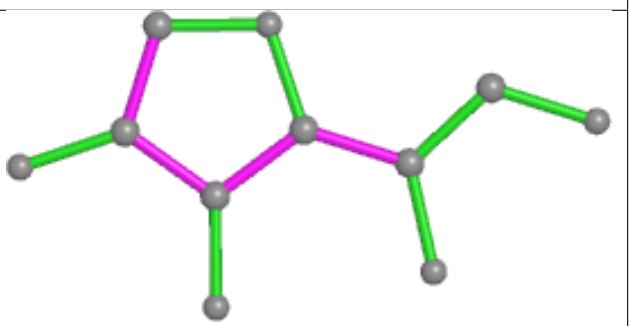


Rings

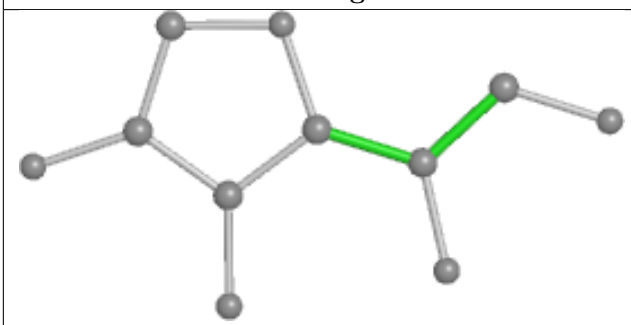
Ligand A1AIO A 2019



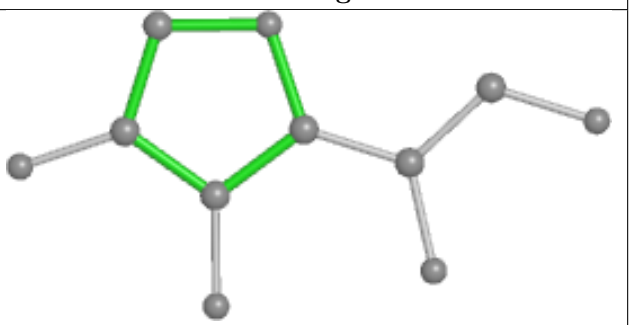
Bond lengths



Bond angles

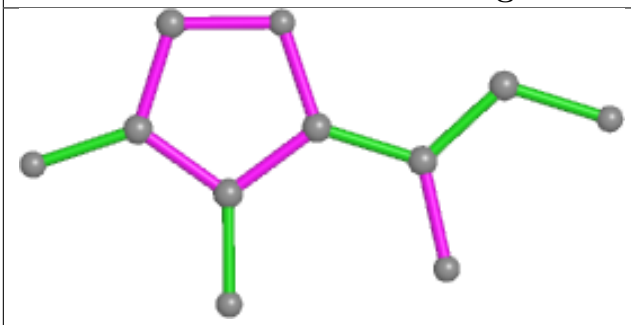


Torsions

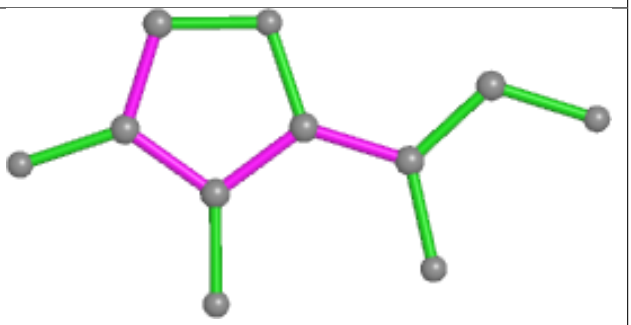


Rings

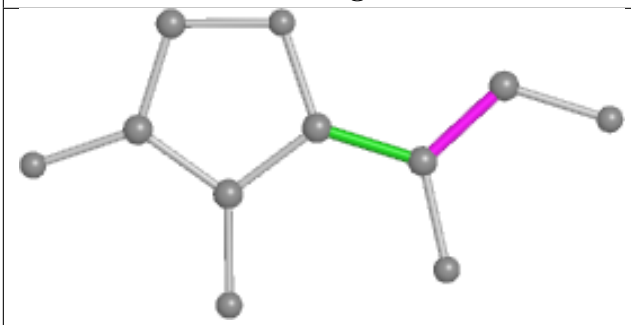
Ligand A1AIO B 2043



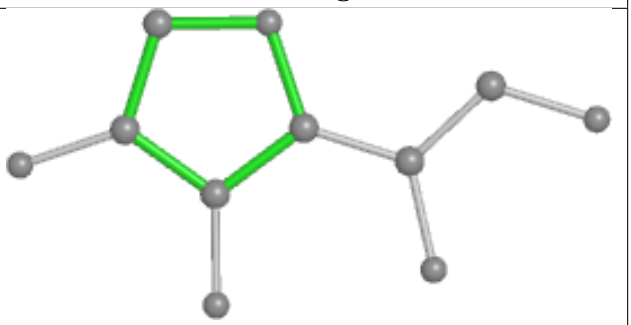
Bond lengths



Bond angles

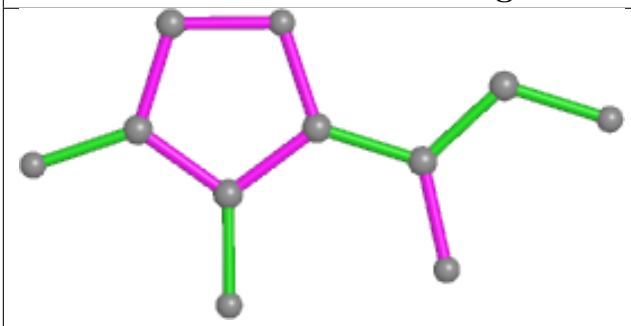


Torsions

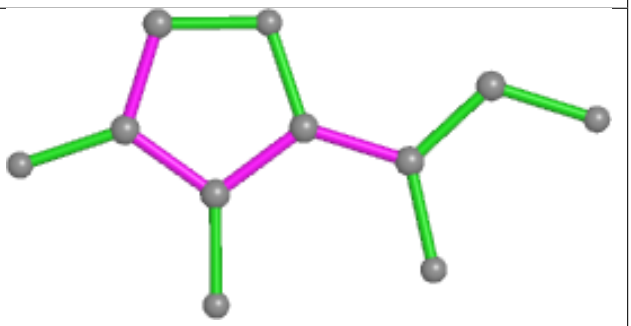


Rings

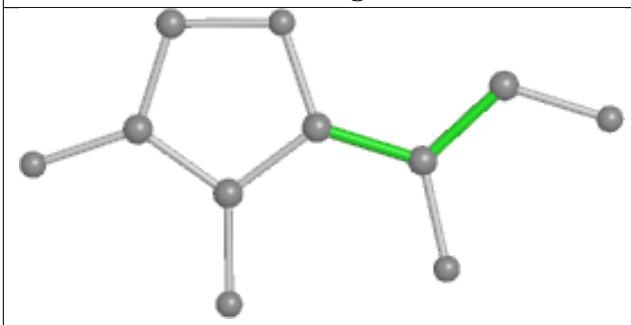
Ligand A1AIO A 2007



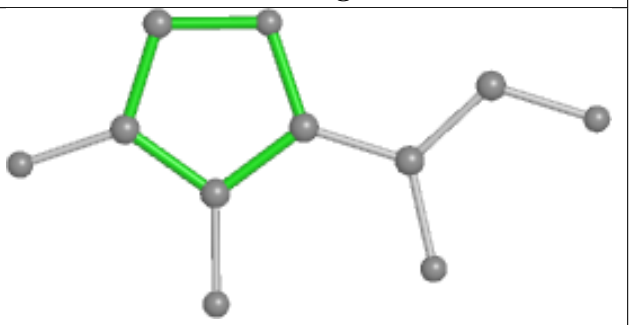
Bond lengths



Bond angles

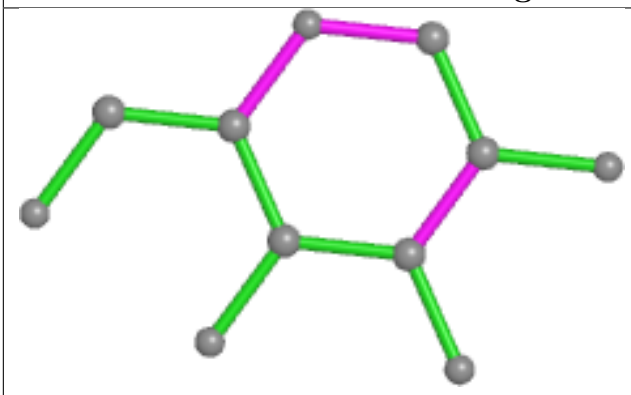


Torsions

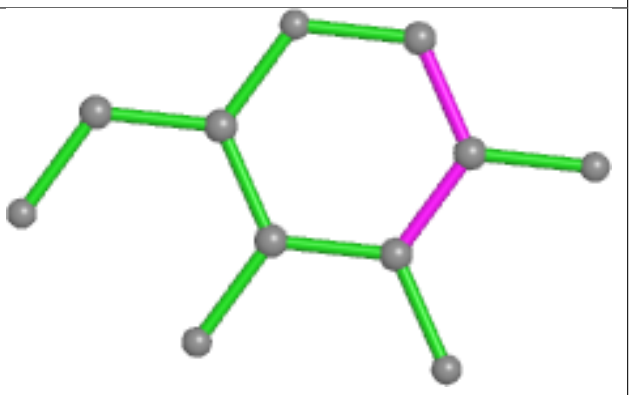


Rings

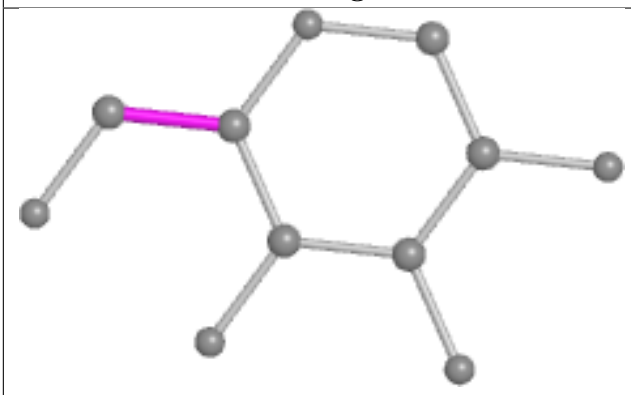
Ligand GLA B 2058



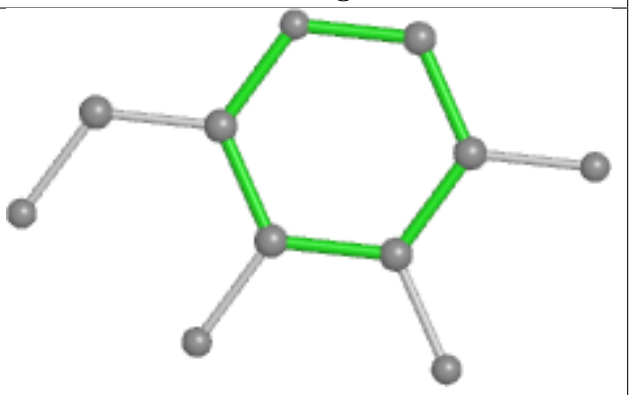
Bond lengths



Bond angles

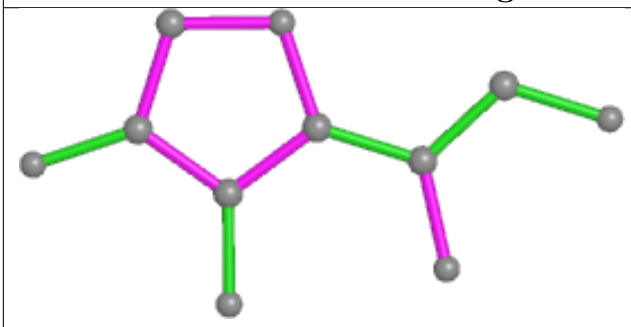


Torsions

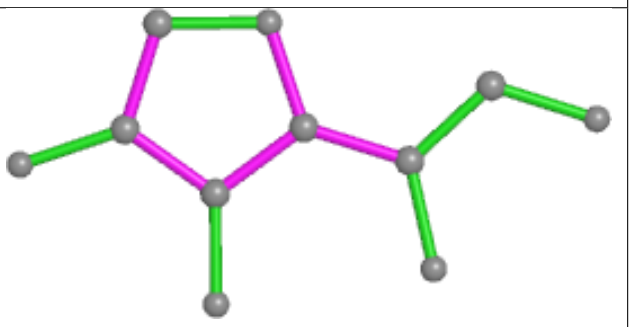


Rings

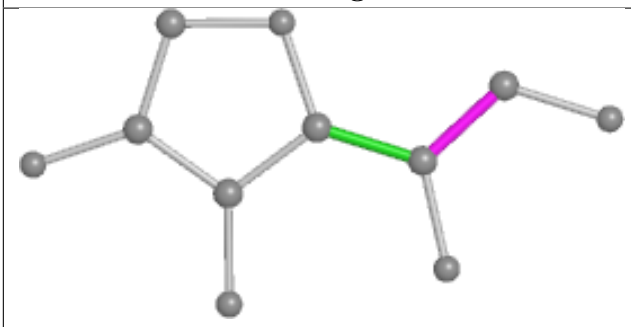
Ligand A1AIO B 2041



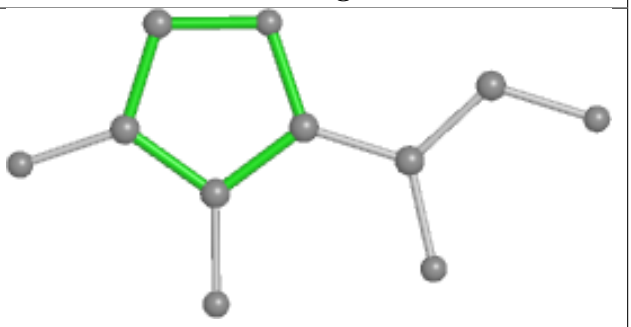
Bond lengths



Bond angles

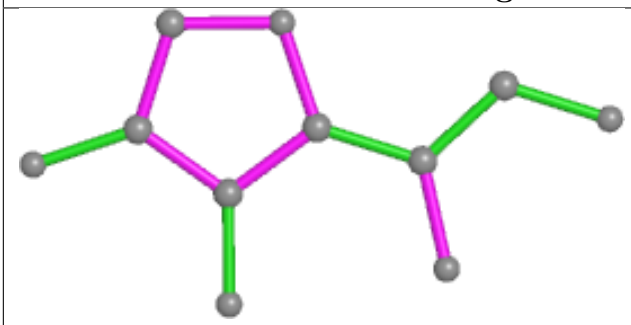


Torsions

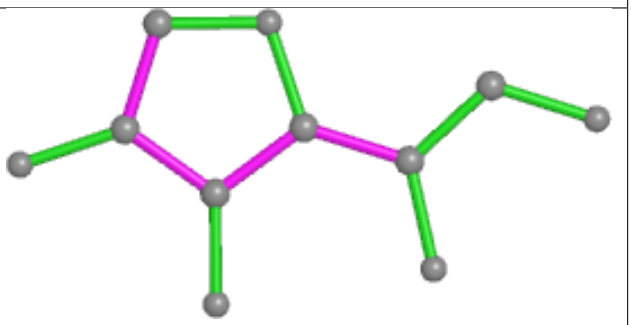


Rings

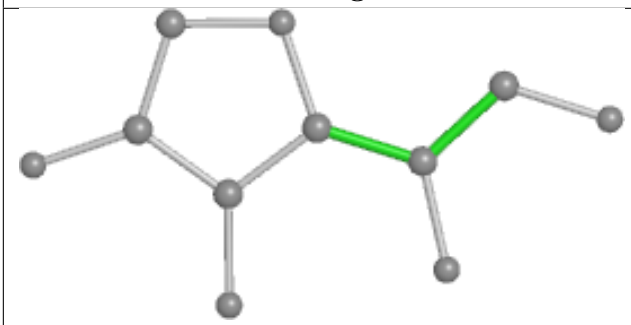
Ligand A1AIO A 2036



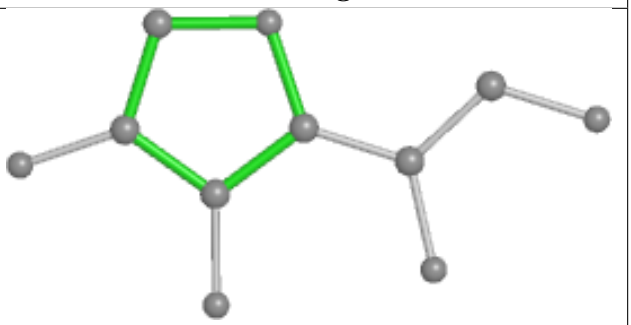
Bond lengths



Bond angles

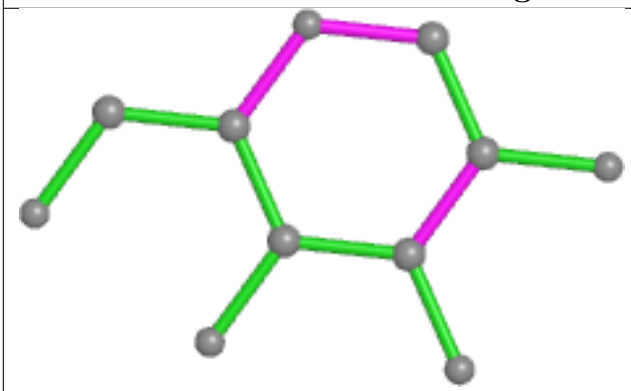


Torsions

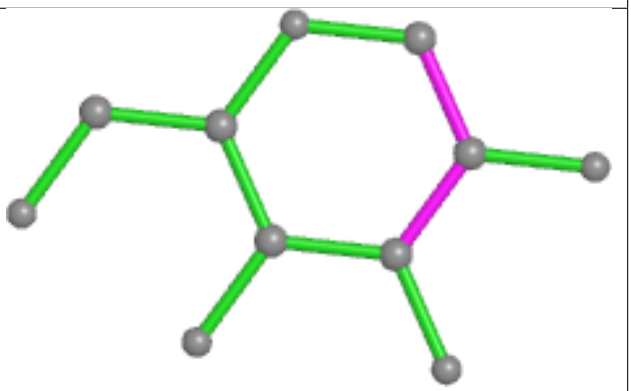


Rings

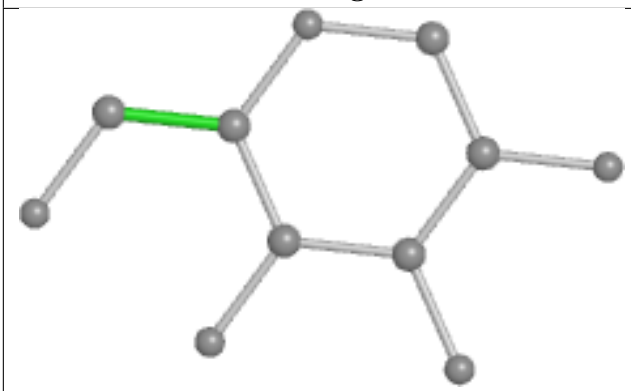
Ligand GLA A 2061



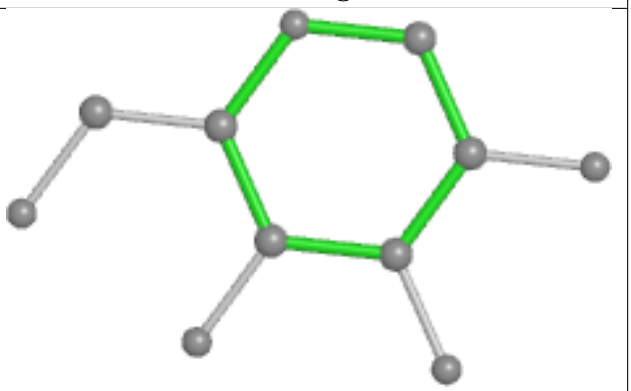
Bond lengths



Bond angles

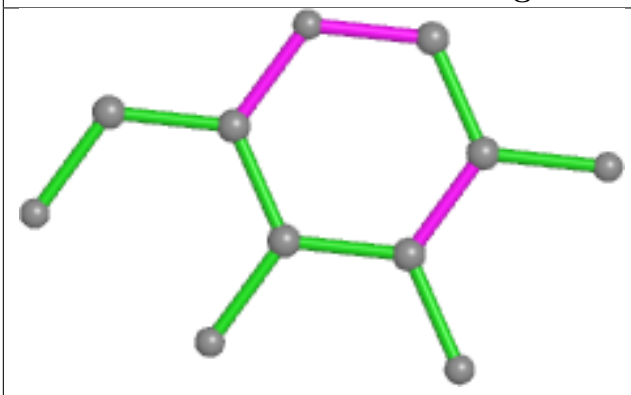


Torsions

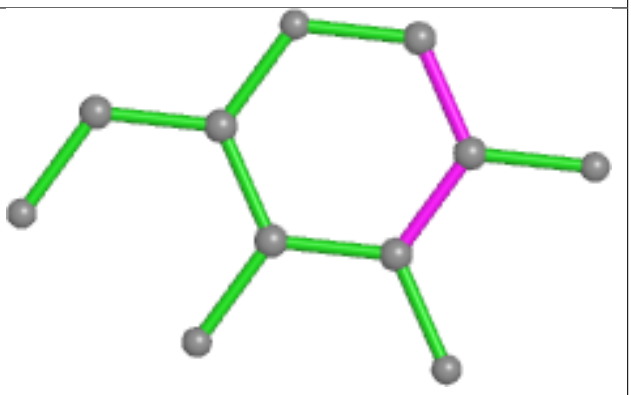


Rings

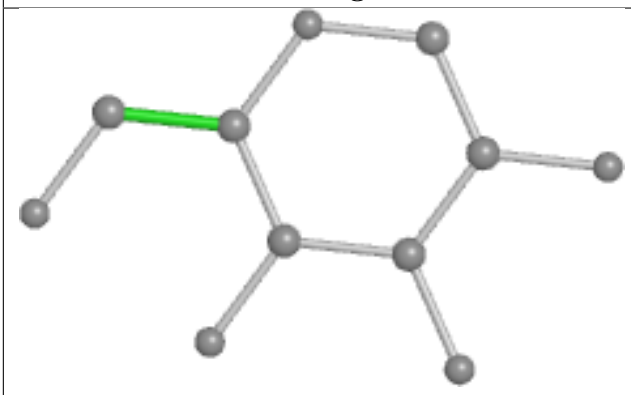
Ligand GLA A 2062



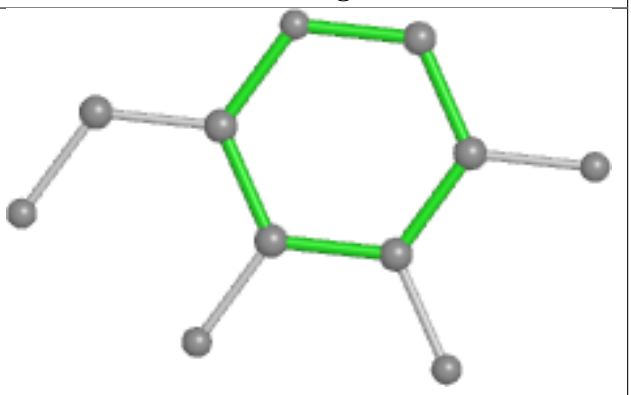
Bond lengths



Bond angles

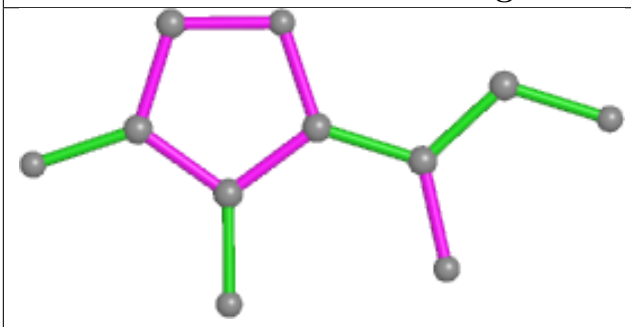


Torsions

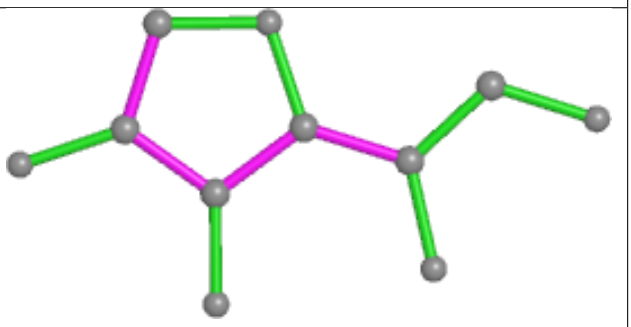


Rings

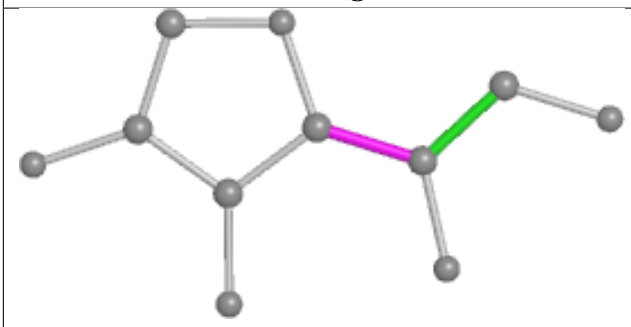
Ligand A1AIO A 2020



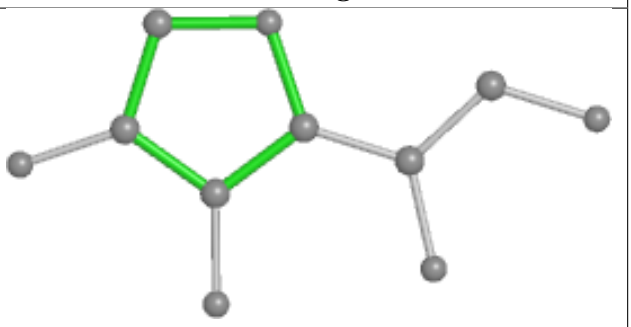
Bond lengths



Bond angles

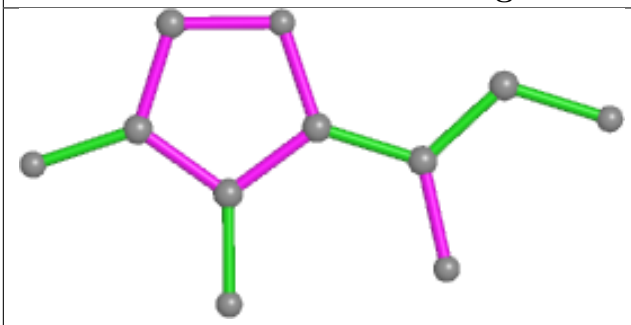


Torsions

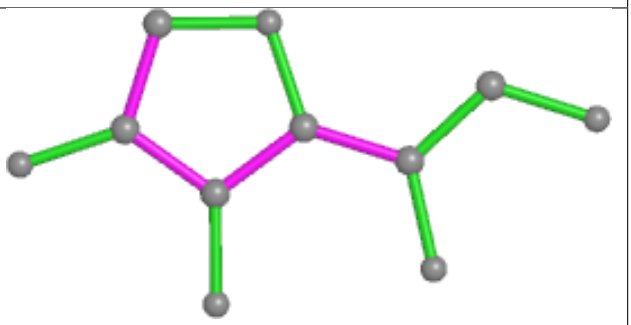


Rings

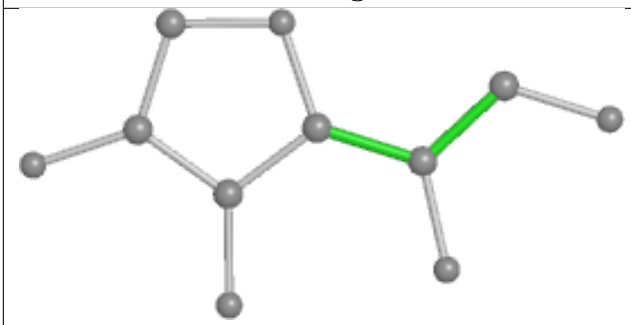
Ligand A1AIO A 2050



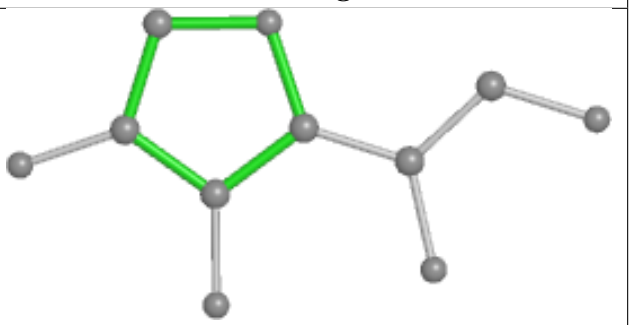
Bond lengths



Bond angles

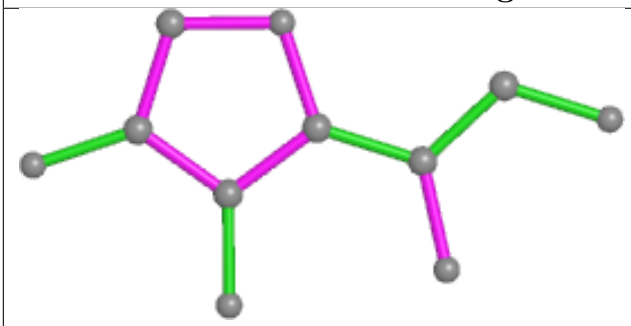


Torsions

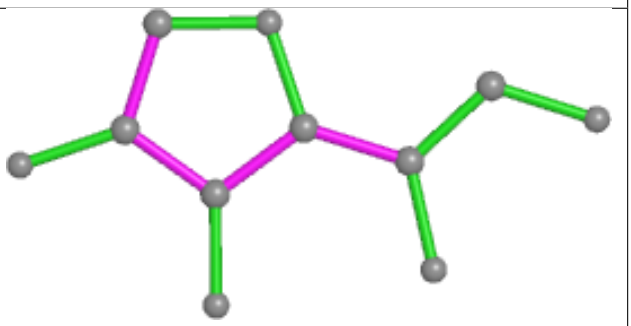


Rings

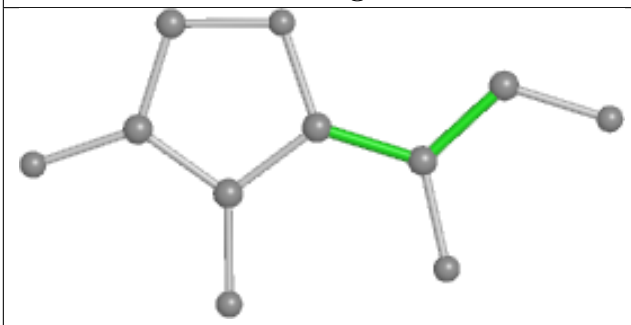
Ligand A1AIO B 2057



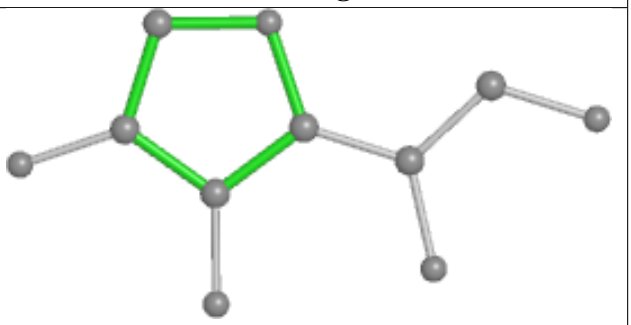
Bond lengths



Bond angles

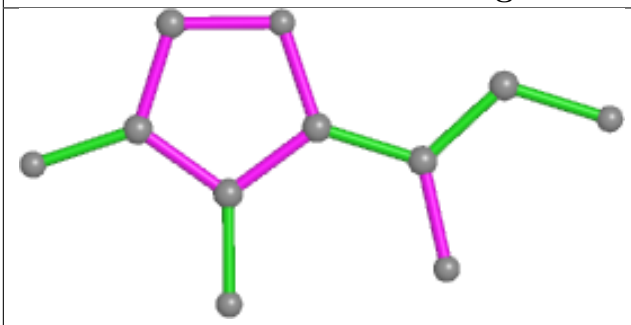


Torsions

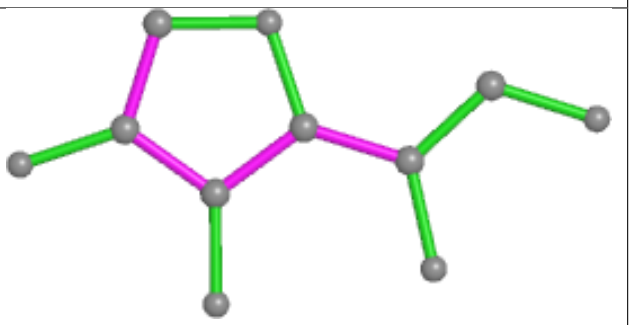


Rings

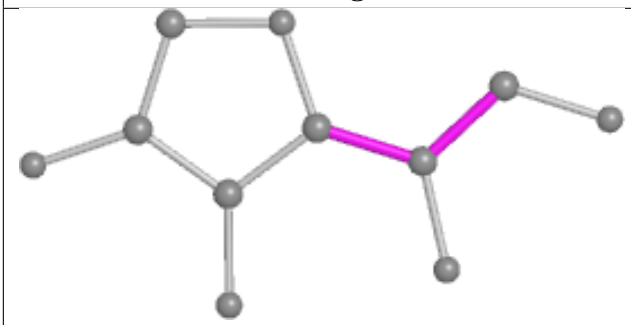
Ligand A1AIO A 2035



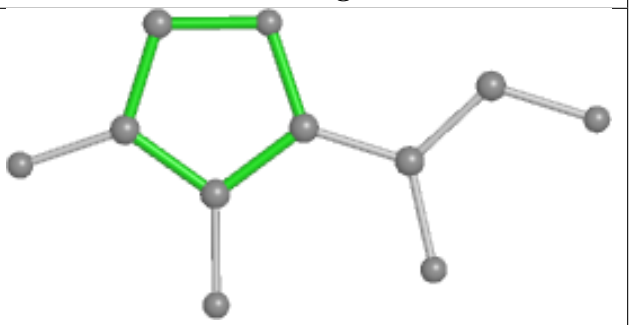
Bond lengths



Bond angles

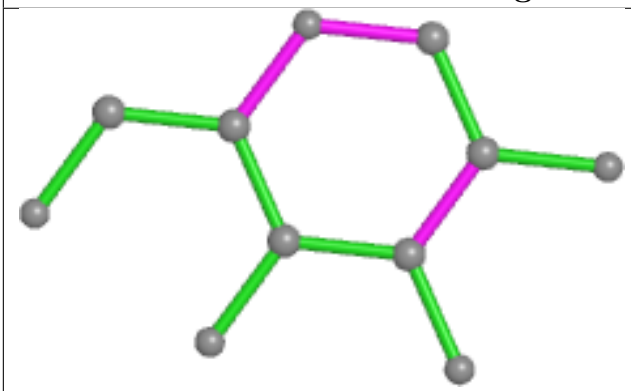


Torsions

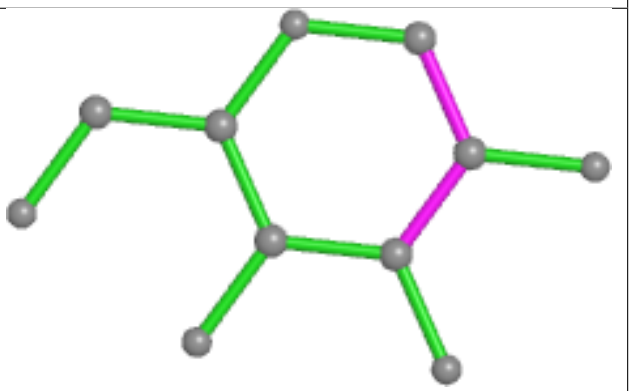


Rings

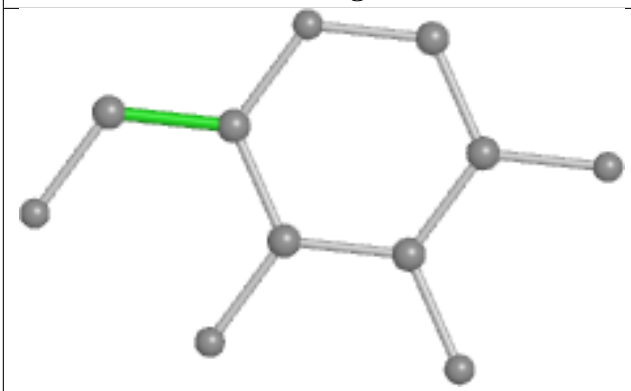
Ligand GLA B 2070



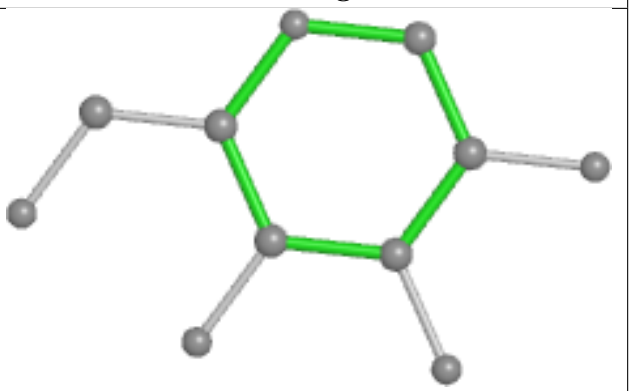
Bond lengths



Bond angles

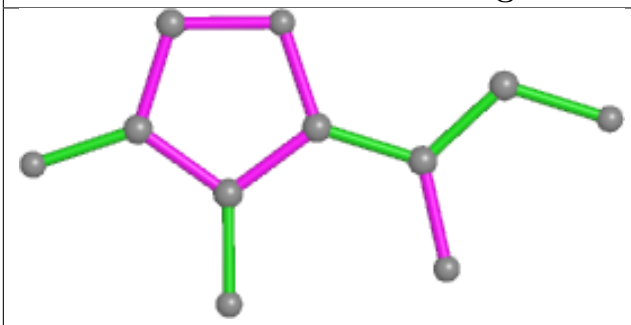


Torsions

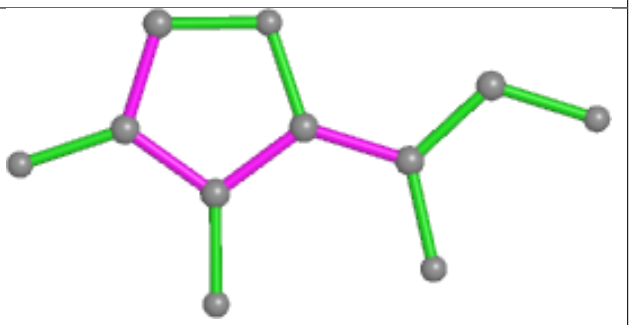


Rings

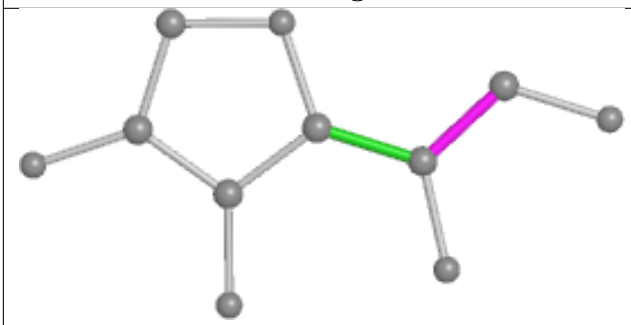
Ligand A1AIO B 2042



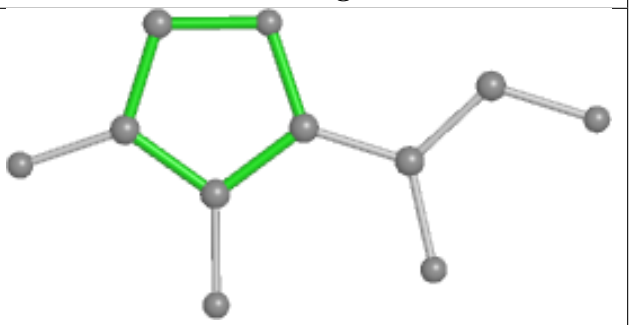
Bond lengths



Bond angles

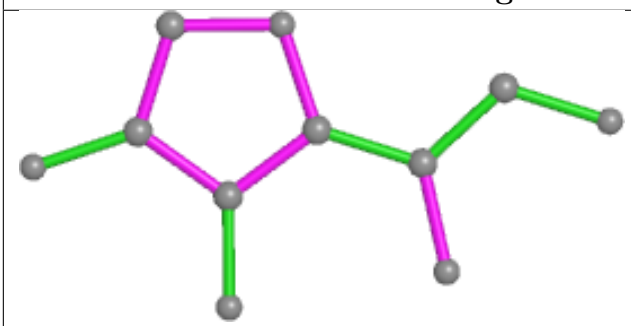


Torsions

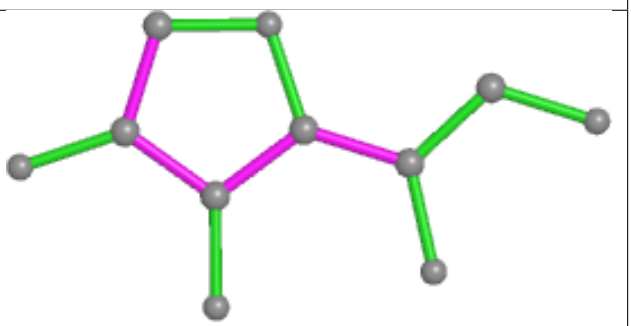


Rings

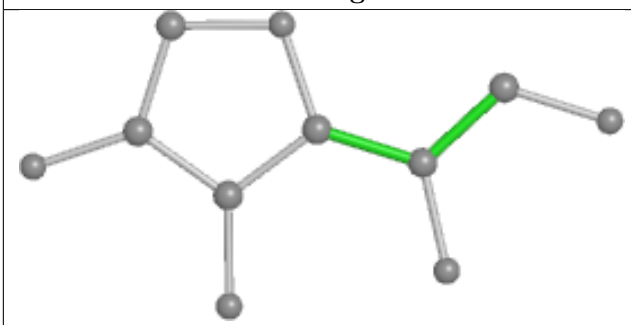
Ligand A1AIO A 2034



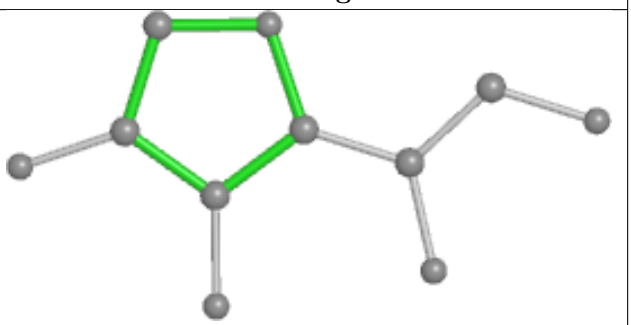
Bond lengths



Bond angles

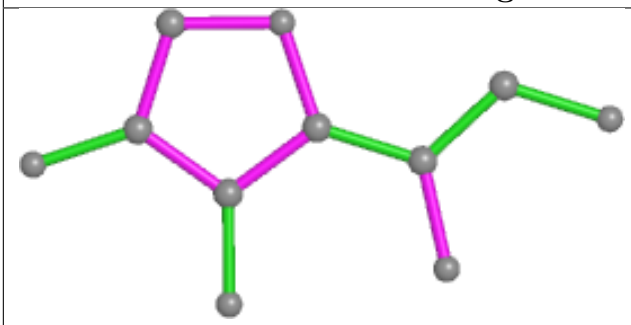


Torsions

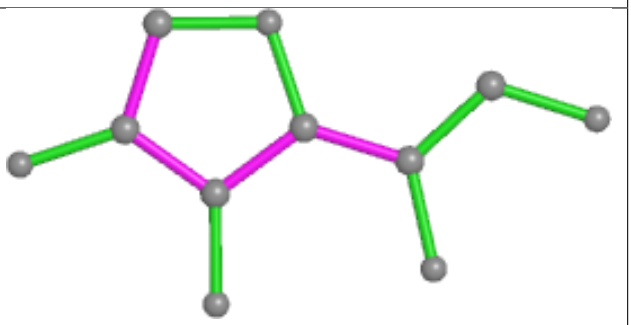


Rings

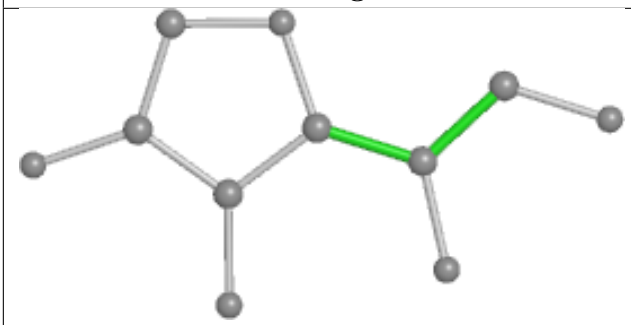
Ligand A1AIO B 2012



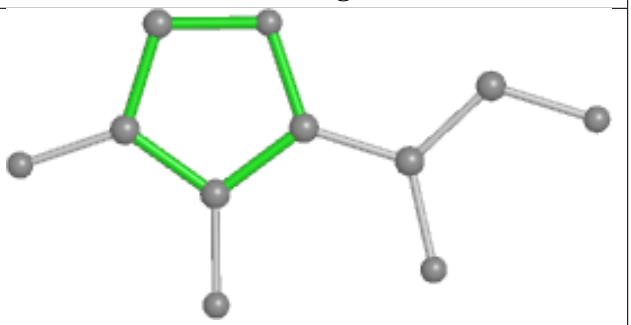
Bond lengths



Bond angles

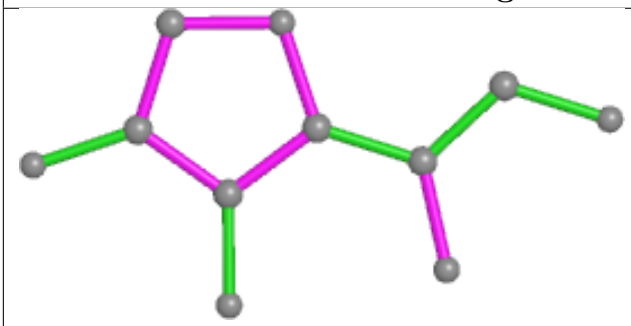


Torsions

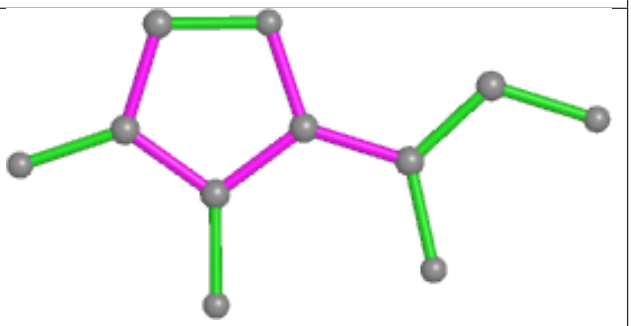


Rings

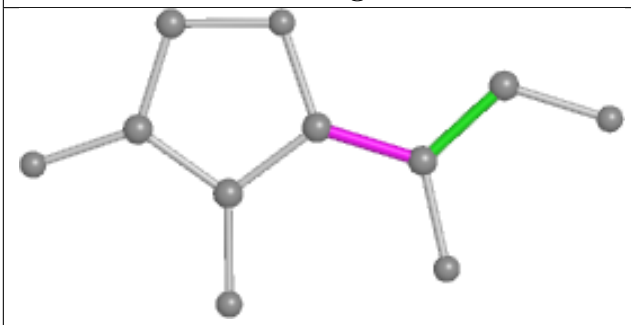
Ligand A1AIO B 2015



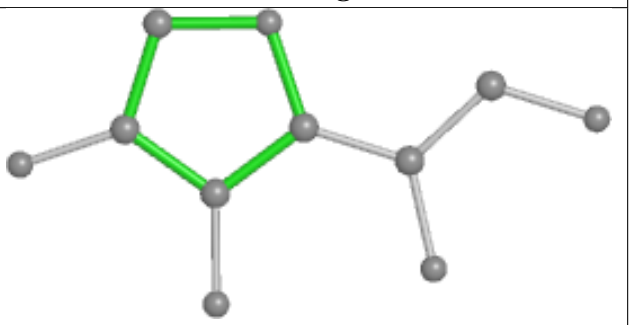
Bond lengths



Bond angles

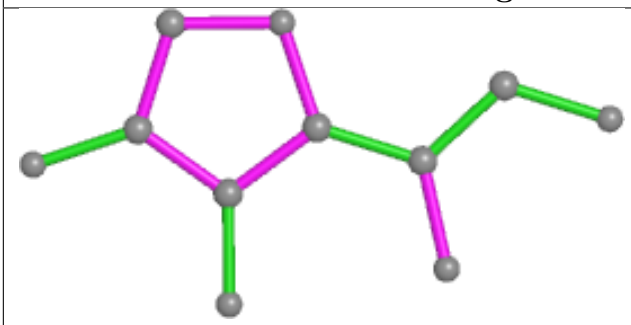


Torsions

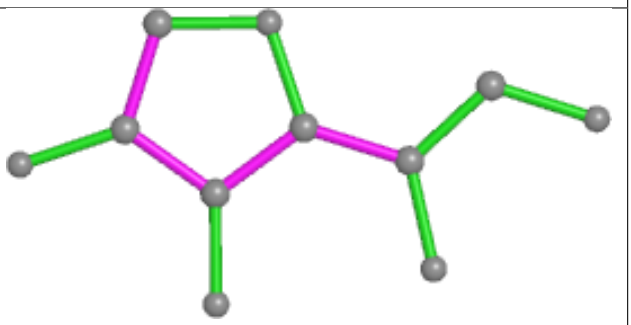


Rings

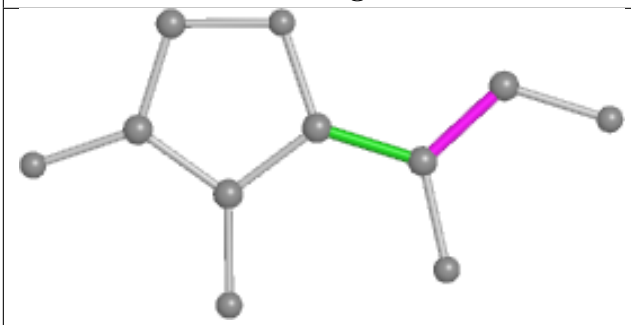
Ligand A1AIO A 2016



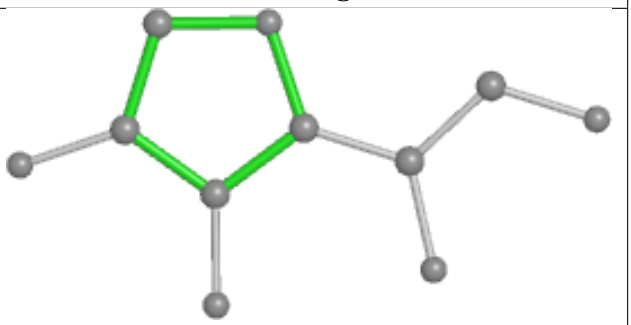
Bond lengths



Bond angles

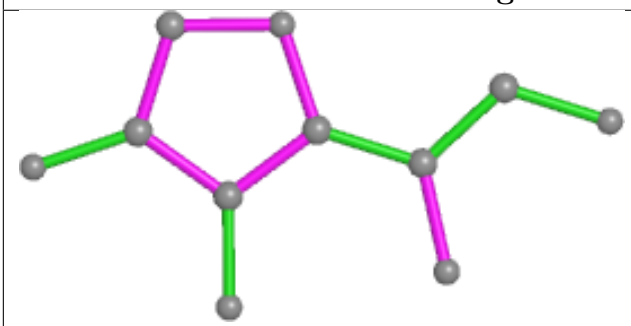


Torsions

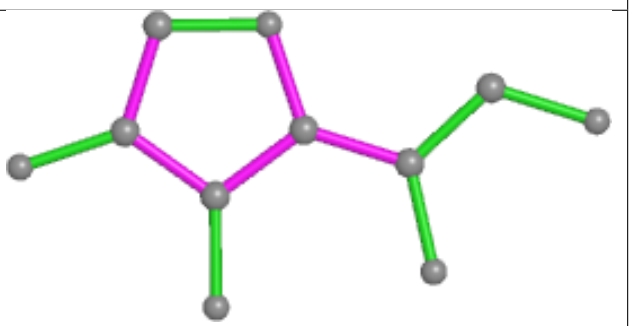


Rings

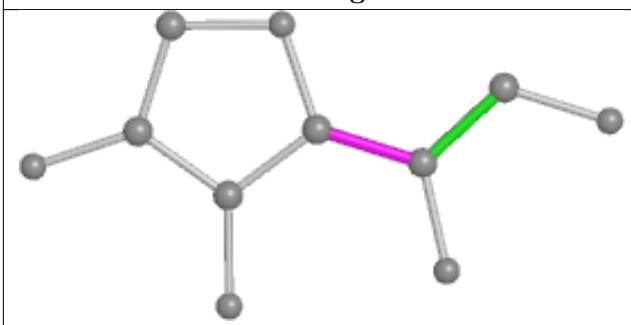
Ligand A1AIO B 2031



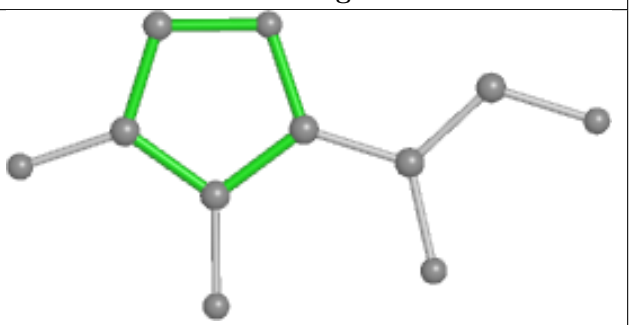
Bond lengths



Bond angles

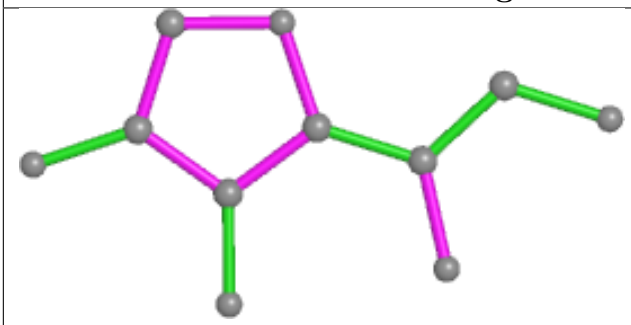


Torsions

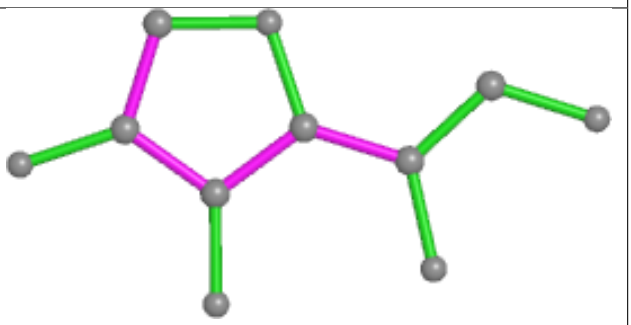


Rings

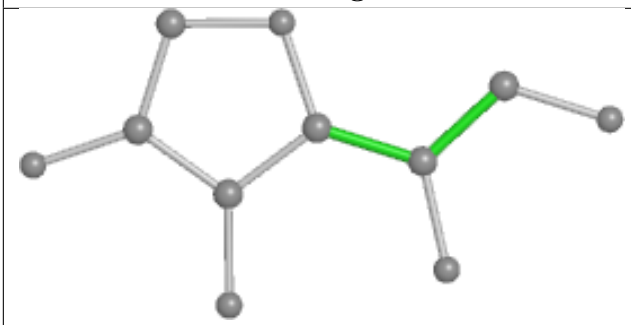
Ligand A1AIO A 2029



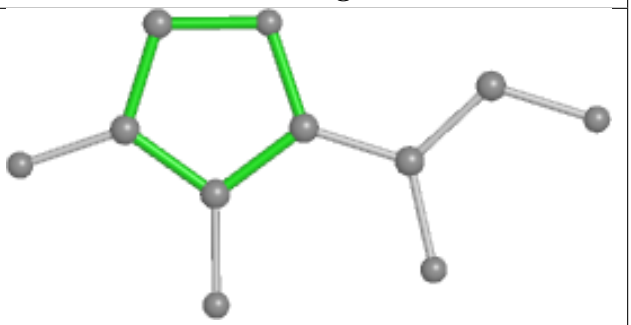
Bond lengths



Bond angles

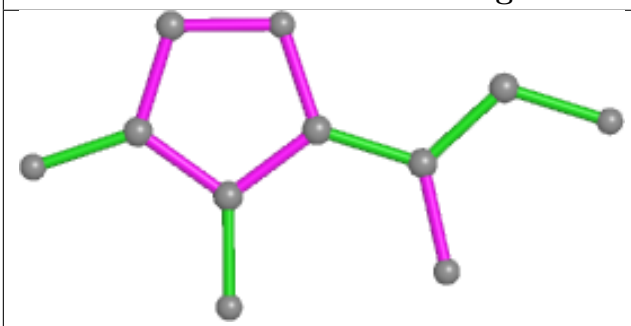


Torsions

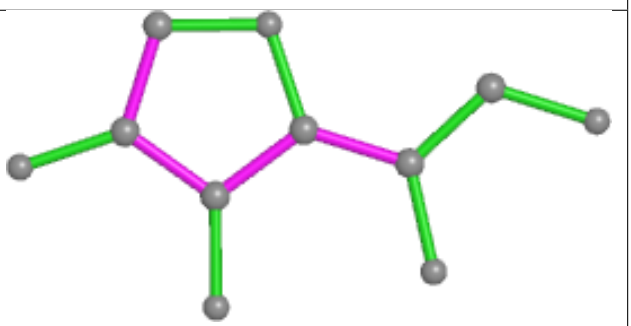


Rings

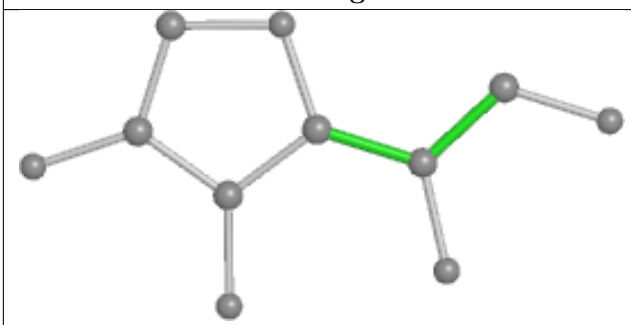
Ligand A1AIO A 2014



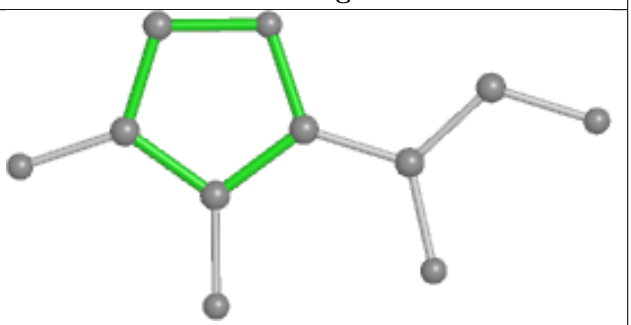
Bond lengths



Bond angles

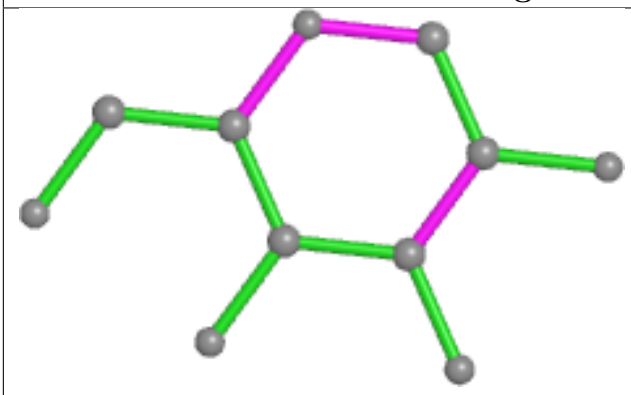


Torsions

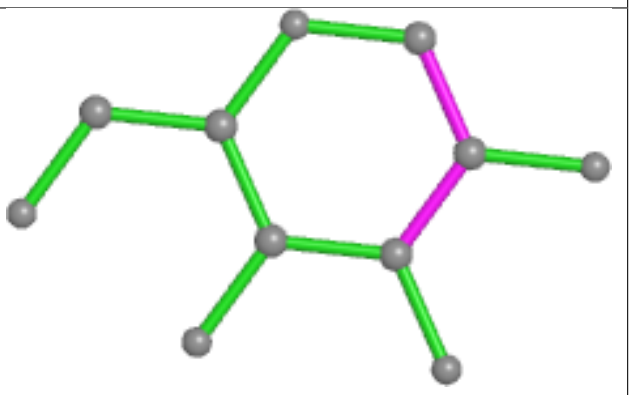


Rings

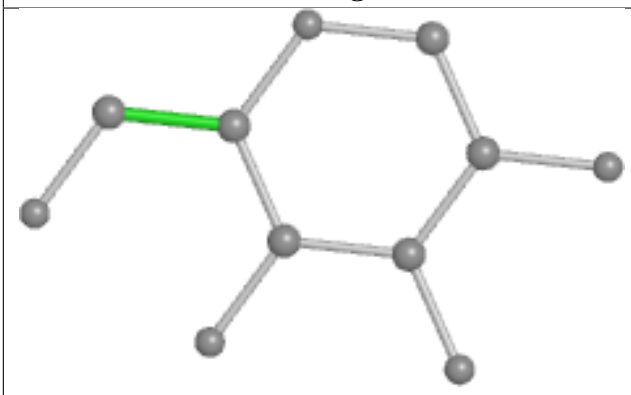
Ligand GLA B 2064



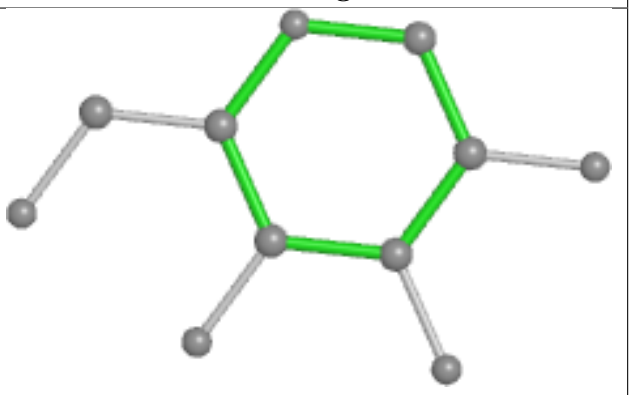
Bond lengths



Bond angles

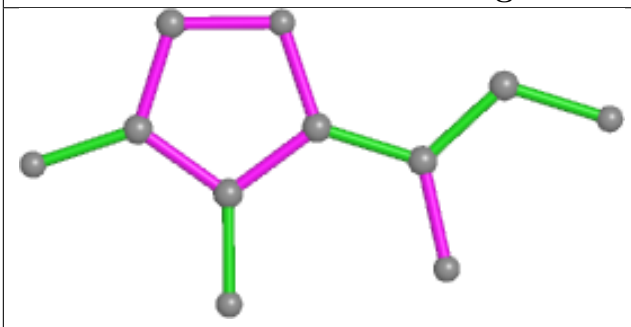


Torsions

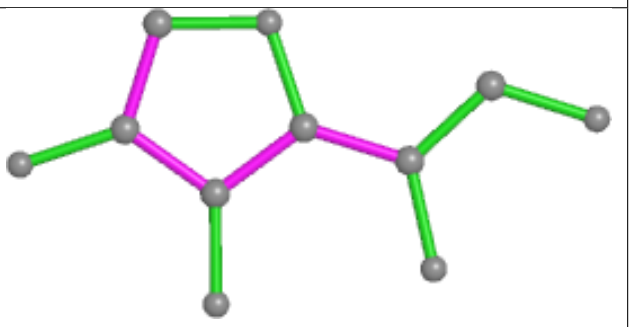


Rings

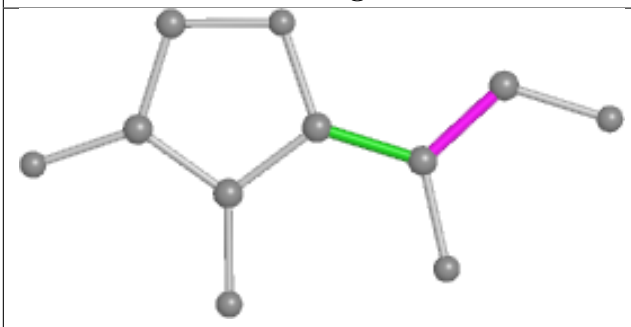
Ligand A1AIO A 2004



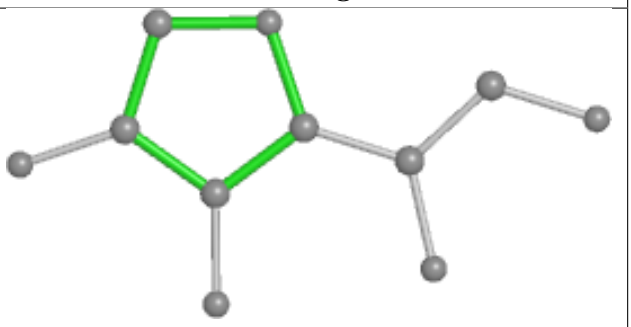
Bond lengths



Bond angles

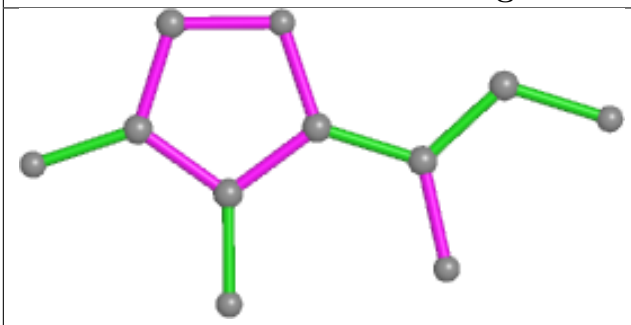


Torsions

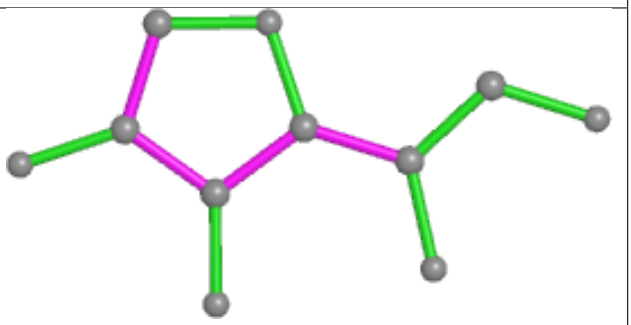


Rings

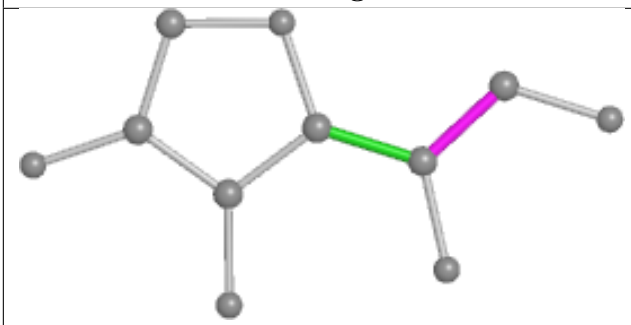
Ligand A1AIO B 2025



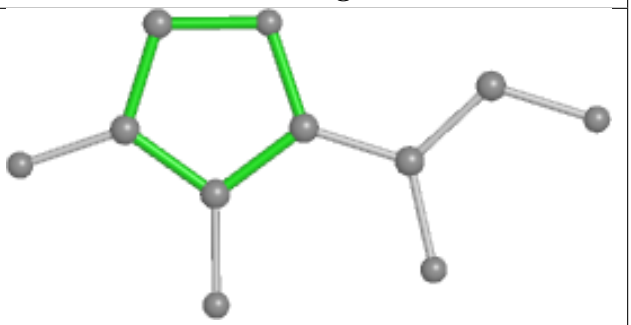
Bond lengths



Bond angles

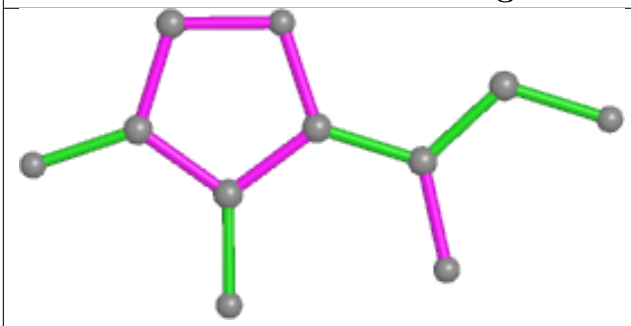


Torsions

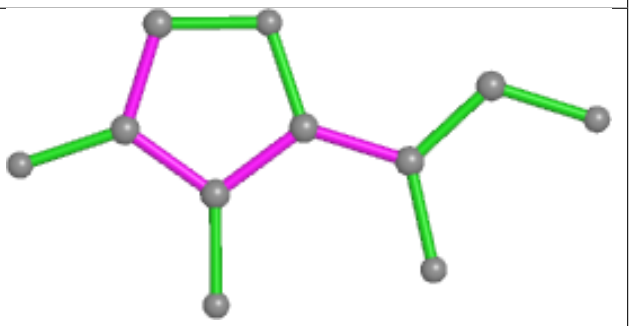


Rings

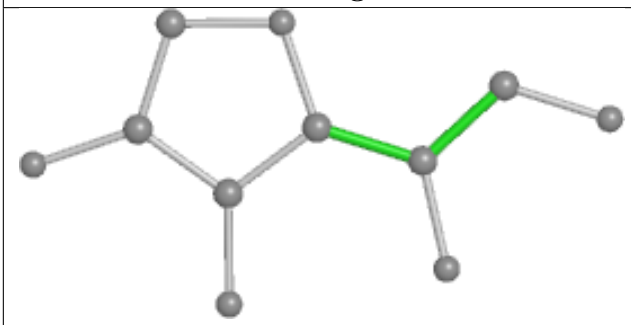
Ligand A1AIO B 2022



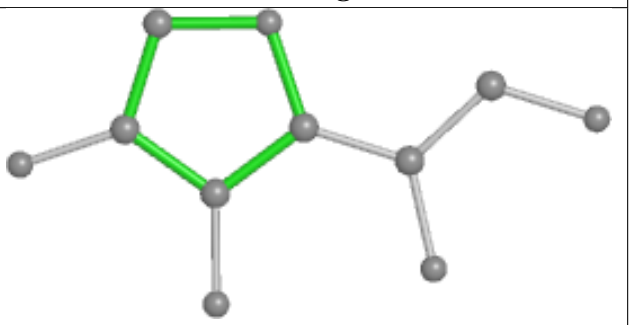
Bond lengths



Bond angles

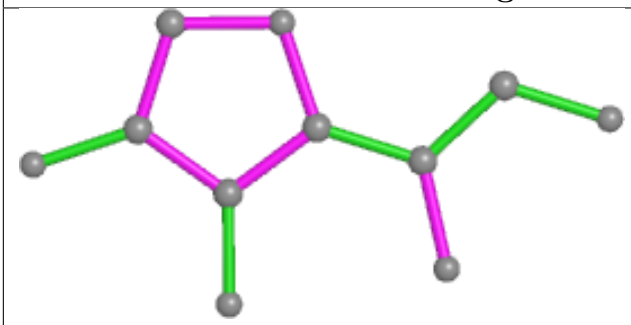


Torsions

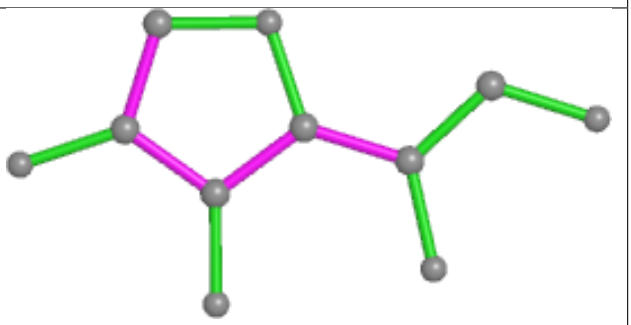


Rings

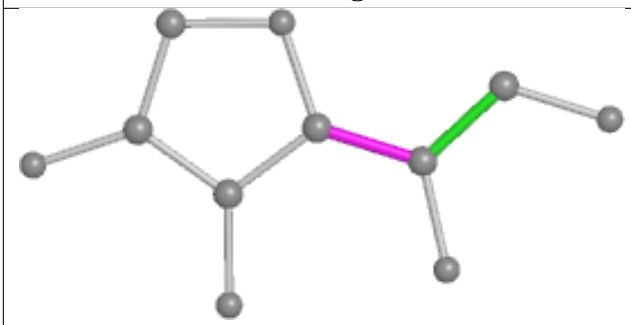
Ligand A1AIO B 2018



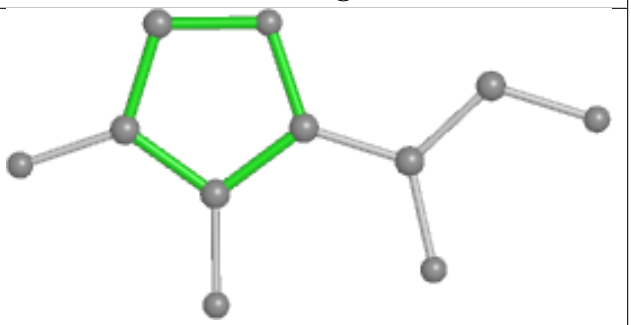
Bond lengths



Bond angles

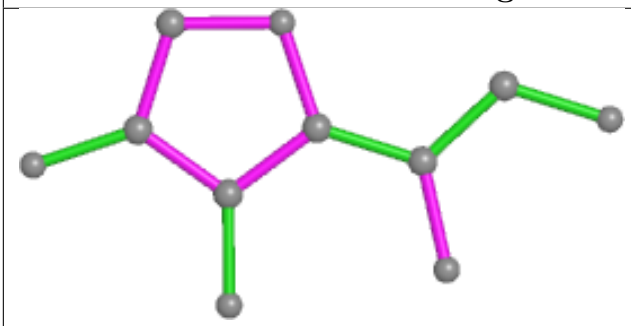


Torsions

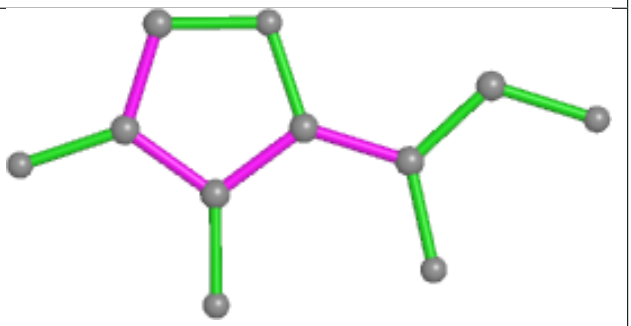


Rings

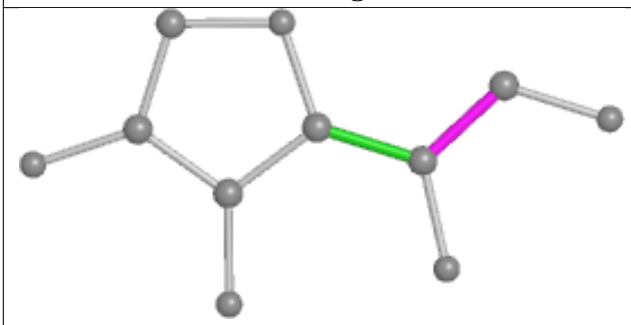
Ligand A1AIO B 2002



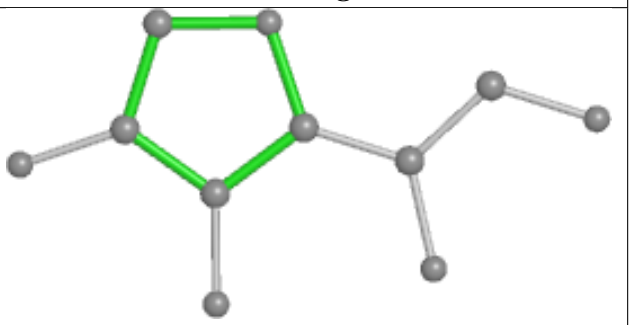
Bond lengths



Bond angles

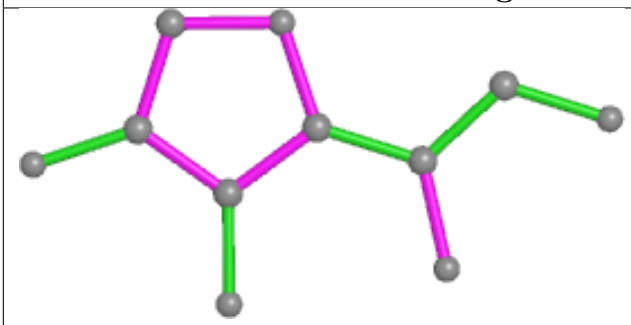


Torsions

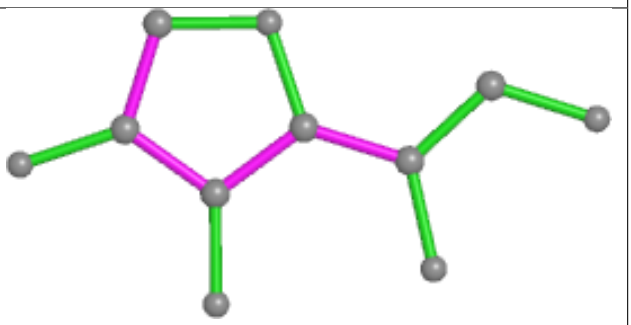


Rings

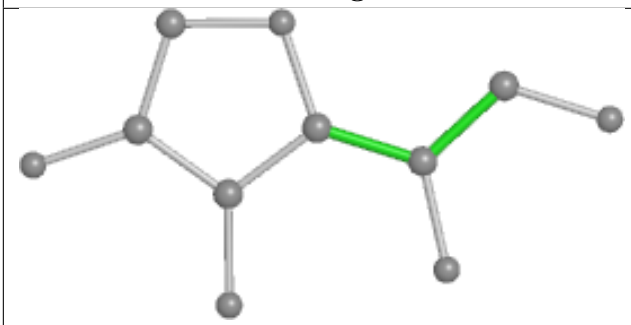
Ligand A1AIO A 2032



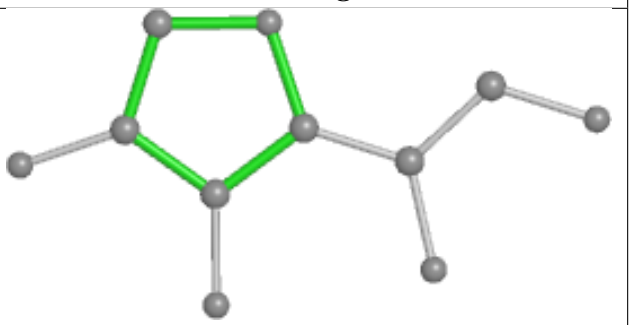
Bond lengths



Bond angles

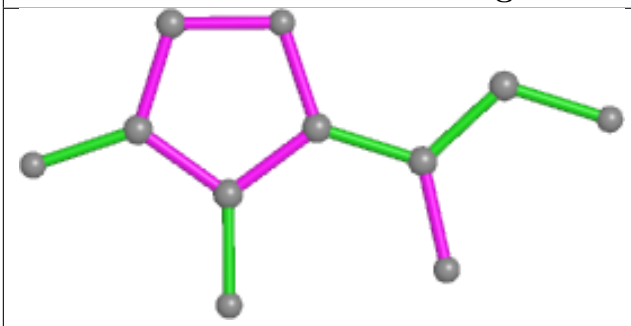


Torsions

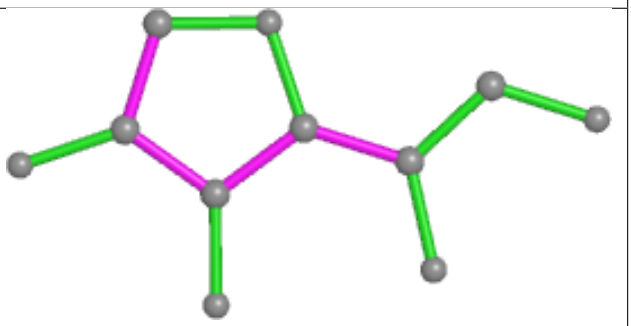


Rings

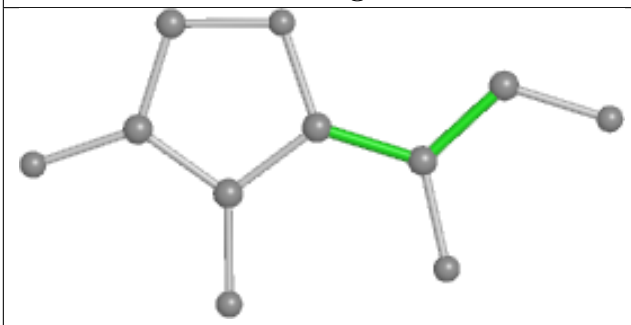
Ligand A1AIO A 2043



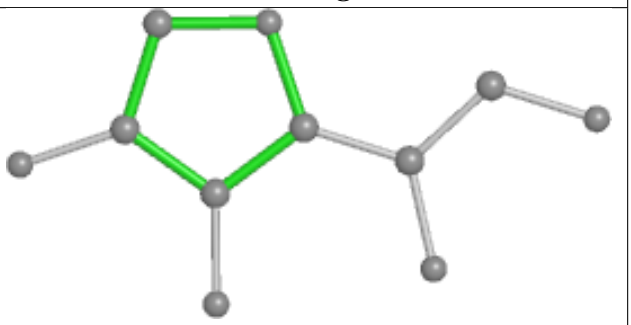
Bond lengths



Bond angles

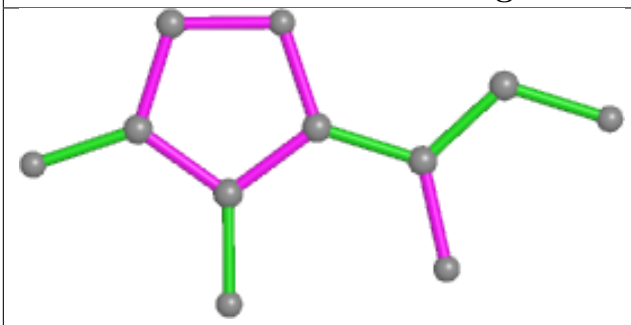


Torsions

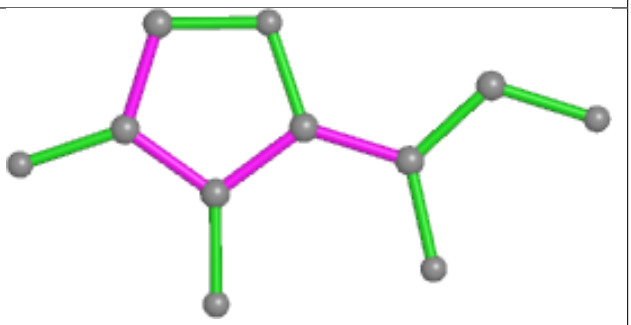


Rings

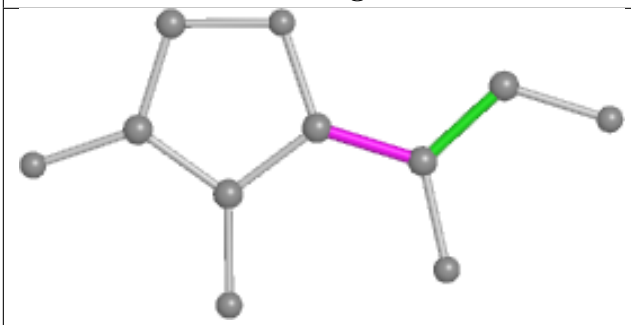
Ligand A1AIO A 2030



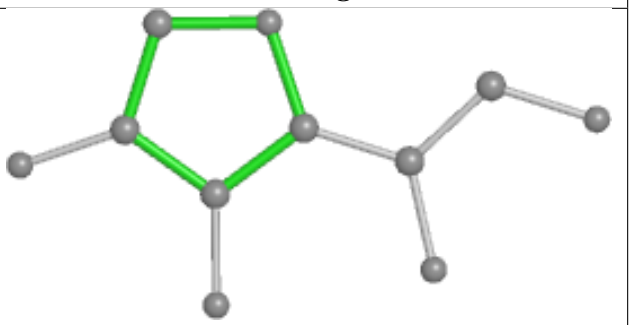
Bond lengths



Bond angles

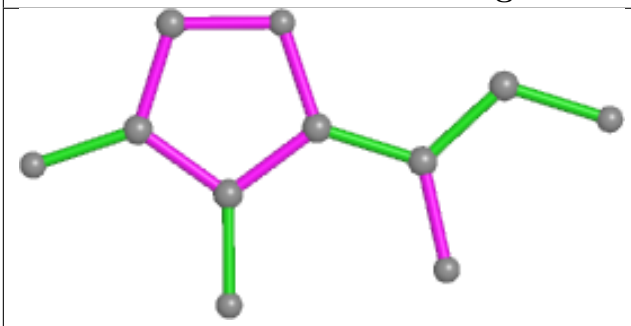


Torsions

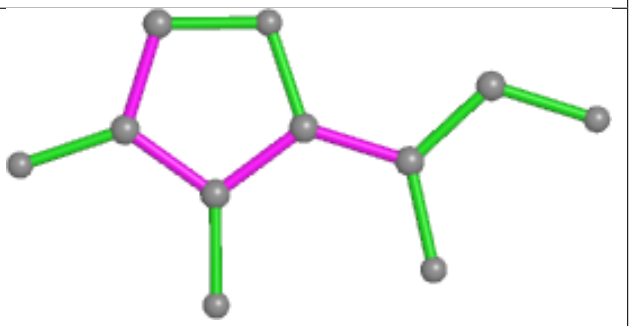


Rings

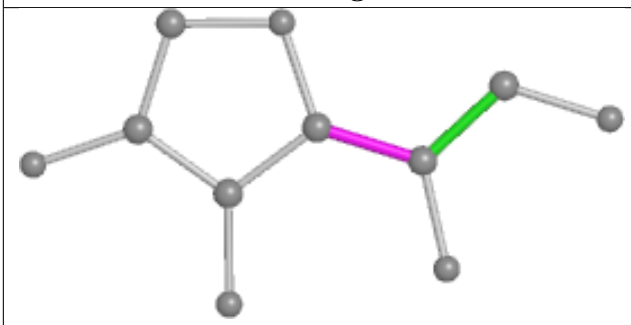
Ligand A1AIO A 2052



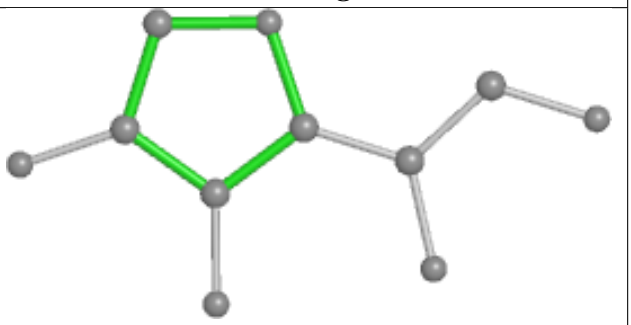
Bond lengths



Bond angles

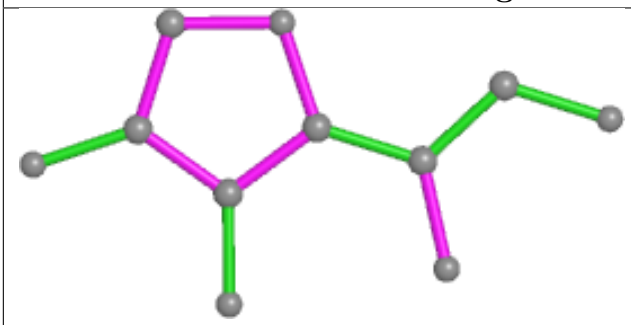


Torsions

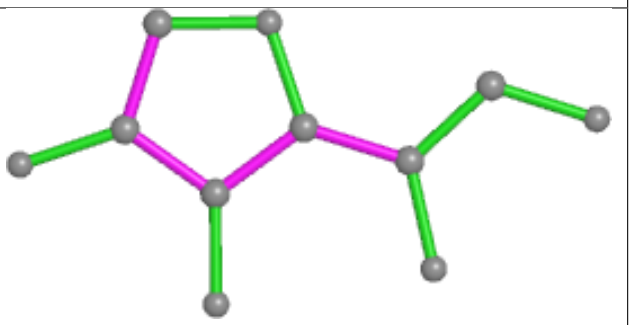


Rings

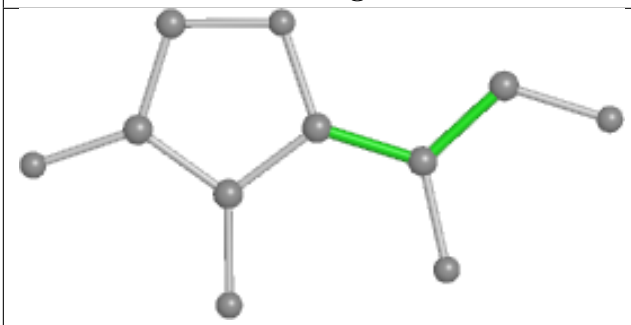
Ligand A1AIO A 2015



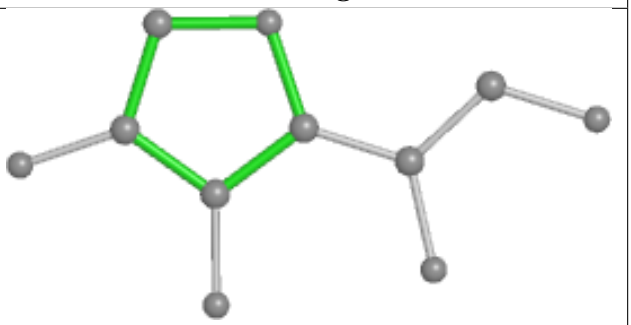
Bond lengths



Bond angles

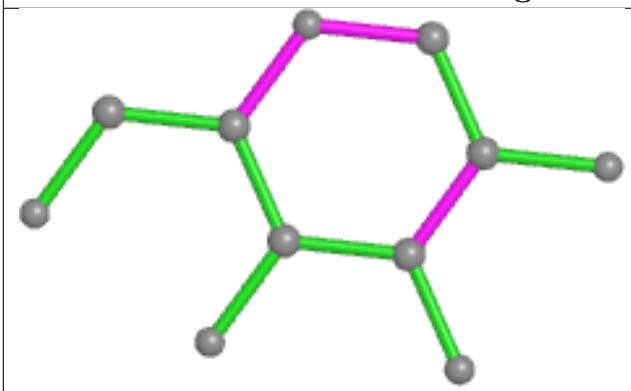


Torsions

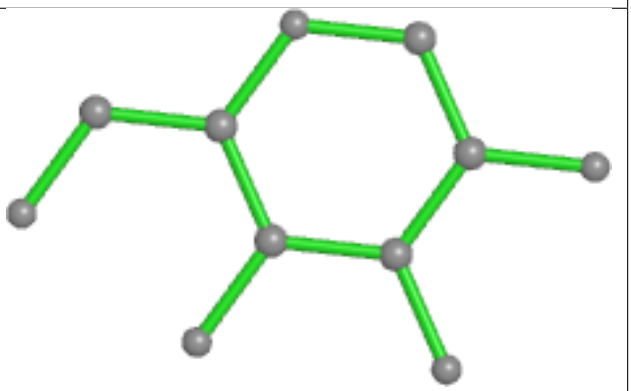


Rings

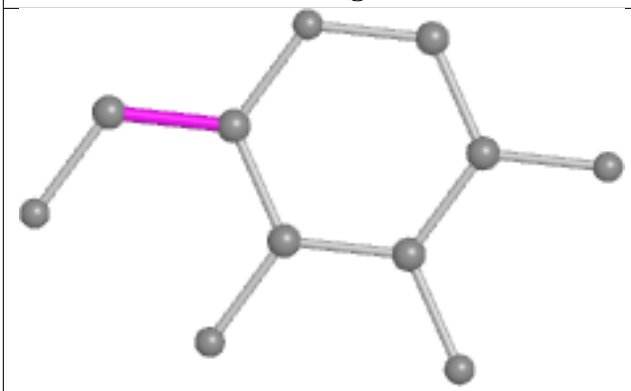
Ligand GLA B 2061



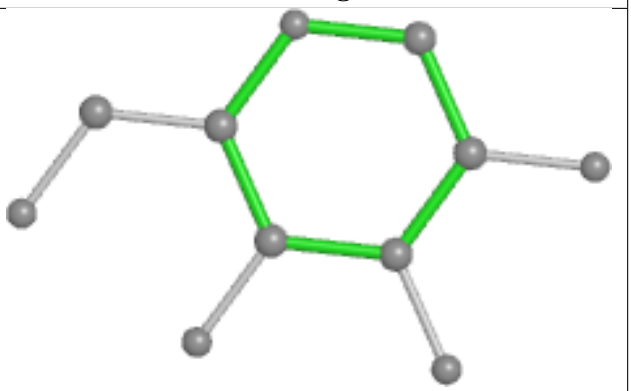
Bond lengths



Bond angles

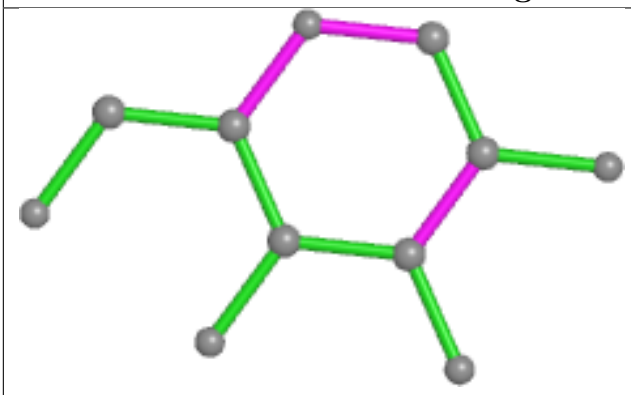


Torsions

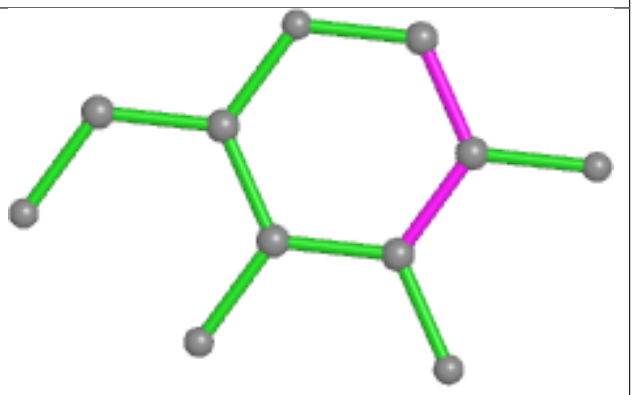


Rings

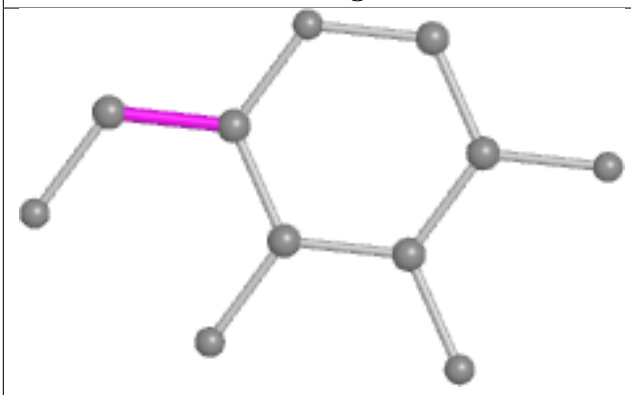
Ligand GLA B 2062



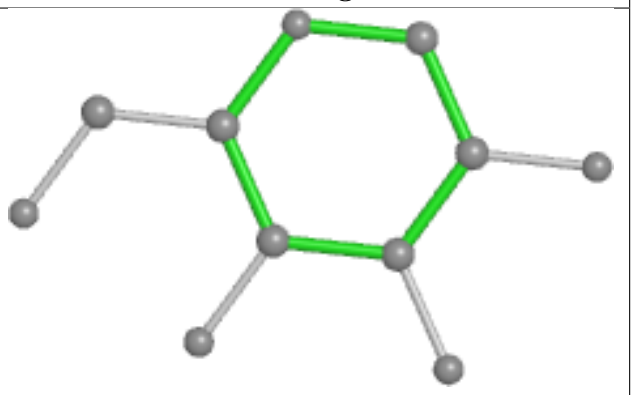
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

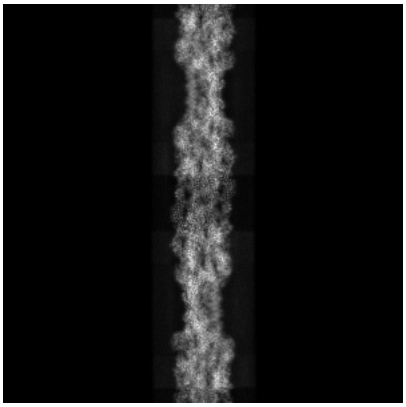
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43892. These allow visual inspection of the internal detail of the map and identification of artifacts.

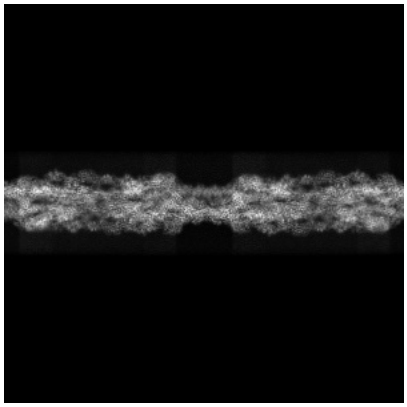
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

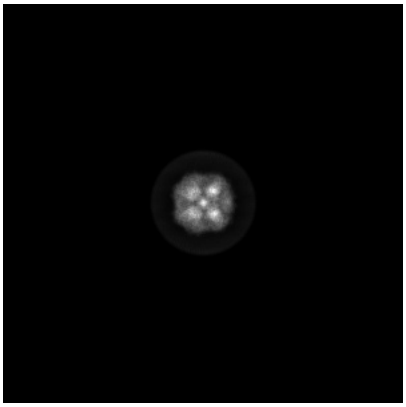
6.1.1 Primary map



X



Y

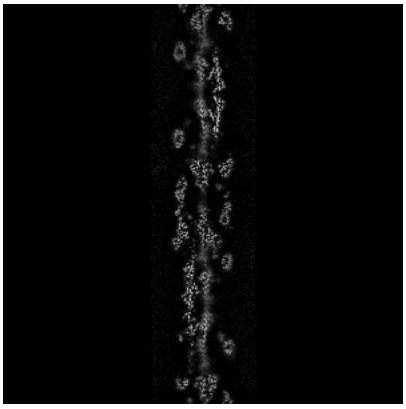


Z

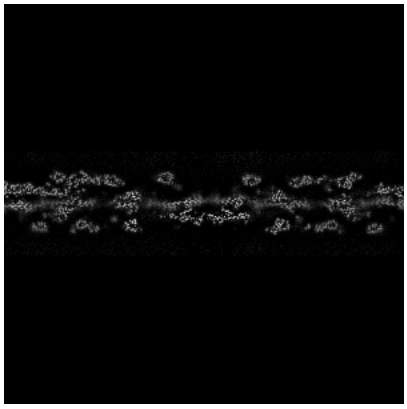
The images above show the map projected in three orthogonal directions.

6.2 Central slices

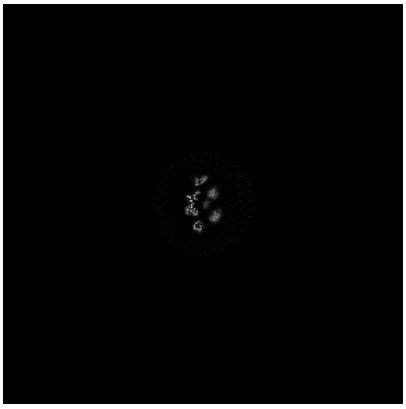
6.2.1 Primary map



X Index: 256



Y Index: 256

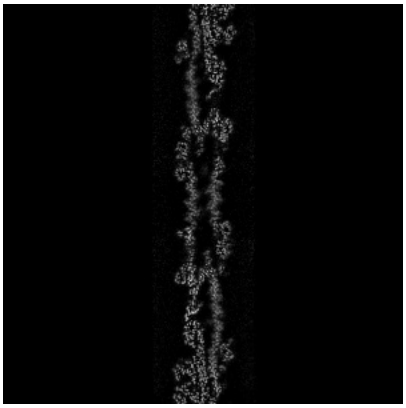


Z Index: 256

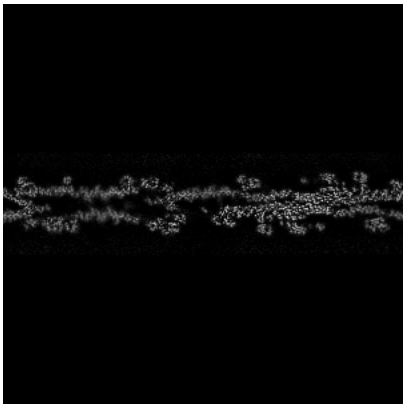
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

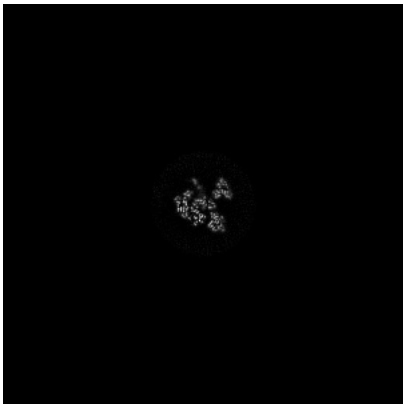
6.3.1 Primary map



X Index: 270



Y Index: 271

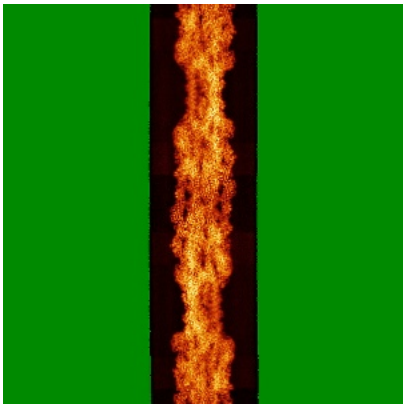


Z Index: 161

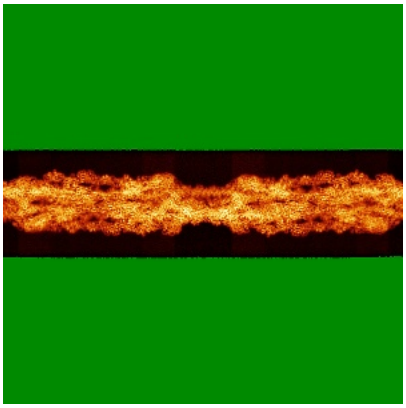
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

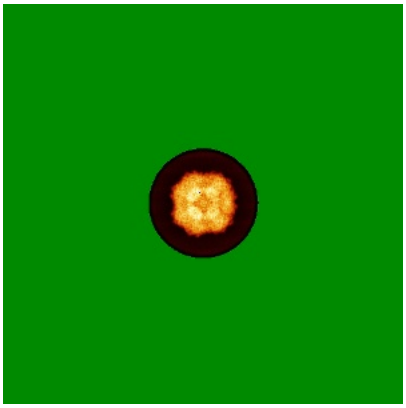
6.4.1 Primary map



X



Y

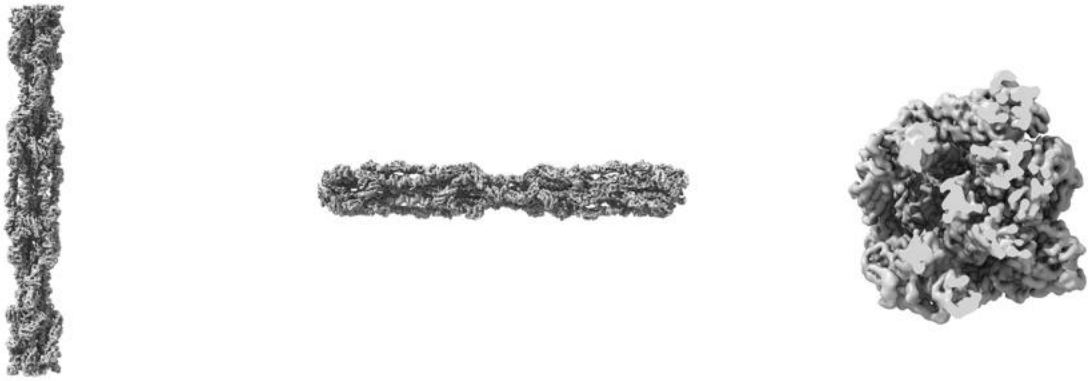


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

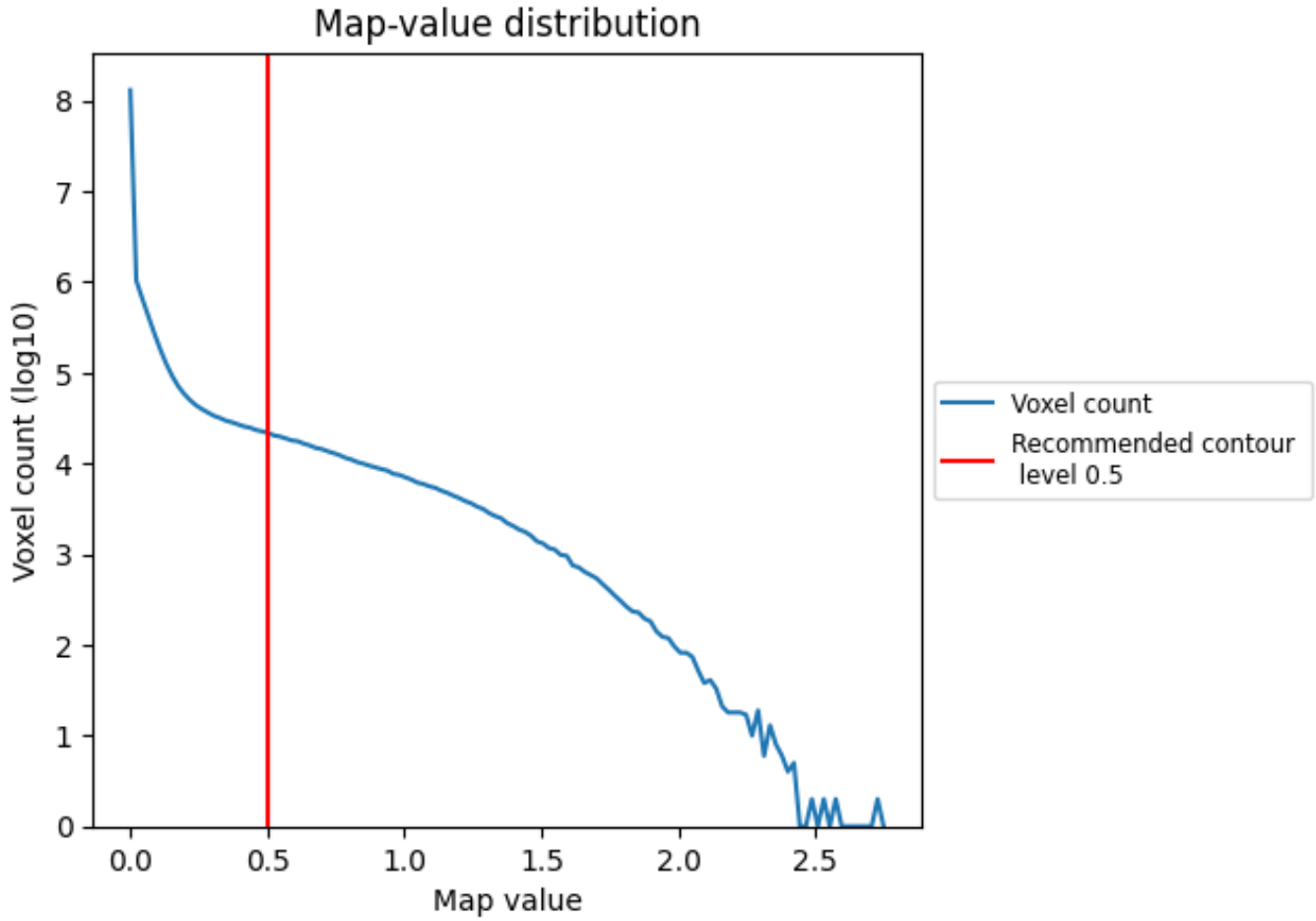
6.6 Mask visualisation (i)

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

7 Map analysis

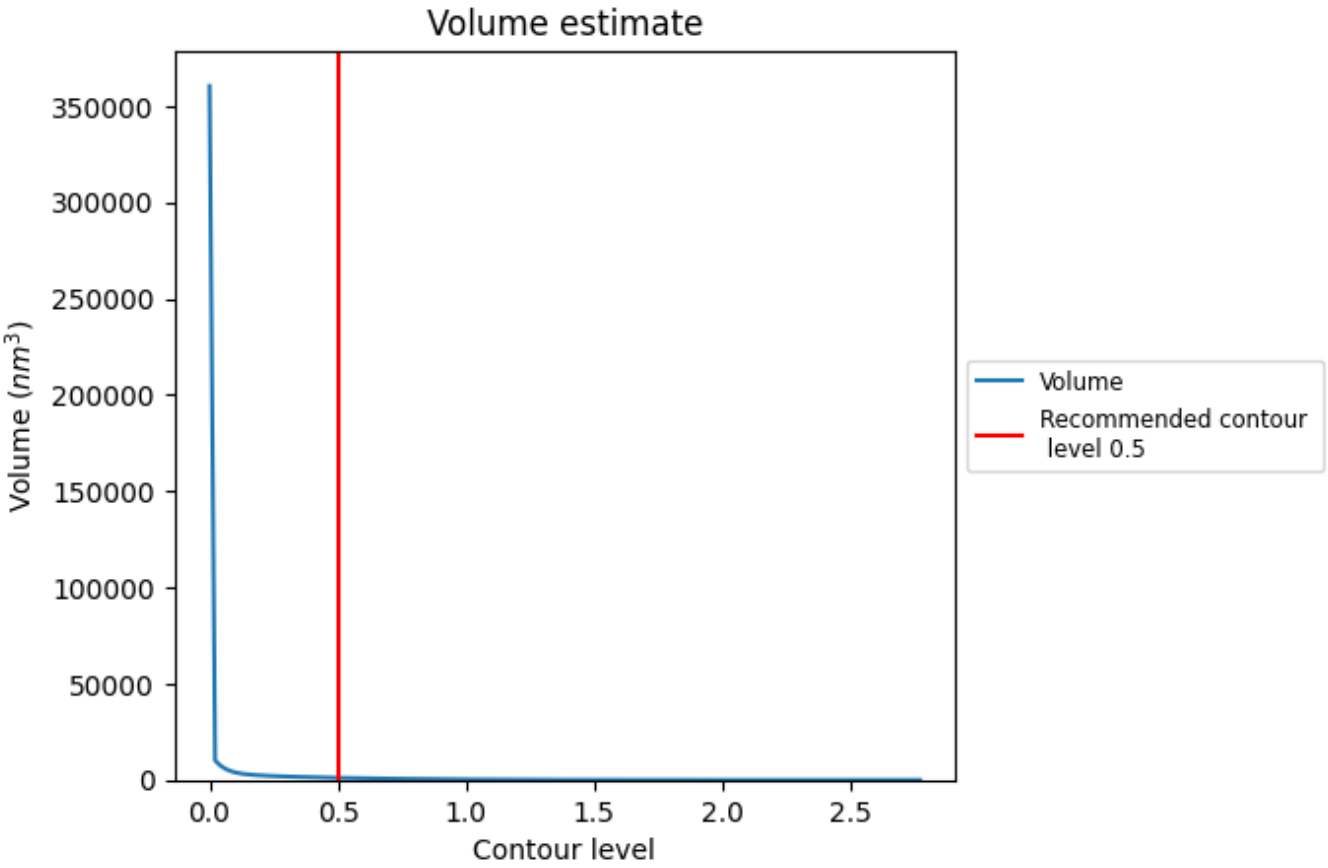
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

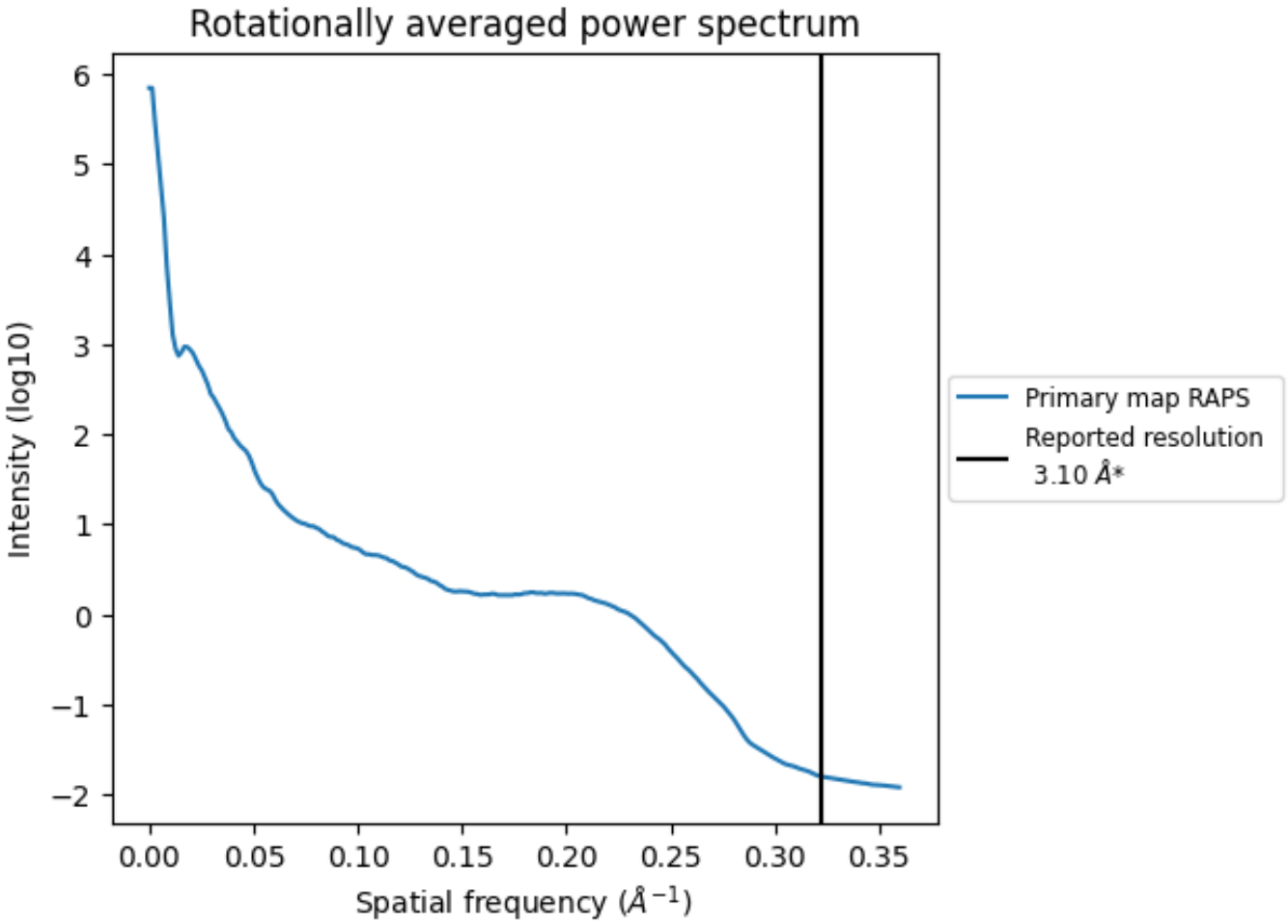
7.2 Volume estimate



The volume at the recommended contour level is 1110 nm^3; this corresponds to an approximate mass of 1002 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

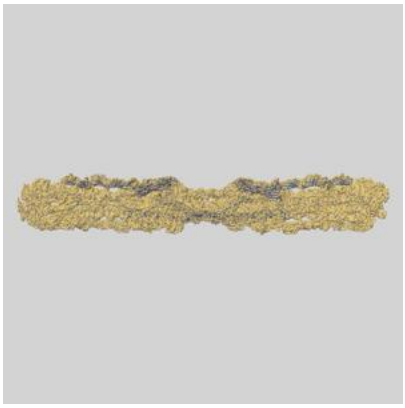
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

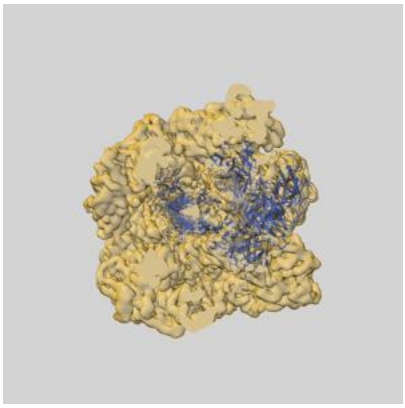
This section contains information regarding the fit between EMDB map EMD-43892 and PDB model 9B4H. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay

X



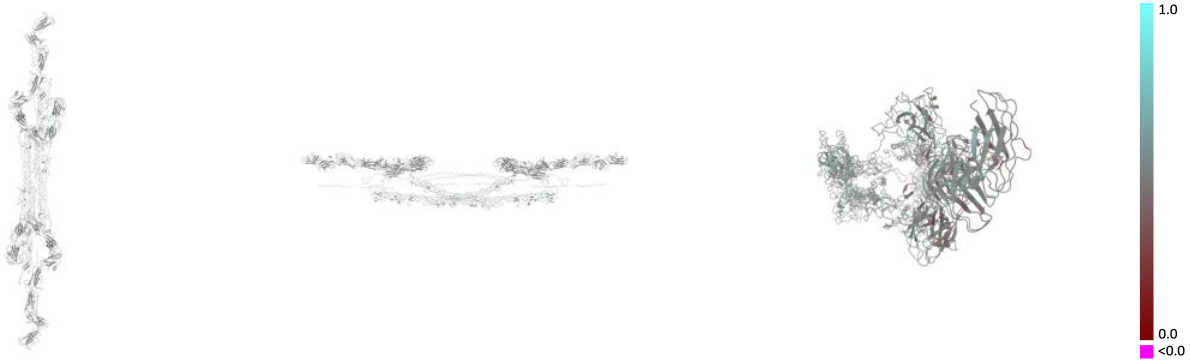
Y



Z

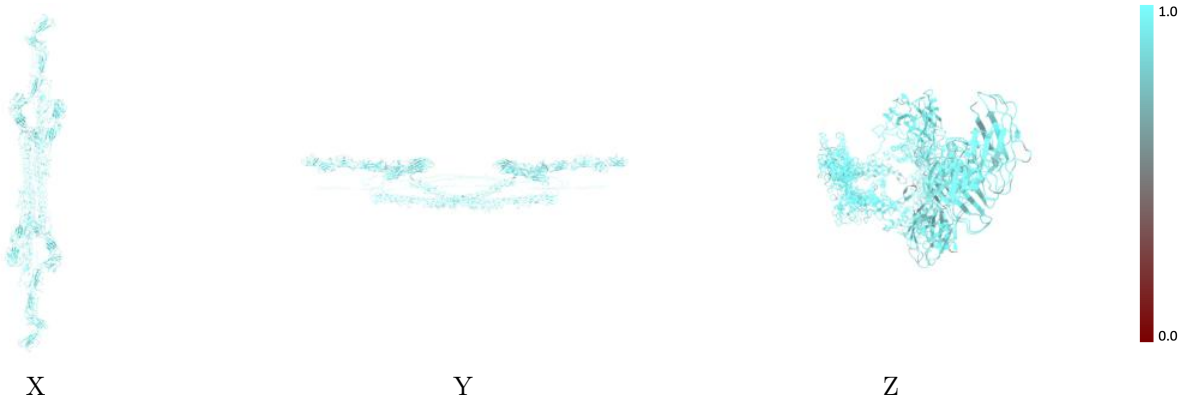
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



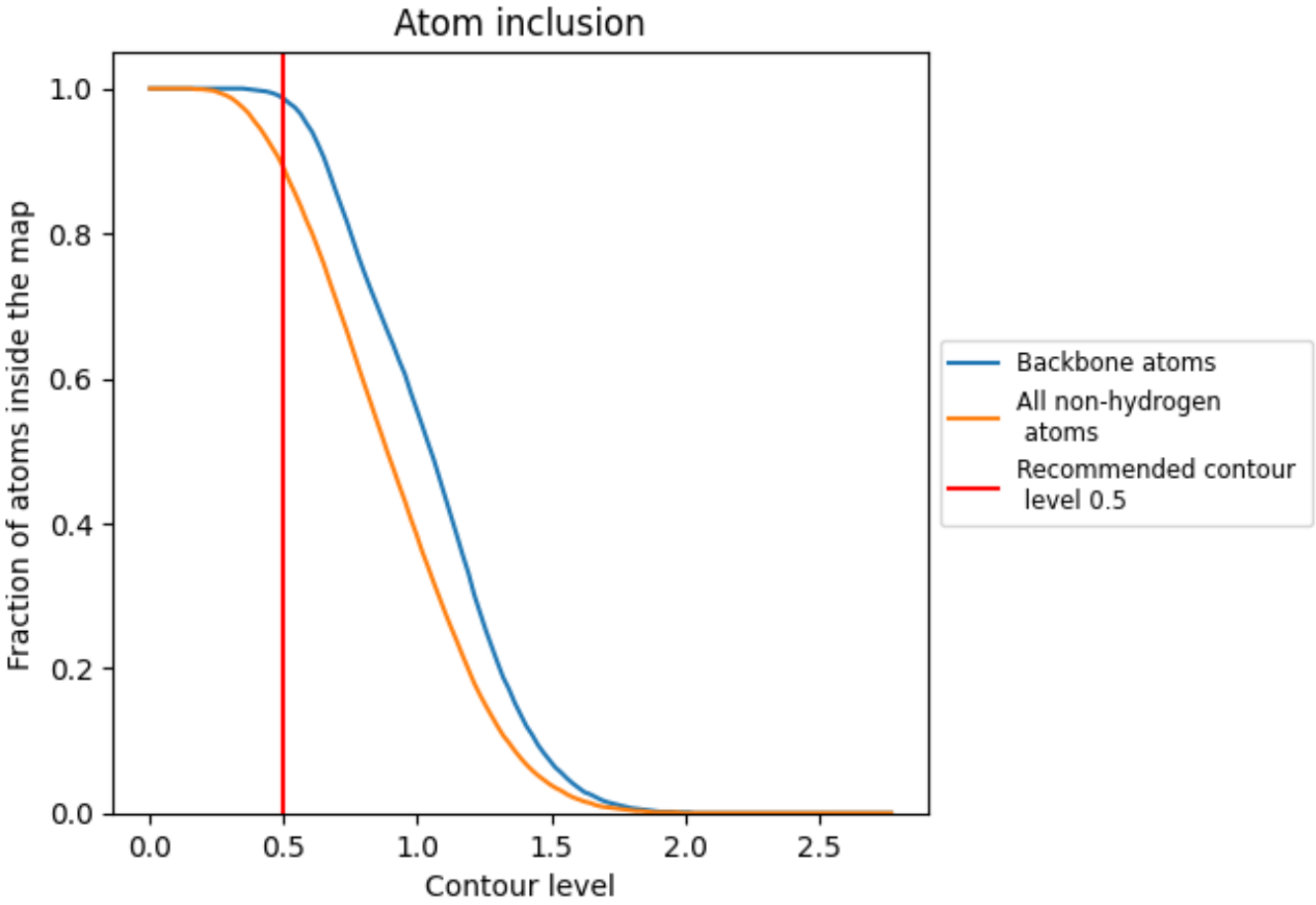
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.4880
A	0.8940	0.4900
A1	0.7140	0.4580
A2	0.8210	0.4630
A3	0.8930	0.5310
A4	0.8330	0.5290
A5	0.8330	0.4860
A6	0.8330	0.4760
A7	1.0000	0.5530
A9	0.8060	0.4870
B	0.8900	0.4890
B0	0.8890	0.4180
B1	0.7780	0.4140
B3	0.8330	0.4690
B4	0.7220	0.4660
B5	0.7220	0.5070
B6	0.8060	0.4670
B7	0.8890	0.4520
B9	0.6670	0.5150
C0	0.8330	0.4270
C1	0.7780	0.4790
C2	0.6670	0.4470
C3	0.9440	0.4330
C4	0.8330	0.4900
C5	0.7220	0.4670
C6	1.0000	0.4270
C7	0.8890	0.4860
C8	0.7780	0.4280
C9	0.7780	0.4180
D0	0.8890	0.4360
D1	0.5560	0.3560
D2	0.6670	0.4780
D3	0.8330	0.5100
D4	0.8330	0.4810
D5	0.7780	0.4830

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
D6	0.9440	0.5310
D7	0.8890	0.4730
D8	0.8330	0.4470
D9	0.8890	0.4850
E0	0.8330	0.4820
E1	0.7780	0.4790
E2	0.6670	0.4360
E3	0.8330	0.4660
E4	0.7220	0.3750
E5	0.7780	0.4620
E6	0.7780	0.4810
E7	0.7220	0.5030
E8	0.8330	0.4950
F0	0.7780	0.4980
F2	0.9440	0.5270
F3	0.9440	0.4910
F5	0.6670	0.4890
F6	0.8890	0.5040
F7	0.9170	0.5100
F8	0.9440	0.5430
X	0.9770	0.4900
a1	0.7500	0.4670
a2	0.7860	0.4180
a3	0.8570	0.5080
a4	0.8330	0.5080
a5	0.8330	0.4650
a6	0.8330	0.4790
a7	1.0000	0.5850
a9	0.8060	0.4960
b0	0.9440	0.4330
b1	0.6670	0.4610
b3	0.9440	0.5280
b4	0.8330	0.4610
b5	0.7780	0.4880
b6	0.8610	0.4400
b7	0.9440	0.4880
b9	0.8330	0.4850
c0	0.8330	0.4050
c1	0.8330	0.4300
c2	0.6670	0.4130
c3	0.9440	0.4320
c4	0.8330	0.4440

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c5	0.7780	0.4640
c6	1.0000	0.3930
c7	0.8890	0.4920
c8	0.8330	0.4650
c9	0.8330	0.4250
d0	0.7780	0.4100
d1	0.6670	0.3850
d2	0.7220	0.4600
d3	0.8890	0.5220
d4	0.8330	0.4840
d5	0.9440	0.5030
d6	0.9440	0.4680
d7	0.8890	0.4480
d8	0.7780	0.4470
d9	0.6670	0.4410
e0	0.8890	0.5090
e1	0.7780	0.5230
e2	0.7780	0.4800
e3	0.8330	0.4630
e4	0.7780	0.3930
e5	0.7780	0.4600
e6	0.8330	0.4700
e7	0.8330	0.4670
e8	0.8330	0.5300
e9	0.8330	0.4940
f0	0.8330	0.4820
f2	0.8890	0.4740
f3	0.9440	0.5090
f5	0.7220	0.5210
f6	0.9440	0.5080
f7	0.9170	0.5290
f8	1.0000	0.5210