Full wwPDB EM Validation Report ⓘ

Aug 29, 2024 – 10:09 PM JST

PDB ID	:	8WLU
EMDB ID	:	EMD-37632
Title	:	Cryo-EM structure of bat RsSHC014 spike glycoprotein
Authors	:	Wang, X.; Qiao, S.
Deposited on	:	2023-10-01
Resolution	:	2.87 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

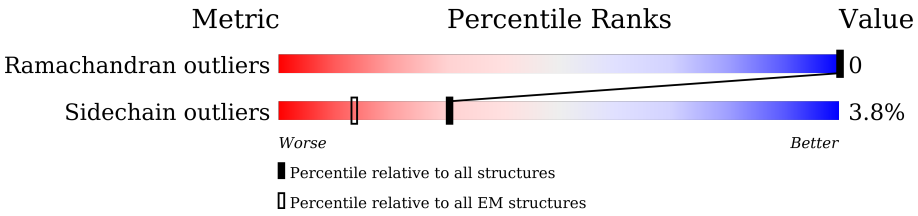
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.87 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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1271	84% · 13%
1	B	1271	84% · 13%
1	C	1271	85% · 13%
2	D	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	100%
2	N	2	50% 50%
2	O	2	100%
2	P	2	100%

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Mol	Chain	Length	Quality of chain
2	Q	2	100%
2	R	2	100%
2	S	2	100%
2	T	2	100%
2	Z	2	100%
2	a	2	100%
2	b	2	100%
2	d	2	50% 50%
2	e	2	100%
2	f	2	100%
2	g	2	100%
2	h	2	100%
2	i	2	100%
2	j	2	100%
2	p	2	100%
2	q	2	100%
2	r	2	100%
2	t	2	50% 50%
2	u	2	100%
2	v	2	100%
2	w	2	100%
2	x	2	100%
2	y	2	100%
3	E	3	100%
3	F	3	100%

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Mol	Chain	Length	Quality of chain
3	G	3	100%
3	H	3	100%
3	I	3	67% 33%
3	M	3	33% 67%
3	U	3	100%
3	V	3	100%
3	W	3	100%
3	X	3	100%
3	Y	3	67% 33%
3	c	3	33% 67%
3	k	3	100%
3	l	3	100%
3	m	3	100%
3	n	3	100%
3	o	3	33% 67%
3	s	3	33% 67%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27438 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1106	Total 8604	C 5477	N 1439	O 1644	S 44	0	0
1	C	1106	Total 8604	C 5477	N 1439	O 1644	S 44	0	0
1	B	1106	Total 8604	C 5477	N 1439	O 1644	S 44	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	969	PRO	LYS	conflict	UNP U5WLK5
A	970	PRO	VAL	conflict	UNP U5WLK5
A	1192	GLY	-	linker	UNP U5WLK5
A	1193	SER	-	linker	UNP U5WLK5
A	1220	LEU	-	expression tag	UNP A0A346FJN8
A	1221	GLY	-	expression tag	UNP A0A346FJN8
A	1222	ARG	-	expression tag	UNP A0A346FJN8
A	1223	SER	-	expression tag	UNP A0A346FJN8
A	1224	LEU	-	expression tag	UNP A0A346FJN8
A	1225	GLU	-	expression tag	UNP A0A346FJN8
A	1226	VAL	-	expression tag	UNP A0A346FJN8
A	1227	LEU	-	expression tag	UNP A0A346FJN8
A	1228	PHE	-	expression tag	UNP A0A346FJN8
A	1229	GLN	-	expression tag	UNP A0A346FJN8
A	1230	GLY	-	expression tag	UNP A0A346FJN8
A	1231	PRO	-	expression tag	UNP A0A346FJN8
A	1232	GLY	-	expression tag	UNP A0A346FJN8
A	1233	HIS	-	expression tag	UNP A0A346FJN8
A	1234	HIS	-	expression tag	UNP A0A346FJN8
A	1235	HIS	-	expression tag	UNP A0A346FJN8
A	1236	HIS	-	expression tag	UNP A0A346FJN8
A	1237	HIS	-	expression tag	UNP A0A346FJN8
A	1238	HIS	-	expression tag	UNP A0A346FJN8
A	1239	HIS	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	HIS	-	expression tag	UNP A0A346FJN8
A	1241	SER	-	expression tag	UNP A0A346FJN8
A	1242	ALA	-	expression tag	UNP A0A346FJN8
A	1243	TRP	-	expression tag	UNP A0A346FJN8
A	1244	SER	-	expression tag	UNP A0A346FJN8
A	1245	HIS	-	expression tag	UNP A0A346FJN8
A	1246	PRO	-	expression tag	UNP A0A346FJN8
A	1247	GLN	-	expression tag	UNP A0A346FJN8
A	1248	PHE	-	expression tag	UNP A0A346FJN8
A	1249	GLU	-	expression tag	UNP A0A346FJN8
A	1250	LYS	-	expression tag	UNP A0A346FJN8
A	1251	GLY	-	expression tag	UNP A0A346FJN8
A	1252	GLY	-	expression tag	UNP A0A346FJN8
A	1253	GLY	-	expression tag	UNP A0A346FJN8
A	1254	SER	-	expression tag	UNP A0A346FJN8
A	1255	GLY	-	expression tag	UNP A0A346FJN8
A	1256	GLY	-	expression tag	UNP A0A346FJN8
A	1257	GLY	-	expression tag	UNP A0A346FJN8
A	1258	GLY	-	expression tag	UNP A0A346FJN8
A	1259	SER	-	expression tag	UNP A0A346FJN8
A	1260	GLY	-	expression tag	UNP A0A346FJN8
A	1261	GLY	-	expression tag	UNP A0A346FJN8
A	1262	SER	-	expression tag	UNP A0A346FJN8
A	1263	ALA	-	expression tag	UNP A0A346FJN8
A	1264	TRP	-	expression tag	UNP A0A346FJN8
A	1265	SER	-	expression tag	UNP A0A346FJN8
A	1266	HIS	-	expression tag	UNP A0A346FJN8
A	1267	PRO	-	expression tag	UNP A0A346FJN8
A	1268	GLN	-	expression tag	UNP A0A346FJN8
A	1269	PHE	-	expression tag	UNP A0A346FJN8
A	1270	GLU	-	expression tag	UNP A0A346FJN8
A	1271	LYS	-	expression tag	UNP A0A346FJN8
C	969	PRO	LYS	conflict	UNP U5WLK5
C	970	PRO	VAL	conflict	UNP U5WLK5
C	1192	GLY	-	linker	UNP U5WLK5
C	1193	SER	-	linker	UNP U5WLK5
C	1220	LEU	-	expression tag	UNP A0A346FJN8
C	1221	GLY	-	expression tag	UNP A0A346FJN8
C	1222	ARG	-	expression tag	UNP A0A346FJN8
C	1223	SER	-	expression tag	UNP A0A346FJN8
C	1224	LEU	-	expression tag	UNP A0A346FJN8
C	1225	GLU	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	VAL	-	expression tag	UNP A0A346FJN8
C	1227	LEU	-	expression tag	UNP A0A346FJN8
C	1228	PHE	-	expression tag	UNP A0A346FJN8
C	1229	GLN	-	expression tag	UNP A0A346FJN8
C	1230	GLY	-	expression tag	UNP A0A346FJN8
C	1231	PRO	-	expression tag	UNP A0A346FJN8
C	1232	GLY	-	expression tag	UNP A0A346FJN8
C	1233	HIS	-	expression tag	UNP A0A346FJN8
C	1234	HIS	-	expression tag	UNP A0A346FJN8
C	1235	HIS	-	expression tag	UNP A0A346FJN8
C	1236	HIS	-	expression tag	UNP A0A346FJN8
C	1237	HIS	-	expression tag	UNP A0A346FJN8
C	1238	HIS	-	expression tag	UNP A0A346FJN8
C	1239	HIS	-	expression tag	UNP A0A346FJN8
C	1240	HIS	-	expression tag	UNP A0A346FJN8
C	1241	SER	-	expression tag	UNP A0A346FJN8
C	1242	ALA	-	expression tag	UNP A0A346FJN8
C	1243	TRP	-	expression tag	UNP A0A346FJN8
C	1244	SER	-	expression tag	UNP A0A346FJN8
C	1245	HIS	-	expression tag	UNP A0A346FJN8
C	1246	PRO	-	expression tag	UNP A0A346FJN8
C	1247	GLN	-	expression tag	UNP A0A346FJN8
C	1248	PHE	-	expression tag	UNP A0A346FJN8
C	1249	GLU	-	expression tag	UNP A0A346FJN8
C	1250	LYS	-	expression tag	UNP A0A346FJN8
C	1251	GLY	-	expression tag	UNP A0A346FJN8
C	1252	GLY	-	expression tag	UNP A0A346FJN8
C	1253	GLY	-	expression tag	UNP A0A346FJN8
C	1254	SER	-	expression tag	UNP A0A346FJN8
C	1255	GLY	-	expression tag	UNP A0A346FJN8
C	1256	GLY	-	expression tag	UNP A0A346FJN8
C	1257	GLY	-	expression tag	UNP A0A346FJN8
C	1258	GLY	-	expression tag	UNP A0A346FJN8
C	1259	SER	-	expression tag	UNP A0A346FJN8
C	1260	GLY	-	expression tag	UNP A0A346FJN8
C	1261	GLY	-	expression tag	UNP A0A346FJN8
C	1262	SER	-	expression tag	UNP A0A346FJN8
C	1263	ALA	-	expression tag	UNP A0A346FJN8
C	1264	TRP	-	expression tag	UNP A0A346FJN8
C	1265	SER	-	expression tag	UNP A0A346FJN8
C	1266	HIS	-	expression tag	UNP A0A346FJN8
C	1267	PRO	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	GLN	-	expression tag	UNP A0A346FJN8
C	1269	PHE	-	expression tag	UNP A0A346FJN8
C	1270	GLU	-	expression tag	UNP A0A346FJN8
C	1271	LYS	-	expression tag	UNP A0A346FJN8
B	969	PRO	LYS	conflict	UNP U5WLK5
B	970	PRO	VAL	conflict	UNP U5WLK5
B	1192	GLY	-	linker	UNP U5WLK5
B	1193	SER	-	linker	UNP U5WLK5
B	1220	LEU	-	expression tag	UNP A0A346FJN8
B	1221	GLY	-	expression tag	UNP A0A346FJN8
B	1222	ARG	-	expression tag	UNP A0A346FJN8
B	1223	SER	-	expression tag	UNP A0A346FJN8
B	1224	LEU	-	expression tag	UNP A0A346FJN8
B	1225	GLU	-	expression tag	UNP A0A346FJN8
B	1226	VAL	-	expression tag	UNP A0A346FJN8
B	1227	LEU	-	expression tag	UNP A0A346FJN8
B	1228	PHE	-	expression tag	UNP A0A346FJN8
B	1229	GLN	-	expression tag	UNP A0A346FJN8
B	1230	GLY	-	expression tag	UNP A0A346FJN8
B	1231	PRO	-	expression tag	UNP A0A346FJN8
B	1232	GLY	-	expression tag	UNP A0A346FJN8
B	1233	HIS	-	expression tag	UNP A0A346FJN8
B	1234	HIS	-	expression tag	UNP A0A346FJN8
B	1235	HIS	-	expression tag	UNP A0A346FJN8
B	1236	HIS	-	expression tag	UNP A0A346FJN8
B	1237	HIS	-	expression tag	UNP A0A346FJN8
B	1238	HIS	-	expression tag	UNP A0A346FJN8
B	1239	HIS	-	expression tag	UNP A0A346FJN8
B	1240	HIS	-	expression tag	UNP A0A346FJN8
B	1241	SER	-	expression tag	UNP A0A346FJN8
B	1242	ALA	-	expression tag	UNP A0A346FJN8
B	1243	TRP	-	expression tag	UNP A0A346FJN8
B	1244	SER	-	expression tag	UNP A0A346FJN8
B	1245	HIS	-	expression tag	UNP A0A346FJN8
B	1246	PRO	-	expression tag	UNP A0A346FJN8
B	1247	GLN	-	expression tag	UNP A0A346FJN8
B	1248	PHE	-	expression tag	UNP A0A346FJN8
B	1249	GLU	-	expression tag	UNP A0A346FJN8
B	1250	LYS	-	expression tag	UNP A0A346FJN8
B	1251	GLY	-	expression tag	UNP A0A346FJN8
B	1252	GLY	-	expression tag	UNP A0A346FJN8
B	1253	GLY	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1254	SER	-	expression tag	UNP A0A346FJN8
B	1255	GLY	-	expression tag	UNP A0A346FJN8
B	1256	GLY	-	expression tag	UNP A0A346FJN8
B	1257	GLY	-	expression tag	UNP A0A346FJN8
B	1258	GLY	-	expression tag	UNP A0A346FJN8
B	1259	SER	-	expression tag	UNP A0A346FJN8
B	1260	GLY	-	expression tag	UNP A0A346FJN8
B	1261	GLY	-	expression tag	UNP A0A346FJN8
B	1262	SER	-	expression tag	UNP A0A346FJN8
B	1263	ALA	-	expression tag	UNP A0A346FJN8
B	1264	TRP	-	expression tag	UNP A0A346FJN8
B	1265	SER	-	expression tag	UNP A0A346FJN8
B	1266	HIS	-	expression tag	UNP A0A346FJN8
B	1267	PRO	-	expression tag	UNP A0A346FJN8
B	1268	GLN	-	expression tag	UNP A0A346FJN8
B	1269	PHE	-	expression tag	UNP A0A346FJN8
B	1270	GLU	-	expression tag	UNP A0A346FJN8
B	1271	LYS	-	expression tag	UNP A0A346FJN8

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		
2	i	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	p	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	r	2	Total	C	N	O	0	0
			28	16	2	10		
2	t	2	Total	C	N	O	0	0
			28	16	2	10		
2	u	2	Total	C	N	O	0	0
			28	16	2	10		
2	v	2	Total	C	N	O	0	0
			28	16	2	10		
2	w	2	Total	C	N	O	0	0
			28	16	2	10		

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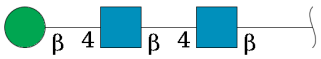
Mol	Chain	Residues	Atoms	AltConf	Trace
2	x	2	Total C N O 28 16 2 10	0	0
2	y	2	Total C N O 28 16 2 10	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
3	E	3	Total C N O 39 22 2 15	0	0
3	F	3	Total C N O 39 22 2 15	0	0
3	G	3	Total C N O 39 22 2 15	0	0
3	H	3	Total C N O 39 22 2 15	0	0
3	I	3	Total C N O 39 22 2 15	0	0
3	M	3	Total C N O 39 22 2 15	0	0
3	U	3	Total C N O 39 22 2 15	0	0
3	V	3	Total C N O 39 22 2 15	0	0
3	W	3	Total C N O 39 22 2 15	0	0
3	X	3	Total C N O 39 22 2 15	0	0
3	Y	3	Total C N O 39 22 2 15	0	0
3	c	3	Total C N O 39 22 2 15	0	0
3	k	3	Total C N O 39 22 2 15	0	0
3	l	3	Total C N O 39 22 2 15	0	0
3	m	3	Total C N O 39 22 2 15	0	0

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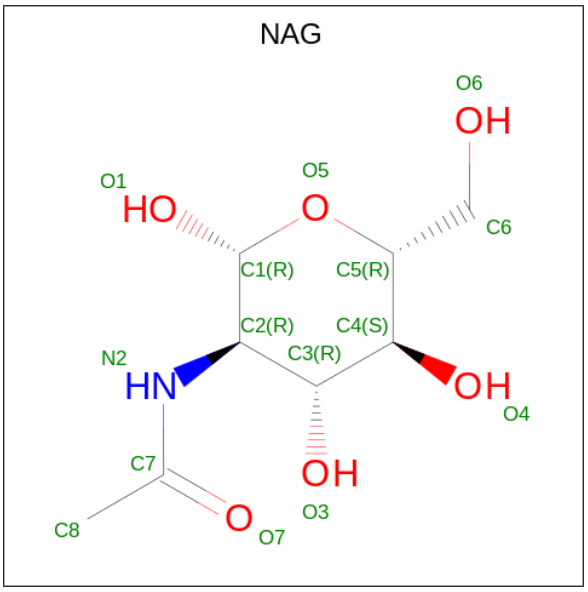
Mol	Chain	Residues	Atoms	AltConf	Trace
3	n	3	Total C N O 39 22 2 15	0	0
3	o	3	Total C N O 39 22 2 15	0	0
3	s	3	Total C N O 39 22 2 15	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



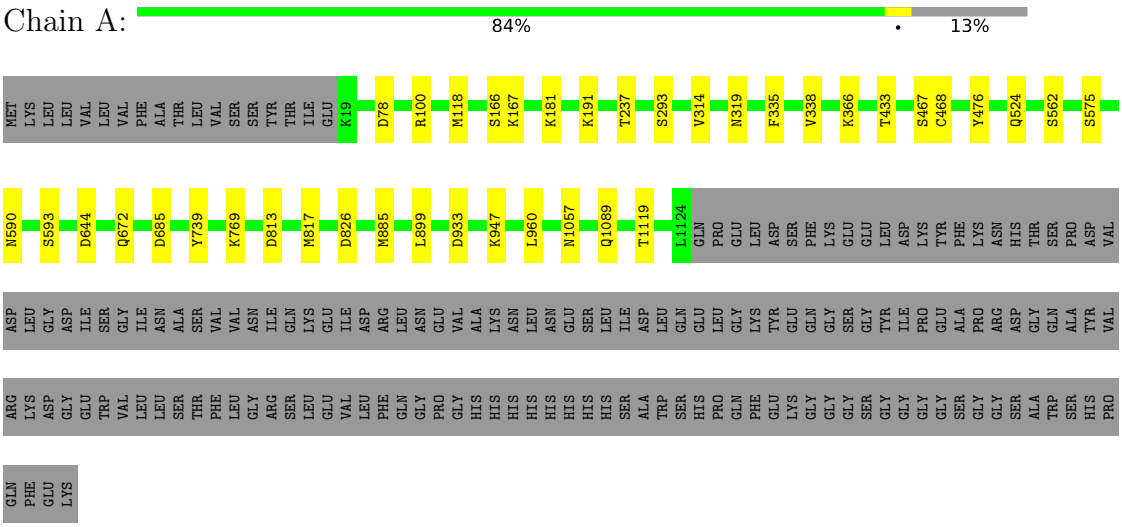
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0

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. 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. 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.

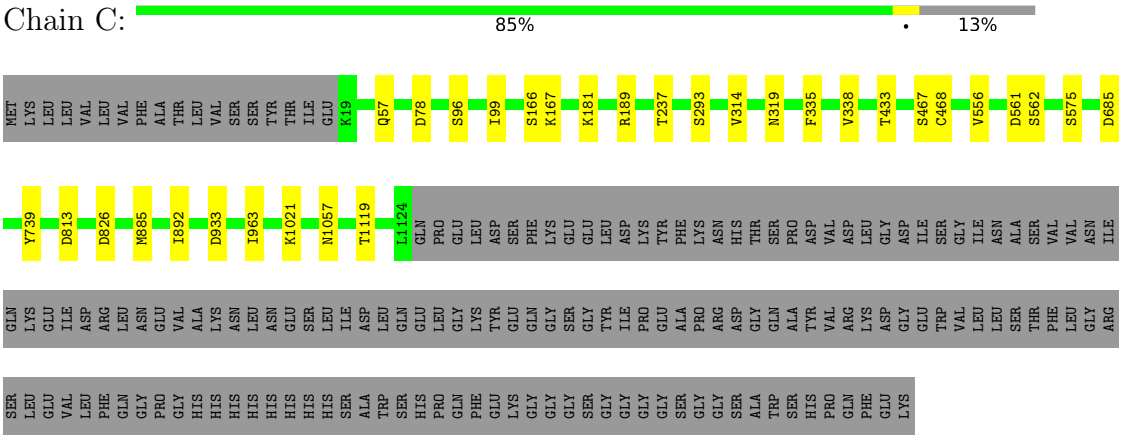
• Molecule 1: Spike glycoprotein,Fibritin

Chain A:



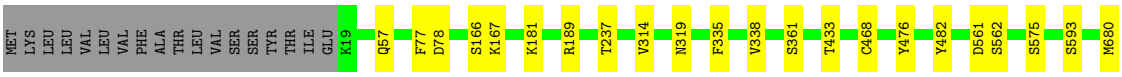
• Molecule 1: Spike glycoprotein,Fibritin

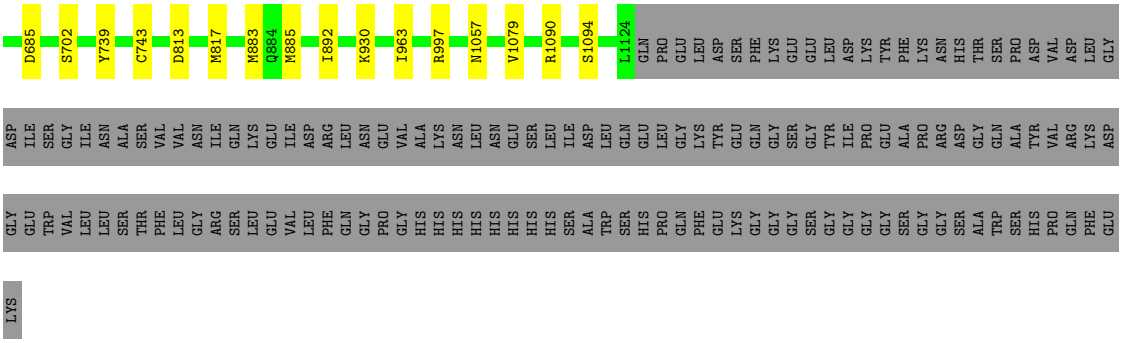
Chain C:



• Molecule 1: Spike glycoprotein,Fibritin

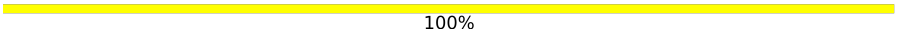
Chain B:





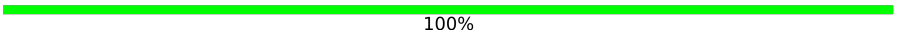
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



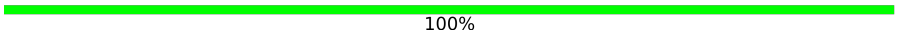
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



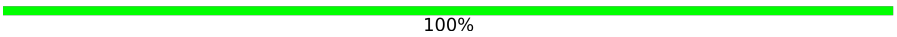
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:

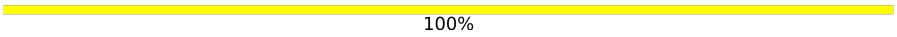


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

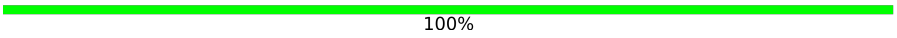
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



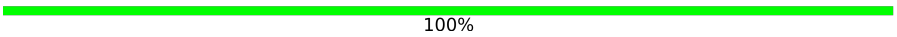
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



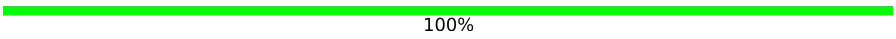
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



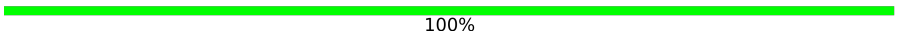
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



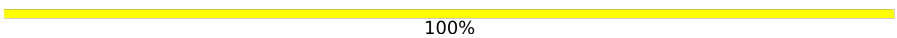
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



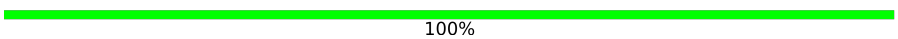
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



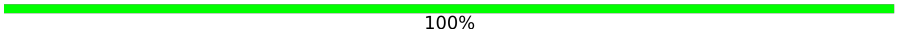
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



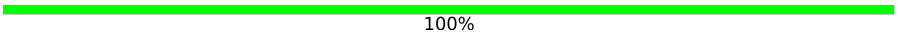
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



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

Chain b:

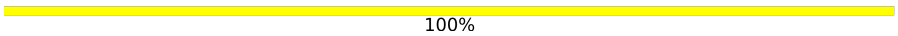


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

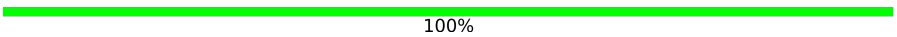
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



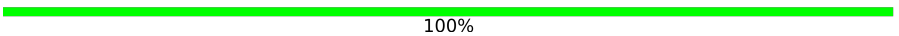
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



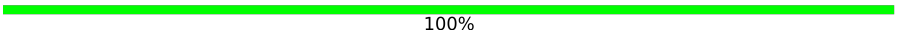
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



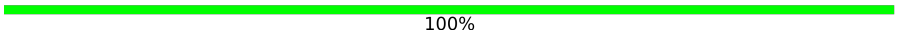
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



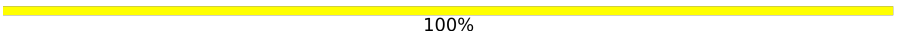
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



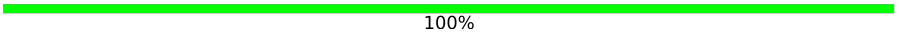
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



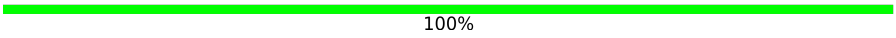
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



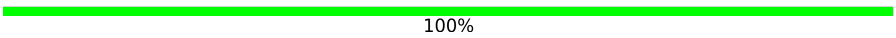
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



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

Chain r:

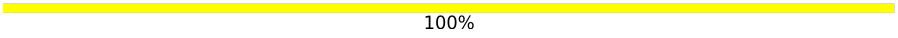


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

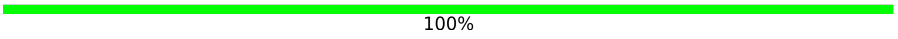
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



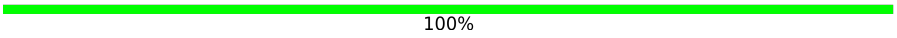
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



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

Chain w:

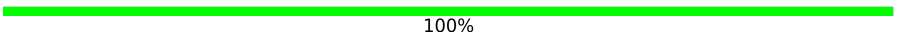


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

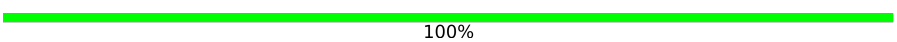
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:

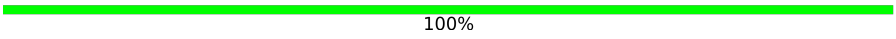


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

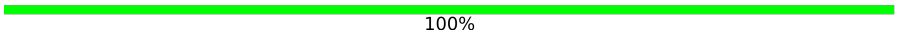
Chain E:



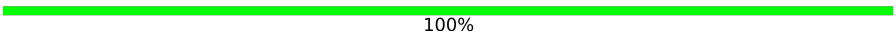
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

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

Chain G: 

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

Chain H: 

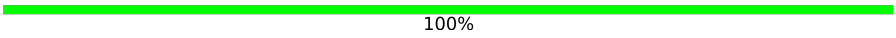
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

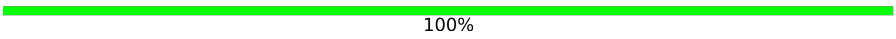
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

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

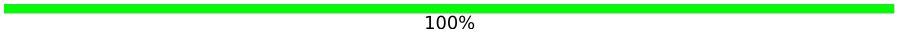
Chain U: 

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

Chain V: 

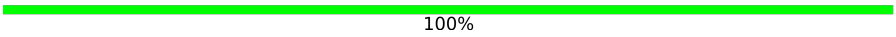
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain X:

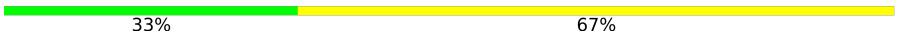


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

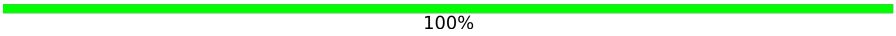
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



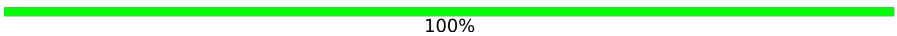
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



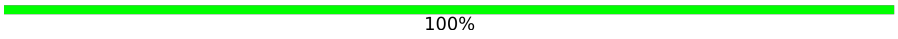
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



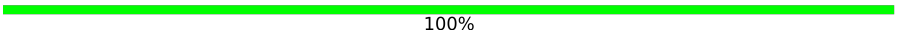
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



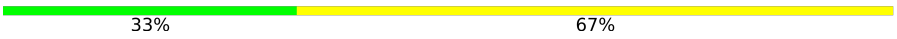
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



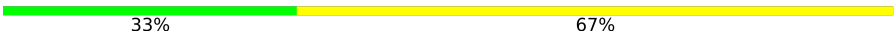
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	0/8810	0.51	0/11997
1	B	0.27	0/8810	0.50	0/11997
1	C	0.27	0/8810	0.51	0/11997
All	All	0.27	0/26430	0.51	0/35991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1104/1271 (87%)	1074 (97%)	30 (3%)	0	100	100
1	B	1104/1271 (87%)	1078 (98%)	26 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1104/1271 (87%)	1077 (98%)	27 (2%)	0	100	100
All	All	3312/3813 (87%)	3229 (98%)	83 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	960/1099 (87%)	921 (96%)	39 (4%)	26	57
1	B	960/1099 (87%)	922 (96%)	38 (4%)	27	58
1	C	960/1099 (87%)	928 (97%)	32 (3%)	33	65
All	All	2880/3297 (87%)	2771 (96%)	109 (4%)	30	60

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	A	100	ARG
1	A	118	MET
1	A	166	SER
1	A	167	LYS
1	A	181	LYS
1	A	191	LYS
1	A	237	THR
1	A	293	SER
1	A	314	VAL
1	A	319	ASN
1	A	335	PHE
1	A	338	VAL
1	A	366	LYS
1	A	433	THR
1	A	467	SER
1	A	468	CYS

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Mol	Chain	Res	Type
1	A	476	TYR
1	A	524	GLN
1	A	562	SER
1	A	575	SER
1	A	590	ASN
1	A	593	SER
1	A	644	ASP
1	A	672	GLN
1	A	685	ASP
1	A	739	TYR
1	A	769	LYS
1	A	813	ASP
1	A	817	MET
1	A	826	ASP
1	A	885	MET
1	A	899	LEU
1	A	933	ASP
1	A	947	LYS
1	A	960	LEU
1	A	1057	ASN
1	A	1089	GLN
1	A	1119	THR
1	C	57	GLN
1	C	78	ASP
1	C	96	SER
1	C	99	ILE
1	C	166	SER
1	C	167	LYS
1	C	181	LYS
1	C	189	ARG
1	C	237	THR
1	C	293	SER
1	C	314	VAL
1	C	319	ASN
1	C	335	PHE
1	C	338	VAL
1	C	433	THR
1	C	467	SER
1	C	468	CYS
1	C	556	VAL
1	C	561	ASP
1	C	562	SER

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Mol	Chain	Res	Type
1	C	575	SER
1	C	685	ASP
1	C	739	TYR
1	C	813	ASP
1	C	826	ASP
1	C	885	MET
1	C	892	ILE
1	C	933	ASP
1	C	963	ILE
1	C	1021	LYS
1	C	1057	ASN
1	C	1119	THR
1	B	57	GLN
1	B	77	PHE
1	B	78	ASP
1	B	166	SER
1	B	167	LYS
1	B	181	LYS
1	B	189	ARG
1	B	237	THR
1	B	314	VAL
1	B	319	ASN
1	B	335	PHE
1	B	338	VAL
1	B	361	SER
1	B	433	THR
1	B	468	CYS
1	B	476	TYR
1	B	482	TYR
1	B	561	ASP
1	B	562	SER
1	B	575	SER
1	B	593	SER
1	B	680	MET
1	B	685	ASP
1	B	702	SER
1	B	739	TYR
1	B	743	CYS
1	B	813	ASP
1	B	817	MET
1	B	883	MET
1	B	885	MET

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Mol	Chain	Res	Type
1	B	892	ILE
1	B	930	LYS
1	B	963	ILE
1	B	997	ARG
1	B	1057	ASN
1	B	1079	VAL
1	B	1090	ARG
1	B	1094	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	948	GLN
1	C	722	ASN
1	C	948	GLN
1	B	940	GLN
1	B	948	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

114 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	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.73	0	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	2	2	14,14,15	0.18	0	17,19,21	0.67	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.40	0
3	BMA	E	3	3	11,11,12	0.59	0	15,15,17	0.76	0
3	NAG	F	1	3,1	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	F	2	3	14,14,15	0.19	0	17,19,21	0.51	0
3	BMA	F	3	3	11,11,12	0.51	0	15,15,17	0.76	0
3	NAG	G	1	3,1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	G	2	3	14,14,15	0.17	0	17,19,21	0.47	0
3	BMA	G	3	3	11,11,12	0.69	0	15,15,17	0.70	0
3	NAG	H	1	3,1	14,14,15	0.35	0	17,19,21	0.47	0
3	NAG	H	2	3	14,14,15	0.35	0	17,19,21	0.40	0
3	BMA	H	3	3	11,11,12	0.55	0	15,15,17	0.73	0
3	NAG	I	1	3,1	14,14,15	0.44	0	17,19,21	0.45	0
3	NAG	I	2	3	14,14,15	0.65	1 (7%)	17,19,21	0.82	0
3	BMA	I	3	3	11,11,12	0.70	0	15,15,17	1.00	0
2	NAG	J	1	2,1	14,14,15	0.16	0	17,19,21	0.53	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.34	0
2	NAG	K	1	2,1	14,14,15	0.22	0	17,19,21	0.39	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	L	1	2,1	14,14,15	0.43	0	17,19,21	0.39	0
2	NAG	L	2	2	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	M	1	3,1	14,14,15	0.37	0	17,19,21	1.29	2 (11%)
3	NAG	M	2	3	14,14,15	0.67	1 (7%)	17,19,21	0.97	2 (11%)
3	BMA	M	3	3	11,11,12	0.76	0	15,15,17	0.91	0
2	NAG	N	1	2,1	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
2	NAG	N	2	2	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	O	1	2,1	14,14,15	0.55	0	17,19,21	1.40	2 (11%)
2	NAG	O	2	2	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
2	NAG	P	1	2,1	14,14,15	0.23	0	17,19,21	0.34	0
2	NAG	P	2	2	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	Q	1	2,1	14,14,15	0.28	0	17,19,21	0.33	0
2	NAG	Q	2	2	14,14,15	0.30	0	17,19,21	0.41	0
2	NAG	R	1	2,1	14,14,15	0.19	0	17,19,21	0.53	0
2	NAG	R	2	2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	S	1	2,1	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	S	2	2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	T	1	2,1	14,14,15	0.77	1 (7%)	17,19,21	1.13	2 (11%)
2	NAG	T	2	2	14,14,15	0.16	0	17,19,21	0.68	1 (5%)
3	NAG	U	1	3,1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	U	3	3	11,11,12	0.58	0	15,15,17	0.74	0
3	NAG	V	1	3,1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	V	2	3	14,14,15	0.20	0	17,19,21	0.51	0
3	BMA	V	3	3	11,11,12	0.51	0	15,15,17	0.75	0
3	NAG	W	1	3,1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	W	2	3	14,14,15	0.16	0	17,19,21	0.49	0
3	BMA	W	3	3	11,11,12	0.69	0	15,15,17	0.68	0
3	NAG	X	1	3,1	14,14,15	0.28	0	17,19,21	0.52	0
3	NAG	X	2	3	14,14,15	0.33	0	17,19,21	0.40	0
3	BMA	X	3	3	11,11,12	0.54	0	15,15,17	0.76	0
3	NAG	Y	1	3,1	14,14,15	0.52	0	17,19,21	0.48	0
3	NAG	Y	2	3	14,14,15	0.65	1 (7%)	17,19,21	0.84	0
3	BMA	Y	3	3	11,11,12	0.69	0	15,15,17	1.00	0
2	NAG	Z	1	2,1	14,14,15	0.17	0	17,19,21	0.50	0
2	NAG	Z	2	2	14,14,15	0.23	0	17,19,21	0.35	0
2	NAG	a	1	2,1	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	a	2	2	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	b	1	2,1	14,14,15	0.41	0	17,19,21	0.41	0
2	NAG	b	2	2	14,14,15	0.28	0	17,19,21	0.42	0
3	NAG	c	1	3,1	14,14,15	0.37	0	17,19,21	1.30	2 (11%)
3	NAG	c	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.98	2 (11%)
3	BMA	c	3	3	11,11,12	0.74	0	15,15,17	0.92	0
2	NAG	d	1	2,1	14,14,15	0.27	0	17,19,21	0.72	1 (5%)
2	NAG	d	2	2	14,14,15	0.33	0	17,19,21	0.47	0
2	NAG	e	1	2,1	14,14,15	0.55	0	17,19,21	1.40	2 (11%)
2	NAG	e	2	2	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
2	NAG	f	1	2,1	14,14,15	0.18	0	17,19,21	0.35	0
2	NAG	f	2	2	14,14,15	0.24	0	17,19,21	0.54	0
2	NAG	g	1	2,1	14,14,15	0.28	0	17,19,21	0.33	0
2	NAG	g	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	h	1	2,1	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	h	2	2	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	i	1	2,1	14,14,15	0.27	0	17,19,21	0.42	0
2	NAG	i	2	2	14,14,15	0.15	0	17,19,21	0.43	0
2	NAG	j	1	2,1	14,14,15	0.74	0	17,19,21	1.12	2 (11%)
2	NAG	j	2	2	14,14,15	0.15	0	17,19,21	0.70	1 (5%)
3	NAG	k	1	3,1	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	k	2	3	14,14,15	0.28	0	17,19,21	0.40	0
3	BMA	k	3	3	11,11,12	0.58	0	15,15,17	0.74	0
3	NAG	l	1	3,1	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	l	2	3	14,14,15	0.20	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	l	3	3	11,11,12	0.49	0	15,15,17	0.77	0
3	NAG	m	1	3,1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	m	2	3	14,14,15	0.18	0	17,19,21	0.45	0
3	BMA	m	3	3	11,11,12	0.69	0	15,15,17	0.69	0
3	NAG	n	1	3,1	14,14,15	0.33	0	17,19,21	0.51	0
3	NAG	n	2	3	14,14,15	0.33	0	17,19,21	0.40	0
3	BMA	n	3	3	11,11,12	0.55	0	15,15,17	0.74	0
3	NAG	o	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.63	0
3	NAG	o	2	3	14,14,15	0.73	1 (7%)	17,19,21	0.92	1 (5%)
3	BMA	o	3	3	11,11,12	0.73	0	15,15,17	0.96	0
2	NAG	p	1	2,1	14,14,15	0.18	0	17,19,21	0.51	0
2	NAG	p	2	2	14,14,15	0.24	0	17,19,21	0.35	0
2	NAG	q	1	2,1	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	q	2	2	14,14,15	0.19	0	17,19,21	0.39	0
2	NAG	r	1	2,1	14,14,15	0.39	0	17,19,21	0.38	0
2	NAG	r	2	2	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	s	1	3,1	14,14,15	0.38	0	17,19,21	1.31	2 (11%)
3	NAG	s	2	3	14,14,15	0.64	1 (7%)	17,19,21	0.98	2 (11%)
3	BMA	s	3	3	11,11,12	0.73	0	15,15,17	0.90	0
2	NAG	t	1	2,1	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
2	NAG	t	2	2	14,14,15	0.33	0	17,19,21	0.49	0
2	NAG	u	1	2,1	14,14,15	0.55	0	17,19,21	1.40	2 (11%)
2	NAG	u	2	2	14,14,15	0.43	0	17,19,21	0.80	1 (5%)
2	NAG	v	1	2,1	14,14,15	0.19	0	17,19,21	0.35	0
2	NAG	v	2	2	14,14,15	0.24	0	17,19,21	0.53	0
2	NAG	w	1	2,1	14,14,15	0.26	0	17,19,21	0.33	0
2	NAG	w	2	2	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	x	1	2,1	14,14,15	0.25	0	17,19,21	0.52	0
2	NAG	x	2	2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	y	1	2,1	14,14,15	0.30	0	17,19,21	0.45	0
2	NAG	y	2	2	14,14,15	0.16	0	17,19,21	0.42	0

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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	O	2	2	-	4/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	2/2/19/22	0/1/1/1
3	NAG	W	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	NAG	X	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	2/2/19/22	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	NAG	a	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	2/2/19/22	0/1/1/1
2	NAG	d	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1
2	NAG	e	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	e	2	2	-	4/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	NAG	g	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	0/6/23/26	0/1/1/1
2	NAG	i	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	i	2	2	-	0/6/23/26	0/1/1/1
2	NAG	j	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	j	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	k	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	k	2	3	-	0/6/23/26	0/1/1/1
3	BMA	k	3	3	-	0/2/19/22	0/1/1/1
3	NAG	l	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	l	2	3	-	0/6/23/26	0/1/1/1
3	BMA	l	3	3	-	2/2/19/22	0/1/1/1
3	NAG	m	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	0/6/23/26	0/1/1/1
3	BMA	m	3	3	-	0/2/19/22	0/1/1/1
3	NAG	n	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	BMA	n	3	3	-	0/2/19/22	0/1/1/1
3	NAG	o	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	o	2	3	-	4/6/23/26	0/1/1/1
3	BMA	o	3	3	-	2/2/19/22	0/1/1/1
2	NAG	p	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	p	2	2	-	2/6/23/26	0/1/1/1
2	NAG	q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	r	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	r	2	2	-	1/6/23/26	0/1/1/1
3	NAG	s	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	s	2	3	-	2/6/23/26	0/1/1/1
3	BMA	s	3	3	-	2/2/19/22	0/1/1/1
2	NAG	t	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	t	2	2	-	2/6/23/26	0/1/1/1
2	NAG	u	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	u	2	2	-	4/6/23/26	0/1/1/1
2	NAG	v	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	v	2	2	-	0/6/23/26	0/1/1/1
2	NAG	w	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	w	2	2	-	0/6/23/26	0/1/1/1
2	NAG	x	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	x	2	2	-	0/6/23/26	0/1/1/1
2	NAG	y	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	y	2	2	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	o	2	NAG	O5-C1	-2.59	1.39	1.43
3	c	2	NAG	O5-C1	-2.41	1.39	1.43
3	o	1	NAG	O5-C1	-2.41	1.39	1.43
3	M	2	NAG	O5-C1	-2.28	1.40	1.43
3	Y	2	NAG	O5-C1	-2.27	1.40	1.43
3	I	2	NAG	O5-C1	-2.26	1.40	1.43
3	s	2	NAG	O5-C1	-2.19	1.40	1.43
2	T	1	NAG	O5-C1	2.12	1.47	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	s	1	NAG	C2-N2-C7	4.32	129.05	122.90
3	c	1	NAG	C2-N2-C7	4.31	129.03	122.90
3	M	1	NAG	C2-N2-C7	4.29	129.01	122.90
2	e	1	NAG	C2-N2-C7	4.23	128.93	122.90
2	u	1	NAG	C2-N2-C7	4.23	128.92	122.90
2	O	1	NAG	C2-N2-C7	4.20	128.88	122.90
2	D	1	NAG	C1-O5-C5	3.11	116.41	112.19
2	j	1	NAG	C1-O5-C5	3.08	116.37	112.19
2	T	1	NAG	C1-O5-C5	3.06	116.34	112.19
2	e	2	NAG	C1-O5-C5	2.98	116.23	112.19
2	u	2	NAG	C1-O5-C5	2.87	116.08	112.19
2	O	2	NAG	C1-O5-C5	2.82	116.02	112.19
2	N	1	NAG	C1-O5-C5	2.61	115.73	112.19
2	t	1	NAG	C1-O5-C5	2.56	115.66	112.19
2	d	1	NAG	C1-O5-C5	2.55	115.65	112.19
2	j	2	NAG	C1-O5-C5	2.48	115.55	112.19
2	T	2	NAG	C1-O5-C5	2.42	115.47	112.19
2	D	2	NAG	C1-O5-C5	2.35	115.37	112.19
3	c	2	NAG	C3-C4-C5	2.18	114.13	110.24
3	s	2	NAG	C3-C4-C5	2.18	114.13	110.24
3	M	2	NAG	C3-C4-C5	2.18	114.12	110.24
2	T	1	NAG	O4-C4-C5	2.13	114.58	109.30
3	c	1	NAG	C1-C2-N2	2.10	114.08	110.49
3	c	2	NAG	O4-C4-C3	-2.10	105.49	110.35
3	o	2	NAG	O4-C4-C3	-2.10	105.50	110.35
3	s	1	NAG	C1-C2-N2	2.09	114.06	110.49
3	s	2	NAG	O4-C4-C3	-2.08	105.54	110.35
2	j	1	NAG	O4-C4-C5	2.07	114.44	109.30
2	D	1	NAG	O4-C4-C5	2.07	114.43	109.30
3	M	1	NAG	C1-C2-N2	2.07	114.02	110.49
2	O	1	NAG	O4-C4-C3	2.05	115.08	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	1	NAG	O4-C4-C3	2.04	115.06	110.35
3	M	2	NAG	O4-C4-C3	-2.04	105.64	110.35
2	u	1	NAG	O4-C4-C3	2.01	114.99	110.35

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	1	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	s	1	NAG	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	o	3	BMA	C4-C5-C6-O6
3	Y	3	BMA	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	t	2	NAG	O5-C5-C6-O6
2	u	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	o	3	BMA	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
3	s	1	NAG	C4-C5-C6-O6
3	Y	3	BMA	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	u	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	T	2	NAG	C8-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
2	e	1	NAG	C8-C7-N2-C2
2	e	1	NAG	O7-C7-N2-C2
2	e	2	NAG	C8-C7-N2-C2
2	e	2	NAG	O7-C7-N2-C2
2	j	2	NAG	C8-C7-N2-C2
2	j	2	NAG	O7-C7-N2-C2
2	u	1	NAG	C8-C7-N2-C2
2	u	1	NAG	O7-C7-N2-C2
2	u	2	NAG	C8-C7-N2-C2
2	u	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	c	1	NAG	C8-C7-N2-C2
3	c	1	NAG	O7-C7-N2-C2
3	l	1	NAG	C8-C7-N2-C2
3	l	1	NAG	O7-C7-N2-C2
3	m	1	NAG	C8-C7-N2-C2
3	m	1	NAG	O7-C7-N2-C2
3	o	1	NAG	C8-C7-N2-C2
3	o	1	NAG	O7-C7-N2-C2
3	o	2	NAG	C8-C7-N2-C2
3	o	2	NAG	O7-C7-N2-C2
3	s	1	NAG	C8-C7-N2-C2
3	s	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	j	1	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
2	j	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	p	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
3	l	3	BMA	C4-C5-C6-O6
3	n	1	NAG	C4-C5-C6-O6
3	V	3	BMA	C4-C5-C6-O6
3	n	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	p	2	NAG	O5-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
3	c	3	BMA	C4-C5-C6-O6
3	s	3	BMA	C4-C5-C6-O6
2	t	2	NAG	C4-C5-C6-O6
3	l	3	BMA	O5-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	i	1	NAG	C4-C5-C6-O6
2	y	1	NAG	C4-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6

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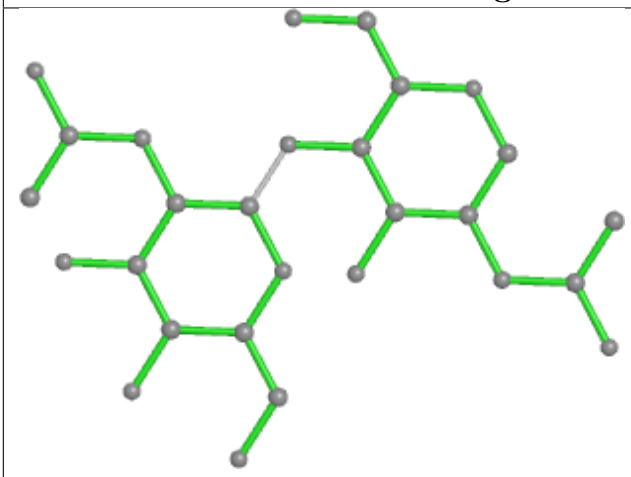
Mol	Chain	Res	Type	Atoms
3	X	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	y	1	NAG	O5-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
2	x	1	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C3-C2-N2-C7
2	e	1	NAG	C3-C2-N2-C7
2	u	1	NAG	C3-C2-N2-C7
2	R	1	NAG	O5-C5-C6-O6
3	c	3	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
3	s	3	BMA	O5-C5-C6-O6
3	M	2	NAG	C1-C2-N2-C7
2	N	2	NAG	C4-C5-C6-O6
2	x	1	NAG	O5-C5-C6-O6
3	c	2	NAG	C1-C2-N2-C7
3	s	2	NAG	C1-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	M	2	NAG	C3-C2-N2-C7
3	c	1	NAG	C3-C2-N2-C7
3	c	2	NAG	C3-C2-N2-C7
3	s	1	NAG	C3-C2-N2-C7
3	s	2	NAG	C3-C2-N2-C7
2	r	2	NAG	O5-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6

There are no ring outliers.

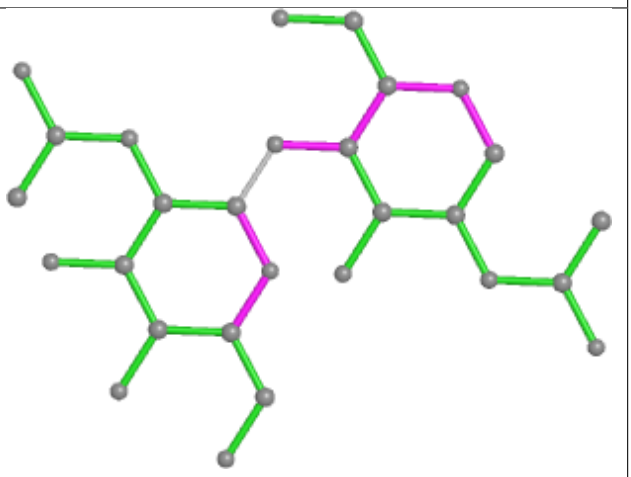
No monomer is involved in short contacts.

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

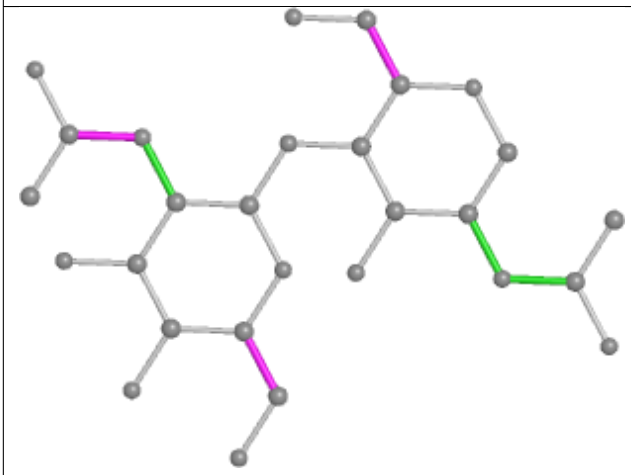
Oligosaccharide Chain D



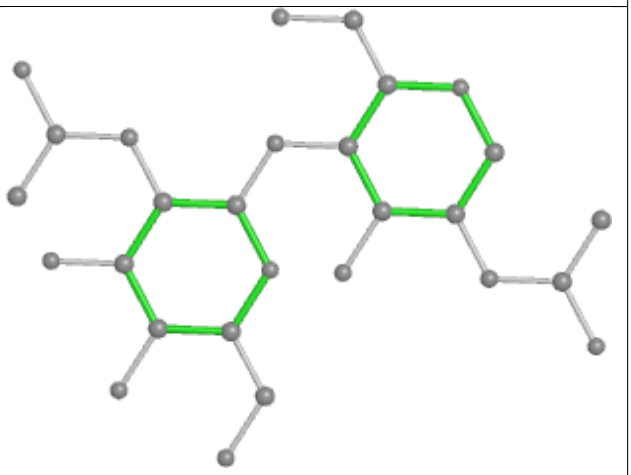
Bond lengths



Bond angles

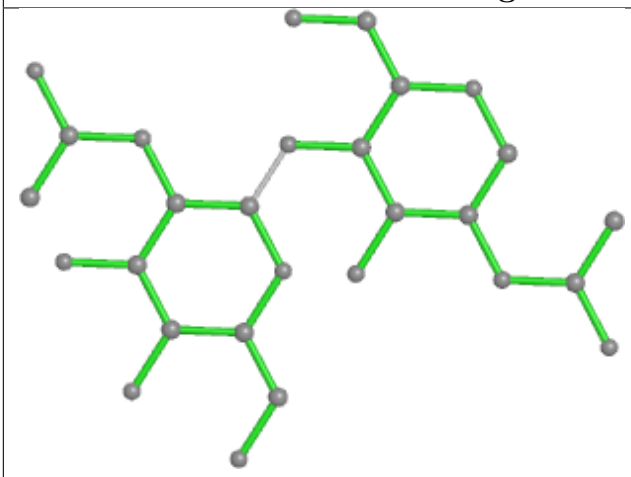


Torsions

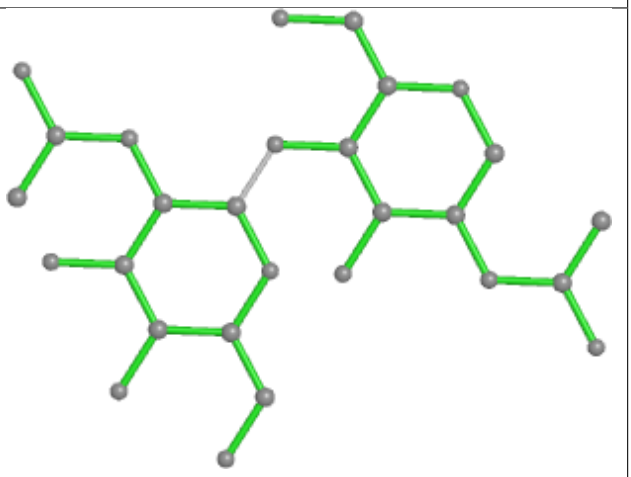


Rings

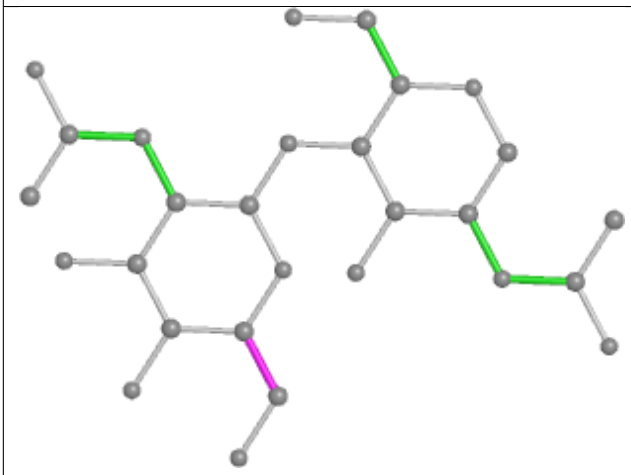
Oligosaccharide Chain J



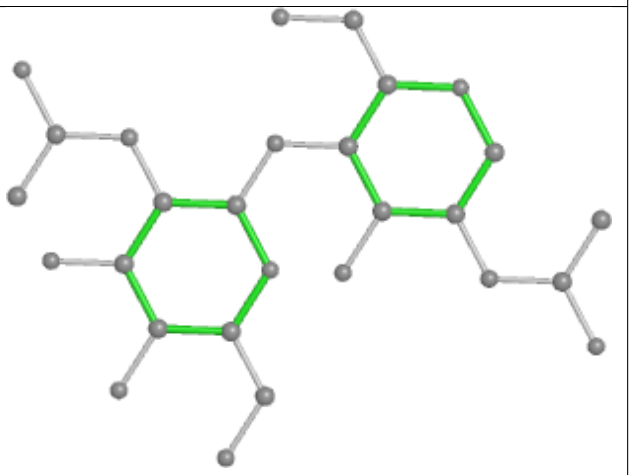
Bond lengths



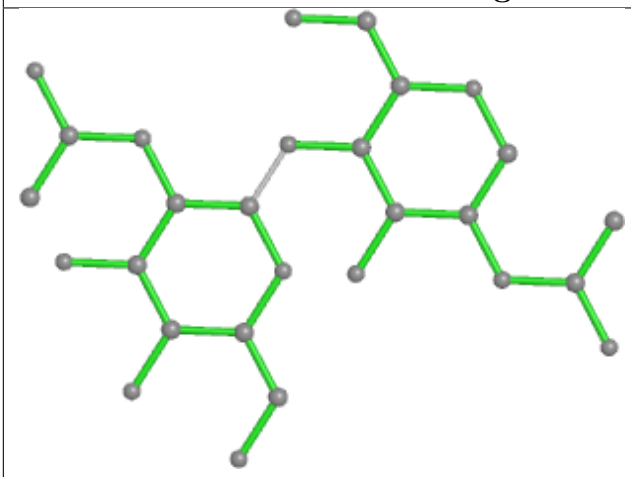
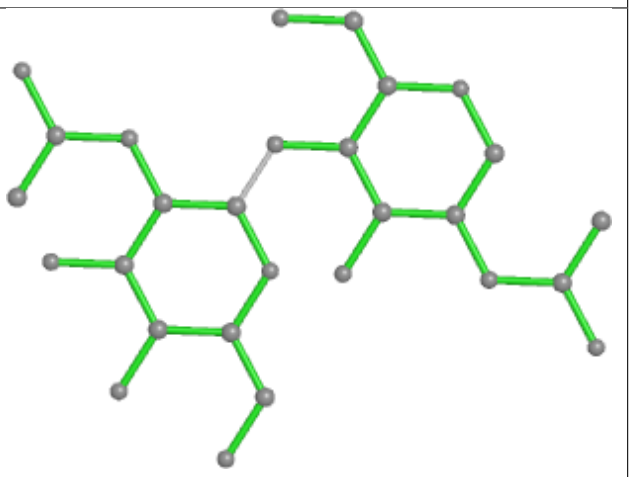
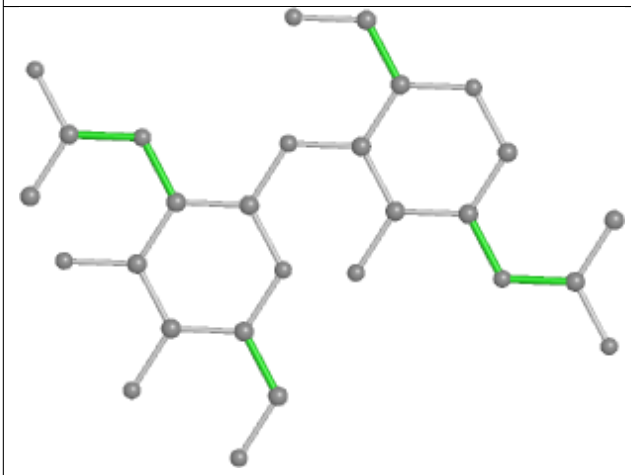
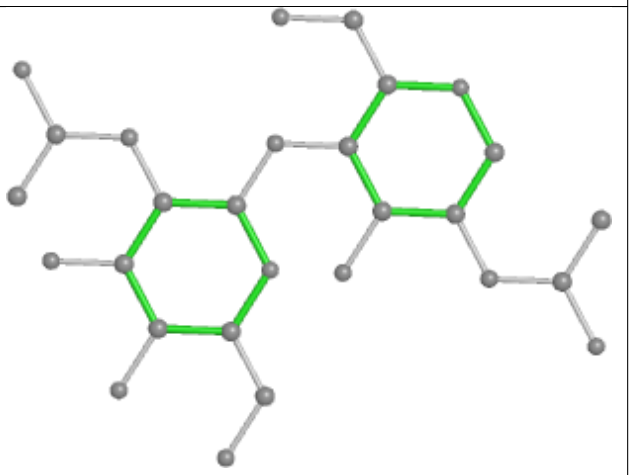
Bond angles



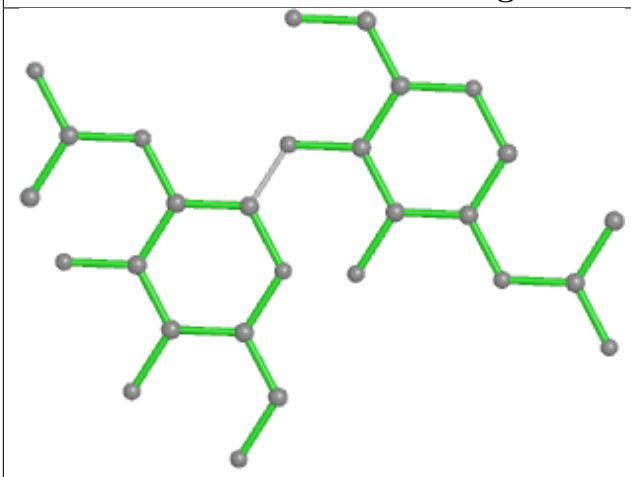
Torsions



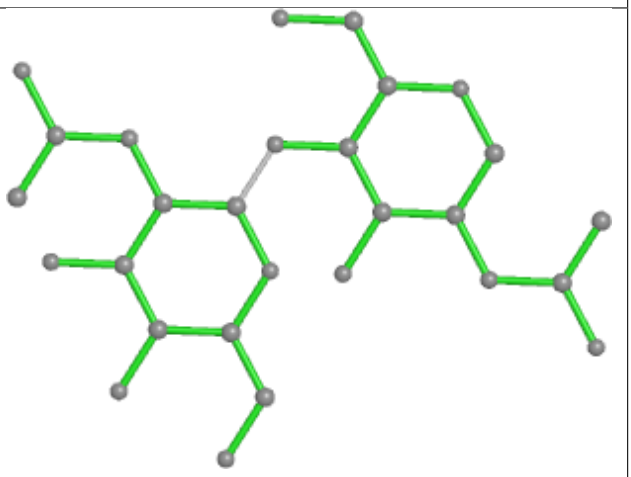
Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

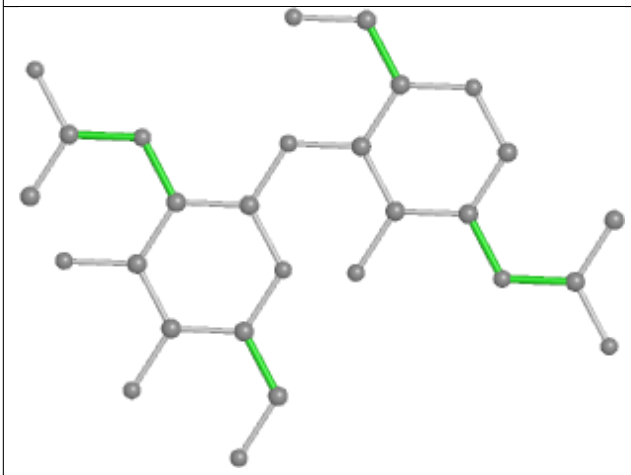
Oligosaccharide Chain L



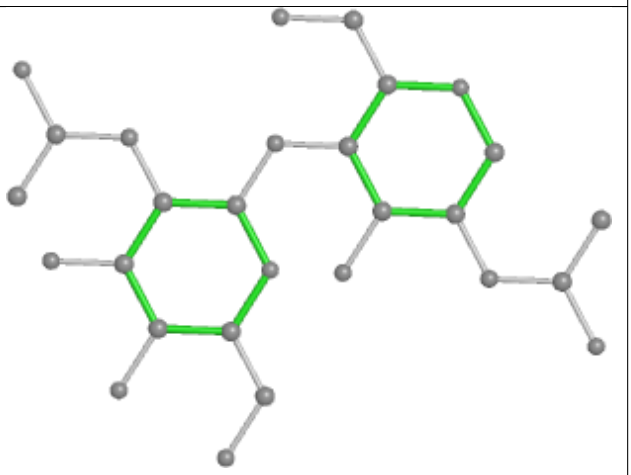
Bond lengths



Bond angles

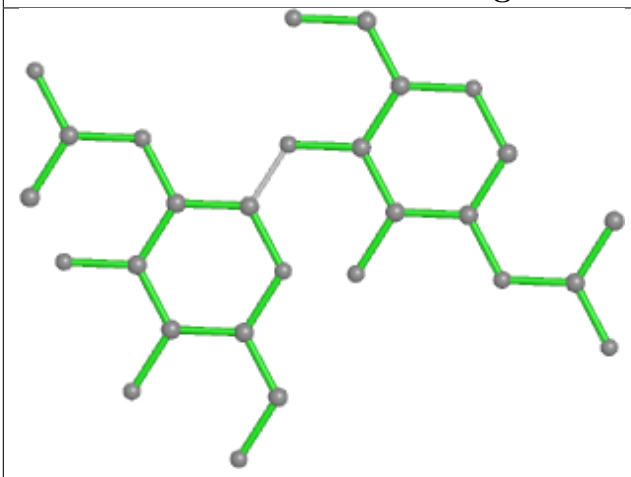


Torsions



Rings

Oligosaccharide Chain N



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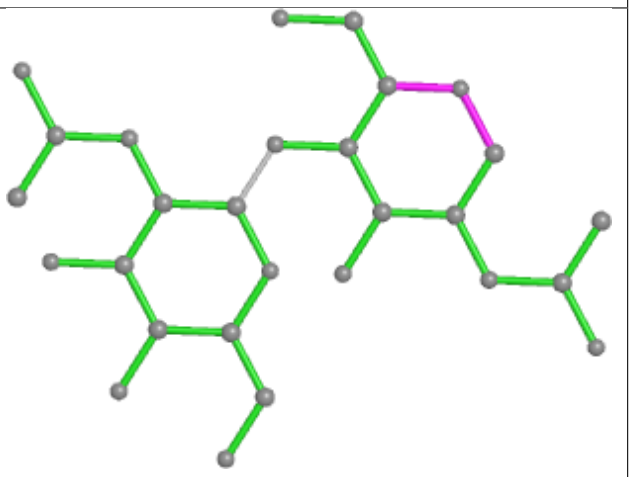
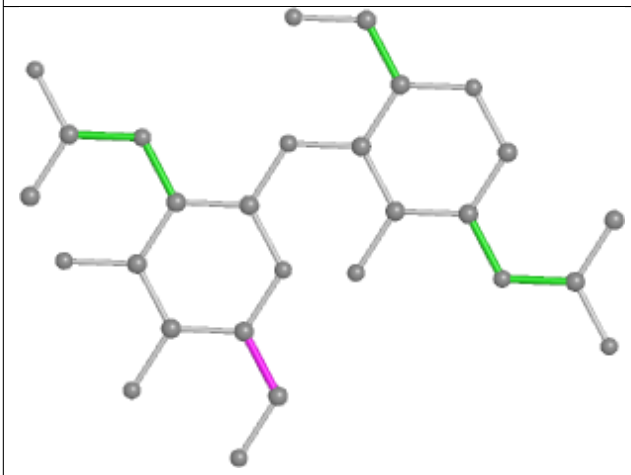
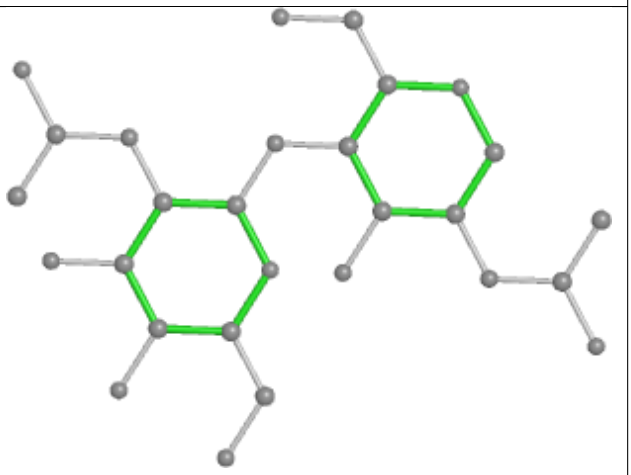


Bond angles

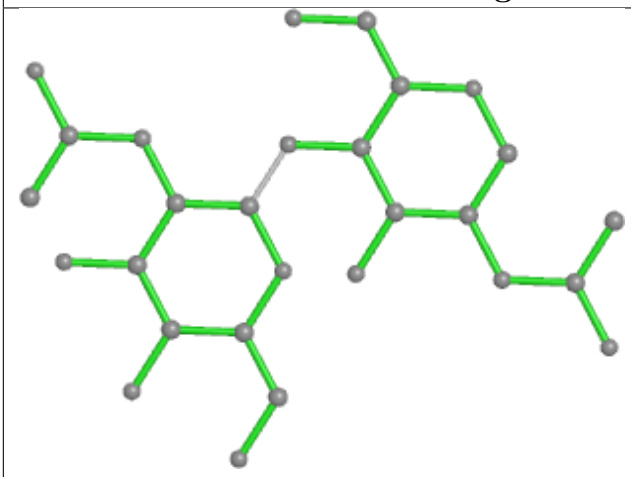


Torsions

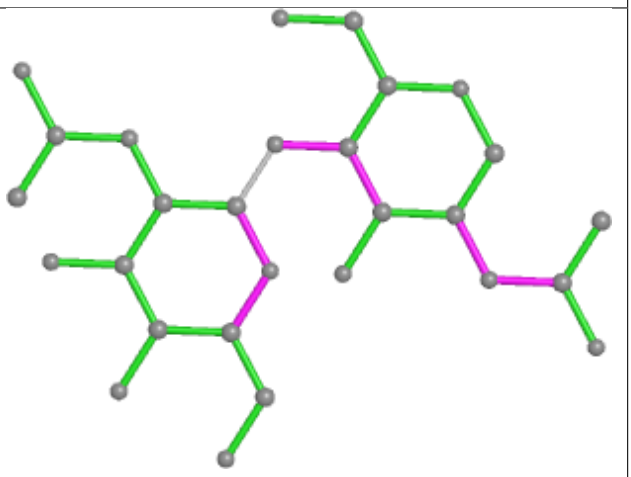


Rings

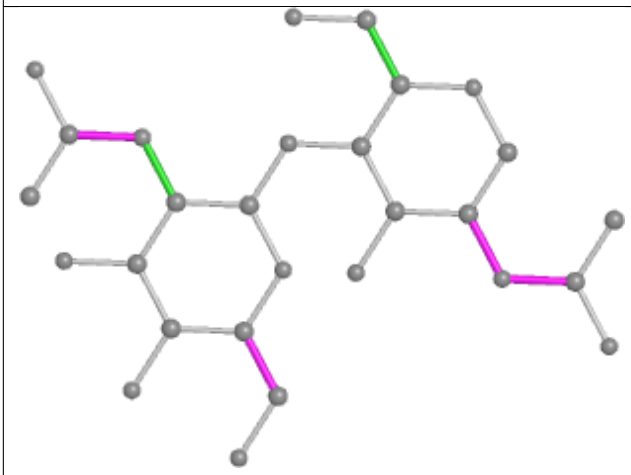
Oligosaccharide Chain O



Bond lengths



Bond angles



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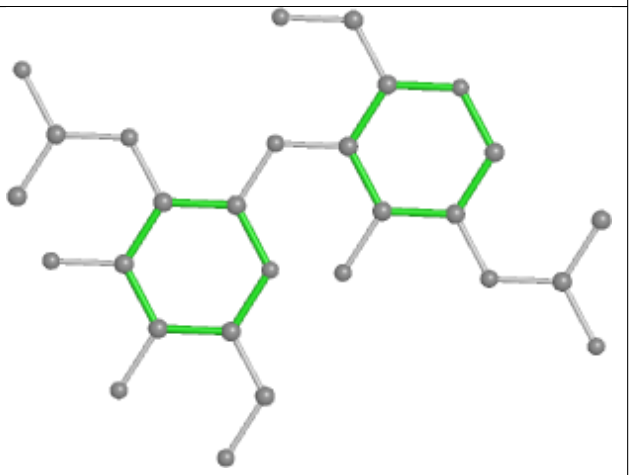
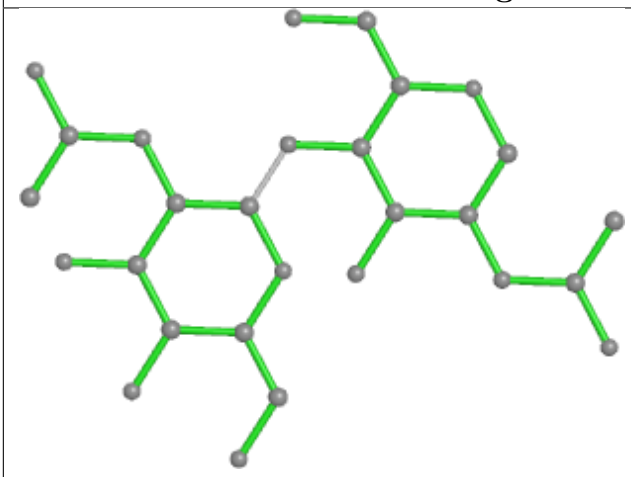
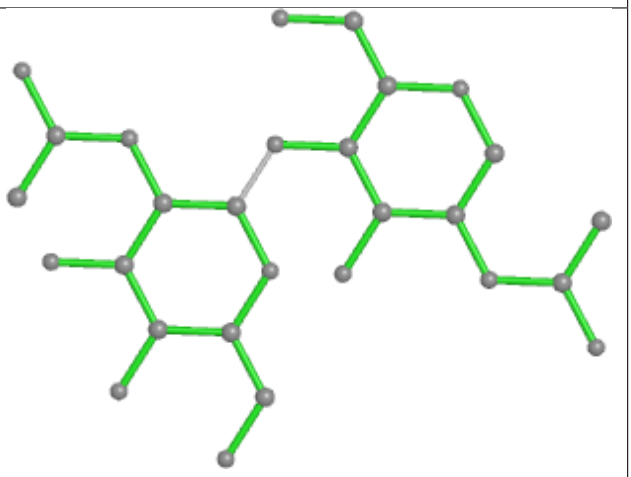


Rings

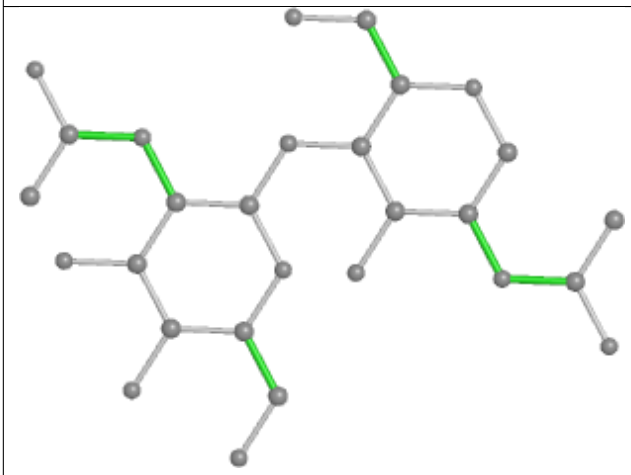
Oligosaccharide Chain P



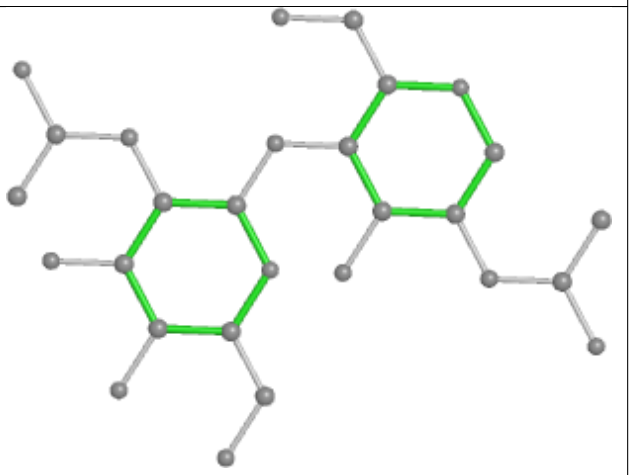
Bond lengths



Bond angles

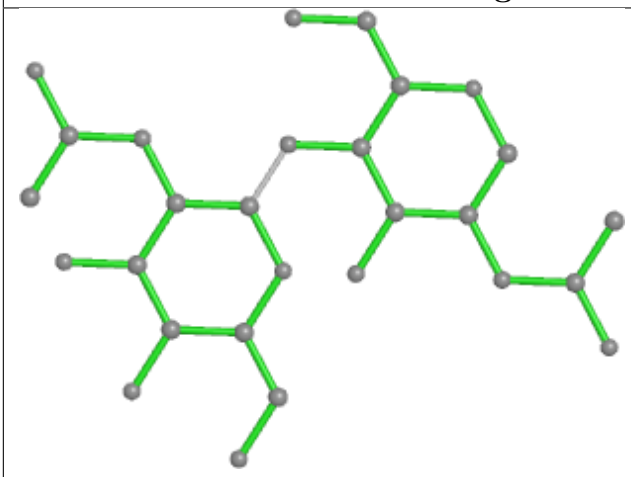


Torsions

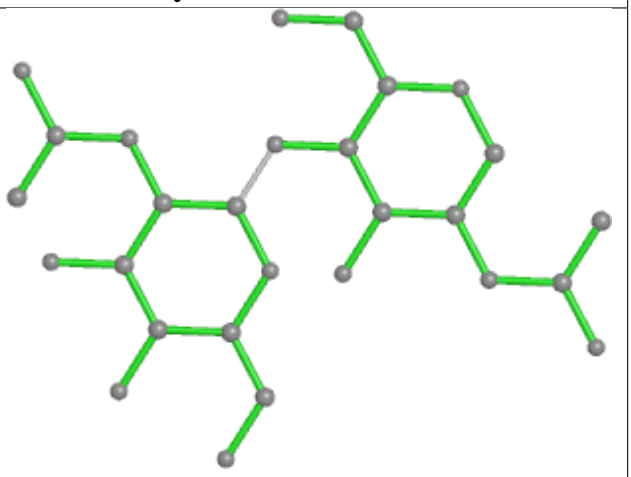


Rings

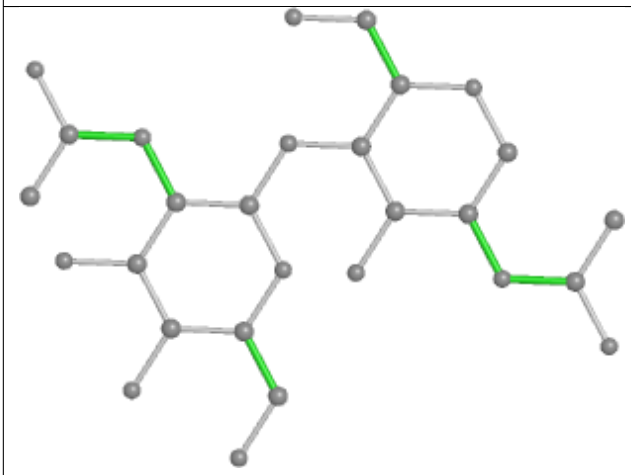
Oligosaccharide Chain Q



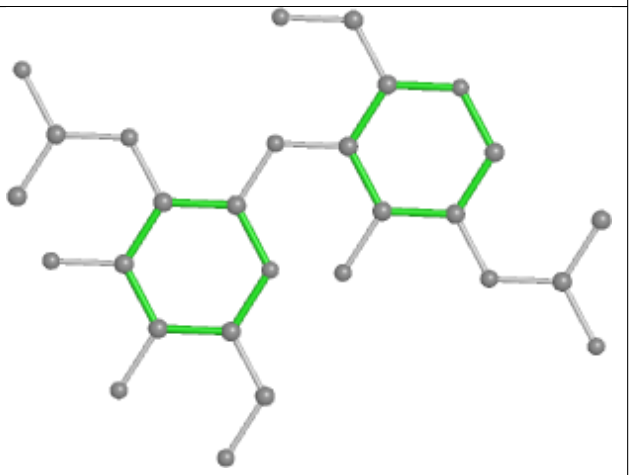
Bond lengths



Bond angles

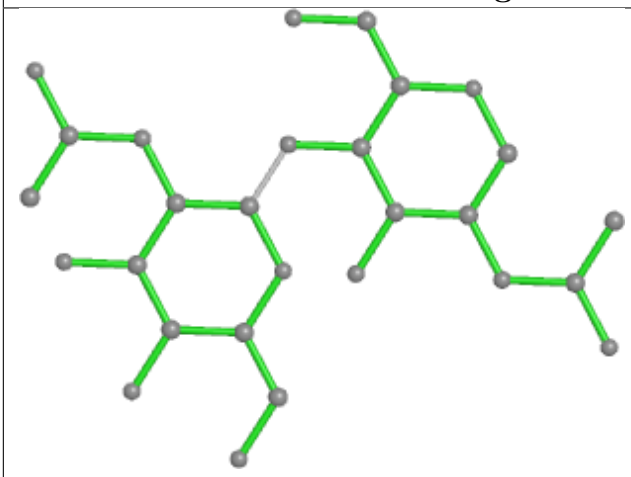


Torsions

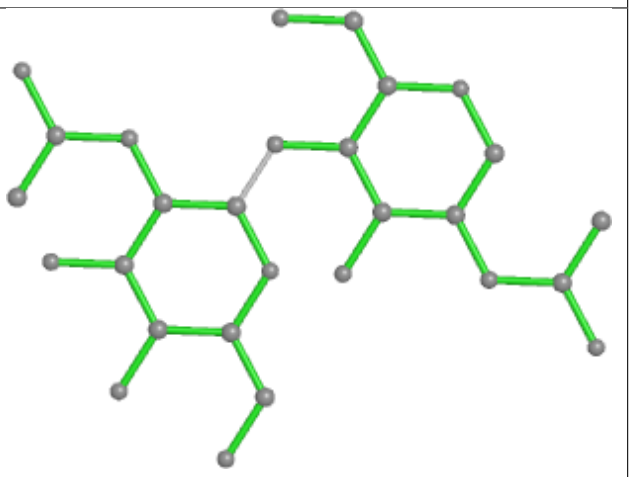


Rings

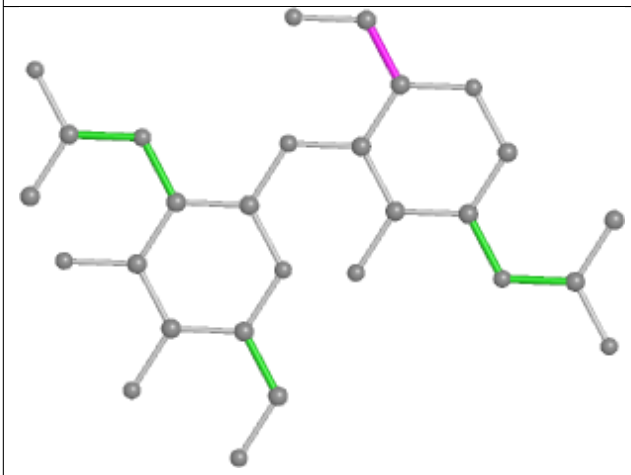
Oligosaccharide Chain R



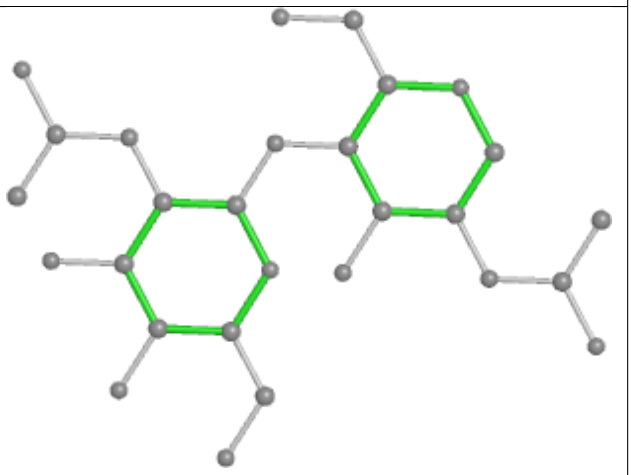
Bond lengths



Bond angles

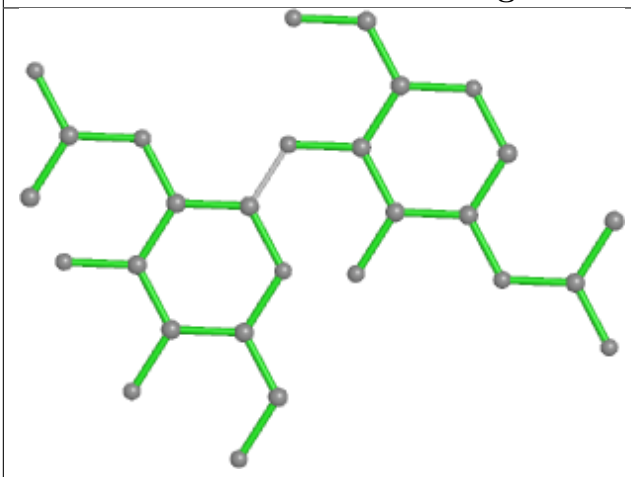


Torsions

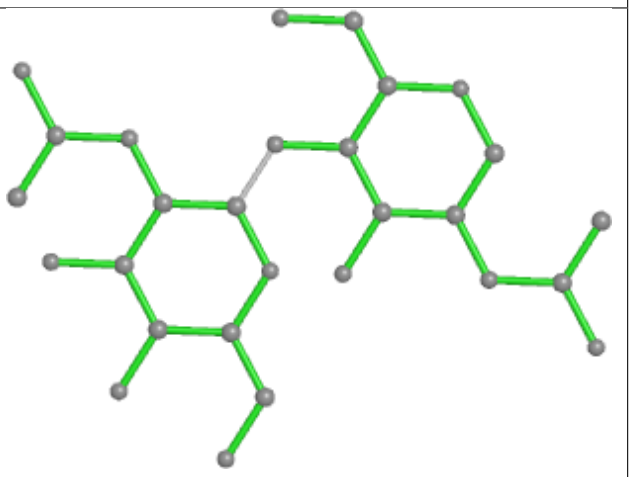


Rings

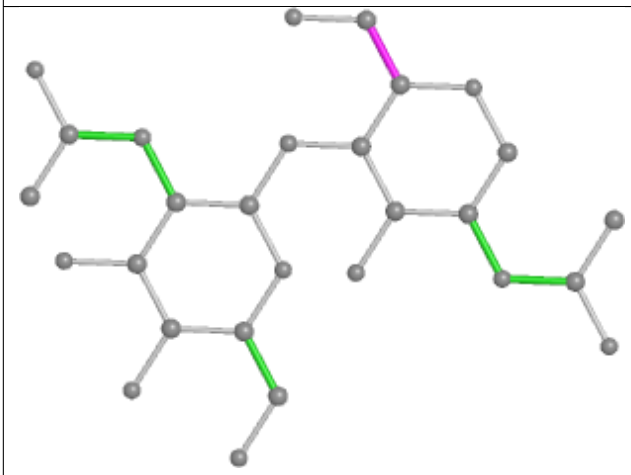
Oligosaccharide Chain S



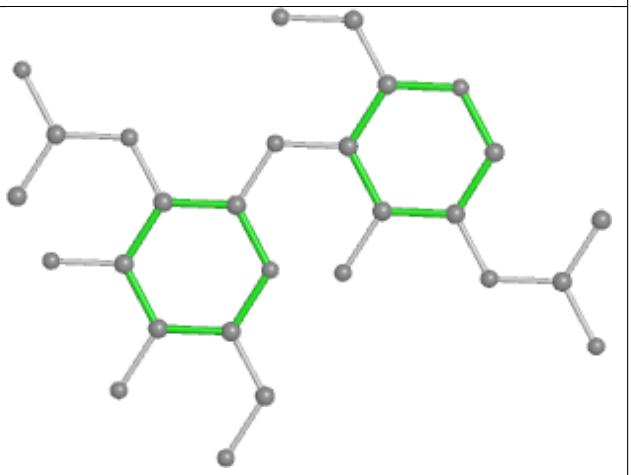
Bond lengths



Bond angles

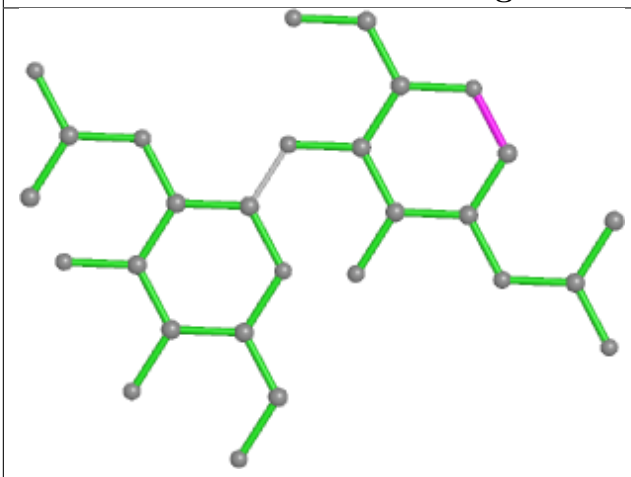


Torsions

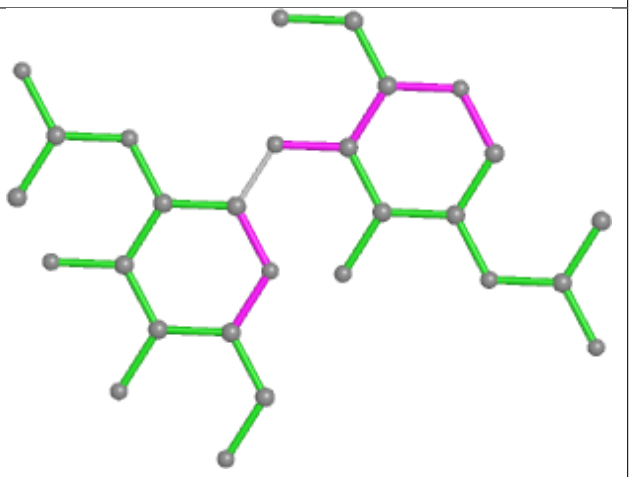


Rings

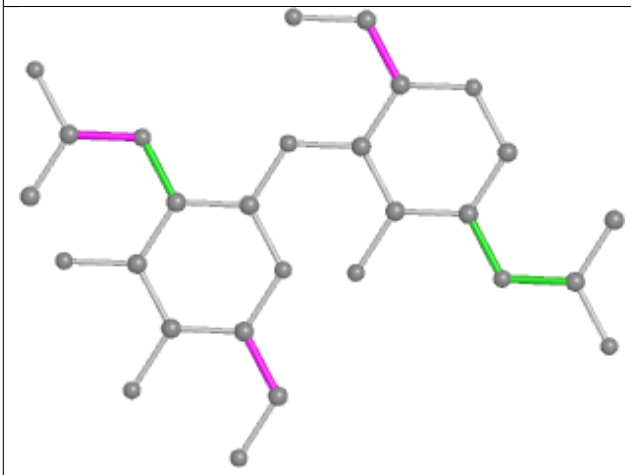
Oligosaccharide Chain T



Bond lengths



Bond angles



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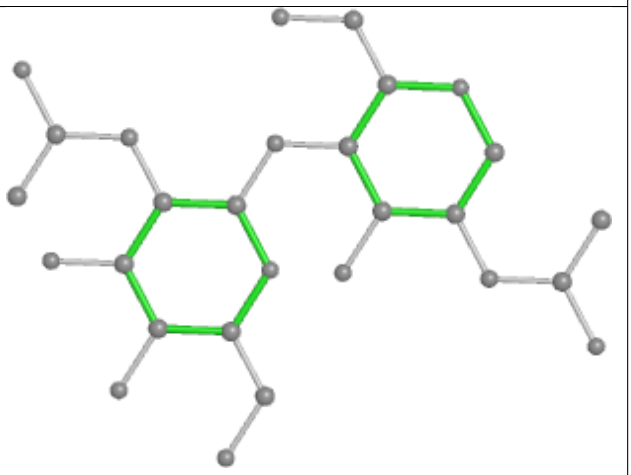
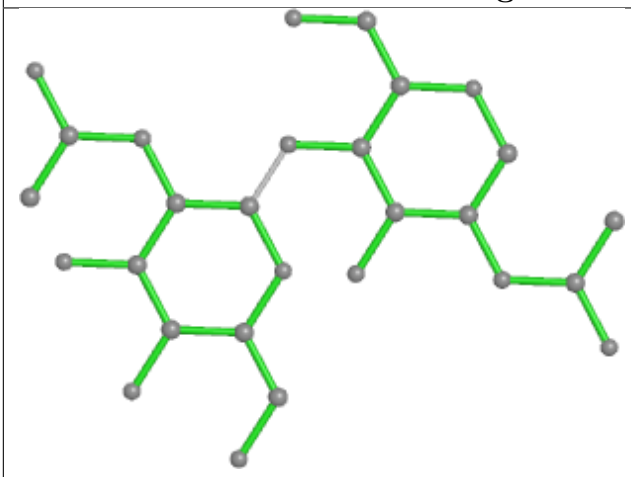


Rings

Oligosaccharide Chain Z



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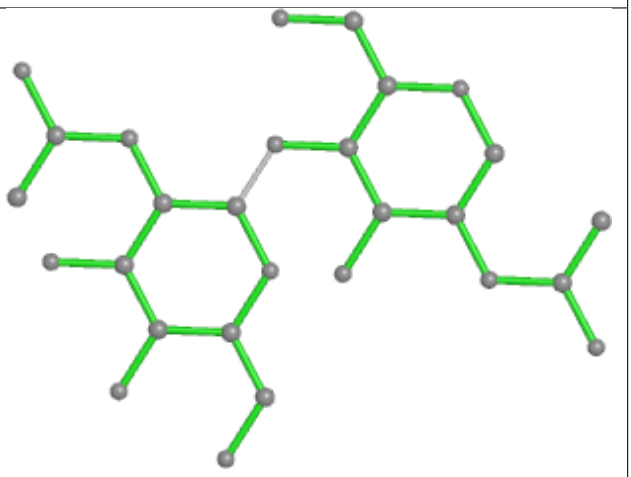
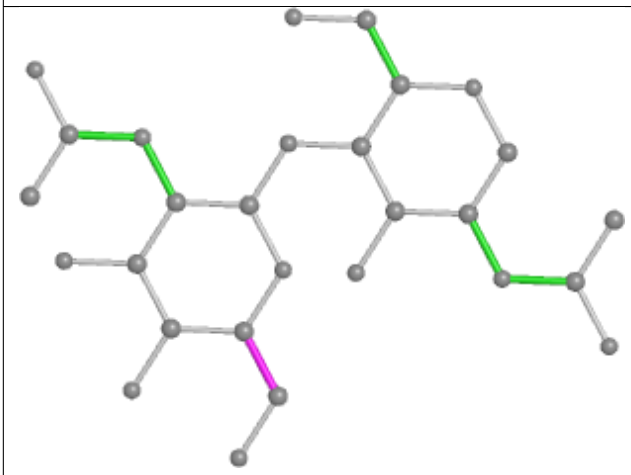
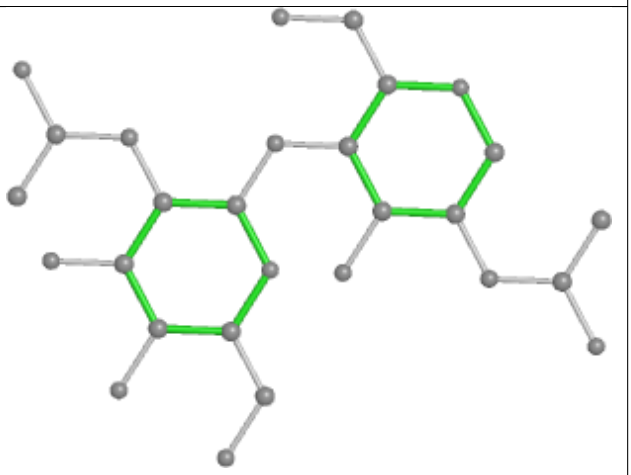


Bond angles

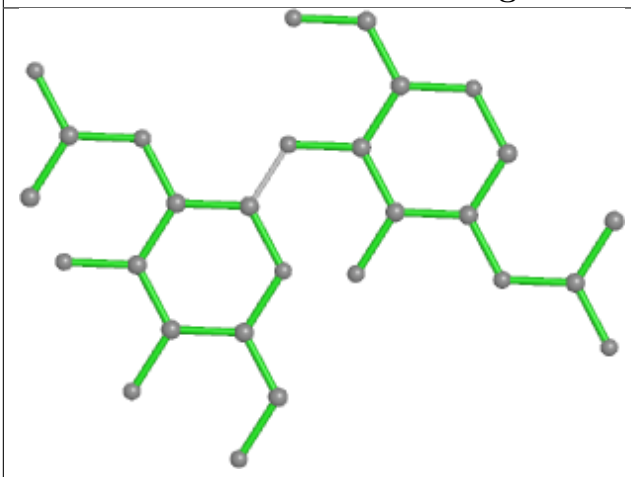


Torsions

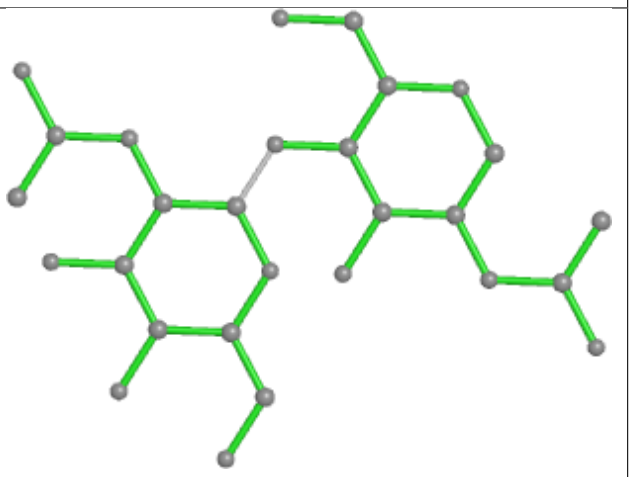


Rings

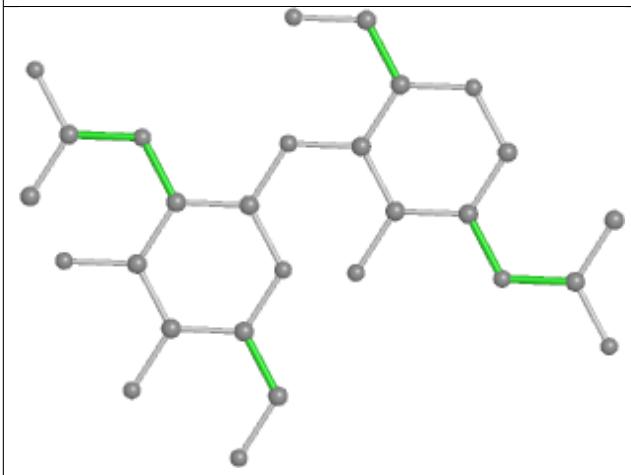
Oligosaccharide Chain a



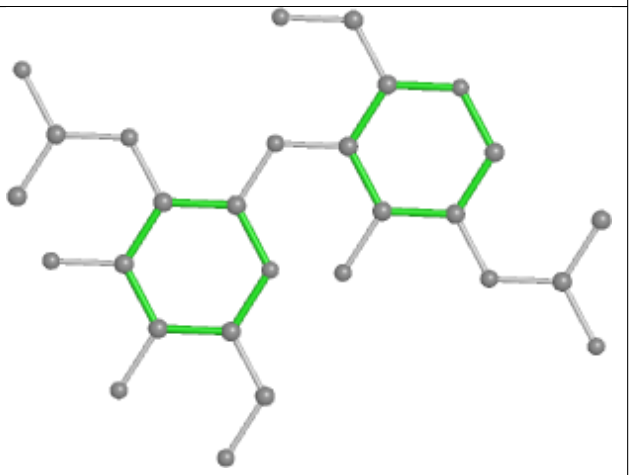
Bond lengths



Bond angles

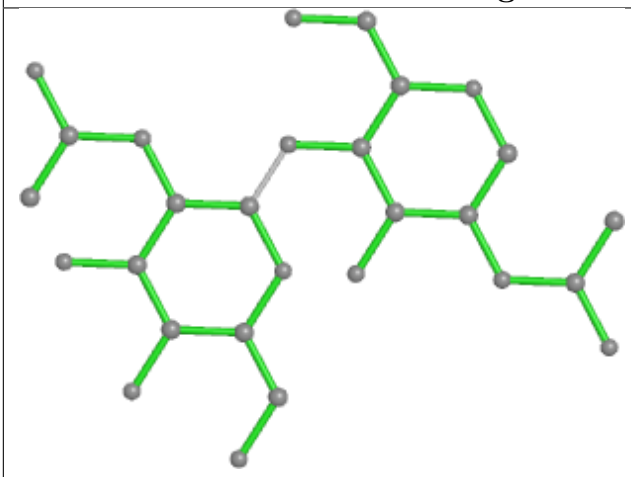


Torsions

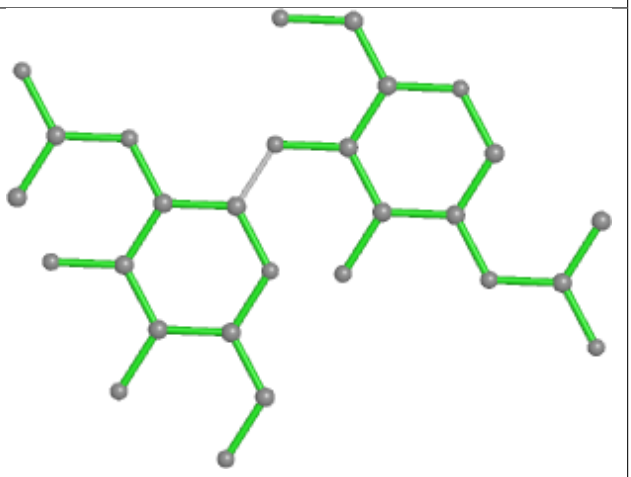


Rings

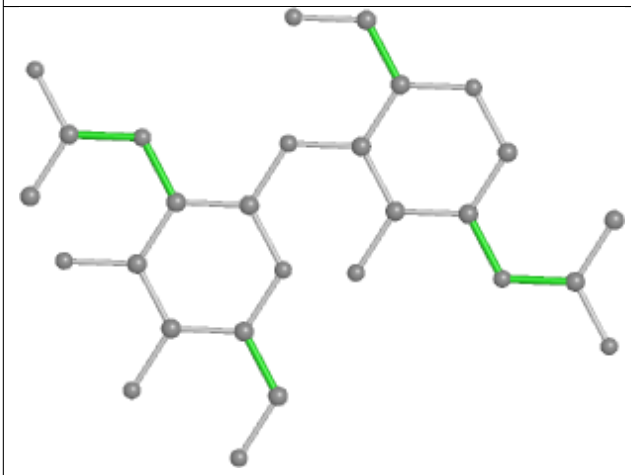
Oligosaccharide Chain b



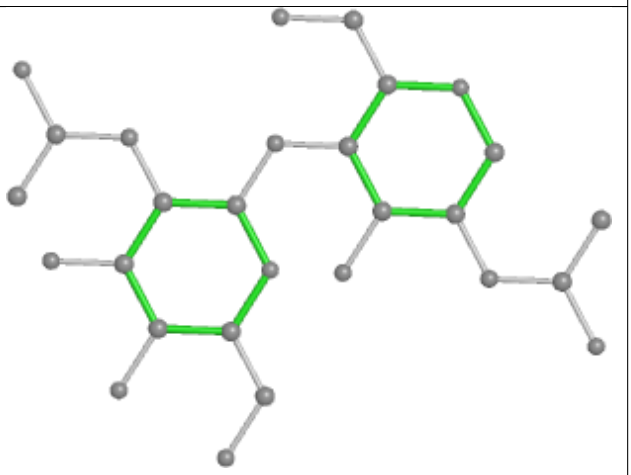
Bond lengths



Bond angles

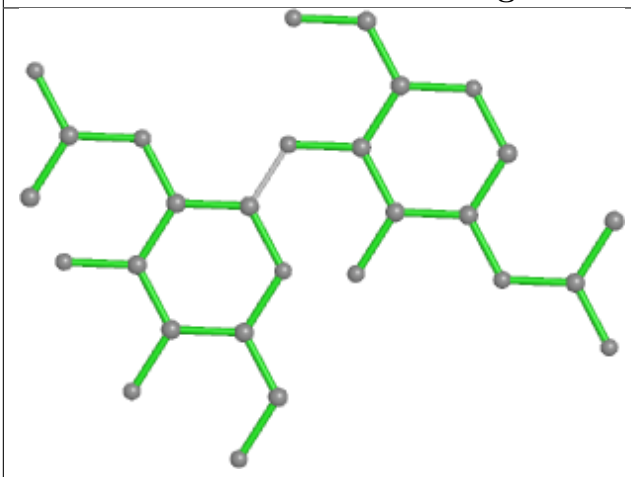


Torsions

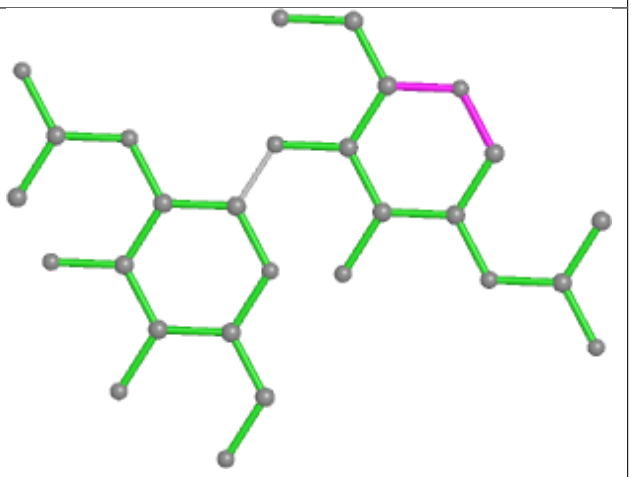


Rings

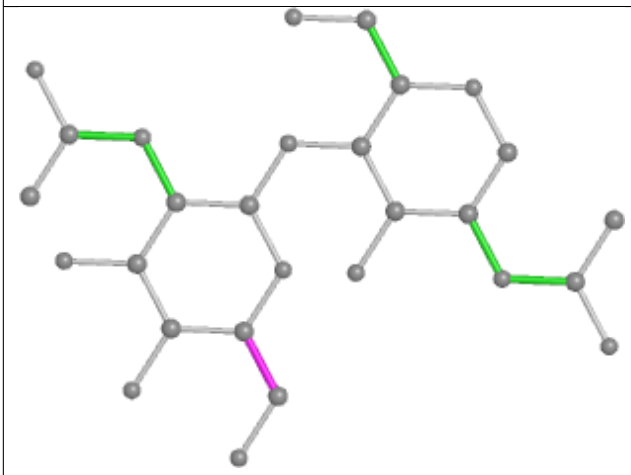
Oligosaccharide Chain d



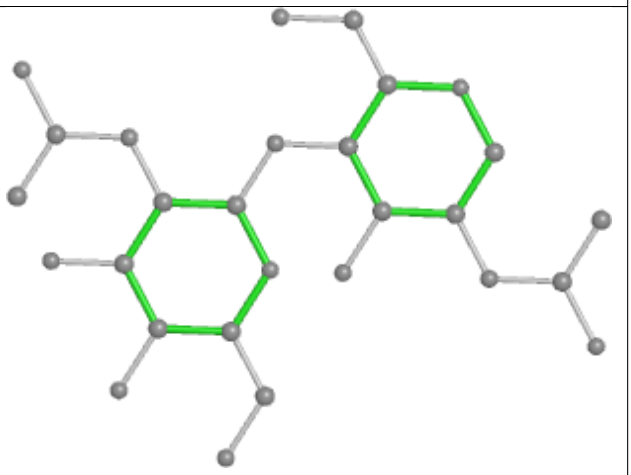
Bond lengths



Bond angles

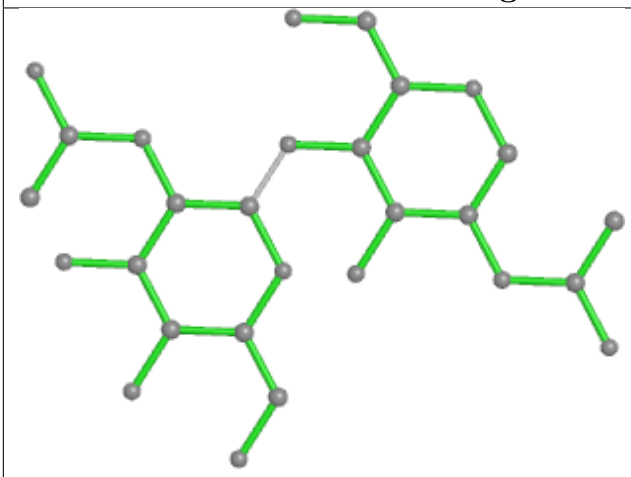


Torsions



Rings

Oligosaccharide Chain e



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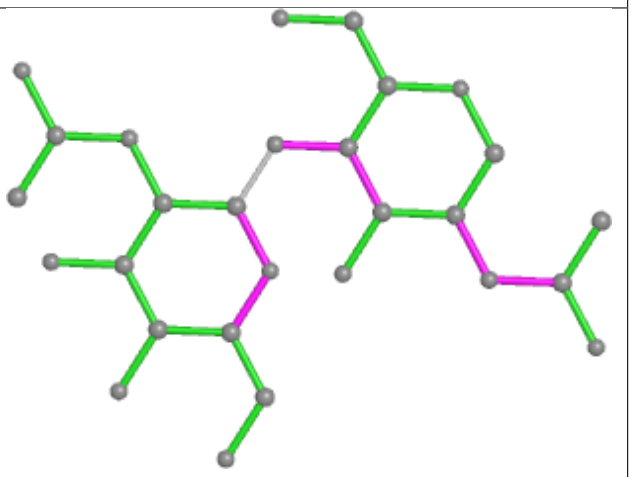
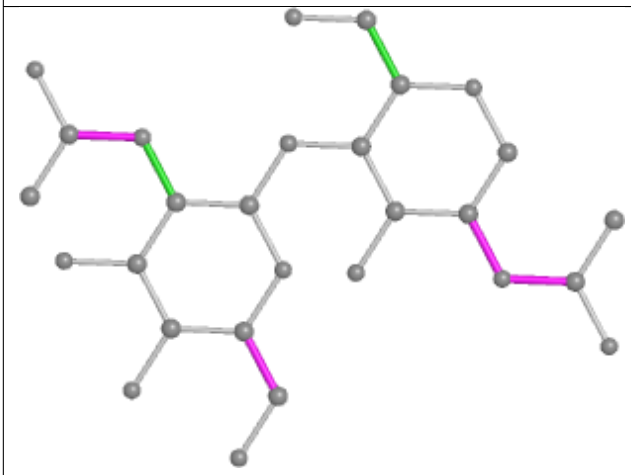


Bond angles



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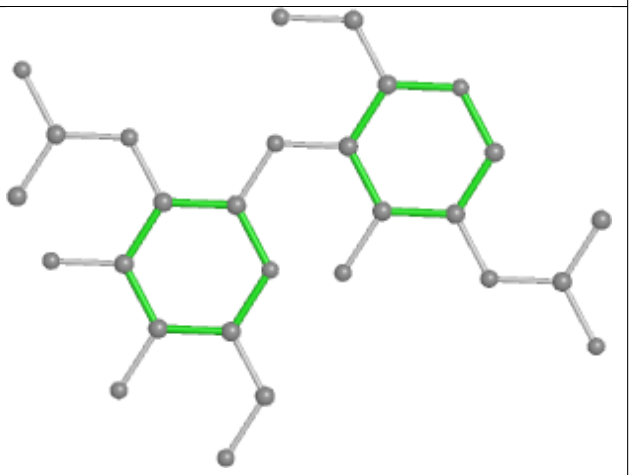
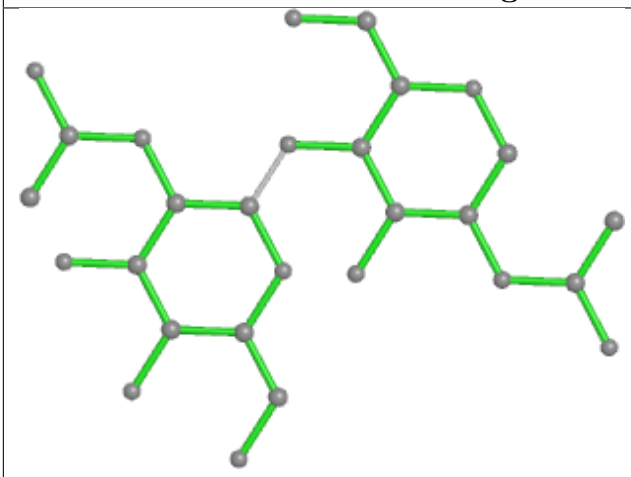


Rings

Oligosaccharide Chain f



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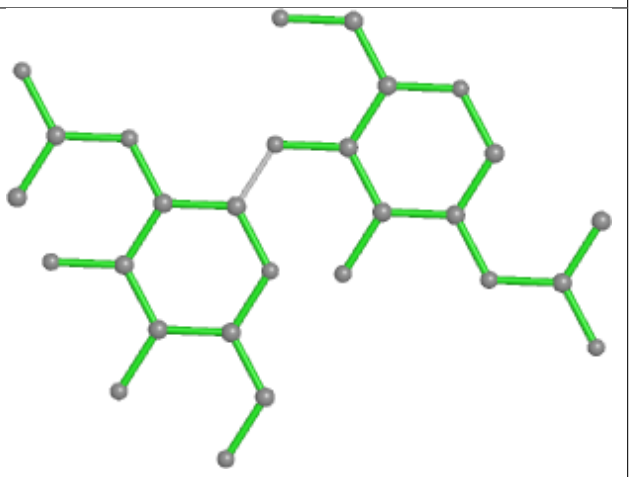

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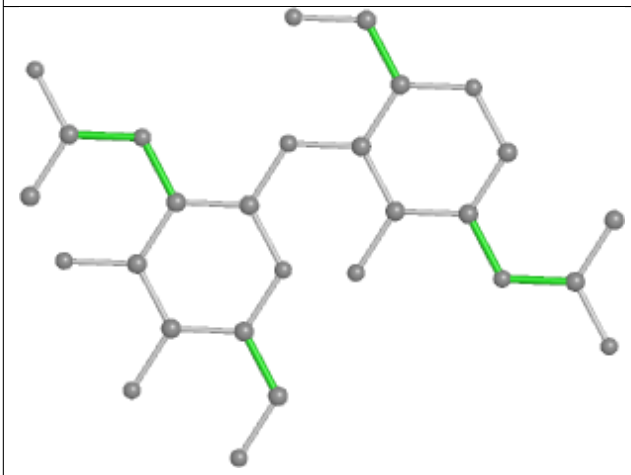

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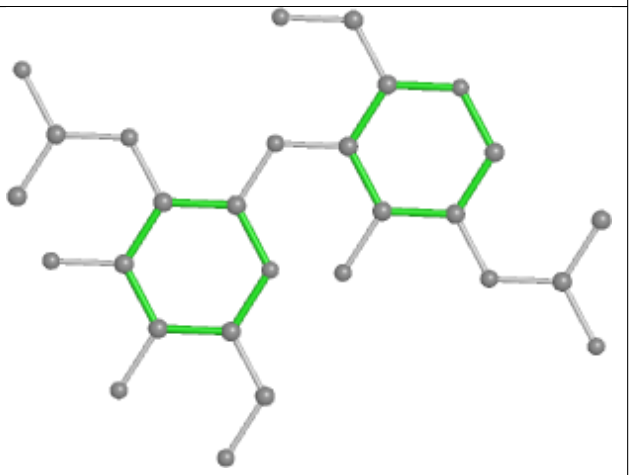
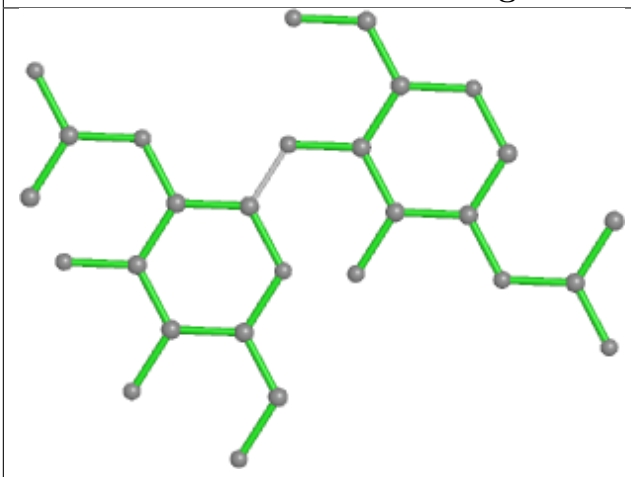


Rings

Oligosaccharide Chain g



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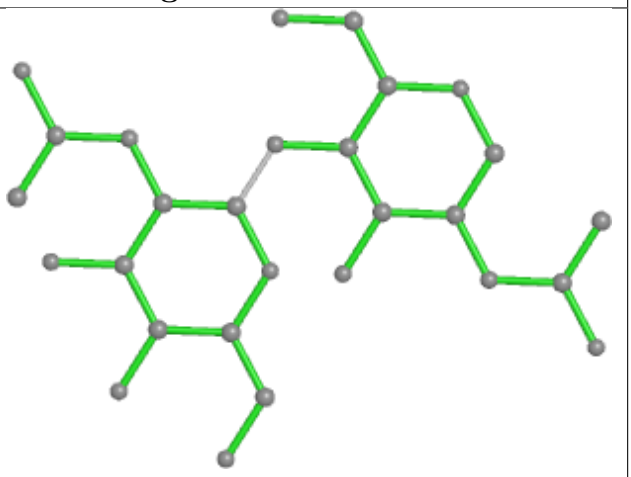

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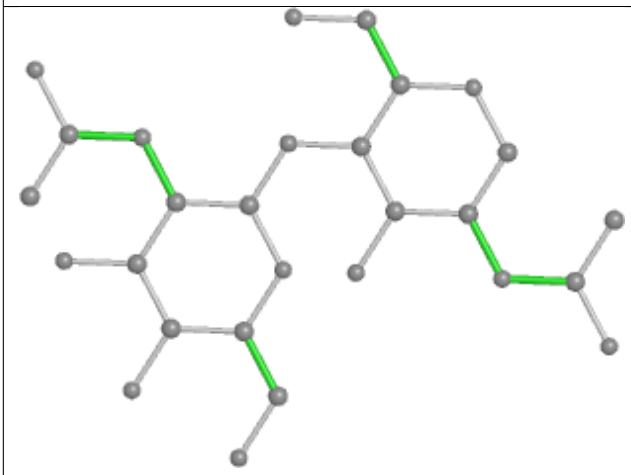

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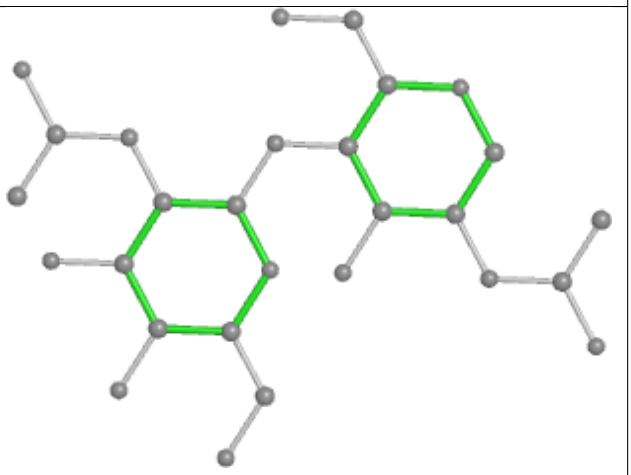
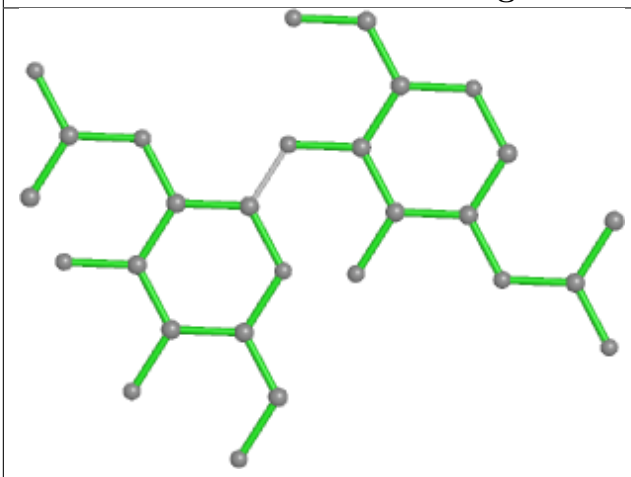


Rings

Oligosaccharide Chain h



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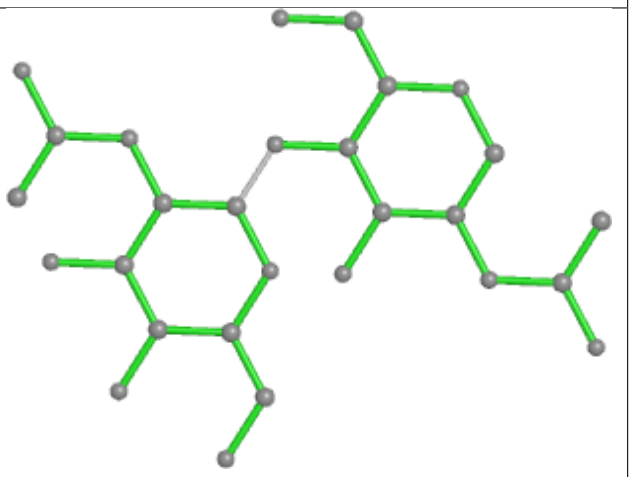
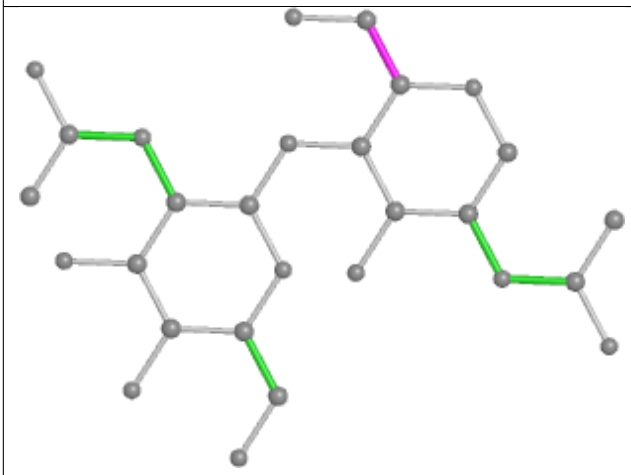


Bond angles



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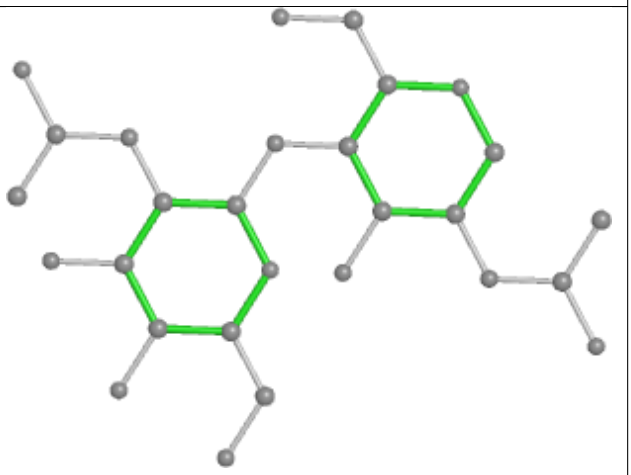
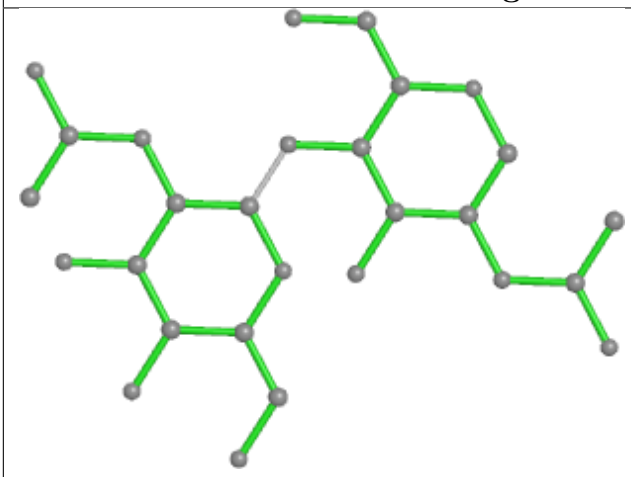


Rings

Oligosaccharide Chain i



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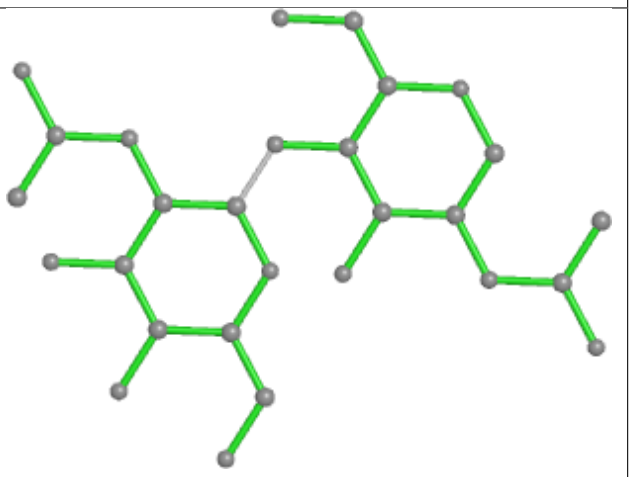

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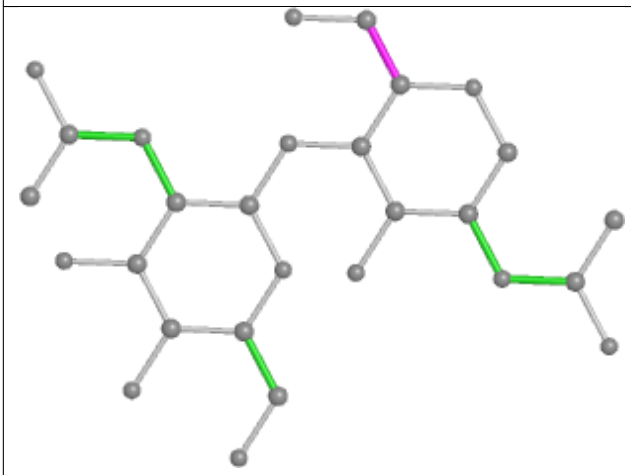

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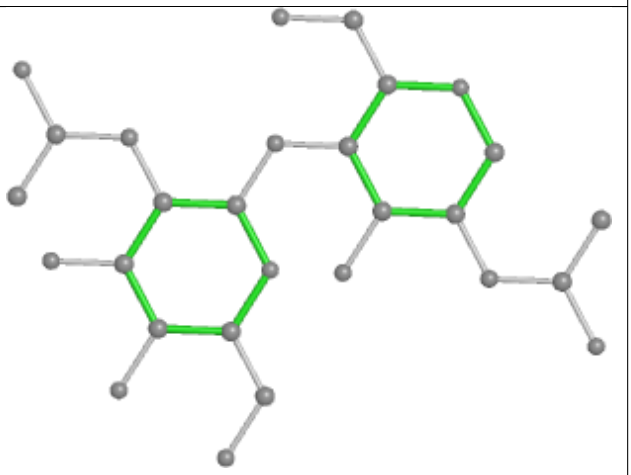
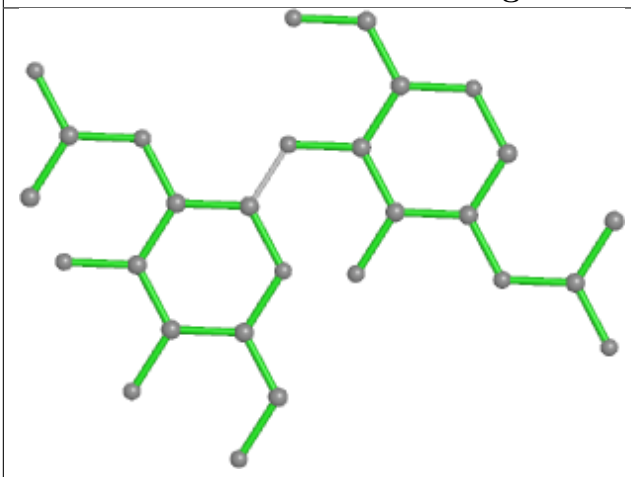


Rings

Oligosaccharide Chain j



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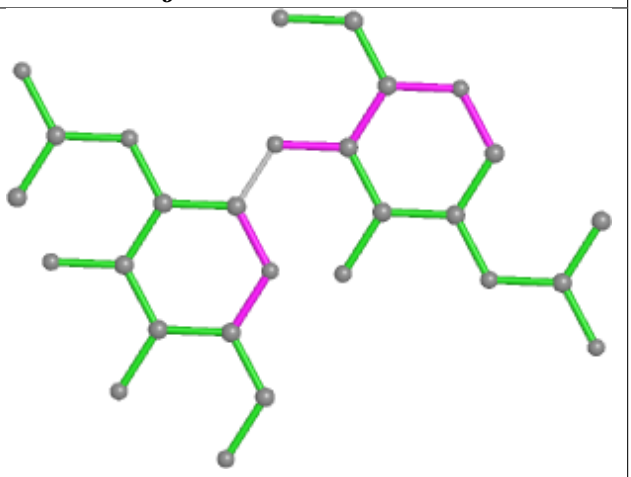

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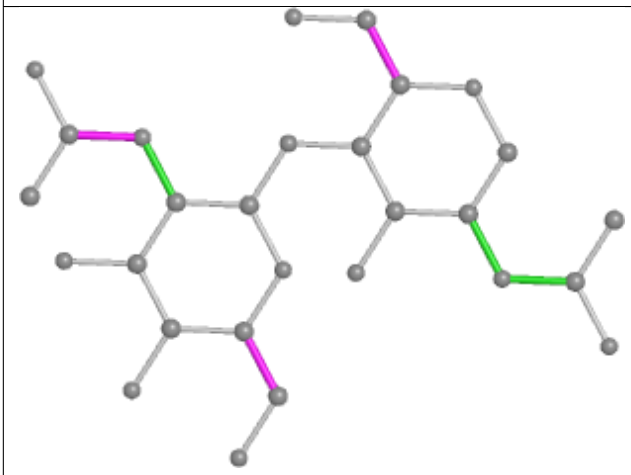

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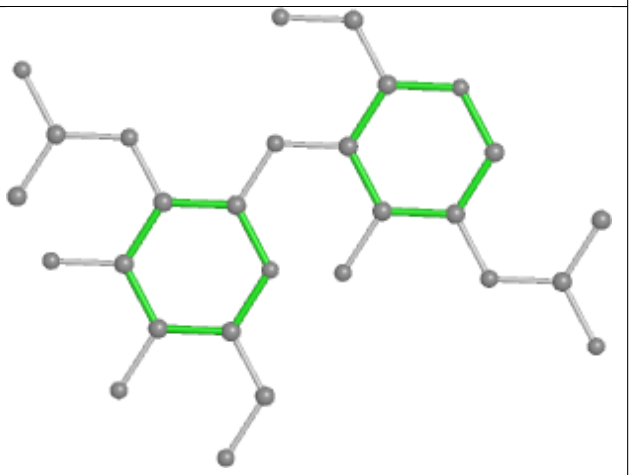
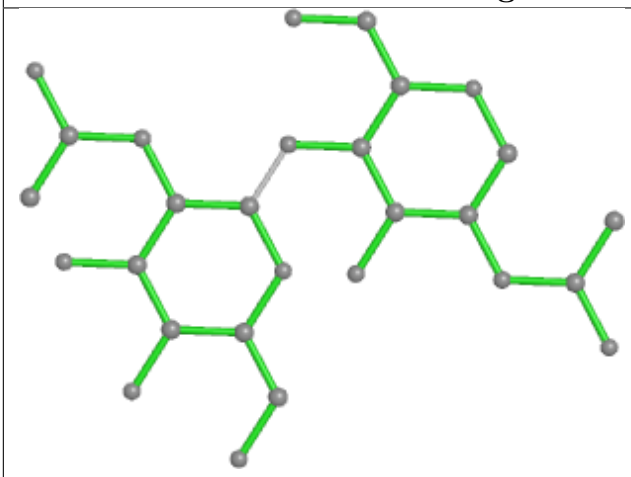


Rings

Oligosaccharide Chain p



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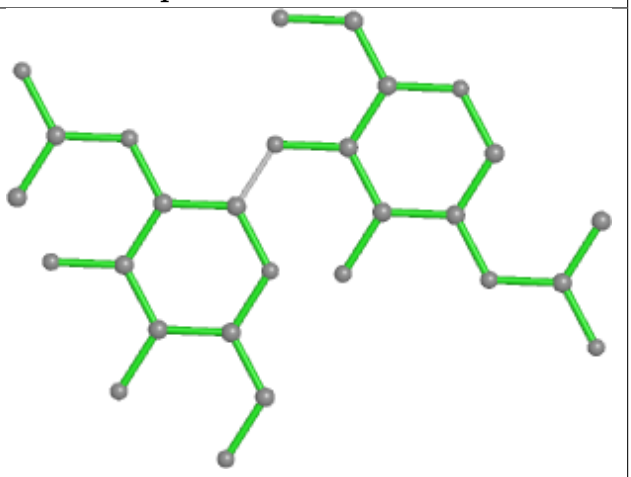

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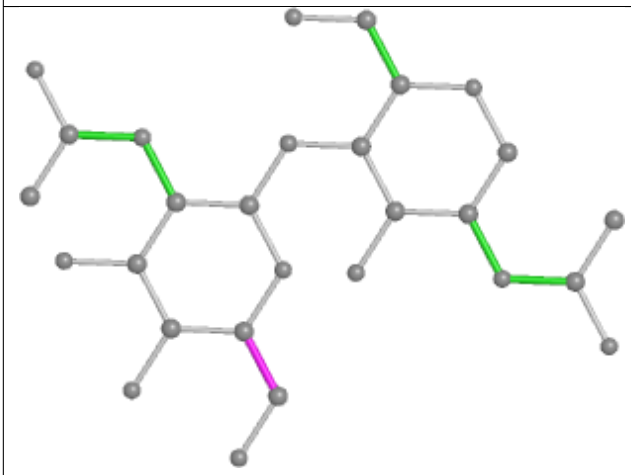

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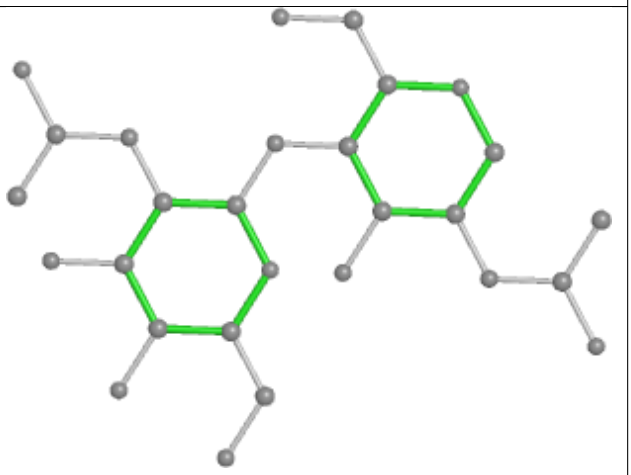
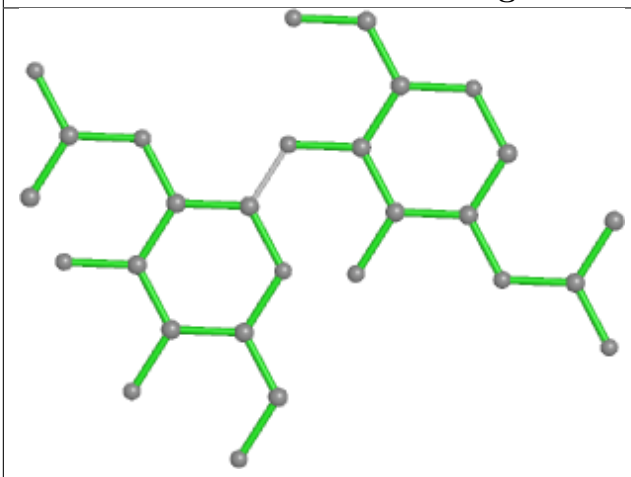


Rings

Oligosaccharide Chain q



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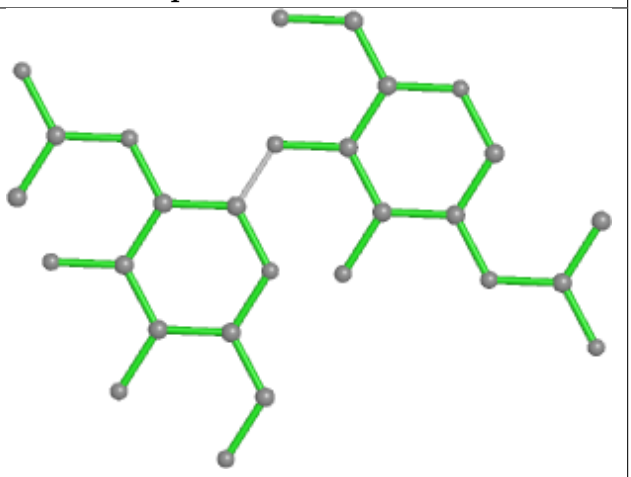
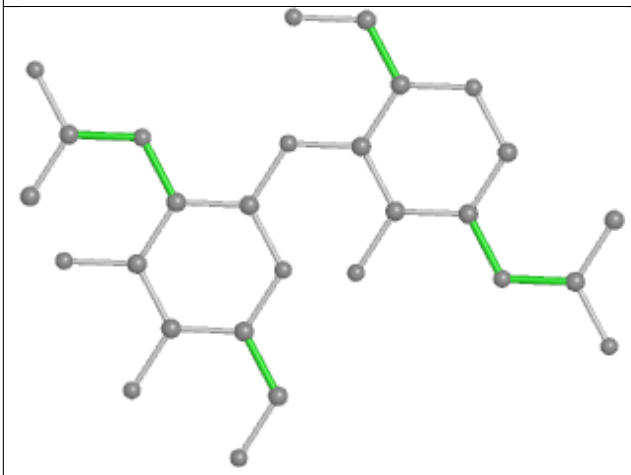


Bond angles



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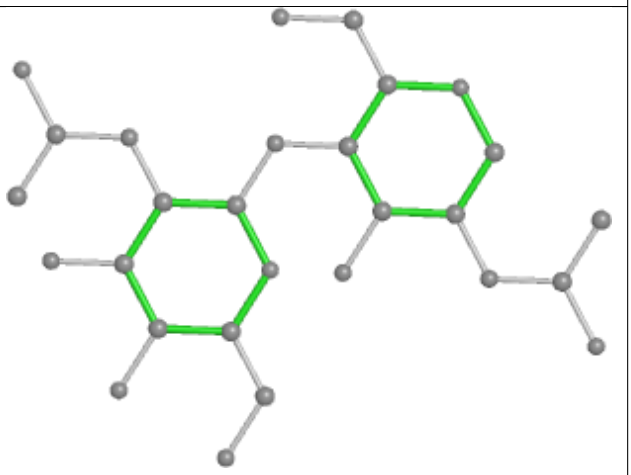
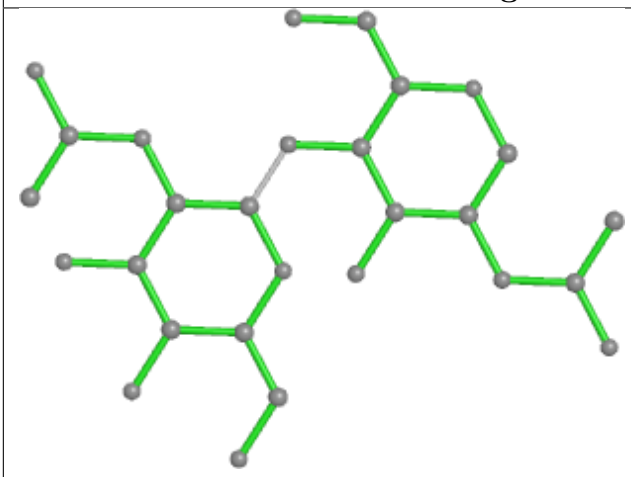


Rings

Oligosaccharide Chain r



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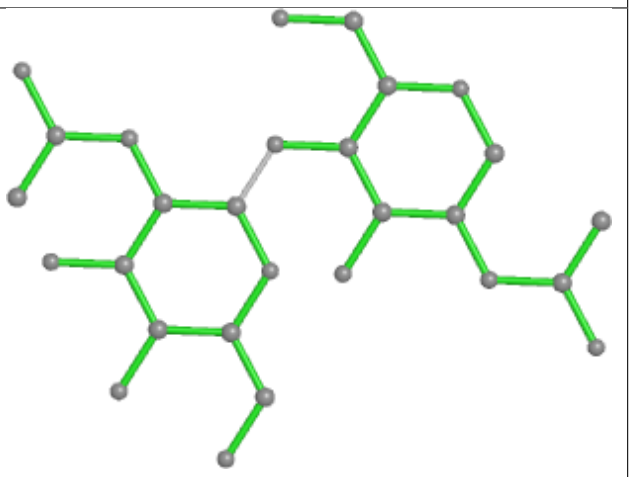

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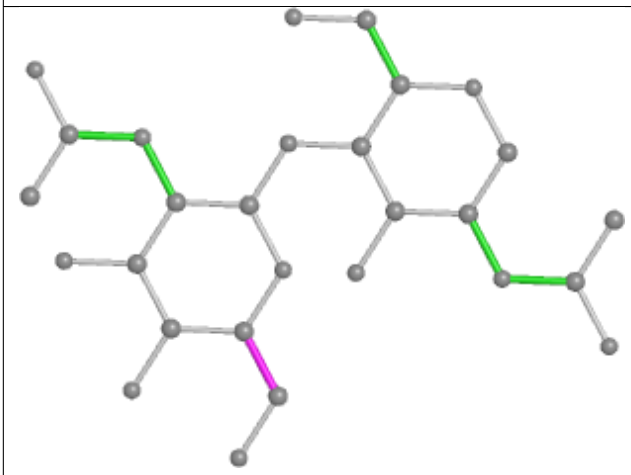

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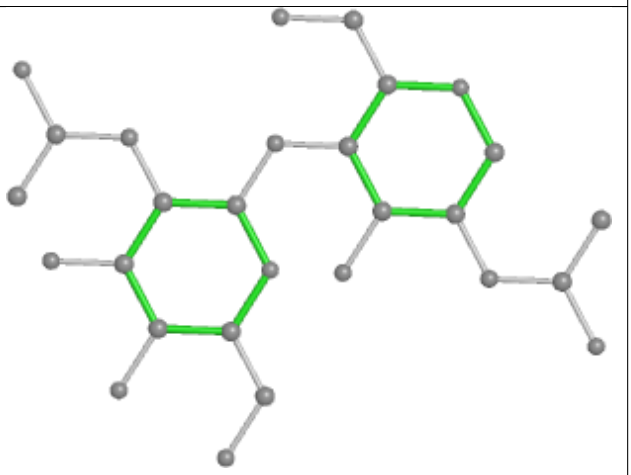
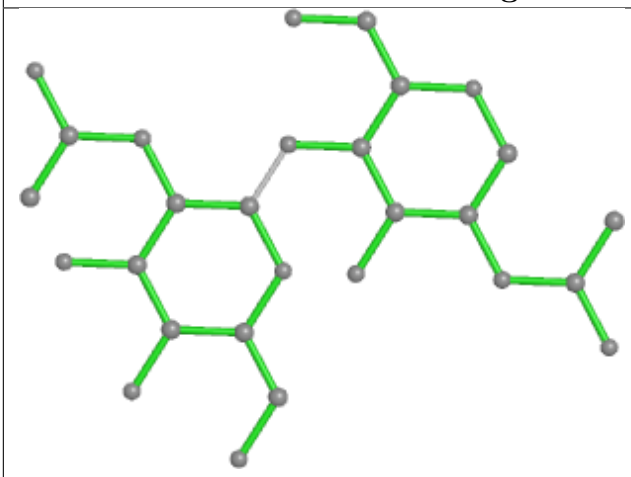


Rings

Oligosaccharide Chain t



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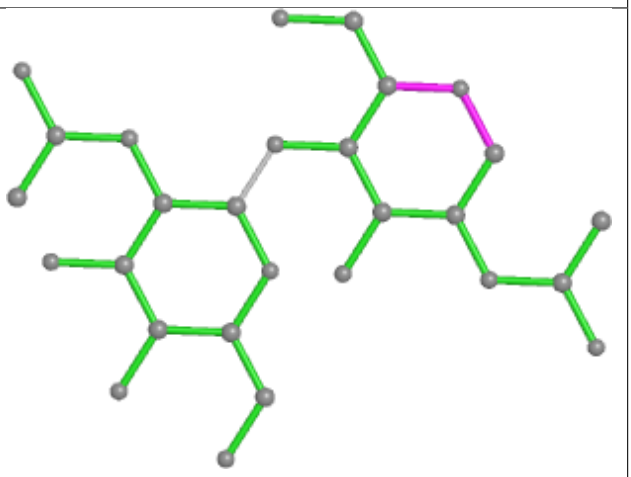

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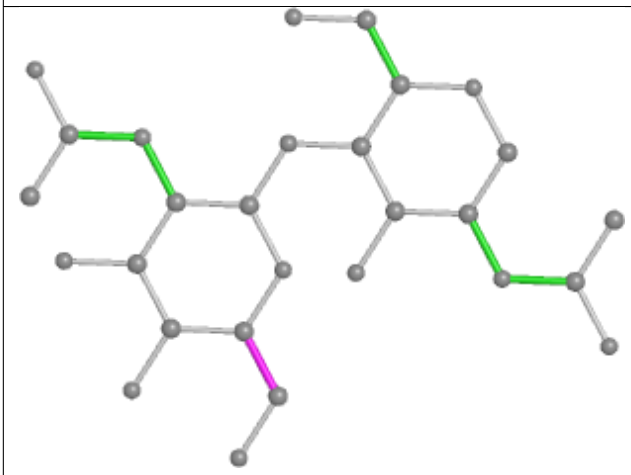

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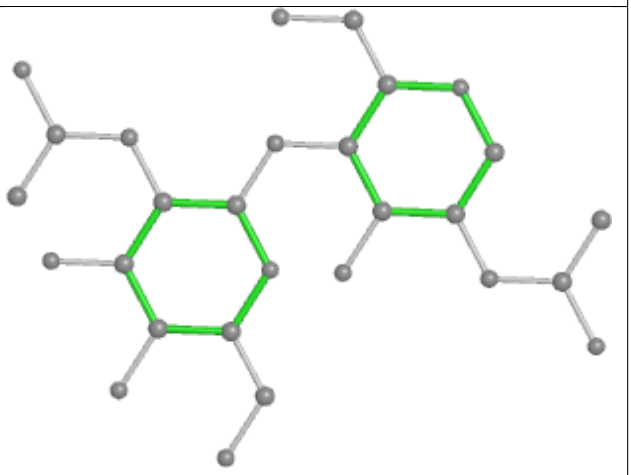
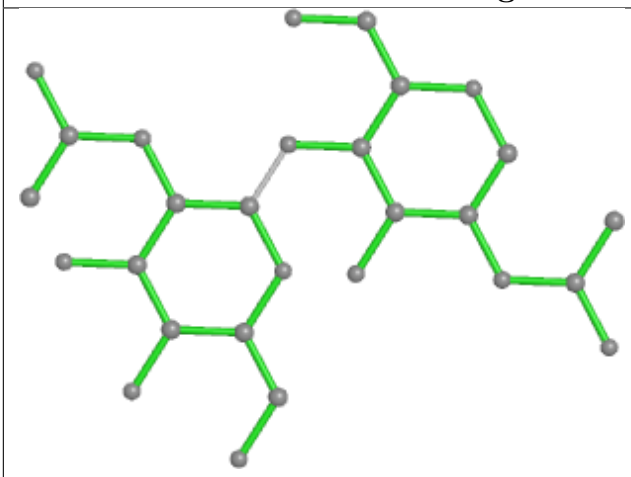


Rings

Oligosaccharide Chain u



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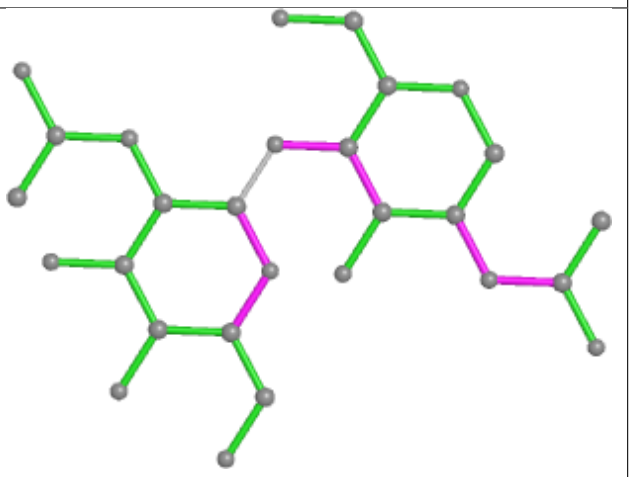

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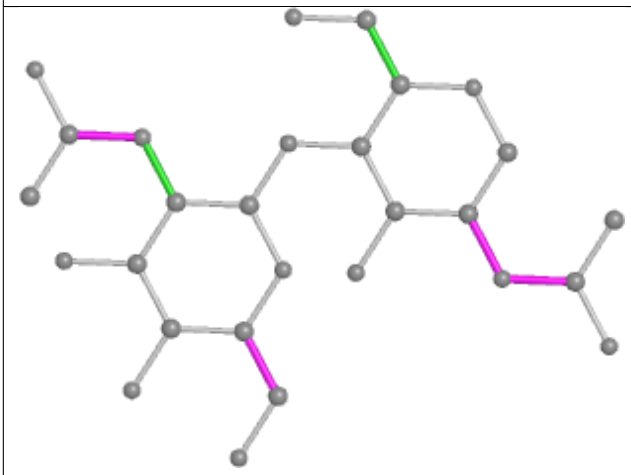

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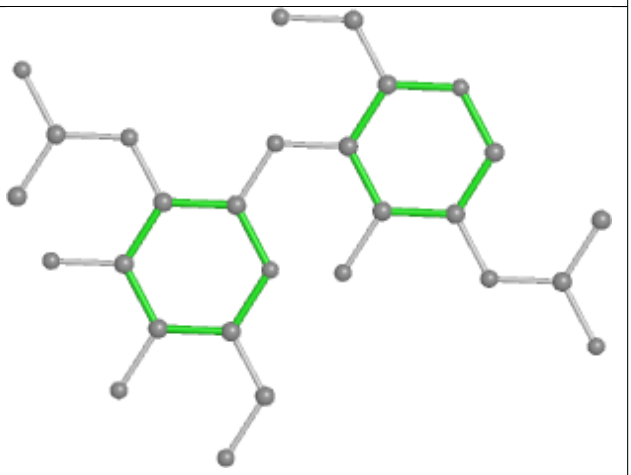
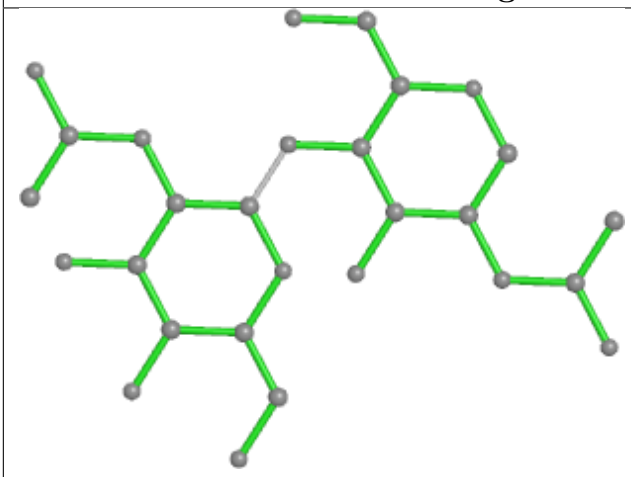


Rings

Oligosaccharide Chain v



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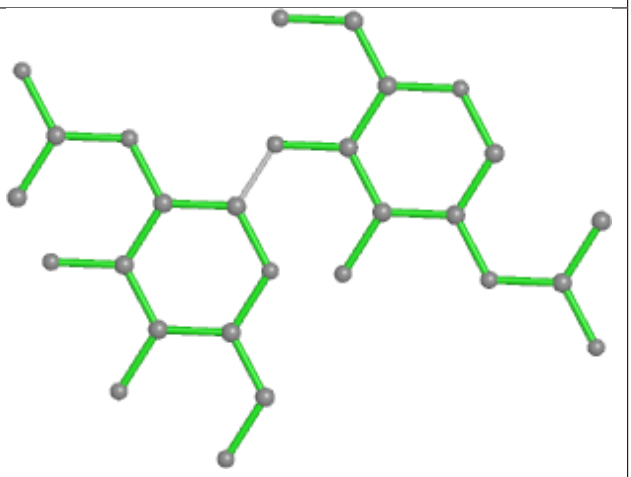

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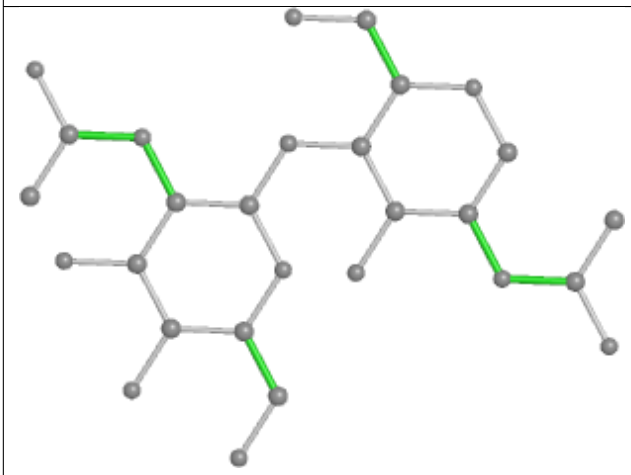
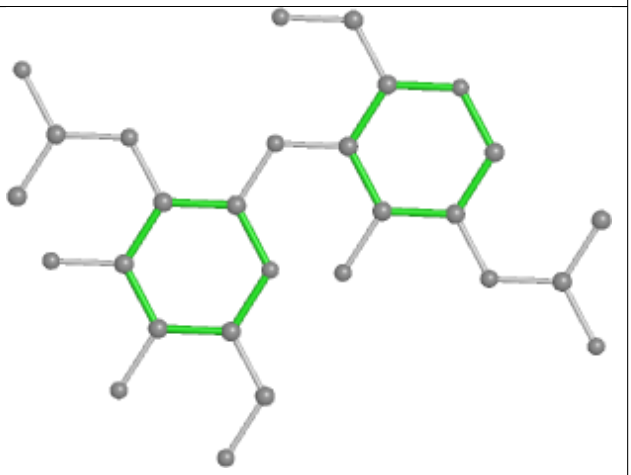
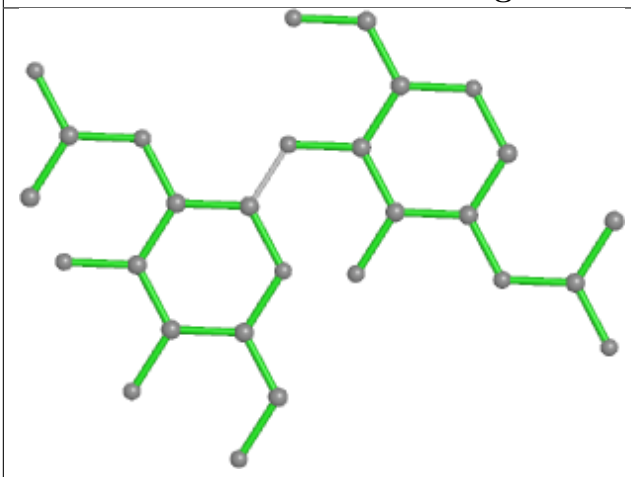


Torsions



Rings

Oligosaccharide Chain w



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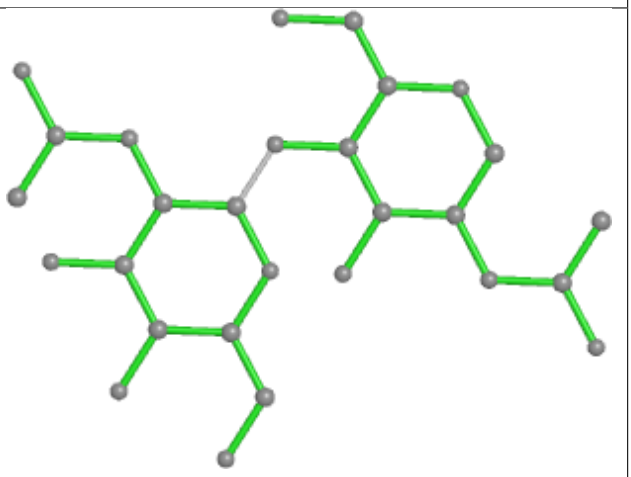
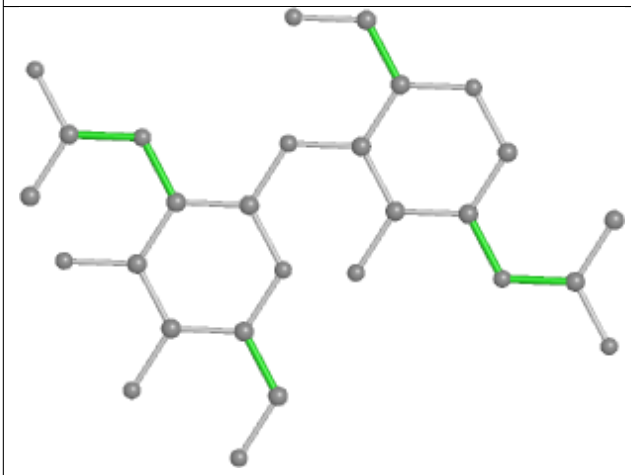


Bond angles



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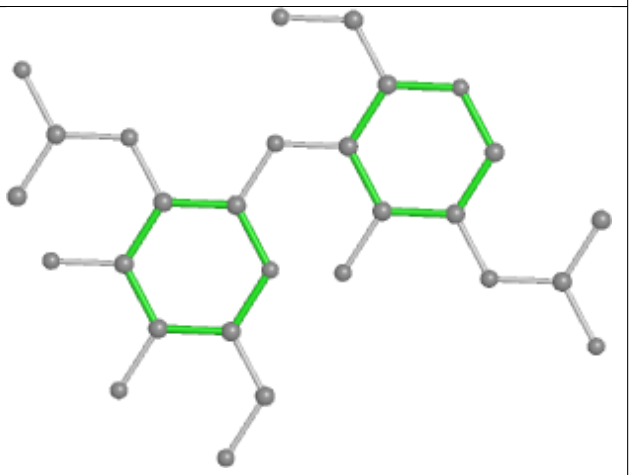
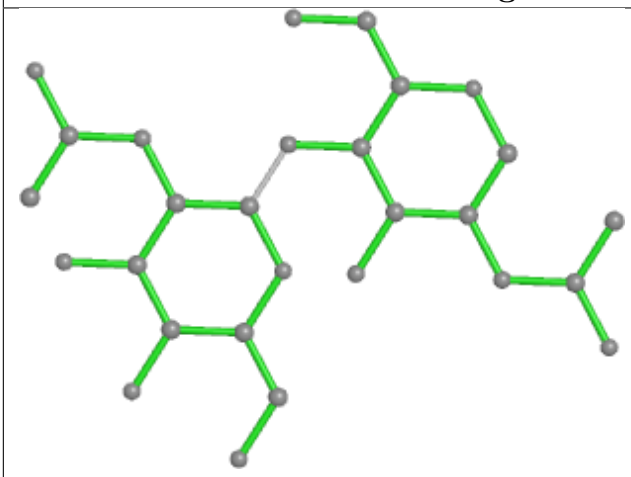


Rings

Oligosaccharide Chain x



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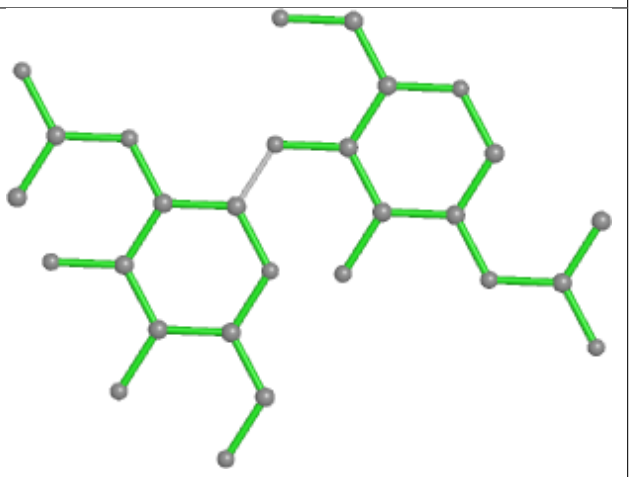
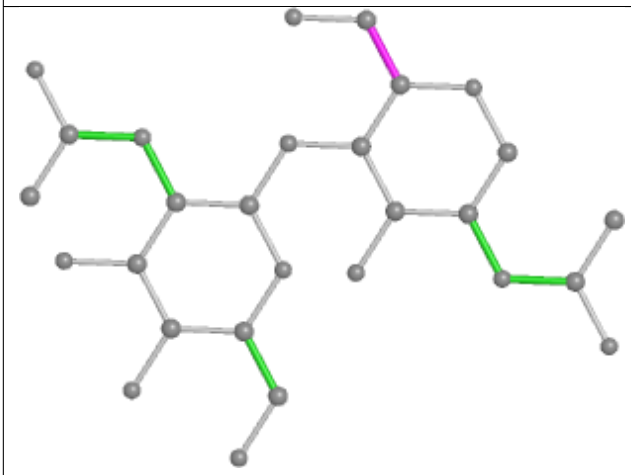


Bond angles



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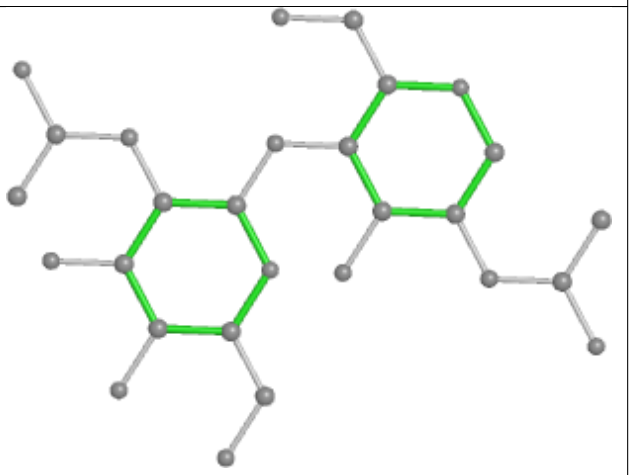
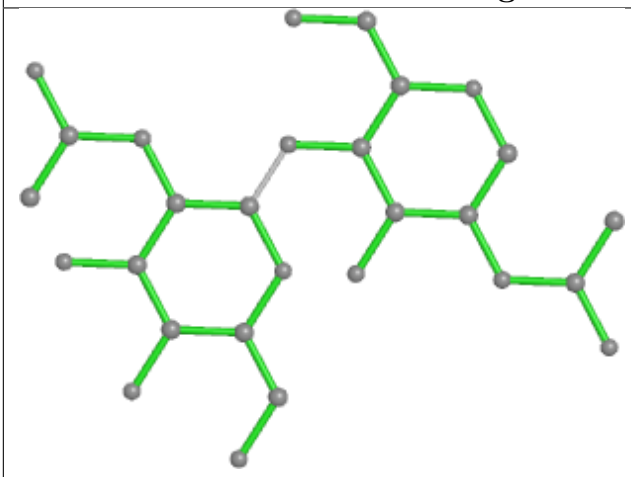
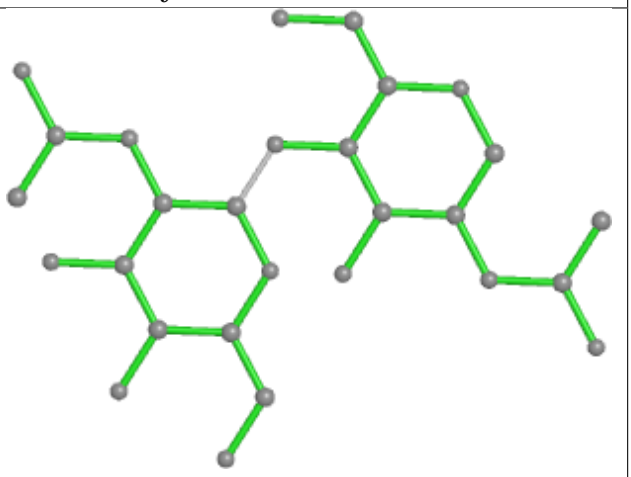


Rings

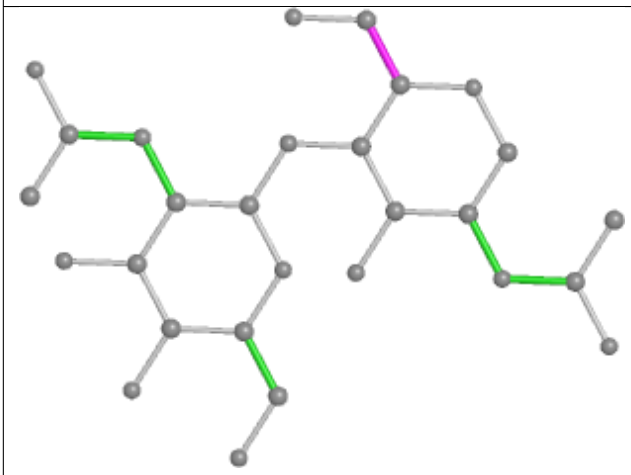
Oligosaccharide Chain y



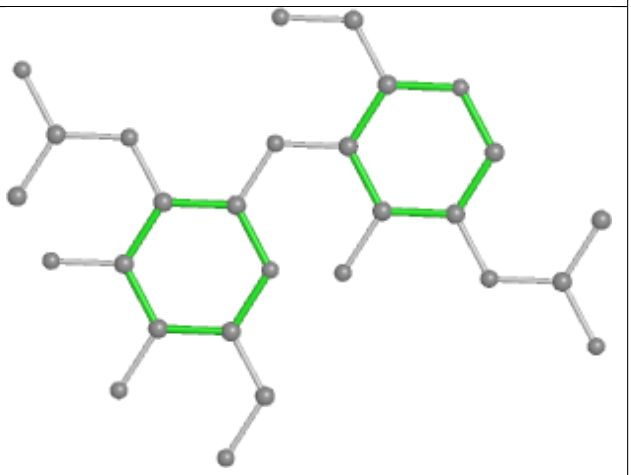
Bond lengths



Bond angles

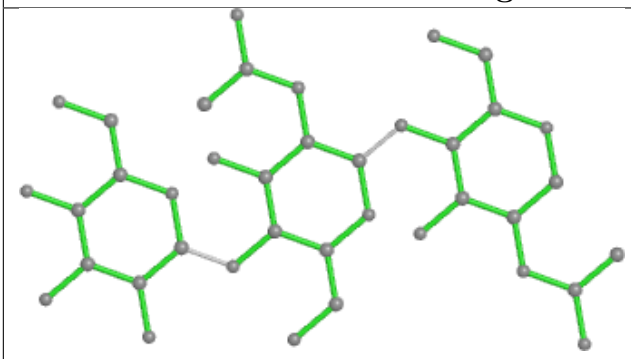


Torsions



Rings

Oligosaccharide Chain E



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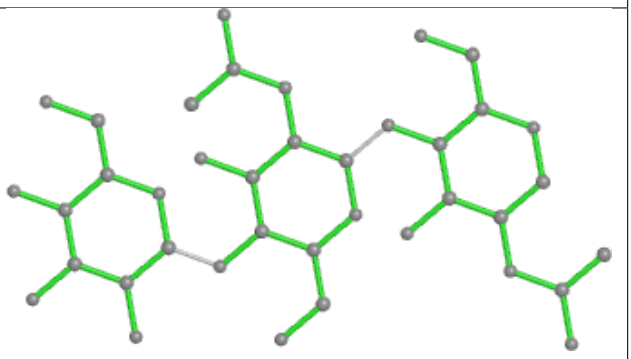
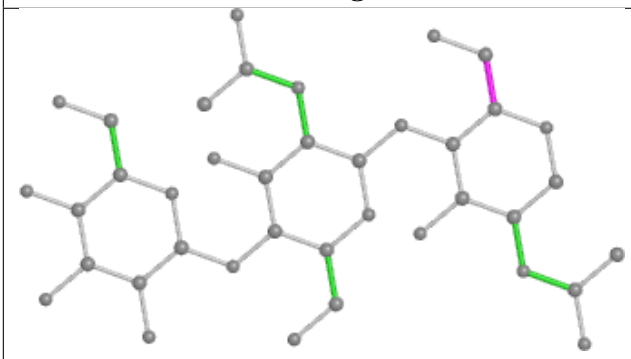


Bond angles



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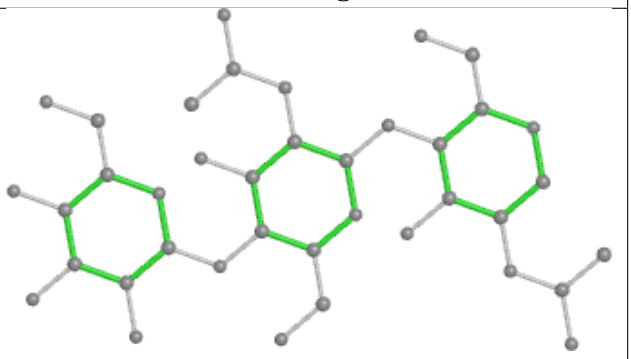
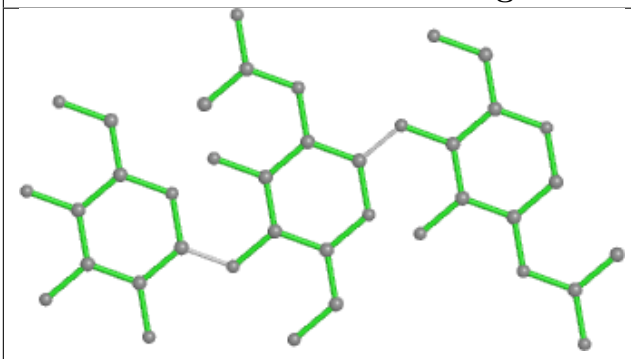


Rings

Oligosaccharide Chain F



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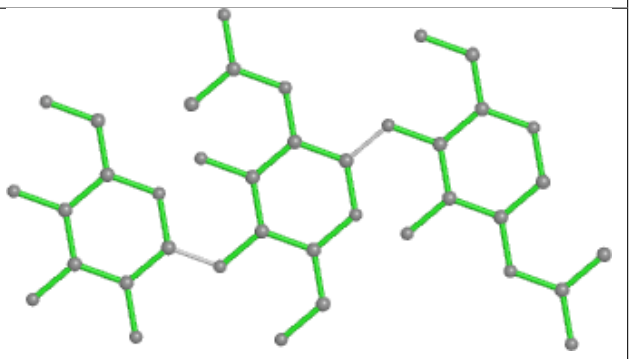
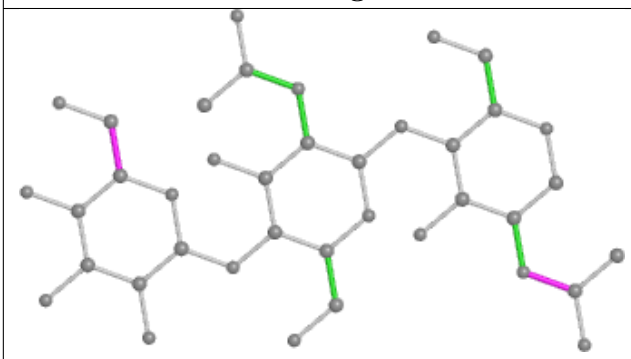


Bond angles



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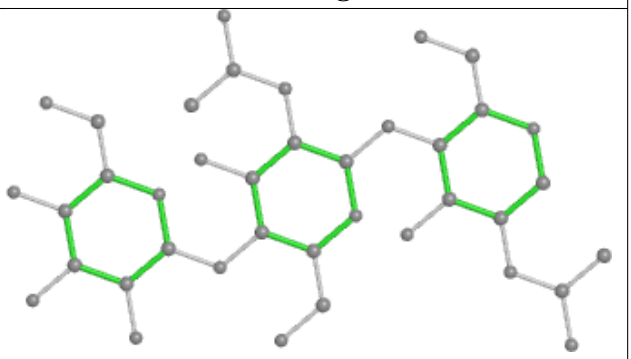
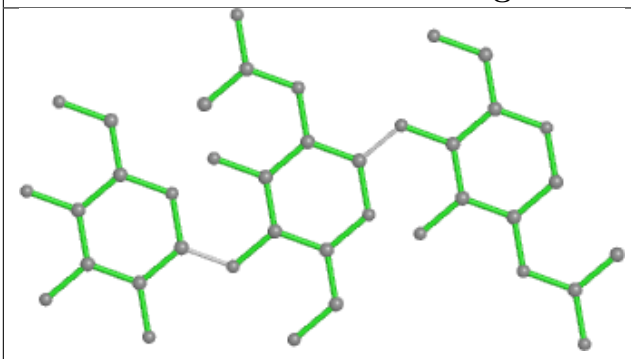


Rings

Oligosaccharide Chain G



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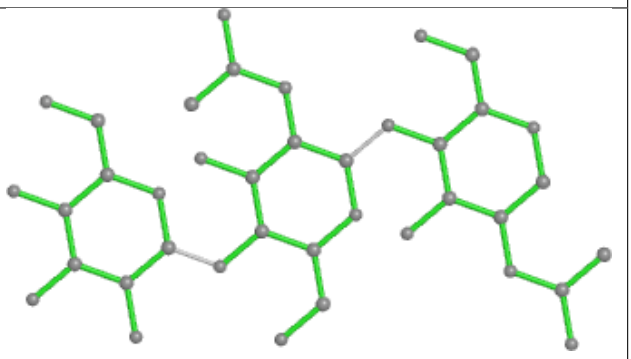
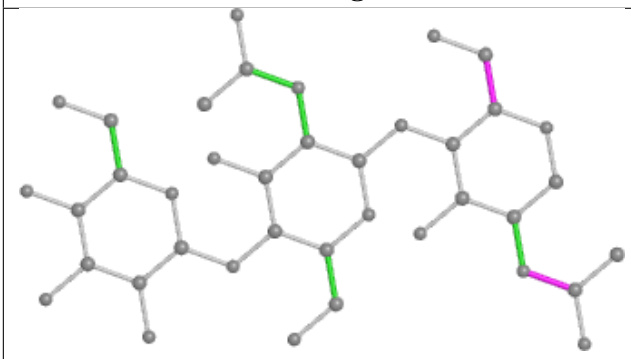


Bond angles



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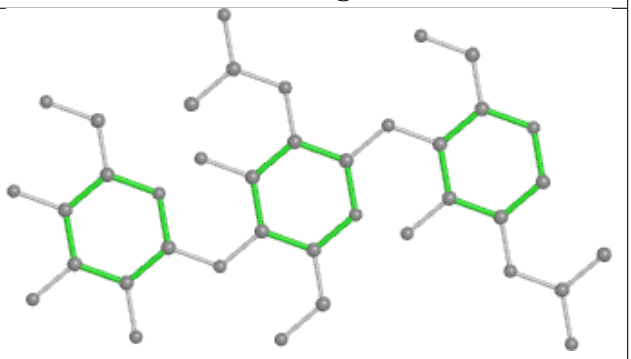
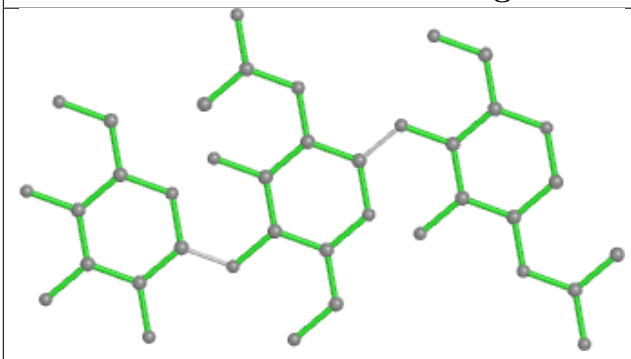


Rings

Oligosaccharide Chain H



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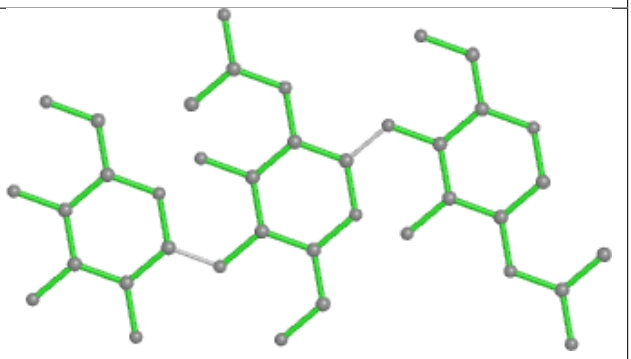
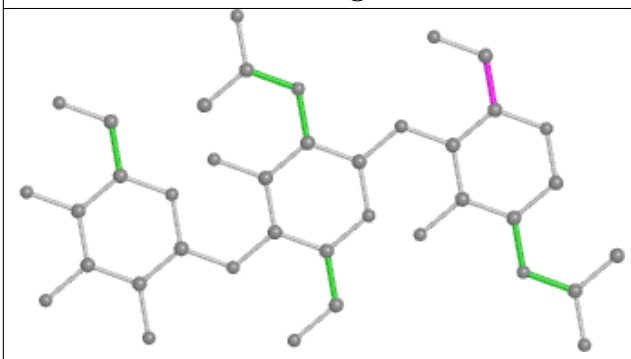


Bond angles



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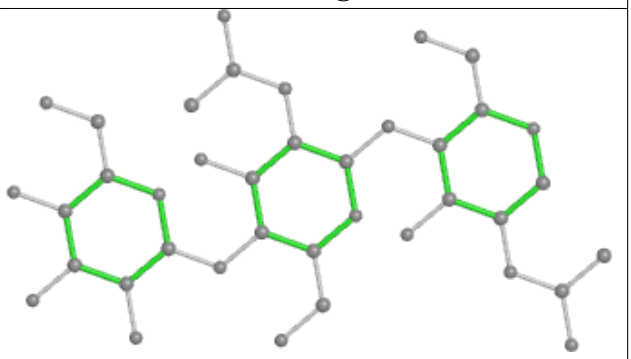
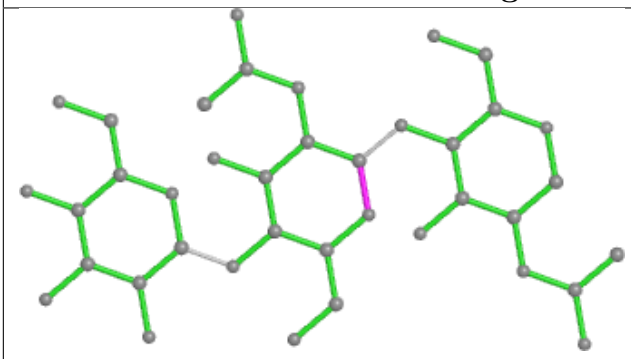


Rings

Oligosaccharide Chain I



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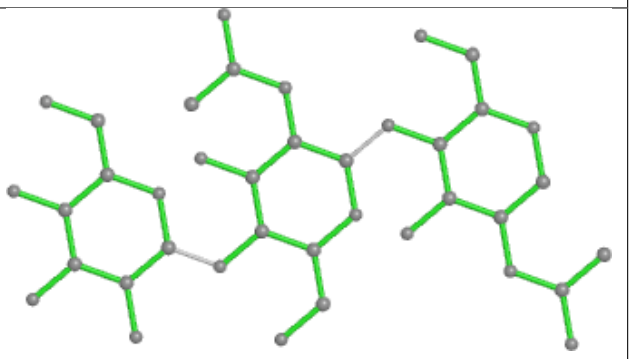
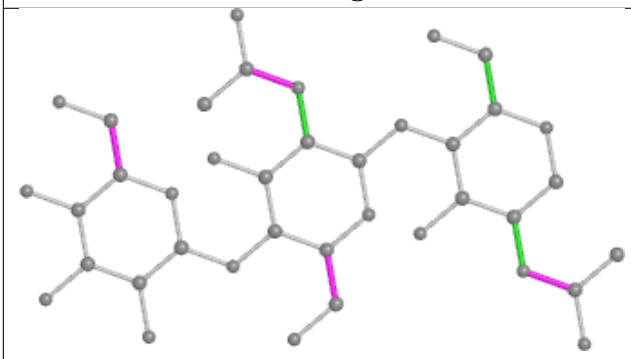


Bond angles



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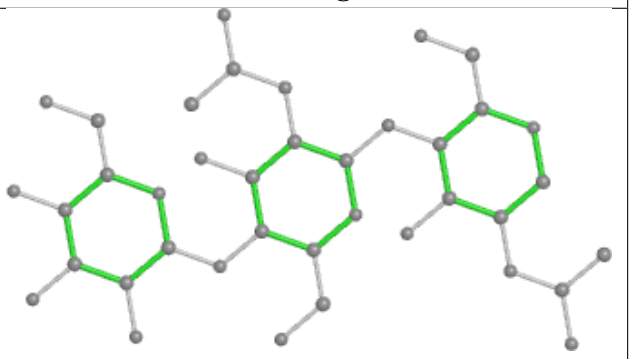
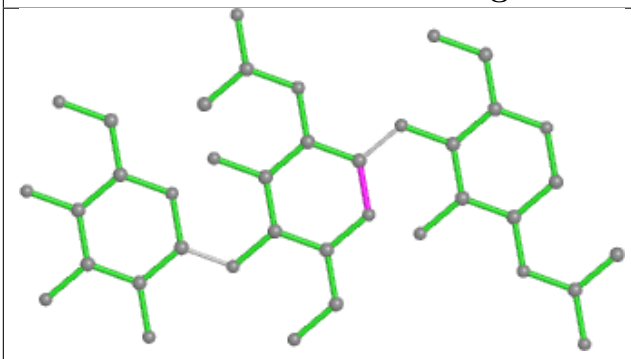


Rings

Oligosaccharide Chain M



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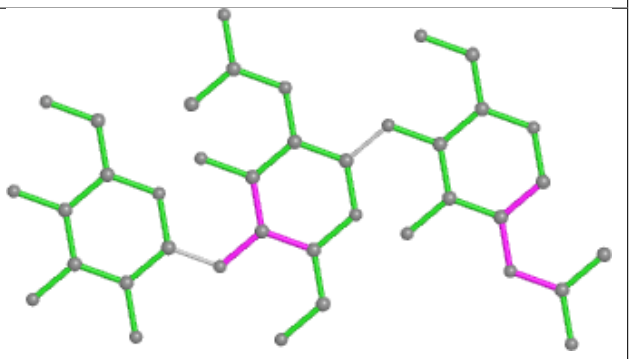
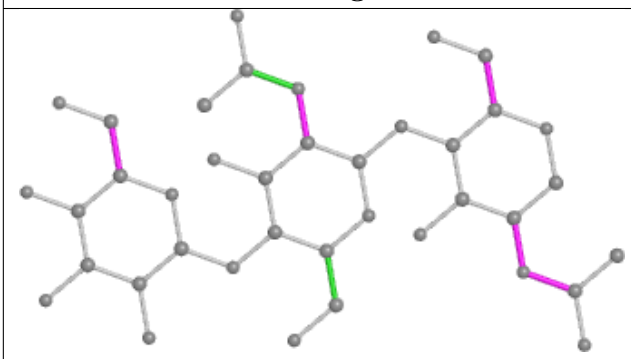
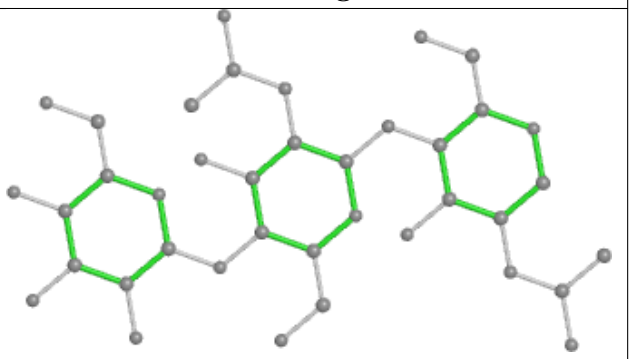


Bond angles

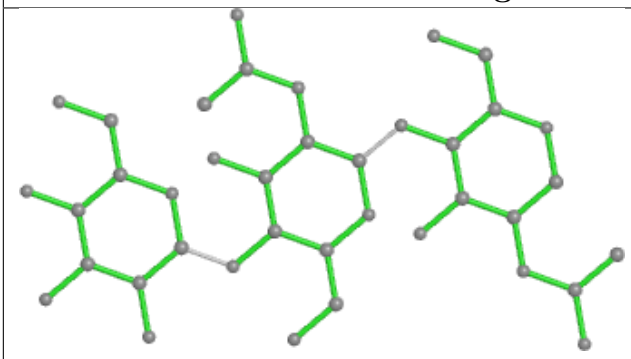


Torsions



Rings

Oligosaccharide Chain U



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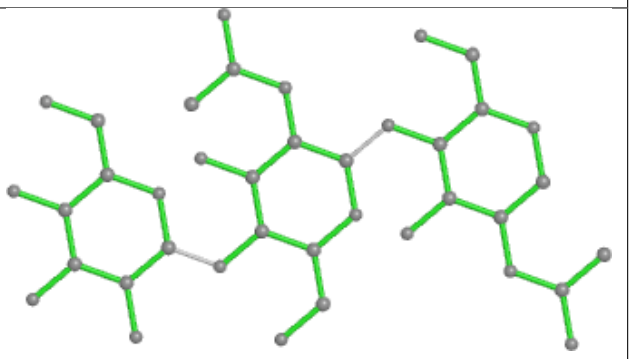
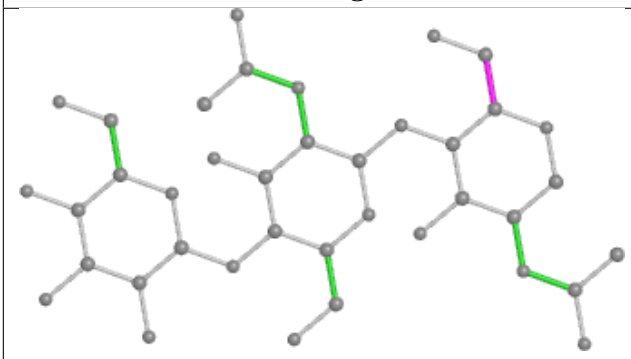


Bond angles



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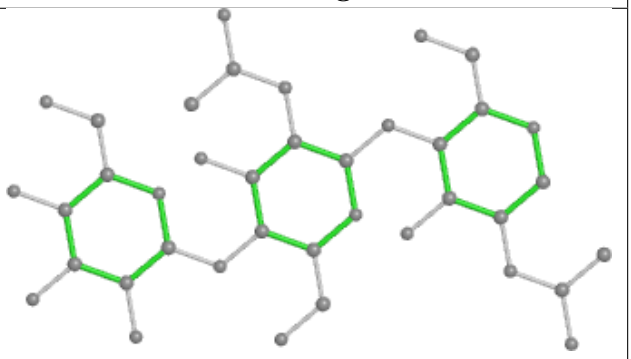
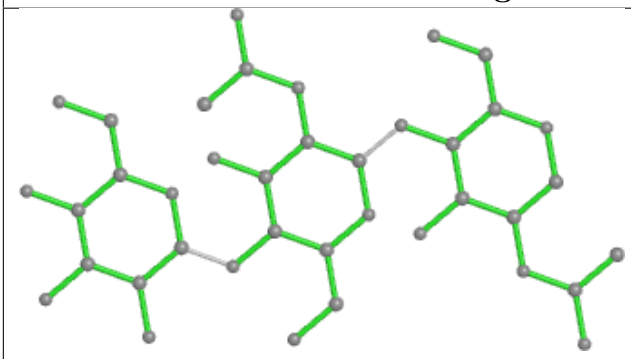


Rings

Oligosaccharide Chain V



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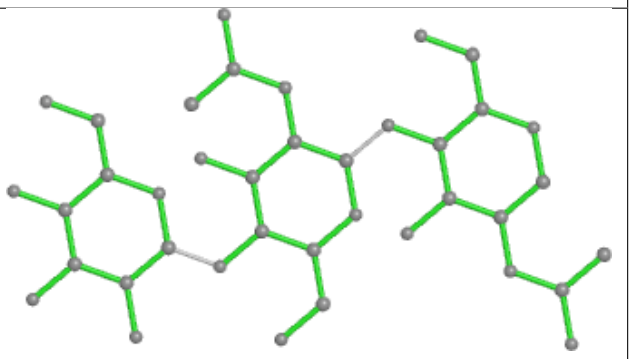
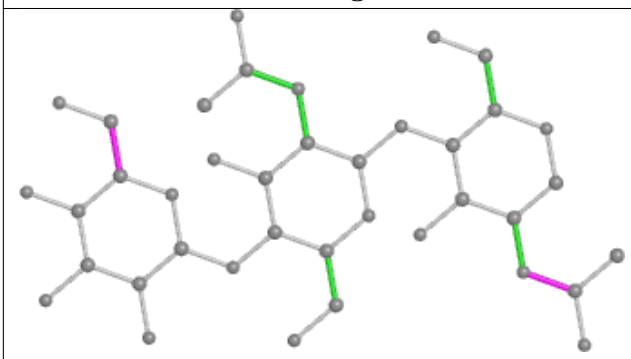


Bond angles



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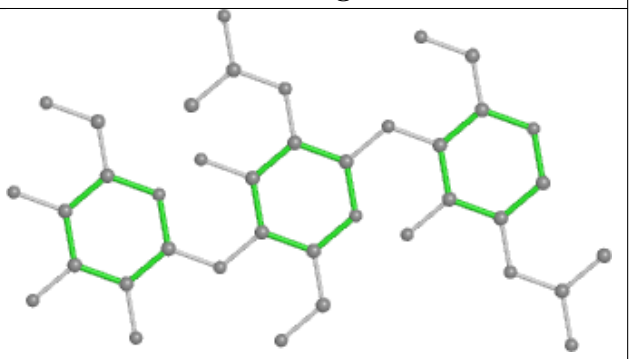
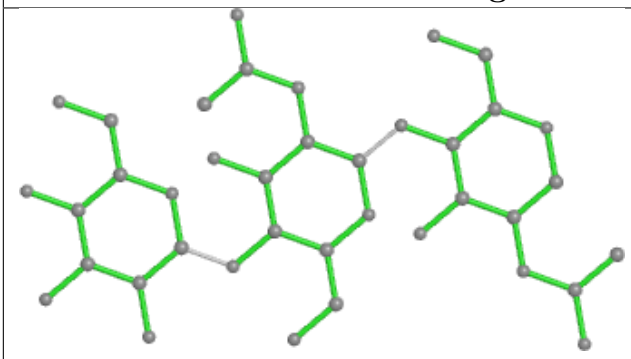


Rings

Oligosaccharide Chain W



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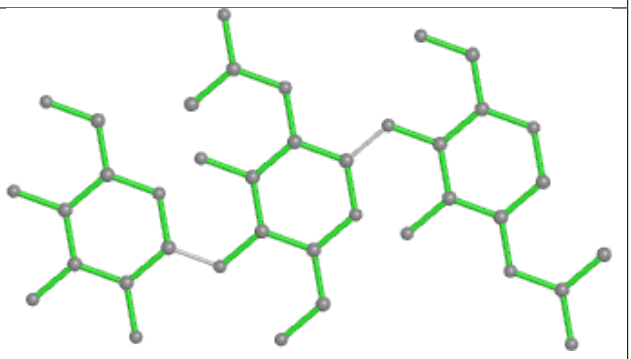
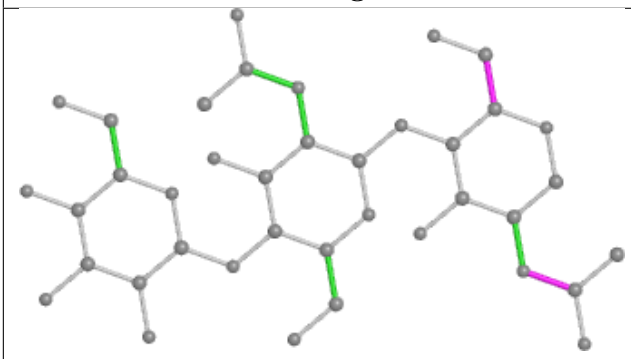
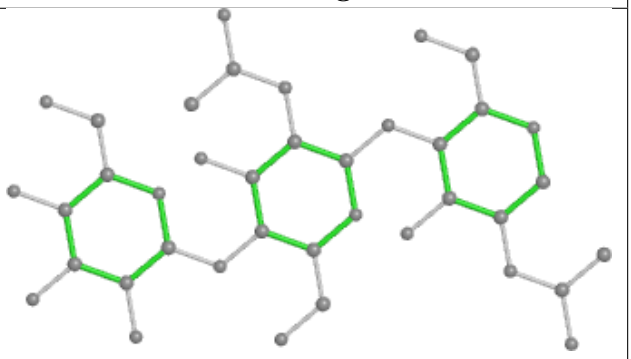


Bond angles

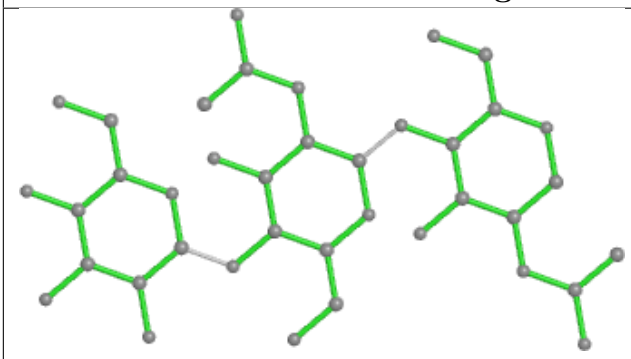


Torsions



Rings

Oligosaccharide Chain X



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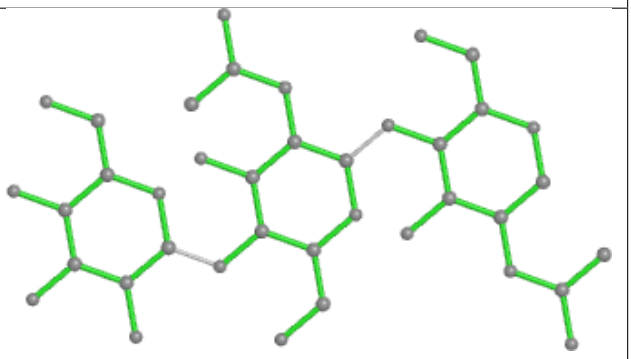
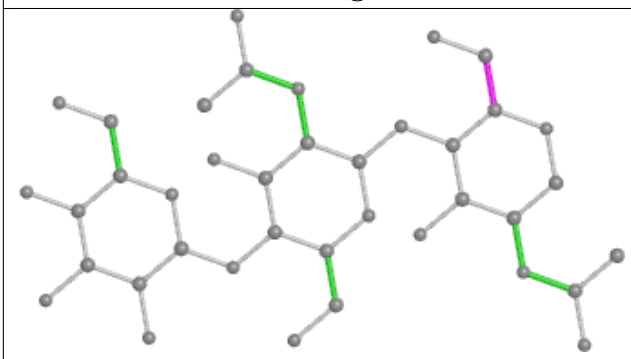


Bond angles



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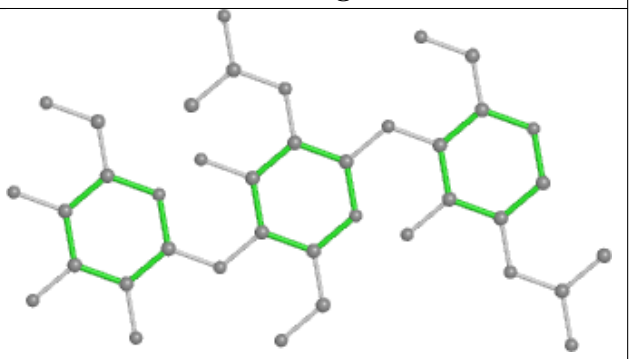
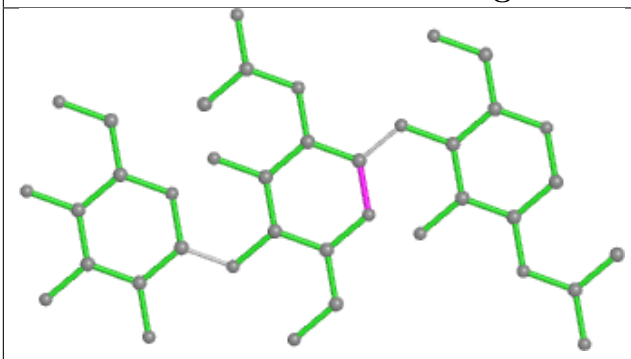


Rings

Oligosaccharide Chain Y



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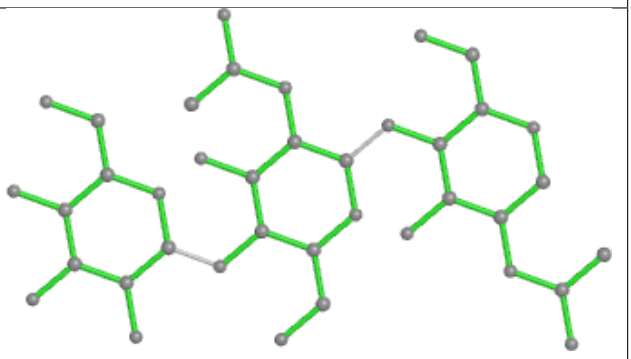
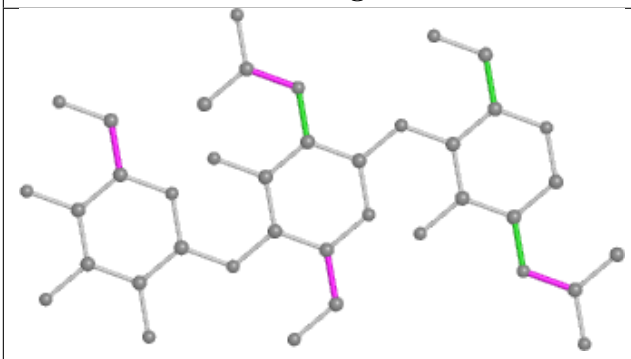


Bond angles



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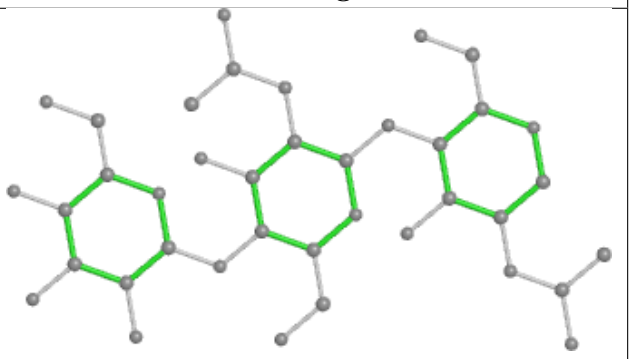
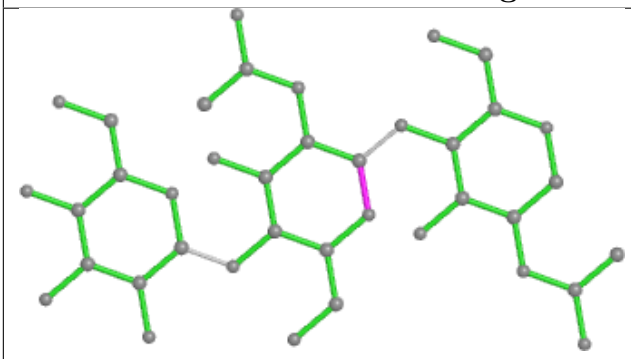


Rings

Oligosaccharide Chain c



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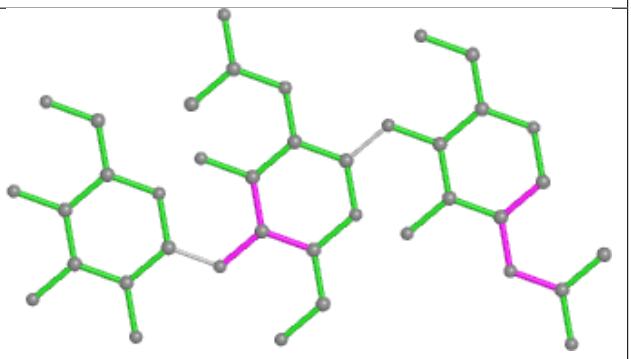
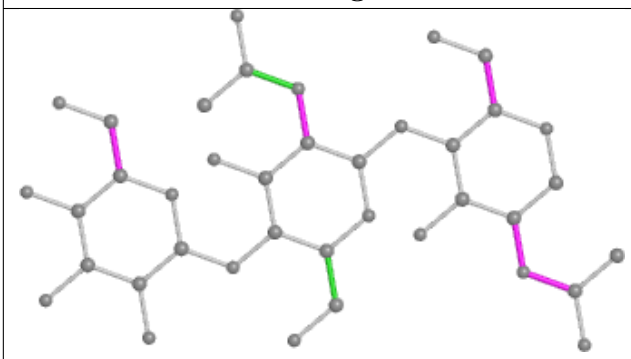
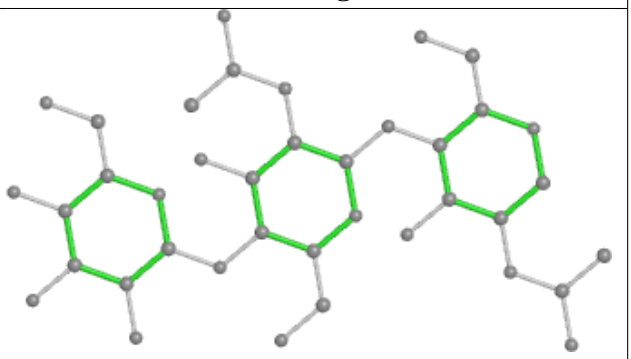


Bond angles

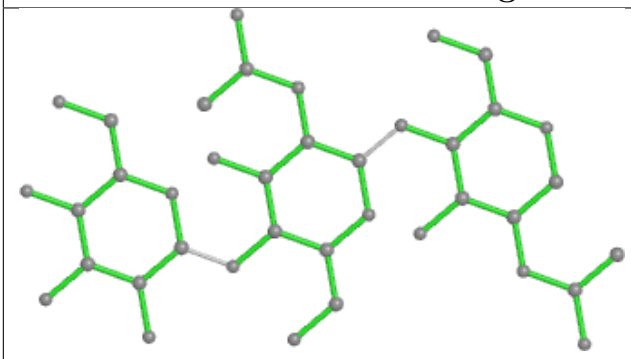


Torsions

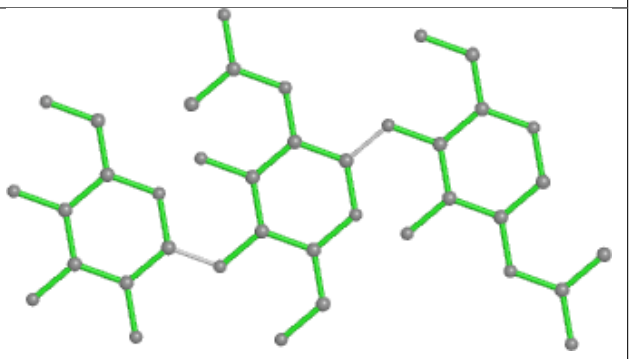


Rings

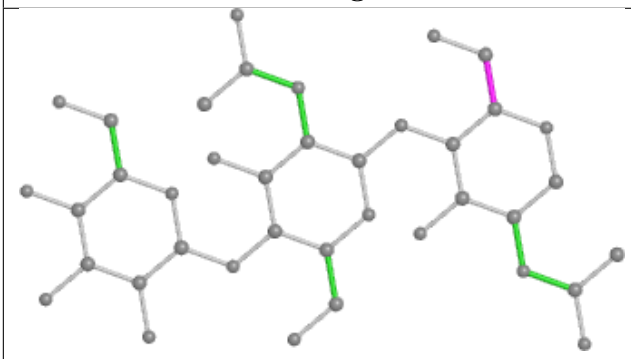
Oligosaccharide Chain k



Bond lengths



Bond angles



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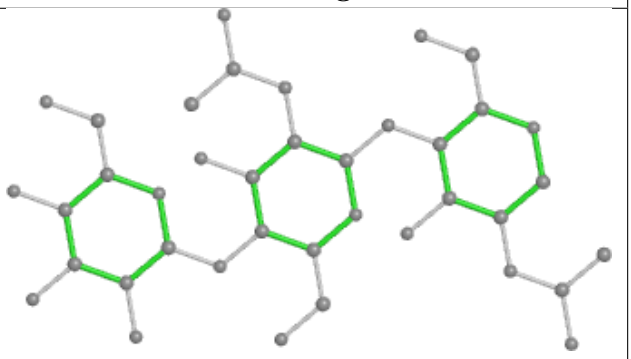
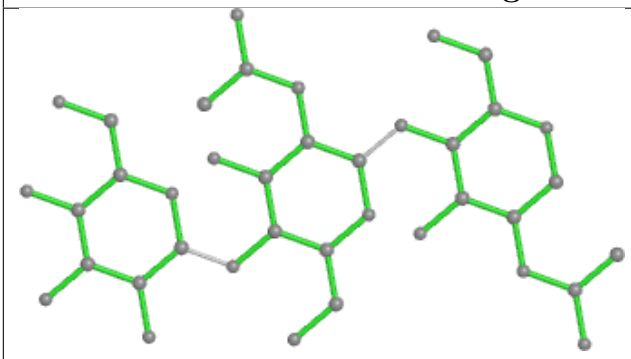
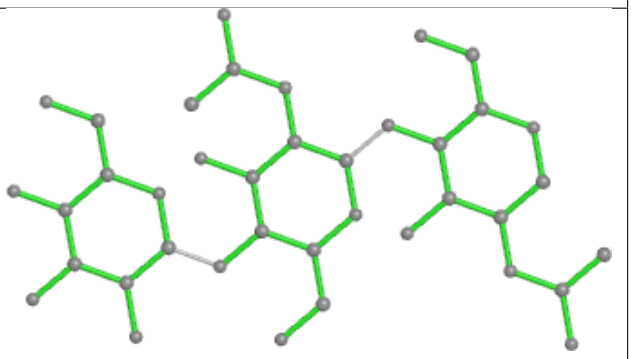


Rings

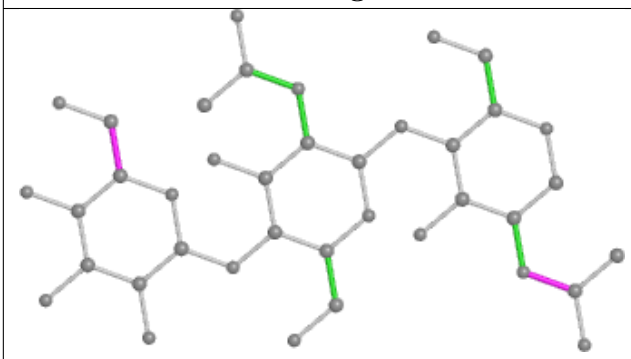
Oligosaccharide Chain l



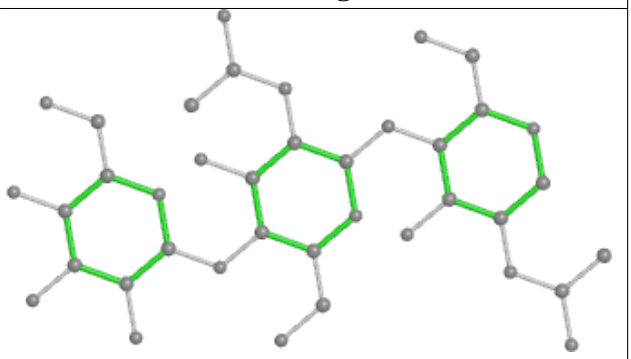
Bond lengths



Bond angles

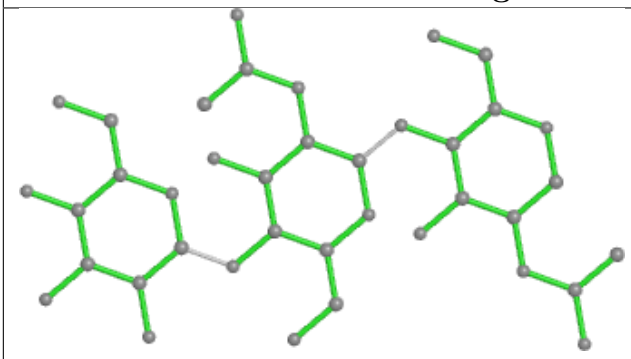


Torsions

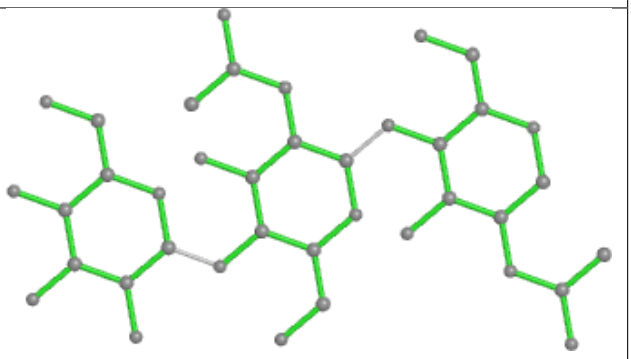


Rings

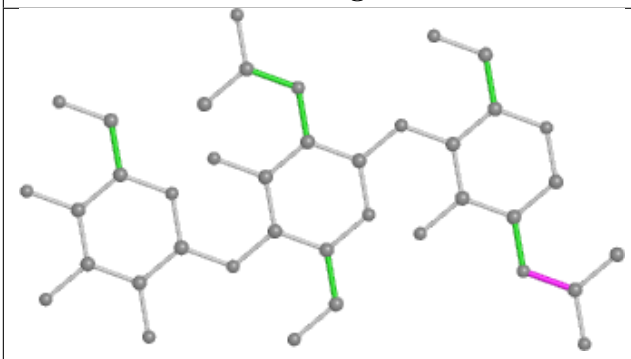
Oligosaccharide Chain m



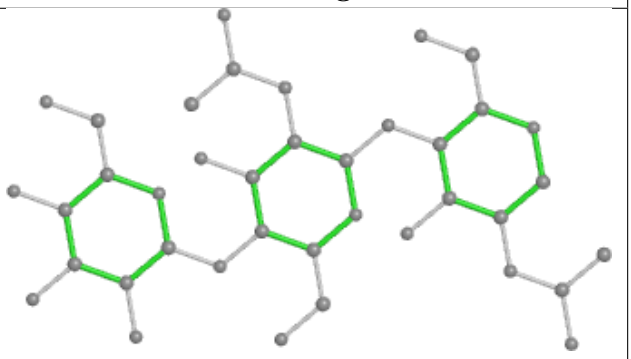
Bond lengths



Bond angles

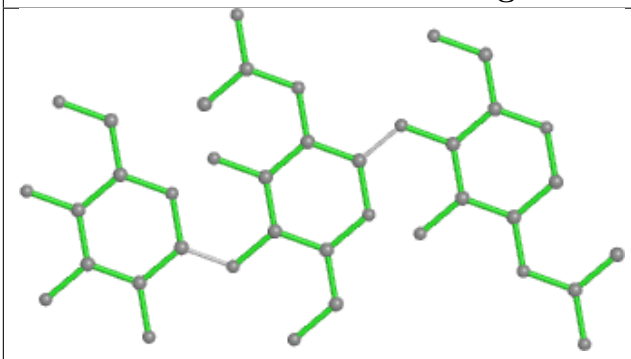


Torsions

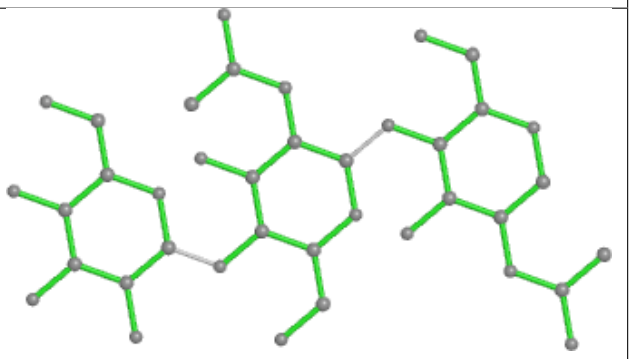


Rings

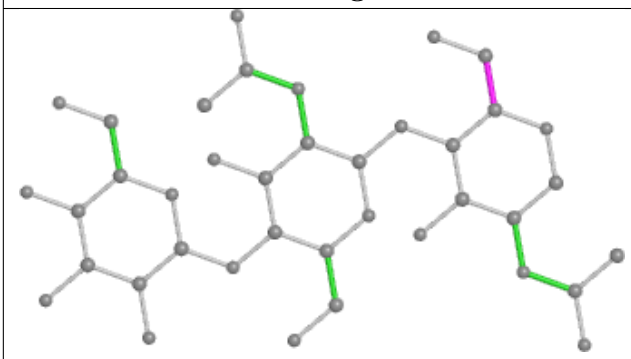
Oligosaccharide Chain n



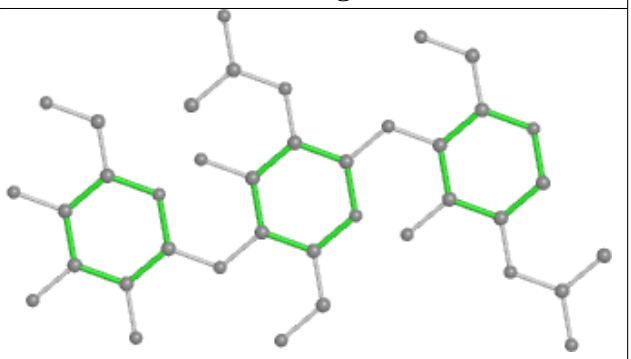
Bond lengths



Bond angles

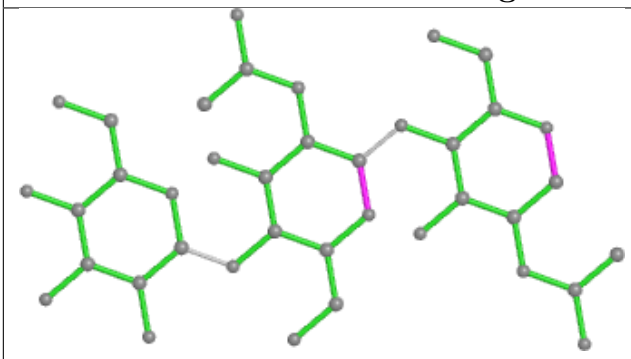


Torsions

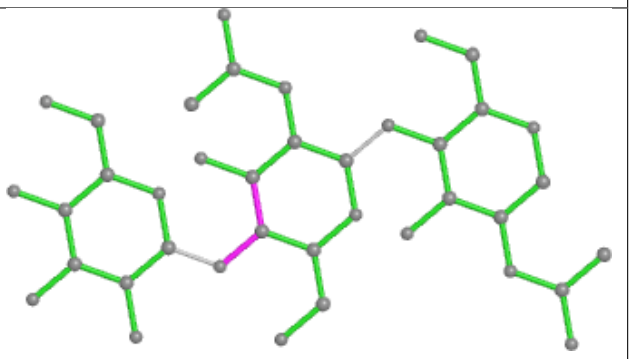


Rings

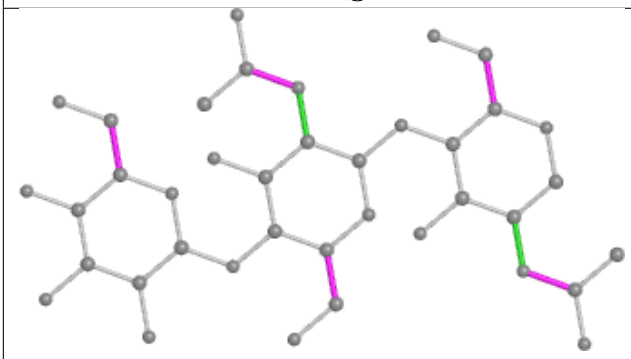
Oligosaccharide Chain o



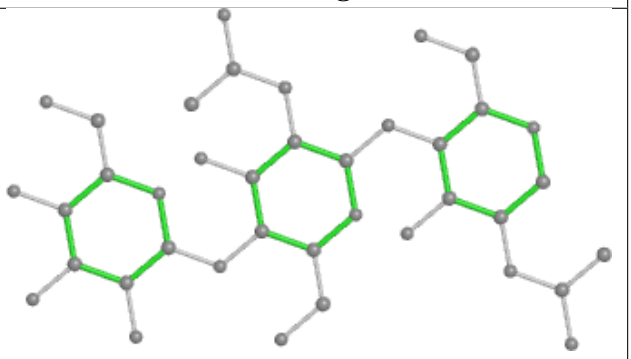
Bond lengths



Bond angles

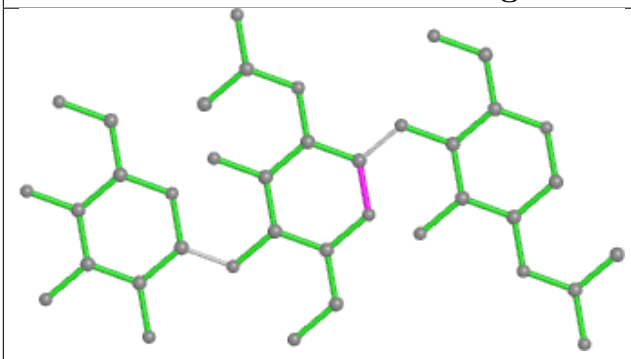


Torsions

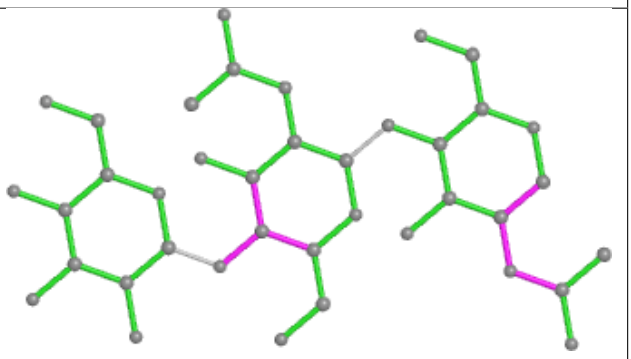


Rings

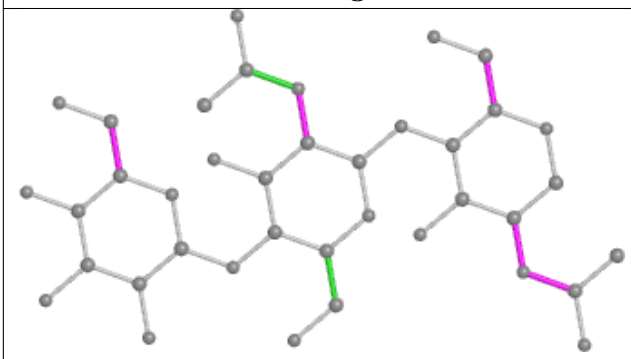
Oligosaccharide Chain s



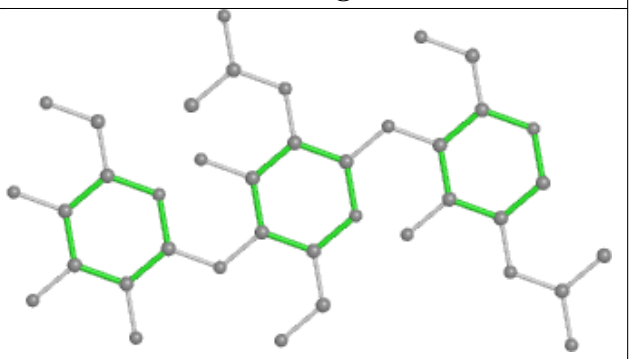
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
4	NAG	C	1302	1	14,14,15	0.73	1 (7%)	17,19,21	0.68	1 (5%)
4	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	0.35	0
4	NAG	A	1302	1	14,14,15	0.83	1 (7%)	17,19,21	0.50	0
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.35	0
4	NAG	B	1302	1	14,14,15	0.29	0	17,19,21	0.36	0
4	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.34	0

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
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	NAG	C1-C2	2.87	1.56	1.52
4	C	1302	NAG	C1-C2	2.49	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1302	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1301	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	C	1302	NAG	C8-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	C1-C2-N2-C7
4	B	1301	NAG	C1-C2-N2-C7
4	C	1301	NAG	C1-C2-N2-C7
4	B	1302	NAG	O5-C5-C6-O6
4	A	1301	NAG	C3-C2-N2-C7
4	C	1301	NAG	C3-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.