wwPDB EM Validation Summary Report (i)

Nov 13, 2022 – 08:04 PM EST

PDB ID	:	7JJJ
EMDB ID	:	EMD-22354
Title	:	Structure of SARS-CoV-2 3Q-2P full-length dimers of spike trimers
Authors	:	Bangaru, S.; Turner, H.L.; Ozorowski, G.; Antanasijevic, A.; Ward, A.B.
Deposited on	:	2020-07-26
Resolution	:	4.50 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

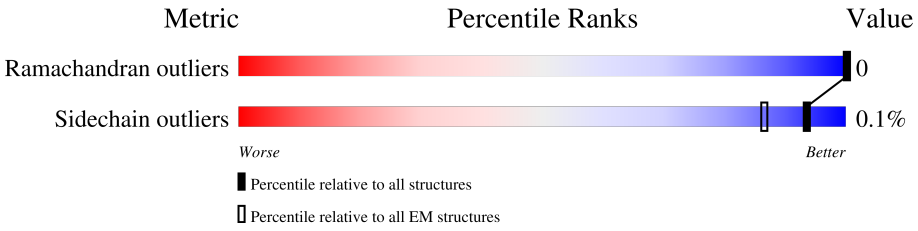
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1273	86% · 12%
1	B	1273	5% 85% · 13%
1	C	1273	5% 85% · 13%
1	D	1273	86% · 12%
1	E	1273	5% 85% · 13%
1	F	1273	5% 85% · 13%
2	0	2	100%
2	1	2	100%
2	2	2	50% 100%

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Mol	Chain	Length	Quality of chain
2	3	2	100%
2	4	2	100%
2	5	2	100%
2	7	2	100% 100%
2	8	2	50% 100%
2	9	2	50% 100%
2	AA	2	50% 100%
2	BA	2	100% 100%
2	CA	2	50% 100%
2	DA	2	50% 100%
2	EA	2	50% 100%
2	FA	2	50% 100%
2	G	2	50% 100%
2	GA	2	100%
2	H	2	50% 100%
2	HA	2	100%
2	I	2	50% 100%
2	IA	2	50% 100%
2	J	2	50% 100%
2	JA	2	50% 100%
2	K	2	50% 100%
2	KA	2	50% 100%
2	L	2	50% 100%
2	LA	2	50% 100%
2	M	2	100%

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Mol	Chain	Length	Quality of chain
2	MA	2	100% 100%
2	N	2	100%
2	NA	2	50% 100%
2	O	2	50% 100%
2	OA	2	50% 100%
2	P	2	100%
2	PA	2	100% 100%
2	Q	2	100%
2	QA	2	50% 100%
2	R	2	100%
2	RA	2	100% 100%
2	SA	2	100%
2	T	2	100% 100%
2	TA	2	100%
2	U	2	50% 100%
2	UA	2	50% 100%
2	V	2	50% 100%
2	VA	2	100%
2	W	2	50% 100%
2	WA	2	100%
2	X	2	100% 100%
2	Y	2	50% 100%
2	Z	2	50% 100%
2	a	2	50% 100%
2	b	2	50% 100%

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Mol	Chain	Length	Quality of chain
2	c	2	100%
2	d	2	100%
2	e	2	50% 100%
2	f	2	50% 100%
2	g	2	50% 100%
2	h	2	50% 100%
2	i	2	100% 100%
2	j	2	50% 100%
2	k	2	50% 100%
2	l	2	100% 100%
2	m	2	50% 100%
2	n	2	100% 100%
2	o	2	100%
2	p	2	100%
2	q	2	50% 100%
2	r	2	100%
2	s	2	100%
2	u	2	50% 100%
2	v	2	50% 100%
2	w	2	50% 100%
2	x	2	50% 100%
2	y	2	50% 100%
2	z	2	50% 100%
3	6	3	33% 100%
3	S	3	33% 100%

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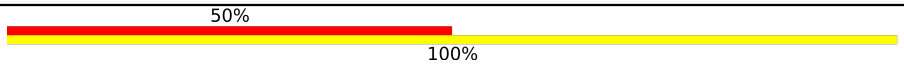
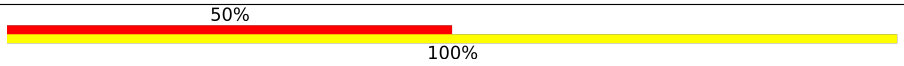
Mol	Chain	Length	Quality of chain
4	XA	4	
4	t	4	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 54614 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1120	Total	C	N	O	S	0	0
			8739	5570	1461	1668	40		
1	B	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		
1	C	1108	Total	C	N	O	S	0	0
			8648	5511	1446	1651	40		
1	D	1120	Total	C	N	O	S	0	0
			8739	5570	1461	1668	40		
1	E	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		
1	F	1108	Total	C	N	O	S	0	0
			8648	5511	1446	1651	40		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLN	ARG	engineered mutation	UNP P0DTC2
A	683	GLN	ARG	engineered mutation	UNP P0DTC2
A	685	GLN	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLN	ARG	engineered mutation	UNP P0DTC2
B	683	GLN	ARG	engineered mutation	UNP P0DTC2
B	685	GLN	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLN	ARG	engineered mutation	UNP P0DTC2
C	683	GLN	ARG	engineered mutation	UNP P0DTC2
C	685	GLN	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	682	GLN	ARG	engineered mutation	UNP P0DTC2
D	683	GLN	ARG	engineered mutation	UNP P0DTC2
D	685	GLN	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
E	682	GLN	ARG	engineered mutation	UNP P0DTC2
E	683	GLN	ARG	engineered mutation	UNP P0DTC2
E	685	GLN	ARG	engineered mutation	UNP P0DTC2
E	986	PRO	LYS	engineered mutation	UNP P0DTC2
E	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	682	GLN	ARG	engineered mutation	UNP P0DTC2
F	683	GLN	ARG	engineered mutation	UNP P0DTC2
F	685	GLN	ARG	engineered mutation	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2

- 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	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	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	M	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	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		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	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	c	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	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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	m	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		
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	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		
2	x	2	Total	C	N	O	0	0
			28	16	2	10		
2	y	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	0	2	Total	C	N	O	0	0
			28	16	2	10		
2	1	2	Total	C	N	O	0	0
			28	16	2	10		
2	2	2	Total	C	N	O	0	0
			28	16	2	10		
2	3	2	Total	C	N	O	0	0
			28	16	2	10		
2	4	2	Total	C	N	O	0	0
			28	16	2	10		
2	5	2	Total	C	N	O	0	0
			28	16	2	10		
2	7	2	Total	C	N	O	0	0
			28	16	2	10		
2	8	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	9	2	Total	C	N	O	0	0
			28	16	2	10		
2	AA	2	Total	C	N	O	0	0
			28	16	2	10		
2	BA	2	Total	C	N	O	0	0
			28	16	2	10		
2	CA	2	Total	C	N	O	0	0
			28	16	2	10		
2	DA	2	Total	C	N	O	0	0
			28	16	2	10		
2	EA	2	Total	C	N	O	0	0
			28	16	2	10		
2	FA	2	Total	C	N	O	0	0
			28	16	2	10		
2	GA	2	Total	C	N	O	0	0
			28	16	2	10		
2	HA	2	Total	C	N	O	0	0
			28	16	2	10		
2	IA	2	Total	C	N	O	0	0
			28	16	2	10		
2	JA	2	Total	C	N	O	0	0
			28	16	2	10		
2	KA	2	Total	C	N	O	0	0
			28	16	2	10		
2	LA	2	Total	C	N	O	0	0
			28	16	2	10		
2	MA	2	Total	C	N	O	0	0
			28	16	2	10		
2	NA	2	Total	C	N	O	0	0
			28	16	2	10		
2	OA	2	Total	C	N	O	0	0
			28	16	2	10		
2	PA	2	Total	C	N	O	0	0
			28	16	2	10		
2	QA	2	Total	C	N	O	0	0
			28	16	2	10		
2	RA	2	Total	C	N	O	0	0
			28	16	2	10		
2	SA	2	Total	C	N	O	0	0
			28	16	2	10		
2	TA	2	Total	C	N	O	0	0
			28	16	2	10		

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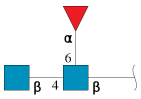
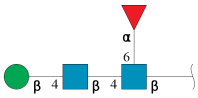
Mol	Chain	Residues	Atoms				AltConf	Trace
2	UA	2	Total	C	N	O	0	0
			28	16	2	10		
2	VA	2	Total	C	N	O	0	0
			28	16	2	10		
2	WA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



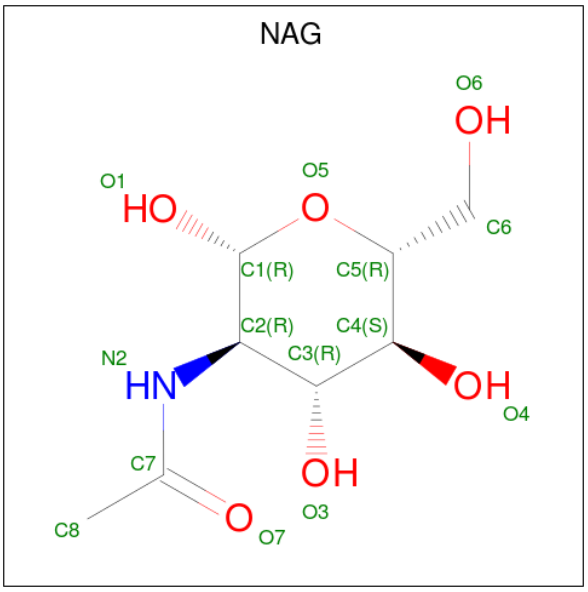
Mol	Chain	Residues	Atoms				AltConf	Trace
3	S	3	Total	C	N	O	0	0
			38	22	2	14		
3	6	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	t	4	Total	C	N	O	0	0
			49	28	2	19		
4	XA	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			42	24	3	15	
5	A	1	Total	C	N	O	0
			42	24	3	15	
5	A	1	Total	C	N	O	0
			42	24	3	15	
5	B	1	Total	C	N	O	0
			28	16	2	10	
5	B	1	Total	C	N	O	0
			28	16	2	10	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			28	16	2	10	
5	E	1	Total	C	N	O	0
			28	16	2	10	
5	F	1	Total	C	N	O	0
			42	24	3	15	

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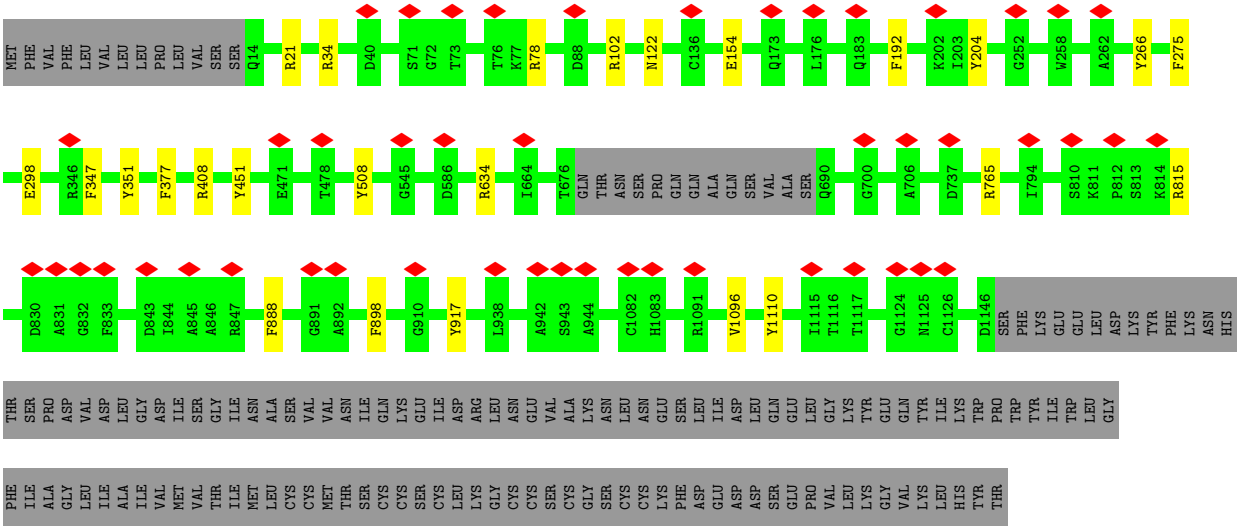
Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			42	24	3	15	
5	F	1	Total	C	N	O	0
			42	24	3	15	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

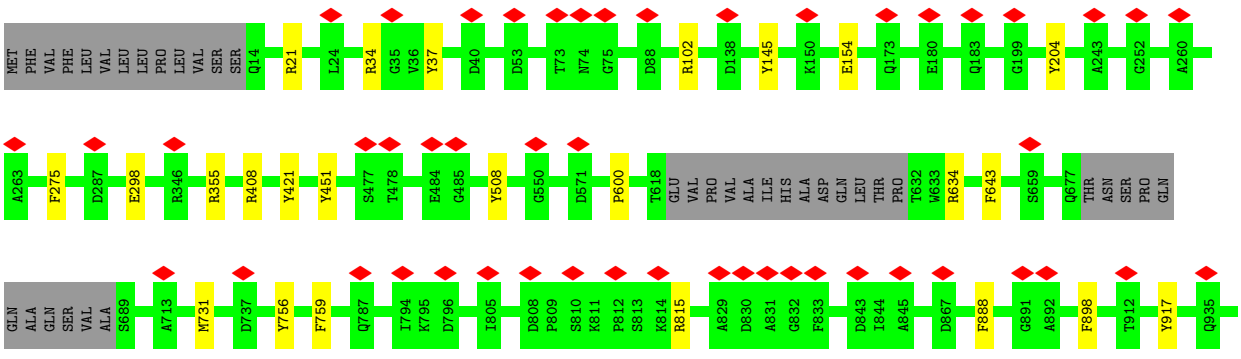
• Molecule 1: Spike glycoprotein

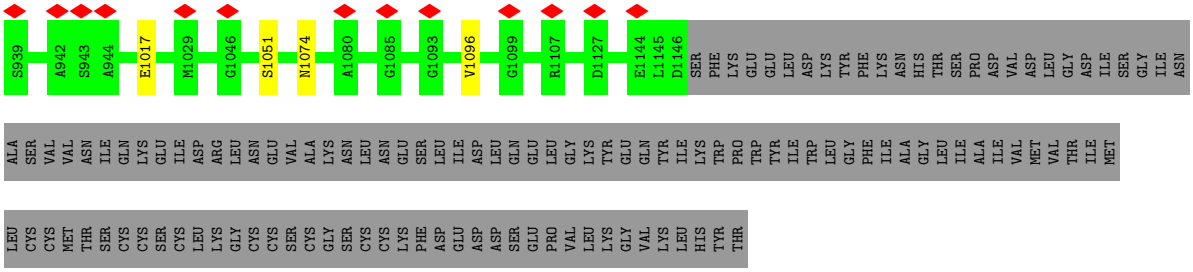
Chain A:



• Molecule 1: Spike glycoprotein

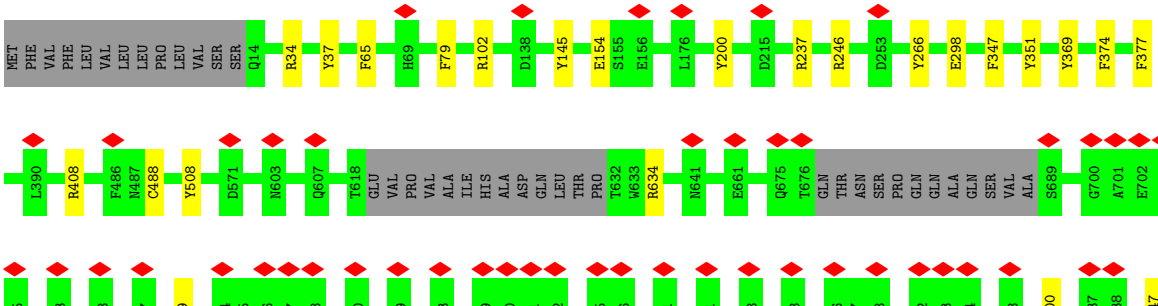
Chain B:





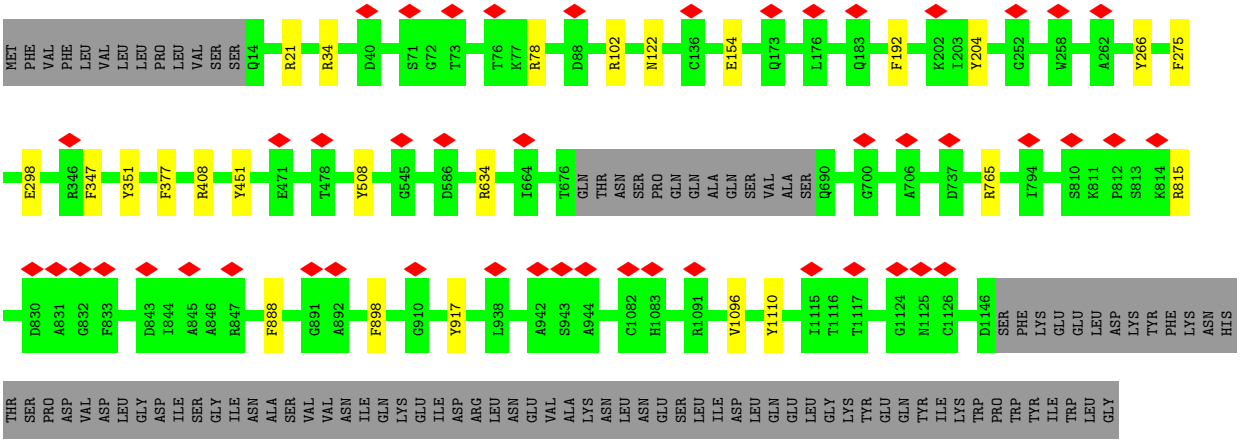
• Molecule 1: Spike glycoprotein

Chain C:



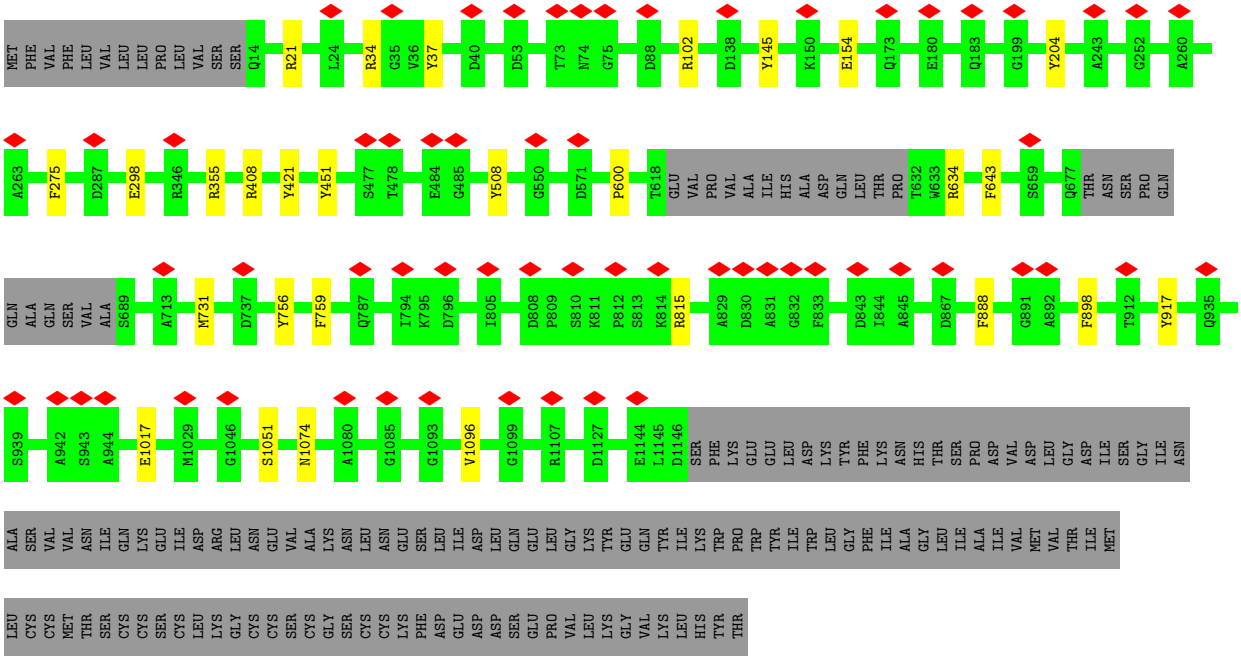
• Molecule 1: Spike glycoprotein

Chain D:



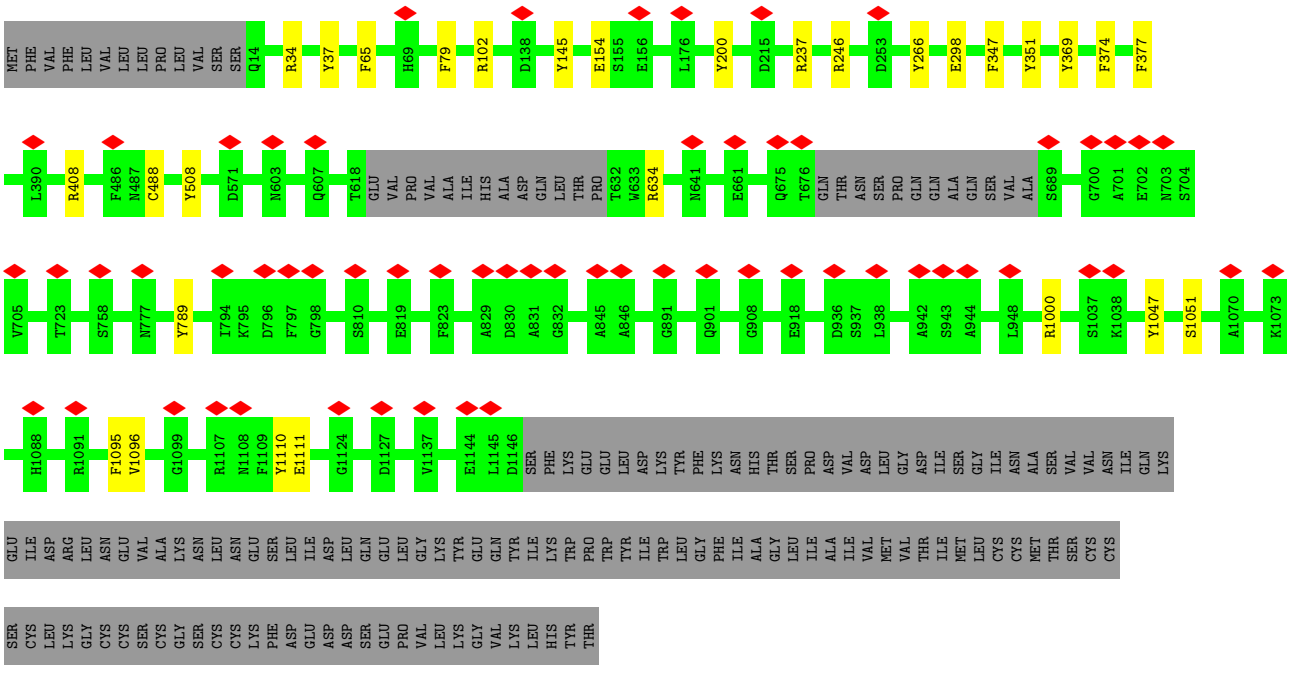
• Molecule 1: Spike glycoprotein

Chain E:



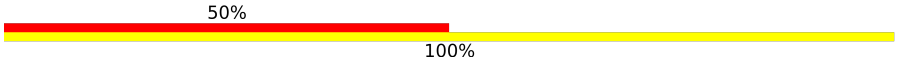
• Molecule 1: Spike glycoprotein

Chain F:



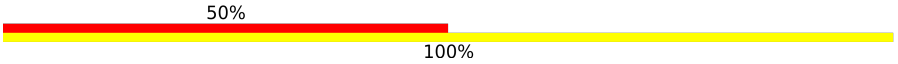
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

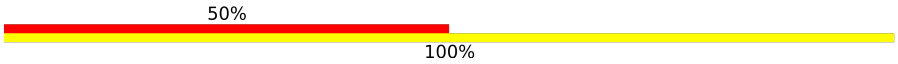


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:

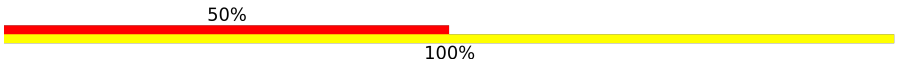


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

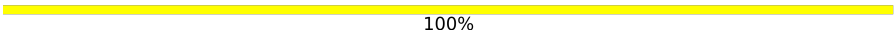
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



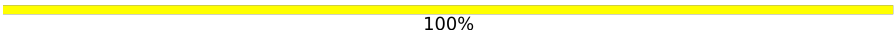
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



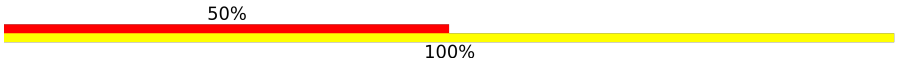
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



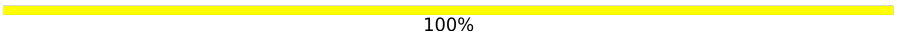
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



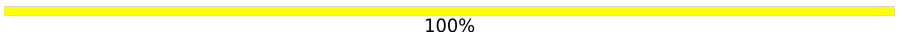
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



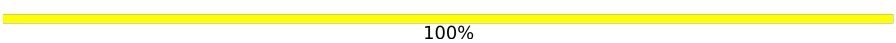
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



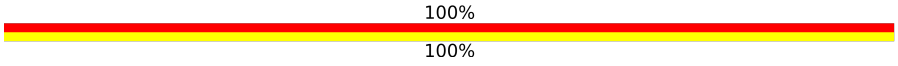
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain T:

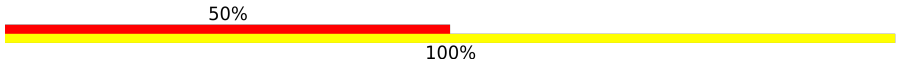


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

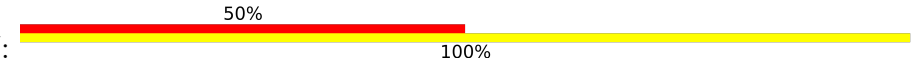
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



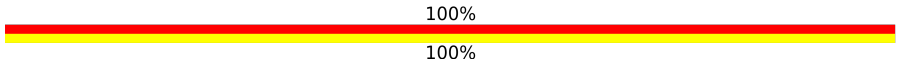
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



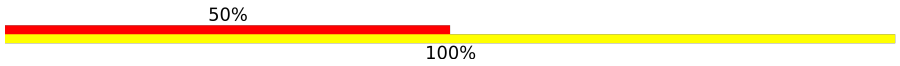
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



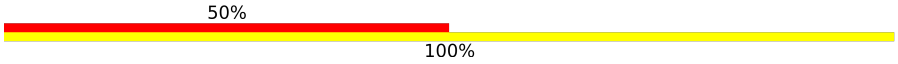
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



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

Chain Z:

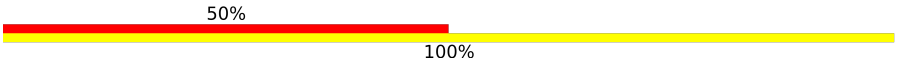


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

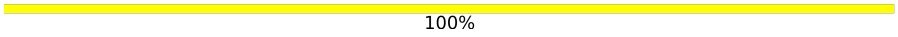
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



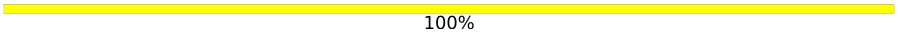
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain d:

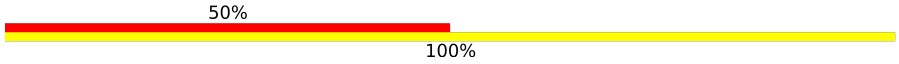


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

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

Chain f:

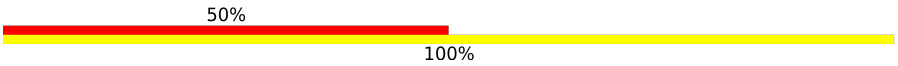


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

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

Chain h:

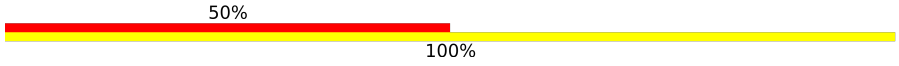


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

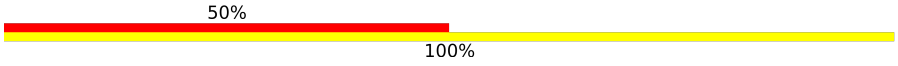
Chain k:

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

Chain l:

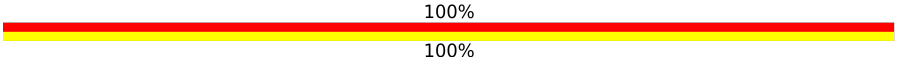
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



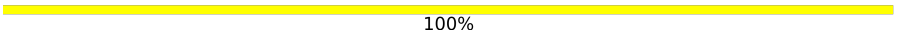
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



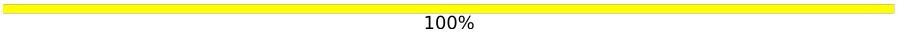
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



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

Chain p:

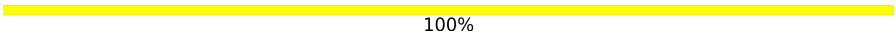


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

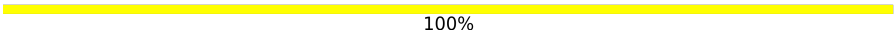
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



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

Chain s:

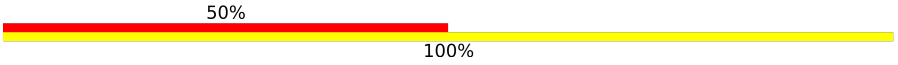


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

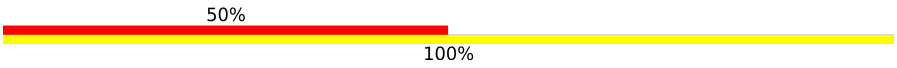
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



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

Chain w:

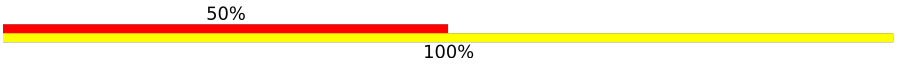


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

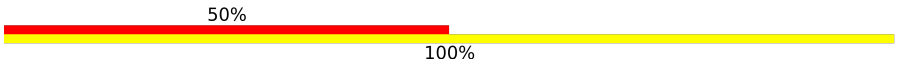
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:



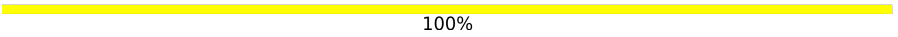
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



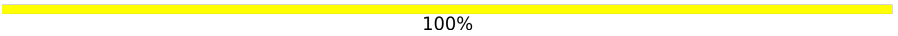
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:



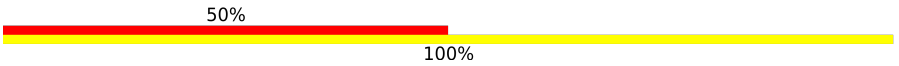
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:



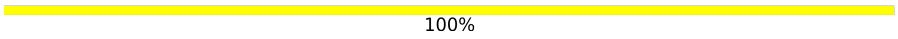
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



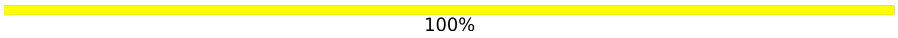
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



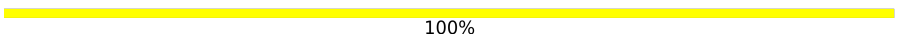
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:



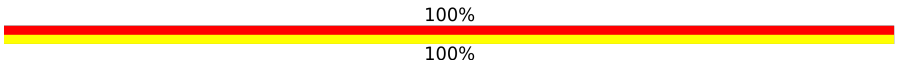
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



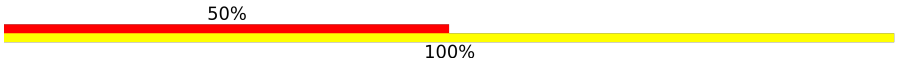
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:



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

Chain 8:



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

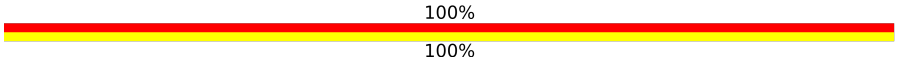
Chain 9:

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

Chain AA:

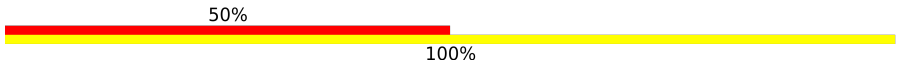
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:



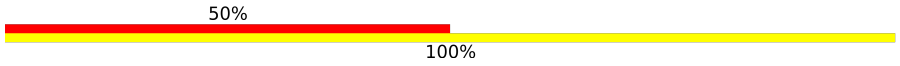
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:



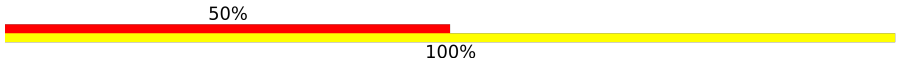
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:



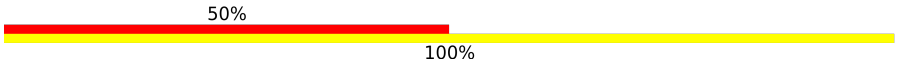
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:



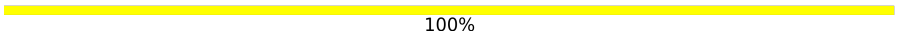
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:



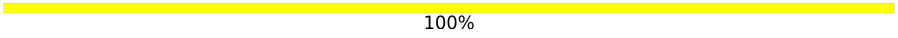
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:



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

Chain HA:

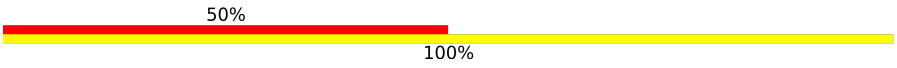


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:

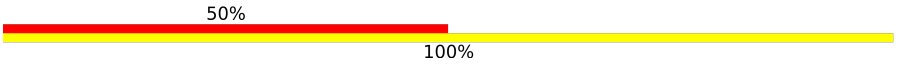
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:



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

Chain KA:

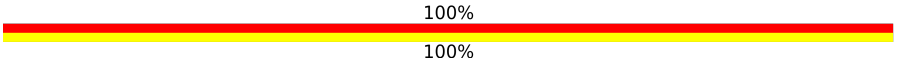


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:

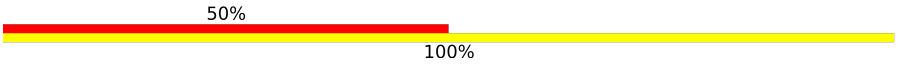
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA:



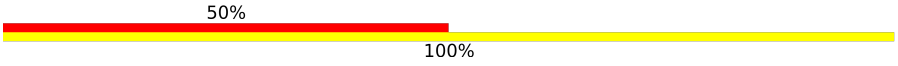
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:



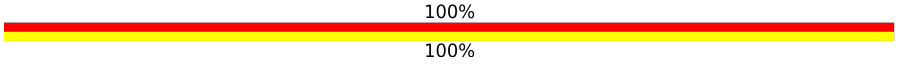
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA:



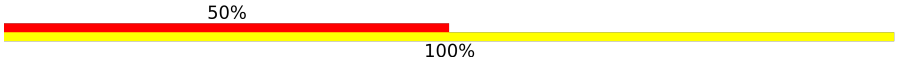
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA:



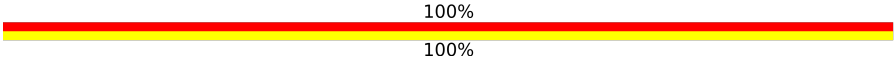
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain QA:



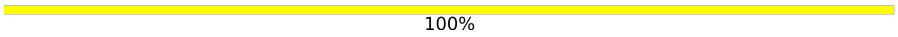
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RA:



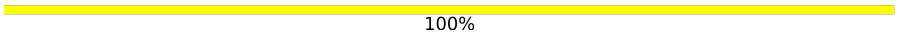
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SA:



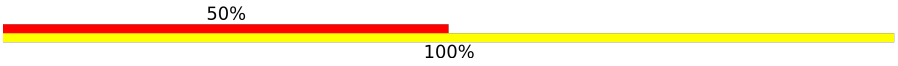
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TA:



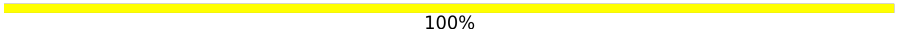
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain UA:



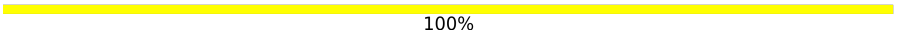
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain VA:



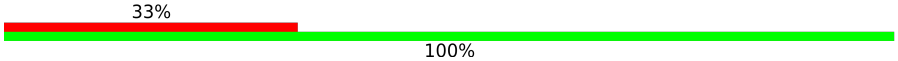
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain WA:



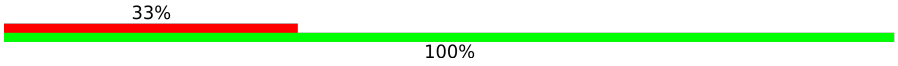
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:

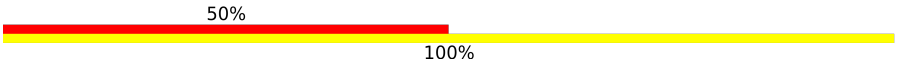


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain XA:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	15411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	529.0, 529.0, 529.0	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.98	9/8945 (0.1%)	0.93	19/12182 (0.2%)
1	B	0.97	9/8859 (0.1%)	0.94	22/12059 (0.2%)
1	C	1.00	20/8850 (0.2%)	0.93	16/12047 (0.1%)
1	D	0.98	9/8945 (0.1%)	0.93	19/12182 (0.2%)
1	E	0.97	9/8859 (0.1%)	0.94	22/12059 (0.2%)
1	F	1.00	20/8850 (0.2%)	0.93	16/12047 (0.1%)
All	All	0.98	76/53308 (0.1%)	0.94	114/72576 (0.2%)

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	TYR	CB-CG	-7.75	1.40	1.51
1	D	351	TYR	CB-CG	-7.75	1.40	1.51
1	A	1096	VAL	CB-CG2	-7.57	1.36	1.52
1	D	1096	VAL	CB-CG2	-7.57	1.36	1.52
1	B	37	TYR	CB-CG	-7.11	1.41	1.51

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	246	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	F	246	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	B	102	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	E	102	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	204	TYR	CB-CG-CD2	-8.74	115.75	121.00

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	1116/1273 (88%)	1097 (98%)	19 (2%)	0	100	100
1	B	1103/1273 (87%)	1073 (97%)	30 (3%)	0	100	100
1	C	1102/1273 (87%)	1083 (98%)	19 (2%)	0	100	100
1	D	1116/1273 (88%)	1097 (98%)	19 (2%)	0	100	100
1	E	1103/1273 (87%)	1073 (97%)	30 (3%)	0	100	100
1	F	1102/1273 (87%)	1083 (98%)	19 (2%)	0	100	100
All	All	6642/7638 (87%)	6506 (98%)	136 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	973/1112 (88%)	972 (100%)	1 (0%)	93	96
1	B	964/1112 (87%)	963 (100%)	1 (0%)	93	96
1	C	963/1112 (87%)	963 (100%)	0	100	100
1	D	973/1112 (88%)	972 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	964/1112 (87%)	963 (100%)	1 (0%)	93 96
1	F	963/1112 (87%)	963 (100%)	0	100 100
All	All	5800/6672 (87%)	5796 (100%)	4 (0%)	93 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	B	1074	ASN
1	D	122	ASN
1	E	1074	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	69	HIS
1	F	146	HIS
1	F	1010	GLN
1	F	188	ASN
1	C	1010	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)

166 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	0	1	1,2	14,14,15	2.17	6 (42%)	17,19,21	1.19	1 (5%)
2	NAG	0	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.84	1 (5%)
2	NAG	1	1	1,2	14,14,15	2.11	6 (42%)	17,19,21	1.14	3 (17%)
2	NAG	1	2	2	14,14,15	1.89	5 (35%)	17,19,21	0.85	0
2	NAG	2	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	0.94	1 (5%)
2	NAG	2	2	2	14,14,15	1.98	7 (50%)	17,19,21	0.88	1 (5%)
2	NAG	3	1	1,2	14,14,15	2.08	7 (50%)	17,19,21	1.49	3 (17%)
2	NAG	3	2	2	14,14,15	2.05	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	4	1	1,2	14,14,15	2.17	6 (42%)	17,19,21	1.09	0
2	NAG	4	2	2	14,14,15	1.99	5 (35%)	17,19,21	0.86	1 (5%)
2	NAG	5	1	1,2	14,14,15	2.06	5 (35%)	17,19,21	1.26	3 (17%)
2	NAG	5	2	2	14,14,15	1.95	6 (42%)	17,19,21	1.00	1 (5%)
3	NAG	6	1	1,3	14,14,15	0.38	0	17,19,21	0.62	0
3	NAG	6	2	3	14,14,15	0.37	0	17,19,21	0.38	0
3	FUC	6	3	3	10,10,11	0.28	0	14,14,16	0.35	0
2	NAG	7	1	1,2	14,14,15	2.15	7 (50%)	17,19,21	1.17	1 (5%)
2	NAG	7	2	2	14,14,15	2.02	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	8	1	1,2	14,14,15	2.08	7 (50%)	17,19,21	1.10	1 (5%)
2	NAG	8	2	2	14,14,15	1.94	6 (42%)	17,19,21	0.86	1 (5%)
2	NAG	9	1	1,2	14,14,15	2.12	7 (50%)	17,19,21	1.15	2 (11%)
2	NAG	9	2	2	14,14,15	2.03	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	AA	1	1,2	14,14,15	2.12	6 (42%)	17,19,21	1.00	1 (5%)
2	NAG	AA	2	2	14,14,15	2.00	7 (50%)	17,19,21	0.91	1 (5%)
2	NAG	BA	1	1,2	14,14,15	2.07	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	BA	2	2	14,14,15	2.03	7 (50%)	17,19,21	0.81	0
2	NAG	CA	1	1,2	14,14,15	2.17	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	CA	2	2	14,14,15	2.03	5 (35%)	17,19,21	0.80	0
2	NAG	DA	1	1,2	14,14,15	2.25	7 (50%)	17,19,21	1.21	3 (17%)
2	NAG	DA	2	2	14,14,15	1.98	4 (28%)	17,19,21	0.94	1 (5%)
2	NAG	EA	1	1,2	14,14,15	2.21	5 (35%)	17,19,21	0.92	0
2	NAG	EA	2	2	14,14,15	1.92	6 (42%)	17,19,21	0.92	1 (5%)
2	NAG	FA	1	1,2	14,14,15	2.14	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	FA	2	2	14,14,15	1.98	7 (50%)	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	G	1	1,2	14,14,15	2.07	5 (35%)	17,19,21	1.03	1 (5%)
2	NAG	G	2	2	14,14,15	1.92	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	GA	1	1,2	14,14,15	1.96	6 (42%)	17,19,21	1.29	1 (5%)
2	NAG	GA	2	2	14,14,15	2.02	4 (28%)	17,19,21	0.96	2 (11%)
2	NAG	H	1	1,2	14,14,15	2.02	7 (50%)	17,19,21	1.04	0
2	NAG	H	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.91	1 (5%)
2	NAG	HA	1	1,2	14,14,15	2.07	5 (35%)	17,19,21	1.13	2 (11%)
2	NAG	HA	2	2	14,14,15	1.89	5 (35%)	17,19,21	0.82	1 (5%)
2	NAG	I	1	1,2	14,14,15	2.23	6 (42%)	17,19,21	1.20	1 (5%)
2	NAG	I	2	2	14,14,15	2.08	6 (42%)	17,19,21	0.91	1 (5%)
2	NAG	IA	1	1,2	14,14,15	2.06	6 (42%)	17,19,21	1.18	2 (11%)
2	NAG	IA	2	2	14,14,15	2.01	4 (28%)	17,19,21	0.87	1 (5%)
2	NAG	J	1	1,2	14,14,15	2.16	5 (35%)	17,19,21	1.41	3 (17%)
2	NAG	J	2	2	14,14,15	2.10	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	JA	1	1,2	14,14,15	2.09	5 (35%)	17,19,21	0.98	0
2	NAG	JA	2	2	14,14,15	1.99	5 (35%)	17,19,21	0.84	0
2	NAG	K	1	1,2	14,14,15	2.25	7 (50%)	17,19,21	1.03	1 (5%)
2	NAG	K	2	2	14,14,15	1.90	6 (42%)	17,19,21	0.85	0
2	NAG	KA	1	1,2	14,14,15	2.13	5 (35%)	17,19,21	0.94	1 (5%)
2	NAG	KA	2	2	14,14,15	1.86	6 (42%)	17,19,21	2.06	2 (11%)
2	NAG	L	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	0.96	0
2	NAG	L	2	2	14,14,15	1.84	5 (35%)	17,19,21	0.96	1 (5%)
2	NAG	LA	1	1,2	14,14,15	2.09	6 (42%)	17,19,21	1.13	1 (5%)
2	NAG	LA	2	2	14,14,15	1.93	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	M	1	1,2	14,14,15	2.17	6 (42%)	17,19,21	1.19	1 (5%)
2	NAG	M	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.84	1 (5%)
2	NAG	MA	1	1,2	14,14,15	2.21	7 (50%)	17,19,21	1.06	2 (11%)
2	NAG	MA	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	N	1	1,2	14,14,15	2.11	6 (42%)	17,19,21	1.14	3 (17%)
2	NAG	N	2	2	14,14,15	1.89	5 (35%)	17,19,21	0.85	0
2	NAG	NA	1	1,2	14,14,15	2.19	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	NA	2	2	14,14,15	2.02	7 (50%)	17,19,21	0.96	1 (5%)
2	NAG	O	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	0.94	1 (5%)
2	NAG	O	2	2	14,14,15	1.98	7 (50%)	17,19,21	0.88	1 (5%)
2	NAG	OA	1	1,2	14,14,15	2.12	7 (50%)	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	OA	2	2	14,14,15	2.04	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	P	1	1,2	14,14,15	2.08	7 (50%)	17,19,21	1.49	3 (17%)
2	NAG	P	2	2	14,14,15	2.05	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	PA	1	1,2	14,14,15	2.30	7 (50%)	17,19,21	1.21	1 (5%)
2	NAG	PA	2	2	14,14,15	1.90	5 (35%)	17,19,21	0.93	1 (5%)
2	NAG	Q	1	1,2	14,14,15	2.17	6 (42%)	17,19,21	1.09	0
2	NAG	Q	2	2	14,14,15	1.99	5 (35%)	17,19,21	0.86	1 (5%)
2	NAG	QA	1	1,2	14,14,15	2.06	4 (28%)	17,19,21	1.04	1 (5%)
2	NAG	QA	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.99	1 (5%)
2	NAG	R	1	1,2	14,14,15	2.06	5 (35%)	17,19,21	1.26	3 (17%)
2	NAG	R	2	2	14,14,15	1.95	6 (42%)	17,19,21	1.00	1 (5%)
2	NAG	RA	1	1,2	14,14,15	2.20	6 (42%)	17,19,21	1.03	2 (11%)
2	NAG	RA	2	2	14,14,15	1.97	6 (42%)	17,19,21	0.91	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.38	0	17,19,21	0.62	0
3	NAG	S	2	3	14,14,15	0.39	0	17,19,21	0.39	0
3	FUC	S	3	3	10,10,11	0.29	0	14,14,16	0.34	0
2	NAG	SA	1	1,2	14,14,15	2.04	7 (50%)	17,19,21	1.27	2 (11%)
2	NAG	SA	2	2	14,14,15	1.88	4 (28%)	17,19,21	0.83	1 (5%)
2	NAG	T	1	1,2	14,14,15	2.15	7 (50%)	17,19,21	1.17	1 (5%)
2	NAG	T	2	2	14,14,15	2.02	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	TA	1	1,2	14,14,15	1.97	7 (50%)	17,19,21	1.14	1 (5%)
2	NAG	TA	2	2	14,14,15	1.91	6 (42%)	17,19,21	0.85	1 (5%)
2	NAG	U	1	1,2	14,14,15	2.08	7 (50%)	17,19,21	1.10	1 (5%)
2	NAG	U	2	2	14,14,15	1.94	6 (42%)	17,19,21	0.86	1 (5%)
2	NAG	UA	1	1,2	14,14,15	1.99	6 (42%)	17,19,21	1.21	2 (11%)
2	NAG	UA	2	2	14,14,15	2.06	4 (28%)	17,19,21	0.95	1 (5%)
2	NAG	V	1	1,2	14,14,15	2.12	7 (50%)	17,19,21	1.15	2 (11%)
2	NAG	V	2	2	14,14,15	2.03	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	VA	1	1,2	14,14,15	2.01	4 (28%)	17,19,21	0.91	0
2	NAG	VA	2	2	14,14,15	1.81	5 (35%)	17,19,21	0.98	2 (11%)
2	NAG	W	1	1,2	14,14,15	2.12	6 (42%)	17,19,21	1.00	1 (5%)
2	NAG	W	2	2	14,14,15	2.00	7 (50%)	17,19,21	0.91	1 (5%)
2	NAG	WA	1	1,2	14,14,15	2.02	5 (35%)	17,19,21	1.28	2 (11%)
2	NAG	WA	2	2	14,14,15	2.00	6 (42%)	17,19,21	1.04	2 (11%)
2	NAG	X	1	1,2	14,14,15	2.07	6 (42%)	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	X	2	2	14,14,15	2.03	7 (50%)	17,19,21	0.81	0
4	NAG	XA	1	1,4	14,14,15	1.39	2 (14%)	17,19,21	1.05	1 (5%)
4	NAG	XA	2	4	14,14,15	1.97	6 (42%)	17,19,21	0.94	1 (5%)
4	BMA	XA	3	4	11,11,12	1.91	4 (36%)	15,15,17	0.76	0
4	FUC	XA	4	4	10,10,11	1.95	5 (50%)	14,14,16	0.62	0
2	NAG	Y	1	1,2	14,14,15	2.17	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	Y	2	2	14,14,15	2.03	5 (35%)	17,19,21	0.80	0
2	NAG	Z	1	1,2	14,14,15	2.25	7 (50%)	17,19,21	1.21	3 (17%)
2	NAG	Z	2	2	14,14,15	1.98	4 (28%)	17,19,21	0.94	1 (5%)
2	NAG	a	1	1,2	14,14,15	2.21	5 (35%)	17,19,21	0.92	0
2	NAG	a	2	2	14,14,15	1.92	6 (42%)	17,19,21	0.92	1 (5%)
2	NAG	b	1	1,2	14,14,15	2.14	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	b	2	2	14,14,15	1.98	7 (50%)	17,19,21	0.89	1 (5%)
2	NAG	c	1	1,2	14,14,15	1.96	6 (42%)	17,19,21	1.29	1 (5%)
2	NAG	c	2	2	14,14,15	2.02	4 (28%)	17,19,21	0.96	2 (11%)
2	NAG	d	1	1,2	14,14,15	2.07	5 (35%)	17,19,21	1.13	2 (11%)
2	NAG	d	2	2	14,14,15	1.89	5 (35%)	17,19,21	0.82	1 (5%)
2	NAG	e	1	1,2	14,14,15	2.06	6 (42%)	17,19,21	1.18	2 (11%)
2	NAG	e	2	2	14,14,15	2.01	4 (28%)	17,19,21	0.87	1 (5%)
2	NAG	f	1	1,2	14,14,15	2.09	5 (35%)	17,19,21	0.98	0
2	NAG	f	2	2	14,14,15	1.99	5 (35%)	17,19,21	0.84	0
2	NAG	g	1	1,2	14,14,15	2.13	5 (35%)	17,19,21	0.94	1 (5%)
2	NAG	g	2	2	14,14,15	1.86	6 (42%)	17,19,21	2.06	2 (11%)
2	NAG	h	1	1,2	14,14,15	2.09	6 (42%)	17,19,21	1.13	1 (5%)
2	NAG	h	2	2	14,14,15	1.93	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	i	1	1,2	14,14,15	2.21	7 (50%)	17,19,21	1.06	2 (11%)
2	NAG	i	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	j	1	1,2	14,14,15	2.19	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	j	2	2	14,14,15	2.02	7 (50%)	17,19,21	0.96	1 (5%)
2	NAG	k	1	1,2	14,14,15	2.12	7 (50%)	17,19,21	1.32	2 (11%)
2	NAG	k	2	2	14,14,15	2.04	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	l	1	1,2	14,14,15	2.30	7 (50%)	17,19,21	1.21	1 (5%)
2	NAG	l	2	2	14,14,15	1.90	5 (35%)	17,19,21	0.93	1 (5%)
2	NAG	m	1	1,2	14,14,15	2.06	4 (28%)	17,19,21	1.04	1 (5%)
2	NAG	m	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	n	1	1,2	14,14,15	2.20	6 (42%)	17,19,21	1.03	2 (11%)
2	NAG	n	2	2	14,14,15	1.97	6 (42%)	17,19,21	0.91	1 (5%)
2	NAG	o	1	1,2	14,14,15	2.04	7 (50%)	17,19,21	1.27	2 (11%)
2	NAG	o	2	2	14,14,15	1.88	4 (28%)	17,19,21	0.83	1 (5%)
2	NAG	p	1	1,2	14,14,15	1.97	7 (50%)	17,19,21	1.14	1 (5%)
2	NAG	p	2	2	14,14,15	1.91	6 (42%)	17,19,21	0.85	1 (5%)
2	NAG	q	1	1,2	14,14,15	1.99	6 (42%)	17,19,21	1.21	2 (11%)
2	NAG	q	2	2	14,14,15	2.06	4 (28%)	17,19,21	0.95	1 (5%)
2	NAG	r	1	1,2	14,14,15	2.01	4 (28%)	17,19,21	0.91	0
2	NAG	r	2	2	14,14,15	1.81	5 (35%)	17,19,21	0.98	2 (11%)
2	NAG	s	1	1,2	14,14,15	2.02	5 (35%)	17,19,21	1.28	2 (11%)
2	NAG	s	2	2	14,14,15	2.00	6 (42%)	17,19,21	1.04	2 (11%)
4	NAG	t	1	1,4	14,14,15	1.39	2 (14%)	17,19,21	1.05	1 (5%)
4	NAG	t	2	4	14,14,15	1.97	6 (42%)	17,19,21	0.94	1 (5%)
4	BMA	t	3	4	11,11,12	1.91	4 (36%)	15,15,17	0.76	0
4	FUC	t	4	4	10,10,11	1.95	5 (50%)	14,14,16	0.62	0
2	NAG	u	1	1,2	14,14,15	2.07	5 (35%)	17,19,21	1.03	1 (5%)
2	NAG	u	2	2	14,14,15	1.92	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	v	1	1,2	14,14,15	2.02	7 (50%)	17,19,21	1.04	0
2	NAG	v	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.91	1 (5%)
2	NAG	w	1	1,2	14,14,15	2.23	6 (42%)	17,19,21	1.20	1 (5%)
2	NAG	w	2	2	14,14,15	2.08	6 (42%)	17,19,21	0.91	1 (5%)
2	NAG	x	1	1,2	14,14,15	2.16	5 (35%)	17,19,21	1.41	3 (17%)
2	NAG	x	2	2	14,14,15	2.10	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	y	1	1,2	14,14,15	2.25	7 (50%)	17,19,21	1.03	1 (5%)
2	NAG	y	2	2	14,14,15	1.90	6 (42%)	17,19,21	0.85	0
2	NAG	z	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	0.96	0
2	NAG	z	2	2	14,14,15	1.84	5 (35%)	17,19,21	0.96	1 (5%)

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	0	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0	2	2	-	0/6/23/26	0/1/1/1
2	NAG	1	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	1	2	2	-	0/6/23/26	0/1/1/1
2	NAG	2	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	2	2	2	-	0/6/23/26	0/1/1/1
2	NAG	3	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	3	2	2	-	0/6/23/26	0/1/1/1
2	NAG	4	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	4	2	2	-	0/6/23/26	0/1/1/1
2	NAG	5	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	5	2	2	-	0/6/23/26	0/1/1/1
3	NAG	6	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	6	2	3	-	2/6/23/26	0/1/1/1
3	FUC	6	3	3	-	-	0/1/1/1
2	NAG	7	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	7	2	2	-	0/6/23/26	0/1/1/1
2	NAG	8	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	8	2	2	-	0/6/23/26	0/1/1/1
2	NAG	9	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	9	2	2	-	0/6/23/26	0/1/1/1
2	NAG	AA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	BA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	CA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	DA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	EA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	EA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	FA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	FA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	GA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	HA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	IA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	JA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	JA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	KA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	KA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	LA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	MA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	NA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	NA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	OA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	OA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	PA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	PA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	QA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	QA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	RA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	RA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	S	3	3	-	-	0/1/1/1
2	NAG	SA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	TA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	TA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	UA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	UA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	VA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	VA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	1/6/23/26	0/1/1/1
2	NAG	WA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	WA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
4	NAG	XA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	XA	2	4	-	0/6/23/26	0/1/1/1
4	BMA	XA	3	4	-	0/2/19/22	0/1/1/1
4	FUC	XA	4	4	-	-	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	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	1,2	-	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	f	1	1,2	-	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	1,2	-	0/6/23/26	0/1/1/1

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

The worst 5 of 912 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	1	NAG	C1-C2	5.70	1.60	1.52
2	EA	1	NAG	C1-C2	5.70	1.60	1.52
2	G	1	NAG	C1-C2	5.54	1.60	1.52
2	u	1	NAG	C1-C2	5.54	1.60	1.52
2	L	1	NAG	C1-C2	5.46	1.60	1.52

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	g	2	NAG	C8-C7-N2	6.33	126.82	116.10
2	KA	2	NAG	C8-C7-N2	6.33	126.82	116.10
2	g	2	NAG	O7-C7-N2	-4.20	114.24	121.95
2	KA	2	NAG	O7-C7-N2	-4.20	114.24	121.95
2	o	1	NAG	C1-C2-N2	-3.35	104.76	110.49

There are no chirality outliers.

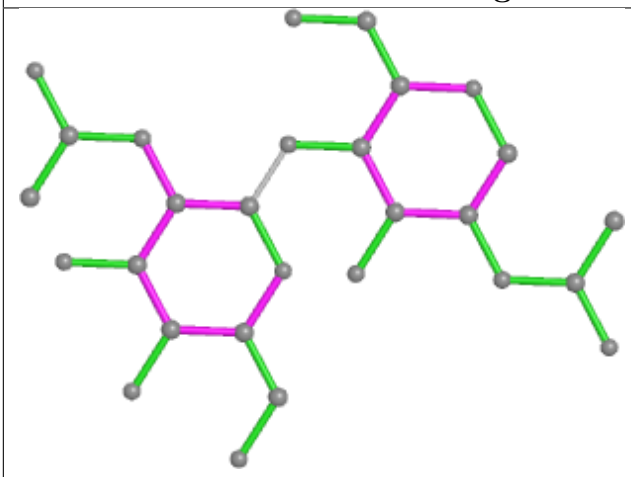
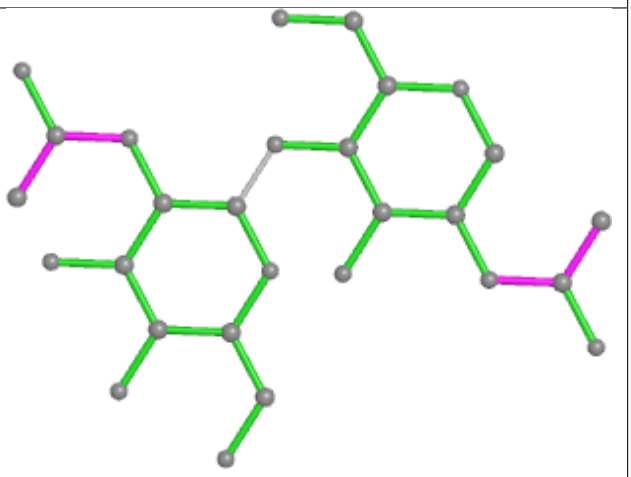
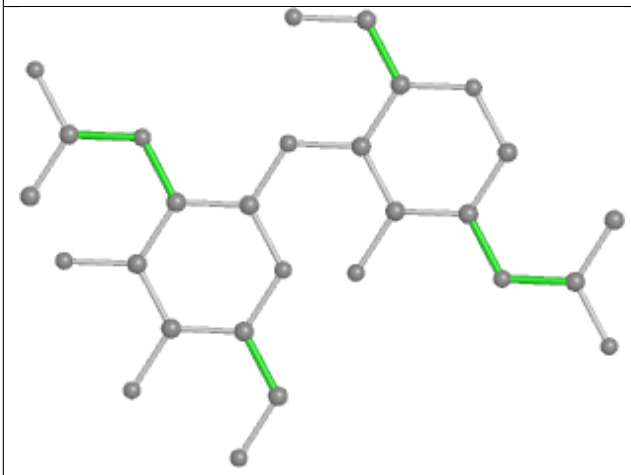
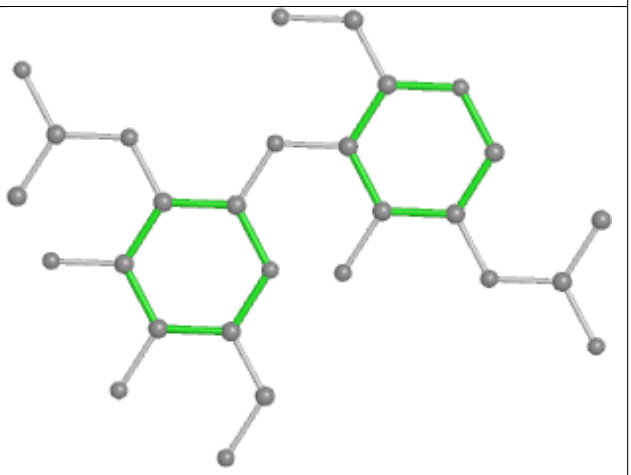
5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C4-C5-C6-O6
3	6	1	NAG	C4-C5-C6-O6
2	g	2	NAG	C8-C7-N2-C2
2	g	2	NAG	O7-C7-N2-C2
2	KA	2	NAG	C8-C7-N2-C2

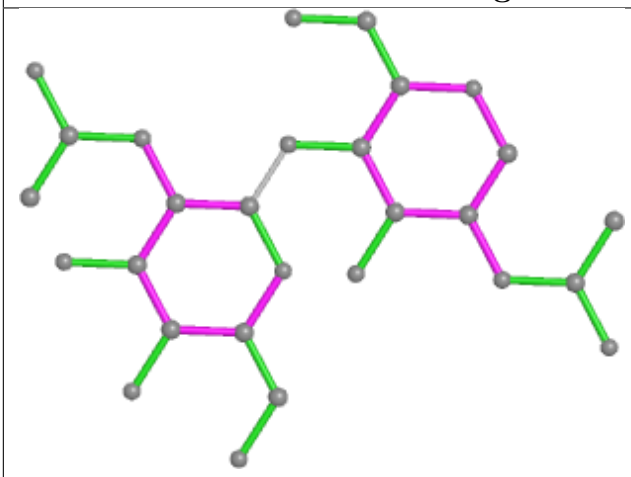
There are no ring outliers.

No monomer is involved in short contacts.

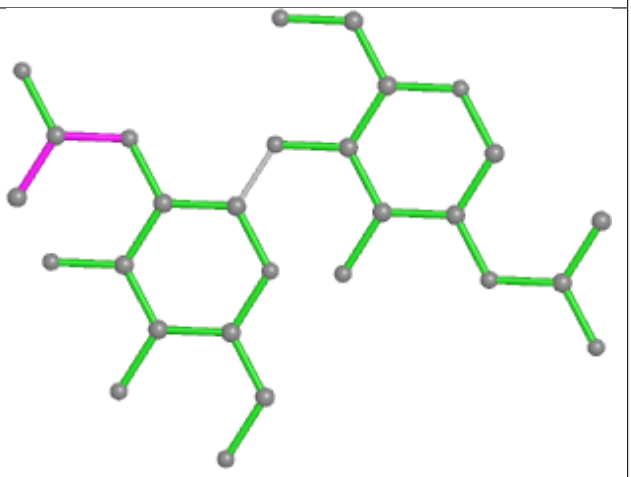
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

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

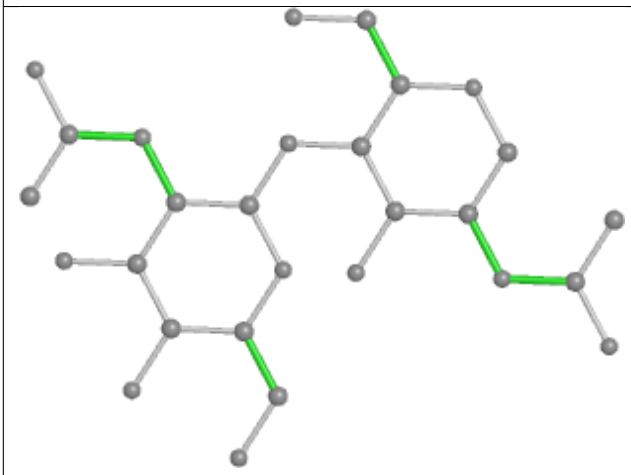
Oligosaccharide Chain H



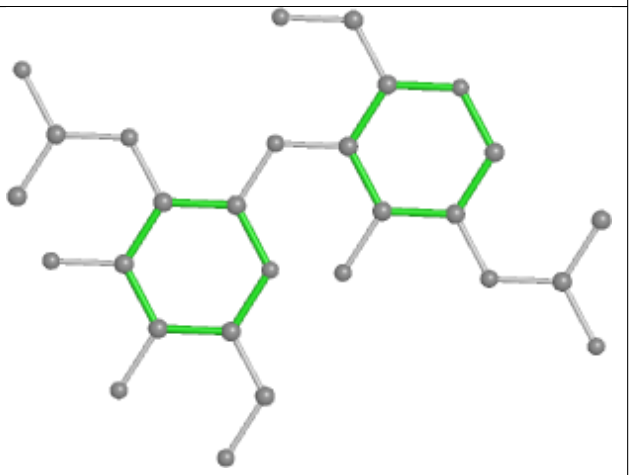
Bond lengths



Bond angles

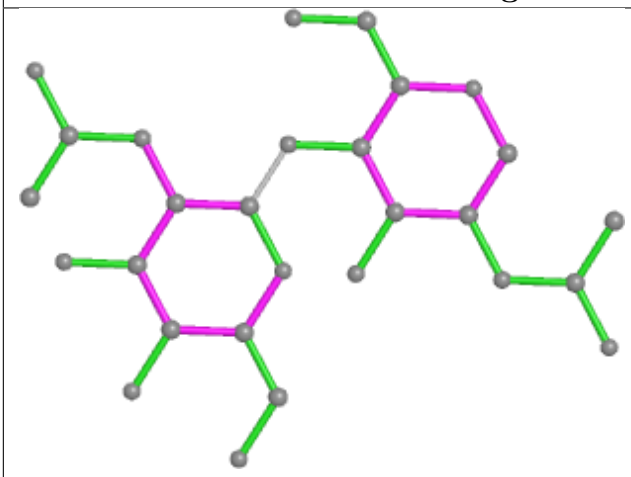


Torsions

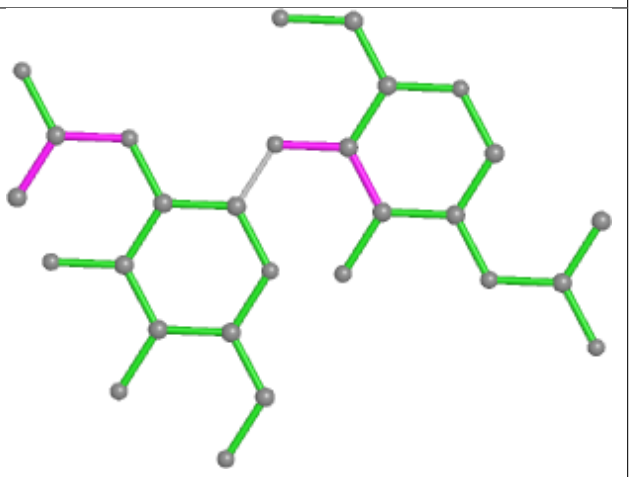


Rings

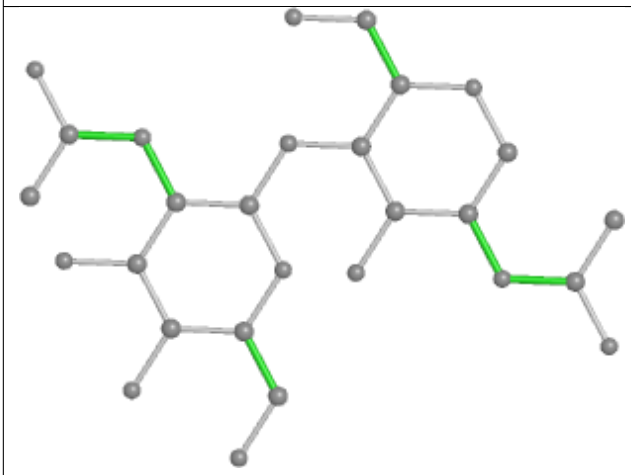
Oligosaccharide Chain I



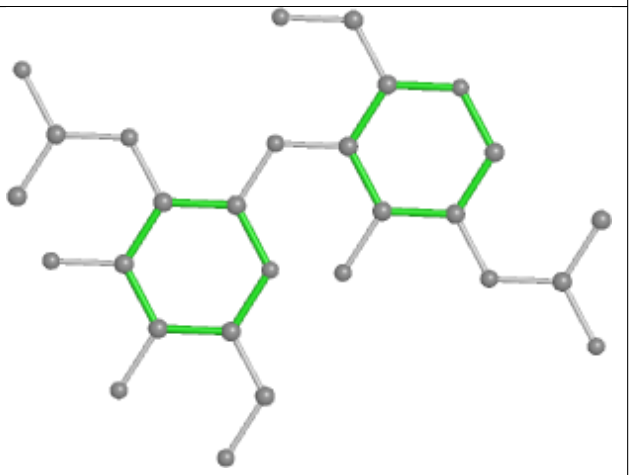
Bond lengths



Bond angles

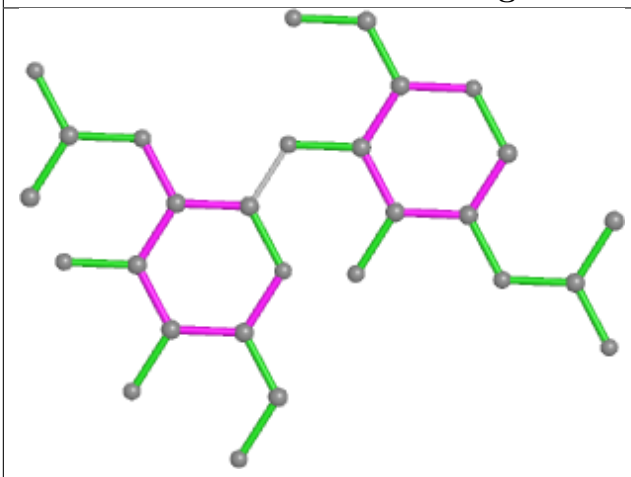


Torsions

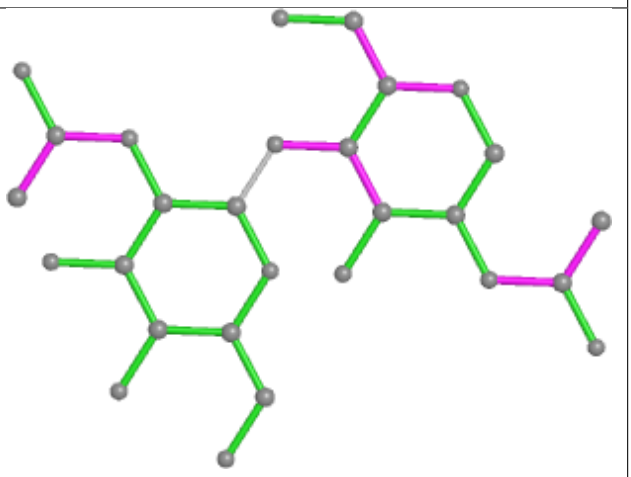


Rings

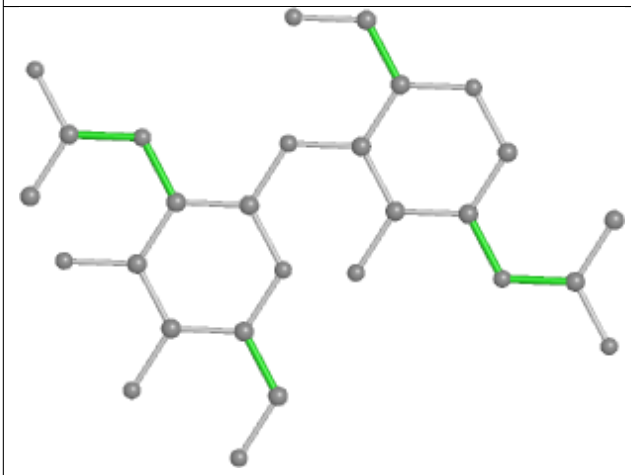
Oligosaccharide Chain J



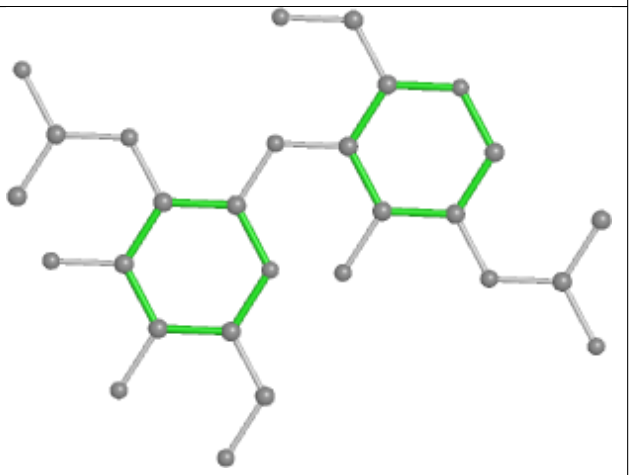
Bond lengths



Bond angles

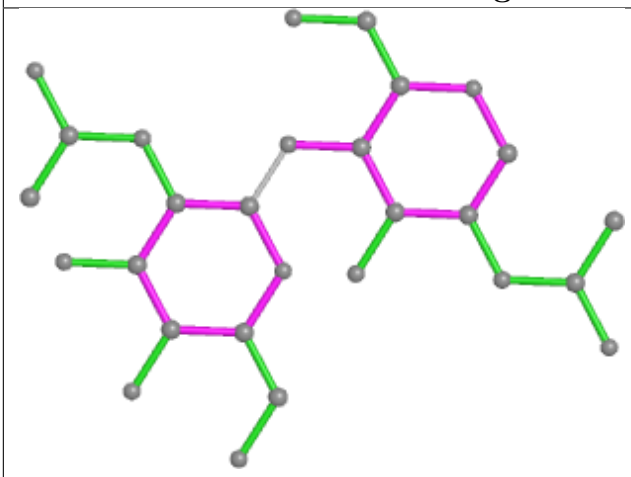


Torsions

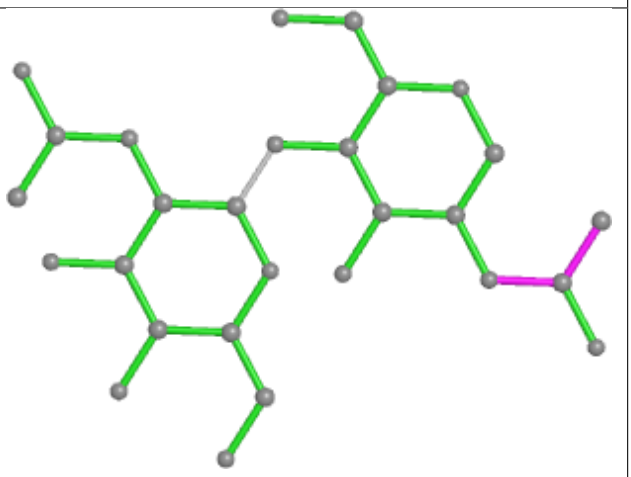


Rings

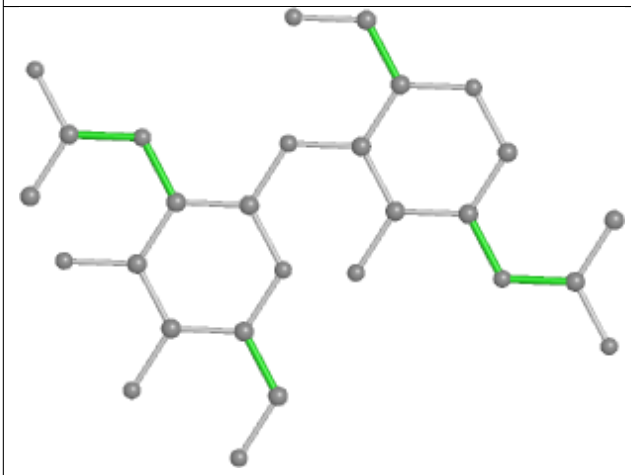
Oligosaccharide Chain K



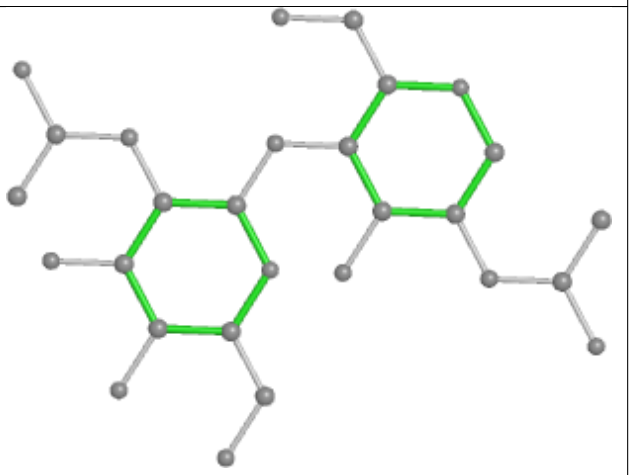
Bond lengths



Bond angles

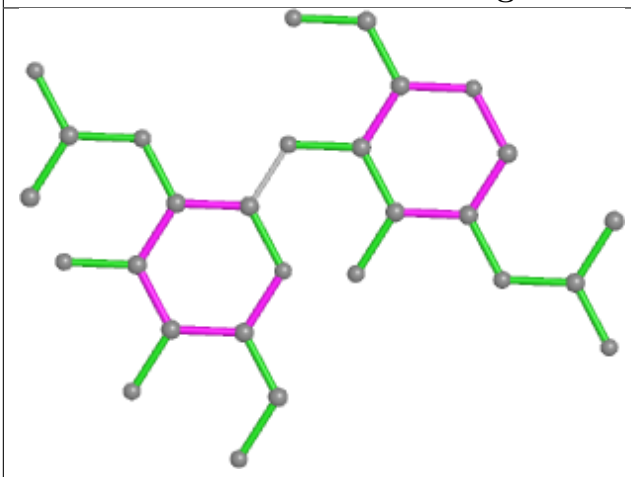


Torsions

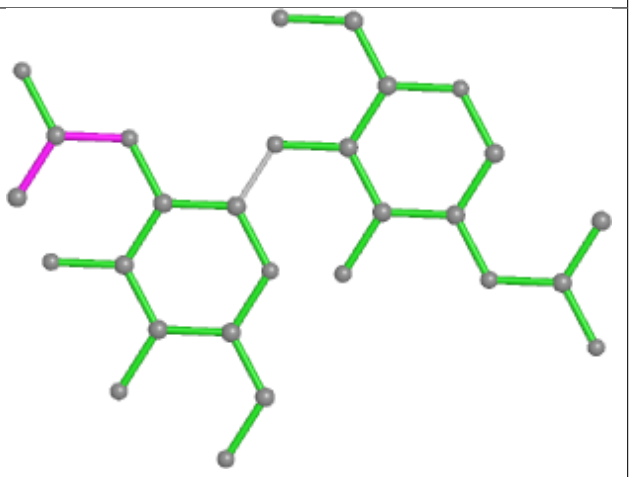


Rings

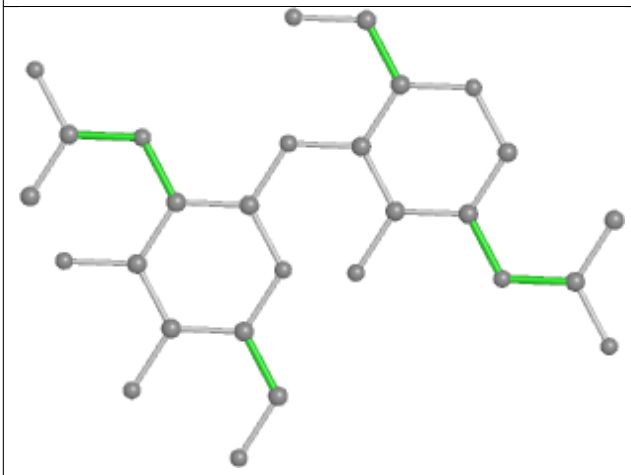
Oligosaccharide Chain L



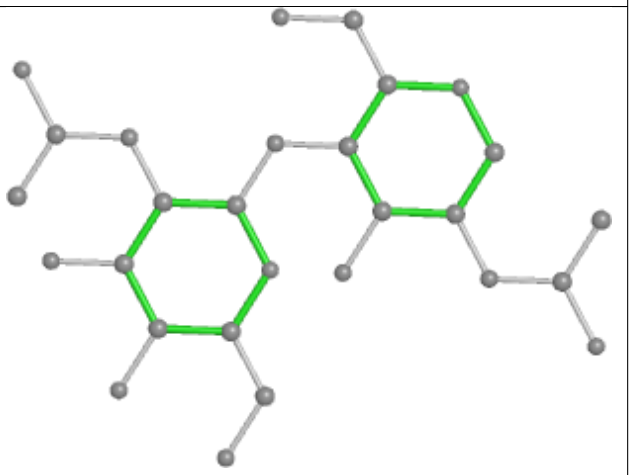
Bond lengths



Bond angles

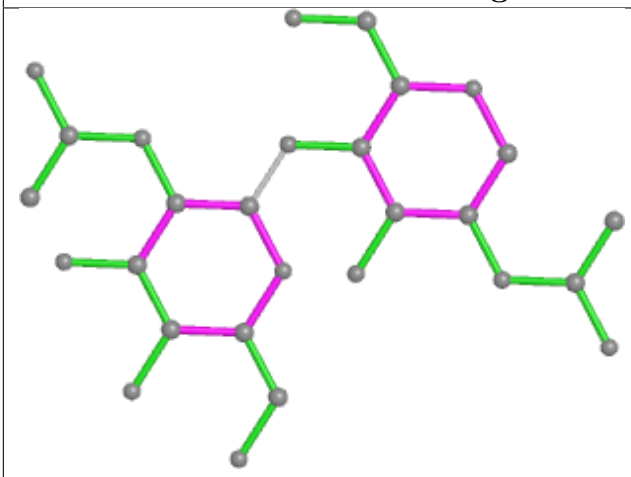


Torsions

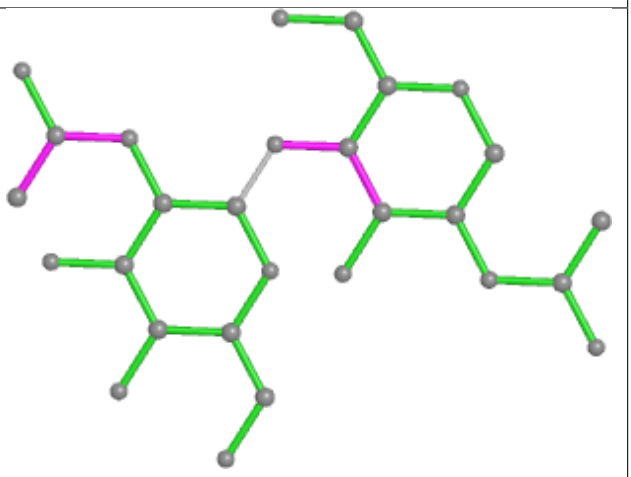


Rings

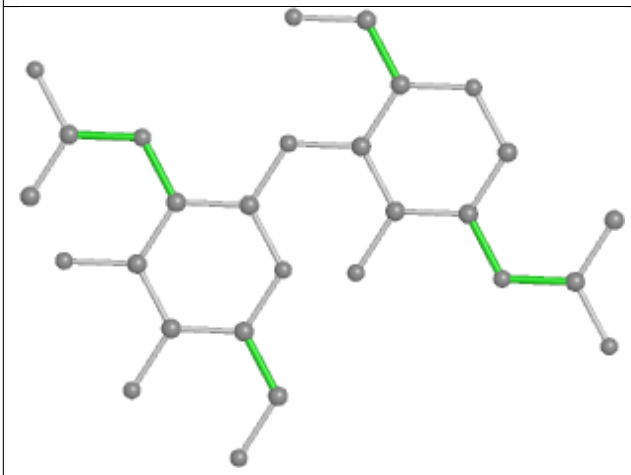
Oligosaccharide Chain M



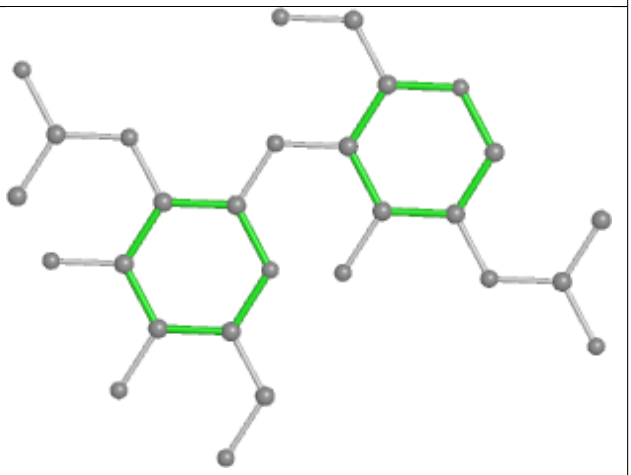
Bond lengths



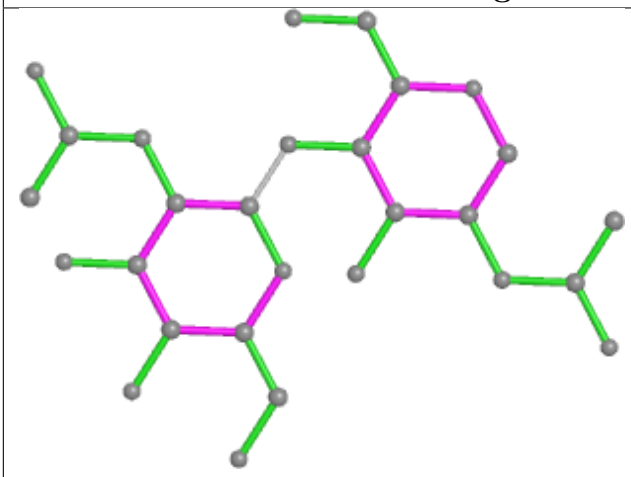
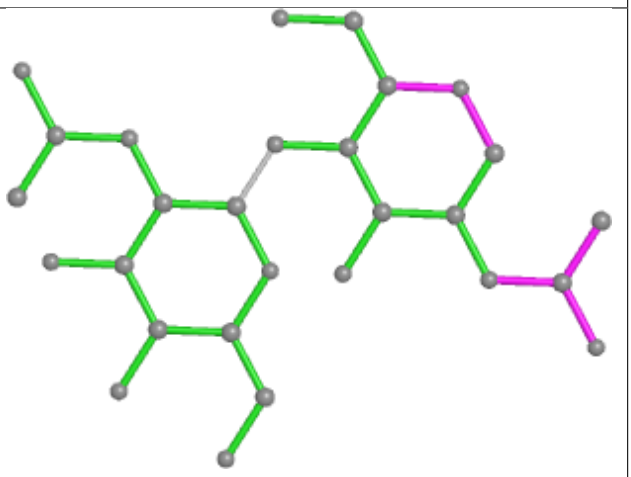
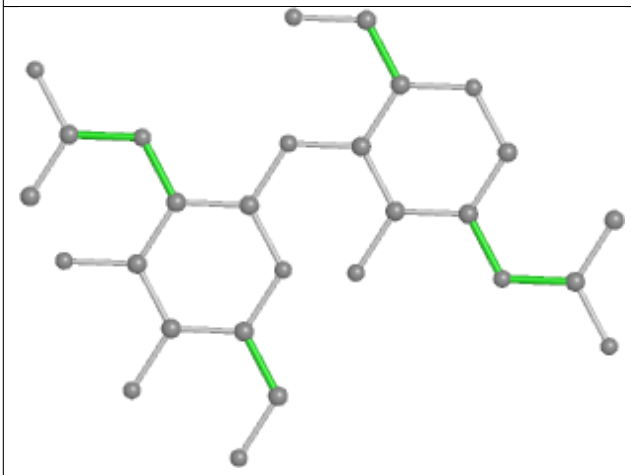
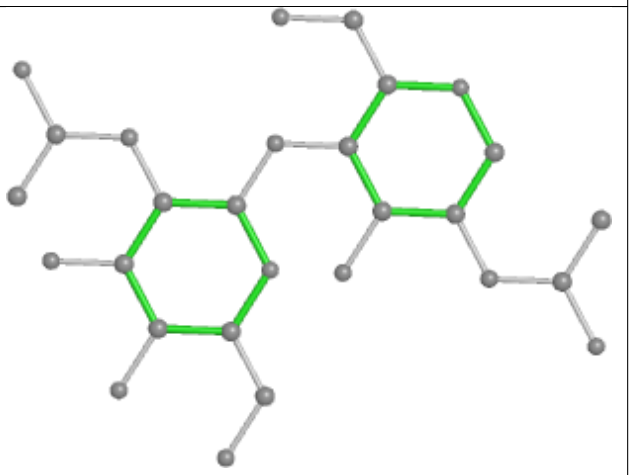
Bond angles

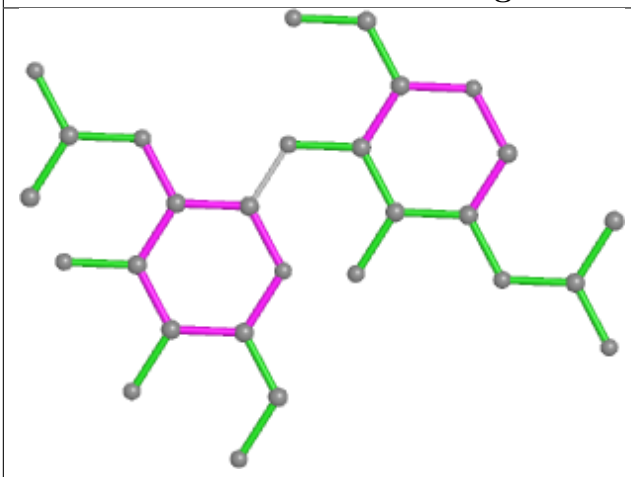
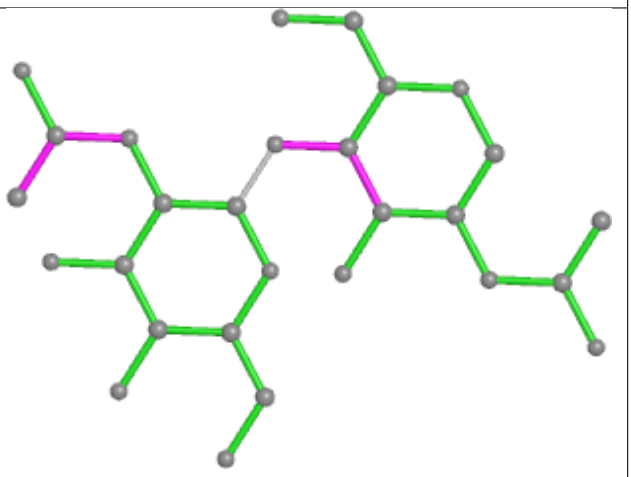
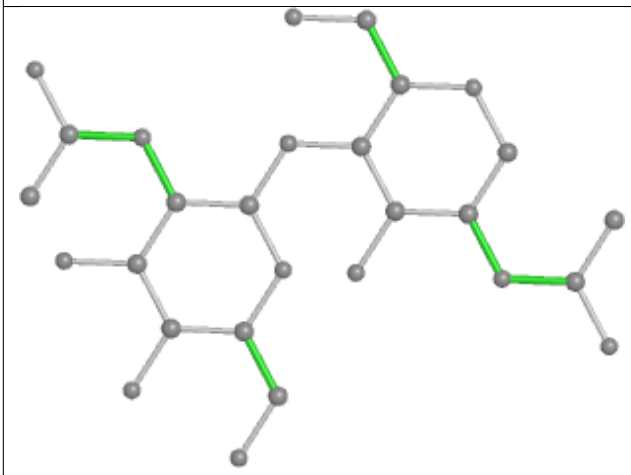
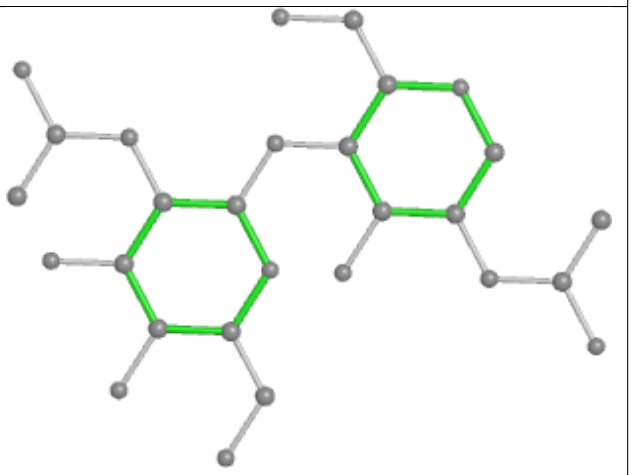


Torsions

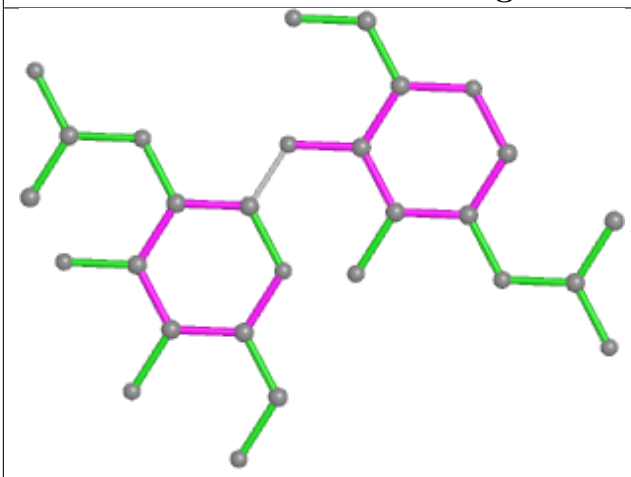


Rings

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

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

Oligosaccharide Chain P



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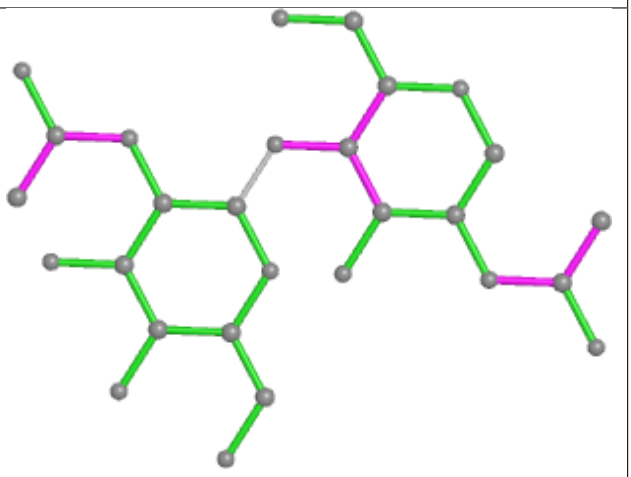
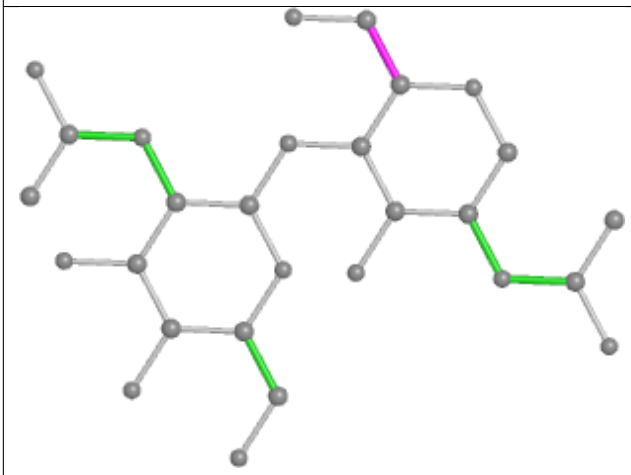
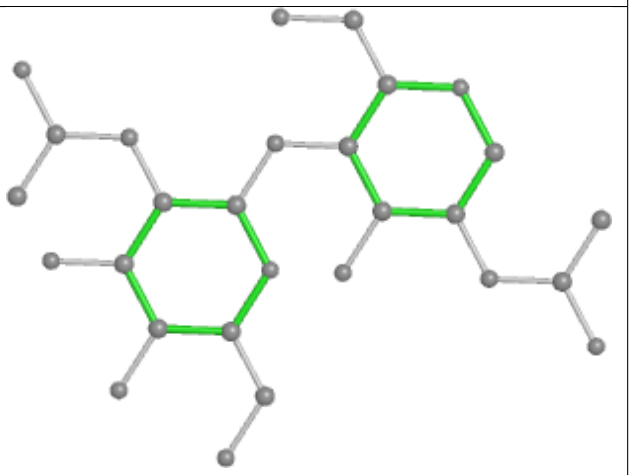


Bond angles

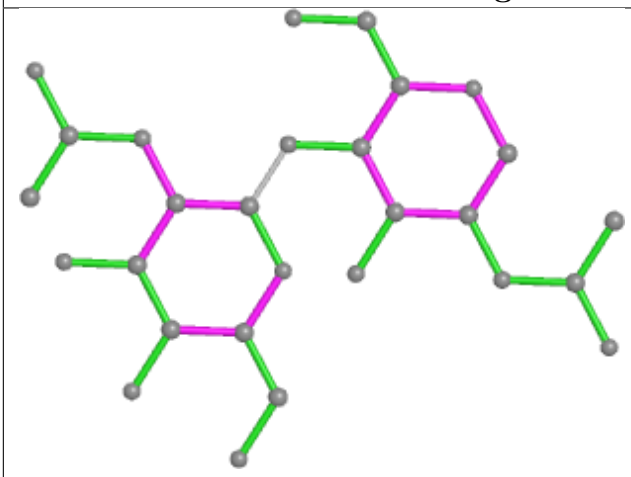


Torsions



Rings

Oligosaccharide Chain Q



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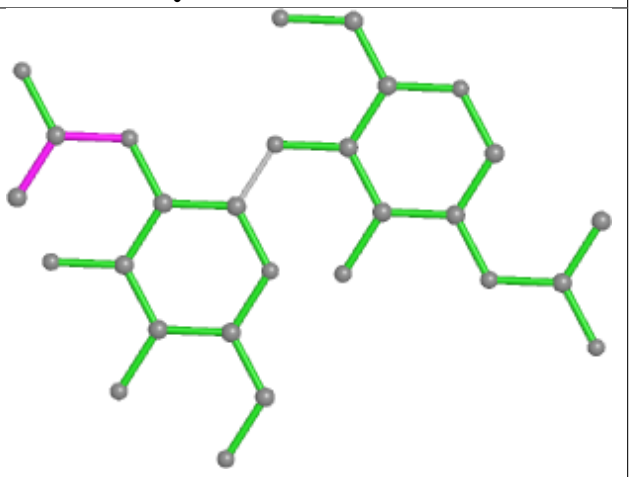

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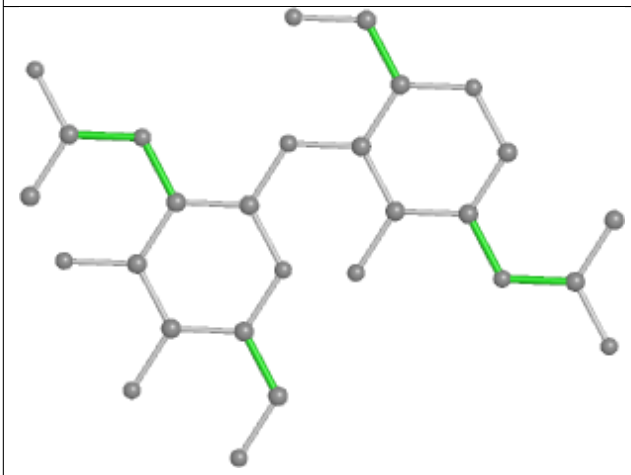
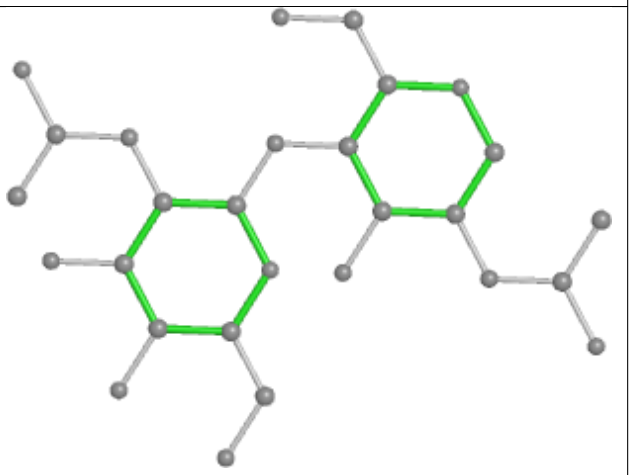
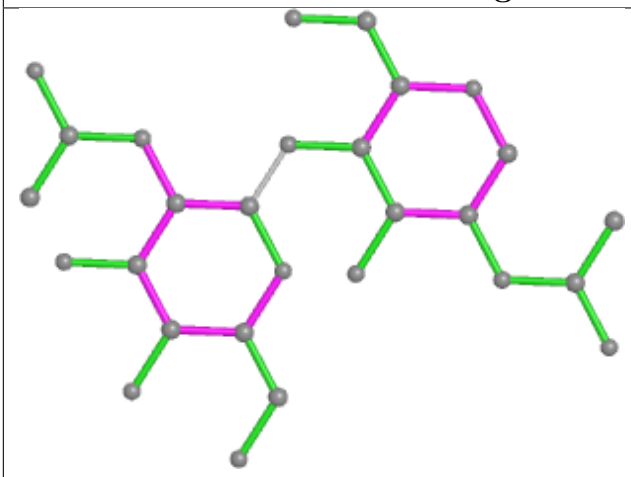


Torsions



Rings

Oligosaccharide Chain R



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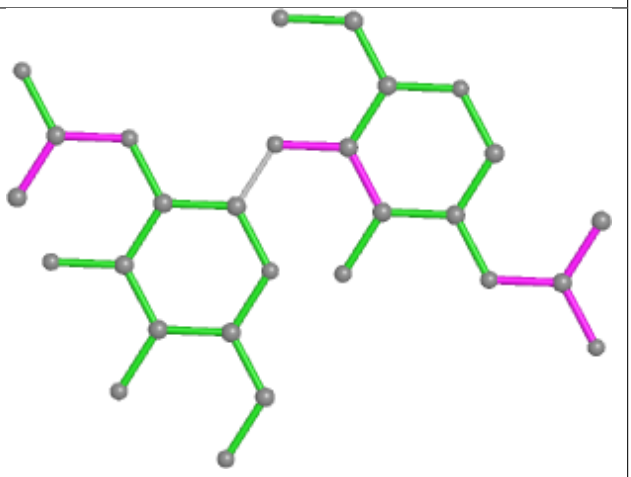
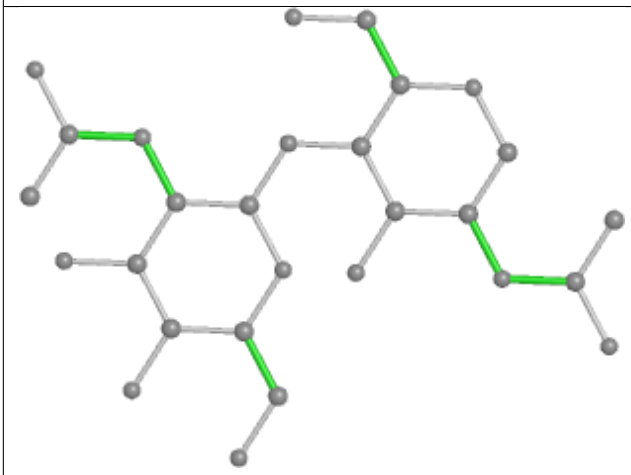
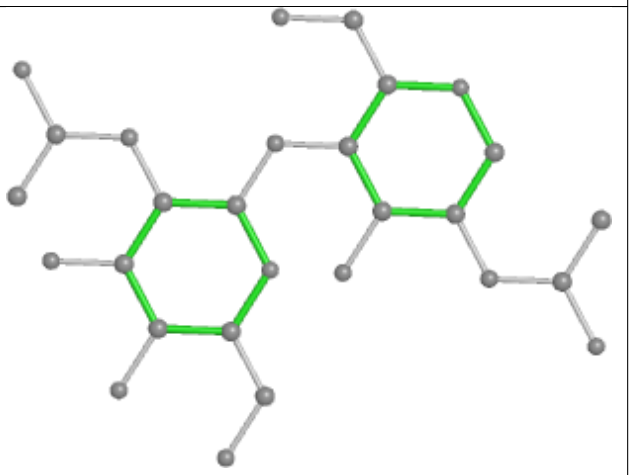


Bond angles

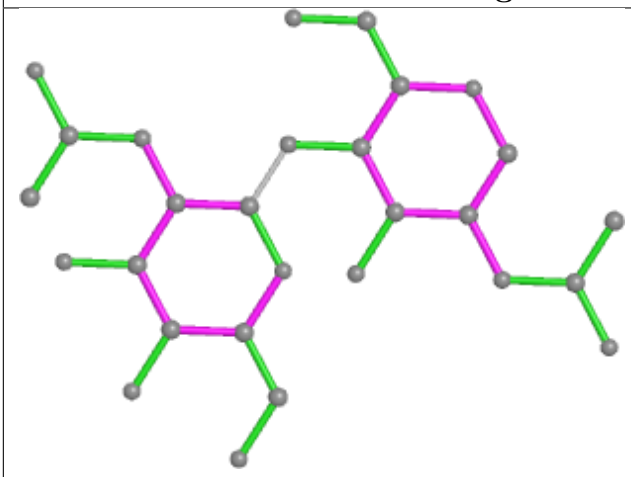


Torsions

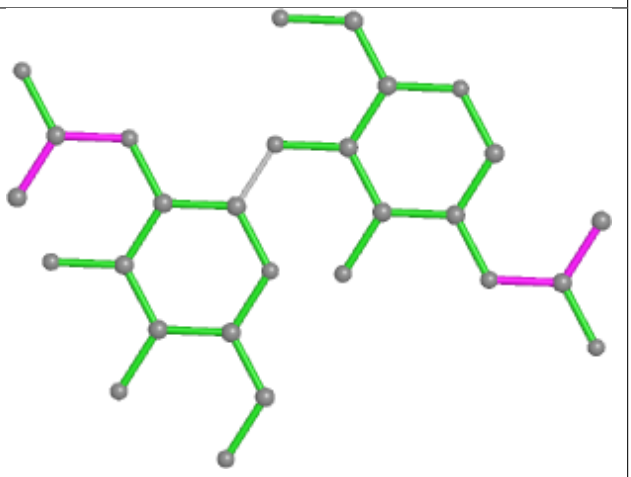


Rings

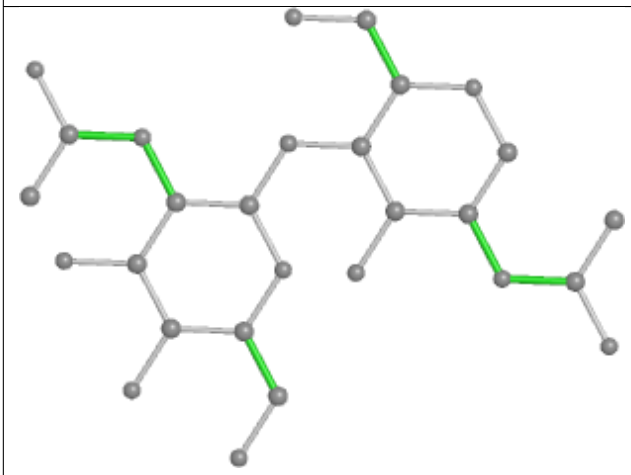
Oligosaccharide Chain T



Bond lengths



Bond angles



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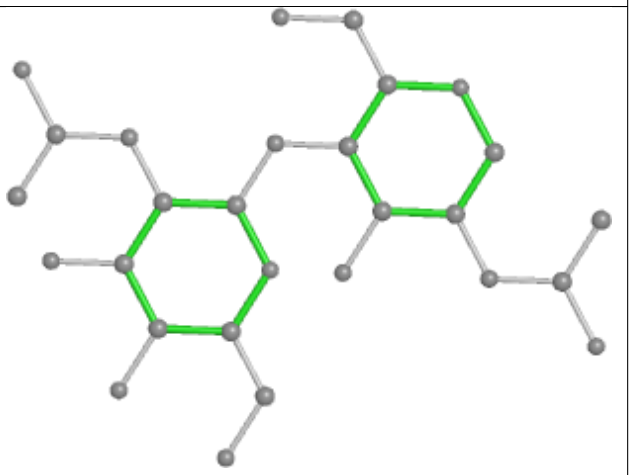
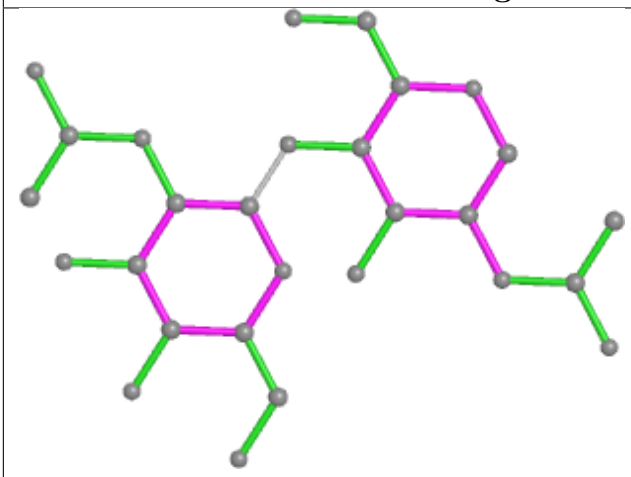


Rings

Oligosaccharide Chain U



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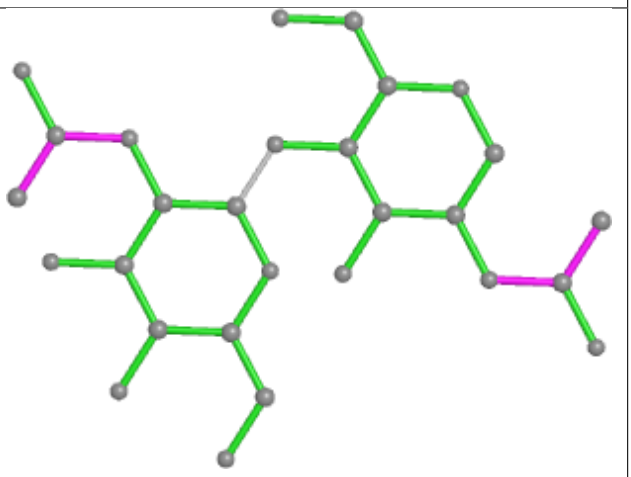

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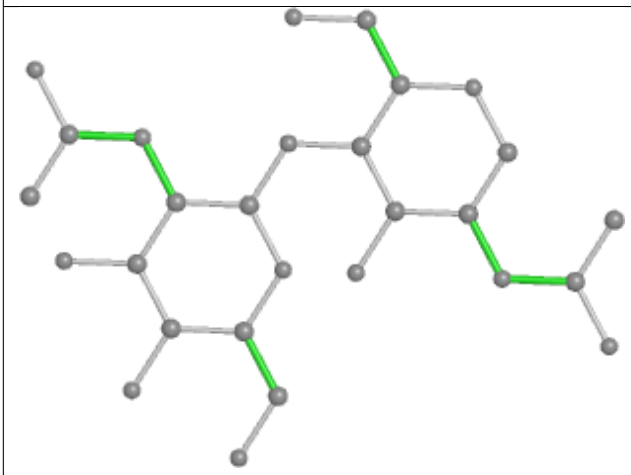
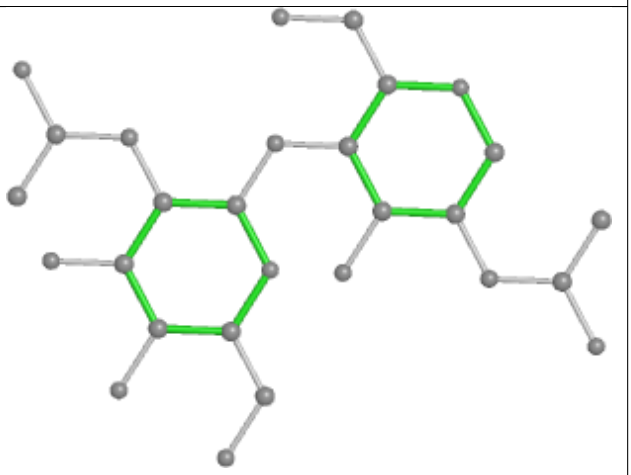
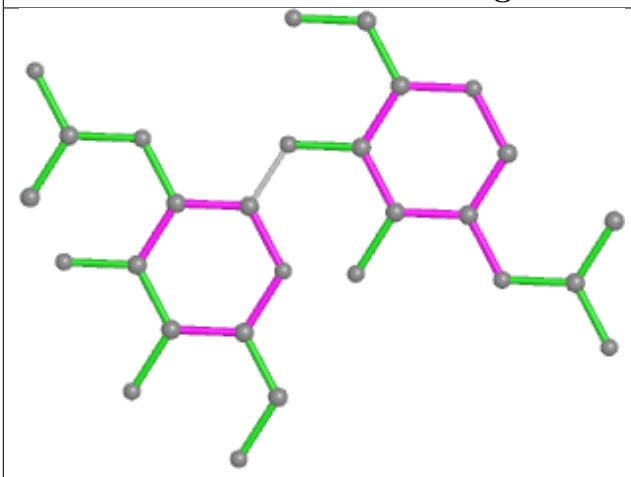


Torsions



Rings

Oligosaccharide Chain V



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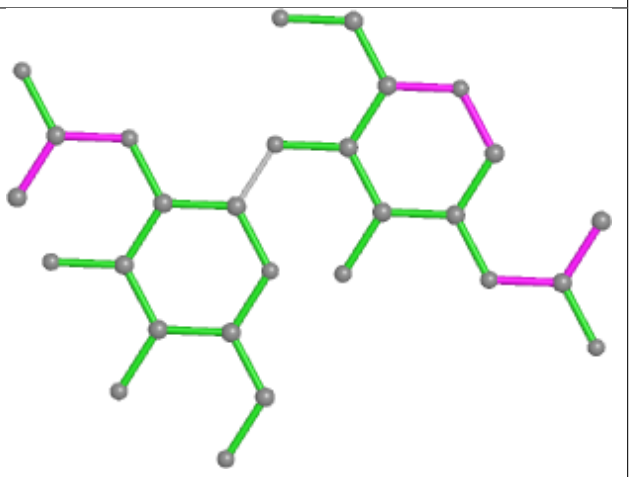
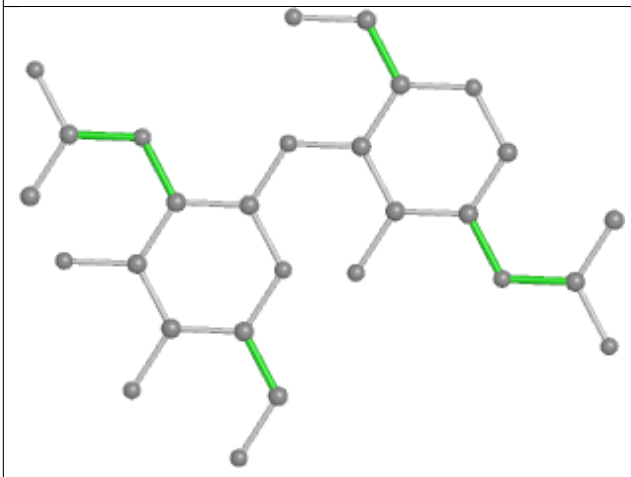


Bond angles



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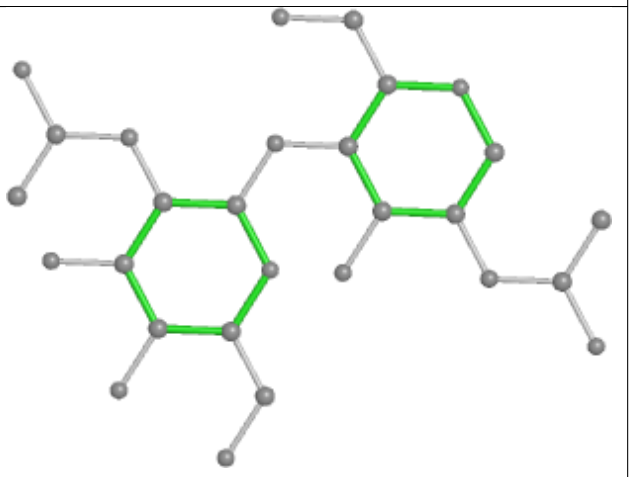
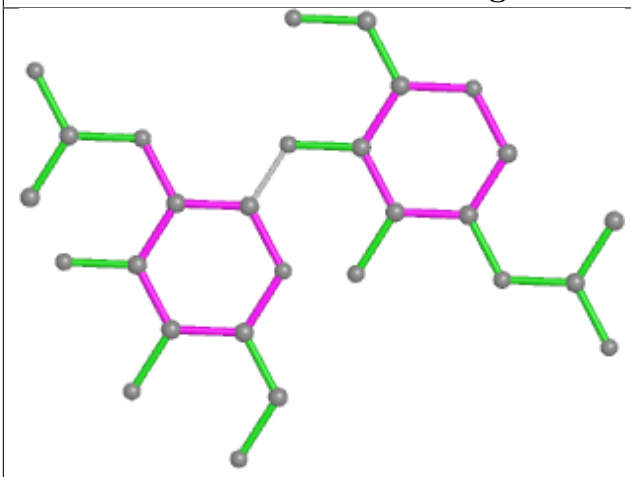


Rings

Oligosaccharide Chain W



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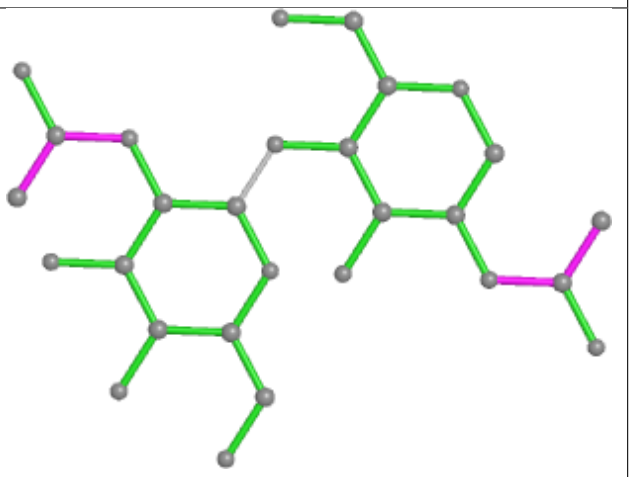
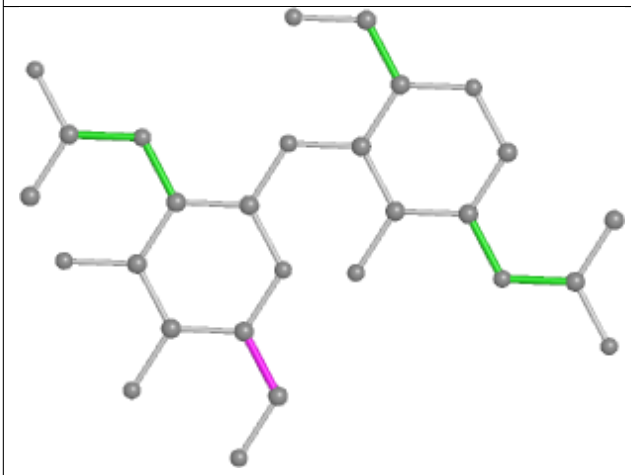
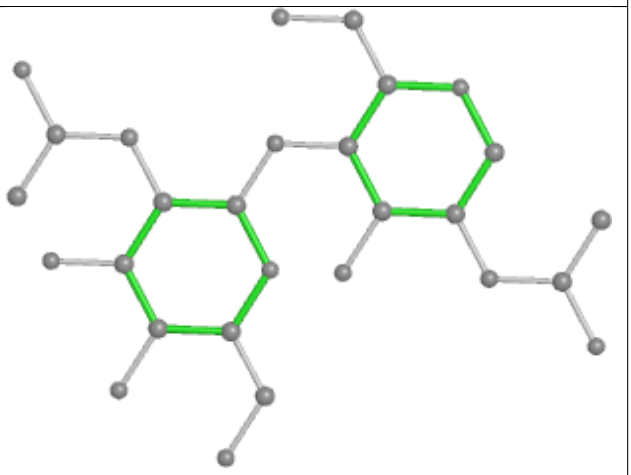


Bond angles

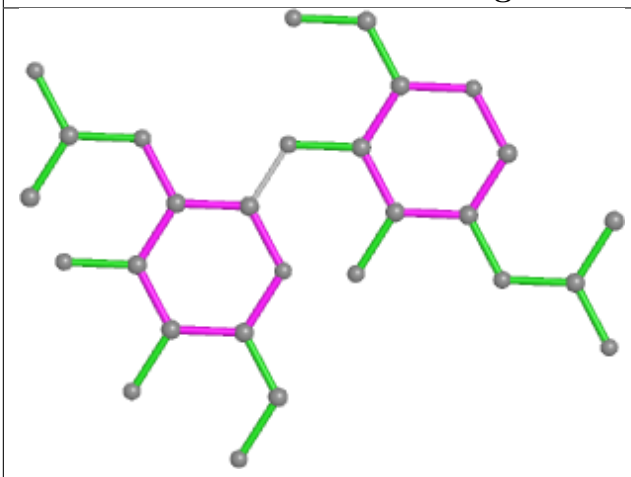


Torsions



Rings

Oligosaccharide Chain X



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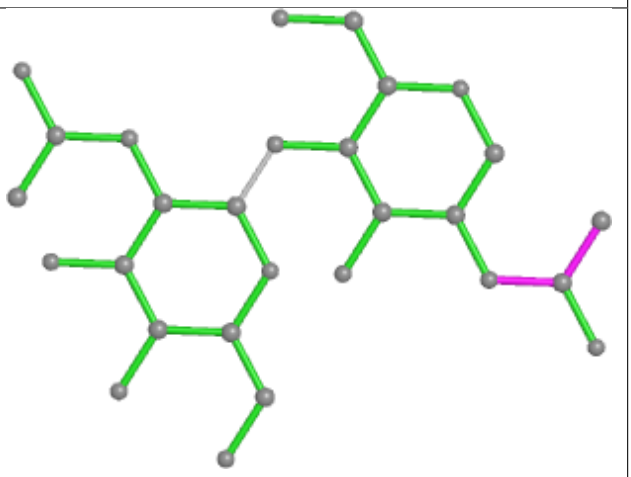
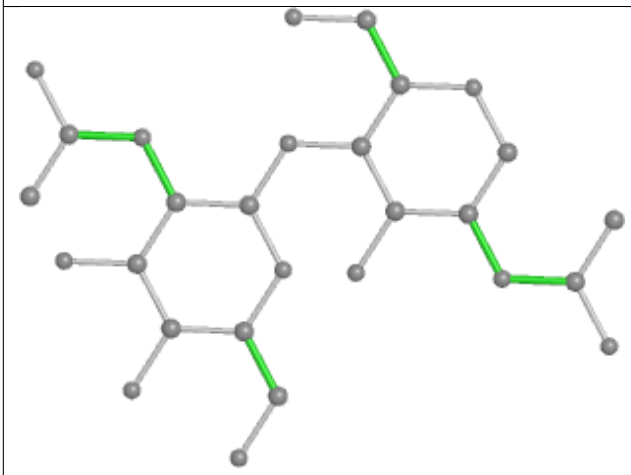
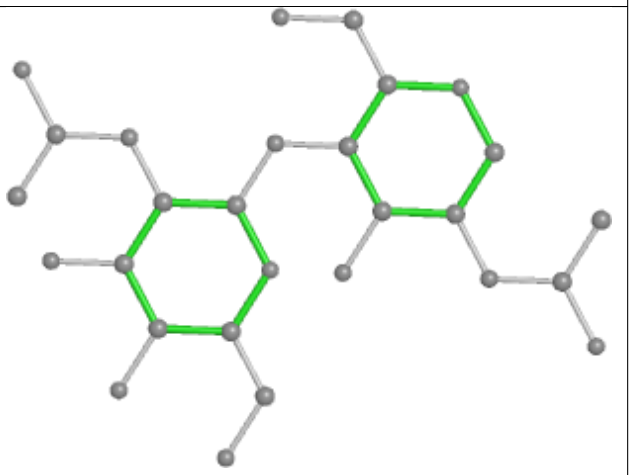


Bond angles

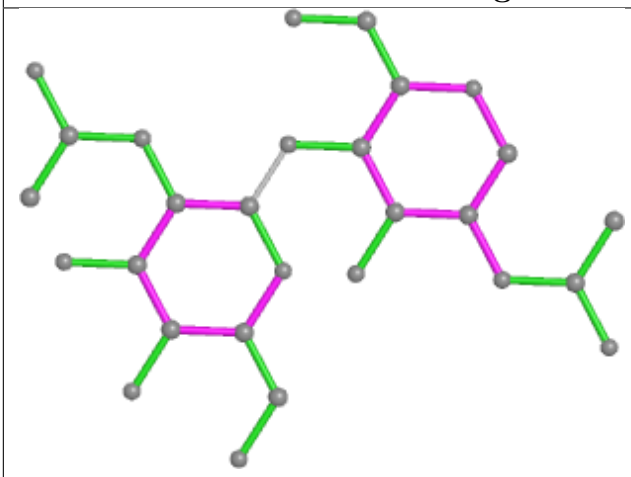


Torsions



Rings

Oligosaccharide Chain Y



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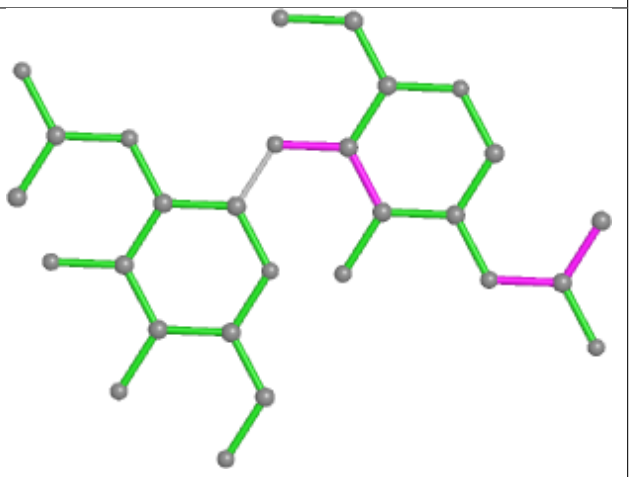
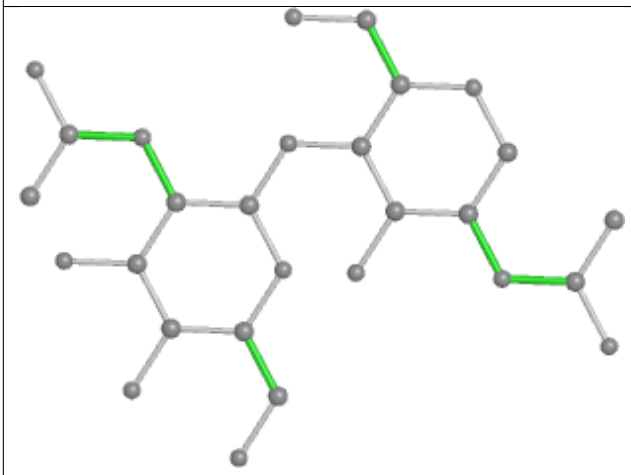


Bond angles



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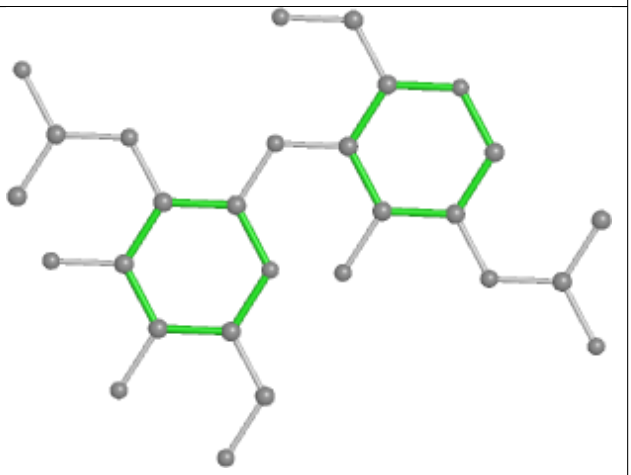
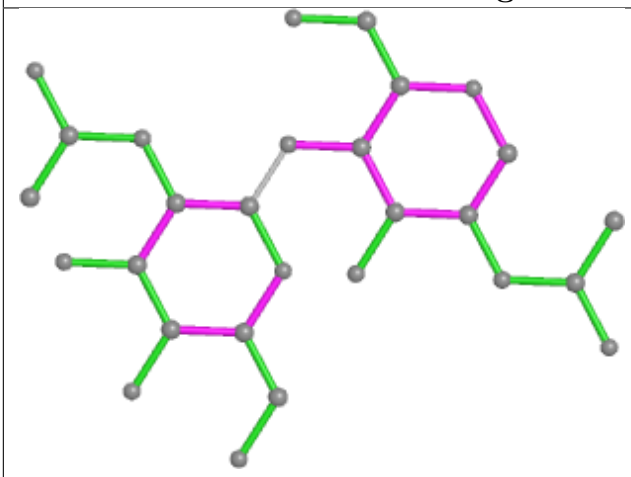


Rings

Oligosaccharide Chain Z



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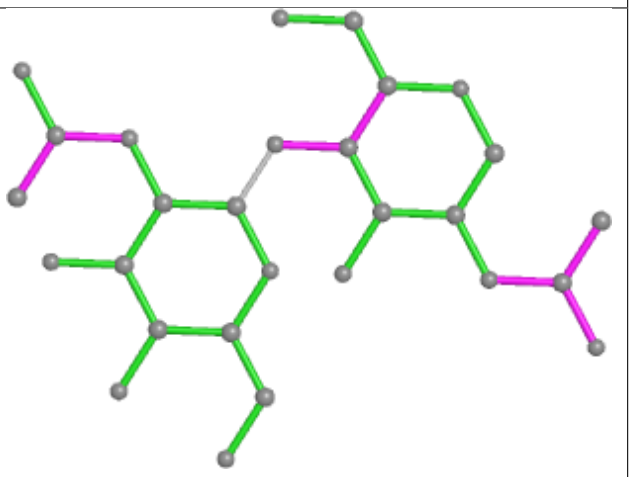
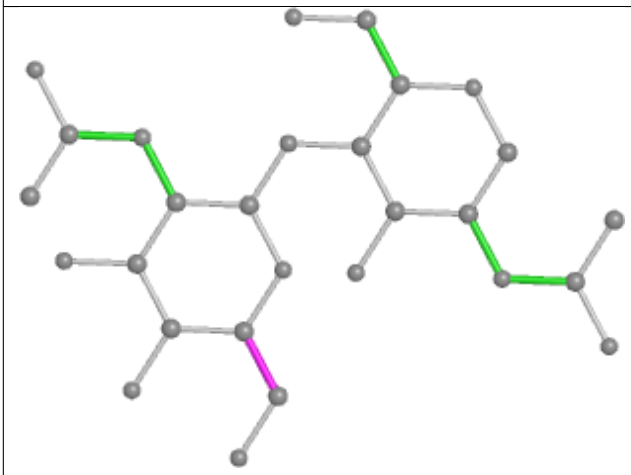
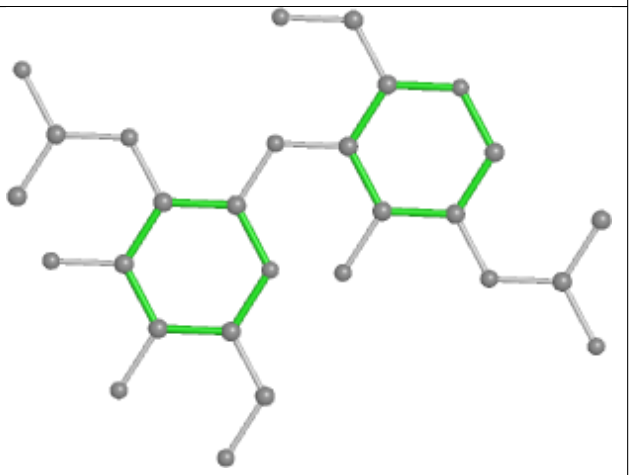


Bond angles

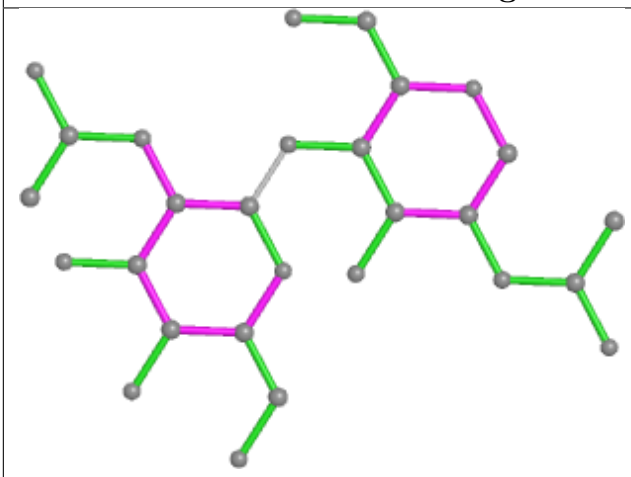


Torsions



Rings

Oligosaccharide Chain a



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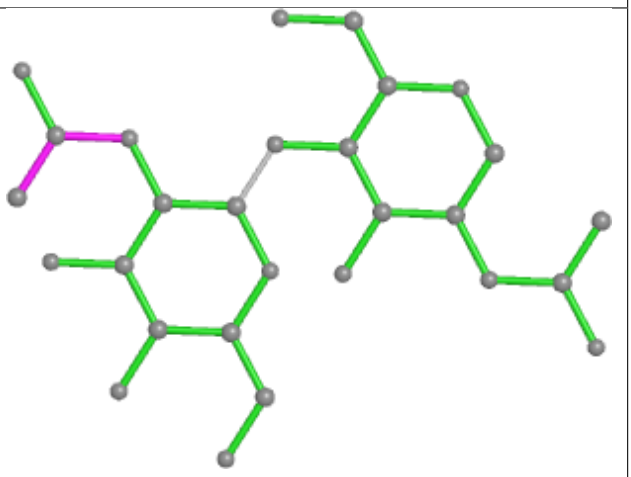
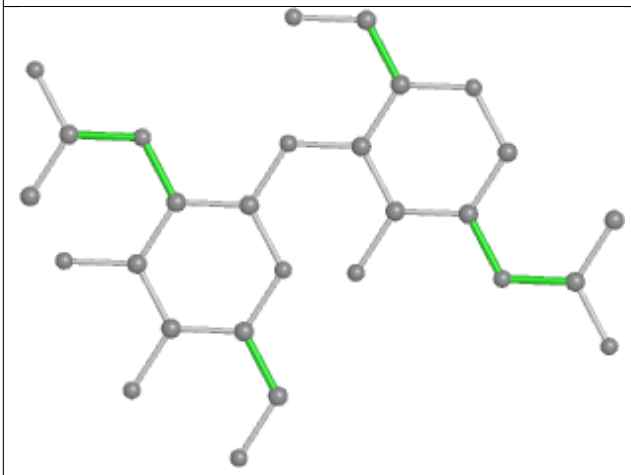


Bond angles



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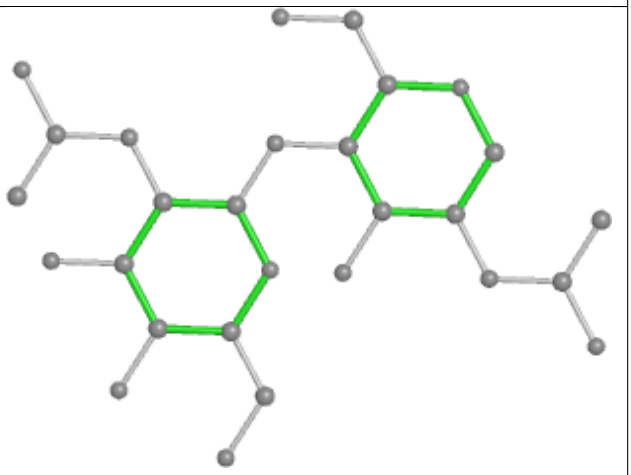
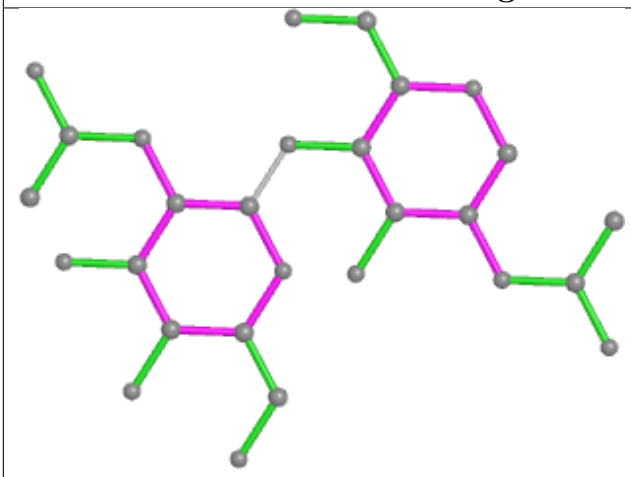


Rings

Oligosaccharide Chain b



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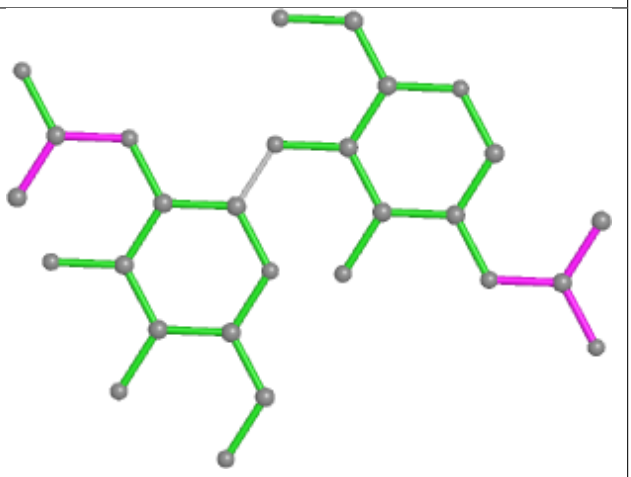
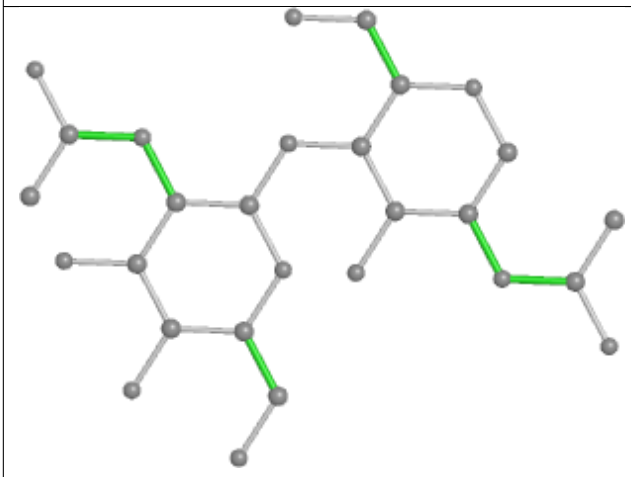
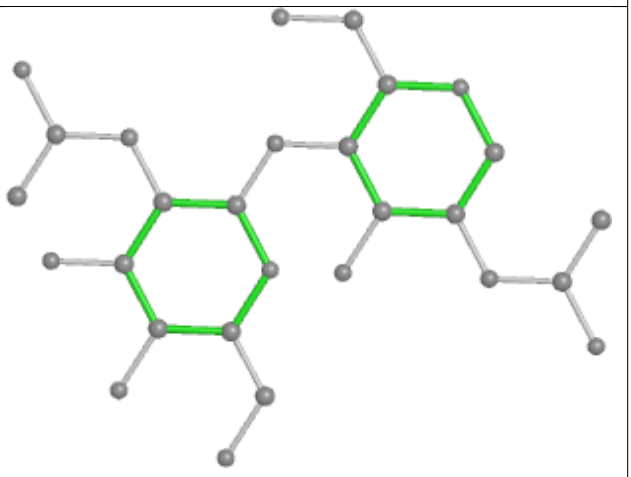


Bond angles

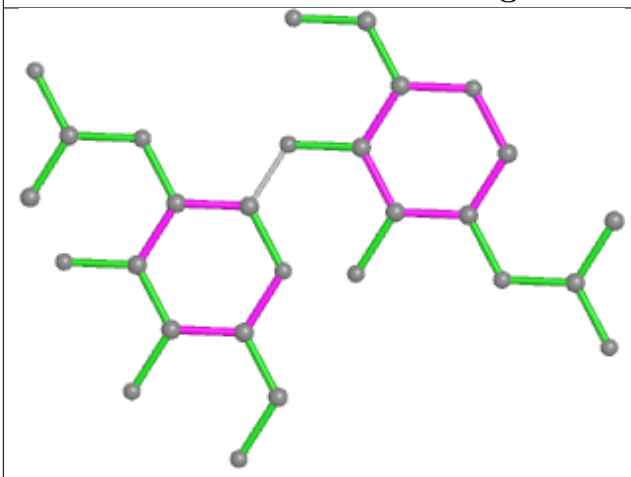


Torsions

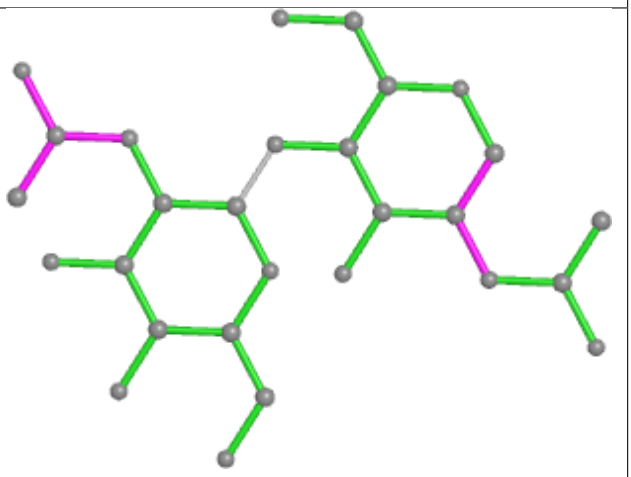


Rings

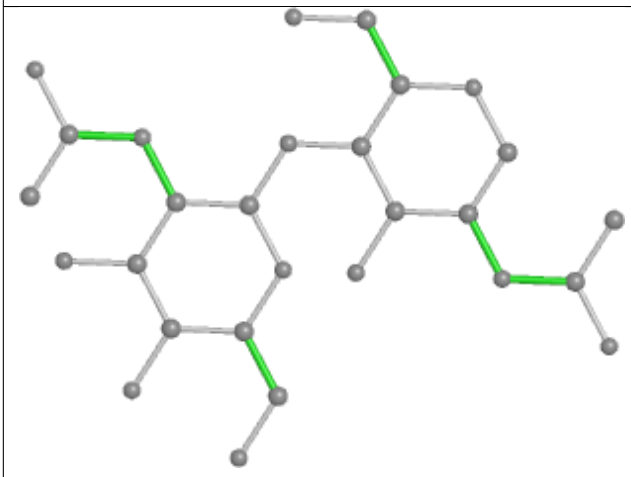
Oligosaccharide Chain c



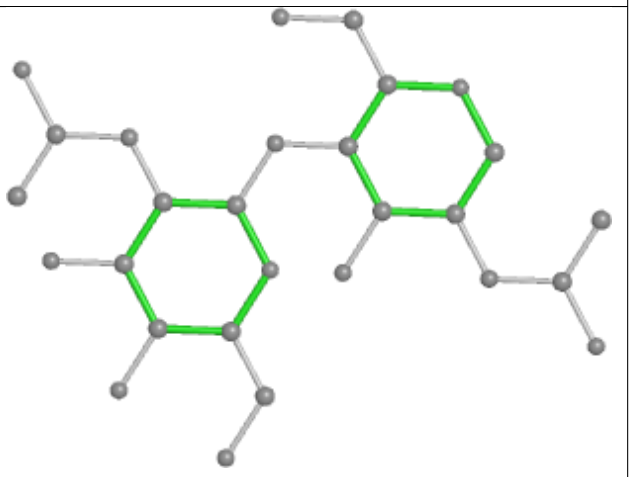
Bond lengths



Bond angles

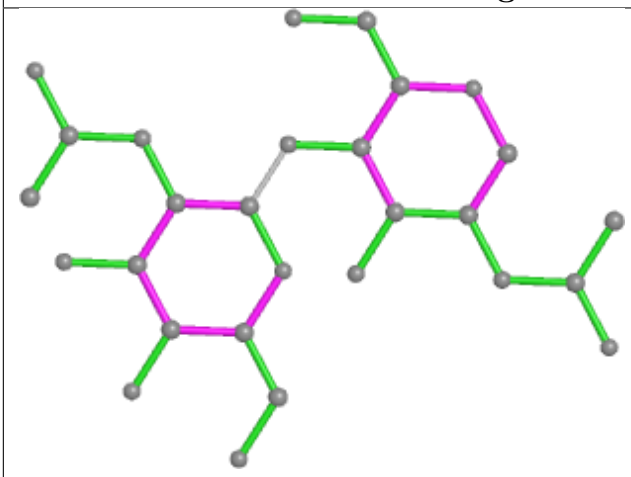


Torsions



Rings

Oligosaccharide Chain d



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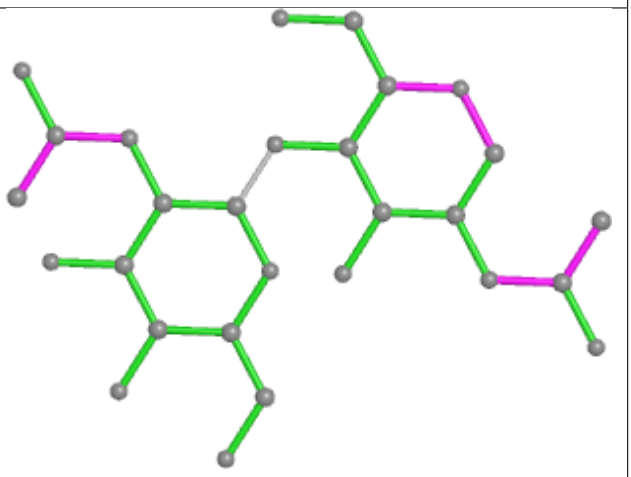

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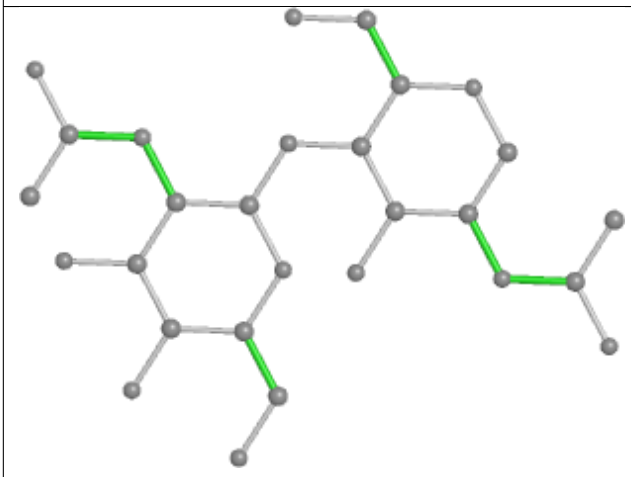

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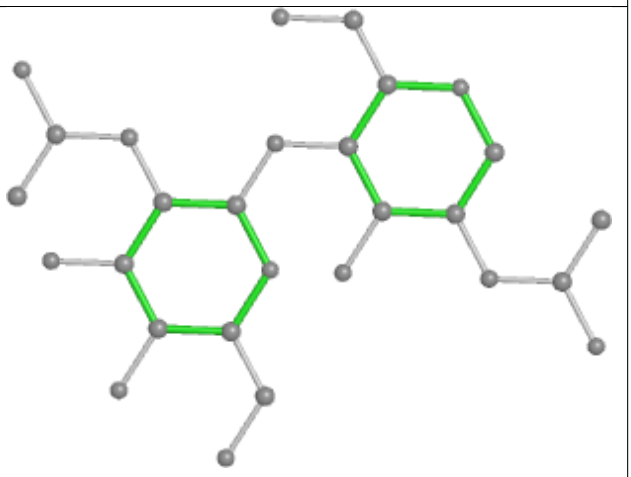
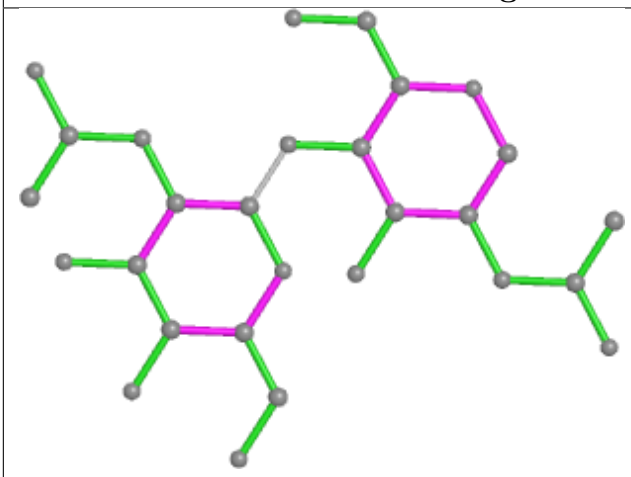


Rings

Oligosaccharide Chain e



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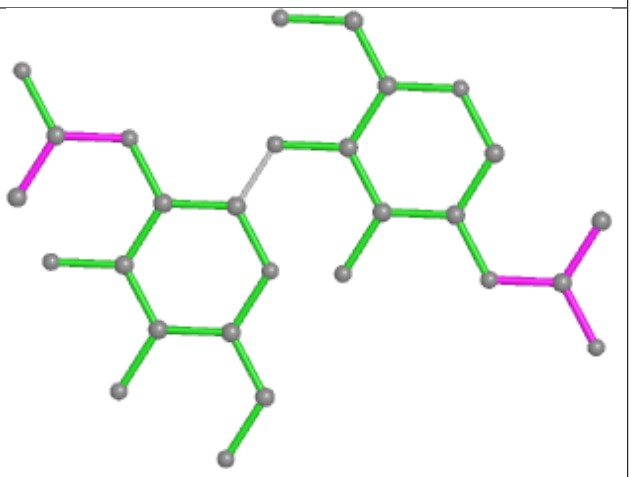

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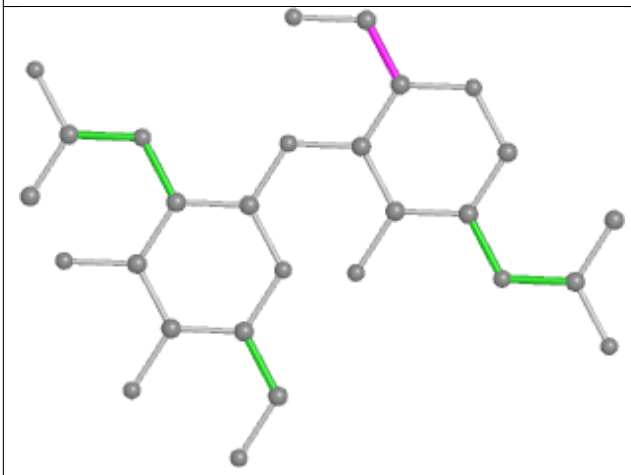

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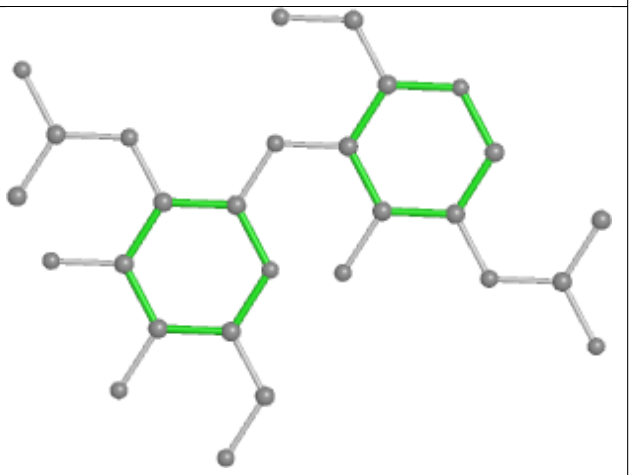
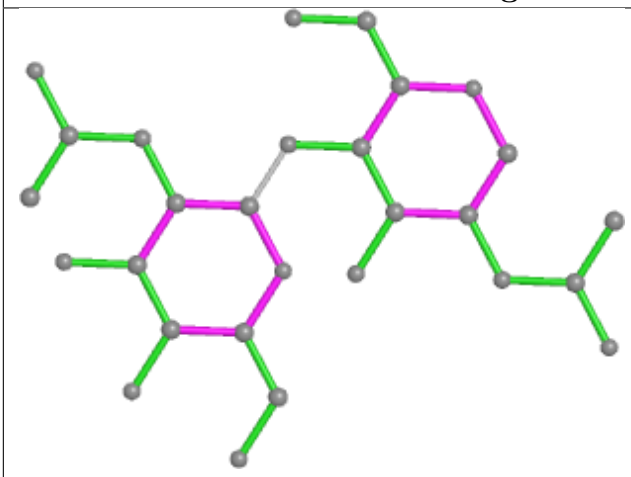


Rings

Oligosaccharide Chain f



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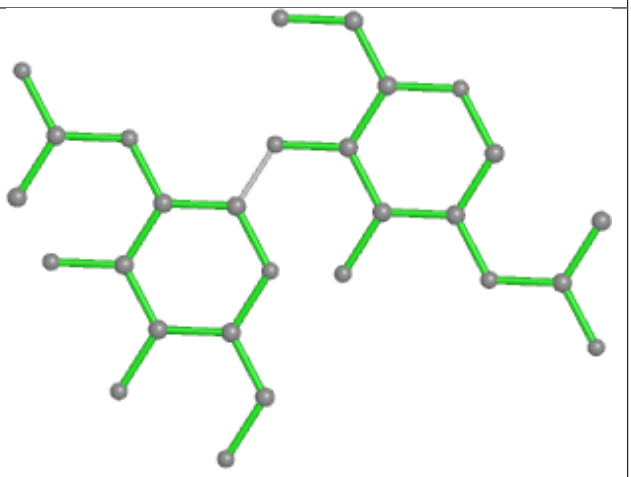

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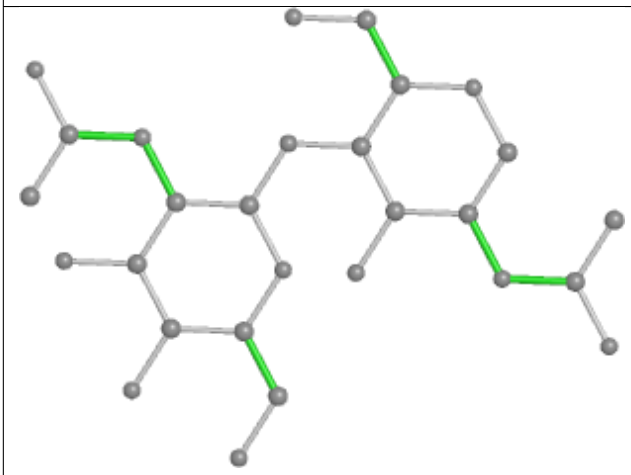

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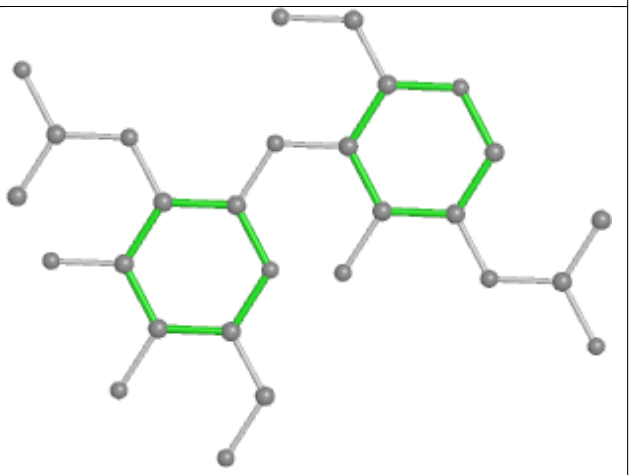
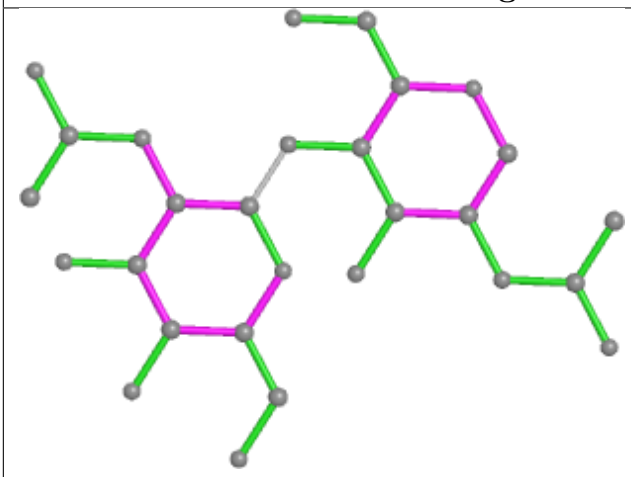


Rings

Oligosaccharide Chain g



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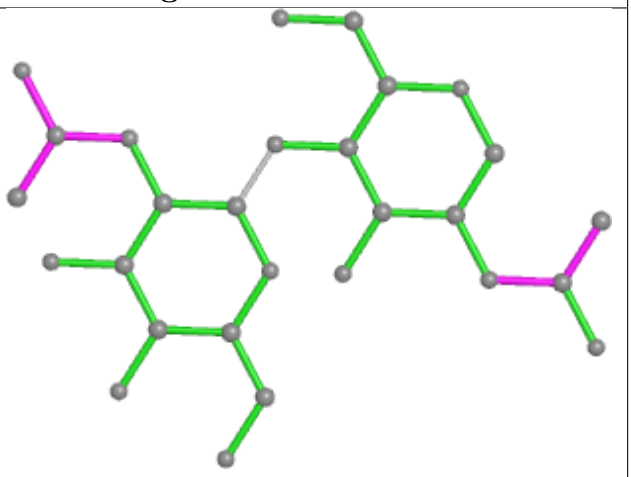
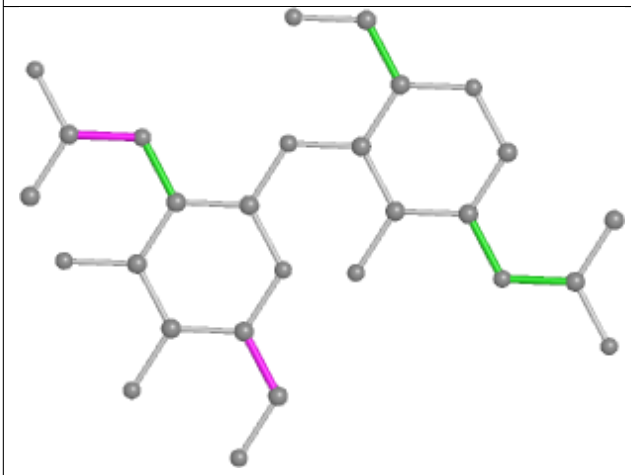


Bond angles



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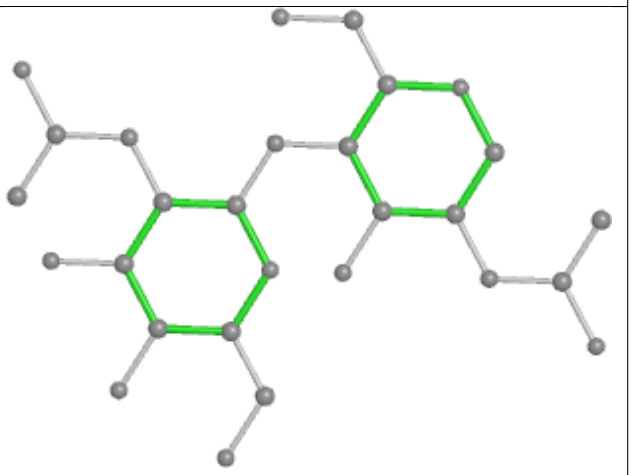
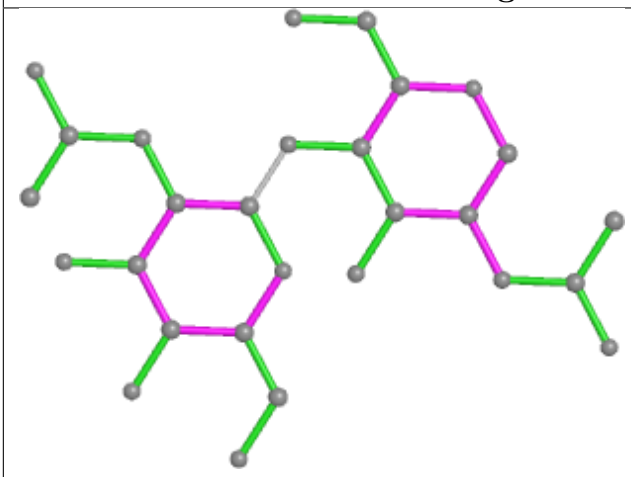


Rings

Oligosaccharide Chain h



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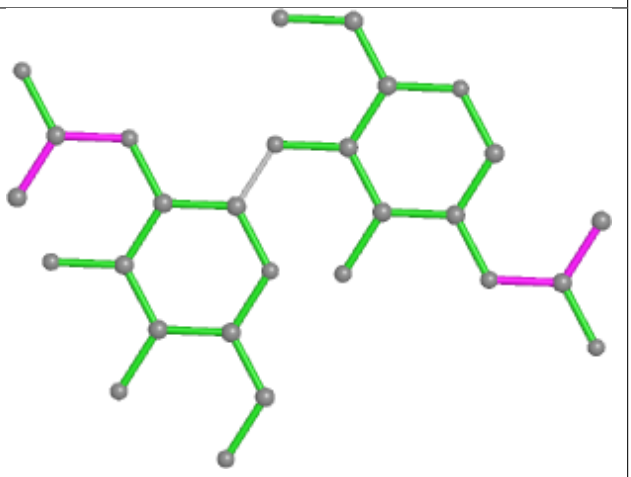

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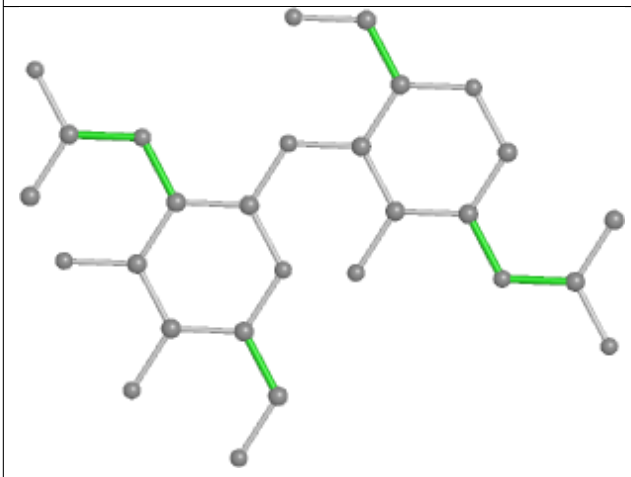

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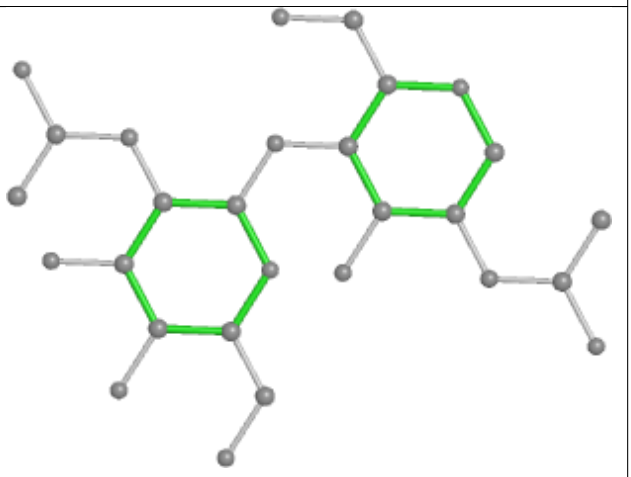
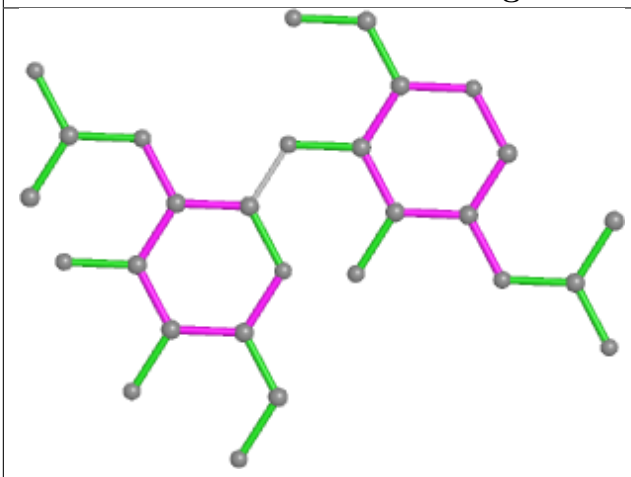


Rings

Oligosaccharide Chain i



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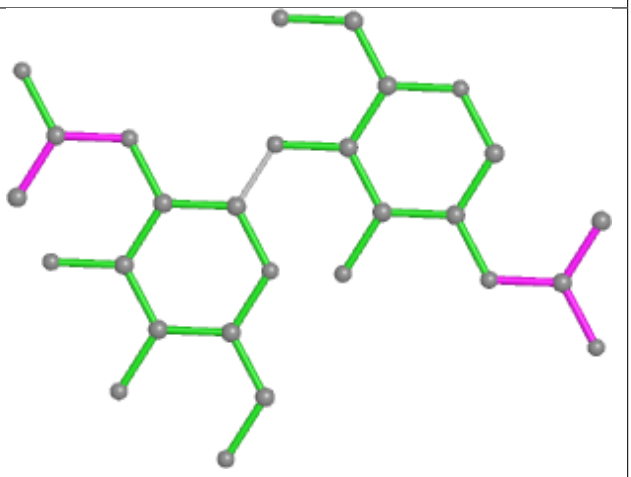

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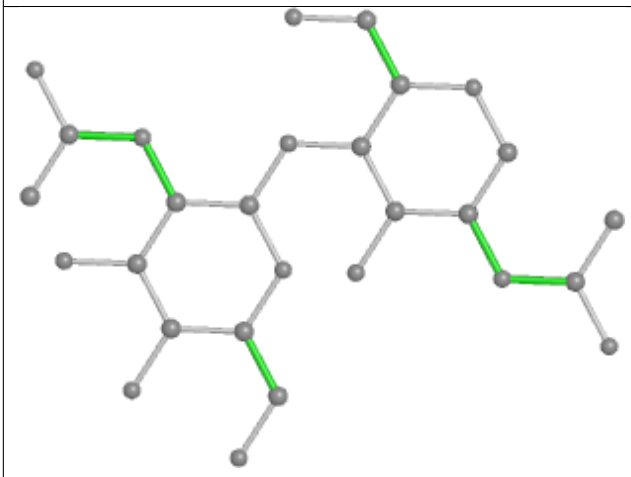

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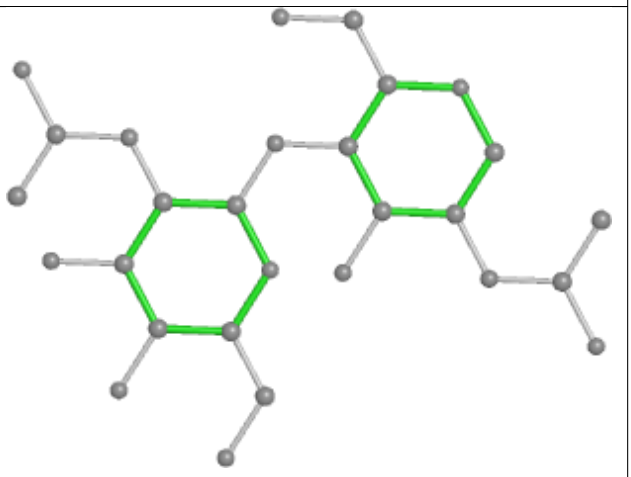
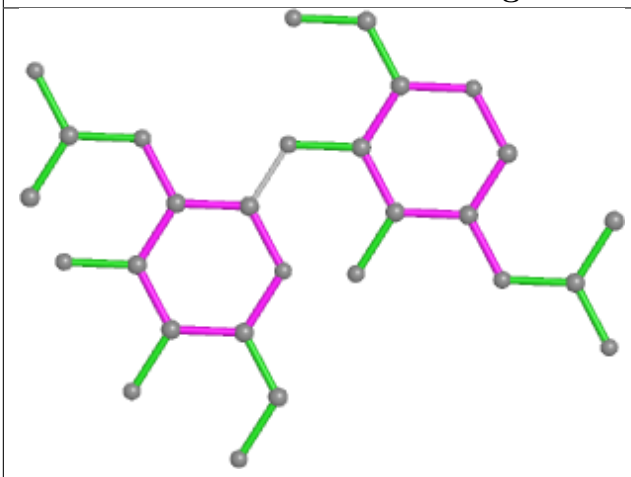


Rings

Oligosaccharide Chain j



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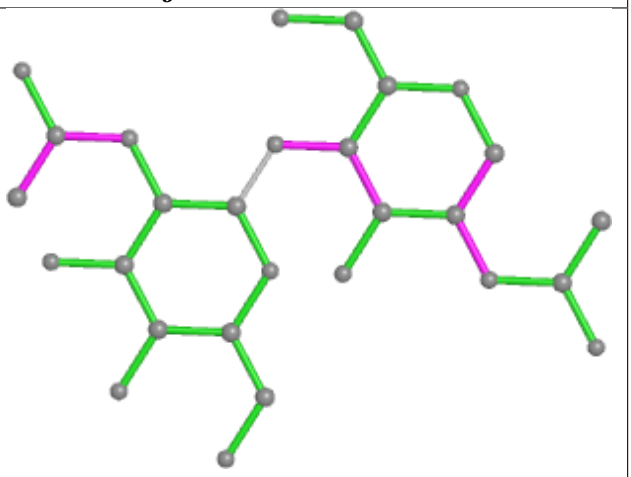
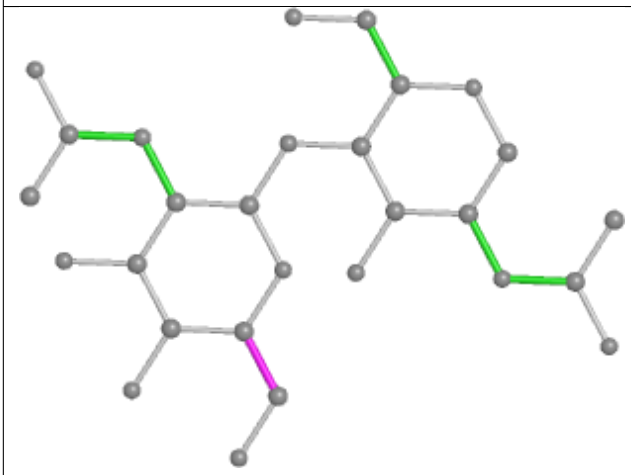


Bond angles



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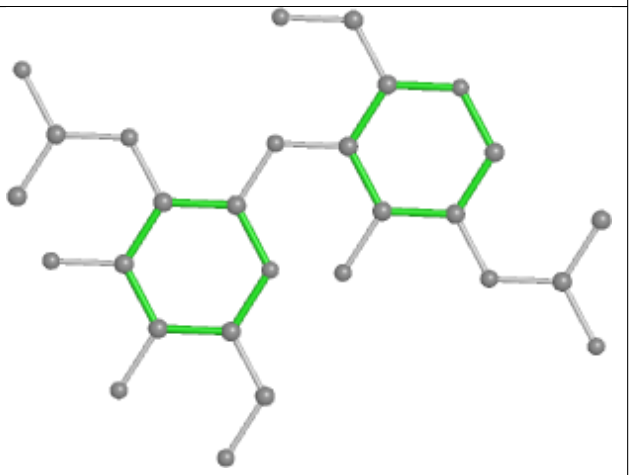
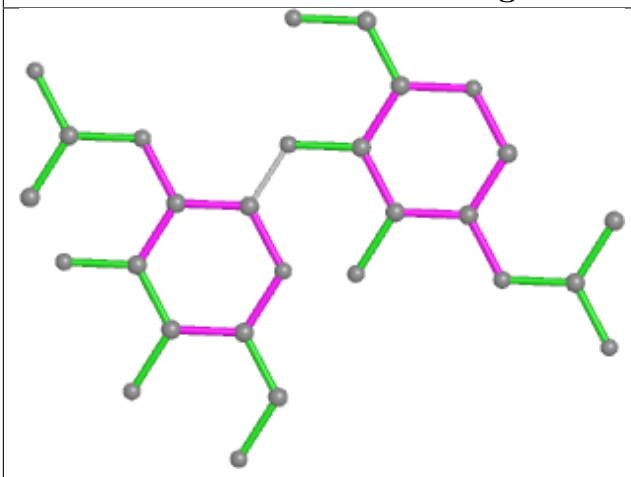


Rings

Oligosaccharide Chain k



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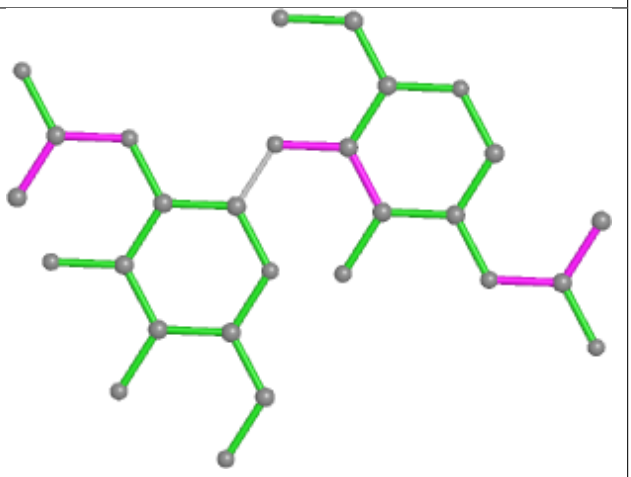
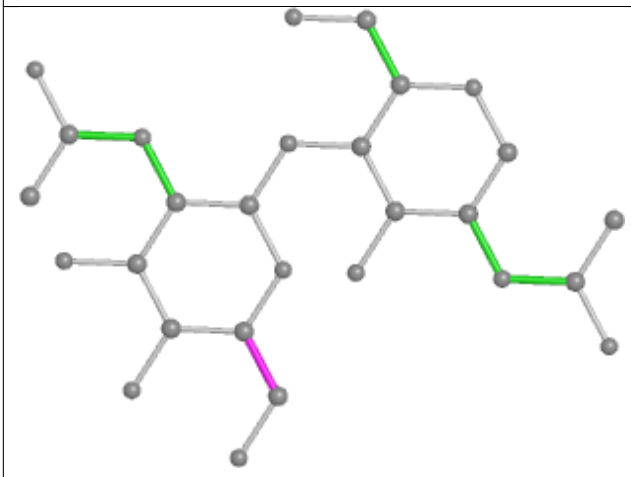


Bond angles



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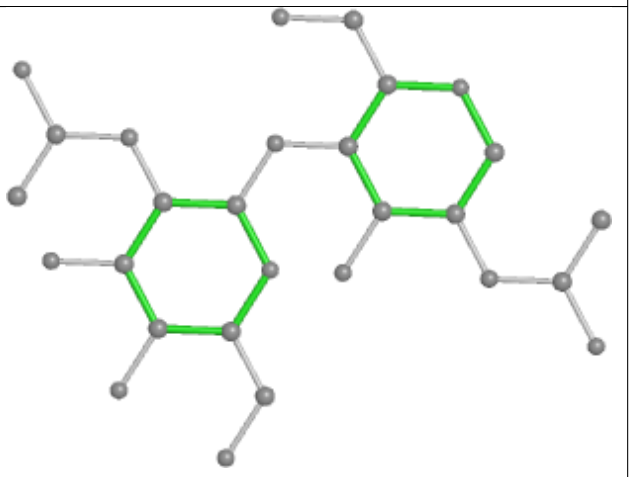
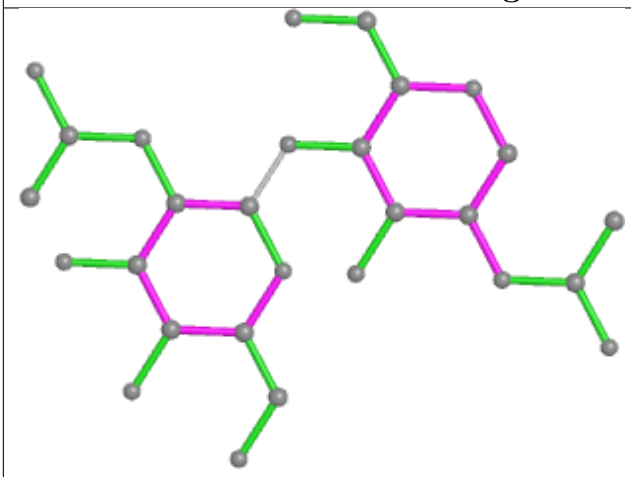


Rings

Oligosaccharide Chain l



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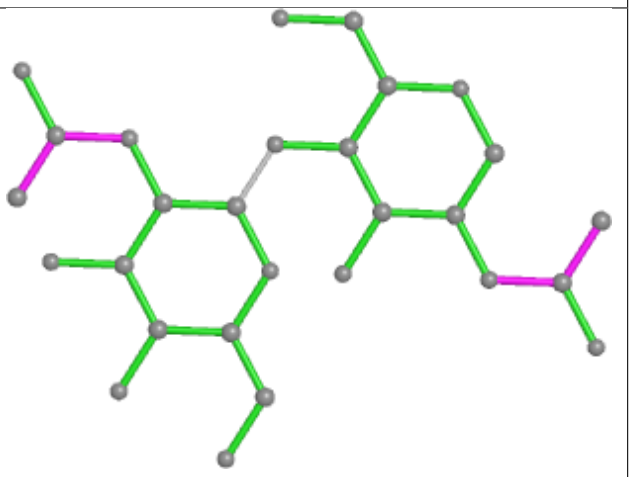
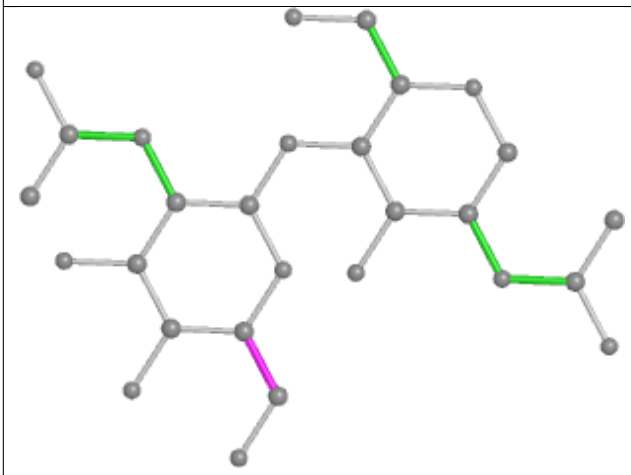


Bond angles



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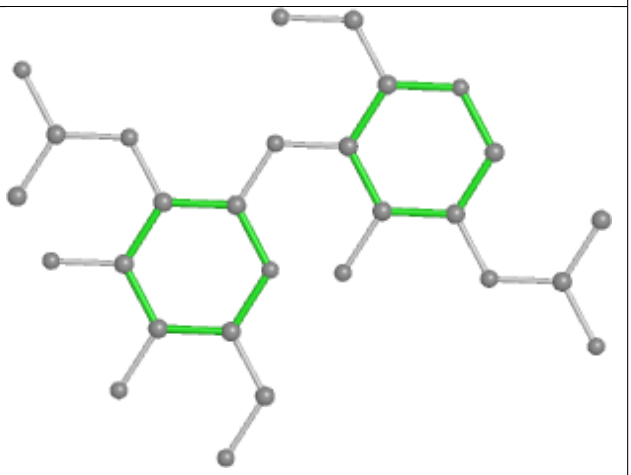
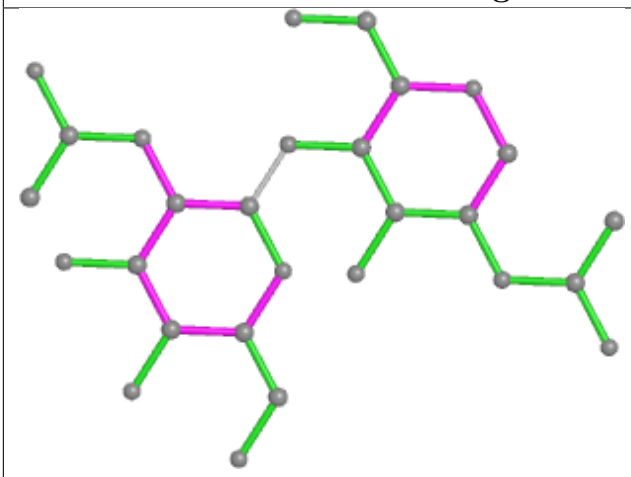


Rings

Oligosaccharide Chain m



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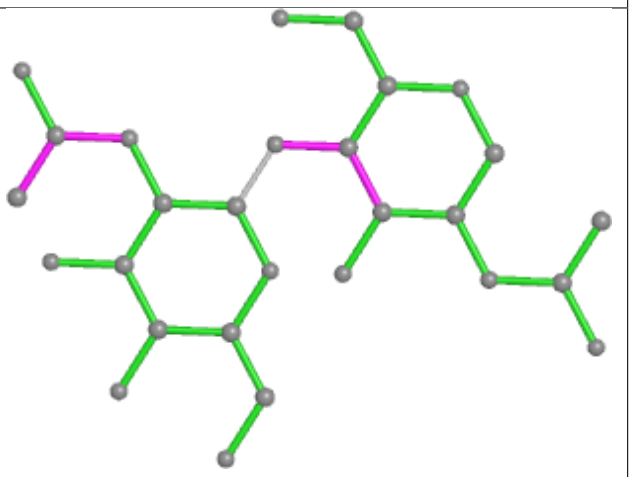
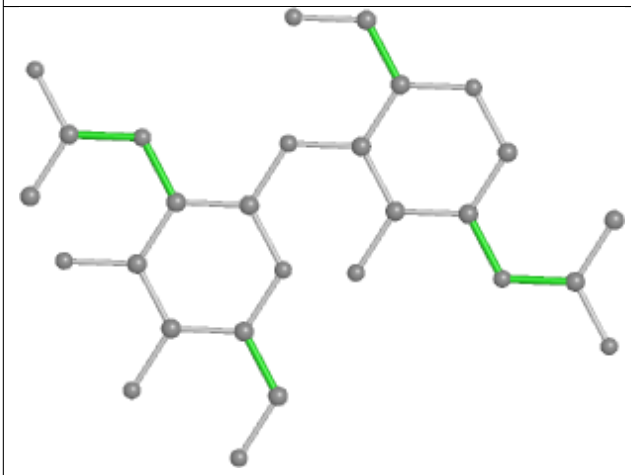


Bond angles



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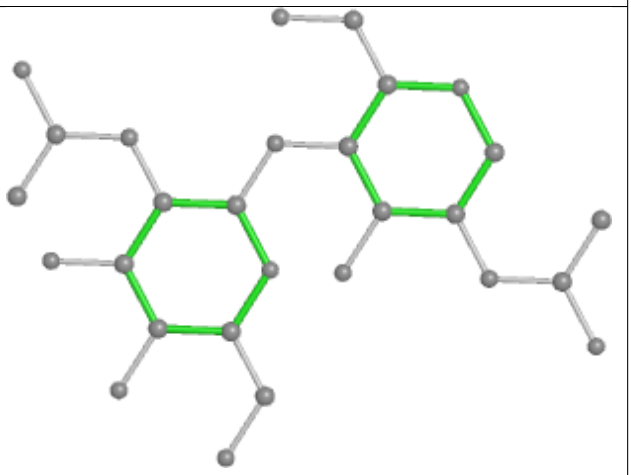
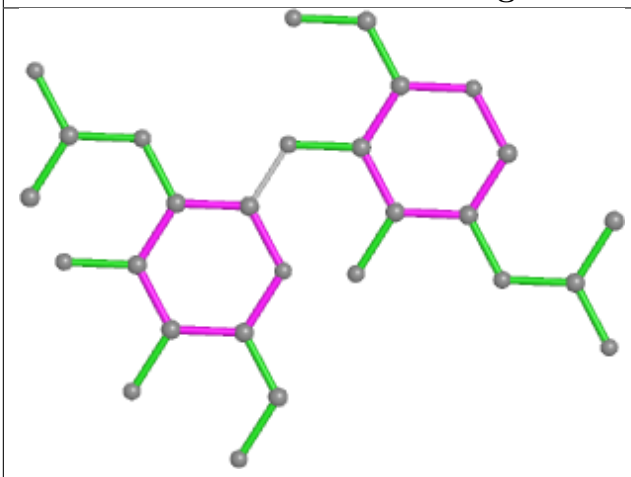


Rings

Oligosaccharide Chain n



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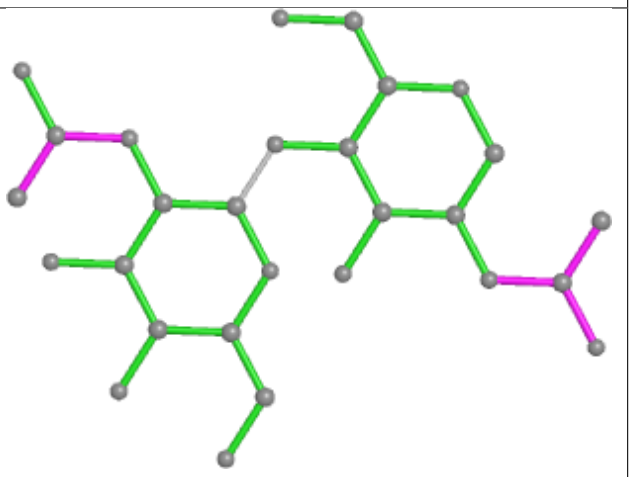
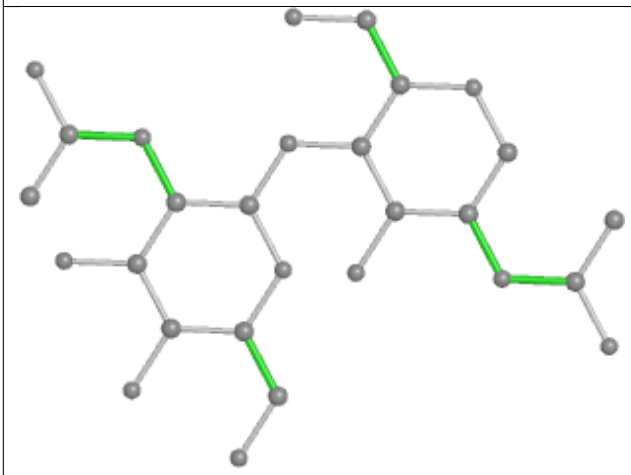


Bond angles



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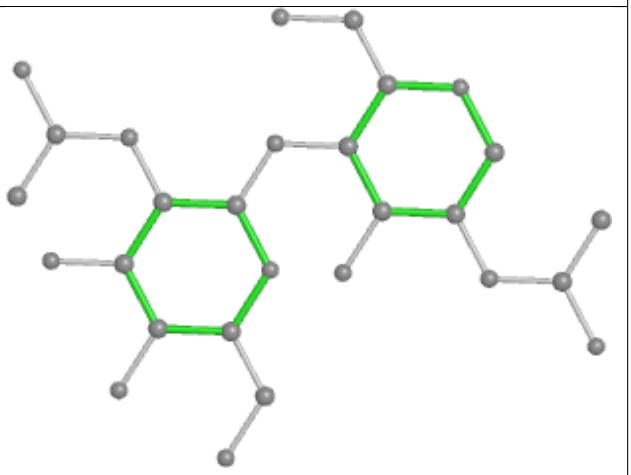
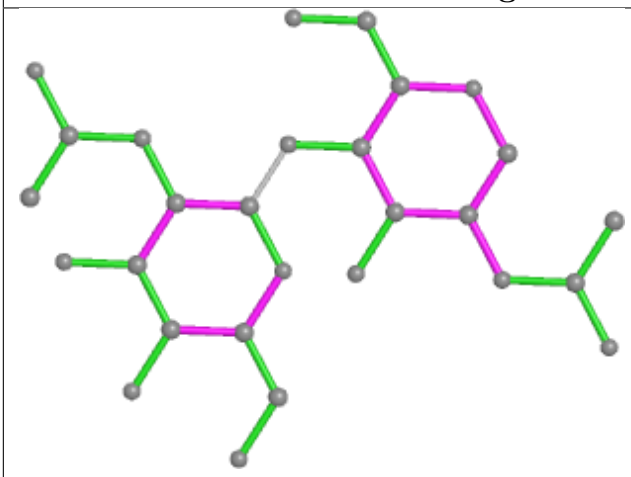


Rings

Oligosaccharide Chain o



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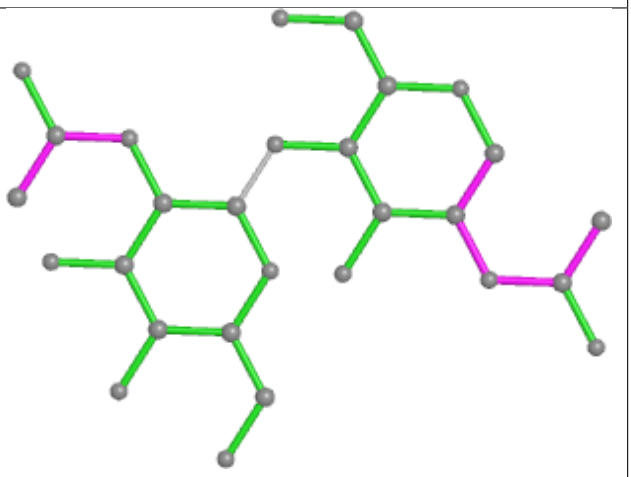
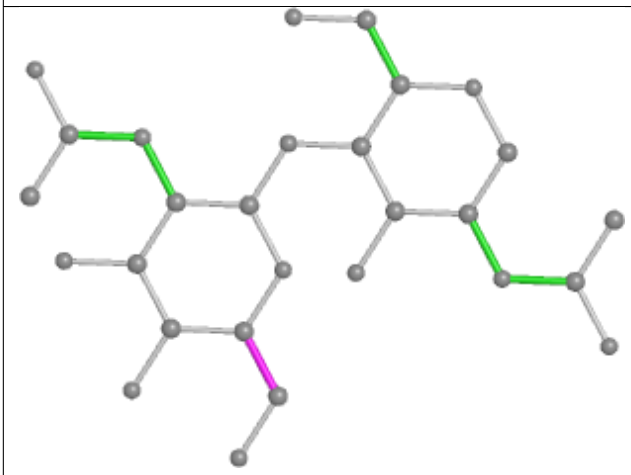
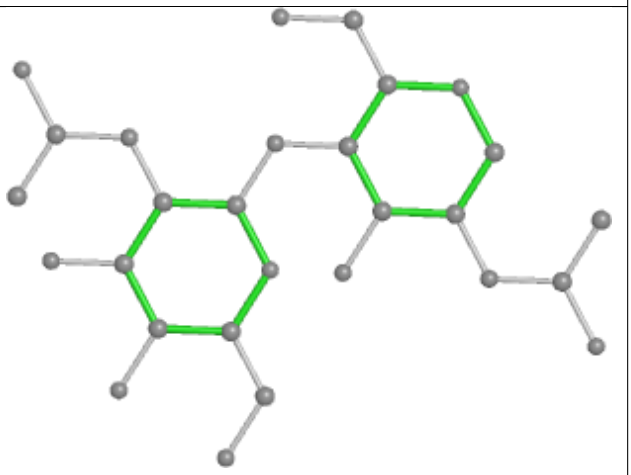


Bond angles

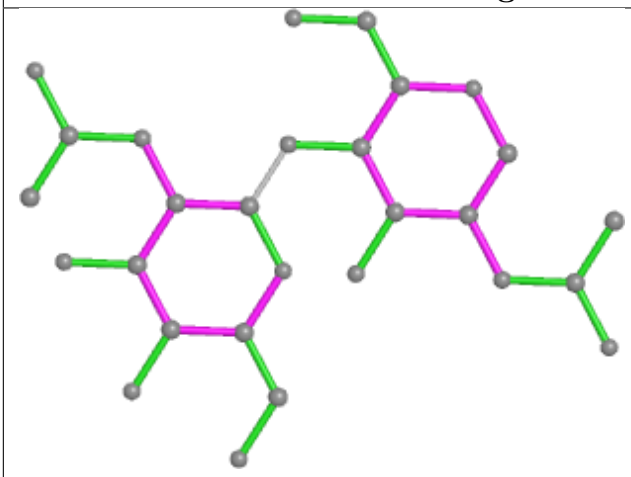


Torsions



Rings

Oligosaccharide Chain p



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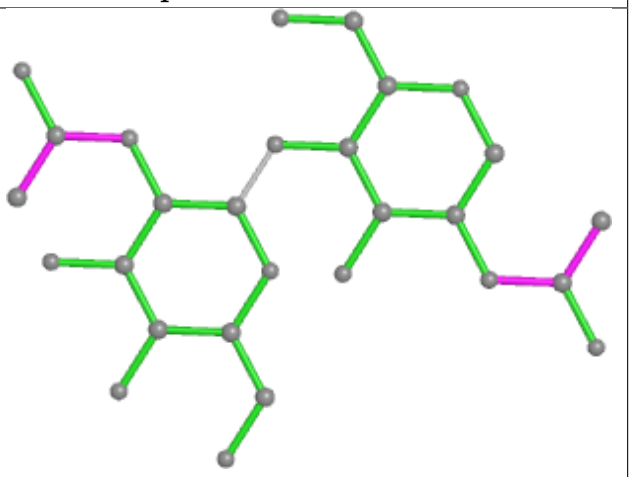
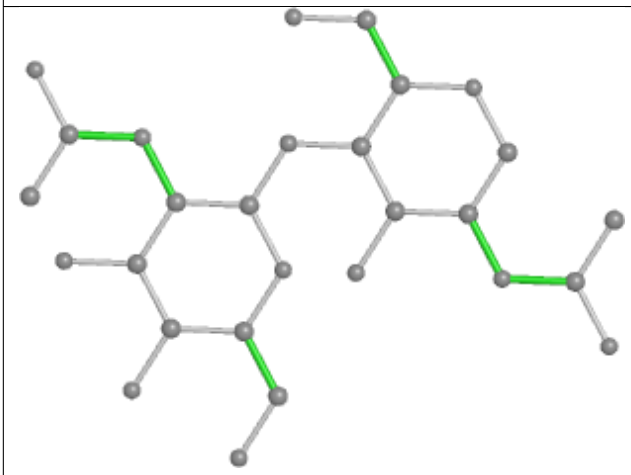
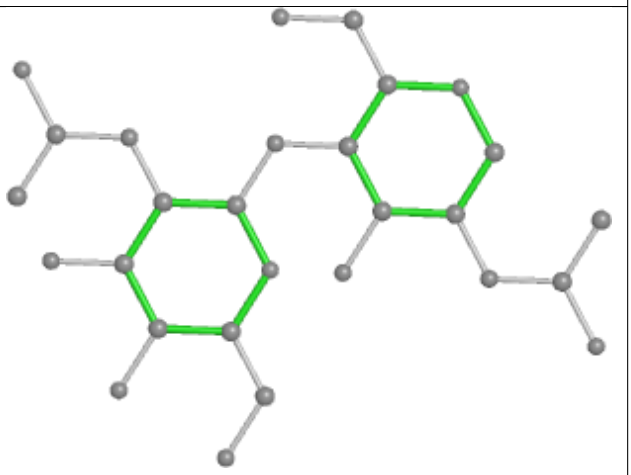


Bond angles

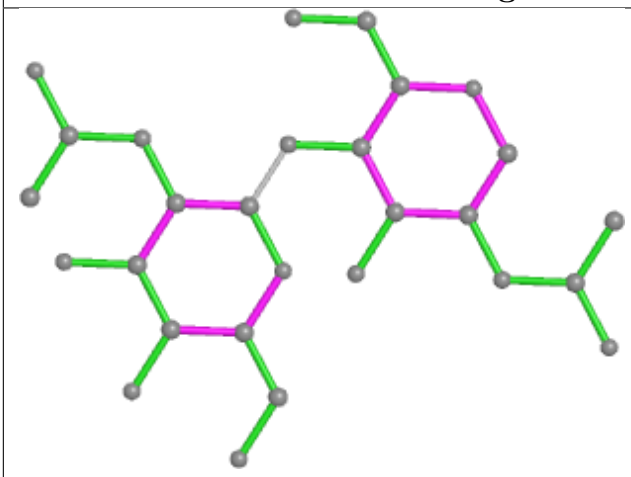


Torsions



Rings

Oligosaccharide Chain q



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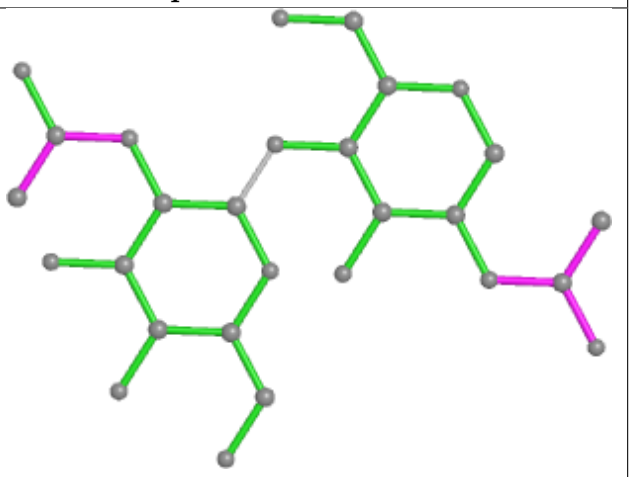
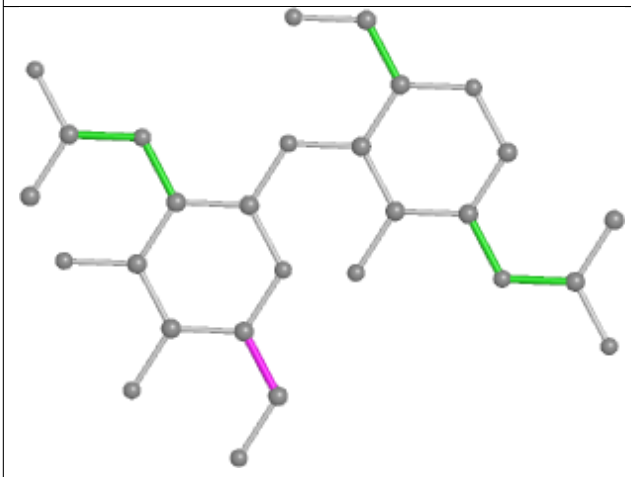


Bond angles



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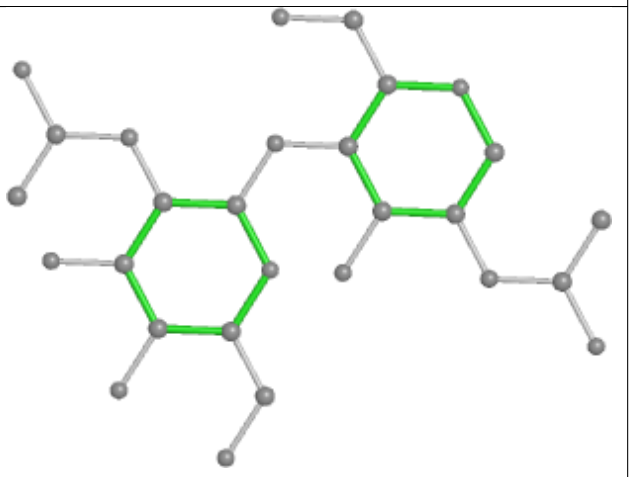
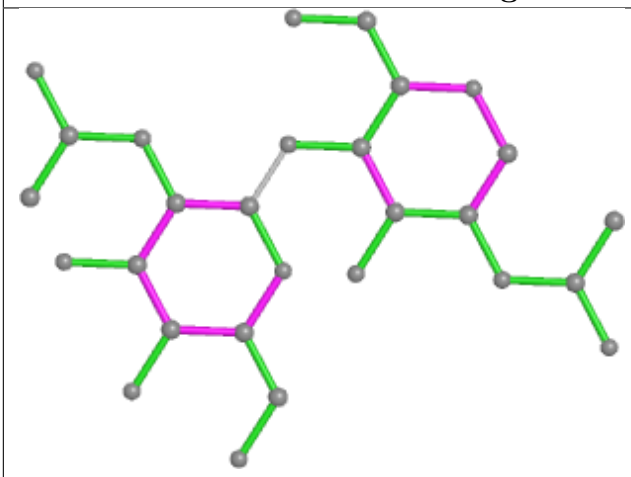
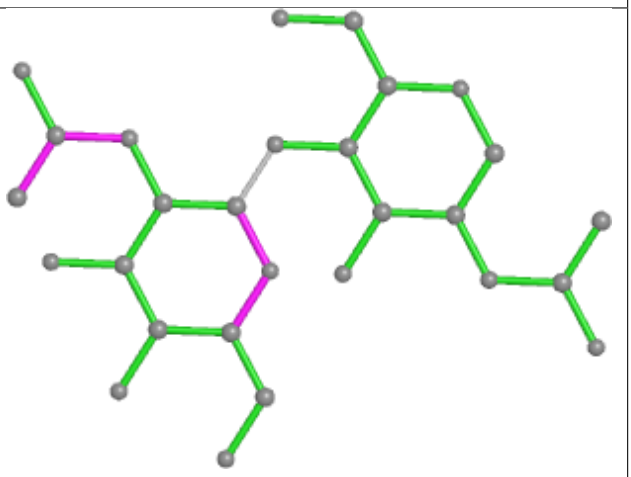


Rings

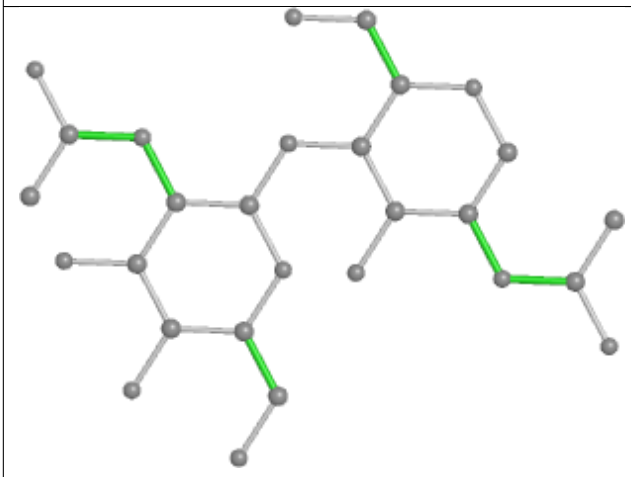
Oligosaccharide Chain r



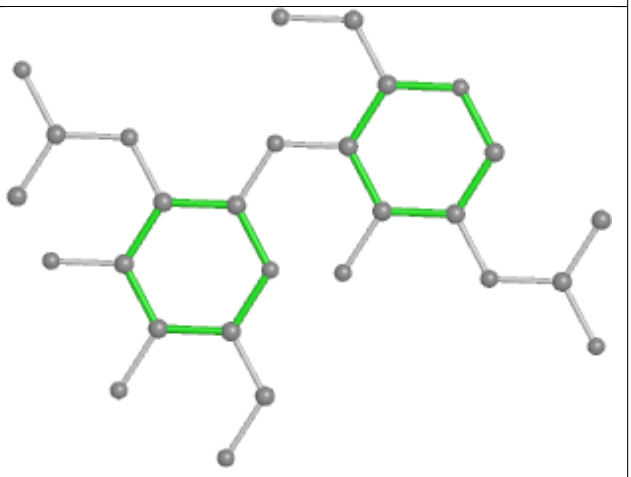
Bond lengths



Bond angles

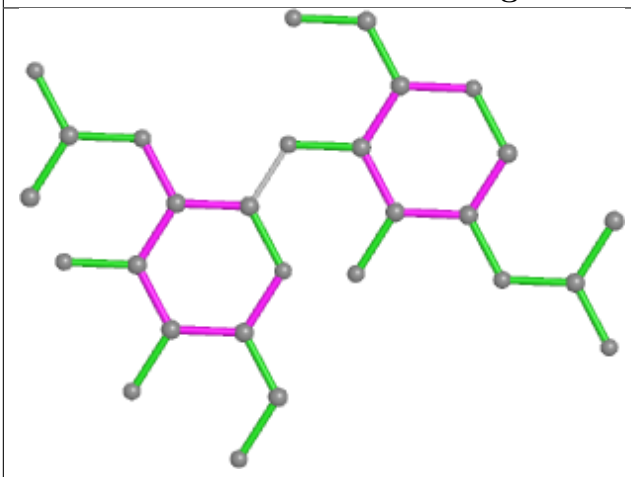


Torsions



Rings

Oligosaccharide Chain s



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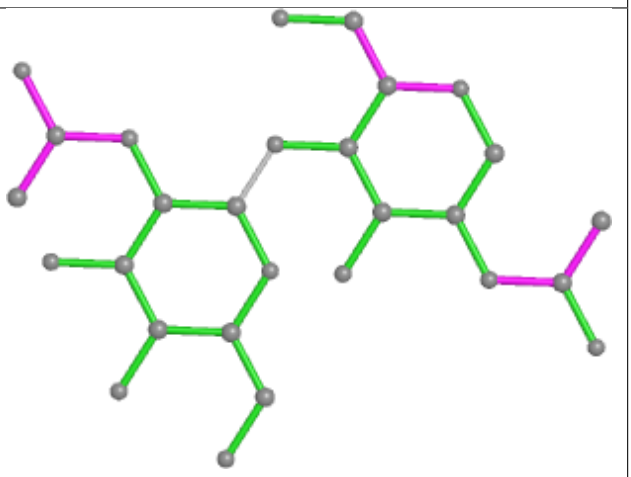

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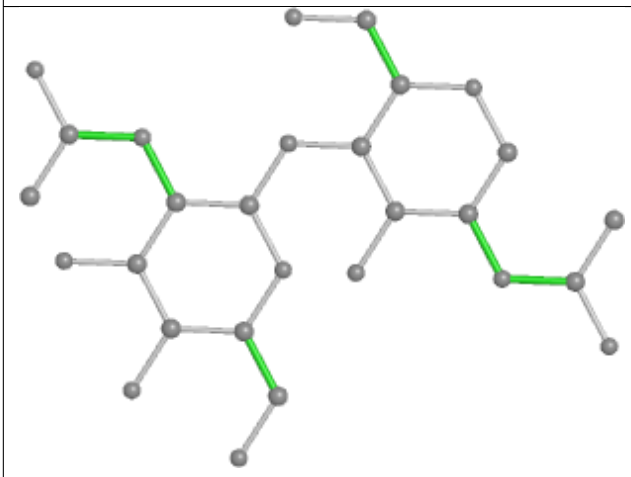

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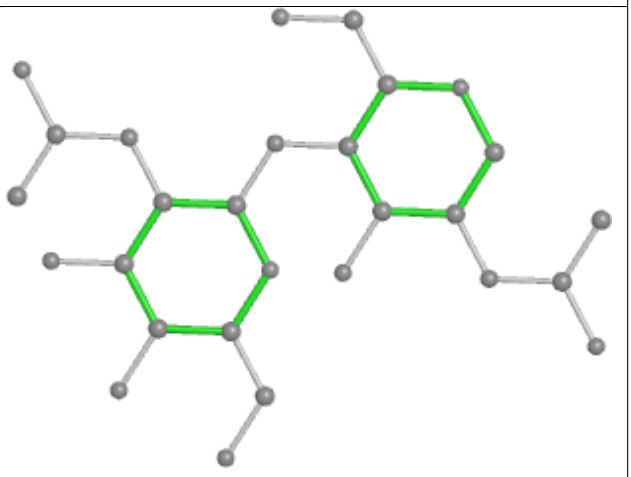
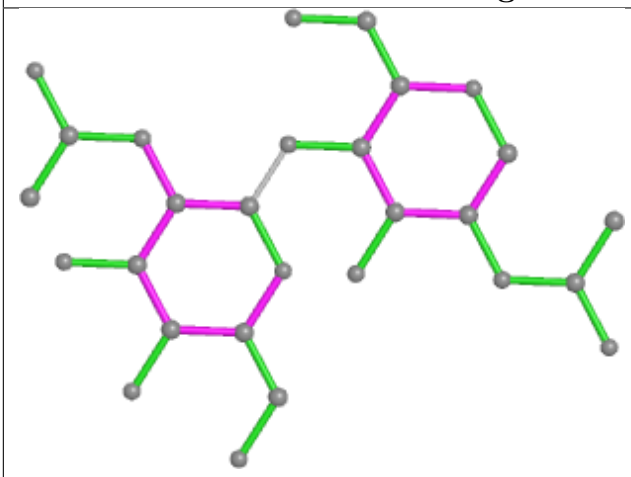


Rings

Oligosaccharide Chain u



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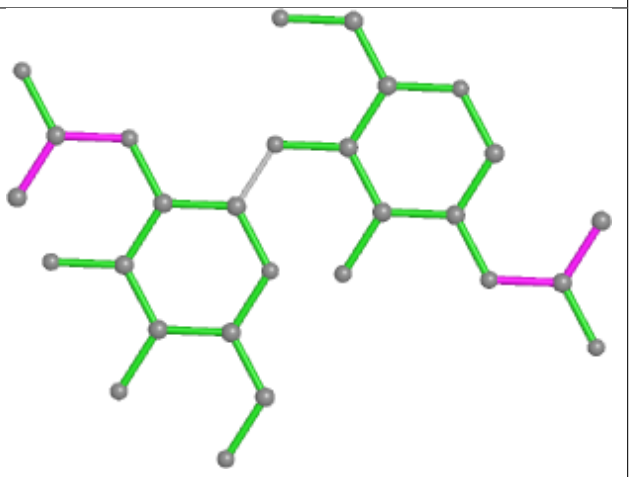
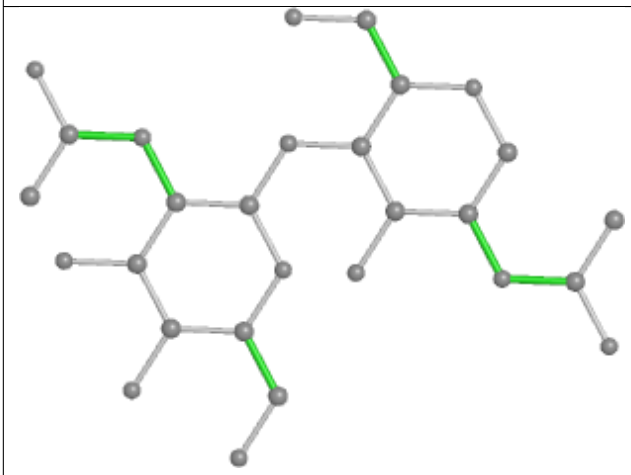


Bond angles



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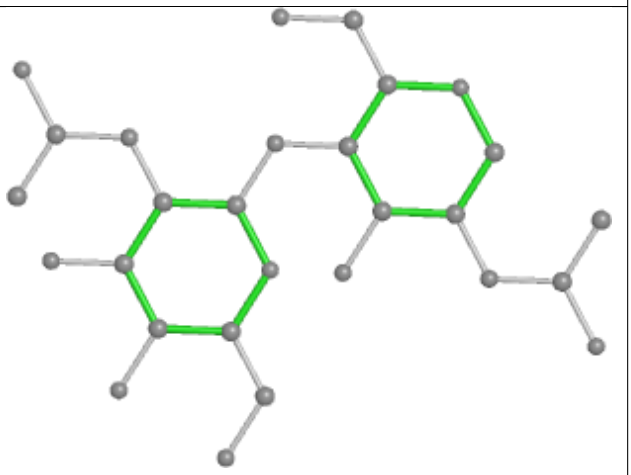
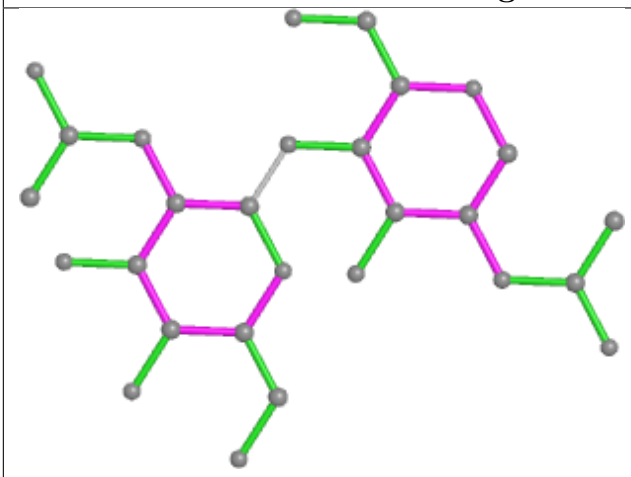


Rings

Oligosaccharide Chain v



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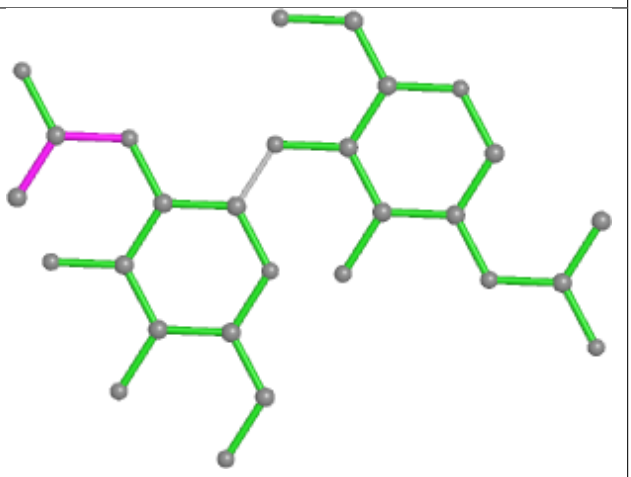

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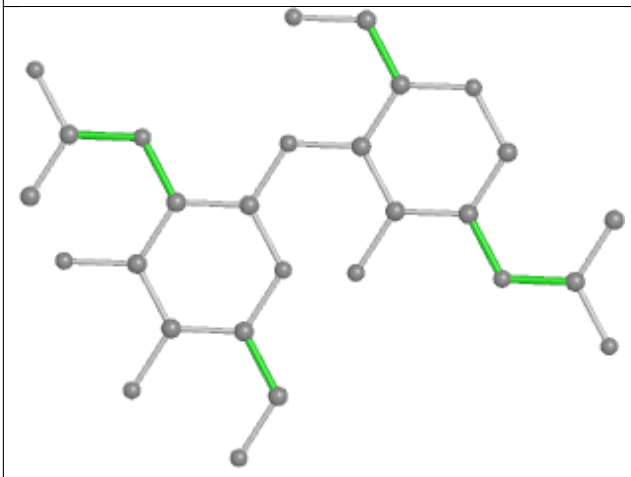

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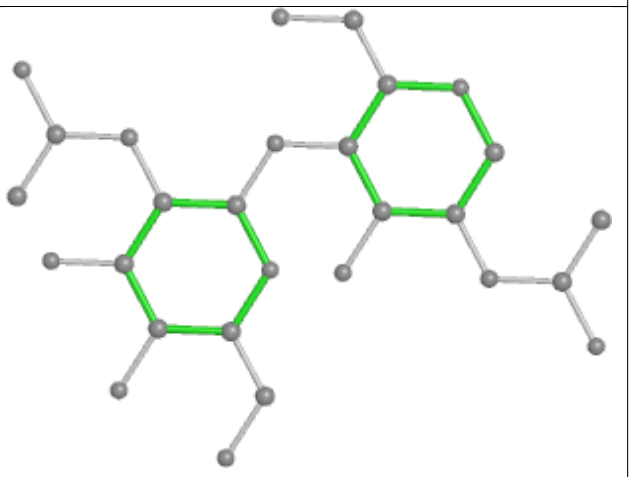
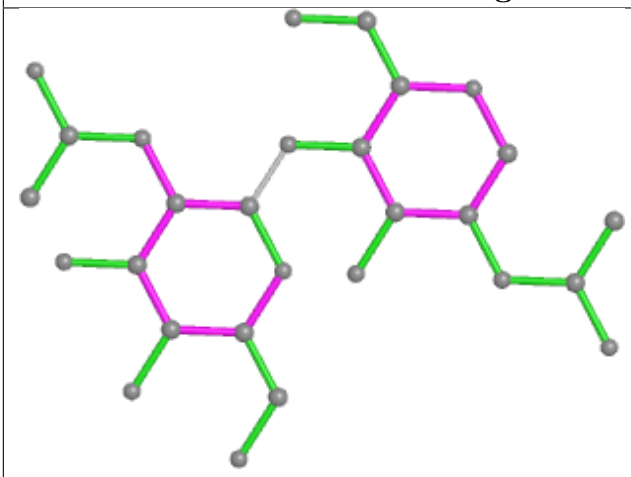


Rings

Oligosaccharide Chain w



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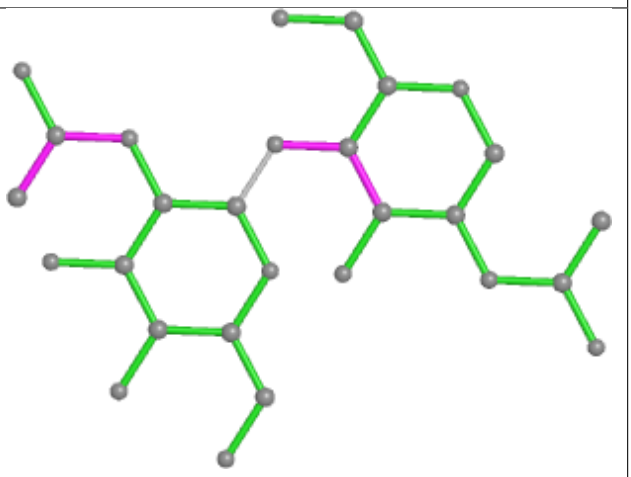
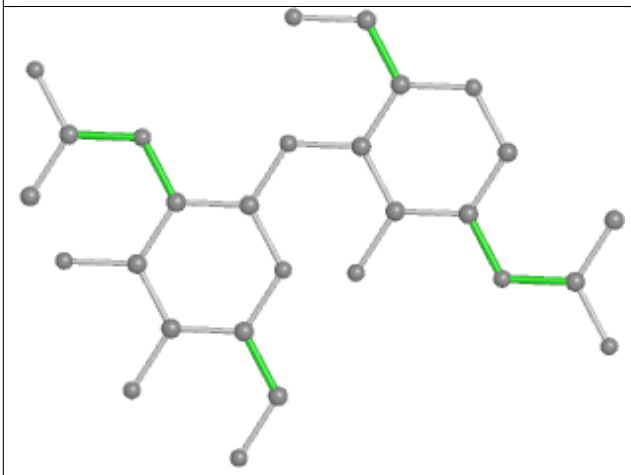


Bond angles



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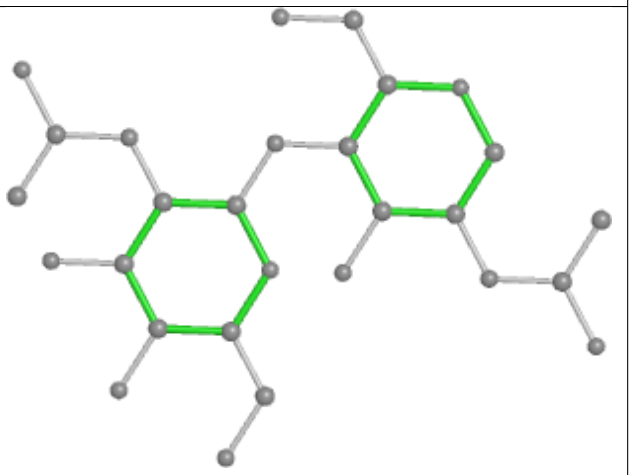
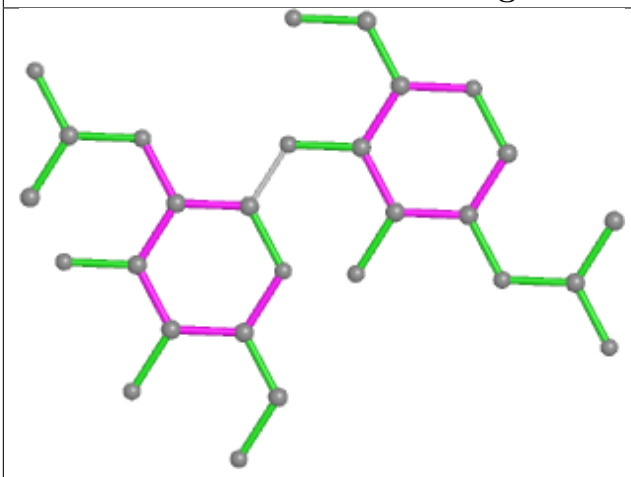


Rings

Oligosaccharide Chain x



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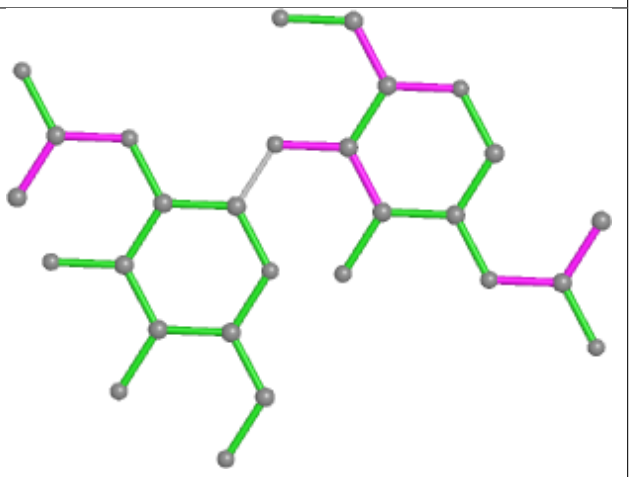
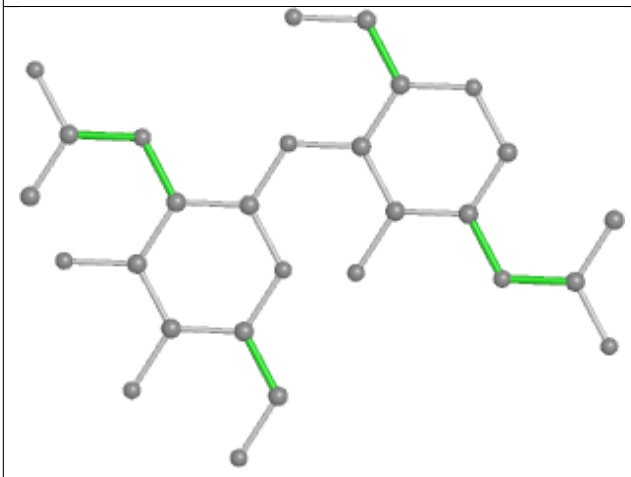


Bond angles



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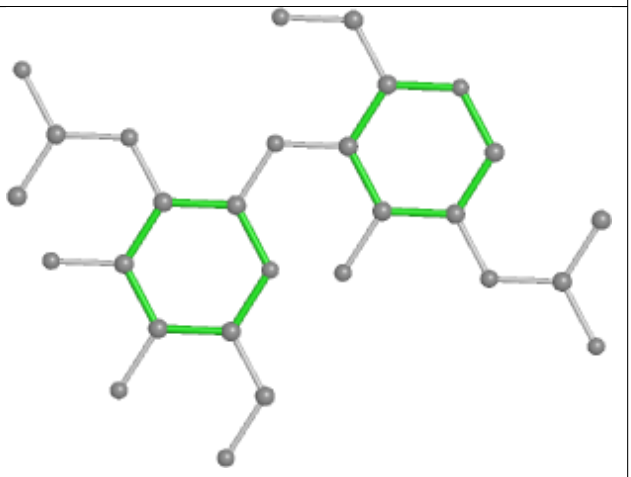
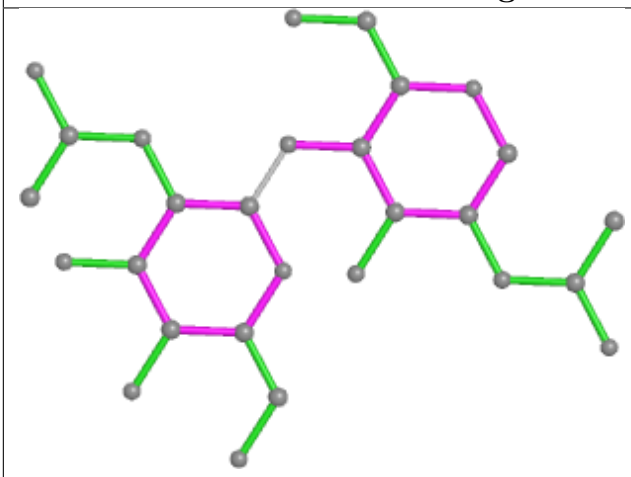


Rings

Oligosaccharide Chain y



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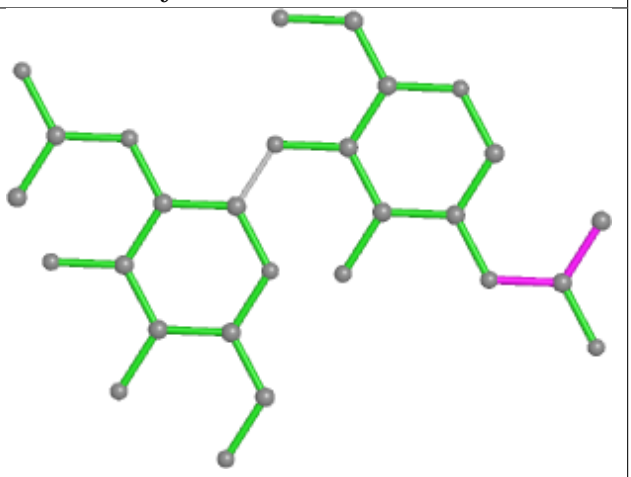
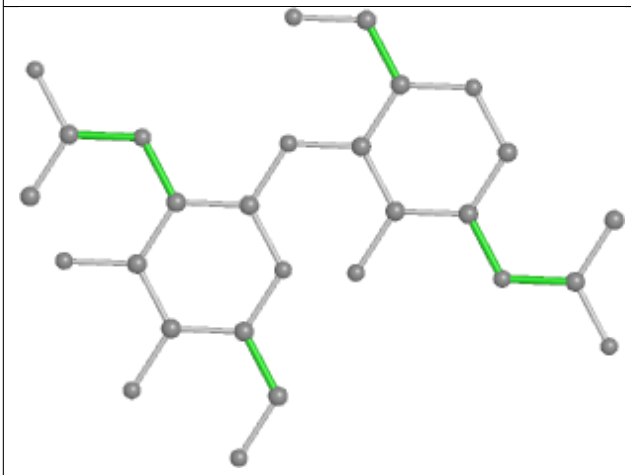


Bond angles



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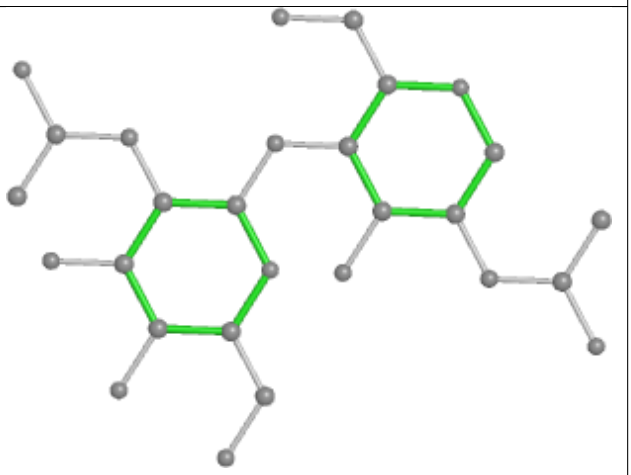
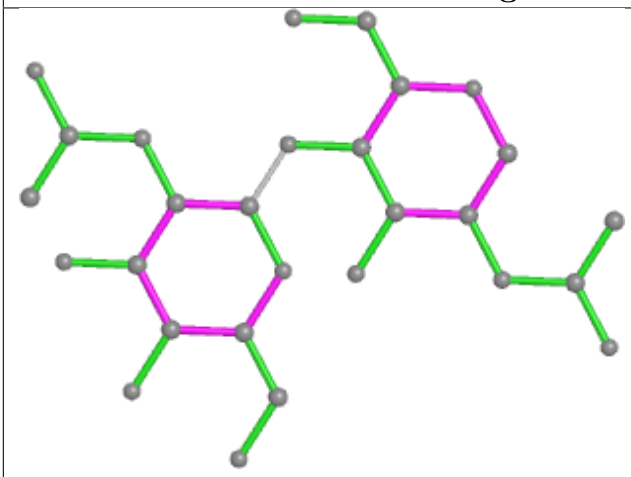


Rings

Oligosaccharide Chain z



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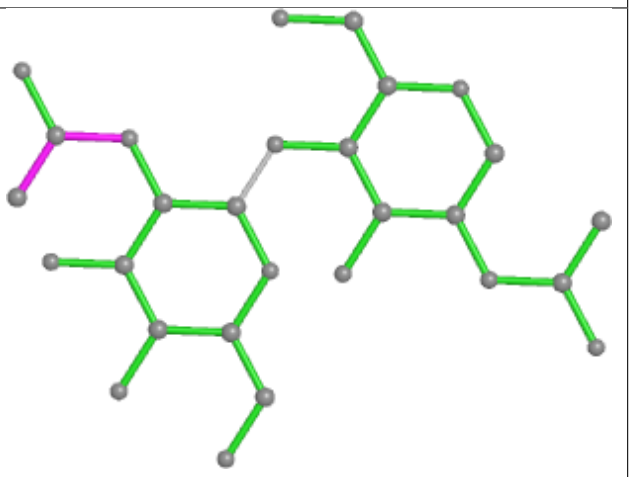

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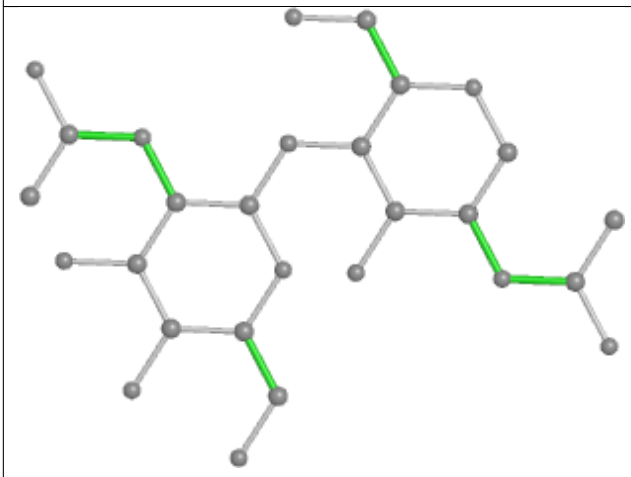

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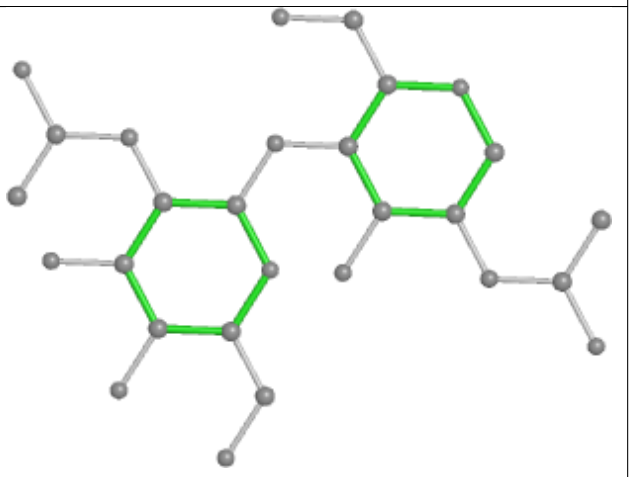
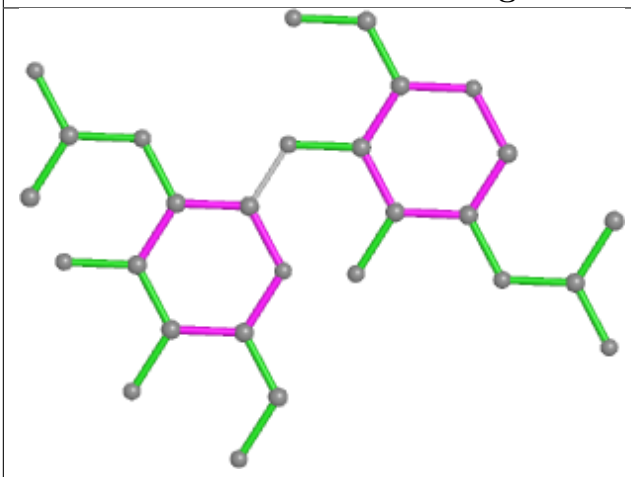


Rings

Oligosaccharide Chain 0



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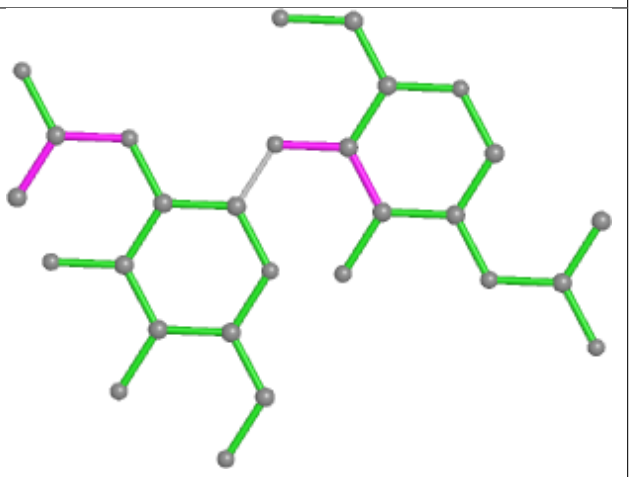
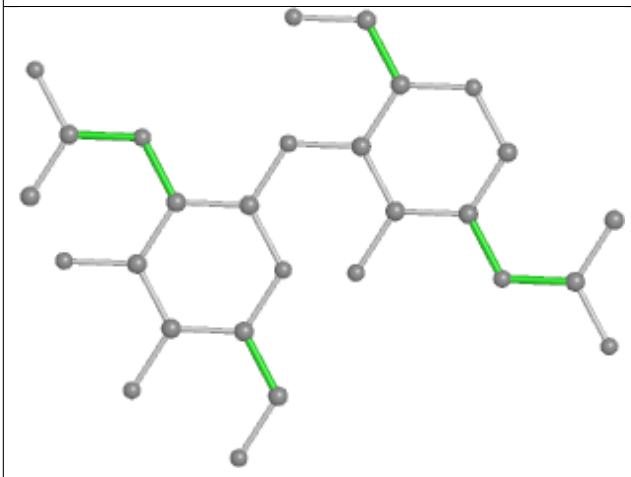


Bond angles



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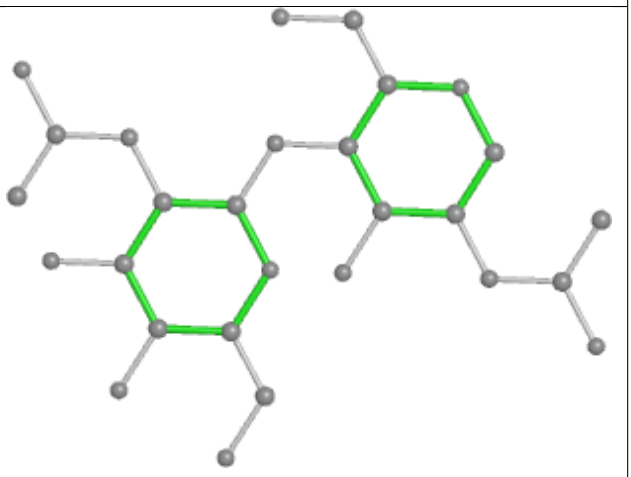
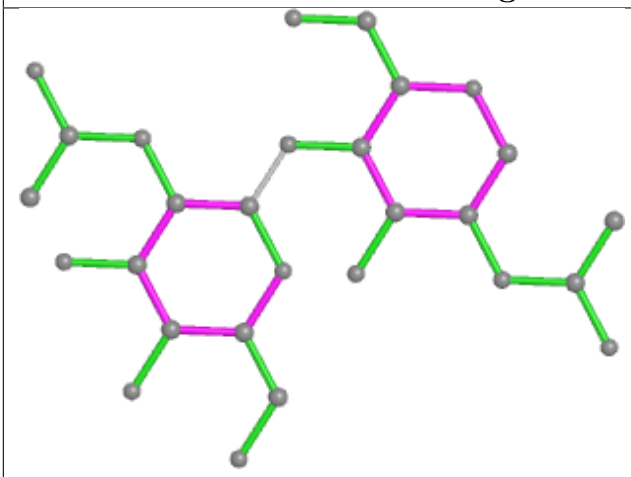


Rings

Oligosaccharide Chain 1



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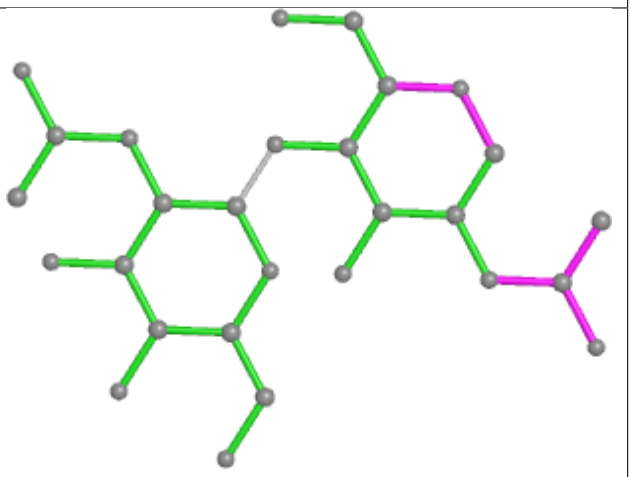

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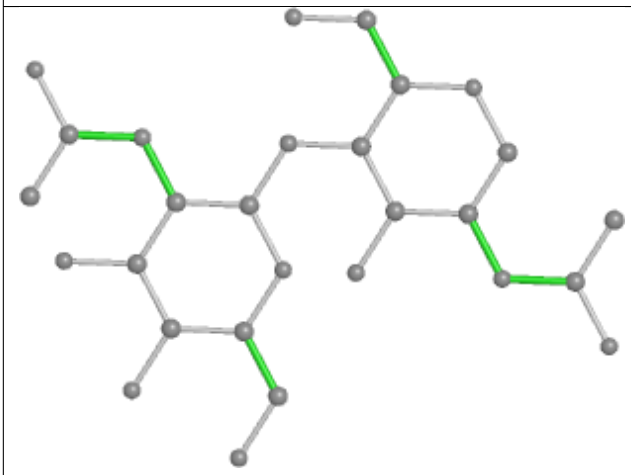

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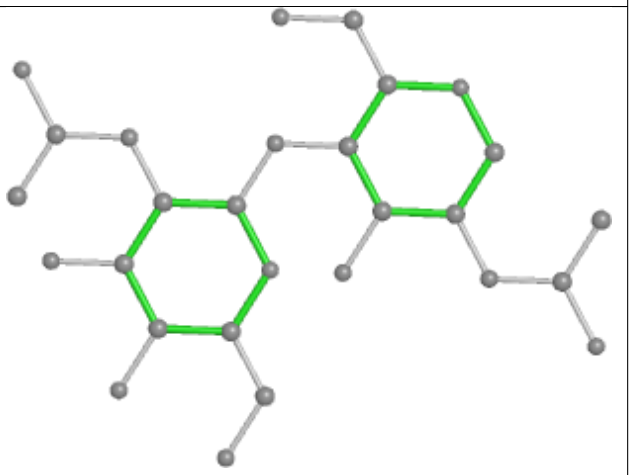
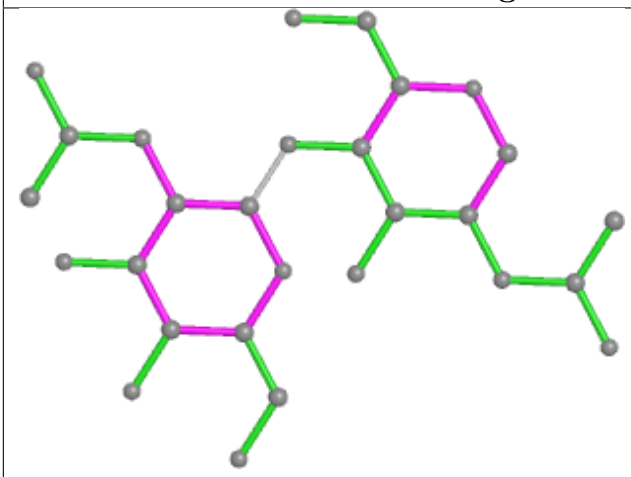


Rings

Oligosaccharide Chain 2



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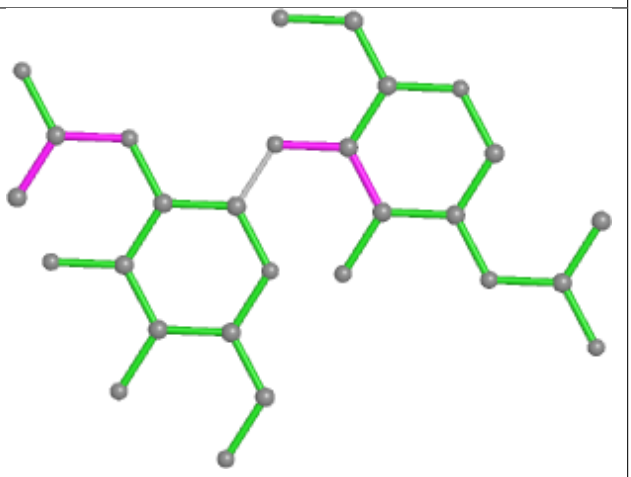

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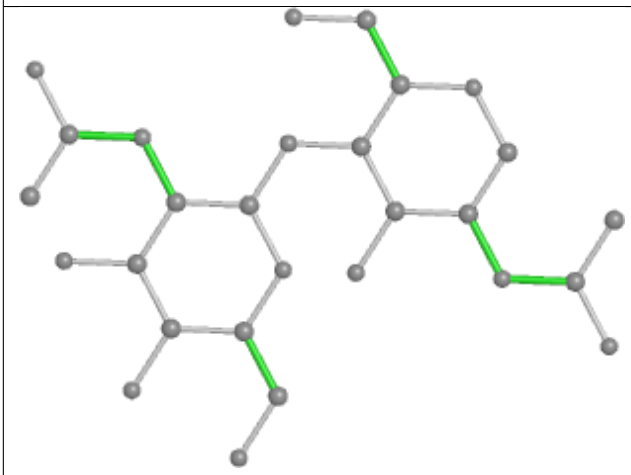

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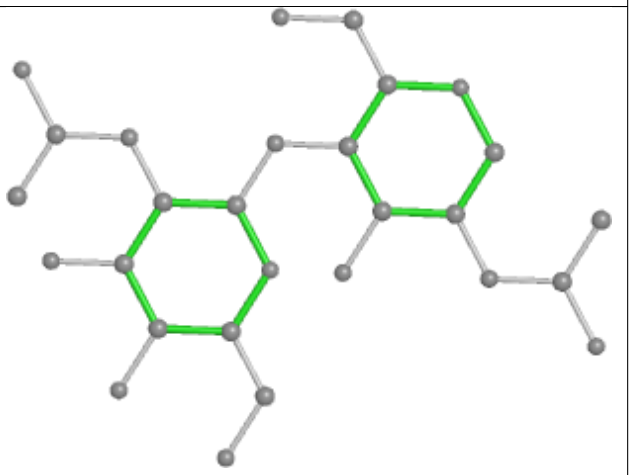
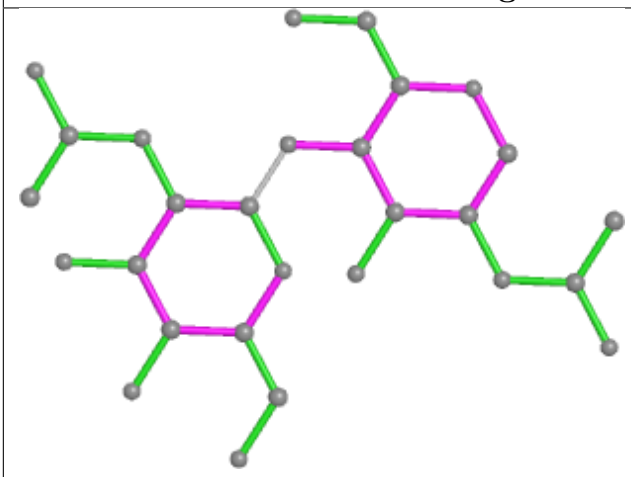


Rings

Oligosaccharide Chain 3



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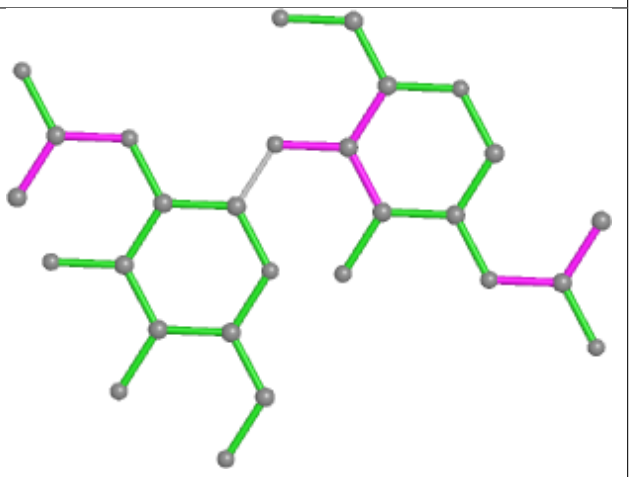

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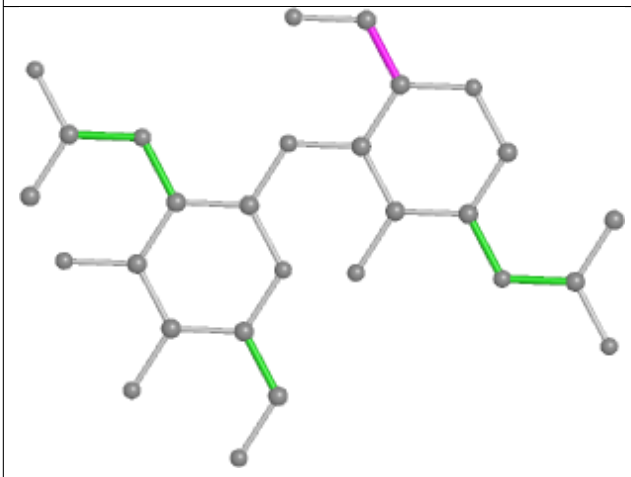

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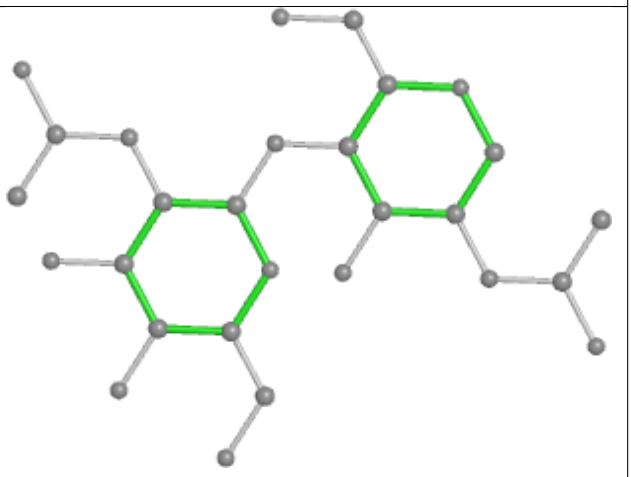
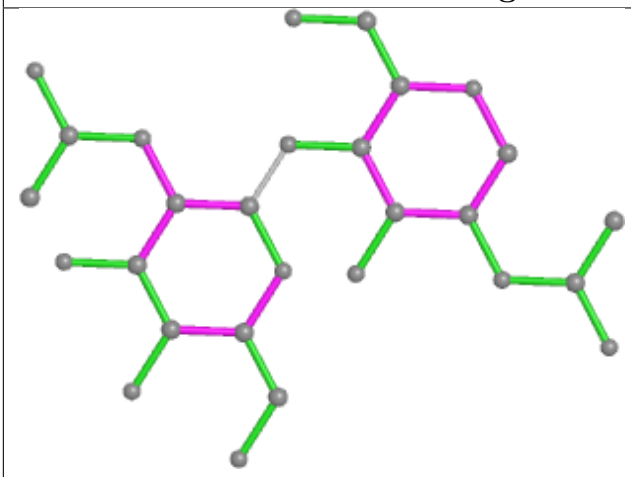


Rings

Oligosaccharide Chain 4



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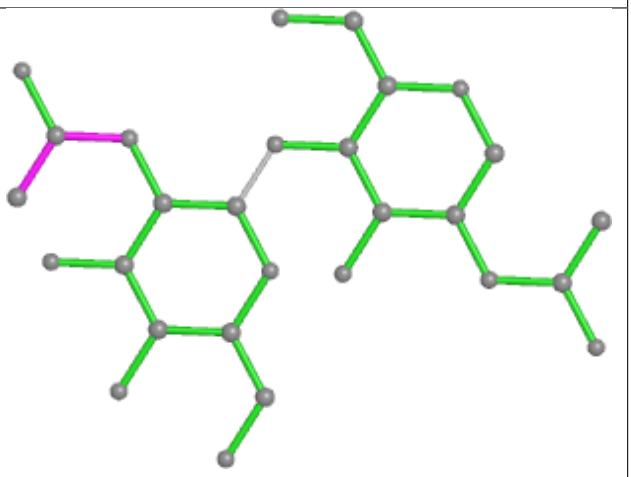
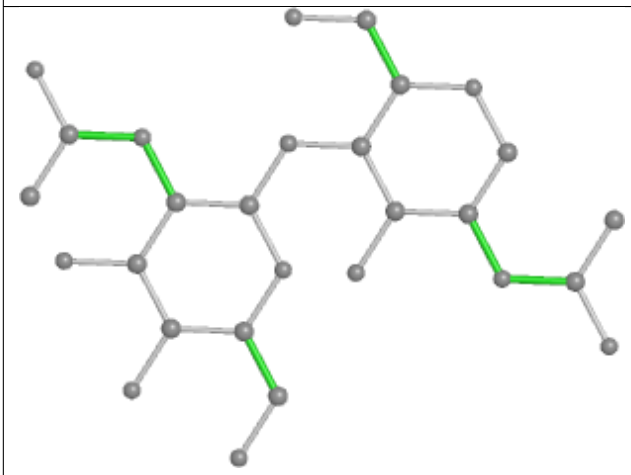
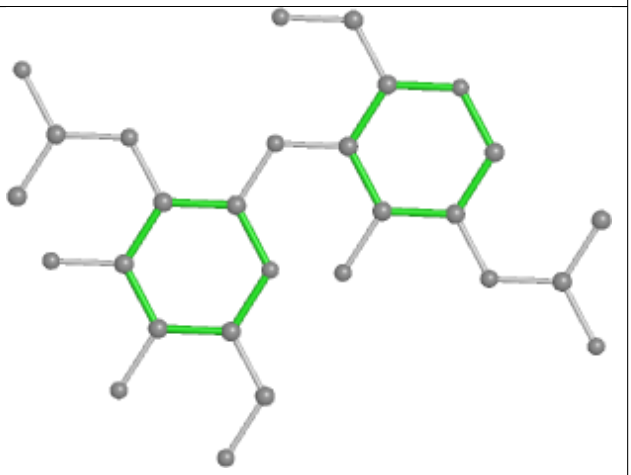


Bond angles

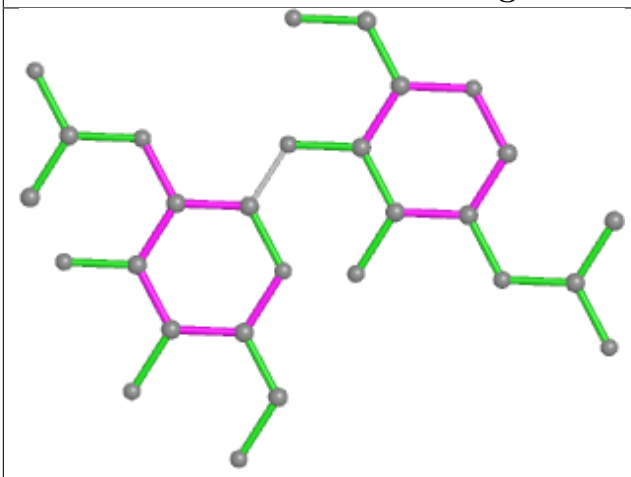


Torsions



Rings

Oligosaccharide Chain 5



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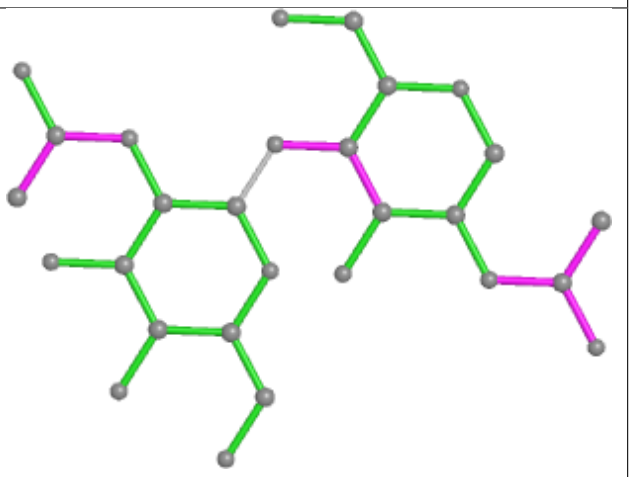
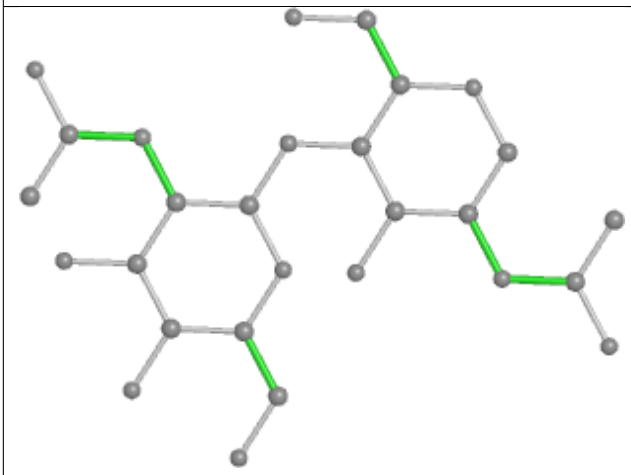


Bond angles



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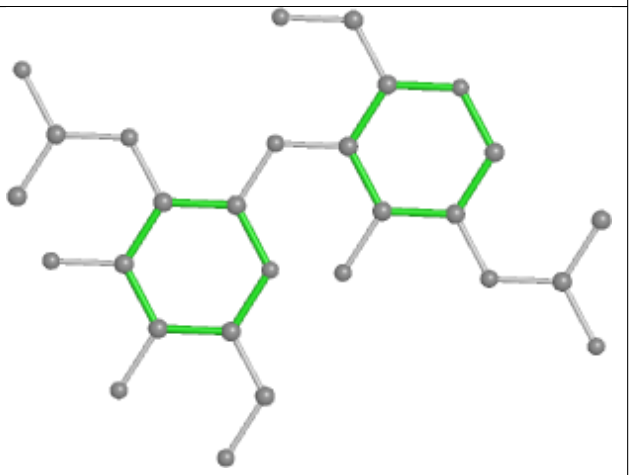
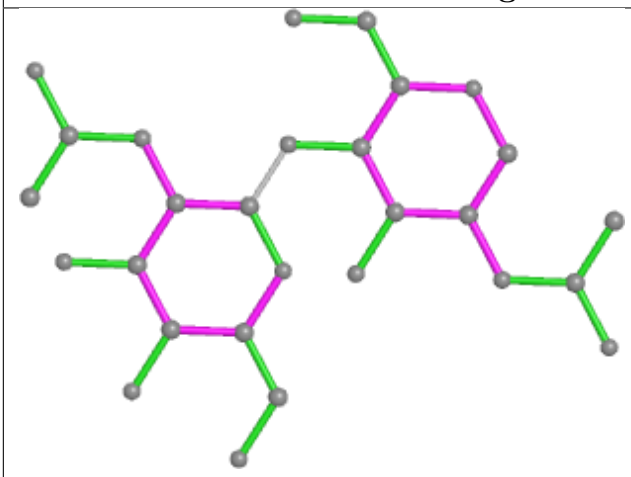


Rings

Oligosaccharide Chain 7



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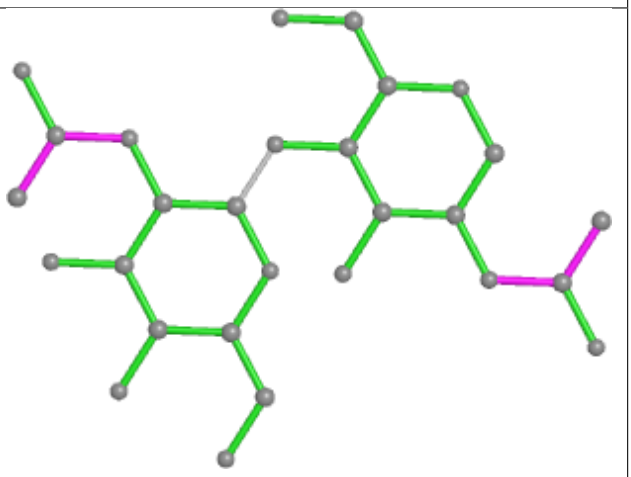
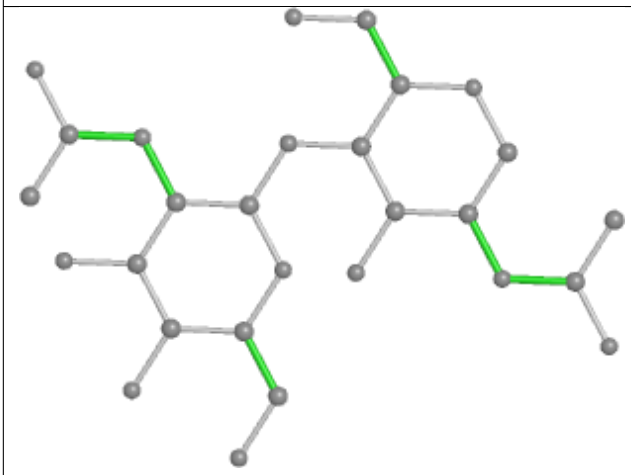
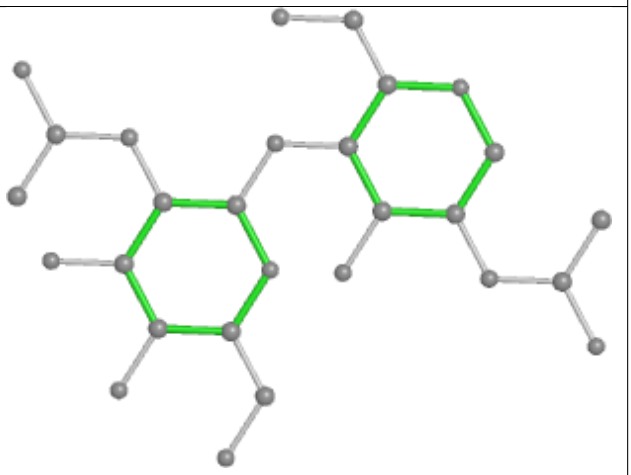


Bond angles

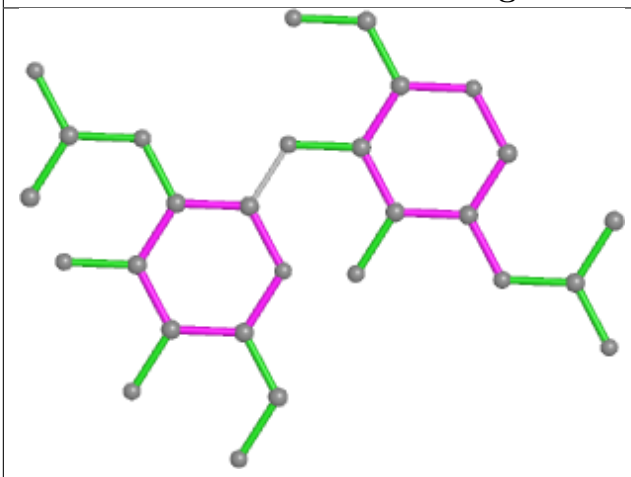


Torsions



Rings

Oligosaccharide Chain 8



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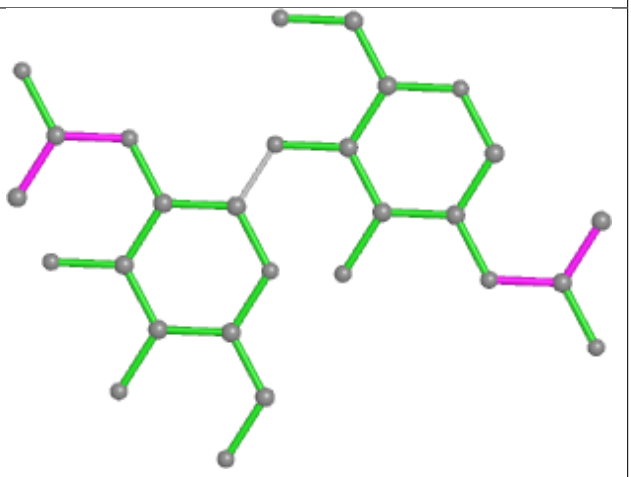
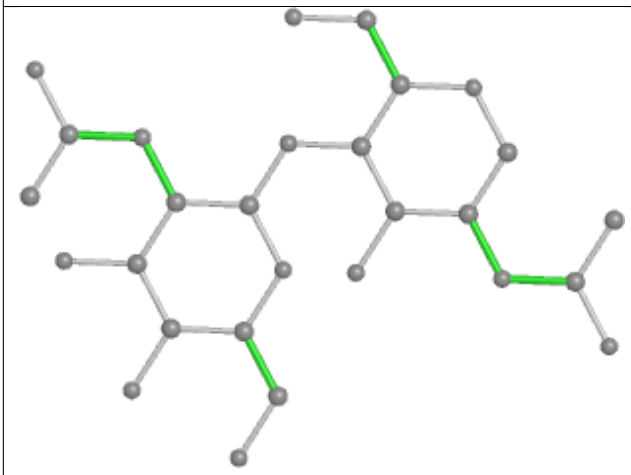


Bond angles



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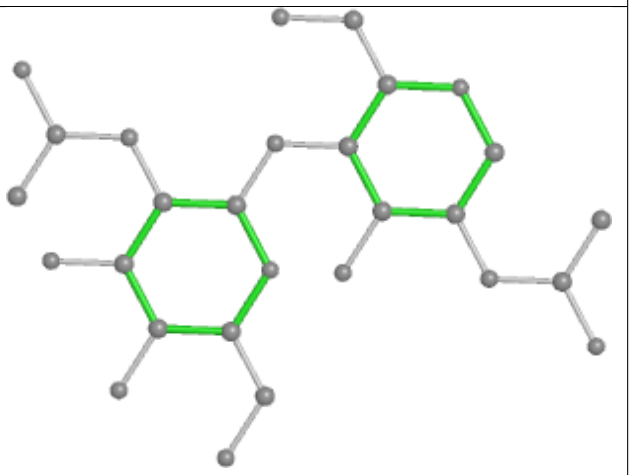
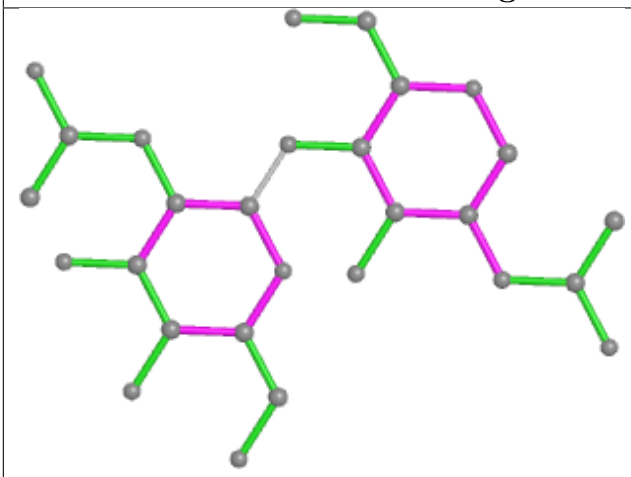


Rings

Oligosaccharide Chain 9



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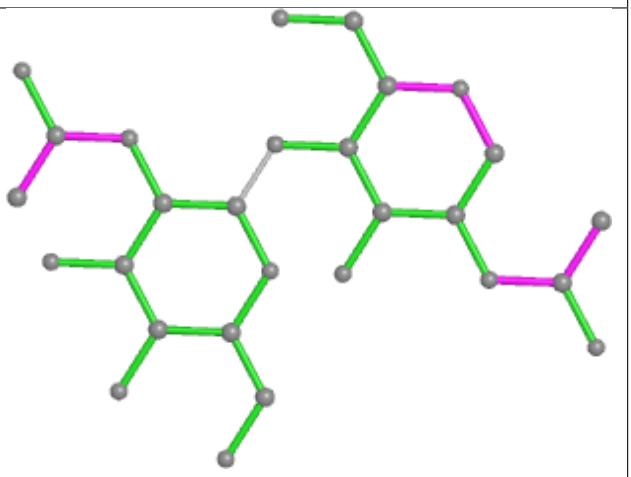
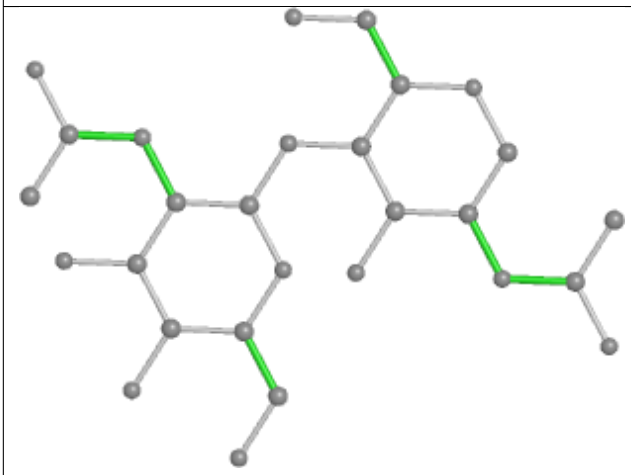


Bond angles



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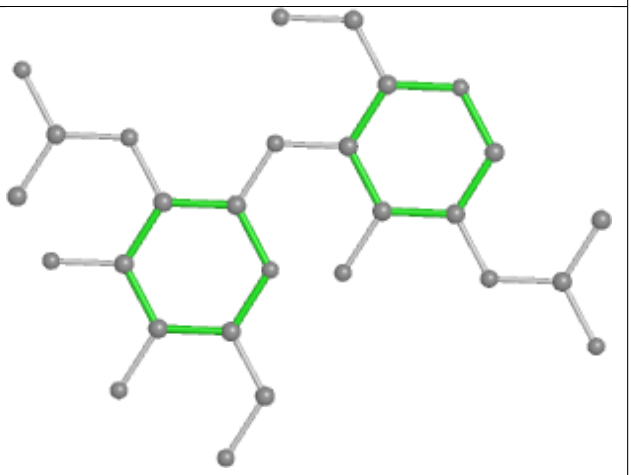
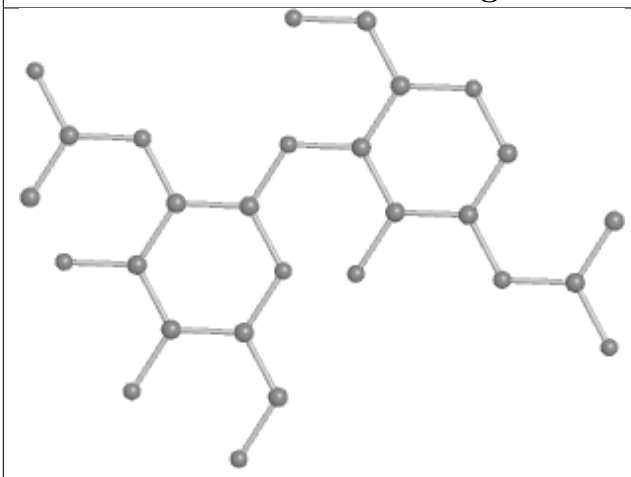


Rings

Oligosaccharide Chain AA



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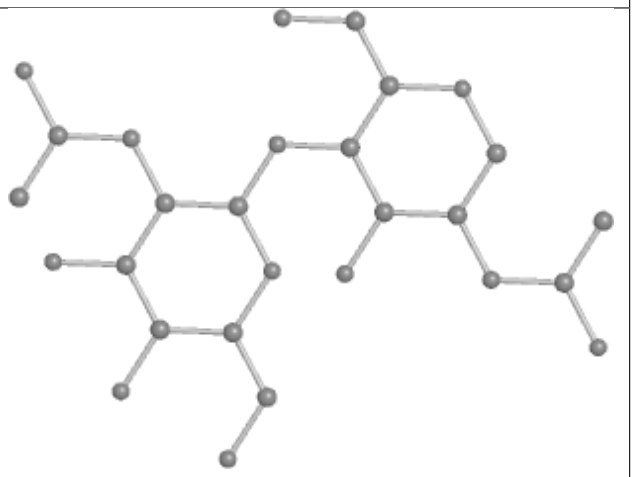

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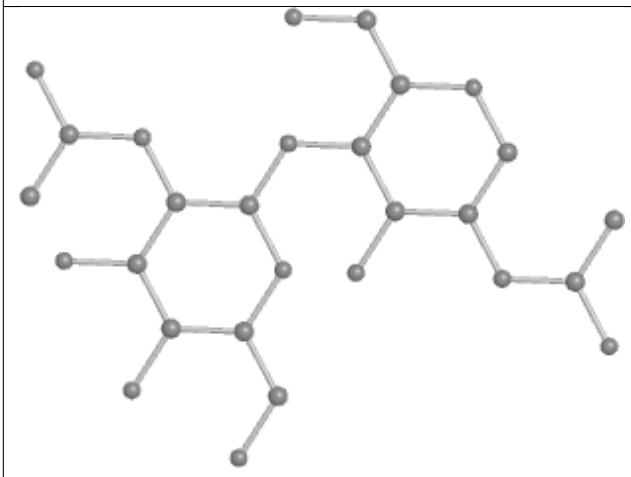

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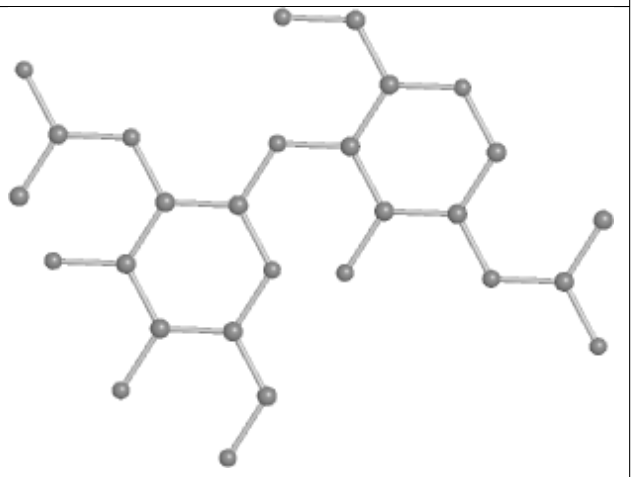
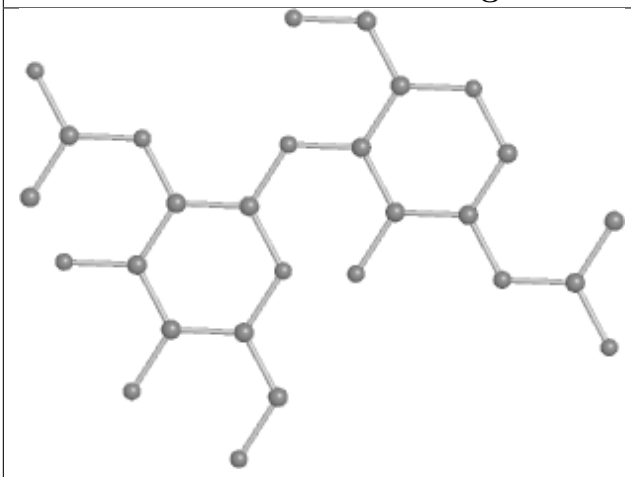


Rings

Oligosaccharide Chain BA



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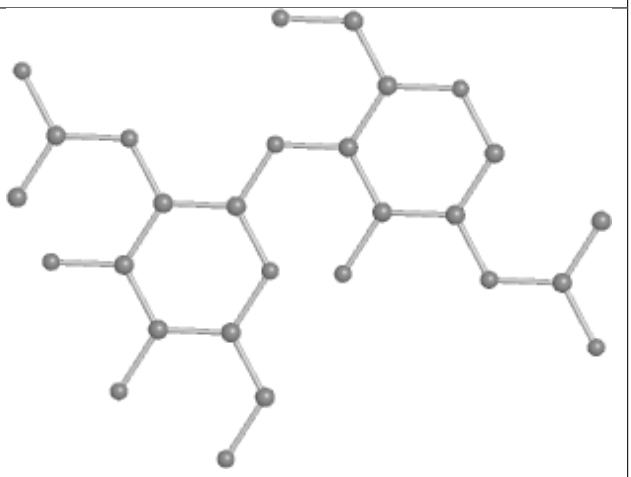
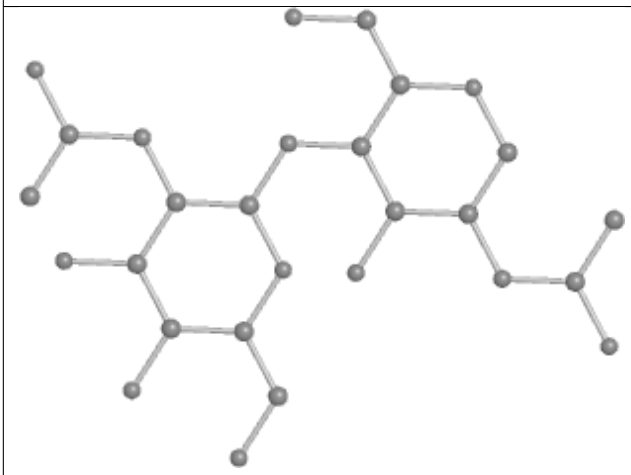


Bond angles



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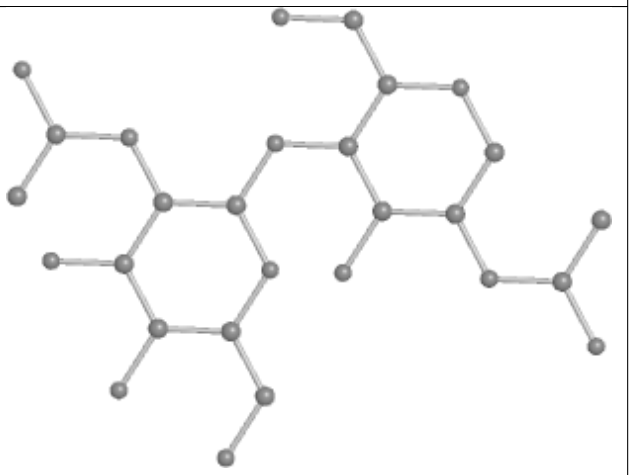
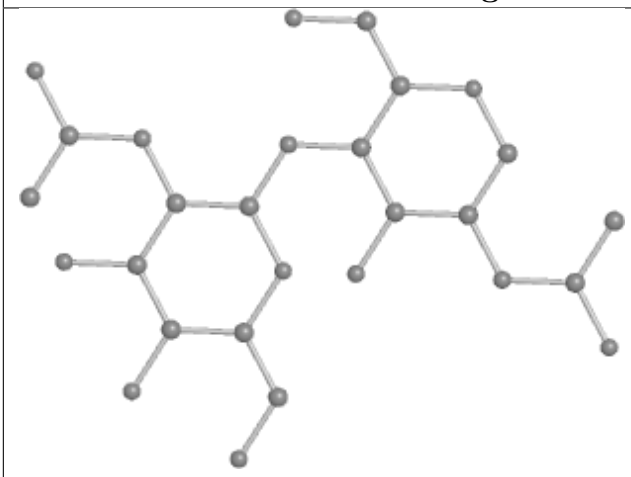


Rings

Oligosaccharide Chain CA



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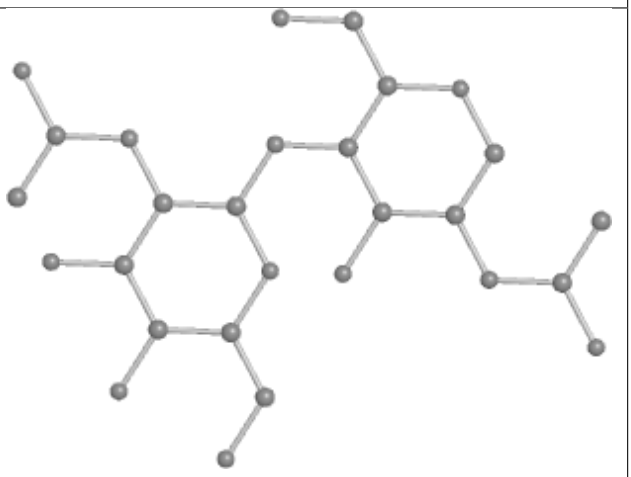

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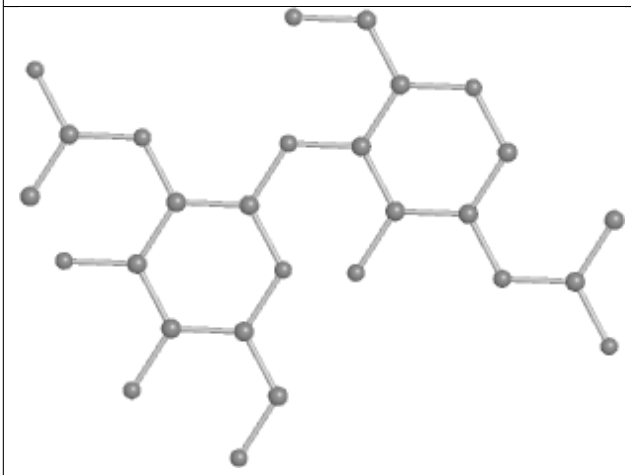

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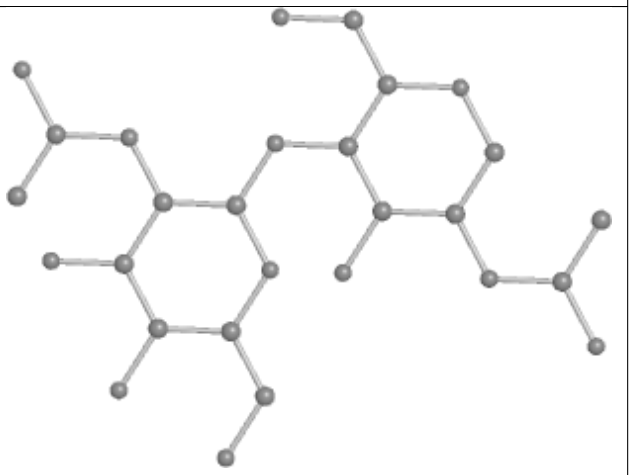
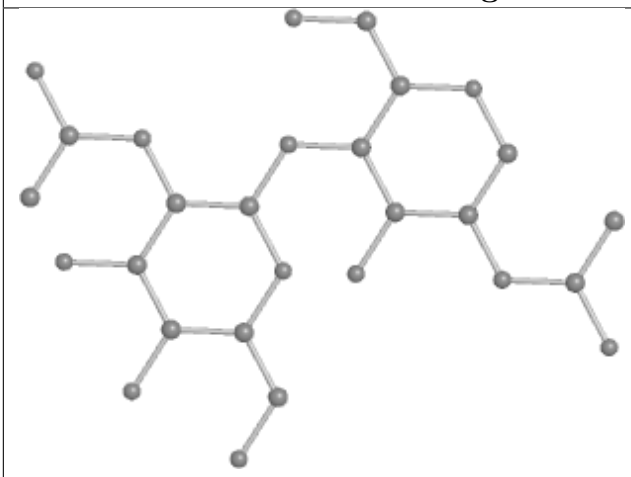


Rings

Oligosaccharide Chain DA



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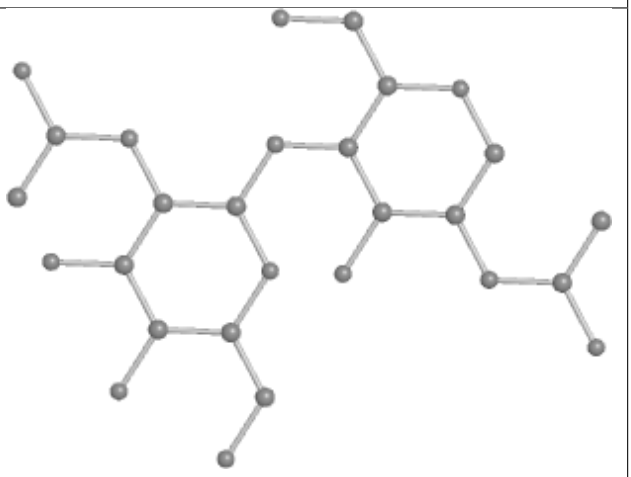
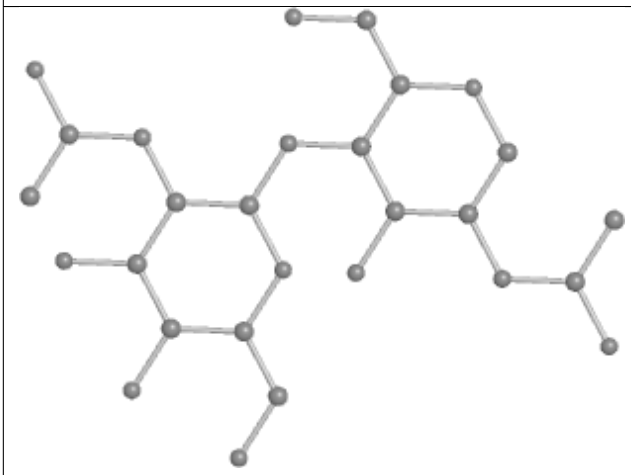


Bond angles



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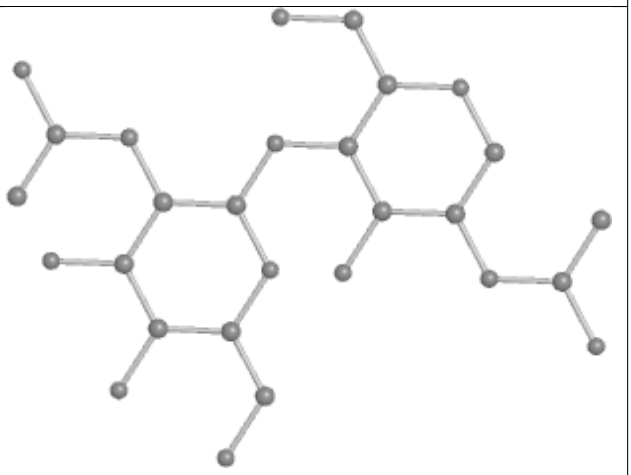
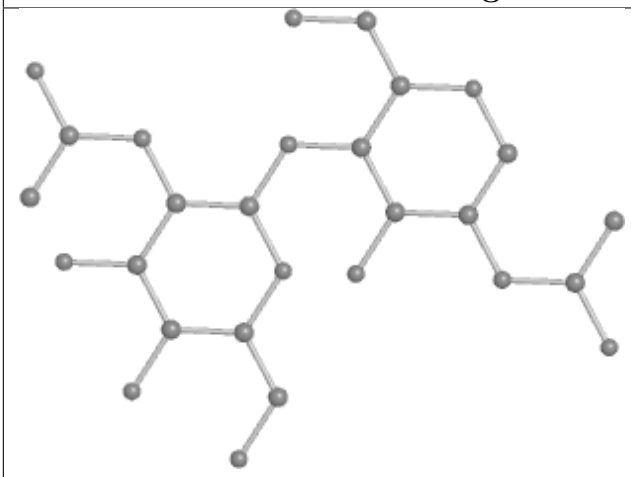


Rings

Oligosaccharide Chain EA



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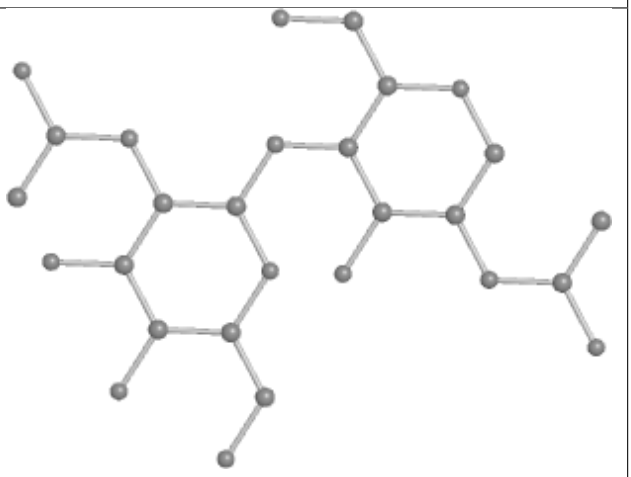
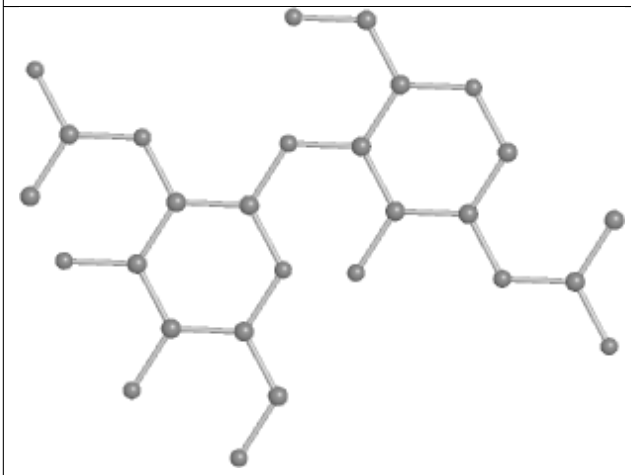


Bond angles



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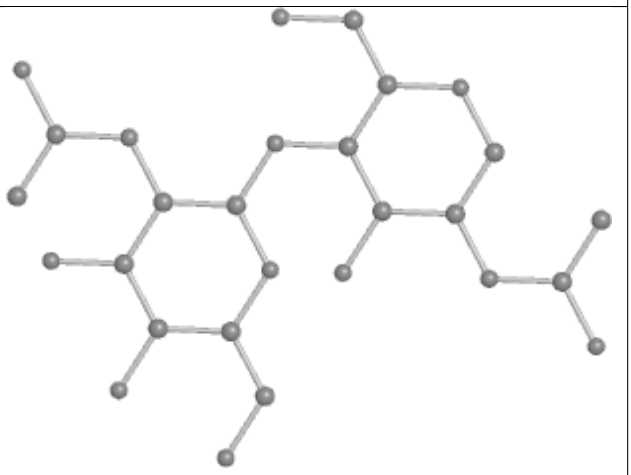
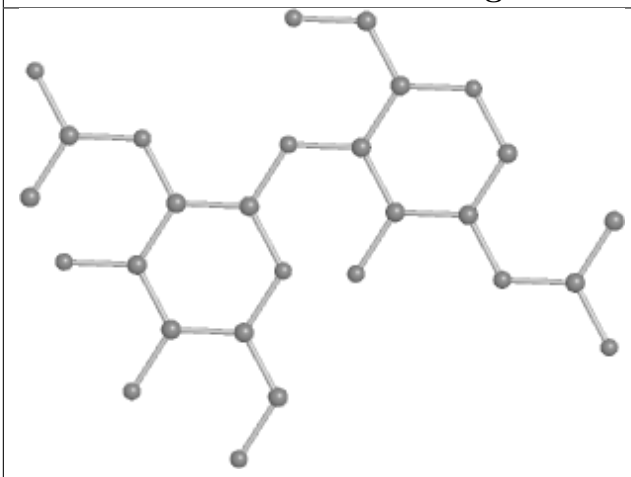


Rings

Oligosaccharide Chain FA



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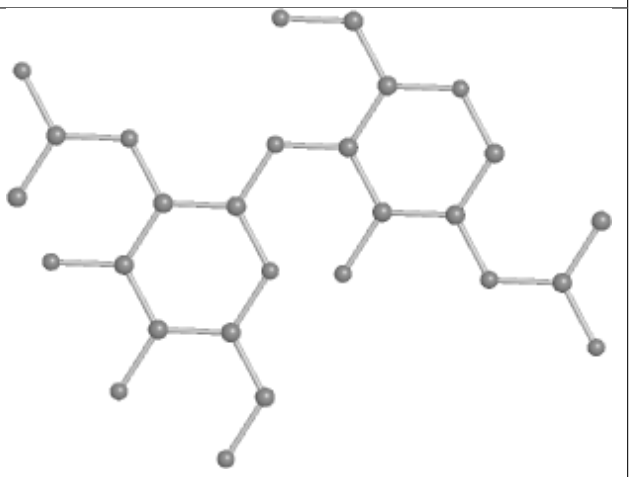
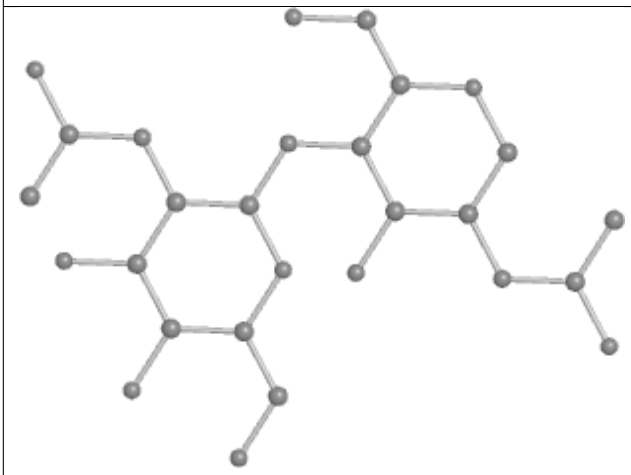


Bond angles



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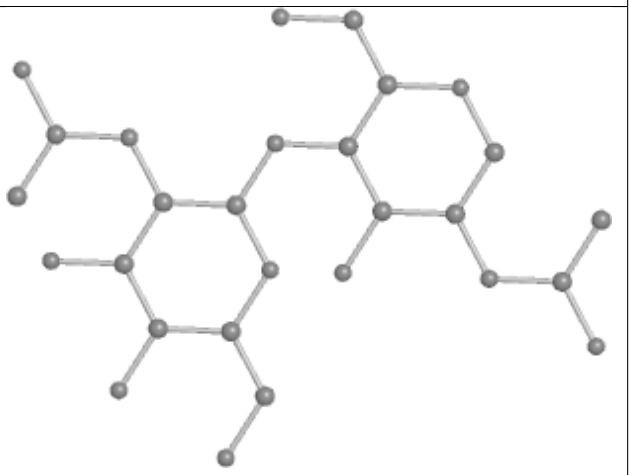
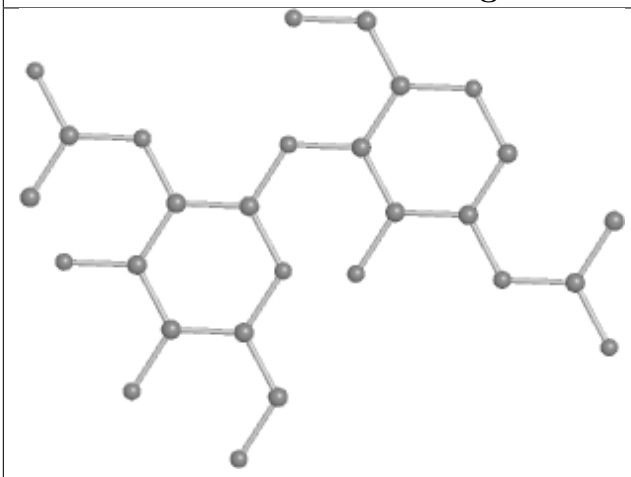


Rings

Oligosaccharide Chain GA



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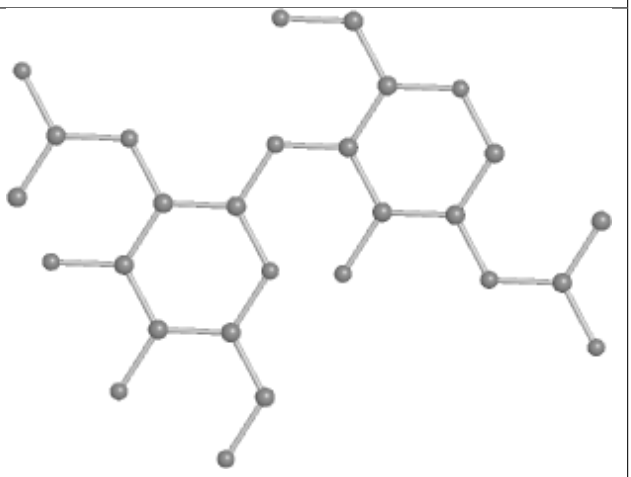

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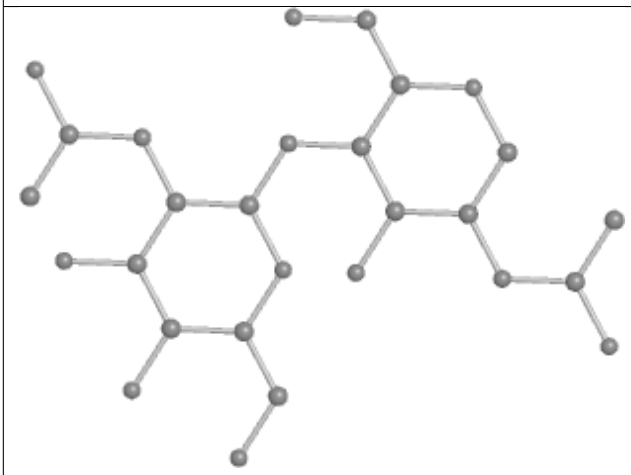

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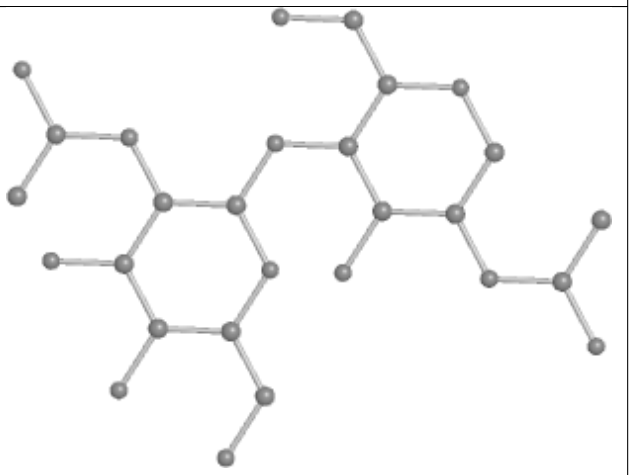
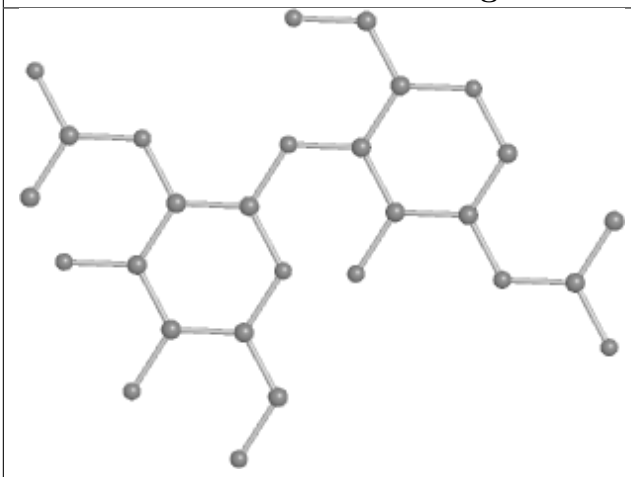


Rings

Oligosaccharide Chain HA



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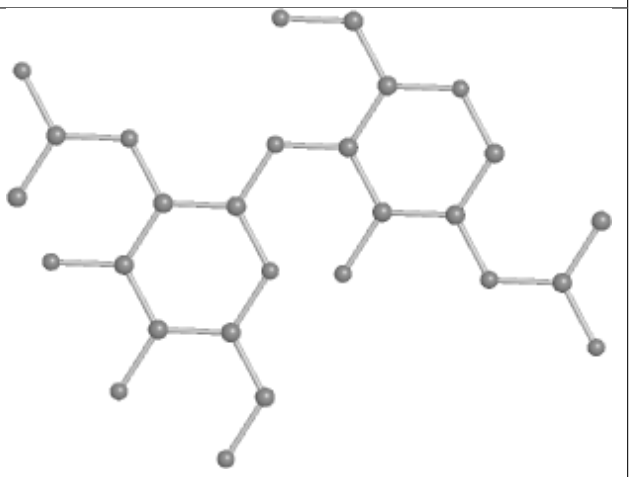
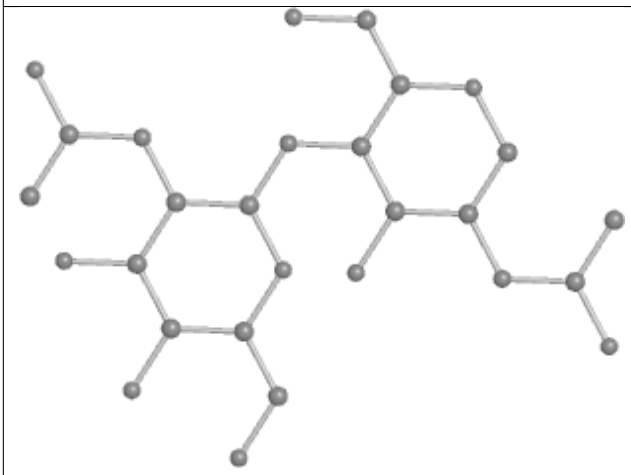


Bond angles



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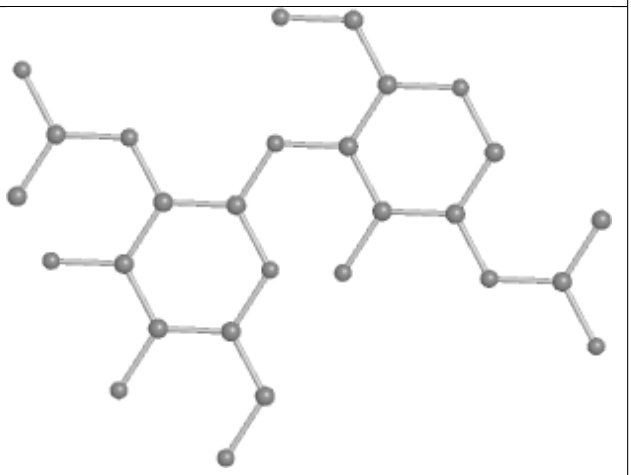
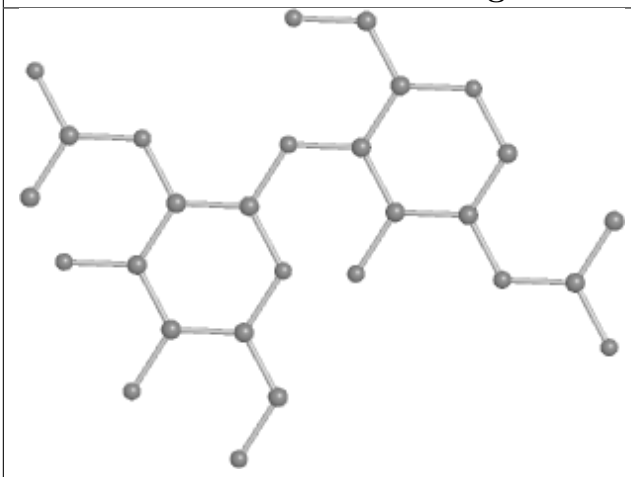


Rings

Oligosaccharide Chain IA



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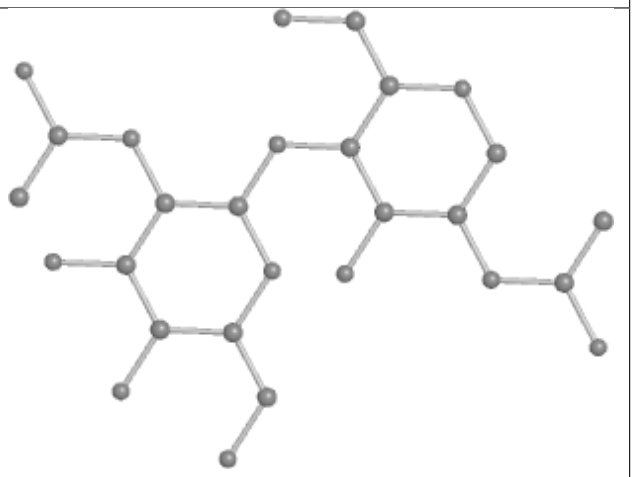

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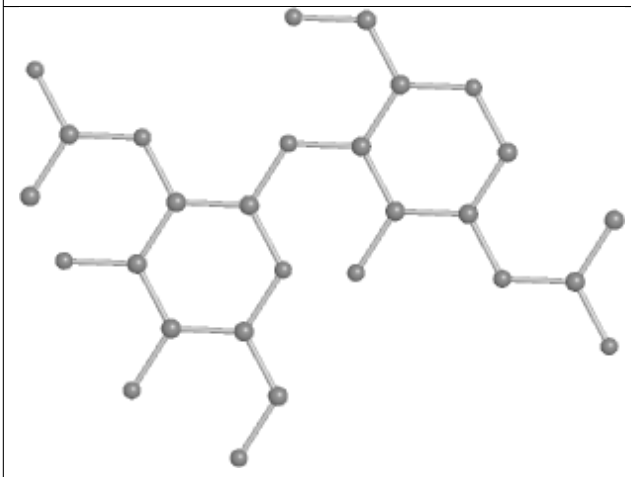

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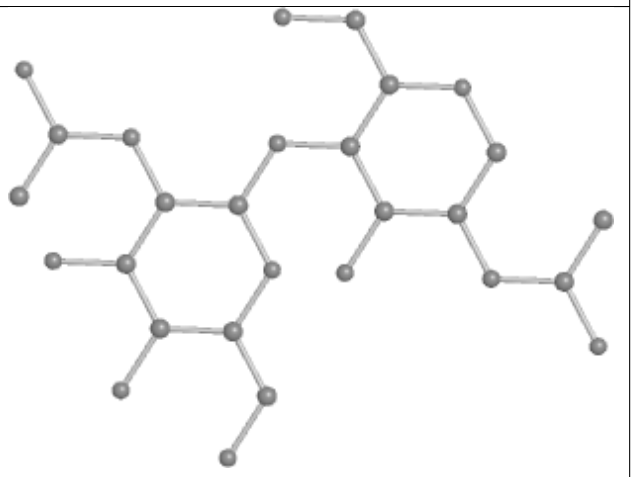
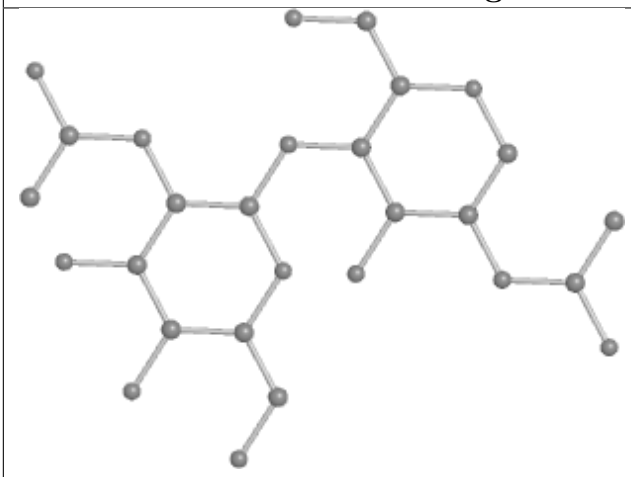


Rings

Oligosaccharide Chain JA



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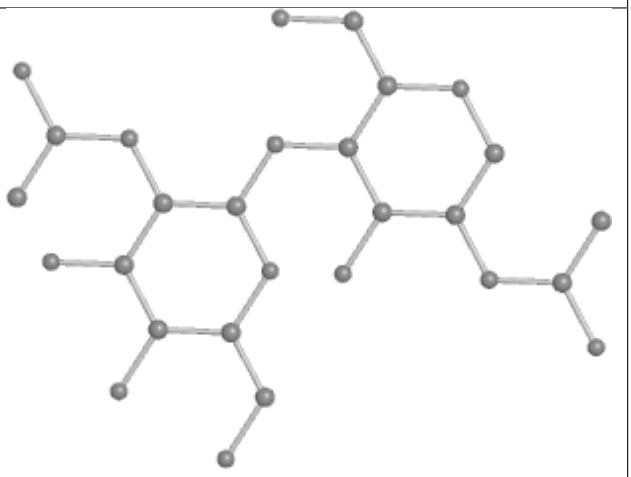
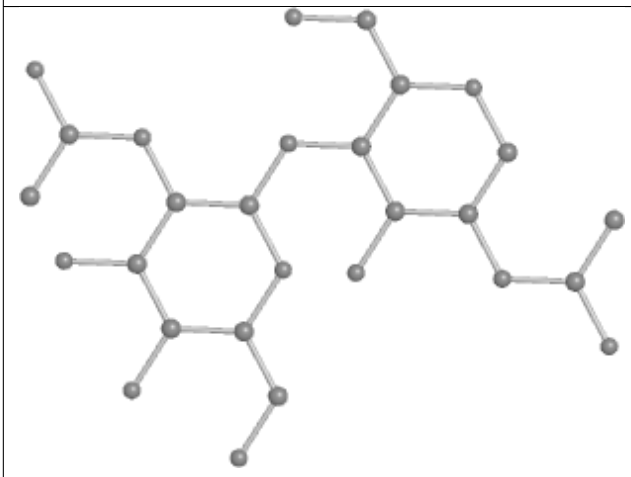


Bond angles



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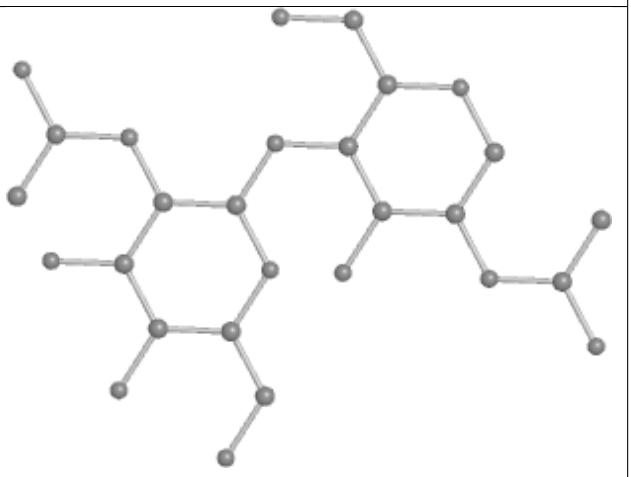
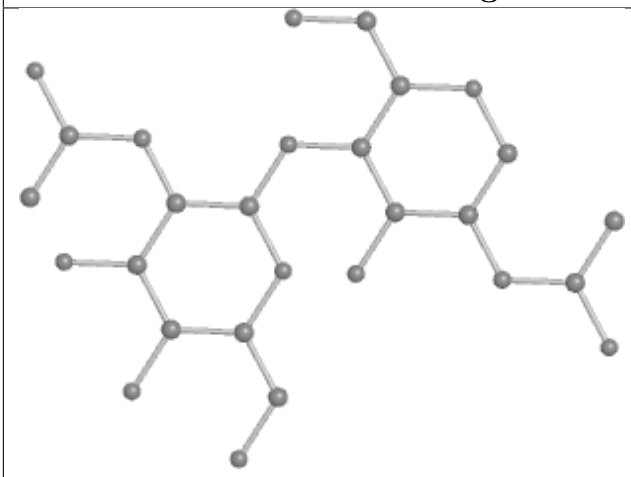
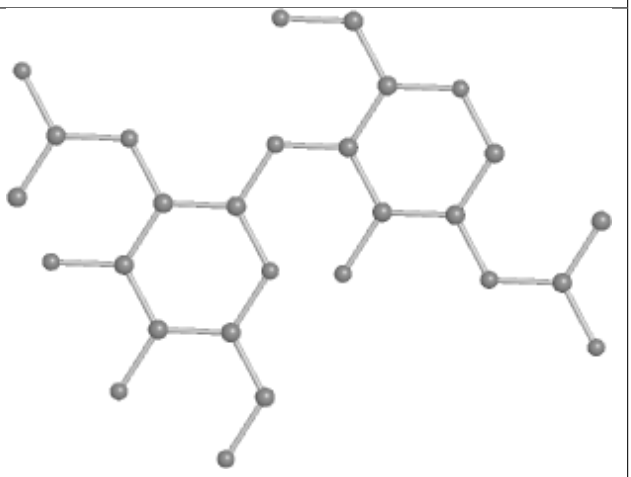


Rings

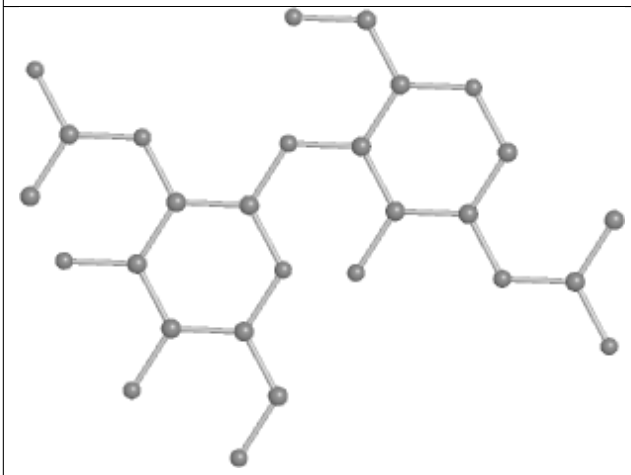
Oligosaccharide Chain KA



Bond lengths



Bond angles



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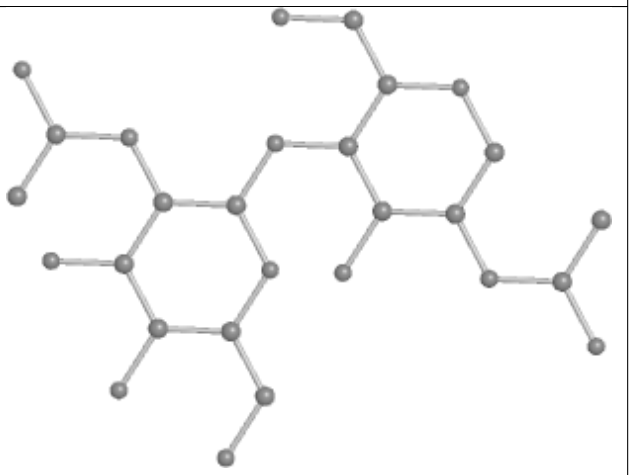
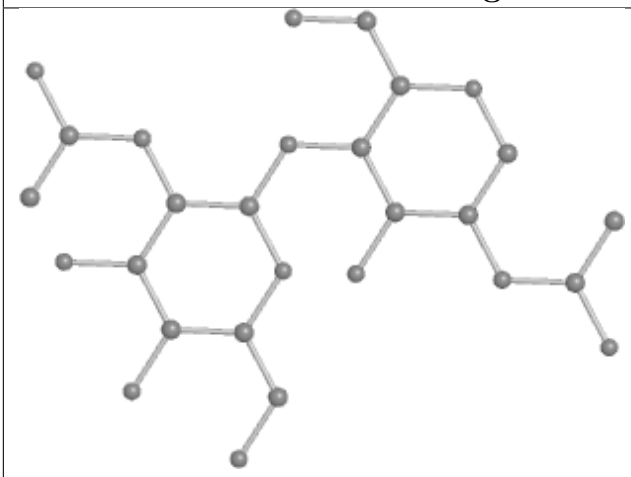
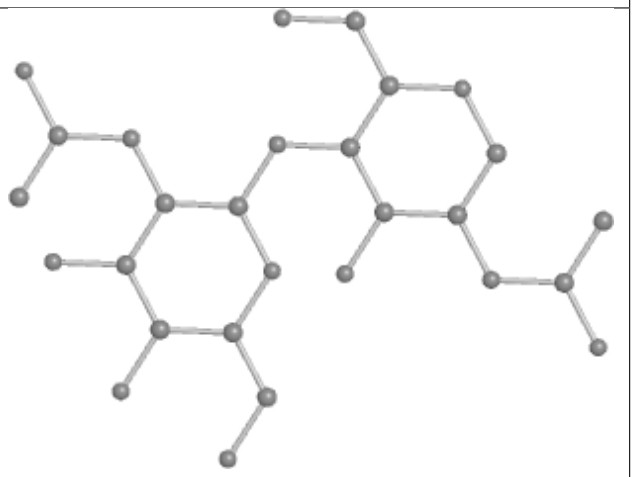


Rings

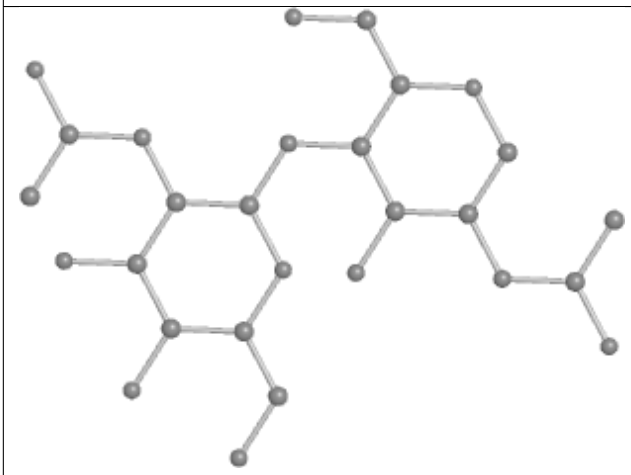
Oligosaccharide Chain LA



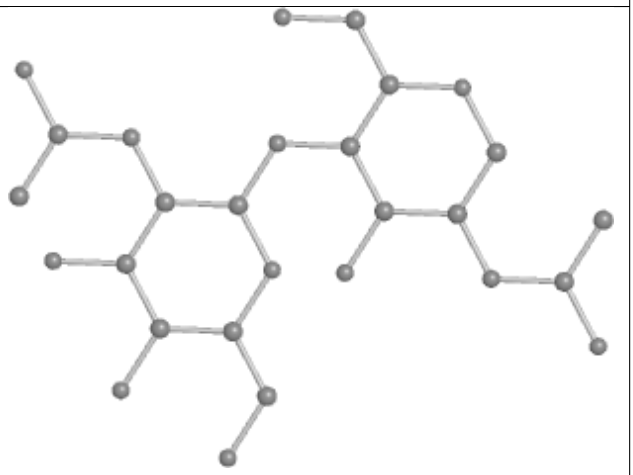
Bond lengths



Bond angles

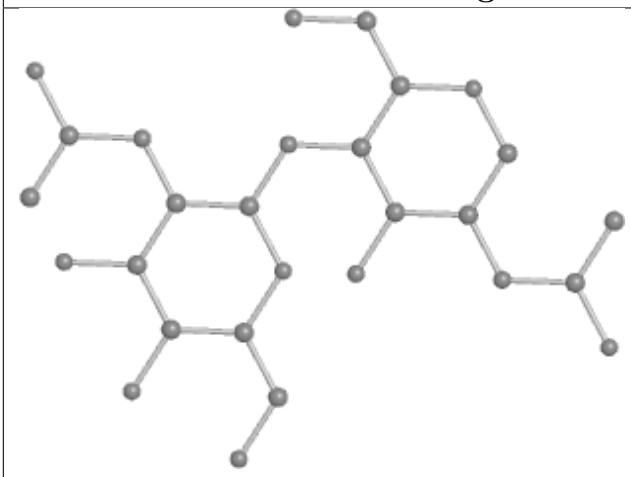


Torsions

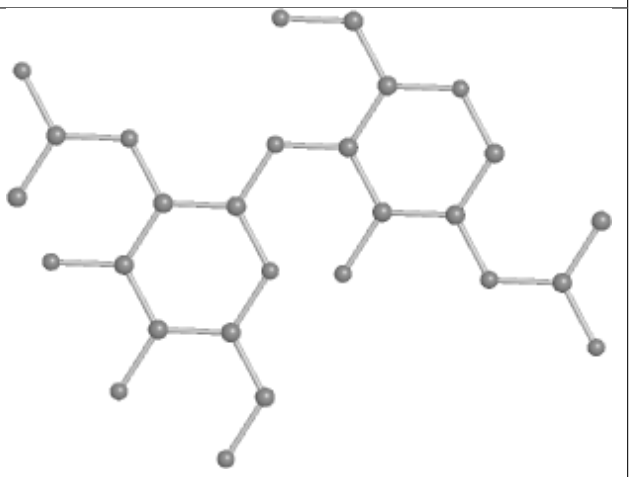


Rings

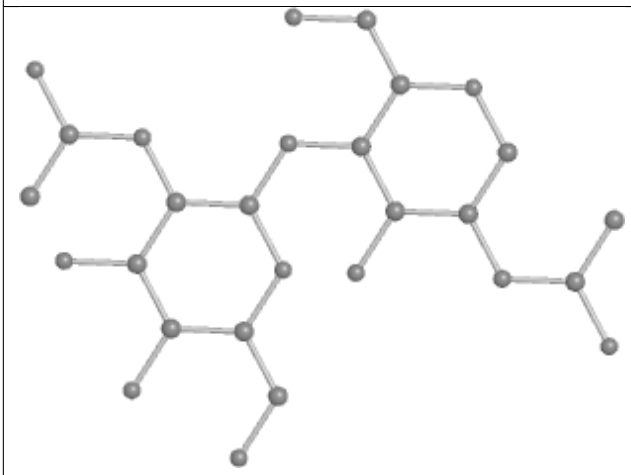
Oligosaccharide Chain MA



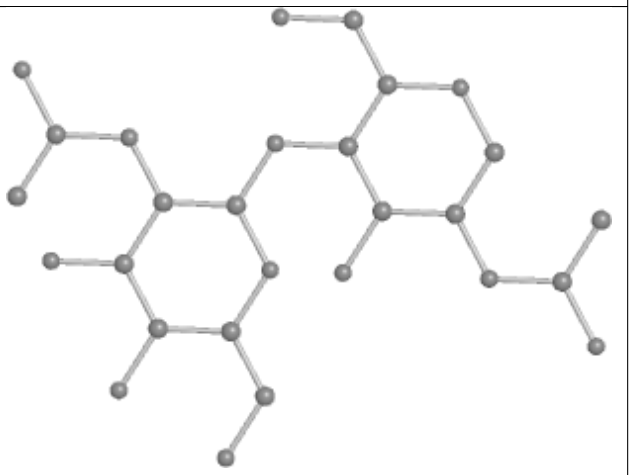
Bond lengths



Bond angles

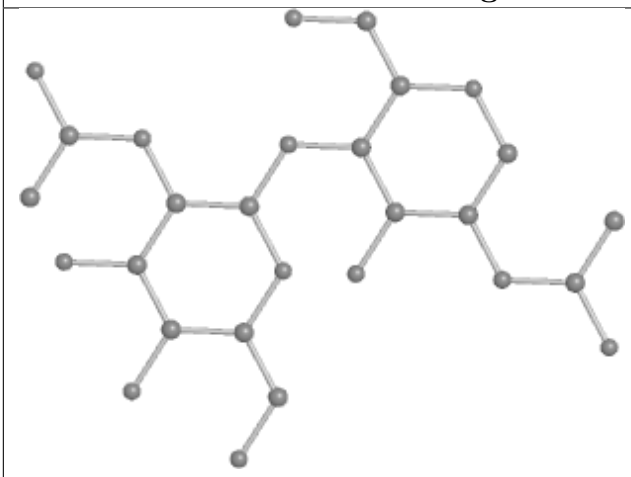


Torsions



Rings

Oligosaccharide Chain NA



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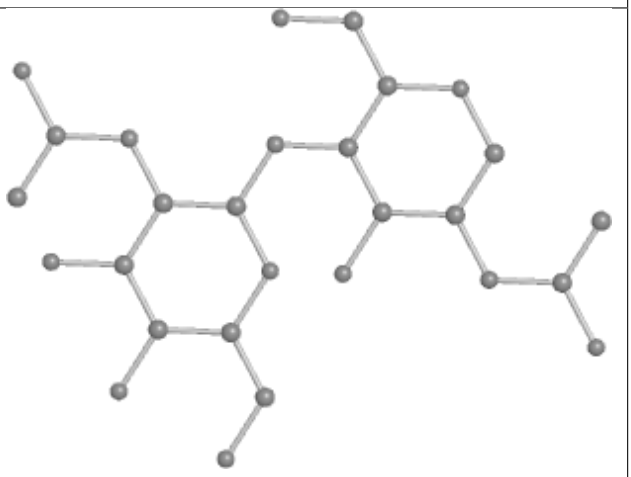

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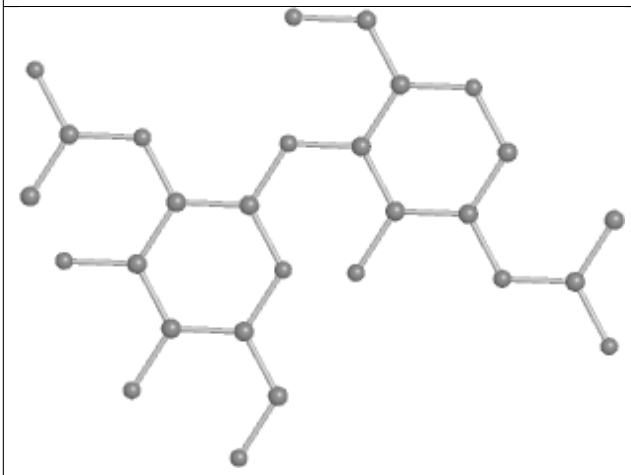

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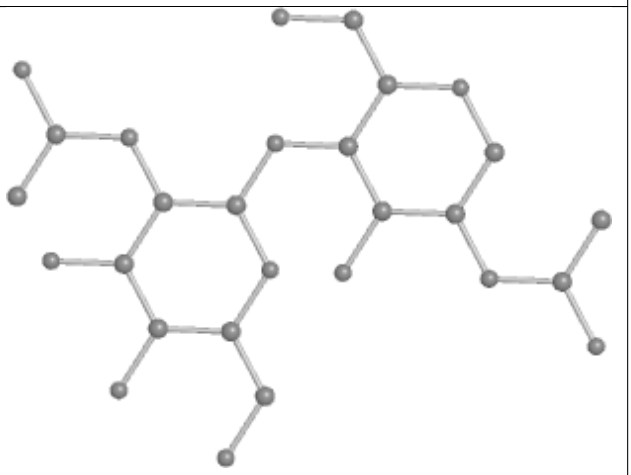
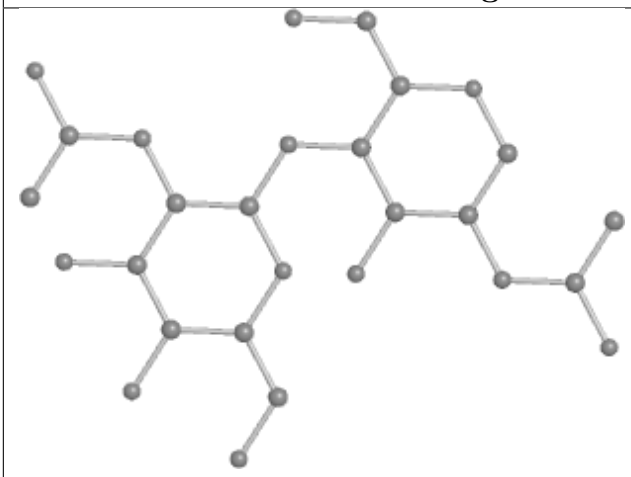


Rings

Oligosaccharide Chain OA



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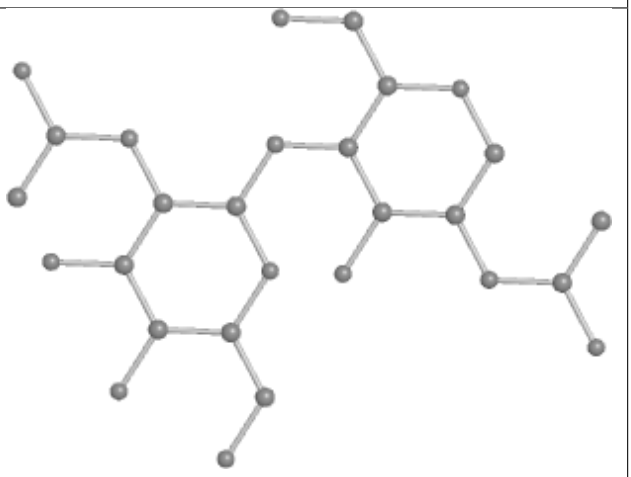
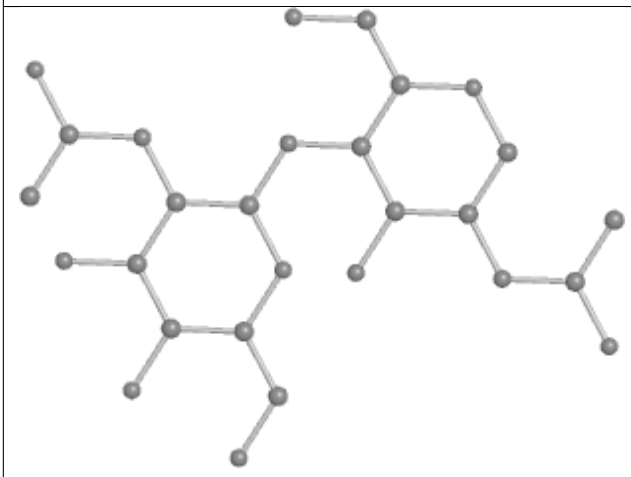
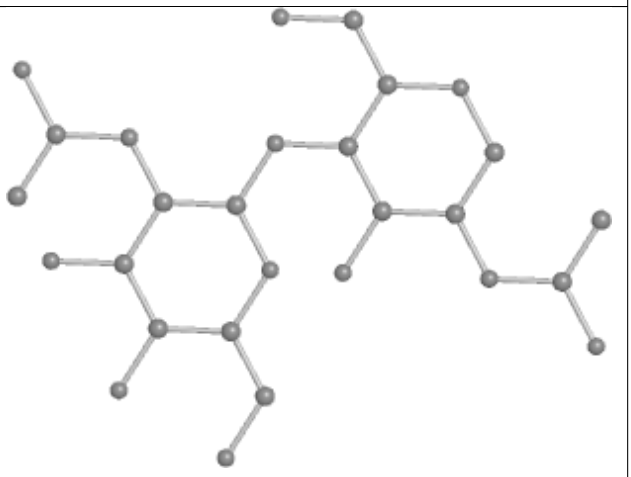


Bond angles

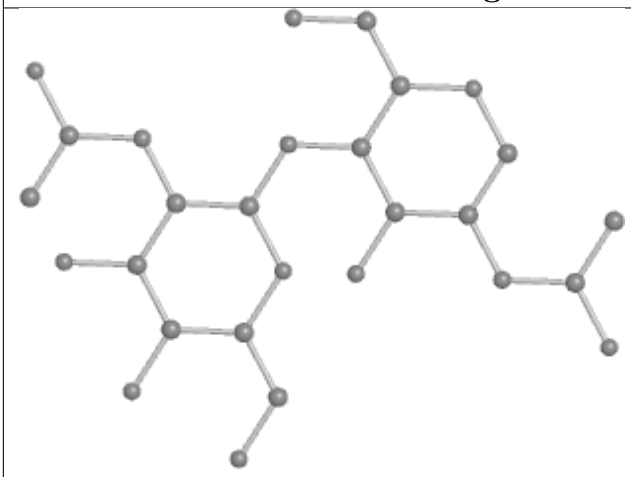


Torsions



Rings

Oligosaccharide Chain PA



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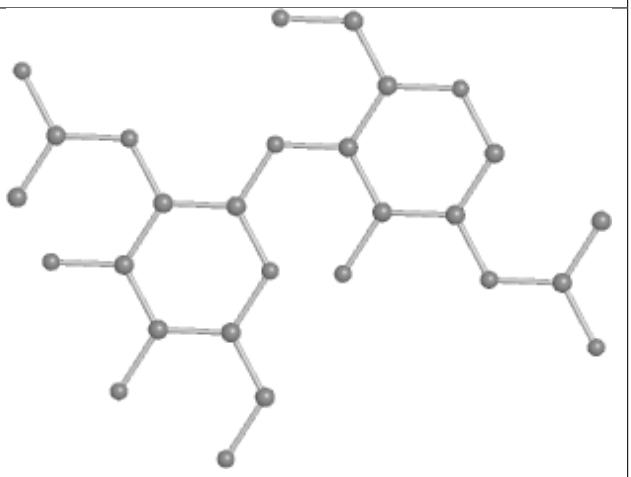

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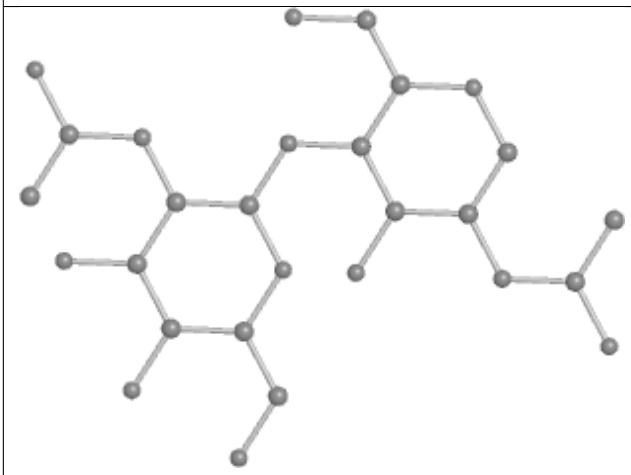
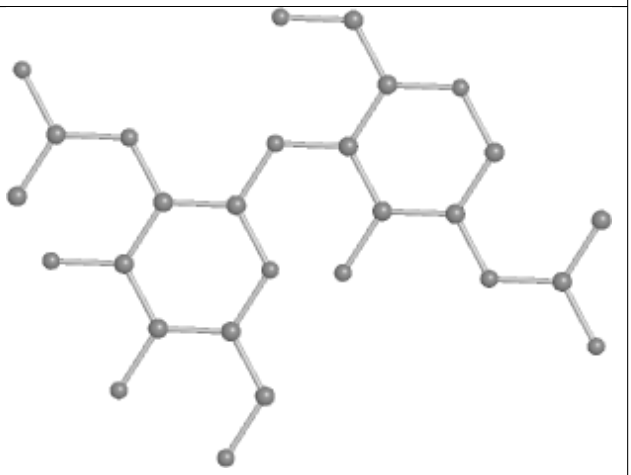
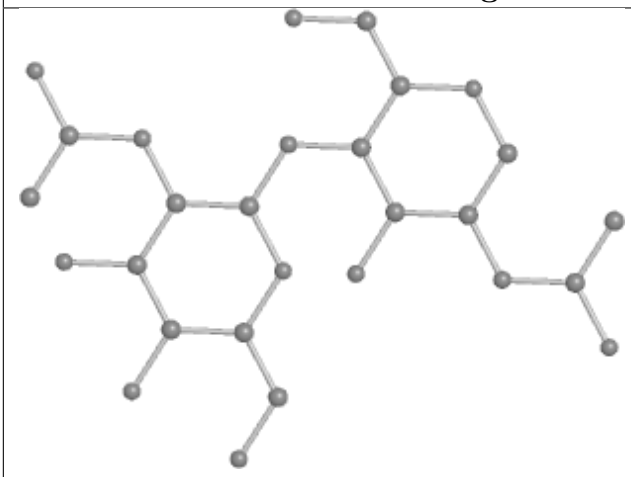


Torsions



Rings

Oligosaccharide Chain QA



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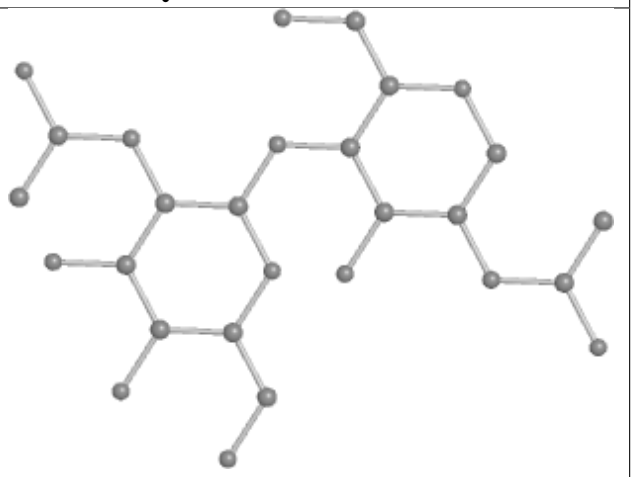
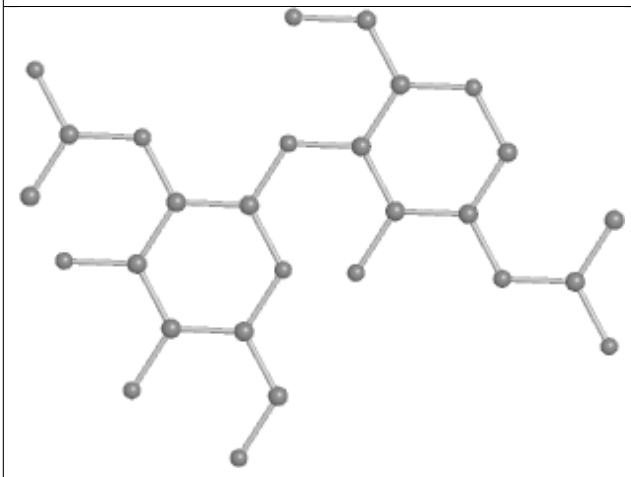


Bond angles



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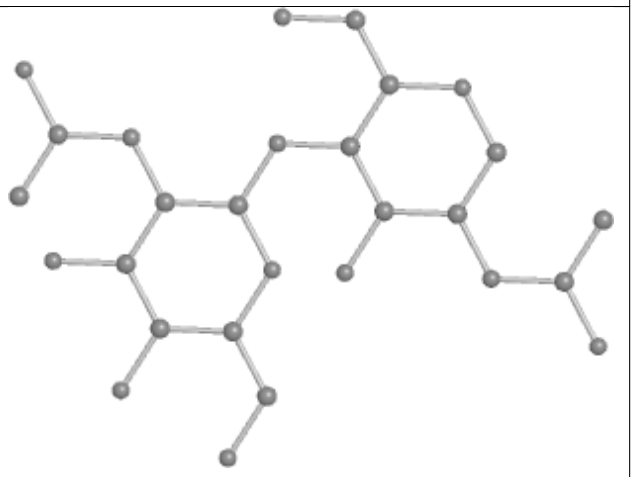
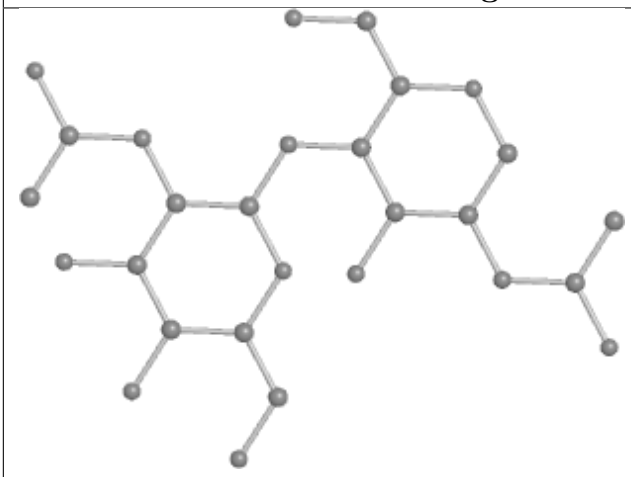


Rings

Oligosaccharide Chain RA



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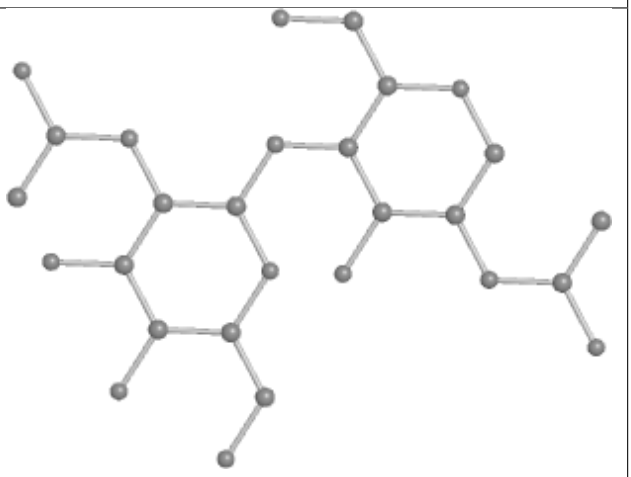
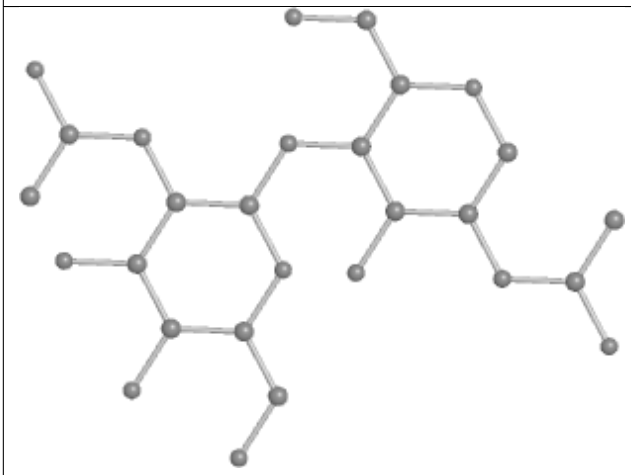


Bond angles



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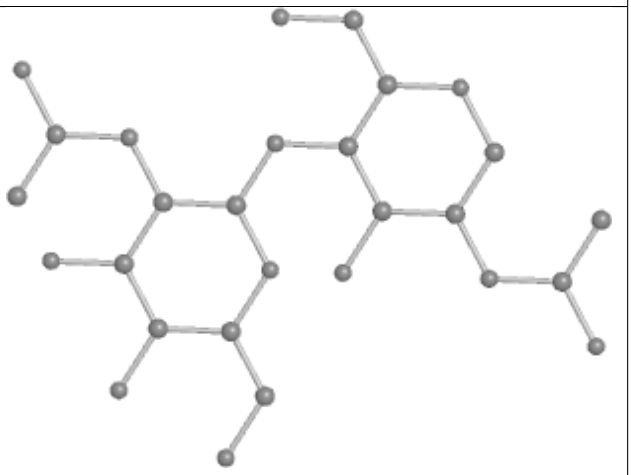
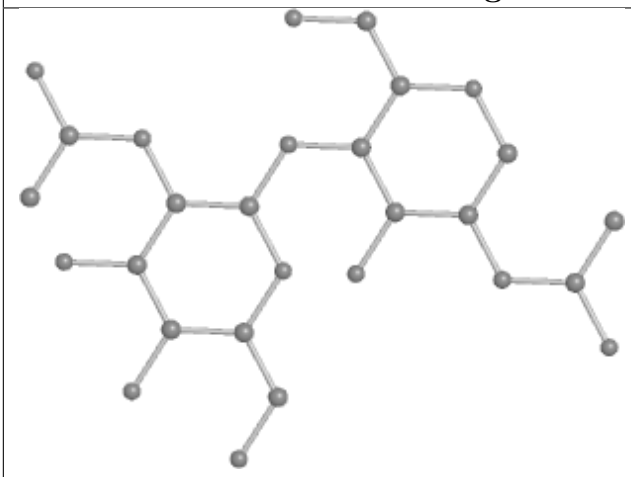


Rings

Oligosaccharide Chain SA



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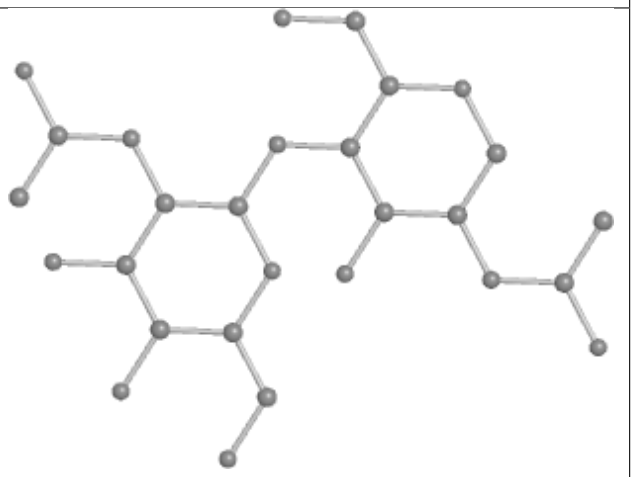
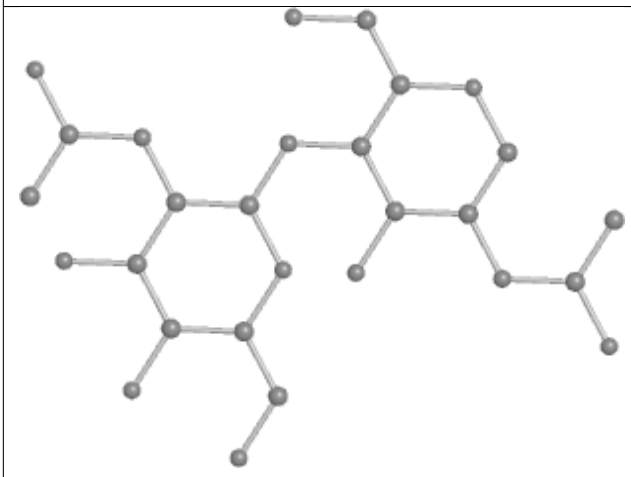


Bond angles



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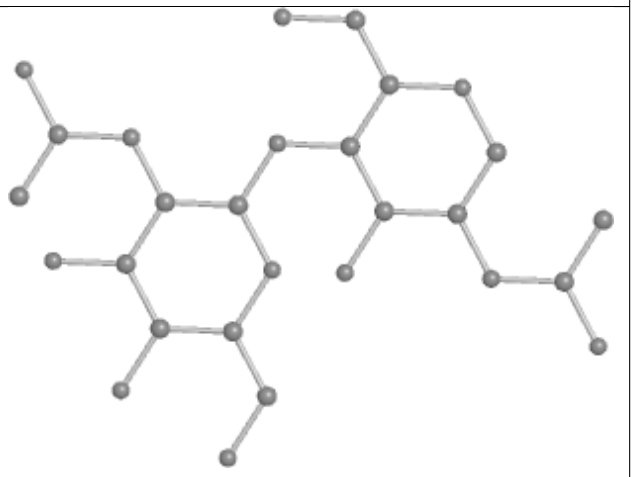
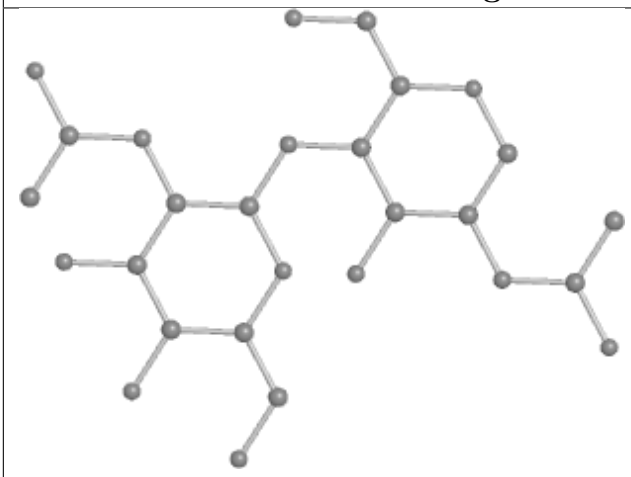


Rings

Oligosaccharide Chain TA



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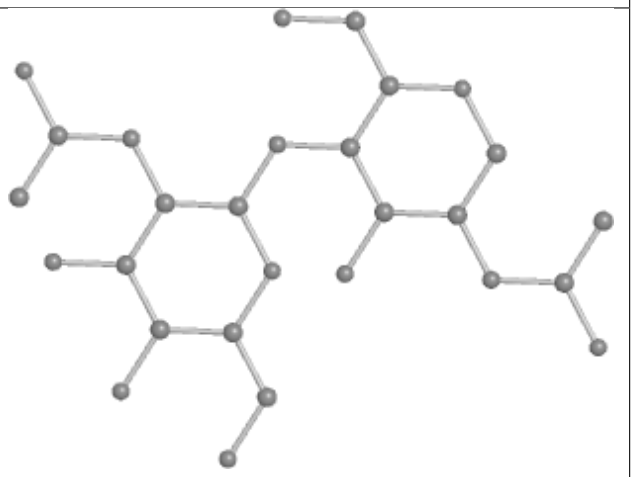

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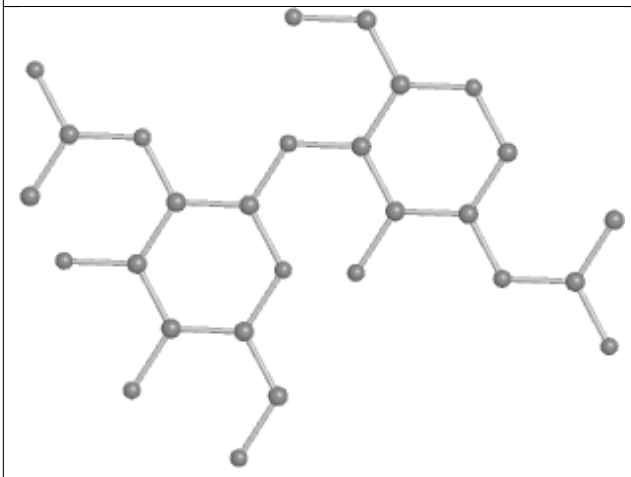

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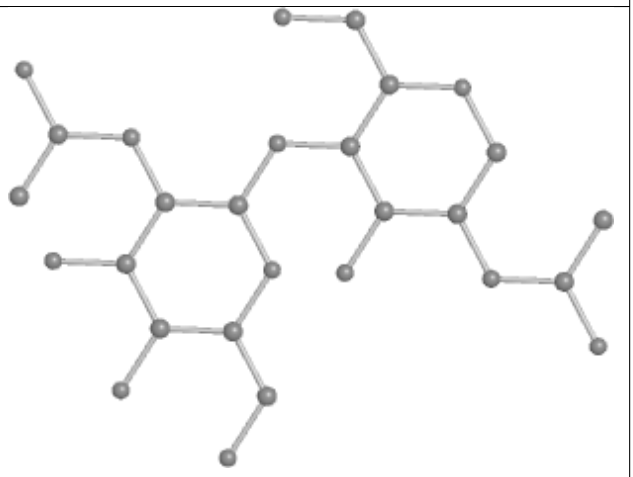
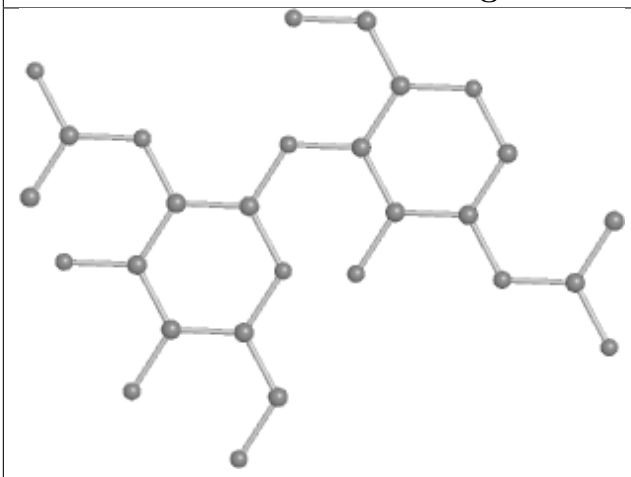


Rings

Oligosaccharide Chain UA



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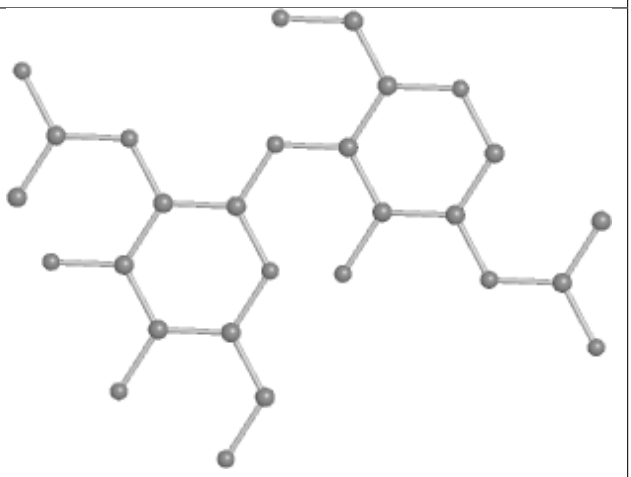
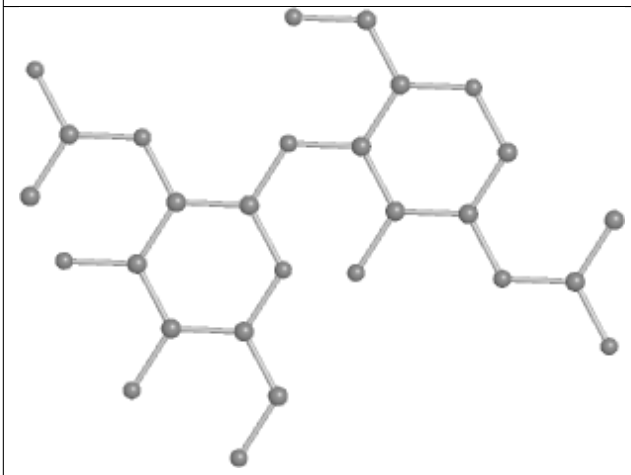


Bond angles



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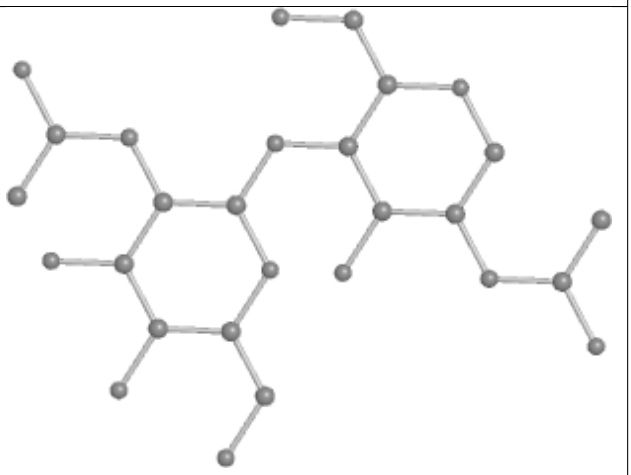
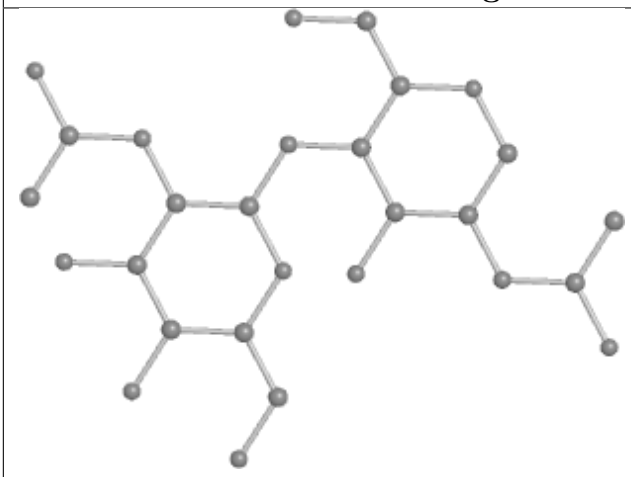


Rings

Oligosaccharide Chain VA



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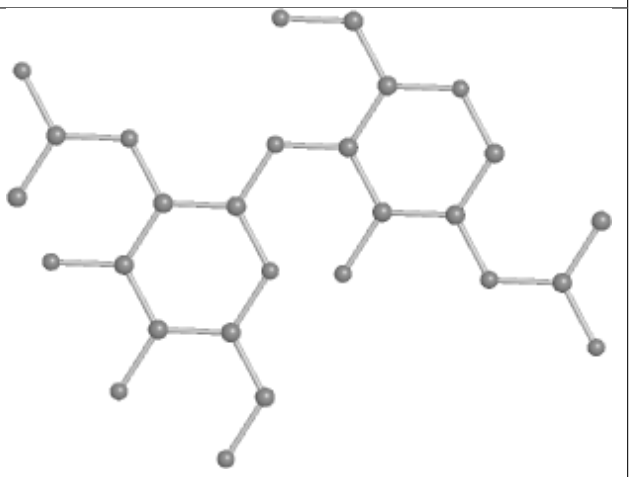
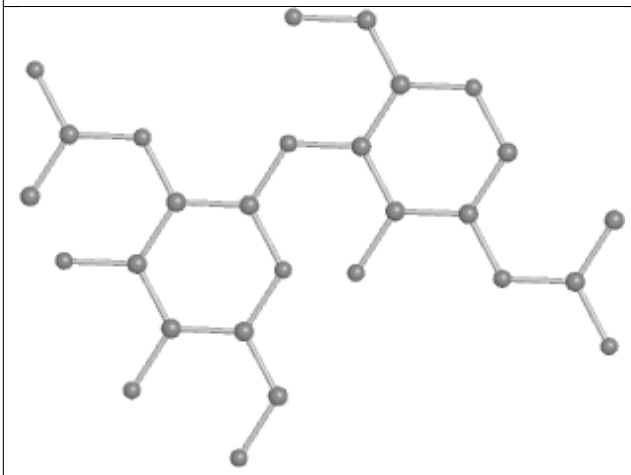


Bond angles



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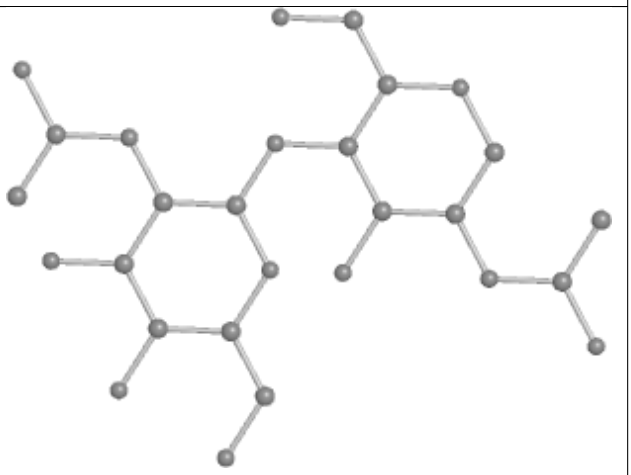
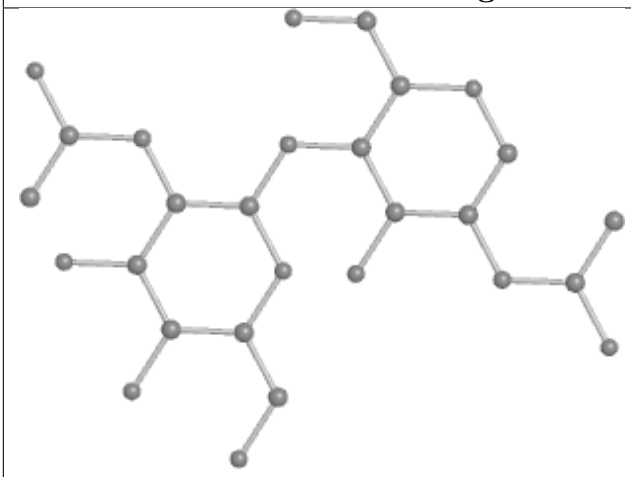


Rings

Oligosaccharide Chain WA



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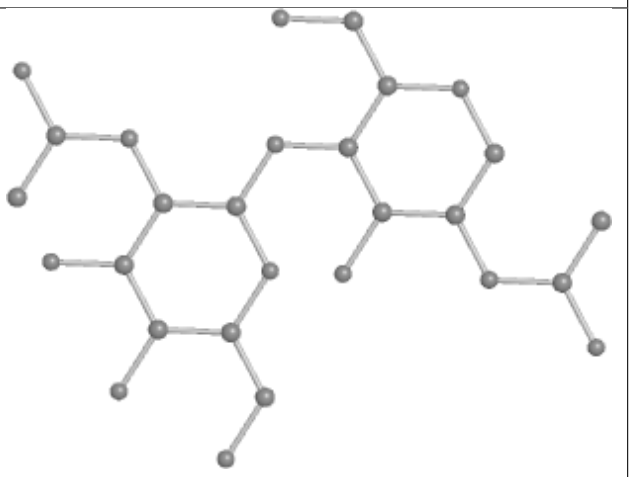
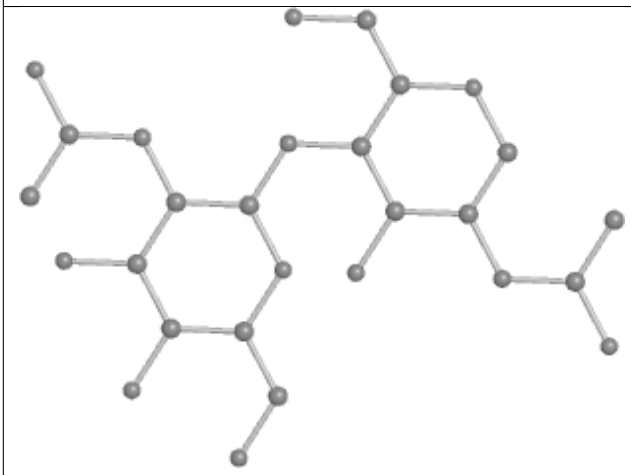


Bond angles



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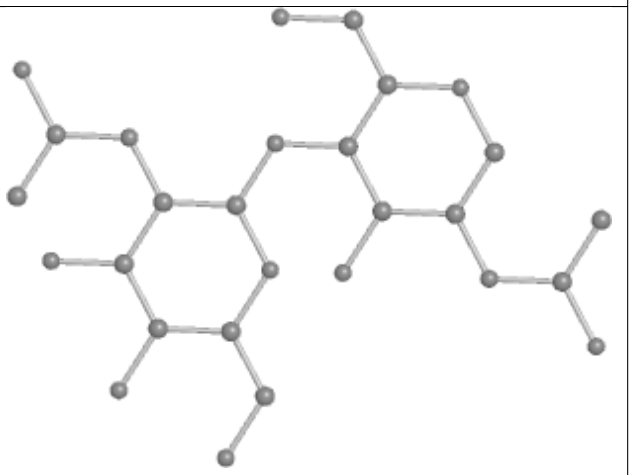
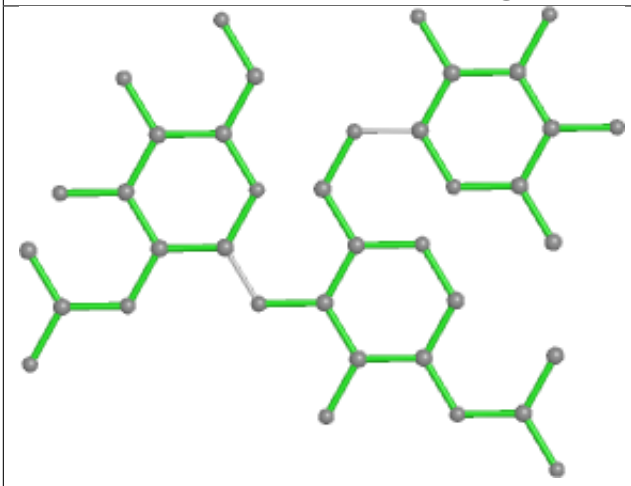


Rings

Oligosaccharide Chain S



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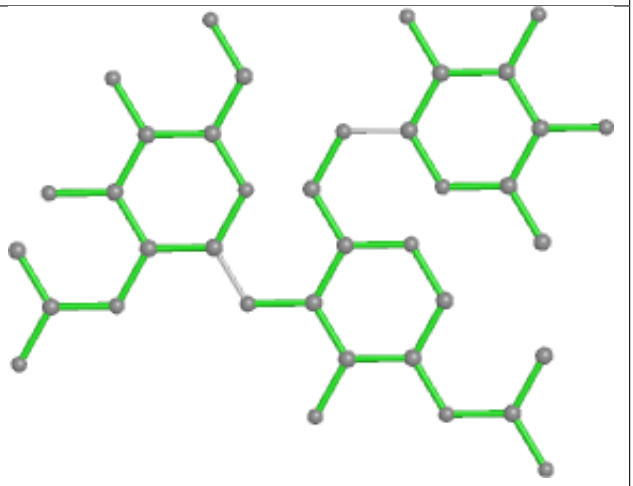
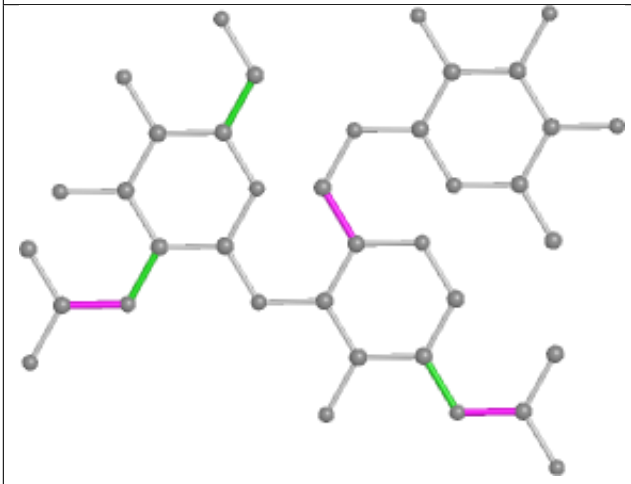


Bond angles



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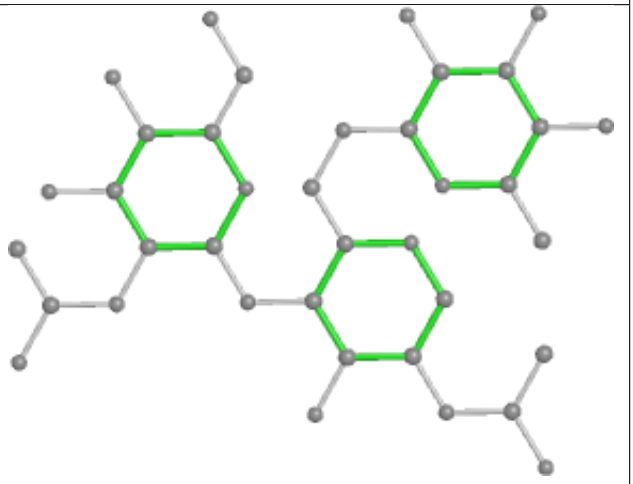
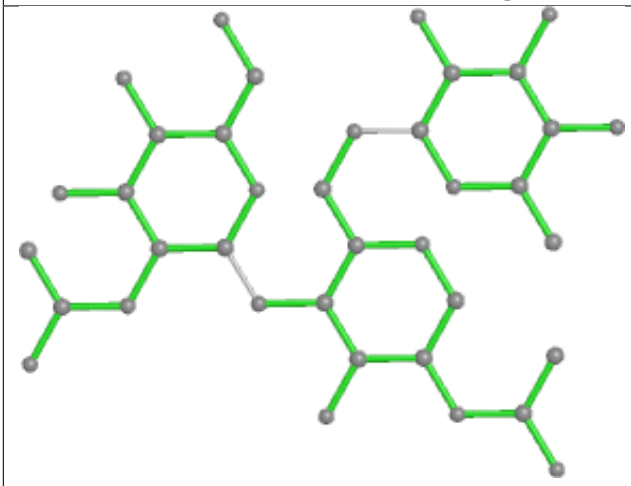


Rings

Oligosaccharide Chain 6



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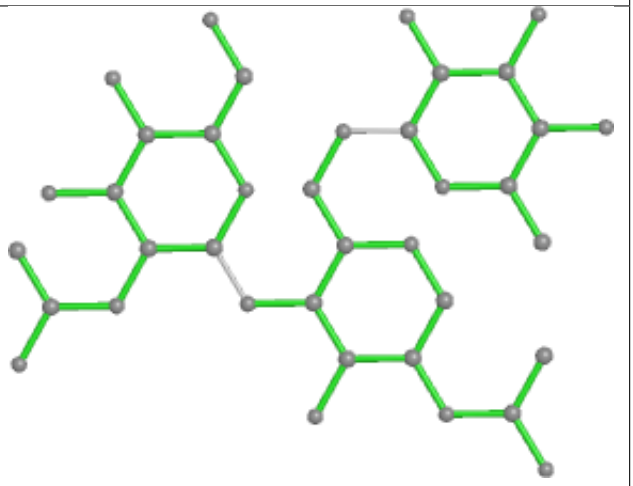
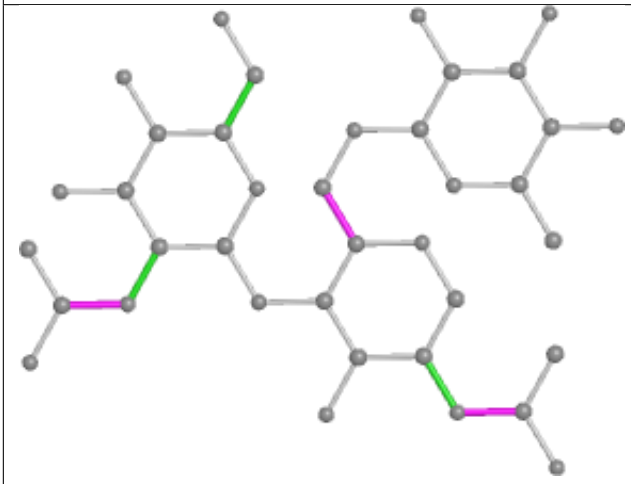
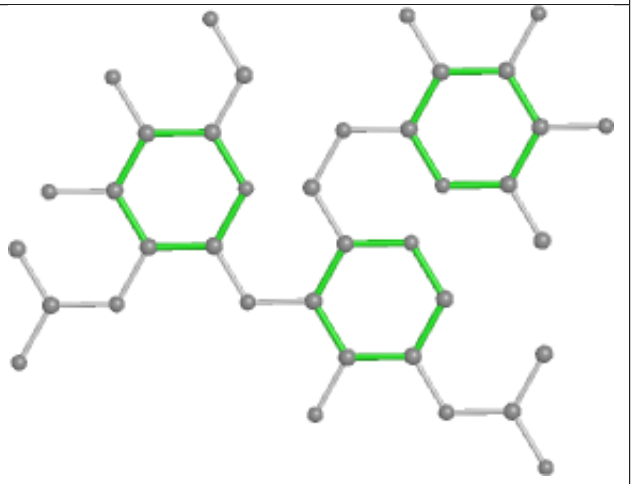


Bond angles

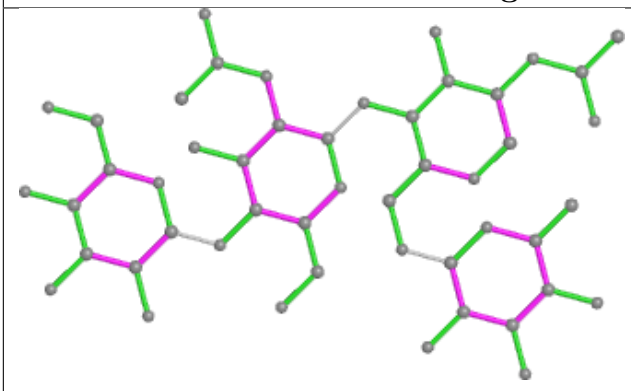


Torsions



Rings

Oligosaccharide Chain t



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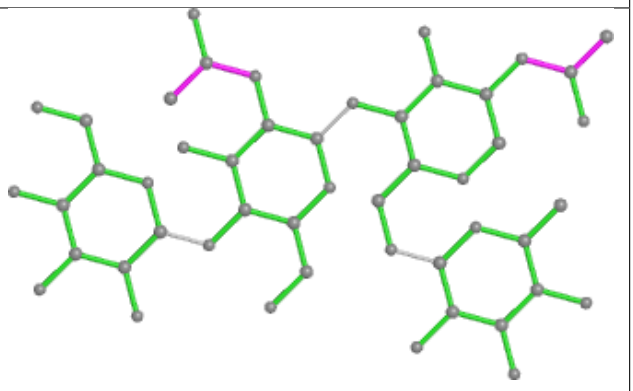
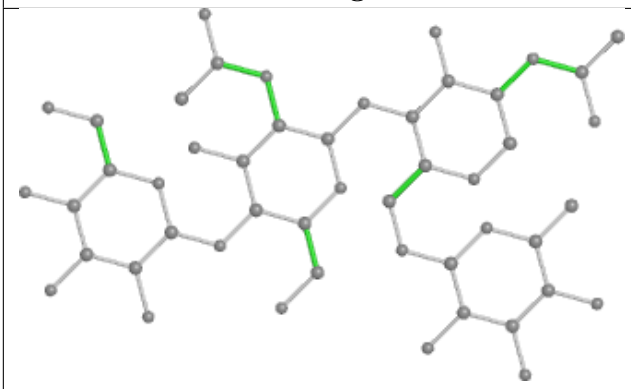
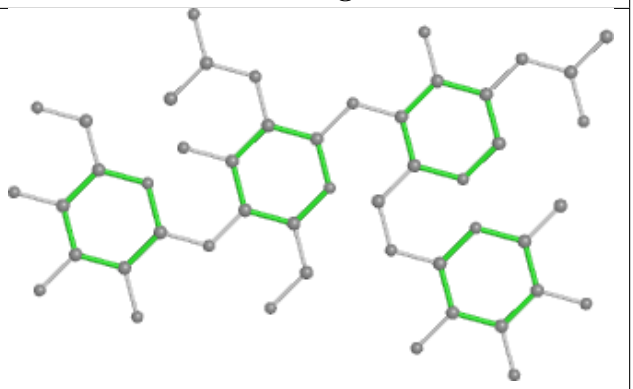


Bond angles

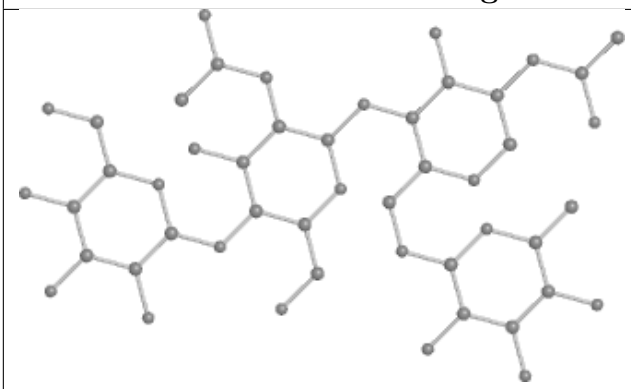


Torsions

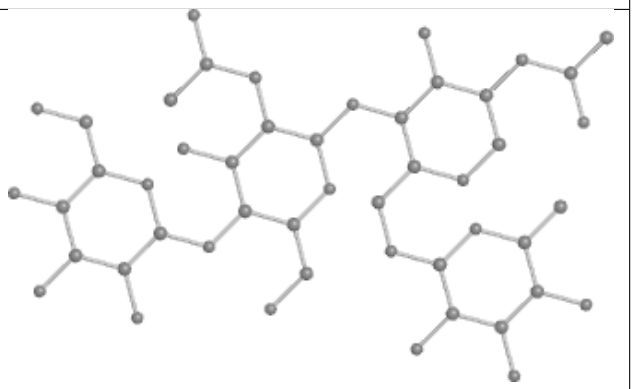


Rings

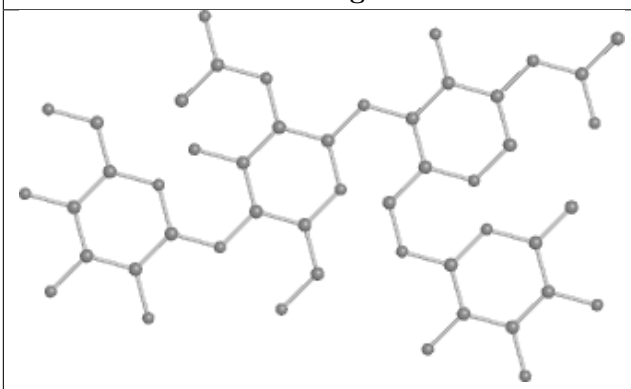
Oligosaccharide Chain XA



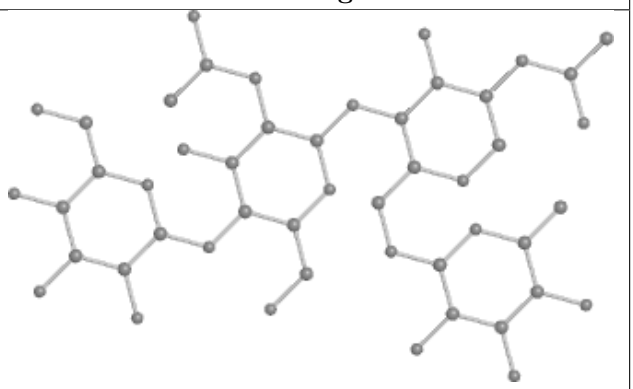
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
5	NAG	C	1301	1	14,14,15	2.10	5 (35%)	17,19,21	0.87	0
5	NAG	C	1302	1	14,14,15	2.06	5 (35%)	17,19,21	6.70	2 (11%)
5	NAG	F	1303	1	14,14,15	1.99	5 (35%)	17,19,21	1.01	2 (11%)
5	NAG	D	1302	1	14,14,15	2.10	6 (42%)	17,19,21	1.01	1 (5%)
5	NAG	F	1302	1	14,14,15	2.06	5 (35%)	17,19,21	6.70	2 (11%)
5	NAG	A	1302	1	14,14,15	2.10	6 (42%)	17,19,21	1.01	1 (5%)
5	NAG	A	1303	1	14,14,15	2.26	5 (35%)	17,19,21	0.94	1 (5%)
5	NAG	B	1301	1	14,14,15	2.13	6 (42%)	17,19,21	0.99	1 (5%)
5	NAG	E	1301	1	14,14,15	2.13	6 (42%)	17,19,21	0.99	1 (5%)
5	NAG	D	1303	1	14,14,15	2.26	5 (35%)	17,19,21	0.94	1 (5%)
5	NAG	A	1301	1	14,14,15	1.96	6 (42%)	17,19,21	6.63	2 (11%)
5	NAG	D	1301	1	14,14,15	1.96	6 (42%)	17,19,21	6.63	2 (11%)
5	NAG	B	1302	1	14,14,15	2.13	5 (35%)	17,19,21	1.02	1 (5%)
5	NAG	F	1301	1	14,14,15	2.10	5 (35%)	17,19,21	0.87	0
5	NAG	C	1303	1	14,14,15	1.99	5 (35%)	17,19,21	1.01	2 (11%)
5	NAG	E	1302	1	14,14,15	2.13	5 (35%)	17,19,21	1.02	1 (5%)

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
5	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	F	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	F	1302	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	E	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	D	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	F	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1302	1	-	0/6/23/26	0/1/1/1

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1303	NAG	C1-C2	5.71	1.60	1.52
5	D	1303	NAG	C1-C2	5.71	1.60	1.52
5	C	1301	NAG	C1-C2	5.34	1.60	1.52
5	F	1301	NAG	C1-C2	5.34	1.60	1.52
5	B	1302	NAG	C1-C2	5.30	1.60	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1302	NAG	C2-N2-C7	27.31	161.78	122.90
5	F	1302	NAG	C2-N2-C7	27.31	161.78	122.90
5	A	1301	NAG	C2-N2-C7	26.90	161.20	122.90
5	D	1301	NAG	C2-N2-C7	26.90	161.20	122.90
5	A	1301	NAG	C8-C7-N2	3.38	121.82	116.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1301	NAG	O5-C5-C6-O6
5	E	1301	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	F	1301	NAG	O5-C5-C6-O6

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.

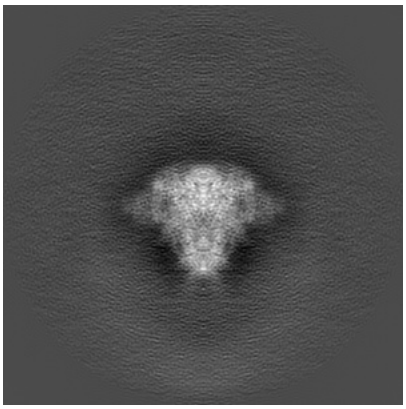
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22354. These allow visual inspection of the internal detail of the map and identification of artifacts.

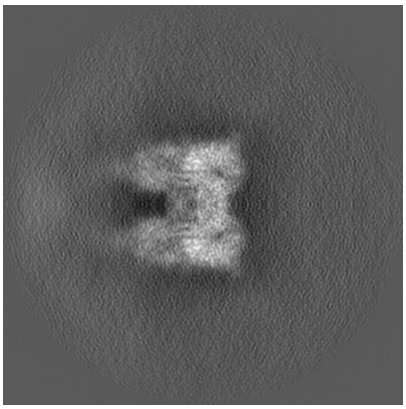
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

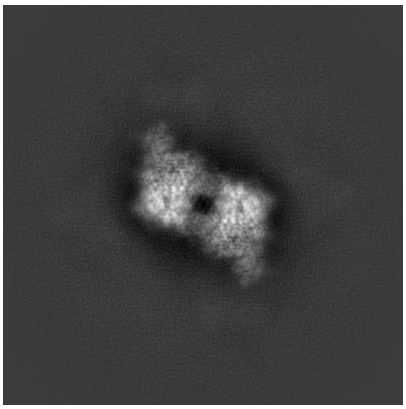
6.1.1 Primary map



X

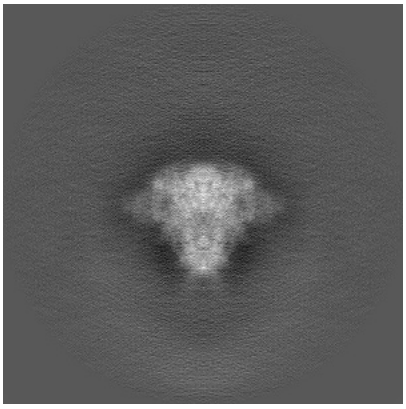


Y

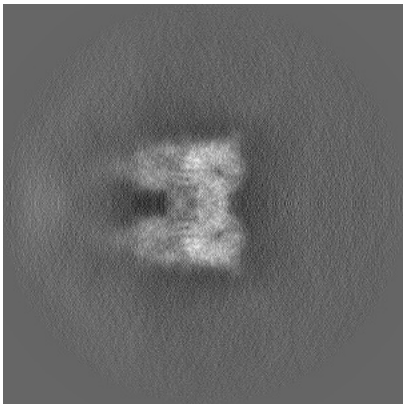


Z

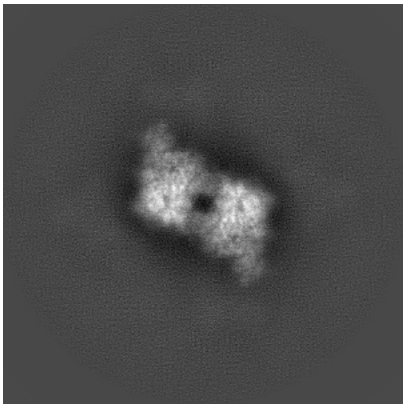
6.1.2 Raw map



X



Y

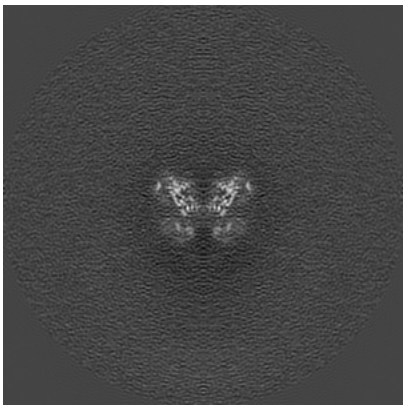


Z

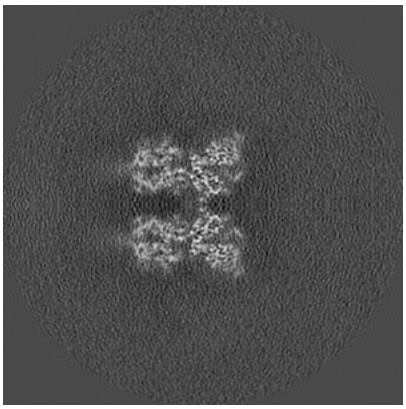
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

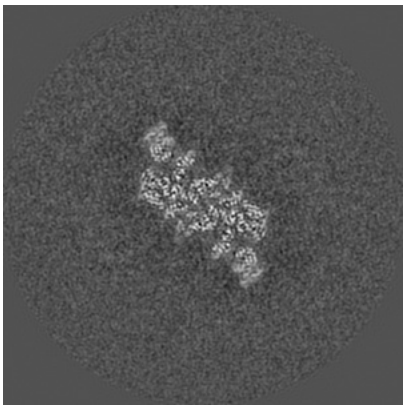
6.2.1 Primary map



X Index: 230

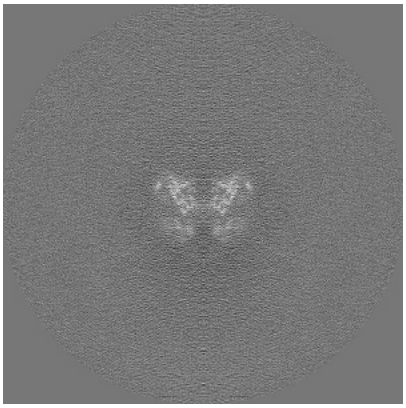


Y Index: 230

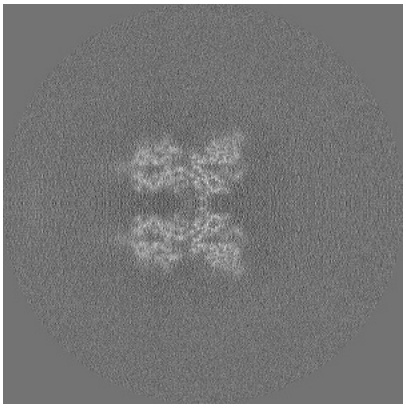


Z Index: 230

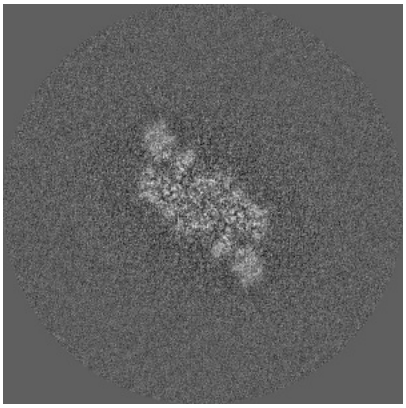
6.2.2 Raw map



X Index: 230



Y Index: 230

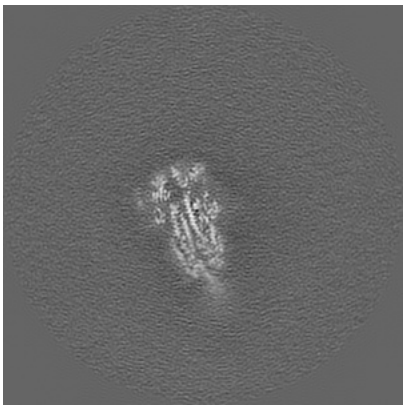


Z Index: 230

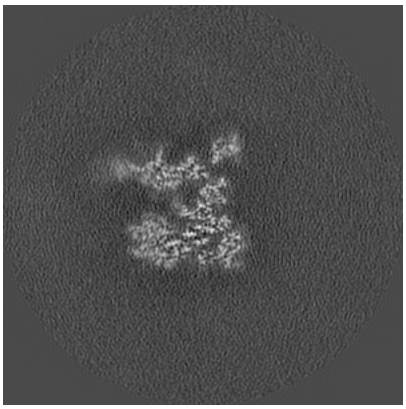
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

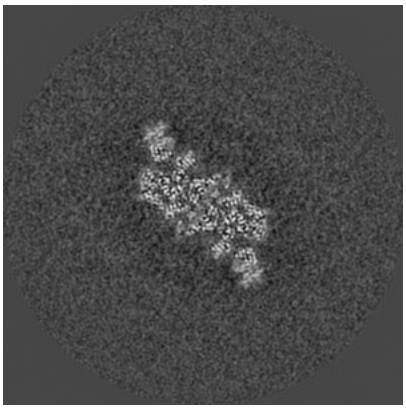
6.3.1 Primary map



X Index: 264

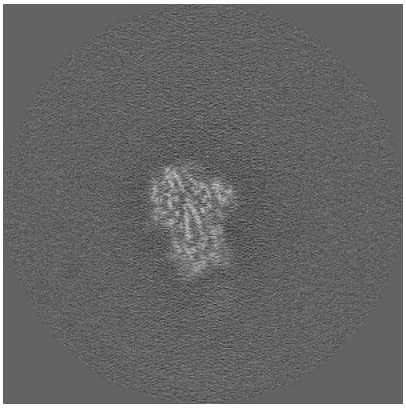


Y Index: 243

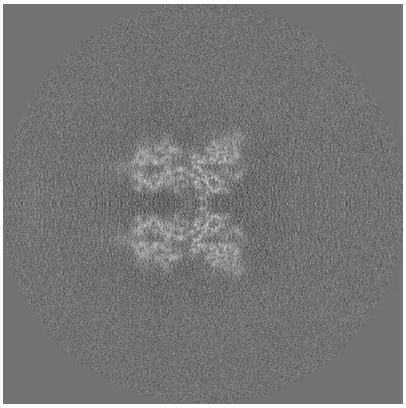


Z Index: 229

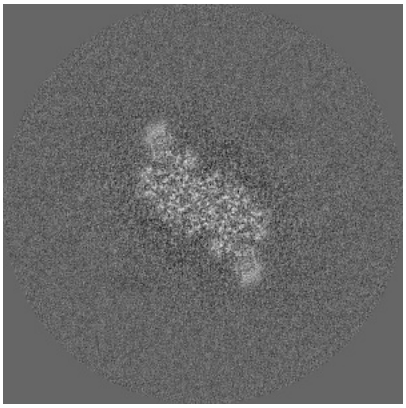
6.3.2 Raw map



X Index: 255



Y Index: 230



Z Index: 227

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

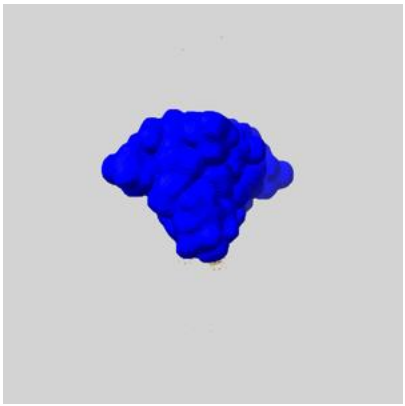
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

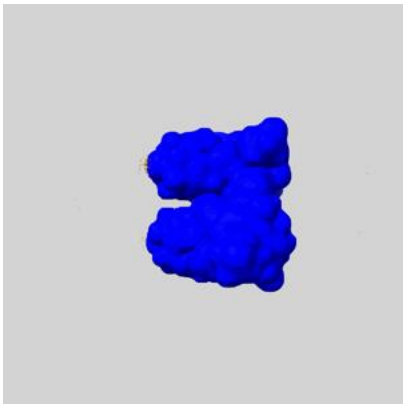
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

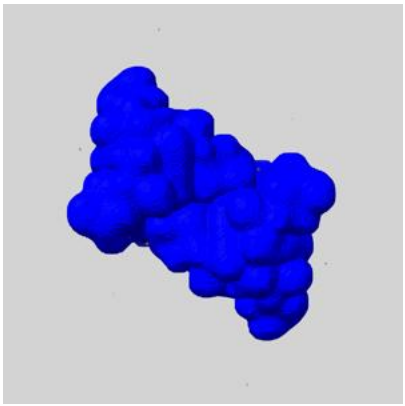
6.5.1 emd_22354_msk_1.map



X



Y

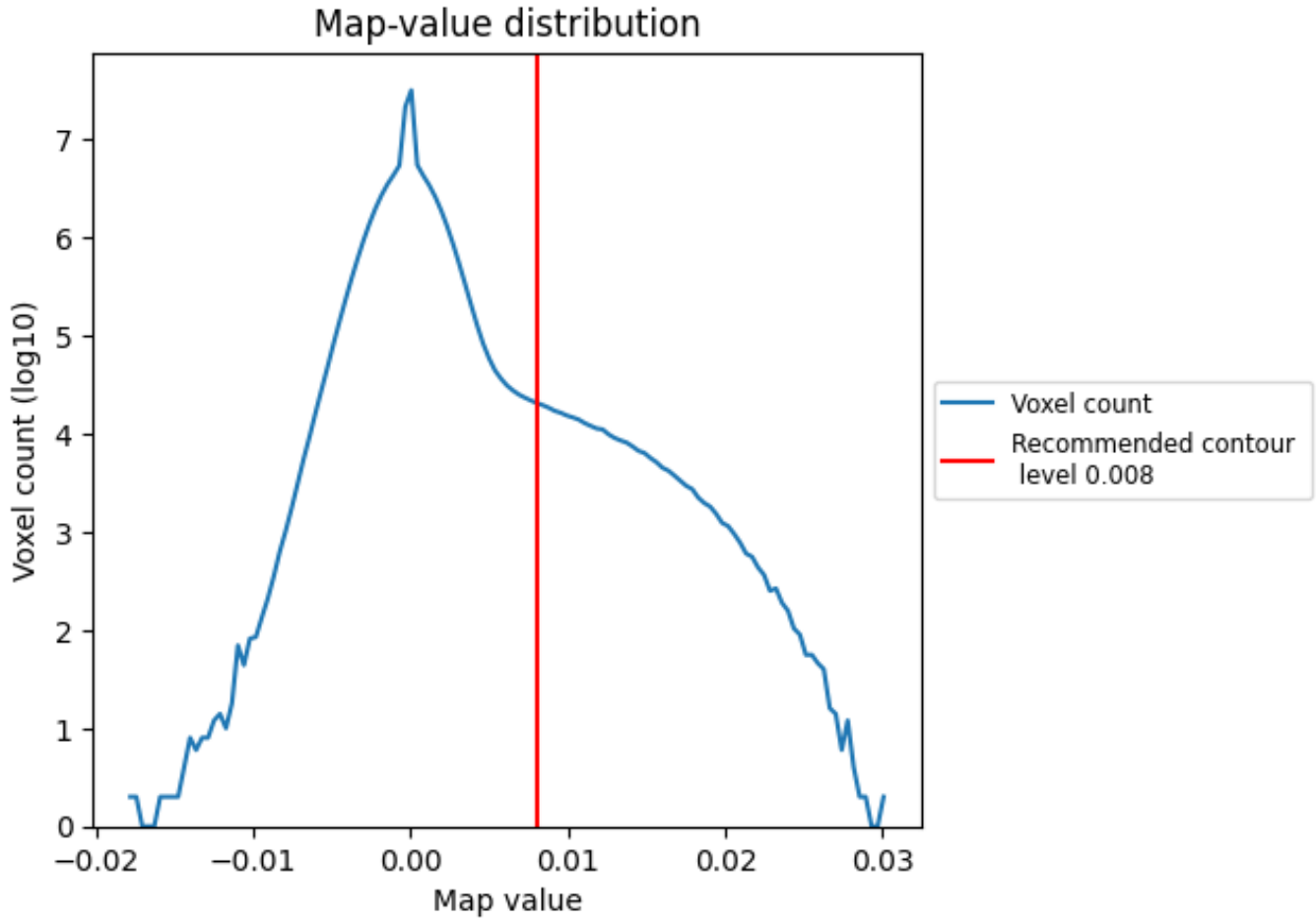


Z

7 Map analysis

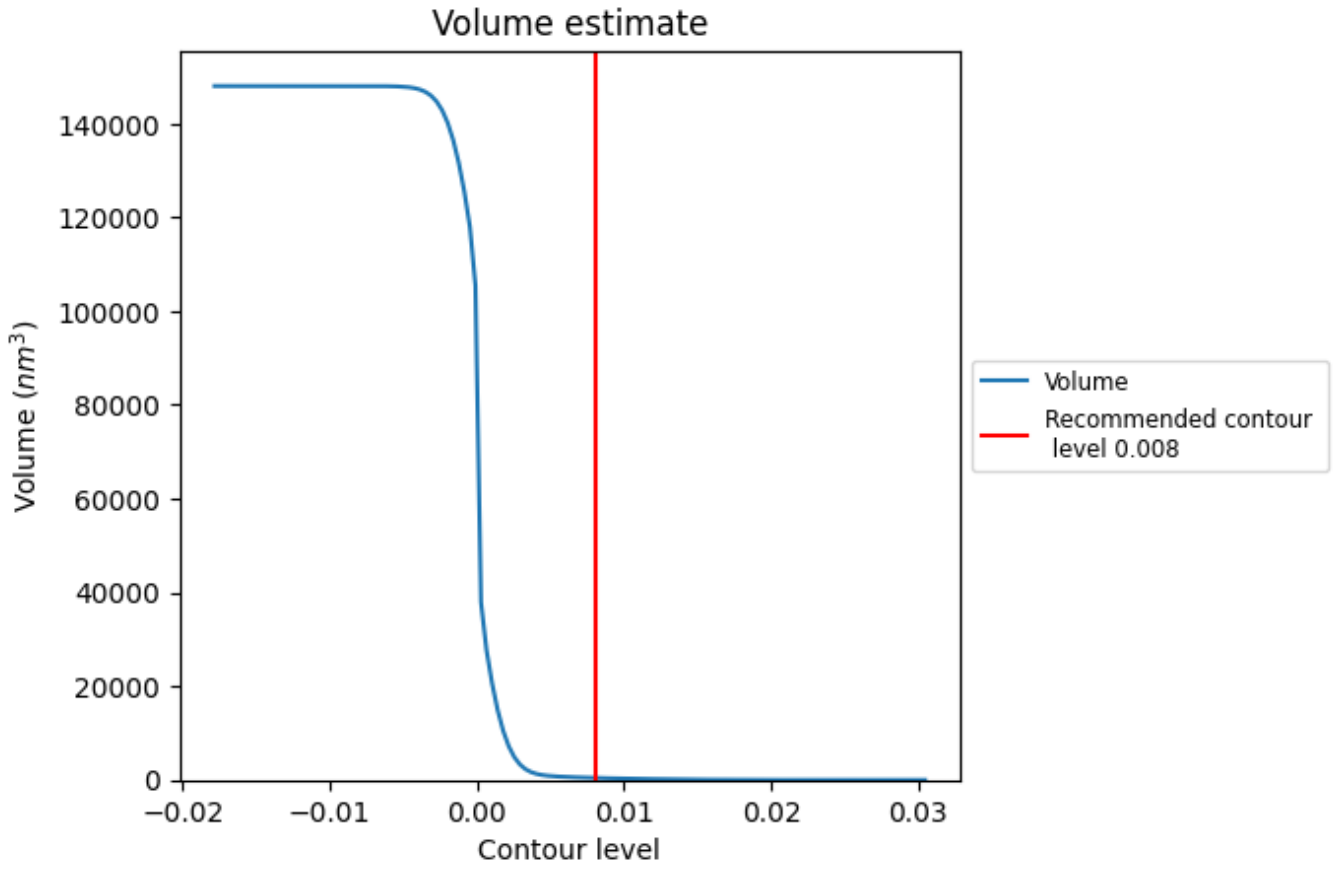
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

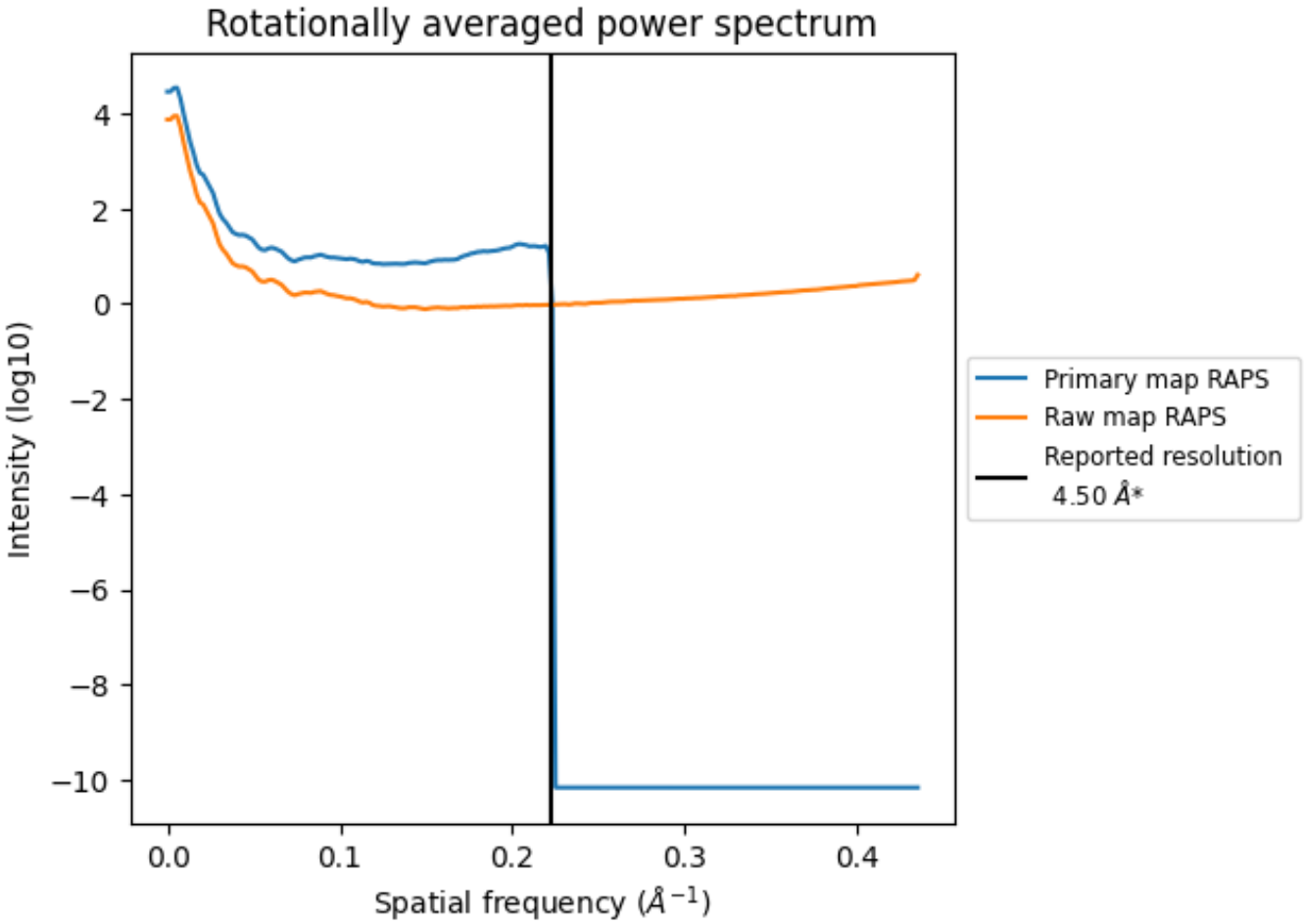
7.2 Volume estimate (i)



The volume at the recommended contour level is 440 nm^3; this corresponds to an approximate mass of 397 kDa.

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

7.3 Rotationally averaged power spectrum (i)

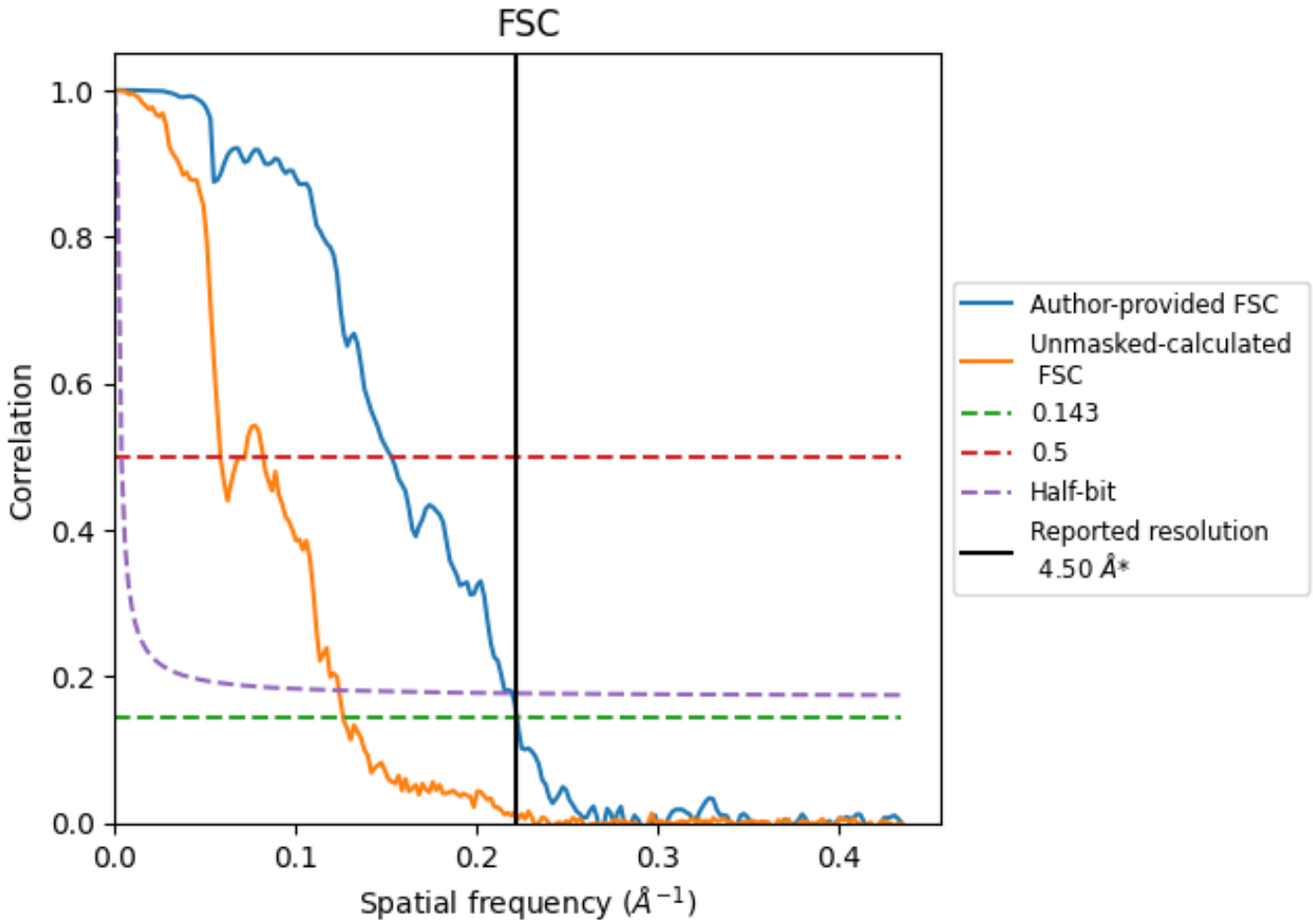


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

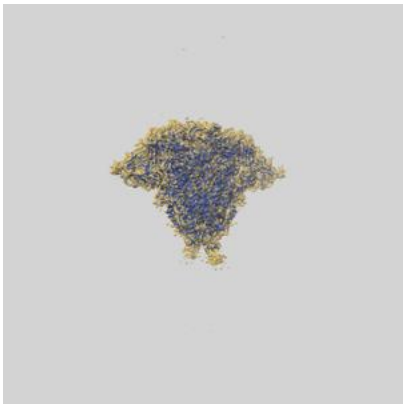
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.54	4.55
Unmasked-calculated*	7.92	17.09	8.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.92 differs from the reported value 4.5 by more than 10 %

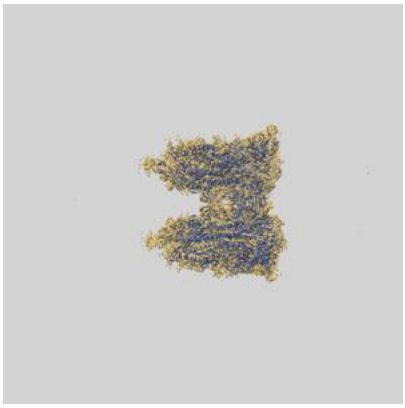
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22354 and PDB model 7JJJ. Per-residue inclusion information can be found in section 3 on page 15.

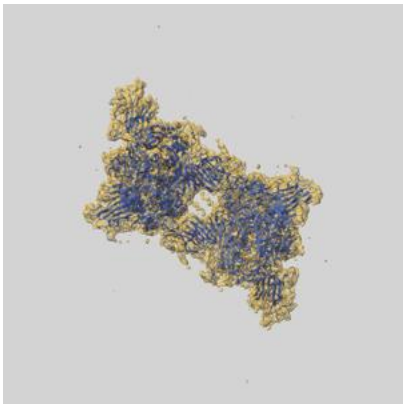
9.1 Map-model overlay



X



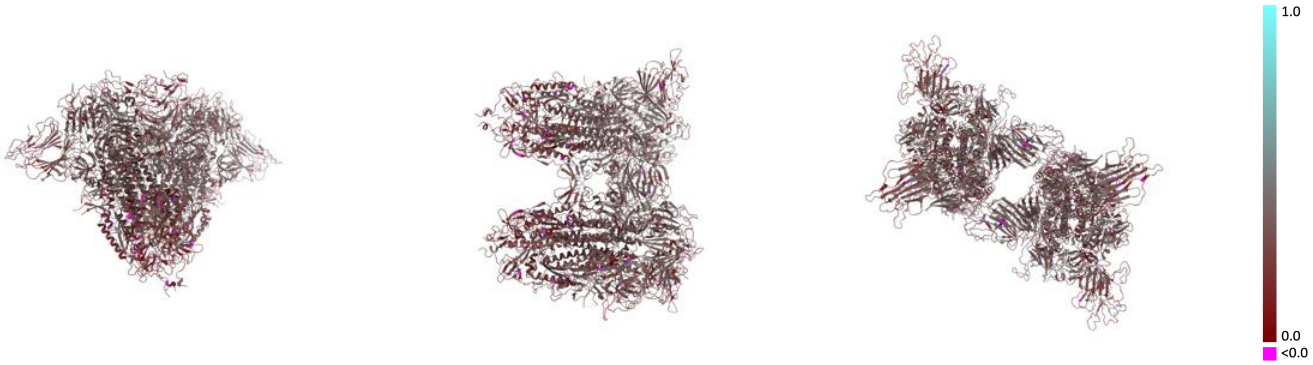
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

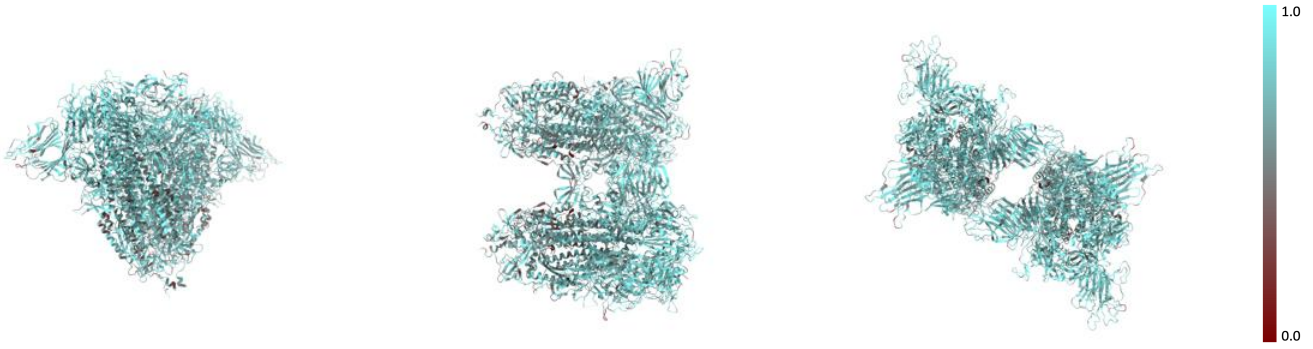
9.2 Q-score mapped to coordinate model



X Y Z

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

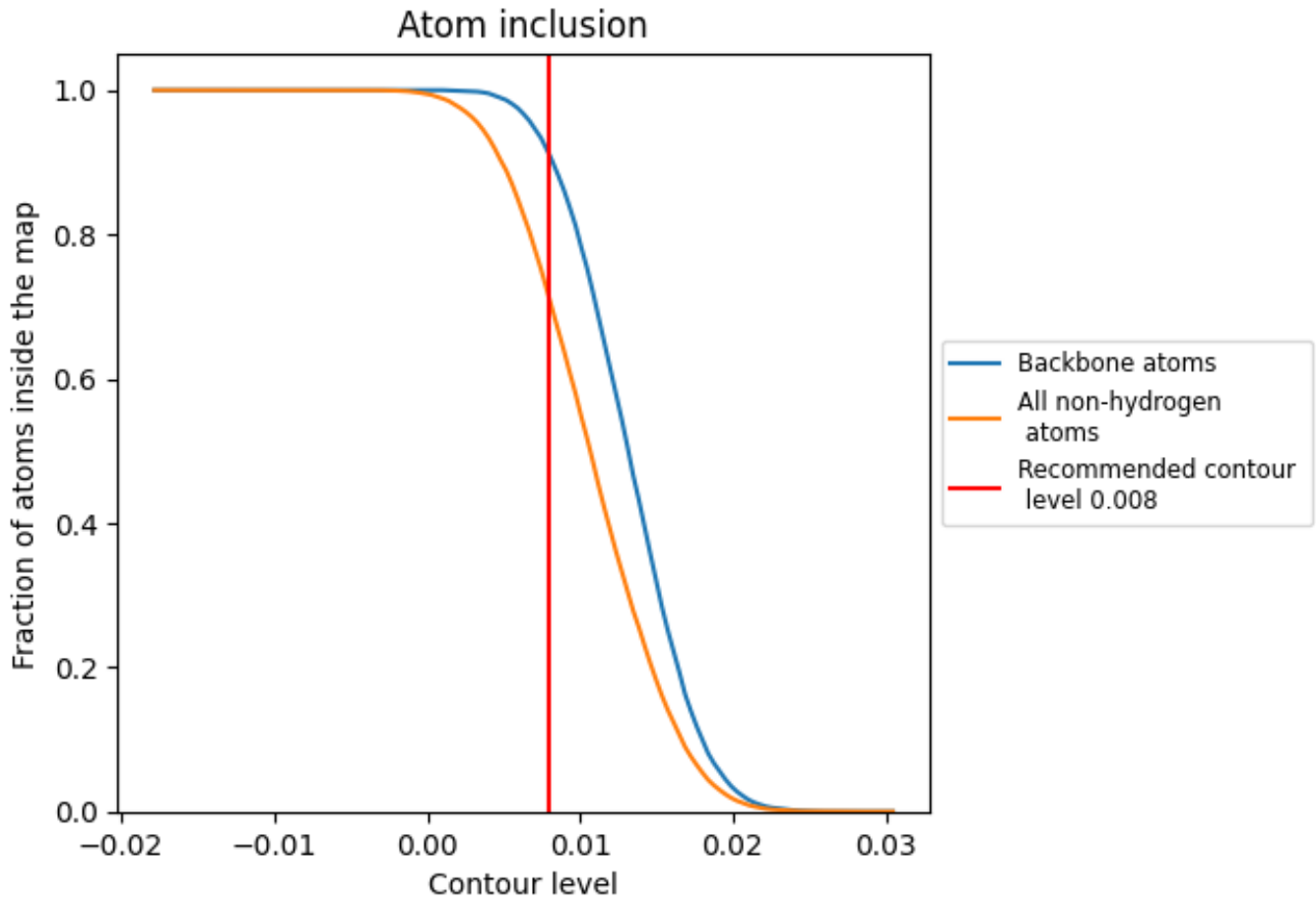
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7104	0.3200
0	0.6429	0.2750
1	0.5357	0.3790
2	0.3571	0.3370
3	0.4286	0.2610
4	0.6429	0.2830
5	0.6429	0.3270
6	0.5000	0.2190
7	0.1786	0.2470
8	0.5714	0.3680
9	0.3214	0.3300
A	0.7263	0.3270
AA	0.3929	0.3050
B	0.7131	0.3110
BA	0.1429	0.1630
C	0.7251	0.3240
CA	0.3571	0.2860
D	0.7263	0.3280
DA	0.3571	0.2380
E	0.7131	0.3100
EA	0.5714	0.3480
F	0.7251	0.3230
FA	0.2500	0.2670
G	0.3929	0.3030
GA	0.7143	0.2740
H	0.4643	0.3080
HA	0.6786	0.3790
I	0.3214	0.2180
IA	0.5714	0.2900
J	0.3929	0.2620
JA	0.5714	0.3220
K	0.3214	0.2850
KA	0.4643	0.2360
L	0.5000	0.2860
LA	0.4643	0.2760

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Chain	Atom inclusion	Q-score
M	0.6429	0.2840
MA	0.0357	0.2080
N	0.5357	0.3940
NA	0.2857	0.2540
O	0.3571	0.3460
OA	0.5357	0.3670
P	0.4286	0.2390
PA	0.2500	0.3730
Q	0.6429	0.2940
QA	0.5714	0.3110
R	0.6429	0.3290
RA	0.2857	0.2880
S	0.5000	0.2410
SA	0.7500	0.3640
T	0.1786	0.2530
TA	0.7143	0.4010
U	0.5714	0.3710
UA	0.6071	0.3140
V	0.3214	0.3480
VA	0.6071	0.3390
W	0.3929	0.2950
WA	0.6786	0.3830
X	0.1429	0.1650
XA	0.3878	0.3570
Y	0.3571	0.2950
Z	0.3571	0.2440
a	0.5714	0.3420
b	0.2500	0.2760
c	0.7143	0.2860
d	0.6786	0.3840
e	0.5714	0.2820
f	0.5714	0.3220
g	0.4643	0.2300
h	0.4643	0.2760
i	0.0357	0.2020
j	0.2857	0.2490
k	0.5357	0.3740
l	0.2500	0.3700
m	0.5714	0.3040
n	0.2857	0.2980
o	0.7500	0.3680
p	0.7143	0.4000

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Chain	Atom inclusion	Q-score
q	0.6071	0.3100
r	0.6071	0.3080
s	0.6786	0.3700
t	0.3878	0.3600
u	0.3929	0.3050
v	0.4643	0.3340
w	0.3214	0.2520
x	0.3929	0.2510
y	0.3214	0.2800
z	0.5000	0.2840