wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID	:	8QX4 / pdb_00008qx4
EMDB ID	:	EMD-18700
Title	:	Sulfolobus acidocaldarius Archaellum filament.
Authors	:	Isupov, M.N.; Gaines, M.; McLaren, M.; Daum, B.
Deposited on	:	2023-10-22
Resolution	:	2.03 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 ⓘ symbol.

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

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

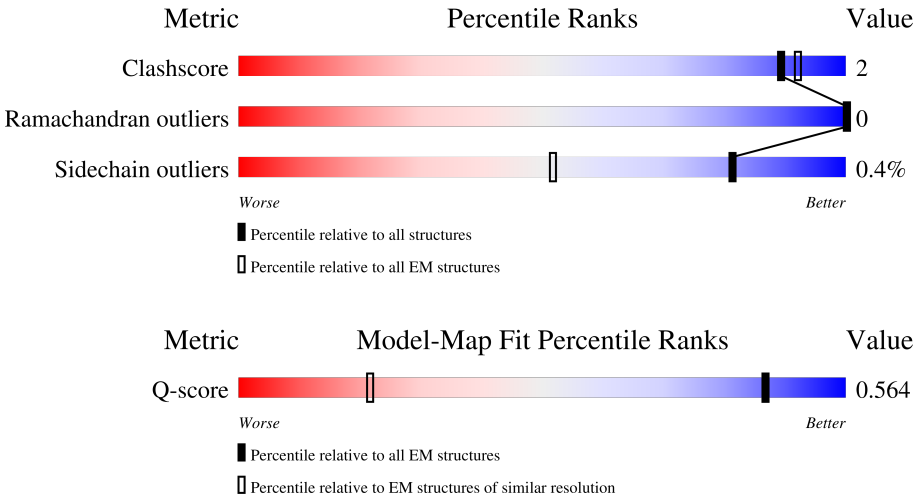
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.03 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1771 (1.55 - 2.53)

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	293	98%
1	B	293	98%
1	C	293	98%
1	D	293	97%

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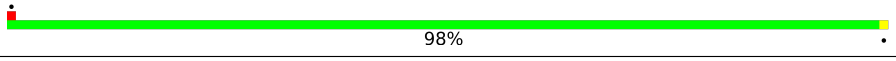
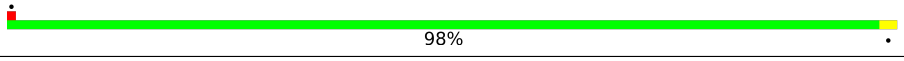
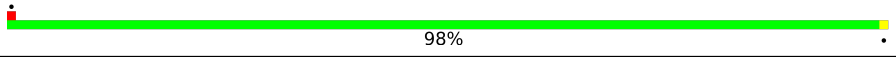
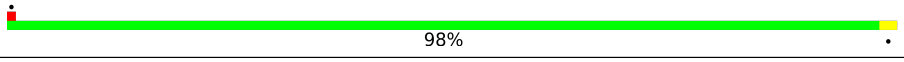
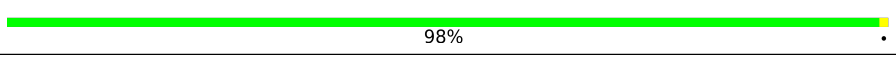
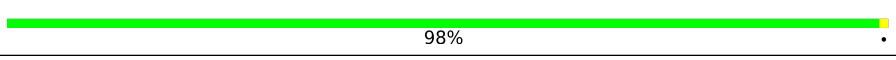
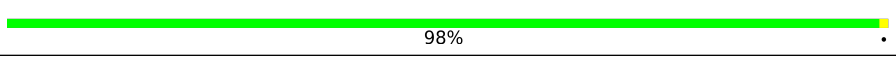
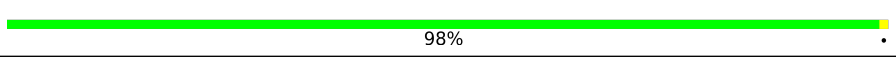
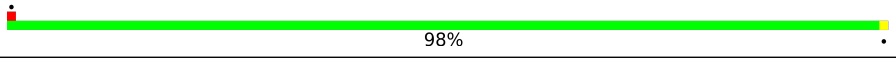
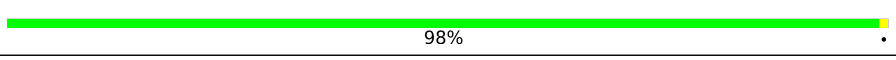
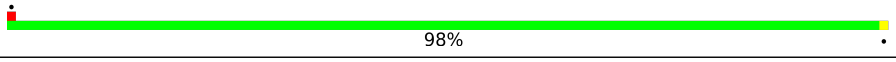
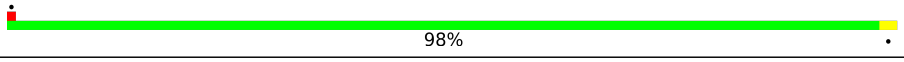
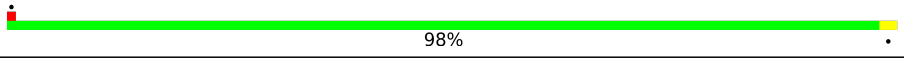
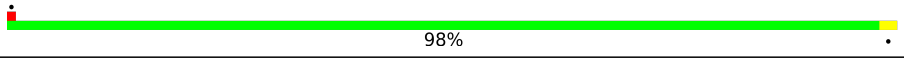
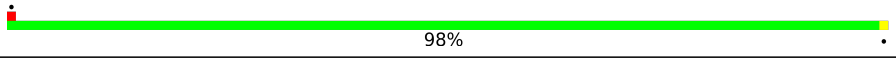
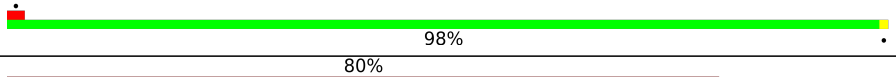
Mol	Chain	Length	Quality of chain
1	E	293	
1	F	293	
1	G	293	
1	H	293	
1	I	293	
1	J	293	
1	K	293	
1	L	293	
1	M	293	
1	N	293	
1	O	293	
1	P	293	
1	Q	293	
1	R	293	
1	S	293	
1	T	293	
2	2A	5	
2	4	5	
2	8A	5	
2	AA	5	
2	EB	5	
2	GA	5	
2	KB	5	
2	MA	5	
2	SA	5	

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Mol	Chain	Length	Quality of chain
2	U	5	80% 20% 80%
2	YA	5	80% 20% 80%
2	a	5	80% 20% 80%
2	eA	5	80% 60% 40%
2	g	5	80% 20% 80%
2	kA	5	80% 20% 80%
2	m	5	80% 60% 40%
2	qA	5	80% 20% 80%
2	s	5	80% 20% 80%
2	wA	5	80% 20% 80%
2	y	5	80% 20% 80%
3	0	6	83% 17% 50% 33%
3	0A	6	67% 67% 33%
3	1A	6	50% 17% 50% 33%
3	2	6	67% 67% 33%
3	3	6	50% 17% 50% 33%
3	3A	6	50% 33% 50% 17%
3	4A	6	83% 17% 50% 33%
3	5	6	50% 33% 50% 17%
3	6	6	83% 17% 50% 33%
3	6A	6	67% 67% 33%
3	7A	6	50% 17% 50% 33%
3	8	6	67% 67% 33%
3	9	6	50% 17% 50% 33%
3	9A	6	50% 33% 50% 17%

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Mol	Chain	Length	Quality of chain
3	AB	6	83% 17% 50% 33%
3	BA	6	50% 33% 50% 17%
3	CA	6	83% 17% 50% 33%
3	CB	6	83% 67% 33%
3	DB	6	50% 17% 50% 33%
3	EA	6	67% 67% 33%
3	FA	6	50% 17% 50% 33%
3	FB	6	50% 33% 50% 17%
3	GB	6	83% 17% 50% 33%
3	HA	6	50% 33% 50% 17%
3	IA	6	83% 17% 50% 33%
3	IB	6	83% 67% 33%
3	JB	6	50% 17% 50% 33%
3	KA	6	67% 67% 33%
3	LA	6	50% 17% 50% 33%
3	LB	6	50% 33% 50% 17%
3	MB	6	100% 17% 50% 33%
3	NA	6	50% 33% 50% 17%
3	OA	6	83% 17% 50% 33%
3	OB	6	100% 67% 33%
3	PB	6	50% 17% 50% 33%
3	QA	6	67% 67% 33%
3	RA	6	50% 17% 50% 33%
3	TA	6	50% 33% 50% 17%
3	UA	6	83% 17% 50% 33%

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Mol	Chain	Length	Quality of chain
3	V	6	50% 33% 50% 17%
3	W	6	83% 17% 50% 33%
3	WA	6	67% 67% 33%
3	XA	6	50% 17% 50% 33%
3	Y	6	67% 67% 33%
3	Z	6	50% 17% 50% 33%
3	ZA	6	50% 33% 50% 17%
3	aA	6	83% 17% 50% 33%
3	b	6	50% 33% 50% 17%
3	c	6	83% 17% 50% 33%
3	cA	6	67% 67% 33%
3	dA	6	50% 17% 50% 33%
3	e	6	67% 67% 33%
3	f	6	50% 17% 50% 33%
3	fA	6	50% 33% 50% 17%
3	gA	6	83% 17% 50% 33%
3	h	6	50% 33% 50% 17%
3	i	6	83% 17% 50% 33%
3	iA	6	67% 67% 33%
3	jA	6	50% 17% 50% 33%
3	k	6	67% 67% 33%
3	l	6	50% 17% 50% 33%
3	lA	6	50% 33% 50% 17%
3	mA	6	83% 17% 50% 33%
3	n	6	50% 33% 50% 17%

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Mol	Chain	Length	Quality of chain
3	o	6	83% 17% 50% 33%
3	oA	6	67% 67% 33%
3	pA	6	50% 17% 50% 33%
3	q	6	67% 50% 50%
3	r	6	50% 17% 50% 33%
3	rA	6	50% 33% 50% 17%
3	sA	6	83% 17% 50% 33%
3	t	6	50% 33% 50% 17%
3	u	6	83% 17% 50% 33%
3	uA	6	67% 67% 33%
3	vA	6	50% 17% 50% 33%
3	w	6	67% 67% 33%
3	x	6	50% 17% 50% 33%
3	xA	6	50% 33% 50% 17%
3	yA	6	83% 17% 50% 33%
3	z	6	50% 33% 50% 17%
4	1	2	50% 50% 50%
4	5A	2	50% 50% 50%
4	7	2	50% 50% 50%
4	BB	2	50% 50% 50%
4	DA	2	50% 50%
4	HB	2	50% 50% 50%
4	JA	2	50% 50%
4	NB	2	50% 50% 50%
4	PA	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
4	VA	2	50% 50% 50%
4	X	2	50% 50% 50%
4	bA	2	50% 50% 50%
4	d	2	50% 50%
4	hA	2	50% 50% 50%
4	j	2	50% 50%
4	nA	2	50% 50% 50%
4	p	2	50% 50%
4	tA	2	50% 50% 50%
4	v	2	50% 50%
4	zA	2	50% 50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51960 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 Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	A	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	B	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	C	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	D	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	E	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	F	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	G	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	I	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	J	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	K	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	L	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	M	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	N	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	O	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	P	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	Q	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	S	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		
1	T	293	Total	C	N	O	S	0	0
			2206	1430	340	433	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	a	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	g	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	m	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	s	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	y	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	4	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	AA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	GA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	MA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	SA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	YA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	eA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	kA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	qA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	wA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	2A	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	8A	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	EB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	KB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	W	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	Y	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	Z	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	b	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	c	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	e	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	f	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	h	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	i	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	k	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	l	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	n	6	Total	C	N	O	S	0	0
			75	40	2	32	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	o	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	q	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	r	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	t	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	u	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	w	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	x	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	z	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	0	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	2	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	3	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	5	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	6	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	8	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	9	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	BA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	CA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	EA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	FA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	HA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	IA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	KA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	LA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	NA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	OA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	QA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	RA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	TA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	UA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	WA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	XA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	ZA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	aA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	cA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	dA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	fA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	gA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	iA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	jA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	lA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	mA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	oA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	pA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	rA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	sA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	uA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	vA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	xA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	yA	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	0A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	1A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	3A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	4A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	6A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	7A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	9A	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	AB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	CB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	DB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	FB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	GB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	IB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	JB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	MB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	OB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
3	PB	6	Total	C	N	O	S	0	0
			75	40	2	32	1		

- Molecule 4 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
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		
4	v	2	Total	C	N	O	0	0
			28	16	2	10		
4	1	2	Total	C	N	O	0	0
			28	16	2	10		
4	7	2	Total	C	N	O	0	0
			28	16	2	10		
4	DA	2	Total	C	N	O	0	0
			28	16	2	10		
4	JA	2	Total	C	N	O	0	0
			28	16	2	10		
4	PA	2	Total	C	N	O	0	0
			28	16	2	10		
4	VA	2	Total	C	N	O	0	0
			28	16	2	10		
4	bA	2	Total	C	N	O	0	0
			28	16	2	10		
4	hA	2	Total	C	N	O	0	0
			28	16	2	10		

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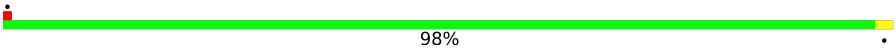
Mol	Chain	Residues	Atoms				AltConf	Trace
4	nA	2	Total	C	N	O	0	0
			28	16	2	10		
4	tA	2	Total	C	N	O	0	0
			28	16	2	10		
4	zA	2	Total	C	N	O	0	0
			28	16	2	10		
4	5A	2	Total	C	N	O	0	0
			28	16	2	10		
4	BB	2	Total	C	N	O	0	0
			28	16	2	10		
4	HB	2	Total	C	N	O	0	0
			28	16	2	10		
4	NB	2	Total	C	N	O	0	0
			28	16	2	10		

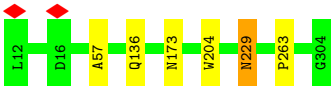
3 Residue-property plots (i)

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: Flagellin

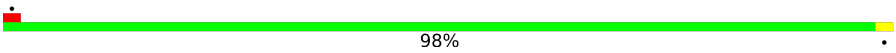
Chain H:

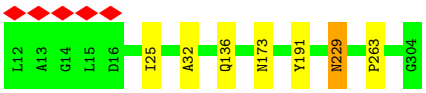




• Molecule 1: Flagellin

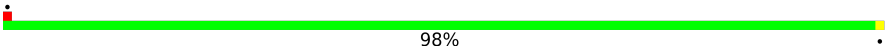
Chain A:





• Molecule 1: Flagellin

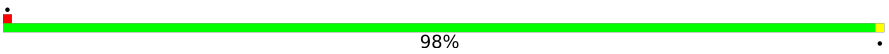
Chain B:





• Molecule 1: Flagellin

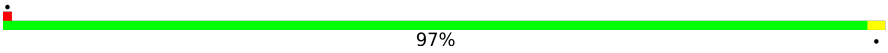
Chain C:

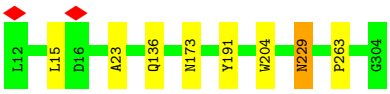




• Molecule 1: Flagellin

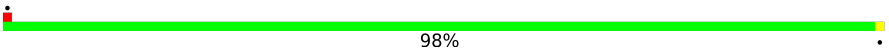
Chain D:





• Molecule 1: Flagellin

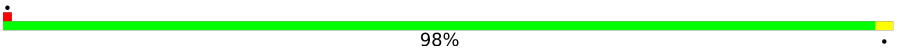
Chain E:





• Molecule 1: Flagellin

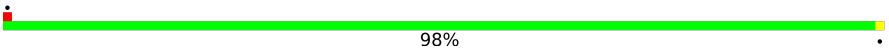
Chain F:





• Molecule 1: Flagellin

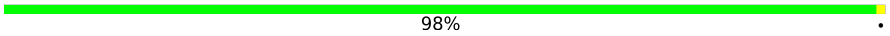
Chain G:

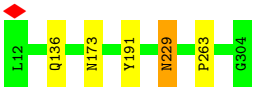




• Molecule 1: Flagellin

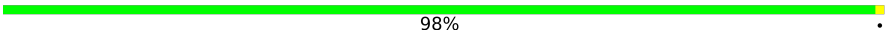
Chain I:

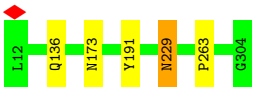




• Molecule 1: Flagellin

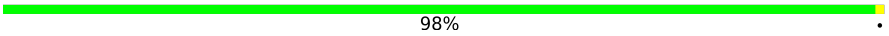
Chain J:

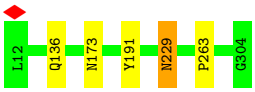




• Molecule 1: Flagellin

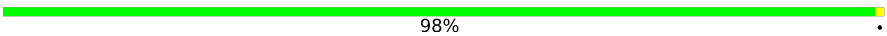
Chain K:





• Molecule 1: Flagellin

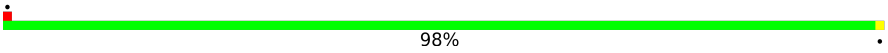
Chain L:

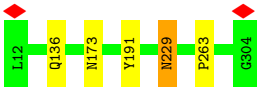




• Molecule 1: Flagellin

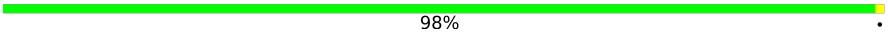
Chain M:

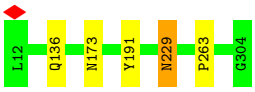




• Molecule 1: Flagellin

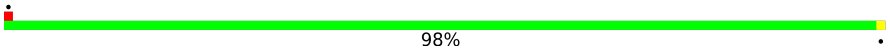
Chain N:





• Molecule 1: Flagellin

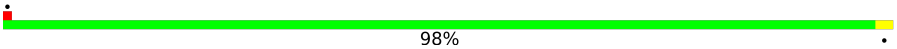
Chain O:





• Molecule 1: Flagellin

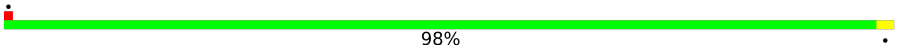
Chain P:





• Molecule 1: Flagellin

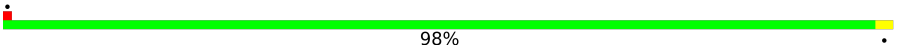
Chain Q:





• Molecule 1: Flagellin

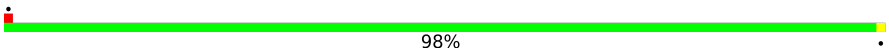
Chain R:





• Molecule 1: Flagellin

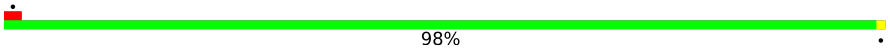
Chain S:

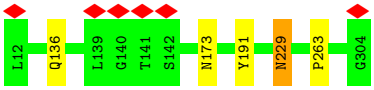




• Molecule 1: Flagellin

Chain T:

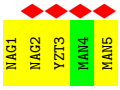




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

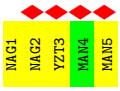




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

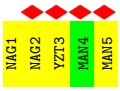




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

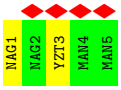




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

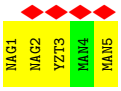




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

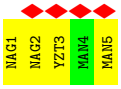




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:

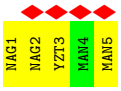




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

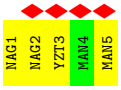




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:

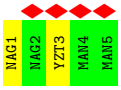




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:

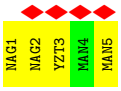




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA:

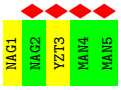




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SA:

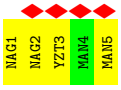




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain YA:

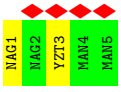




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eA:

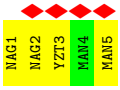




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain kA:

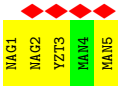




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain qA:

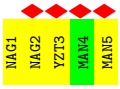




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain wA:

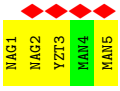




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2A:

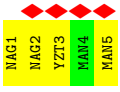




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8A:

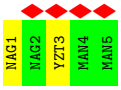




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EB:

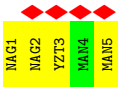




• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KB:

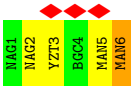




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

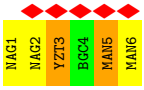




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:





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

Chain Y:

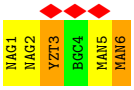




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

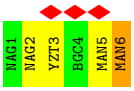




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

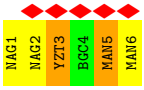




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

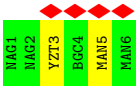




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

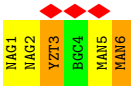




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

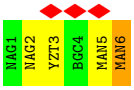




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

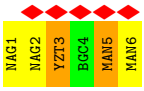




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

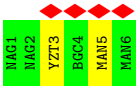




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

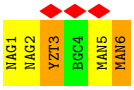




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

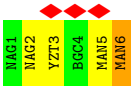




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

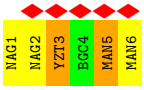




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

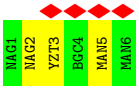




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

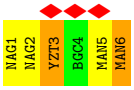




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

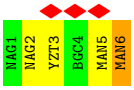




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

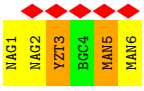




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

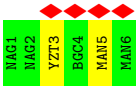




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

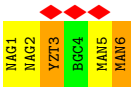




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

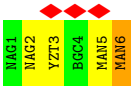




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:

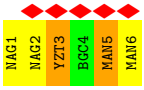




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:





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

Chain 2:

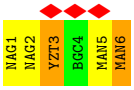




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

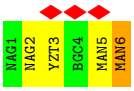
Chain 3:





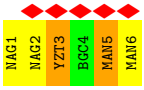
• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5: 



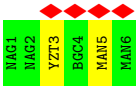
• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6: 



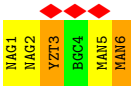
• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8: 



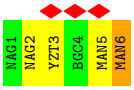
• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9: 



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

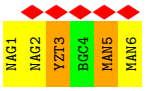
Chain BA: 



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

Chain CA:

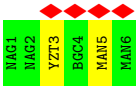




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:

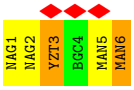




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:

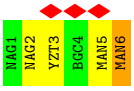




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:

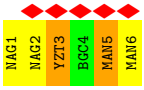




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:

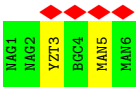




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA:

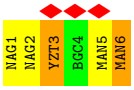




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:

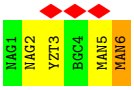




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:

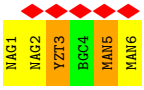




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA:

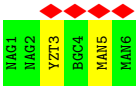




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain QA:

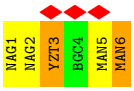




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RA:

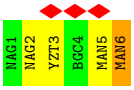




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TA:

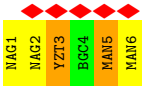




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain UA:





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

Chain WA:

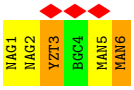




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain XA:

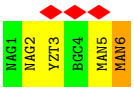




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain ZA:

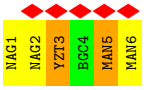




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA:

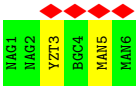




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain cA:

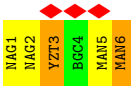




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain dA:

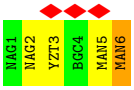




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fA:

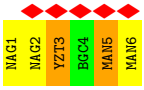




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain gA:

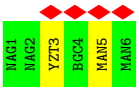




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain iA:

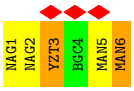




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain jA:

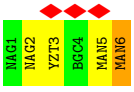




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain lA:

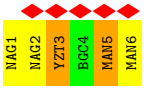




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain mA:

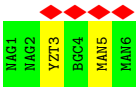




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:

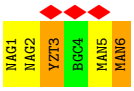




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pA:

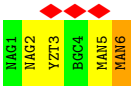




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain rA:

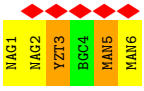




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sA:

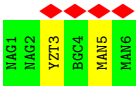




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain uA:

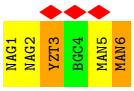




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain vA:

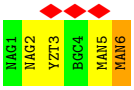




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain xA:

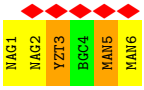




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain yA:

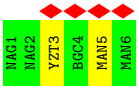




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0A:

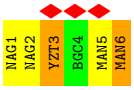




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1A:

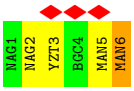




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3A:

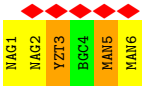




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4A:

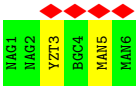




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6A:

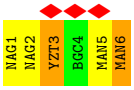




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7A:

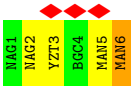




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9A:

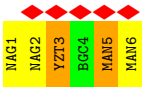




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AB:

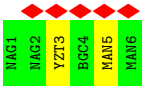




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CB:

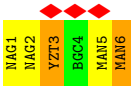




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DB:

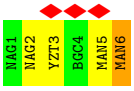




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FB:

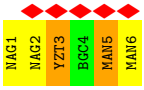




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GB:

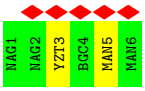




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IB:

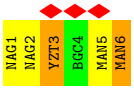




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JB:

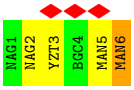




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

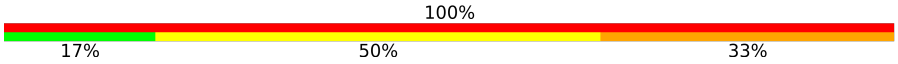
Chain LB:

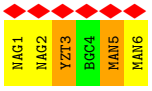




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MB:

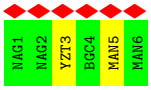




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OB:

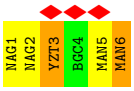




• Molecule 3: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PB:





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

Chain X:





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

Chain d:





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

Chain j:





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

Chain p:





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

Chain v:





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

Chain 1:





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

Chain 7:





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

Chain DA:





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

Chain JA:





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

Chain PA:





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

Chain VA:





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

Chain bA:





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

Chain hA:





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

Chain nA:





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

Chain tA:





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

Chain zA:





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

Chain 5A:





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

Chain BB:





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

Chain HB:





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

Chain NB:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=107.947°, rise=5.433 Å, axial sym=C1	Depositor
Number of segments used	1059736	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	238.752, 238.752, 238.752	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	0/2255	0.98	1/3089 (0.0%)
1	B	0.54	0/2255	0.97	1/3089 (0.0%)
1	C	0.54	0/2255	0.98	1/3089 (0.0%)
1	D	0.54	0/2255	0.97	1/3089 (0.0%)
1	E	0.54	0/2255	0.97	1/3089 (0.0%)
1	F	0.54	0/2255	0.97	1/3089 (0.0%)
1	G	0.54	0/2255	0.97	1/3089 (0.0%)
1	H	0.54	0/2255	0.97	1/3089 (0.0%)
1	I	0.54	0/2255	0.98	1/3089 (0.0%)
1	J	0.54	0/2255	0.97	1/3089 (0.0%)
1	K	0.54	0/2255	0.98	1/3089 (0.0%)
1	L	0.54	0/2255	0.97	1/3089 (0.0%)
1	M	0.54	0/2255	0.98	1/3089 (0.0%)
1	N	0.54	0/2255	0.97	1/3089 (0.0%)
1	O	0.54	0/2255	0.97	1/3089 (0.0%)
1	P	0.54	0/2255	0.97	1/3089 (0.0%)
1	Q	0.54	0/2255	0.97	1/3089 (0.0%)
1	R	0.54	0/2255	0.98	1/3089 (0.0%)
1	S	0.54	0/2255	0.98	1/3089 (0.0%)
1	T	0.54	0/2255	0.98	1/3089 (0.0%)
All	All	0.54	0/45100	0.97	20/61780 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	229	ASN	CB-CA-C	-5.78	101.32	110.86
1	G	229	ASN	CB-CA-C	-5.76	101.36	110.86
1	D	229	ASN	CB-CA-C	-5.75	101.36	110.86
1	J	229	ASN	CB-CA-C	-5.75	101.37	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	229	ASN	CB-CA-C	-5.75	101.37	110.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2206	0	2208	5	0
1	B	2206	0	2208	3	0
1	C	2206	0	2208	3	0
1	D	2206	0	2208	6	0
1	E	2206	0	2208	3	0
1	F	2206	0	2208	5	0
1	G	2206	0	2208	3	0
1	H	2206	0	2208	4	0
1	I	2206	0	2208	3	0
1	J	2206	0	2208	3	0
1	K	2206	0	2208	3	0
1	L	2206	0	2208	3	0
1	M	2206	0	2208	3	0
1	N	2206	0	2208	3	0
1	O	2206	0	2208	3	0
1	P	2206	0	2208	4	0
1	Q	2206	0	2208	4	0
1	R	2206	0	2208	4	0
1	S	2206	0	2208	3	0
1	T	2206	0	2208	3	0
2	2A	64	0	42	1	0
2	4	64	0	42	1	0
2	8A	64	0	42	1	0
2	AA	64	0	42	1	0
2	EB	64	0	42	0	0
2	GA	64	0	42	0	0
2	KB	64	0	42	1	0
2	MA	64	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	SA	64	0	42	0	0
2	U	64	0	42	1	0
2	YA	64	0	42	1	0
2	a	64	0	42	1	0
2	eA	64	0	42	0	0
2	g	64	0	42	1	0
2	kA	64	0	42	1	0
2	m	64	0	42	0	0
2	qA	64	0	42	1	0
2	s	64	0	42	1	0
2	wA	64	0	42	1	0
2	y	64	0	42	1	0
3	0	75	0	52	1	0
3	0A	75	0	52	0	0
3	1A	75	0	52	5	0
3	2	75	0	52	0	0
3	3	75	0	52	5	0
3	3A	75	0	52	2	0
3	4A	75	0	52	1	0
3	5	75	0	52	2	0
3	6	75	0	52	1	0
3	6A	75	0	52	0	0
3	7A	75	0	52	6	0
3	8	75	0	52	0	0
3	9	75	0	52	5	0
3	9A	75	0	52	2	0
3	AB	75	0	52	1	0
3	BA	75	0	52	2	0
3	CA	75	0	52	1	0
3	CB	75	0	52	0	0
3	DB	75	0	52	5	0
3	EA	75	0	52	0	0
3	FA	75	0	52	5	0
3	FB	75	0	52	2	0
3	GB	75	0	52	1	0
3	HA	75	0	52	2	0
3	IA	75	0	52	1	0
3	IB	75	0	52	0	0
3	JB	75	0	52	5	0
3	KA	75	0	52	0	0
3	LA	75	0	52	5	0
3	LB	75	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	MB	75	0	52	1	0
3	NA	75	0	52	2	0
3	OA	75	0	52	1	0
3	OB	75	0	52	0	0
3	PB	75	0	52	5	0
3	QA	75	0	52	0	0
3	RA	75	0	52	5	0
3	TA	75	0	52	2	0
3	UA	75	0	52	1	0
3	V	75	0	52	2	0
3	W	75	0	52	1	0
3	WA	75	0	52	0	0
3	XA	75	0	52	5	0
3	Y	75	0	52	0	0
3	Z	75	0	52	5	0
3	ZA	75	0	52	2	0
3	aA	75	0	52	1	0
3	b	75	0	52	2	0
3	c	75	0	52	1	0
3	cA	75	0	52	0	0
3	dA	75	0	52	5	0
3	e	75	0	52	0	0
3	f	75	0	52	5	0
3	fA	75	0	52	2	0
3	gA	75	0	52	1	0
3	h	75	0	52	2	0
3	i	75	0	52	1	0
3	iA	75	0	52	0	0
3	jA	75	0	52	5	0
3	k	75	0	52	0	0
3	l	75	0	52	5	0
3	lA	75	0	52	2	0
3	mA	75	0	52	1	0
3	n	75	0	52	2	0
3	o	75	0	52	1	0
3	oA	75	0	52	0	0
3	pA	75	0	52	5	0
3	q	75	0	52	1	0
3	r	75	0	52	5	0
3	rA	75	0	52	2	0
3	sA	75	0	52	1	0
3	t	75	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	u	75	0	52	1	0
3	uA	75	0	52	0	0
3	vA	75	0	52	5	0
3	w	75	0	52	0	0
3	x	75	0	52	6	0
3	xA	75	0	52	2	0
3	yA	75	0	52	1	0
3	z	75	0	52	2	0
4	1	28	0	25	0	0
4	5A	28	0	25	0	0
4	7	28	0	25	0	0
4	BB	28	0	25	0	0
4	DA	28	0	25	0	0
4	HB	28	0	25	0	0
4	JA	28	0	25	0	0
4	NB	28	0	25	0	0
4	PA	28	0	25	0	0
4	VA	28	0	25	0	0
4	X	28	0	25	0	0
4	bA	28	0	25	0	0
4	d	28	0	25	0	0
4	hA	28	0	25	0	0
4	j	28	0	25	0	0
4	nA	28	0	25	0	0
4	p	28	0	25	0	0
4	tA	28	0	25	0	0
4	v	28	0	25	0	0
4	zA	28	0	25	0	0
All	All	51960	0	49660	182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 182 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:2:NAG:H61	3:DB:5:MAN:H5	1.86	0.57
3:l:2:NAG:H61	3:l:5:MAN:H5	1.86	0.57
3:vA:2:NAG:H61	3:vA:5:MAN:H5	1.87	0.57
3:Z:2:NAG:H61	3:Z:5:MAN:H5	1.87	0.57
3:dA:2:NAG:H61	3:dA:5:MAN:H5	1.87	0.57

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/293 (95%)	272 (98%)	6 (2%)	0	100	100
1	B	278/293 (95%)	273 (98%)	5 (2%)	0	100	100
1	C	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	D	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	E	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	F	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	G	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	H	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	I	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	J	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	K	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	L	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	M	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	N	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	O	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	P	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	Q	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	R	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	S	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
1	T	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
All	All	5794/5860 (99%)	5675 (98%)	119 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	B	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	C	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	D	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	E	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	F	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	G	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	H	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	I	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	J	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	K	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	L	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	M	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	N	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	O	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	P	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	Q	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	R	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	S	247/247 (100%)	246 (100%)	1 (0%)	84	84
1	T	247/247 (100%)	246 (100%)	1 (0%)	84	84
All	All	4940/4940 (100%)	4920 (100%)	20 (0%)	81	84

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	173	ASN
1	R	173	ASN
1	T	173	ASN

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Mol	Chain	Res	Type
1	S	173	ASN
1	F	173	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	295	GLN
1	T	136	GLN
1	M	166	ASN
1	T	37	ASN
1	R	136	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)

620 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	0	1	1,3	14,14,15	0.34	0	17,19,21	1.51	1 (5%)
3	NAG	0	2	3	14,14,15	0.52	0	17,19,21	2.03	2 (11%)
3	YZT	0	3	3	12,14,15	1.11	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	0	4	3	11,11,12	0.52	0	15,15,17	0.74	0
3	MAN	0	5	3	11,11,12	0.44	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	0	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	0A	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	0A	2	3	14,14,15	0.33	0	17,19,21	0.84	0
3	YZT	0A	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.77	1 (5%)
3	BGC	0A	4	3	11,11,12	0.45	0	15,15,17	0.94	0
3	MAN	0A	5	3	11,11,12	0.57	0	15,15,17	2.09	3 (20%)
3	MAN	0A	6	3	11,11,12	0.35	0	15,15,17	0.71	0
4	NAG	1	1	4,1	14,14,15	0.36	0	17,19,21	0.68	1 (5%)
4	NAG	1	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	1A	1	1,3	14,14,15	0.39	0	17,19,21	1.51	1 (5%)
3	NAG	1A	2	3	14,14,15	0.29	0	17,19,21	0.57	0
3	YZT	1A	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	1A	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	1A	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	1A	6	3	11,11,12	0.29	0	15,15,17	1.23	1 (6%)
3	NAG	2	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	2	2	3	14,14,15	0.31	0	17,19,21	0.83	0
3	YZT	2	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.81	1 (5%)
3	BGC	2	4	3	11,11,12	0.48	0	15,15,17	0.95	0
3	MAN	2	5	3	11,11,12	0.56	0	15,15,17	2.07	3 (20%)
3	MAN	2	6	3	11,11,12	0.34	0	15,15,17	0.69	0
2	NAG	2A	1	2,1	14,14,15	0.37	0	17,19,21	1.35	1 (5%)
2	NAG	2A	2	2	14,14,15	0.30	0	17,19,21	0.65	0
2	YZT	2A	3	2	12,14,15	1.06	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	2A	4	2	11,11,12	0.36	0	15,15,17	0.50	0
2	MAN	2A	5	2	11,11,12	0.22	0	15,15,17	0.51	0
3	NAG	3	1	1,3	14,14,15	0.40	0	17,19,21	1.50	1 (5%)
3	NAG	3	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	YZT	3	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	3	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	3	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	3	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	3A	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	3A	2	3	14,14,15	0.53	0	17,19,21	0.66	0
3	YZT	3A	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	3A	4	3	11,11,12	0.39	0	15,15,17	0.59	0
3	MAN	3A	5	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)
3	MAN	3A	6	3	11,11,12	0.42	0	15,15,17	0.85	1 (6%)
2	NAG	4	1	2,1	14,14,15	0.36	0	17,19,21	1.36	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	4	2	2	14,14,15	0.28	0	17,19,21	0.64	0
2	YZT	4	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	4	4	2	11,11,12	0.36	0	15,15,17	0.51	0
2	MAN	4	5	2	11,11,12	0.23	0	15,15,17	0.52	0
3	NAG	4A	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	4A	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	4A	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	4A	4	3	11,11,12	0.50	0	15,15,17	0.73	0
3	MAN	4A	5	3	11,11,12	0.45	0	15,15,17	1.14	1 (6%)
3	MAN	4A	6	3	11,11,12	0.52	0	15,15,17	1.92	3 (20%)
3	NAG	5	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	5	2	3	14,14,15	0.52	0	17,19,21	0.67	0
3	YZT	5	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	5	4	3	11,11,12	0.37	0	15,15,17	0.58	0
3	MAN	5	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	5	6	3	11,11,12	0.43	0	15,15,17	0.86	1 (6%)
4	NAG	5A	1	4,1	14,14,15	0.37	0	17,19,21	0.71	1 (5%)
4	NAG	5A	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	6	1	1,3	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
3	NAG	6	2	3	14,14,15	0.53	0	17,19,21	2.04	2 (11%)
3	YZT	6	3	3	12,14,15	1.12	1 (8%)	18,21,23	1.07	2 (11%)
3	BGC	6	4	3	11,11,12	0.51	0	15,15,17	0.71	0
3	MAN	6	5	3	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
3	MAN	6	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	6A	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	6A	2	3	14,14,15	0.32	0	17,19,21	0.85	0
3	YZT	6A	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	6A	4	3	11,11,12	0.46	0	15,15,17	0.97	0
3	MAN	6A	5	3	11,11,12	0.60	0	15,15,17	2.03	4 (26%)
3	MAN	6A	6	3	11,11,12	0.33	0	15,15,17	0.71	0
4	NAG	7	1	4,1	14,14,15	0.35	0	17,19,21	0.68	1 (5%)
4	NAG	7	2	4	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	7A	1	1,3	14,14,15	0.39	0	17,19,21	1.52	1 (5%)
3	NAG	7A	2	3	14,14,15	0.30	0	17,19,21	0.58	0
3	YZT	7A	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	7A	4	3	11,11,12	0.30	0	15,15,17	0.60	0
3	MAN	7A	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	7A	6	3	11,11,12	0.29	0	15,15,17	1.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	8	1	1,3	14,14,15	0.34	0	17,19,21	0.66	0
3	NAG	8	2	3	14,14,15	0.32	0	17,19,21	0.84	0
3	YZT	8	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.78	1 (5%)
3	BGC	8	4	3	11,11,12	0.44	0	15,15,17	0.94	0
3	MAN	8	5	3	11,11,12	0.58	0	15,15,17	2.08	3 (20%)
3	MAN	8	6	3	11,11,12	0.34	0	15,15,17	0.71	0
2	NAG	8A	1	2,1	14,14,15	0.37	0	17,19,21	1.36	1 (5%)
2	NAG	8A	2	2	14,14,15	0.29	0	17,19,21	0.65	0
2	YZT	8A	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	8A	4	2	11,11,12	0.36	0	15,15,17	0.50	0
2	MAN	8A	5	2	11,11,12	0.22	0	15,15,17	0.52	0
3	NAG	9	1	1,3	14,14,15	0.40	0	17,19,21	1.50	1 (5%)
3	NAG	9	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	YZT	9	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.03	2 (11%)
3	BGC	9	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	9	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	9	6	3	11,11,12	0.29	0	15,15,17	1.22	1 (6%)
3	NAG	9A	1	1,3	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	9A	2	3	14,14,15	0.53	0	17,19,21	0.66	0
3	YZT	9A	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.11	2 (11%)
3	BGC	9A	4	3	11,11,12	0.38	0	15,15,17	0.59	0
3	MAN	9A	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	9A	6	3	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
2	NAG	AA	1	2,1	14,14,15	0.36	0	17,19,21	1.37	1 (5%)
2	NAG	AA	2	2	14,14,15	0.31	0	17,19,21	0.64	0
2	YZT	AA	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	AA	4	2	11,11,12	0.35	0	15,15,17	0.50	0
2	MAN	AA	5	2	11,11,12	0.23	0	15,15,17	0.51	0
3	NAG	AB	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	AB	2	3	14,14,15	0.52	0	17,19,21	2.05	2 (11%)
3	YZT	AB	3	3	12,14,15	1.13	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	AB	4	3	11,11,12	0.51	0	15,15,17	0.73	0
3	MAN	AB	5	3	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
3	MAN	AB	6	3	11,11,12	0.51	0	15,15,17	1.92	3 (20%)
3	NAG	BA	1	1,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	BA	2	3	14,14,15	0.53	0	17,19,21	0.67	0
3	YZT	BA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	BA	4	3	11,11,12	0.38	0	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	BA	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	BA	6	3	11,11,12	0.42	0	15,15,17	0.84	1 (6%)
4	NAG	BB	1	4,1	14,14,15	0.35	0	17,19,21	0.69	1 (5%)
4	NAG	BB	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	CA	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	CA	2	3	14,14,15	0.52	0	17,19,21	2.05	2 (11%)
3	YZT	CA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	CA	4	3	11,11,12	0.50	0	15,15,17	0.73	0
3	MAN	CA	5	3	11,11,12	0.46	0	15,15,17	1.15	1 (6%)
3	MAN	CA	6	3	11,11,12	0.51	0	15,15,17	1.94	3 (20%)
3	NAG	CB	1	1,3	14,14,15	0.34	0	17,19,21	0.68	0
3	NAG	CB	2	3	14,14,15	0.32	0	17,19,21	0.84	0
3	YZT	CB	3	3	12,14,15	0.76	1 (8%)	18,21,23	0.79	1 (5%)
3	BGC	CB	4	3	11,11,12	0.47	0	15,15,17	0.94	0
3	MAN	CB	5	3	11,11,12	0.58	0	15,15,17	2.08	4 (26%)
3	MAN	CB	6	3	11,11,12	0.35	0	15,15,17	0.72	0
4	NAG	DA	1	4,1	14,14,15	0.35	0	17,19,21	0.69	1 (5%)
4	NAG	DA	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	DB	1	1,3	14,14,15	0.38	0	17,19,21	1.51	1 (5%)
3	NAG	DB	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	YZT	DB	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	DB	4	3	11,11,12	0.32	0	15,15,17	0.60	0
3	MAN	DB	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	DB	6	3	11,11,12	0.29	0	15,15,17	1.23	1 (6%)
3	NAG	EA	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	EA	2	3	14,14,15	0.33	0	17,19,21	0.84	0
3	YZT	EA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	EA	4	3	11,11,12	0.47	0	15,15,17	0.98	0
3	MAN	EA	5	3	11,11,12	0.59	0	15,15,17	2.03	4 (26%)
3	MAN	EA	6	3	11,11,12	0.34	0	15,15,17	0.71	0
2	NAG	EB	1	2,1	14,14,15	0.38	0	17,19,21	1.35	1 (5%)
2	NAG	EB	2	2	14,14,15	0.28	0	17,19,21	0.64	0
2	YZT	EB	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	EB	4	2	11,11,12	0.36	0	15,15,17	0.50	0
2	MAN	EB	5	2	11,11,12	0.23	0	15,15,17	0.52	0
3	NAG	FA	1	1,3	14,14,15	0.41	0	17,19,21	1.50	1 (5%)
3	NAG	FA	2	3	14,14,15	0.30	0	17,19,21	0.59	0
3	YZT	FA	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	FA	4	3	11,11,12	0.32	0	15,15,17	0.60	0
3	MAN	FA	5	3	11,11,12	0.28	0	15,15,17	0.81	0
3	MAN	FA	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	FB	1	1,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	FB	2	3	14,14,15	0.52	0	17,19,21	0.68	0
3	YZT	FB	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	FB	4	3	11,11,12	0.37	0	15,15,17	0.58	0
3	MAN	FB	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	FB	6	3	11,11,12	0.42	0	15,15,17	0.85	1 (6%)
2	NAG	GA	1	2,1	14,14,15	0.37	0	17,19,21	1.34	1 (5%)
2	NAG	GA	2	2	14,14,15	0.27	0	17,19,21	0.64	0
2	YZT	GA	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	GA	4	2	11,11,12	0.35	0	15,15,17	0.50	0
2	MAN	GA	5	2	11,11,12	0.23	0	15,15,17	0.52	0
3	NAG	GB	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	GB	2	3	14,14,15	0.53	0	17,19,21	2.04	2 (11%)
3	YZT	GB	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.07	2 (11%)
3	BGC	GB	4	3	11,11,12	0.51	0	15,15,17	0.75	0
3	MAN	GB	5	3	11,11,12	0.46	0	15,15,17	1.15	1 (6%)
3	MAN	GB	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	HA	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	HA	2	3	14,14,15	0.53	0	17,19,21	0.67	0
3	YZT	HA	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.14	2 (11%)
3	BGC	HA	4	3	11,11,12	0.37	0	15,15,17	0.59	0
3	MAN	HA	5	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)
3	MAN	HA	6	3	11,11,12	0.42	0	15,15,17	0.84	1 (6%)
4	NAG	HB	1	4,1	14,14,15	0.36	0	17,19,21	0.69	1 (5%)
4	NAG	HB	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	IA	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	IA	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	IA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.07	2 (11%)
3	BGC	IA	4	3	11,11,12	0.52	0	15,15,17	0.74	0
3	MAN	IA	5	3	11,11,12	0.45	0	15,15,17	1.16	1 (6%)
3	MAN	IA	6	3	11,11,12	0.51	0	15,15,17	1.92	3 (20%)
3	NAG	IB	1	1,3	14,14,15	0.34	0	17,19,21	0.68	0
3	NAG	IB	2	3	14,14,15	0.32	0	17,19,21	0.82	0
3	YZT	IB	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.79	1 (5%)
3	BGC	IB	4	3	11,11,12	0.45	0	15,15,17	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	IB	5	3	11,11,12	0.59	0	15,15,17	2.04	4 (26%)
3	MAN	IB	6	3	11,11,12	0.33	0	15,15,17	0.68	0
4	NAG	JA	1	4,1	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
4	NAG	JA	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	JB	1	1,3	14,14,15	0.39	0	17,19,21	1.52	1 (5%)
3	NAG	JB	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	YZT	JB	3	3	12,14,15	1.14	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	JB	4	3	11,11,12	0.30	0	15,15,17	0.61	0
3	MAN	JB	5	3	11,11,12	0.29	0	15,15,17	0.80	0
3	MAN	JB	6	3	11,11,12	0.29	0	15,15,17	1.22	1 (6%)
3	NAG	KA	1	1,3	14,14,15	0.35	0	17,19,21	0.67	0
3	NAG	KA	2	3	14,14,15	0.32	0	17,19,21	0.82	0
3	YZT	KA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	KA	4	3	11,11,12	0.45	0	15,15,17	0.94	0
3	MAN	KA	5	3	11,11,12	0.58	0	15,15,17	2.05	4 (26%)
3	MAN	KA	6	3	11,11,12	0.33	0	15,15,17	0.67	0
2	NAG	KB	1	2,1	14,14,15	0.37	0	17,19,21	1.37	1 (5%)
2	NAG	KB	2	2	14,14,15	0.30	0	17,19,21	0.64	0
2	YZT	KB	3	2	12,14,15	1.07	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	KB	4	2	11,11,12	0.35	0	15,15,17	0.51	0
2	MAN	KB	5	2	11,11,12	0.23	0	15,15,17	0.51	0
3	NAG	LA	1	1,3	14,14,15	0.40	0	17,19,21	1.50	1 (5%)
3	NAG	LA	2	3	14,14,15	0.30	0	17,19,21	0.59	0
3	YZT	LA	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	LA	4	3	11,11,12	0.29	0	15,15,17	0.61	0
3	MAN	LA	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	LA	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	LB	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	LB	2	3	14,14,15	0.53	0	17,19,21	0.66	0
3	YZT	LB	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.11	2 (11%)
3	BGC	LB	4	3	11,11,12	0.39	0	15,15,17	0.59	0
3	MAN	LB	5	3	11,11,12	0.37	0	15,15,17	1.17	1 (6%)
3	MAN	LB	6	3	11,11,12	0.42	0	15,15,17	0.85	1 (6%)
2	NAG	MA	1	2,1	14,14,15	0.37	0	17,19,21	1.37	1 (5%)
2	NAG	MA	2	2	14,14,15	0.31	0	17,19,21	0.65	0
2	YZT	MA	3	2	12,14,15	1.07	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	MA	4	2	11,11,12	0.35	0	15,15,17	0.51	0
2	MAN	MA	5	2	11,11,12	0.23	0	15,15,17	0.51	0
3	NAG	MB	1	1,3	14,14,15	0.33	0	17,19,21	1.50	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	MB	2	3	14,14,15	0.53	0	17,19,21	2.04	2 (11%)
3	YZT	MB	3	3	12,14,15	1.11	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	MB	4	3	11,11,12	0.51	0	15,15,17	0.74	0
3	MAN	MB	5	3	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
3	MAN	MB	6	3	11,11,12	0.52	0	15,15,17	1.93	3 (20%)
3	NAG	NA	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	NA	2	3	14,14,15	0.52	0	17,19,21	0.67	0
3	YZT	NA	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.11	2 (11%)
3	BGC	NA	4	3	11,11,12	0.38	0	15,15,17	0.59	0
3	MAN	NA	5	3	11,11,12	0.36	0	15,15,17	1.18	1 (6%)
3	MAN	NA	6	3	11,11,12	0.42	0	15,15,17	0.85	1 (6%)
4	NAG	NB	1	4,1	14,14,15	0.36	0	17,19,21	0.69	1 (5%)
4	NAG	NB	2	4	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	OA	1	1,3	14,14,15	0.33	0	17,19,21	1.50	1 (5%)
3	NAG	OA	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	OA	3	3	12,14,15	1.12	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	OA	4	3	11,11,12	0.52	0	15,15,17	0.74	0
3	MAN	OA	5	3	11,11,12	0.45	0	15,15,17	1.14	1 (6%)
3	MAN	OA	6	3	11,11,12	0.52	0	15,15,17	1.93	3 (20%)
3	NAG	OB	1	1,3	14,14,15	0.35	0	17,19,21	0.68	0
3	NAG	OB	2	3	14,14,15	0.32	0	17,19,21	0.82	0
3	YZT	OB	3	3	12,14,15	0.76	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	OB	4	3	11,11,12	0.49	0	15,15,17	0.97	0
3	MAN	OB	5	3	11,11,12	0.57	0	15,15,17	2.08	3 (20%)
3	MAN	OB	6	3	11,11,12	0.35	0	15,15,17	0.69	0
4	NAG	PA	1	4,1	14,14,15	0.35	0	17,19,21	0.69	1 (5%)
4	NAG	PA	2	4	14,14,15	0.32	0	17,19,21	0.61	0
3	NAG	PB	1	1,3	14,14,15	0.38	0	17,19,21	1.51	1 (5%)
3	NAG	PB	2	3	14,14,15	0.30	0	17,19,21	0.57	0
3	YZT	PB	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	PB	4	3	11,11,12	0.30	0	15,15,17	0.60	0
3	MAN	PB	5	3	11,11,12	0.30	0	15,15,17	0.80	0
3	MAN	PB	6	3	11,11,12	0.29	0	15,15,17	1.23	1 (6%)
3	NAG	QA	1	1,3	14,14,15	0.34	0	17,19,21	0.66	0
3	NAG	QA	2	3	14,14,15	0.33	0	17,19,21	0.82	0
3	YZT	QA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	QA	4	3	11,11,12	0.47	0	15,15,17	0.96	0
3	MAN	QA	5	3	11,11,12	0.58	0	15,15,17	2.08	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	QA	6	3	11,11,12	0.34	0	15,15,17	0.68	0
3	NAG	RA	1	1,3	14,14,15	0.39	0	17,19,21	1.50	1 (5%)
3	NAG	RA	2	3	14,14,15	0.30	0	17,19,21	0.58	0
3	YZT	RA	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	RA	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	RA	5	3	11,11,12	0.29	0	15,15,17	0.80	0
3	MAN	RA	6	3	11,11,12	0.29	0	15,15,17	1.22	1 (6%)
2	NAG	SA	1	2,1	14,14,15	0.38	0	17,19,21	1.35	1 (5%)
2	NAG	SA	2	2	14,14,15	0.28	0	17,19,21	0.64	0
2	YZT	SA	3	2	12,14,15	1.06	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	SA	4	2	11,11,12	0.35	0	15,15,17	0.51	0
2	MAN	SA	5	2	11,11,12	0.22	0	15,15,17	0.52	0
3	NAG	TA	1	1,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	TA	2	3	14,14,15	0.52	0	17,19,21	0.67	0
3	YZT	TA	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	TA	4	3	11,11,12	0.37	0	15,15,17	0.59	0
3	MAN	TA	5	3	11,11,12	0.36	0	15,15,17	1.18	1 (6%)
3	MAN	TA	6	3	11,11,12	0.42	0	15,15,17	0.86	1 (6%)
2	NAG	U	1	2,1	14,14,15	0.37	0	17,19,21	1.37	1 (5%)
2	NAG	U	2	2	14,14,15	0.28	0	17,19,21	0.65	0
2	YZT	U	3	2	12,14,15	1.06	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	U	4	2	11,11,12	0.37	0	15,15,17	0.50	0
2	MAN	U	5	2	11,11,12	0.23	0	15,15,17	0.51	0
3	NAG	UA	1	1,3	14,14,15	0.33	0	17,19,21	1.50	1 (5%)
3	NAG	UA	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	UA	3	3	12,14,15	1.12	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	UA	4	3	11,11,12	0.50	0	15,15,17	0.71	0
3	MAN	UA	5	3	11,11,12	0.44	0	15,15,17	1.15	1 (6%)
3	MAN	UA	6	3	11,11,12	0.51	0	15,15,17	1.92	3 (20%)
3	NAG	V	1	1,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	V	2	3	14,14,15	0.53	0	17,19,21	0.65	0
3	YZT	V	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.12	2 (11%)
3	BGC	V	4	3	11,11,12	0.38	0	15,15,17	0.58	0
3	MAN	V	5	3	11,11,12	0.37	0	15,15,17	1.16	1 (6%)
3	MAN	V	6	3	11,11,12	0.43	0	15,15,17	0.85	1 (6%)
4	NAG	VA	1	4,1	14,14,15	0.36	0	17,19,21	0.68	1 (5%)
4	NAG	VA	2	4	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	W	1	1,3	14,14,15	0.35	0	17,19,21	1.50	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	W	2	3	14,14,15	0.53	0	17,19,21	2.04	2 (11%)
3	YZT	W	3	3	12,14,15	1.12	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	W	4	3	11,11,12	0.52	0	15,15,17	0.73	0
3	MAN	W	5	3	11,11,12	0.44	0	15,15,17	1.14	1 (6%)
3	MAN	W	6	3	11,11,12	0.51	0	15,15,17	1.92	3 (20%)
3	NAG	WA	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	WA	2	3	14,14,15	0.34	0	17,19,21	0.84	0
3	YZT	WA	3	3	12,14,15	0.76	1 (8%)	18,21,23	0.78	1 (5%)
3	BGC	WA	4	3	11,11,12	0.44	0	15,15,17	0.94	0
3	MAN	WA	5	3	11,11,12	0.57	0	15,15,17	2.08	3 (20%)
3	MAN	WA	6	3	11,11,12	0.35	0	15,15,17	0.70	0
4	NAG	X	1	4,1	14,14,15	0.35	0	17,19,21	0.66	1 (5%)
4	NAG	X	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	XA	1	1,3	14,14,15	0.40	0	17,19,21	1.50	1 (5%)
3	NAG	XA	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	YZT	XA	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	XA	4	3	11,11,12	0.30	0	15,15,17	0.61	0
3	MAN	XA	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	XA	6	3	11,11,12	0.31	0	15,15,17	1.23	1 (6%)
3	NAG	Y	1	1,3	14,14,15	0.34	0	17,19,21	0.66	0
3	NAG	Y	2	3	14,14,15	0.33	0	17,19,21	0.84	0
3	YZT	Y	3	3	12,14,15	0.76	1 (8%)	18,21,23	0.79	1 (5%)
3	BGC	Y	4	3	11,11,12	0.46	0	15,15,17	0.95	0
3	MAN	Y	5	3	11,11,12	0.58	0	15,15,17	2.07	4 (26%)
3	MAN	Y	6	3	11,11,12	0.35	0	15,15,17	0.71	0
2	NAG	YA	1	2,1	14,14,15	0.38	0	17,19,21	1.36	1 (5%)
2	NAG	YA	2	2	14,14,15	0.31	0	17,19,21	0.64	0
2	YZT	YA	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	YA	4	2	11,11,12	0.36	0	15,15,17	0.51	0
2	MAN	YA	5	2	11,11,12	0.23	0	15,15,17	0.52	0
3	NAG	Z	1	1,3	14,14,15	0.39	0	17,19,21	1.50	1 (5%)
3	NAG	Z	2	3	14,14,15	0.30	0	17,19,21	0.58	0
3	YZT	Z	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	Z	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	Z	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	Z	6	3	11,11,12	0.30	0	15,15,17	1.23	1 (6%)
3	NAG	ZA	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	ZA	2	3	14,14,15	0.52	0	17,19,21	0.68	0
3	YZT	ZA	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	ZA	4	3	11,11,12	0.38	0	15,15,17	0.60	0
3	MAN	ZA	5	3	11,11,12	0.37	0	15,15,17	1.16	1 (6%)
3	MAN	ZA	6	3	11,11,12	0.42	0	15,15,17	0.84	1 (6%)
2	NAG	a	1	2,1	14,14,15	0.37	0	17,19,21	1.35	1 (5%)
2	NAG	a	2	2	14,14,15	0.27	0	17,19,21	0.64	0
2	YZT	a	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	a	4	2	11,11,12	0.35	0	15,15,17	0.50	0
2	MAN	a	5	2	11,11,12	0.23	0	15,15,17	0.52	0
3	NAG	aA	1	1,3	14,14,15	0.35	0	17,19,21	1.50	1 (5%)
3	NAG	aA	2	3	14,14,15	0.52	0	17,19,21	2.03	2 (11%)
3	YZT	aA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	aA	4	3	11,11,12	0.52	0	15,15,17	0.73	0
3	MAN	aA	5	3	11,11,12	0.45	0	15,15,17	1.14	1 (6%)
3	MAN	aA	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	b	1	1,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	b	2	3	14,14,15	0.53	0	17,19,21	0.66	0
3	YZT	b	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	b	4	3	11,11,12	0.38	0	15,15,17	0.58	0
3	MAN	b	5	3	11,11,12	0.38	0	15,15,17	1.16	1 (6%)
3	MAN	b	6	3	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
4	NAG	bA	1	4,1	14,14,15	0.37	0	17,19,21	0.68	1 (5%)
4	NAG	bA	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	c	1	1,3	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
3	NAG	c	2	3	14,14,15	0.53	0	17,19,21	2.04	2 (11%)
3	YZT	c	3	3	12,14,15	1.11	1 (8%)	18,21,23	1.07	2 (11%)
3	BGC	c	4	3	11,11,12	0.49	0	15,15,17	0.71	0
3	MAN	c	5	3	11,11,12	0.45	0	15,15,17	1.15	1 (6%)
3	MAN	c	6	3	11,11,12	0.50	0	15,15,17	1.92	3 (20%)
3	NAG	cA	1	1,3	14,14,15	0.34	0	17,19,21	0.66	0
3	NAG	cA	2	3	14,14,15	0.32	0	17,19,21	0.84	0
3	YZT	cA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	cA	4	3	11,11,12	0.47	0	15,15,17	0.97	0
3	MAN	cA	5	3	11,11,12	0.59	0	15,15,17	2.03	4 (26%)
3	MAN	cA	6	3	11,11,12	0.32	0	15,15,17	0.70	0
4	NAG	d	1	4,1	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
4	NAG	d	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	dA	1	1,3	14,14,15	0.39	0	17,19,21	1.50	1 (5%)
3	NAG	dA	2	3	14,14,15	0.31	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	YZT	dA	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.03	2 (11%)
3	BGC	dA	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	dA	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	dA	6	3	11,11,12	0.29	0	15,15,17	1.22	1 (6%)
3	NAG	e	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	e	2	3	14,14,15	0.33	0	17,19,21	0.84	0
3	YZT	e	3	3	12,14,15	0.76	1 (8%)	18,21,23	0.78	1 (5%)
3	BGC	e	4	3	11,11,12	0.44	0	15,15,17	0.95	0
3	MAN	e	5	3	11,11,12	0.57	0	15,15,17	2.09	4 (26%)
3	MAN	e	6	3	11,11,12	0.35	0	15,15,17	0.70	0
2	NAG	eA	1	2,1	14,14,15	0.37	0	17,19,21	1.35	1 (5%)
2	NAG	eA	2	2	14,14,15	0.28	0	17,19,21	0.65	0
2	YZT	eA	3	2	12,14,15	1.07	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	eA	4	2	11,11,12	0.37	0	15,15,17	0.50	0
2	MAN	eA	5	2	11,11,12	0.22	0	15,15,17	0.52	0
3	NAG	f	1	1,3	14,14,15	0.38	0	17,19,21	1.51	1 (5%)
3	NAG	f	2	3	14,14,15	0.31	0	17,19,21	0.57	0
3	YZT	f	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	f	4	3	11,11,12	0.30	0	15,15,17	0.61	0
3	MAN	f	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	f	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	fA	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	fA	2	3	14,14,15	0.54	0	17,19,21	0.65	0
3	YZT	fA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.12	2 (11%)
3	BGC	fA	4	3	11,11,12	0.38	0	15,15,17	0.58	0
3	MAN	fA	5	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)
3	MAN	fA	6	3	11,11,12	0.41	0	15,15,17	0.85	1 (6%)
2	NAG	g	1	2,1	14,14,15	0.36	0	17,19,21	1.35	1 (5%)
2	NAG	g	2	2	14,14,15	0.30	0	17,19,21	0.65	0
2	YZT	g	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	g	4	2	11,11,12	0.36	0	15,15,17	0.50	0
2	MAN	g	5	2	11,11,12	0.24	0	15,15,17	0.51	0
3	NAG	gA	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	gA	2	3	14,14,15	0.53	0	17,19,21	2.05	2 (11%)
3	YZT	gA	3	3	12,14,15	1.13	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	gA	4	3	11,11,12	0.50	0	15,15,17	0.72	0
3	MAN	gA	5	3	11,11,12	0.45	0	15,15,17	1.14	1 (6%)
3	MAN	gA	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	h	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	h	2	3	14,14,15	0.53	0	17,19,21	0.67	0
3	YZT	h	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	h	4	3	11,11,12	0.38	0	15,15,17	0.59	0
3	MAN	h	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	h	6	3	11,11,12	0.43	0	15,15,17	0.84	1 (6%)
4	NAG	hA	1	4,1	14,14,15	0.34	0	17,19,21	0.66	1 (5%)
4	NAG	hA	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	i	1	1,3	14,14,15	0.33	0	17,19,21	1.49	1 (5%)
3	NAG	i	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	i	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	i	4	3	11,11,12	0.52	0	15,15,17	0.73	0
3	MAN	i	5	3	11,11,12	0.44	0	15,15,17	1.15	1 (6%)
3	MAN	i	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	iA	1	1,3	14,14,15	0.35	0	17,19,21	0.66	0
3	NAG	iA	2	3	14,14,15	0.34	0	17,19,21	0.83	0
3	YZT	iA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.79	1 (5%)
3	BGC	iA	4	3	11,11,12	0.46	0	15,15,17	0.94	0
3	MAN	iA	5	3	11,11,12	0.57	0	15,15,17	2.07	4 (26%)
3	MAN	iA	6	3	11,11,12	0.34	0	15,15,17	0.72	0
4	NAG	j	1	4,1	14,14,15	0.35	0	17,19,21	0.69	1 (5%)
4	NAG	j	2	4	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	jA	1	1,3	14,14,15	0.39	0	17,19,21	1.51	1 (5%)
3	NAG	jA	2	3	14,14,15	0.30	0	17,19,21	0.58	0
3	YZT	jA	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.03	2 (11%)
3	BGC	jA	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	jA	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	jA	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	k	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0
3	NAG	k	2	3	14,14,15	0.32	0	17,19,21	0.84	0
3	YZT	k	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	k	4	3	11,11,12	0.47	0	15,15,17	0.96	0
3	MAN	k	5	3	11,11,12	0.60	0	15,15,17	2.03	4 (26%)
3	MAN	k	6	3	11,11,12	0.34	0	15,15,17	0.71	0
2	NAG	kA	1	2,1	14,14,15	0.36	0	17,19,21	1.34	1 (5%)
2	NAG	kA	2	2	14,14,15	0.28	0	17,19,21	0.64	0
2	YZT	kA	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	kA	4	2	11,11,12	0.36	0	15,15,17	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	kA	5	2	11,11,12	0.23	0	15,15,17	0.51	0
3	NAG	l	1	1,3	14,14,15	0.40	0	17,19,21	1.52	1 (5%)
3	NAG	l	2	3	14,14,15	0.31	0	17,19,21	0.58	0
3	YZT	l	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	l	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	l	5	3	11,11,12	0.28	0	15,15,17	0.81	0
3	MAN	l	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	lA	1	1,3	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	lA	2	3	14,14,15	0.52	0	17,19,21	0.66	0
3	YZT	lA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	lA	4	3	11,11,12	0.39	0	15,15,17	0.59	0
3	MAN	lA	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	lA	6	3	11,11,12	0.42	0	15,15,17	0.85	1 (6%)
2	NAG	m	1	2,1	14,14,15	0.37	0	17,19,21	1.36	1 (5%)
2	NAG	m	2	2	14,14,15	0.29	0	17,19,21	0.66	0
2	YZT	m	3	2	12,14,15	1.07	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	m	4	2	11,11,12	0.36	0	15,15,17	0.50	0
2	MAN	m	5	2	11,11,12	0.24	0	15,15,17	0.51	0
3	NAG	mA	1	1,3	14,14,15	0.33	0	17,19,21	1.50	1 (5%)
3	NAG	mA	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	mA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.07	2 (11%)
3	BGC	mA	4	3	11,11,12	0.51	0	15,15,17	0.74	0
3	MAN	mA	5	3	11,11,12	0.46	0	15,15,17	1.15	1 (6%)
3	MAN	mA	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	n	1	1,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	n	2	3	14,14,15	0.52	0	17,19,21	0.66	0
3	YZT	n	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.12	2 (11%)
3	BGC	n	4	3	11,11,12	0.37	0	15,15,17	0.58	0
3	MAN	n	5	3	11,11,12	0.35	0	15,15,17	1.17	1 (6%)
3	MAN	n	6	3	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
4	NAG	nA	1	4,1	14,14,15	0.36	0	17,19,21	0.66	1 (5%)
4	NAG	nA	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	o	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	o	2	3	14,14,15	0.53	0	17,19,21	2.03	2 (11%)
3	YZT	o	3	3	12,14,15	1.12	1 (8%)	18,21,23	1.06	2 (11%)
3	BGC	o	4	3	11,11,12	0.50	0	15,15,17	0.73	0
3	MAN	o	5	3	11,11,12	0.44	0	15,15,17	1.14	1 (6%)
3	MAN	o	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	oA	1	1,3	14,14,15	0.35	0	17,19,21	0.67	0
3	NAG	oA	2	3	14,14,15	0.33	0	17,19,21	0.82	0
3	YZT	oA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.79	1 (5%)
3	BGC	oA	4	3	11,11,12	0.46	0	15,15,17	0.94	0
3	MAN	oA	5	3	11,11,12	0.58	0	15,15,17	2.04	4 (26%)
3	MAN	oA	6	3	11,11,12	0.34	0	15,15,17	0.68	0
4	NAG	p	1	4,1	14,14,15	0.35	0	17,19,21	0.66	1 (5%)
4	NAG	p	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	pA	1	1,3	14,14,15	0.39	0	17,19,21	1.51	1 (5%)
3	NAG	pA	2	3	14,14,15	0.28	0	17,19,21	0.58	0
3	YZT	pA	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	pA	4	3	11,11,12	0.30	0	15,15,17	0.60	0
3	MAN	pA	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	pA	6	3	11,11,12	0.31	0	15,15,17	1.22	1 (6%)
3	NAG	q	1	1,3	14,14,15	0.36	0	17,19,21	0.66	0
3	NAG	q	2	3	14,14,15	0.33	0	17,19,21	0.83	0
3	YZT	q	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.79	1 (5%)
3	BGC	q	4	3	11,11,12	0.47	0	15,15,17	0.94	0
3	MAN	q	5	3	11,11,12	0.57	0	15,15,17	2.08	4 (26%)
3	MAN	q	6	3	11,11,12	0.35	0	15,15,17	0.71	0
2	NAG	qA	1	2,1	14,14,15	0.37	0	17,19,21	1.37	1 (5%)
2	NAG	qA	2	2	14,14,15	0.30	0	17,19,21	0.64	0
2	YZT	qA	3	2	12,14,15	1.06	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	qA	4	2	11,11,12	0.35	0	15,15,17	0.51	0
2	MAN	qA	5	2	11,11,12	0.24	0	15,15,17	0.50	0
3	NAG	r	1	1,3	14,14,15	0.40	0	17,19,21	1.51	1 (5%)
3	NAG	r	2	3	14,14,15	0.31	0	17,19,21	0.57	0
3	YZT	r	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	r	4	3	11,11,12	0.31	0	15,15,17	0.60	0
3	MAN	r	5	3	11,11,12	0.28	0	15,15,17	0.80	0
3	MAN	r	6	3	11,11,12	0.30	0	15,15,17	1.22	1 (6%)
3	NAG	rA	1	1,3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	rA	2	3	14,14,15	0.54	0	17,19,21	0.66	0
3	YZT	rA	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.11	2 (11%)
3	BGC	rA	4	3	11,11,12	0.39	0	15,15,17	0.59	0
3	MAN	rA	5	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)
3	MAN	rA	6	3	11,11,12	0.42	0	15,15,17	0.84	1 (6%)
2	NAG	s	1	2,1	14,14,15	0.37	0	17,19,21	1.35	1 (5%)
2	NAG	s	2	2	14,14,15	0.28	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	YZT	s	3	2	12,14,15	1.06	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	s	4	2	11,11,12	0.37	0	15,15,17	0.50	0
2	MAN	s	5	2	11,11,12	0.22	0	15,15,17	0.52	0
3	NAG	sA	1	1,3	14,14,15	0.34	0	17,19,21	1.50	1 (5%)
3	NAG	sA	2	3	14,14,15	0.52	0	17,19,21	2.04	2 (11%)
3	YZT	sA	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	sA	4	3	11,11,12	0.51	0	15,15,17	0.74	0
3	MAN	sA	5	3	11,11,12	0.44	0	15,15,17	1.16	1 (6%)
3	MAN	sA	6	3	11,11,12	0.51	0	15,15,17	1.92	3 (20%)
3	NAG	t	1	1,3	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	t	2	3	14,14,15	0.53	0	17,19,21	0.67	0
3	YZT	t	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	t	4	3	11,11,12	0.38	0	15,15,17	0.59	0
3	MAN	t	5	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)
3	MAN	t	6	3	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
4	NAG	tA	1	4,1	14,14,15	0.35	0	17,19,21	0.67	1 (5%)
4	NAG	tA	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	u	1	1,3	14,14,15	0.33	0	17,19,21	1.50	1 (5%)
3	NAG	u	2	3	14,14,15	0.52	0	17,19,21	2.03	2 (11%)
3	YZT	u	3	3	12,14,15	1.11	1 (8%)	18,21,23	1.08	2 (11%)
3	BGC	u	4	3	11,11,12	0.51	0	15,15,17	0.73	0
3	MAN	u	5	3	11,11,12	0.46	0	15,15,17	1.15	1 (6%)
3	MAN	u	6	3	11,11,12	0.50	0	15,15,17	1.92	3 (20%)
3	NAG	uA	1	1,3	14,14,15	0.35	0	17,19,21	0.67	0
3	NAG	uA	2	3	14,14,15	0.32	0	17,19,21	0.83	0
3	YZT	uA	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	uA	4	3	11,11,12	0.48	0	15,15,17	0.96	0
3	MAN	uA	5	3	11,11,12	0.58	0	15,15,17	2.08	3 (20%)
3	MAN	uA	6	3	11,11,12	0.34	0	15,15,17	0.69	0
4	NAG	v	1	4,1	14,14,15	0.37	0	17,19,21	0.68	1 (5%)
4	NAG	v	2	4	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	vA	1	1,3	14,14,15	0.39	0	17,19,21	1.51	1 (5%)
3	NAG	vA	2	3	14,14,15	0.31	0	17,19,21	0.58	0
3	YZT	vA	3	3	12,14,15	1.16	1 (8%)	18,21,23	1.05	2 (11%)
3	BGC	vA	4	3	11,11,12	0.30	0	15,15,17	0.60	0
3	MAN	vA	5	3	11,11,12	0.30	0	15,15,17	0.79	0
3	MAN	vA	6	3	11,11,12	0.29	0	15,15,17	1.22	1 (6%)
3	NAG	w	1	1,3	14,14,15	0.34	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	w	2	3	14,14,15	0.32	0	17,19,21	0.82	0
3	YZT	w	3	3	12,14,15	0.75	1 (8%)	18,21,23	0.80	1 (5%)
3	BGC	w	4	3	11,11,12	0.44	0	15,15,17	0.94	0
3	MAN	w	5	3	11,11,12	0.58	0	15,15,17	2.04	4 (26%)
3	MAN	w	6	3	11,11,12	0.35	0	15,15,17	0.67	0
2	NAG	wA	1	2,1	14,14,15	0.36	0	17,19,21	1.35	1 (5%)
2	NAG	wA	2	2	14,14,15	0.28	0	17,19,21	0.65	0
2	YZT	wA	3	2	12,14,15	1.05	1 (8%)	18,21,23	1.13	2 (11%)
2	MAN	wA	4	2	11,11,12	0.36	0	15,15,17	0.50	0
2	MAN	wA	5	2	11,11,12	0.23	0	15,15,17	0.51	0
3	NAG	x	1	1,3	14,14,15	0.40	0	17,19,21	1.50	1 (5%)
3	NAG	x	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	YZT	x	3	3	12,14,15	1.15	1 (8%)	18,21,23	1.04	2 (11%)
3	BGC	x	4	3	11,11,12	0.30	0	15,15,17	0.60	0
3	MAN	x	5	3	11,11,12	0.29	0	15,15,17	0.80	0
3	MAN	x	6	3	11,11,12	0.29	0	15,15,17	1.21	1 (6%)
3	NAG	xA	1	1,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	xA	2	3	14,14,15	0.51	0	17,19,21	0.66	0
3	YZT	xA	3	3	12,14,15	1.09	1 (8%)	18,21,23	1.13	2 (11%)
3	BGC	xA	4	3	11,11,12	0.37	0	15,15,17	0.58	0
3	MAN	xA	5	3	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
3	MAN	xA	6	3	11,11,12	0.42	0	15,15,17	0.85	1 (6%)
2	NAG	y	1	2,1	14,14,15	0.38	0	17,19,21	1.36	1 (5%)
2	NAG	y	2	2	14,14,15	0.31	0	17,19,21	0.65	0
2	YZT	y	3	2	12,14,15	1.06	1 (8%)	18,21,23	1.14	2 (11%)
2	MAN	y	4	2	11,11,12	0.35	0	15,15,17	0.51	0
2	MAN	y	5	2	11,11,12	0.24	0	15,15,17	0.50	0
3	NAG	yA	1	1,3	14,14,15	0.34	0	17,19,21	1.49	1 (5%)
3	NAG	yA	2	3	14,14,15	0.52	0	17,19,21	2.05	2 (11%)
3	YZT	yA	3	3	12,14,15	1.11	1 (8%)	18,21,23	1.07	2 (11%)
3	BGC	yA	4	3	11,11,12	0.50	0	15,15,17	0.71	0
3	MAN	yA	5	3	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
3	MAN	yA	6	3	11,11,12	0.51	0	15,15,17	1.93	3 (20%)
3	NAG	z	1	1,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	z	2	3	14,14,15	0.53	0	17,19,21	0.67	0
3	YZT	z	3	3	12,14,15	1.10	1 (8%)	18,21,23	1.12	2 (11%)
3	BGC	z	4	3	11,11,12	0.37	0	15,15,17	0.59	0
3	MAN	z	5	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	z	6	3	11,11,12	0.41	0	15,15,17	0.85	1 (6%)
4	NAG	zA	1	4,1	14,14,15	0.36	0	17,19,21	0.68	1 (5%)
4	NAG	zA	2	4	14,14,15	0.30	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	0	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	0	2	3	-	0/6/23/26	0/1/1/1
3	YZT	0	3	3	-	0/5/22/25	0/1/1/1
3	BGC	0	4	3	-	2/2/19/22	0/1/1/1
3	MAN	0	5	3	-	0/2/19/22	0/1/1/1
3	MAN	0	6	3	-	0/2/19/22	0/1/1/1
3	NAG	0A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	0A	2	3	-	0/6/23/26	0/1/1/1
3	YZT	0A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	0A	4	3	-	2/2/19/22	0/1/1/1
3	MAN	0A	5	3	-	0/2/19/22	0/1/1/1
3	MAN	0A	6	3	-	2/2/19/22	0/1/1/1
4	NAG	1	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	1	2	4	-	1/6/23/26	0/1/1/1
3	NAG	1A	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	1A	2	3	-	2/6/23/26	0/1/1/1
3	YZT	1A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	1A	4	3	-	0/2/19/22	0/1/1/1
3	MAN	1A	5	3	-	0/2/19/22	0/1/1/1
3	MAN	1A	6	3	-	0/2/19/22	0/1/1/1
3	NAG	2	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	2	2	3	-	0/6/23/26	0/1/1/1
3	YZT	2	3	3	-	0/5/22/25	0/1/1/1
3	BGC	2	4	3	-	2/2/19/22	0/1/1/1
3	MAN	2	5	3	-	0/2/19/22	0/1/1/1
3	MAN	2	6	3	-	2/2/19/22	0/1/1/1
2	NAG	2A	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	2A	2	2	-	2/6/23/26	0/1/1/1
2	YZT	2A	3	2	-	2/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	2A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	2A	5	2	-	0/2/19/22	0/1/1/1
3	NAG	3	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	3	2	3	-	2/6/23/26	0/1/1/1
3	YZT	3	3	3	-	0/5/22/25	0/1/1/1
3	BGC	3	4	3	-	0/2/19/22	0/1/1/1
3	MAN	3	5	3	-	0/2/19/22	0/1/1/1
3	MAN	3	6	3	-	0/2/19/22	0/1/1/1
3	NAG	3A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	3A	2	3	-	0/6/23/26	0/1/1/1
3	YZT	3A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	3A	4	3	-	0/2/19/22	0/1/1/1
3	MAN	3A	5	3	-	2/2/19/22	0/1/1/1
3	MAN	3A	6	3	-	0/2/19/22	0/1/1/1
2	NAG	4	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	4	2	2	-	2/6/23/26	0/1/1/1
2	YZT	4	3	2	-	2/5/22/25	0/1/1/1
2	MAN	4	4	2	-	0/2/19/22	0/1/1/1
2	MAN	4	5	2	-	0/2/19/22	0/1/1/1
3	NAG	4A	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	4A	2	3	-	0/6/23/26	0/1/1/1
3	YZT	4A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	4A	4	3	-	2/2/19/22	0/1/1/1
3	MAN	4A	5	3	-	0/2/19/22	0/1/1/1
3	MAN	4A	6	3	-	0/2/19/22	0/1/1/1
3	NAG	5	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	5	2	3	-	0/6/23/26	0/1/1/1
3	YZT	5	3	3	-	0/5/22/25	0/1/1/1
3	BGC	5	4	3	-	0/2/19/22	0/1/1/1
3	MAN	5	5	3	-	2/2/19/22	0/1/1/1
3	MAN	5	6	3	-	0/2/19/22	0/1/1/1
4	NAG	5A	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	5A	2	4	-	1/6/23/26	0/1/1/1
3	NAG	6	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	6	2	3	-	0/6/23/26	0/1/1/1
3	YZT	6	3	3	-	0/5/22/25	0/1/1/1
3	BGC	6	4	3	-	2/2/19/22	0/1/1/1
3	MAN	6	5	3	-	0/2/19/22	0/1/1/1
3	MAN	6	6	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	6A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	6A	2	3	-	0/6/23/26	0/1/1/1
3	YZT	6A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	6A	4	3	-	2/2/19/22	0/1/1/1
3	MAN	6A	5	3	-	0/2/19/22	0/1/1/1
3	MAN	6A	6	3	-	2/2/19/22	0/1/1/1
4	NAG	7	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	7	2	4	-	1/6/23/26	0/1/1/1
3	NAG	7A	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	7A	2	3	-	2/6/23/26	0/1/1/1
3	YZT	7A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	7A	4	3	-	0/2/19/22	0/1/1/1
3	MAN	7A	5	3	-	0/2/19/22	0/1/1/1
3	MAN	7A	6	3	-	0/2/19/22	0/1/1/1
3	NAG	8	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	8	2	3	-	0/6/23/26	0/1/1/1
3	YZT	8	3	3	-	0/5/22/25	0/1/1/1
3	BGC	8	4	3	-	2/2/19/22	0/1/1/1
3	MAN	8	5	3	-	0/2/19/22	0/1/1/1
3	MAN	8	6	3	-	2/2/19/22	0/1/1/1
2	NAG	8A	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	8A	2	2	-	2/6/23/26	0/1/1/1
2	YZT	8A	3	2	-	2/5/22/25	0/1/1/1
2	MAN	8A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	8A	5	2	-	0/2/19/22	0/1/1/1
3	NAG	9	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	9	2	3	-	2/6/23/26	0/1/1/1
3	YZT	9	3	3	-	0/5/22/25	0/1/1/1
3	BGC	9	4	3	-	0/2/19/22	0/1/1/1
3	MAN	9	5	3	-	0/2/19/22	0/1/1/1
3	MAN	9	6	3	-	0/2/19/22	0/1/1/1
3	NAG	9A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	9A	2	3	-	0/6/23/26	0/1/1/1
3	YZT	9A	3	3	-	0/5/22/25	0/1/1/1
3	BGC	9A	4	3	-	0/2/19/22	0/1/1/1
3	MAN	9A	5	3	-	2/2/19/22	0/1/1/1
3	MAN	9A	6	3	-	0/2/19/22	0/1/1/1
2	NAG	AA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YZT	AA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	AA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	AA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	AB	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	AB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	AB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	AB	4	3	-	2/2/19/22	0/1/1/1
3	MAN	AB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	AB	6	3	-	0/2/19/22	0/1/1/1
3	NAG	BA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	BA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	BA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	BA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	BA	6	3	-	0/2/19/22	0/1/1/1
4	NAG	BB	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	BB	2	4	-	1/6/23/26	0/1/1/1
3	NAG	CA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	CA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	CA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	CA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	CA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	CA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	CB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	CB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	CB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	CB	4	3	-	2/2/19/22	0/1/1/1
3	MAN	CB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	CB	6	3	-	2/2/19/22	0/1/1/1
4	NAG	DA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	DA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	DB	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	DB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	DB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	DB	4	3	-	0/2/19/22	0/1/1/1
3	MAN	DB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	DB	6	3	-	0/2/19/22	0/1/1/1
3	NAG	EA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	EA	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YZT	EA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	EA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	EA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	EA	6	3	-	2/2/19/22	0/1/1/1
2	NAG	EB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	EB	2	2	-	2/6/23/26	0/1/1/1
2	YZT	EB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	EB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	EB	5	2	-	0/2/19/22	0/1/1/1
3	NAG	FA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	FA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	FA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	FA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	FA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	FA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	FB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	FB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	FB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	FB	4	3	-	0/2/19/22	0/1/1/1
3	MAN	FB	5	3	-	2/2/19/22	0/1/1/1
3	MAN	FB	6	3	-	0/2/19/22	0/1/1/1
2	NAG	GA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	GA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	GA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	GA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	GB	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	GB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	GB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	GB	4	3	-	2/2/19/22	0/1/1/1
3	MAN	GB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	GB	6	3	-	0/2/19/22	0/1/1/1
3	NAG	HA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	HA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	HA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	HA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	HA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	HA	6	3	-	0/2/19/22	0/1/1/1
4	NAG	HB	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	HB	2	4	-	1/6/23/26	0/1/1/1
3	NAG	IA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	IA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	IA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	IA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	IA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	IA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	IB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	IB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	IB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	IB	4	3	-	2/2/19/22	0/1/1/1
3	MAN	IB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	IB	6	3	-	2/2/19/22	0/1/1/1
4	NAG	JA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	JA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	JB	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	JB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	JB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	JB	4	3	-	0/2/19/22	0/1/1/1
3	MAN	JB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	JB	6	3	-	0/2/19/22	0/1/1/1
3	NAG	KA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	KA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	KA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	KA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	KA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	KA	6	3	-	2/2/19/22	0/1/1/1
2	NAG	KB	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	KB	2	2	-	2/6/23/26	0/1/1/1
2	YZT	KB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	KB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	KB	5	2	-	0/2/19/22	0/1/1/1
3	NAG	LA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	LA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	LA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	LA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	LA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	LA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	LB	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	LB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	LB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	LB	4	3	-	0/2/19/22	0/1/1/1
3	MAN	LB	5	3	-	2/2/19/22	0/1/1/1
3	MAN	LB	6	3	-	0/2/19/22	0/1/1/1
2	NAG	MA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	MA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	MA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	MA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	MB	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	MB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	MB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	MB	4	3	-	2/2/19/22	0/1/1/1
3	MAN	MB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	MB	6	3	-	0/2/19/22	0/1/1/1
3	NAG	NA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	NA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	NA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	NA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	NA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	NA	6	3	-	0/2/19/22	0/1/1/1
4	NAG	NB	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	NB	2	4	-	1/6/23/26	0/1/1/1
3	NAG	OA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	OA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	OA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	OA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	OA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	OA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	OB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	OB	2	3	-	0/6/23/26	0/1/1/1
3	YZT	OB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	OB	4	3	-	2/2/19/22	0/1/1/1
3	MAN	OB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	OB	6	3	-	2/2/19/22	0/1/1/1
4	NAG	PA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	PA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	PB	1	1,3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	PB	2	3	-	2/6/23/26	0/1/1/1
3	YZT	PB	3	3	-	0/5/22/25	0/1/1/1
3	BGC	PB	4	3	-	0/2/19/22	0/1/1/1
3	MAN	PB	5	3	-	0/2/19/22	0/1/1/1
3	MAN	PB	6	3	-	0/2/19/22	0/1/1/1
3	NAG	QA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	QA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	QA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	QA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	QA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	QA	6	3	-	2/2/19/22	0/1/1/1
3	NAG	RA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	RA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	RA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	RA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	RA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	RA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	SA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	SA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	SA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	SA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	TA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	TA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	TA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	TA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	TA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	TA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	YZT	U	3	2	-	2/5/22/25	0/1/1/1
2	MAN	U	4	2	-	0/2/19/22	0/1/1/1
2	MAN	U	5	2	-	0/2/19/22	0/1/1/1
3	NAG	UA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	UA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	UA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	UA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	UA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	UA	6	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	YZT	V	3	3	-	0/5/22/25	0/1/1/1
3	BGC	V	4	3	-	0/2/19/22	0/1/1/1
3	MAN	V	5	3	-	2/2/19/22	0/1/1/1
3	MAN	V	6	3	-	0/2/19/22	0/1/1/1
4	NAG	VA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	VA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	YZT	W	3	3	-	0/5/22/25	0/1/1/1
3	BGC	W	4	3	-	2/2/19/22	0/1/1/1
3	MAN	W	5	3	-	0/2/19/22	0/1/1/1
3	MAN	W	6	3	-	0/2/19/22	0/1/1/1
3	NAG	WA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	WA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	WA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	WA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	WA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	WA	6	3	-	2/2/19/22	0/1/1/1
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	1/6/23/26	0/1/1/1
3	NAG	XA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	XA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	XA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	XA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	XA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	XA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	YZT	Y	3	3	-	0/5/22/25	0/1/1/1
3	BGC	Y	4	3	-	2/2/19/22	0/1/1/1
3	MAN	Y	5	3	-	0/2/19/22	0/1/1/1
3	MAN	Y	6	3	-	2/2/19/22	0/1/1/1
2	NAG	YA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	YA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	YA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	YA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	YA	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Z	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	YZT	Z	3	3	-	0/5/22/25	0/1/1/1
3	BGC	Z	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Z	5	3	-	0/2/19/22	0/1/1/1
3	MAN	Z	6	3	-	0/2/19/22	0/1/1/1
3	NAG	ZA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	ZA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	ZA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	ZA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	ZA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	ZA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	a	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1
2	YZT	a	3	2	-	2/5/22/25	0/1/1/1
2	MAN	a	4	2	-	0/2/19/22	0/1/1/1
2	MAN	a	5	2	-	0/2/19/22	0/1/1/1
3	NAG	aA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	aA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	aA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	aA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	aA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	aA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	b	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
3	YZT	b	3	3	-	0/5/22/25	0/1/1/1
3	BGC	b	4	3	-	0/2/19/22	0/1/1/1
3	MAN	b	5	3	-	2/2/19/22	0/1/1/1
3	MAN	b	6	3	-	0/2/19/22	0/1/1/1
4	NAG	bA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	bA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	YZT	c	3	3	-	0/5/22/25	0/1/1/1
3	BGC	c	4	3	-	2/2/19/22	0/1/1/1
3	MAN	c	5	3	-	0/2/19/22	0/1/1/1
3	MAN	c	6	3	-	0/2/19/22	0/1/1/1
3	NAG	cA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	cA	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YZT	cA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	cA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	cA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	cA	6	3	-	2/2/19/22	0/1/1/1
4	NAG	d	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	1/6/23/26	0/1/1/1
3	NAG	dA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	dA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	dA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	dA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	dA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	dA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	e	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	YZT	e	3	3	-	0/5/22/25	0/1/1/1
3	BGC	e	4	3	-	2/2/19/22	0/1/1/1
3	MAN	e	5	3	-	0/2/19/22	0/1/1/1
3	MAN	e	6	3	-	2/2/19/22	0/1/1/1
2	NAG	eA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	eA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	eA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	eA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	eA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	f	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	YZT	f	3	3	-	0/5/22/25	0/1/1/1
3	BGC	f	4	3	-	0/2/19/22	0/1/1/1
3	MAN	f	5	3	-	0/2/19/22	0/1/1/1
3	MAN	f	6	3	-	0/2/19/22	0/1/1/1
3	NAG	fA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	fA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	fA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	fA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	fA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	fA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	g	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	YZT	g	3	2	-	2/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	g	4	2	-	0/2/19/22	0/1/1/1
2	MAN	g	5	2	-	0/2/19/22	0/1/1/1
3	NAG	gA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	gA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	gA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	gA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	gA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	gA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	h	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
3	YZT	h	3	3	-	0/5/22/25	0/1/1/1
3	BGC	h	4	3	-	0/2/19/22	0/1/1/1
3	MAN	h	5	3	-	2/2/19/22	0/1/1/1
3	MAN	h	6	3	-	0/2/19/22	0/1/1/1
4	NAG	hA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	hA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	i	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	i	2	3	-	0/6/23/26	0/1/1/1
3	YZT	i	3	3	-	0/5/22/25	0/1/1/1
3	BGC	i	4	3	-	2/2/19/22	0/1/1/1
3	MAN	i	5	3	-	0/2/19/22	0/1/1/1
3	MAN	i	6	3	-	0/2/19/22	0/1/1/1
3	NAG	iA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	iA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	iA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	iA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	iA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	iA	6	3	-	2/2/19/22	0/1/1/1
4	NAG	j	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	1/6/23/26	0/1/1/1
3	NAG	jA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	jA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	jA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	jA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	jA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	jA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	k	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	0/6/23/26	0/1/1/1
3	YZT	k	3	3	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	k	4	3	-	2/2/19/22	0/1/1/1
3	MAN	k	5	3	-	0/2/19/22	0/1/1/1
3	MAN	k	6	3	-	2/2/19/22	0/1/1/1
2	NAG	kA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	kA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	kA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	kA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	kA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	l	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	YZT	l	3	3	-	0/5/22/25	0/1/1/1
3	BGC	l	4	3	-	0/2/19/22	0/1/1/1
3	MAN	l	5	3	-	0/2/19/22	0/1/1/1
3	MAN	l	6	3	-	0/2/19/22	0/1/1/1
3	NAG	lA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	lA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	lA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	lA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	lA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	lA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	m	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	YZT	m	3	2	-	2/5/22/25	0/1/1/1
2	MAN	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	m	5	2	-	0/2/19/22	0/1/1/1
3	NAG	mA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	mA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	mA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	mA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	mA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	mA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	n	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	YZT	n	3	3	-	0/5/22/25	0/1/1/1
3	BGC	n	4	3	-	0/2/19/22	0/1/1/1
3	MAN	n	5	3	-	2/2/19/22	0/1/1/1
3	MAN	n	6	3	-	0/2/19/22	0/1/1/1
4	NAG	nA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	nA	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	o	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	o	2	3	-	0/6/23/26	0/1/1/1
3	YZT	o	3	3	-	0/5/22/25	0/1/1/1
3	BGC	o	4	3	-	2/2/19/22	0/1/1/1
3	MAN	o	5	3	-	0/2/19/22	0/1/1/1
3	MAN	o	6	3	-	0/2/19/22	0/1/1/1
3	NAG	oA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	oA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	oA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	oA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	oA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	oA	6	3	-	2/2/19/22	0/1/1/1
4	NAG	p	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	1/6/23/26	0/1/1/1
3	NAG	pA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	pA	2	3	-	2/6/23/26	0/1/1/1
3	YZT	pA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	pA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	pA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	pA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	YZT	q	3	3	-	0/5/22/25	0/1/1/1
3	BGC	q	4	3	-	2/2/19/22	0/1/1/1
3	MAN	q	5	3	-	0/2/19/22	0/1/1/1
3	MAN	q	6	3	-	2/2/19/22	0/1/1/1
2	NAG	qA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	qA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	qA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	qA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	r	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	r	2	3	-	2/6/23/26	0/1/1/1
3	YZT	r	3	3	-	0/5/22/25	0/1/1/1
3	BGC	r	4	3	-	0/2/19/22	0/1/1/1
3	MAN	r	5	3	-	0/2/19/22	0/1/1/1
3	MAN	r	6	3	-	0/2/19/22	0/1/1/1
3	NAG	rA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	rA	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YZT	rA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	rA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	rA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	rA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	s	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
2	YZT	s	3	2	-	2/5/22/25	0/1/1/1
2	MAN	s	4	2	-	0/2/19/22	0/1/1/1
2	MAN	s	5	2	-	0/2/19/22	0/1/1/1
3	NAG	sA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	sA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	sA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	sA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	sA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	sA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	t	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	t	2	3	-	0/6/23/26	0/1/1/1
3	YZT	t	3	3	-	0/5/22/25	0/1/1/1
3	BGC	t	4	3	-	0/2/19/22	0/1/1/1
3	MAN	t	5	3	-	2/2/19/22	0/1/1/1
3	MAN	t	6	3	-	0/2/19/22	0/1/1/1
4	NAG	tA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	tA	2	4	-	1/6/23/26	0/1/1/1
3	NAG	u	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	u	2	3	-	0/6/23/26	0/1/1/1
3	YZT	u	3	3	-	0/5/22/25	0/1/1/1
3	BGC	u	4	3	-	2/2/19/22	0/1/1/1
3	MAN	u	5	3	-	0/2/19/22	0/1/1/1
3	MAN	u	6	3	-	0/2/19/22	0/1/1/1
3	NAG	uA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	uA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	uA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	uA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	uA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	uA	6	3	-	2/2/19/22	0/1/1/1
4	NAG	v	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	v	2	4	-	1/6/23/26	0/1/1/1
3	NAG	vA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	vA	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YZT	vA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	vA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	vA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	vA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	w	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	w	2	3	-	0/6/23/26	0/1/1/1
3	YZT	w	3	3	-	0/5/22/25	0/1/1/1
3	BGC	w	4	3	-	2/2/19/22	0/1/1/1
3	MAN	w	5	3	-	0/2/19/22	0/1/1/1
3	MAN	w	6	3	-	2/2/19/22	0/1/1/1
2	NAG	wA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	2/6/23/26	0/1/1/1
2	YZT	wA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	wA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	wA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	x	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	x	2	3	-	2/6/23/26	0/1/1/1
3	YZT	x	3	3	-	0/5/22/25	0/1/1/1
3	BGC	x	4	3	-	0/2/19/22	0/1/1/1
3	MAN	x	5	3	-	0/2/19/22	0/1/1/1
3	MAN	x	6	3	-	0/2/19/22	0/1/1/1
3	NAG	xA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	xA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	xA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	xA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	xA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	xA	6	3	-	0/2/19/22	0/1/1/1
2	NAG	y	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	y	2	2	-	2/6/23/26	0/1/1/1
2	YZT	y	3	2	-	2/5/22/25	0/1/1/1
2	MAN	y	4	2	-	0/2/19/22	0/1/1/1
2	MAN	y	5	2	-	0/2/19/22	0/1/1/1
3	NAG	yA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	yA	2	3	-	0/6/23/26	0/1/1/1
3	YZT	yA	3	3	-	0/5/22/25	0/1/1/1
3	BGC	yA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	yA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	yA	6	3	-	0/2/19/22	0/1/1/1
3	NAG	z	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	z	2	3	-	0/6/23/26	0/1/1/1
3	YZT	z	3	3	-	0/5/22/25	0/1/1/1
3	BGC	z	4	3	-	0/2/19/22	0/1/1/1
3	MAN	z	5	3	-	2/2/19/22	0/1/1/1
3	MAN	z	6	3	-	0/2/19/22	0/1/1/1
4	NAG	zA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	zA	2	4	-	1/6/23/26	0/1/1/1

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	XA	3	YZT	O2S6-S6	3.80	1.55	1.45
3	FA	3	YZT	O2S6-S6	3.80	1.55	1.45
3	RA	3	YZT	O2S6-S6	3.80	1.55	1.45
3	3	3	YZT	O2S6-S6	3.78	1.55	1.45
3	r	3	YZT	O2S6-S6	3.78	1.55	1.45

The worst 5 of 513 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	yA	2	NAG	C1-O5-C5	7.29	121.96	112.19
3	AB	2	NAG	C1-O5-C5	7.29	121.95	112.19
3	gA	2	NAG	C1-O5-C5	7.28	121.95	112.19
3	CA	2	NAG	C1-O5-C5	7.28	121.94	112.19
3	i	2	NAG	C1-O5-C5	7.27	121.93	112.19

There are no chirality outliers.

5 of 520 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	U	3	YZT	O5-C5-C6-S6
2	a	3	YZT	O5-C5-C6-S6
2	g	3	YZT	O5-C5-C6-S6
2	m	3	YZT	O5-C5-C6-S6
2	s	3	YZT	O5-C5-C6-S6

There are no ring outliers.

191 monomers are involved in 158 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1A	3	YZT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	RA	2	NAG	2	0
3	sA	5	MAN	1	0
3	Z	2	NAG	2	0
3	FA	5	MAN	3	0
3	BA	2	NAG	1	0
3	9	2	NAG	2	0
3	jA	6	MAN	2	0
2	2A	2	NAG	1	0
3	Z	6	MAN	2	0
3	OA	5	MAN	1	0
3	xA	6	MAN	1	0
3	3	3	YZT	1	0
3	NA	2	NAG	1	0
3	jA	3	YZT	1	0
3	RA	6	MAN	2	0
3	JB	5	MAN	3	0
3	u	5	MAN	1	0
3	l	5	MAN	3	0
3	GB	5	MAN	1	0
3	IA	3	YZT	1	0
3	7A	2	NAG	2	0
2	a	5	MAN	1	0
3	Z	3	YZT	1	0
3	NA	6	MAN	1	0
3	pA	6	MAN	2	0
3	RA	3	YZT	1	0
3	vA	5	MAN	3	0
3	PB	5	MAN	3	0
3	9	6	MAN	2	0
3	dA	3	YZT	1	0
3	pA	3	YZT	1	0
2	AA	5	MAN	1	0
3	TA	2	NAG	1	0
3	9A	6	MAN	1	0
2	a	2	NAG	1	0
3	mA	3	YZT	1	0
3	XA	6	MAN	2	0
3	gA	5	MAN	1	0
3	PB	2	NAG	2	0
3	9	5	MAN	3	0
3	x	3	YZT	1	0
2	AA	2	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	5	6	MAN	1	0
3	XA	3	YZT	1	0
2	kA	2	NAG	1	0
3	u	3	YZT	1	0
3	t	6	MAN	1	0
3	x	5	MAN	3	0
2	KB	5	MAN	1	0
2	qA	2	NAG	1	0
2	U	5	MAN	1	0
3	W	3	YZT	1	0
3	sA	3	YZT	1	0
3	7A	6	MAN	3	0
3	6	5	MAN	1	0
3	i	5	MAN	1	0
3	FA	2	NAG	2	0
3	f	3	YZT	1	0
3	n	6	MAN	1	0
3	7A	3	YZT	1	0
3	x	6	MAN	3	0
3	DB	2	NAG	2	0
3	r	3	YZT	1	0
2	KB	2	NAG	1	0
3	LB	2	NAG	1	0
3	o	5	MAN	1	0
2	wA	2	NAG	1	0
3	vA	2	NAG	2	0
3	PB	3	YZT	1	0
3	c	5	MAN	1	0
2	wA	5	MAN	1	0
2	8A	2	NAG	1	0
3	f	6	MAN	2	0
3	DB	6	MAN	2	0
2	y	2	NAG	1	0
3	XA	2	NAG	2	0
3	DB	5	MAN	3	0
3	z	2	NAG	1	0
3	9	3	YZT	1	0
3	FB	6	MAN	1	0
2	MA	5	MAN	1	0
3	3	6	MAN	2	0
3	z	6	MAN	1	0
3	0	3	YZT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	0	5	MAN	1	0
3	1A	6	MAN	2	0
3	LA	3	YZT	1	0
2	g	5	MAN	1	0
3	jA	5	MAN	3	0
3	LA	5	MAN	3	0
3	JB	6	MAN	2	0
3	r	5	MAN	3	0
3	pA	5	MAN	3	0
2	YA	5	MAN	1	0
3	pA	2	NAG	2	0
2	2A	5	MAN	1	0
3	lA	6	MAN	1	0
3	rA	6	MAN	1	0
3	6	3	YZT	1	0
2	8A	5	MAN	1	0
3	q	2	NAG	1	0
3	LA	6	MAN	2	0
3	RA	5	MAN	3	0
3	dA	6	MAN	2	0
3	3A	2	NAG	1	0
3	Z	5	MAN	3	0
2	MA	2	NAG	1	0
3	3	5	MAN	3	0
3	1A	5	MAN	3	0
3	ZA	2	NAG	1	0
3	FA	3	YZT	1	0
3	AB	5	MAN	1	0
3	xA	2	NAG	1	0
3	f	5	MAN	3	0
3	mA	5	MAN	1	0
3	UA	3	YZT	1	0
3	UA	5	MAN	1	0
3	n	2	NAG	1	0
3	fA	6	MAN	1	0
3	HA	2	NAG	1	0
3	TA	6	MAN	1	0
3	V	2	NAG	1	0
3	fA	2	NAG	1	0
3	DB	3	YZT	1	0
3	CA	3	YZT	1	0
3	aA	5	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	OA	3	YZT	1	0
3	V	6	MAN	1	0
3	l	6	MAN	2	0
3	t	2	NAG	1	0
3	W	5	MAN	1	0
3	HA	6	MAN	1	0
3	JB	3	YZT	1	0
3	dA	5	MAN	3	0
3	l	3	YZT	1	0
3	GB	3	YZT	1	0
3	c	3	YZT	1	0
2	s	5	MAN	1	0
3	7A	5	MAN	3	0
3	jA	2	NAG	2	0
3	b	6	MAN	1	0
3	r	2	NAG	2	0
2	YA	2	NAG	1	0
3	IA	5	MAN	1	0
3	MB	3	YZT	1	0
3	h	6	MAN	1	0
3	x	2	NAG	2	0
3	BA	6	MAN	1	0
3	3A	6	MAN	1	0
3	r	6	MAN	2	0
3	4A	5	MAN	1	0
3	PB	6	MAN	2	0
3	LA	2	NAG	2	0
3	yA	5	MAN	1	0
3	lA	2	NAG	1	0
3	i	3	YZT	1	0
3	1A	2	NAG	2	0
3	MB	5	MAN	1	0
3	gA	3	YZT	1	0
3	LB	6	MAN	1	0
3	aA	3	YZT	1	0
3	f	2	NAG	2	0
3	5	2	NAG	1	0
2	U	2	NAG	1	0
3	yA	3	YZT	1	0
3	ZA	6	MAN	1	0
2	g	2	NAG	1	0
3	FA	6	MAN	2	0

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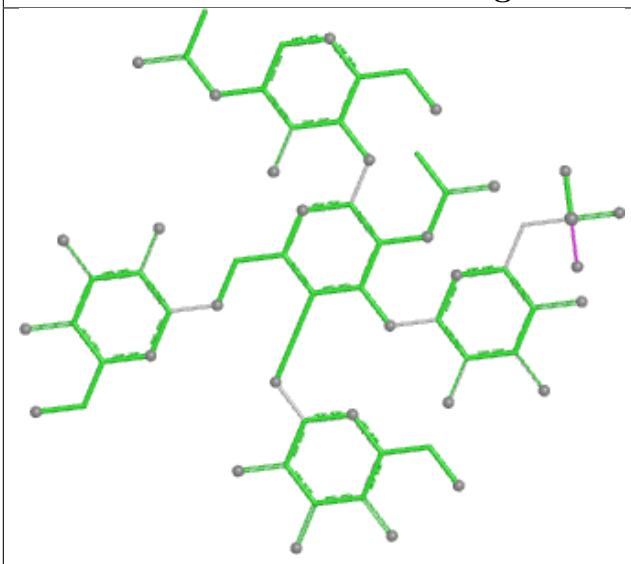
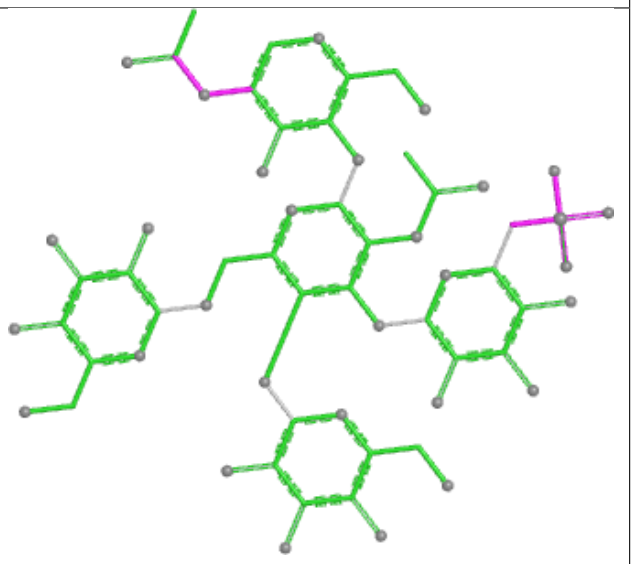
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4	5	MAN	1	0
3	AB	3	YZT	1	0
2	4	2	NAG	1	0
3	XA	5	MAN	3	0
3	FB	2	NAG	1	0
3	vA	3	YZT	1	0
3	3	2	NAG	2	0
3	9A	2	NAG	1	0
3	o	3	YZT	1	0
3	b	2	NAG	1	0
3	dA	2	NAG	2	0
3	l	2	NAG	2	0
3	vA	6	MAN	2	0
2	kA	5	MAN	1	0
2	s	2	NAG	1	0
3	h	2	NAG	1	0
3	4A	3	YZT	1	0
2	y	5	MAN	1	0
3	CA	5	MAN	1	0
2	qA	5	MAN	1	0
3	rA	2	NAG	1	0
3	JB	2	NAG	2	0

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

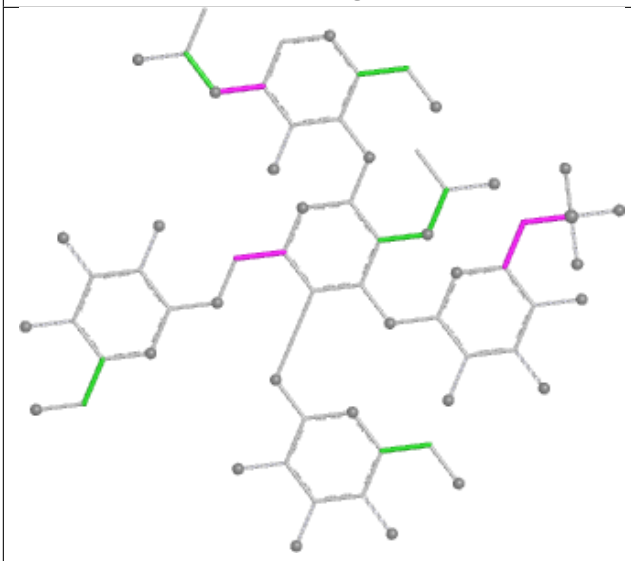
Oligosaccharide Chain U



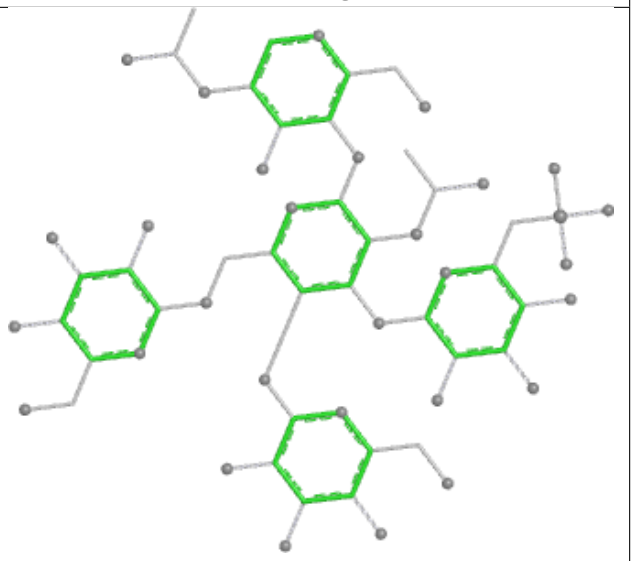
Bond lengths



Bond angles

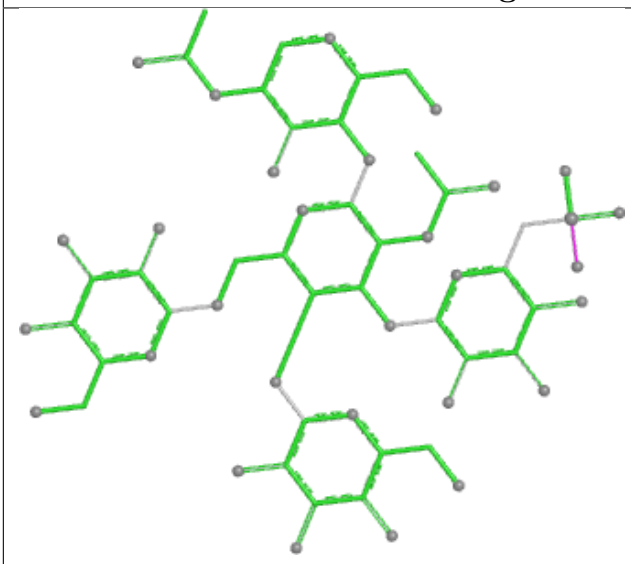


Torsions



Rings

Oligosaccharide Chain a



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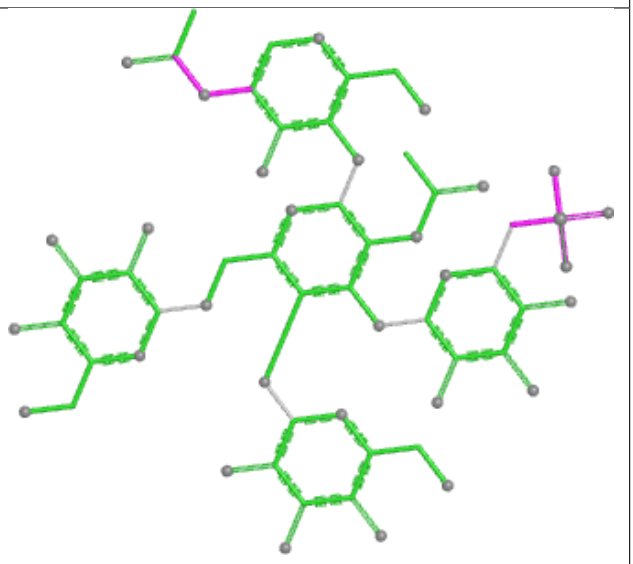
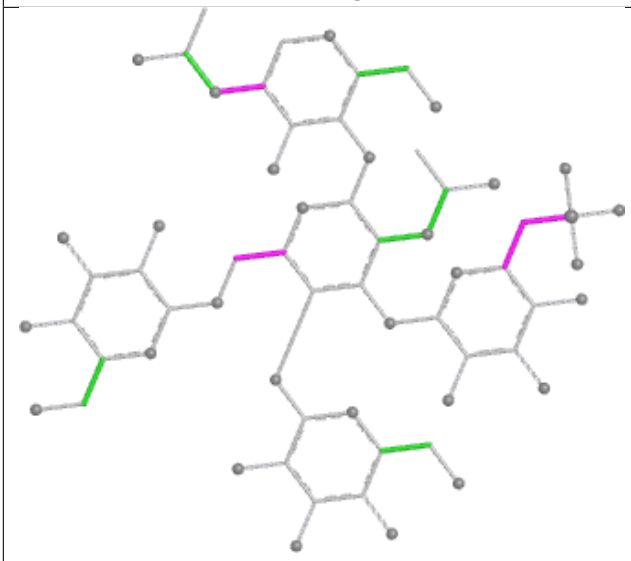
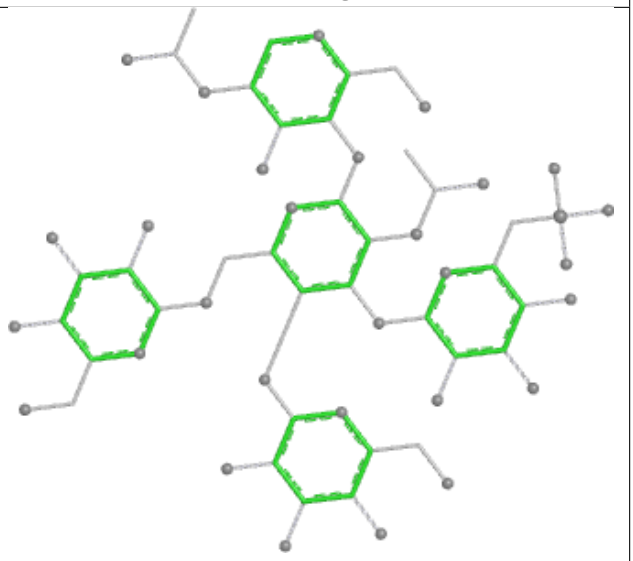


Bond angles

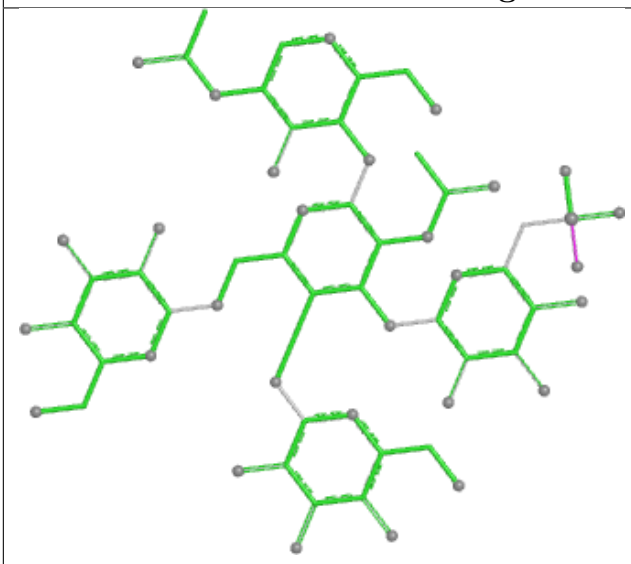


Torsions

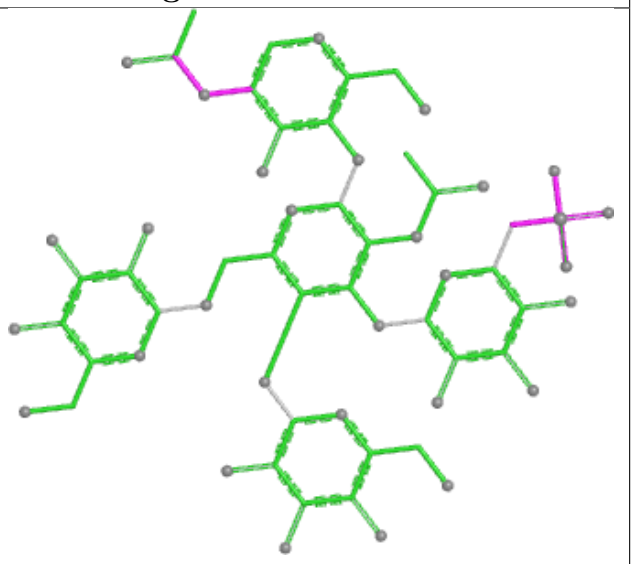


Rings

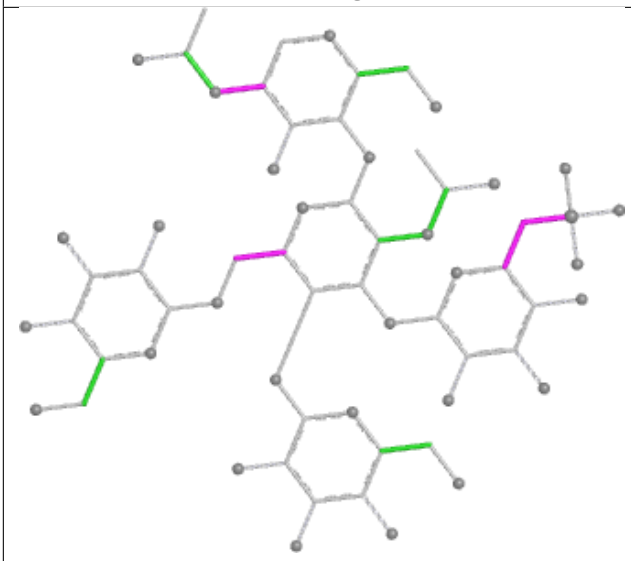
Oligosaccharide Chain g



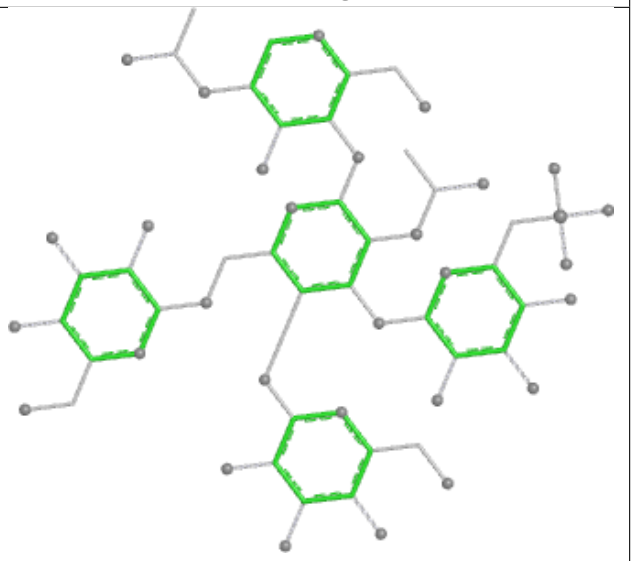
Bond lengths



Bond angles

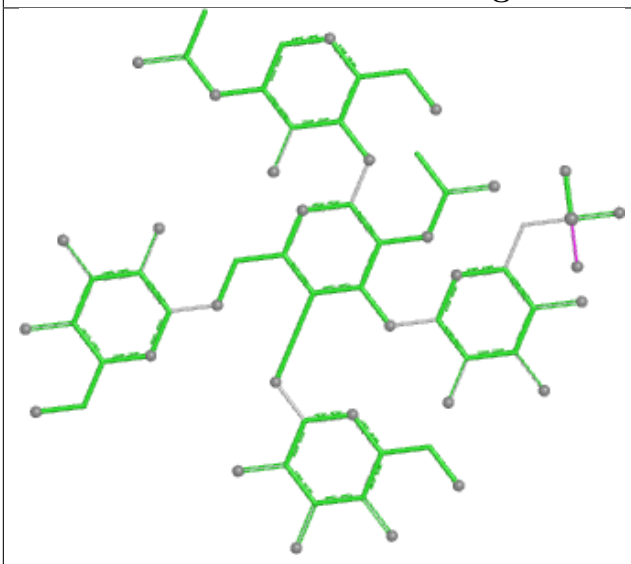


Torsions

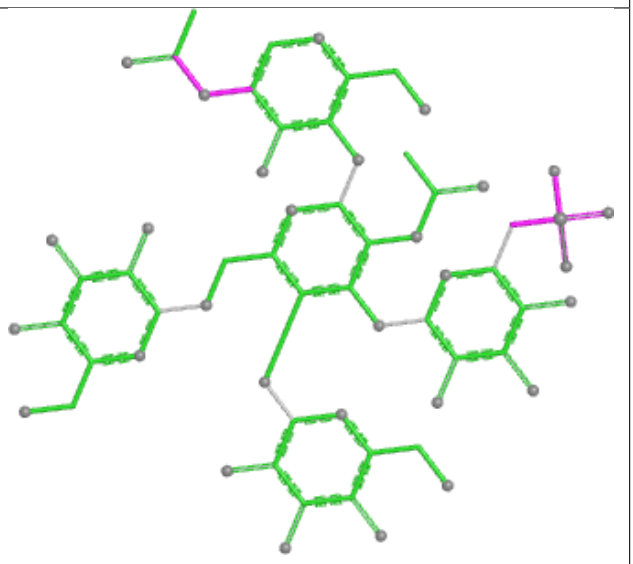


Rings

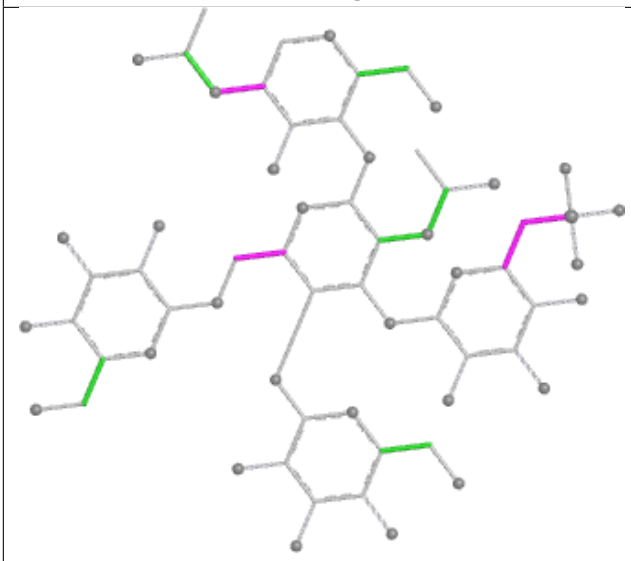
Oligosaccharide Chain m



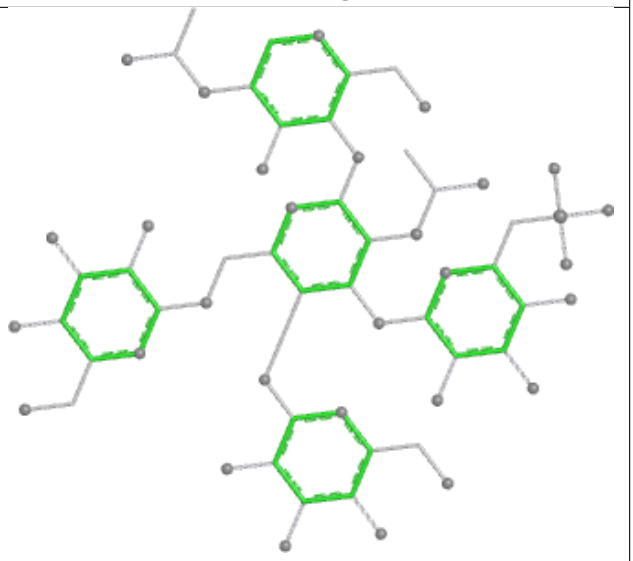
Bond lengths



Bond angles

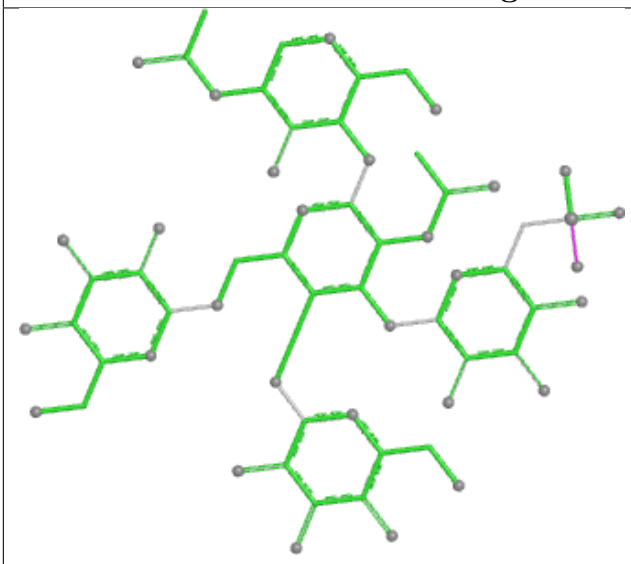


Torsions

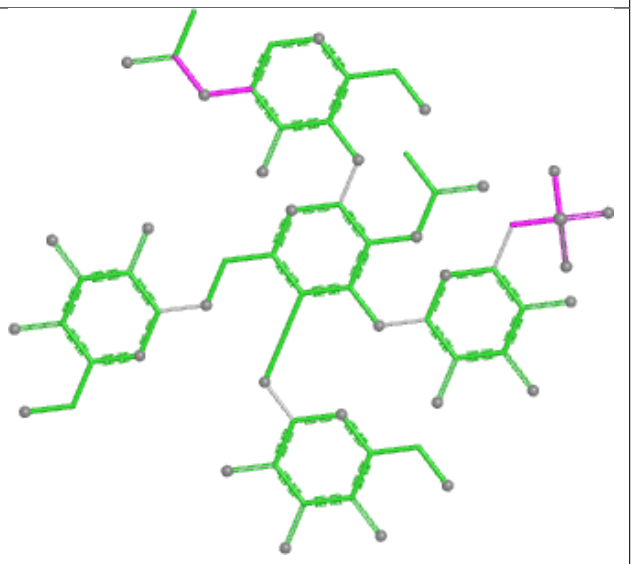


Rings

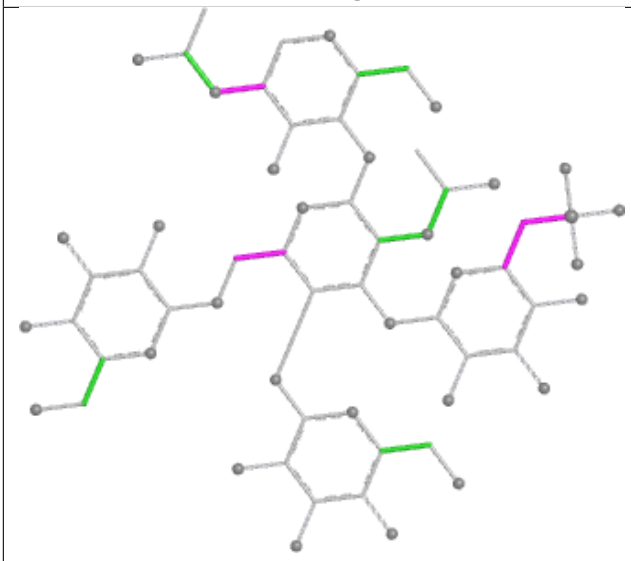
Oligosaccharide Chain s



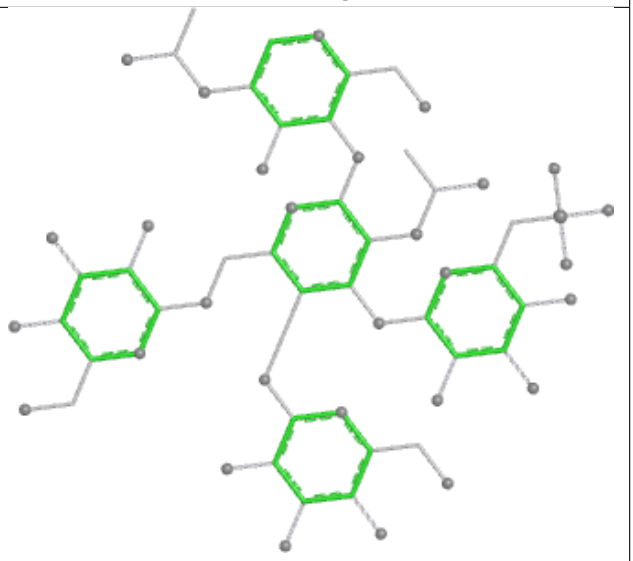
Bond lengths



Bond angles

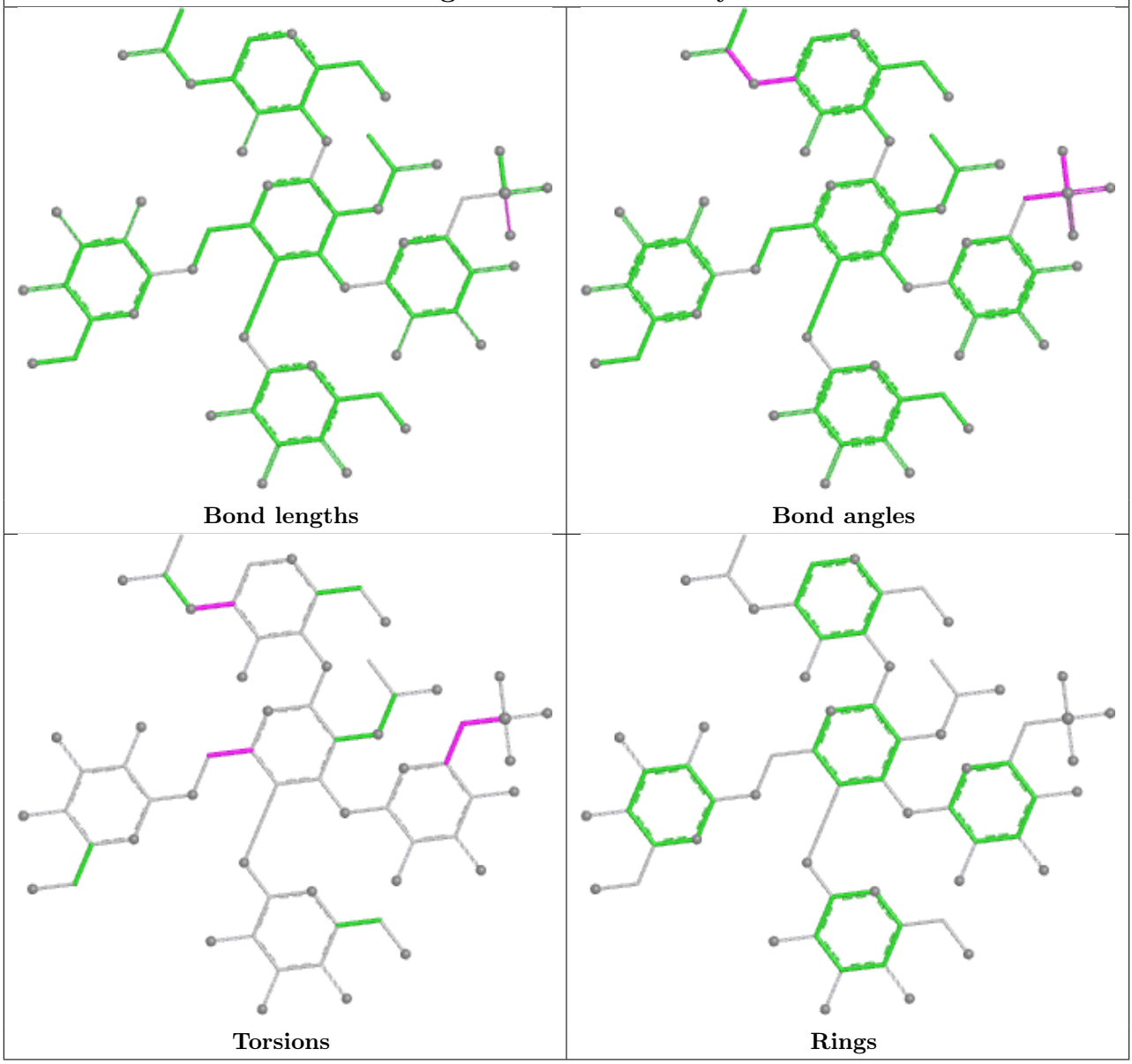


Torsions



Rings

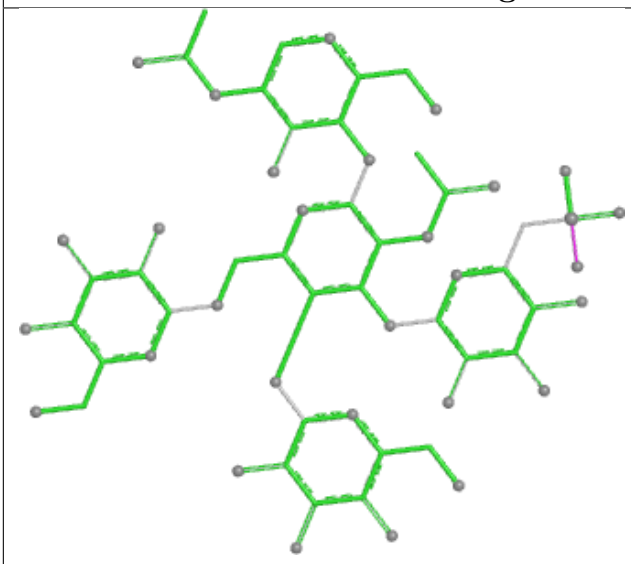
Oligosaccharide Chain y



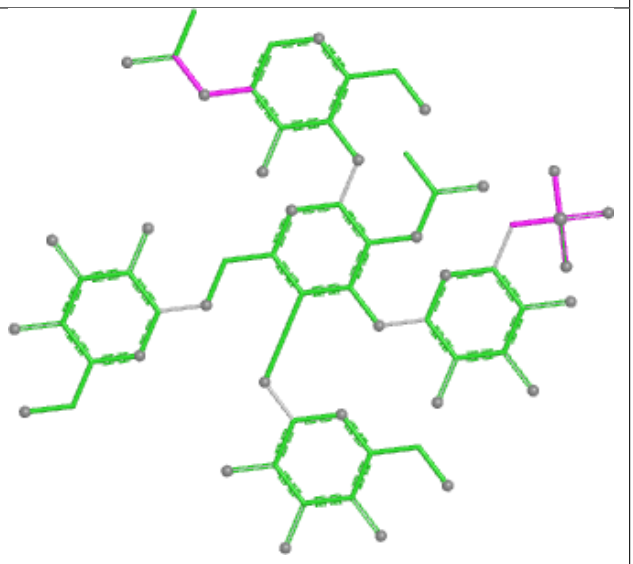
Bond lengths | **Bond angles**

Torsions | **Rings**

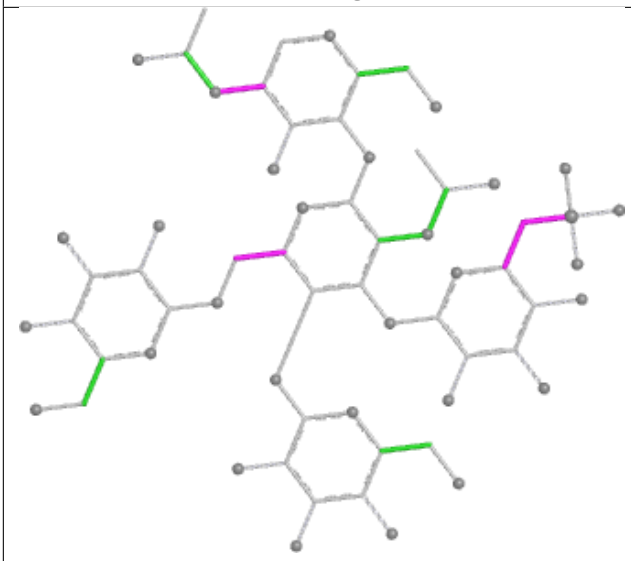
Oligosaccharide Chain 4



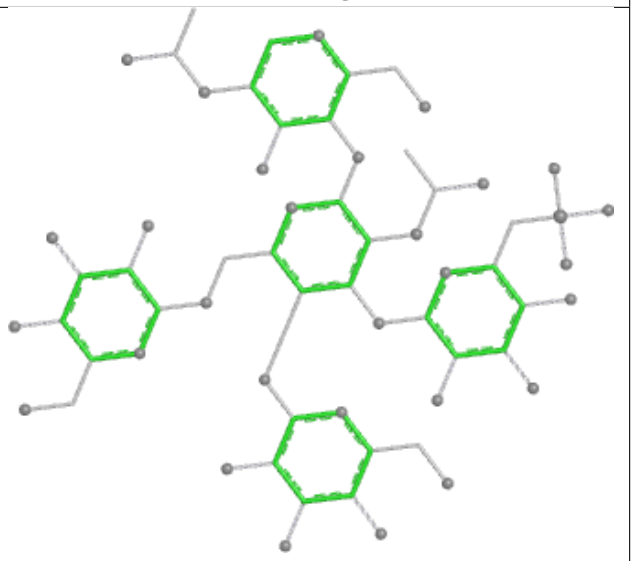
Bond lengths



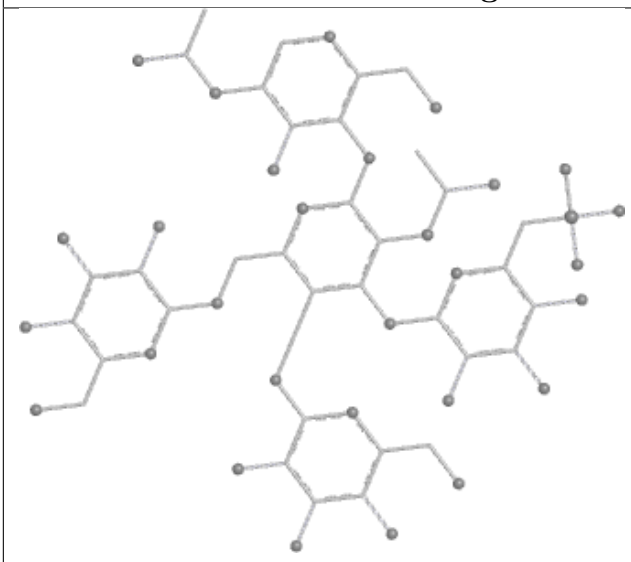
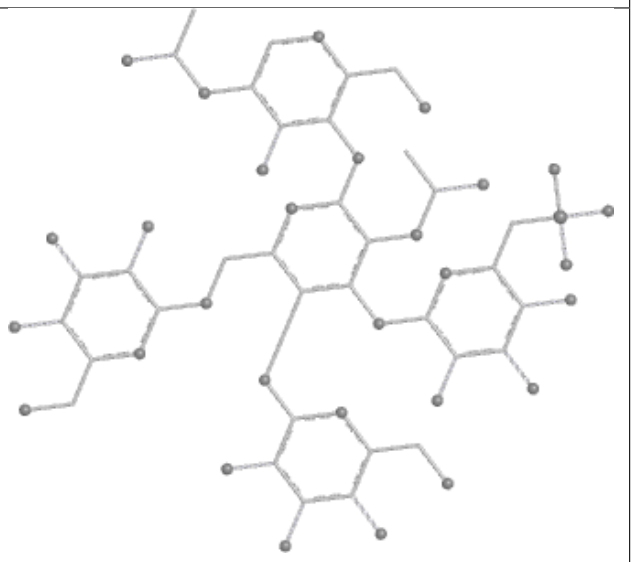
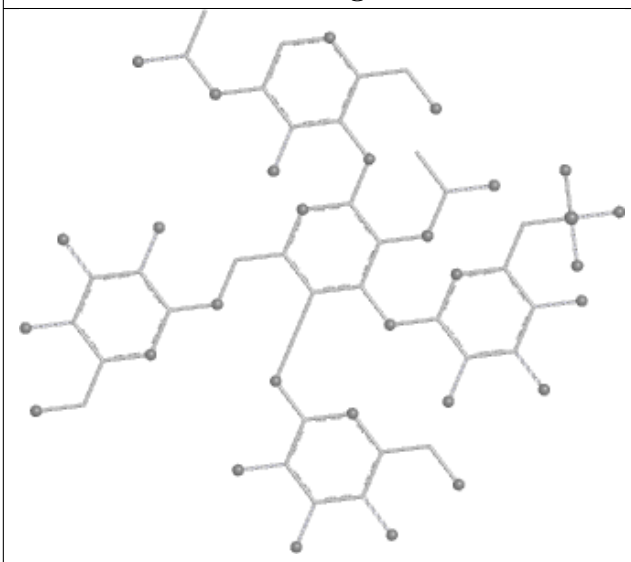
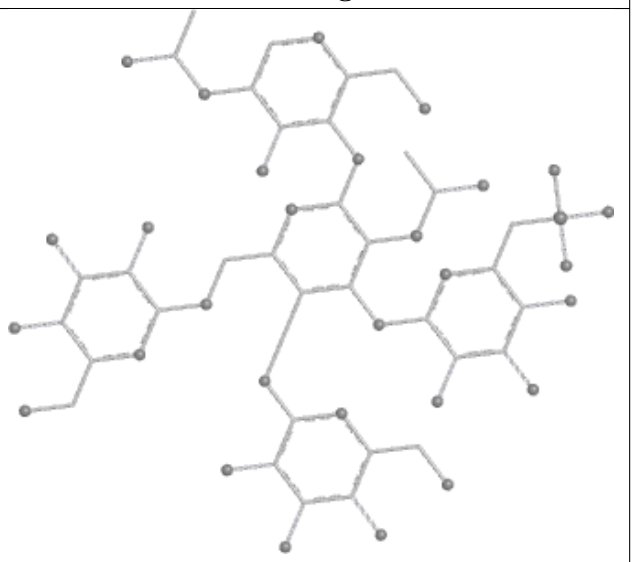
Bond angles



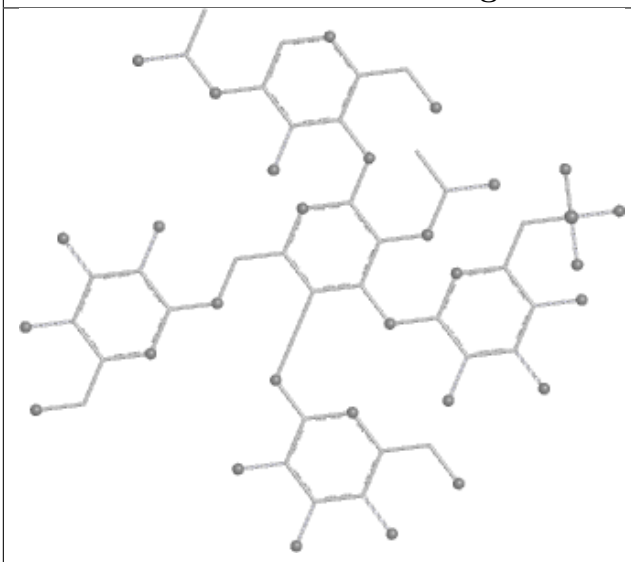
Torsions



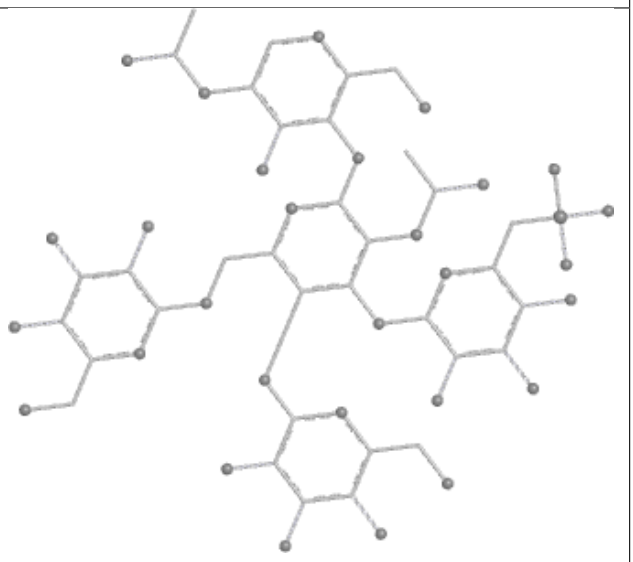
Rings

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

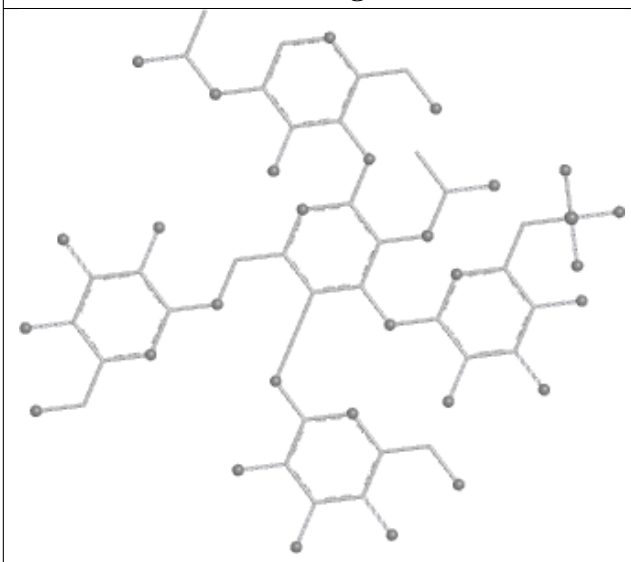
Oligosaccharide Chain GA



Bond lengths



Bond angles



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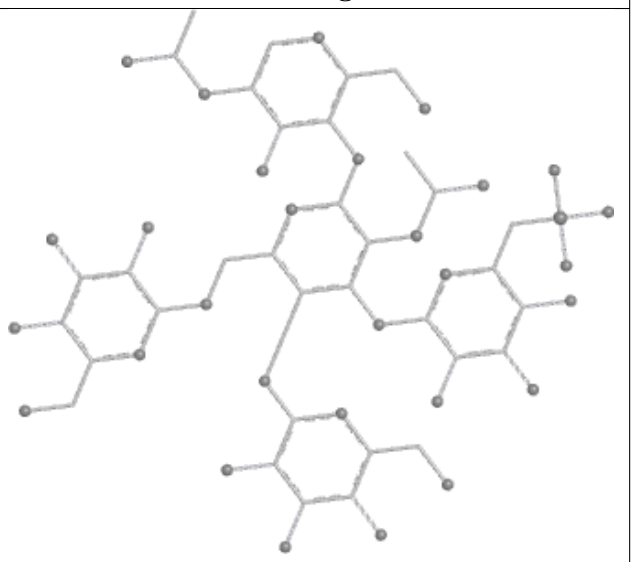
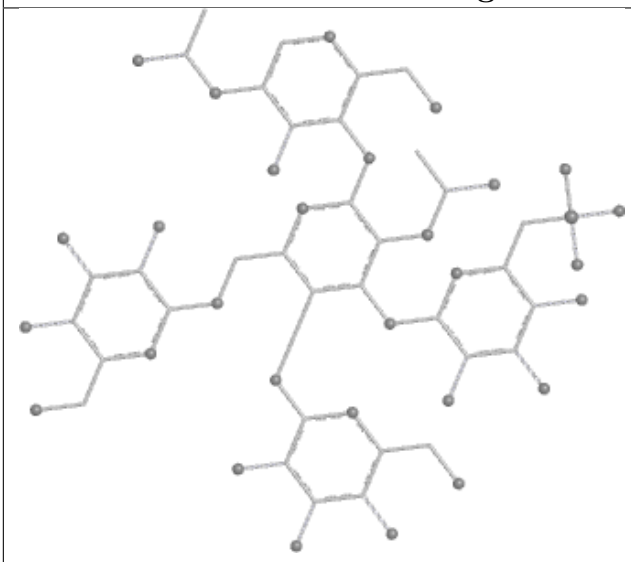
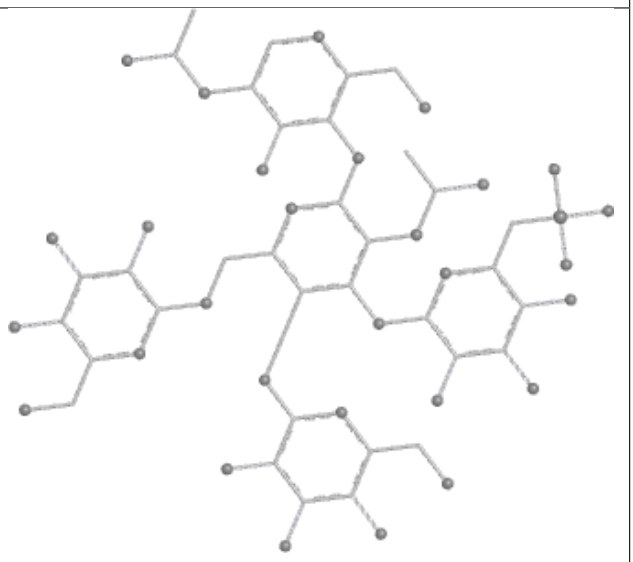


Rings

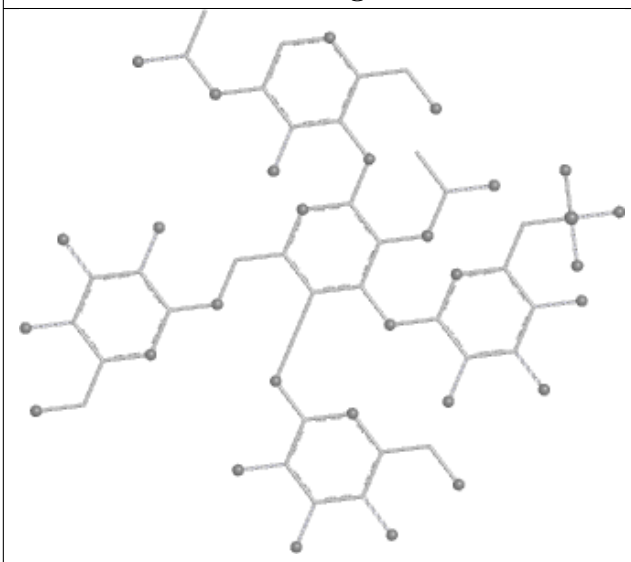
Oligosaccharide Chain MA



Bond lengths



Bond angles



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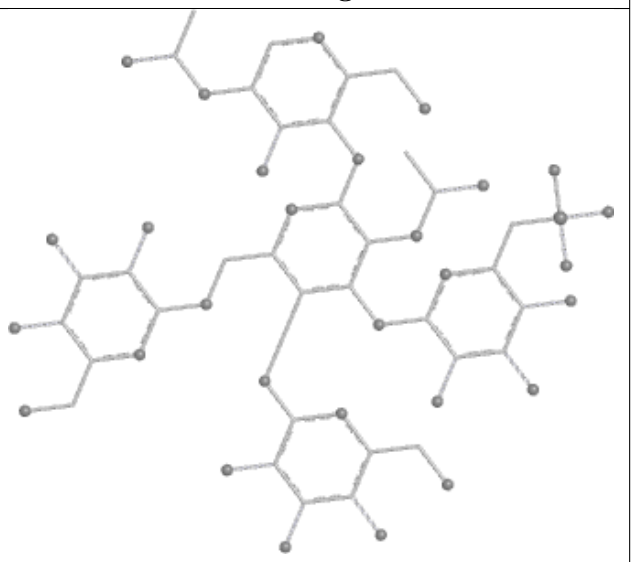
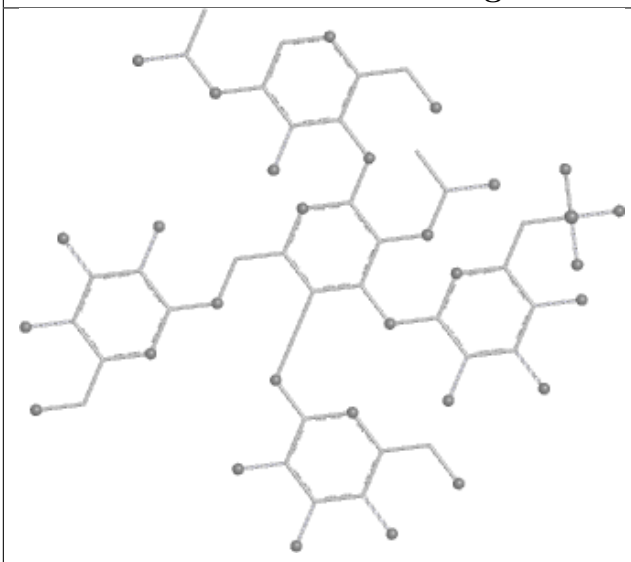
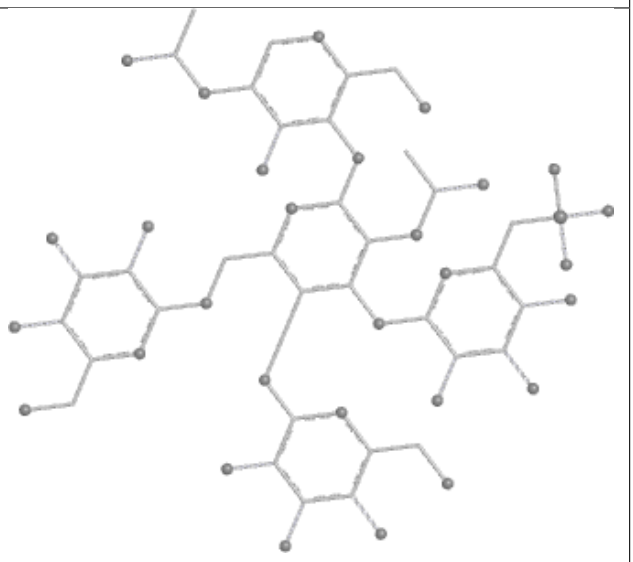
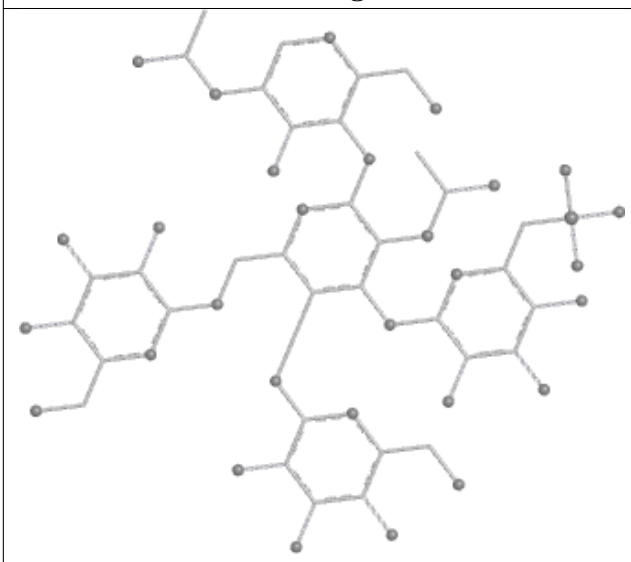
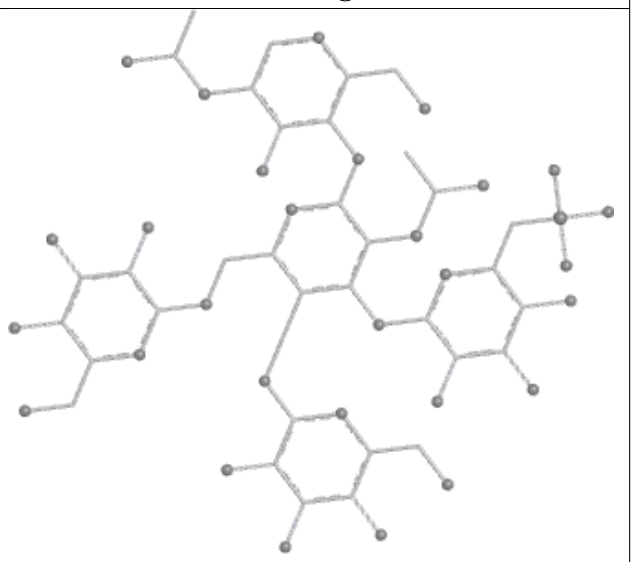
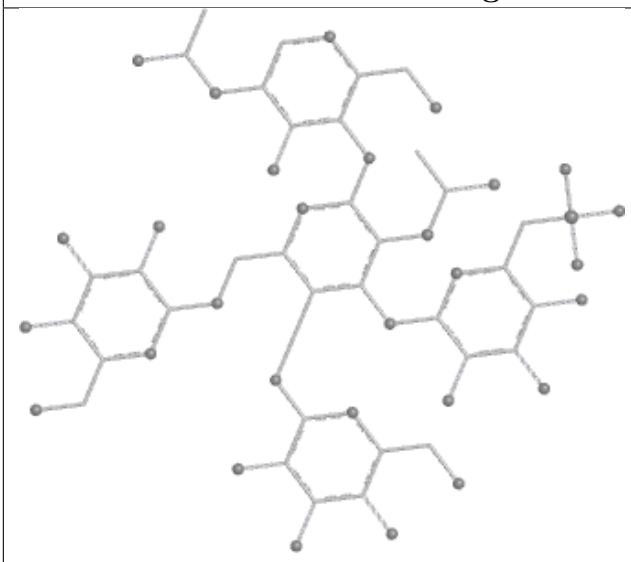
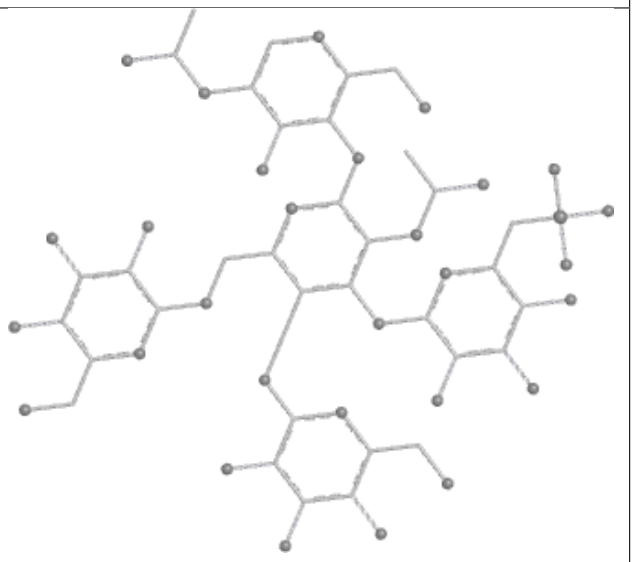
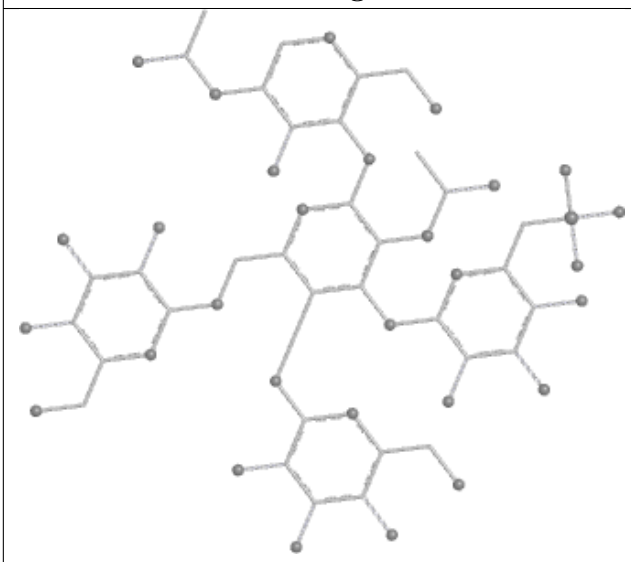
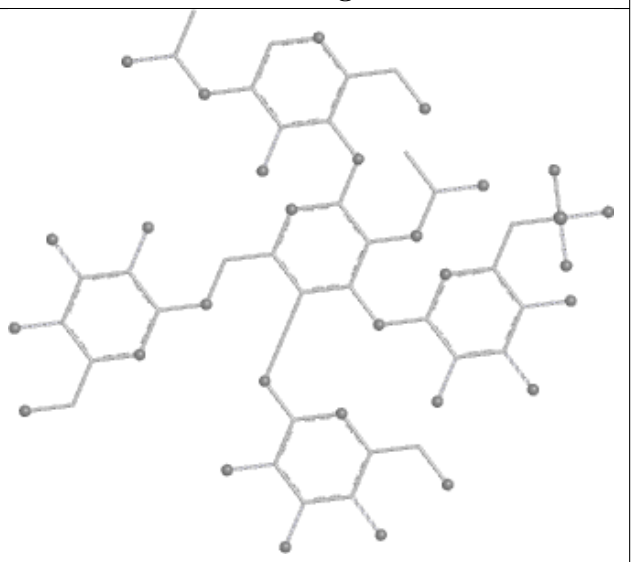
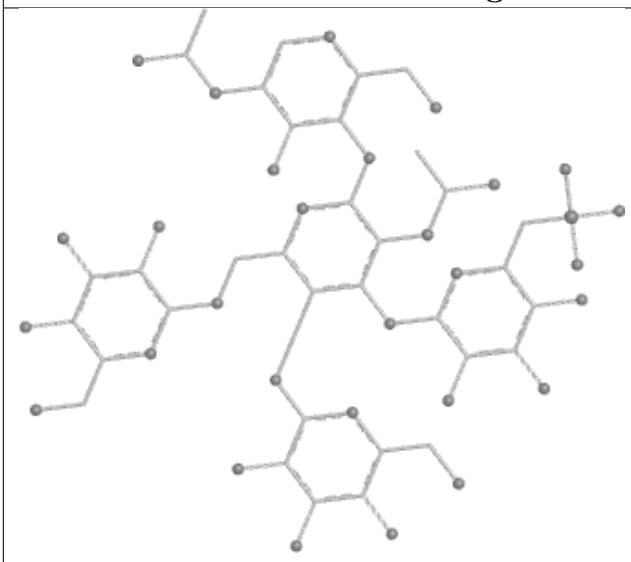


Rings

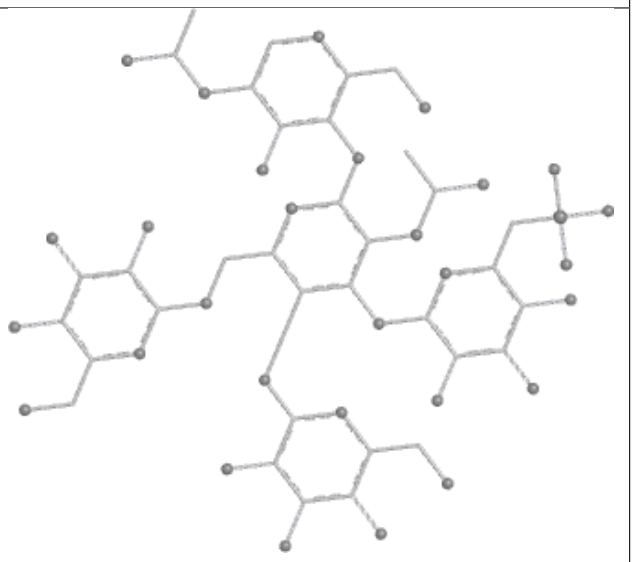
Oligosaccharide Chain SA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

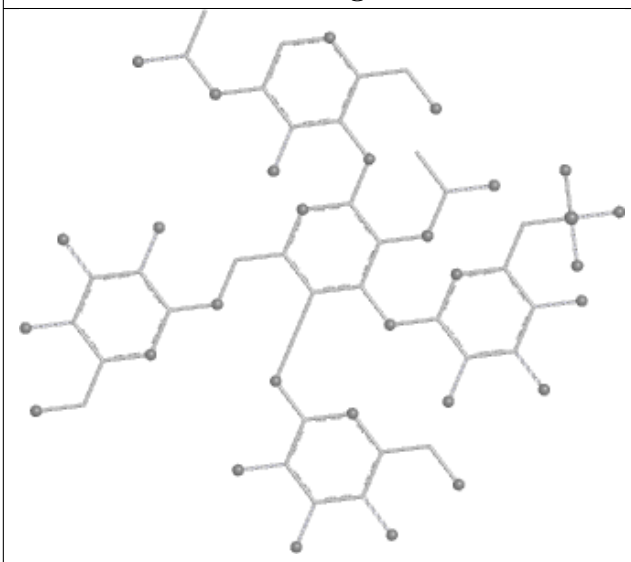
Oligosaccharide Chain eA



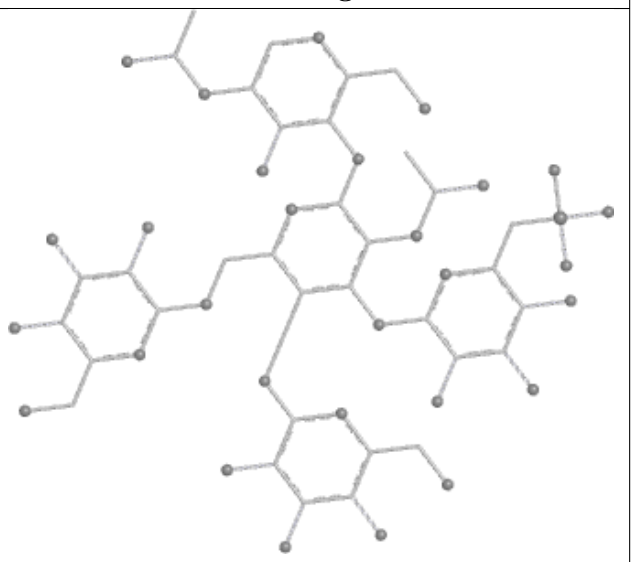
Bond lengths



Bond angles

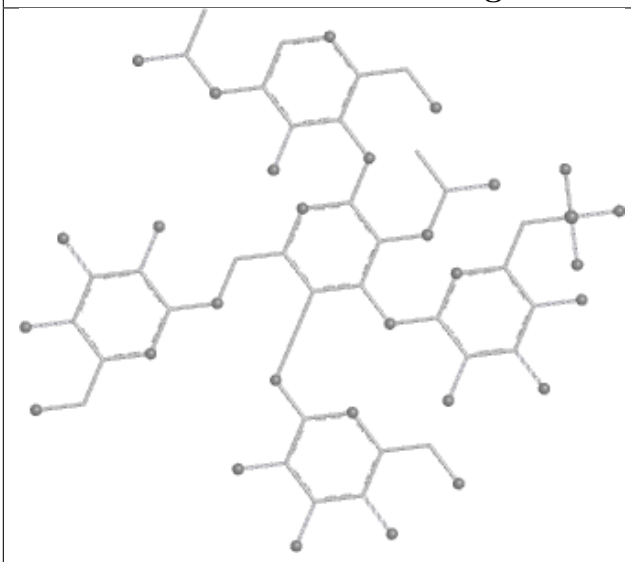


Torsions



Rings

Oligosaccharide Chain kA



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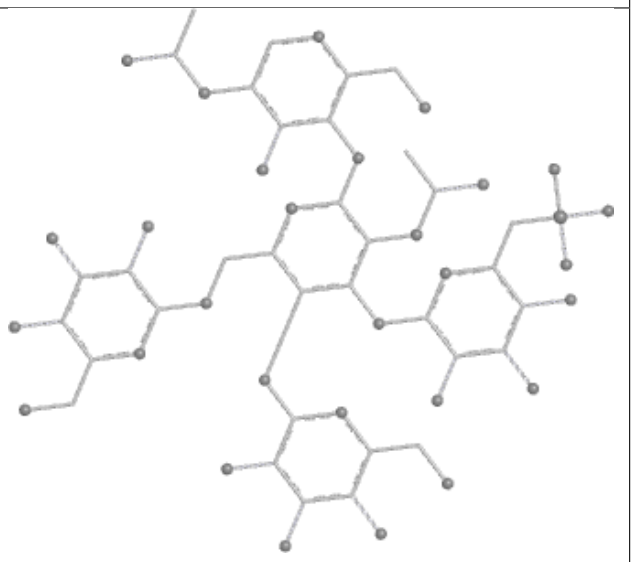

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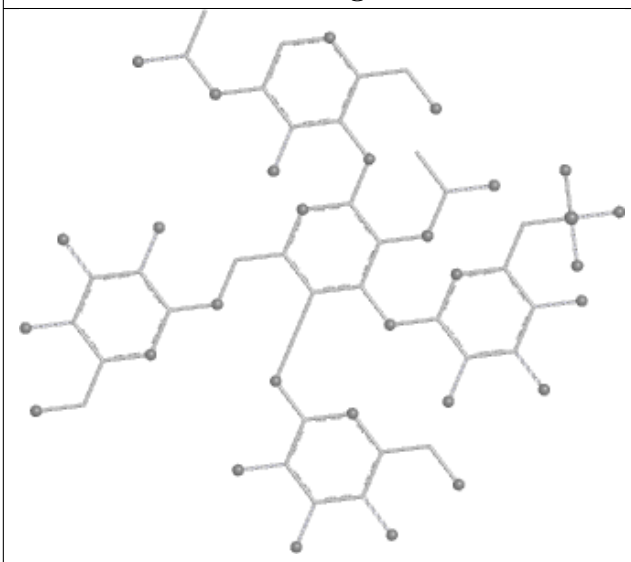

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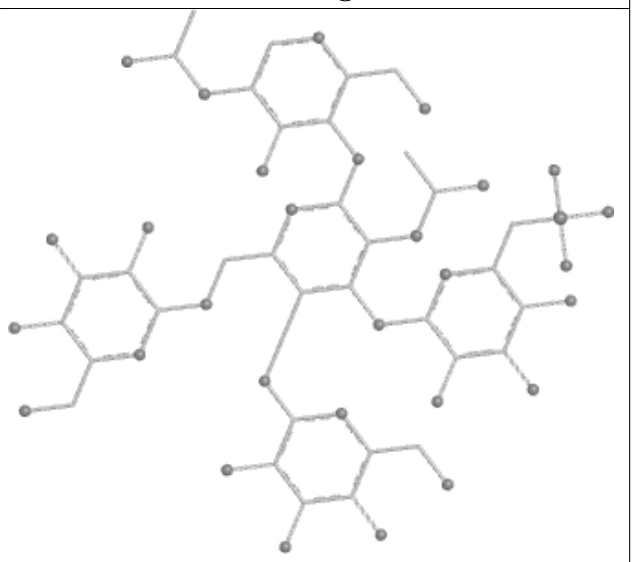
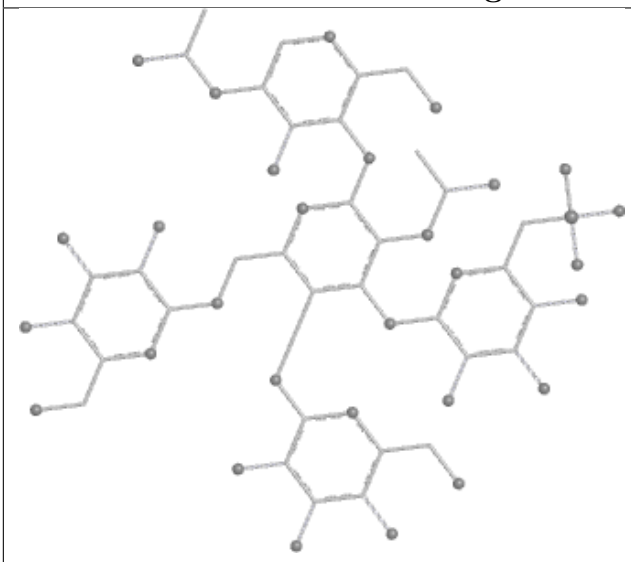


Rings

Oligosaccharide Chain qA



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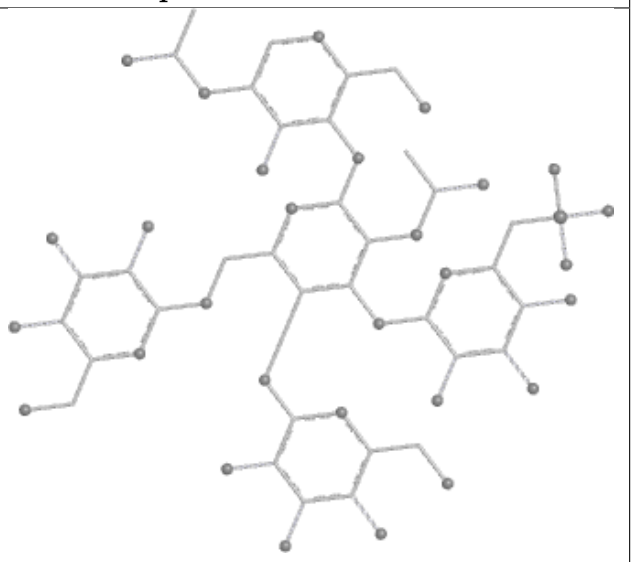
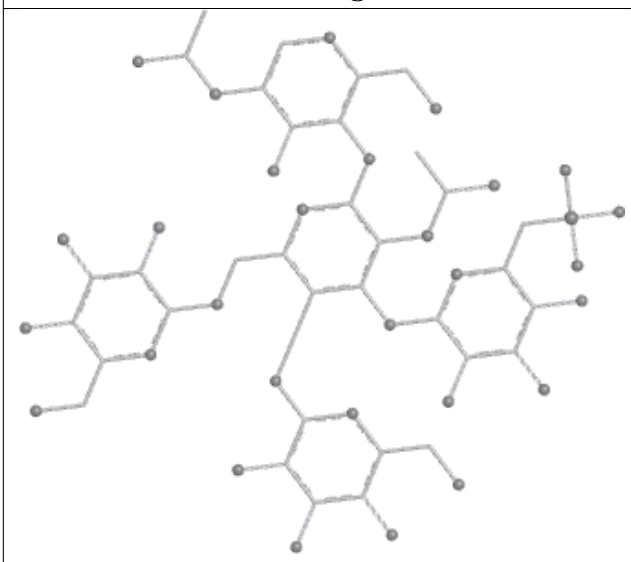


Bond angles



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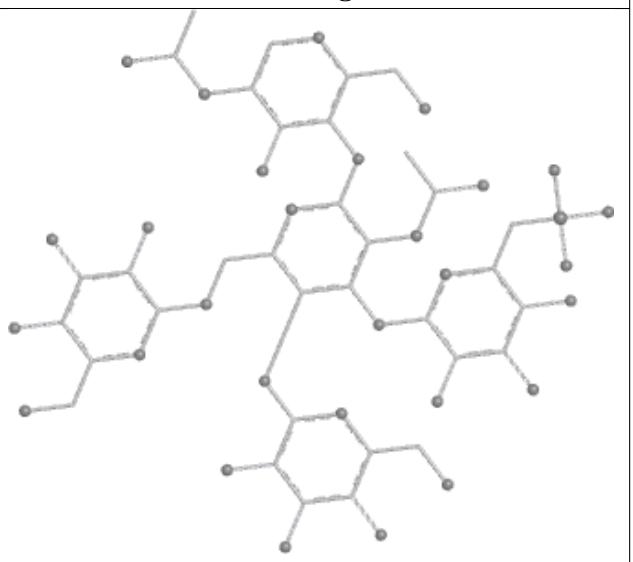
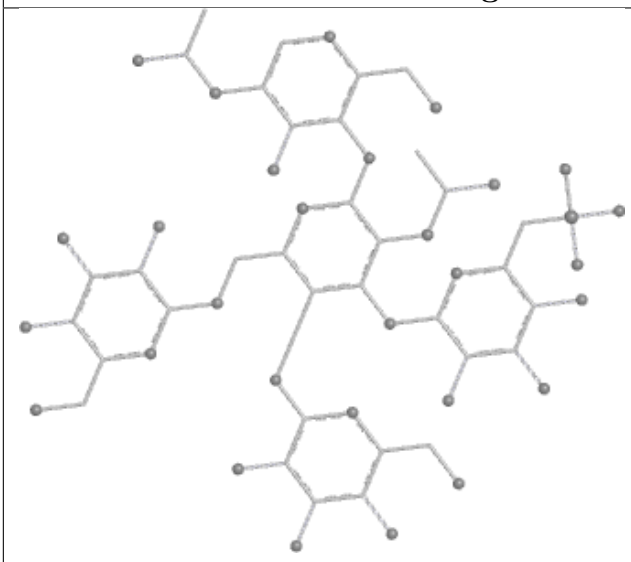
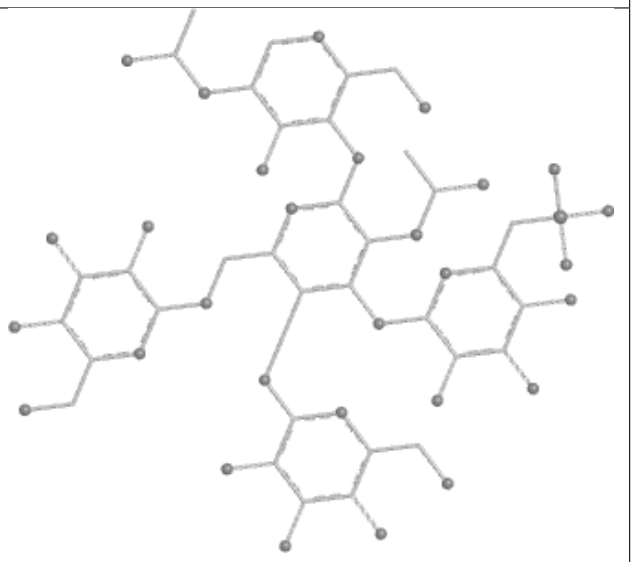
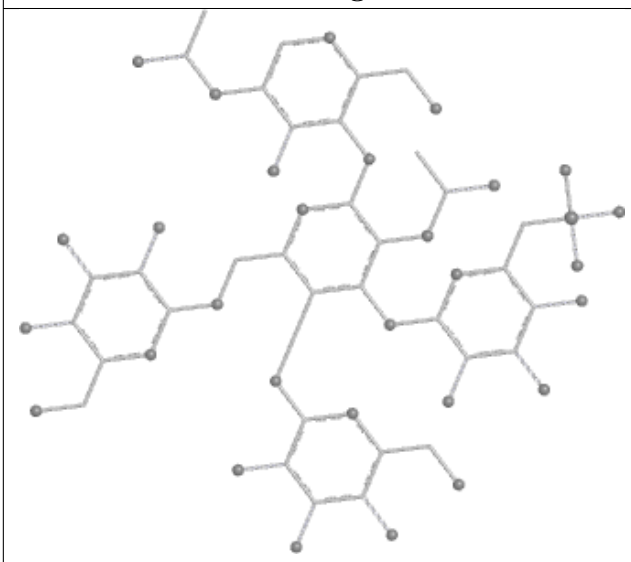
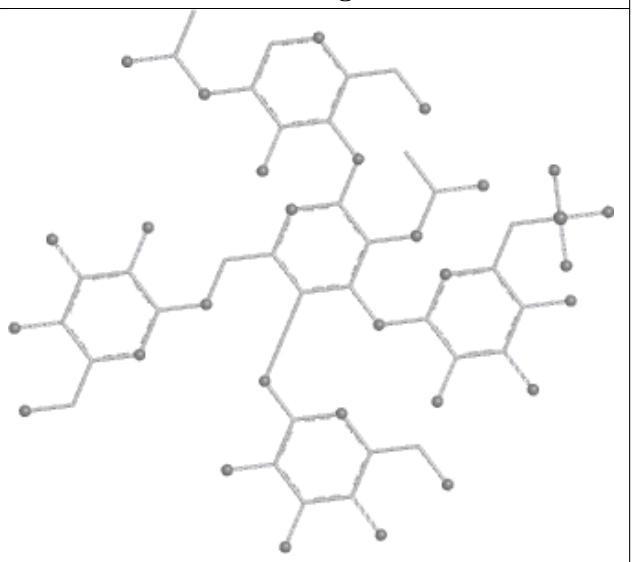
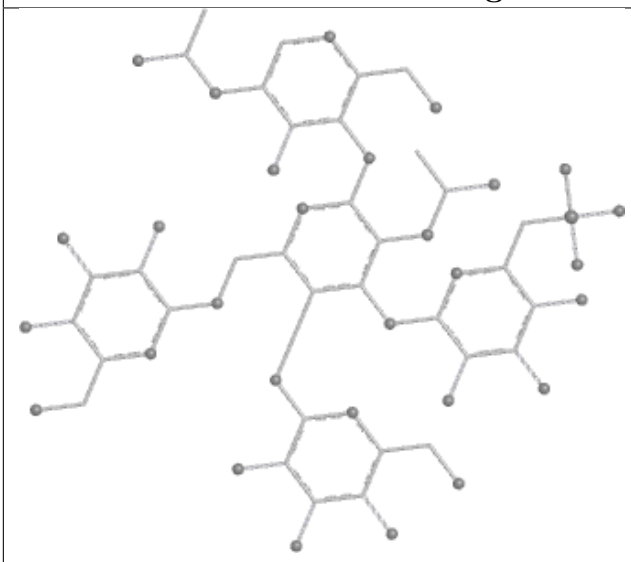


Rings

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

Oligosaccharide Chain 2A



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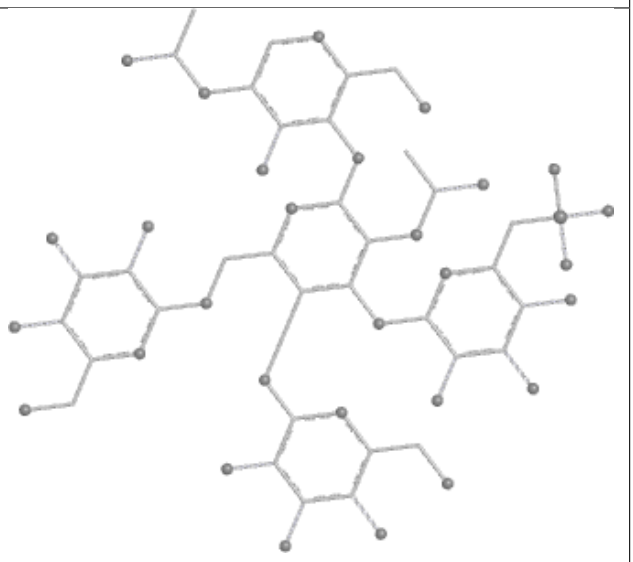
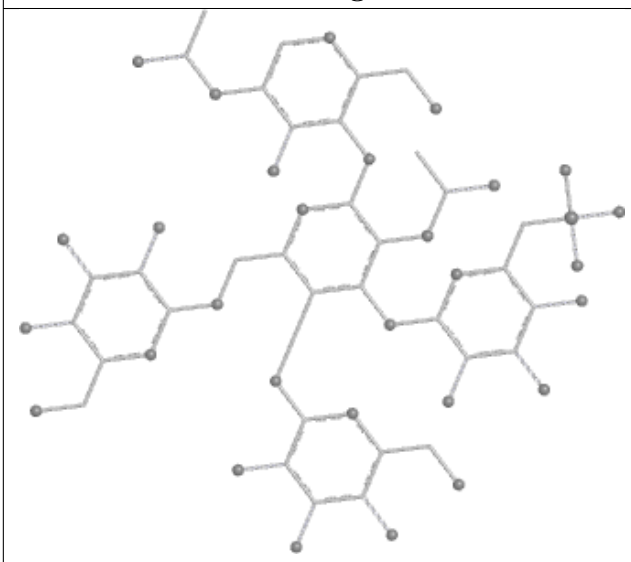
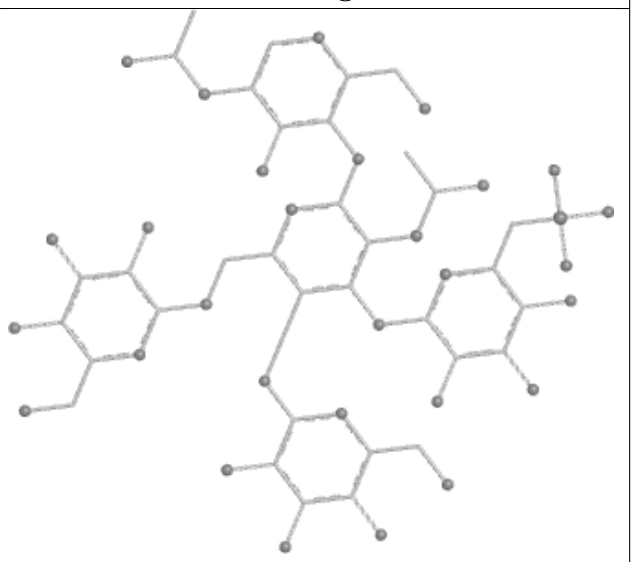


Bond angles

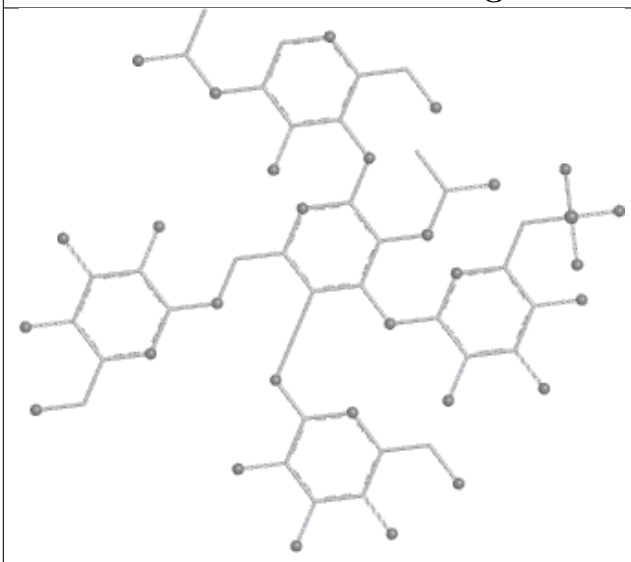


Torsions



Rings

Oligosaccharide Chain 8A



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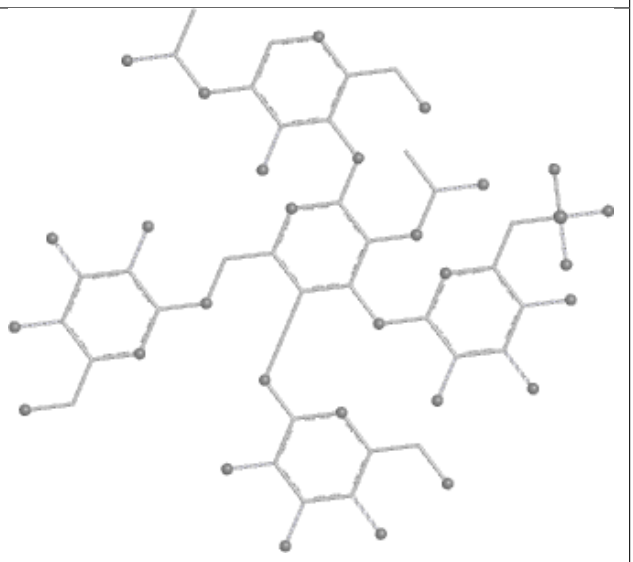
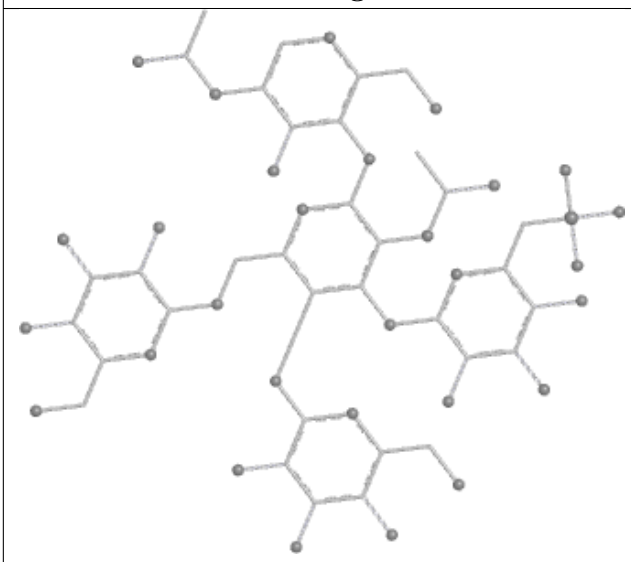


Bond angles



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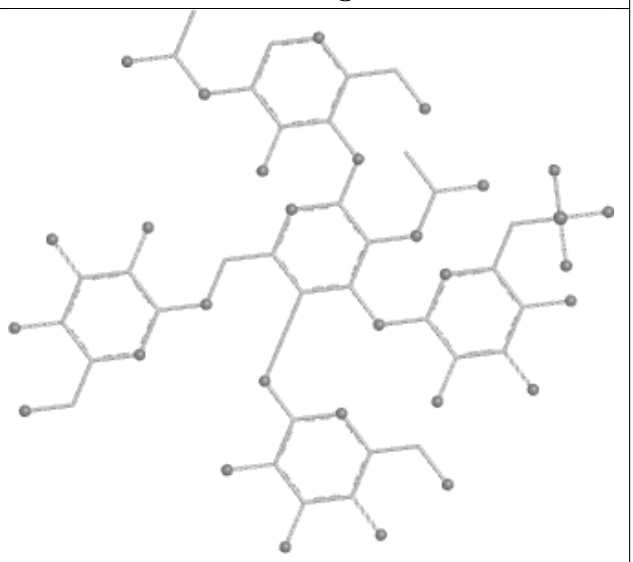
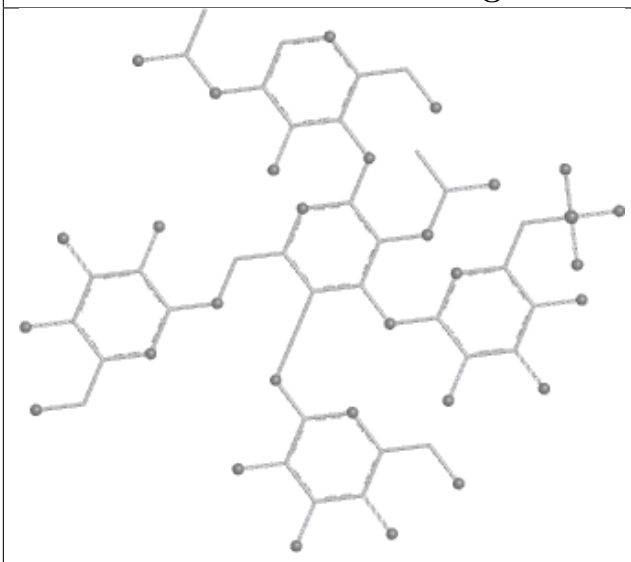
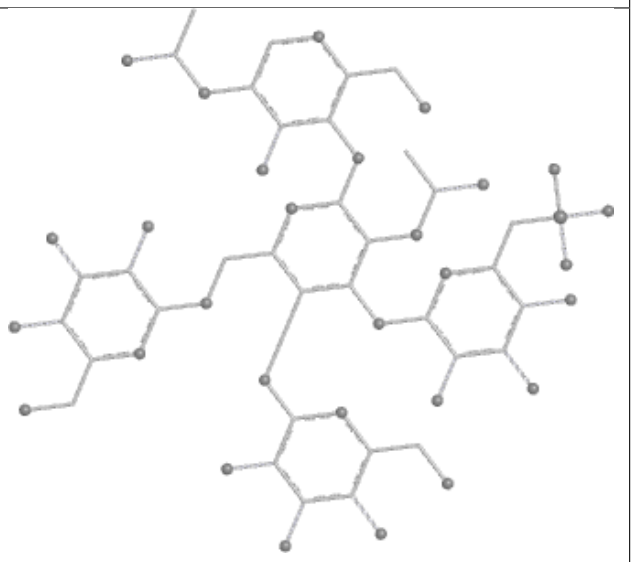


Rings

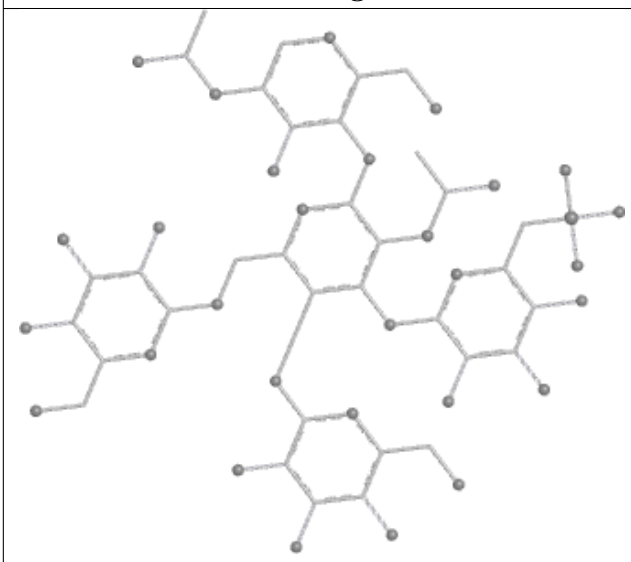
Oligosaccharide Chain EB



Bond lengths



Bond angles



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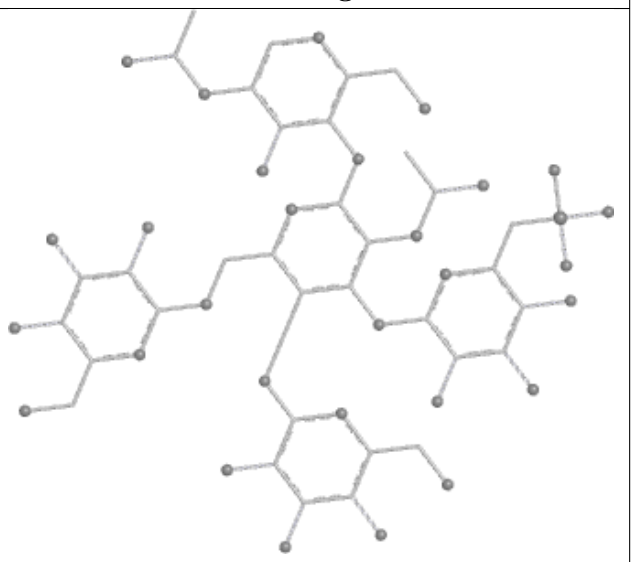
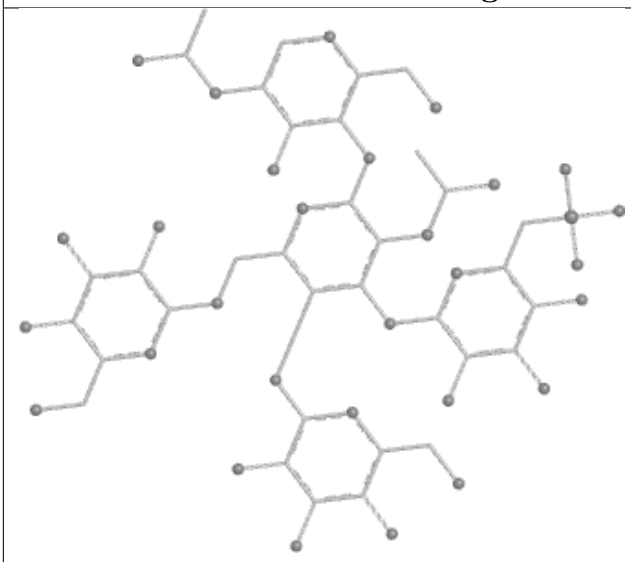
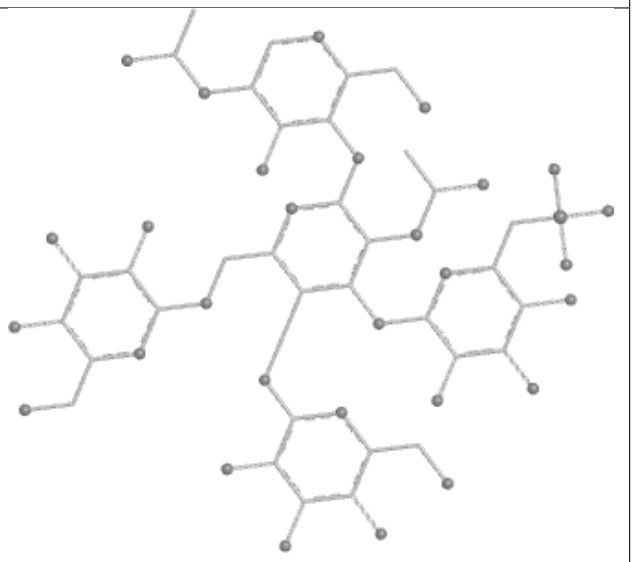


Rings

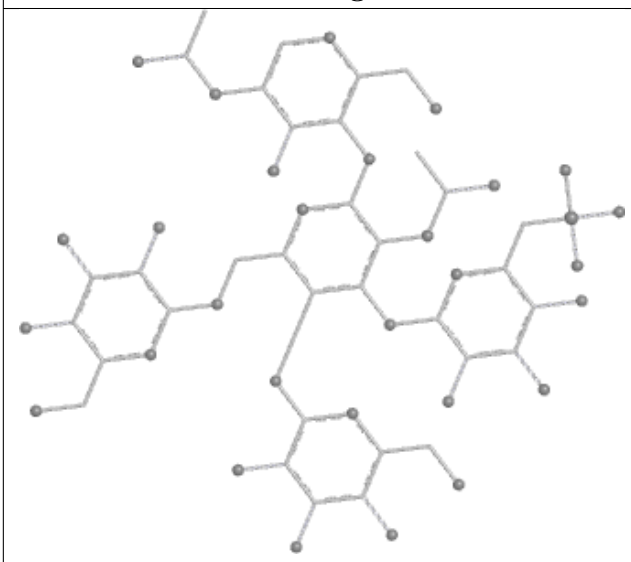
Oligosaccharide Chain KB



Bond lengths



Bond angles



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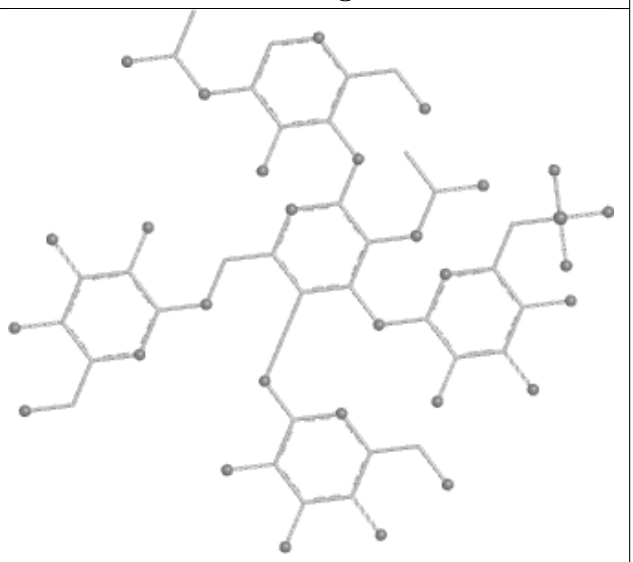
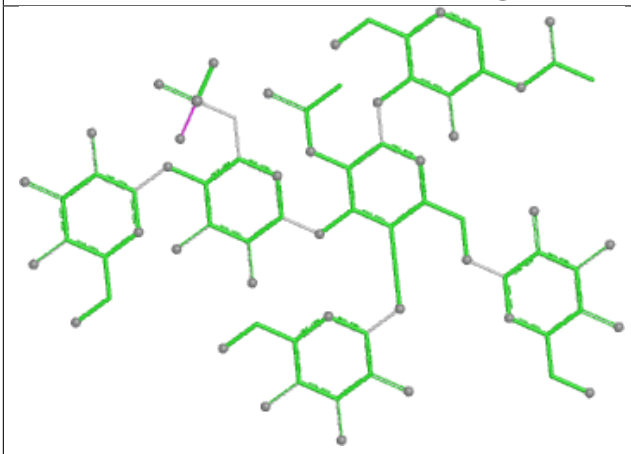
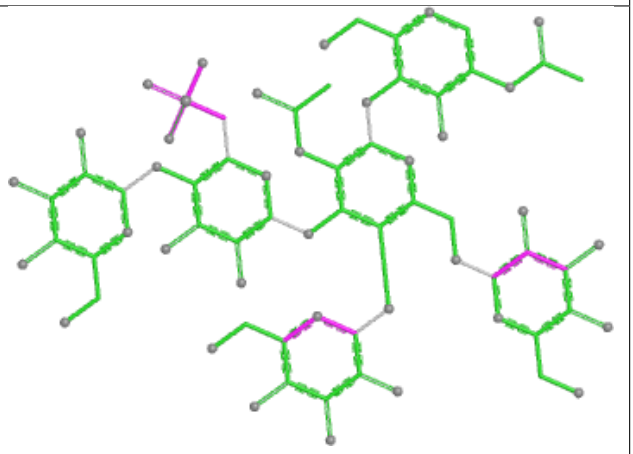


Rings

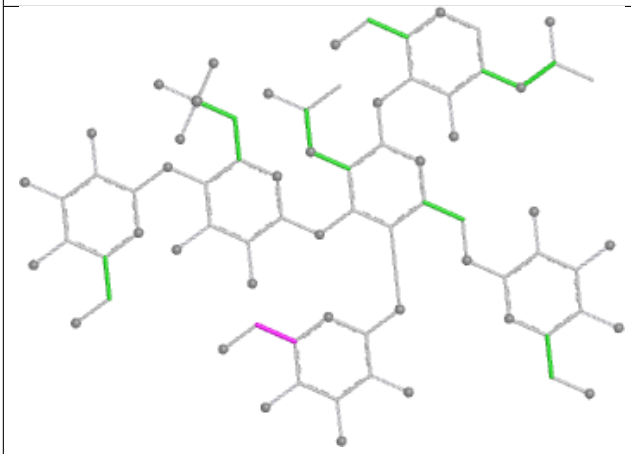
Oligosaccharide Chain V



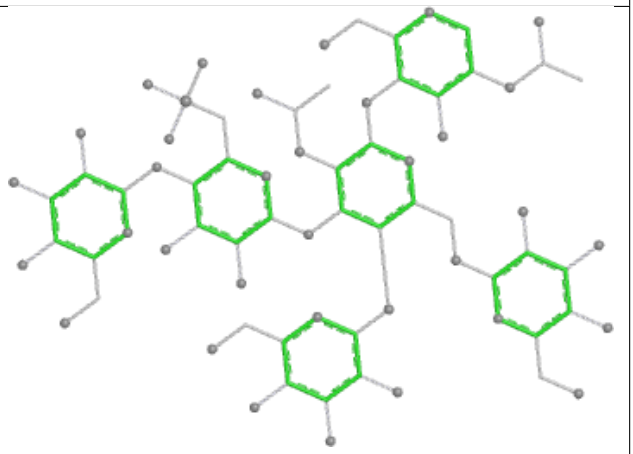
Bond lengths



Bond angles

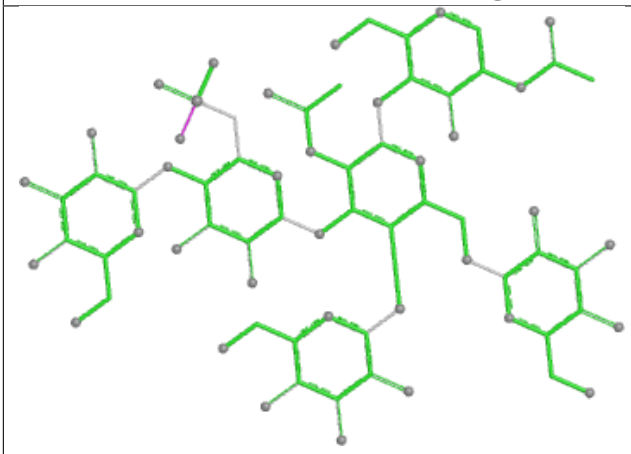


Torsions



Rings

Oligosaccharide Chain W



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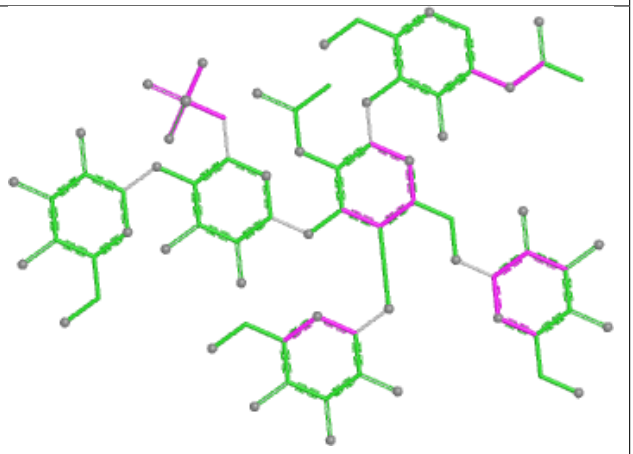

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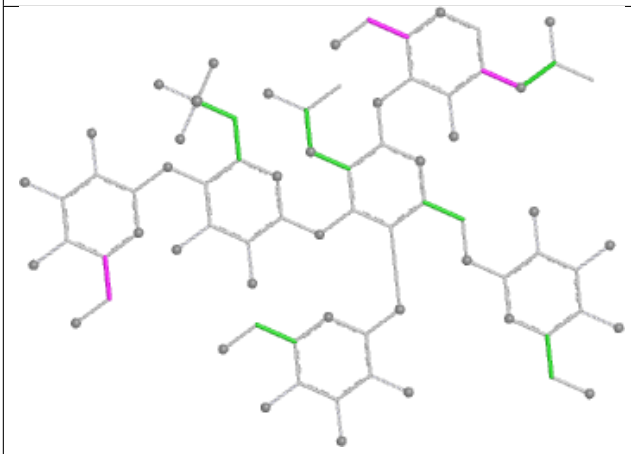

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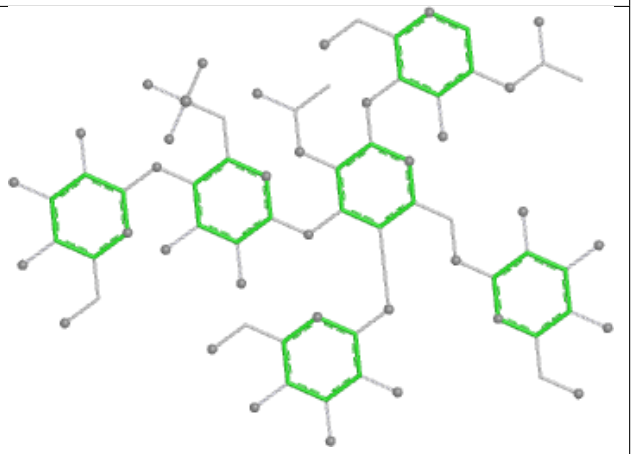
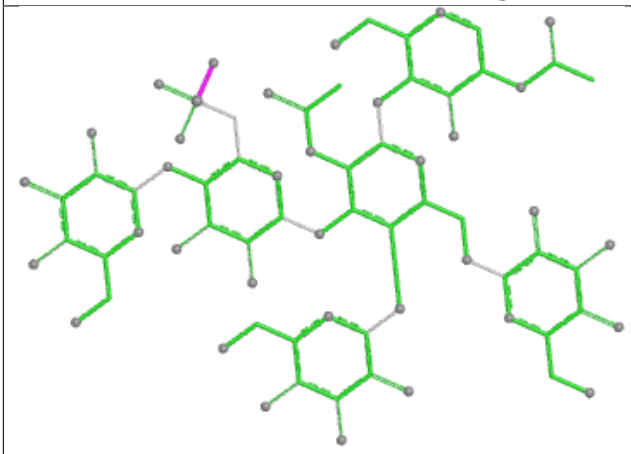


Rings

Oligosaccharide Chain Y



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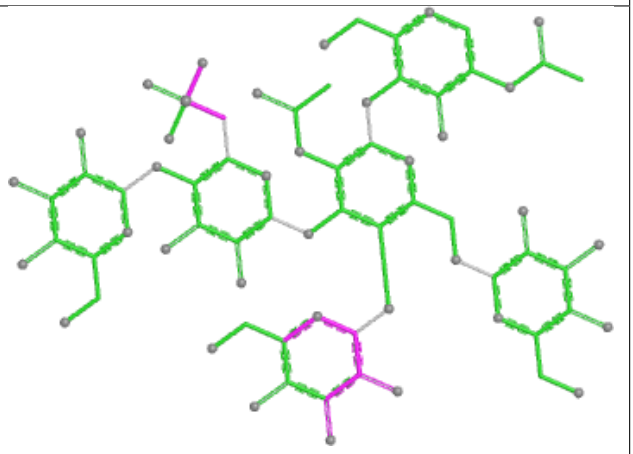

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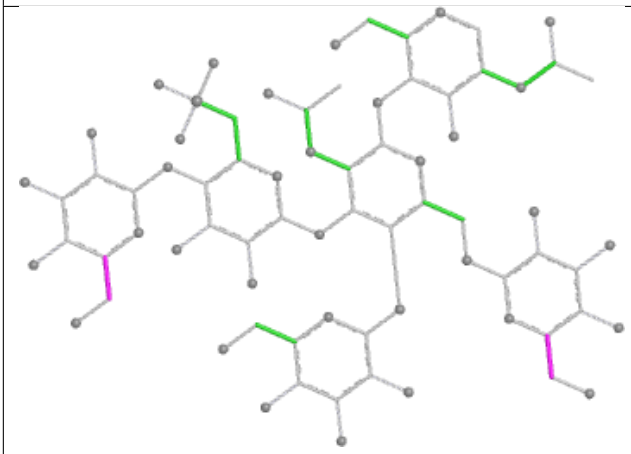

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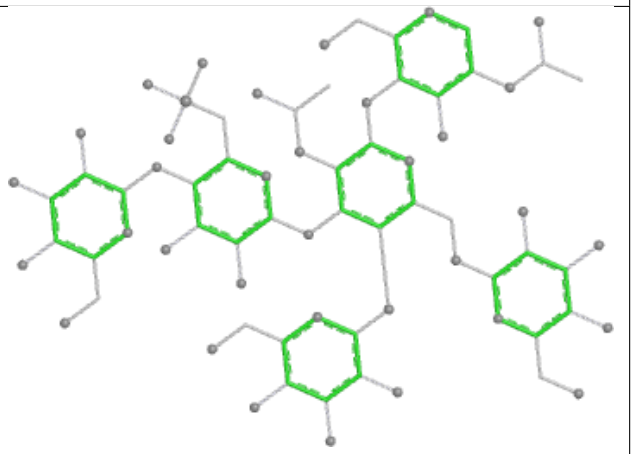
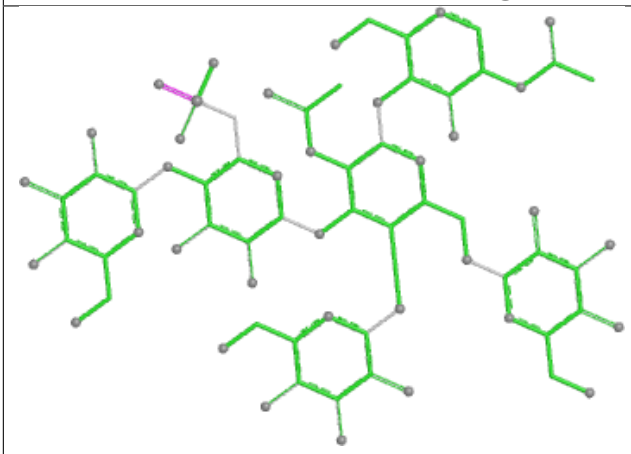


Rings

Oligosaccharide Chain Z



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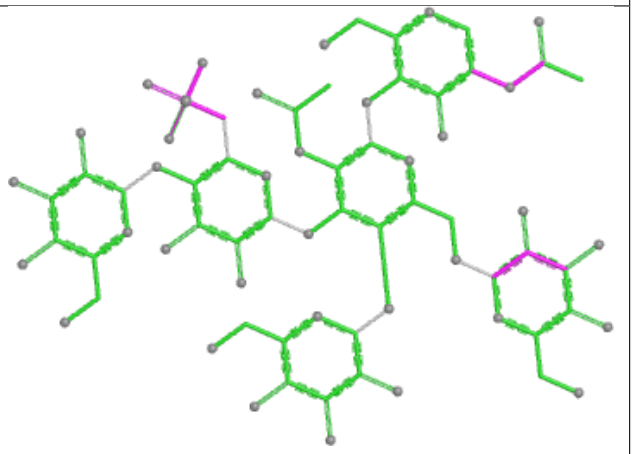
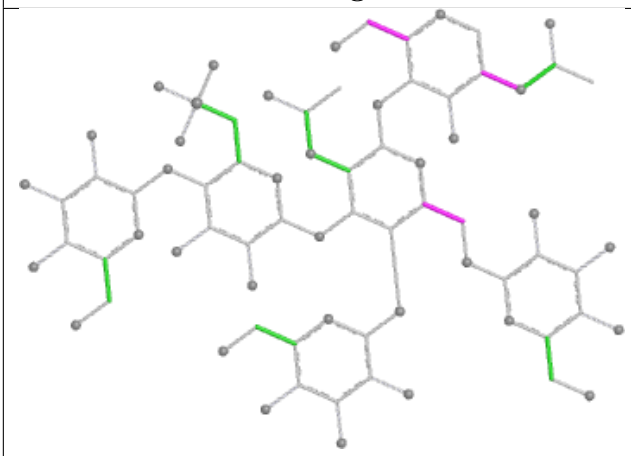


Bond angles



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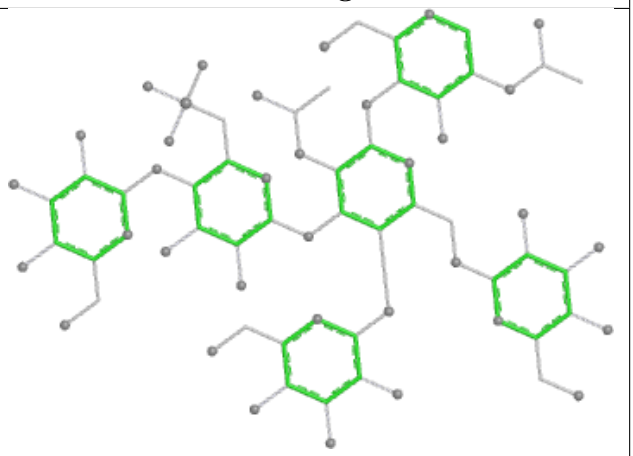
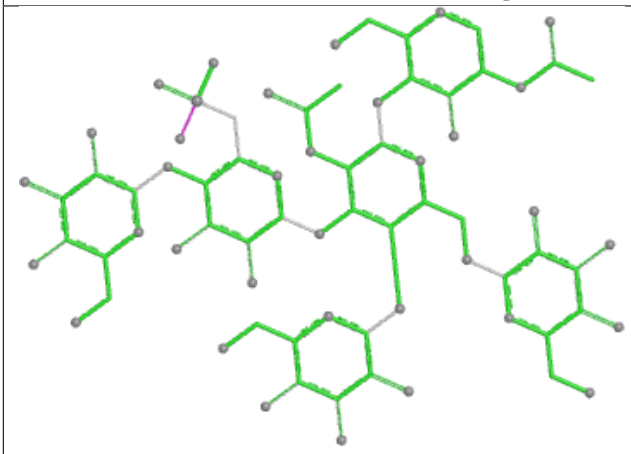


Rings

Oligosaccharide Chain b



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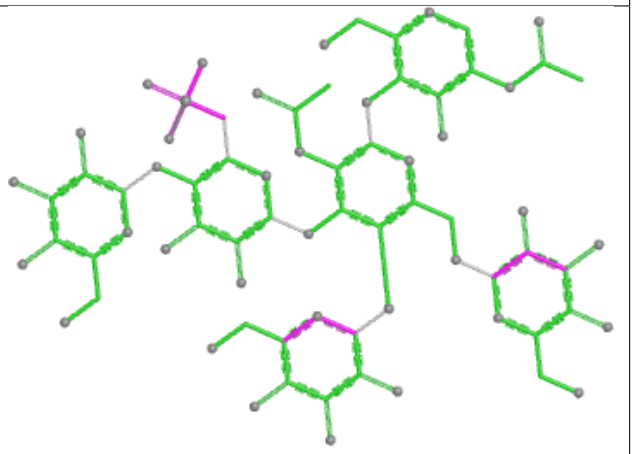

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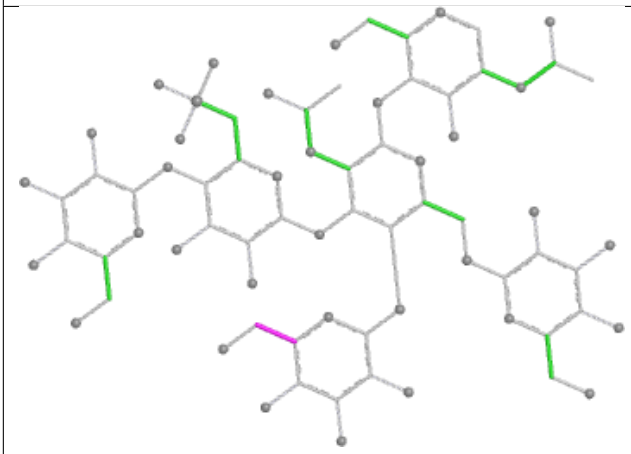

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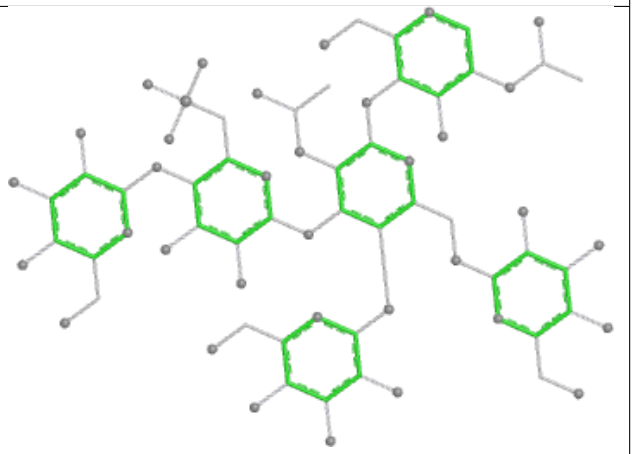
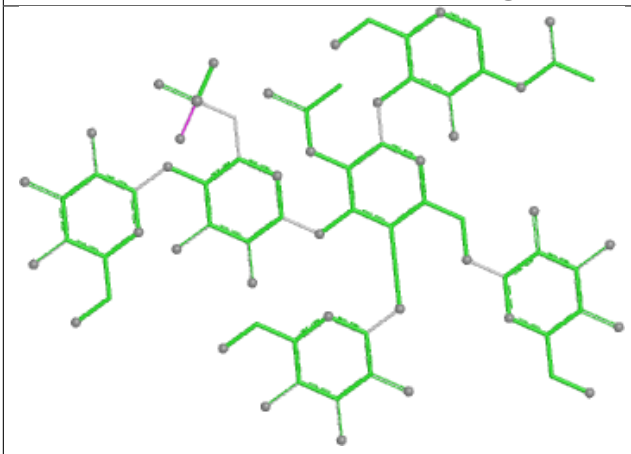


Rings

Oligosaccharide Chain c



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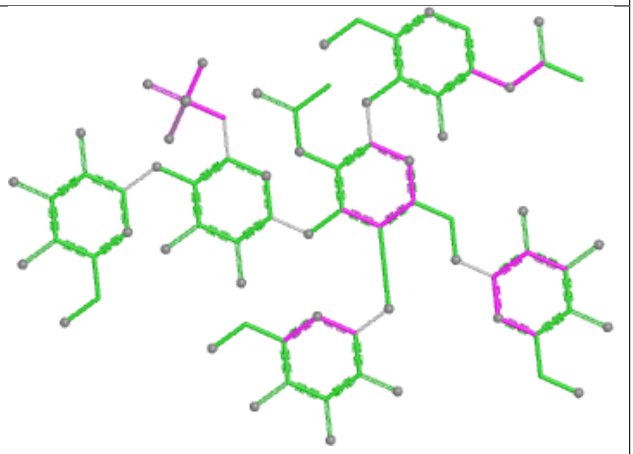

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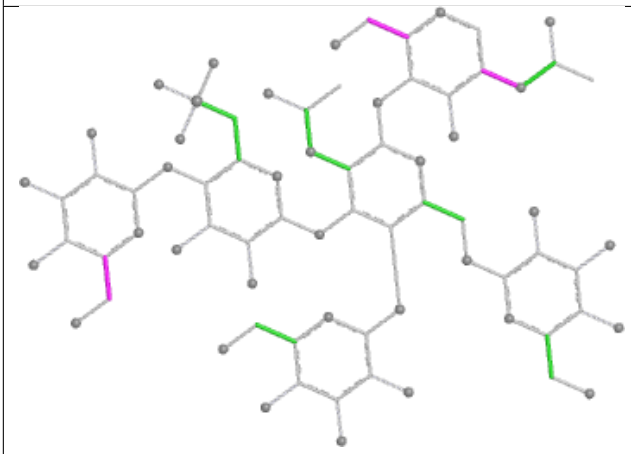

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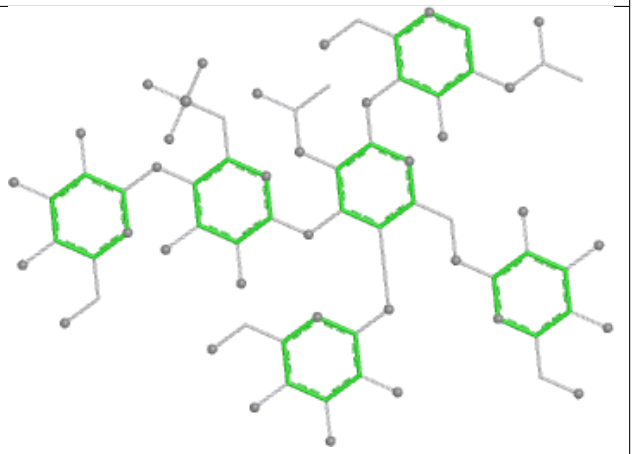
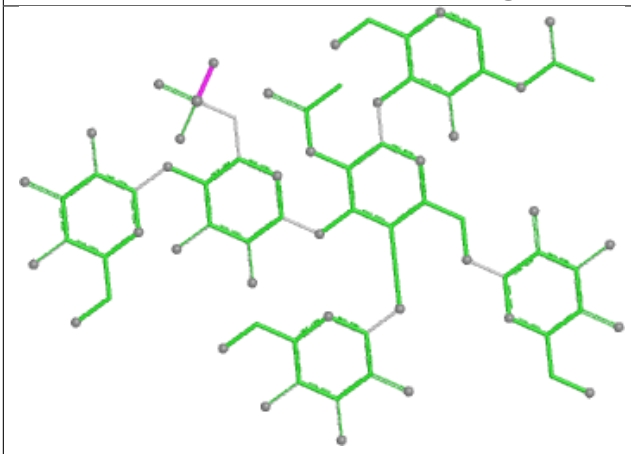


Rings

Oligosaccharide Chain e



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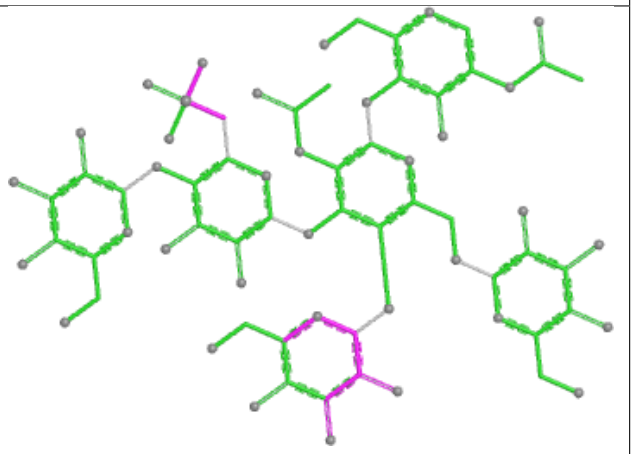
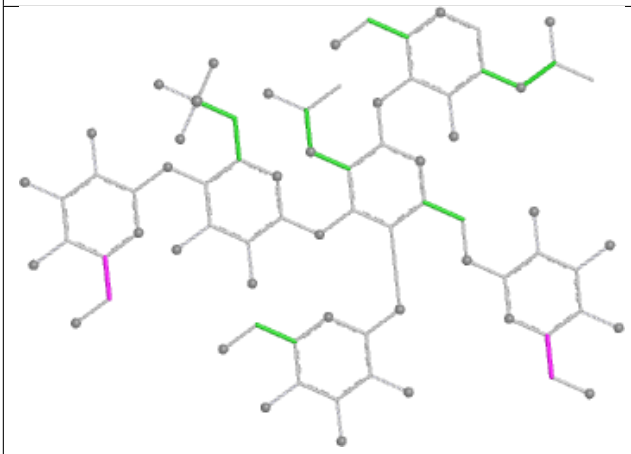


Bond angles



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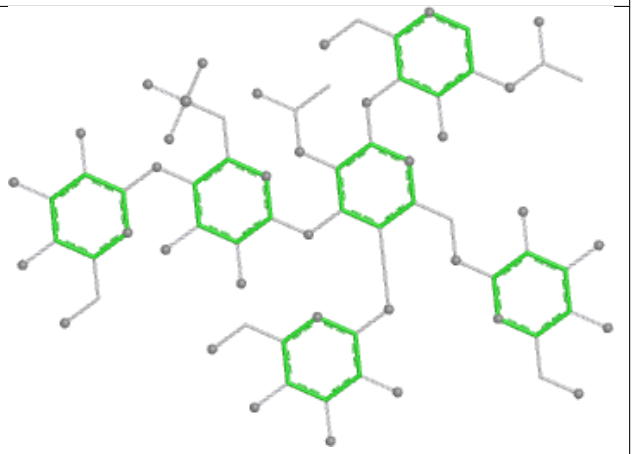
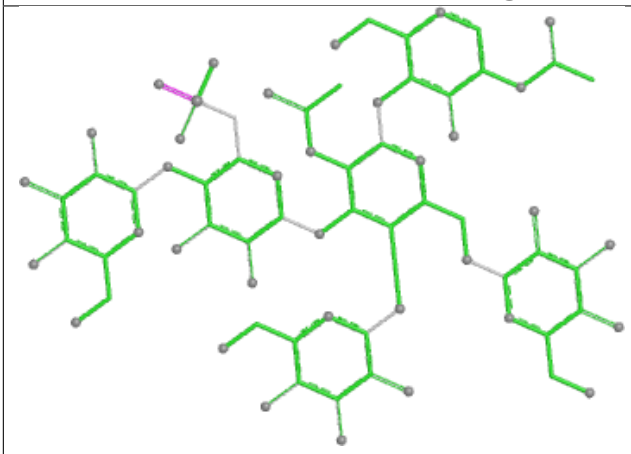


Rings

Oligosaccharide Chain f



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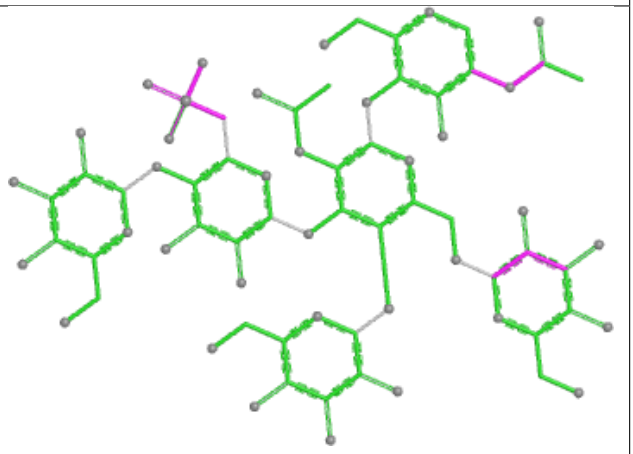
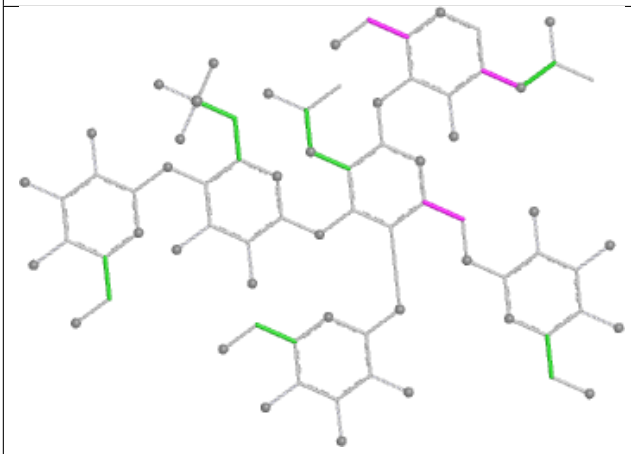


Bond angles



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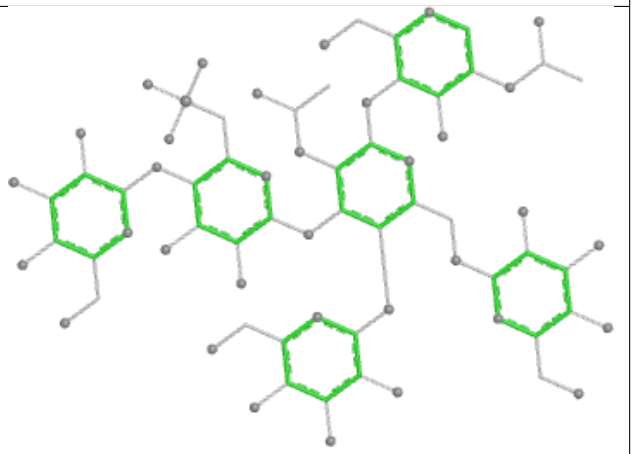
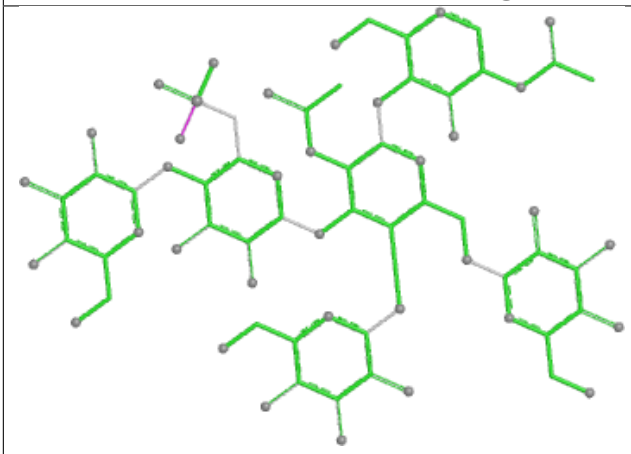


Rings

Oligosaccharide Chain h



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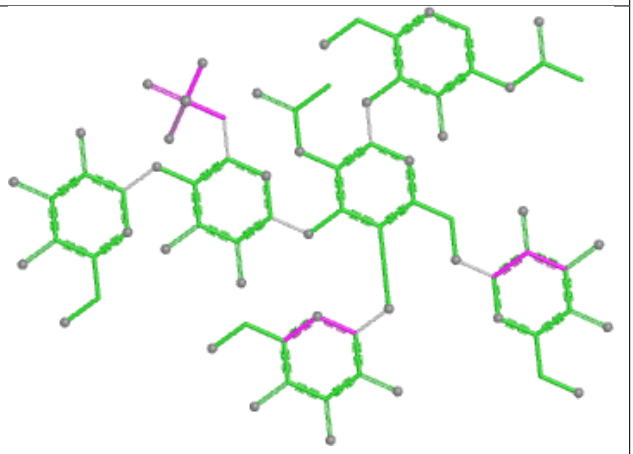
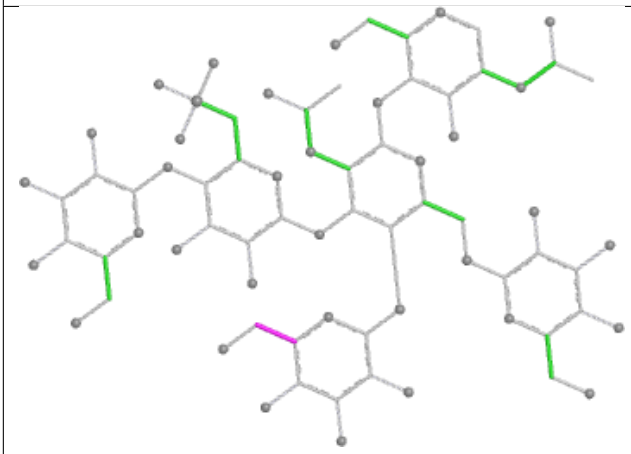


Bond angles



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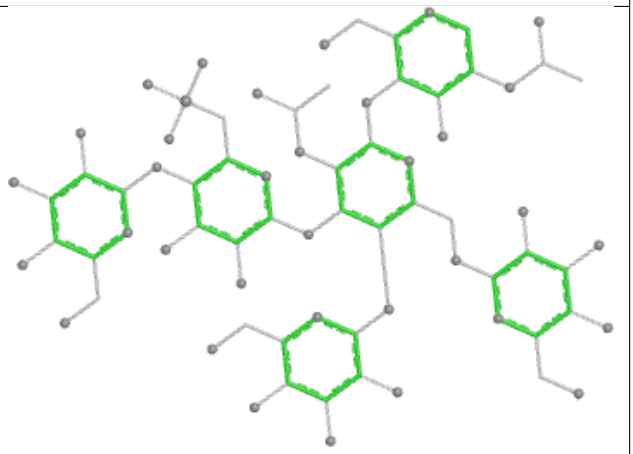
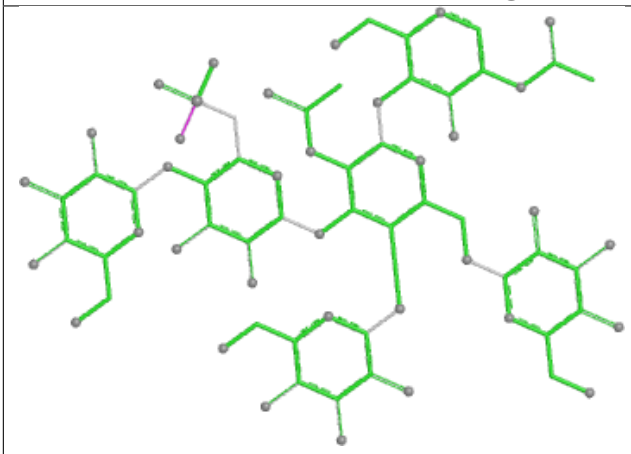


Rings

Oligosaccharide Chain i



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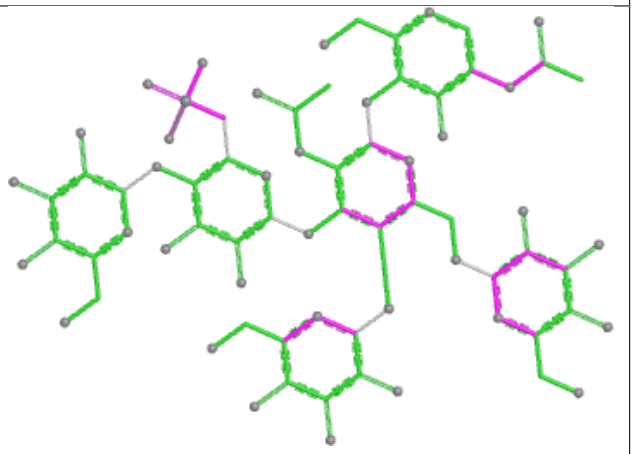

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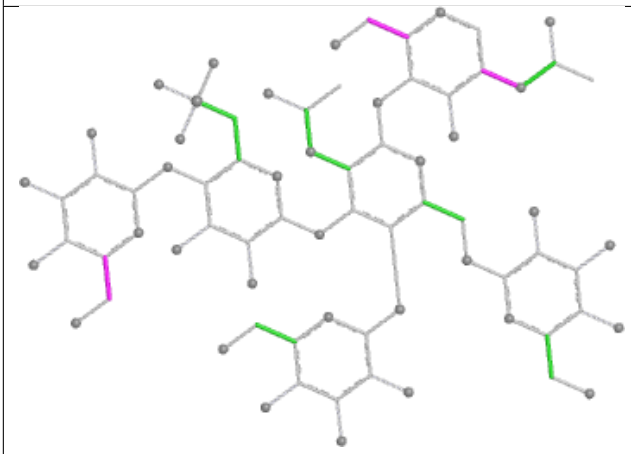

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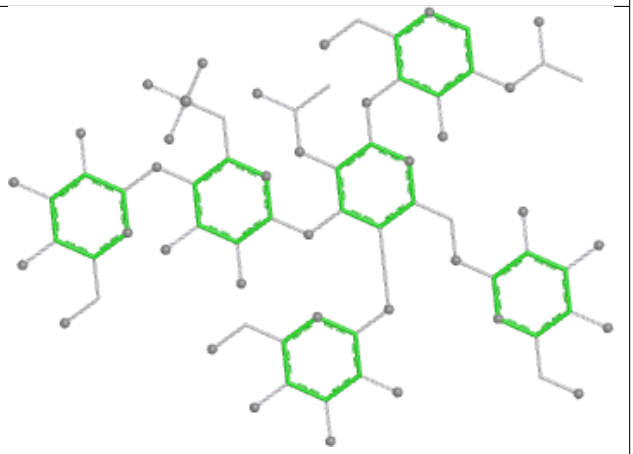
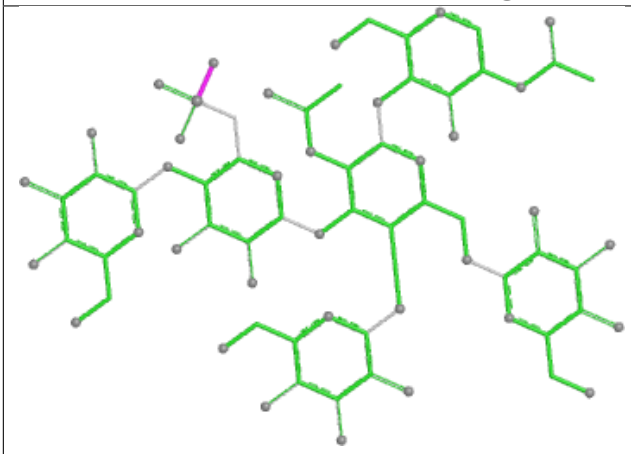


Rings

Oligosaccharide Chain k



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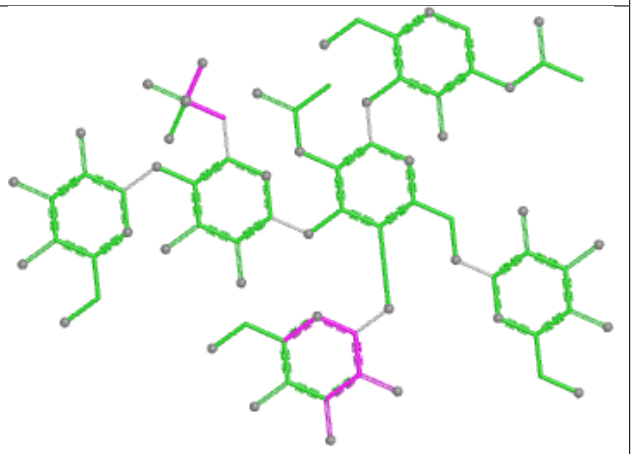

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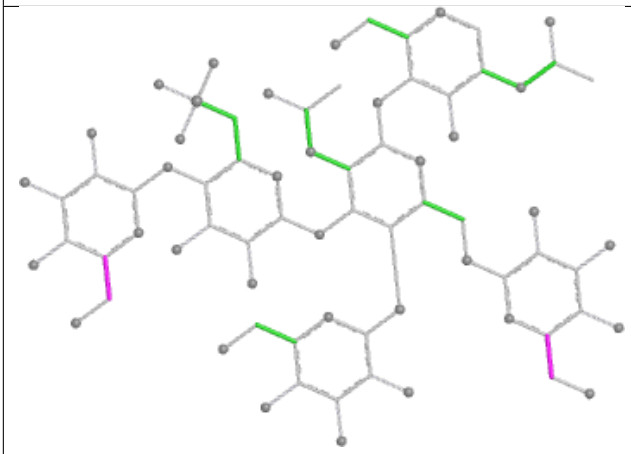

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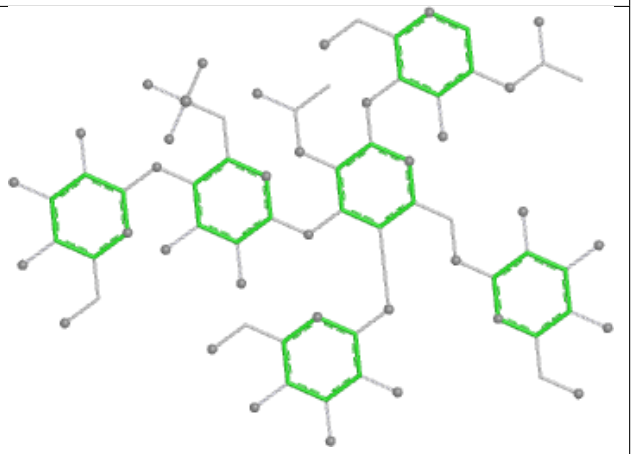
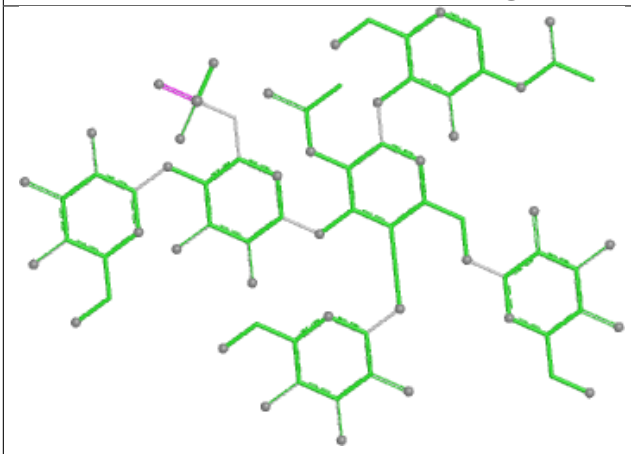


Rings

Oligosaccharide Chain l



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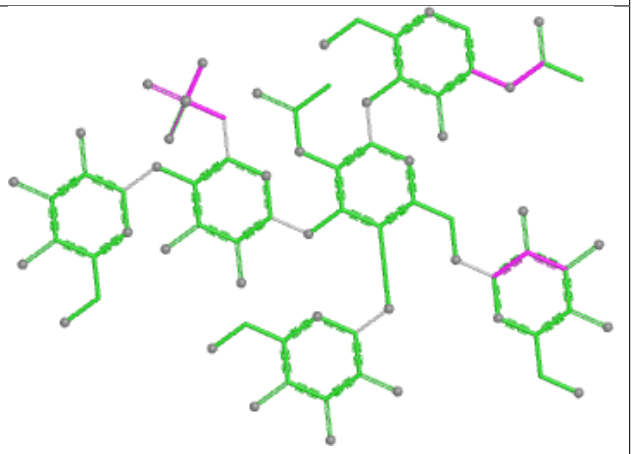

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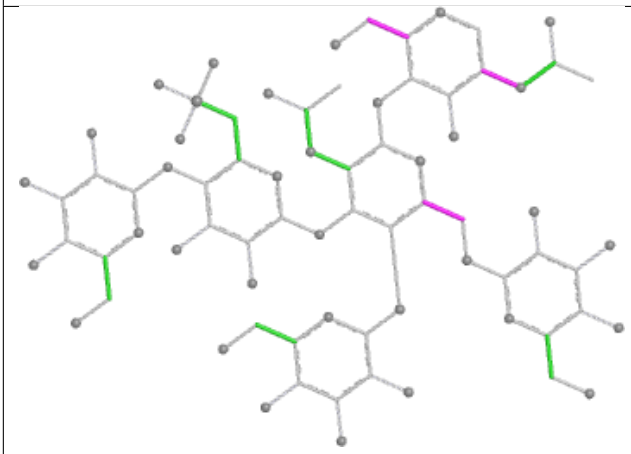

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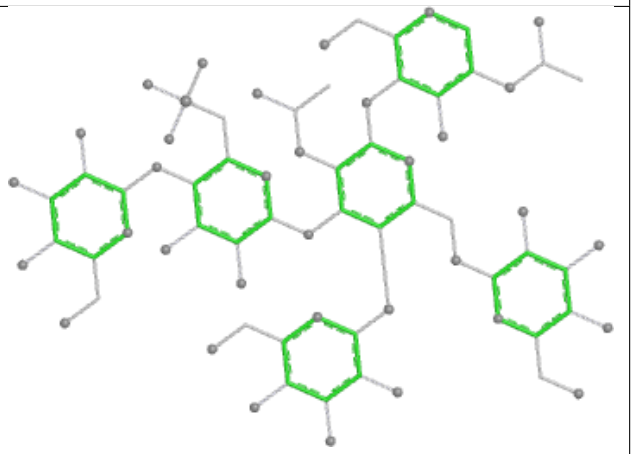
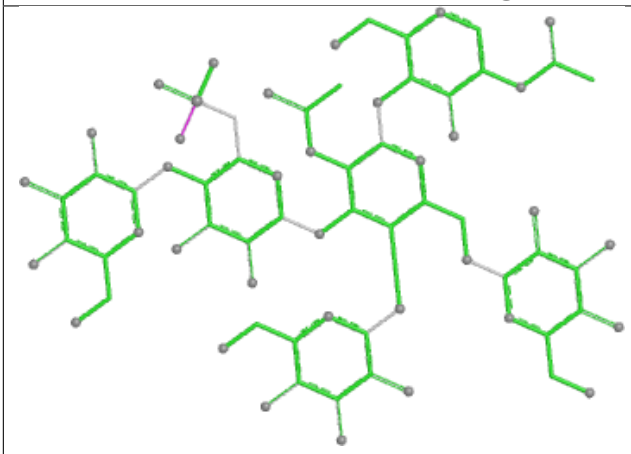


Rings

Oligosaccharide Chain n



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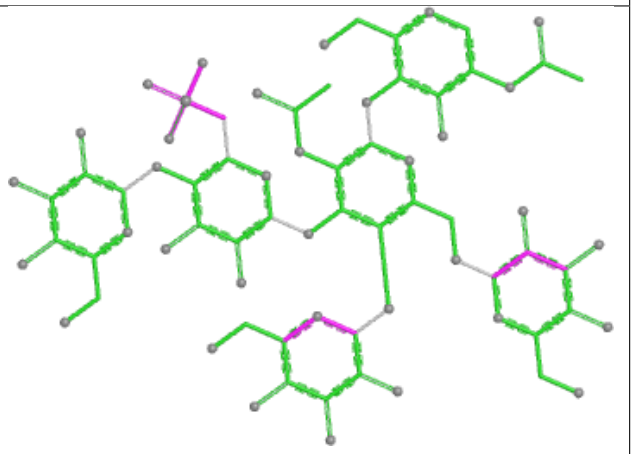
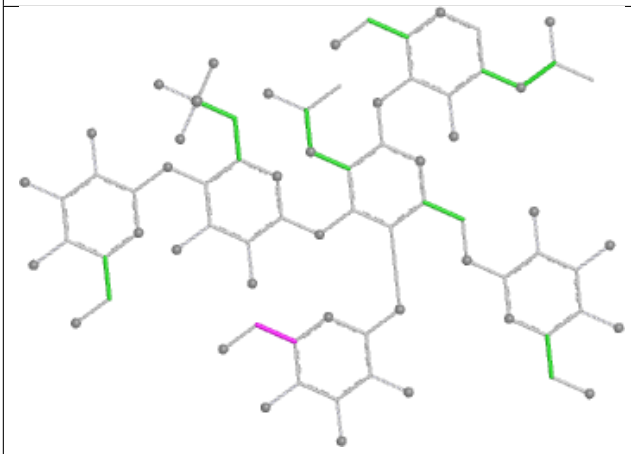


Bond angles



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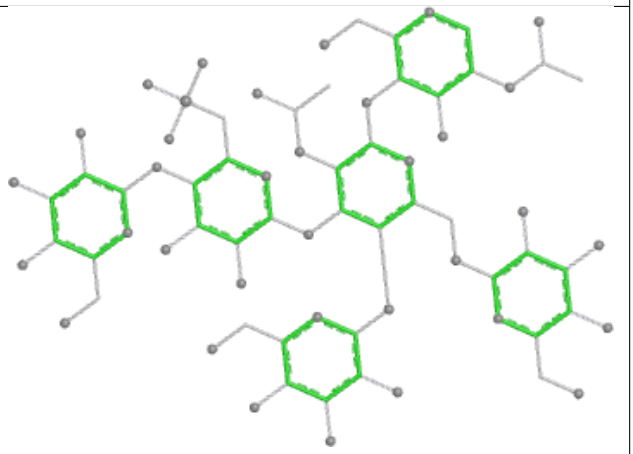
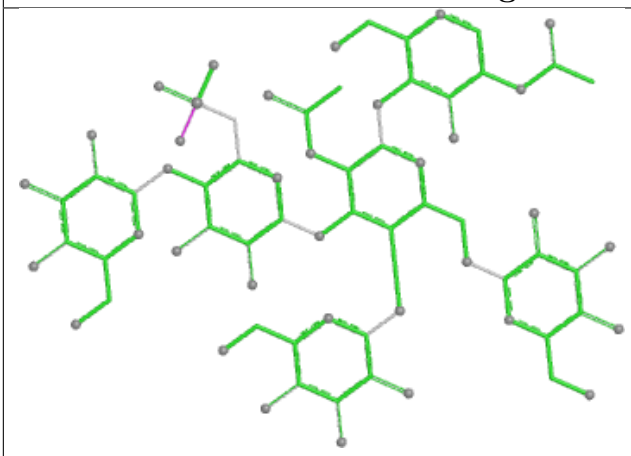
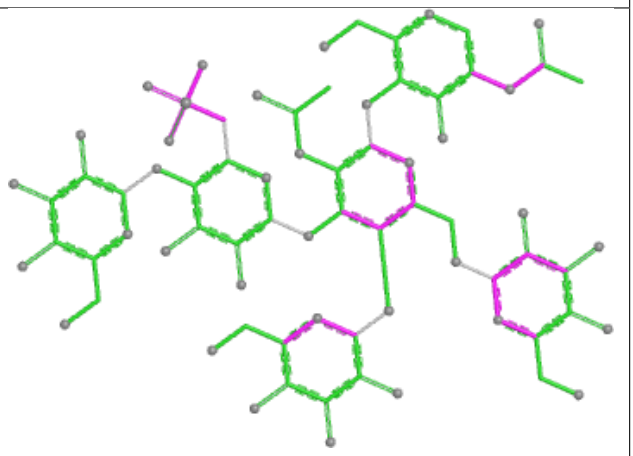


Rings

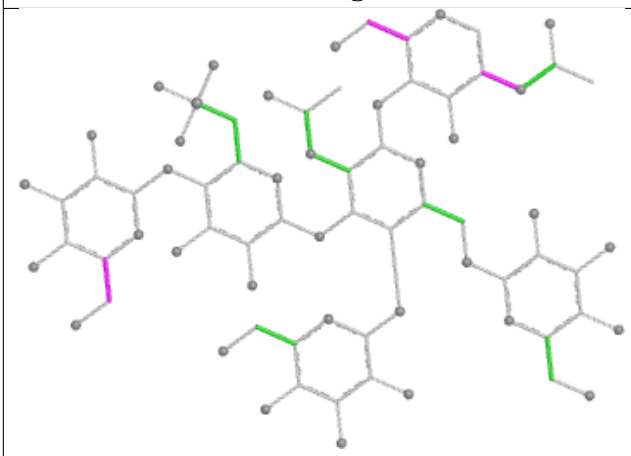
Oligosaccharide Chain o



Bond lengths



Bond angles



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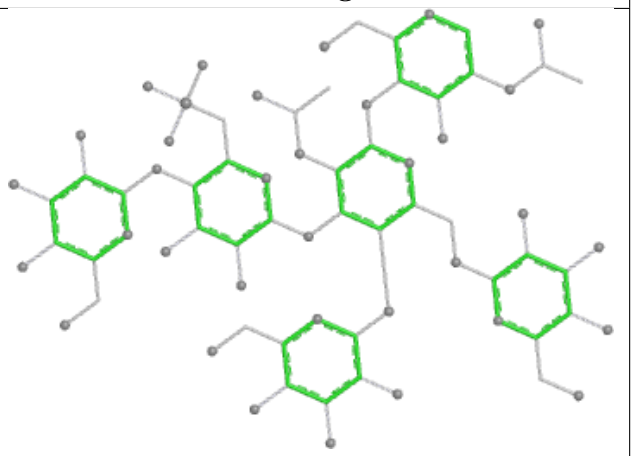
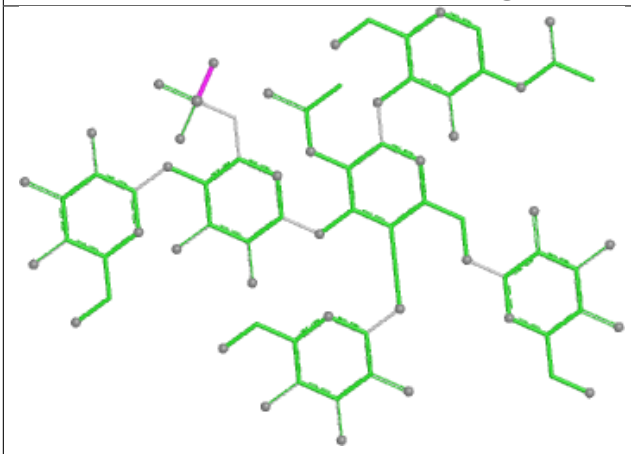
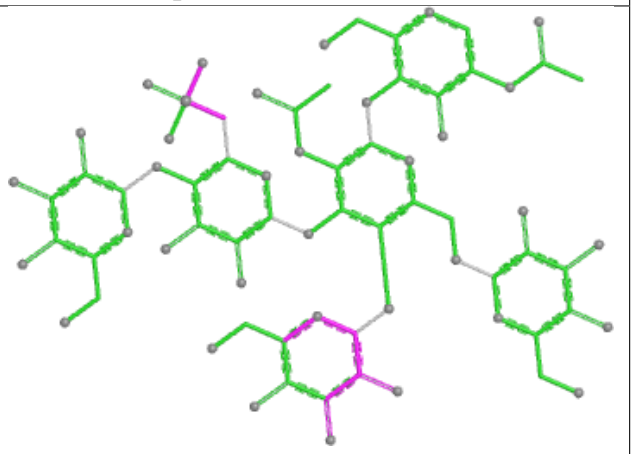


Rings

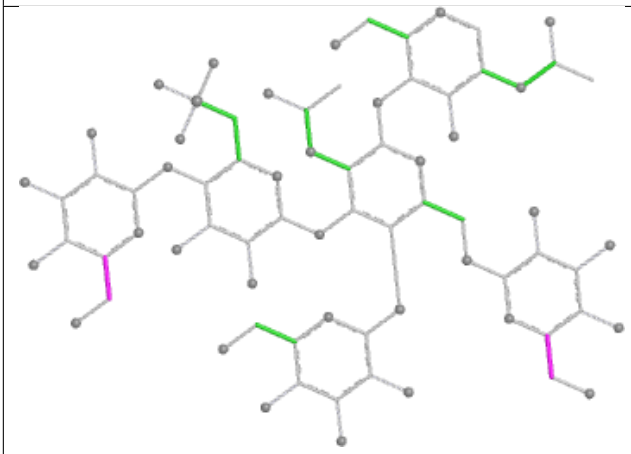
Oligosaccharide Chain q



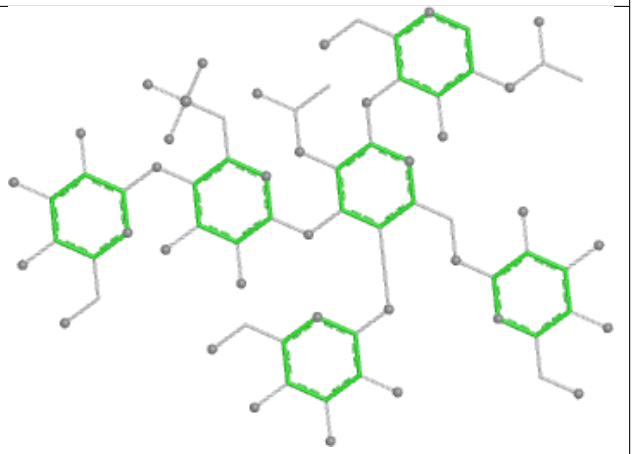
Bond lengths



Bond angles

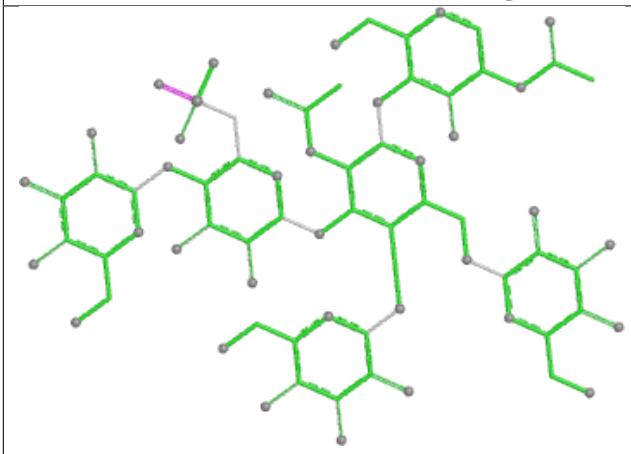


Torsions



Rings

Oligosaccharide Chain r



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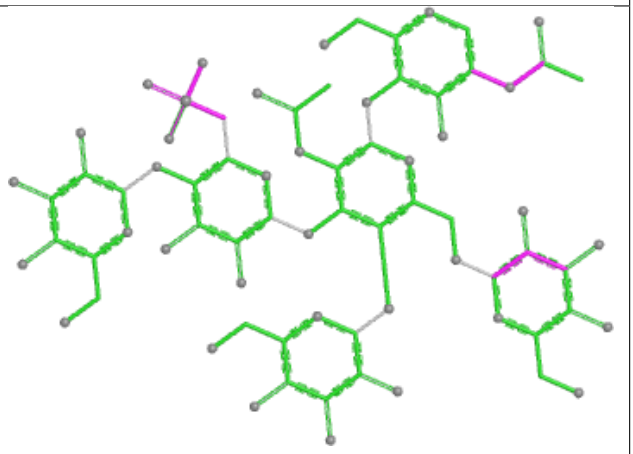

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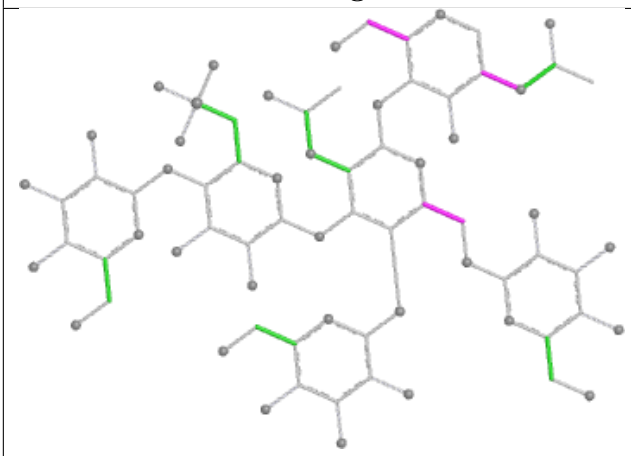

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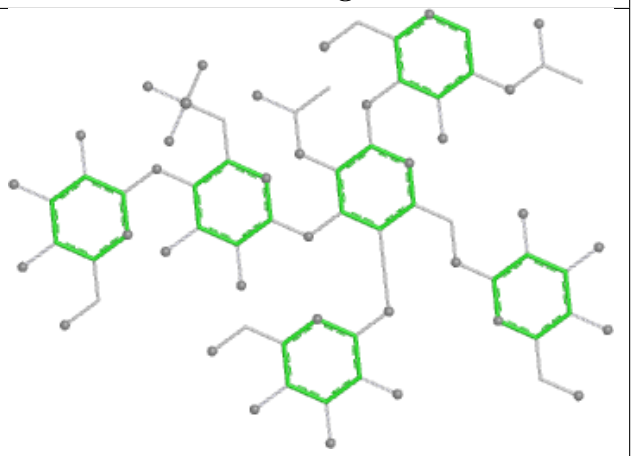
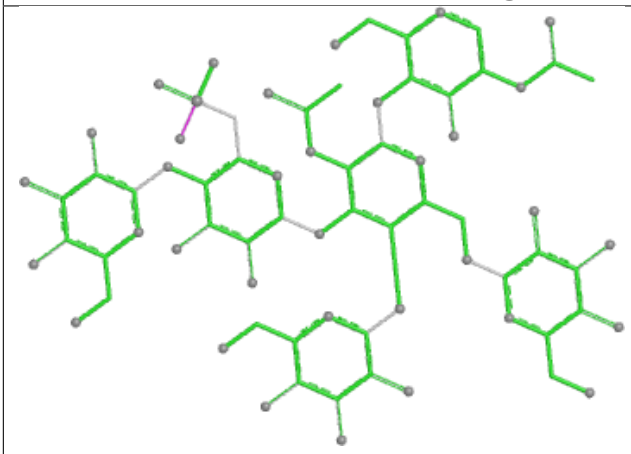


Rings

Oligosaccharide Chain t



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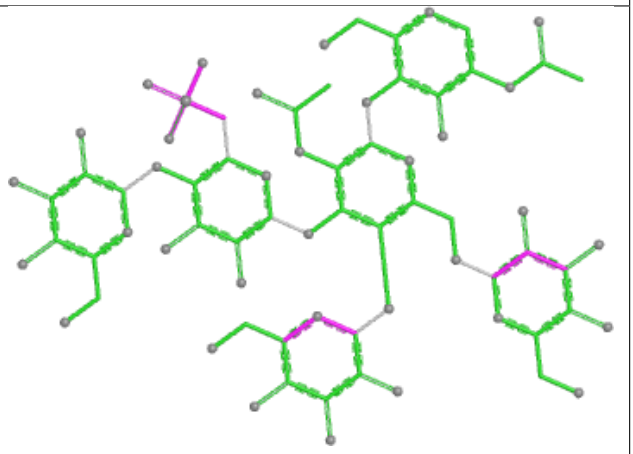

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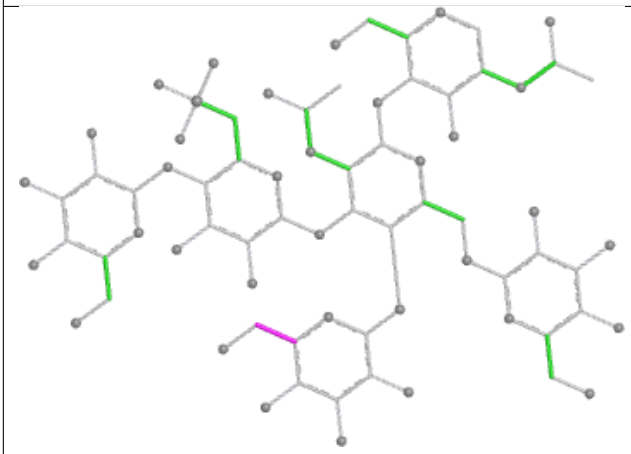

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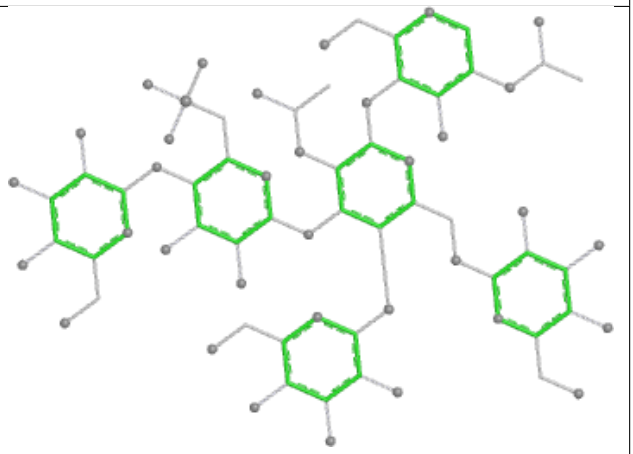
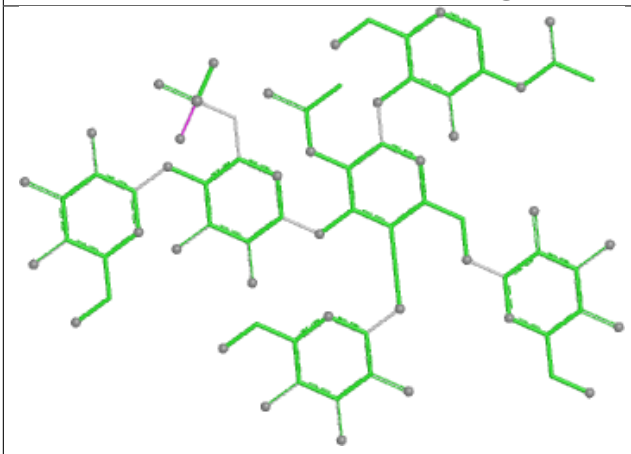


Rings

Oligosaccharide Chain u



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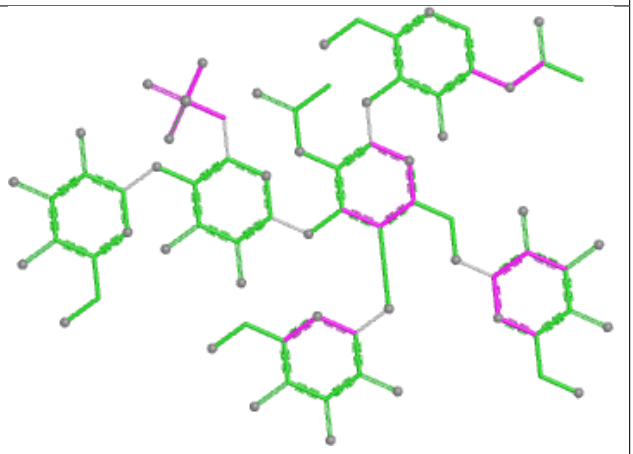

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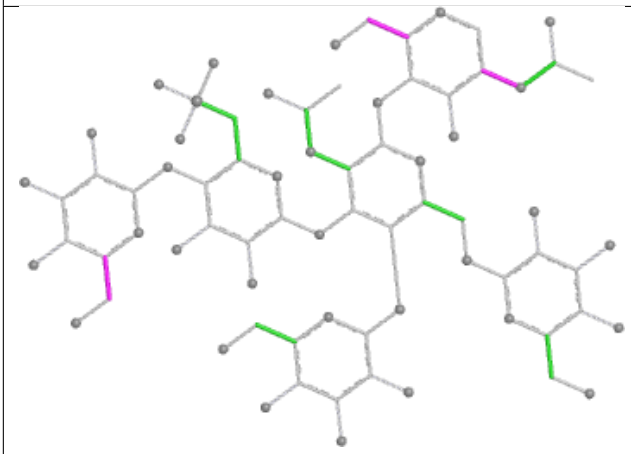

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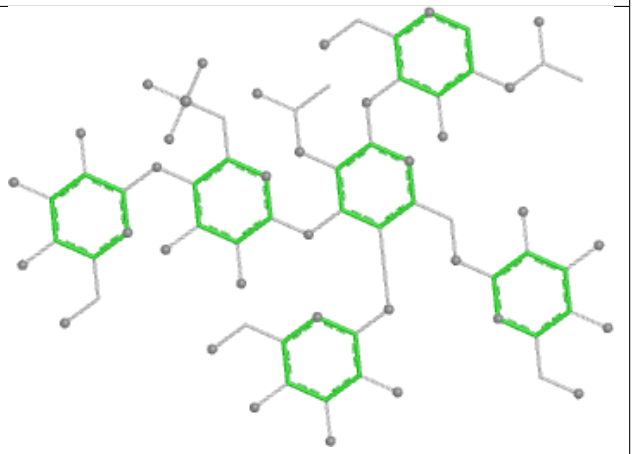
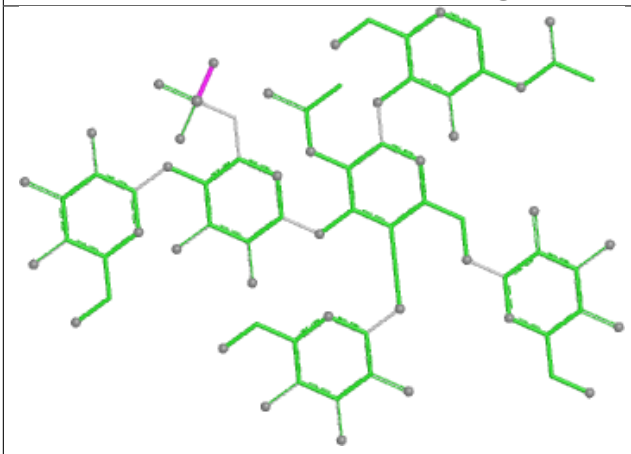


Rings

Oligosaccharide Chain w



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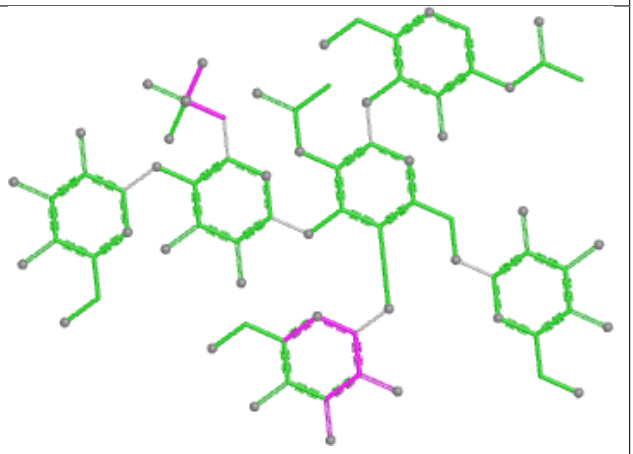

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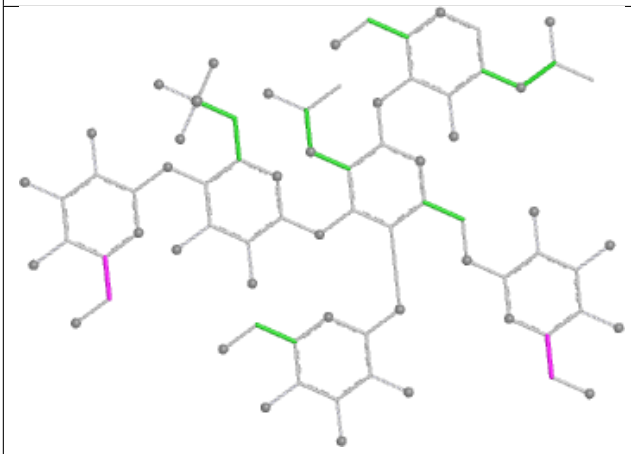

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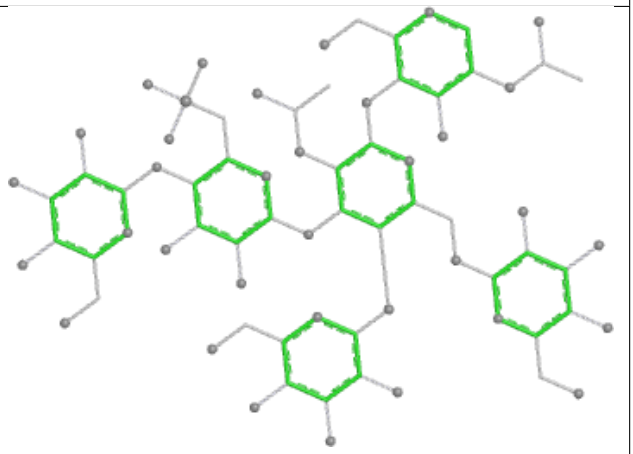
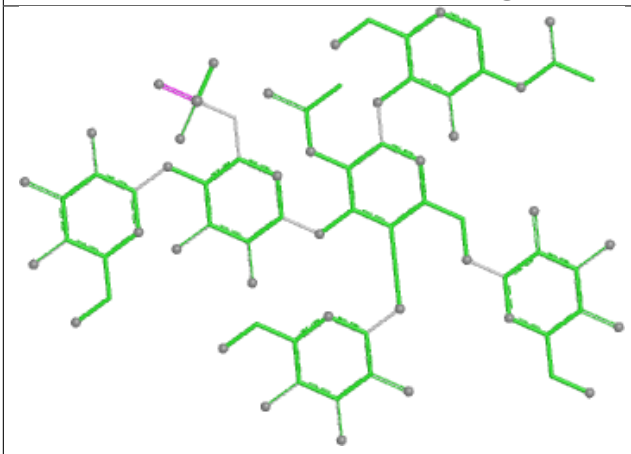


Rings

Oligosaccharide Chain x



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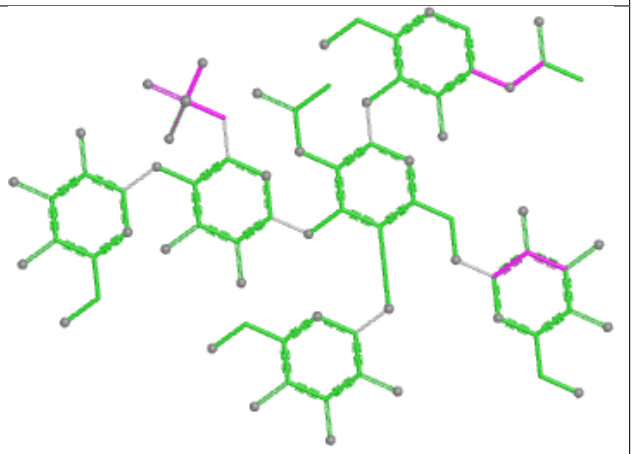
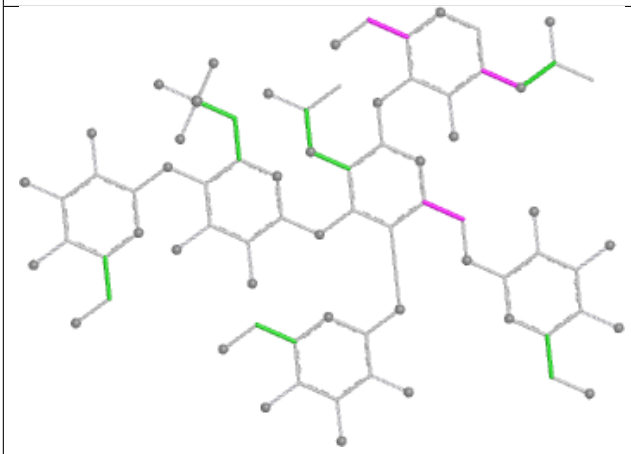


Bond angles



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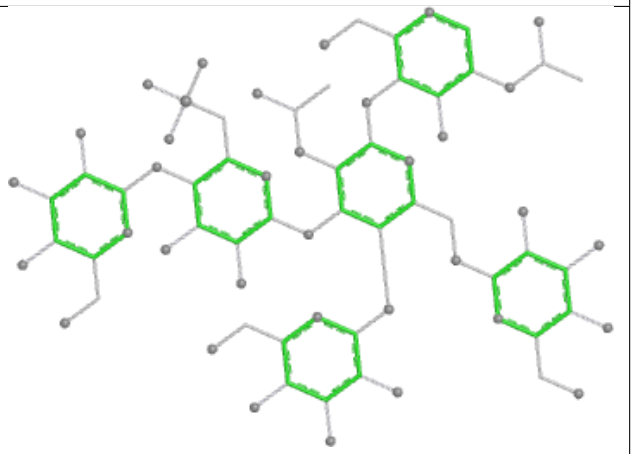
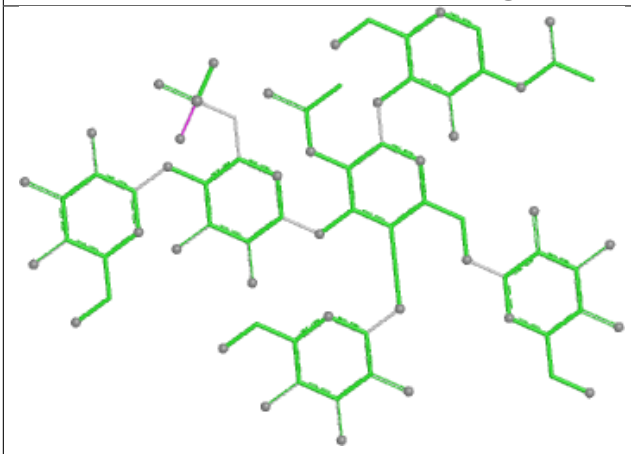


Rings

Oligosaccharide Chain z



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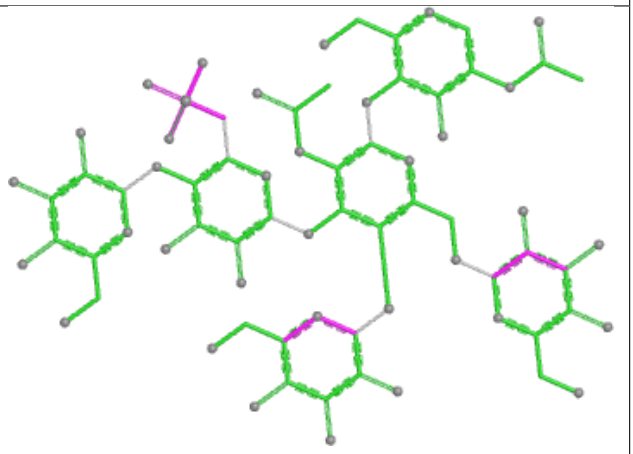
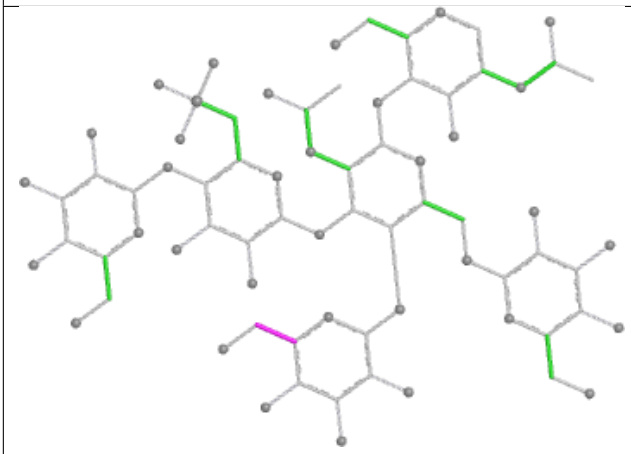


Bond angles



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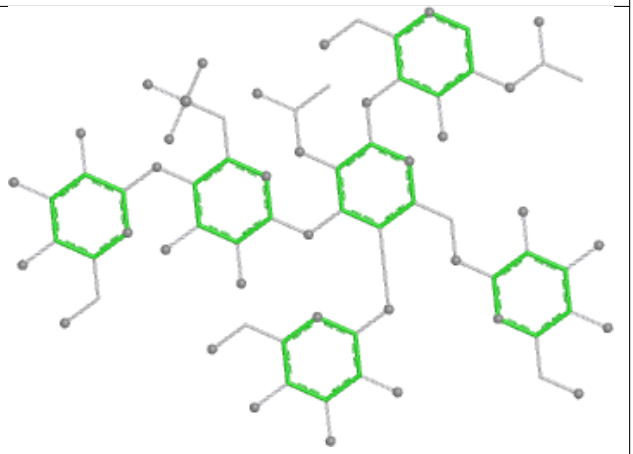
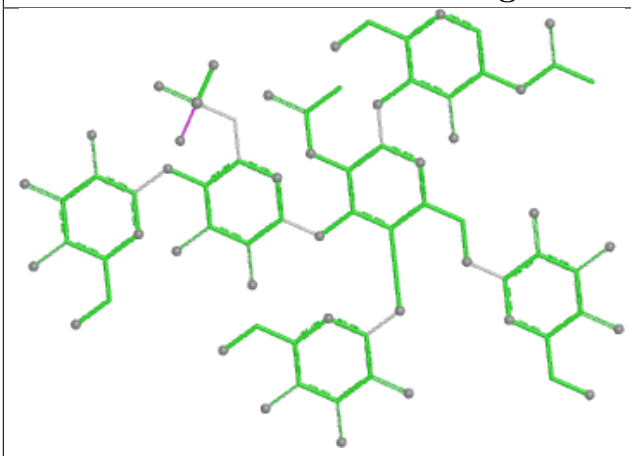


Rings

Oligosaccharide Chain 0



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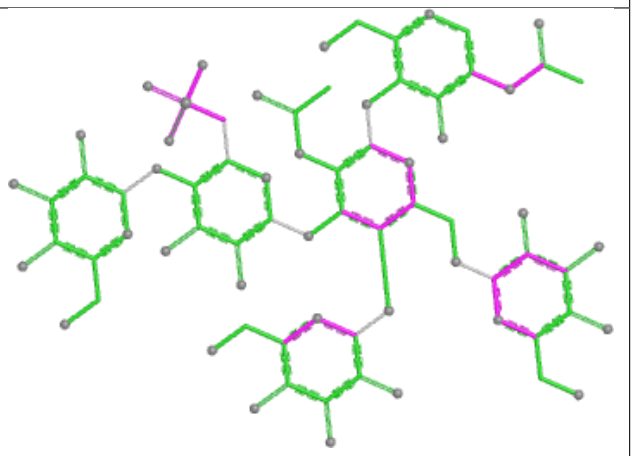
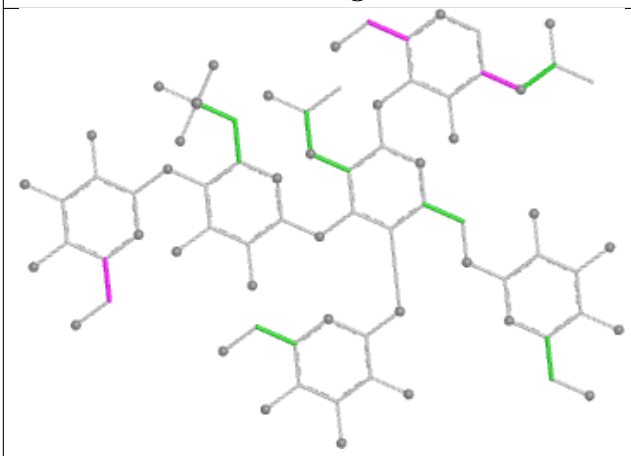


Bond angles



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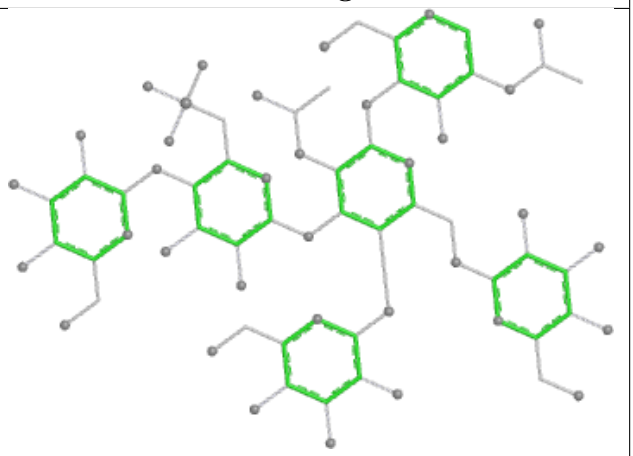
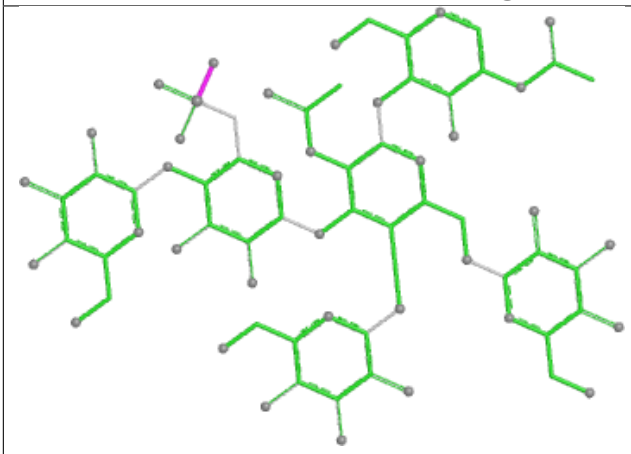


Rings

Oligosaccharide Chain 2



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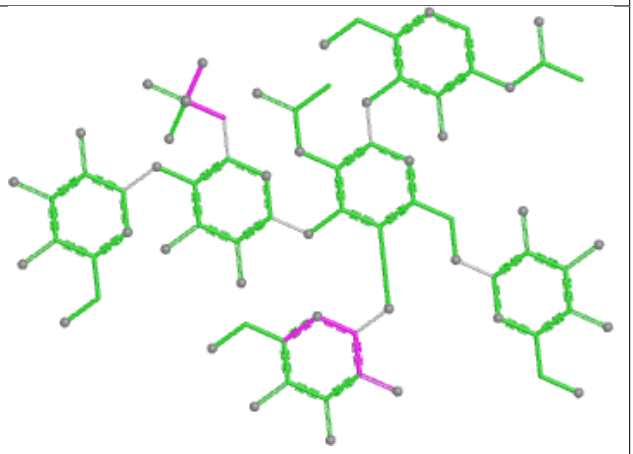

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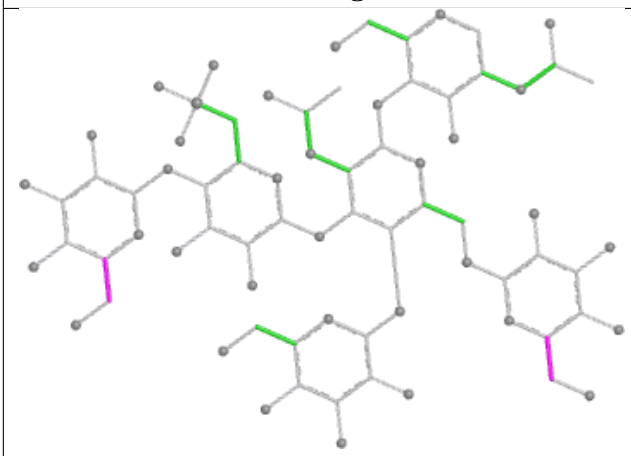

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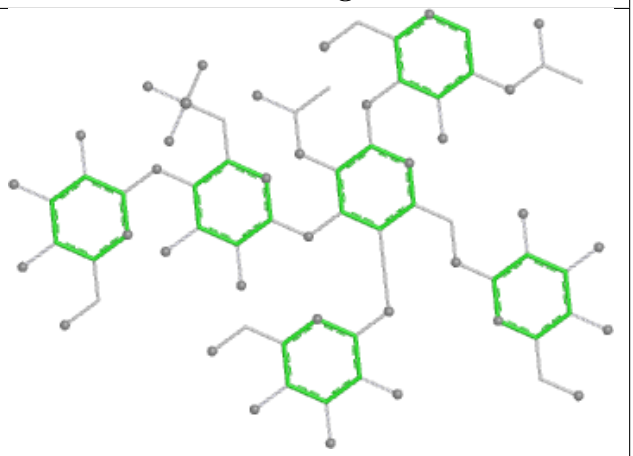
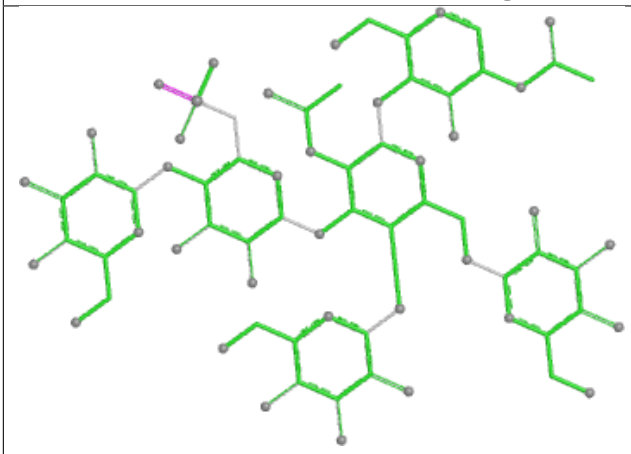


Rings

Oligosaccharide Chain 3



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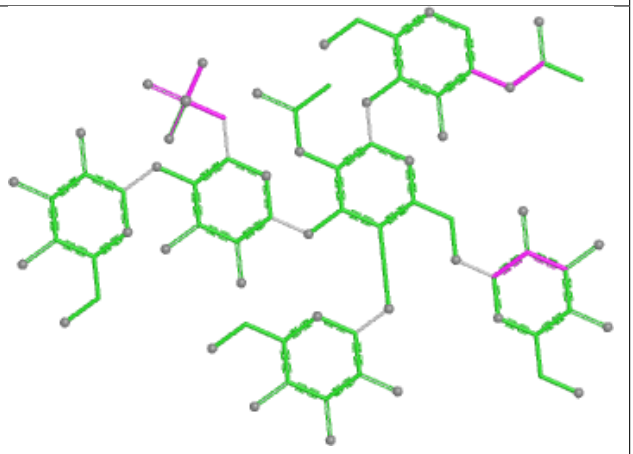

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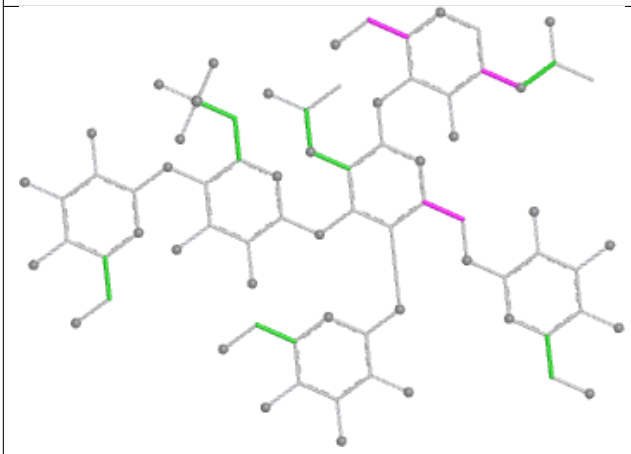

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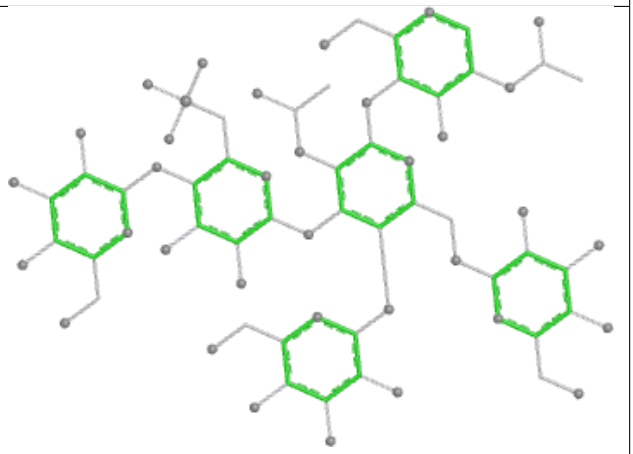
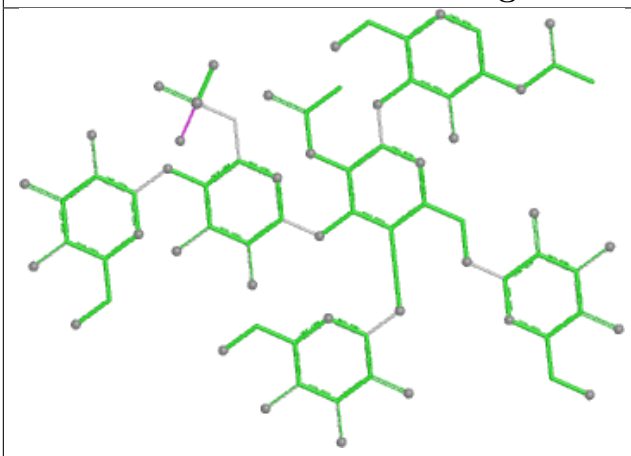


Rings

Oligosaccharide Chain 5



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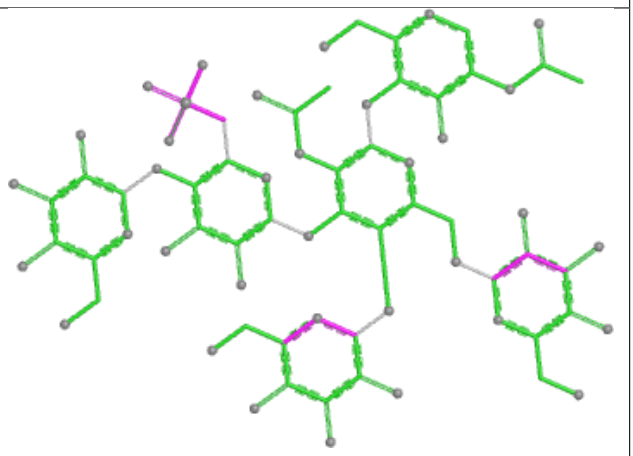

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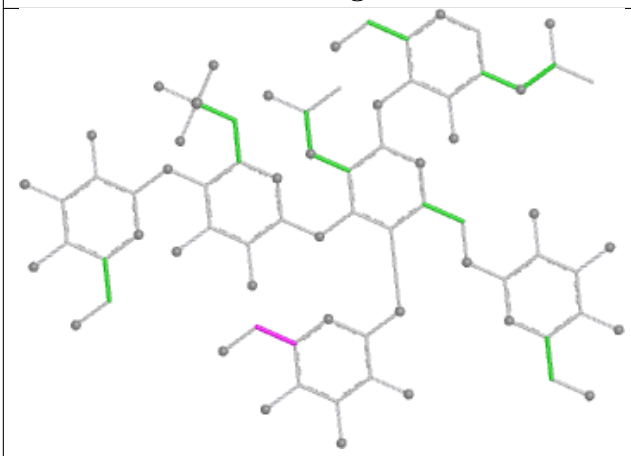

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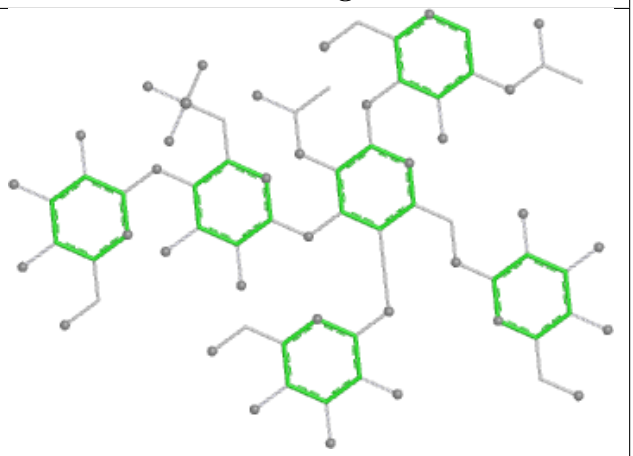
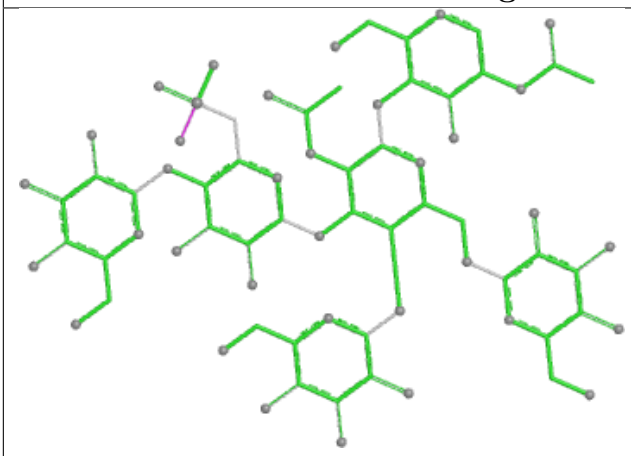


Rings

Oligosaccharide Chain 6



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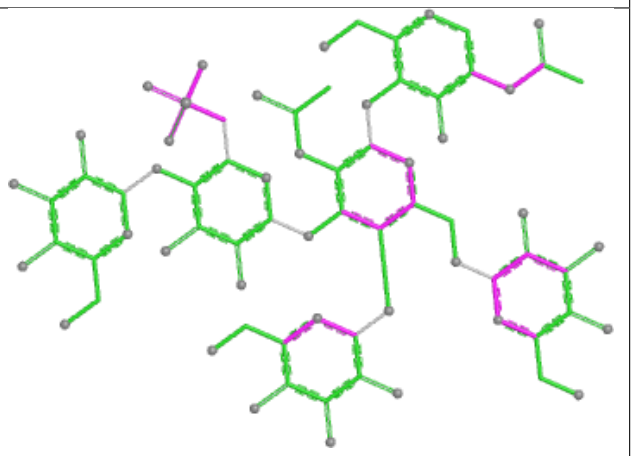

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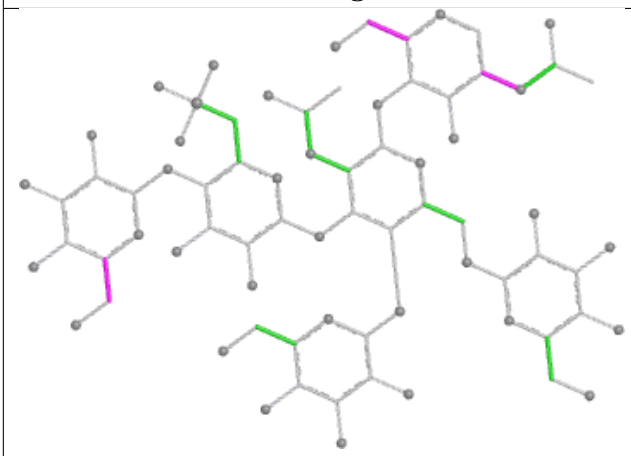

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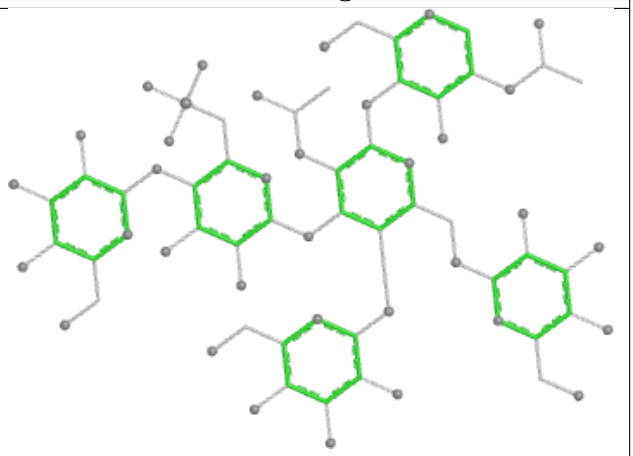
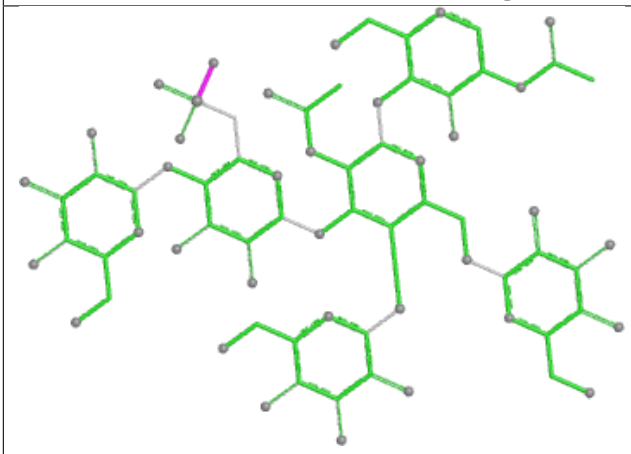


Rings

Oligosaccharide Chain 8



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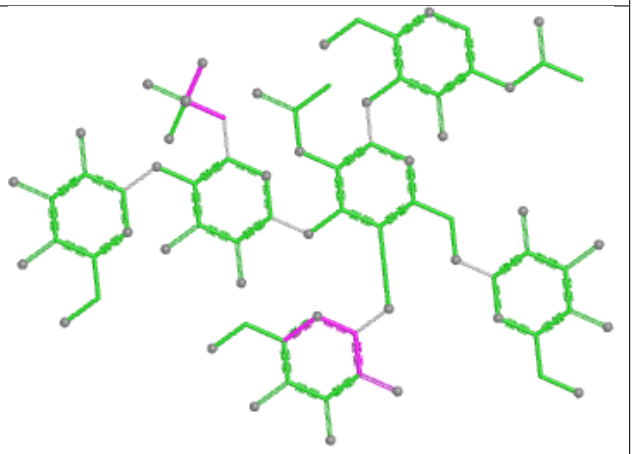

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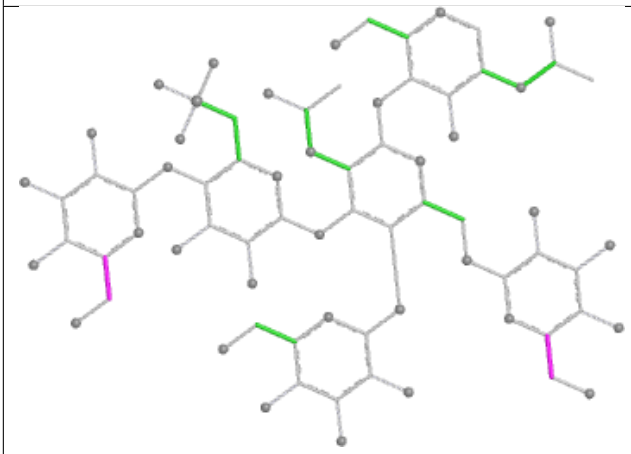

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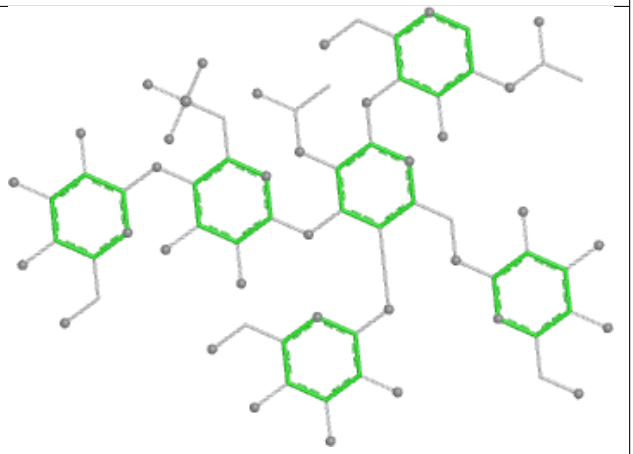
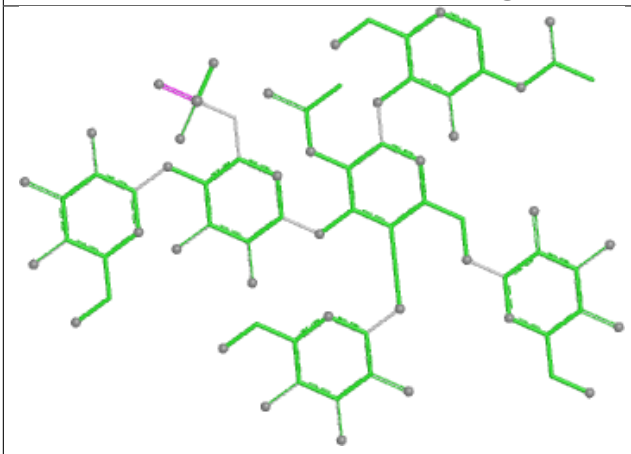


Rings

Oligosaccharide Chain 9



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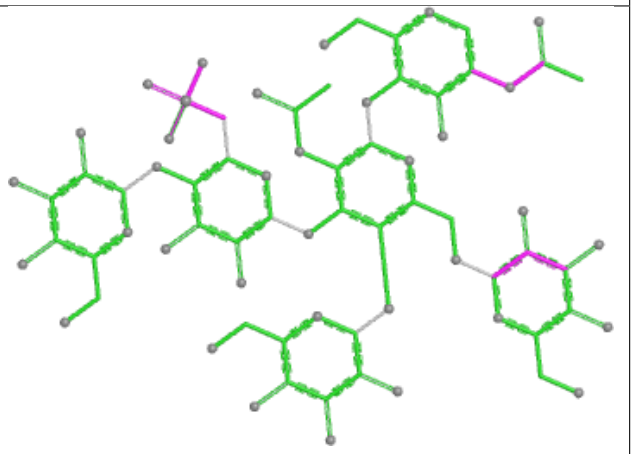

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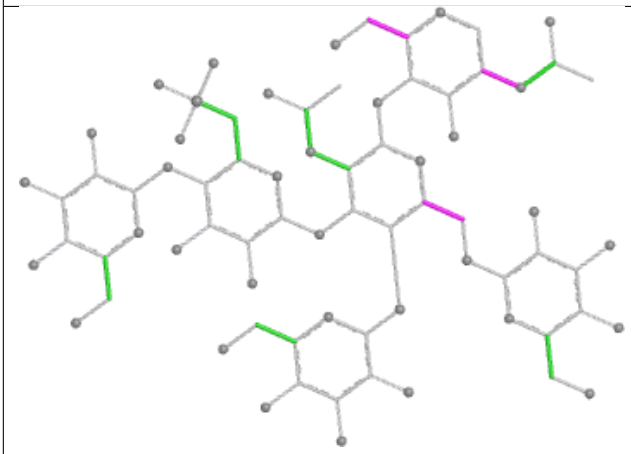

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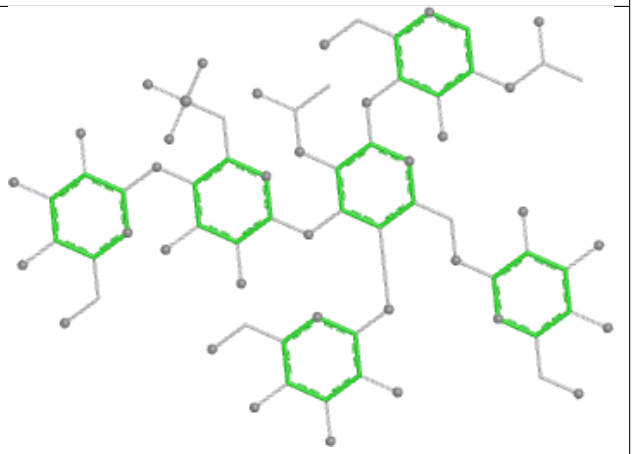
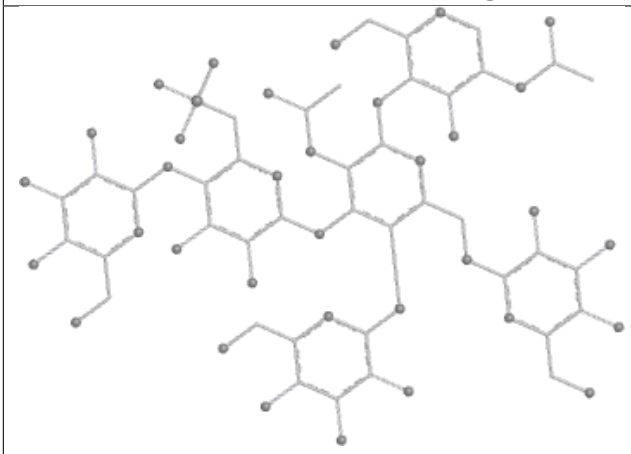


Rings

Oligosaccharide Chain BA



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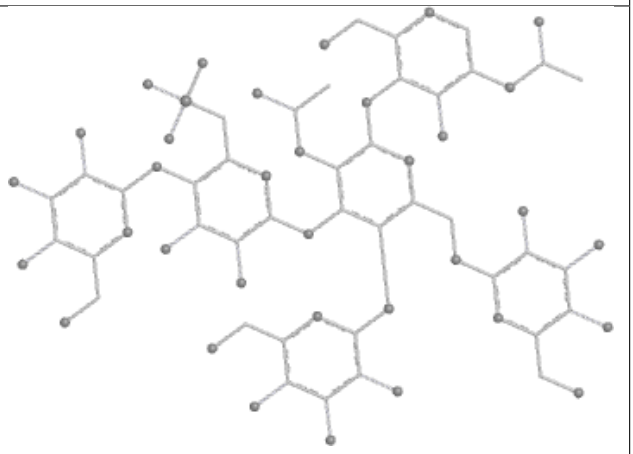
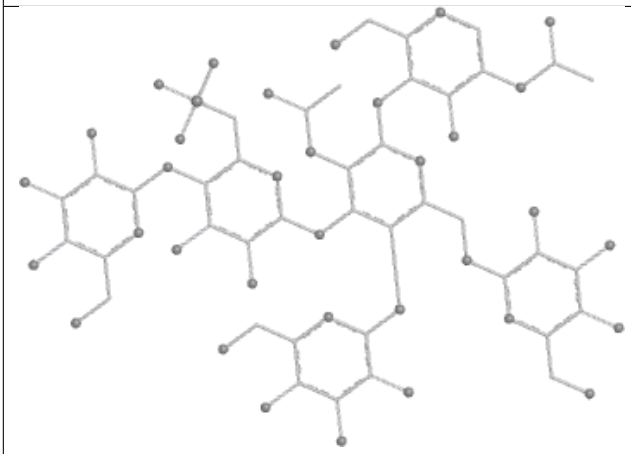


Bond angles



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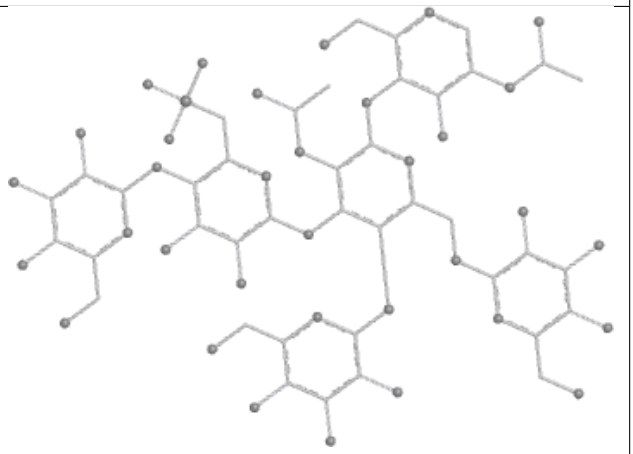
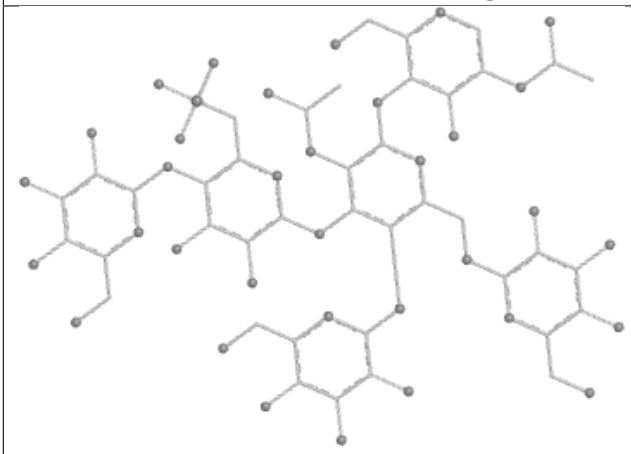


Rings

Oligosaccharide Chain CA



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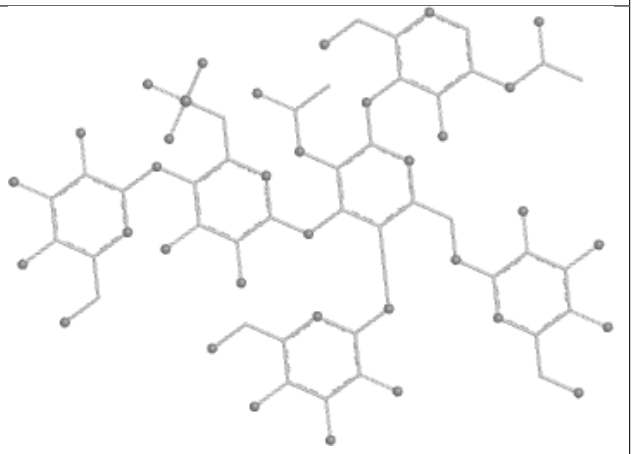
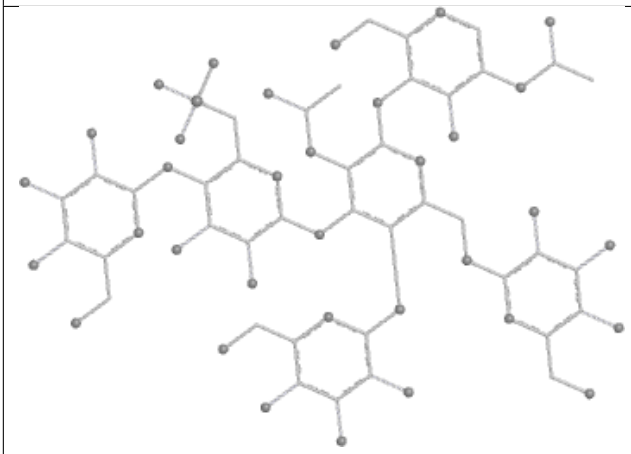
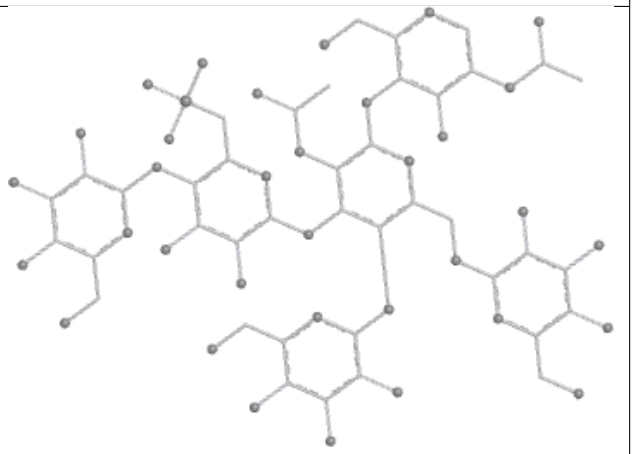


Bond angles

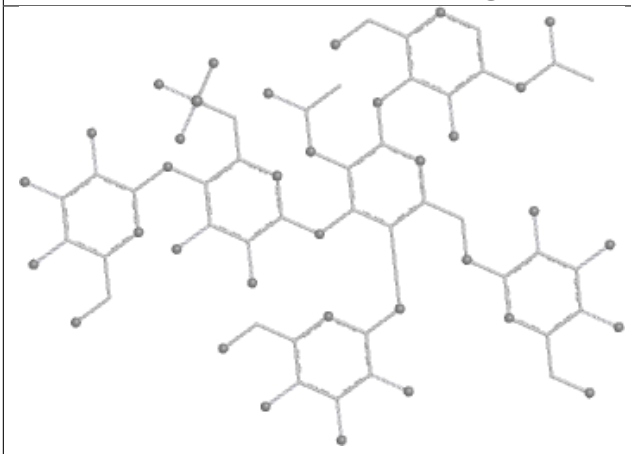


Torsions



Rings

Oligosaccharide Chain EA



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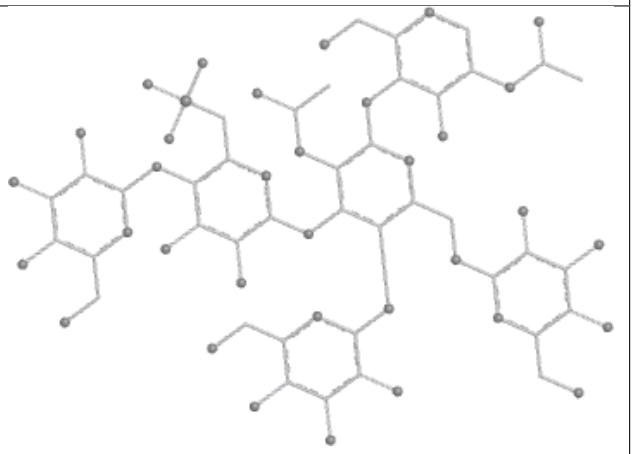
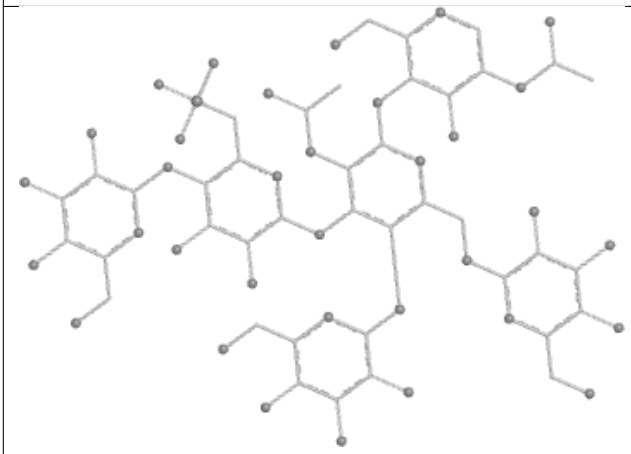


Bond angles



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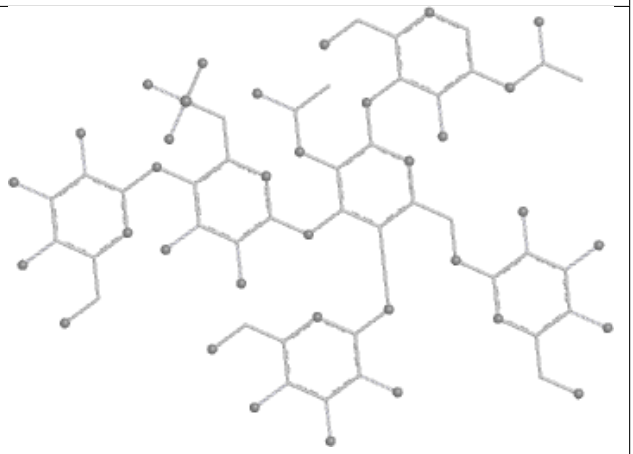
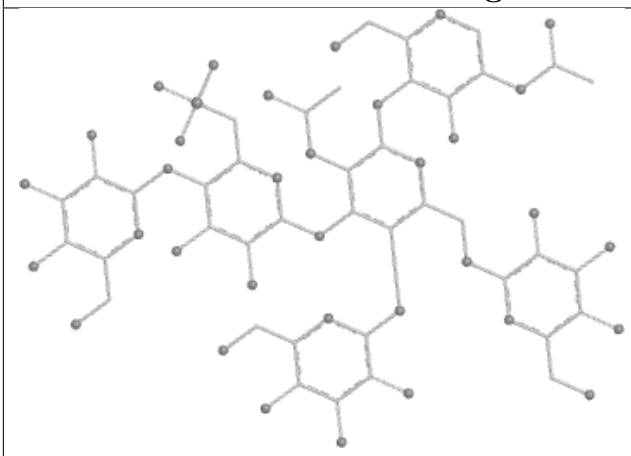


Rings

Oligosaccharide Chain FA



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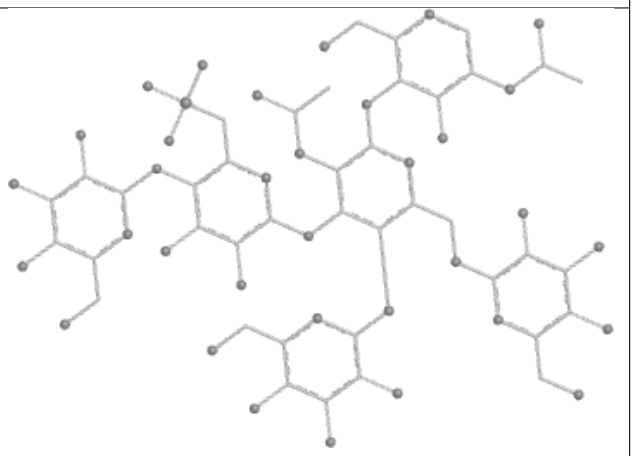

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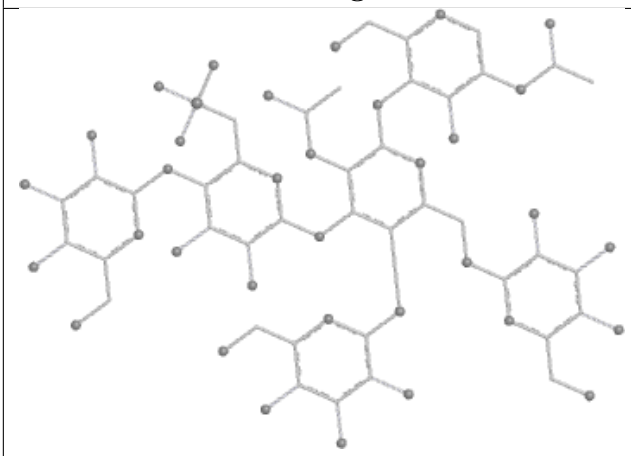

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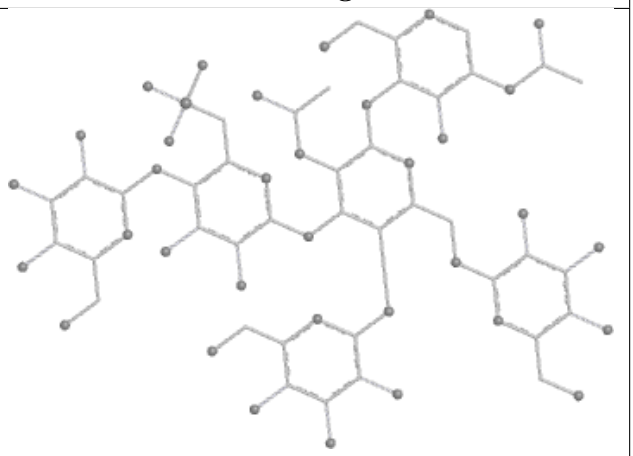
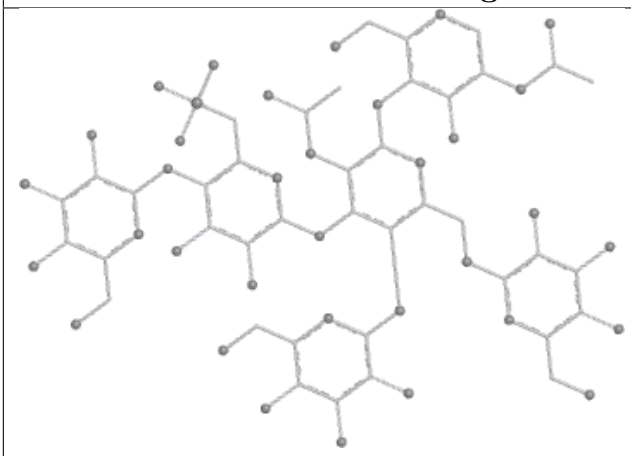


Rings

Oligosaccharide Chain HA



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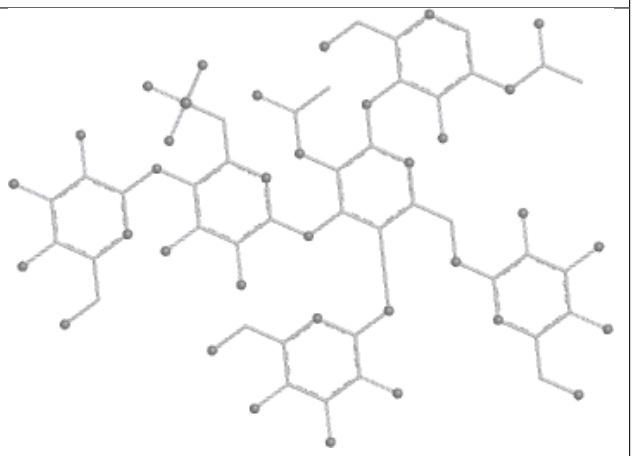

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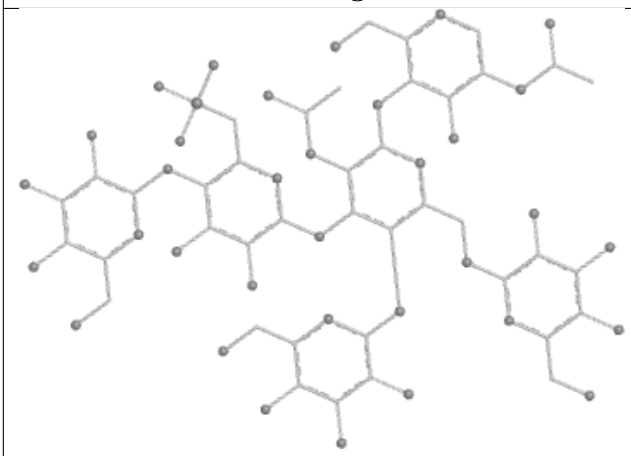

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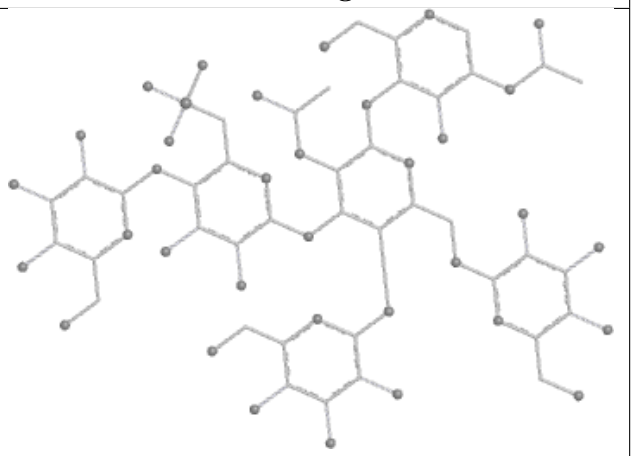
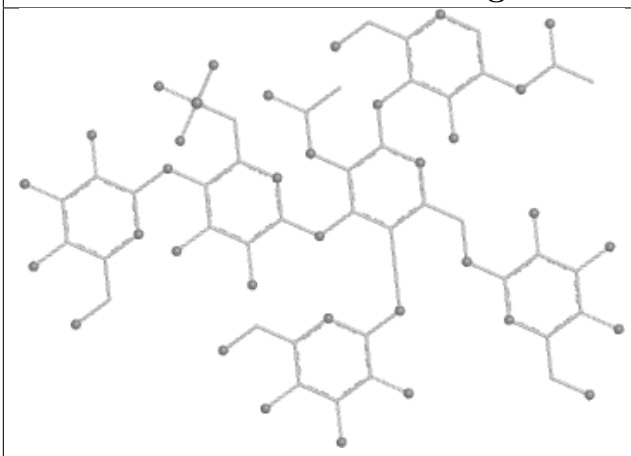


Rings

Oligosaccharide Chain IA



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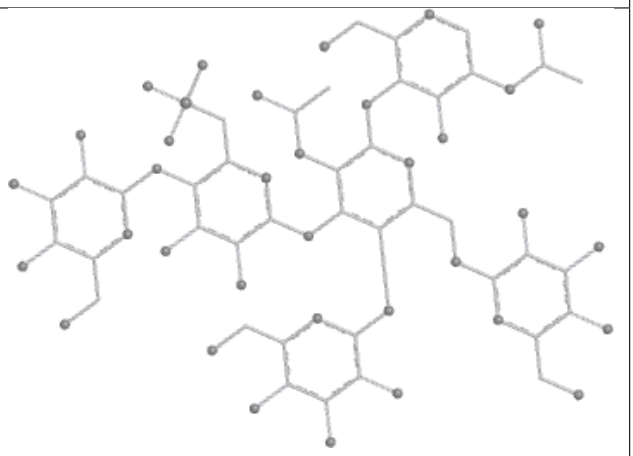

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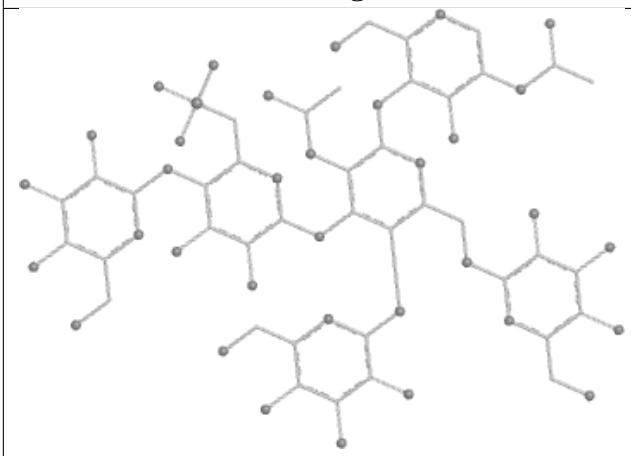

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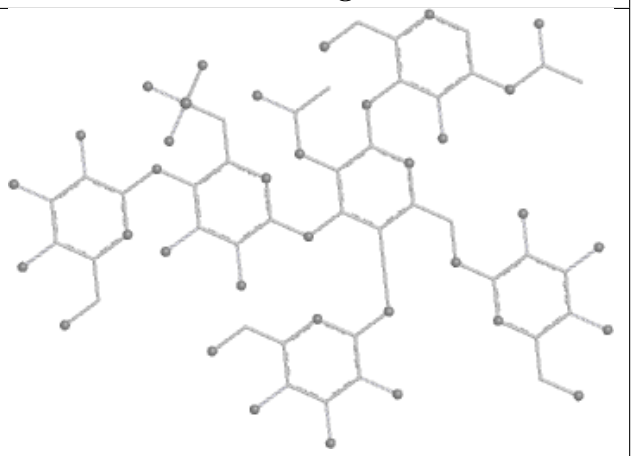
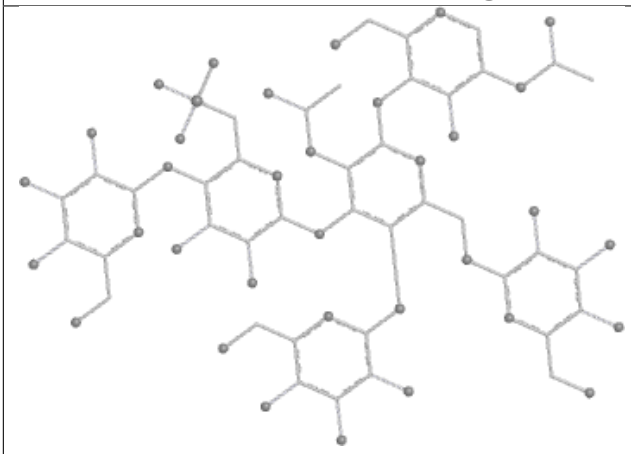


Rings

Oligosaccharide Chain KA



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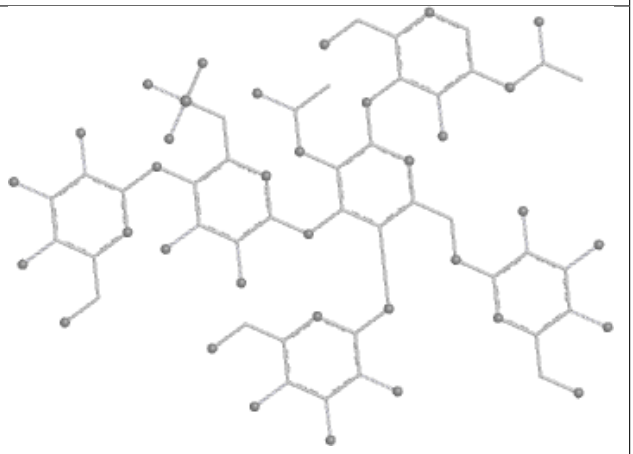

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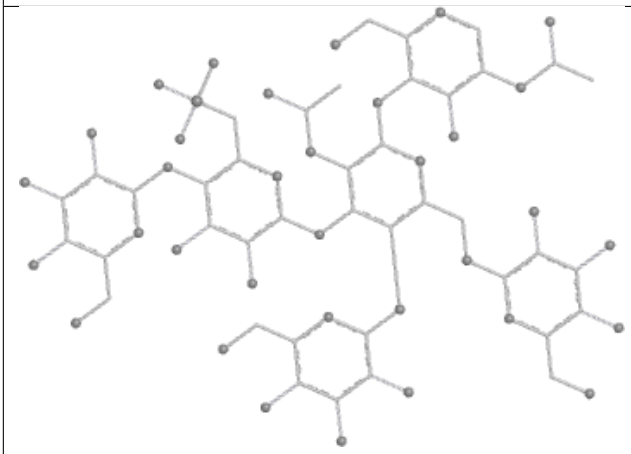

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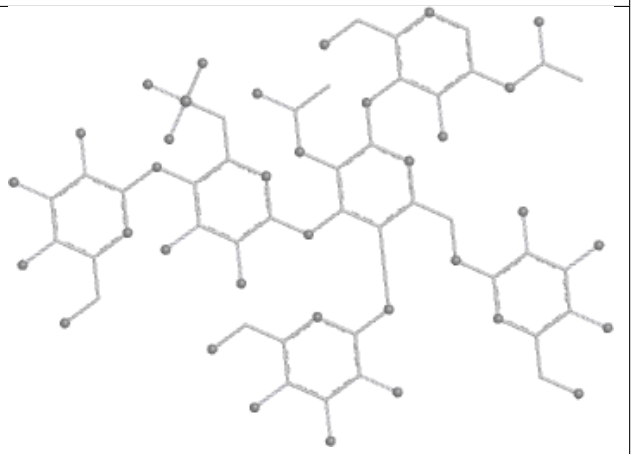
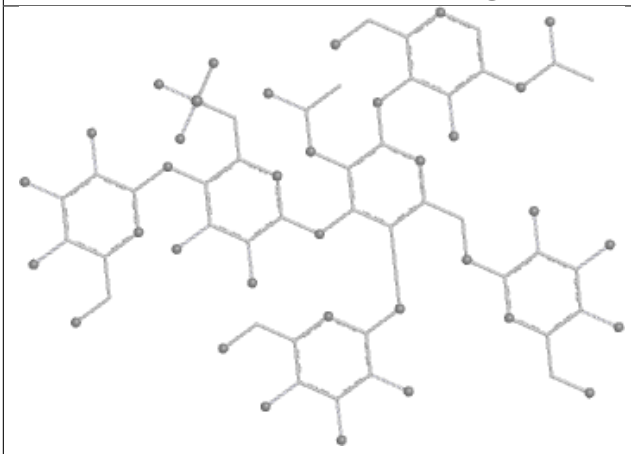


Rings

Oligosaccharide Chain LA



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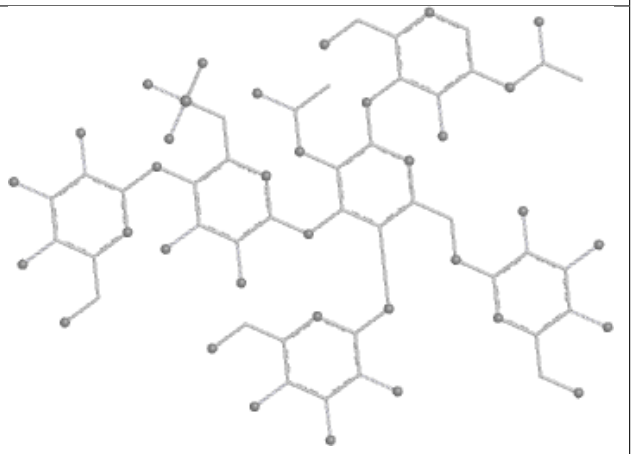
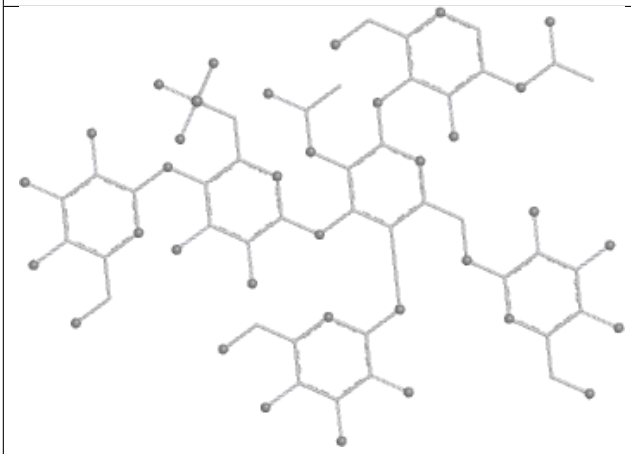


Bond angles



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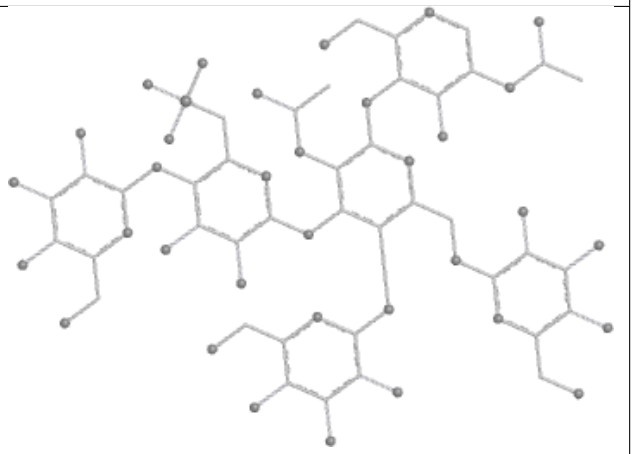
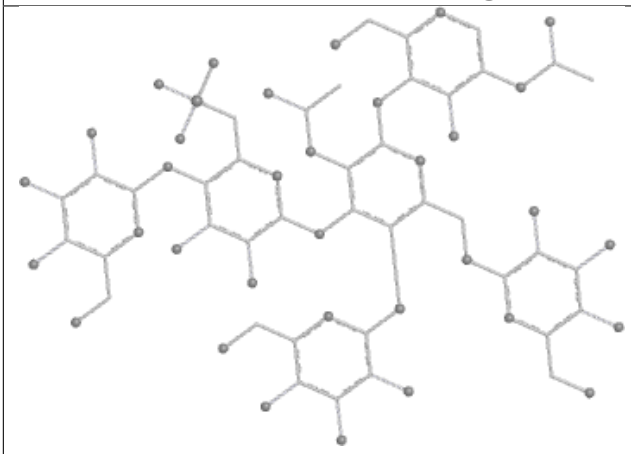


Rings

Oligosaccharide Chain NA



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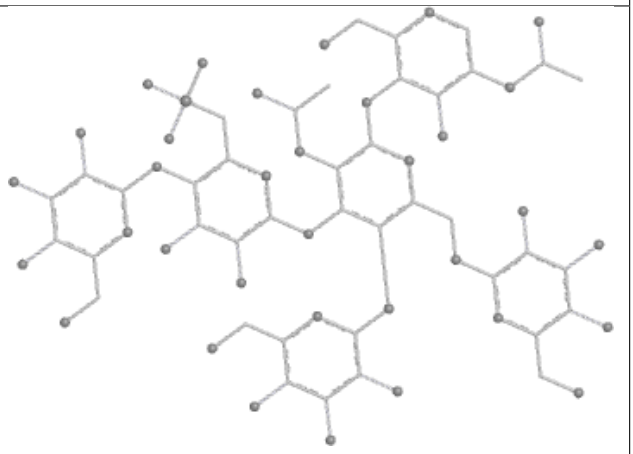

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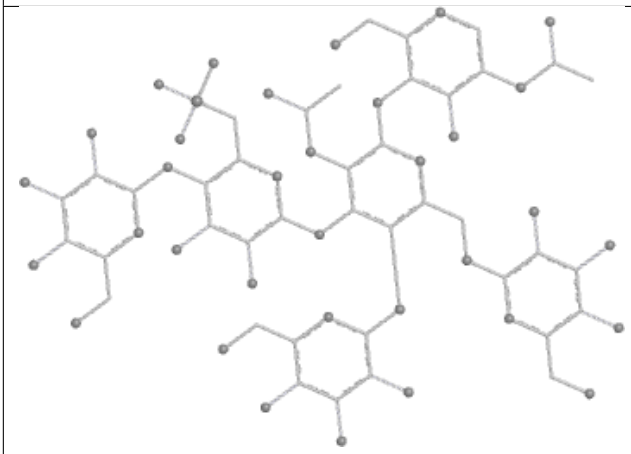

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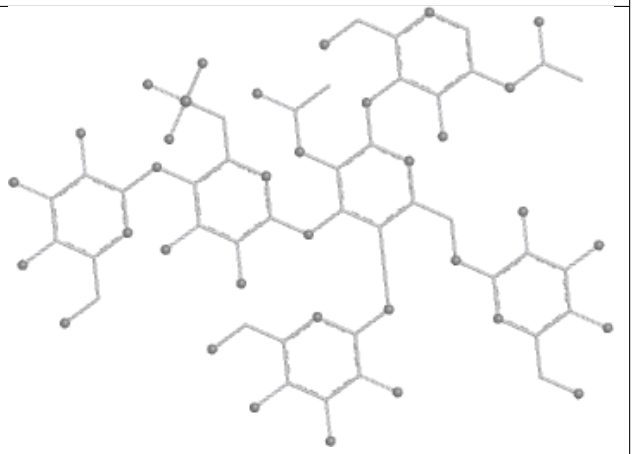
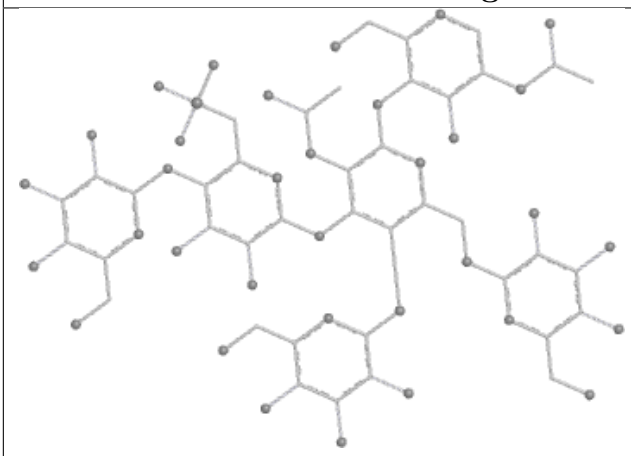


Rings

Oligosaccharide Chain OA



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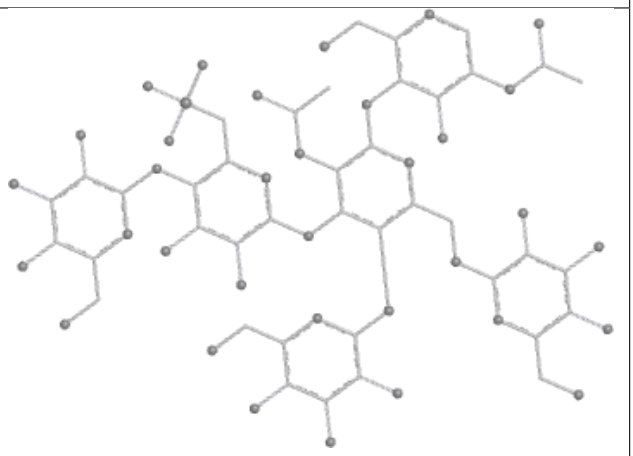
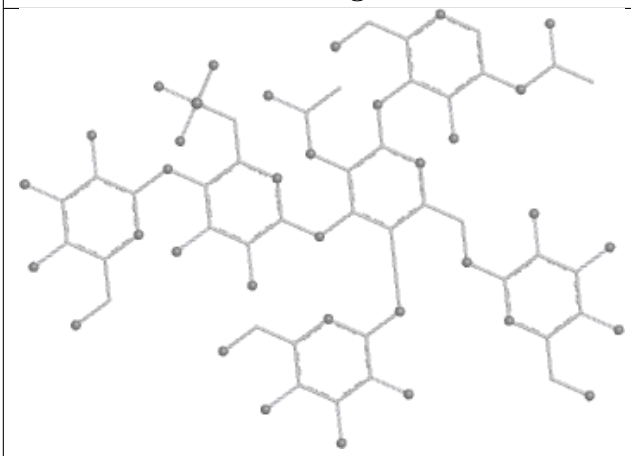


Bond angles



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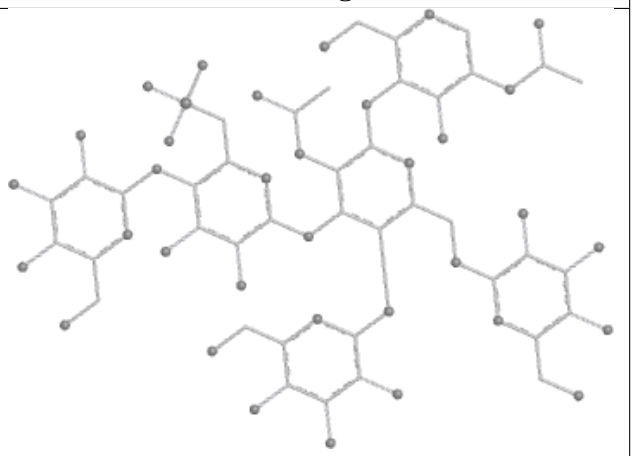
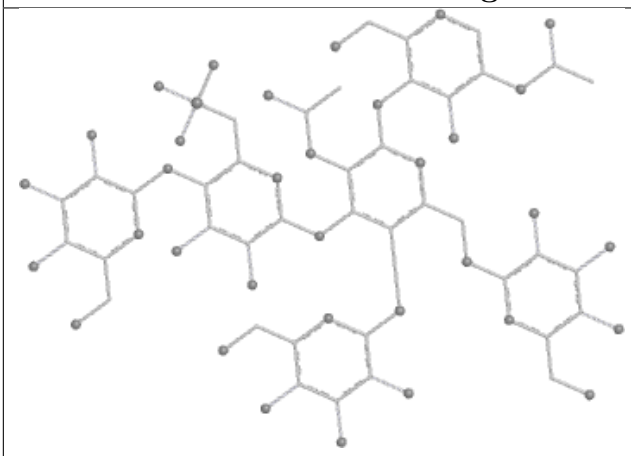


Rings

Oligosaccharide Chain QA



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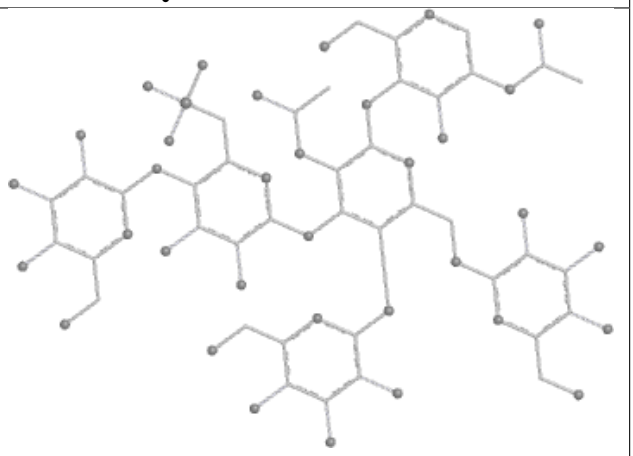

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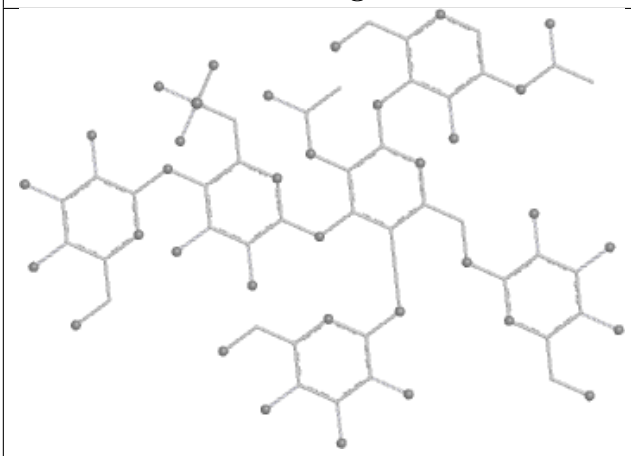

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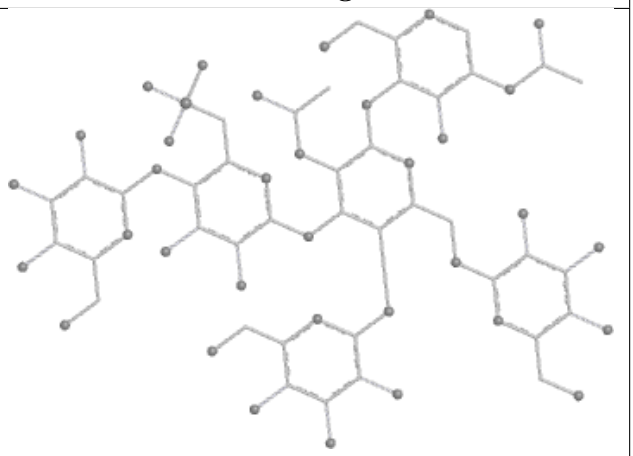
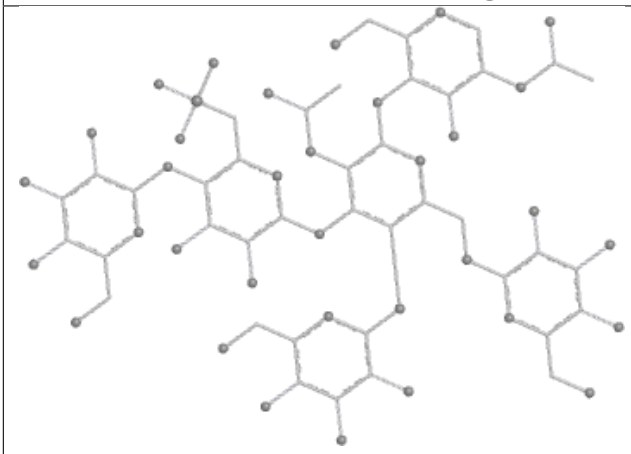


Rings

Oligosaccharide Chain RA



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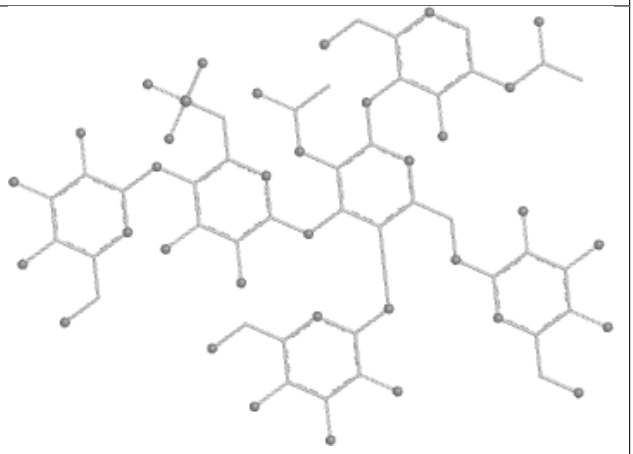
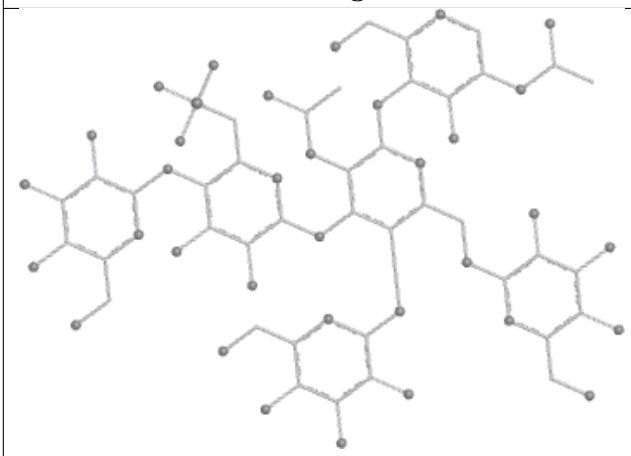


Bond angles



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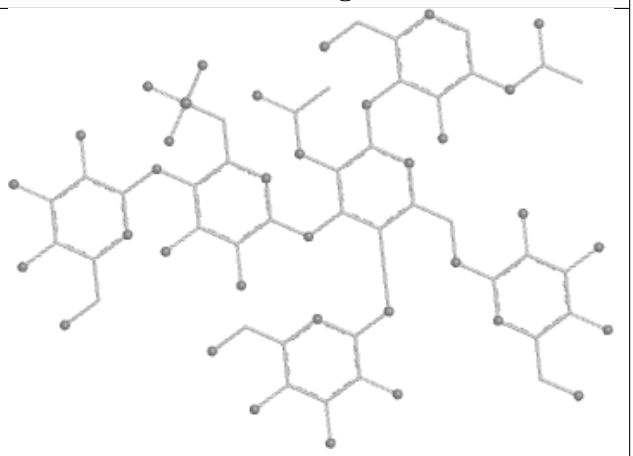
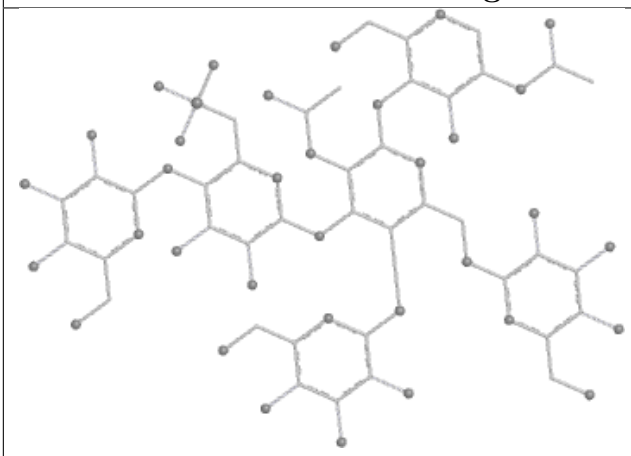


Rings

Oligosaccharide Chain TA



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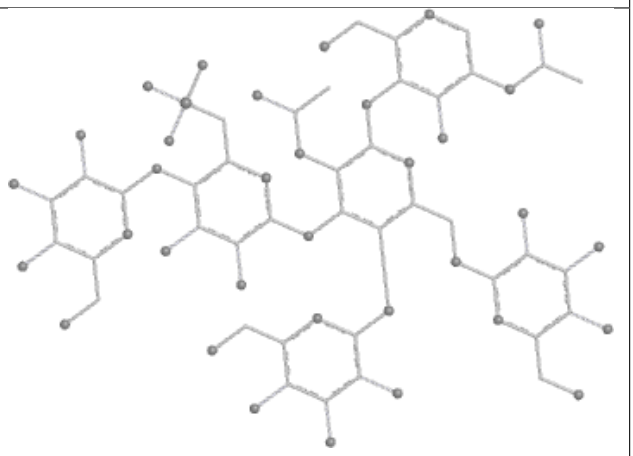
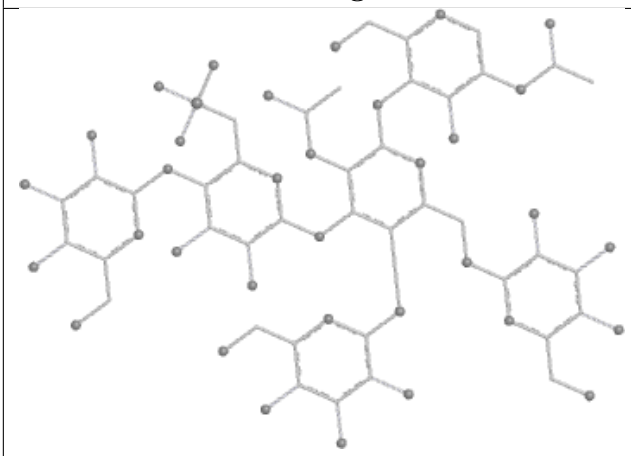


Bond angles



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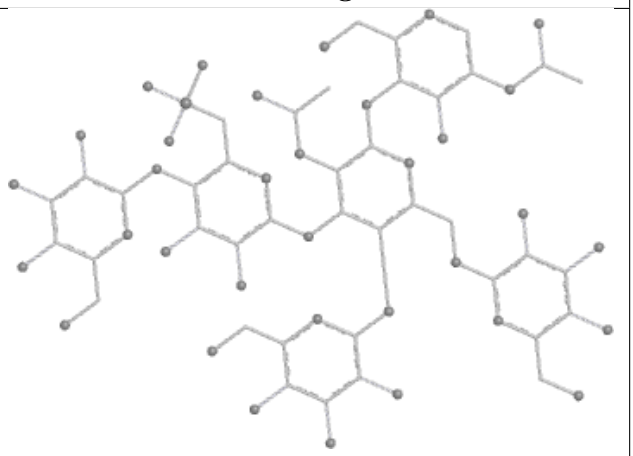
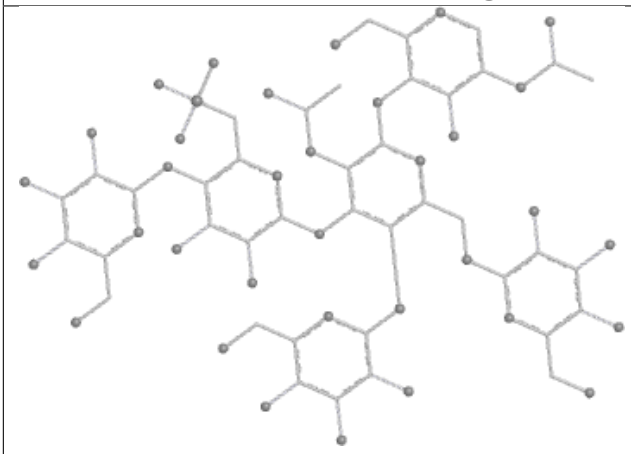


Rings

Oligosaccharide Chain UA



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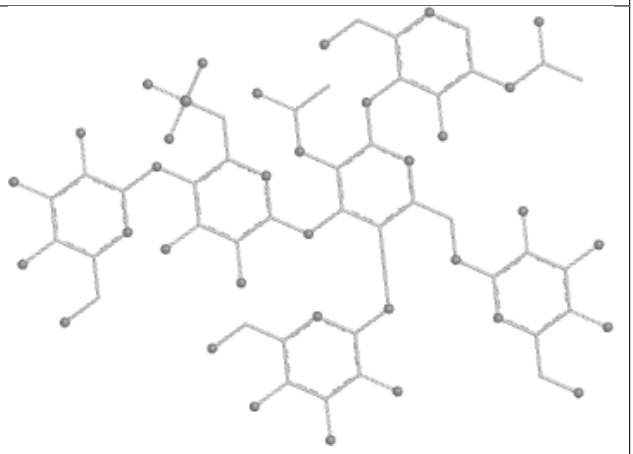

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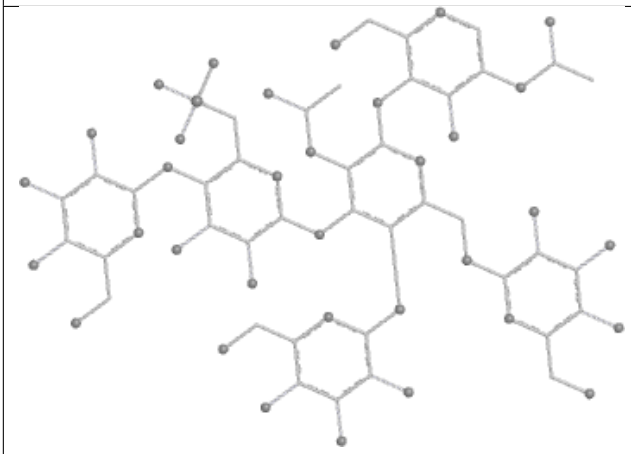

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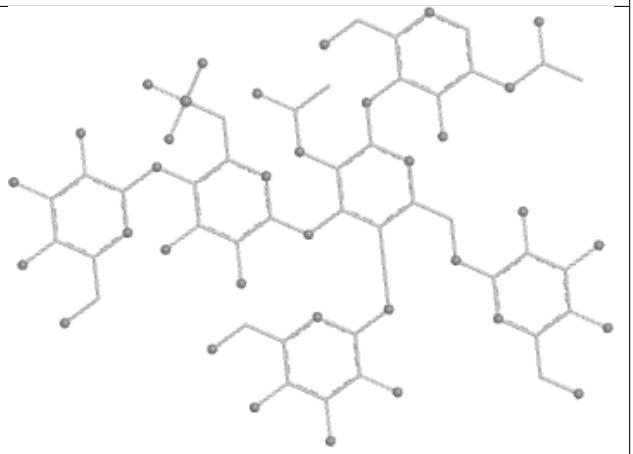
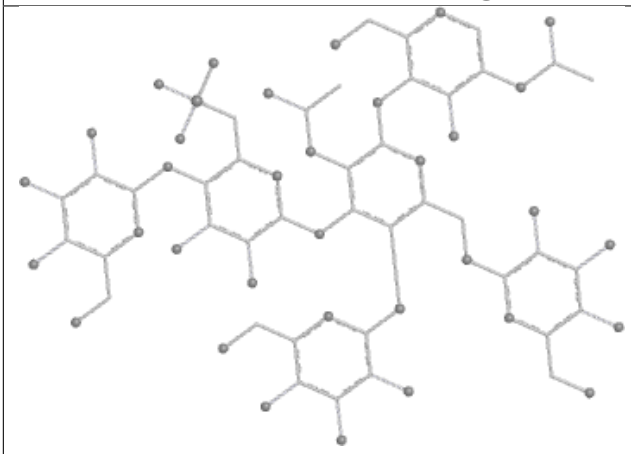


Rings

Oligosaccharide Chain WA



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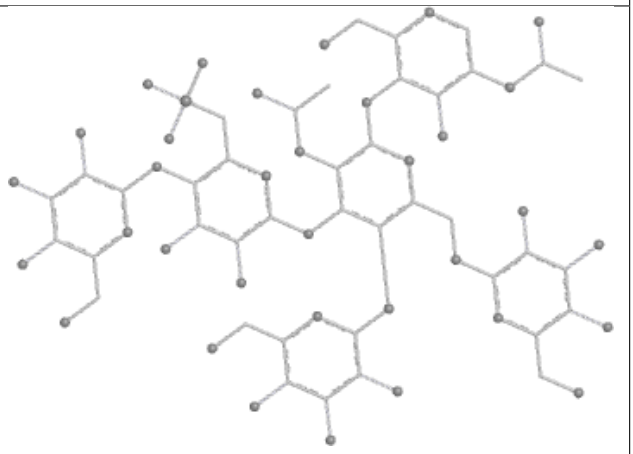
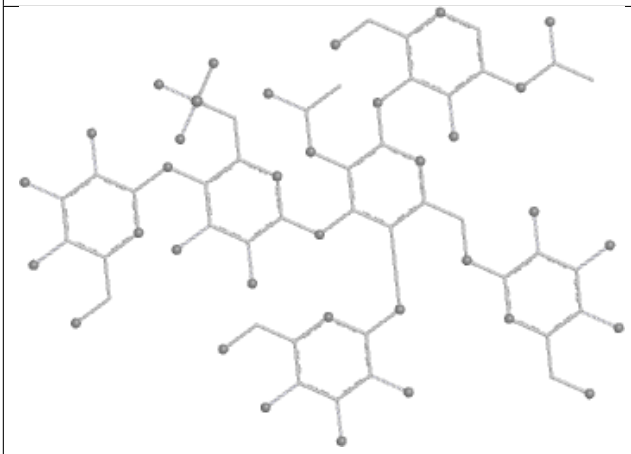


Bond angles



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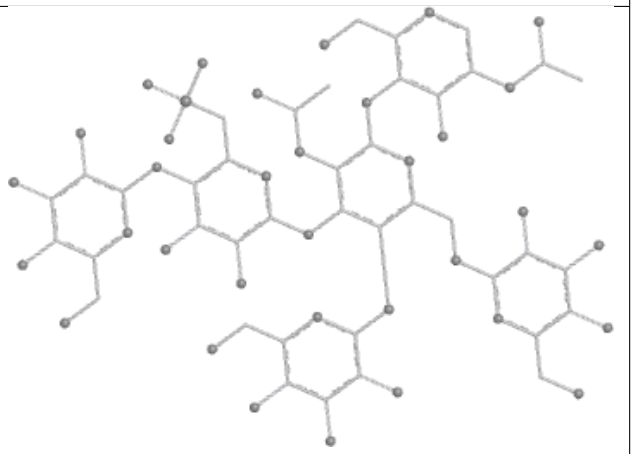
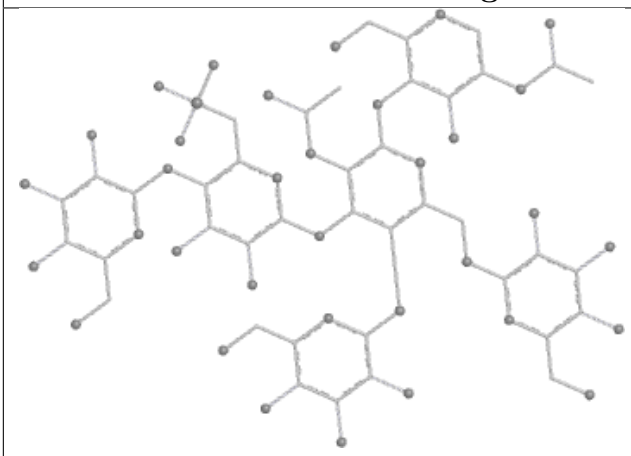


Rings

Oligosaccharide Chain XA



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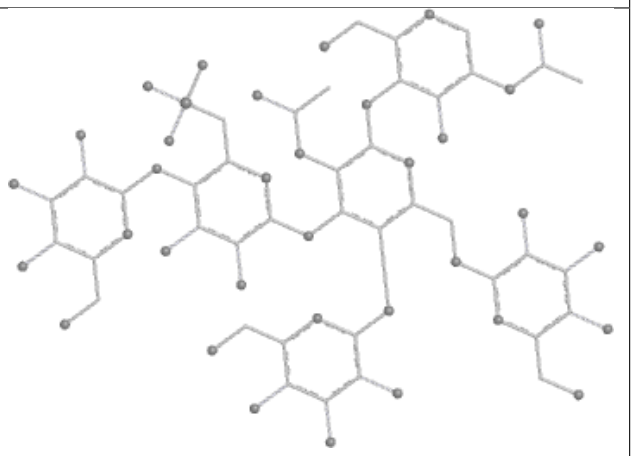
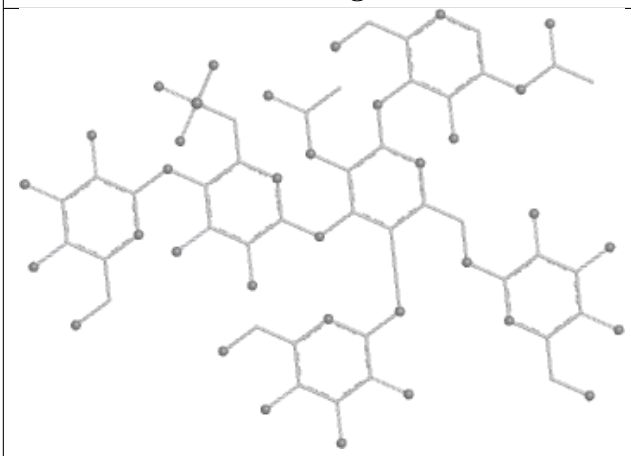


Bond angles



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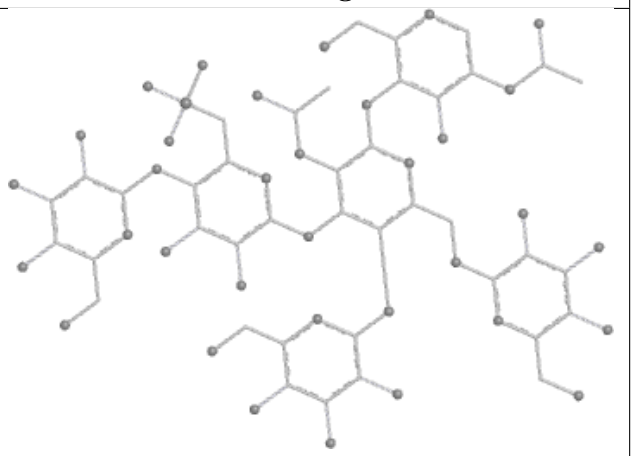
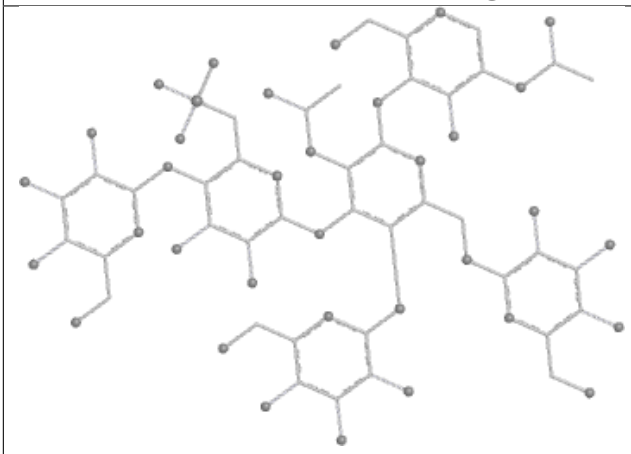


Rings

Oligosaccharide Chain ZA



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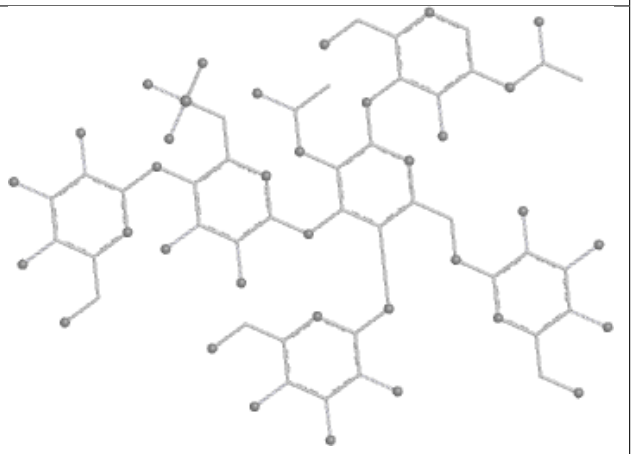
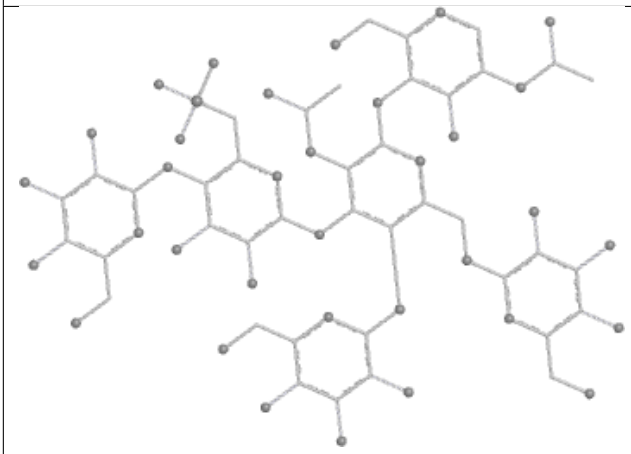
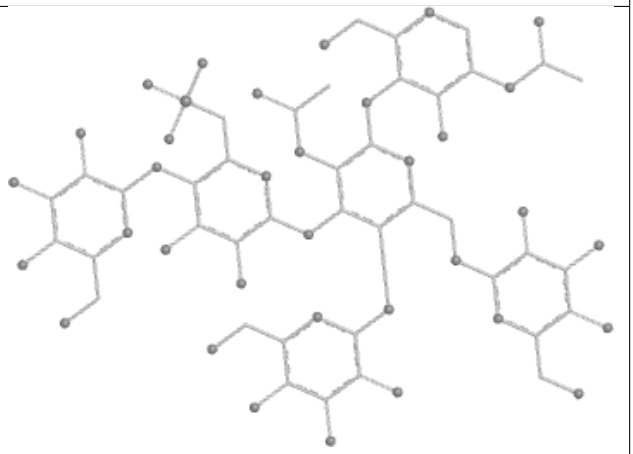


Bond angles

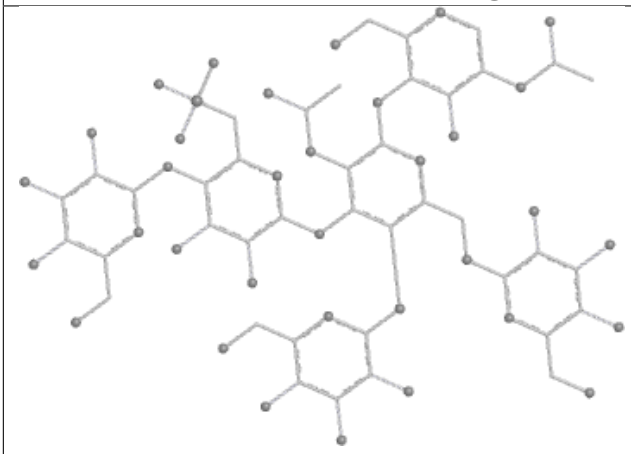


Torsions



Rings

Oligosaccharide Chain aA



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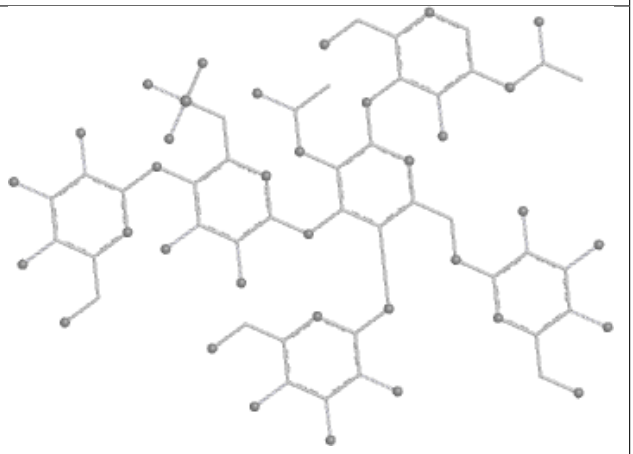

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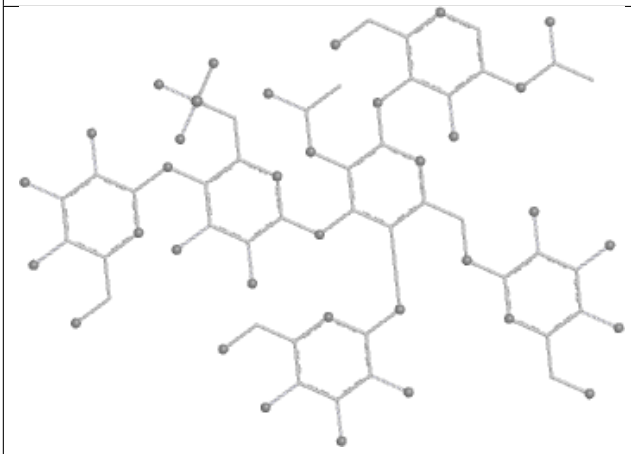

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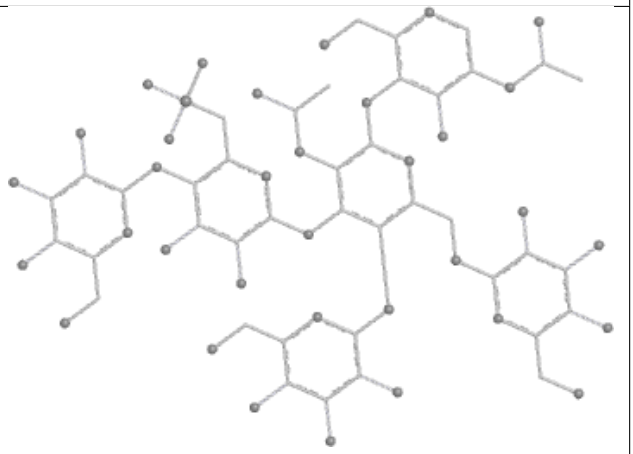
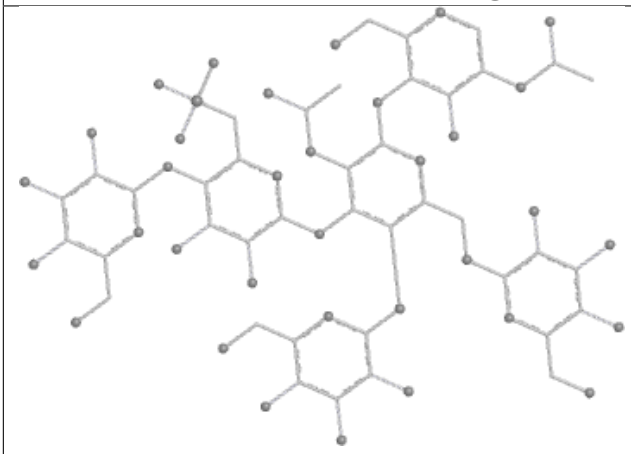


Rings

Oligosaccharide Chain cA



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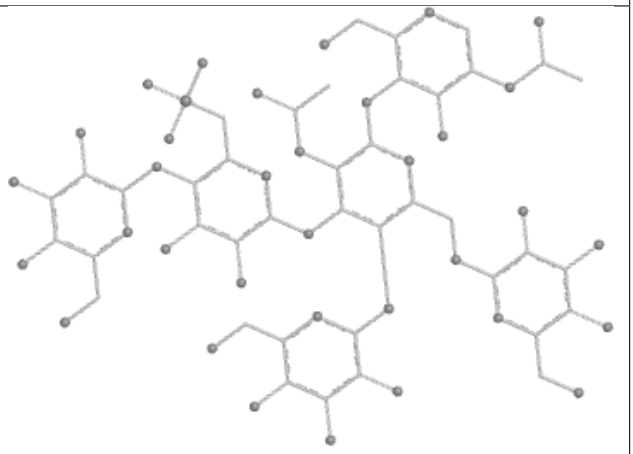

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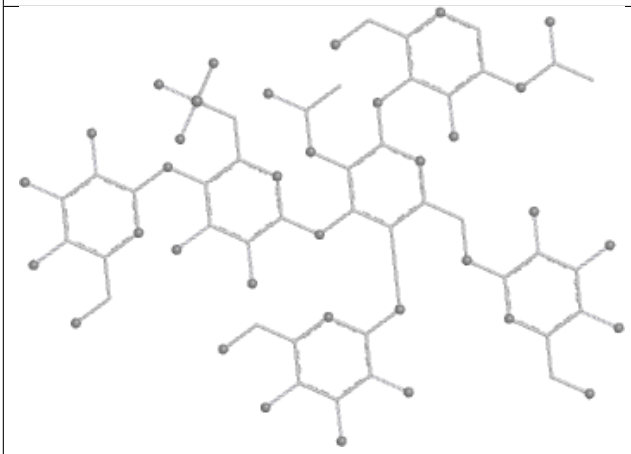

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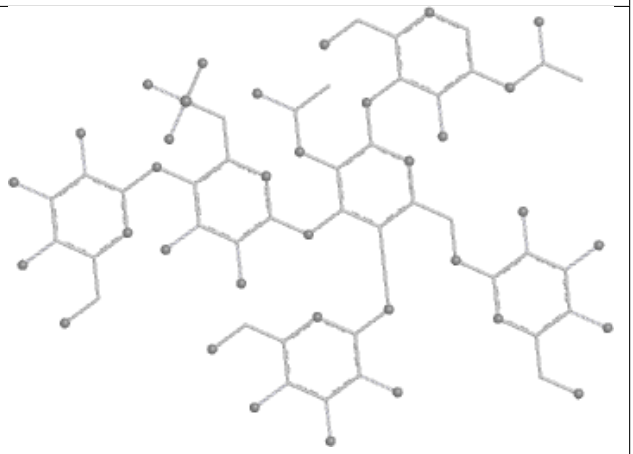
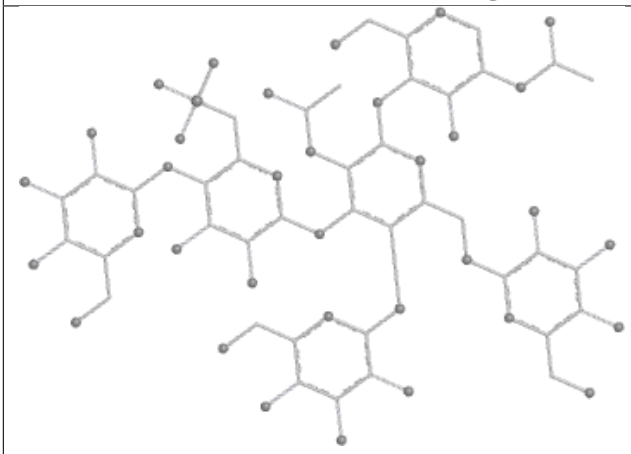


Rings

Oligosaccharide Chain dA



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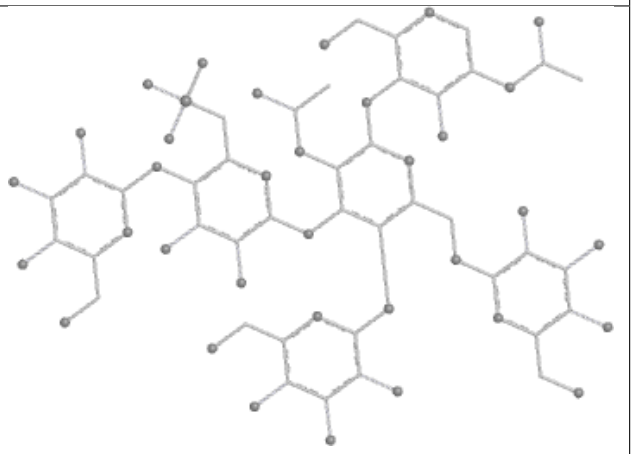

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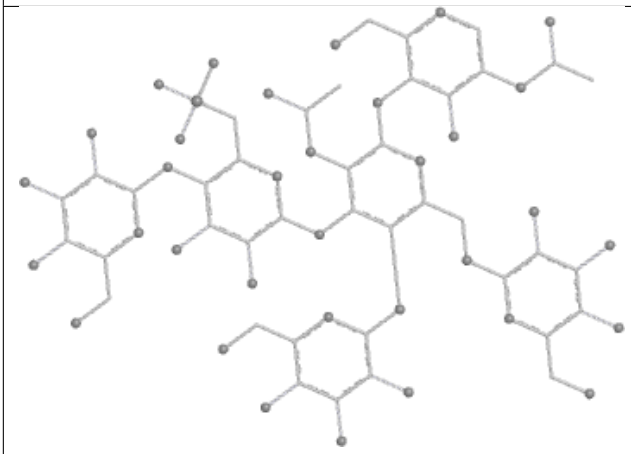

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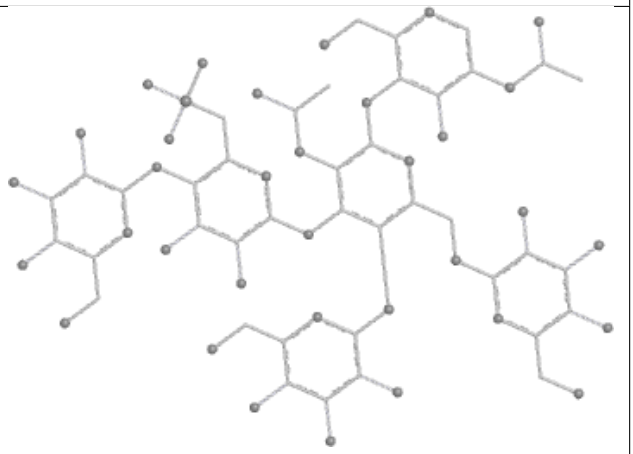
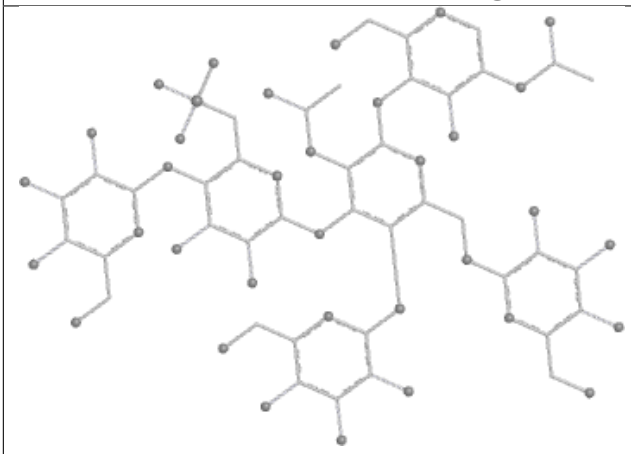


Rings

Oligosaccharide Chain fA



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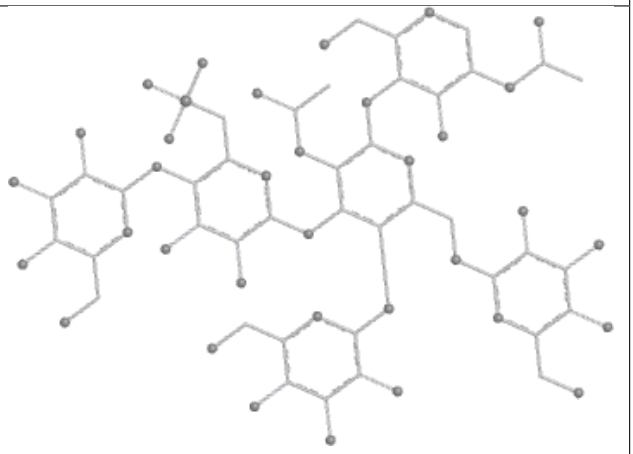

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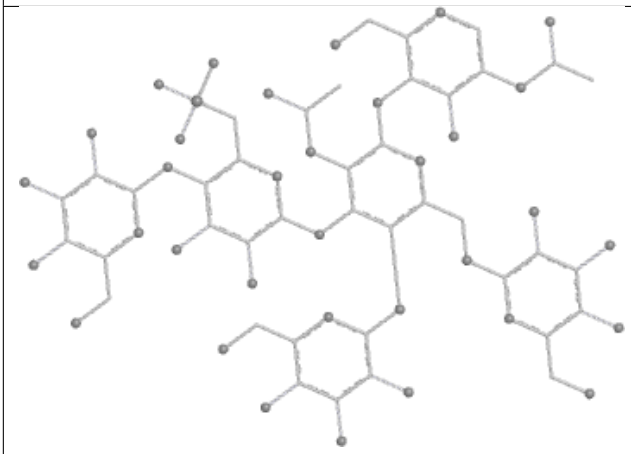

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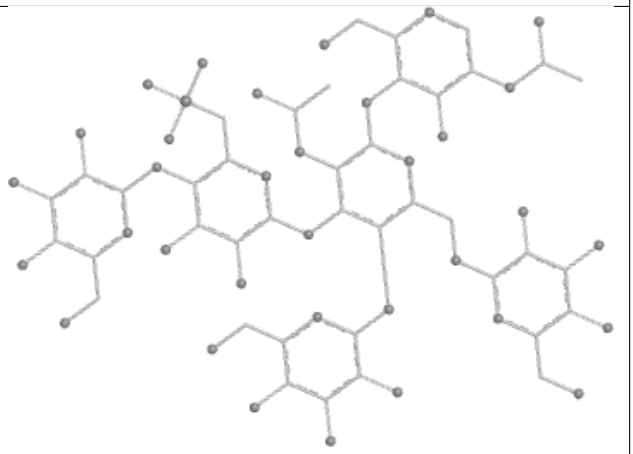
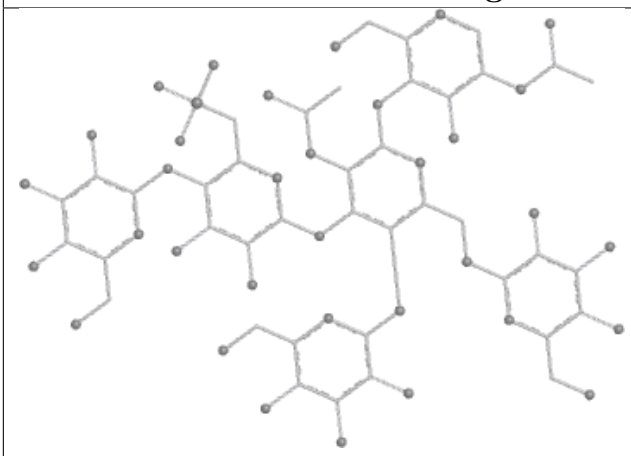


Rings

Oligosaccharide Chain gA



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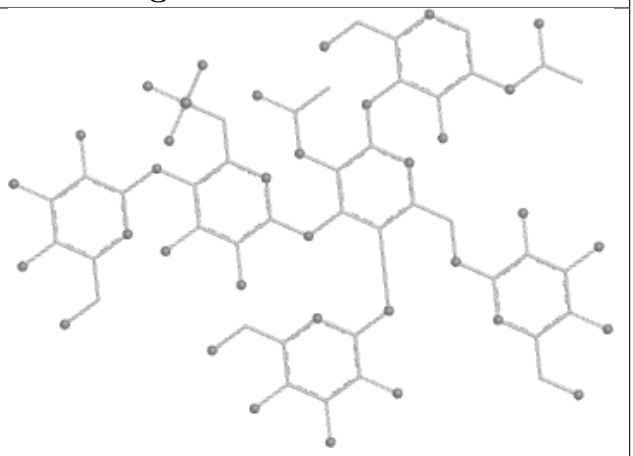

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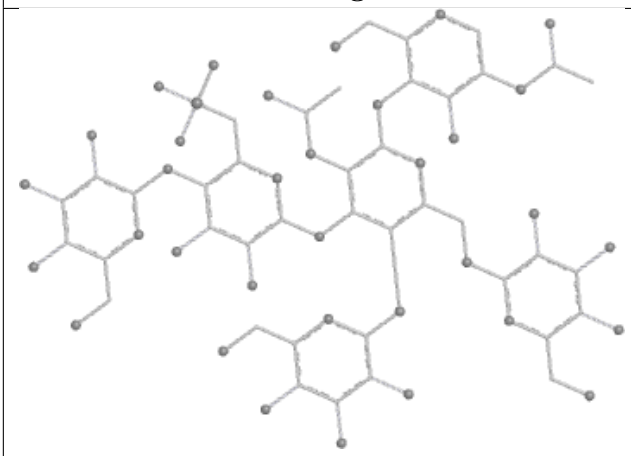

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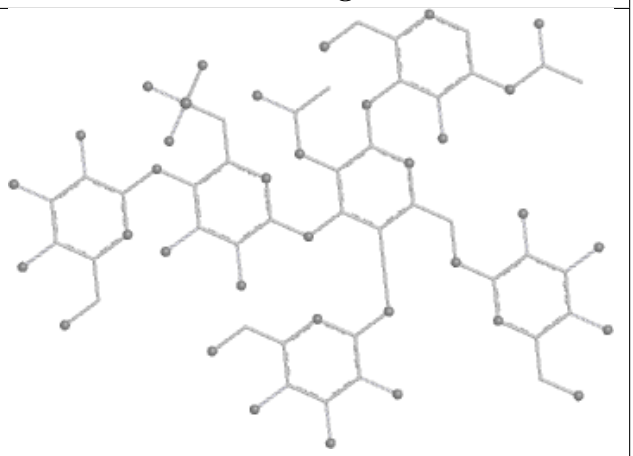
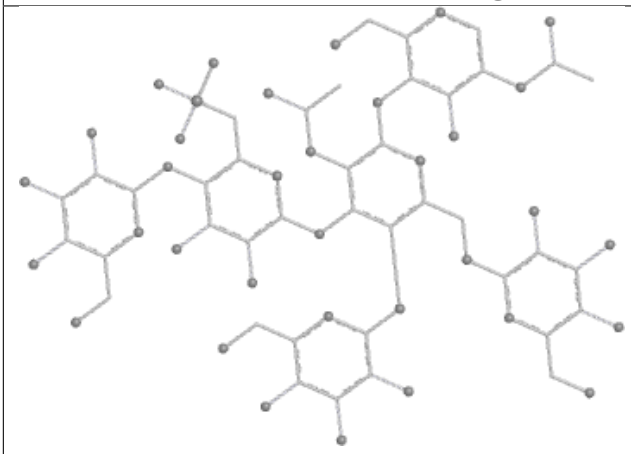


Rings

Oligosaccharide Chain iA



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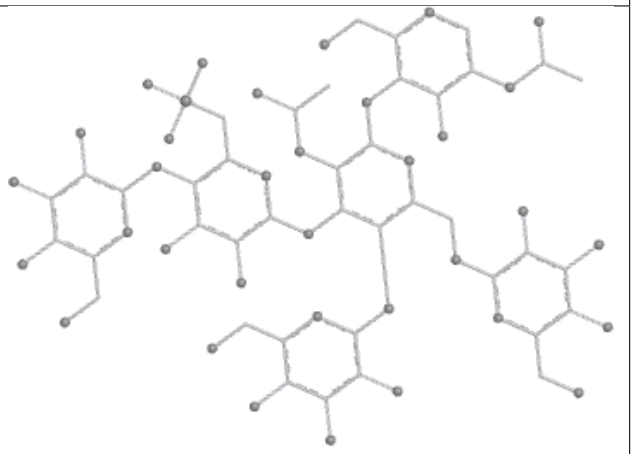

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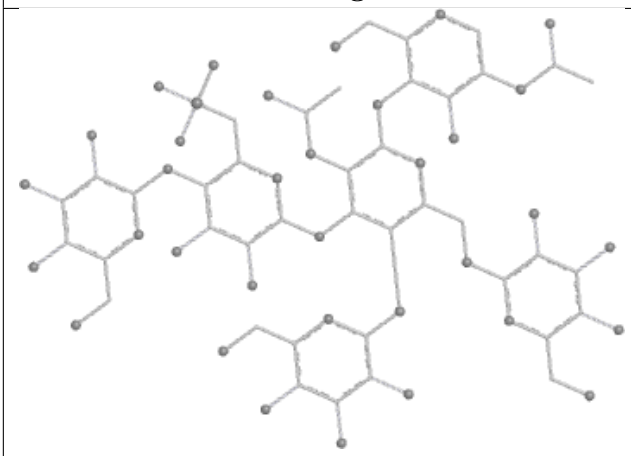

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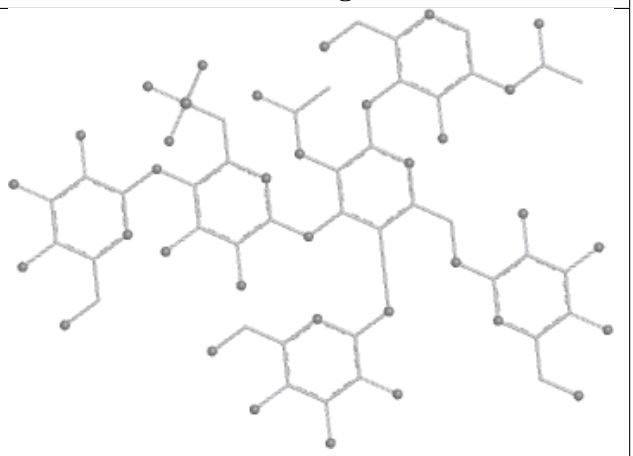
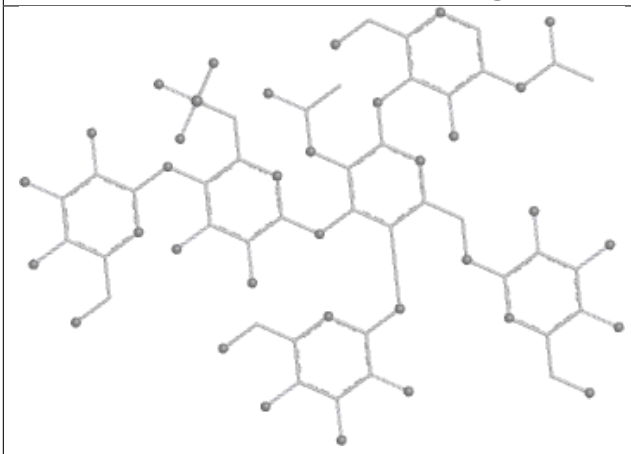


Rings

Oligosaccharide Chain jA



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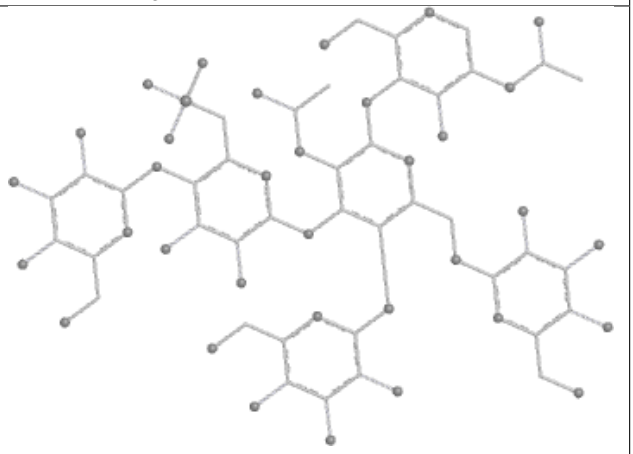

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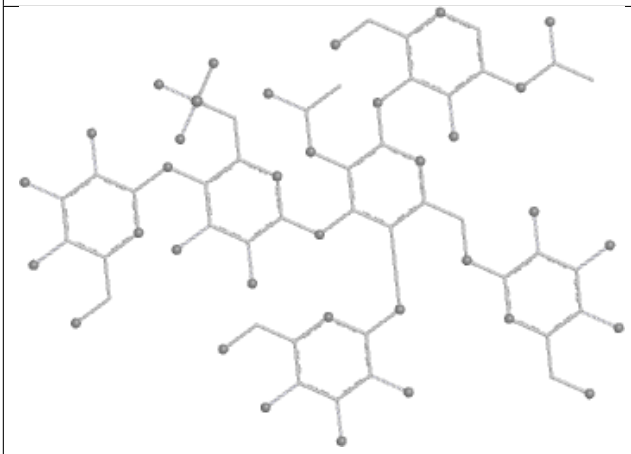

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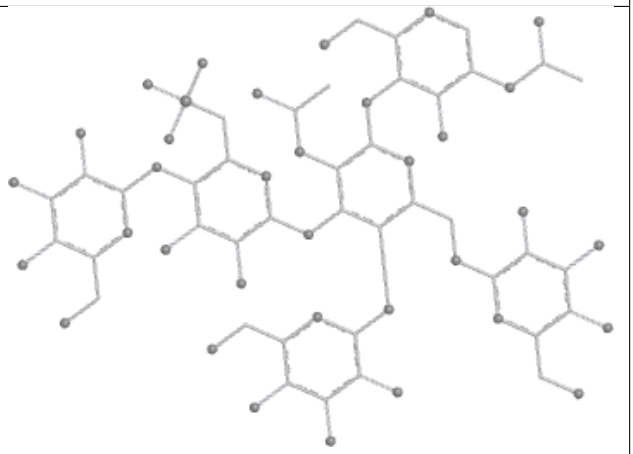
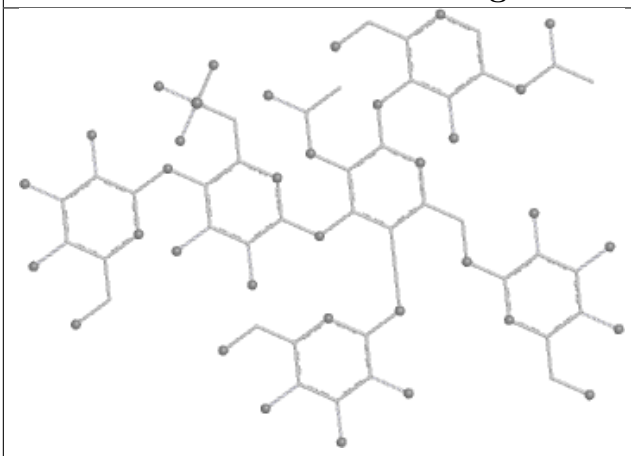


Rings

Oligosaccharide Chain lA



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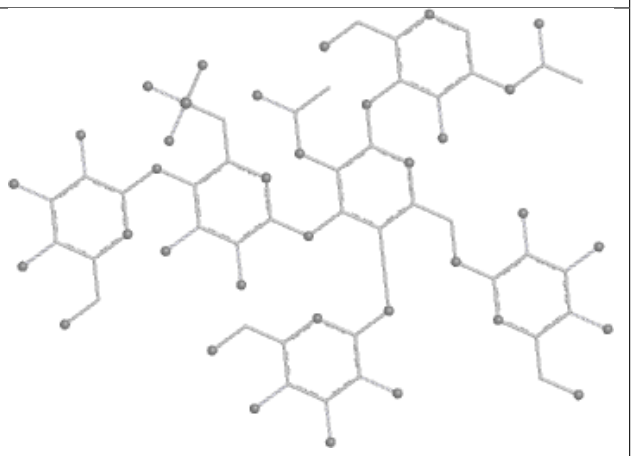

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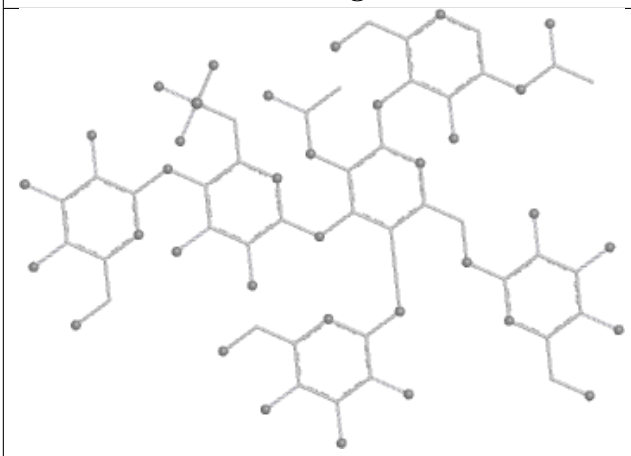

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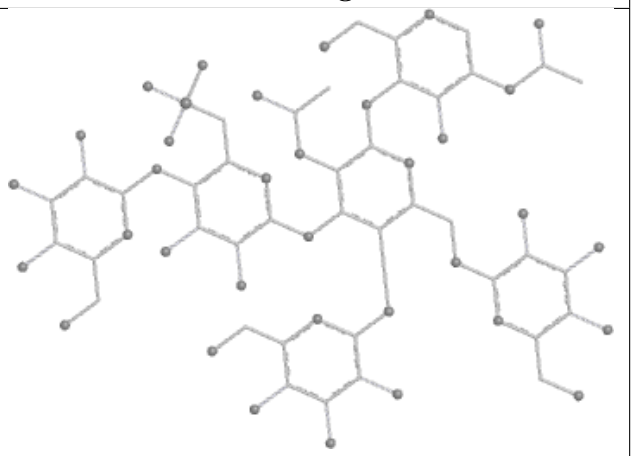
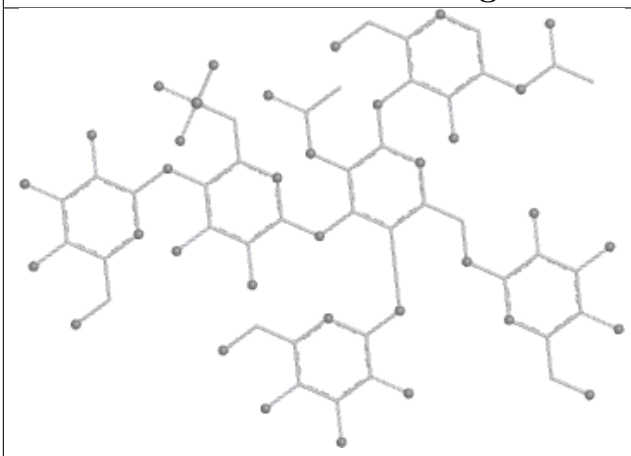


Rings

Oligosaccharide Chain mA



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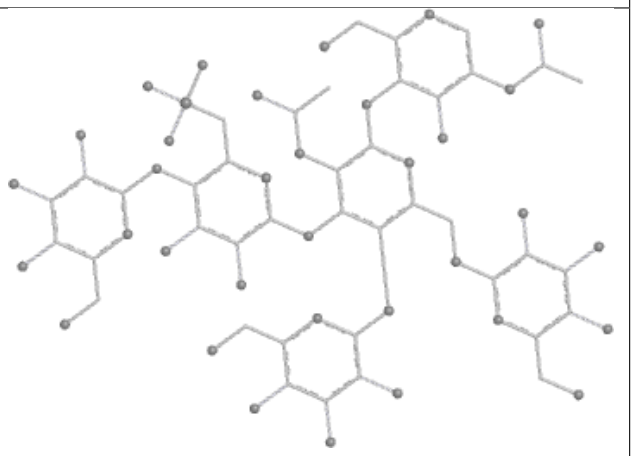

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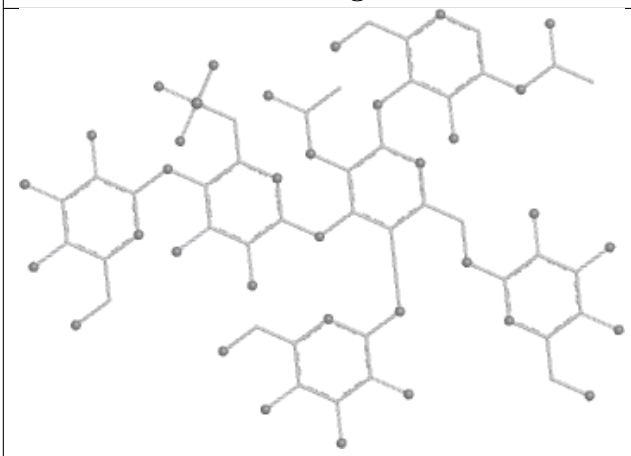

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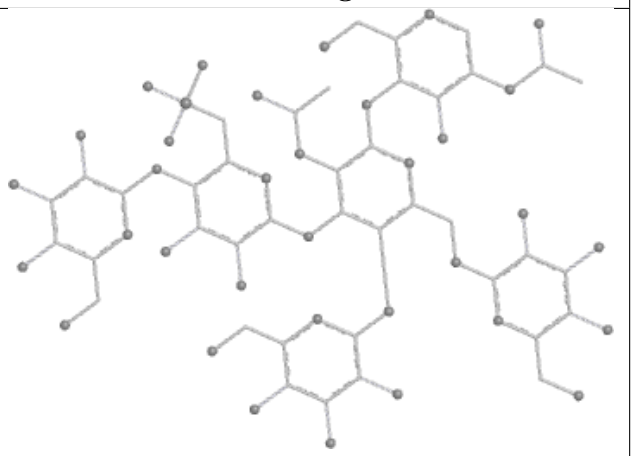
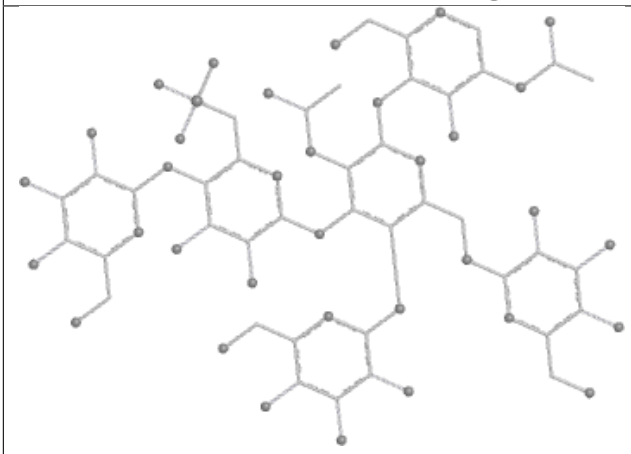


Rings

Oligosaccharide Chain oA



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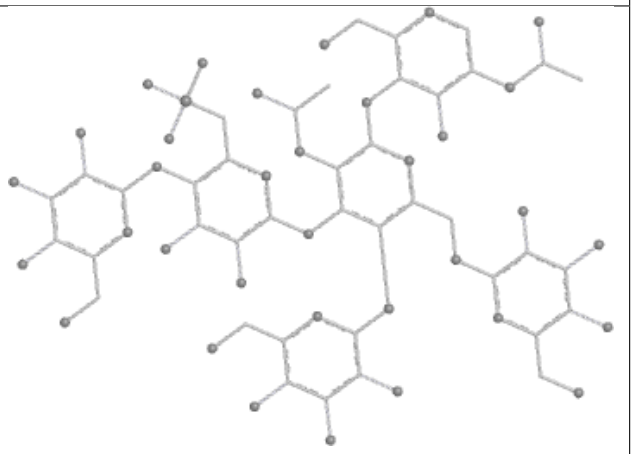

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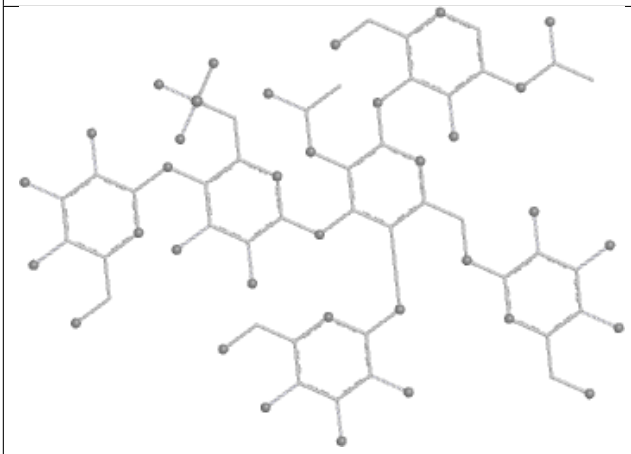

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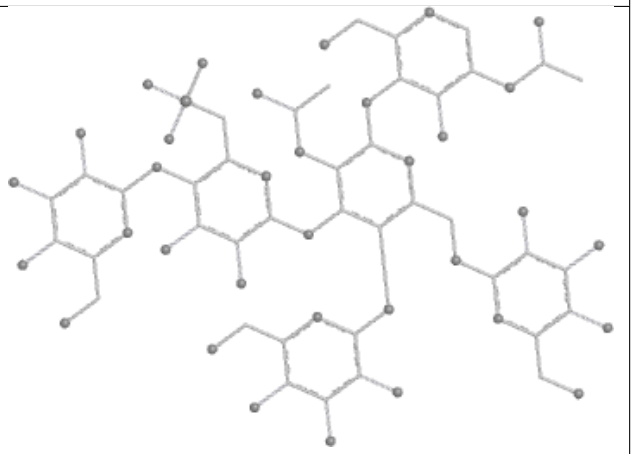
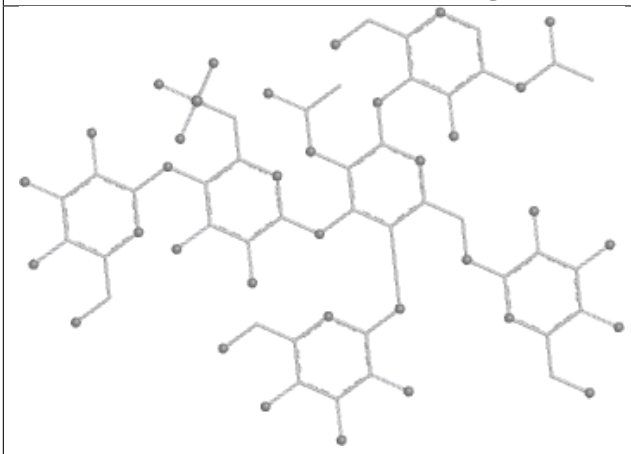


Rings

Oligosaccharide Chain pA



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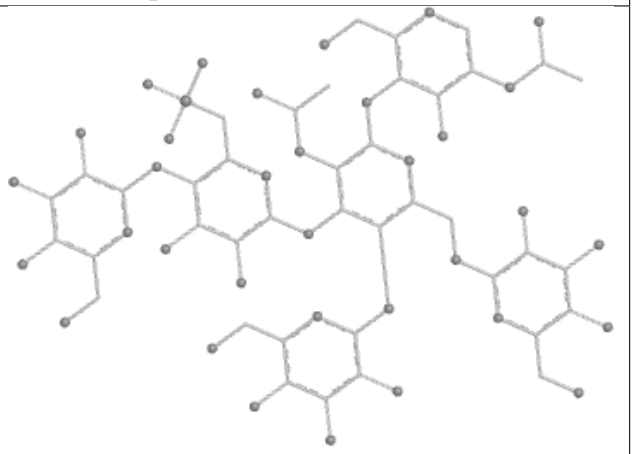

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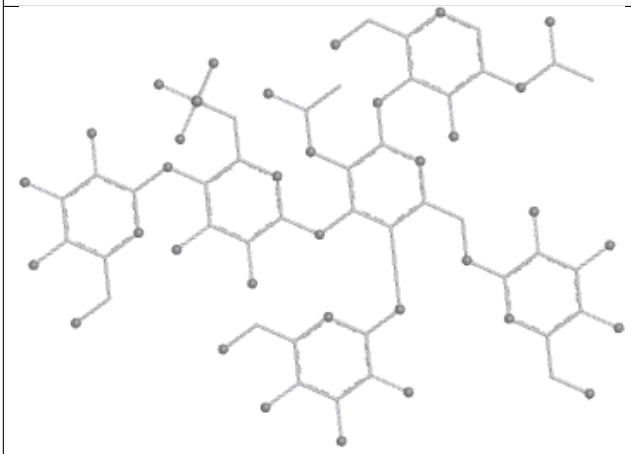

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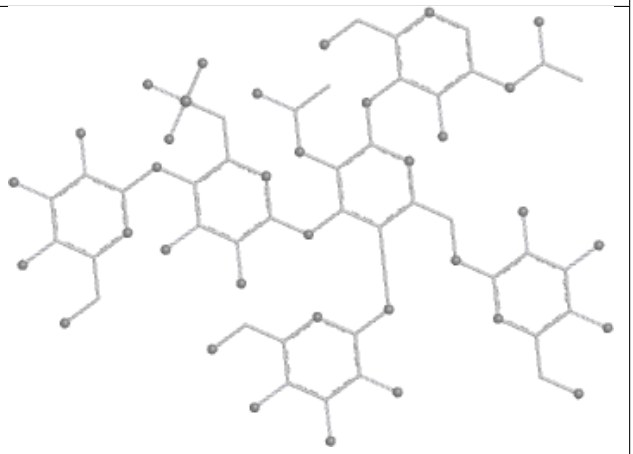
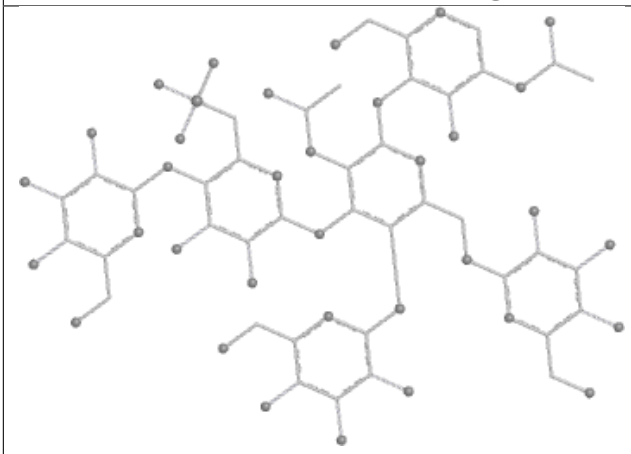


Rings

Oligosaccharide Chain rA



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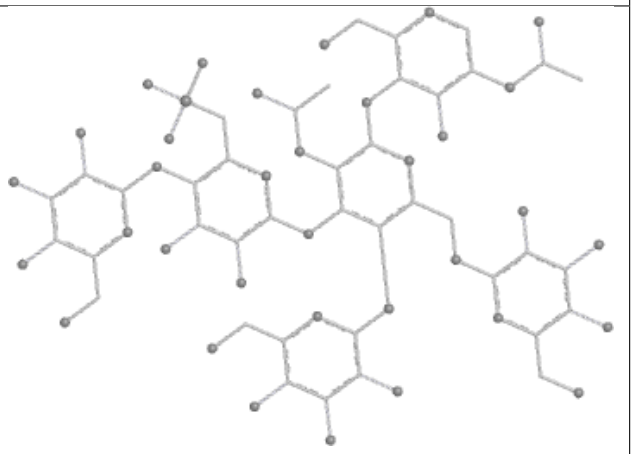
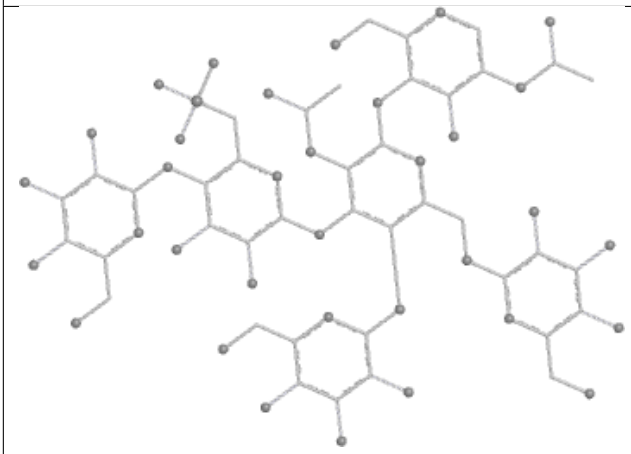


Bond angles



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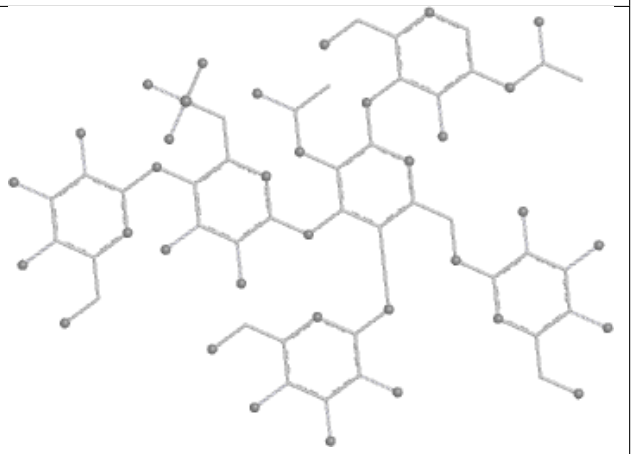
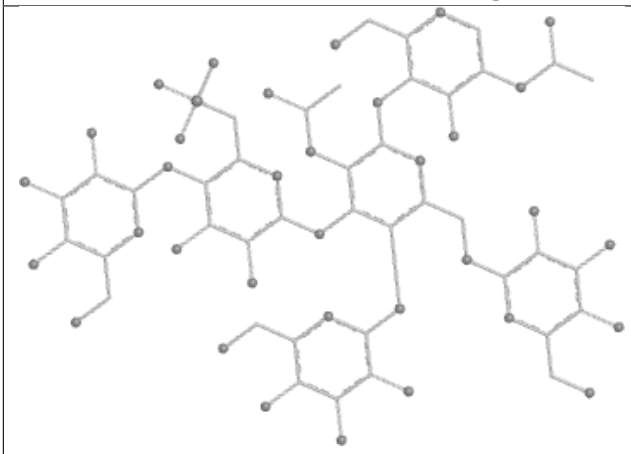


Rings

Oligosaccharide Chain sA



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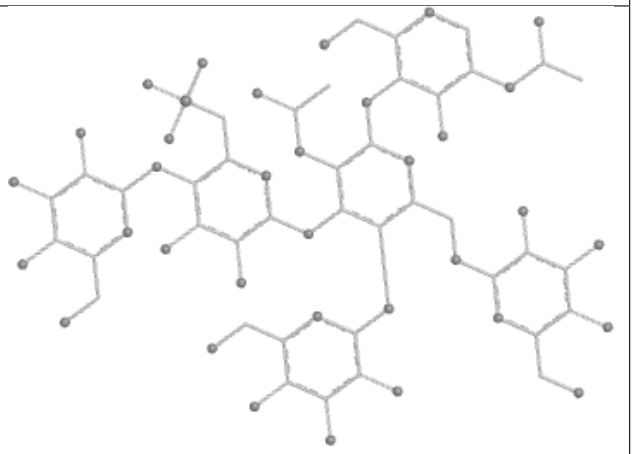
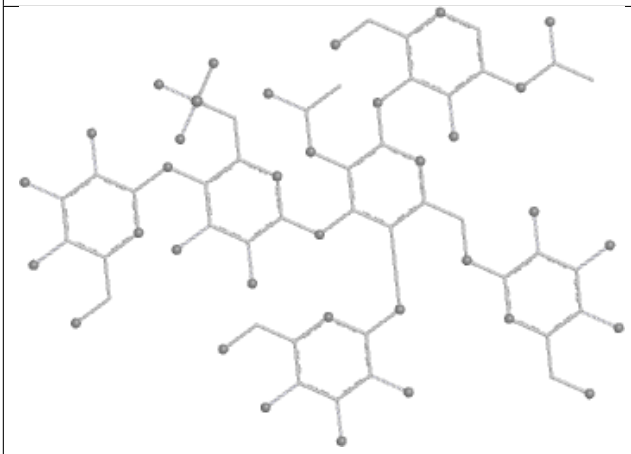


Bond angles



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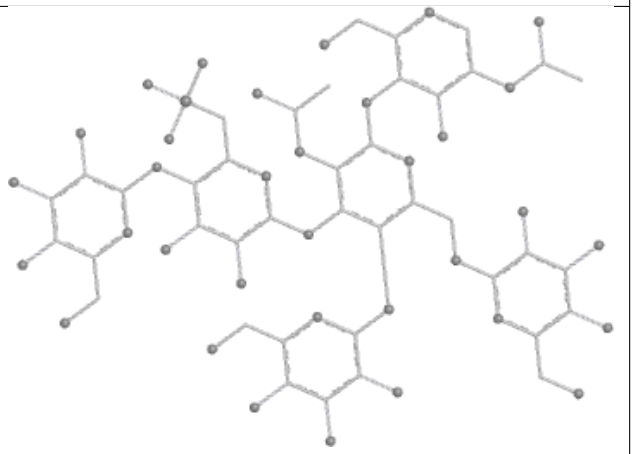
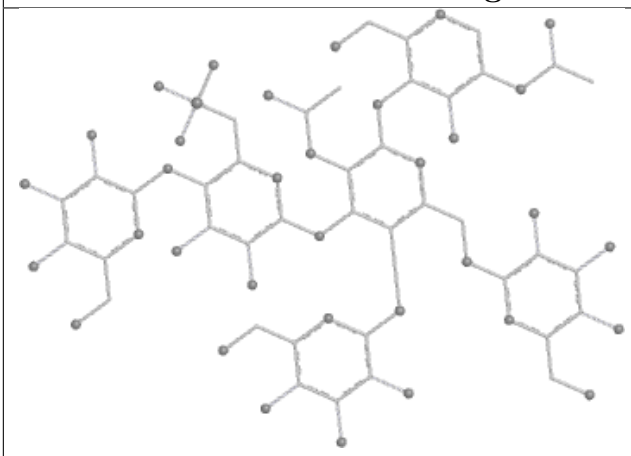
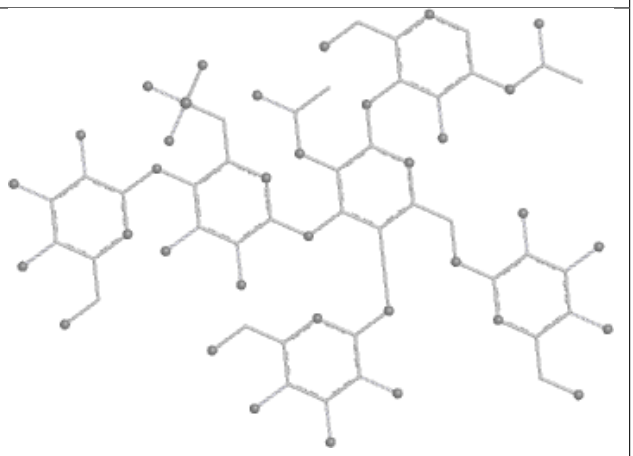


Rings

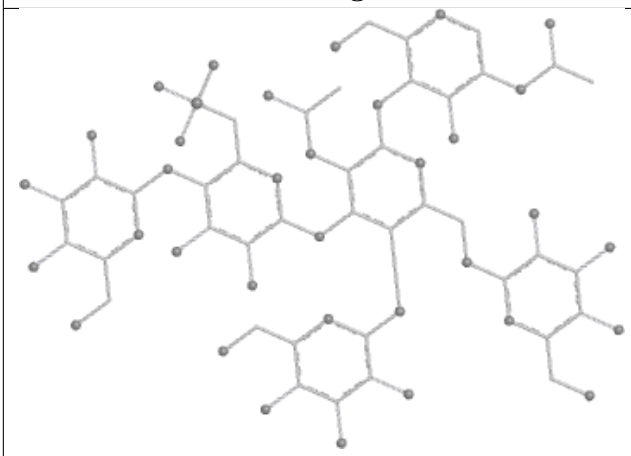
Oligosaccharide Chain uA



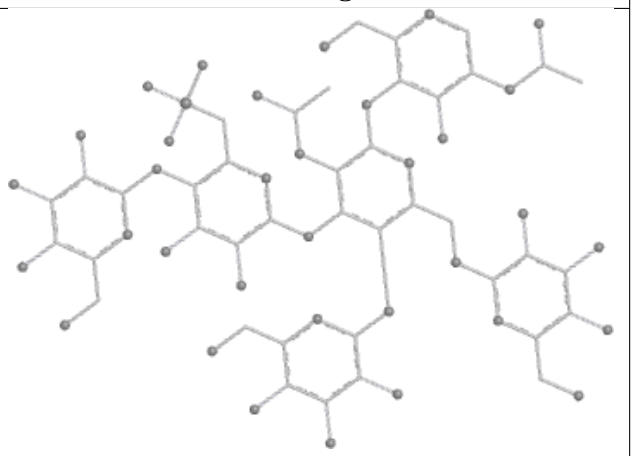
Bond lengths



Bond angles

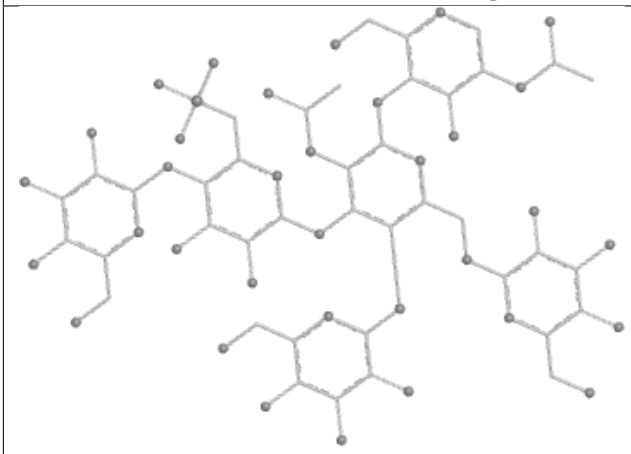


Torsions

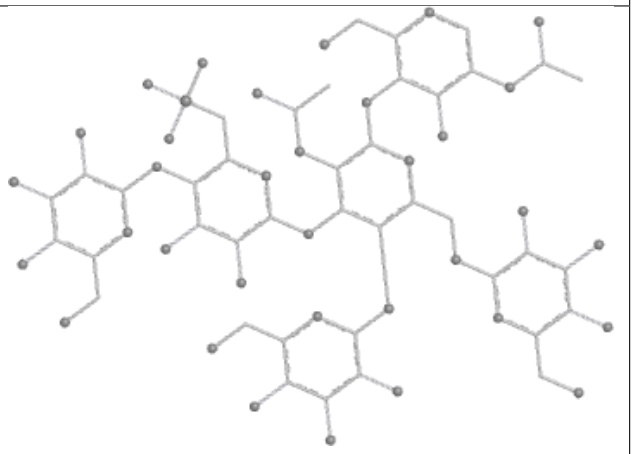


Rings

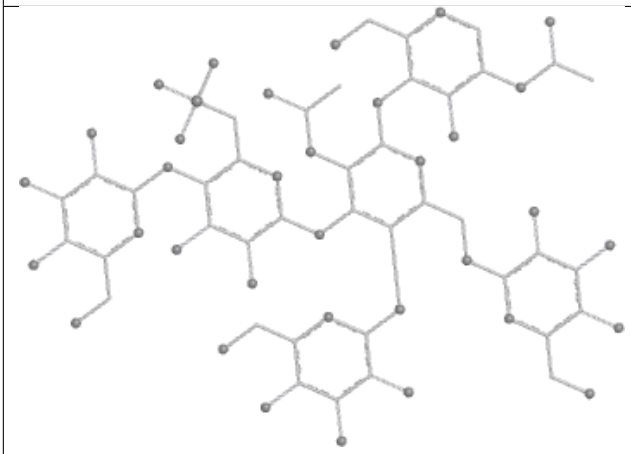
Oligosaccharide Chain vA



Bond lengths



Bond angles



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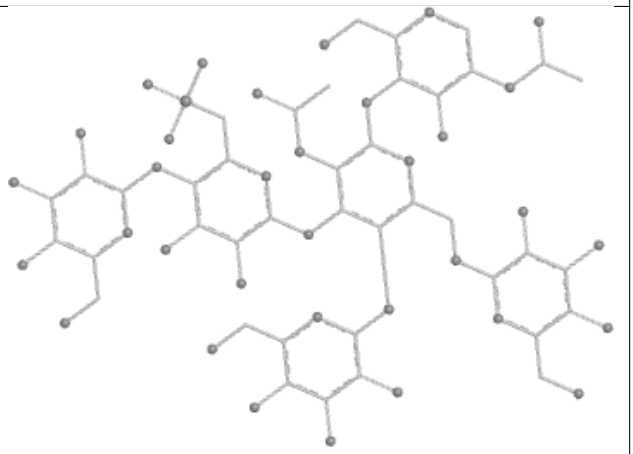
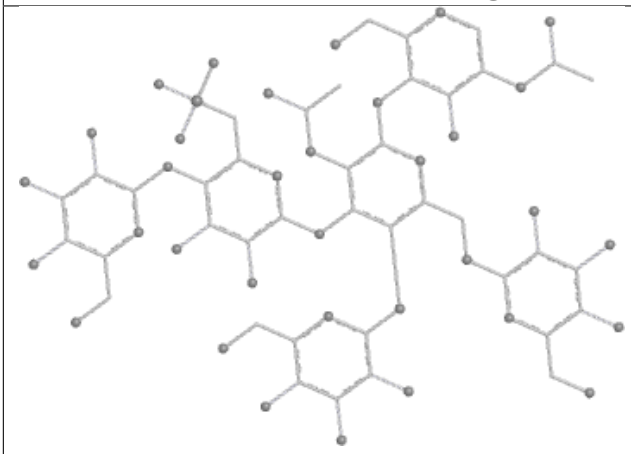


Rings

Oligosaccharide Chain xA



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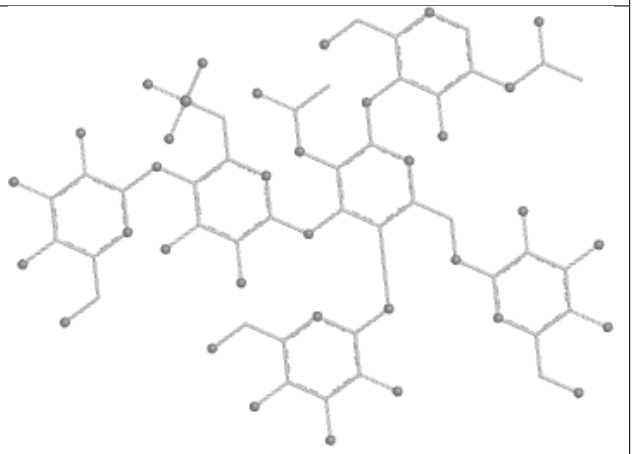
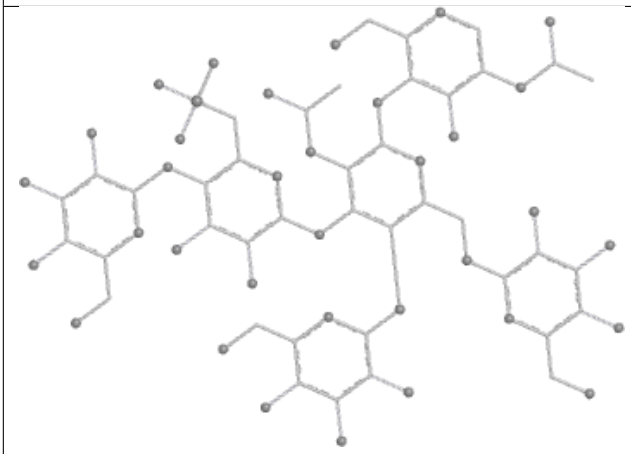


Bond angles



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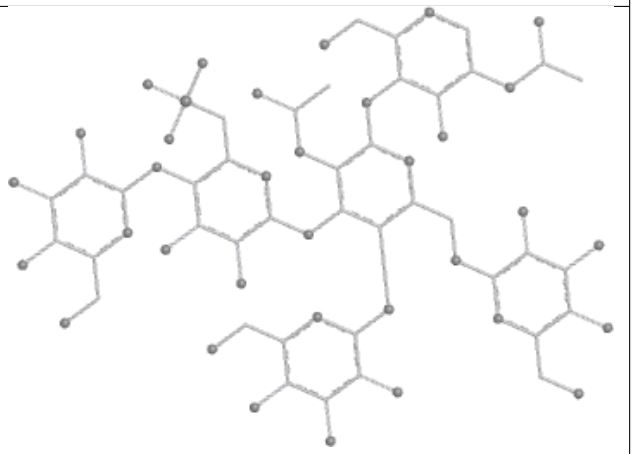
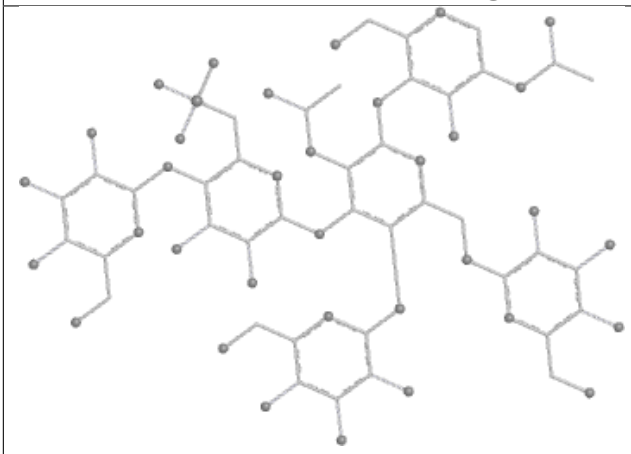


Rings

Oligosaccharide Chain yA



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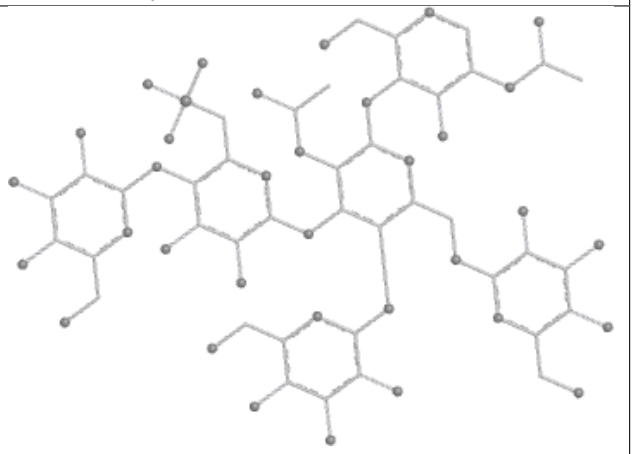
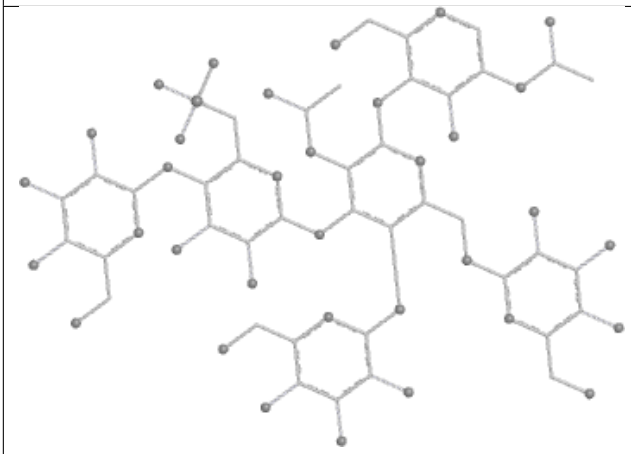


Bond angles



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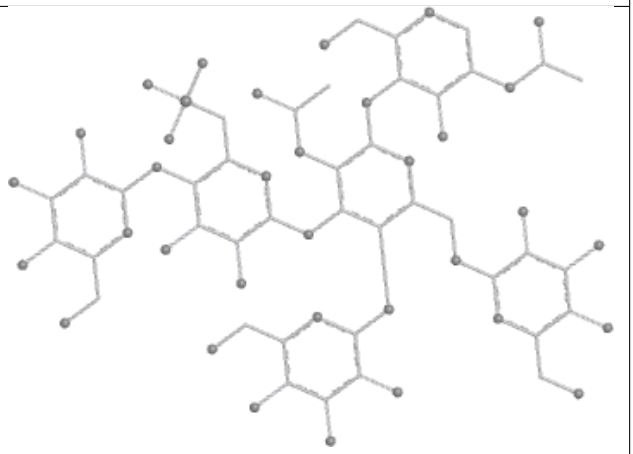
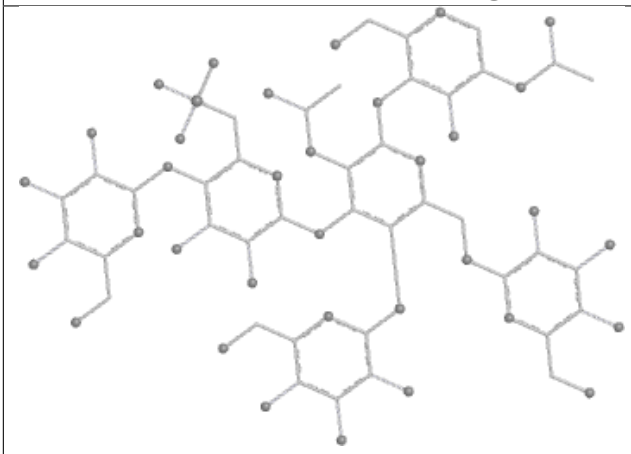


Rings

Oligosaccharide Chain 0A



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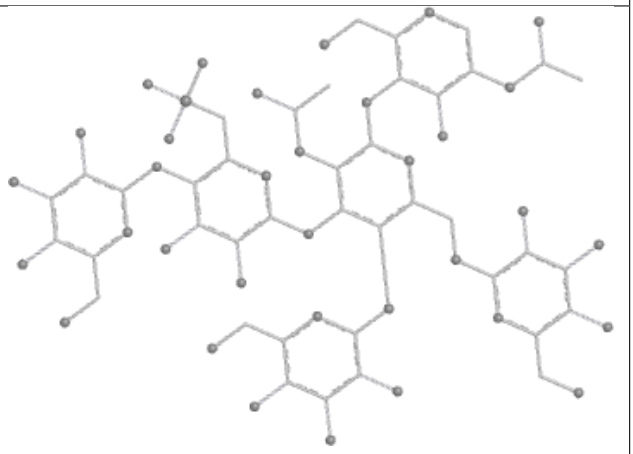
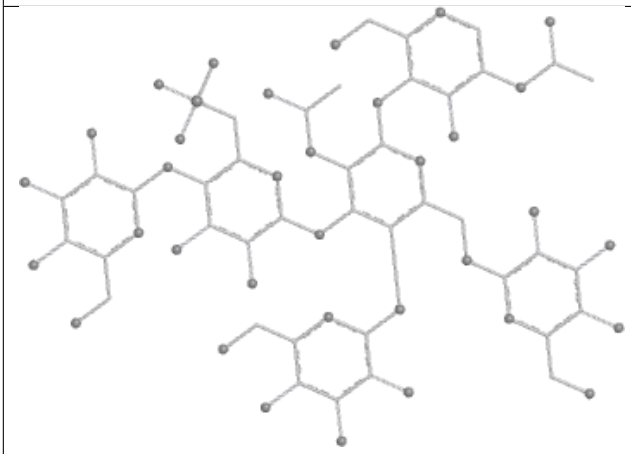


Bond angles



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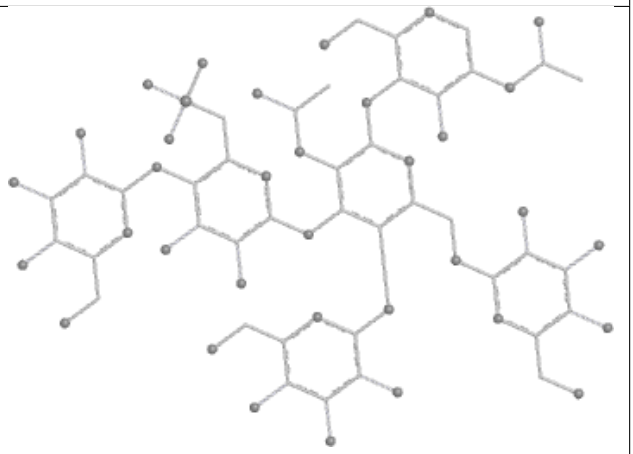
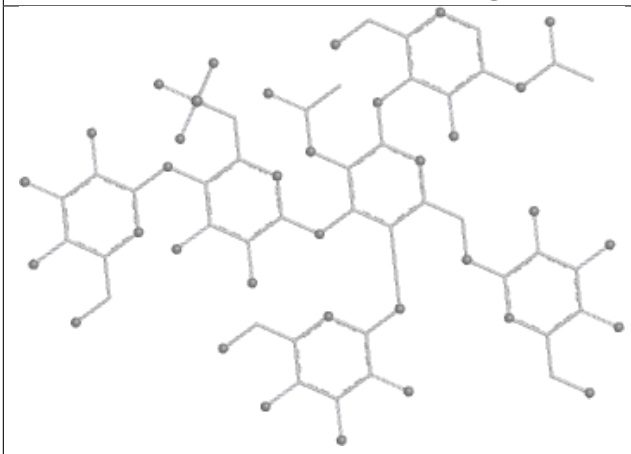


Rings

Oligosaccharide Chain 1A



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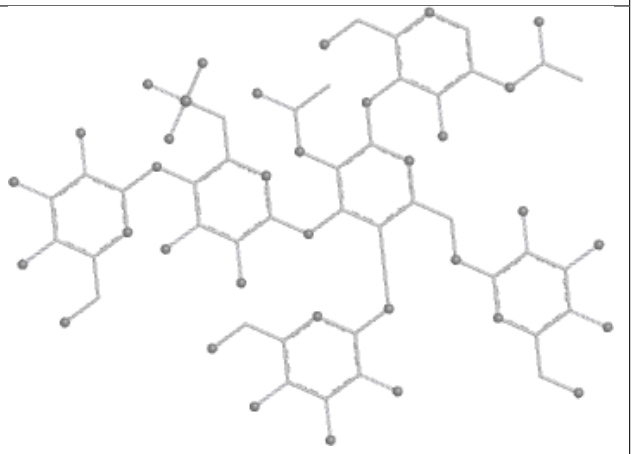
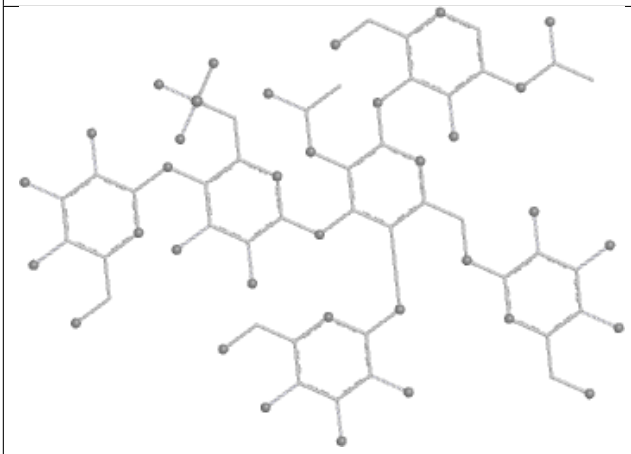


Bond angles



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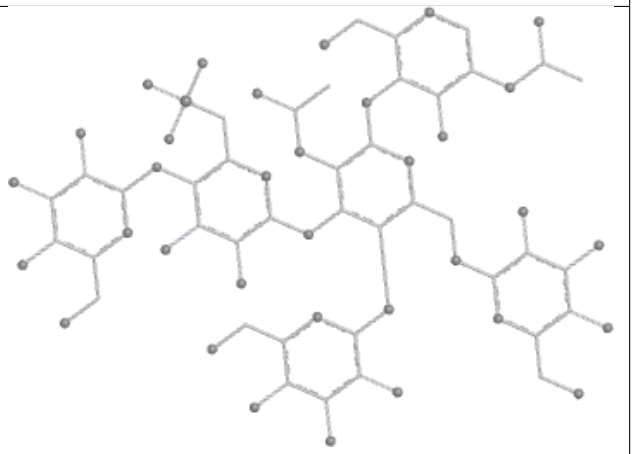
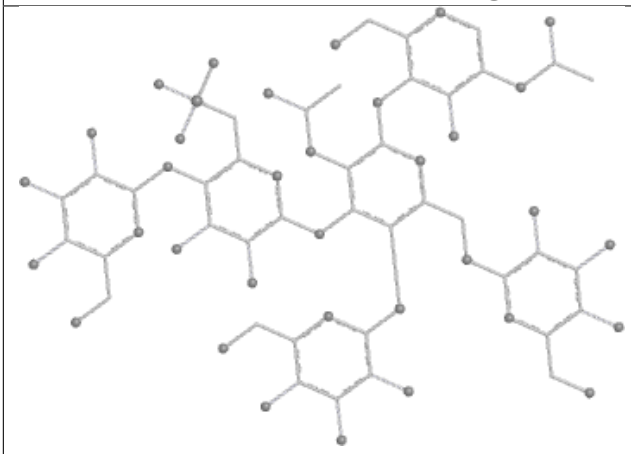


Rings

Oligosaccharide Chain 3A



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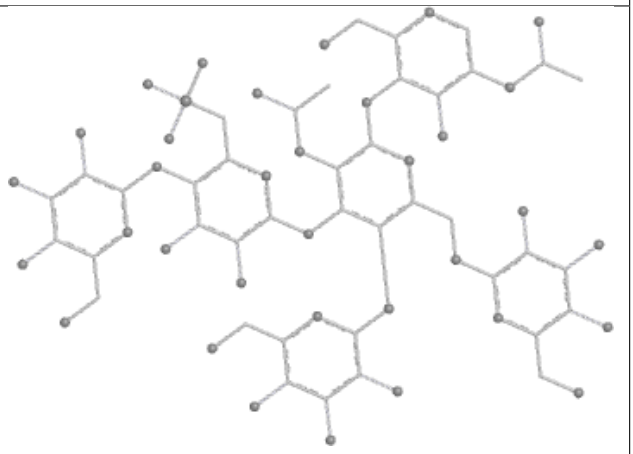
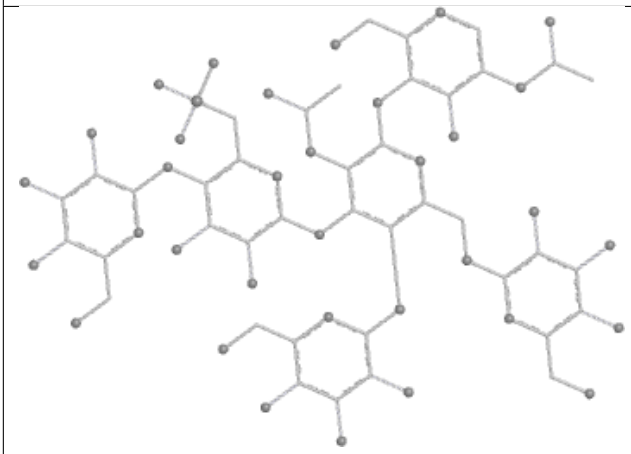


Bond angles



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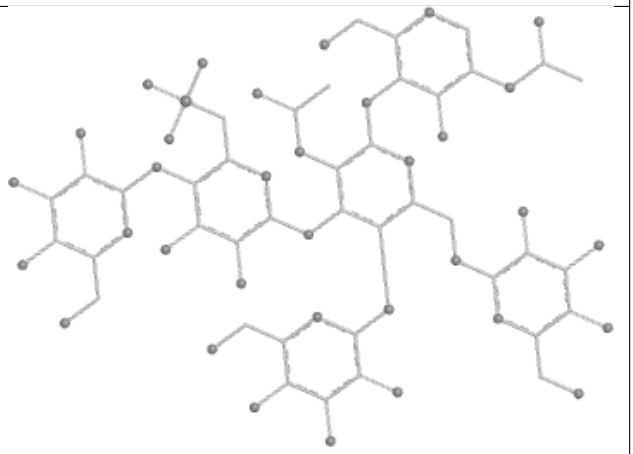
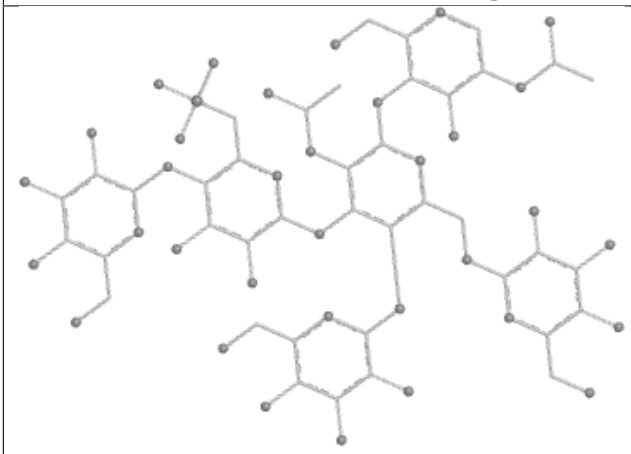


Rings

Oligosaccharide Chain 4A



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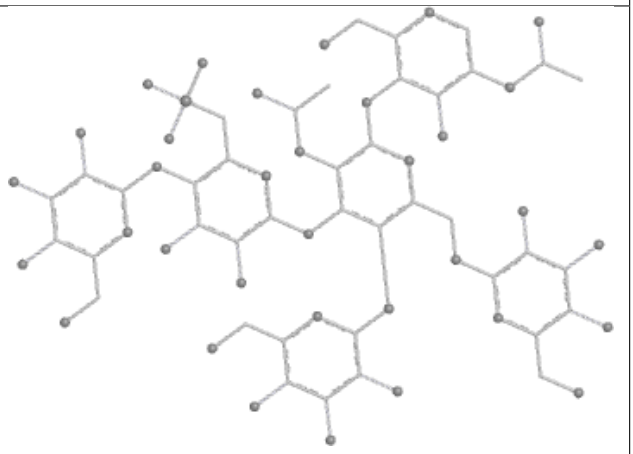
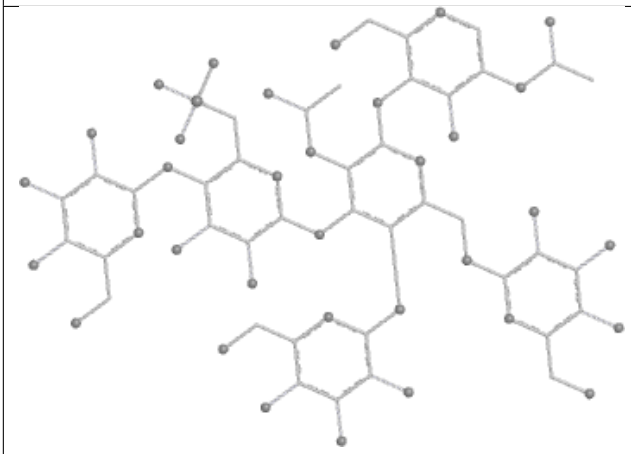


Bond angles



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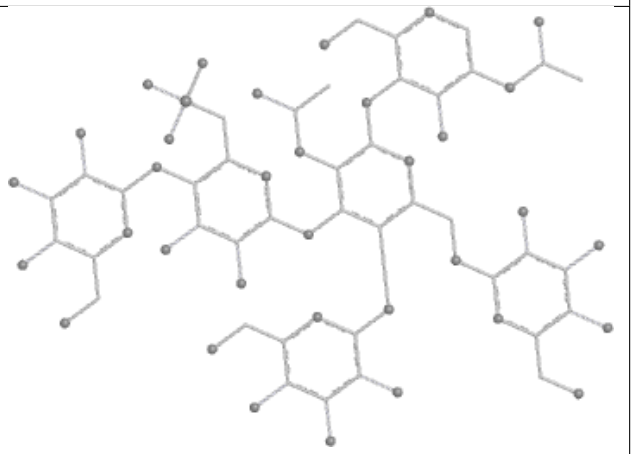
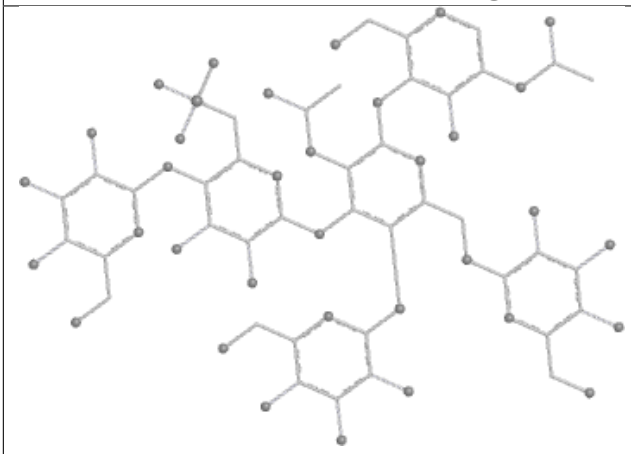


Rings

Oligosaccharide Chain 6A



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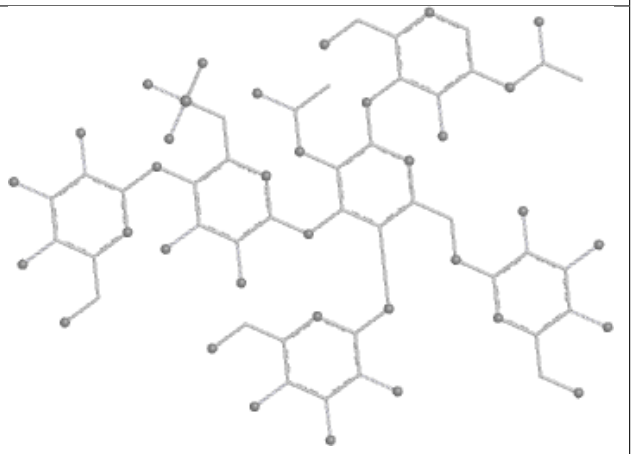

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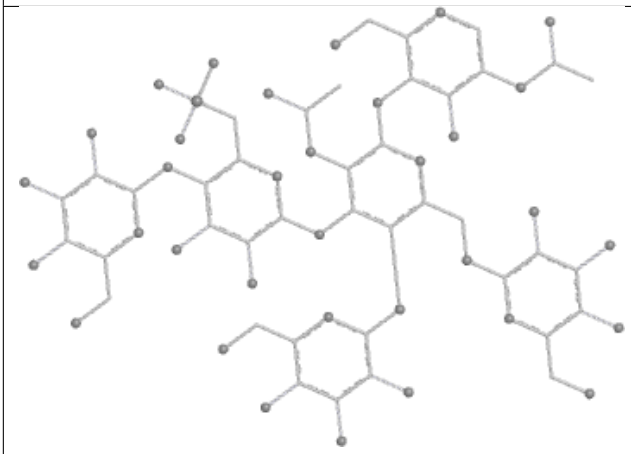

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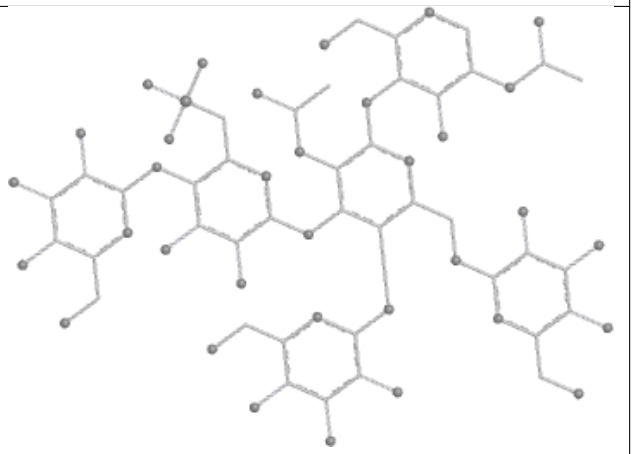
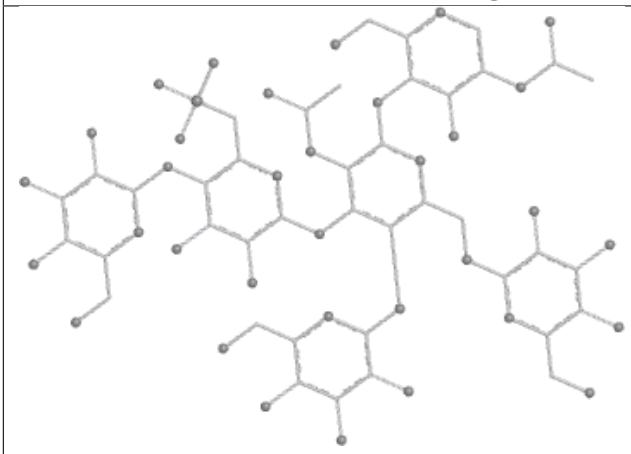


Rings

Oligosaccharide Chain 7A



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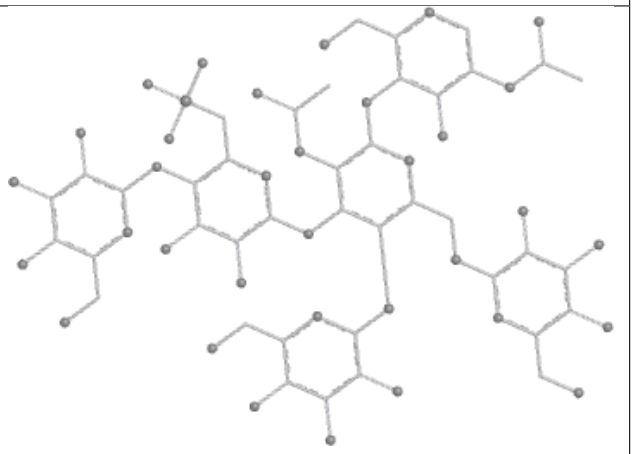

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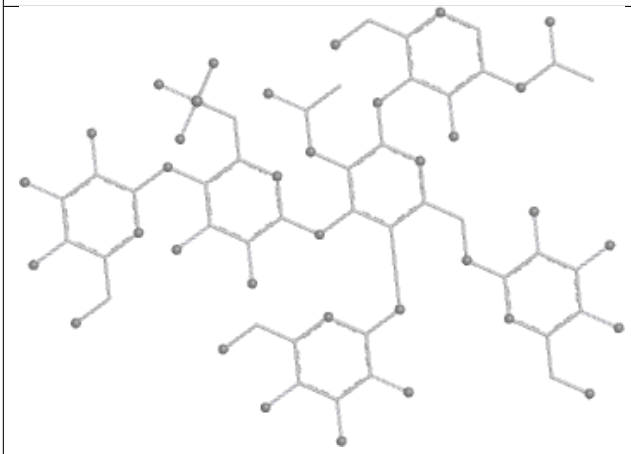

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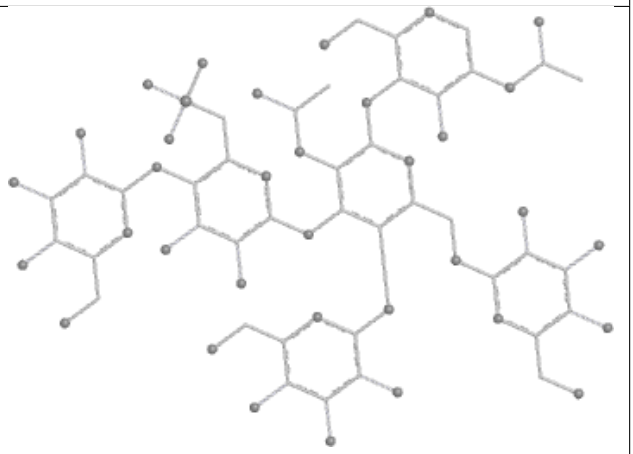
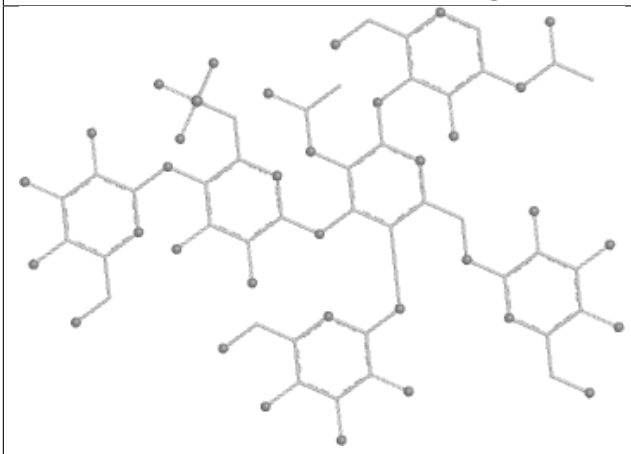


Rings

Oligosaccharide Chain 9A



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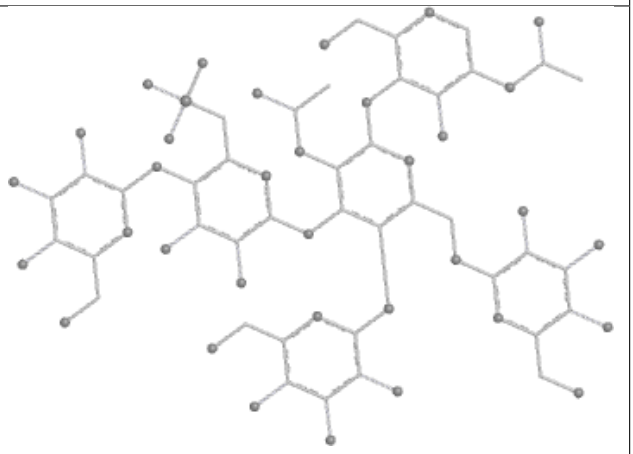

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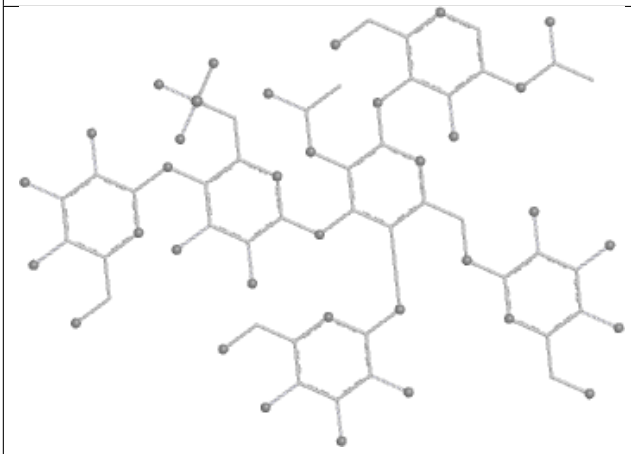

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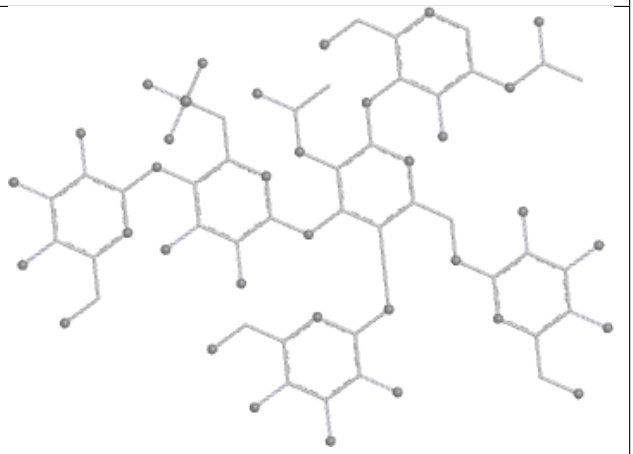
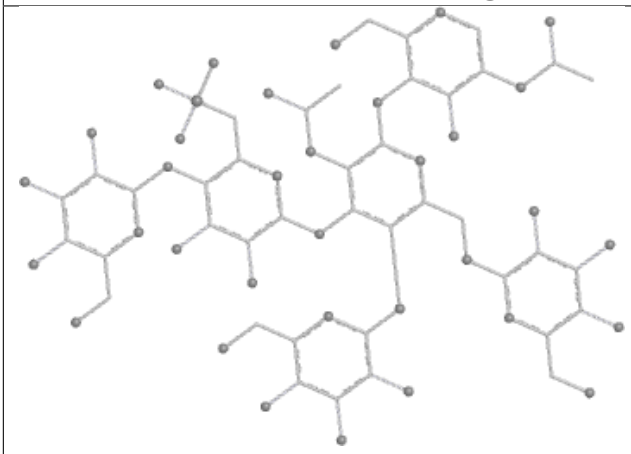


Rings

Oligosaccharide Chain AB



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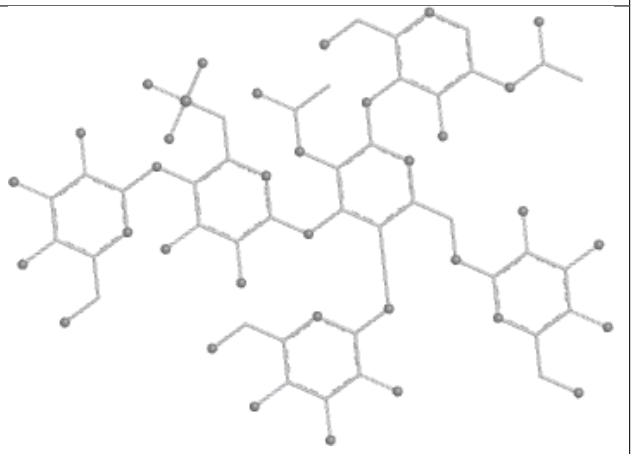

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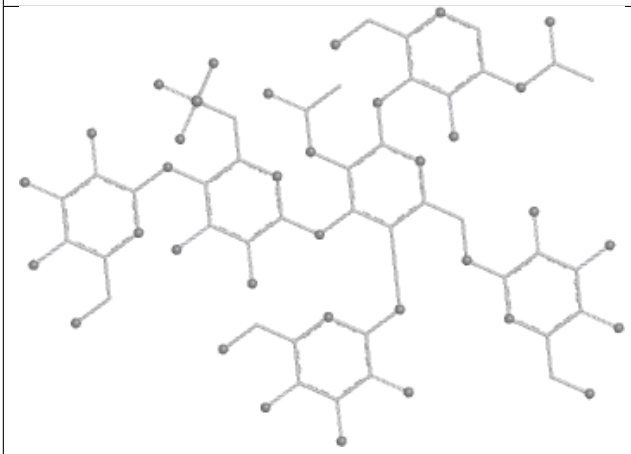

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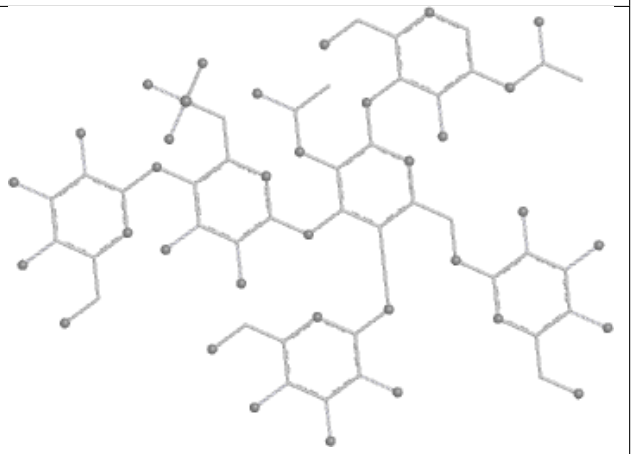
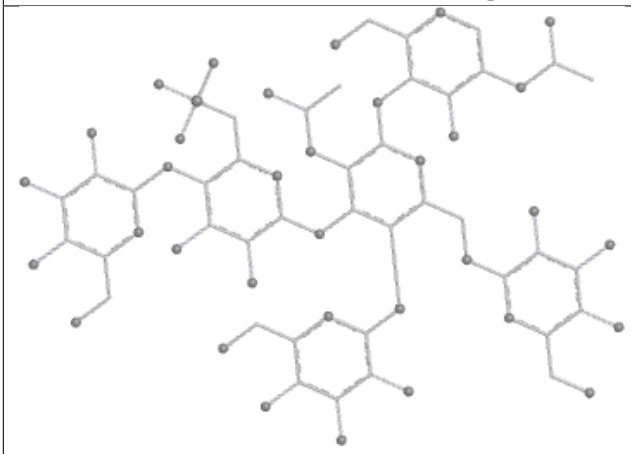


Rings

Oligosaccharide Chain CB



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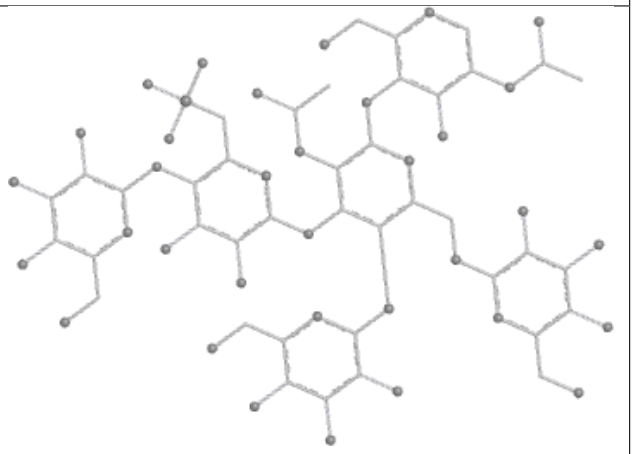

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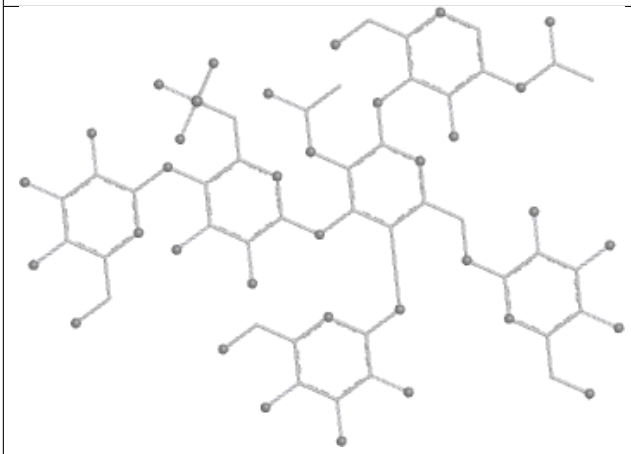

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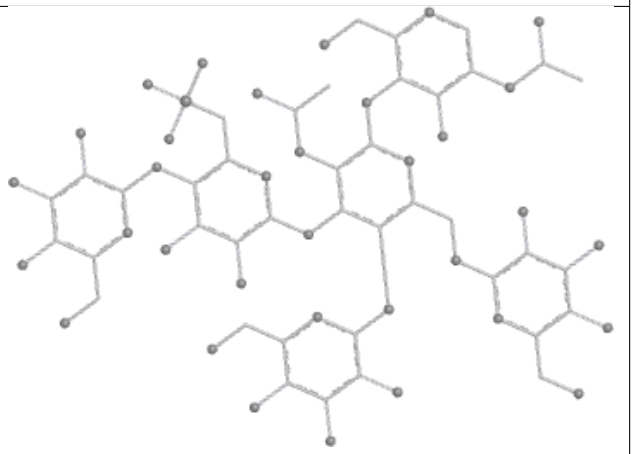
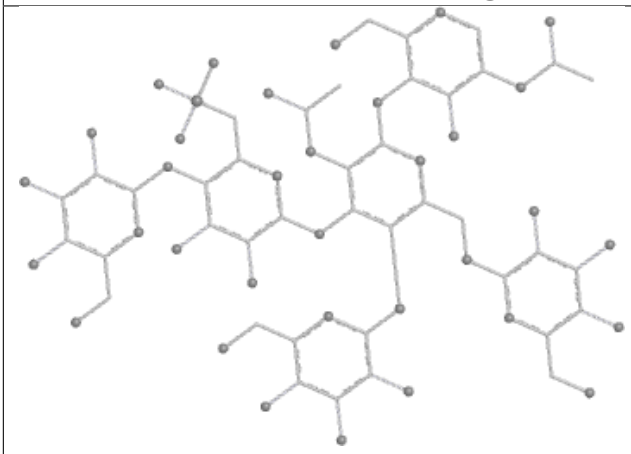


Rings

Oligosaccharide Chain DB



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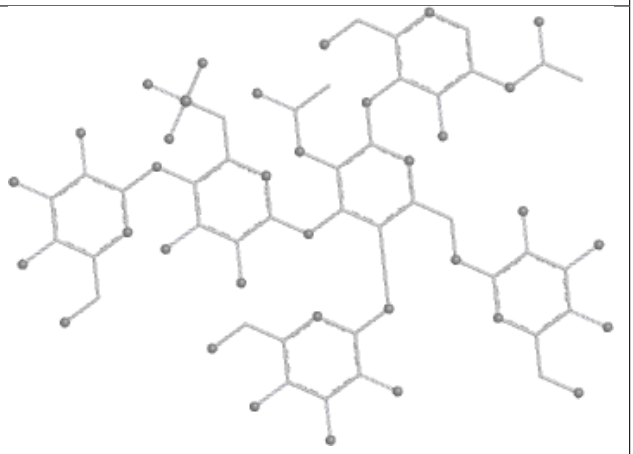
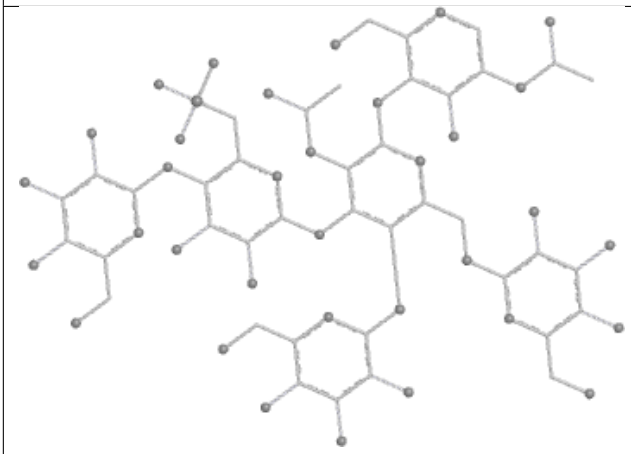


Bond angles



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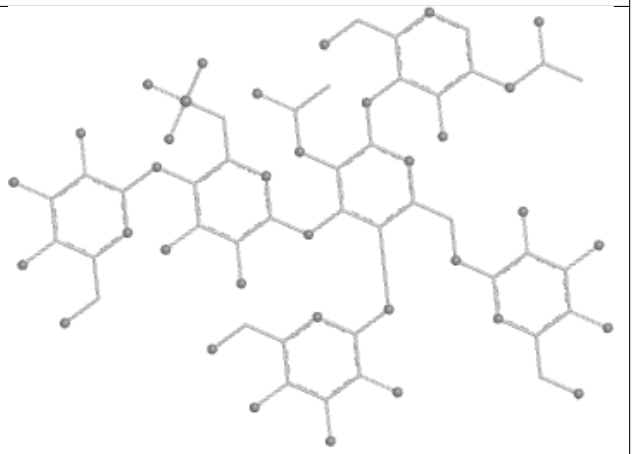
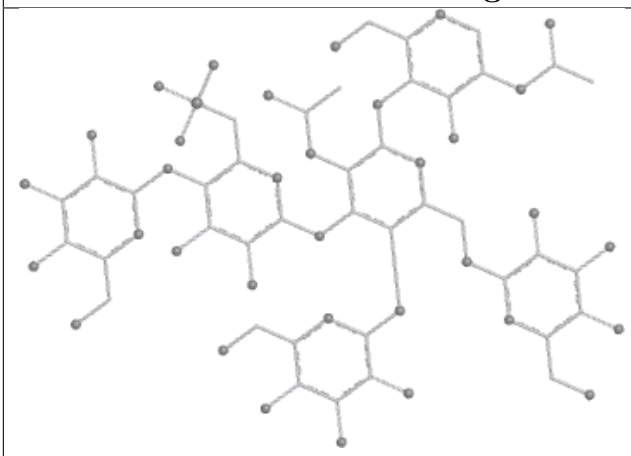


Rings

Oligosaccharide Chain FB



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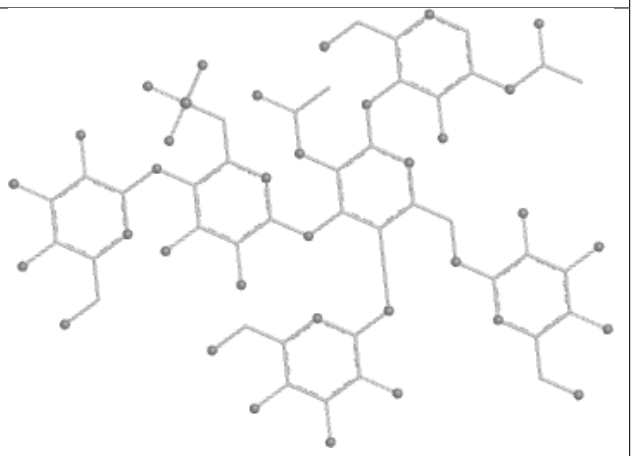
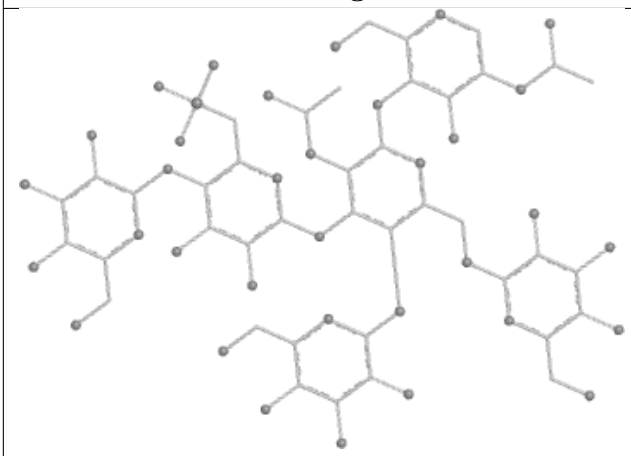


Bond angles



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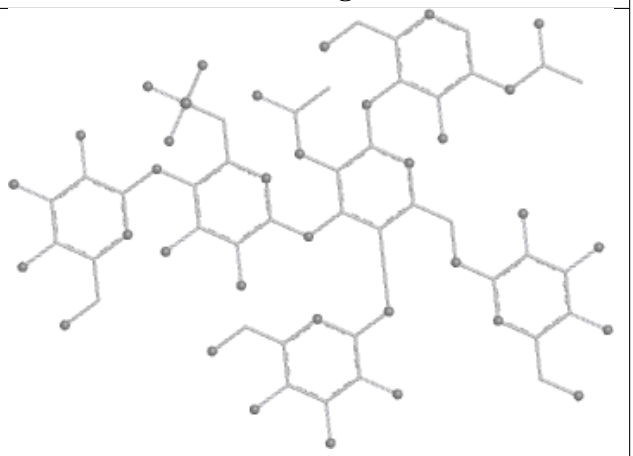
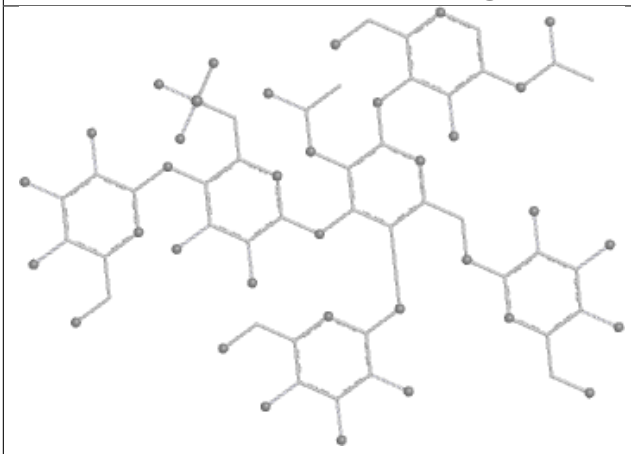
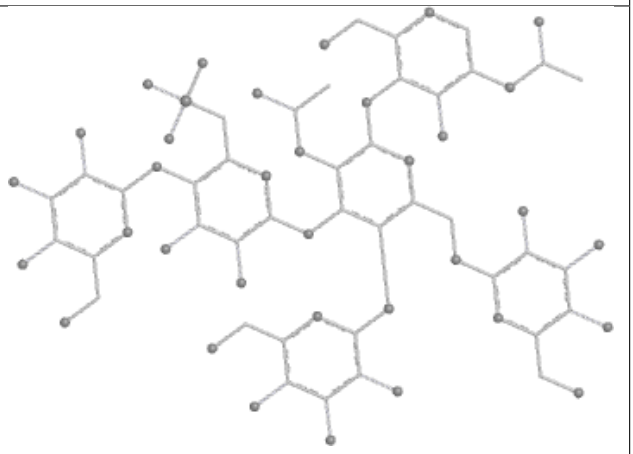


Rings

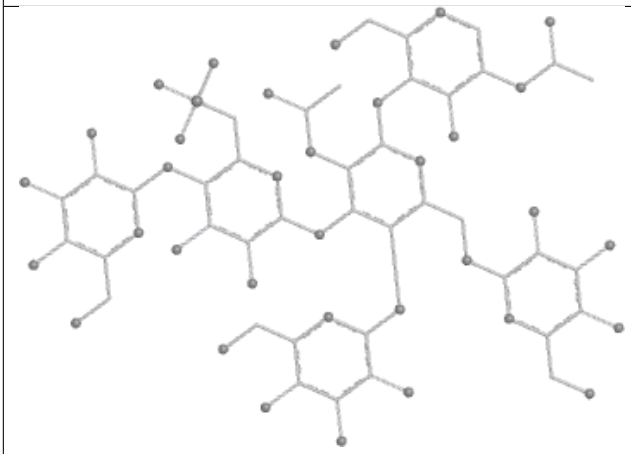
Oligosaccharide Chain GB



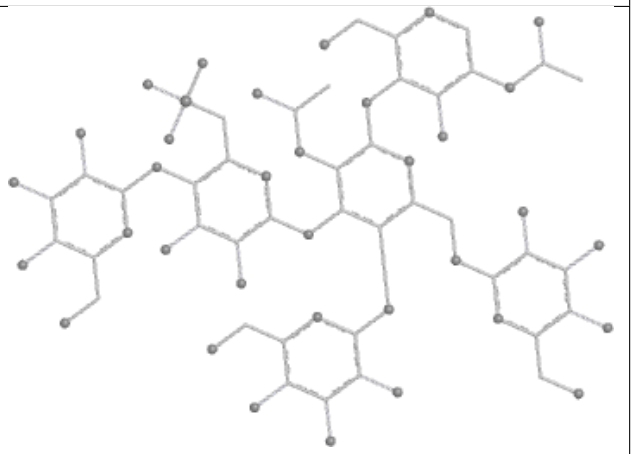
Bond lengths



Bond angles

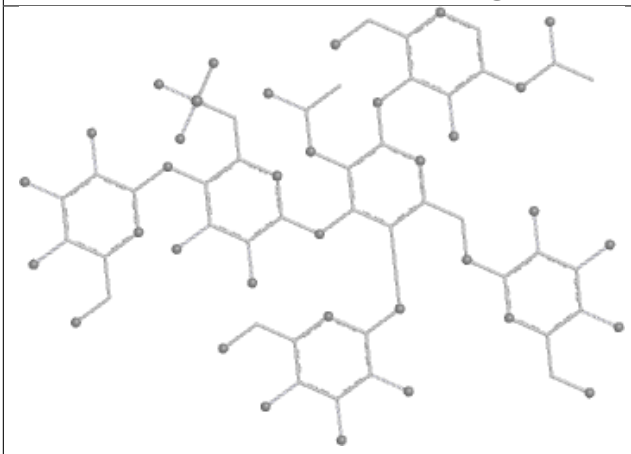


Torsions



Rings

Oligosaccharide Chain IB



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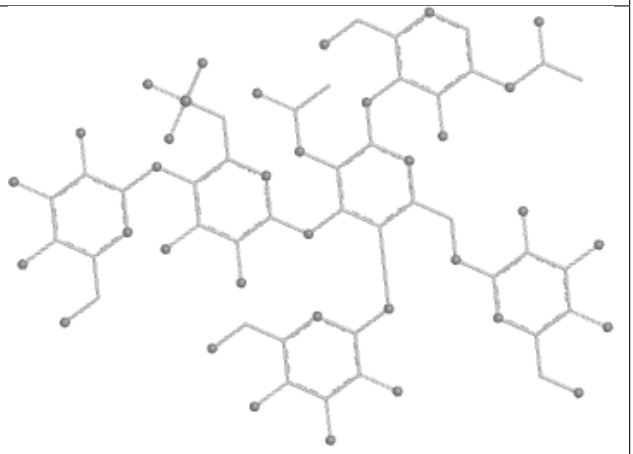
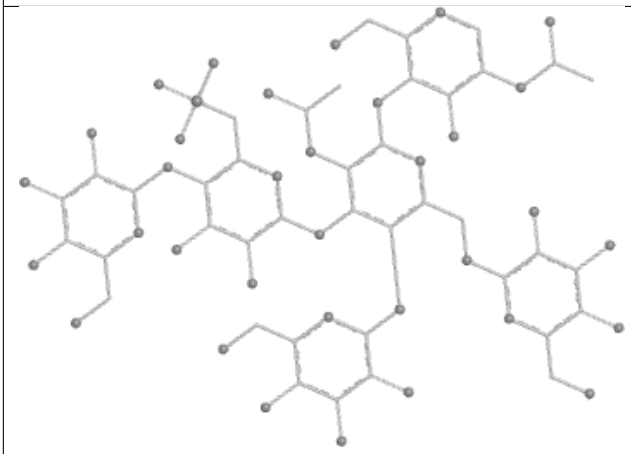


Bond angles



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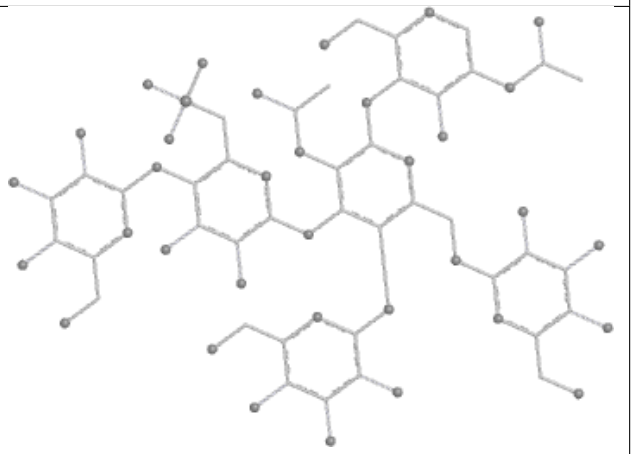
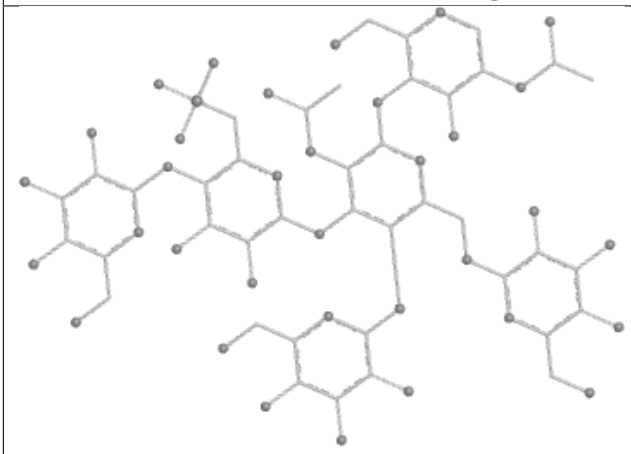


Rings

Oligosaccharide Chain JB



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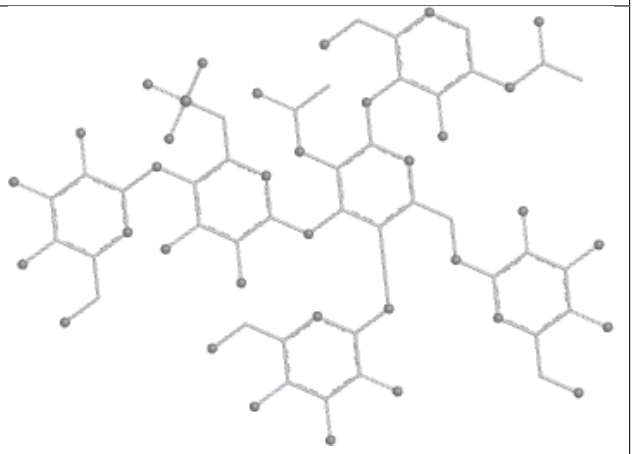
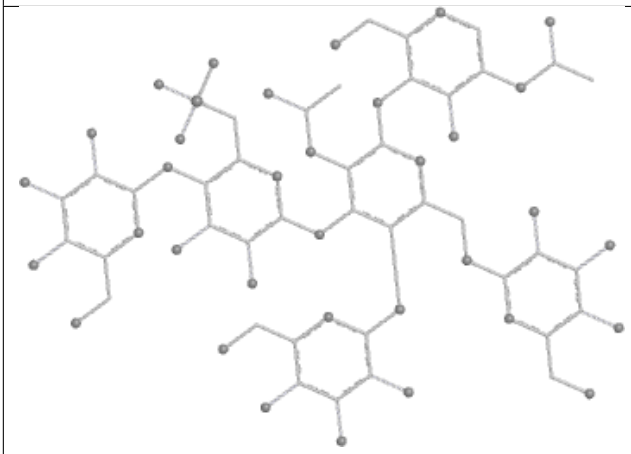


Bond angles



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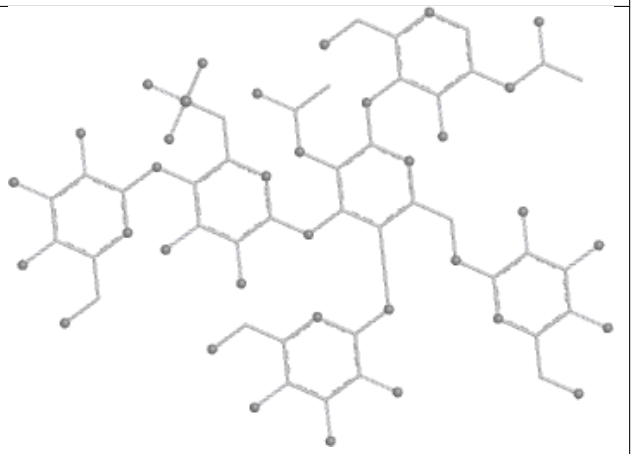
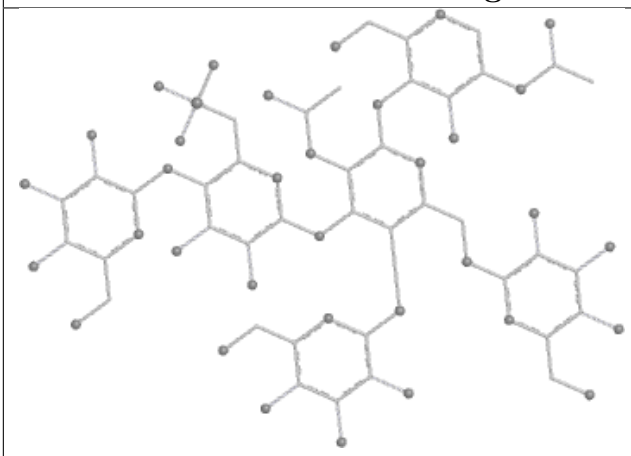


Rings

Oligosaccharide Chain LB



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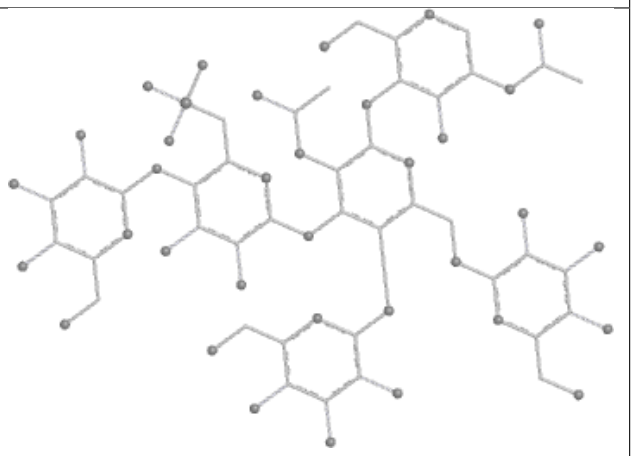

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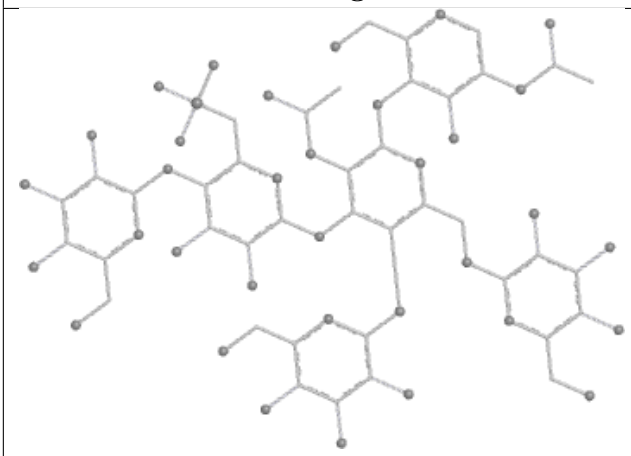

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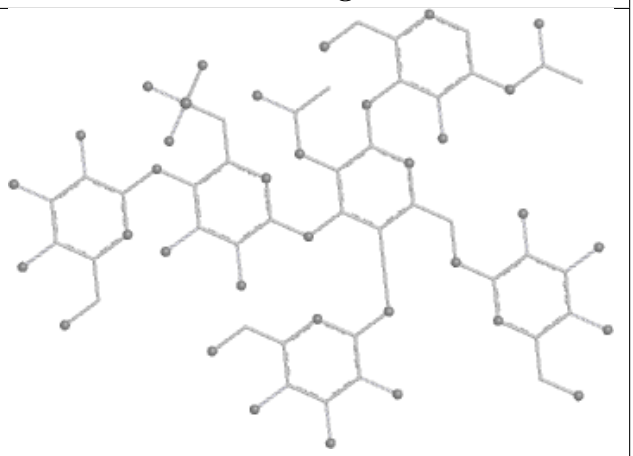
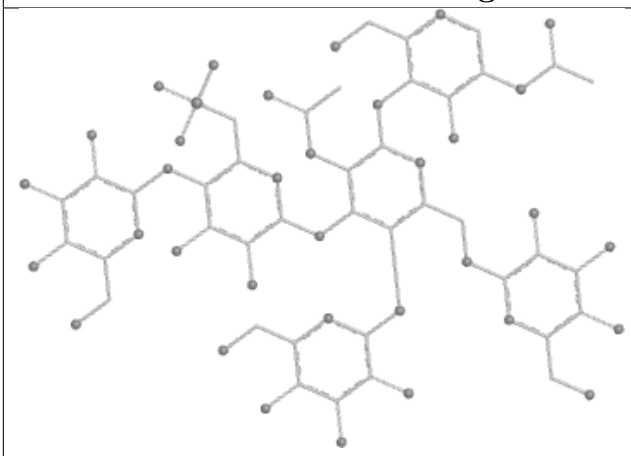


Rings

Oligosaccharide Chain MB



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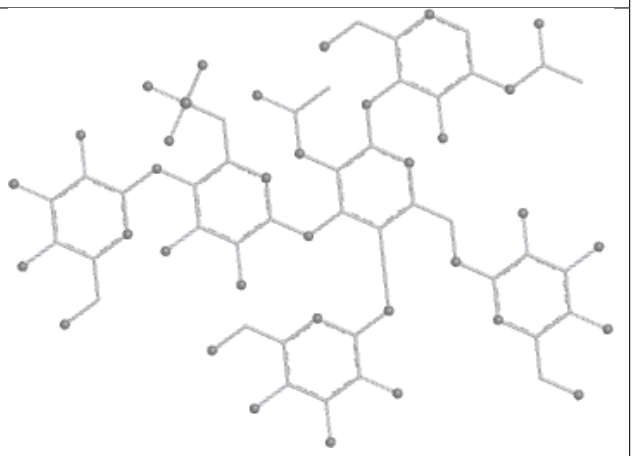
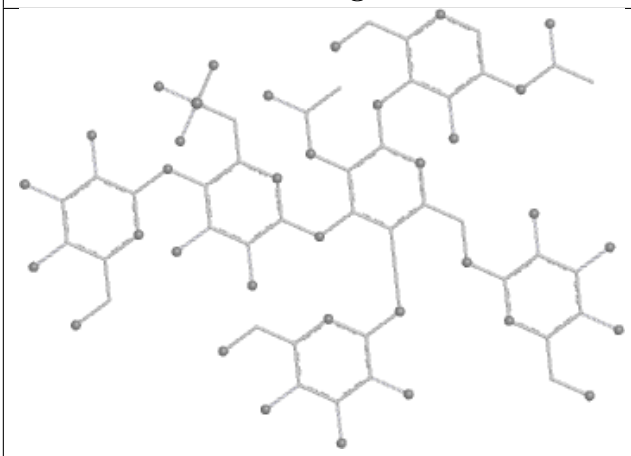


Bond angles



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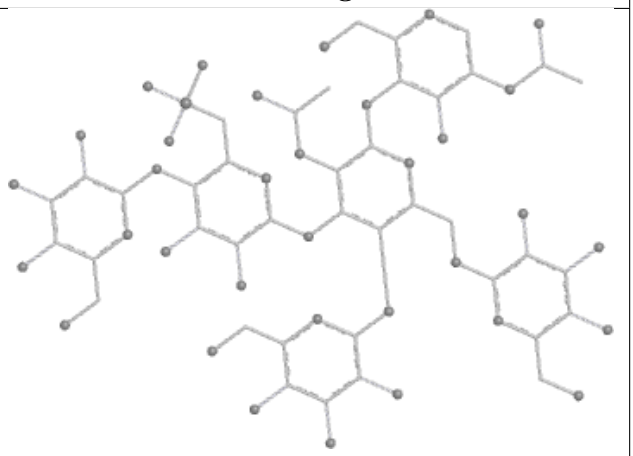
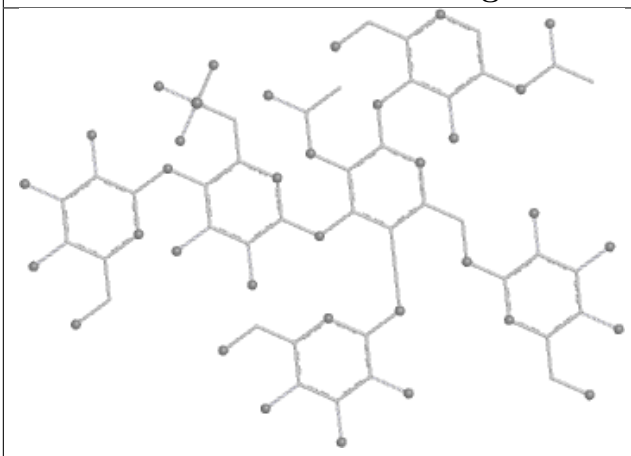


Rings

Oligosaccharide Chain OB



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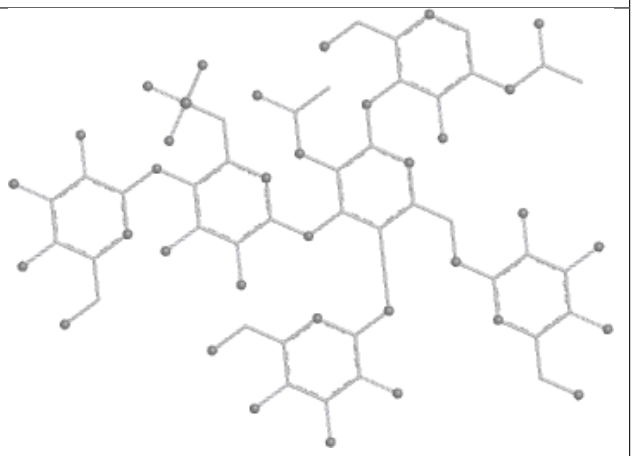
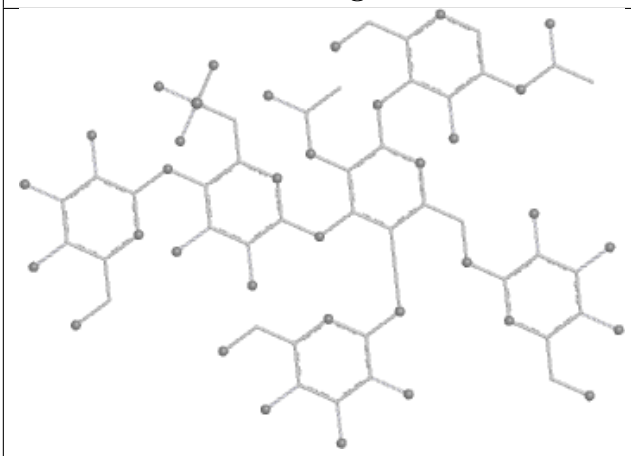


Bond angles



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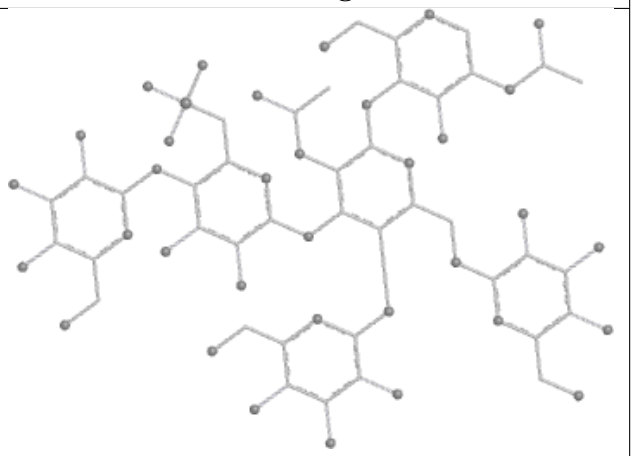
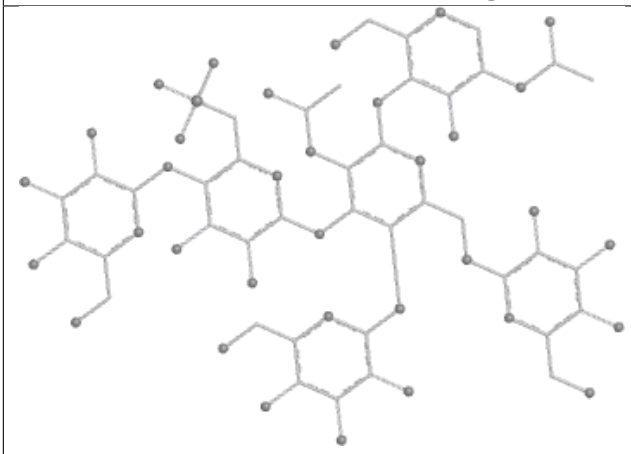


Rings

Oligosaccharide Chain PB



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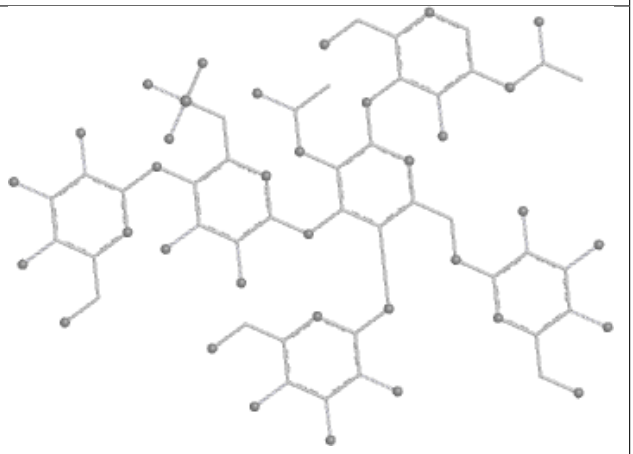
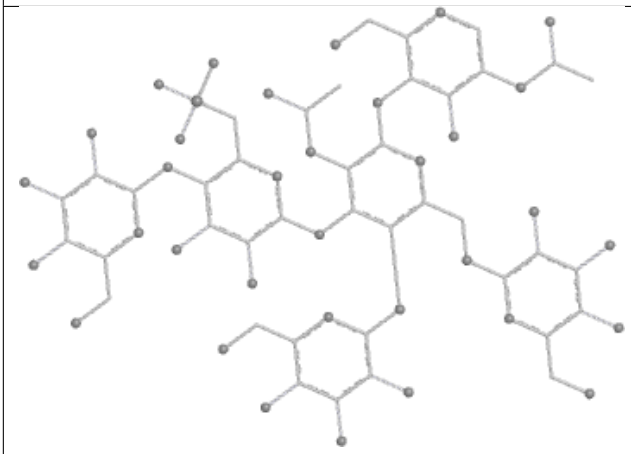


Bond angles



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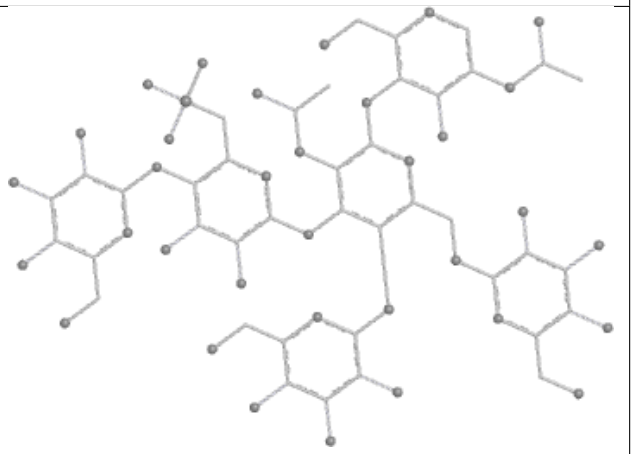
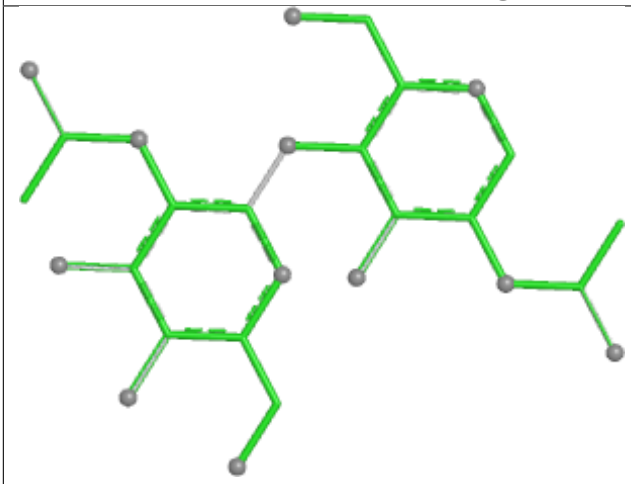


Rings

Oligosaccharide Chain X



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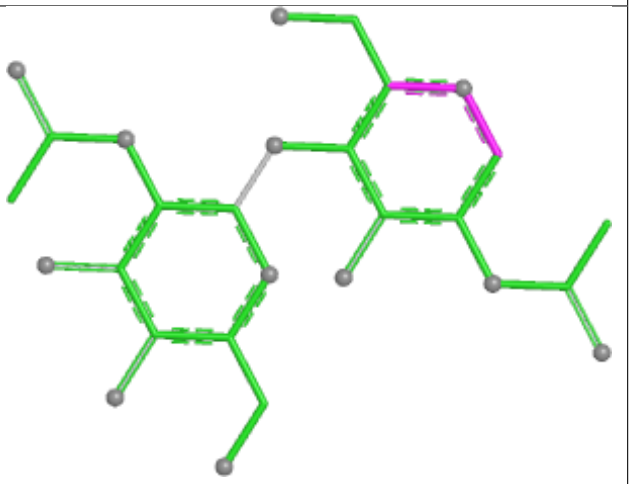

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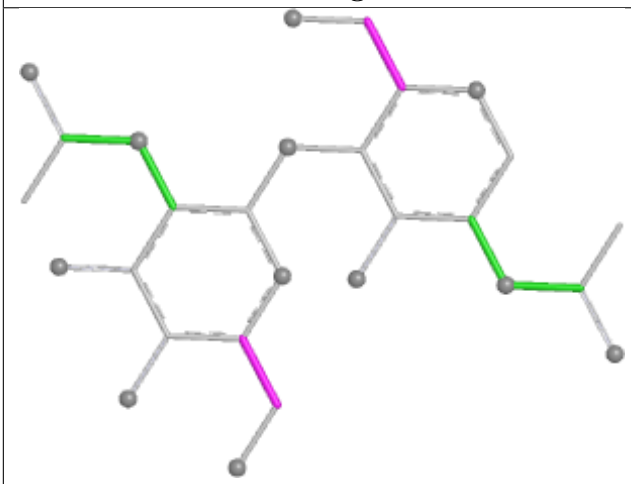

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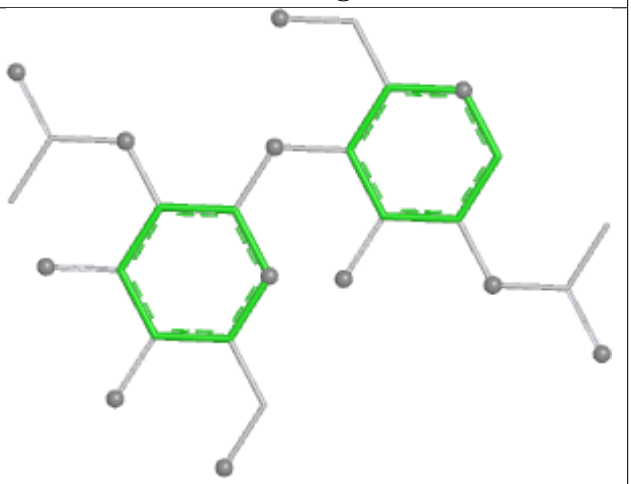
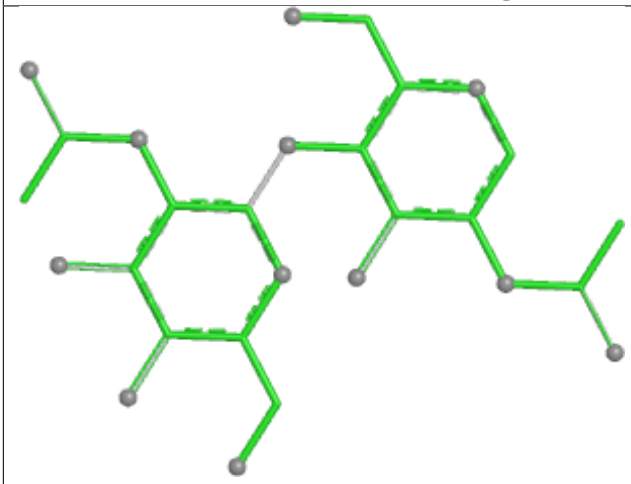


Rings

Oligosaccharide Chain d



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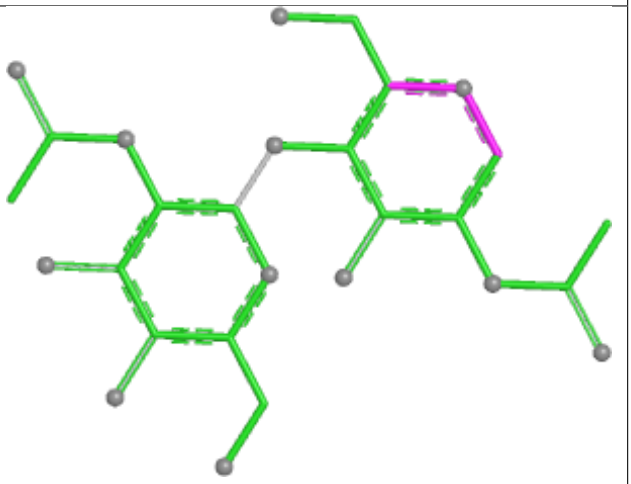
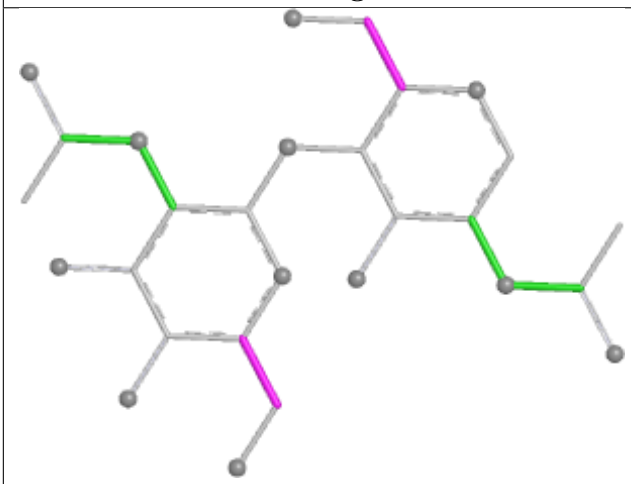


Bond angles



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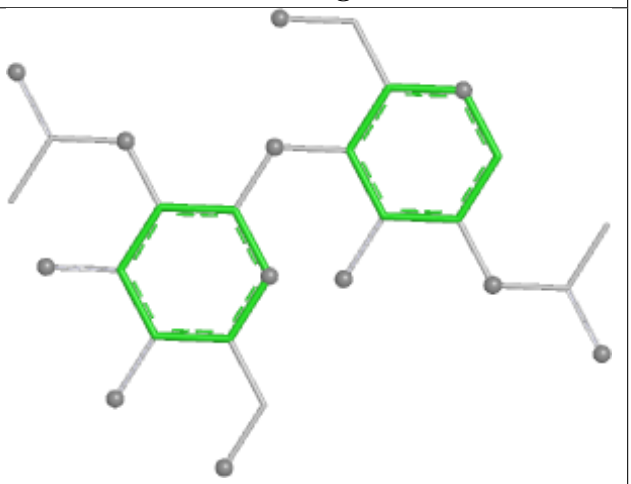
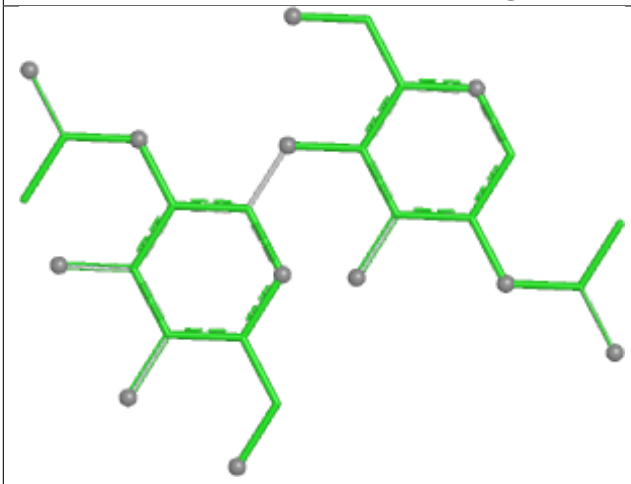


Rings

Oligosaccharide Chain j



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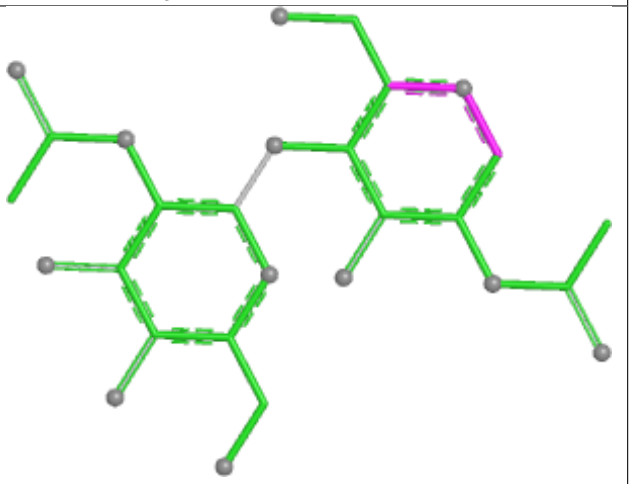

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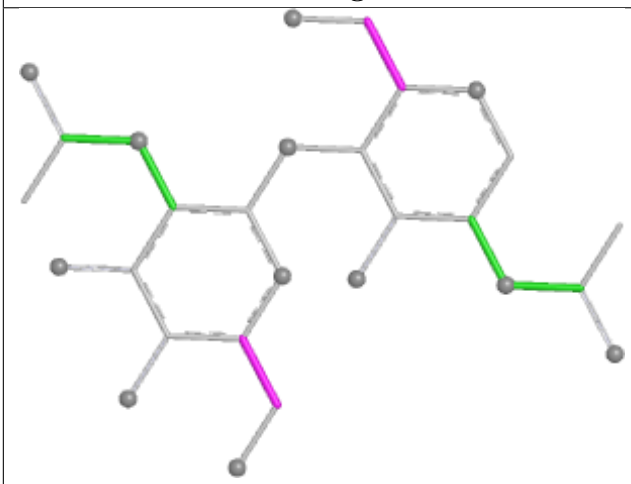

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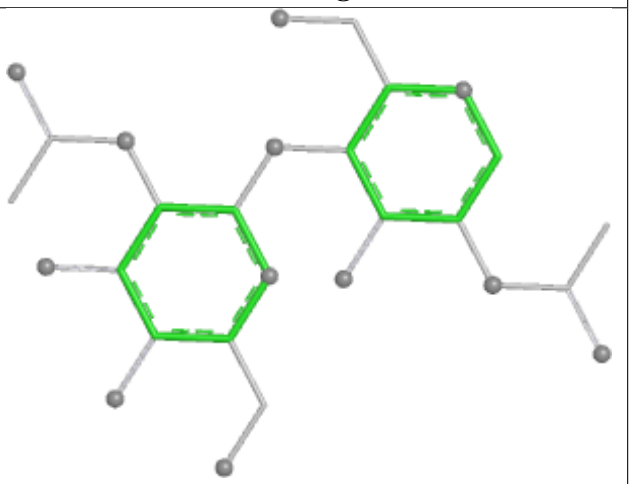
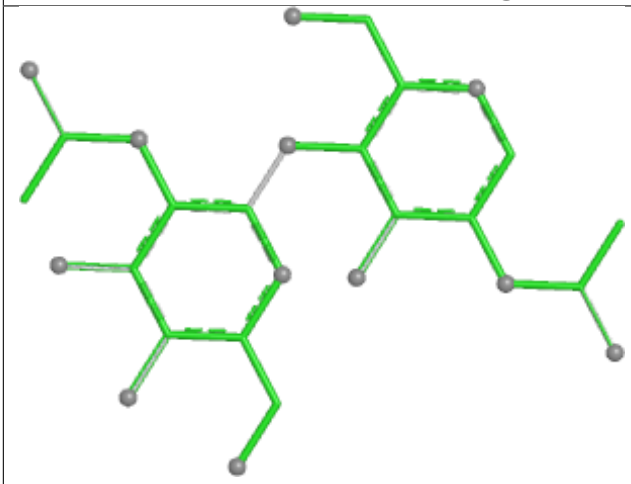


Rings

Oligosaccharide Chain p



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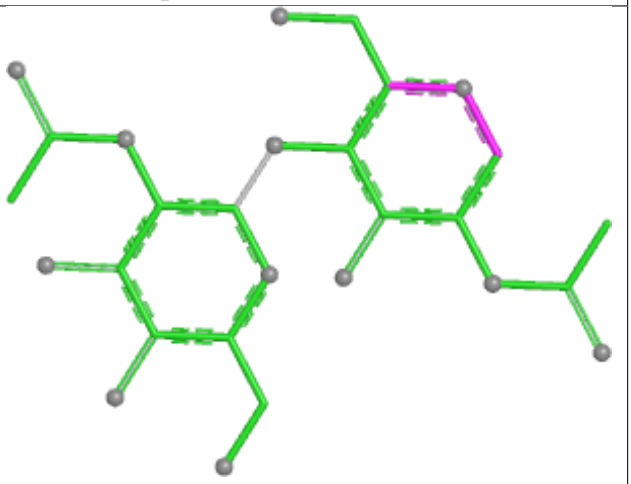

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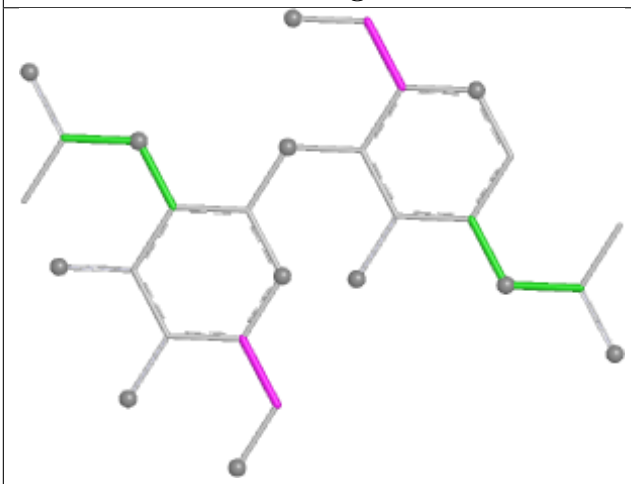

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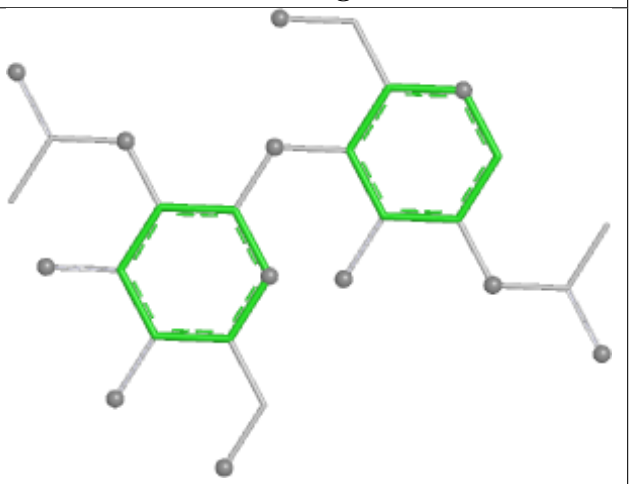
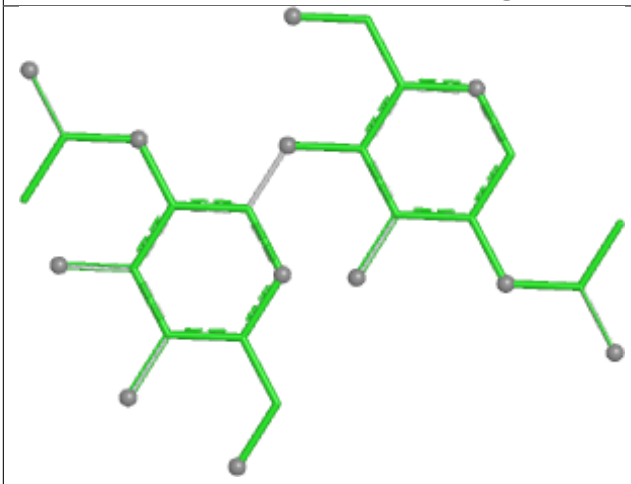


Rings

Oligosaccharide Chain v



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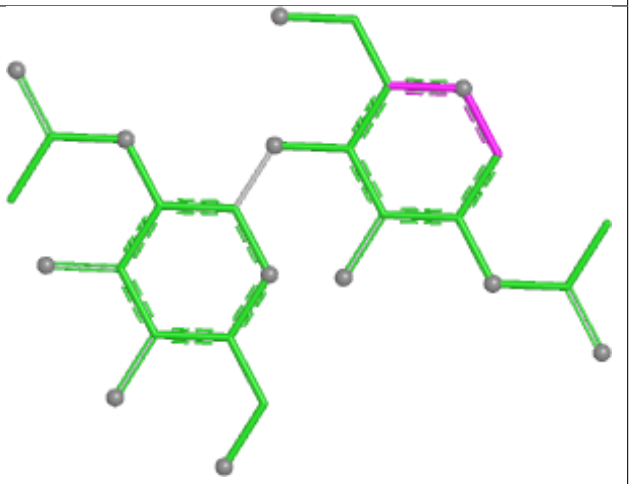

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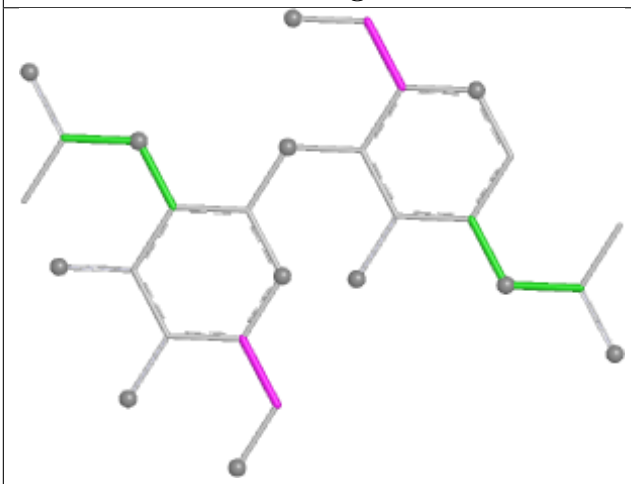

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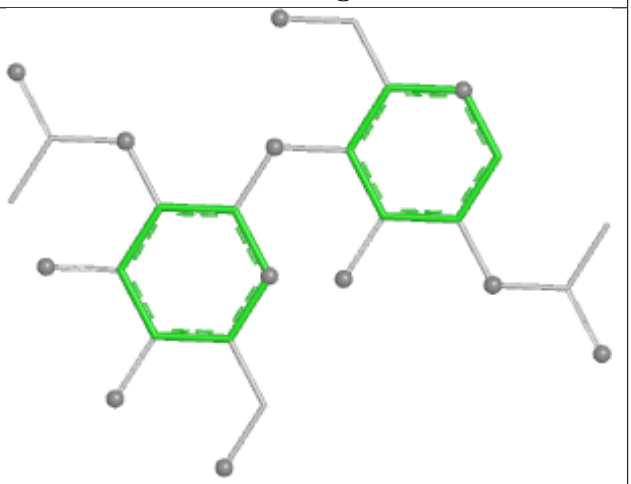
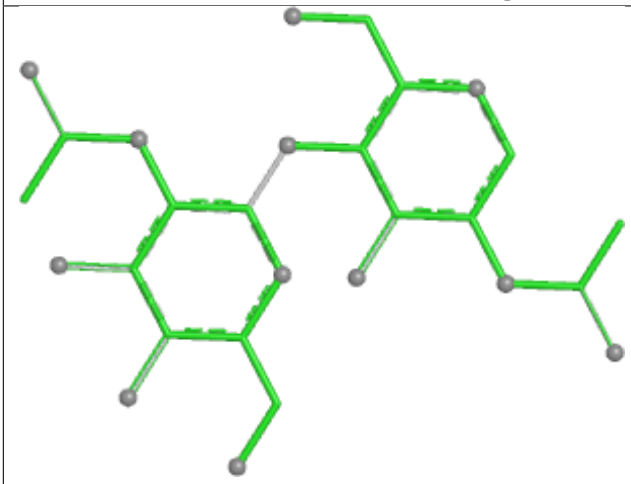


Rings

Oligosaccharide Chain 1



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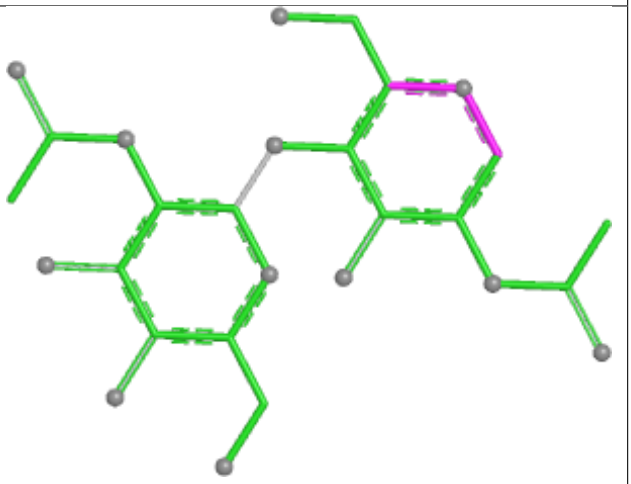

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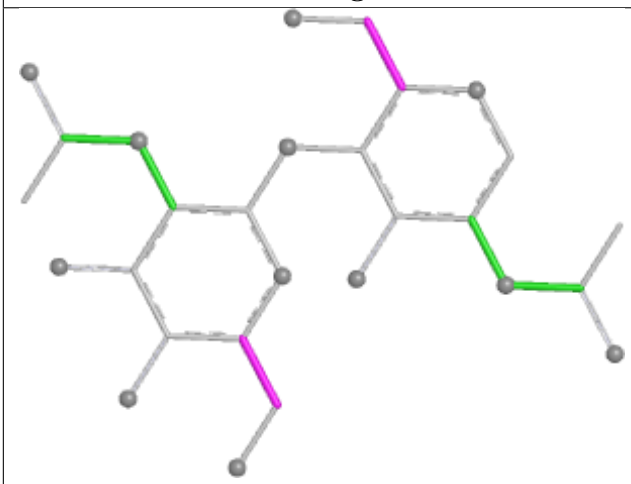

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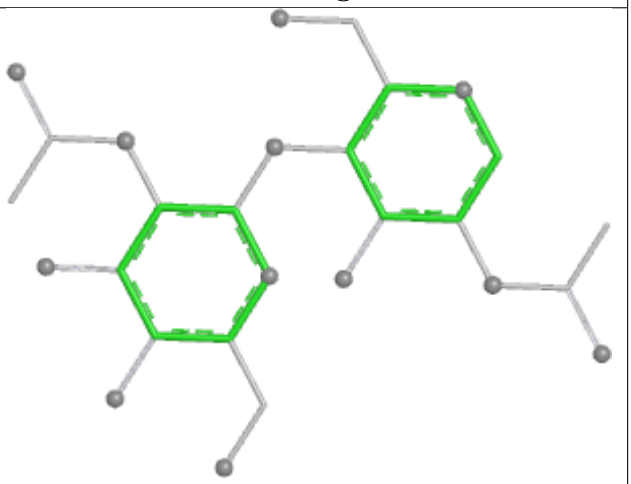
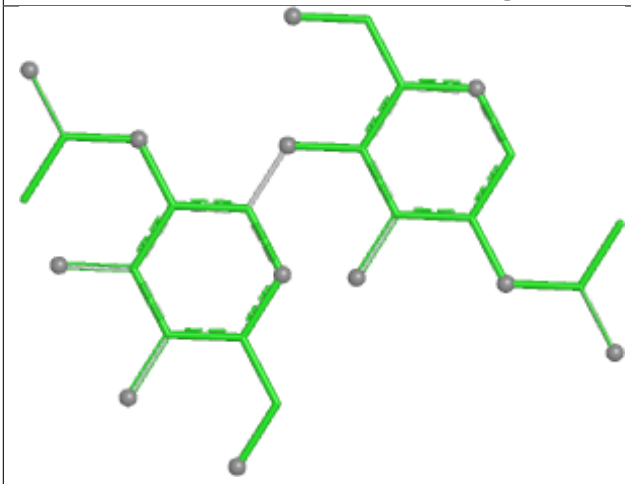


Rings

Oligosaccharide Chain 7



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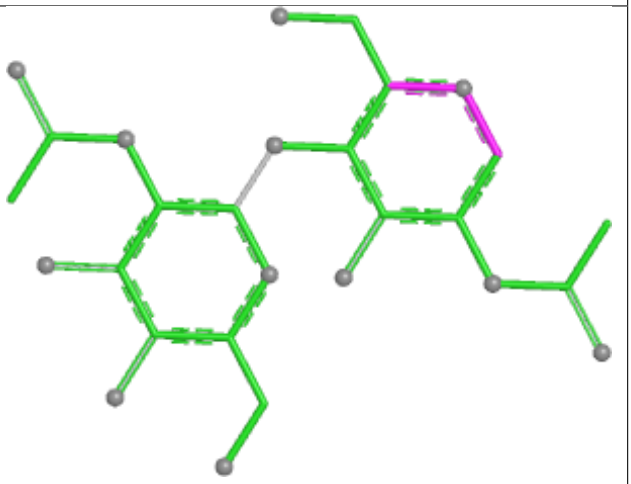
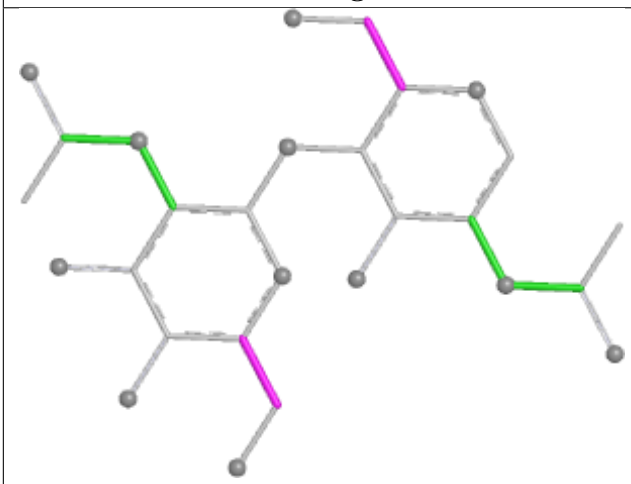


Bond angles



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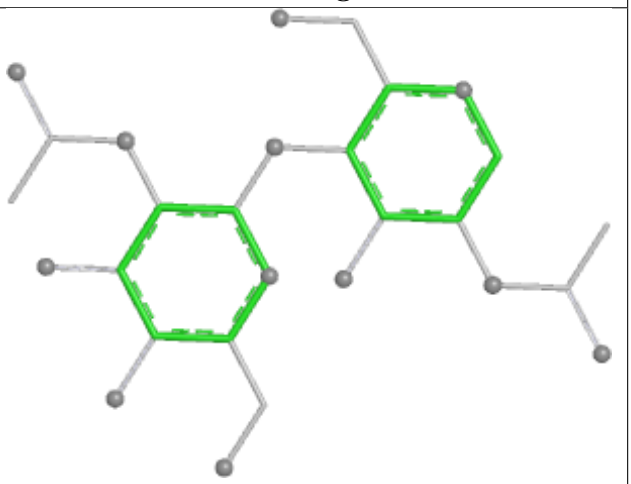
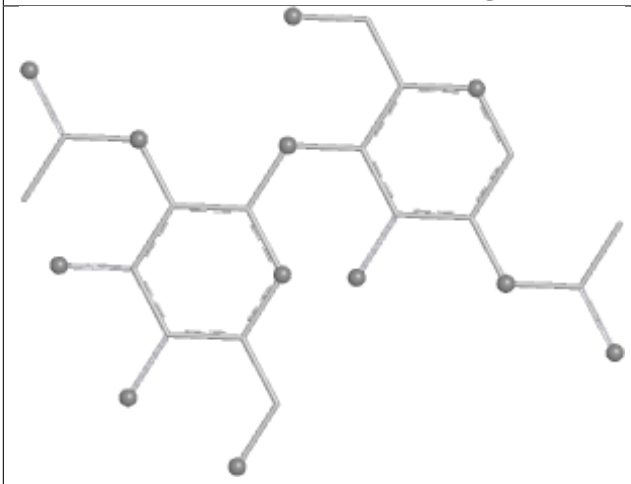
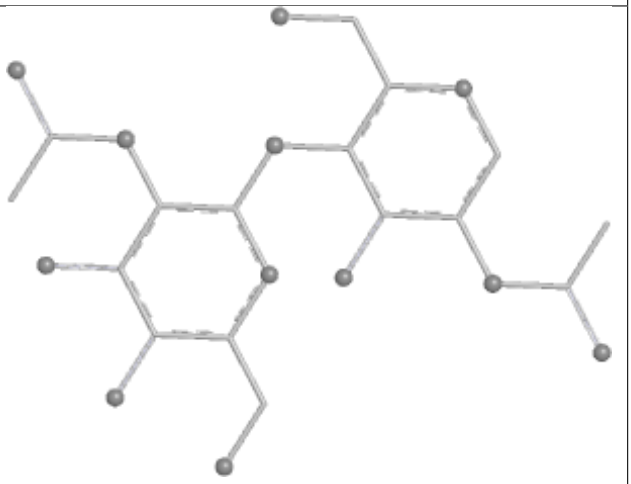


Rings

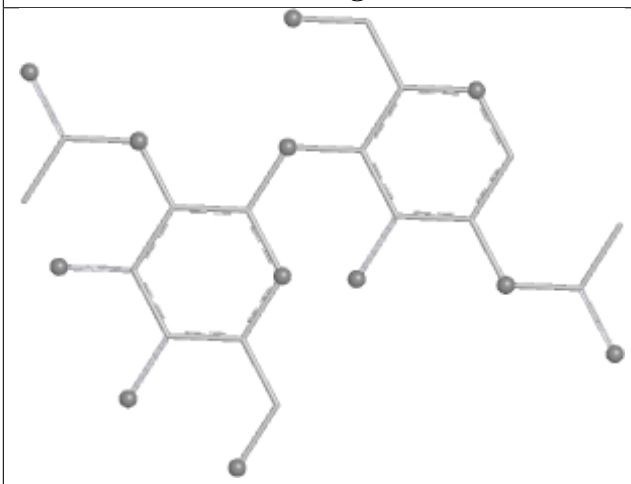
Oligosaccharide Chain DA



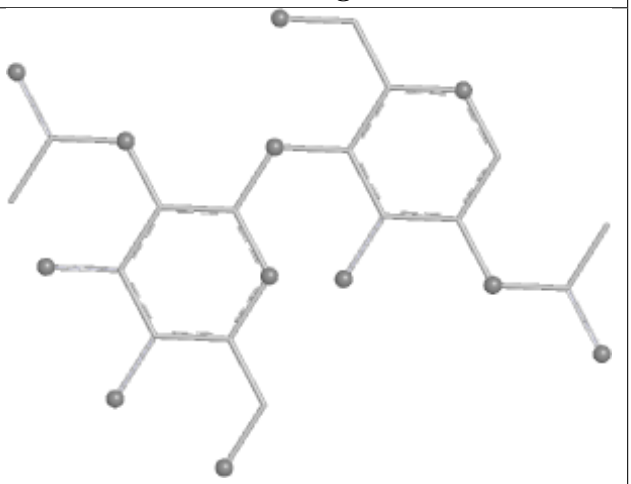
Bond lengths



Bond angles

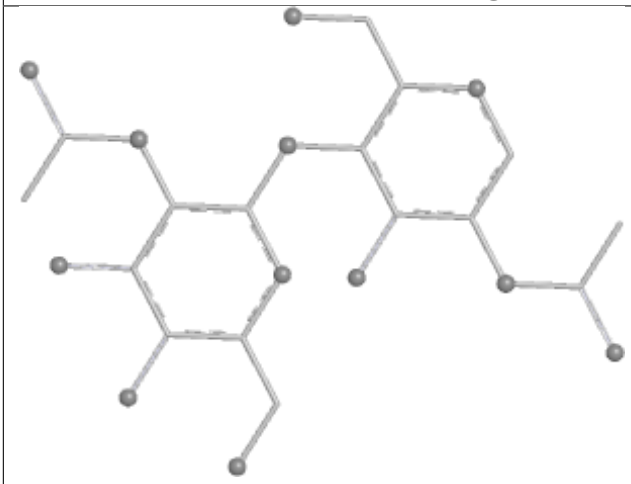


Torsions

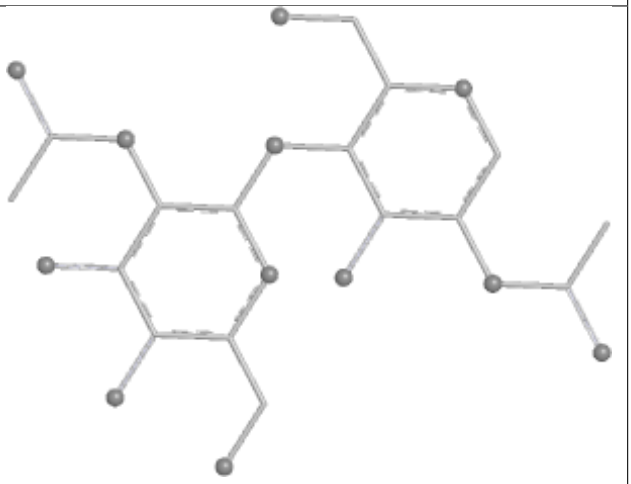


Rings

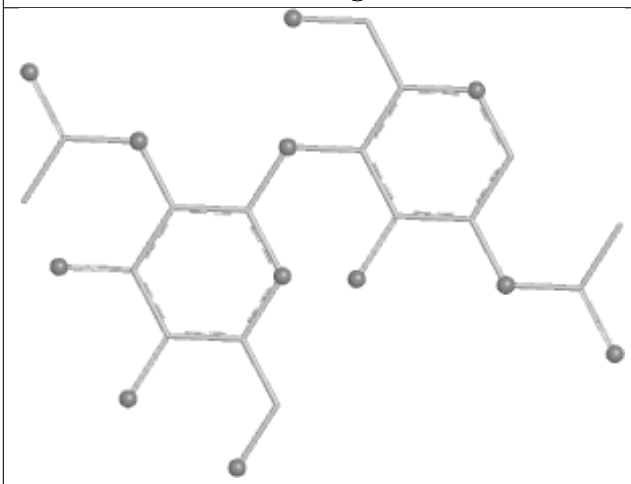
Oligosaccharide Chain JA



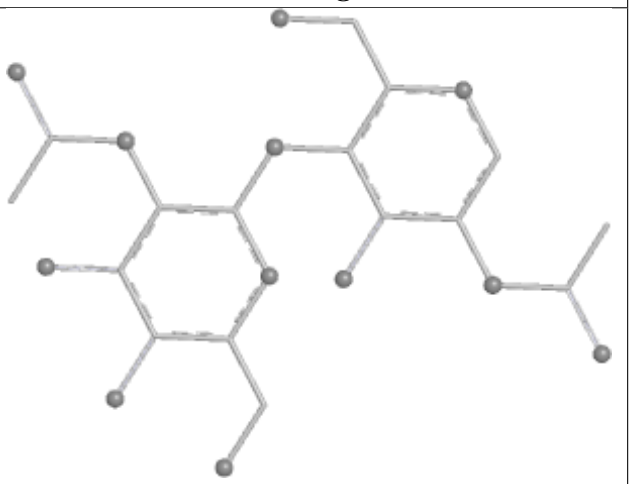
Bond lengths



Bond angles

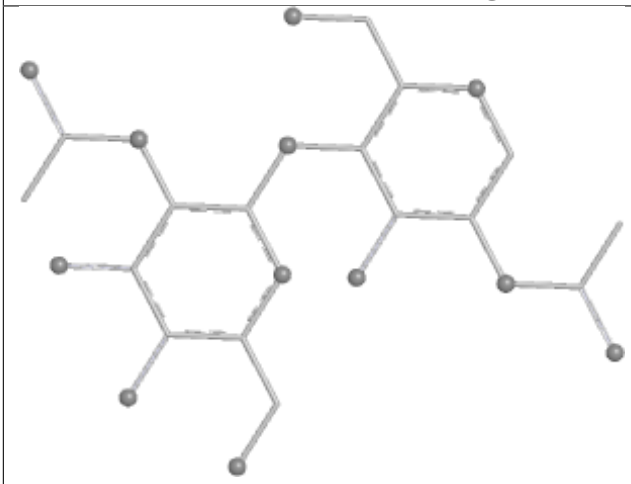


Torsions



Rings

Oligosaccharide Chain PA



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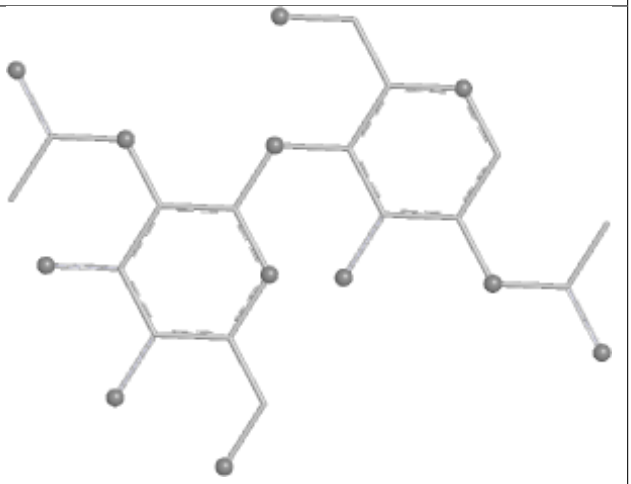
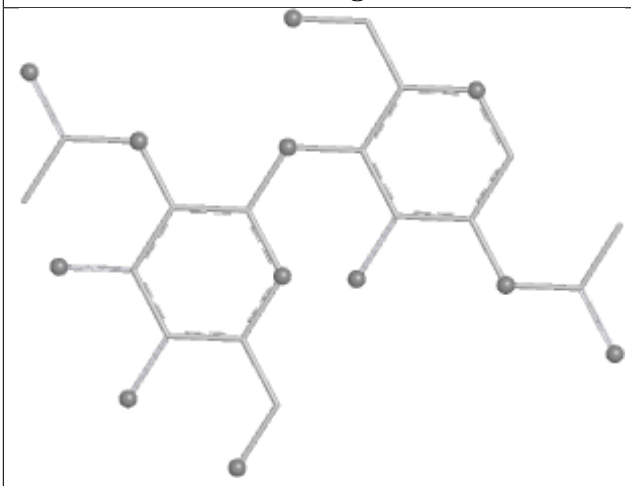
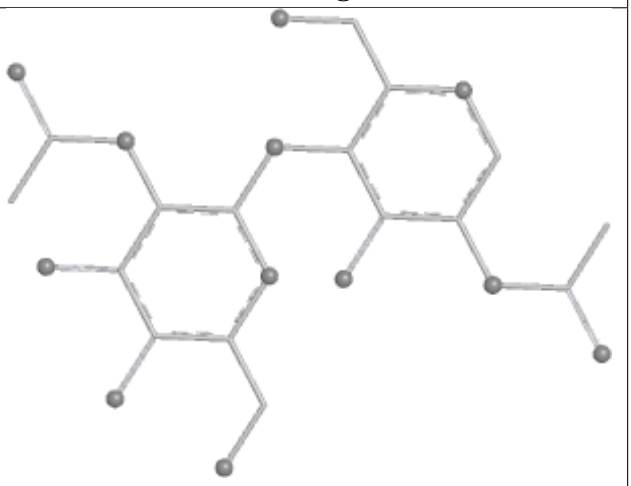


Bond angles

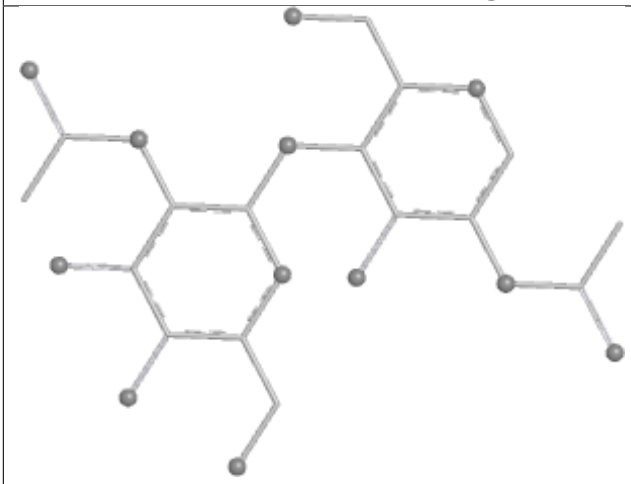


Torsions

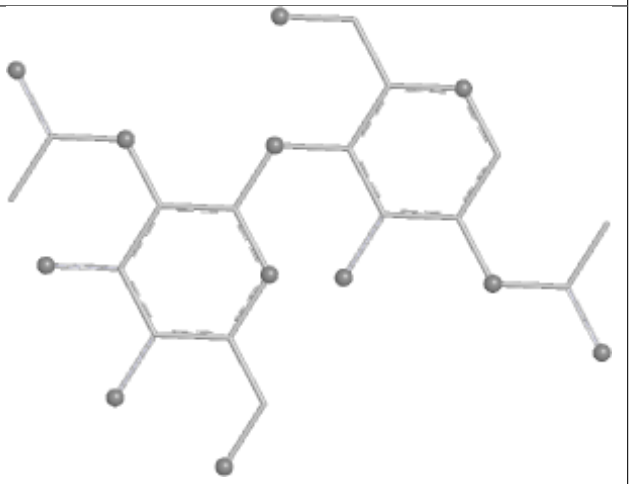


Rings

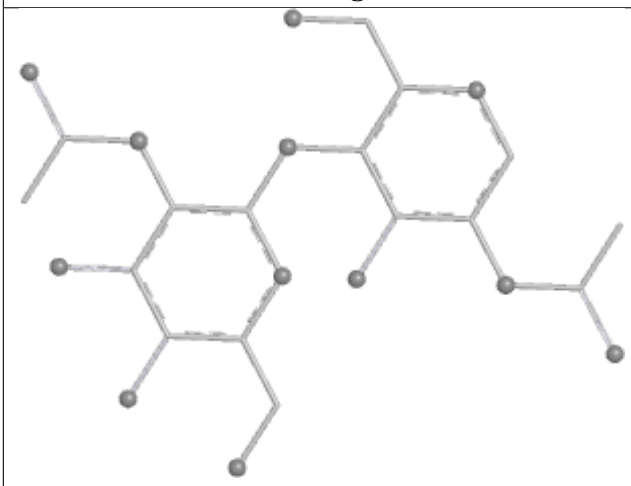
Oligosaccharide Chain VA



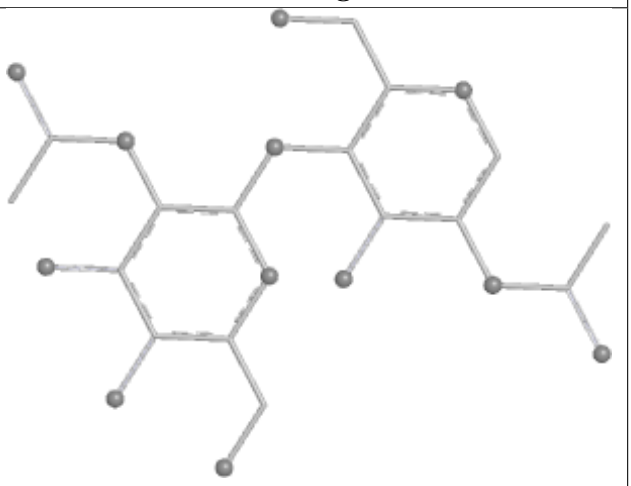
Bond lengths



Bond angles

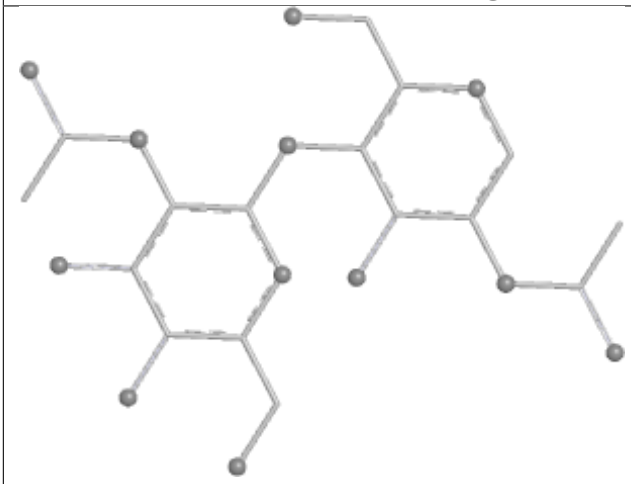


Torsions

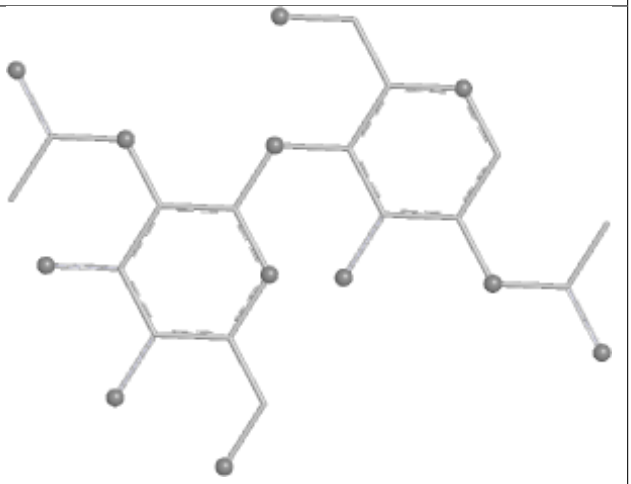


Rings

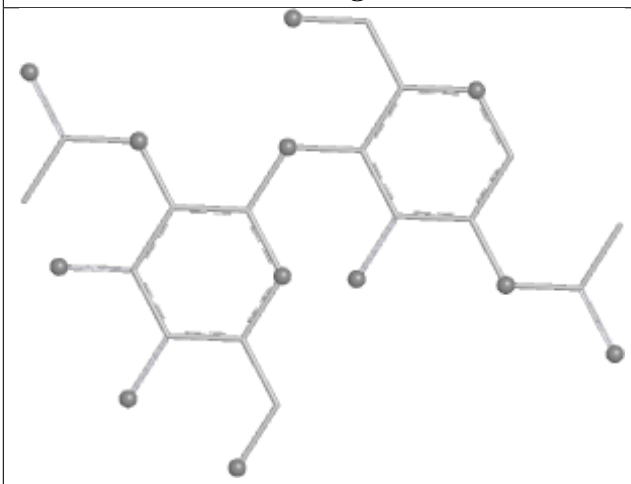
Oligosaccharide Chain bA



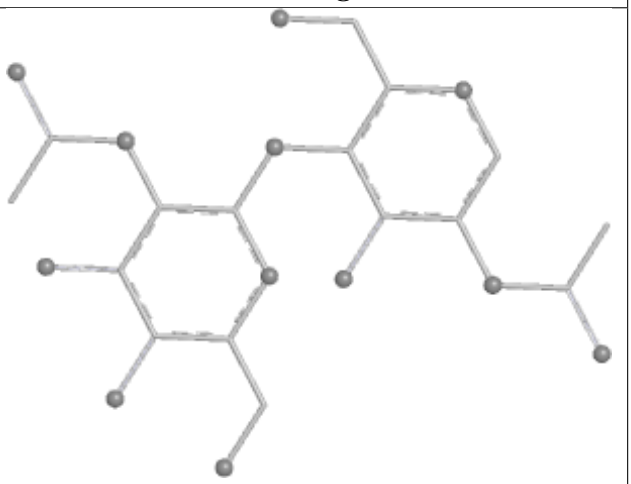
Bond lengths



Bond angles

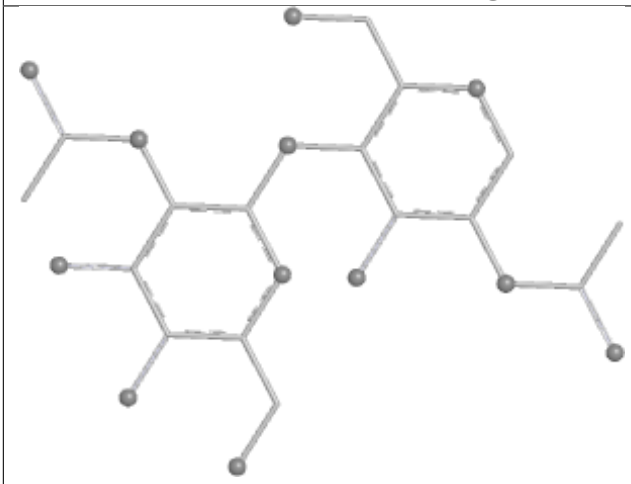


Torsions

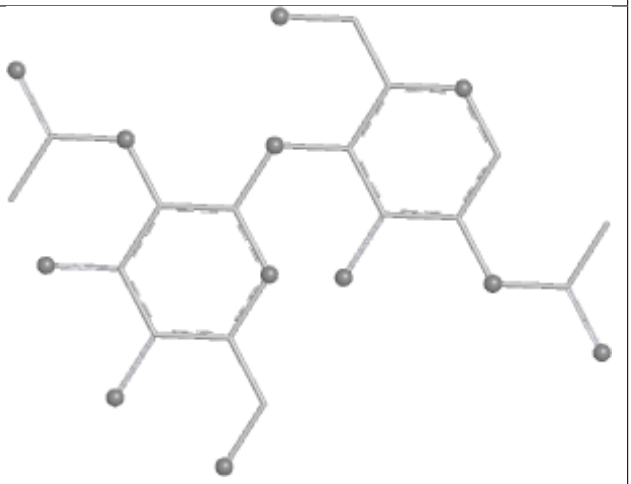


Rings

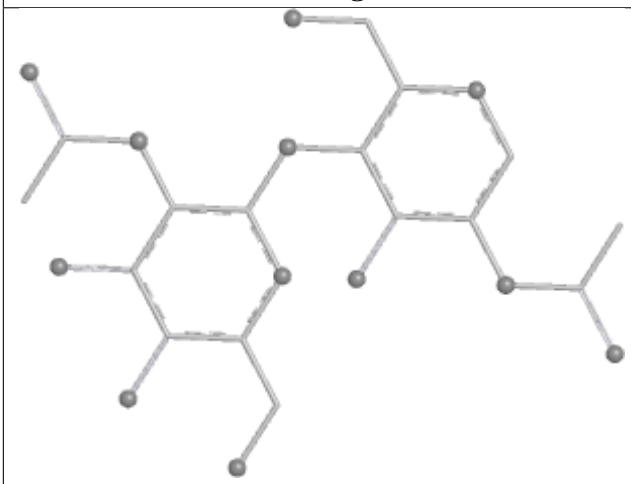
Oligosaccharide Chain hA



Bond lengths



Bond angles



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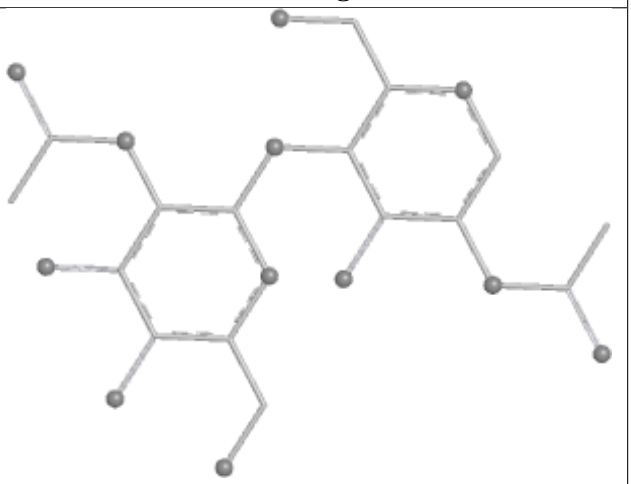
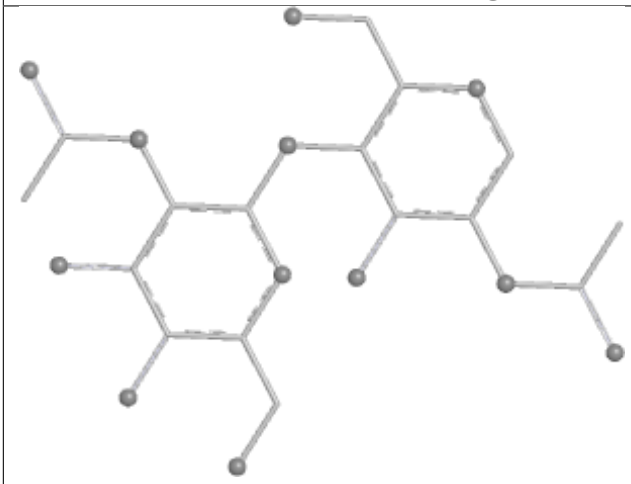
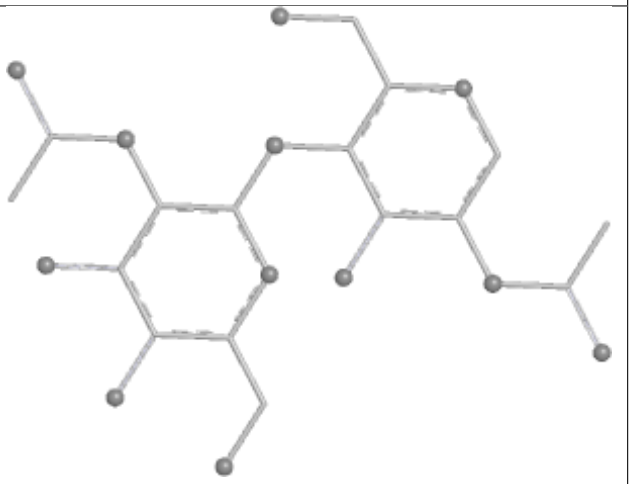


Rings

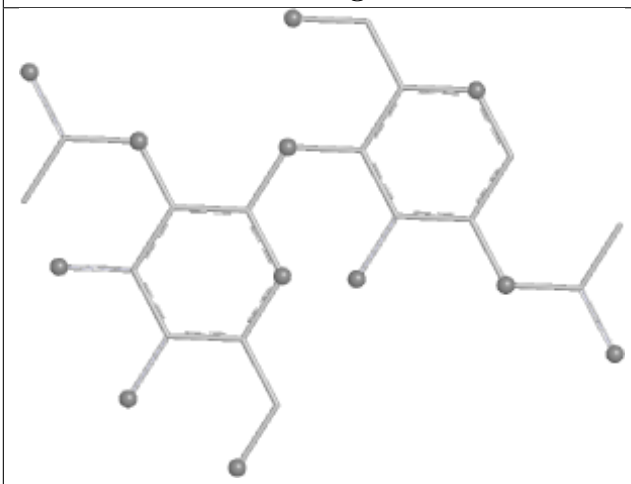
Oligosaccharide Chain nA



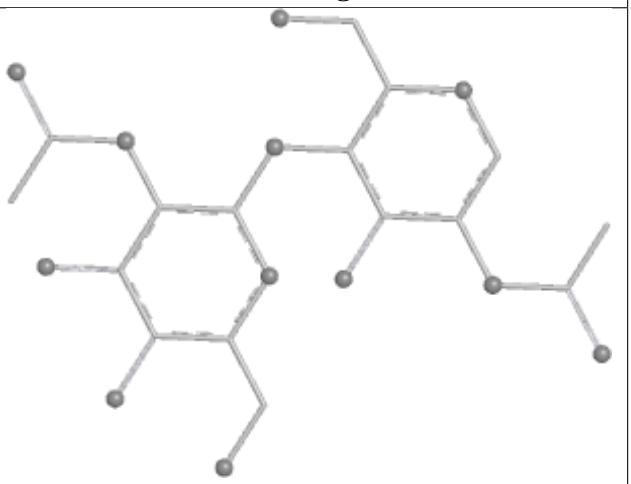
Bond lengths



Bond angles

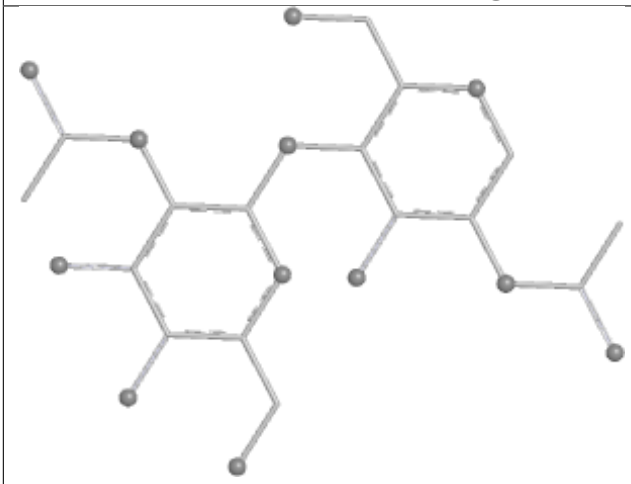


Torsions

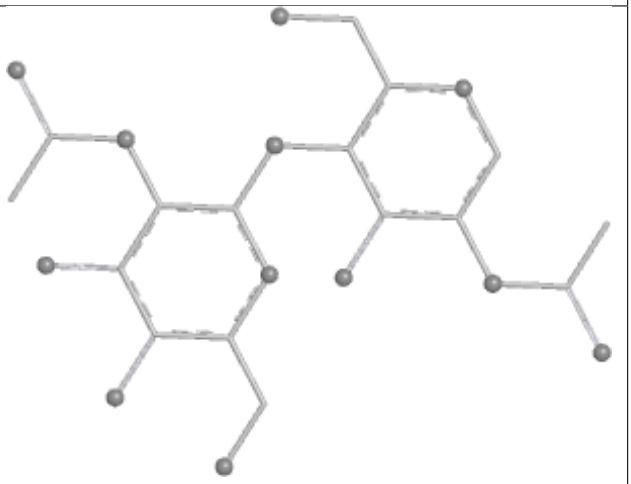


Rings

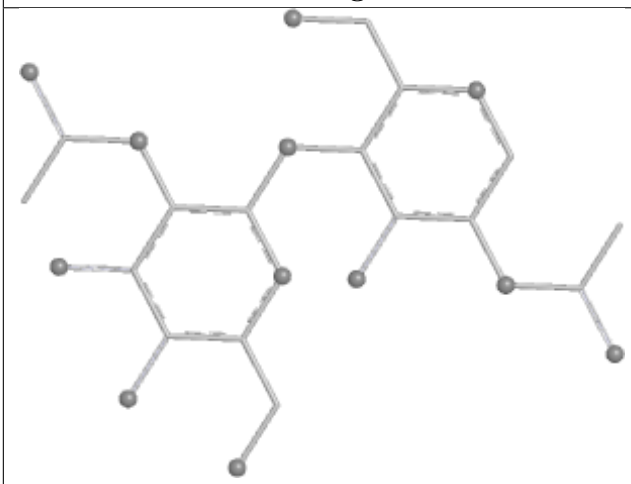
Oligosaccharide Chain tA



Bond lengths



Bond angles



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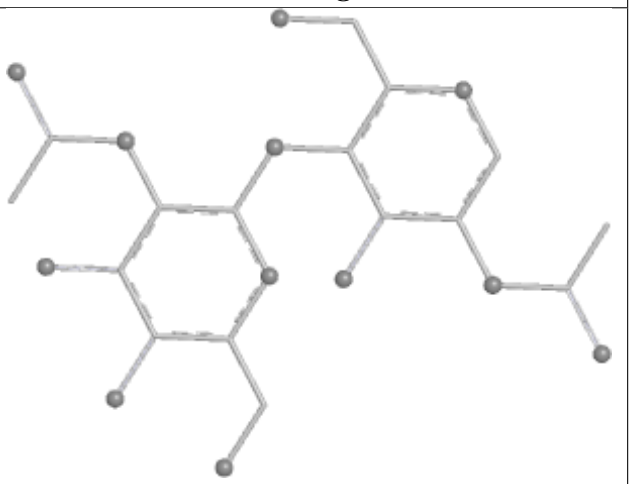
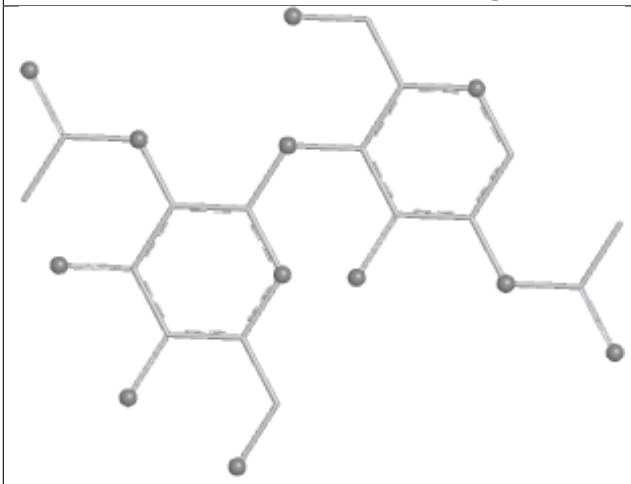
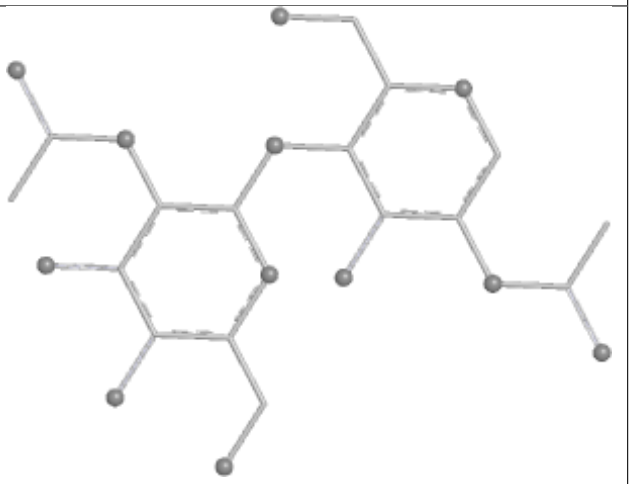


Rings

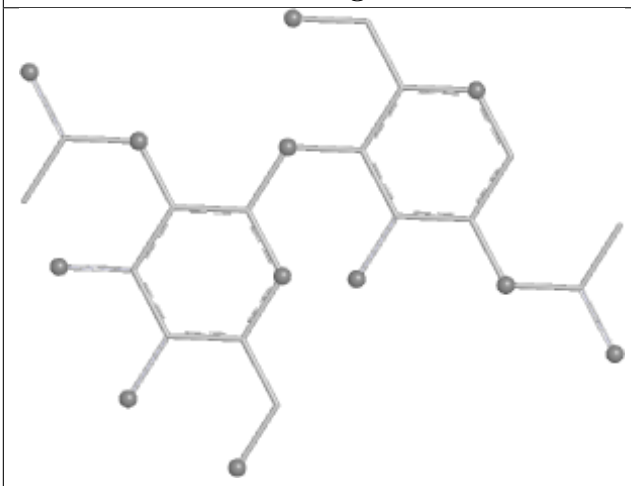
Oligosaccharide Chain zA



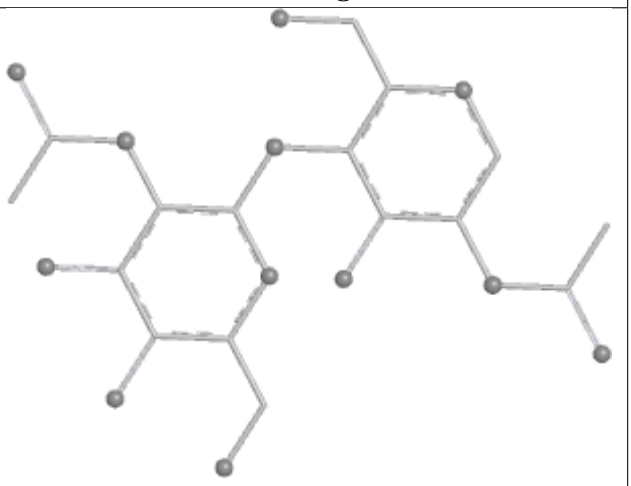
Bond lengths



Bond angles

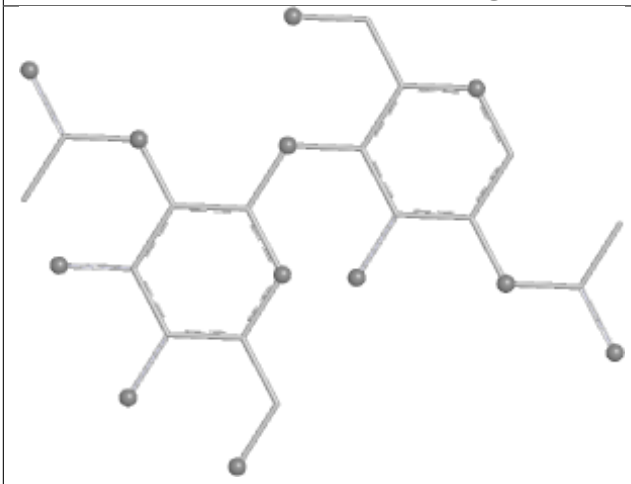


Torsions

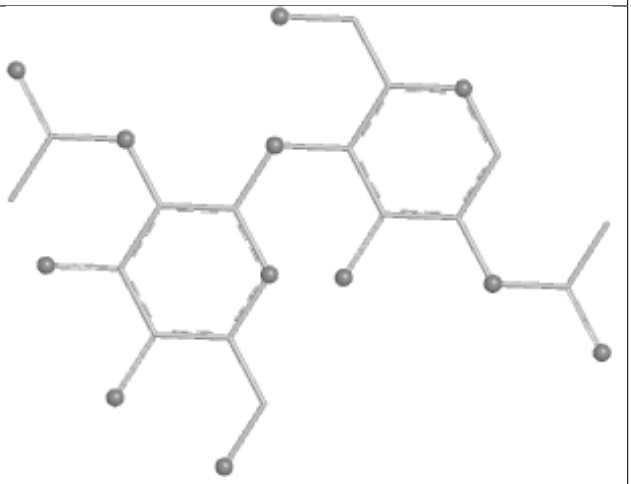


Rings

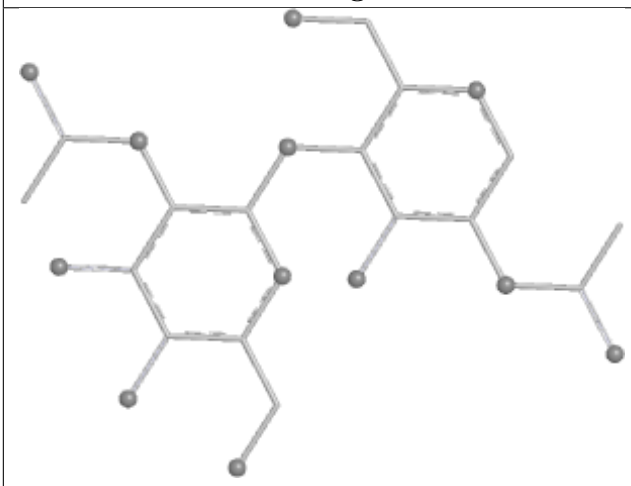
Oligosaccharide Chain 5A



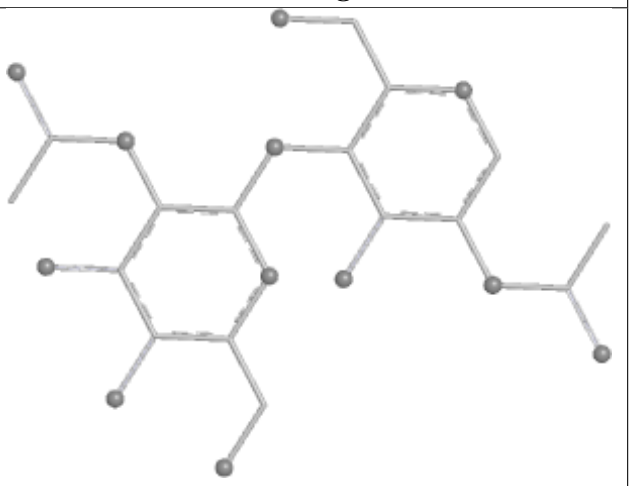
Bond lengths



Bond angles

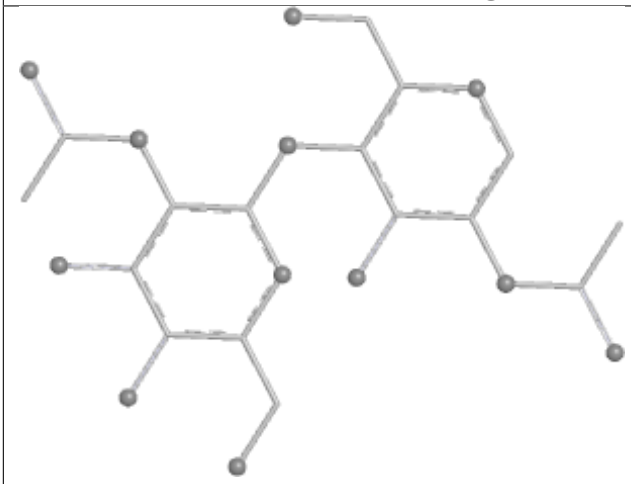


Torsions

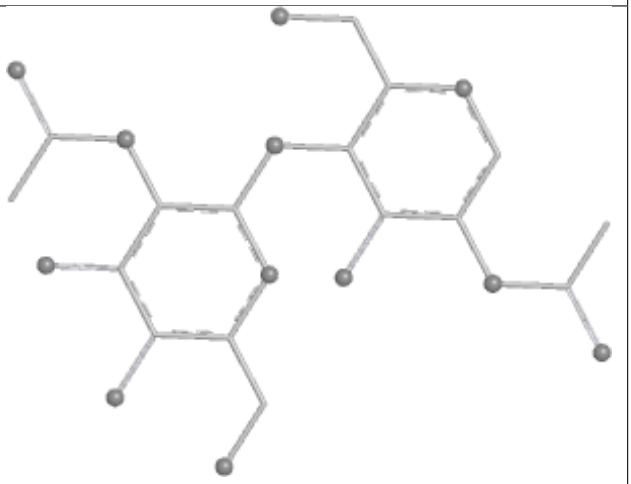


Rings

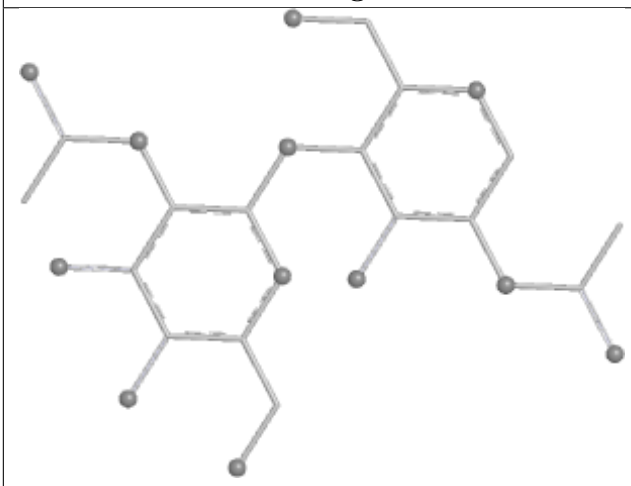
Oligosaccharide Chain BB



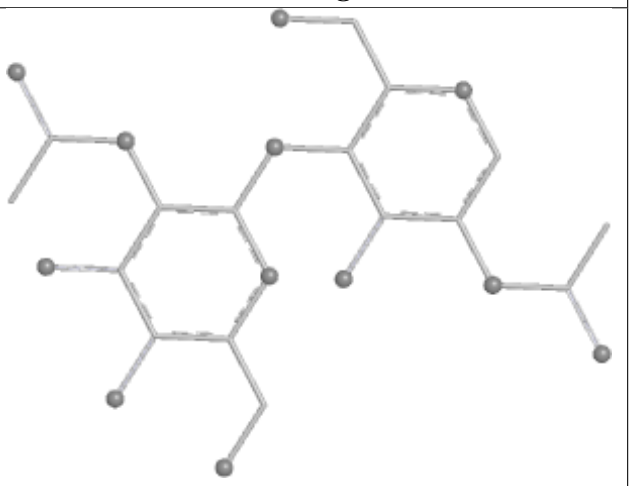
Bond lengths



Bond angles

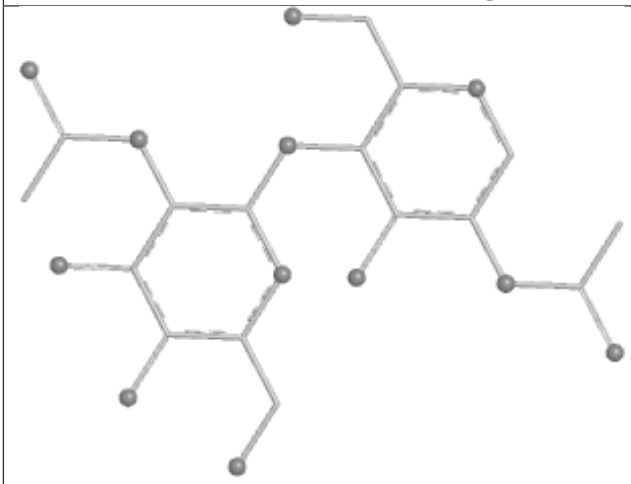


Torsions

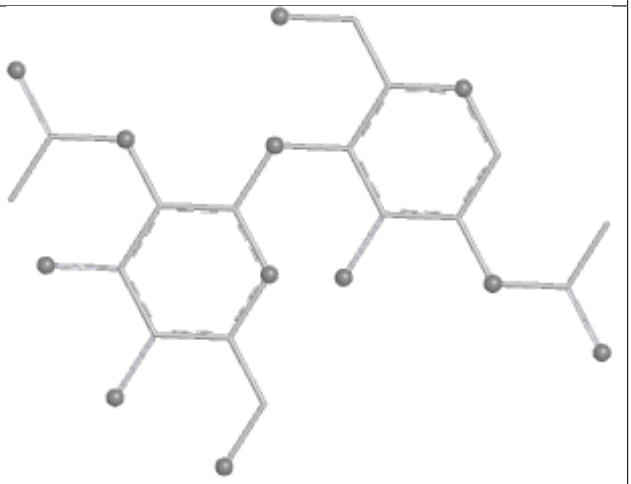


Rings

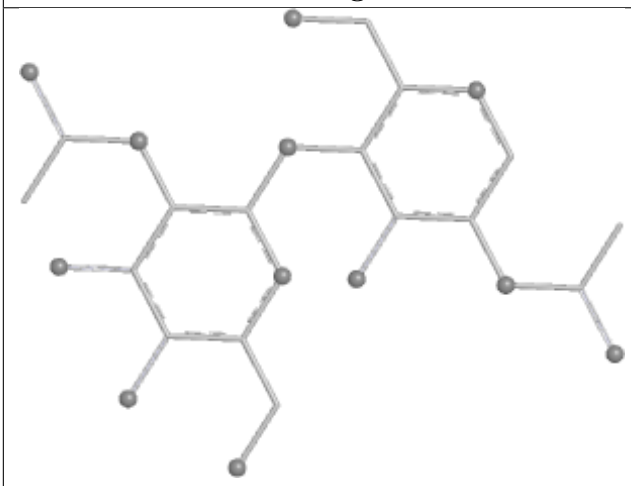
Oligosaccharide Chain HB



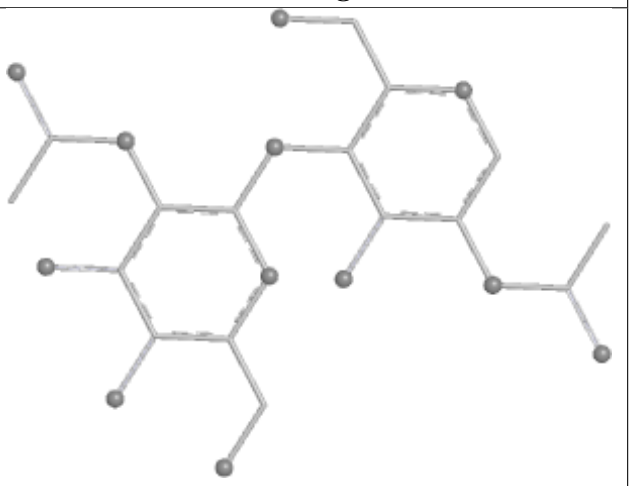
Bond lengths



Bond angles

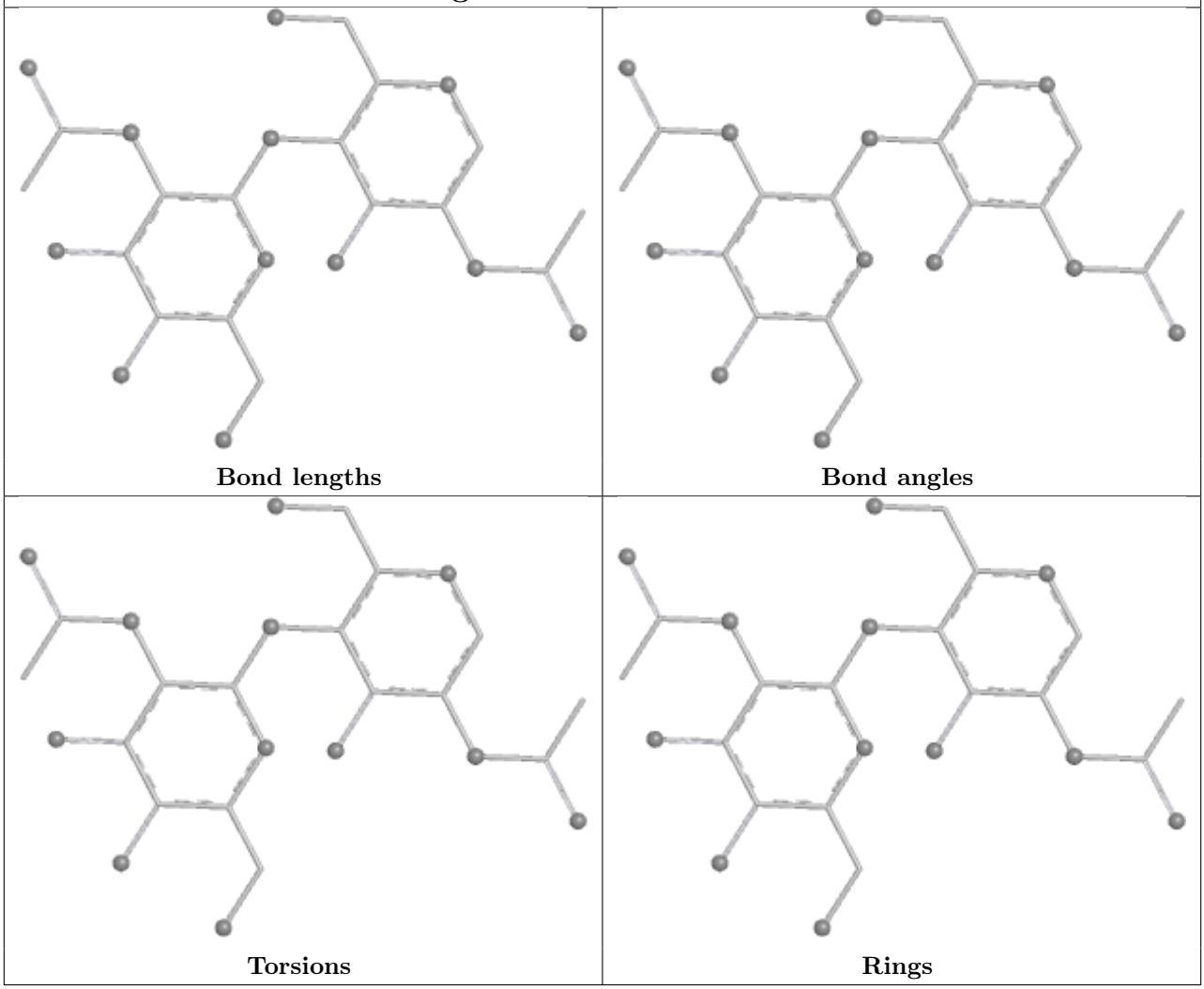


Torsions



Rings

Oligosaccharide Chain NB



5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

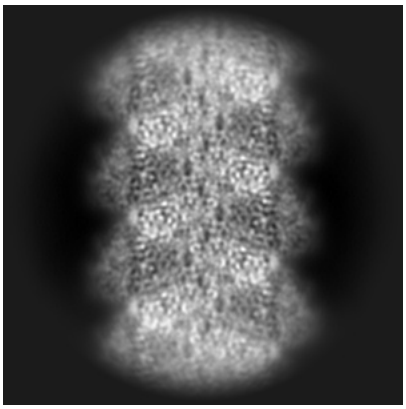
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18700. These allow visual inspection of the internal detail of the map and identification of artifacts.

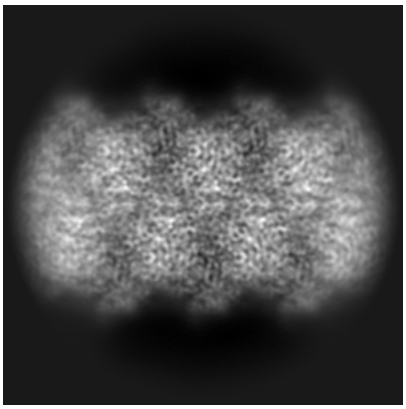
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

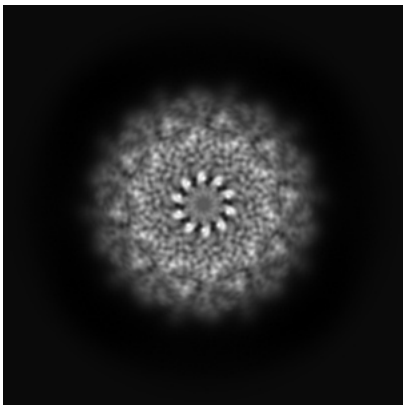
6.1.1 Primary map



X

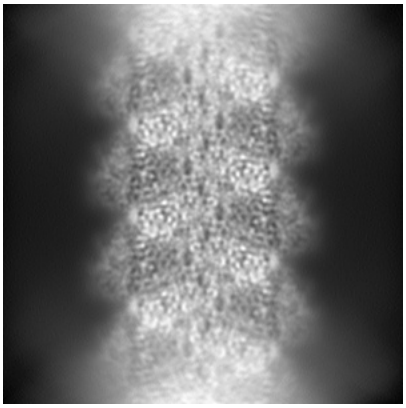


Y

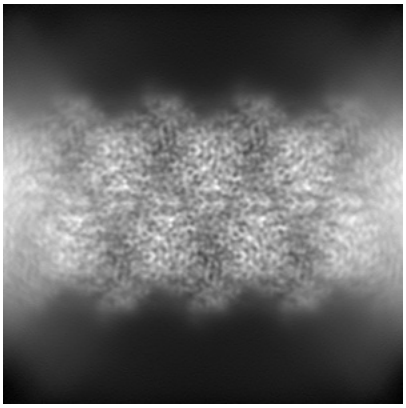


Z

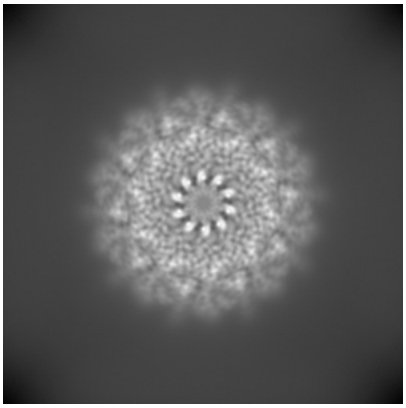
6.1.2 Raw map



X



Y

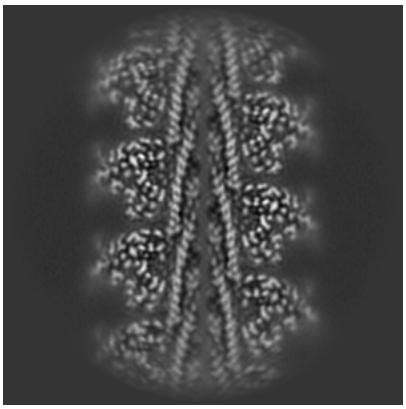


Z

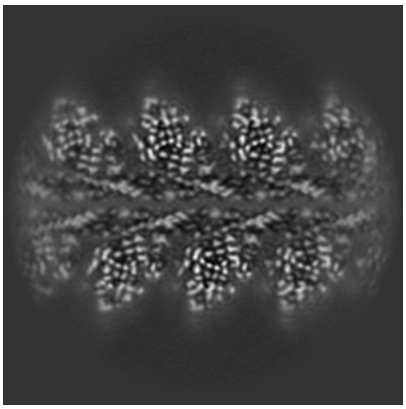
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

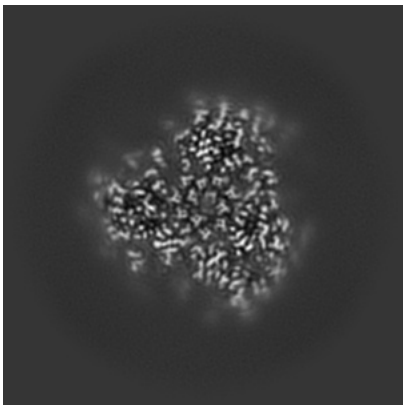
6.2.1 Primary map



X Index: 144

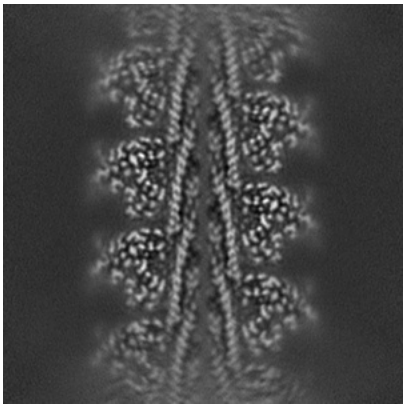


Y Index: 144

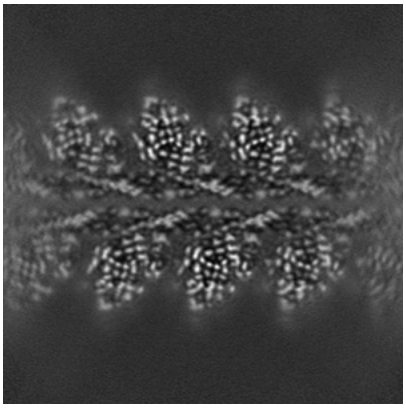


Z Index: 144

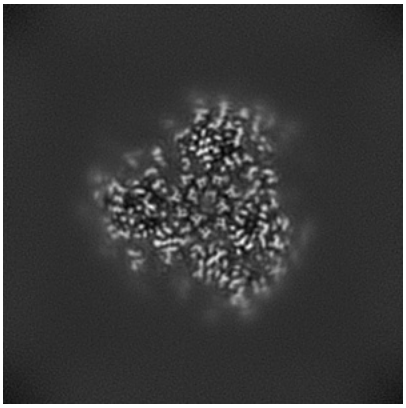
6.2.2 Raw map



X Index: 144



Y Index: 144

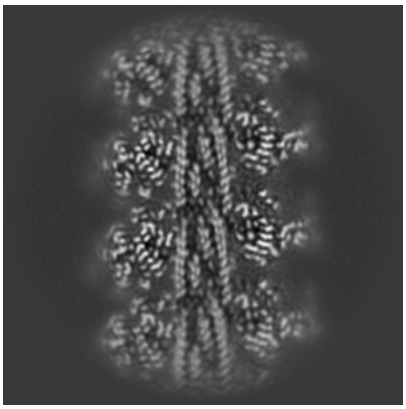


Z Index: 144

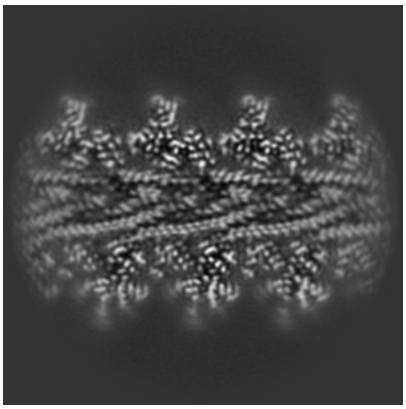
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

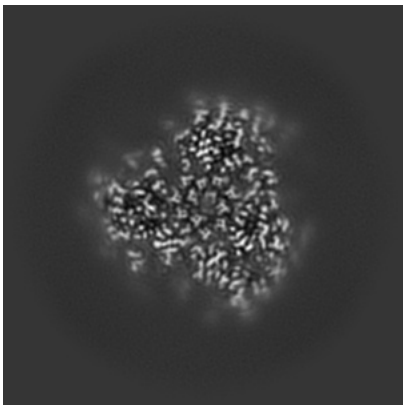
6.3.1 Primary map



X Index: 133

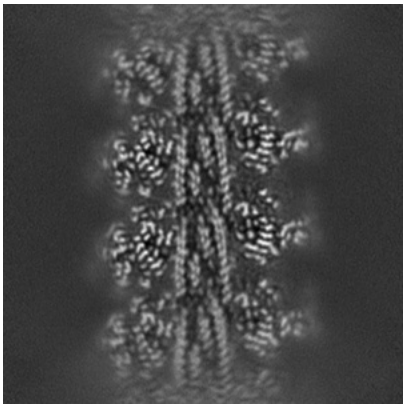


Y Index: 137

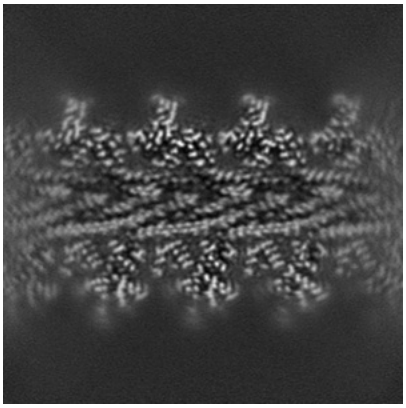


Z Index: 144

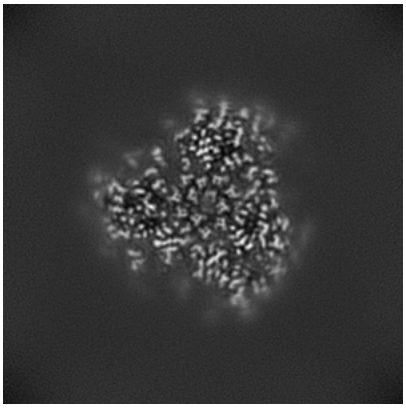
6.3.2 Raw map



X Index: 133



Y Index: 136

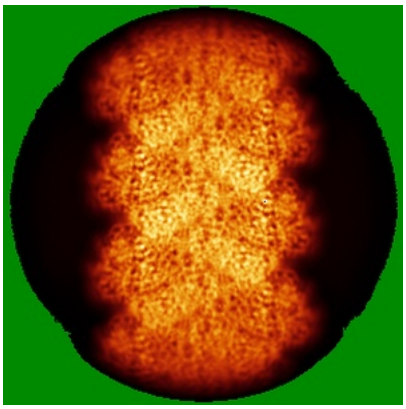


Z Index: 144

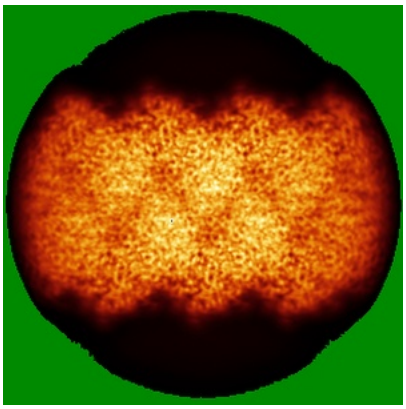
The images above show the largest variance slices of the map in three orthogonal directions.

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

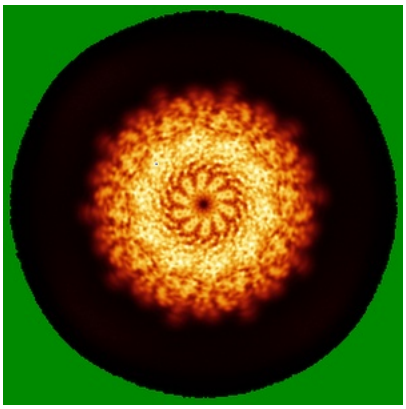
6.4.1 Primary map



X

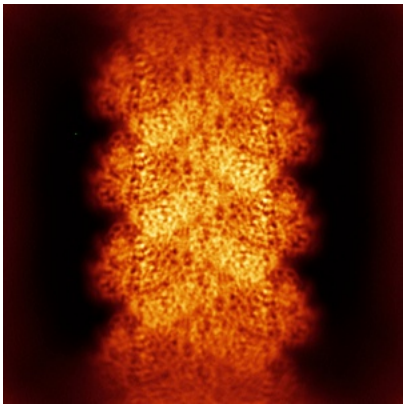


Y

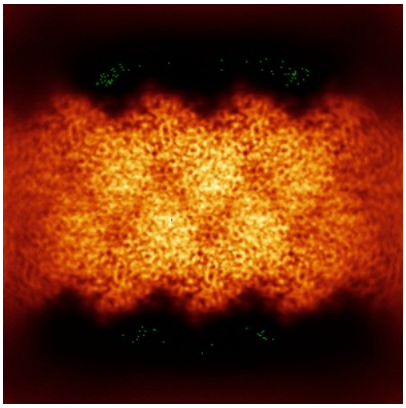


Z

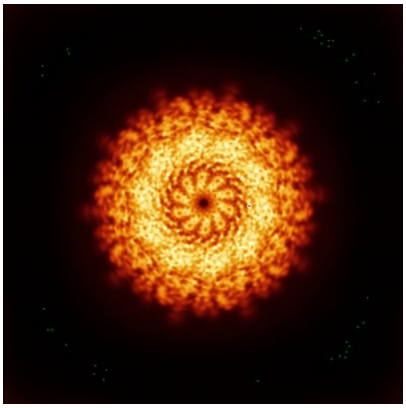
6.4.2 Raw map



X



Y

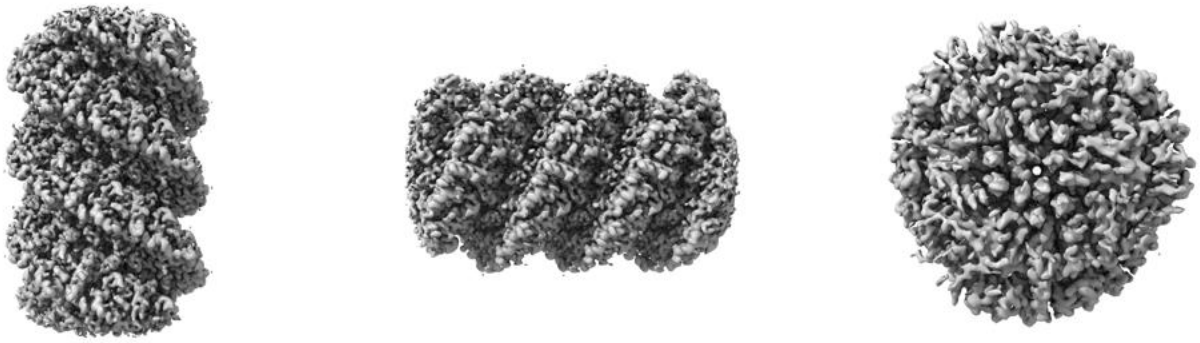


Z

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

6.5 Orthogonal surface views (i)

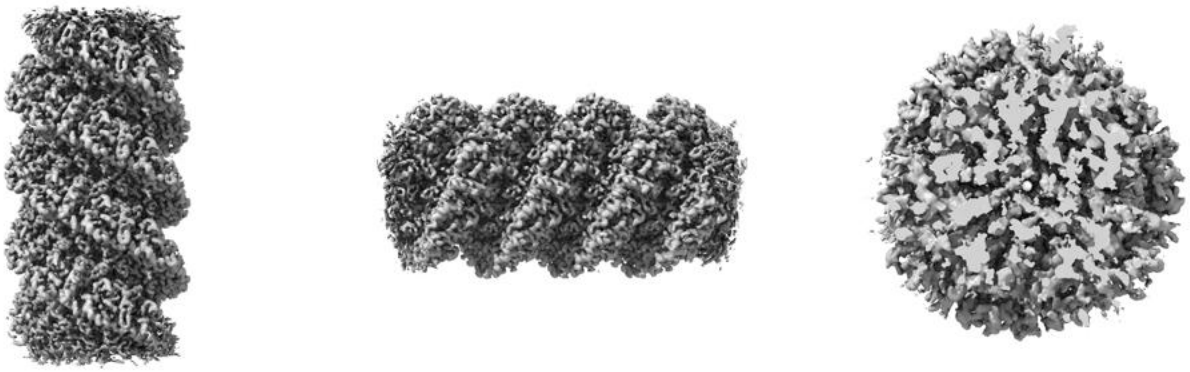
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

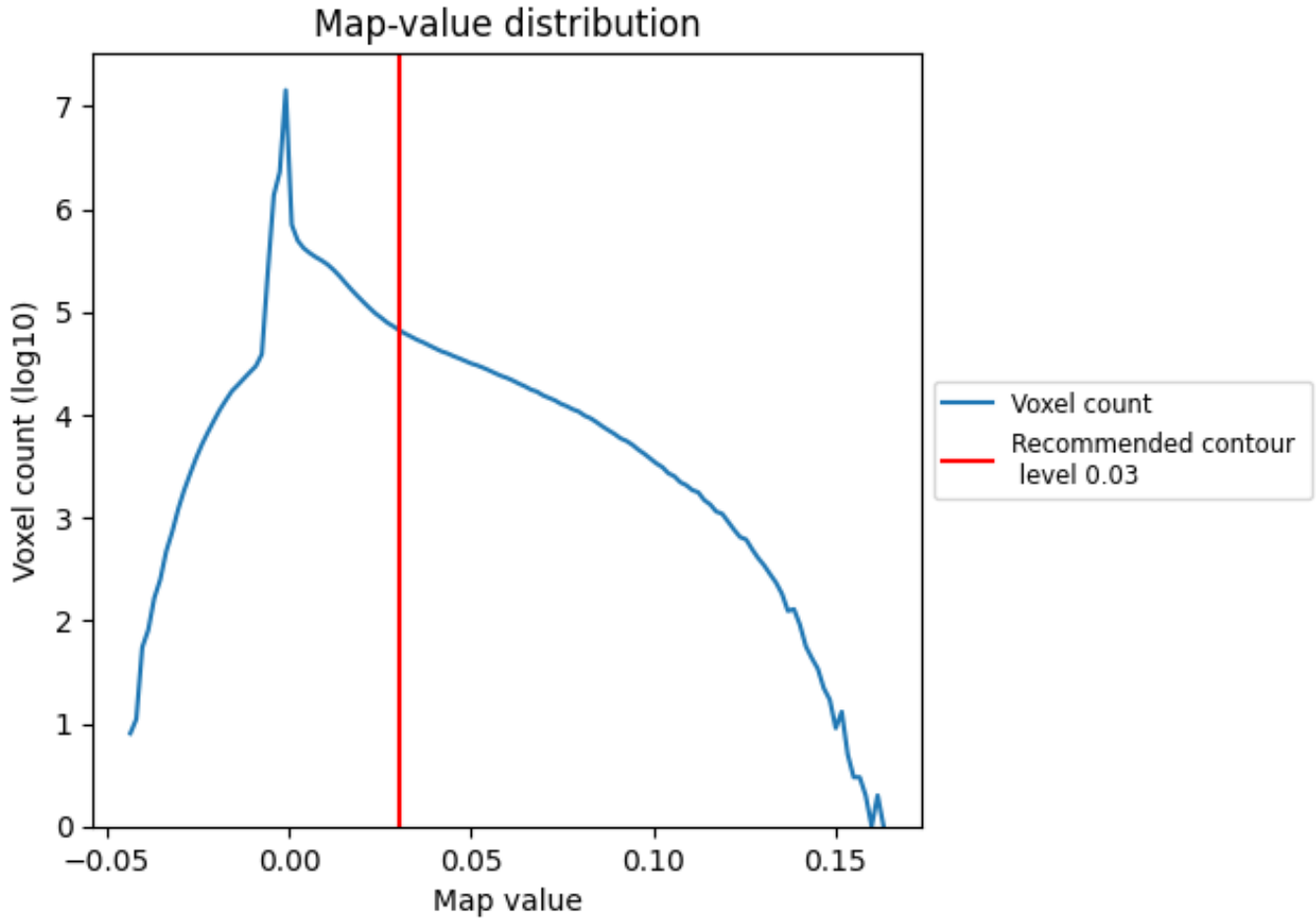
6.6 Mask visualisation (i)

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

7 Map analysis

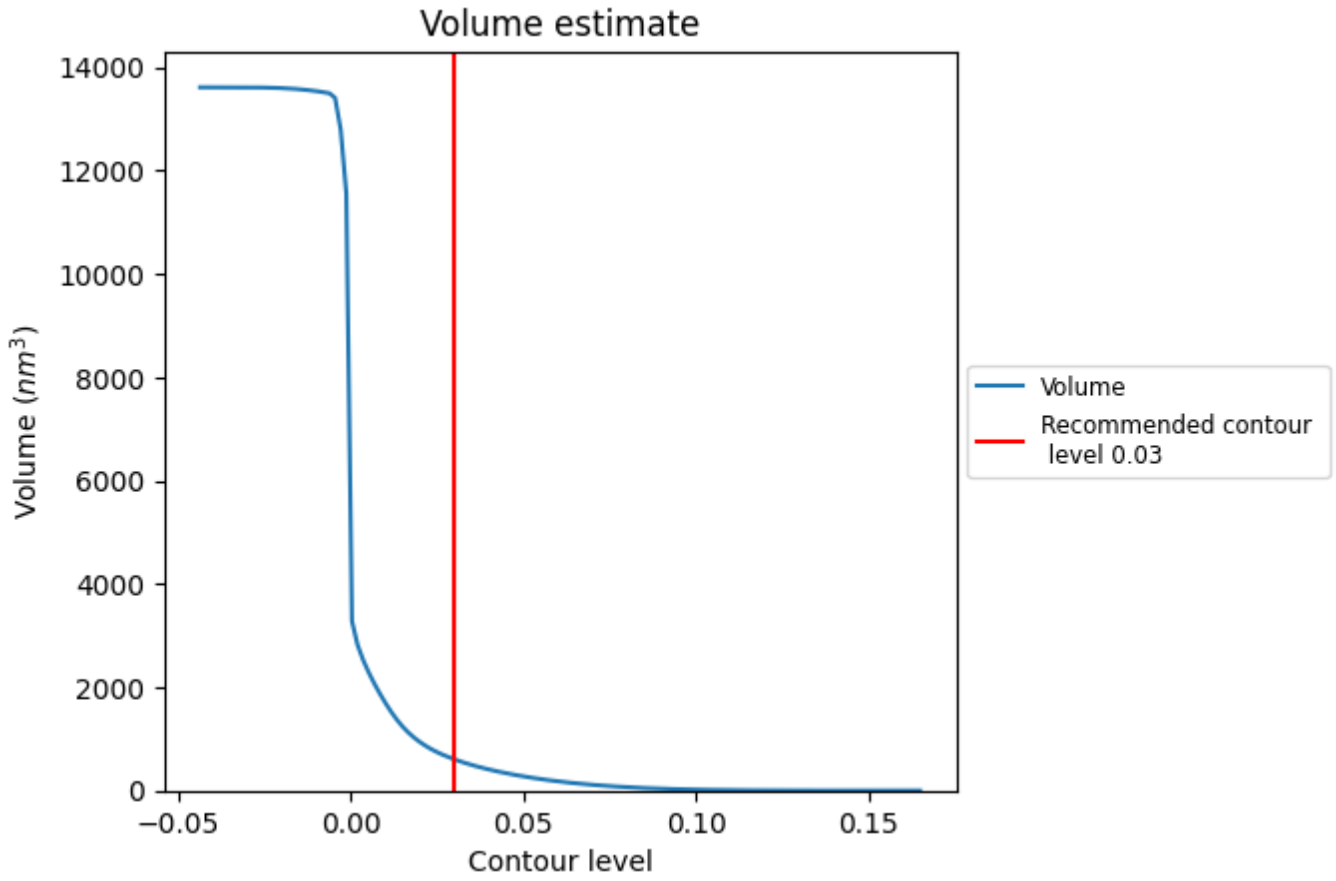
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

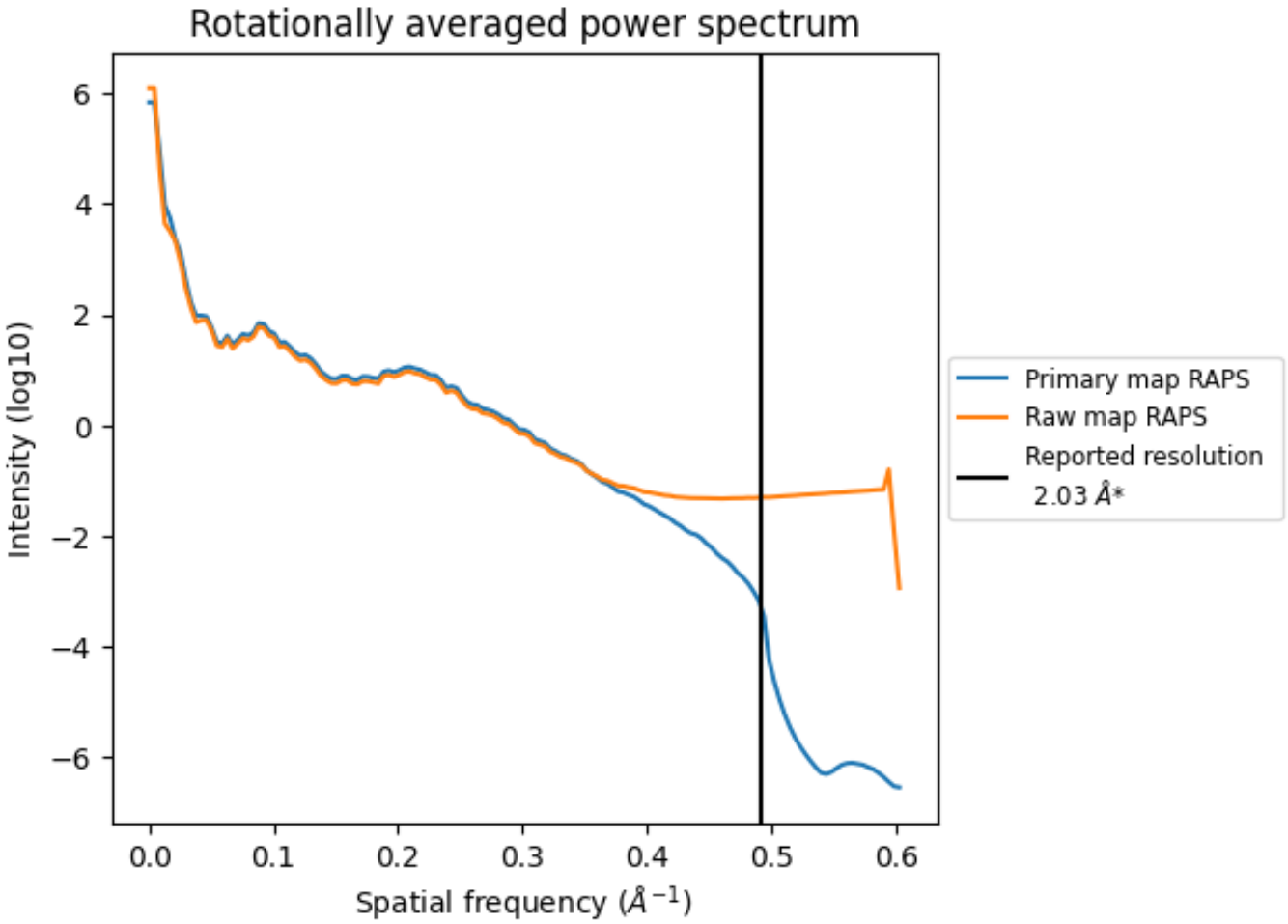
7.2 Volume estimate (i)



The volume at the recommended contour level is 604 nm^3; this corresponds to an approximate mass of 546 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)

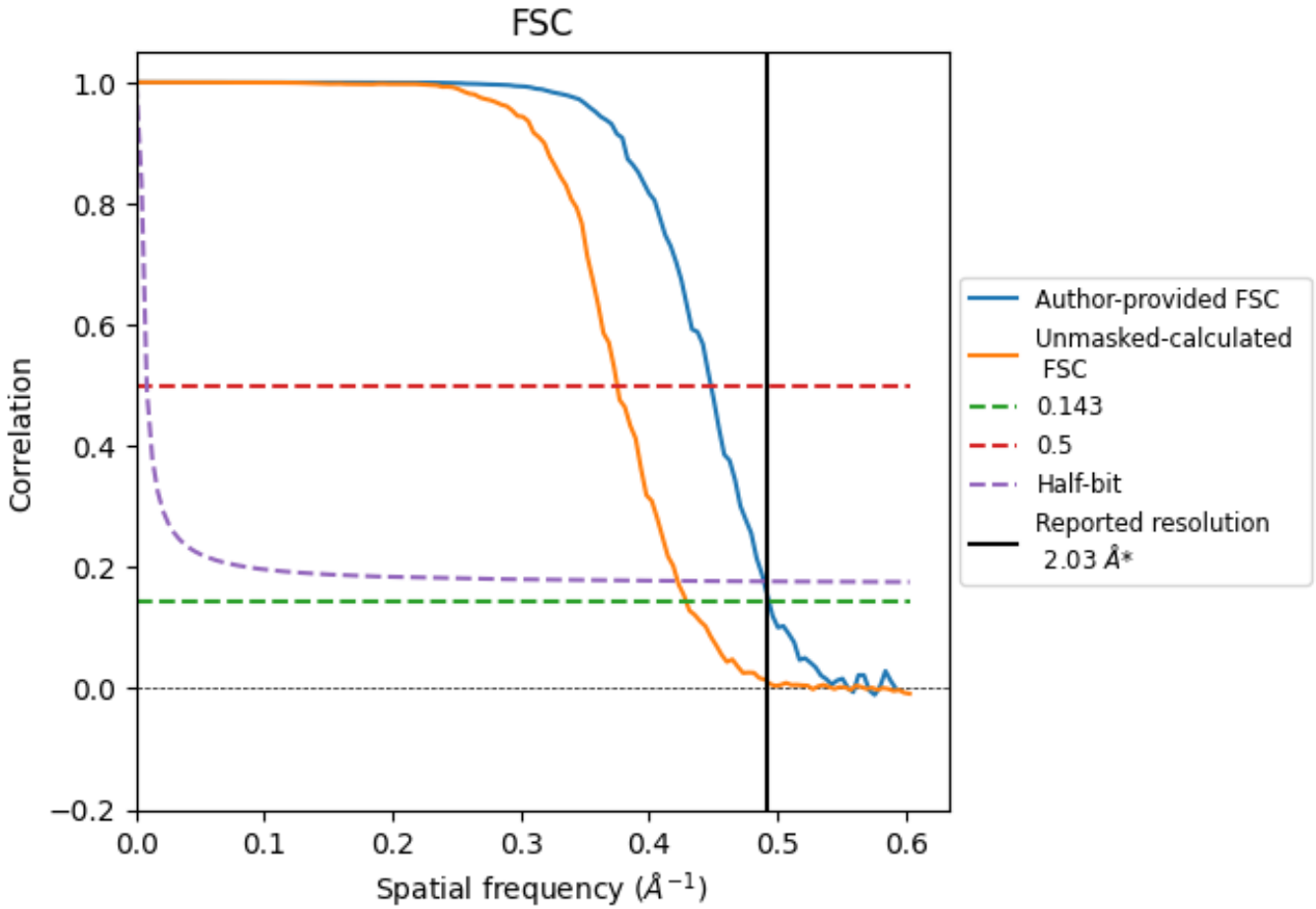


*Reported resolution corresponds to spatial frequency of 0.493 Å^{-1}

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 0.493 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.03	-	-
Author-provided FSC curve	2.03	2.23	2.04
Unmasked-calculated*	2.33	2.67	2.37

*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 2.33 differs from the reported value 2.03 by more than 10 %

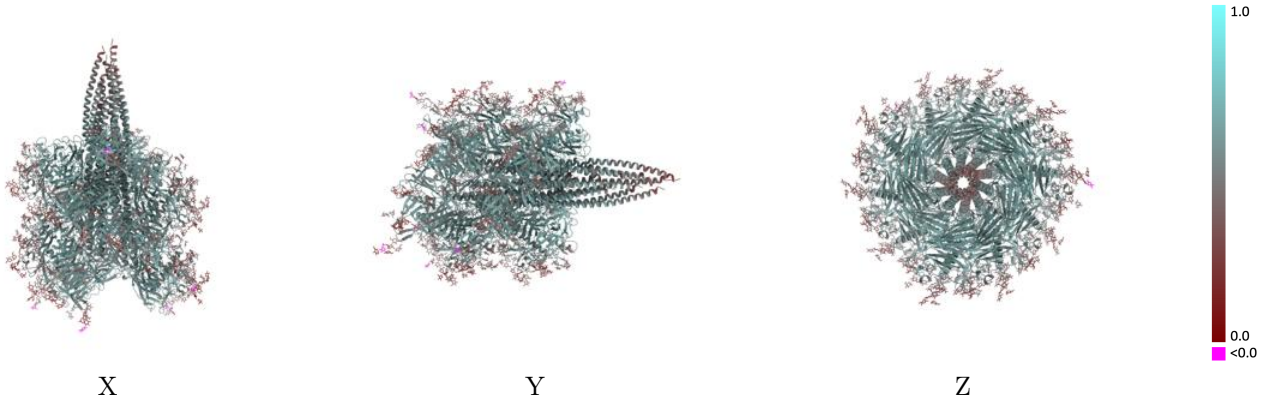
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18700 and PDB model 8QX4. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay

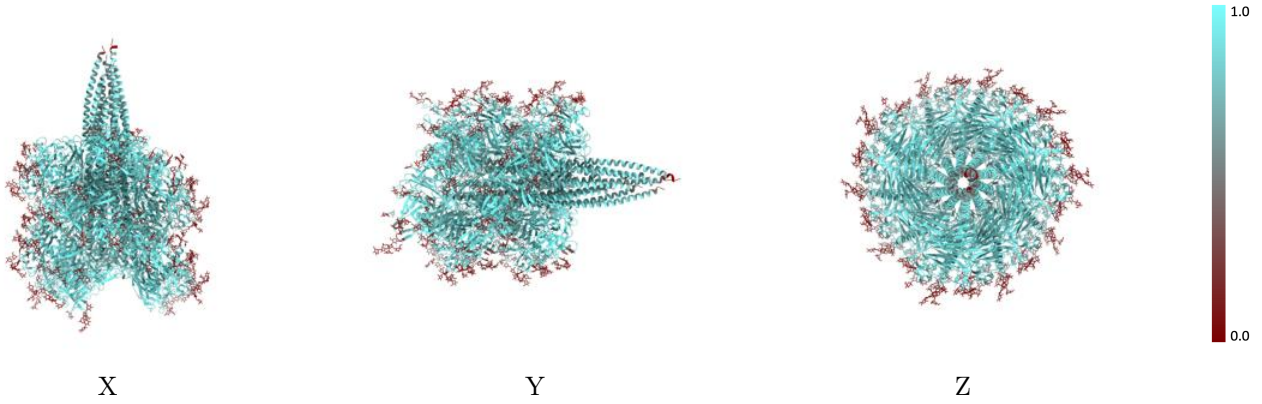
This section was not generated.

9.2 Q-score mapped to coordinate model



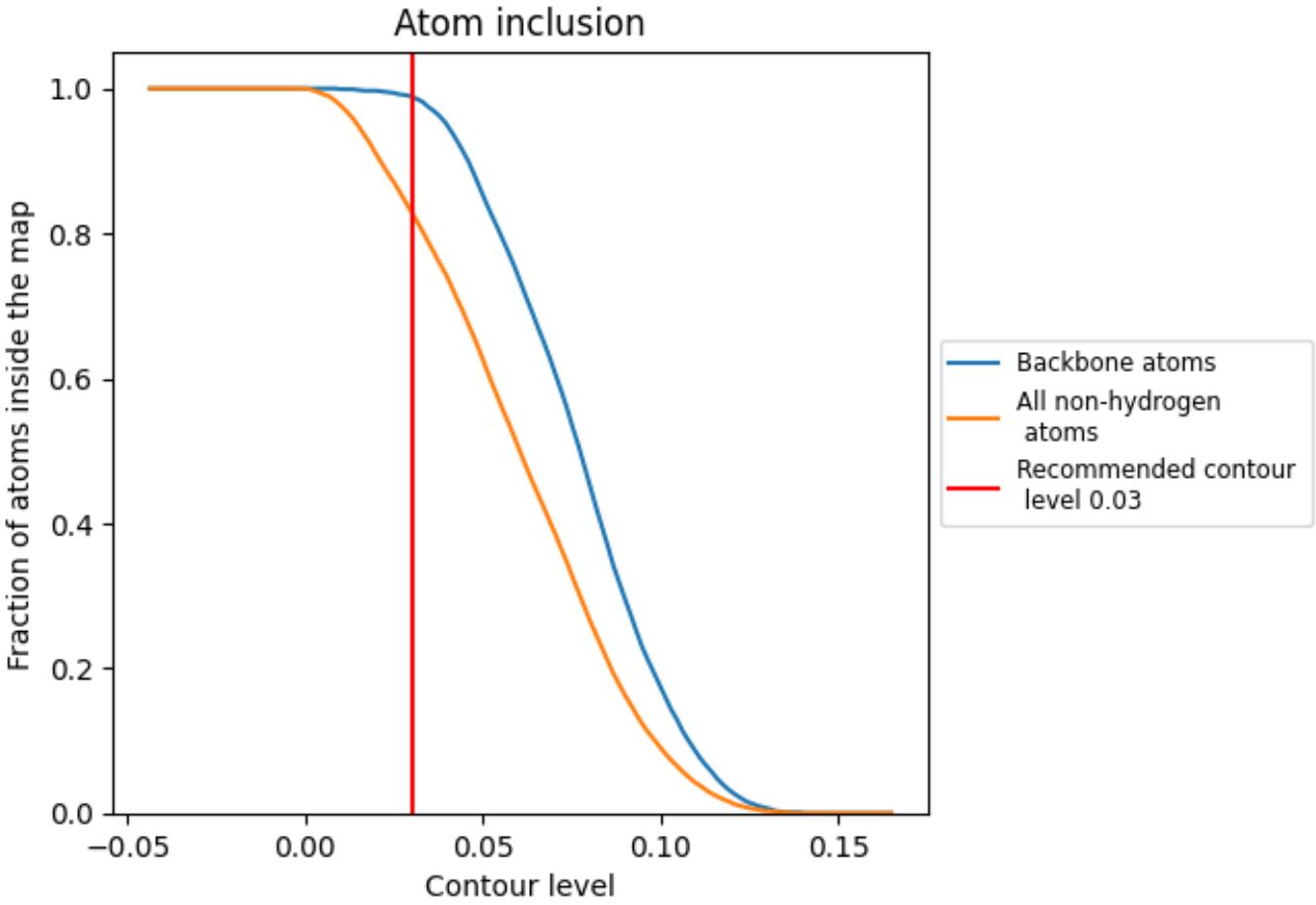
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 83% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.5640
0	0.1470	0.2310
0A	0.2930	0.2560
1	0.5710	0.4760
1A	0.5600	0.4370
2	0.3200	0.3150
2A	0.1410	0.3670
3	0.5600	0.4470
3A	0.4670	0.4500
4	0.1720	0.3860
4A	0.1470	0.2100
5	0.4930	0.4730
5A	0.6070	0.4860
6	0.1330	0.2510
6A	0.2930	0.2440
7	0.5710	0.4620
7A	0.5600	0.4150
8	0.3070	0.3200
8A	0.1410	0.3600
9	0.5600	0.4550
9A	0.4530	0.4430
A	0.9020	0.5930
AA	0.1560	0.3850
AB	0.1470	0.1990
B	0.9090	0.5950
BA	0.4930	0.4550
BB	0.5710	0.4820
C	0.9130	0.5970
CA	0.1330	0.2510
CB	0.2130	0.2140
D	0.9160	0.6020
DA	0.6070	0.4730
DB	0.5600	0.4120
E	0.9160	0.6050
EA	0.3070	0.3140



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Chain	Atom inclusion	Q-score
EB	0.1250	0.3610
F	0.9170	0.6050
FA	0.5600	0.4450
FB	0.4400	0.4580
G	0.9230	0.6060
GA	0.1560	0.3850
GB	0.1330	0.1730
H	0.9210	0.6090
HA	0.4930	0.4680
HB	0.5360	0.4280
I	0.9240	0.6060
IA	0.1330	0.2390
IB	0.1200	0.1620
J	0.9240	0.6070
JA	0.6070	0.4800
JB	0.5600	0.4240
K	0.9230	0.6080
KA	0.3070	0.2880
KB	0.1090	0.3640
L	0.9260	0.6060
LA	0.5730	0.4510
LB	0.4270	0.4550
M	0.9220	0.6020
MA	0.1560	0.3940
MB	0.0530	0.1610
N	0.9230	0.6040
NA	0.4930	0.4500
NB	0.3570	0.3990
O	0.9170	0.6020
OA	0.1330	0.2160
OB	0.0400	0.1370
P	0.9180	0.5970
PA	0.5710	0.4740
PB	0.5330	0.4070
Q	0.9180	0.5960
QA	0.3200	0.2750
R	0.9090	0.5920
RA	0.5730	0.4390
S	0.9100	0.5870
SA	0.1560	0.3730
T	0.8940	0.5820
TA	0.4930	0.4440

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Chain	Atom inclusion	Q-score
U	0.1560	0.3810
UA	0.1330	0.2120
V	0.4930	0.4450
VA	0.5710	0.4900
W	0.1470	0.2350
WA	0.3200	0.2760
X	0.5710	0.4840
XA	0.5600	0.4250
Y	0.2930	0.2940
YA	0.1560	0.3730
Z	0.5730	0.4360
ZA	0.4800	0.4630
a	0.1720	0.3850
aA	0.1330	0.2100
b	0.4800	0.4610
bA	0.5710	0.5080
c	0.1330	0.2130
cA	0.3070	0.2780
d	0.6070	0.4700
dA	0.5600	0.4440
e	0.2930	0.3080
eA	0.1560	0.3810
f	0.5470	0.4420
fA	0.4930	0.4600
g	0.1880	0.3720
gA	0.1470	0.2010
h	0.4800	0.4810
hA	0.5710	0.4840
i	0.1330	0.2130
iA	0.3200	0.2680
j	0.6070	0.4810
jA	0.5600	0.4290
k	0.2930	0.3070
kA	0.1410	0.3710
l	0.5870	0.4570
lA	0.4800	0.4510
m	0.1880	0.3880
mA	0.1470	0.1870
n	0.4930	0.4840
nA	0.6070	0.4720
o	0.1470	0.2220
oA	0.3200	0.2530

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Chain	Atom inclusion	Q-score
p	0.6070	0.4680
pA	0.5600	0.4220
q	0.2930	0.3210
qA	0.1410	0.3730
r	0.5600	0.4570
rA	0.4800	0.4510
s	0.1880	0.3850
sA	0.1470	0.2080
t	0.4930	0.4700
tA	0.6070	0.4890
u	0.1470	0.2230
uA	0.3200	0.2540
v	0.6070	0.4580
vA	0.5600	0.4260
w	0.3070	0.3130
wA	0.1410	0.3630
x	0.5470	0.4420
xA	0.4530	0.4610
y	0.1720	0.3700
yA	0.1470	0.2170
z	0.4930	0.4650
zA	0.5710	0.4730