Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 11:47 AM EDT

PDB ID	:	9NAJ
EMDB ID	:	EMD-49196
Title	:	LuIII VLP - Glycan [3's(LN)3]
Authors	:	Busuttil, K.B.; Bennett, A.B.
Deposited on	:	2025-02-12
Resolution	:	2.66 Å(reported)

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

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

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

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

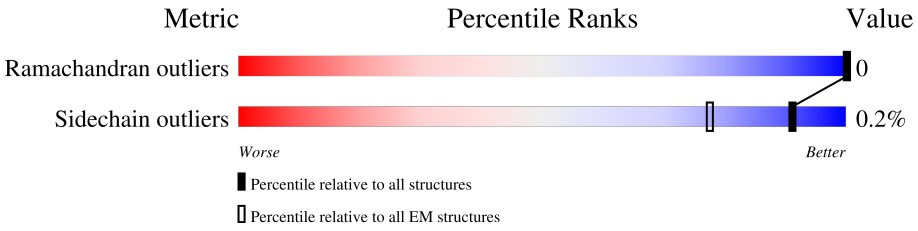
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.66 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	1	551	100%
1	2	551	100%
1	3	551	100%
1	4	551	100%
1	5	551	100%
1	6	551	100%
1	7	551	100%
1	8	551	100%
1	A	551	100%

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Mol	Chain	Length	Quality of chain
1	B	551	100%
1	C	551	100%
1	D	551	100%
1	E	551	100%
1	F	551	100%
1	G	551	100%
1	H	551	100%
1	I	551	100%
1	J	551	100%
1	K	551	100%
1	L	551	100%
1	M	551	100%
1	N	551	100%
1	O	551	100%
1	P	551	100%
1	Q	551	100%
1	R	551	100%
1	S	551	100%
1	T	551	100%
1	U	551	100%
1	V	551	100%
1	W	551	100%
1	X	551	100%
1	Y	551	100%
1	Z	551	100%

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Mol	Chain	Length	Quality of chain
1	a	551	100%
1	b	551	100%
1	c	551	100%
1	d	551	100%
1	e	551	100%
1	f	551	100%
1	g	551	100%
1	h	551	100%
1	i	551	100%
1	j	551	100%
1	k	551	100%
1	l	551	100%
1	m	551	100%
1	n	551	100%
1	o	551	100%
1	p	551	100%
1	q	551	100%
1	r	551	100%
1	s	551	100%
1	t	551	100%
1	u	551	100%
1	v	551	100%
1	w	551	100%
1	x	551	100%
1	y	551	100%

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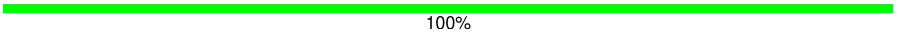
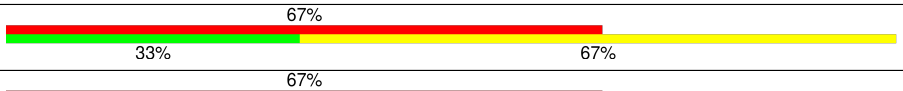
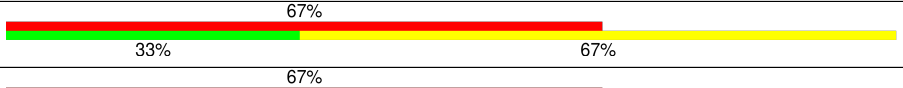
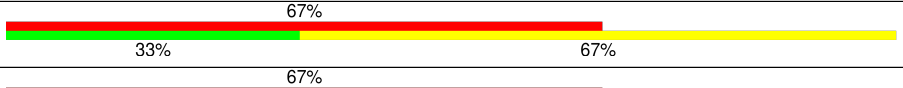
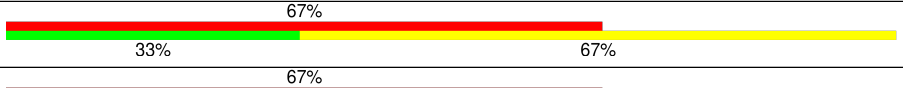
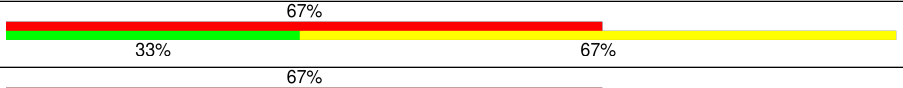
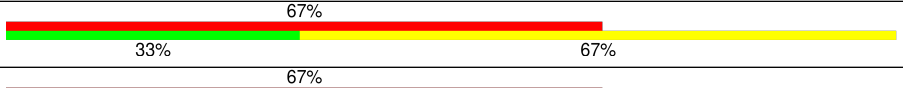
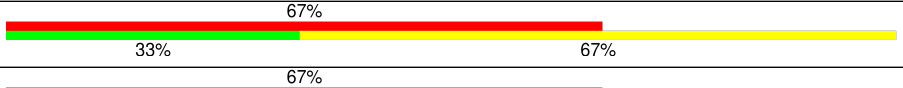
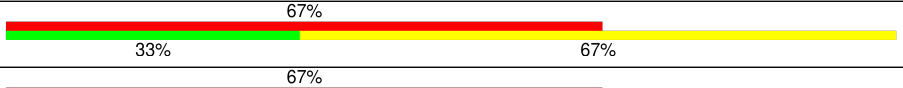
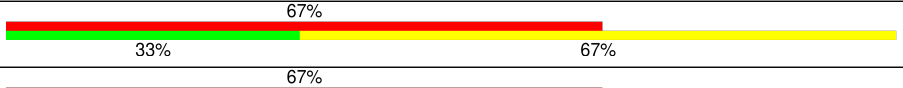
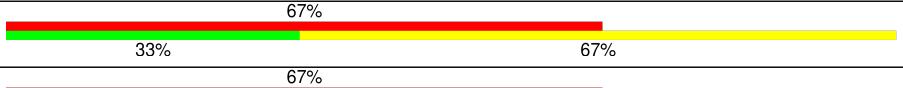
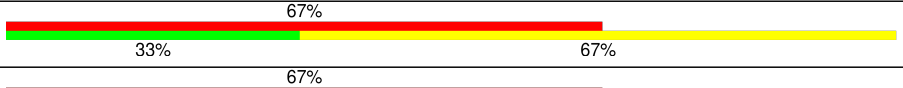
Mol	Chain	Length	Quality of chain
1	z	551	
2	0	3	
2	0A	3	
2	1B	3	
2	3A	3	
2	4B	3	
2	6A	3	
2	7B	3	
2	9A	3	
2	AC	3	
2	BA	3	
2	CB	3	
2	DC	3	
2	EA	3	
2	FB	3	
2	GC	3	
2	HA	3	
2	IB	3	
2	JC	3	
2	KA	3	
2	LB	3	
2	MC	3	
2	NA	3	
2	OB	3	
2	PC	3	

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Mol	Chain	Length	Quality of chain
2	QA	3	67% 33% 67%
2	RB	3	67% 33% 67%
2	SC	3	67% 33% 67%
2	TA	3	67% 33% 67%
2	UB	3	67% 33% 67%
2	VC	3	67% 33% 67%
2	WA	3	67% 33% 67%
2	XB	3	67% 33% 67%
2	YC	3	67% 33% 67%
2	ZA	3	67% 33% 67%
2	aB	3	67% 33% 67%
2	bC	3	67% 33% 67%
2	cA	3	67% 33% 67%
2	dB	3	67% 33% 67%
2	eC	3	67% 33% 67%
2	fA	3	67% 33% 67%
2	gB	3	67% 33% 67%
2	hC	3	67% 33% 67%
2	iA	3	67% 33% 67%
2	jB	3	67% 33% 67%
2	kC	3	67% 33% 67%
2	lA	3	67% 33% 67%
2	mB	3	67% 33% 67%
2	nC	3	67% 33% 67%
2	oA	3	67% 33% 67%

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Mol	Chain	Length	Quality of chain
2	pB	3	67% 33% 67%
2	qC	3	67% 33% 67%
2	rA	3	67% 33% 67%
2	sB	3	67% 33% 67%
2	tC	3	67% 33% 67%
2	uA	3	67% 33% 67%
2	vB	3	67% 33% 67%
2	wC	3	67% 33% 67%
2	xA	3	67% 33% 67%
2	yB	3	67% 33% 67%
2	zC	3	67% 33% 67%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 266820 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	B	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	C	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	D	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	E	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	F	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	G	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	H	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	I	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	J	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	K	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	L	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	M	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	N	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	O	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	P	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	Q	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	S	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	T	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	U	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	V	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	W	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	X	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	Y	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	Z	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	a	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	b	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	c	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	d	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	e	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	f	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	g	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	h	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	i	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	j	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	k	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	l	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	n	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	o	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	p	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	q	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	r	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	s	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	t	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	u	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	v	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	w	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	x	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	y	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	z	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	1	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	2	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	3	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	4	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	5	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	6	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	7	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		

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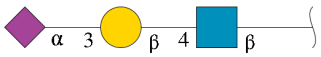
Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	0	3	Total	C	N	O	0	0
			46	25	2	19		
2	BA	3	Total	C	N	O	0	0
			46	25	2	19		
2	EA	3	Total	C	N	O	0	0
			46	25	2	19		
2	HA	3	Total	C	N	O	0	0
			46	25	2	19		
2	KA	3	Total	C	N	O	0	0
			46	25	2	19		
2	NA	3	Total	C	N	O	0	0
			46	25	2	19		
2	QA	3	Total	C	N	O	0	0
			46	25	2	19		
2	TA	3	Total	C	N	O	0	0
			46	25	2	19		
2	WA	3	Total	C	N	O	0	0
			46	25	2	19		
2	ZA	3	Total	C	N	O	0	0
			46	25	2	19		
2	cA	3	Total	C	N	O	0	0
			46	25	2	19		
2	fA	3	Total	C	N	O	0	0
			46	25	2	19		
2	iA	3	Total	C	N	O	0	0
			46	25	2	19		
2	lA	3	Total	C	N	O	0	0
			46	25	2	19		
2	oA	3	Total	C	N	O	0	0
			46	25	2	19		
2	rA	3	Total	C	N	O	0	0
			46	25	2	19		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	uA	3	Total	C	N	O	0	0
			46	25	2	19		
2	xA	3	Total	C	N	O	0	0
			46	25	2	19		
2	0A	3	Total	C	N	O	0	0
			46	25	2	19		
2	3A	3	Total	C	N	O	0	0
			46	25	2	19		
2	6A	3	Total	C	N	O	0	0
			46	25	2	19		
2	9A	3	Total	C	N	O	0	0
			46	25	2	19		
2	CB	3	Total	C	N	O	0	0
			46	25	2	19		
2	FB	3	Total	C	N	O	0	0
			46	25	2	19		
2	IB	3	Total	C	N	O	0	0
			46	25	2	19		
2	LB	3	Total	C	N	O	0	0
			46	25	2	19		
2	OB	3	Total	C	N	O	0	0
			46	25	2	19		
2	RB	3	Total	C	N	O	0	0
			46	25	2	19		
2	UB	3	Total	C	N	O	0	0
			46	25	2	19		
2	XB	3	Total	C	N	O	0	0
			46	25	2	19		
2	aB	3	Total	C	N	O	0	0
			46	25	2	19		
2	dB	3	Total	C	N	O	0	0
			46	25	2	19		
2	gB	3	Total	C	N	O	0	0
			46	25	2	19		
2	jB	3	Total	C	N	O	0	0
			46	25	2	19		
2	mB	3	Total	C	N	O	0	0
			46	25	2	19		
2	pB	3	Total	C	N	O	0	0
			46	25	2	19		
2	sB	3	Total	C	N	O	0	0
			46	25	2	19		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	vB	3	Total	C	N	O	0	0
			46	25	2	19		
2	yB	3	Total	C	N	O	0	0
			46	25	2	19		
2	1B	3	Total	C	N	O	0	0
			46	25	2	19		
2	4B	3	Total	C	N	O	0	0
			46	25	2	19		
2	7B	3	Total	C	N	O	0	0
			46	25	2	19		
2	AC	3	Total	C	N	O	0	0
			46	25	2	19		
2	DC	3	Total	C	N	O	0	0
			46	25	2	19		
2	GC	3	Total	C	N	O	0	0
			46	25	2	19		
2	JC	3	Total	C	N	O	0	0
			46	25	2	19		
2	MC	3	Total	C	N	O	0	0
			46	25	2	19		
2	PC	3	Total	C	N	O	0	0
			46	25	2	19		
2	SC	3	Total	C	N	O	0	0
			46	25	2	19		
2	VC	3	Total	C	N	O	0	0
			46	25	2	19		
2	YC	3	Total	C	N	O	0	0
			46	25	2	19		
2	bC	3	Total	C	N	O	0	0
			46	25	2	19		
2	eC	3	Total	C	N	O	0	0
			46	25	2	19		
2	hC	3	Total	C	N	O	0	0
			46	25	2	19		
2	kC	3	Total	C	N	O	0	0
			46	25	2	19		
2	nC	3	Total	C	N	O	0	0
			46	25	2	19		
2	qC	3	Total	C	N	O	0	0
			46	25	2	19		
2	tC	3	Total	C	N	O	0	0
			46	25	2	19		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	wC	3	Total	C	N	O	0	0
			46	25	2	19		
2	zC	3	Total	C	N	O	0	0
			46	25	2	19		

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: Capsid protein VP1

Chain A:

- Molecule 1: Capsid protein VP1

Chain B:

- Molecule 1: Capsid protein VP1

Chain C:

- Molecule 1: Capsid protein VP1

Chain D:

- Molecule 1: Capsid protein VP1

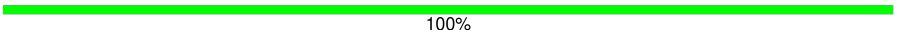
Chain E:

- Molecule 1: Capsid protein VP1

Chain F:

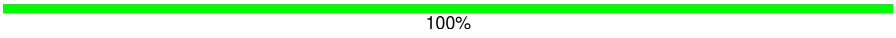
- Molecule 1: Capsid protein VP1

Chain G:



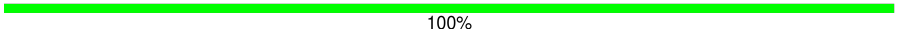
- Molecule 1: Capsid protein VP1

Chain H:



- Molecule 1: Capsid protein VP1

Chain I:

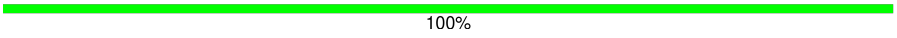


- Molecule 1: Capsid protein VP1

Chain J:

- Molecule 1: Capsid protein VP1

Chain K:



- Molecule 1: Capsid protein VP1

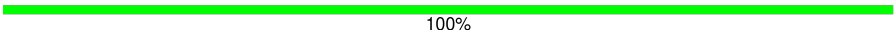
Chain L:

- Molecule 1: Capsid protein VP1

Chain M:

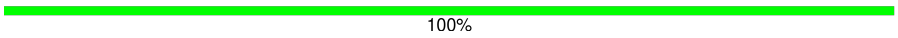
• Molecule 1: Capsid protein VP1

Chain N:



• Molecule 1: Capsid protein VP1

Chain O:

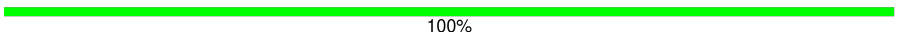


• Molecule 1: Capsid protein VP1

Chain P:

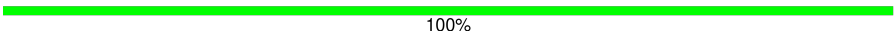
• Molecule 1: Capsid protein VP1

Chain Q:



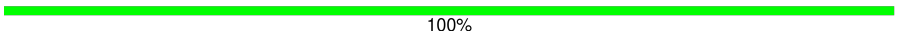
• Molecule 1: Capsid protein VP1

Chain R:



• Molecule 1: Capsid protein VP1

Chain S:

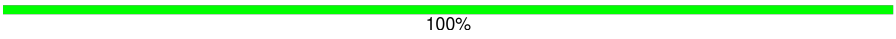


• Molecule 1: Capsid protein VP1

Chain T:

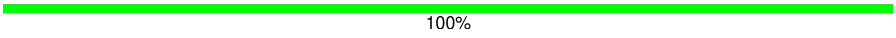
- Molecule 1: Capsid protein VP1

Chain U:



- Molecule 1: Capsid protein VP1

Chain V:

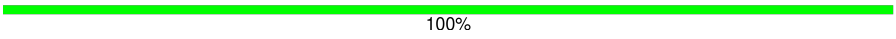


- Molecule 1: Capsid protein VP1

Chain W:

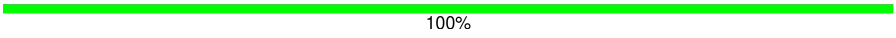
- Molecule 1: Capsid protein VP1

Chain X:



- Molecule 1: Capsid protein VP1

Chain Y:



- Molecule 1: Capsid protein VP1

Chain Z:

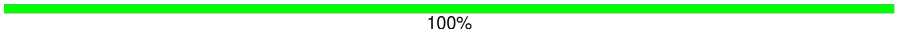
- Molecule 1: Capsid protein VP1

Chain a: 

• Molecule 1: Capsid protein VP1

Chain b: 

• Molecule 1: Capsid protein VP1

Chain c: 

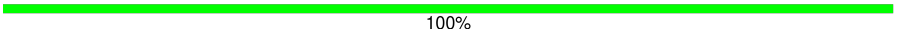
• Molecule 1: Capsid protein VP1

Chain d: 

• Molecule 1: Capsid protein VP1

Chain e: 

• Molecule 1: Capsid protein VP1

Chain f: 

• Molecule 1: Capsid protein VP1

Chain g: 

• Molecule 1: Capsid protein VP1

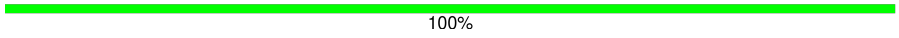
Chain h:

• Molecule 1: Capsid protein VP1

Chain i:

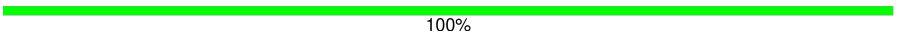
• Molecule 1: Capsid protein VP1

Chain j:



• Molecule 1: Capsid protein VP1

Chain k:

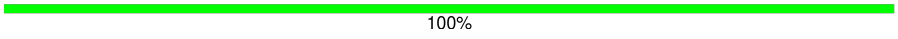


• Molecule 1: Capsid protein VP1

Chain l:

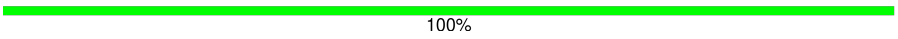
• Molecule 1: Capsid protein VP1

Chain m:



• Molecule 1: Capsid protein VP1

Chain n:

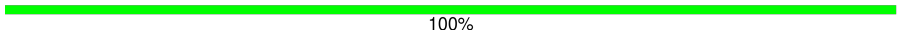


• Molecule 1: Capsid protein VP1

Chain o:

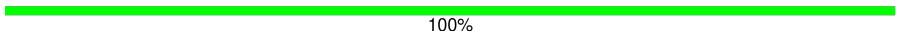
- Molecule 1: Capsid protein VP1

Chain p:



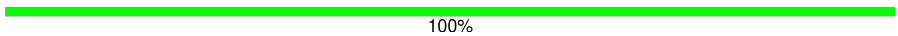
- Molecule 1: Capsid protein VP1

Chain q:



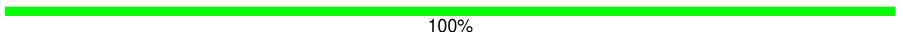
- Molecule 1: Capsid protein VP1

Chain r:



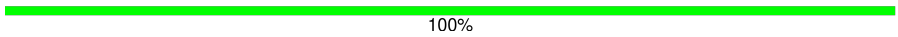
- Molecule 1: Capsid protein VP1

Chain s:



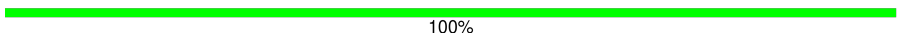
- Molecule 1: Capsid protein VP1

Chain t:



- Molecule 1: Capsid protein VP1

Chain u:



- Molecule 1: Capsid protein VP1

Chain v: 100%

• Molecule 1: Capsid protein VP1

Chain w: 100%

• Molecule 1: Capsid protein VP1

Chain x: 100%

• Molecule 1: Capsid protein VP1

Chain y: 100%

• Molecule 1: Capsid protein VP1

Chain z: 100%

• Molecule 1: Capsid protein VP1

Chain 1: 100%

• Molecule 1: Capsid protein VP1

Chain 2: 100%

• Molecule 1: Capsid protein VP1

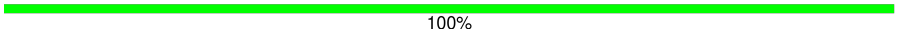
Chain 3:

• Molecule 1: Capsid protein VP1

Chain 4:

• Molecule 1: Capsid protein VP1

Chain 5:



• Molecule 1: Capsid protein VP1

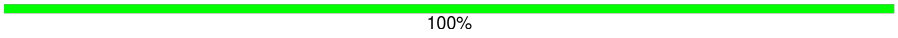
Chain 6:

• Molecule 1: Capsid protein VP1

Chain 7:

• Molecule 1: Capsid protein VP1

Chain 8:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain QA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain WA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain ZA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain cA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain iA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain lA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain rA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain uA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain xA:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0A:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3A:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6A:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9A:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain UB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain XB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain dB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain gB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain jB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain mB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain vB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain yB:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1B:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4B:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7B:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain VC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain YC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain hC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain kC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain nC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain qC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain tC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain wC:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain zC:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38079	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 ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	890	Depositor
Maximum defocus (nm)	3110	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	17.398	Depositor
Minimum map value	-9.306	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	441.84003, 441.84003, 441.84003	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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, SIA, GAL

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	1	0.53	0/4530	0.54	0/6196
1	2	0.53	0/4530	0.54	0/6196
1	3	0.53	0/4530	0.54	0/6196
1	4	0.53	0/4530	0.54	0/6196
1	5	0.53	0/4530	0.54	0/6196
1	6	0.53	0/4530	0.54	0/6196
1	7	0.53	0/4530	0.54	0/6196
1	8	0.53	0/4530	0.54	0/6196
1	A	0.53	0/4530	0.54	0/6196
1	B	0.53	0/4530	0.54	0/6196
1	C	0.53	0/4530	0.54	0/6196
1	D	0.53	0/4530	0.54	0/6196
1	E	0.53	0/4530	0.54	0/6196
1	F	0.53	0/4530	0.54	0/6196
1	G	0.53	0/4530	0.54	0/6196
1	H	0.53	0/4530	0.54	0/6196
1	I	0.53	0/4530	0.54	0/6196
1	J	0.53	0/4530	0.54	0/6196
1	K	0.53	0/4530	0.54	0/6196
1	L	0.53	0/4530	0.54	0/6196
1	M	0.53	0/4530	0.54	0/6196
1	N	0.53	0/4530	0.54	0/6196
1	O	0.53	0/4530	0.54	0/6196
1	P	0.53	0/4530	0.54	0/6196
1	Q	0.53	0/4530	0.54	0/6196
1	R	0.53	0/4530	0.54	0/6196
1	S	0.53	0/4530	0.54	0/6196
1	T	0.53	0/4530	0.54	0/6196
1	U	0.53	0/4530	0.54	0/6196
1	V	0.53	0/4530	0.54	0/6196
1	W	0.53	0/4530	0.54	0/6196
1	X	0.53	0/4530	0.54	0/6196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	Y	0.53	0/4530	0.54	0/6196
1	Z	0.53	0/4530	0.54	0/6196
1	a	0.53	0/4530	0.54	0/6196
1	b	0.53	0/4530	0.54	0/6196
1	c	0.53	0/4530	0.54	0/6196
1	d	0.53	0/4530	0.54	0/6196
1	e	0.53	0/4530	0.54	0/6196
1	f	0.53	0/4530	0.54	0/6196
1	g	0.53	0/4530	0.54	0/6196
1	h	0.53	0/4530	0.54	0/6196
1	i	0.53	0/4530	0.54	0/6196
1	j	0.53	0/4530	0.54	0/6196
1	k	0.53	0/4530	0.54	0/6196
1	l	0.53	0/4530	0.54	0/6196
1	m	0.53	0/4530	0.54	0/6196
1	n	0.53	0/4530	0.54	0/6196
1	o	0.53	0/4530	0.54	0/6196
1	p	0.53	0/4530	0.54	0/6196
1	q	0.53	0/4530	0.54	0/6196
1	r	0.53	0/4530	0.54	0/6196
1	s	0.53	0/4530	0.54	0/6196
1	t	0.53	0/4530	0.54	0/6196
1	u	0.53	0/4530	0.54	0/6196
1	v	0.53	0/4530	0.54	0/6196
1	w	0.53	0/4530	0.54	0/6196
1	x	0.53	0/4530	0.54	0/6196
1	y	0.53	0/4530	0.54	0/6196
1	z	0.53	0/4530	0.54	0/6196
All	All	0.53	0/271800	0.54	0/371760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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	1	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	2	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	3	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	4	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	5	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	6	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	7	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	8	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	A	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	B	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	C	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	D	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	E	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	F	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	G	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	H	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	I	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	J	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	K	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	L	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	M	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	N	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	O	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	P	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	Q	550/551 (100%)	540 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	S	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	T	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	U	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	V	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	W	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	X	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	Y	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	Z	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	a	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	b	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	c	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	d	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	e	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	f	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	g	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	h	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	i	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	j	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	k	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	l	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	m	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	n	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	o	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	p	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	q	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	r	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	s	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	t	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	u	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	v	550/551 (100%)	540 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	x	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	y	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	z	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
All	All	33000/33060 (100%)	32391 (98%)	609 (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	1	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	2	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	3	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	4	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	5	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	6	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	7	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	8	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	A	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	B	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	C	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	D	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	E	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	F	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	G	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	H	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	I	480/479 (100%)	479 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	K	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	L	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	M	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	N	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	O	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	P	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	Q	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	R	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	S	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	T	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	U	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	V	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	W	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	X	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	Y	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	Z	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	a	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	b	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	c	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	d	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	e	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	f	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	g	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	h	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	i	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	j	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	k	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	l	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	m	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	n	480/479 (100%)	479 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	p	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	q	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	r	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	s	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	t	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	u	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	v	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	w	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	x	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	y	480/479 (100%)	479 (100%)	1 (0%)	92	97
1	z	480/479 (100%)	479 (100%)	1 (0%)	92	97
All	All	28800/28740 (100%)	28740 (100%)	60 (0%)	91	97

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	LEU
1	B	480	LEU
1	C	480	LEU
1	D	480	LEU
1	E	480	LEU
1	F	480	LEU
1	G	480	LEU
1	H	480	LEU
1	I	480	LEU
1	J	480	LEU
1	K	480	LEU
1	L	480	LEU
1	M	480	LEU
1	N	480	LEU
1	O	480	LEU
1	P	480	LEU
1	Q	480	LEU
1	R	480	LEU
1	S	480	LEU
1	T	480	LEU
1	U	480	LEU

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Mol	Chain	Res	Type
1	V	480	LEU
1	W	480	LEU
1	X	480	LEU
1	Y	480	LEU
1	Z	480	LEU
1	a	480	LEU
1	b	480	LEU
1	c	480	LEU
1	d	480	LEU
1	e	480	LEU
1	f	480	LEU
1	g	480	LEU
1	h	480	LEU
1	i	480	LEU
1	j	480	LEU
1	k	480	LEU
1	l	480	LEU
1	m	480	LEU
1	n	480	LEU
1	o	480	LEU
1	p	480	LEU
1	q	480	LEU
1	r	480	LEU
1	s	480	LEU
1	t	480	LEU
1	u	480	LEU
1	v	480	LEU
1	w	480	LEU
1	x	480	LEU
1	y	480	LEU
1	z	480	LEU
1	1	480	LEU
1	2	480	LEU
1	3	480	LEU
1	4	480	LEU
1	5	480	LEU
1	6	480	LEU
1	7	480	LEU
1	8	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	74	ASN
1	A	80	ASN
1	A	149	ASN
1	A	251	ASN
1	A	287	HIS
1	A	342	HIS
1	A	368	HIS
1	A	381	GLN
1	A	391	ASN
1	A	409	ASN
1	A	430	ASN
1	A	441	HIS
1	A	457	HIS
1	A	495	GLN
1	A	511	ASN
1	A	547	GLN
1	A	552	ASN
1	A	585	ASN
1	B	49	ASN
1	B	74	ASN
1	B	80	ASN
1	B	149	ASN
1	B	251	ASN
1	B	287	HIS
1	B	342	HIS
1	B	368	HIS
1	B	381	GLN
1	B	391	ASN
1	B	409	ASN
1	B	430	ASN
1	B	441	HIS
1	B	457	HIS
1	B	495	GLN
1	B	511	ASN
1	B	547	GLN
1	B	552	ASN
1	B	585	ASN
1	C	49	ASN
1	C	74	ASN
1	C	80	ASN
1	C	149	ASN
1	C	251	ASN

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Mol	Chain	Res	Type
1	C	287	HIS
1	C	342	HIS
1	C	368	HIS
1	C	381	GLN
1	C	391	ASN
1	C	409	ASN
1	C	430	ASN
1	C	441	HIS
1	C	457	HIS
1	C	495	GLN
1	C	511	ASN
1	C	547	GLN
1	C	552	ASN
1	C	585	ASN
1	D	49	ASN
1	D	74	ASN
1	D	80	ASN
1	D	149	ASN
1	D	251	ASN
1	D	287	HIS
1	D	342	HIS
1	D	368	HIS
1	D	381	GLN
1	D	391	ASN
1	D	409	ASN
1	D	430	ASN
1	D	441	HIS
1	D	457	HIS
1	D	495	GLN
1	D	511	ASN
1	D	547	GLN
1	D	552	ASN
1	D	585	ASN
1	E	49	ASN
1	E	74	ASN
1	E	80	ASN
1	E	149	ASN
1	E	251	ASN
1	E	287	HIS
1	E	342	HIS
1	E	368	HIS
1	E	381	GLN

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Mol	Chain	Res	Type
1	E	391	ASN
1	E	409	ASN
1	E	430	ASN
1	E	441	HIS
1	E	457	HIS
1	E	495	GLN
1	E	511	ASN
1	E	547	GLN
1	E	552	ASN
1	E	585	ASN
1	F	49	ASN
1	F	74	ASN
1	F	80	ASN
1	F	149	ASN
1	F	251	ASN
1	F	287	HIS
1	F	342	HIS
1	F	368	HIS
1	F	381	GLN
1	F	391	ASN
1	F	409	ASN
1	F	430	ASN
1	F	441	HIS
1	F	457	HIS
1	F	495	GLN
1	F	511	ASN
1	F	547	GLN
1	F	552	ASN
1	F	585	ASN
1	G	49	ASN
1	G	74	ASN
1	G	80	ASN
1	G	149	ASN
1	G	251	ASN
1	G	287	HIS
1	G	342	HIS
1	G	368	HIS
1	G	381	GLN
1	G	391	ASN
1	G	409	ASN
1	G	430	ASN
1	G	441	HIS

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Mol	Chain	Res	Type
1	G	457	HIS
1	G	495	GLN
1	G	511	ASN
1	G	547	GLN
1	G	552	ASN
1	G	585	ASN
1	H	49	ASN
1	H	74	ASN
1	H	80	ASN
1	H	149	ASN
1	H	251	ASN
1	H	287	HIS
1	H	342	HIS
1	H	368	HIS
1	H	381	GLN
1	H	391	ASN
1	H	409	ASN
1	H	430	ASN
1	H	441	HIS
1	H	457	HIS
1	H	495	GLN
1	H	511	ASN
1	H	547	GLN
1	H	552	ASN
1	H	585	ASN
1	I	49	ASN
1	I	74	ASN
1	I	80	ASN
1	I	149	ASN
1	I	251	ASN
1	I	287	HIS
1	I	342	HIS
1	I	368	HIS
1	I	381	GLN
1	I	391	ASN
1	I	409	ASN
1	I	430	ASN
1	I	441	HIS
1	I	457	HIS
1	I	495	GLN
1	I	511	ASN
1	I	547	GLN

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Mol	Chain	Res	Type
1	I	552	ASN
1	I	585	ASN
1	J	49	ASN
1	J	74	ASN
1	J	80	ASN
1	J	149	ASN
1	J	251	ASN
1	J	287	HIS
1	J	342	HIS
1	J	368	HIS
1	J	381	GLN
1	J	391	ASN
1	J	409	ASN
1	J	430	ASN
1	J	441	HIS
1	J	457	HIS
1	J	495	GLN
1	J	511	ASN
1	J	547	GLN
1	J	552	ASN
1	J	585	ASN
1	K	49	ASN
1	K	74	ASN
1	K	80	ASN
1	K	149	ASN
1	K	251	ASN
1	K	287	HIS
1	K	342	HIS
1	K	368	HIS
1	K	381	GLN
1	K	391	ASN
1	K	409	ASN
1	K	430	ASN
1	K	441	HIS
1	K	457	HIS
1	K	495	GLN
1	K	511	ASN
1	K	547	GLN
1	K	552	ASN
1	K	585	ASN
1	L	49	ASN
1	L	74	ASN

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Mol	Chain	Res	Type
1	L	80	ASN
1	L	149	ASN
1	L	251	ASN
1	L	287	HIS
1	L	342	HIS
1	L	368	HIS
1	L	381	GLN
1	L	391	ASN
1	L	409	ASN
1	L	430	ASN
1	L	441	HIS
1	L	457	HIS
1	L	495	GLN
1	L	511	ASN
1	L	547	GLN
1	L	552	ASN
1	L	585	ASN
1	M	49	ASN
1	M	74	ASN
1	M	80	ASN
1	M	149	ASN
1	M	251	ASN
1	M	287	HIS
1	M	342	HIS
1	M	368	HIS
1	M	381	GLN
1	M	391	ASN
1	M	409	ASN
1	M	430	ASN
1	M	441	HIS
1	M	457	HIS
1	M	495	GLN
1	M	511	ASN
1	M	547	GLN
1	M	552	ASN
1	M	585	ASN
1	N	49	ASN
1	N	74	ASN
1	N	80	ASN
1	N	149	ASN
1	N	251	ASN
1	N	287	HIS

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Mol	Chain	Res	Type
1	N	342	HIS
1	N	368	HIS
1	N	381	GLN
1	N	391	ASN
1	N	409	ASN
1	N	430	ASN
1	N	441	HIS
1	N	457	HIS
1	N	495	GLN
1	N	511	ASN
1	N	547	GLN
1	N	552	ASN
1	N	585	ASN
1	O	49	ASN
1	O	74	ASN
1	O	80	ASN
1	O	149	ASN
1	O	251	ASN
1	O	287	HIS
1	O	342	HIS
1	O	368	HIS
1	O	381	GLN
1	O	391	ASN
1	O	409	ASN
1	O	430	ASN
1	O	441	HIS
1	O	457	HIS
1	O	495	GLN
1	O	511	ASN
1	O	547	GLN
1	O	552	ASN
1	O	585	ASN
1	P	49	ASN
1	P	74	ASN
1	P	80	ASN
1	P	149	ASN
1	P	251	ASN
1	P	287	HIS
1	P	342	HIS
1	P	368	HIS
1	P	381	GLN
1	P	391	ASN

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Mol	Chain	Res	Type
1	P	409	ASN
1	P	430	ASN
1	P	441	HIS
1	P	457	HIS
1	P	495	GLN
1	P	511	ASN
1	P	547	GLN
1	P	552	ASN
1	P	585	ASN
1	Q	49	ASN
1	Q	74	ASN
1	Q	80	ASN
1	Q	149	ASN
1	Q	251	ASN
1	Q	287	HIS
1	Q	342	HIS
1	Q	368	HIS
1	Q	381	GLN
1	Q	391	ASN
1	Q	409	ASN
1	Q	430	ASN
1	Q	441	HIS
1	Q	457	HIS
1	Q	495	GLN
1	Q	511	ASN
1	Q	547	GLN
1	Q	552	ASN
1	Q	585	ASN
1	R	49	ASN
1	R	74	ASN
1	R	80	ASN
1	R	149	ASN
1	R	251	ASN
1	R	287	HIS
1	R	342	HIS
1	R	368	HIS
1	R	381	GLN
1	R	391	ASN
1	R	409	ASN
1	R	430	ASN
1	R	441	HIS
1	R	457	HIS

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Mol	Chain	Res	Type
1	R	495	GLN
1	R	511	ASN
1	R	547	GLN
1	R	552	ASN
1	R	585	ASN
1	S	49	ASN
1	S	74	ASN
1	S	80	ASN
1	S	149	ASN
1	S	251	ASN
1	S	287	HIS
1	S	342	HIS
1	S	368	HIS
1	S	381	GLN
1	S	391	ASN
1	S	409	ASN
1	S	430	ASN
1	S	441	HIS
1	S	457	HIS
1	S	495	GLN
1	S	511	ASN
1	S	547	GLN
1	S	552	ASN
1	S	585	ASN
1	T	49	ASN
1	T	74	ASN
1	T	80	ASN
1	T	149	ASN
1	T	251	ASN
1	T	287	HIS
1	T	342	HIS
1	T	368	HIS
1	T	381	GLN
1	T	391	ASN
1	T	409	ASN
1	T	430	ASN
1	T	441	HIS
1	T	457	HIS
1	T	495	GLN
1	T	511	ASN
1	T	547	GLN
1	T	552	ASN

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Mol	Chain	Res	Type
1	T	585	ASN
1	U	49	ASN
1	U	74	ASN
1	U	80	ASN
1	U	149	ASN
1	U	251	ASN
1	U	287	HIS
1	U	342	HIS
1	U	368	HIS
1	U	381	GLN
1	U	391	ASN
1	U	409	ASN
1	U	430	ASN
1	U	441	HIS
1	U	457	HIS
1	U	495	GLN
1	U	511	ASN
1	U	547	GLN
1	U	552	ASN
1	U	585	ASN
1	V	49	ASN
1	V	74	ASN
1	V	80	ASN
1	V	251	ASN
1	V	287	HIS
1	V	342	HIS
1	V	368	HIS
1	V	381	GLN
1	V	391	ASN
1	V	409	ASN
1	V	430	ASN
1	V	441	HIS
1	V	457	HIS
1	V	495	GLN
1	V	511	ASN
1	V	547	GLN
1	V	552	ASN
1	V	585	ASN
1	W	49	ASN
1	W	74	ASN
1	W	80	ASN
1	W	149	ASN

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Mol	Chain	Res	Type
1	W	251	ASN
1	W	287	HIS
1	W	342	HIS
1	W	368	HIS
1	W	381	GLN
1	W	391	ASN
1	W	409	ASN
1	W	430	ASN
1	W	441	HIS
1	W	457	HIS
1	W	495	GLN
1	W	511	ASN
1	W	547	GLN
1	W	552	ASN
1	W	585	ASN
1	X	49	ASN
1	X	74	ASN
1	X	80	ASN
1	X	149	ASN
1	X	251	ASN
1	X	287	HIS
1	X	342	HIS
1	X	368	HIS
1	X	381	GLN
1	X	391	ASN
1	X	409	ASN
1	X	430	ASN
1	X	441	HIS
1	X	457	HIS
1	X	495	GLN
1	X	511	ASN
1	X	547	GLN
1	X	552	ASN
1	X	585	ASN
1	Y	49	ASN
1	Y	74	ASN
1	Y	80	ASN
1	Y	149	ASN
1	Y	251	ASN
1	Y	287	HIS
1	Y	342	HIS
1	Y	368	HIS

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Mol	Chain	Res	Type
1	Y	381	GLN
1	Y	391	ASN
1	Y	409	ASN
1	Y	430	ASN
1	Y	441	HIS
1	Y	457	HIS
1	Y	495	GLN
1	Y	511	ASN
1	Y	547	GLN
1	Y	552	ASN
1	Y	585	ASN
1	Z	49	ASN
1	Z	74	ASN
1	Z	80	ASN
1	Z	149	ASN
1	Z	251	ASN
1	Z	287	HIS
1	Z	342	HIS
1	Z	368	HIS
1	Z	381	GLN
1	Z	391	ASN
1	Z	409	ASN
1	Z	430	ASN
1	Z	441	HIS
1	Z	457	HIS
1	Z	495	GLN
1	Z	511	ASN
1	Z	547	GLN
1	Z	552	ASN
1	Z	585	ASN
1	a	49	ASN
1	a	74	ASN
1	a	80	ASN
1	a	149	ASN
1	a	251	ASN
1	a	287	HIS
1	a	342	HIS
1	a	368	HIS
1	a	381	GLN
1	a	391	ASN
1	a	409	ASN
1	a	430	ASN

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Mol	Chain	Res	Type
1	a	441	HIS
1	a	457	HIS
1	a	495	GLN
1	a	511	ASN
1	a	547	GLN
1	a	552	ASN
1	a	585	ASN
1	b	49	ASN
1	b	74	ASN
1	b	80	ASN
1	b	149	ASN
1	b	251	ASN
1	b	287	HIS
1	b	342	HIS
1	b	368	HIS
1	b	381	GLN
1	b	391	ASN
1	b	409	ASN
1	b	430	ASN
1	b	441	HIS
1	b	457	HIS
1	b	495	GLN
1	b	511	ASN
1	b	547	GLN
1	b	552	ASN
1	b	585	ASN
1	c	49	ASN
1	c	74	ASN
1	c	80	ASN
1	c	149	ASN
1	c	251	ASN
1	c	287	HIS
1	c	342	HIS
1	c	368	HIS
1	c	381	GLN
1	c	391	ASN
1	c	409	ASN
1	c	430	ASN
1	c	441	HIS
1	c	457	HIS
1	c	495	GLN
1	c	511	ASN

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Mol	Chain	Res	Type
1	c	547	GLN
1	c	552	ASN
1	c	585	ASN
1	d	49	ASN
1	d	74	ASN
1	d	80	ASN
1	d	149	ASN
1	d	251	ASN
1	d	287	HIS
1	d	342	HIS
1	d	368	HIS
1	d	381	GLN
1	d	391	ASN
1	d	409	ASN
1	d	430	ASN
1	d	441	HIS
1	d	457	HIS
1	d	495	GLN
1	d	511	ASN
1	d	547	GLN
1	d	552	ASN
1	d	585	ASN
1	e	49	ASN
1	e	74	ASN
1	e	80	ASN
1	e	149	ASN
1	e	251	ASN
1	e	287	HIS
1	e	342	HIS
1	e	368	HIS
1	e	381	GLN
1	e	391	ASN
1	e	409	ASN
1	e	430	ASN
1	e	441	HIS
1	e	457	HIS
1	e	495	GLN
1	e	511	ASN
1	e	547	GLN
1	e	552	ASN
1	e	585	ASN
1	f	49	ASN

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Mol	Chain	Res	Type
1	f	74	ASN
1	f	80	ASN
1	f	149	ASN
1	f	251	ASN
1	f	287	HIS
1	f	342	HIS
1	f	368	HIS
1	f	381	GLN
1	f	391	ASN
1	f	409	ASN
1	f	430	ASN
1	f	441	HIS
1	f	457	HIS
1	f	495	GLN
1	f	511	ASN
1	f	547	GLN
1	f	552	ASN
1	f	585	ASN
1	g	49	ASN
1	g	74	ASN
1	g	80	ASN
1	g	149	ASN
1	g	251	ASN
1	g	287	HIS
1	g	342	HIS
1	g	368	HIS
1	g	381	GLN
1	g	391	ASN
1	g	409	ASN
1	g	430	ASN
1	g	441	HIS
1	g	457	HIS
1	g	495	GLN
1	g	511	ASN
1	g	547	GLN
1	g	552	ASN
1	g	585	ASN
1	h	49	ASN
1	h	74	ASN
1	h	80	ASN
1	h	149	ASN
1	h	251	ASN

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Mol	Chain	Res	Type
1	h	287	HIS
1	h	342	HIS
1	h	368	HIS
1	h	381	GLN
1	h	391	ASN
1	h	409	ASN
1	h	430	ASN
1	h	441	HIS
1	h	457	HIS
1	h	495	GLN
1	h	511	ASN
1	h	547	GLN
1	h	552	ASN
1	h	585	ASN
1	i	49	ASN
1	i	74	ASN
1	i	80	ASN
1	i	149	ASN
1	i	251	ASN
1	i	287	HIS
1	i	342	HIS
1	i	368	HIS
1	i	381	GLN
1	i	391	ASN
1	i	409	ASN
1	i	430	ASN
1	i	441	HIS
1	i	457	HIS
1	i	495	GLN
1	i	511	ASN
1	i	547	GLN
1	i	552	ASN
1	i	585	ASN
1	j	49	ASN
1	j	74	ASN
1	j	80	ASN
1	j	149	ASN
1	j	251	ASN
1	j	287	HIS
1	j	342	HIS
1	j	368	HIS
1	j	381	GLN

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Mol	Chain	Res	Type
1	j	391	ASN
1	j	409	ASN
1	j	430	ASN
1	j	441	HIS
1	j	457	HIS
1	j	495	GLN
1	j	511	ASN
1	j	547	GLN
1	j	552	ASN
1	j	585	ASN
1	k	49	ASN
1	k	74	ASN
1	k	80	ASN
1	k	149	ASN
1	k	251	ASN
1	k	287	HIS
1	k	342	HIS
1	k	368	HIS
1	k	381	GLN
1	k	391	ASN
1	k	409	ASN
1	k	430	ASN
1	k	441	HIS
1	k	457	HIS
1	k	495	GLN
1	k	511	ASN
1	k	547	GLN
1	k	552	ASN
1	k	585	ASN
1	l	49	ASN
1	l	74	ASN
1	l	80	ASN
1	l	149	ASN
1	l	251	ASN
1	l	287	HIS
1	l	342	HIS
1	l	368	HIS
1	l	381	GLN
1	l	391	ASN
1	l	409	ASN
1	l	430	ASN
1	l	441	HIS

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Mol	Chain	Res	Type
1	l	457	HIS
1	l	495	GLN
1	l	511	ASN
1	l	547	GLN
1	l	552	ASN
1	l	585	ASN
1	m	49	ASN
1	m	74	ASN
1	m	80	ASN
1	m	149	ASN
1	m	251	ASN
1	m	287	HIS
1	m	342	HIS
1	m	368	HIS
1	m	381	GLN
1	m	391	ASN
1	m	409	ASN
1	m	430	ASN
1	m	441	HIS
1	m	457	HIS
1	m	495	GLN
1	m	511	ASN
1	m	547	GLN
1	m	552	ASN
1	m	585	ASN
1	n	49	ASN
1	n	74	ASN
1	n	80	ASN
1	n	149	ASN
1	n	251	ASN
1	n	287	HIS
1	n	342	HIS
1	n	368	HIS
1	n	381	GLN
1	n	391	ASN
1	n	409	ASN
1	n	430	ASN
1	n	441	HIS
1	n	457	HIS
1	n	495	GLN
1	n	511	ASN
1	n	547	GLN

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Mol	Chain	Res	Type
1	n	552	ASN
1	n	585	ASN
1	o	49	ASN
1	o	74	ASN
1	o	80	ASN
1	o	149	ASN
1	o	251	ASN
1	o	287	HIS
1	o	342	HIS
1	o	368	HIS
1	o	381	GLN
1	o	391	ASN
1	o	409	ASN
1	o	430	ASN
1	o	441	HIS
1	o	457	HIS
1	o	495	GLN
1	o	511	ASN
1	o	547	GLN
1	o	552	ASN
1	o	585	ASN
1	p	49	ASN
1	p	74	ASN
1	p	80	ASN
1	p	251	ASN
1	p	287	HIS
1	p	342	HIS
1	p	368	HIS
1	p	381	GLN
1	p	391	ASN
1	p	409	ASN
1	p	430	ASN
1	p	441	HIS
1	p	457	HIS
1	p	495	GLN
1	p	511	ASN
1	p	547	GLN
1	p	552	ASN
1	p	585	ASN
1	q	49	ASN
1	q	74	ASN
1	q	80	ASN

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Mol	Chain	Res	Type
1	q	149	ASN
1	q	251	ASN
1	q	287	HIS
1	q	342	HIS
1	q	368	HIS
1	q	381	GLN
1	q	391	ASN
1	q	409	ASN
1	q	430	ASN
1	q	441	HIS
1	q	457	HIS
1	q	495	GLN
1	q	511	ASN
1	q	547	GLN
1	q	552	ASN
1	q	585	ASN
1	r	49	ASN
1	r	74	ASN
1	r	80	ASN
1	r	149	ASN
1	r	251	ASN
1	r	287	HIS
1	r	342	HIS
1	r	368	HIS
1	r	381	GLN
1	r	391	ASN
1	r	409	ASN
1	r	430	ASN
1	r	441	HIS
1	r	457	HIS
1	r	495	GLN
1	r	511	ASN
1	r	547	GLN
1	r	552	ASN
1	r	585	ASN
1	s	49	ASN
1	s	80	ASN
1	s	149	ASN
1	s	251	ASN
1	s	287	HIS
1	s	342	HIS
1	s	368	HIS

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Mol	Chain	Res	Type
1	s	381	GLN
1	s	391	ASN
1	s	409	ASN
1	s	430	ASN
1	s	441	HIS
1	s	457	HIS
1	s	495	GLN
1	s	511	ASN
1	s	547	GLN
1	s	552	ASN
1	s	585	ASN
1	t	49	ASN
1	t	74	ASN
1	t	80	ASN
1	t	149	ASN
1	t	251	ASN
1	t	287	HIS
1	t	342	HIS
1	t	368	HIS
1	t	381	GLN
1	t	391	ASN
1	t	409	ASN
1	t	430	ASN
1	t	441	HIS
1	t	457	HIS
1	t	495	GLN
1	t	511	ASN
1	t	547	GLN
1	t	552	ASN
1	t	585	ASN
1	u	49	ASN
1	u	74	ASN
1	u	80	ASN
1	u	149	ASN
1	u	251	ASN
1	u	287	HIS
1	u	342	HIS
1	u	368	HIS
1	u	381	GLN
1	u	391	ASN
1	u	409	ASN
1	u	430	ASN

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Mol	Chain	Res	Type
1	u	441	HIS
1	u	457	HIS
1	u	495	GLN
1	u	511	ASN
1	u	547	GLN
1	u	552	ASN
1	u	585	ASN
1	v	49	ASN
1	v	74	ASN
1	v	80	ASN
1	v	149	ASN
1	v	251	ASN
1	v	287	HIS
1	v	342	HIS
1	v	368	HIS
1	v	381	GLN
1	v	391	ASN
1	v	409	ASN
1	v	430	ASN
1	v	441	HIS
1	v	457	HIS
1	v	495	GLN
1	v	511	ASN
1	v	547	GLN
1	v	552	ASN
1	v	585	ASN
1	w	49	ASN
1	w	74	ASN
1	w	80	ASN
1	w	149	ASN
1	w	251	ASN
1	w	287	HIS
1	w	342	HIS
1	w	368	HIS
1	w	381	GLN
1	w	391	ASN
1	w	409	ASN
1	w	430	ASN
1	w	441	HIS
1	w	457	HIS
1	w	495	GLN
1	w	511	ASN

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Mol	Chain	Res	Type
1	w	547	GLN
1	w	552	ASN
1	w	585	ASN
1	x	49	ASN
1	x	74	ASN
1	x	80	ASN
1	x	149	ASN
1	x	251	ASN
1	x	287	HIS
1	x	342	HIS
1	x	368	HIS
1	x	381	GLN
1	x	391	ASN
1	x	409	ASN
1	x	430	ASN
1	x	441	HIS
1	x	457	HIS
1	x	495	GLN
1	x	511	ASN
1	x	547	GLN
1	x	552	ASN
1	x	585	ASN
1	y	49	ASN
1	y	74	ASN
1	y	80	ASN
1	y	149	ASN
1	y	251	ASN
1	y	287	HIS
1	y	342	HIS
1	y	368	HIS
1	y	381	GLN
1	y	391	ASN
1	y	409	ASN
1	y	430	ASN
1	y	441	HIS
1	y	457	HIS
1	y	495	GLN
1	y	511	ASN
1	y	547	GLN
1	y	552	ASN
1	y	585	ASN
1	z	49	ASN

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Mol	Chain	Res	Type
1	z	74	ASN
1	z	80	ASN
1	z	149	ASN
1	z	251	ASN
1	z	287	HIS
1	z	342	HIS
1	z	368	HIS
1	z	381	GLN
1	z	391	ASN
1	z	409	ASN
1	z	430	ASN
1	z	441	HIS
1	z	457	HIS
1	z	495	GLN
1	z	511	ASN
1	z	547	GLN
1	z	552	ASN
1	z	585	ASN
1	1	49	ASN
1	1	74	ASN
1	1	80	ASN
1	1	149	ASN
1	1	251	ASN
1	1	287	HIS
1	1	342	HIS
1	1	368	HIS
1	1	381	GLN
1	1	391	ASN
1	1	409	ASN
1	1	430	ASN
1	1	441	HIS
1	1	457	HIS
1	1	495	GLN
1	1	511	ASN
1	1	547	GLN
1	1	552	ASN
1	1	585	ASN
1	2	49	ASN
1	2	74	ASN
1	2	80	ASN
1	2	149	ASN
1	2	251	ASN

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Mol	Chain	Res	Type
1	2	287	HIS
1	2	342	HIS
1	2	368	HIS
1	2	381	GLN
1	2	391	ASN
1	2	409	ASN
1	2	430	ASN
1	2	441	HIS
1	2	457	HIS
1	2	495	GLN
1	2	511	ASN
1	2	547	GLN
1	2	552	ASN
1	2	585	ASN
1	3	49	ASN
1	3	74	ASN
1	3	80	ASN
1	3	149	ASN
1	3	251	ASN
1	3	287	HIS
1	3	342	HIS
1	3	368	HIS
1	3	381	GLN
1	3	391	ASN
1	3	409	ASN
1	3	430	ASN
1	3	441	HIS
1	3	457	HIS
1	3	495	GLN
1	3	511	ASN
1	3	547	GLN
1	3	552	ASN
1	3	585	ASN
1	4	49	ASN
1	4	74	ASN
1	4	80	ASN
1	4	149	ASN
1	4	251	ASN
1	4	287	HIS
1	4	342	HIS
1	4	368	HIS
1	4	381	GLN

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Mol	Chain	Res	Type
1	4	391	ASN
1	4	409	ASN
1	4	430	ASN
1	4	441	HIS
1	4	457	HIS
1	4	495	GLN
1	4	511	ASN
1	4	547	GLN
1	4	552	ASN
1	4	585	ASN
1	5	49	ASN
1	5	74	ASN
1	5	80	ASN
1	5	149	ASN
1	5	251	ASN
1	5	287	HIS
1	5	342	HIS
1	5	368	HIS
1	5	381	GLN
1	5	391	ASN
1	5	409	ASN
1	5	430	ASN
1	5	441	HIS
1	5	457	HIS
1	5	495	GLN
1	5	511	ASN
1	5	547	GLN
1	5	552	ASN
1	5	585	ASN
1	6	49	ASN
1	6	74	ASN
1	6	80	ASN
1	6	149	ASN
1	6	251	ASN
1	6	287	HIS
1	6	342	HIS
1	6	368	HIS
1	6	381	GLN
1	6	391	ASN
1	6	409	ASN
1	6	430	ASN
1	6	441	HIS

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Mol	Chain	Res	Type
1	6	457	HIS
1	6	495	GLN
1	6	511	ASN
1	6	547	GLN
1	6	552	ASN
1	6	585	ASN
1	7	49	ASN
1	7	74	ASN
1	7	80	ASN
1	7	149	ASN
1	7	251	ASN
1	7	287	HIS
1	7	342	HIS
1	7	368	HIS
1	7	381	GLN
1	7	391	ASN
1	7	409	ASN
1	7	430	ASN
1	7	441	HIS
1	7	457	HIS
1	7	495	GLN
1	7	511	ASN
1	7	547	GLN
1	7	552	ASN
1	7	585	ASN
1	8	49	ASN
1	8	74	ASN
1	8	80	ASN
1	8	149	ASN
1	8	251	ASN
1	8	287	HIS
1	8	342	HIS
1	8	368	HIS
1	8	381	GLN
1	8	391	ASN
1	8	409	ASN
1	8	430	ASN
1	8	441	HIS
1	8	457	HIS
1	8	495	GLN
1	8	511	ASN
1	8	547	GLN

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Mol	Chain	Res	Type
1	8	552	ASN
1	8	585	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

180 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	0	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	0	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	0	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	0A	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	0A	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	0A	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	1B	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	1B	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	1B	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	3A	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	3A	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	3A	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	4B	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	4B	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SIA	4B	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	6A	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	6A	2	2	11,11,12	1.13	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	6A	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	7B	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	7B	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	7B	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	9A	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	9A	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	9A	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	AC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	AC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	AC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	BA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	BA	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	BA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	CB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	CB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	CB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	DC	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	DC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	DC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	EA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	EA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	EA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	FB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	FB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	FB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	GC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	GC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	GC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	HA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	HA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	HA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	IB	1	2	15,15,15	0.14	0	21,21,21	0.17	0
2	GAL	IB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	IB	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	JC	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	JC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	JC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	KA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	KA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	KA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	LB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	LB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	LB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	MC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	MC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	MC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	NA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	NA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	NA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	OB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	OB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	OB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	PC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	PC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	PC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	QA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	QA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	QA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	RB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	RB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	RB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	SC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	SC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	SC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	TA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	TA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	TA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	UB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	UB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	UB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	VC	1	2	15,15,15	0.12	0	21,21,21	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	VC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	VC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	WA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	WA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	WA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	XB	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	XB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	XB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	YC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	YC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	YC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	ZA	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	ZA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	ZA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	aB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	aB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	aB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	bC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	bC	2	2	11,11,12	1.13	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	bC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	cA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	cA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	cA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	dB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	dB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	dB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	eC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	eC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	eC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	fA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	fA	2	2	11,11,12	1.13	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	fA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	gB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	gB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	gB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	hC	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	hC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SIA	hC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	iA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	iA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	iA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	jB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	jB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	jB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	kC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	kC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	kC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	lA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	lA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	lA	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	mB	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	mB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	mB	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	nC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	nC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	nC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	oA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	oA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	oA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	pB	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	pB	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	pB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	qC	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	qC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	qC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	rA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	rA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	rA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	sB	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	sB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	sB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	tC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	tC	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.64	2 (13%)
2	SIA	tC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	uA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	uA	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	uA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	vB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	vB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	vB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	wC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	wC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	wC	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	xA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	xA	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	xA	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	yB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	yB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	yB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	zC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	zC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	zC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0	1	2	-	2/6/26/26	0/1/1/1
2	GAL	0	2	2	-	1/2/19/22	0/1/1/1
2	SIA	0	3	2	-	3/18/34/38	0/1/1/1
2	NAG	0A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	0A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	0A	3	2	-	3/18/34/38	0/1/1/1
2	NAG	1B	1	2	-	2/6/26/26	0/1/1/1
2	GAL	1B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	1B	3	2	-	3/18/34/38	0/1/1/1
2	NAG	3A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	3A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	3A	3	2	-	3/18/34/38	0/1/1/1
2	NAG	4B	1	2	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	4B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	4B	3	2	-	3/18/34/38	0/1/1/1
2	NAG	6A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	6A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	6A	3	2	-	3/18/34/38	0/1/1/1
2	NAG	7B	1	2	-	2/6/26/26	0/1/1/1
2	GAL	7B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	7B	3	2	-	3/18/34/38	0/1/1/1
2	NAG	9A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	9A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	9A	3	2	-	3/18/34/38	0/1/1/1
2	NAG	AC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	AC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	AC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	BA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	BA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	BA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	CB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	CB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	CB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	DC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	DC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	DC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	EA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	EA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	EA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	FB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	FB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	FB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	GC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	GC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	GC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	HA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	HA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	HA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	IB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	IB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	IB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	JC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	JC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	JC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	KA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	KA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	KA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	LB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	LB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	LB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	MC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	MC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	MC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	NA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	NA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	NA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	OB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	OB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	OB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	PC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	PC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	PC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	QA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	QA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	QA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	RB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	RB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	RB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	SC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	SC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	SC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	TA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	TA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	TA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	UB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	UB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	UB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	VC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	VC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	VC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	WA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	WA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	WA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	XB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	XB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	XB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	YC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	YC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	YC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	ZA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	ZA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	ZA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	aB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	aB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	aB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	bC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	bC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	bC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	cA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	cA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	cA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	dB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	dB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	dB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	eC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	eC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	eC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	fA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	fA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	fA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	gB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	gB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	gB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	hC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	hC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	hC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	iA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	iA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	iA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	jB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	jB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	jB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	kC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	kC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	kC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	lA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	lA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	lA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	mB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	mB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	mB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	nC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	nC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	nC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	oA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	oA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	oA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	pB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	pB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	pB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	qC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	qC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	qC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	rA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	rA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	rA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	sB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	sB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	sB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	tC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	tC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	tC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	uA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	uA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	uA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	vB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	vB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	vB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	wC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	wC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	wC	3	2	-	3/18/34/38	0/1/1/1
2	NAG	xA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	xA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	xA	3	2	-	3/18/34/38	0/1/1/1
2	NAG	yB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	yB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	yB	3	2	-	3/18/34/38	0/1/1/1
2	NAG	zC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	zC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	zC	3	2	-	3/18/34/38	0/1/1/1

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	RB	3	SIA	C2-C1	5.68	1.59	1.52
2	UB	3	SIA	C2-C1	5.68	1.59	1.52
2	xA	3	SIA	C2-C1	5.67	1.59	1.52
2	eC	3	SIA	C2-C1	5.67	1.59	1.52
2	pB	3	SIA	C2-C1	5.66	1.59	1.52
2	AC	3	SIA	C2-C1	5.65	1.59	1.52
2	GC	3	SIA	C2-C1	5.65	1.59	1.52
2	rA	3	SIA	C2-C1	5.64	1.59	1.52
2	sB	3	SIA	C2-C1	5.64	1.59	1.52
2	qC	3	SIA	C2-C1	5.64	1.59	1.52
2	ZA	3	SIA	C2-C1	5.63	1.59	1.52
2	fA	3	SIA	C2-C1	5.63	1.59	1.52
2	0A	3	SIA	C2-C1	5.63	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6A	3	SIA	C2-C1	5.63	1.59	1.52
2	bC	3	SIA	C2-C1	5.63	1.59	1.52
2	hC	3	SIA	C2-C1	5.63	1.59	1.52
2	0	3	SIA	C2-C1	5.61	1.59	1.52
2	BA	3	SIA	C2-C1	5.61	1.59	1.52
2	NA	3	SIA	C2-C1	5.61	1.59	1.52
2	OB	3	SIA	C2-C1	5.61	1.59	1.52
2	XB	3	SIA	C2-C1	5.61	1.59	1.52
2	aB	3	SIA	C2-C1	5.61	1.59	1.52
2	dB	3	SIA	C2-C1	5.61	1.59	1.52
2	1B	3	SIA	C2-C1	5.61	1.59	1.52
2	PC	3	SIA	C2-C1	5.61	1.59	1.52
2	YC	3	SIA	C2-C1	5.61	1.59	1.52
2	kC	3	SIA	C2-C1	5.61	1.59	1.52
2	KA	3	SIA	C2-C1	5.61	1.59	1.52
2	QA	3	SIA	C2-C1	5.61	1.59	1.52
2	iA	3	SIA	C2-C1	5.61	1.59	1.52
2	oA	3	SIA	C2-C1	5.61	1.59	1.52
2	FB	3	SIA	C2-C1	5.61	1.59	1.52
2	LB	3	SIA	C2-C1	5.61	1.59	1.52
2	jB	3	SIA	C2-C1	5.61	1.59	1.52
2	vB	3	SIA	C2-C1	5.61	1.59	1.52
2	4B	3	SIA	C2-C1	5.61	1.59	1.52
2	JC	3	SIA	C2-C1	5.61	1.59	1.52
2	SC	3	SIA	C2-C1	5.61	1.59	1.52
2	zC	3	SIA	C2-C1	5.61	1.59	1.52
2	EA	3	SIA	C2-C1	5.61	1.59	1.52
2	WA	3	SIA	C2-C1	5.61	1.59	1.52
2	cA	3	SIA	C2-C1	5.61	1.59	1.52
2	3A	3	SIA	C2-C1	5.61	1.59	1.52
2	9A	3	SIA	C2-C1	5.61	1.59	1.52
2	gB	3	SIA	C2-C1	5.61	1.59	1.52
2	yB	3	SIA	C2-C1	5.61	1.59	1.52
2	7B	3	SIA	C2-C1	5.61	1.59	1.52
2	nC	3	SIA	C2-C1	5.61	1.59	1.52
2	uA	3	SIA	C2-C1	5.60	1.59	1.52
2	MC	3	SIA	C2-C1	5.60	1.59	1.52
2	VC	3	SIA	C2-C1	5.60	1.59	1.52
2	mB	3	SIA	C2-C1	5.59	1.59	1.52
2	HA	3	SIA	C2-C1	5.57	1.59	1.52
2	TA	3	SIA	C2-C1	5.57	1.59	1.52
2	lA	3	SIA	C2-C1	5.57	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CB	3	SIA	C2-C1	5.57	1.59	1.52
2	IB	3	SIA	C2-C1	5.57	1.59	1.52
2	tC	3	SIA	C2-C1	5.57	1.59	1.52
2	wC	3	SIA	C2-C1	5.57	1.59	1.52
2	DC	3	SIA	C2-C1	5.56	1.59	1.52
2	yB	2	GAL	C1-C2	2.55	1.58	1.52
2	ZA	2	GAL	C1-C2	2.54	1.58	1.52
2	0A	2	GAL	C1-C2	2.54	1.58	1.52
2	AC	2	GAL	C1-C2	2.54	1.58	1.52
2	DC	2	GAL	C1-C2	2.54	1.58	1.52
2	hC	2	GAL	C1-C2	2.54	1.58	1.52
2	BA	2	GAL	C1-C2	2.54	1.58	1.52
2	fA	2	GAL	C1-C2	2.54	1.58	1.52
2	xA	2	GAL	C1-C2	2.54	1.58	1.52
2	6A	2	GAL	C1-C2	2.54	1.58	1.52
2	bC	2	GAL	C1-C2	2.54	1.58	1.52
2	eC	2	GAL	C1-C2	2.54	1.58	1.52
2	jB	2	GAL	C1-C2	2.54	1.58	1.52
2	SC	2	GAL	C1-C2	2.54	1.58	1.52
2	KA	2	GAL	C1-C2	2.53	1.58	1.52
2	oA	2	GAL	C1-C2	2.53	1.58	1.52
2	vB	2	GAL	C1-C2	2.53	1.58	1.52
2	WA	2	GAL	C1-C2	2.53	1.58	1.52
2	cA	2	GAL	C1-C2	2.53	1.58	1.52
2	uA	2	GAL	C1-C2	2.53	1.58	1.52
2	3A	2	GAL	C1-C2	2.53	1.58	1.52
2	MC	2	GAL	C1-C2	2.53	1.58	1.52
2	VC	2	GAL	C1-C2	2.53	1.58	1.52
2	nC	2	GAL	C1-C2	2.53	1.58	1.52
2	HA	2	GAL	C1-C2	2.53	1.58	1.52
2	TA	2	GAL	C1-C2	2.53	1.58	1.52
2	lA	2	GAL	C1-C2	2.53	1.58	1.52
2	rA	2	GAL	C1-C2	2.53	1.58	1.52
2	CB	2	GAL	C1-C2	2.53	1.58	1.52
2	IB	2	GAL	C1-C2	2.53	1.58	1.52
2	pB	2	GAL	C1-C2	2.53	1.58	1.52
2	sB	2	GAL	C1-C2	2.53	1.58	1.52
2	qC	2	GAL	C1-C2	2.53	1.58	1.52
2	tC	2	GAL	C1-C2	2.53	1.58	1.52
2	wC	2	GAL	C1-C2	2.53	1.58	1.52
2	0	2	GAL	C1-C2	2.53	1.58	1.52
2	NA	2	GAL	C1-C2	2.53	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	OB	2	GAL	C1-C2	2.53	1.58	1.52
2	RB	2	GAL	C1-C2	2.53	1.58	1.52
2	UB	2	GAL	C1-C2	2.53	1.58	1.52
2	XB	2	GAL	C1-C2	2.53	1.58	1.52
2	aB	2	GAL	C1-C2	2.53	1.58	1.52
2	dB	2	GAL	C1-C2	2.53	1.58	1.52
2	1B	2	GAL	C1-C2	2.53	1.58	1.52
2	PC	2	GAL	C1-C2	2.53	1.58	1.52
2	YC	2	GAL	C1-C2	2.53	1.58	1.52
2	kC	2	GAL	C1-C2	2.52	1.58	1.52
2	mB	2	GAL	C1-C2	2.50	1.58	1.52
2	EA	2	GAL	C1-C2	2.50	1.58	1.52
2	9A	2	GAL	C1-C2	2.50	1.58	1.52
2	gB	2	GAL	C1-C2	2.50	1.58	1.52
2	7B	2	GAL	C1-C2	2.50	1.58	1.52
2	GC	2	GAL	C1-C2	2.50	1.58	1.52
2	QA	2	GAL	C1-C2	2.49	1.58	1.52
2	iA	2	GAL	C1-C2	2.49	1.58	1.52
2	FB	2	GAL	C1-C2	2.49	1.58	1.52
2	LB	2	GAL	C1-C2	2.49	1.58	1.52
2	4B	2	GAL	C1-C2	2.49	1.58	1.52
2	JC	2	GAL	C1-C2	2.49	1.58	1.52
2	zC	2	GAL	C1-C2	2.49	1.58	1.52
2	fA	2	GAL	C2-C3	2.22	1.55	1.52
2	6A	2	GAL	C2-C3	2.22	1.55	1.52
2	GC	2	GAL	C2-C3	2.22	1.55	1.52
2	bC	2	GAL	C2-C3	2.22	1.55	1.52
2	QA	2	GAL	C2-C3	2.21	1.55	1.52
2	iA	2	GAL	C2-C3	2.21	1.55	1.52
2	FB	2	GAL	C2-C3	2.21	1.55	1.52
2	4B	2	GAL	C2-C3	2.21	1.55	1.52
2	HA	2	GAL	C2-C3	2.21	1.55	1.52
2	lA	2	GAL	C2-C3	2.21	1.55	1.52
2	CB	2	GAL	C2-C3	2.21	1.55	1.52
2	IB	2	GAL	C2-C3	2.21	1.55	1.52
2	mB	2	GAL	C2-C3	2.21	1.55	1.52
2	tC	2	GAL	C2-C3	2.21	1.55	1.52
2	wC	2	GAL	C2-C3	2.21	1.55	1.52
2	EA	2	GAL	C2-C3	2.21	1.55	1.52
2	WA	2	GAL	C2-C3	2.21	1.55	1.52
2	ZA	2	GAL	C2-C3	2.21	1.55	1.52
2	9A	2	GAL	C2-C3	2.21	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	gB	2	GAL	C2-C3	2.21	1.55	1.52
2	7B	2	GAL	C2-C3	2.21	1.55	1.52
2	TA	2	GAL	C2-C3	2.20	1.55	1.52
2	rA	2	GAL	C2-C3	2.20	1.55	1.52
2	sB	2	GAL	C2-C3	2.20	1.55	1.52
2	oA	2	GAL	C2-C3	2.18	1.55	1.52
2	LB	2	GAL	C2-C3	2.18	1.55	1.52
2	vB	2	GAL	C2-C3	2.18	1.55	1.52
2	zC	2	GAL	C2-C3	2.18	1.55	1.52
2	0	2	GAL	C2-C3	2.18	1.55	1.52
2	NA	2	GAL	C2-C3	2.18	1.55	1.52
2	OB	2	GAL	C2-C3	2.18	1.55	1.52
2	RB	2	GAL	C2-C3	2.18	1.55	1.52
2	UB	2	GAL	C2-C3	2.18	1.55	1.52
2	XB	2	GAL	C2-C3	2.18	1.55	1.52
2	aB	2	GAL	C2-C3	2.18	1.55	1.52
2	dB	2	GAL	C2-C3	2.18	1.55	1.52
2	1B	2	GAL	C2-C3	2.18	1.55	1.52
2	PC	2	GAL	C2-C3	2.18	1.55	1.52
2	YC	2	GAL	C2-C3	2.18	1.55	1.52
2	kC	2	GAL	C2-C3	2.18	1.55	1.52
2	KA	2	GAL	C2-C3	2.17	1.55	1.52
2	yB	2	GAL	C2-C3	2.17	1.55	1.52
2	VC	2	GAL	C2-C3	2.17	1.55	1.52
2	AC	2	GAL	C2-C3	2.17	1.55	1.52
2	0A	2	GAL	C2-C3	2.16	1.55	1.52
2	DC	2	GAL	C2-C3	2.16	1.55	1.52
2	hC	2	GAL	C2-C3	2.16	1.55	1.52
2	jB	2	GAL	C2-C3	2.16	1.55	1.52
2	cA	2	GAL	C2-C3	2.15	1.55	1.52
2	uA	2	GAL	C2-C3	2.15	1.55	1.52
2	3A	2	GAL	C2-C3	2.15	1.55	1.52
2	MC	2	GAL	C2-C3	2.15	1.55	1.52
2	nC	2	GAL	C2-C3	2.15	1.55	1.52
2	pB	2	GAL	C2-C3	2.14	1.55	1.52
2	qC	2	GAL	C2-C3	2.14	1.55	1.52
2	JC	2	GAL	C2-C3	2.13	1.55	1.52
2	SC	2	GAL	C2-C3	2.13	1.55	1.52
2	BA	2	GAL	C2-C3	2.13	1.55	1.52
2	xA	2	GAL	C2-C3	2.13	1.55	1.52
2	eC	2	GAL	C2-C3	2.13	1.55	1.52

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BA	3	SIA	O1A-C1-C2	-5.04	111.96	122.85
2	xA	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	eC	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	cA	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	3A	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	nC	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	RB	3	SIA	O1A-C1-C2	-5.03	111.99	122.85
2	UB	3	SIA	O1A-C1-C2	-5.03	111.99	122.85
2	pB	3	SIA	O1A-C1-C2	-5.02	111.99	122.85
2	QA	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	LB	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	zC	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	KA	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	EA	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	9A	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	gB	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	7B	3	SIA	O1A-C1-C2	-5.02	112.00	122.85
2	fA	3	SIA	O1A-C1-C2	-5.02	112.01	122.85
2	6A	3	SIA	O1A-C1-C2	-5.02	112.01	122.85
2	bC	3	SIA	O1A-C1-C2	-5.02	112.01	122.85
2	sB	3	SIA	O1A-C1-C2	-5.02	112.01	122.85
2	WA	3	SIA	O1A-C1-C2	-5.01	112.02	122.85
2	vB	3	SIA	O1A-C1-C2	-5.01	112.02	122.85
2	rA	3	SIA	O1A-C1-C2	-5.01	112.03	122.85
2	DC	3	SIA	O1A-C1-C2	-5.01	112.03	122.85
2	qC	3	SIA	O1A-C1-C2	-5.01	112.03	122.85
2	0	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	NA	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	OB	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	XB	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	aB	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	dB	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	PC	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	YC	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	kC	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	mB	3	SIA	O1A-C1-C2	-5.00	112.04	122.85
2	ZA	3	SIA	O1A-C1-C2	-5.00	112.05	122.85
2	0A	3	SIA	O1A-C1-C2	-5.00	112.05	122.85
2	yB	3	SIA	O1A-C1-C2	-5.00	112.05	122.85
2	hC	3	SIA	O1A-C1-C2	-5.00	112.05	122.85
2	HA	3	SIA	O1A-C1-C2	-5.00	112.06	122.85
2	CB	3	SIA	O1A-C1-C2	-5.00	112.06	122.85
2	tC	3	SIA	O1A-C1-C2	-5.00	112.06	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	lA	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	IB	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	wC	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	iA	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	oA	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	FB	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	jB	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	4B	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	JC	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	SC	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	AC	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	GC	3	SIA	O1A-C1-C2	-4.99	112.06	122.85
2	1B	3	SIA	O1A-C1-C2	-4.99	112.07	122.85
2	TA	3	SIA	O1A-C1-C2	-4.98	112.08	122.85
2	uA	3	SIA	O1A-C1-C2	-4.98	112.08	122.85
2	MC	3	SIA	O1A-C1-C2	-4.98	112.08	122.85
2	VC	3	SIA	O1A-C1-C2	-4.98	112.08	122.85
2	lA	2	GAL	C1-O5-C5	4.29	117.94	112.19
2	IB	2	GAL	C1-O5-C5	4.29	117.94	112.19
2	tC	2	GAL	C1-O5-C5	4.29	117.94	112.19
2	wC	2	GAL	C1-O5-C5	4.29	117.94	112.19
2	SC	2	GAL	C1-O5-C5	4.29	117.93	112.19
2	GC	2	GAL	C1-O5-C5	4.28	117.92	112.19
2	rA	2	GAL	C1-O5-C5	4.28	117.92	112.19
2	qC	2	GAL	C1-O5-C5	4.28	117.92	112.19
2	TA	2	GAL	C1-O5-C5	4.27	117.91	112.19
2	sB	2	GAL	C1-O5-C5	4.27	117.91	112.19
2	WA	2	GAL	C1-O5-C5	4.26	117.90	112.19
2	VC	2	GAL	C1-O5-C5	4.26	117.90	112.19
2	AC	2	GAL	C1-O5-C5	4.26	117.90	112.19
2	fA	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	6A	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	bC	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	KA	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	jB	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	vB	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	0	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	NA	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	RB	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	UB	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	XB	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	aB	2	GAL	C1-O5-C5	4.26	117.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	dB	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	1B	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	PC	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	YC	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	kC	2	GAL	C1-O5-C5	4.26	117.89	112.19
2	OB	2	GAL	C1-O5-C5	4.25	117.89	112.19
2	pB	2	GAL	C1-O5-C5	4.25	117.89	112.19
2	3A	2	GAL	C1-O5-C5	4.25	117.89	112.19
2	BA	2	GAL	C1-O5-C5	4.25	117.88	112.19
2	xA	2	GAL	C1-O5-C5	4.25	117.88	112.19
2	eC	2	GAL	C1-O5-C5	4.25	117.88	112.19
2	CB	2	GAL	C1-O5-C5	4.25	117.88	112.19
2	HA	2	GAL	C1-O5-C5	4.25	117.88	112.19
2	ZA	2	GAL	C1-O5-C5	4.24	117.87	112.19
2	QA	2	GAL	C1-O5-C5	4.24	117.87	112.19
2	EA	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	cA	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	uA	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	9A	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	gB	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	7B	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	MC	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	nC	2	GAL	C1-O5-C5	4.24	117.86	112.19
2	0A	2	GAL	C1-O5-C5	4.23	117.86	112.19
2	DC	2	GAL	C1-O5-C5	4.23	117.86	112.19
2	hC	2	GAL	C1-O5-C5	4.23	117.86	112.19
2	oA	2	GAL	C1-O5-C5	4.23	117.85	112.19
2	yB	2	GAL	C1-O5-C5	4.22	117.85	112.19
2	iA	2	GAL	C1-O5-C5	4.22	117.84	112.19
2	FB	2	GAL	C1-O5-C5	4.22	117.84	112.19
2	LB	2	GAL	C1-O5-C5	4.22	117.84	112.19
2	4B	2	GAL	C1-O5-C5	4.22	117.84	112.19
2	zC	2	GAL	C1-O5-C5	4.22	117.84	112.19
2	mB	2	GAL	C1-O5-C5	4.21	117.83	112.19
2	JC	2	GAL	C1-O5-C5	4.21	117.83	112.19
2	jB	2	GAL	C1-C2-C3	3.43	114.64	109.64
2	SC	2	GAL	C1-C2-C3	3.42	114.63	109.64
2	WA	2	GAL	C1-C2-C3	3.42	114.63	109.64
2	HA	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	lA	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	CB	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	IB	2	GAL	C1-C2-C3	3.42	114.62	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	tC	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	wC	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	cA	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	uA	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	0A	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	3A	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	DC	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	MC	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	hC	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	nC	2	GAL	C1-C2-C3	3.42	114.62	109.64
2	JC	2	GAL	C1-C2-C3	3.41	114.61	109.64
2	EA	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	QA	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	iA	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	9A	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	FB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	gB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	4B	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	TA	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	rA	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	sB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	0	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	NA	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	OB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	RB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	UB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	XB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	aB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	dB	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	1B	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	PC	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	YC	2	GAL	C1-C2-C3	3.40	114.60	109.64
2	mB	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	LB	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	zC	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	ZA	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	fA	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	6A	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	VC	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	bC	2	GAL	C1-C2-C3	3.40	114.59	109.64
2	pB	2	GAL	C1-C2-C3	3.39	114.59	109.64
2	qC	2	GAL	C1-C2-C3	3.39	114.59	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	oA	2	GAL	C1-C2-C3	3.39	114.59	109.64
2	vB	2	GAL	C1-C2-C3	3.39	114.59	109.64
2	BA	2	GAL	C1-C2-C3	3.39	114.58	109.64
2	xA	2	GAL	C1-C2-C3	3.39	114.58	109.64
2	eC	2	GAL	C1-C2-C3	3.39	114.58	109.64
2	GC	2	GAL	C1-C2-C3	3.39	114.58	109.64
2	7B	2	GAL	C1-C2-C3	3.39	114.58	109.64
2	kC	2	GAL	C1-C2-C3	3.38	114.57	109.64
2	yB	2	GAL	C1-C2-C3	3.38	114.57	109.64
2	AC	2	GAL	C1-C2-C3	3.38	114.56	109.64
2	KA	2	GAL	C1-C2-C3	3.37	114.55	109.64
2	LB	3	SIA	O1B-C1-O1A	2.41	129.55	124.08
2	zC	3	SIA	O1B-C1-O1A	2.41	129.55	124.08
2	KA	3	SIA	O1B-C1-O1A	2.40	129.53	124.08
2	xA	3	SIA	O1B-C1-O1A	2.40	129.52	124.08
2	eC	3	SIA	O1B-C1-O1A	2.40	129.52	124.08
2	QA	3	SIA	O1B-C1-O1A	2.40	129.51	124.08
2	RB	3	SIA	O1B-C1-O1A	2.39	129.51	124.08
2	UB	3	SIA	O1B-C1-O1A	2.39	129.51	124.08
2	pB	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	sB	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	cA	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	3A	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	nC	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	fA	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	6A	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	bC	3	SIA	O1B-C1-O1A	2.39	129.50	124.08
2	vB	3	SIA	O1B-C1-O1A	2.38	129.49	124.08
2	AC	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	BA	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	EA	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	9A	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	gB	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	7B	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	rA	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	qC	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	GC	3	SIA	O1B-C1-O1A	2.38	129.48	124.08
2	HA	3	SIA	O1B-C1-O1A	2.38	129.47	124.08
2	CB	3	SIA	O1B-C1-O1A	2.38	129.47	124.08
2	tC	3	SIA	O1B-C1-O1A	2.38	129.47	124.08
2	lA	3	SIA	O1B-C1-O1A	2.38	129.47	124.08
2	IB	3	SIA	O1B-C1-O1A	2.38	129.47	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	wC	3	SIA	O1B-C1-O1A	2.38	129.47	124.08
2	0	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	NA	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	OB	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	XB	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	aB	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	PC	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	YC	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	kC	3	SIA	O1B-C1-O1A	2.37	129.47	124.08
2	ZA	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	WA	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	uA	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	MC	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	VC	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	0A	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	DC	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	hC	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
2	JC	3	SIA	O1B-C1-O1A	2.37	129.45	124.08
2	dB	3	SIA	O1B-C1-O1A	2.36	129.44	124.08
2	yB	3	SIA	O1B-C1-O1A	2.36	129.44	124.08
2	mB	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	1B	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	iA	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	oA	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	FB	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	jB	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	4B	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	SC	3	SIA	O1B-C1-O1A	2.36	129.43	124.08
2	TA	3	SIA	O1B-C1-O1A	2.35	129.41	124.08
2	BA	3	SIA	O1B-C1-C2	2.25	118.56	112.71
2	dB	3	SIA	O1B-C1-C2	2.24	118.52	112.71
2	mB	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	WA	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	7B	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	DC	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	EA	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	cA	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	3A	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	9A	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	gB	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	yB	3	SIA	O1B-C1-C2	2.23	118.52	112.71
2	nC	3	SIA	O1B-C1-C2	2.23	118.52	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	TA	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	iA	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	oA	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	FB	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	jB	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	4B	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	SC	3	SIA	O1B-C1-C2	2.23	118.51	112.71
2	pB	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	RB	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	UB	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	xA	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	eC	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	0A	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	hC	3	SIA	O1B-C1-C2	2.23	118.50	112.71
2	0	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	NA	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	OB	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	XB	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	aB	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	1B	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	PC	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	YC	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	kC	3	SIA	O1B-C1-C2	2.22	118.50	112.71
2	ZA	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	fA	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	6A	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	bC	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	rA	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	qC	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	QA	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	sB	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	vB	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	JC	3	SIA	O1B-C1-C2	2.22	118.49	112.71
2	HA	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	KA	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	lA	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	CB	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	IB	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	tC	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	wC	3	SIA	O1B-C1-C2	2.22	118.47	112.71
2	uA	3	SIA	O1B-C1-C2	2.21	118.46	112.71
2	GC	3	SIA	O1B-C1-C2	2.21	118.46	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	MC	3	SIA	O1B-C1-C2	2.21	118.46	112.71
2	VC	3	SIA	O1B-C1-C2	2.21	118.46	112.71
2	AC	3	SIA	O1B-C1-C2	2.21	118.46	112.71
2	LB	3	SIA	O1B-C1-C2	2.21	118.45	112.71
2	zC	3	SIA	O1B-C1-C2	2.21	118.45	112.71
2	JC	3	SIA	C6-C5-N5	-2.16	107.47	110.91
2	yB	3	SIA	C6-C5-N5	-2.15	107.47	110.91
2	GC	3	SIA	C6-C5-N5	-2.15	107.47	110.91
2	sB	3	SIA	C6-C5-N5	-2.15	107.47	110.91
2	YC	3	SIA	C6-C5-N5	-2.15	107.47	110.91
2	mB	3	SIA	C6-C5-N5	-2.15	107.48	110.91
2	VC	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	WA	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	cA	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	7B	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	nC	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	TA	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	rA	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	qC	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	ZA	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	fA	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	6A	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	AC	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	bC	3	SIA	C6-C5-N5	-2.14	107.49	110.91
2	OB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	kC	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	iA	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	oA	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	FB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	jB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	4B	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	SC	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	QA	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	3A	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	0	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	NA	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	RB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	UB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	XB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	aB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	dB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	1B	3	SIA	C6-C5-N5	-2.14	107.50	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	PC	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	EA	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	9A	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	gB	3	SIA	C6-C5-N5	-2.14	107.50	110.91
2	0A	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	hC	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	KA	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	uA	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	LB	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	MC	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	zC	3	SIA	C6-C5-N5	-2.13	107.50	110.91
2	BA	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	xA	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	DC	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	eC	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	HA	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	CB	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	pB	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	tC	3	SIA	C6-C5-N5	-2.13	107.51	110.91
2	vB	3	SIA	C6-C5-N5	-2.12	107.52	110.91
2	lA	3	SIA	C6-C5-N5	-2.12	107.53	110.91
2	IB	3	SIA	C6-C5-N5	-2.12	107.53	110.91
2	wC	3	SIA	C6-C5-N5	-2.12	107.53	110.91

There are no chirality outliers.

All (360) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	0	3	SIA	O8-C8-C9-O9
2	BA	3	SIA	O8-C8-C9-O9
2	EA	3	SIA	O8-C8-C9-O9
2	HA	3	SIA	O8-C8-C9-O9
2	KA	3	SIA	O8-C8-C9-O9
2	NA	3	SIA	O8-C8-C9-O9
2	QA	3	SIA	O8-C8-C9-O9
2	TA	3	SIA	O8-C8-C9-O9
2	WA	3	SIA	O8-C8-C9-O9
2	ZA	3	SIA	O8-C8-C9-O9
2	cA	3	SIA	O8-C8-C9-O9
2	fA	3	SIA	O8-C8-C9-O9
2	iA	3	SIA	O8-C8-C9-O9
2	lA	3	SIA	O8-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
2	oA	3	SIA	O8-C8-C9-O9
2	rA	3	SIA	O8-C8-C9-O9
2	uA	3	SIA	O8-C8-C9-O9
2	xA	3	SIA	O8-C8-C9-O9
2	0A	3	SIA	O8-C8-C9-O9
2	3A	3	SIA	O8-C8-C9-O9
2	6A	3	SIA	O8-C8-C9-O9
2	9A	3	SIA	O8-C8-C9-O9
2	CB	3	SIA	O8-C8-C9-O9
2	FB	3	SIA	O8-C8-C9-O9
2	IB	3	SIA	O8-C8-C9-O9
2	LB	3	SIA	O8-C8-C9-O9
2	OB	3	SIA	O8-C8-C9-O9
2	RB	3	SIA	O8-C8-C9-O9
2	UB	3	SIA	O8-C8-C9-O9
2	XB	3	SIA	O8-C8-C9-O9
2	aB	3	SIA	O8-C8-C9-O9
2	dB	3	SIA	O8-C8-C9-O9
2	gB	3	SIA	O8-C8-C9-O9
2	jB	3	SIA	O8-C8-C9-O9
2	mB	3	SIA	O8-C8-C9-O9
2	pB	3	SIA	O8-C8-C9-O9
2	sB	3	SIA	O8-C8-C9-O9
2	vB	3	SIA	O8-C8-C9-O9
2	yB	3	SIA	O8-C8-C9-O9
2	1B	3	SIA	O8-C8-C9-O9
2	4B	3	SIA	O8-C8-C9-O9
2	7B	3	SIA	O8-C8-C9-O9
2	AC	3	SIA	O8-C8-C9-O9
2	DC	3	SIA	O8-C8-C9-O9
2	GC	3	SIA	O8-C8-C9-O9
2	JC	3	SIA	O8-C8-C9-O9
2	MC	3	SIA	O8-C8-C9-O9
2	PC	3	SIA	O8-C8-C9-O9
2	SC	3	SIA	O8-C8-C9-O9
2	VC	3	SIA	O8-C8-C9-O9
2	YC	3	SIA	O8-C8-C9-O9
2	bC	3	SIA	O8-C8-C9-O9
2	eC	3	SIA	O8-C8-C9-O9
2	hC	3	SIA	O8-C8-C9-O9
2	kC	3	SIA	O8-C8-C9-O9
2	nC	3	SIA	O8-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
2	qC	3	SIA	O8-C8-C9-O9
2	tC	3	SIA	O8-C8-C9-O9
2	wC	3	SIA	O8-C8-C9-O9
2	zC	3	SIA	O8-C8-C9-O9
2	0	1	NAG	C8-C7-N2-C2
2	0	1	NAG	O7-C7-N2-C2
2	BA	1	NAG	C8-C7-N2-C2
2	BA	1	NAG	O7-C7-N2-C2
2	EA	1	NAG	C8-C7-N2-C2
2	EA	1	NAG	O7-C7-N2-C2
2	HA	1	NAG	C8-C7-N2-C2
2	HA	1	NAG	O7-C7-N2-C2
2	KA	1	NAG	C8-C7-N2-C2
2	KA	1	NAG	O7-C7-N2-C2
2	NA	1	NAG	C8-C7-N2-C2
2	NA	1	NAG	O7-C7-N2-C2
2	QA	1	NAG	C8-C7-N2-C2
2	QA	1	NAG	O7-C7-N2-C2
2	TA	1	NAG	C8-C7-N2-C2
2	TA	1	NAG	O7-C7-N2-C2
2	WA	1	NAG	C8-C7-N2-C2
2	WA	1	NAG	O7-C7-N2-C2
2	ZA	1	NAG	C8-C7-N2-C2
2	ZA	1	NAG	O7-C7-N2-C2
2	cA	1	NAG	C8-C7-N2-C2
2	cA	1	NAG	O7-C7-N2-C2
2	fA	1	NAG	C8-C7-N2-C2
2	fA	1	NAG	O7-C7-N2-C2
2	iA	1	NAG	C8-C7-N2-C2
2	iA	1	NAG	O7-C7-N2-C2
2	lA	1	NAG	C8-C7-N2-C2
2	lA	1	NAG	O7-C7-N2-C2
2	oA	1	NAG	C8-C7-N2-C2
2	oA	1	NAG	O7-C7-N2-C2
2	rA	1	NAG	C8-C7-N2-C2
2	rA	1	NAG	O7-C7-N2-C2
2	uA	1	NAG	C8-C7-N2-C2
2	uA	1	NAG	O7-C7-N2-C2
2	xA	1	NAG	C8-C7-N2-C2
2	xA	1	NAG	O7-C7-N2-C2
2	0A	1	NAG	C8-C7-N2-C2
2	0A	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	3A	1	NAG	C8-C7-N2-C2
2	3A	1	NAG	O7-C7-N2-C2
2	6A	1	NAG	C8-C7-N2-C2
2	6A	1	NAG	O7-C7-N2-C2
2	9A	1	NAG	C8-C7-N2-C2
2	9A	1	NAG	O7-C7-N2-C2
2	CB	1	NAG	C8-C7-N2-C2
2	CB	1	NAG	O7-C7-N2-C2
2	FB	1	NAG	C8-C7-N2-C2
2	FB	1	NAG	O7-C7-N2-C2
2	IB	1	NAG	C8-C7-N2-C2
2	IB	1	NAG	O7-C7-N2-C2
2	LB	1	NAG	C8-C7-N2-C2
2	LB	1	NAG	O7-C7-N2-C2
2	OB	1	NAG	C8-C7-N2-C2
2	OB	1	NAG	O7-C7-N2-C2
2	RB	1	NAG	C8-C7-N2-C2
2	RB	1	NAG	O7-C7-N2-C2
2	UB	1	NAG	C8-C7-N2-C2
2	UB	1	NAG	O7-C7-N2-C2
2	XB	1	NAG	C8-C7-N2-C2
2	XB	1	NAG	O7-C7-N2-C2
2	aB	1	NAG	C8-C7-N2-C2
2	aB	1	NAG	O7-C7-N2-C2
2	dB	1	NAG	C8-C7-N2-C2
2	dB	1	NAG	O7-C7-N2-C2
2	gB	1	NAG	C8-C7-N2-C2
2	gB	1	NAG	O7-C7-N2-C2
2	jB	1	NAG	C8-C7-N2-C2
2	jB	1	NAG	O7-C7-N2-C2
2	mB	1	NAG	C8-C7-N2-C2
2	mB	1	NAG	O7-C7-N2-C2
2	pB	1	NAG	C8-C7-N2-C2
2	pB	1	NAG	O7-C7-N2-C2
2	sB	1	NAG	C8-C7-N2-C2
2	sB	1	NAG	O7-C7-N2-C2
2	vB	1	NAG	C8-C7-N2-C2
2	vB	1	NAG	O7-C7-N2-C2
2	yB	1	NAG	C8-C7-N2-C2
2	yB	1	NAG	O7-C7-N2-C2
2	1B	1	NAG	C8-C7-N2-C2
2	1B	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	4B	1	NAG	C8-C7-N2-C2
2	4B	1	NAG	O7-C7-N2-C2
2	7B	1	NAG	C8-C7-N2-C2
2	7B	1	NAG	O7-C7-N2-C2
2	AC	1	NAG	C8-C7-N2-C2
2	AC	1	NAG	O7-C7-N2-C2
2	DC	1	NAG	C8-C7-N2-C2
2	DC	1	NAG	O7-C7-N2-C2
2	GC	1	NAG	C8-C7-N2-C2
2	GC	1	NAG	O7-C7-N2-C2
2	JC	1	NAG	C8-C7-N2-C2
2	JC	1	NAG	O7-C7-N2-C2
2	MC	1	NAG	C8-C7-N2-C2
2	MC	1	NAG	O7-C7-N2-C2
2	PC	1	NAG	C8-C7-N2-C2
2	PC	1	NAG	O7-C7-N2-C2
2	SC	1	NAG	C8-C7-N2-C2
2	SC	1	NAG	O7-C7-N2-C2
2	VC	1	NAG	C8-C7-N2-C2
2	VC	1	NAG	O7-C7-N2-C2
2	YC	1	NAG	C8-C7-N2-C2
2	YC	1	NAG	O7-C7-N2-C2
2	bC	1	NAG	C8-C7-N2-C2
2	bC	1	NAG	O7-C7-N2-C2
2	eC	1	NAG	C8-C7-N2-C2
2	eC	1	NAG	O7-C7-N2-C2
2	hC	1	NAG	C8-C7-N2-C2
2	hC	1	NAG	O7-C7-N2-C2
2	kC	1	NAG	C8-C7-N2-C2
2	kC	1	NAG	O7-C7-N2-C2
2	nC	1	NAG	C8-C7-N2-C2
2	nC	1	NAG	O7-C7-N2-C2
2	qC	1	NAG	C8-C7-N2-C2
2	qC	1	NAG	O7-C7-N2-C2
2	tC	1	NAG	C8-C7-N2-C2
2	tC	1	NAG	O7-C7-N2-C2
2	wC	1	NAG	C8-C7-N2-C2
2	wC	1	NAG	O7-C7-N2-C2
2	zC	1	NAG	C8-C7-N2-C2
2	zC	1	NAG	O7-C7-N2-C2
2	0	3	SIA	C7-C8-C9-O9
2	BA	3	SIA	C7-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
2	EA	3	SIA	C7-C8-C9-O9
2	HA	3	SIA	C7-C8-C9-O9
2	KA	3	SIA	C7-C8-C9-O9
2	NA	3	SIA	C7-C8-C9-O9
2	QA	3	SIA	C7-C8-C9-O9
2	TA	3	SIA	C7-C8-C9-O9
2	WA	3	SIA	C7-C8-C9-O9
2	ZA	3	SIA	C7-C8-C9-O9
2	cA	3	SIA	C7-C8-C9-O9
2	fA	3	SIA	C7-C8-C9-O9
2	iA	3	SIA	C7-C8-C9-O9
2	lA	3	SIA	C7-C8-C9-O9
2	oA	3	SIA	C7-C8-C9-O9
2	rA	3	SIA	C7-C8-C9-O9
2	uA	3	SIA	C7-C8-C9-O9
2	xA	3	SIA	C7-C8-C9-O9
2	0A	3	SIA	C7-C8-C9-O9
2	3A	3	SIA	C7-C8-C9-O9
2	6A	3	SIA	C7-C8-C9-O9
2	9A	3	SIA	C7-C8-C9-O9
2	CB	3	SIA	C7-C8-C9-O9
2	FB	3	SIA	C7-C8-C9-O9
2	IB	3	SIA	C7-C8-C9-O9
2	LB	3	SIA	C7-C8-C9-O9
2	OB	3	SIA	C7-C8-C9-O9
2	RB	3	SIA	C7-C8-C9-O9
2	UB	3	SIA	C7-C8-C9-O9
2	XB	3	SIA	C7-C8-C9-O9
2	aB	3	SIA	C7-C8-C9-O9
2	dB	3	SIA	C7-C8-C9-O9
2	gB	3	SIA	C7-C8-C9-O9
2	jB	3	SIA	C7-C8-C9-O9
2	mB	3	SIA	C7-C8-C9-O9
2	pB	3	SIA	C7-C8-C9-O9
2	sB	3	SIA	C7-C8-C9-O9
2	vB	3	SIA	C7-C8-C9-O9
2	yB	3	SIA	C7-C8-C9-O9
2	1B	3	SIA	C7-C8-C9-O9
2	4B	3	SIA	C7-C8-C9-O9
2	7B	3	SIA	C7-C8-C9-O9
2	AC	3	SIA	C7-C8-C9-O9
2	DC	3	SIA	C7-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
2	GC	3	SIA	C7-C8-C9-O9
2	JC	3	SIA	C7-C8-C9-O9
2	MC	3	SIA	C7-C8-C9-O9
2	PC	3	SIA	C7-C8-C9-O9
2	SC	3	SIA	C7-C8-C9-O9
2	VC	3	SIA	C7-C8-C9-O9
2	YC	3	SIA	C7-C8-C9-O9
2	bC	3	SIA	C7-C8-C9-O9
2	eC	3	SIA	C7-C8-C9-O9
2	hC	3	SIA	C7-C8-C9-O9
2	kC	3	SIA	C7-C8-C9-O9
2	nC	3	SIA	C7-C8-C9-O9
2	qC	3	SIA	C7-C8-C9-O9
2	tC	3	SIA	C7-C8-C9-O9
2	wC	3	SIA	C7-C8-C9-O9
2	zC	3	SIA	C7-C8-C9-O9
2	0	2	GAL	O5-C5-C6-O6
2	BA	2	GAL	O5-C5-C6-O6
2	EA	2	GAL	O5-C5-C6-O6
2	HA	2	GAL	O5-C5-C6-O6
2	KA	2	GAL	O5-C5-C6-O6
2	NA	2	GAL	O5-C5-C6-O6
2	QA	2	GAL	O5-C5-C6-O6
2	TA	2	GAL	O5-C5-C6-O6
2	WA	2	GAL	O5-C5-C6-O6
2	ZA	2	GAL	O5-C5-C6-O6
2	cA	2	GAL	O5-C5-C6-O6
2	fA	2	GAL	O5-C5-C6-O6
2	iA	2	GAL	O5-C5-C6-O6
2	lA	2	GAL	O5-C5-C6-O6
2	oA	2	GAL	O5-C5-C6-O6
2	rA	2	GAL	O5-C5-C6-O6
2	uA	2	GAL	O5-C5-C6-O6
2	xA	2	GAL	O5-C5-C6-O6
2	0A	2	GAL	O5-C5-C6-O6
2	3A	2	GAL	O5-C5-C6-O6
2	6A	2	GAL	O5-C5-C6-O6
2	9A	2	GAL	O5-C5-C6-O6
2	CB	2	GAL	O5-C5-C6-O6
2	FB	2	GAL	O5-C5-C6-O6
2	IB	2	GAL	O5-C5-C6-O6
2	LB	2	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	OB	2	GAL	O5-C5-C6-O6
2	RB	2	GAL	O5-C5-C6-O6
2	UB	2	GAL	O5-C5-C6-O6
2	XB	2	GAL	O5-C5-C6-O6
2	aB	2	GAL	O5-C5-C6-O6
2	dB	2	GAL	O5-C5-C6-O6
2	gB	2	GAL	O5-C5-C6-O6
2	jB	2	GAL	O5-C5-C6-O6
2	mB	2	GAL	O5-C5-C6-O6
2	pB	2	GAL	O5-C5-C6-O6
2	sB	2	GAL	O5-C5-C6-O6
2	vB	2	GAL	O5-C5-C6-O6
2	yB	2	GAL	O5-C5-C6-O6
2	1B	2	GAL	O5-C5-C6-O6
2	4B	2	GAL	O5-C5-C6-O6
2	7B	2	GAL	O5-C5-C6-O6
2	AC	2	GAL	O5-C5-C6-O6
2	DC	2	GAL	O5-C5-C6-O6
2	GC	2	GAL	O5-C5-C6-O6
2	JC	2	GAL	O5-C5-C6-O6
2	MC	2	GAL	O5-C5-C6-O6
2	PC	2	GAL	O5-C5-C6-O6
2	SC	2	GAL	O5-C5-C6-O6
2	VC	2	GAL	O5-C5-C6-O6
2	YC	2	GAL	O5-C5-C6-O6
2	bC	2	GAL	O5-C5-C6-O6
2	eC	2	GAL	O5-C5-C6-O6
2	hC	2	GAL	O5-C5-C6-O6
2	kC	2	GAL	O5-C5-C6-O6
2	nC	2	GAL	O5-C5-C6-O6
2	qC	2	GAL	O5-C5-C6-O6
2	tC	2	GAL	O5-C5-C6-O6
2	wC	2	GAL	O5-C5-C6-O6
2	zC	2	GAL	O5-C5-C6-O6
2	0	3	SIA	C4-C5-N5-C10
2	BA	3	SIA	C4-C5-N5-C10
2	EA	3	SIA	C4-C5-N5-C10
2	HA	3	SIA	C4-C5-N5-C10
2	KA	3	SIA	C4-C5-N5-C10
2	NA	3	SIA	C4-C5-N5-C10
2	QA	3	SIA	C4-C5-N5-C10
2	TA	3	SIA	C4-C5-N5-C10

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Mol	Chain	Res	Type	Atoms
2	WA	3	SIA	C4-C5-N5-C10
2	ZA	3	SIA	C4-C5-N5-C10
2	cA	3	SIA	C4-C5-N5-C10
2	fA	3	SIA	C4-C5-N5-C10
2	iA	3	SIA	C4-C5-N5-C10
2	lA	3	SIA	C4-C5-N5-C10
2	oA	3	SIA	C4-C5-N5-C10
2	rA	3	SIA	C4-C5-N5-C10
2	uA	3	SIA	C4-C5-N5-C10
2	xA	3	SIA	C4-C5-N5-C10
2	0A	3	SIA	C4-C5-N5-C10
2	3A	3	SIA	C4-C5-N5-C10
2	6A	3	SIA	C4-C5-N5-C10
2	9A	3	SIA	C4-C5-N5-C10
2	CB	3	SIA	C4-C5-N5-C10
2	FB	3	SIA	C4-C5-N5-C10
2	IB	3	SIA	C4-C5-N5-C10
2	LB	3	SIA	C4-C5-N5-C10
2	OB	3	SIA	C4-C5-N5-C10
2	RB	3	SIA	C4-C5-N5-C10
2	UB	3	SIA	C4-C5-N5-C10
2	XB	3	SIA	C4-C5-N5-C10
2	aB	3	SIA	C4-C5-N5-C10
2	dB	3	SIA	C4-C5-N5-C10
2	gB	3	SIA	C4-C5-N5-C10
2	jB	3	SIA	C4-C5-N5-C10
2	mB	3	SIA	C4-C5-N5-C10
2	pB	3	SIA	C4-C5-N5-C10
2	sB	3	SIA	C4-C5-N5-C10
2	vB	3	SIA	C4-C5-N5-C10
2	yB	3	SIA	C4-C5-N5-C10
2	1B	3	SIA	C4-C5-N5-C10
2	4B	3	SIA	C4-C5-N5-C10
2	7B	3	SIA	C4-C5-N5-C10
2	AC	3	SIA	C4-C5-N5-C10
2	DC	3	SIA	C4-C5-N5-C10
2	GC	3	SIA	C4-C5-N5-C10
2	JC	3	SIA	C4-C5-N5-C10
2	MC	3	SIA	C4-C5-N5-C10
2	PC	3	SIA	C4-C5-N5-C10
2	SC	3	SIA	C4-C5-N5-C10
2	VC	3	SIA	C4-C5-N5-C10

Continued on next page...

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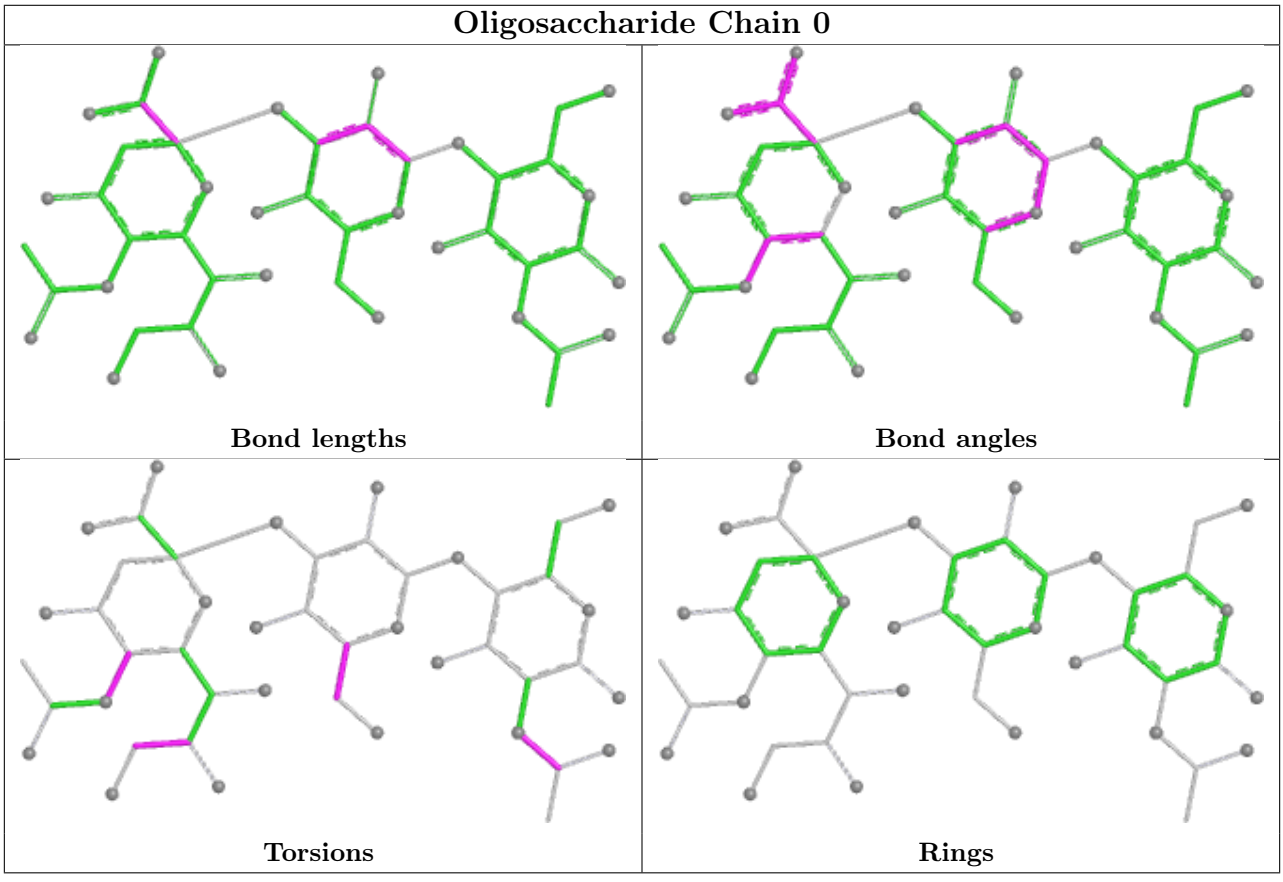
Mol	Chain	Res	Type	Atoms
2	YC	3	SIA	C4-C5-N5-C10
2	bC	3	SIA	C4-C5-N5-C10
2	eC	3	SIA	C4-C5-N5-C10
2	hC	3	SIA	C4-C5-N5-C10
2	kC	3	SIA	C4-C5-N5-C10
2	nC	3	SIA	C4-C5-N5-C10
2	qC	3	SIA	C4-C5-N5-C10
2	tC	3	SIA	C4-C5-N5-C10
2	wC	3	SIA	C4-C5-N5-C10
2	zC	3	SIA	C4-C5-N5-C10

There are no ring outliers.

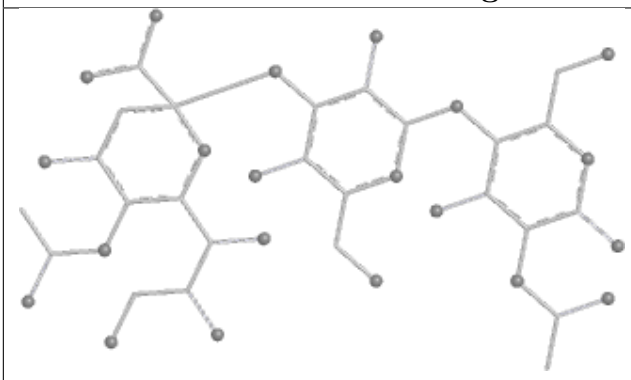
No monomer is involved in short contacts.

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

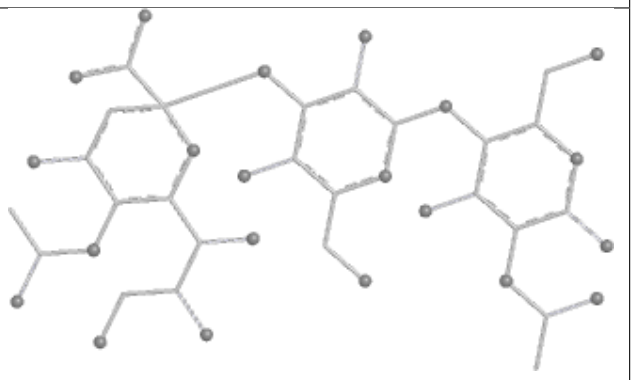
Oligosaccharide Chain 0



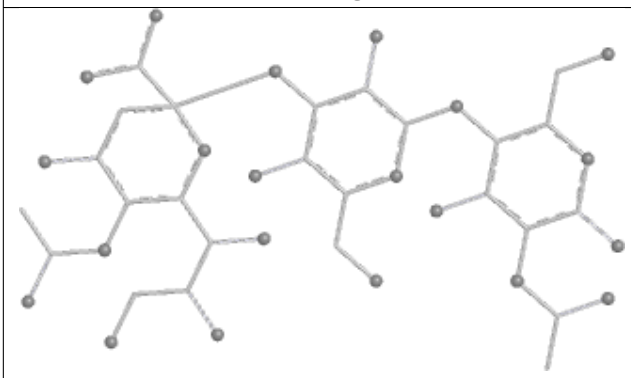
Oligosaccharide Chain BA



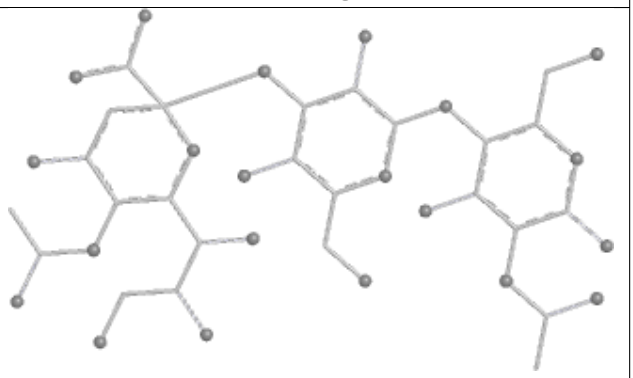
Bond lengths



Bond angles

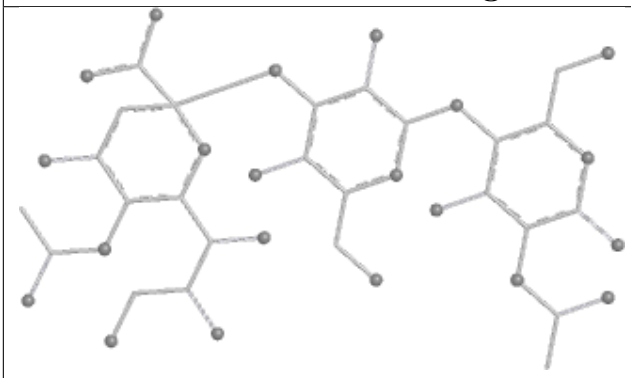


Torsions

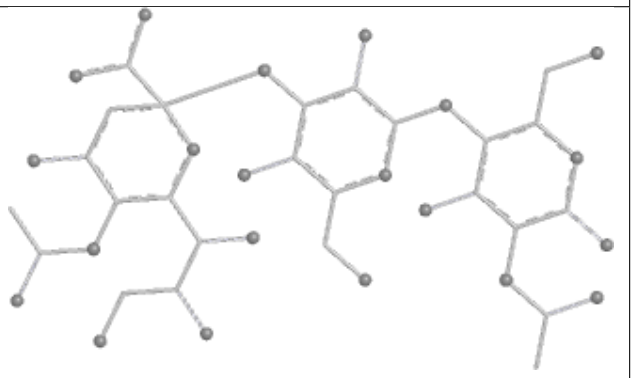


Rings

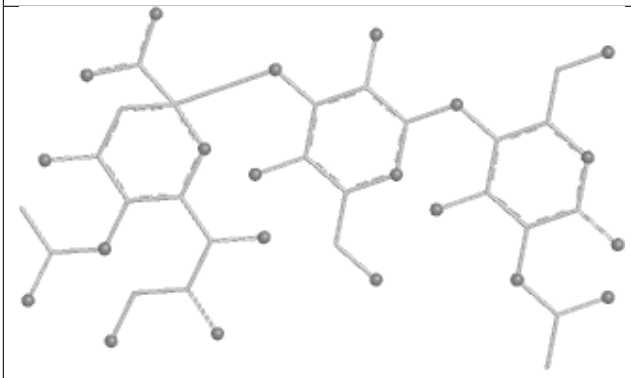
Oligosaccharide Chain EA



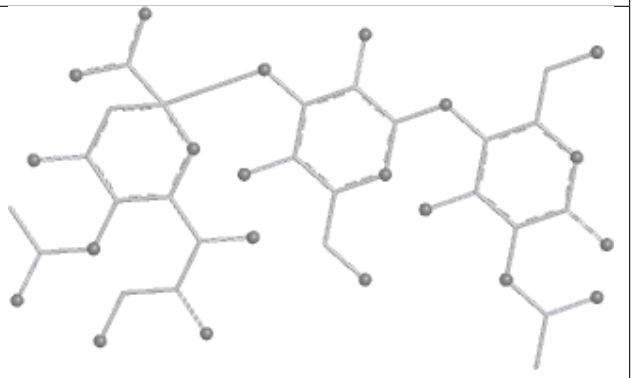
Bond lengths



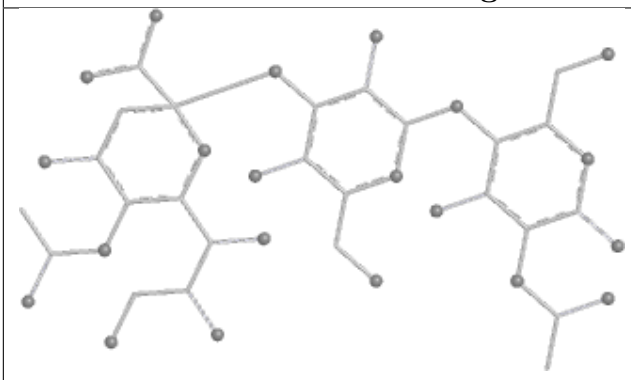
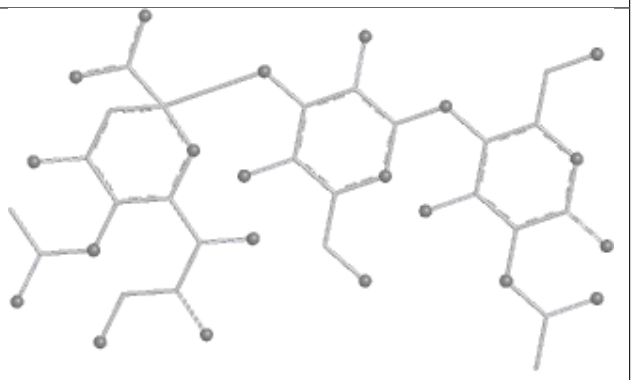
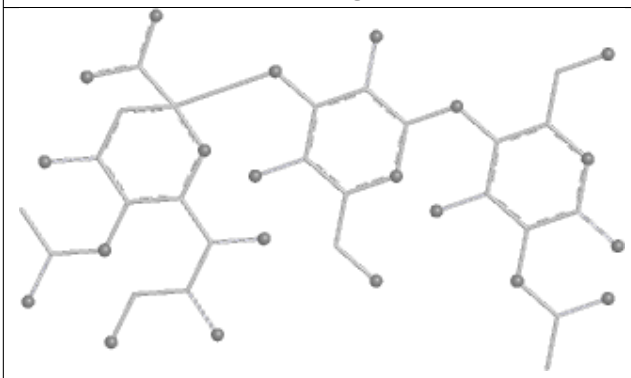
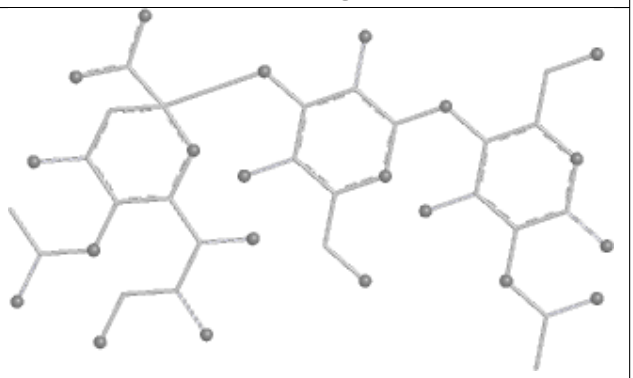
Bond angles

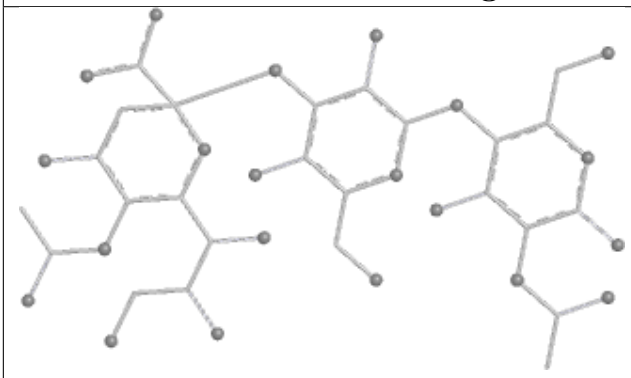
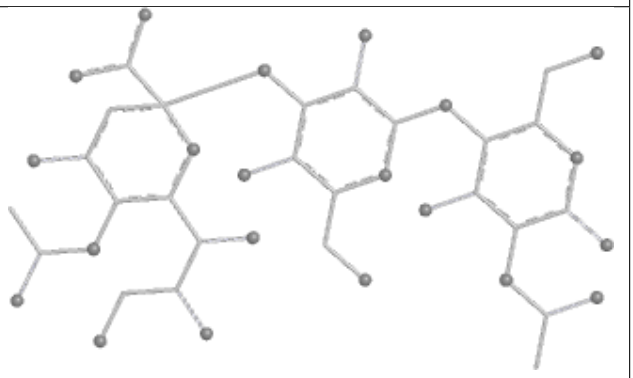
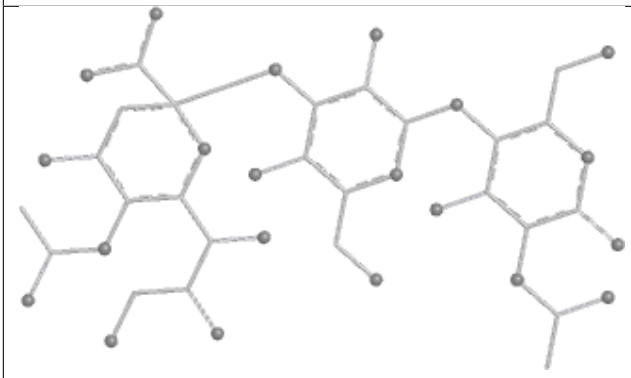
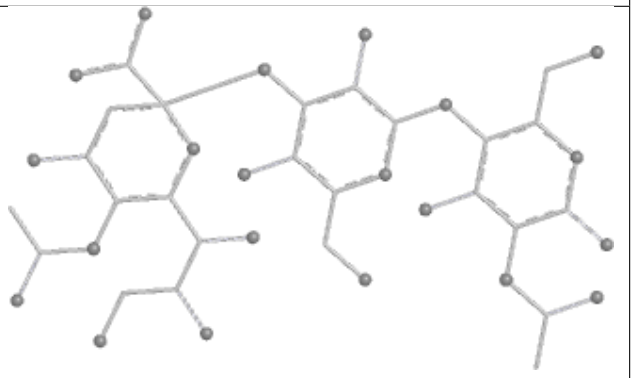


Torsions

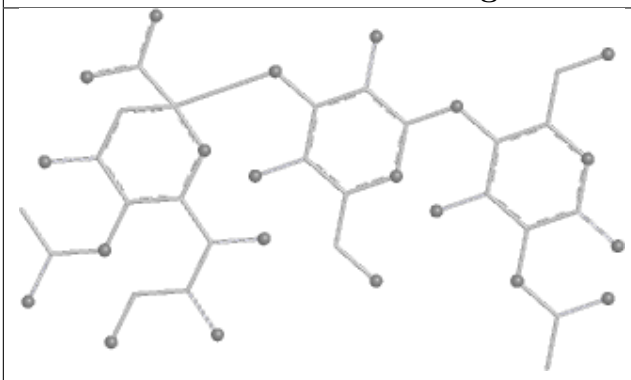


Rings

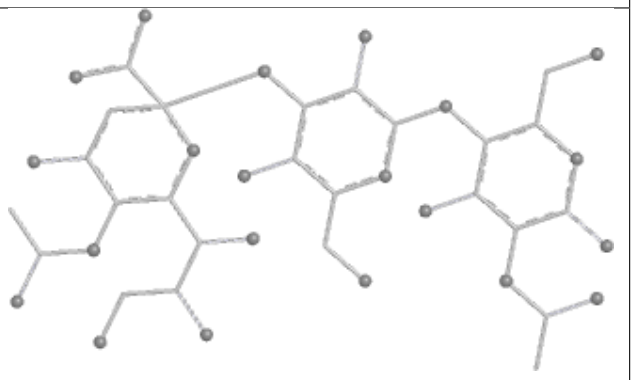
Oligosaccharide Chain HA	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

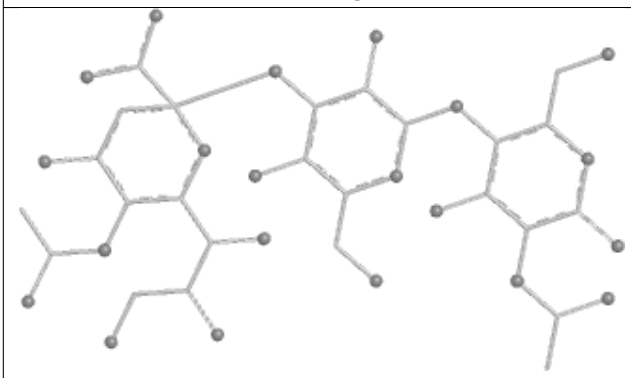
Oligosaccharide Chain NA



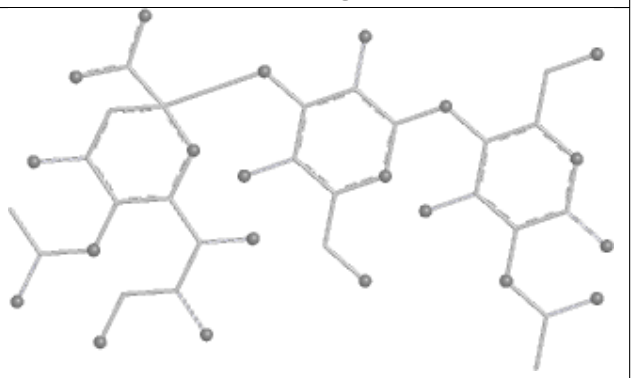
Bond lengths



Bond angles

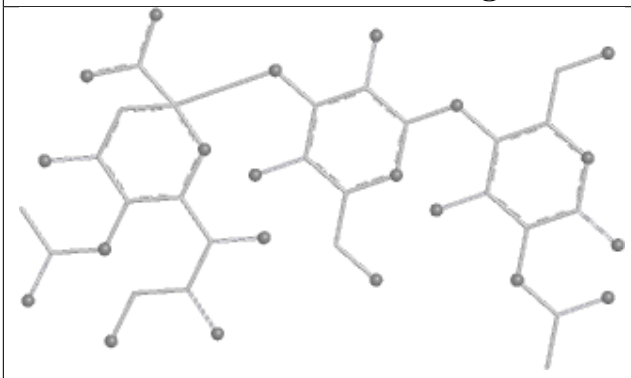


Torsions

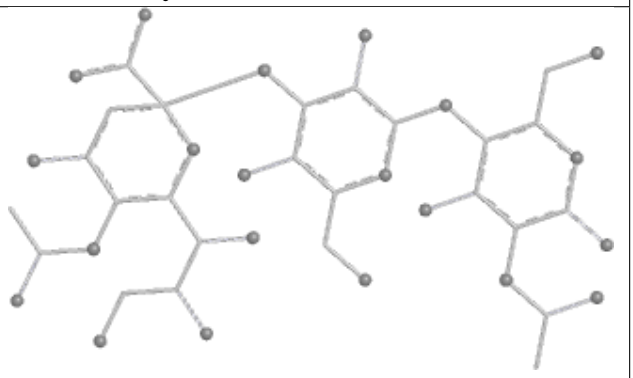


Rings

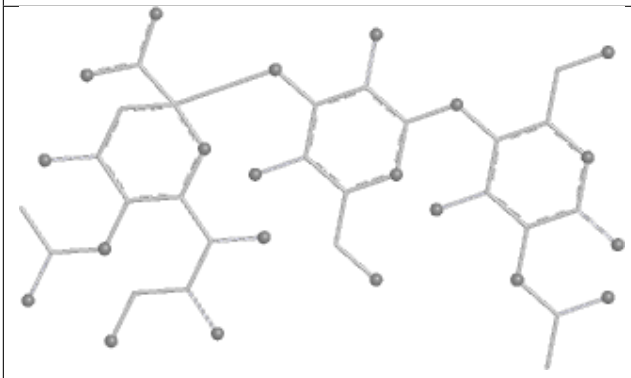
Oligosaccharide Chain QA



Bond lengths



Bond angles



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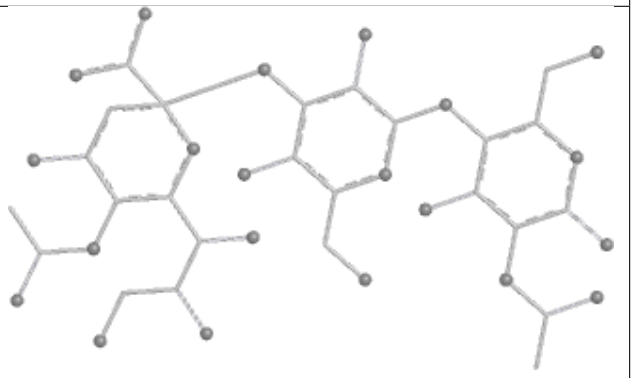
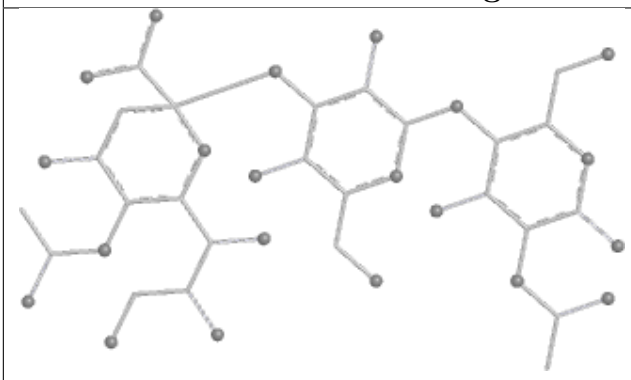
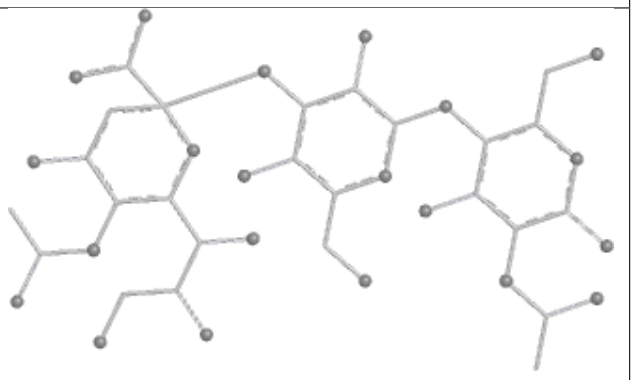


Rings

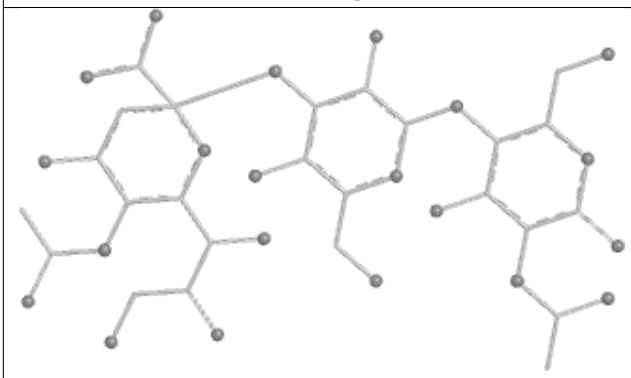
Oligosaccharide Chain TA



Bond lengths



Bond angles



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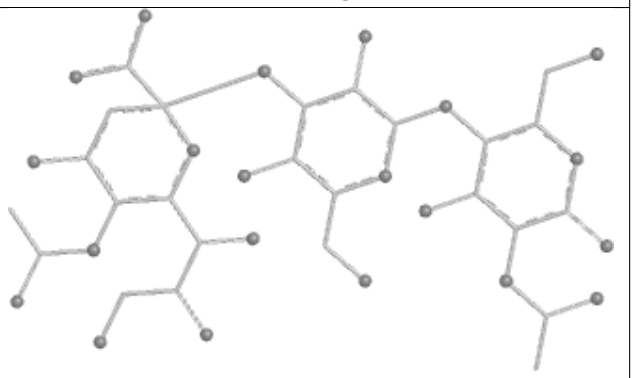
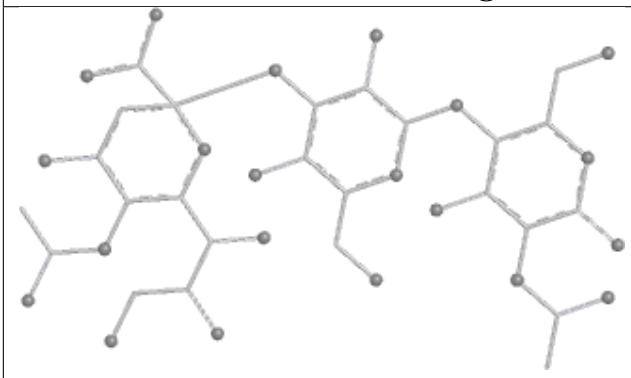
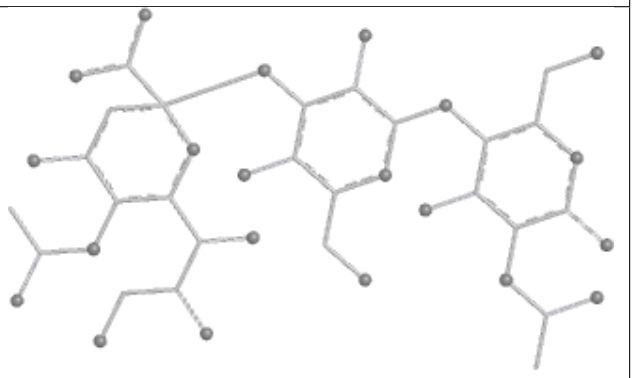


Rings

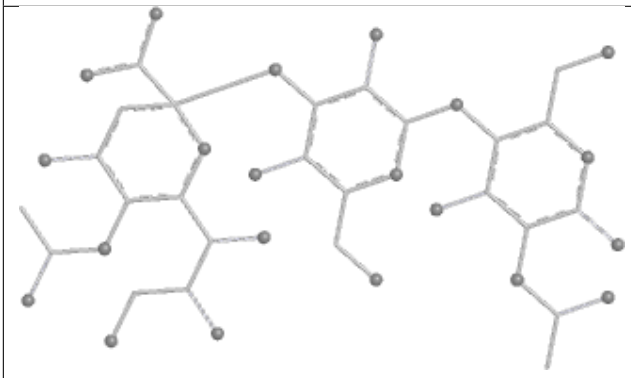
Oligosaccharide Chain WA



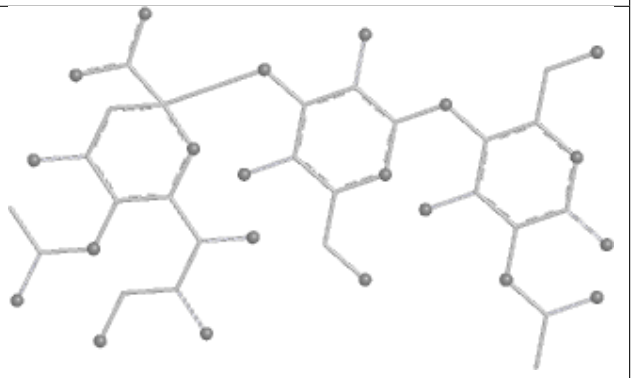
Bond lengths



Bond angles

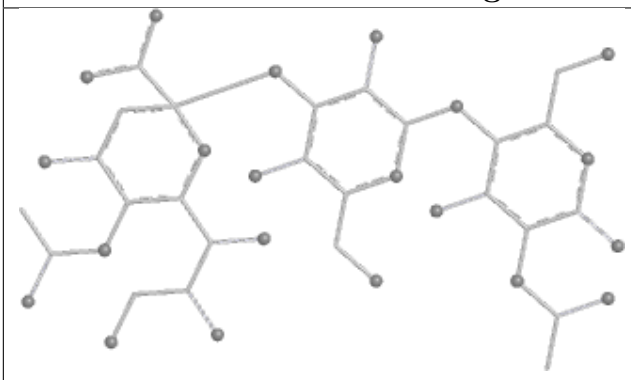


Torsions

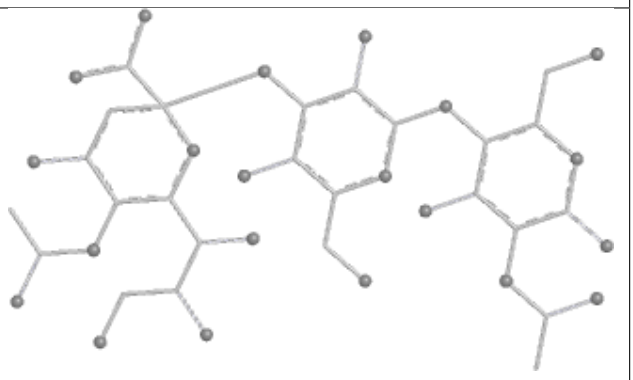


Rings

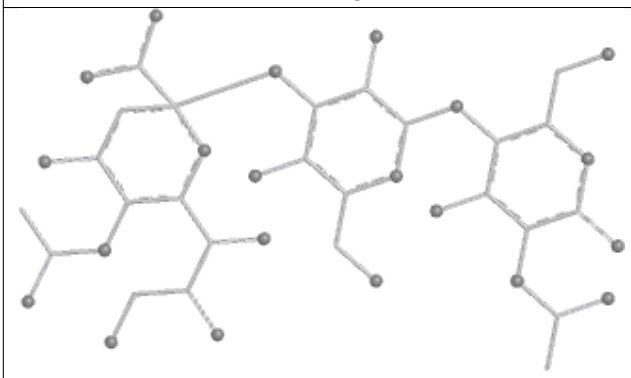
Oligosaccharide Chain ZA



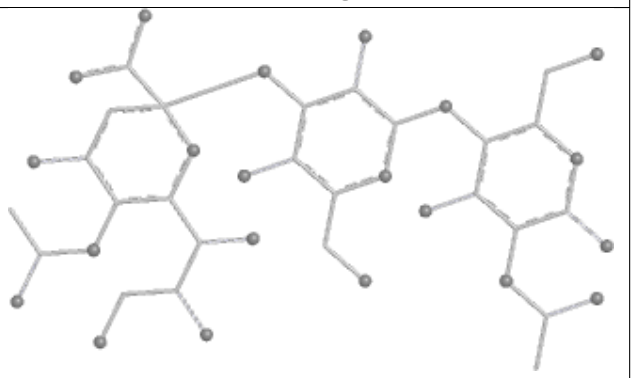
Bond lengths



Bond angles

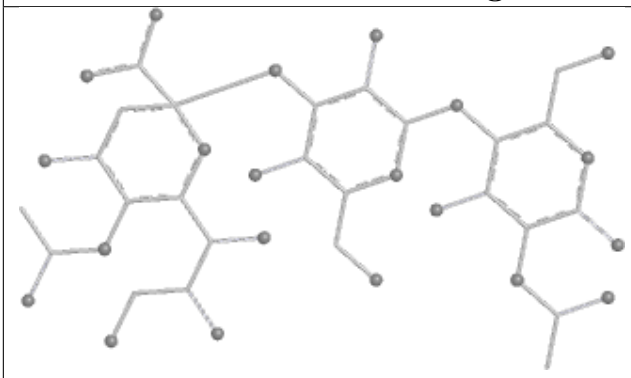


Torsions

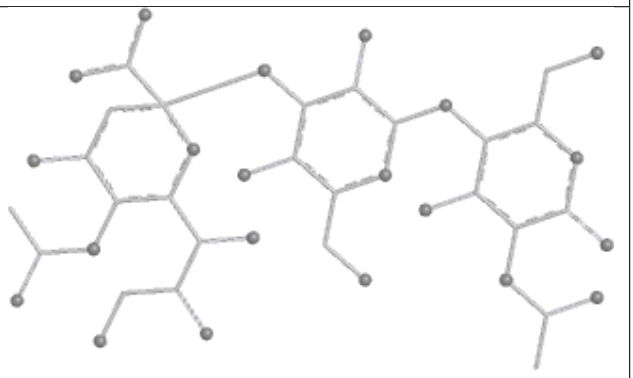


Rings

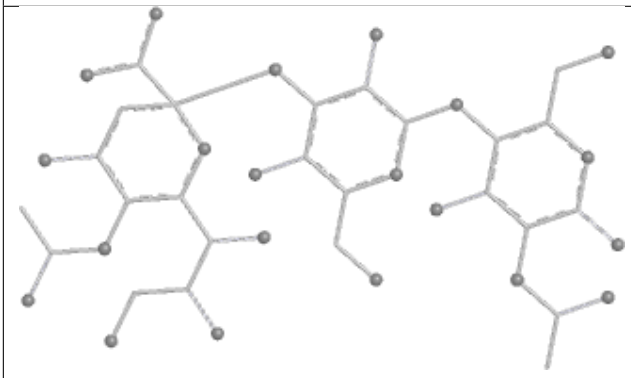
Oligosaccharide Chain cA



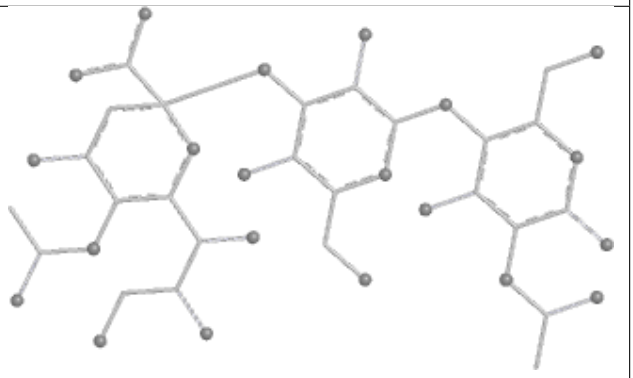
Bond lengths



Bond angles

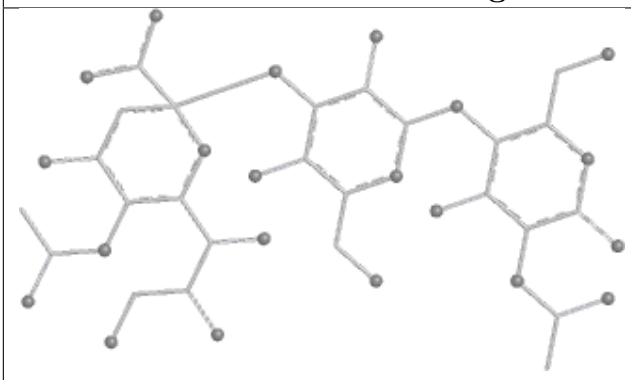


Torsions

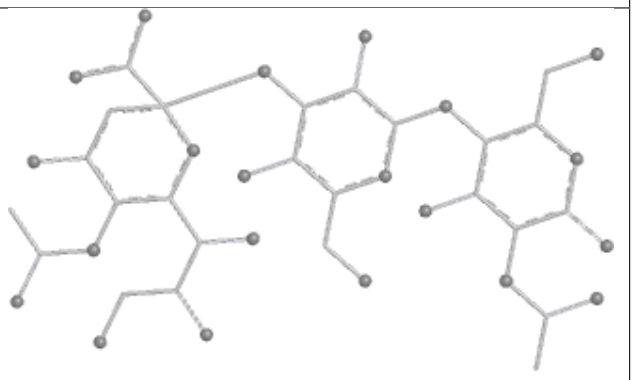


Rings

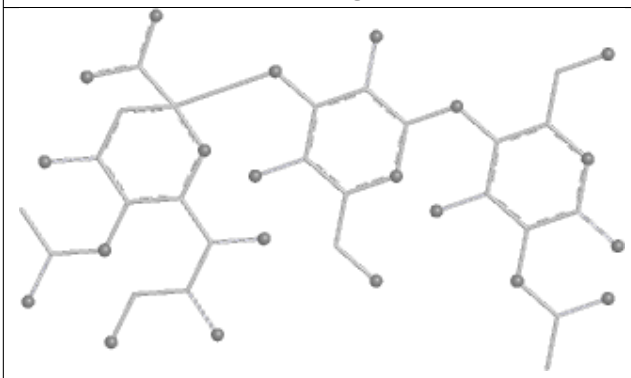
Oligosaccharide Chain fA



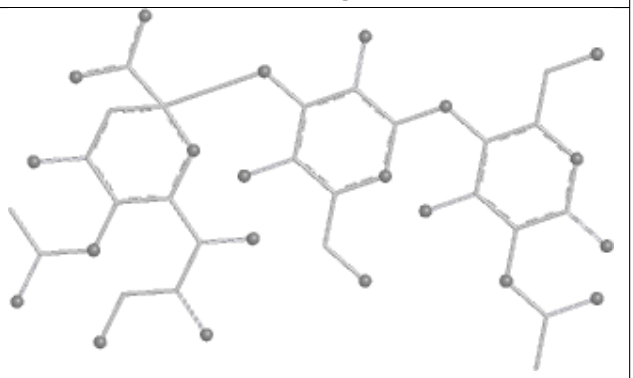
Bond lengths



Bond angles

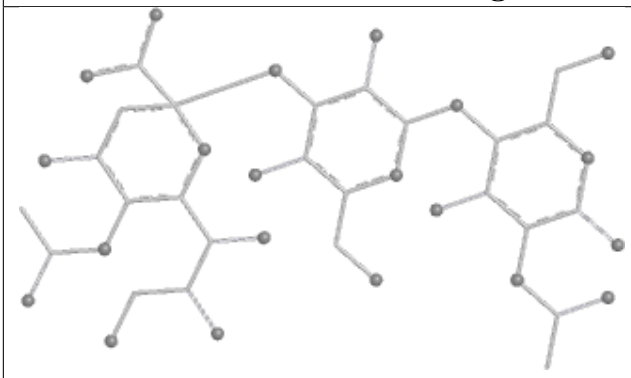


Torsions

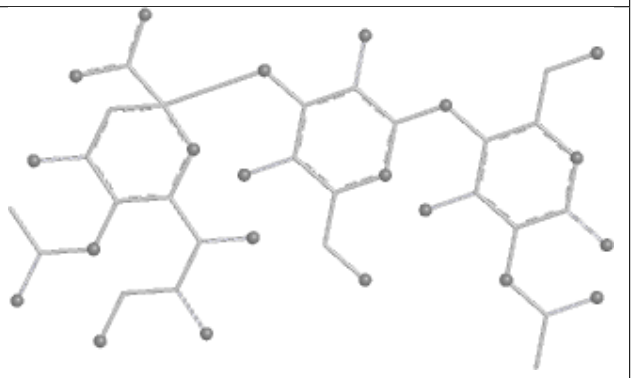


Rings

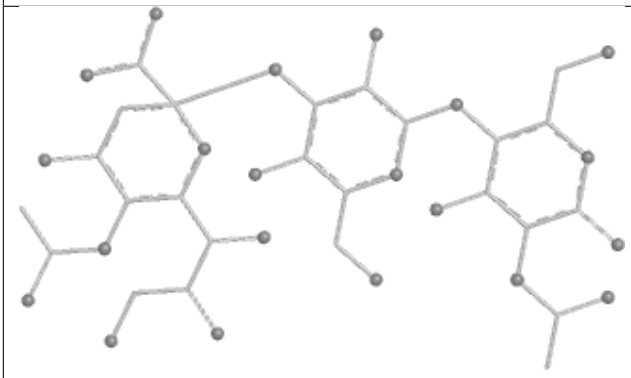
Oligosaccharide Chain iA



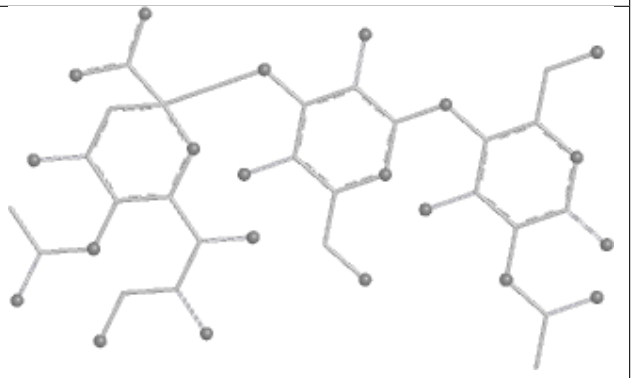
Bond lengths



Bond angles

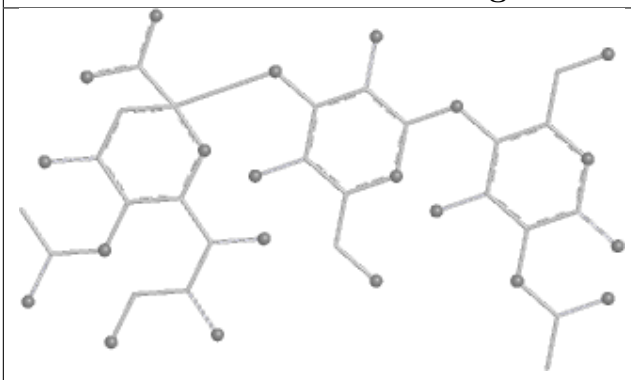


Torsions

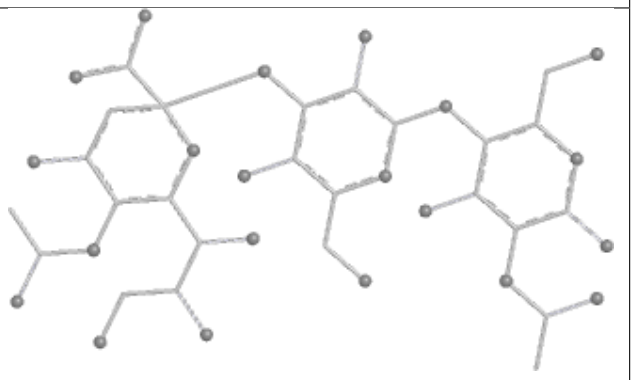


Rings

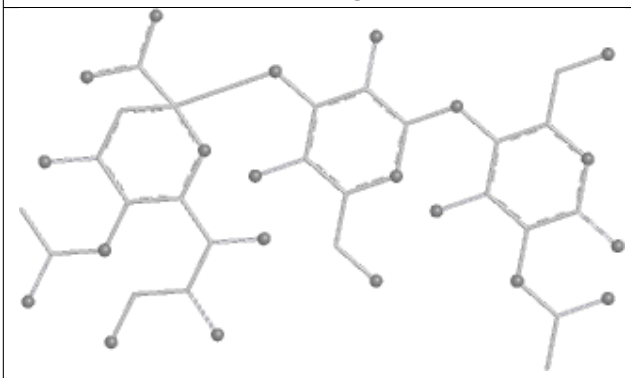
Oligosaccharide Chain lA



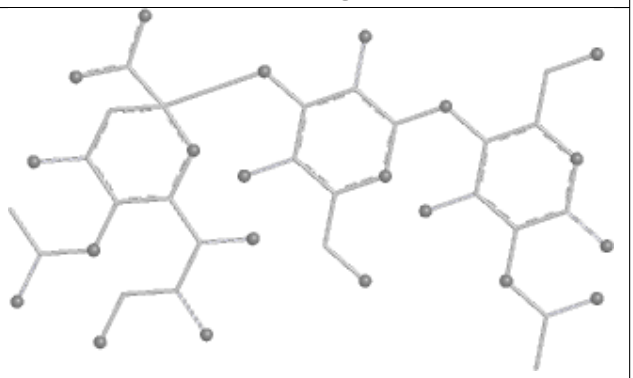
Bond lengths



Bond angles

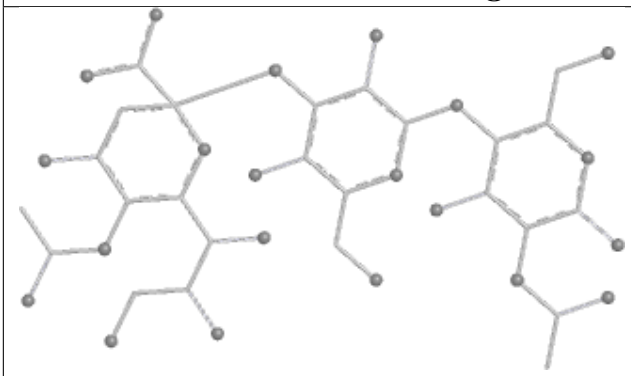


Torsions

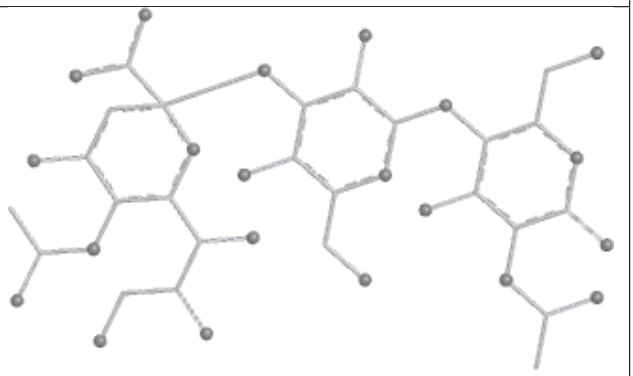


Rings

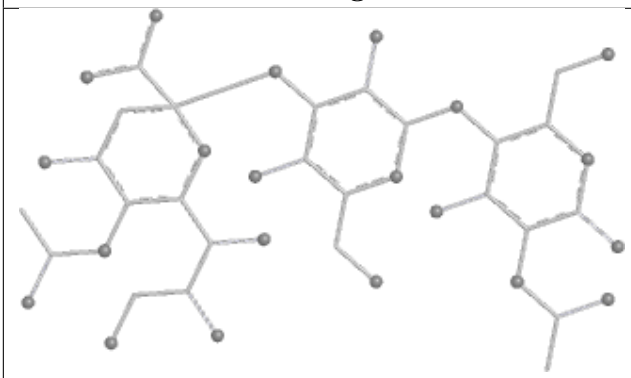
Oligosaccharide Chain oA



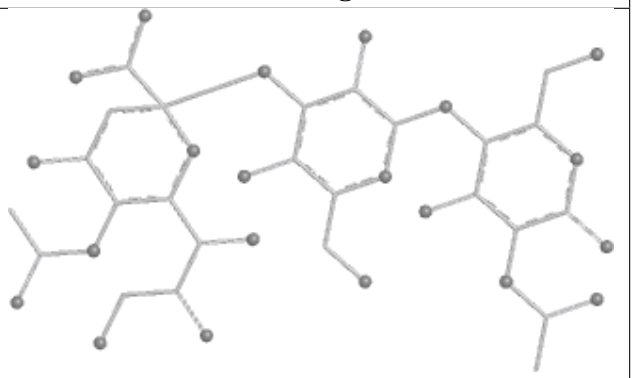
Bond lengths



Bond angles

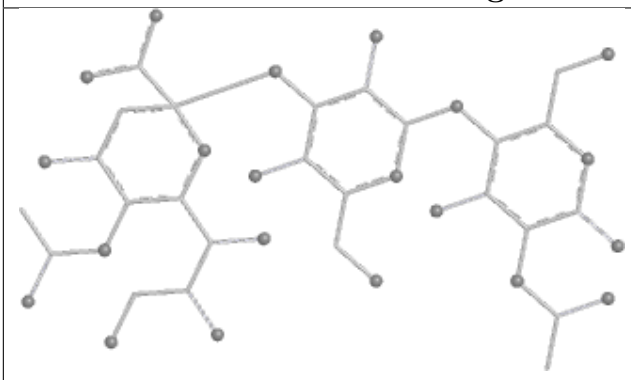


Torsions



Rings

Oligosaccharide Chain rA



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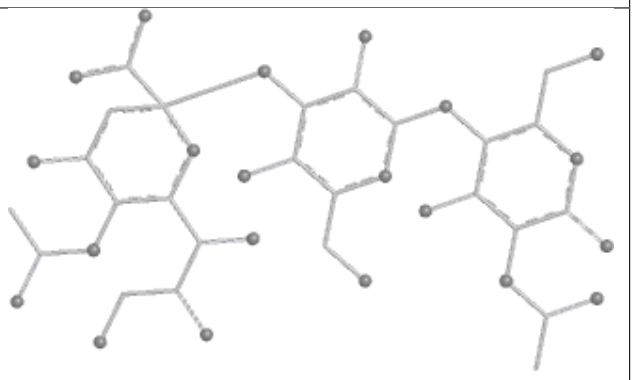
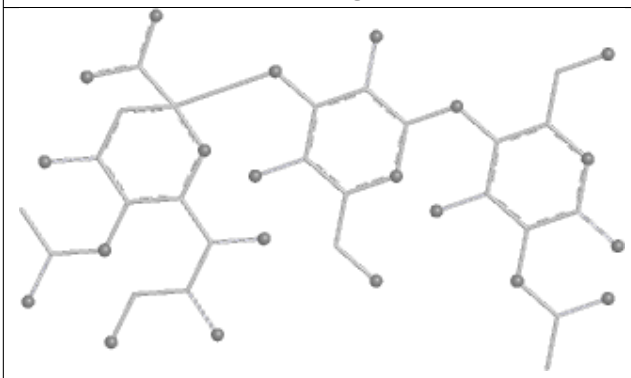


Bond angles



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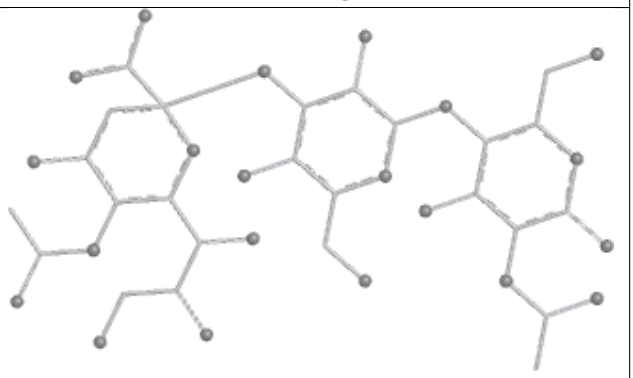
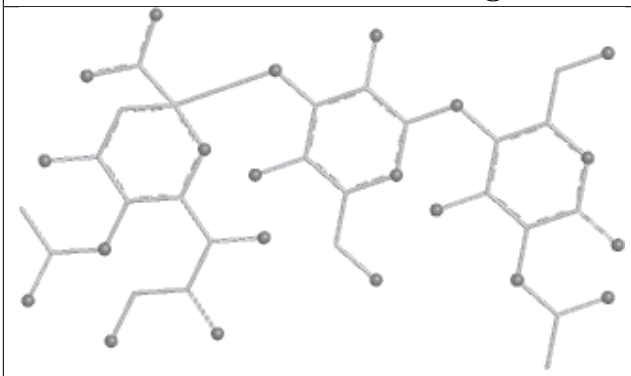


Rings

Oligosaccharide Chain uA



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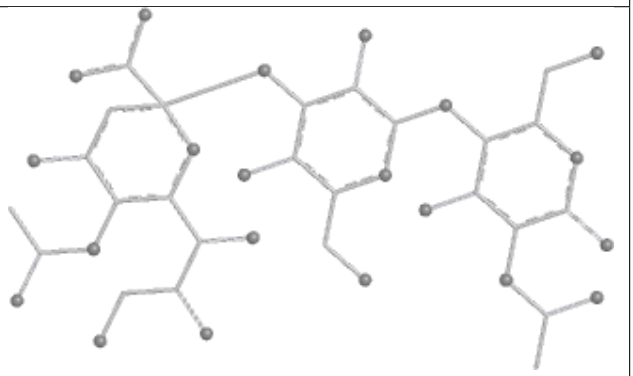
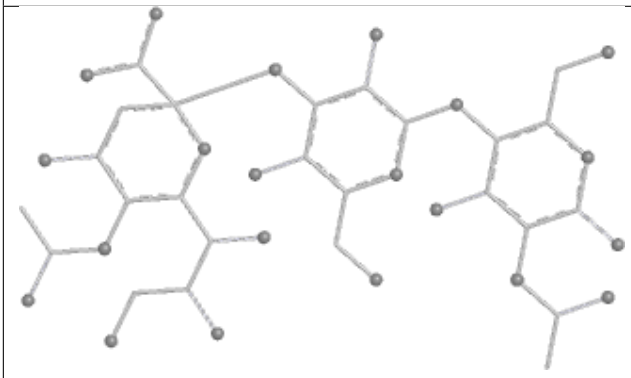
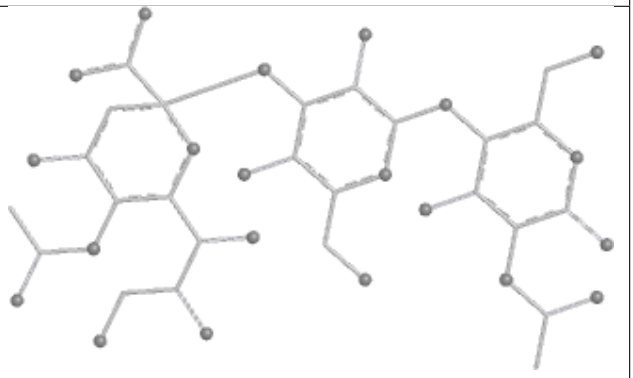


Bond angles

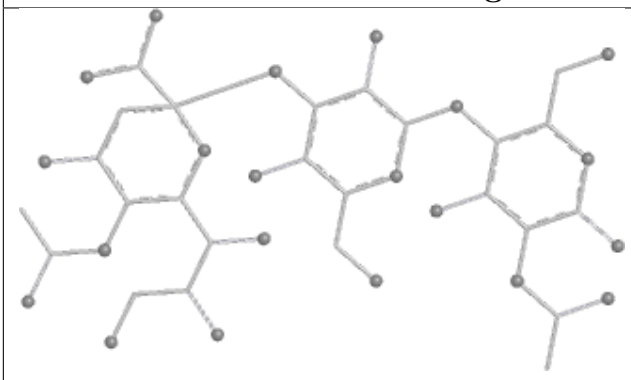


Torsions



Rings

Oligosaccharide Chain xA



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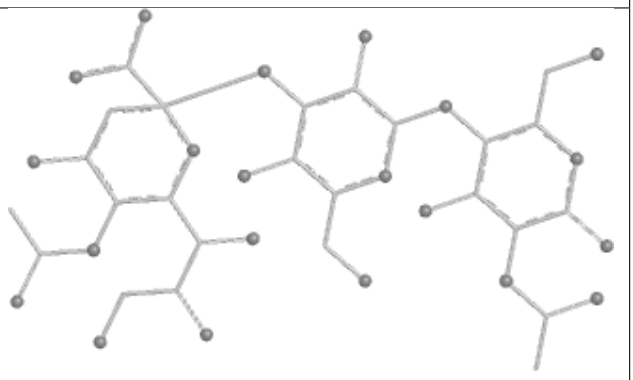
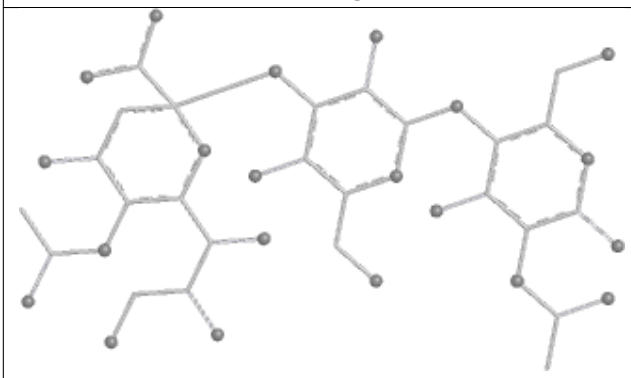
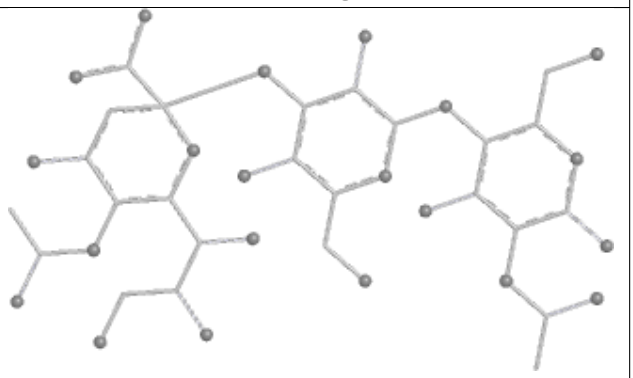


Bond angles

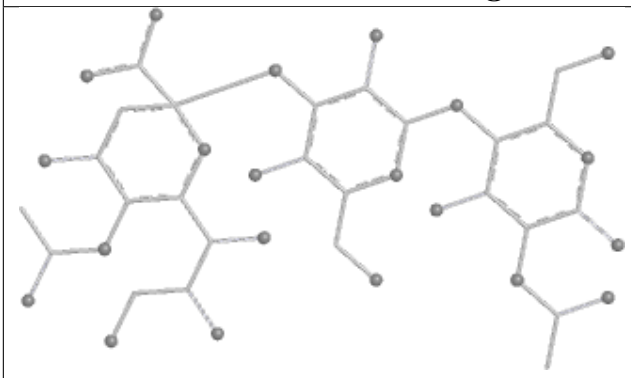


Torsions



Rings

Oligosaccharide Chain 0A



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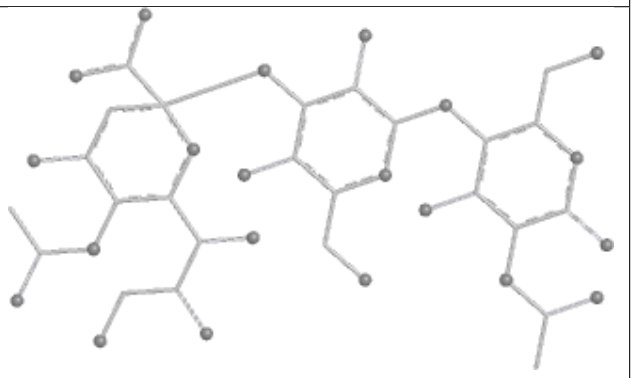
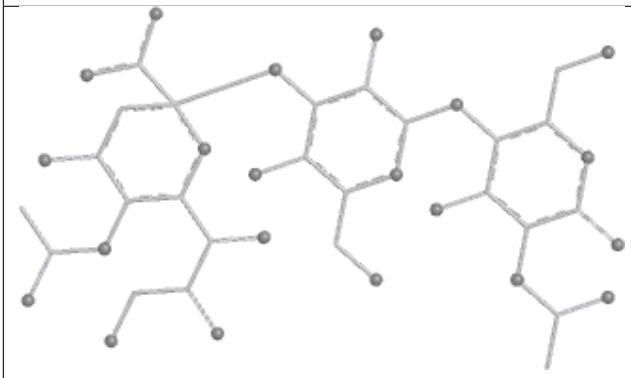


Bond angles



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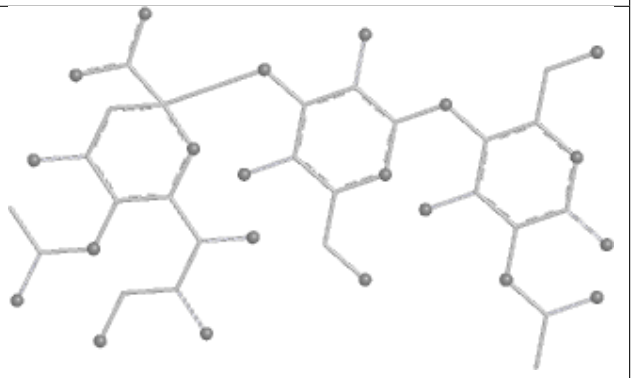
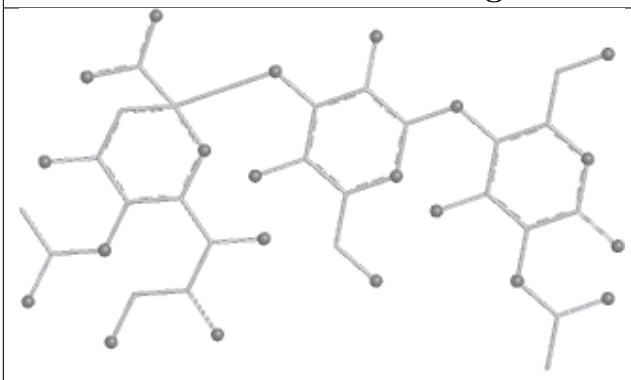


Rings

Oligosaccharide Chain 3A



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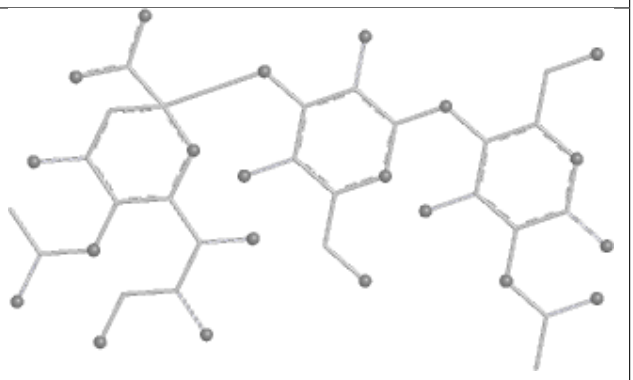
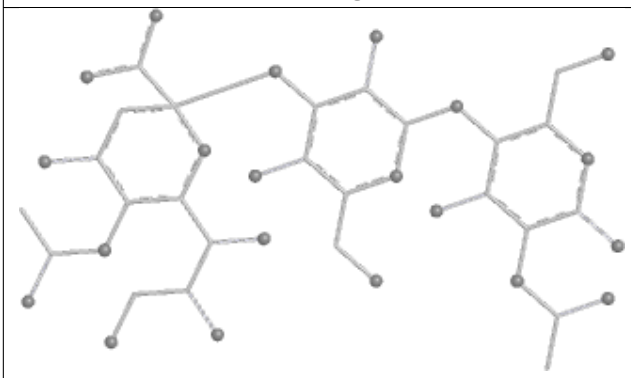


Bond angles



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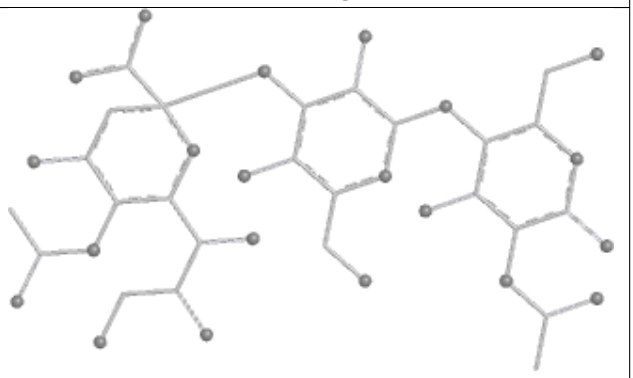
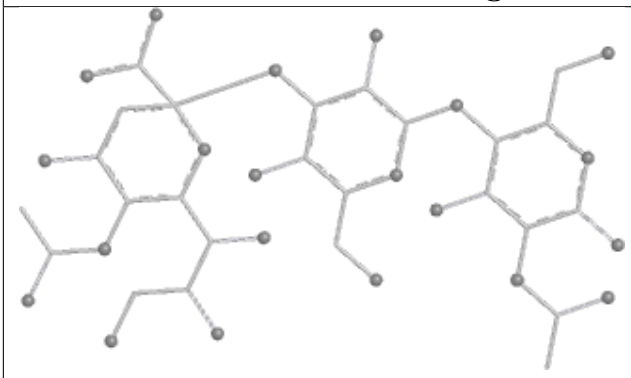


Rings

Oligosaccharide Chain 6A



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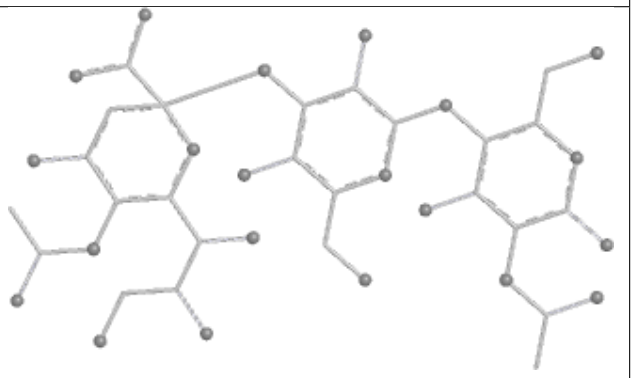
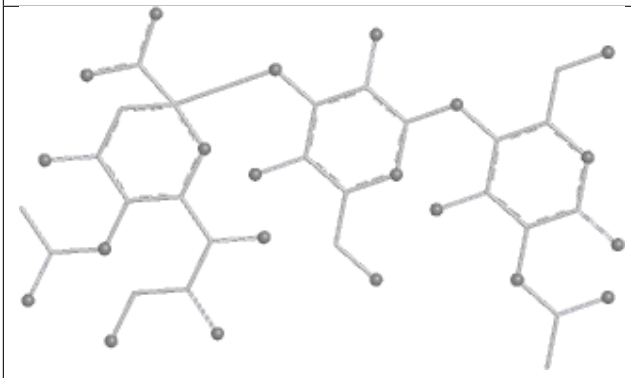


Bond angles



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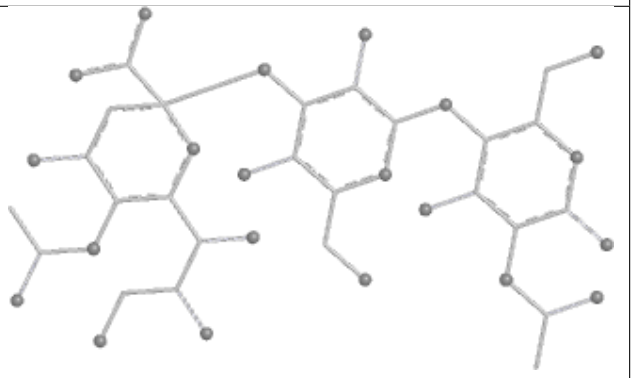
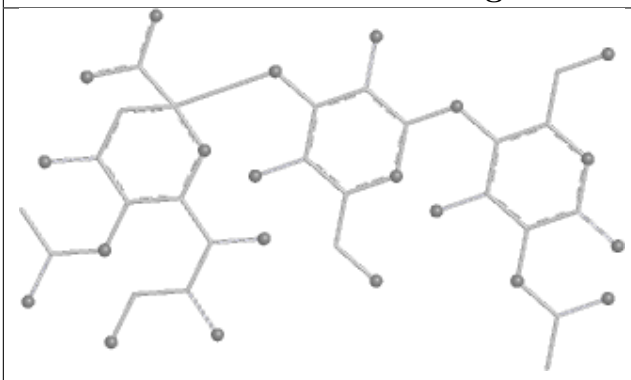


Rings

Oligosaccharide Chain 9A



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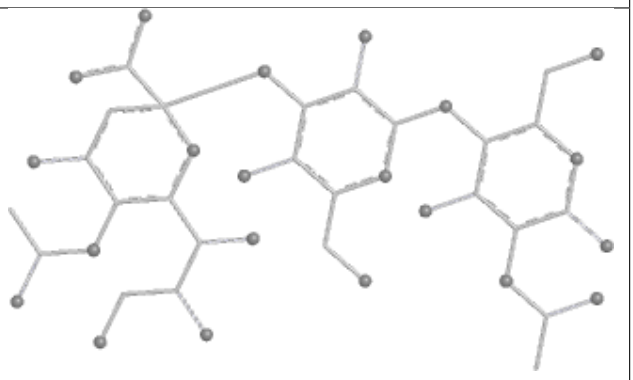
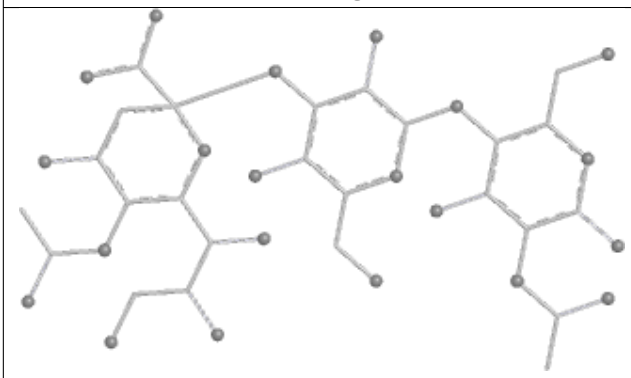


Bond angles



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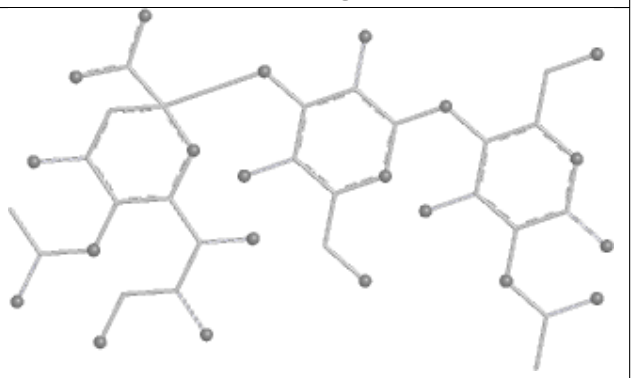
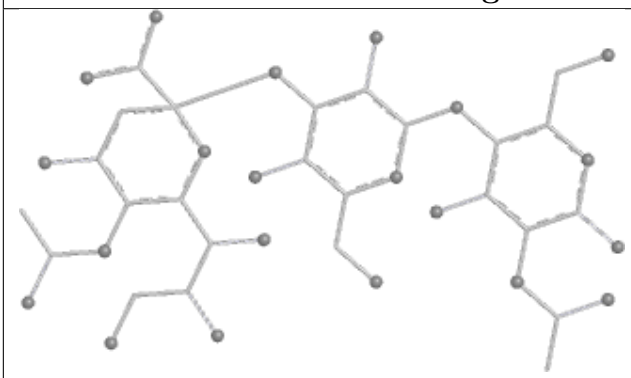


Rings

Oligosaccharide Chain CB



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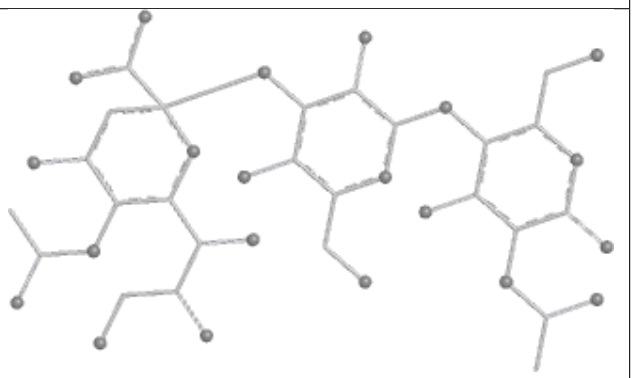
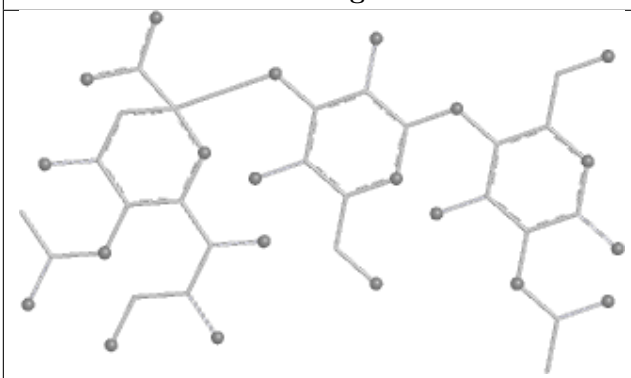


Bond angles



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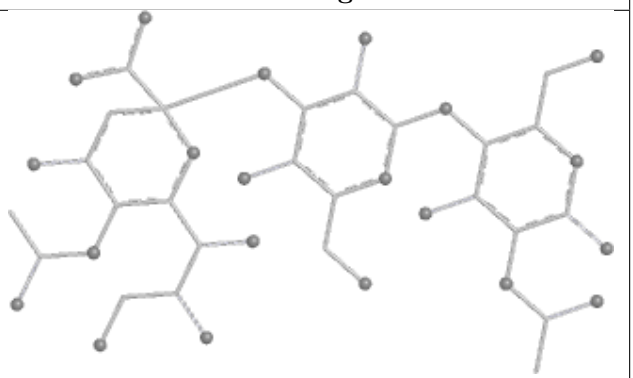
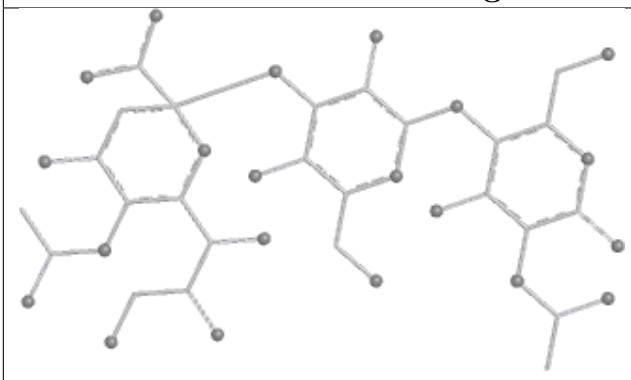


Rings

Oligosaccharide Chain FB



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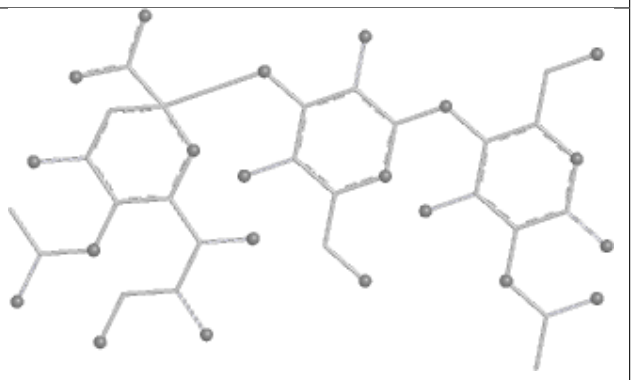
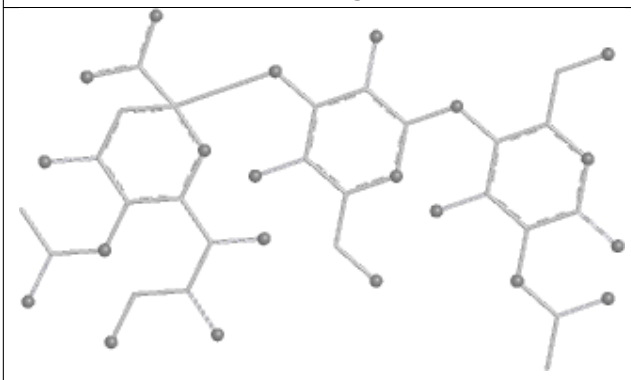
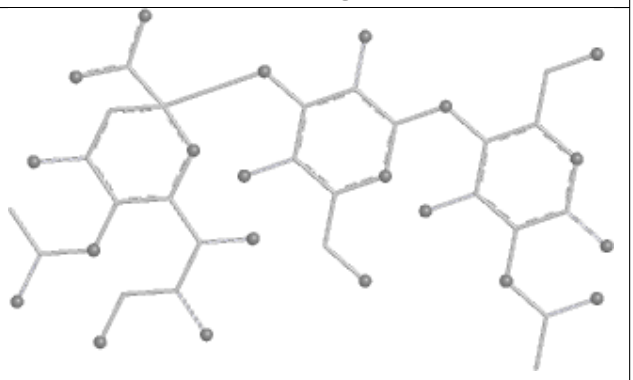


Bond angles

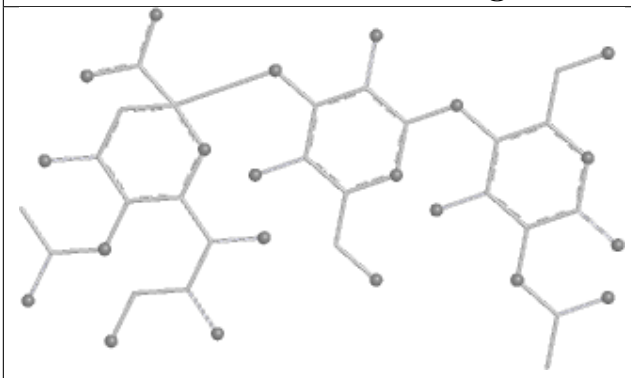


Torsions

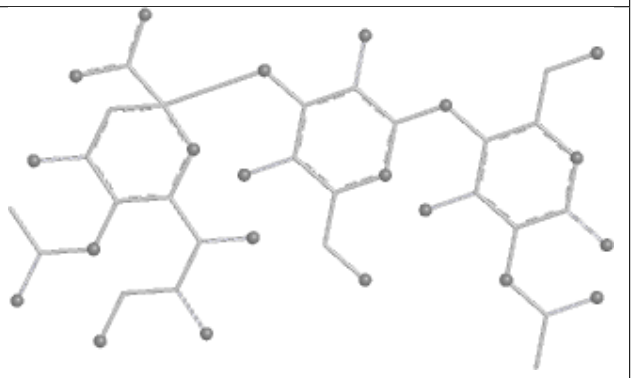


Rings

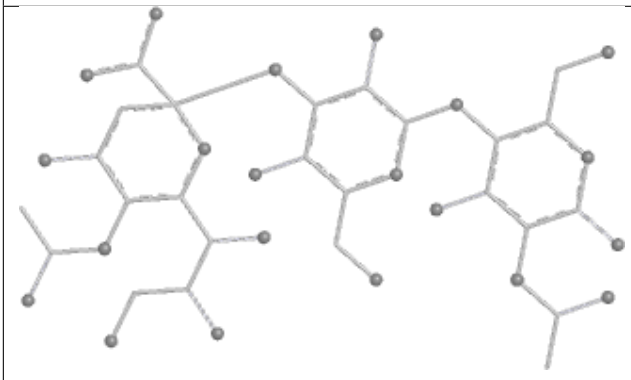
Oligosaccharide Chain IB



Bond lengths



Bond angles



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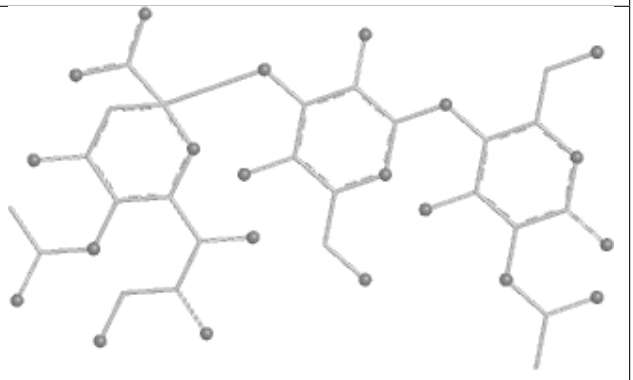
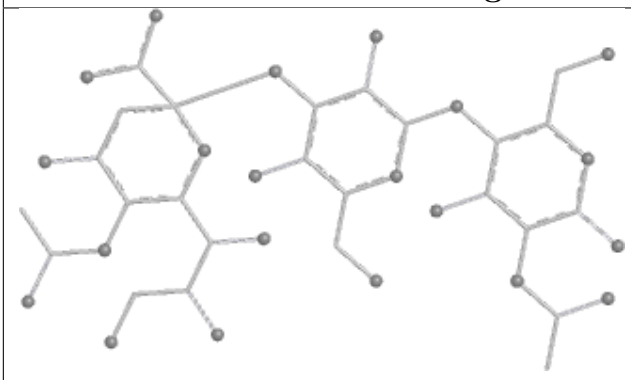


Rings

Oligosaccharide Chain LB



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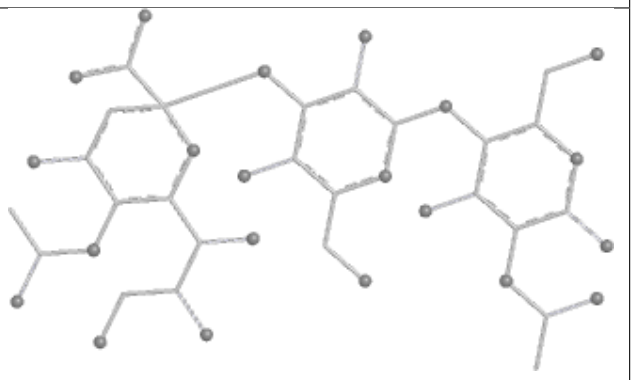
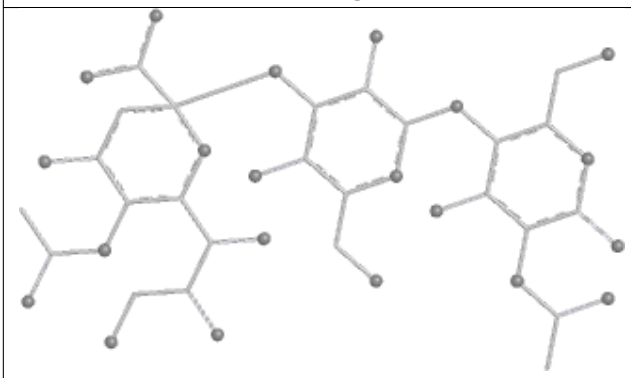


Bond angles



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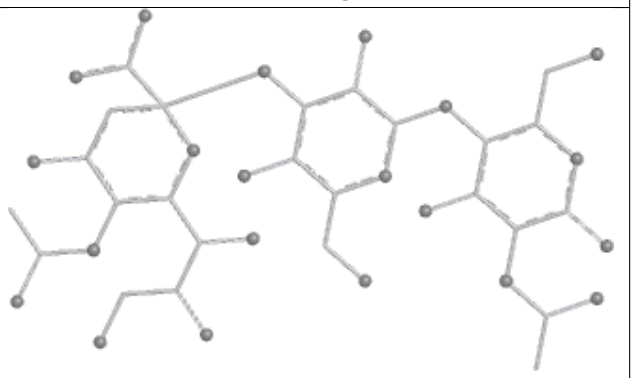
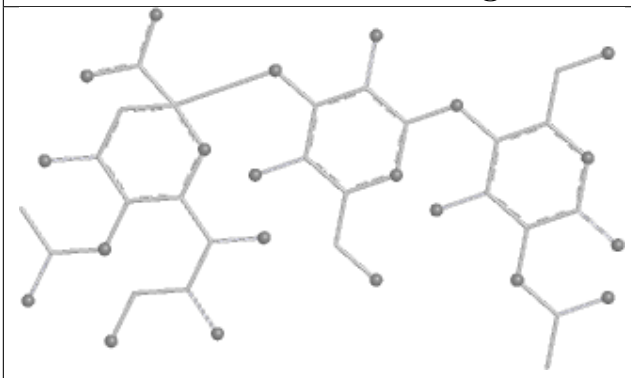


Rings

Oligosaccharide Chain OB



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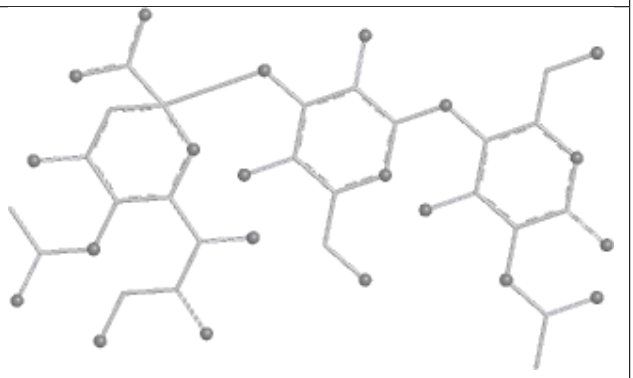
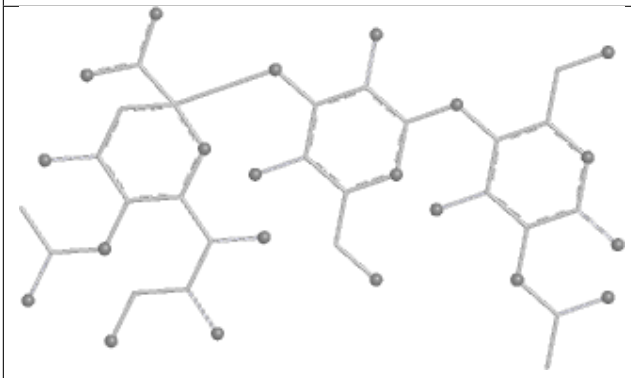


Bond angles



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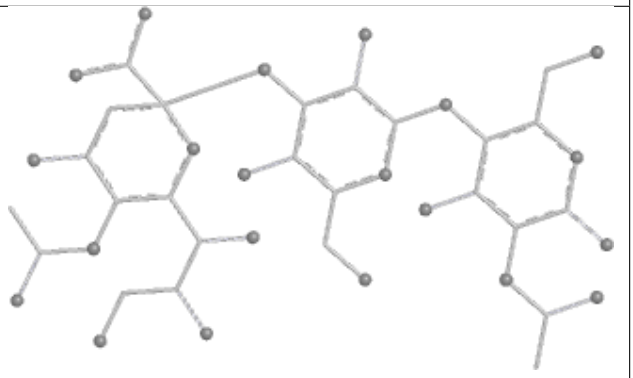
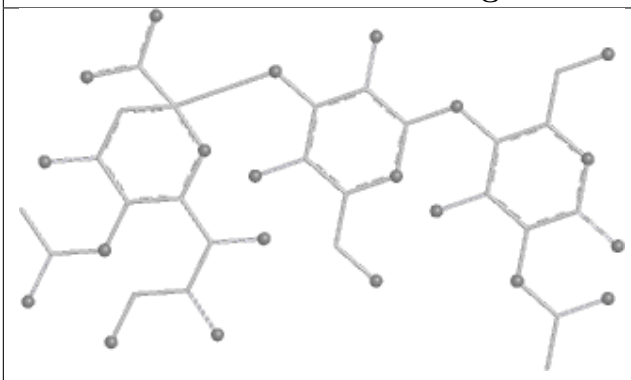


Rings

Oligosaccharide Chain RB



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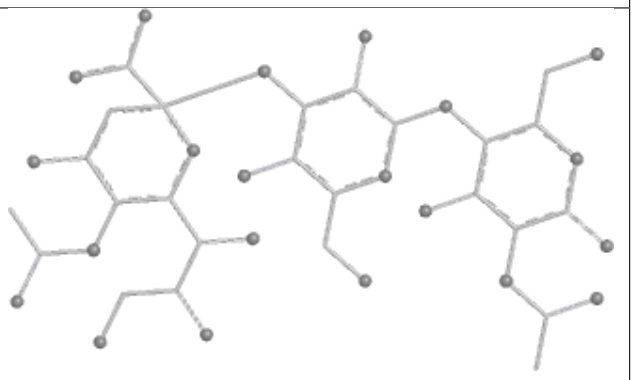
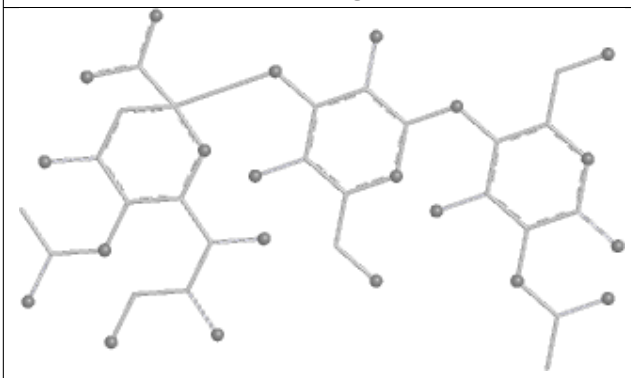


Bond angles



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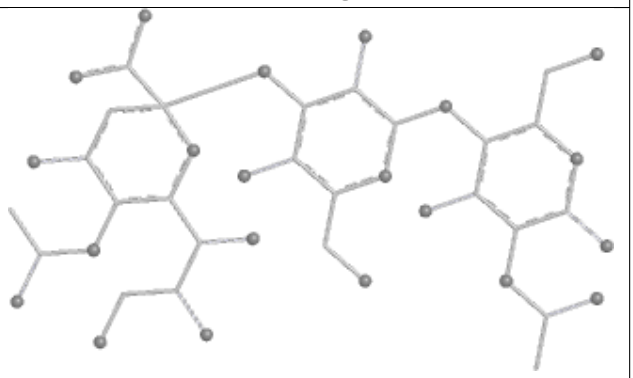
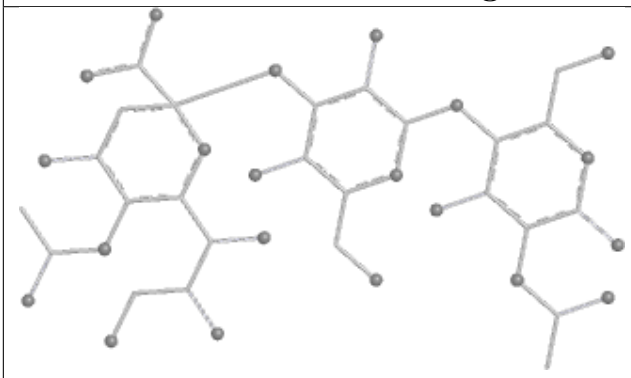


Rings

Oligosaccharide Chain UB



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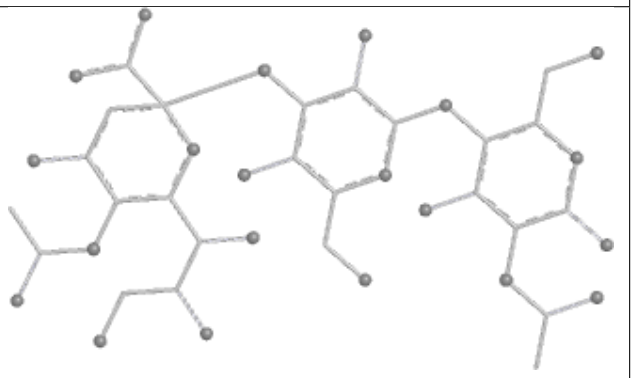
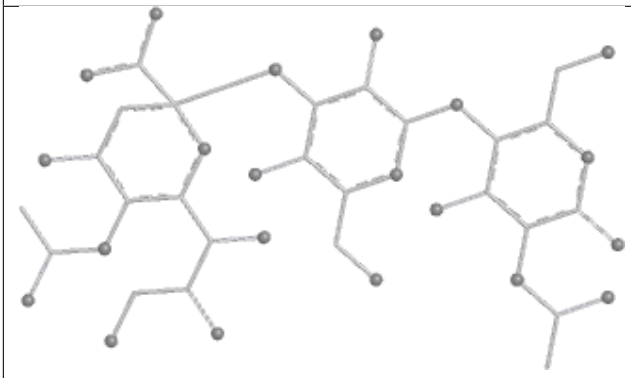


Bond angles



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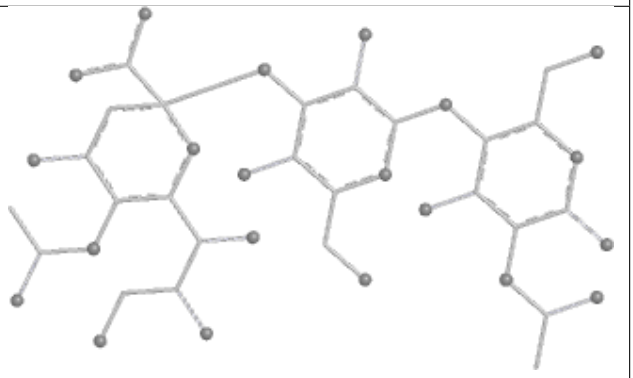
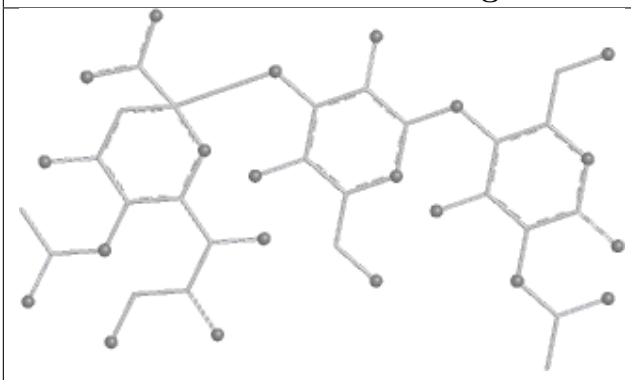
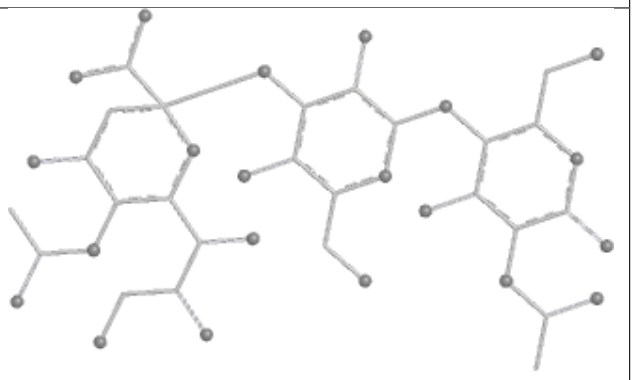


Rings

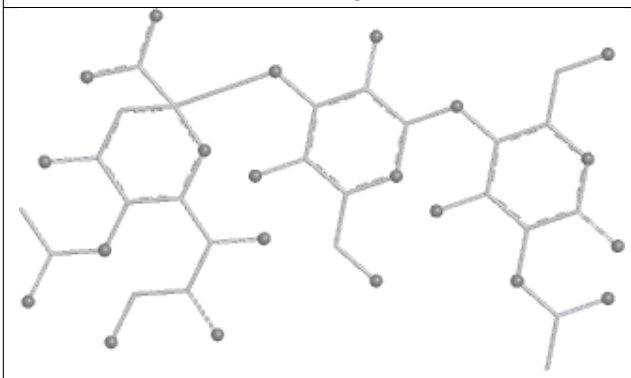
Oligosaccharide Chain XB



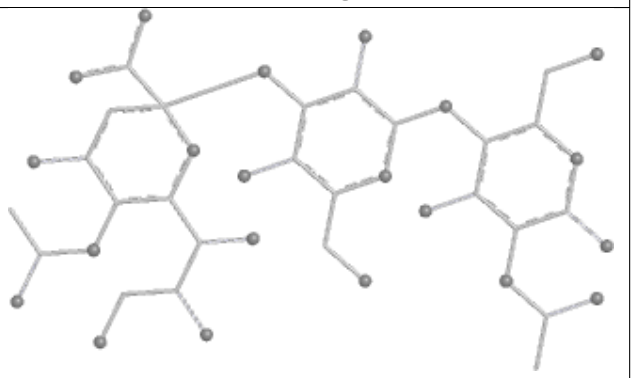
Bond lengths



Bond angles

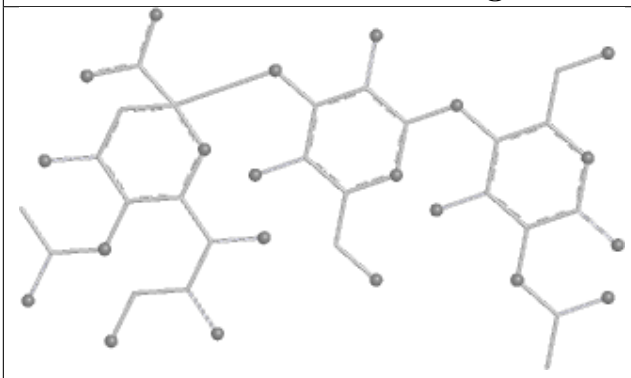


Torsions



Rings

Oligosaccharide Chain aB



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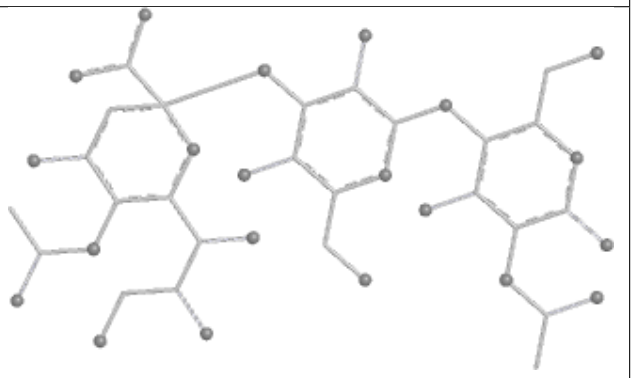

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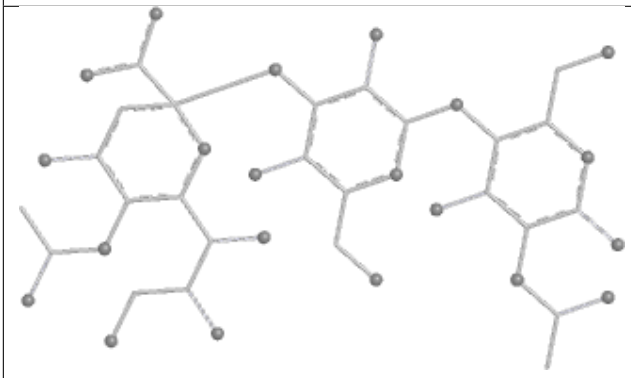

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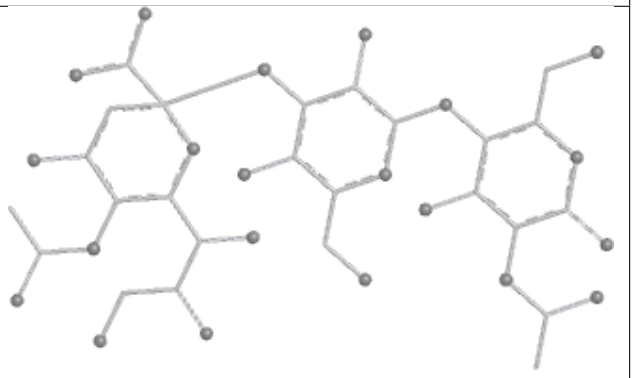
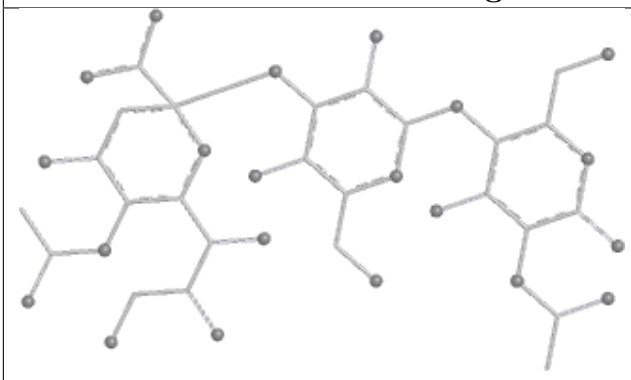


Rings

Oligosaccharide Chain dB



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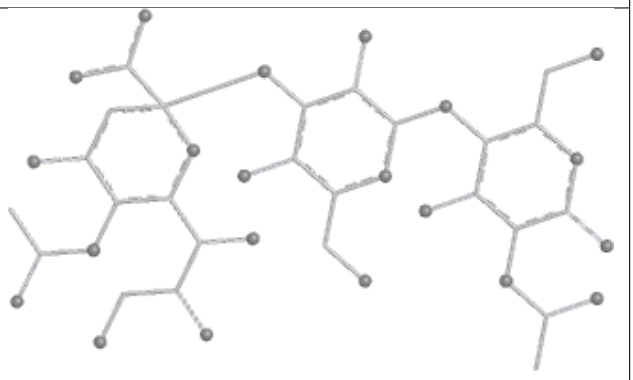
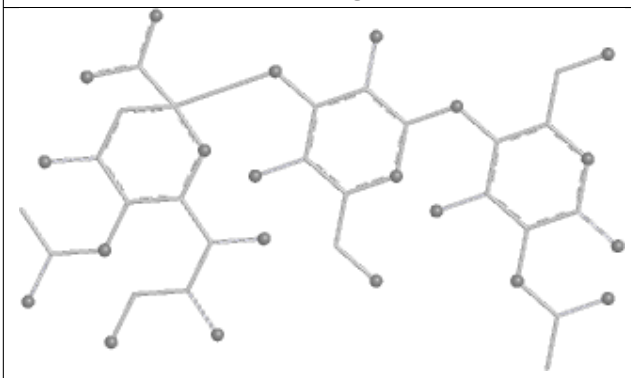


Bond angles



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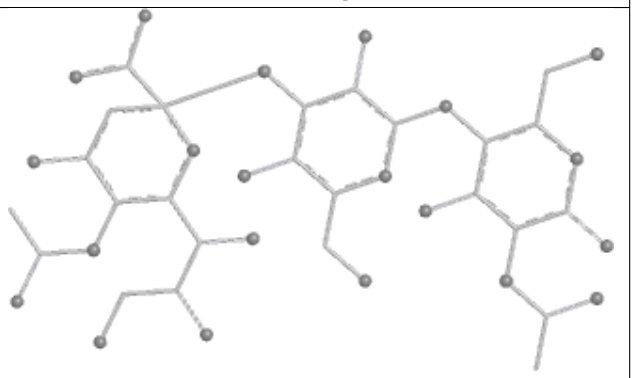
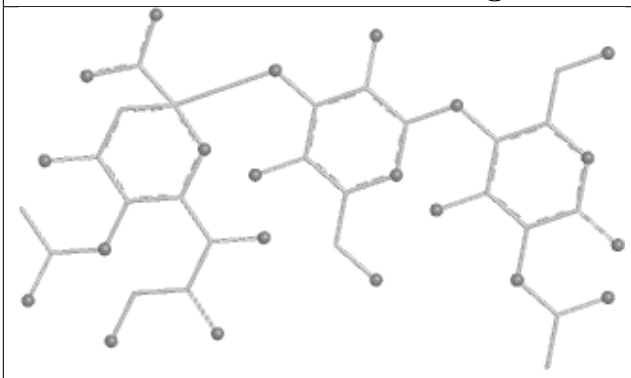


Rings

Oligosaccharide Chain gB



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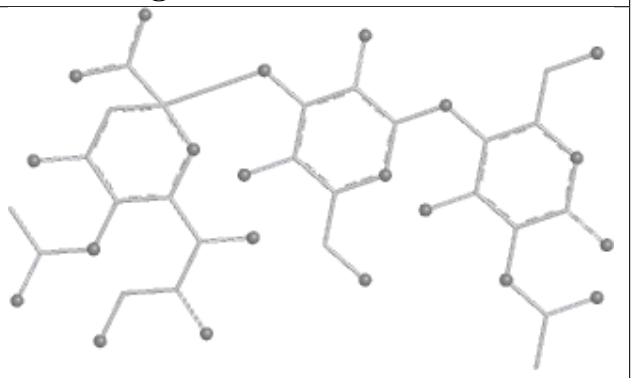

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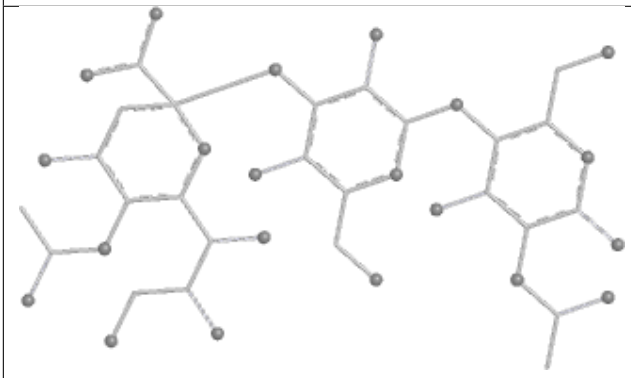

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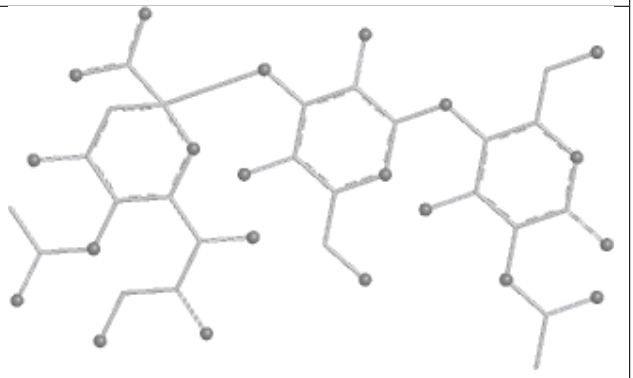
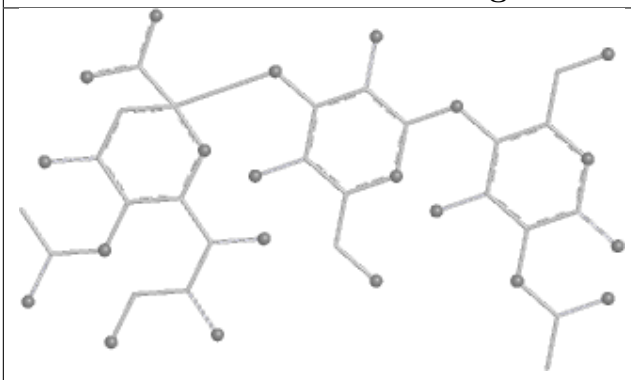


Rings

Oligosaccharide Chain jB



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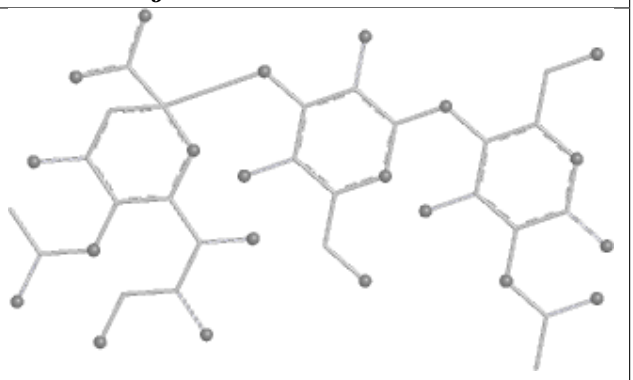

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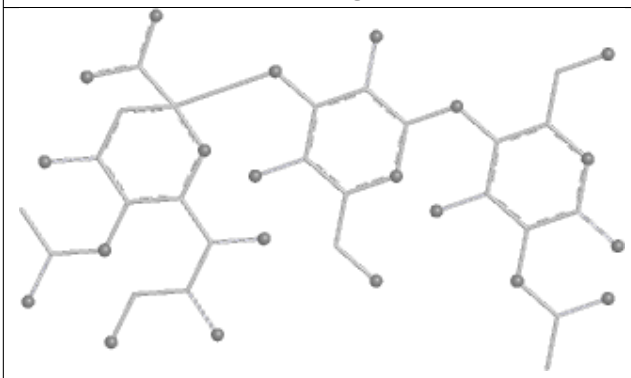

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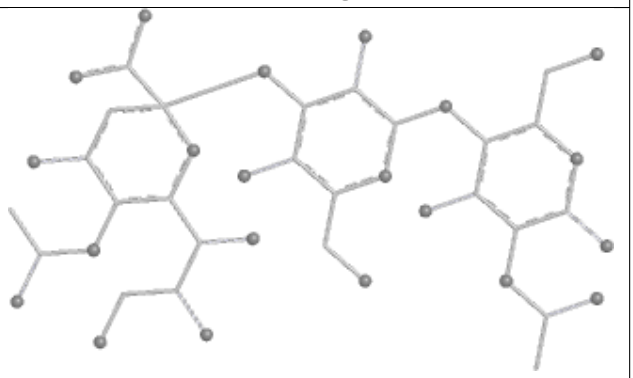
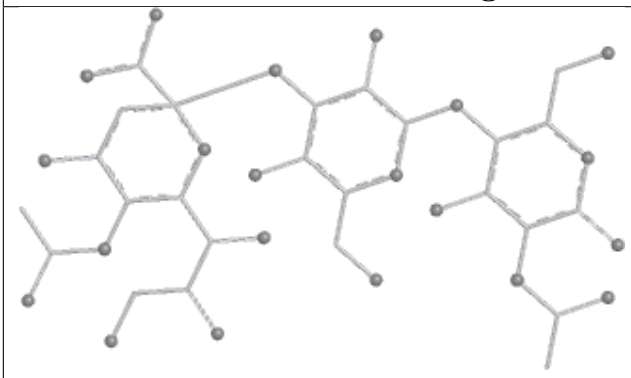


Rings

Oligosaccharide Chain mB



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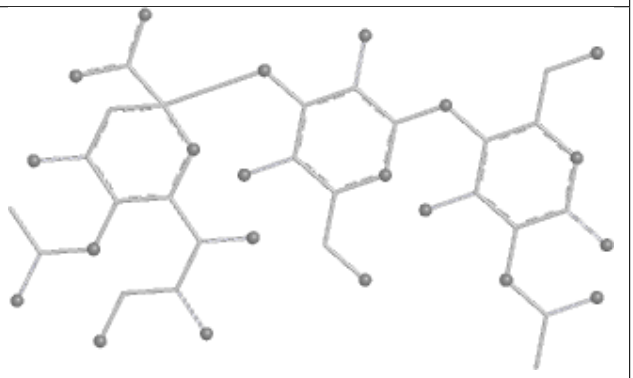
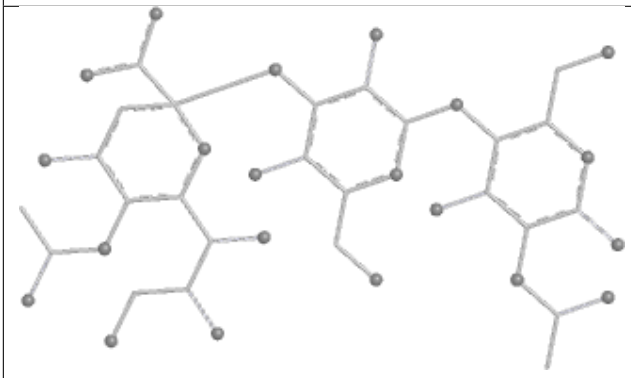


Bond angles



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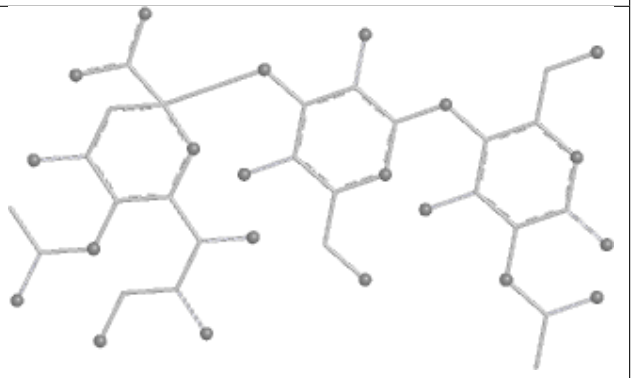
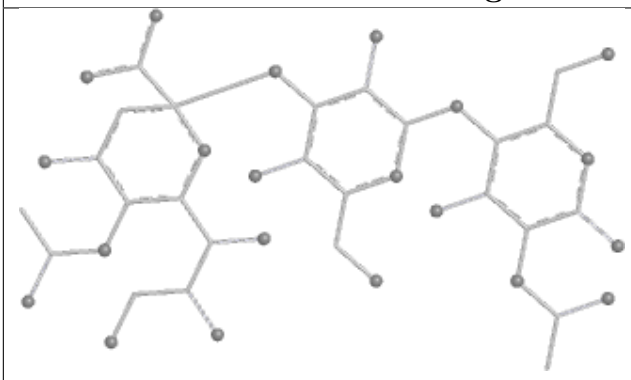


Rings

Oligosaccharide Chain pB



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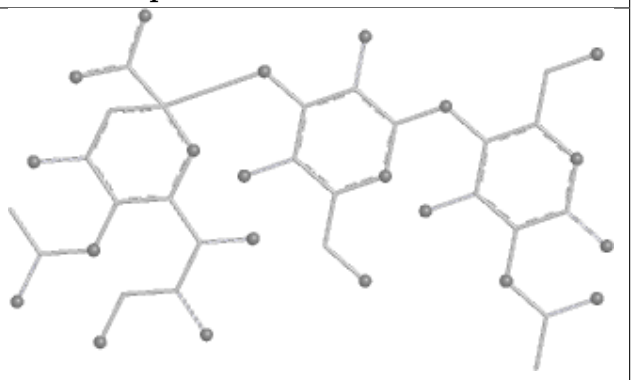

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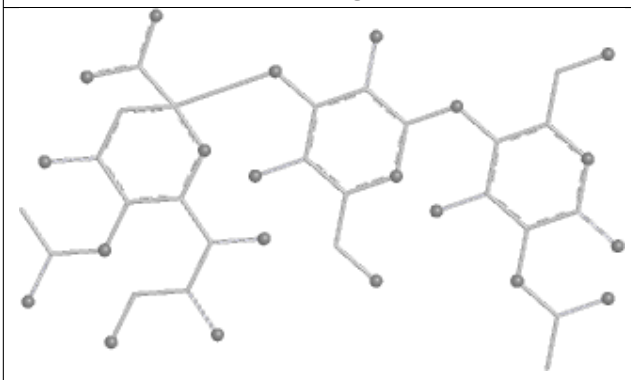

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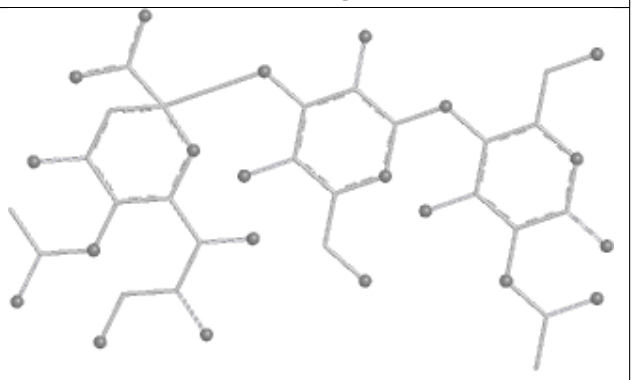
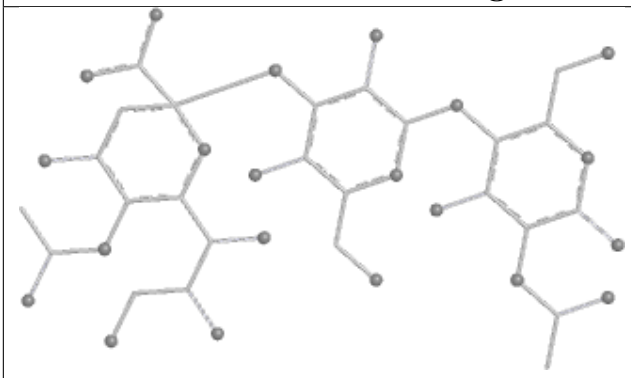


Rings

Oligosaccharide Chain sB



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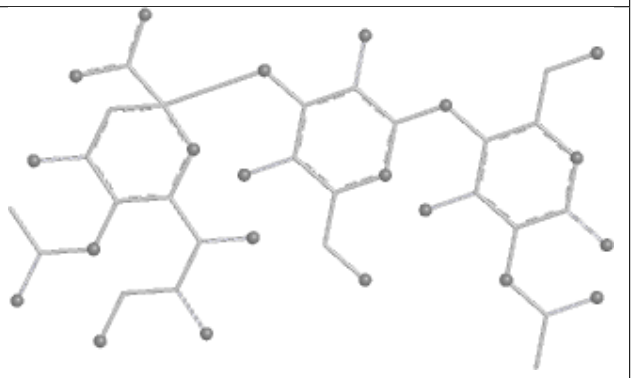
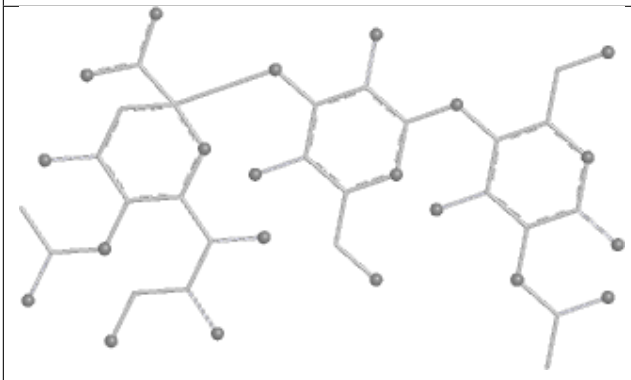


Bond angles



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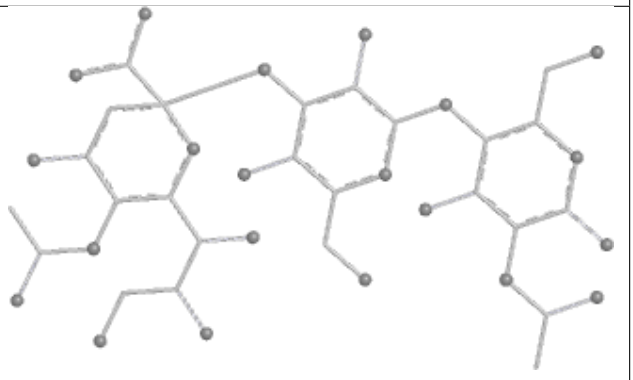
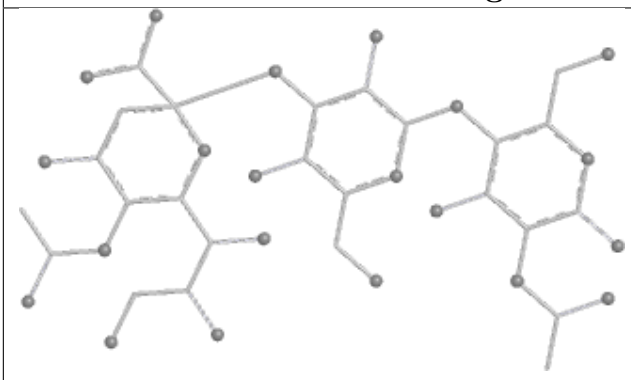


Rings

Oligosaccharide Chain vB



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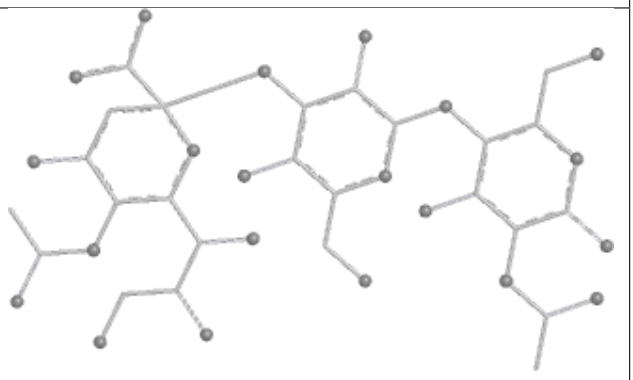
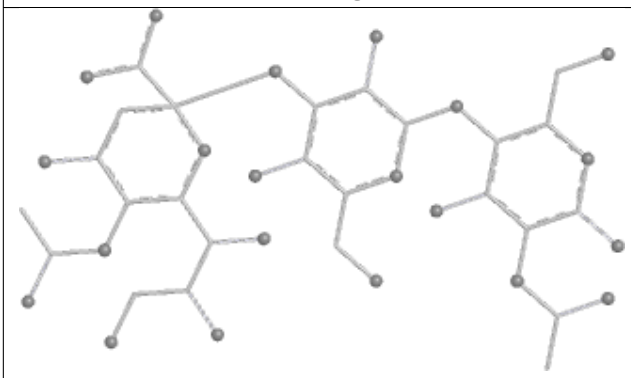


Bond angles



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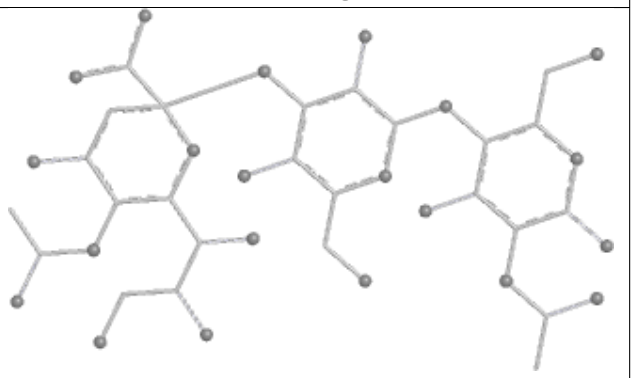
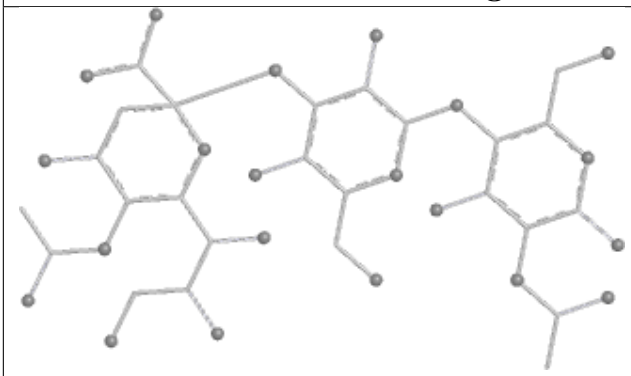


Rings

Oligosaccharide Chain yB



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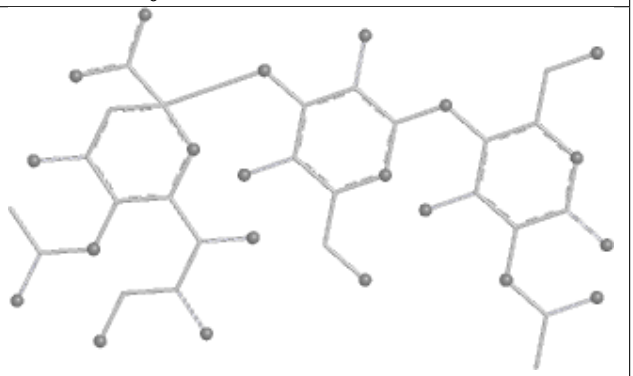
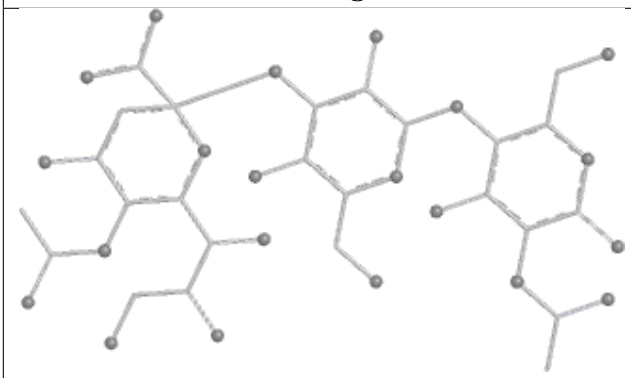


Bond angles



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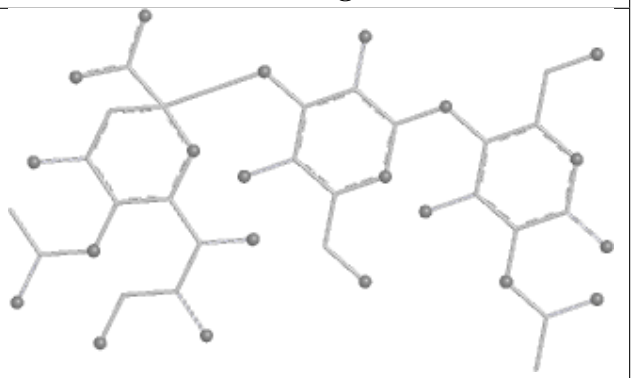
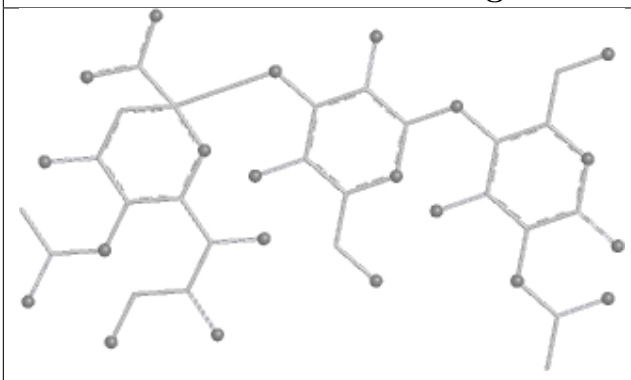


Rings

Oligosaccharide Chain 1B



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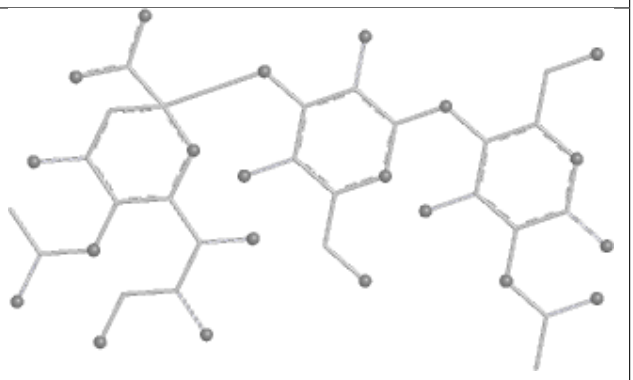
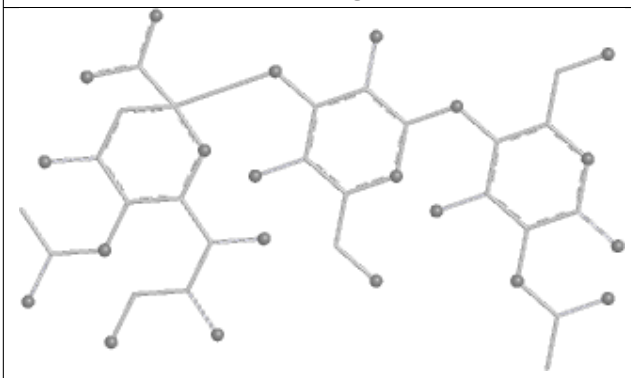


Bond angles



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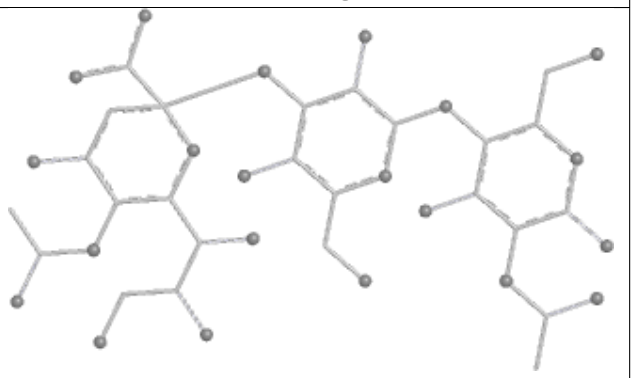
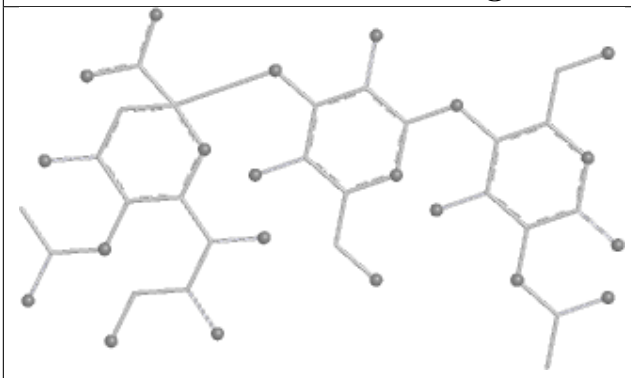


Rings

Oligosaccharide Chain 4B



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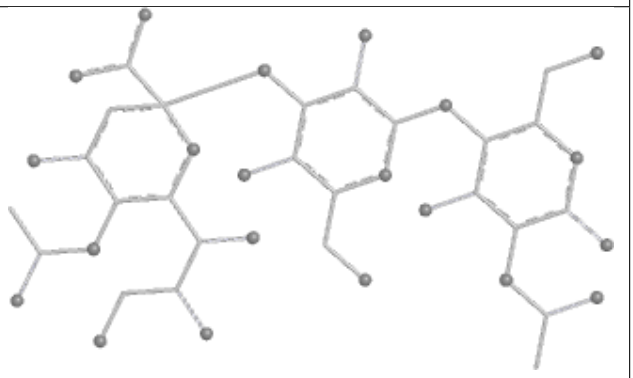
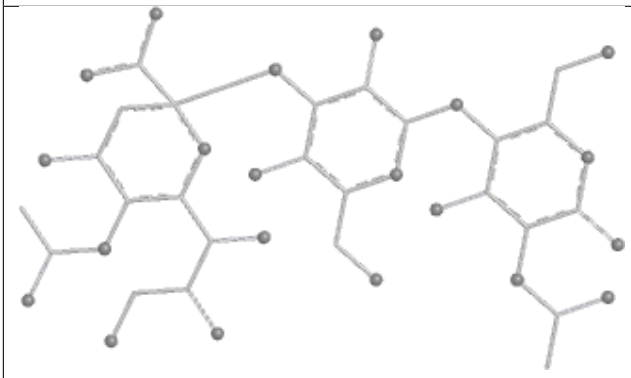


Bond angles



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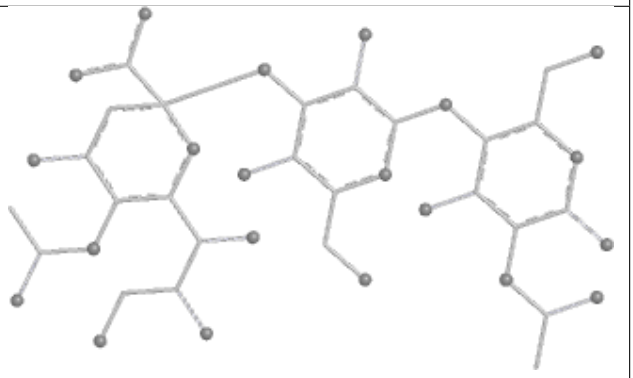
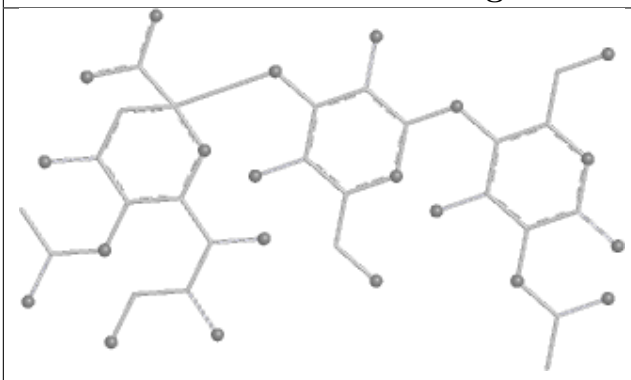
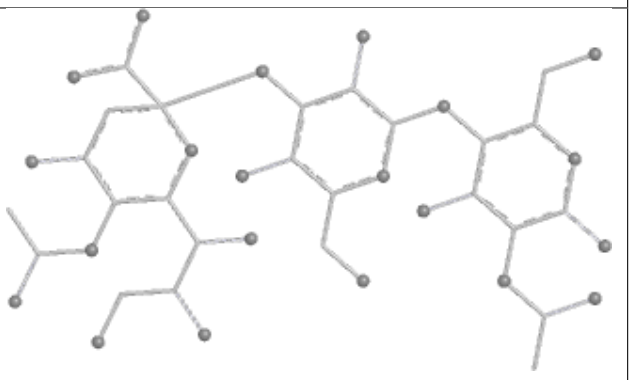
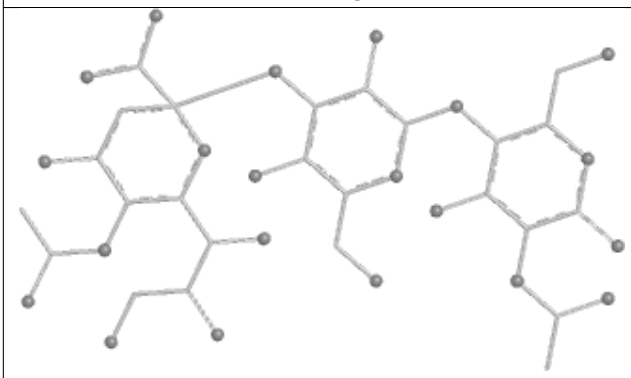
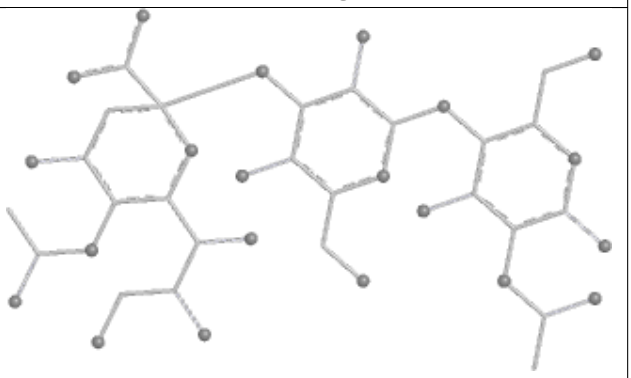
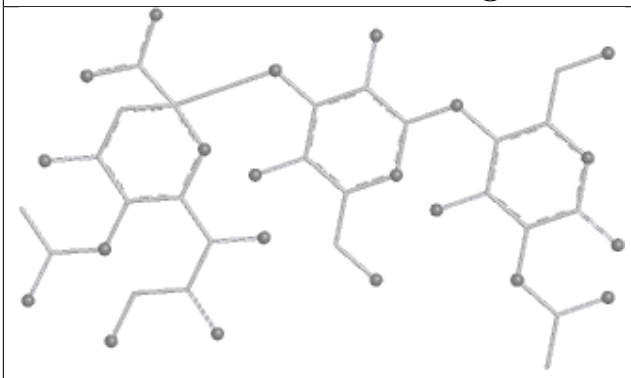
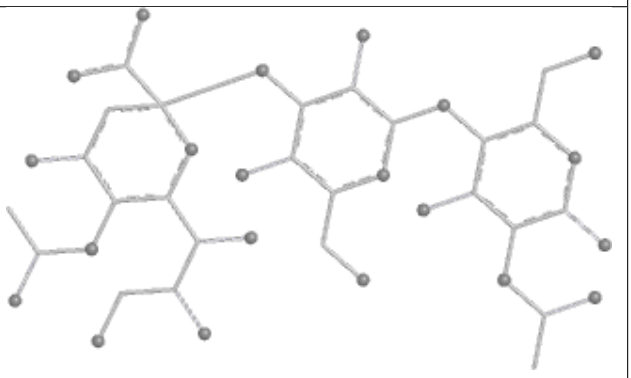
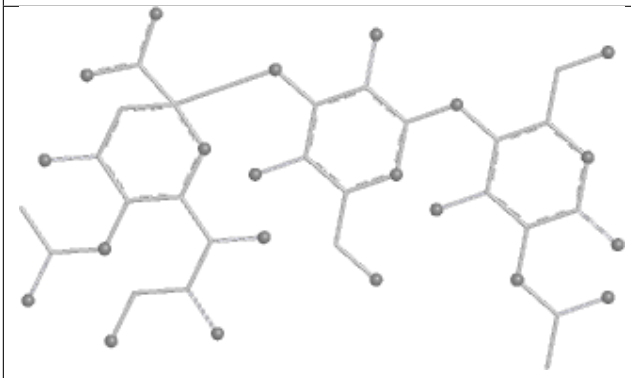
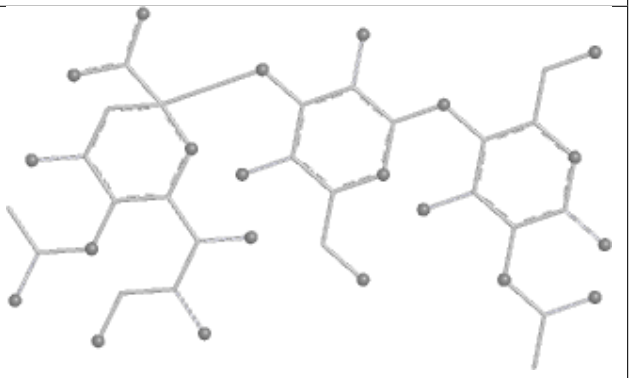
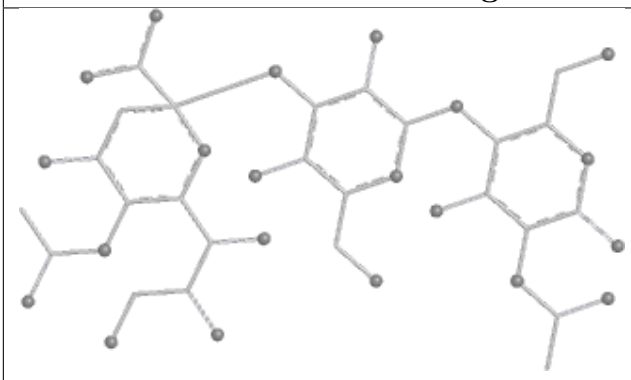


Rings

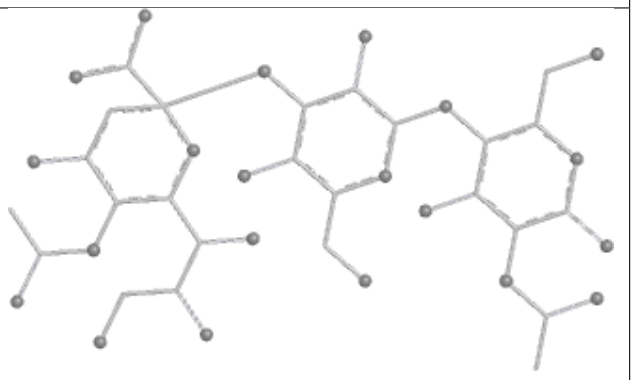
Oligosaccharide Chain 7B	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

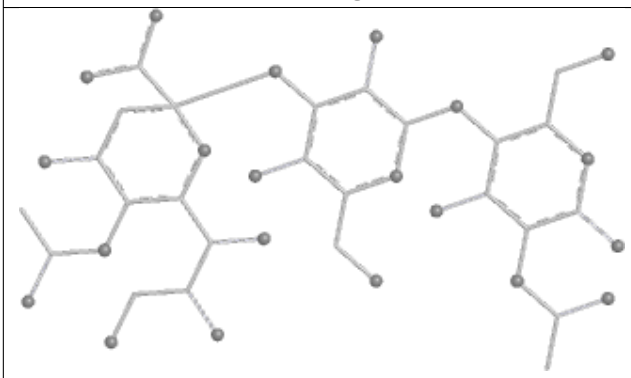
Oligosaccharide Chain DC



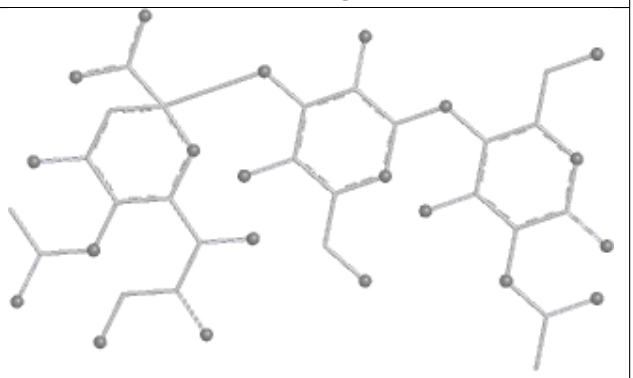
Bond lengths



Bond angles

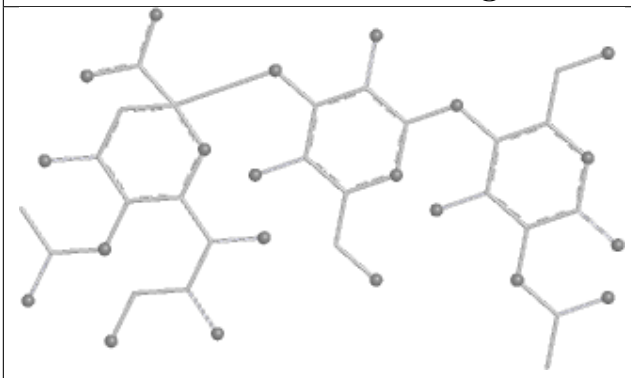


Torsions

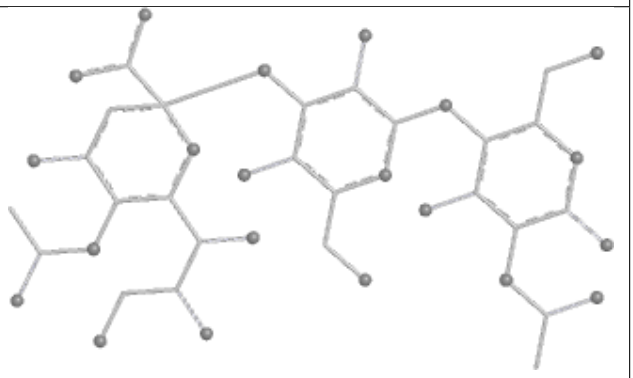


Rings

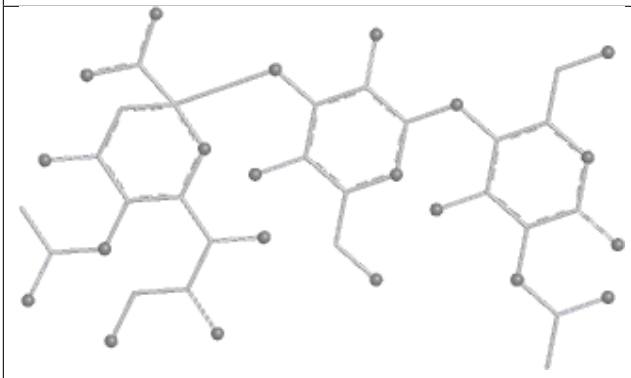
Oligosaccharide Chain GC



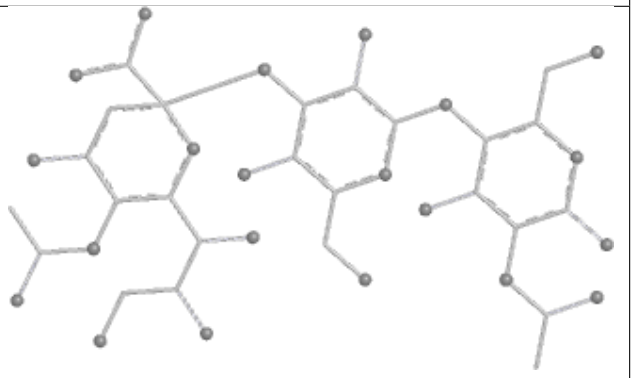
Bond lengths



Bond angles

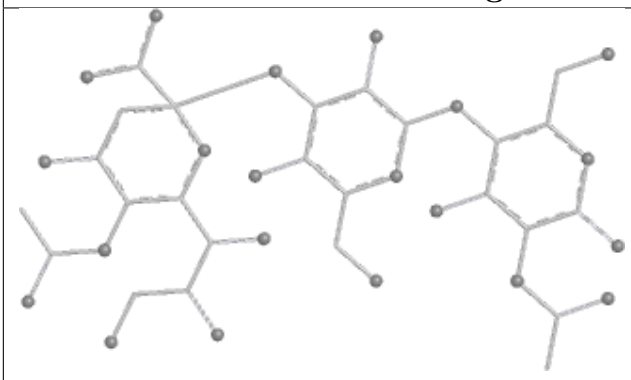


Torsions



Rings

Oligosaccharide Chain JC



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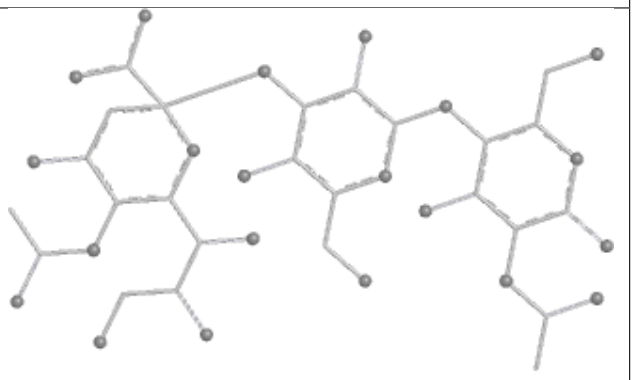
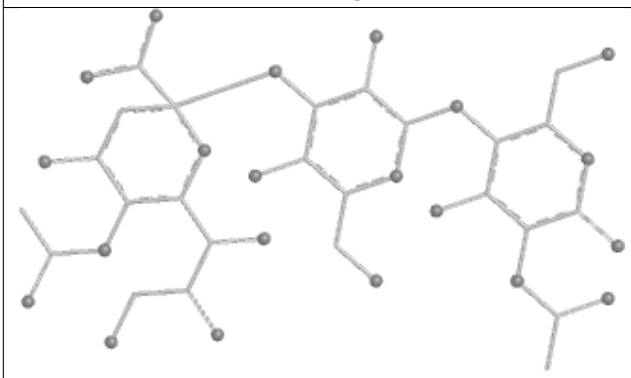


Bond angles



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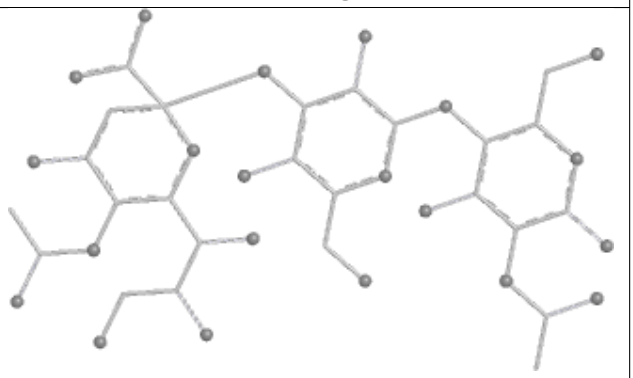
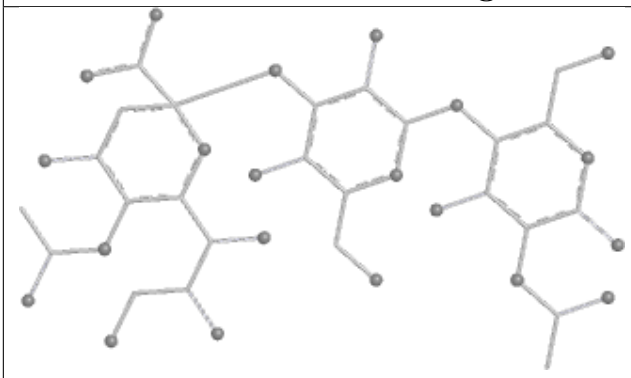


Rings

Oligosaccharide Chain MC



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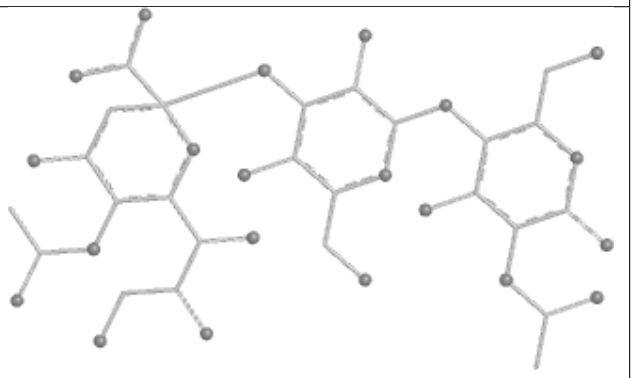
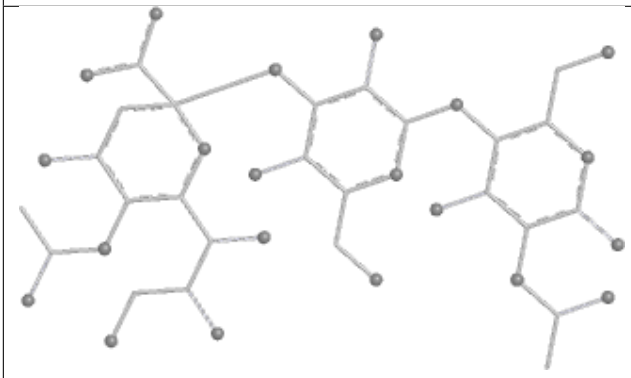


Bond angles



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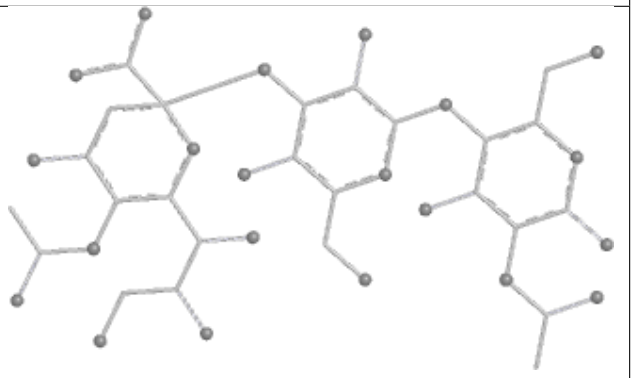
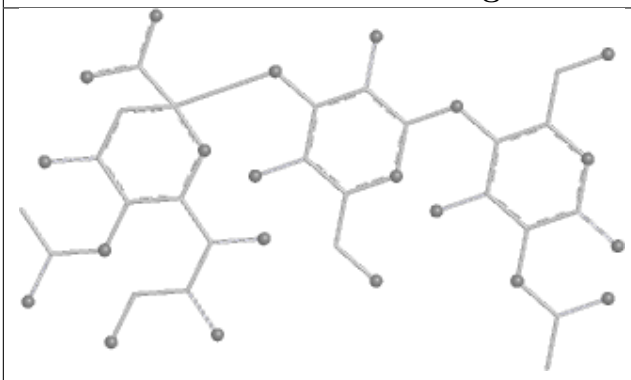


Rings

Oligosaccharide Chain PC



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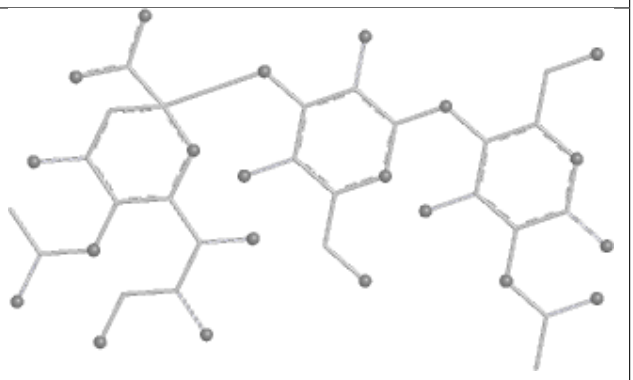
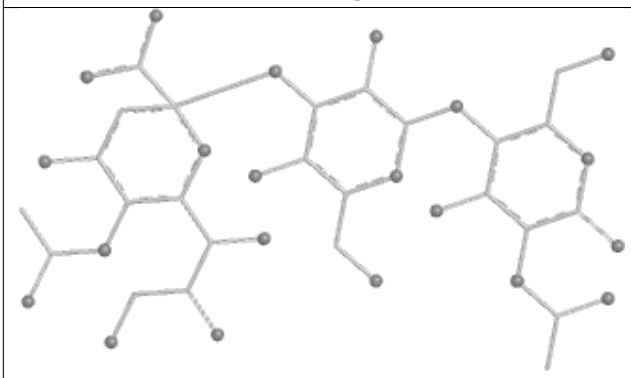


Bond angles



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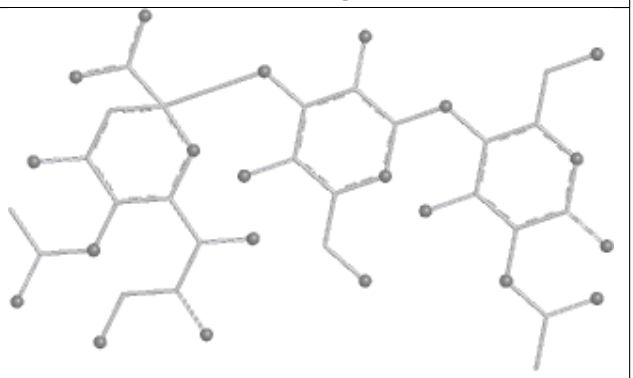
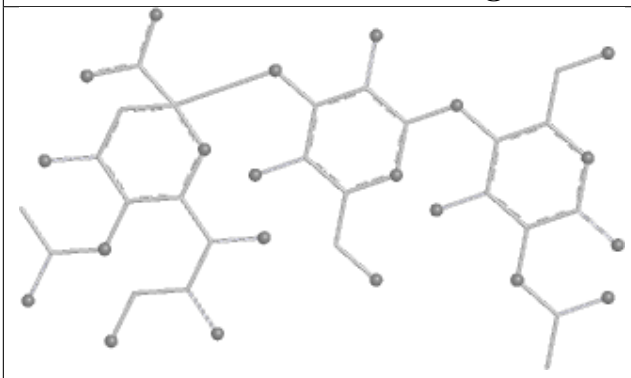


Rings

Oligosaccharide Chain SC



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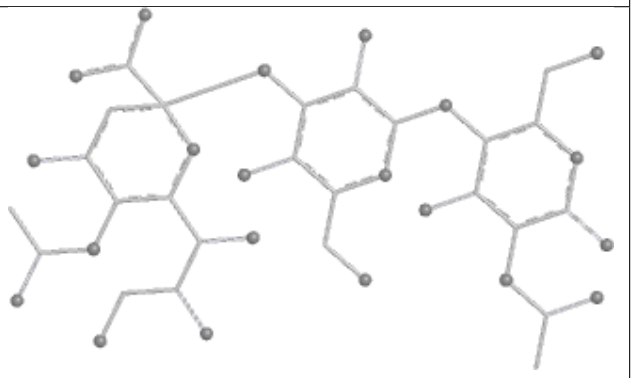

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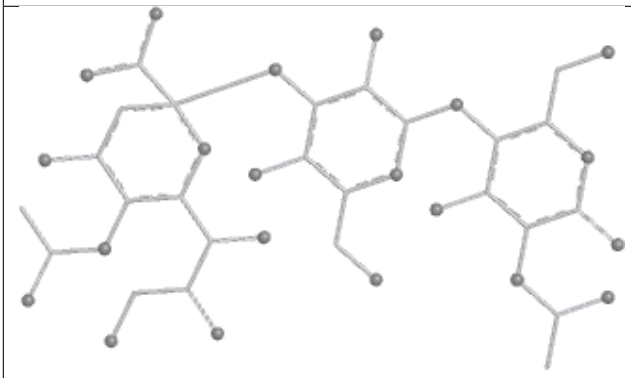

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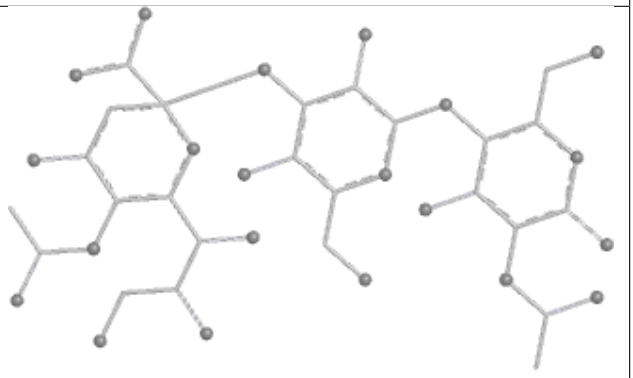
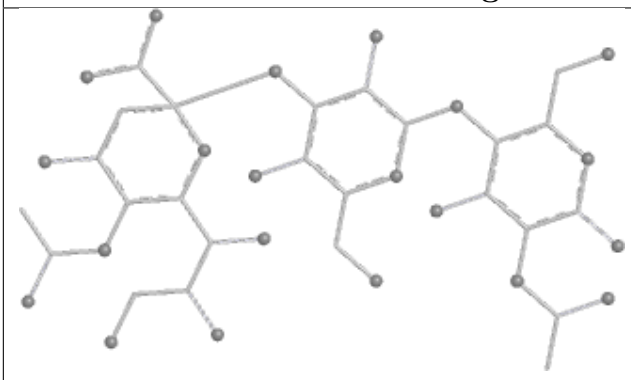


Rings

Oligosaccharide Chain VC



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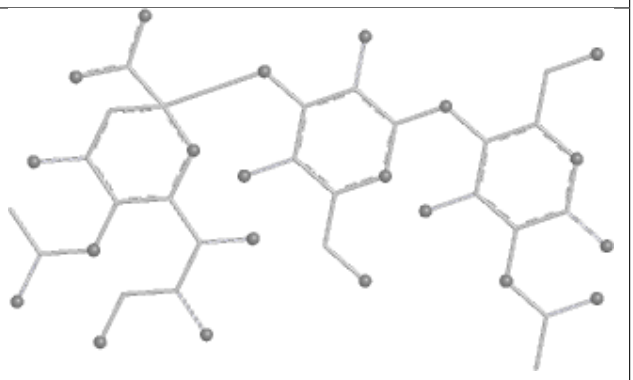
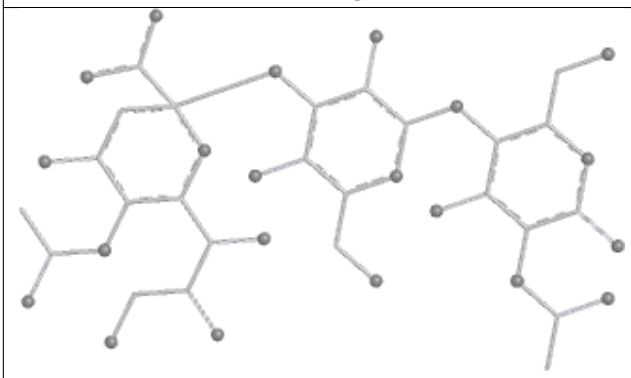


Bond angles



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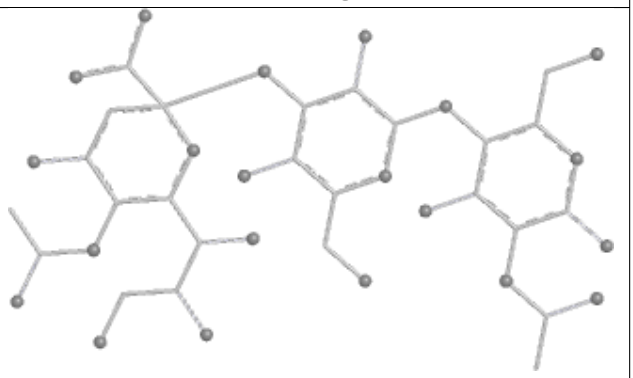
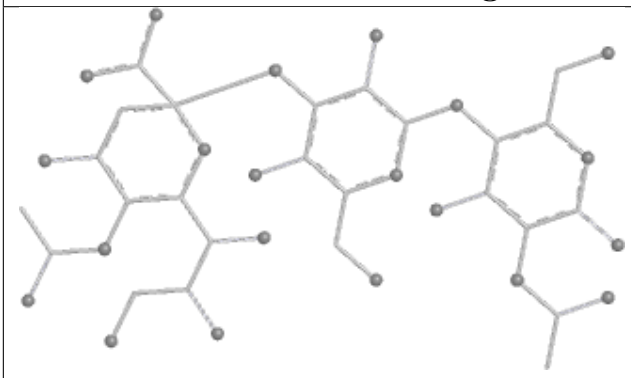


Rings

Oligosaccharide Chain YC



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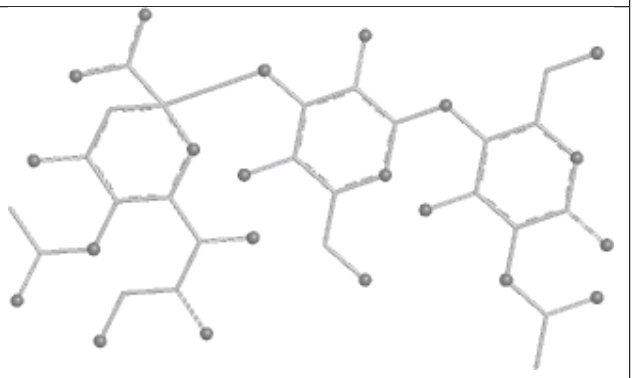
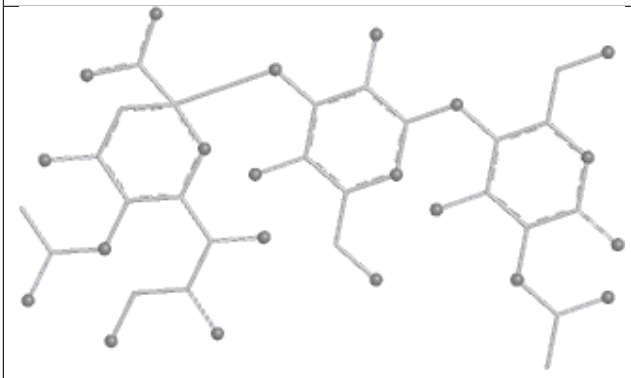


Bond angles



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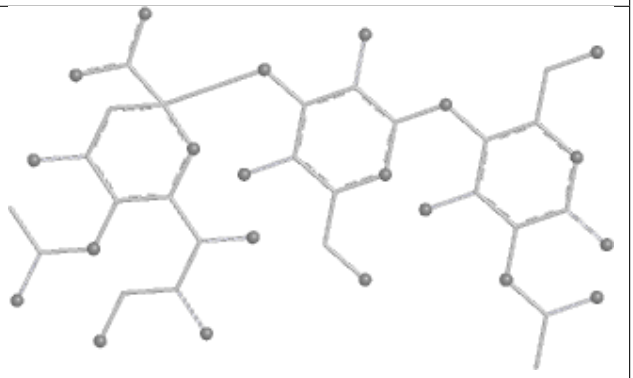
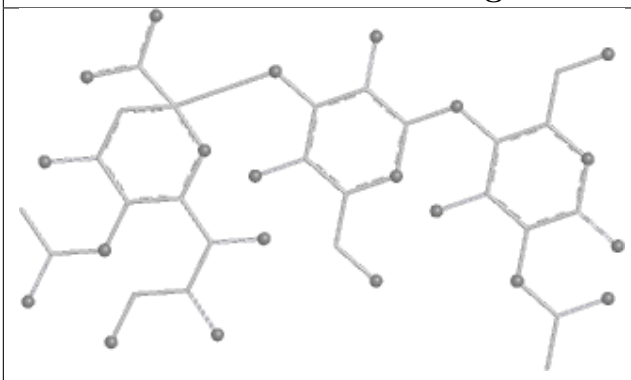


Rings

Oligosaccharide Chain bC



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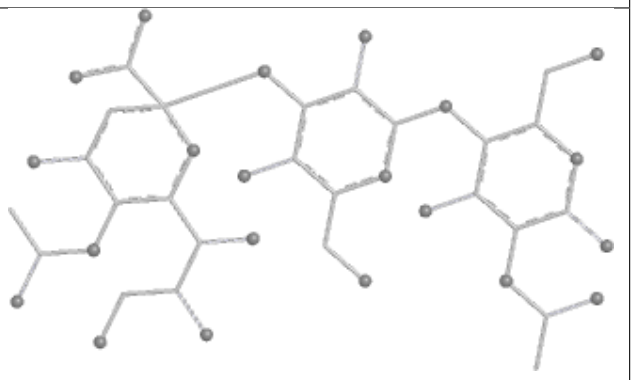
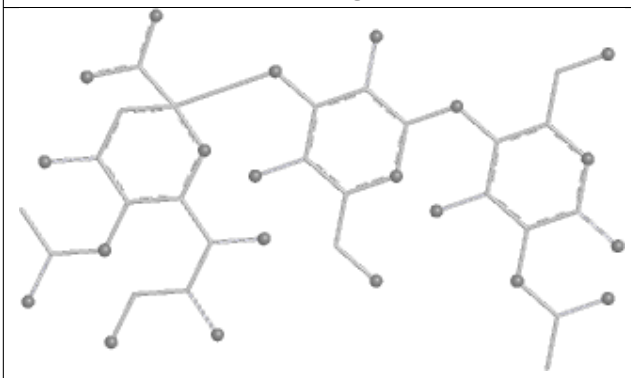


Bond angles



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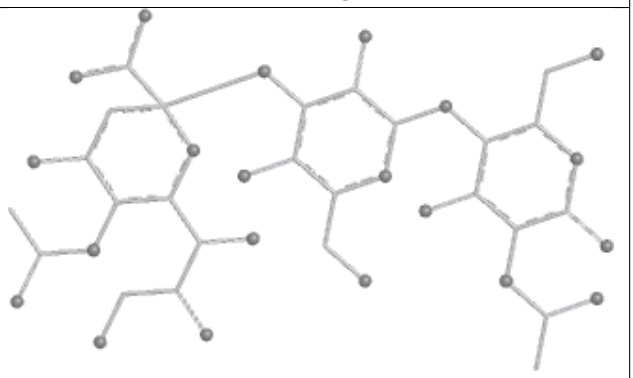
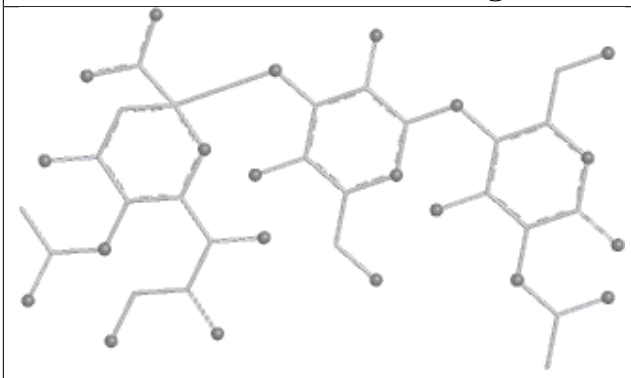


Rings

Oligosaccharide Chain eC



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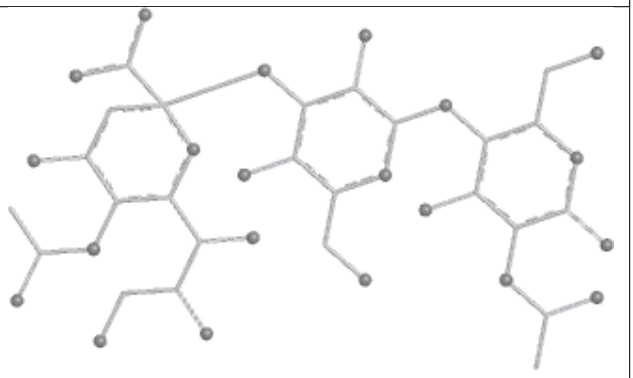
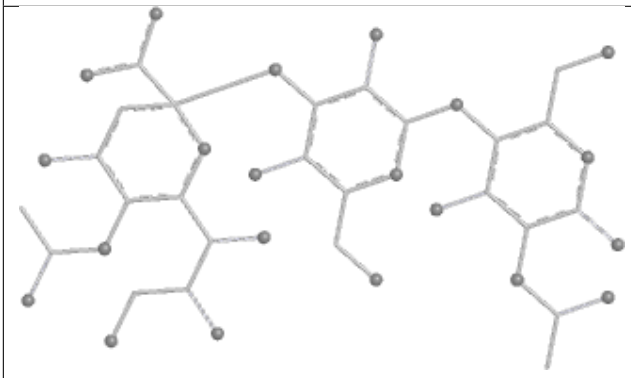


Bond angles



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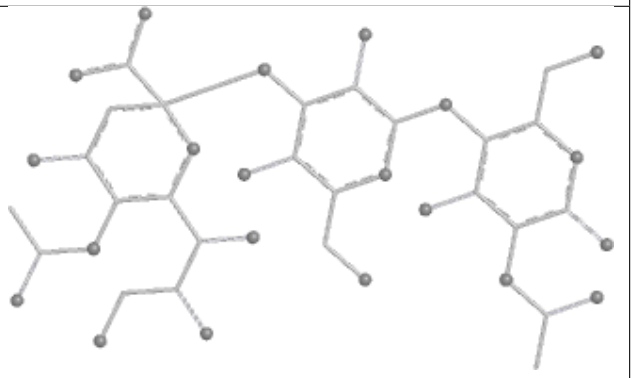
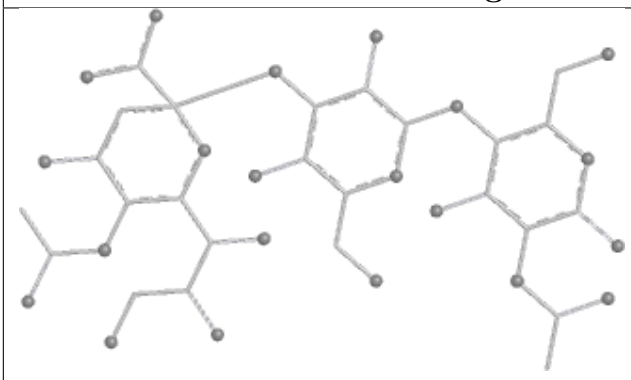


Rings

Oligosaccharide Chain hC



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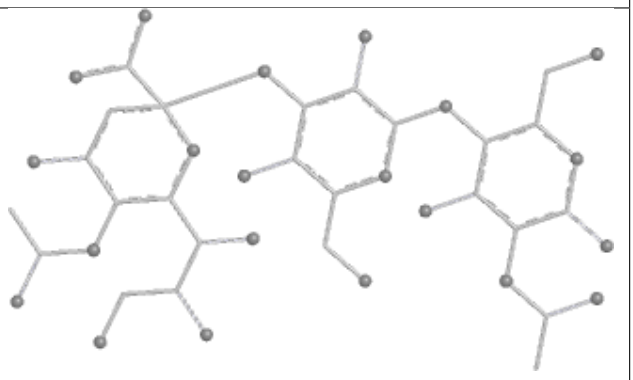
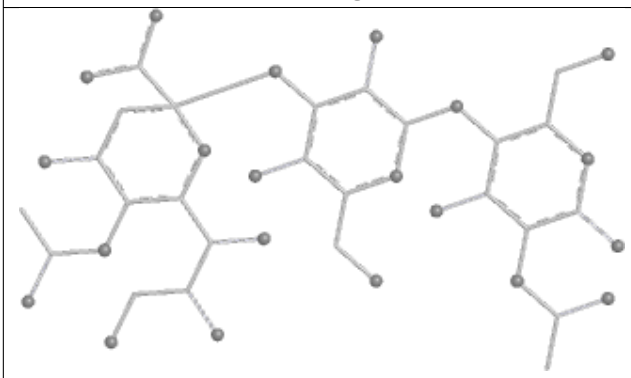


Bond angles



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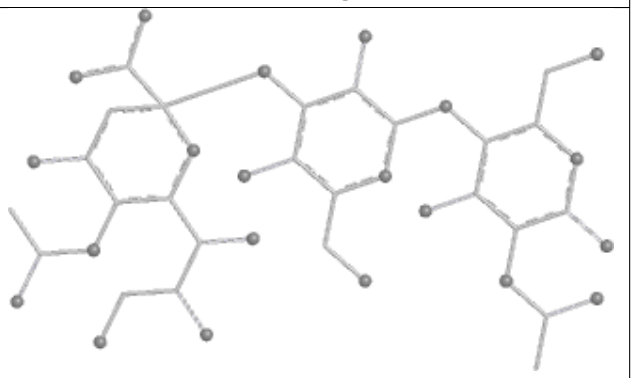
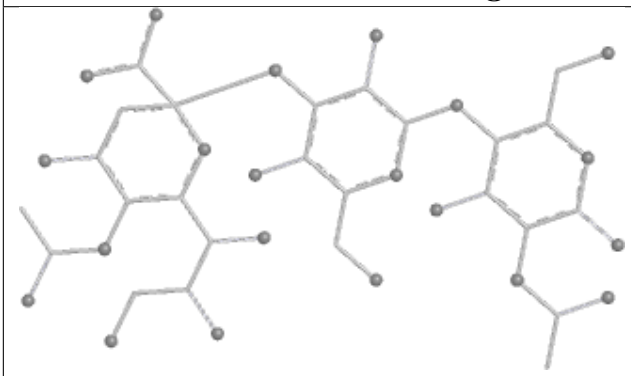


Rings

Oligosaccharide Chain kC



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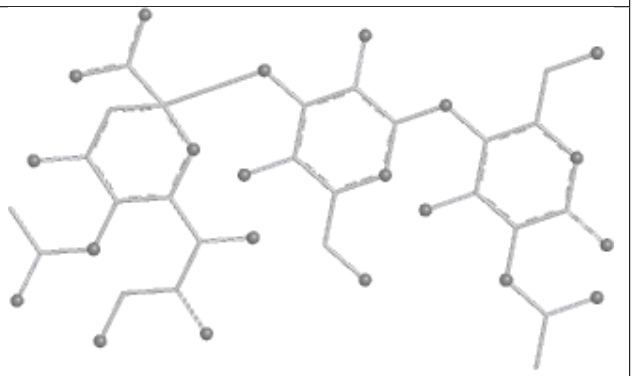

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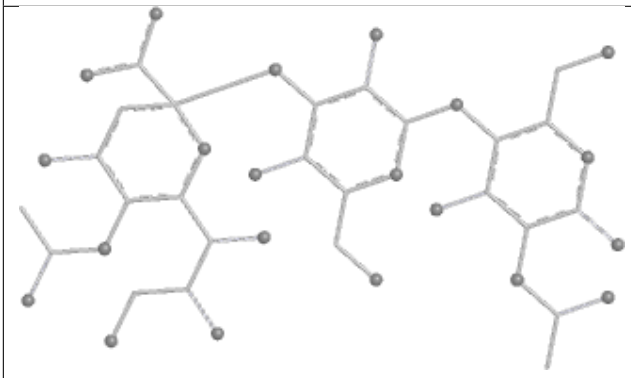

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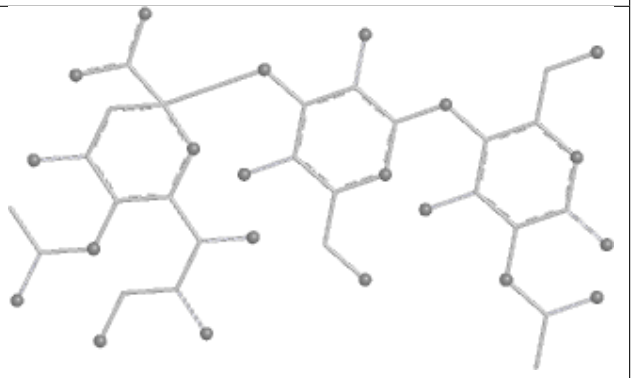
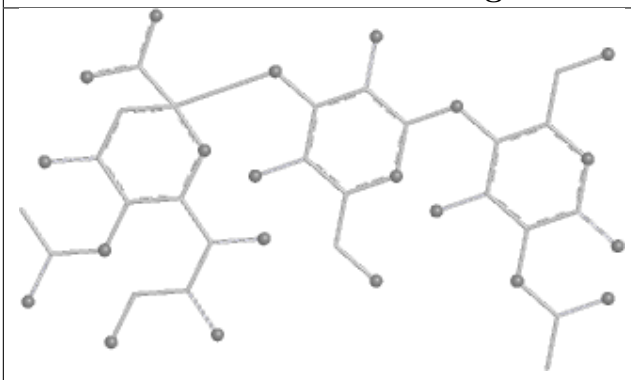


Rings

Oligosaccharide Chain nC



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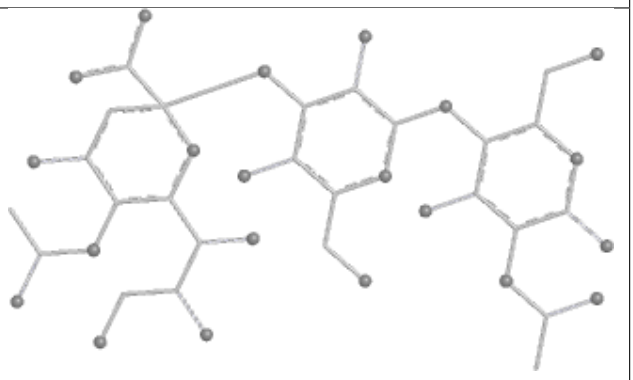
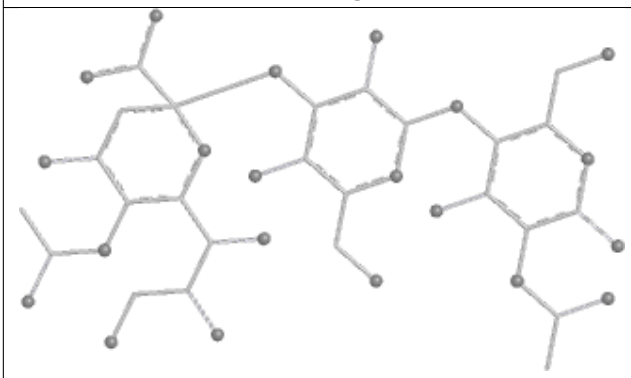


Bond angles



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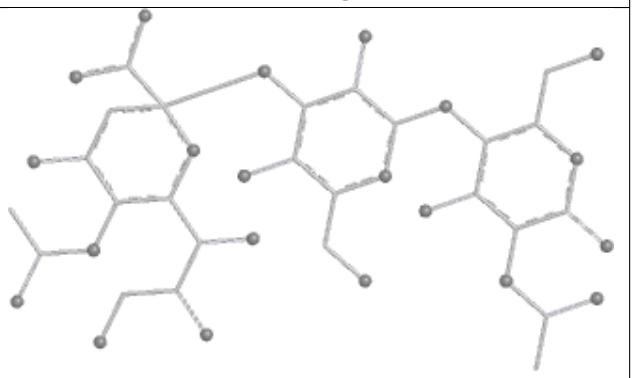
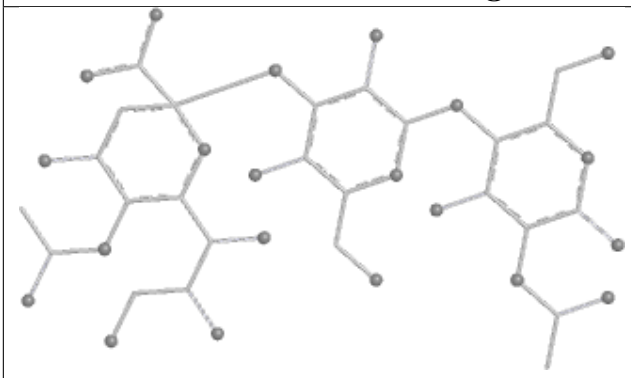


Rings

Oligosaccharide Chain qC



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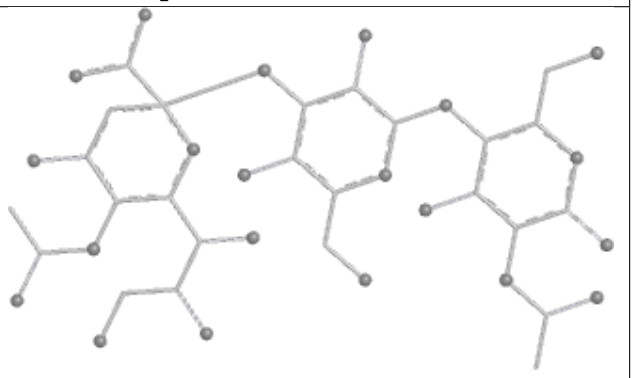
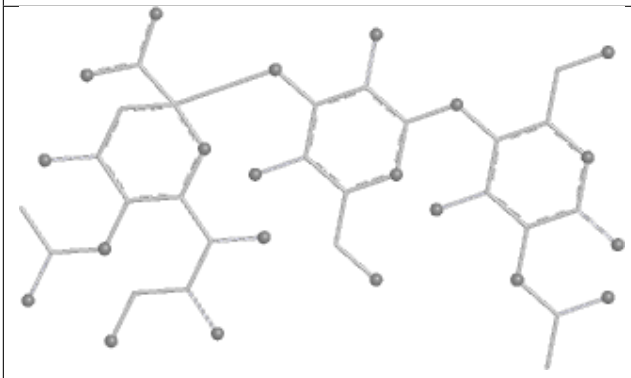


Bond angles



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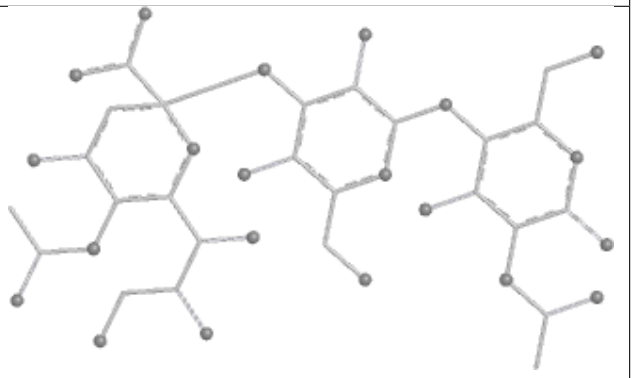
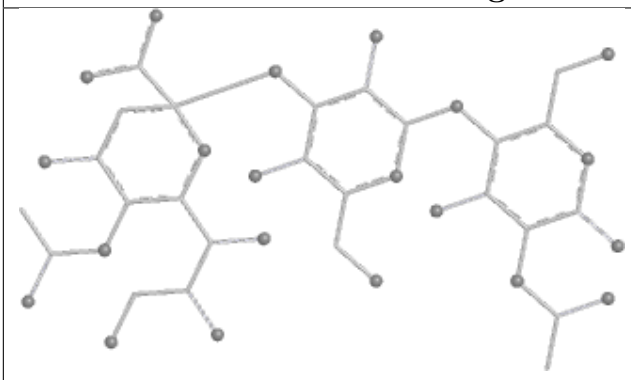
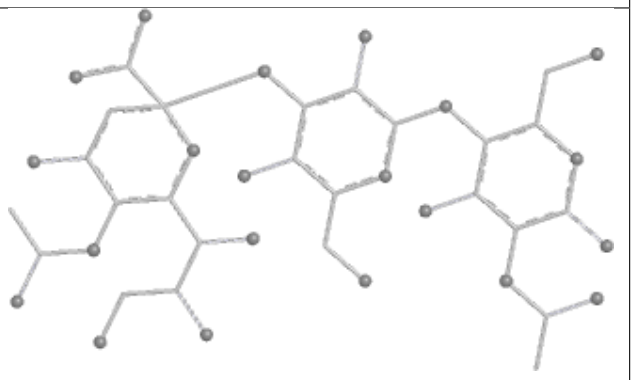


Rings

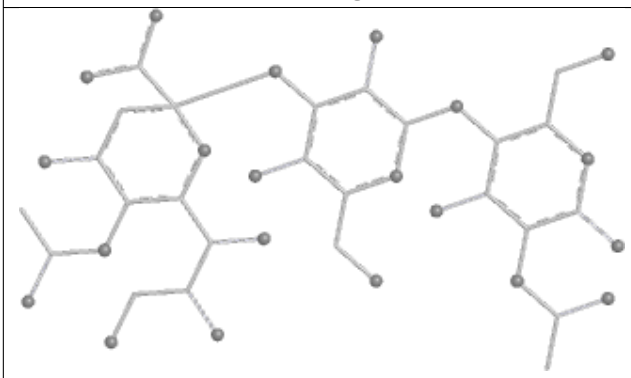
Oligosaccharide Chain tC



Bond lengths



Bond angles



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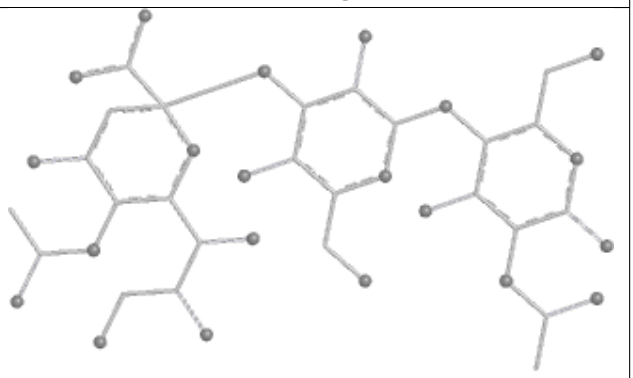
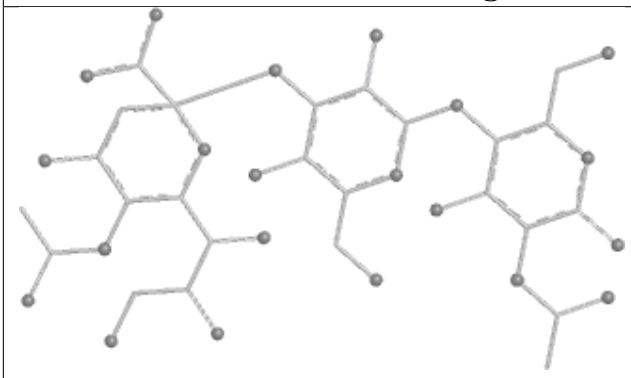


Rings

Oligosaccharide Chain wC



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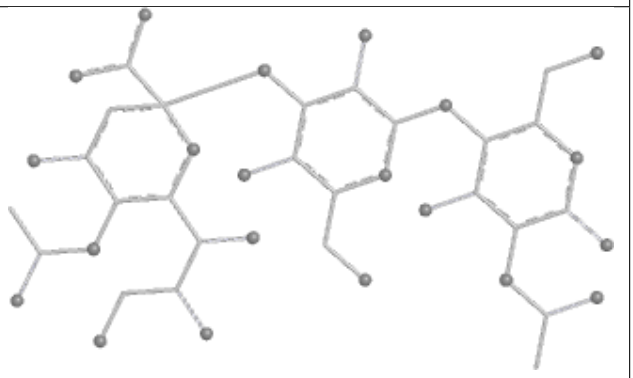
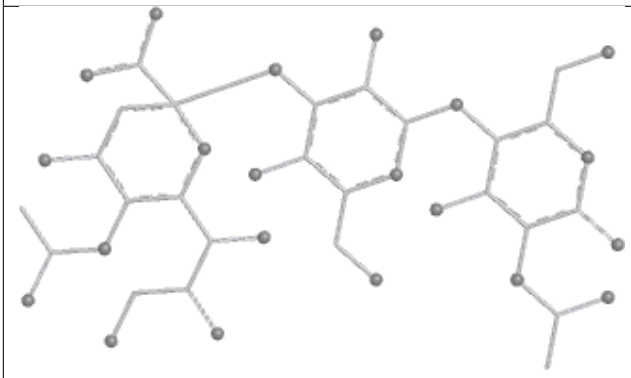


Bond angles



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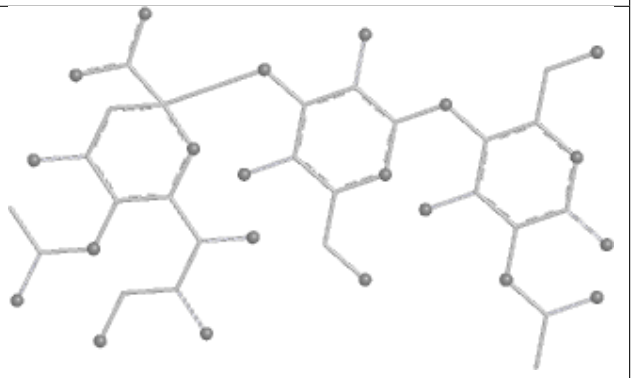
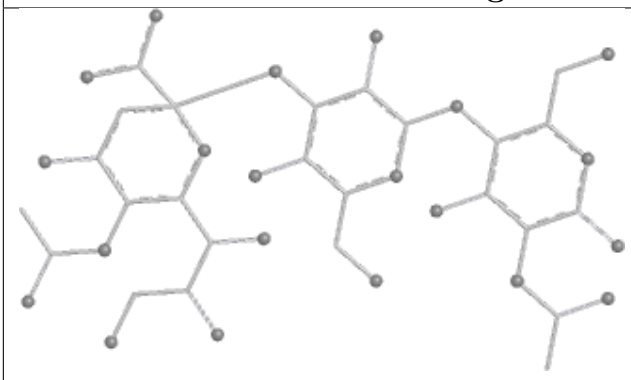
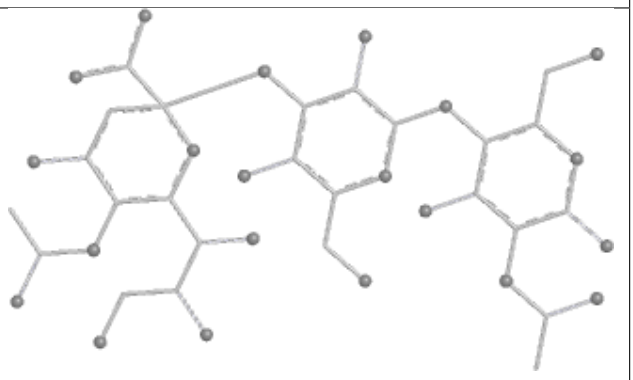
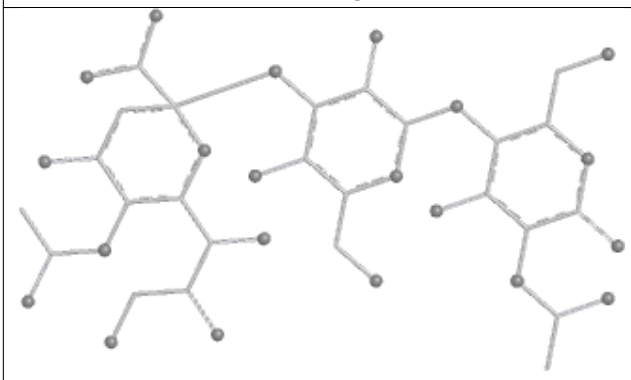
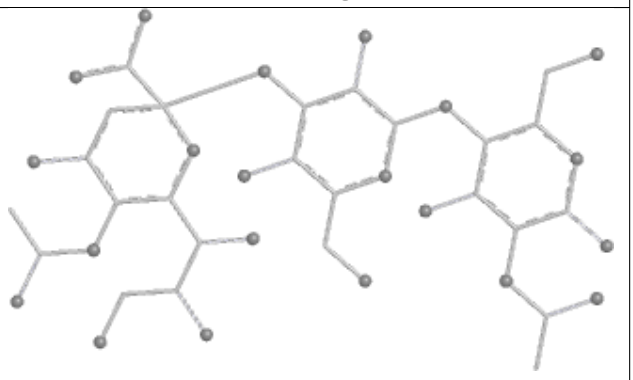


Rings

Oligosaccharide Chain zC	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

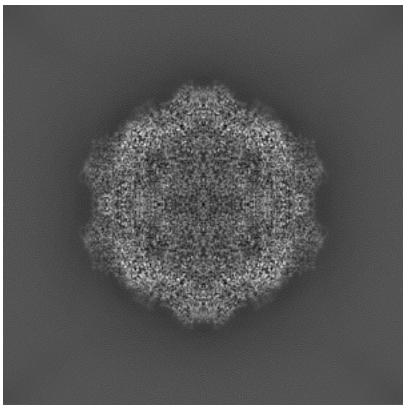
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49196. These allow visual inspection of the internal detail of the map and identification of artifacts.

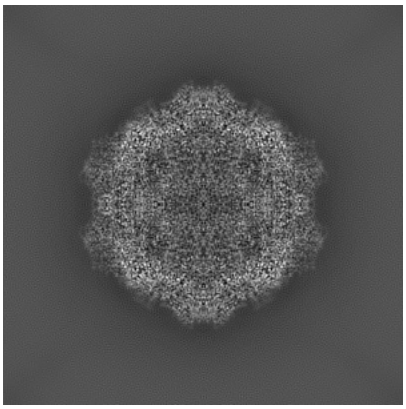
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

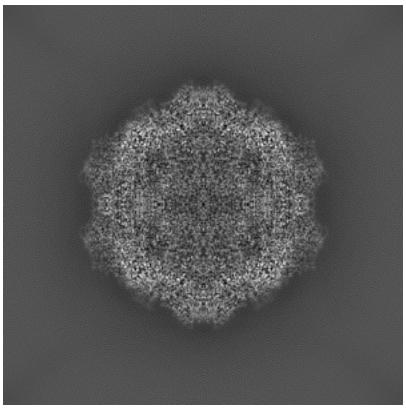
6.1.1 Primary map



X

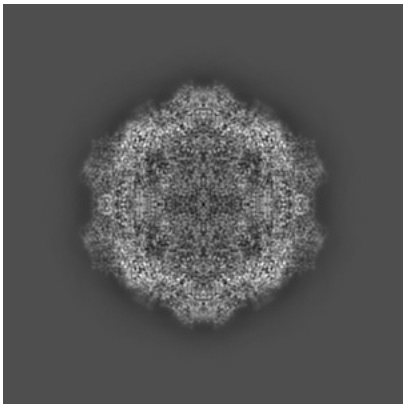


Y

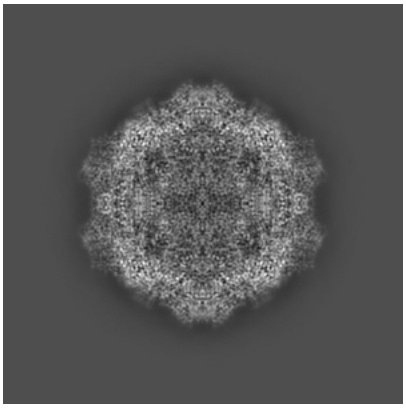


Z

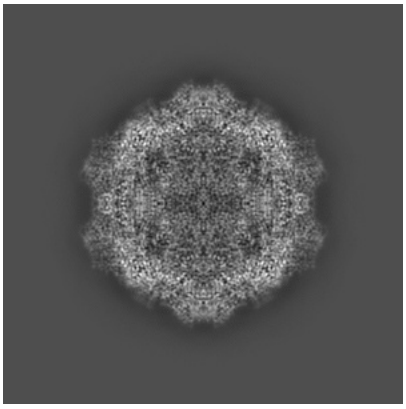
6.1.2 Raw map



X



Y

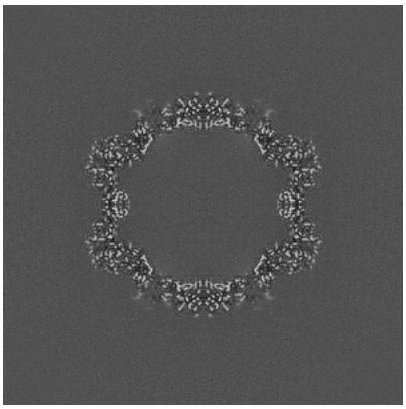


Z

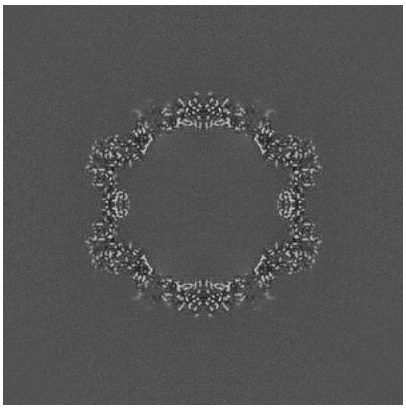
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

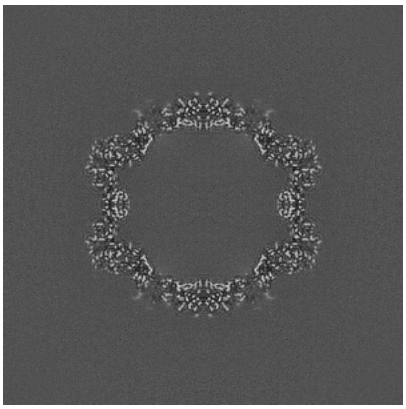
6.2.1 Primary map



X Index: 210

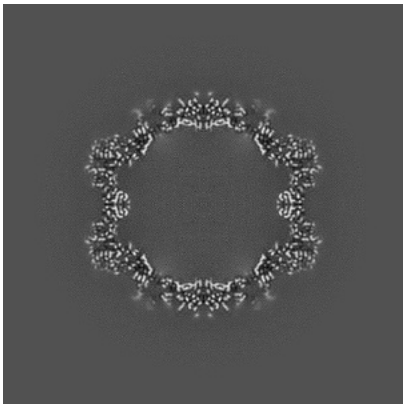


Y Index: 210

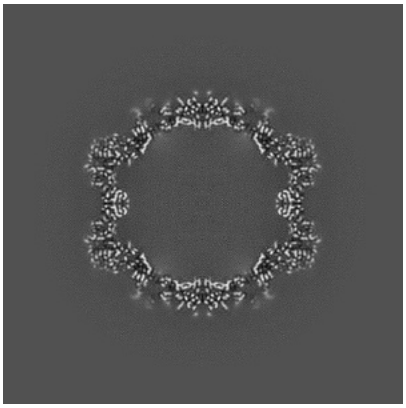


Z Index: 210

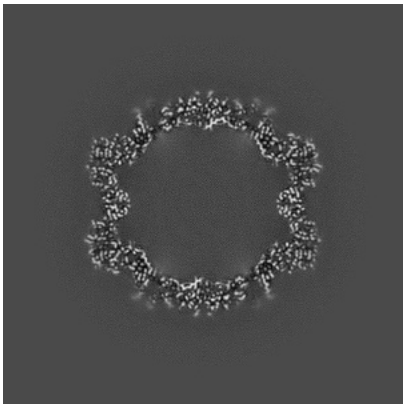
6.2.2 Raw map



X Index: 210



Y Index: 210

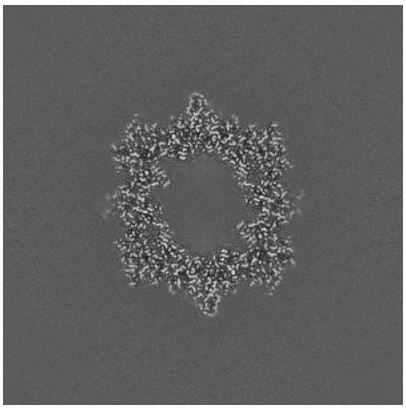


Z Index: 210

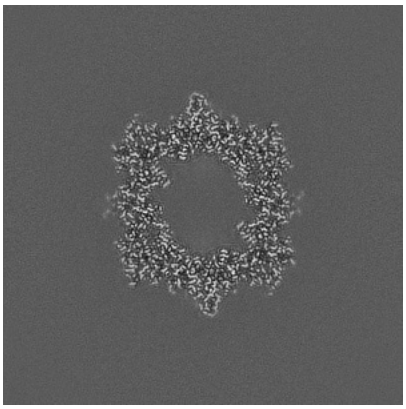
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

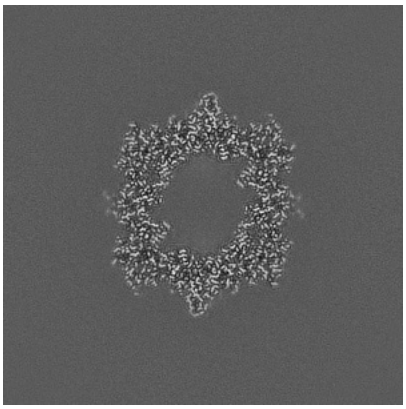
6.3.1 Primary map



X Index: 275

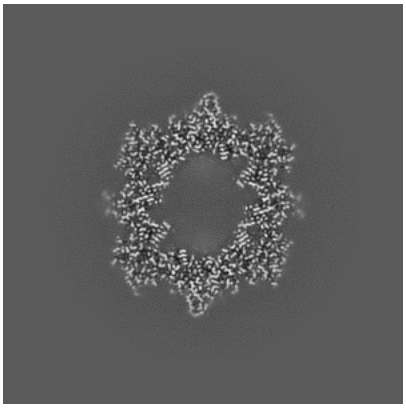


Y Index: 275

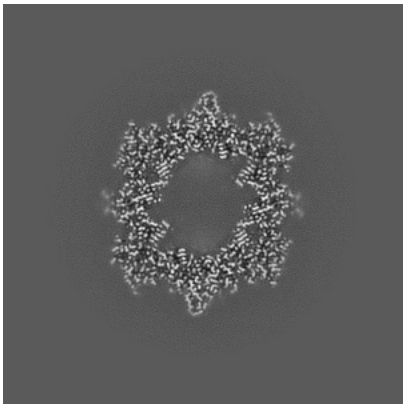


Z Index: 145

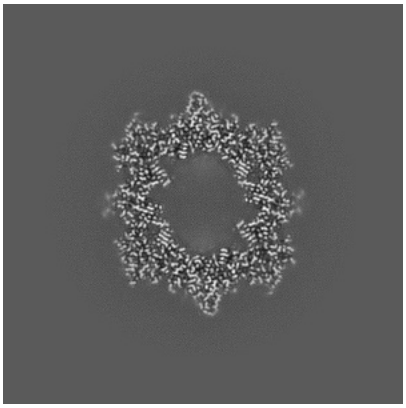
6.3.2 Raw map



X Index: 145



Y Index: 145

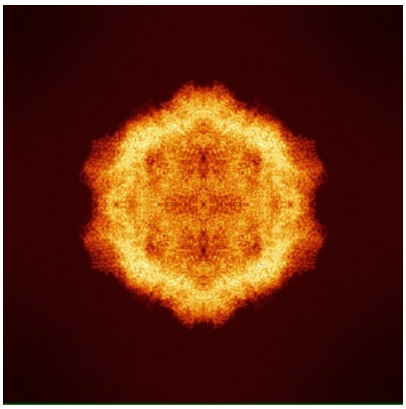


Z Index: 274

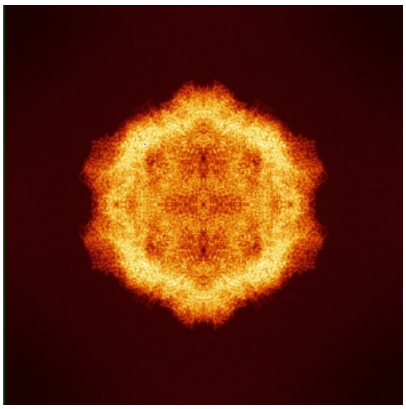
The images above show the largest variance slices of the map in three orthogonal directions.

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

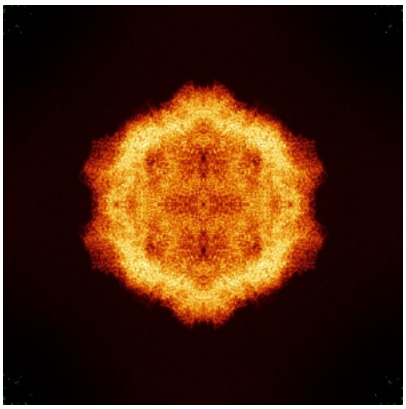
6.4.1 Primary map



X

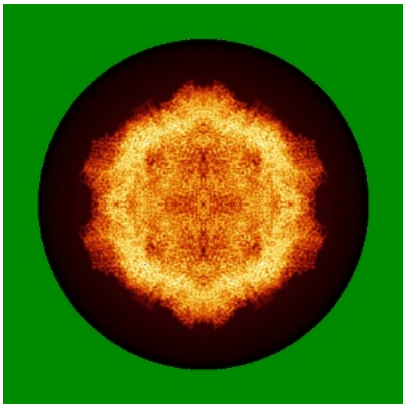


Y

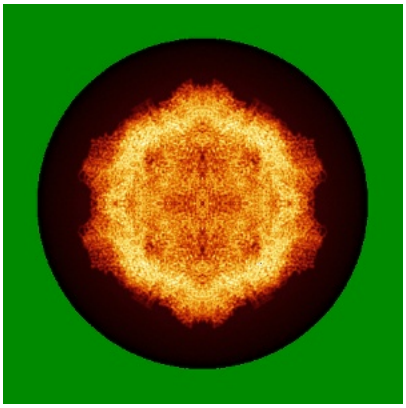


Z

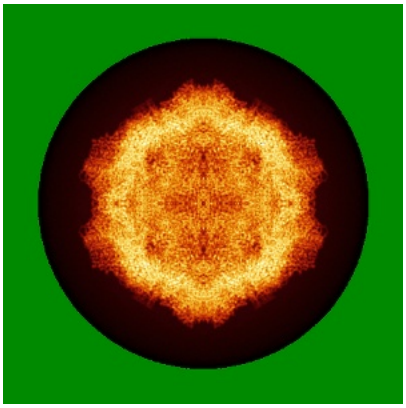
6.4.2 Raw map



X



Y

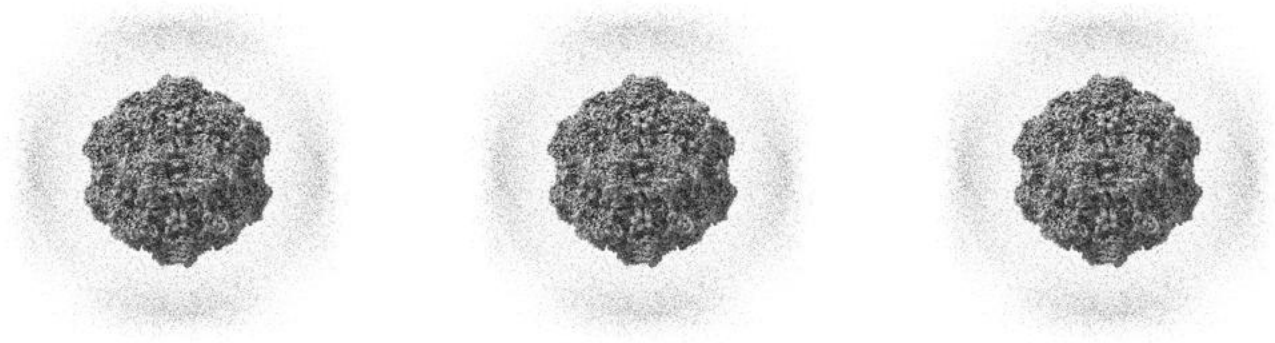


Z

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)

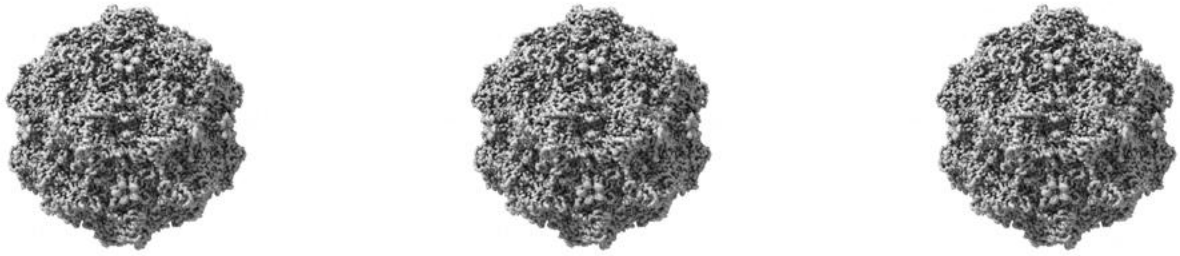
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

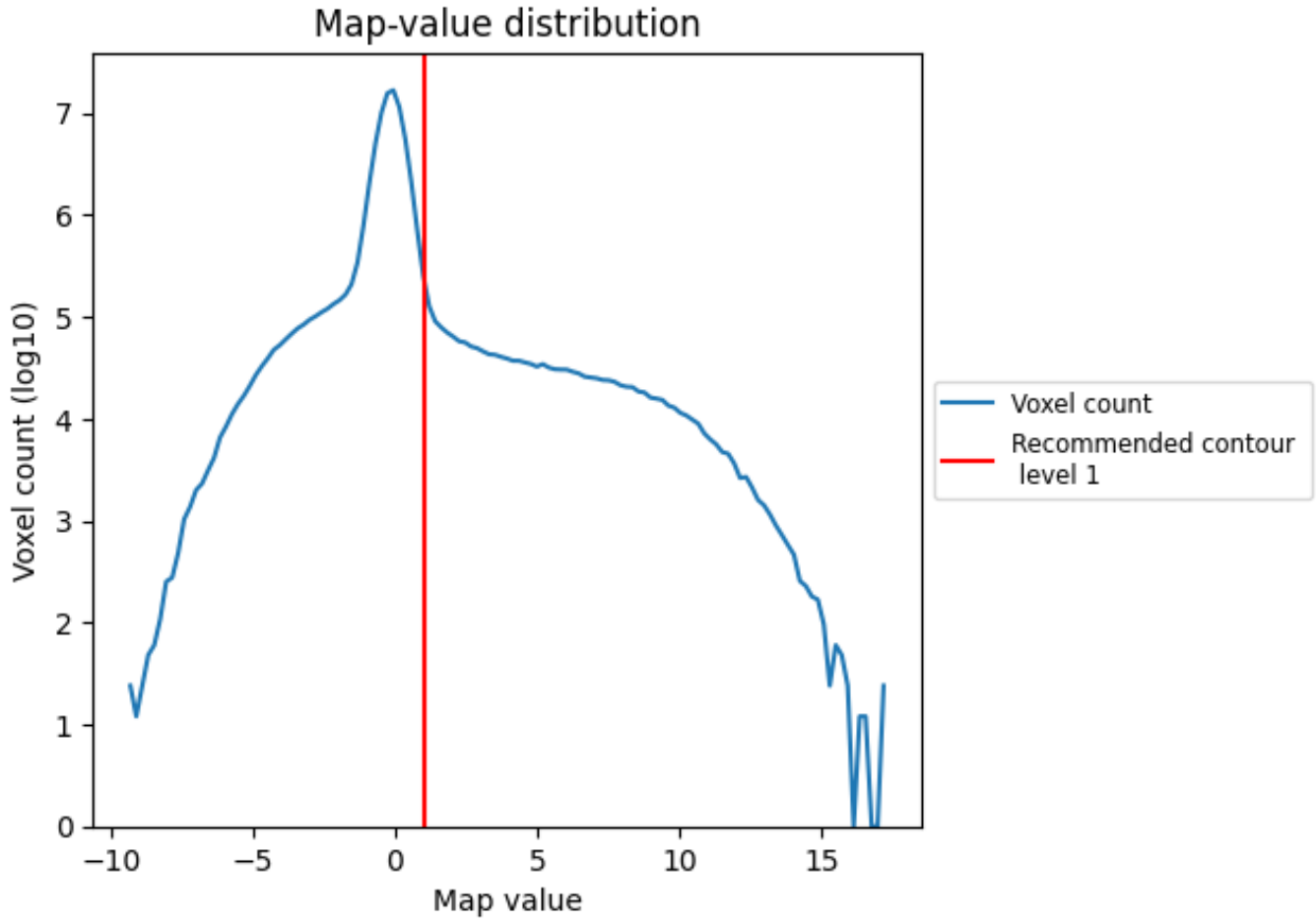
6.6 Mask visualisation (i)

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

7 Map analysis

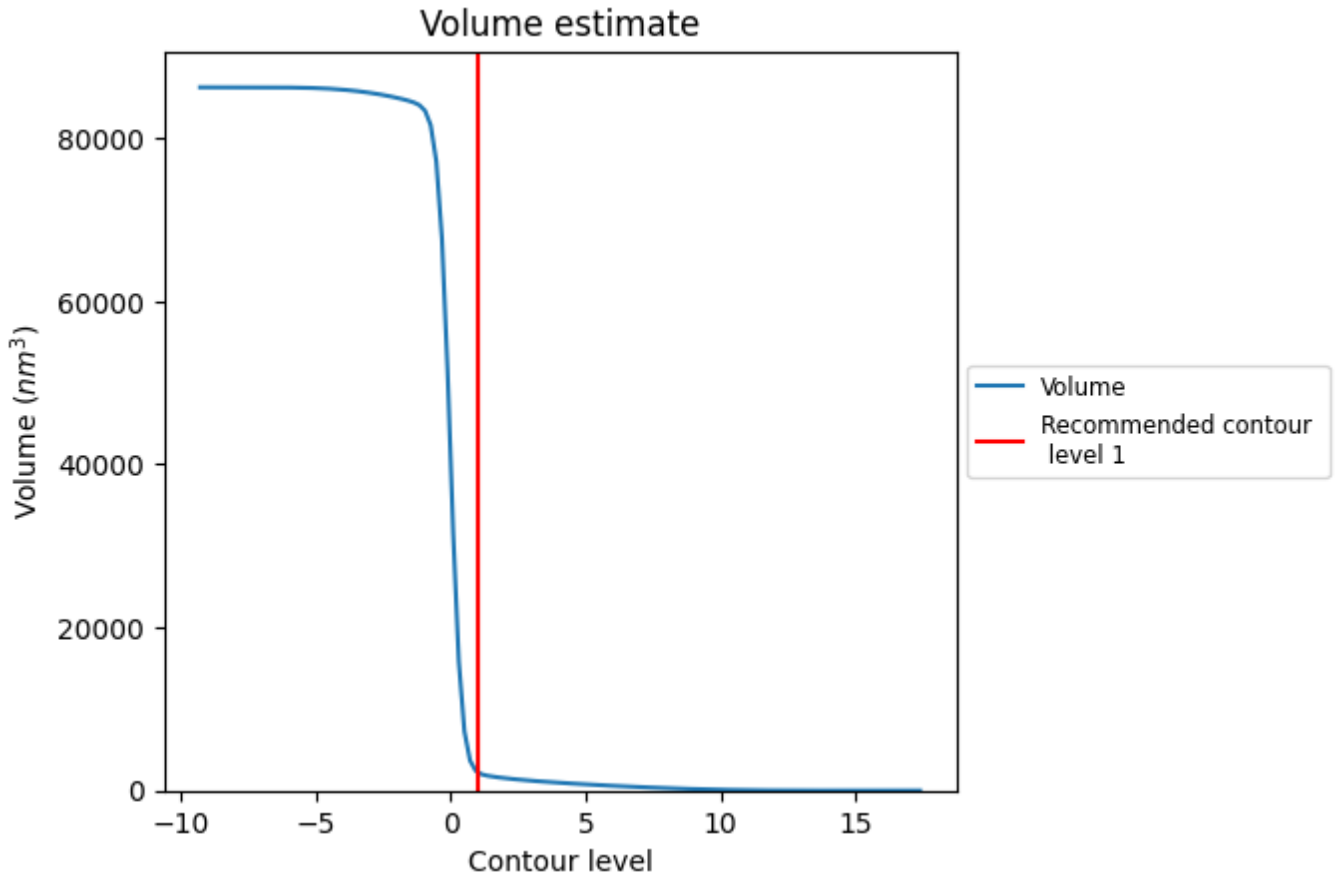
This section contains the results of statistical analysis of the map.

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.

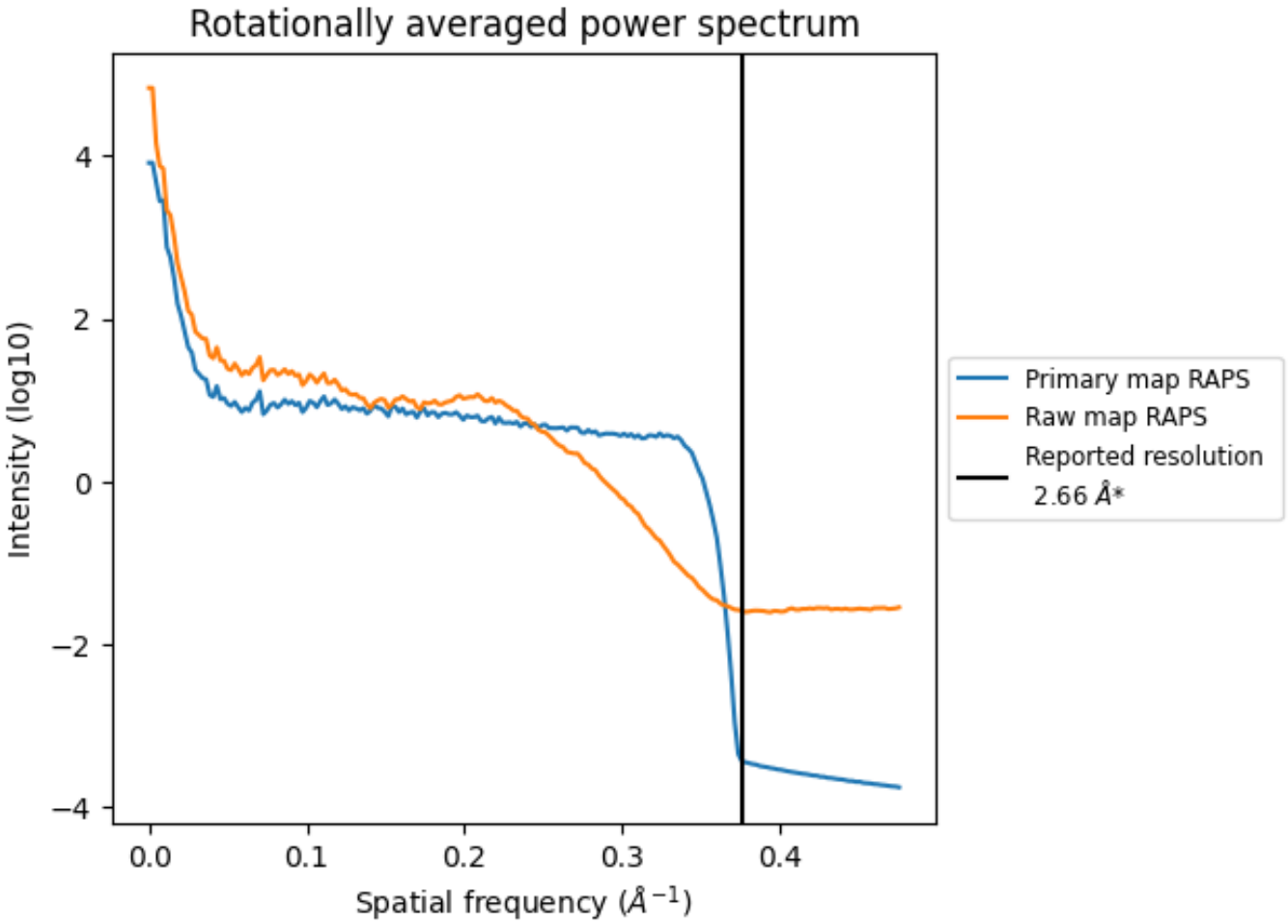
7.2 Volume estimate



The volume at the recommended contour level is 2263 nm^3; this corresponds to an approximate mass of 2045 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)

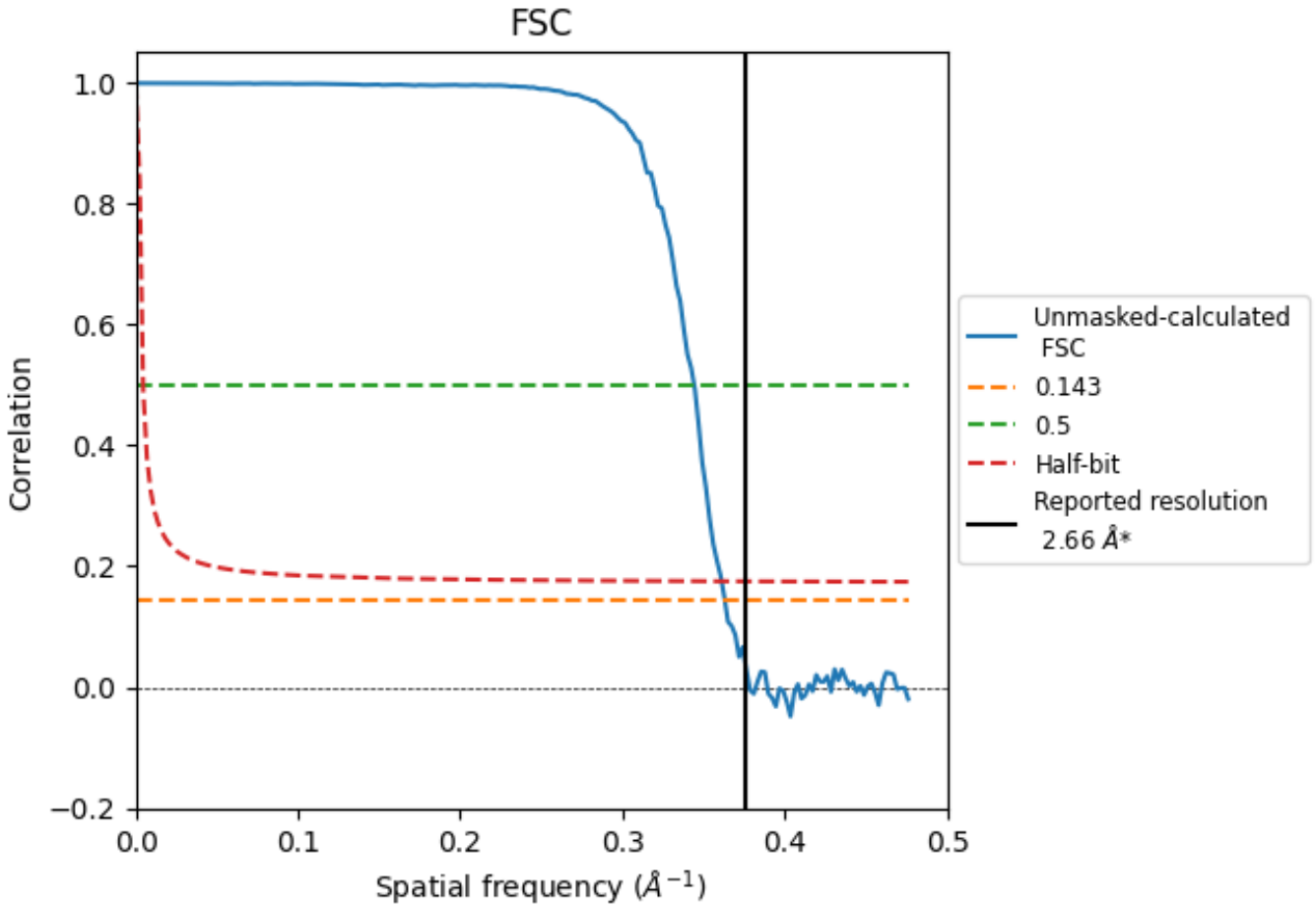


*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

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 0.376 Å^{-1}

8.2 Resolution estimates (i)

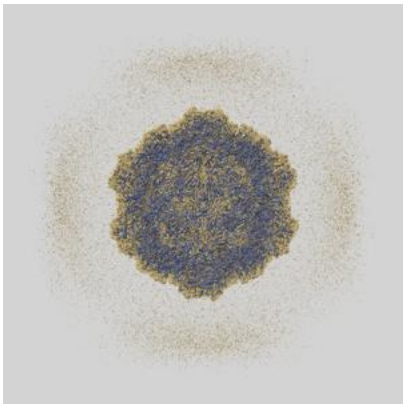
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.75	2.91	2.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

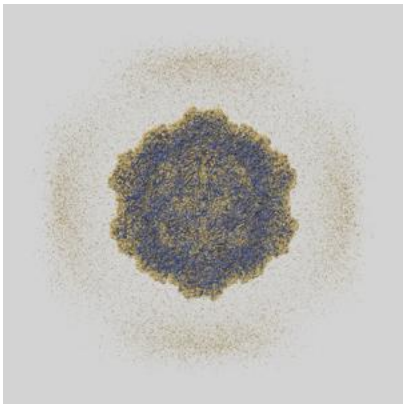
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49196 and PDB model 9NAJ. Per-residue inclusion information can be found in section 3 on page 15.

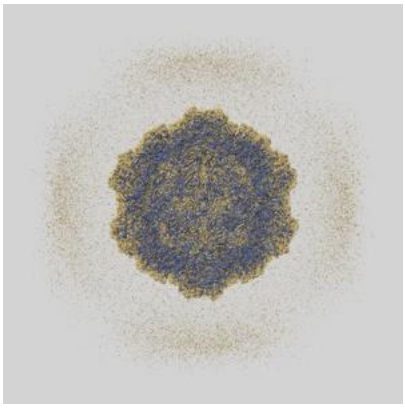
9.1 Map-model overlay



X



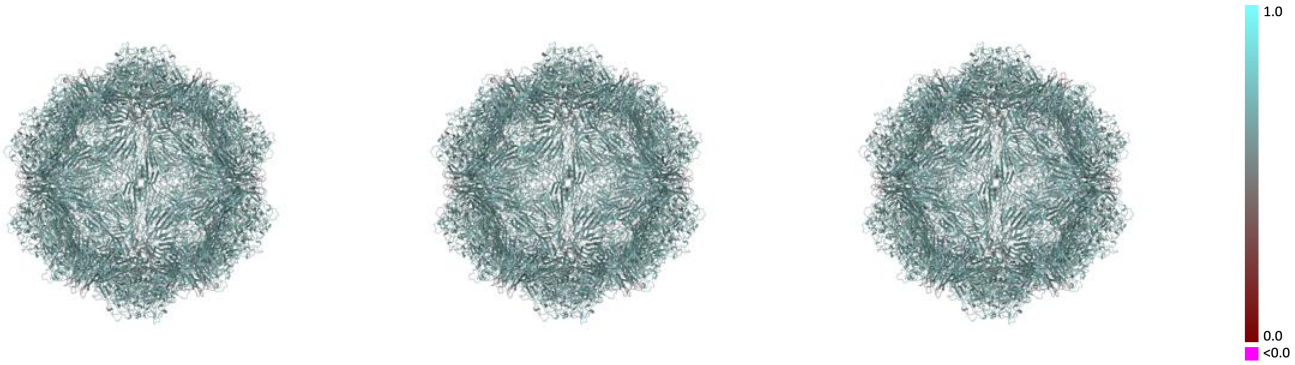
Y



Z

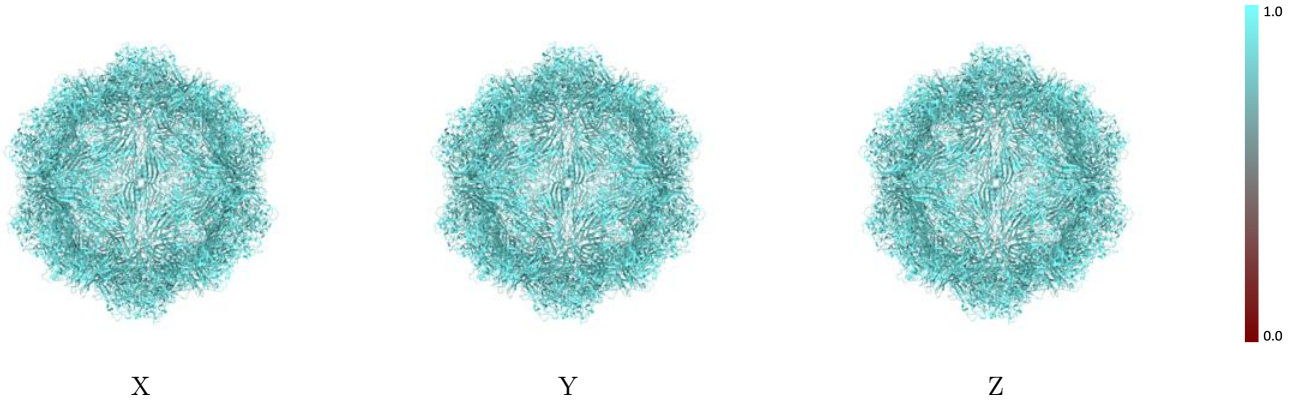
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



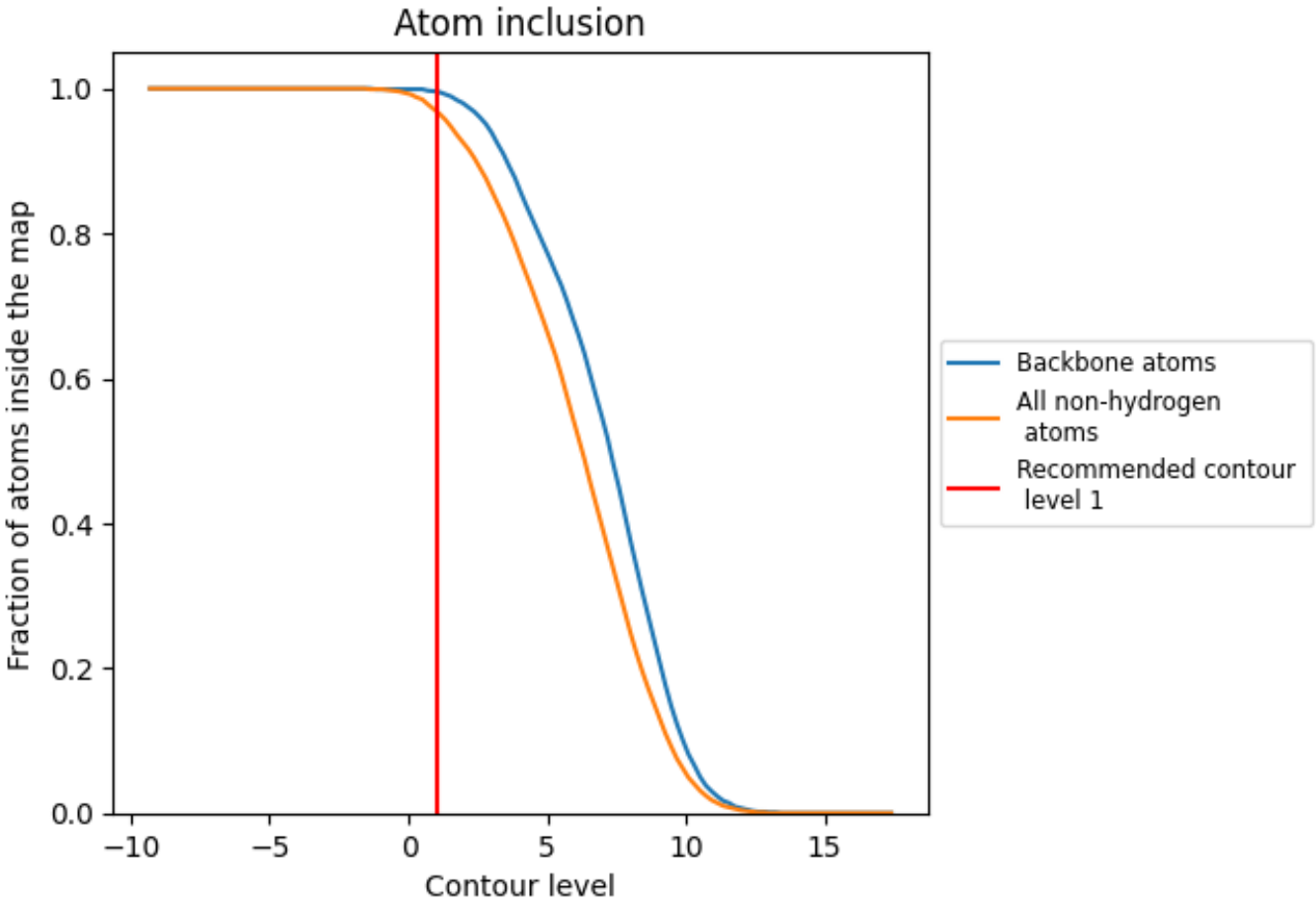
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9690	0.6280
0	0.3700	0.3930
0A	0.3700	0.3870
1	0.9740	0.6300
1B	0.3700	0.4030
2	0.9740	0.6300
3	0.9740	0.6300
3A	0.3480	0.3730
4	0.9770	0.6300
4B	0.3700	0.3880
5	0.9760	0.6290
6	0.9760	0.6300
6A	0.3700	0.3970
7	0.9760	0.6300
7B	0.3480	0.3820
8	0.9740	0.6300
9A	0.3480	0.3830
A	0.9740	0.6300
AC	0.3700	0.3860
B	0.9740	0.6300
BA	0.3700	0.3910
C	0.9770	0.6300
CB	0.3480	0.3820
D	0.9760	0.6300
DC	0.3700	0.3800
E	0.9740	0.6320
EA	0.3480	0.3770
F	0.9740	0.6300
FB	0.3700	0.3810
G	0.9740	0.6300
GC	0.3700	0.3840
H	0.9760	0.6300
HA	0.3480	0.3760
I	0.9770	0.6300
IB	0.3480	0.3770

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Chain	Atom inclusion	Q-score
J	0.9740	0.6300
JC	0.3700	0.3860
K	0.9770	0.6290
KA	0.3700	0.3830
L	0.9740	0.6300
LB	0.3700	0.3920
M	0.9740	0.6310
MC	0.3480	0.3670
N	0.9760	0.6310
NA	0.3700	0.3890
O	0.9740	0.6310
OB	0.3700	0.3950
P	0.9760	0.6310
PC	0.3700	0.3950
Q	0.9770	0.6300
QA	0.3700	0.3850
R	0.9740	0.6310
RB	0.3700	0.3940
S	0.9740	0.6310
SC	0.3700	0.3800
T	0.9770	0.6310
TA	0.3480	0.3810
U	0.9740	0.6300
UB	0.3700	0.3780
V	0.9770	0.6300
VC	0.3480	0.3770
W	0.9760	0.6300
WA	0.3480	0.3780
X	0.9740	0.6300
XB	0.3700	0.3830
Y	0.9760	0.6310
YC	0.3700	0.3910
Z	0.9740	0.6300
ZA	0.3700	0.3950
a	0.9740	0.6300
aB	0.3700	0.3940
b	0.9740	0.6300
bC	0.3700	0.3850
c	0.9740	0.6300
cA	0.3480	0.3710
d	0.9740	0.6300
dB	0.3700	0.3910

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Chain	Atom inclusion	Q-score
e	0.9740	0.6300
eC	0.3700	0.3870
f	0.9740	0.6310
fA	0.3700	0.3890
g	0.9770	0.6300
gB	0.3480	0.3720
h	0.9740	0.6300
hC	0.3700	0.3950
i	0.9760	0.6310
iA	0.3700	0.3860
j	0.9760	0.6300
jB	0.3700	0.3940
k	0.9760	0.6300
kC	0.3700	0.3910
l	0.9740	0.6300
lA	0.3480	0.3790
m	0.9770	0.6300
mB	0.3480	0.3730
n	0.9740	0.6290
nC	0.3480	0.3710
o	0.9740	0.6300
oA	0.3700	0.3800
p	0.9770	0.6290
pB	0.3480	0.3750
q	0.9740	0.6300
qC	0.3480	0.3650
r	0.9740	0.6300
rA	0.3480	0.3670
s	0.9740	0.6310
sB	0.3480	0.3790
t	0.9740	0.6300
tC	0.3480	0.3770
u	0.9770	0.6300
uA	0.3480	0.3780
v	0.9740	0.6300
vB	0.3700	0.3870
w	0.9740	0.6310
wC	0.3480	0.3700
x	0.9770	0.6290
xA	0.3700	0.3920
y	0.9740	0.6300
yB	0.3480	0.3640

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Chain	Atom inclusion	Q-score
z	0.9740	0.6300
zC	0.3700	0.3870