Full wwPDB EM Validation Report ⓘ

Jan 28, 2025 – 12:41 pm GMT

PDB ID	:	9EV0
EMDB ID	:	EMD-19990
Title	:	Structure of the AAP filament of Sulfolobus acidocaldarius strain MW039 (delta agl3 mutant).
Authors	:	Daum, B.; Isupov, M.N.; Gaines, M.; McLaren, M.; Mollat, C.
Deposited on	:	2024-03-28
Resolution	:	2.38 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:

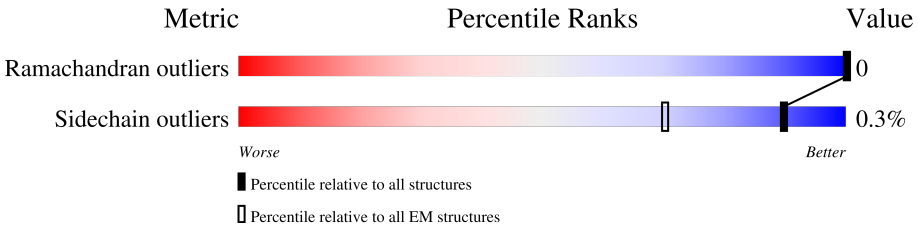
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.38 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	A	141	100%
1	B	141	100%
1	C	141	99%
1	D	141	100%
1	E	141	100%
1	F	141	99%
1	G	141	100%
1	H	141	100%
1	I	141	99%

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Mol	Chain	Length	Quality of chain
1	J	141	100%
1	K	141	100%
1	L	141	99%
1	M	141	100%
1	N	141	100%
1	O	141	99%
1	P	141	100%
1	Q	141	100%
1	R	141	99%
1	S	141	100%
1	T	141	100%
1	U	141	99%
1	V	141	100%
1	W	141	100%
1	X	141	99%
1	Y	141	5% 100%
1	Z	141	100%
1	a	141	99%
1	b	141	7% 100%
1	c	141	6% 100%
1	d	141	6% 99%
2	0	3	33% 100%
2	0A	3	67% 100%
2	1	3	100% 33% 67%
2	1A	3	67% 100%

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Mol	Chain	Length	Quality of chain
2	2	3	67% 33% 67%
2	2A	3	100% 33% 67%
2	3	3	67% 100%
2	3A	3	100% 100%
2	4	3	100% 33% 67%
2	4A	3	100% 100%
2	5	3	100% 33% 67%
2	5A	3	100% 33% 67%
2	6	3	67% 100%
2	7	3	100% 33% 67%
2	8	3	67% 33% 67%
2	9	3	67% 33% 67%
2	AA	3	100% 33% 67%
2	BA	3	67% 33% 67%
2	CA	3	67% 33% 67%
2	DA	3	100% 33% 67%
2	EA	3	67% 33% 67%
2	FA	3	67% 33% 67%
2	GA	3	100% 33% 67%
2	HA	3	67% 33% 67%
2	IA	3	67% 33% 67%
2	JA	3	100% 33% 67%
2	KA	3	67% 33% 67%
2	LA	3	67% 33% 67%
2	MA	3	100% 33% 67%

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Mol	Chain	Length	Quality of chain
2	NA	3	67% 33% 67%
2	OA	3	67% 33% 67%
2	PA	3	100% 33% 67%
2	QA	3	67% 33% 67%
2	RA	3	67% 33% 67%
2	SA	3	100% 33% 67%
2	TA	3	67% 33% 67%
2	UA	3	67% 33% 67%
2	VA	3	100% 33% 67%
2	WA	3	67% 100%
2	XA	3	67% 33% 67%
2	YA	3	100% 33% 67%
2	ZA	3	100% 33% 67%
2	aA	3	100% 33% 67%
2	bA	3	100% 33% 67%
2	cA	3	33% 100%
2	dA	3	67% 100%
2	e	3	67% 33% 67%
2	eA	3	100% 33% 67%
2	f	3	33% 100%
2	fA	3	33% 100%
2	g	3	100% 33% 67%
2	gA	3	67% 100%
2	h	3	67% 33% 67%
2	hA	3	100% 33% 67%

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Mol	Chain	Length	Quality of chain
2	i	3	33% 100%
2	iA	3	33% 100%
2	j	3	100% 33% 67%
2	jA	3	67% 100%
2	k	3	67% 33% 67%
2	kA	3	100% 33% 67%
2	l	3	33% 100%
2	lA	3	33% 100%
2	m	3	100% 33% 67%
2	mA	3	67% 100%
2	n	3	67% 33% 67%
2	nA	3	100% 33% 67%
2	o	3	33% 100%
2	oA	3	33% 100%
2	p	3	100% 33% 67%
2	pA	3	67% 100%
2	q	3	67% 33% 67%
2	qA	3	100% 33% 67%
2	r	3	33% 100%
2	rA	3	33% 100%
2	s	3	100% 33% 67%
2	sA	3	67% 100%
2	t	3	67% 33% 67%
2	tA	3	100% 33% 67%
2	u	3	33% 100%

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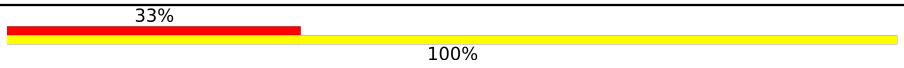
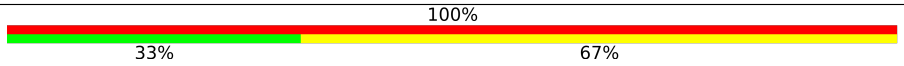
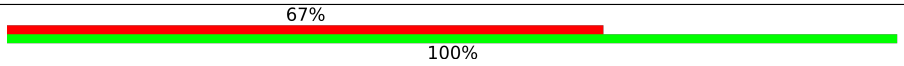
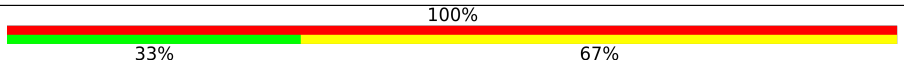
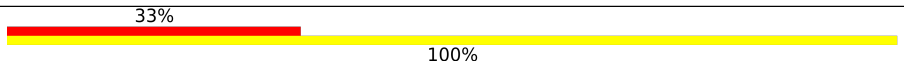
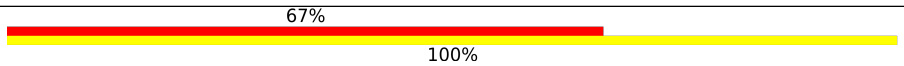
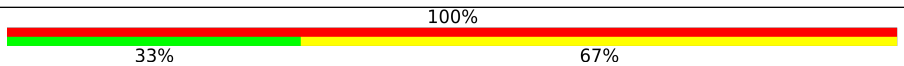
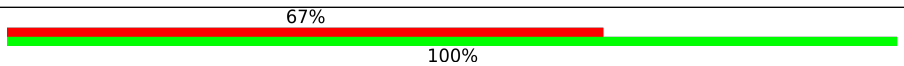
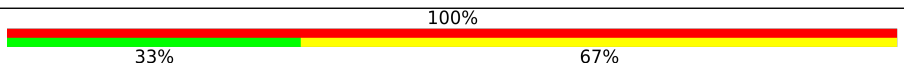
Mol	Chain	Length	Quality of chain
2	uA	3	
2	v	3	
2	vA	3	
2	w	3	
2	wA	3	
2	x	3	
2	xA	3	
2	y	3	
2	yA	3	
2	z	3	
2	zA	3	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 33540 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 DUF4352 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	141	Total	C	N	O	0	0
			1001	639	165	197		
1	A	141	Total	C	N	O	0	0
			1001	639	165	197		
1	D	141	Total	C	N	O	0	0
			1001	639	165	197		
1	J	141	Total	C	N	O	0	0
			1001	639	165	197		
1	M	141	Total	C	N	O	0	0
			1001	639	165	197		
1	P	141	Total	C	N	O	0	0
			1001	639	165	197		
1	S	141	Total	C	N	O	0	0
			1001	639	165	197		
1	V	141	Total	C	N	O	0	0
			1001	639	165	197		
1	Y	141	Total	C	N	O	0	0
			1001	639	165	197		
1	b	141	Total	C	N	O	0	0
			1001	639	165	197		
1	H	141	Total	C	N	O	0	0
			1001	639	165	197		
1	B	141	Total	C	N	O	0	0
			1001	639	165	197		
1	E	141	Total	C	N	O	0	0
			1001	639	165	197		
1	K	141	Total	C	N	O	0	0
			1001	639	165	197		
1	N	141	Total	C	N	O	0	0
			1001	639	165	197		
1	Q	141	Total	C	N	O	0	0
			1001	639	165	197		
1	T	141	Total	C	N	O	0	0
			1001	639	165	197		

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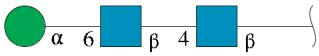
Mol	Chain	Residues	Atoms				AltConf	Trace
1	W	141	Total	C	N	O	0	0
			1001	639	165	197		
1	Z	141	Total	C	N	O	0	0
			1001	639	165	197		
1	c	141	Total	C	N	O	0	0
			1001	639	165	197		
1	I	141	Total	C	N	O	0	0
			1001	639	165	197		
1	C	141	Total	C	N	O	0	0
			1001	639	165	197		
1	F	141	Total	C	N	O	0	0
			1001	639	165	197		
1	L	141	Total	C	N	O	0	0
			1001	639	165	197		
1	O	141	Total	C	N	O	0	0
			1001	639	165	197		
1	R	141	Total	C	N	O	0	0
			1001	639	165	197		
1	U	141	Total	C	N	O	0	0
			1001	639	165	197		
1	X	141	Total	C	N	O	0	0
			1001	639	165	197		
1	a	141	Total	C	N	O	0	0
			1001	639	165	197		
1	d	141	Total	C	N	O	0	0
			1001	639	165	197		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	e	3	Total	C	N	O	0	0
			39	22	2	15		
2	f	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	3	Total	C	N	O	0	0
			39	22	2	15		
2	h	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	i	3	Total	C	N	O	0	0
			39	22	2	15		
2	j	3	Total	C	N	O	0	0
			39	22	2	15		
2	k	3	Total	C	N	O	0	0
			39	22	2	15		
2	l	3	Total	C	N	O	0	0
			39	22	2	15		
2	m	3	Total	C	N	O	0	0
			39	22	2	15		
2	n	3	Total	C	N	O	0	0
			39	22	2	15		
2	o	3	Total	C	N	O	0	0
			39	22	2	15		
2	p	3	Total	C	N	O	0	0
			39	22	2	15		
2	q	3	Total	C	N	O	0	0
			39	22	2	15		
2	r	3	Total	C	N	O	0	0
			39	22	2	15		
2	s	3	Total	C	N	O	0	0
			39	22	2	15		
2	t	3	Total	C	N	O	0	0
			39	22	2	15		
2	u	3	Total	C	N	O	0	0
			39	22	2	15		
2	v	3	Total	C	N	O	0	0
			39	22	2	15		
2	w	3	Total	C	N	O	0	0
			39	22	2	15		
2	x	3	Total	C	N	O	0	0
			39	22	2	15		
2	y	3	Total	C	N	O	0	0
			39	22	2	15		
2	z	3	Total	C	N	O	0	0
			39	22	2	15		
2	0	3	Total	C	N	O	0	0
			39	22	2	15		
2	1	3	Total	C	N	O	0	0
			39	22	2	15		
2	2	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	3	Total	C	N	O	0	0
			39	22	2	15		
2	4	3	Total	C	N	O	0	0
			39	22	2	15		
2	5	3	Total	C	N	O	0	0
			39	22	2	15		
2	6	3	Total	C	N	O	0	0
			39	22	2	15		
2	7	3	Total	C	N	O	0	0
			39	22	2	15		
2	8	3	Total	C	N	O	0	0
			39	22	2	15		
2	9	3	Total	C	N	O	0	0
			39	22	2	15		
2	AA	3	Total	C	N	O	0	0
			39	22	2	15		
2	BA	3	Total	C	N	O	0	0
			39	22	2	15		
2	CA	3	Total	C	N	O	0	0
			39	22	2	15		
2	DA	3	Total	C	N	O	0	0
			39	22	2	15		
2	EA	3	Total	C	N	O	0	0
			39	22	2	15		
2	FA	3	Total	C	N	O	0	0
			39	22	2	15		
2	GA	3	Total	C	N	O	0	0
			39	22	2	15		
2	HA	3	Total	C	N	O	0	0
			39	22	2	15		
2	IA	3	Total	C	N	O	0	0
			39	22	2	15		
2	JA	3	Total	C	N	O	0	0
			39	22	2	15		
2	KA	3	Total	C	N	O	0	0
			39	22	2	15		
2	LA	3	Total	C	N	O	0	0
			39	22	2	15		
2	MA	3	Total	C	N	O	0	0
			39	22	2	15		
2	NA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	OA	3	Total	C	N	O	0	0
			39	22	2	15		
2	PA	3	Total	C	N	O	0	0
			39	22	2	15		
2	QA	3	Total	C	N	O	0	0
			39	22	2	15		
2	RA	3	Total	C	N	O	0	0
			39	22	2	15		
2	SA	3	Total	C	N	O	0	0
			39	22	2	15		
2	TA	3	Total	C	N	O	0	0
			39	22	2	15		
2	UA	3	Total	C	N	O	0	0
			39	22	2	15		
2	VA	3	Total	C	N	O	0	0
			39	22	2	15		
2	WA	3	Total	C	N	O	0	0
			39	22	2	15		
2	XA	3	Total	C	N	O	0	0
			39	22	2	15		
2	YA	3	Total	C	N	O	0	0
			39	22	2	15		
2	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
2	aA	3	Total	C	N	O	0	0
			39	22	2	15		
2	bA	3	Total	C	N	O	0	0
			39	22	2	15		
2	cA	3	Total	C	N	O	0	0
			39	22	2	15		
2	dA	3	Total	C	N	O	0	0
			39	22	2	15		
2	eA	3	Total	C	N	O	0	0
			39	22	2	15		
2	fA	3	Total	C	N	O	0	0
			39	22	2	15		
2	gA	3	Total	C	N	O	0	0
			39	22	2	15		
2	hA	3	Total	C	N	O	0	0
			39	22	2	15		
2	iA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	jA	3	Total	C	N	O	0	0
			39	22	2	15		
2	kA	3	Total	C	N	O	0	0
			39	22	2	15		
2	lA	3	Total	C	N	O	0	0
			39	22	2	15		
2	mA	3	Total	C	N	O	0	0
			39	22	2	15		
2	nA	3	Total	C	N	O	0	0
			39	22	2	15		
2	oA	3	Total	C	N	O	0	0
			39	22	2	15		
2	pA	3	Total	C	N	O	0	0
			39	22	2	15		
2	qA	3	Total	C	N	O	0	0
			39	22	2	15		
2	rA	3	Total	C	N	O	0	0
			39	22	2	15		
2	sA	3	Total	C	N	O	0	0
			39	22	2	15		
2	tA	3	Total	C	N	O	0	0
			39	22	2	15		
2	uA	3	Total	C	N	O	0	0
			39	22	2	15		
2	vA	3	Total	C	N	O	0	0
			39	22	2	15		
2	wA	3	Total	C	N	O	0	0
			39	22	2	15		
2	xA	3	Total	C	N	O	0	0
			39	22	2	15		
2	yA	3	Total	C	N	O	0	0
			39	22	2	15		
2	zA	3	Total	C	N	O	0	0
			39	22	2	15		
2	0A	3	Total	C	N	O	0	0
			39	22	2	15		
2	1A	3	Total	C	N	O	0	0
			39	22	2	15		
2	2A	3	Total	C	N	O	0	0
			39	22	2	15		
2	3A	3	Total	C	N	O	0	0
			39	22	2	15		

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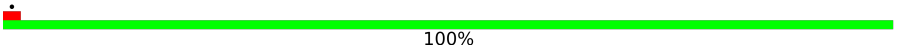
Mol	Chain	Residues	Atoms				AltConf	Trace
2	4A	3	Total	C	N	O	0	0
			39	22	2	15		
2	5A	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots (i)

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

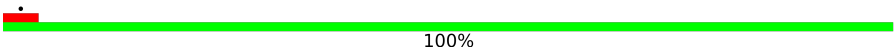
- Molecule 1: DUF4352 domain-containing protein

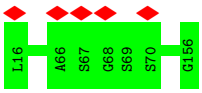
Chain G:



- Molecule 1: DUF4352 domain-containing protein

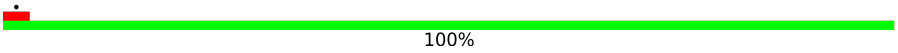
Chain A:

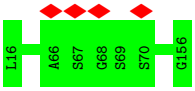




- Molecule 1: DUF4352 domain-containing protein

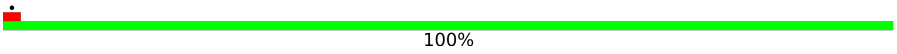
Chain D:

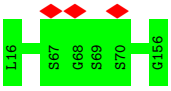




- Molecule 1: DUF4352 domain-containing protein

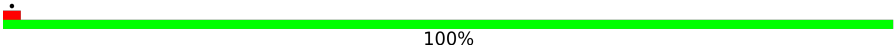
Chain J:

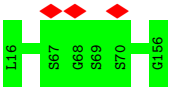




- Molecule 1: DUF4352 domain-containing protein

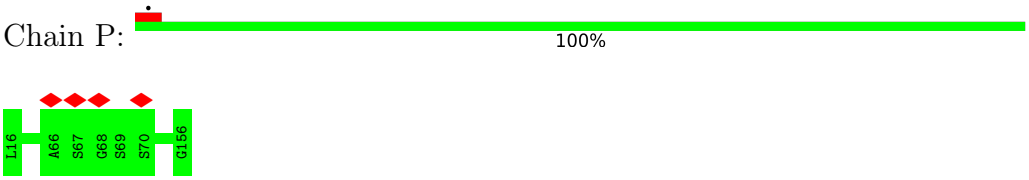
Chain M:





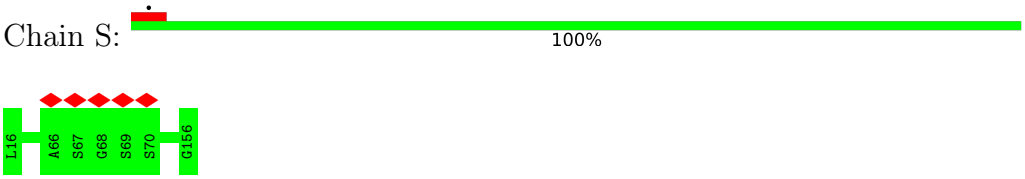
• Molecule 1: DUF4352 domain-containing protein

Chain P:



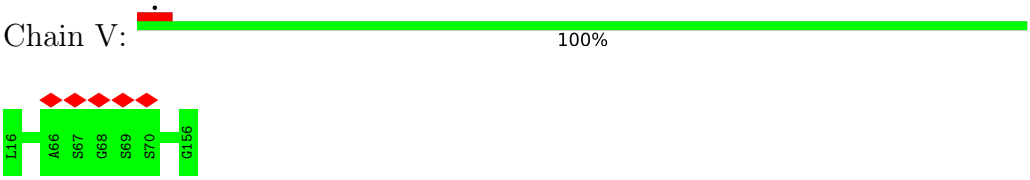
• Molecule 1: DUF4352 domain-containing protein

Chain S:



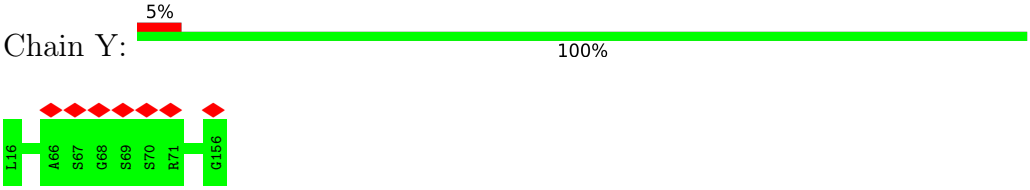
• Molecule 1: DUF4352 domain-containing protein

Chain V:



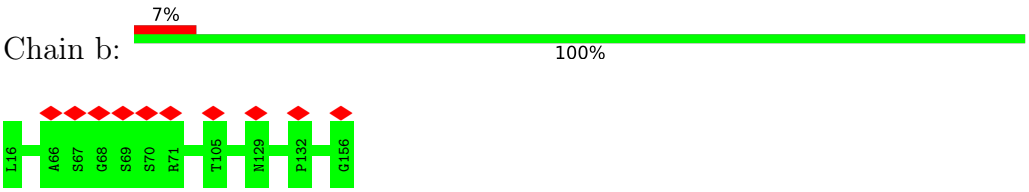
• Molecule 1: DUF4352 domain-containing protein

Chain Y:



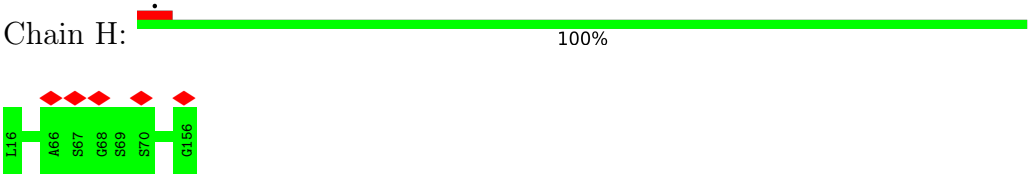
• Molecule 1: DUF4352 domain-containing protein

Chain b:



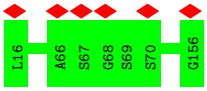
• Molecule 1: DUF4352 domain-containing protein

Chain H:



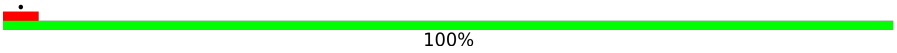
• Molecule 1: DUF4352 domain-containing protein

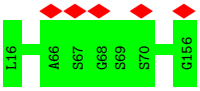
Chain B:



• Molecule 1: DUF4352 domain-containing protein

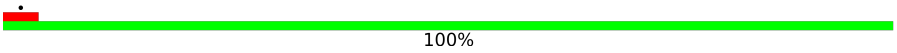
Chain E:

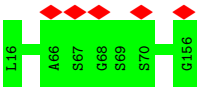




• Molecule 1: DUF4352 domain-containing protein

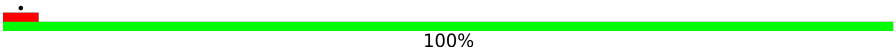
Chain K:

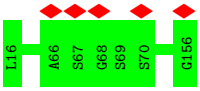




• Molecule 1: DUF4352 domain-containing protein

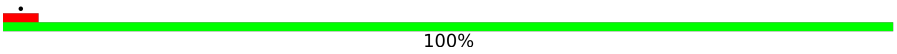
Chain N:

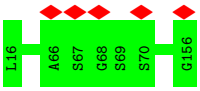




• Molecule 1: DUF4352 domain-containing protein

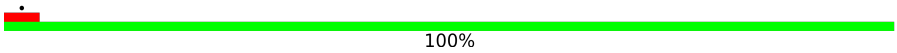
Chain Q:

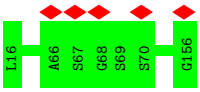




• Molecule 1: DUF4352 domain-containing protein

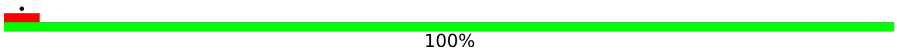
Chain T:

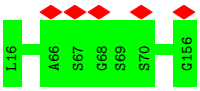




• Molecule 1: DUF4352 domain-containing protein

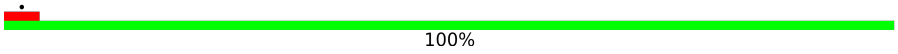
Chain W:

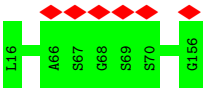




• Molecule 1: DUF4352 domain-containing protein

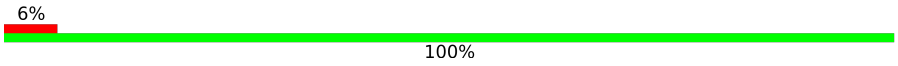
Chain Z:

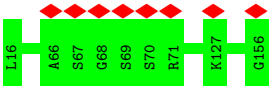




• Molecule 1: DUF4352 domain-containing protein

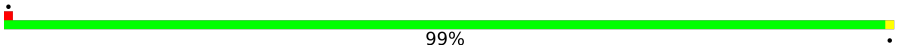
Chain c:

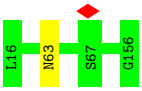




• Molecule 1: DUF4352 domain-containing protein

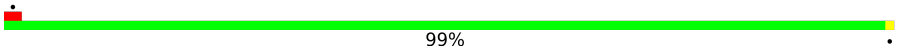
Chain I:

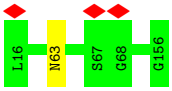




• Molecule 1: DUF4352 domain-containing protein

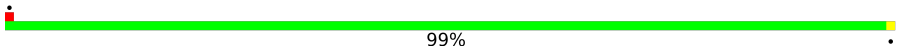
Chain C:

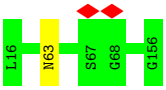




• Molecule 1: DUF4352 domain-containing protein

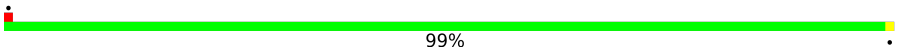
Chain F:

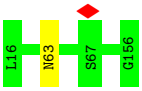




• Molecule 1: DUF4352 domain-containing protein

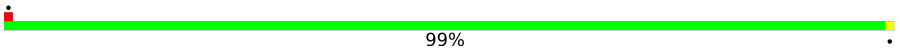
Chain L:

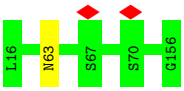




• Molecule 1: DUF4352 domain-containing protein

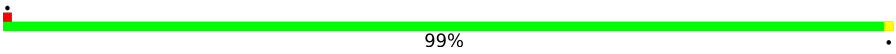
Chain O:

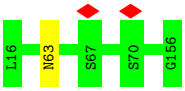




• Molecule 1: DUF4352 domain-containing protein

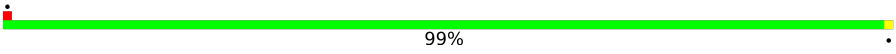
Chain R:

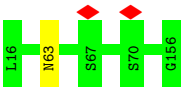




• Molecule 1: DUF4352 domain-containing protein

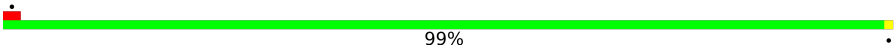
Chain U:

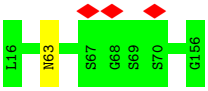




• Molecule 1: DUF4352 domain-containing protein

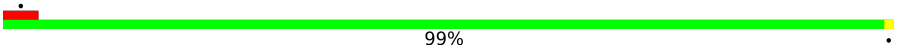
Chain X:

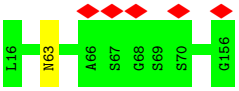




• Molecule 1: DUF4352 domain-containing protein

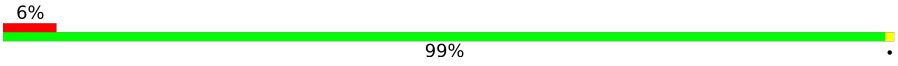
Chain a:

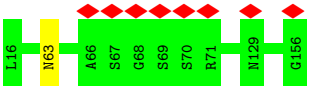




• Molecule 1: DUF4352 domain-containing protein

Chain d:



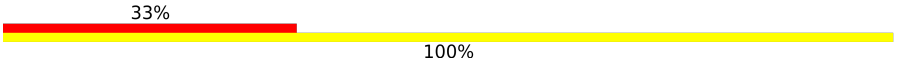


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

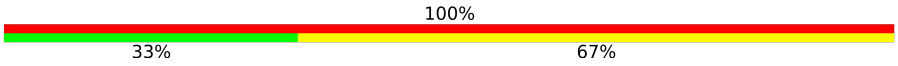
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



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

Chain g:

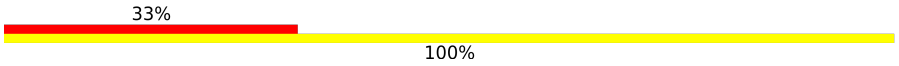


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

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

Chain i:



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

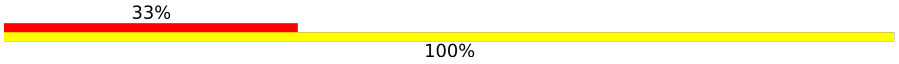
Chain j:

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

Chain k:

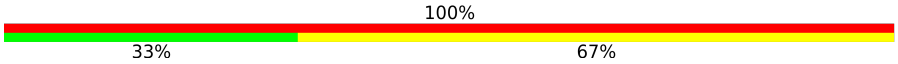
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



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

Chain m:

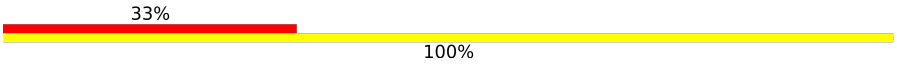


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

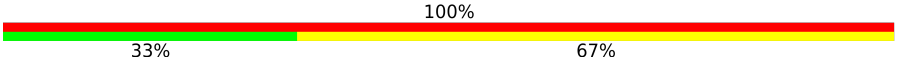
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



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

Chain p:

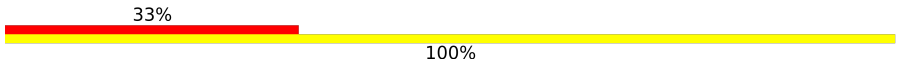


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

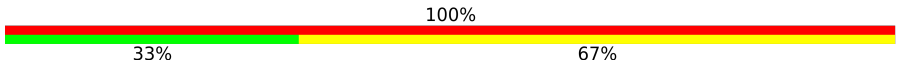
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



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

Chain s:

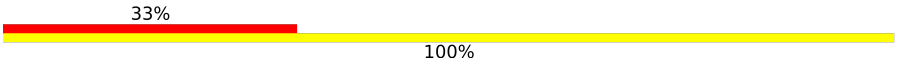


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

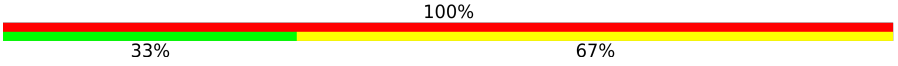
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



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

Chain v:

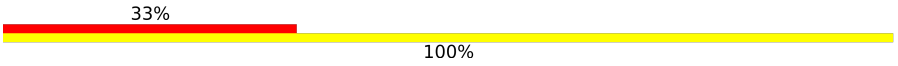


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

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

Chain x:



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

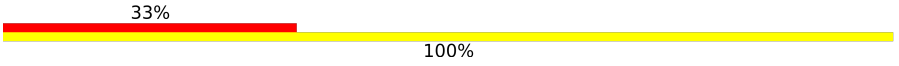
Chain y:

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

Chain z:

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

Chain 0:



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

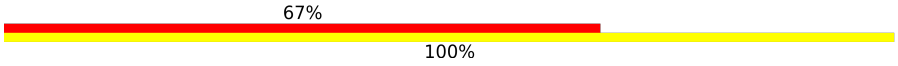
Chain 1:

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

Chain 2:

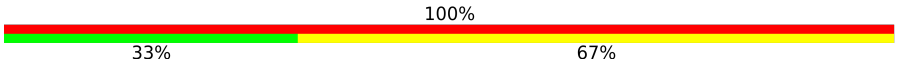
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



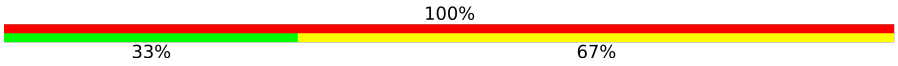
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:



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

Chain 5:

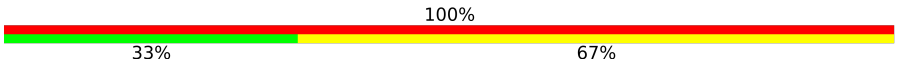


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:

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

Chain 7:



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

Chain 8:

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

Chain 9:

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

Chain AA:

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

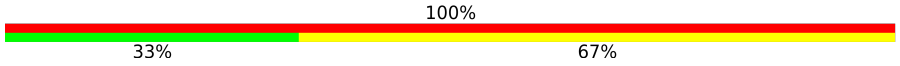
Chain BA:

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

Chain CA:

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

Chain DA:



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

Chain EA:

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

Chain FA:

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

Chain GA:

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

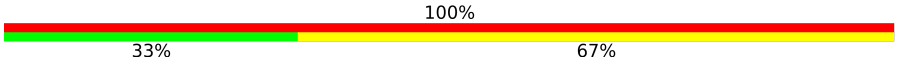
Chain HA:

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

Chain IA:

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

Chain JA:



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

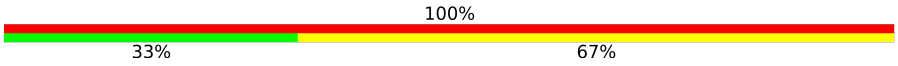
Chain KA:

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

Chain LA:

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

Chain MA:



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

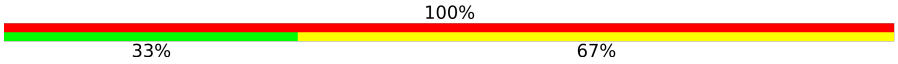
Chain NA:

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

Chain OA:

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

Chain PA:



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

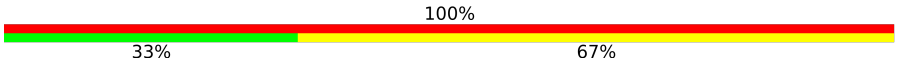
Chain QA:

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

Chain RA:

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

Chain SA:



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

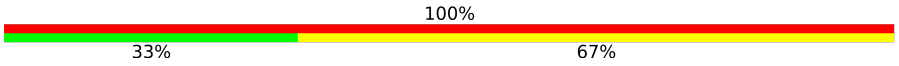
Chain TA:

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

Chain UA:

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

Chain VA:



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

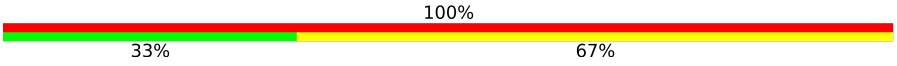
Chain WA:

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

Chain XA:

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

Chain YA:

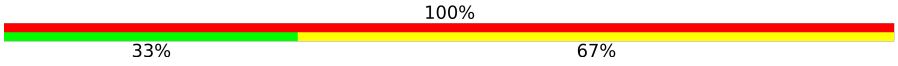


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain ZA:

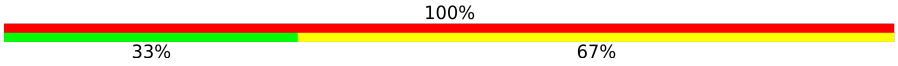
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA:



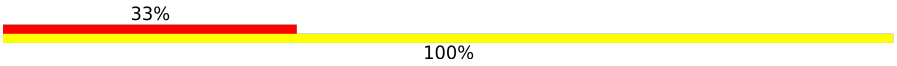
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bA:



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

Chain cA:

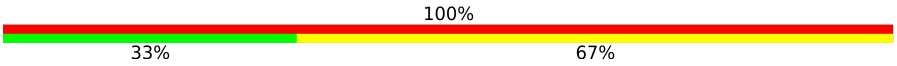


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain dA:

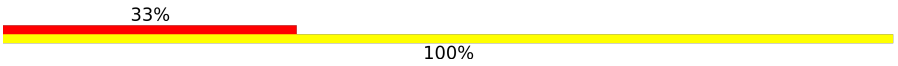
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eA:



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

Chain fA:



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

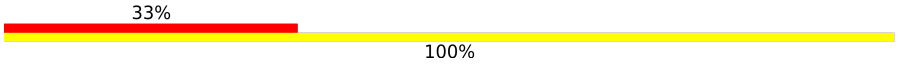
Chain gA:

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

Chain hA:

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

Chain iA:

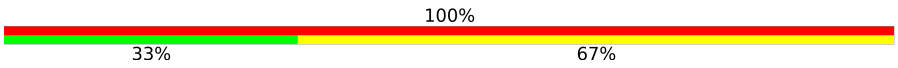


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain jA:

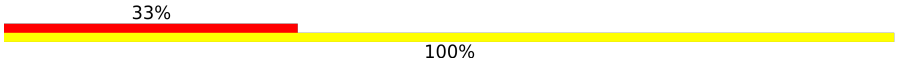
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain kA:



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

Chain lA:

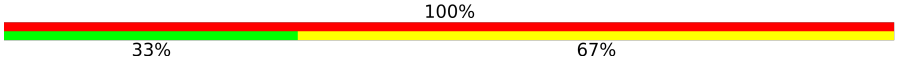


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain mA:

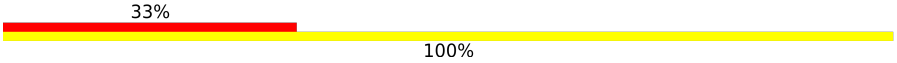
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain nA:



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

Chain oA:

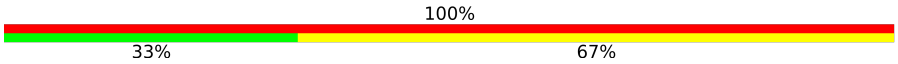


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pA:

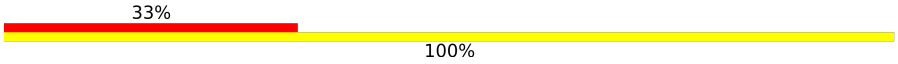
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain qA:



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

Chain rA:

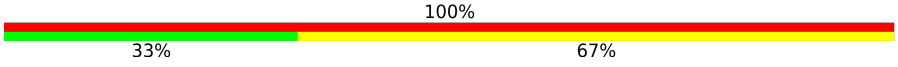


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sA:

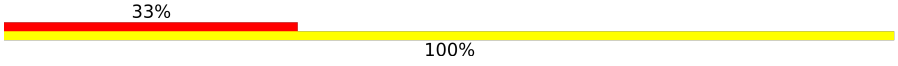
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain tA:



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

Chain uA:



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

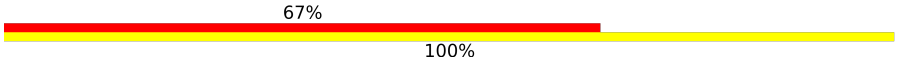
Chain vA:

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

Chain wA:

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

Chain xA:

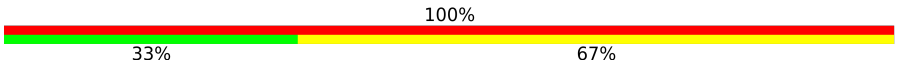


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain yA:

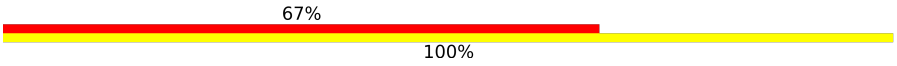
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain zA:



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

Chain 0A:

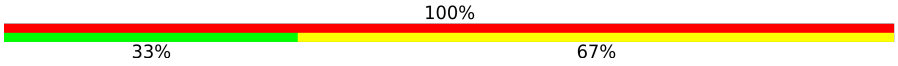


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1A:

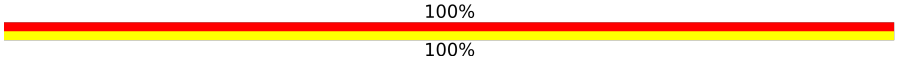
• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2A:



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

Chain 3A:

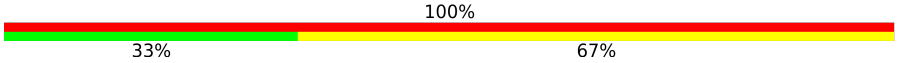


• Molecule 2: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4A:

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

Chain 5A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-39.953°, rise=15.282 Å, axial sym=C1	Depositor
Number of segments used	691479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	265.248, 265.248, 265.248	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92099994, 0.92099994, 0.92099994	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.36	0/1019	0.69	0/1396
1	B	0.36	0/1019	0.66	0/1396
1	C	0.36	0/1019	0.69	0/1396
1	D	0.36	0/1019	0.69	0/1396
1	E	0.36	0/1019	0.66	0/1396
1	F	0.36	0/1019	0.69	0/1396
1	G	0.36	0/1019	0.69	0/1396
1	H	0.36	0/1019	0.66	0/1396
1	I	0.36	0/1019	0.69	0/1396
1	J	0.36	0/1019	0.69	0/1396
1	K	0.36	0/1019	0.66	0/1396
1	L	0.36	0/1019	0.69	0/1396
1	M	0.36	0/1019	0.69	0/1396
1	N	0.36	0/1019	0.66	0/1396
1	O	0.36	0/1019	0.69	0/1396
1	P	0.36	0/1019	0.69	0/1396
1	Q	0.36	0/1019	0.66	0/1396
1	R	0.36	0/1019	0.69	0/1396
1	S	0.36	0/1019	0.69	0/1396
1	T	0.36	0/1019	0.66	0/1396
1	U	0.36	0/1019	0.69	0/1396
1	V	0.36	0/1019	0.69	0/1396
1	W	0.36	0/1019	0.66	0/1396
1	X	0.36	0/1019	0.69	0/1396
1	Y	0.36	0/1019	0.69	0/1396
1	Z	0.36	0/1019	0.66	0/1396
1	a	0.36	0/1019	0.69	0/1396
1	b	0.36	0/1019	0.69	0/1396
1	c	0.36	0/1019	0.66	0/1396
1	d	0.36	0/1019	0.69	0/1396
All	All	0.36	0/30570	0.68	0/41880

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	A	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	B	139/141 (99%)	139 (100%)	0	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	D	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	E	139/141 (99%)	139 (100%)	0	0	100	100
1	F	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	G	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	H	139/141 (99%)	139 (100%)	0	0	100	100
1	I	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	J	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	K	139/141 (99%)	139 (100%)	0	0	100	100
1	L	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	M	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	N	139/141 (99%)	139 (100%)	0	0	100	100
1	O	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	P	139/141 (99%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	139/141 (99%)	139 (100%)	0	0	100	100
1	R	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	S	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	T	139/141 (99%)	139 (100%)	0	0	100	100
1	U	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	V	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	W	139/141 (99%)	139 (100%)	0	0	100	100
1	X	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Y	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Z	139/141 (99%)	139 (100%)	0	0	100	100
1	a	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	b	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	c	139/141 (99%)	139 (100%)	0	0	100	100
1	d	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
All	All	4170/4230 (99%)	4150 (100%)	20 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/110 (100%)	110 (100%)	0	100	100
1	B	110/110 (100%)	110 (100%)	0	100	100
1	C	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	D	110/110 (100%)	110 (100%)	0	100	100
1	E	110/110 (100%)	110 (100%)	0	100	100
1	F	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	G	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	110/110 (100%)	110 (100%)	0	100	100
1	I	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	J	110/110 (100%)	110 (100%)	0	100	100
1	K	110/110 (100%)	110 (100%)	0	100	100
1	L	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	M	110/110 (100%)	110 (100%)	0	100	100
1	N	110/110 (100%)	110 (100%)	0	100	100
1	O	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	P	110/110 (100%)	110 (100%)	0	100	100
1	Q	110/110 (100%)	110 (100%)	0	100	100
1	R	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	S	110/110 (100%)	110 (100%)	0	100	100
1	T	110/110 (100%)	110 (100%)	0	100	100
1	U	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	V	110/110 (100%)	110 (100%)	0	100	100
1	W	110/110 (100%)	110 (100%)	0	100	100
1	X	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	Y	110/110 (100%)	110 (100%)	0	100	100
1	Z	110/110 (100%)	110 (100%)	0	100	100
1	a	110/110 (100%)	109 (99%)	1 (1%)	75	87
1	b	110/110 (100%)	110 (100%)	0	100	100
1	c	110/110 (100%)	110 (100%)	0	100	100
1	d	110/110 (100%)	109 (99%)	1 (1%)	75	87
All	All	3300/3300 (100%)	3290 (100%)	10 (0%)	90	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	63	ASN
1	C	63	ASN
1	F	63	ASN
1	L	63	ASN
1	O	63	ASN
1	R	63	ASN

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Mol	Chain	Res	Type
1	U	63	ASN
1	X	63	ASN
1	a	63	ASN
1	d	63	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

270 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	2,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	0	2	2	14,14,15	0.28	0	17,19,21	1.33	2 (11%)
2	MAN	0	3	2	11,11,12	1.39	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	0A	1	2,1	14,14,15	0.70	0	17,19,21	1.44	3 (17%)
2	NAG	0A	2	2	14,14,15	0.60	0	17,19,21	1.37	1 (5%)
2	MAN	0A	3	2	11,11,12	0.80	0	15,15,17	1.09	1 (6%)
2	NAG	1	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.77	0
2	NAG	1	2	2	14,14,15	0.30	0	17,19,21	0.64	1 (5%)
2	MAN	1	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	1A	1	2,1	14,14,15	0.51	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	1A	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	1A	3	2	11,11,12	0.42	0	15,15,17	0.59	0
2	NAG	2	1	2,1	14,14,15	0.37	0	17,19,21	1.00	1 (5%)
2	NAG	2	2	2	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
2	MAN	2	3	2	11,11,12	0.46	0	15,15,17	0.79	0
2	NAG	2A	1	2,1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	NAG	2A	2	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	MAN	2A	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	3	1	2,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	3	2	2	14,14,15	0.28	0	17,19,21	1.32	2 (11%)
2	MAN	3	3	2	11,11,12	1.38	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	3A	1	2,1	14,14,15	0.70	0	17,19,21	1.44	3 (17%)
2	NAG	3A	2	2	14,14,15	0.60	0	17,19,21	1.37	1 (5%)
2	MAN	3A	3	2	11,11,12	0.80	0	15,15,17	1.09	1 (6%)
2	NAG	4	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.77	0
2	NAG	4	2	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
2	MAN	4	3	2	11,11,12	0.46	0	15,15,17	0.68	0
2	NAG	4A	1	2,1	14,14,15	0.51	0	17,19,21	0.64	0
2	NAG	4A	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	4A	3	2	11,11,12	0.44	0	15,15,17	0.59	0
2	NAG	5	1	2,1	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
2	NAG	5	2	2	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
2	MAN	5	3	2	11,11,12	0.45	0	15,15,17	0.79	0
2	NAG	5A	1	2,1	14,14,15	0.27	0	17,19,21	0.99	1 (5%)
2	NAG	5A	2	2	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
2	MAN	5A	3	2	11,11,12	0.45	0	15,15,17	0.69	0
2	NAG	6	1	2,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	6	2	2	14,14,15	0.27	0	17,19,21	1.33	2 (11%)
2	MAN	6	3	2	11,11,12	1.37	2 (18%)	15,15,17	3.77	9 (60%)
2	NAG	7	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.77	0
2	NAG	7	2	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
2	MAN	7	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	8	1	2,1	14,14,15	0.36	0	17,19,21	1.42	1 (5%)
2	NAG	8	2	2	14,14,15	0.33	0	17,19,21	1.09	2 (11%)
2	MAN	8	3	2	11,11,12	0.36	0	15,15,17	0.85	0
2	NAG	9	1	2,1	14,14,15	0.65	0	17,19,21	0.67	0
2	NAG	9	2	2	14,14,15	0.53	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	9	3	2	11,11,12	0.26	0	15,15,17	0.77	1 (6%)
2	NAG	AA	1	2,1	14,14,15	0.30	0	17,19,21	1.27	1 (5%)
2	NAG	AA	2	2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	MAN	AA	3	2	11,11,12	0.42	0	15,15,17	0.73	0
2	NAG	BA	1	2,1	14,14,15	0.36	0	17,19,21	1.42	1 (5%)
2	NAG	BA	2	2	14,14,15	0.33	0	17,19,21	1.08	2 (11%)
2	MAN	BA	3	2	11,11,12	0.36	0	15,15,17	0.85	0
2	NAG	CA	1	2,1	14,14,15	0.65	0	17,19,21	0.66	0
2	NAG	CA	2	2	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
2	MAN	CA	3	2	11,11,12	0.26	0	15,15,17	0.77	1 (6%)
2	NAG	DA	1	2,1	14,14,15	0.30	0	17,19,21	1.27	1 (5%)
2	NAG	DA	2	2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	MAN	DA	3	2	11,11,12	0.41	0	15,15,17	0.73	0
2	NAG	EA	1	2,1	14,14,15	0.37	0	17,19,21	1.42	1 (5%)
2	NAG	EA	2	2	14,14,15	0.32	0	17,19,21	1.09	2 (11%)
2	MAN	EA	3	2	11,11,12	0.36	0	15,15,17	0.84	0
2	NAG	FA	1	2,1	14,14,15	0.66	0	17,19,21	0.67	0
2	NAG	FA	2	2	14,14,15	0.52	0	17,19,21	0.85	1 (5%)
2	MAN	FA	3	2	11,11,12	0.26	0	15,15,17	0.77	1 (6%)
2	NAG	GA	1	2,1	14,14,15	0.30	0	17,19,21	1.26	1 (5%)
2	NAG	GA	2	2	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
2	MAN	GA	3	2	11,11,12	0.41	0	15,15,17	0.73	0
2	NAG	HA	1	2,1	14,14,15	0.38	0	17,19,21	1.42	1 (5%)
2	NAG	HA	2	2	14,14,15	0.33	0	17,19,21	1.09	2 (11%)
2	MAN	HA	3	2	11,11,12	0.36	0	15,15,17	0.85	0
2	NAG	IA	1	2,1	14,14,15	0.65	0	17,19,21	0.67	0
2	NAG	IA	2	2	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
2	MAN	IA	3	2	11,11,12	0.28	0	15,15,17	0.77	1 (6%)
2	NAG	JA	1	2,1	14,14,15	0.29	0	17,19,21	1.26	1 (5%)
2	NAG	JA	2	2	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
2	MAN	JA	3	2	11,11,12	0.41	0	15,15,17	0.73	0
2	NAG	KA	1	2,1	14,14,15	0.38	0	17,19,21	1.42	1 (5%)
2	NAG	KA	2	2	14,14,15	0.34	0	17,19,21	1.08	2 (11%)
2	MAN	KA	3	2	11,11,12	0.37	0	15,15,17	0.85	0
2	NAG	LA	1	2,1	14,14,15	0.65	0	17,19,21	0.67	0
2	NAG	LA	2	2	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
2	MAN	LA	3	2	11,11,12	0.27	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	MA	1	2,1	14,14,15	0.31	0	17,19,21	1.27	1 (5%)
2	NAG	MA	2	2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	MAN	MA	3	2	11,11,12	0.42	0	15,15,17	0.73	0
2	NAG	NA	1	2,1	14,14,15	0.37	0	17,19,21	1.42	1 (5%)
2	NAG	NA	2	2	14,14,15	0.33	0	17,19,21	1.08	2 (11%)
2	MAN	NA	3	2	11,11,12	0.35	0	15,15,17	0.85	0
2	NAG	OA	1	2,1	14,14,15	0.65	0	17,19,21	0.67	0
2	NAG	OA	2	2	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
2	MAN	OA	3	2	11,11,12	0.26	0	15,15,17	0.77	1 (6%)
2	NAG	PA	1	2,1	14,14,15	0.31	0	17,19,21	1.27	1 (5%)
2	NAG	PA	2	2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	MAN	PA	3	2	11,11,12	0.42	0	15,15,17	0.73	0
2	NAG	QA	1	2,1	14,14,15	0.36	0	17,19,21	1.42	1 (5%)
2	NAG	QA	2	2	14,14,15	0.34	0	17,19,21	1.09	2 (11%)
2	MAN	QA	3	2	11,11,12	0.37	0	15,15,17	0.84	0
2	NAG	RA	1	2,1	14,14,15	0.66	0	17,19,21	0.67	0
2	NAG	RA	2	2	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
2	MAN	RA	3	2	11,11,12	0.26	0	15,15,17	0.77	1 (6%)
2	NAG	SA	1	2,1	14,14,15	0.30	0	17,19,21	1.26	1 (5%)
2	NAG	SA	2	2	14,14,15	0.27	0	17,19,21	0.65	1 (5%)
2	MAN	SA	3	2	11,11,12	0.41	0	15,15,17	0.73	0
2	NAG	TA	1	2,1	14,14,15	0.37	0	17,19,21	1.42	1 (5%)
2	NAG	TA	2	2	14,14,15	0.33	0	17,19,21	1.09	2 (11%)
2	MAN	TA	3	2	11,11,12	0.36	0	15,15,17	0.85	0
2	NAG	UA	1	2,1	14,14,15	0.65	0	17,19,21	0.66	0
2	NAG	UA	2	2	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
2	MAN	UA	3	2	11,11,12	0.27	0	15,15,17	0.77	1 (6%)
2	NAG	VA	1	2,1	14,14,15	0.31	0	17,19,21	1.28	1 (5%)
2	NAG	VA	2	2	14,14,15	0.27	0	17,19,21	0.65	1 (5%)
2	MAN	VA	3	2	11,11,12	0.42	0	15,15,17	0.73	0
2	NAG	WA	1	2,1	14,14,15	0.37	0	17,19,21	1.42	1 (5%)
2	NAG	WA	2	2	14,14,15	0.34	0	17,19,21	1.09	2 (11%)
2	MAN	WA	3	2	11,11,12	0.37	0	15,15,17	0.85	1 (6%)
2	NAG	XA	1	2,1	14,14,15	0.67	0	17,19,21	0.66	0
2	NAG	XA	2	2	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
2	MAN	XA	3	2	11,11,12	0.27	0	15,15,17	0.76	1 (6%)
2	NAG	YA	1	2,1	14,14,15	0.30	0	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	YA	2	2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
2	MAN	YA	3	2	11,11,12	0.41	0	15,15,17	0.74	0
2	NAG	ZA	1	2,1	14,14,15	0.38	0	17,19,21	1.42	1 (5%)
2	NAG	ZA	2	2	14,14,15	0.32	0	17,19,21	1.08	2 (11%)
2	MAN	ZA	3	2	11,11,12	0.36	0	15,15,17	0.85	0
2	NAG	aA	1	2,1	14,14,15	0.65	0	17,19,21	0.66	0
2	NAG	aA	2	2	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
2	MAN	aA	3	2	11,11,12	0.27	0	15,15,17	0.78	1 (6%)
2	NAG	bA	1	2,1	14,14,15	0.31	0	17,19,21	1.27	1 (5%)
2	NAG	bA	2	2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
2	MAN	bA	3	2	11,11,12	0.42	0	15,15,17	0.73	0
2	NAG	cA	1	2,1	14,14,15	0.71	0	17,19,21	1.44	3 (17%)
2	NAG	cA	2	2	14,14,15	0.60	0	17,19,21	1.37	1 (5%)
2	MAN	cA	3	2	11,11,12	0.80	0	15,15,17	1.10	1 (6%)
2	NAG	dA	1	2,1	14,14,15	0.52	0	17,19,21	0.64	0
2	NAG	dA	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	dA	3	2	11,11,12	0.44	0	15,15,17	0.59	0
2	NAG	e	1	2,1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	e	2	2	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
2	MAN	e	3	2	11,11,12	0.45	0	15,15,17	0.79	0
2	NAG	eA	1	2,1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	NAG	eA	2	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	MAN	eA	3	2	11,11,12	0.46	0	15,15,17	0.68	0
2	NAG	f	1	2,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	f	2	2	14,14,15	0.28	0	17,19,21	1.33	2 (11%)
2	MAN	f	3	2	11,11,12	1.38	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	fA	1	2,1	14,14,15	0.71	0	17,19,21	1.45	3 (17%)
2	NAG	fA	2	2	14,14,15	0.60	0	17,19,21	1.37	1 (5%)
2	MAN	fA	3	2	11,11,12	0.79	0	15,15,17	1.09	1 (6%)
2	NAG	g	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.77	0
2	NAG	g	2	2	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
2	MAN	g	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	gA	1	2,1	14,14,15	0.51	0	17,19,21	0.63	0
2	NAG	gA	2	2	14,14,15	0.36	0	17,19,21	0.68	0
2	MAN	gA	3	2	11,11,12	0.43	0	15,15,17	0.59	0
2	NAG	h	1	2,1	14,14,15	0.36	0	17,19,21	1.01	1 (5%)
2	NAG	h	2	2	14,14,15	0.56	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	h	3	2	11,11,12	0.44	0	15,15,17	0.79	0
2	NAG	hA	1	2,1	14,14,15	0.30	0	17,19,21	1.00	1 (5%)
2	NAG	hA	2	2	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
2	MAN	hA	3	2	11,11,12	0.45	0	15,15,17	0.68	0
2	NAG	i	1	2,1	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
2	NAG	i	2	2	14,14,15	0.27	0	17,19,21	1.33	2 (11%)
2	MAN	i	3	2	11,11,12	1.39	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	iA	1	2,1	14,14,15	0.71	0	17,19,21	1.45	3 (17%)
2	NAG	iA	2	2	14,14,15	0.61	0	17,19,21	1.36	1 (5%)
2	MAN	iA	3	2	11,11,12	0.81	0	15,15,17	1.09	1 (6%)
2	NAG	j	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.77	0
2	NAG	j	2	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
2	MAN	j	3	2	11,11,12	0.48	0	15,15,17	0.68	0
2	NAG	jA	1	2,1	14,14,15	0.52	0	17,19,21	0.64	0
2	NAG	jA	2	2	14,14,15	0.35	0	17,19,21	0.67	0
2	MAN	jA	3	2	11,11,12	0.44	0	15,15,17	0.59	0
2	NAG	k	1	2,1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	k	2	2	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
2	MAN	k	3	2	11,11,12	0.44	0	15,15,17	0.79	0
2	NAG	kA	1	2,1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	NAG	kA	2	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	MAN	kA	3	2	11,11,12	0.45	0	15,15,17	0.69	0
2	NAG	l	1	2,1	14,14,15	0.59	0	17,19,21	1.35	2 (11%)
2	NAG	l	2	2	14,14,15	0.27	0	17,19,21	1.33	2 (11%)
2	MAN	l	3	2	11,11,12	1.38	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	lA	1	2,1	14,14,15	0.71	0	17,19,21	1.45	3 (17%)
2	NAG	lA	2	2	14,14,15	0.60	0	17,19,21	1.36	1 (5%)
2	MAN	lA	3	2	11,11,12	0.79	0	15,15,17	1.09	1 (6%)
2	NAG	m	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.77	0
2	NAG	m	2	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
2	MAN	m	3	2	11,11,12	0.48	0	15,15,17	0.68	0
2	NAG	mA	1	2,1	14,14,15	0.53	0	17,19,21	0.64	0
2	NAG	mA	2	2	14,14,15	0.34	0	17,19,21	0.68	0
2	MAN	mA	3	2	11,11,12	0.45	0	15,15,17	0.59	0
2	NAG	n	1	2,1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	n	2	2	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
2	MAN	n	3	2	11,11,12	0.45	0	15,15,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	nA	1	2,1	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
2	NAG	nA	2	2	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
2	MAN	nA	3	2	11,11,12	0.46	0	15,15,17	0.68	0
2	NAG	o	1	2,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	o	2	2	14,14,15	0.28	0	17,19,21	1.33	2 (11%)
2	MAN	o	3	2	11,11,12	1.39	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	oA	1	2,1	14,14,15	0.71	0	17,19,21	1.44	3 (17%)
2	NAG	oA	2	2	14,14,15	0.61	0	17,19,21	1.37	1 (5%)
2	MAN	oA	3	2	11,11,12	0.81	0	15,15,17	1.10	1 (6%)
2	NAG	p	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.77	0
2	NAG	p	2	2	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
2	MAN	p	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	pA	1	2,1	14,14,15	0.52	0	17,19,21	0.63	0
2	NAG	pA	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	pA	3	2	11,11,12	0.45	0	15,15,17	0.60	0
2	NAG	q	1	2,1	14,14,15	0.36	0	17,19,21	1.01	1 (5%)
2	NAG	q	2	2	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
2	MAN	q	3	2	11,11,12	0.46	0	15,15,17	0.79	0
2	NAG	qA	1	2,1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	NAG	qA	2	2	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
2	MAN	qA	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	r	1	2,1	14,14,15	0.59	0	17,19,21	1.35	2 (11%)
2	NAG	r	2	2	14,14,15	0.28	0	17,19,21	1.33	2 (11%)
2	MAN	r	3	2	11,11,12	1.38	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	rA	1	2,1	14,14,15	0.72	0	17,19,21	1.44	3 (17%)
2	NAG	rA	2	2	14,14,15	0.61	0	17,19,21	1.36	1 (5%)
2	MAN	rA	3	2	11,11,12	0.80	0	15,15,17	1.10	1 (6%)
2	NAG	s	1	2,1	14,14,15	0.66	1 (7%)	17,19,21	0.77	0
2	NAG	s	2	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
2	MAN	s	3	2	11,11,12	0.48	0	15,15,17	0.68	0
2	NAG	sA	1	2,1	14,14,15	0.52	0	17,19,21	0.64	0
2	NAG	sA	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	sA	3	2	11,11,12	0.43	0	15,15,17	0.60	0
2	NAG	t	1	2,1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	t	2	2	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
2	MAN	t	3	2	11,11,12	0.44	0	15,15,17	0.79	0
2	NAG	tA	1	2,1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	tA	2	2	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
2	MAN	tA	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	u	1	2,1	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
2	NAG	u	2	2	14,14,15	0.29	0	17,19,21	1.33	2 (11%)
2	MAN	u	3	2	11,11,12	1.38	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	uA	1	2,1	14,14,15	0.71	0	17,19,21	1.44	3 (17%)
2	NAG	uA	2	2	14,14,15	0.59	0	17,19,21	1.37	1 (5%)
2	MAN	uA	3	2	11,11,12	0.80	0	15,15,17	1.09	1 (6%)
2	NAG	v	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.77	0
2	NAG	v	2	2	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
2	MAN	v	3	2	11,11,12	0.47	0	15,15,17	0.68	0
2	NAG	vA	1	2,1	14,14,15	0.50	0	17,19,21	0.64	0
2	NAG	vA	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	vA	3	2	11,11,12	0.45	0	15,15,17	0.59	0
2	NAG	w	1	2,1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	w	2	2	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
2	MAN	w	3	2	11,11,12	0.45	0	15,15,17	0.79	0
2	NAG	wA	1	2,1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	NAG	wA	2	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	MAN	wA	3	2	11,11,12	0.46	0	15,15,17	0.68	0
2	NAG	x	1	2,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	x	2	2	14,14,15	0.28	0	17,19,21	1.33	2 (11%)
2	MAN	x	3	2	11,11,12	1.37	2 (18%)	15,15,17	3.76	9 (60%)
2	NAG	xA	1	2,1	14,14,15	0.70	0	17,19,21	1.44	3 (17%)
2	NAG	xA	2	2	14,14,15	0.61	0	17,19,21	1.36	1 (5%)
2	MAN	xA	3	2	11,11,12	0.81	0	15,15,17	1.10	1 (6%)
2	NAG	y	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.77	0
2	NAG	y	2	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
2	MAN	y	3	2	11,11,12	0.47	0	15,15,17	0.69	0
2	NAG	yA	1	2,1	14,14,15	0.53	0	17,19,21	0.63	0
2	NAG	yA	2	2	14,14,15	0.35	0	17,19,21	0.68	0
2	MAN	yA	3	2	11,11,12	0.44	0	15,15,17	0.59	0
2	NAG	z	1	2,1	14,14,15	0.37	0	17,19,21	1.00	1 (5%)
2	NAG	z	2	2	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
2	MAN	z	3	2	11,11,12	0.45	0	15,15,17	0.79	0
2	NAG	zA	1	2,1	14,14,15	0.27	0	17,19,21	0.99	1 (5%)
2	NAG	zA	2	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	zA	3	2	11,11,12	0.46	0	15,15,17	0.69	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	5	3	2	-	0/2/19/22	0/1/1/1
2	NAG	5A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	5A	2	2	-	2/6/23/26	0/1/1/1
2	MAN	5A	3	2	-	0/2/19/22	0/1/1/1
2	NAG	6	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	6	2	2	-	3/6/23/26	0/1/1/1
2	MAN	6	3	2	-	0/2/19/22	0/1/1/1
2	NAG	7	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	7	2	2	-	2/6/23/26	0/1/1/1
2	MAN	7	3	2	-	0/2/19/22	0/1/1/1
2	NAG	8	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	8	2	2	-	2/6/23/26	0/1/1/1
2	MAN	8	3	2	-	0/2/19/22	0/1/1/1
2	NAG	9	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	9	2	2	-	3/6/23/26	0/1/1/1
2	MAN	9	3	2	-	2/2/19/22	0/1/1/1
2	NAG	AA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	AA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	BA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	BA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	CA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	CA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	DA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	DA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	EA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	EA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	EA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	FA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	FA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	FA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	GA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	GA	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	HA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	HA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	IA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	IA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	JA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	JA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	JA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	KA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	KA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	KA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	LA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	LA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	MA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	MA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	NA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	NA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	NA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	OA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	OA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	OA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	PA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	PA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	PA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	QA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	QA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	QA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	RA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	RA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	RA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	SA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	SA	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	TA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	TA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	TA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	UA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	UA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	UA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	VA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	VA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	VA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	WA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	WA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	WA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	XA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	XA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	XA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	YA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	YA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	YA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	ZA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	ZA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	ZA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	aA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	aA	2	2	-	3/6/23/26	0/1/1/1
2	MAN	aA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	bA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	bA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	bA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	cA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	cA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	cA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	dA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	dA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	dA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	e	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	e	2	2	-	3/6/23/26	0/1/1/1
2	MAN	e	3	2	-	0/2/19/22	0/1/1/1
2	NAG	eA	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	eA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	eA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	3/6/23/26	0/1/1/1
2	MAN	f	3	2	-	0/2/19/22	0/1/1/1
2	NAG	fA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	fA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	fA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	g	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	MAN	g	3	2	-	0/2/19/22	0/1/1/1
2	NAG	gA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	gA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	gA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	h	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	h	2	2	-	3/6/23/26	0/1/1/1
2	MAN	h	3	2	-	0/2/19/22	0/1/1/1
2	NAG	hA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	hA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	hA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	i	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	i	2	2	-	3/6/23/26	0/1/1/1
2	MAN	i	3	2	-	0/2/19/22	0/1/1/1
2	NAG	iA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	iA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	iA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	j	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	j	2	2	-	2/6/23/26	0/1/1/1
2	MAN	j	3	2	-	0/2/19/22	0/1/1/1
2	NAG	jA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	jA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	jA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	k	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	k	2	2	-	3/6/23/26	0/1/1/1
2	MAN	k	3	2	-	0/2/19/22	0/1/1/1
2	NAG	kA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	kA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	kA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	l	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	l	2	2	-	3/6/23/26	0/1/1/1
2	MAN	l	3	2	-	0/2/19/22	0/1/1/1
2	NAG	lA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	lA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	lA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	m	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	MAN	m	3	2	-	0/2/19/22	0/1/1/1
2	NAG	mA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	mA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	mA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	n	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	n	2	2	-	3/6/23/26	0/1/1/1
2	MAN	n	3	2	-	0/2/19/22	0/1/1/1
2	NAG	nA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	nA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	nA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	o	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	3/6/23/26	0/1/1/1
2	MAN	o	3	2	-	0/2/19/22	0/1/1/1
2	NAG	oA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	oA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	oA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	p	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	p	2	2	-	2/6/23/26	0/1/1/1
2	MAN	p	3	2	-	0/2/19/22	0/1/1/1
2	NAG	pA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	pA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	pA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	q	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	q	2	2	-	3/6/23/26	0/1/1/1
2	MAN	q	3	2	-	0/2/19/22	0/1/1/1
2	NAG	qA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	qA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	r	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	r	2	2	-	3/6/23/26	0/1/1/1
2	MAN	r	3	2	-	0/2/19/22	0/1/1/1
2	NAG	rA	1	2,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	rA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	rA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	s	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
2	MAN	s	3	2	-	0/2/19/22	0/1/1/1
2	NAG	sA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	sA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	sA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	t	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	t	2	2	-	3/6/23/26	0/1/1/1
2	MAN	t	3	2	-	0/2/19/22	0/1/1/1
2	NAG	tA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	tA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	tA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	u	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	u	2	2	-	3/6/23/26	0/1/1/1
2	MAN	u	3	2	-	0/2/19/22	0/1/1/1
2	NAG	uA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	uA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	uA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	v	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	v	2	2	-	2/6/23/26	0/1/1/1
2	MAN	v	3	2	-	0/2/19/22	0/1/1/1
2	NAG	vA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	vA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	vA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	w	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	w	2	2	-	3/6/23/26	0/1/1/1
2	MAN	w	3	2	-	0/2/19/22	0/1/1/1
2	NAG	wA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	wA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	x	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	x	2	2	-	3/6/23/26	0/1/1/1
2	MAN	x	3	2	-	0/2/19/22	0/1/1/1
2	NAG	xA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	xA	2	2	-	4/6/23/26	0/1/1/1
2	MAN	xA	3	2	-	2/2/19/22	0/1/1/1
2	NAG	y	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	y	2	2	-	2/6/23/26	0/1/1/1
2	MAN	y	3	2	-	0/2/19/22	0/1/1/1
2	NAG	yA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	yA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	z	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	z	2	2	-	3/6/23/26	0/1/1/1
2	MAN	z	3	2	-	0/2/19/22	0/1/1/1
2	NAG	zA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	zA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	zA	3	2	-	0/2/19/22	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	3	MAN	O2-C2	2.86	1.49	1.43
2	o	3	MAN	O2-C2	2.86	1.49	1.43
2	6	3	MAN	O2-C2	2.84	1.49	1.43
2	r	3	MAN	O2-C2	2.84	1.49	1.43
2	i	3	MAN	O2-C2	2.84	1.49	1.43
2	u	3	MAN	O2-C2	2.84	1.49	1.43
2	f	3	MAN	O2-C2	2.83	1.49	1.43
2	0	3	MAN	O2-C2	2.83	1.49	1.43
2	l	3	MAN	O2-C2	2.81	1.49	1.43
2	x	3	MAN	O2-C2	2.81	1.49	1.43
2	0	3	MAN	C2-C3	2.55	1.56	1.52
2	i	3	MAN	C2-C3	2.54	1.56	1.52
2	l	3	MAN	C2-C3	2.53	1.56	1.52
2	o	3	MAN	C2-C3	2.52	1.56	1.52
2	f	3	MAN	C2-C3	2.51	1.56	1.52
2	u	3	MAN	C2-C3	2.50	1.56	1.52
2	x	3	MAN	C2-C3	2.50	1.56	1.52
2	3	3	MAN	C2-C3	2.49	1.56	1.52
2	r	3	MAN	C2-C3	2.49	1.56	1.52
2	6	3	MAN	C2-C3	2.47	1.56	1.52
2	4	1	NAG	O5-C1	-2.17	1.40	1.43
2	y	1	NAG	O5-C1	-2.17	1.40	1.43
2	j	1	NAG	O5-C1	-2.15	1.40	1.43
2	g	1	NAG	O5-C1	-2.14	1.40	1.43
2	p	1	NAG	O5-C1	-2.14	1.40	1.43
2	m	1	NAG	O5-C1	-2.13	1.40	1.43
2	v	1	NAG	O5-C1	-2.12	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	1	NAG	O5-C1	-2.12	1.40	1.43
2	1	1	NAG	O5-C1	-2.11	1.40	1.43
2	s	1	NAG	O5-C1	-2.10	1.40	1.43

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	3	MAN	O2-C2-C3	8.27	126.70	110.14
2	r	3	MAN	O2-C2-C3	8.25	126.67	110.14
2	3	3	MAN	O2-C2-C3	8.25	126.67	110.14
2	l	3	MAN	O2-C2-C3	8.25	126.67	110.14
2	x	3	MAN	O2-C2-C3	8.25	126.67	110.14
2	f	3	MAN	O2-C2-C3	8.25	126.66	110.14
2	i	3	MAN	O2-C2-C3	8.24	126.65	110.14
2	0	3	MAN	O2-C2-C3	8.24	126.64	110.14
2	o	3	MAN	O2-C2-C3	8.24	126.64	110.14
2	u	3	MAN	O2-C2-C3	8.23	126.63	110.14
2	u	3	MAN	O5-C5-C6	-7.81	94.95	107.20
2	i	3	MAN	O5-C5-C6	-7.80	94.97	107.20
2	f	3	MAN	O5-C5-C6	-7.80	94.98	107.20
2	0	3	MAN	O5-C5-C6	-7.80	94.98	107.20
2	6	3	MAN	O5-C5-C6	-7.79	94.98	107.20
2	o	3	MAN	O5-C5-C6	-7.79	94.98	107.20
2	x	3	MAN	O5-C5-C6	-7.79	94.99	107.20
2	r	3	MAN	O5-C5-C6	-7.79	94.99	107.20
2	3	3	MAN	O5-C5-C6	-7.79	95.00	107.20
2	l	3	MAN	O5-C5-C6	-7.78	95.00	107.20
2	VA	1	NAG	C1-O5-C5	5.02	119.00	112.19
2	PA	1	NAG	C1-O5-C5	5.02	118.99	112.19
2	AA	1	NAG	C1-O5-C5	4.99	118.96	112.19
2	MA	1	NAG	C1-O5-C5	4.99	118.96	112.19
2	bA	1	NAG	C1-O5-C5	4.99	118.96	112.19
2	DA	1	NAG	C1-O5-C5	4.99	118.95	112.19
2	YA	1	NAG	C1-O5-C5	4.98	118.94	112.19
2	SA	1	NAG	C1-O5-C5	4.96	118.92	112.19
2	JA	1	NAG	C1-O5-C5	4.95	118.90	112.19
2	GA	1	NAG	C1-O5-C5	4.94	118.89	112.19
2	NA	1	NAG	C2-N2-C7	4.45	129.24	122.90
2	EA	1	NAG	C2-N2-C7	4.42	129.20	122.90
2	KA	1	NAG	C2-N2-C7	4.42	129.19	122.90
2	QA	1	NAG	C2-N2-C7	4.42	129.19	122.90
2	ZA	1	NAG	C2-N2-C7	4.42	129.19	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	HA	1	NAG	C2-N2-C7	4.41	129.19	122.90
2	8	1	NAG	C2-N2-C7	4.41	129.18	122.90
2	WA	1	NAG	C2-N2-C7	4.40	129.18	122.90
2	BA	1	NAG	C2-N2-C7	4.40	129.17	122.90
2	TA	1	NAG	C2-N2-C7	4.39	129.15	122.90
2	0A	2	NAG	C1-O5-C5	4.26	117.96	112.19
2	oA	2	NAG	C1-O5-C5	4.25	117.95	112.19
2	fA	2	NAG	C1-O5-C5	4.24	117.94	112.19
2	iA	2	NAG	C1-O5-C5	4.24	117.93	112.19
2	3A	2	NAG	C1-O5-C5	4.24	117.93	112.19
2	cA	2	NAG	C1-O5-C5	4.23	117.93	112.19
2	uA	2	NAG	C1-O5-C5	4.23	117.92	112.19
2	rA	2	NAG	C1-O5-C5	4.22	117.91	112.19
2	lA	2	NAG	C1-O5-C5	4.22	117.91	112.19
2	xA	2	NAG	C1-O5-C5	4.21	117.89	112.19
2	u	3	MAN	O3-C3-C2	4.01	117.67	109.99
2	l	3	MAN	O3-C3-C2	4.00	117.65	109.99
2	6	3	MAN	O3-C3-C2	3.99	117.64	109.99
2	o	3	MAN	O3-C3-C2	3.99	117.64	109.99
2	f	3	MAN	O3-C3-C2	3.99	117.64	109.99
2	3	3	MAN	O3-C3-C2	3.99	117.63	109.99
2	r	3	MAN	O3-C3-C2	3.99	117.63	109.99
2	x	3	MAN	O3-C3-C2	3.99	117.63	109.99
2	i	3	MAN	O3-C3-C2	3.98	117.62	109.99
2	0	3	MAN	O3-C3-C2	3.98	117.61	109.99
2	u	3	MAN	C1-C2-C3	3.97	114.55	109.67
2	r	3	MAN	C1-C2-C3	3.97	114.54	109.67
2	6	3	MAN	C1-C2-C3	3.96	114.53	109.67
2	f	3	MAN	C1-C2-C3	3.95	114.52	109.67
2	3	3	MAN	C1-C2-C3	3.94	114.51	109.67
2	o	3	MAN	C1-C2-C3	3.94	114.51	109.67
2	i	3	MAN	C1-C2-C3	3.94	114.51	109.67
2	l	3	MAN	C1-C2-C3	3.94	114.51	109.67
2	0	3	MAN	C1-C2-C3	3.94	114.51	109.67
2	x	3	MAN	C1-C2-C3	3.94	114.50	109.67
2	iA	1	NAG	C2-N2-C7	3.84	128.38	122.90
2	lA	1	NAG	C2-N2-C7	3.82	128.34	122.90
2	uA	1	NAG	C2-N2-C7	3.81	128.33	122.90
2	oA	1	NAG	C2-N2-C7	3.81	128.33	122.90
2	0A	1	NAG	C2-N2-C7	3.81	128.33	122.90
2	cA	1	NAG	C2-N2-C7	3.81	128.32	122.90
2	xA	1	NAG	C2-N2-C7	3.80	128.32	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	fA	1	NAG	C2-N2-C7	3.80	128.31	122.90
2	3	3	MAN	O4-C4-C5	-3.80	99.87	109.30
2	3A	1	NAG	C2-N2-C7	3.80	128.31	122.90
2	0	3	MAN	O4-C4-C5	-3.79	99.88	109.30
2	x	3	MAN	O4-C4-C5	-3.79	99.89	109.30
2	u	3	MAN	O4-C4-C5	-3.78	99.90	109.30
2	rA	1	NAG	C2-N2-C7	3.78	128.29	122.90
2	o	3	MAN	O4-C4-C5	-3.78	99.91	109.30
2	6	3	MAN	O4-C4-C5	-3.78	99.91	109.30
2	f	3	MAN	O4-C4-C5	-3.78	99.91	109.30
2	r	3	MAN	O4-C4-C5	-3.78	99.92	109.30
2	i	3	MAN	O4-C4-C5	-3.77	99.93	109.30
2	l	3	MAN	O4-C4-C5	-3.77	99.93	109.30
2	i	3	MAN	O5-C1-C2	3.60	116.33	110.77
2	0	3	MAN	O5-C1-C2	3.60	116.32	110.77
2	6	3	MAN	O5-C1-C2	3.60	116.32	110.77
2	o	3	MAN	O5-C1-C2	3.59	116.31	110.77
2	l	3	MAN	O5-C1-C2	3.59	116.31	110.77
2	3	3	MAN	O5-C1-C2	3.59	116.31	110.77
2	f	3	MAN	O5-C1-C2	3.58	116.30	110.77
2	x	3	MAN	O5-C1-C2	3.57	116.29	110.77
2	r	3	MAN	O5-C1-C2	3.57	116.28	110.77
2	u	3	MAN	O5-C1-C2	3.57	116.28	110.77
2	kA	1	NAG	C1-O5-C5	3.48	116.91	112.19
2	2A	1	NAG	C1-O5-C5	3.48	116.90	112.19
2	tA	1	NAG	C1-O5-C5	3.47	116.90	112.19
2	hA	1	NAG	C1-O5-C5	3.47	116.90	112.19
2	eA	1	NAG	C1-O5-C5	3.47	116.89	112.19
2	nA	1	NAG	C1-O5-C5	3.46	116.89	112.19
2	wA	1	NAG	C1-O5-C5	3.46	116.88	112.19
2	qA	1	NAG	C1-O5-C5	3.45	116.87	112.19
2	5A	1	NAG	C1-O5-C5	3.45	116.86	112.19
2	zA	1	NAG	C1-O5-C5	3.42	116.83	112.19
2	l	1	NAG	O5-C1-C2	-3.38	105.94	111.29
2	r	1	NAG	O5-C1-C2	-3.36	105.98	111.29
2	3	1	NAG	O5-C1-C2	-3.35	105.99	111.29
2	0	1	NAG	O5-C1-C2	-3.35	106.00	111.29
2	x	1	NAG	O5-C1-C2	-3.35	106.00	111.29
2	f	1	NAG	O5-C1-C2	-3.35	106.00	111.29
2	u	1	NAG	O5-C1-C2	-3.35	106.00	111.29
2	i	1	NAG	O5-C1-C2	-3.34	106.01	111.29
2	6	1	NAG	O5-C1-C2	-3.34	106.01	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	o	1	NAG	O5-C1-C2	-3.33	106.02	111.29
2	x	2	NAG	C2-N2-C7	3.15	127.38	122.90
2	u	2	NAG	C2-N2-C7	3.13	127.36	122.90
2	r	2	NAG	C2-N2-C7	3.13	127.36	122.90
2	i	2	NAG	C2-N2-C7	3.12	127.35	122.90
2	f	2	NAG	C2-N2-C7	3.11	127.34	122.90
2	6	2	NAG	C2-N2-C7	3.11	127.33	122.90
2	3	2	NAG	C2-N2-C7	3.10	127.31	122.90
2	0	2	NAG	C2-N2-C7	3.09	127.31	122.90
2	o	2	NAG	C2-N2-C7	3.09	127.30	122.90
2	l	2	NAG	C2-N2-C7	3.09	127.30	122.90
2	oA	3	MAN	O2-C2-C1	-2.97	103.08	109.15
2	o	2	NAG	C1-O5-C5	-2.97	108.17	112.19
2	6	2	NAG	C1-O5-C5	-2.95	108.20	112.19
2	rA	3	MAN	O2-C2-C1	-2.95	103.12	109.15
2	r	1	NAG	C3-C4-C5	2.94	115.49	110.24
2	3	1	NAG	C3-C4-C5	2.94	115.49	110.24
2	cA	3	MAN	O2-C2-C1	-2.94	103.14	109.15
2	fA	3	MAN	O2-C2-C1	-2.94	103.14	109.15
2	uA	3	MAN	O2-C2-C1	-2.94	103.14	109.15
2	x	2	NAG	C1-O5-C5	-2.94	108.21	112.19
2	l	2	NAG	C1-O5-C5	-2.94	108.21	112.19
2	u	1	NAG	C3-C4-C5	2.93	115.47	110.24
2	f	2	NAG	C1-O5-C5	-2.93	108.22	112.19
2	0	2	NAG	C1-O5-C5	-2.93	108.22	112.19
2	xA	3	MAN	O2-C2-C1	-2.93	103.15	109.15
2	o	1	NAG	C3-C4-C5	2.93	115.46	110.24
2	i	1	NAG	C3-C4-C5	2.93	115.46	110.24
2	3A	3	MAN	O2-C2-C1	-2.93	103.16	109.15
2	x	3	MAN	O3-C3-C4	-2.93	103.58	110.35
2	iA	3	MAN	O2-C2-C1	-2.92	103.17	109.15
2	6	1	NAG	C3-C4-C5	2.92	115.45	110.24
2	0A	3	MAN	O2-C2-C1	-2.92	103.17	109.15
2	r	2	NAG	C1-O5-C5	-2.92	108.23	112.19
2	lA	3	MAN	O2-C2-C1	-2.92	103.18	109.15
2	f	1	NAG	C3-C4-C5	2.92	115.44	110.24
2	3	2	NAG	C1-O5-C5	-2.91	108.24	112.19
2	6	3	MAN	O3-C3-C4	-2.91	103.61	110.35
2	0	3	MAN	O3-C3-C4	-2.91	103.62	110.35
2	u	3	MAN	O3-C3-C4	-2.91	103.62	110.35
2	i	2	NAG	C1-O5-C5	-2.91	108.25	112.19
2	l	1	NAG	C3-C4-C5	2.91	115.43	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	r	3	MAN	O3-C3-C4	-2.91	103.62	110.35
2	f	3	MAN	O3-C3-C4	-2.91	103.63	110.35
2	x	1	NAG	C3-C4-C5	2.91	115.42	110.24
2	3	3	MAN	O3-C3-C4	-2.90	103.64	110.35
2	i	3	MAN	O3-C3-C4	-2.90	103.65	110.35
2	l	3	MAN	O3-C3-C4	-2.90	103.65	110.35
2	u	2	NAG	C1-O5-C5	-2.90	108.27	112.19
2	0	1	NAG	C3-C4-C5	2.90	115.40	110.24
2	o	3	MAN	O3-C3-C4	-2.89	103.66	110.35
2	k	1	NAG	C1-O5-C5	2.89	116.10	112.19
2	t	1	NAG	C1-O5-C5	2.86	116.07	112.19
2	e	1	NAG	C1-O5-C5	2.85	116.05	112.19
2	n	1	NAG	C1-O5-C5	2.85	116.05	112.19
2	q	1	NAG	C1-O5-C5	2.85	116.05	112.19
2	5	1	NAG	C1-O5-C5	2.85	116.05	112.19
2	2	1	NAG	C1-O5-C5	2.84	116.04	112.19
2	w	1	NAG	C1-O5-C5	2.84	116.03	112.19
2	h	1	NAG	C1-O5-C5	2.83	116.03	112.19
2	z	1	NAG	C1-O5-C5	2.82	116.02	112.19
2	fA	1	NAG	C1-O5-C5	2.82	116.02	112.19
2	lA	1	NAG	C1-O5-C5	2.82	116.01	112.19
2	xA	1	NAG	C1-O5-C5	2.80	115.99	112.19
2	rA	1	NAG	C1-O5-C5	2.80	115.98	112.19
2	3A	1	NAG	C1-O5-C5	2.80	115.98	112.19
2	cA	1	NAG	C1-O5-C5	2.79	115.98	112.19
2	0A	1	NAG	C1-O5-C5	2.79	115.97	112.19
2	iA	1	NAG	C1-O5-C5	2.79	115.97	112.19
2	uA	1	NAG	C1-O5-C5	2.79	115.97	112.19
2	oA	1	NAG	C1-O5-C5	2.78	115.95	112.19
2	TA	2	NAG	O7-C7-C8	-2.67	117.09	122.06
2	WA	2	NAG	O7-C7-C8	-2.67	117.10	122.06
2	BA	2	NAG	O7-C7-C8	-2.66	117.11	122.06
2	QA	2	NAG	O7-C7-C8	-2.66	117.11	122.06
2	ZA	2	NAG	O7-C7-C8	-2.66	117.11	122.06
2	EA	2	NAG	O7-C7-C8	-2.66	117.11	122.06
2	8	2	NAG	O7-C7-C8	-2.66	117.12	122.06
2	KA	2	NAG	O7-C7-C8	-2.65	117.13	122.06
2	NA	2	NAG	O7-C7-C8	-2.65	117.14	122.06
2	HA	2	NAG	O7-C7-C8	-2.65	117.14	122.06
2	i	3	MAN	C3-C4-C5	2.57	114.83	110.24
2	0	3	MAN	C3-C4-C5	2.57	114.82	110.24
2	l	3	MAN	C3-C4-C5	2.57	114.81	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	x	3	MAN	C3-C4-C5	2.56	114.81	110.24
2	3	3	MAN	C3-C4-C5	2.56	114.81	110.24
2	f	3	MAN	C3-C4-C5	2.56	114.80	110.24
2	o	3	MAN	C3-C4-C5	2.56	114.80	110.24
2	6	3	MAN	C3-C4-C5	2.55	114.79	110.24
2	u	3	MAN	C3-C4-C5	2.55	114.78	110.24
2	r	3	MAN	C3-C4-C5	2.54	114.78	110.24
2	k	2	NAG	O7-C7-C8	-2.45	117.52	122.06
2	w	2	NAG	O7-C7-C8	-2.45	117.52	122.06
2	h	2	NAG	O7-C7-C8	-2.43	117.54	122.06
2	2	2	NAG	O7-C7-C8	-2.43	117.54	122.06
2	e	2	NAG	O7-C7-C8	-2.43	117.54	122.06
2	q	2	NAG	O7-C7-C8	-2.43	117.55	122.06
2	t	2	NAG	O7-C7-C8	-2.43	117.55	122.06
2	n	2	NAG	O7-C7-C8	-2.43	117.55	122.06
2	z	2	NAG	O7-C7-C8	-2.43	117.55	122.06
2	5	2	NAG	O7-C7-C8	-2.43	117.55	122.06
2	x	3	MAN	C2-C3-C4	2.33	114.93	110.89
2	r	3	MAN	C2-C3-C4	2.33	114.93	110.89
2	u	3	MAN	C2-C3-C4	2.33	114.92	110.89
2	6	3	MAN	C2-C3-C4	2.33	114.92	110.89
2	i	3	MAN	C2-C3-C4	2.32	114.92	110.89
2	3	3	MAN	C2-C3-C4	2.32	114.92	110.89
2	f	3	MAN	C2-C3-C4	2.32	114.91	110.89
2	l	3	MAN	C2-C3-C4	2.32	114.91	110.89
2	o	3	MAN	C2-C3-C4	2.32	114.91	110.89
2	0	3	MAN	C2-C3-C4	2.32	114.91	110.89
2	zA	2	NAG	C1-O5-C5	2.30	115.31	112.19
2	kA	2	NAG	C1-O5-C5	2.30	115.31	112.19
2	2A	2	NAG	C1-O5-C5	2.29	115.29	112.19
2	wA	2	NAG	C1-O5-C5	2.28	115.28	112.19
2	qA	2	NAG	C1-O5-C5	2.28	115.28	112.19
2	eA	2	NAG	C1-O5-C5	2.28	115.28	112.19
2	nA	2	NAG	C1-O5-C5	2.27	115.27	112.19
2	tA	2	NAG	C1-O5-C5	2.27	115.27	112.19
2	GA	2	NAG	C1-O5-C5	2.26	115.26	112.19
2	5A	2	NAG	C1-O5-C5	2.26	115.25	112.19
2	hA	2	NAG	C1-O5-C5	2.25	115.24	112.19
2	bA	2	NAG	C1-O5-C5	2.24	115.23	112.19
2	MA	2	NAG	C1-O5-C5	2.23	115.21	112.19
2	HA	2	NAG	C2-N2-C7	-2.22	119.74	122.90
2	AA	2	NAG	C1-O5-C5	2.21	115.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	KA	2	NAG	C2-N2-C7	-2.21	119.75	122.90
2	QA	2	NAG	C2-N2-C7	-2.21	119.75	122.90
2	JA	2	NAG	C1-O5-C5	2.21	115.19	112.19
2	SA	2	NAG	C1-O5-C5	2.21	115.18	112.19
2	BA	2	NAG	C2-N2-C7	-2.21	119.76	122.90
2	YA	2	NAG	C1-O5-C5	2.21	115.18	112.19
2	8	2	NAG	C2-N2-C7	-2.20	119.77	122.90
2	EA	2	NAG	C2-N2-C7	-2.20	119.77	122.90
2	VA	2	NAG	C1-O5-C5	2.20	115.17	112.19
2	PA	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	DA	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	TA	2	NAG	C2-N2-C7	-2.19	119.79	122.90
2	ZA	2	NAG	C2-N2-C7	-2.18	119.79	122.90
2	1	2	NAG	C1-O5-C5	2.18	115.14	112.19
2	aA	3	MAN	O5-C5-C6	2.18	110.62	107.20
2	NA	2	NAG	C2-N2-C7	-2.18	119.81	122.90
2	WA	2	NAG	C2-N2-C7	-2.17	119.81	122.90
2	p	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	RA	2	NAG	C1-O5-C5	2.16	115.12	112.19
2	IA	3	MAN	O5-C5-C6	2.16	110.58	107.20
2	OA	3	MAN	O5-C5-C6	2.16	110.58	107.20
2	IA	2	NAG	C1-O5-C5	2.16	115.11	112.19
2	LA	3	MAN	O5-C5-C6	2.15	110.58	107.20
2	CA	2	NAG	C1-O5-C5	2.15	115.10	112.19
2	UA	3	MAN	O5-C5-C6	2.14	110.56	107.20
2	v	2	NAG	C1-O5-C5	2.14	115.09	112.19
2	9	3	MAN	O5-C5-C6	2.14	110.56	107.20
2	FA	3	MAN	O5-C5-C6	2.13	110.55	107.20
2	m	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	OA	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	XA	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	s	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	LA	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	g	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	j	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	CA	3	MAN	O5-C5-C6	2.13	110.54	107.20
2	4	2	NAG	C1-O5-C5	2.12	115.07	112.19
2	9	2	NAG	C1-O5-C5	2.12	115.07	112.19
2	RA	3	MAN	O5-C5-C6	2.12	110.53	107.20
2	XA	3	MAN	O5-C5-C6	2.12	110.53	107.20
2	7	2	NAG	C1-O5-C5	2.12	115.06	112.19
2	aA	2	NAG	C1-O5-C5	2.11	115.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	y	2	NAG	C1-O5-C5	2.10	115.04	112.19
2	UA	2	NAG	C1-O5-C5	2.10	115.04	112.19
2	FA	2	NAG	C1-O5-C5	2.09	115.02	112.19
2	3A	1	NAG	O7-C7-N2	2.06	125.74	121.95
2	fA	1	NAG	O7-C7-N2	2.05	125.72	121.95
2	rA	1	NAG	O7-C7-N2	2.04	125.71	121.95
2	cA	1	NAG	O7-C7-N2	2.04	125.69	121.95
2	oA	1	NAG	O7-C7-N2	2.03	125.69	121.95
2	iA	1	NAG	O7-C7-N2	2.03	125.68	121.95
2	xA	1	NAG	O7-C7-N2	2.03	125.68	121.95
2	0A	1	NAG	O7-C7-N2	2.03	125.68	121.95
2	lA	1	NAG	O7-C7-N2	2.03	125.68	121.95
2	uA	1	NAG	O7-C7-N2	2.02	125.67	121.95
2	WA	3	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (350) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	f	2	NAG	C3-C2-N2-C7
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
2	i	2	NAG	C3-C2-N2-C7
2	i	2	NAG	C8-C7-N2-C2
2	i	2	NAG	O7-C7-N2-C2
2	l	2	NAG	C3-C2-N2-C7
2	l	2	NAG	C8-C7-N2-C2
2	l	2	NAG	O7-C7-N2-C2
2	o	2	NAG	C3-C2-N2-C7
2	o	2	NAG	C8-C7-N2-C2
2	o	2	NAG	O7-C7-N2-C2
2	r	2	NAG	C3-C2-N2-C7
2	r	2	NAG	C8-C7-N2-C2
2	r	2	NAG	O7-C7-N2-C2
2	u	2	NAG	C3-C2-N2-C7
2	u	2	NAG	C8-C7-N2-C2
2	u	2	NAG	O7-C7-N2-C2
2	x	2	NAG	C3-C2-N2-C7
2	x	2	NAG	C8-C7-N2-C2
2	x	2	NAG	O7-C7-N2-C2
2	0	2	NAG	C3-C2-N2-C7
2	0	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	0	2	NAG	O7-C7-N2-C2
2	3	2	NAG	C3-C2-N2-C7
2	3	2	NAG	C8-C7-N2-C2
2	3	2	NAG	O7-C7-N2-C2
2	6	2	NAG	C3-C2-N2-C7
2	6	2	NAG	C8-C7-N2-C2
2	6	2	NAG	O7-C7-N2-C2
2	9	2	NAG	C3-C2-N2-C7
2	CA	2	NAG	C3-C2-N2-C7
2	FA	2	NAG	C3-C2-N2-C7
2	IA	2	NAG	C3-C2-N2-C7
2	LA	2	NAG	C3-C2-N2-C7
2	OA	2	NAG	C3-C2-N2-C7
2	RA	2	NAG	C3-C2-N2-C7
2	UA	2	NAG	C3-C2-N2-C7
2	XA	2	NAG	C3-C2-N2-C7
2	aA	2	NAG	C3-C2-N2-C7
2	cA	2	NAG	O5-C5-C6-O6
2	fA	2	NAG	O5-C5-C6-O6
2	iA	2	NAG	O5-C5-C6-O6
2	lA	2	NAG	O5-C5-C6-O6
2	oA	2	NAG	O5-C5-C6-O6
2	rA	2	NAG	O5-C5-C6-O6
2	uA	2	NAG	O5-C5-C6-O6
2	xA	2	NAG	O5-C5-C6-O6
2	0A	2	NAG	O5-C5-C6-O6
2	3A	2	NAG	O5-C5-C6-O6
2	9	2	NAG	O5-C5-C6-O6
2	CA	2	NAG	O5-C5-C6-O6
2	FA	2	NAG	O5-C5-C6-O6
2	IA	2	NAG	O5-C5-C6-O6
2	LA	2	NAG	O5-C5-C6-O6
2	OA	2	NAG	O5-C5-C6-O6
2	RA	2	NAG	O5-C5-C6-O6
2	UA	2	NAG	O5-C5-C6-O6
2	XA	2	NAG	O5-C5-C6-O6
2	aA	2	NAG	O5-C5-C6-O6
2	AA	1	NAG	O5-C5-C6-O6
2	DA	1	NAG	O5-C5-C6-O6
2	GA	1	NAG	O5-C5-C6-O6
2	JA	1	NAG	O5-C5-C6-O6
2	MA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	PA	1	NAG	O5-C5-C6-O6
2	SA	1	NAG	O5-C5-C6-O6
2	VA	1	NAG	O5-C5-C6-O6
2	YA	1	NAG	O5-C5-C6-O6
2	bA	1	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
2	p	2	NAG	O5-C5-C6-O6
2	s	2	NAG	O5-C5-C6-O6
2	v	2	NAG	O5-C5-C6-O6
2	y	2	NAG	O5-C5-C6-O6
2	1	2	NAG	O5-C5-C6-O6
2	4	2	NAG	O5-C5-C6-O6
2	7	2	NAG	O5-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	p	2	NAG	C4-C5-C6-O6
2	s	2	NAG	C4-C5-C6-O6
2	v	2	NAG	C4-C5-C6-O6
2	y	2	NAG	C4-C5-C6-O6
2	1	2	NAG	C4-C5-C6-O6
2	4	2	NAG	C4-C5-C6-O6
2	7	2	NAG	C4-C5-C6-O6
2	9	2	NAG	C4-C5-C6-O6
2	CA	2	NAG	C4-C5-C6-O6
2	FA	2	NAG	C4-C5-C6-O6
2	IA	2	NAG	C4-C5-C6-O6
2	LA	2	NAG	C4-C5-C6-O6
2	OA	2	NAG	C4-C5-C6-O6
2	RA	2	NAG	C4-C5-C6-O6
2	UA	2	NAG	C4-C5-C6-O6
2	XA	2	NAG	C4-C5-C6-O6
2	aA	2	NAG	C4-C5-C6-O6
2	eA	2	NAG	O5-C5-C6-O6
2	hA	2	NAG	O5-C5-C6-O6
2	kA	2	NAG	O5-C5-C6-O6
2	nA	2	NAG	O5-C5-C6-O6
2	qA	2	NAG	O5-C5-C6-O6
2	tA	2	NAG	O5-C5-C6-O6
2	wA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	zA	2	NAG	O5-C5-C6-O6
2	2A	2	NAG	O5-C5-C6-O6
2	5A	2	NAG	O5-C5-C6-O6
2	AA	2	NAG	O5-C5-C6-O6
2	DA	2	NAG	O5-C5-C6-O6
2	GA	2	NAG	O5-C5-C6-O6
2	JA	2	NAG	O5-C5-C6-O6
2	MA	2	NAG	O5-C5-C6-O6
2	PA	2	NAG	O5-C5-C6-O6
2	SA	2	NAG	O5-C5-C6-O6
2	VA	2	NAG	O5-C5-C6-O6
2	YA	2	NAG	O5-C5-C6-O6
2	bA	2	NAG	O5-C5-C6-O6
2	cA	3	MAN	O5-C5-C6-O6
2	fA	3	MAN	O5-C5-C6-O6
2	iA	3	MAN	O5-C5-C6-O6
2	lA	3	MAN	O5-C5-C6-O6
2	oA	3	MAN	O5-C5-C6-O6
2	rA	3	MAN	O5-C5-C6-O6
2	uA	3	MAN	O5-C5-C6-O6
2	xA	3	MAN	O5-C5-C6-O6
2	0A	3	MAN	O5-C5-C6-O6
2	3A	3	MAN	O5-C5-C6-O6
2	cA	2	NAG	C4-C5-C6-O6
2	fA	2	NAG	C4-C5-C6-O6
2	iA	2	NAG	C4-C5-C6-O6
2	lA	2	NAG	C4-C5-C6-O6
2	oA	2	NAG	C4-C5-C6-O6
2	rA	2	NAG	C4-C5-C6-O6
2	uA	2	NAG	C4-C5-C6-O6
2	xA	2	NAG	C4-C5-C6-O6
2	0A	2	NAG	C4-C5-C6-O6
2	3A	2	NAG	C4-C5-C6-O6
2	aA	1	NAG	O5-C5-C6-O6
2	AA	1	NAG	C4-C5-C6-O6
2	DA	1	NAG	C4-C5-C6-O6
2	GA	1	NAG	C4-C5-C6-O6
2	JA	1	NAG	C4-C5-C6-O6
2	MA	1	NAG	C4-C5-C6-O6
2	PA	1	NAG	C4-C5-C6-O6
2	SA	1	NAG	C4-C5-C6-O6
2	VA	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	YA	1	NAG	C4-C5-C6-O6
2	bA	1	NAG	C4-C5-C6-O6
2	9	1	NAG	O5-C5-C6-O6
2	BA	2	NAG	O5-C5-C6-O6
2	CA	1	NAG	O5-C5-C6-O6
2	FA	1	NAG	O5-C5-C6-O6
2	IA	1	NAG	O5-C5-C6-O6
2	LA	1	NAG	O5-C5-C6-O6
2	OA	1	NAG	O5-C5-C6-O6
2	RA	1	NAG	O5-C5-C6-O6
2	UA	1	NAG	O5-C5-C6-O6
2	WA	2	NAG	O5-C5-C6-O6
2	XA	1	NAG	O5-C5-C6-O6
2	8	2	NAG	O5-C5-C6-O6
2	EA	2	NAG	O5-C5-C6-O6
2	HA	2	NAG	O5-C5-C6-O6
2	KA	2	NAG	O5-C5-C6-O6
2	NA	2	NAG	O5-C5-C6-O6
2	QA	2	NAG	O5-C5-C6-O6
2	TA	2	NAG	O5-C5-C6-O6
2	ZA	2	NAG	O5-C5-C6-O6
2	IA	3	MAN	O5-C5-C6-O6
2	RA	3	MAN	O5-C5-C6-O6
2	9	3	MAN	O5-C5-C6-O6
2	CA	3	MAN	O5-C5-C6-O6
2	FA	3	MAN	O5-C5-C6-O6
2	LA	3	MAN	O5-C5-C6-O6
2	OA	3	MAN	O5-C5-C6-O6
2	UA	3	MAN	O5-C5-C6-O6
2	XA	3	MAN	O5-C5-C6-O6
2	aA	3	MAN	O5-C5-C6-O6
2	AA	2	NAG	C4-C5-C6-O6
2	DA	2	NAG	C4-C5-C6-O6
2	GA	2	NAG	C4-C5-C6-O6
2	JA	2	NAG	C4-C5-C6-O6
2	MA	2	NAG	C4-C5-C6-O6
2	PA	2	NAG	C4-C5-C6-O6
2	SA	2	NAG	C4-C5-C6-O6
2	VA	2	NAG	C4-C5-C6-O6
2	YA	2	NAG	C4-C5-C6-O6
2	bA	2	NAG	C4-C5-C6-O6
2	eA	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	hA	2	NAG	C4-C5-C6-O6
2	kA	2	NAG	C4-C5-C6-O6
2	nA	2	NAG	C4-C5-C6-O6
2	qA	2	NAG	C4-C5-C6-O6
2	tA	2	NAG	C4-C5-C6-O6
2	wA	2	NAG	C4-C5-C6-O6
2	zA	2	NAG	C4-C5-C6-O6
2	2A	2	NAG	C4-C5-C6-O6
2	5A	2	NAG	C4-C5-C6-O6
2	9	1	NAG	C4-C5-C6-O6
2	CA	1	NAG	C4-C5-C6-O6
2	FA	1	NAG	C4-C5-C6-O6
2	IA	1	NAG	C4-C5-C6-O6
2	LA	1	NAG	C4-C5-C6-O6
2	OA	1	NAG	C4-C5-C6-O6
2	RA	1	NAG	C4-C5-C6-O6
2	UA	1	NAG	C4-C5-C6-O6
2	XA	1	NAG	C4-C5-C6-O6
2	aA	1	NAG	C4-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
2	n	2	NAG	O5-C5-C6-O6
2	q	2	NAG	O5-C5-C6-O6
2	t	2	NAG	O5-C5-C6-O6
2	w	2	NAG	O5-C5-C6-O6
2	z	2	NAG	O5-C5-C6-O6
2	2	2	NAG	O5-C5-C6-O6
2	5	2	NAG	O5-C5-C6-O6
2	cA	2	NAG	C8-C7-N2-C2
2	fA	2	NAG	C8-C7-N2-C2
2	iA	2	NAG	C8-C7-N2-C2
2	iA	2	NAG	O7-C7-N2-C2
2	lA	2	NAG	C8-C7-N2-C2
2	lA	2	NAG	O7-C7-N2-C2
2	oA	2	NAG	C8-C7-N2-C2
2	rA	2	NAG	C8-C7-N2-C2
2	uA	2	NAG	C8-C7-N2-C2
2	uA	2	NAG	O7-C7-N2-C2
2	xA	2	NAG	C8-C7-N2-C2
2	xA	2	NAG	O7-C7-N2-C2
2	0A	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	3A	2	NAG	C8-C7-N2-C2
2	cA	2	NAG	O7-C7-N2-C2
2	fA	2	NAG	O7-C7-N2-C2
2	oA	2	NAG	O7-C7-N2-C2
2	rA	2	NAG	O7-C7-N2-C2
2	0A	2	NAG	O7-C7-N2-C2
2	3A	2	NAG	O7-C7-N2-C2
2	CA	3	MAN	C4-C5-C6-O6
2	XA	3	MAN	C4-C5-C6-O6
2	9	3	MAN	C4-C5-C6-O6
2	LA	3	MAN	C4-C5-C6-O6
2	OA	3	MAN	C4-C5-C6-O6
2	RA	3	MAN	C4-C5-C6-O6
2	aA	3	MAN	C4-C5-C6-O6
2	FA	3	MAN	C4-C5-C6-O6
2	IA	3	MAN	C4-C5-C6-O6
2	UA	3	MAN	C4-C5-C6-O6
2	EA	1	NAG	C4-C5-C6-O6
2	NA	1	NAG	C4-C5-C6-O6
2	QA	1	NAG	C4-C5-C6-O6
2	ZA	1	NAG	C4-C5-C6-O6
2	8	1	NAG	C4-C5-C6-O6
2	HA	1	NAG	C4-C5-C6-O6
2	KA	1	NAG	C4-C5-C6-O6
2	TA	1	NAG	C4-C5-C6-O6
2	BA	1	NAG	C4-C5-C6-O6
2	WA	1	NAG	C4-C5-C6-O6
2	BA	2	NAG	C4-C5-C6-O6
2	NA	2	NAG	C4-C5-C6-O6
2	ZA	2	NAG	C4-C5-C6-O6
2	8	2	NAG	C4-C5-C6-O6
2	EA	2	NAG	C4-C5-C6-O6
2	HA	2	NAG	C4-C5-C6-O6
2	KA	2	NAG	C4-C5-C6-O6
2	QA	2	NAG	C4-C5-C6-O6
2	TA	2	NAG	C4-C5-C6-O6
2	WA	2	NAG	C4-C5-C6-O6
2	8	1	NAG	O5-C5-C6-O6
2	BA	1	NAG	O5-C5-C6-O6
2	EA	1	NAG	O5-C5-C6-O6
2	HA	1	NAG	O5-C5-C6-O6
2	KA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	NA	1	NAG	O5-C5-C6-O6
2	QA	1	NAG	O5-C5-C6-O6
2	TA	1	NAG	O5-C5-C6-O6
2	WA	1	NAG	O5-C5-C6-O6
2	ZA	1	NAG	O5-C5-C6-O6
2	iA	3	MAN	C4-C5-C6-O6
2	oA	3	MAN	C4-C5-C6-O6
2	rA	3	MAN	C4-C5-C6-O6
2	xA	3	MAN	C4-C5-C6-O6
2	cA	3	MAN	C4-C5-C6-O6
2	fA	3	MAN	C4-C5-C6-O6
2	uA	3	MAN	C4-C5-C6-O6
2	3A	3	MAN	C4-C5-C6-O6
2	lA	3	MAN	C4-C5-C6-O6
2	0A	3	MAN	C4-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	w	2	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
2	q	2	NAG	C4-C5-C6-O6
2	t	2	NAG	C4-C5-C6-O6
2	5	2	NAG	C4-C5-C6-O6
2	2	2	NAG	C4-C5-C6-O6
2	z	2	NAG	C4-C5-C6-O6
2	e	2	NAG	C3-C2-N2-C7
2	h	2	NAG	C3-C2-N2-C7
2	k	2	NAG	C3-C2-N2-C7
2	n	2	NAG	C3-C2-N2-C7
2	q	2	NAG	C3-C2-N2-C7
2	t	2	NAG	C3-C2-N2-C7
2	w	2	NAG	C3-C2-N2-C7
2	z	2	NAG	C3-C2-N2-C7
2	2	2	NAG	C3-C2-N2-C7
2	5	2	NAG	C3-C2-N2-C7
2	8	1	NAG	C3-C2-N2-C7
2	BA	1	NAG	C3-C2-N2-C7
2	EA	1	NAG	C3-C2-N2-C7
2	HA	1	NAG	C3-C2-N2-C7
2	KA	1	NAG	C3-C2-N2-C7
2	NA	1	NAG	C3-C2-N2-C7
2	QA	1	NAG	C3-C2-N2-C7

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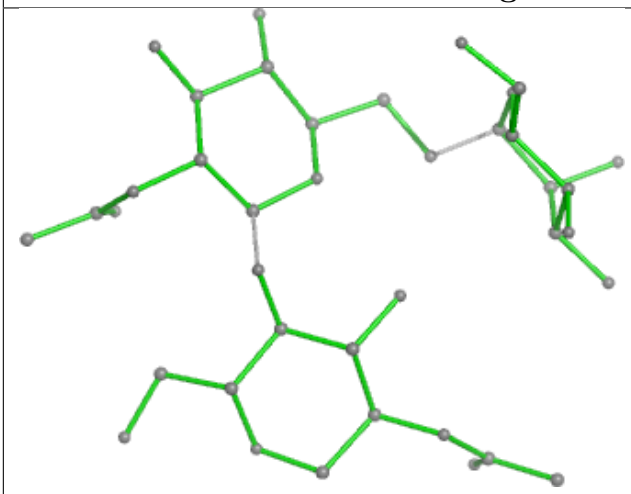
Mol	Chain	Res	Type	Atoms
2	TA	1	NAG	C3-C2-N2-C7
2	WA	1	NAG	C3-C2-N2-C7
2	ZA	1	NAG	C3-C2-N2-C7
2	cA	1	NAG	C3-C2-N2-C7
2	fA	1	NAG	C3-C2-N2-C7
2	iA	1	NAG	C3-C2-N2-C7
2	lA	1	NAG	C3-C2-N2-C7
2	oA	1	NAG	C3-C2-N2-C7
2	rA	1	NAG	C3-C2-N2-C7
2	uA	1	NAG	C3-C2-N2-C7
2	xA	1	NAG	C3-C2-N2-C7
2	0A	1	NAG	C3-C2-N2-C7
2	3A	1	NAG	C3-C2-N2-C7
2	4A	2	NAG	O5-C5-C6-O6
2	gA	2	NAG	O5-C5-C6-O6
2	vA	2	NAG	O5-C5-C6-O6
2	yA	2	NAG	O5-C5-C6-O6
2	1A	2	NAG	O5-C5-C6-O6
2	dA	2	NAG	O5-C5-C6-O6
2	mA	2	NAG	O5-C5-C6-O6
2	sA	2	NAG	O5-C5-C6-O6
2	pA	2	NAG	O5-C5-C6-O6
2	jA	2	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
2	q	1	NAG	O5-C5-C6-O6
2	5	1	NAG	O5-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
2	w	1	NAG	O5-C5-C6-O6
2	t	1	NAG	O5-C5-C6-O6
2	z	1	NAG	O5-C5-C6-O6
2	2	1	NAG	O5-C5-C6-O6

There are no ring outliers.

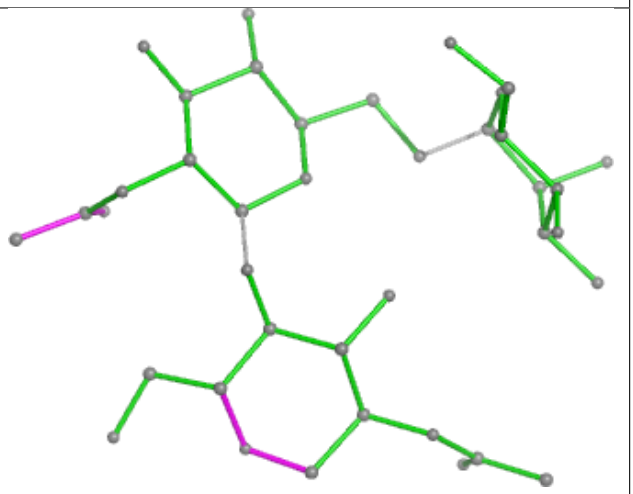
No monomer is involved in short contacts.

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

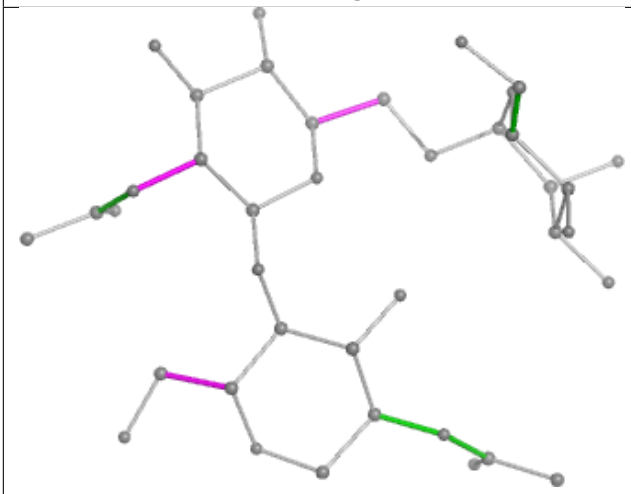
Oligosaccharide Chain e



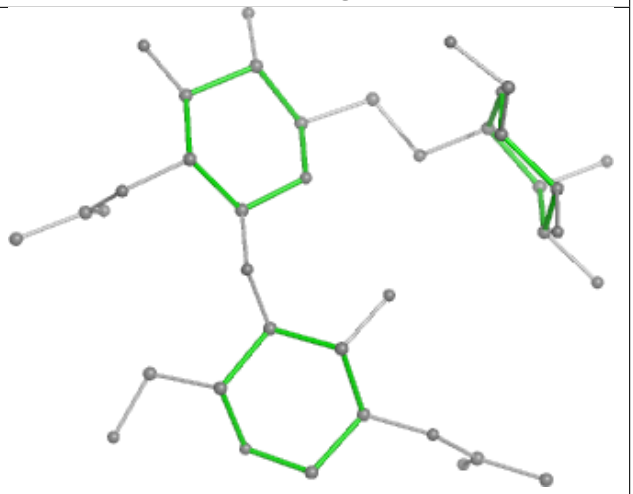
Bond lengths



Bond angles

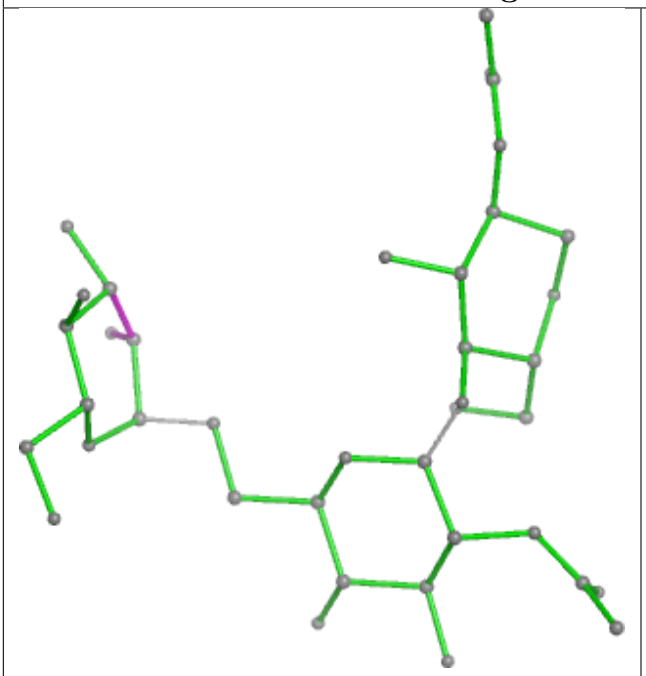


Torsions

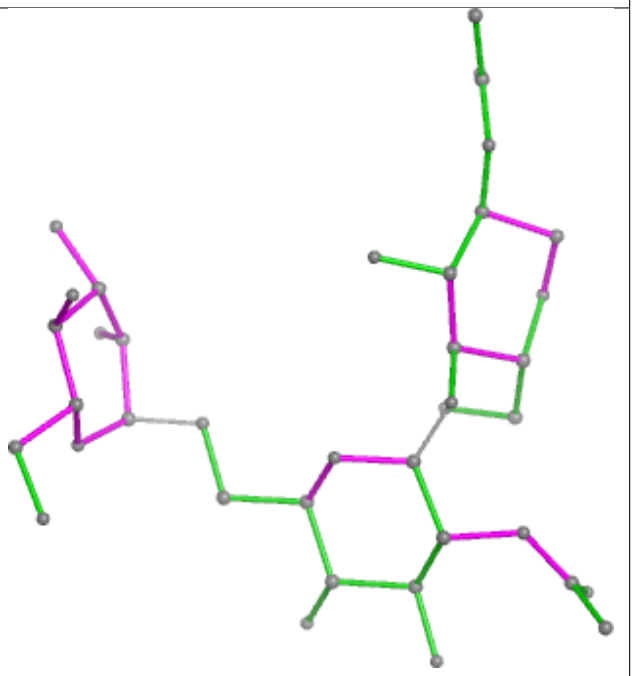


Rings

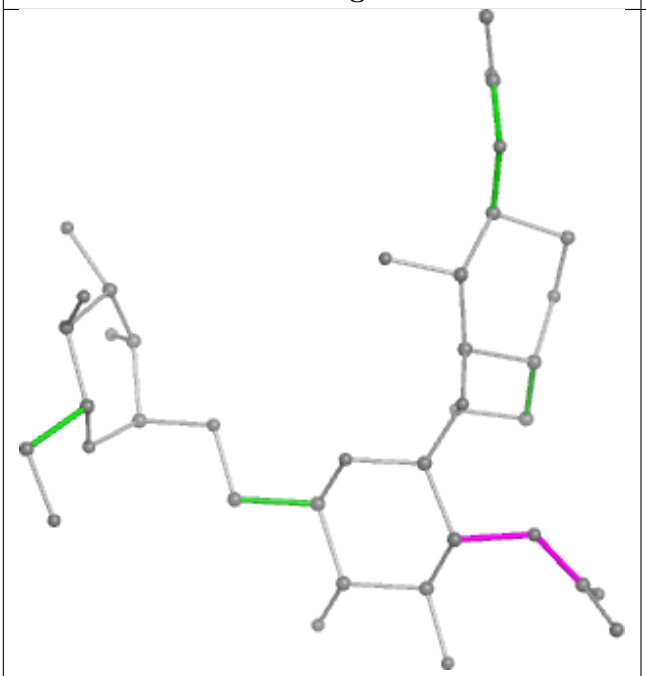
Oligosaccharide Chain f



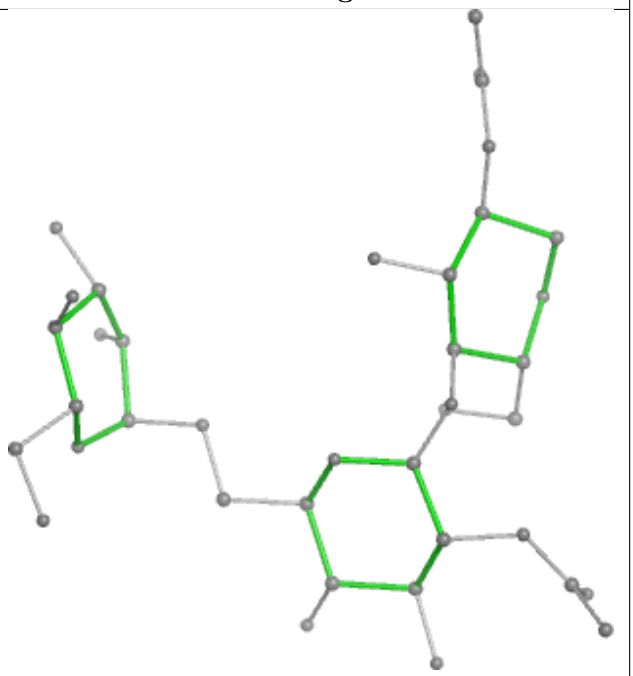
Bond lengths



Bond angles

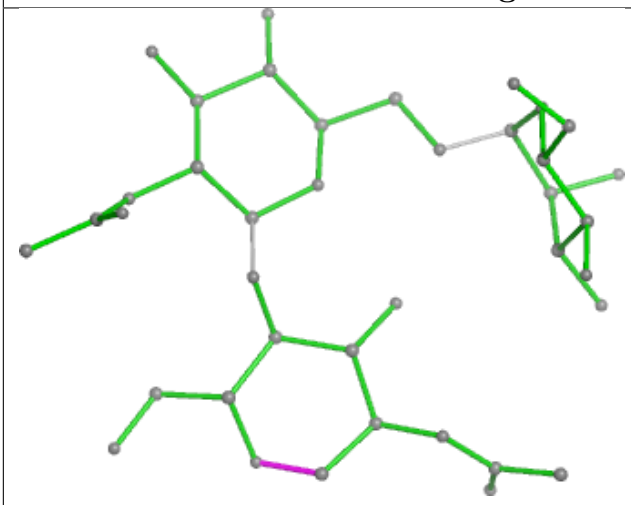


Torsions

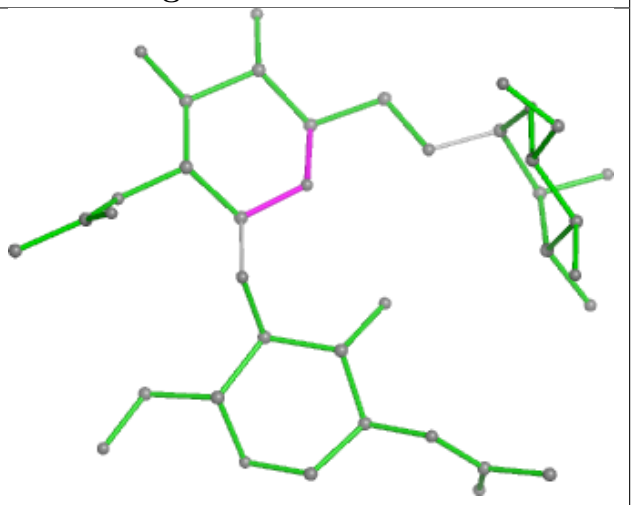


Rings

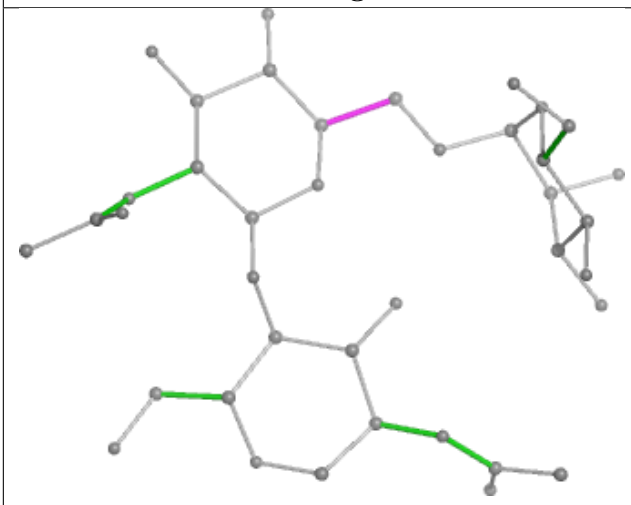
Oligosaccharide Chain g



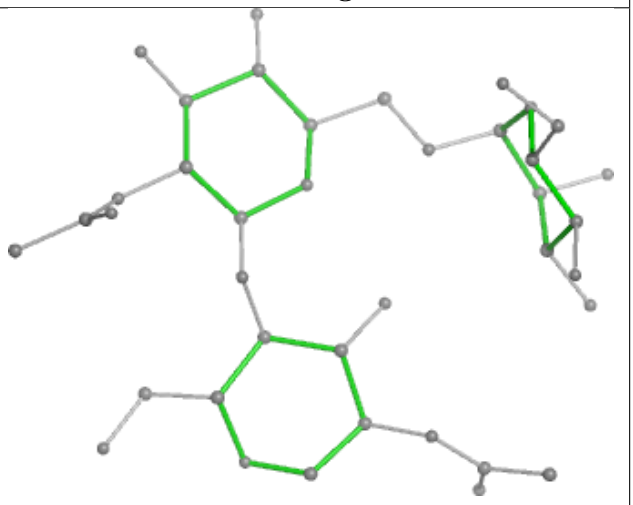
Bond lengths



Bond angles

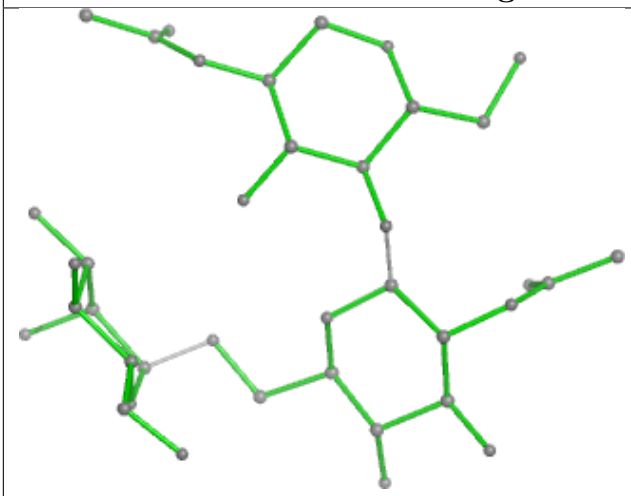


Torsions

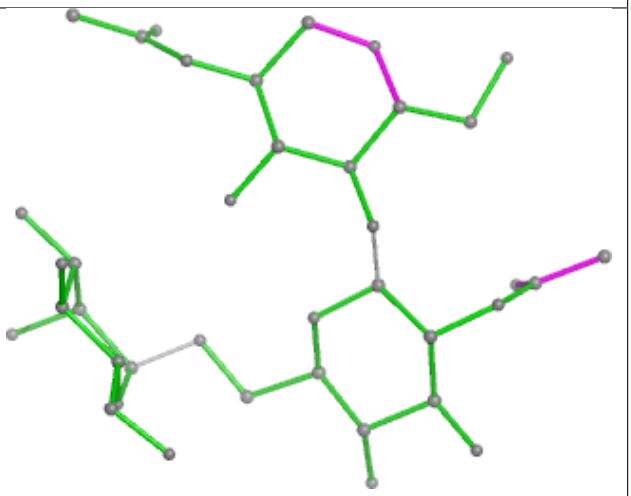


Rings

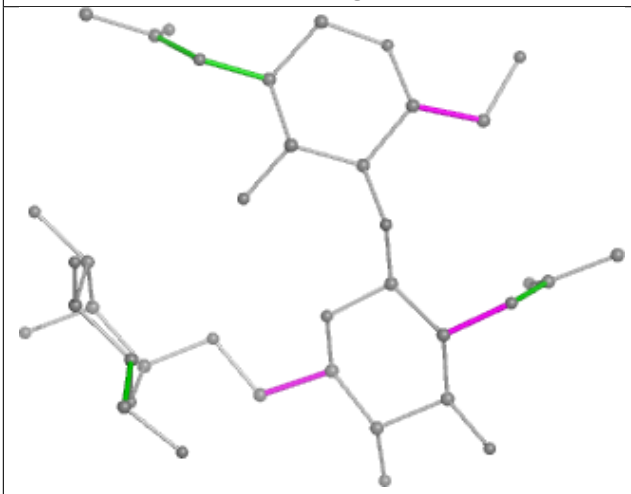
Oligosaccharide Chain h



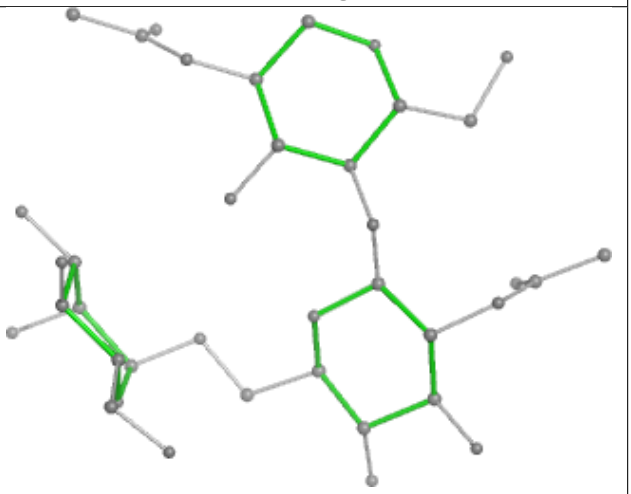
Bond lengths



Bond angles

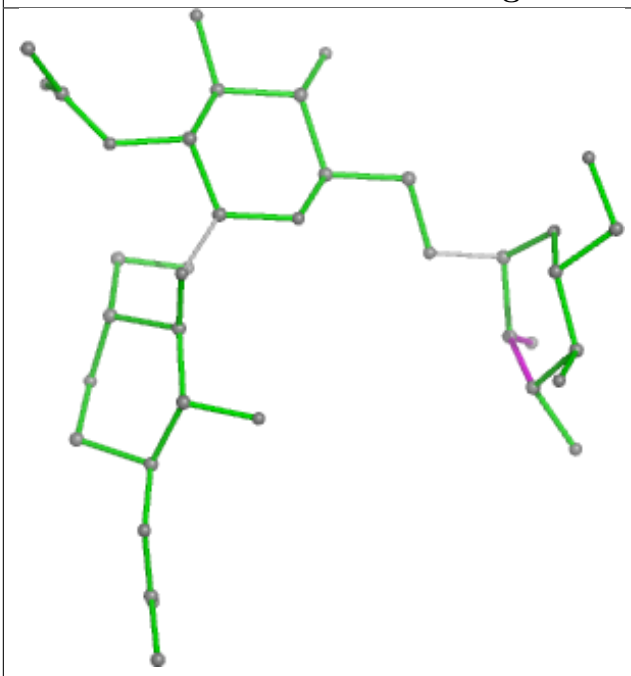


Torsions

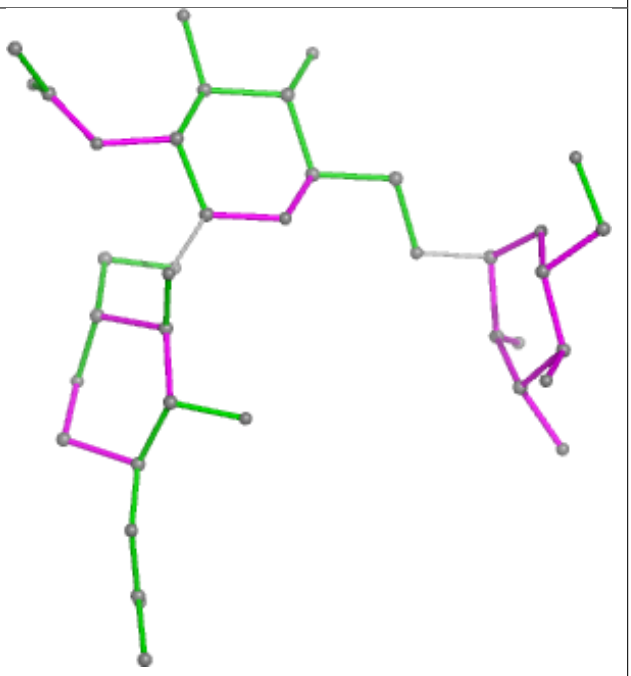


Rings

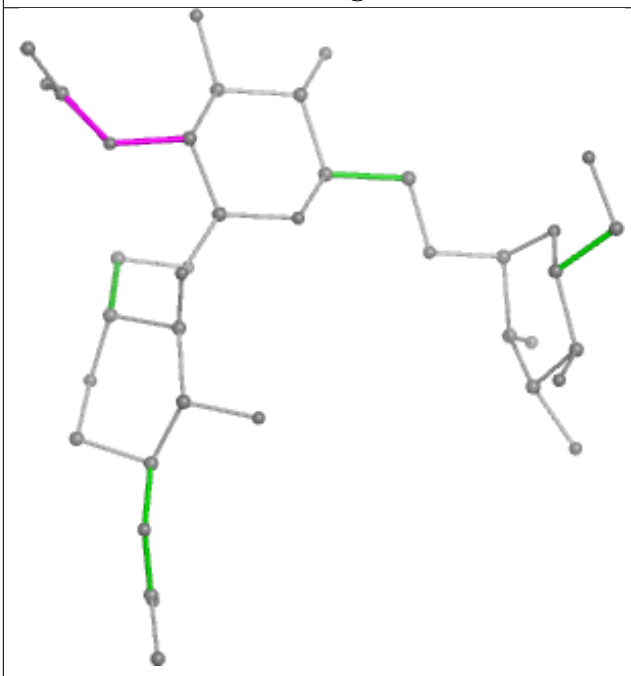
Oligosaccharide Chain i



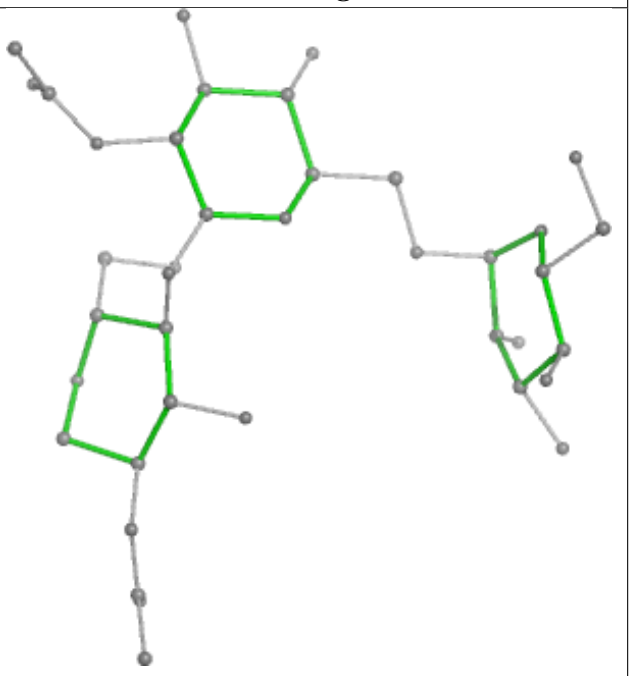
Bond lengths



Bond angles

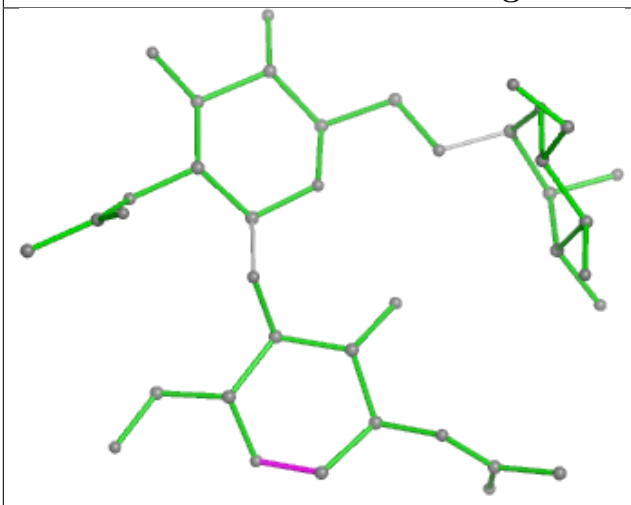


Torsions

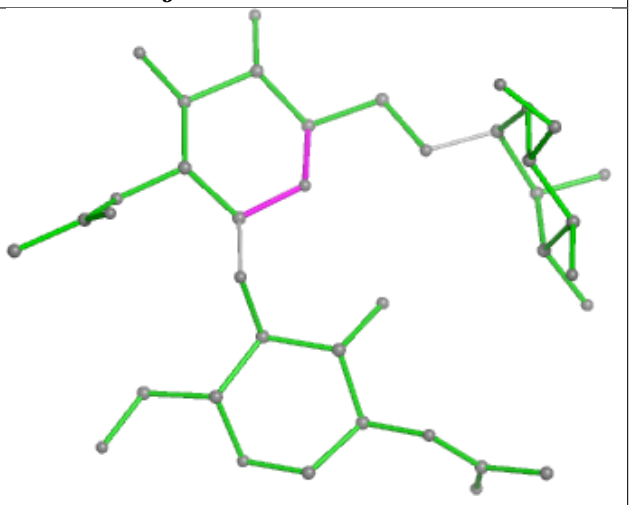


Rings

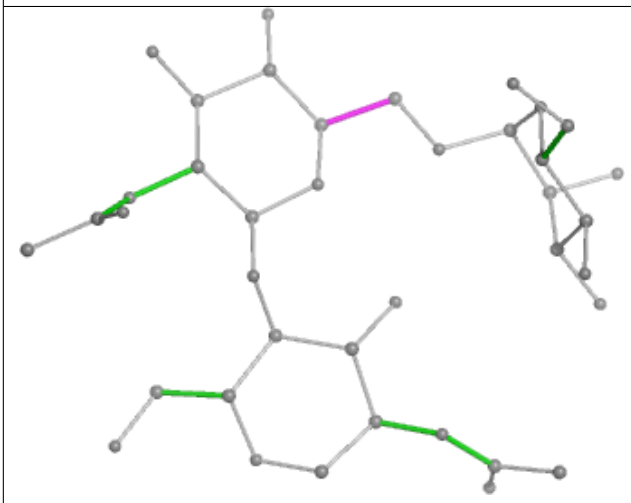
Oligosaccharide Chain j



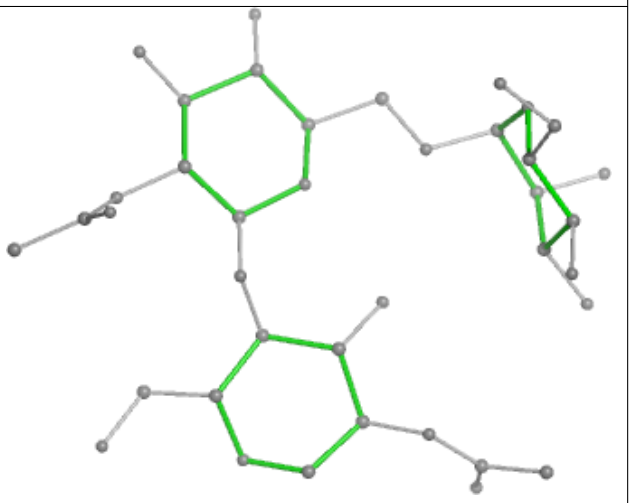
Bond lengths



Bond angles

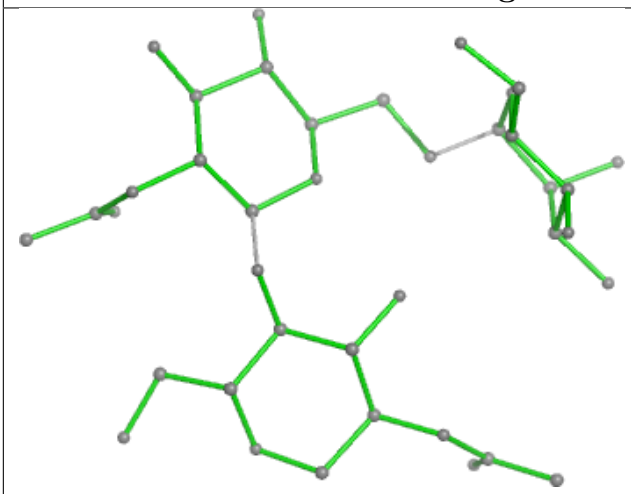


Torsions

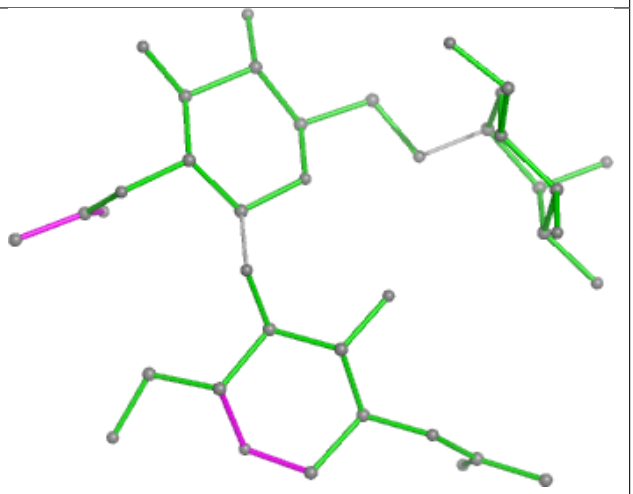


Rings

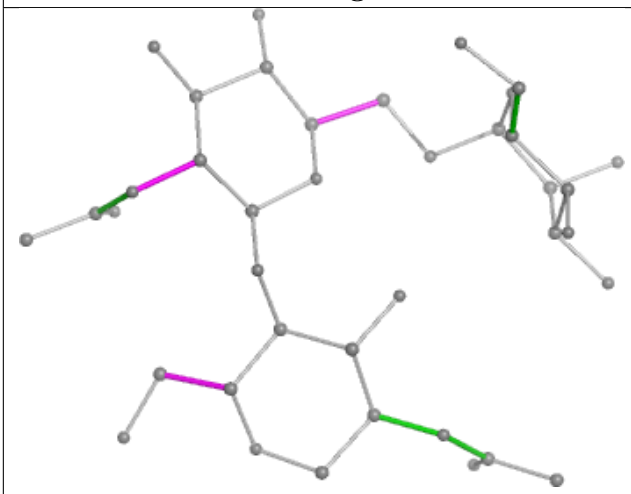
Oligosaccharide Chain k



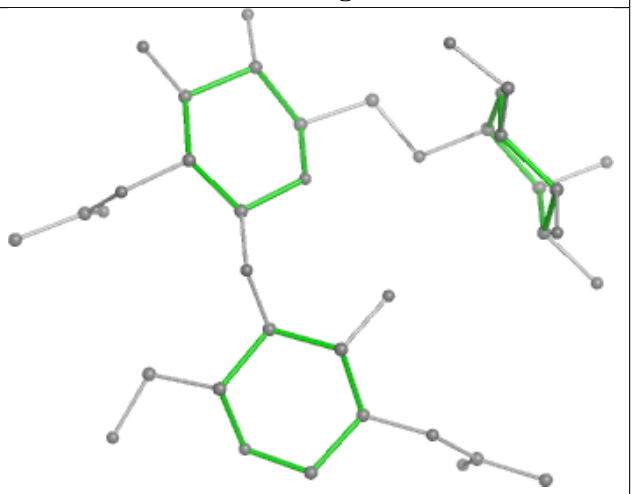
Bond lengths



Bond angles

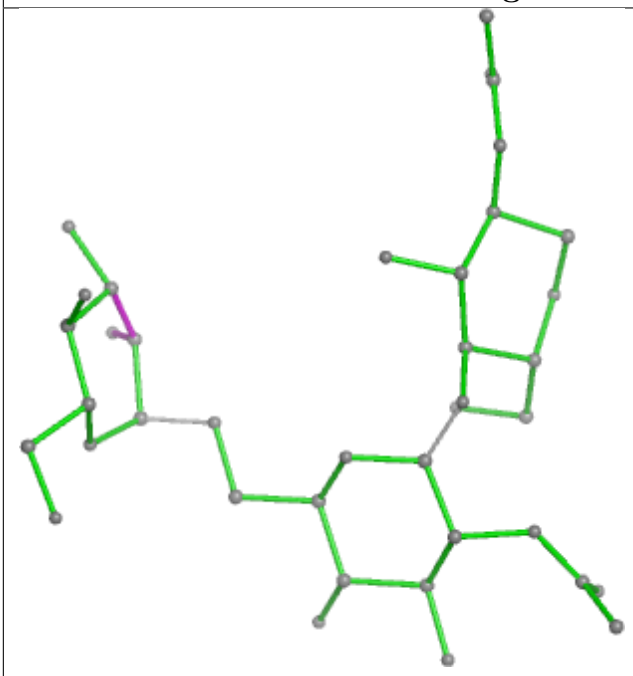


Torsions



Rings

Oligosaccharide Chain l



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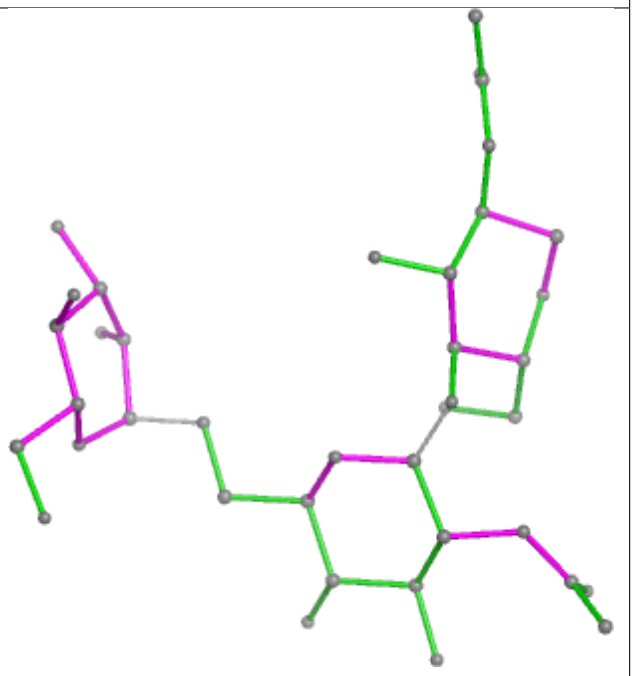

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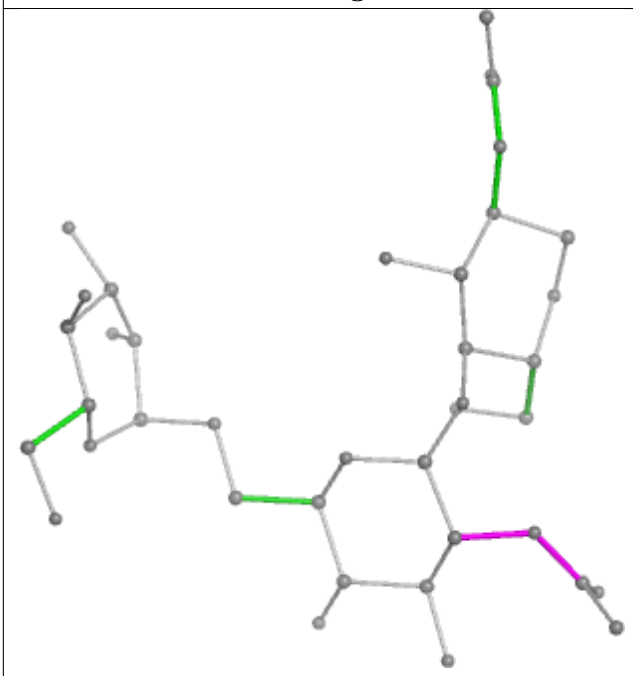
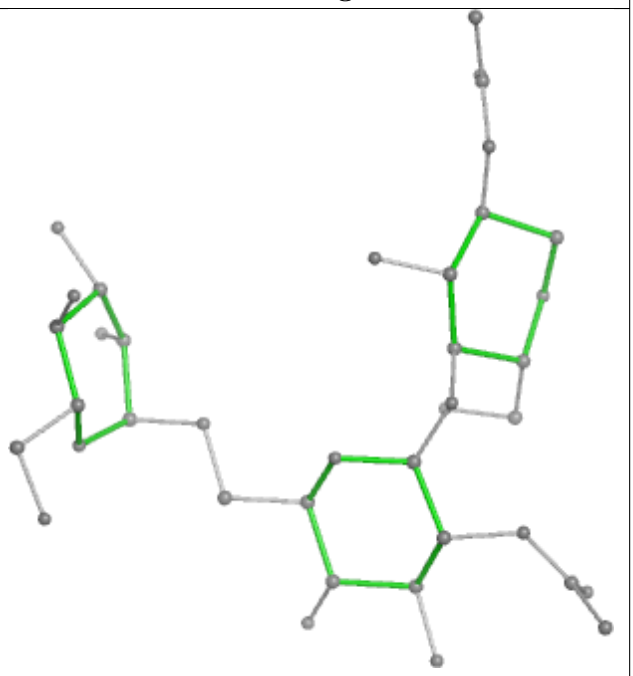
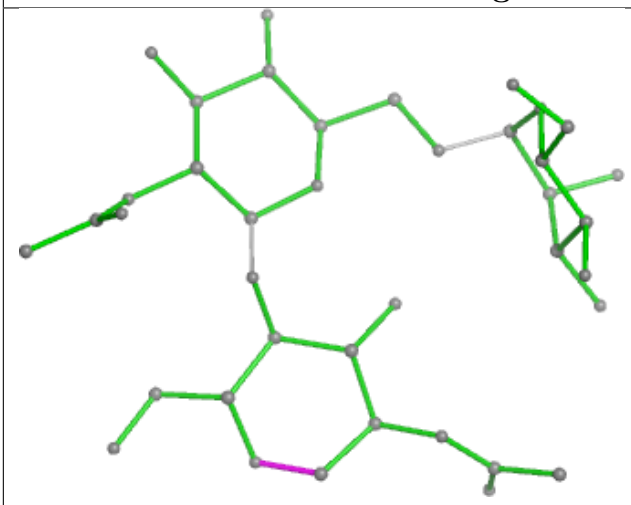


Torsions



Rings

Oligosaccharide Chain m



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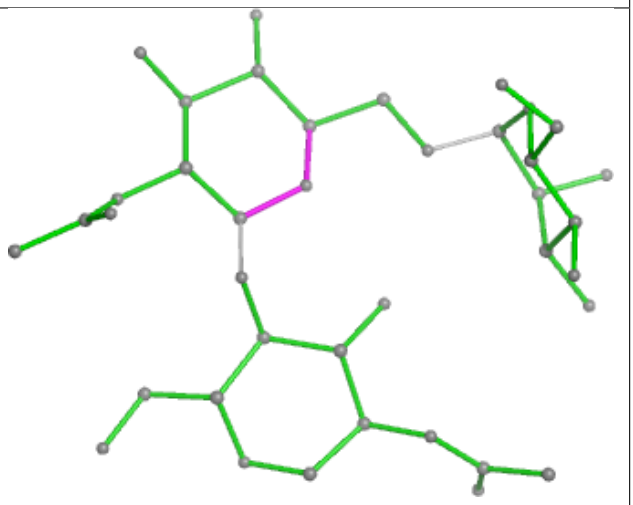

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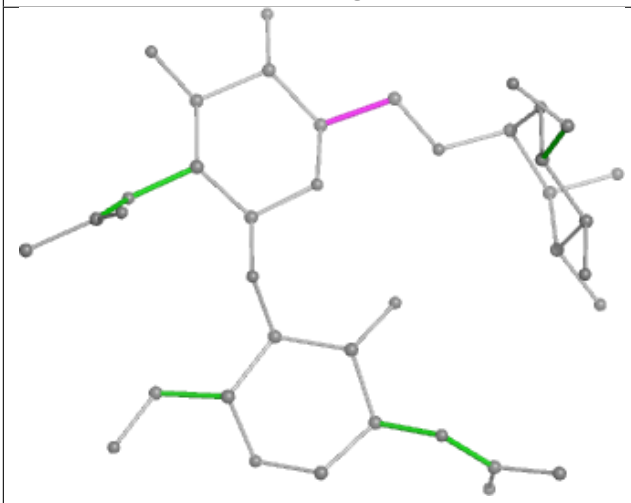

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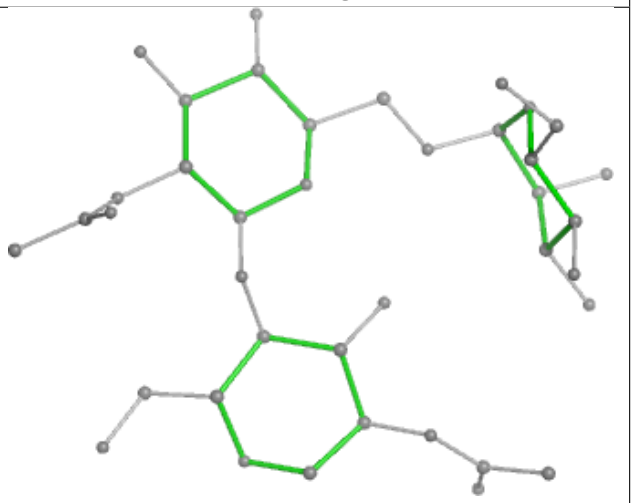
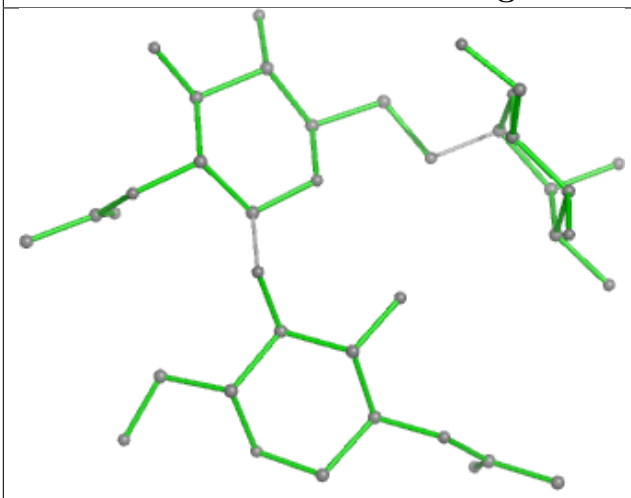


Rings

Oligosaccharide Chain n



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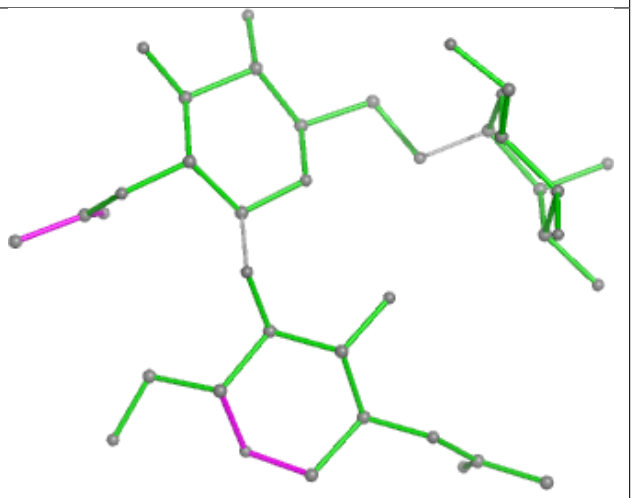

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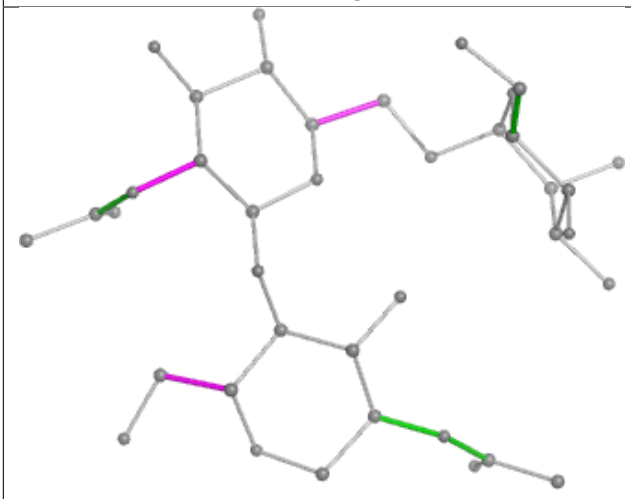

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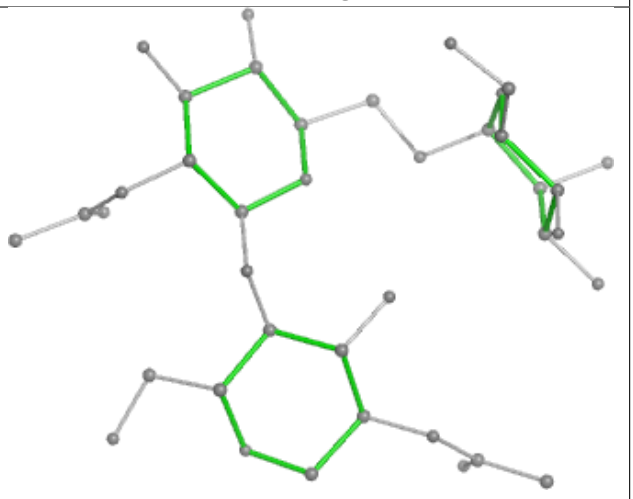
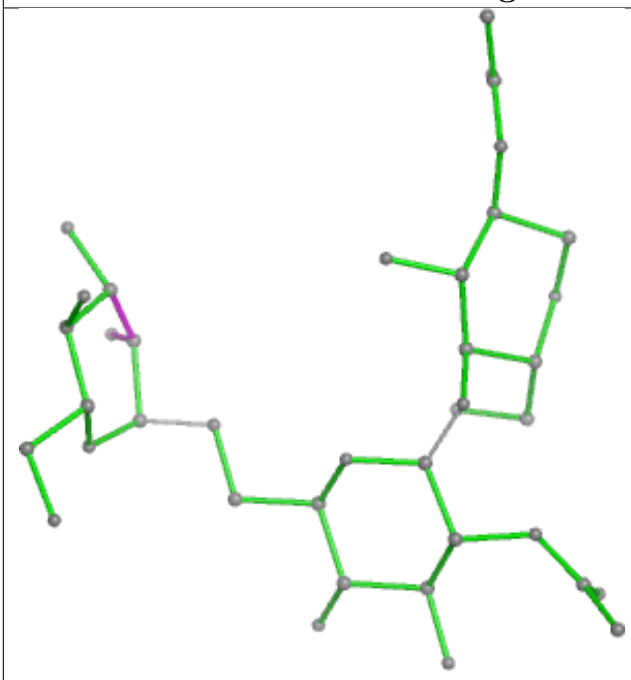


Rings

Oligosaccharide Chain o



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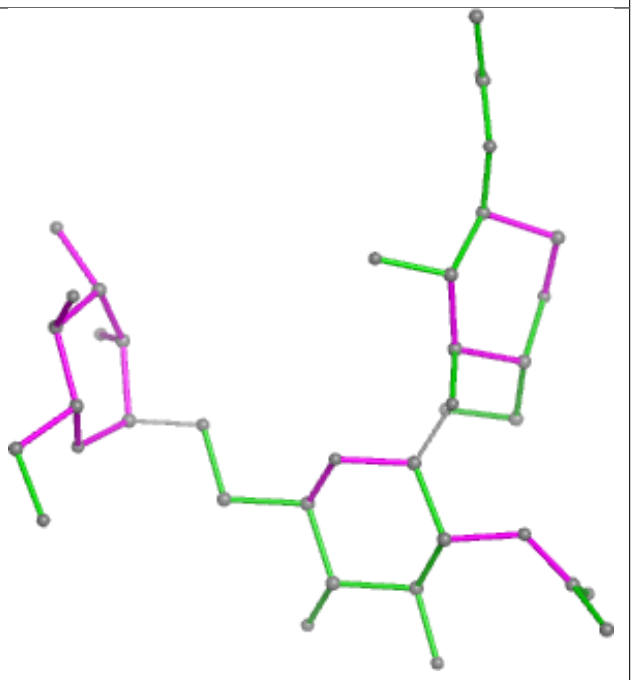

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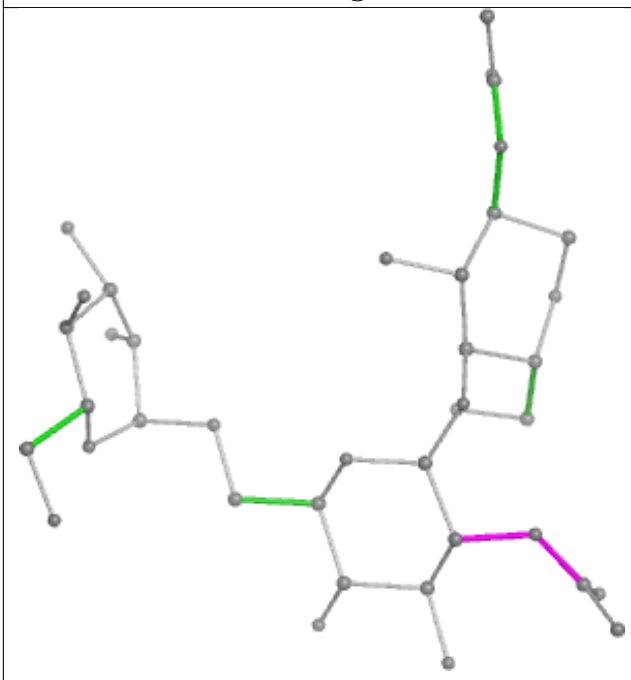

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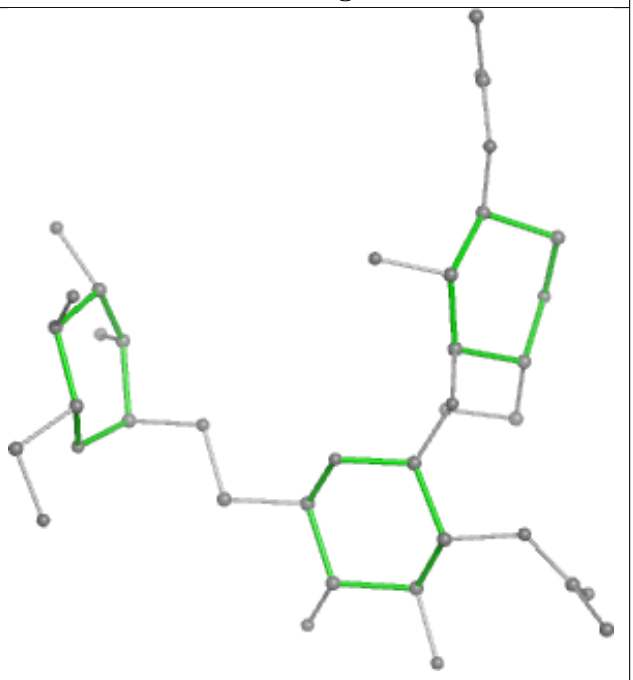
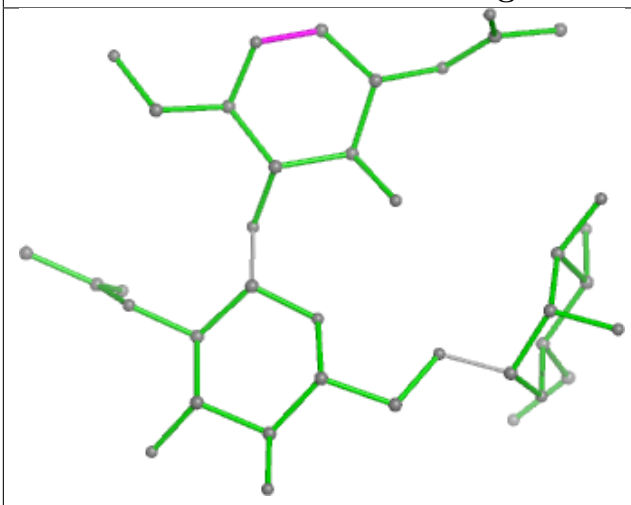


Rings

Oligosaccharide Chain p



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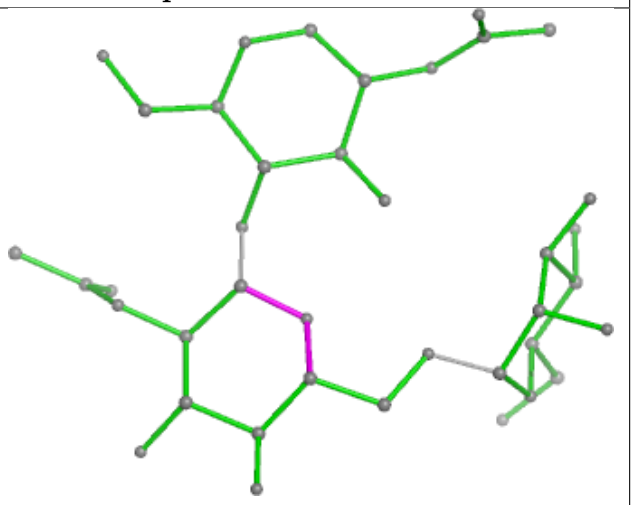

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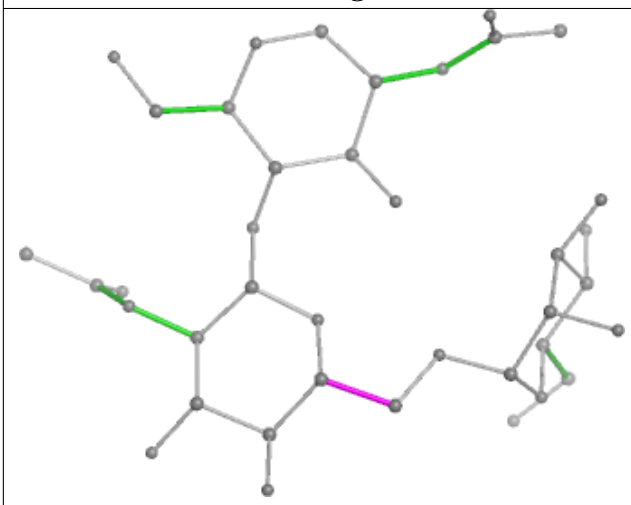

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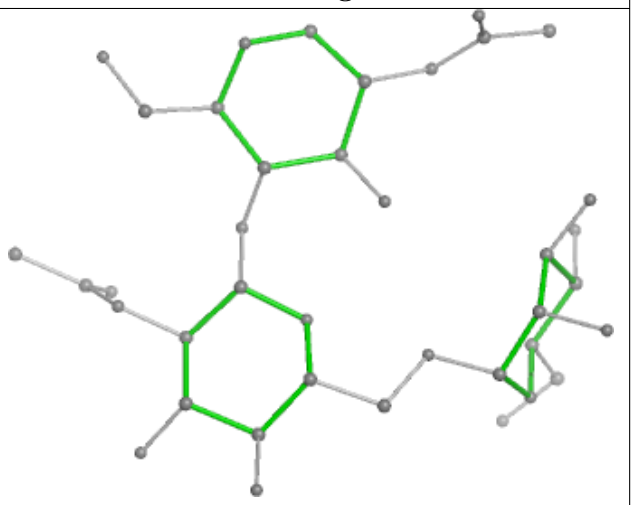
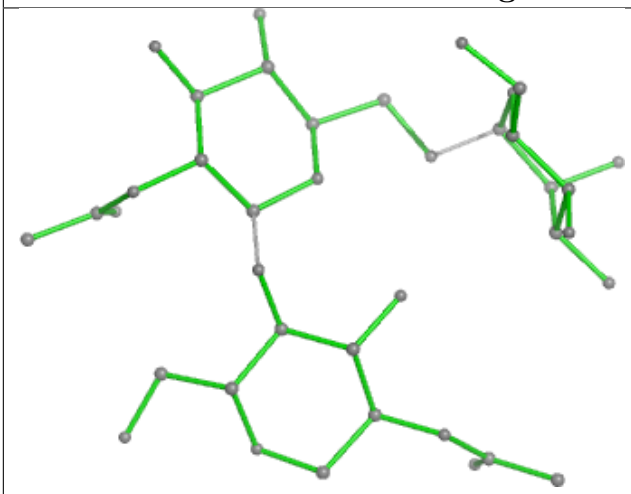


Rings

Oligosaccharide Chain q



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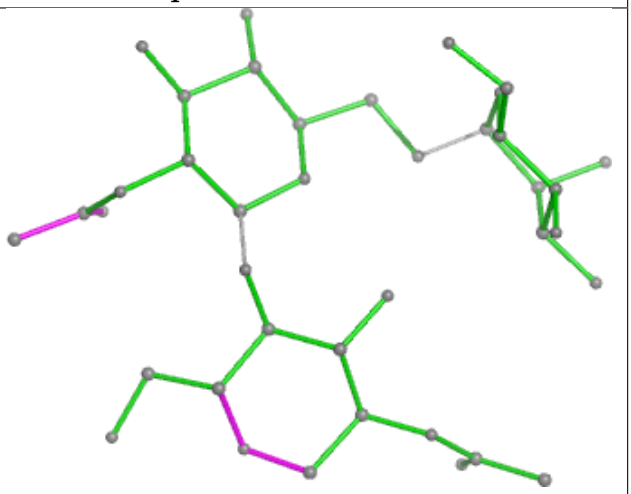
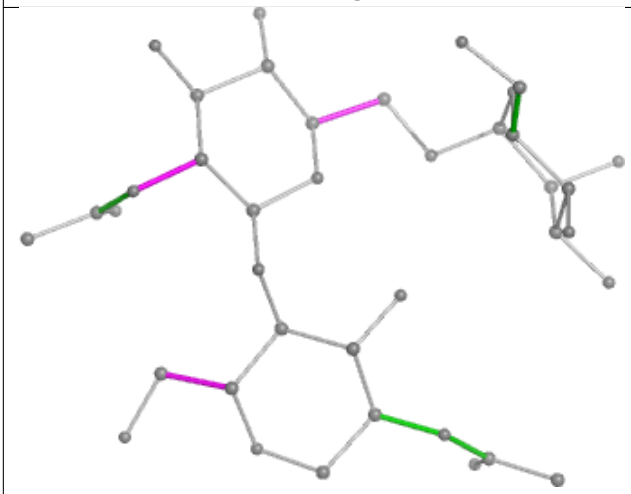


Bond angles



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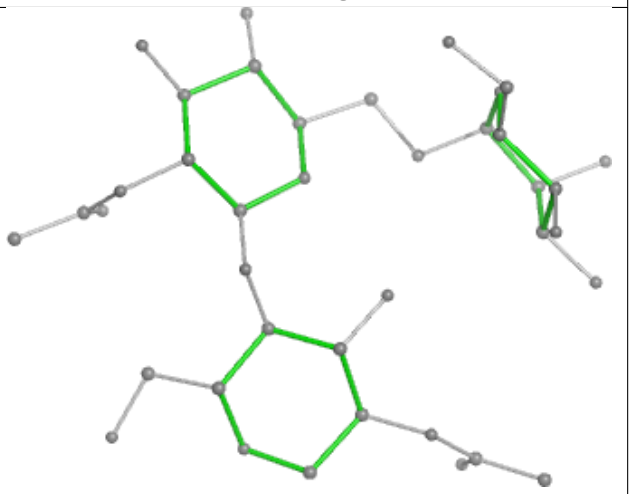
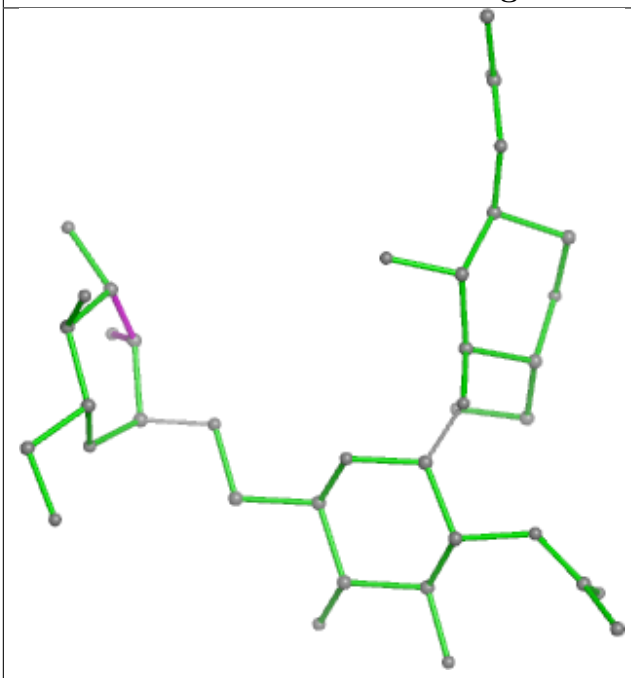


Rings

Oligosaccharide Chain r



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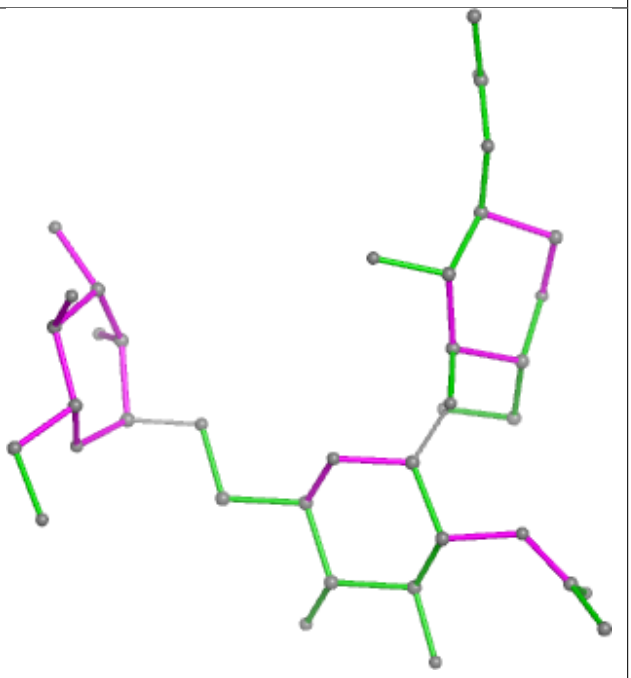
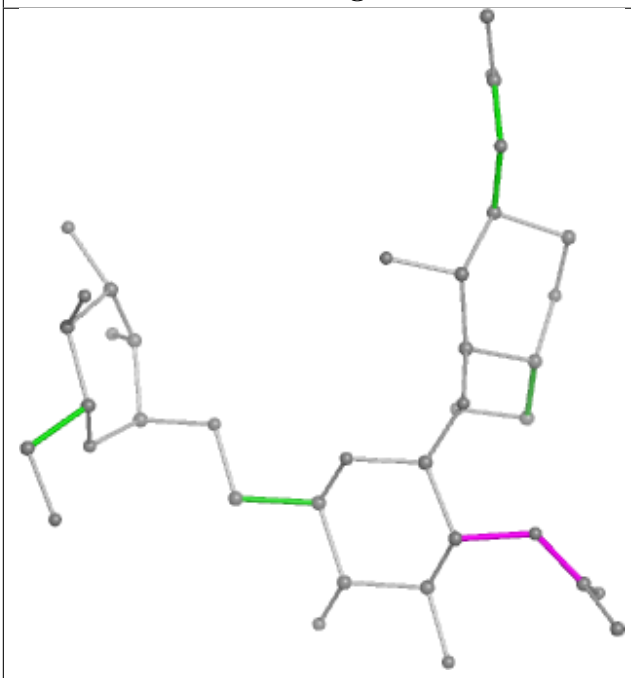


Bond angles



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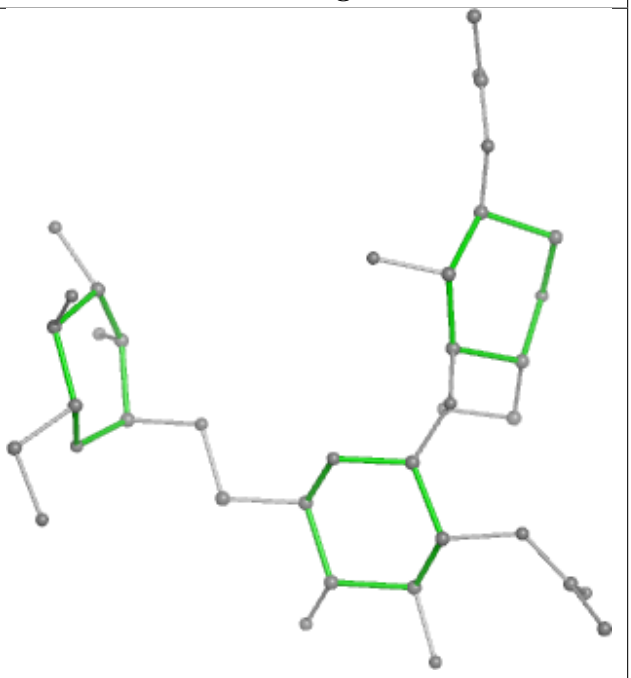
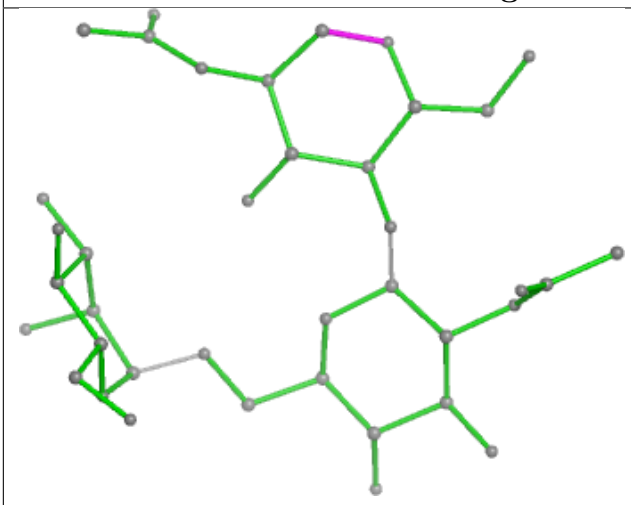


Rings

Oligosaccharide Chain s



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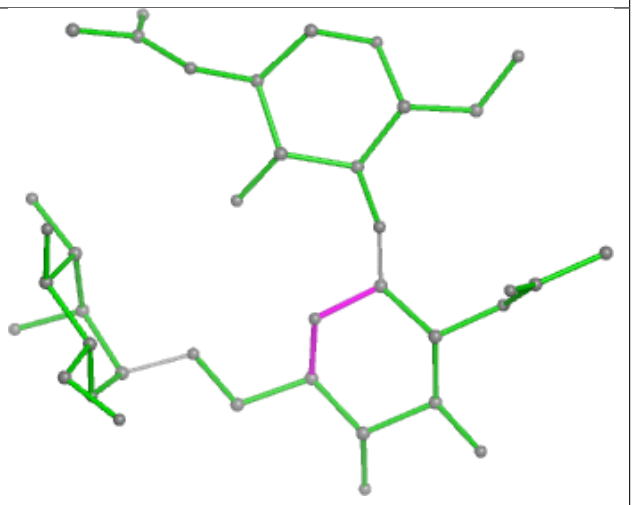
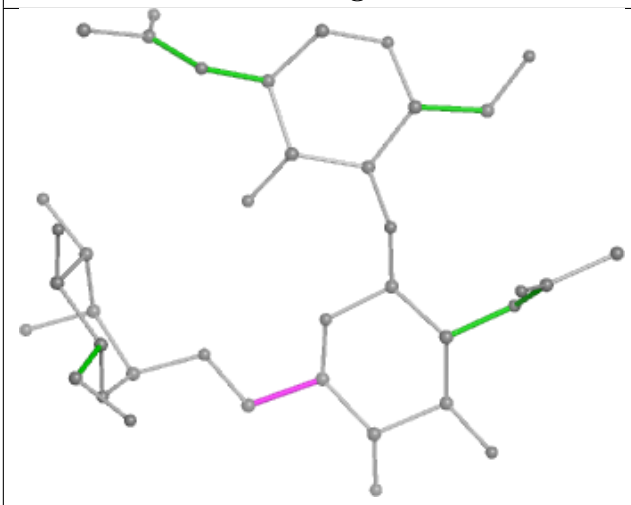


Bond angles



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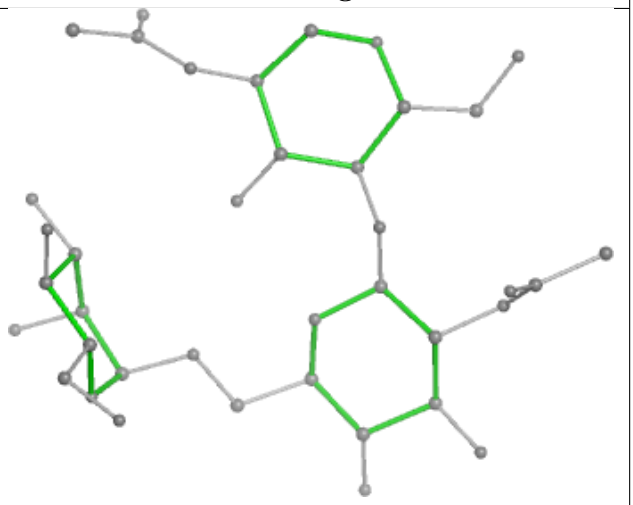
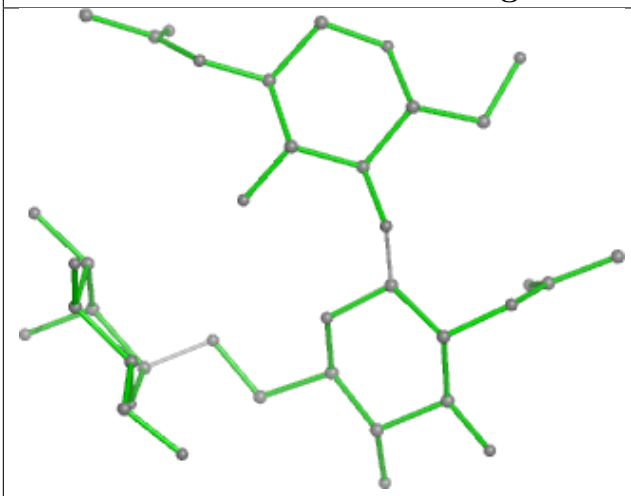


Rings

Oligosaccharide Chain t



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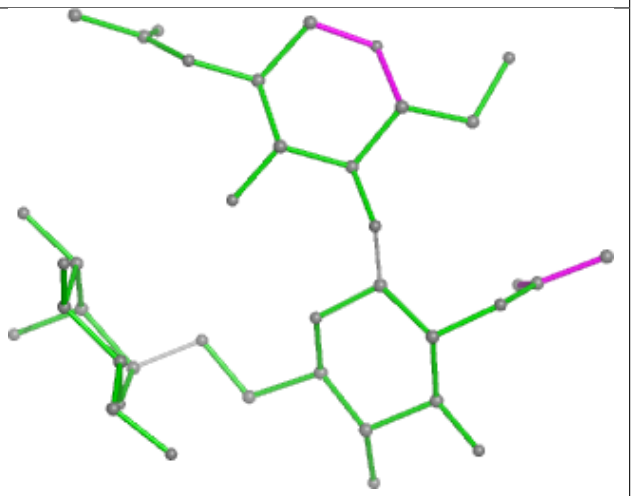

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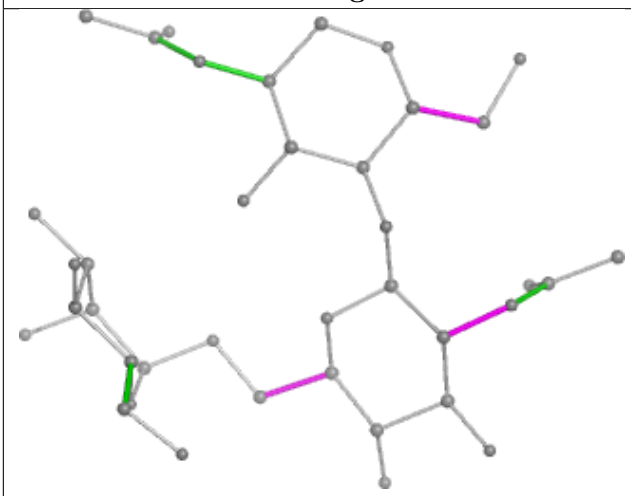
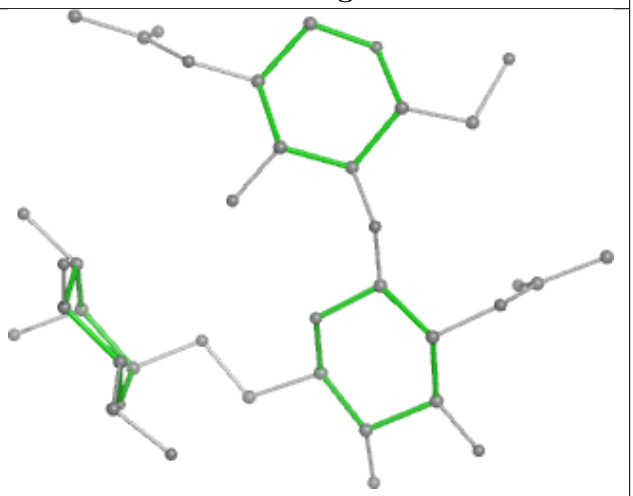
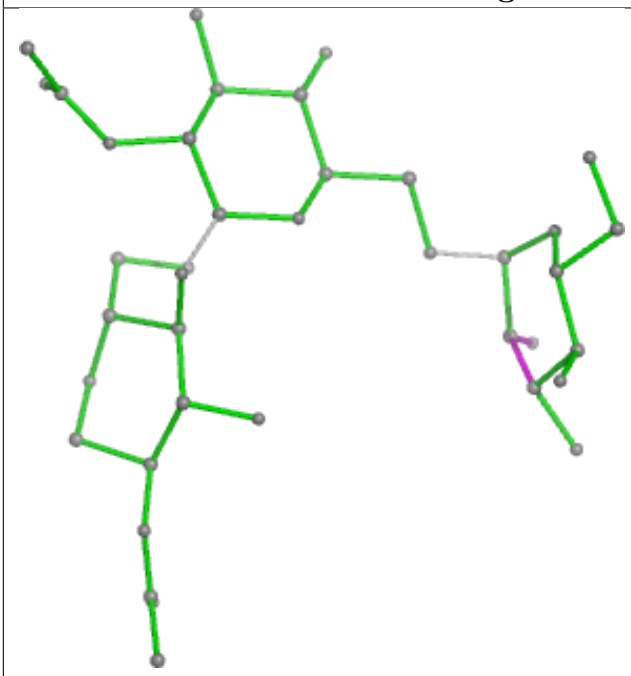


Torsions



Rings

Oligosaccharide Chain u



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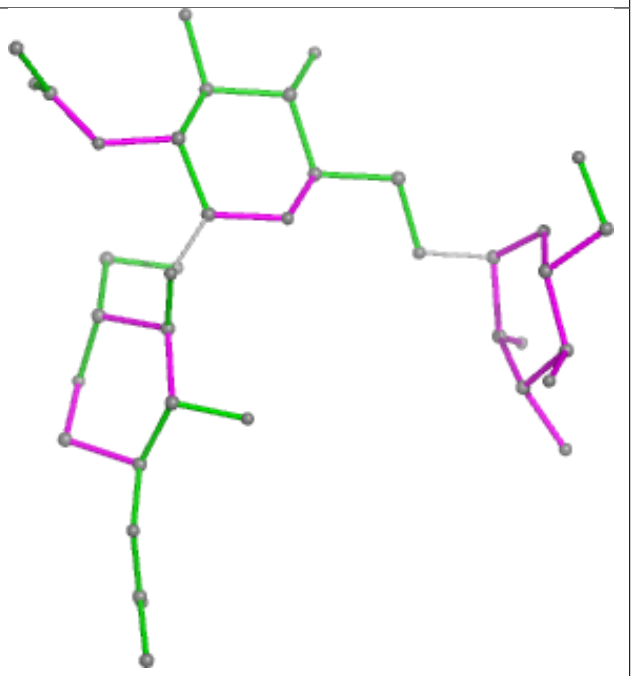
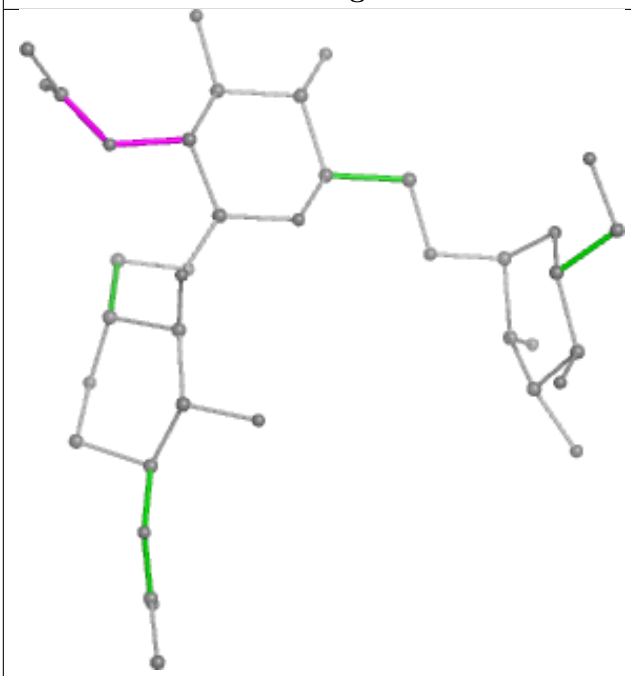


Bond angles



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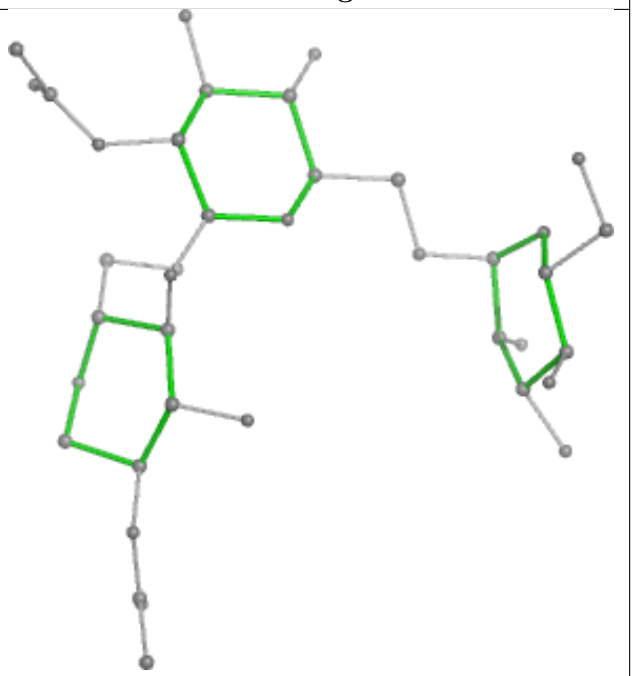
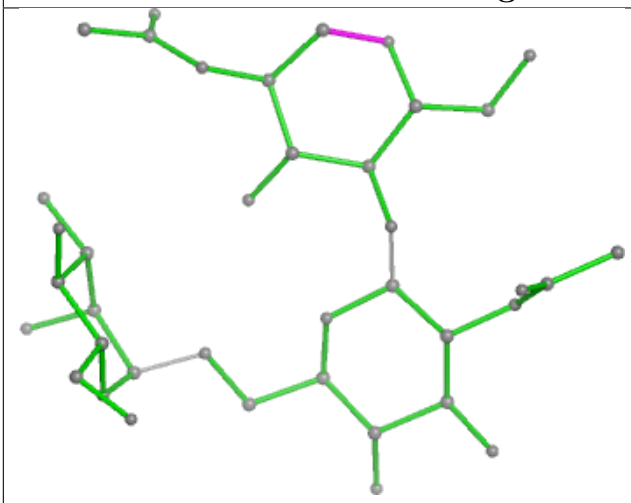


Rings

Oligosaccharide Chain v



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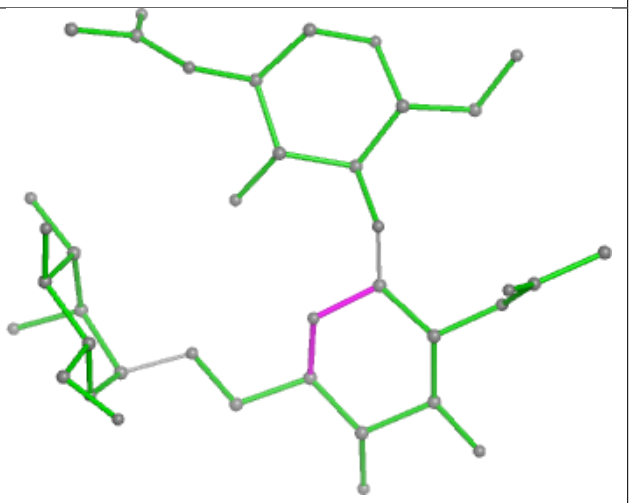
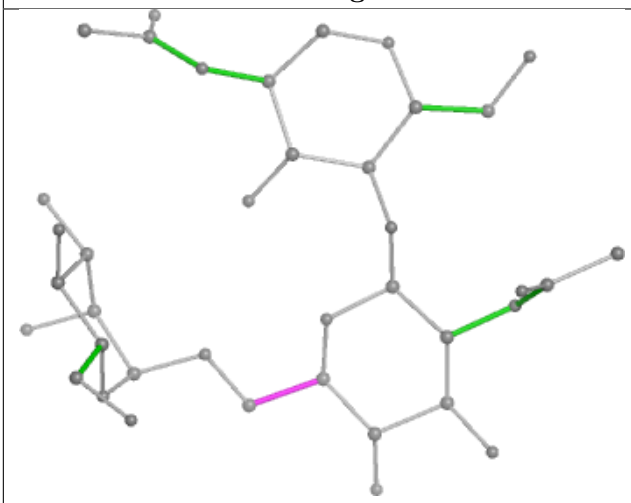


Bond angles



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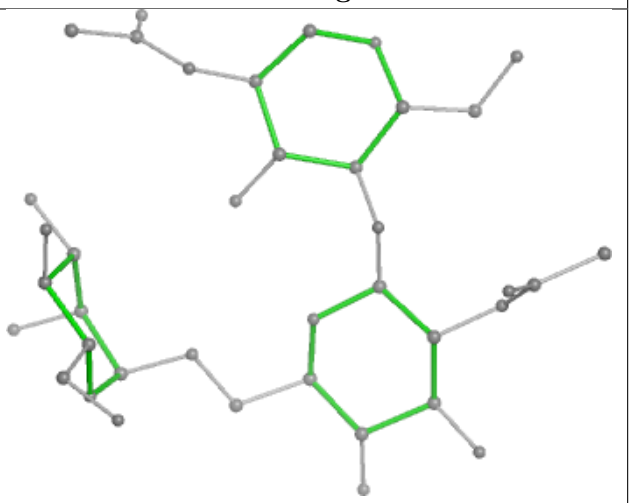
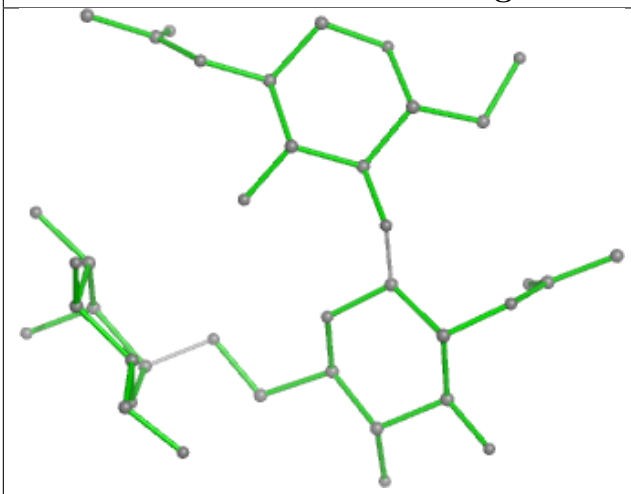


Rings

Oligosaccharide Chain w



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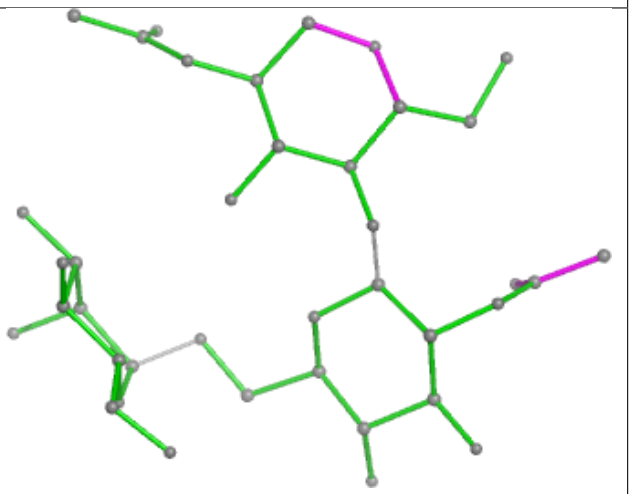
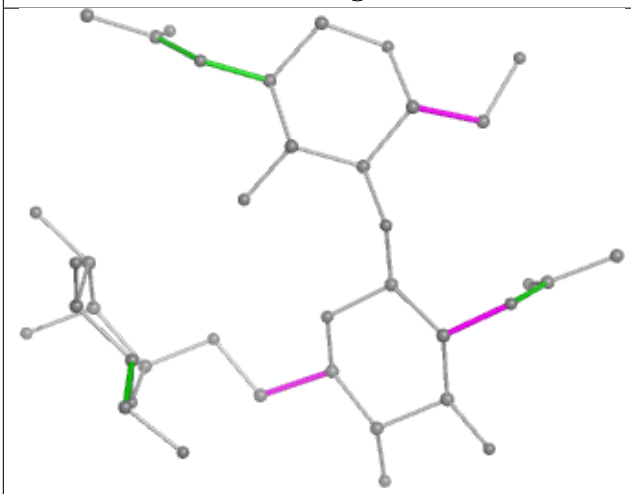
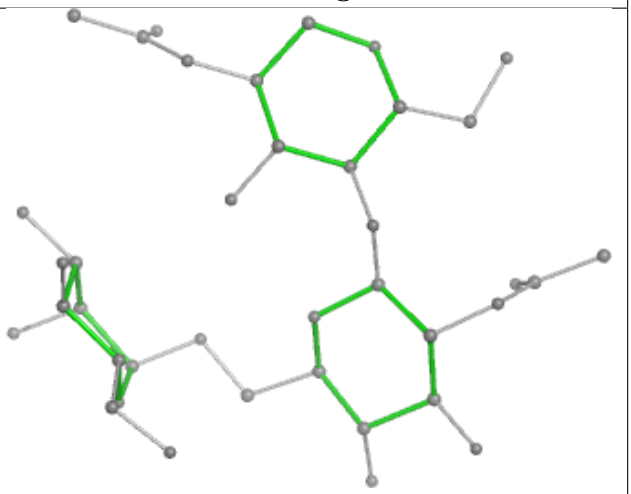


Bond angles

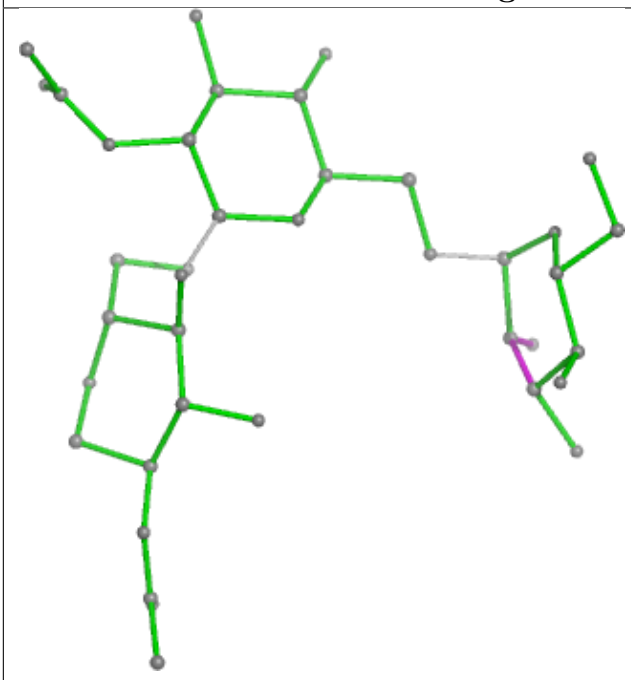


Torsions

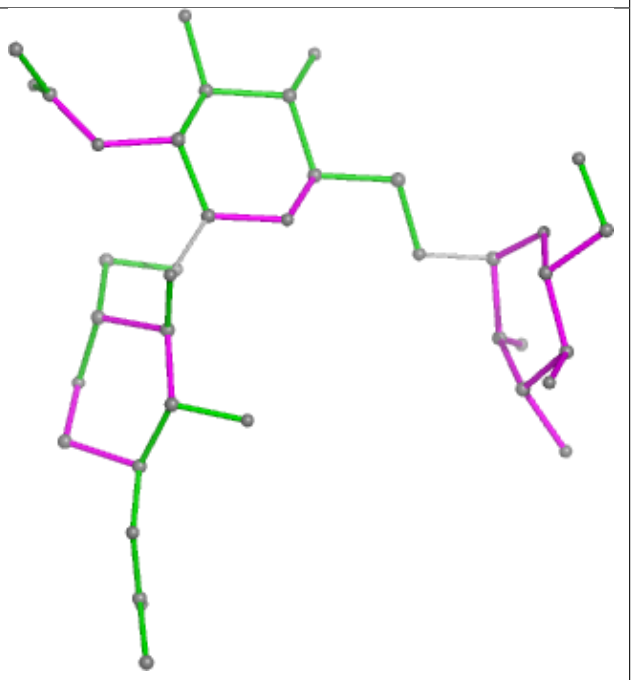


Rings

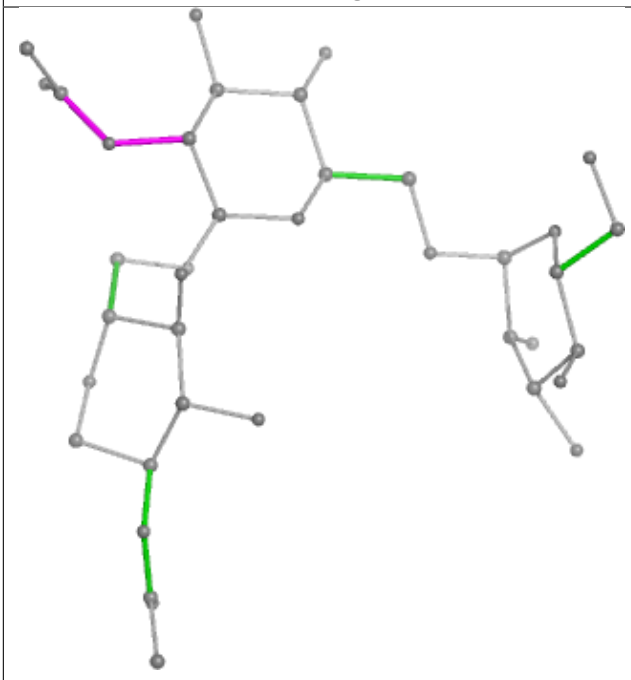
Oligosaccharide Chain x



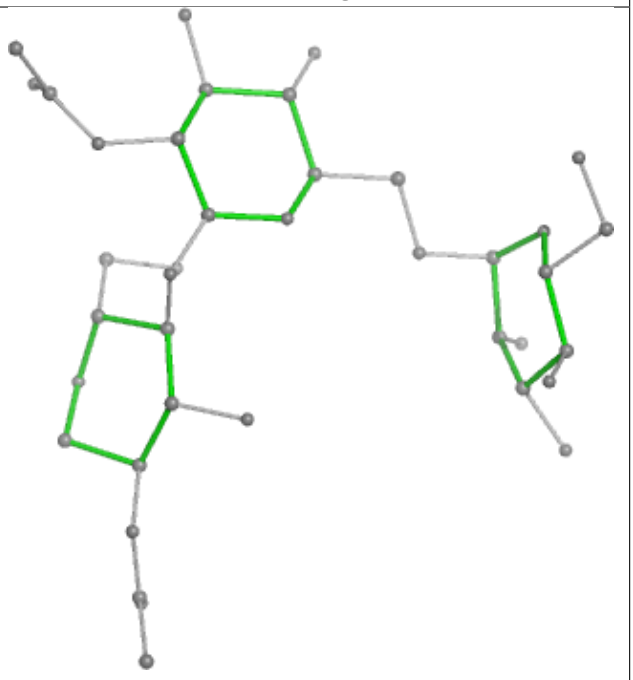
Bond lengths



Bond angles

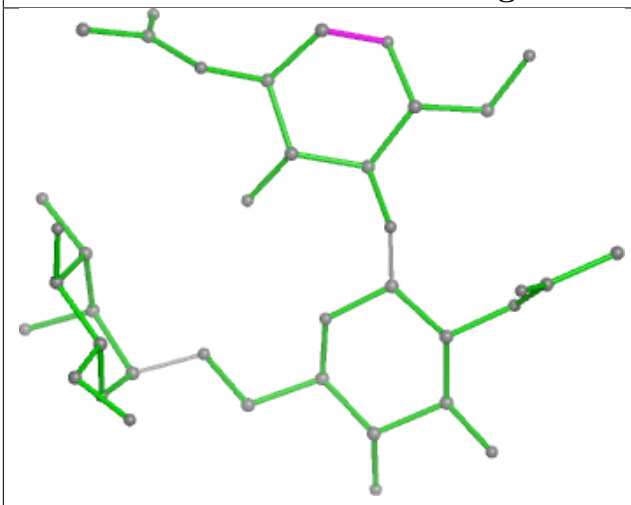


Torsions

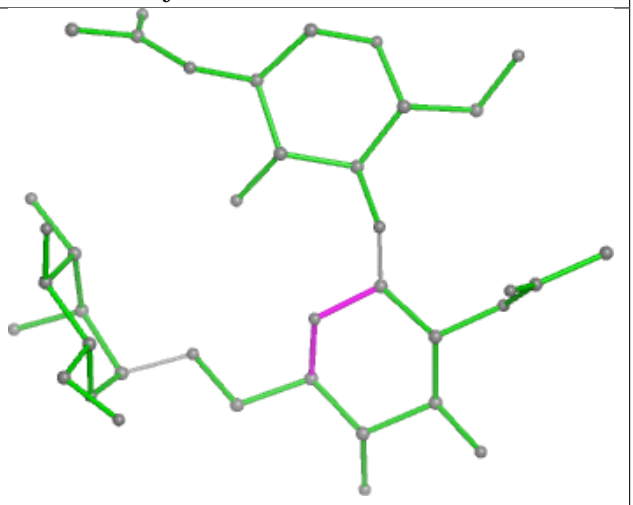


Rings

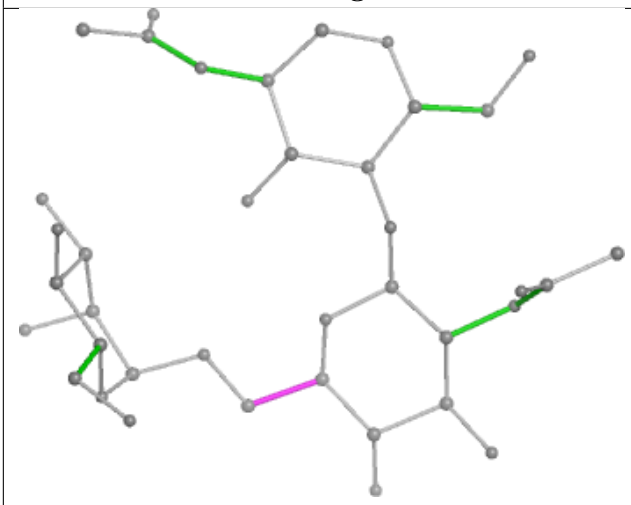
Oligosaccharide Chain y



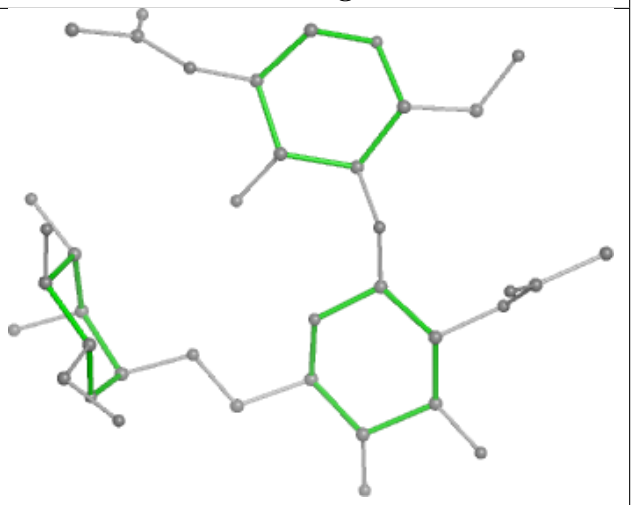
Bond lengths



Bond angles

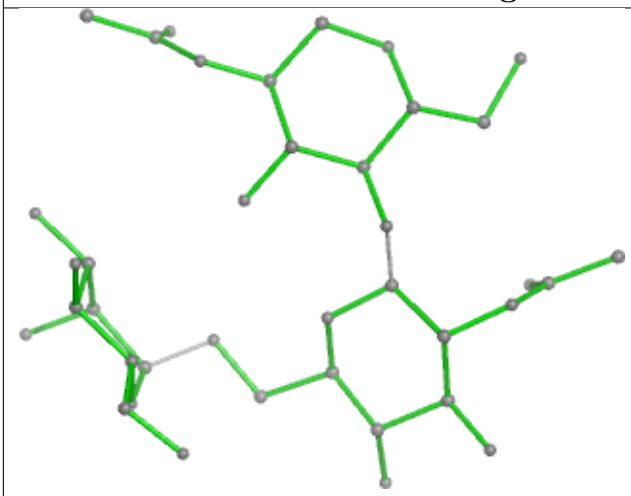


Torsions

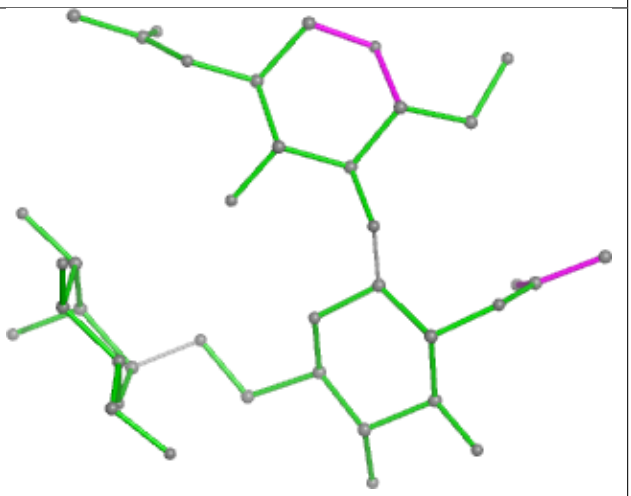


Rings

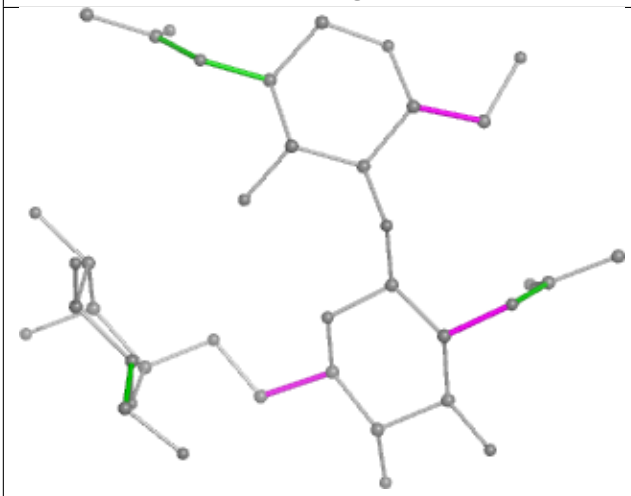
Oligosaccharide Chain z



Bond lengths



Bond angles



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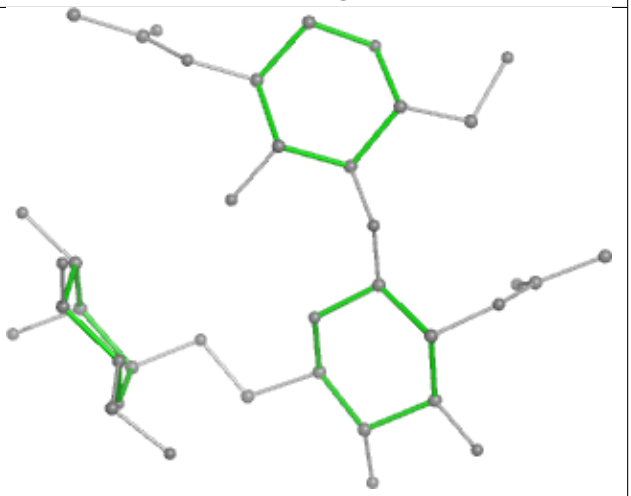
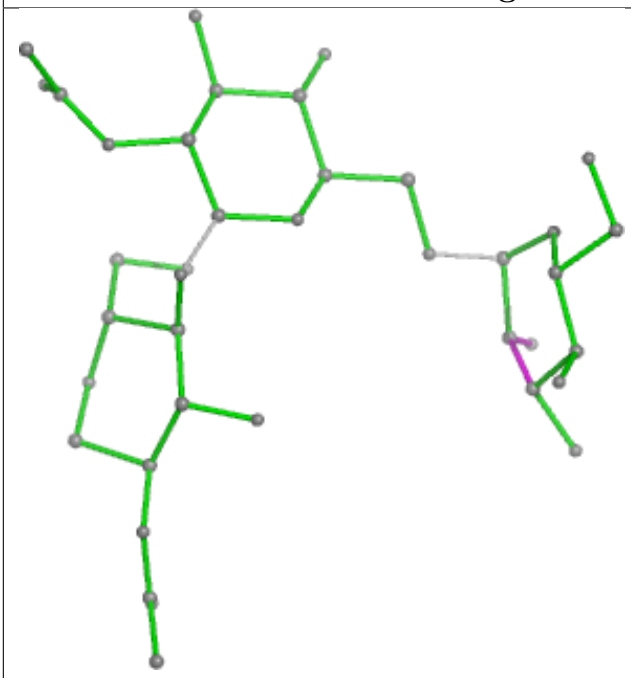


Rings

Oligosaccharide Chain 0



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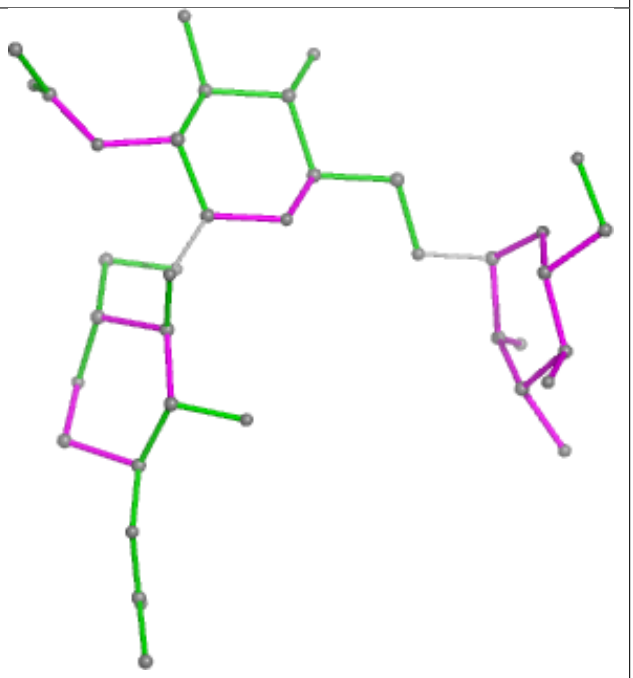
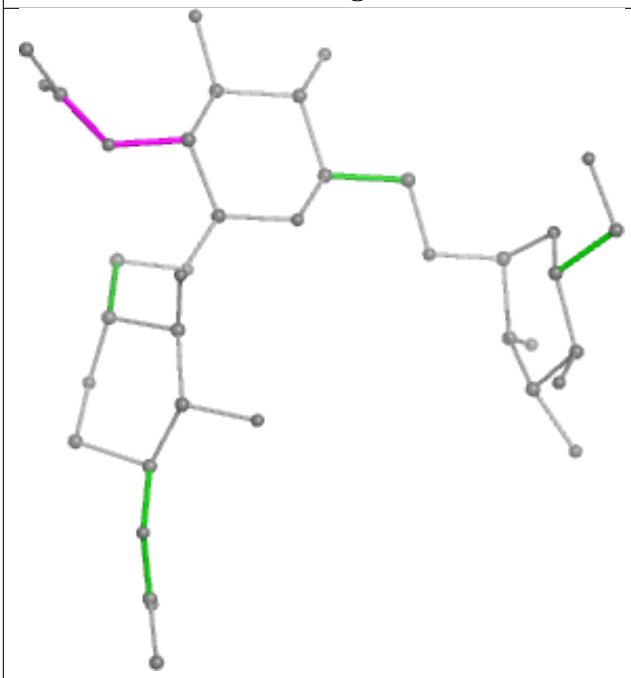


Bond angles



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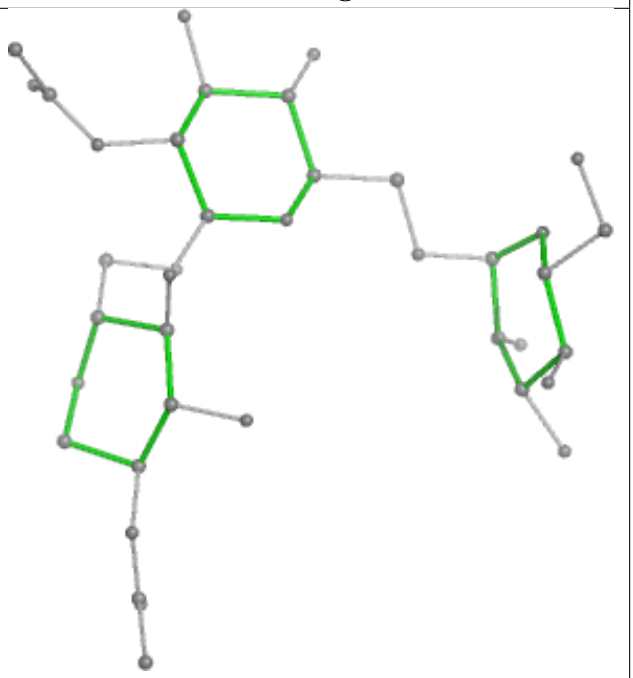
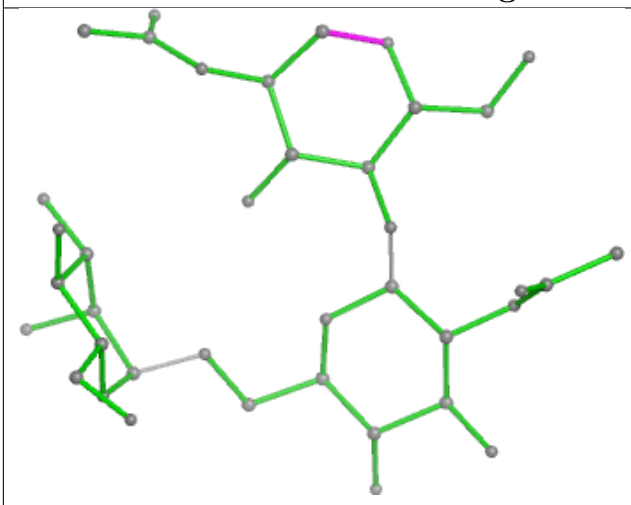


Rings

Oligosaccharide Chain 1



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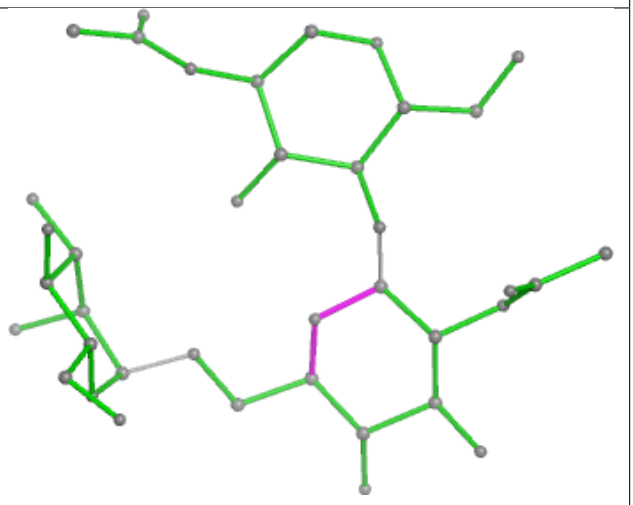
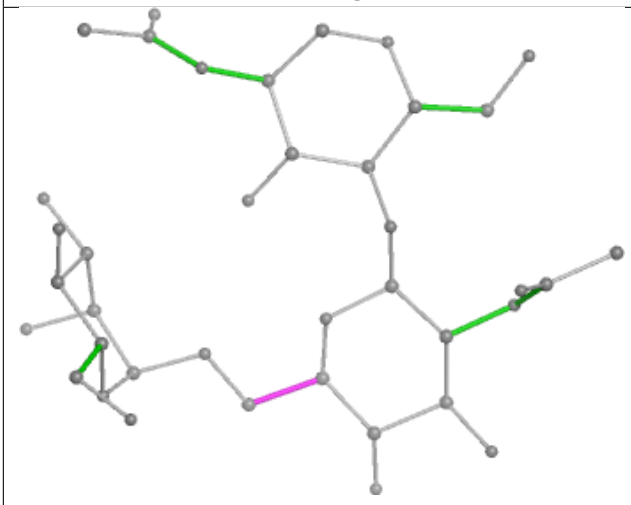


Bond angles



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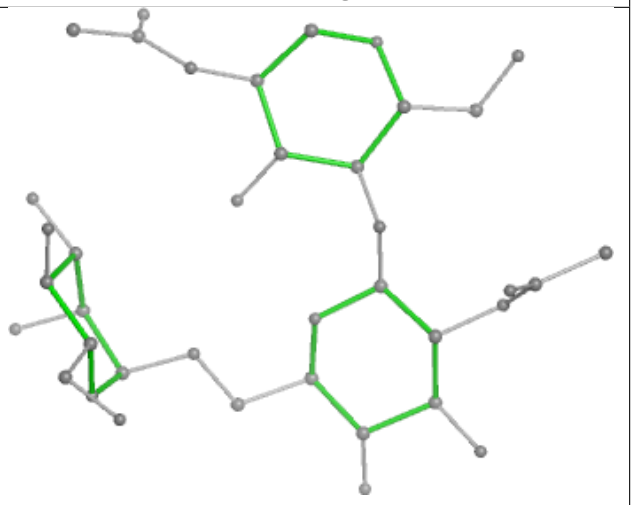
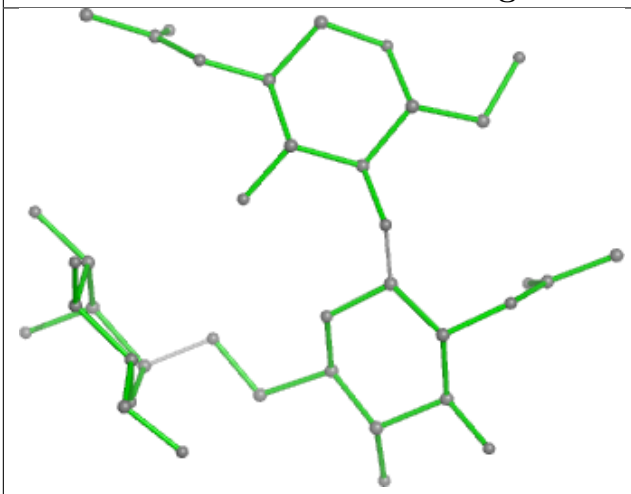


Rings

Oligosaccharide Chain 2



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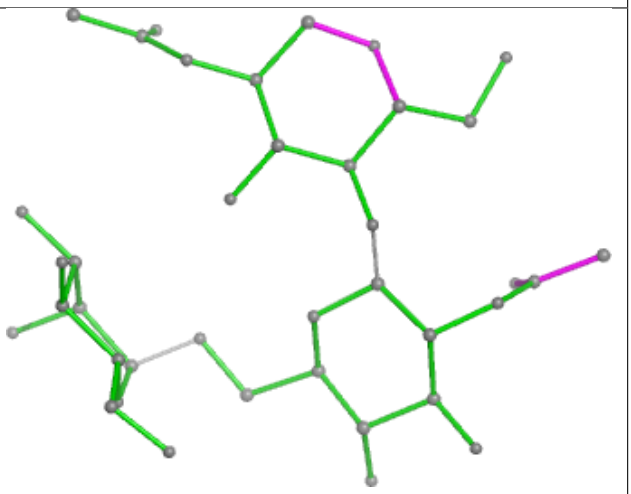
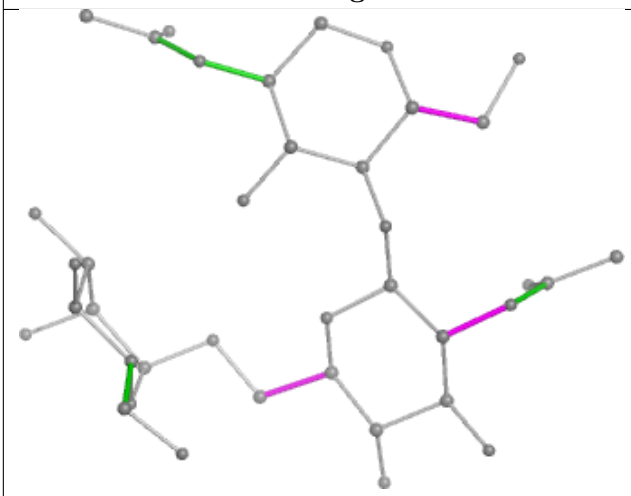


Bond angles



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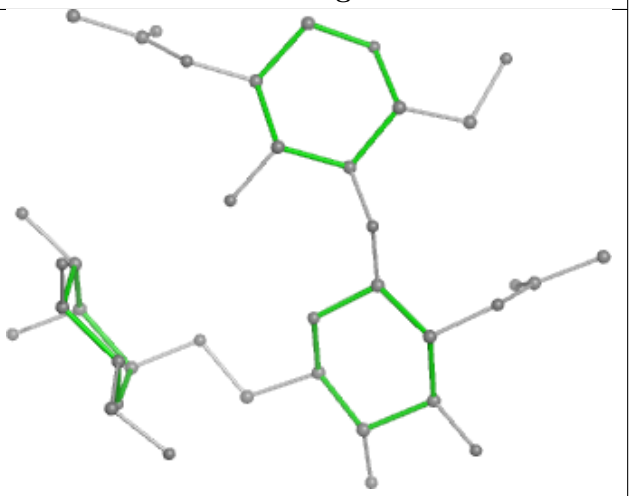
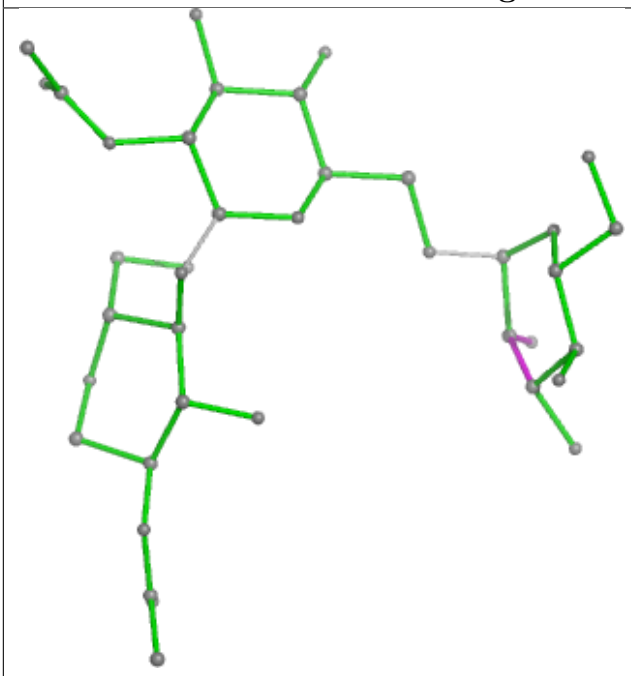


Rings

Oligosaccharide Chain 3



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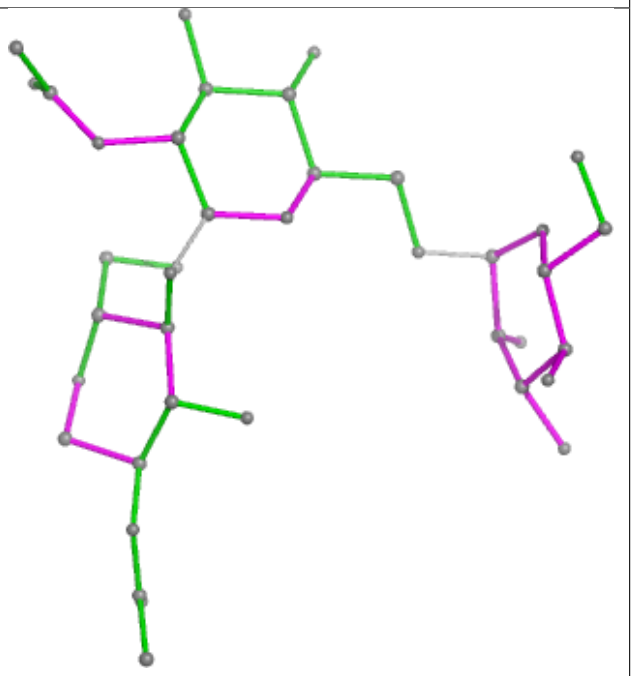
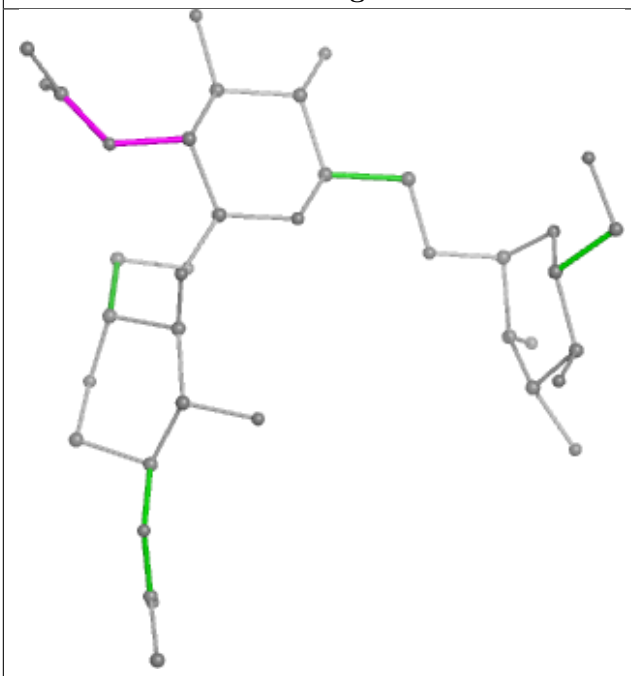


Bond angles



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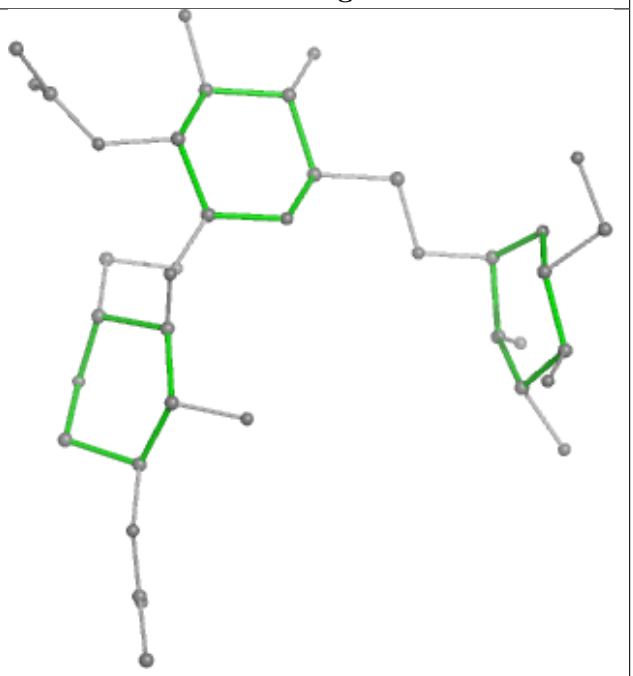
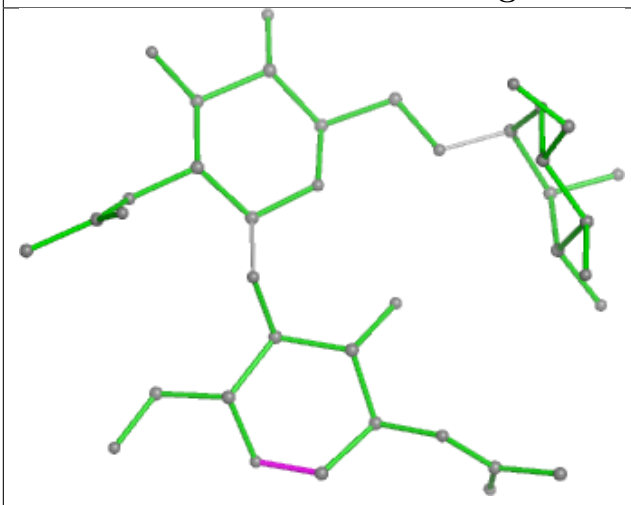
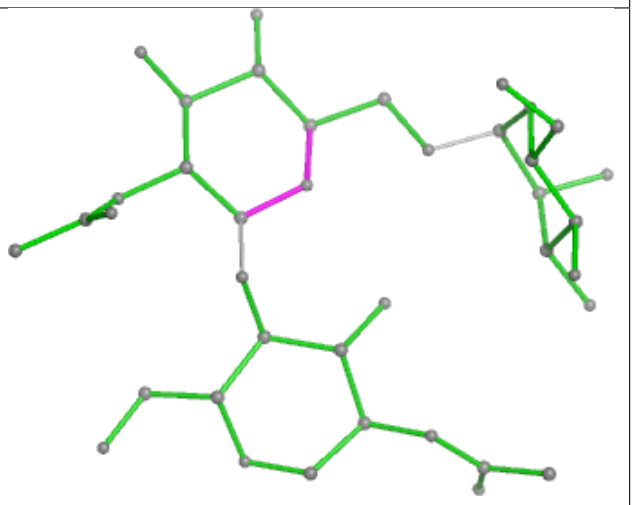
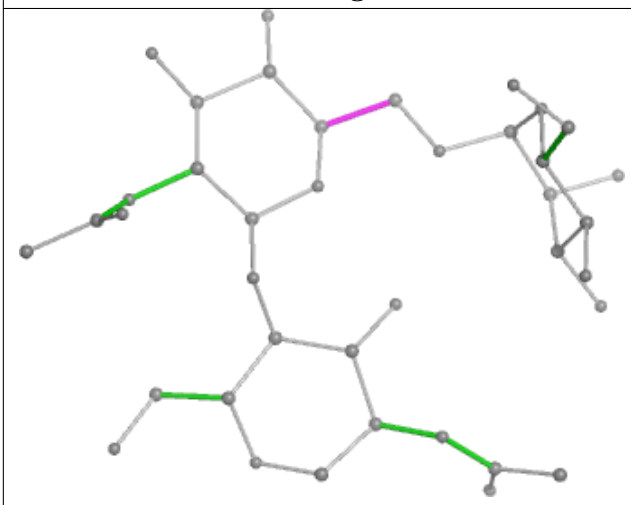
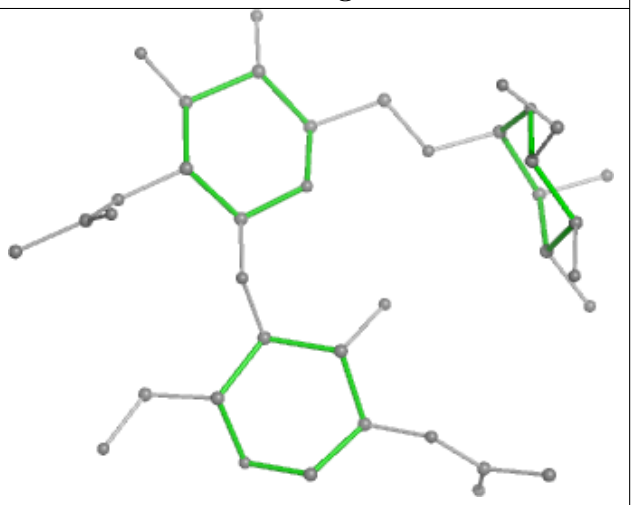
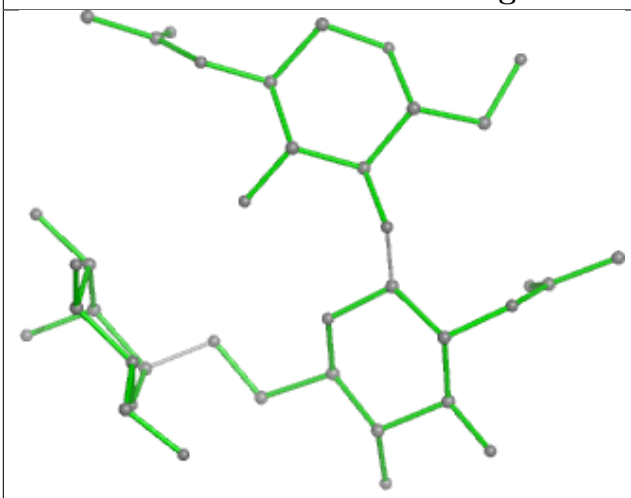


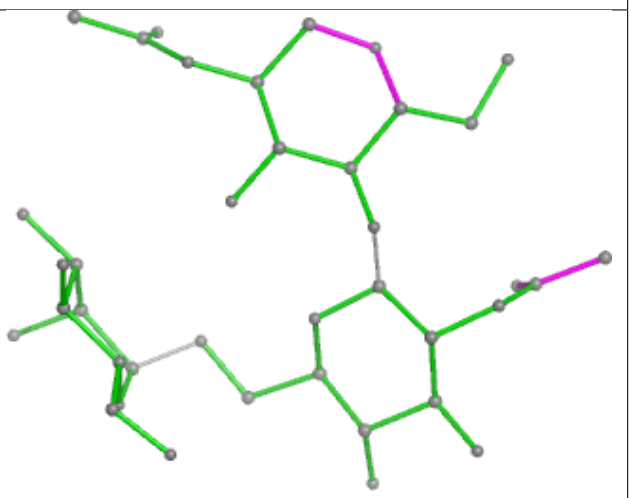
Rings

Oligosaccharide Chain 4	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

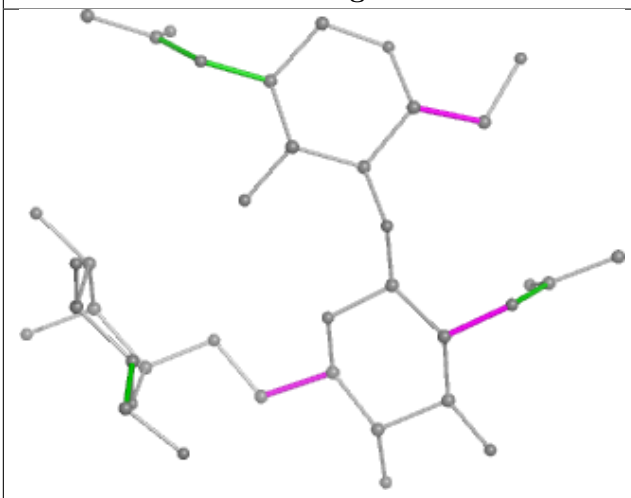
Oligosaccharide Chain 5



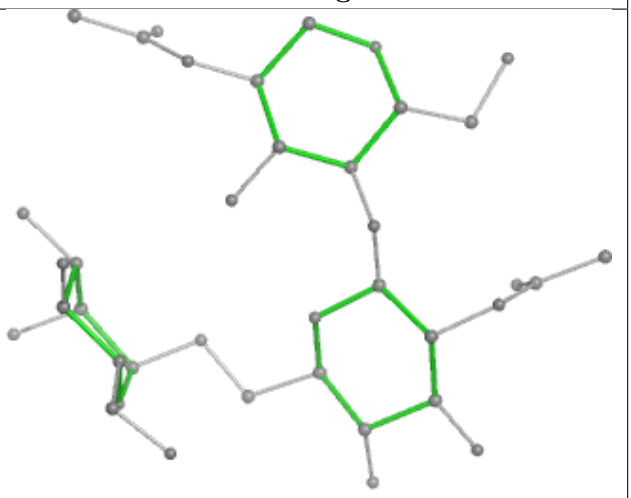
Bond lengths



Bond angles

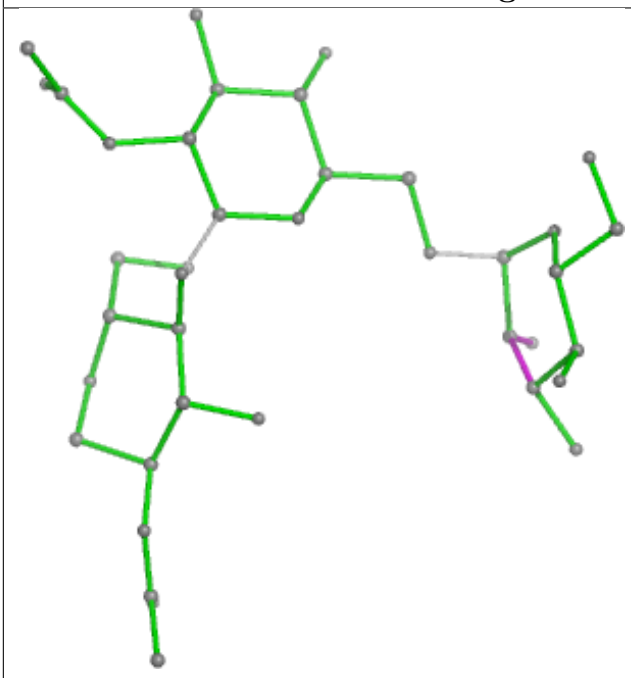


Torsions



Rings

Oligosaccharide Chain 6



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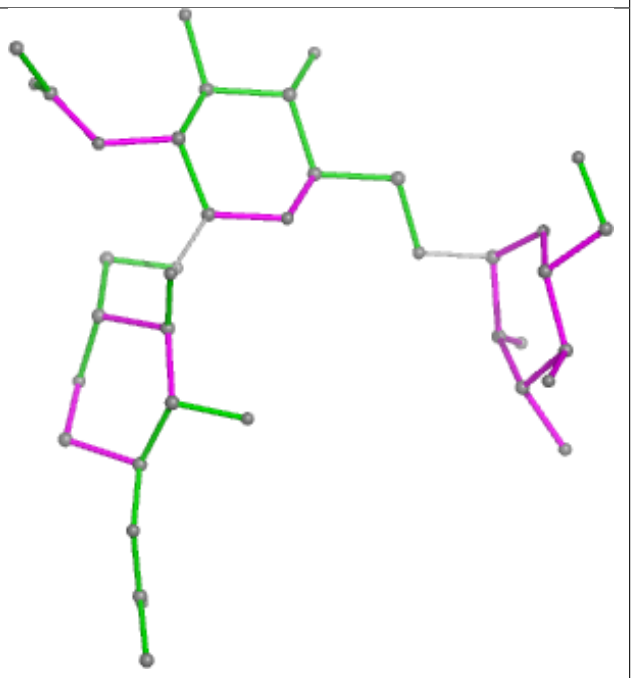
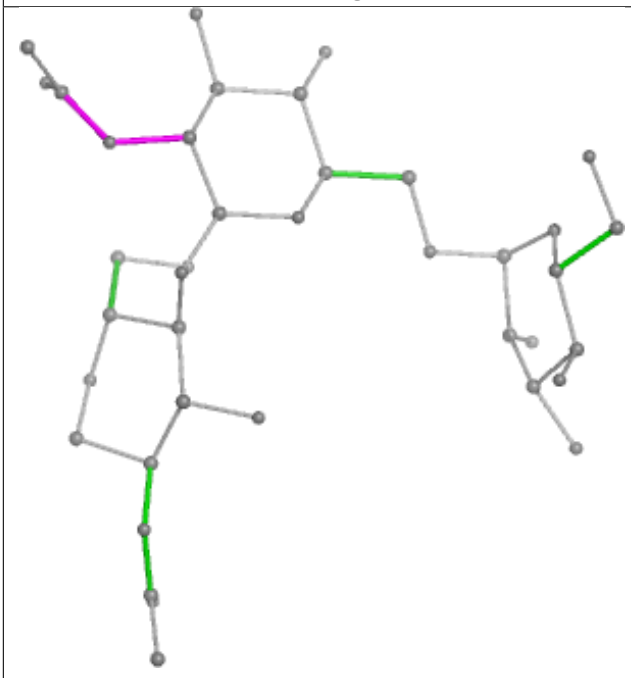


Bond angles



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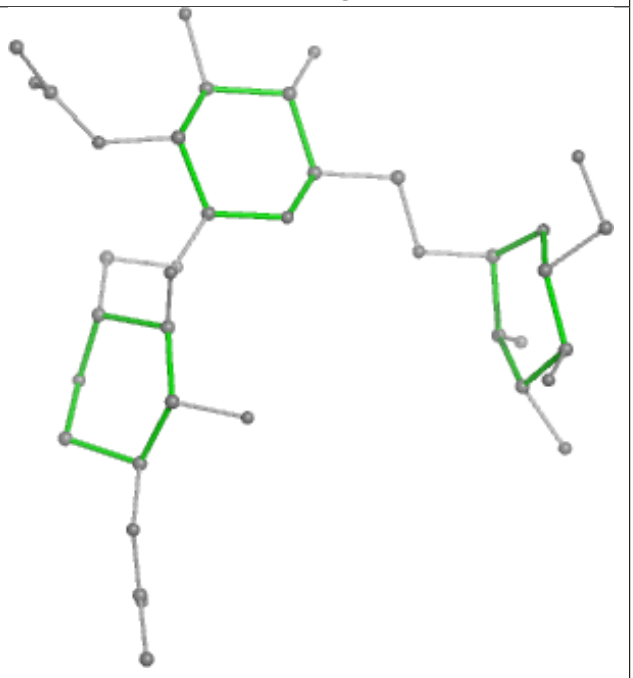
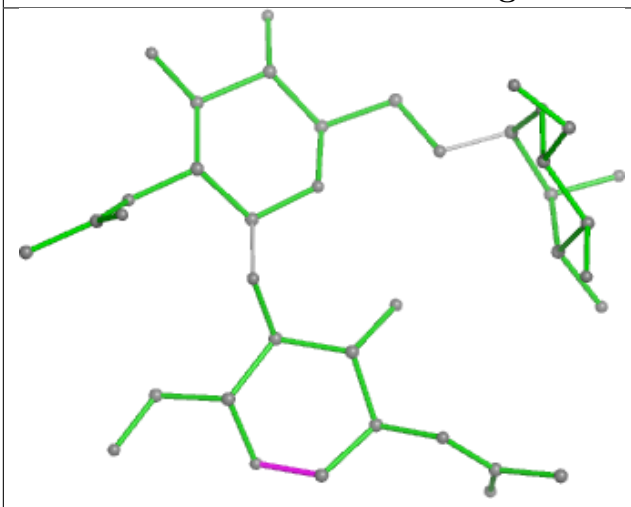


Rings

Oligosaccharide Chain 7



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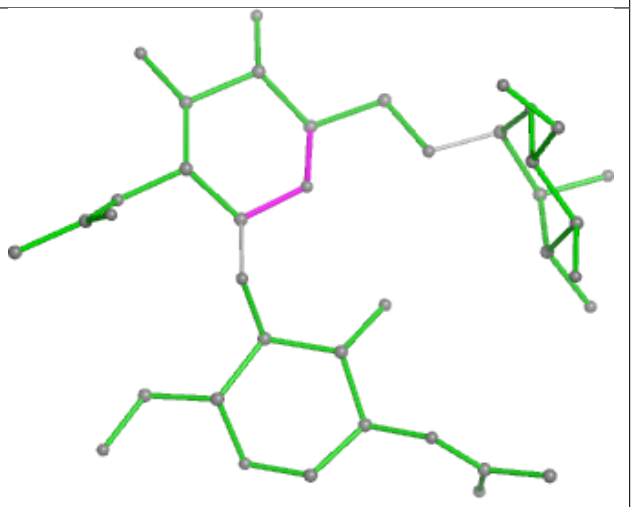
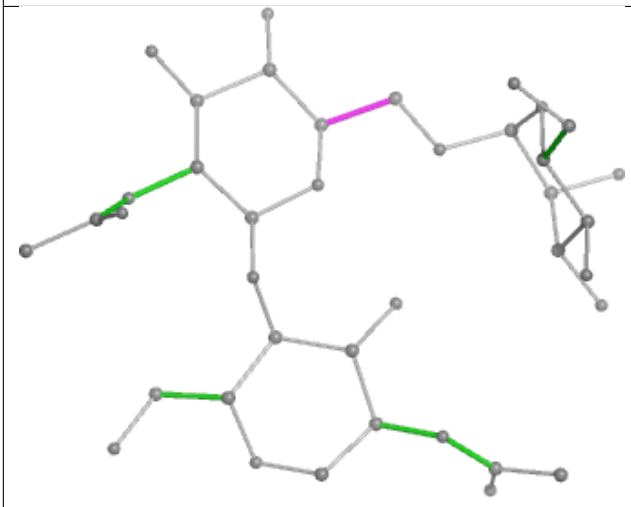


Bond angles



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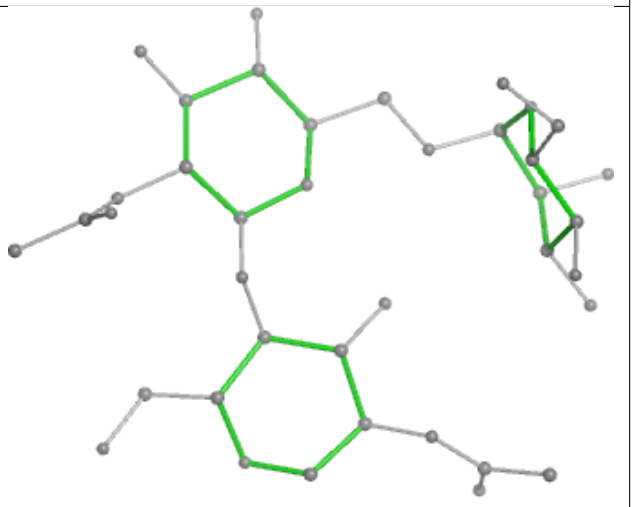
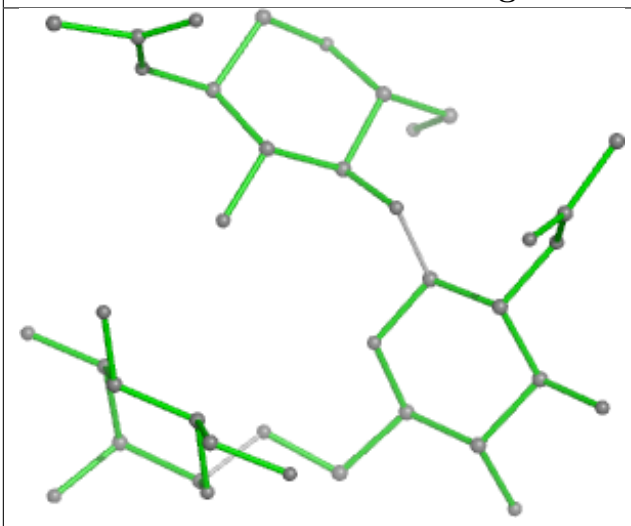
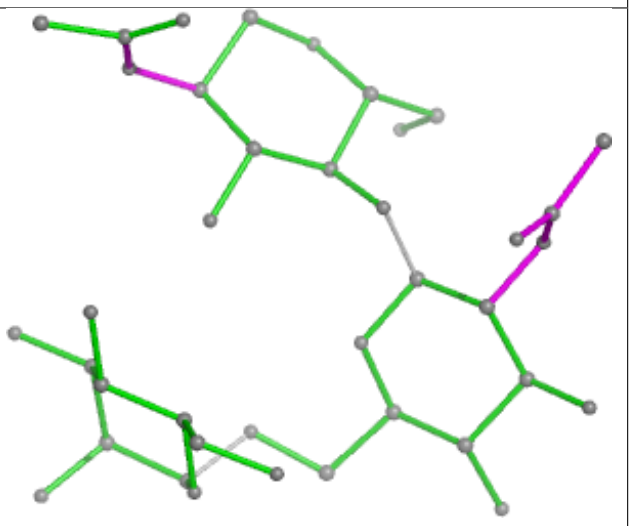


Rings

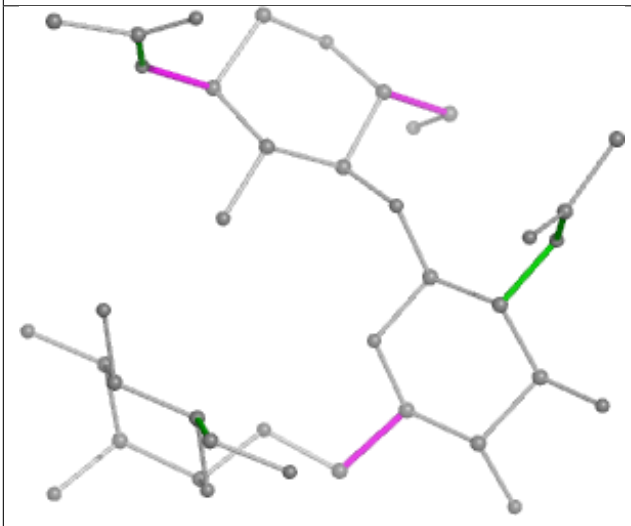
Oligosaccharide Chain 8



Bond lengths



Bond angles



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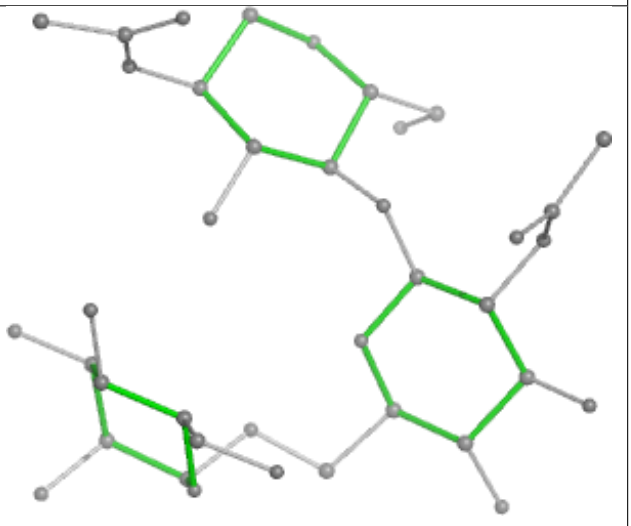
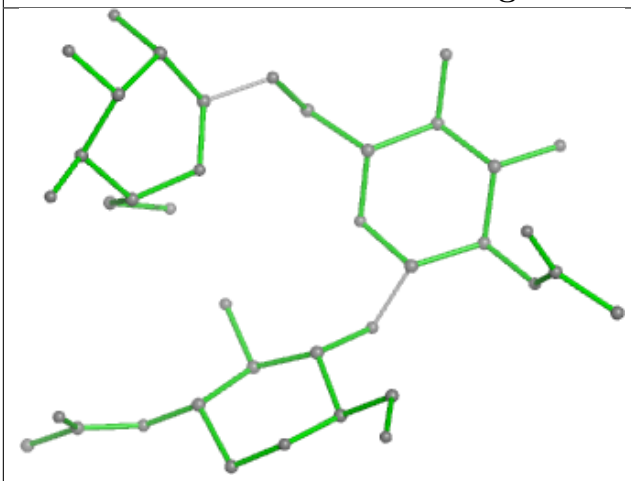


Rings

Oligosaccharide Chain 9



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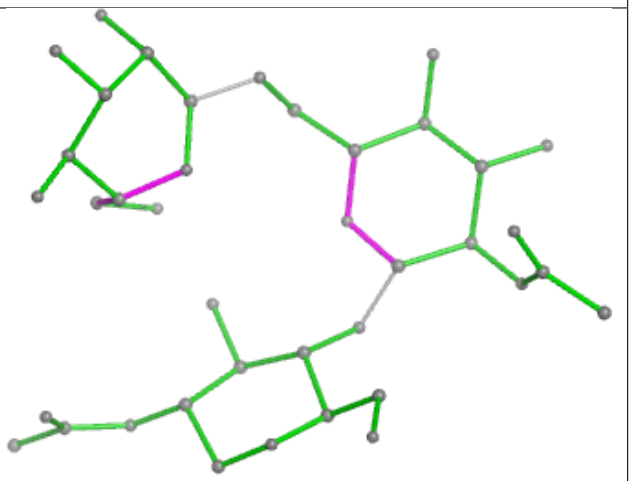
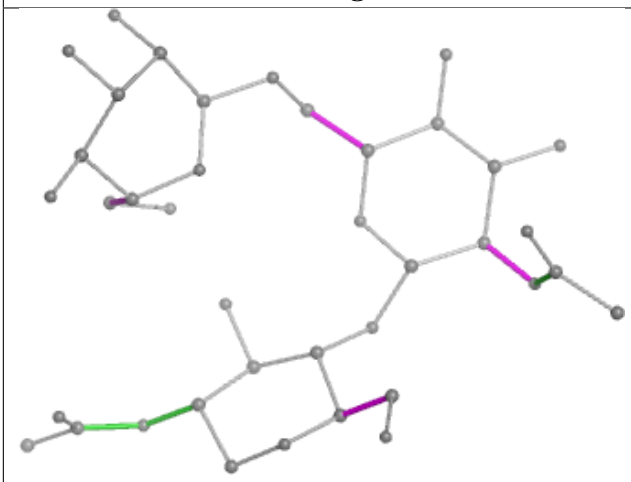


Bond angles



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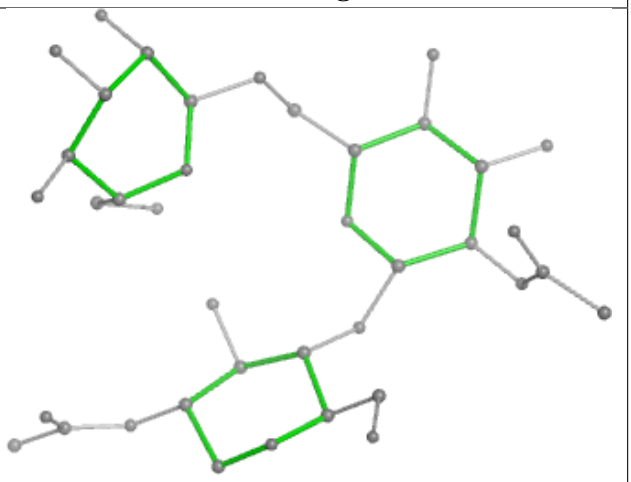
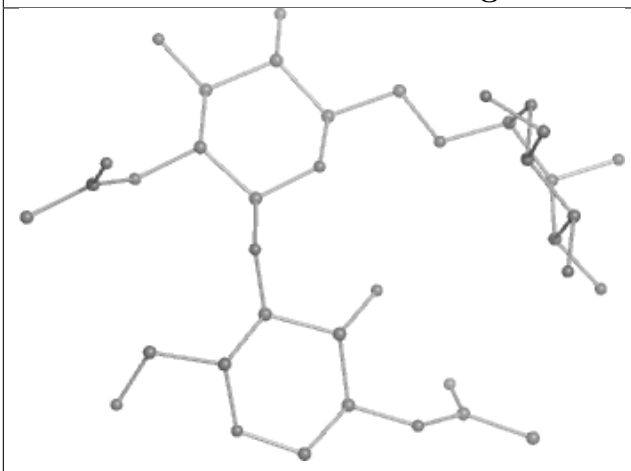


Rings

Oligosaccharide Chain AA



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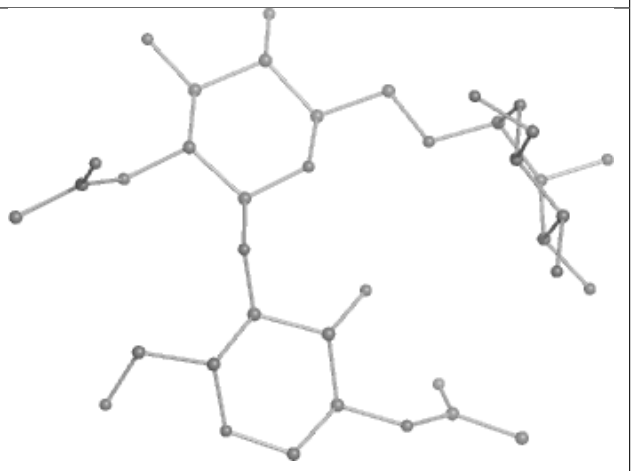
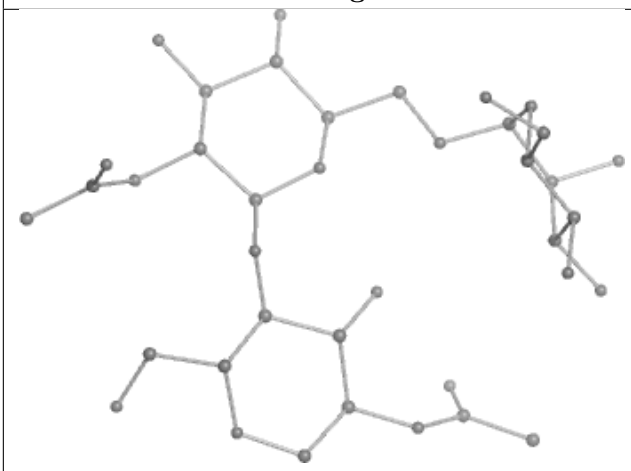


Bond angles



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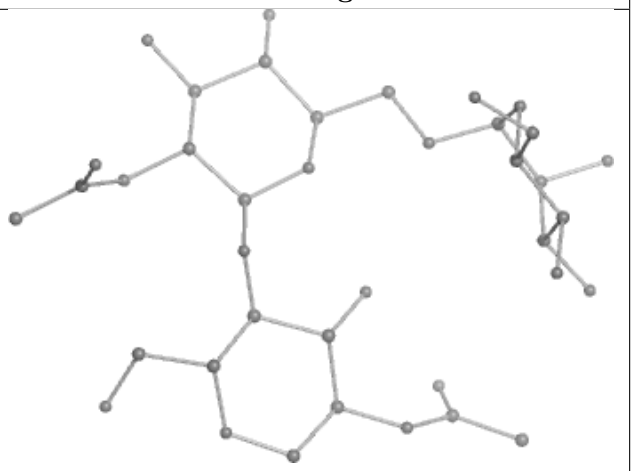
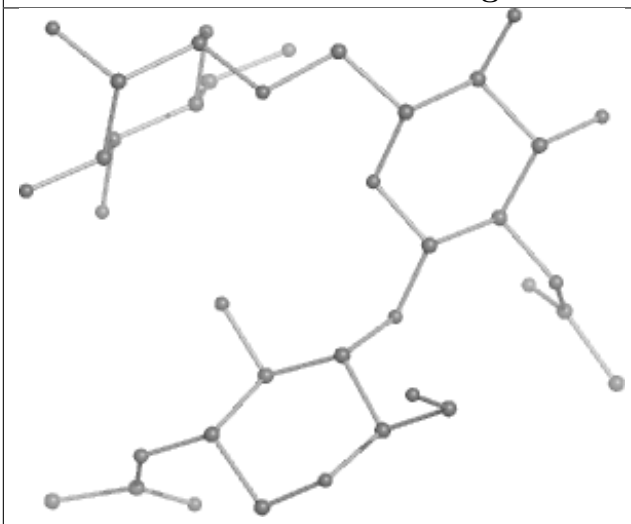
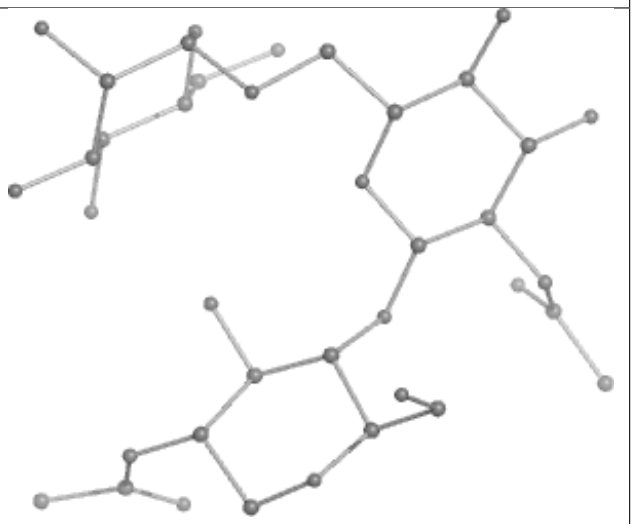


Rings

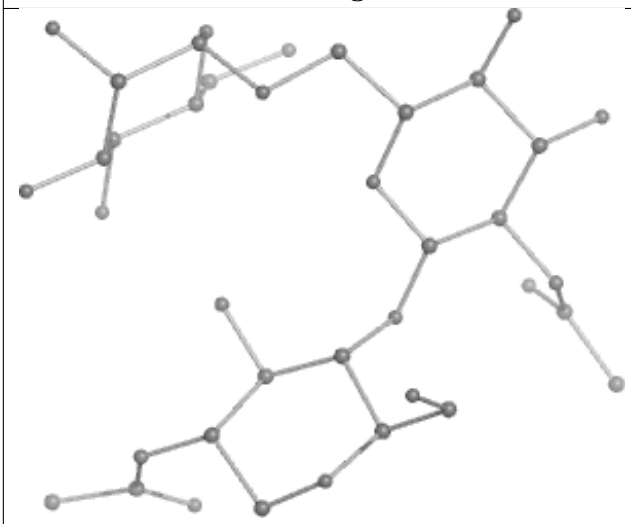
Oligosaccharide Chain BA



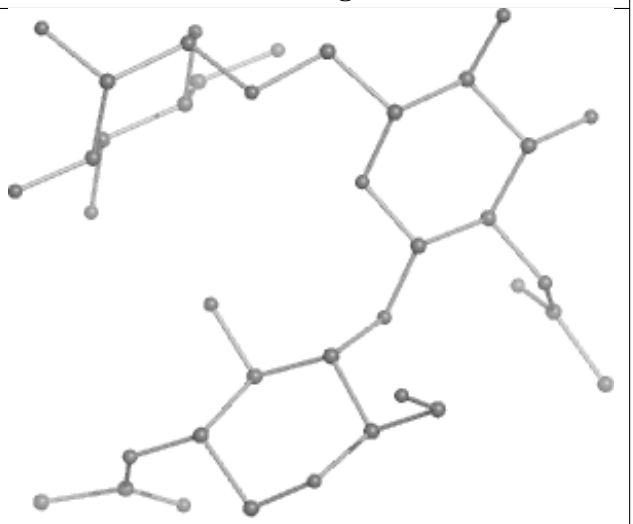
Bond lengths



Bond angles

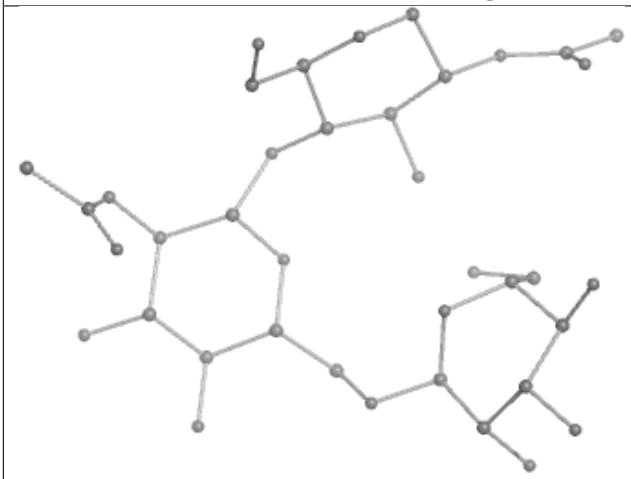


Torsions

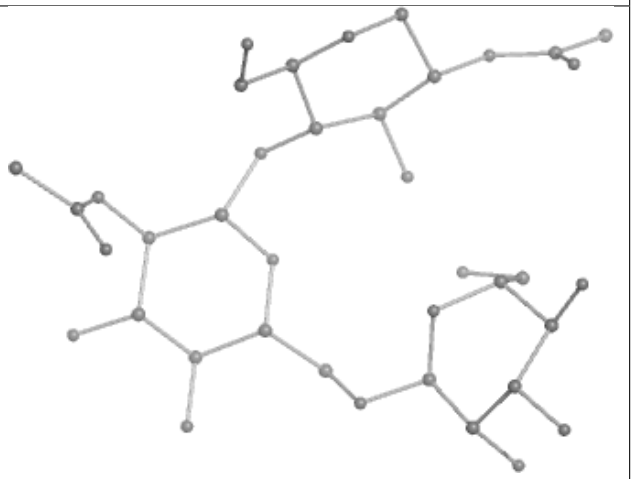


Rings

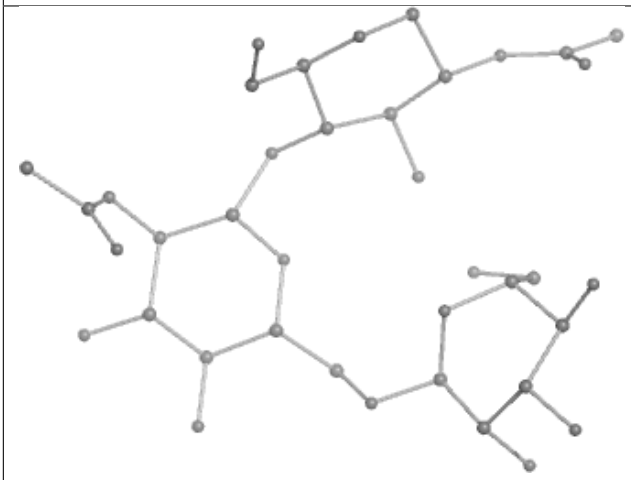
Oligosaccharide Chain CA



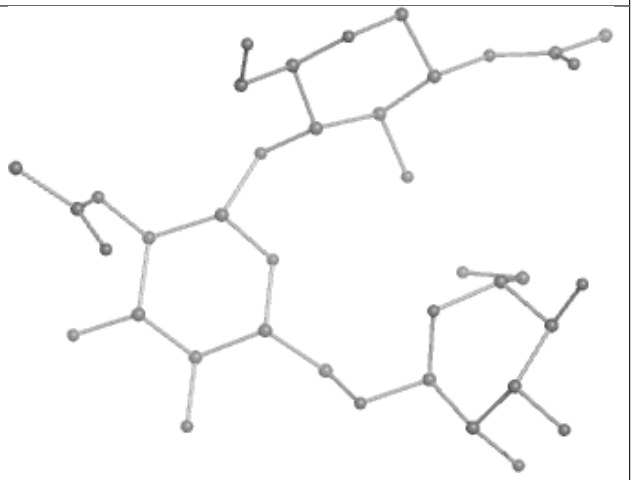
Bond lengths



Bond angles

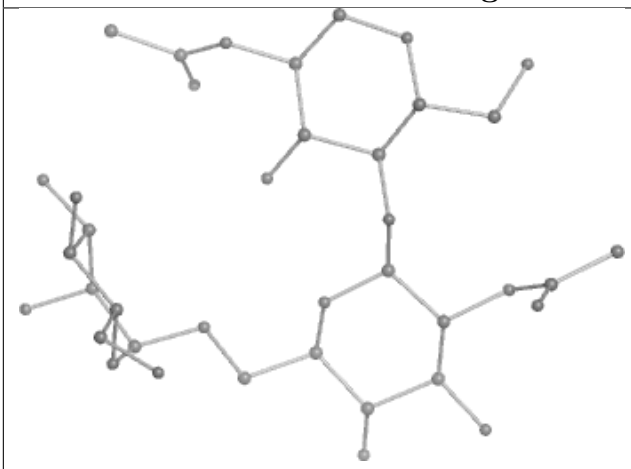


Torsions

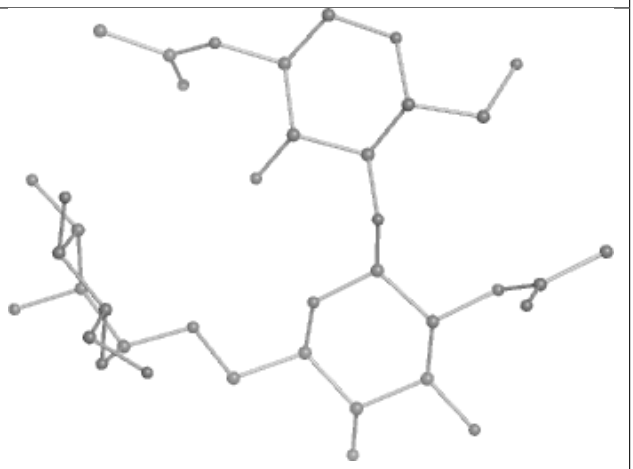


Rings

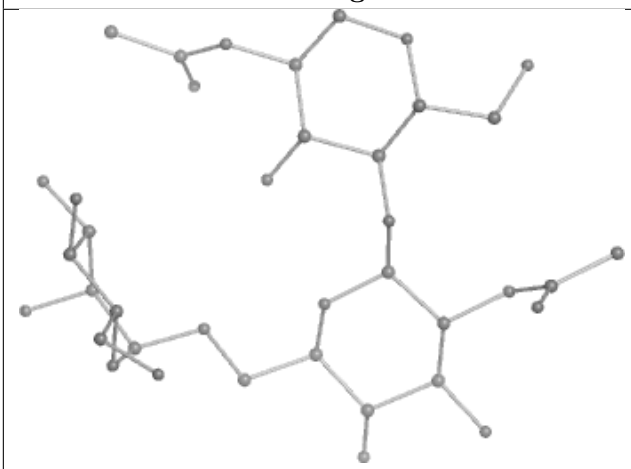
Oligosaccharide Chain DA



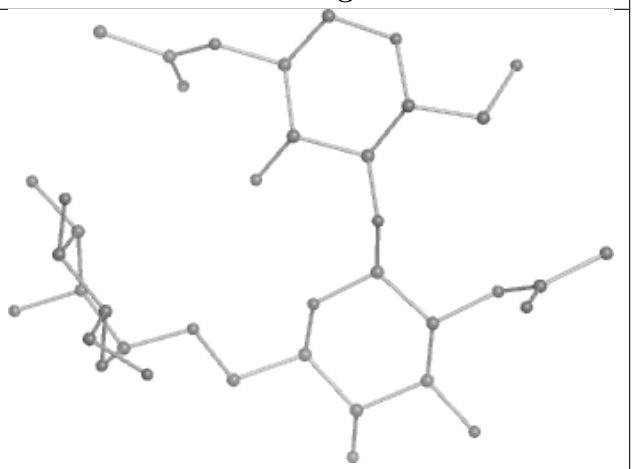
Bond lengths



Bond angles

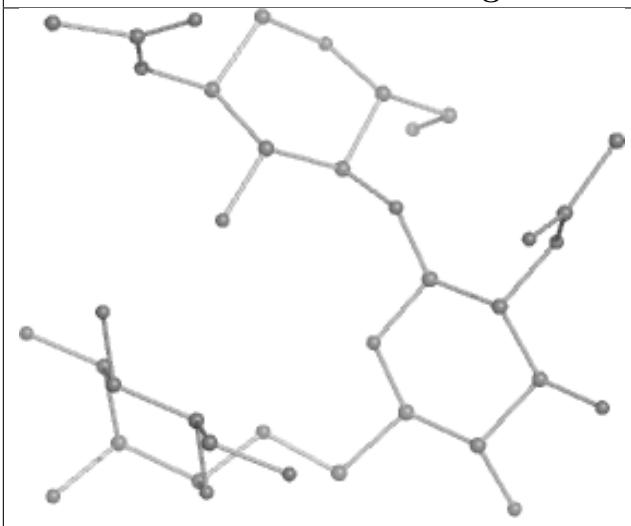


Torsions



Rings

Oligosaccharide Chain EA



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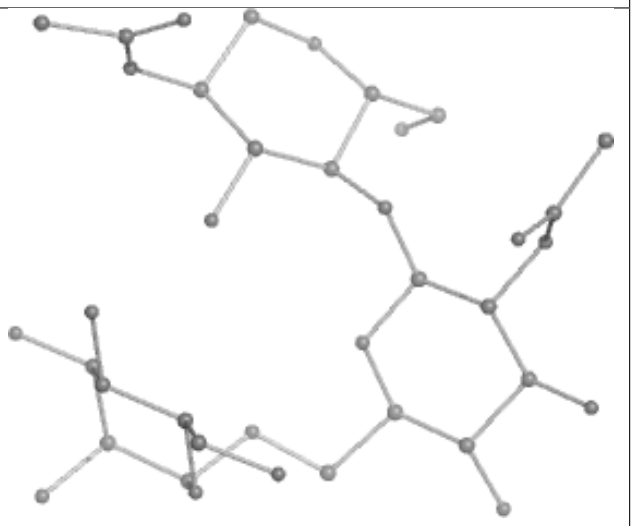
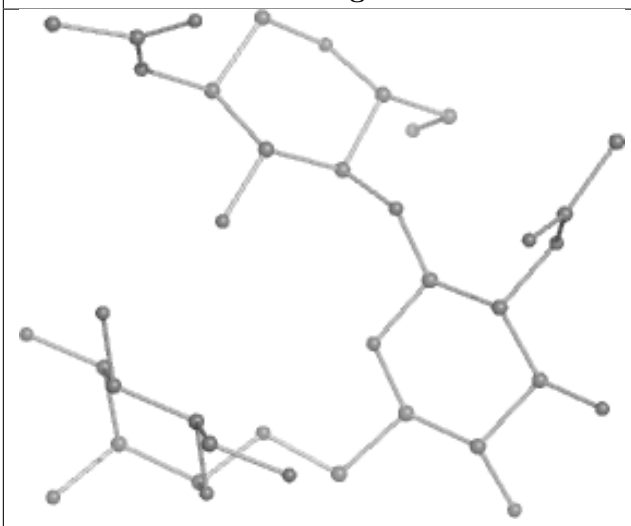


Bond angles



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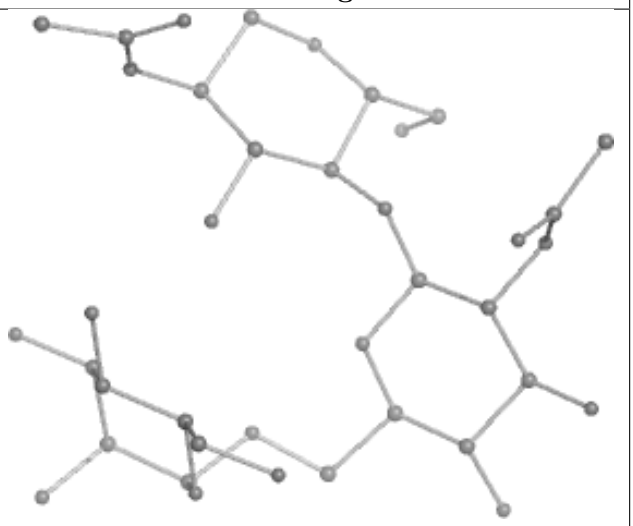
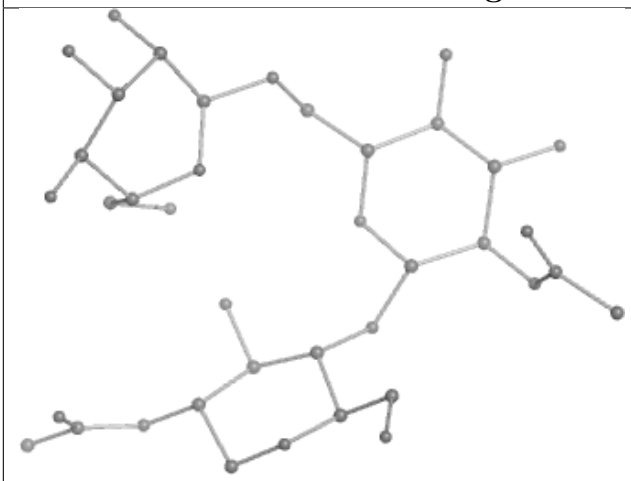


Rings

Oligosaccharide Chain FA



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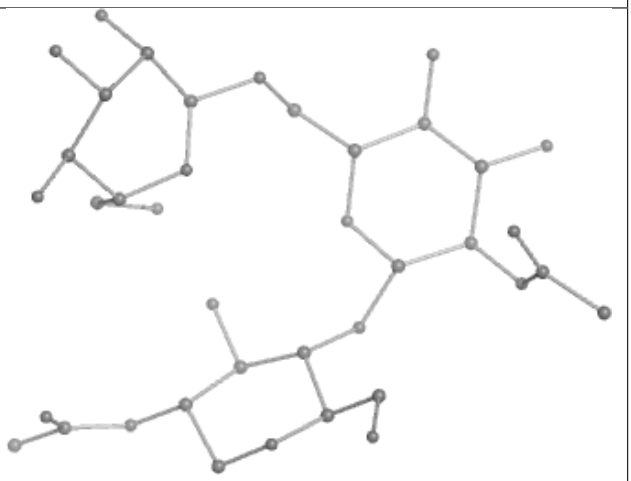
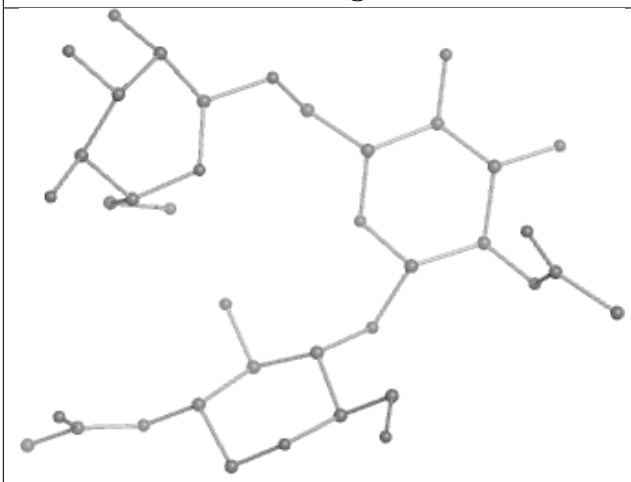


Bond angles



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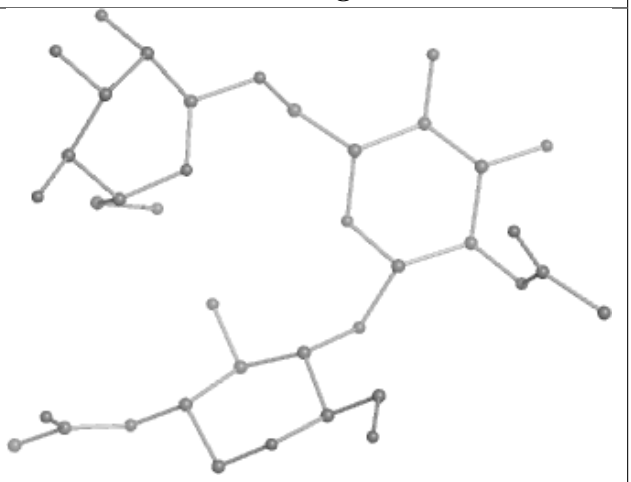
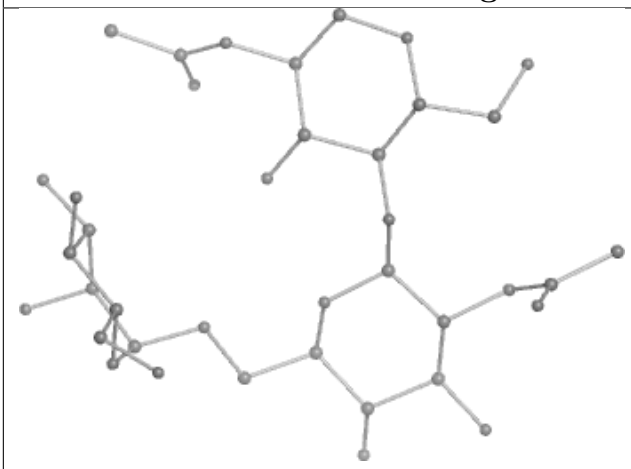


Rings

Oligosaccharide Chain GA



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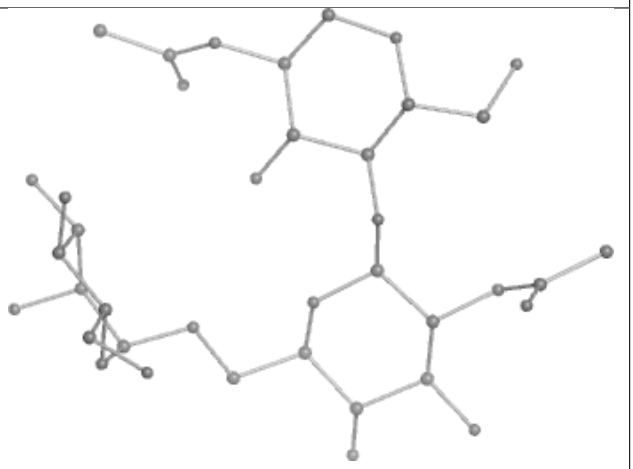
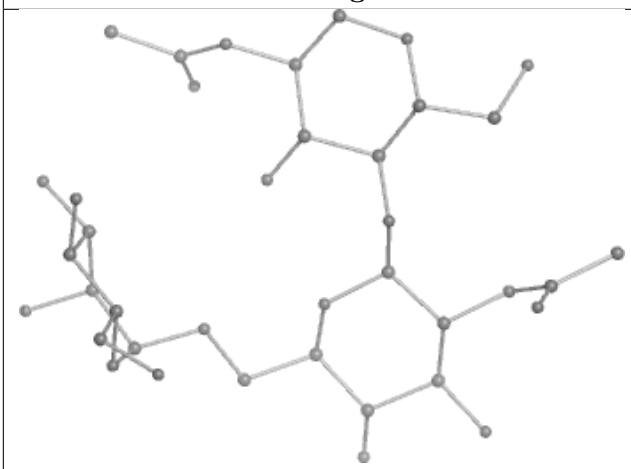
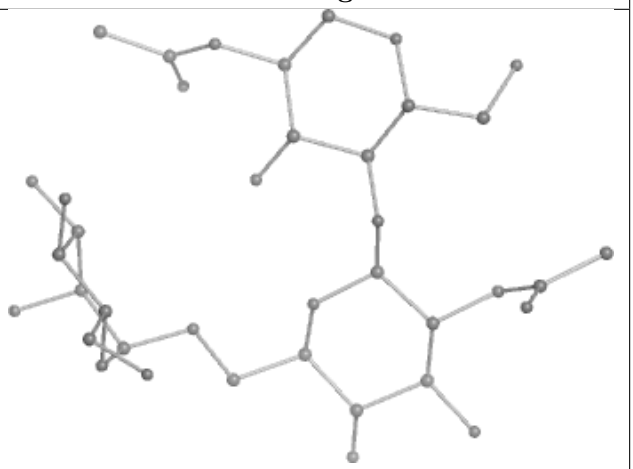


Bond angles

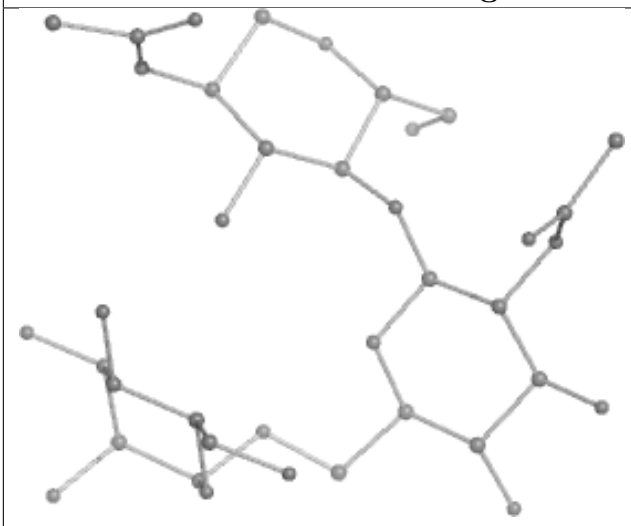


Torsions

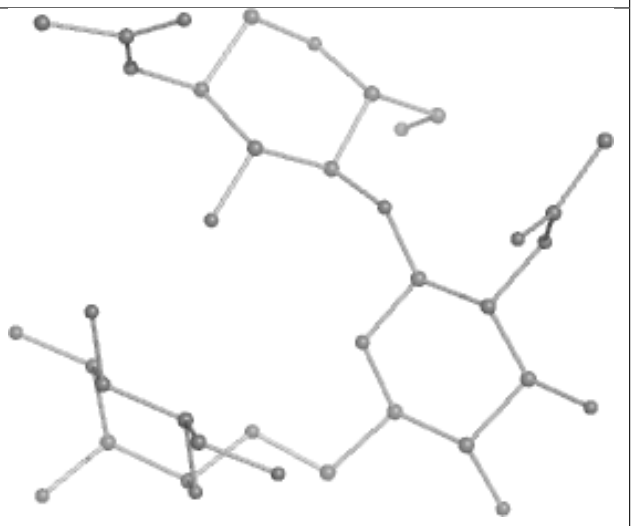


Rings

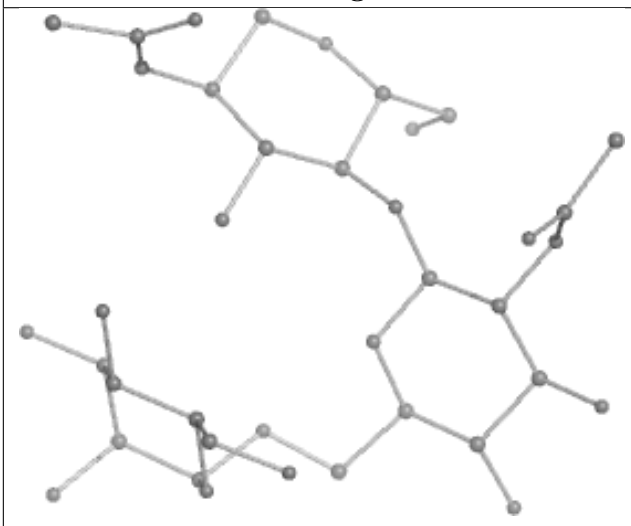
Oligosaccharide Chain HA



Bond lengths



Bond angles



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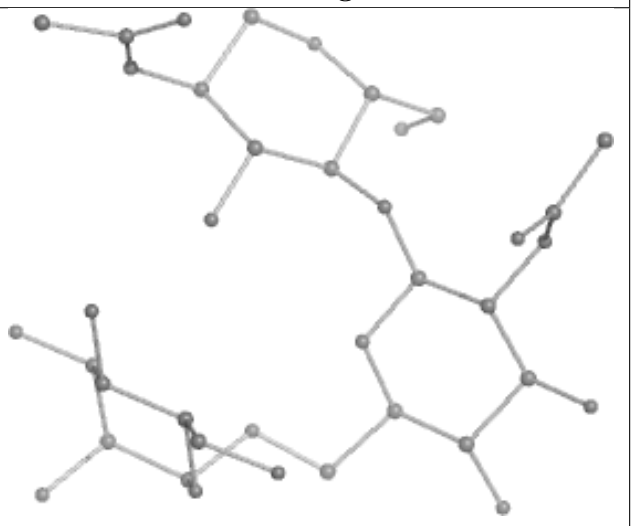
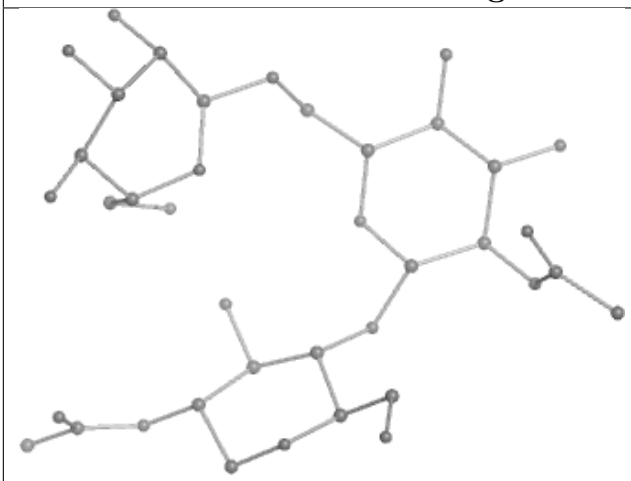


Rings

Oligosaccharide Chain IA



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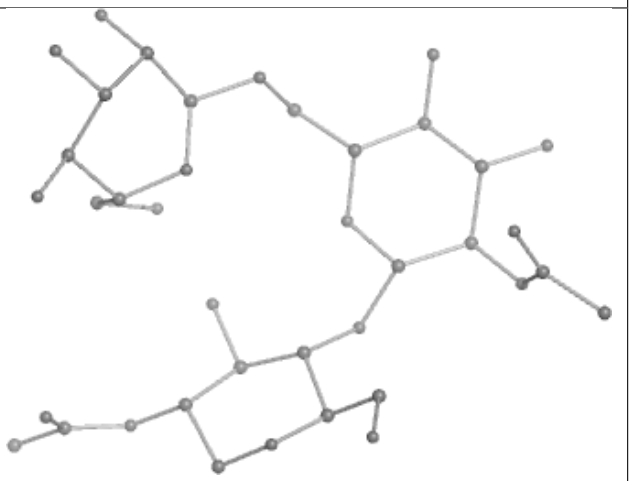
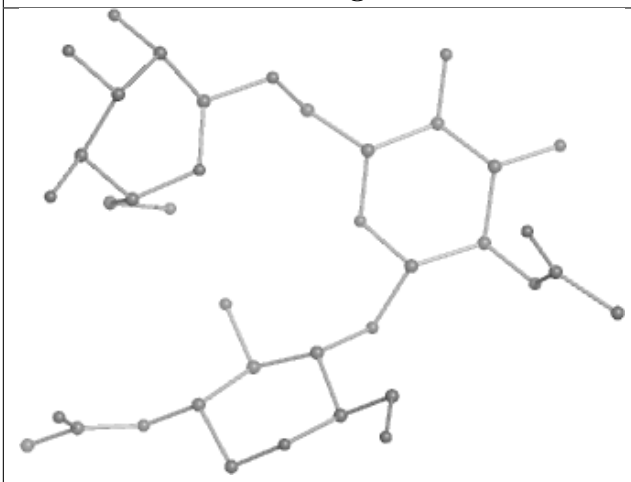


Bond angles



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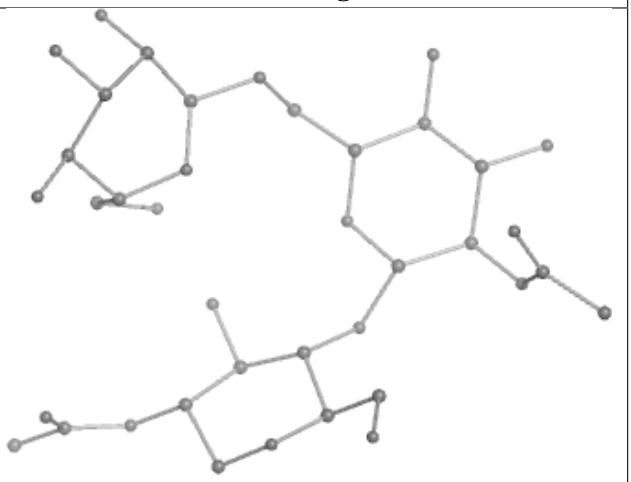
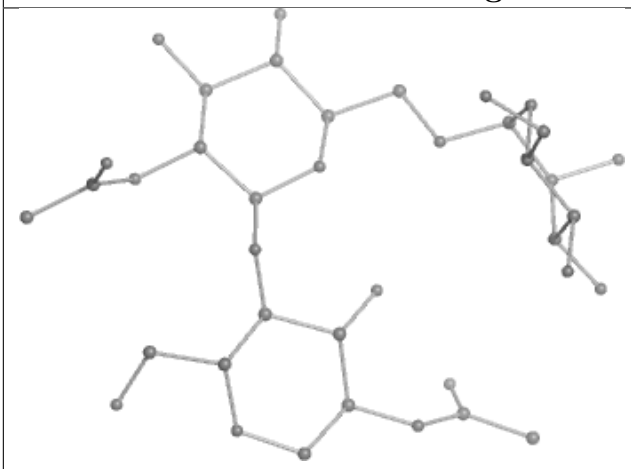


Rings

Oligosaccharide Chain JA



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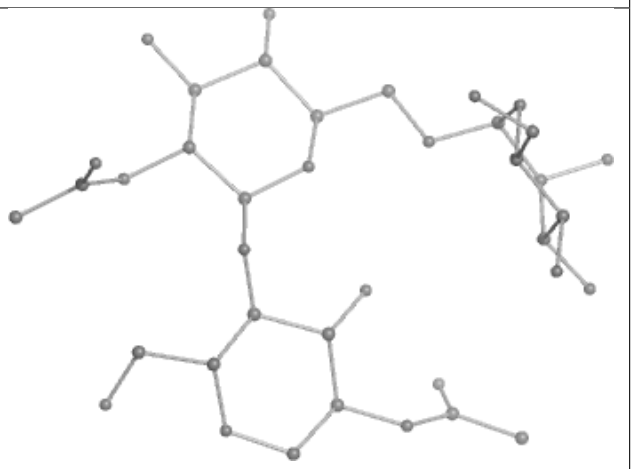
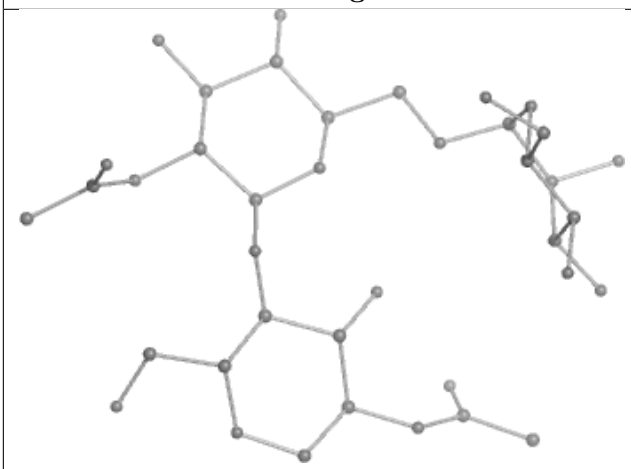


Bond angles



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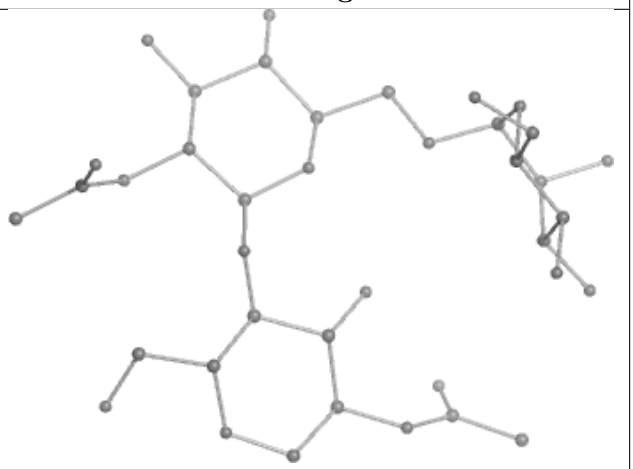
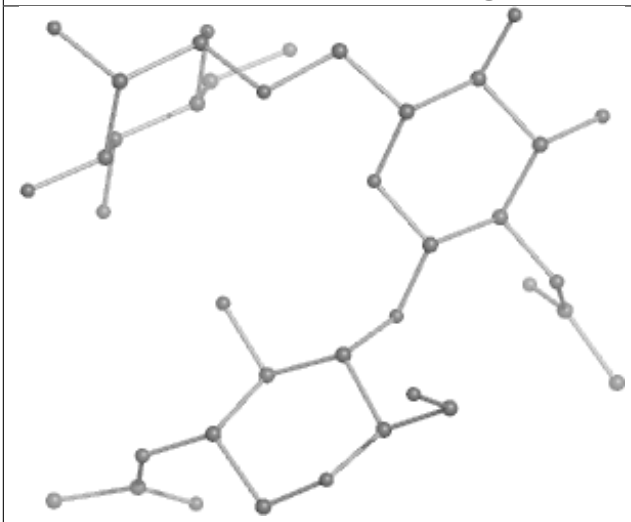


Rings

Oligosaccharide Chain KA



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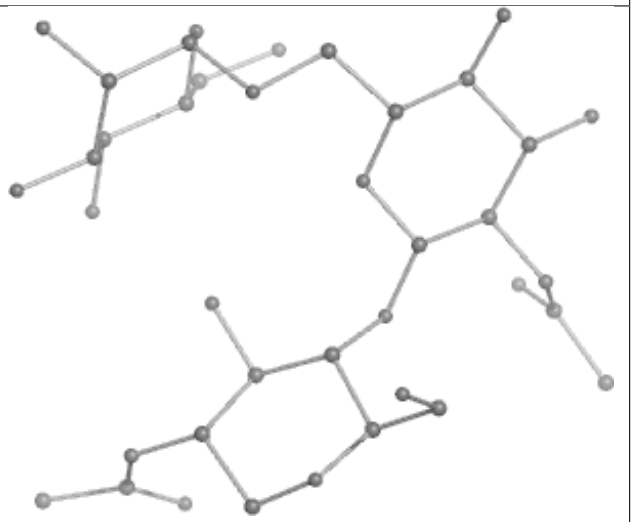
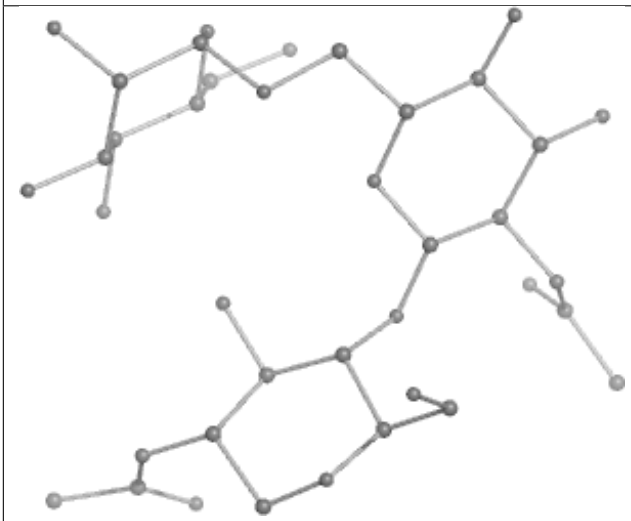


Bond angles



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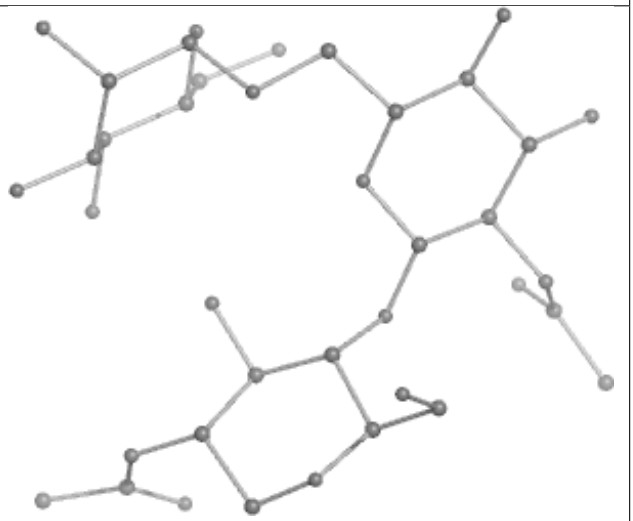
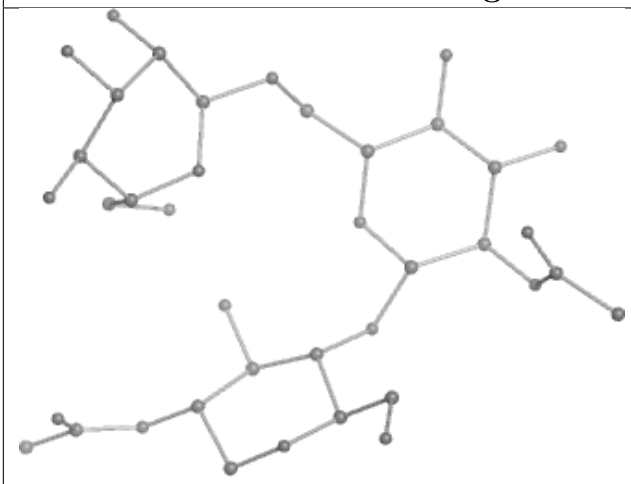


Rings

Oligosaccharide Chain LA



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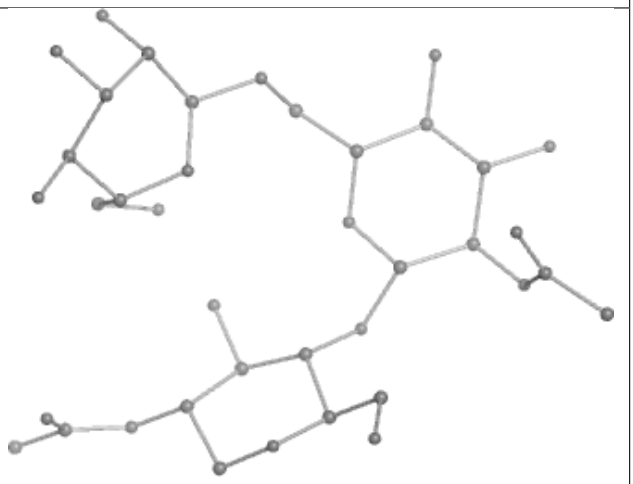
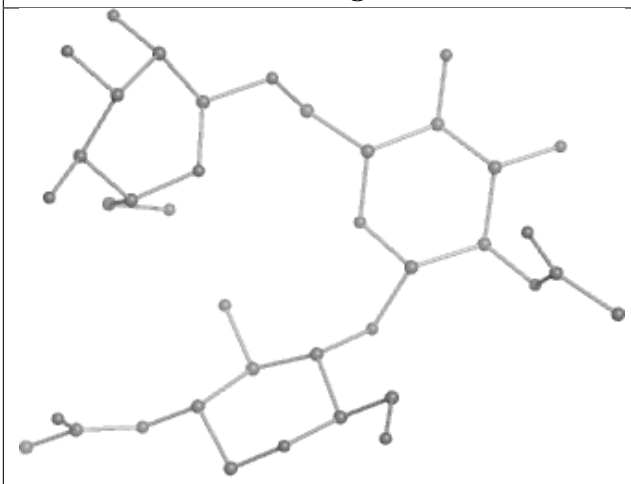
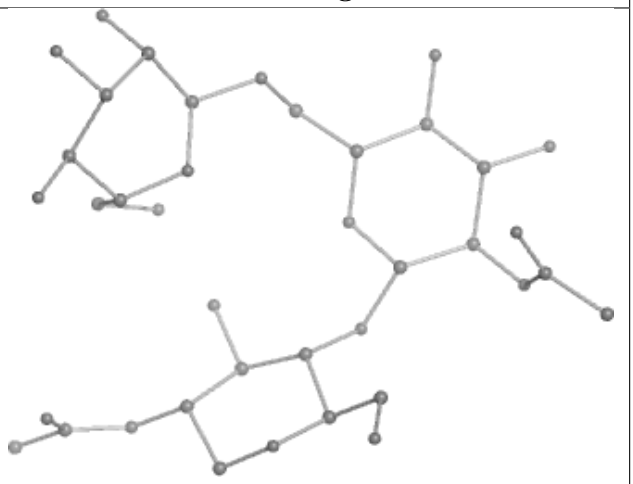


Bond angles

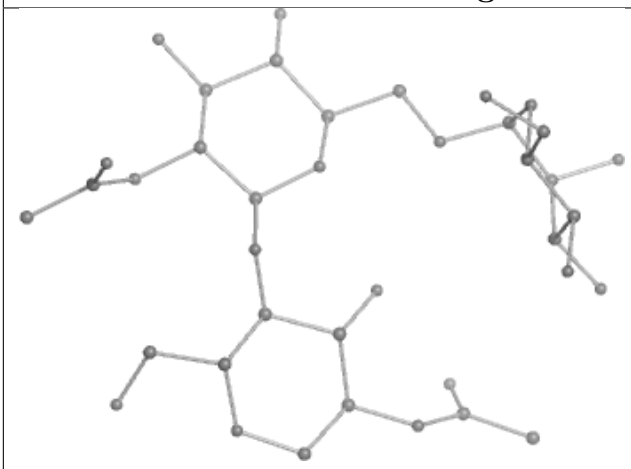


Torsions



Rings

Oligosaccharide Chain MA



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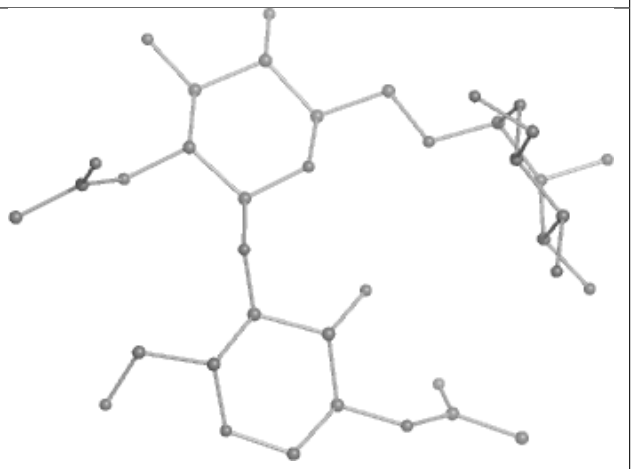
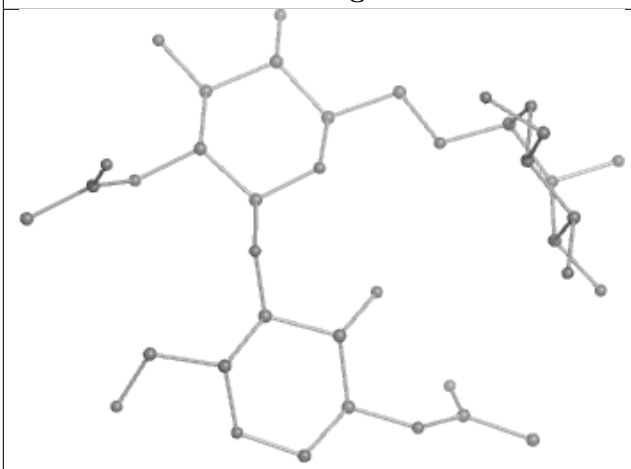
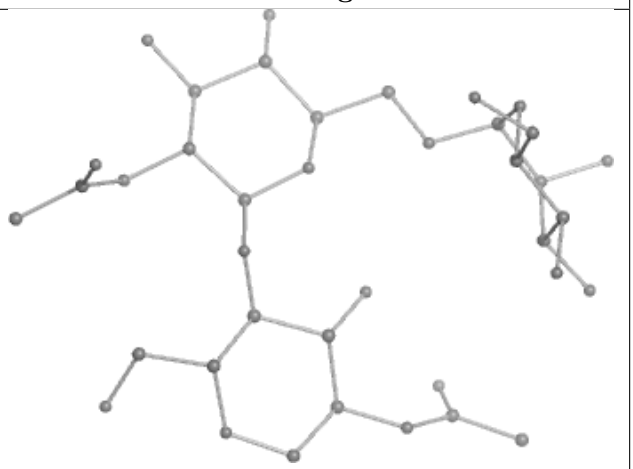


Bond angles

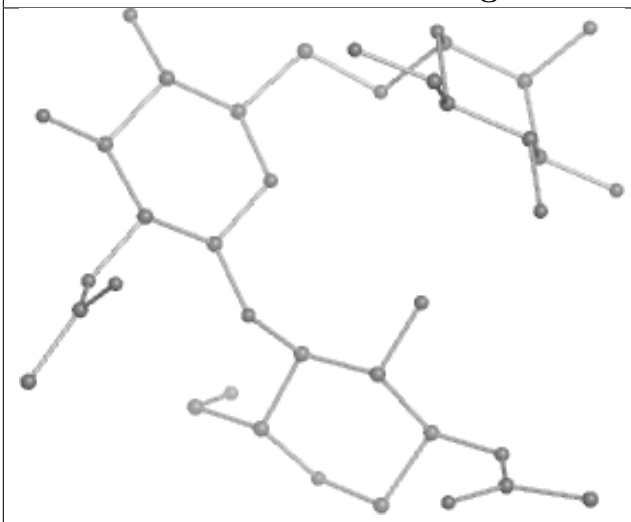


Torsions



Rings

Oligosaccharide Chain NA



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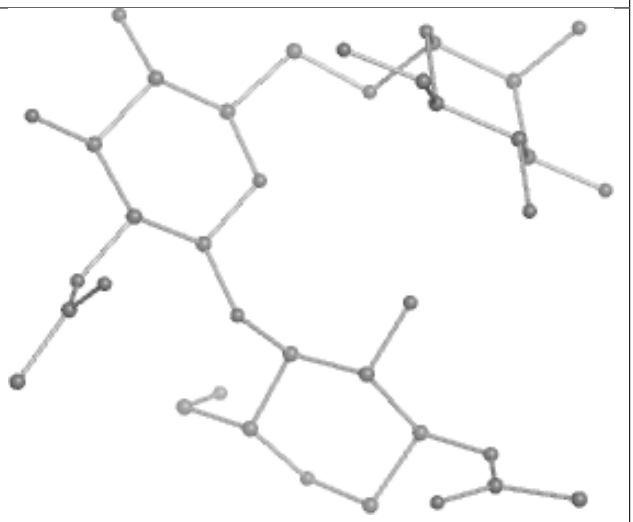
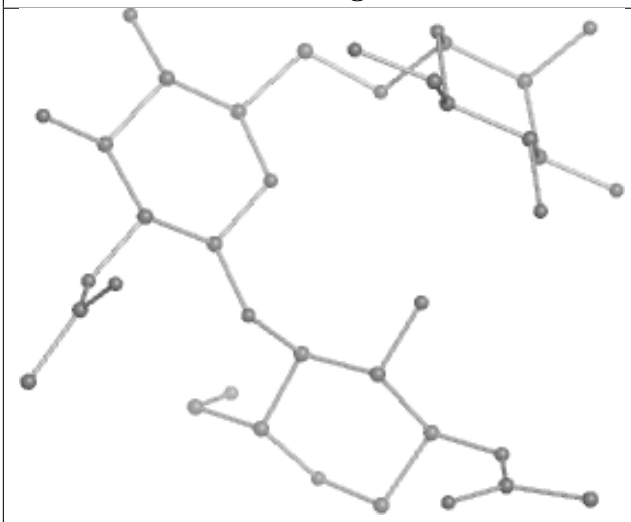
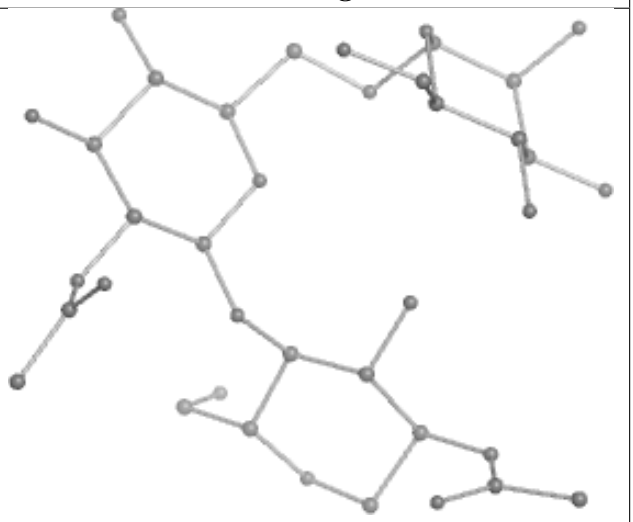


Bond angles

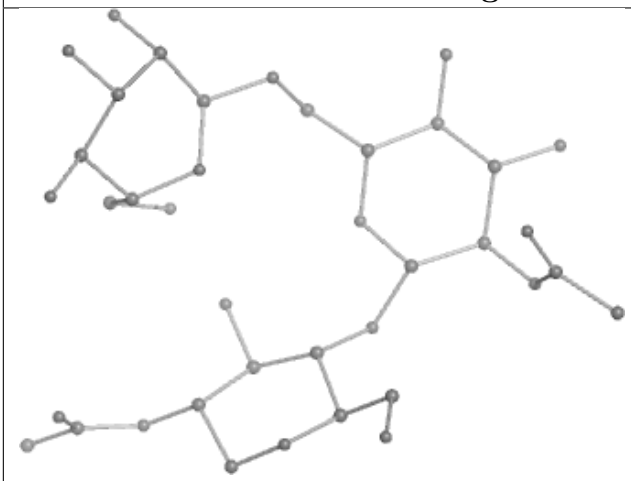


Torsions



Rings

Oligosaccharide Chain OA



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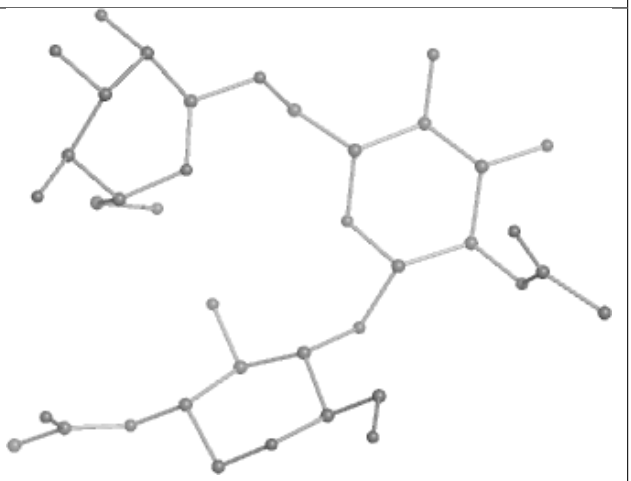
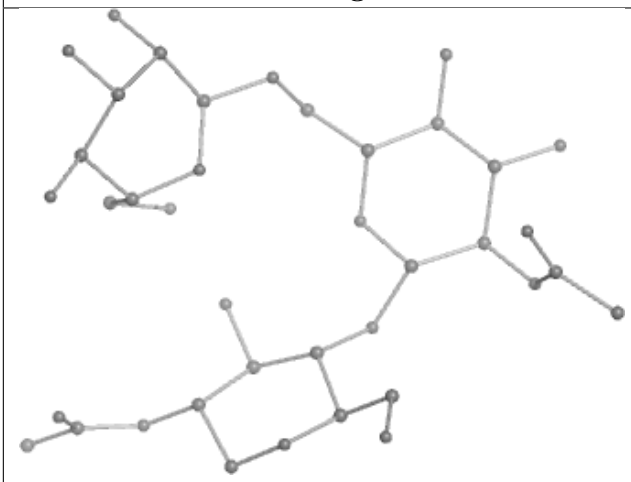
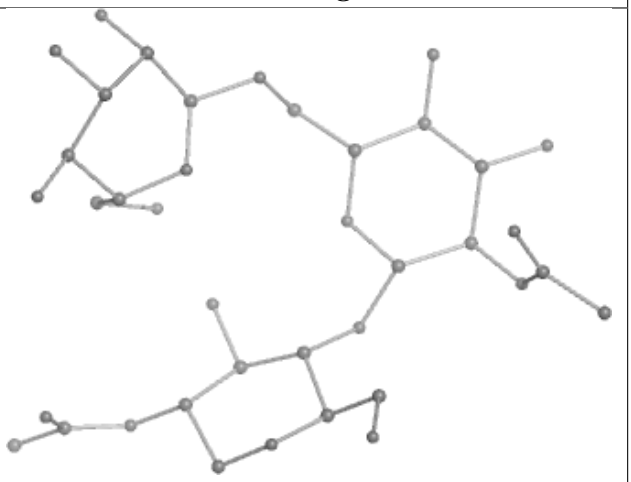


Bond angles

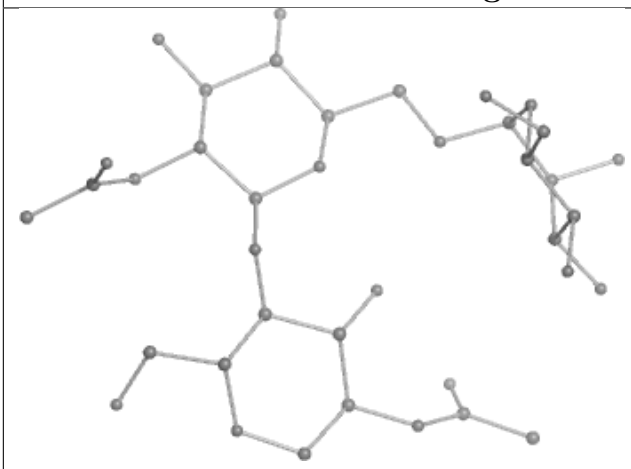


Torsions

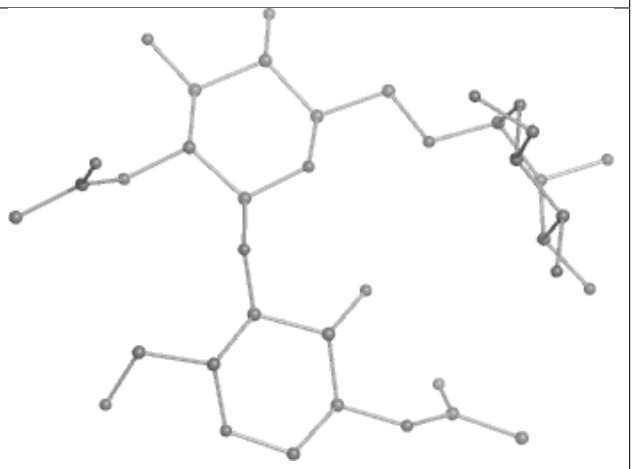


Rings

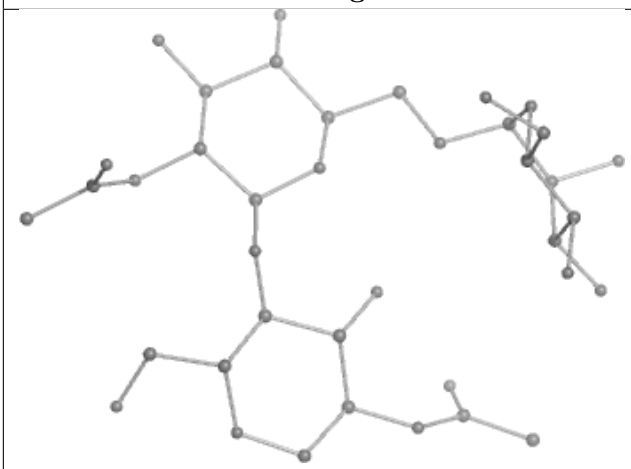
Oligosaccharide Chain PA



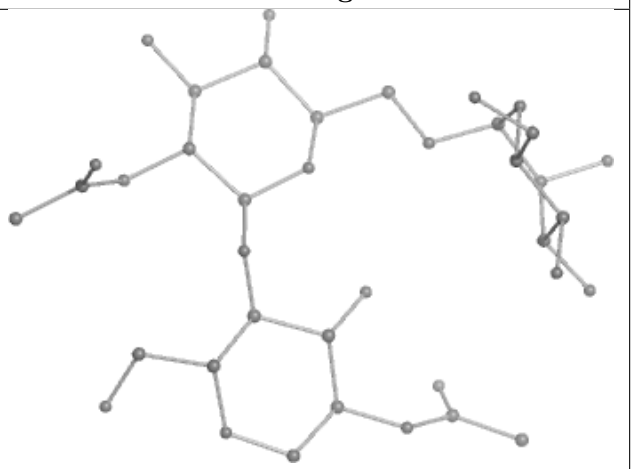
Bond lengths



Bond angles

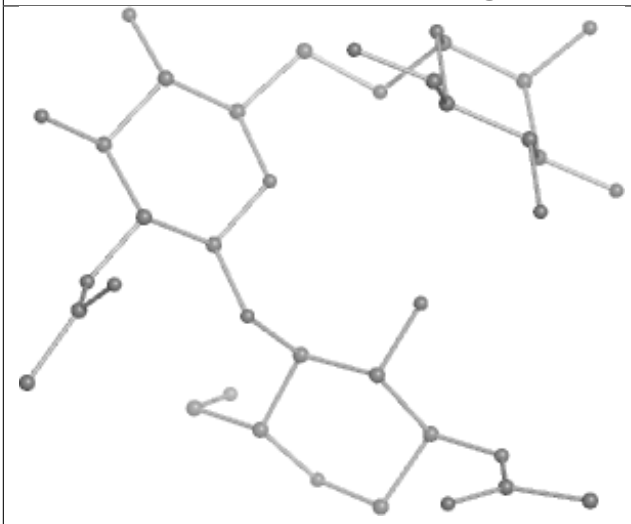


Torsions

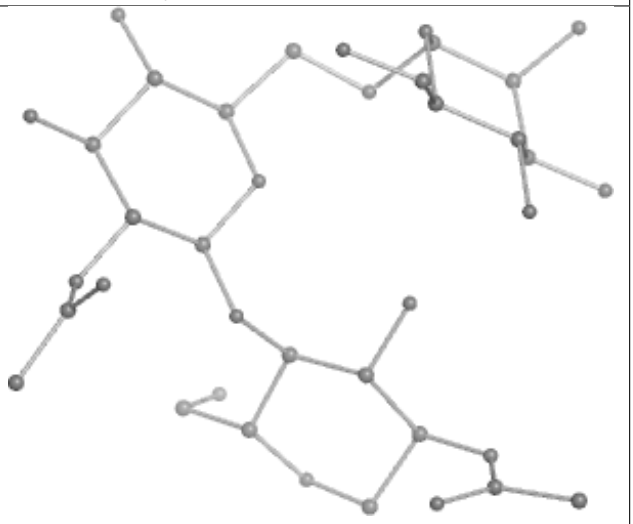


Rings

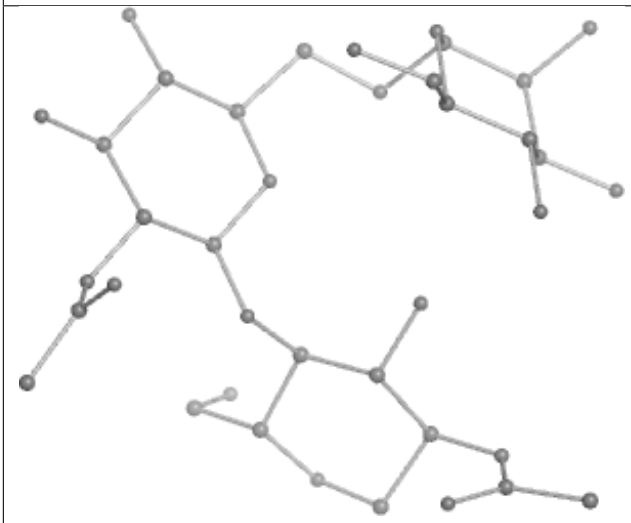
Oligosaccharide Chain QA



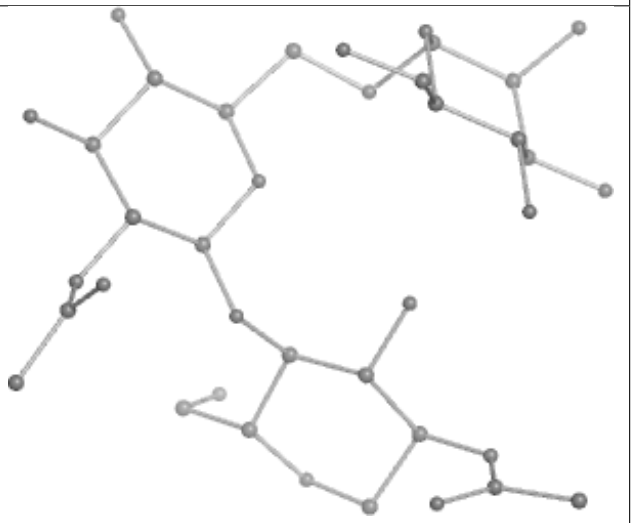
Bond lengths



Bond angles

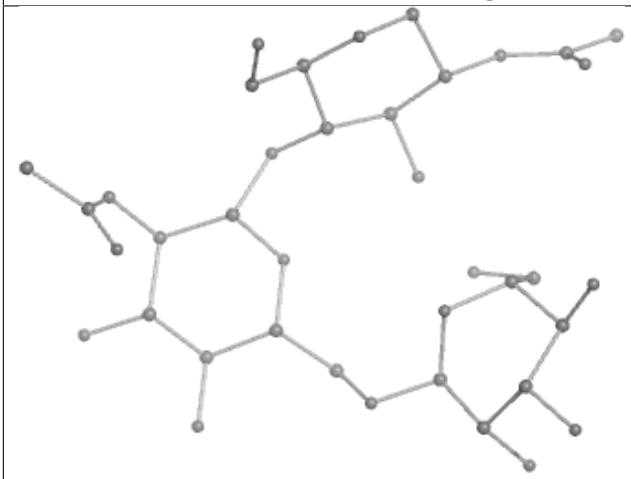


Torsions

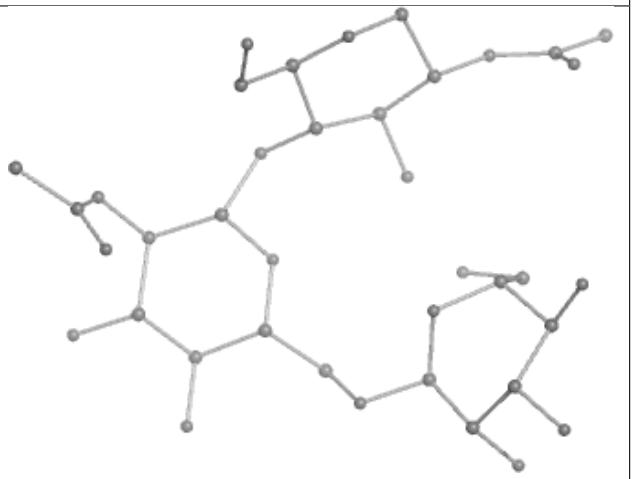


Rings

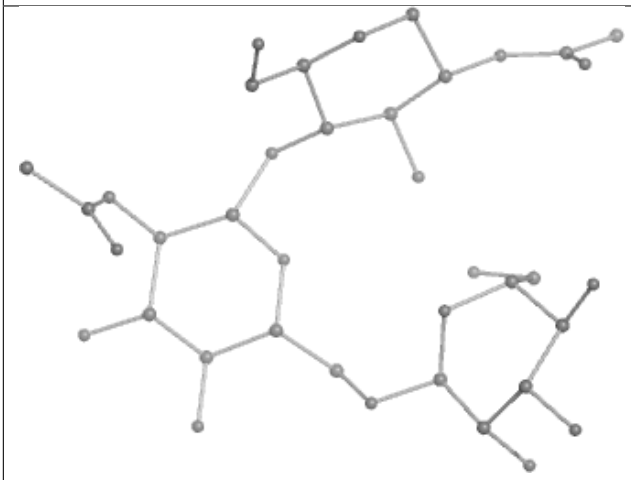
Oligosaccharide Chain RA



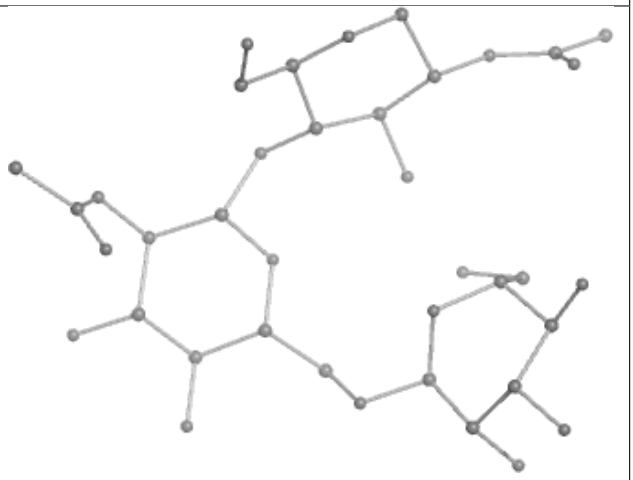
Bond lengths



Bond angles

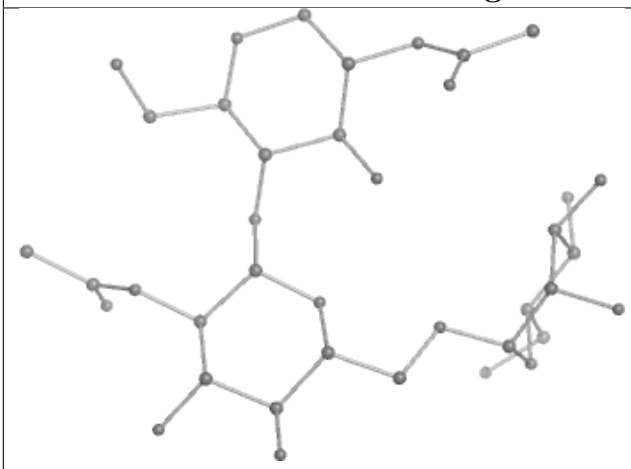


Torsions

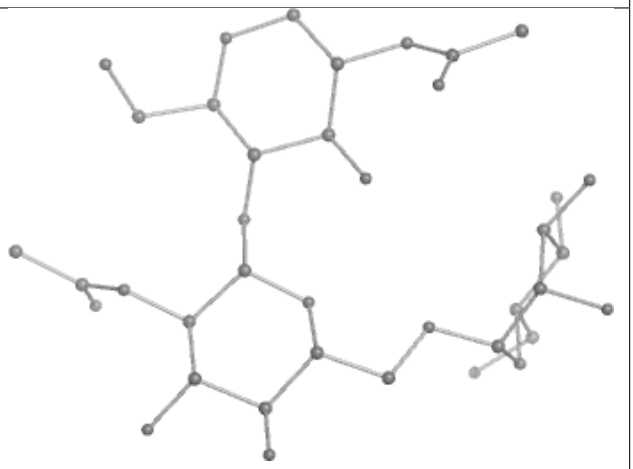


Rings

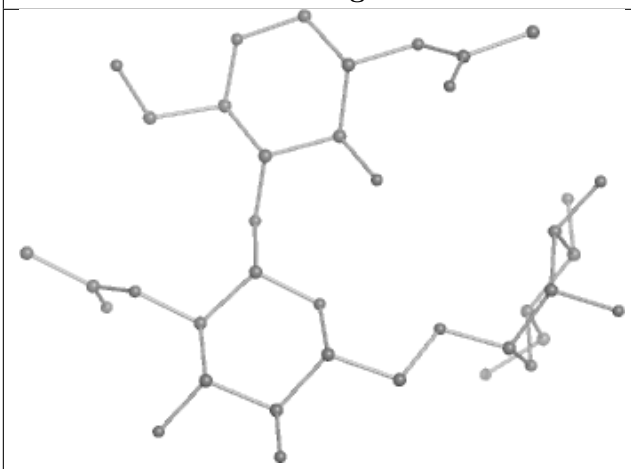
Oligosaccharide Chain SA



Bond lengths



Bond angles



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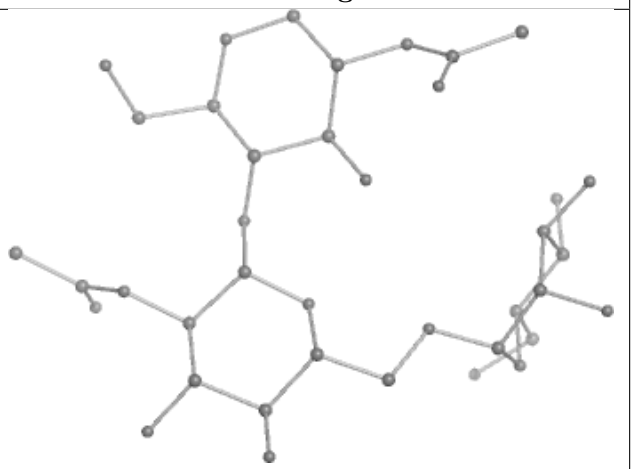
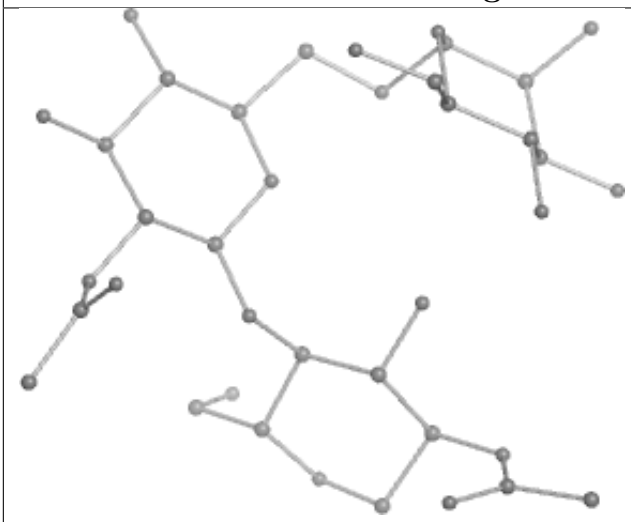


Rings

Oligosaccharide Chain TA



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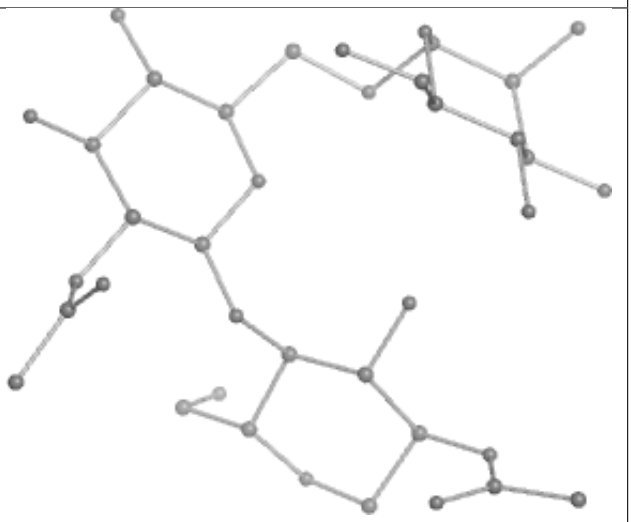
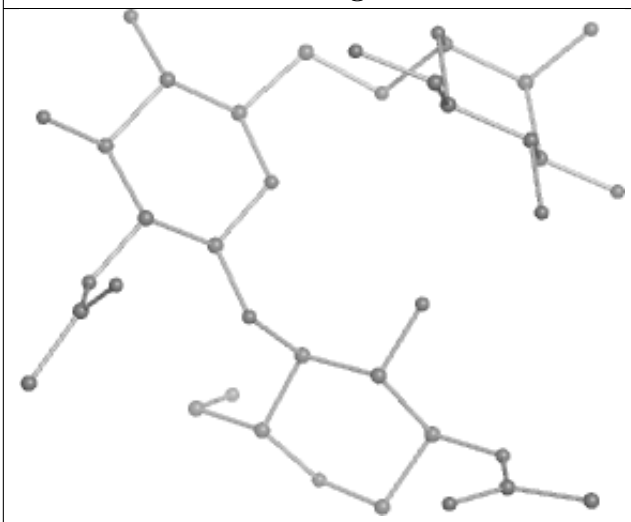


Bond angles



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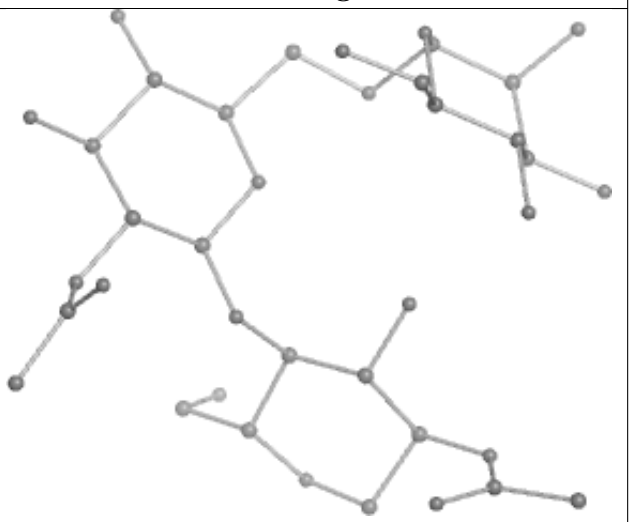
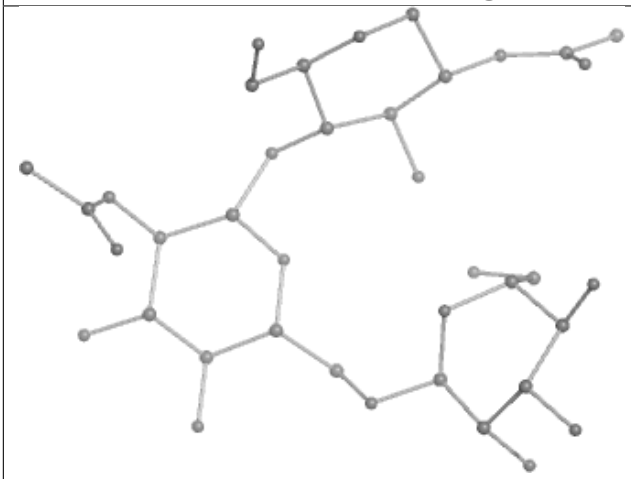


Rings

Oligosaccharide Chain UA



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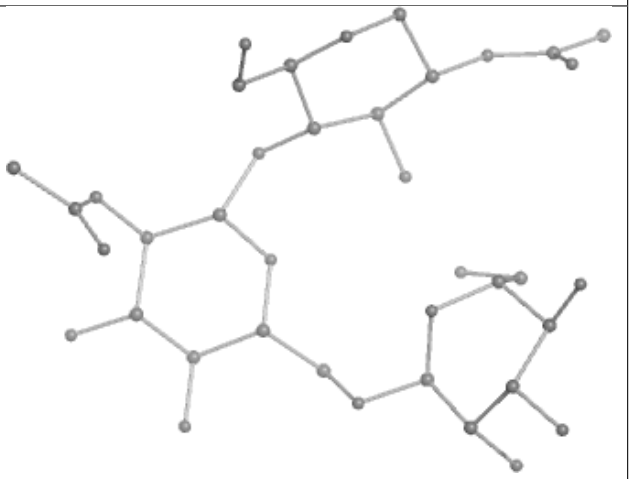
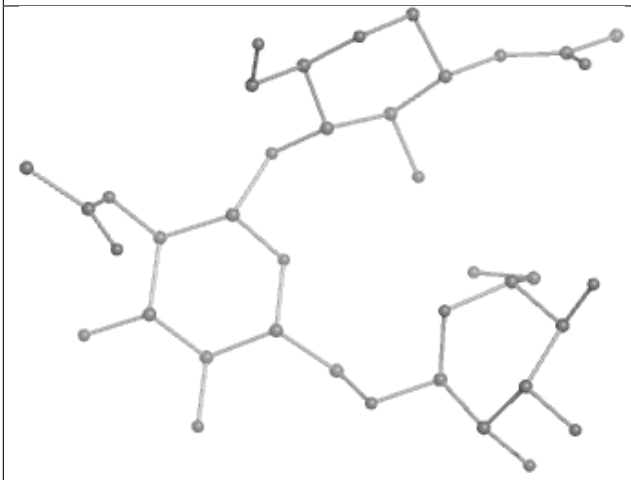


Bond angles



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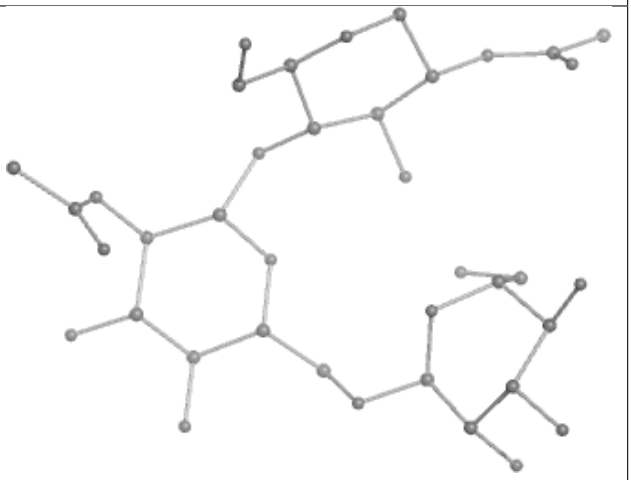
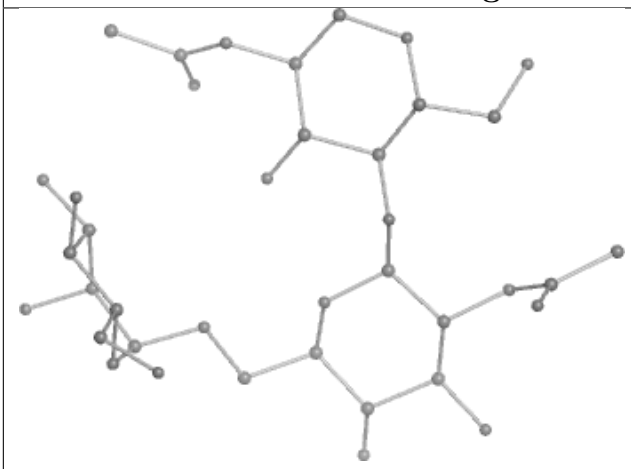


Rings

Oligosaccharide Chain VA



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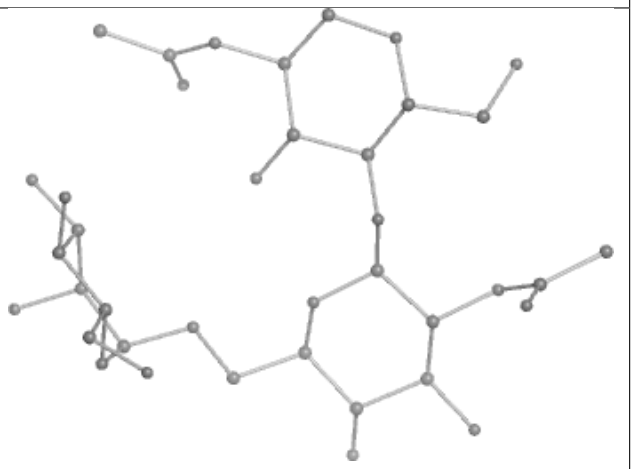
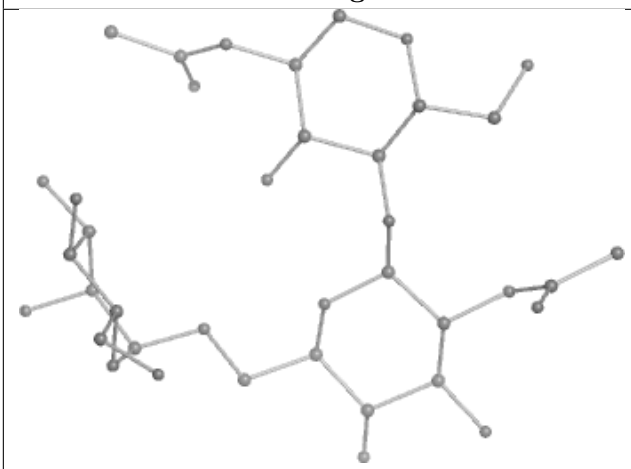


Bond angles



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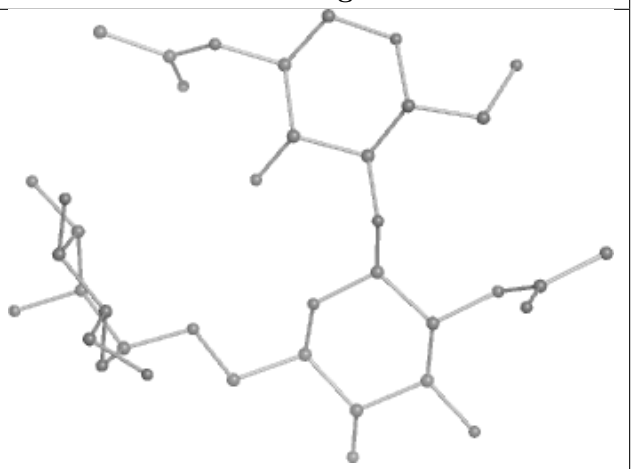
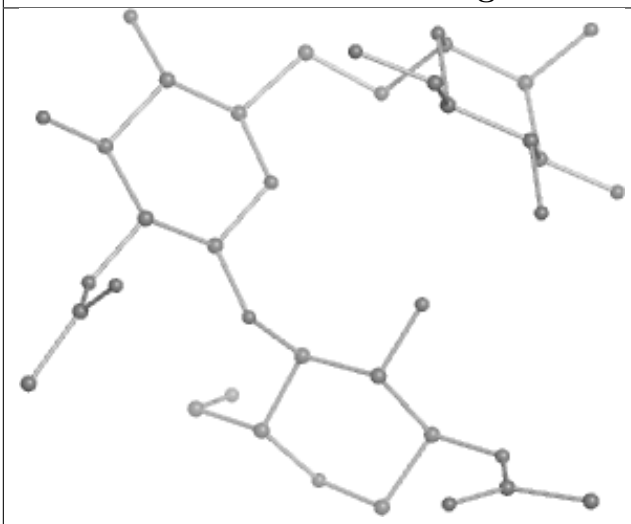


Rings

Oligosaccharide Chain WA



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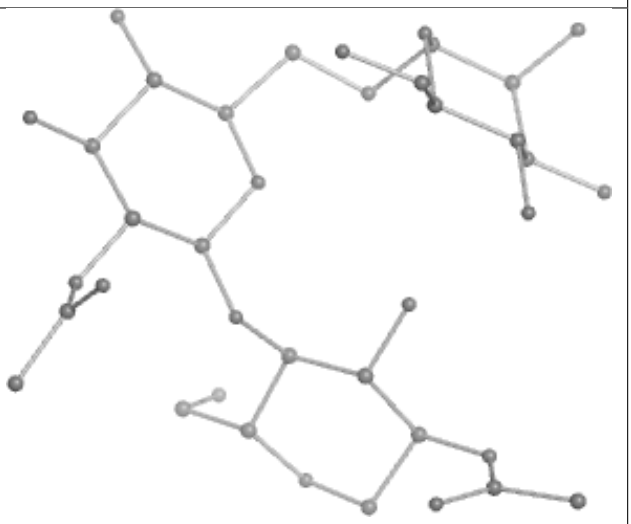
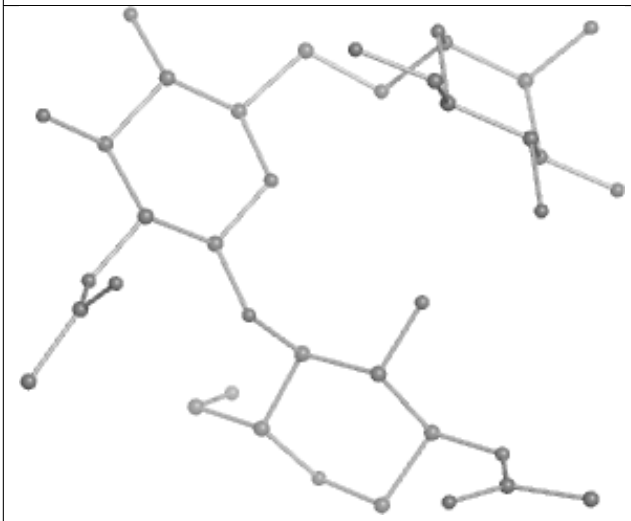


Bond angles



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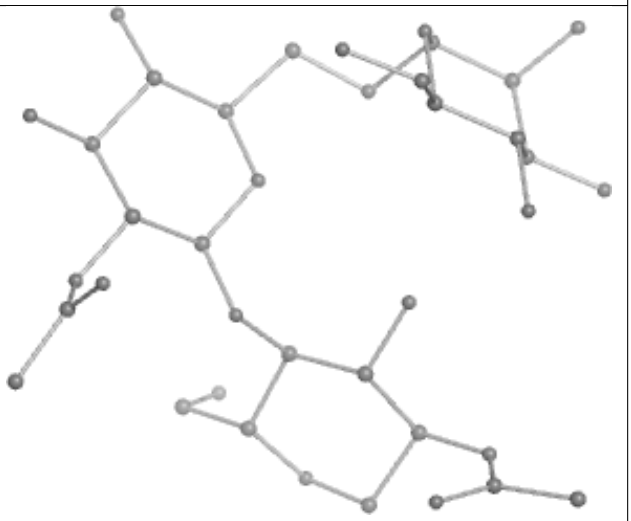
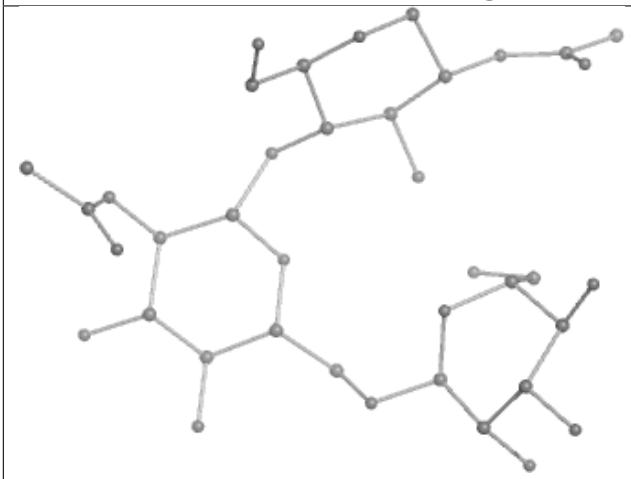


Rings

Oligosaccharide Chain XA



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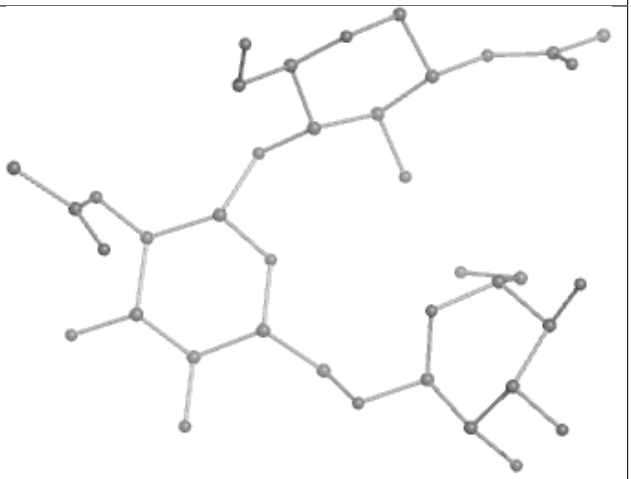
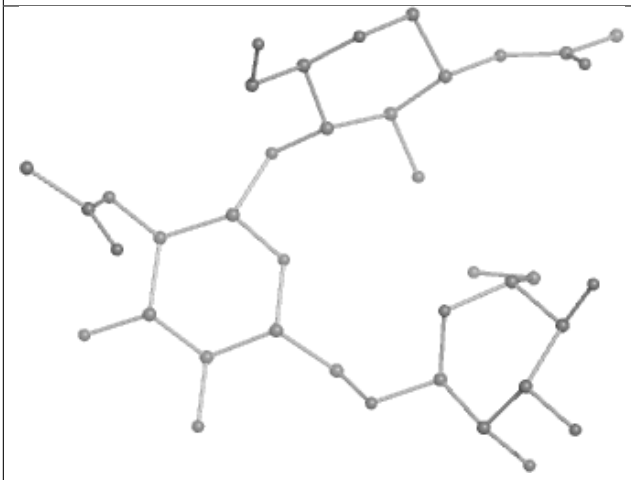


Bond angles



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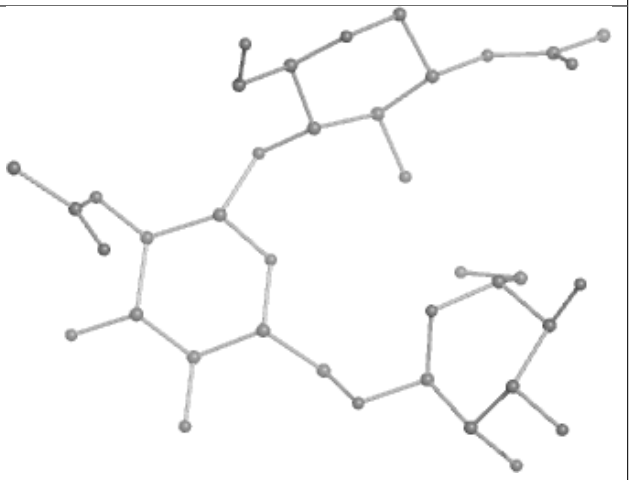
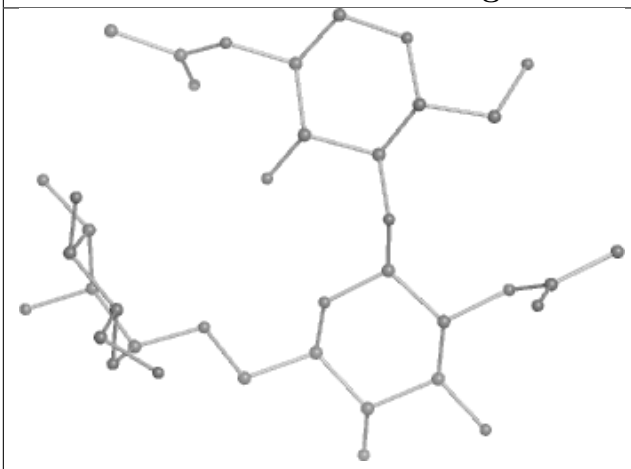


Rings

Oligosaccharide Chain YA



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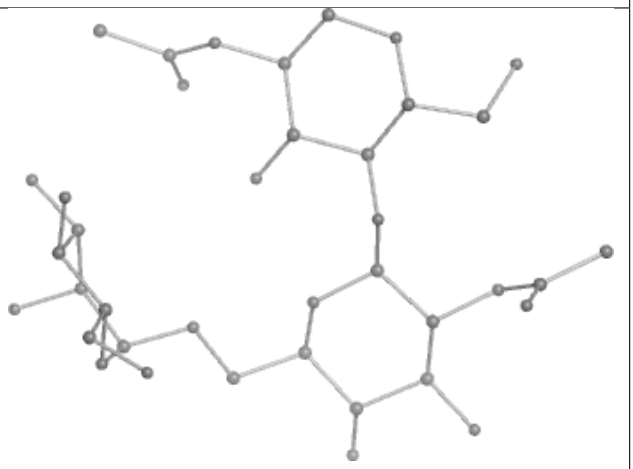
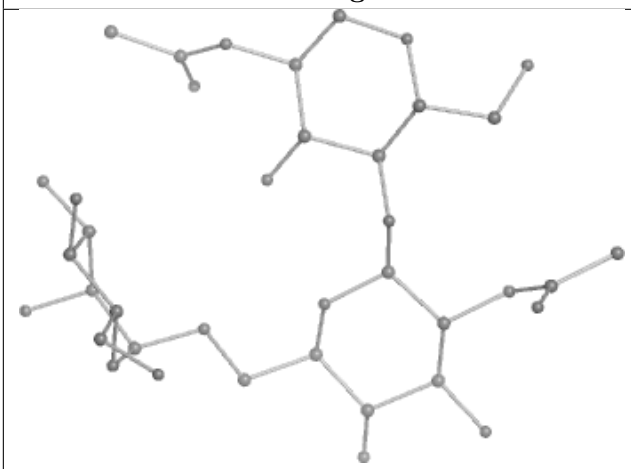


Bond angles



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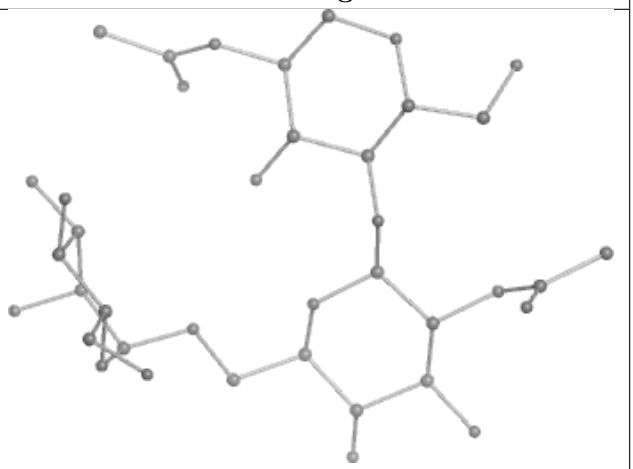
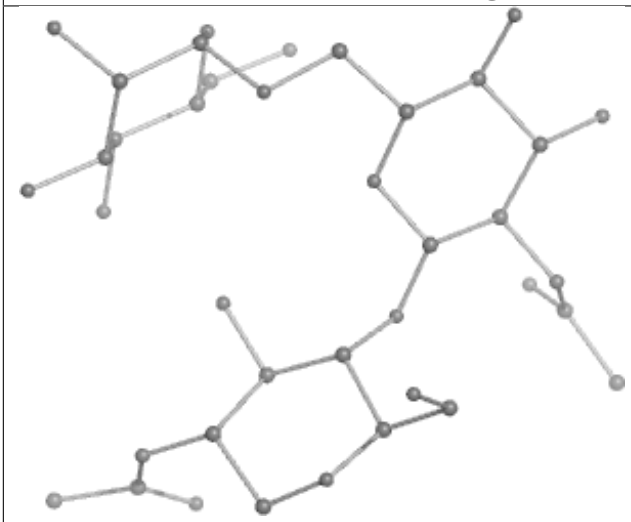


Rings

Oligosaccharide Chain ZA



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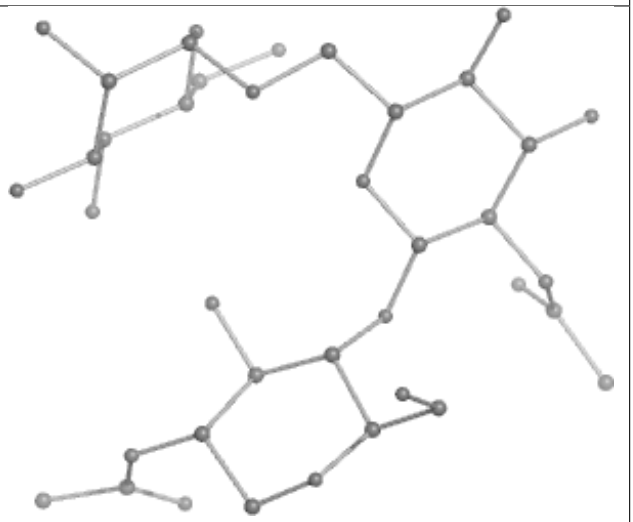

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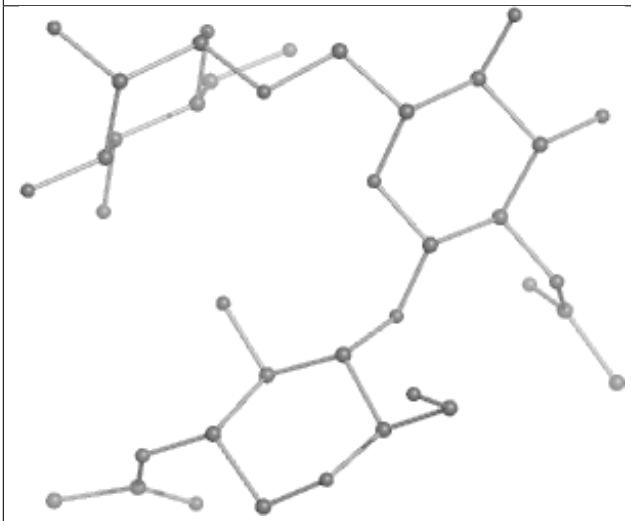

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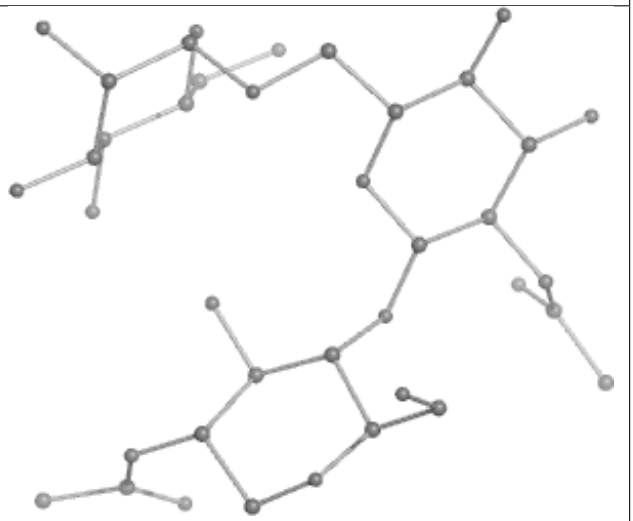
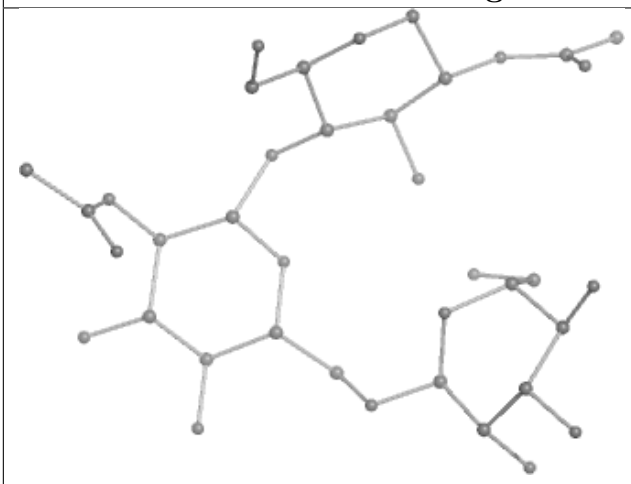


Rings

Oligosaccharide Chain aA



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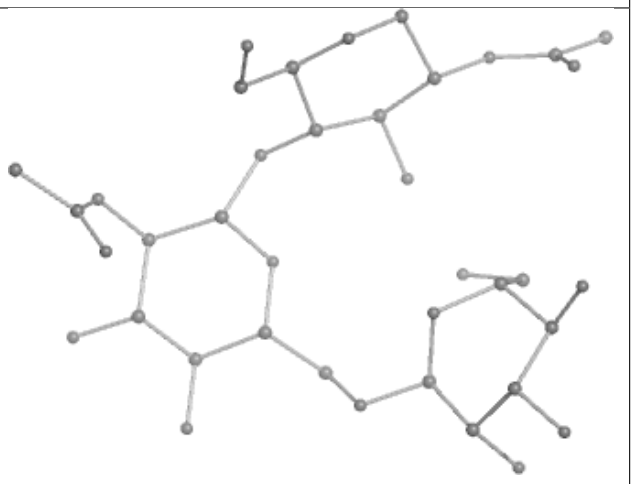
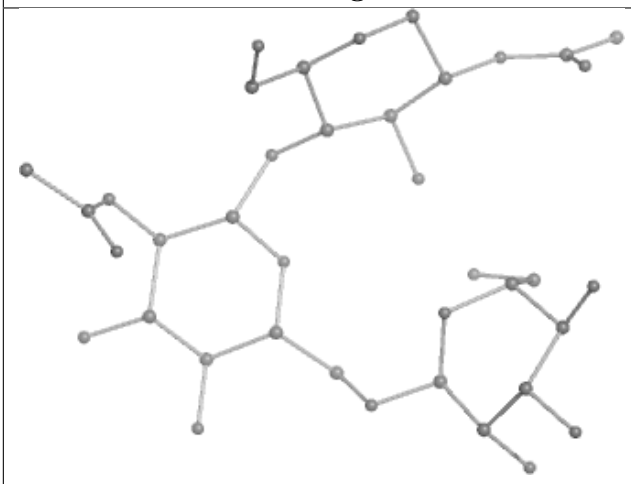


Bond angles



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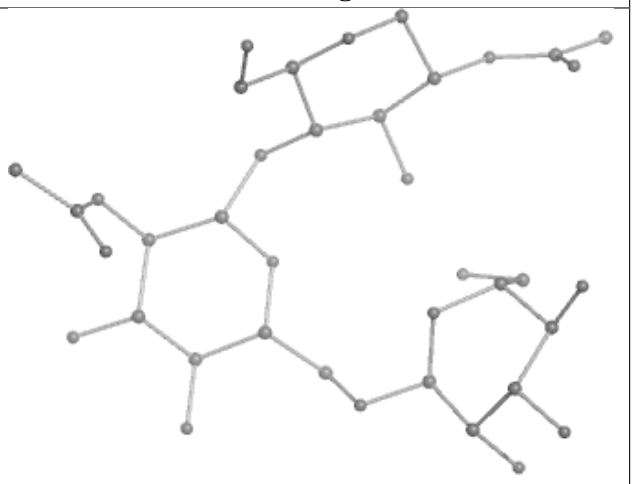
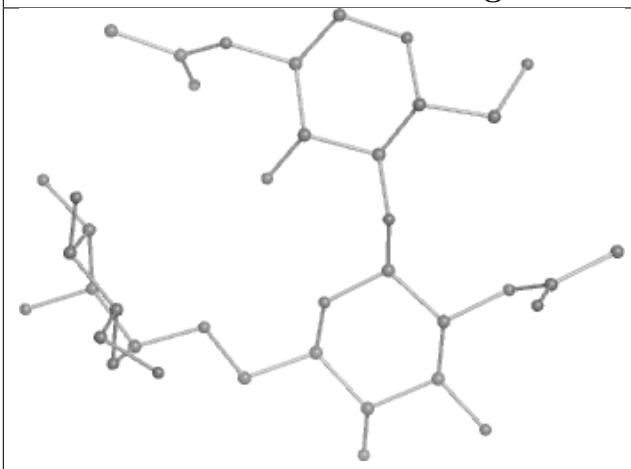


Rings

Oligosaccharide Chain bA



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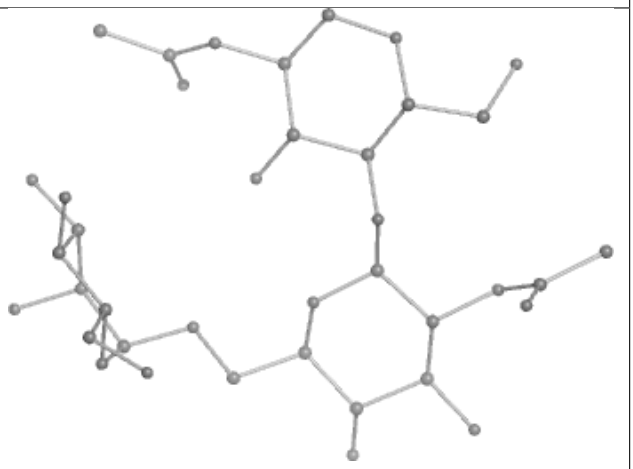
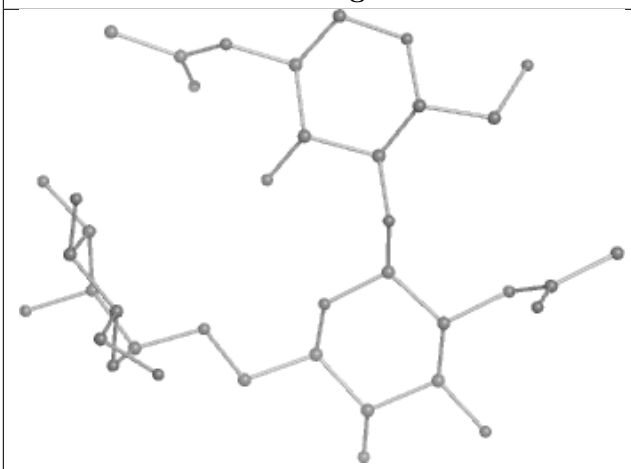
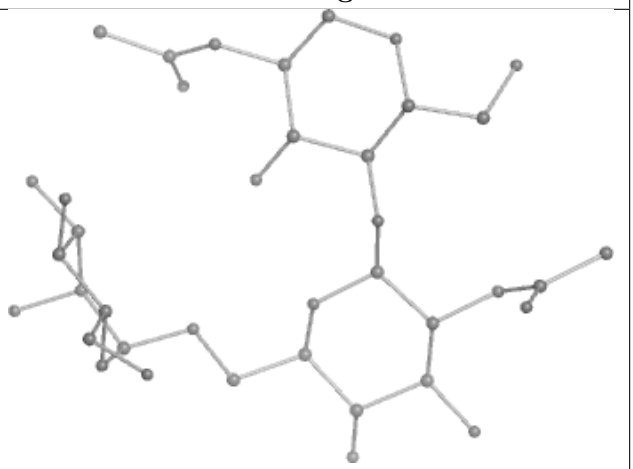


Bond angles

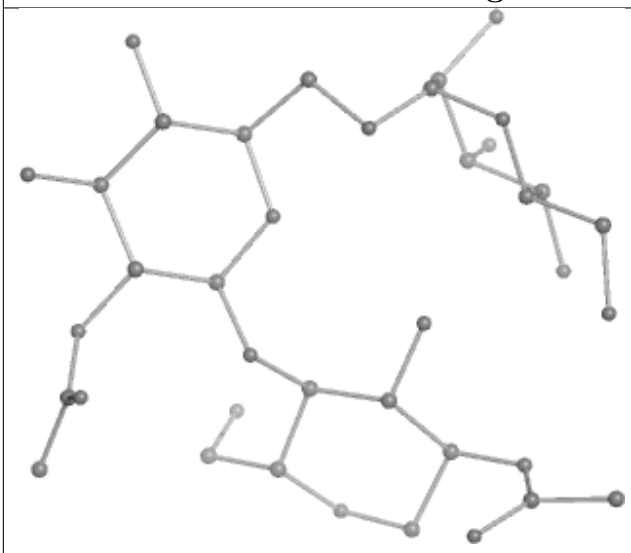


Torsions



Rings

Oligosaccharide Chain cA



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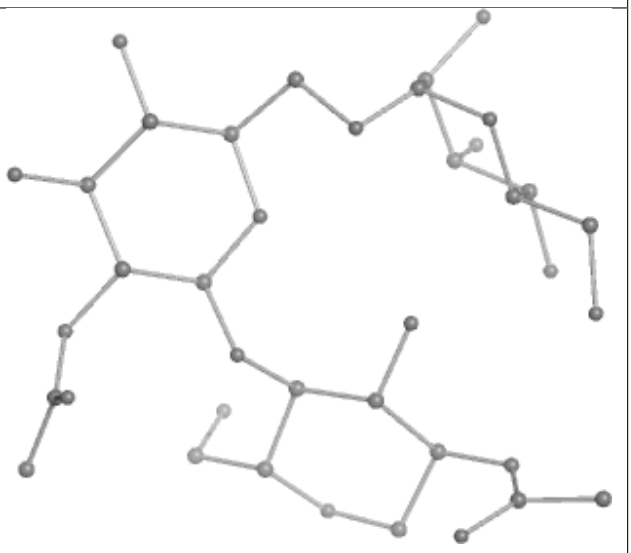
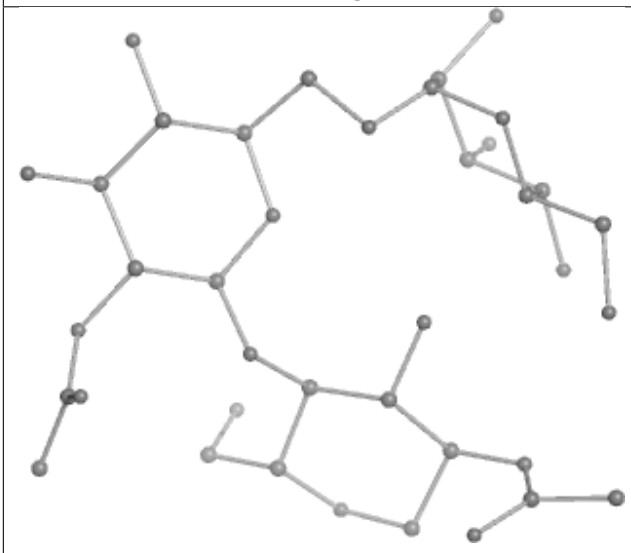


Bond angles



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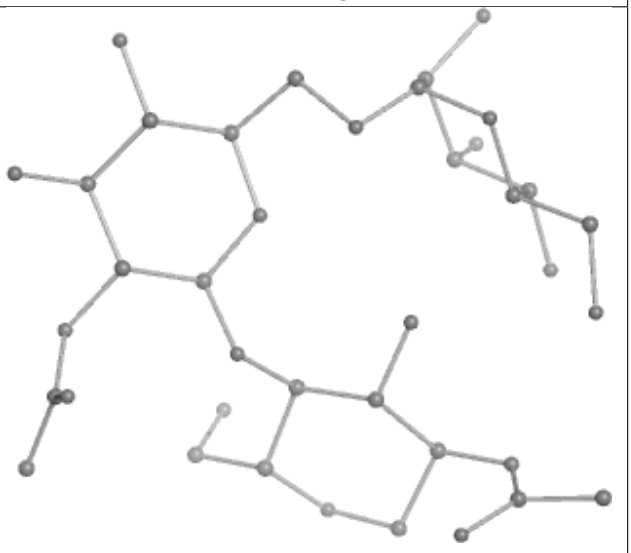
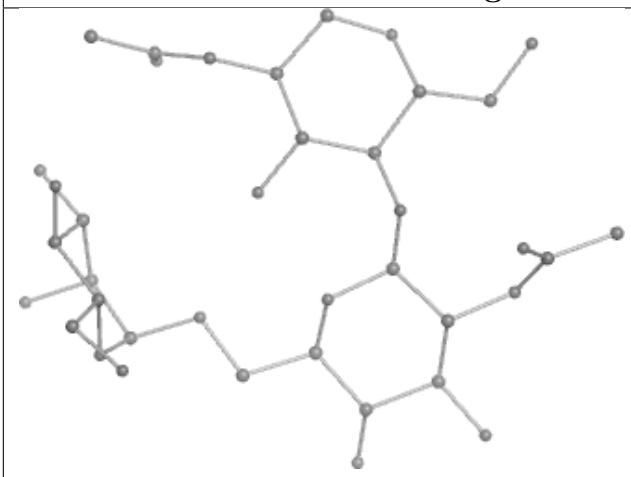


Rings

Oligosaccharide Chain dA



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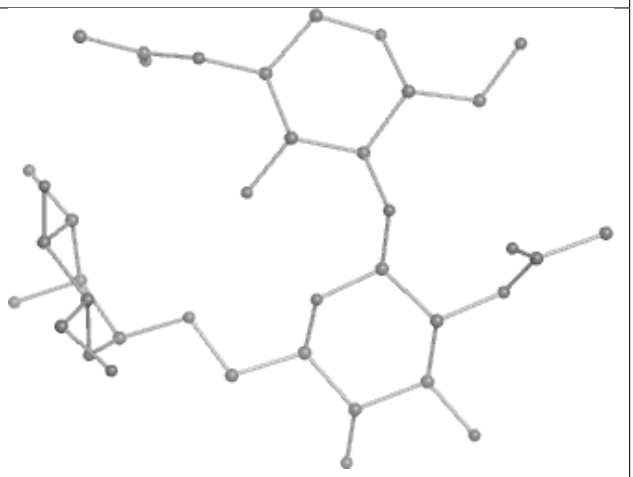
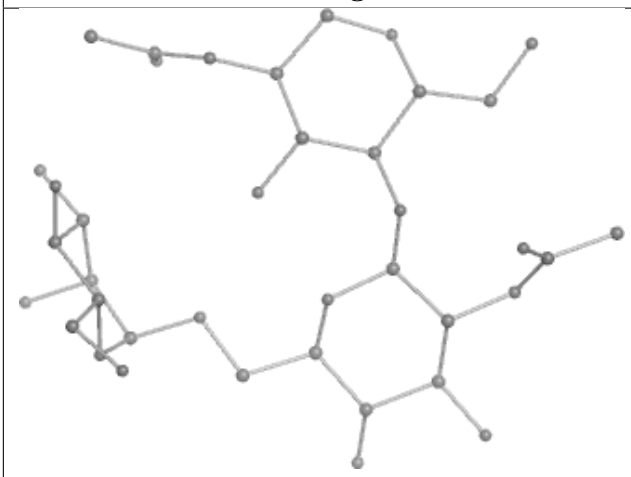


Bond angles



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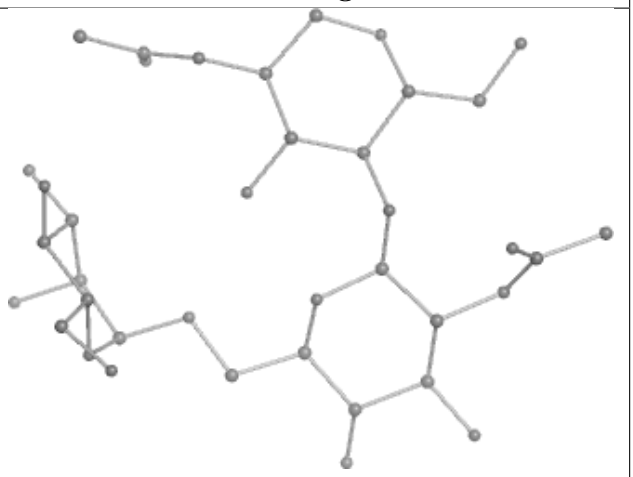
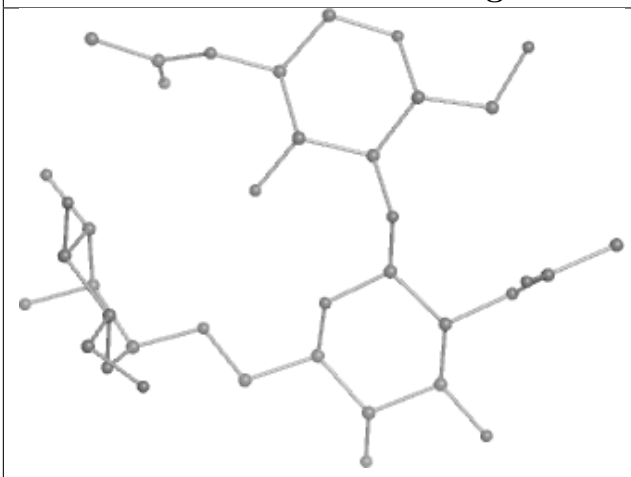
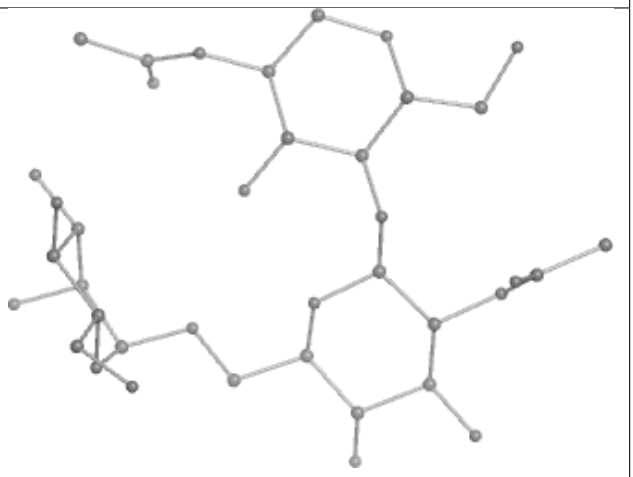


Rings

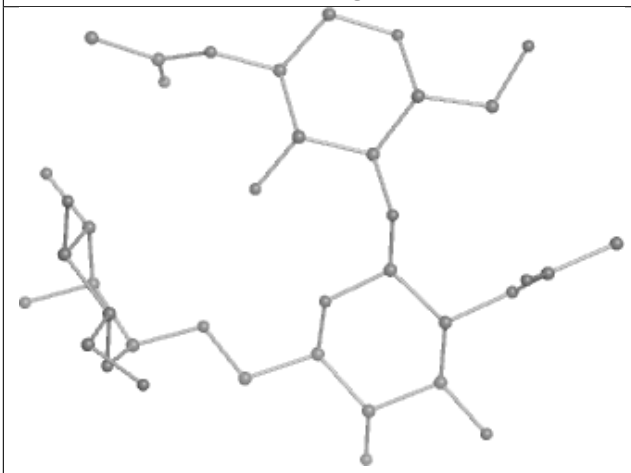
Oligosaccharide Chain eA



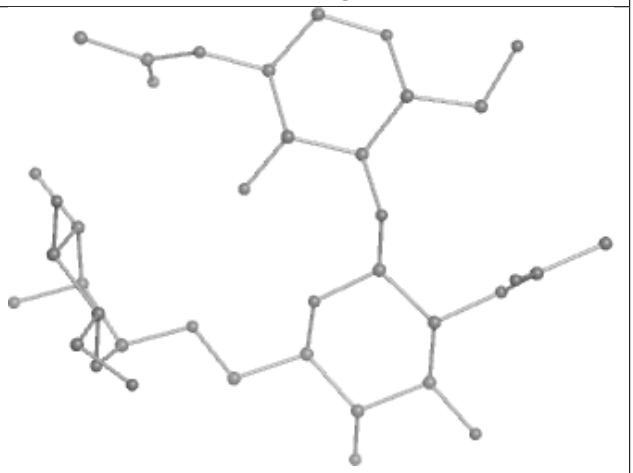
Bond lengths



Bond angles

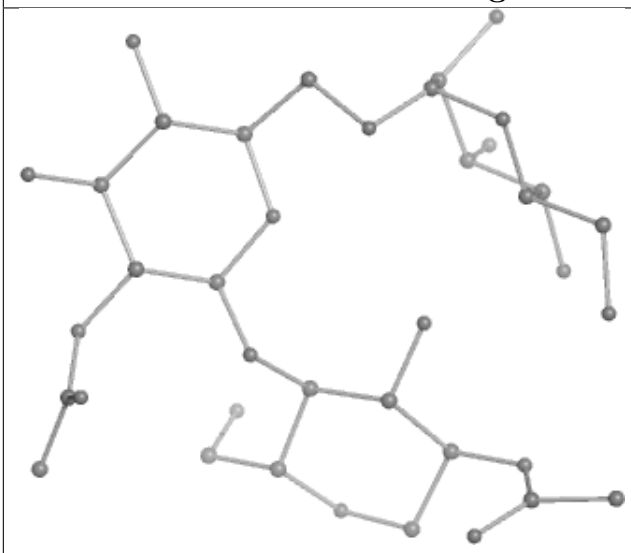


Torsions

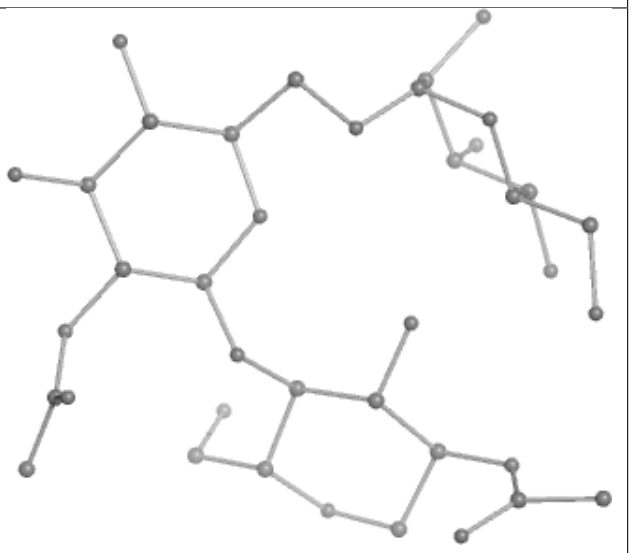


Rings

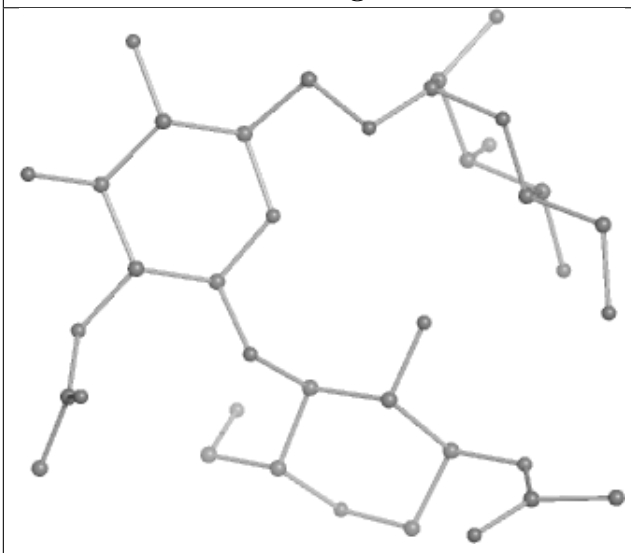
Oligosaccharide Chain fA



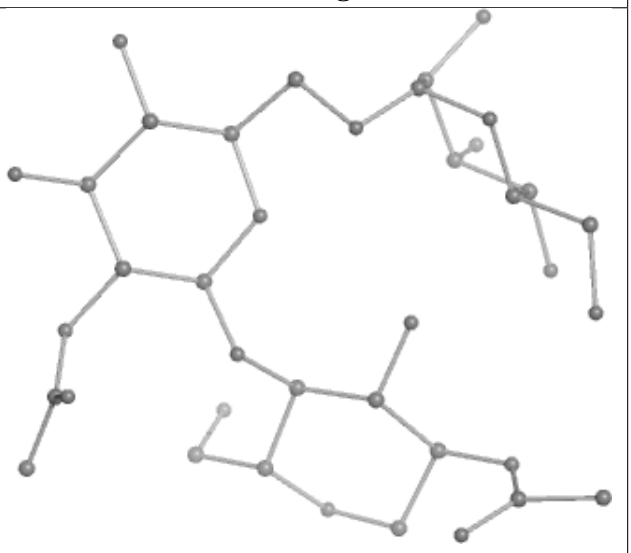
Bond lengths



Bond angles

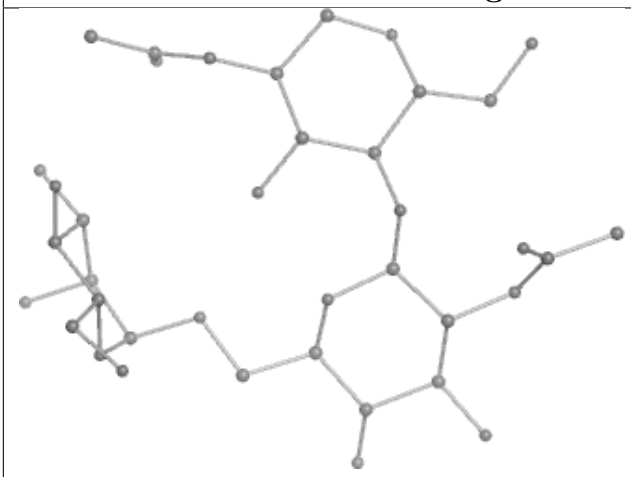


Torsions

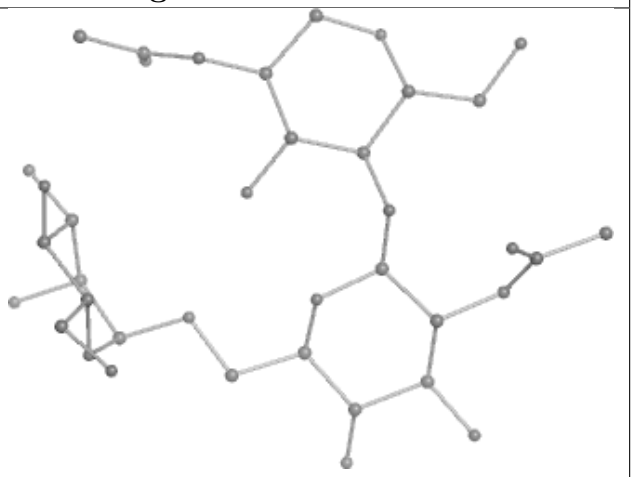


Rings

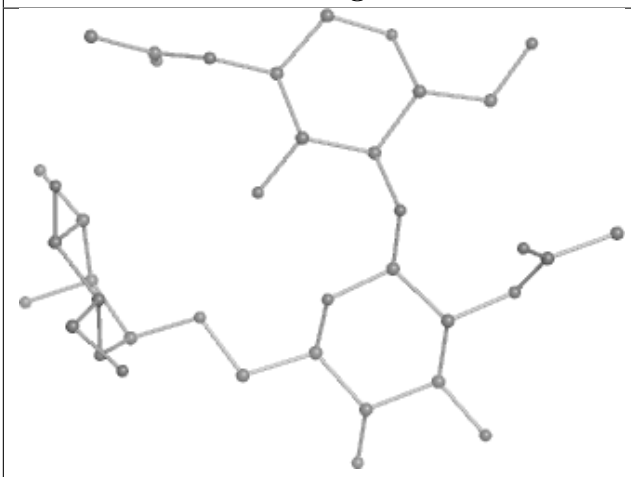
Oligosaccharide Chain gA



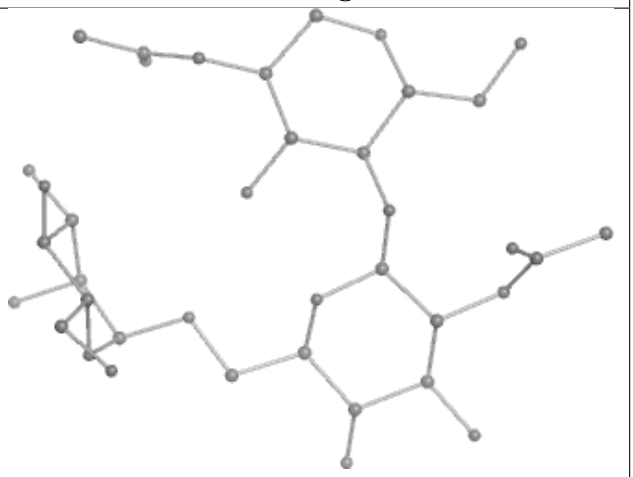
Bond lengths



Bond angles

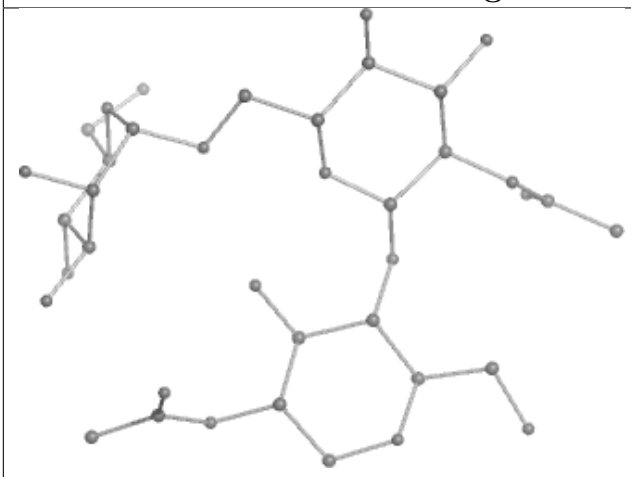


Torsions



Rings

Oligosaccharide Chain hA



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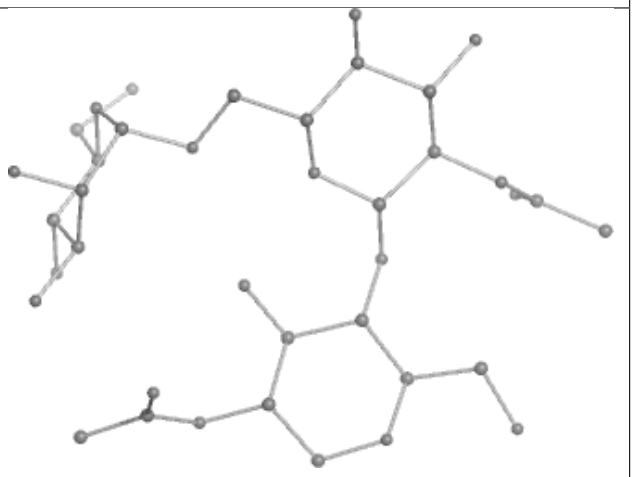
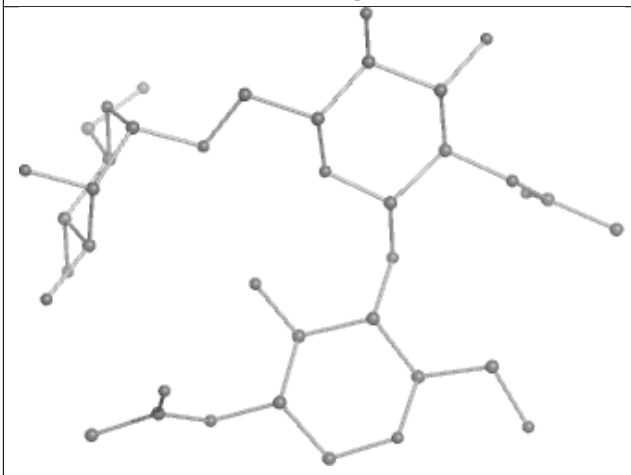
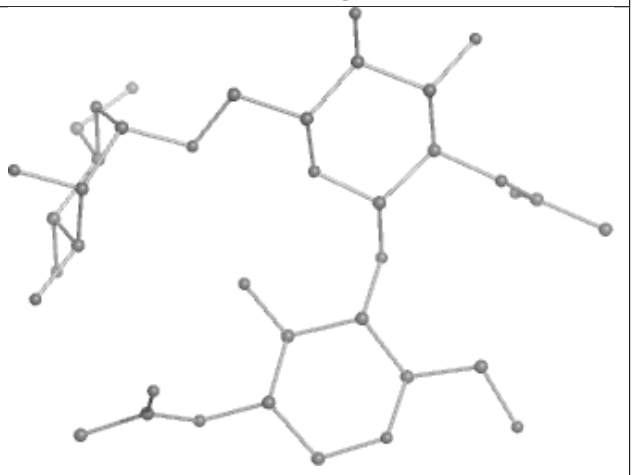


Bond angles

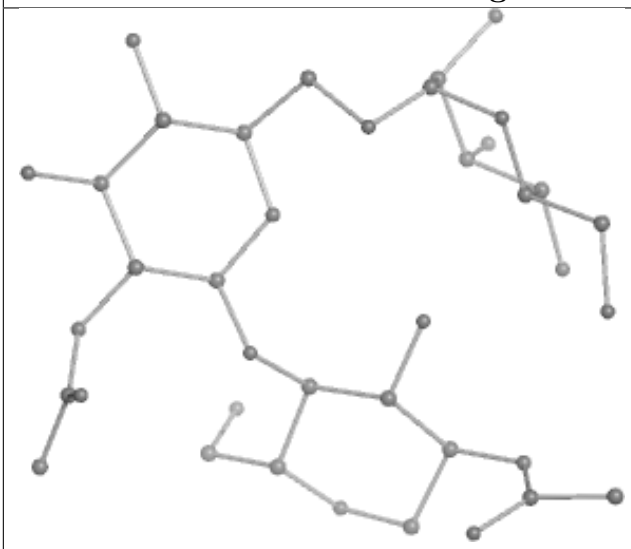


Torsions



Rings

Oligosaccharide Chain iA



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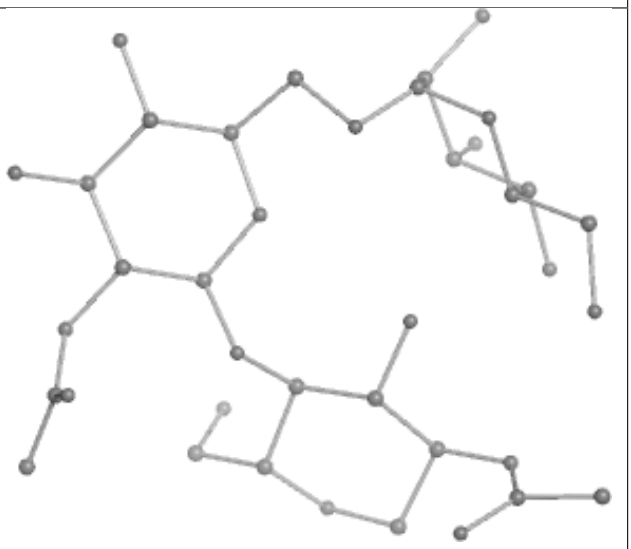
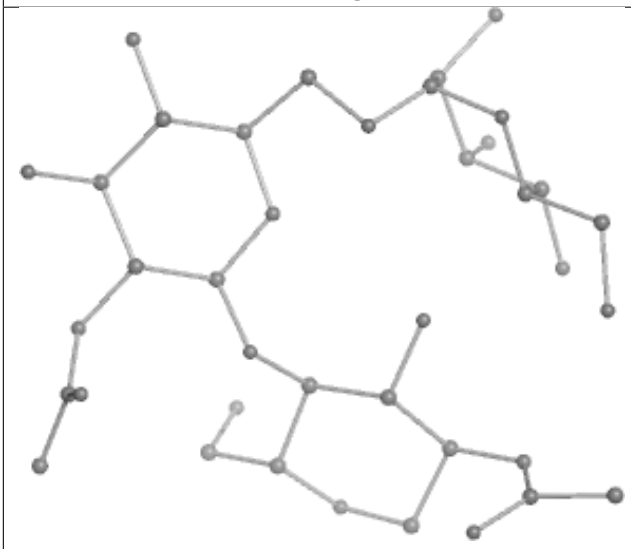


Bond angles



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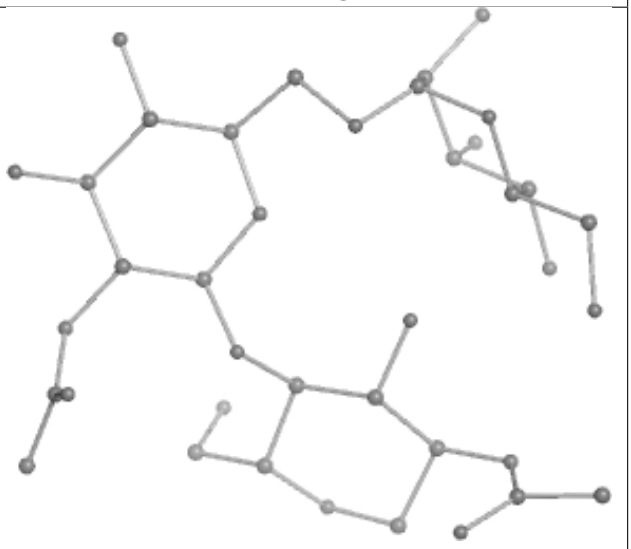
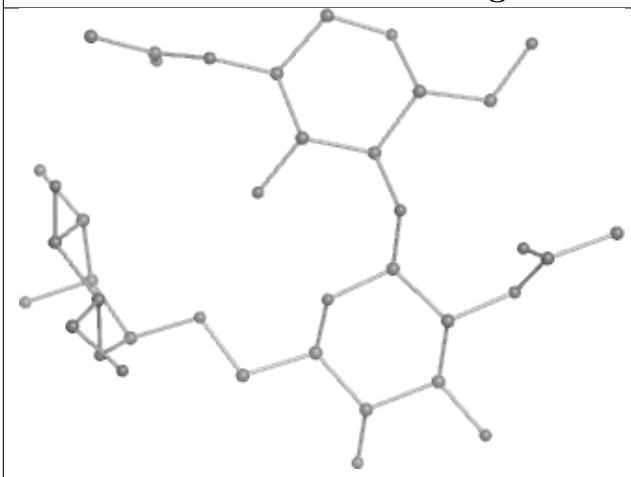


Rings

Oligosaccharide Chain jA



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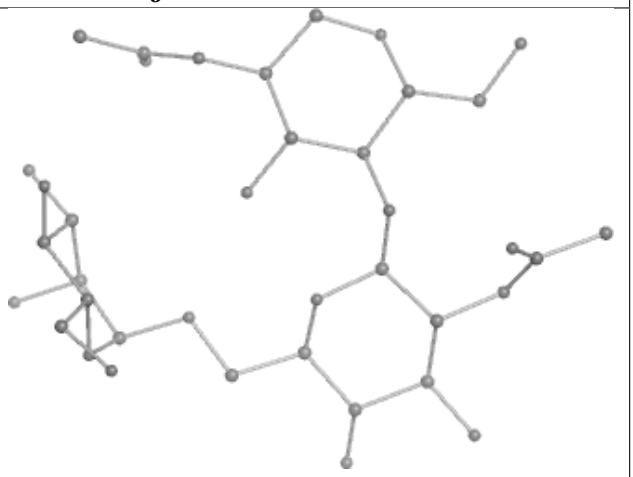
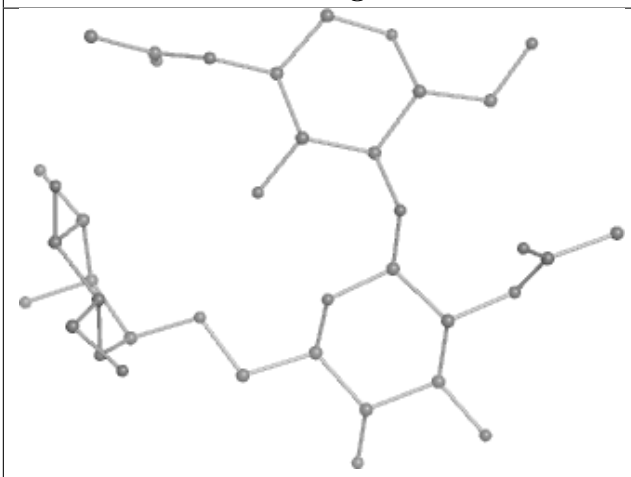
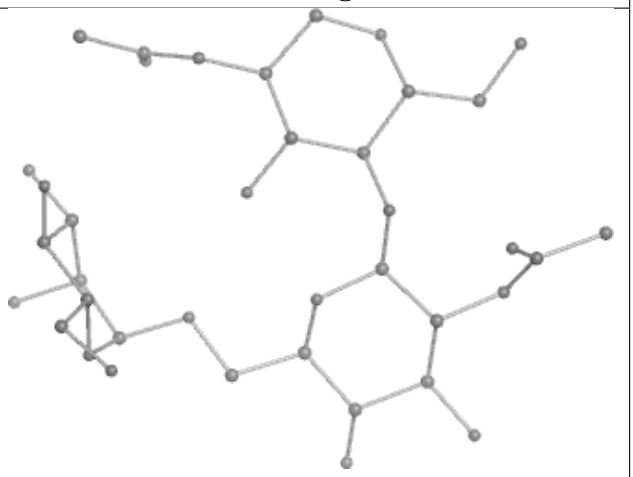


Bond angles

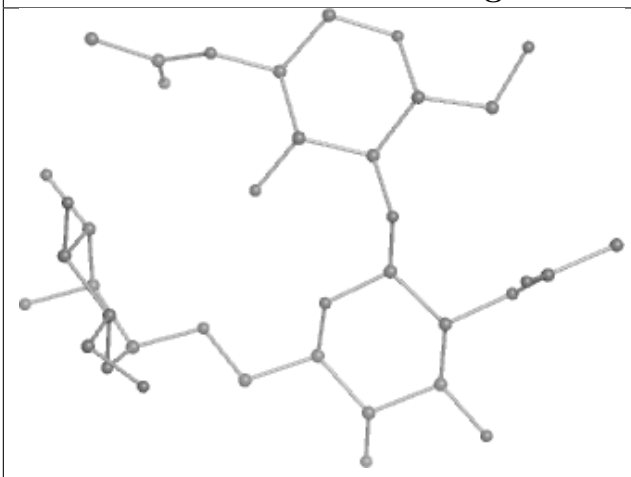


Torsions

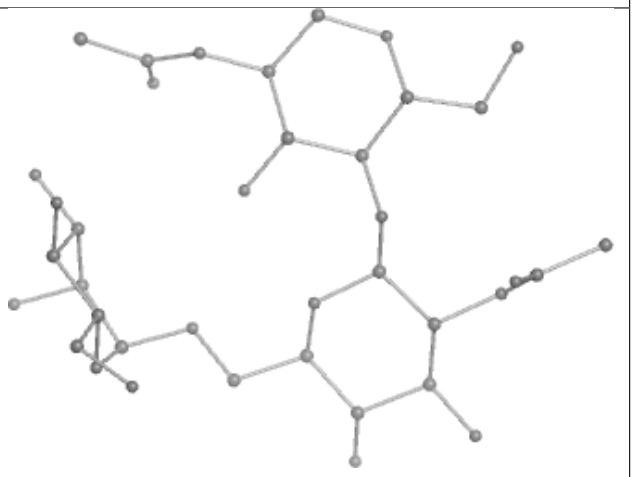


Rings

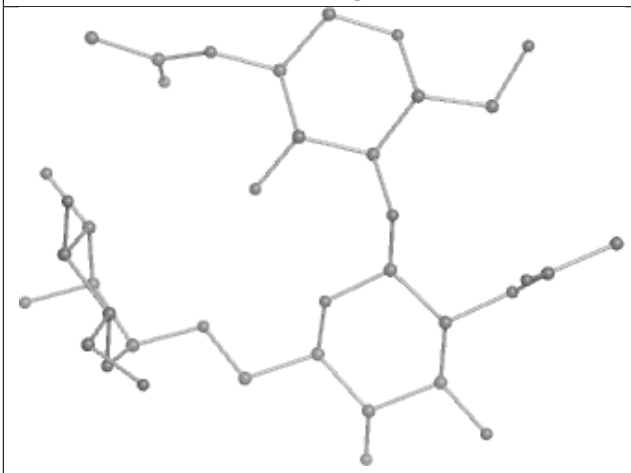
Oligosaccharide Chain kA



Bond lengths



Bond angles



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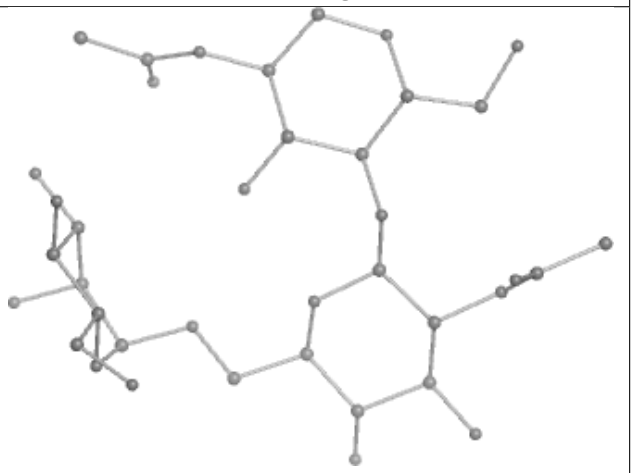
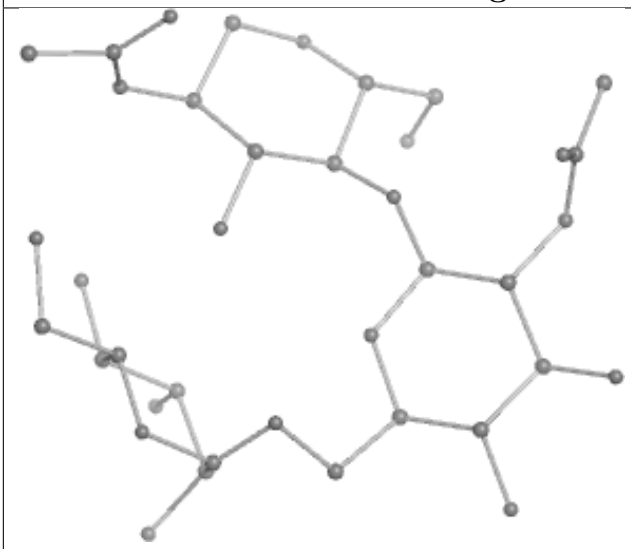


Rings

Oligosaccharide Chain lA



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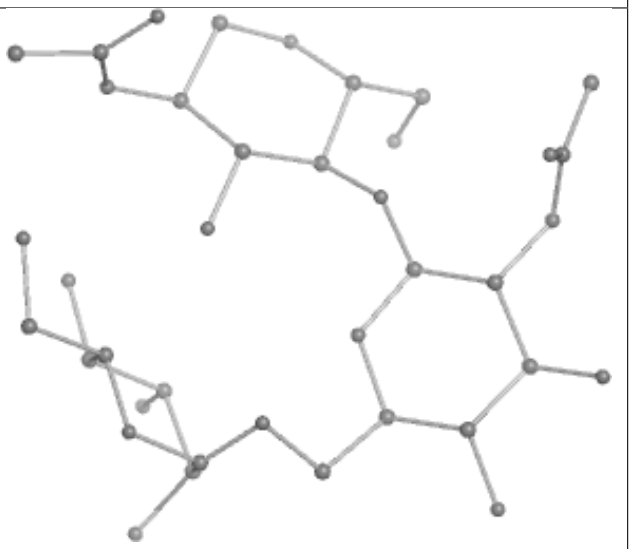
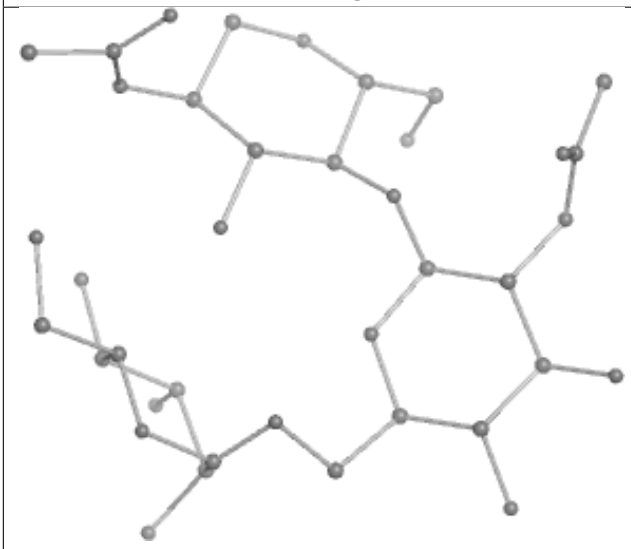


Bond angles



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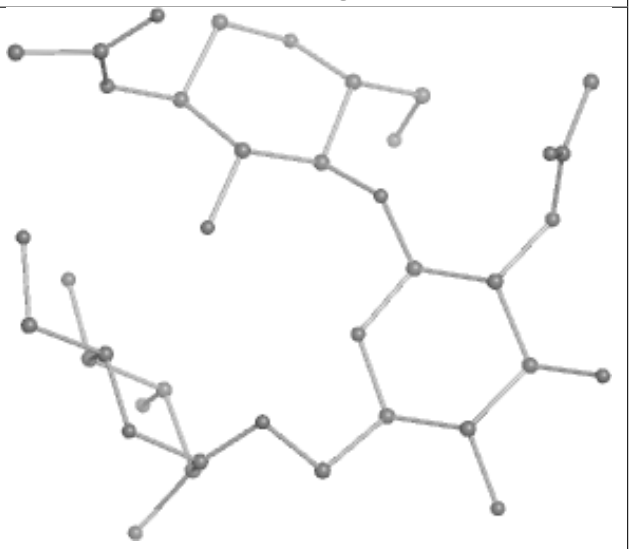
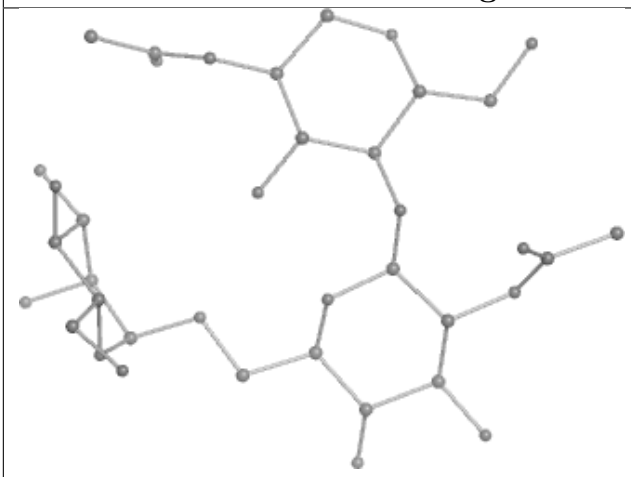


Rings

Oligosaccharide Chain mA



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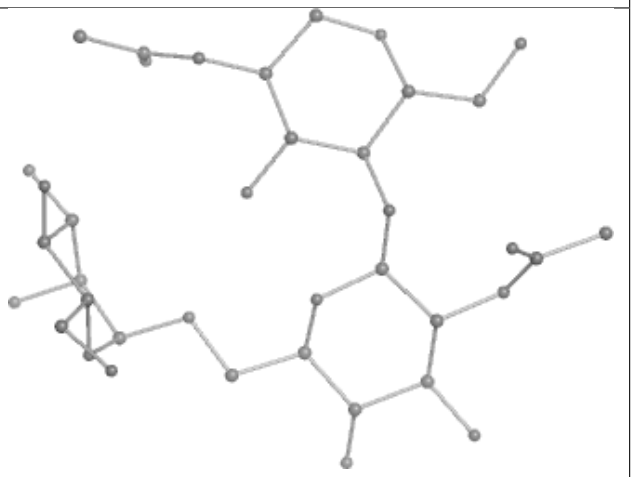
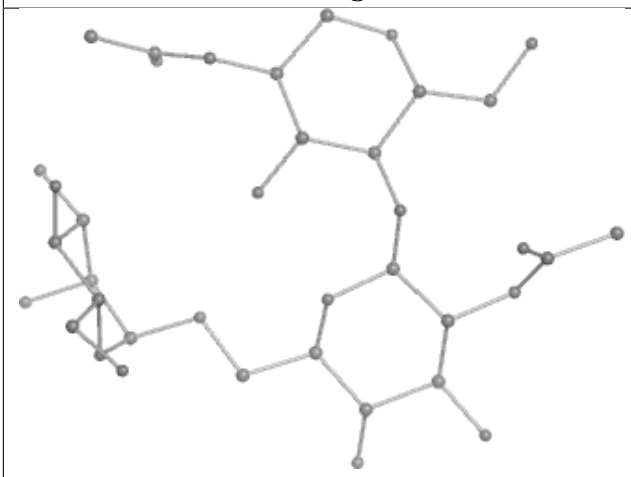
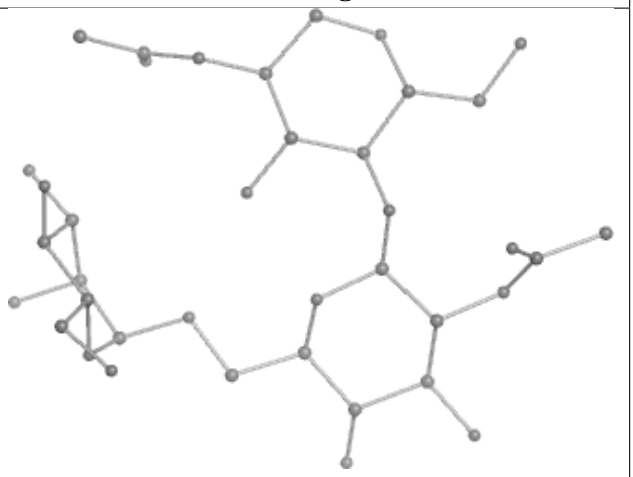


Bond angles

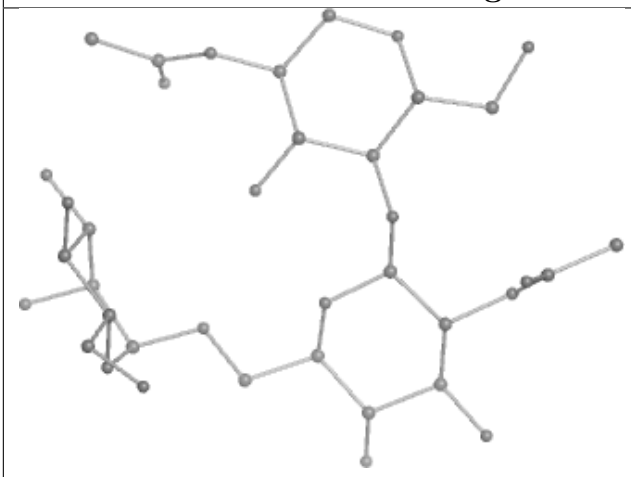


Torsions



Rings

Oligosaccharide Chain nA



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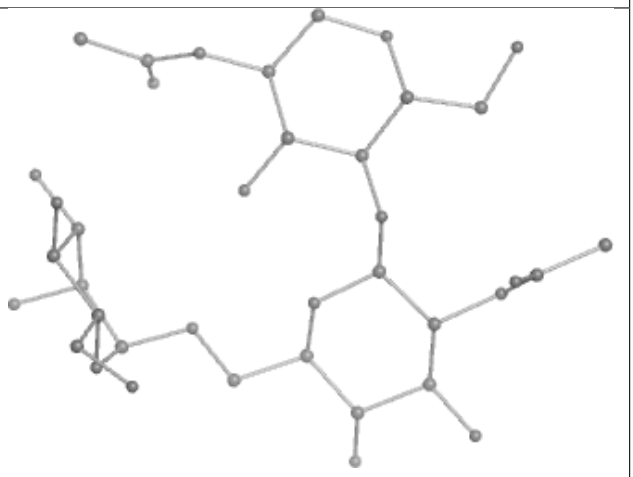
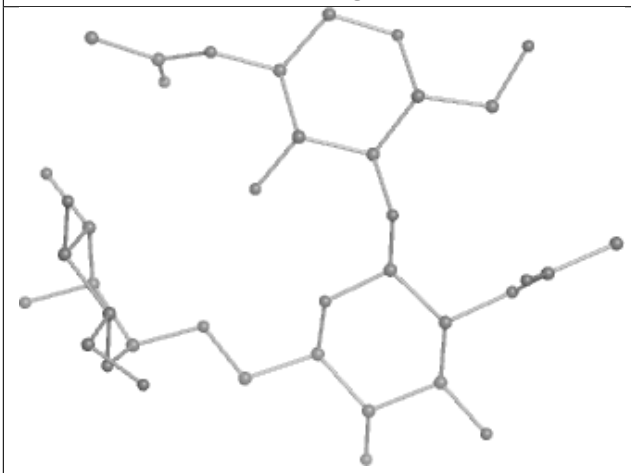


Bond angles



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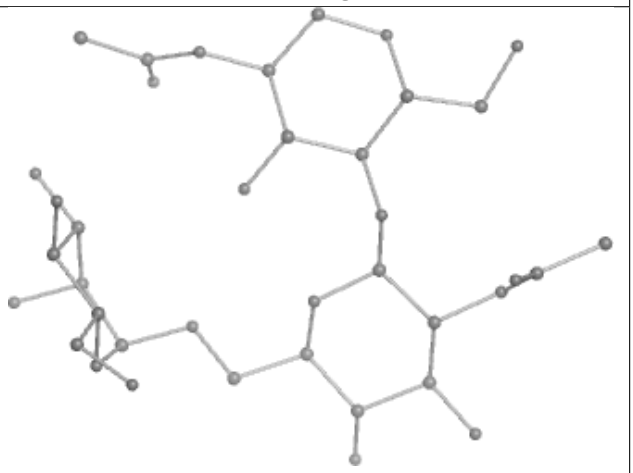
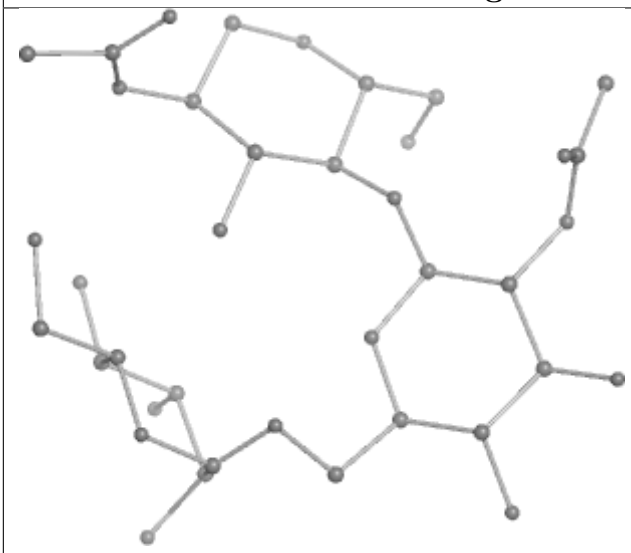


Rings

Oligosaccharide Chain oA



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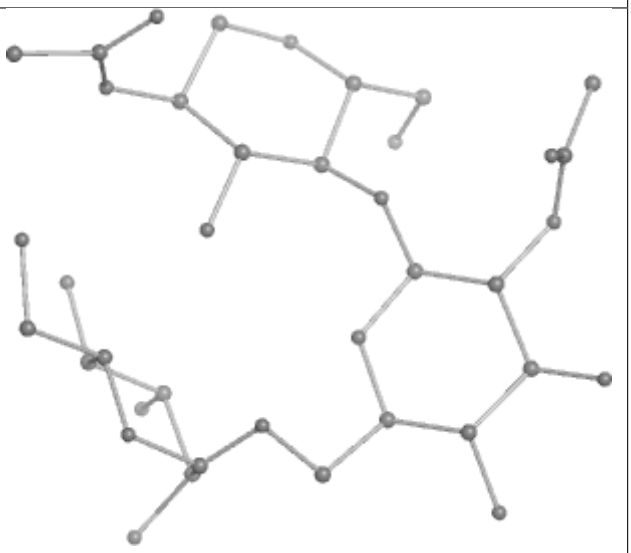
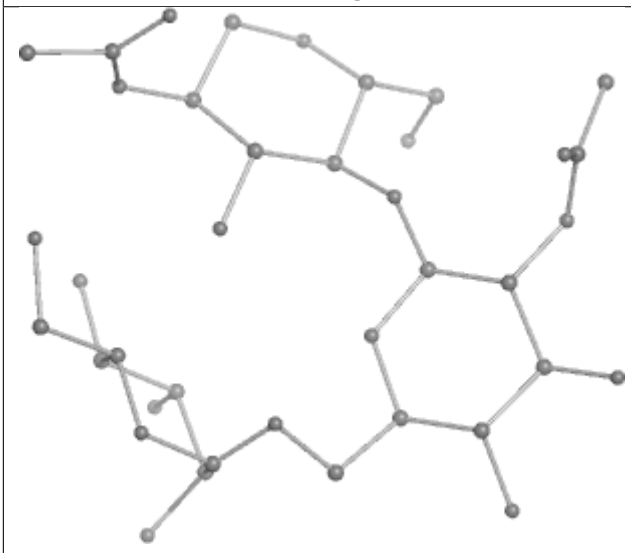
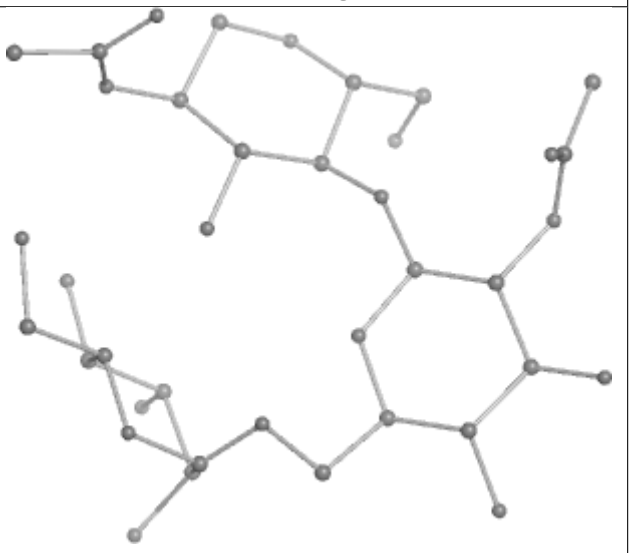


Bond angles

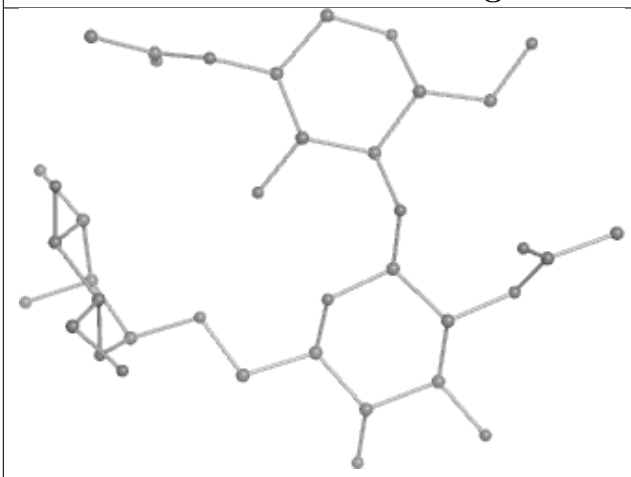


Torsions



Rings

Oligosaccharide Chain pA



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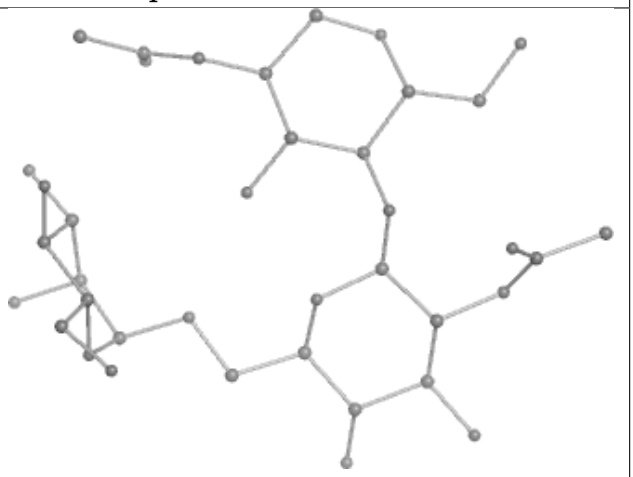
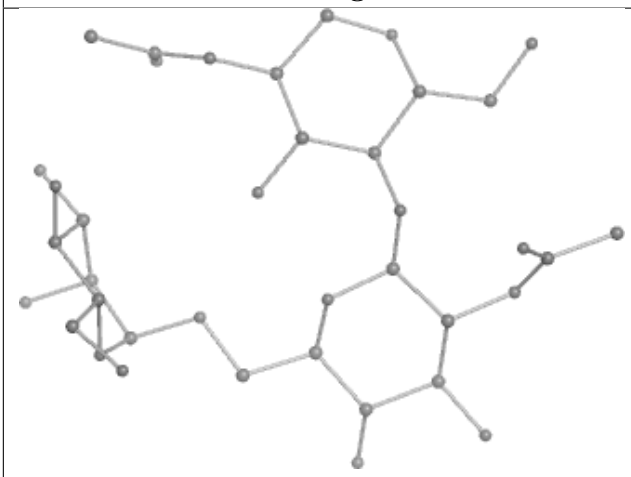
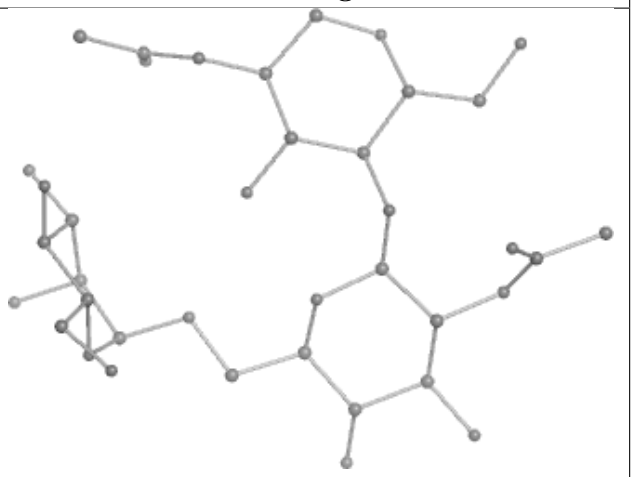


Bond angles

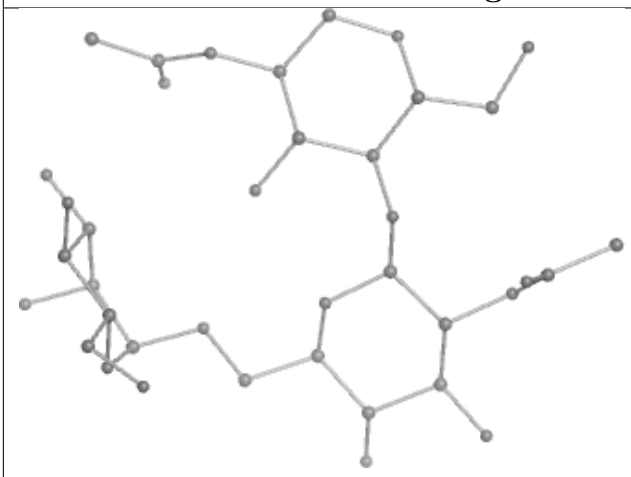


Torsions



Rings

Oligosaccharide Chain qA



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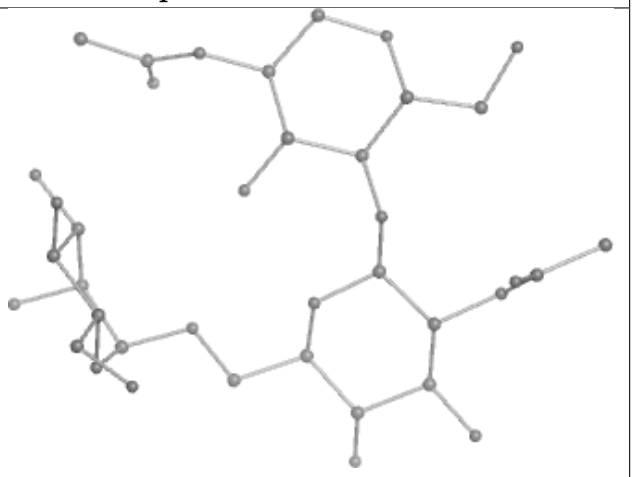
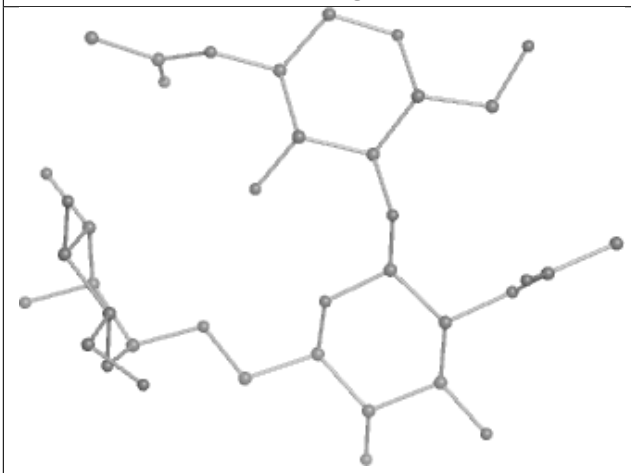
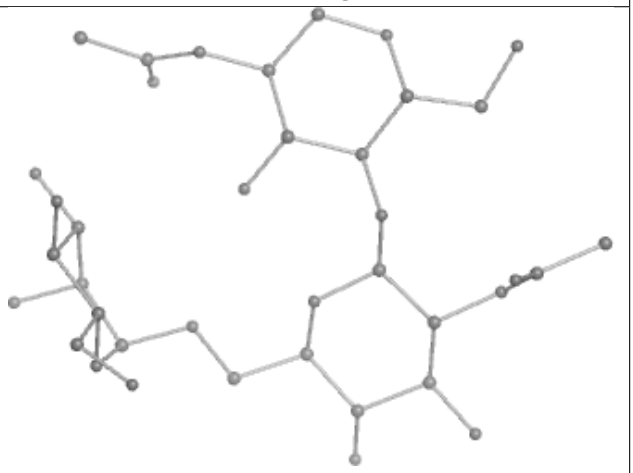


Bond angles

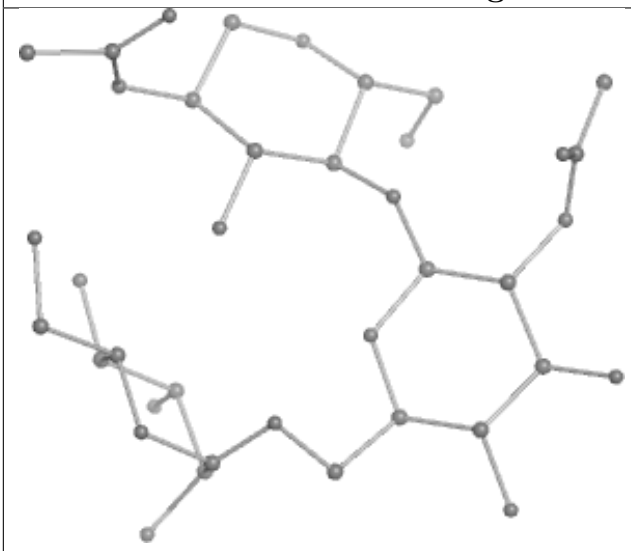


Torsions



Rings

Oligosaccharide Chain rA



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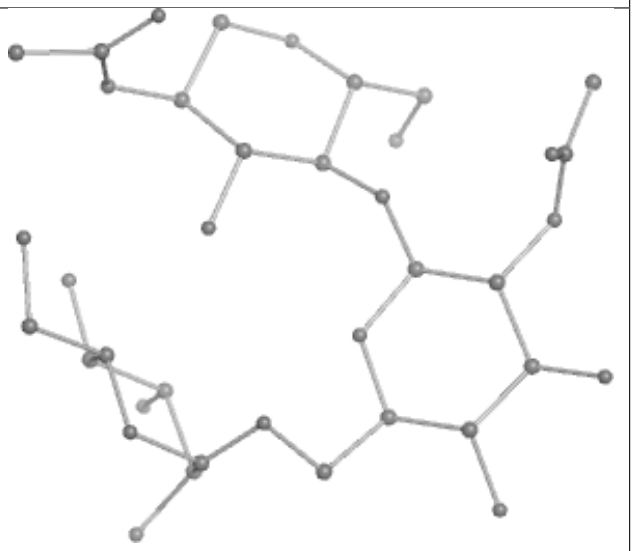
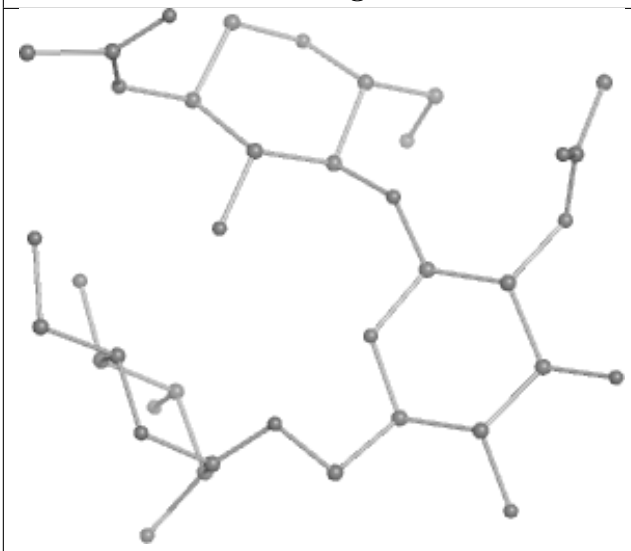
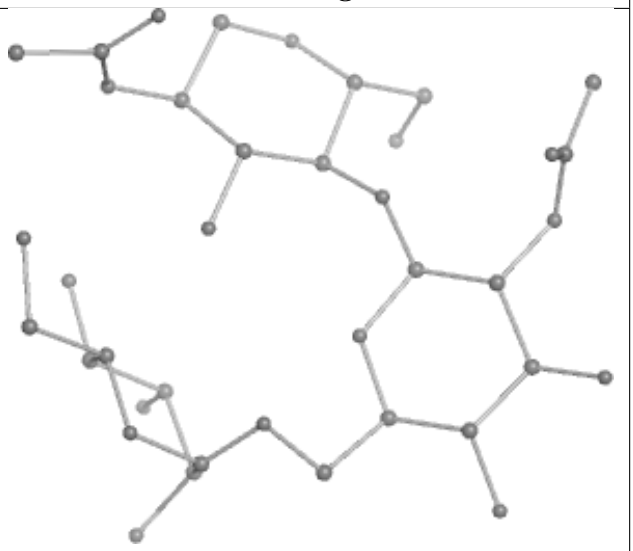


Bond angles

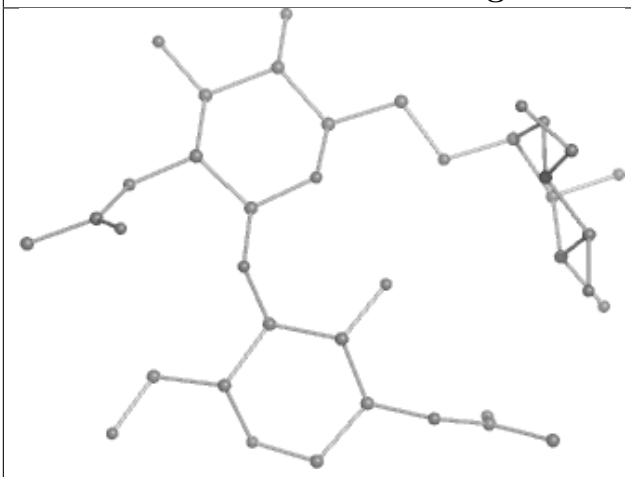


Torsions

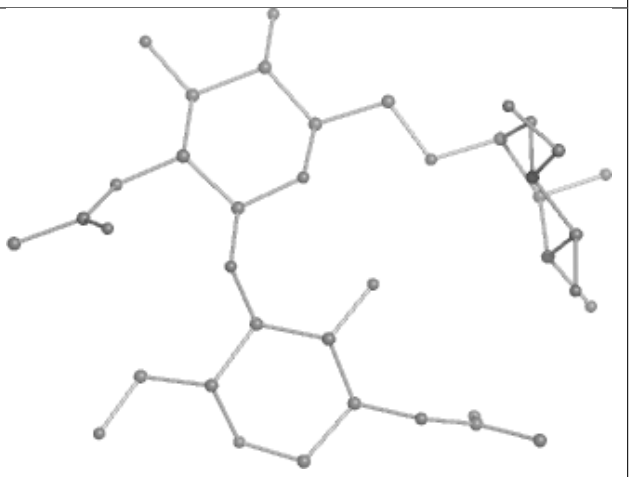


Rings

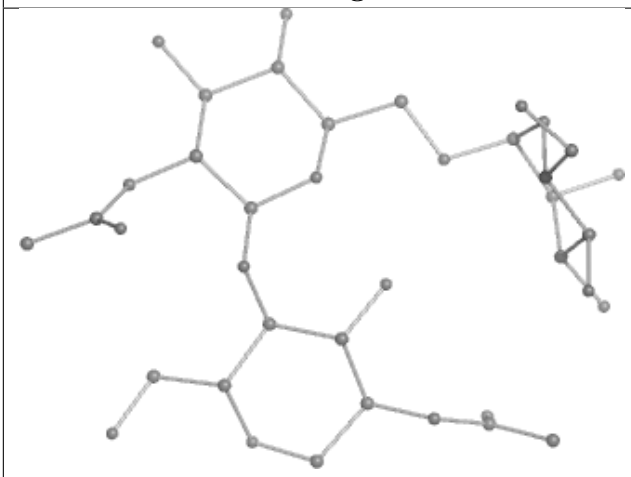
Oligosaccharide Chain sA



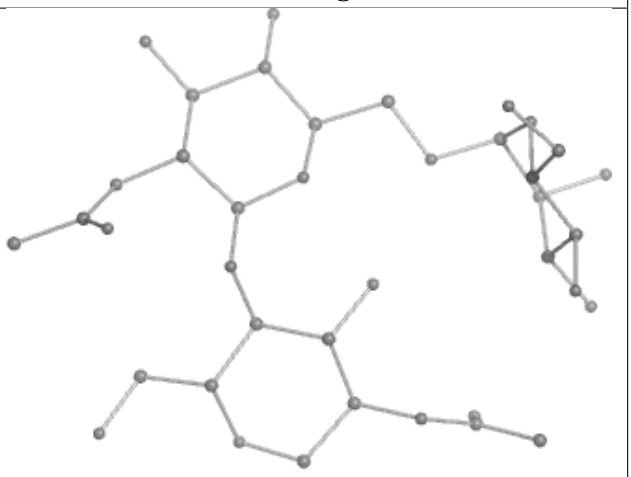
Bond lengths



Bond angles

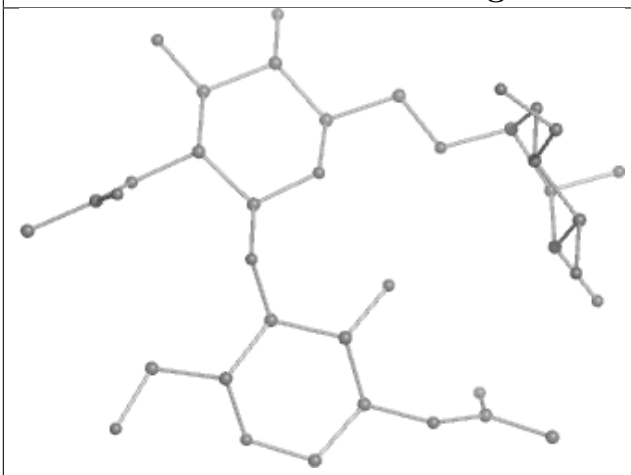


Torsions

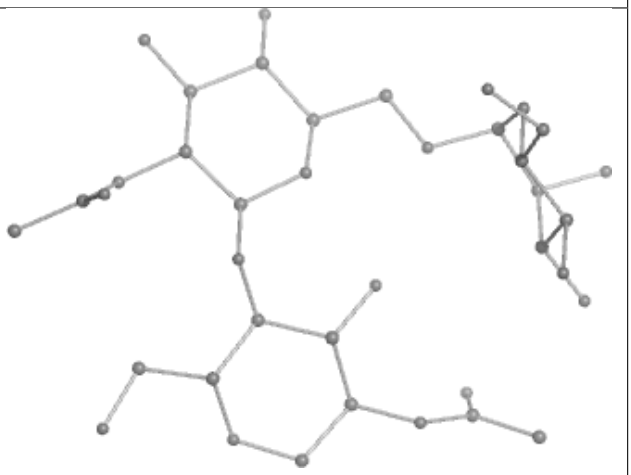


Rings

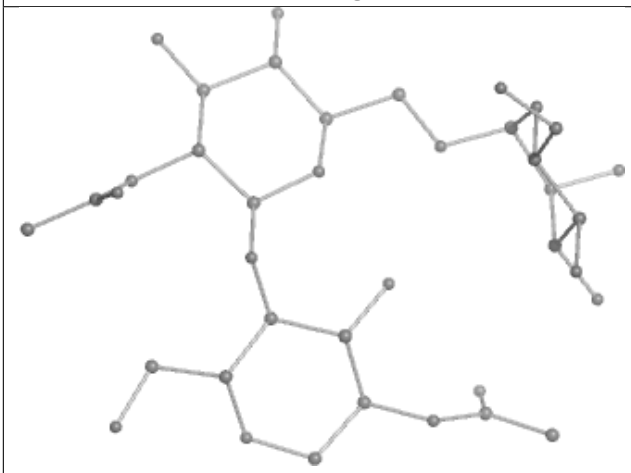
Oligosaccharide Chain tA



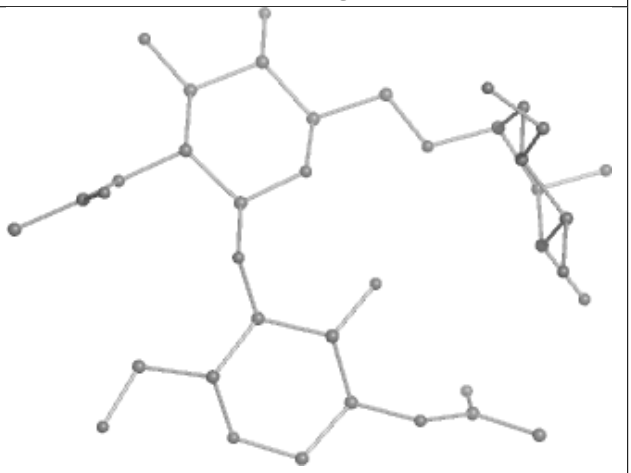
Bond lengths



Bond angles

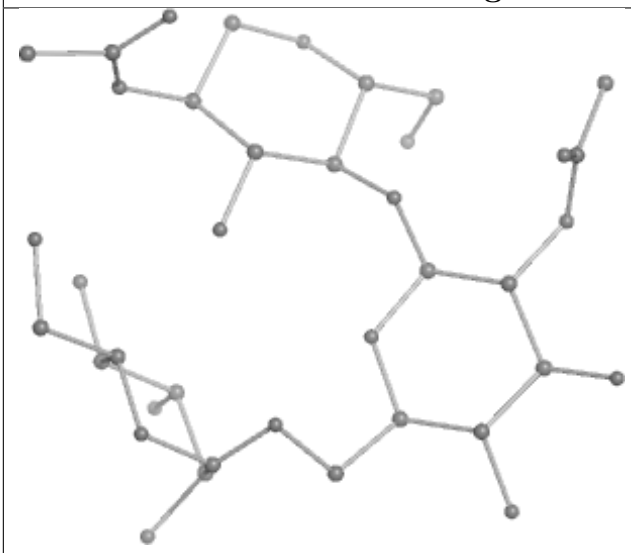


Torsions

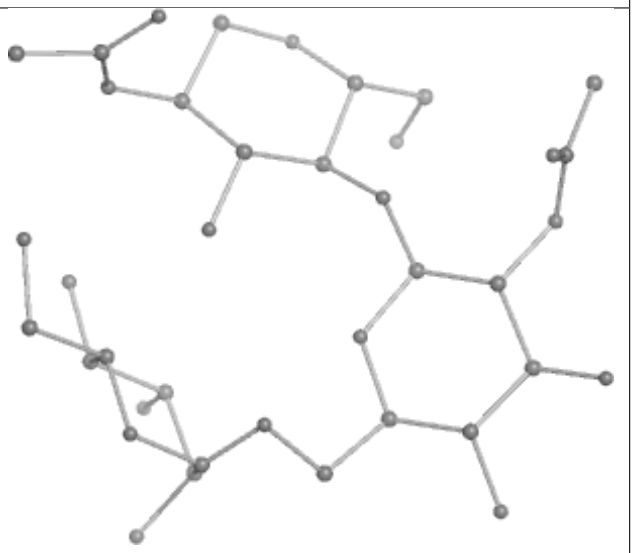


Rings

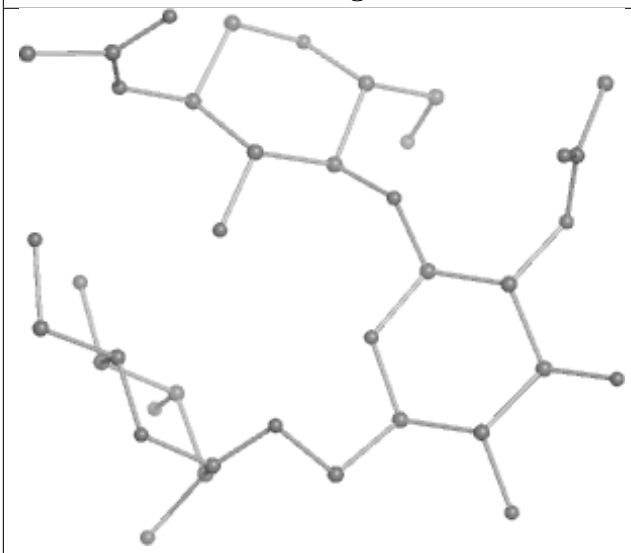
Oligosaccharide Chain uA



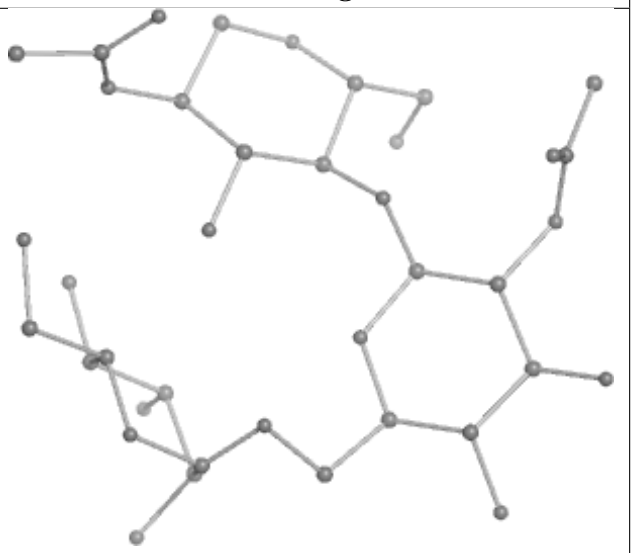
Bond lengths



Bond angles

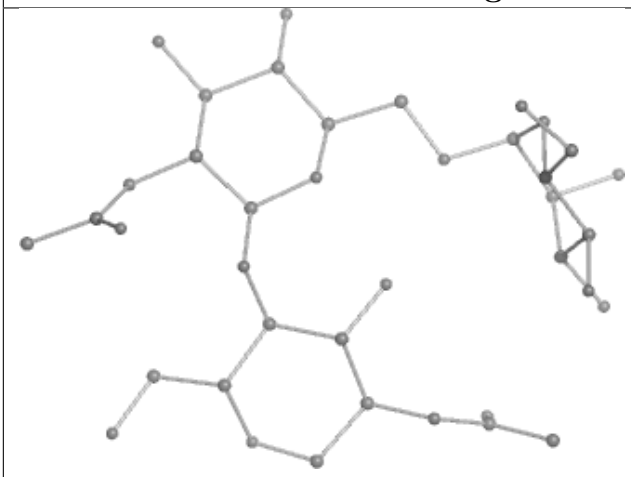


Torsions

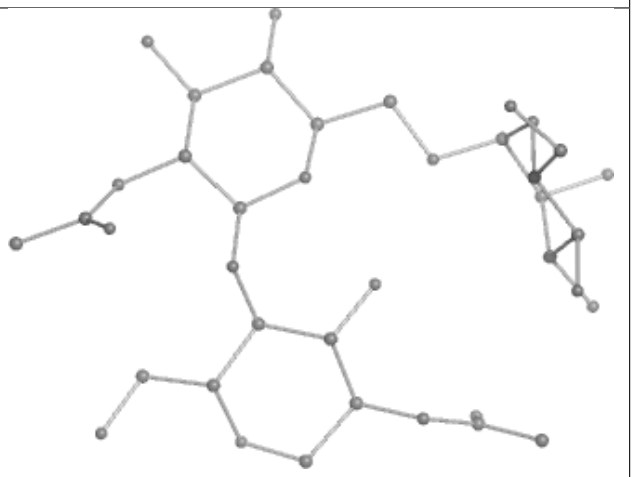


Rings

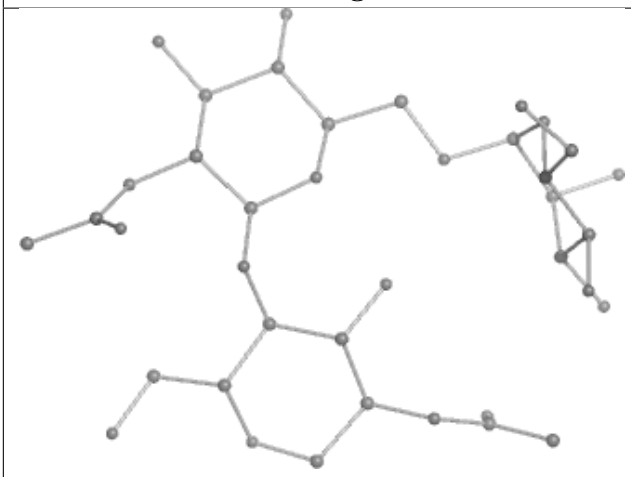
Oligosaccharide Chain vA



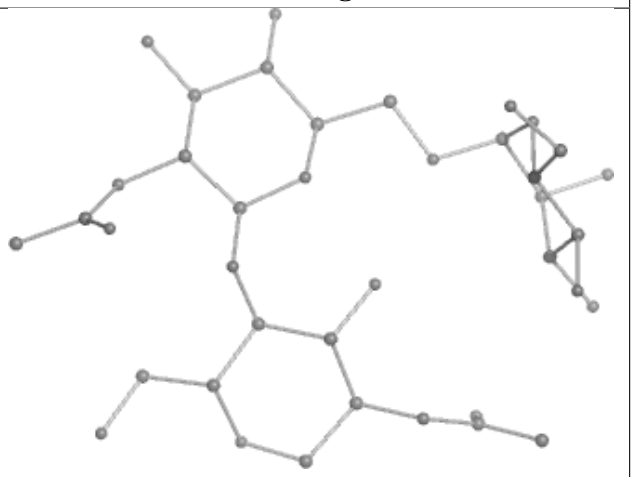
Bond lengths



Bond angles

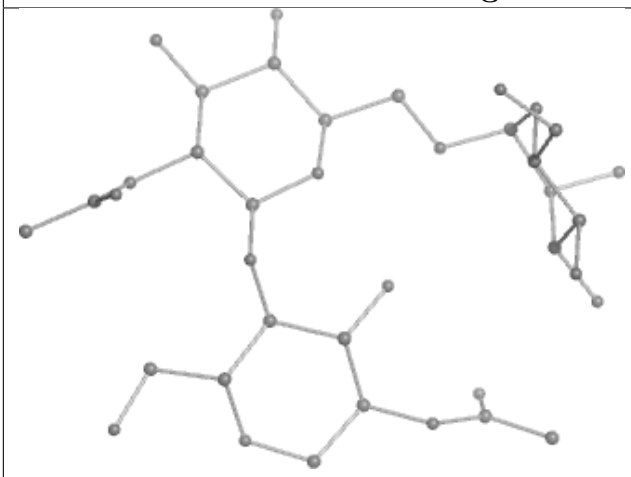


Torsions

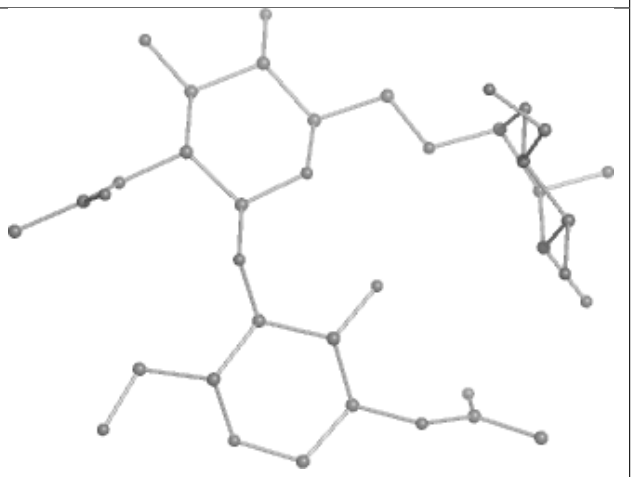


Rings

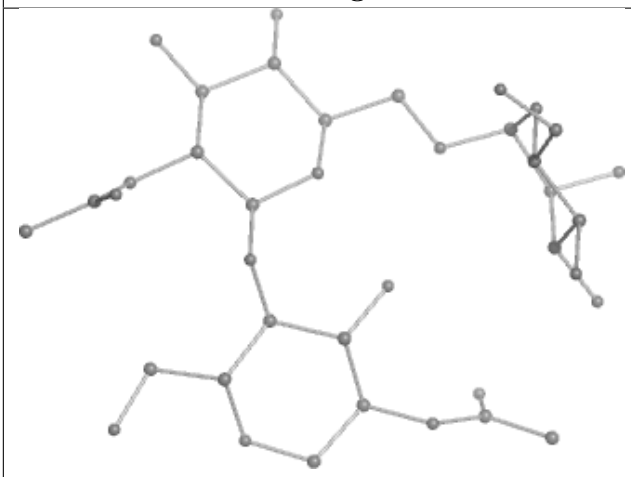
Oligosaccharide Chain wA



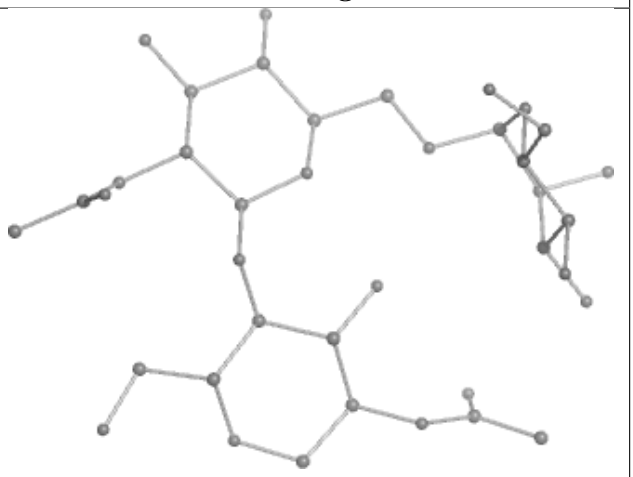
Bond lengths



Bond angles

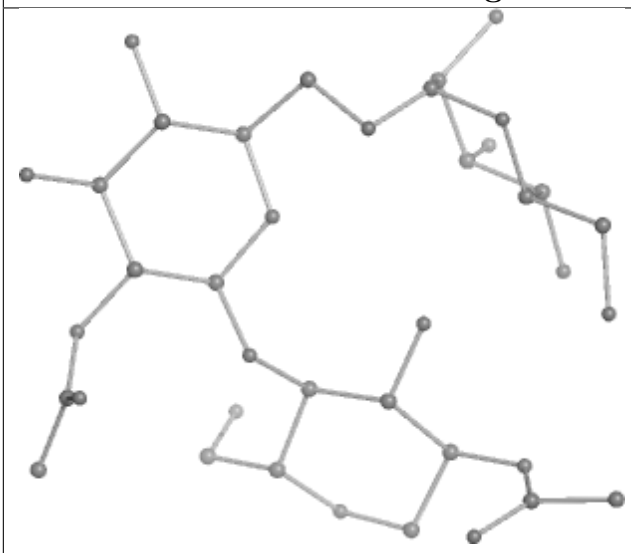


Torsions

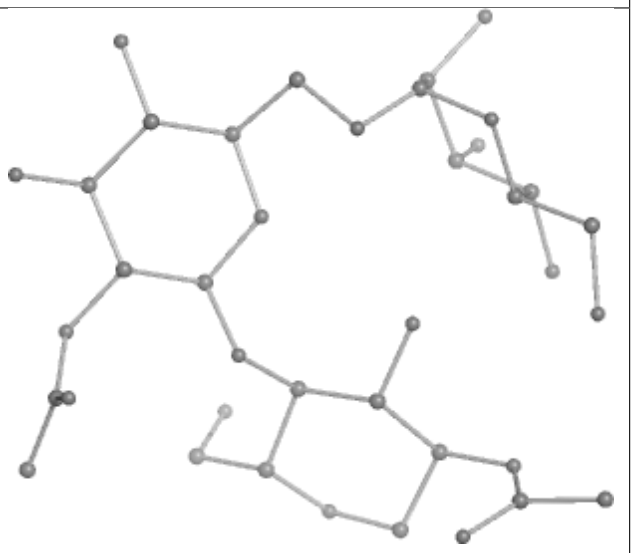


Rings

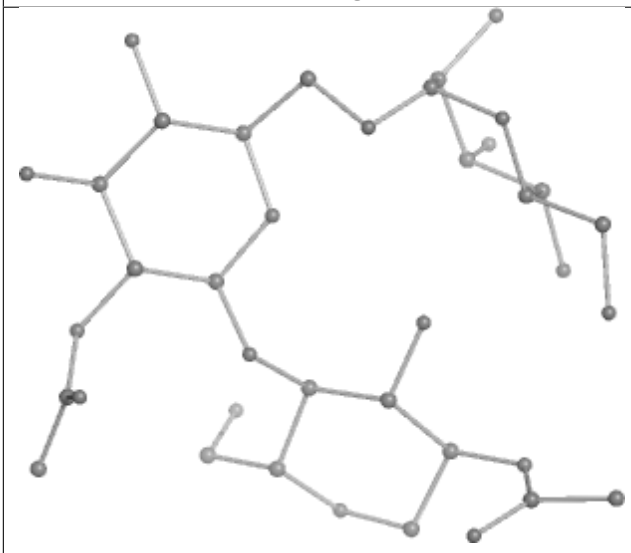
Oligosaccharide Chain xA



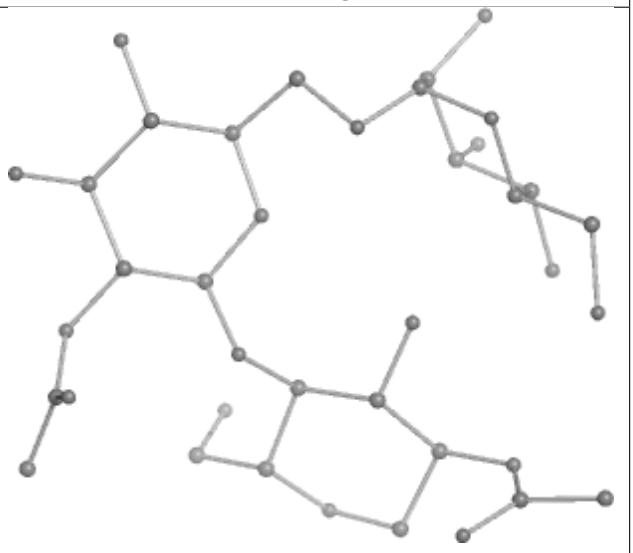
Bond lengths



Bond angles

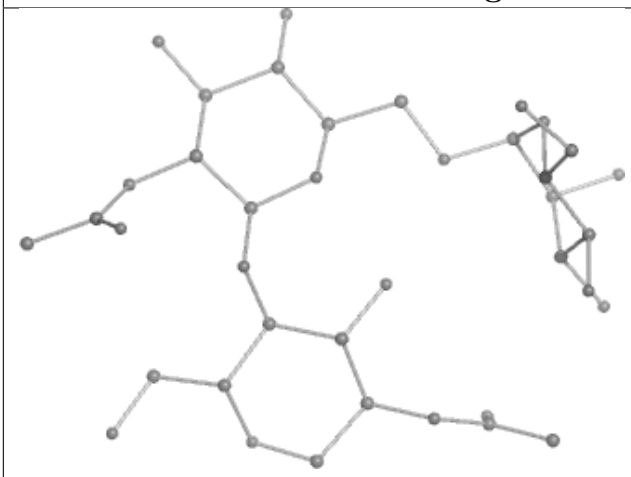


Torsions

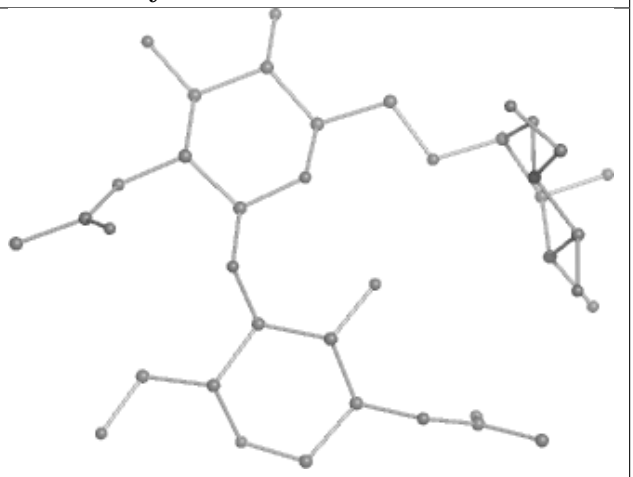


Rings

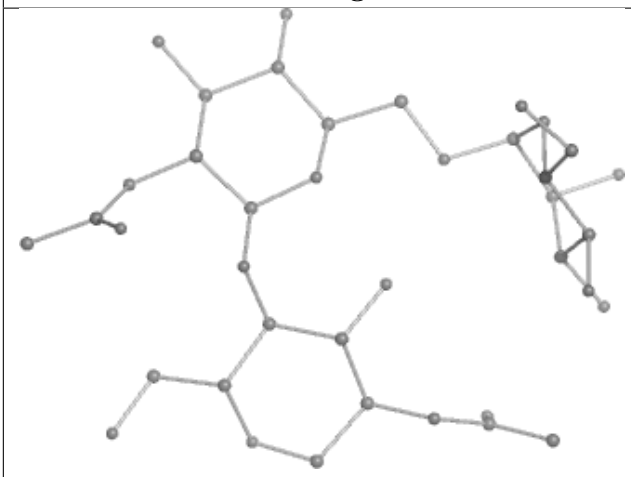
Oligosaccharide Chain yA



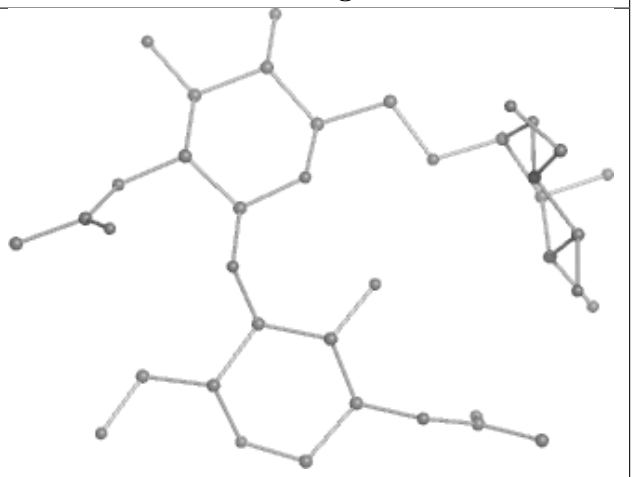
Bond lengths



Bond angles

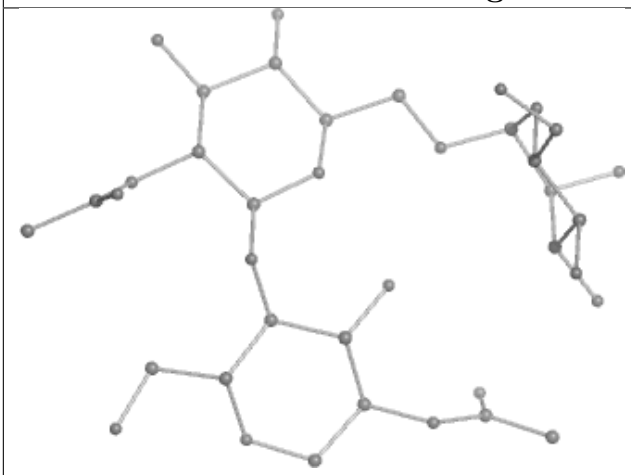


Torsions

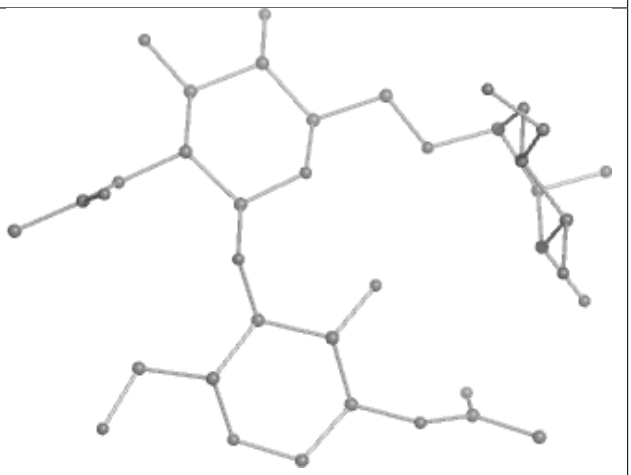


Rings

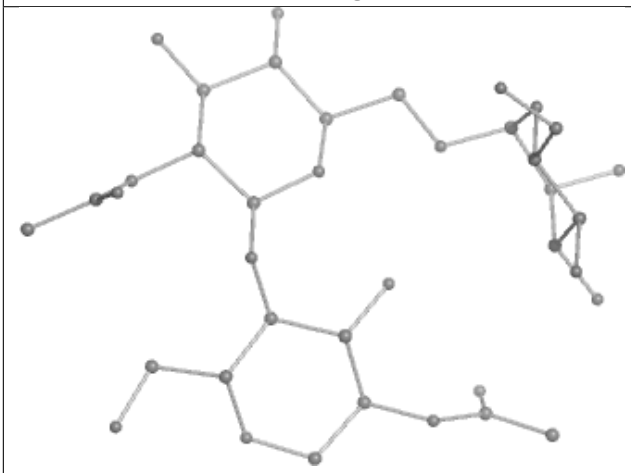
Oligosaccharide Chain zA



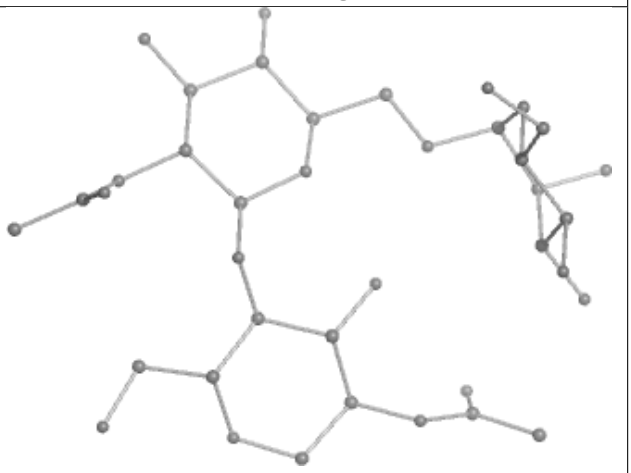
Bond lengths



Bond angles

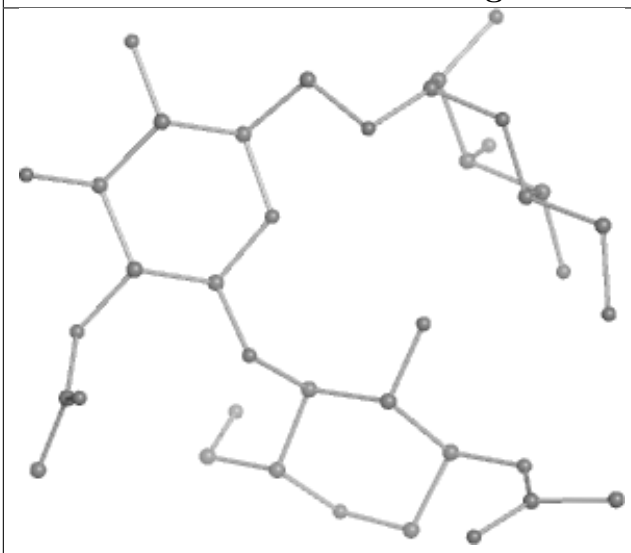


Torsions

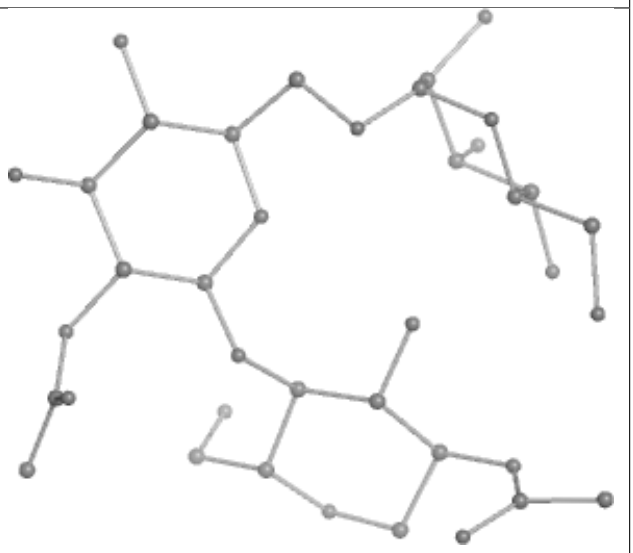


Rings

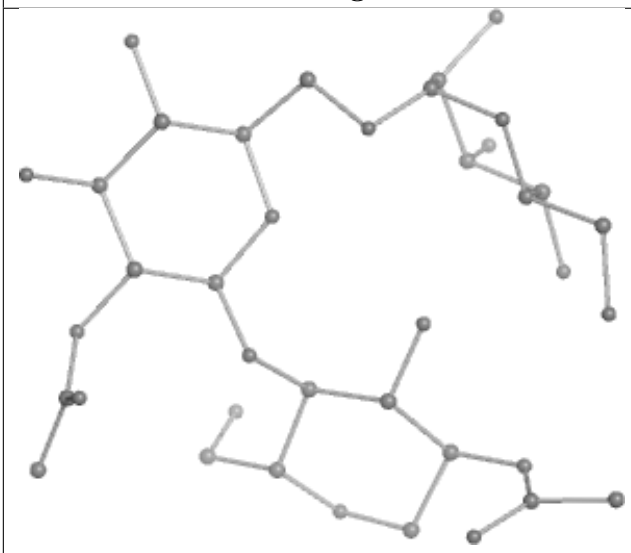
Oligosaccharide Chain 0A



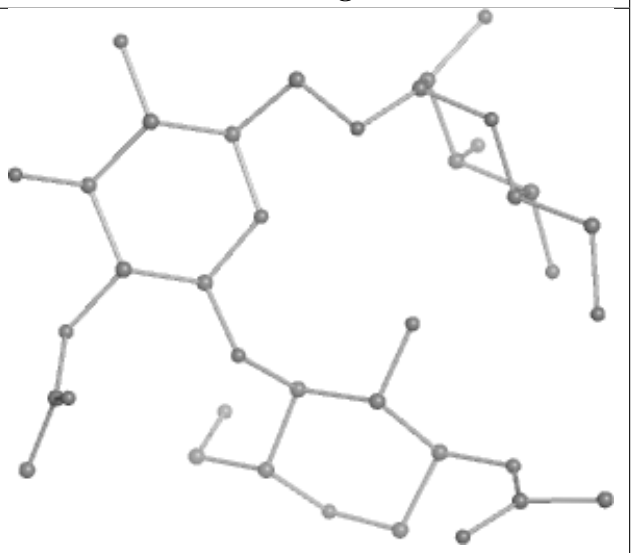
Bond lengths



Bond angles

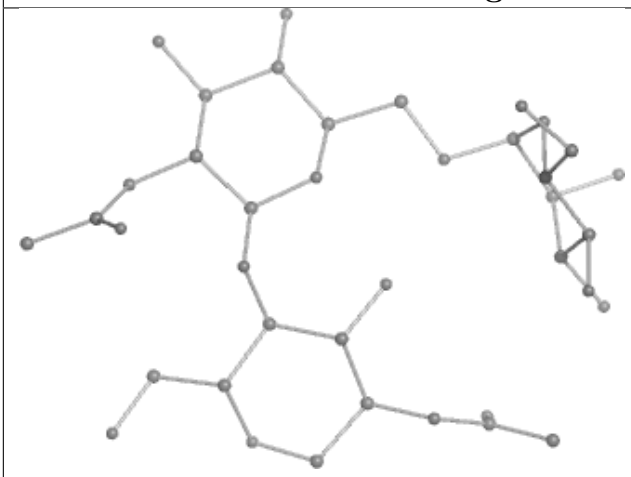


Torsions

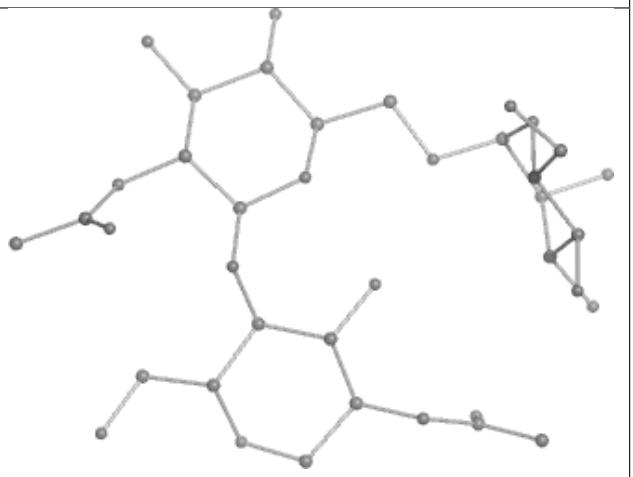


Rings

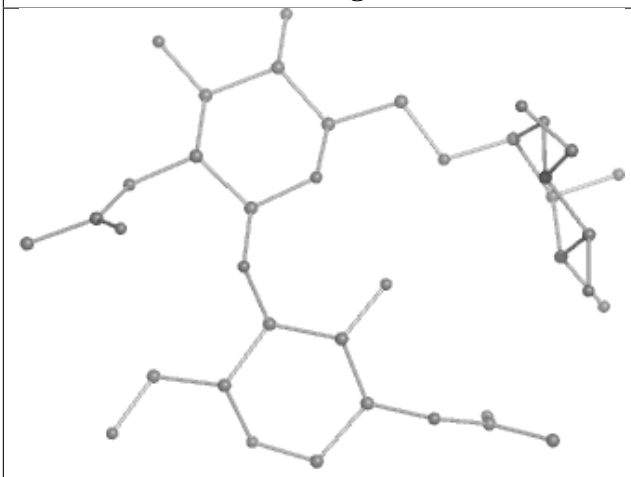
Oligosaccharide Chain 1A



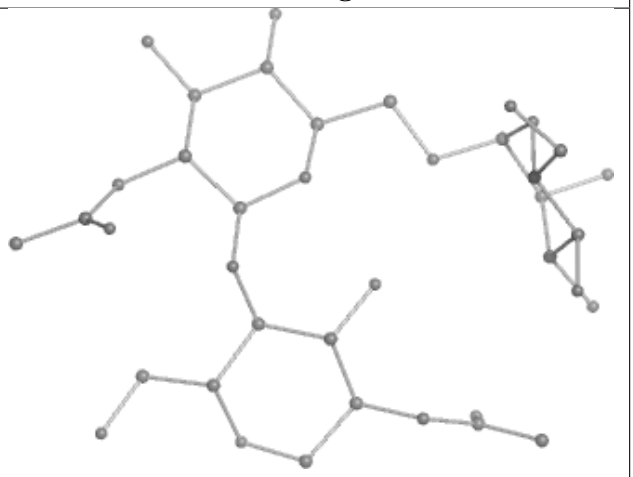
Bond lengths



Bond angles

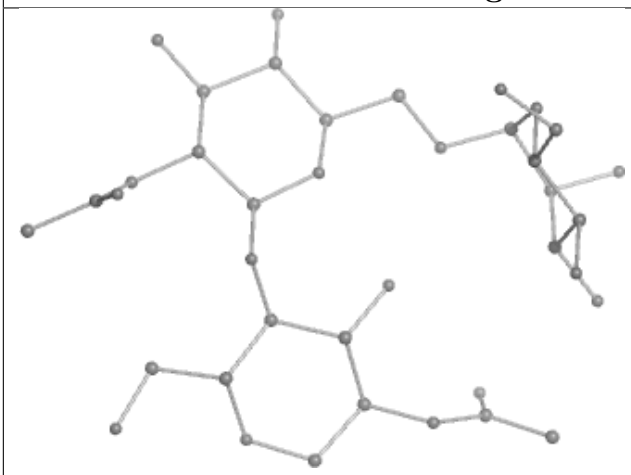


Torsions

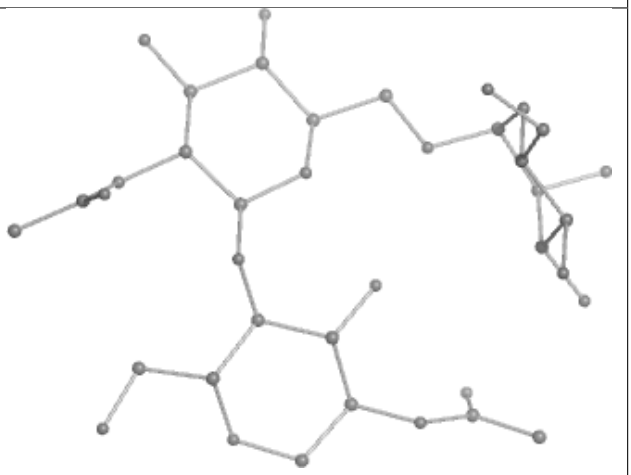


Rings

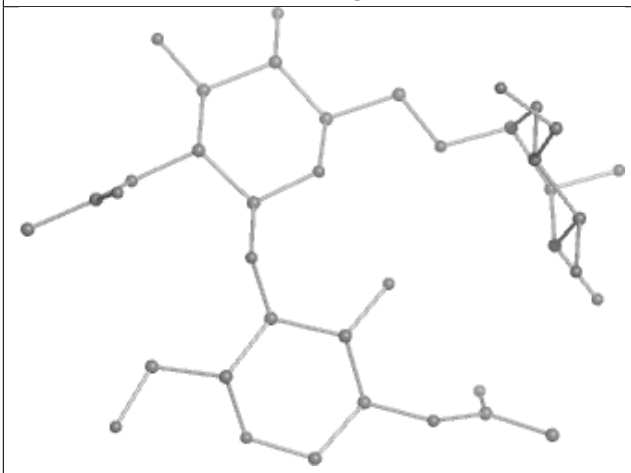
Oligosaccharide Chain 2A



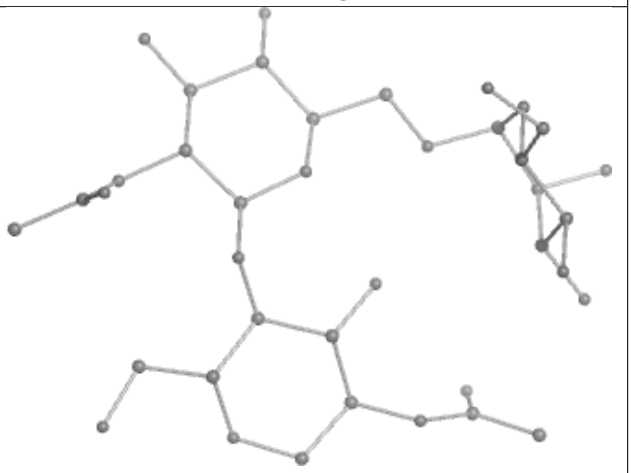
Bond lengths



Bond angles

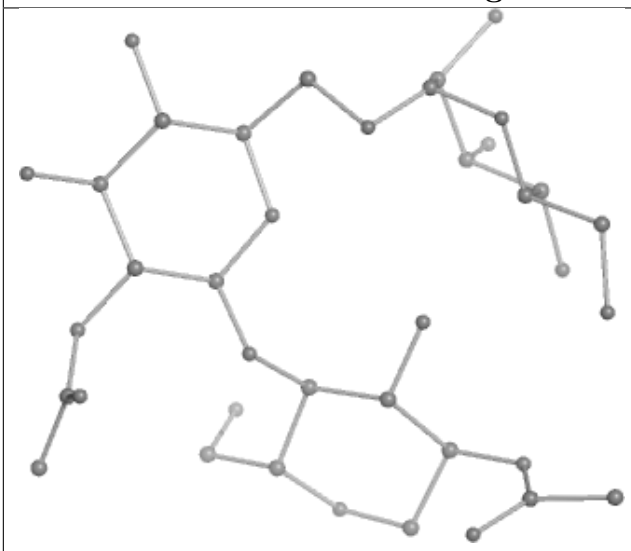


Torsions

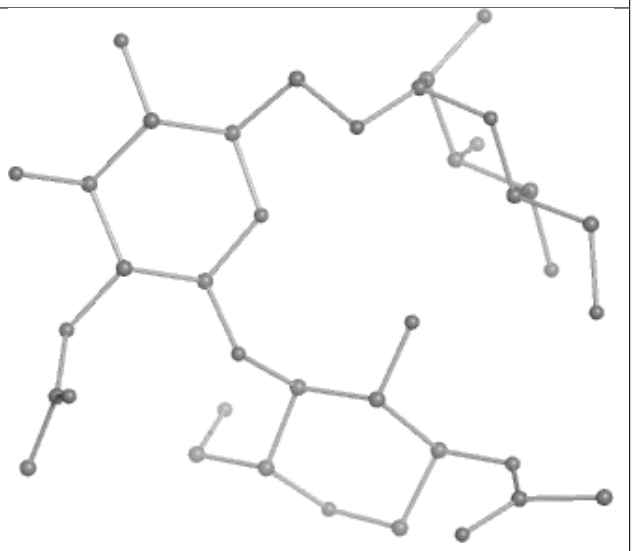


Rings

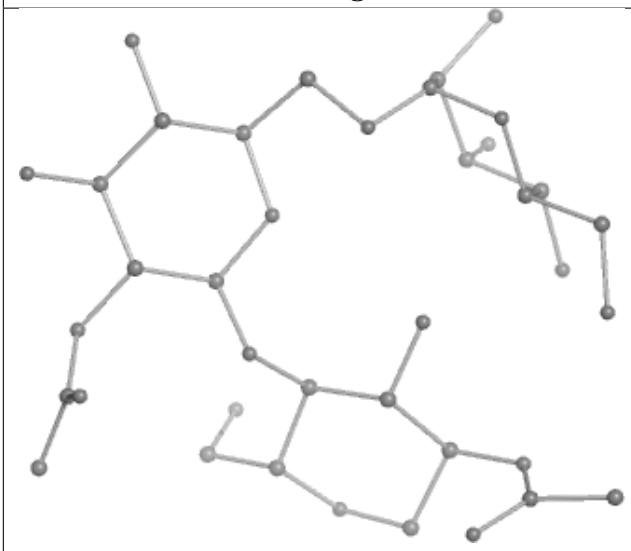
Oligosaccharide Chain 3A



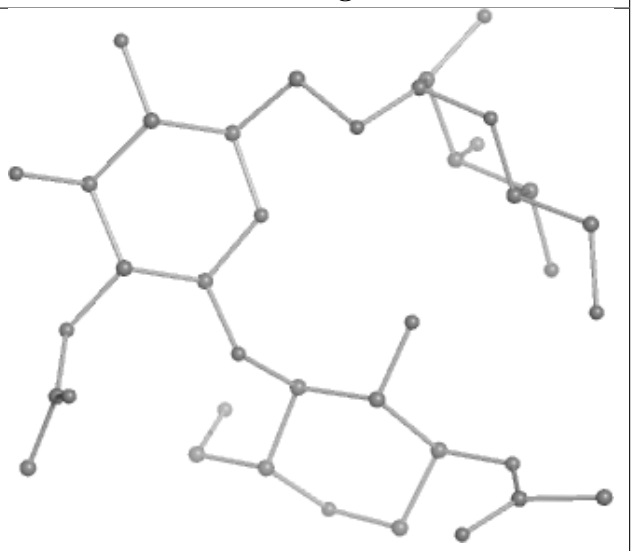
Bond lengths



Bond angles

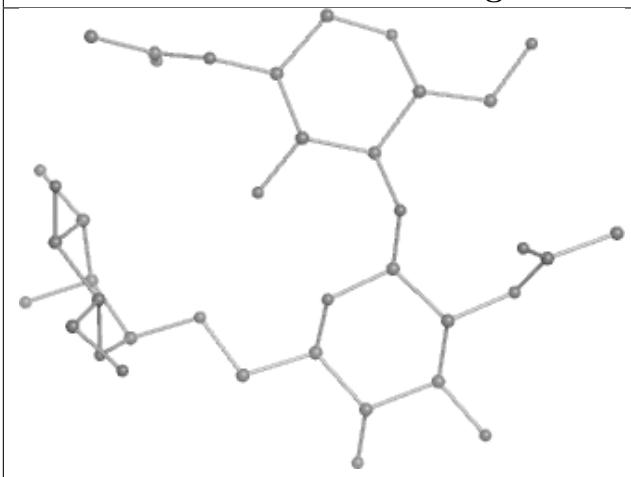


Torsions

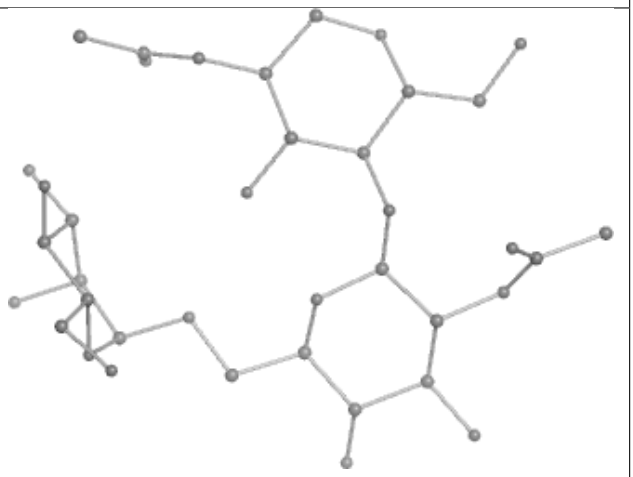


Rings

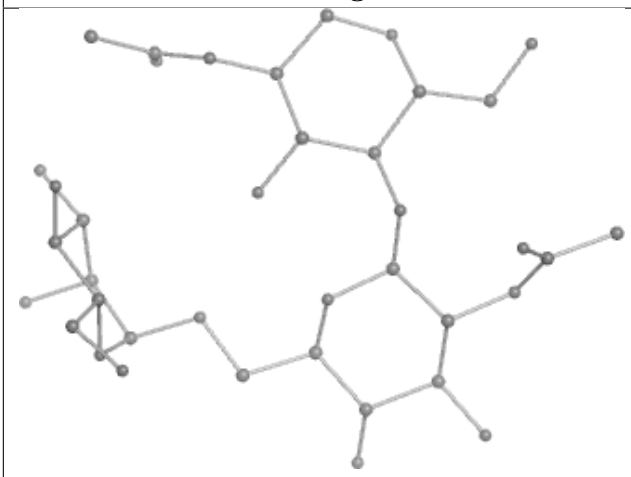
Oligosaccharide Chain 4A



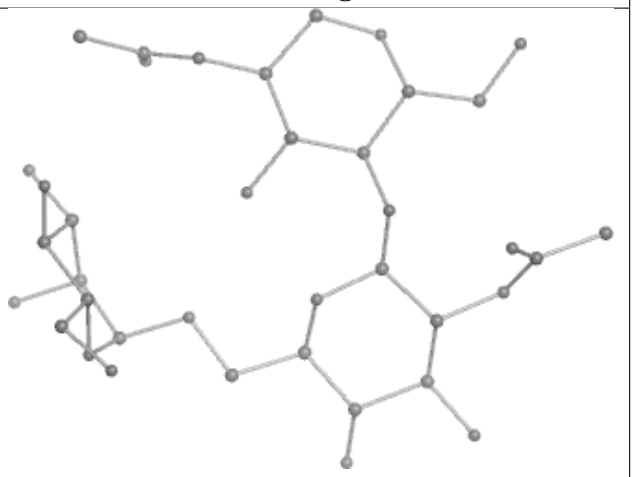
Bond lengths



Bond angles

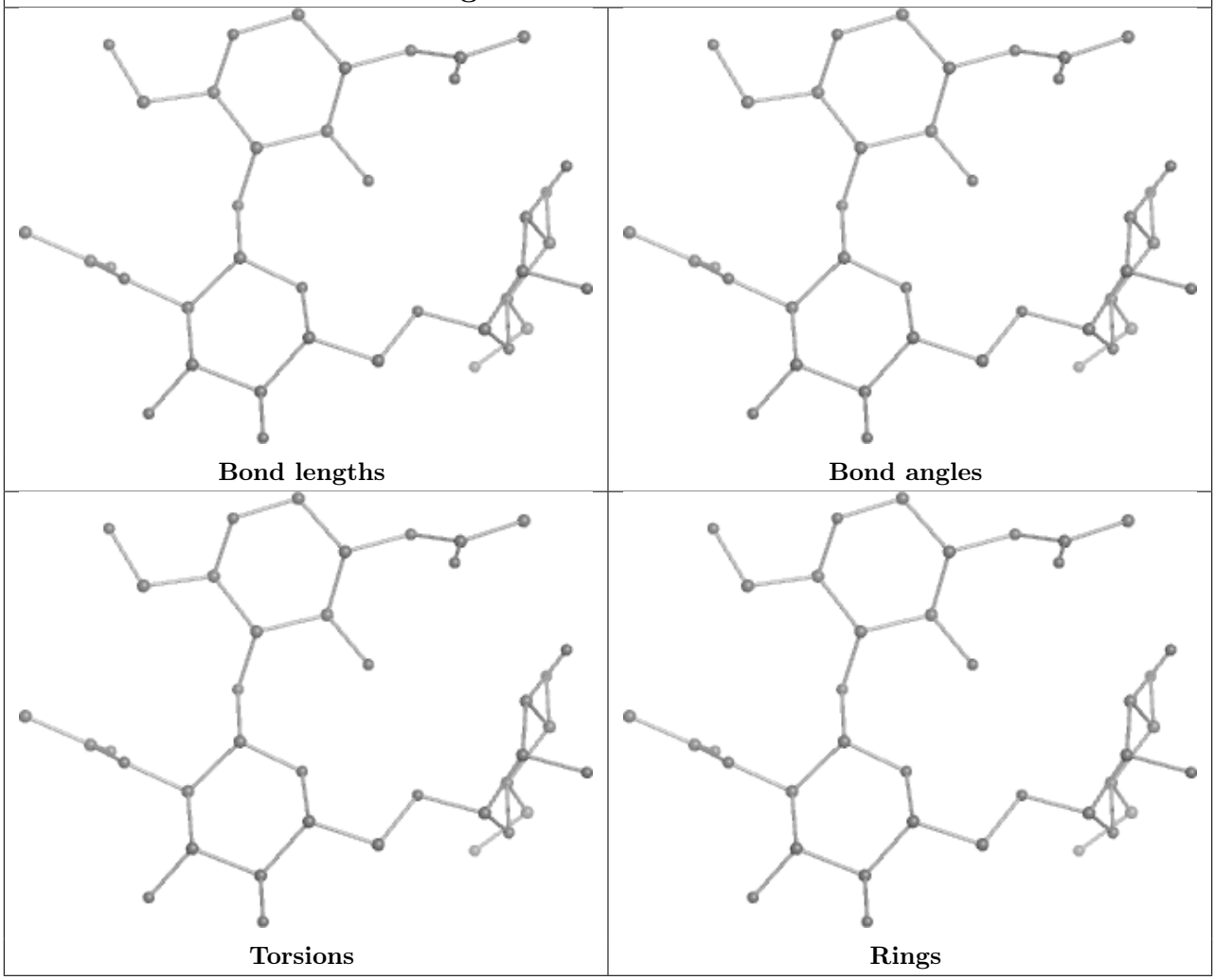


Torsions



Rings

Oligosaccharide Chain 5A



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

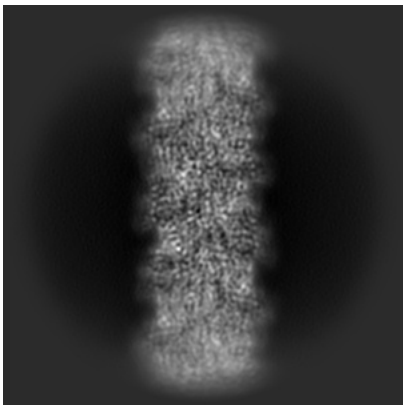
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19990. These allow visual inspection of the internal detail of the map and identification of artifacts.

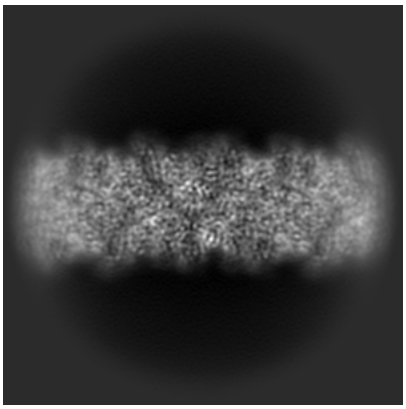
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

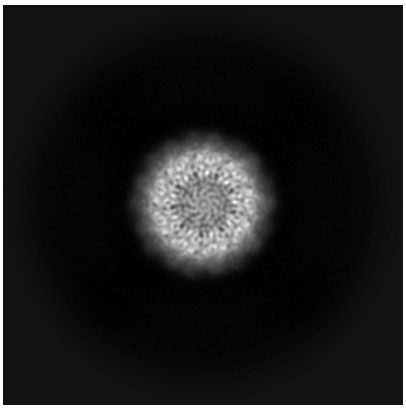
6.1.1 Primary map



X

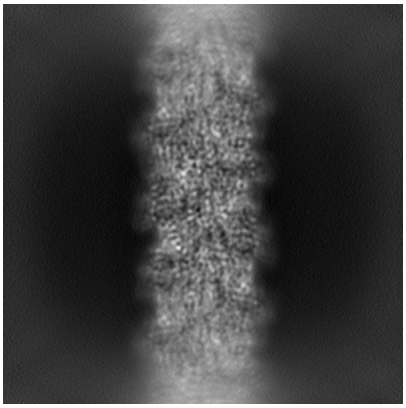


Y

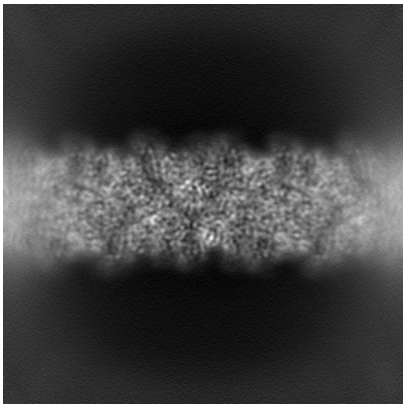


Z

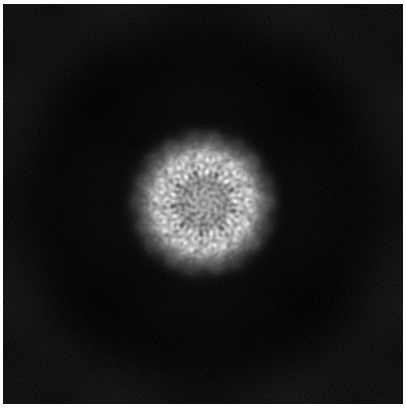
6.1.2 Raw map



X



Y

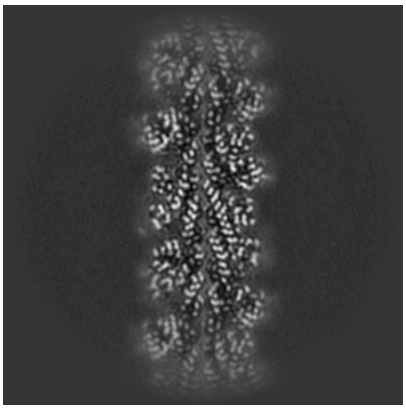


Z

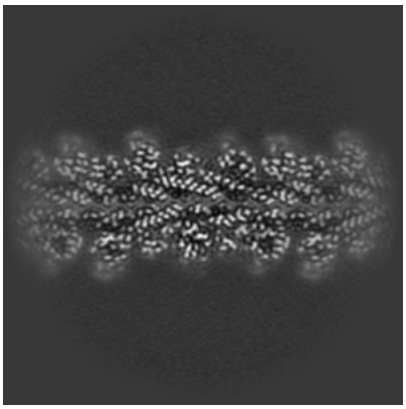
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

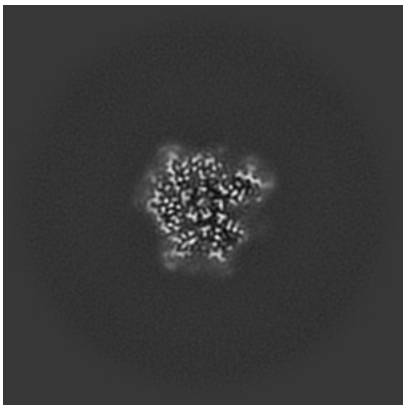
6.2.1 Primary map



X Index: 144

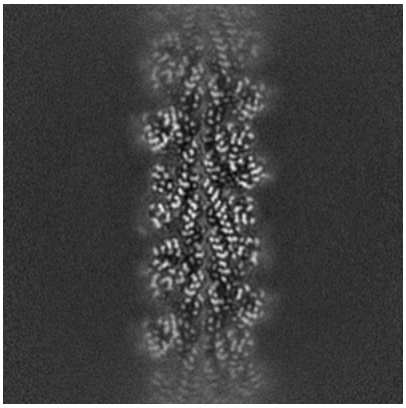


Y Index: 144

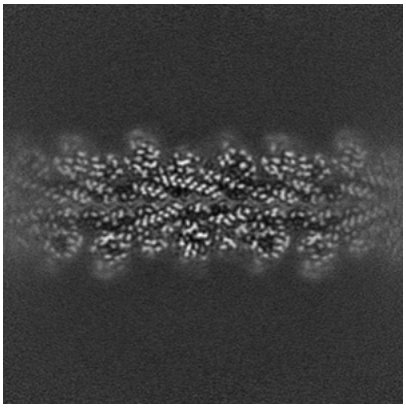


Z Index: 144

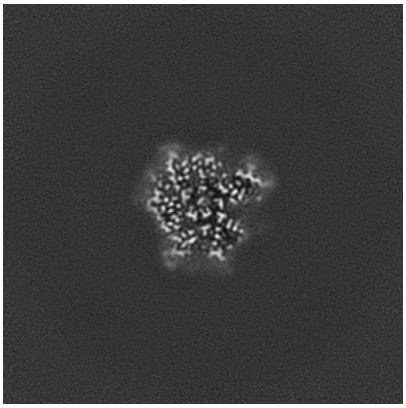
6.2.2 Raw map



X Index: 144



Y Index: 144

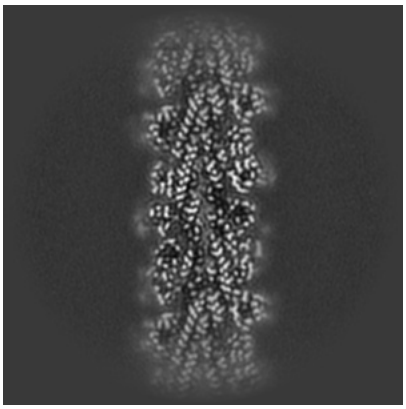


Z Index: 144

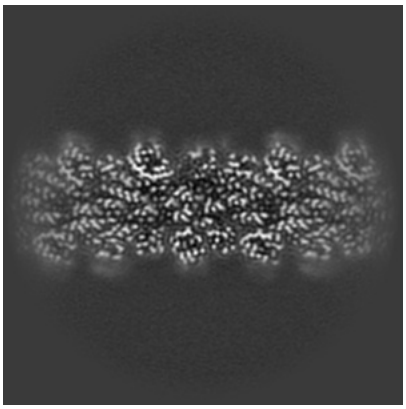
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

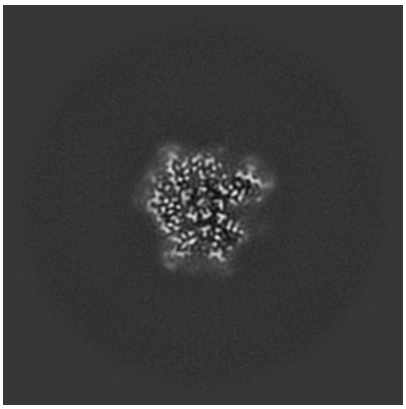
6.3.1 Primary map



X Index: 147

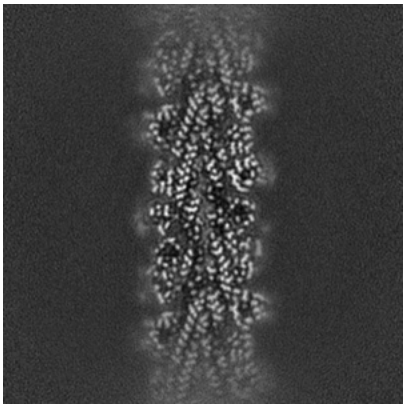


Y Index: 150

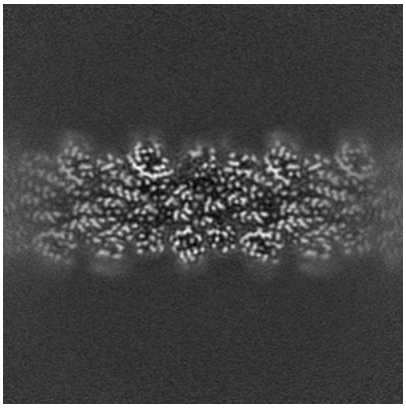


Z Index: 144

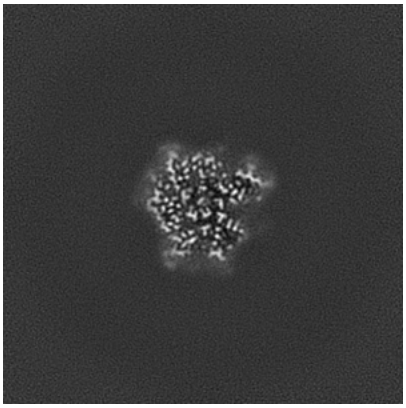
6.3.2 Raw map



X Index: 147



Y Index: 150

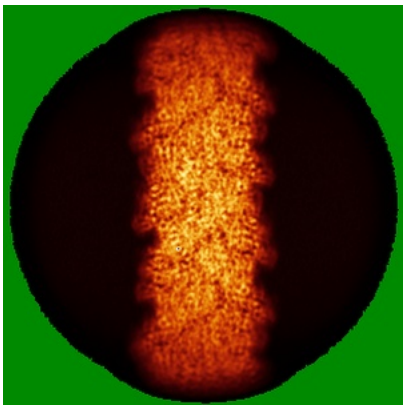


Z Index: 144

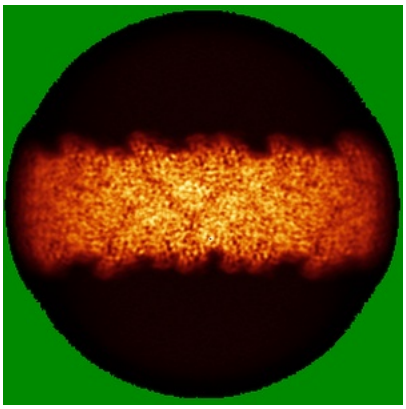
The images above show the largest variance slices of the map in three orthogonal directions.

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

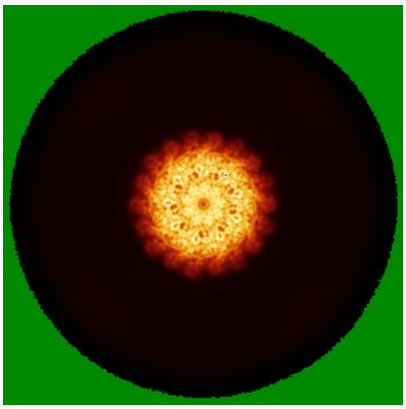
6.4.1 Primary map



X

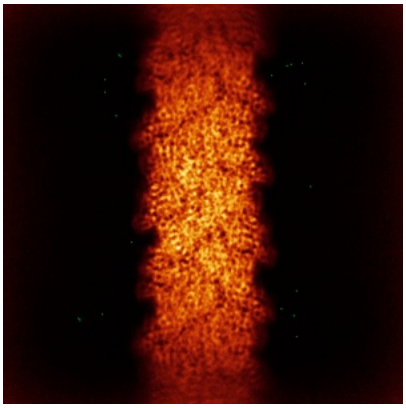


Y

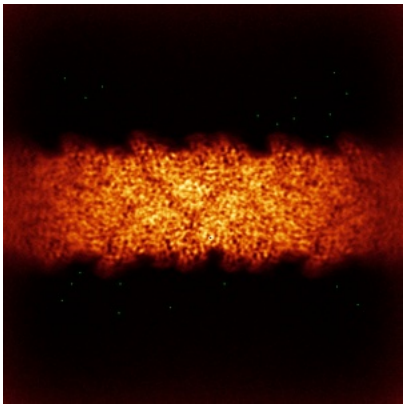


Z

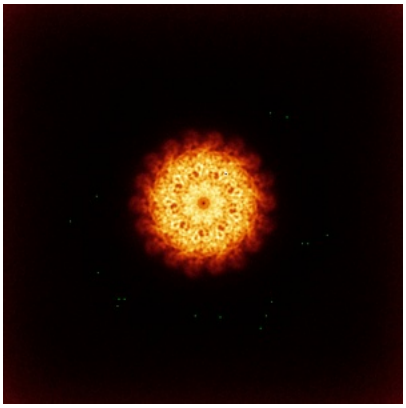
6.4.2 Raw map



X



Y

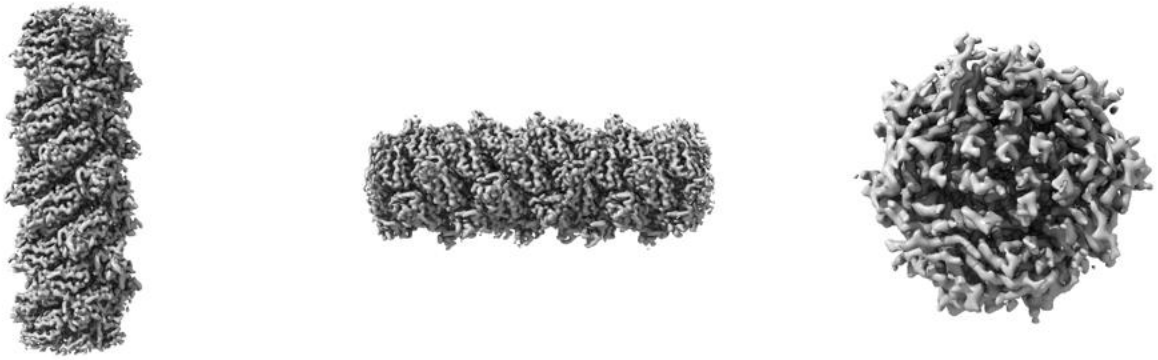


Z

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

6.5 Orthogonal surface views (i)

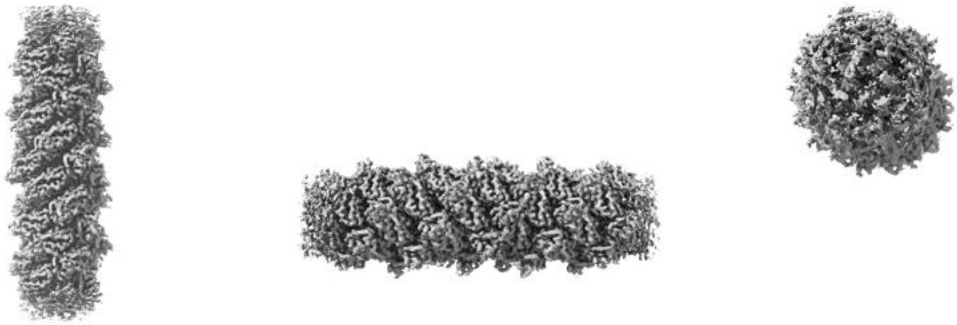
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

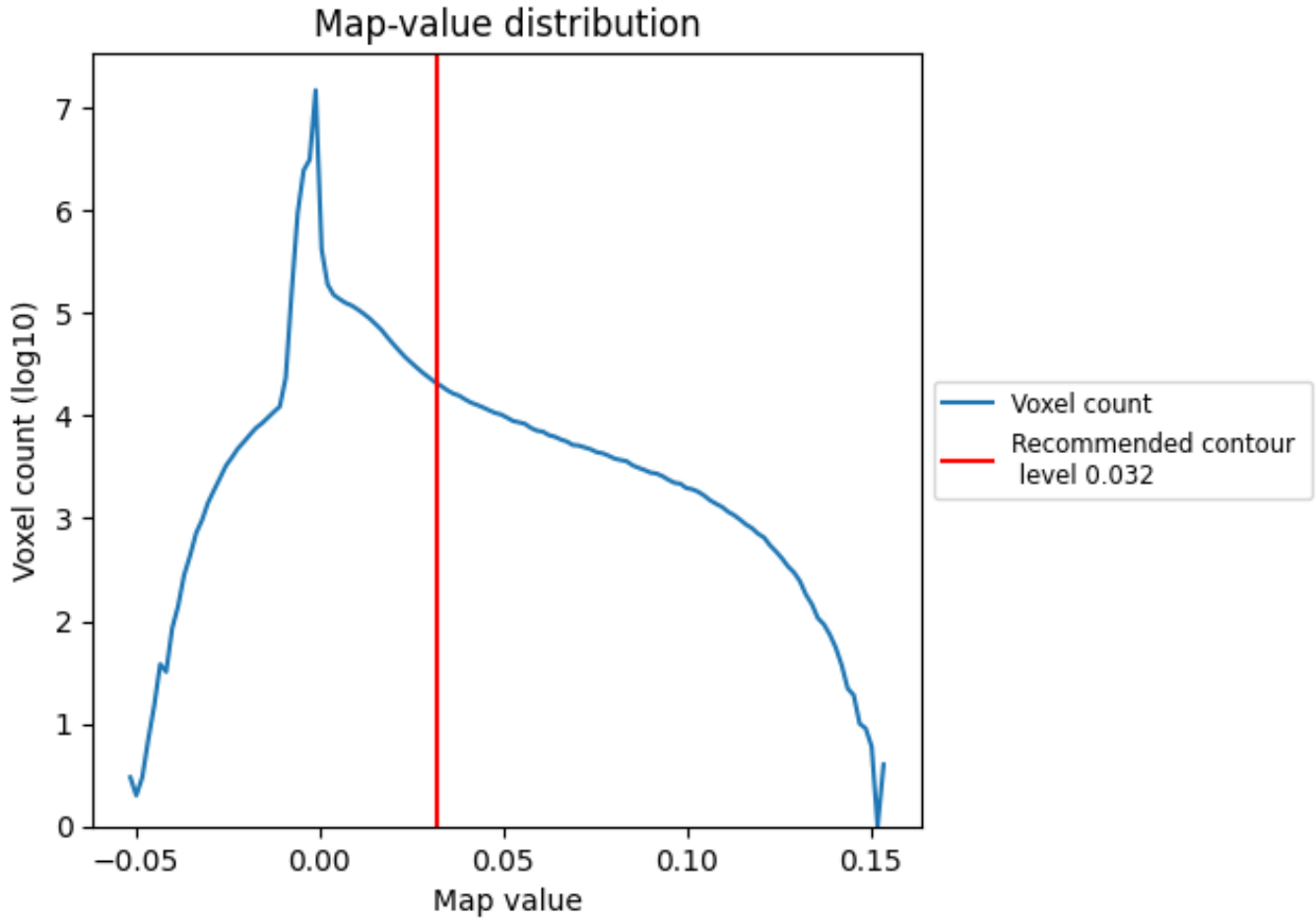
6.6 Mask visualisation (i)

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

7 Map analysis

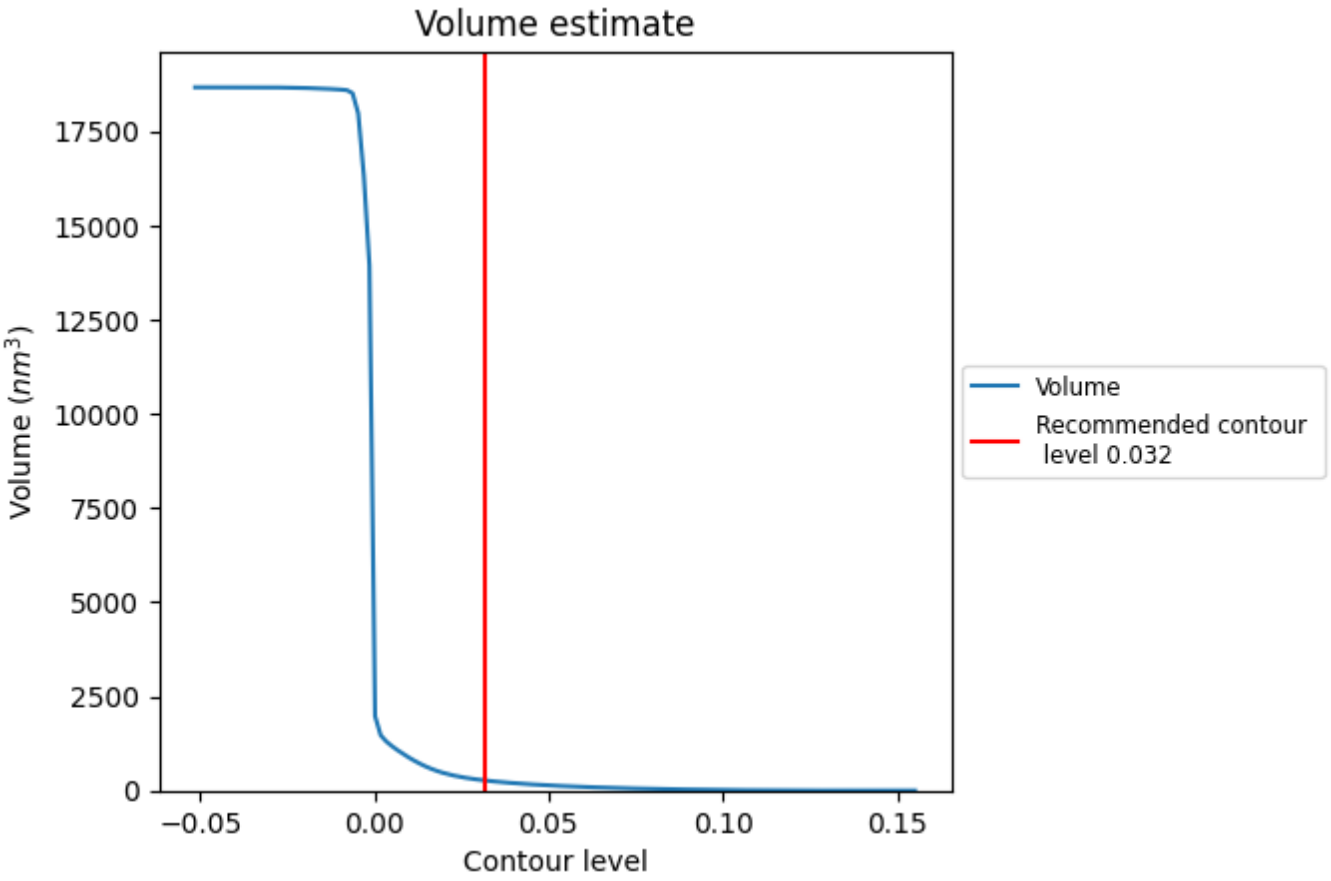
This section contains the results of statistical analysis of the map.

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.

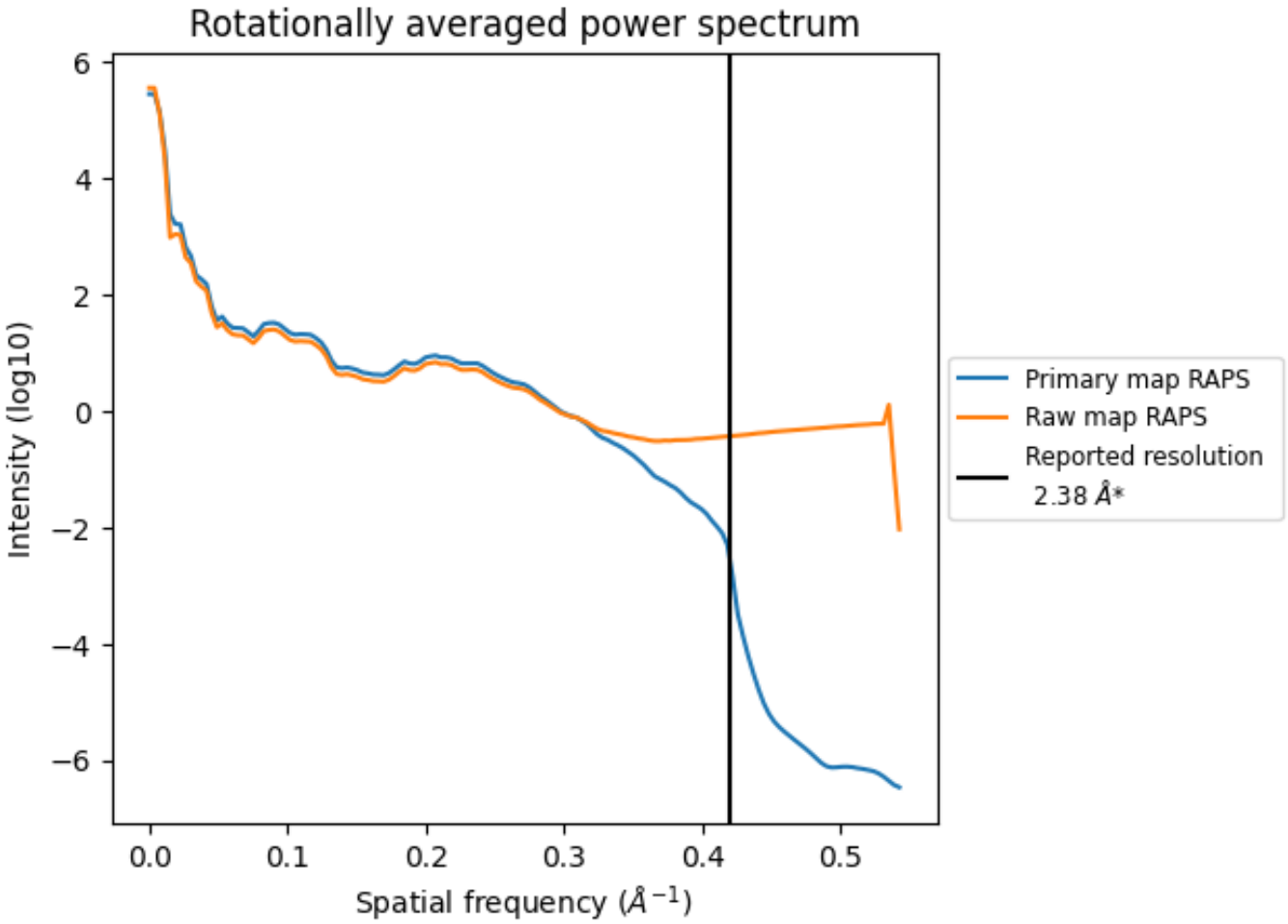
7.2 Volume estimate



The volume at the recommended contour level is 266 nm^3; this corresponds to an approximate mass of 240 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)

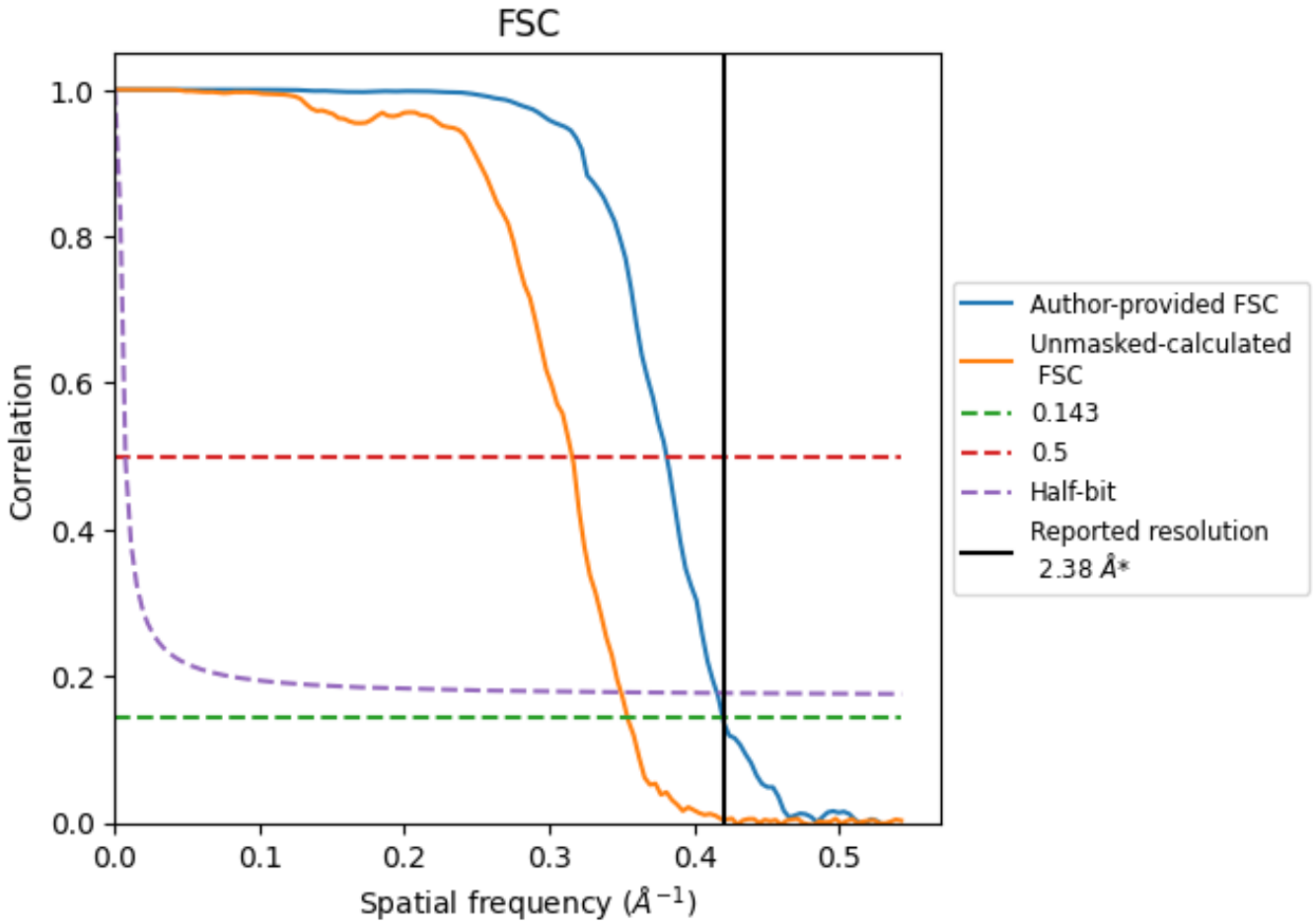


*Reported resolution corresponds to spatial frequency of 0.420 Å^{-1}

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 0.420 Å^{-1}

8.2 Resolution estimates (i)

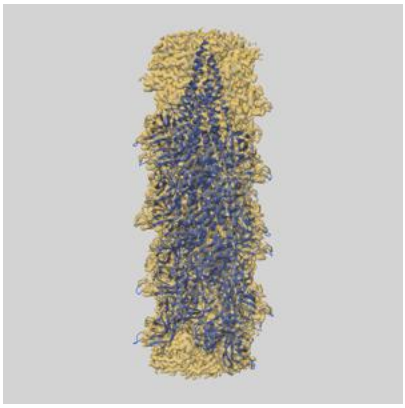
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	2.38	2.63	2.41
Unmasked-calculated*	2.82	3.17	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.82 differs from the reported value 2.38 by more than 10 %

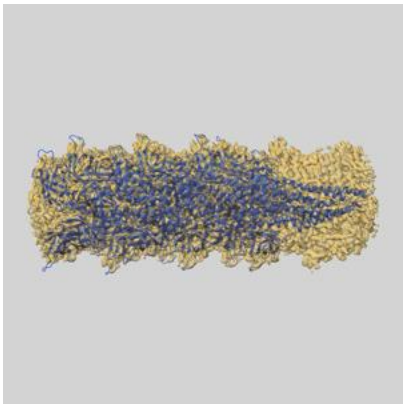
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19990 and PDB model 9EV0. Per-residue inclusion information can be found in section 3 on page 15.

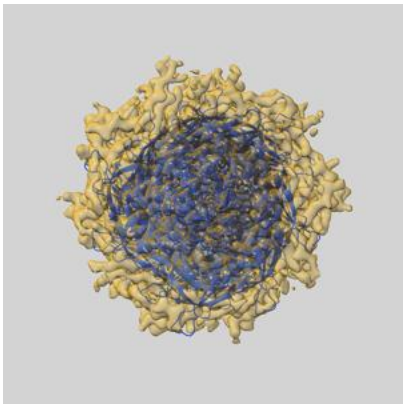
9.1 Map-model overlay



X



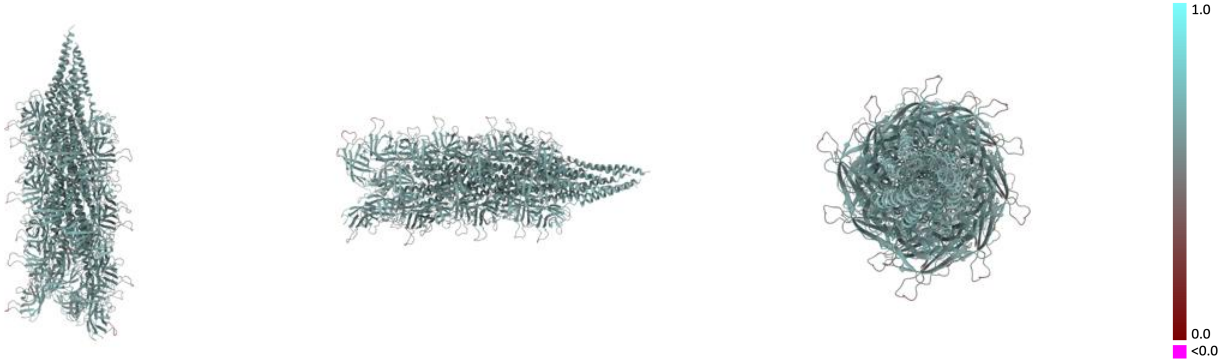
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

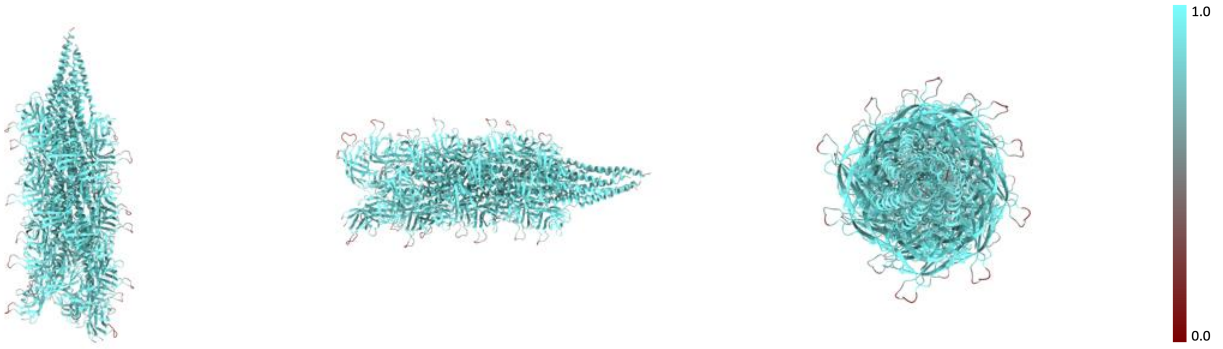
9.2 Q-score mapped to coordinate model



X Y Z

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

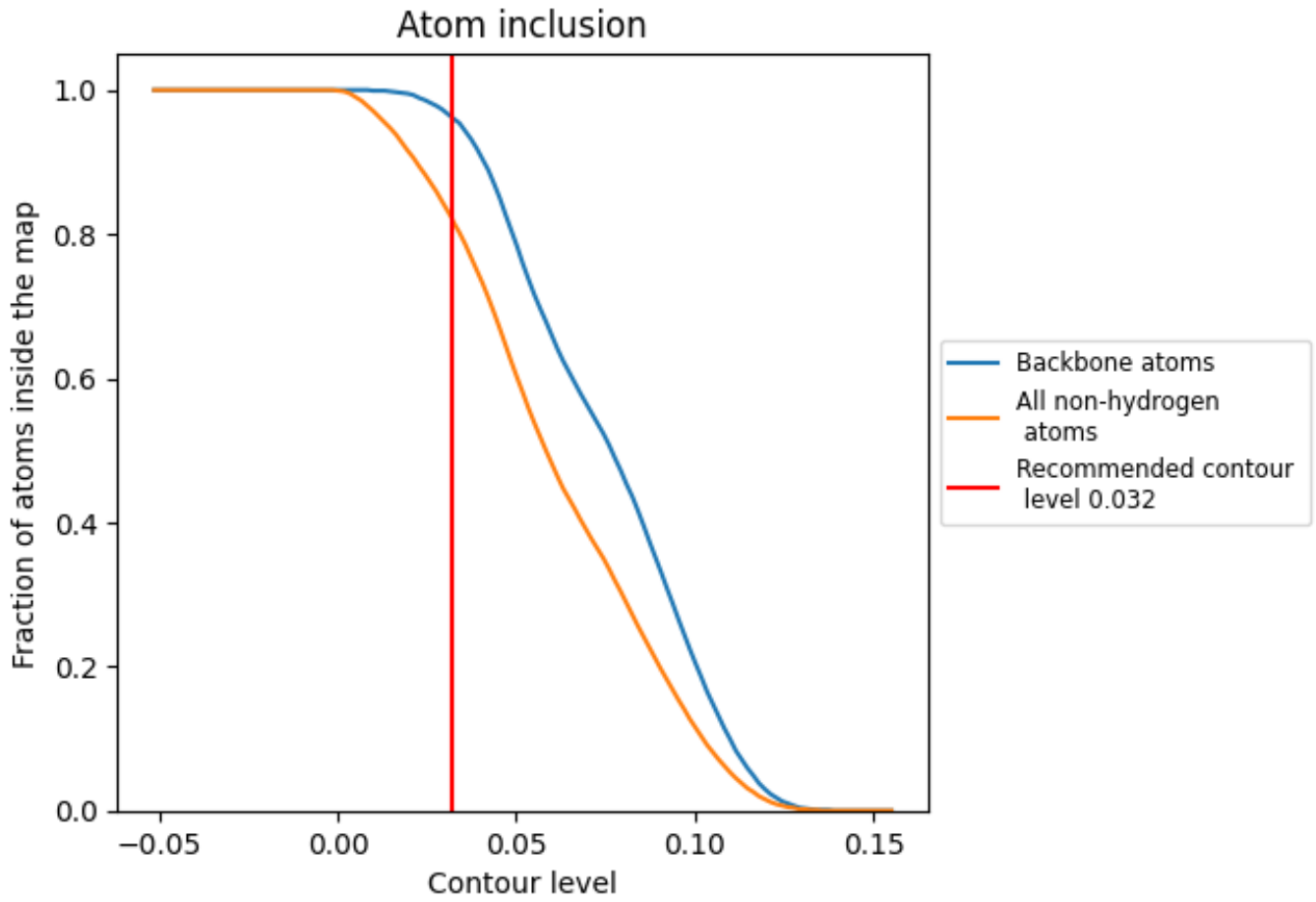
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.5560
0	0.4360	0.3670
0A	0.3080	0.3100
1	0.0000	0.1590
1A	0.1540	0.2720
2	0.1790	0.2530
2A	0.0000	0.2180
3	0.3330	0.3430
3A	0.1030	0.2580
4	0.0000	0.1500
4A	0.0770	0.2630
5	0.0510	0.1750
5A	0.0000	0.1890
6	0.2050	0.3130
7	0.0000	0.0930
8	0.2310	0.2990
9	0.2050	0.2460
A	0.8910	0.5910
AA	0.0000	0.1920
B	0.8510	0.5680
BA	0.2310	0.3070
C	0.9010	0.5960
CA	0.2050	0.2590
D	0.9070	0.5990
DA	0.0000	0.1810
E	0.8710	0.5730
EA	0.2310	0.3140
F	0.9170	0.6040
FA	0.2050	0.2560
G	0.9200	0.6040
GA	0.0000	0.2100
H	0.8970	0.5800
HA	0.2560	0.3380
I	0.9280	0.6040
IA	0.1790	0.2380

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Chain	Atom inclusion	Q-score
J	0.9200	0.6040
JA	0.0000	0.1820
K	0.9060	0.5810
KA	0.2560	0.3300
L	0.9300	0.6060
LA	0.1790	0.2130
M	0.9200	0.6060
MA	0.0000	0.1700
N	0.9050	0.5860
NA	0.2560	0.3320
O	0.9340	0.6080
OA	0.1790	0.2230
P	0.9150	0.6010
PA	0.0000	0.1710
Q	0.9040	0.5810
QA	0.2560	0.3080
R	0.9330	0.6040
RA	0.1790	0.2260
S	0.9080	0.5970
SA	0.0000	0.1810
T	0.8940	0.5780
TA	0.2310	0.2940
U	0.9240	0.6020
UA	0.1790	0.2160
V	0.9000	0.5910
VA	0.0000	0.1740
W	0.8860	0.5750
WA	0.1790	0.2420
X	0.9120	0.5980
XA	0.1790	0.2350
Y	0.8730	0.5850
YA	0.0000	0.1970
Z	0.8650	0.5730
ZA	0.1030	0.2030
a	0.8920	0.5930
aA	0.1030	0.2030
b	0.8200	0.5760
bA	0.0000	0.1250
c	0.8230	0.5650
cA	0.4620	0.3080
d	0.8350	0.5820
dA	0.2050	0.3000

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Chain	Atom inclusion	Q-score
e	0.2560	0.2370
eA	0.0000	0.2670
f	0.5640	0.3730
fA	0.4620	0.2920
g	0.0260	0.2160
gA	0.2050	0.2860
h	0.2560	0.2520
hA	0.0000	0.2860
i	0.4620	0.3680
iA	0.4620	0.3050
j	0.0000	0.2060
jA	0.2050	0.2810
k	0.2820	0.2500
kA	0.0000	0.2870
l	0.5130	0.3710
lA	0.4620	0.3220
m	0.0260	0.2570
mA	0.2050	0.3080
n	0.2820	0.2470
nA	0.0000	0.2730
o	0.5380	0.3750
oA	0.4870	0.3240
p	0.0260	0.2060
pA	0.2050	0.2950
q	0.2820	0.2490
qA	0.0000	0.2340
r	0.4870	0.3670
rA	0.4620	0.3520
s	0.0260	0.1860
sA	0.2050	0.2990
t	0.2560	0.2880
tA	0.0000	0.2350
u	0.4870	0.3810
uA	0.4360	0.3530
v	0.0260	0.2190
vA	0.1790	0.2730
w	0.2820	0.2730
wA	0.0000	0.2040
x	0.4620	0.3850
xA	0.4100	0.3230
y	0.0260	0.1840
yA	0.2050	0.2630

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Chain	Atom inclusion	Q-score
z	0.2050	0.2640
zA	0.0000	0.2350