Full wwPDB EM Validation Report ⓘ

Jan 28, 2025 – 12:49 pm GMT

PDB ID	:	9ETS
EMDB ID	:	EMD-19960
Title	:	Sulfolobus acidocaldarius AAP filament
Authors	:	Daum, B.; Isupov, M.N.; Gaines, M.; McLaren, M.; Mollat, C.
Deposited on	:	2024-03-26
Resolution	:	2.60 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:

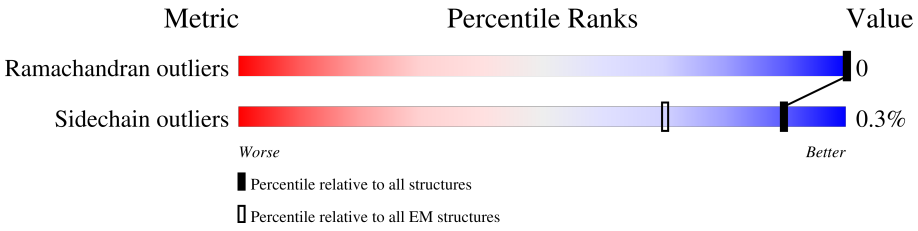
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.60 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	99%
1	C	141	100%
1	D	141	100%
1	E	141	99%
1	F	141	100%
1	G	141	100%
1	H	141	99%
1	I	141	100%

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Mol	Chain	Length	Quality of chain
1	J	141	100%
1	K	141	99%
1	L	141	100%
1	M	141	100%
1	N	141	99%
1	O	141	100%
1	P	141	100%
1	Q	141	99%
1	R	141	100%
1	S	141	100%
1	T	141	99%
1	U	141	100%
1	V	141	100%
1	W	141	99%
1	X	141	100%
1	Y	141	100%
1	Z	141	99%
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	5% 100%

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Mol	Chain	Length	Quality of chain
1	i	141	99%
1	j	141	100%
1	l	141	14% 99%
2	0	5	60% 20% 80%
2	1	5	80% 80% 20%
2	1A	5	60% 20% 80%
2	3	5	60% 40% 60%
2	4	5	80% 80% 20%
2	4A	5	60% 20% 80%
2	6	5	80% 20% 80%
2	7	5	80% 80% 20%
2	7A	5	60% 20% 80%
2	9	5	80% 20% 80%
2	AA	5	80% 80% 20%
2	AB	5	60% 20% 80%
2	CA	5	80% 20% 80%
2	DA	5	80% 80% 20%
2	DB	5	60% 20% 80%
2	FA	5	80% 20% 80%
2	GA	5	80% 80% 20%
2	GB	5	60% 20% 80%
2	IA	5	80% 20% 80%
2	JA	5	80% 80% 20%
2	JB	5	60% 20% 80%
2	LA	5	40% 20% 80%

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Mol	Chain	Length	Quality of chain
2	MB	5	60% 20% 80%
2	OA	5	40% 20% 80%
2	PB	5	60% 20% 80%
2	RA	5	40% 20% 80%
2	SB	5	80% 20% 80%
2	UA	5	40% 20% 80%
2	VB	5	100% 20% 80%
2	XA	5	40% 20% 80%
2	aA	5	40% 20% 80%
2	dA	5	40% 20% 80%
2	gA	5	40% 20% 80%
2	jA	5	40% 20% 80%
2	k	5	80% 20% 80%
2	m	5	80% 80% 20%
2	mA	5	60% 20% 80%
2	o	5	80% 20% 80%
2	p	5	80% 80% 20%
2	pA	5	60% 20% 80%
2	r	5	80% 20% 80%
2	s	5	80% 80% 20%
2	sA	5	80% 20% 80%
2	u	5	60% 20% 80%
2	v	5	80% 80% 20%
2	vA	5	60% 20% 80%
2	x	5	60% 40% 60%

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Mol	Chain	Length	Quality of chain
2	y	5	80% 80% 20%
2	yA	5	60% 20% 80%
3	0A	3	100% 33% 67%
3	2	3	100% 100%
3	3A	3	100% 33% 67%
3	5	3	100% 100%
3	6A	3	100% 33% 67%
3	8	3	100% 100%
3	9A	3	100% 67% 33%
3	BA	3	100% 100%
3	CB	3	100% 33% 67%
3	EA	3	100% 100%
3	FB	3	100% 33% 67%
3	HA	3	100% 67% 33%
3	IB	3	100% 33% 67%
3	KA	3	100% 100%
3	LB	3	100% 33% 67%
3	NA	3	67% 33% 67%
3	OB	3	100% 33% 67%
3	QA	3	67% 33% 67%
3	RB	3	100% 33% 67%
3	TA	3	67% 33% 67%
3	UB	3	100% 33% 67%
3	WA	3	67% 33% 67%
3	XB	3	100% 33% 67%

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Mol	Chain	Length	Quality of chain
3	ZA	3	67% 33% 67%
3	cA	3	67% 33% 67%
3	fA	3	67% 33% 67%
3	iA	3	67% 33% 67%
3	lA	3	67% 33% 67%
3	n	3	67% 100%
3	oA	3	100% 33% 67%
3	q	3	100% 100%
3	rA	3	100% 33% 67%
3	t	3	67% 100%
3	uA	3	100% 33% 67%
3	w	3	67% 100%
3	xA	3	100% 33% 67%
3	z	3	100% 100%
4	2A	4	75% 75% 25%
4	5A	4	75% 75% 25%
4	8A	4	75% 75% 25%
4	BB	4	75% 75% 25%
4	EB	4	75% 75% 25%
4	HB	4	75% 75% 25%
4	KB	4	75% 75% 25%
4	MA	4	75% 50% 50%
4	NB	4	75% 75% 25%
4	PA	4	75% 50% 50%
4	QB	4	75% 75% 25%

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Mol	Chain	Length	Quality of chain
4	SA	4	75% 50% 50%
4	TB	4	75% 75% 25%
4	VA	4	75% 50% 50%
4	WB	4	100% 75% 25%
4	YA	4	75% 50% 50%
4	bA	4	75% 75% 25%
4	eA	4	75% 75% 25%
4	hA	4	75% 50% 50%
4	kA	4	75% 50% 50%
4	nA	4	75% 50% 50%
4	qA	4	75% 75% 25%
4	tA	4	75% 75% 25%
4	wA	4	75% 75% 25%
4	zA	4	75% 75% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 42941 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	e	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	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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		
1	g	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	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		
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	f	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	l	141	Total	C	N	O	0	0
			1001	639	165	197		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	m	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	o	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	p	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	r	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	s	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	u	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	v	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	x	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	y	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	0	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	1	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	3	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	4	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	6	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	7	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	9	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	AA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	CA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	DA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	FA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	GA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	JA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	LA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	OA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	RA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	UA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	XA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	aA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	dA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	gA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	jA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	mA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	pA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	sA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	vA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	yA	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	1A	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	4A	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	7A	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	AB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	DB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		

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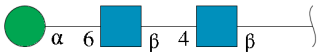
Mol	Chain	Residues	Atoms					AltConf	Trace
2	GB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	JB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	MB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	PB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	SB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		
2	VB	5	Total	C	N	O	S	0	0
			64	34	2	27	1		

- Molecule 3 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
3	n	3	Total	C	N	O	0	0
			39	22	2	15		
3	q	3	Total	C	N	O	0	0
			39	22	2	15		
3	t	3	Total	C	N	O	0	0
			39	22	2	15		
3	w	3	Total	C	N	O	0	0
			39	22	2	15		
3	z	3	Total	C	N	O	0	0
			39	22	2	15		
3	2	3	Total	C	N	O	0	0
			39	22	2	15		
3	5	3	Total	C	N	O	0	0
			39	22	2	15		
3	8	3	Total	C	N	O	0	0
			39	22	2	15		
3	BA	3	Total	C	N	O	0	0
			39	22	2	15		
3	EA	3	Total	C	N	O	0	0
			39	22	2	15		
3	HA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	KA	3	Total	C	N	O	0	0
			39	22	2	15		
3	NA	3	Total	C	N	O	0	0
			39	22	2	15		
3	QA	3	Total	C	N	O	0	0
			39	22	2	15		
3	TA	3	Total	C	N	O	0	0
			39	22	2	15		
3	WA	3	Total	C	N	O	0	0
			39	22	2	15		
3	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
3	cA	3	Total	C	N	O	0	0
			39	22	2	15		
3	fA	3	Total	C	N	O	0	0
			39	22	2	15		
3	iA	3	Total	C	N	O	0	0
			39	22	2	15		
3	lA	3	Total	C	N	O	0	0
			39	22	2	15		
3	oA	3	Total	C	N	O	0	0
			39	22	2	15		
3	rA	3	Total	C	N	O	0	0
			39	22	2	15		
3	uA	3	Total	C	N	O	0	0
			39	22	2	15		
3	xA	3	Total	C	N	O	0	0
			39	22	2	15		
3	0A	3	Total	C	N	O	0	0
			39	22	2	15		
3	3A	3	Total	C	N	O	0	0
			39	22	2	15		
3	6A	3	Total	C	N	O	0	0
			39	22	2	15		
3	9A	3	Total	C	N	O	0	0
			39	22	2	15		
3	CB	3	Total	C	N	O	0	0
			39	22	2	15		
3	FB	3	Total	C	N	O	0	0
			39	22	2	15		
3	IB	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	LB	3	Total	C	N	O	0	0
			39	22	2	15		
3	OB	3	Total	C	N	O	0	0
			39	22	2	15		
3	RB	3	Total	C	N	O	0	0
			39	22	2	15		
3	UB	3	Total	C	N	O	0	0
			39	22	2	15		
3	XB	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[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
4	MA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	PA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	SA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	VA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	YA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	bA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	eA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	hA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	kA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	nA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	qA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	tA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	wA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		

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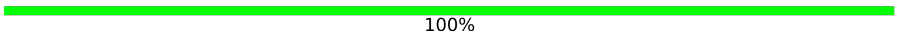
Mol	Chain	Residues	Atoms					AltConf	Trace
4	zA	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	2A	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	5A	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	8A	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	BB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	EB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	HB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	KB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	NB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	QB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	TB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		
4	WB	4	Total	C	N	O	S	0	0
			53	28	2	22	1		

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

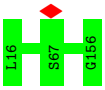
Chain G:



There are no outlier residues recorded for this chain.

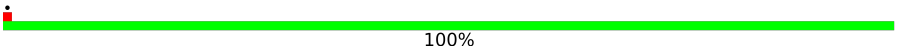
• Molecule 1: DUF4352 domain-containing protein

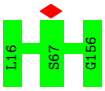
Chain A:



• Molecule 1: DUF4352 domain-containing protein

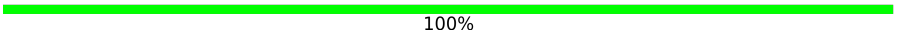
Chain D:





• Molecule 1: DUF4352 domain-containing protein

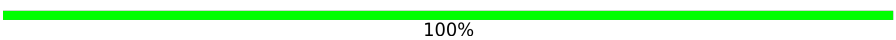
Chain J:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

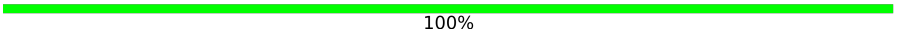
Chain M:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

Chain P:



There are no outlier residues recorded for this chain.

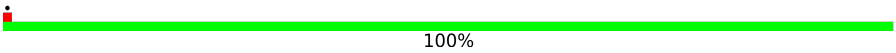
• Molecule 1: DUF4352 domain-containing protein

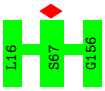
Chain S:

There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

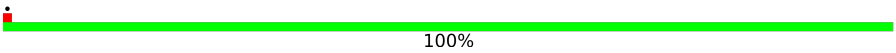
Chain V:

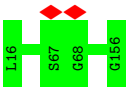




• Molecule 1: DUF4352 domain-containing protein

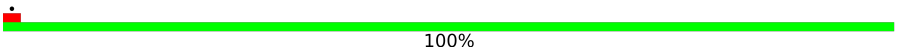
Chain Y:

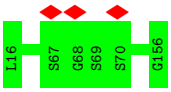




• Molecule 1: DUF4352 domain-containing protein

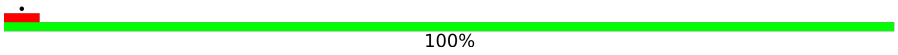
Chain b:

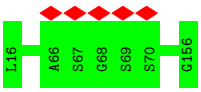




• Molecule 1: DUF4352 domain-containing protein

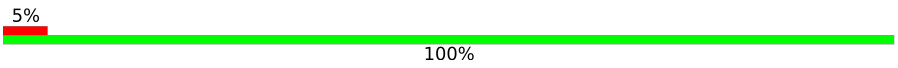
Chain e:

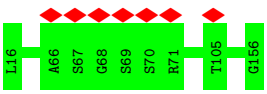




• Molecule 1: DUF4352 domain-containing protein

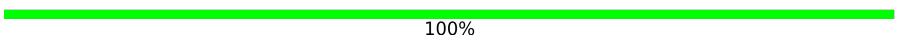
Chain h:





• Molecule 1: DUF4352 domain-containing protein

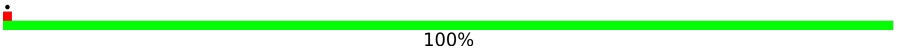
Chain I:

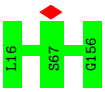


There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

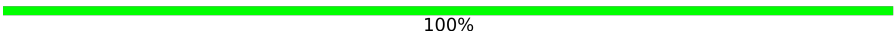
Chain C:





• Molecule 1: DUF4352 domain-containing protein

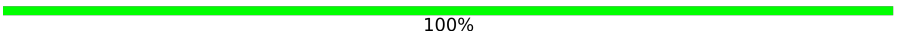
Chain F:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

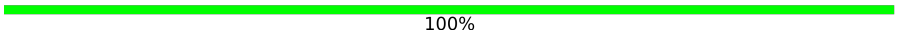
Chain L:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

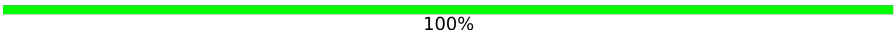
Chain O:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

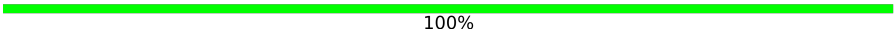
Chain R:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

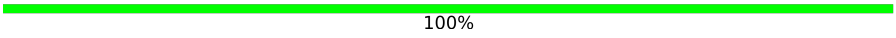
Chain U:



There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

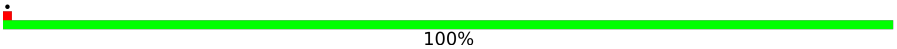
Chain X:

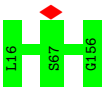


There are no outlier residues recorded for this chain.

• Molecule 1: DUF4352 domain-containing protein

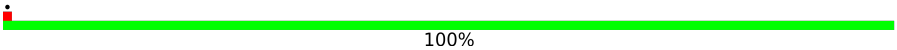
Chain a:

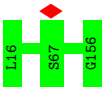




• Molecule 1: DUF4352 domain-containing protein

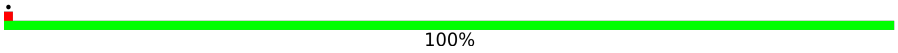
Chain d:

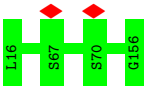




• Molecule 1: DUF4352 domain-containing protein

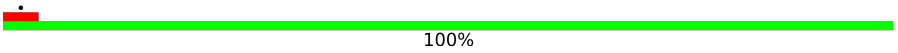
Chain g:

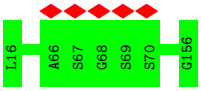




• Molecule 1: DUF4352 domain-containing protein

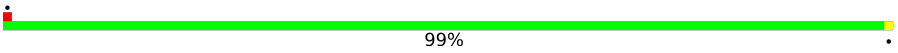
Chain j:

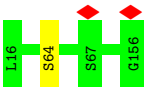




• Molecule 1: DUF4352 domain-containing protein

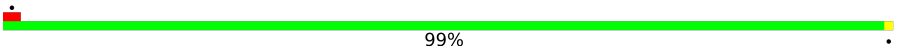
Chain H:

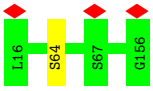




• Molecule 1: DUF4352 domain-containing protein

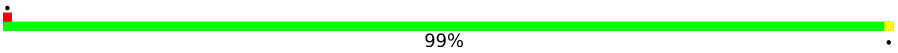
Chain B:

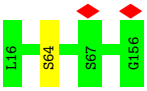




• Molecule 1: DUF4352 domain-containing protein

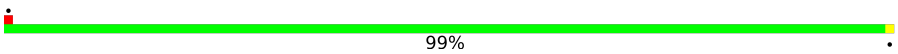
Chain E:

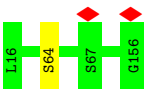




• Molecule 1: DUF4352 domain-containing protein

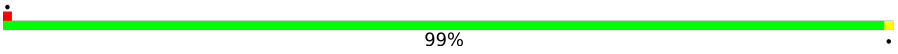
Chain K:

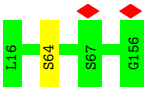




• Molecule 1: DUF4352 domain-containing protein

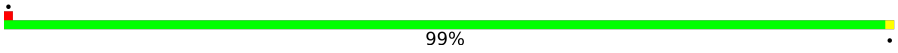
Chain N:

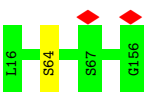




• Molecule 1: DUF4352 domain-containing protein

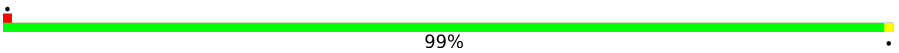
Chain Q:

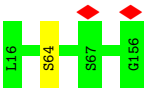




• Molecule 1: DUF4352 domain-containing protein

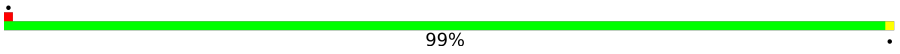
Chain T:

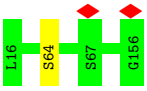




• Molecule 1: DUF4352 domain-containing protein

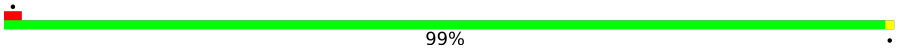
Chain W:

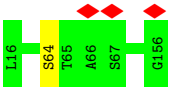




• Molecule 1: DUF4352 domain-containing protein

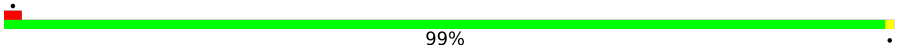
Chain Z:

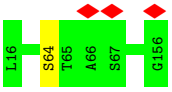




• Molecule 1: DUF4352 domain-containing protein

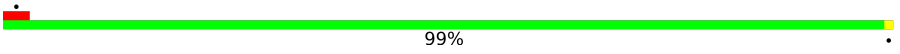
Chain c:

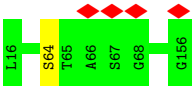




• Molecule 1: DUF4352 domain-containing protein

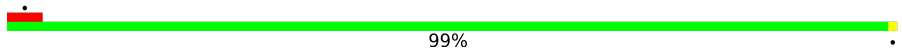
Chain f:

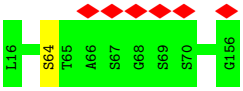




• Molecule 1: DUF4352 domain-containing protein

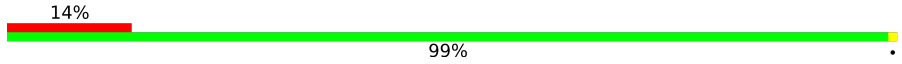
Chain i:

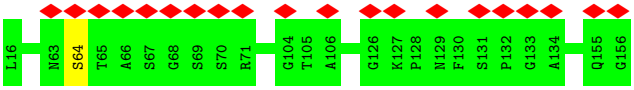




• Molecule 1: DUF4352 domain-containing protein

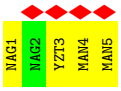
Chain l:





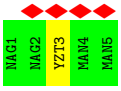
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



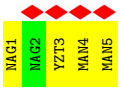
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



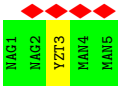
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



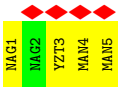
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



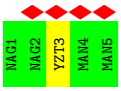
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



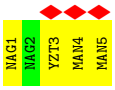
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



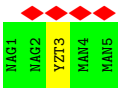
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



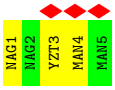
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



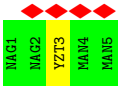
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



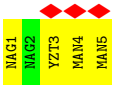
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:



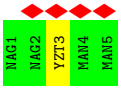
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:



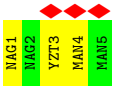
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:



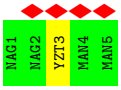
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



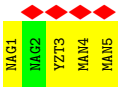
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:



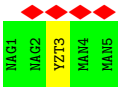
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6: 



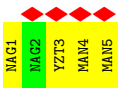
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7: 



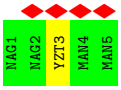
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9: 



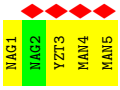
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA: 



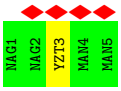
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA: 



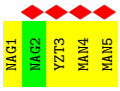
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:



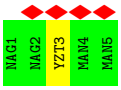
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:



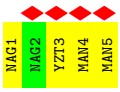
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:



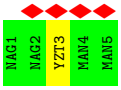
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:



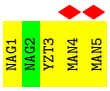
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:



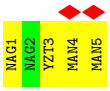
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:



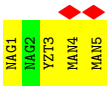
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA:



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

Chain RA:

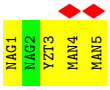


• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain UA:

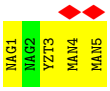
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain XA:



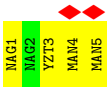
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA:



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

Chain dA:

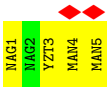


• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain gA:

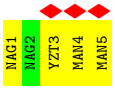
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain jA:



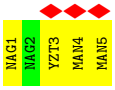
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain mA:



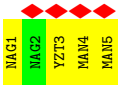
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pA:



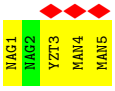
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sA:



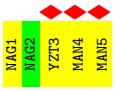
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain vA:



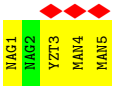
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain yA:



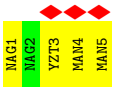
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1A:



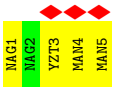
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4A: 



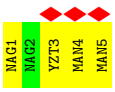
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7A: 



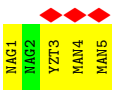
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AB: 



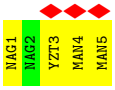
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DB: 



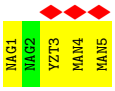
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GB: 



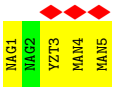
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JB:



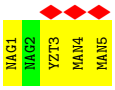
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MB:



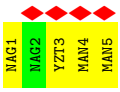
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PB:



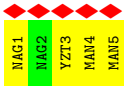
• Molecule 2: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SB:



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

Chain VB:



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

Chain n:

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

Chain q:

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

Chain t:

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

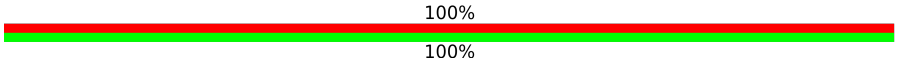
Chain w:

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

Chain z:

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

Chain 2:



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

Chain 5:

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

Chain 8:

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

Chain BA:

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

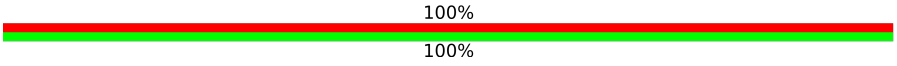
Chain EA:

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

Chain HA:

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

Chain KA:



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

Chain NA:

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

Chain QA:

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

Chain TA:

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

Chain WA:

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

Chain ZA:

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

Chain cA:

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

Chain fA:

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

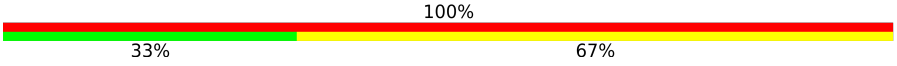
Chain iA:

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

Chain lA:

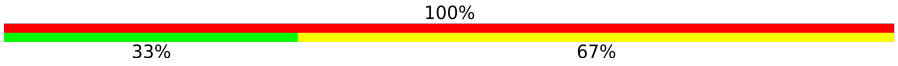
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:



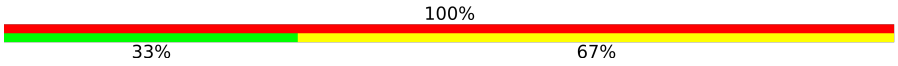
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain rA:



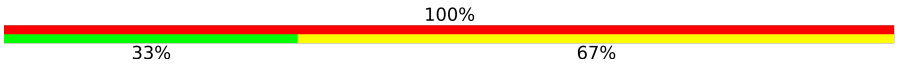
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain uA:



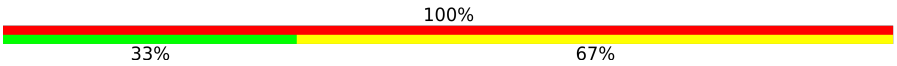
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain xA:



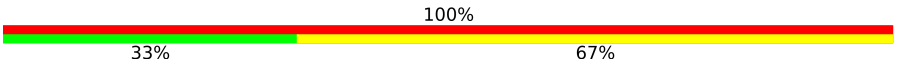
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0A:



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

Chain 3A:



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

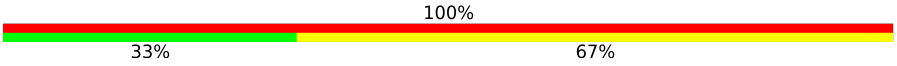
Chain 6A:

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

Chain 9A:

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

Chain CB:



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

Chain FB:

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

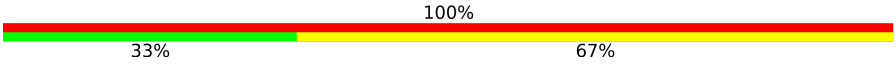
Chain IB:

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

Chain LB:

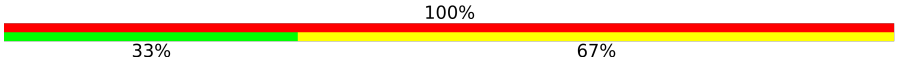
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OB:



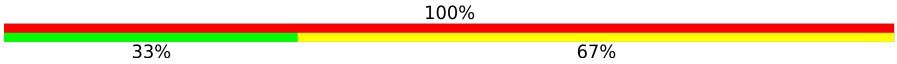
• Molecule 3: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RB:



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

Chain UB:



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

Chain XB:

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

Chain MA:

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

Chain PA:

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

Chain SA:

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

Chain VA:

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

Chain YA:

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

Chain bA:

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

Chain eA:

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

Chain hA:

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

Chain kA:

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

Chain nA:

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

Chain qA:

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

Chain tA:

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

Chain wA:

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

Chain zA:

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

Chain 2A: 

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

Chain 5A: 

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

Chain 8A: 

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

Chain BB: 

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

Chain EB: 

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

Chain HB:

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

Chain KB:

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

Chain NB:

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

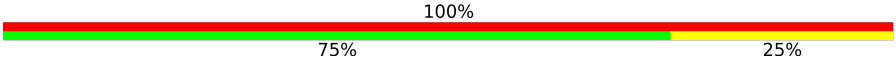
Chain QB:

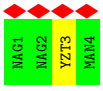
• Molecule 4: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TB:

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

Chain WB:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-39.86°, rise=15.52 Å, axial sym=C1	Depositor
Number of segments used	505862	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 ($e^-/Å^2$)	40.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.169	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.041	Depositor
Map size (Å)	308.73602, 308.73602, 308.73602	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YZT, 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	0.34	0/1019	0.63	0/1396
1	B	0.34	0/1019	0.61	0/1396
1	C	0.34	0/1019	0.63	0/1396
1	D	0.34	0/1019	0.63	0/1396
1	E	0.34	0/1019	0.61	0/1396
1	F	0.34	0/1019	0.63	0/1396
1	G	0.34	0/1019	0.63	0/1396
1	H	0.34	0/1019	0.61	0/1396
1	I	0.34	0/1019	0.63	0/1396
1	J	0.34	0/1019	0.63	0/1396
1	K	0.34	0/1019	0.61	0/1396
1	L	0.34	0/1019	0.64	0/1396
1	M	0.34	0/1019	0.63	0/1396
1	N	0.35	0/1019	0.61	0/1396
1	O	0.34	0/1019	0.64	0/1396
1	P	0.34	0/1019	0.63	0/1396
1	Q	0.34	0/1019	0.61	0/1396
1	R	0.34	0/1019	0.63	0/1396
1	S	0.34	0/1019	0.63	0/1396
1	T	0.34	0/1019	0.61	0/1396
1	U	0.34	0/1019	0.64	0/1396
1	V	0.34	0/1019	0.63	0/1396
1	W	0.35	0/1019	0.61	0/1396
1	X	0.33	0/1019	0.64	0/1396
1	Y	0.34	0/1019	0.63	0/1396
1	Z	0.34	0/1019	0.61	0/1396
1	a	0.33	0/1019	0.63	0/1396
1	b	0.34	0/1019	0.63	0/1396
1	c	0.34	0/1019	0.61	0/1396
1	d	0.34	0/1019	0.63	0/1396
1	e	0.34	0/1019	0.63	0/1396
1	f	0.34	0/1019	0.61	0/1396

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	g	0.34	0/1019	0.63	0/1396
1	h	0.34	0/1019	0.63	0/1396
1	i	0.35	0/1019	0.60	0/1396
1	j	0.34	0/1019	0.63	0/1396
1	l	0.34	0/1019	0.60	0/1396
All	All	0.34	0/37703	0.62	0/51652

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%)	138 (99%)	1 (1%)	0	100	100
1	C	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	D	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	E	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	F	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	G	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	H	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	I	139/141 (99%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	K	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	L	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	M	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	N	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	O	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	P	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Q	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	R	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	S	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	T	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	U	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	V	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	W	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	X	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	Y	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	Z	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	a	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	b	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	c	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	d	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	e	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	f	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	g	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	h	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	i	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	j	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	l	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
All	All	5143/5217 (99%)	5094 (99%)	49 (1%)	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%)	109 (99%)	1 (1%)	75 90
1	C	110/110 (100%)	110 (100%)	0	100 100
1	D	110/110 (100%)	110 (100%)	0	100 100
1	E	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	F	110/110 (100%)	110 (100%)	0	100 100
1	G	110/110 (100%)	110 (100%)	0	100 100
1	H	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	I	110/110 (100%)	110 (100%)	0	100 100
1	J	110/110 (100%)	110 (100%)	0	100 100
1	K	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	L	110/110 (100%)	110 (100%)	0	100 100
1	M	110/110 (100%)	110 (100%)	0	100 100
1	N	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	O	110/110 (100%)	110 (100%)	0	100 100
1	P	110/110 (100%)	110 (100%)	0	100 100
1	Q	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	R	110/110 (100%)	110 (100%)	0	100 100
1	S	110/110 (100%)	110 (100%)	0	100 100
1	T	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	U	110/110 (100%)	110 (100%)	0	100 100
1	V	110/110 (100%)	110 (100%)	0	100 100
1	W	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	X	110/110 (100%)	110 (100%)	0	100 100
1	Y	110/110 (100%)	110 (100%)	0	100 100
1	Z	110/110 (100%)	109 (99%)	1 (1%)	75 90

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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 90
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 90
1	g	110/110 (100%)	110 (100%)	0	100 100
1	h	110/110 (100%)	110 (100%)	0	100 100
1	i	110/110 (100%)	109 (99%)	1 (1%)	75 90
1	j	110/110 (100%)	110 (100%)	0	100 100
1	l	110/110 (100%)	109 (99%)	1 (1%)	75 90
All	All	4070/4070 (100%)	4057 (100%)	13 (0%)	90 97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	64	SER
1	B	64	SER
1	E	64	SER
1	K	64	SER
1	N	64	SER
1	Q	64	SER
1	T	64	SER
1	W	64	SER
1	Z	64	SER
1	c	64	SER
1	f	64	SER
1	i	64	SER
1	l	64	SER

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 (i)

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

5.5 Carbohydrates (i)

456 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	0.30	0	17,19,21	0.88	1 (5%)
2	NAG	0	2	2	14,14,15	0.47	0	17,19,21	0.68	0
2	YZT	0	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.79	1 (5%)
2	MAN	0	4	2	11,11,12	0.46	0	15,15,17	0.86	1 (6%)
2	MAN	0	5	2	11,11,12	0.46	0	15,15,17	0.90	1 (6%)
3	NAG	0A	1	3,1	14,14,15	0.25	0	17,19,21	0.93	1 (5%)
3	NAG	0A	2	3	14,14,15	0.28	0	17,19,21	0.62	1 (5%)
3	MAN	0A	3	3	11,11,12	0.44	0	15,15,17	0.77	0
2	NAG	1	1	2,1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	1	2	2	14,14,15	0.46	0	17,19,21	0.75	0
2	YZT	1	3	2	13,14,15	1.17	1 (7%)	18,21,23	1.22	2 (11%)
2	MAN	1	4	2	11,11,12	0.58	0	15,15,17	0.66	0
2	MAN	1	5	2	11,11,12	0.45	0	15,15,17	0.76	0
2	NAG	1A	1	2,1	14,14,15	0.37	0	17,19,21	1.43	1 (5%)
2	NAG	1A	2	2	14,14,15	0.37	0	17,19,21	0.79	0
2	YZT	1A	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.21	2 (11%)
2	MAN	1A	4	2	11,11,12	0.34	0	15,15,17	0.90	1 (6%)
2	MAN	1A	5	2	11,11,12	0.40	0	15,15,17	0.97	1 (6%)
3	NAG	2	1	3,1	14,14,15	0.49	0	17,19,21	0.67	0
3	NAG	2	2	3	14,14,15	0.28	0	17,19,21	0.57	0
3	MAN	2	3	3	11,11,12	0.48	0	15,15,17	0.71	0
4	NAG	2A	1	4,1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	2A	2	4	14,14,15	0.45	0	17,19,21	0.65	0
4	YZT	2A	3	4	13,14,15	1.20	1 (7%)	18,21,23	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	2A	4	4	11,11,12	0.45	0	15,15,17	0.71	0
2	NAG	3	1	2,1	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
2	NAG	3	2	2	14,14,15	0.47	0	17,19,21	0.68	0
2	YZT	3	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.76	1 (5%)
2	MAN	3	4	2	11,11,12	0.45	0	15,15,17	0.89	1 (6%)
2	MAN	3	5	2	11,11,12	0.45	0	15,15,17	0.89	0
3	NAG	3A	1	3,1	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
3	NAG	3A	2	3	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
3	MAN	3A	3	3	11,11,12	0.44	0	15,15,17	0.75	0
2	NAG	4	1	2,1	14,14,15	0.26	0	17,19,21	0.51	0
2	NAG	4	2	2	14,14,15	0.45	0	17,19,21	0.75	0
2	YZT	4	3	2	13,14,15	1.16	1 (7%)	18,21,23	1.21	2 (11%)
2	MAN	4	4	2	11,11,12	0.58	0	15,15,17	0.66	0
2	MAN	4	5	2	11,11,12	0.44	0	15,15,17	0.76	0
2	NAG	4A	1	2,1	14,14,15	0.37	0	17,19,21	1.45	2 (11%)
2	NAG	4A	2	2	14,14,15	0.36	0	17,19,21	0.79	0
2	YZT	4A	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.25	2 (11%)
2	MAN	4A	4	2	11,11,12	0.34	0	15,15,17	0.89	1 (6%)
2	MAN	4A	5	2	11,11,12	0.39	0	15,15,17	0.95	1 (6%)
3	NAG	5	1	3,1	14,14,15	0.49	0	17,19,21	0.68	0
3	NAG	5	2	3	14,14,15	0.29	0	17,19,21	0.57	0
3	MAN	5	3	3	11,11,12	0.48	0	15,15,17	0.71	0
4	NAG	5A	1	4,1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	5A	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	YZT	5A	3	4	13,14,15	1.18	1 (7%)	18,21,23	1.06	2 (11%)
4	MAN	5A	4	4	11,11,12	0.43	0	15,15,17	0.73	0
2	NAG	6	1	2,1	14,14,15	0.30	0	17,19,21	0.87	1 (5%)
2	NAG	6	2	2	14,14,15	0.46	0	17,19,21	0.68	0
2	YZT	6	3	2	13,14,15	0.68	1 (7%)	18,21,23	0.78	1 (5%)
2	MAN	6	4	2	11,11,12	0.45	0	15,15,17	0.87	1 (6%)
2	MAN	6	5	2	11,11,12	0.45	0	15,15,17	0.89	1 (6%)
3	NAG	6A	1	3,1	14,14,15	0.26	0	17,19,21	0.95	1 (5%)
3	NAG	6A	2	3	14,14,15	0.28	0	17,19,21	0.63	1 (5%)
3	MAN	6A	3	3	11,11,12	0.43	0	15,15,17	0.75	0
2	NAG	7	1	2,1	14,14,15	0.28	0	17,19,21	0.53	0
2	NAG	7	2	2	14,14,15	0.45	0	17,19,21	0.75	0
2	YZT	7	3	2	13,14,15	1.18	1 (7%)	18,21,23	1.21	2 (11%)
2	MAN	7	4	2	11,11,12	0.56	0	15,15,17	0.64	0
2	MAN	7	5	2	11,11,12	0.43	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	7A	1	2,1	14,14,15	0.34	0	17,19,21	1.43	2 (11%)
2	NAG	7A	2	2	14,14,15	0.35	0	17,19,21	0.78	0
2	YZT	7A	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.24	2 (11%)
2	MAN	7A	4	2	11,11,12	0.35	0	15,15,17	0.86	1 (6%)
2	MAN	7A	5	2	11,11,12	0.39	0	15,15,17	0.94	1 (6%)
3	NAG	8	1	3,1	14,14,15	0.48	0	17,19,21	0.69	0
3	NAG	8	2	3	14,14,15	0.27	0	17,19,21	0.55	0
3	MAN	8	3	3	11,11,12	0.48	0	15,15,17	0.71	0
4	NAG	8A	1	4,1	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	8A	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	YZT	8A	3	4	13,14,15	1.19	1 (7%)	18,21,23	1.03	2 (11%)
4	MAN	8A	4	4	11,11,12	0.45	0	15,15,17	0.70	0
2	NAG	9	1	2,1	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
2	NAG	9	2	2	14,14,15	0.46	0	17,19,21	0.68	0
2	YZT	9	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.79	1 (5%)
2	MAN	9	4	2	11,11,12	0.47	0	15,15,17	0.90	1 (6%)
2	MAN	9	5	2	11,11,12	0.45	0	15,15,17	0.89	1 (6%)
3	NAG	9A	1	3,1	14,14,15	0.25	0	17,19,21	0.90	1 (5%)
3	NAG	9A	2	3	14,14,15	0.27	0	17,19,21	0.58	0
3	MAN	9A	3	3	11,11,12	0.43	0	15,15,17	0.77	0
2	NAG	AA	1	2,1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	AA	2	2	14,14,15	0.46	0	17,19,21	0.72	0
2	YZT	AA	3	2	13,14,15	1.17	1 (7%)	18,21,23	1.20	2 (11%)
2	MAN	AA	4	2	11,11,12	0.60	0	15,15,17	0.70	0
2	MAN	AA	5	2	11,11,12	0.42	0	15,15,17	0.77	0
2	NAG	AB	1	2,1	14,14,15	0.36	0	17,19,21	1.47	2 (11%)
2	NAG	AB	2	2	14,14,15	0.37	0	17,19,21	0.79	0
2	YZT	AB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.21	2 (11%)
2	MAN	AB	4	2	11,11,12	0.34	0	15,15,17	0.85	1 (6%)
2	MAN	AB	5	2	11,11,12	0.38	0	15,15,17	0.96	1 (6%)
3	NAG	BA	1	3,1	14,14,15	0.49	0	17,19,21	0.69	0
3	NAG	BA	2	3	14,14,15	0.27	0	17,19,21	0.57	0
3	MAN	BA	3	3	11,11,12	0.49	0	15,15,17	0.70	0
4	NAG	BB	1	4,1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	BB	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	YZT	BB	3	4	13,14,15	1.19	1 (7%)	18,21,23	1.03	2 (11%)
4	MAN	BB	4	4	11,11,12	0.44	0	15,15,17	0.71	0
2	NAG	CA	1	2,1	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
2	NAG	CA	2	2	14,14,15	0.48	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	YZT	CA	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.79	1 (5%)
2	MAN	CA	4	2	11,11,12	0.46	0	15,15,17	0.86	1 (6%)
2	MAN	CA	5	2	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
3	NAG	CB	1	3,1	14,14,15	0.25	0	17,19,21	0.96	1 (5%)
3	NAG	CB	2	3	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
3	MAN	CB	3	3	11,11,12	0.45	0	15,15,17	0.74	0
2	NAG	DA	1	2,1	14,14,15	0.26	0	17,19,21	0.51	0
2	NAG	DA	2	2	14,14,15	0.47	0	17,19,21	0.74	0
2	YZT	DA	3	2	13,14,15	1.16	1 (7%)	18,21,23	1.20	2 (11%)
2	MAN	DA	4	2	11,11,12	0.58	0	15,15,17	0.69	0
2	MAN	DA	5	2	11,11,12	0.45	0	15,15,17	0.76	0
2	NAG	DB	1	2,1	14,14,15	0.35	0	17,19,21	1.41	2 (11%)
2	NAG	DB	2	2	14,14,15	0.35	0	17,19,21	0.79	0
2	YZT	DB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.19	2 (11%)
2	MAN	DB	4	2	11,11,12	0.36	0	15,15,17	0.85	1 (6%)
2	MAN	DB	5	2	11,11,12	0.39	0	15,15,17	0.93	1 (6%)
3	NAG	EA	1	3,1	14,14,15	0.50	0	17,19,21	0.68	0
3	NAG	EA	2	3	14,14,15	0.29	0	17,19,21	0.57	0
3	MAN	EA	3	3	11,11,12	0.48	0	15,15,17	0.70	0
4	NAG	EB	1	4,1	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	EB	2	4	14,14,15	0.46	0	17,19,21	0.64	0
4	YZT	EB	3	4	13,14,15	1.20	1 (7%)	18,21,23	1.04	2 (11%)
4	MAN	EB	4	4	11,11,12	0.44	0	15,15,17	0.72	0
2	NAG	FA	1	2,1	14,14,15	0.29	0	17,19,21	0.86	1 (5%)
2	NAG	FA	2	2	14,14,15	0.46	0	17,19,21	0.67	0
2	YZT	FA	3	2	13,14,15	0.71	1 (7%)	18,21,23	0.78	1 (5%)
2	MAN	FA	4	2	11,11,12	0.46	0	15,15,17	0.88	1 (6%)
2	MAN	FA	5	2	11,11,12	0.45	0	15,15,17	0.89	1 (6%)
3	NAG	FB	1	3,1	14,14,15	0.24	0	17,19,21	0.87	1 (5%)
3	NAG	FB	2	3	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
3	MAN	FB	3	3	11,11,12	0.44	0	15,15,17	0.78	0
2	NAG	GA	1	2,1	14,14,15	0.24	0	17,19,21	0.51	0
2	NAG	GA	2	2	14,14,15	0.44	0	17,19,21	0.75	0
2	YZT	GA	3	2	13,14,15	1.15	1 (7%)	18,21,23	1.22	2 (11%)
2	MAN	GA	4	2	11,11,12	0.57	0	15,15,17	0.66	0
2	MAN	GA	5	2	11,11,12	0.44	0	15,15,17	0.74	0
2	NAG	GB	1	2,1	14,14,15	0.35	0	17,19,21	1.42	2 (11%)
2	NAG	GB	2	2	14,14,15	0.35	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	YZT	GB	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.20	2 (11%)
2	MAN	GB	4	2	11,11,12	0.35	0	15,15,17	0.87	1 (6%)
2	MAN	GB	5	2	11,11,12	0.38	0	15,15,17	0.93	1 (6%)
3	NAG	HA	1	3,1	14,14,15	0.50	0	17,19,21	0.68	0
3	NAG	HA	2	3	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
3	MAN	HA	3	3	11,11,12	0.48	0	15,15,17	0.70	0
4	NAG	HB	1	4,1	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	HB	2	4	14,14,15	0.46	0	17,19,21	0.62	0
4	YZT	HB	3	4	13,14,15	1.19	1 (7%)	18,21,23	1.05	2 (11%)
4	MAN	HB	4	4	11,11,12	0.44	0	15,15,17	0.73	0
2	NAG	IA	1	2,1	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
2	NAG	IA	2	2	14,14,15	0.48	0	17,19,21	0.69	0
2	YZT	IA	3	2	13,14,15	0.69	1 (7%)	18,21,23	0.76	1 (5%)
2	MAN	IA	4	2	11,11,12	0.46	0	15,15,17	0.88	1 (6%)
2	MAN	IA	5	2	11,11,12	0.45	0	15,15,17	0.88	1 (6%)
3	NAG	IB	1	3,1	14,14,15	0.26	0	17,19,21	0.95	1 (5%)
3	NAG	IB	2	3	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
3	MAN	IB	3	3	11,11,12	0.42	0	15,15,17	0.77	0
2	NAG	JA	1	2,1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	JA	2	2	14,14,15	0.44	0	17,19,21	0.74	0
2	YZT	JA	3	2	13,14,15	1.16	1 (7%)	18,21,23	1.21	2 (11%)
2	MAN	JA	4	2	11,11,12	0.54	0	15,15,17	0.64	0
2	MAN	JA	5	2	11,11,12	0.43	0	15,15,17	0.76	0
2	NAG	JB	1	2,1	14,14,15	0.36	0	17,19,21	1.38	1 (5%)
2	NAG	JB	2	2	14,14,15	0.35	0	17,19,21	0.77	0
2	YZT	JB	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.25	2 (11%)
2	MAN	JB	4	2	11,11,12	0.34	0	15,15,17	0.87	1 (6%)
2	MAN	JB	5	2	11,11,12	0.39	0	15,15,17	0.95	1 (6%)
3	NAG	KA	1	3,1	14,14,15	0.47	0	17,19,21	0.68	0
3	NAG	KA	2	3	14,14,15	0.28	0	17,19,21	0.57	0
3	MAN	KA	3	3	11,11,12	0.48	0	15,15,17	0.70	0
4	NAG	KB	1	4,1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	KB	2	4	14,14,15	0.45	0	17,19,21	0.64	0
4	YZT	KB	3	4	13,14,15	1.19	1 (7%)	18,21,23	1.05	2 (11%)
4	MAN	KB	4	4	11,11,12	0.44	0	15,15,17	0.71	0
2	NAG	LA	1	2,1	14,14,15	0.35	0	17,19,21	1.32	1 (5%)
2	NAG	LA	2	2	14,14,15	0.37	0	17,19,21	0.74	0
2	YZT	LA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.39	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	LA	4	2	11,11,12	0.65	0	15,15,17	1.12	1 (6%)
2	MAN	LA	5	2	11,11,12	0.57	0	15,15,17	1.16	2 (13%)
3	NAG	LB	1	3,1	14,14,15	0.26	0	17,19,21	0.90	1 (5%)
3	NAG	LB	2	3	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
3	MAN	LB	3	3	11,11,12	0.44	0	15,15,17	0.77	0
4	NAG	MA	1	4,1	14,14,15	0.30	0	17,19,21	0.55	0
4	NAG	MA	2	4	14,14,15	0.45	0	17,19,21	0.81	1 (5%)
4	YZT	MA	3	4	13,14,15	1.22	1 (7%)	18,21,23	1.33	3 (16%)
4	MAN	MA	4	4	11,11,12	0.40	0	15,15,17	0.68	0
2	NAG	MB	1	2,1	14,14,15	0.35	0	17,19,21	1.40	1 (5%)
2	NAG	MB	2	2	14,14,15	0.37	0	17,19,21	0.78	0
2	YZT	MB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.22	2 (11%)
2	MAN	MB	4	2	11,11,12	0.35	0	15,15,17	0.86	1 (6%)
2	MAN	MB	5	2	11,11,12	0.38	0	15,15,17	0.96	1 (6%)
3	NAG	NA	1	3,1	14,14,15	0.25	0	17,19,21	0.76	1 (5%)
3	NAG	NA	2	3	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
3	MAN	NA	3	3	11,11,12	0.43	0	15,15,17	0.73	0
4	NAG	NB	1	4,1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	NB	2	4	14,14,15	0.46	0	17,19,21	0.63	0
4	YZT	NB	3	4	13,14,15	1.19	1 (7%)	18,21,23	1.03	2 (11%)
4	MAN	NB	4	4	11,11,12	0.44	0	15,15,17	0.71	0
2	NAG	OA	1	2,1	14,14,15	0.33	0	17,19,21	1.35	1 (5%)
2	NAG	OA	2	2	14,14,15	0.36	0	17,19,21	0.73	0
2	YZT	OA	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.30	2 (11%)
2	MAN	OA	4	2	11,11,12	0.65	0	15,15,17	1.08	1 (6%)
2	MAN	OA	5	2	11,11,12	0.58	0	15,15,17	1.13	2 (13%)
3	NAG	OB	1	3,1	14,14,15	0.25	0	17,19,21	0.93	1 (5%)
3	NAG	OB	2	3	14,14,15	0.29	0	17,19,21	0.63	1 (5%)
3	MAN	OB	3	3	11,11,12	0.45	0	15,15,17	0.77	0
4	NAG	PA	1	4,1	14,14,15	0.30	0	17,19,21	0.55	0
4	NAG	PA	2	4	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
4	YZT	PA	3	4	13,14,15	1.24	1 (7%)	18,21,23	1.33	3 (16%)
4	MAN	PA	4	4	11,11,12	0.40	0	15,15,17	0.68	0
2	NAG	PB	1	2,1	14,14,15	0.37	0	17,19,21	1.41	1 (5%)
2	NAG	PB	2	2	14,14,15	0.36	0	17,19,21	0.79	0
2	YZT	PB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.19	2 (11%)
2	MAN	PB	4	2	11,11,12	0.34	0	15,15,17	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	PB	5	2	11,11,12	0.39	0	15,15,17	0.95	1 (6%)
3	NAG	QA	1	3,1	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
3	NAG	QA	2	3	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
3	MAN	QA	3	3	11,11,12	0.41	0	15,15,17	0.74	0
4	NAG	QB	1	4,1	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	QB	2	4	14,14,15	0.46	0	17,19,21	0.64	0
4	YZT	QB	3	4	13,14,15	1.20	1 (7%)	18,21,23	1.05	2 (11%)
4	MAN	QB	4	4	11,11,12	0.45	0	15,15,17	0.71	0
2	NAG	RA	1	2,1	14,14,15	0.34	0	17,19,21	1.36	1 (5%)
2	NAG	RA	2	2	14,14,15	0.36	0	17,19,21	0.72	0
2	YZT	RA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.35	2 (11%)
2	MAN	RA	4	2	11,11,12	0.66	0	15,15,17	1.13	1 (6%)
2	MAN	RA	5	2	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
3	NAG	RB	1	3,1	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
3	NAG	RB	2	3	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
3	MAN	RB	3	3	11,11,12	0.43	0	15,15,17	0.75	0
4	NAG	SA	1	4,1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	SA	2	4	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
4	YZT	SA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.31	3 (16%)
4	MAN	SA	4	4	11,11,12	0.38	0	15,15,17	0.69	0
2	NAG	SB	1	2,1	14,14,15	0.37	0	17,19,21	1.43	1 (5%)
2	NAG	SB	2	2	14,14,15	0.36	0	17,19,21	0.79	0
2	YZT	SB	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.18	2 (11%)
2	MAN	SB	4	2	11,11,12	0.34	0	15,15,17	0.87	1 (6%)
2	MAN	SB	5	2	11,11,12	0.39	0	15,15,17	0.92	1 (6%)
3	NAG	TA	1	3,1	14,14,15	0.26	0	17,19,21	0.74	1 (5%)
3	NAG	TA	2	3	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
3	MAN	TA	3	3	11,11,12	0.42	0	15,15,17	0.75	0
4	NAG	TB	1	4,1	14,14,15	0.32	0	17,19,21	0.45	0
4	NAG	TB	2	4	14,14,15	0.45	0	17,19,21	0.61	0
4	YZT	TB	3	4	13,14,15	1.20	1 (7%)	18,21,23	1.05	2 (11%)
4	MAN	TB	4	4	11,11,12	0.44	0	15,15,17	0.73	0
2	NAG	UA	1	2,1	14,14,15	0.35	0	17,19,21	1.35	1 (5%)
2	NAG	UA	2	2	14,14,15	0.35	0	17,19,21	0.71	0
2	YZT	UA	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.34	2 (11%)
2	MAN	UA	4	2	11,11,12	0.64	0	15,15,17	1.10	1 (6%)
2	MAN	UA	5	2	11,11,12	0.57	0	15,15,17	1.16	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	UB	1	3,1	14,14,15	0.25	0	17,19,21	0.90	1 (5%)
3	NAG	UB	2	3	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
3	MAN	UB	3	3	11,11,12	0.42	0	15,15,17	0.80	0
4	NAG	VA	1	4,1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	VA	2	4	14,14,15	0.45	0	17,19,21	0.82	1 (5%)
4	YZT	VA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.33	3 (16%)
4	MAN	VA	4	4	11,11,12	0.42	0	15,15,17	0.66	0
2	NAG	VB	1	2,1	14,14,15	0.38	0	17,19,21	1.42	1 (5%)
2	NAG	VB	2	2	14,14,15	0.37	0	17,19,21	0.77	0
2	YZT	VB	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.23	2 (11%)
2	MAN	VB	4	2	11,11,12	0.34	0	15,15,17	0.88	1 (6%)
2	MAN	VB	5	2	11,11,12	0.38	0	15,15,17	0.93	1 (6%)
3	NAG	WA	1	3,1	14,14,15	0.26	0	17,19,21	0.73	1 (5%)
3	NAG	WA	2	3	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
3	MAN	WA	3	3	11,11,12	0.44	0	15,15,17	0.72	0
4	NAG	WB	1	4,1	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	WB	2	4	14,14,15	0.46	0	17,19,21	0.62	0
4	YZT	WB	3	4	13,14,15	1.20	1 (7%)	18,21,23	1.06	2 (11%)
4	MAN	WB	4	4	11,11,12	0.43	0	15,15,17	0.72	0
2	NAG	XA	1	2,1	14,14,15	0.34	0	17,19,21	1.37	1 (5%)
2	NAG	XA	2	2	14,14,15	0.36	0	17,19,21	0.72	0
2	YZT	XA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.32	2 (11%)
2	MAN	XA	4	2	11,11,12	0.63	0	15,15,17	1.09	1 (6%)
2	MAN	XA	5	2	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
3	NAG	XB	1	3,1	14,14,15	0.27	0	17,19,21	0.94	1 (5%)
3	NAG	XB	2	3	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
3	MAN	XB	3	3	11,11,12	0.43	0	15,15,17	0.75	0
4	NAG	YA	1	4,1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	YA	2	4	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
4	YZT	YA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.33	3 (16%)
4	MAN	YA	4	4	11,11,12	0.40	0	15,15,17	0.68	0
3	NAG	ZA	1	3,1	14,14,15	0.26	0	17,19,21	0.73	1 (5%)
3	NAG	ZA	2	3	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
3	MAN	ZA	3	3	11,11,12	0.42	0	15,15,17	0.72	0
2	NAG	aA	1	2,1	14,14,15	0.33	0	17,19,21	1.35	1 (5%)
2	NAG	aA	2	2	14,14,15	0.37	0	17,19,21	0.71	0
2	YZT	aA	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	aA	4	2	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
2	MAN	aA	5	2	11,11,12	0.58	0	15,15,17	1.16	2 (13%)
4	NAG	bA	1	4,1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	bA	2	4	14,14,15	0.47	0	17,19,21	0.81	0
4	YZT	bA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.31	3 (16%)
4	MAN	bA	4	4	11,11,12	0.39	0	15,15,17	0.70	0
3	NAG	cA	1	3,1	14,14,15	0.26	0	17,19,21	0.74	1 (5%)
3	NAG	cA	2	3	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
3	MAN	cA	3	3	11,11,12	0.42	0	15,15,17	0.74	0
2	NAG	dA	1	2,1	14,14,15	0.34	0	17,19,21	1.36	1 (5%)
2	NAG	dA	2	2	14,14,15	0.37	0	17,19,21	0.72	0
2	YZT	dA	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.40	2 (11%)
2	MAN	dA	4	2	11,11,12	0.66	0	15,15,17	1.14	1 (6%)
2	MAN	dA	5	2	11,11,12	0.57	0	15,15,17	1.16	2 (13%)
4	NAG	eA	1	4,1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	eA	2	4	14,14,15	0.46	0	17,19,21	0.81	0
4	YZT	eA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.32	3 (16%)
4	MAN	eA	4	4	11,11,12	0.39	0	15,15,17	0.68	0
3	NAG	fA	1	3,1	14,14,15	0.25	0	17,19,21	0.74	1 (5%)
3	NAG	fA	2	3	14,14,15	0.28	0	17,19,21	0.62	1 (5%)
3	MAN	fA	3	3	11,11,12	0.43	0	15,15,17	0.74	0
2	NAG	gA	1	2,1	14,14,15	0.36	0	17,19,21	1.36	1 (5%)
2	NAG	gA	2	2	14,14,15	0.35	0	17,19,21	0.73	0
2	YZT	gA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.39	2 (11%)
2	MAN	gA	4	2	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
2	MAN	gA	5	2	11,11,12	0.56	0	15,15,17	1.18	2 (13%)
4	NAG	hA	1	4,1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	hA	2	4	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
4	YZT	hA	3	4	13,14,15	1.24	1 (7%)	18,21,23	1.32	3 (16%)
4	MAN	hA	4	4	11,11,12	0.41	0	15,15,17	0.67	0
3	NAG	iA	1	3,1	14,14,15	0.25	0	17,19,21	0.75	1 (5%)
3	NAG	iA	2	3	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
3	MAN	iA	3	3	11,11,12	0.43	0	15,15,17	0.72	0
2	NAG	jA	1	2,1	14,14,15	0.36	0	17,19,21	1.40	1 (5%)
2	NAG	jA	2	2	14,14,15	0.35	0	17,19,21	0.71	0
2	YZT	jA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.34	2 (11%)
2	MAN	jA	4	2	11,11,12	0.64	0	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	jA	5	2	11,11,12	0.57	0	15,15,17	1.17	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.30	0	17,19,21	0.89	1 (5%)
2	NAG	k	2	2	14,14,15	0.48	0	17,19,21	0.69	0
2	YZT	k	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.78	1 (5%)
2	MAN	k	4	2	11,11,12	0.44	0	15,15,17	0.88	1 (6%)
2	MAN	k	5	2	11,11,12	0.45	0	15,15,17	0.89	1 (6%)
4	NAG	kA	1	4,1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	kA	2	4	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
4	YZT	kA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.32	3 (16%)
4	MAN	kA	4	4	11,11,12	0.41	0	15,15,17	0.68	0
3	NAG	lA	1	3,1	14,14,15	0.27	0	17,19,21	0.73	1 (5%)
3	NAG	lA	2	3	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
3	MAN	lA	3	3	11,11,12	0.43	0	15,15,17	0.71	0
2	NAG	m	1	2,1	14,14,15	0.27	0	17,19,21	0.54	0
2	NAG	m	2	2	14,14,15	0.45	0	17,19,21	0.73	0
2	YZT	m	3	2	13,14,15	1.17	1 (7%)	18,21,23	1.23	2 (11%)
2	MAN	m	4	2	11,11,12	0.55	0	15,15,17	0.64	0
2	MAN	m	5	2	11,11,12	0.43	0	15,15,17	0.76	0
2	NAG	mA	1	2,1	14,14,15	0.36	0	17,19,21	1.38	1 (5%)
2	NAG	mA	2	2	14,14,15	0.36	0	17,19,21	0.72	0
2	YZT	mA	3	2	13,14,15	1.06	1 (7%)	18,21,23	1.34	2 (11%)
2	MAN	mA	4	2	11,11,12	0.63	0	15,15,17	1.08	1 (6%)
2	MAN	mA	5	2	11,11,12	0.59	0	15,15,17	1.13	2 (13%)
3	NAG	n	1	3,1	14,14,15	0.48	0	17,19,21	0.68	0
3	NAG	n	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	MAN	n	3	3	11,11,12	0.48	0	15,15,17	0.71	0
4	NAG	nA	1	4,1	14,14,15	0.27	0	17,19,21	0.53	0
4	NAG	nA	2	4	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
4	YZT	nA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.32	3 (16%)
4	MAN	nA	4	4	11,11,12	0.39	0	15,15,17	0.68	0
2	NAG	o	1	2,1	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
2	NAG	o	2	2	14,14,15	0.47	0	17,19,21	0.68	0
2	YZT	o	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.82	1 (5%)
2	MAN	o	4	2	11,11,12	0.47	0	15,15,17	0.86	1 (6%)
2	MAN	o	5	2	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
3	NAG	oA	1	3,1	14,14,15	0.26	0	17,19,21	0.72	1 (5%)
3	NAG	oA	2	3	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
3	MAN	oA	3	3	11,11,12	0.43	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	p	1	2,1	14,14,15	0.29	0	17,19,21	0.54	0
2	NAG	p	2	2	14,14,15	0.46	0	17,19,21	0.73	0
2	YZT	p	3	2	13,14,15	1.16	1 (7%)	18,21,23	1.20	2 (11%)
2	MAN	p	4	2	11,11,12	0.59	0	15,15,17	0.68	0
2	MAN	p	5	2	11,11,12	0.44	0	15,15,17	0.77	0
2	NAG	pA	1	2,1	14,14,15	0.36	0	17,19,21	1.41	1 (5%)
2	NAG	pA	2	2	14,14,15	0.36	0	17,19,21	0.71	0
2	YZT	pA	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.39	2 (11%)
2	MAN	pA	4	2	11,11,12	0.64	0	15,15,17	1.10	1 (6%)
2	MAN	pA	5	2	11,11,12	0.58	0	15,15,17	1.16	2 (13%)
3	NAG	q	1	3,1	14,14,15	0.48	0	17,19,21	0.68	0
3	NAG	q	2	3	14,14,15	0.29	0	17,19,21	0.56	0
3	MAN	q	3	3	11,11,12	0.49	0	15,15,17	0.72	0
4	NAG	qA	1	4,1	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	qA	2	4	14,14,15	0.47	0	17,19,21	0.81	0
4	YZT	qA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.31	3 (16%)
4	MAN	qA	4	4	11,11,12	0.38	0	15,15,17	0.69	0
2	NAG	r	1	2,1	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
2	NAG	r	2	2	14,14,15	0.48	0	17,19,21	0.67	0
2	YZT	r	3	2	13,14,15	0.71	1 (7%)	18,21,23	0.80	1 (5%)
2	MAN	r	4	2	11,11,12	0.46	0	15,15,17	0.88	1 (6%)
2	MAN	r	5	2	11,11,12	0.44	0	15,15,17	0.89	1 (6%)
3	NAG	rA	1	3,1	14,14,15	0.27	0	17,19,21	0.74	1 (5%)
3	NAG	rA	2	3	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
3	MAN	rA	3	3	11,11,12	0.41	0	15,15,17	0.74	0
2	NAG	s	1	2,1	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	s	2	2	14,14,15	0.45	0	17,19,21	0.74	0
2	YZT	s	3	2	13,14,15	1.15	1 (7%)	18,21,23	1.23	2 (11%)
2	MAN	s	4	2	11,11,12	0.58	0	15,15,17	0.65	0
2	MAN	s	5	2	11,11,12	0.44	0	15,15,17	0.74	0
2	NAG	sA	1	2,1	14,14,15	0.36	0	17,19,21	1.38	1 (5%)
2	NAG	sA	2	2	14,14,15	0.37	0	17,19,21	0.70	0
2	YZT	sA	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.43	2 (11%)
2	MAN	sA	4	2	11,11,12	0.64	0	15,15,17	1.11	1 (6%)
2	MAN	sA	5	2	11,11,12	0.59	0	15,15,17	1.16	2 (13%)
3	NAG	t	1	3,1	14,14,15	0.49	0	17,19,21	0.68	0
3	NAG	t	2	3	14,14,15	0.27	0	17,19,21	0.58	0
3	MAN	t	3	3	11,11,12	0.49	0	15,15,17	0.71	0
4	NAG	tA	1	4,1	14,14,15	0.28	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	tA	2	4	14,14,15	0.45	0	17,19,21	0.81	0
4	YZT	tA	3	4	13,14,15	1.23	1 (7%)	18,21,23	1.34	3 (16%)
4	MAN	tA	4	4	11,11,12	0.40	0	15,15,17	0.66	0
2	NAG	u	1	2,1	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
2	NAG	u	2	2	14,14,15	0.48	0	17,19,21	0.68	0
2	YZT	u	3	2	13,14,15	0.68	1 (7%)	18,21,23	0.78	1 (5%)
2	MAN	u	4	2	11,11,12	0.45	0	15,15,17	0.90	1 (6%)
2	MAN	u	5	2	11,11,12	0.45	0	15,15,17	0.89	1 (6%)
3	NAG	uA	1	3,1	14,14,15	0.25	0	17,19,21	0.74	1 (5%)
3	NAG	uA	2	3	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
3	MAN	uA	3	3	11,11,12	0.44	0	15,15,17	0.74	0
2	NAG	v	1	2,1	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	v	2	2	14,14,15	0.46	0	17,19,21	0.74	0
2	YZT	v	3	2	13,14,15	1.18	1 (7%)	18,21,23	1.22	2 (11%)
2	MAN	v	4	2	11,11,12	0.58	0	15,15,17	0.67	0
2	MAN	v	5	2	11,11,12	0.43	0	15,15,17	0.77	0
2	NAG	vA	1	2,1	14,14,15	0.35	0	17,19,21	1.43	2 (11%)
2	NAG	vA	2	2	14,14,15	0.35	0	17,19,21	0.79	0
2	YZT	vA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.20	2 (11%)
2	MAN	vA	4	2	11,11,12	0.36	0	15,15,17	0.88	1 (6%)
2	MAN	vA	5	2	11,11,12	0.39	0	15,15,17	0.92	1 (6%)
3	NAG	w	1	3,1	14,14,15	0.48	0	17,19,21	0.68	0
3	NAG	w	2	3	14,14,15	0.27	0	17,19,21	0.58	0
3	MAN	w	3	3	11,11,12	0.50	0	15,15,17	0.72	0
4	NAG	wA	1	4,1	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	wA	2	4	14,14,15	0.45	0	17,19,21	0.62	0
4	YZT	wA	3	4	13,14,15	1.19	1 (7%)	18,21,23	1.04	2 (11%)
4	MAN	wA	4	4	11,11,12	0.44	0	15,15,17	0.73	0
2	NAG	x	1	2,1	14,14,15	0.29	0	17,19,21	0.89	1 (5%)
2	NAG	x	2	2	14,14,15	0.48	0	17,19,21	0.68	0
2	YZT	x	3	2	13,14,15	0.70	1 (7%)	18,21,23	0.79	1 (5%)
2	MAN	x	4	2	11,11,12	0.45	0	15,15,17	0.87	1 (6%)
2	MAN	x	5	2	11,11,12	0.45	0	15,15,17	0.89	0
3	NAG	xA	1	3,1	14,14,15	0.26	0	17,19,21	0.91	1 (5%)
3	NAG	xA	2	3	14,14,15	0.27	0	17,19,21	0.62	1 (5%)
3	MAN	xA	3	3	11,11,12	0.42	0	15,15,17	0.79	0
2	NAG	y	1	2,1	14,14,15	0.29	0	17,19,21	0.50	0
2	NAG	y	2	2	14,14,15	0.46	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	YZT	y	3	2	13,14,15	1.17	1 (7%)	18,21,23	1.21	2 (11%)
2	MAN	y	4	2	11,11,12	0.59	0	15,15,17	0.71	0
2	MAN	y	5	2	11,11,12	0.43	0	15,15,17	0.77	0
2	NAG	yA	1	2,1	14,14,15	0.37	0	17,19,21	1.41	2 (11%)
2	NAG	yA	2	2	14,14,15	0.35	0	17,19,21	0.79	0
2	YZT	yA	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.24	2 (11%)
2	MAN	yA	4	2	11,11,12	0.34	0	15,15,17	0.86	1 (6%)
2	MAN	yA	5	2	11,11,12	0.39	0	15,15,17	0.94	1 (6%)
3	NAG	z	1	3,1	14,14,15	0.47	0	17,19,21	0.68	0
3	NAG	z	2	3	14,14,15	0.27	0	17,19,21	0.56	0
3	MAN	z	3	3	11,11,12	0.49	0	15,15,17	0.72	0
4	NAG	zA	1	4,1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	zA	2	4	14,14,15	0.46	0	17,19,21	0.64	0
4	YZT	zA	3	4	13,14,15	1.20	1 (7%)	18,21,23	1.03	2 (11%)
4	MAN	zA	4	4	11,11,12	0.44	0	15,15,17	0.71	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	-	1/6/23/26	0/1/1/1
2	NAG	0	2	2	-	3/6/23/26	0/1/1/1
2	YZT	0	3	2	-	0/5/22/25	0/1/1/1
2	MAN	0	4	2	-	0/2/19/22	0/1/1/1
2	MAN	0	5	2	-	0/2/19/22	0/1/1/1
3	NAG	0A	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	0A	2	3	-	2/6/23/26	0/1/1/1
3	MAN	0A	3	3	-	0/2/19/22	0/1/1/1
2	NAG	1	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	1	2	2	-	0/6/23/26	0/1/1/1
2	YZT	1	3	2	-	0/5/22/25	0/1/1/1
2	MAN	1	4	2	-	0/2/19/22	0/1/1/1
2	MAN	1	5	2	-	0/2/19/22	0/1/1/1
2	NAG	1A	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	1A	2	2	-	2/6/23/26	0/1/1/1
2	YZT	1A	3	2	-	0/5/22/25	0/1/1/1
2	MAN	1A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	1A	5	2	-	0/2/19/22	0/1/1/1

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	UB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	UB	3	3	-	0/2/19/22	0/1/1/1
4	NAG	VA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	VA	2	4	-	1/6/23/26	0/1/1/1
4	YZT	VA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	VA	4	4	-	0/2/19/22	0/1/1/1
2	NAG	VB	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	VB	2	2	-	2/6/23/26	0/1/1/1
2	YZT	VB	3	2	-	0/5/22/25	0/1/1/1
2	MAN	VB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	VB	5	2	-	0/2/19/22	0/1/1/1
3	NAG	WA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	WA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	WA	3	3	-	0/2/19/22	0/1/1/1
4	NAG	WB	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	WB	2	4	-	2/6/23/26	0/1/1/1
4	YZT	WB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	WB	4	4	-	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	-	0/6/23/26	0/1/1/1
2	YZT	XA	3	2	-	0/5/22/25	0/1/1/1
2	MAN	XA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	XA	5	2	-	0/2/19/22	0/1/1/1
3	NAG	XB	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	XB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	XB	3	3	-	0/2/19/22	0/1/1/1
4	NAG	YA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	YA	2	4	-	1/6/23/26	0/1/1/1
4	YZT	YA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	YA	4	4	-	0/2/19/22	0/1/1/1
3	NAG	ZA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	ZA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	ZA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	aA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	aA	2	2	-	0/6/23/26	0/1/1/1
2	YZT	aA	3	2	-	0/5/22/25	0/1/1/1
2	MAN	aA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	aA	5	2	-	0/2/19/22	0/1/1/1
4	NAG	bA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	bA	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	YZT	bA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	bA	4	4	-	0/2/19/22	0/1/1/1
3	NAG	cA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	cA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	cA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	dA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	dA	2	2	-	0/6/23/26	0/1/1/1
2	YZT	dA	3	2	-	0/5/22/25	0/1/1/1
2	MAN	dA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	dA	5	2	-	0/2/19/22	0/1/1/1
4	NAG	eA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	eA	2	4	-	1/6/23/26	0/1/1/1
4	YZT	eA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	eA	4	4	-	0/2/19/22	0/1/1/1
3	NAG	fA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	fA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	fA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	gA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	gA	2	2	-	0/6/23/26	0/1/1/1
2	YZT	gA	3	2	-	0/5/22/25	0/1/1/1
2	MAN	gA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	gA	5	2	-	0/2/19/22	0/1/1/1
4	NAG	hA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	hA	2	4	-	1/6/23/26	0/1/1/1
4	YZT	hA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	hA	4	4	-	0/2/19/22	0/1/1/1
3	NAG	iA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	iA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	iA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	jA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	jA	2	2	-	0/6/23/26	0/1/1/1
2	YZT	jA	3	2	-	0/5/22/25	0/1/1/1
2	MAN	jA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	jA	5	2	-	0/2/19/22	0/1/1/1
2	NAG	k	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	3/6/23/26	0/1/1/1
2	YZT	k	3	2	-	0/5/22/25	0/1/1/1
2	MAN	k	4	2	-	0/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	0/1/1/1
4	NAG	kA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	kA	2	4	-	1/6/23/26	0/1/1/1

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	zA	4	4	-	0/2/19/22	0/1/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	TB	3	YZT	O3S6-S6	3.67	1.55	1.45
4	WB	3	YZT	O3S6-S6	3.64	1.55	1.45
4	EB	3	YZT	O3S6-S6	3.63	1.55	1.45
2	1	3	YZT	O2S6-S6	3.63	1.55	1.45
4	QB	3	YZT	O3S6-S6	3.63	1.55	1.45
4	wA	3	YZT	O3S6-S6	3.63	1.55	1.45
4	zA	3	YZT	O3S6-S6	3.62	1.55	1.45
4	2A	3	YZT	O3S6-S6	3.62	1.55	1.45
4	HB	3	YZT	O3S6-S6	3.62	1.55	1.45
2	y	3	YZT	O2S6-S6	3.62	1.55	1.45
2	7	3	YZT	O2S6-S6	3.62	1.55	1.45
2	p	3	YZT	O2S6-S6	3.61	1.55	1.45
4	NB	3	YZT	O3S6-S6	3.61	1.55	1.45
4	8A	3	YZT	O3S6-S6	3.60	1.55	1.45
2	m	3	YZT	O2S6-S6	3.60	1.55	1.45
4	BB	3	YZT	O3S6-S6	3.60	1.55	1.45
2	AA	3	YZT	O2S6-S6	3.60	1.55	1.45
2	DA	3	YZT	O2S6-S6	3.60	1.55	1.45
2	4	3	YZT	O2S6-S6	3.60	1.55	1.45
2	v	3	YZT	O2S6-S6	3.60	1.55	1.45
2	JA	3	YZT	O2S6-S6	3.59	1.55	1.45
4	KB	3	YZT	O3S6-S6	3.59	1.55	1.45
4	5A	3	YZT	O3S6-S6	3.59	1.55	1.45
2	s	3	YZT	O2S6-S6	3.59	1.55	1.45
2	GA	3	YZT	O2S6-S6	3.57	1.55	1.45
2	UA	3	YZT	O2S6-S6	3.52	1.55	1.45
2	LA	3	YZT	O2S6-S6	3.50	1.55	1.45
2	gA	3	YZT	O2S6-S6	3.49	1.55	1.45
2	jA	3	YZT	O2S6-S6	3.48	1.55	1.45
4	PA	3	YZT	O2S6-S6	3.48	1.55	1.45
2	XA	3	YZT	O2S6-S6	3.47	1.55	1.45
4	SA	3	YZT	O2S6-S6	3.47	1.55	1.45
4	tA	3	YZT	O2S6-S6	3.47	1.55	1.45
2	dA	3	YZT	O2S6-S6	3.46	1.55	1.45
4	hA	3	YZT	O2S6-S6	3.46	1.55	1.45
2	sA	3	YZT	O2S6-S6	3.46	1.55	1.45
2	RA	3	YZT	O2S6-S6	3.46	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	bA	3	YZT	O2S6-S6	3.46	1.55	1.45
2	pA	3	YZT	O2S6-S6	3.45	1.55	1.45
2	OA	3	YZT	O2S6-S6	3.45	1.55	1.45
4	eA	3	YZT	O2S6-S6	3.44	1.55	1.45
4	nA	3	YZT	O2S6-S6	3.44	1.55	1.45
4	VA	3	YZT	O2S6-S6	3.44	1.55	1.45
4	YA	3	YZT	O2S6-S6	3.44	1.55	1.45
4	qA	3	YZT	O2S6-S6	3.44	1.55	1.45
4	kA	3	YZT	O2S6-S6	3.43	1.55	1.45
2	mA	3	YZT	O2S6-S6	3.43	1.55	1.45
2	aA	3	YZT	O2S6-S6	3.43	1.55	1.45
4	MA	3	YZT	O2S6-S6	3.42	1.55	1.45
2	1A	3	YZT	O2S6-S6	3.35	1.54	1.45
2	MB	3	YZT	O2S6-S6	3.35	1.54	1.45
2	DB	3	YZT	O2S6-S6	3.34	1.54	1.45
2	AB	3	YZT	O2S6-S6	3.33	1.54	1.45
2	PB	3	YZT	O2S6-S6	3.33	1.54	1.45
2	yA	3	YZT	O2S6-S6	3.32	1.54	1.45
2	7A	3	YZT	O2S6-S6	3.30	1.54	1.45
2	JB	3	YZT	O2S6-S6	3.30	1.54	1.45
2	SB	3	YZT	O2S6-S6	3.29	1.54	1.45
2	VB	3	YZT	O2S6-S6	3.28	1.54	1.45
2	vA	3	YZT	O2S6-S6	3.28	1.54	1.45
2	4A	3	YZT	O2S6-S6	3.28	1.54	1.45
2	GB	3	YZT	O2S6-S6	3.25	1.54	1.45
2	r	3	YZT	O1S6-S6	2.22	1.55	1.47
2	FA	3	YZT	O1S6-S6	2.21	1.55	1.47
2	CA	3	YZT	O1S6-S6	2.20	1.55	1.47
2	o	3	YZT	O1S6-S6	2.19	1.55	1.47
2	0	3	YZT	O1S6-S6	2.19	1.55	1.47
2	3	3	YZT	O1S6-S6	2.18	1.55	1.47
2	k	3	YZT	O1S6-S6	2.18	1.55	1.47
2	IA	3	YZT	O1S6-S6	2.17	1.55	1.47
2	x	3	YZT	O1S6-S6	2.16	1.55	1.47
2	9	3	YZT	O1S6-S6	2.14	1.55	1.47
2	6	3	YZT	O1S6-S6	2.13	1.55	1.47
2	u	3	YZT	O1S6-S6	2.10	1.55	1.47

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	sA	3	YZT	O2S6-S6-C6	-4.73	101.32	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	dA	3	YZT	O2S6-S6-C6	-4.60	101.47	106.94
2	pA	1	NAG	C2-N2-C7	4.60	129.45	122.90
2	AB	1	NAG	C2-N2-C7	4.58	129.42	122.90
2	gA	3	YZT	O2S6-S6-C6	-4.57	101.51	106.94
2	pA	3	YZT	O2S6-S6-C6	-4.56	101.52	106.94
2	SB	1	NAG	C2-N2-C7	4.55	129.38	122.90
2	LA	3	YZT	O2S6-S6-C6	-4.55	101.53	106.94
2	4A	1	NAG	C2-N2-C7	4.53	129.35	122.90
2	sA	1	NAG	C2-N2-C7	4.52	129.34	122.90
2	jA	1	NAG	C2-N2-C7	4.50	129.31	122.90
2	1A	1	NAG	C2-N2-C7	4.48	129.28	122.90
2	VB	1	NAG	C2-N2-C7	4.48	129.28	122.90
2	PB	1	NAG	C2-N2-C7	4.46	129.25	122.90
2	yA	1	NAG	C2-N2-C7	4.43	129.21	122.90
2	vA	1	NAG	C2-N2-C7	4.42	129.20	122.90
2	7A	1	NAG	C2-N2-C7	4.40	129.17	122.90
2	mA	1	NAG	C2-N2-C7	4.39	129.15	122.90
2	MB	1	NAG	C2-N2-C7	4.36	129.11	122.90
2	GB	1	NAG	C2-N2-C7	4.35	129.10	122.90
2	RA	3	YZT	O2S6-S6-C6	-4.34	101.78	106.94
2	DB	1	NAG	C2-N2-C7	4.33	129.07	122.90
2	gA	1	NAG	C2-N2-C7	4.32	129.06	122.90
2	dA	1	NAG	C2-N2-C7	4.32	129.05	122.90
2	jA	3	YZT	O2S6-S6-C6	-4.30	101.83	106.94
2	RA	1	NAG	C2-N2-C7	4.29	129.01	122.90
2	mA	3	YZT	O2S6-S6-C6	-4.27	101.86	106.94
2	UA	3	YZT	O2S6-S6-C6	-4.26	101.87	106.94
2	aA	3	YZT	O2S6-S6-C6	-4.26	101.88	106.94
2	JB	1	NAG	C2-N2-C7	4.24	128.94	122.90
2	XA	1	NAG	C2-N2-C7	4.24	128.94	122.90
2	OA	1	NAG	C2-N2-C7	4.23	128.92	122.90
2	UA	1	NAG	C2-N2-C7	4.19	128.87	122.90
2	aA	1	NAG	C2-N2-C7	4.17	128.85	122.90
2	XA	3	YZT	O2S6-S6-C6	-4.16	102.00	106.94
2	LA	1	NAG	C2-N2-C7	4.12	128.78	122.90
2	OA	3	YZT	O2S6-S6-C6	-4.06	102.11	106.94
4	tA	3	YZT	O2S6-S6-C6	-3.73	102.50	106.94
4	MA	3	YZT	O2S6-S6-C6	-3.69	102.55	106.94
4	eA	3	YZT	O2S6-S6-C6	-3.68	102.57	106.94
3	IB	1	NAG	C1-O5-C5	3.66	117.16	112.19
4	YA	3	YZT	O2S6-S6-C6	-3.66	102.59	106.94
3	CB	1	NAG	C1-O5-C5	3.65	117.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	VA	3	YZT	O2S6-S6-C6	-3.64	102.61	106.94
4	SA	3	YZT	O2S6-S6-C6	-3.61	102.64	106.94
4	kA	3	YZT	O2S6-S6-C6	-3.61	102.64	106.94
3	6A	1	NAG	C1-O5-C5	3.60	117.08	112.19
4	PA	3	YZT	O2S6-S6-C6	-3.60	102.67	106.94
4	nA	3	YZT	O2S6-S6-C6	-3.58	102.68	106.94
3	XB	1	NAG	C1-O5-C5	3.58	117.05	112.19
3	0A	1	NAG	C1-O5-C5	3.57	117.03	112.19
4	qA	3	YZT	O2S6-S6-C6	-3.57	102.69	106.94
3	OB	1	NAG	C1-O5-C5	3.57	117.03	112.19
4	hA	3	YZT	O2S6-S6-C6	-3.56	102.70	106.94
4	bA	3	YZT	O2S6-S6-C6	-3.56	102.71	106.94
3	xA	1	NAG	C1-O5-C5	3.48	116.91	112.19
3	UB	1	NAG	C1-O5-C5	3.48	116.90	112.19
2	aA	5	MAN	C1-O5-C5	3.44	116.85	112.19
2	gA	5	MAN	C1-O5-C5	3.43	116.84	112.19
3	9A	1	NAG	C1-O5-C5	3.42	116.82	112.19
2	jA	5	MAN	C1-O5-C5	3.42	116.82	112.19
3	LB	1	NAG	C1-O5-C5	3.41	116.81	112.19
2	dA	5	MAN	C1-O5-C5	3.40	116.80	112.19
3	3A	1	NAG	C1-O5-C5	3.39	116.79	112.19
2	pA	5	MAN	C1-O5-C5	3.39	116.78	112.19
2	RA	5	MAN	C1-O5-C5	3.39	116.78	112.19
3	RB	1	NAG	C1-O5-C5	3.38	116.77	112.19
2	XA	5	MAN	C1-O5-C5	3.37	116.76	112.19
2	sA	5	MAN	C1-O5-C5	3.36	116.75	112.19
2	LA	5	MAN	C1-O5-C5	3.35	116.73	112.19
2	UA	5	MAN	C1-O5-C5	3.34	116.71	112.19
2	JB	3	YZT	O2S6-S6-C6	-3.32	102.99	106.94
2	mA	5	MAN	C1-O5-C5	3.32	116.69	112.19
2	OA	5	MAN	C1-O5-C5	3.31	116.67	112.19
2	4A	3	YZT	O2S6-S6-C6	-3.30	103.02	106.94
3	FB	1	NAG	C1-O5-C5	3.29	116.65	112.19
2	7A	3	YZT	O2S6-S6-C6	-3.25	103.07	106.94
2	VB	3	YZT	O2S6-S6-C6	-3.20	103.14	106.94
2	yA	3	YZT	O2S6-S6-C6	-3.19	103.15	106.94
2	s	3	YZT	O2S6-S6-C6	-3.16	103.18	106.94
2	m	3	YZT	O2S6-S6-C6	-3.15	103.20	106.94
2	vA	3	YZT	O2S6-S6-C6	-3.09	103.26	106.94
2	MB	3	YZT	O2S6-S6-C6	-3.09	103.26	106.94
2	y	3	YZT	O2S6-S6-C6	-3.09	103.26	106.94
2	4	3	YZT	O2S6-S6-C6	-3.09	103.27	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	JA	3	YZT	O2S6-S6-C6	-3.08	103.28	106.94
2	1	3	YZT	O2S6-S6-C6	-3.06	103.30	106.94
2	AA	3	YZT	O2S6-S6-C6	-3.06	103.31	106.94
2	GA	3	YZT	O2S6-S6-C6	-3.05	103.31	106.94
2	v	3	YZT	O2S6-S6-C6	-3.05	103.32	106.94
2	AB	3	YZT	O2S6-S6-C6	-3.04	103.33	106.94
2	1A	3	YZT	O2S6-S6-C6	-3.04	103.33	106.94
2	p	3	YZT	O2S6-S6-C6	-3.03	103.33	106.94
2	DA	3	YZT	O2S6-S6-C6	-3.01	103.36	106.94
2	7	3	YZT	O2S6-S6-C6	-3.01	103.36	106.94
2	DB	3	YZT	O2S6-S6-C6	-3.00	103.38	106.94
2	GB	3	YZT	O2S6-S6-C6	-2.99	103.39	106.94
2	yA	3	YZT	O1S6-S6-O3S6	2.97	118.52	111.27
2	SB	3	YZT	O2S6-S6-C6	-2.97	103.42	106.94
2	MB	3	YZT	O1S6-S6-O3S6	2.94	118.46	111.27
2	GB	3	YZT	O1S6-S6-O3S6	2.93	118.43	111.27
2	JB	3	YZT	O1S6-S6-O3S6	2.92	118.41	111.27
2	PB	3	YZT	O1S6-S6-O3S6	2.92	118.41	111.27
2	7A	3	YZT	O1S6-S6-O3S6	2.92	118.40	111.27
2	XA	3	YZT	O1S6-S6-O3S6	2.91	118.40	111.27
2	AB	3	YZT	O1S6-S6-O3S6	2.90	118.37	111.27
4	tA	3	YZT	O1S6-S6-O3S6	2.90	118.37	111.27
2	4A	3	YZT	O1S6-S6-O3S6	2.90	118.36	111.27
2	VB	3	YZT	O1S6-S6-O3S6	2.90	118.36	111.27
2	PB	3	YZT	O2S6-S6-C6	-2.90	103.50	106.94
2	aA	3	YZT	O1S6-S6-O3S6	2.90	118.35	111.27
2	dA	3	YZT	O1S6-S6-O3S6	2.90	118.35	111.27
2	OA	3	YZT	O1S6-S6-O3S6	2.89	118.34	111.27
2	UA	3	YZT	O1S6-S6-O3S6	2.89	118.34	111.27
2	LA	3	YZT	O1S6-S6-O3S6	2.89	118.34	111.27
2	jA	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
4	qA	3	YZT	O1S6-S6-O3S6	2.89	118.33	111.27
2	gA	3	YZT	O1S6-S6-O3S6	2.89	118.32	111.27
4	eA	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
4	kA	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
4	PA	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
4	VA	3	YZT	O1S6-S6-O3S6	2.88	118.32	111.27
4	SA	3	YZT	O1S6-S6-O3S6	2.88	118.31	111.27
4	hA	3	YZT	O1S6-S6-O3S6	2.88	118.31	111.27
2	RA	3	YZT	O1S6-S6-O3S6	2.88	118.30	111.27
4	bA	3	YZT	O1S6-S6-O3S6	2.87	118.29	111.27
4	nA	3	YZT	O1S6-S6-O3S6	2.87	118.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	pA	3	YZT	O1S6-S6-O3S6	2.87	118.28	111.27
2	1A	3	YZT	O1S6-S6-O3S6	2.87	118.28	111.27
2	mA	3	YZT	O1S6-S6-O3S6	2.86	118.27	111.27
2	sA	3	YZT	O1S6-S6-O3S6	2.86	118.27	111.27
4	MA	3	YZT	O1S6-S6-O3S6	2.86	118.26	111.27
4	YA	3	YZT	O1S6-S6-O3S6	2.86	118.26	111.27
2	SB	3	YZT	O1S6-S6-O3S6	2.85	118.25	111.27
2	DB	3	YZT	O1S6-S6-O3S6	2.85	118.24	111.27
2	vA	3	YZT	O1S6-S6-O3S6	2.82	118.16	111.27
2	o	3	YZT	O1S6-S6-C6	-2.80	101.28	105.74
2	0	3	YZT	O1S6-S6-C6	-2.70	101.44	105.74
2	CA	3	YZT	O1S6-S6-C6	-2.70	101.44	105.74
2	r	3	YZT	O1S6-S6-C6	-2.68	101.47	105.74
2	x	3	YZT	O1S6-S6-C6	-2.67	101.48	105.74
4	WB	3	YZT	O1S6-S6-O2S6	2.67	117.79	111.27
4	QB	3	YZT	O1S6-S6-O2S6	2.66	117.78	111.27
2	9	3	YZT	O1S6-S6-C6	-2.66	101.50	105.74
2	s	3	YZT	O1S6-S6-O3S6	2.66	117.77	111.27
4	5A	3	YZT	O1S6-S6-O2S6	2.65	117.75	111.27
4	KB	3	YZT	O1S6-S6-O2S6	2.64	117.73	111.27
4	TB	3	YZT	O1S6-S6-O2S6	2.64	117.73	111.27
4	8A	3	YZT	O1S6-S6-O2S6	2.64	117.72	111.27
4	NB	3	YZT	O1S6-S6-O2S6	2.63	117.69	111.27
2	GA	3	YZT	O1S6-S6-O3S6	2.62	117.69	111.27
4	zA	3	YZT	O1S6-S6-O2S6	2.62	117.68	111.27
4	HB	3	YZT	O1S6-S6-O2S6	2.62	117.67	111.27
4	2A	3	YZT	O1S6-S6-O2S6	2.62	117.67	111.27
4	EB	3	YZT	O1S6-S6-O2S6	2.62	117.67	111.27
2	u	3	YZT	O1S6-S6-C6	-2.62	101.57	105.74
2	1	3	YZT	O1S6-S6-O3S6	2.62	117.67	111.27
2	p	3	YZT	O1S6-S6-O3S6	2.61	117.66	111.27
4	wA	3	YZT	O1S6-S6-O2S6	2.61	117.66	111.27
2	m	3	YZT	O1S6-S6-O3S6	2.61	117.65	111.27
2	y	3	YZT	O1S6-S6-O3S6	2.61	117.64	111.27
2	FA	3	YZT	O1S6-S6-C6	-2.60	101.59	105.74
2	v	3	YZT	O1S6-S6-O3S6	2.60	117.64	111.27
2	4	3	YZT	O1S6-S6-O3S6	2.60	117.64	111.27
4	BB	3	YZT	O1S6-S6-O2S6	2.60	117.64	111.27
2	7	3	YZT	O1S6-S6-O3S6	2.59	117.60	111.27
2	JA	3	YZT	O1S6-S6-O3S6	2.59	117.59	111.27
2	AA	3	YZT	O1S6-S6-O3S6	2.58	117.59	111.27
2	6	3	YZT	O1S6-S6-C6	-2.58	101.64	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DA	3	YZT	O1S6-S6-O3S6	2.57	117.55	111.27
2	k	3	YZT	O1S6-S6-C6	-2.54	101.69	105.74
2	3	3	YZT	O1S6-S6-C6	-2.51	101.74	105.74
4	5A	3	YZT	O3S6-S6-C6	-2.50	103.97	106.94
2	jA	4	MAN	O5-C1-C2	2.47	114.58	110.77
2	pA	4	MAN	O5-C1-C2	2.47	114.58	110.77
2	sA	4	MAN	O5-C1-C2	2.46	114.57	110.77
4	WB	3	YZT	O3S6-S6-C6	-2.46	104.02	106.94
2	gA	4	MAN	O5-C1-C2	2.45	114.56	110.77
2	IA	3	YZT	O1S6-S6-C6	-2.45	101.83	105.74
2	mA	4	MAN	O5-C1-C2	2.45	114.56	110.77
2	UA	4	MAN	O5-C1-C2	2.45	114.55	110.77
2	1A	4	MAN	C1-O5-C5	2.45	115.51	112.19
4	HB	3	YZT	O3S6-S6-C6	-2.44	104.04	106.94
2	aA	4	MAN	O5-C1-C2	2.44	114.53	110.77
2	u	4	MAN	C1-O5-C5	2.43	115.49	112.19
2	XA	4	MAN	O5-C1-C2	2.42	114.51	110.77
2	9	4	MAN	C1-O5-C5	2.41	115.45	112.19
2	dA	4	MAN	O5-C1-C2	2.40	114.48	110.77
2	4A	4	MAN	C1-O5-C5	2.40	115.44	112.19
2	vA	4	MAN	C1-O5-C5	2.40	115.44	112.19
2	LA	4	MAN	O5-C1-C2	2.39	114.47	110.77
2	OA	4	MAN	O5-C1-C2	2.38	114.45	110.77
2	k	4	MAN	C1-O5-C5	2.38	115.42	112.19
2	RA	4	MAN	O5-C1-C2	2.38	114.44	110.77
2	VB	4	MAN	C1-O5-C5	2.37	115.41	112.19
2	IA	4	MAN	C1-O5-C5	2.37	115.40	112.19
2	3	4	MAN	C1-O5-C5	2.36	115.39	112.19
2	JB	4	MAN	C1-O5-C5	2.36	115.39	112.19
2	SB	4	MAN	C1-O5-C5	2.36	115.39	112.19
2	FA	4	MAN	C1-O5-C5	2.36	115.39	112.19
2	CA	4	MAN	C1-O5-C5	2.36	115.39	112.19
2	x	4	MAN	C1-O5-C5	2.35	115.38	112.19
2	r	4	MAN	C1-O5-C5	2.35	115.38	112.19
4	2A	3	YZT	O3S6-S6-C6	-2.35	104.15	106.94
2	6	4	MAN	C1-O5-C5	2.34	115.37	112.19
4	wA	3	YZT	O3S6-S6-C6	-2.34	104.16	106.94
2	GB	4	MAN	C1-O5-C5	2.33	115.35	112.19
2	1A	5	MAN	C1-O5-C5	2.33	115.35	112.19
4	QB	3	YZT	O3S6-S6-C6	-2.32	104.18	106.94
2	7A	4	MAN	C1-O5-C5	2.32	115.34	112.19
4	KB	3	YZT	O3S6-S6-C6	-2.32	104.18	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BB	3	YZT	O3S6-S6-C6	-2.32	104.18	106.94
2	LA	5	MAN	C2-C3-C4	2.31	114.90	110.89
4	EB	3	YZT	O3S6-S6-C6	-2.31	104.19	106.94
2	sA	5	MAN	C2-C3-C4	2.31	114.90	110.89
4	TB	3	YZT	O3S6-S6-C6	-2.31	104.19	106.94
2	o	4	MAN	C1-O5-C5	2.31	115.32	112.19
3	WA	2	NAG	C1-O5-C5	2.31	115.32	112.19
3	rA	2	NAG	C1-O5-C5	2.31	115.32	112.19
2	MB	4	MAN	C1-O5-C5	2.31	115.32	112.19
3	TA	2	NAG	C1-O5-C5	2.30	115.31	112.19
2	gA	5	MAN	C2-C3-C4	2.30	114.88	110.89
2	AB	5	MAN	C1-O5-C5	2.30	115.31	112.19
2	yA	4	MAN	C1-O5-C5	2.30	115.31	112.19
2	UA	5	MAN	C2-C3-C4	2.29	114.87	110.89
2	PB	5	MAN	C1-O5-C5	2.29	115.29	112.19
3	cA	2	NAG	C1-O5-C5	2.29	115.29	112.19
2	0	4	MAN	C1-O5-C5	2.28	115.28	112.19
2	4A	5	MAN	C1-O5-C5	2.28	115.28	112.19
2	MB	5	MAN	C1-O5-C5	2.27	115.27	112.19
2	DB	4	MAN	C1-O5-C5	2.27	115.27	112.19
3	ZA	2	NAG	C1-O5-C5	2.27	115.26	112.19
2	jA	5	MAN	C2-C3-C4	2.26	114.81	110.89
4	zA	3	YZT	O3S6-S6-C6	-2.26	104.26	106.94
3	NA	1	NAG	C1-O5-C5	2.26	115.25	112.19
4	NB	3	YZT	O3S6-S6-C6	-2.25	104.26	106.94
2	AB	4	MAN	C1-O5-C5	2.25	115.24	112.19
2	JB	5	MAN	C1-O5-C5	2.24	115.23	112.19
2	PB	4	MAN	C1-O5-C5	2.24	115.22	112.19
2	yA	5	MAN	C1-O5-C5	2.24	115.22	112.19
2	VB	5	MAN	C1-O5-C5	2.24	115.22	112.19
2	k	1	NAG	C1-O5-C5	2.24	115.22	112.19
3	iA	1	NAG	C1-O5-C5	2.23	115.22	112.19
3	RB	2	NAG	C1-O5-C5	2.23	115.22	112.19
3	fA	1	NAG	C1-O5-C5	2.23	115.22	112.19
3	CB	2	NAG	C1-O5-C5	2.23	115.22	112.19
3	TA	1	NAG	C1-O5-C5	2.23	115.21	112.19
2	dA	5	MAN	C2-C3-C4	2.22	114.74	110.89
3	rA	1	NAG	C1-O5-C5	2.22	115.20	112.19
3	3A	2	NAG	C1-O5-C5	2.22	115.20	112.19
2	DB	5	MAN	C1-O5-C5	2.22	115.20	112.19
3	lA	2	NAG	C1-O5-C5	2.22	115.20	112.19
4	8A	3	YZT	O3S6-S6-C6	-2.21	104.31	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	QA	2	NAG	C1-O5-C5	2.21	115.19	112.19
3	XB	2	NAG	C1-O5-C5	2.21	115.18	112.19
2	XA	5	MAN	C2-C3-C4	2.21	114.72	110.89
3	WA	1	NAG	C1-O5-C5	2.20	115.18	112.19
3	uA	1	NAG	C1-O5-C5	2.20	115.17	112.19
2	RA	5	MAN	C2-C3-C4	2.20	114.70	110.89
2	pA	5	MAN	C2-C3-C4	2.20	114.70	110.89
4	YA	3	YZT	O5-C1-C2	-2.20	107.38	110.77
2	6	1	NAG	C1-O5-C5	2.20	115.17	112.19
2	SB	5	MAN	C1-O5-C5	2.19	115.16	112.19
2	GB	5	MAN	C1-O5-C5	2.19	115.16	112.19
2	7A	5	MAN	C1-O5-C5	2.19	115.16	112.19
3	6A	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	vA	5	MAN	C1-O5-C5	2.18	115.15	112.19
4	nA	3	YZT	O5-C1-C2	-2.18	107.41	110.77
2	3	1	NAG	C1-O5-C5	2.18	115.14	112.19
2	mA	5	MAN	C2-C3-C4	2.17	114.65	110.89
4	PA	3	YZT	O5-C1-C2	-2.17	107.43	110.77
2	aA	5	MAN	C2-C3-C4	2.16	114.64	110.89
2	OA	5	MAN	C2-C3-C4	2.16	114.63	110.89
3	cA	1	NAG	C1-O5-C5	2.16	115.12	112.19
3	oA	2	NAG	C1-O5-C5	2.16	115.11	112.19
3	OB	2	NAG	C1-O5-C5	2.15	115.11	112.19
3	IB	2	NAG	C1-O5-C5	2.15	115.11	112.19
3	lA	1	NAG	C1-O5-C5	2.15	115.11	112.19
4	VA	3	YZT	O5-C1-C2	-2.15	107.45	110.77
2	0	1	NAG	C1-O5-C5	2.15	115.11	112.19
2	GB	1	NAG	O5-C1-C2	-2.15	107.89	111.29
3	ZA	1	NAG	C1-O5-C5	2.15	115.10	112.19
4	bA	3	YZT	O5-C1-C2	-2.13	107.48	110.77
4	hA	3	YZT	O5-C1-C2	-2.13	107.48	110.77
3	uA	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	AB	1	NAG	O5-C1-C2	-2.13	107.93	111.29
2	r	1	NAG	C1-O5-C5	2.12	115.07	112.19
4	tA	3	YZT	O5-C1-C2	-2.12	107.49	110.77
2	u	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	x	1	NAG	C1-O5-C5	2.11	115.05	112.19
4	MA	3	YZT	O5-C1-C2	-2.11	107.52	110.77
3	QA	1	NAG	C1-O5-C5	2.11	115.05	112.19
3	0A	2	NAG	C1-O5-C5	2.11	115.05	112.19
2	DB	1	NAG	O5-C1-C2	-2.10	107.97	111.29
2	vA	1	NAG	O5-C1-C2	-2.10	107.97	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	fA	2	NAG	C1-O5-C5	2.10	115.03	112.19
2	4A	1	NAG	O5-C1-C2	-2.10	107.98	111.29
2	7A	1	NAG	O5-C1-C2	-2.09	107.98	111.29
3	UB	2	NAG	C1-O5-C5	2.09	115.03	112.19
3	NA	2	NAG	C1-O5-C5	2.09	115.02	112.19
4	kA	3	YZT	O5-C1-C2	-2.09	107.55	110.77
3	oA	1	NAG	C1-O5-C5	2.09	115.02	112.19
2	9	1	NAG	C1-O5-C5	2.09	115.02	112.19
2	FA	1	NAG	C1-O5-C5	2.09	115.02	112.19
2	o	1	NAG	C1-O5-C5	2.09	115.02	112.19
3	xA	2	NAG	C1-O5-C5	2.08	115.01	112.19
4	qA	3	YZT	O5-C1-C2	-2.08	107.56	110.77
3	LB	2	NAG	C1-O5-C5	2.07	115.00	112.19
2	o	5	MAN	C1-O5-C5	2.07	114.99	112.19
2	CA	1	NAG	C1-O5-C5	2.07	114.99	112.19
3	FB	2	NAG	C1-O5-C5	2.06	114.98	112.19
4	eA	3	YZT	O5-C1-C2	-2.06	107.59	110.77
2	k	5	MAN	C1-O5-C5	2.05	114.97	112.19
2	u	5	MAN	C1-O5-C5	2.04	114.96	112.19
3	HA	2	NAG	C1-O5-C5	2.04	114.96	112.19
3	iA	2	NAG	C1-O5-C5	2.04	114.96	112.19
2	0	5	MAN	C1-O5-C5	2.04	114.96	112.19
4	MA	2	NAG	O3-C3-C2	2.04	113.69	109.47
2	9	5	MAN	C1-O5-C5	2.04	114.96	112.19
4	SA	3	YZT	O5-C1-C2	-2.03	107.63	110.77
2	r	5	MAN	C1-O5-C5	2.03	114.95	112.19
2	yA	1	NAG	O5-C1-C2	-2.03	108.08	111.29
4	PA	2	NAG	O3-C3-C2	2.03	113.66	109.47
4	VA	2	NAG	O3-C3-C2	2.03	113.66	109.47
4	YA	2	NAG	O3-C3-C2	2.02	113.65	109.47
2	FA	5	MAN	C1-O5-C5	2.02	114.93	112.19
2	CA	5	MAN	C1-O5-C5	2.02	114.93	112.19
4	kA	2	NAG	O3-C3-C2	2.02	113.64	109.47
4	hA	2	NAG	O3-C3-C2	2.02	113.64	109.47
2	6	5	MAN	C1-O5-C5	2.01	114.92	112.19
2	IA	5	MAN	C1-O5-C5	2.01	114.92	112.19
2	IA	1	NAG	C1-O5-C5	2.01	114.92	112.19
4	SA	2	NAG	O3-C3-C2	2.01	113.62	109.47
4	nA	2	NAG	O3-C3-C2	2.00	113.61	109.47

There are no chirality outliers.

All (283) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	LB	1	NAG	O5-C5-C6-O6
3	3A	1	NAG	O5-C5-C6-O6
3	xA	1	NAG	O5-C5-C6-O6
3	0A	1	NAG	O5-C5-C6-O6
3	6A	1	NAG	O5-C5-C6-O6
3	9A	1	NAG	O5-C5-C6-O6
3	CB	1	NAG	O5-C5-C6-O6
3	FB	1	NAG	O5-C5-C6-O6
3	IB	1	NAG	O5-C5-C6-O6
3	OB	1	NAG	O5-C5-C6-O6
3	RB	1	NAG	O5-C5-C6-O6
3	UB	1	NAG	O5-C5-C6-O6
3	XB	1	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	q	2	NAG	O5-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	w	2	NAG	O5-C5-C6-O6
3	z	2	NAG	O5-C5-C6-O6
3	2	2	NAG	O5-C5-C6-O6
3	5	2	NAG	O5-C5-C6-O6
3	8	2	NAG	O5-C5-C6-O6
3	BA	2	NAG	O5-C5-C6-O6
3	EA	2	NAG	O5-C5-C6-O6
3	HA	2	NAG	O5-C5-C6-O6
3	KA	2	NAG	O5-C5-C6-O6
3	NA	2	NAG	O5-C5-C6-O6
3	iA	2	NAG	O5-C5-C6-O6
3	n	2	NAG	C4-C5-C6-O6
3	q	2	NAG	C4-C5-C6-O6
3	t	2	NAG	C4-C5-C6-O6
3	w	2	NAG	C4-C5-C6-O6
3	z	2	NAG	C4-C5-C6-O6
3	2	2	NAG	C4-C5-C6-O6
3	5	2	NAG	C4-C5-C6-O6
3	8	2	NAG	C4-C5-C6-O6
3	BA	2	NAG	C4-C5-C6-O6
3	EA	2	NAG	C4-C5-C6-O6
3	HA	2	NAG	C4-C5-C6-O6
3	KA	2	NAG	C4-C5-C6-O6
3	QA	2	NAG	O5-C5-C6-O6
3	TA	2	NAG	O5-C5-C6-O6
3	WA	2	NAG	O5-C5-C6-O6
3	ZA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	cA	2	NAG	O5-C5-C6-O6
3	fA	2	NAG	O5-C5-C6-O6
3	lA	2	NAG	O5-C5-C6-O6
3	oA	2	NAG	O5-C5-C6-O6
3	rA	2	NAG	O5-C5-C6-O6
3	uA	2	NAG	O5-C5-C6-O6
3	xA	2	NAG	O5-C5-C6-O6
3	0A	2	NAG	O5-C5-C6-O6
3	3A	2	NAG	O5-C5-C6-O6
3	6A	2	NAG	O5-C5-C6-O6
3	9A	2	NAG	O5-C5-C6-O6
3	CB	2	NAG	O5-C5-C6-O6
3	FB	2	NAG	O5-C5-C6-O6
3	IB	2	NAG	O5-C5-C6-O6
3	LB	2	NAG	O5-C5-C6-O6
3	OB	2	NAG	O5-C5-C6-O6
3	RB	2	NAG	O5-C5-C6-O6
3	UB	2	NAG	O5-C5-C6-O6
3	XB	2	NAG	O5-C5-C6-O6
3	3A	1	NAG	C4-C5-C6-O6
3	6A	1	NAG	C4-C5-C6-O6
3	9A	1	NAG	C4-C5-C6-O6
3	FB	1	NAG	C4-C5-C6-O6
3	LB	1	NAG	C4-C5-C6-O6
3	RB	1	NAG	C4-C5-C6-O6
3	XB	1	NAG	C4-C5-C6-O6
3	xA	1	NAG	C4-C5-C6-O6
3	0A	1	NAG	C4-C5-C6-O6
3	CB	1	NAG	C4-C5-C6-O6
3	IB	1	NAG	C4-C5-C6-O6
3	OB	1	NAG	C4-C5-C6-O6
3	UB	1	NAG	C4-C5-C6-O6
2	vA	2	NAG	O5-C5-C6-O6
2	yA	2	NAG	O5-C5-C6-O6
2	7A	2	NAG	O5-C5-C6-O6
2	DB	2	NAG	O5-C5-C6-O6
2	GB	2	NAG	O5-C5-C6-O6
2	JB	2	NAG	O5-C5-C6-O6
3	NA	2	NAG	C4-C5-C6-O6
3	WA	2	NAG	C4-C5-C6-O6
3	fA	2	NAG	C4-C5-C6-O6
3	iA	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	oA	2	NAG	C4-C5-C6-O6
3	rA	2	NAG	C4-C5-C6-O6
3	0A	2	NAG	C4-C5-C6-O6
3	3A	2	NAG	C4-C5-C6-O6
3	6A	2	NAG	C4-C5-C6-O6
3	9A	2	NAG	C4-C5-C6-O6
3	CB	2	NAG	C4-C5-C6-O6
3	IB	2	NAG	C4-C5-C6-O6
3	LB	2	NAG	C4-C5-C6-O6
3	OB	2	NAG	C4-C5-C6-O6
3	XB	2	NAG	C4-C5-C6-O6
2	1A	2	NAG	O5-C5-C6-O6
2	4A	2	NAG	O5-C5-C6-O6
2	AB	2	NAG	O5-C5-C6-O6
2	MB	2	NAG	O5-C5-C6-O6
2	PB	2	NAG	O5-C5-C6-O6
2	SB	2	NAG	O5-C5-C6-O6
2	VB	2	NAG	O5-C5-C6-O6
3	QA	2	NAG	C4-C5-C6-O6
3	TA	2	NAG	C4-C5-C6-O6
3	ZA	2	NAG	C4-C5-C6-O6
3	cA	2	NAG	C4-C5-C6-O6
3	lA	2	NAG	C4-C5-C6-O6
3	uA	2	NAG	C4-C5-C6-O6
3	xA	2	NAG	C4-C5-C6-O6
3	FB	2	NAG	C4-C5-C6-O6
3	RB	2	NAG	C4-C5-C6-O6
3	UB	2	NAG	C4-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
2	r	2	NAG	O5-C5-C6-O6
2	3	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
4	wA	2	NAG	O5-C5-C6-O6
4	zA	2	NAG	O5-C5-C6-O6
4	2A	1	NAG	O5-C5-C6-O6
4	2A	2	NAG	O5-C5-C6-O6
4	5A	2	NAG	O5-C5-C6-O6
4	8A	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	BB	1	NAG	O5-C5-C6-O6
4	BB	2	NAG	O5-C5-C6-O6
4	EB	2	NAG	O5-C5-C6-O6
4	HB	2	NAG	O5-C5-C6-O6
4	KB	2	NAG	O5-C5-C6-O6
4	NB	2	NAG	O5-C5-C6-O6
4	QB	1	NAG	O5-C5-C6-O6
4	QB	2	NAG	O5-C5-C6-O6
4	WB	2	NAG	O5-C5-C6-O6
2	u	2	NAG	O5-C5-C6-O6
2	x	2	NAG	O5-C5-C6-O6
2	0	2	NAG	O5-C5-C6-O6
2	6	2	NAG	O5-C5-C6-O6
4	TB	2	NAG	O5-C5-C6-O6
4	NB	1	NAG	O5-C5-C6-O6
4	zA	1	NAG	O5-C5-C6-O6
4	EB	1	NAG	O5-C5-C6-O6
4	wA	1	NAG	O5-C5-C6-O6
4	HB	1	NAG	O5-C5-C6-O6
4	KB	1	NAG	O5-C5-C6-O6
4	TB	1	NAG	O5-C5-C6-O6
4	5A	1	NAG	O5-C5-C6-O6
4	8A	1	NAG	O5-C5-C6-O6
4	WB	1	NAG	O5-C5-C6-O6
2	7A	1	NAG	C4-C5-C6-O6
2	vA	1	NAG	C4-C5-C6-O6
2	yA	1	NAG	C4-C5-C6-O6
2	4A	1	NAG	C4-C5-C6-O6
2	AB	1	NAG	C4-C5-C6-O6
2	DB	1	NAG	C4-C5-C6-O6
2	JB	1	NAG	C4-C5-C6-O6
2	1A	1	NAG	C4-C5-C6-O6
2	GB	1	NAG	C4-C5-C6-O6
2	MB	1	NAG	C4-C5-C6-O6
2	PB	1	NAG	C4-C5-C6-O6
2	SB	1	NAG	C4-C5-C6-O6
2	VB	1	NAG	C4-C5-C6-O6
2	VB	2	NAG	C4-C5-C6-O6
2	7A	1	NAG	O5-C5-C6-O6
2	4A	2	NAG	C4-C5-C6-O6
2	AB	2	NAG	C4-C5-C6-O6
2	MB	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	PB	2	NAG	C4-C5-C6-O6
2	SB	2	NAG	C4-C5-C6-O6
2	GB	2	NAG	C4-C5-C6-O6
2	1A	2	NAG	C4-C5-C6-O6
2	7A	2	NAG	C4-C5-C6-O6
2	vA	2	NAG	C4-C5-C6-O6
2	yA	2	NAG	C4-C5-C6-O6
2	DB	2	NAG	C4-C5-C6-O6
2	JB	2	NAG	C4-C5-C6-O6
2	AB	1	NAG	O5-C5-C6-O6
2	DB	1	NAG	O5-C5-C6-O6
2	4A	1	NAG	O5-C5-C6-O6
2	vA	1	NAG	O5-C5-C6-O6
2	yA	1	NAG	O5-C5-C6-O6
2	MB	1	NAG	O5-C5-C6-O6
2	GB	1	NAG	O5-C5-C6-O6
2	1A	1	NAG	O5-C5-C6-O6
2	JB	1	NAG	O5-C5-C6-O6
2	PB	1	NAG	O5-C5-C6-O6
2	SB	1	NAG	O5-C5-C6-O6
2	VB	1	NAG	O5-C5-C6-O6
4	TB	2	NAG	C4-C5-C6-O6
4	WB	2	NAG	C4-C5-C6-O6
4	HB	2	NAG	C4-C5-C6-O6
4	NB	2	NAG	C4-C5-C6-O6
4	KB	2	NAG	C4-C5-C6-O6
4	QB	2	NAG	C4-C5-C6-O6
4	wA	2	NAG	C4-C5-C6-O6
4	5A	2	NAG	C4-C5-C6-O6
4	8A	2	NAG	C4-C5-C6-O6
4	EB	2	NAG	C4-C5-C6-O6
4	BB	2	NAG	C4-C5-C6-O6
4	zA	2	NAG	C4-C5-C6-O6
4	2A	2	NAG	C4-C5-C6-O6
4	2A	1	NAG	C4-C5-C6-O6
4	QB	1	NAG	C4-C5-C6-O6
2	x	2	NAG	C4-C5-C6-O6
4	BB	1	NAG	C4-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
2	o	2	NAG	C4-C5-C6-O6
2	u	2	NAG	C4-C5-C6-O6
2	0	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	3	2	NAG	C4-C5-C6-O6
2	6	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
4	NB	1	NAG	C4-C5-C6-O6
2	r	2	NAG	C4-C5-C6-O6
4	zA	1	NAG	C4-C5-C6-O6
4	wA	1	NAG	C4-C5-C6-O6
4	EB	1	NAG	C4-C5-C6-O6
4	KB	1	NAG	C4-C5-C6-O6
4	HB	1	NAG	C4-C5-C6-O6
4	TB	1	NAG	C4-C5-C6-O6
4	5A	1	NAG	C4-C5-C6-O6
4	8A	1	NAG	C4-C5-C6-O6
2	k	2	NAG	C3-C2-N2-C7
2	o	2	NAG	C3-C2-N2-C7
2	r	2	NAG	C3-C2-N2-C7
2	u	2	NAG	C3-C2-N2-C7
2	x	2	NAG	C3-C2-N2-C7
2	0	2	NAG	C3-C2-N2-C7
2	3	2	NAG	C3-C2-N2-C7
2	6	2	NAG	C3-C2-N2-C7
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	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	aA	1	NAG	C3-C2-N2-C7
2	dA	1	NAG	C3-C2-N2-C7
2	gA	1	NAG	C3-C2-N2-C7
2	jA	1	NAG	C3-C2-N2-C7
2	mA	1	NAG	C3-C2-N2-C7
2	pA	1	NAG	C3-C2-N2-C7
2	sA	1	NAG	C3-C2-N2-C7
2	vA	1	NAG	C3-C2-N2-C7
2	yA	1	NAG	C3-C2-N2-C7

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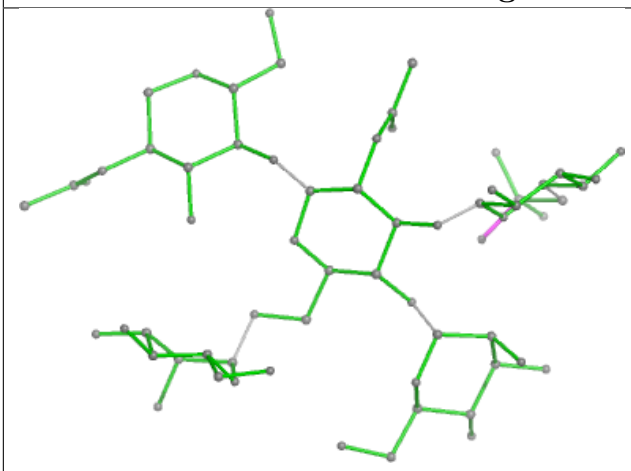
Mol	Chain	Res	Type	Atoms
2	1A	1	NAG	C3-C2-N2-C7
2	4A	1	NAG	C3-C2-N2-C7
2	7A	1	NAG	C3-C2-N2-C7
2	AB	1	NAG	C3-C2-N2-C7
2	DB	1	NAG	C3-C2-N2-C7
2	GB	1	NAG	C3-C2-N2-C7
2	JB	1	NAG	C3-C2-N2-C7
2	MB	1	NAG	C3-C2-N2-C7
2	PB	1	NAG	C3-C2-N2-C7
2	SB	1	NAG	C3-C2-N2-C7
2	VB	1	NAG	C3-C2-N2-C7
4	WB	1	NAG	C4-C5-C6-O6
4	tA	2	NAG	O5-C5-C6-O6
4	bA	2	NAG	O5-C5-C6-O6
4	qA	2	NAG	O5-C5-C6-O6
4	VA	2	NAG	O5-C5-C6-O6
4	MA	2	NAG	O5-C5-C6-O6
4	PA	2	NAG	O5-C5-C6-O6
4	hA	2	NAG	O5-C5-C6-O6
4	SA	2	NAG	O5-C5-C6-O6
2	3	1	NAG	O5-C5-C6-O6
2	9	1	NAG	O5-C5-C6-O6
4	eA	2	NAG	O5-C5-C6-O6
4	nA	2	NAG	O5-C5-C6-O6
2	6	1	NAG	O5-C5-C6-O6
2	o	1	NAG	O5-C5-C6-O6
4	YA	2	NAG	O5-C5-C6-O6
4	kA	2	NAG	O5-C5-C6-O6
2	0	1	NAG	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6

There are no ring outliers.

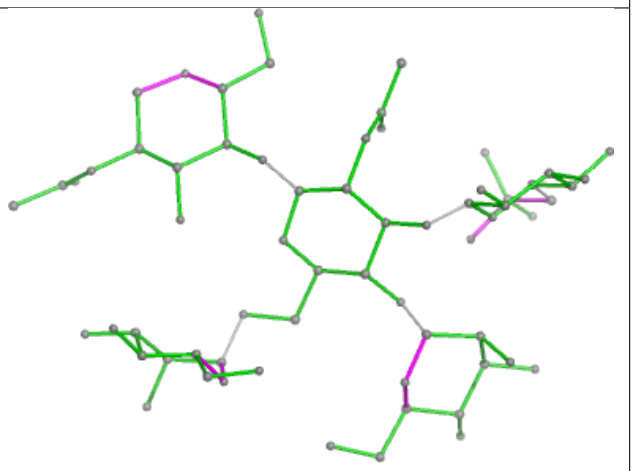
No monomer is involved in short contacts.

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

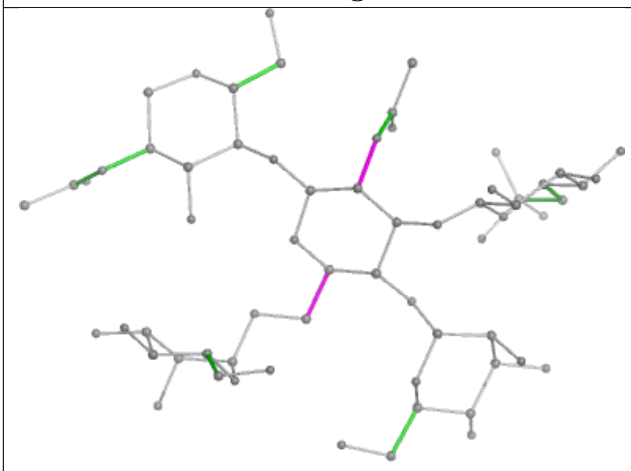
Oligosaccharide Chain k



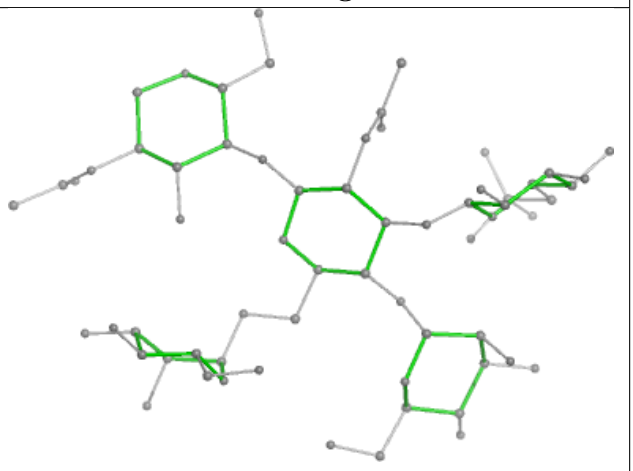
Bond lengths



Bond angles

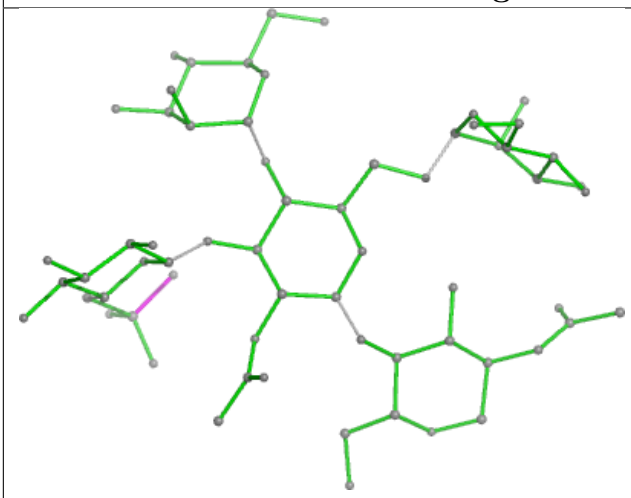


Torsions

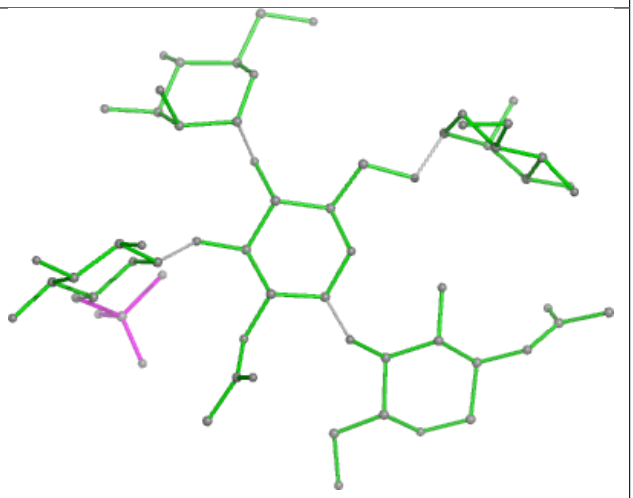


Rings

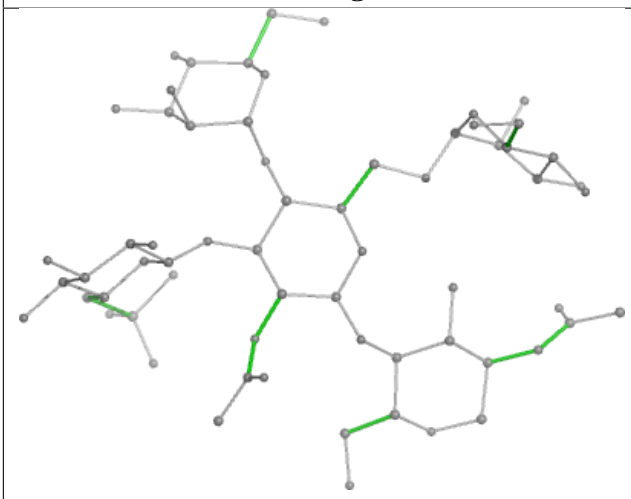
Oligosaccharide Chain m



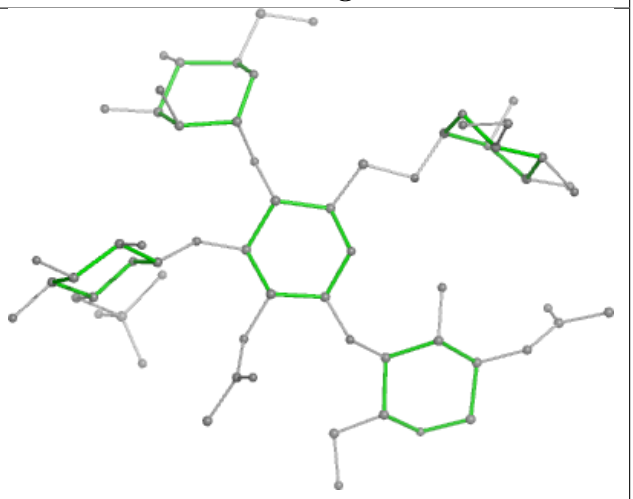
Bond lengths



Bond angles

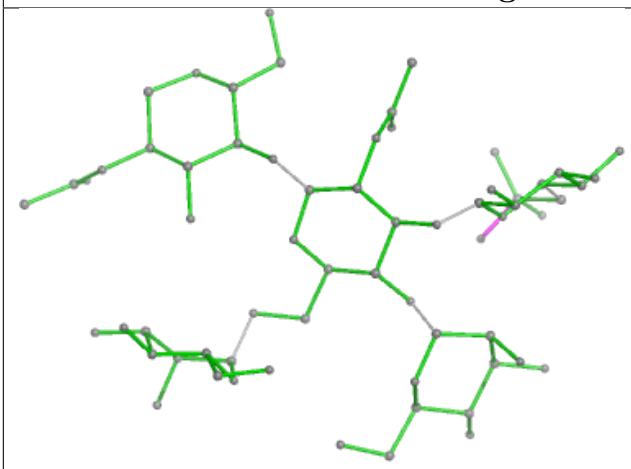


Torsions

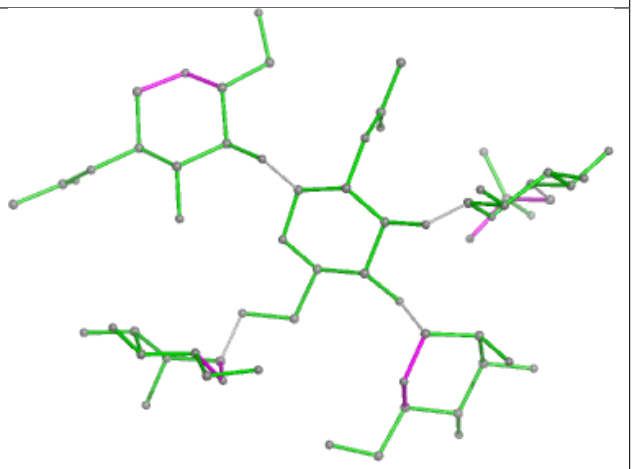


Rings

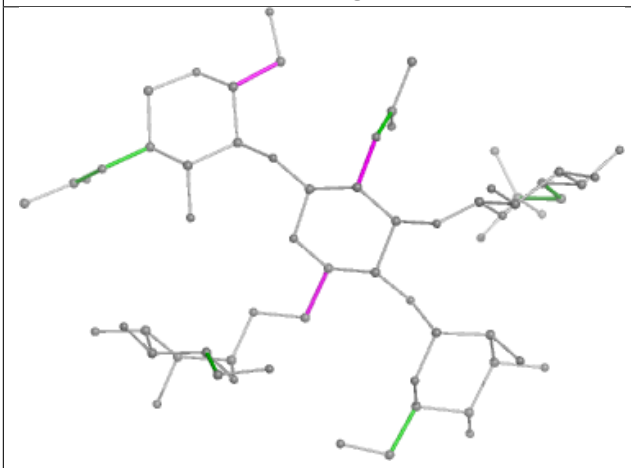
Oligosaccharide Chain o



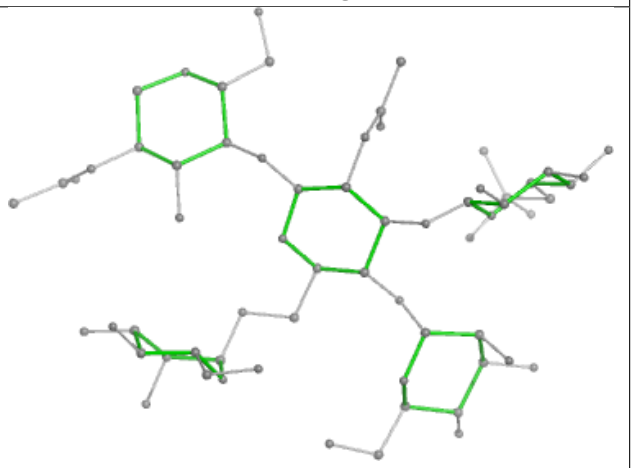
Bond lengths



Bond angles

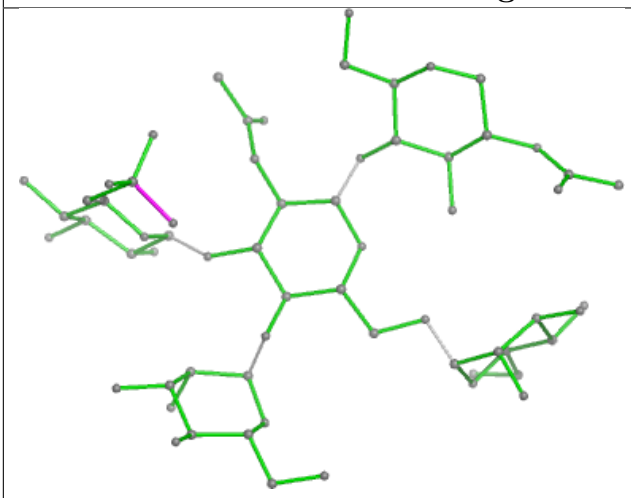


Torsions

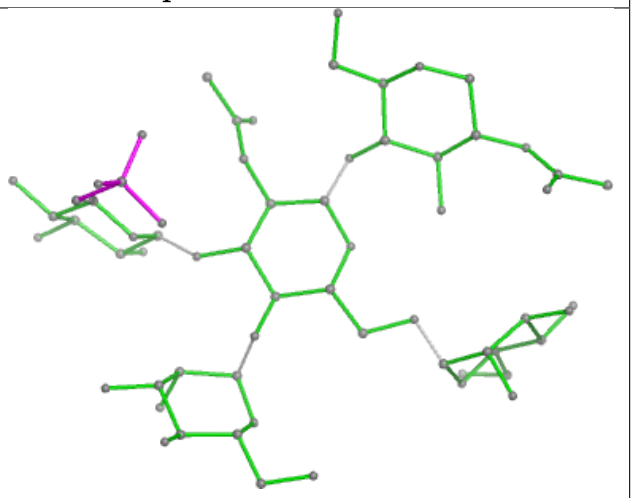


Rings

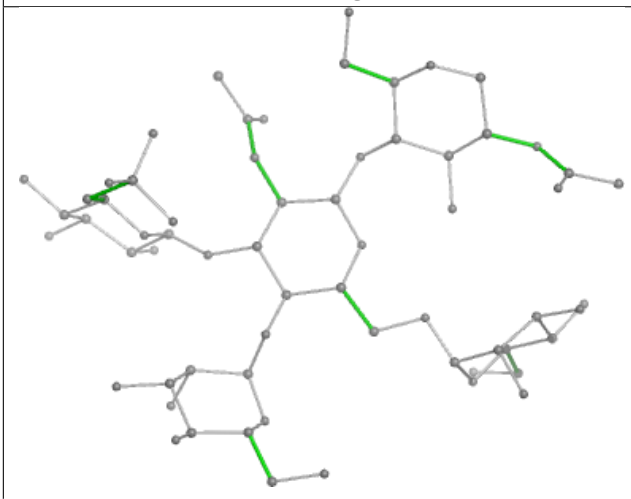
Oligosaccharide Chain p



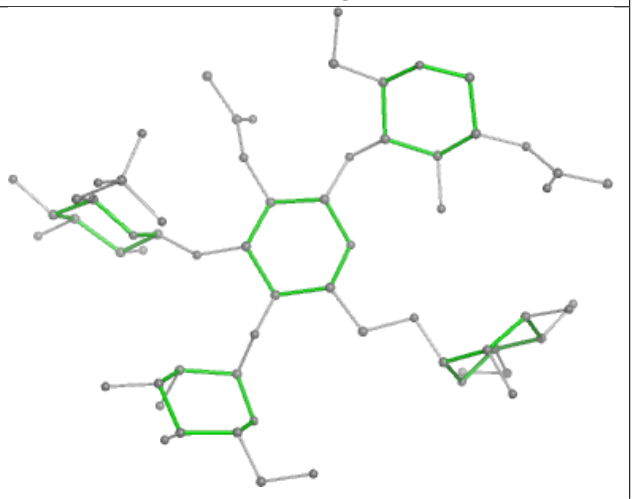
Bond lengths



Bond angles

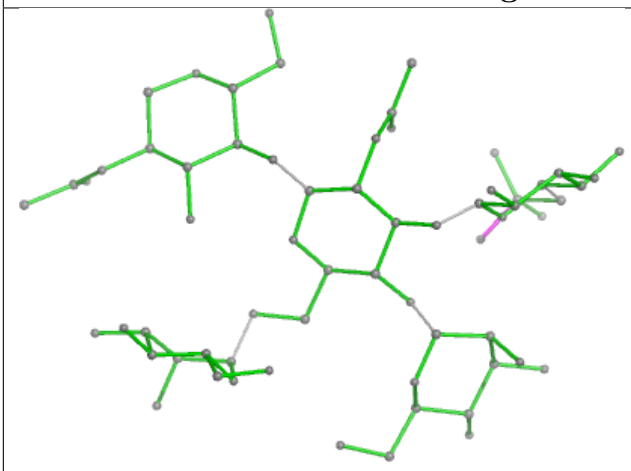


Torsions

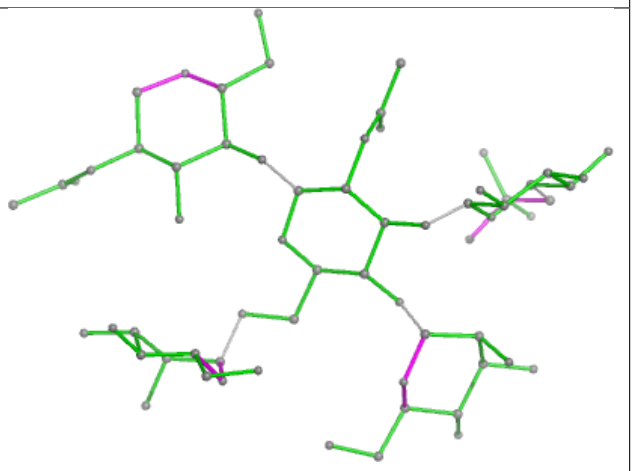


Rings

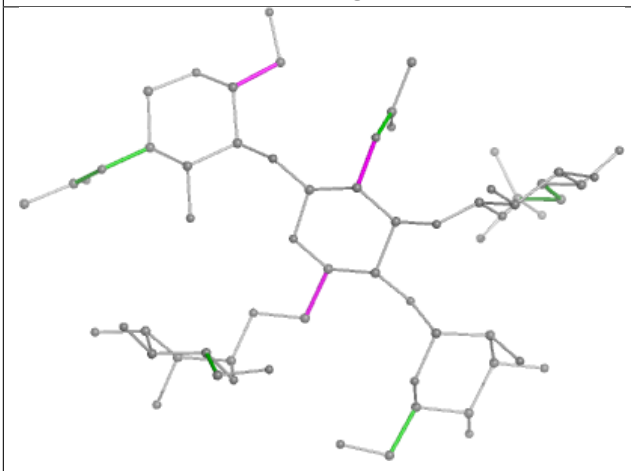
Oligosaccharide Chain r



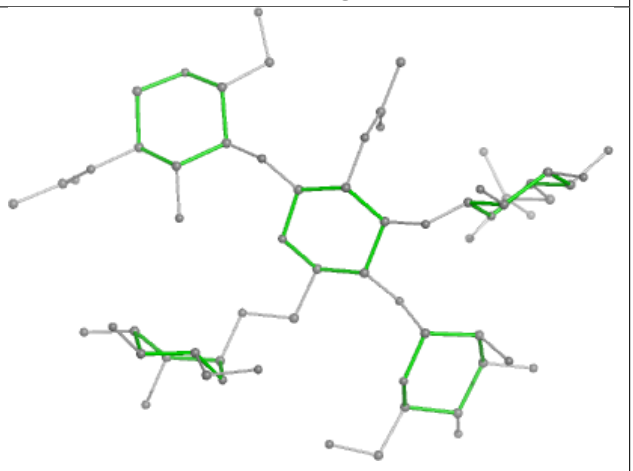
Bond lengths



Bond angles

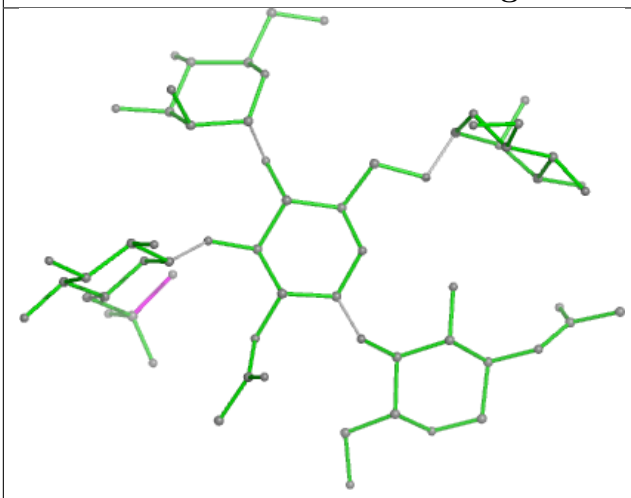


Torsions

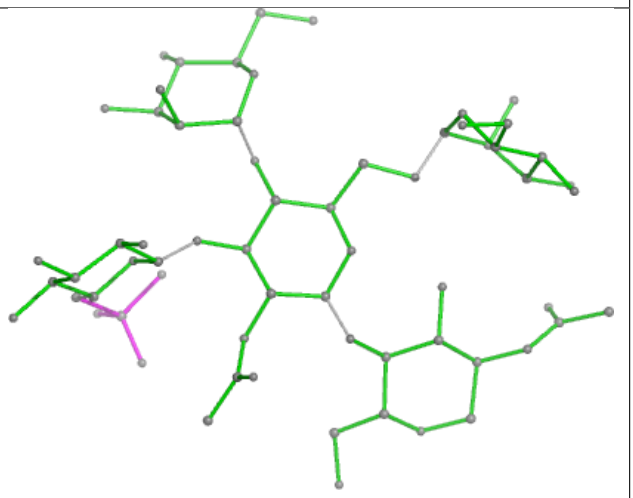


Rings

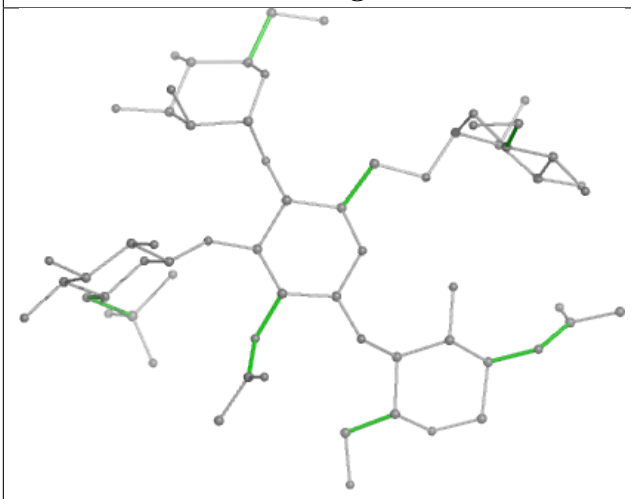
Oligosaccharide Chain s



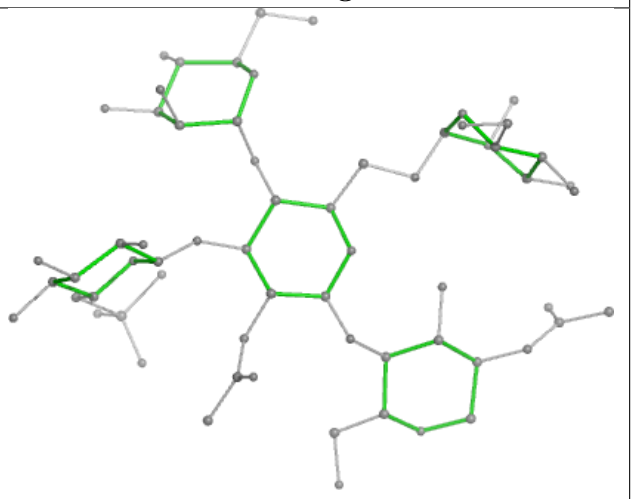
Bond lengths



Bond angles

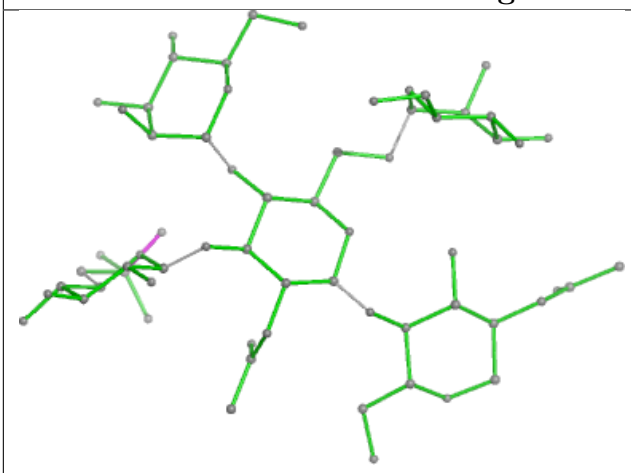


Torsions

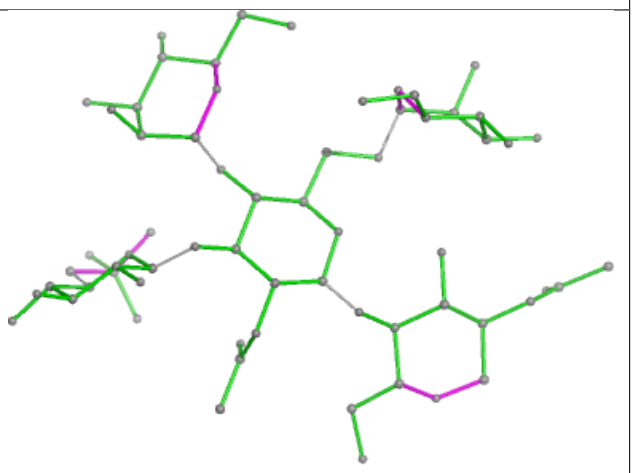


Rings

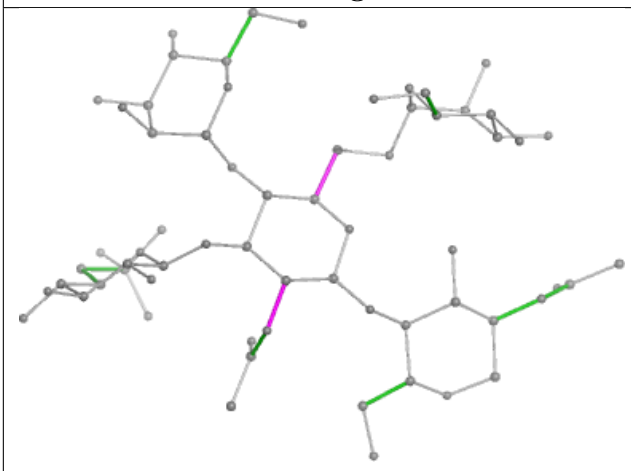
Oligosaccharide Chain u



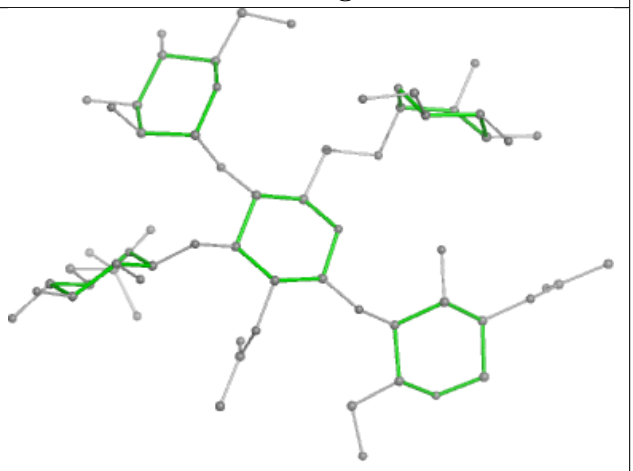
Bond lengths



Bond angles

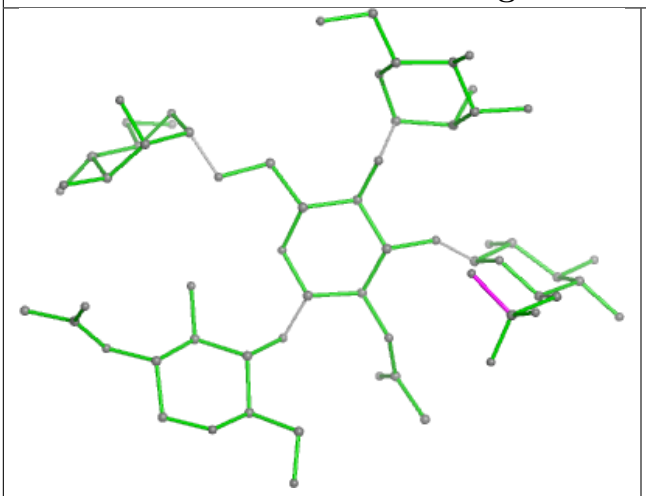


Torsions

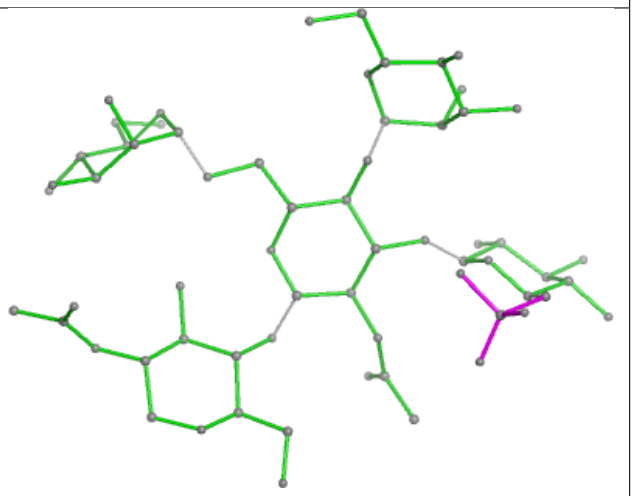


Rings

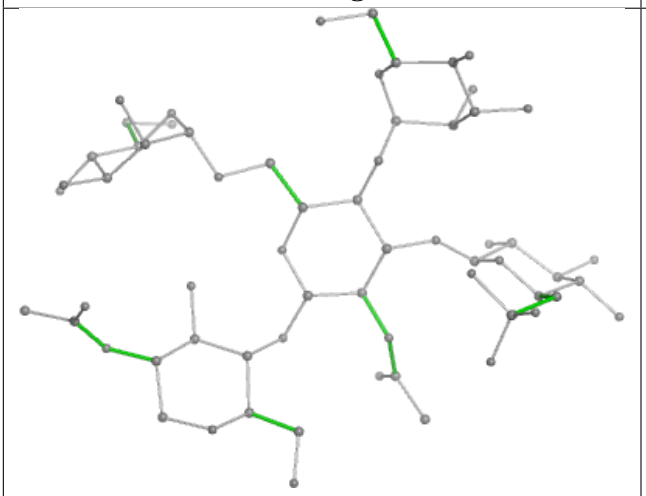
Oligosaccharide Chain v



Bond lengths



Bond angles



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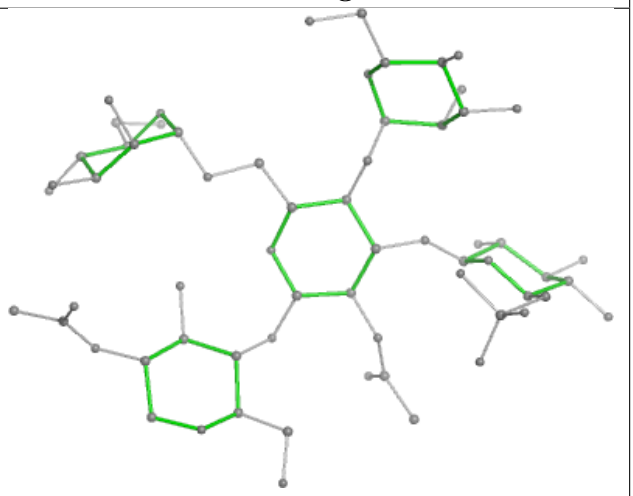
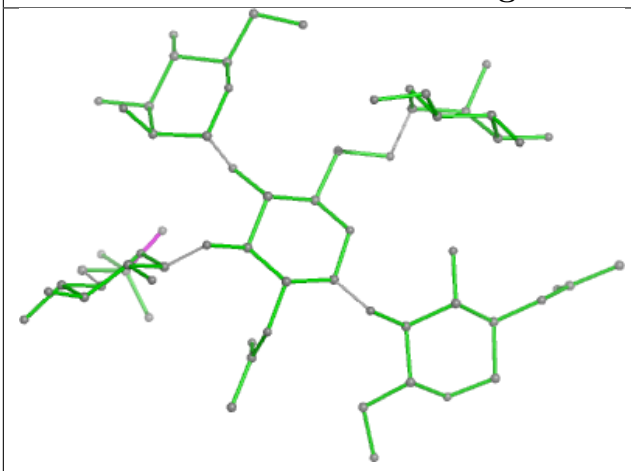
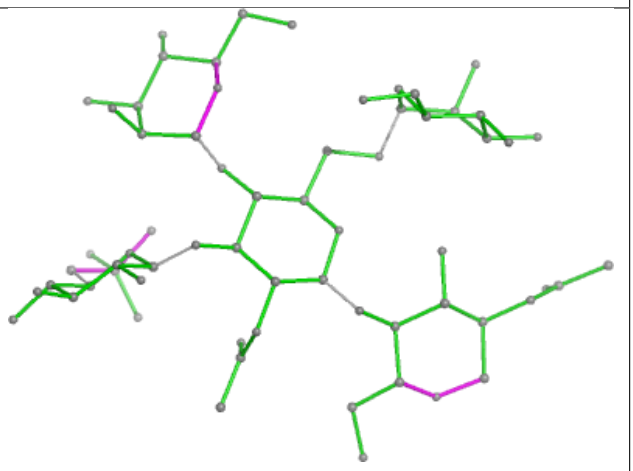


Rings

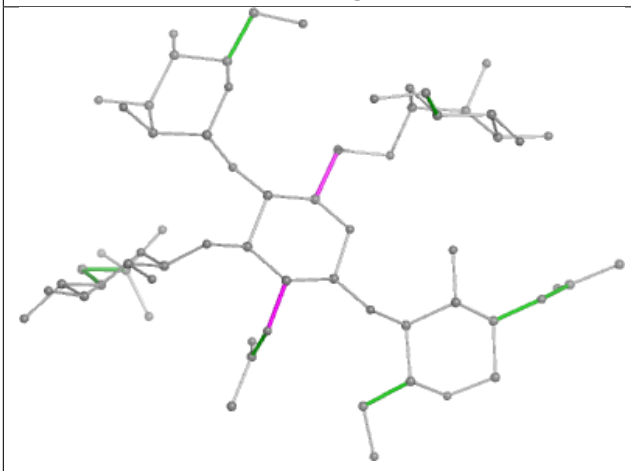
Oligosaccharide Chain x



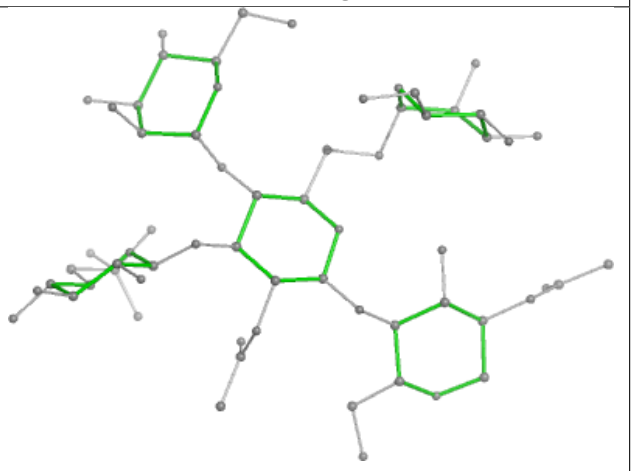
Bond lengths



Bond angles

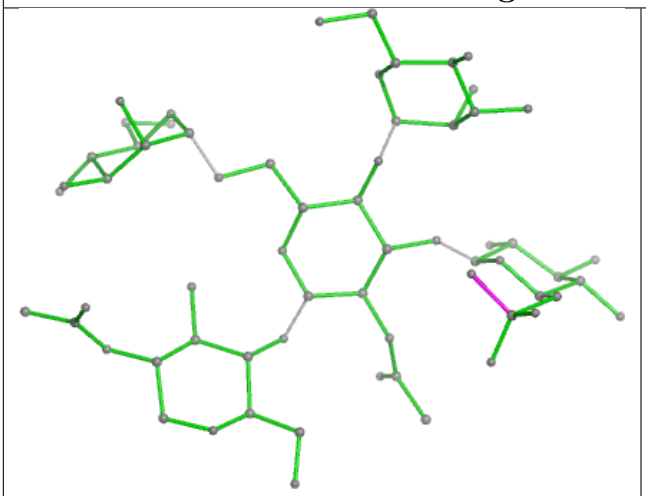


Torsions

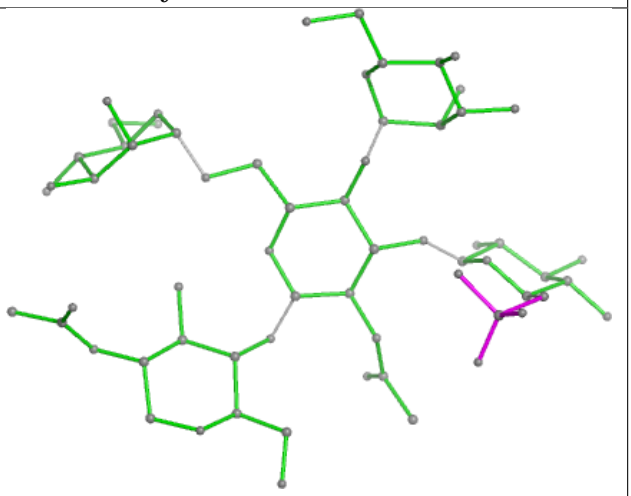


Rings

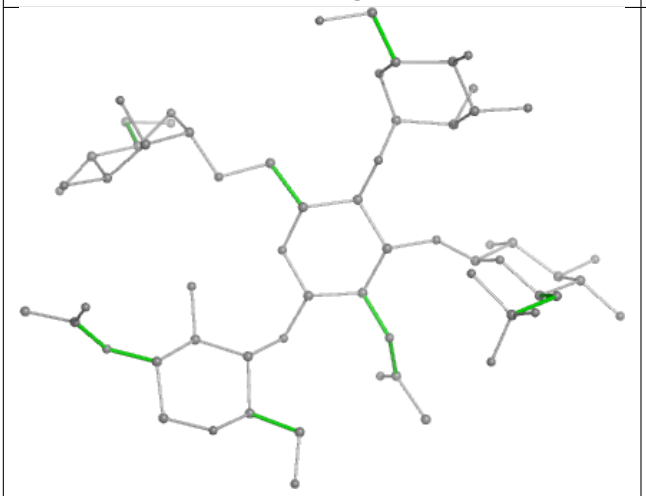
Oligosaccharide Chain y



Bond lengths



Bond angles



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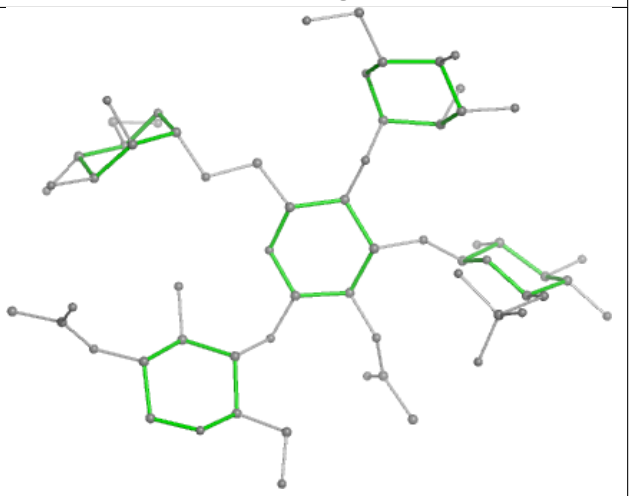
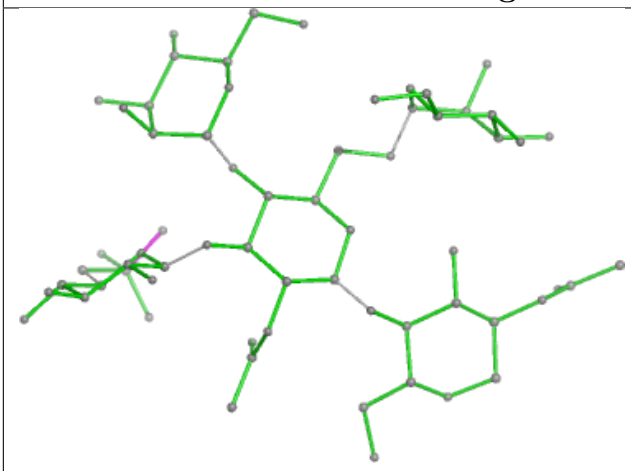


Rings

Oligosaccharide Chain 0



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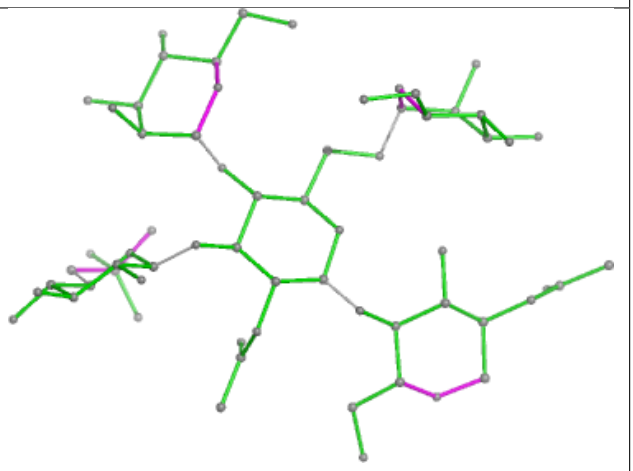
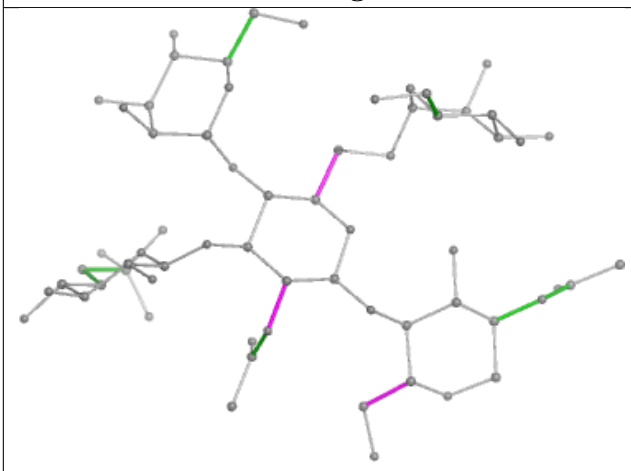


Bond angles



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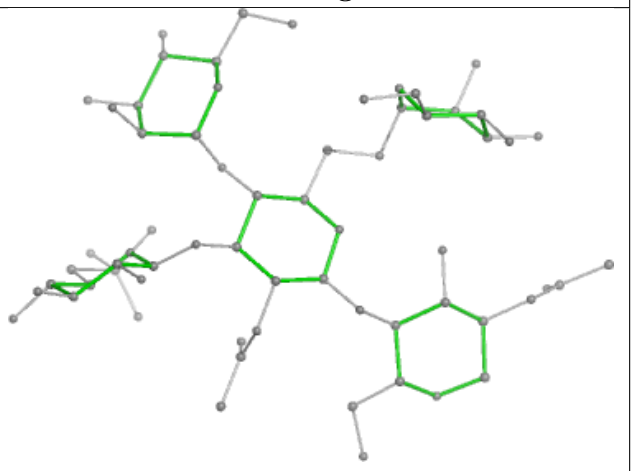
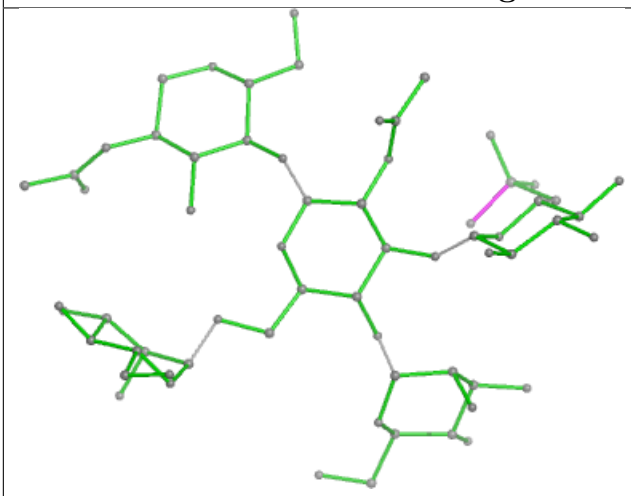


Rings

Oligosaccharide Chain 1



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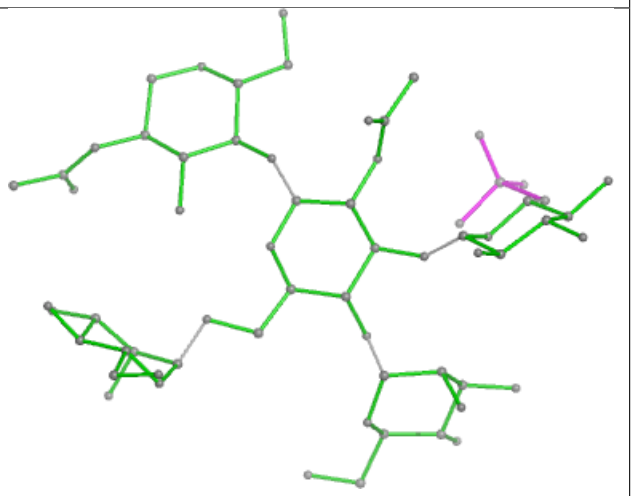

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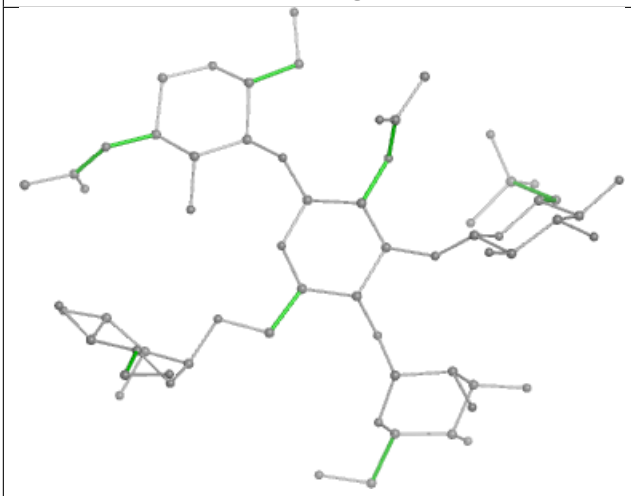

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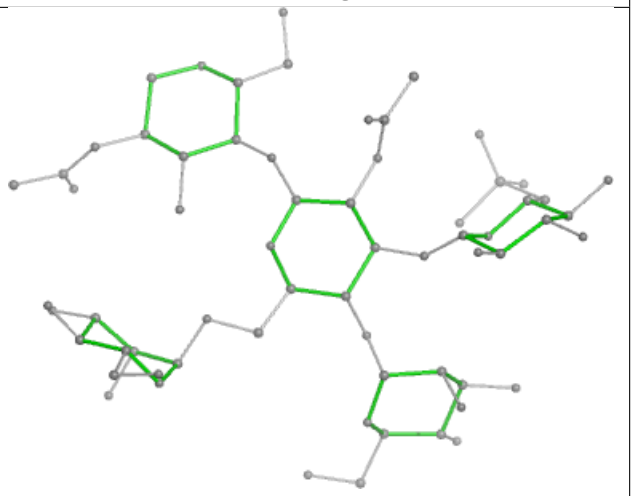
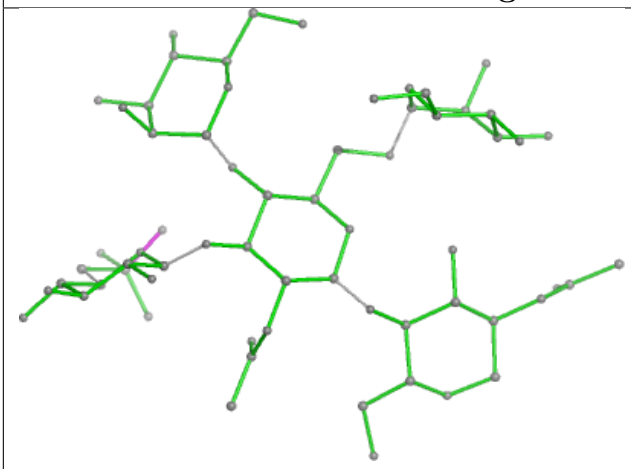


Rings

Oligosaccharide Chain 3



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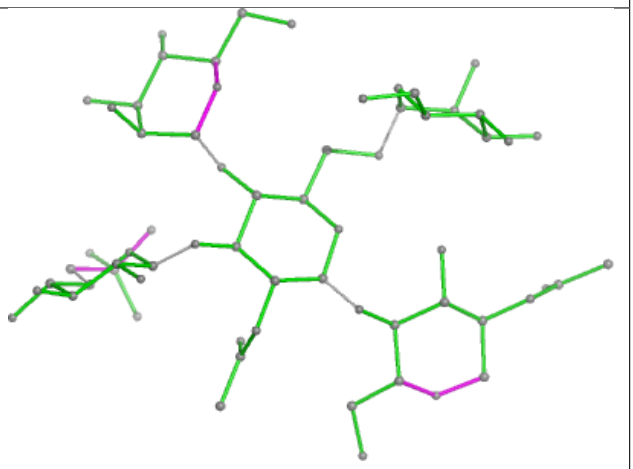
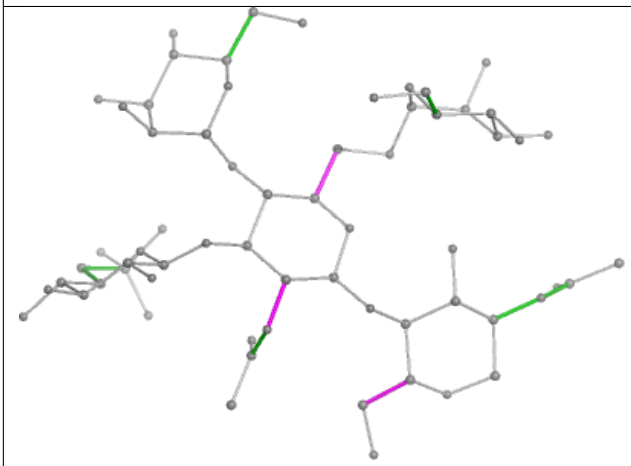


Bond angles



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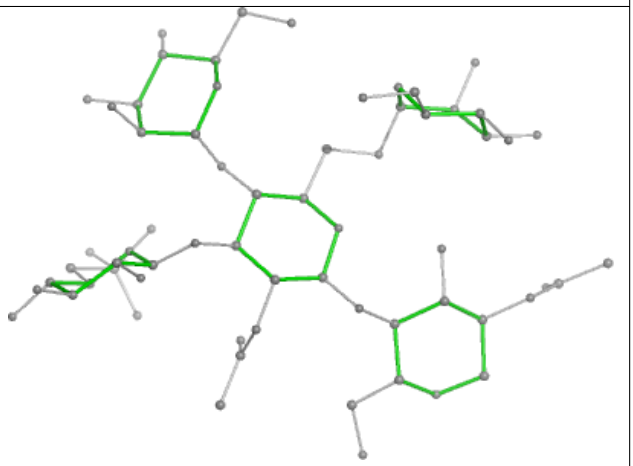
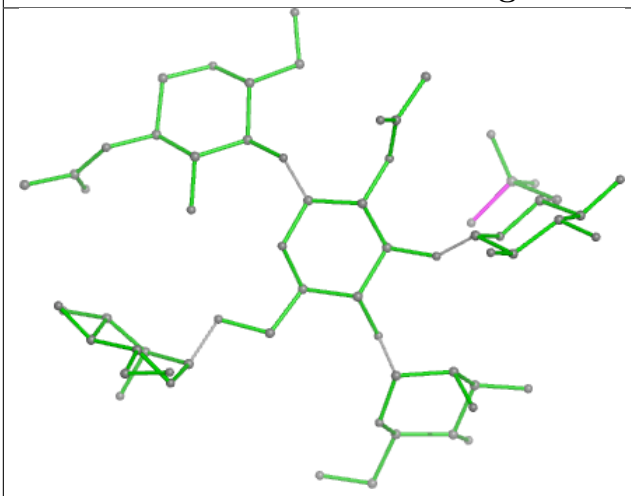
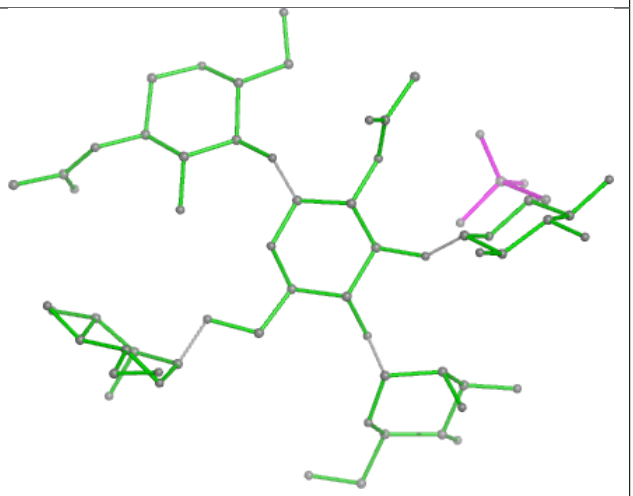
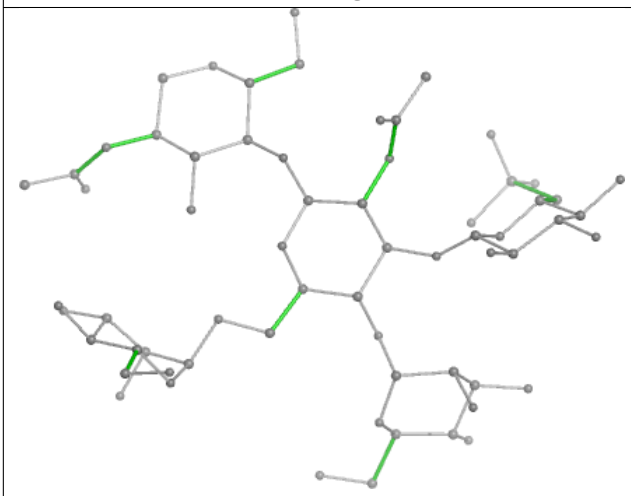
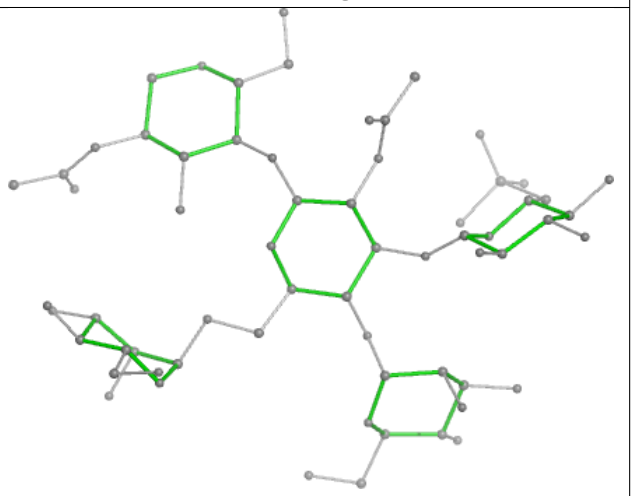
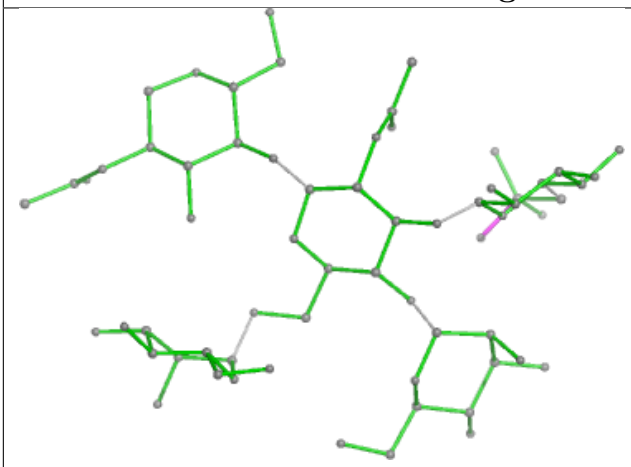


Rings

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

Oligosaccharide Chain 6



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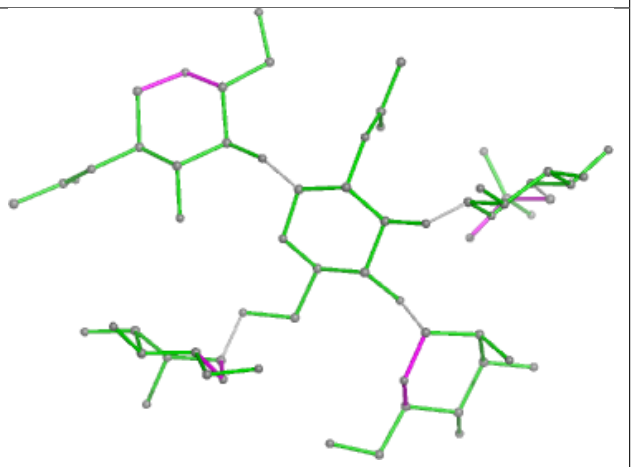
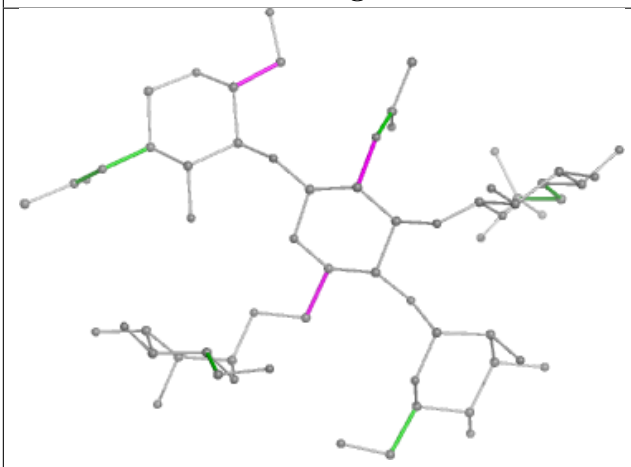


Bond angles



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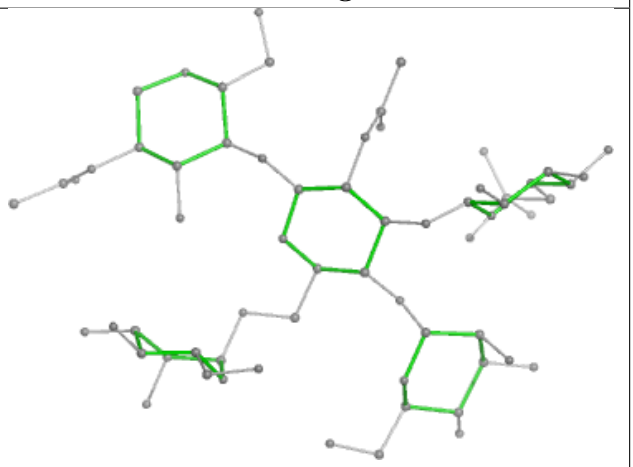
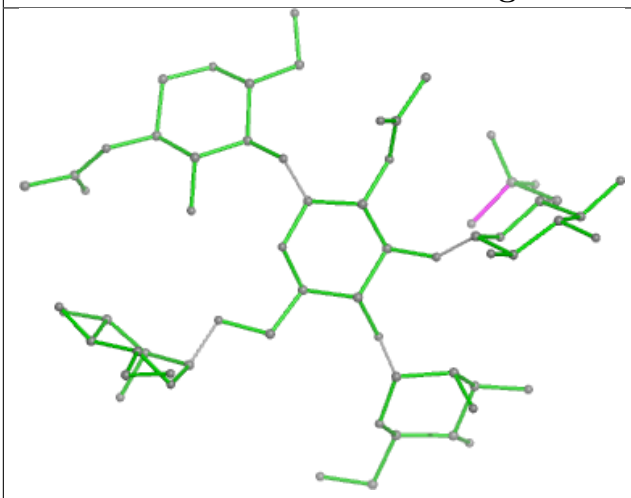


Rings

Oligosaccharide Chain 7



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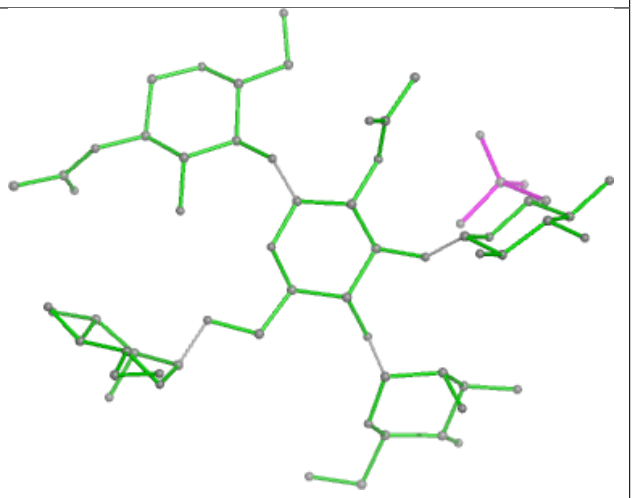
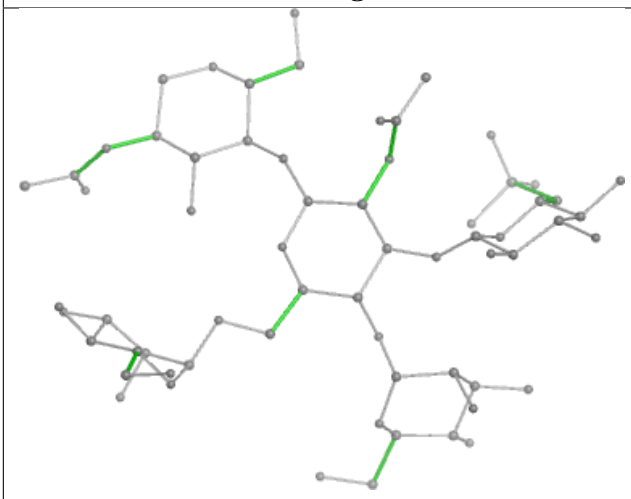


Bond angles



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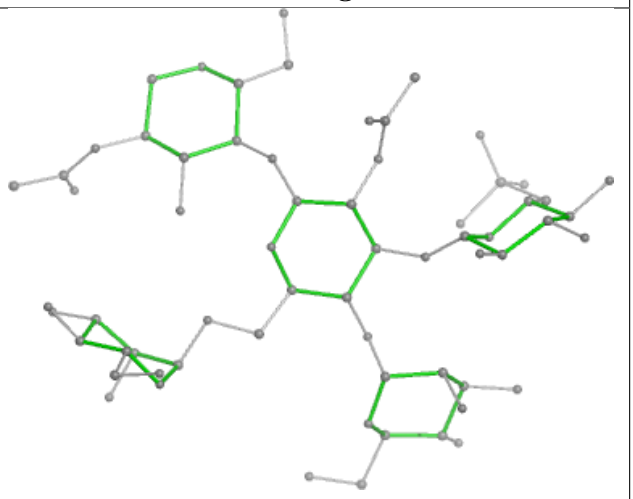
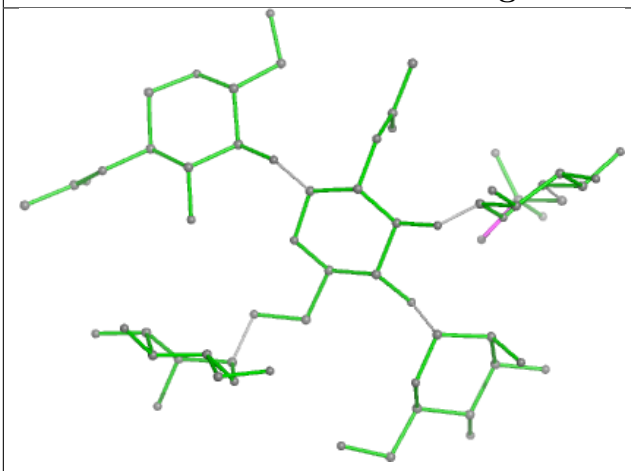


Rings

Oligosaccharide Chain 9



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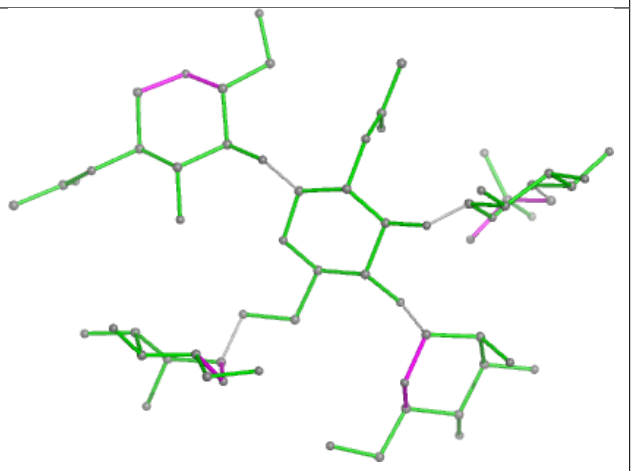

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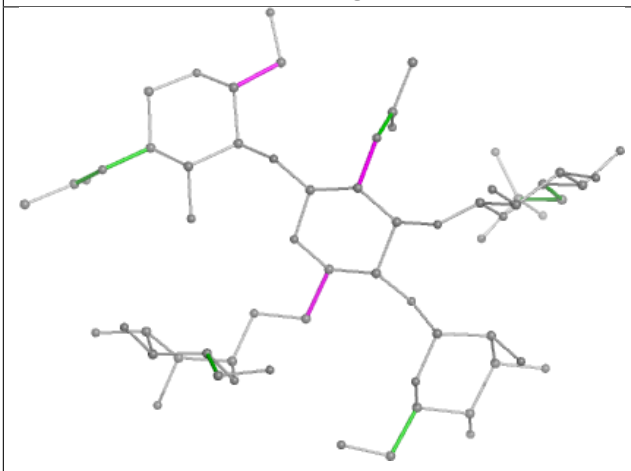

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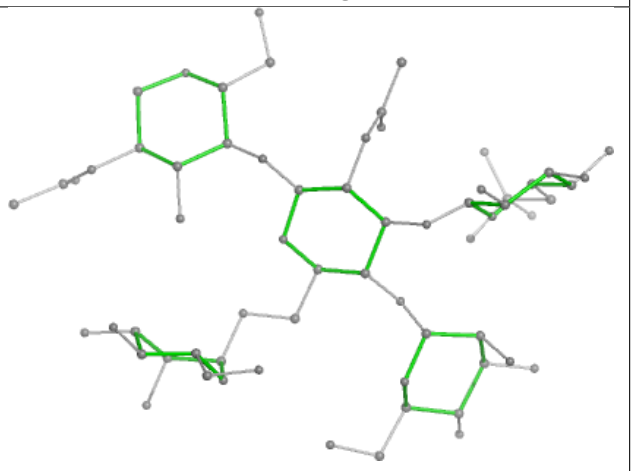
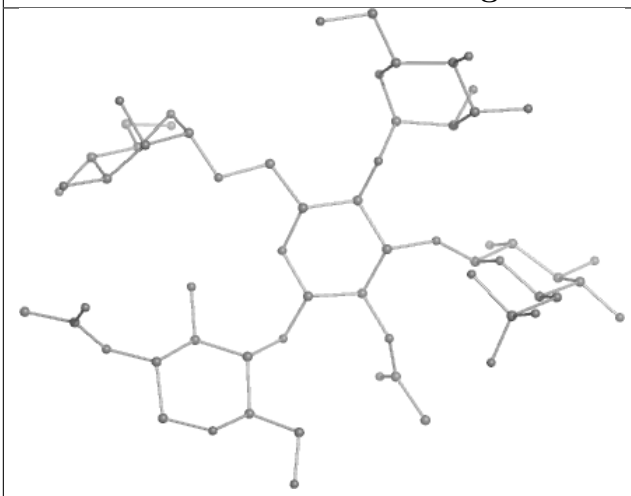


Rings

Oligosaccharide Chain AA



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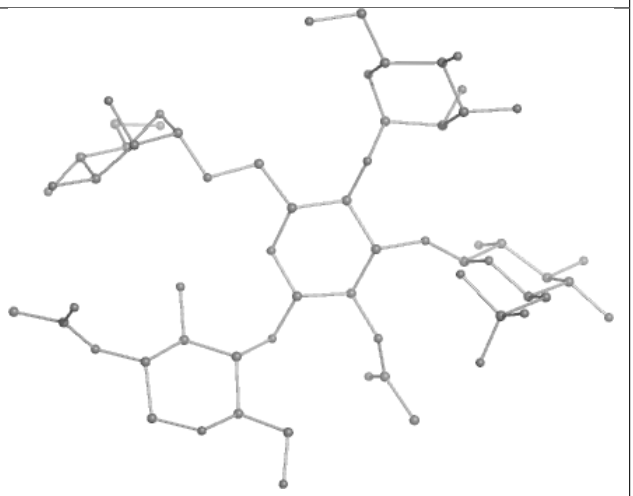
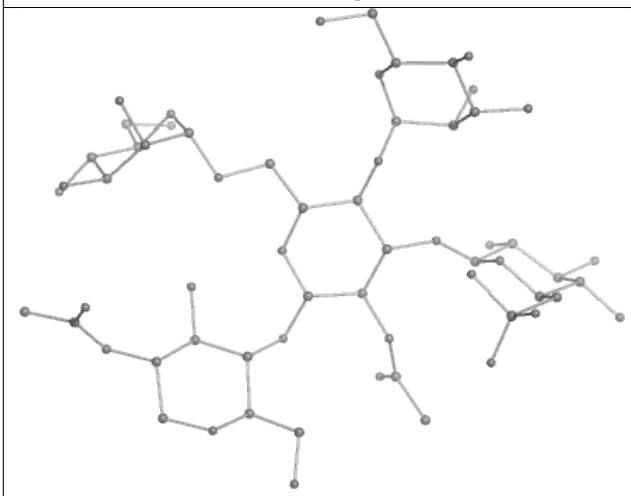


Bond angles



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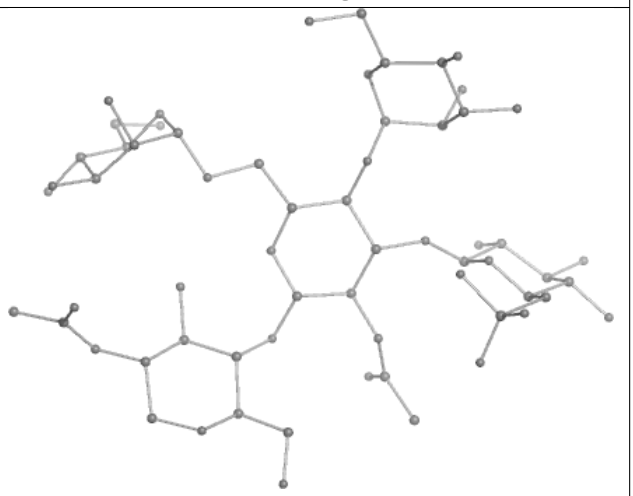
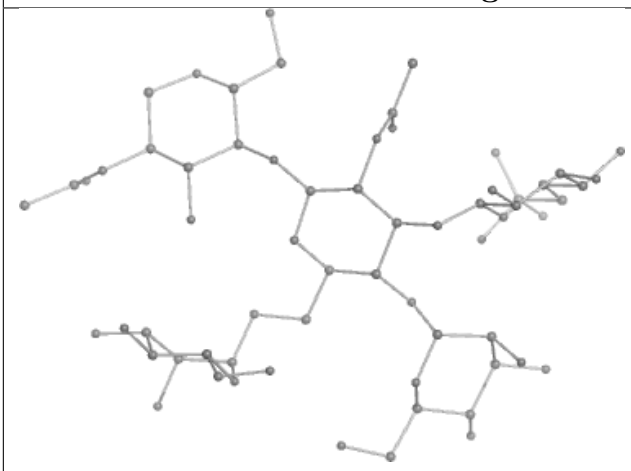


Rings

Oligosaccharide Chain CA



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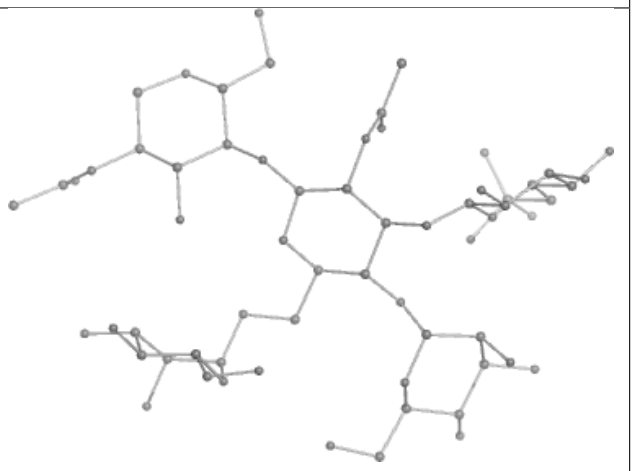

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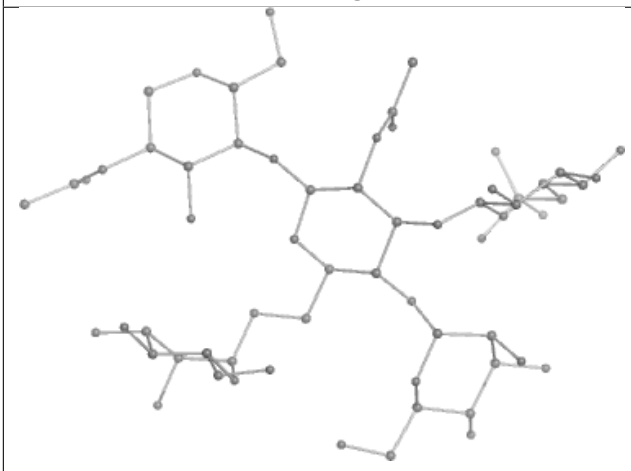

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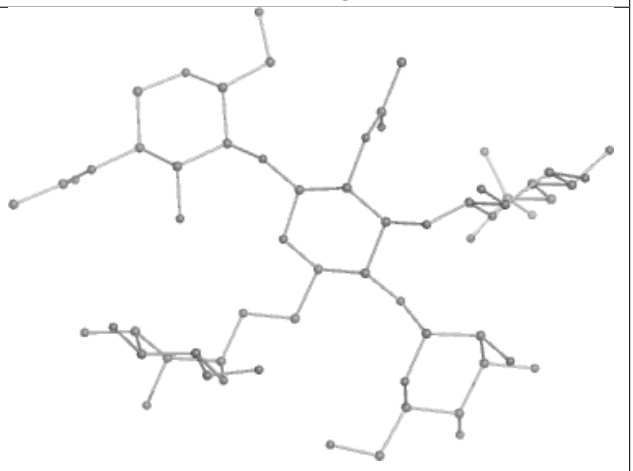
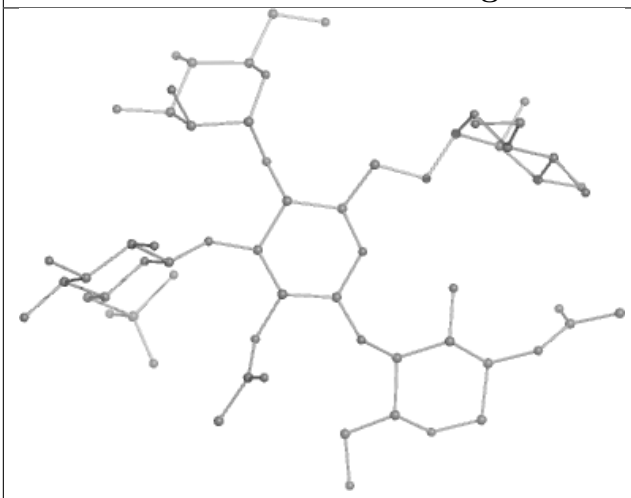


Rings

Oligosaccharide Chain DA



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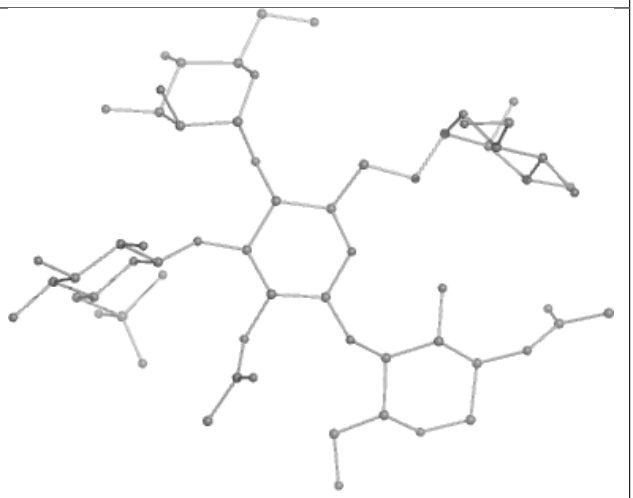
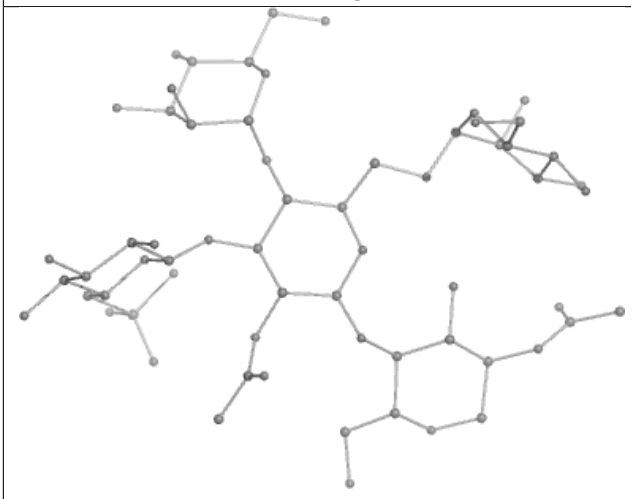


Bond angles



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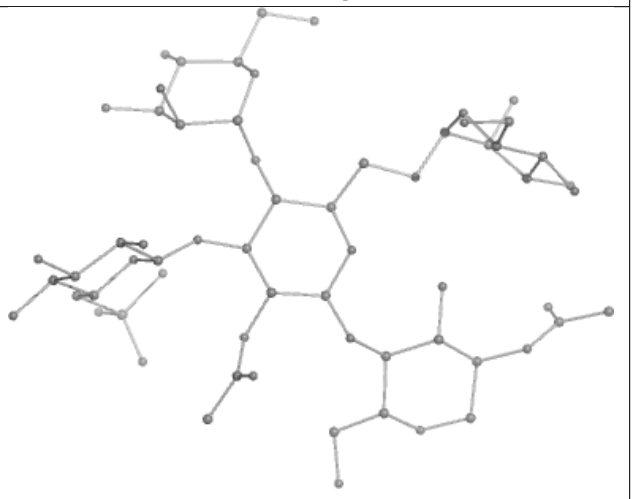
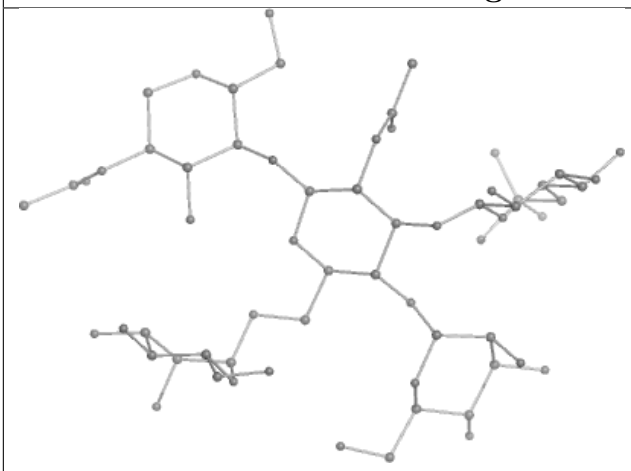


Rings

Oligosaccharide Chain FA



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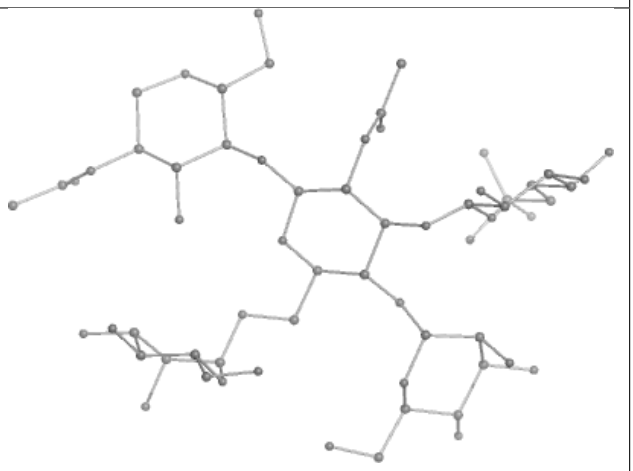
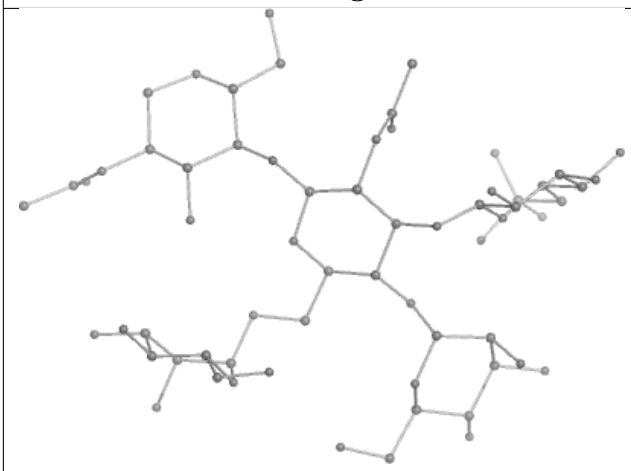


Bond angles



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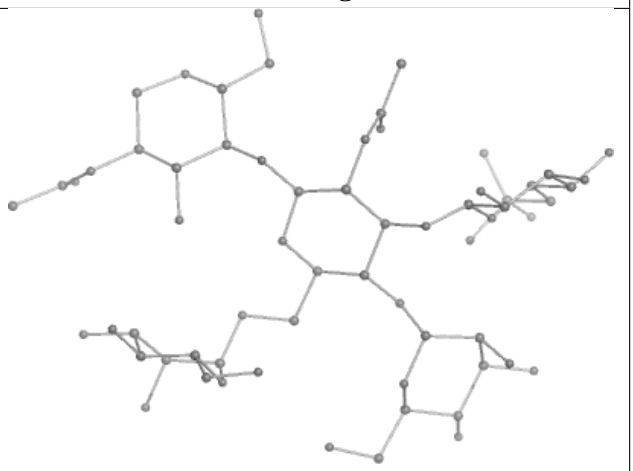
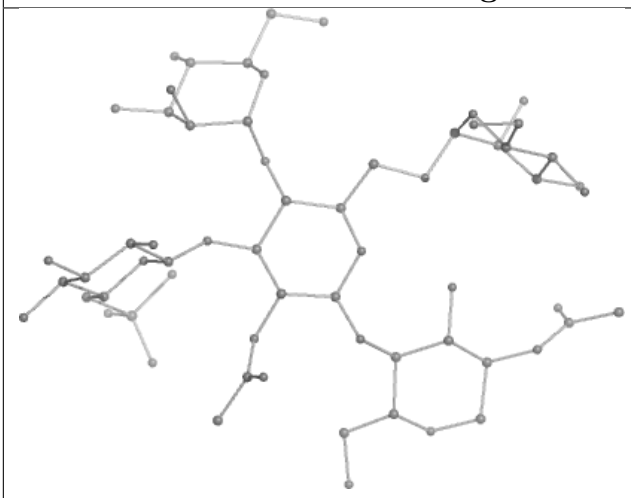


Rings

Oligosaccharide Chain GA



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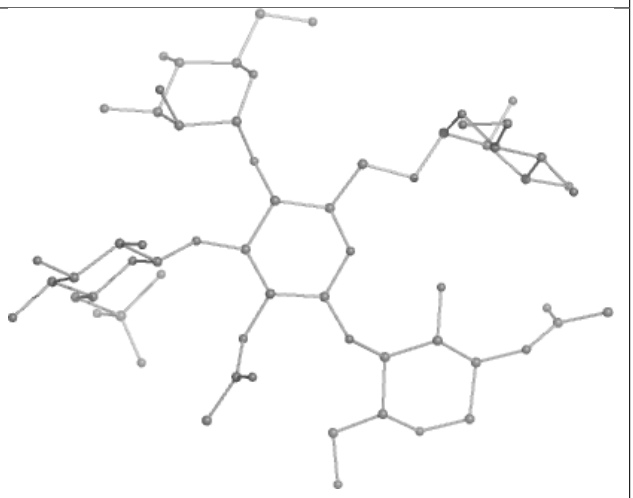
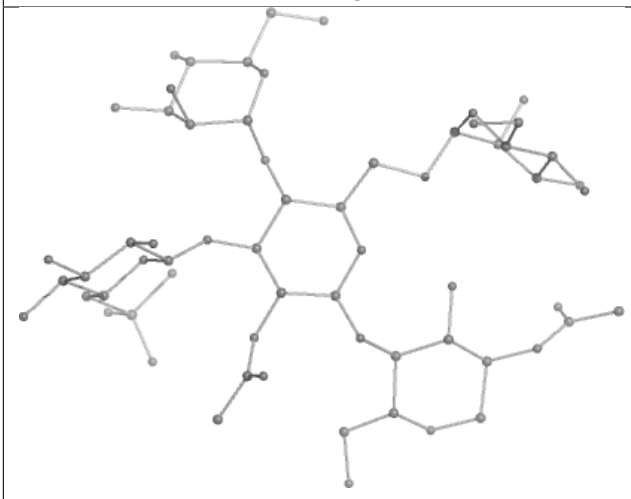


Bond angles



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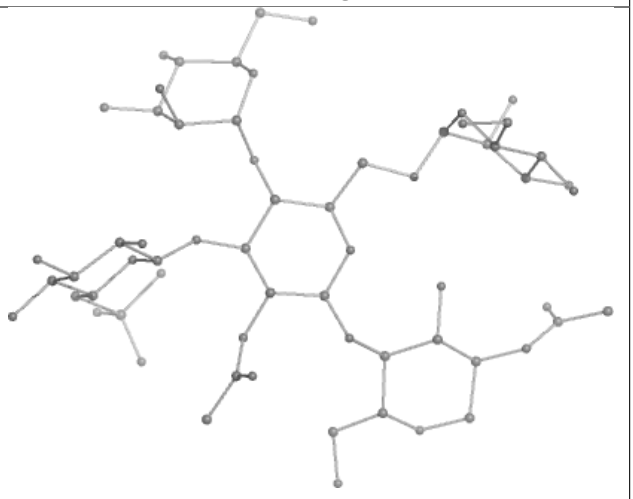
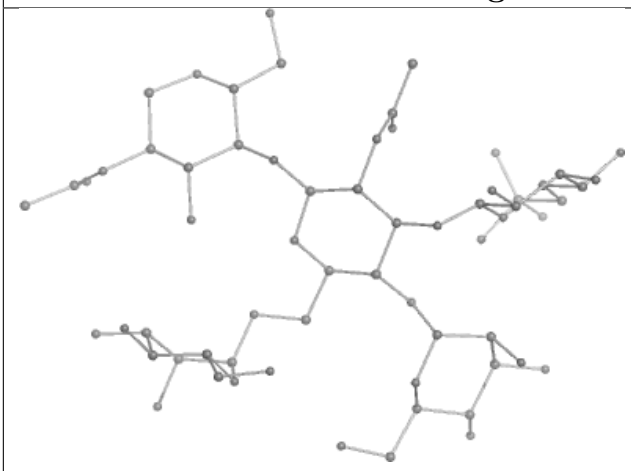
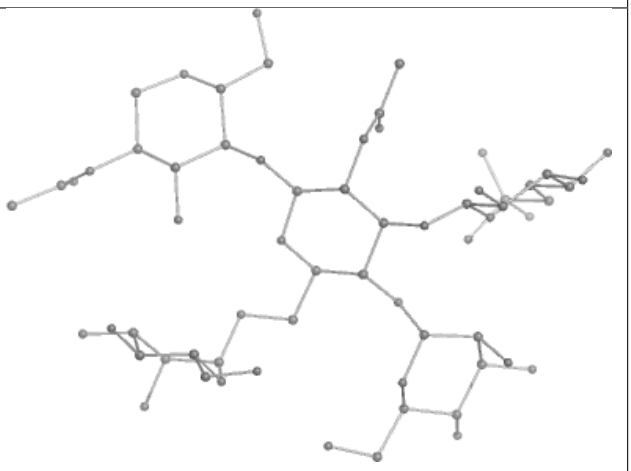


Rings

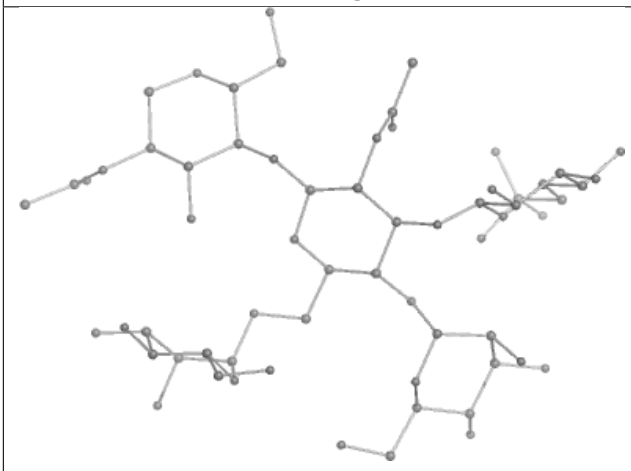
Oligosaccharide Chain IA



Bond lengths



Bond angles



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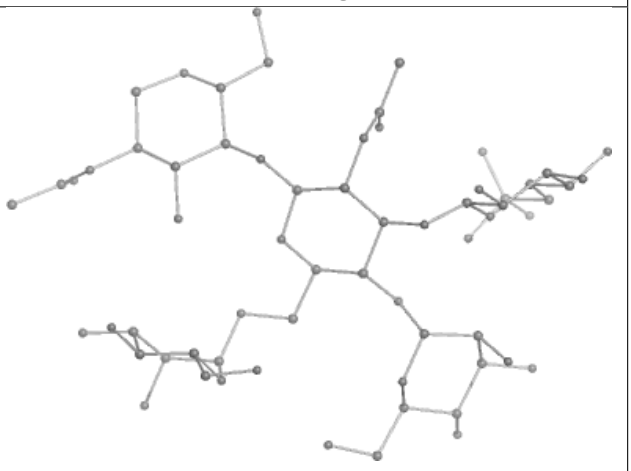
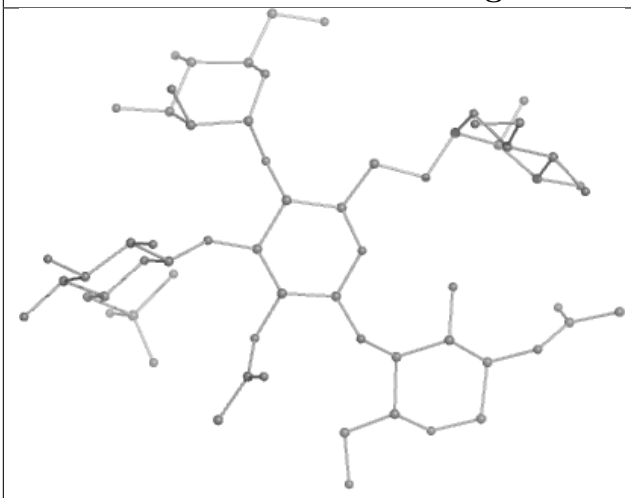


Rings

Oligosaccharide Chain JA



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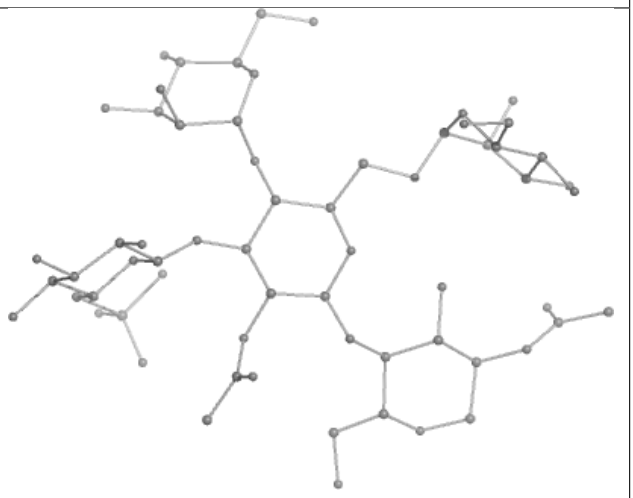
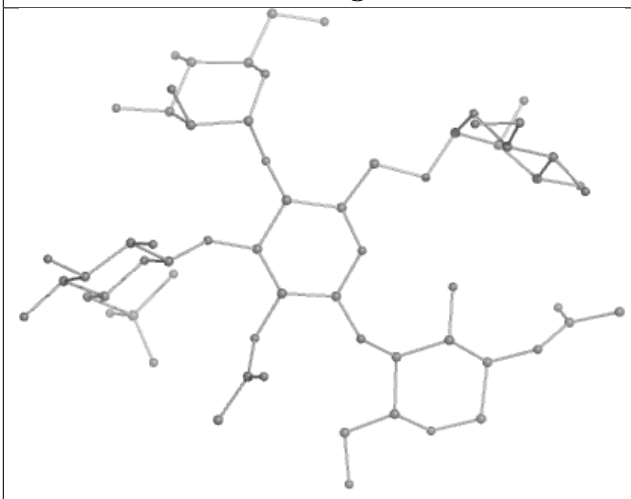


Bond angles



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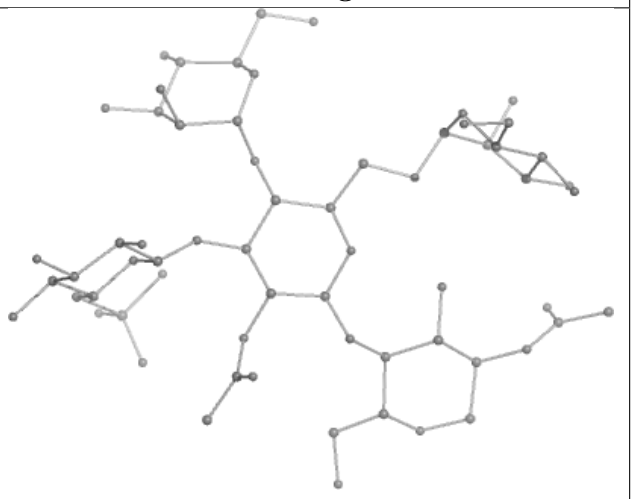
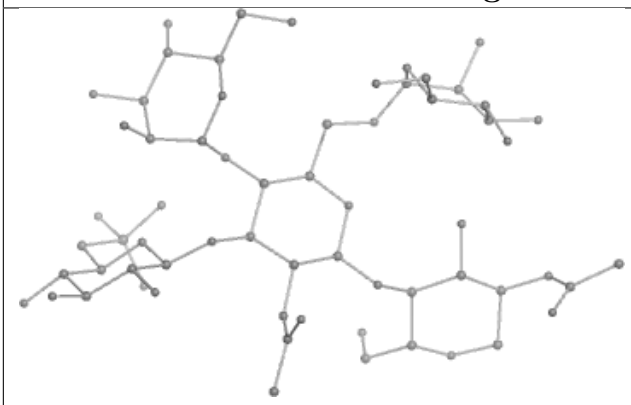
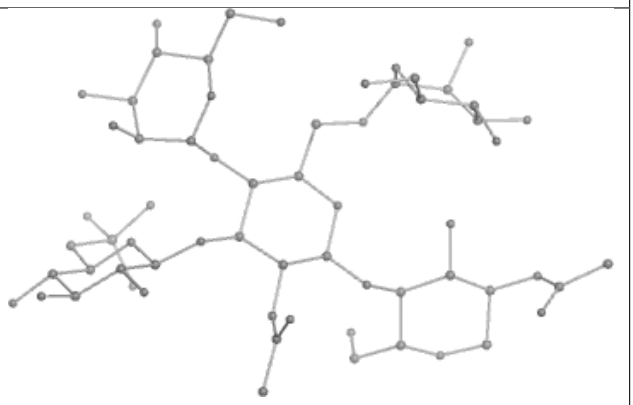


Rings

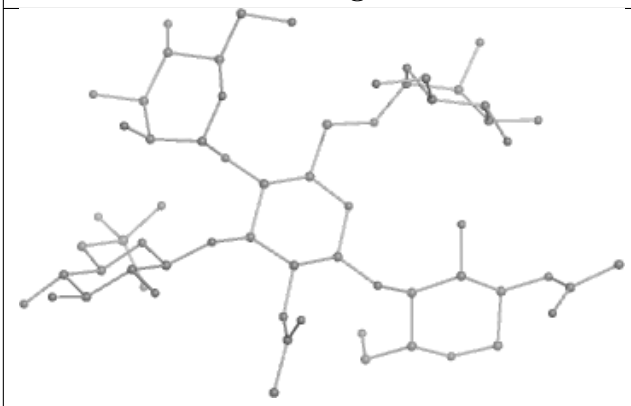
Oligosaccharide Chain LA



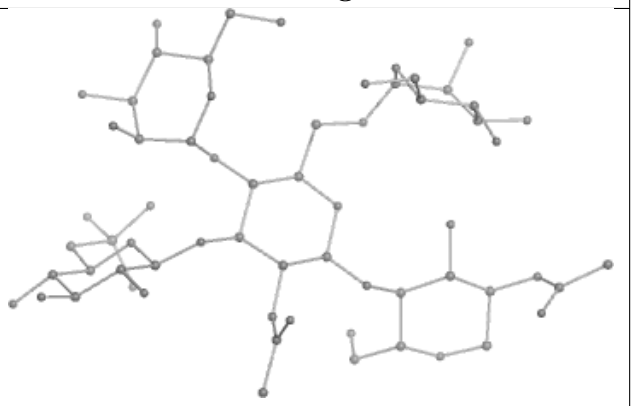
Bond lengths



Bond angles

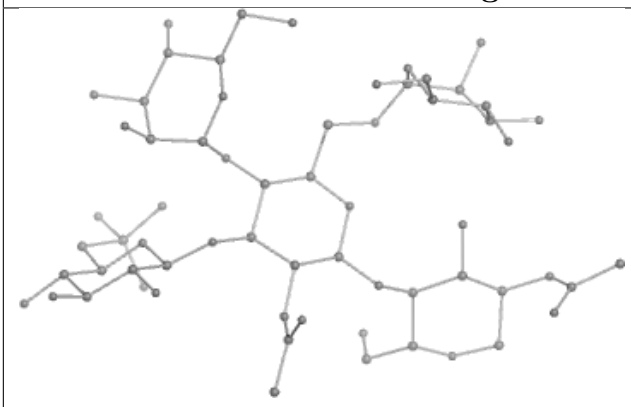


Torsions



Rings

Oligosaccharide Chain OA



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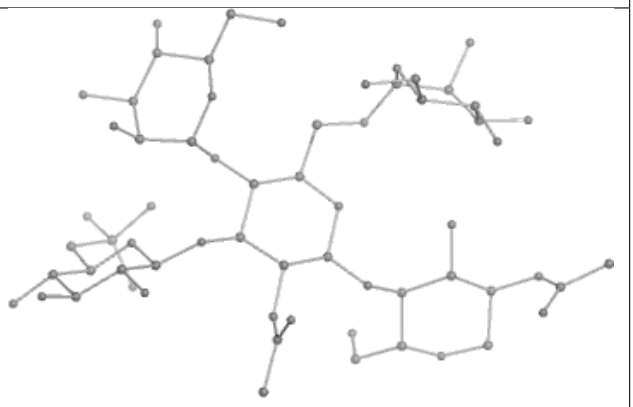

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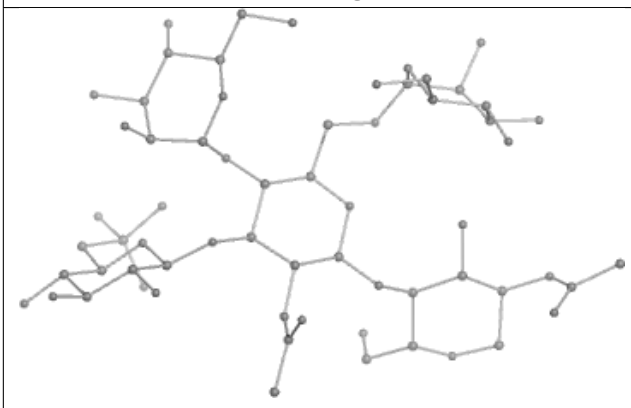

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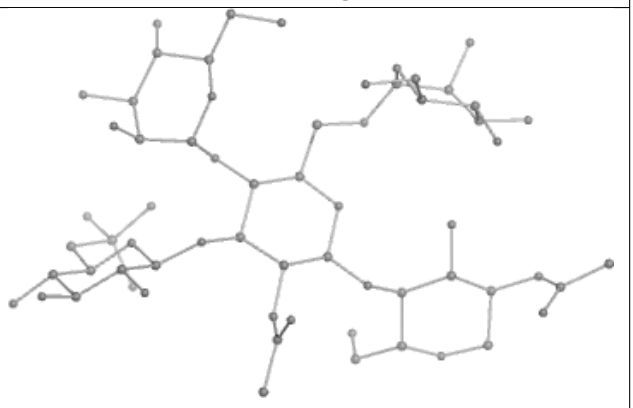
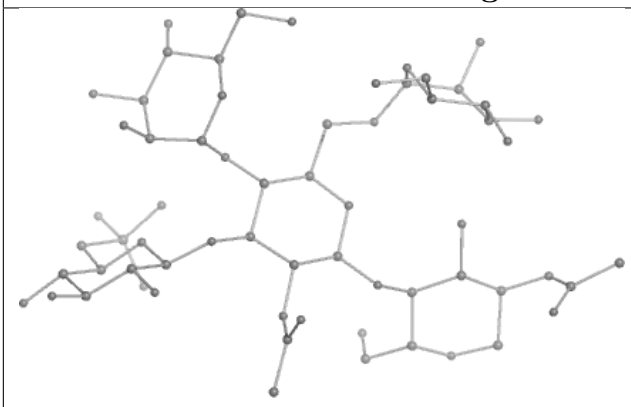


Rings

Oligosaccharide Chain RA



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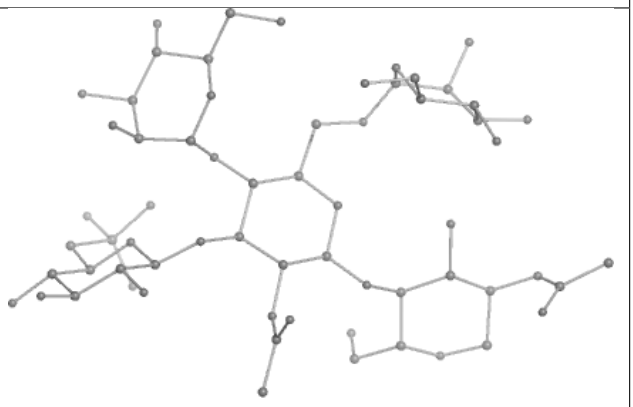
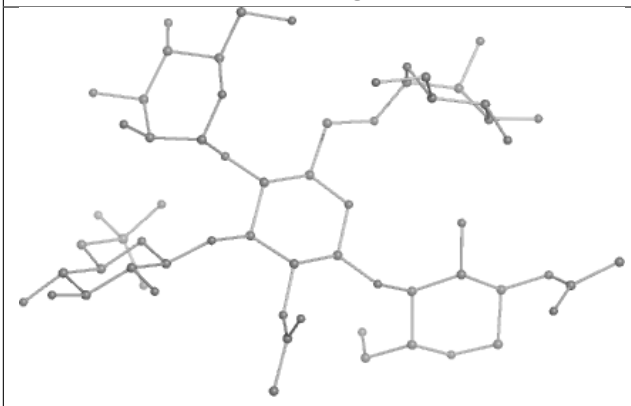
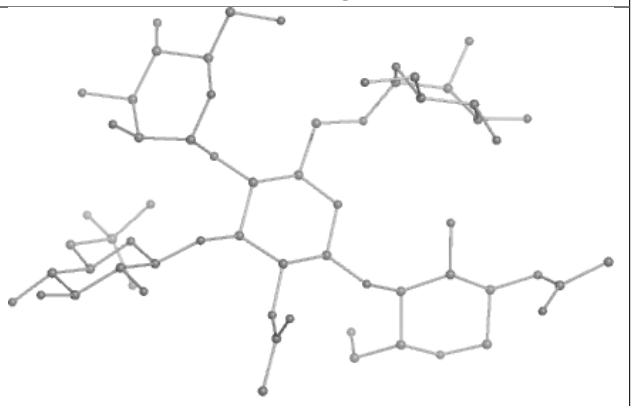


Bond angles

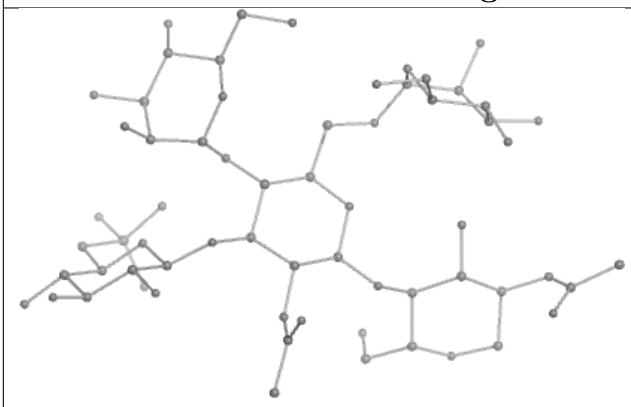


Torsions



Rings

Oligosaccharide Chain UA



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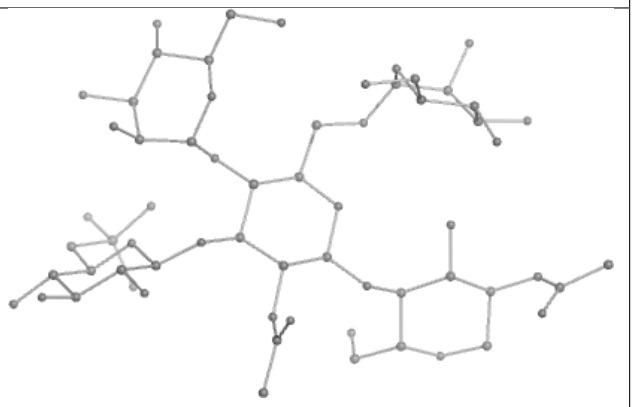
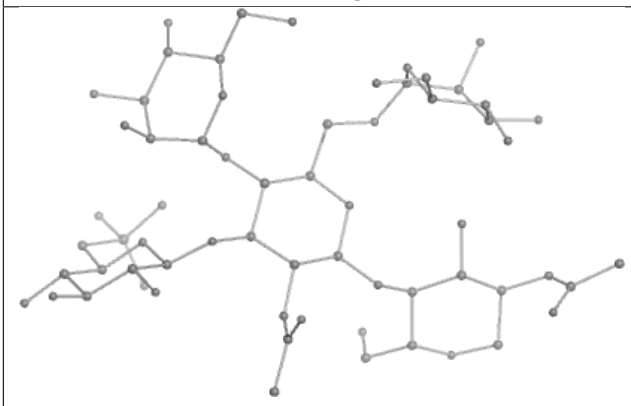
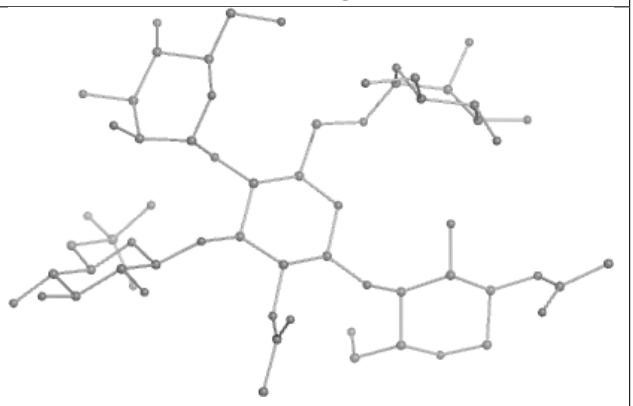


Bond angles

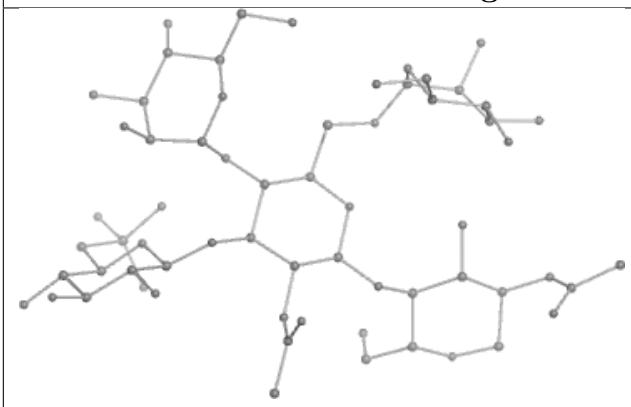


Torsions



Rings

Oligosaccharide Chain XA



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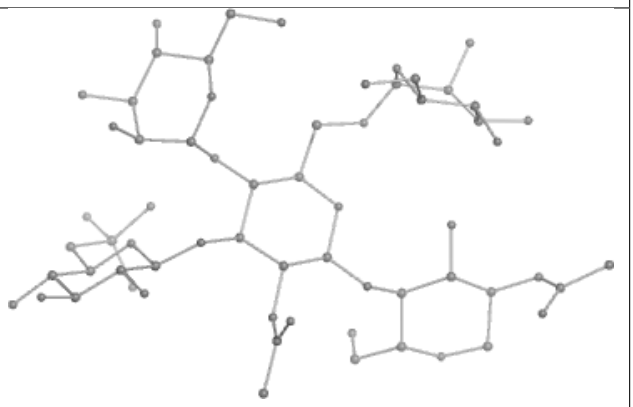
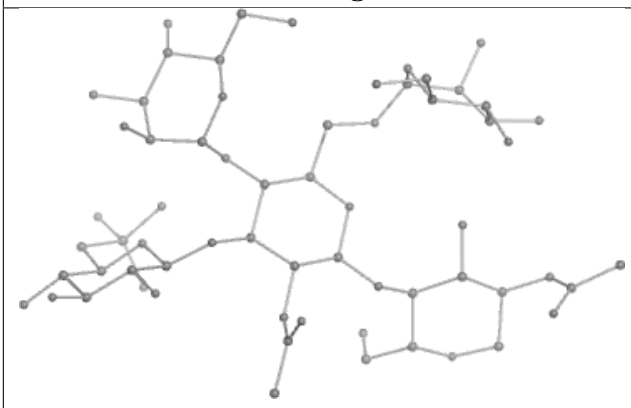


Bond angles



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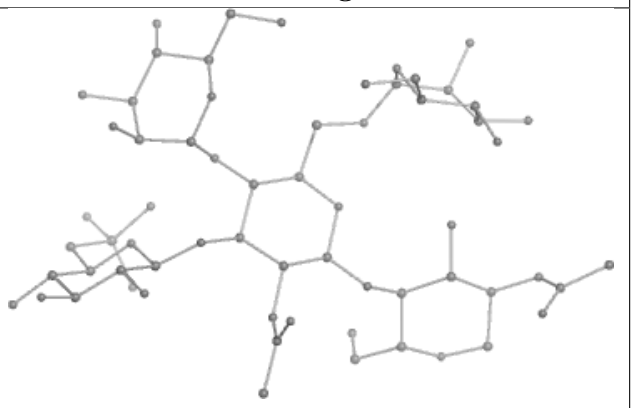
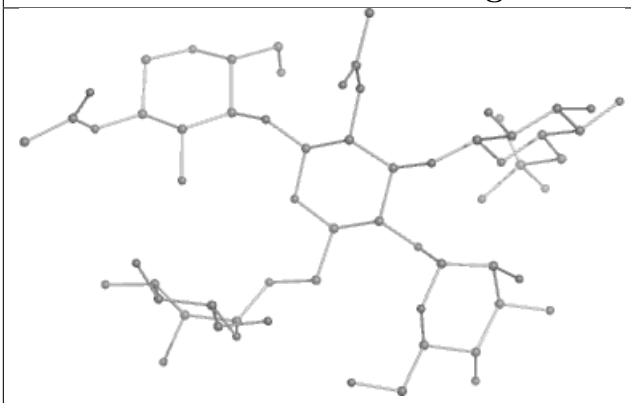


Rings

Oligosaccharide Chain aA



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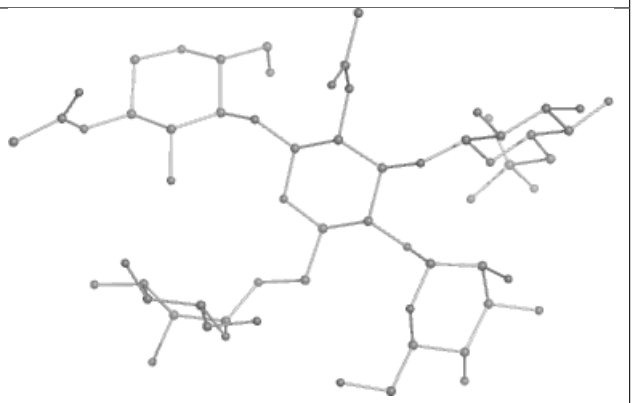
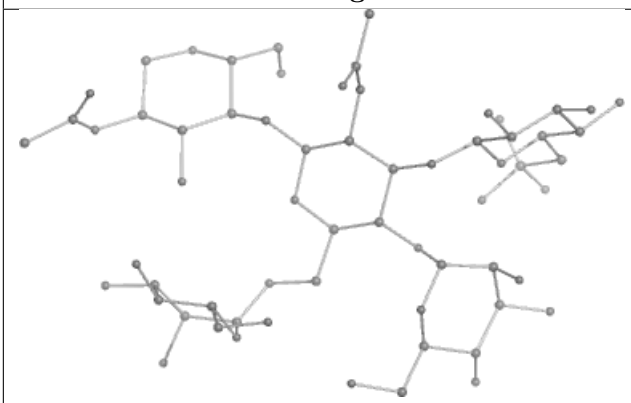


Bond angles



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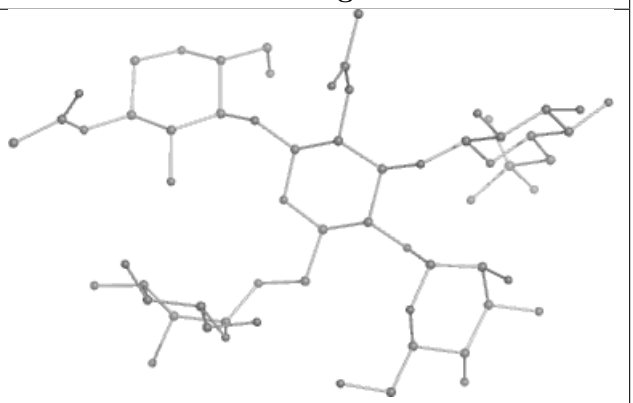
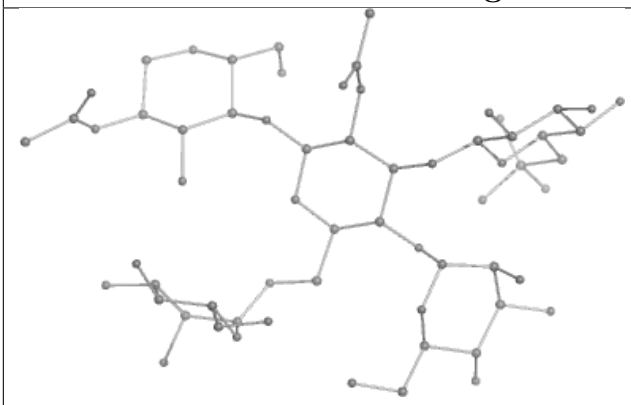


Rings

Oligosaccharide Chain dA



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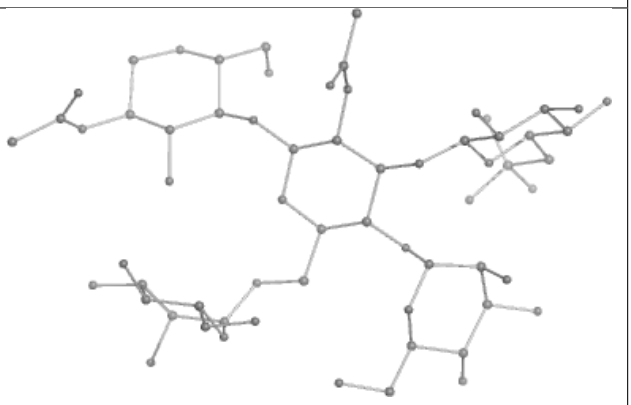
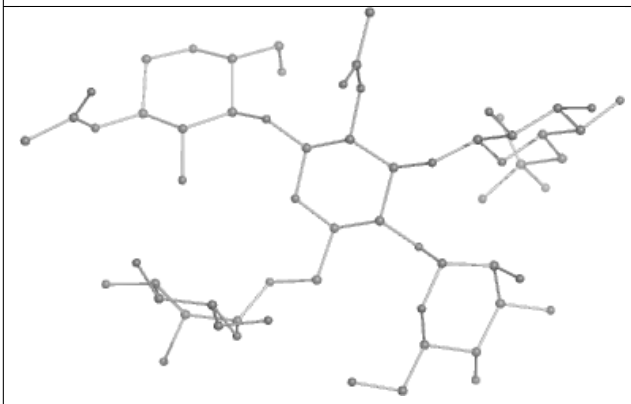


Bond angles



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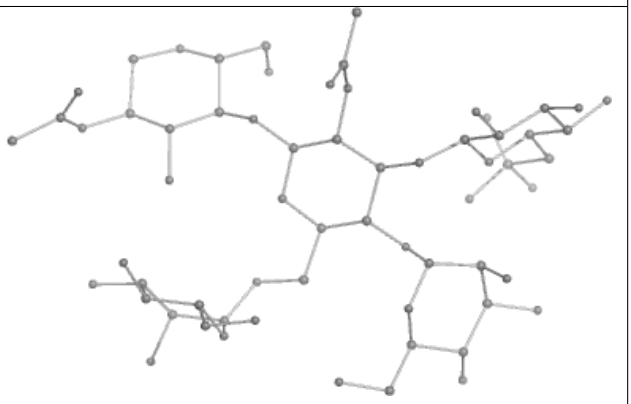
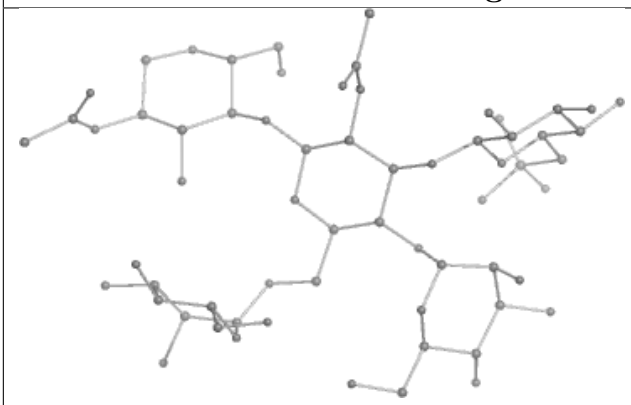


Rings

Oligosaccharide Chain gA



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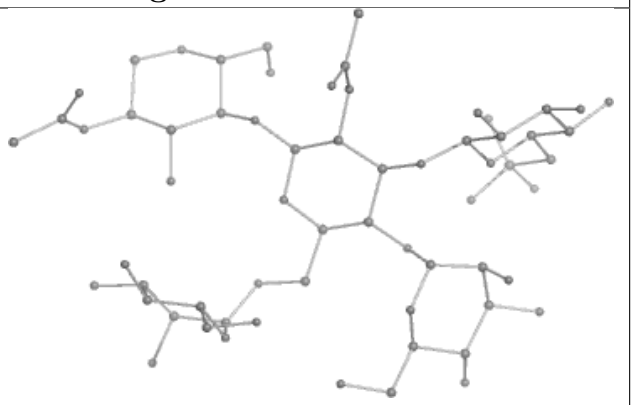

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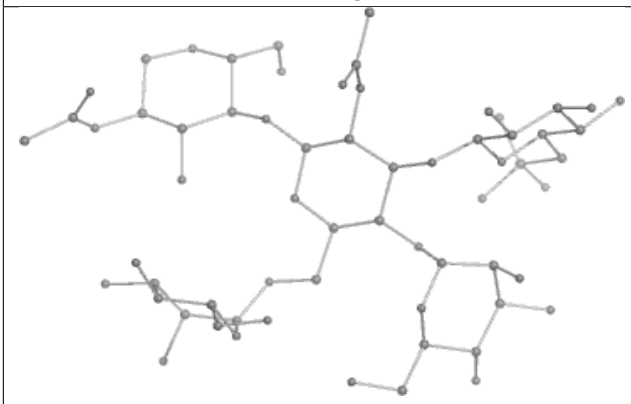

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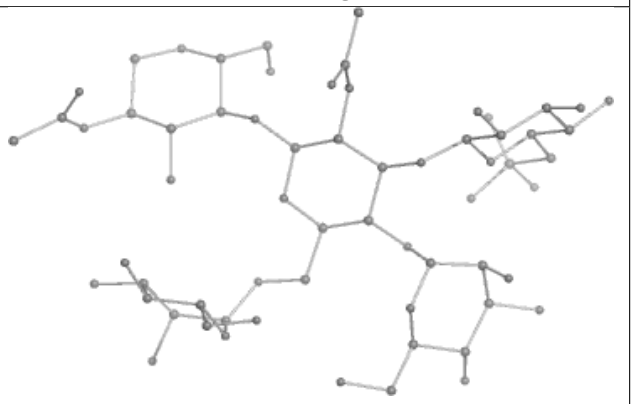
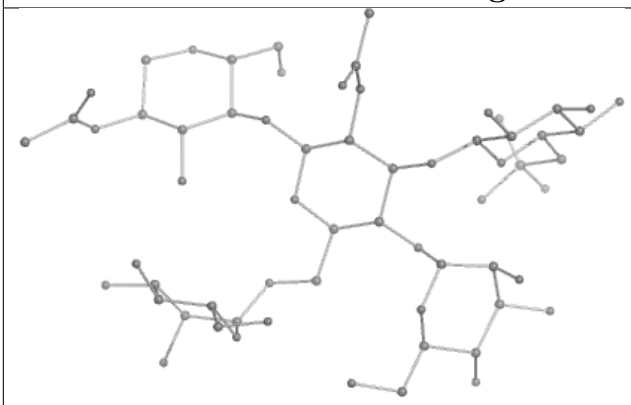


Rings

Oligosaccharide Chain jA



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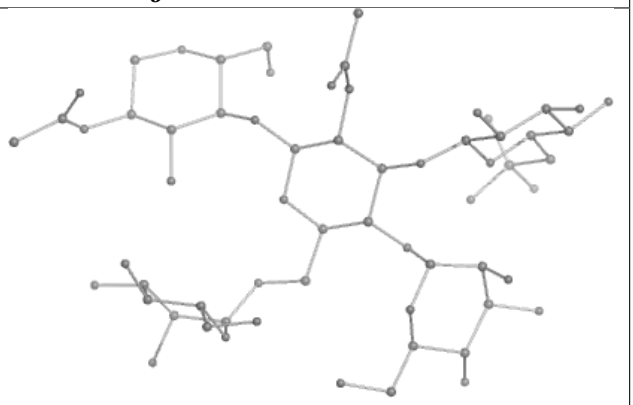
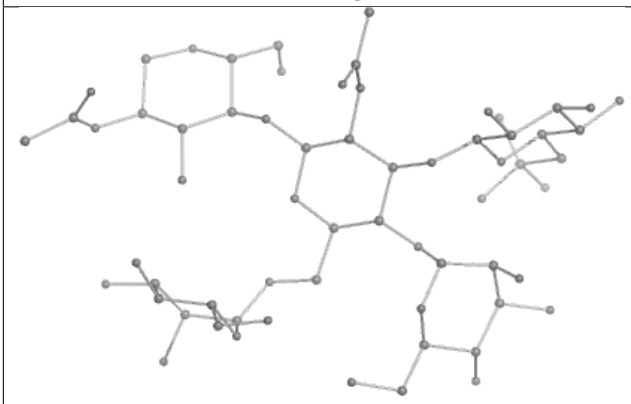


Bond angles



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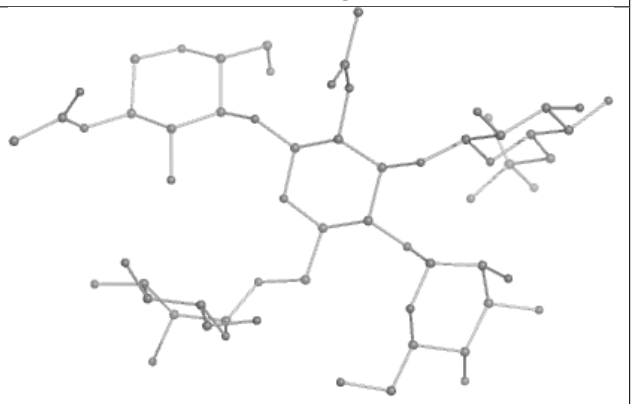
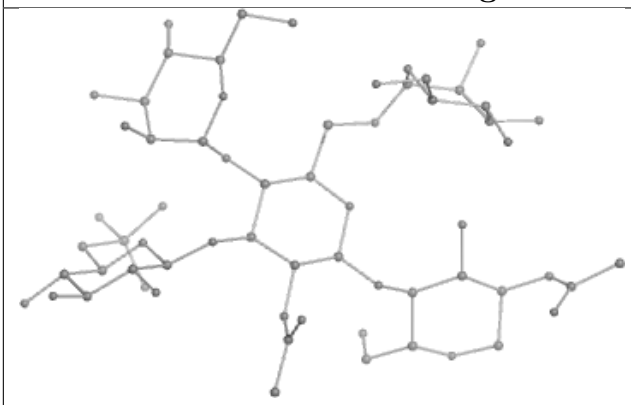
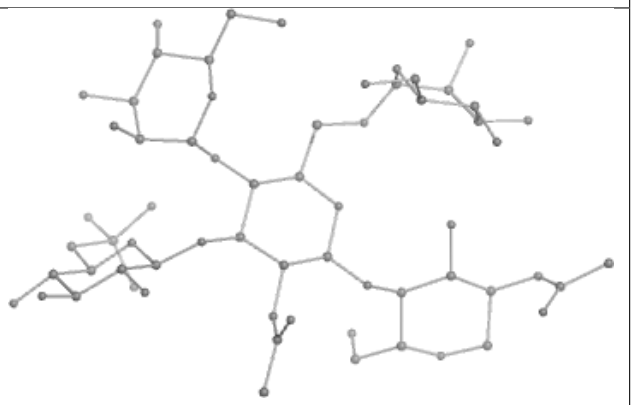


Rings

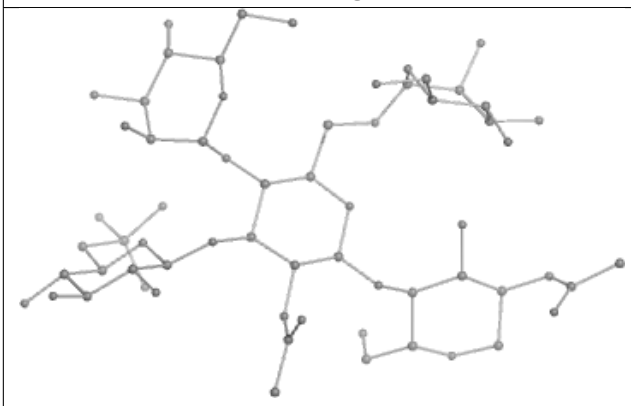
Oligosaccharide Chain mA



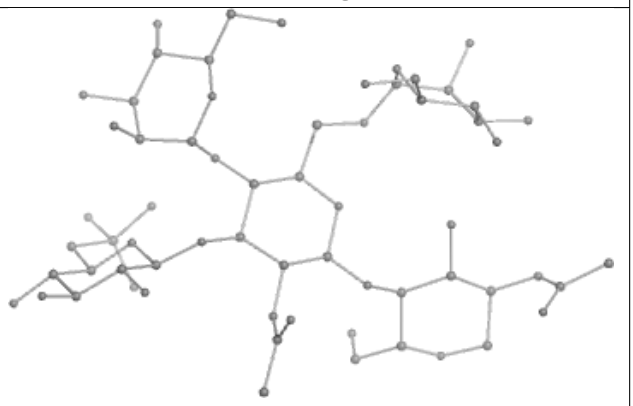
Bond lengths



Bond angles

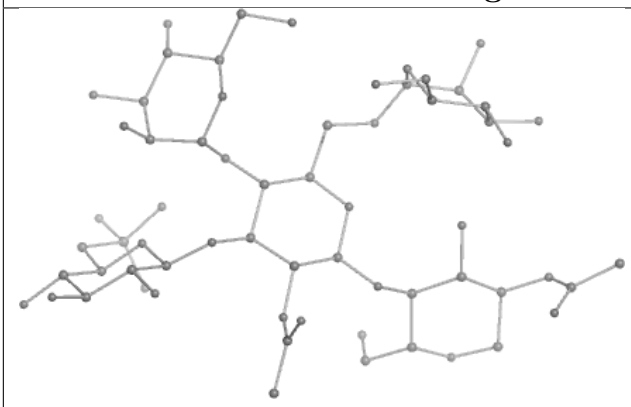


Torsions

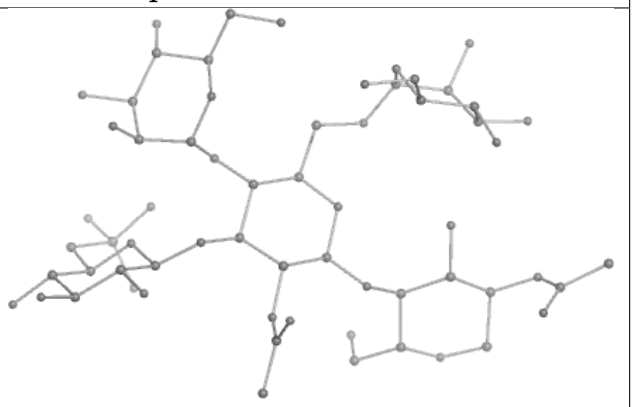


Rings

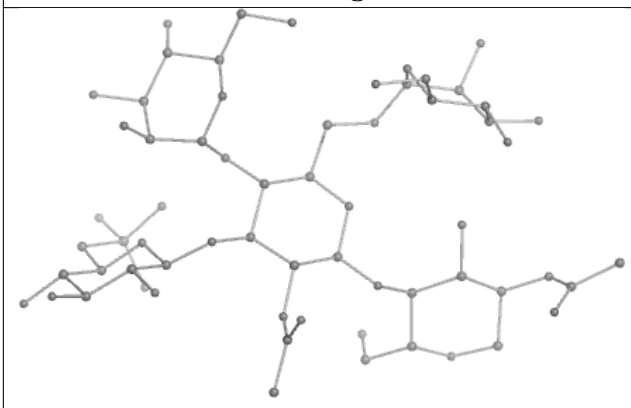
Oligosaccharide Chain pA



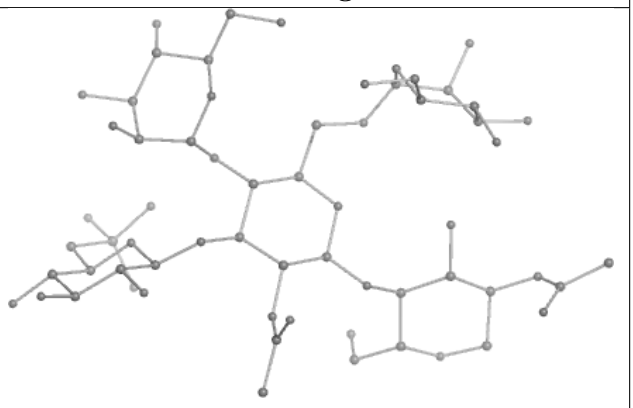
Bond lengths



Bond angles

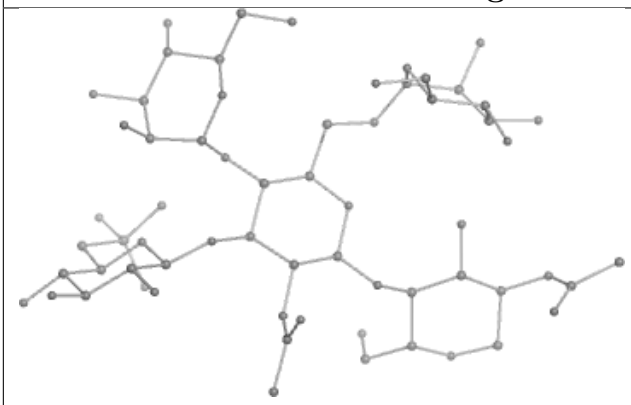


Torsions



Rings

Oligosaccharide Chain sA



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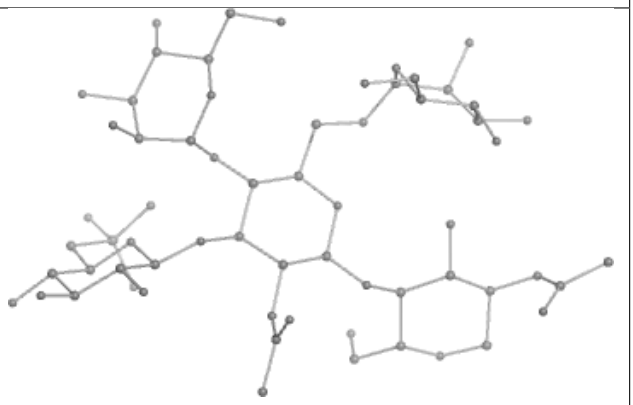
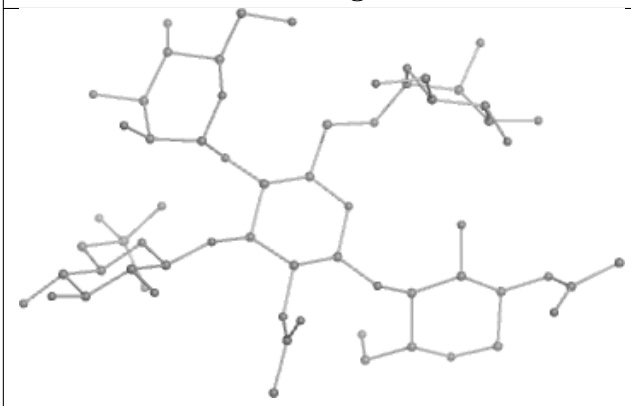


Bond angles



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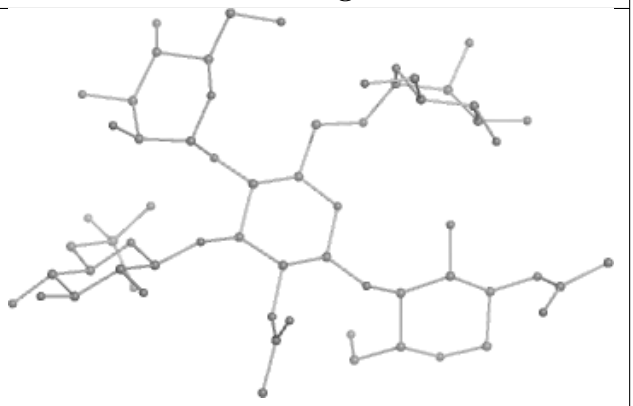
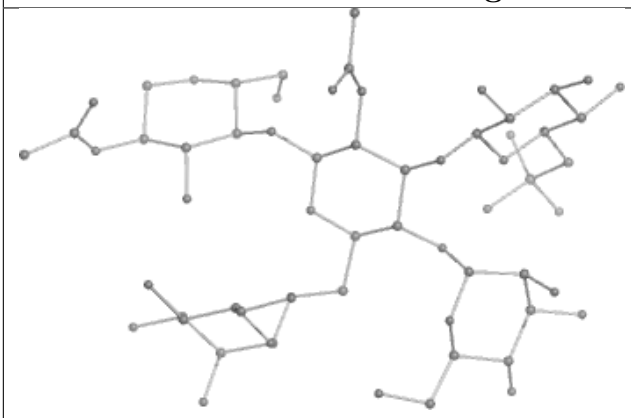
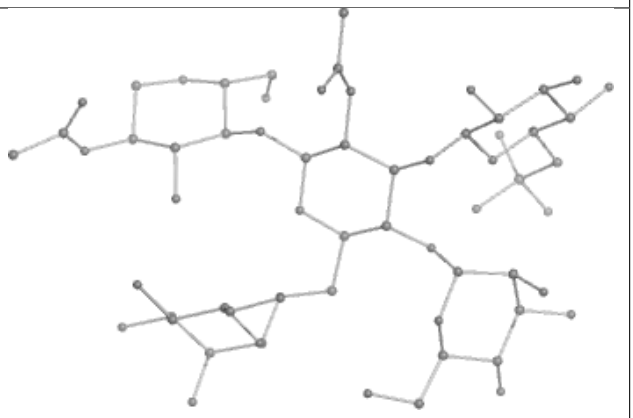
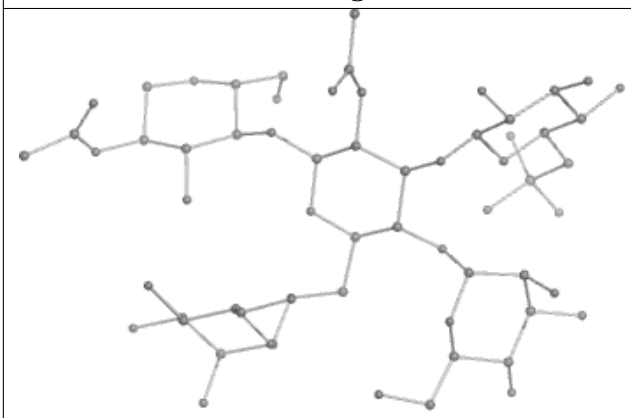
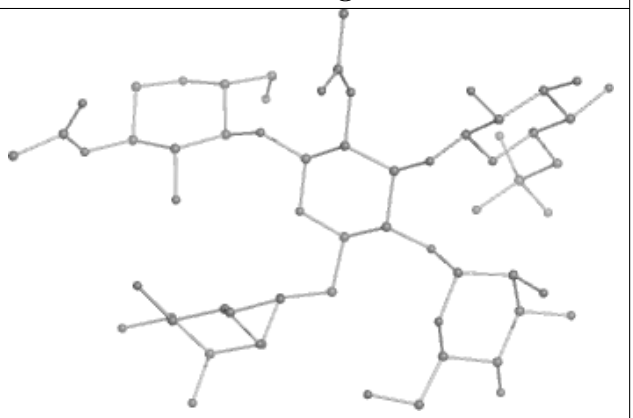
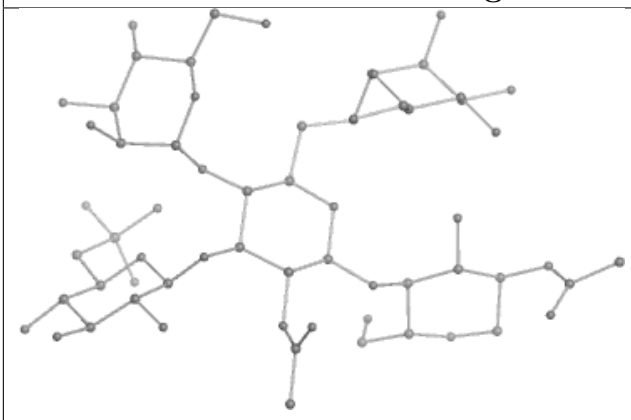


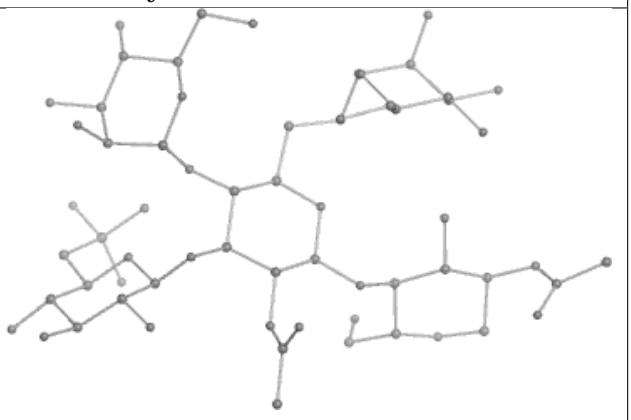
Rings

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

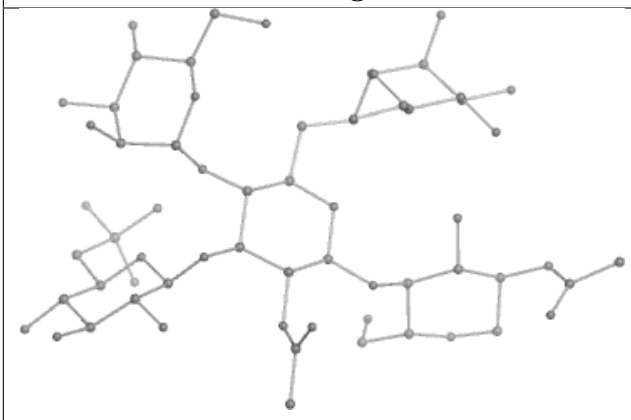
Oligosaccharide Chain yA



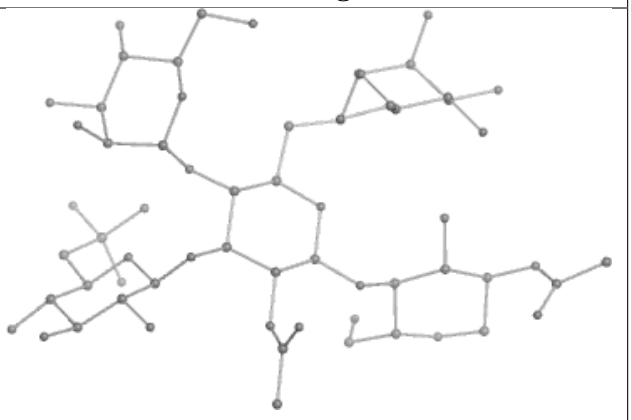
Bond lengths



Bond angles

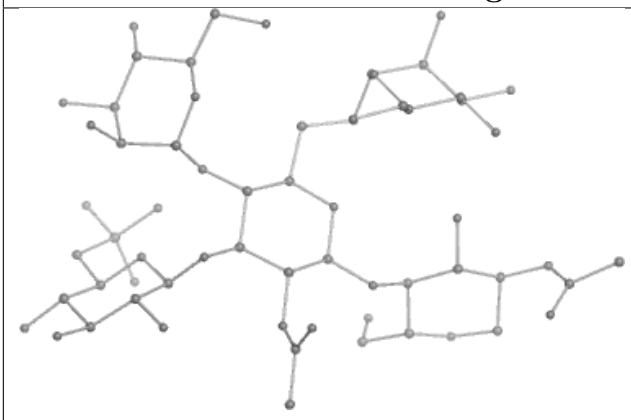


Torsions



Rings

Oligosaccharide Chain 1A



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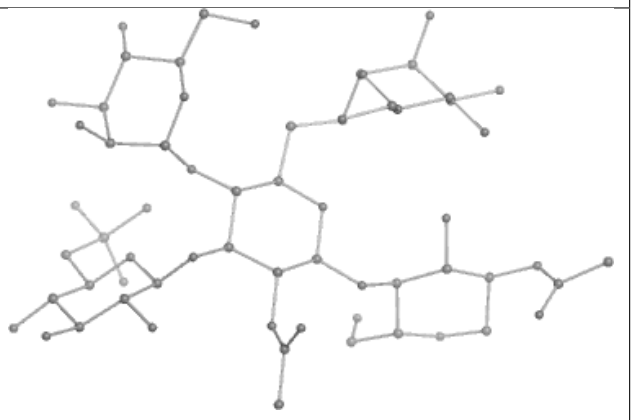
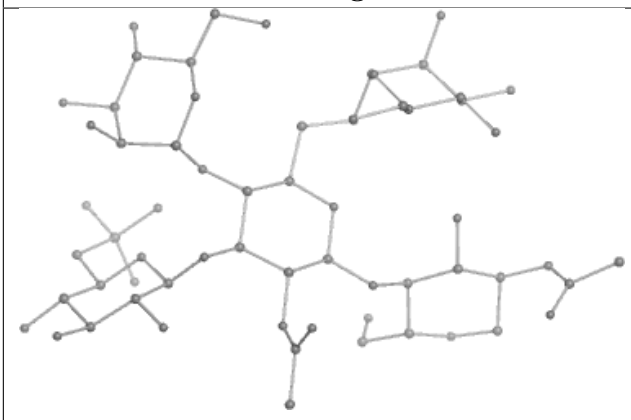


Bond angles



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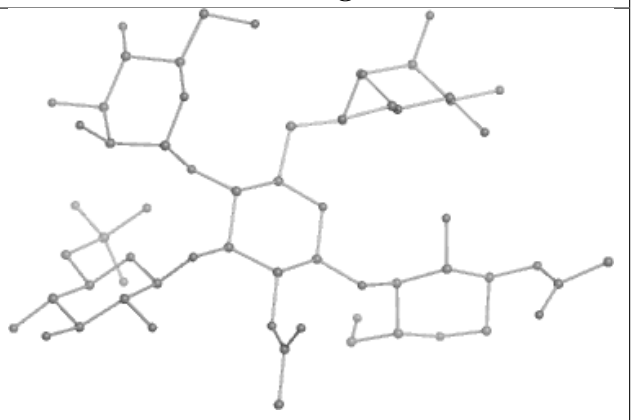
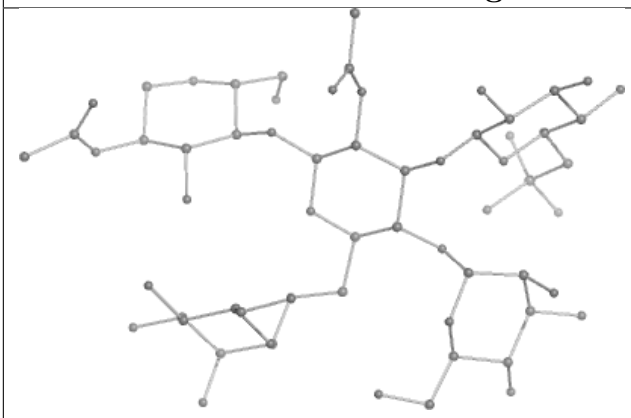
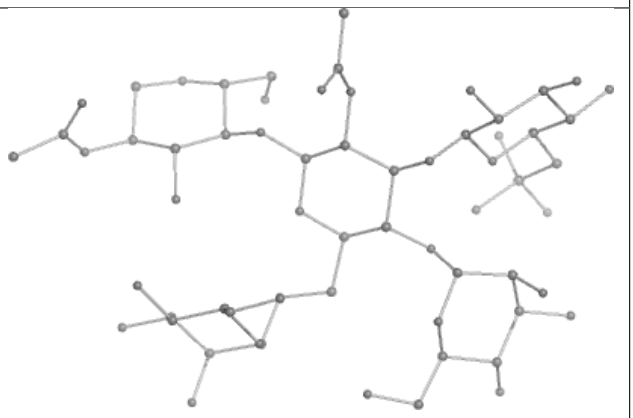


Rings

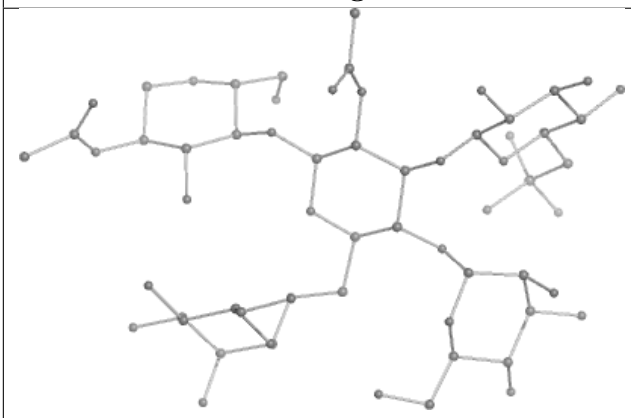
Oligosaccharide Chain 4A



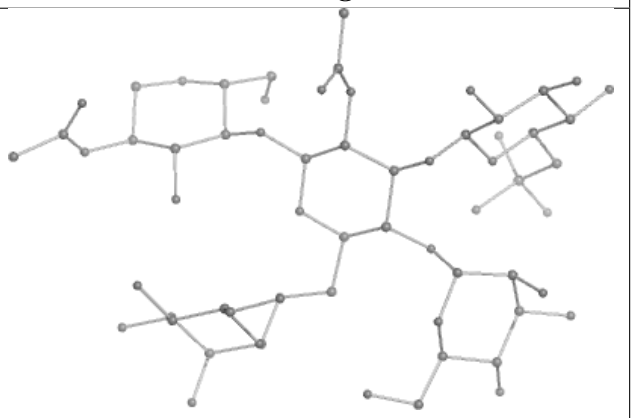
Bond lengths



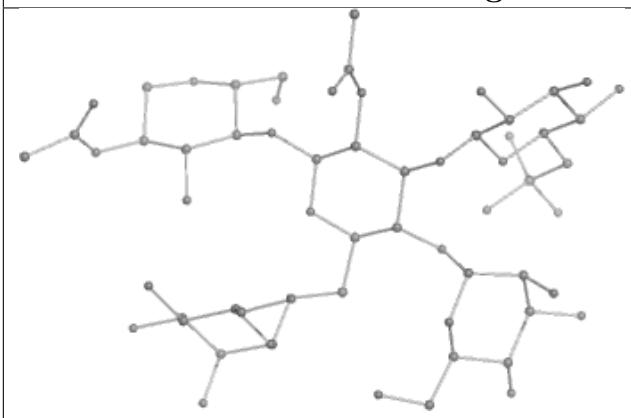
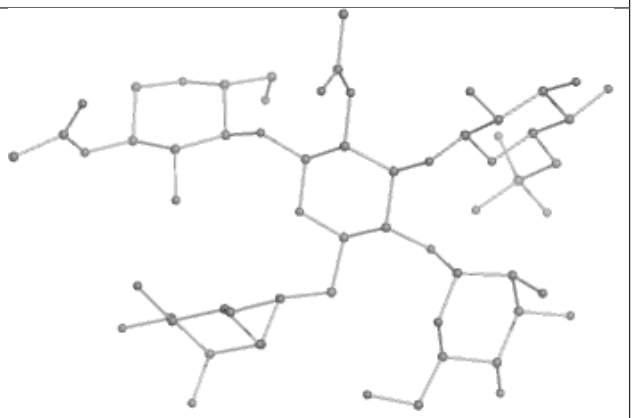
Bond angles



Torsions



Rings

Oligosaccharide Chain 7A	
	
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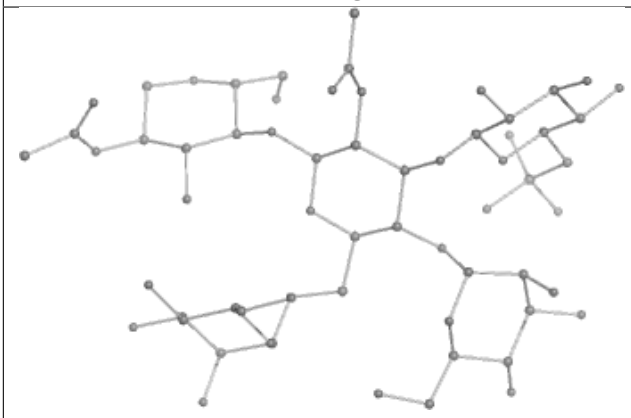
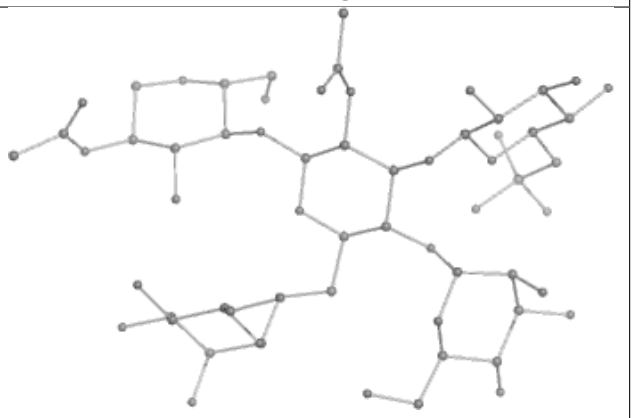
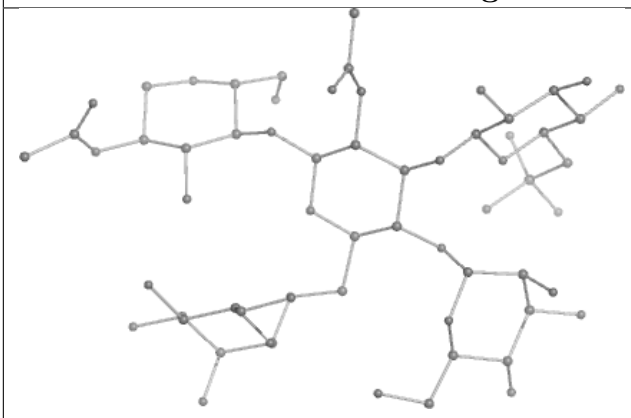
	
Torsions	**Rings**

Oligosaccharide Chain AB



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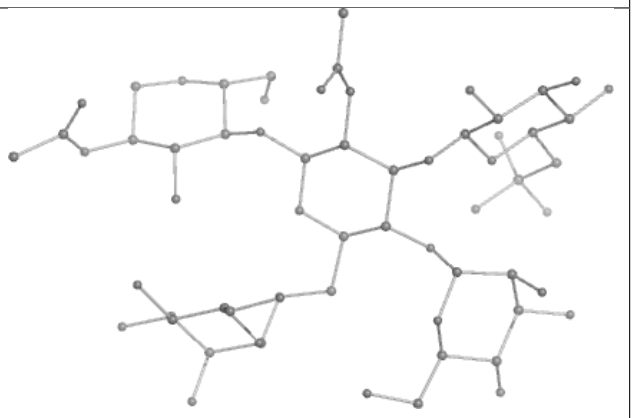
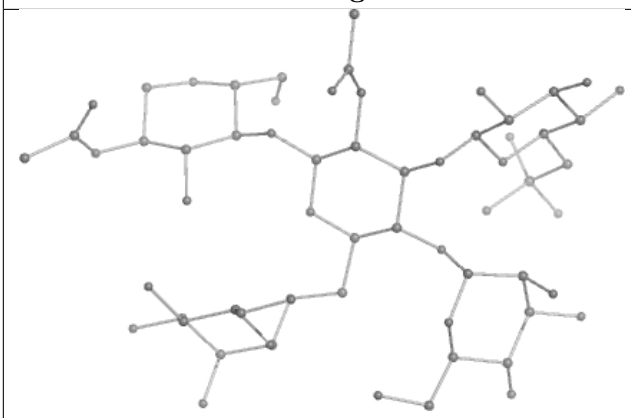
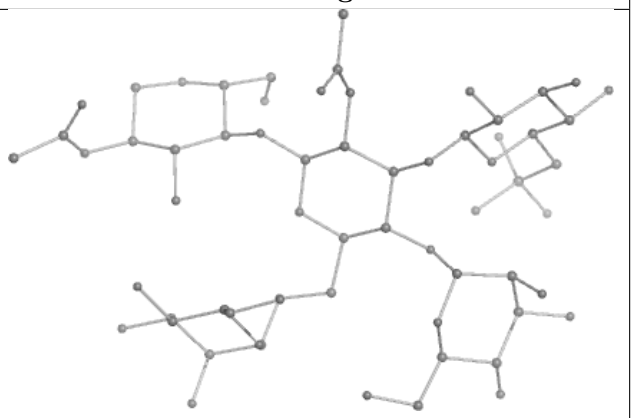


Bond angles

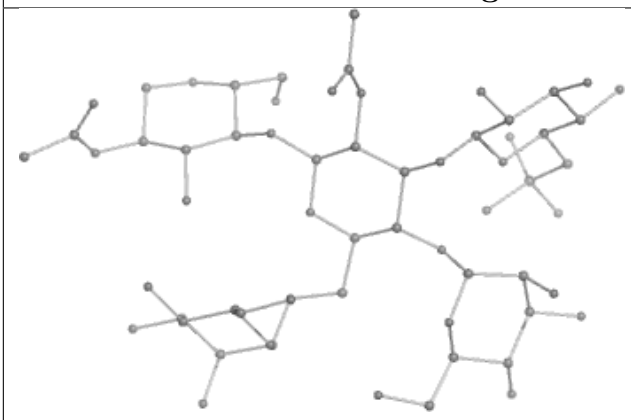


Torsions



Rings

Oligosaccharide Chain DB



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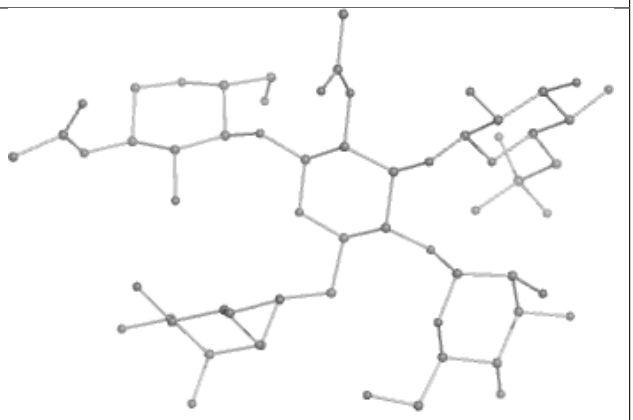

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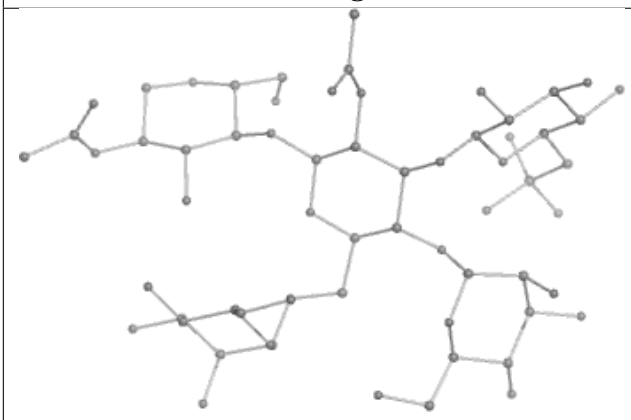

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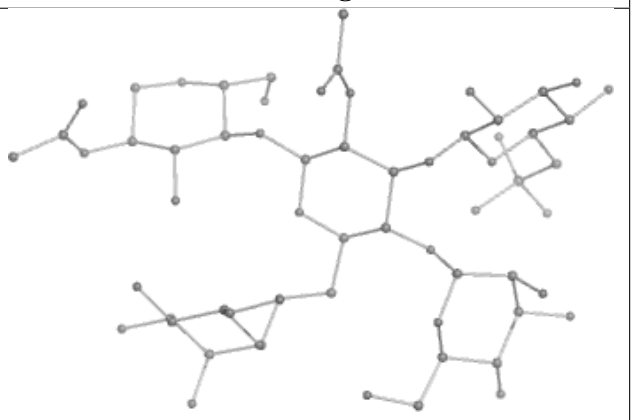
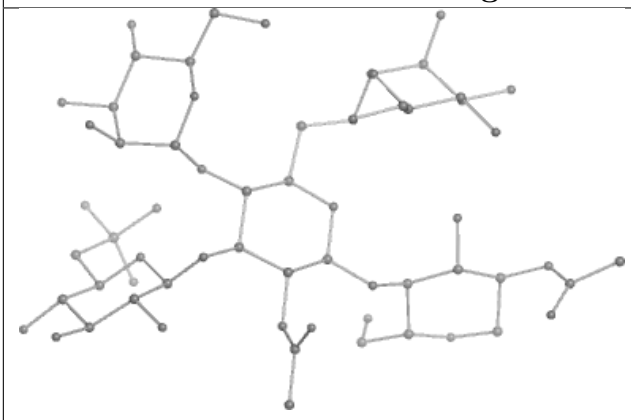


Rings

Oligosaccharide Chain GB



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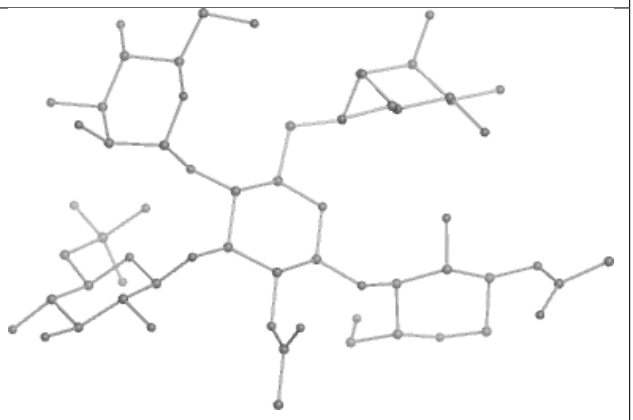
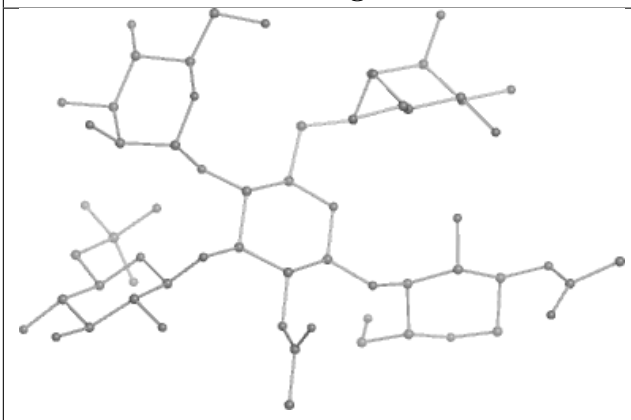


Bond angles



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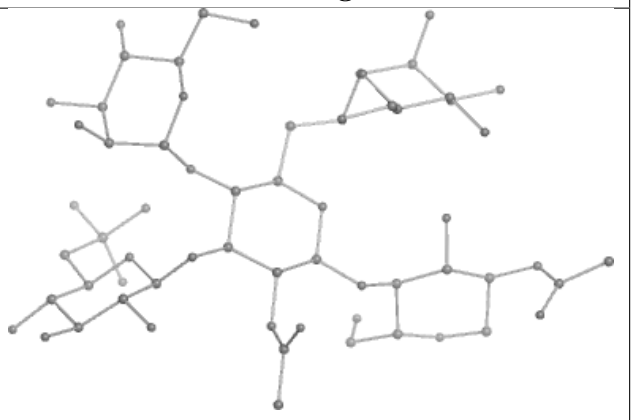
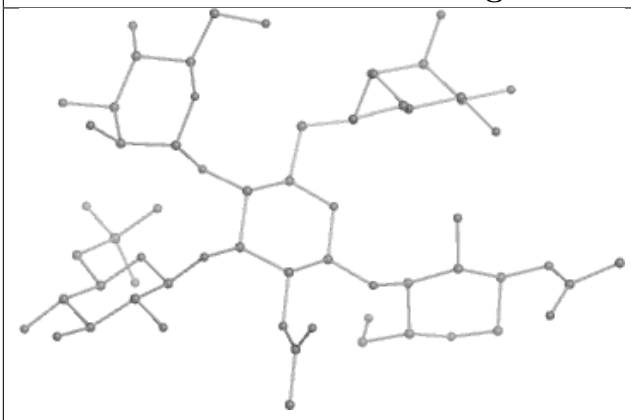


Rings

Oligosaccharide Chain JB



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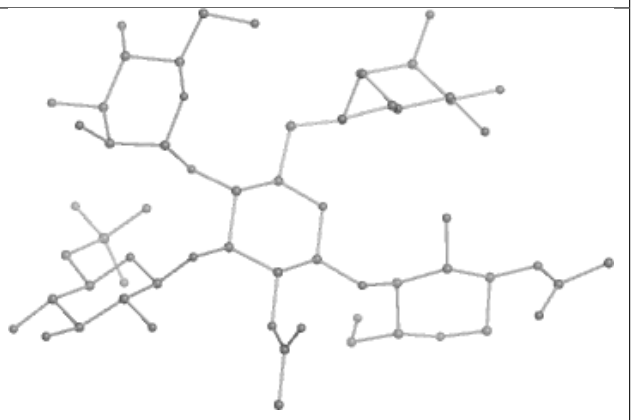
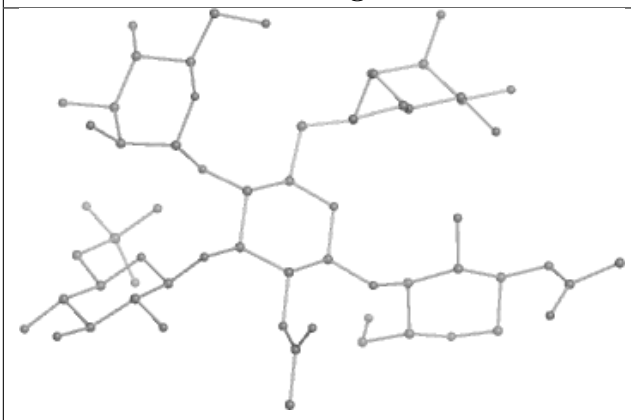


Bond angles



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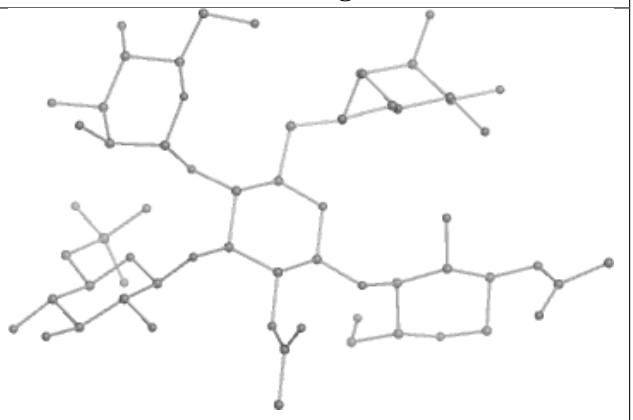
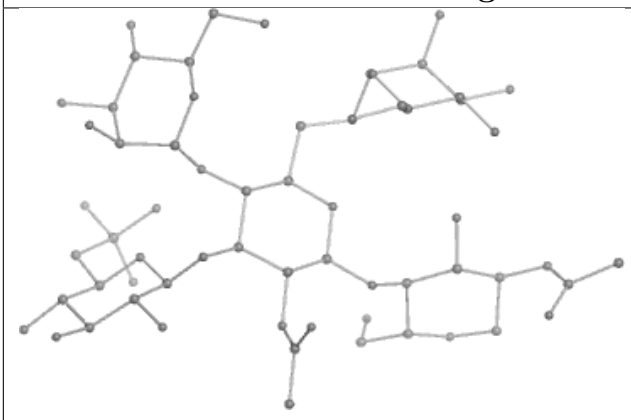


Rings

Oligosaccharide Chain MB



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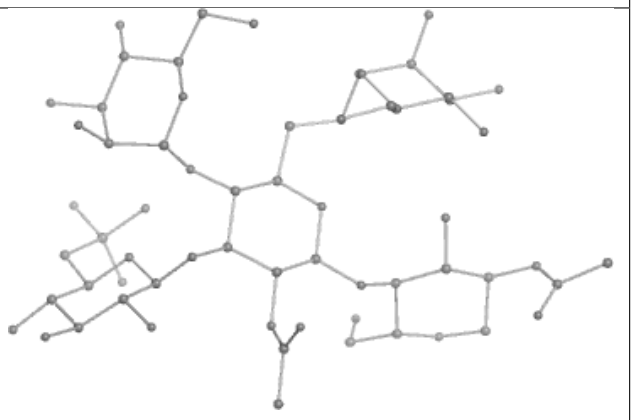
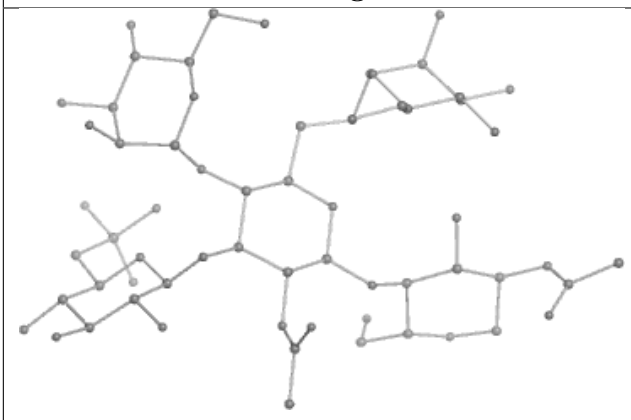


Bond angles



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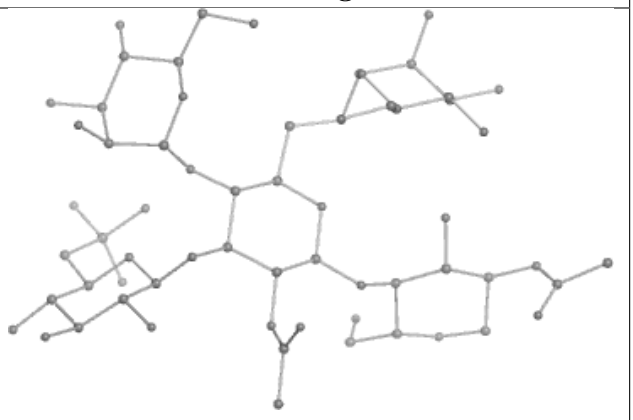
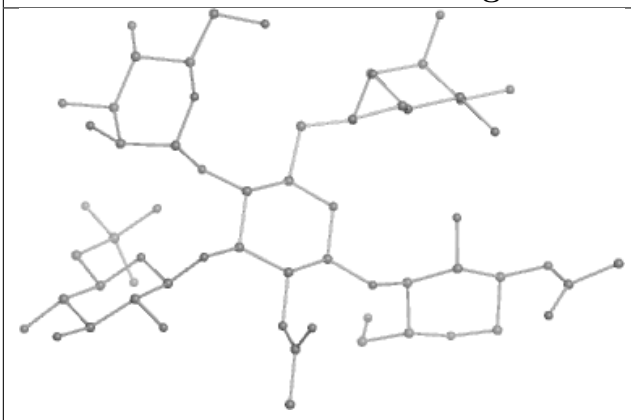


Rings

Oligosaccharide Chain PB



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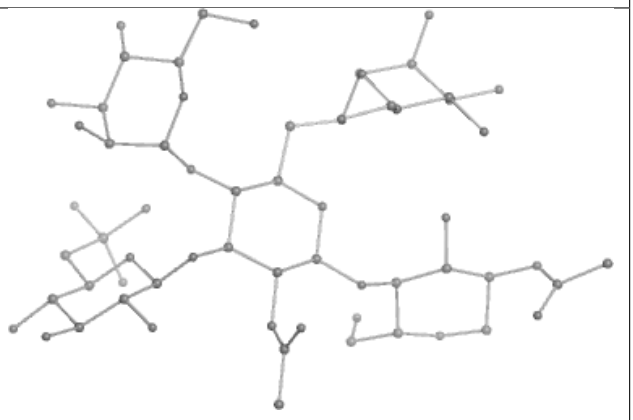

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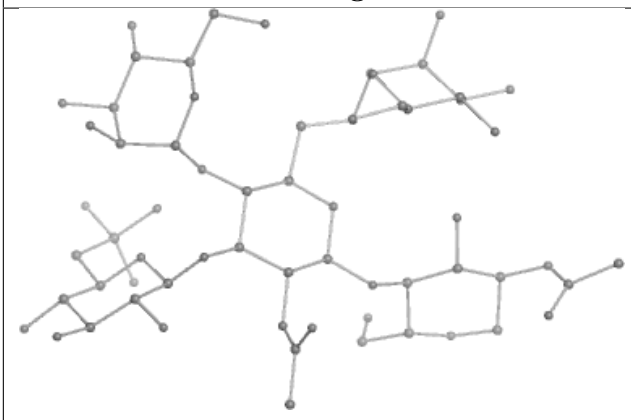

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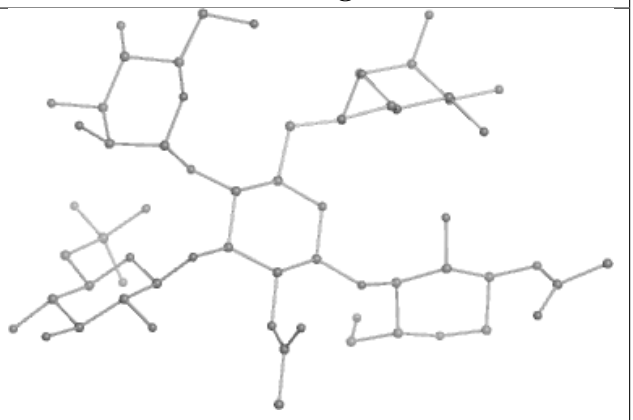
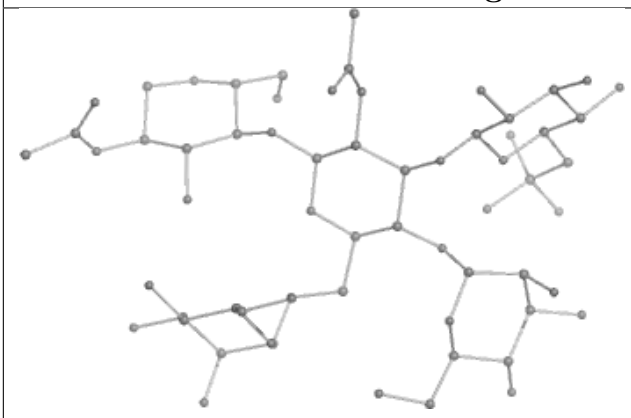


Rings

Oligosaccharide Chain SB



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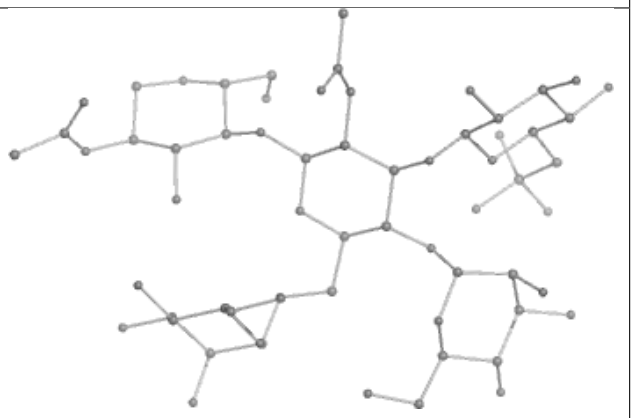
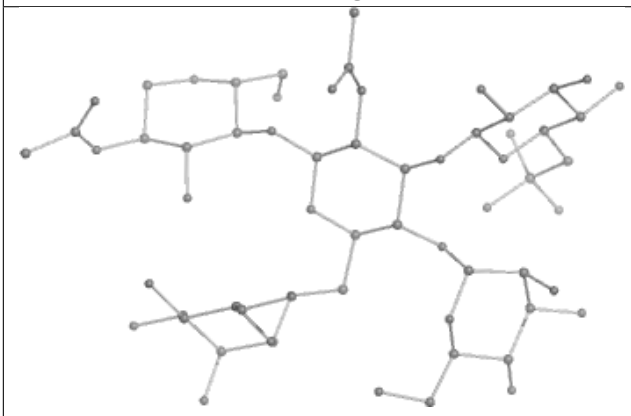


Bond angles



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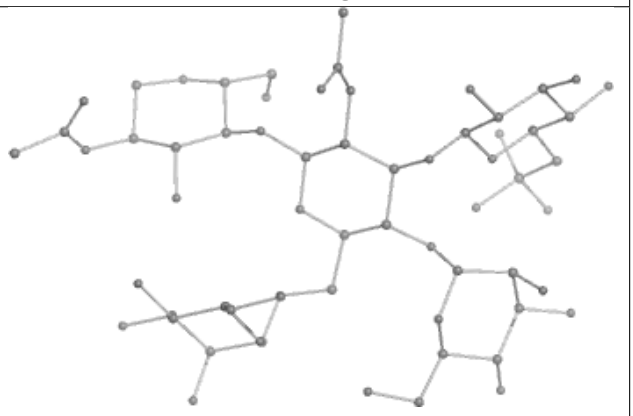
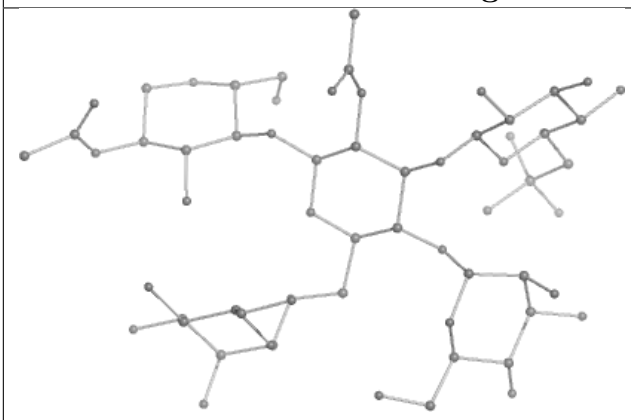


Rings

Oligosaccharide Chain VB



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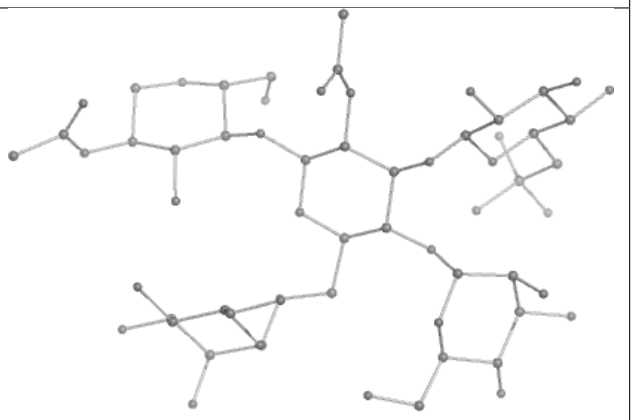
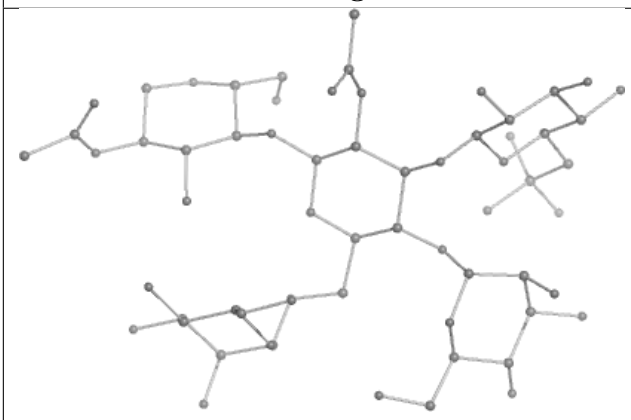


Bond angles



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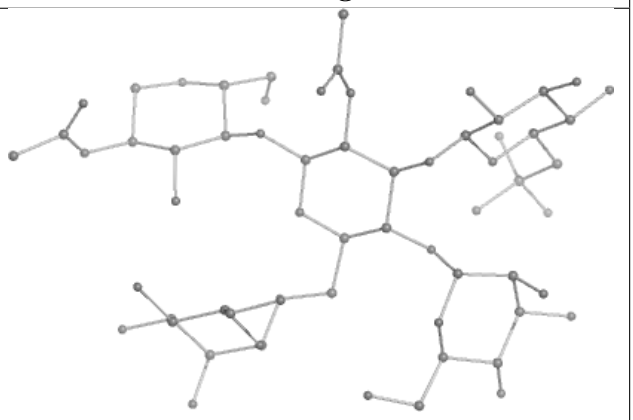
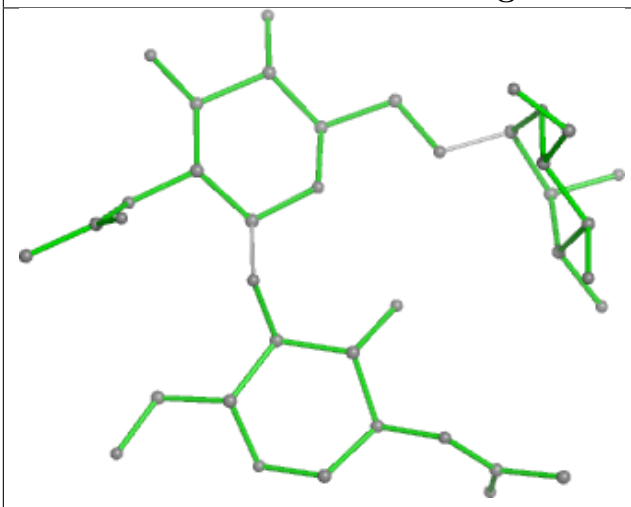


Rings

Oligosaccharide Chain n



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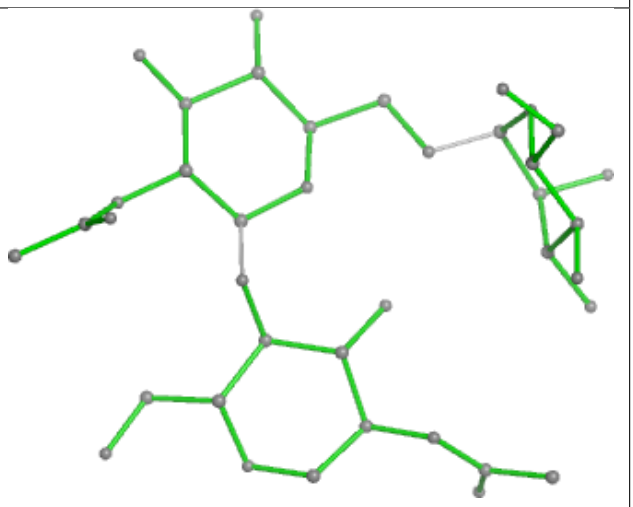

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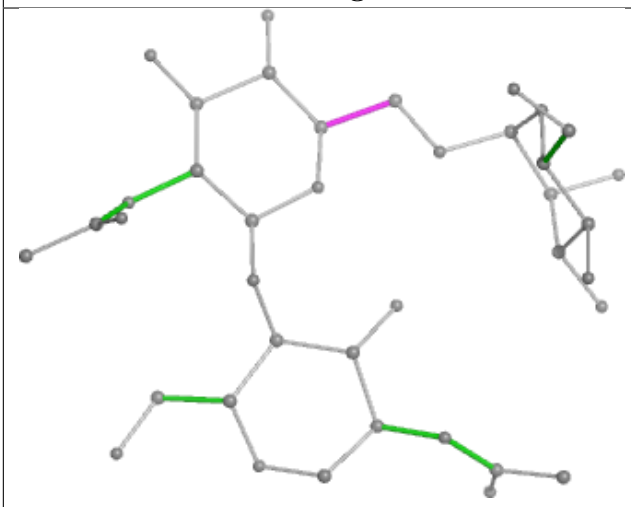

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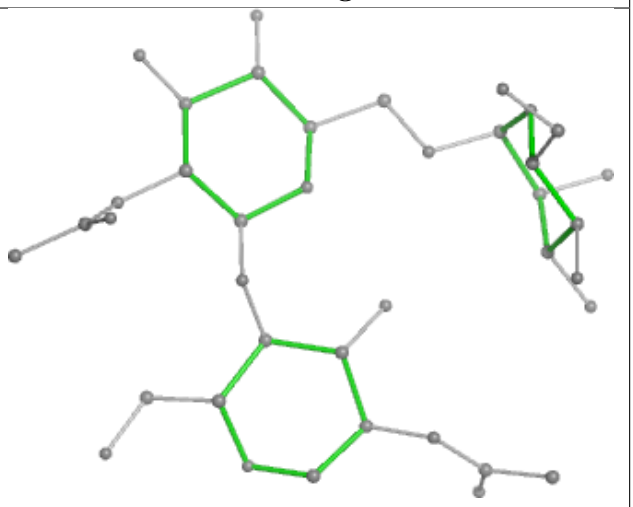
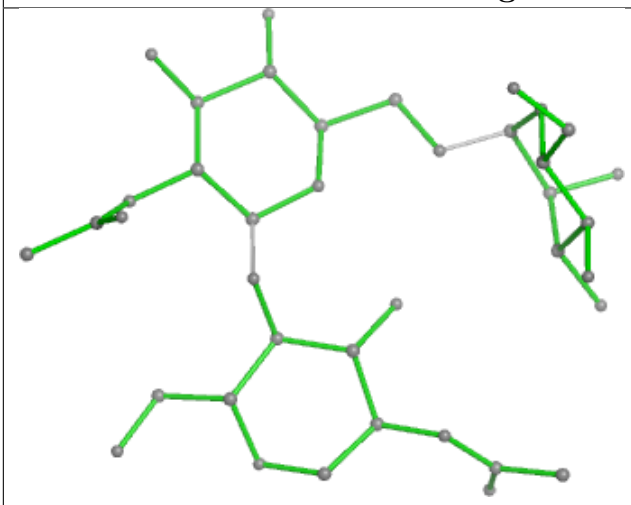


Rings

Oligosaccharide Chain q



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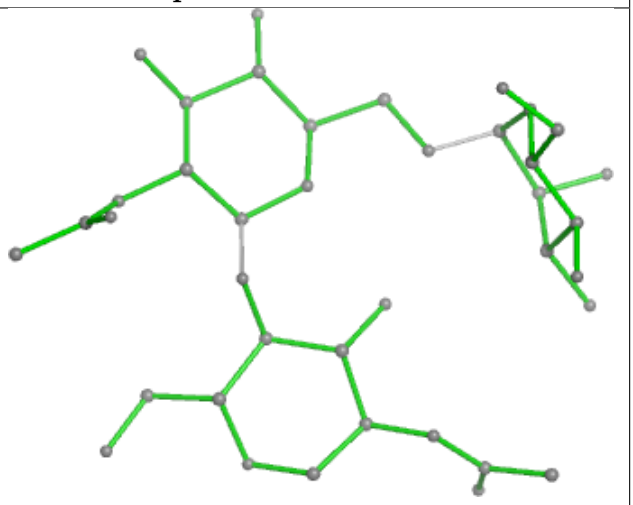
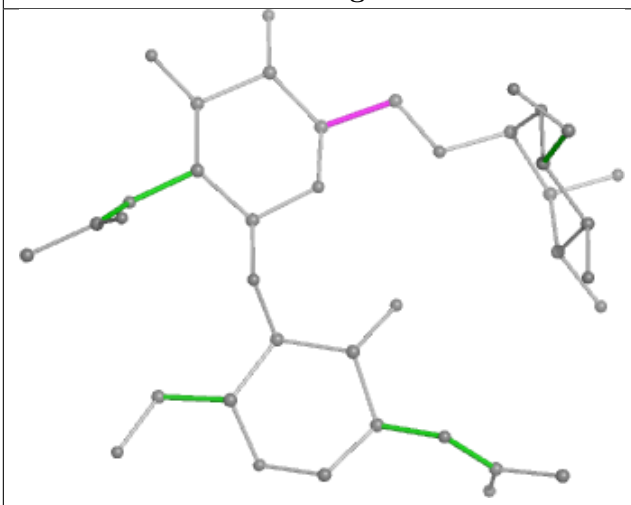


Bond angles



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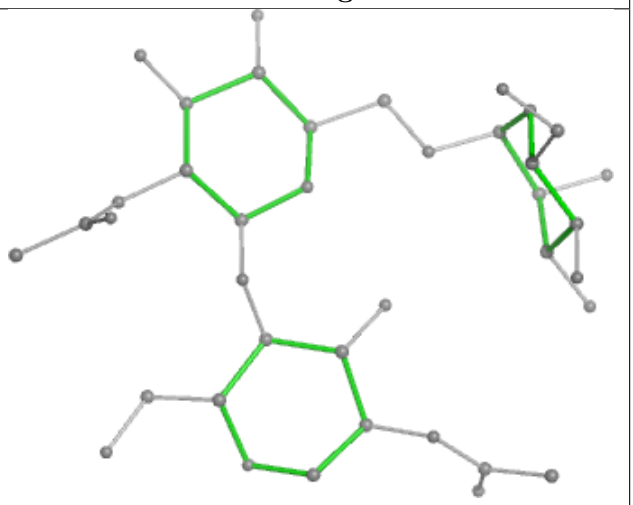
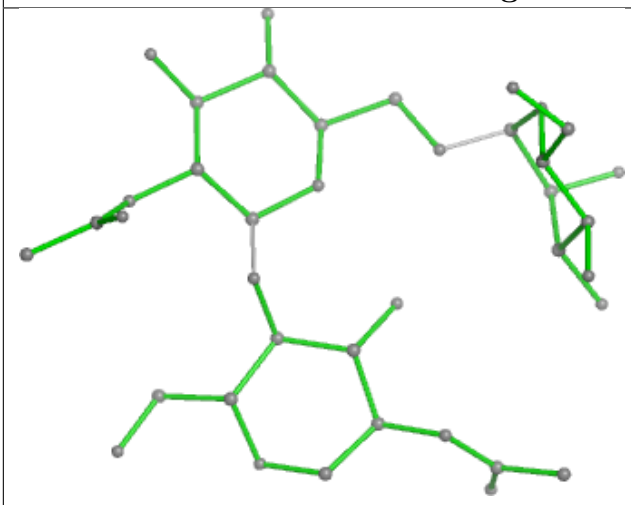


Rings

Oligosaccharide Chain t



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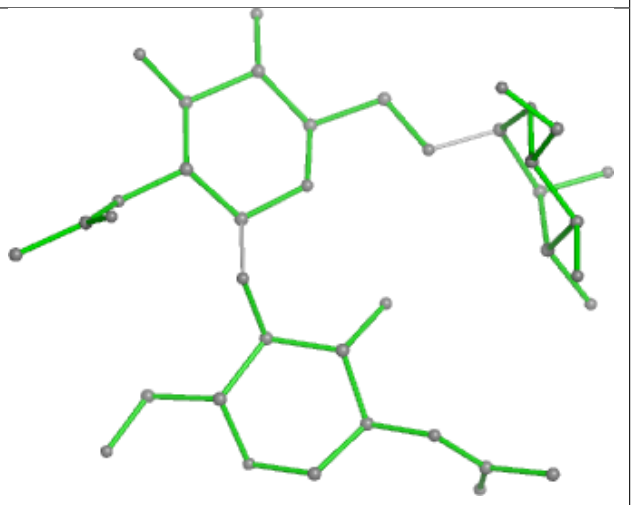

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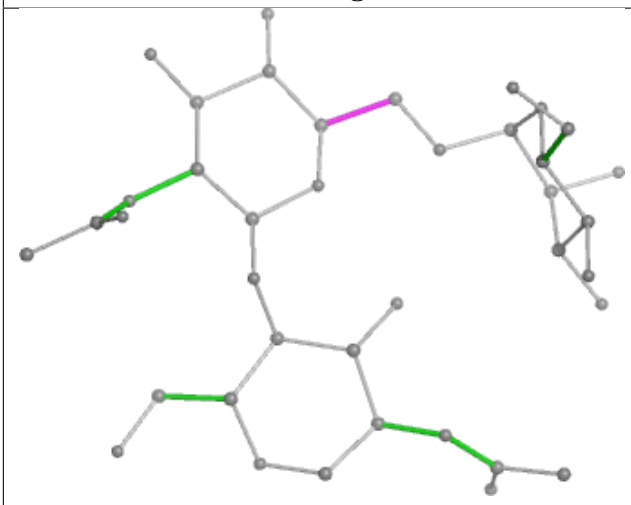

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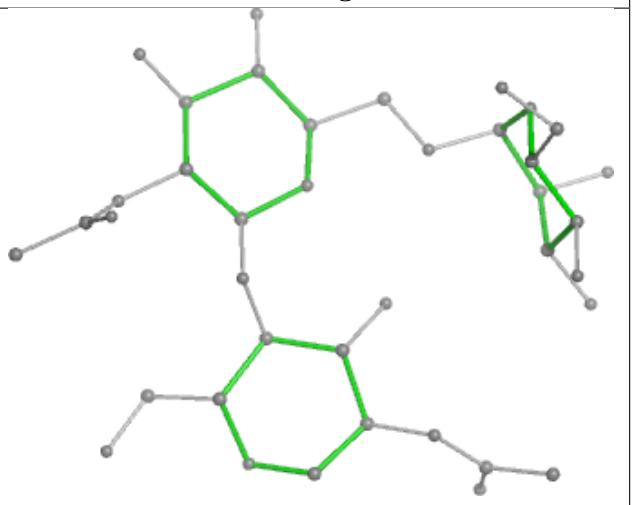
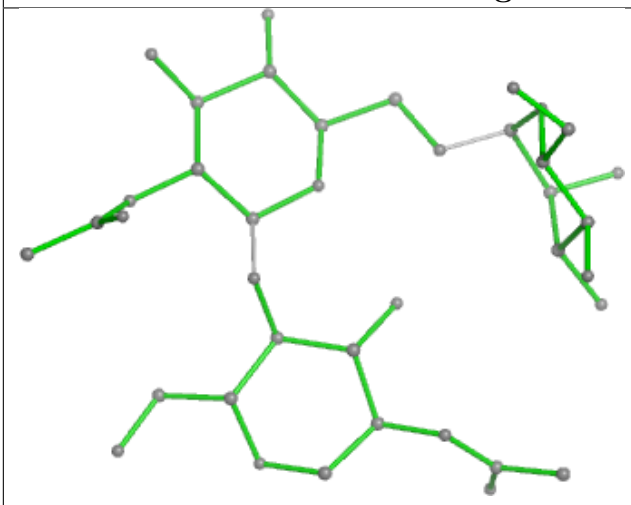


Rings

Oligosaccharide Chain w



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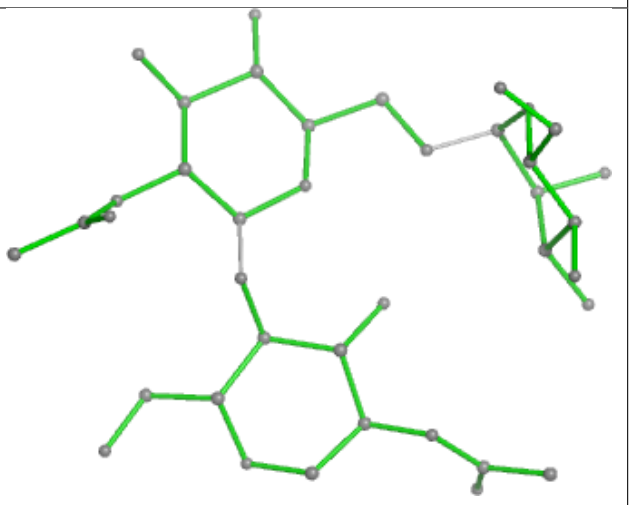
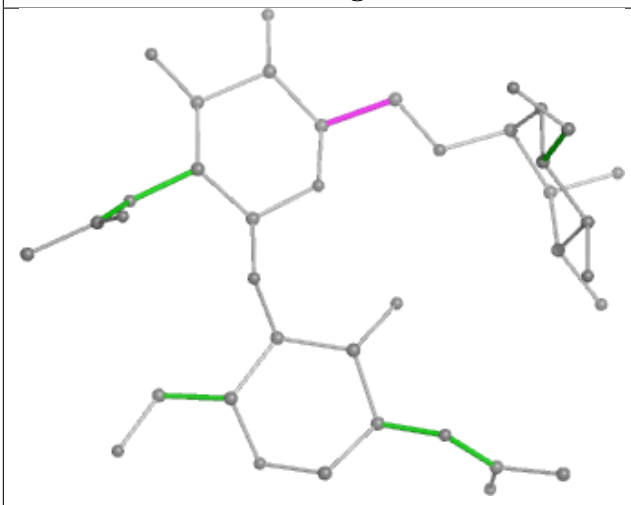


Bond angles



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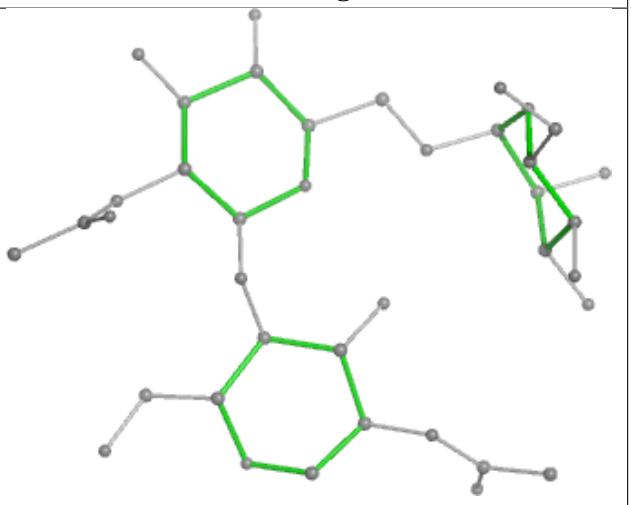
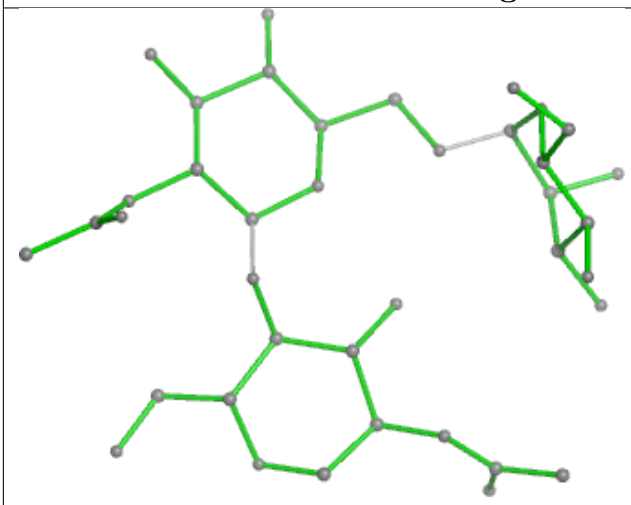


Rings

Oligosaccharide Chain z



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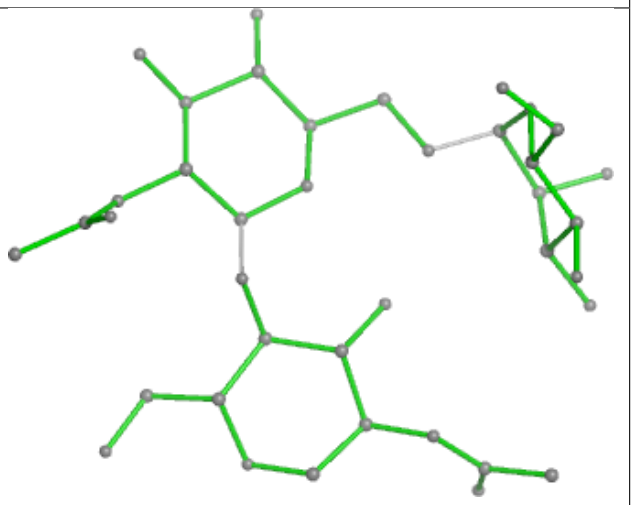
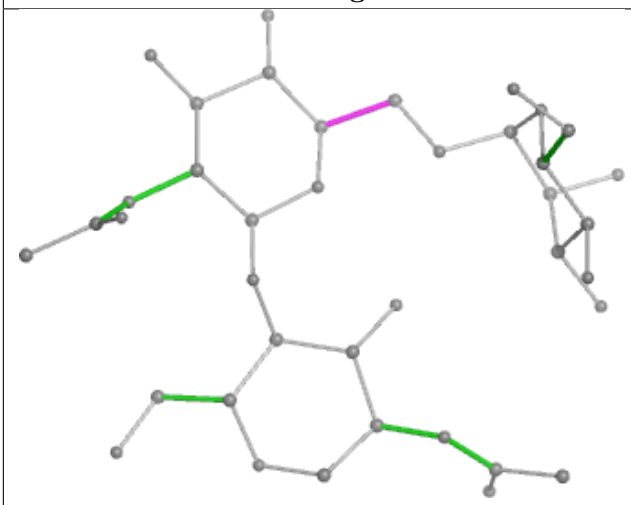


Bond angles



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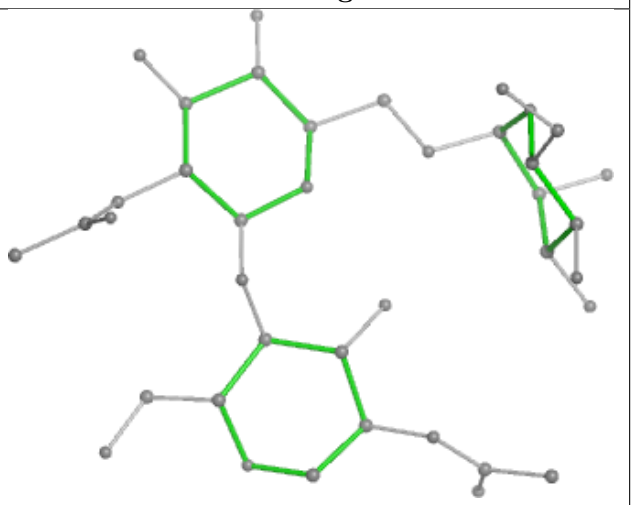
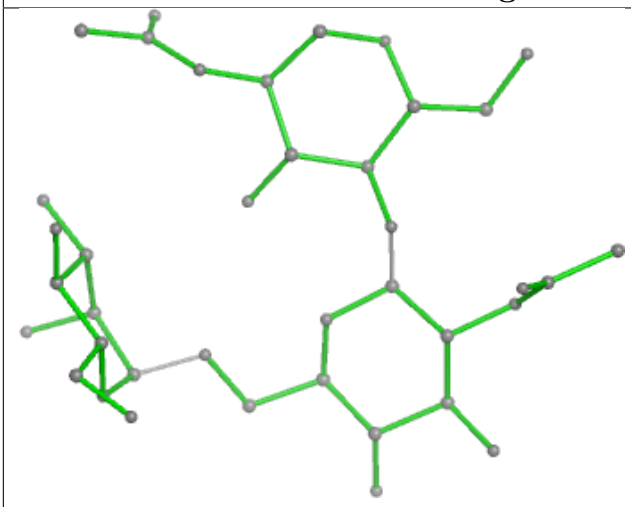
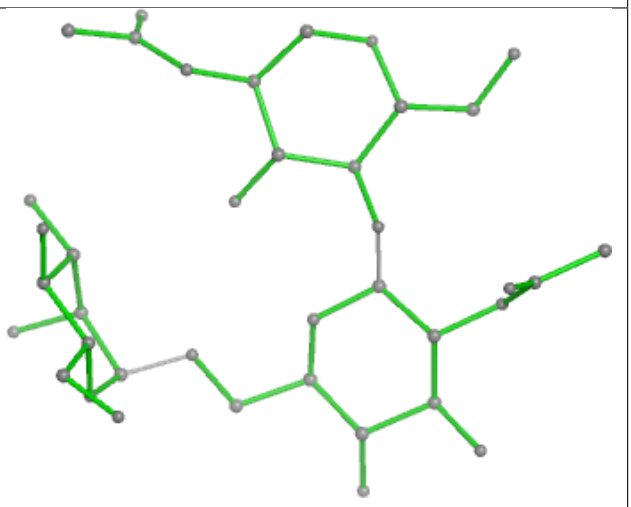


Rings

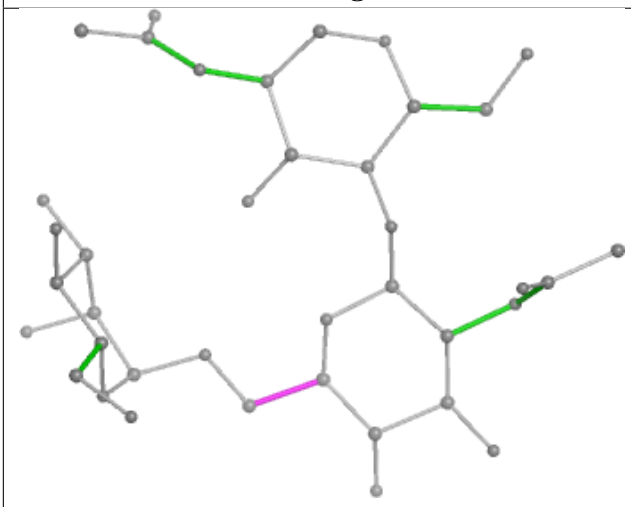
Oligosaccharide Chain 2



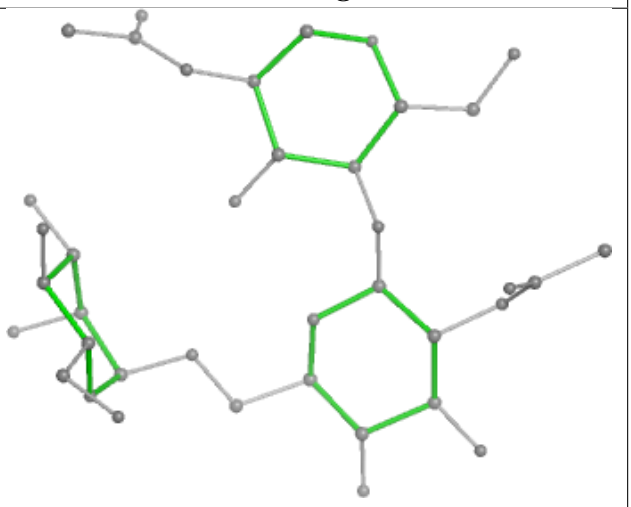
Bond lengths



Bond angles

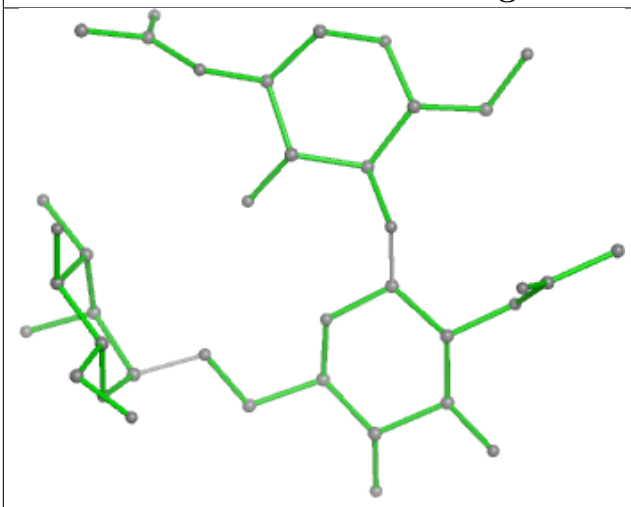


Torsions

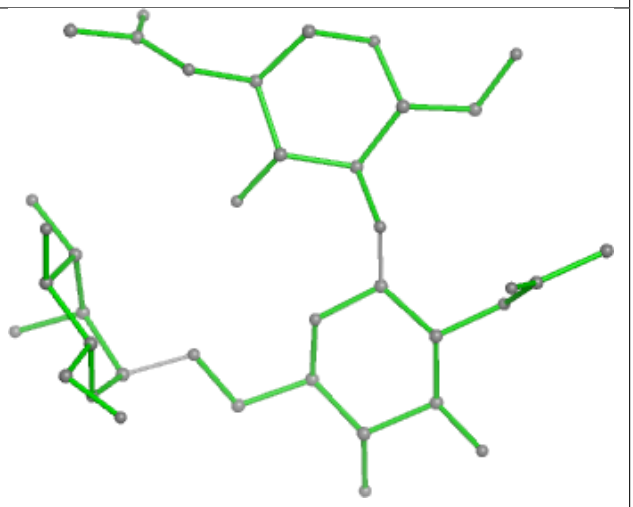


Rings

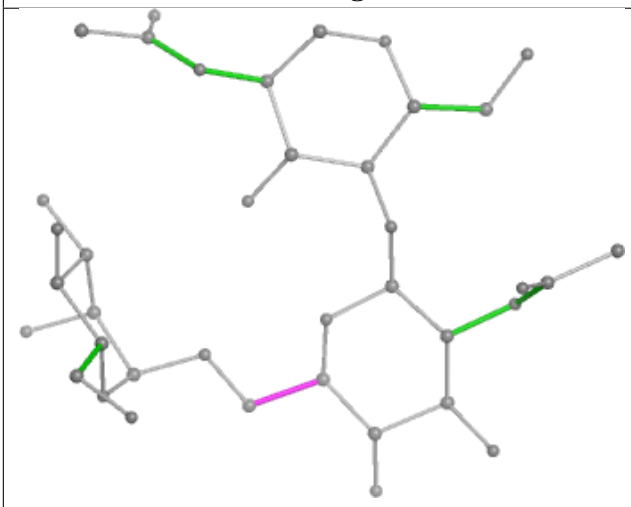
Oligosaccharide Chain 5



Bond lengths



Bond angles



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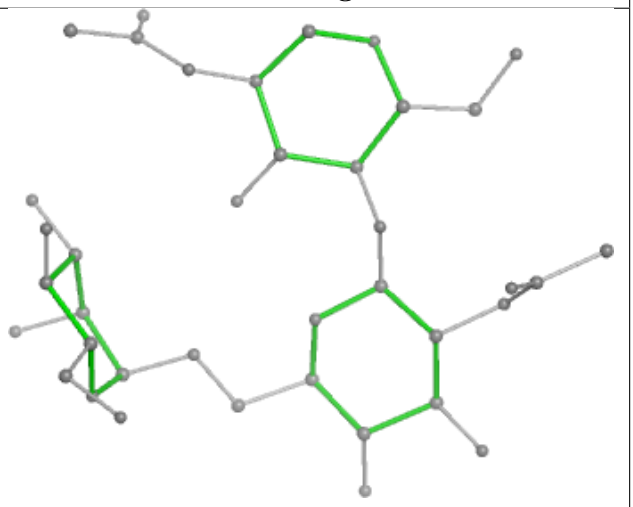
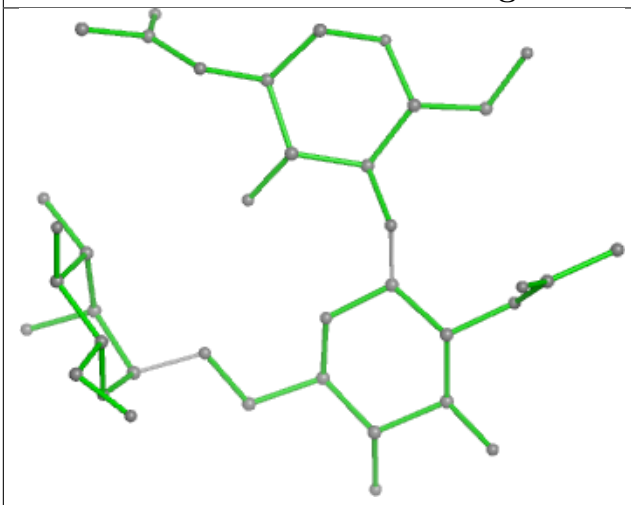


Rings

Oligosaccharide Chain 8



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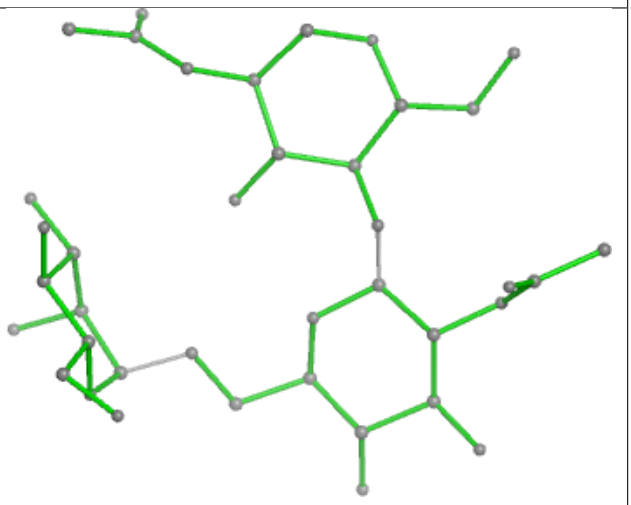
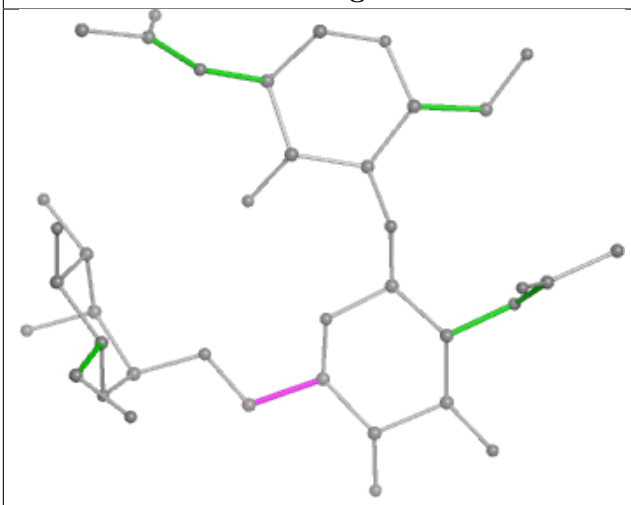


Bond angles



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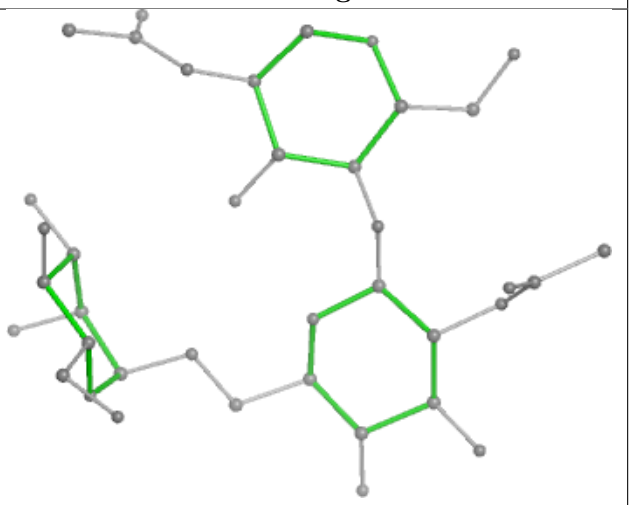
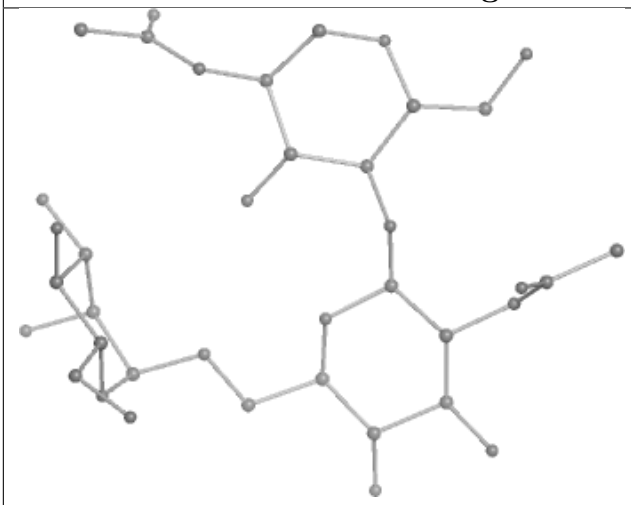


Rings

Oligosaccharide Chain BA



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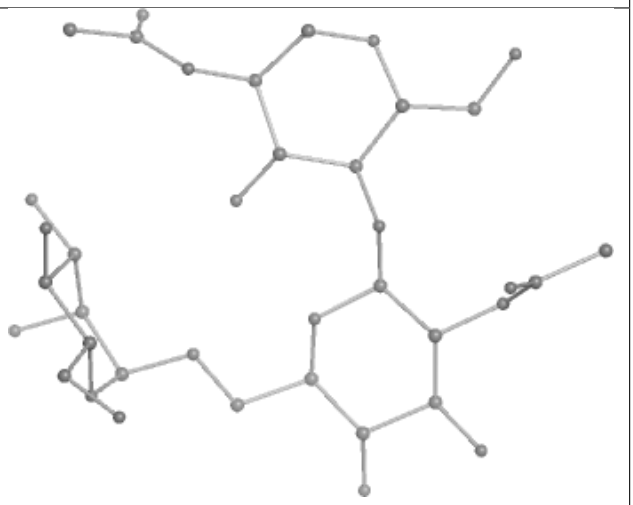
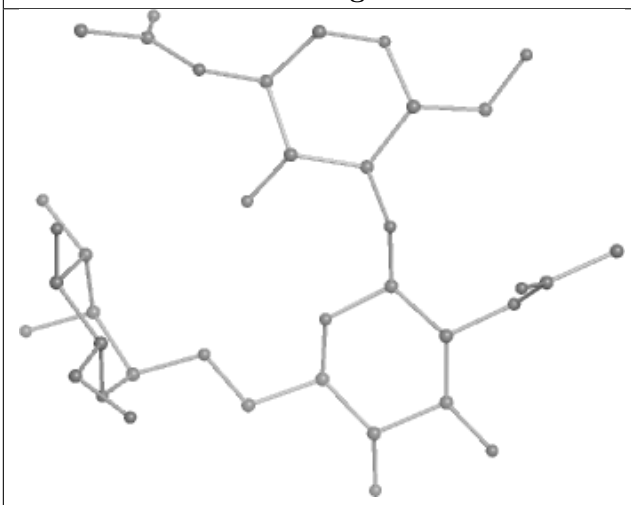


Bond angles



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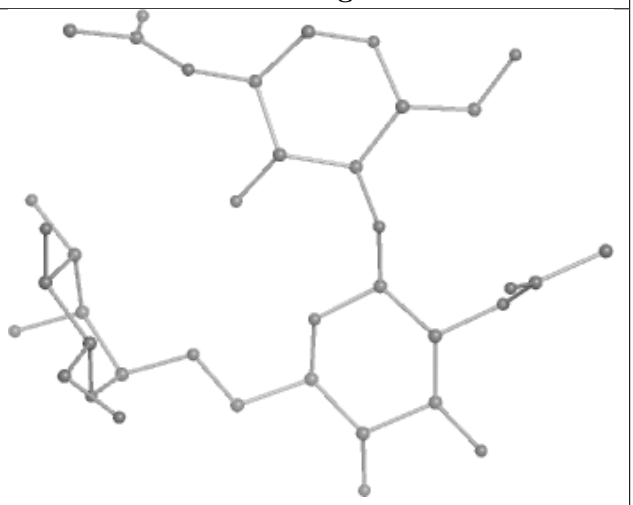
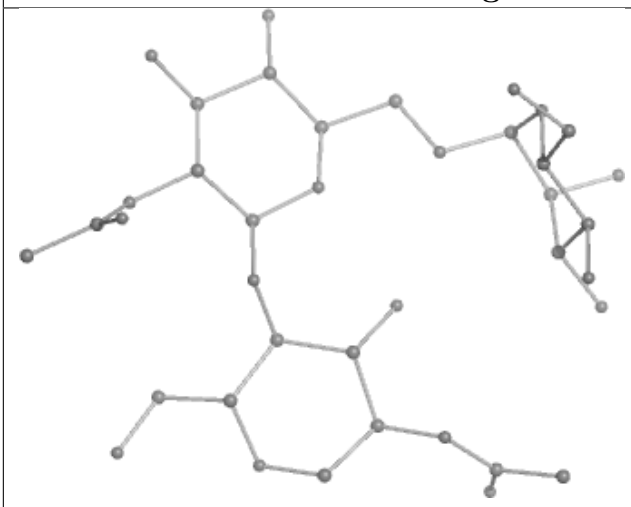


Rings

Oligosaccharide Chain EA



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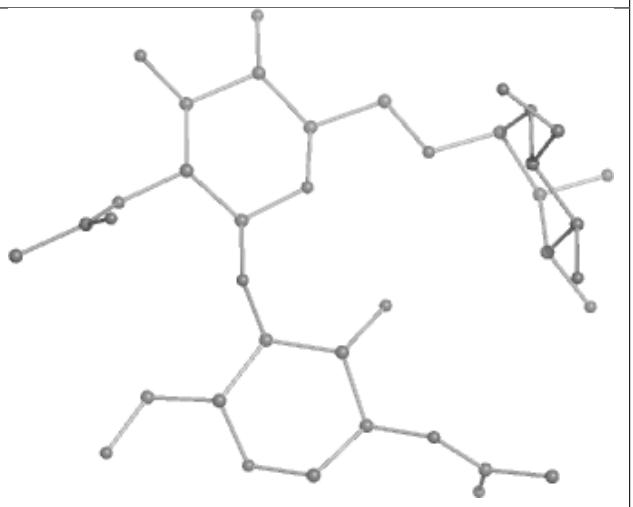
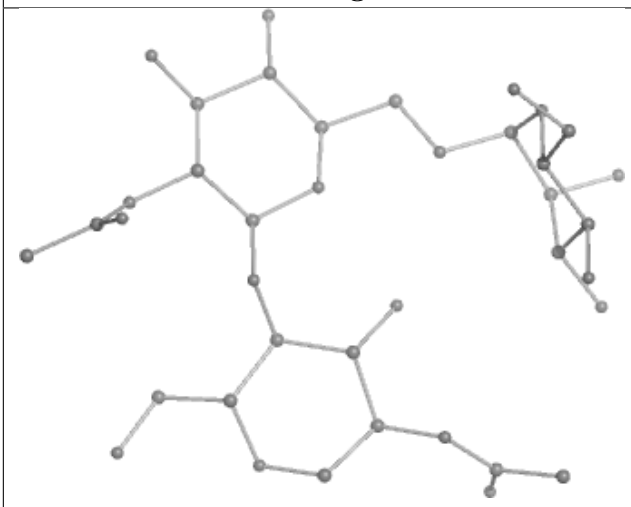


Bond angles



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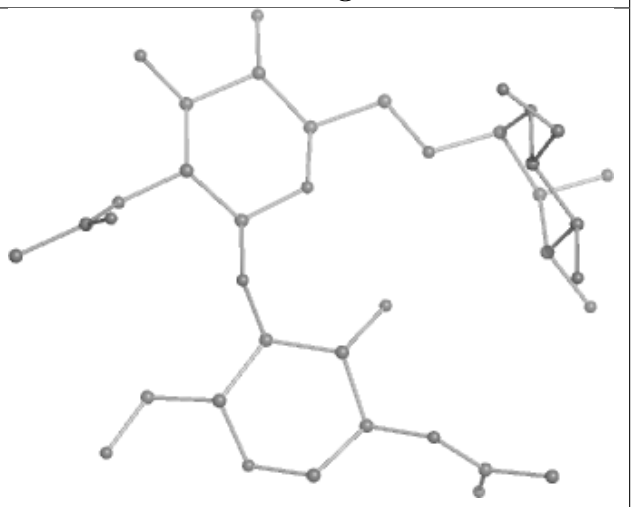
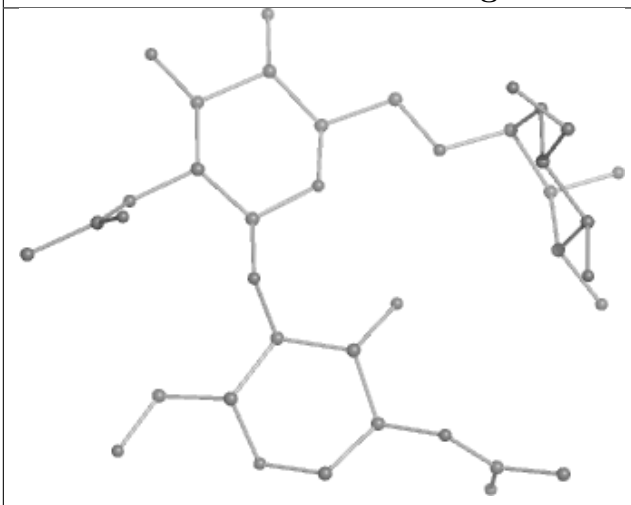
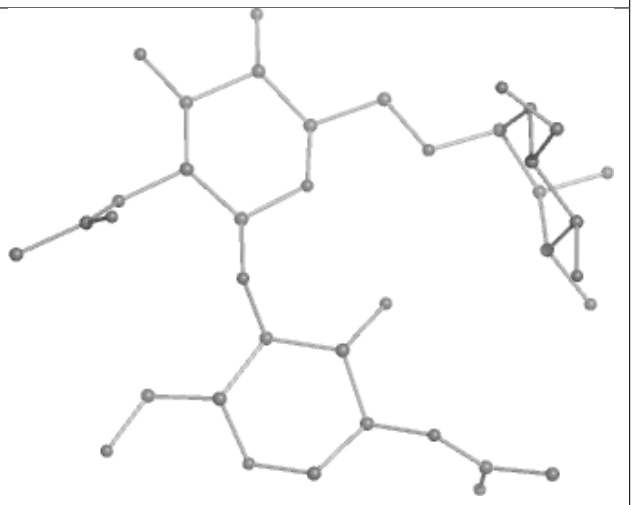


Rings

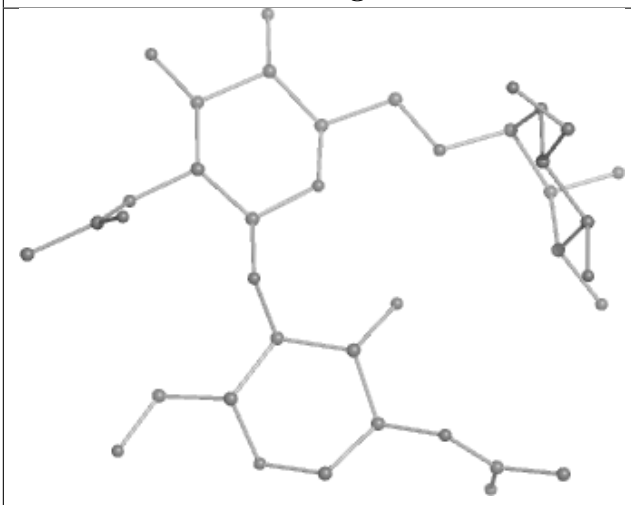
Oligosaccharide Chain HA



Bond lengths



Bond angles



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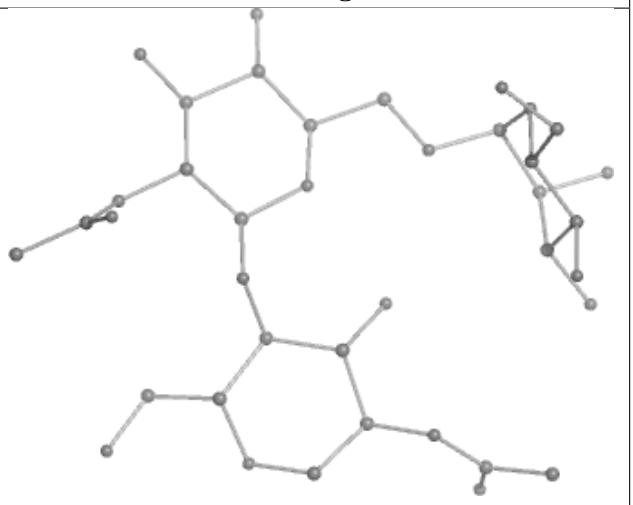
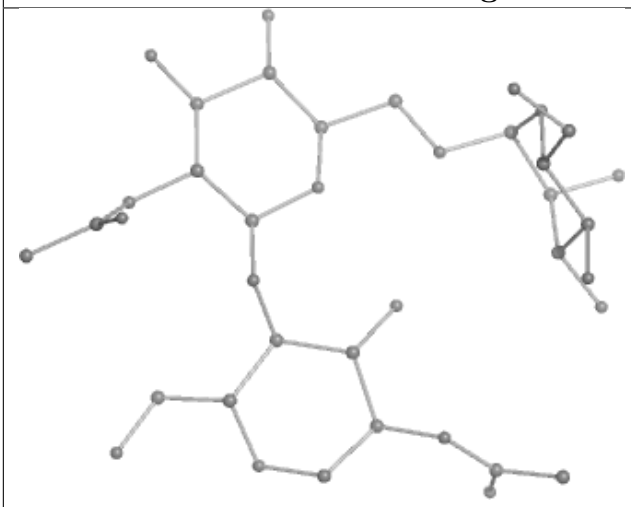


Rings

Oligosaccharide Chain KA



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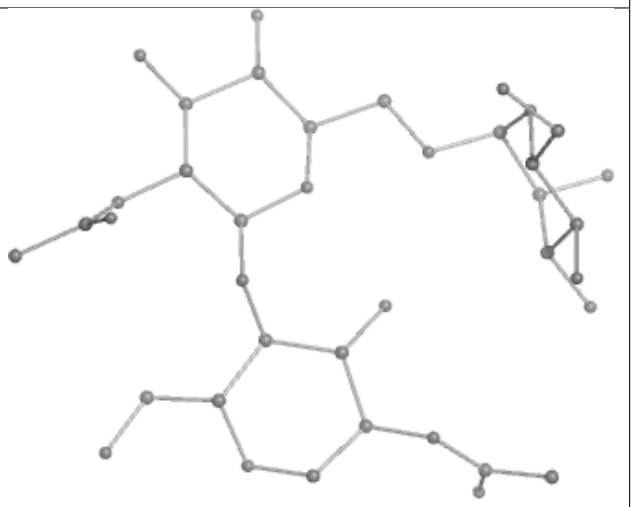
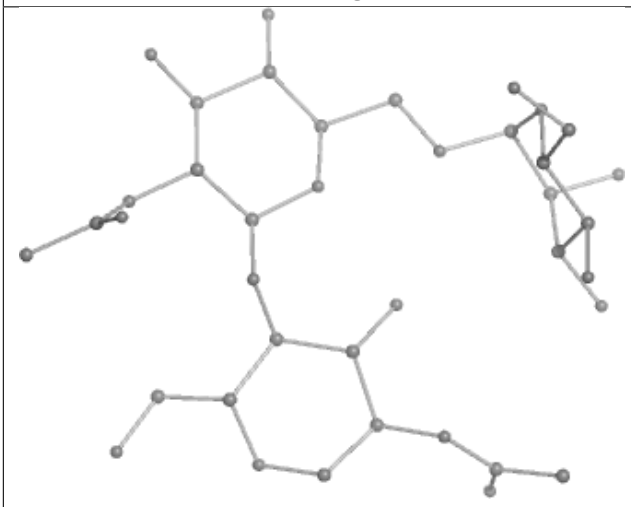


Bond angles



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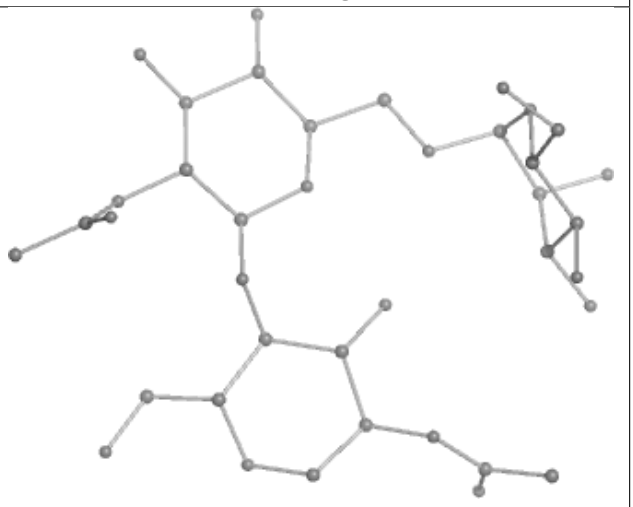
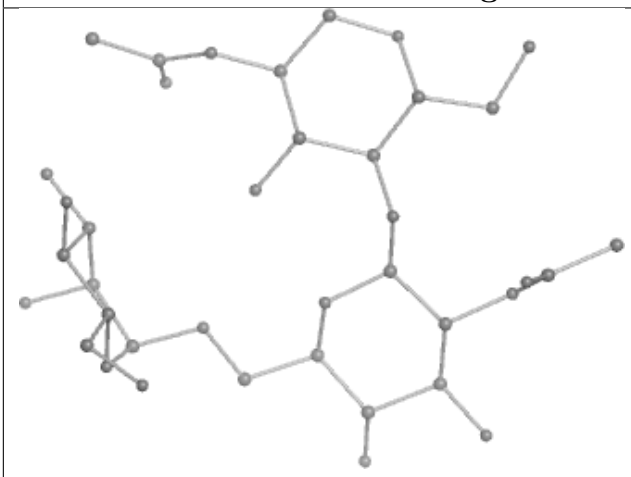


Rings

Oligosaccharide Chain NA



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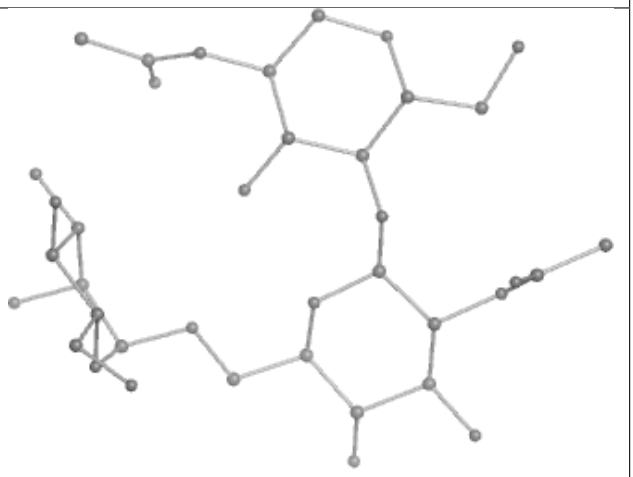
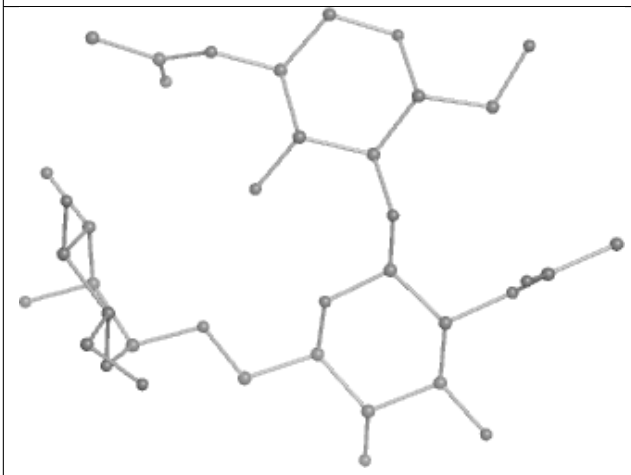


Bond angles



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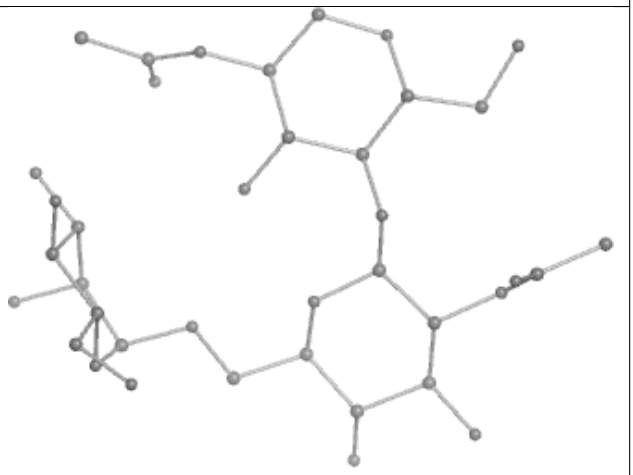
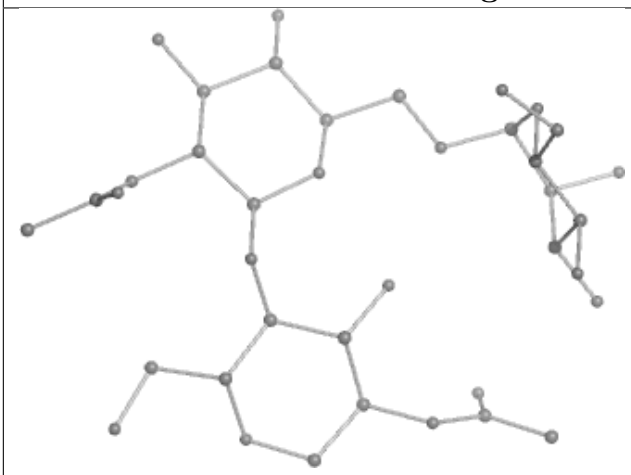


Rings

Oligosaccharide Chain QA



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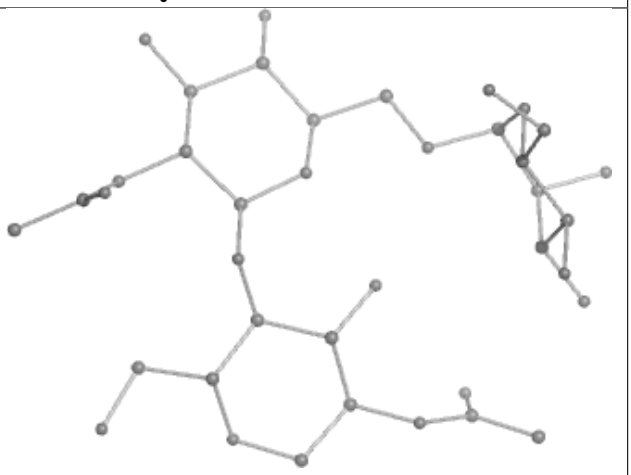
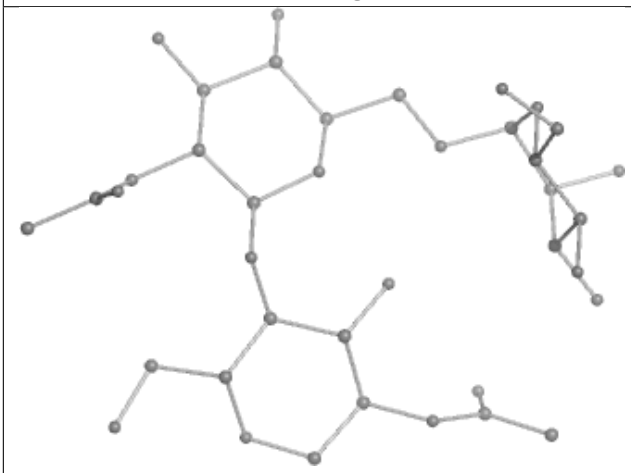


Bond angles



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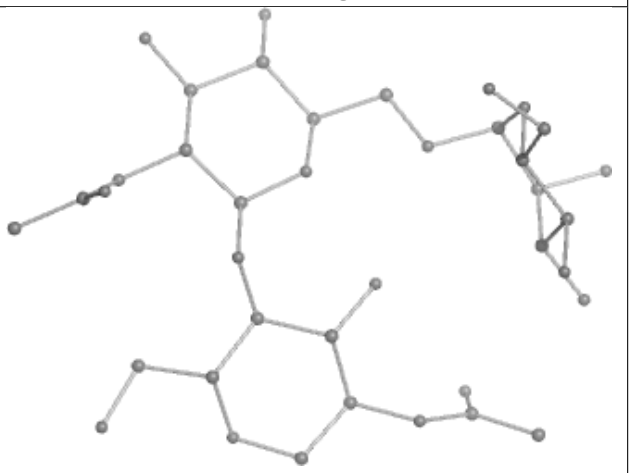
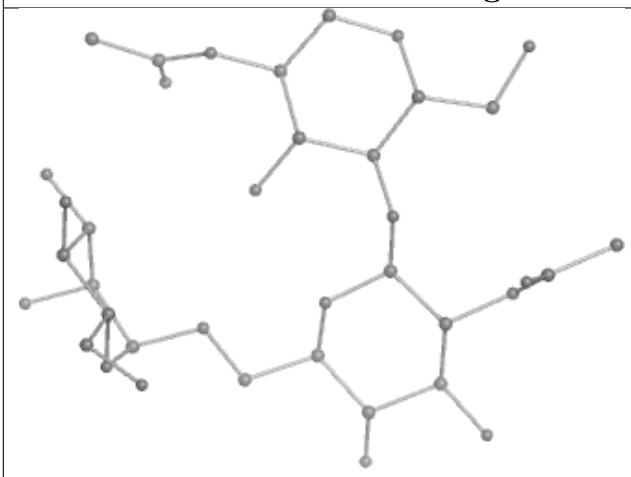


Rings

Oligosaccharide Chain TA



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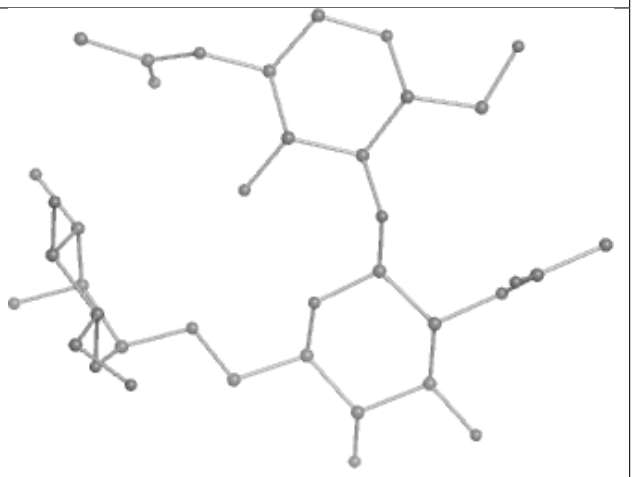
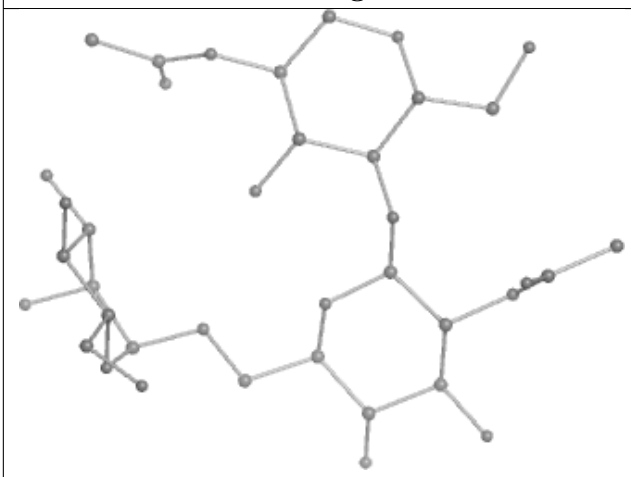


Bond angles



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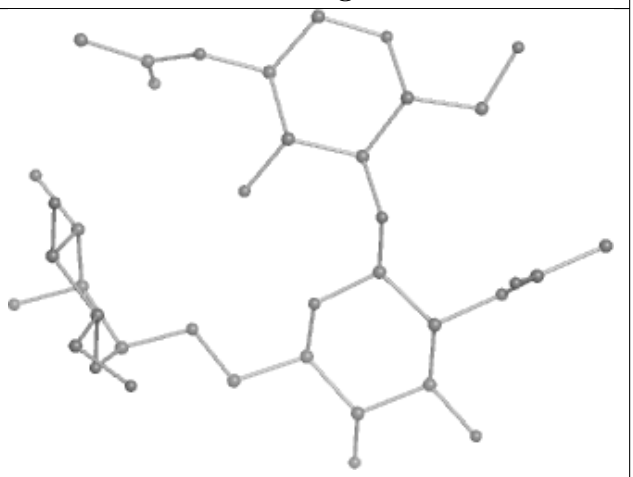
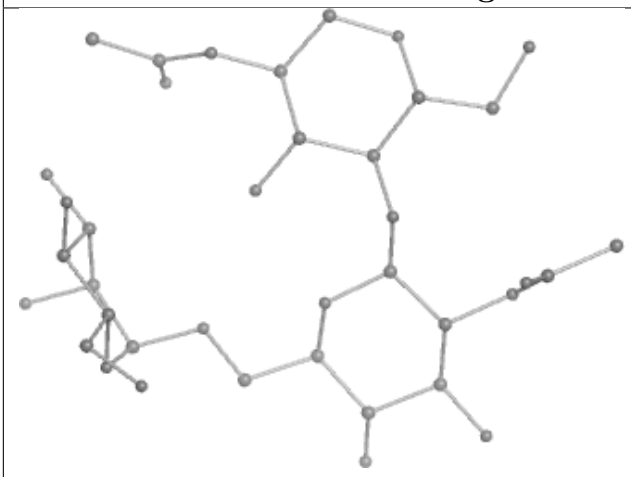


Rings

Oligosaccharide Chain WA



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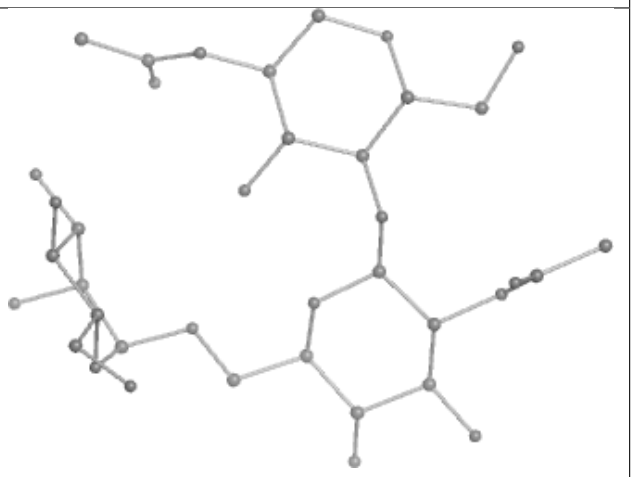
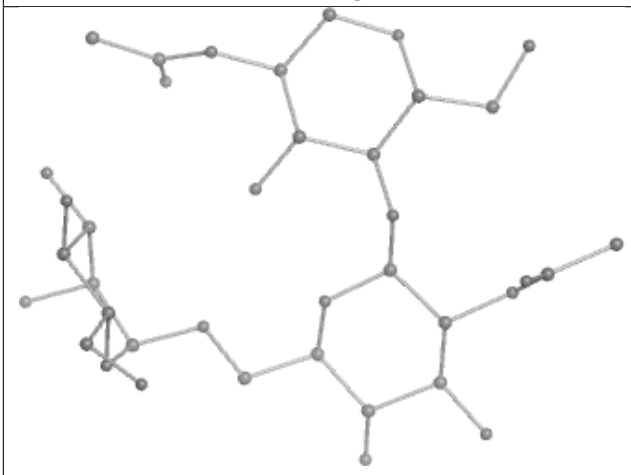


Bond angles



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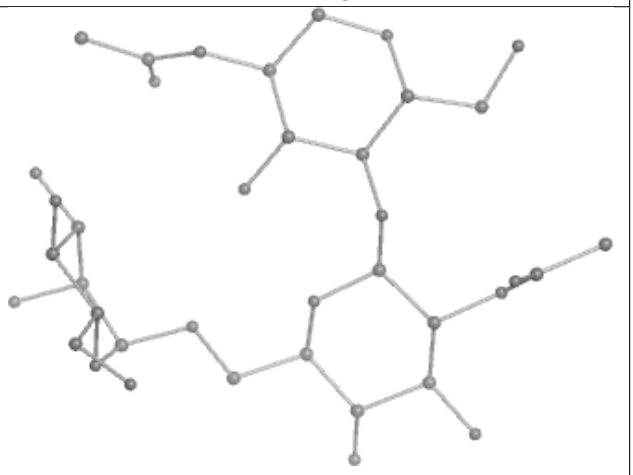
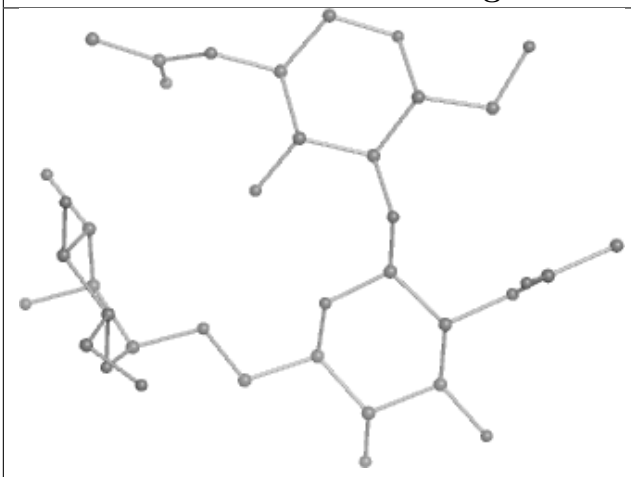


Rings

Oligosaccharide Chain ZA



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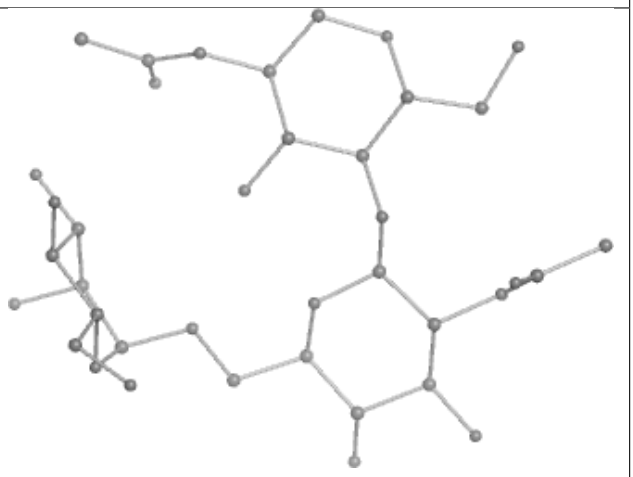
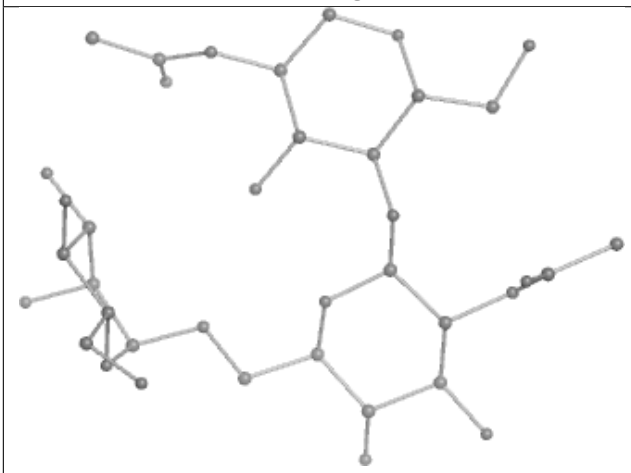


Bond angles



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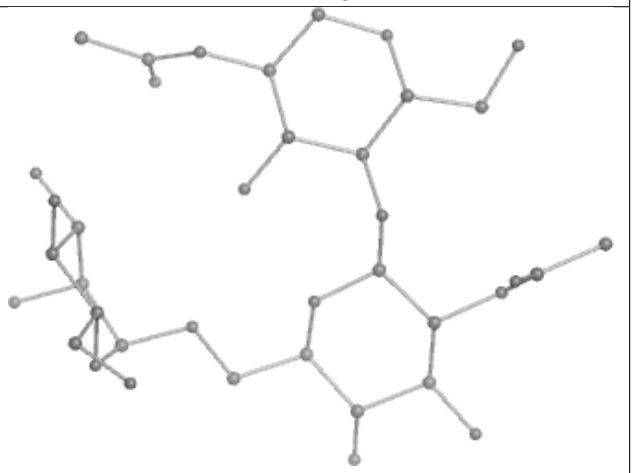
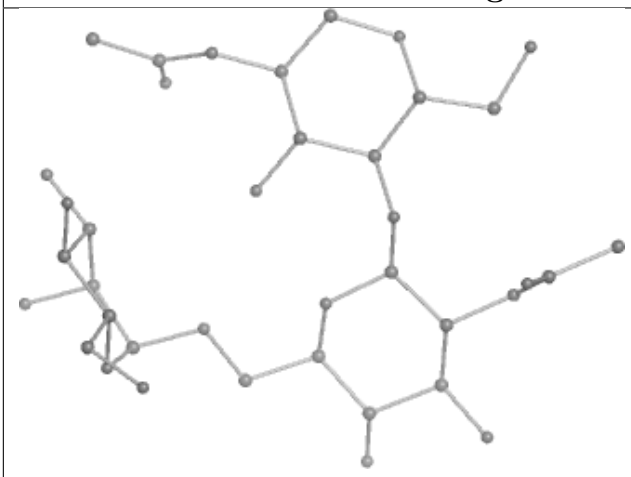


Rings

Oligosaccharide Chain cA



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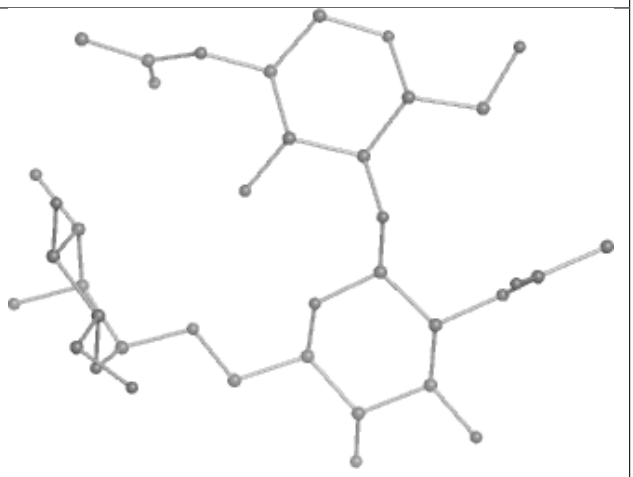
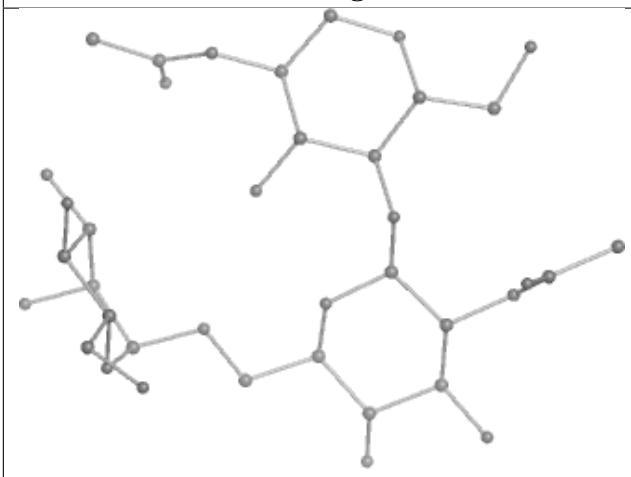


Bond angles



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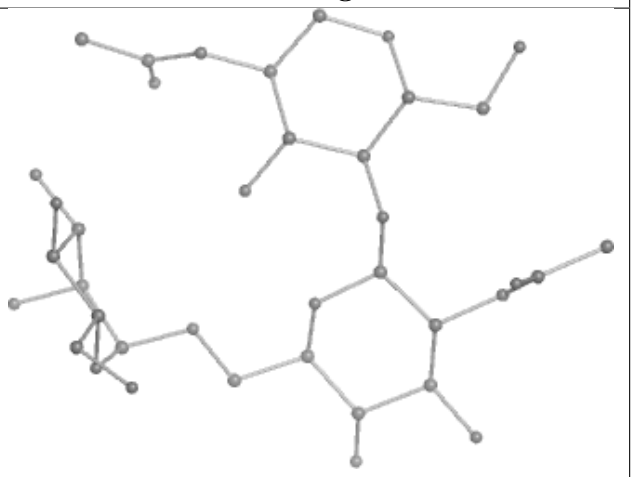
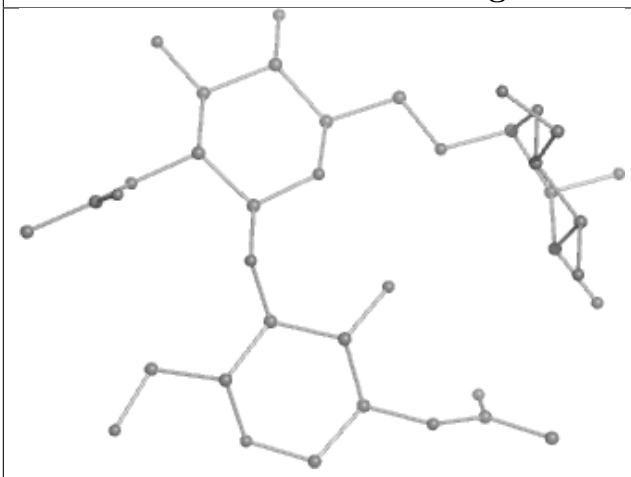


Rings

Oligosaccharide Chain fA



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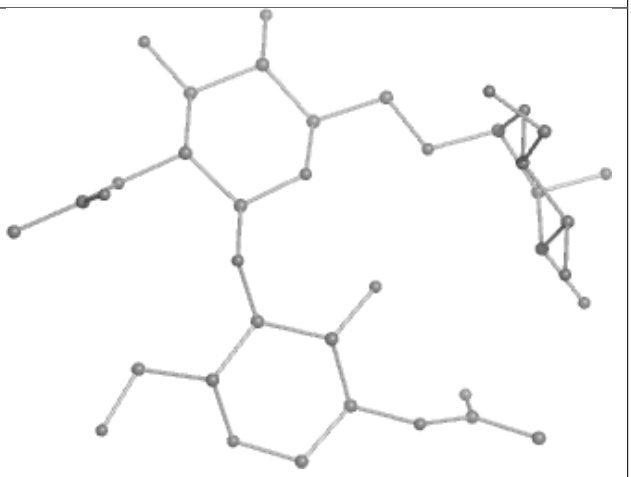
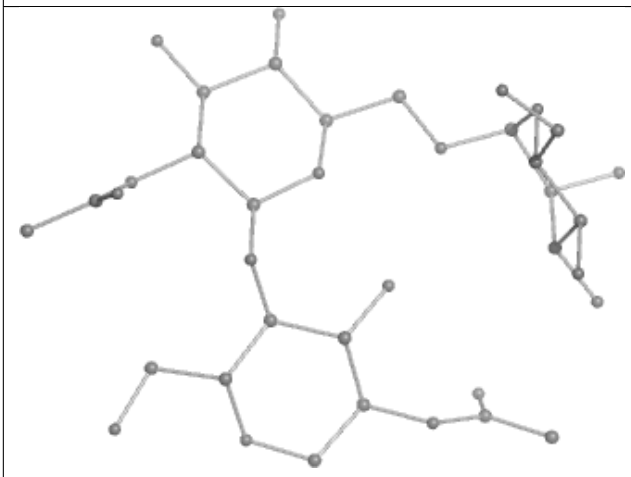
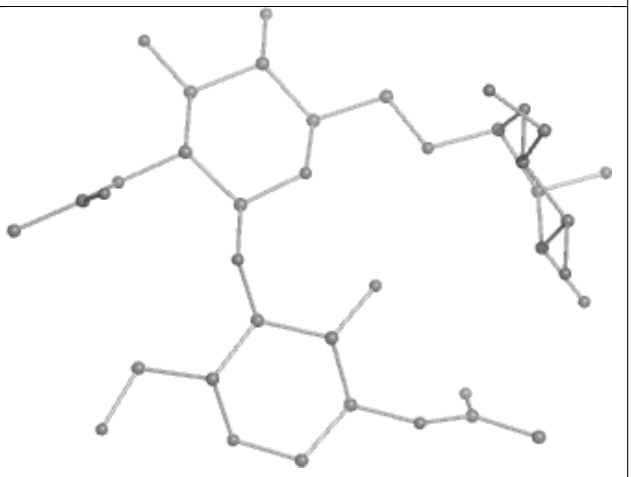


Bond angles

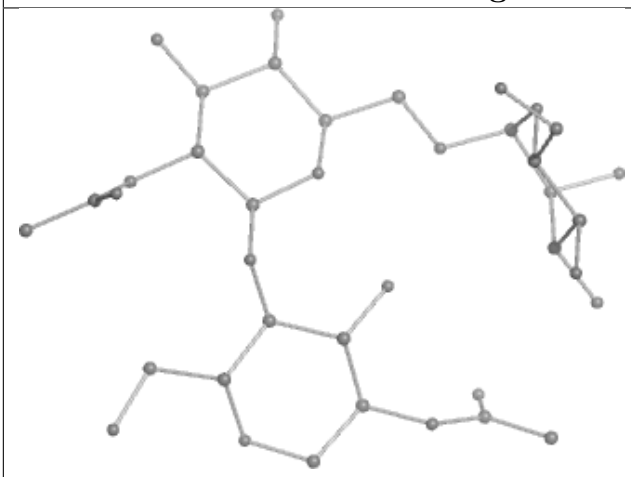


Torsions

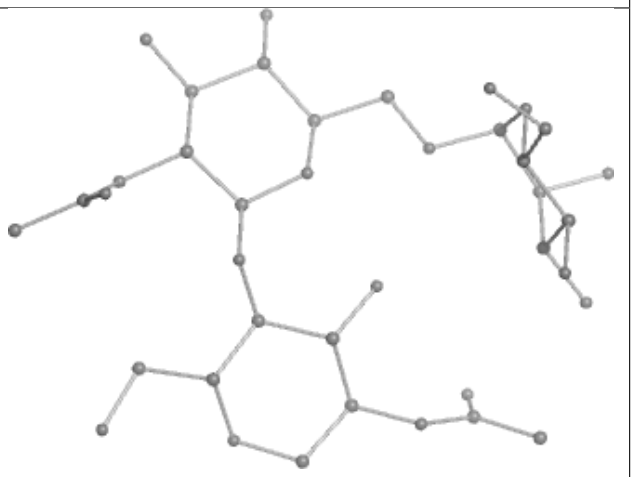


Rings

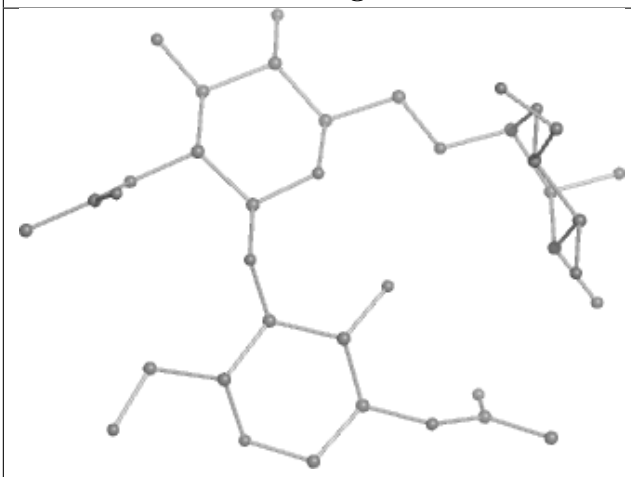
Oligosaccharide Chain iA



Bond lengths



Bond angles



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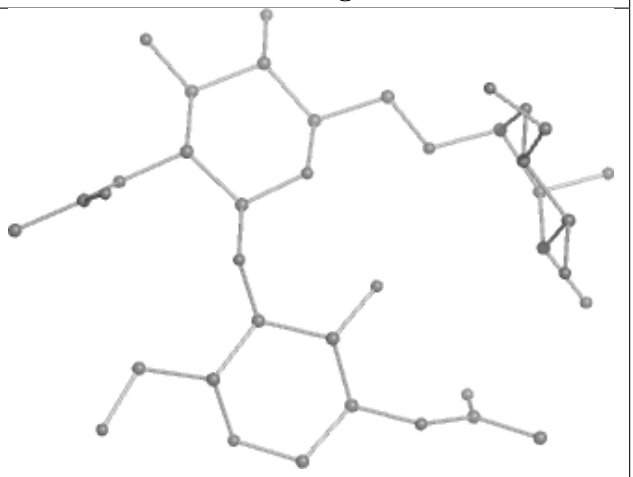
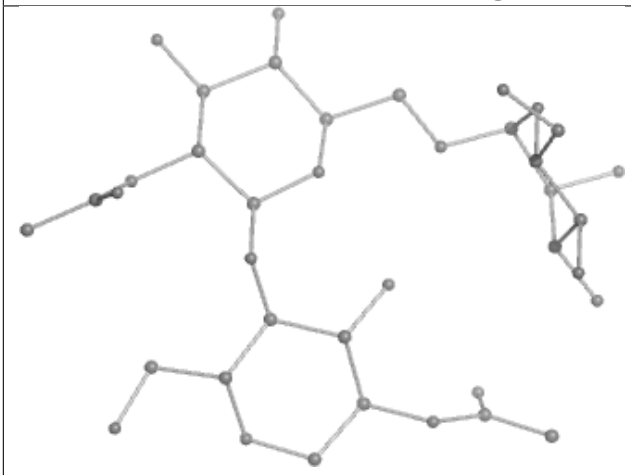
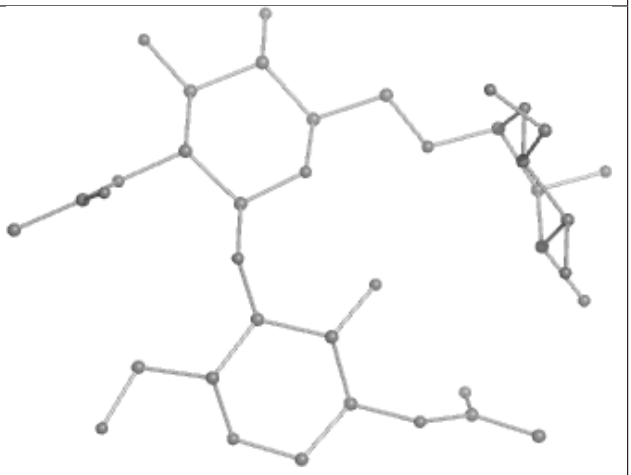


Rings

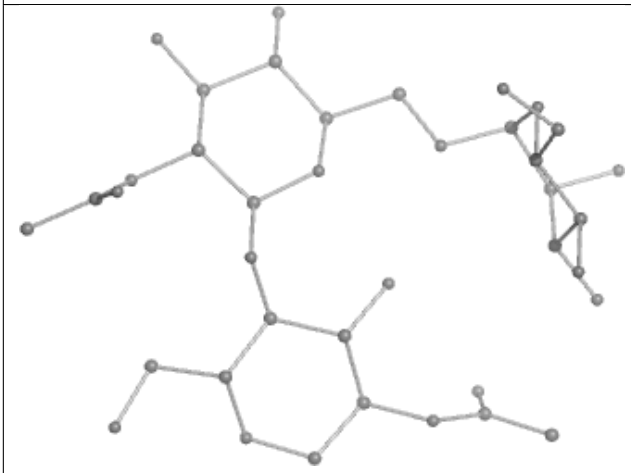
Oligosaccharide Chain lA



Bond lengths



Bond angles



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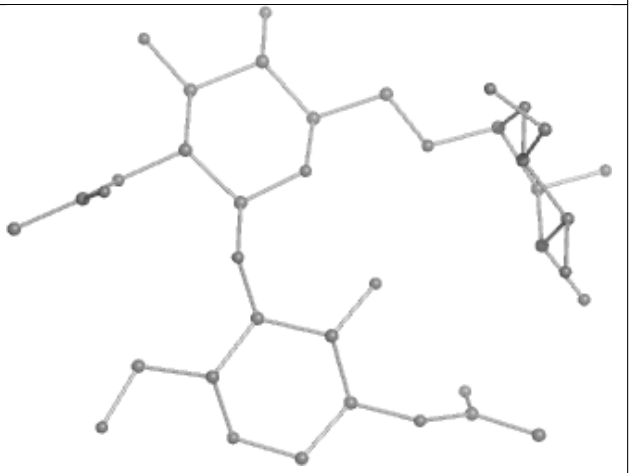
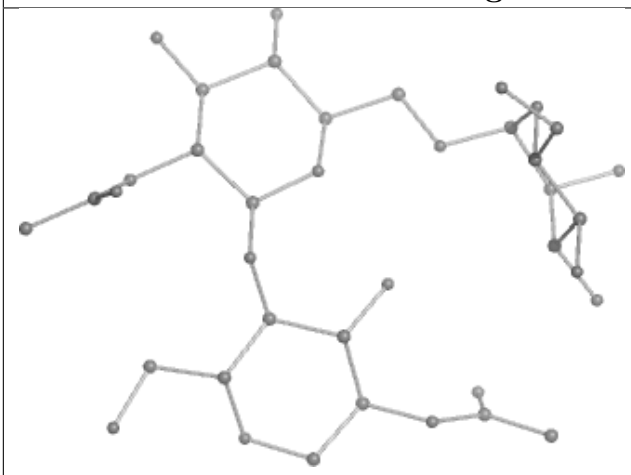
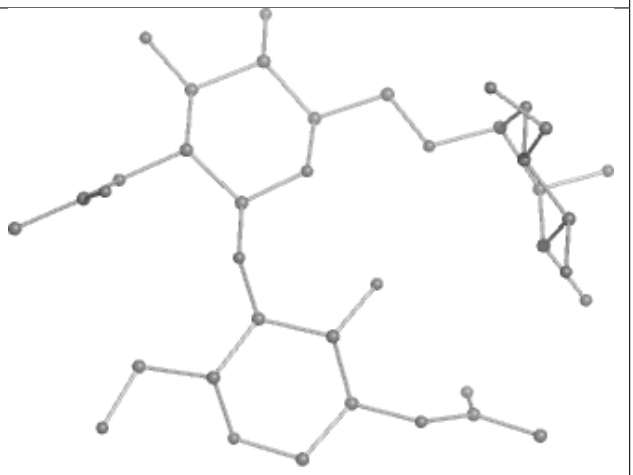


Rings

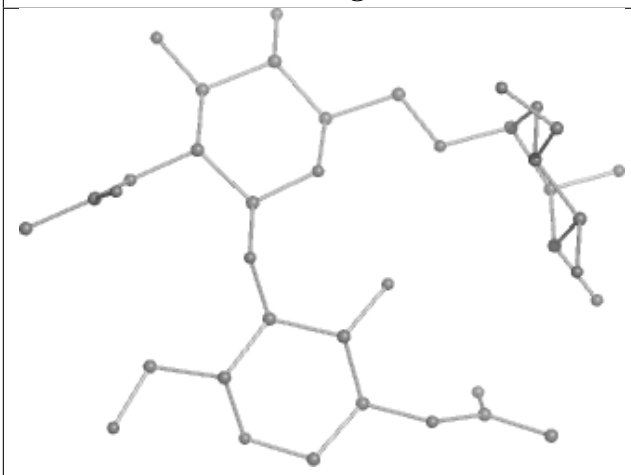
Oligosaccharide Chain oA



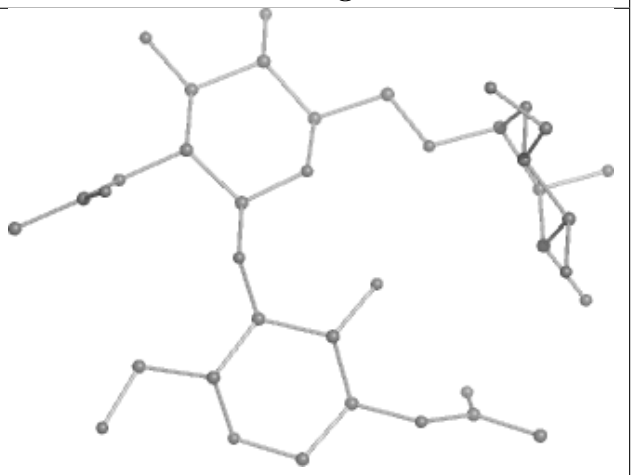
Bond lengths



Bond angles

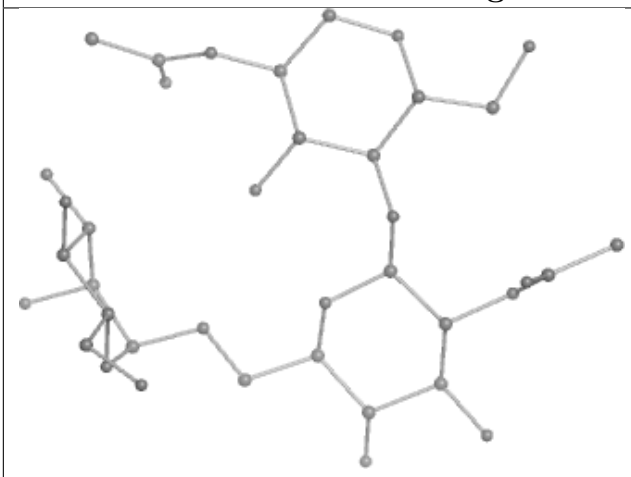


Torsions



Rings

Oligosaccharide Chain rA



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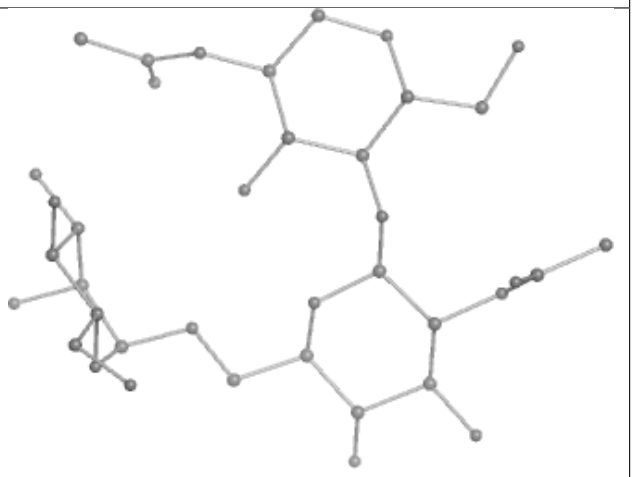
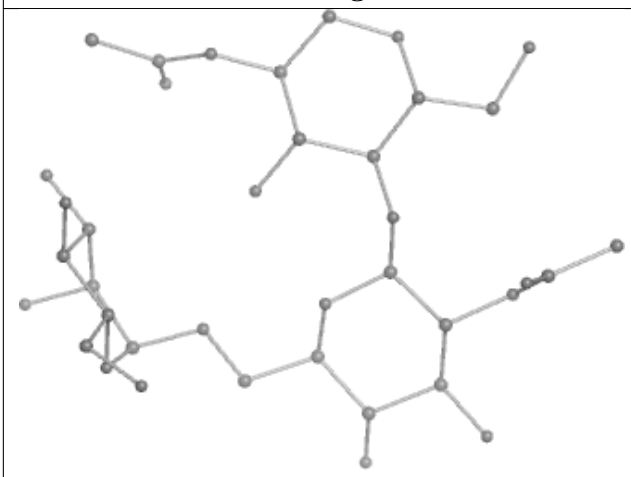
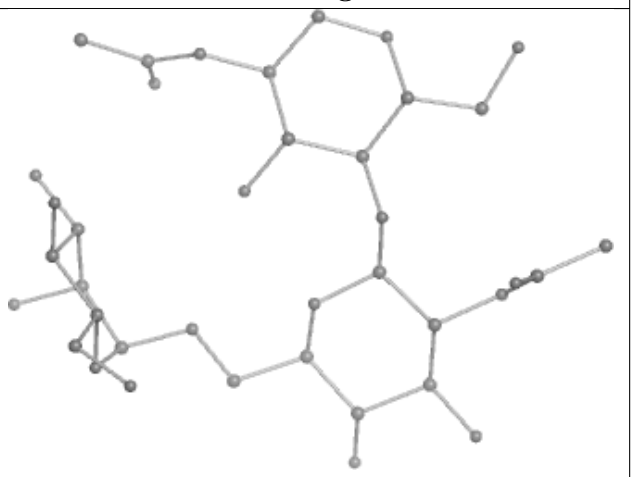


Bond angles

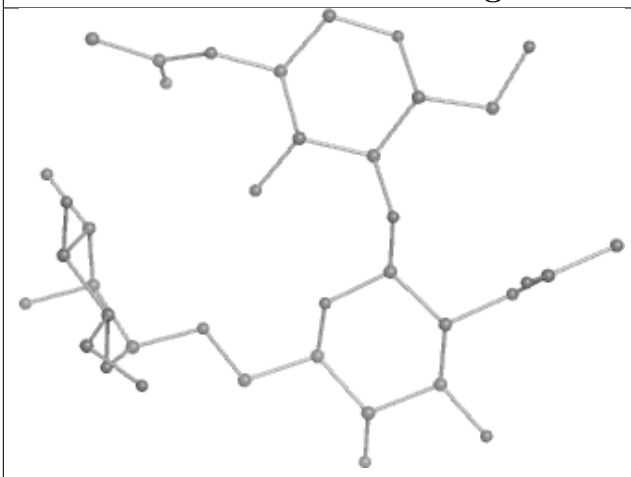


Torsions



Rings

Oligosaccharide Chain uA



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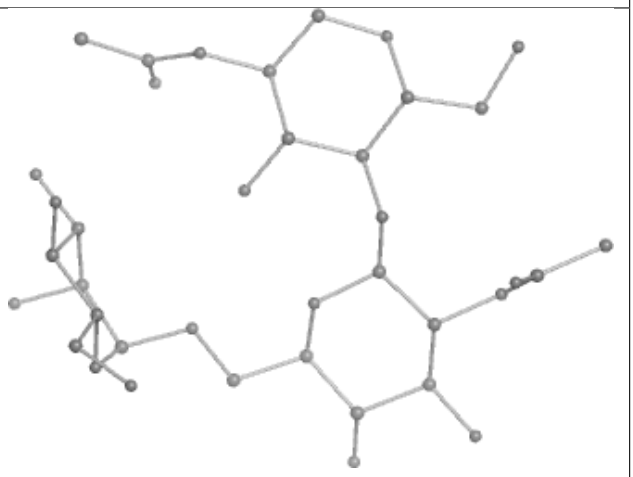
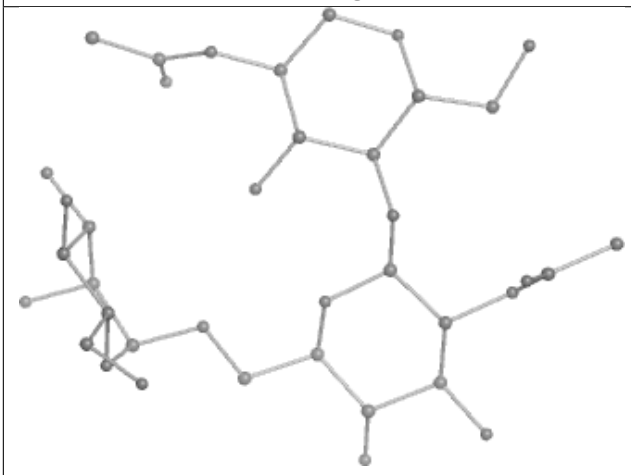
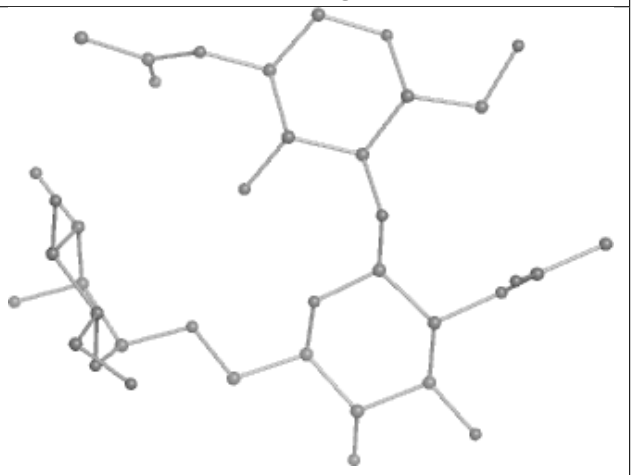


Bond angles

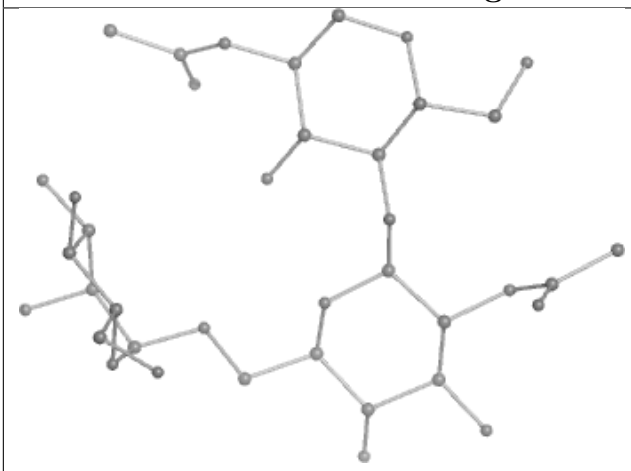


Torsions



Rings

Oligosaccharide Chain xA



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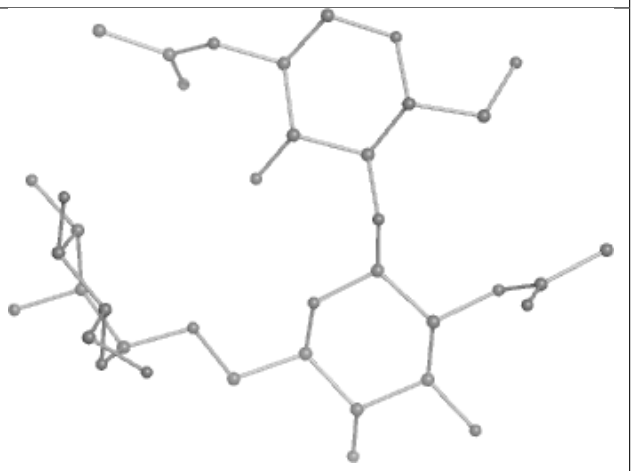
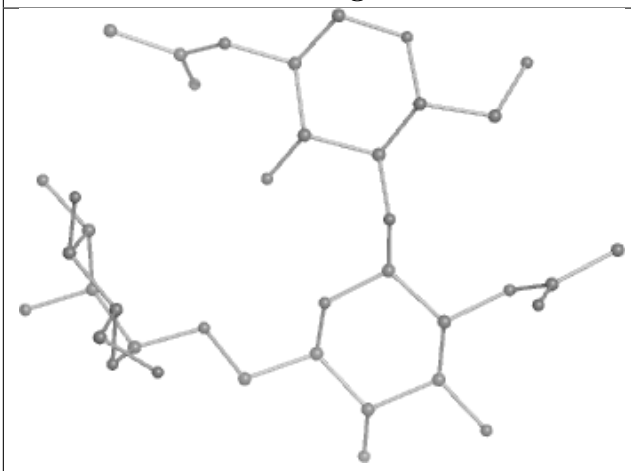
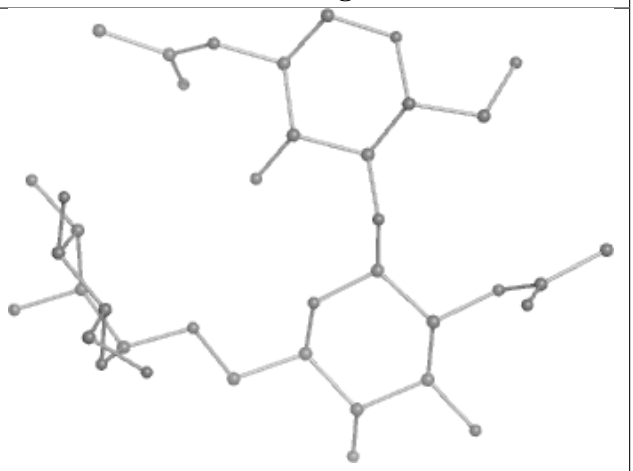


Bond angles

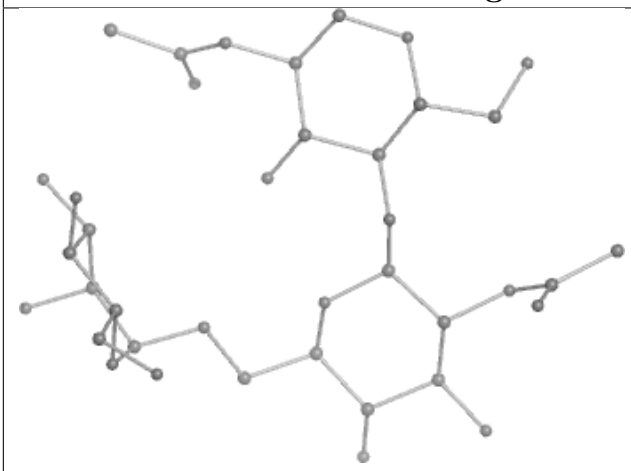


Torsions



Rings

Oligosaccharide Chain 0A



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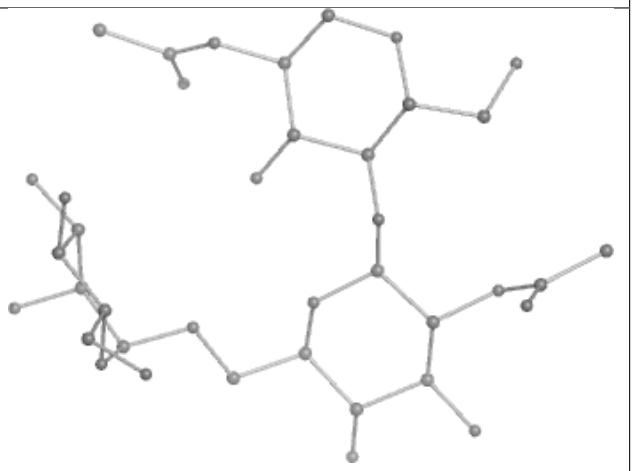
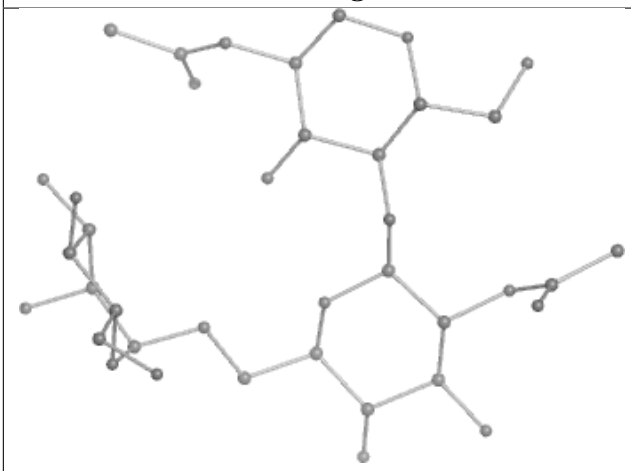


Bond angles



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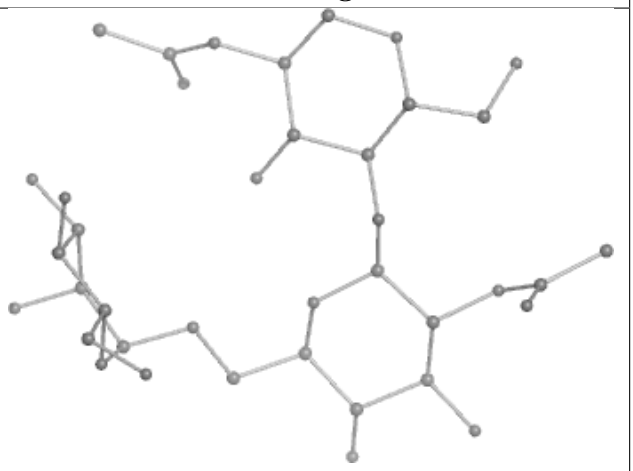
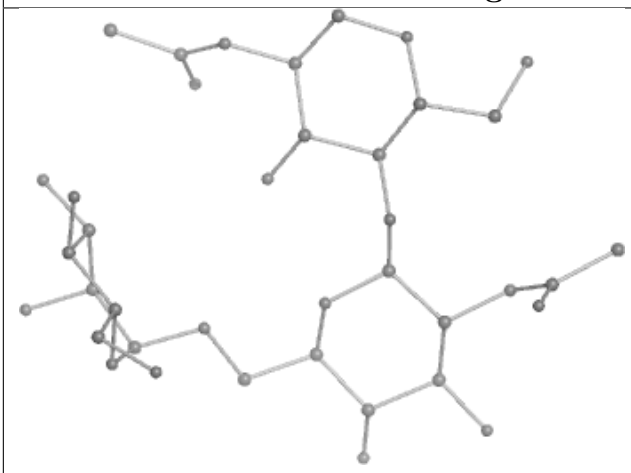


Rings

Oligosaccharide Chain 3A



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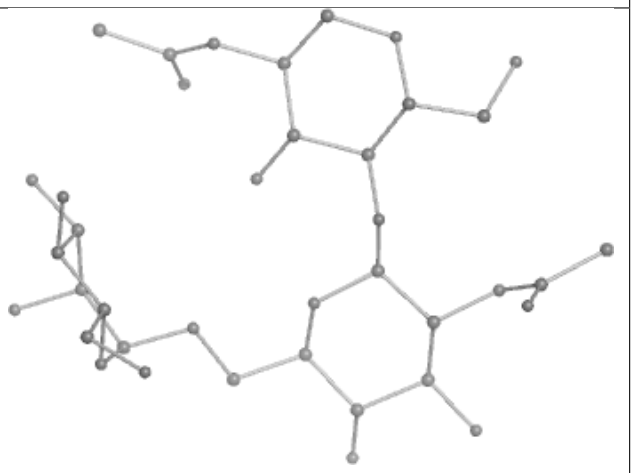
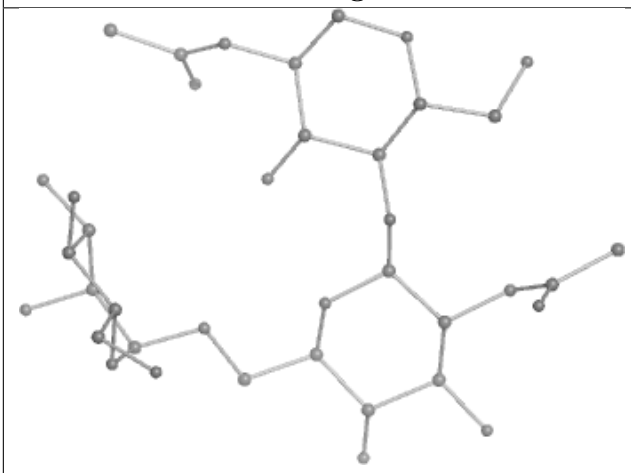


Bond angles



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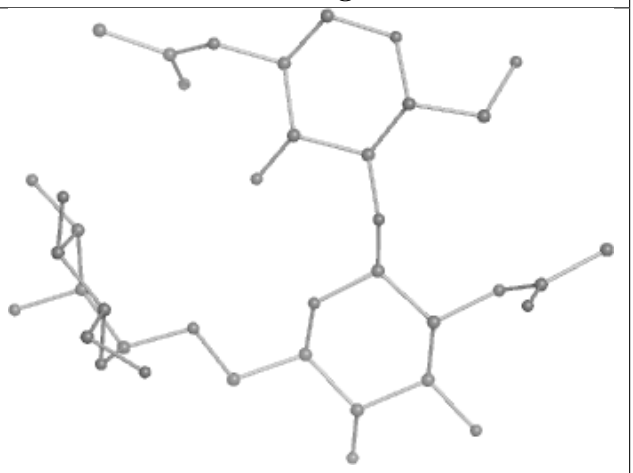
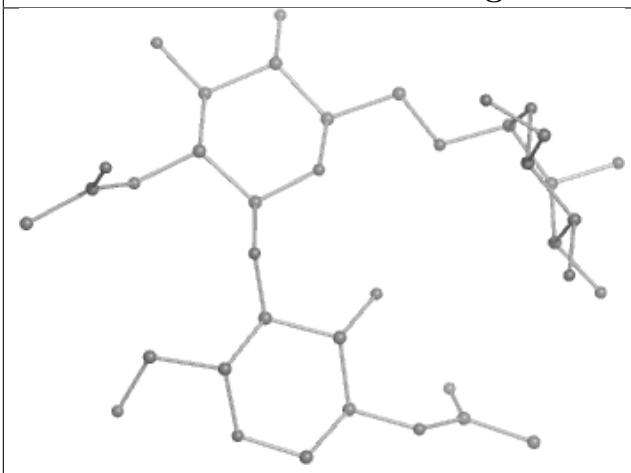


Rings

Oligosaccharide Chain 6A



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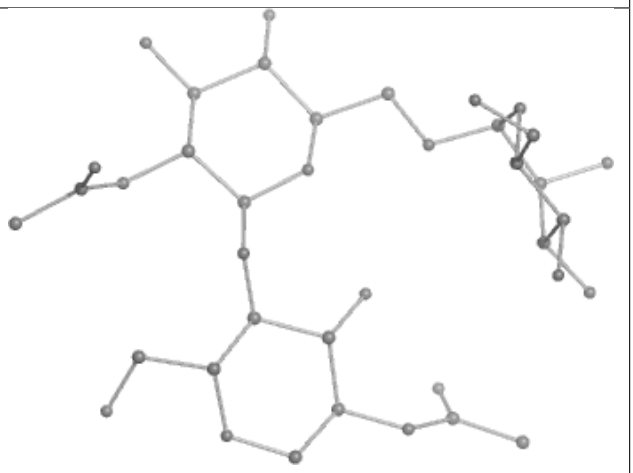
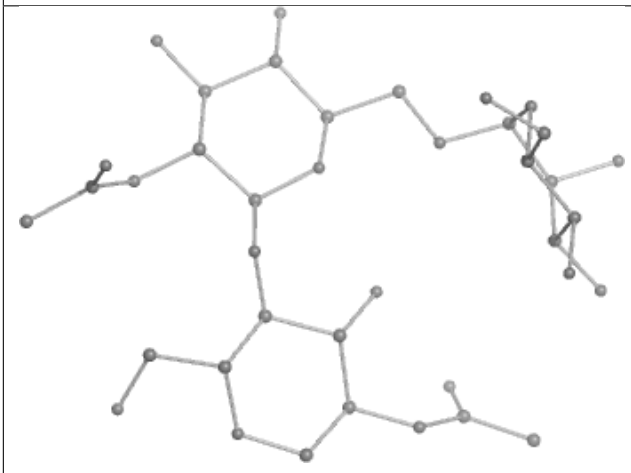


Bond angles



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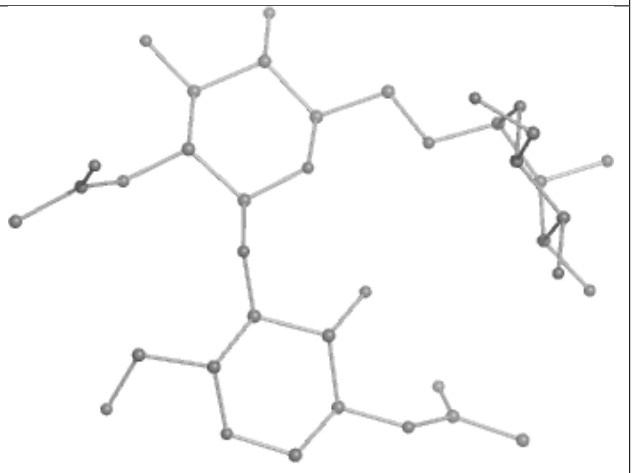
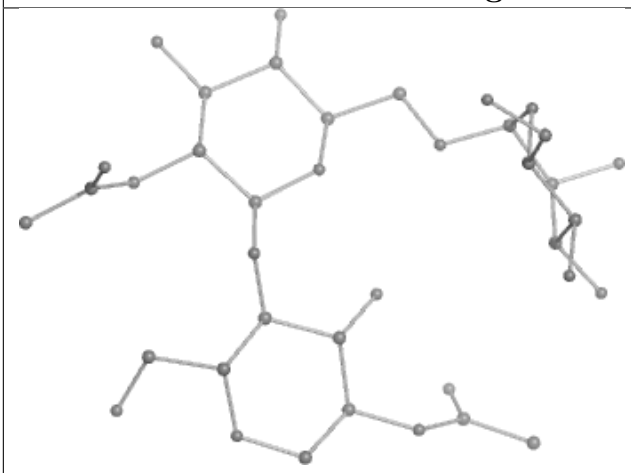


Rings

Oligosaccharide Chain 9A



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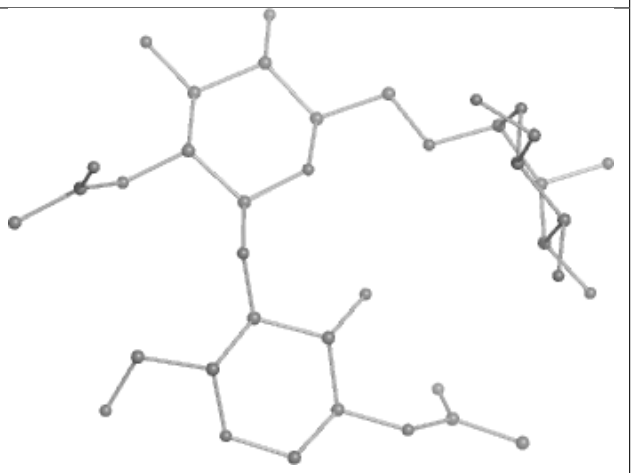
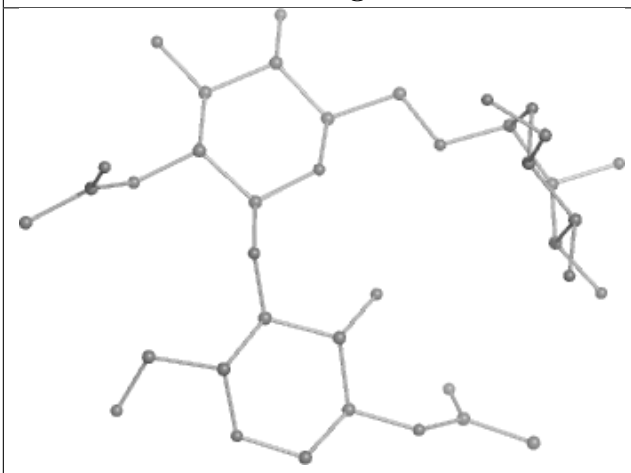


Bond angles



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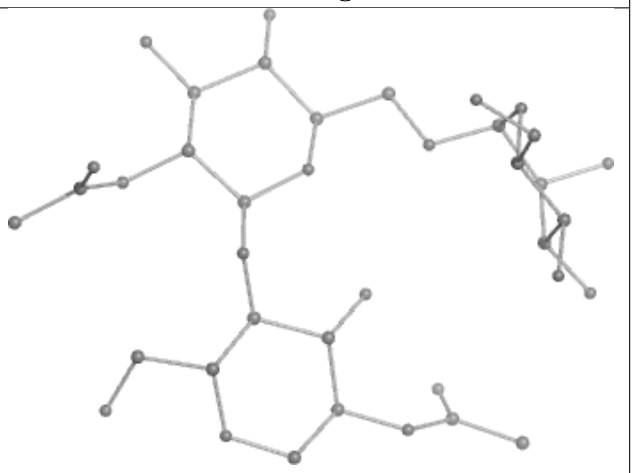
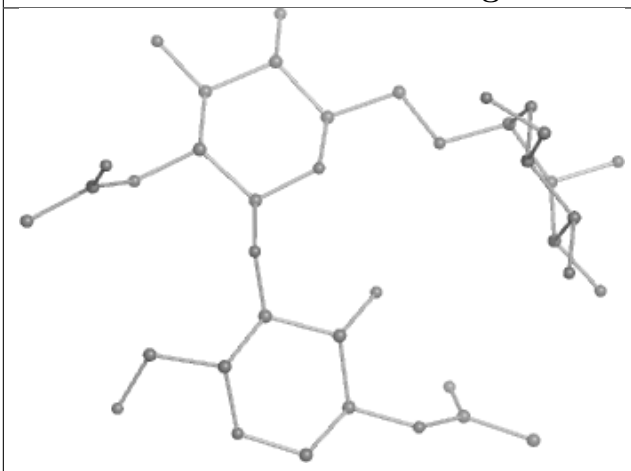


Rings

Oligosaccharide Chain CB



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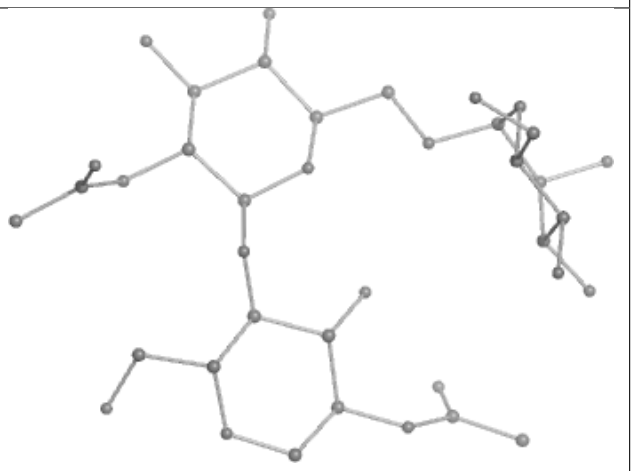
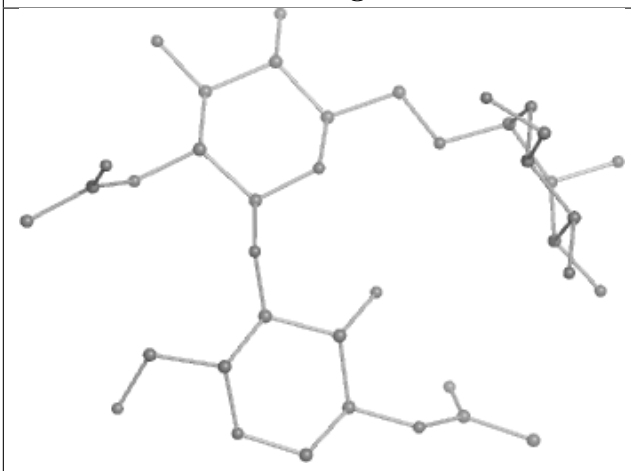
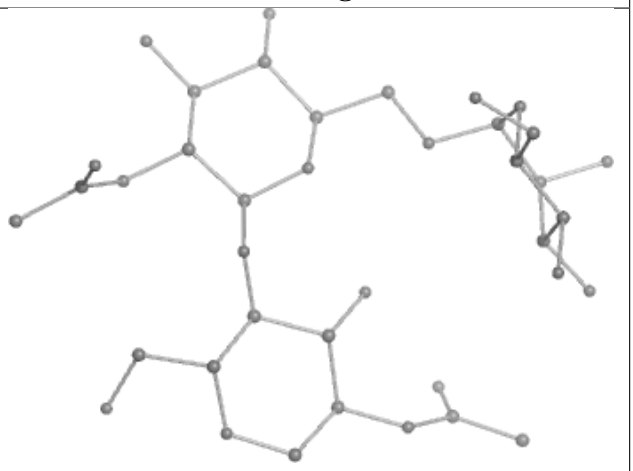


Bond angles

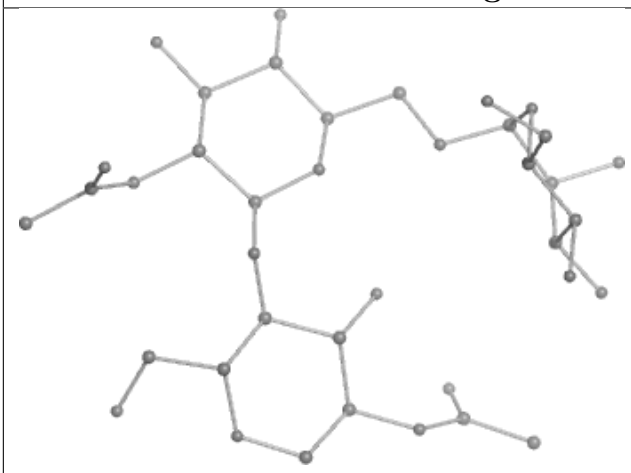


Torsions



Rings

Oligosaccharide Chain FB



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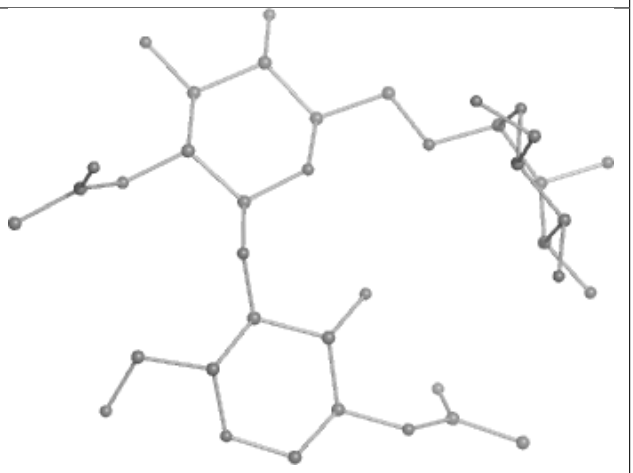
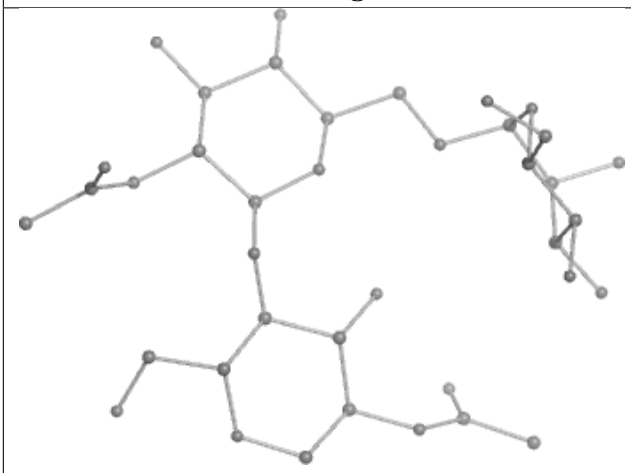
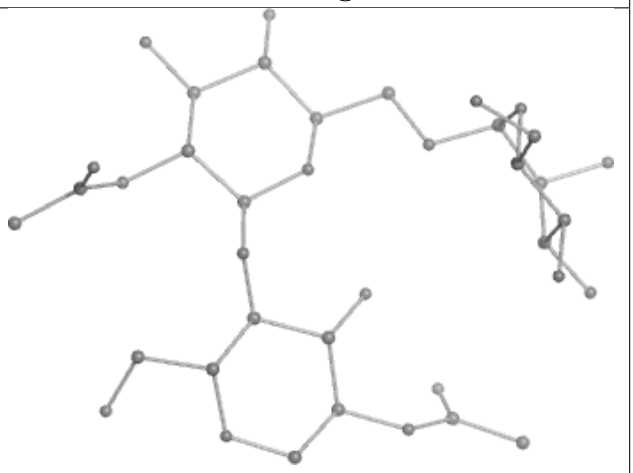


Bond angles

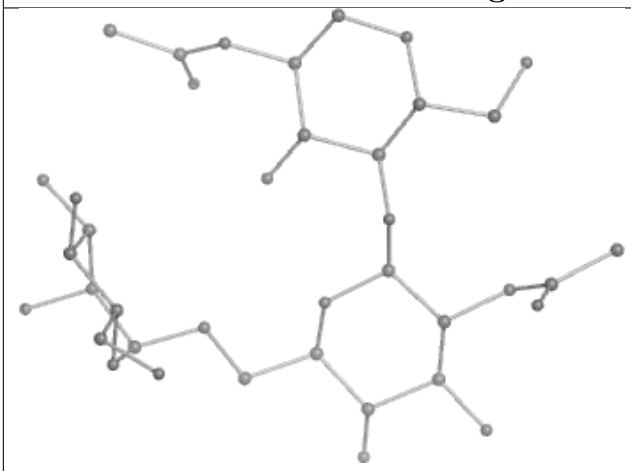


Torsions



Rings

Oligosaccharide Chain IB



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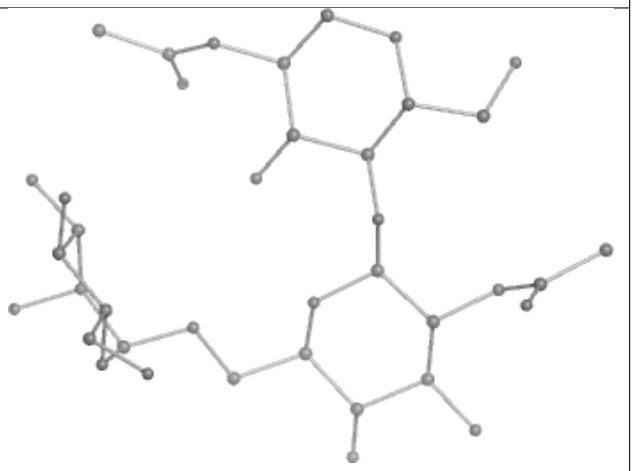
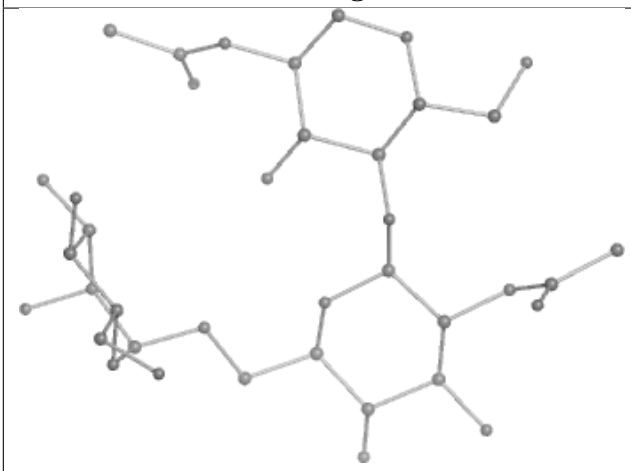
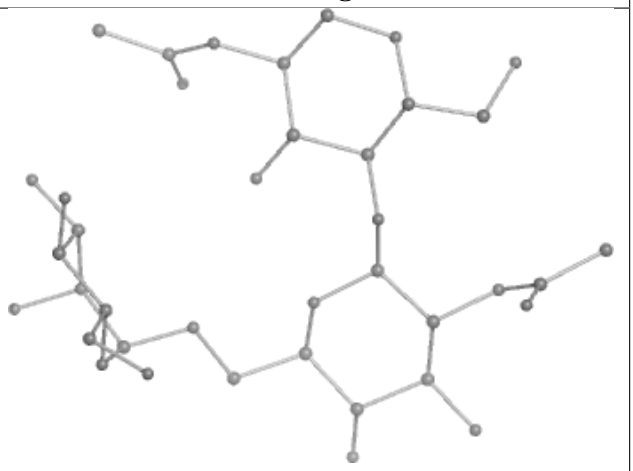


Bond angles

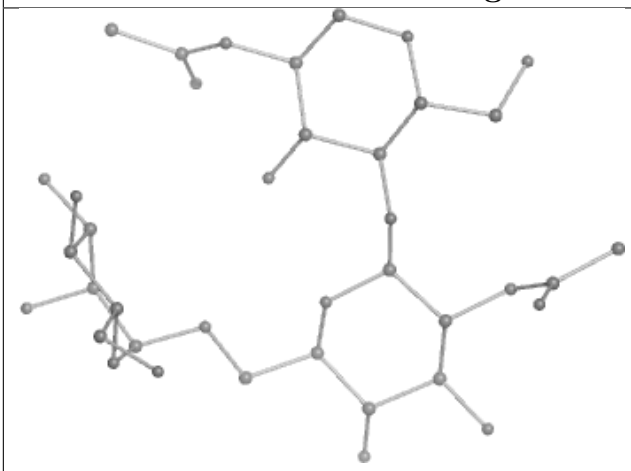


Torsions



Rings

Oligosaccharide Chain LB



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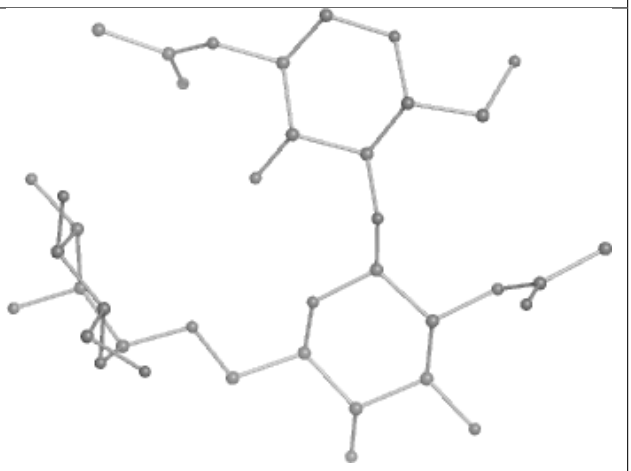
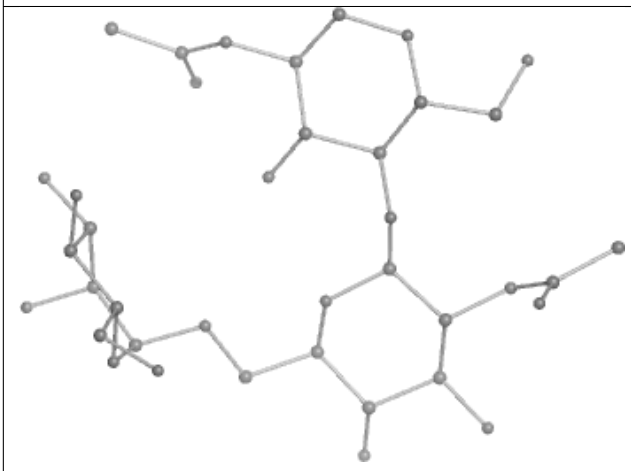
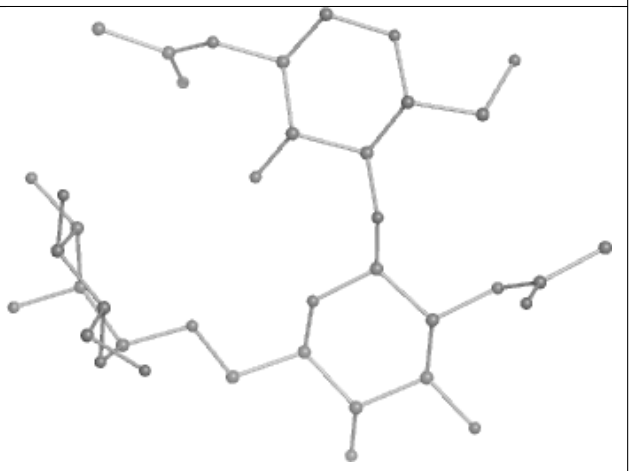


Bond angles

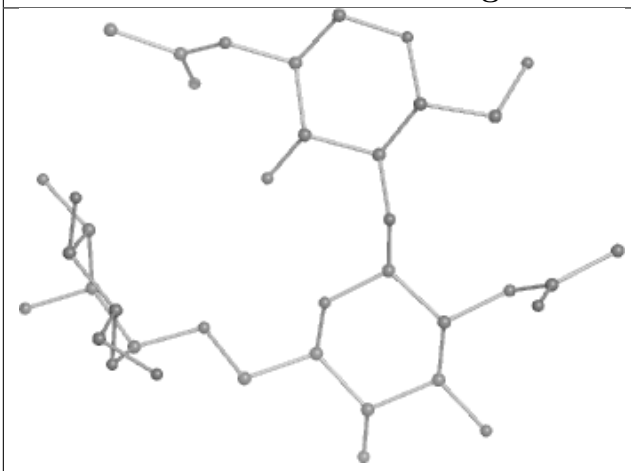


Torsions



Rings

Oligosaccharide Chain OB



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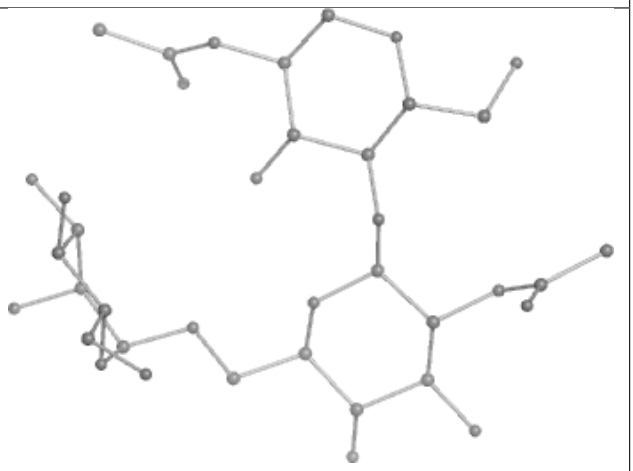
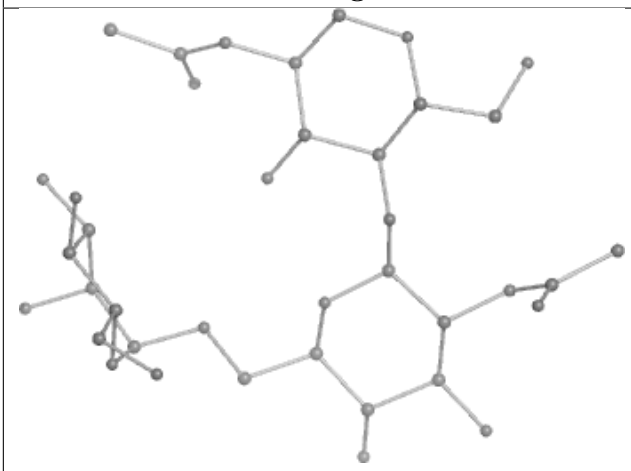
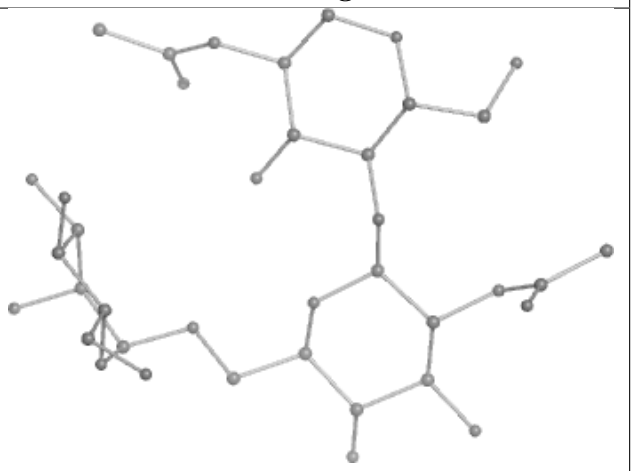


Bond angles

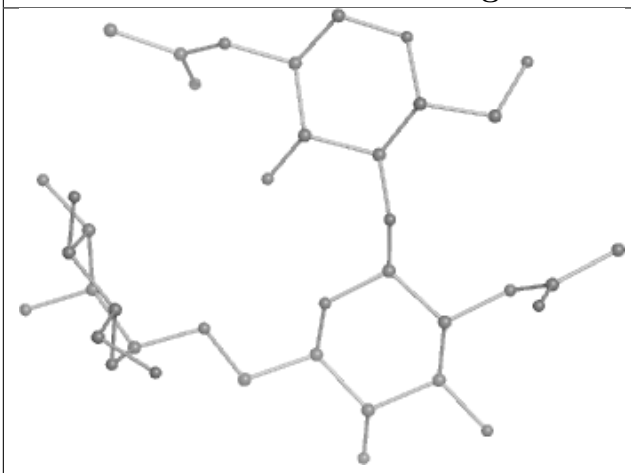


Torsions

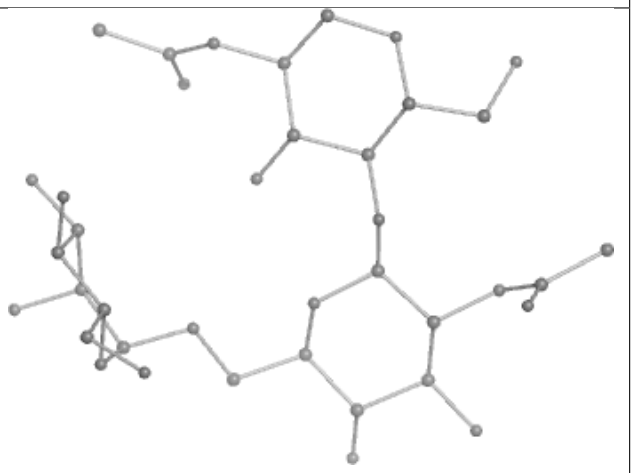


Rings

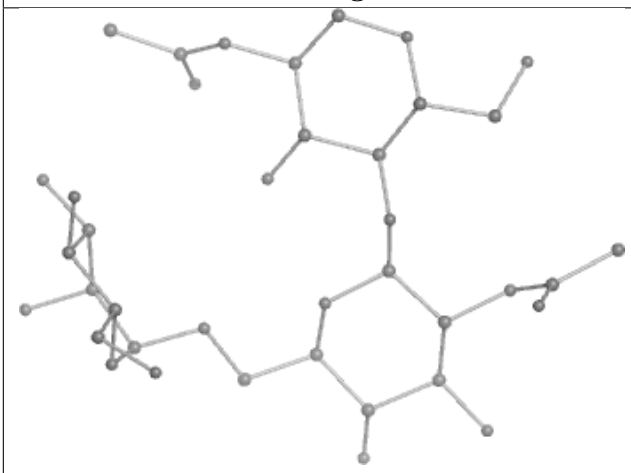
Oligosaccharide Chain RB



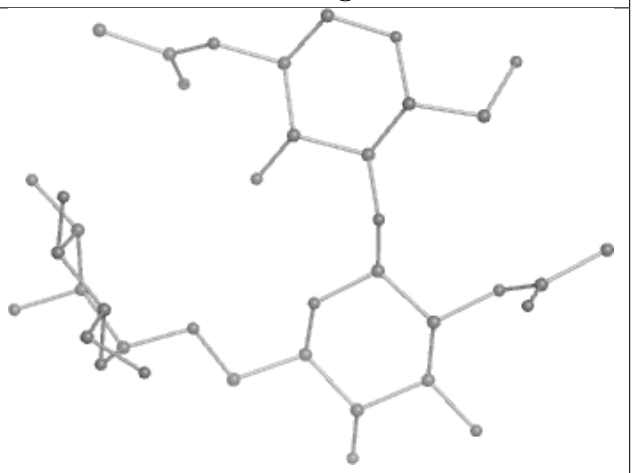
Bond lengths



Bond angles

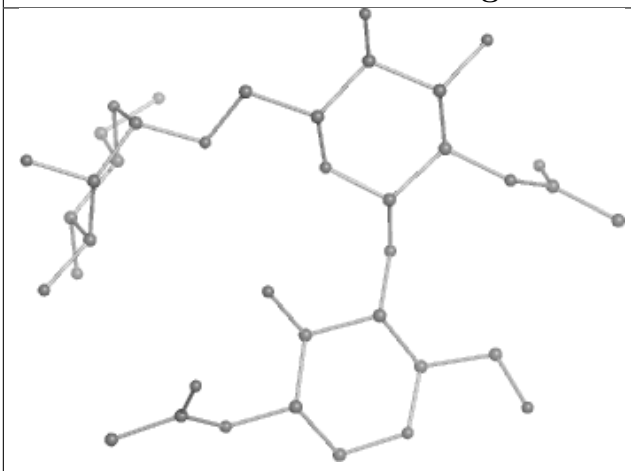


Torsions

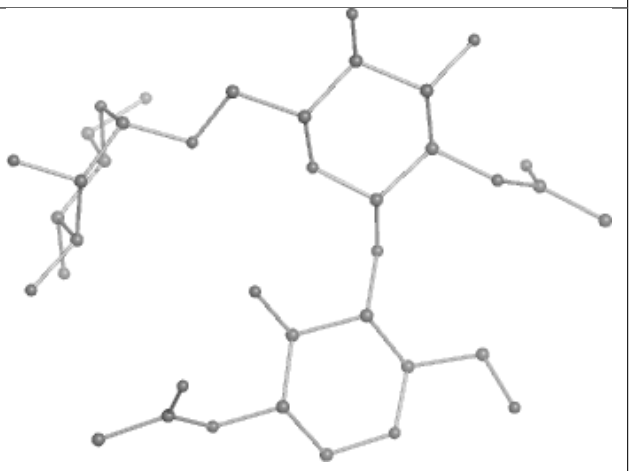


Rings

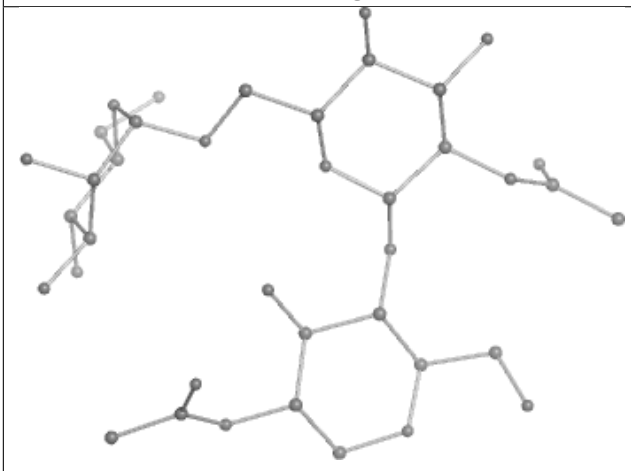
Oligosaccharide Chain UB



Bond lengths



Bond angles



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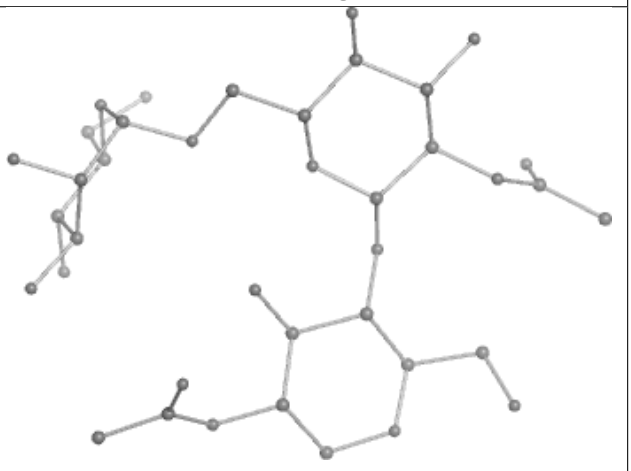
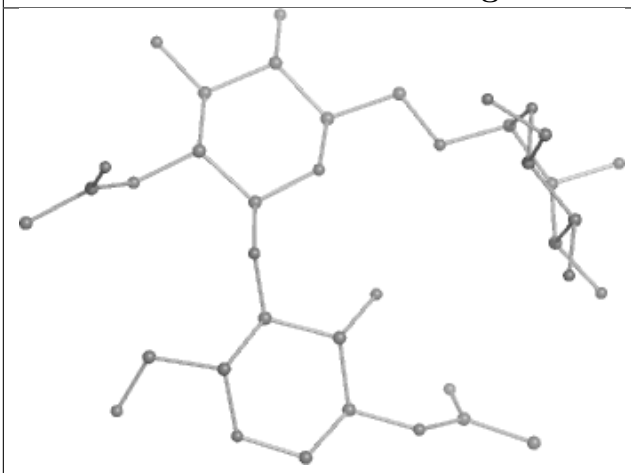
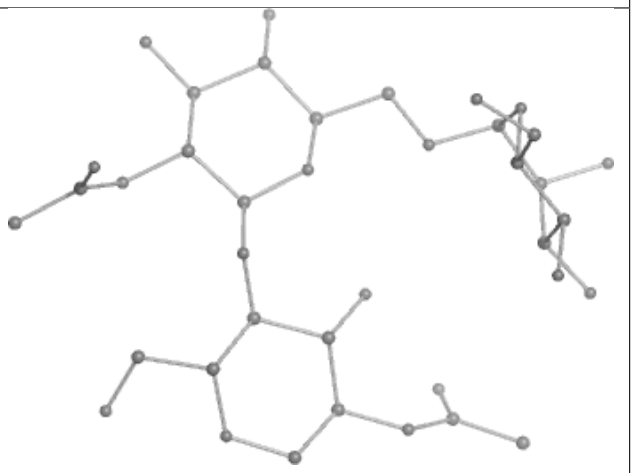


Rings

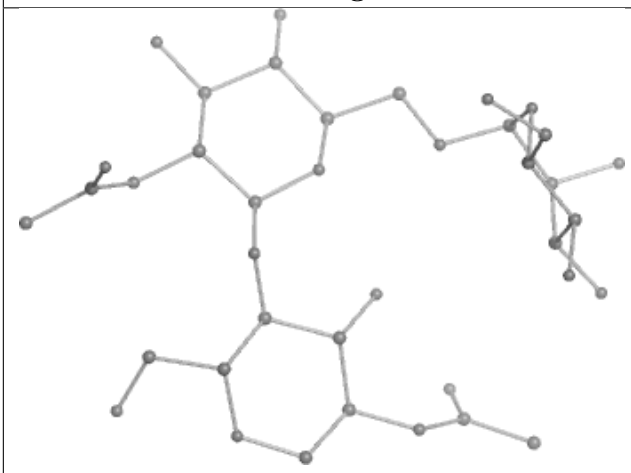
Oligosaccharide Chain XB



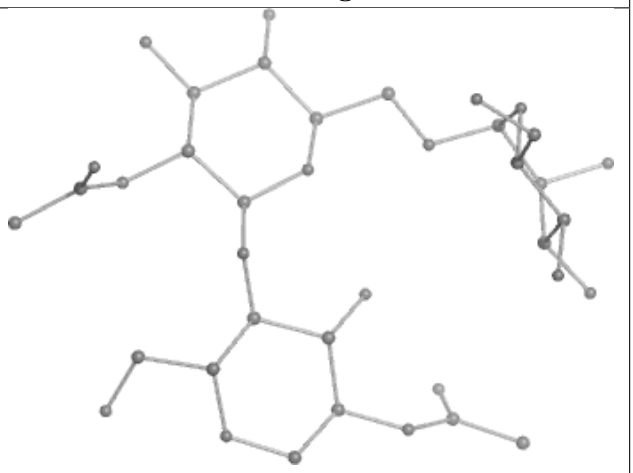
Bond lengths



Bond angles

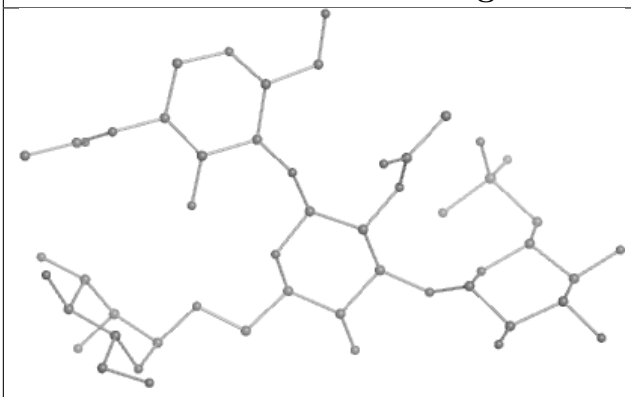


Torsions

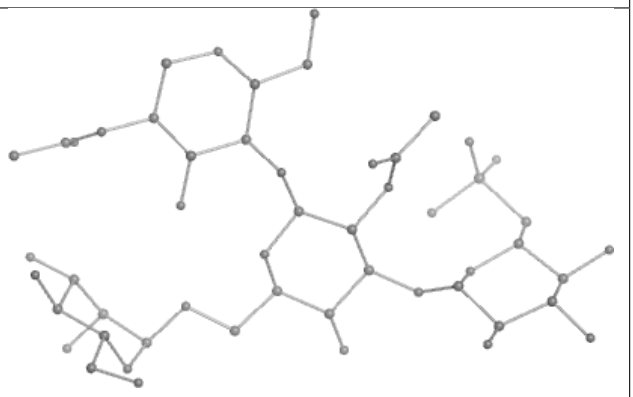


Rings

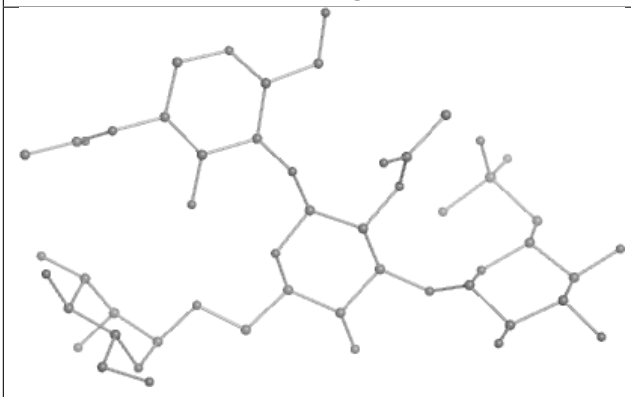
Oligosaccharide Chain MA



Bond lengths



Bond angles



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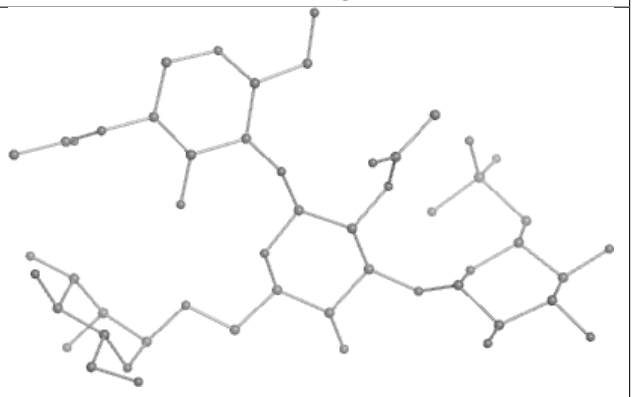
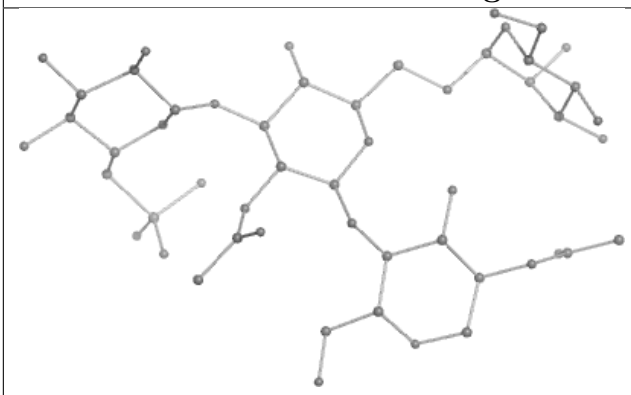


Rings

Oligosaccharide Chain PA



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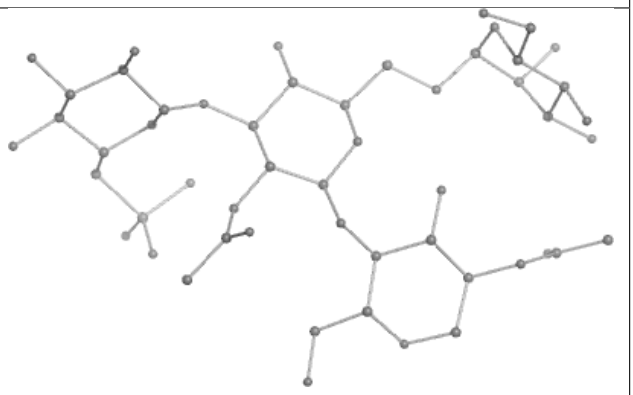
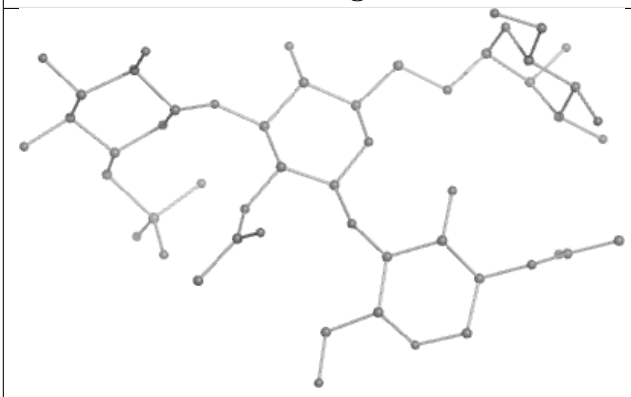
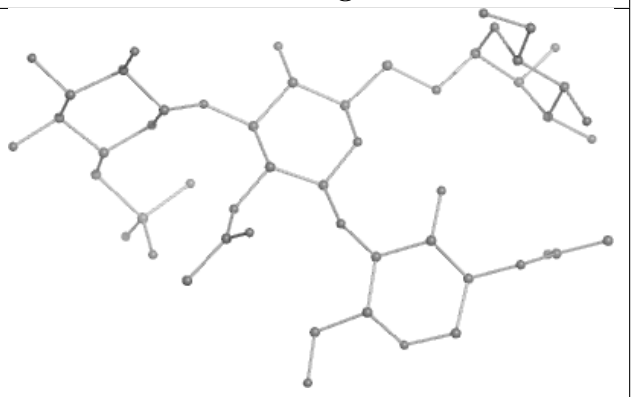


Bond angles

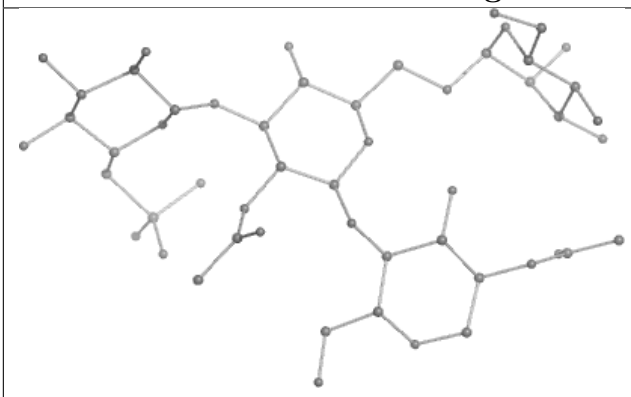


Torsions



Rings

Oligosaccharide Chain SA



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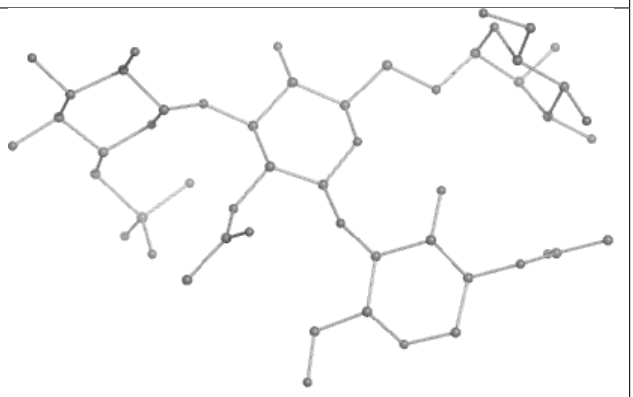
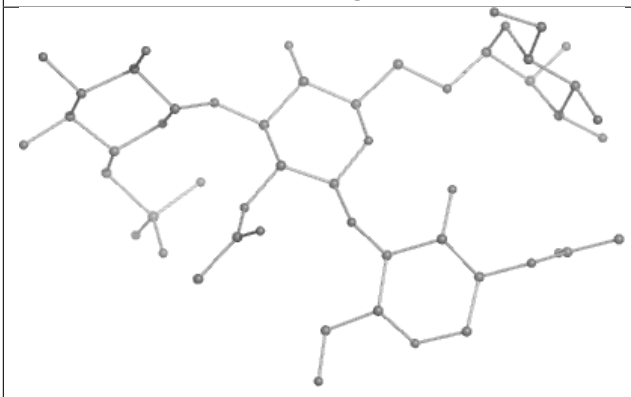
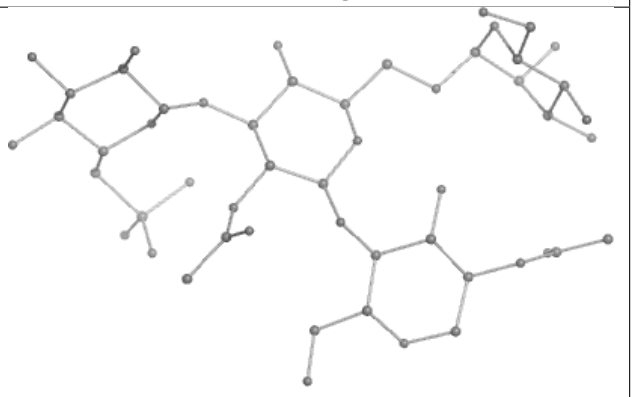


Bond angles

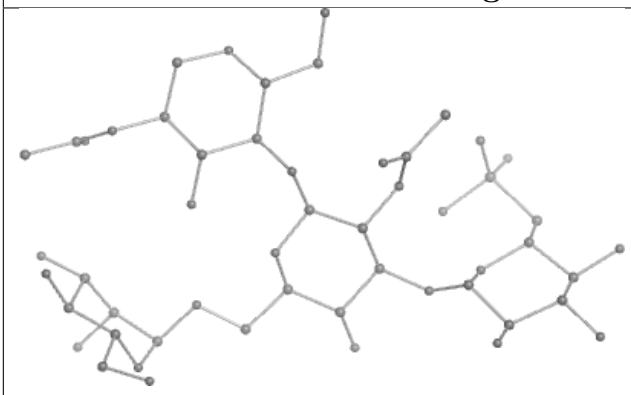


Torsions

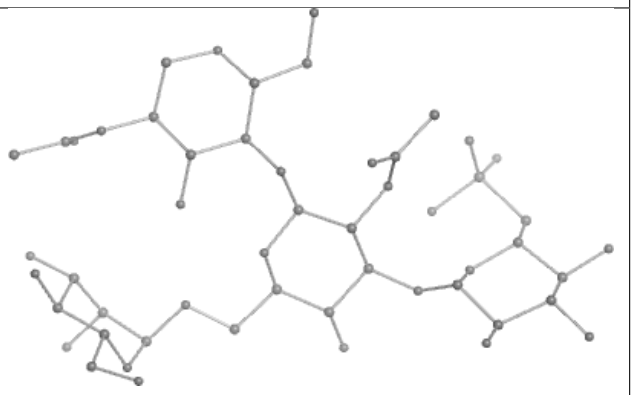


Rings

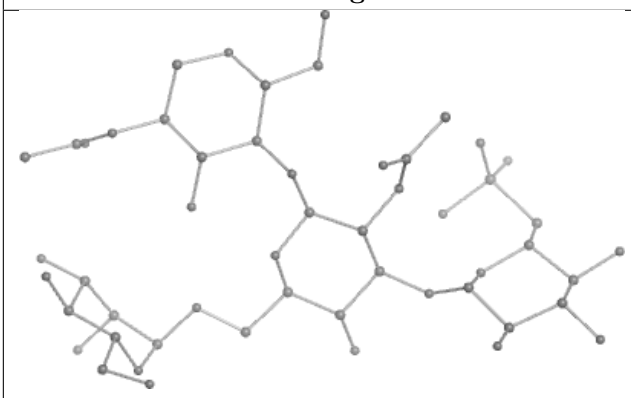
Oligosaccharide Chain VA



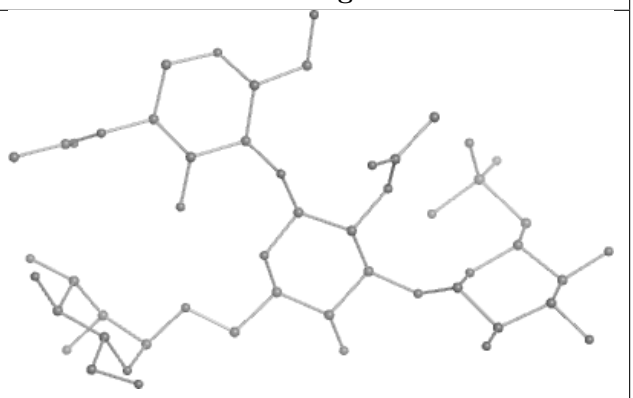
Bond lengths



Bond angles

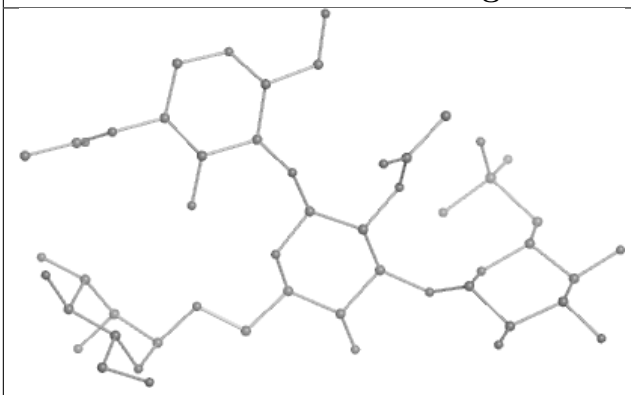


Torsions



Rings

Oligosaccharide Chain YA



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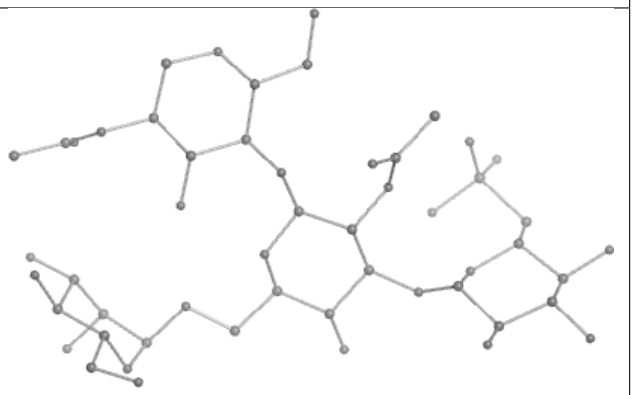
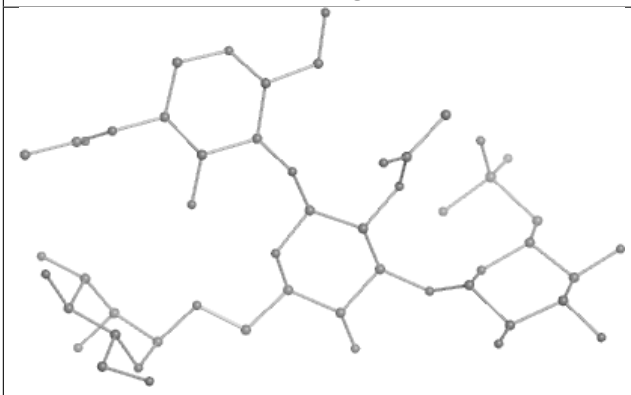


Bond angles



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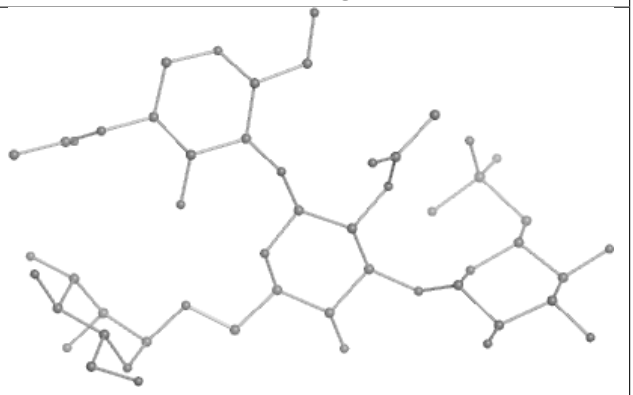
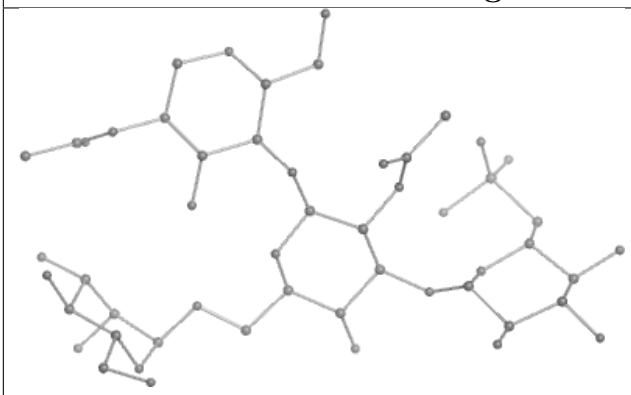


Rings

Oligosaccharide Chain bA



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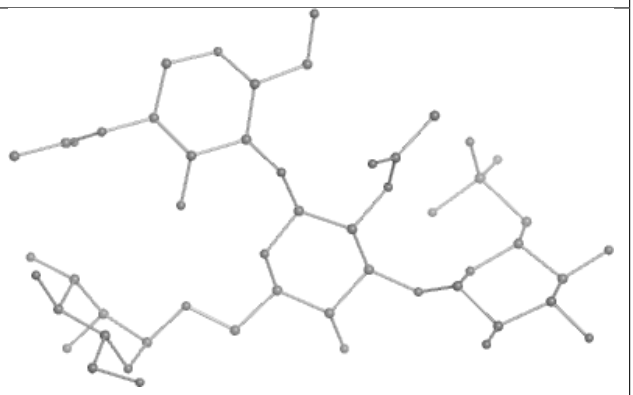
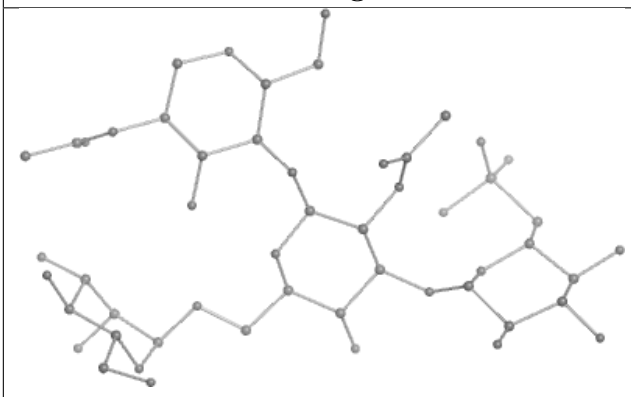
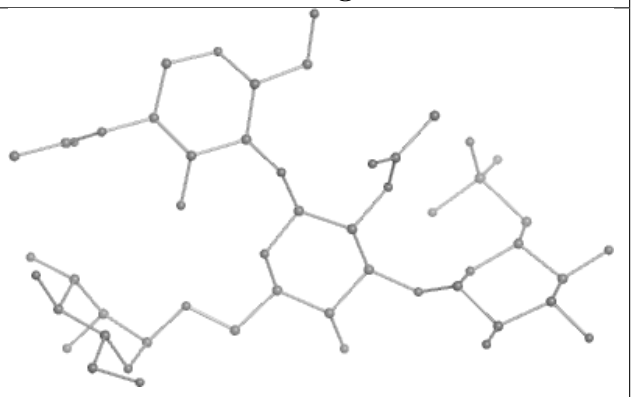


Bond angles

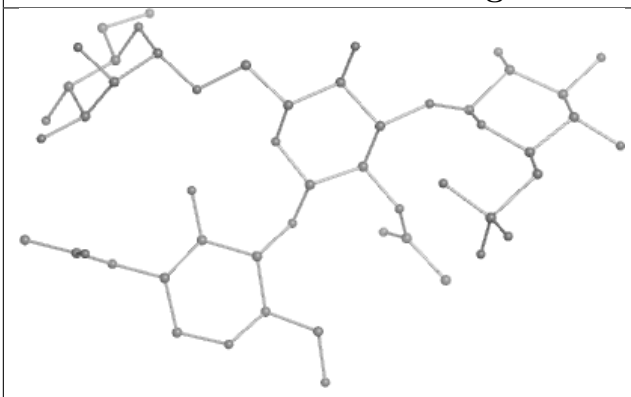


Torsions



Rings

Oligosaccharide Chain eA



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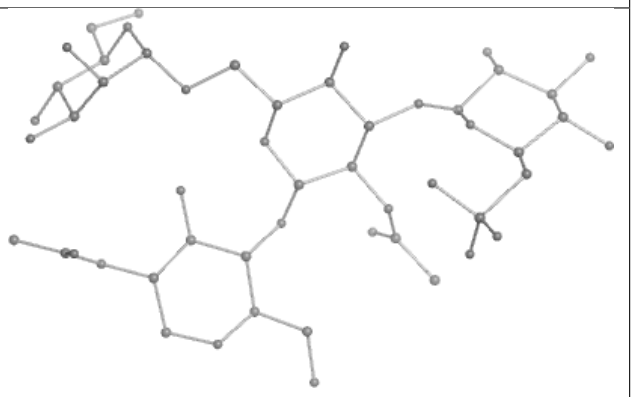
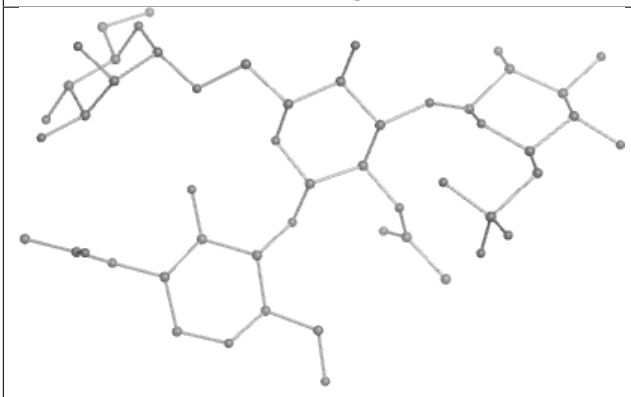


Bond angles



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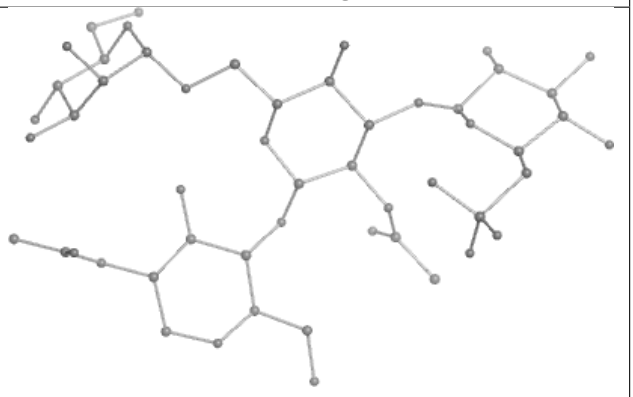
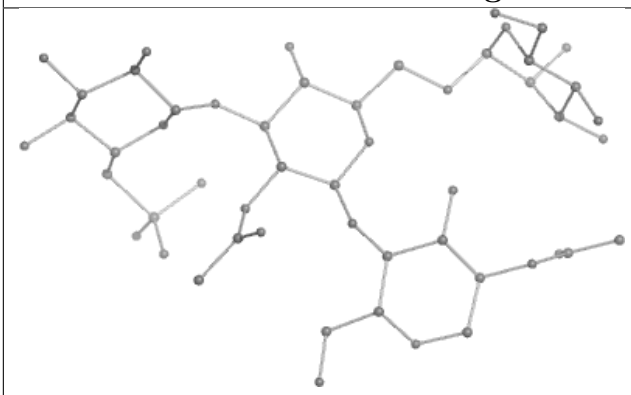


Rings

Oligosaccharide Chain hA



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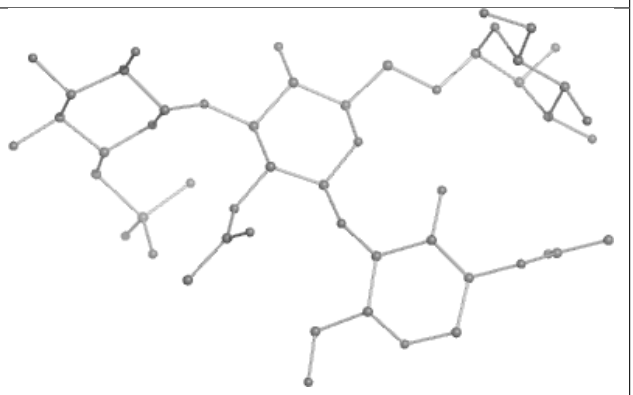
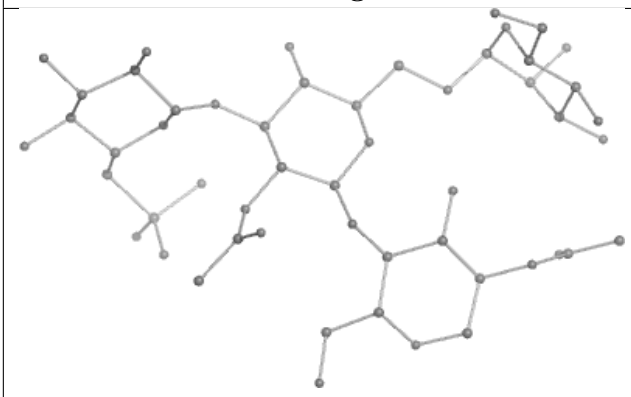


Bond angles



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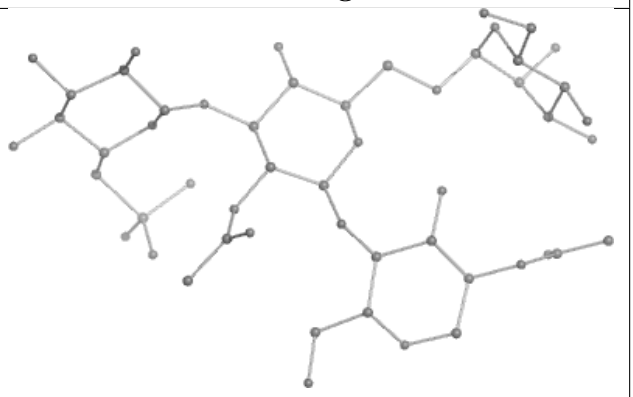
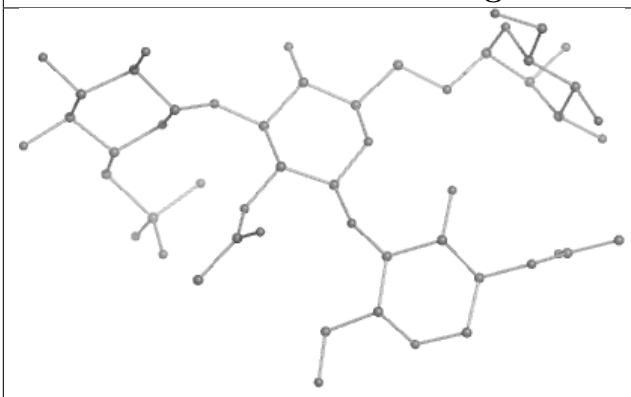


Rings

Oligosaccharide Chain kA



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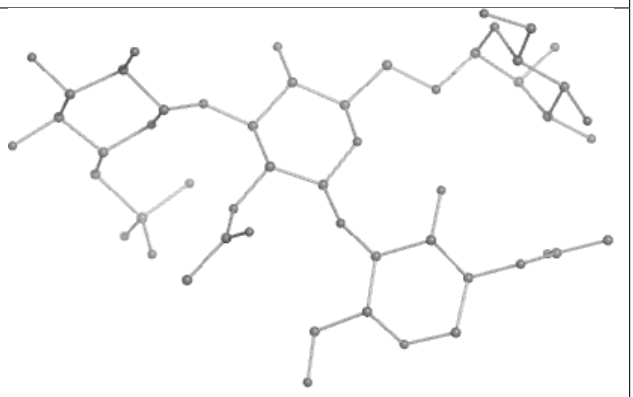
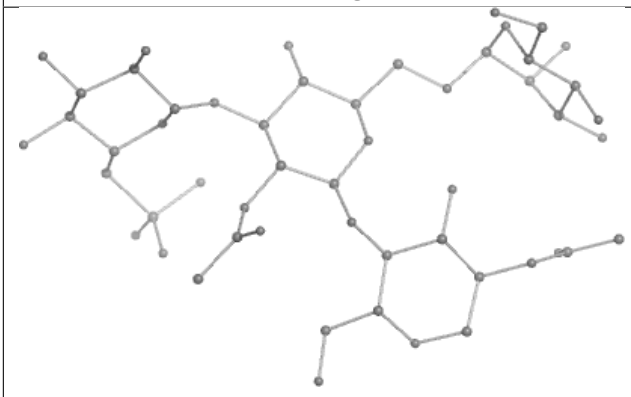


Bond angles



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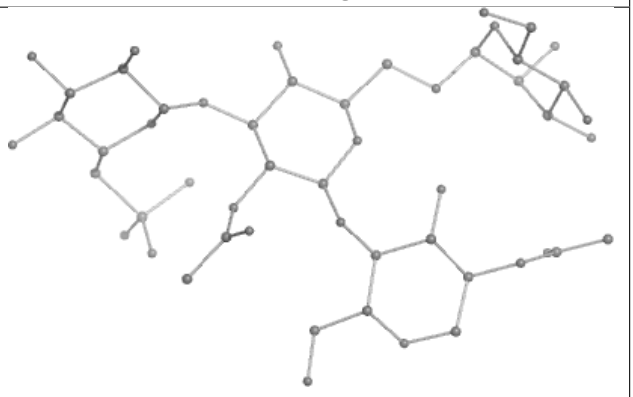
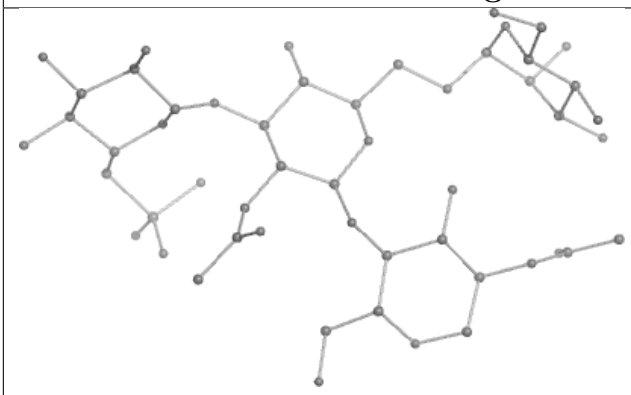
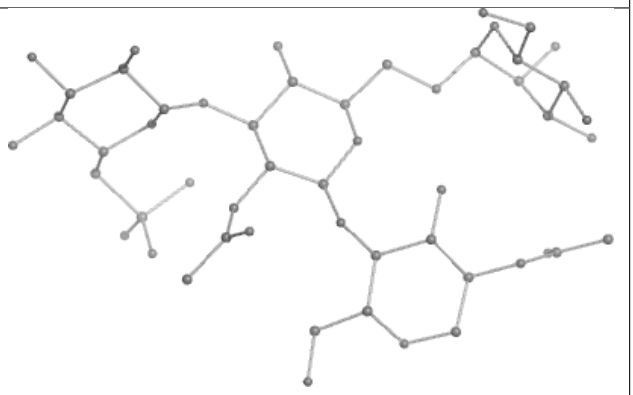


Rings

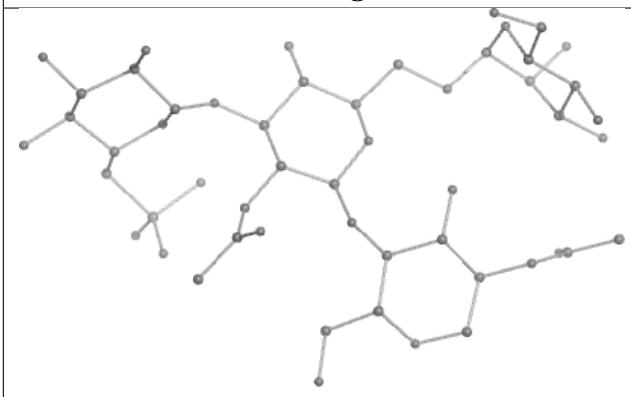
Oligosaccharide Chain nA



Bond lengths



Bond angles



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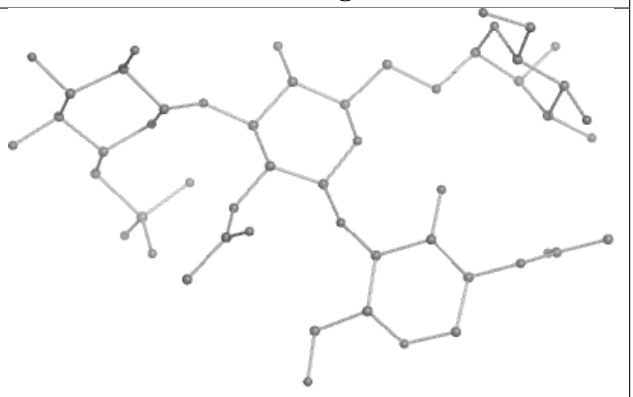
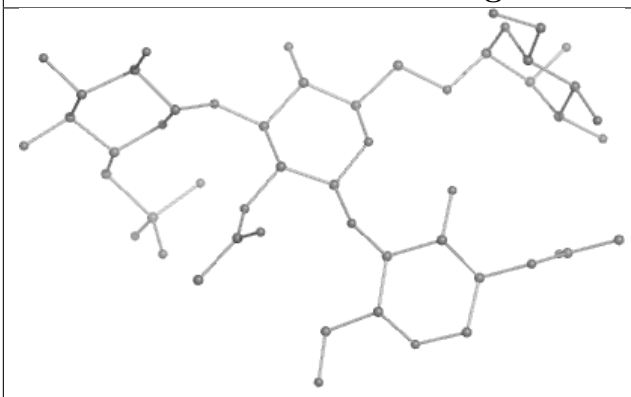


Rings

Oligosaccharide Chain qA



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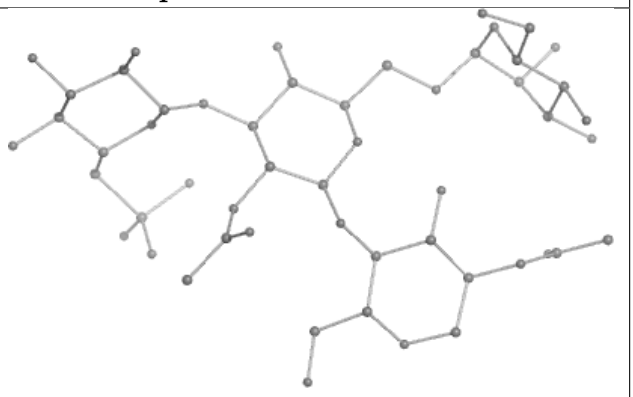
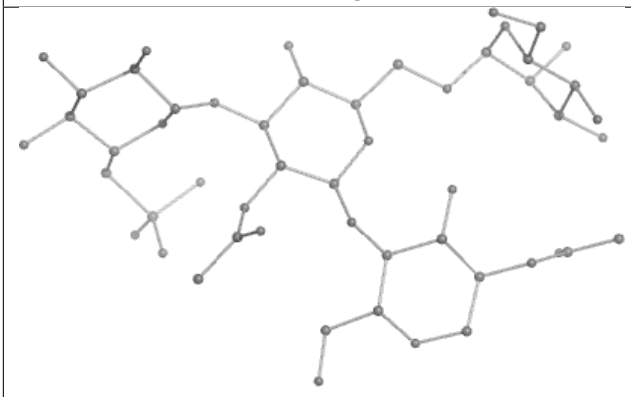


Bond angles



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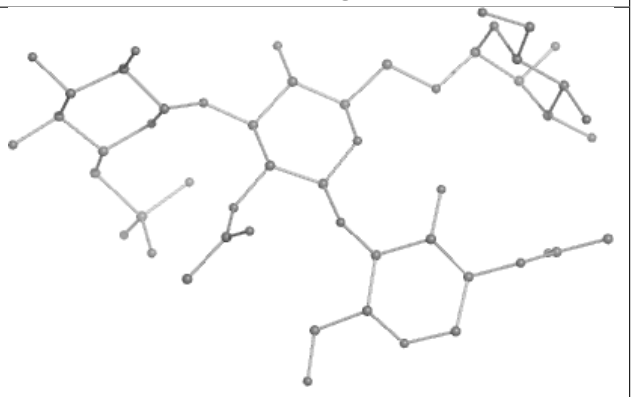
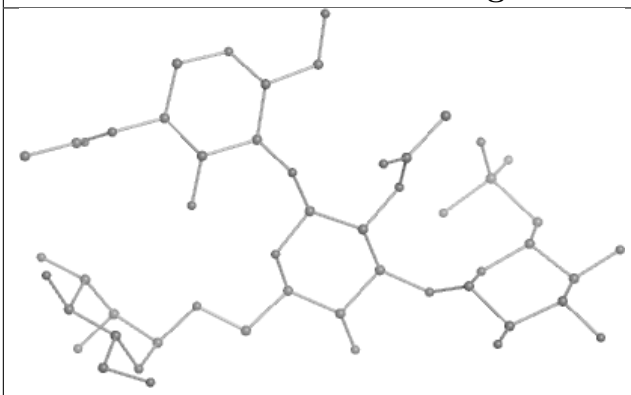


Rings

Oligosaccharide Chain tA



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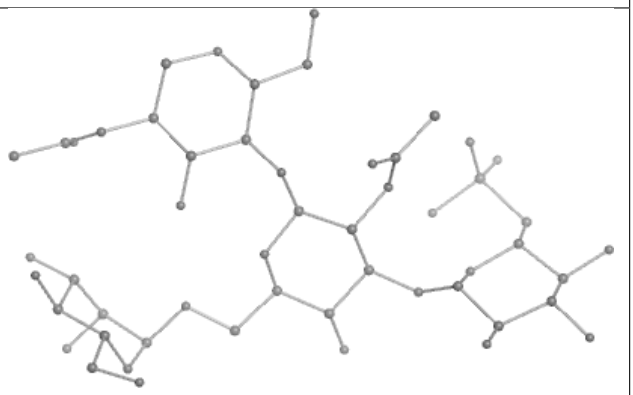
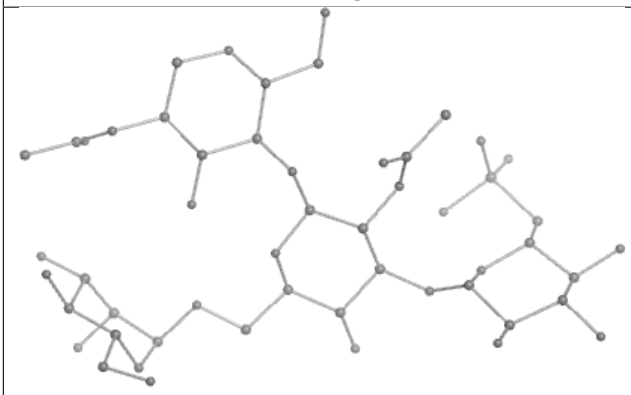
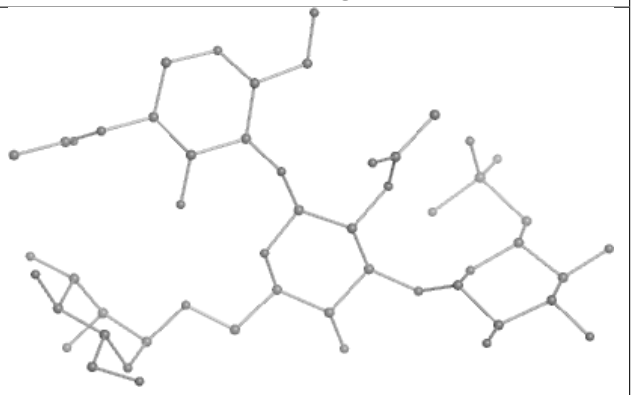


Bond angles

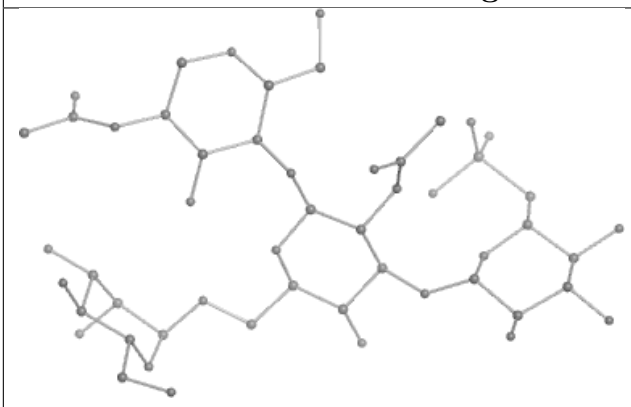


Torsions



Rings

Oligosaccharide Chain wA



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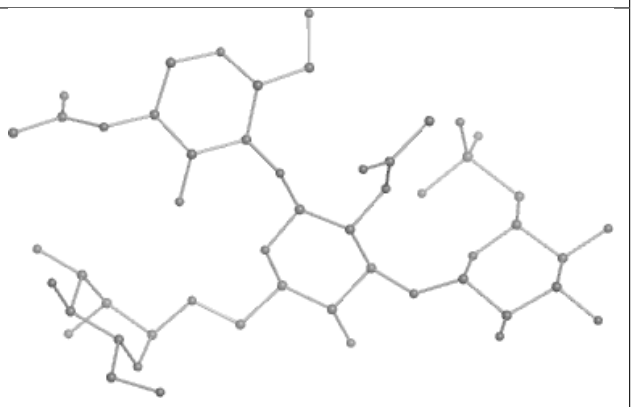
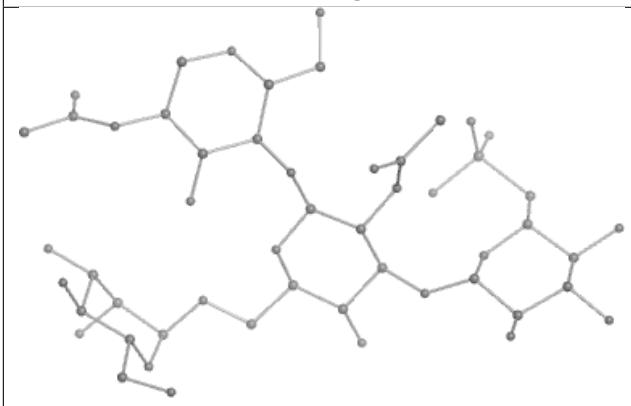


Bond angles



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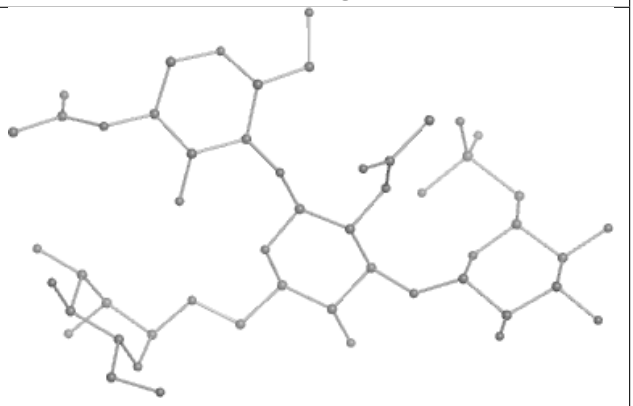
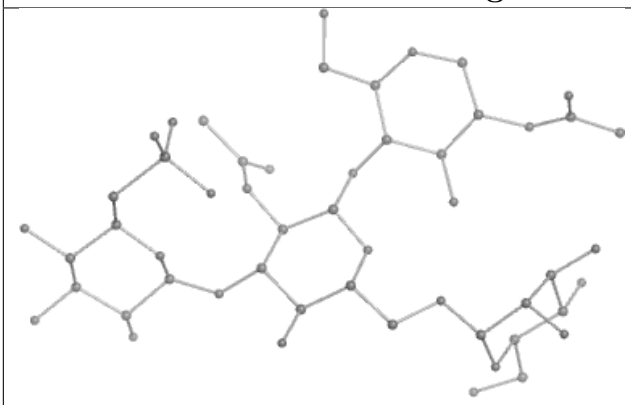
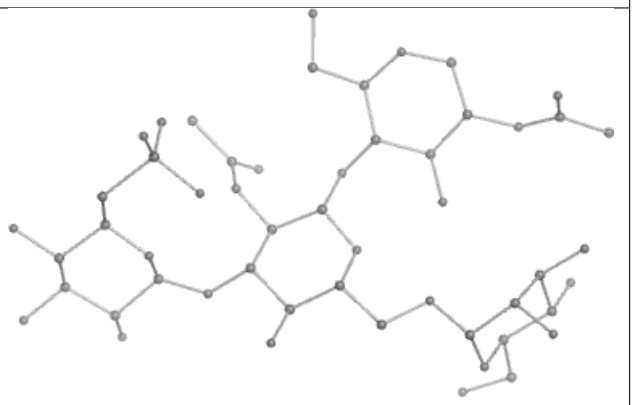


Rings

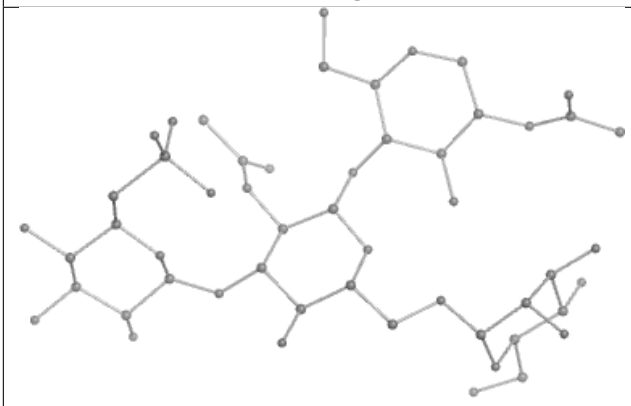
Oligosaccharide Chain zA



Bond lengths



Bond angles



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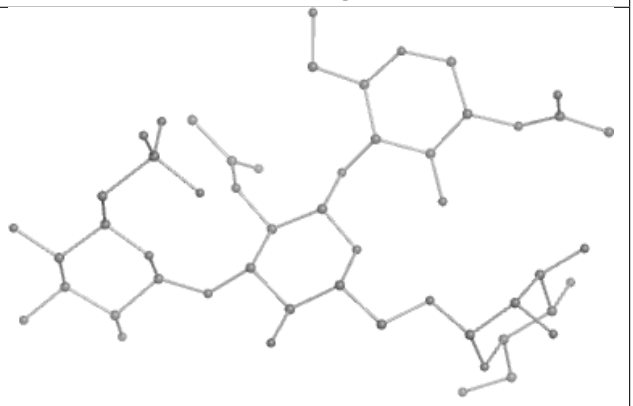
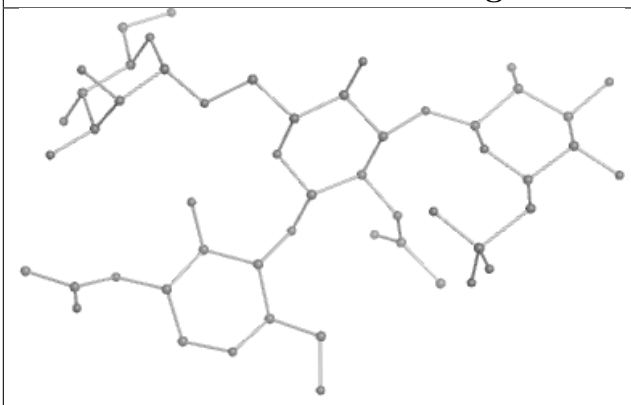
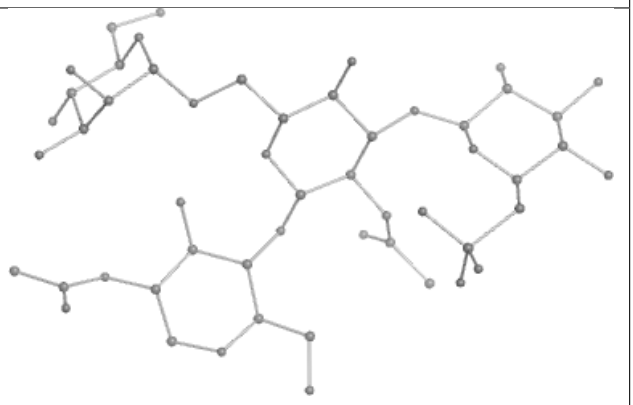


Rings

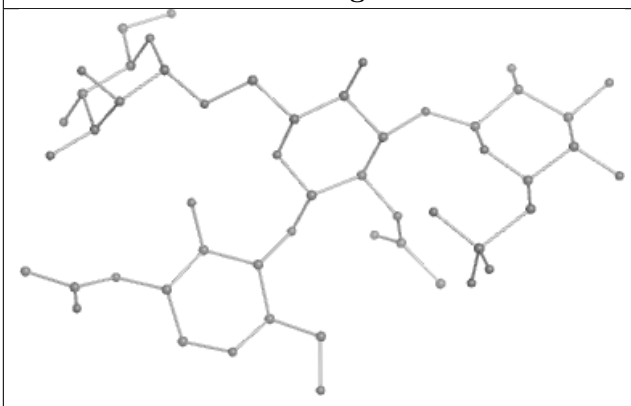
Oligosaccharide Chain 2A



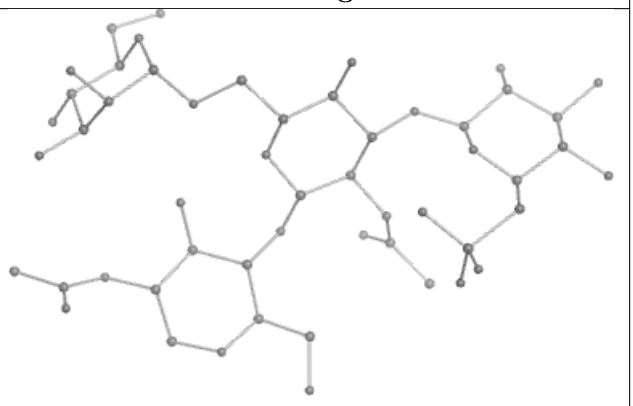
Bond lengths



Bond angles

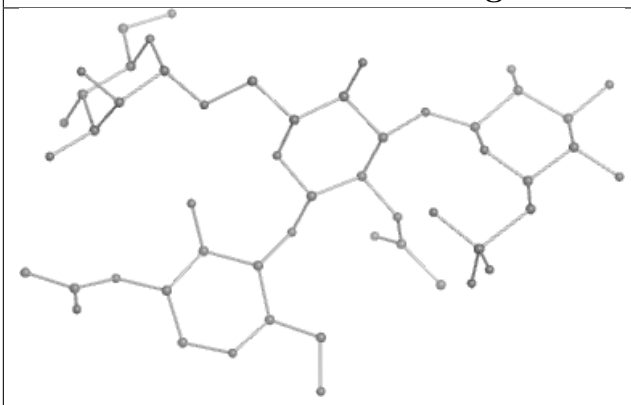


Torsions

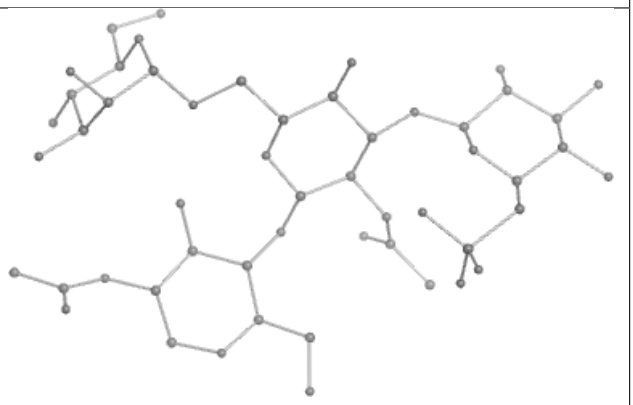


Rings

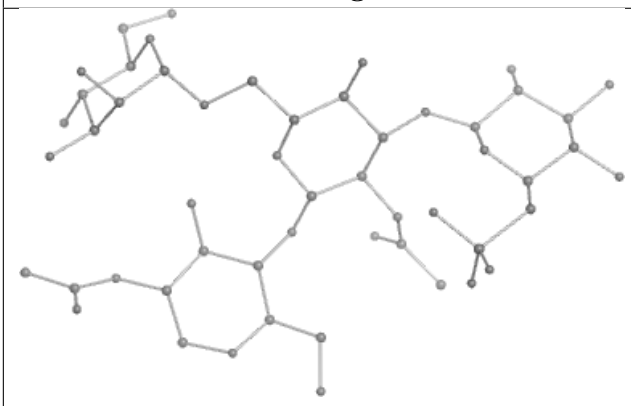
Oligosaccharide Chain 5A



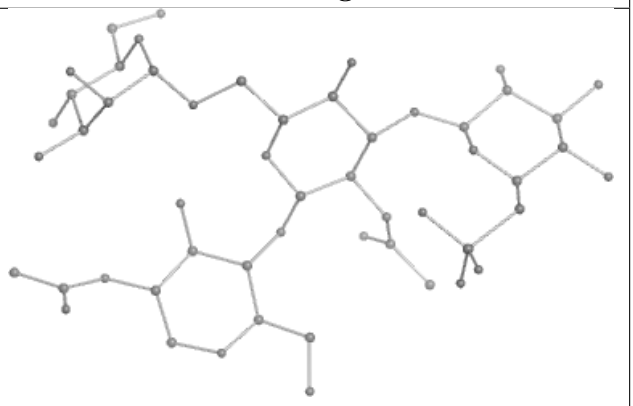
Bond lengths



Bond angles

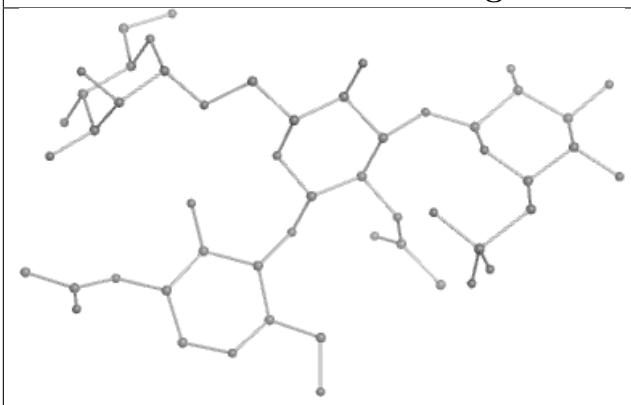


Torsions

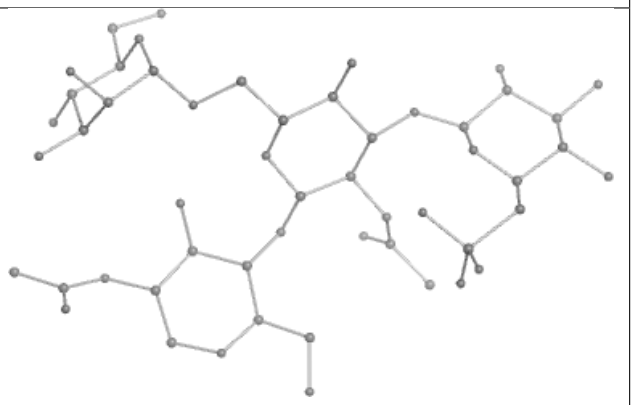


Rings

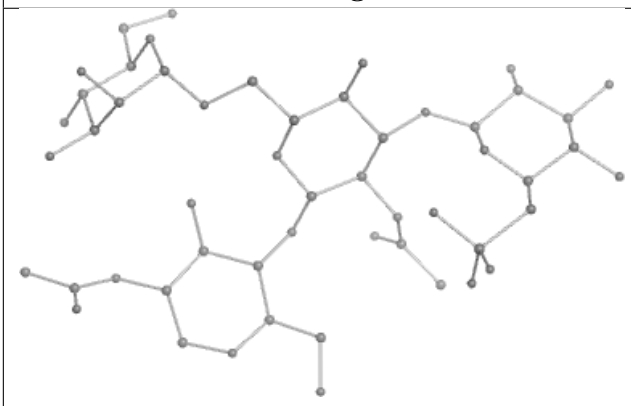
Oligosaccharide Chain 8A



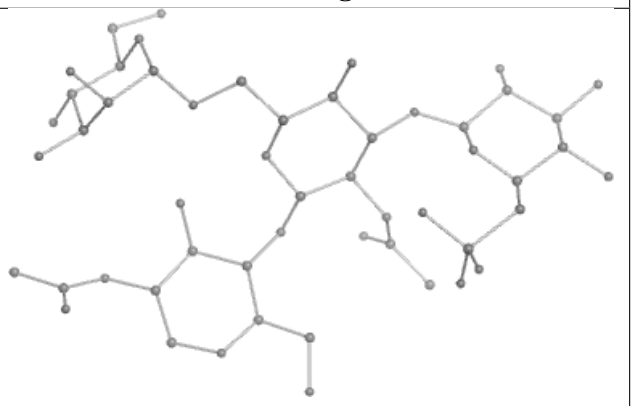
Bond lengths



Bond angles

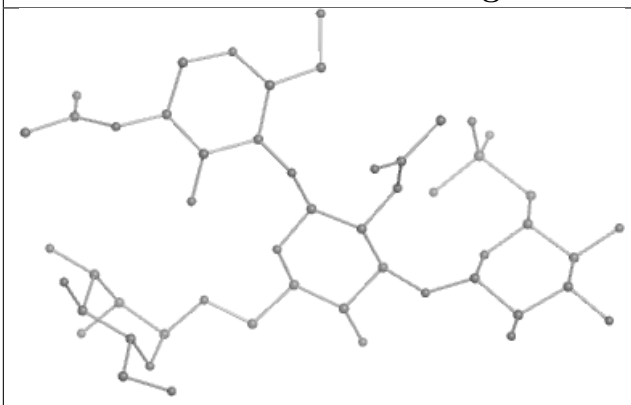


Torsions

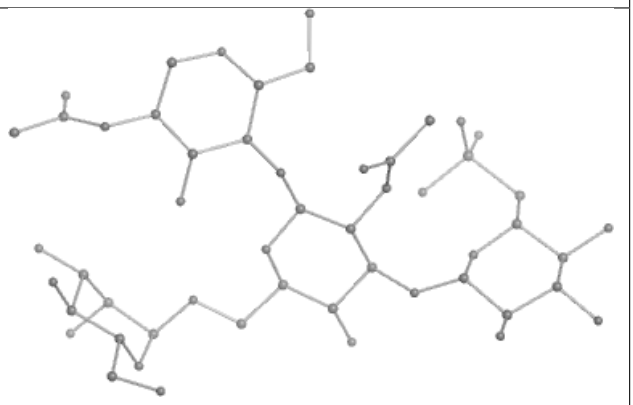


Rings

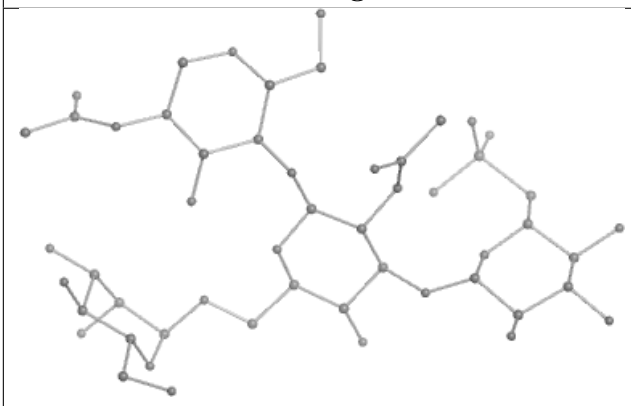
Oligosaccharide Chain BB



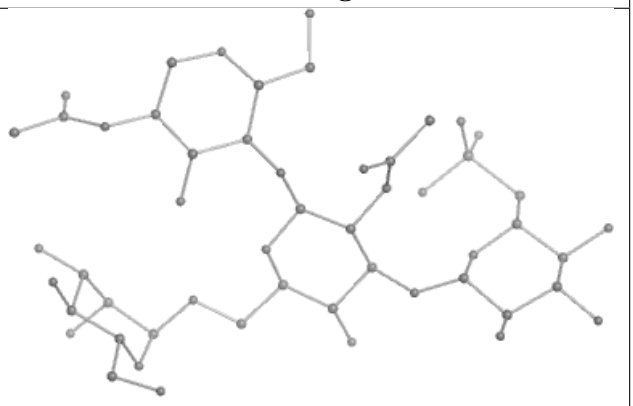
Bond lengths



Bond angles

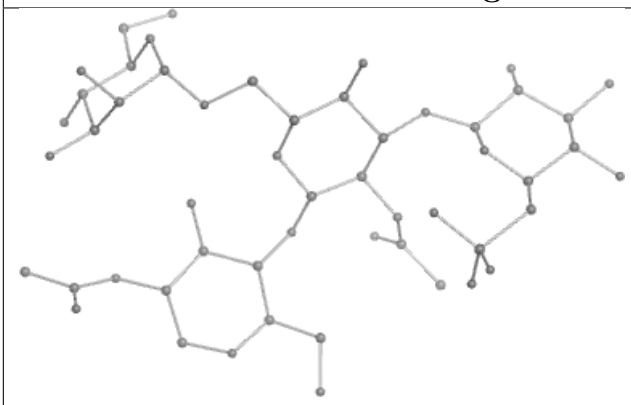


Torsions

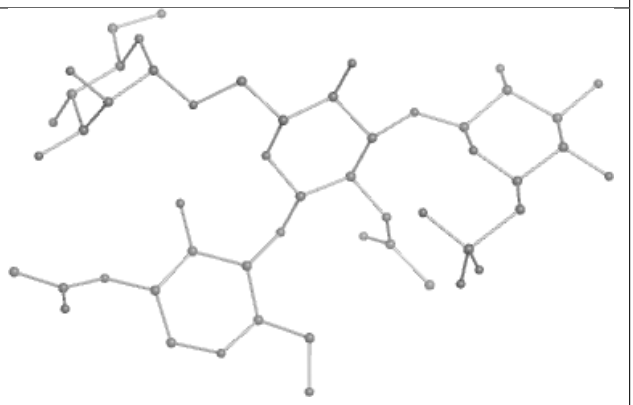


Rings

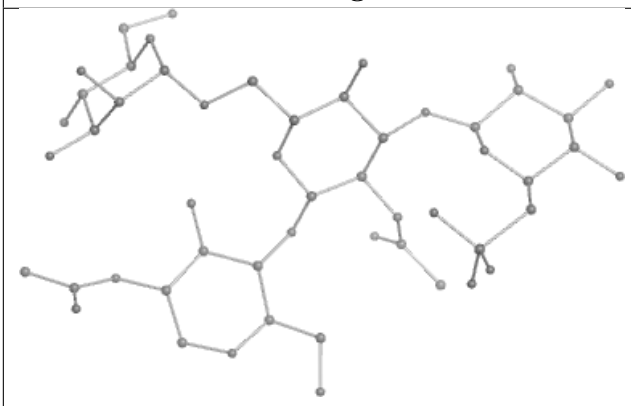
Oligosaccharide Chain EB



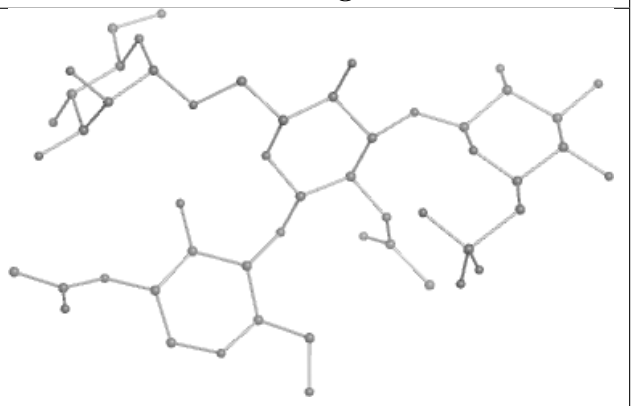
Bond lengths



Bond angles

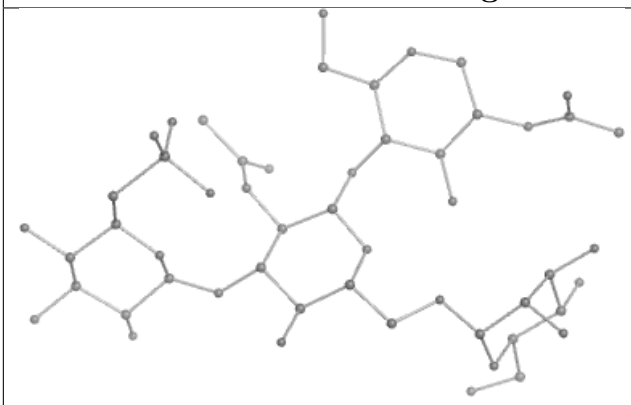


Torsions

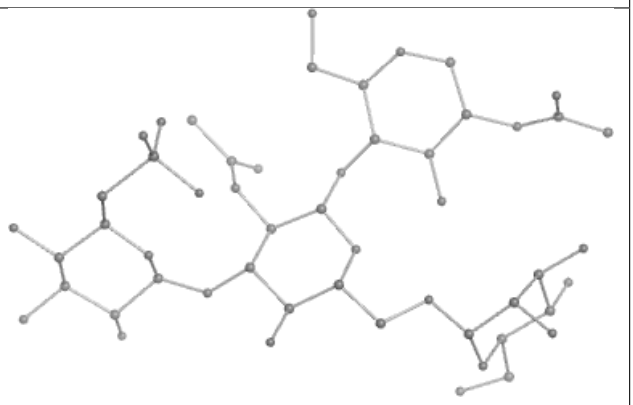


Rings

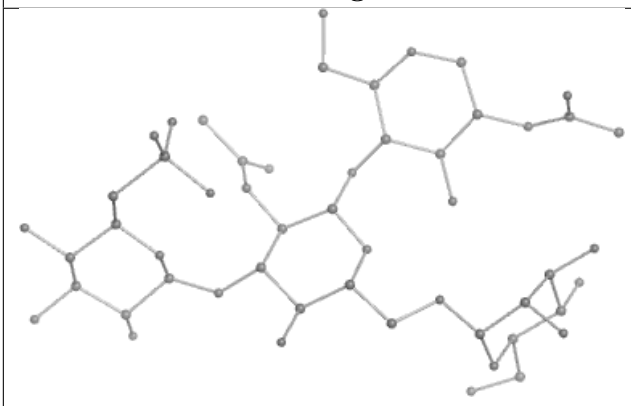
Oligosaccharide Chain HB



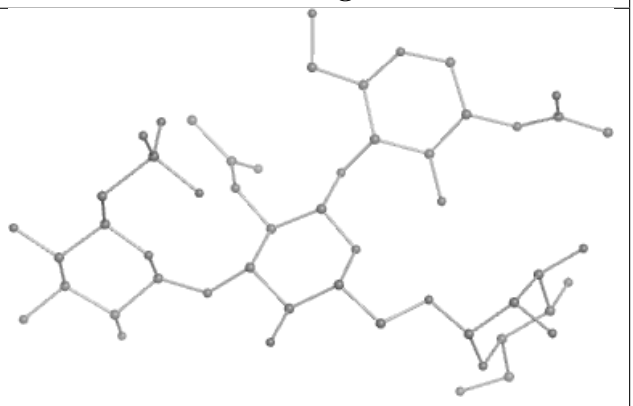
Bond lengths



Bond angles

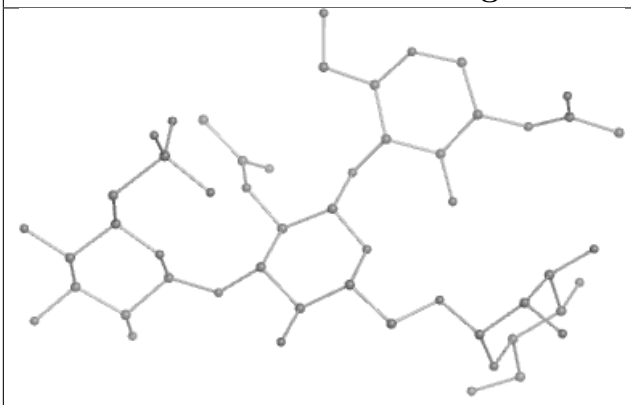


Torsions

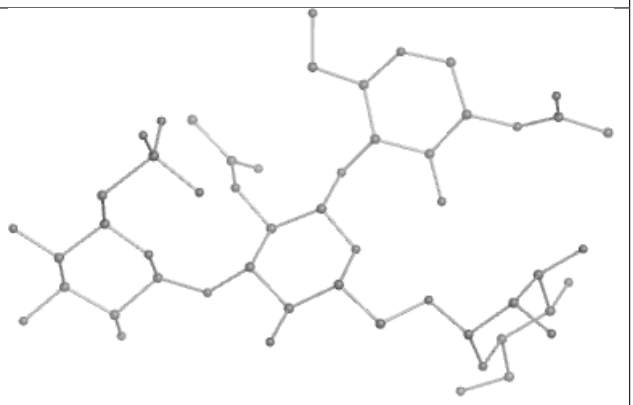


Rings

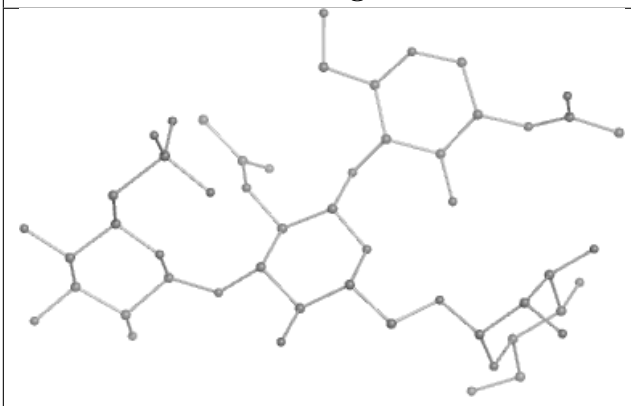
Oligosaccharide Chain KB



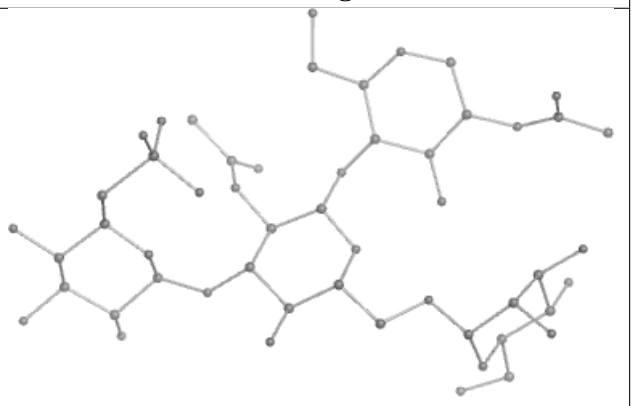
Bond lengths



Bond angles

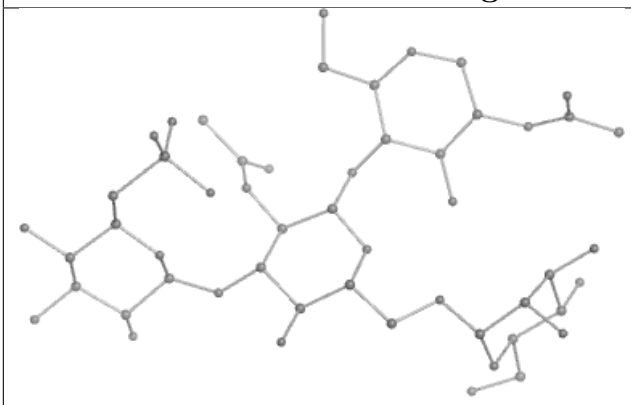


Torsions

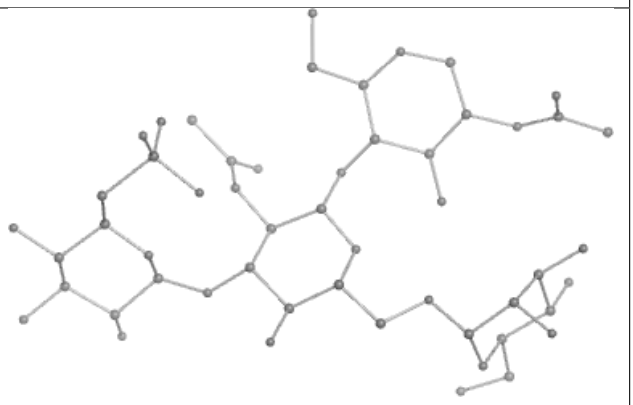


Rings

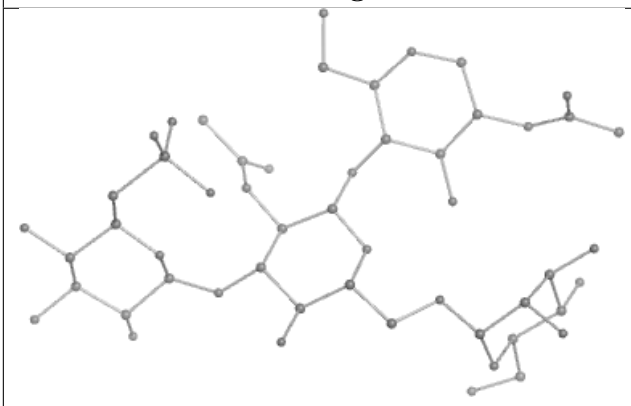
Oligosaccharide Chain NB



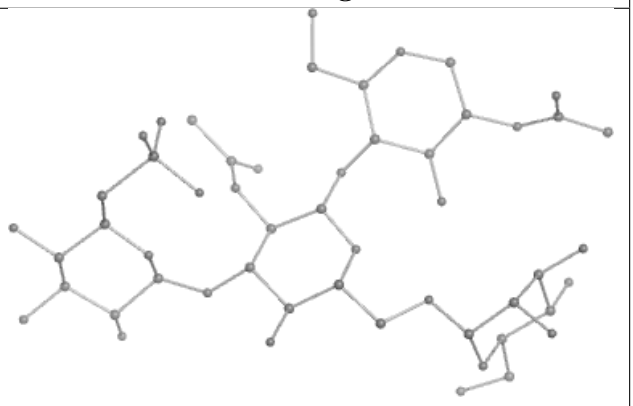
Bond lengths



Bond angles

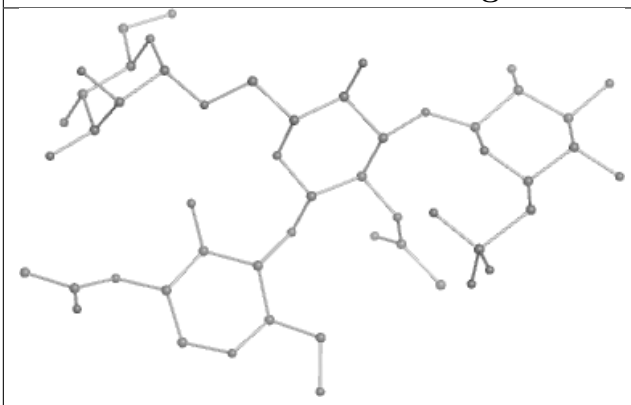


Torsions

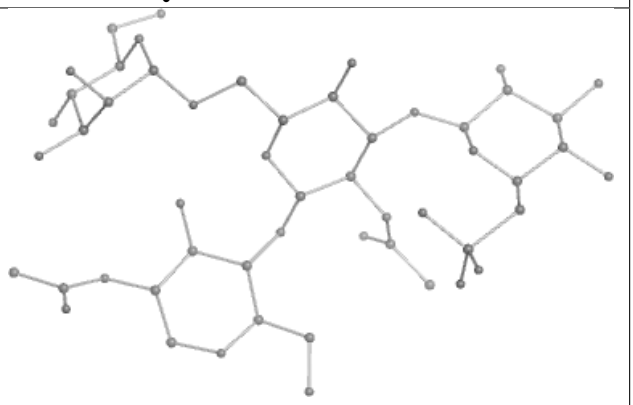


Rings

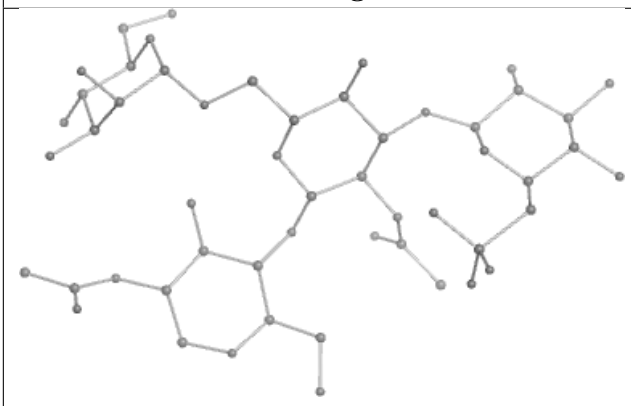
Oligosaccharide Chain QB



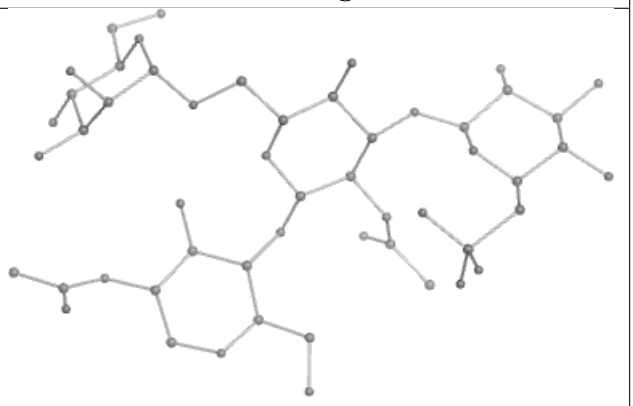
Bond lengths



Bond angles

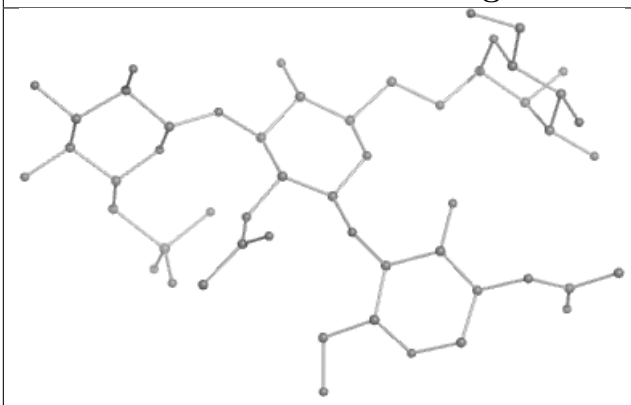


Torsions

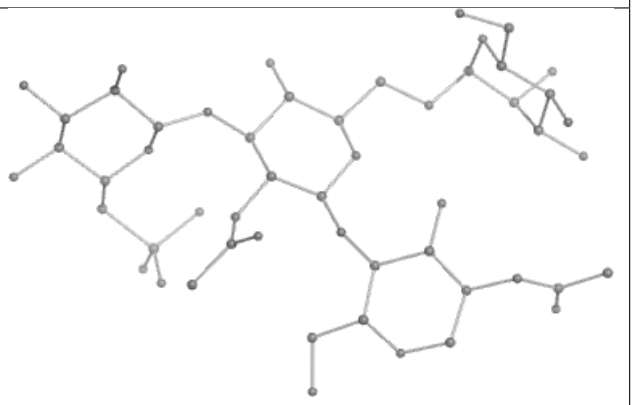


Rings

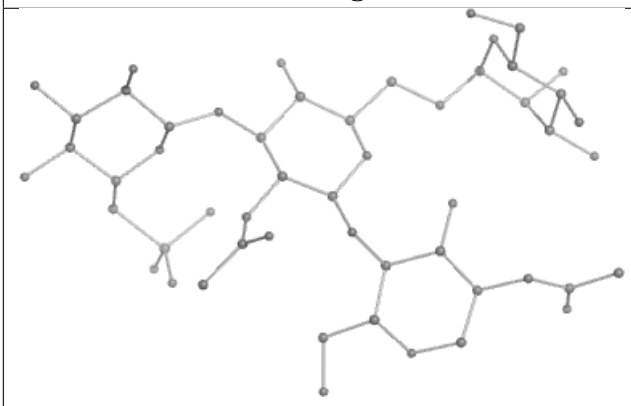
Oligosaccharide Chain TB



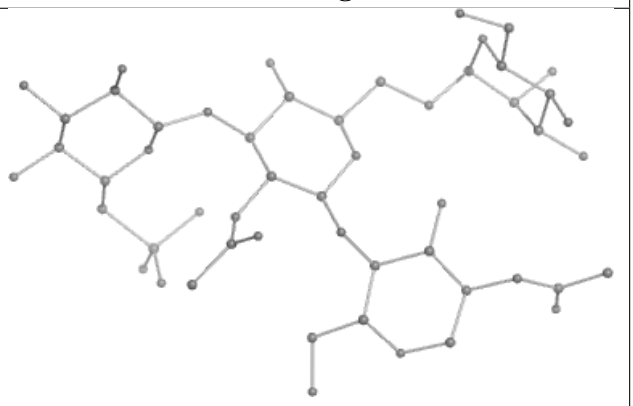
Bond lengths



Bond angles

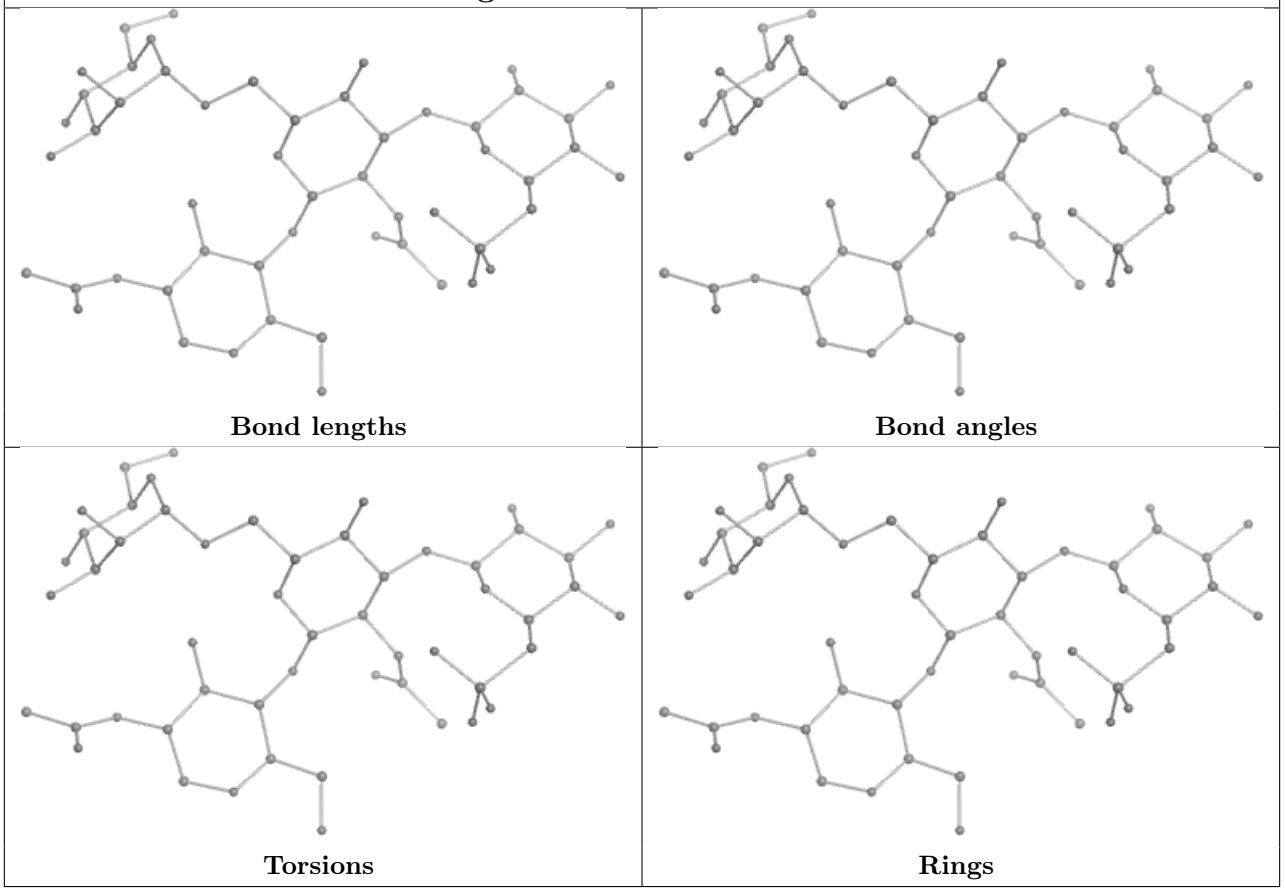


Torsions



Rings

Oligosaccharide Chain WB



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.

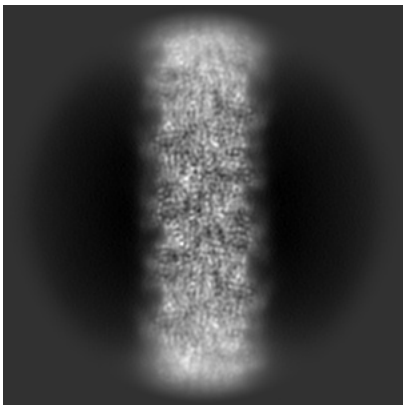
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19960. These allow visual inspection of the internal detail of the map and identification of artifacts.

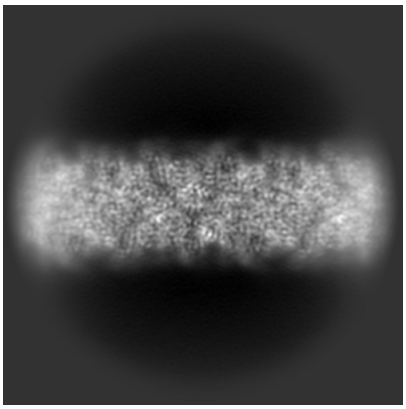
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

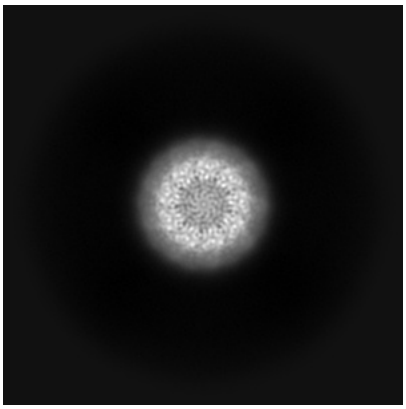
6.1.1 Primary map



X

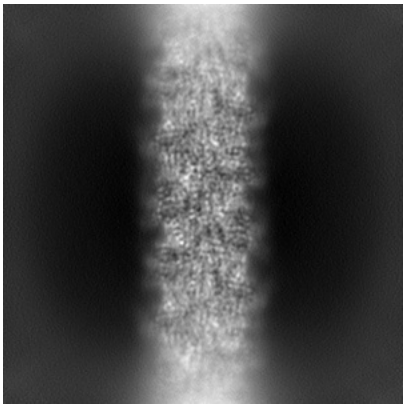


Y

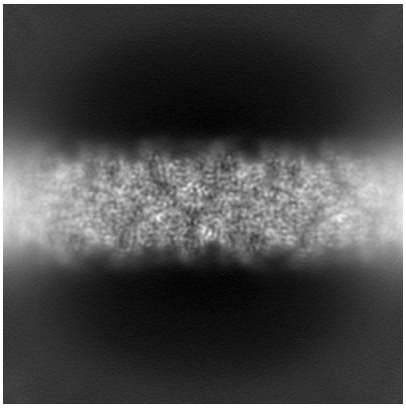


Z

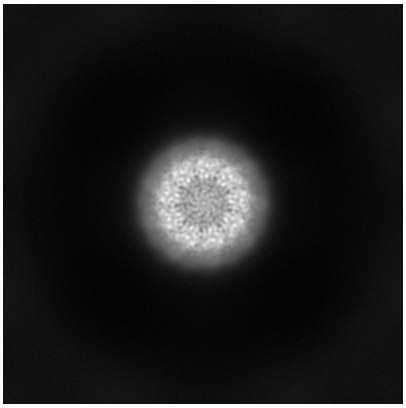
6.1.2 Raw map



X



Y

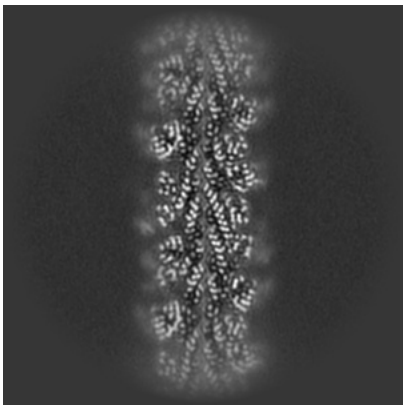


Z

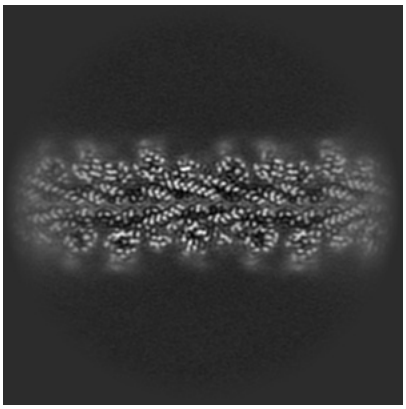
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

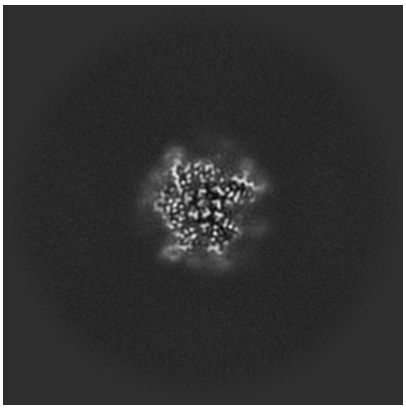
6.2.1 Primary map



X Index: 144

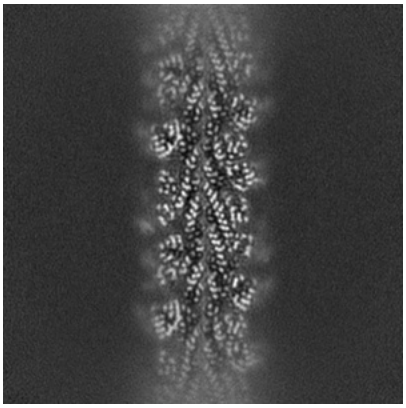


Y Index: 144

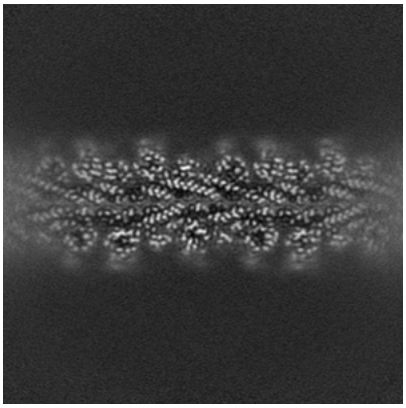


Z Index: 144

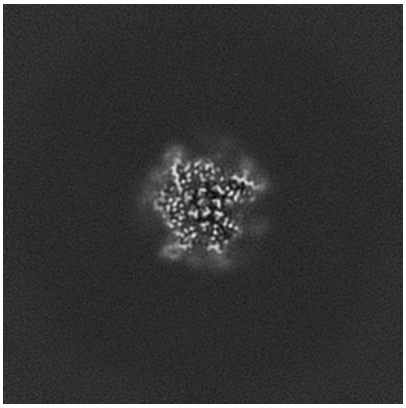
6.2.2 Raw map



X Index: 144



Y Index: 144

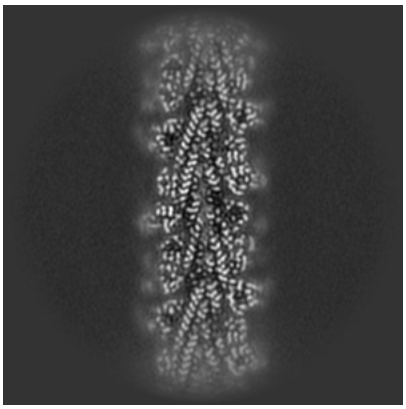


Z Index: 144

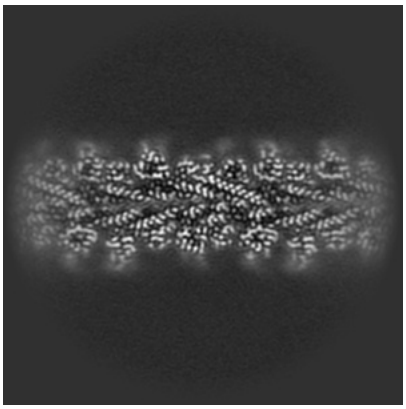
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

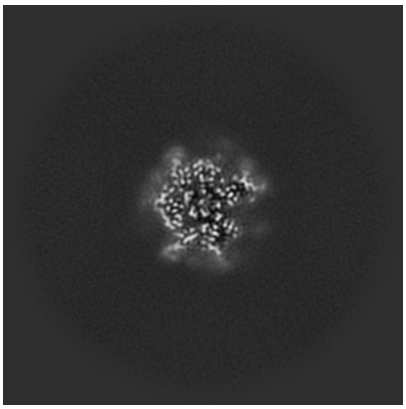
6.3.1 Primary map



X Index: 147

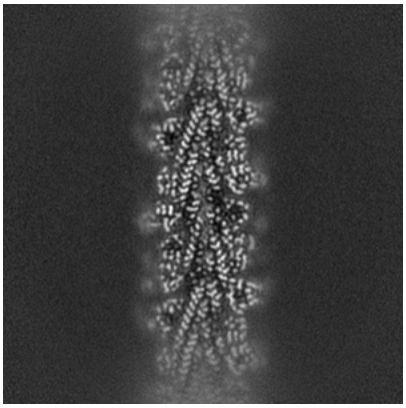


Y Index: 146

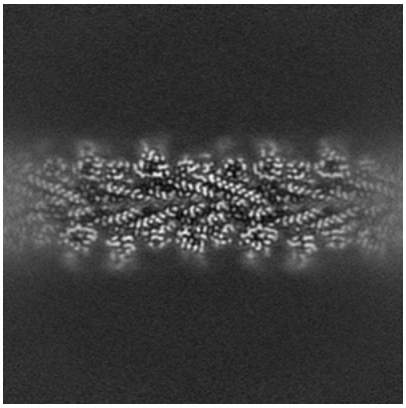


Z Index: 143

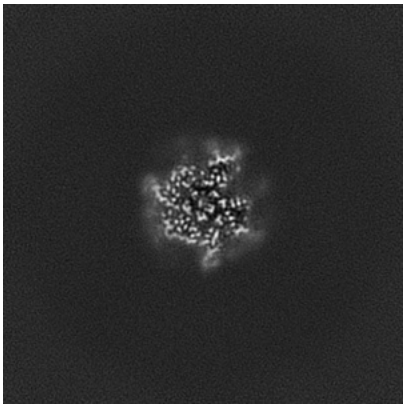
6.3.2 Raw map



X Index: 147



Y Index: 146

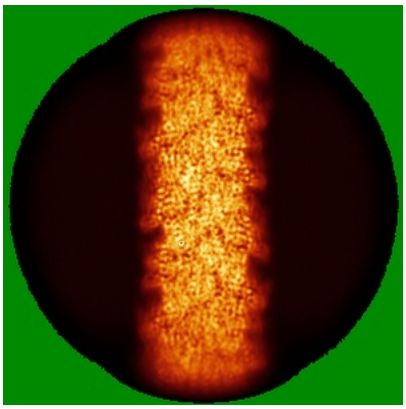


Z Index: 129

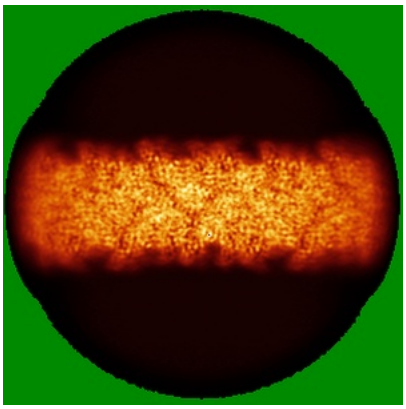
The images above show the largest variance slices of the map in three orthogonal directions.

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

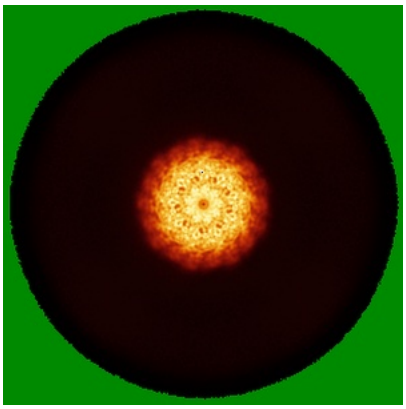
6.4.1 Primary map



X

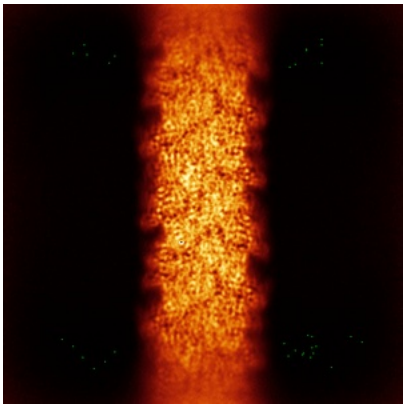


Y

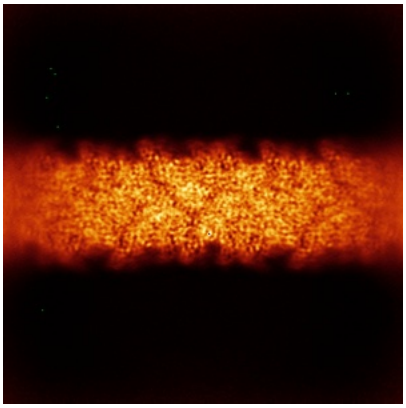


Z

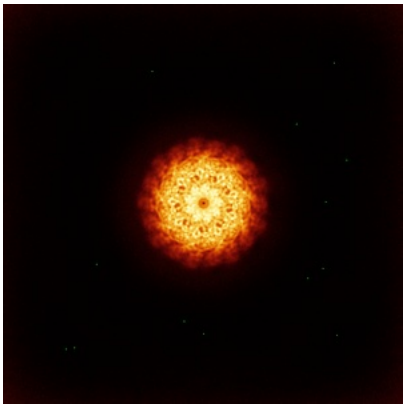
6.4.2 Raw map



X



Y

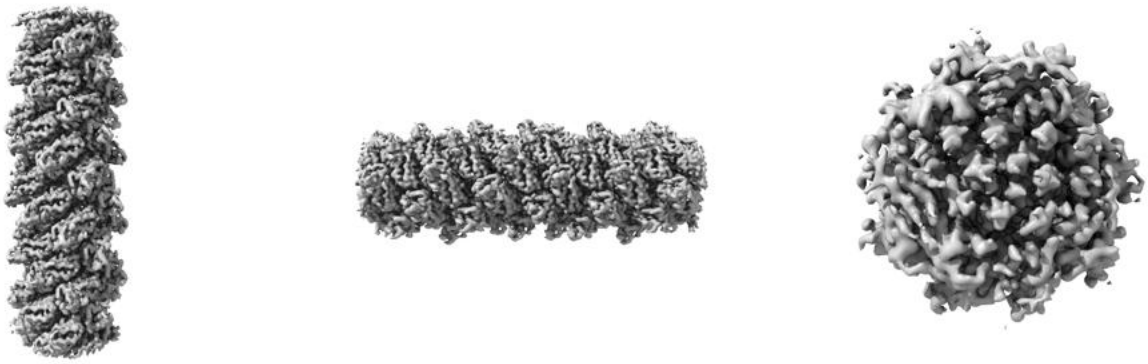


Z

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)

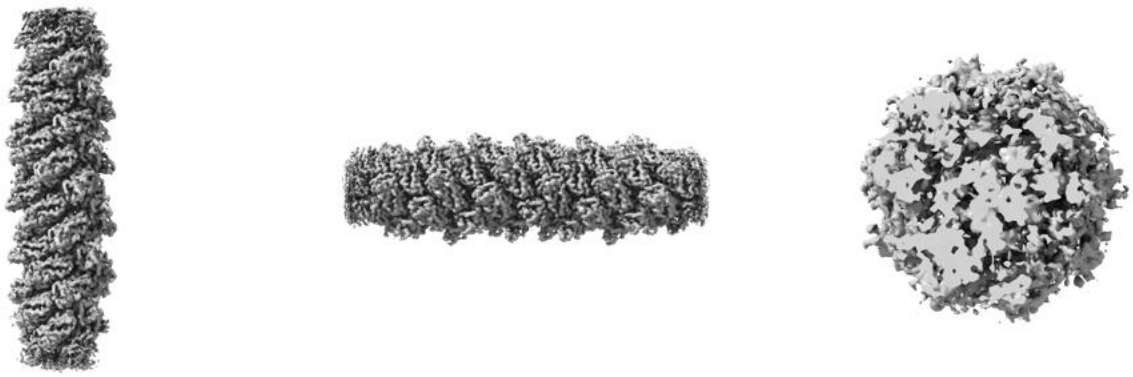
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.041. 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.

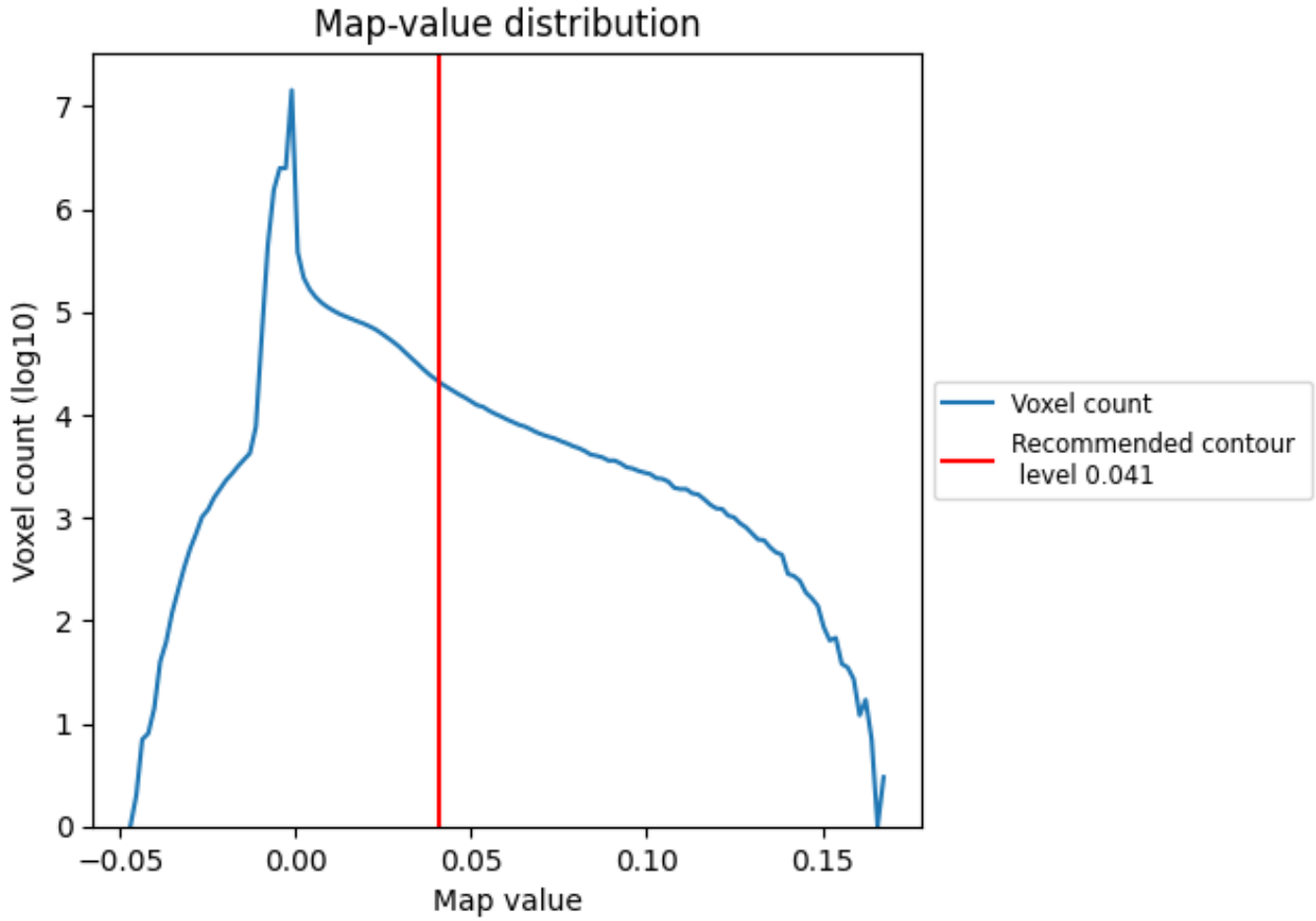
6.6 Mask visualisation (i)

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

7 Map analysis

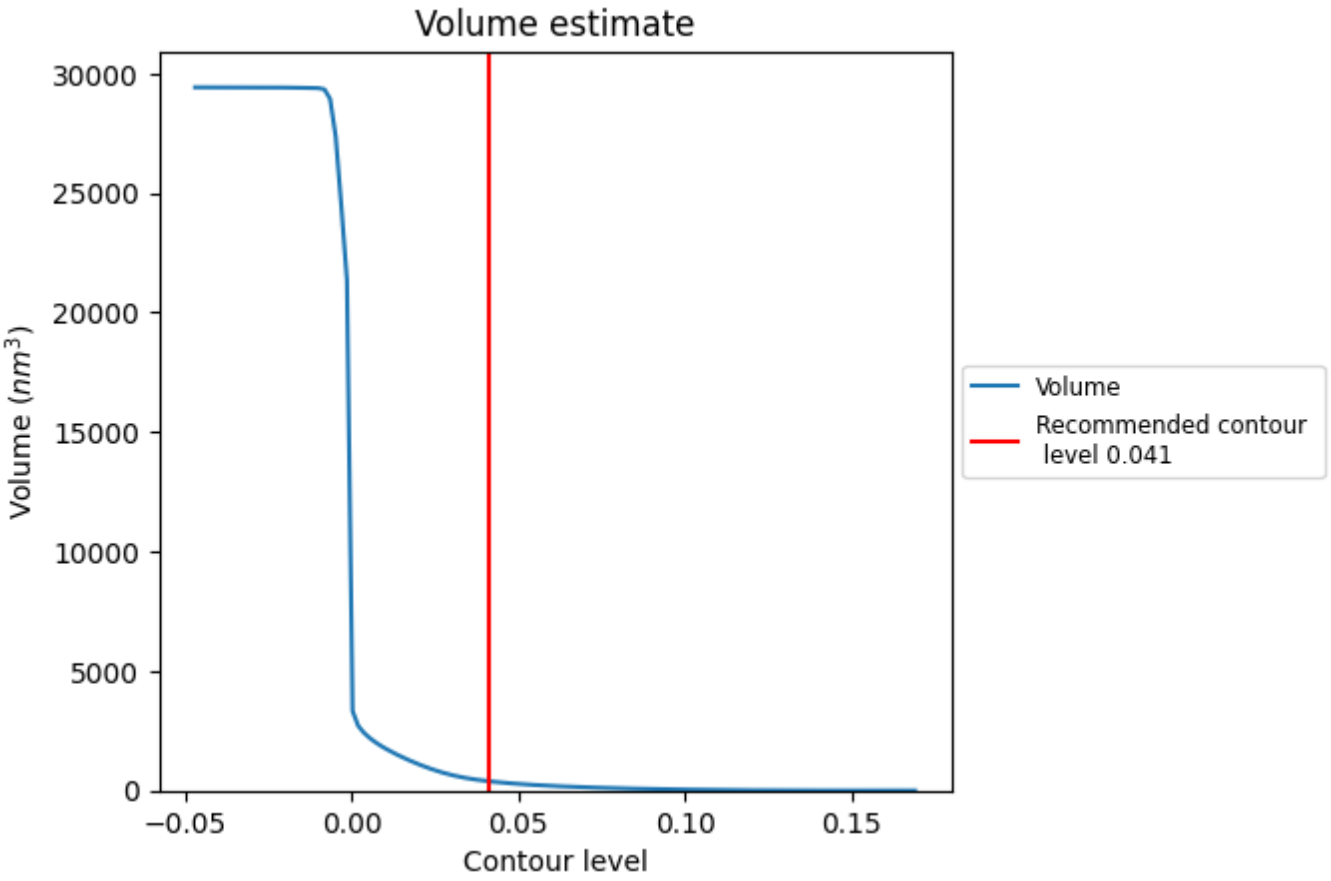
This section contains the results of statistical analysis of the map.

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.

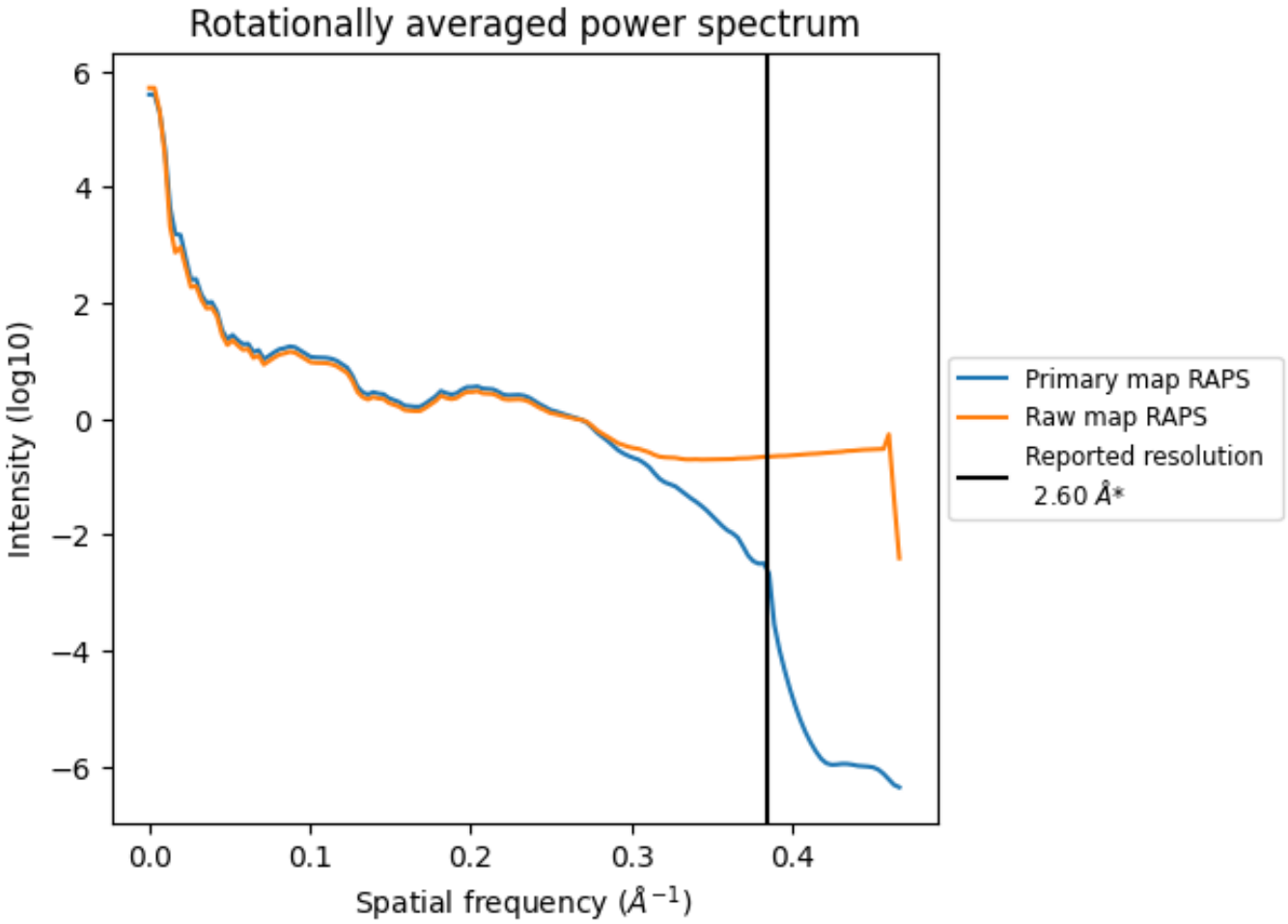
7.2 Volume estimate



The volume at the recommended contour level is 393 nm^3; this corresponds to an approximate mass of 355 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)

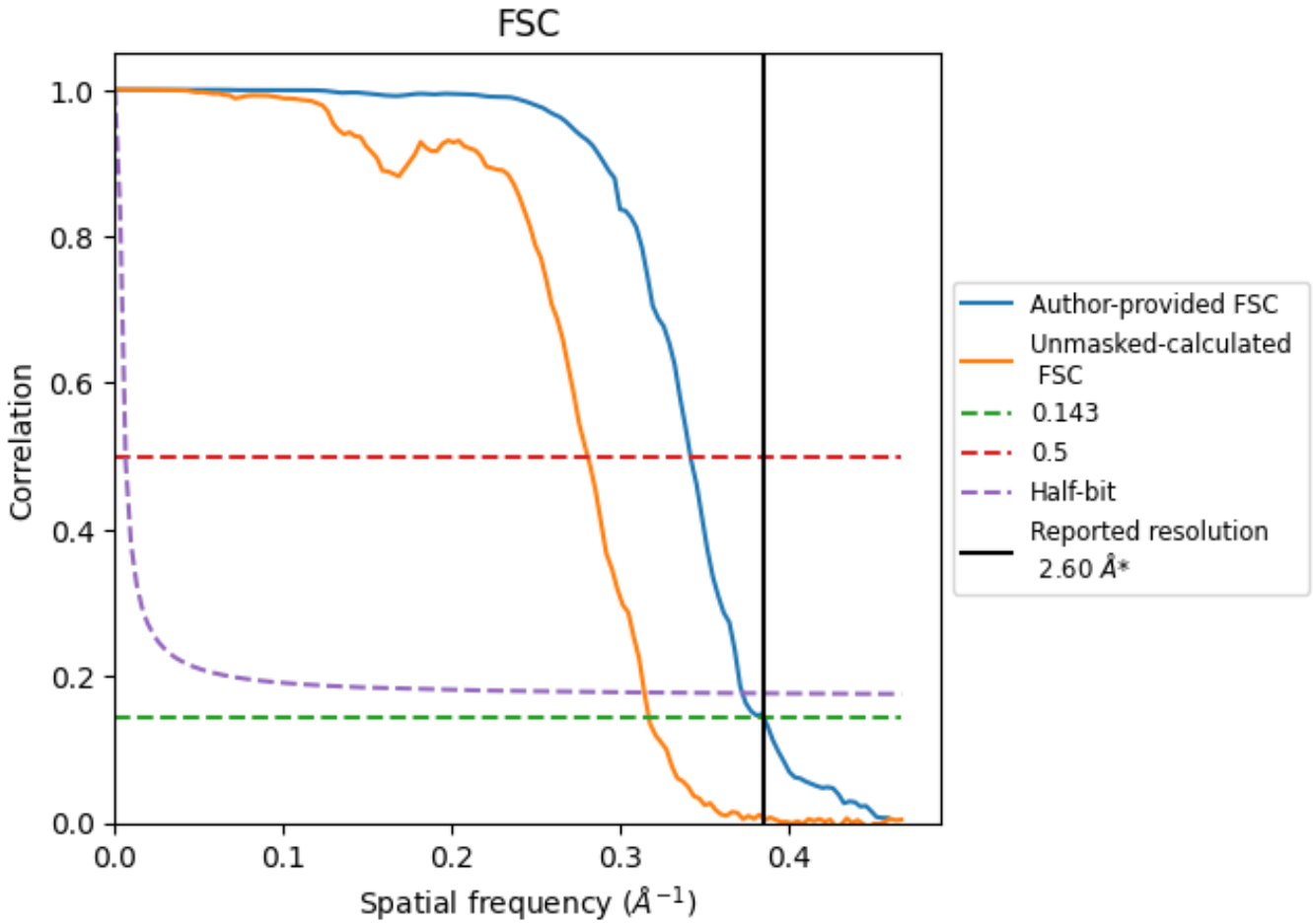


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

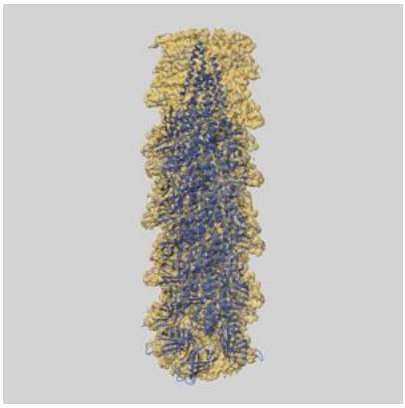
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	2.93	2.69
Unmasked-calculated*	3.16	3.57	3.18

*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 3.16 differs from the reported value 2.6 by more than 10 %

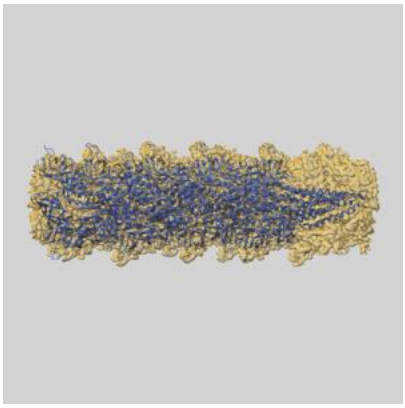
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19960 and PDB model 9ETS. Per-residue inclusion information can be found in section 3 on page 17.

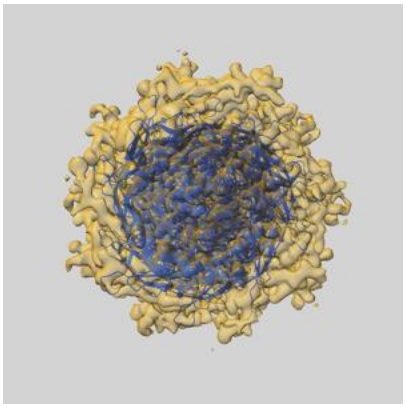
9.1 Map-model overlay



X



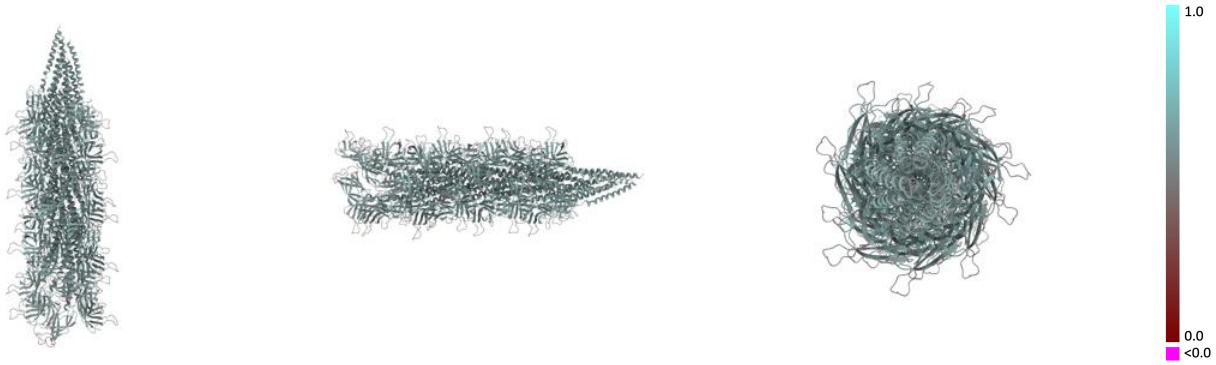
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.041 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.

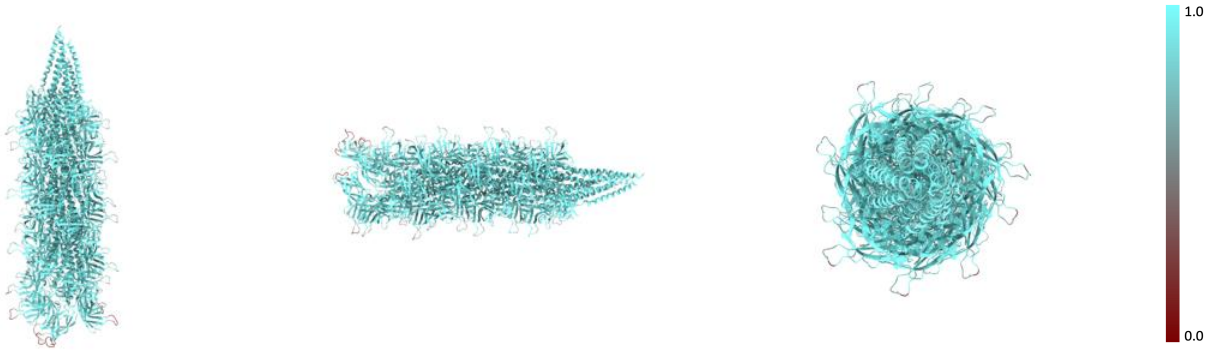
9.2 Q-score mapped to coordinate model



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.

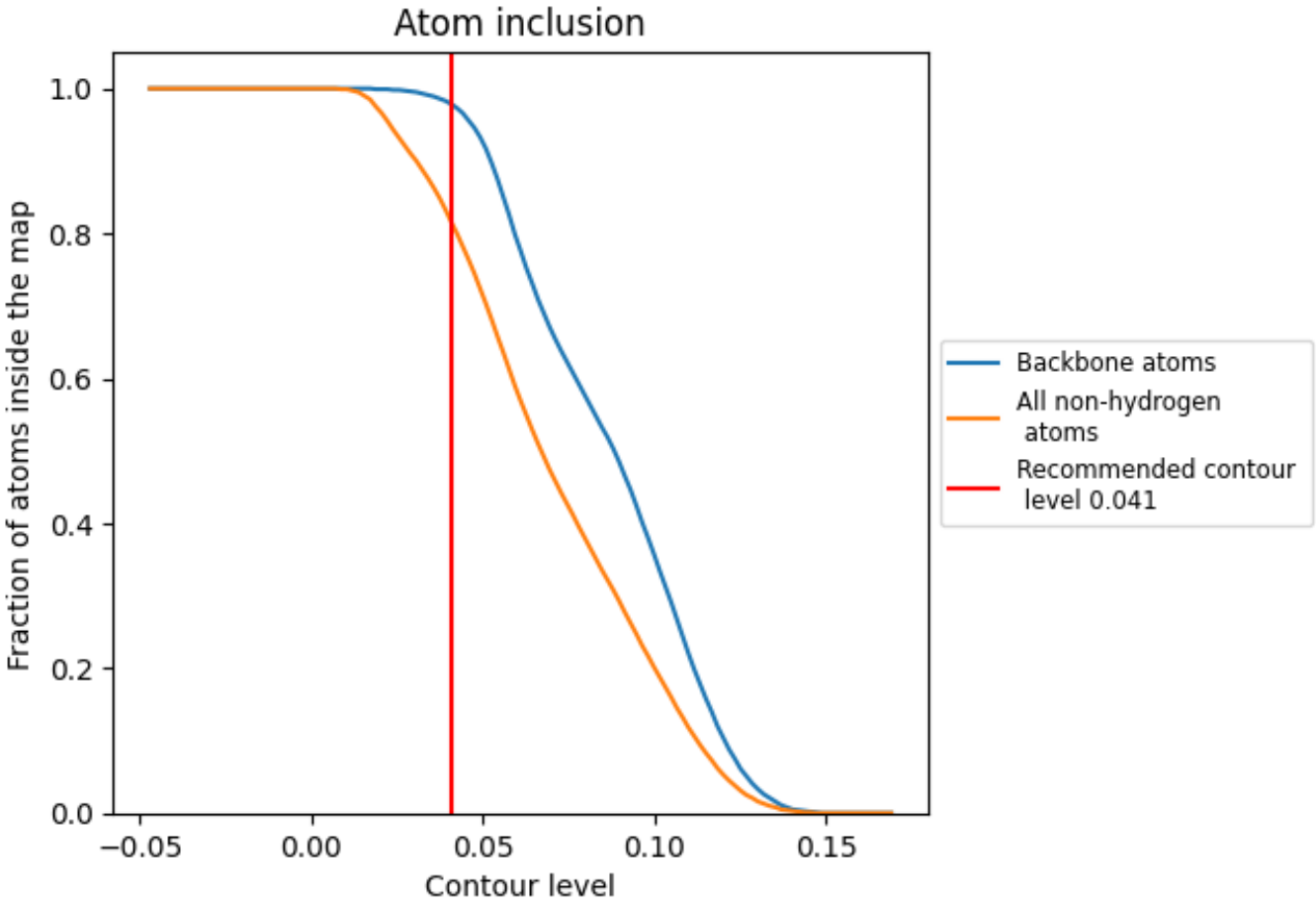
9.3 Atom inclusion mapped to coordinate model



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 (0.041).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 81% 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 (0.041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.5170
0	0.3440	0.2500
0A	0.0770	0.2110
1	0.1560	0.2500
1A	0.3280	0.3230
2	0.1280	0.1750
2A	0.1890	0.2050
3	0.3280	0.2360
3A	0.1030	0.2440
4	0.1560	0.2460
4A	0.3590	0.3220
5	0.0510	0.1780
5A	0.1890	0.2190
6	0.2810	0.2290
6A	0.1280	0.2390
7	0.1560	0.2450
7A	0.3280	0.3430
8	0.0510	0.1960
8A	0.1700	0.2170
9	0.2810	0.2160
9A	0.1280	0.2110
A	0.9120	0.5600
AA	0.1720	0.2620
AB	0.3280	0.3190
B	0.8900	0.5420
BA	0.0260	0.1650
BB	0.1510	0.1780
C	0.9170	0.5650
CA	0.2030	0.1870
CB	0.1030	0.2230
D	0.9130	0.5660
DA	0.1720	0.2660
DB	0.3280	0.3210
E	0.9010	0.5480
EA	0.0260	0.1780

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Chain	Atom inclusion	Q-score
EB	0.1510	0.1750
F	0.9230	0.5690
FA	0.1880	0.1700
FB	0.1030	0.2300
G	0.9190	0.5690
GA	0.1250	0.2120
GB	0.3440	0.3220
H	0.9090	0.5540
HA	0.0000	0.1750
HB	0.1510	0.1410
I	0.9370	0.5740
IA	0.1090	0.1630
IB	0.1030	0.2630
J	0.9200	0.5740
JA	0.1090	0.1680
JB	0.3120	0.3240
K	0.9100	0.5510
KA	0.0000	0.1310
KB	0.1700	0.1460
L	0.9400	0.5750
LA	0.5470	0.3580
LB	0.1030	0.3060
M	0.9200	0.5730
MA	0.2640	0.3160
MB	0.3120	0.2870
N	0.9090	0.5540
NA	0.1540	0.3390
NB	0.1510	0.1580
O	0.9420	0.5780
OA	0.5160	0.3620
OB	0.1030	0.2980
P	0.9210	0.5710
PA	0.2260	0.3310
PB	0.2810	0.2730
Q	0.9100	0.5560
QA	0.1540	0.3060
QB	0.1320	0.1260
R	0.9370	0.5770
RA	0.5160	0.3480
RB	0.0770	0.2800
S	0.9180	0.5670
SA	0.2450	0.3110

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Chain	Atom inclusion	Q-score
SB	0.1410	0.2030
T	0.9160	0.5560
TA	0.1540	0.3380
TB	0.1320	0.1440
U	0.9420	0.5760
UA	0.5310	0.3710
UB	0.0000	0.2190
V	0.9150	0.5660
VA	0.2830	0.2830
VB	0.0000	0.1380
W	0.9140	0.5530
WA	0.1790	0.3190
WB	0.0190	0.1070
X	0.9380	0.5710
XA	0.5310	0.3860
XB	0.0000	0.2150
Y	0.9090	0.5620
YA	0.2640	0.2700
Z	0.9130	0.5510
ZA	0.1790	0.2770
a	0.9340	0.5680
aA	0.5470	0.3840
b	0.8980	0.5550
bA	0.2450	0.2890
c	0.9030	0.5490
cA	0.1790	0.2770
d	0.9280	0.5640
dA	0.5310	0.3840
e	0.8940	0.5500
eA	0.3210	0.2840
f	0.8910	0.5420
fA	0.1790	0.2940
g	0.9090	0.5570
gA	0.5310	0.3920
h	0.8660	0.5400
hA	0.3020	0.2810
i	0.8690	0.5350
iA	0.1540	0.2790
j	0.8790	0.5490
jA	0.4530	0.3910
k	0.2810	0.2000
kA	0.2640	0.2870

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Chain	Atom inclusion	Q-score
l	0.7530	0.5140
lA	0.1540	0.2560
m	0.1560	0.2150
mA	0.4060	0.3620
n	0.1540	0.1420
nA	0.2070	0.2740
o	0.2810	0.2360
oA	0.1280	0.2470
p	0.1410	0.2090
pA	0.3590	0.3190
q	0.1280	0.1470
qA	0.1890	0.2650
r	0.2810	0.2340
rA	0.1280	0.2500
s	0.1560	0.2010
sA	0.2340	0.2350
t	0.1790	0.1440
tA	0.1510	0.2280
u	0.3120	0.2290
uA	0.0770	0.2540
v	0.1560	0.2250
vA	0.3120	0.3270
w	0.1540	0.1360
wA	0.1700	0.2290
x	0.3590	0.2450
xA	0.1280	0.2270
y	0.1560	0.2440
yA	0.3120	0.2920
z	0.1030	0.1380
zA	0.1700	0.1130