wwPDB EM Validation Summary Report

Dec 21, 2024 – 03:44 pm GMT

PDB ID	:	8REY
EMDB ID	:	EMD-19112
Title	:	Cuniculiplasma divulgatum filament
Authors	:	Isupov, M.N.; Gaines, M.; Daum, B.; McLaren, M.
Deposited on	:	2023-12-12
Resolution	:	2.61 Å(reported)

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

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

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

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

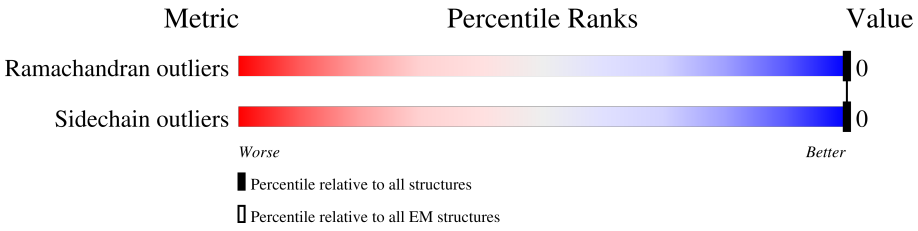
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.61 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	135	100%
1	B	135	100%
1	C	135	100%
1	D	135	100%
1	E	135	100%
1	F	135	100%
1	G	135	100%
1	H	135	100%
1	I	135	100%

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Mol	Chain	Length	Quality of chain
1	J	135	100%
1	K	135	100%
1	L	135	100%
1	M	135	100%
1	N	135	100%
1	O	135	100%
1	P	135	100%
1	Q	135	100%
1	R	135	100%
1	S	135	100%
1	T	135	100%
1	U	135	100%
1	V	135	100%
1	W	135	100%
1	X	135	100%
1	Y	135	100%
1	Z	135	100%
1	a	135	100%
1	b	135	100%
1	c	135	100%
1	d	135	100%
1	e	135	100%
1	f	135	100%
1	g	135	100%
1	h	135	100%

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Mol	Chain	Length	Quality of chain
1	i	135	100%
1	j	135	5% 100%
2	0	7	43% 71% 29%
2	0A	7	57% 57% 43%
2	0B	7	71% 57% 43%
2	2	7	57% 57% 43%
2	2A	7	43% 71% 29%
2	2B	7	71% 57% 43%
2	4	7	43% 71% 29%
2	4A	7	57% 57% 43%
2	6	7	57% 57% 43%
2	6A	7	43% 71% 29%
2	8	7	43% 71% 29%
2	8A	7	57% 57% 43%
2	AA	7	57% 57% 43%
2	AB	7	43% 71% 29%
2	CA	7	43% 71% 29%
2	CB	7	57% 57% 43%
2	EA	7	57% 57% 43%
2	EB	7	43% 57% 43%
2	GA	7	43% 57% 43%
2	GB	7	57% 57% 43%
2	IA	7	57% 57% 43%
2	IB	7	43% 57% 43%
2	KA	7	43% 71% 29%

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Mol	Chain	Length	Quality of chain
2	KB	7	57% 57% 43%
2	MA	7	57% 57% 43%
2	MB	7	43% 71% 29%
2	OA	7	29% 71% 29%
2	OB	7	57% 57% 43%
2	QA	7	57% 57% 43%
2	QB	7	43% 71% 29%
2	SA	7	29% 71% 29%
2	SB	7	57% 57% 43%
2	UA	7	57% 57% 43%
2	UB	7	43% 57% 43%
2	WA	7	43% 71% 29%
2	WB	7	57% 57% 43%
2	YA	7	57% 57% 43%
2	YB	7	43% 57% 43%
2	aA	7	29% 71% 29%
2	aB	7	57% 57% 43%
2	cA	7	57% 57% 43%
2	cB	7	43% 57% 43%
2	eA	7	29% 71% 29%
2	eB	7	57% 57% 43%
2	gA	7	57% 57% 43%
2	gB	7	43% 57% 43%
2	iA	7	29% 71% 29%
2	iB	7	57% 57% 43%

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Mol	Chain	Length	Quality of chain
2	k	7	29% 57% 43%
2	kA	7	57% 57% 43%
2	kB	7	57% 57% 43%
2	m	7	57% 57% 43%
2	mA	7	29% 71% 29%
2	mB	7	71% 57% 43%
2	o	7	43% 71% 29%
2	oA	7	57% 57% 43%
2	oB	7	57% 71% 29%
2	q	7	57% 57% 43%
2	qA	7	29% 57% 43%
2	qB	7	57% 57% 43%
2	s	7	43% 71% 29%
2	sA	7	57% 57% 43%
2	sB	7	57% 71% 29%
2	u	7	57% 57% 43%
2	uA	7	29% 71% 29%
2	uB	7	71% 57% 43%
2	w	7	43% 57% 43%
2	wA	7	57% 57% 43%
2	wB	7	57% 57% 43%
2	y	7	57% 57% 43%
2	yA	7	43% 71% 29%
2	yB	7	71% 57% 43%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40140 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellin-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	M	135	Total 951	C 603	N 148	O 200	0	0
1	C	135	Total 951	C 603	N 148	O 200	0	0
1	A	135	Total 951	C 603	N 148	O 200	0	0
1	B	135	Total 951	C 603	N 148	O 200	0	0
1	D	135	Total 951	C 603	N 148	O 200	0	0
1	E	135	Total 951	C 603	N 148	O 200	0	0
1	F	135	Total 951	C 603	N 148	O 200	0	0
1	G	135	Total 951	C 603	N 148	O 200	0	0
1	H	135	Total 951	C 603	N 148	O 200	0	0
1	I	135	Total 951	C 603	N 148	O 200	0	0
1	J	135	Total 951	C 603	N 148	O 200	0	0
1	K	135	Total 951	C 603	N 148	O 200	0	0
1	L	135	Total 951	C 603	N 148	O 200	0	0
1	N	135	Total 951	C 603	N 148	O 200	0	0
1	O	135	Total 951	C 603	N 148	O 200	0	0
1	P	135	Total 951	C 603	N 148	O 200	0	0
1	Q	135	Total 951	C 603	N 148	O 200	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	135	Total 951	C 603	N 148	O 200	0	0
1	S	135	Total 951	C 603	N 148	O 200	0	0
1	T	135	Total 951	C 603	N 148	O 200	0	0
1	U	135	Total 951	C 603	N 148	O 200	0	0
1	V	135	Total 951	C 603	N 148	O 200	0	0
1	W	135	Total 951	C 603	N 148	O 200	0	0
1	X	135	Total 951	C 603	N 148	O 200	0	0
1	Y	135	Total 951	C 603	N 148	O 200	0	0
1	Z	135	Total 951	C 603	N 148	O 200	0	0
1	a	135	Total 951	C 603	N 148	O 200	0	0
1	b	135	Total 951	C 603	N 148	O 200	0	0
1	c	135	Total 951	C 603	N 148	O 200	0	0
1	d	135	Total 951	C 603	N 148	O 200	0	0
1	e	135	Total 951	C 603	N 148	O 200	0	0
1	f	135	Total 951	C 603	N 148	O 200	0	0
1	g	135	Total 951	C 603	N 148	O 200	0	0
1	h	135	Total 951	C 603	N 148	O 200	0	0
1	i	135	Total 951	C 603	N 148	O 200	0	0
1	j	135	Total 951	C 603	N 148	O 200	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	k	7	Total	C	O	S	0	0
			82	43	38	1		
2	m	7	Total	C	O	S	0	0
			82	43	38	1		
2	o	7	Total	C	O	S	0	0
			82	43	38	1		
2	q	7	Total	C	O	S	0	0
			82	43	38	1		
2	s	7	Total	C	O	S	0	0
			82	43	38	1		
2	u	7	Total	C	O	S	0	0
			82	43	38	1		
2	w	7	Total	C	O	S	0	0
			82	43	38	1		
2	y	7	Total	C	O	S	0	0
			82	43	38	1		
2	0	7	Total	C	O	S	0	0
			82	43	38	1		
2	2	7	Total	C	O	S	0	0
			82	43	38	1		
2	4	7	Total	C	O	S	0	0
			82	43	38	1		
2	6	7	Total	C	O	S	0	0
			82	43	38	1		
2	8	7	Total	C	O	S	0	0
			82	43	38	1		
2	AA	7	Total	C	O	S	0	0
			82	43	38	1		
2	CA	7	Total	C	O	S	0	0
			82	43	38	1		
2	EA	7	Total	C	O	S	0	0
			82	43	38	1		
2	GA	7	Total	C	O	S	0	0
			82	43	38	1		
2	IA	7	Total	C	O	S	0	0
			82	43	38	1		
2	KA	7	Total	C	O	S	0	0
			82	43	38	1		
2	MA	7	Total	C	O	S	0	0
			82	43	38	1		
2	OA	7	Total	C	O	S	0	0
			82	43	38	1		
2	QA	7	Total	C	O	S	0	0
			82	43	38	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	SA	7	Total	C	O	S	0	0
			82	43	38	1		
2	UA	7	Total	C	O	S	0	0
			82	43	38	1		
2	WA	7	Total	C	O	S	0	0
			82	43	38	1		
2	YA	7	Total	C	O	S	0	0
			82	43	38	1		
2	aA	7	Total	C	O	S	0	0
			82	43	38	1		
2	cA	7	Total	C	O	S	0	0
			82	43	38	1		
2	eA	7	Total	C	O	S	0	0
			82	43	38	1		
2	gA	7	Total	C	O	S	0	0
			82	43	38	1		
2	iA	7	Total	C	O	S	0	0
			82	43	38	1		
2	kA	7	Total	C	O	S	0	0
			82	43	38	1		
2	mA	7	Total	C	O	S	0	0
			82	43	38	1		
2	oA	7	Total	C	O	S	0	0
			82	43	38	1		
2	qA	7	Total	C	O	S	0	0
			82	43	38	1		
2	sA	7	Total	C	O	S	0	0
			82	43	38	1		
2	uA	7	Total	C	O	S	0	0
			82	43	38	1		
2	wA	7	Total	C	O	S	0	0
			82	43	38	1		
2	yA	7	Total	C	O	S	0	0
			82	43	38	1		
2	0A	7	Total	C	O	S	0	0
			82	43	38	1		
2	2A	7	Total	C	O	S	0	0
			82	43	38	1		
2	4A	7	Total	C	O	S	0	0
			82	43	38	1		
2	6A	7	Total	C	O	S	0	0
			82	43	38	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	8A	7	Total	C	O	S	0	0
			82	43	38	1		
2	AB	7	Total	C	O	S	0	0
			82	43	38	1		
2	CB	7	Total	C	O	S	0	0
			82	43	38	1		
2	EB	7	Total	C	O	S	0	0
			82	43	38	1		
2	GB	7	Total	C	O	S	0	0
			82	43	38	1		
2	IB	7	Total	C	O	S	0	0
			82	43	38	1		
2	KB	7	Total	C	O	S	0	0
			82	43	38	1		
2	MB	7	Total	C	O	S	0	0
			82	43	38	1		
2	OB	7	Total	C	O	S	0	0
			82	43	38	1		
2	QB	7	Total	C	O	S	0	0
			82	43	38	1		
2	SB	7	Total	C	O	S	0	0
			82	43	38	1		
2	UB	7	Total	C	O	S	0	0
			82	43	38	1		
2	WB	7	Total	C	O	S	0	0
			82	43	38	1		
2	YB	7	Total	C	O	S	0	0
			82	43	38	1		
2	aB	7	Total	C	O	S	0	0
			82	43	38	1		
2	cB	7	Total	C	O	S	0	0
			82	43	38	1		
2	eB	7	Total	C	O	S	0	0
			82	43	38	1		
2	gB	7	Total	C	O	S	0	0
			82	43	38	1		
2	iB	7	Total	C	O	S	0	0
			82	43	38	1		
2	kB	7	Total	C	O	S	0	0
			82	43	38	1		
2	mB	7	Total	C	O	S	0	0
			82	43	38	1		

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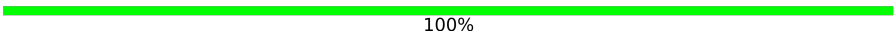
Mol	Chain	Residues	Atoms				AltConf	Trace
2	oB	7	Total	C	O	S	0	0
			82	43	38	1		
2	qB	7	Total	C	O	S	0	0
			82	43	38	1		
2	sB	7	Total	C	O	S	0	0
			82	43	38	1		
2	uB	7	Total	C	O	S	0	0
			82	43	38	1		
2	wB	7	Total	C	O	S	0	0
			82	43	38	1		
2	yB	7	Total	C	O	S	0	0
			82	43	38	1		
2	0B	7	Total	C	O	S	0	0
			82	43	38	1		
2	2B	7	Total	C	O	S	0	0
			82	43	38	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: Flagellin-like protein

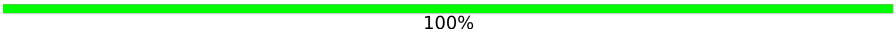
Chain M:



There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

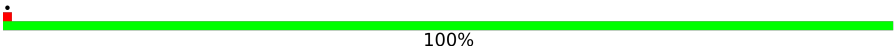
Chain C:



There are no outlier residues recorded for this chain.

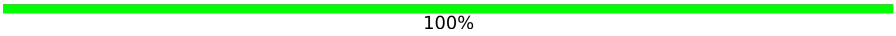
• Molecule 1: Flagellin-like protein

Chain A:



• Molecule 1: Flagellin-like protein

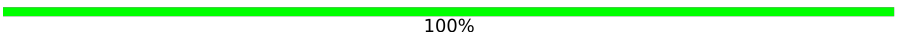
Chain B:



There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

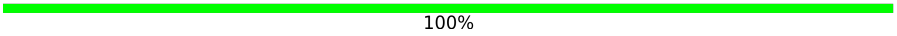
Chain D:



There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain E:



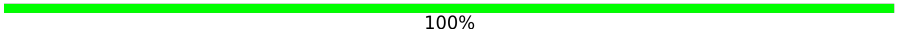
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain F: 

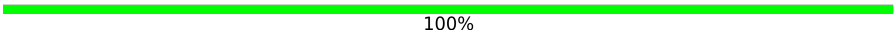
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain G: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain H: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain I: 

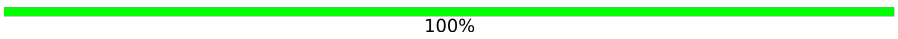
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain J: 

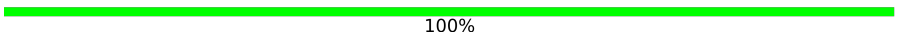
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain K: 

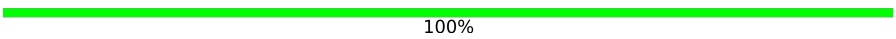
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain L: 

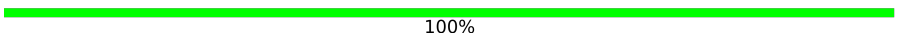
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain N: 

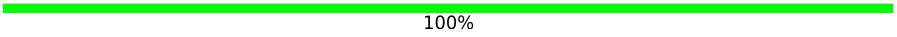
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain O: 

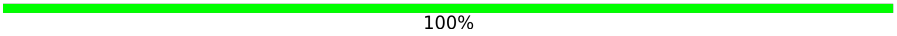
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain P: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain Q: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain R: 

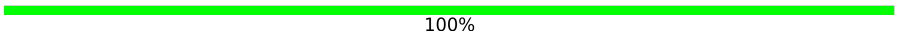
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain S: 

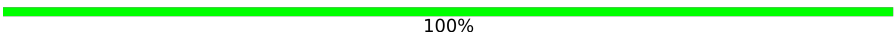
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain T: 

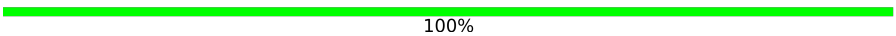
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain U: 

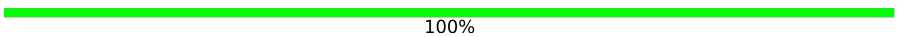
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain V: 

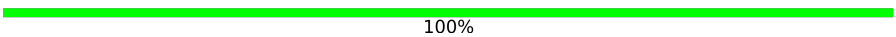
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain W: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain X: 

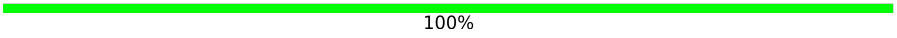
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain Y: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain Z: 

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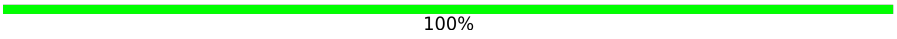
• Molecule 1: Flagellin-like protein

Chain a: 

There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain b: 

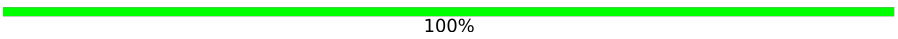
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain c: 

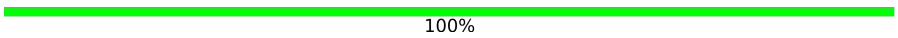
There are no outlier residues recorded for this chain.

• Molecule 1: Flagellin-like protein

Chain d: 

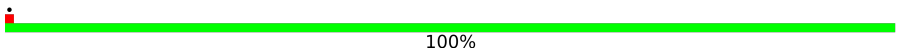
There are no outlier residues recorded for this chain.

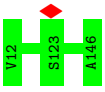
• Molecule 1: Flagellin-like protein

Chain e: 

There are no outlier residues recorded for this chain.

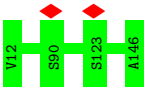
• Molecule 1: Flagellin-like protein

Chain f: 



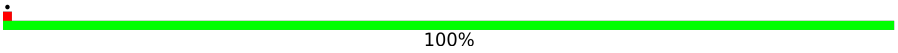
• Molecule 1: Flagellin-like protein

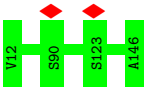
Chain g: 



• Molecule 1: Flagellin-like protein

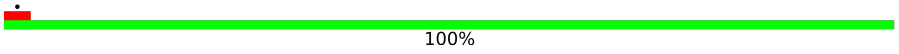
Chain h:

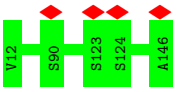




• Molecule 1: Flagellin-like protein

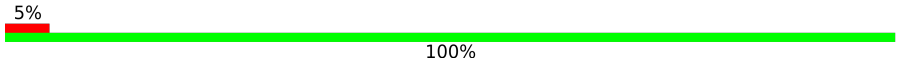
Chain i:

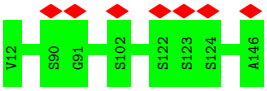




• Molecule 1: Flagellin-like protein

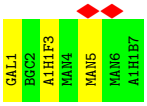
Chain j:





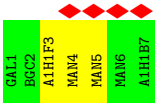
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain k:



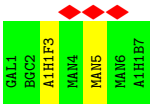
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain m:



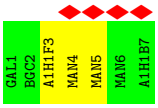
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain o:



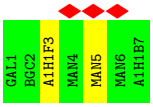
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain q:



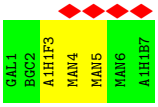
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain s:



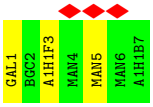
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain u:



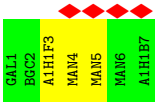
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain w:



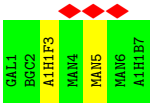
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain y:



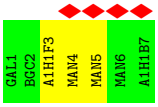
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 0:



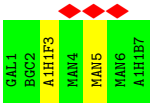
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 2:



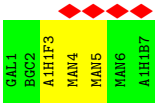
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 4:



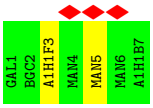
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 6:



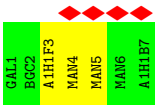
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 8:



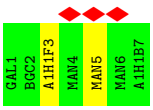
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain AA:



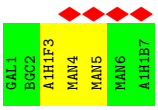
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain CA:



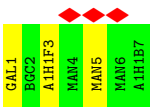
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain EA:



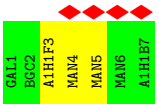
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain GA:



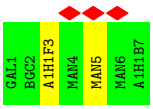
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain IA:



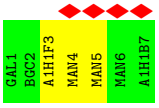
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain KA:



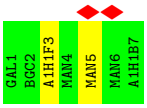
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain MA:



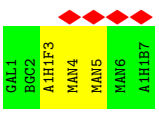
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain OA:



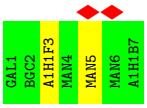
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain QA:



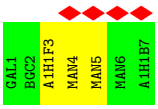
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain SA:



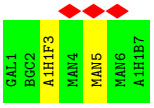
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain UA:



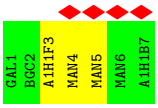
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain WA:



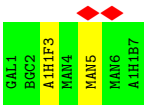
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain YA:



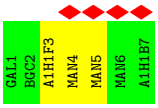
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain aA:



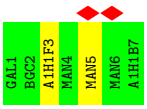
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain cA:



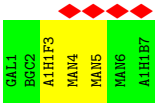
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain eA:



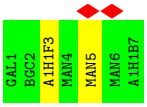
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain gA:



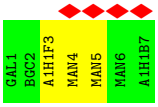
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain iA:



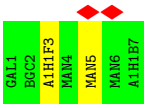
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain kA:



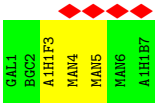
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain mA:



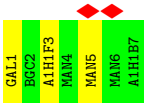
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain oA:



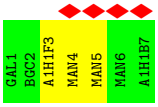
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain qA:



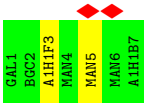
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain sA:



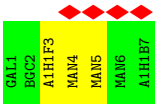
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain uA:



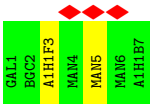
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain wA:



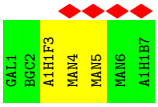
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain yA:



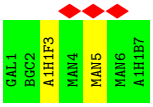
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 0A:



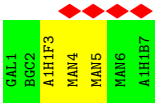
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 2A:



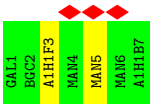
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 4A:



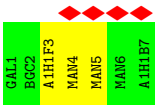
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 6A:



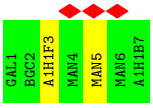
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 8A:



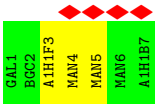
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain AB:



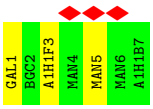
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain CB:



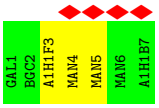
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain EB:



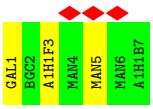
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain GB:



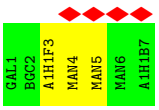
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain IB:



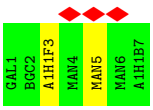
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain KB:



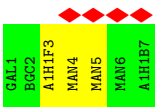
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain MB:



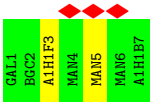
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain OB:



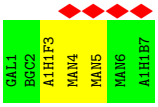
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain QB:



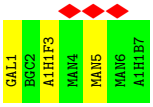
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain SB:



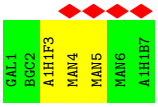
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain UB:



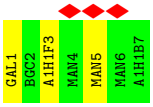
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain WB:



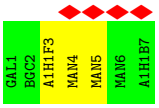
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain YB:



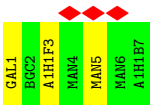
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain aB:



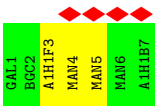
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain cB:



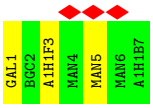
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain eB:



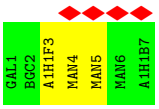
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain gB:



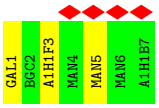
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain iB:



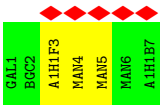
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain kB:



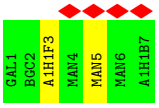
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain mB:



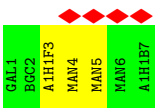
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain oB:



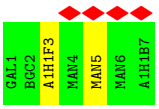
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain qB:



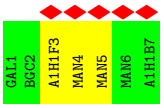
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain sB:



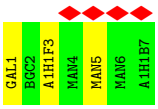
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain uB:



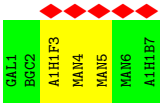
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain wB:



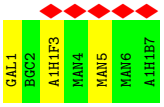
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain yB:



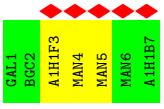
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[D-glycero-beta-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain 0B:



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

Chain 2B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=106.047°, rise=5.188 Å, axial sym=C1	Depositor
Number of segments used	645487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	51.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, A1H1B, GAL, A1H1F, BGC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.36	0/963	0.59	0/1318
1	B	0.36	0/963	0.59	0/1318
1	C	0.36	0/963	0.58	0/1318
1	D	0.36	0/963	0.59	0/1318
1	E	0.36	0/963	0.59	0/1318
1	F	0.36	0/963	0.59	0/1318
1	G	0.36	0/963	0.59	0/1318
1	H	0.36	0/963	0.59	0/1318
1	I	0.36	0/963	0.59	0/1318
1	J	0.36	0/963	0.59	0/1318
1	K	0.36	0/963	0.59	0/1318
1	L	0.36	0/963	0.59	0/1318
1	M	0.36	0/963	0.59	0/1318
1	N	0.36	0/963	0.59	0/1318
1	O	0.36	0/963	0.59	0/1318
1	P	0.36	0/963	0.59	0/1318
1	Q	0.36	0/963	0.59	0/1318
1	R	0.36	0/963	0.59	0/1318
1	S	0.36	0/963	0.59	0/1318
1	T	0.36	0/963	0.59	0/1318
1	U	0.36	0/963	0.59	0/1318
1	V	0.36	0/963	0.59	0/1318
1	W	0.36	0/963	0.59	0/1318
1	X	0.36	0/963	0.59	0/1318
1	Y	0.36	0/963	0.59	0/1318
1	Z	0.36	0/963	0.59	0/1318
1	a	0.36	0/963	0.59	0/1318
1	b	0.36	0/963	0.59	0/1318
1	c	0.36	0/963	0.59	0/1318
1	d	0.36	0/963	0.59	0/1318
1	e	0.36	0/963	0.59	0/1318
1	f	0.36	0/963	0.59	0/1318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	g	0.36	0/963	0.59	0/1318
1	h	0.36	0/963	0.59	0/1318
1	i	0.36	0/963	0.59	0/1318
1	j	0.36	0/963	0.59	0/1318
All	All	0.36	0/34668	0.59	0/47448

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	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	B	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	C	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	D	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	E	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	F	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	G	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	H	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	I	133/135 (98%)	130 (98%)	3 (2%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	K	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	L	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	M	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	N	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	O	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	P	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	Q	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	R	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	S	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	T	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	U	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	V	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	W	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	X	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	Y	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	a	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	b	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	c	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	d	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	e	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	f	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	g	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	h	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	i	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	j	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
All	All	4788/4860 (98%)	4680 (98%)	108 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/110 (100%)	110 (100%)	0	100	100
1	B	110/110 (100%)	110 (100%)	0	100	100
1	C	110/110 (100%)	110 (100%)	0	100	100
1	D	110/110 (100%)	110 (100%)	0	100	100
1	E	110/110 (100%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100

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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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
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%)	110 (100%)	0	100	100
1	j	110/110 (100%)	110 (100%)	0	100	100
All	All	3960/3960 (100%)	3960 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

504 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	GAL	0	1	1,2	11,11,12	0.34	0	15,15,17	0.97	0
2	BGC	0	2	2	11,11,12	0.19	0	15,15,17	0.59	0
2	A1H1F	0	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.05	3 (16%)
2	MAN	0	4	2	11,11,12	0.46	0	15,15,17	0.80	0
2	MAN	0	5	2	11,11,12	0.45	0	15,15,17	1.26	1 (6%)
2	MAN	0	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	0	7	2	13,13,14	0.40	0	17,18,20	0.61	0
2	GAL	0A	1	1,2	11,11,12	0.38	0	15,15,17	0.72	0
2	BGC	0A	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	0A	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.63	4 (22%)
2	MAN	0A	4	2	11,11,12	0.71	0	15,15,17	1.25	2 (13%)
2	MAN	0A	5	2	11,11,12	0.42	0	15,15,17	1.32	1 (6%)
2	MAN	0A	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	0A	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	0B	1	1,2	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
2	BGC	0B	2	2	11,11,12	0.20	0	15,15,17	0.56	0
2	A1H1F	0B	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.02	3 (16%)
2	MAN	0B	4	2	11,11,12	0.45	0	15,15,17	0.79	0
2	MAN	0B	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	0B	6	2	11,11,12	0.50	0	15,15,17	0.72	0
2	A1H1B	0B	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	2	1	1,2	11,11,12	0.38	0	15,15,17	0.72	0
2	BGC	2	2	2	11,11,12	0.26	0	15,15,17	0.69	0
2	A1H1F	2	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	2	4	2	11,11,12	0.72	0	15,15,17	1.20	1 (6%)
2	MAN	2	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	2	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	2	7	2	13,13,14	0.42	0	17,18,20	0.57	0
2	GAL	2A	1	1,2	11,11,12	0.34	0	15,15,17	0.97	0
2	BGC	2A	2	2	11,11,12	0.20	0	15,15,17	0.60	0
2	A1H1F	2A	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	2A	4	2	11,11,12	0.45	0	15,15,17	0.81	0
2	MAN	2A	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	2A	6	2	11,11,12	0.49	0	15,15,17	0.73	0
2	A1H1B	2A	7	2	13,13,14	0.39	0	17,18,20	0.61	0
2	GAL	2B	1	1,2	11,11,12	0.42	0	15,15,17	0.74	0
2	BGC	2B	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	2B	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.61	4 (22%)
2	MAN	2B	4	2	11,11,12	0.70	0	15,15,17	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	2B	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	2B	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	2B	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	4	1	1,2	11,11,12	0.34	0	15,15,17	0.93	0
2	BGC	4	2	2	11,11,12	0.19	0	15,15,17	0.62	0
2	A1H1F	4	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.05	3 (16%)
2	MAN	4	4	2	11,11,12	0.44	0	15,15,17	0.81	0
2	MAN	4	5	2	11,11,12	0.43	0	15,15,17	1.28	1 (6%)
2	MAN	4	6	2	11,11,12	0.50	0	15,15,17	0.74	0
2	A1H1B	4	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	4A	1	1,2	11,11,12	0.38	0	15,15,17	0.69	0
2	BGC	4A	2	2	11,11,12	0.27	0	15,15,17	0.70	0
2	A1H1F	4A	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	4A	4	2	11,11,12	0.73	0	15,15,17	1.20	1 (6%)
2	MAN	4A	5	2	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
2	MAN	4A	6	2	11,11,12	0.54	0	15,15,17	0.75	0
2	A1H1B	4A	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	6	1	1,2	11,11,12	0.39	0	15,15,17	0.69	0
2	BGC	6	2	2	11,11,12	0.25	0	15,15,17	0.68	0
2	A1H1F	6	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.64	4 (22%)
2	MAN	6	4	2	11,11,12	0.70	0	15,15,17	1.21	1 (6%)
2	MAN	6	5	2	11,11,12	0.43	0	15,15,17	1.34	1 (6%)
2	MAN	6	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	6	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	6A	1	1,2	11,11,12	0.35	0	15,15,17	0.91	0
2	BGC	6A	2	2	11,11,12	0.19	0	15,15,17	0.62	0
2	A1H1F	6A	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	6A	4	2	11,11,12	0.44	0	15,15,17	0.80	0
2	MAN	6A	5	2	11,11,12	0.43	0	15,15,17	1.28	1 (6%)
2	MAN	6A	6	2	11,11,12	0.51	0	15,15,17	0.73	0
2	A1H1B	6A	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	8	1	1,2	11,11,12	0.32	0	15,15,17	0.90	0
2	BGC	8	2	2	11,11,12	0.20	0	15,15,17	0.57	0
2	A1H1F	8	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.02	3 (16%)
2	MAN	8	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	8	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	8	6	2	11,11,12	0.49	0	15,15,17	0.74	0
2	A1H1B	8	7	2	13,13,14	0.40	0	17,18,20	0.63	0
2	GAL	8A	1	1,2	11,11,12	0.39	0	15,15,17	0.67	0
2	BGC	8A	2	2	11,11,12	0.25	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A1H1F	8A	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.64	4 (22%)
2	MAN	8A	4	2	11,11,12	0.70	0	15,15,17	1.21	1 (6%)
2	MAN	8A	5	2	11,11,12	0.43	0	15,15,17	1.34	1 (6%)
2	MAN	8A	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	8A	7	2	13,13,14	0.44	0	17,18,20	0.57	0
2	GAL	AA	1	1,2	11,11,12	0.36	0	15,15,17	0.70	0
2	BGC	AA	2	2	11,11,12	0.26	0	15,15,17	0.70	0
2	A1H1F	AA	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	AA	4	2	11,11,12	0.72	0	15,15,17	1.22	2 (13%)
2	MAN	AA	5	2	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
2	MAN	AA	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	AA	7	2	13,13,14	0.42	0	17,18,20	0.55	0
2	GAL	AB	1	1,2	11,11,12	0.30	0	15,15,17	0.91	0
2	BGC	AB	2	2	11,11,12	0.21	0	15,15,17	0.57	0
2	A1H1F	AB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	2 (11%)
2	MAN	AB	4	2	11,11,12	0.46	0	15,15,17	0.82	0
2	MAN	AB	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	AB	6	2	11,11,12	0.49	0	15,15,17	0.74	0
2	A1H1B	AB	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	CA	1	1,2	11,11,12	0.32	0	15,15,17	0.92	0
2	BGC	CA	2	2	11,11,12	0.21	0	15,15,17	0.59	0
2	A1H1F	CA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	CA	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	CA	5	2	11,11,12	0.45	0	15,15,17	1.27	1 (6%)
2	MAN	CA	6	2	11,11,12	0.50	0	15,15,17	0.72	0
2	A1H1B	CA	7	2	13,13,14	0.39	0	17,18,20	0.63	0
2	GAL	CB	1	1,2	11,11,12	0.36	0	15,15,17	0.71	0
2	BGC	CB	2	2	11,11,12	0.25	0	15,15,17	0.70	0
2	A1H1F	CB	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.61	3 (16%)
2	MAN	CB	4	2	11,11,12	0.73	0	15,15,17	1.23	2 (13%)
2	MAN	CB	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	CB	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	CB	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	EA	1	1,2	11,11,12	0.38	0	15,15,17	0.69	0
2	BGC	EA	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	EA	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.62	4 (22%)
2	MAN	EA	4	2	11,11,12	0.72	0	15,15,17	1.17	1 (6%)
2	MAN	EA	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	EA	6	2	11,11,12	0.54	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A1H1B	EA	7	2	13,13,14	0.43	0	17,18,20	0.57	0
2	GAL	EB	1	1,2	11,11,12	0.32	0	15,15,17	0.93	1 (6%)
2	BGC	EB	2	2	11,11,12	0.20	0	15,15,17	0.58	0
2	A1H1F	EB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	EB	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	EB	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	EB	6	2	11,11,12	0.50	0	15,15,17	0.72	0
2	A1H1B	EB	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	GA	1	1,2	11,11,12	0.36	0	15,15,17	1.00	1 (6%)
2	BGC	GA	2	2	11,11,12	0.20	0	15,15,17	0.59	0
2	A1H1F	GA	3	2	13,14,15	1.01	1 (7%)	18,21,23	1.05	3 (16%)
2	MAN	GA	4	2	11,11,12	0.46	0	15,15,17	0.84	0
2	MAN	GA	5	2	11,11,12	0.43	0	15,15,17	1.26	1 (6%)
2	MAN	GA	6	2	11,11,12	0.49	0	15,15,17	0.73	0
2	A1H1B	GA	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	GB	1	1,2	11,11,12	0.38	0	15,15,17	0.71	0
2	BGC	GB	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	GB	3	2	13,14,15	1.12	1 (7%)	18,21,23	1.65	4 (22%)
2	MAN	GB	4	2	11,11,12	0.72	0	15,15,17	1.19	1 (6%)
2	MAN	GB	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	GB	6	2	11,11,12	0.54	0	15,15,17	0.74	0
2	A1H1B	GB	7	2	13,13,14	0.43	0	17,18,20	0.57	0
2	GAL	IA	1	1,2	11,11,12	0.40	0	15,15,17	0.73	0
2	BGC	IA	2	2	11,11,12	0.24	0	15,15,17	0.70	0
2	A1H1F	IA	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	IA	4	2	11,11,12	0.70	0	15,15,17	1.24	2 (13%)
2	MAN	IA	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	IA	6	2	11,11,12	0.50	0	15,15,17	0.76	0
2	A1H1B	IA	7	2	13,13,14	0.42	0	17,18,20	0.55	0
2	GAL	IB	1	1,2	11,11,12	0.37	0	15,15,17	1.02	1 (6%)
2	BGC	IB	2	2	11,11,12	0.20	0	15,15,17	0.60	0
2	A1H1F	IB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	2 (11%)
2	MAN	IB	4	2	11,11,12	0.45	0	15,15,17	0.83	0
2	MAN	IB	5	2	11,11,12	0.43	0	15,15,17	1.26	1 (6%)
2	MAN	IB	6	2	11,11,12	0.50	0	15,15,17	0.73	0
2	A1H1B	IB	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	KA	1	1,2	11,11,12	0.35	0	15,15,17	0.96	0
2	BGC	KA	2	2	11,11,12	0.19	0	15,15,17	0.60	0
2	A1H1F	KA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	KA	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	KA	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	KA	6	2	11,11,12	0.50	0	15,15,17	0.72	0
2	A1H1B	KA	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	KB	1	1,2	11,11,12	0.41	0	15,15,17	0.73	0
2	BGC	KB	2	2	11,11,12	0.24	0	15,15,17	0.70	0
2	A1H1F	KB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.62	5 (27%)
2	MAN	KB	4	2	11,11,12	0.71	0	15,15,17	1.24	2 (13%)
2	MAN	KB	5	2	11,11,12	0.41	0	15,15,17	1.33	1 (6%)
2	MAN	KB	6	2	11,11,12	0.51	0	15,15,17	0.75	0
2	A1H1B	KB	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	MA	1	1,2	11,11,12	0.38	0	15,15,17	0.74	0
2	BGC	MA	2	2	11,11,12	0.26	0	15,15,17	0.70	0
2	A1H1F	MA	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.61	3 (16%)
2	MAN	MA	4	2	11,11,12	0.71	0	15,15,17	1.20	1 (6%)
2	MAN	MA	5	2	11,11,12	0.46	0	15,15,17	1.32	1 (6%)
2	MAN	MA	6	2	11,11,12	0.54	0	15,15,17	0.74	0
2	A1H1B	MA	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	MB	1	1,2	11,11,12	0.35	0	15,15,17	0.96	0
2	BGC	MB	2	2	11,11,12	0.20	0	15,15,17	0.57	0
2	A1H1F	MB	3	2	13,14,15	0.99	1 (7%)	18,21,23	1.03	2 (11%)
2	MAN	MB	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	MB	5	2	11,11,12	0.45	0	15,15,17	1.26	1 (6%)
2	MAN	MB	6	2	11,11,12	0.52	0	15,15,17	0.73	0
2	A1H1B	MB	7	2	13,13,14	0.39	0	17,18,20	0.63	0
2	GAL	OA	1	1,2	11,11,12	0.34	0	15,15,17	0.92	0
2	BGC	OA	2	2	11,11,12	0.20	0	15,15,17	0.62	0
2	A1H1F	OA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	OA	4	2	11,11,12	0.46	0	15,15,17	0.81	0
2	MAN	OA	5	2	11,11,12	0.43	0	15,15,17	1.28	1 (6%)
2	MAN	OA	6	2	11,11,12	0.49	0	15,15,17	0.73	0
2	A1H1B	OA	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	OB	1	1,2	11,11,12	0.39	0	15,15,17	0.74	0
2	BGC	OB	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	OB	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.61	3 (16%)
2	MAN	OB	4	2	11,11,12	0.72	0	15,15,17	1.19	1 (6%)
2	MAN	OB	5	2	11,11,12	0.44	0	15,15,17	1.31	1 (6%)
2	MAN	OB	6	2	11,11,12	0.54	0	15,15,17	0.75	0
2	A1H1B	OB	7	2	13,13,14	0.43	0	17,18,20	0.55	0
2	GAL	QA	1	1,2	11,11,12	0.36	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	QA	2	2	11,11,12	0.25	0	15,15,17	0.68	0
2	A1H1F	QA	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.63	4 (22%)
2	MAN	QA	4	2	11,11,12	0.70	0	15,15,17	1.23	1 (6%)
2	MAN	QA	5	2	11,11,12	0.42	0	15,15,17	1.34	1 (6%)
2	MAN	QA	6	2	11,11,12	0.51	0	15,15,17	0.75	0
2	A1H1B	QA	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	QB	1	1,2	11,11,12	0.32	0	15,15,17	0.92	0
2	BGC	QB	2	2	11,11,12	0.20	0	15,15,17	0.60	0
2	A1H1F	QB	3	2	13,14,15	1.01	1 (7%)	18,21,23	1.05	3 (16%)
2	MAN	QB	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	QB	5	2	11,11,12	0.42	0	15,15,17	1.28	1 (6%)
2	MAN	QB	6	2	11,11,12	0.50	0	15,15,17	0.74	0
2	A1H1B	QB	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	SA	1	1,2	11,11,12	0.32	0	15,15,17	0.92	0
2	BGC	SA	2	2	11,11,12	0.21	0	15,15,17	0.59	0
2	A1H1F	SA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	SA	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	SA	5	2	11,11,12	0.44	0	15,15,17	1.27	1 (6%)
2	MAN	SA	6	2	11,11,12	0.49	0	15,15,17	0.73	0
2	A1H1B	SA	7	2	13,13,14	0.40	0	17,18,20	0.61	0
2	GAL	SB	1	1,2	11,11,12	0.36	0	15,15,17	0.70	0
2	BGC	SB	2	2	11,11,12	0.26	0	15,15,17	0.67	0
2	A1H1F	SB	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.63	4 (22%)
2	MAN	SB	4	2	11,11,12	0.70	0	15,15,17	1.22	1 (6%)
2	MAN	SB	5	2	11,11,12	0.42	0	15,15,17	1.33	1 (6%)
2	MAN	SB	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	SB	7	2	13,13,14	0.43	0	17,18,20	0.57	0
2	GAL	UA	1	1,2	11,11,12	0.37	0	15,15,17	0.69	0
2	BGC	UA	2	2	11,11,12	0.26	0	15,15,17	0.70	0
2	A1H1F	UA	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.59	3 (16%)
2	MAN	UA	4	2	11,11,12	0.73	0	15,15,17	1.22	1 (6%)
2	MAN	UA	5	2	11,11,12	0.46	0	15,15,17	1.32	1 (6%)
2	MAN	UA	6	2	11,11,12	0.52	0	15,15,17	0.74	0
2	A1H1B	UA	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	UB	1	1,2	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
2	BGC	UB	2	2	11,11,12	0.21	0	15,15,17	0.57	0
2	A1H1F	UB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	UB	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	UB	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	UB	6	2	11,11,12	0.50	0	15,15,17	0.74	0
2	A1H1B	UB	7	2	13,13,14	0.39	0	17,18,20	0.61	0
2	GAL	WA	1	1,2	11,11,12	0.33	0	15,15,17	0.88	0
2	BGC	WA	2	2	11,11,12	0.20	0	15,15,17	0.61	0
2	A1H1F	WA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	WA	4	2	11,11,12	0.46	0	15,15,17	0.81	0
2	MAN	WA	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	WA	6	2	11,11,12	0.50	0	15,15,17	0.72	0
2	A1H1B	WA	7	2	13,13,14	0.39	0	17,18,20	0.63	0
2	GAL	WB	1	1,2	11,11,12	0.37	0	15,15,17	0.69	0
2	BGC	WB	2	2	11,11,12	0.26	0	15,15,17	0.70	0
2	A1H1F	WB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.59	3 (16%)
2	MAN	WB	4	2	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
2	MAN	WB	5	2	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
2	MAN	WB	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	WB	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	YA	1	1,2	11,11,12	0.37	0	15,15,17	0.69	0
2	BGC	YA	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	YA	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.63	4 (22%)
2	MAN	YA	4	2	11,11,12	0.72	0	15,15,17	1.18	1 (6%)
2	MAN	YA	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	YA	6	2	11,11,12	0.54	0	15,15,17	0.73	0
2	A1H1B	YA	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	YB	1	1,2	11,11,12	0.34	0	15,15,17	0.91	1 (6%)
2	BGC	YB	2	2	11,11,12	0.20	0	15,15,17	0.59	0
2	A1H1F	YB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	YB	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	YB	5	2	11,11,12	0.44	0	15,15,17	1.27	1 (6%)
2	MAN	YB	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	YB	7	2	13,13,14	0.40	0	17,18,20	0.63	0
2	GAL	aA	1	1,2	11,11,12	0.34	0	15,15,17	0.97	0
2	BGC	aA	2	2	11,11,12	0.20	0	15,15,17	0.60	0
2	A1H1F	aA	3	2	13,14,15	0.99	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	aA	4	2	11,11,12	0.44	0	15,15,17	0.80	0
2	MAN	aA	5	2	11,11,12	0.45	0	15,15,17	1.26	1 (6%)
2	MAN	aA	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	aA	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	aB	1	1,2	11,11,12	0.39	0	15,15,17	0.72	0
2	BGC	aB	2	2	11,11,12	0.25	0	15,15,17	0.68	0
2	A1H1F	aB	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.64	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	aB	4	2	11,11,12	0.69	0	15,15,17	1.19	1 (6%)
2	MAN	aB	5	2	11,11,12	0.43	0	15,15,17	1.33	1 (6%)
2	MAN	aB	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	aB	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	cA	1	1,2	11,11,12	0.38	0	15,15,17	0.72	0
2	BGC	cA	2	2	11,11,12	0.25	0	15,15,17	0.70	0
2	A1H1F	cA	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.61	4 (22%)
2	MAN	cA	4	2	11,11,12	0.73	0	15,15,17	1.19	1 (6%)
2	MAN	cA	5	2	11,11,12	0.46	0	15,15,17	1.32	1 (6%)
2	MAN	cA	6	2	11,11,12	0.54	0	15,15,17	0.74	0
2	A1H1B	cA	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	cB	1	1,2	11,11,12	0.32	0	15,15,17	0.96	1 (6%)
2	BGC	cB	2	2	11,11,12	0.21	0	15,15,17	0.56	0
2	A1H1F	cB	3	2	13,14,15	1.01	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	cB	4	2	11,11,12	0.46	0	15,15,17	0.83	0
2	MAN	cB	5	2	11,11,12	0.42	0	15,15,17	1.26	1 (6%)
2	MAN	cB	6	2	11,11,12	0.49	0	15,15,17	0.72	0
2	A1H1B	cB	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	eA	1	1,2	11,11,12	0.36	0	15,15,17	1.00	0
2	BGC	eA	2	2	11,11,12	0.21	0	15,15,17	0.64	0
2	A1H1F	eA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	eA	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	eA	5	2	11,11,12	0.42	0	15,15,17	1.28	1 (6%)
2	MAN	eA	6	2	11,11,12	0.50	0	15,15,17	0.72	0
2	A1H1B	eA	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	eB	1	1,2	11,11,12	0.39	0	15,15,17	0.74	0
2	BGC	eB	2	2	11,11,12	0.24	0	15,15,17	0.70	0
2	A1H1F	eB	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.60	5 (27%)
2	MAN	eB	4	2	11,11,12	0.72	0	15,15,17	1.25	2 (13%)
2	MAN	eB	5	2	11,11,12	0.43	0	15,15,17	1.31	1 (6%)
2	MAN	eB	6	2	11,11,12	0.50	0	15,15,17	0.75	0
2	A1H1B	eB	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	gA	1	1,2	11,11,12	0.38	0	15,15,17	0.72	0
2	BGC	gA	2	2	11,11,12	0.25	0	15,15,17	0.68	0
2	A1H1F	gA	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.62	4 (22%)
2	MAN	gA	4	2	11,11,12	0.71	0	15,15,17	1.23	1 (6%)
2	MAN	gA	5	2	11,11,12	0.42	0	15,15,17	1.34	1 (6%)
2	MAN	gA	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	gA	7	2	13,13,14	0.42	0	17,18,20	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	gB	1	1,2	11,11,12	0.33	0	15,15,17	1.01	1 (6%)
2	BGC	gB	2	2	11,11,12	0.20	0	15,15,17	0.58	0
2	A1H1F	gB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	gB	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	gB	5	2	11,11,12	0.45	0	15,15,17	1.25	1 (6%)
2	MAN	gB	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	gB	7	2	13,13,14	0.40	0	17,18,20	0.61	0
2	GAL	iA	1	1,2	11,11,12	0.31	0	15,15,17	0.92	0
2	BGC	iA	2	2	11,11,12	0.21	0	15,15,17	0.58	0
2	A1H1F	iA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	iA	4	2	11,11,12	0.46	0	15,15,17	0.81	0
2	MAN	iA	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	iA	6	2	11,11,12	0.50	0	15,15,17	0.73	0
2	A1H1B	iA	7	2	13,13,14	0.41	0	17,18,20	0.62	0
2	GAL	iB	1	1,2	11,11,12	0.39	0	15,15,17	0.76	0
2	BGC	iB	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	iB	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	iB	4	2	11,11,12	0.72	0	15,15,17	1.19	1 (6%)
2	MAN	iB	5	2	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
2	MAN	iB	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	iB	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	k	1	1,2	11,11,12	0.34	0	15,15,17	0.91	1 (6%)
2	BGC	k	2	2	11,11,12	0.20	0	15,15,17	0.58	0
2	A1H1F	k	3	2	13,14,15	1.01	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	k	4	2	11,11,12	0.45	0	15,15,17	0.83	0
2	MAN	k	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	k	6	2	11,11,12	0.50	0	15,15,17	0.74	0
2	A1H1B	k	7	2	13,13,14	0.39	0	17,18,20	0.63	0
2	GAL	kA	1	1,2	11,11,12	0.38	0	15,15,17	0.70	0
2	BGC	kA	2	2	11,11,12	0.27	0	15,15,17	0.71	0
2	A1H1F	kA	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	kA	4	2	11,11,12	0.72	0	15,15,17	1.22	1 (6%)
2	MAN	kA	5	2	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
2	MAN	kA	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	kA	7	2	13,13,14	0.42	0	17,18,20	0.57	0
2	GAL	kB	1	1,2	11,11,12	0.35	0	15,15,17	1.00	1 (6%)
2	BGC	kB	2	2	11,11,12	0.19	0	15,15,17	0.60	0
2	A1H1F	kB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	kB	4	2	11,11,12	0.46	0	15,15,17	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	kB	5	2	11,11,12	0.42	0	15,15,17	1.28	1 (6%)
2	MAN	kB	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	kB	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	m	1	1,2	11,11,12	0.37	0	15,15,17	0.72	0
2	BGC	m	2	2	11,11,12	0.26	0	15,15,17	0.70	0
2	A1H1F	m	3	2	13,14,15	1.08	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	m	4	2	11,11,12	0.71	0	15,15,17	1.24	2 (13%)
2	MAN	m	5	2	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
2	MAN	m	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	m	7	2	13,13,14	0.43	0	17,18,20	0.55	0
2	GAL	mA	1	1,2	11,11,12	0.32	0	15,15,17	0.86	0
2	BGC	mA	2	2	11,11,12	0.20	0	15,15,17	0.59	0
2	A1H1F	mA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	mA	4	2	11,11,12	0.45	0	15,15,17	0.81	0
2	MAN	mA	5	2	11,11,12	0.44	0	15,15,17	1.27	1 (6%)
2	MAN	mA	6	2	11,11,12	0.52	0	15,15,17	0.73	0
2	A1H1B	mA	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	mB	1	1,2	11,11,12	0.39	0	15,15,17	0.73	0
2	BGC	mB	2	2	11,11,12	0.25	0	15,15,17	0.67	0
2	A1H1F	mB	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.63	4 (22%)
2	MAN	mB	4	2	11,11,12	0.70	0	15,15,17	1.23	1 (6%)
2	MAN	mB	5	2	11,11,12	0.42	0	15,15,17	1.34	1 (6%)
2	MAN	mB	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	mB	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	o	1	1,2	11,11,12	0.37	0	15,15,17	0.98	0
2	BGC	o	2	2	11,11,12	0.19	0	15,15,17	0.60	0
2	A1H1F	o	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	o	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	o	5	2	11,11,12	0.43	0	15,15,17	1.27	1 (6%)
2	MAN	o	6	2	11,11,12	0.48	0	15,15,17	0.73	0
2	A1H1B	o	7	2	13,13,14	0.39	0	17,18,20	0.63	0
2	GAL	oA	1	1,2	11,11,12	0.37	0	15,15,17	0.65	0
2	BGC	oA	2	2	11,11,12	0.26	0	15,15,17	0.68	0
2	A1H1F	oA	3	2	13,14,15	1.10	1 (7%)	18,21,23	1.64	4 (22%)
2	MAN	oA	4	2	11,11,12	0.71	0	15,15,17	1.22	1 (6%)
2	MAN	oA	5	2	11,11,12	0.43	0	15,15,17	1.34	1 (6%)
2	MAN	oA	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	oA	7	2	13,13,14	0.44	0	17,18,20	0.57	0
2	GAL	oB	1	1,2	11,11,12	0.31	0	15,15,17	0.95	0
2	BGC	oB	2	2	11,11,12	0.20	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A1H1F	oB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	oB	4	2	11,11,12	0.46	0	15,15,17	0.81	0
2	MAN	oB	5	2	11,11,12	0.45	0	15,15,17	1.26	1 (6%)
2	MAN	oB	6	2	11,11,12	0.50	0	15,15,17	0.73	0
2	A1H1B	oB	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	q	1	1,2	11,11,12	0.40	0	15,15,17	0.74	0
2	BGC	q	2	2	11,11,12	0.24	0	15,15,17	0.69	0
2	A1H1F	q	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.62	5 (27%)
2	MAN	q	4	2	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
2	MAN	q	5	2	11,11,12	0.42	0	15,15,17	1.33	1 (6%)
2	MAN	q	6	2	11,11,12	0.53	0	15,15,17	0.75	0
2	A1H1B	q	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	qA	1	1,2	11,11,12	0.33	0	15,15,17	0.96	1 (6%)
2	BGC	qA	2	2	11,11,12	0.21	0	15,15,17	0.58	0
2	A1H1F	qA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	2 (11%)
2	MAN	qA	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	qA	5	2	11,11,12	0.44	0	15,15,17	1.27	1 (6%)
2	MAN	qA	6	2	11,11,12	0.48	0	15,15,17	0.74	0
2	A1H1B	qA	7	2	13,13,14	0.40	0	17,18,20	0.61	0
2	GAL	qB	1	1,2	11,11,12	0.39	0	15,15,17	0.70	0
2	BGC	qB	2	2	11,11,12	0.25	0	15,15,17	0.70	0
2	A1H1F	qB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.59	3 (16%)
2	MAN	qB	4	2	11,11,12	0.70	0	15,15,17	1.23	1 (6%)
2	MAN	qB	5	2	11,11,12	0.46	0	15,15,17	1.31	1 (6%)
2	MAN	qB	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	qB	7	2	13,13,14	0.43	0	17,18,20	0.55	0
2	GAL	s	1	1,2	11,11,12	0.32	0	15,15,17	0.94	0
2	BGC	s	2	2	11,11,12	0.20	0	15,15,17	0.56	0
2	A1H1F	s	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.02	3 (16%)
2	MAN	s	4	2	11,11,12	0.45	0	15,15,17	0.83	0
2	MAN	s	5	2	11,11,12	0.43	0	15,15,17	1.26	1 (6%)
2	MAN	s	6	2	11,11,12	0.49	0	15,15,17	0.72	0
2	A1H1B	s	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	sA	1	1,2	11,11,12	0.38	0	15,15,17	0.71	0
2	BGC	sA	2	2	11,11,12	0.25	0	15,15,17	0.71	0
2	A1H1F	sA	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.61	3 (16%)
2	MAN	sA	4	2	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
2	MAN	sA	5	2	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
2	MAN	sA	6	2	11,11,12	0.52	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A1H1B	sA	7	2	13,13,14	0.42	0	17,18,20	0.54	0
2	GAL	sB	1	1,2	11,11,12	0.31	0	15,15,17	0.91	0
2	BGC	sB	2	2	11,11,12	0.19	0	15,15,17	0.56	0
2	A1H1F	sB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	sB	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	sB	5	2	11,11,12	0.43	0	15,15,17	1.27	1 (6%)
2	MAN	sB	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	sB	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	u	1	1,2	11,11,12	0.38	0	15,15,17	0.72	0
2	BGC	u	2	2	11,11,12	0.25	0	15,15,17	0.70	0
2	A1H1F	u	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.60	3 (16%)
2	MAN	u	4	2	11,11,12	0.71	0	15,15,17	1.25	2 (13%)
2	MAN	u	5	2	11,11,12	0.45	0	15,15,17	1.31	1 (6%)
2	MAN	u	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	u	7	2	13,13,14	0.42	0	17,18,20	0.55	0
2	GAL	uA	1	1,2	11,11,12	0.36	0	15,15,17	0.90	0
2	BGC	uA	2	2	11,11,12	0.20	0	15,15,17	0.60	0
2	A1H1F	uA	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.03	3 (16%)
2	MAN	uA	4	2	11,11,12	0.45	0	15,15,17	0.81	0
2	MAN	uA	5	2	11,11,12	0.44	0	15,15,17	1.26	1 (6%)
2	MAN	uA	6	2	11,11,12	0.51	0	15,15,17	0.72	0
2	A1H1B	uA	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	uB	1	1,2	11,11,12	0.36	0	15,15,17	0.70	0
2	BGC	uB	2	2	11,11,12	0.24	0	15,15,17	0.68	0
2	A1H1F	uB	3	2	13,14,15	1.11	1 (7%)	18,21,23	1.63	4 (22%)
2	MAN	uB	4	2	11,11,12	0.70	0	15,15,17	1.21	1 (6%)
2	MAN	uB	5	2	11,11,12	0.44	0	15,15,17	1.33	1 (6%)
2	MAN	uB	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	uB	7	2	13,13,14	0.43	0	17,18,20	0.56	0
2	GAL	w	1	1,2	11,11,12	0.35	0	15,15,17	0.93	1 (6%)
2	BGC	w	2	2	11,11,12	0.19	0	15,15,17	0.59	0
2	A1H1F	w	3	2	13,14,15	1.01	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	w	4	2	11,11,12	0.45	0	15,15,17	0.80	0
2	MAN	w	5	2	11,11,12	0.44	0	15,15,17	1.27	1 (6%)
2	MAN	w	6	2	11,11,12	0.51	0	15,15,17	0.71	0
2	A1H1B	w	7	2	13,13,14	0.39	0	17,18,20	0.62	0
2	GAL	wA	1	1,2	11,11,12	0.39	0	15,15,17	0.74	0
2	BGC	wA	2	2	11,11,12	0.25	0	15,15,17	0.69	0
2	A1H1F	wA	3	2	13,14,15	1.12	1 (7%)	18,21,23	1.62	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	wA	4	2	11,11,12	0.71	0	15,15,17	1.18	1 (6%)
2	MAN	wA	5	2	11,11,12	0.45	0	15,15,17	1.33	1 (6%)
2	MAN	wA	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	wA	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	wB	1	1,2	11,11,12	0.33	0	15,15,17	0.97	1 (6%)
2	BGC	wB	2	2	11,11,12	0.20	0	15,15,17	0.56	0
2	A1H1F	wB	3	2	13,14,15	1.00	1 (7%)	18,21,23	1.02	3 (16%)
2	MAN	wB	4	2	11,11,12	0.46	0	15,15,17	0.82	0
2	MAN	wB	5	2	11,11,12	0.43	0	15,15,17	1.25	1 (6%)
2	MAN	wB	6	2	11,11,12	0.49	0	15,15,17	0.72	0
2	A1H1B	wB	7	2	13,13,14	0.41	0	17,18,20	0.61	0
2	GAL	y	1	1,2	11,11,12	0.39	0	15,15,17	0.74	0
2	BGC	y	2	2	11,11,12	0.26	0	15,15,17	0.68	0
2	A1H1F	y	3	2	13,14,15	1.12	1 (7%)	18,21,23	1.62	4 (22%)
2	MAN	y	4	2	11,11,12	0.72	0	15,15,17	1.17	1 (6%)
2	MAN	y	5	2	11,11,12	0.45	0	15,15,17	1.33	1 (6%)
2	MAN	y	6	2	11,11,12	0.53	0	15,15,17	0.74	0
2	A1H1B	y	7	2	13,13,14	0.42	0	17,18,20	0.56	0
2	GAL	yA	1	1,2	11,11,12	0.34	0	15,15,17	0.92	0
2	BGC	yA	2	2	11,11,12	0.21	0	15,15,17	0.58	0
2	A1H1F	yA	3	2	13,14,15	1.01	1 (7%)	18,21,23	1.04	3 (16%)
2	MAN	yA	4	2	11,11,12	0.46	0	15,15,17	0.82	0
2	MAN	yA	5	2	11,11,12	0.42	0	15,15,17	1.28	1 (6%)
2	MAN	yA	6	2	11,11,12	0.48	0	15,15,17	0.73	0
2	A1H1B	yA	7	2	13,13,14	0.40	0	17,18,20	0.62	0
2	GAL	yB	1	1,2	11,11,12	0.40	0	15,15,17	0.71	0
2	BGC	yB	2	2	11,11,12	0.23	0	15,15,17	0.69	0
2	A1H1F	yB	3	2	13,14,15	1.09	1 (7%)	18,21,23	1.59	3 (16%)
2	MAN	yB	4	2	11,11,12	0.71	0	15,15,17	1.26	2 (13%)
2	MAN	yB	5	2	11,11,12	0.44	0	15,15,17	1.31	1 (6%)
2	MAN	yB	6	2	11,11,12	0.52	0	15,15,17	0.75	0
2	A1H1B	yB	7	2	13,13,14	0.42	0	17,18,20	0.55	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	GAL	0	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	0	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	0	3	2	-	1/5/22/25	0/1/1/1
2	MAN	0	4	2	-	1/2/19/22	0/1/1/1
2	MAN	0	5	2	-	0/2/19/22	1/1/1/1
2	MAN	0	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	0	7	2	-	0/6/23/26	0/1/1/1
2	GAL	0A	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	0A	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	0A	3	2	-	2/5/22/25	0/1/1/1
2	MAN	0A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	0A	5	2	-	0/2/19/22	1/1/1/1
2	MAN	0A	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	0A	7	2	-	0/6/23/26	0/1/1/1
2	GAL	0B	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	0B	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	0B	3	2	-	1/5/22/25	0/1/1/1
2	MAN	0B	4	2	-	1/2/19/22	0/1/1/1
2	MAN	0B	5	2	-	0/2/19/22	1/1/1/1
2	MAN	0B	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	0B	7	2	-	0/6/23/26	0/1/1/1
2	GAL	2	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	2	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	2	3	2	-	2/5/22/25	0/1/1/1
2	MAN	2	4	2	-	0/2/19/22	0/1/1/1
2	MAN	2	5	2	-	0/2/19/22	1/1/1/1
2	MAN	2	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	2	7	2	-	0/6/23/26	0/1/1/1
2	GAL	2A	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	2A	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	2A	3	2	-	1/5/22/25	0/1/1/1
2	MAN	2A	4	2	-	1/2/19/22	0/1/1/1
2	MAN	2A	5	2	-	0/2/19/22	1/1/1/1
2	MAN	2A	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	2A	7	2	-	0/6/23/26	0/1/1/1
2	GAL	2B	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	2B	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	2B	3	2	-	2/5/22/25	0/1/1/1
2	MAN	2B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	2B	5	2	-	0/2/19/22	1/1/1/1
2	MAN	2B	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	2B	7	2	-	0/6/23/26	0/1/1/1
2	GAL	4	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	4	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	4	3	2	-	1/5/22/25	0/1/1/1
2	MAN	4	4	2	-	1/2/19/22	0/1/1/1
2	MAN	4	5	2	-	0/2/19/22	1/1/1/1
2	MAN	4	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	4	7	2	-	0/6/23/26	0/1/1/1
2	GAL	4A	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	4A	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	4A	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	4A	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	4A	7	2	-	0/6/23/26	0/1/1/1
2	GAL	6	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	6	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	6	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	6	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	6	7	2	-	0/6/23/26	0/1/1/1
2	GAL	6A	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	6A	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	6A	3	2	-	1/5/22/25	0/1/1/1
2	MAN	6A	4	2	-	1/2/19/22	0/1/1/1
2	MAN	6A	5	2	-	0/2/19/22	1/1/1/1
2	MAN	6A	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	6A	7	2	-	0/6/23/26	0/1/1/1
2	GAL	8	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	8	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	8	3	2	-	1/5/22/25	0/1/1/1
2	MAN	8	4	2	-	1/2/19/22	0/1/1/1
2	MAN	8	5	2	-	0/2/19/22	1/1/1/1
2	MAN	8	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	8	7	2	-	0/6/23/26	0/1/1/1
2	GAL	8A	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	8A	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	8A	3	2	-	2/5/22/25	0/1/1/1
2	MAN	8A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	8A	5	2	-	0/2/19/22	1/1/1/1
2	MAN	8A	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	8A	7	2	-	0/6/23/26	0/1/1/1
2	GAL	AA	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	AA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	AA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	AA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	AA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	AA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	AA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	AB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	AB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	AB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	AB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	AB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	AB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	AB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	CA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	CA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	CA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	CA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	CA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	CA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	CA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	CB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	CB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	CB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	CB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	CB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	CB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	CB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	EA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	EA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	EA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	EA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	EA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	EA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	EA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	EB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	EB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	EB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	EB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	EB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	EB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	EB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	GA	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	GA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	GA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	GA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	GA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	GA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	GA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	GB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	GB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	GB	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	GB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	GB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	IA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	IA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	IA	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	IA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	IA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	IB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	IB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	IB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	IB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	IB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	IB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	IB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	KA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	KA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	KA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	KA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	KA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	KA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	KA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	KB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	KB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	KB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	KB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	KB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	KB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	KB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	MA	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	MA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	MA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	MA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	MA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	MA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	MA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	MB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	MB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	MB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	MB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	MB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	MB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	MB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	OA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	OA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	OA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	OA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	OA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	OA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	OA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	OB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	OB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	OB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	OB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	OB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	OB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	OB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	QA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	QA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	QA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	QA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	QA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	QA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	QA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	QB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	QB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	QB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	QB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	QB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	QB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	QB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	SA	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	SA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	SA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	SA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	SA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	SA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	SA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	SB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	SB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	SB	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	SB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	SB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	UA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	UA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	UA	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	UA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	UA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	UB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	UB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	UB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	UB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	UB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	UB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	UB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	WA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	WA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	WA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	WA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	WA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	WA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	WA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	WB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	WB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	WB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	WB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	WB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	WB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	WB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	YA	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	YA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	YA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	YA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	YA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	YA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	YA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	YB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	YB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	YB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	YB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	YB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	YB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	YB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	aA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	aA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	aA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	aA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	aA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	aA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	aA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	aB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	aB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	aB	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	aB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	aB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	cA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	cA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	cA	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	cA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	cA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	cB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	cB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	cB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	cB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	cB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	cB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	cB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	eA	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	eA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	eA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	eA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	eA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	eA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	eA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	eB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	eB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	eB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	eB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	eB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	eB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	eB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	gA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	gA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	gA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	gA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	gA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	gA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	gA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	gB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	gB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	gB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	gB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	gB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	gB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	gB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	iA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	iA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	iA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	iA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	iA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	iA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	iA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	iB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	iB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	iB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	iB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	iB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	iB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	iB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	k	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	k	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	k	3	2	-	1/5/22/25	0/1/1/1
2	MAN	k	4	2	-	1/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	1/1/1/1
2	MAN	k	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	k	7	2	-	0/6/23/26	0/1/1/1
2	GAL	kA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	kA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	kA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	kA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	kA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	kA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	kA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	kB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	kB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	kB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	kB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	kB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	kB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	kB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	m	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	m	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	m	3	2	-	2/5/22/25	0/1/1/1
2	MAN	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	m	5	2	-	0/2/19/22	1/1/1/1
2	MAN	m	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	m	7	2	-	0/6/23/26	0/1/1/1
2	GAL	mA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	mA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	mA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	mA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	mA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	mA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	mA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	mB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	mB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	mB	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	mB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	mB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	o	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	o	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	o	3	2	-	1/5/22/25	0/1/1/1
2	MAN	o	4	2	-	1/2/19/22	0/1/1/1
2	MAN	o	5	2	-	0/2/19/22	1/1/1/1
2	MAN	o	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	o	7	2	-	0/6/23/26	0/1/1/1
2	GAL	oA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	oA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	oA	3	2	-	2/5/22/25	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	1/1/1/1
2	MAN	oA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	oA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	oB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	oB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	oB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	oB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	oB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	oB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	oB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	q	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	q	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	q	3	2	-	2/5/22/25	0/1/1/1
2	MAN	q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	q	5	2	-	0/2/19/22	1/1/1/1
2	MAN	q	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	q	7	2	-	0/6/23/26	0/1/1/1
2	GAL	qA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	qA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	qA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	qA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	qA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	qA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	qA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	qB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	qB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	qB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	qB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	qB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	qB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	qB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	s	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	s	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	s	3	2	-	1/5/22/25	0/1/1/1
2	MAN	s	4	2	-	1/2/19/22	0/1/1/1
2	MAN	s	5	2	-	0/2/19/22	1/1/1/1
2	MAN	s	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	s	7	2	-	0/6/23/26	0/1/1/1
2	GAL	sA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	sA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	sA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	sA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	sA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	sA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	sA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	sB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	sB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	sB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	sB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	sB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	sB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	sB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	u	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	u	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	u	3	2	-	2/5/22/25	0/1/1/1
2	MAN	u	4	2	-	0/2/19/22	0/1/1/1
2	MAN	u	5	2	-	0/2/19/22	1/1/1/1
2	MAN	u	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	u	7	2	-	0/6/23/26	0/1/1/1
2	GAL	uA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	uA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	uA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	uA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	uA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	uA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	uA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	uB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	uB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	uB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	uB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	uB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	uB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	uB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	w	1	1,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	w	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	w	3	2	-	1/5/22/25	0/1/1/1
2	MAN	w	4	2	-	1/2/19/22	0/1/1/1
2	MAN	w	5	2	-	0/2/19/22	1/1/1/1
2	MAN	w	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	w	7	2	-	0/6/23/26	0/1/1/1
2	GAL	wA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	wA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	wA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	wA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	wA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	wA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	wA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	wB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	wB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	wB	3	2	-	1/5/22/25	0/1/1/1
2	MAN	wB	4	2	-	1/2/19/22	0/1/1/1
2	MAN	wB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	wB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	wB	7	2	-	0/6/23/26	0/1/1/1
2	GAL	y	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	y	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	y	3	2	-	2/5/22/25	0/1/1/1
2	MAN	y	4	2	-	0/2/19/22	0/1/1/1
2	MAN	y	5	2	-	0/2/19/22	1/1/1/1
2	MAN	y	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	y	7	2	-	0/6/23/26	0/1/1/1
2	GAL	yA	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	yA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	yA	3	2	-	1/5/22/25	0/1/1/1
2	MAN	yA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	yA	5	2	-	0/2/19/22	1/1/1/1
2	MAN	yA	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	yA	7	2	-	0/6/23/26	0/1/1/1
2	GAL	yB	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	yB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	yB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	yB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	yB	5	2	-	0/2/19/22	1/1/1/1
2	MAN	yB	6	2	-	0/2/19/22	0/1/1/1
2	A1H1B	yB	7	2	-	0/6/23/26	0/1/1/1

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4A	3	A1H1F	C6-S6	-3.10	1.66	1.77
2	WB	3	A1H1F	C6-S6	-3.09	1.66	1.77
2	MA	3	A1H1F	C6-S6	-3.09	1.66	1.77
2	wA	3	A1H1F	C6-S6	-3.08	1.66	1.77
2	y	3	A1H1F	C6-S6	-3.08	1.66	1.77

The worst 5 of 368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	mB	3	A1H1F	C1-O5-C5	-4.69	105.84	112.19
2	oA	3	A1H1F	C1-O5-C5	-4.68	105.85	112.19
2	8A	3	A1H1F	C1-O5-C5	-4.67	105.86	112.19
2	SB	3	A1H1F	C1-O5-C5	-4.66	105.88	112.19
2	QA	3	A1H1F	C1-O5-C5	-4.66	105.88	112.19

There are no chirality outliers.

5 of 144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	m	3	A1H1F	C4-C5-C6-S6
2	q	3	A1H1F	C4-C5-C6-S6
2	u	3	A1H1F	C4-C5-C6-S6
2	y	3	A1H1F	C4-C5-C6-S6
2	2	3	A1H1F	C4-C5-C6-S6

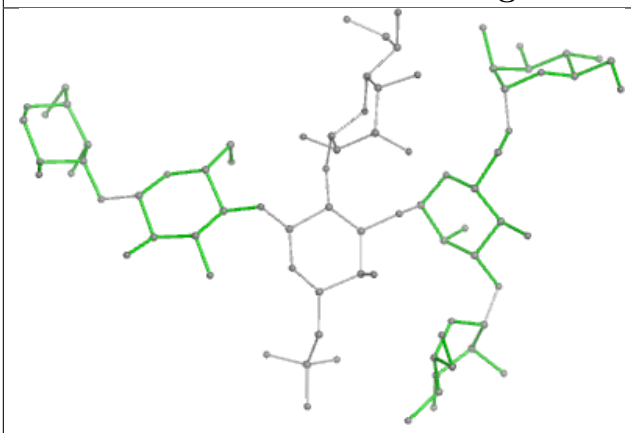
5 of 72 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	IB	5	MAN	C1-C2-C3-C4-C5-O5
2	MB	5	MAN	C1-C2-C3-C4-C5-O5
2	UB	5	MAN	C1-C2-C3-C4-C5-O5
2	eA	5	MAN	C1-C2-C3-C4-C5-O5
2	yA	5	MAN	C1-C2-C3-C4-C5-O5

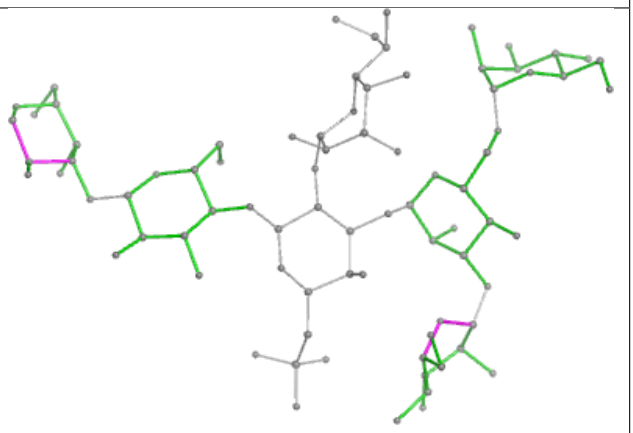
No monomer is involved in short contacts.

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

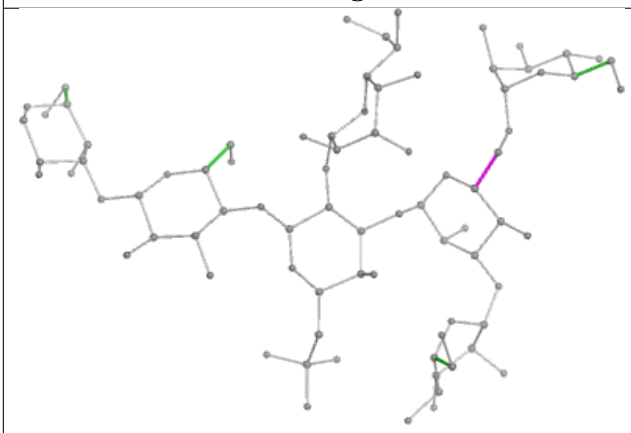
Oligosaccharide Chain k



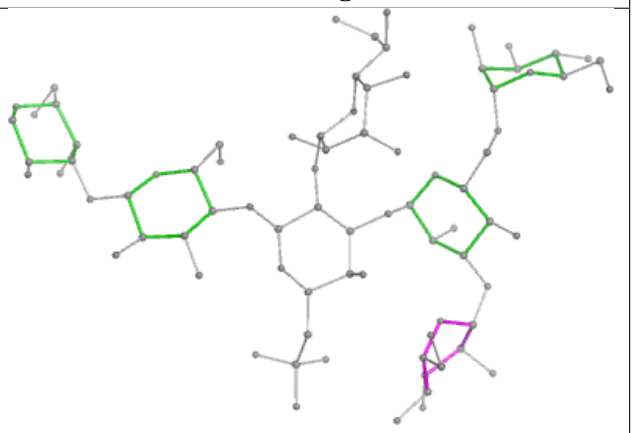
Bond lengths



Bond angles

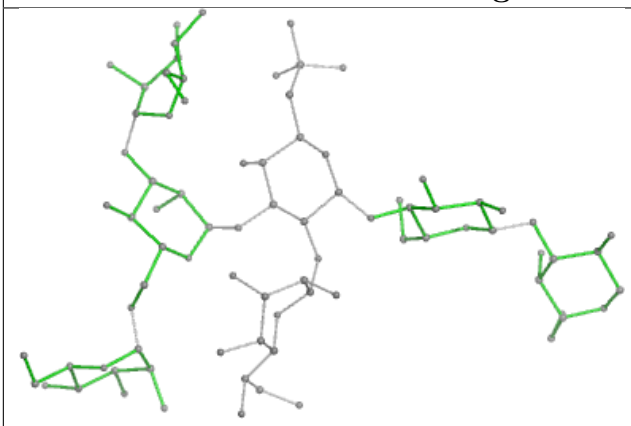


Torsions

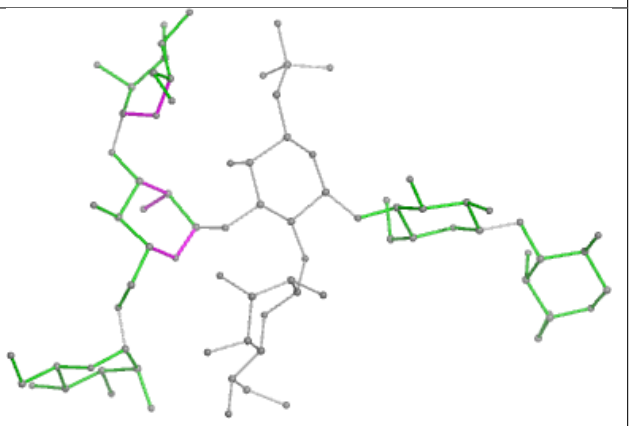


Rings

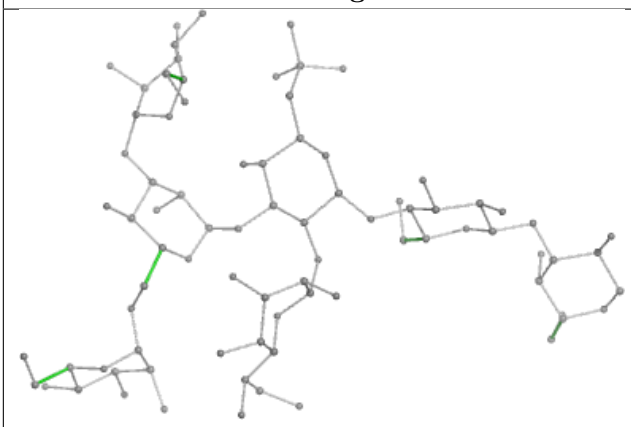
Oligosaccharide Chain m



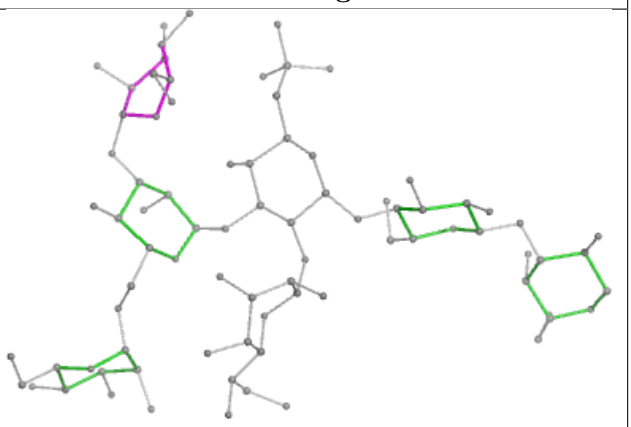
Bond lengths



Bond angles

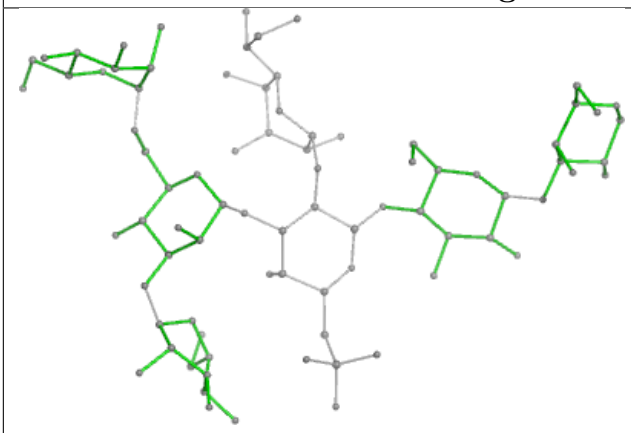


Torsions

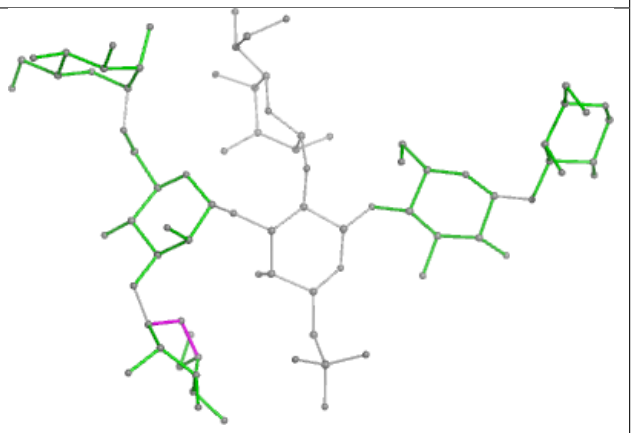


Rings

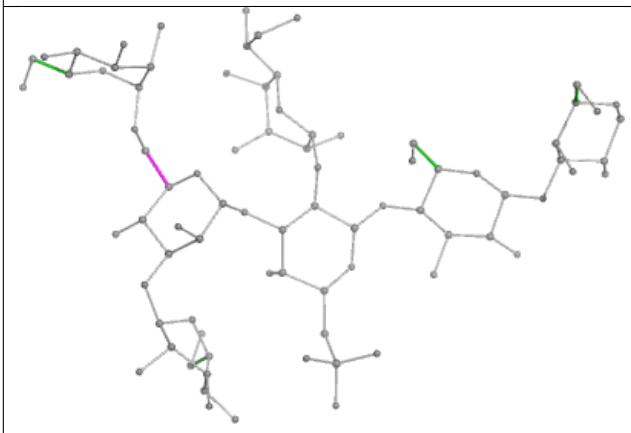
Oligosaccharide Chain o



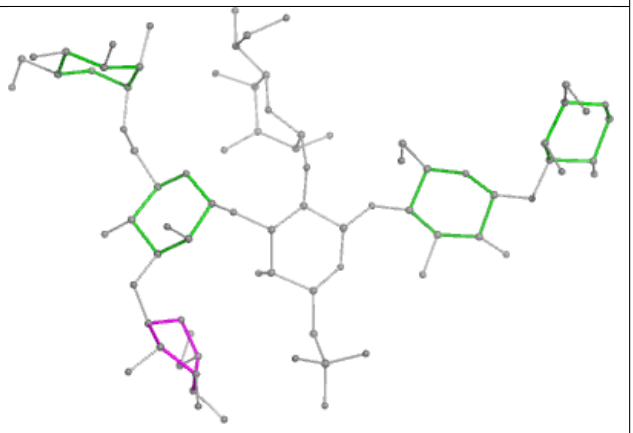
Bond lengths



Bond angles

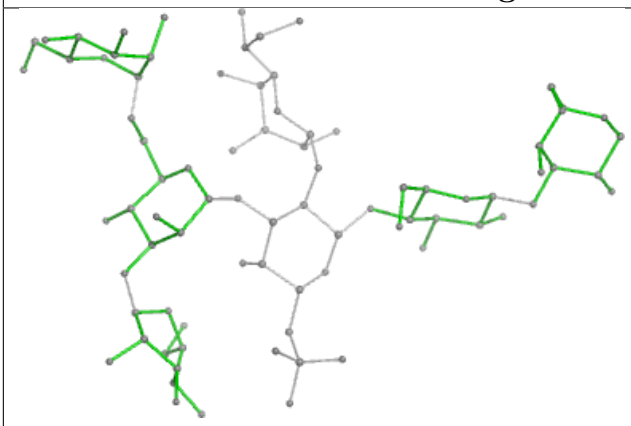


Torsions

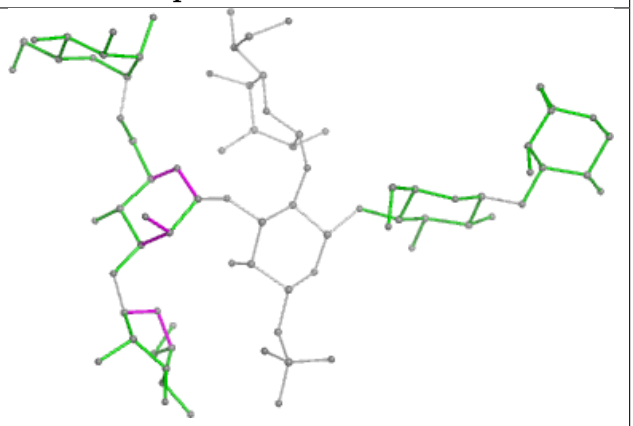


Rings

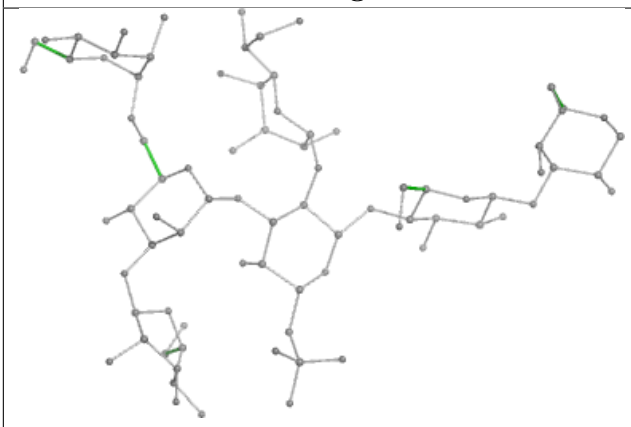
Oligosaccharide Chain q



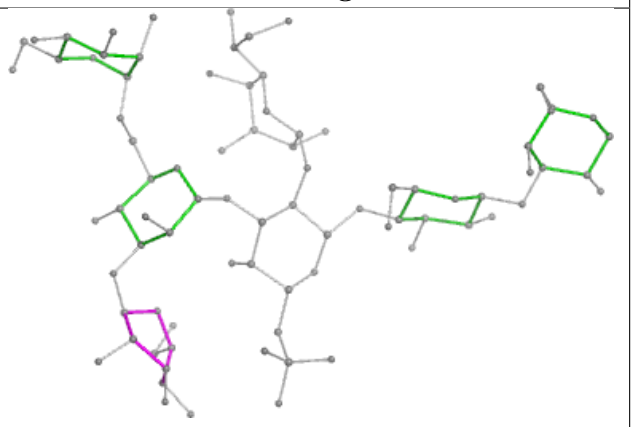
Bond lengths



Bond angles

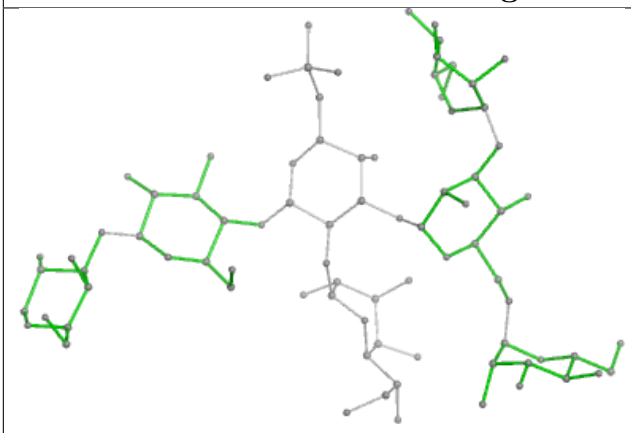


Torsions



Rings

Oligosaccharide Chain s



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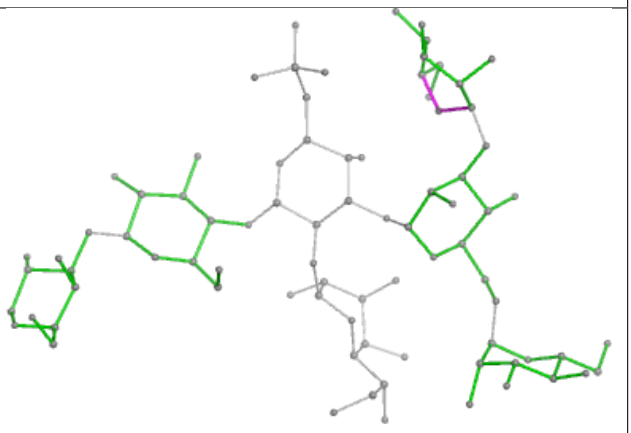
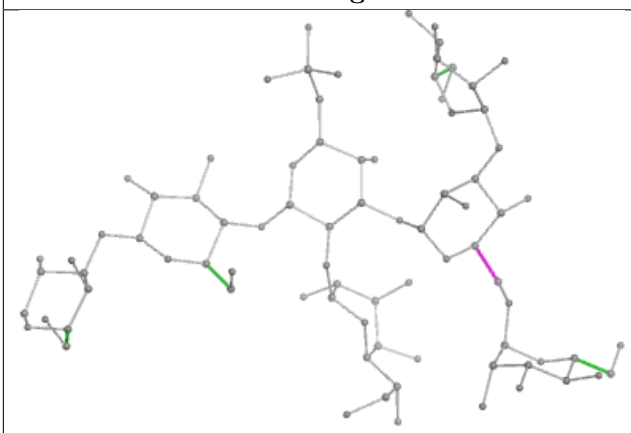


Bond angles



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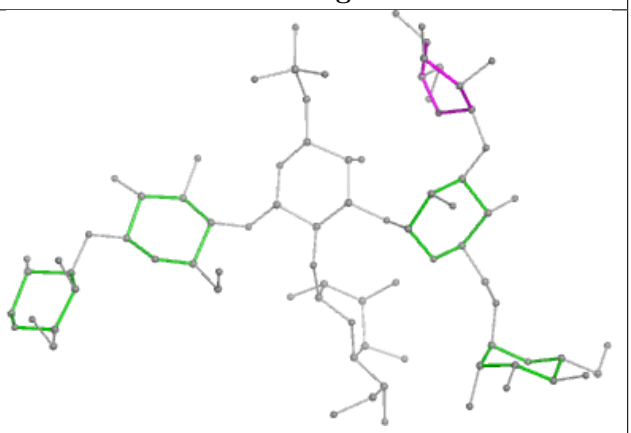
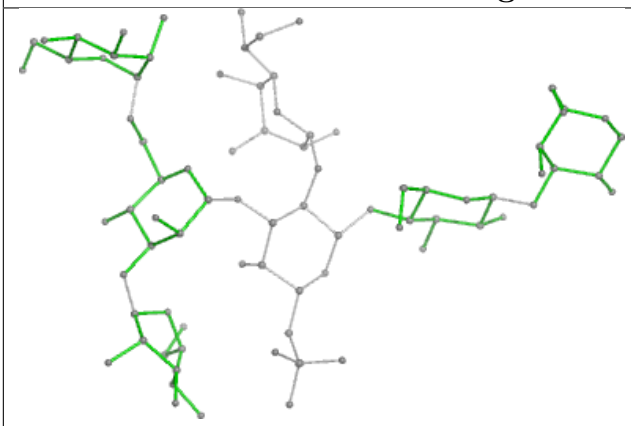


Rings

Oligosaccharide Chain u



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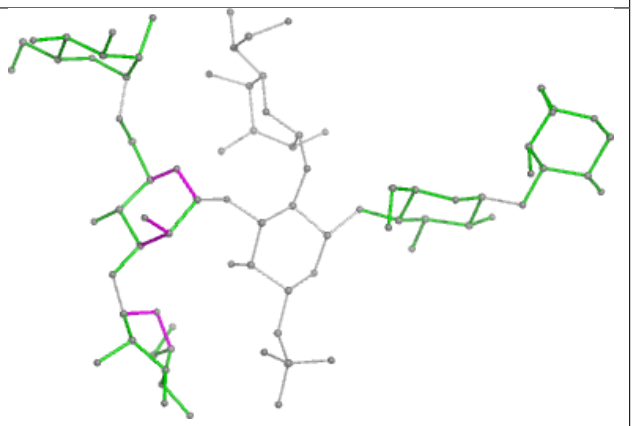
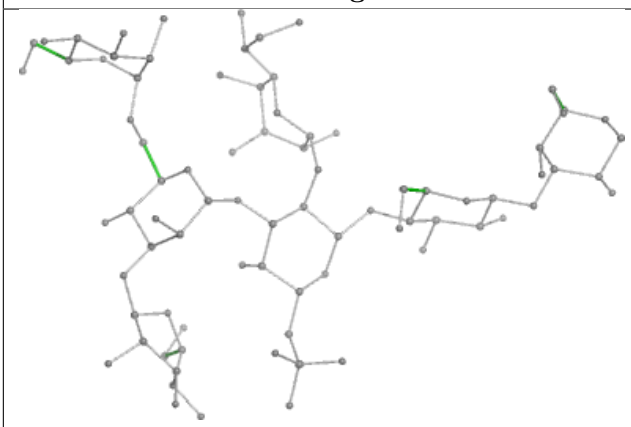


Bond angles



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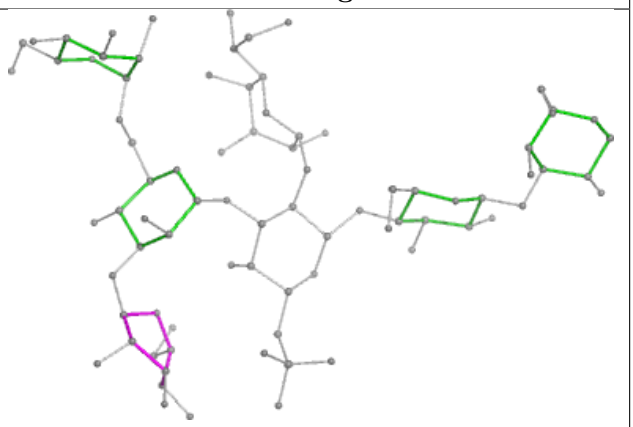
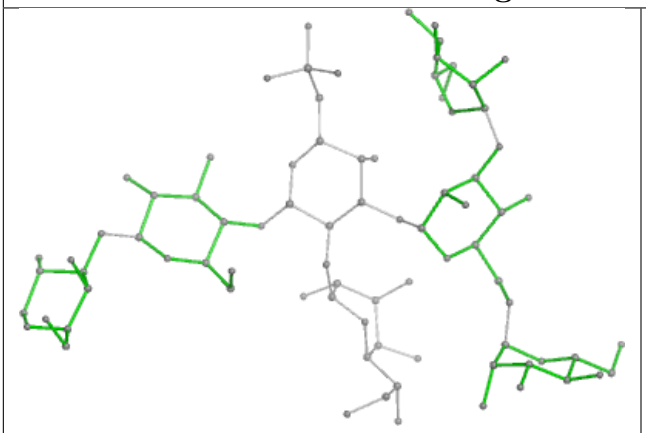


Rings

Oligosaccharide Chain w



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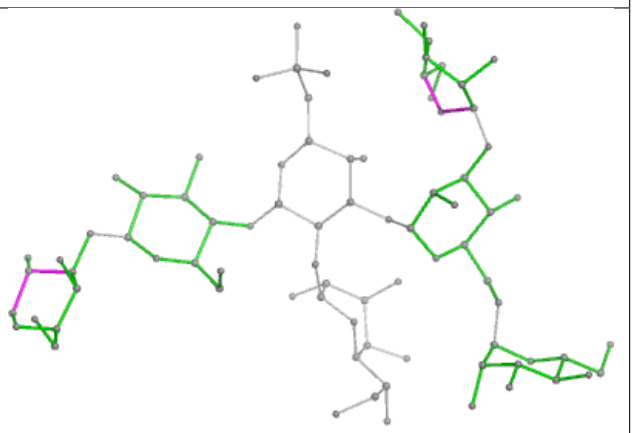
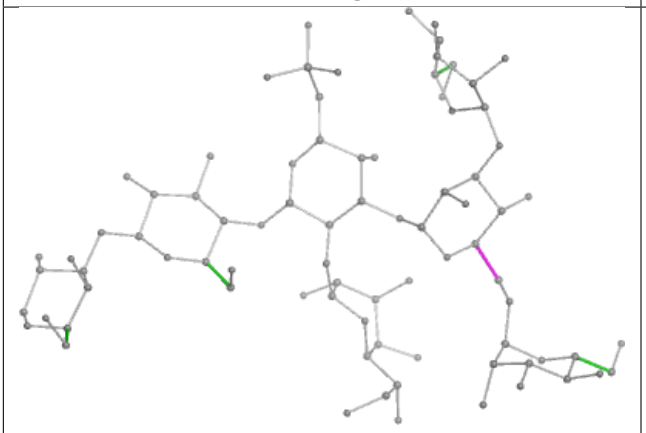


Bond angles



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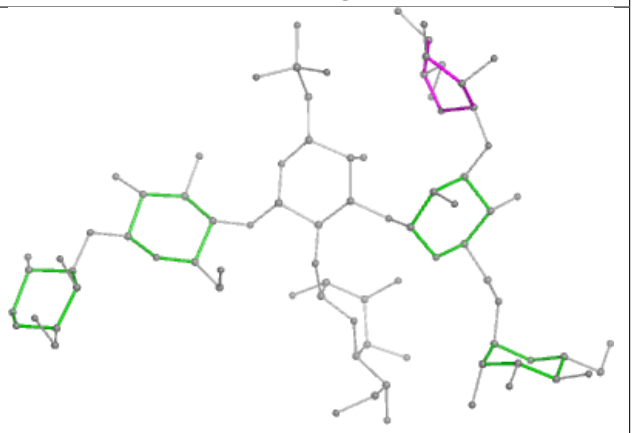
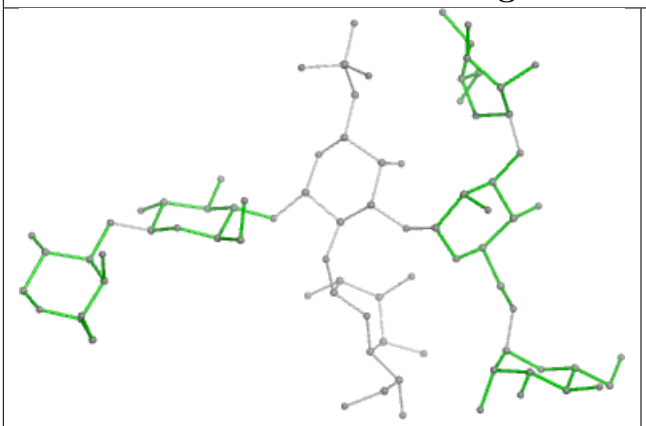


Rings

Oligosaccharide Chain y



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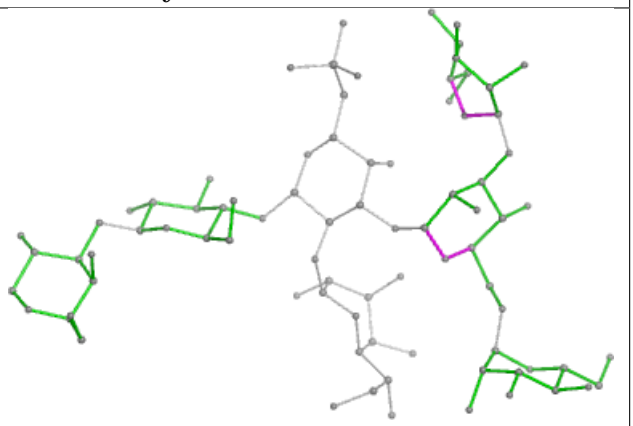
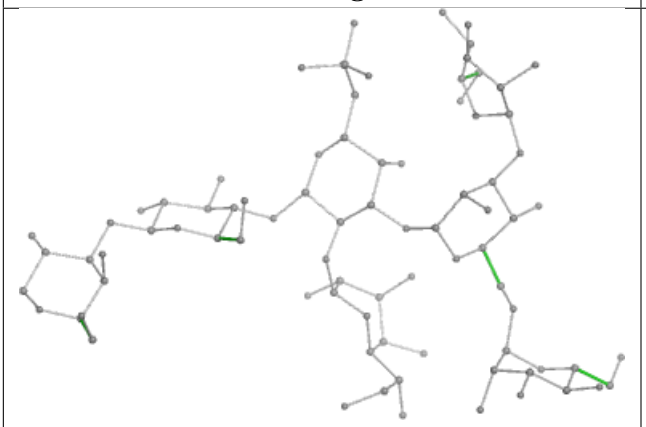


Bond angles



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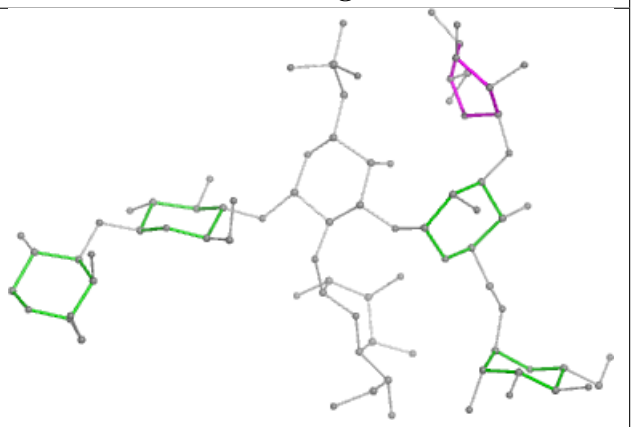
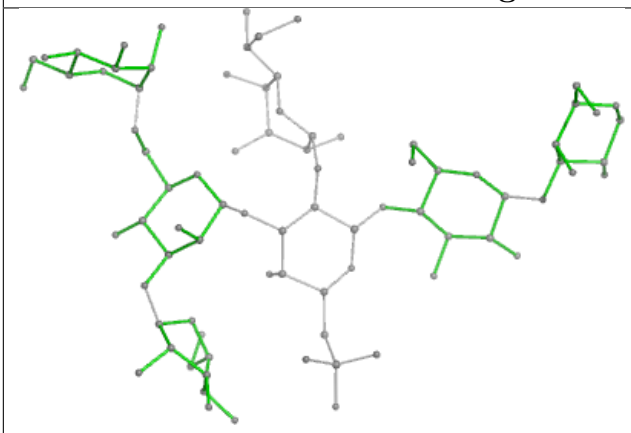


Rings

Oligosaccharide Chain 0



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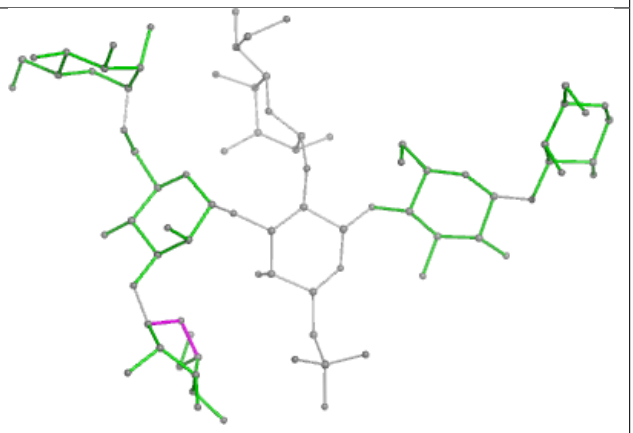
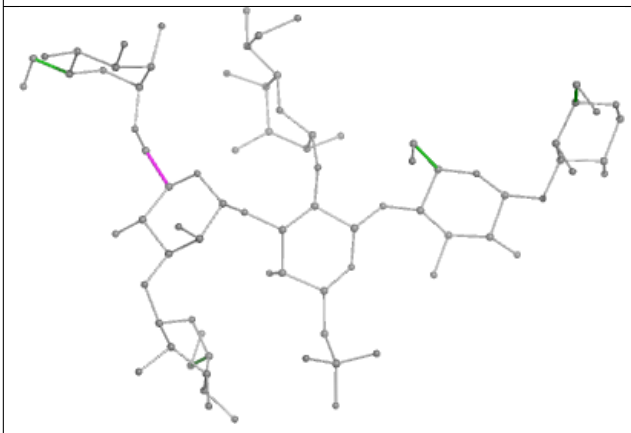


Bond angles



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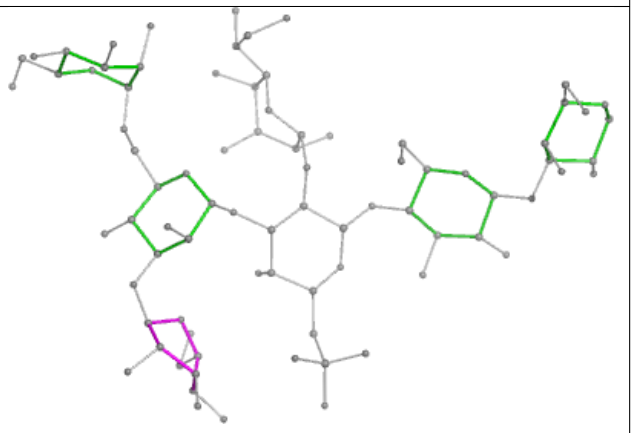
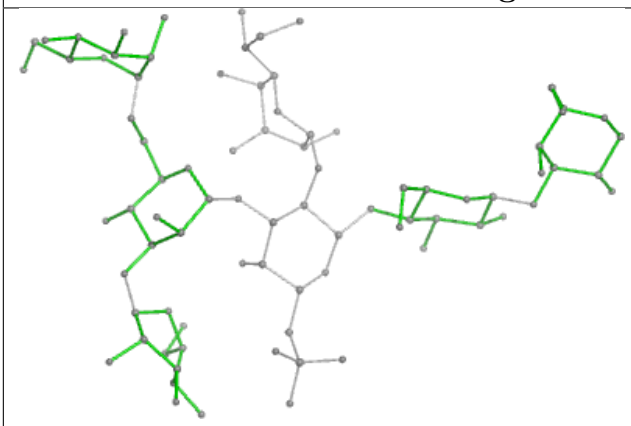


Rings

Oligosaccharide Chain 2



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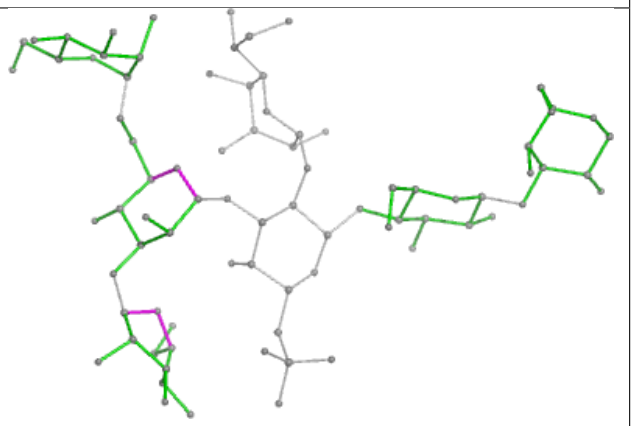
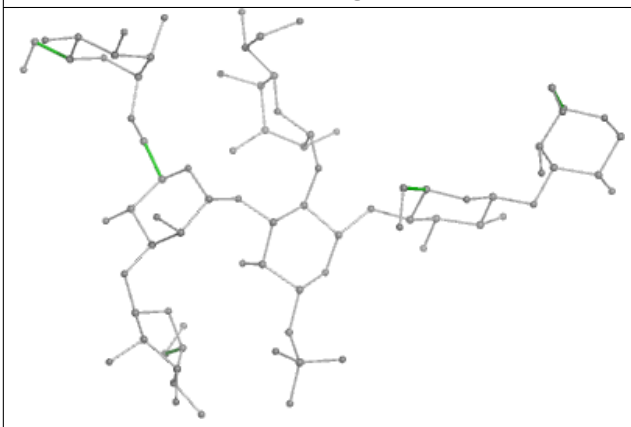


Bond angles



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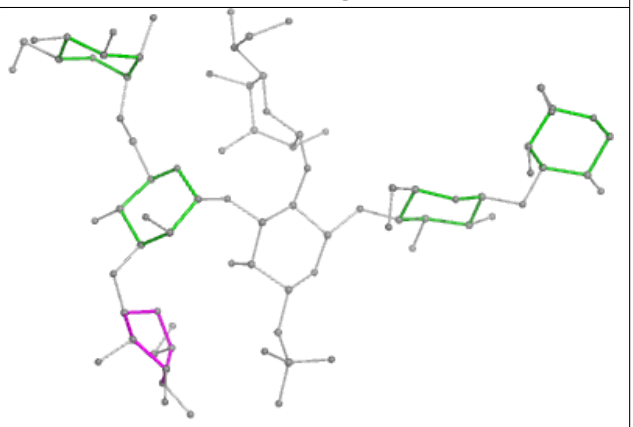
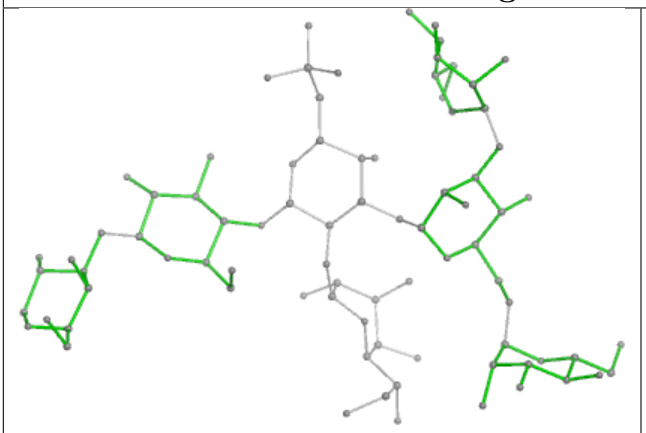


Rings

Oligosaccharide Chain 4



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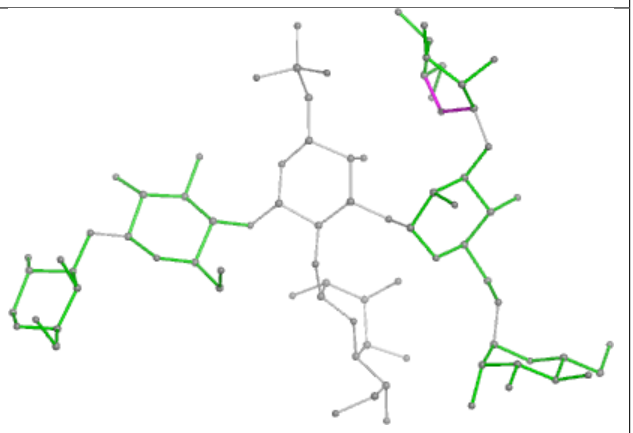
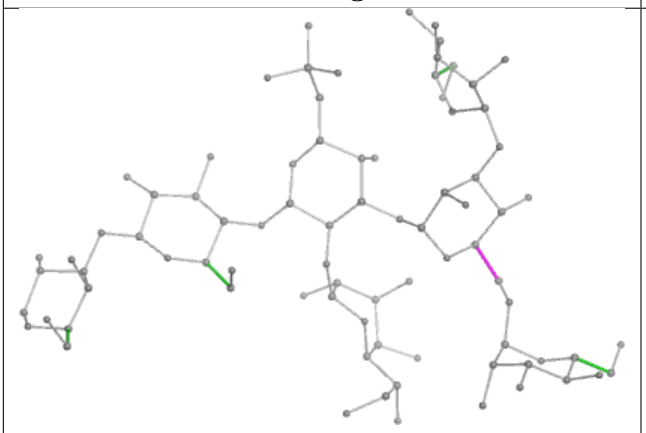


Bond angles



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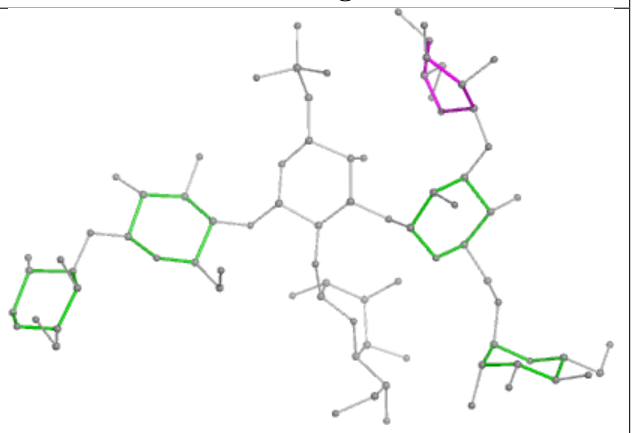
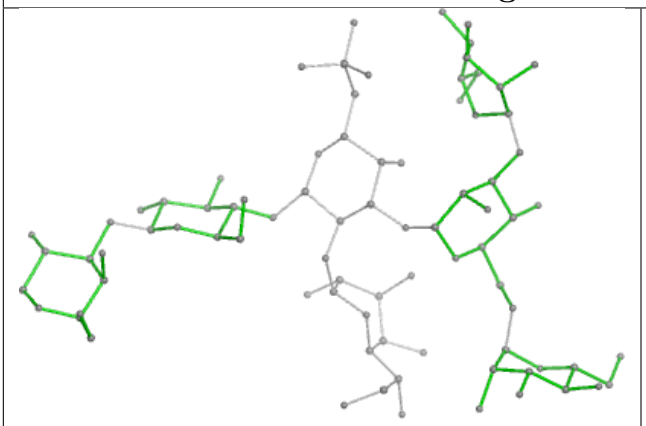


Rings

Oligosaccharide Chain 6



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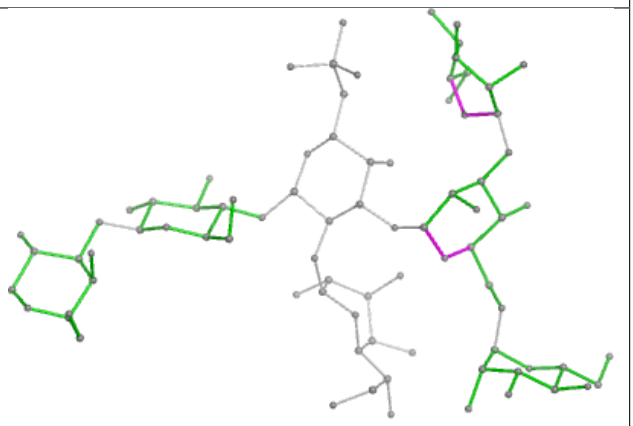
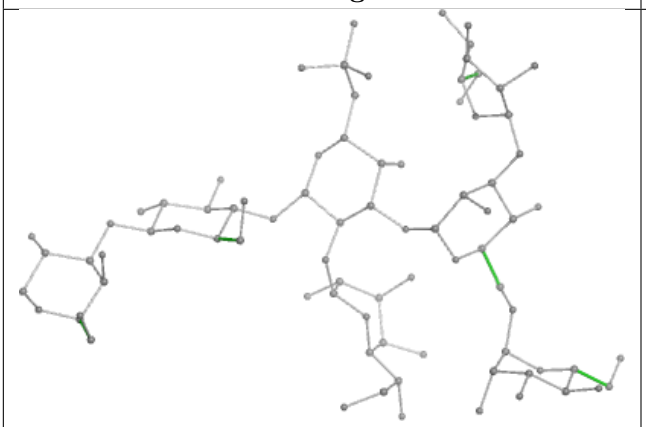


Bond angles



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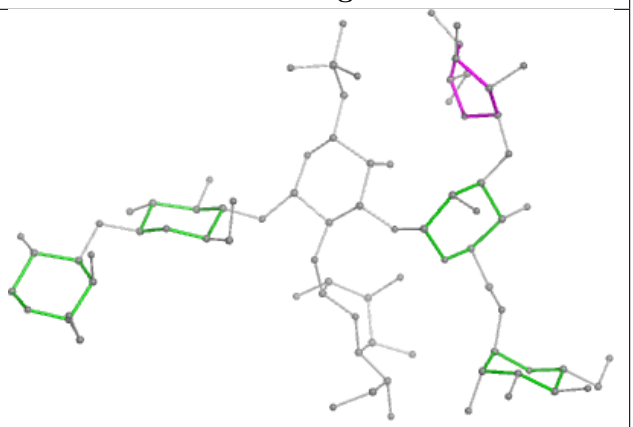
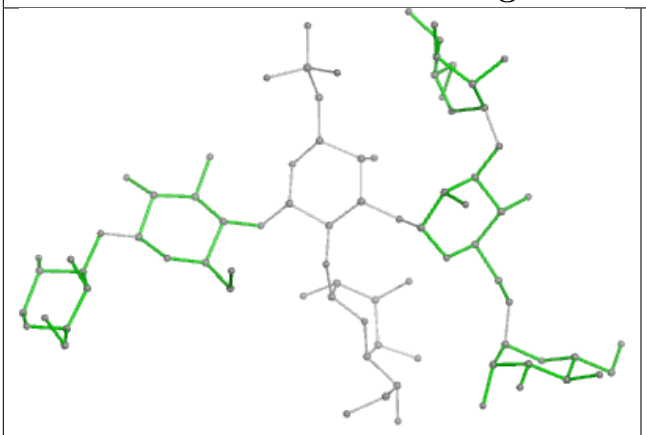


Rings

Oligosaccharide Chain 8



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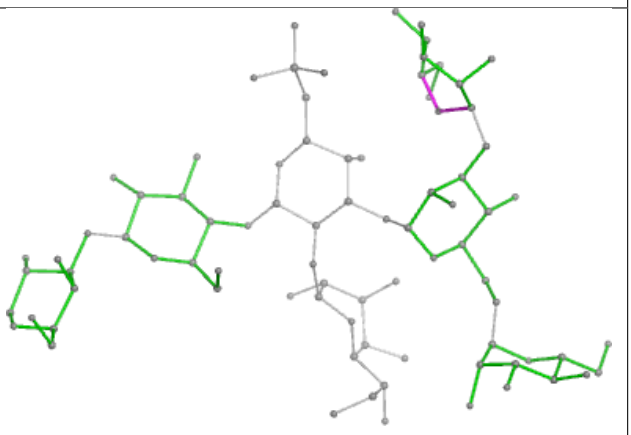
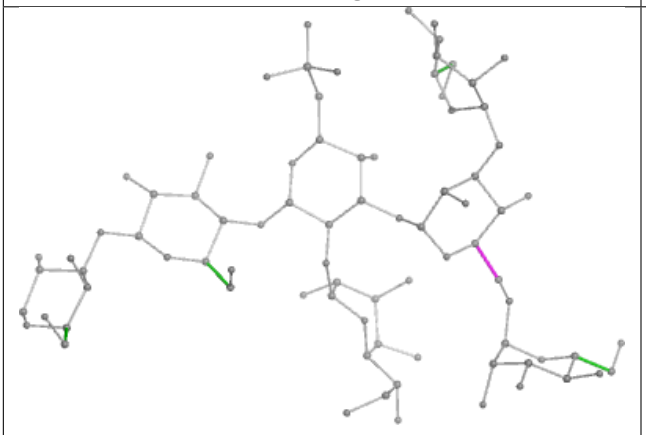


Bond angles



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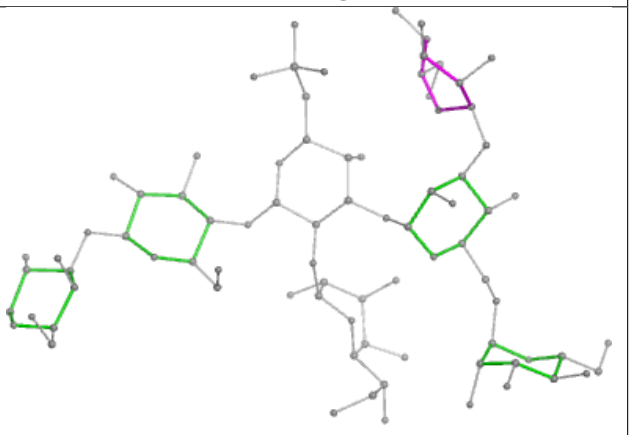
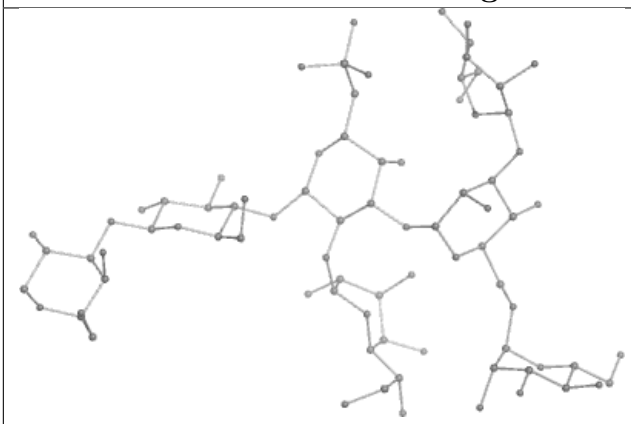


Rings

Oligosaccharide Chain AA



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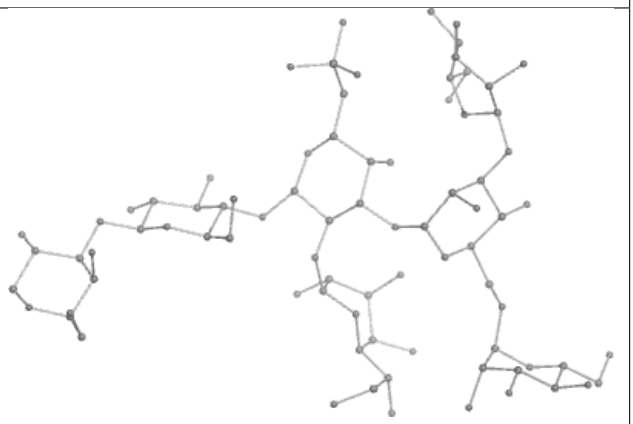
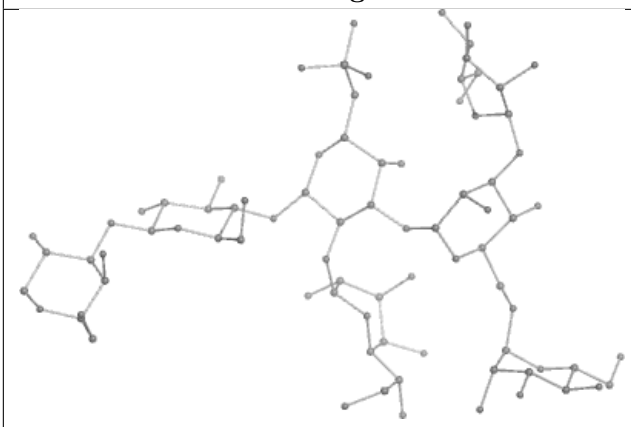
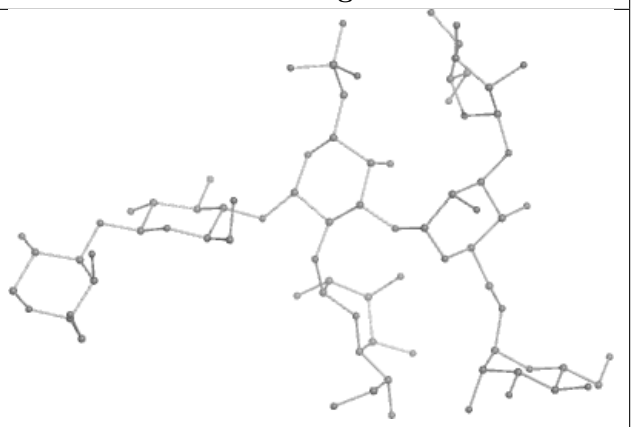


Bond angles

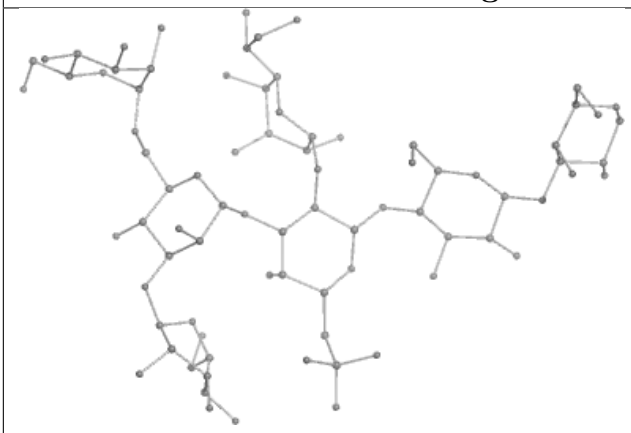


Torsions



Rings

Oligosaccharide Chain CA



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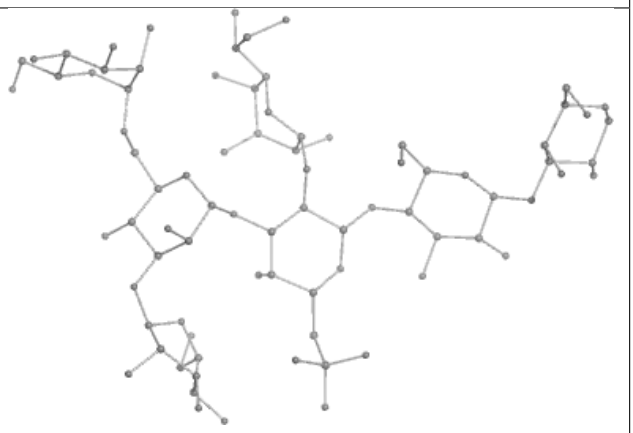
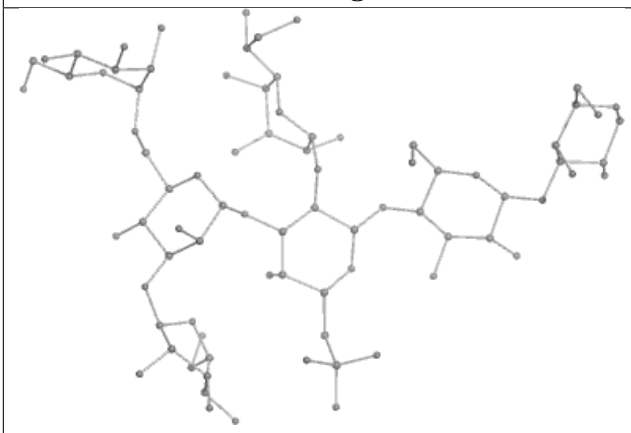


Bond angles



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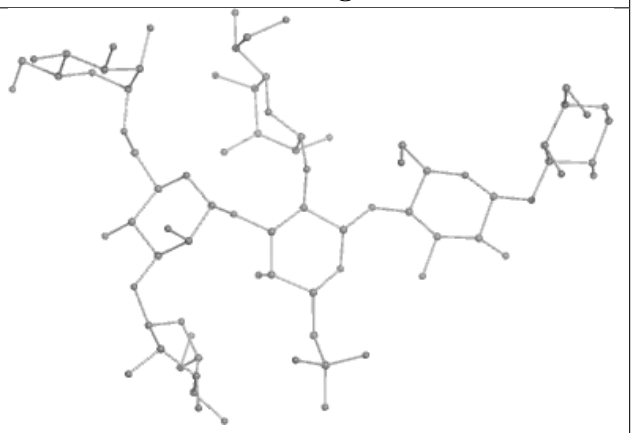
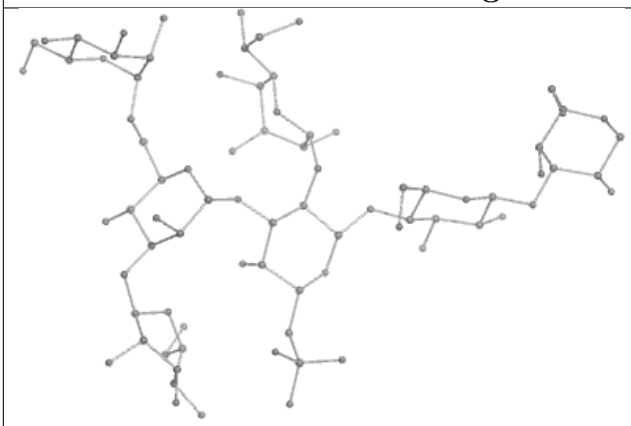


Rings

Oligosaccharide Chain EA



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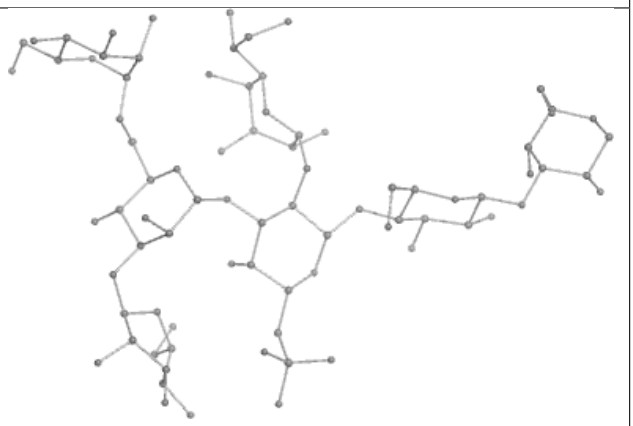
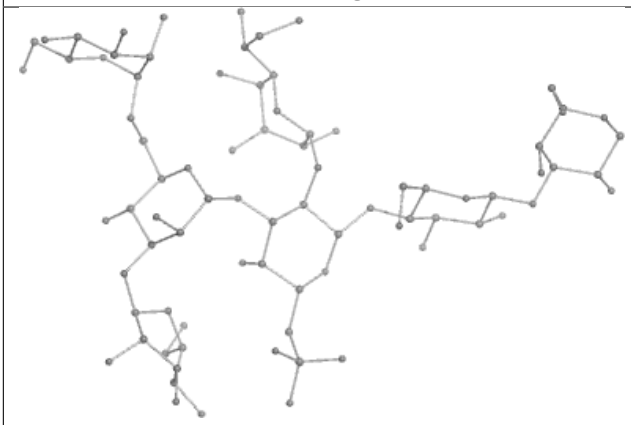
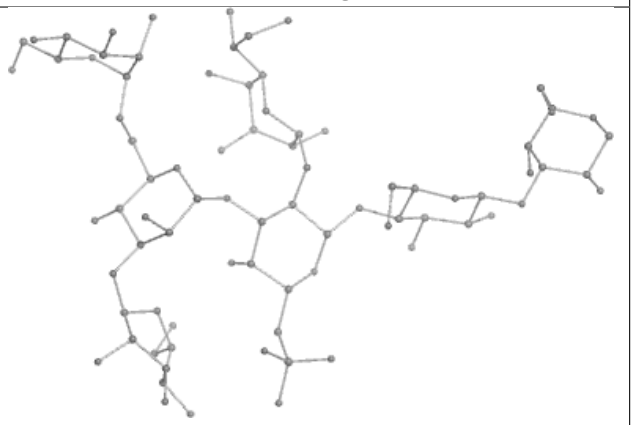


Bond angles

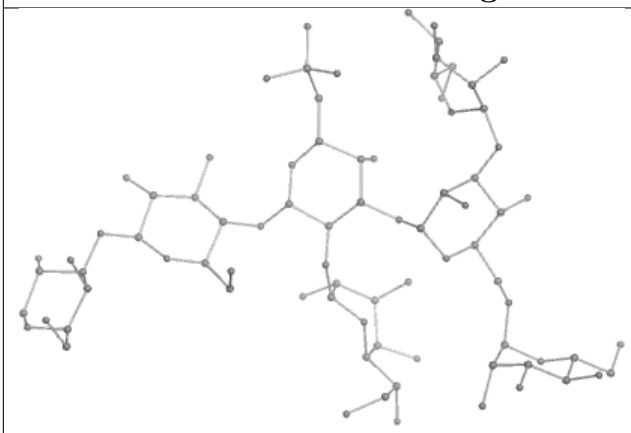


Torsions



Rings

Oligosaccharide Chain GA



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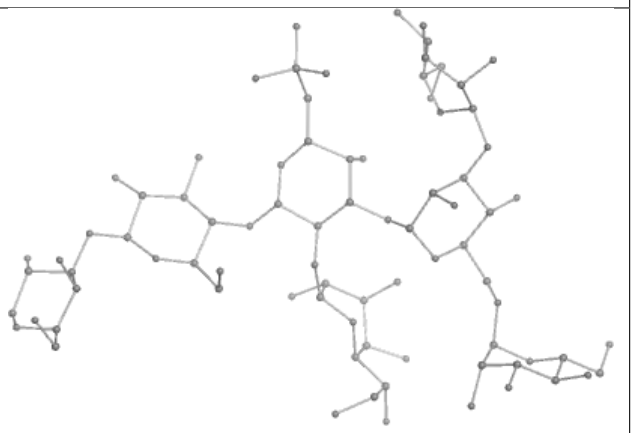
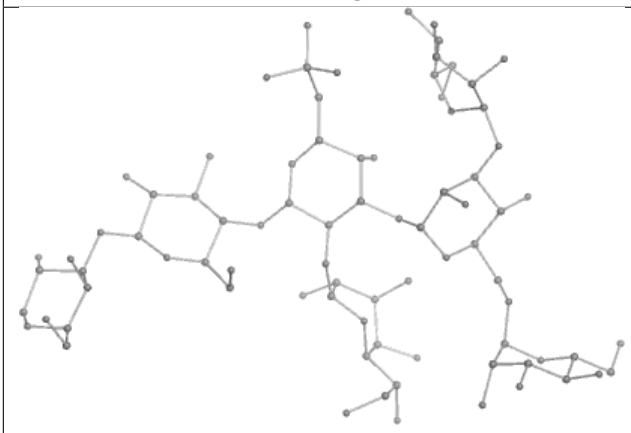
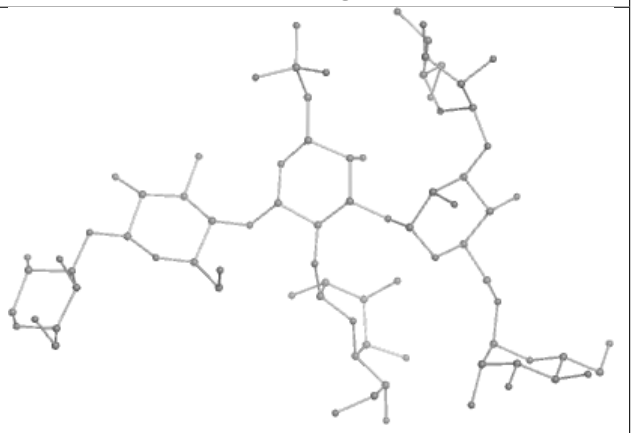


Bond angles

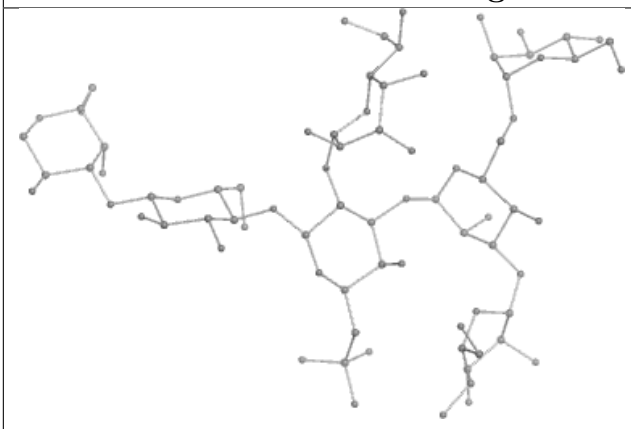


Torsions



Rings

Oligosaccharide Chain IA



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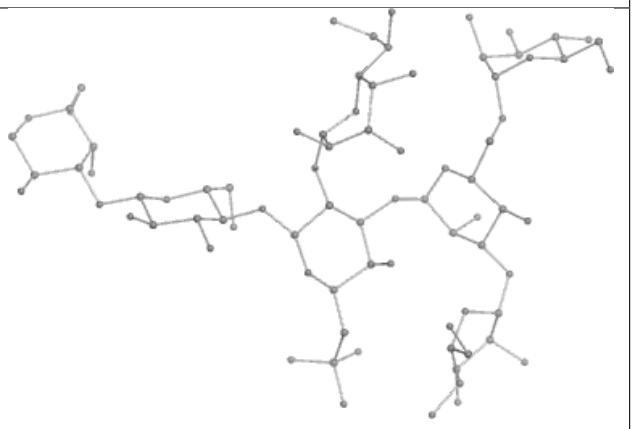
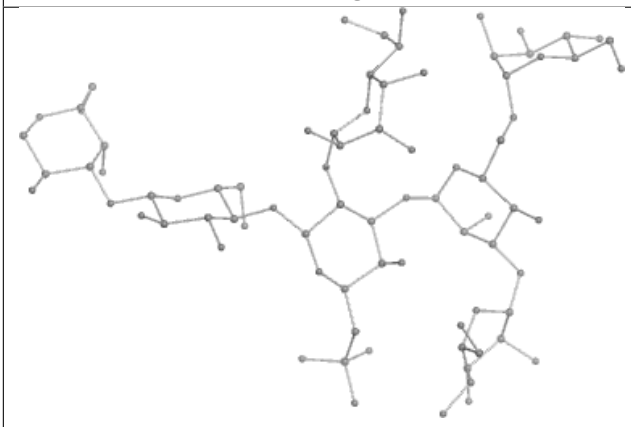
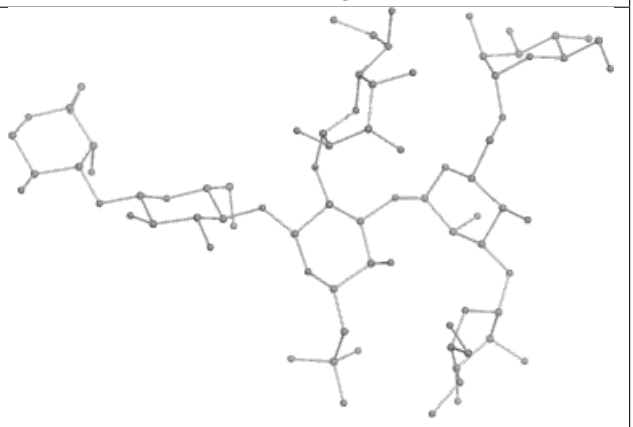


Bond angles

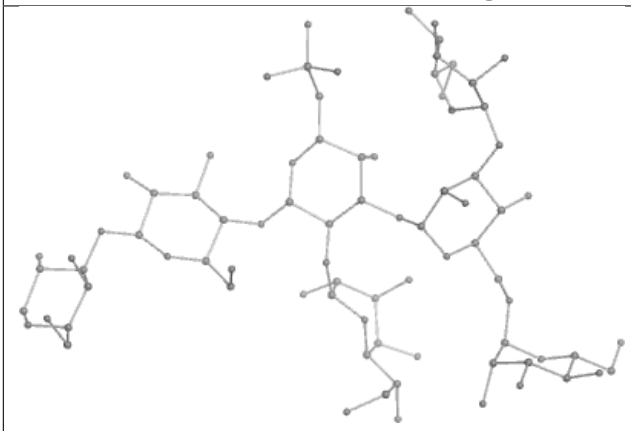


Torsions

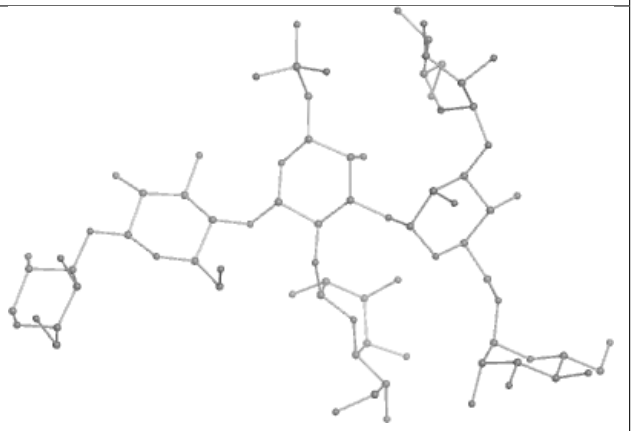


Rings

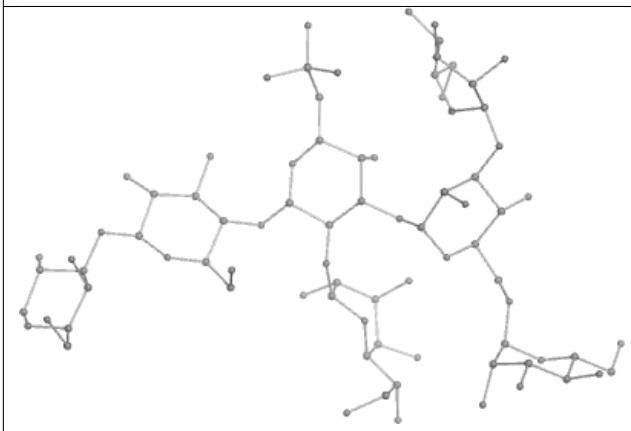
Oligosaccharide Chain KA



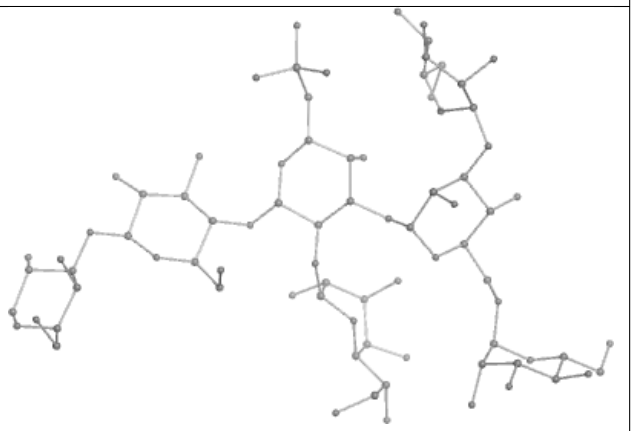
Bond lengths



Bond angles

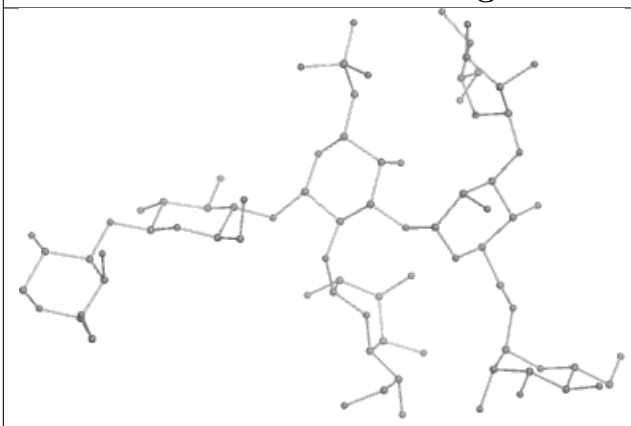


Torsions



Rings

Oligosaccharide Chain MA



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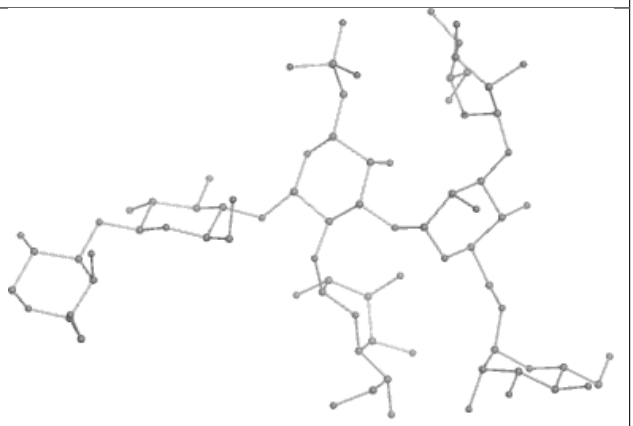

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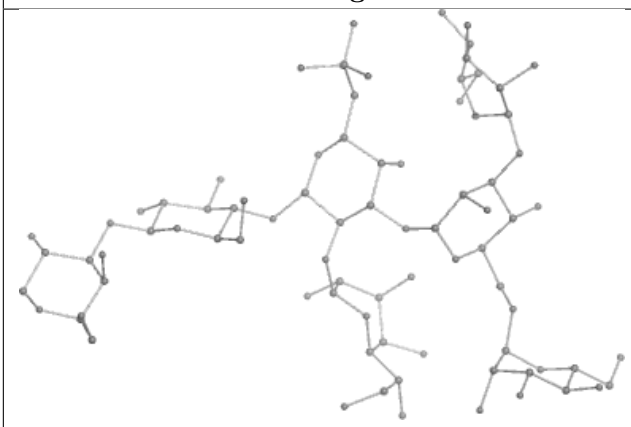

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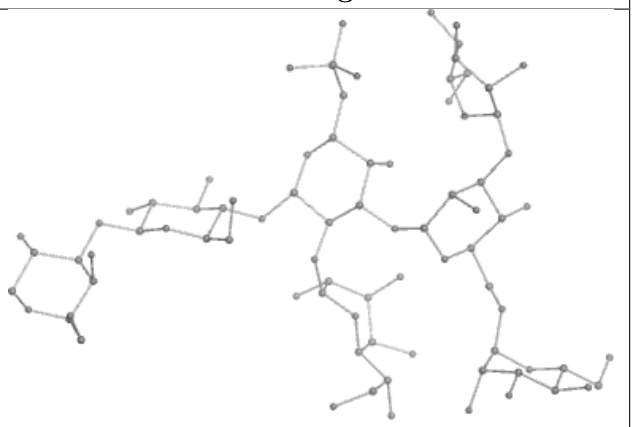
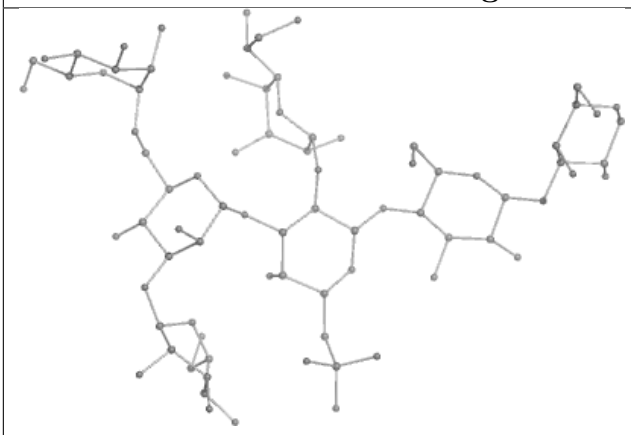


Rings

Oligosaccharide Chain OA



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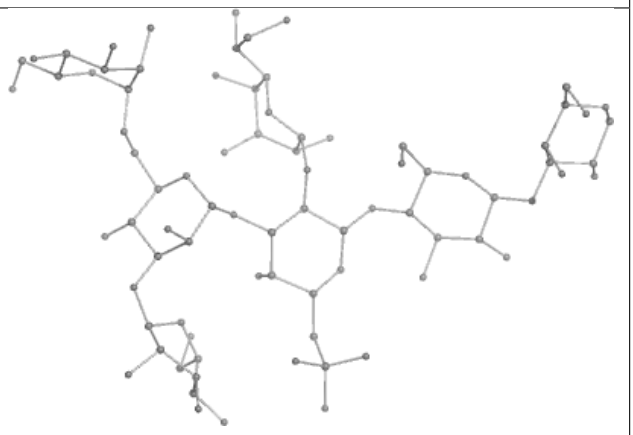
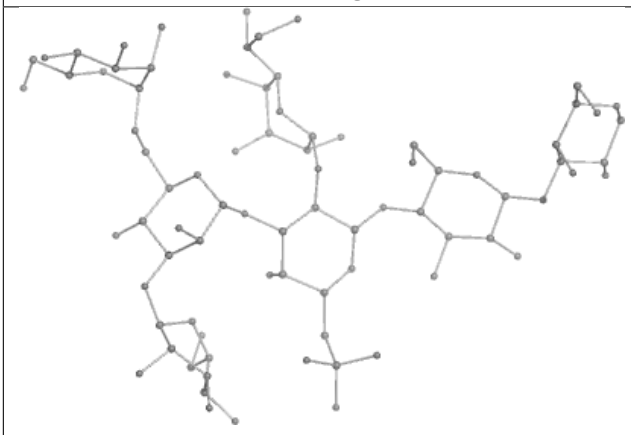


Bond angles



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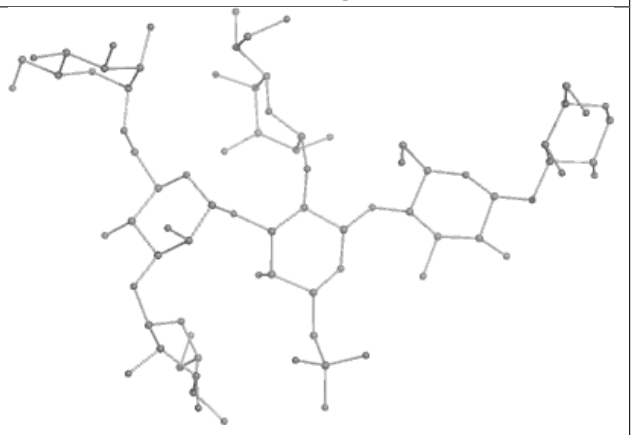
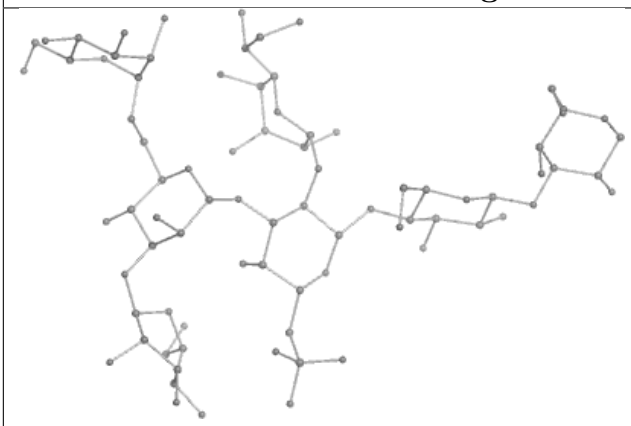


Rings

Oligosaccharide Chain QA



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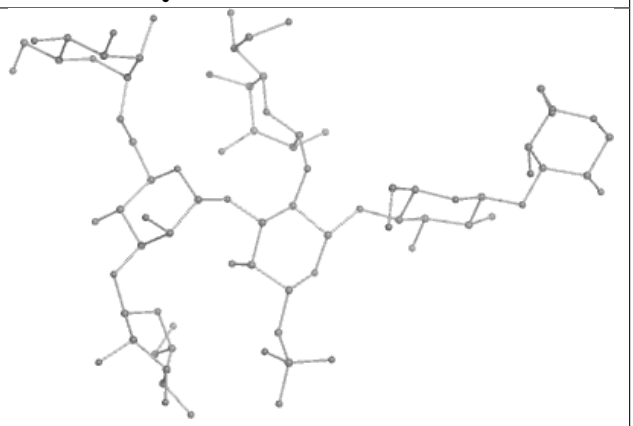
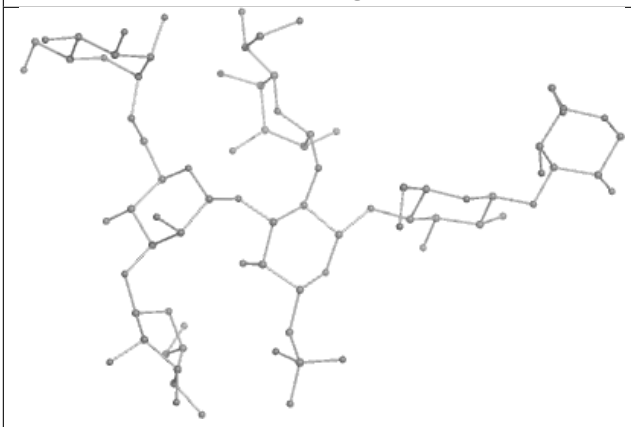


Bond angles



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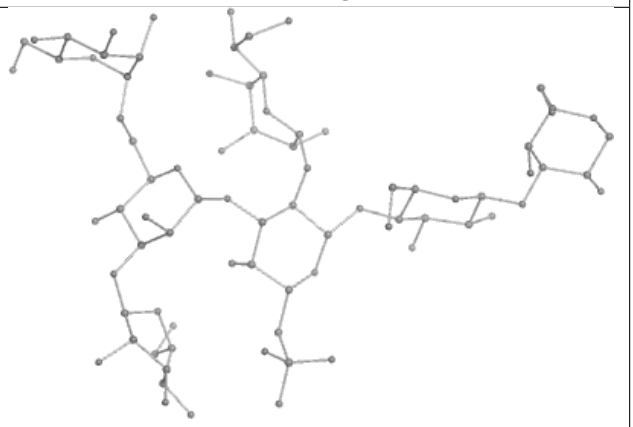
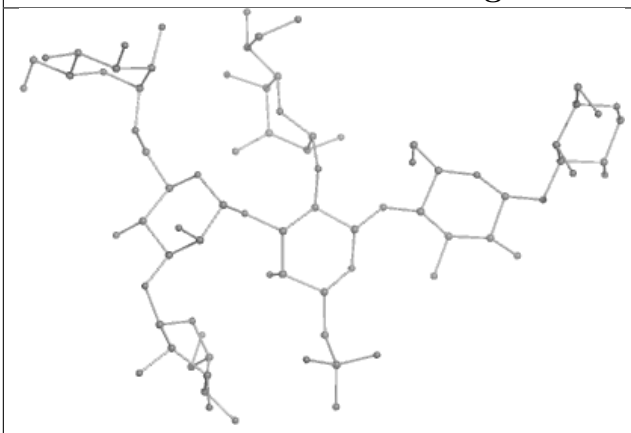


Rings

Oligosaccharide Chain SA



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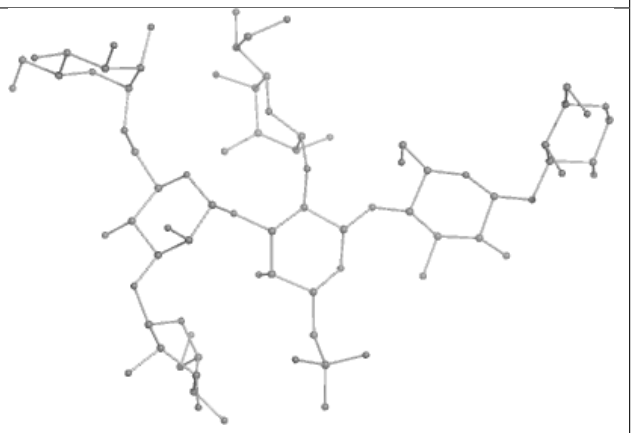
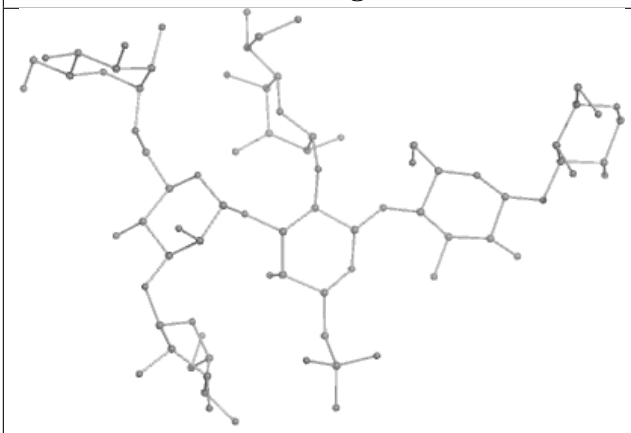


Bond angles



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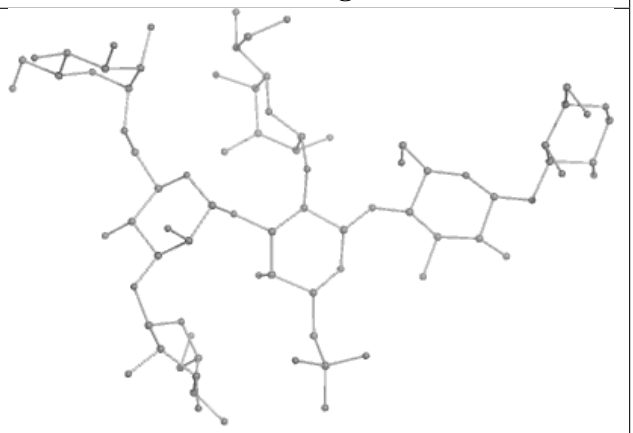
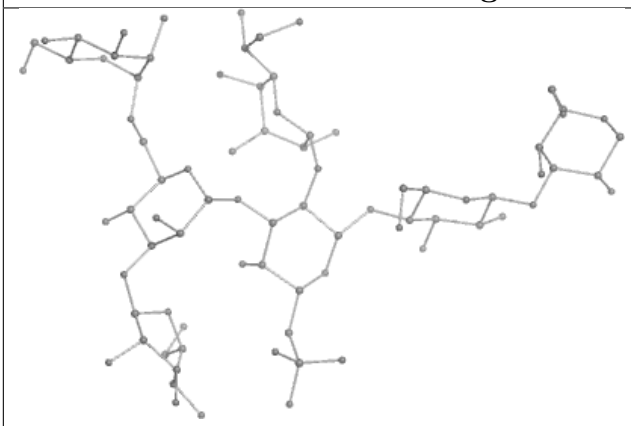


Rings

Oligosaccharide Chain UA



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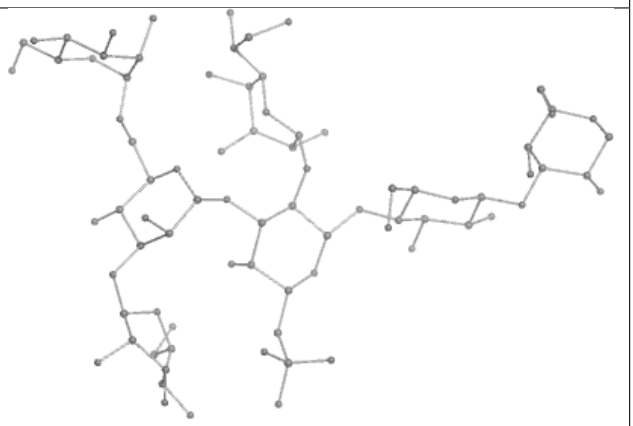
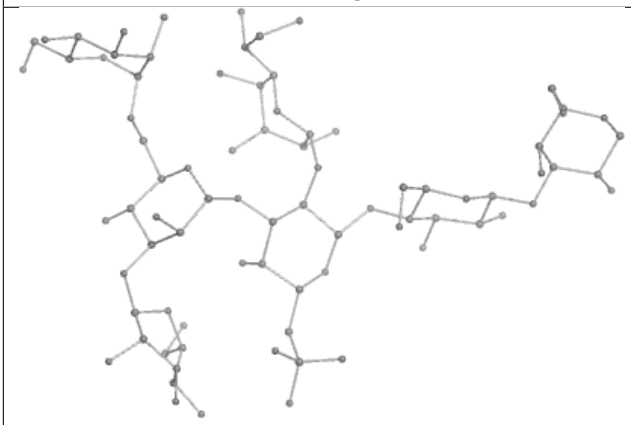


Bond angles



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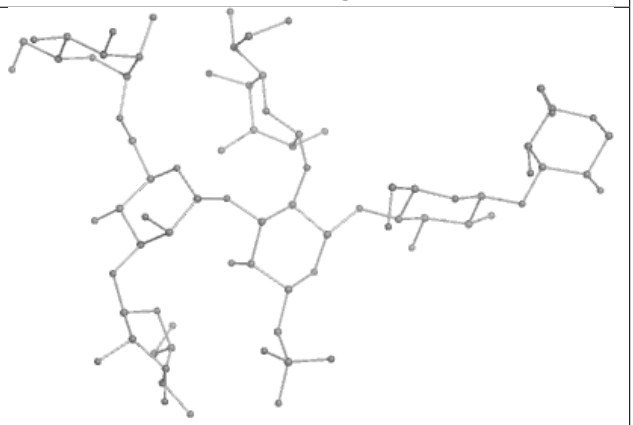
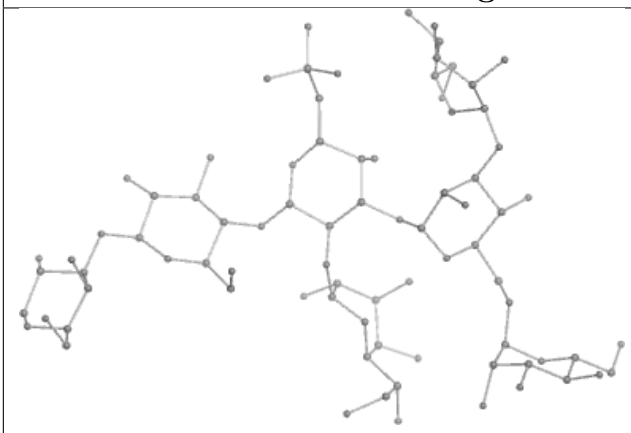


Rings

Oligosaccharide Chain WA



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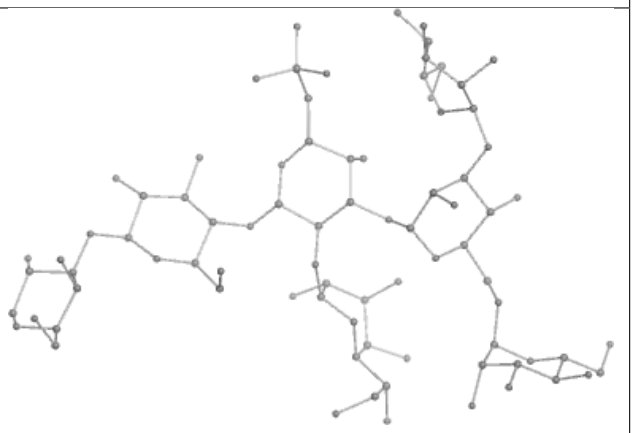
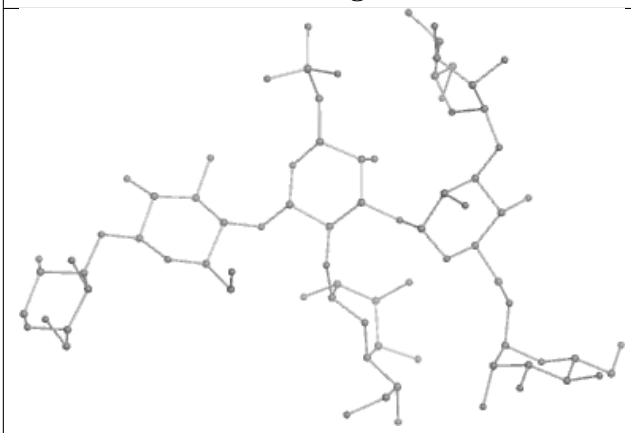


Bond angles



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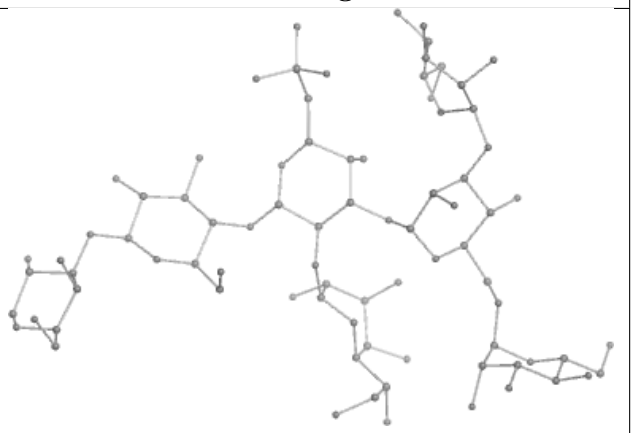
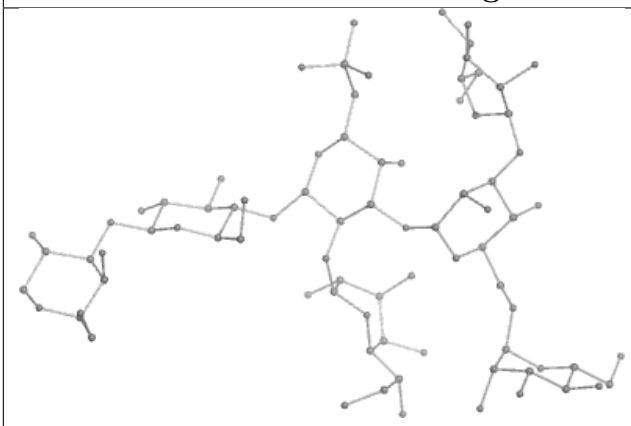


Rings

Oligosaccharide Chain YA



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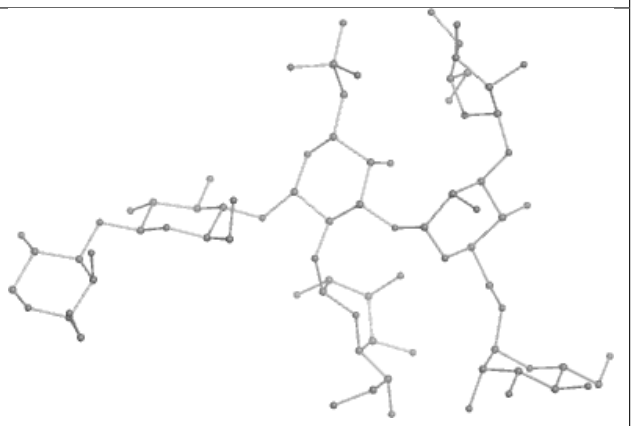
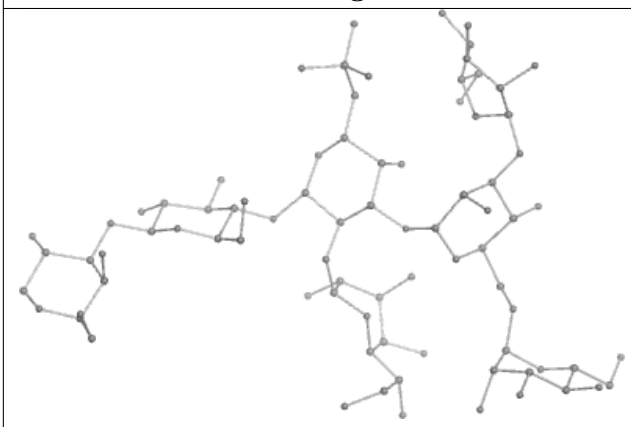


Bond angles



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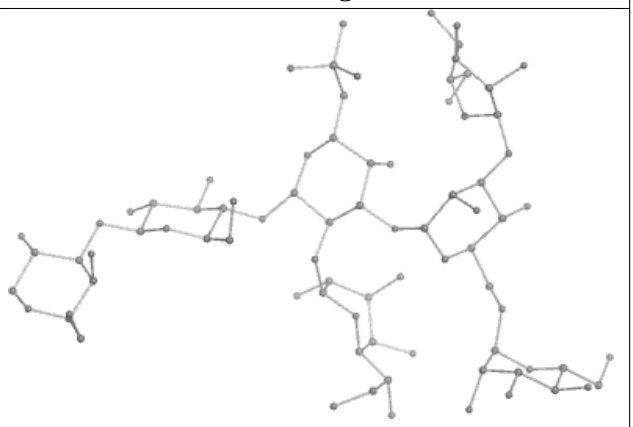
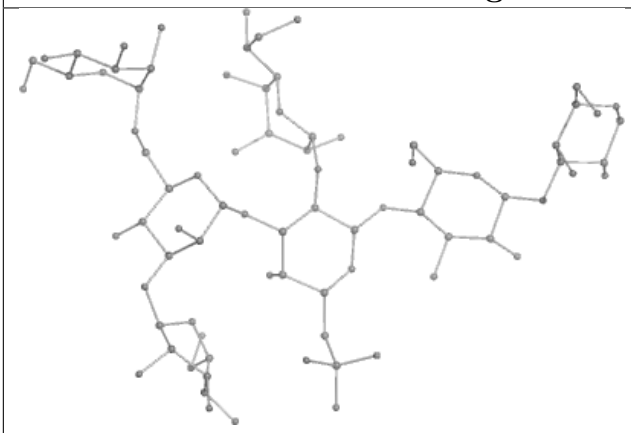


Rings

Oligosaccharide Chain aA



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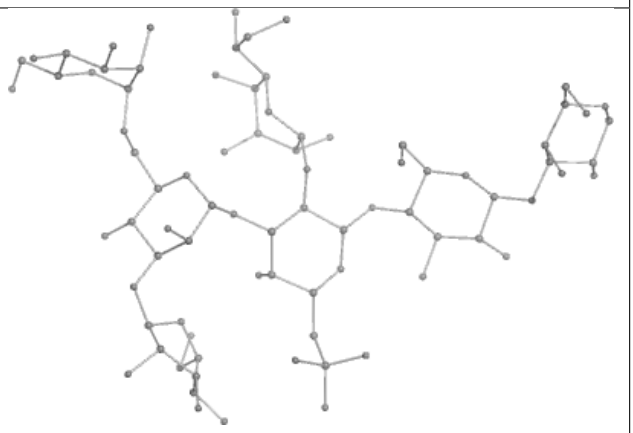
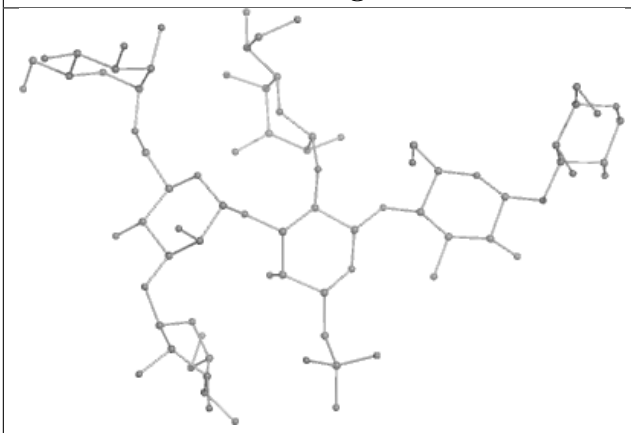
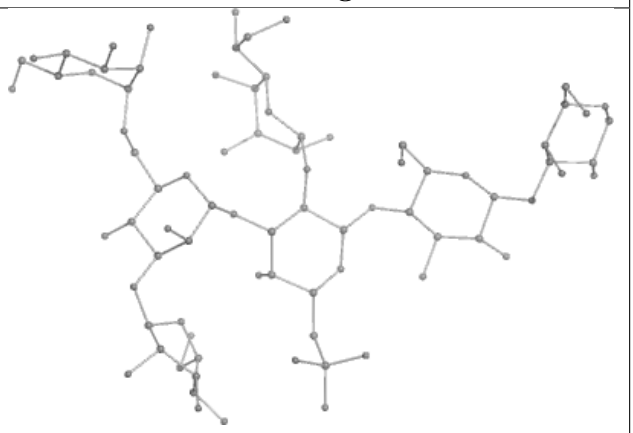


Bond angles

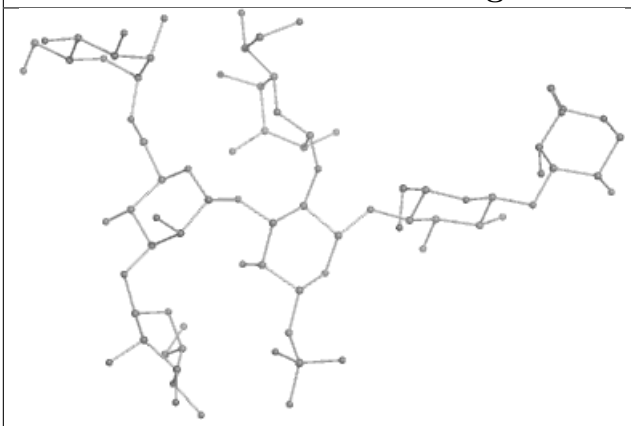


Torsions



Rings

Oligosaccharide Chain cA



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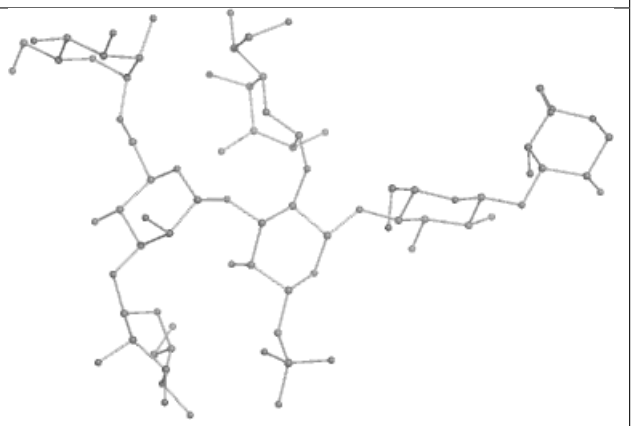
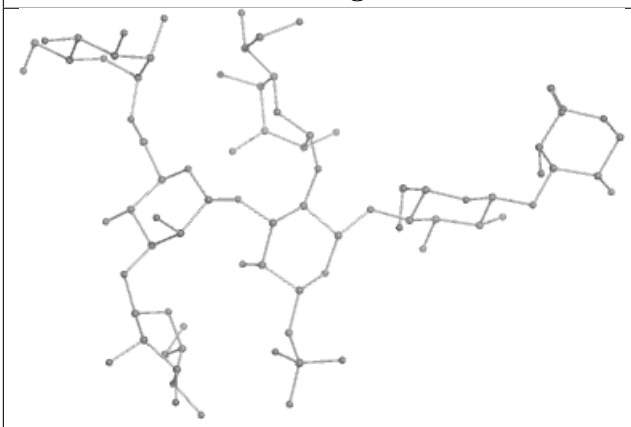
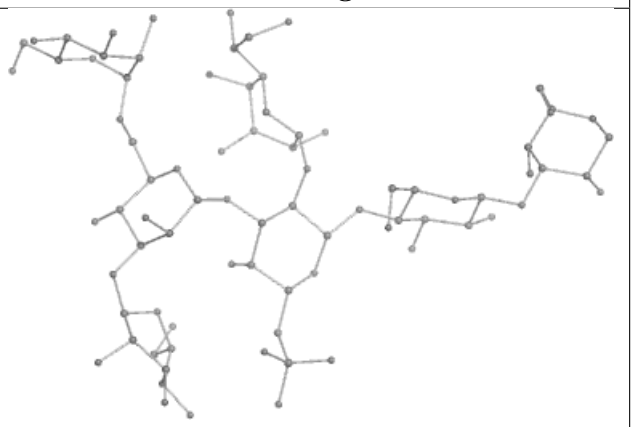


Bond angles

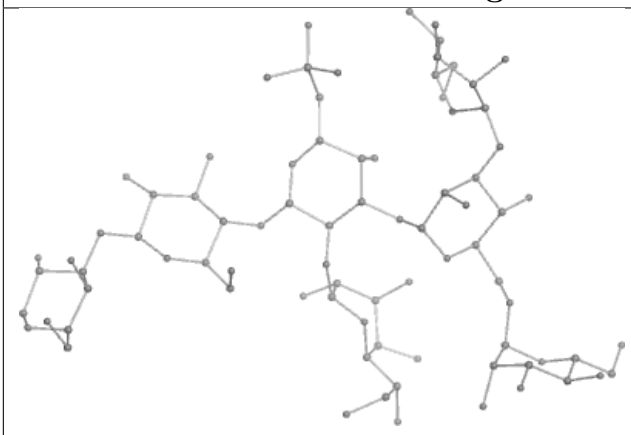


Torsions



Rings

Oligosaccharide Chain eA



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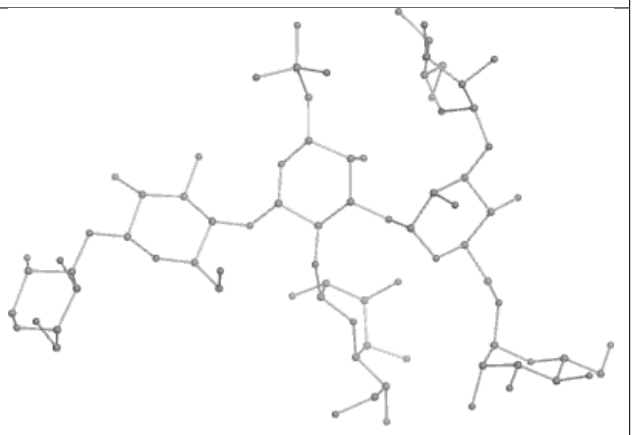
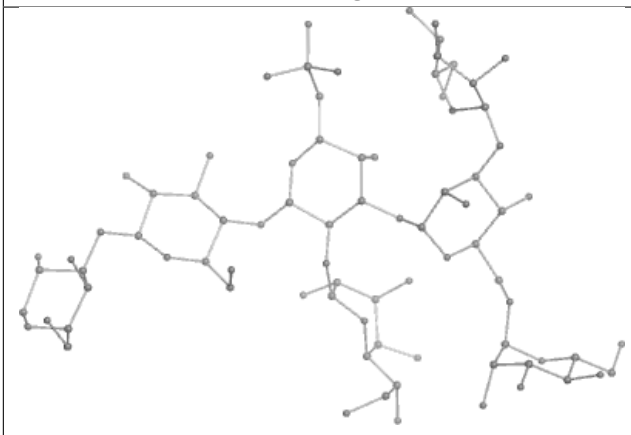


Bond angles



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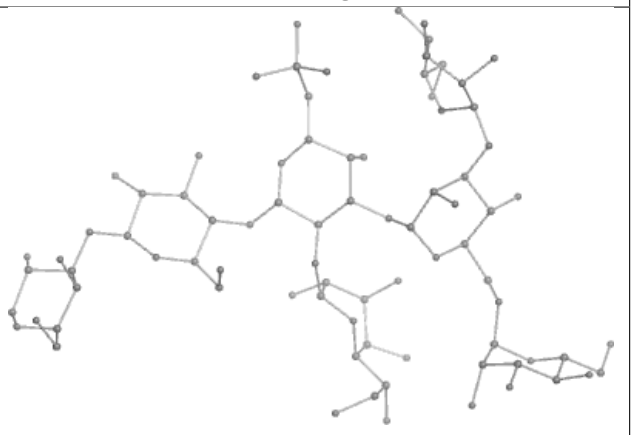
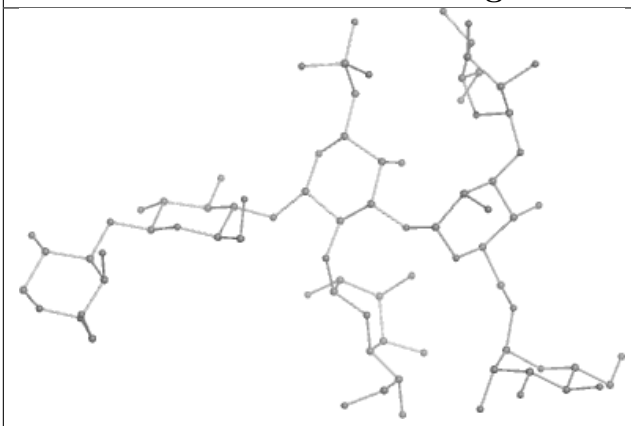


Rings

Oligosaccharide Chain gA



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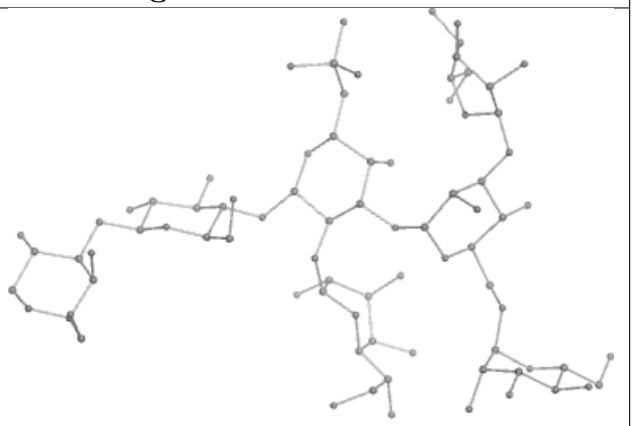
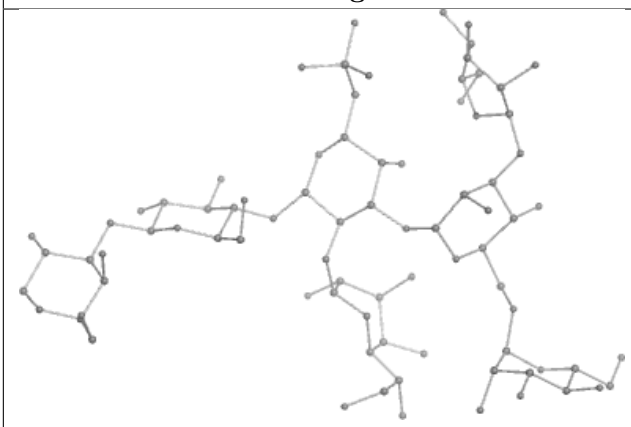


Bond angles



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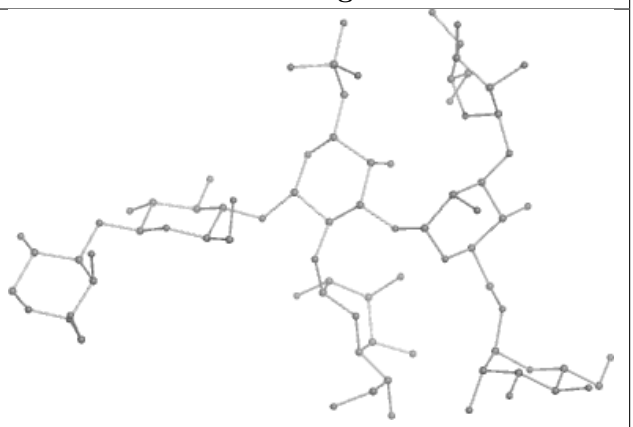
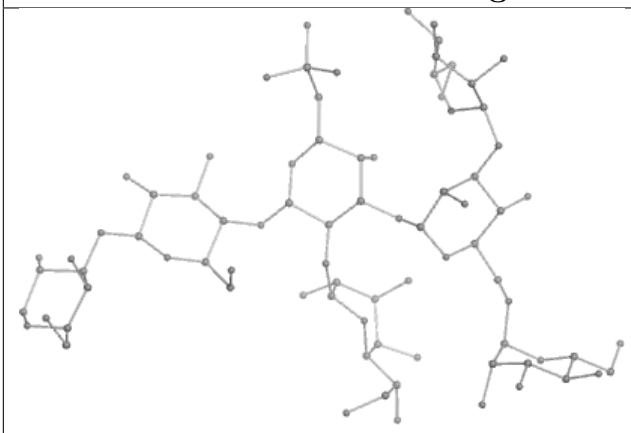
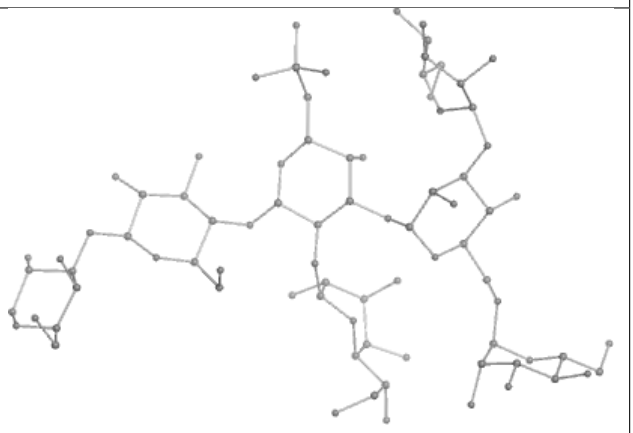


Rings

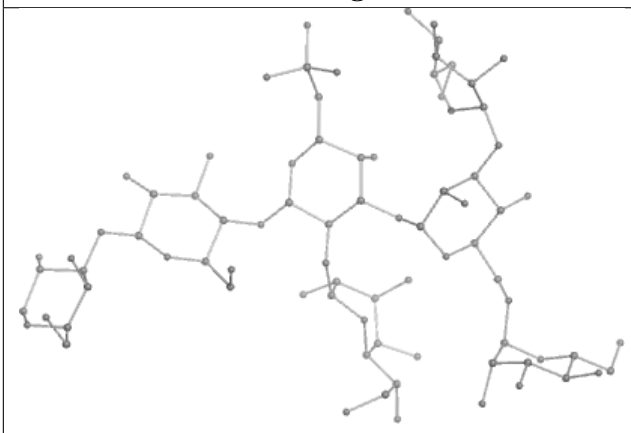
Oligosaccharide Chain iA



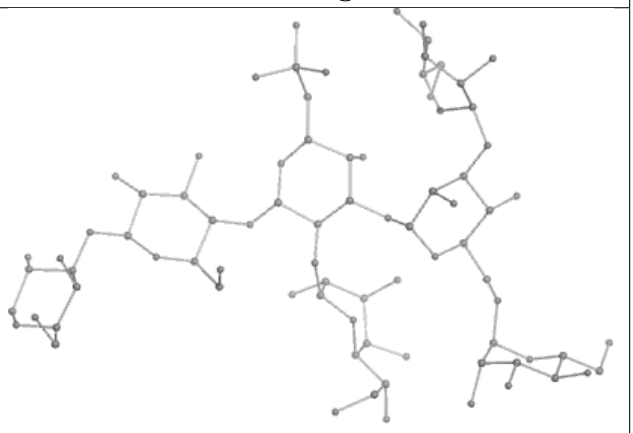
Bond lengths



Bond angles

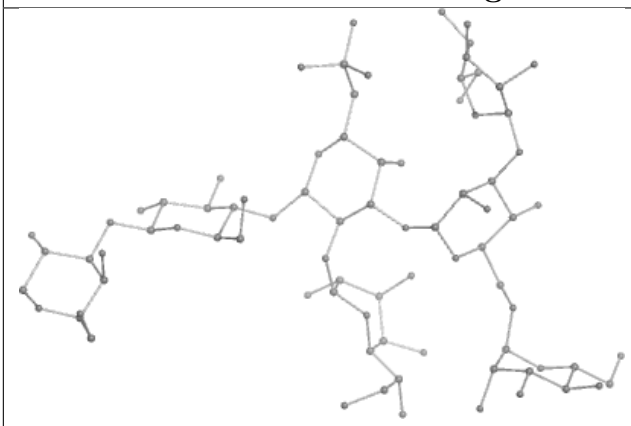


Torsions

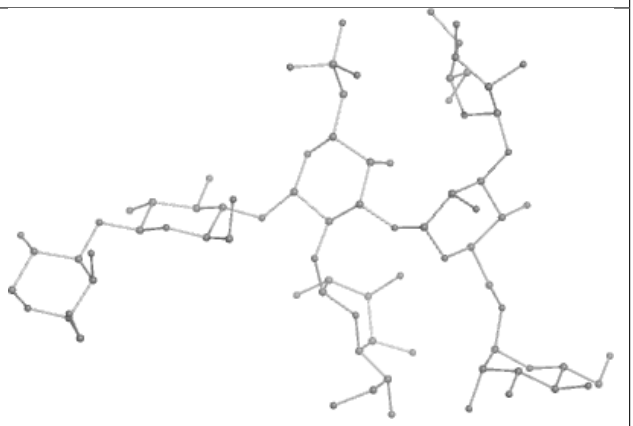


Rings

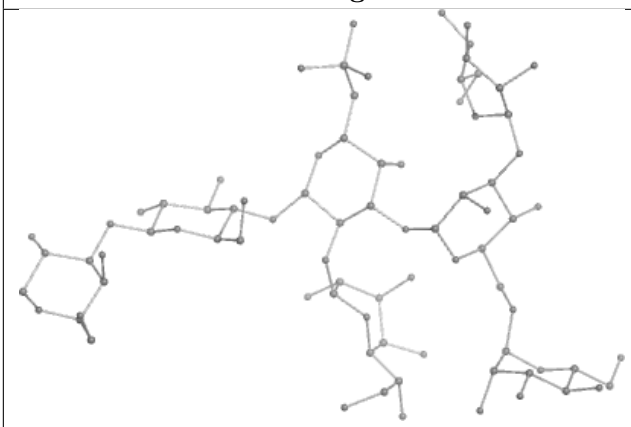
Oligosaccharide Chain kA



Bond lengths



Bond angles



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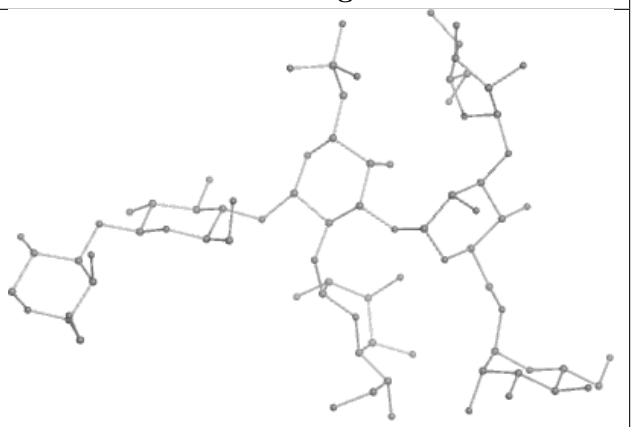
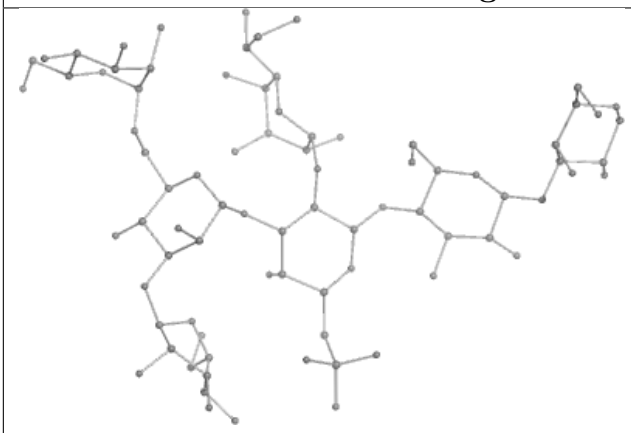
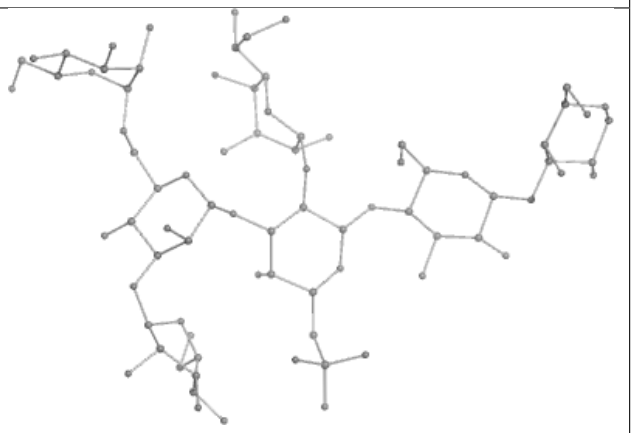


Rings

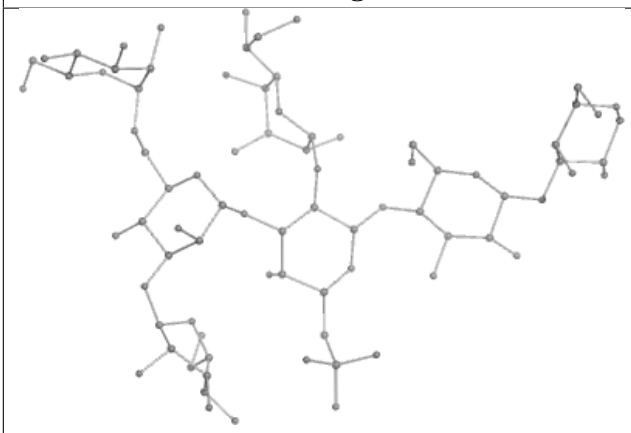
Oligosaccharide Chain mA



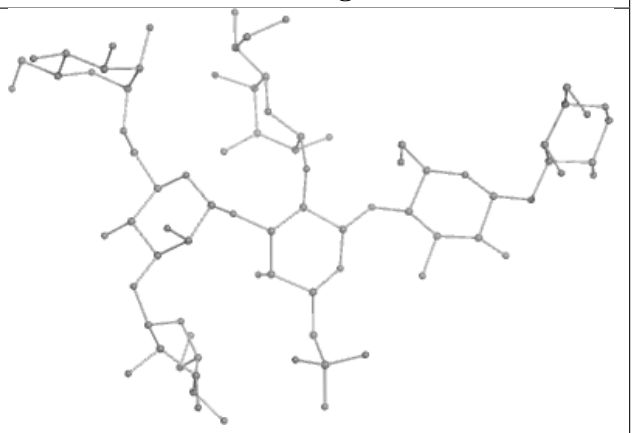
Bond lengths



Bond angles

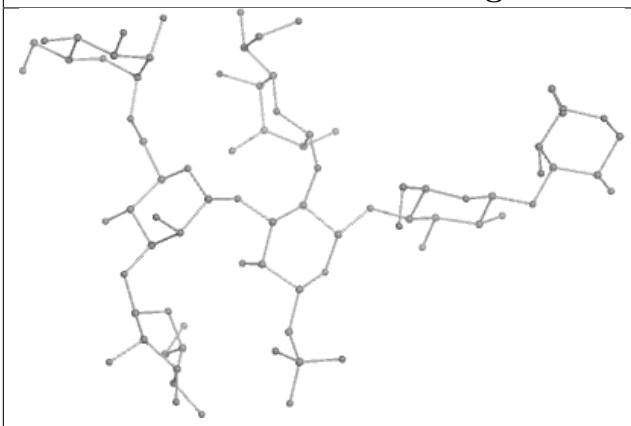


Torsions



Rings

Oligosaccharide Chain oA



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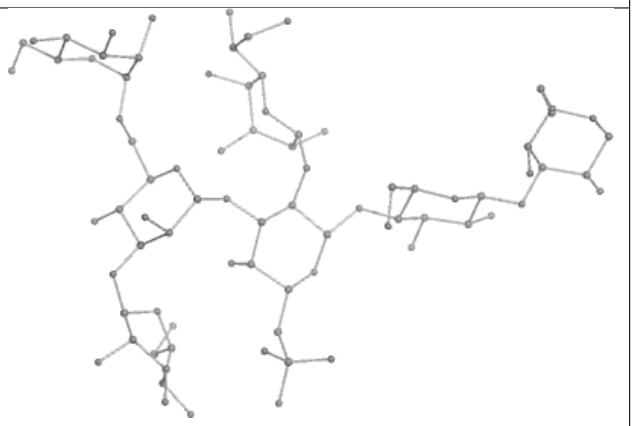
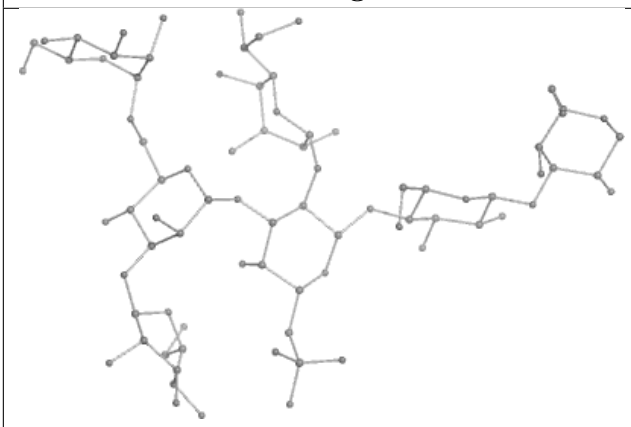


Bond angles



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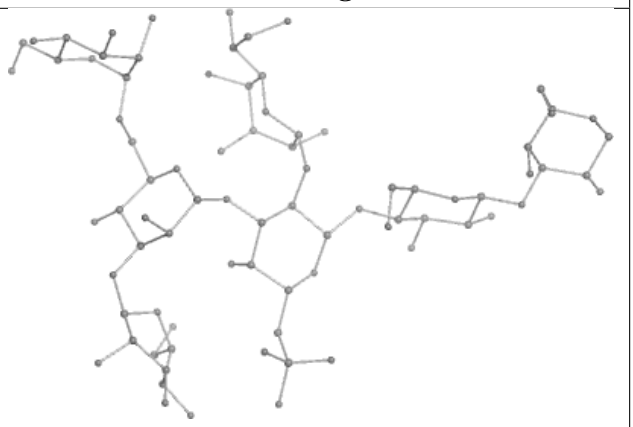
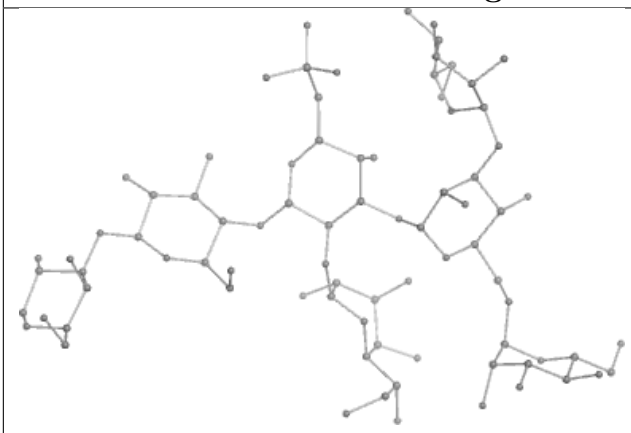


Rings

Oligosaccharide Chain qA



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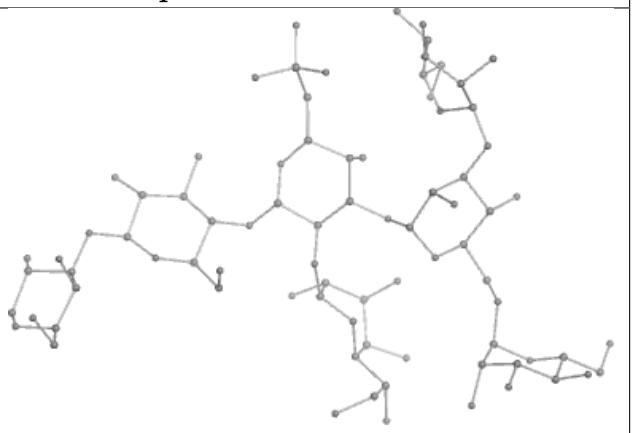
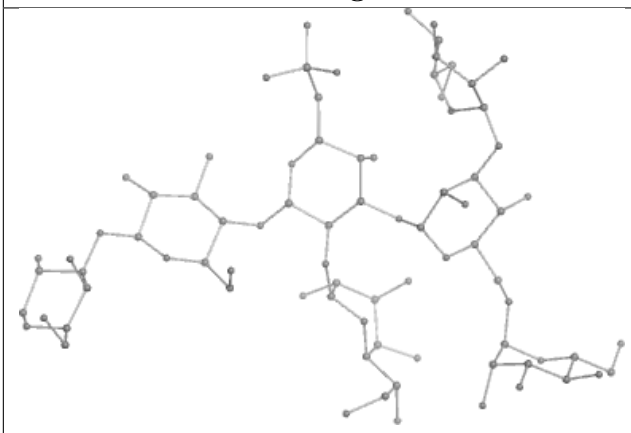
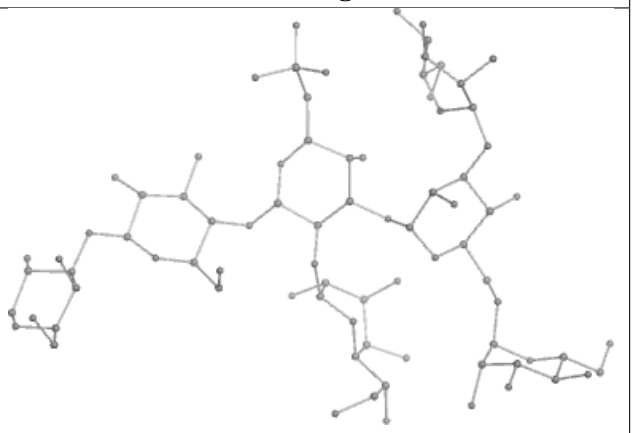


Bond angles

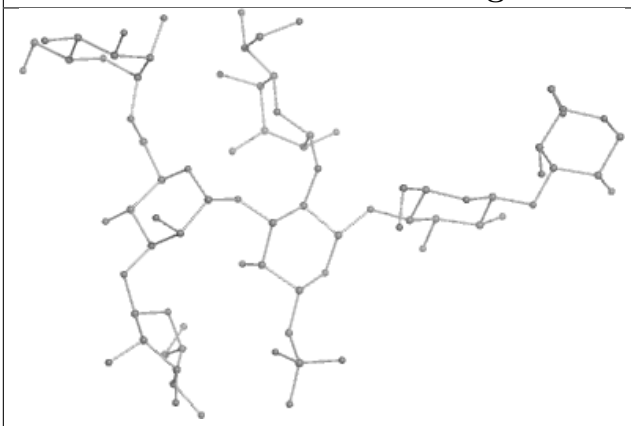


Torsions



Rings

Oligosaccharide Chain sA



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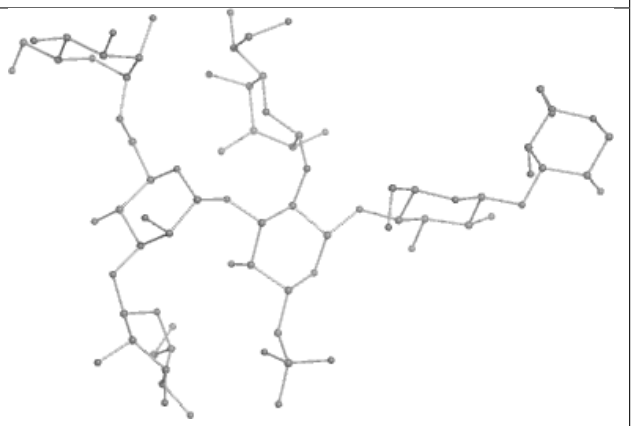
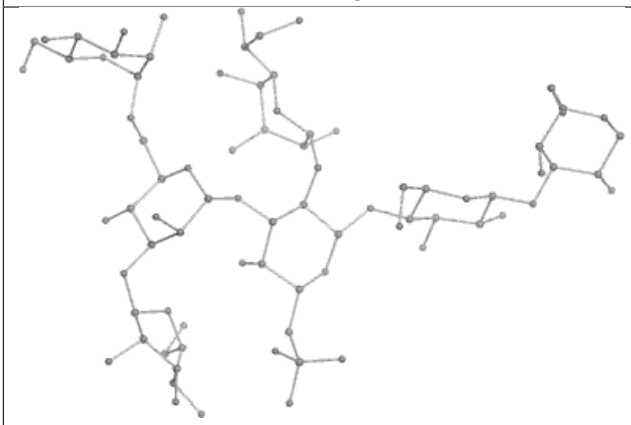
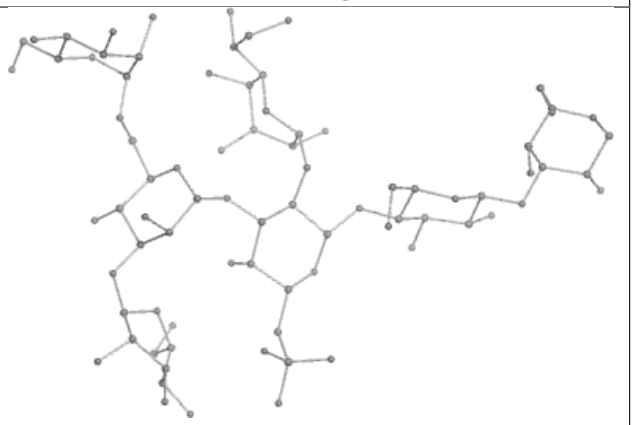


Bond angles

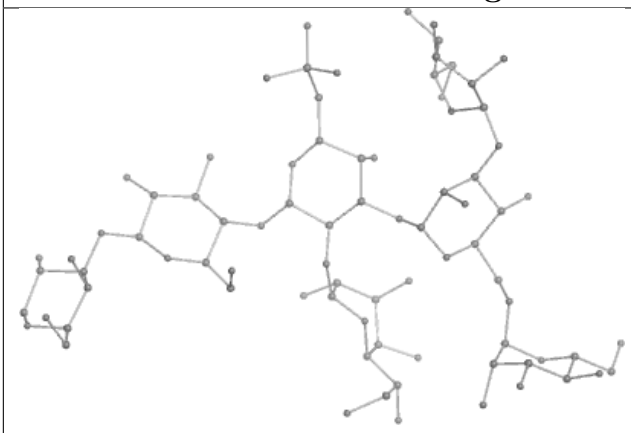


Torsions



Rings

Oligosaccharide Chain uA



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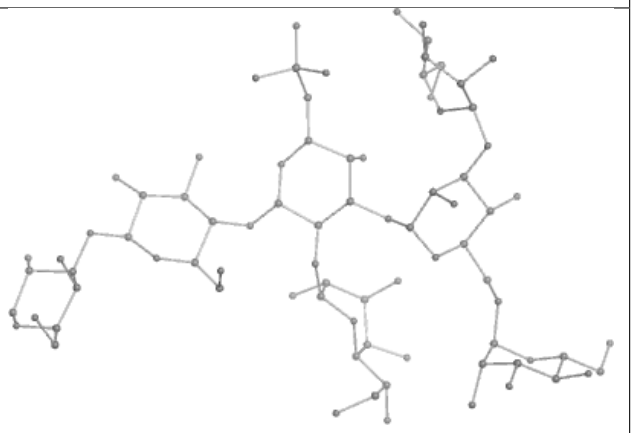
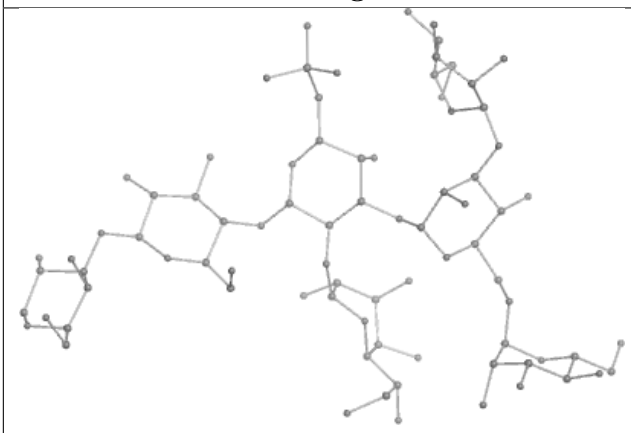


Bond angles



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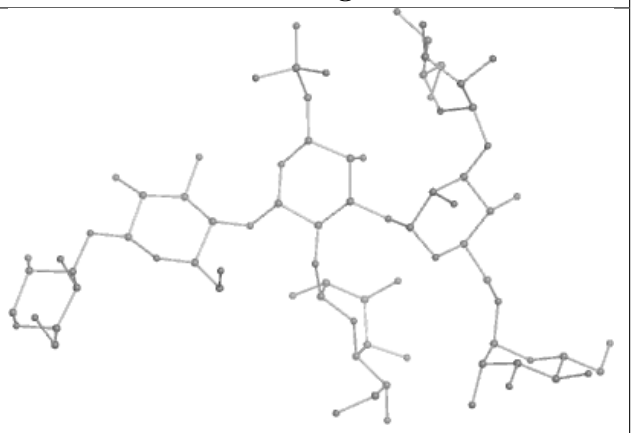
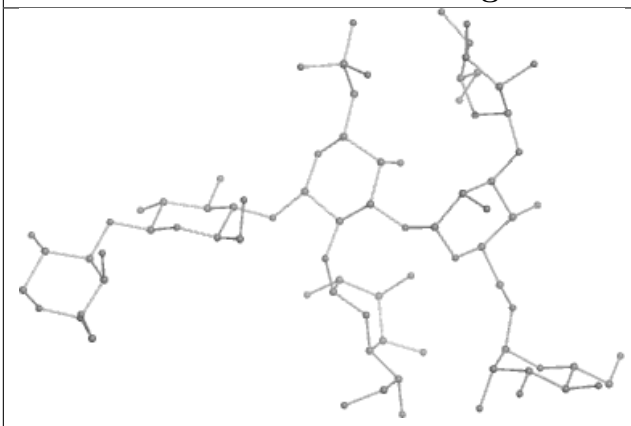


Rings

Oligosaccharide Chain wA



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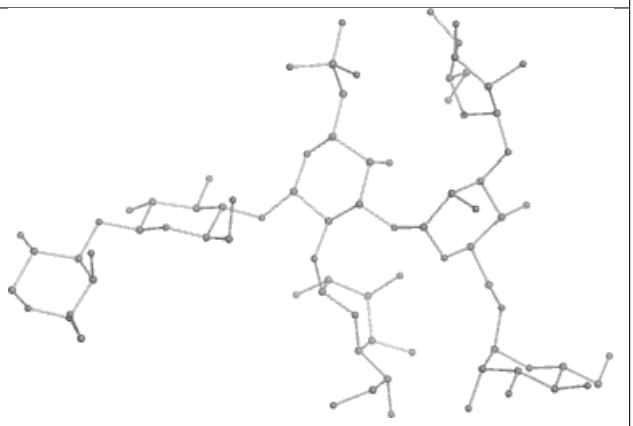
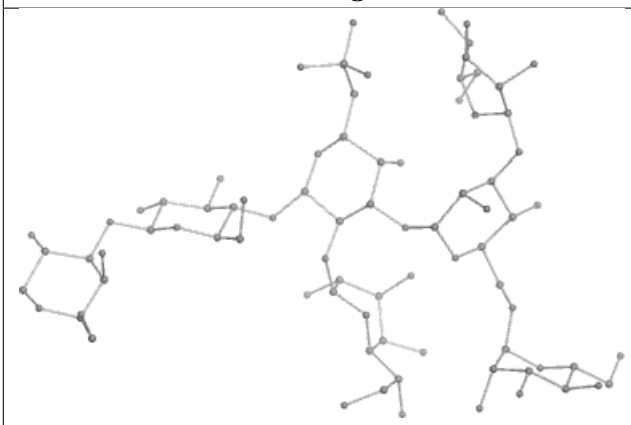


Bond angles



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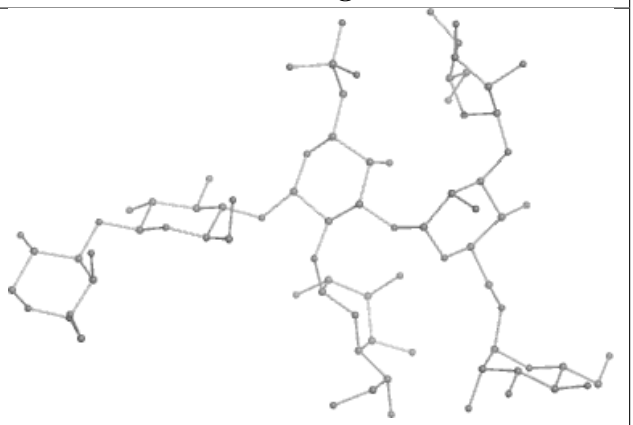
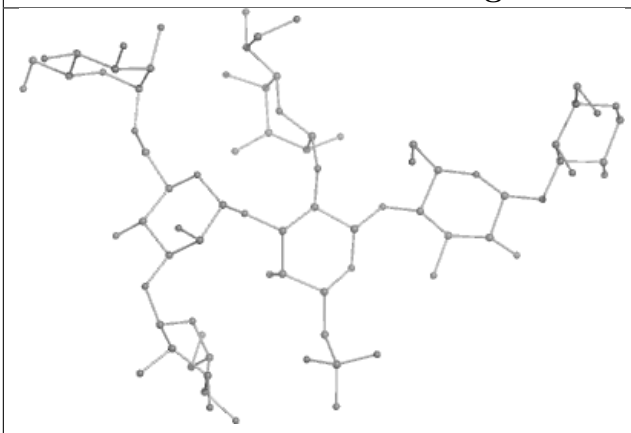


Rings

Oligosaccharide Chain yA



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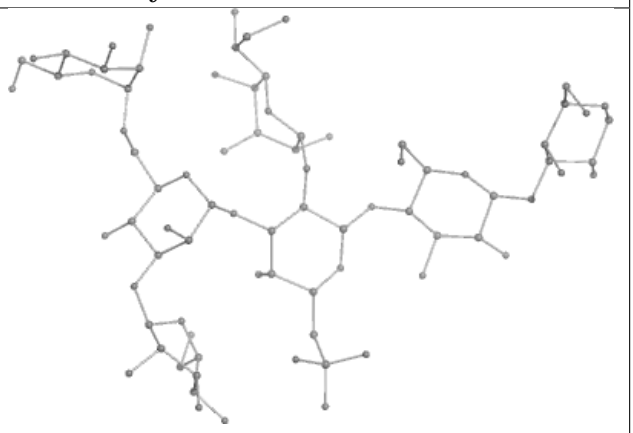
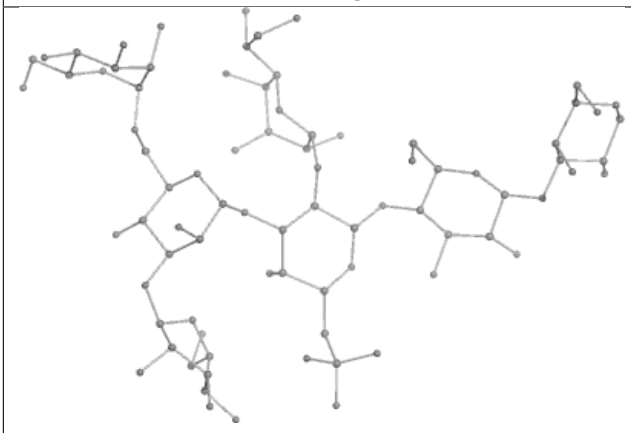


Bond angles



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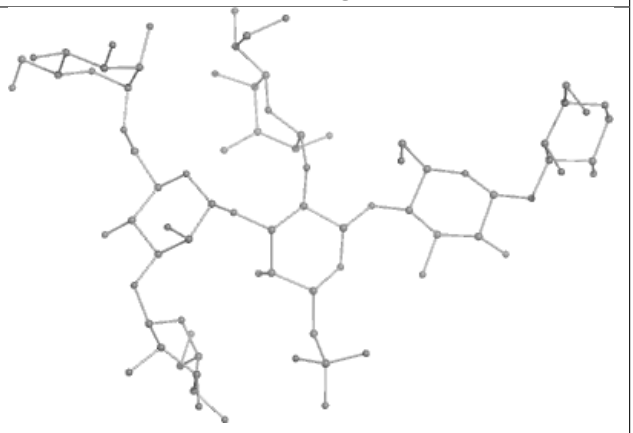
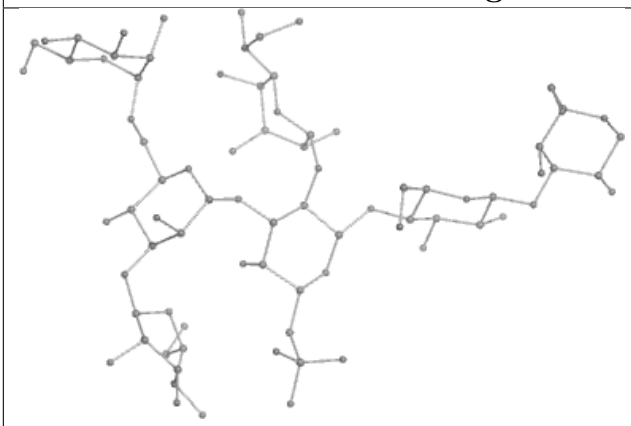


Rings

Oligosaccharide Chain 0A



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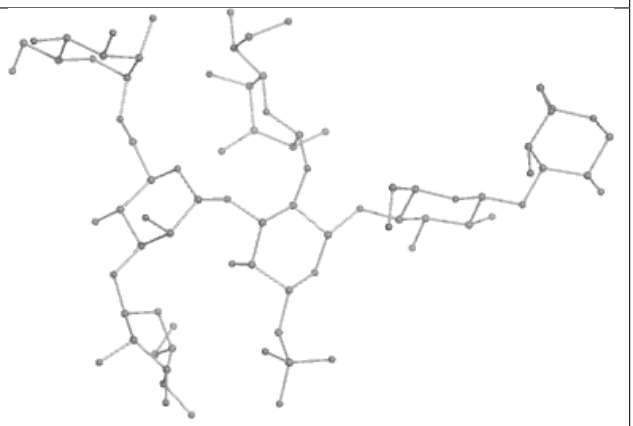
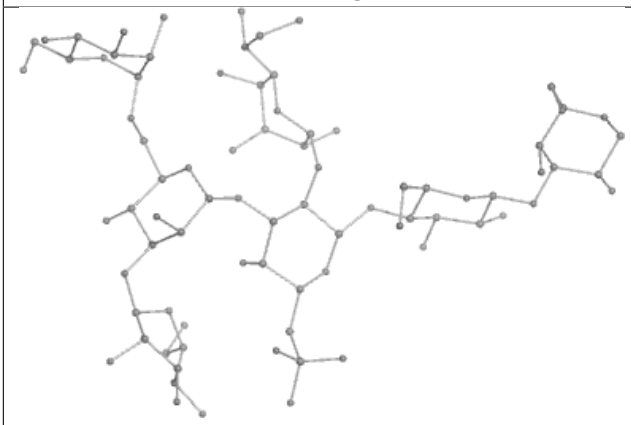
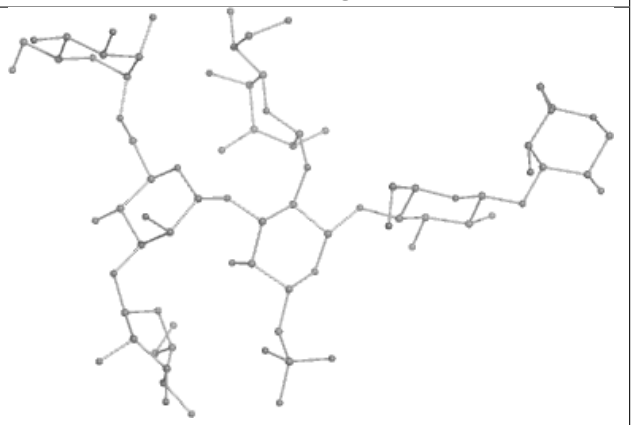


Bond angles

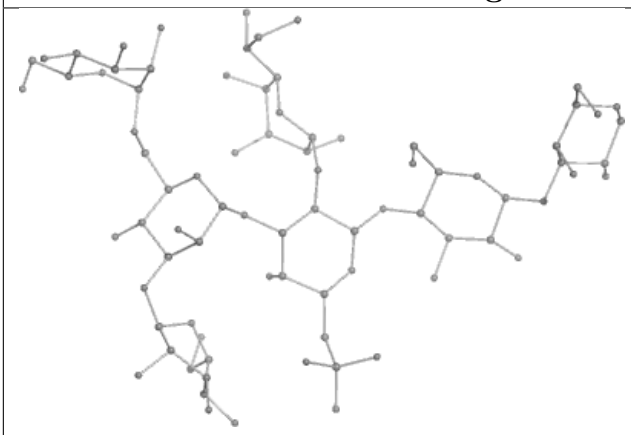


Torsions



Rings

Oligosaccharide Chain 2A



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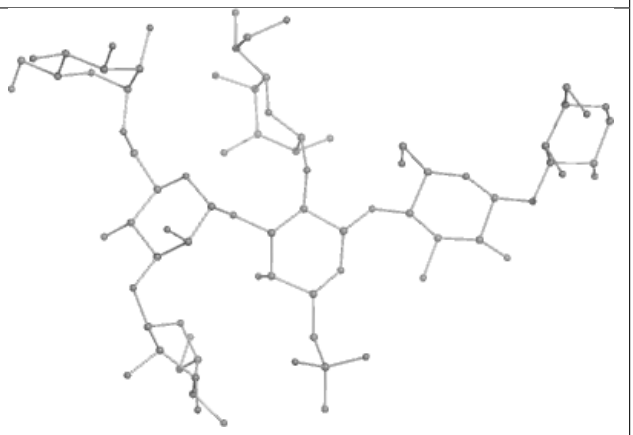
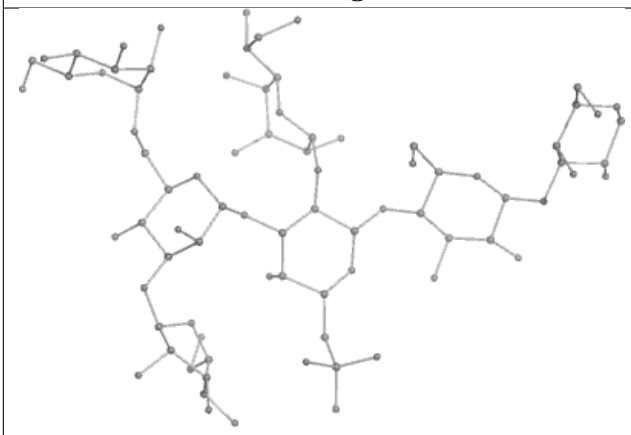


Bond angles



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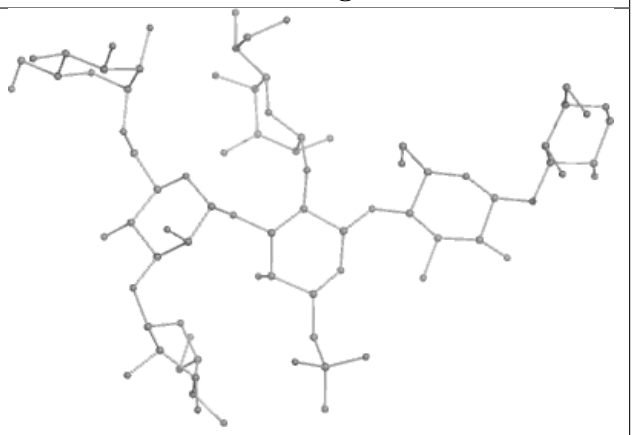
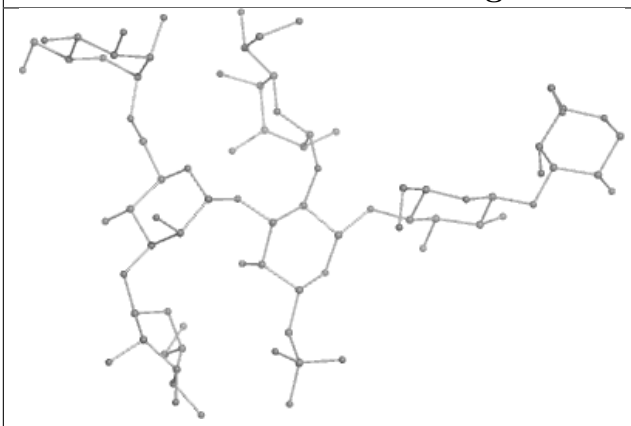


Rings

Oligosaccharide Chain 4A



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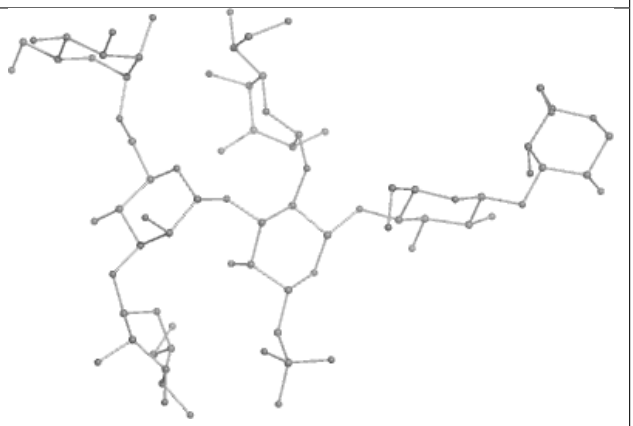
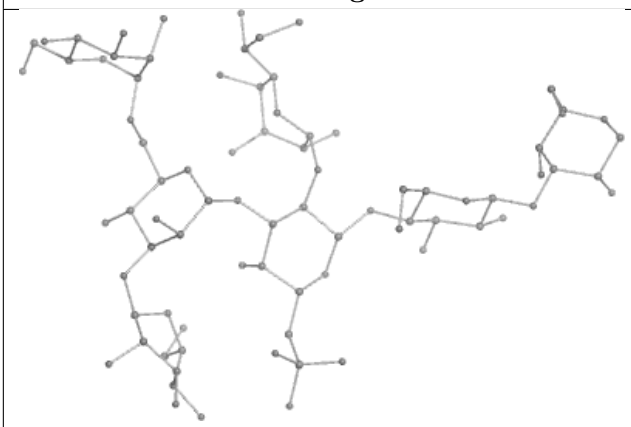
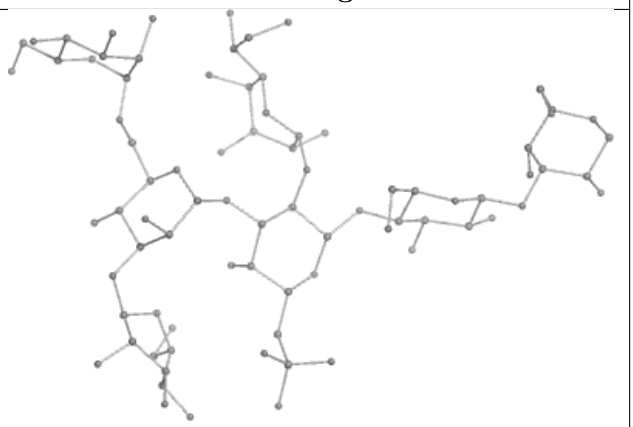


Bond angles

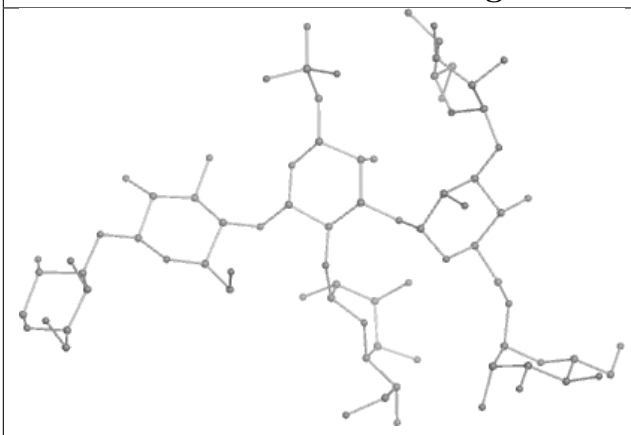


Torsions



Rings

Oligosaccharide Chain 6A



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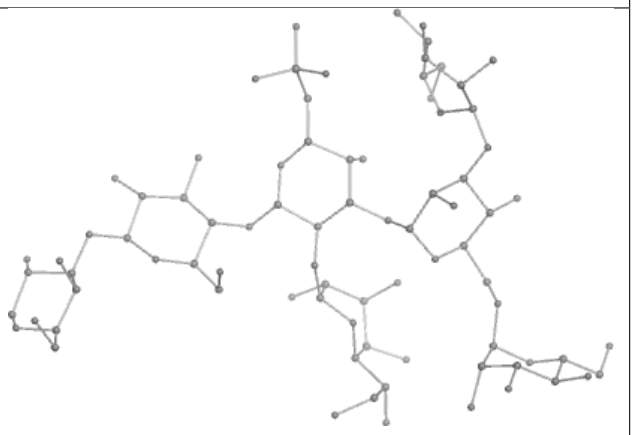
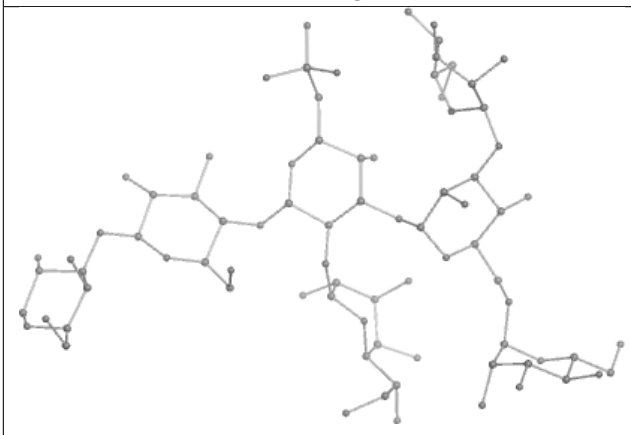
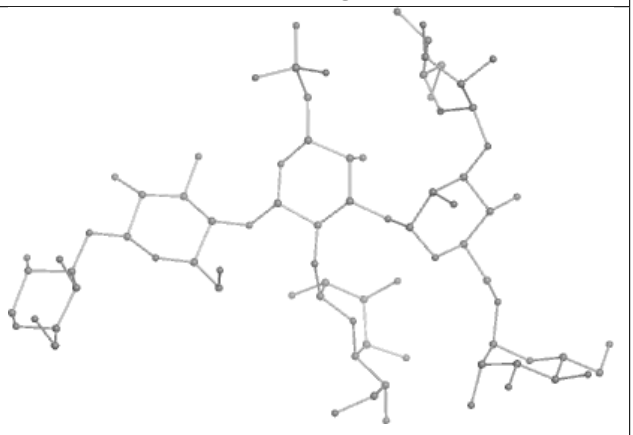


Bond angles

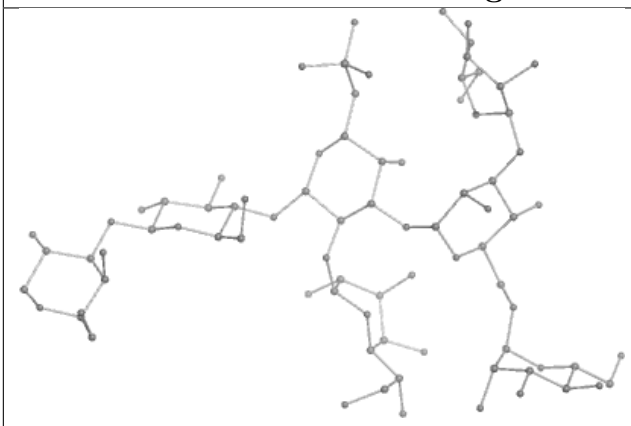


Torsions



Rings

Oligosaccharide Chain 8A



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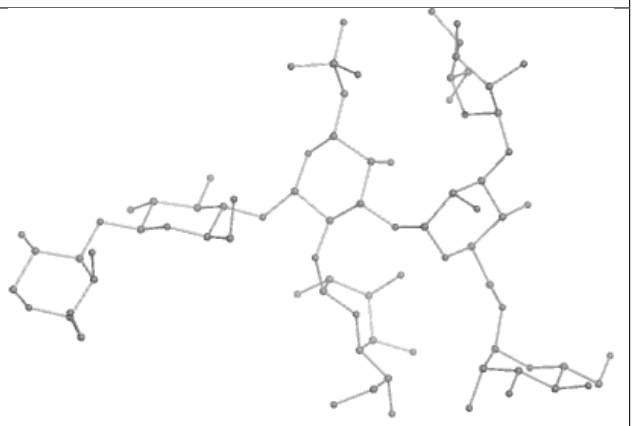
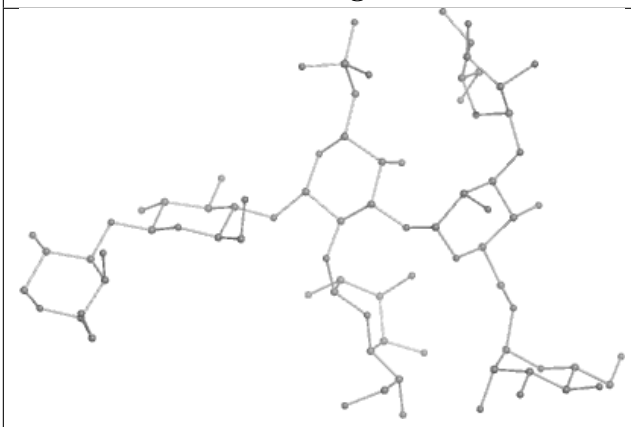
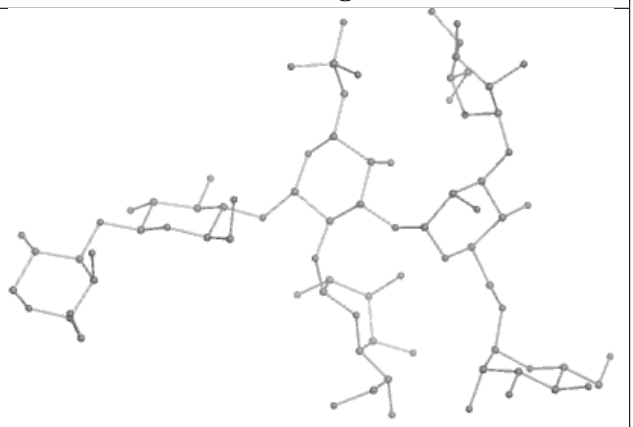


Bond angles

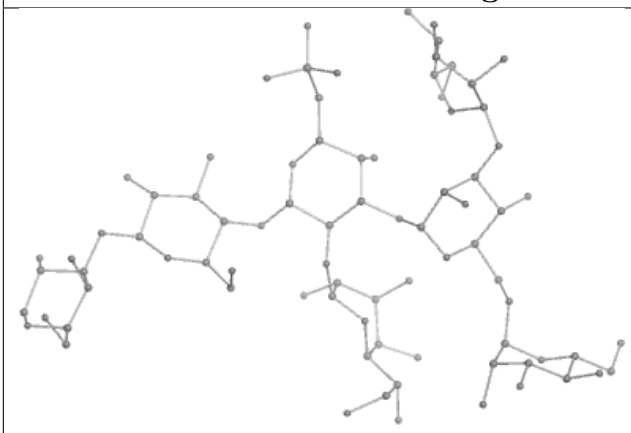


Torsions

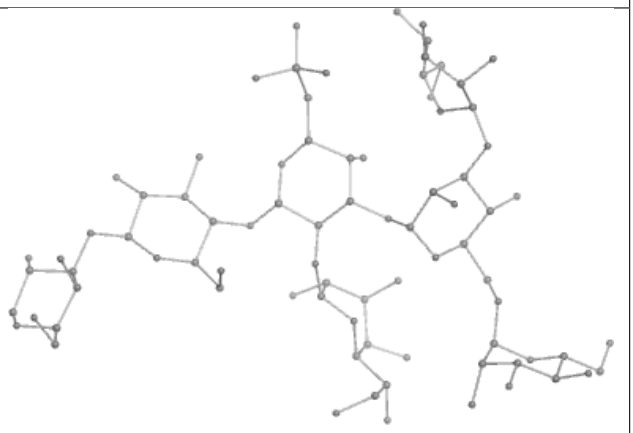


Rings

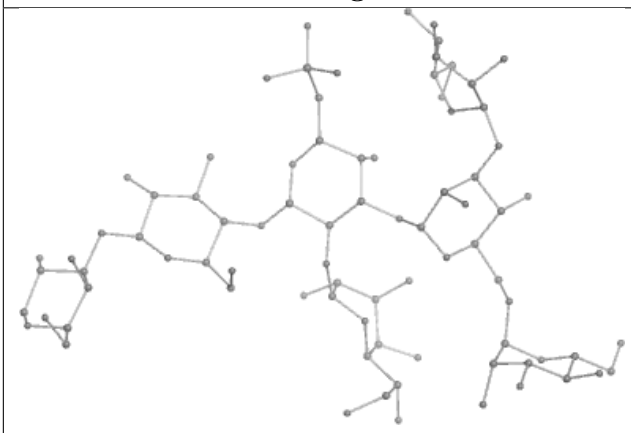
Oligosaccharide Chain AB



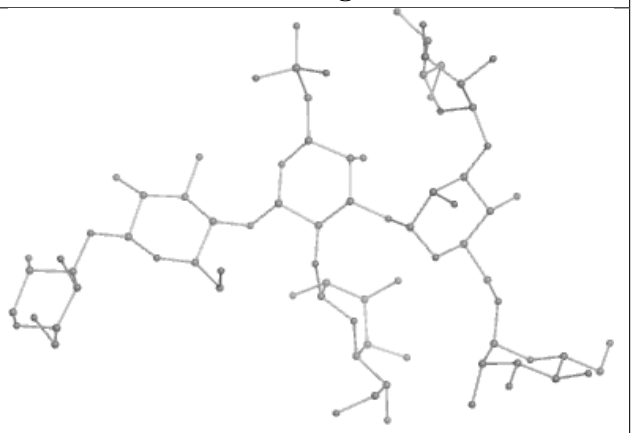
Bond lengths



Bond angles

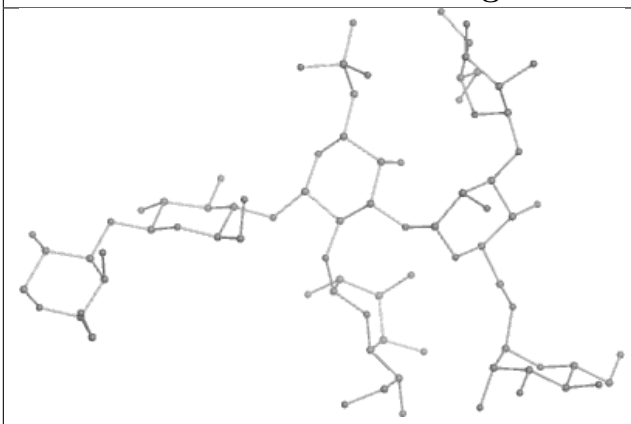


Torsions

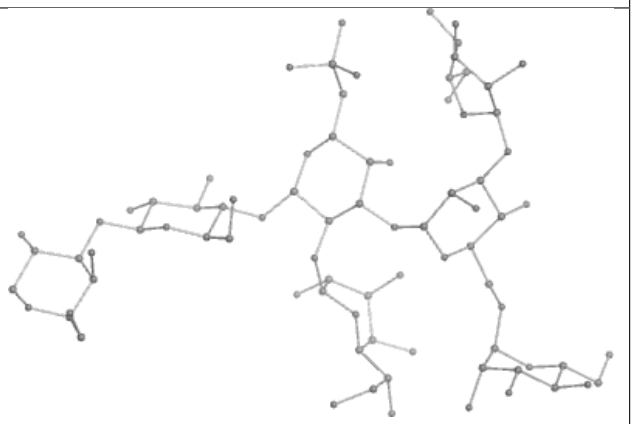


Rings

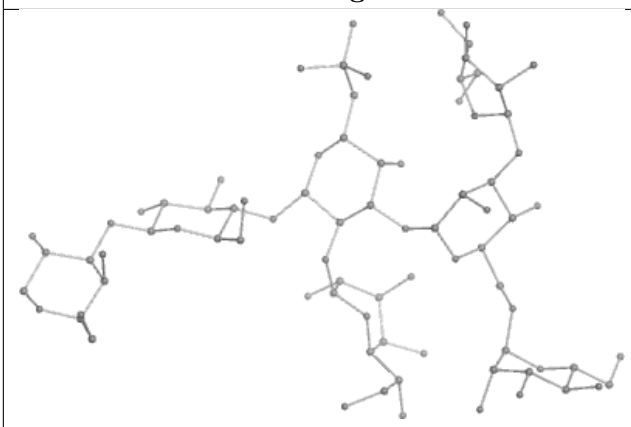
Oligosaccharide Chain CB



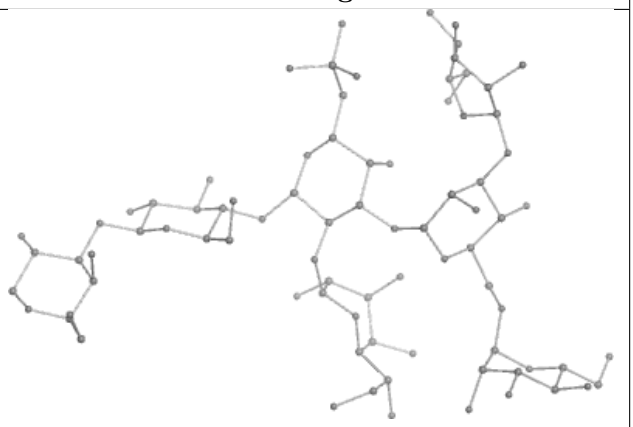
Bond lengths



Bond angles

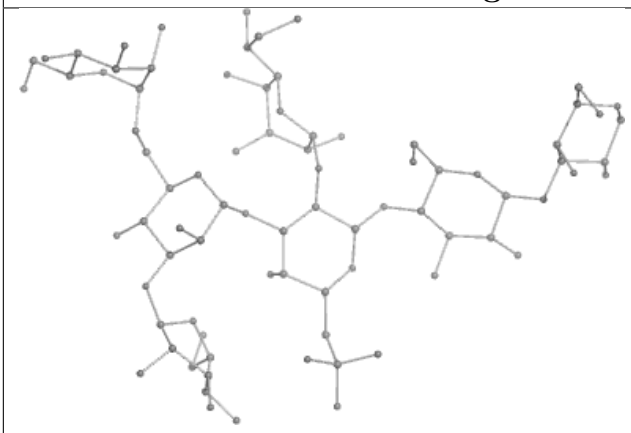


Torsions

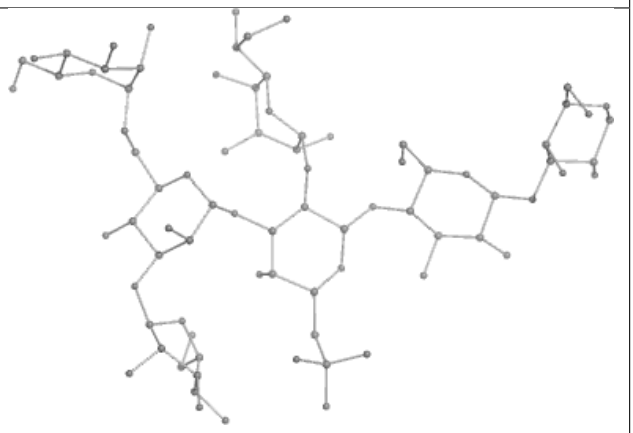


Rings

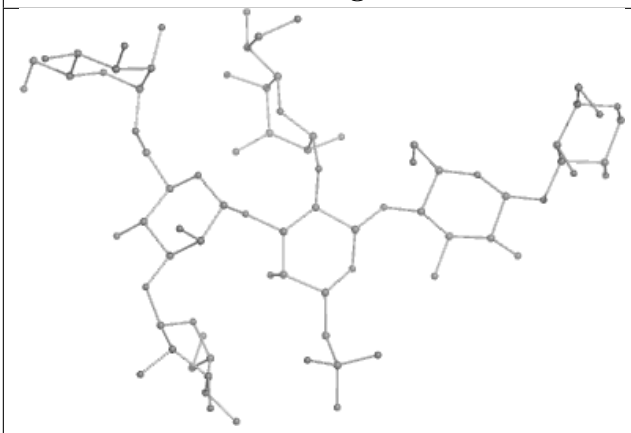
Oligosaccharide Chain EB



Bond lengths



Bond angles



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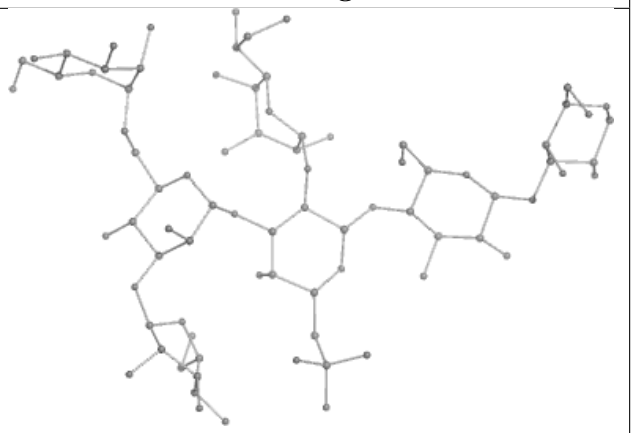
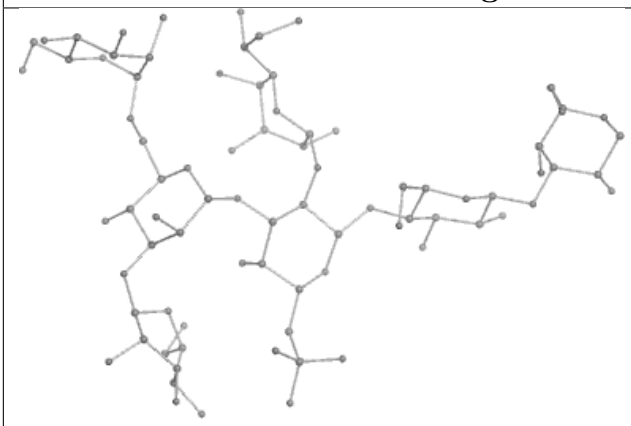
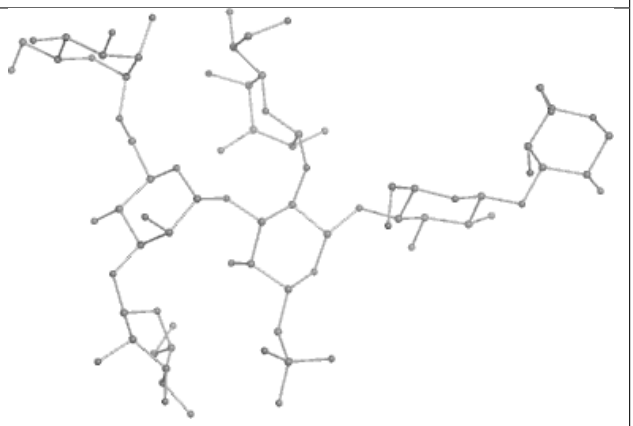


Rings

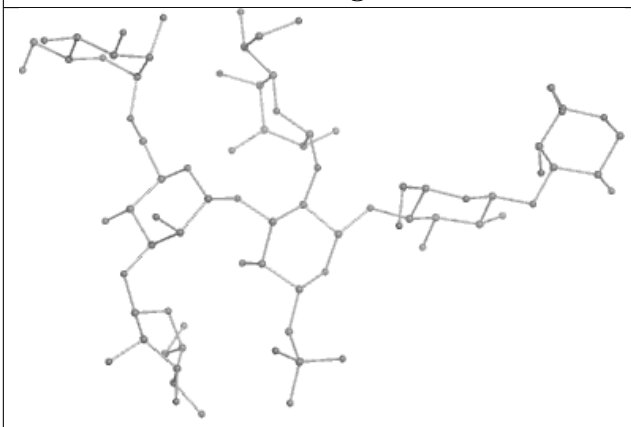
Oligosaccharide Chain GB



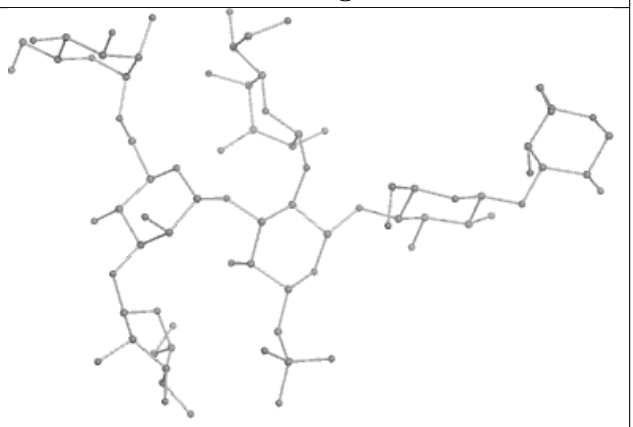
Bond lengths



Bond angles

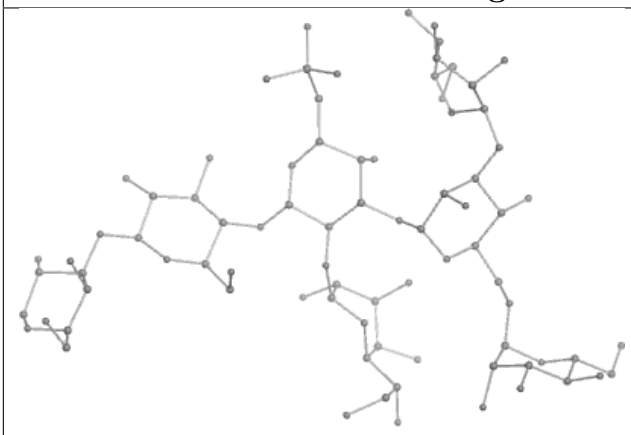


Torsions



Rings

Oligosaccharide Chain IB



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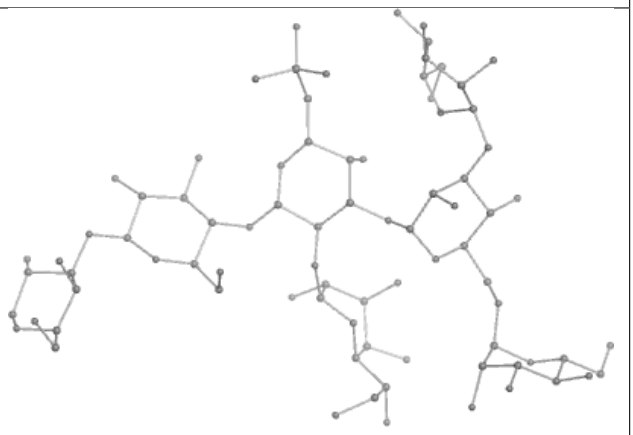
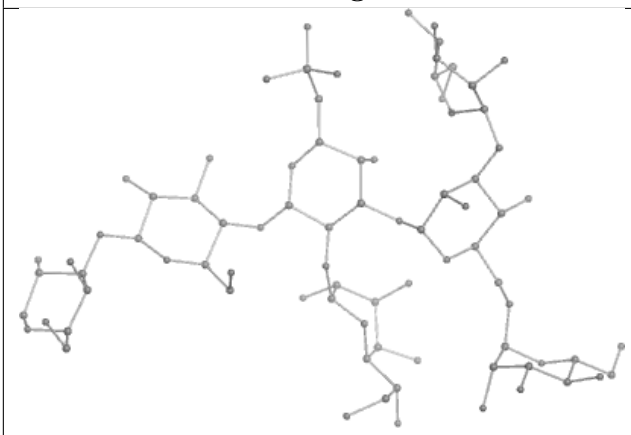
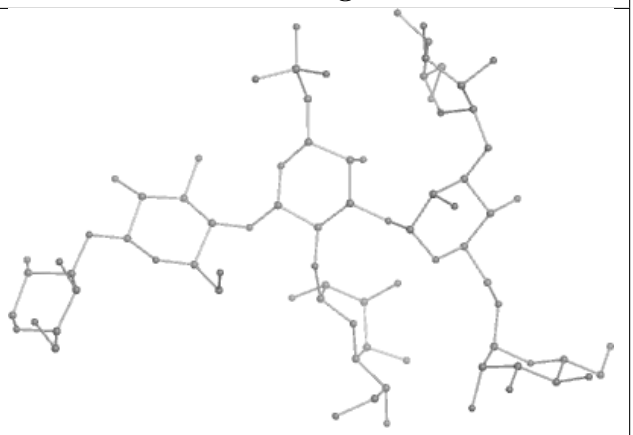


Bond angles

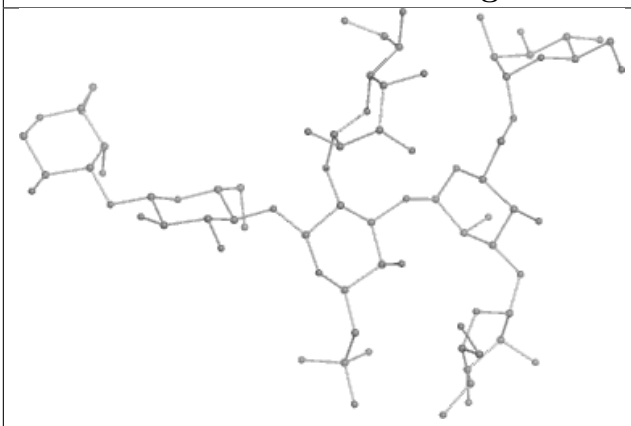


Torsions



Rings

Oligosaccharide Chain KB



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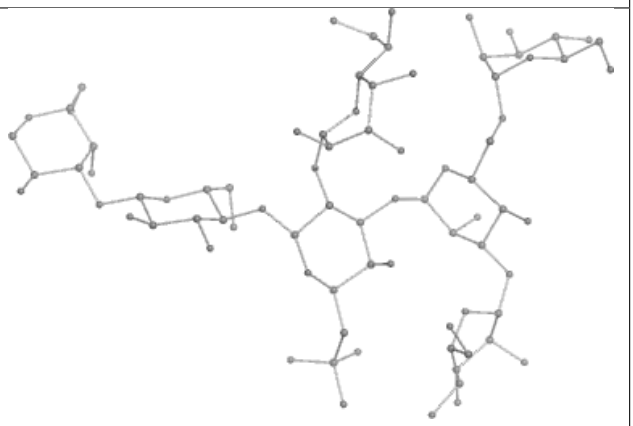
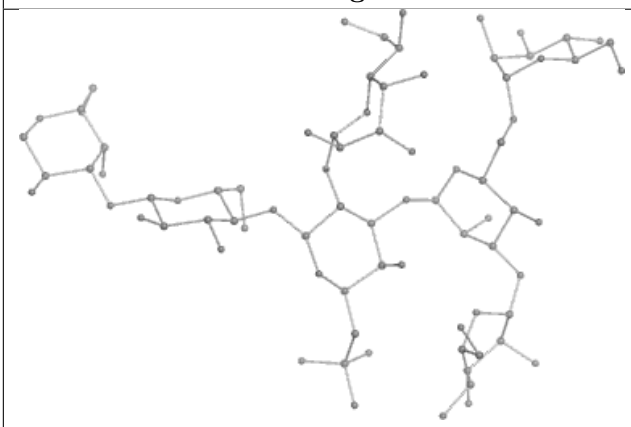


Bond angles



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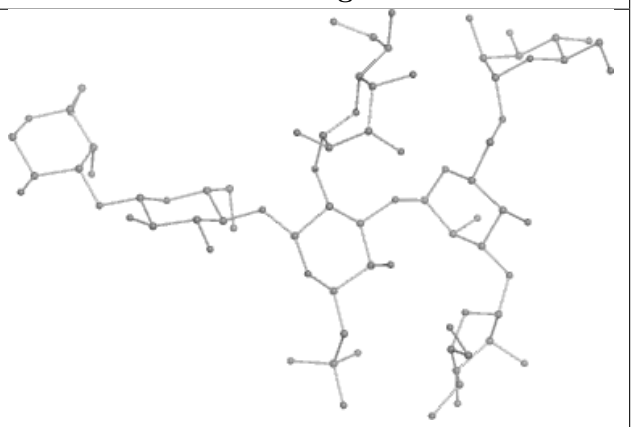
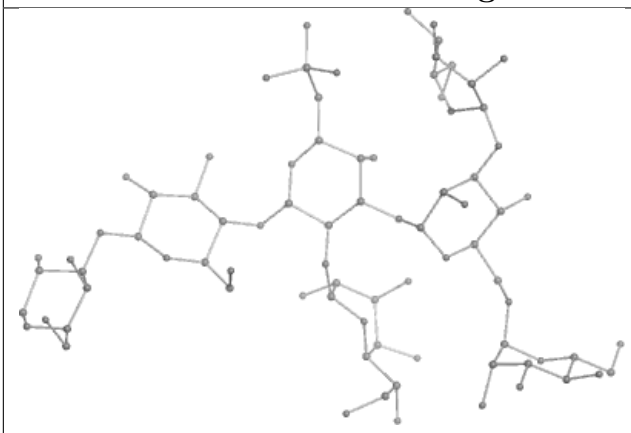


Rings

Oligosaccharide Chain MB



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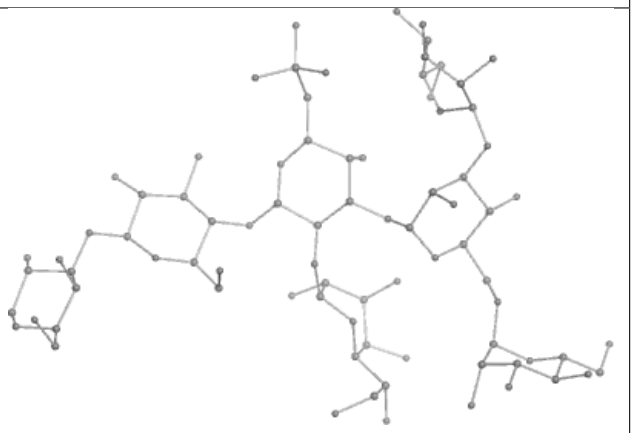
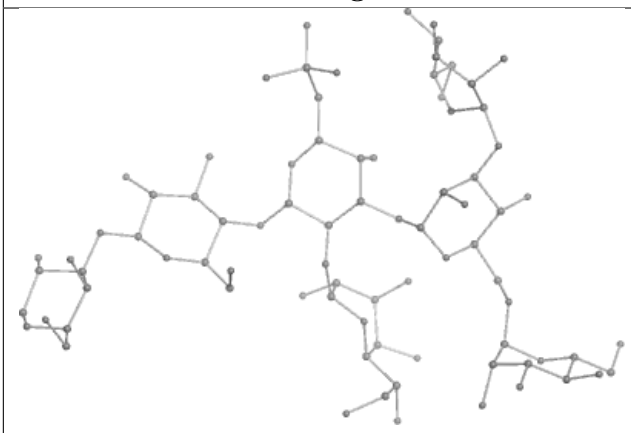
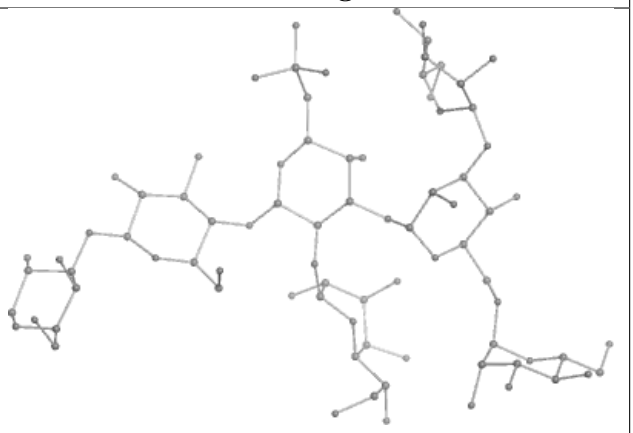


Bond angles

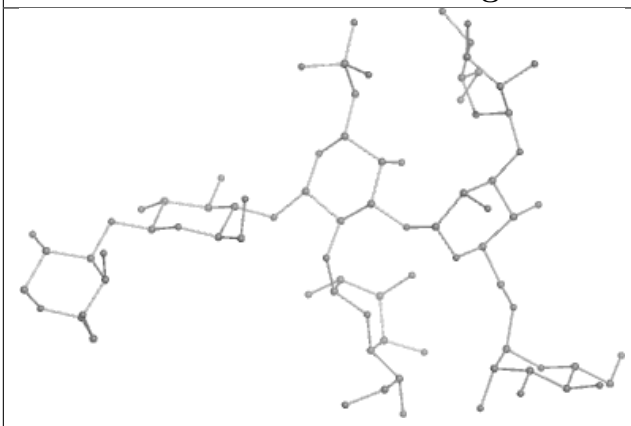


Torsions



Rings

Oligosaccharide Chain OB



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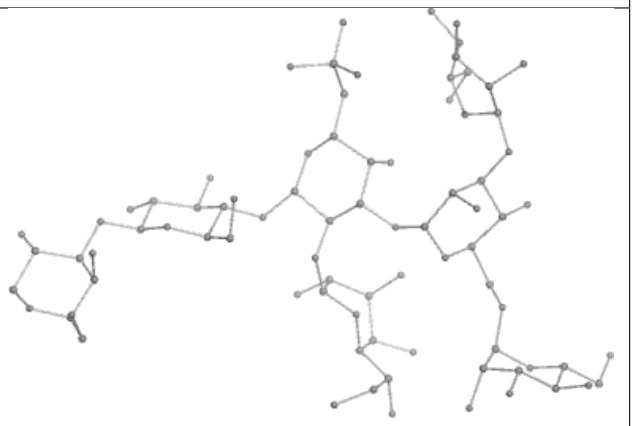
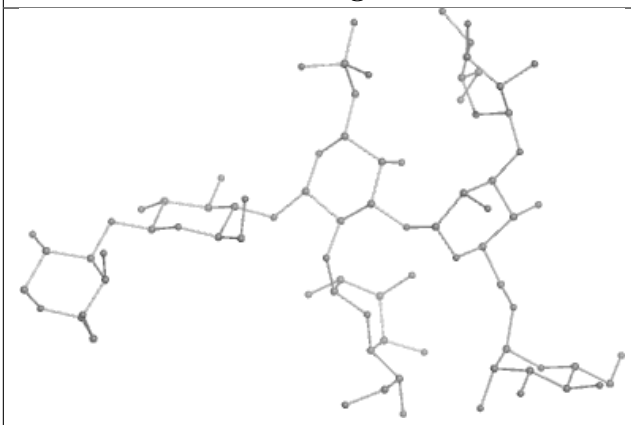


Bond angles



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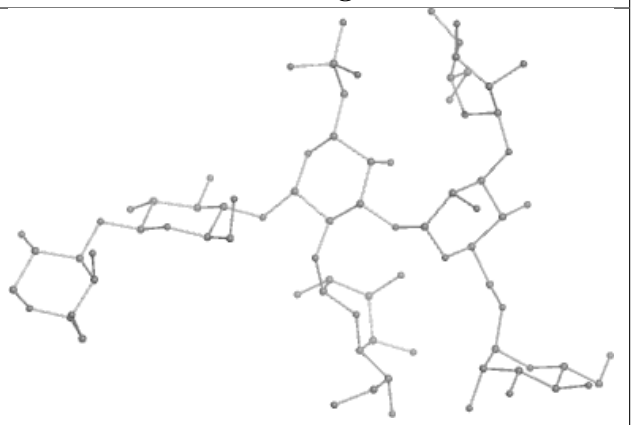
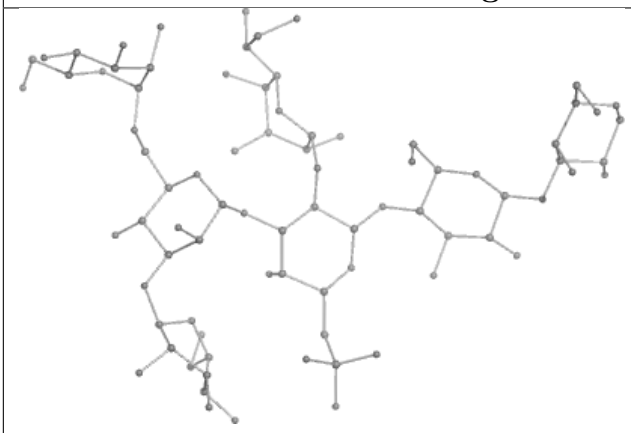


Rings

Oligosaccharide Chain QB



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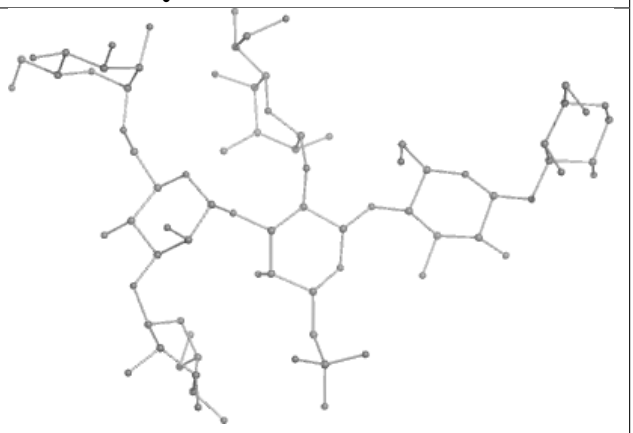
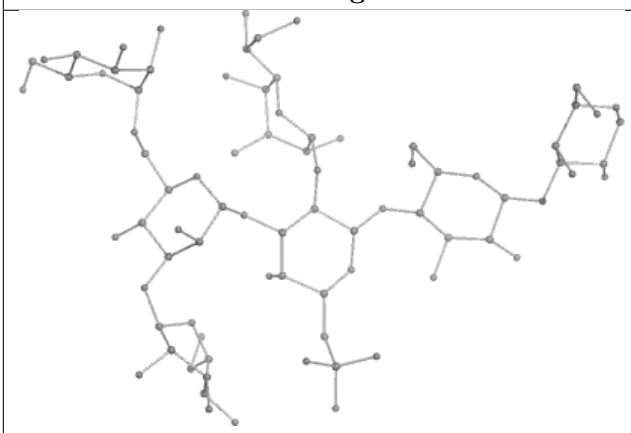
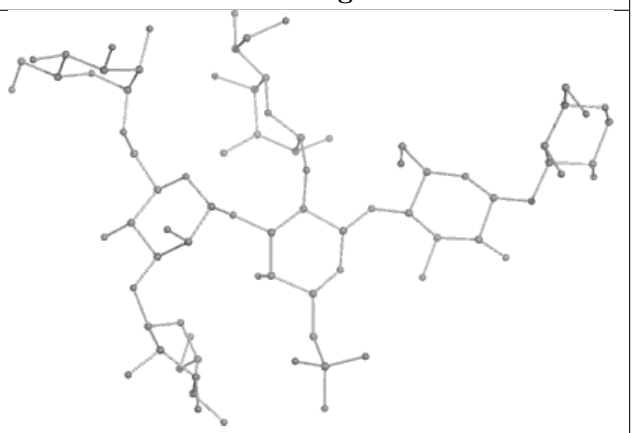


Bond angles

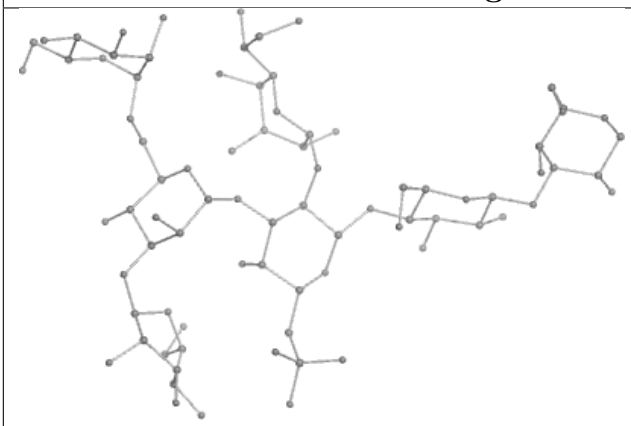


Torsions



Rings

Oligosaccharide Chain SB



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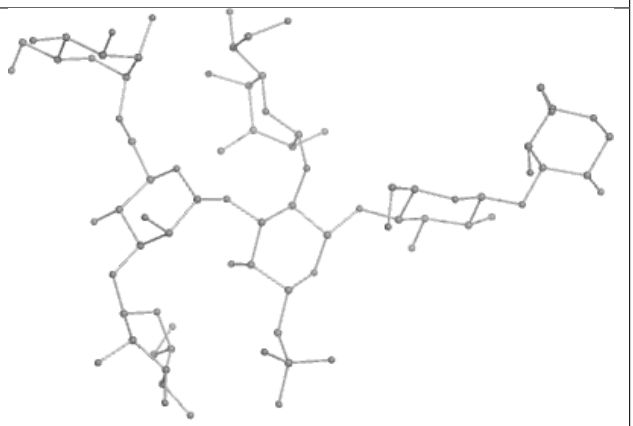
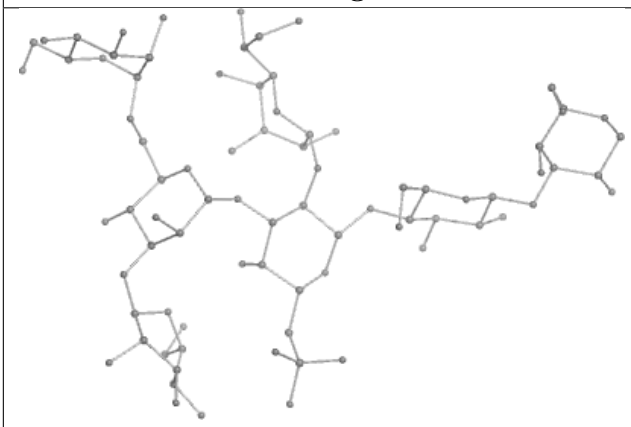


Bond angles



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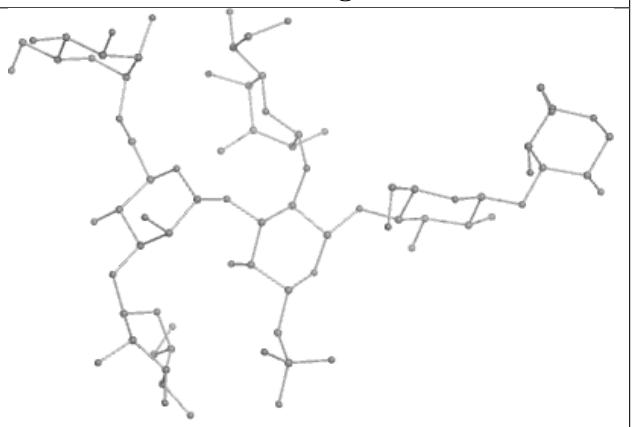
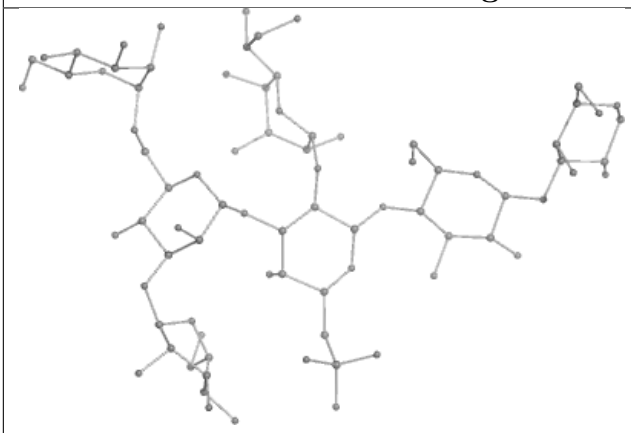


Rings

Oligosaccharide Chain UB



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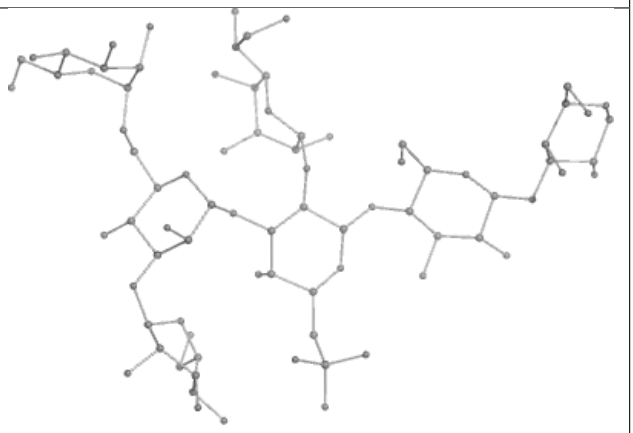
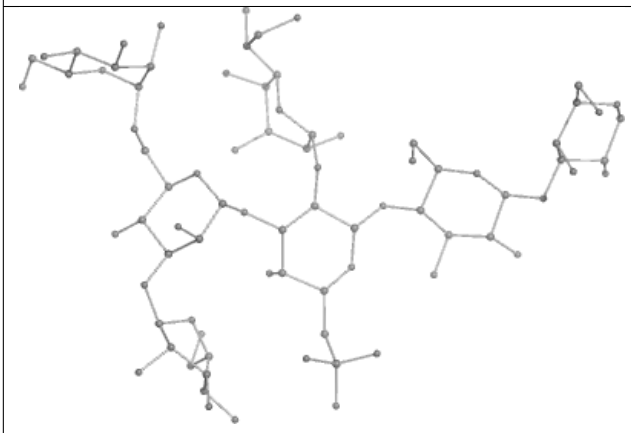
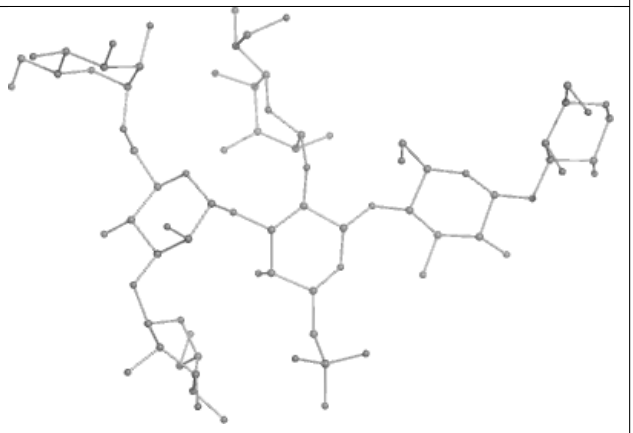


Bond angles

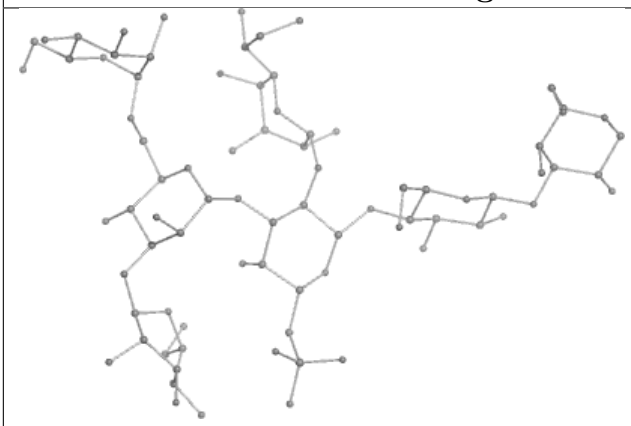


Torsions

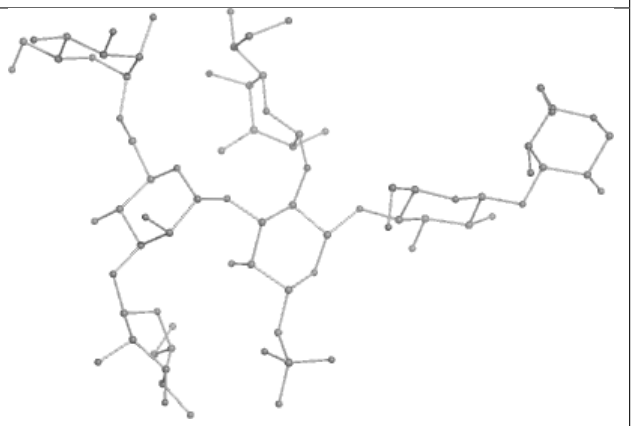


Rings

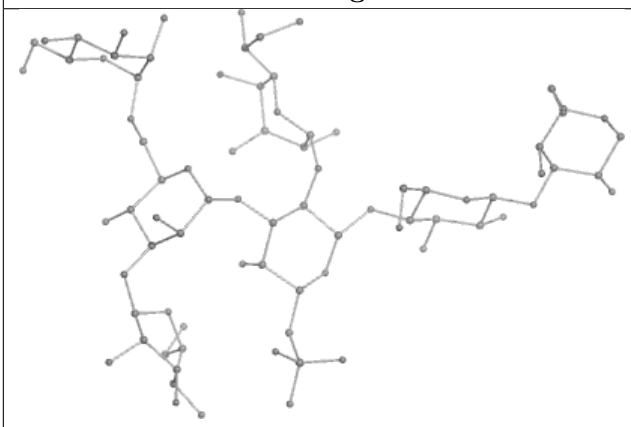
Oligosaccharide Chain WB



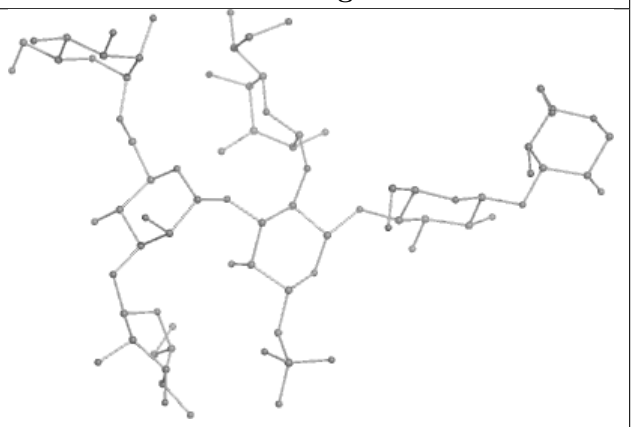
Bond lengths



Bond angles

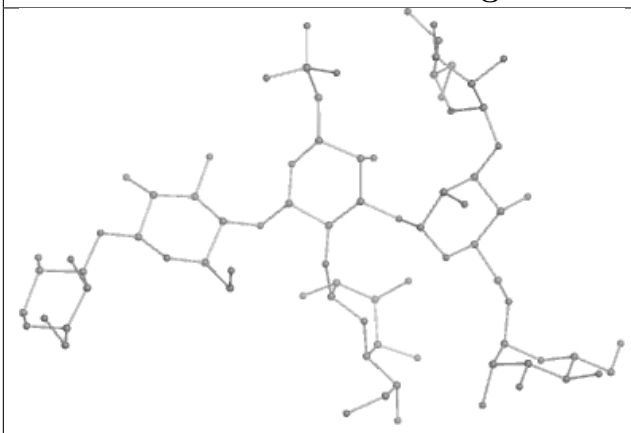


Torsions



Rings

Oligosaccharide Chain YB



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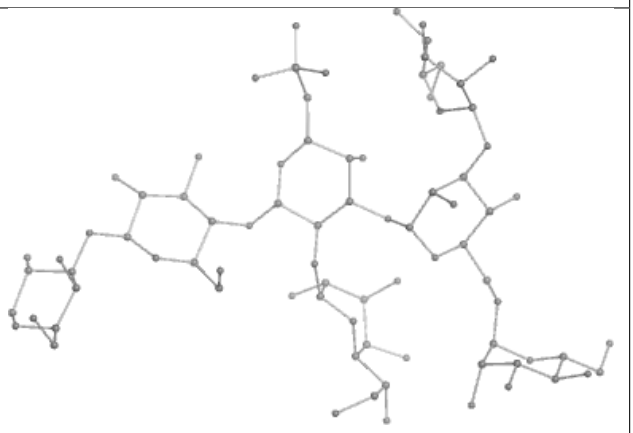
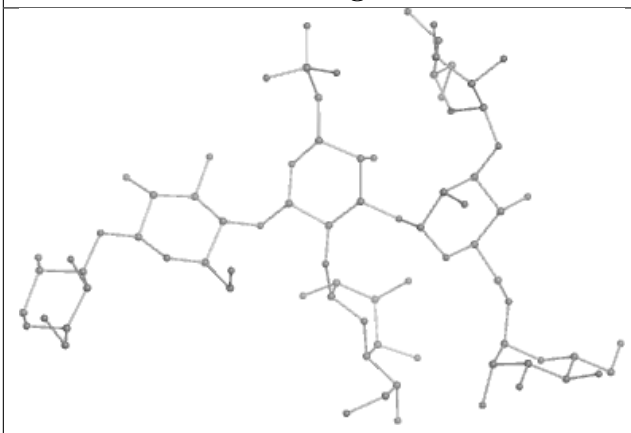
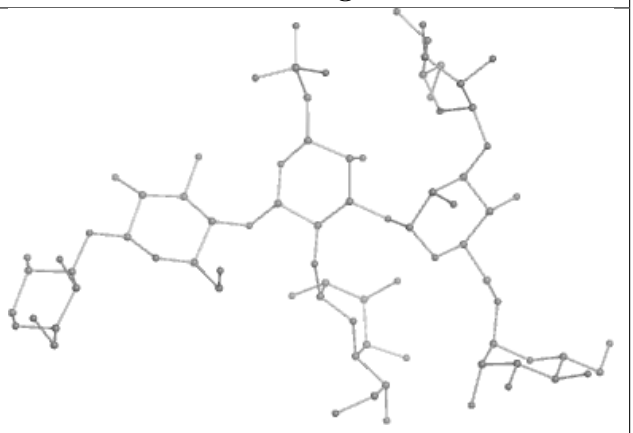


Bond angles

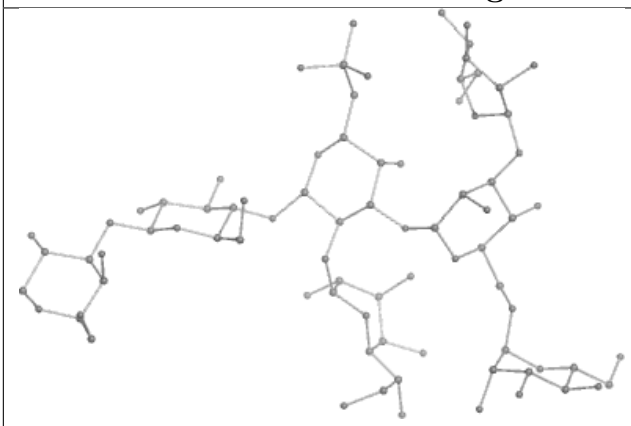


Torsions



Rings

Oligosaccharide Chain aB



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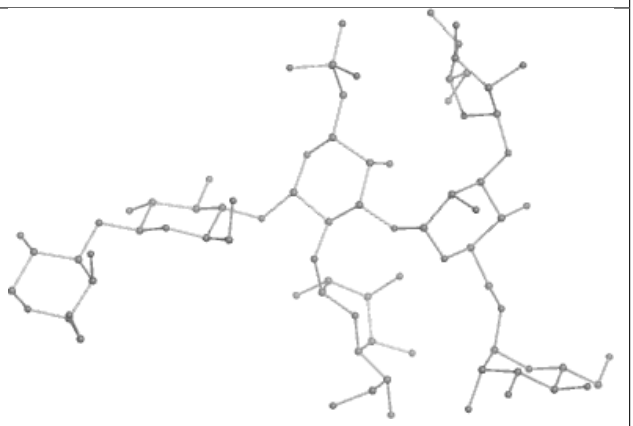
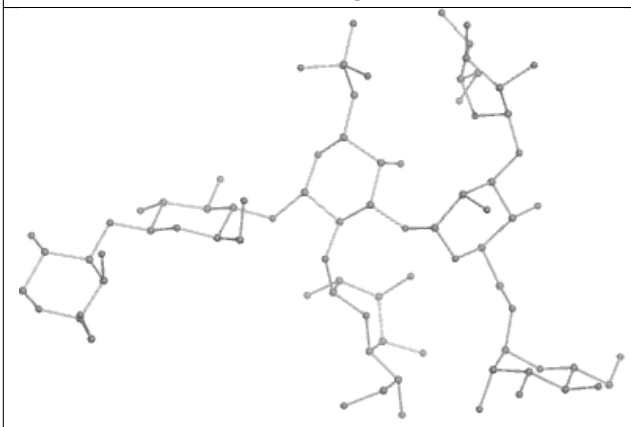
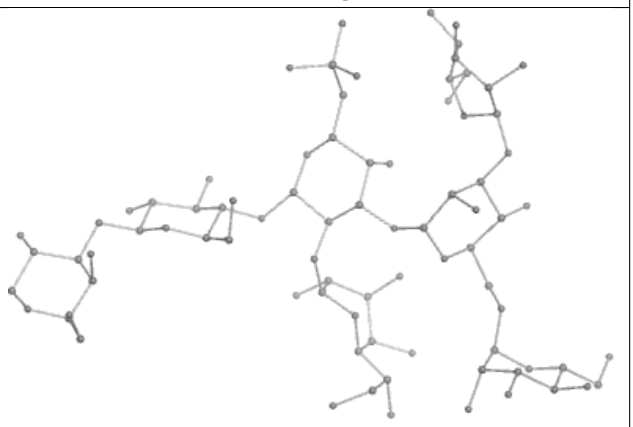


Bond angles

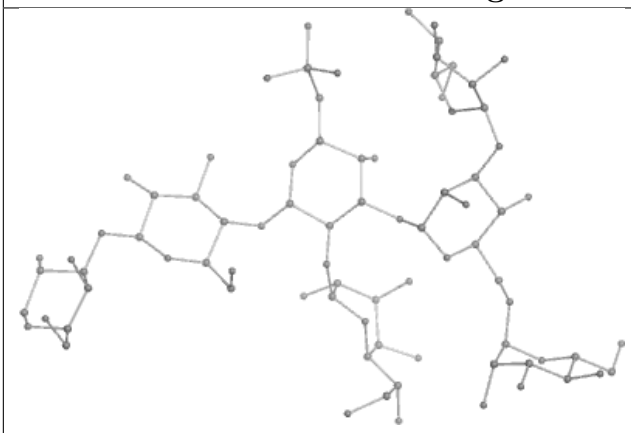


Torsions



Rings

Oligosaccharide Chain cB



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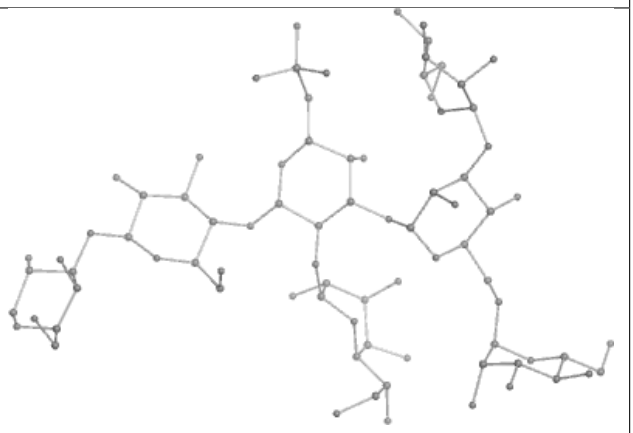
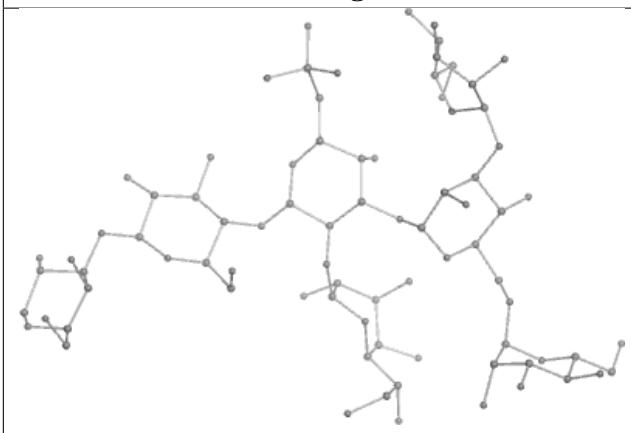
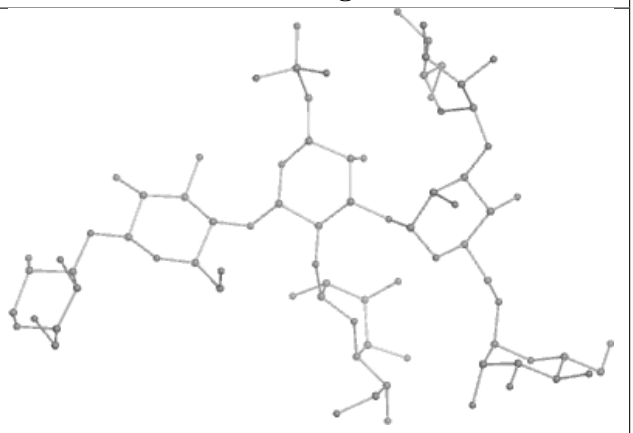


Bond angles

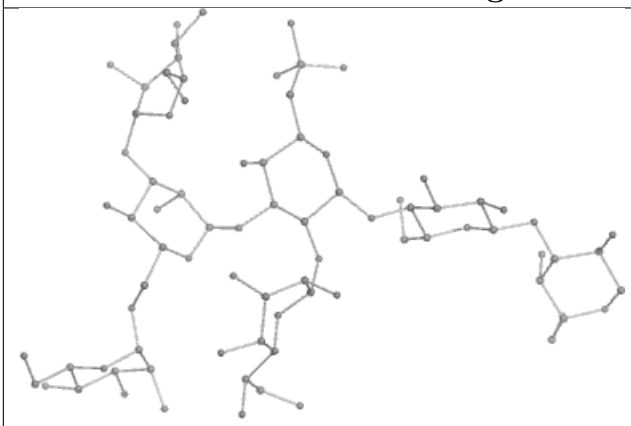


Torsions

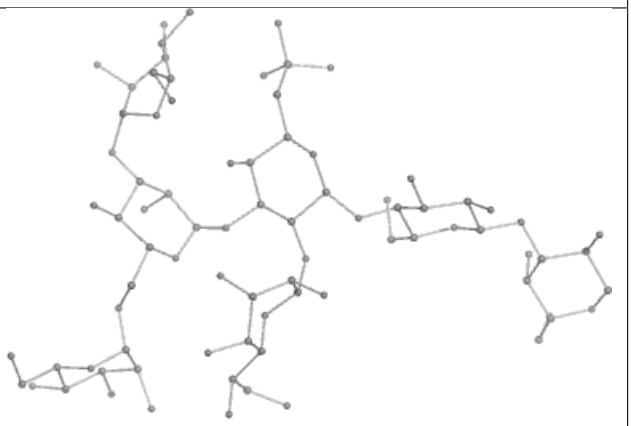


Rings

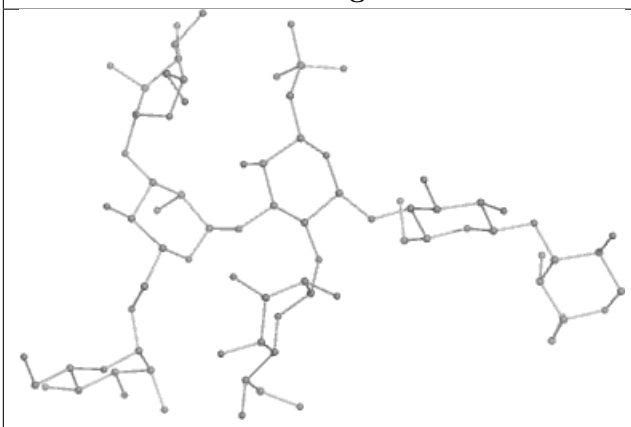
Oligosaccharide Chain eB



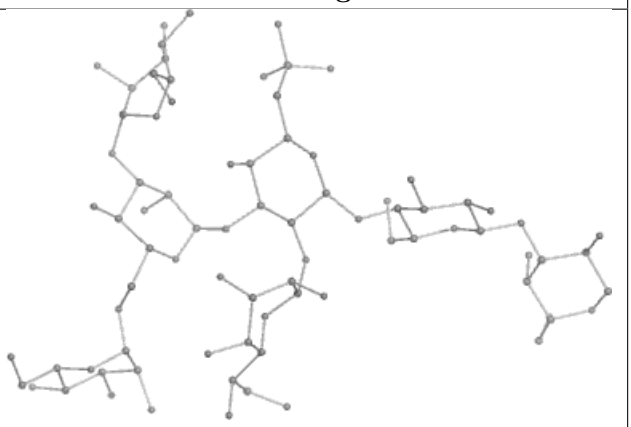
Bond lengths



Bond angles

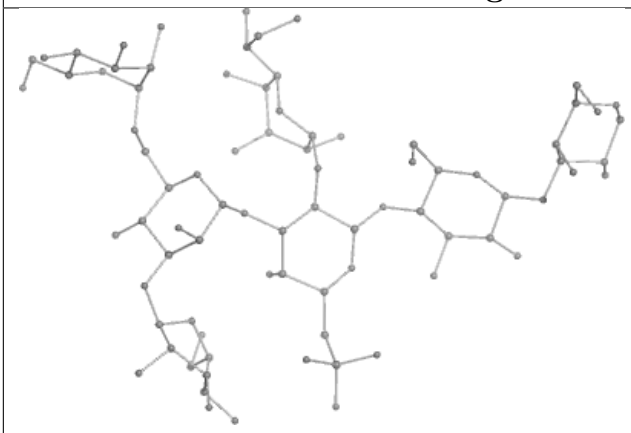


Torsions

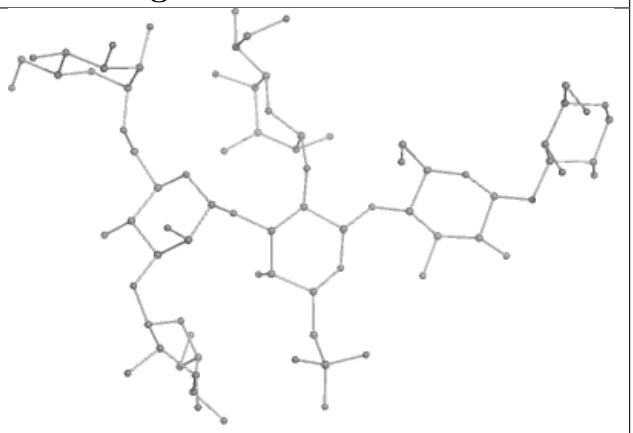


Rings

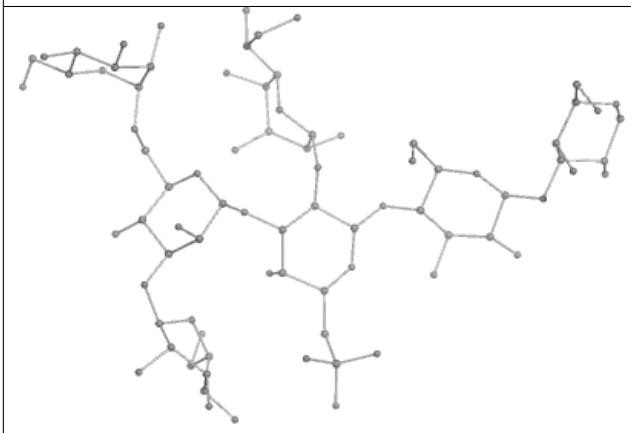
Oligosaccharide Chain gB



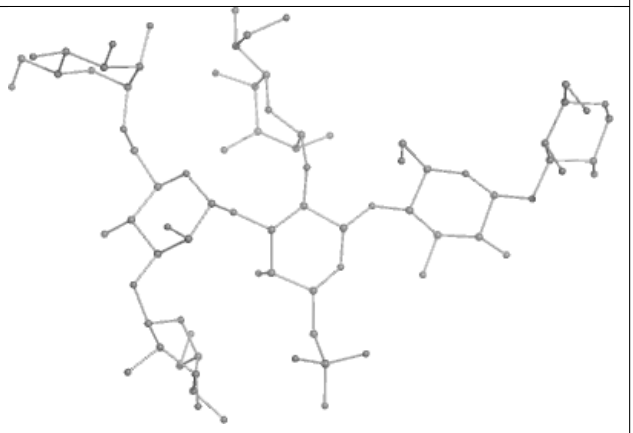
Bond lengths



Bond angles

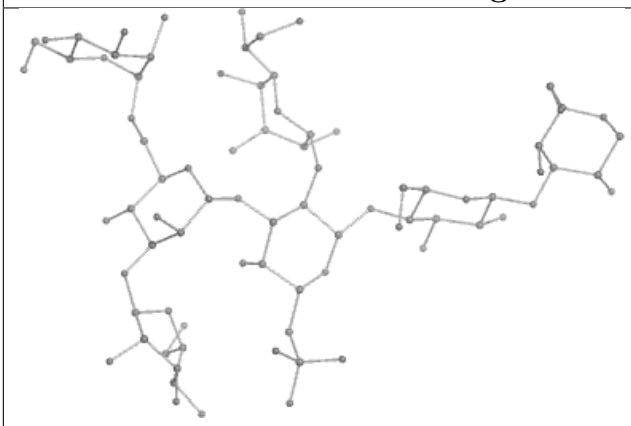


Torsions

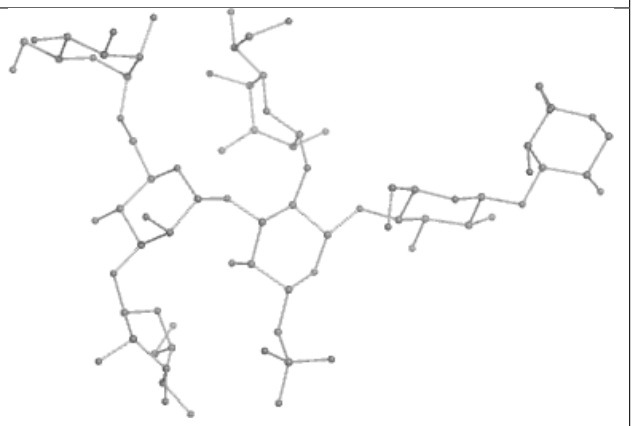


Rings

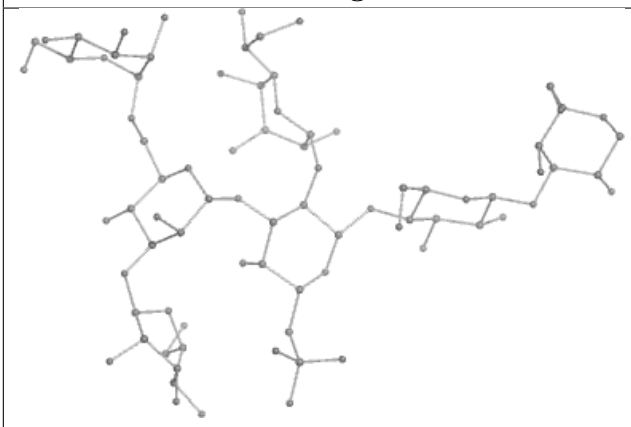
Oligosaccharide Chain iB



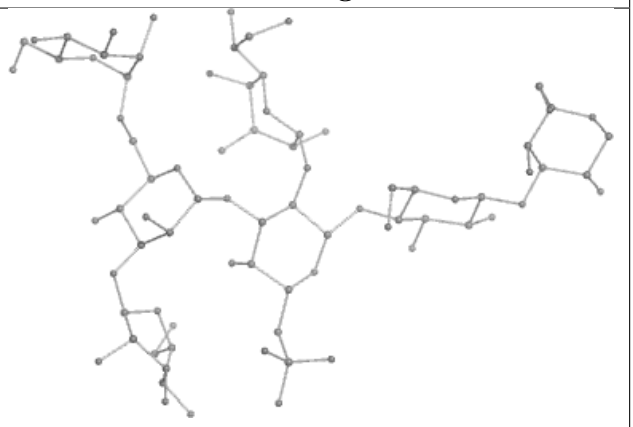
Bond lengths



Bond angles

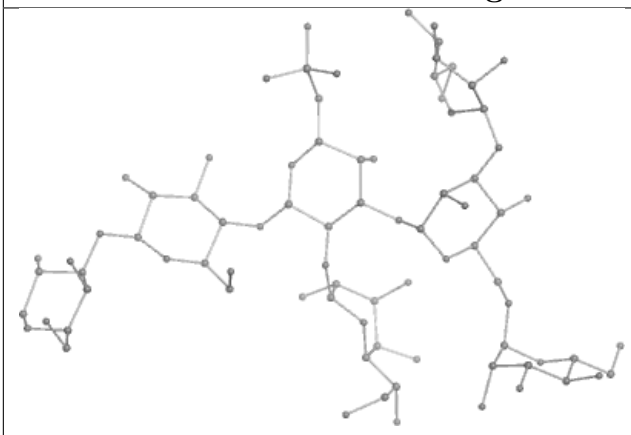


Torsions

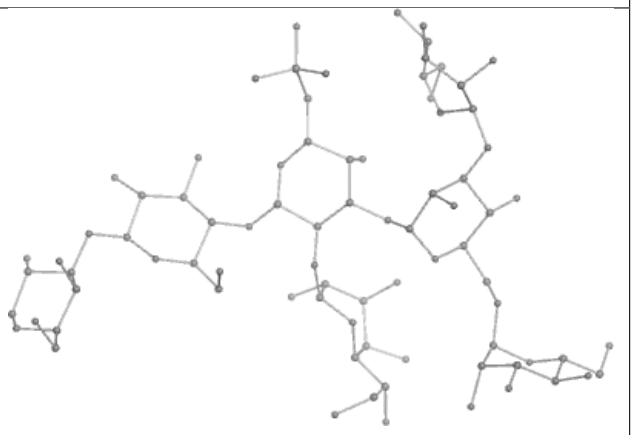


Rings

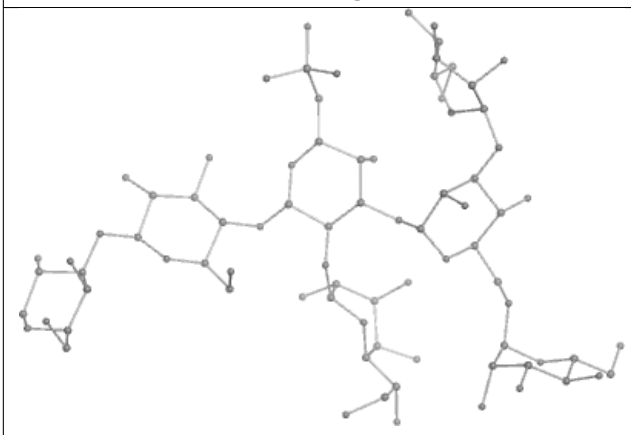
Oligosaccharide Chain kB



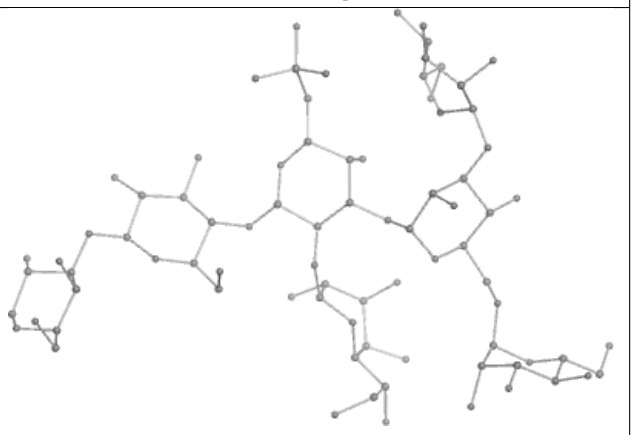
Bond lengths



Bond angles

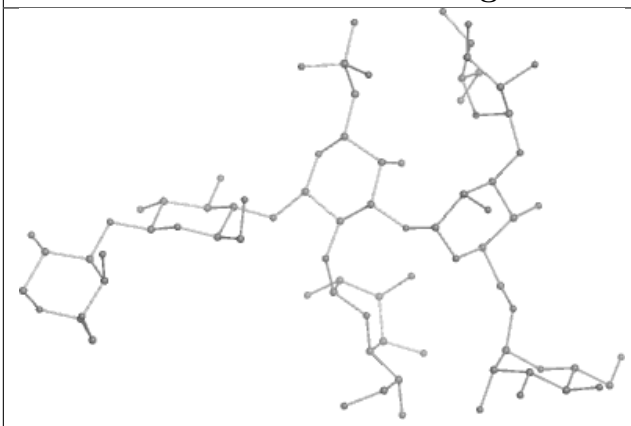


Torsions

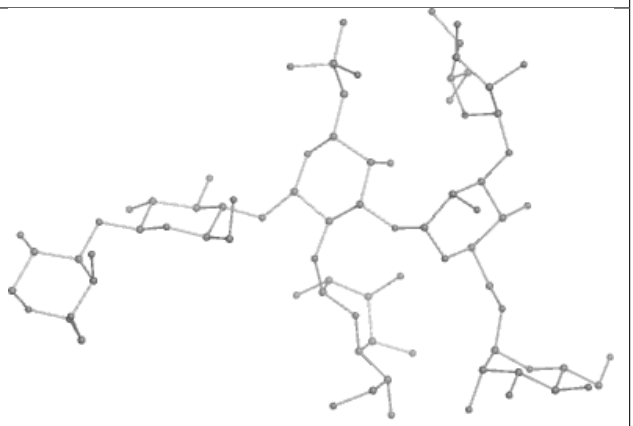


Rings

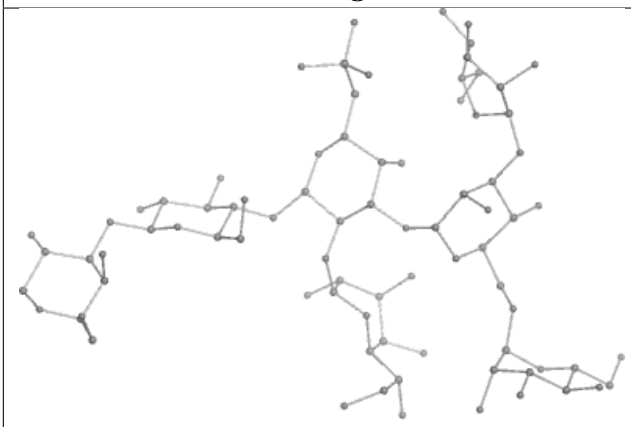
Oligosaccharide Chain mB



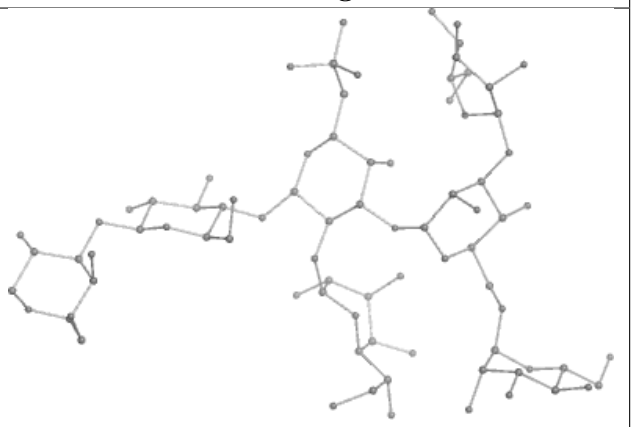
Bond lengths



Bond angles

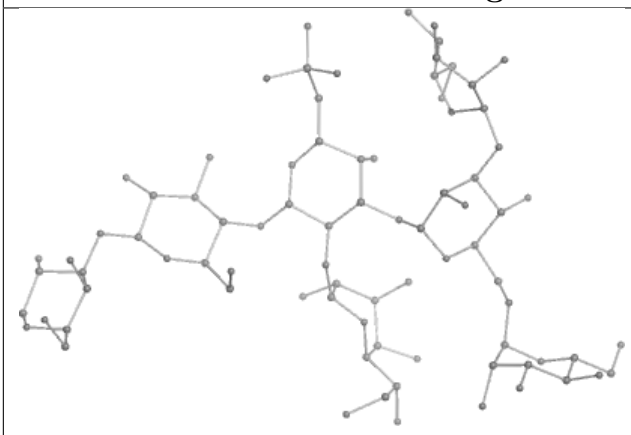


Torsions

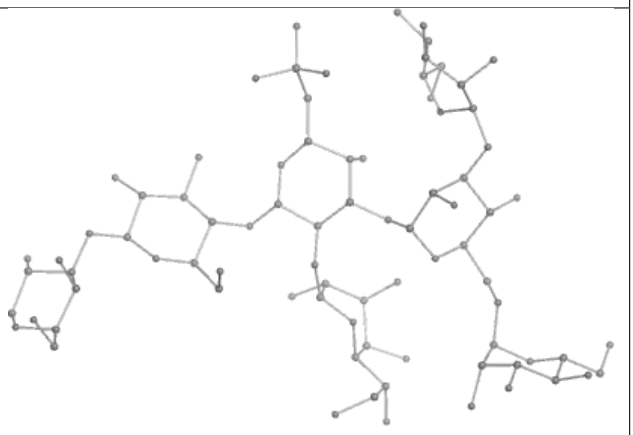


Rings

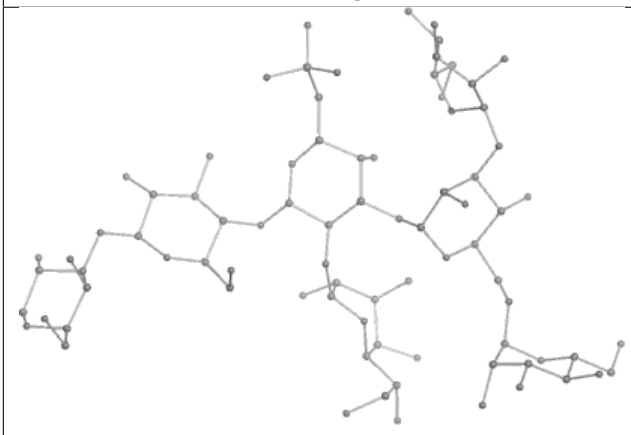
Oligosaccharide Chain oB



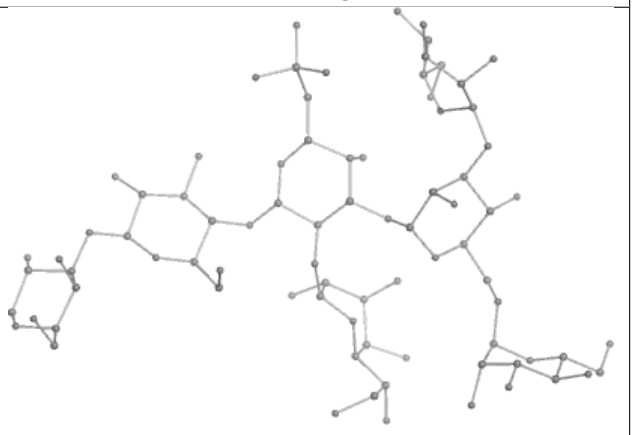
Bond lengths



Bond angles

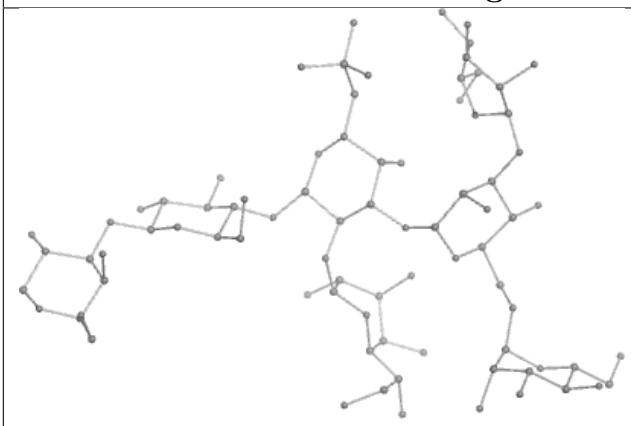


Torsions

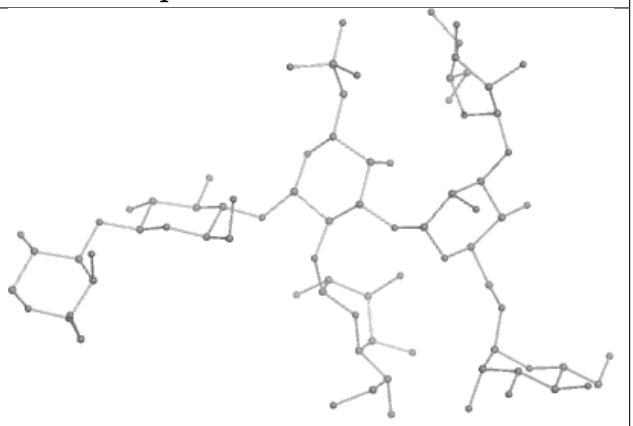


Rings

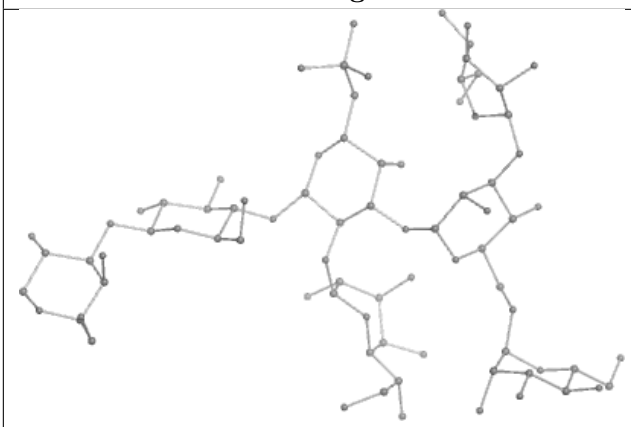
Oligosaccharide Chain qB



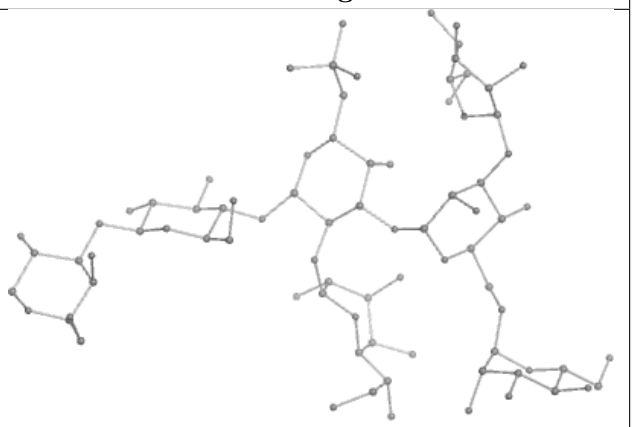
Bond lengths



Bond angles

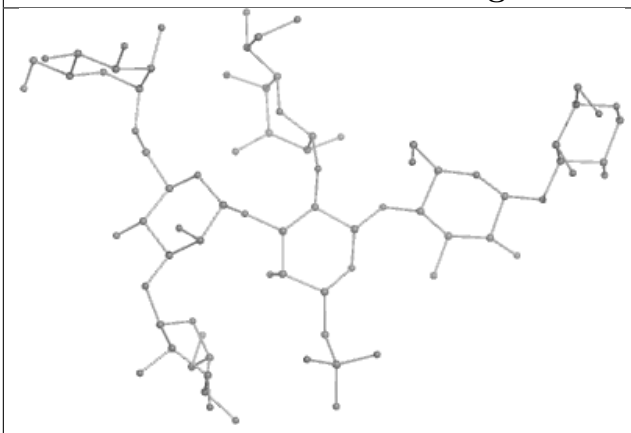


Torsions

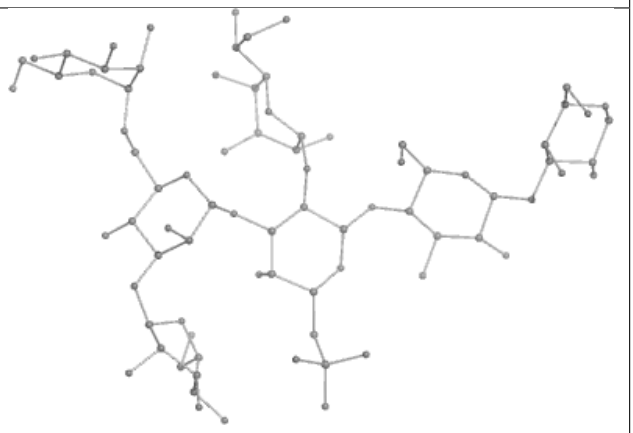


Rings

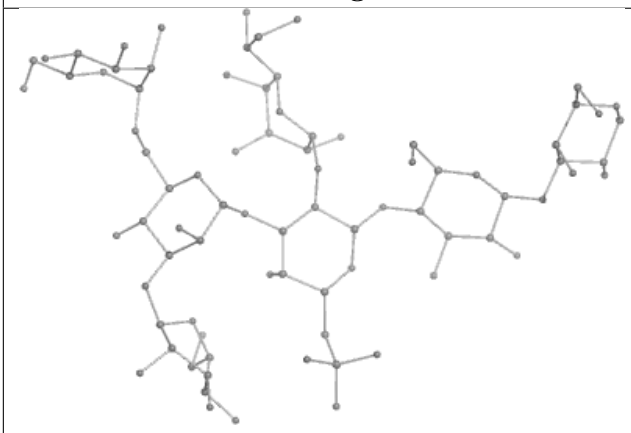
Oligosaccharide Chain sB



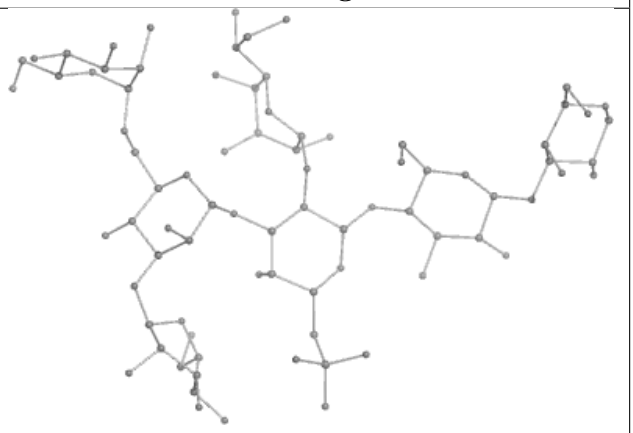
Bond lengths



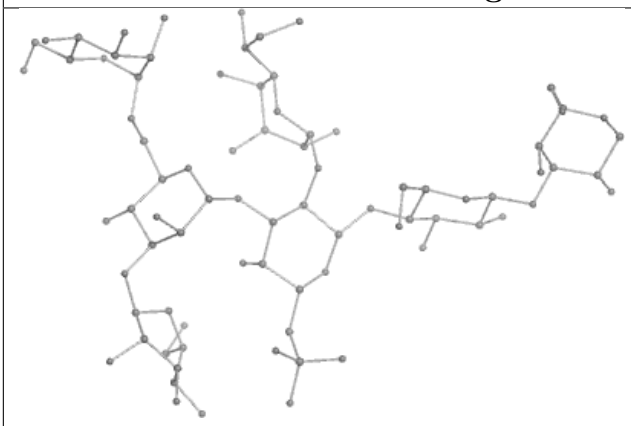
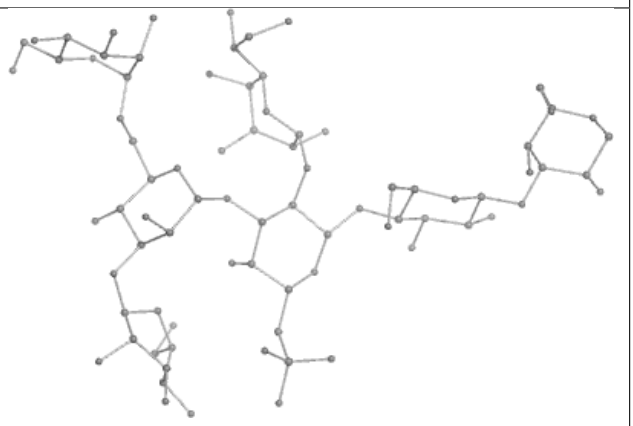
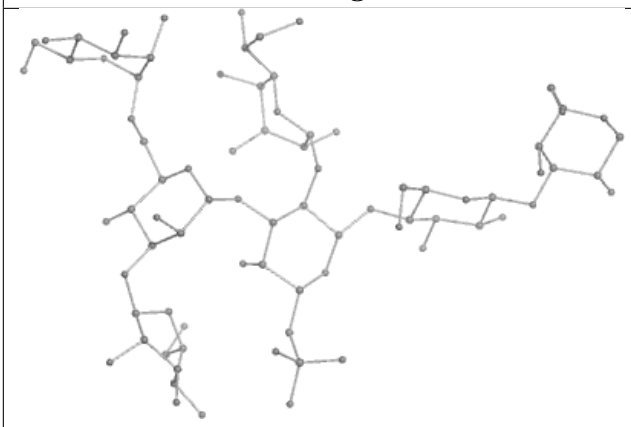
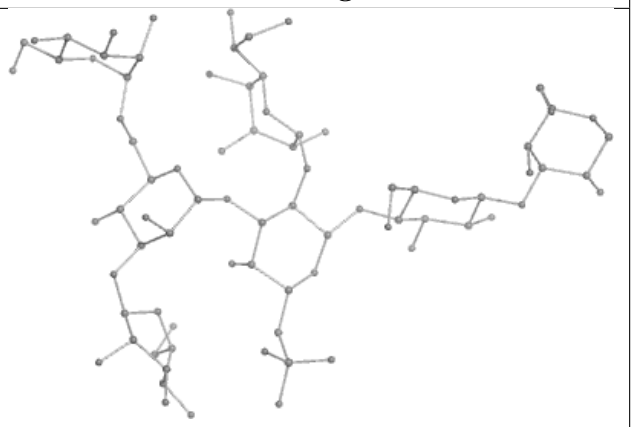
Bond angles



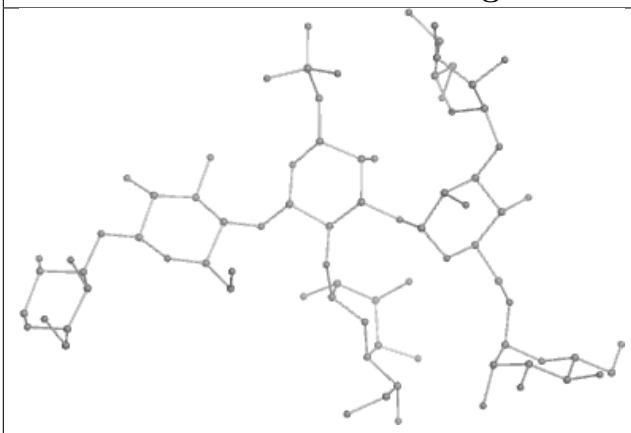
Torsions



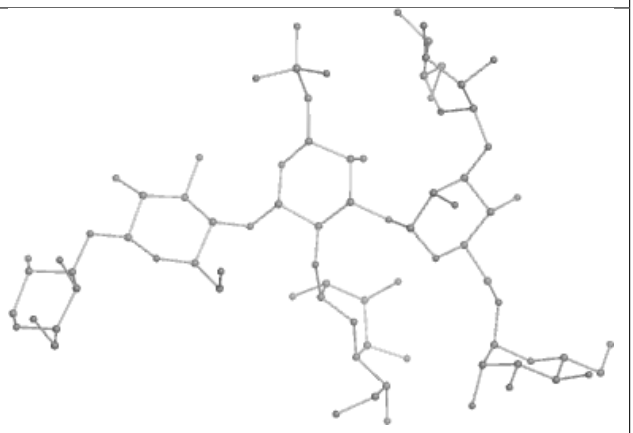
Rings

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

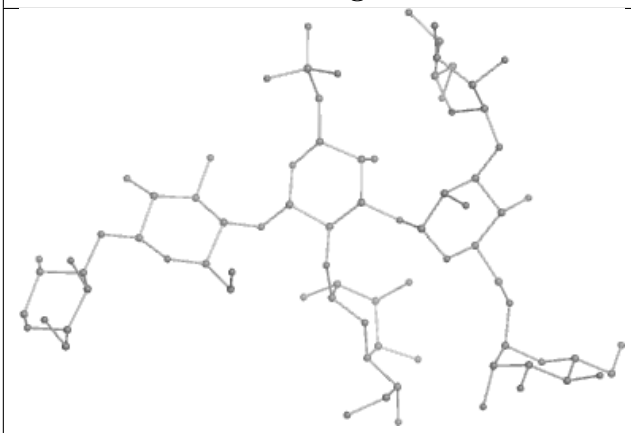
Oligosaccharide Chain wB



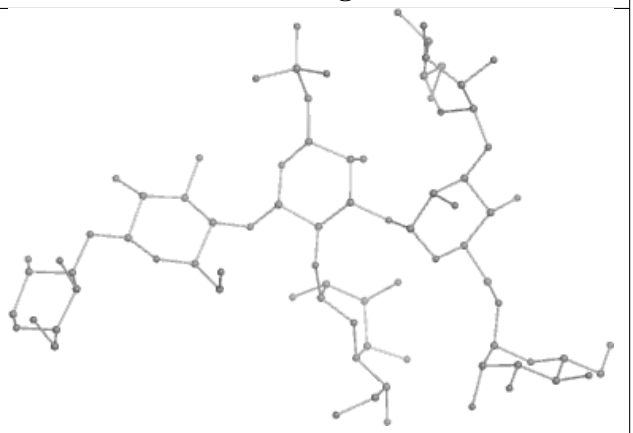
Bond lengths



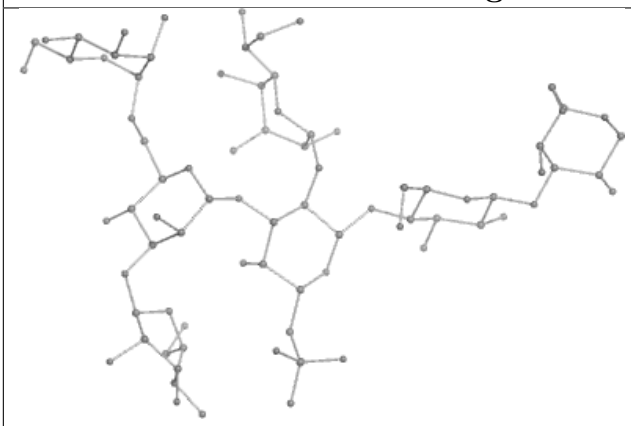
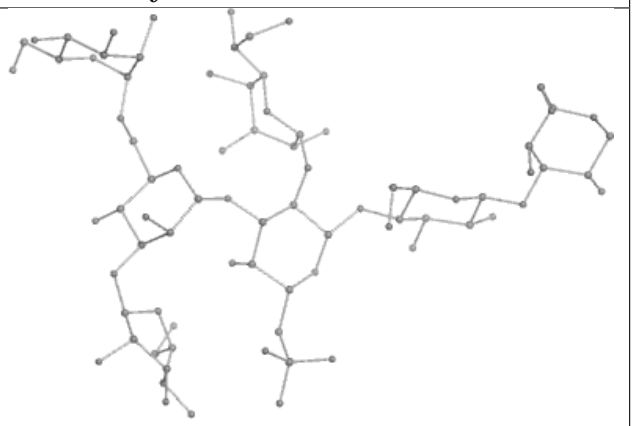
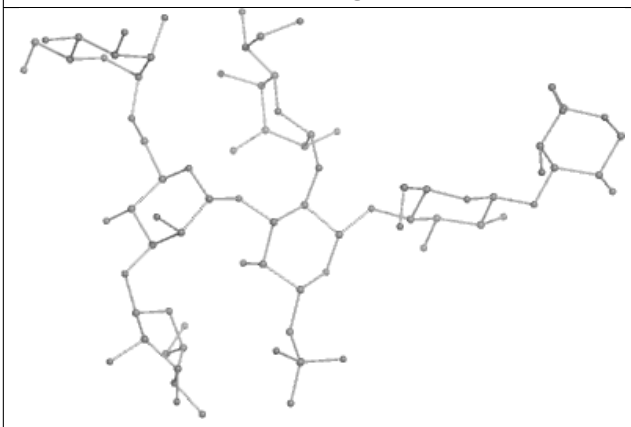
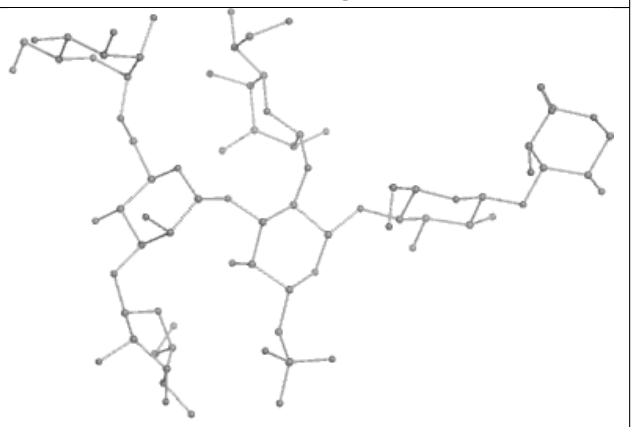
Bond angles



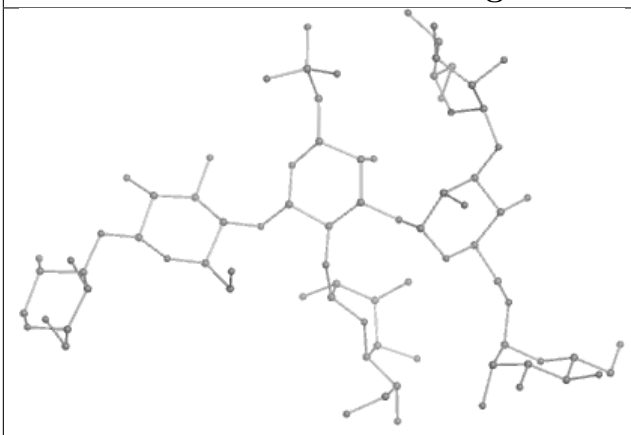
Torsions



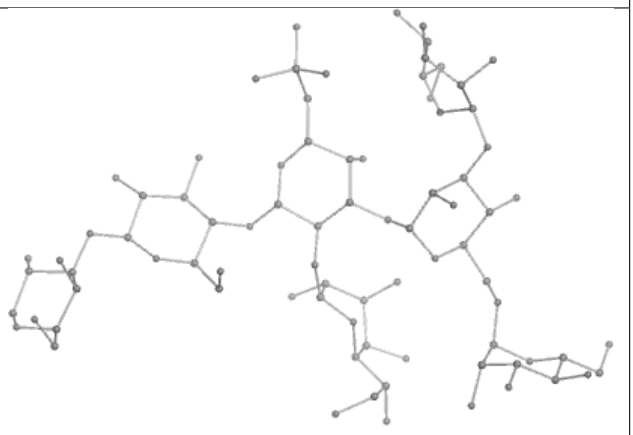
Rings

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

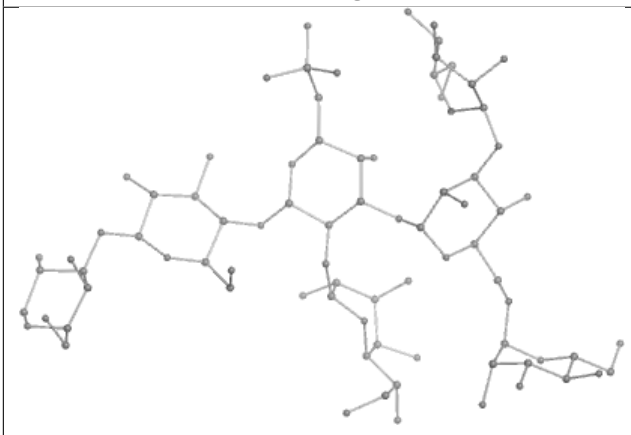
Oligosaccharide Chain 0B



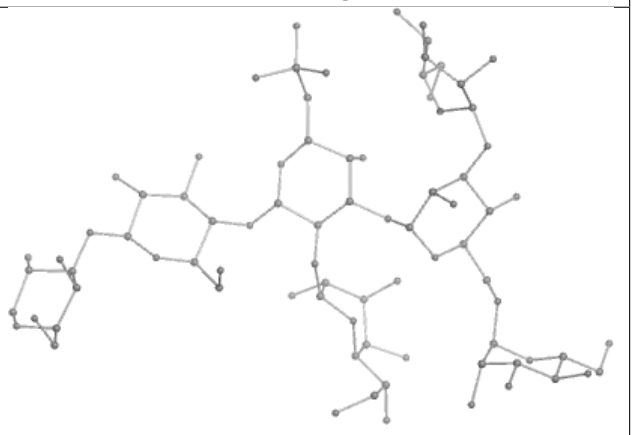
Bond lengths



Bond angles

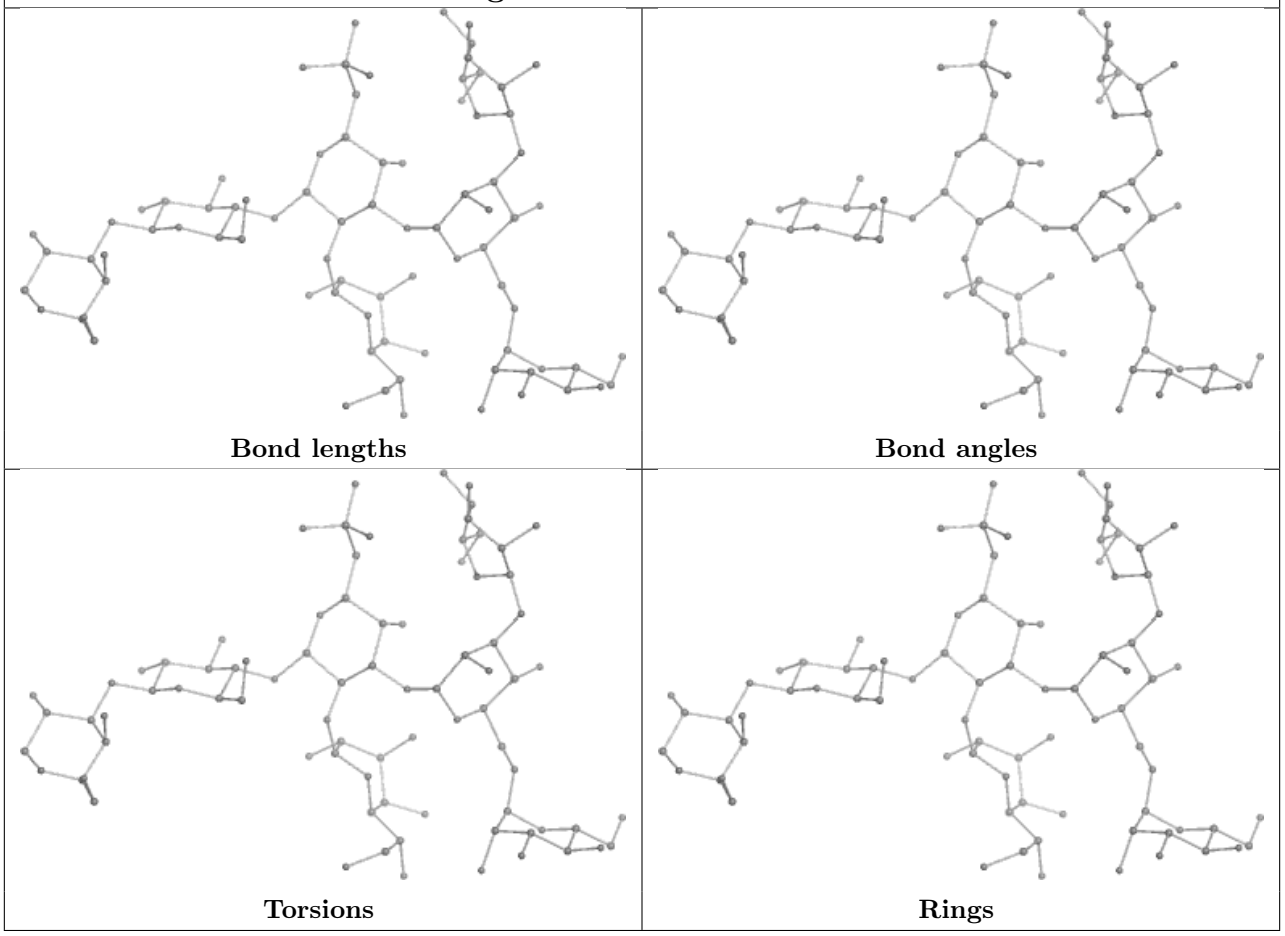


Torsions



Rings

Oligosaccharide Chain 2B



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.

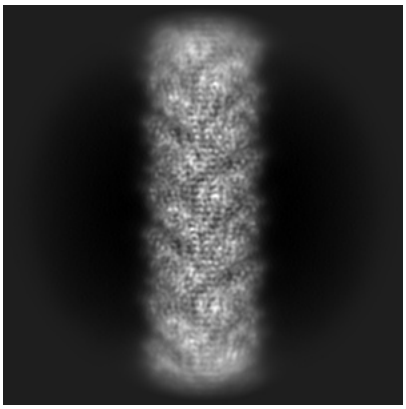
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19112. These allow visual inspection of the internal detail of the map and identification of artifacts.

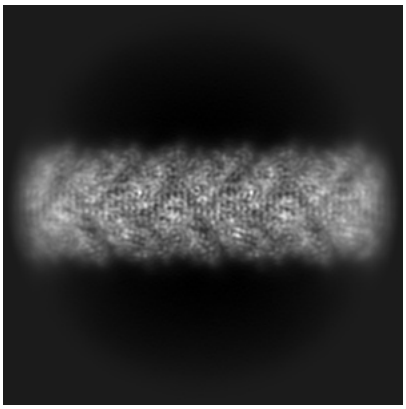
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

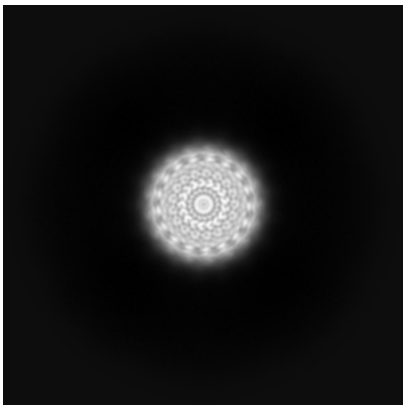
6.1.1 Primary map



X

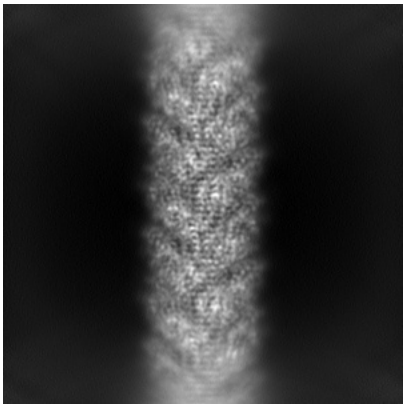


Y

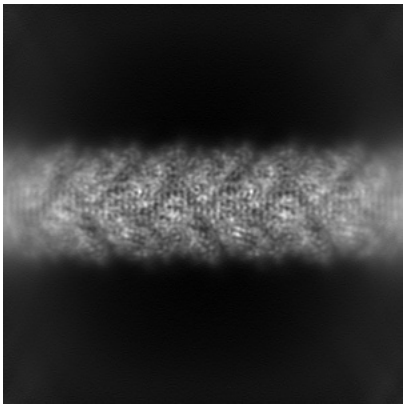


Z

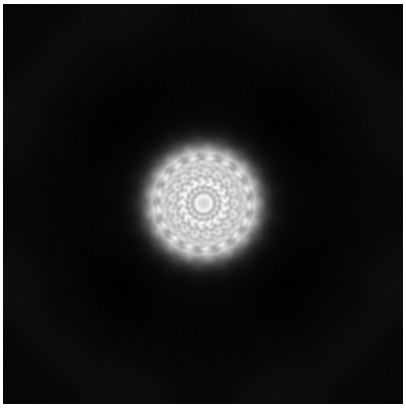
6.1.2 Raw map



X



Y

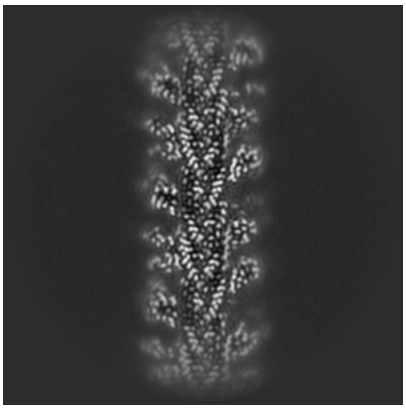


Z

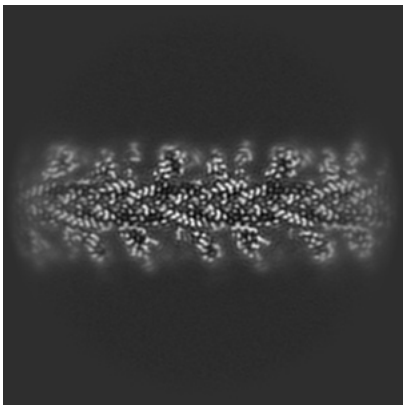
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

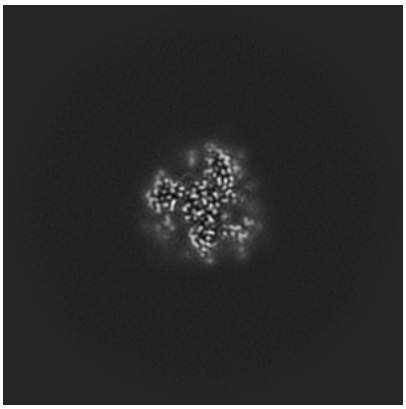
6.2.1 Primary map



X Index: 150

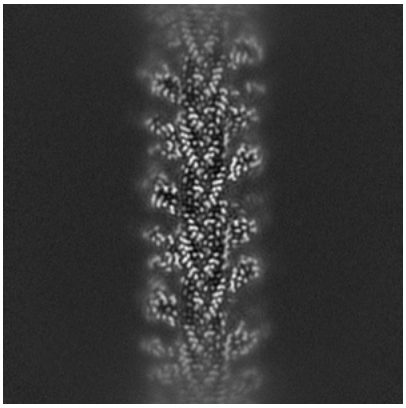


Y Index: 150

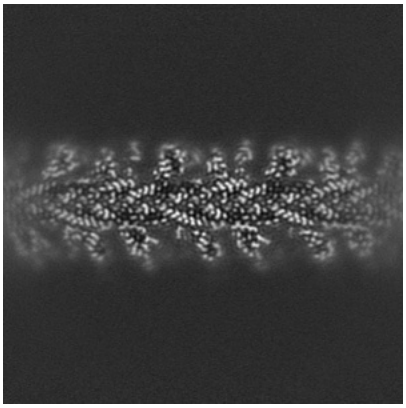


Z Index: 150

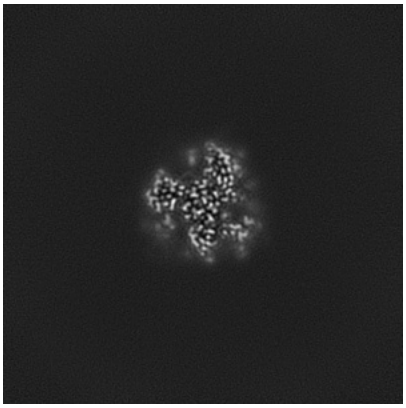
6.2.2 Raw map



X Index: 150



Y Index: 150

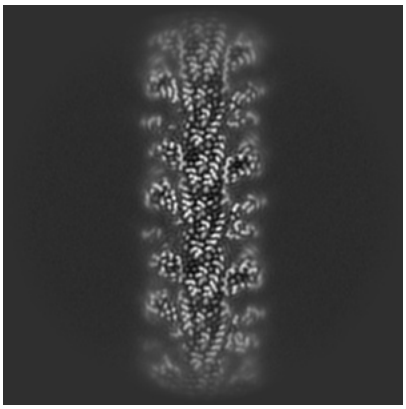


Z Index: 150

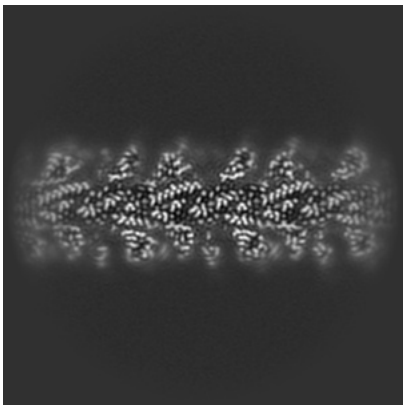
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

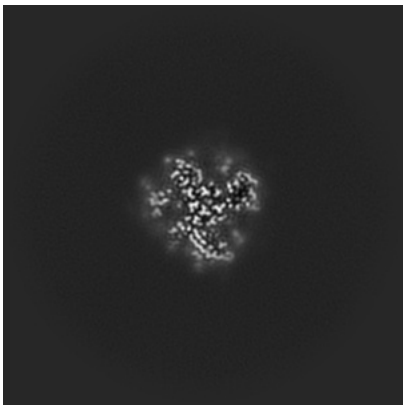
6.3.1 Primary map



X Index: 155

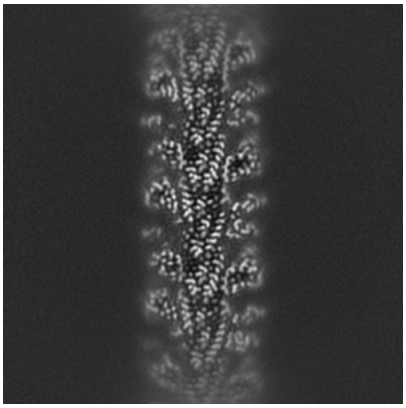


Y Index: 144

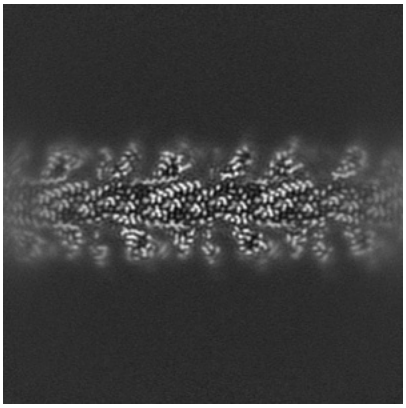


Z Index: 161

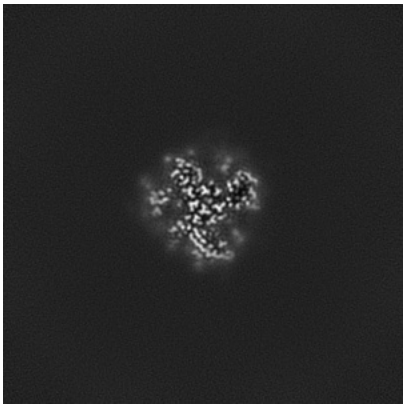
6.3.2 Raw map



X Index: 155



Y Index: 145

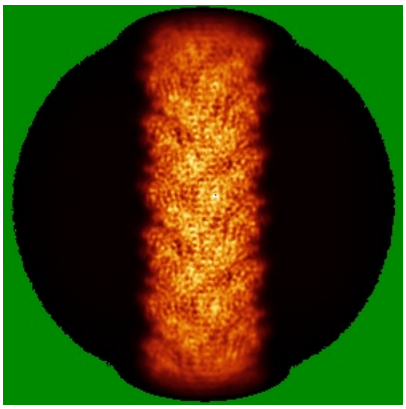


Z Index: 161

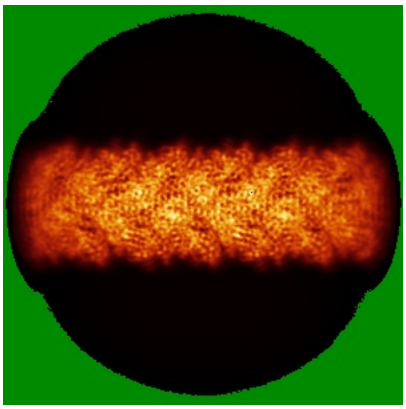
The images above show the largest variance slices of the map in three orthogonal directions.

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

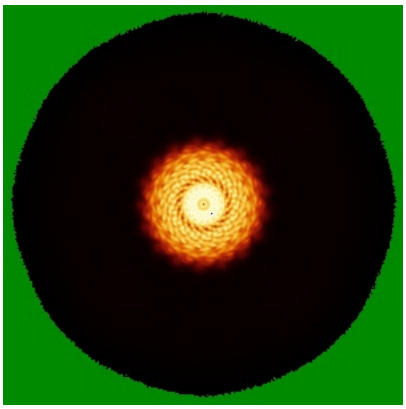
6.4.1 Primary map



X

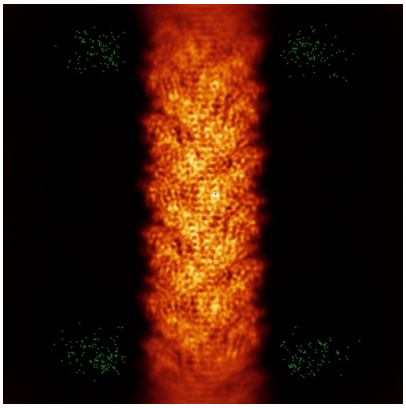


Y

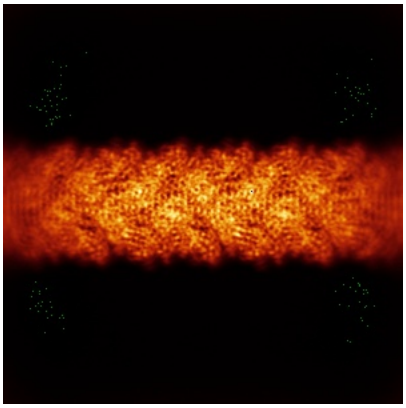


Z

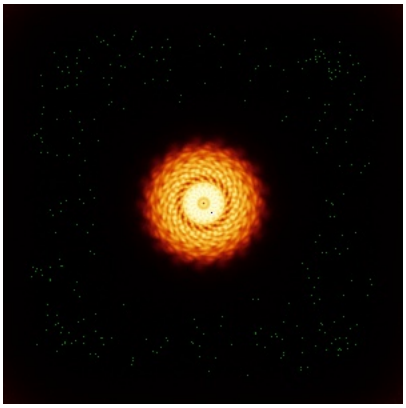
6.4.2 Raw map



X



Y

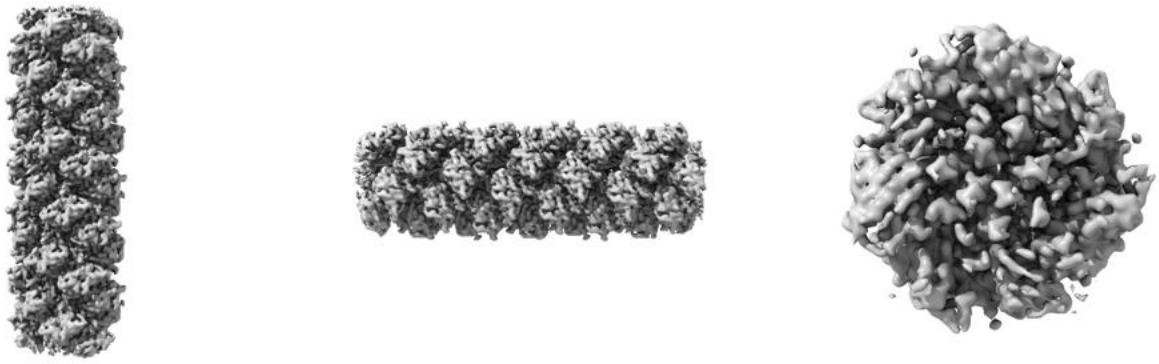


Z

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)

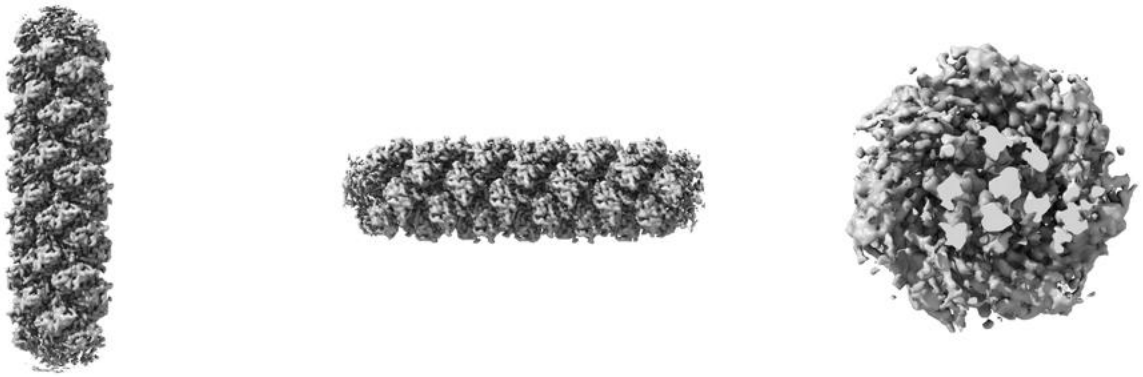
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

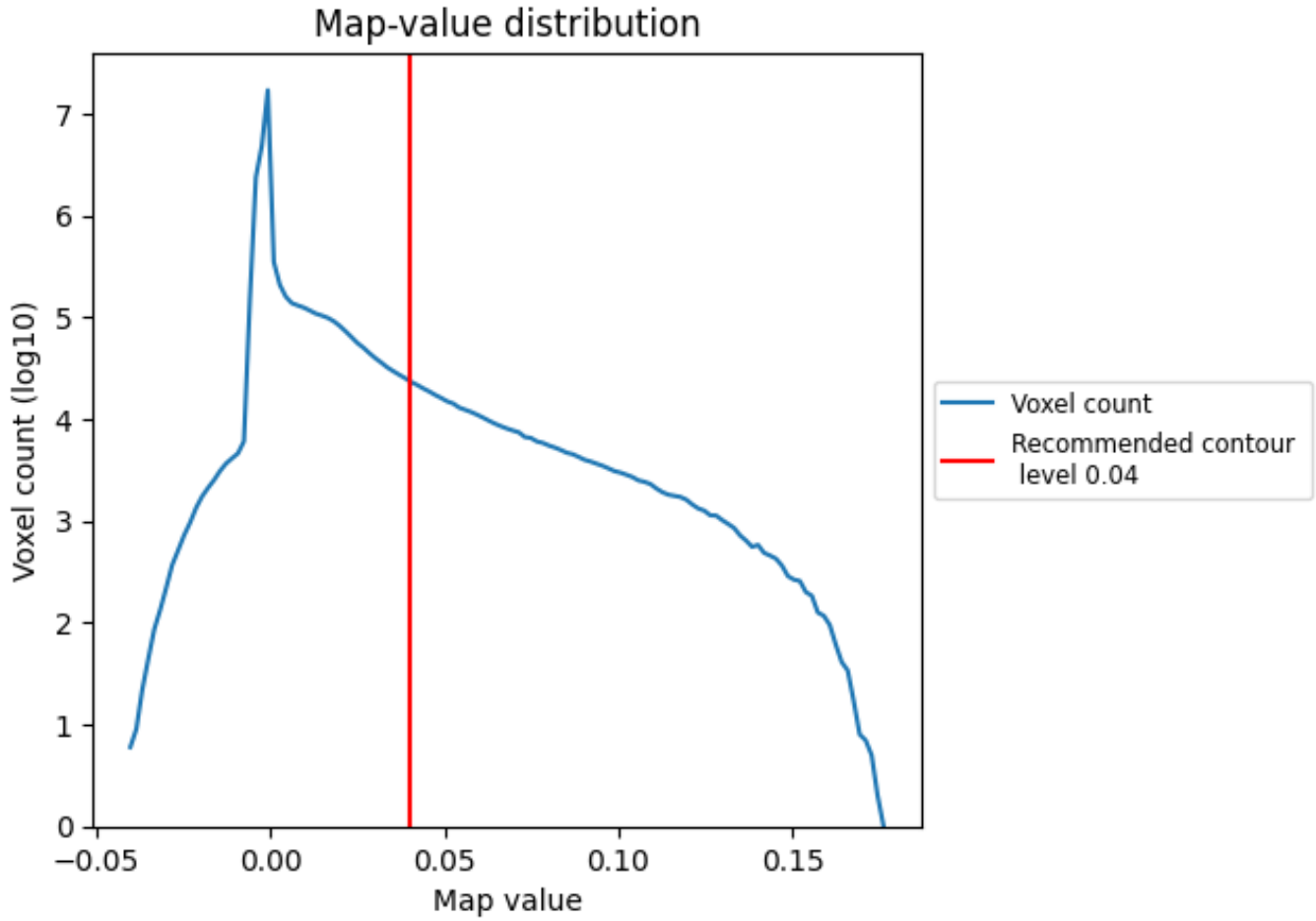
6.6 Mask visualisation (i)

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

7 Map analysis

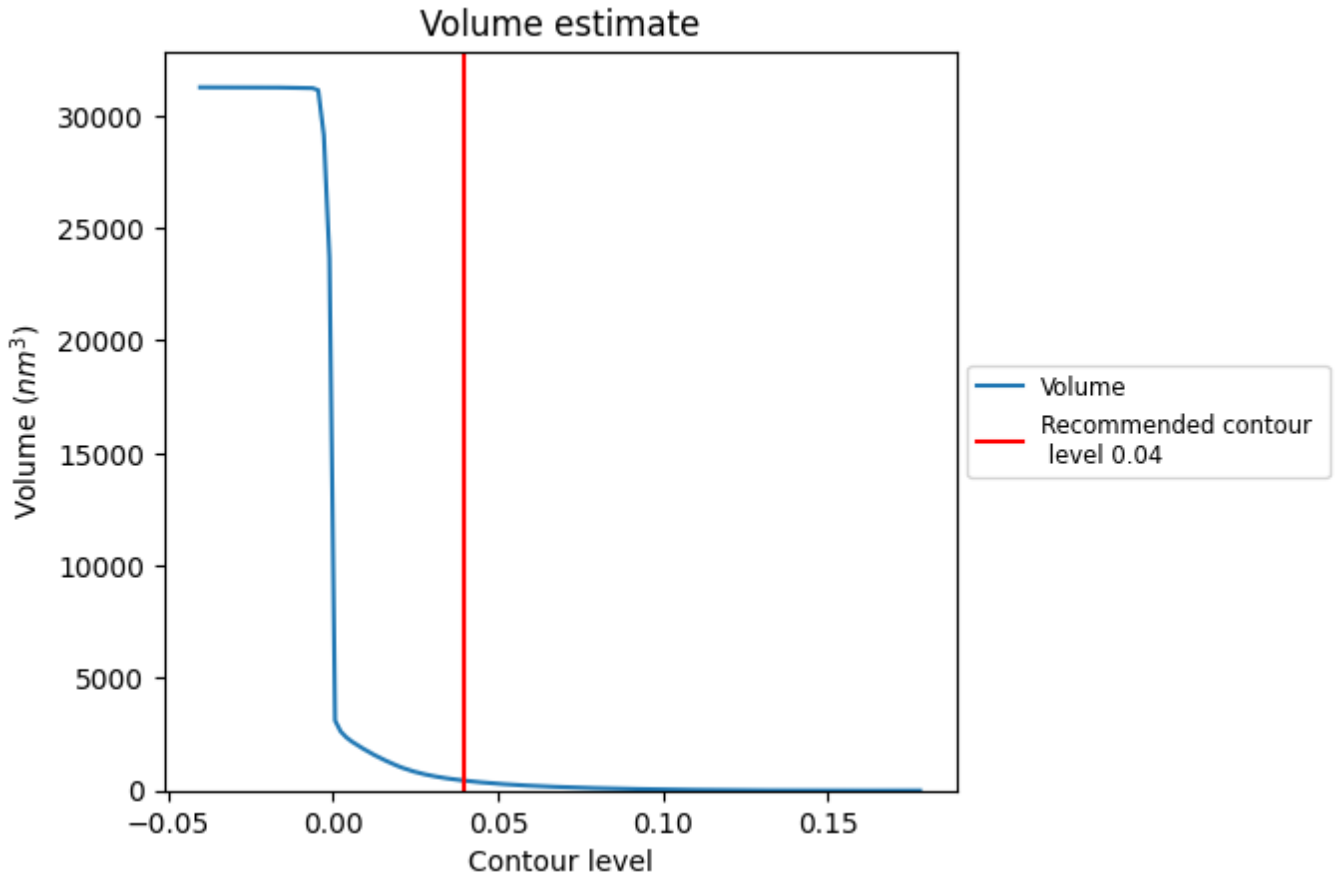
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

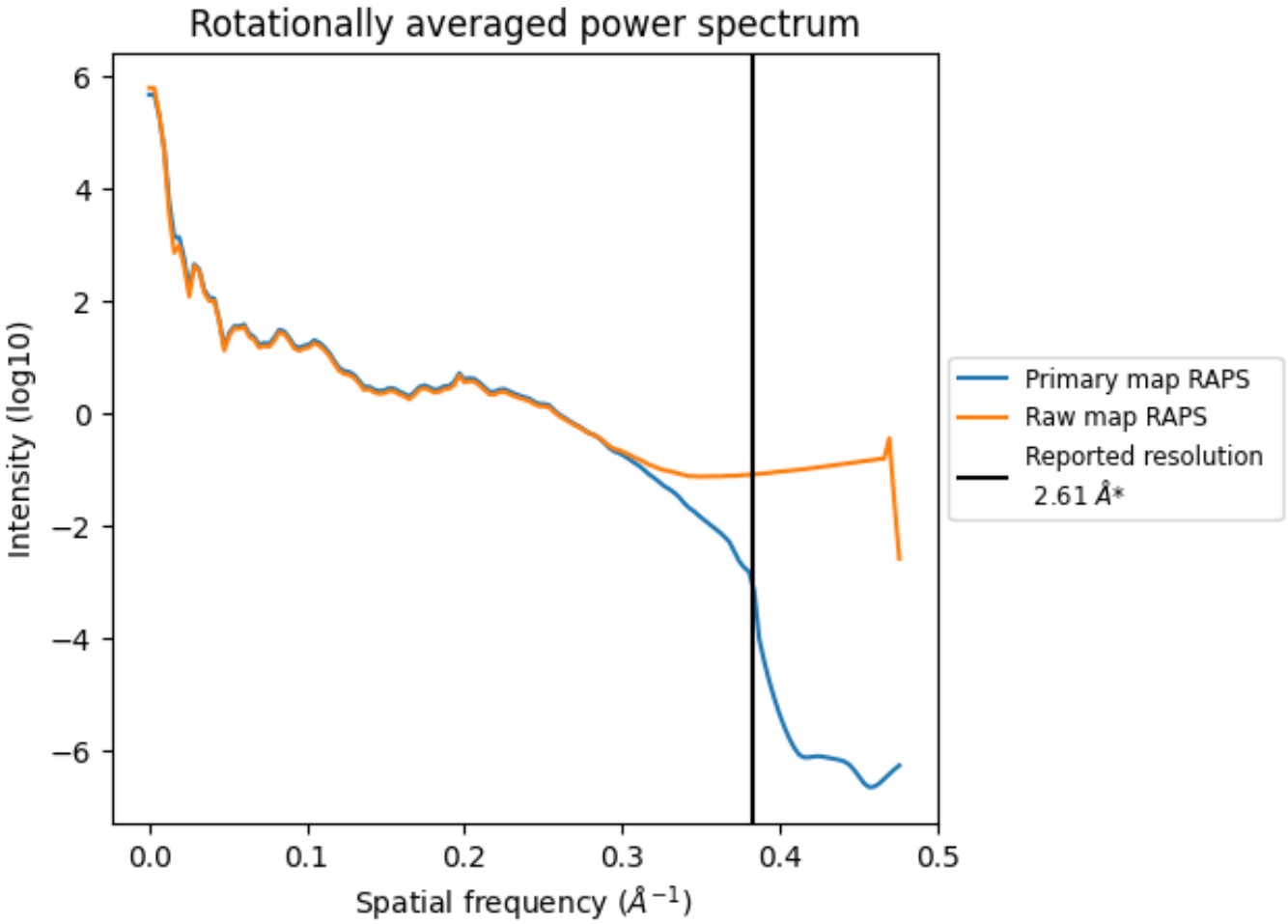
7.2 Volume estimate (i)



The volume at the recommended contour level is 439 nm^3; this corresponds to an approximate mass of 397 kDa.

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

7.3 Rotationally averaged power spectrum (i)

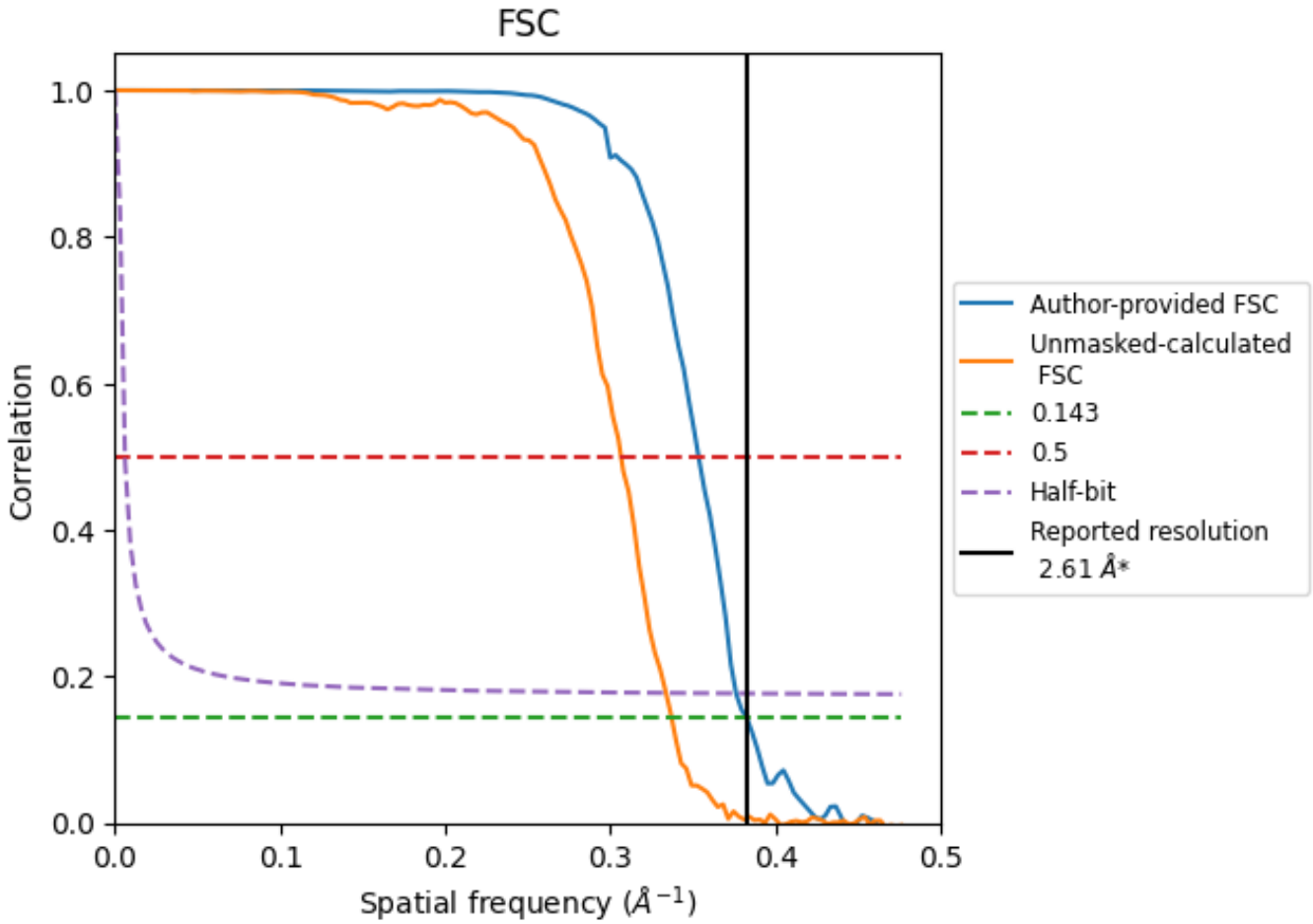


*Reported resolution corresponds to spatial frequency of 0.383 Å^{-1}

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 0.383 Å^{-1}

8.2 Resolution estimates (i)

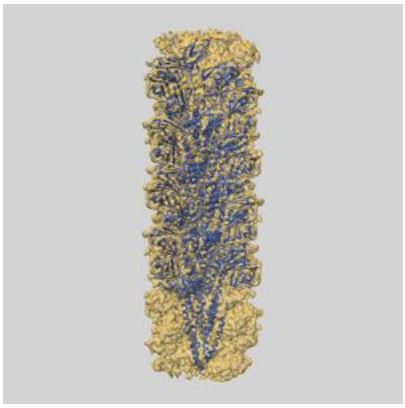
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.61	2.83	2.66
Unmasked-calculated*	2.97	3.26	3.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.97 differs from the reported value 2.61 by more than 10 %

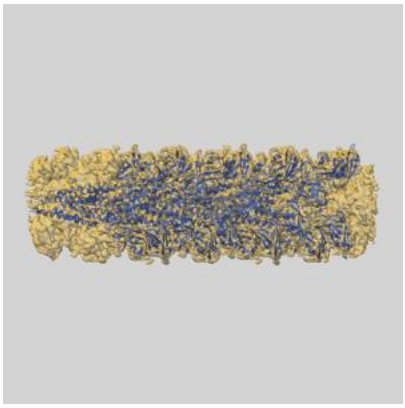
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19112 and PDB model 8REY. Per-residue inclusion information can be found in section 3 on page 13.

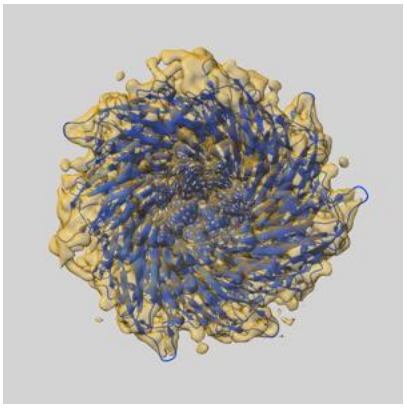
9.1 Map-model overlay



X



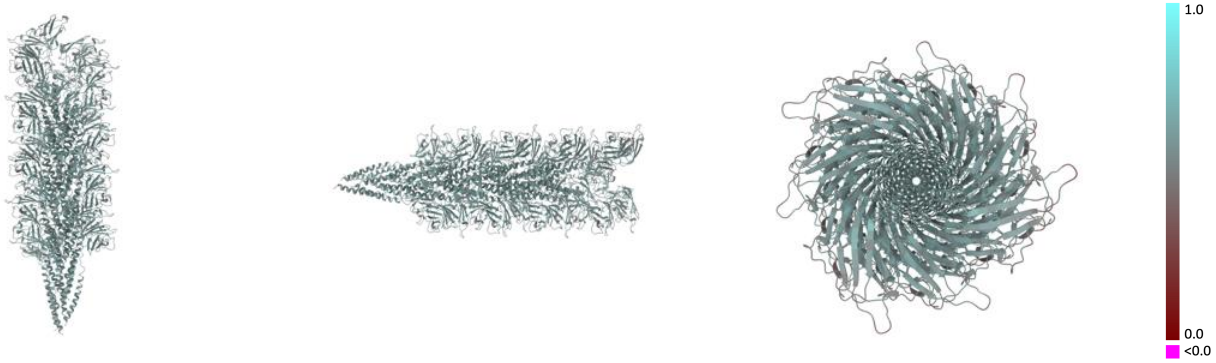
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

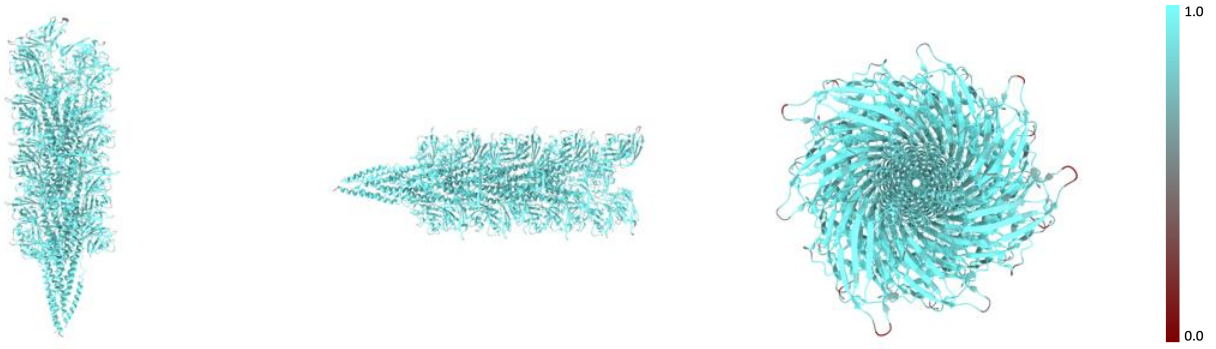
9.2 Q-score mapped to coordinate model



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.

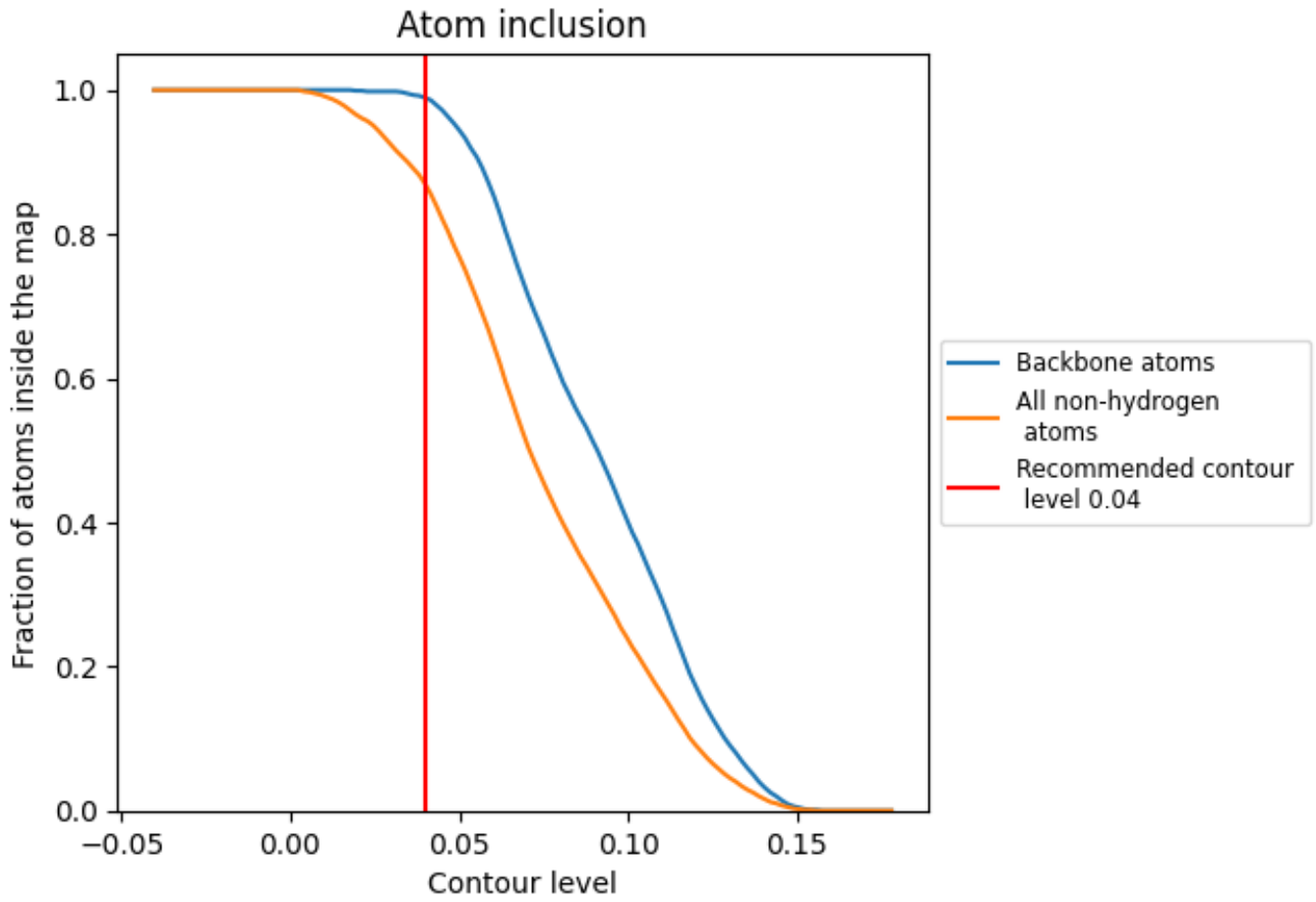
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 87% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.5300
0	0.5370	0.3460
0A	0.3540	0.2990
0B	0.1710	0.2680
2	0.3420	0.3070
2A	0.5610	0.3390
2B	0.1950	0.2390
4	0.5370	0.3330
4A	0.3540	0.2910
6	0.3540	0.3060
6A	0.5490	0.3230
8	0.5370	0.3560
8A	0.3540	0.2820
A	0.9260	0.5550
AA	0.3420	0.3170
AB	0.5240	0.3440
B	0.9360	0.5600
C	0.9450	0.5660
CA	0.5490	0.3500
CB	0.3170	0.2850
D	0.9490	0.5670
E	0.9490	0.5700
EA	0.3420	0.3220
EB	0.5120	0.3420
F	0.9540	0.5750
G	0.9570	0.5750
GA	0.5610	0.3460
GB	0.3660	0.2940
H	0.9540	0.5740
I	0.9560	0.5770
IA	0.3540	0.3170
IB	0.5240	0.3230
J	0.9590	0.5800
K	0.9580	0.5770
KA	0.5610	0.3480

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Chain	Atom inclusion	Q-score
KB	0.3420	0.2840
L	0.9570	0.5760
M	0.9590	0.5790
MA	0.3540	0.3170
MB	0.5240	0.3260
N	0.9600	0.5790
O	0.9580	0.5750
OA	0.5610	0.3590
OB	0.3420	0.2840
P	0.9580	0.5790
Q	0.9580	0.5780
QA	0.3420	0.3130
QB	0.5000	0.3430
R	0.9590	0.5750
S	0.9590	0.5760
SA	0.5730	0.3440
SB	0.3420	0.2890
T	0.9580	0.5770
U	0.9560	0.5760
UA	0.3540	0.3080
UB	0.5000	0.3290
V	0.9530	0.5720
W	0.9590	0.5750
WA	0.5490	0.3330
WB	0.2930	0.2800
X	0.9550	0.5720
Y	0.9540	0.5690
YA	0.3540	0.3100
YB	0.5120	0.3170
Z	0.9490	0.5680
a	0.9530	0.5680
aA	0.5610	0.3500
aB	0.3290	0.2680
b	0.9440	0.5640
c	0.9430	0.5600
cA	0.3780	0.3150
cB	0.5000	0.3340
d	0.9440	0.5580
e	0.9440	0.5560
eA	0.5730	0.3330
eB	0.2930	0.2840
f	0.9370	0.5530

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Chain	Atom inclusion	Q-score
g	0.9240	0.5510
gA	0.3780	0.3020
gB	0.4510	0.3220
h	0.9130	0.5480
i	0.9040	0.5420
iA	0.5610	0.3510
iB	0.2930	0.2880
j	0.8810	0.5360
k	0.5610	0.3510
kA	0.3540	0.3040
kB	0.4020	0.3140
m	0.3540	0.3070
mA	0.5610	0.3550
mB	0.2810	0.2630
o	0.5240	0.3510
oA	0.3660	0.3120
oB	0.3660	0.3220
q	0.3420	0.3080
qA	0.5730	0.3280
qB	0.2680	0.2590
s	0.5370	0.3360
sA	0.3780	0.2950
sB	0.3540	0.3300
u	0.3290	0.3020
uA	0.5610	0.3340
uB	0.2070	0.2640
w	0.5370	0.3420
wA	0.3420	0.2890
wB	0.3170	0.2970
y	0.3290	0.2960
yA	0.5370	0.3490
yB	0.1950	0.2460