Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 04:33 am GMT

PDB ID	:	8QQD
EMDB ID	:	EMD-18588
Title	:	CryoEM structure of the type IV pilin PilA4 from Thermus thermophilus
Authors	:	Gold, V.A.M.; Neuhaus, A.; Gaines, M.; Isupov, M.; McLaren, M.
Deposited on	:	2023-10-04
Resolution	:	2.40 Å(reported)

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

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

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

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

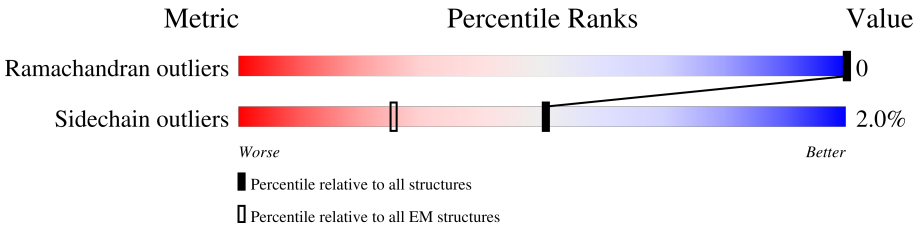
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.40 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	125	98%
1	B	125	98%
1	C	125	98%
1	D	125	98%
1	E	125	98%
1	F	125	98%
1	G	125	98%
1	H	125	98%
1	I	125	98%

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Mol	Chain	Length	Quality of chain
1	J	125	98%
1	K	125	98%
1	L	125	98%
1	M	125	98%
1	N	125	98%
1	O	125	98%
1	P	125	98%
1	Q	125	98%
1	R	125	98%
1	S	125	98%
1	T	125	98%
1	U	125	98%
1	V	125	98%
1	W	125	98%
1	X	125	98%
1	Y	125	98%
1	Z	125	98%
1	a	125	98%
1	b	125	98%
1	c	125	98%
1	d	125	98%
1	e	125	98%
1	f	125	98%
1	g	125	98%
1	h	125	98%

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Mol	Chain	Length	Quality of chain
1	i	125	98%
1	j	125	98%
1	k	125	98%
1	l	125	98%
1	m	125	98%
1	n	125	98%
1	o	125	98%
1	p	125	98%
1	q	125	98%
1	r	125	98%
1	s	125	98%
2	1	2	100%
2	1D	2	100%
2	3A	2	100%
2	3E	2	100%
2	5B	2	100%
2	7C	2	100%
2	9	2	50% 100%
2	9D	2	100%
2	BB	2	100%
2	BF	2	100%
2	DC	2	100%
2	FD	2	100%
2	HA	2	100%
2	HE	2	100%

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Mol	Chain	Length	Quality of chain
2	JB	2	100%
2	JF	2	100%
2	LC	2	100%
2	ND	2	100%
2	PA	2	100%
2	PE	2	100%
2	RB	2	100%
2	RF	2	100%
2	TC	2	100%
2	VD	2	100%
2	XA	2	100%
2	XE	2	100%
2	ZB	2	100%
2	ZF	2	100%
2	bC	2	100%
2	dD	2	100%
2	fA	2	100%
2	fE	2	100%
2	hB	2	100%
2	jC	2	100%
2	lD	2	100%
2	nA	2	100%
2	nE	2	100%
2	pB	2	100%
2	rC	2	100%

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Mol	Chain	Length	Quality of chain
2	t	2	100%
2	tD	2	100%
2	vA	2	100%
2	vE	2	100%
2	xB	2	100%
2	zC	2	100%
3	0B	4	25% 75%
3	2C	4	25% 75%
3	4	4	25% 25% 75%
3	4D	4	25% 75%
3	6A	4	25% 75%
3	6E	4	25% 75%
3	8B	4	25% 75%
3	AD	4	25% 75%
3	CA	4	25% 25% 75%
3	CE	4	25% 75%
3	EB	4	25% 75%
3	EF	4	25% 75%
3	GC	4	25% 75%
3	ID	4	25% 75%
3	KA	4	25% 75%
3	KE	4	25% 75%
3	MB	4	25% 75%
3	MF	4	25% 75%
3	OC	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	QD	4	25% 75%
3	SA	4	25% 75%
3	SE	4	25% 75%
3	UB	4	25% 75%
3	UF	4	25% 75%
3	WC	4	25% 75%
3	YD	4	25% 75%
3	aA	4	25% 75%
3	aE	4	25% 75%
3	cB	4	25% 75%
3	cF	4	25% 75%
3	eC	4	25% 75%
3	gD	4	25% 75%
3	iA	4	25% 75%
3	iE	4	25% 75%
3	kB	4	25% 75%
3	mC	4	25% 75%
3	oD	4	25% 75%
3	qA	4	25% 75%
3	qE	4	25% 75%
3	sB	4	25% 75%
3	uC	4	25% 75%
3	w	4	25% 75%
3	wD	4	25% 75%
3	yA	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	yE	4	25% 75%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 47025 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 Type IV wide pilus major component PilA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	A	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	B	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	C	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	D	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	E	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	F	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	G	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	H	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	I	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	J	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	K	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	L	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	M	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	N	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	O	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	P	125	Total	C	N	O	S	0	0
			931	594	152	181	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	R	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	S	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	T	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	U	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	V	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	W	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	X	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	Y	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	Z	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	a	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	b	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	c	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	e	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	f	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	g	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	h	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	i	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	j	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	k	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	l	125	Total	C	N	O	S	0	0
			931	594	152	181	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	n	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	o	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	p	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	q	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	r	125	Total	C	N	O	S	0	0
			931	594	152	181	4		
1	s	125	Total	C	N	O	S	0	0
			931	594	152	181	4		

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	t	2	Total	C	N	O	0	0
			28	16	2	10		
2	1	2	Total	C	N	O	0	0
			28	16	2	10		
2	9	2	Total	C	N	O	0	0
			28	16	2	10		
2	HA	2	Total	C	N	O	0	0
			28	16	2	10		
2	PA	2	Total	C	N	O	0	0
			28	16	2	10		
2	XA	2	Total	C	N	O	0	0
			28	16	2	10		
2	fA	2	Total	C	N	O	0	0
			28	16	2	10		
2	nA	2	Total	C	N	O	0	0
			28	16	2	10		
2	vA	2	Total	C	N	O	0	0
			28	16	2	10		
2	3A	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	BB	2	Total	C	N	O	0	0
			28	16	2	10		
2	JB	2	Total	C	N	O	0	0
			28	16	2	10		
2	RB	2	Total	C	N	O	0	0
			28	16	2	10		
2	ZB	2	Total	C	N	O	0	0
			28	16	2	10		
2	hB	2	Total	C	N	O	0	0
			28	16	2	10		
2	pB	2	Total	C	N	O	0	0
			28	16	2	10		
2	xB	2	Total	C	N	O	0	0
			28	16	2	10		
2	5B	2	Total	C	N	O	0	0
			28	16	2	10		
2	DC	2	Total	C	N	O	0	0
			28	16	2	10		
2	LC	2	Total	C	N	O	0	0
			28	16	2	10		
2	TC	2	Total	C	N	O	0	0
			28	16	2	10		
2	bC	2	Total	C	N	O	0	0
			28	16	2	10		
2	jC	2	Total	C	N	O	0	0
			28	16	2	10		
2	rC	2	Total	C	N	O	0	0
			28	16	2	10		
2	zC	2	Total	C	N	O	0	0
			28	16	2	10		
2	7C	2	Total	C	N	O	0	0
			28	16	2	10		
2	FD	2	Total	C	N	O	0	0
			28	16	2	10		
2	ND	2	Total	C	N	O	0	0
			28	16	2	10		
2	VD	2	Total	C	N	O	0	0
			28	16	2	10		
2	dD	2	Total	C	N	O	0	0
			28	16	2	10		
2	lD	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms	AltConf	Trace
2	tD	2	Total C N O 28 16 2 10	0	0
2	1D	2	Total C N O 28 16 2 10	0	0
2	9D	2	Total C N O 28 16 2 10	0	0
2	HE	2	Total C N O 28 16 2 10	0	0
2	PE	2	Total C N O 28 16 2 10	0	0
2	XE	2	Total C N O 28 16 2 10	0	0
2	fE	2	Total C N O 28 16 2 10	0	0
2	nE	2	Total C N O 28 16 2 10	0	0
2	vE	2	Total C N O 28 16 2 10	0	0
2	3E	2	Total C N O 28 16 2 10	0	0
2	BF	2	Total C N O 28 16 2 10	0	0
2	JF	2	Total C N O 28 16 2 10	0	0
2	RF	2	Total C N O 28 16 2 10	0	0
2	ZF	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is an oligosaccharide called 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	w	4	Total C N O 61 35 5 21	0	0
3	4	4	Total C N O 61 35 5 21	0	0
3	CA	4	Total C N O 61 35 5 21	0	0
3	KA	4	Total C N O 61 35 5 21	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	SA	4	Total	C	N	O	0	0
			61	35	5	21		
3	aA	4	Total	C	N	O	0	0
			61	35	5	21		
3	iA	4	Total	C	N	O	0	0
			61	35	5	21		
3	qA	4	Total	C	N	O	0	0
			61	35	5	21		
3	yA	4	Total	C	N	O	0	0
			61	35	5	21		
3	6A	4	Total	C	N	O	0	0
			61	35	5	21		
3	EB	4	Total	C	N	O	0	0
			61	35	5	21		
3	MB	4	Total	C	N	O	0	0
			61	35	5	21		
3	UB	4	Total	C	N	O	0	0
			61	35	5	21		
3	cB	4	Total	C	N	O	0	0
			61	35	5	21		
3	kB	4	Total	C	N	O	0	0
			61	35	5	21		
3	sB	4	Total	C	N	O	0	0
			61	35	5	21		
3	0B	4	Total	C	N	O	0	0
			61	35	5	21		
3	8B	4	Total	C	N	O	0	0
			61	35	5	21		
3	GC	4	Total	C	N	O	0	0
			61	35	5	21		
3	OC	4	Total	C	N	O	0	0
			61	35	5	21		
3	WC	4	Total	C	N	O	0	0
			61	35	5	21		
3	eC	4	Total	C	N	O	0	0
			61	35	5	21		
3	mC	4	Total	C	N	O	0	0
			61	35	5	21		
3	uC	4	Total	C	N	O	0	0
			61	35	5	21		
3	2C	4	Total	C	N	O	0	0
			61	35	5	21		

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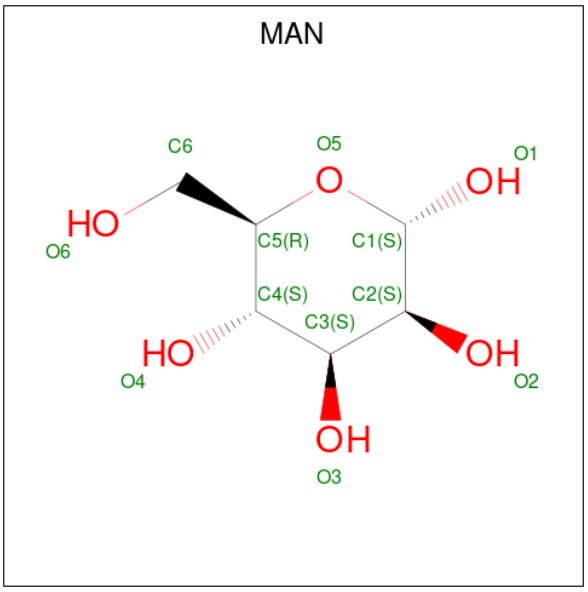
Mol	Chain	Residues	Atoms				AltConf	Trace
3	AD	4	Total	C	N	O	0	0
			61	35	5	21		
3	ID	4	Total	C	N	O	0	0
			61	35	5	21		
3	QD	4	Total	C	N	O	0	0
			61	35	5	21		
3	YD	4	Total	C	N	O	0	0
			61	35	5	21		
3	gD	4	Total	C	N	O	0	0
			61	35	5	21		
3	oD	4	Total	C	N	O	0	0
			61	35	5	21		
3	wD	4	Total	C	N	O	0	0
			61	35	5	21		
3	4D	4	Total	C	N	O	0	0
			61	35	5	21		
3	CE	4	Total	C	N	O	0	0
			61	35	5	21		
3	KE	4	Total	C	N	O	0	0
			61	35	5	21		
3	SE	4	Total	C	N	O	0	0
			61	35	5	21		
3	aE	4	Total	C	N	O	0	0
			61	35	5	21		
3	iE	4	Total	C	N	O	0	0
			61	35	5	21		
3	qE	4	Total	C	N	O	0	0
			61	35	5	21		
3	yE	4	Total	C	N	O	0	0
			61	35	5	21		
3	6E	4	Total	C	N	O	0	0
			61	35	5	21		
3	EF	4	Total	C	N	O	0	0
			61	35	5	21		
3	MF	4	Total	C	N	O	0	0
			61	35	5	21		
3	UF	4	Total	C	N	O	0	0
			61	35	5	21		
3	cF	4	Total	C	N	O	0	0
			61	35	5	21		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
4	d	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	B	1	Total	C	O	0
			11	6	5	
4	C	1	Total	C	O	0
			11	6	5	
4	D	1	Total	C	O	0
			11	6	5	
4	E	1	Total	C	O	0
			11	6	5	
4	F	1	Total	C	O	0
			11	6	5	
4	G	1	Total	C	O	0
			11	6	5	
4	H	1	Total	C	O	0
			11	6	5	
4	I	1	Total	C	O	0
			11	6	5	
4	J	1	Total	C	O	0
			11	6	5	
4	K	1	Total	C	O	0
			11	6	5	
4	L	1	Total	C	O	0
			11	6	5	
4	M	1	Total	C	O	0
			11	6	5	

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Mol	Chain	Residues	Atoms	AltConf
4	N	1	Total C O 11 6 5	0
4	O	1	Total C O 11 6 5	0
4	P	1	Total C O 11 6 5	0
4	Q	1	Total C O 11 6 5	0
4	R	1	Total C O 11 6 5	0
4	S	1	Total C O 11 6 5	0
4	T	1	Total C O 11 6 5	0
4	U	1	Total C O 11 6 5	0
4	V	1	Total C O 11 6 5	0
4	W	1	Total C O 11 6 5	0
4	X	1	Total C O 11 6 5	0
4	Y	1	Total C O 11 6 5	0
4	Z	1	Total C O 11 6 5	0
4	a	1	Total C O 11 6 5	0
4	b	1	Total C O 11 6 5	0
4	c	1	Total C O 11 6 5	0
4	e	1	Total C O 11 6 5	0
4	f	1	Total C O 11 6 5	0
4	g	1	Total C O 11 6 5	0
4	h	1	Total C O 11 6 5	0
4	i	1	Total C O 11 6 5	0

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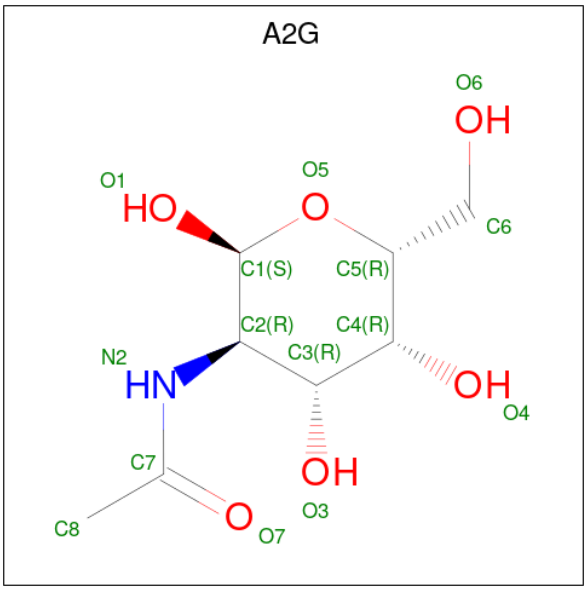
Mol	Chain	Residues	Atoms	AltConf
4	j	1	Total C O 11 6 5	0
4	k	1	Total C O 11 6 5	0
4	l	1	Total C O 11 6 5	0
4	m	1	Total C O 11 6 5	0
4	n	1	Total C O 11 6 5	0
4	o	1	Total C O 11 6 5	0
4	p	1	Total C O 11 6 5	0
4	q	1	Total C O 11 6 5	0
4	r	1	Total C O 11 6 5	0
4	s	1	Total C O 11 6 5	0

- Molecule 5 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	d	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	K	1	Total	C	N	O	0
			14	8	1	5	
5	L	1	Total	C	N	O	0
			14	8	1	5	
5	M	1	Total	C	N	O	0
			14	8	1	5	
5	N	1	Total	C	N	O	0
			14	8	1	5	
5	O	1	Total	C	N	O	0
			14	8	1	5	
5	P	1	Total	C	N	O	0
			14	8	1	5	
5	Q	1	Total	C	N	O	0
			14	8	1	5	
5	R	1	Total	C	N	O	0
			14	8	1	5	
5	S	1	Total	C	N	O	0
			14	8	1	5	
5	T	1	Total	C	N	O	0
			14	8	1	5	
5	U	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	V	1	Total	C	N	O	0
			14	8	1	5	
5	W	1	Total	C	N	O	0
			14	8	1	5	
5	X	1	Total	C	N	O	0
			14	8	1	5	
5	Y	1	Total	C	N	O	0
			14	8	1	5	
5	Z	1	Total	C	N	O	0
			14	8	1	5	
5	a	1	Total	C	N	O	0
			14	8	1	5	
5	b	1	Total	C	N	O	0
			14	8	1	5	
5	c	1	Total	C	N	O	0
			14	8	1	5	
5	e	1	Total	C	N	O	0
			14	8	1	5	
5	f	1	Total	C	N	O	0
			14	8	1	5	
5	g	1	Total	C	N	O	0
			14	8	1	5	
5	h	1	Total	C	N	O	0
			14	8	1	5	
5	i	1	Total	C	N	O	0
			14	8	1	5	
5	j	1	Total	C	N	O	0
			14	8	1	5	
5	k	1	Total	C	N	O	0
			14	8	1	5	
5	l	1	Total	C	N	O	0
			14	8	1	5	
5	m	1	Total	C	N	O	0
			14	8	1	5	
5	n	1	Total	C	N	O	0
			14	8	1	5	
5	o	1	Total	C	N	O	0
			14	8	1	5	
5	p	1	Total	C	N	O	0
			14	8	1	5	
5	q	1	Total	C	N	O	0
			14	8	1	5	

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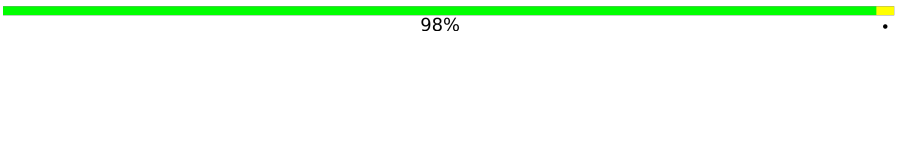
Mol	Chain	Residues	Atoms				AltConf
5	r	1	Total	C	N	O	0
			14	8	1	5	
5	s	1	Total	C	N	O	0
			14	8	1	5	

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.

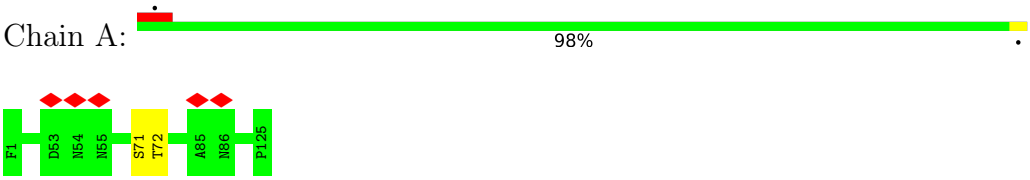
• Molecule 1: Type IV wide pilus major component PilA4

Chain d:



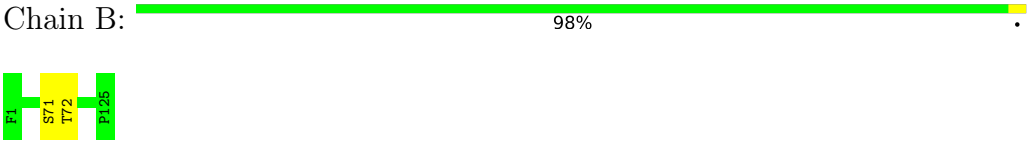
• Molecule 1: Type IV wide pilus major component PilA4

Chain A:



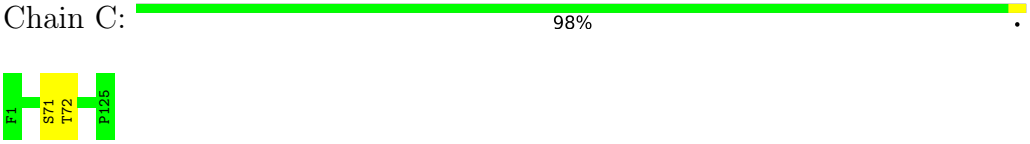
• Molecule 1: Type IV wide pilus major component PilA4

Chain B:



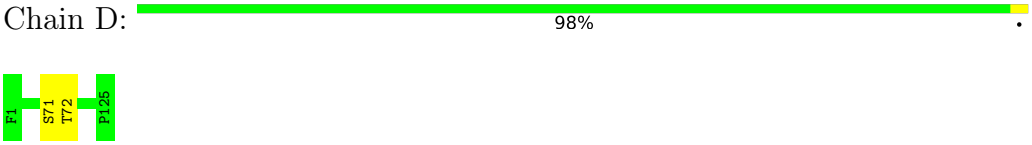
• Molecule 1: Type IV wide pilus major component PilA4

Chain C:



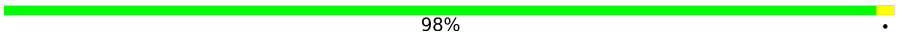
• Molecule 1: Type IV wide pilus major component PilA4

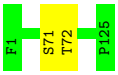
Chain D:



• Molecule 1: Type IV wide pilus major component PilA4

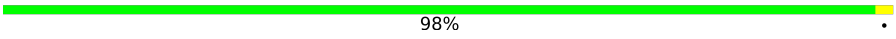
Chain E:

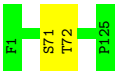




• Molecule 1: Type IV wide pilus major component PilA4

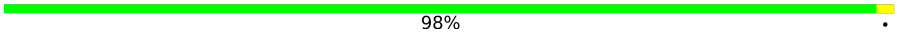
Chain F:

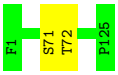




• Molecule 1: Type IV wide pilus major component PilA4

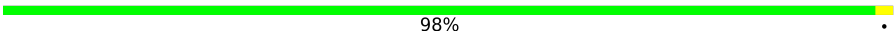
Chain G:

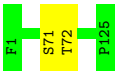




• Molecule 1: Type IV wide pilus major component PilA4

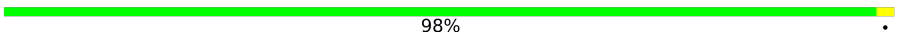
Chain H:

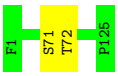




• Molecule 1: Type IV wide pilus major component PilA4

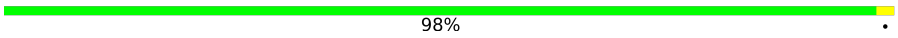
Chain I:

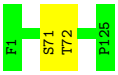




• Molecule 1: Type IV wide pilus major component PilA4

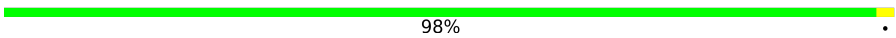
Chain J:

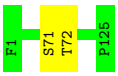




• Molecule 1: Type IV wide pilus major component PilA4

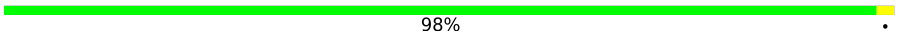
Chain K:

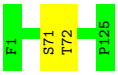




• Molecule 1: Type IV wide pilus major component PilA4

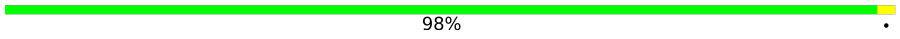
Chain L:

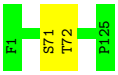




• Molecule 1: Type IV wide pilus major component PilA4

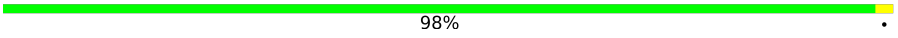
Chain M:

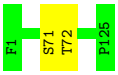




• Molecule 1: Type IV wide pilus major component PilA4

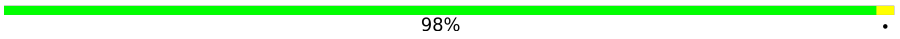
Chain N:

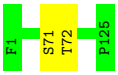




• Molecule 1: Type IV wide pilus major component PilA4

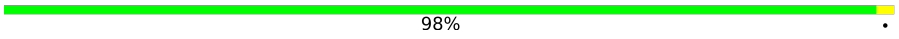
Chain O:

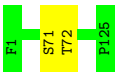




• Molecule 1: Type IV wide pilus major component PilA4

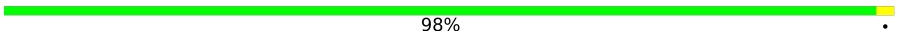
Chain P:

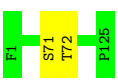




• Molecule 1: Type IV wide pilus major component PilA4

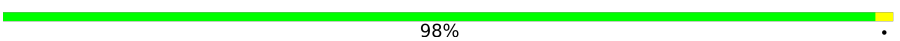
Chain Q:

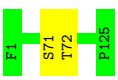




• Molecule 1: Type IV wide pilus major component PilA4

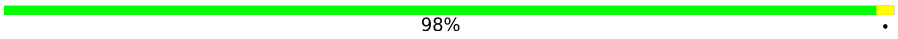
Chain R:

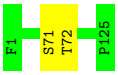




• Molecule 1: Type IV wide pilus major component PilA4

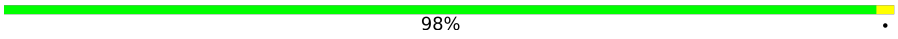
Chain S:

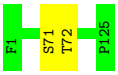




• Molecule 1: Type IV wide pilus major component PilA4

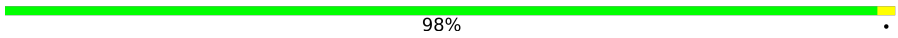
Chain T:

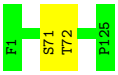




• Molecule 1: Type IV wide pilus major component PilA4

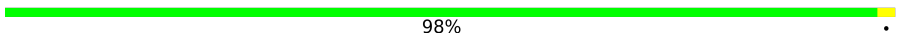
Chain U:

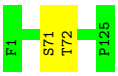




• Molecule 1: Type IV wide pilus major component PilA4

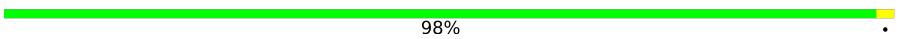
Chain V:

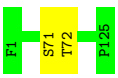




• Molecule 1: Type IV wide pilus major component PilA4

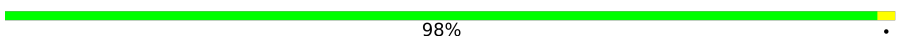
Chain W:





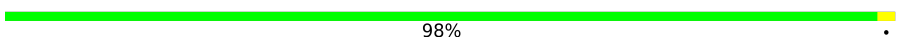
• Molecule 1: Type IV wide pilus major component PilA4

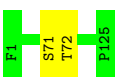
Chain X:



• Molecule 1: Type IV wide pilus major component PilA4

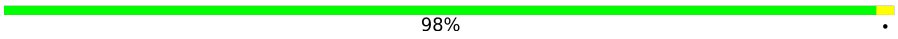
Chain Y:

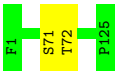




• Molecule 1: Type IV wide pilus major component PilA4

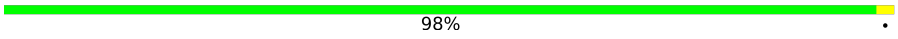
Chain Z:

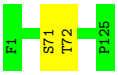




• Molecule 1: Type IV wide pilus major component PilA4

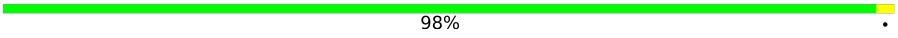
Chain a:

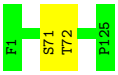




• Molecule 1: Type IV wide pilus major component PilA4

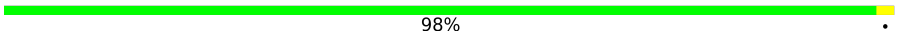
Chain b:

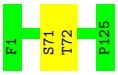




• Molecule 1: Type IV wide pilus major component PilA4

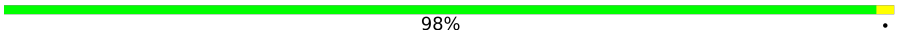
Chain c:

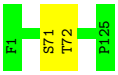




• Molecule 1: Type IV wide pilus major component PilA4

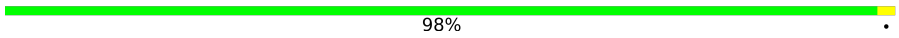
Chain e:

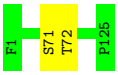




• Molecule 1: Type IV wide pilus major component PilA4

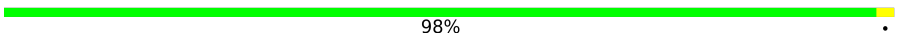
Chain f:

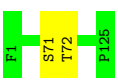




• Molecule 1: Type IV wide pilus major component PilA4

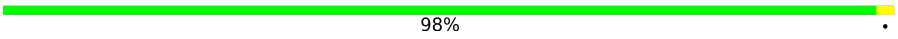
Chain g:

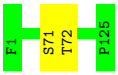




• Molecule 1: Type IV wide pilus major component PilA4

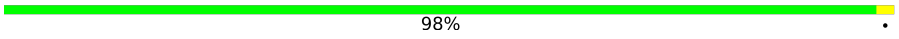
Chain h:

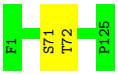




• Molecule 1: Type IV wide pilus major component PilA4

Chain i:





• Molecule 1: Type IV wide pilus major component PilA4

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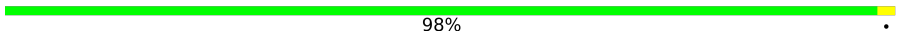
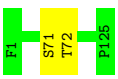
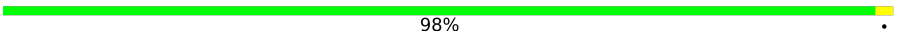
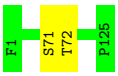




• Molecule 1: Type IV wide pilus major component PilA4

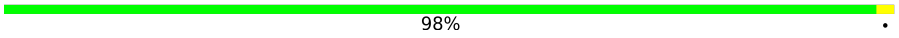
Chain k:

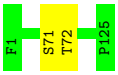




• Molecule 1: Type IV wide pilus major component PilA4

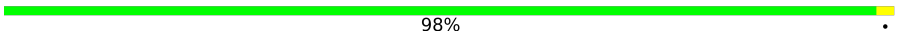
Chain l:

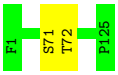




• Molecule 1: Type IV wide pilus major component PilA4

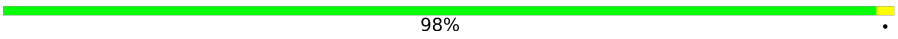
Chain m:

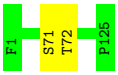




• Molecule 1: Type IV wide pilus major component PilA4

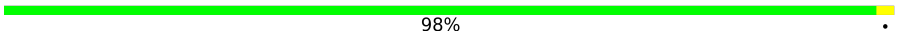
Chain n:

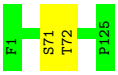




• Molecule 1: Type IV wide pilus major component PilA4

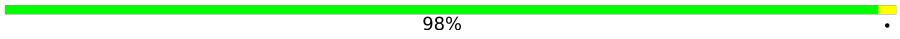
Chain o:

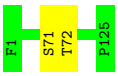




• Molecule 1: Type IV wide pilus major component PilA4

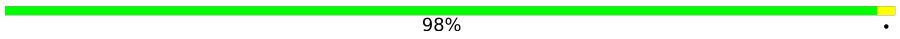
Chain p:

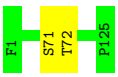




• Molecule 1: Type IV wide pilus major component PilA4

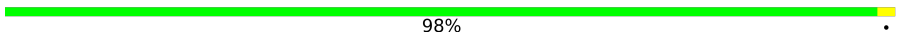
Chain q:

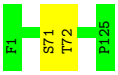




• Molecule 1: Type IV wide pilus major component PilA4

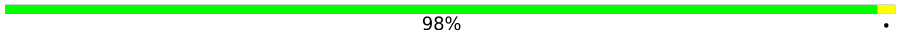
Chain r:

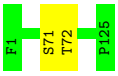




• Molecule 1: Type IV wide pilus major component PilA4

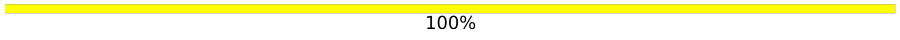
Chain s:





• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain t:

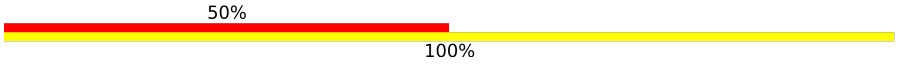


• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 1:

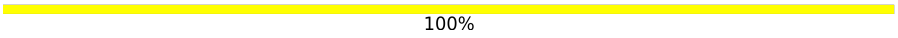
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 9:



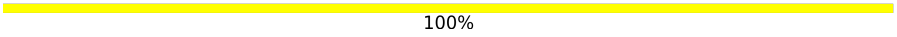
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain HA:



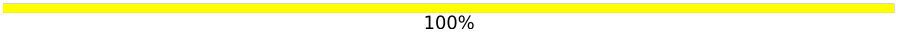
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain PA:



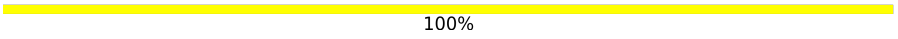
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain XA:



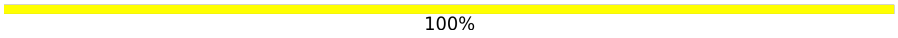
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain fA:



• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain nA:



• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain vA: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 3A: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain BB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain JB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain RB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain ZB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain hB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain pB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain xB: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 5B: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain DC: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain LC: 100%

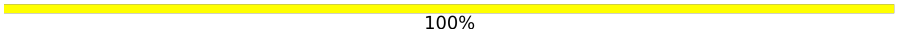
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain TC: 100%

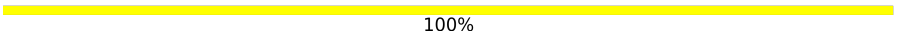
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain bC: 100%

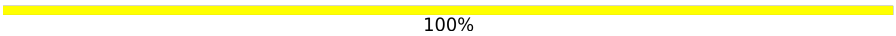
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain jC: 

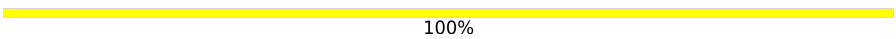
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain rC: 

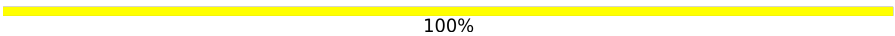
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain zC: 

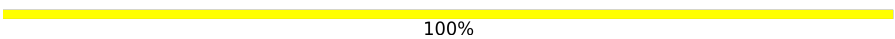
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 7C: 

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain FD: 

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain ND: 

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain VD: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain dD: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain lD: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain tD: 100%

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 1D: 100%

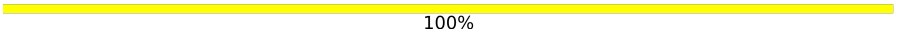
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 9D: 100%

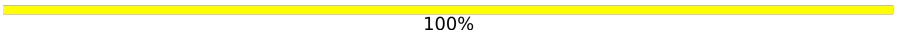
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain HE: 100%

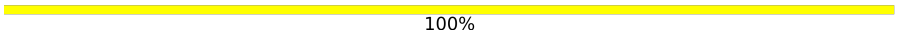
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain PE: 

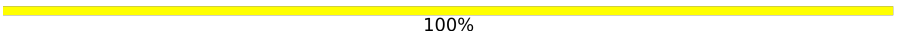
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain XE: 

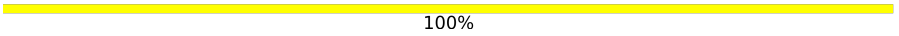
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain fE: 

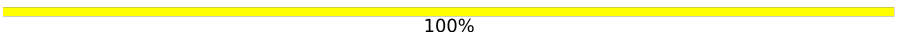
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain nE: 

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

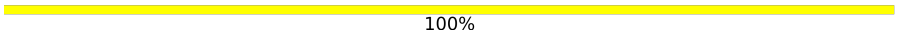
Chain vE: 

• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 3E: 

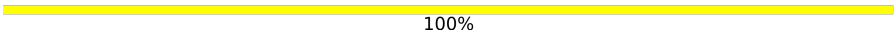
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain BF:



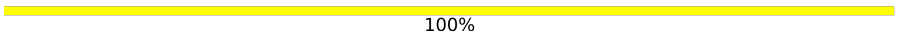
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain JF:



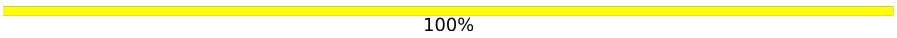
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain RF:



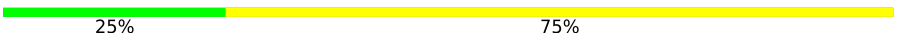
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain ZF:



• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain w:



• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

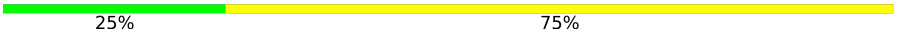
Chain 4:

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain CA:

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain KA:

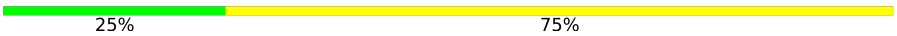


• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain SA:

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain aA:

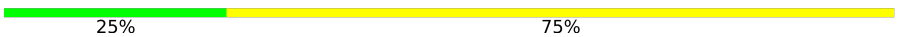


• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain iA:

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain qA:



• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain yA: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 6A: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain EB: 

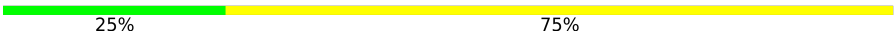
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain MB: 

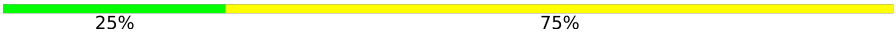
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain UB: 

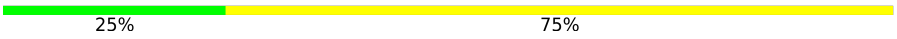
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain cB: 

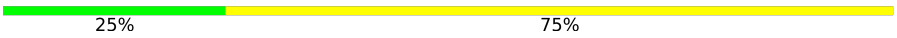
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain kB: 

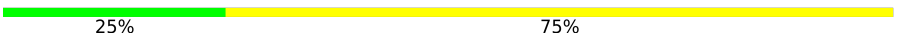
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain sB: 

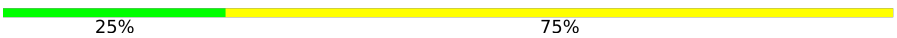
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 0B: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

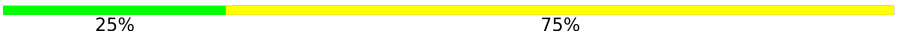
Chain 8B: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain GC: 

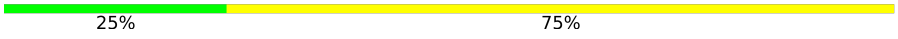
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain OC:



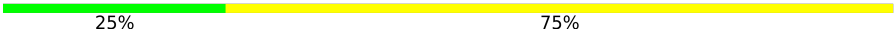
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain WC:



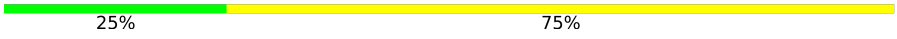
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain eC:



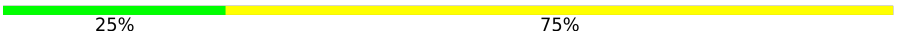
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain mC:



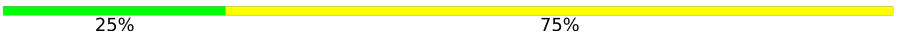
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain uC:



• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

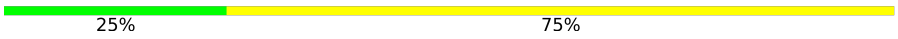
Chain 2C:



• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain AD: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain ID: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain QD: 

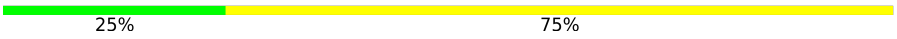
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain YD: 

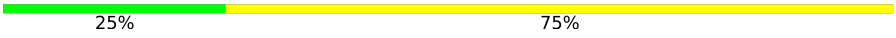
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain gD: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain oD: 

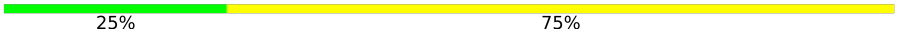
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain wD: 

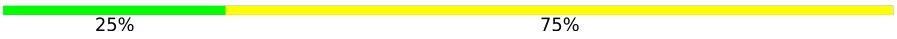
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 4D: 

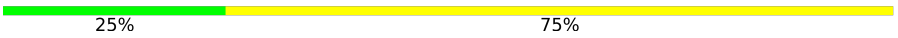
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain CE: 

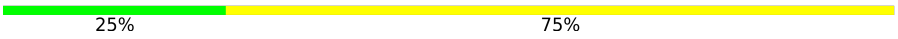
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain KE: 

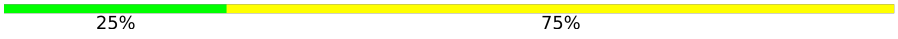
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain SE: 

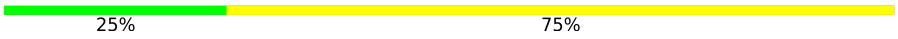
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain aE: 

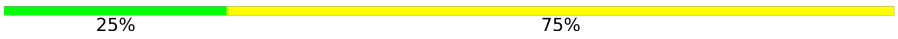
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain iE: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain qE: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain yE: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain 6E: 

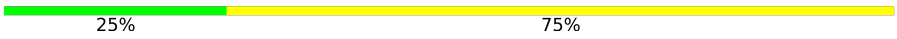
• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain EF: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain MF: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain UF: 

• Molecule 3: 7-Acetamido-5-acetimidoyl-3,5,7,9-tetradeoxy-L-glycero-L-manno-nonulosonic aci-(1-4)-alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain cF: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=92.36°, rise=9.242 Å, axial sym=C1	Depositor
Number of segments used	654248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.343	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	536.576, 536.576, 536.576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: WT8, A2G, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/947	0.67	0/1294
1	B	0.39	0/947	0.67	0/1294
1	C	0.39	0/947	0.67	0/1294
1	D	0.39	0/947	0.67	0/1294
1	E	0.39	0/947	0.67	0/1294
1	F	0.39	0/947	0.67	0/1294
1	G	0.39	0/947	0.67	0/1294
1	H	0.39	0/947	0.67	0/1294
1	I	0.39	0/947	0.67	0/1294
1	J	0.39	0/947	0.67	0/1294
1	K	0.39	0/947	0.67	0/1294
1	L	0.39	0/947	0.67	0/1294
1	M	0.39	0/947	0.67	0/1294
1	N	0.39	0/947	0.67	0/1294
1	O	0.39	0/947	0.67	0/1294
1	P	0.39	0/947	0.67	0/1294
1	Q	0.39	0/947	0.67	0/1294
1	R	0.39	0/947	0.67	0/1294
1	S	0.39	0/947	0.67	0/1294
1	T	0.39	0/947	0.67	0/1294
1	U	0.39	0/947	0.67	0/1294
1	V	0.39	0/947	0.67	0/1294
1	W	0.39	0/947	0.67	0/1294
1	X	0.39	0/947	0.67	0/1294
1	Y	0.39	0/947	0.67	0/1294
1	Z	0.39	0/947	0.67	0/1294
1	a	0.39	0/947	0.67	0/1294
1	b	0.39	0/947	0.67	0/1294
1	c	0.39	0/947	0.67	0/1294
1	d	0.39	0/947	0.67	0/1294
1	e	0.39	0/947	0.67	0/1294
1	f	0.39	0/947	0.67	0/1294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	g	0.39	0/947	0.67	0/1294
1	h	0.39	0/947	0.67	0/1294
1	i	0.39	0/947	0.67	0/1294
1	j	0.39	0/947	0.67	0/1294
1	k	0.39	0/947	0.67	0/1294
1	l	0.39	0/947	0.67	0/1294
1	m	0.39	0/947	0.67	0/1294
1	n	0.39	0/947	0.67	0/1294
1	o	0.39	0/947	0.67	0/1294
1	p	0.39	0/947	0.67	0/1294
1	q	0.39	0/947	0.67	0/1294
1	r	0.39	0/947	0.67	0/1294
1	s	0.39	0/947	0.67	0/1294
All	All	0.39	0/42615	0.67	0/58230

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	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	B	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	C	123/125 (98%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	E	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	F	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	G	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	H	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	I	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	J	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	K	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	M	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	N	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	O	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	P	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	Q	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	R	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	S	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	T	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	U	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	V	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	W	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	X	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	Y	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	Z	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	a	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	b	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	c	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	d	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	e	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	f	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	g	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	h	123/125 (98%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	j	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	k	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	l	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	m	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	n	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	o	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	p	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	q	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	r	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	s	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
All	All	5535/5625 (98%)	5445 (98%)	90 (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	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	B	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	C	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	D	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	E	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	F	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	G	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	H	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	I	102/102 (100%)	100 (98%)	2 (2%)	50	70
1	J	102/102 (100%)	100 (98%)	2 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	L	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	M	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	N	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	O	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	P	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	Q	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	R	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	S	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	T	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	U	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	V	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	W	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	X	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	Y	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	Z	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	a	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	b	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	c	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	d	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	e	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	f	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	g	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	h	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	i	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	j	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	k	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	l	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	m	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	n	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	o	102/102 (100%)	100 (98%)	2 (2%)	50 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	p	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	q	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	r	102/102 (100%)	100 (98%)	2 (2%)	50 70
1	s	102/102 (100%)	100 (98%)	2 (2%)	50 70
All	All	4590/4590 (100%)	4500 (98%)	90 (2%)	50 70

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	d	71	SER
1	d	72	THR
1	A	71	SER
1	A	72	THR
1	B	71	SER
1	B	72	THR
1	C	71	SER
1	C	72	THR
1	D	71	SER
1	D	72	THR
1	E	71	SER
1	E	72	THR
1	F	71	SER
1	F	72	THR
1	G	71	SER
1	G	72	THR
1	H	71	SER
1	H	72	THR
1	I	71	SER
1	I	72	THR
1	J	71	SER
1	J	72	THR
1	K	71	SER
1	K	72	THR
1	L	71	SER
1	L	72	THR
1	M	71	SER
1	M	72	THR
1	N	71	SER
1	N	72	THR
1	O	71	SER
1	O	72	THR

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Mol	Chain	Res	Type
1	P	71	SER
1	P	72	THR
1	Q	71	SER
1	Q	72	THR
1	R	71	SER
1	R	72	THR
1	S	71	SER
1	S	72	THR
1	T	71	SER
1	T	72	THR
1	U	71	SER
1	U	72	THR
1	V	71	SER
1	V	72	THR
1	W	71	SER
1	W	72	THR
1	X	71	SER
1	X	72	THR
1	Y	71	SER
1	Y	72	THR
1	Z	71	SER
1	Z	72	THR
1	a	71	SER
1	a	72	THR
1	b	71	SER
1	b	72	THR
1	c	71	SER
1	c	72	THR
1	e	71	SER
1	e	72	THR
1	f	71	SER
1	f	72	THR
1	g	71	SER
1	g	72	THR
1	h	71	SER
1	h	72	THR
1	i	71	SER
1	i	72	THR
1	j	71	SER
1	j	72	THR
1	k	71	SER
1	k	72	THR

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Mol	Chain	Res	Type
1	l	71	SER
1	l	72	THR
1	m	71	SER
1	m	72	THR
1	n	71	SER
1	n	72	THR
1	o	71	SER
1	o	72	THR
1	p	71	SER
1	p	72	THR
1	q	71	SER
1	q	72	THR
1	r	71	SER
1	r	72	THR
1	s	71	SER
1	s	72	THR

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)

270 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	0B	1	3,1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
3	A2G	0B	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	0B	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	0B	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	1	1	1,2	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
2	A2G	1	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	1D	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	1D	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	2C	1	3,1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
3	A2G	2C	2	3	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
3	MAN	2C	3	3	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
3	WT8	2C	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	3A	1	1,2	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
2	A2G	3A	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	3E	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	3E	2	2	14,14,15	0.86	0	17,19,21	1.47	2 (11%)
3	A2G	4	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	4	2	3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	MAN	4	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	4	4	3	20,22,23	0.57	0	21,31,34	0.80	0
3	A2G	4D	1	3,1	14,14,15	0.45	0	17,19,21	1.25	2 (11%)
3	A2G	4D	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	4D	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	4D	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	5B	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	5B	2	2	14,14,15	0.84	0	17,19,21	1.47	2 (11%)
3	A2G	6A	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	6A	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	6A	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	6A	4	3	20,22,23	0.59	0	21,31,34	0.80	0
3	A2G	6E	1	3,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	A2G	6E	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	6E	3	3	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
3	WT8	6E	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	7C	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	7C	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	8B	1	3,1	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
3	A2G	8B	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	8B	3	3	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
3	WT8	8B	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	9	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	9	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	9D	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	9D	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	AD	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	AD	2	3	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
3	MAN	AD	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	AD	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	BB	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	BB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	BF	1	1,2	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
2	A2G	BF	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	CA	1	3,1	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
3	A2G	CA	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	CA	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	CA	4	3	20,22,23	0.58	0	21,31,34	0.79	0
3	A2G	CE	1	3,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	A2G	CE	2	3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	MAN	CE	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	CE	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	DC	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	DC	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	EB	1	3,1	14,14,15	0.49	0	17,19,21	1.25	2 (11%)
3	A2G	EB	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	EB	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	EB	4	3	20,22,23	0.57	0	21,31,34	0.79	0
3	A2G	EF	1	3,1	14,14,15	0.48	0	17,19,21	1.25	2 (11%)
3	A2G	EF	2	3	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
3	MAN	EF	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	EF	4	3	20,22,23	0.57	0	21,31,34	0.80	0
2	A2G	FD	1	1,2	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
2	A2G	FD	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	GC	1	3,1	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
3	A2G	GC	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	GC	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	GC	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	HA	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	HA	2	2	14,14,15	0.84	0	17,19,21	1.47	2 (11%)
2	A2G	HE	1	1,2	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
2	A2G	HE	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	ID	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	ID	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	ID	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	ID	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	JB	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	JB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	JF	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	JF	2	2	14,14,15	0.86	0	17,19,21	1.47	2 (11%)
3	A2G	KA	1	3,1	14,14,15	0.48	0	17,19,21	1.25	2 (11%)
3	A2G	KA	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	KA	3	3	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
3	WT8	KA	4	3	20,22,23	0.58	0	21,31,34	0.80	0
3	A2G	KE	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	KE	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	KE	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	KE	4	3	20,22,23	0.57	0	21,31,34	0.80	0
2	A2G	LC	1	1,2	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
2	A2G	LC	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	MB	1	3,1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
3	A2G	MB	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	MB	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	MB	4	3	20,22,23	0.58	0	21,31,34	0.80	0
3	A2G	MF	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	MF	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	MF	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	MF	4	3	20,22,23	0.57	0	21,31,34	0.80	0
2	A2G	ND	1	1,2	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
2	A2G	ND	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	OC	1	3,1	14,14,15	0.49	0	17,19,21	1.25	2 (11%)
3	A2G	OC	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	OC	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	OC	4	3	20,22,23	0.59	0	21,31,34	0.80	0
2	A2G	PA	1	1,2	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
2	A2G	PA	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	PE	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	PE	2	2	14,14,15	0.84	0	17,19,21	1.47	2 (11%)
3	A2G	QD	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	QD	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	QD	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	QD	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	RB	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	RB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	RF	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	RF	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	SA	1	3,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	A2G	SA	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	SA	3	3	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
3	WT8	SA	4	3	20,22,23	0.58	0	21,31,34	0.79	0
3	A2G	SE	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	SE	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	SE	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	SE	4	3	20,22,23	0.57	0	21,31,34	0.79	0
2	A2G	TC	1	1,2	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
2	A2G	TC	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	UB	1	3,1	14,14,15	0.48	0	17,19,21	1.25	2 (11%)
3	A2G	UB	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	UB	3	3	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
3	WT8	UB	4	3	20,22,23	0.58	0	21,31,34	0.79	0
3	A2G	UF	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	UF	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	UF	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	UF	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	VD	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	VD	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	WC	1	3,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	A2G	WC	2	3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	MAN	WC	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	WC	4	3	20,22,23	0.57	0	21,31,34	0.80	0
2	A2G	XA	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	XA	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	XE	1	1,2	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
2	A2G	XE	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	YD	1	3,1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
3	A2G	YD	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	YD	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	YD	4	3	20,22,23	0.57	0	21,31,34	0.79	0
2	A2G	ZB	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	ZB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	ZF	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	ZF	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	aA	1	3,1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
3	A2G	aA	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	aA	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	aA	4	3	20,22,23	0.58	0	21,31,34	0.79	0
3	A2G	aE	1	3,1	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
3	A2G	aE	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	aE	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	aE	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	bC	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	bC	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	cB	1	3,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	A2G	cB	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	cB	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	cB	4	3	20,22,23	0.57	0	21,31,34	0.79	0
3	A2G	cF	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	cF	2	3	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
3	MAN	cF	3	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
3	WT8	cF	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	dD	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	dD	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	eC	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	eC	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	eC	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	eC	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	fA	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	fA	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	fE	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	fE	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	gD	1	3,1	14,14,15	0.48	0	17,19,21	1.25	2 (11%)
3	A2G	gD	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	gD	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	gD	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	hB	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	hB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	iA	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	iA	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	iA	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	iA	4	3	20,22,23	0.58	0	21,31,34	0.79	0
3	A2G	iE	1	3,1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
3	A2G	iE	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	iE	3	3	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
3	WT8	iE	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	jC	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	jC	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	kB	1	3,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	A2G	kB	2	3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	MAN	kB	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	kB	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	lD	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	lD	2	2	14,14,15	0.84	0	17,19,21	1.47	2 (11%)
3	A2G	mC	1	3,1	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
3	A2G	mC	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	mC	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	mC	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	nA	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	nA	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A2G	nE	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	nE	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	oD	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	oD	2	3	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	MAN	oD	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	oD	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	pB	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	pB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	qA	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	qA	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	qA	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	qA	4	3	20,22,23	0.57	0	21,31,34	0.80	0
3	A2G	qE	1	3,1	14,14,15	0.48	0	17,19,21	1.25	2 (11%)
3	A2G	qE	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
3	MAN	qE	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	qE	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	rC	1	1,2	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
2	A2G	rC	2	2	14,14,15	0.84	0	17,19,21	1.47	2 (11%)
3	A2G	sB	1	3,1	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
3	A2G	sB	2	3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	MAN	sB	3	3	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
3	WT8	sB	4	3	20,22,23	0.58	0	21,31,34	0.80	0
2	A2G	t	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	t	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
2	A2G	tD	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	tD	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	uC	1	3,1	14,14,15	0.48	0	17,19,21	1.25	2 (11%)
3	A2G	uC	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	uC	3	3	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
3	WT8	uC	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	vA	1	1,2	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
2	A2G	vA	2	2	14,14,15	0.86	0	17,19,21	1.47	2 (11%)
2	A2G	vE	1	1,2	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
2	A2G	vE	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	w	1	3,1	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
3	A2G	w	2	3	14,14,15	0.62	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	w	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	w	4	3	20,22,23	0.58	0	21,31,34	0.80	0
3	A2G	wD	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	wD	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	wD	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	wD	4	3	20,22,23	0.57	0	21,31,34	0.79	0
2	A2G	xB	1	1,2	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	A2G	xB	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	A2G	yA	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	yA	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	yA	3	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
3	WT8	yA	4	3	20,22,23	0.57	0	21,31,34	0.80	0
3	A2G	yE	1	3,1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
3	A2G	yE	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	MAN	yE	3	3	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
3	WT8	yE	4	3	20,22,23	0.58	0	21,31,34	0.79	0
2	A2G	zC	1	1,2	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
2	A2G	zC	2	2	14,14,15	0.85	0	17,19,21	1.47	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	0B	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	0B	2	3	-	2/6/23/26	0/1/1/1
3	MAN	0B	3	3	-	0/2/19/22	0/1/1/1
3	WT8	0B	4	3	-	3/20/36/40	0/1/1/1
2	A2G	1	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	1	2	2	-	2/6/23/26	0/1/1/1
2	A2G	1D	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	1D	2	2	-	2/6/23/26	0/1/1/1
3	A2G	2C	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	2C	2	3	-	1/6/23/26	0/1/1/1
3	MAN	2C	3	3	-	0/2/19/22	0/1/1/1
3	WT8	2C	4	3	-	3/20/36/40	0/1/1/1
2	A2G	3A	1	1,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	3A	2	2	-	2/6/23/26	0/1/1/1
2	A2G	3E	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	3E	2	2	-	2/6/23/26	0/1/1/1
3	A2G	4	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	4	2	3	-	1/6/23/26	0/1/1/1
3	MAN	4	3	3	-	0/2/19/22	0/1/1/1
3	WT8	4	4	3	-	3/20/36/40	0/1/1/1
3	A2G	4D	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	4D	2	3	-	2/6/23/26	0/1/1/1
3	MAN	4D	3	3	-	0/2/19/22	0/1/1/1
3	WT8	4D	4	3	-	3/20/36/40	0/1/1/1
2	A2G	5B	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	5B	2	2	-	2/6/23/26	0/1/1/1
3	A2G	6A	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	6A	2	3	-	1/6/23/26	0/1/1/1
3	MAN	6A	3	3	-	0/2/19/22	0/1/1/1
3	WT8	6A	4	3	-	3/20/36/40	0/1/1/1
3	A2G	6E	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	6E	2	3	-	1/6/23/26	0/1/1/1
3	MAN	6E	3	3	-	0/2/19/22	0/1/1/1
3	WT8	6E	4	3	-	3/20/36/40	0/1/1/1
2	A2G	7C	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	7C	2	2	-	2/6/23/26	0/1/1/1
3	A2G	8B	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	8B	2	3	-	2/6/23/26	0/1/1/1
3	MAN	8B	3	3	-	0/2/19/22	0/1/1/1
3	WT8	8B	4	3	-	3/20/36/40	0/1/1/1
2	A2G	9	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	9	2	2	-	2/6/23/26	0/1/1/1
2	A2G	9D	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	9D	2	2	-	2/6/23/26	0/1/1/1
3	A2G	AD	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	AD	2	3	-	2/6/23/26	0/1/1/1
3	MAN	AD	3	3	-	0/2/19/22	0/1/1/1
3	WT8	AD	4	3	-	3/20/36/40	0/1/1/1
2	A2G	BB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	BB	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	BF	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	BF	2	2	-	2/6/23/26	0/1/1/1
3	A2G	CA	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	CA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	CA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	CA	4	3	-	3/20/36/40	0/1/1/1
3	A2G	CE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	CE	2	3	-	2/6/23/26	0/1/1/1
3	MAN	CE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	CE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	DC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	DC	2	2	-	2/6/23/26	0/1/1/1
3	A2G	EB	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	EB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	EB	3	3	-	0/2/19/22	0/1/1/1
3	WT8	EB	4	3	-	3/20/36/40	0/1/1/1
3	A2G	EF	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	EF	2	3	-	2/6/23/26	0/1/1/1
3	MAN	EF	3	3	-	0/2/19/22	0/1/1/1
3	WT8	EF	4	3	-	3/20/36/40	0/1/1/1
2	A2G	FD	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	FD	2	2	-	2/6/23/26	0/1/1/1
3	A2G	GC	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	GC	2	3	-	1/6/23/26	0/1/1/1
3	MAN	GC	3	3	-	0/2/19/22	0/1/1/1
3	WT8	GC	4	3	-	3/20/36/40	0/1/1/1
2	A2G	HA	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	HA	2	2	-	2/6/23/26	0/1/1/1
2	A2G	HE	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	HE	2	2	-	2/6/23/26	0/1/1/1
3	A2G	ID	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	ID	2	3	-	1/6/23/26	0/1/1/1
3	MAN	ID	3	3	-	0/2/19/22	0/1/1/1
3	WT8	ID	4	3	-	3/20/36/40	0/1/1/1
2	A2G	JB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	JB	2	2	-	2/6/23/26	0/1/1/1
2	A2G	JF	1	1,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	JF	2	2	-	2/6/23/26	0/1/1/1
3	A2G	KA	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	KA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	KA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	KA	4	3	-	3/20/36/40	0/1/1/1
3	A2G	KE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	KE	2	3	-	1/6/23/26	0/1/1/1
3	MAN	KE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	KE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	LC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	LC	2	2	-	2/6/23/26	0/1/1/1
3	A2G	MB	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	MB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	MB	3	3	-	0/2/19/22	0/1/1/1
3	WT8	MB	4	3	-	3/20/36/40	0/1/1/1
3	A2G	MF	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	MF	2	3	-	2/6/23/26	0/1/1/1
3	MAN	MF	3	3	-	0/2/19/22	0/1/1/1
3	WT8	MF	4	3	-	3/20/36/40	0/1/1/1
2	A2G	ND	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	ND	2	2	-	2/6/23/26	0/1/1/1
3	A2G	OC	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	OC	2	3	-	2/6/23/26	0/1/1/1
3	MAN	OC	3	3	-	0/2/19/22	0/1/1/1
3	WT8	OC	4	3	-	3/20/36/40	0/1/1/1
2	A2G	PA	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	PA	2	2	-	2/6/23/26	0/1/1/1
2	A2G	PE	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	PE	2	2	-	2/6/23/26	0/1/1/1
3	A2G	QD	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	QD	2	3	-	1/6/23/26	0/1/1/1
3	MAN	QD	3	3	-	0/2/19/22	0/1/1/1
3	WT8	QD	4	3	-	3/20/36/40	0/1/1/1
2	A2G	RB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	RB	2	2	-	2/6/23/26	0/1/1/1
2	A2G	RF	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	RF	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	SA	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	SA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	SA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	SA	4	3	-	3/20/36/40	0/1/1/1
3	A2G	SE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	SE	2	3	-	2/6/23/26	0/1/1/1
3	MAN	SE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	SE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	TC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	TC	2	2	-	2/6/23/26	0/1/1/1
3	A2G	UB	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	UB	2	3	-	1/6/23/26	0/1/1/1
3	MAN	UB	3	3	-	0/2/19/22	0/1/1/1
3	WT8	UB	4	3	-	3/20/36/40	0/1/1/1
3	A2G	UF	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	UF	2	3	-	2/6/23/26	0/1/1/1
3	MAN	UF	3	3	-	0/2/19/22	0/1/1/1
3	WT8	UF	4	3	-	3/20/36/40	0/1/1/1
2	A2G	VD	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	VD	2	2	-	2/6/23/26	0/1/1/1
3	A2G	WC	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	WC	2	3	-	1/6/23/26	0/1/1/1
3	MAN	WC	3	3	-	0/2/19/22	0/1/1/1
3	WT8	WC	4	3	-	3/20/36/40	0/1/1/1
2	A2G	XA	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	XA	2	2	-	2/6/23/26	0/1/1/1
2	A2G	XE	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	XE	2	2	-	2/6/23/26	0/1/1/1
3	A2G	YD	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	YD	2	3	-	2/6/23/26	0/1/1/1
3	MAN	YD	3	3	-	0/2/19/22	0/1/1/1
3	WT8	YD	4	3	-	3/20/36/40	0/1/1/1
2	A2G	ZB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	ZB	2	2	-	2/6/23/26	0/1/1/1
2	A2G	ZF	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	ZF	2	2	-	2/6/23/26	0/1/1/1
3	A2G	aA	1	3,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	aA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	aA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	aA	4	3	-	3/20/36/40	0/1/1/1
3	A2G	aE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	aE	2	3	-	2/6/23/26	0/1/1/1
3	MAN	aE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	aE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	bC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	bC	2	2	-	2/6/23/26	0/1/1/1
3	A2G	cB	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	cB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	cB	3	3	-	0/2/19/22	0/1/1/1
3	WT8	cB	4	3	-	3/20/36/40	0/1/1/1
3	A2G	cF	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	cF	2	3	-	2/6/23/26	0/1/1/1
3	MAN	cF	3	3	-	0/2/19/22	0/1/1/1
3	WT8	cF	4	3	-	3/20/36/40	0/1/1/1
2	A2G	dD	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	dD	2	2	-	2/6/23/26	0/1/1/1
3	A2G	eC	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	eC	2	3	-	2/6/23/26	0/1/1/1
3	MAN	eC	3	3	-	0/2/19/22	0/1/1/1
3	WT8	eC	4	3	-	3/20/36/40	0/1/1/1
2	A2G	fA	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	fA	2	2	-	2/6/23/26	0/1/1/1
2	A2G	fE	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	fE	2	2	-	2/6/23/26	0/1/1/1
3	A2G	gD	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	gD	2	3	-	2/6/23/26	0/1/1/1
3	MAN	gD	3	3	-	0/2/19/22	0/1/1/1
3	WT8	gD	4	3	-	3/20/36/40	0/1/1/1
2	A2G	hB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	hB	2	2	-	2/6/23/26	0/1/1/1
3	A2G	iA	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	iA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	iA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	iA	4	3	-	3/20/36/40	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	iE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	iE	2	3	-	2/6/23/26	0/1/1/1
3	MAN	iE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	iE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	jC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	jC	2	2	-	2/6/23/26	0/1/1/1
3	A2G	kB	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	kB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	kB	3	3	-	0/2/19/22	0/1/1/1
3	WT8	kB	4	3	-	3/20/36/40	0/1/1/1
2	A2G	lD	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	lD	2	2	-	2/6/23/26	0/1/1/1
3	A2G	mC	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	mC	2	3	-	1/6/23/26	0/1/1/1
3	MAN	mC	3	3	-	0/2/19/22	0/1/1/1
3	WT8	mC	4	3	-	3/20/36/40	0/1/1/1
2	A2G	nA	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	nA	2	2	-	2/6/23/26	0/1/1/1
2	A2G	nE	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	nE	2	2	-	2/6/23/26	0/1/1/1
3	A2G	oD	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	oD	2	3	-	2/6/23/26	0/1/1/1
3	MAN	oD	3	3	-	0/2/19/22	0/1/1/1
3	WT8	oD	4	3	-	3/20/36/40	0/1/1/1
2	A2G	pB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	pB	2	2	-	2/6/23/26	0/1/1/1
3	A2G	qA	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	qA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	qA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	qA	4	3	-	3/20/36/40	0/1/1/1
3	A2G	qE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	qE	2	3	-	1/6/23/26	0/1/1/1
3	MAN	qE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	qE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	rC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	rC	2	2	-	2/6/23/26	0/1/1/1
3	A2G	sB	1	3,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	sB	2	3	-	2/6/23/26	0/1/1/1
3	MAN	sB	3	3	-	0/2/19/22	0/1/1/1
3	WT8	sB	4	3	-	3/20/36/40	0/1/1/1
2	A2G	t	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	t	2	2	-	2/6/23/26	0/1/1/1
2	A2G	tD	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	tD	2	2	-	2/6/23/26	0/1/1/1
3	A2G	uC	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	uC	2	3	-	2/6/23/26	0/1/1/1
3	MAN	uC	3	3	-	0/2/19/22	0/1/1/1
3	WT8	uC	4	3	-	3/20/36/40	0/1/1/1
2	A2G	vA	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	vA	2	2	-	2/6/23/26	0/1/1/1
2	A2G	vE	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	vE	2	2	-	2/6/23/26	0/1/1/1
3	A2G	w	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	w	2	3	-	2/6/23/26	0/1/1/1
3	MAN	w	3	3	-	0/2/19/22	0/1/1/1
3	WT8	w	4	3	-	3/20/36/40	0/1/1/1
3	A2G	wD	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	wD	2	3	-	2/6/23/26	0/1/1/1
3	MAN	wD	3	3	-	0/2/19/22	0/1/1/1
3	WT8	wD	4	3	-	3/20/36/40	0/1/1/1
2	A2G	xB	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	xB	2	2	-	2/6/23/26	0/1/1/1
3	A2G	yA	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	yA	2	3	-	2/6/23/26	0/1/1/1
3	MAN	yA	3	3	-	0/2/19/22	0/1/1/1
3	WT8	yA	4	3	-	3/20/36/40	0/1/1/1
3	A2G	yE	1	3,1	-	1/6/23/26	0/1/1/1
3	A2G	yE	2	3	-	2/6/23/26	0/1/1/1
3	MAN	yE	3	3	-	0/2/19/22	0/1/1/1
3	WT8	yE	4	3	-	3/20/36/40	0/1/1/1
2	A2G	zC	1	1,2	-	3/6/23/26	0/1/1/1
2	A2G	zC	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	cB	1	A2G	O3-C3-C2	4.06	117.87	109.47
3	qA	1	A2G	O3-C3-C2	4.06	117.87	109.47
3	UB	1	A2G	O3-C3-C2	4.06	117.87	109.47
3	kB	1	A2G	O3-C3-C2	4.06	117.86	109.47
3	CA	1	A2G	O3-C3-C2	4.06	117.86	109.47
3	8B	1	A2G	O3-C3-C2	4.06	117.86	109.47
3	GC	1	A2G	O3-C3-C2	4.06	117.86	109.47
3	6A	1	A2G	O3-C3-C2	4.06	117.86	109.47
3	YD	1	A2G	O3-C3-C2	4.06	117.86	109.47
3	CE	1	A2G	O3-C3-C2	4.05	117.86	109.47
3	yA	1	A2G	O3-C3-C2	4.05	117.85	109.47
3	6E	1	A2G	O3-C3-C2	4.05	117.85	109.47
3	iE	1	A2G	O3-C3-C2	4.05	117.85	109.47
3	wD	1	A2G	O3-C3-C2	4.05	117.85	109.47
3	SE	1	A2G	O3-C3-C2	4.05	117.85	109.47
3	WC	1	A2G	O3-C3-C2	4.05	117.85	109.47
3	mC	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	yE	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	aA	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	KE	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	iA	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	4D	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	SA	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	4	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	QD	1	A2G	O3-C3-C2	4.05	117.84	109.47
3	oD	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	eC	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	UF	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	MB	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	2C	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	aE	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	qE	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	w	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	sB	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	0B	1	A2G	O3-C3-C2	4.04	117.83	109.47
3	cF	1	A2G	O3-C3-C2	4.04	117.82	109.47
3	KA	1	A2G	O3-C3-C2	4.04	117.82	109.47
3	EF	1	A2G	O3-C3-C2	4.04	117.82	109.47
3	MF	1	A2G	O3-C3-C2	4.04	117.82	109.47
3	ID	1	A2G	O3-C3-C2	4.03	117.81	109.47
3	gD	1	A2G	O3-C3-C2	4.03	117.81	109.47
3	uC	1	A2G	O3-C3-C2	4.03	117.81	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	OC	1	A2G	O3-C3-C2	4.03	117.81	109.47
3	AD	1	A2G	O3-C3-C2	4.03	117.80	109.47
3	EB	1	A2G	O3-C3-C2	4.03	117.80	109.47
2	dD	2	A2G	O4-C4-C5	3.52	118.05	109.30
2	xB	2	A2G	O4-C4-C5	3.52	118.04	109.30
2	TC	2	A2G	O4-C4-C5	3.52	118.04	109.30
2	fA	2	A2G	O4-C4-C5	3.51	118.03	109.30
2	pB	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	JB	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	XA	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	3A	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	LC	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	9D	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	PE	2	A2G	O4-C4-C5	3.51	118.02	109.30
2	PA	2	A2G	O4-C4-C5	3.51	118.01	109.30
2	7C	2	A2G	O4-C4-C5	3.51	118.01	109.30
2	HE	2	A2G	O4-C4-C5	3.51	118.01	109.30
2	vE	2	A2G	O4-C4-C5	3.51	118.01	109.30
2	zC	2	A2G	O4-C4-C5	3.51	118.01	109.30
2	nA	2	A2G	O4-C4-C5	3.51	118.01	109.30
2	1D	2	A2G	O4-C4-C5	3.51	118.00	109.30
2	HA	2	A2G	O4-C4-C5	3.50	118.00	109.30
2	t	2	A2G	O4-C4-C5	3.50	118.00	109.30
2	lD	2	A2G	O4-C4-C5	3.50	118.00	109.30
2	rC	2	A2G	O4-C4-C5	3.50	117.99	109.30
2	tD	2	A2G	O4-C4-C5	3.50	117.99	109.30
2	1	2	A2G	O4-C4-C5	3.50	117.99	109.30
2	bC	2	A2G	O4-C4-C5	3.50	117.99	109.30
2	BF	2	A2G	O4-C4-C5	3.50	117.99	109.30
2	ZF	2	A2G	O4-C4-C5	3.50	117.99	109.30
2	ND	2	A2G	O4-C4-C5	3.50	117.98	109.30
2	5B	2	A2G	O4-C4-C5	3.50	117.98	109.30
2	hB	2	A2G	O4-C4-C5	3.50	117.98	109.30
2	fE	2	A2G	O4-C4-C5	3.50	117.98	109.30
2	FD	2	A2G	O4-C4-C5	3.50	117.98	109.30
2	nE	2	A2G	O4-C4-C5	3.50	117.98	109.30
2	VD	2	A2G	O4-C4-C5	3.49	117.97	109.30
2	BB	2	A2G	O4-C4-C5	3.49	117.97	109.30
2	vA	2	A2G	O4-C4-C5	3.49	117.97	109.30
2	RB	2	A2G	O4-C4-C5	3.49	117.97	109.30
2	JF	2	A2G	O4-C4-C5	3.49	117.97	109.30
2	jC	2	A2G	O4-C4-C5	3.49	117.96	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9	2	A2G	O4-C4-C5	3.49	117.96	109.30
2	ZB	2	A2G	O4-C4-C5	3.49	117.96	109.30
2	XE	2	A2G	O4-C4-C5	3.49	117.96	109.30
2	RF	2	A2G	O4-C4-C5	3.49	117.95	109.30
2	DC	2	A2G	O4-C4-C5	3.49	117.95	109.30
2	3E	2	A2G	O4-C4-C5	3.48	117.94	109.30
3	mC	2	A2G	C4-C3-C2	3.23	115.75	111.02
3	wD	2	A2G	C4-C3-C2	3.23	115.75	111.02
3	UB	2	A2G	C4-C3-C2	3.22	115.73	111.02
3	EB	2	A2G	C4-C3-C2	3.21	115.73	111.02
3	SA	2	A2G	C4-C3-C2	3.21	115.73	111.02
3	yE	2	A2G	C4-C3-C2	3.21	115.72	111.02
3	ID	2	A2G	C4-C3-C2	3.21	115.72	111.02
3	6E	2	A2G	C4-C3-C2	3.21	115.72	111.02
3	UF	2	A2G	C4-C3-C2	3.20	115.72	111.02
3	aE	2	A2G	C4-C3-C2	3.20	115.71	111.02
3	CA	2	A2G	C4-C3-C2	3.20	115.71	111.02
3	0B	2	A2G	C4-C3-C2	3.20	115.70	111.02
3	4	2	A2G	C4-C3-C2	3.20	115.70	111.02
3	8B	2	A2G	C4-C3-C2	3.20	115.70	111.02
3	EF	2	A2G	C4-C3-C2	3.20	115.70	111.02
3	YD	2	A2G	C4-C3-C2	3.19	115.70	111.02
3	KE	2	A2G	C4-C3-C2	3.19	115.70	111.02
3	KA	2	A2G	C4-C3-C2	3.19	115.70	111.02
3	yA	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	2C	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	w	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	cB	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	kB	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	CE	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	SE	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	uC	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	aA	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	qA	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	cF	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	OC	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	MF	2	A2G	C4-C3-C2	3.19	115.69	111.02
3	MB	2	A2G	C4-C3-C2	3.18	115.69	111.02
3	AD	2	A2G	C4-C3-C2	3.18	115.69	111.02
3	iA	2	A2G	C4-C3-C2	3.18	115.68	111.02
3	WC	2	A2G	C4-C3-C2	3.18	115.68	111.02
3	qE	2	A2G	C4-C3-C2	3.18	115.68	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	gD	2	A2G	C4-C3-C2	3.18	115.68	111.02
3	iE	2	A2G	C4-C3-C2	3.18	115.68	111.02
3	QD	2	A2G	C4-C3-C2	3.17	115.67	111.02
3	eC	2	A2G	C4-C3-C2	3.17	115.67	111.02
3	sB	2	A2G	C4-C3-C2	3.17	115.67	111.02
3	4D	2	A2G	C4-C3-C2	3.17	115.66	111.02
3	oD	2	A2G	C4-C3-C2	3.16	115.65	111.02
3	6A	2	A2G	C4-C3-C2	3.16	115.65	111.02
3	GC	2	A2G	C4-C3-C2	3.16	115.64	111.02
3	GC	1	A2G	O5-C1-C2	-2.86	106.78	111.29
3	sB	1	A2G	O5-C1-C2	-2.85	106.78	111.29
3	wD	1	A2G	O5-C1-C2	-2.85	106.79	111.29
3	SA	1	A2G	O5-C1-C2	-2.84	106.80	111.29
3	CA	1	A2G	O5-C1-C2	-2.84	106.80	111.29
3	eC	1	A2G	O5-C1-C2	-2.84	106.80	111.29
3	KE	1	A2G	O5-C1-C2	-2.84	106.81	111.29
3	CE	1	A2G	O5-C1-C2	-2.84	106.81	111.29
3	EB	1	A2G	O5-C1-C2	-2.84	106.81	111.29
3	yA	1	A2G	O5-C1-C2	-2.84	106.81	111.29
3	kB	1	A2G	O5-C1-C2	-2.84	106.81	111.29
3	0B	1	A2G	O5-C1-C2	-2.83	106.81	111.29
3	qE	1	A2G	O5-C1-C2	-2.83	106.81	111.29
3	aE	1	A2G	O5-C1-C2	-2.83	106.81	111.29
3	gD	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	WC	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	qA	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	6E	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	8B	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	SE	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	yE	1	A2G	O5-C1-C2	-2.83	106.82	111.29
3	6A	1	A2G	O5-C1-C2	-2.83	106.83	111.29
3	mC	1	A2G	O5-C1-C2	-2.83	106.83	111.29
3	EF	1	A2G	O5-C1-C2	-2.83	106.83	111.29
3	w	1	A2G	O5-C1-C2	-2.82	106.83	111.29
3	uC	1	A2G	O5-C1-C2	-2.82	106.83	111.29
3	cB	1	A2G	O5-C1-C2	-2.82	106.83	111.29
3	cF	1	A2G	O5-C1-C2	-2.82	106.83	111.29
3	iE	1	A2G	O5-C1-C2	-2.82	106.83	111.29
3	2C	1	A2G	O5-C1-C2	-2.82	106.84	111.29
3	UF	1	A2G	O5-C1-C2	-2.82	106.84	111.29
3	aA	1	A2G	O5-C1-C2	-2.82	106.84	111.29
3	YD	1	A2G	O5-C1-C2	-2.82	106.84	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4	1	A2G	O5-C1-C2	-2.82	106.84	111.29
3	QD	1	A2G	O5-C1-C2	-2.82	106.84	111.29
3	OC	1	A2G	O5-C1-C2	-2.81	106.84	111.29
3	ID	1	A2G	O5-C1-C2	-2.81	106.85	111.29
3	iA	1	A2G	O5-C1-C2	-2.81	106.85	111.29
3	4D	1	A2G	O5-C1-C2	-2.81	106.85	111.29
3	MF	1	A2G	O5-C1-C2	-2.80	106.86	111.29
3	KA	1	A2G	O5-C1-C2	-2.80	106.86	111.29
3	oD	1	A2G	O5-C1-C2	-2.80	106.86	111.29
3	MB	1	A2G	O5-C1-C2	-2.80	106.87	111.29
3	UB	1	A2G	O5-C1-C2	-2.80	106.87	111.29
3	AD	1	A2G	O5-C1-C2	-2.80	106.87	111.29
3	8B	3	MAN	O2-C2-C3	-2.42	105.30	110.14
3	SE	3	MAN	O2-C2-C3	-2.42	105.30	110.14
3	uC	3	MAN	O2-C2-C3	-2.41	105.31	110.14
3	0B	3	MAN	O2-C2-C3	-2.41	105.31	110.14
3	iA	3	MAN	O2-C2-C3	-2.41	105.31	110.14
3	wD	3	MAN	O2-C2-C3	-2.41	105.32	110.14
3	EB	3	MAN	O2-C2-C3	-2.41	105.32	110.14
3	ID	3	MAN	O2-C2-C3	-2.41	105.32	110.14
3	kB	3	MAN	O2-C2-C3	-2.41	105.32	110.14
3	yA	3	MAN	O2-C2-C3	-2.40	105.32	110.14
3	eC	3	MAN	O2-C2-C3	-2.40	105.32	110.14
3	GC	3	MAN	O2-C2-C3	-2.40	105.32	110.14
3	4D	3	MAN	O2-C2-C3	-2.40	105.32	110.14
3	aA	3	MAN	O2-C2-C3	-2.40	105.32	110.14
3	2C	3	MAN	O2-C2-C3	-2.40	105.33	110.14
3	cB	3	MAN	O2-C2-C3	-2.40	105.33	110.14
3	qE	3	MAN	O2-C2-C3	-2.40	105.33	110.14
3	OC	3	MAN	O2-C2-C3	-2.40	105.33	110.14
3	YD	3	MAN	O2-C2-C3	-2.40	105.33	110.14
3	UB	3	MAN	O2-C2-C3	-2.40	105.33	110.14
3	4	3	MAN	O2-C2-C3	-2.40	105.34	110.14
3	CA	3	MAN	O2-C2-C3	-2.40	105.34	110.14
3	oD	3	MAN	O2-C2-C3	-2.40	105.34	110.14
2	1	2	A2G	C6-C5-C4	2.40	118.62	113.00
3	6A	3	MAN	O2-C2-C3	-2.40	105.34	110.14
3	EF	3	MAN	O2-C2-C3	-2.40	105.34	110.14
3	MB	3	MAN	O2-C2-C3	-2.39	105.34	110.14
3	w	3	MAN	O2-C2-C3	-2.39	105.34	110.14
3	AD	3	MAN	O2-C2-C3	-2.39	105.34	110.14
3	MF	3	MAN	O2-C2-C3	-2.39	105.34	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	pB	2	A2G	C6-C5-C4	2.39	118.61	113.00
2	1D	2	A2G	C6-C5-C4	2.39	118.60	113.00
2	ND	2	A2G	C6-C5-C4	2.39	118.60	113.00
2	3A	2	A2G	C6-C5-C4	2.39	118.60	113.00
3	KA	3	MAN	O2-C2-C3	-2.39	105.36	110.14
3	QD	3	MAN	O2-C2-C3	-2.39	105.36	110.14
3	CE	3	MAN	O2-C2-C3	-2.39	105.36	110.14
2	5B	2	A2G	C6-C5-C4	2.39	118.59	113.00
2	FD	2	A2G	C6-C5-C4	2.39	118.59	113.00
2	RF	2	A2G	C6-C5-C4	2.39	118.59	113.00
2	nE	2	A2G	C6-C5-C4	2.38	118.59	113.00
3	mC	3	MAN	O2-C2-C3	-2.38	105.36	110.14
3	KE	3	MAN	O2-C2-C3	-2.38	105.36	110.14
2	HA	2	A2G	C6-C5-C4	2.38	118.59	113.00
3	6E	3	MAN	O2-C2-C3	-2.38	105.36	110.14
3	aE	3	MAN	O2-C2-C3	-2.38	105.36	110.14
3	UF	3	MAN	O2-C2-C3	-2.38	105.37	110.14
3	iE	3	MAN	O2-C2-C3	-2.38	105.37	110.14
2	TC	2	A2G	C6-C5-C4	2.38	118.58	113.00
2	tD	2	A2G	C6-C5-C4	2.38	118.58	113.00
3	qA	3	MAN	O2-C2-C3	-2.38	105.37	110.14
2	BF	2	A2G	C6-C5-C4	2.38	118.58	113.00
2	9	2	A2G	C6-C5-C4	2.38	118.58	113.00
2	rC	2	A2G	C6-C5-C4	2.38	118.58	113.00
2	9D	2	A2G	C6-C5-C4	2.38	118.58	113.00
3	yE	3	MAN	O2-C2-C3	-2.38	105.37	110.14
2	dD	2	A2G	C6-C5-C4	2.38	118.58	113.00
3	SA	3	MAN	O2-C2-C3	-2.38	105.37	110.14
2	PA	2	A2G	C6-C5-C4	2.38	118.57	113.00
2	fE	2	A2G	C6-C5-C4	2.38	118.57	113.00
2	nA	2	A2G	C6-C5-C4	2.38	118.57	113.00
2	vE	2	A2G	C6-C5-C4	2.38	118.57	113.00
2	t	2	A2G	C6-C5-C4	2.38	118.57	113.00
3	WC	3	MAN	O2-C2-C3	-2.38	105.38	110.14
3	sB	3	MAN	O2-C2-C3	-2.38	105.38	110.14
2	XA	2	A2G	C6-C5-C4	2.38	118.57	113.00
2	ZB	2	A2G	C6-C5-C4	2.38	118.57	113.00
2	zC	2	A2G	C6-C5-C4	2.37	118.57	113.00
2	HE	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	3E	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	jC	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	RB	2	A2G	C6-C5-C4	2.37	118.56	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DC	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	LC	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	BB	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	7C	2	A2G	C6-C5-C4	2.37	118.56	113.00
2	bC	2	A2G	C6-C5-C4	2.37	118.56	113.00
3	gD	3	MAN	C1-O5-C5	2.37	115.40	112.19
2	ZF	2	A2G	C6-C5-C4	2.37	118.55	113.00
2	hB	2	A2G	C6-C5-C4	2.37	118.55	113.00
2	vA	2	A2G	C6-C5-C4	2.37	118.55	113.00
2	xB	2	A2G	C6-C5-C4	2.37	118.55	113.00
3	cF	3	MAN	O2-C2-C3	-2.37	105.40	110.14
2	fA	2	A2G	C6-C5-C4	2.37	118.55	113.00
2	XE	2	A2G	C6-C5-C4	2.37	118.54	113.00
3	KA	3	MAN	C1-O5-C5	2.36	115.40	112.19
3	sB	3	MAN	C1-O5-C5	2.36	115.39	112.19
3	EF	3	MAN	C1-O5-C5	2.36	115.39	112.19
3	2C	3	MAN	C1-O5-C5	2.36	115.39	112.19
2	JF	2	A2G	C6-C5-C4	2.36	118.53	113.00
2	lD	2	A2G	C6-C5-C4	2.36	118.53	113.00
3	gD	3	MAN	O2-C2-C3	-2.36	105.41	110.14
2	JB	2	A2G	C6-C5-C4	2.36	118.53	113.00
2	PE	2	A2G	C6-C5-C4	2.36	118.53	113.00
3	8B	3	MAN	C1-O5-C5	2.36	115.39	112.19
2	VD	2	A2G	C6-C5-C4	2.36	118.52	113.00
3	UF	3	MAN	C1-O5-C5	2.36	115.38	112.19
3	MB	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	OC	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	UB	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	cB	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	AD	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	CE	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	kB	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	qA	3	MAN	C1-O5-C5	2.35	115.38	112.19
3	0B	3	MAN	C1-O5-C5	2.35	115.37	112.19
3	uC	3	MAN	C1-O5-C5	2.35	115.37	112.19
3	iE	3	MAN	C1-O5-C5	2.35	115.37	112.19
3	w	3	MAN	C1-O5-C5	2.34	115.37	112.19
3	WC	3	MAN	C1-O5-C5	2.34	115.37	112.19
3	MF	3	MAN	C1-O5-C5	2.34	115.37	112.19
3	wD	3	MAN	C1-O5-C5	2.34	115.36	112.19
3	aE	3	MAN	C1-O5-C5	2.34	115.36	112.19
3	ID	3	MAN	C1-O5-C5	2.34	115.36	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SE	3	MAN	C1-O5-C5	2.34	115.36	112.19
3	6E	3	MAN	C1-O5-C5	2.33	115.36	112.19
3	mC	3	MAN	C1-O5-C5	2.33	115.35	112.19
3	oD	3	MAN	C1-O5-C5	2.33	115.35	112.19
3	eC	3	MAN	C1-O5-C5	2.33	115.35	112.19
3	aA	3	MAN	C1-O5-C5	2.33	115.35	112.19
2	vE	1	A2G	C4-C3-C2	2.33	114.43	111.02
2	LC	1	A2G	C4-C3-C2	2.33	114.43	111.02
3	SA	3	MAN	C1-O5-C5	2.33	115.35	112.19
3	EB	3	MAN	C1-O5-C5	2.33	115.35	112.19
2	HE	1	A2G	C4-C3-C2	2.33	114.43	111.02
3	iA	3	MAN	C1-O5-C5	2.33	115.34	112.19
3	6A	3	MAN	C1-O5-C5	2.33	115.34	112.19
2	BB	1	A2G	C4-C3-C2	2.33	114.43	111.02
2	ND	1	A2G	C4-C3-C2	2.33	114.43	111.02
3	4	3	MAN	C1-O5-C5	2.32	115.34	112.19
3	QD	3	MAN	C1-O5-C5	2.32	115.34	112.19
3	GC	3	MAN	C1-O5-C5	2.32	115.34	112.19
3	4D	3	MAN	C1-O5-C5	2.32	115.34	112.19
3	cF	3	MAN	C1-O5-C5	2.32	115.34	112.19
3	YD	3	MAN	C1-O5-C5	2.32	115.34	112.19
3	yE	3	MAN	C1-O5-C5	2.32	115.33	112.19
2	9	1	A2G	C4-C3-C2	2.32	114.41	111.02
3	CA	3	MAN	C1-O5-C5	2.32	115.33	112.19
2	9D	1	A2G	C4-C3-C2	2.32	114.41	111.02
2	RB	1	A2G	C4-C3-C2	2.31	114.41	111.02
2	3E	1	A2G	C4-C3-C2	2.31	114.41	111.02
3	yA	3	MAN	C1-O5-C5	2.31	115.33	112.19
3	qE	3	MAN	C1-O5-C5	2.31	115.33	112.19
2	3A	1	A2G	C4-C3-C2	2.31	114.41	111.02
2	XE	1	A2G	C4-C3-C2	2.31	114.40	111.02
2	ZF	1	A2G	C4-C3-C2	2.31	114.40	111.02
2	XA	1	A2G	C4-C3-C2	2.31	114.40	111.02
3	KE	3	MAN	C1-O5-C5	2.31	115.32	112.19
2	ZB	1	A2G	C4-C3-C2	2.31	114.40	111.02
2	TC	1	A2G	C4-C3-C2	2.31	114.40	111.02
2	PE	1	A2G	C4-C3-C2	2.31	114.40	111.02
2	VD	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	tD	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	FD	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	vA	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	fE	1	A2G	C4-C3-C2	2.30	114.39	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	jC	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	5B	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	t	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	7C	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	bC	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	rC	1	A2G	C4-C3-C2	2.30	114.39	111.02
2	PA	1	A2G	C4-C3-C2	2.29	114.38	111.02
2	pB	1	A2G	C4-C3-C2	2.29	114.38	111.02
2	RF	1	A2G	C4-C3-C2	2.29	114.38	111.02
2	nA	1	A2G	C4-C3-C2	2.29	114.38	111.02
2	DC	1	A2G	C4-C3-C2	2.29	114.38	111.02
2	nE	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	BF	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	1	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	HA	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	lD	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	dD	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	zC	1	A2G	C4-C3-C2	2.29	114.37	111.02
2	hB	1	A2G	C4-C3-C2	2.28	114.36	111.02
2	fA	1	A2G	C4-C3-C2	2.28	114.36	111.02
2	xB	1	A2G	C4-C3-C2	2.28	114.36	111.02
2	1D	1	A2G	C4-C3-C2	2.27	114.35	111.02
2	JF	1	A2G	C4-C3-C2	2.27	114.34	111.02
2	JB	1	A2G	C4-C3-C2	2.26	114.33	111.02
3	cF	2	A2G	O5-C5-C4	-2.09	105.75	110.83
3	2C	2	A2G	O5-C5-C4	-2.07	105.78	110.83
3	qE	2	A2G	O5-C5-C4	-2.07	105.79	110.83
3	MF	2	A2G	O5-C5-C4	-2.07	105.79	110.83
3	qA	2	A2G	O5-C5-C4	-2.07	105.79	110.83
3	UB	2	A2G	O5-C5-C4	-2.07	105.80	110.83
3	4D	2	A2G	O5-C5-C4	-2.07	105.80	110.83
3	aE	2	A2G	O5-C5-C4	-2.07	105.80	110.83
3	CA	2	A2G	O5-C5-C4	-2.07	105.80	110.83
3	ID	2	A2G	O5-C5-C4	-2.07	105.80	110.83
3	cB	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	oD	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	0B	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	GC	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	uC	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	sB	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	yE	2	A2G	O5-C5-C4	-2.06	105.81	110.83
3	MB	2	A2G	O5-C5-C4	-2.06	105.82	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	QD	2	A2G	O5-C5-C4	-2.06	105.82	110.83
3	8B	2	A2G	O5-C5-C4	-2.06	105.82	110.83
3	6E	2	A2G	O5-C5-C4	-2.06	105.82	110.83
3	4	2	A2G	O5-C5-C4	-2.06	105.82	110.83
3	aA	2	A2G	O5-C5-C4	-2.06	105.83	110.83
3	iE	2	A2G	O5-C5-C4	-2.06	105.83	110.83
3	SA	2	A2G	O5-C5-C4	-2.06	105.83	110.83
3	w	2	A2G	O5-C5-C4	-2.06	105.83	110.83
3	gD	2	A2G	O5-C5-C4	-2.05	105.83	110.83
3	CE	2	A2G	O5-C5-C4	-2.05	105.83	110.83
3	mC	2	A2G	O5-C5-C4	-2.05	105.83	110.83
3	KA	2	A2G	O5-C5-C4	-2.05	105.83	110.83
3	wD	2	A2G	O5-C5-C4	-2.05	105.83	110.83
3	SE	2	A2G	O5-C5-C4	-2.05	105.83	110.83
3	YD	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	OC	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	EB	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	iA	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	yA	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	6A	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	EF	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	UF	2	A2G	O5-C5-C4	-2.05	105.84	110.83
3	WC	2	A2G	O5-C5-C4	-2.05	105.85	110.83
3	eC	2	A2G	O5-C5-C4	-2.05	105.85	110.83
3	AD	2	A2G	O5-C5-C4	-2.04	105.86	110.83
3	kB	2	A2G	O5-C5-C4	-2.04	105.88	110.83
3	KE	2	A2G	O5-C5-C4	-2.03	105.88	110.83

There are no chirality outliers.

All (483) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	t	1	A2G	C3-C2-N2-C7
2	t	1	A2G	O7-C7-N2-C2
2	t	1	A2G	C8-C7-N2-C2
2	1	1	A2G	C3-C2-N2-C7
2	1	1	A2G	O7-C7-N2-C2
2	1	1	A2G	C8-C7-N2-C2
2	9	1	A2G	C3-C2-N2-C7
2	9	1	A2G	O7-C7-N2-C2
2	9	1	A2G	C8-C7-N2-C2
2	HA	1	A2G	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	HA	1	A2G	O7-C7-N2-C2
2	HA	1	A2G	C8-C7-N2-C2
2	PA	1	A2G	C3-C2-N2-C7
2	PA	1	A2G	O7-C7-N2-C2
2	PA	1	A2G	C8-C7-N2-C2
2	XA	1	A2G	C3-C2-N2-C7
2	XA	1	A2G	O7-C7-N2-C2
2	XA	1	A2G	C8-C7-N2-C2
2	fA	1	A2G	C3-C2-N2-C7
2	fA	1	A2G	O7-C7-N2-C2
2	fA	1	A2G	C8-C7-N2-C2
2	nA	1	A2G	C3-C2-N2-C7
2	nA	1	A2G	O7-C7-N2-C2
2	nA	1	A2G	C8-C7-N2-C2
2	vA	1	A2G	C3-C2-N2-C7
2	vA	1	A2G	O7-C7-N2-C2
2	vA	1	A2G	C8-C7-N2-C2
2	3A	1	A2G	C3-C2-N2-C7
2	3A	1	A2G	O7-C7-N2-C2
2	3A	1	A2G	C8-C7-N2-C2
2	BB	1	A2G	C3-C2-N2-C7
2	BB	1	A2G	O7-C7-N2-C2
2	BB	1	A2G	C8-C7-N2-C2
2	JB	1	A2G	C3-C2-N2-C7
2	JB	1	A2G	O7-C7-N2-C2
2	JB	1	A2G	C8-C7-N2-C2
2	RB	1	A2G	C3-C2-N2-C7
2	RB	1	A2G	O7-C7-N2-C2
2	RB	1	A2G	C8-C7-N2-C2
2	ZB	1	A2G	C3-C2-N2-C7
2	ZB	1	A2G	O7-C7-N2-C2
2	ZB	1	A2G	C8-C7-N2-C2
2	hB	1	A2G	C3-C2-N2-C7
2	hB	1	A2G	O7-C7-N2-C2
2	hB	1	A2G	C8-C7-N2-C2
2	pB	1	A2G	C3-C2-N2-C7
2	pB	1	A2G	O7-C7-N2-C2
2	pB	1	A2G	C8-C7-N2-C2
2	xB	1	A2G	C3-C2-N2-C7
2	xB	1	A2G	O7-C7-N2-C2
2	xB	1	A2G	C8-C7-N2-C2
2	5B	1	A2G	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	5B	1	A2G	O7-C7-N2-C2
2	5B	1	A2G	C8-C7-N2-C2
2	DC	1	A2G	C3-C2-N2-C7
2	DC	1	A2G	O7-C7-N2-C2
2	DC	1	A2G	C8-C7-N2-C2
2	LC	1	A2G	C3-C2-N2-C7
2	LC	1	A2G	O7-C7-N2-C2
2	LC	1	A2G	C8-C7-N2-C2
2	TC	1	A2G	C3-C2-N2-C7
2	TC	1	A2G	O7-C7-N2-C2
2	TC	1	A2G	C8-C7-N2-C2
2	bC	1	A2G	C3-C2-N2-C7
2	bC	1	A2G	O7-C7-N2-C2
2	bC	1	A2G	C8-C7-N2-C2
2	jC	1	A2G	C3-C2-N2-C7
2	jC	1	A2G	O7-C7-N2-C2
2	jC	1	A2G	C8-C7-N2-C2
2	rC	1	A2G	C3-C2-N2-C7
2	rC	1	A2G	O7-C7-N2-C2
2	rC	1	A2G	C8-C7-N2-C2
2	zC	1	A2G	C3-C2-N2-C7
2	zC	1	A2G	O7-C7-N2-C2
2	zC	1	A2G	C8-C7-N2-C2
2	7C	1	A2G	C3-C2-N2-C7
2	7C	1	A2G	O7-C7-N2-C2
2	7C	1	A2G	C8-C7-N2-C2
2	FD	1	A2G	C3-C2-N2-C7
2	FD	1	A2G	O7-C7-N2-C2
2	FD	1	A2G	C8-C7-N2-C2
2	ND	1	A2G	C3-C2-N2-C7
2	ND	1	A2G	O7-C7-N2-C2
2	ND	1	A2G	C8-C7-N2-C2
2	VD	1	A2G	C3-C2-N2-C7
2	VD	1	A2G	O7-C7-N2-C2
2	VD	1	A2G	C8-C7-N2-C2
2	dD	1	A2G	C3-C2-N2-C7
2	dD	1	A2G	O7-C7-N2-C2
2	dD	1	A2G	C8-C7-N2-C2
2	lD	1	A2G	C3-C2-N2-C7
2	lD	1	A2G	O7-C7-N2-C2
2	lD	1	A2G	C8-C7-N2-C2
2	tD	1	A2G	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	tD	1	A2G	O7-C7-N2-C2
2	tD	1	A2G	C8-C7-N2-C2
2	1D	1	A2G	C3-C2-N2-C7
2	1D	1	A2G	O7-C7-N2-C2
2	1D	1	A2G	C8-C7-N2-C2
2	9D	1	A2G	C3-C2-N2-C7
2	9D	1	A2G	O7-C7-N2-C2
2	9D	1	A2G	C8-C7-N2-C2
2	HE	1	A2G	C3-C2-N2-C7
2	HE	1	A2G	O7-C7-N2-C2
2	HE	1	A2G	C8-C7-N2-C2
2	PE	1	A2G	C3-C2-N2-C7
2	PE	1	A2G	O7-C7-N2-C2
2	PE	1	A2G	C8-C7-N2-C2
2	XE	1	A2G	C3-C2-N2-C7
2	XE	1	A2G	O7-C7-N2-C2
2	XE	1	A2G	C8-C7-N2-C2
2	fE	1	A2G	C3-C2-N2-C7
2	fE	1	A2G	O7-C7-N2-C2
2	fE	1	A2G	C8-C7-N2-C2
2	nE	1	A2G	C3-C2-N2-C7
2	nE	1	A2G	O7-C7-N2-C2
2	nE	1	A2G	C8-C7-N2-C2
2	vE	1	A2G	C3-C2-N2-C7
2	vE	1	A2G	O7-C7-N2-C2
2	vE	1	A2G	C8-C7-N2-C2
2	3E	1	A2G	C3-C2-N2-C7
2	3E	1	A2G	O7-C7-N2-C2
2	3E	1	A2G	C8-C7-N2-C2
2	BF	1	A2G	C3-C2-N2-C7
2	BF	1	A2G	O7-C7-N2-C2
2	BF	1	A2G	C8-C7-N2-C2
2	JF	1	A2G	C3-C2-N2-C7
2	JF	1	A2G	O7-C7-N2-C2
2	JF	1	A2G	C8-C7-N2-C2
2	RF	1	A2G	C3-C2-N2-C7
2	RF	1	A2G	O7-C7-N2-C2
2	RF	1	A2G	C8-C7-N2-C2
2	ZF	1	A2G	C3-C2-N2-C7
2	ZF	1	A2G	O7-C7-N2-C2
2	ZF	1	A2G	C8-C7-N2-C2
3	w	1	A2G	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	4	1	A2G	O5-C5-C6-O6
3	CA	1	A2G	O5-C5-C6-O6
3	KA	1	A2G	O5-C5-C6-O6
3	SA	1	A2G	O5-C5-C6-O6
3	aA	1	A2G	O5-C5-C6-O6
3	iA	1	A2G	O5-C5-C6-O6
3	qA	1	A2G	O5-C5-C6-O6
3	yA	1	A2G	O5-C5-C6-O6
3	6A	1	A2G	O5-C5-C6-O6
3	EB	1	A2G	O5-C5-C6-O6
3	MB	1	A2G	O5-C5-C6-O6
3	UB	1	A2G	O5-C5-C6-O6
3	cB	1	A2G	O5-C5-C6-O6
3	kB	1	A2G	O5-C5-C6-O6
3	sB	1	A2G	O5-C5-C6-O6
3	0B	1	A2G	O5-C5-C6-O6
3	8B	1	A2G	O5-C5-C6-O6
3	GC	1	A2G	O5-C5-C6-O6
3	OC	1	A2G	O5-C5-C6-O6
3	WC	1	A2G	O5-C5-C6-O6
3	eC	1	A2G	O5-C5-C6-O6
3	mC	1	A2G	O5-C5-C6-O6
3	uC	1	A2G	O5-C5-C6-O6
3	2C	1	A2G	O5-C5-C6-O6
3	AD	1	A2G	O5-C5-C6-O6
3	ID	1	A2G	O5-C5-C6-O6
3	QD	1	A2G	O5-C5-C6-O6
3	YD	1	A2G	O5-C5-C6-O6
3	gD	1	A2G	O5-C5-C6-O6
3	oD	1	A2G	O5-C5-C6-O6
3	wD	1	A2G	O5-C5-C6-O6
3	4D	1	A2G	O5-C5-C6-O6
3	CE	1	A2G	O5-C5-C6-O6
3	KE	1	A2G	O5-C5-C6-O6
3	SE	1	A2G	O5-C5-C6-O6
3	aE	1	A2G	O5-C5-C6-O6
3	iE	1	A2G	O5-C5-C6-O6
3	qE	1	A2G	O5-C5-C6-O6
3	yE	1	A2G	O5-C5-C6-O6
3	6E	1	A2G	O5-C5-C6-O6
3	EF	1	A2G	O5-C5-C6-O6
3	MF	1	A2G	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	UF	1	A2G	O5-C5-C6-O6
3	cF	1	A2G	O5-C5-C6-O6
3	w	4	WT8	O5-C1-C10-O11
3	4	4	WT8	O5-C1-C10-O11
3	CA	4	WT8	O5-C1-C10-O11
3	KA	4	WT8	O5-C1-C10-O11
3	SA	4	WT8	O5-C1-C10-O11
3	aA	4	WT8	O5-C1-C10-O11
3	iA	4	WT8	O5-C1-C10-O11
3	qA	4	WT8	O5-C1-C10-O11
3	yA	4	WT8	O5-C1-C10-O11
3	6A	4	WT8	O5-C1-C10-O11
3	EB	4	WT8	O5-C1-C10-O11
3	MB	4	WT8	O5-C1-C10-O11
3	UB	4	WT8	O5-C1-C10-O11
3	cB	4	WT8	O5-C1-C10-O11
3	kB	4	WT8	O5-C1-C10-O11
3	sB	4	WT8	O5-C1-C10-O11
3	0B	4	WT8	O5-C1-C10-O11
3	8B	4	WT8	O5-C1-C10-O11
3	GC	4	WT8	O5-C1-C10-O11
3	OC	4	WT8	O5-C1-C10-O11
3	WC	4	WT8	O5-C1-C10-O11
3	eC	4	WT8	O5-C1-C10-O11
3	mC	4	WT8	O5-C1-C10-O11
3	uC	4	WT8	O5-C1-C10-O11
3	2C	4	WT8	O5-C1-C10-O11
3	AD	4	WT8	O5-C1-C10-O11
3	ID	4	WT8	O5-C1-C10-O11
3	QD	4	WT8	O5-C1-C10-O11
3	YD	4	WT8	O5-C1-C10-O11
3	gD	4	WT8	O5-C1-C10-O11
3	oD	4	WT8	O5-C1-C10-O11
3	wD	4	WT8	O5-C1-C10-O11
3	4D	4	WT8	O5-C1-C10-O11
3	CE	4	WT8	O5-C1-C10-O11
3	KE	4	WT8	O5-C1-C10-O11
3	SE	4	WT8	O5-C1-C10-O11
3	aE	4	WT8	O5-C1-C10-O11
3	iE	4	WT8	O5-C1-C10-O11
3	qE	4	WT8	O5-C1-C10-O11
3	yE	4	WT8	O5-C1-C10-O11

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Mol	Chain	Res	Type	Atoms
3	6E	4	WT8	O5-C1-C10-O11
3	EF	4	WT8	O5-C1-C10-O11
3	MF	4	WT8	O5-C1-C10-O11
3	UF	4	WT8	O5-C1-C10-O11
3	cF	4	WT8	O5-C1-C10-O11
2	9	2	A2G	C8-C7-N2-C2
2	bC	2	A2G	C8-C7-N2-C2
2	7C	2	A2G	C8-C7-N2-C2
2	fE	2	A2G	C8-C7-N2-C2
2	1	2	A2G	C8-C7-N2-C2
2	fA	2	A2G	C8-C7-N2-C2
2	BB	2	A2G	C8-C7-N2-C2
2	ZB	2	A2G	C8-C7-N2-C2
2	xB	2	A2G	C8-C7-N2-C2
2	VD	2	A2G	C8-C7-N2-C2
2	XE	2	A2G	C8-C7-N2-C2
2	nE	2	A2G	C8-C7-N2-C2
2	t	2	A2G	C8-C7-N2-C2
2	HA	2	A2G	C8-C7-N2-C2
2	PA	2	A2G	C8-C7-N2-C2
2	XA	2	A2G	C8-C7-N2-C2
2	nA	2	A2G	C8-C7-N2-C2
2	vA	2	A2G	C8-C7-N2-C2
2	3A	2	A2G	C8-C7-N2-C2
2	JB	2	A2G	C8-C7-N2-C2
2	RB	2	A2G	C8-C7-N2-C2
2	hB	2	A2G	C8-C7-N2-C2
2	pB	2	A2G	C8-C7-N2-C2
2	5B	2	A2G	C8-C7-N2-C2
2	DC	2	A2G	C8-C7-N2-C2
2	LC	2	A2G	C8-C7-N2-C2
2	TC	2	A2G	C8-C7-N2-C2
2	jC	2	A2G	C8-C7-N2-C2
2	rC	2	A2G	C8-C7-N2-C2
2	zC	2	A2G	C8-C7-N2-C2
2	FD	2	A2G	C8-C7-N2-C2
2	ND	2	A2G	C8-C7-N2-C2
2	dD	2	A2G	C8-C7-N2-C2
2	lD	2	A2G	C8-C7-N2-C2
2	tD	2	A2G	C8-C7-N2-C2
2	1D	2	A2G	C8-C7-N2-C2
2	9D	2	A2G	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	HE	2	A2G	C8-C7-N2-C2
2	PE	2	A2G	C8-C7-N2-C2
2	vE	2	A2G	C8-C7-N2-C2
2	3E	2	A2G	C8-C7-N2-C2
2	BF	2	A2G	C8-C7-N2-C2
2	JF	2	A2G	C8-C7-N2-C2
2	RF	2	A2G	C8-C7-N2-C2
2	ZF	2	A2G	C8-C7-N2-C2
3	w	4	WT8	C2-C1-C10-O11
3	w	4	WT8	C2-C1-C10-O12
3	4	4	WT8	C2-C1-C10-O11
3	4	4	WT8	C2-C1-C10-O12
3	CA	4	WT8	C2-C1-C10-O11
3	CA	4	WT8	C2-C1-C10-O12
3	KA	4	WT8	C2-C1-C10-O11
3	KA	4	WT8	C2-C1-C10-O12
3	SA	4	WT8	C2-C1-C10-O11
3	SA	4	WT8	C2-C1-C10-O12
3	aA	4	WT8	C2-C1-C10-O11
3	aA	4	WT8	C2-C1-C10-O12
3	iA	4	WT8	C2-C1-C10-O11
3	iA	4	WT8	C2-C1-C10-O12
3	qA	4	WT8	C2-C1-C10-O11
3	qA	4	WT8	C2-C1-C10-O12
3	yA	4	WT8	C2-C1-C10-O11
3	yA	4	WT8	C2-C1-C10-O12
3	6A	4	WT8	C2-C1-C10-O11
3	6A	4	WT8	C2-C1-C10-O12
3	EB	4	WT8	C2-C1-C10-O11
3	EB	4	WT8	C2-C1-C10-O12
3	MB	4	WT8	C2-C1-C10-O11
3	MB	4	WT8	C2-C1-C10-O12
3	UB	4	WT8	C2-C1-C10-O11
3	UB	4	WT8	C2-C1-C10-O12
3	cB	4	WT8	C2-C1-C10-O11
3	cB	4	WT8	C2-C1-C10-O12
3	kB	4	WT8	C2-C1-C10-O11
3	kB	4	WT8	C2-C1-C10-O12
3	sB	4	WT8	C2-C1-C10-O11
3	sB	4	WT8	C2-C1-C10-O12
3	0B	4	WT8	C2-C1-C10-O11
3	0B	4	WT8	C2-C1-C10-O12

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Mol	Chain	Res	Type	Atoms
3	8B	4	WT8	C2-C1-C10-O11
3	8B	4	WT8	C2-C1-C10-O12
3	GC	4	WT8	C2-C1-C10-O11
3	GC	4	WT8	C2-C1-C10-O12
3	OC	4	WT8	C2-C1-C10-O11
3	OC	4	WT8	C2-C1-C10-O12
3	WC	4	WT8	C2-C1-C10-O11
3	WC	4	WT8	C2-C1-C10-O12
3	eC	4	WT8	C2-C1-C10-O11
3	eC	4	WT8	C2-C1-C10-O12
3	mC	4	WT8	C2-C1-C10-O11
3	mC	4	WT8	C2-C1-C10-O12
3	uC	4	WT8	C2-C1-C10-O11
3	uC	4	WT8	C2-C1-C10-O12
3	2C	4	WT8	C2-C1-C10-O11
3	2C	4	WT8	C2-C1-C10-O12
3	AD	4	WT8	C2-C1-C10-O11
3	AD	4	WT8	C2-C1-C10-O12
3	ID	4	WT8	C2-C1-C10-O11
3	ID	4	WT8	C2-C1-C10-O12
3	QD	4	WT8	C2-C1-C10-O11
3	QD	4	WT8	C2-C1-C10-O12
3	YD	4	WT8	C2-C1-C10-O11
3	YD	4	WT8	C2-C1-C10-O12
3	gD	4	WT8	C2-C1-C10-O11
3	gD	4	WT8	C2-C1-C10-O12
3	oD	4	WT8	C2-C1-C10-O11
3	oD	4	WT8	C2-C1-C10-O12
3	wD	4	WT8	C2-C1-C10-O11
3	wD	4	WT8	C2-C1-C10-O12
3	4D	4	WT8	C2-C1-C10-O11
3	4D	4	WT8	C2-C1-C10-O12
3	CE	4	WT8	C2-C1-C10-O11
3	CE	4	WT8	C2-C1-C10-O12
3	KE	4	WT8	C2-C1-C10-O11
3	KE	4	WT8	C2-C1-C10-O12
3	SE	4	WT8	C2-C1-C10-O11
3	SE	4	WT8	C2-C1-C10-O12
3	aE	4	WT8	C2-C1-C10-O11
3	aE	4	WT8	C2-C1-C10-O12
3	iE	4	WT8	C2-C1-C10-O11
3	iE	4	WT8	C2-C1-C10-O12

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Mol	Chain	Res	Type	Atoms
3	qE	4	WT8	C2-C1-C10-O11
3	qE	4	WT8	C2-C1-C10-O12
3	yE	4	WT8	C2-C1-C10-O11
3	yE	4	WT8	C2-C1-C10-O12
3	6E	4	WT8	C2-C1-C10-O11
3	6E	4	WT8	C2-C1-C10-O12
3	EF	4	WT8	C2-C1-C10-O11
3	EF	4	WT8	C2-C1-C10-O12
3	MF	4	WT8	C2-C1-C10-O11
3	MF	4	WT8	C2-C1-C10-O12
3	UF	4	WT8	C2-C1-C10-O11
3	UF	4	WT8	C2-C1-C10-O12
3	cF	4	WT8	C2-C1-C10-O11
3	cF	4	WT8	C2-C1-C10-O12
2	9	2	A2G	O7-C7-N2-C2
2	HA	2	A2G	O7-C7-N2-C2
2	XA	2	A2G	O7-C7-N2-C2
2	fA	2	A2G	O7-C7-N2-C2
2	nA	2	A2G	O7-C7-N2-C2
2	vA	2	A2G	O7-C7-N2-C2
2	BB	2	A2G	O7-C7-N2-C2
2	RB	2	A2G	O7-C7-N2-C2
2	pB	2	A2G	O7-C7-N2-C2
2	5B	2	A2G	O7-C7-N2-C2
2	TC	2	A2G	O7-C7-N2-C2
2	bC	2	A2G	O7-C7-N2-C2
2	FD	2	A2G	O7-C7-N2-C2
2	dD	2	A2G	O7-C7-N2-C2
2	tD	2	A2G	O7-C7-N2-C2
2	9D	2	A2G	O7-C7-N2-C2
2	HE	2	A2G	O7-C7-N2-C2
2	PE	2	A2G	O7-C7-N2-C2
2	fE	2	A2G	O7-C7-N2-C2
2	nE	2	A2G	O7-C7-N2-C2
2	BF	2	A2G	O7-C7-N2-C2
2	JF	2	A2G	O7-C7-N2-C2
2	t	2	A2G	O7-C7-N2-C2
2	1	2	A2G	O7-C7-N2-C2
2	PA	2	A2G	O7-C7-N2-C2
2	3A	2	A2G	O7-C7-N2-C2
2	JB	2	A2G	O7-C7-N2-C2
2	ZB	2	A2G	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	hB	2	A2G	O7-C7-N2-C2
2	xB	2	A2G	O7-C7-N2-C2
2	DC	2	A2G	O7-C7-N2-C2
2	LC	2	A2G	O7-C7-N2-C2
2	jC	2	A2G	O7-C7-N2-C2
2	rC	2	A2G	O7-C7-N2-C2
2	zC	2	A2G	O7-C7-N2-C2
2	7C	2	A2G	O7-C7-N2-C2
2	ND	2	A2G	O7-C7-N2-C2
2	VD	2	A2G	O7-C7-N2-C2
2	lD	2	A2G	O7-C7-N2-C2
2	1D	2	A2G	O7-C7-N2-C2
2	XE	2	A2G	O7-C7-N2-C2
2	vE	2	A2G	O7-C7-N2-C2
2	3E	2	A2G	O7-C7-N2-C2
2	RF	2	A2G	O7-C7-N2-C2
2	ZF	2	A2G	O7-C7-N2-C2
3	OC	2	A2G	C8-C7-N2-C2
3	cF	2	A2G	C8-C7-N2-C2
3	8B	2	A2G	C8-C7-N2-C2
3	mC	2	A2G	C8-C7-N2-C2
3	YD	2	A2G	C8-C7-N2-C2
3	gD	2	A2G	C8-C7-N2-C2
3	KA	2	A2G	C8-C7-N2-C2
3	6A	2	A2G	C8-C7-N2-C2
3	wD	2	A2G	C8-C7-N2-C2
3	CE	2	A2G	C8-C7-N2-C2
3	iE	2	A2G	C8-C7-N2-C2
3	MF	2	A2G	C8-C7-N2-C2
3	UF	2	A2G	C8-C7-N2-C2
3	w	2	A2G	C8-C7-N2-C2
3	4	2	A2G	C8-C7-N2-C2
3	CA	2	A2G	C8-C7-N2-C2
3	SA	2	A2G	C8-C7-N2-C2
3	aA	2	A2G	C8-C7-N2-C2
3	iA	2	A2G	C8-C7-N2-C2
3	qA	2	A2G	C8-C7-N2-C2
3	yA	2	A2G	C8-C7-N2-C2
3	EB	2	A2G	C8-C7-N2-C2
3	MB	2	A2G	C8-C7-N2-C2
3	UB	2	A2G	C8-C7-N2-C2
3	cB	2	A2G	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	kB	2	A2G	C8-C7-N2-C2
3	sB	2	A2G	C8-C7-N2-C2
3	0B	2	A2G	C8-C7-N2-C2
3	GC	2	A2G	C8-C7-N2-C2
3	WC	2	A2G	C8-C7-N2-C2
3	eC	2	A2G	C8-C7-N2-C2
3	uC	2	A2G	C8-C7-N2-C2
3	2C	2	A2G	C8-C7-N2-C2
3	AD	2	A2G	C8-C7-N2-C2
3	ID	2	A2G	C8-C7-N2-C2
3	QD	2	A2G	C8-C7-N2-C2
3	oD	2	A2G	C8-C7-N2-C2
3	4D	2	A2G	C8-C7-N2-C2
3	KE	2	A2G	C8-C7-N2-C2
3	SE	2	A2G	C8-C7-N2-C2
3	aE	2	A2G	C8-C7-N2-C2
3	qE	2	A2G	C8-C7-N2-C2
3	yE	2	A2G	C8-C7-N2-C2
3	6E	2	A2G	C8-C7-N2-C2
3	EF	2	A2G	C8-C7-N2-C2
3	gD	2	A2G	O7-C7-N2-C2
3	w	2	A2G	O7-C7-N2-C2
3	CA	2	A2G	O7-C7-N2-C2
3	KA	2	A2G	O7-C7-N2-C2
3	SA	2	A2G	O7-C7-N2-C2
3	aA	2	A2G	O7-C7-N2-C2
3	iA	2	A2G	O7-C7-N2-C2
3	qA	2	A2G	O7-C7-N2-C2
3	yA	2	A2G	O7-C7-N2-C2
3	EB	2	A2G	O7-C7-N2-C2
3	MB	2	A2G	O7-C7-N2-C2
3	cB	2	A2G	O7-C7-N2-C2
3	kB	2	A2G	O7-C7-N2-C2
3	sB	2	A2G	O7-C7-N2-C2
3	0B	2	A2G	O7-C7-N2-C2
3	8B	2	A2G	O7-C7-N2-C2
3	OC	2	A2G	O7-C7-N2-C2
3	eC	2	A2G	O7-C7-N2-C2
3	uC	2	A2G	O7-C7-N2-C2
3	AD	2	A2G	O7-C7-N2-C2
3	YD	2	A2G	O7-C7-N2-C2
3	oD	2	A2G	O7-C7-N2-C2

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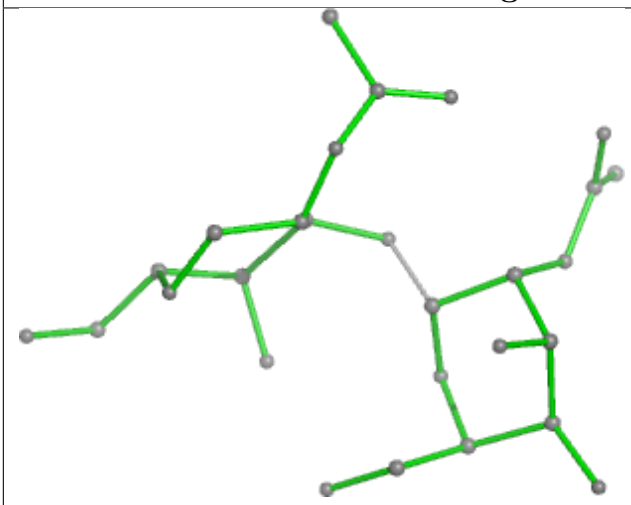
Mol	Chain	Res	Type	Atoms
3	wD	2	A2G	O7-C7-N2-C2
3	4D	2	A2G	O7-C7-N2-C2
3	CE	2	A2G	O7-C7-N2-C2
3	SE	2	A2G	O7-C7-N2-C2
3	aE	2	A2G	O7-C7-N2-C2
3	iE	2	A2G	O7-C7-N2-C2
3	yE	2	A2G	O7-C7-N2-C2
3	EF	2	A2G	O7-C7-N2-C2
3	MF	2	A2G	O7-C7-N2-C2
3	UF	2	A2G	O7-C7-N2-C2
3	cF	2	A2G	O7-C7-N2-C2

There are no ring outliers.

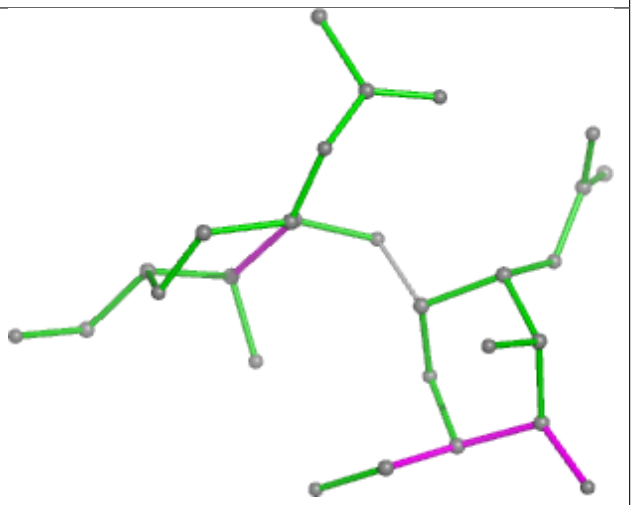
No monomer is involved in short contacts.

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

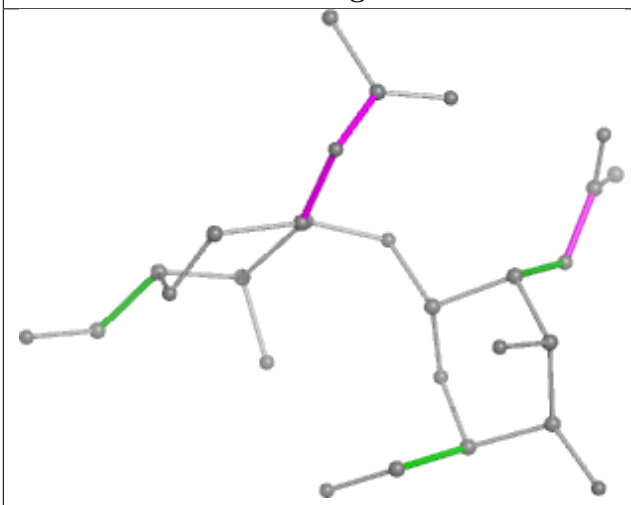
Oligosaccharide Chain t



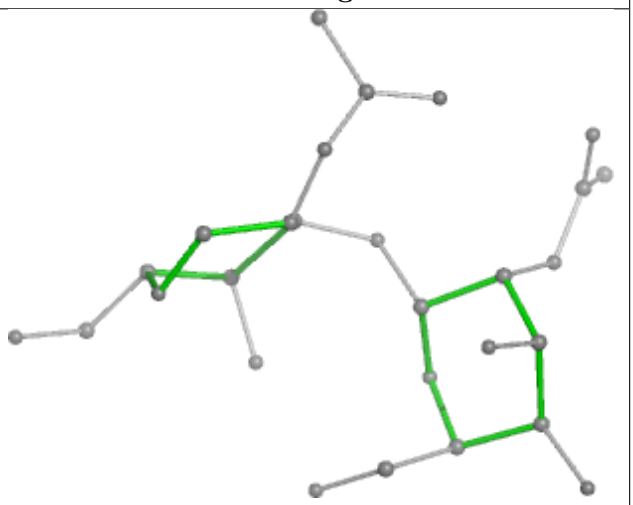
Bond lengths



Bond angles

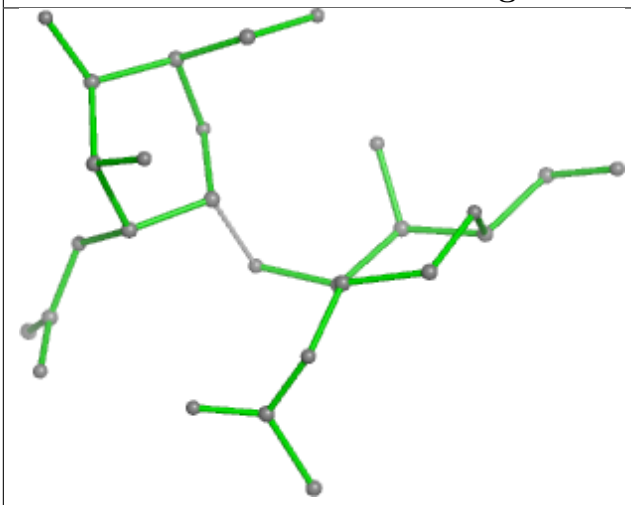


Torsions



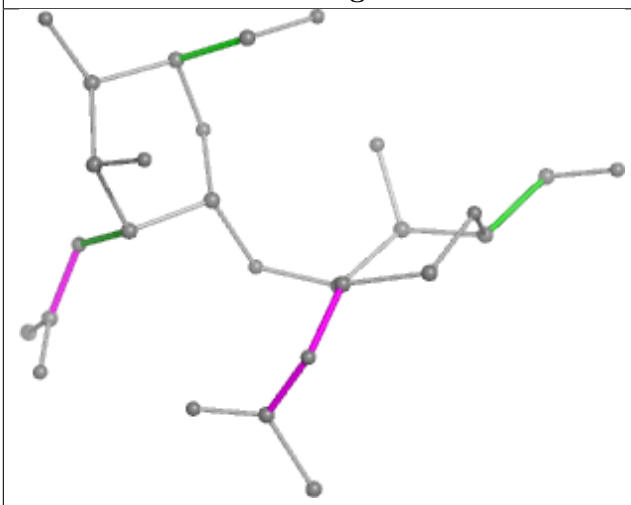
Rings

Oligosaccharide Chain 1

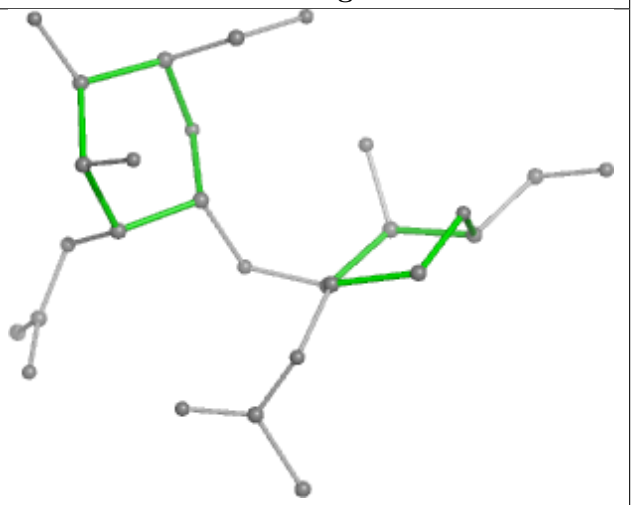


Bond lengths

Bond angles

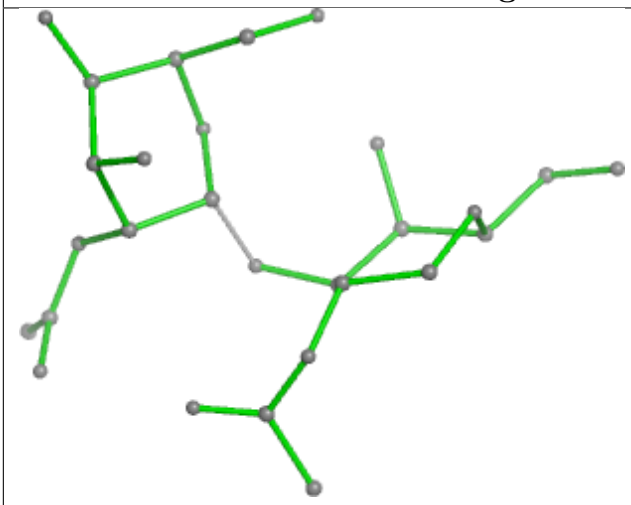


Torsions



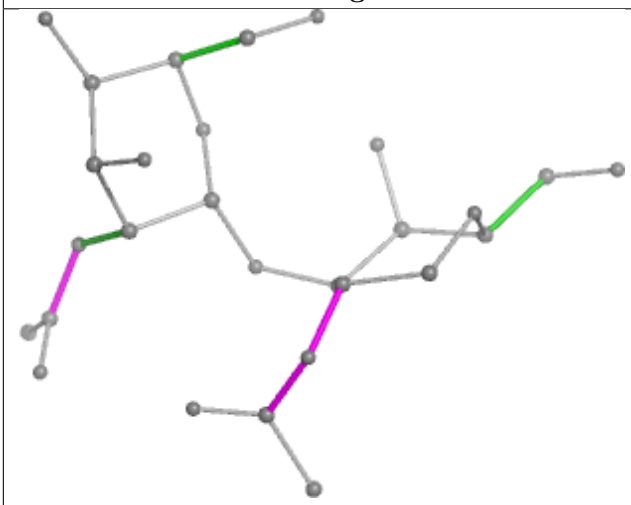
Rings

Oligosaccharide Chain 9

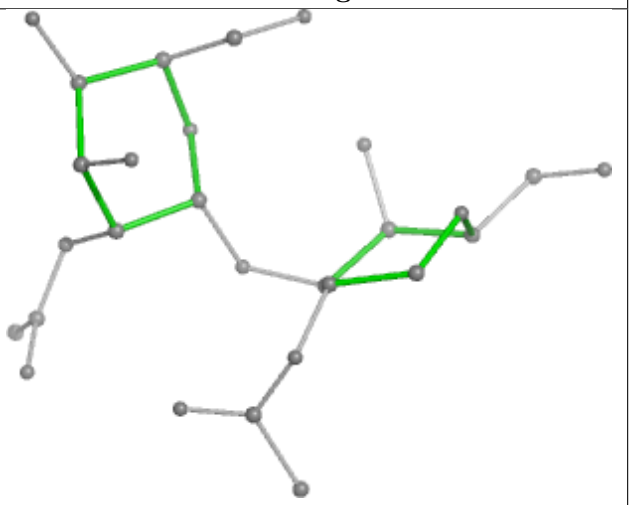


Bond lengths

Bond angles

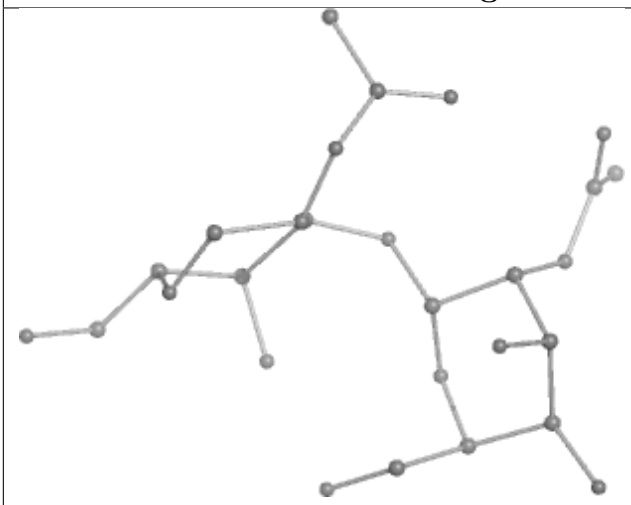


Torsions

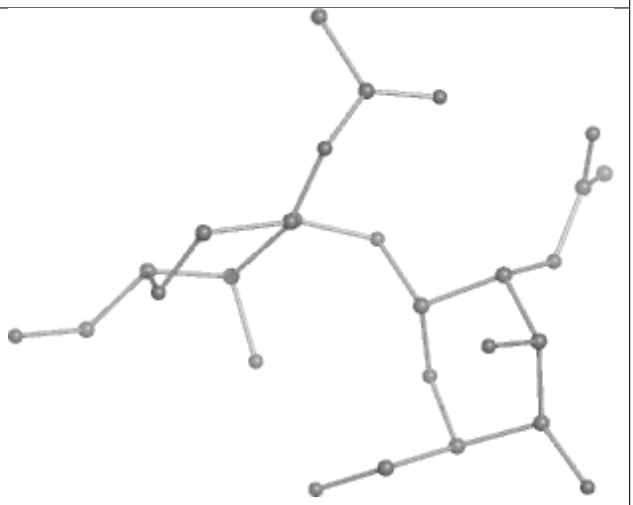


Rings

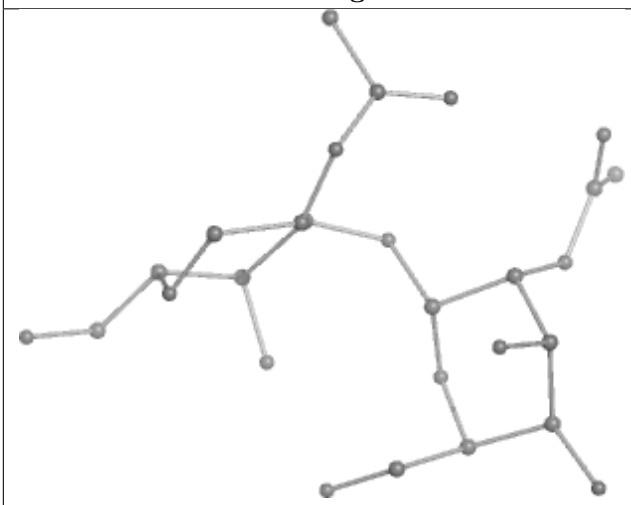
Oligosaccharide Chain HA



Bond lengths



Bond angles



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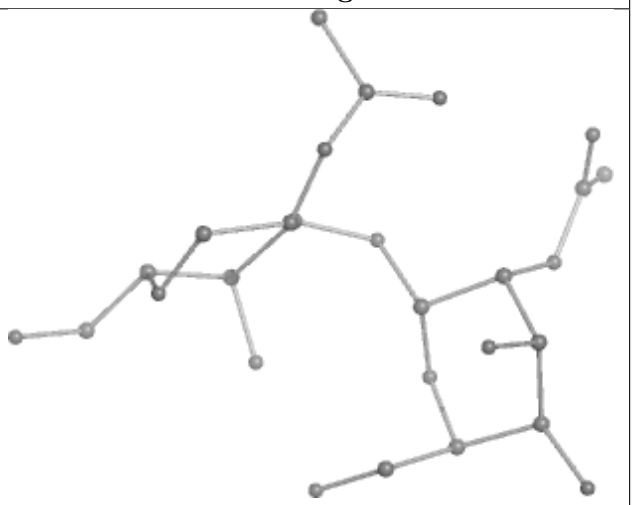
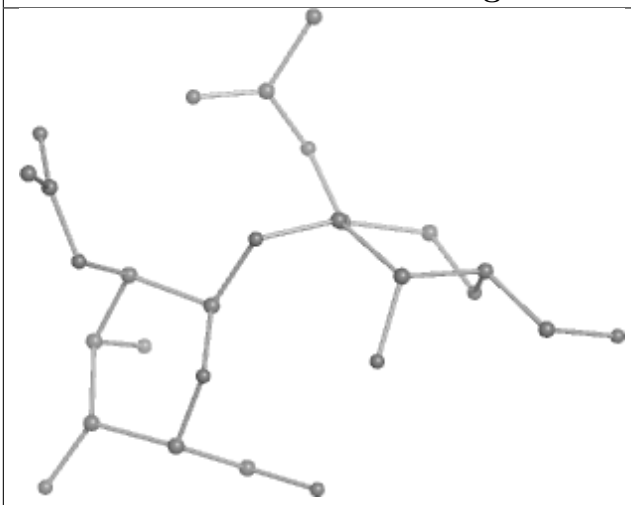


Rings

Oligosaccharide Chain PA



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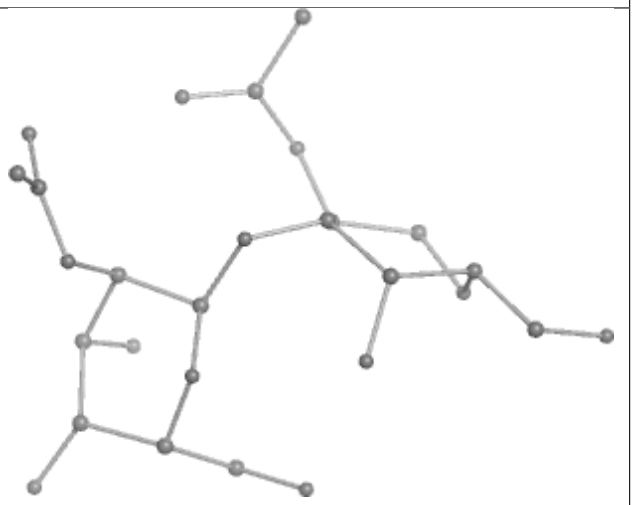
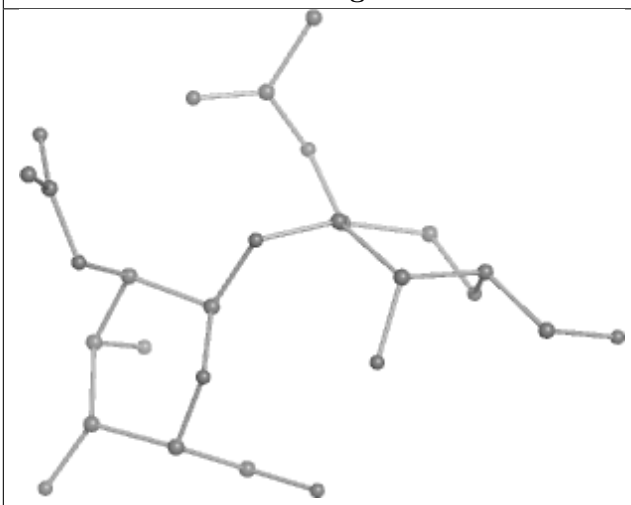


Bond angles



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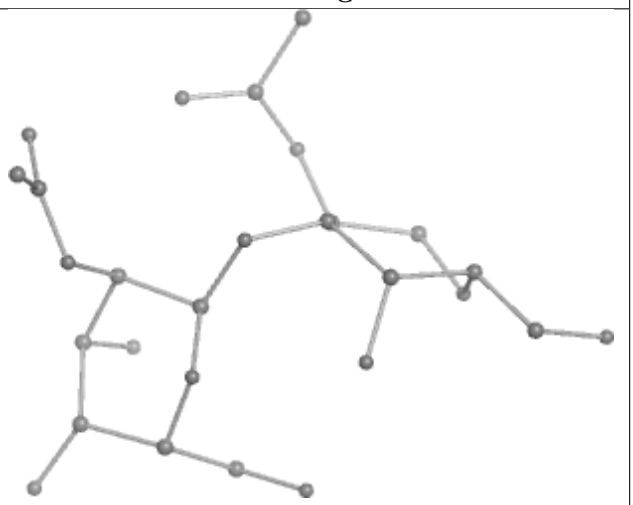
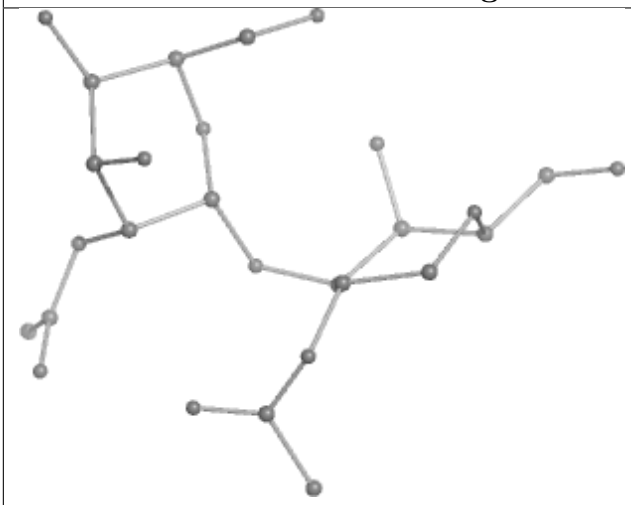


Rings

Oligosaccharide Chain XA



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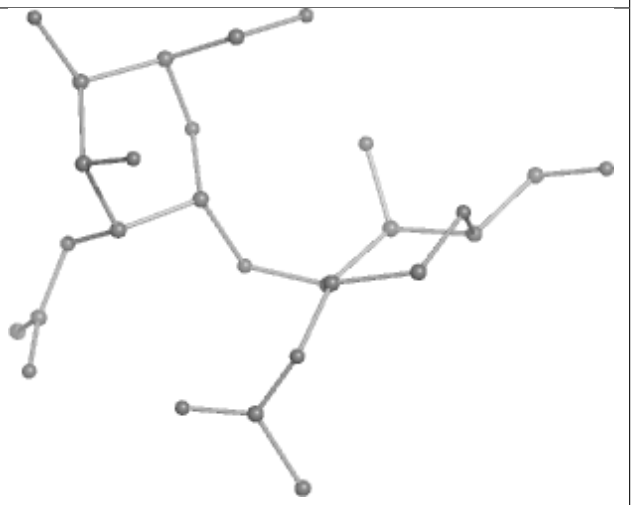

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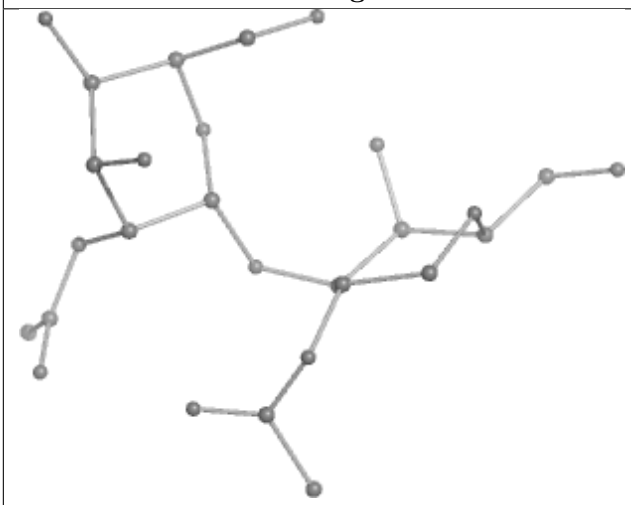

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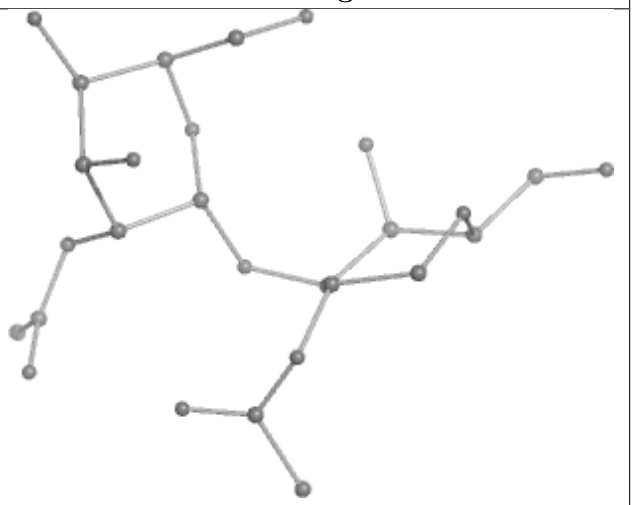
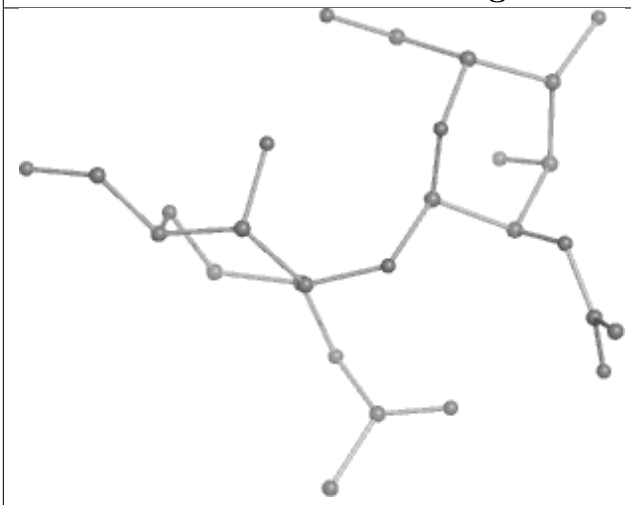


Rings

Oligosaccharide Chain fA



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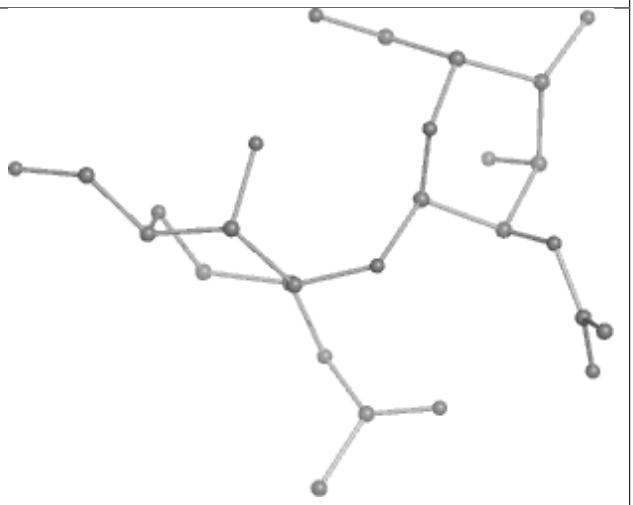
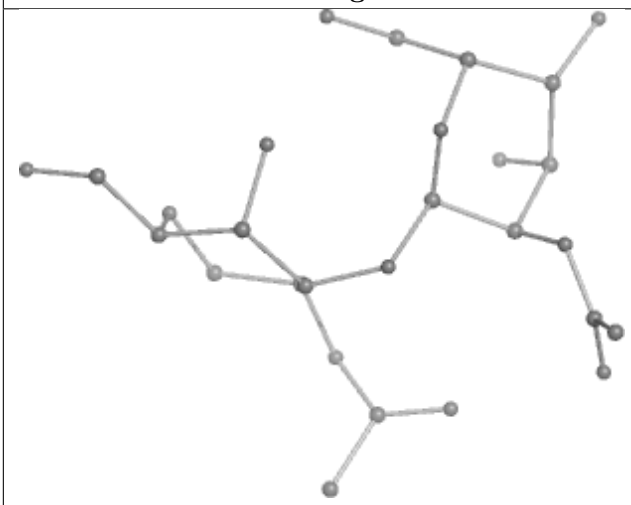


Bond angles



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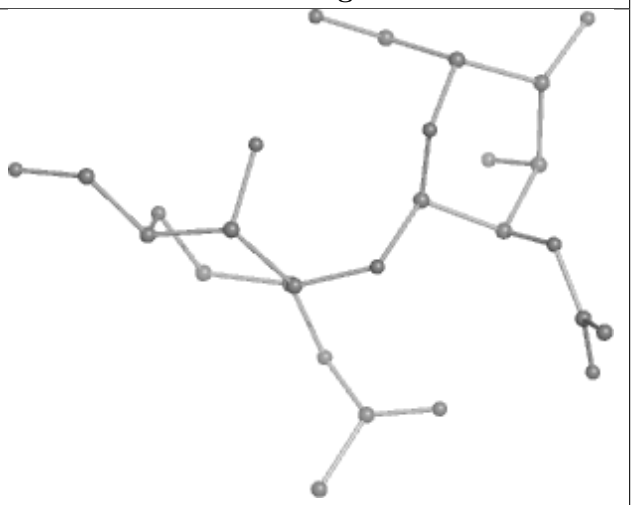
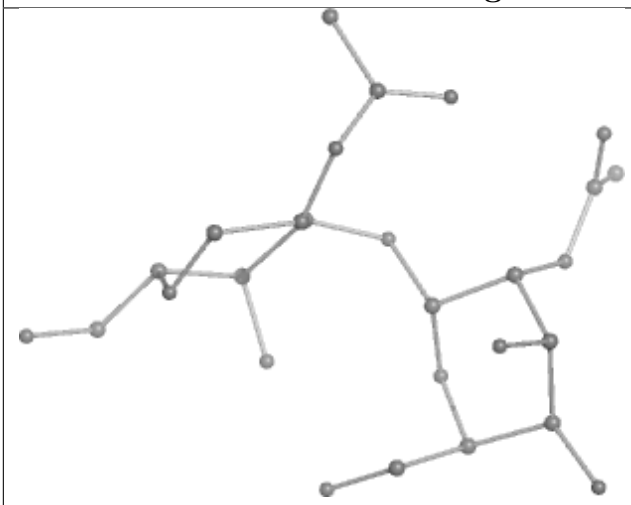


Rings

Oligosaccharide Chain nA



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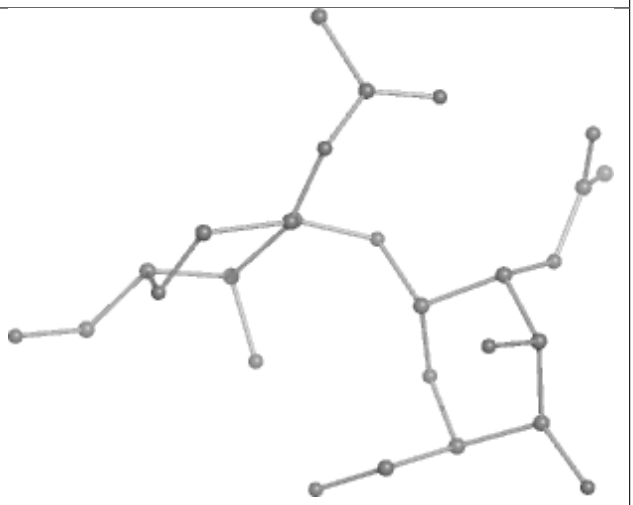
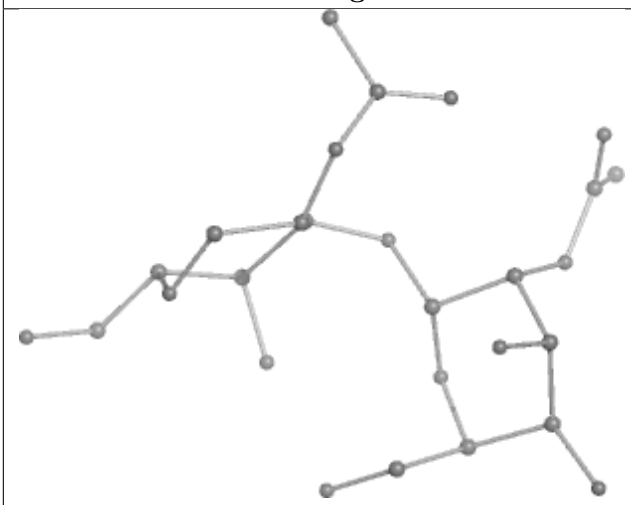


Bond angles



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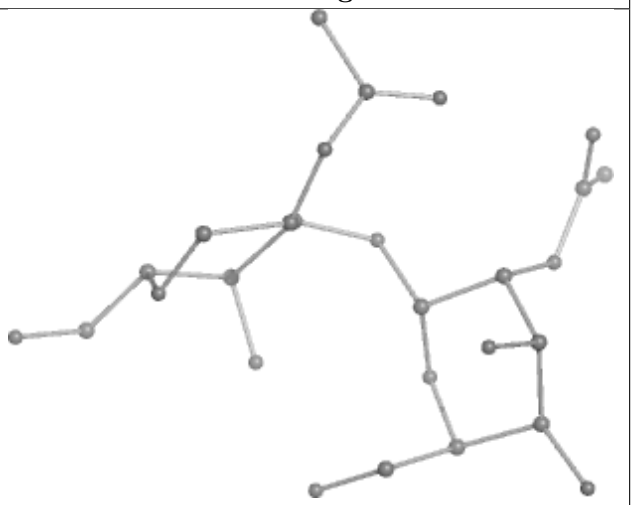
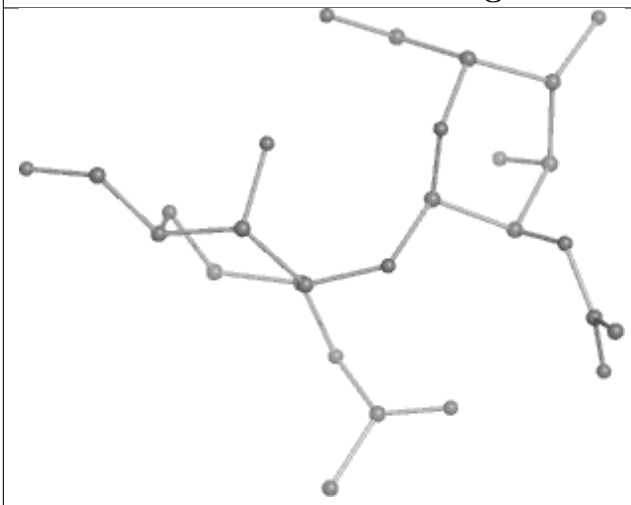


Rings

Oligosaccharide Chain vA



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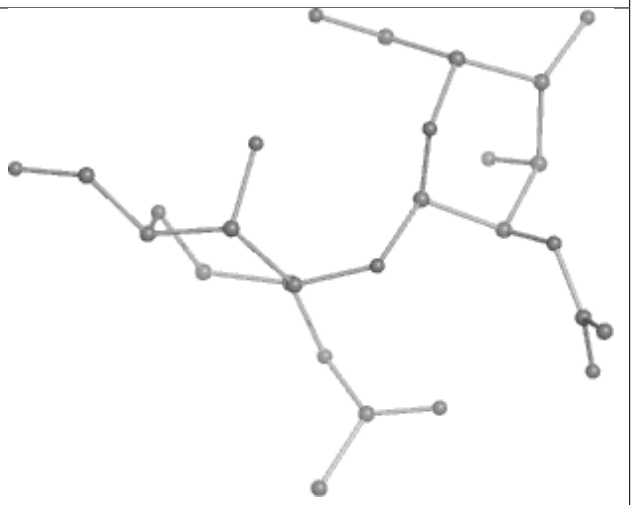
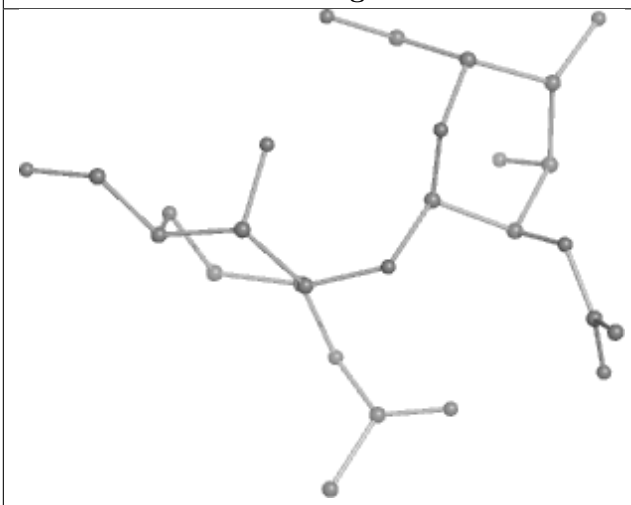


Bond angles



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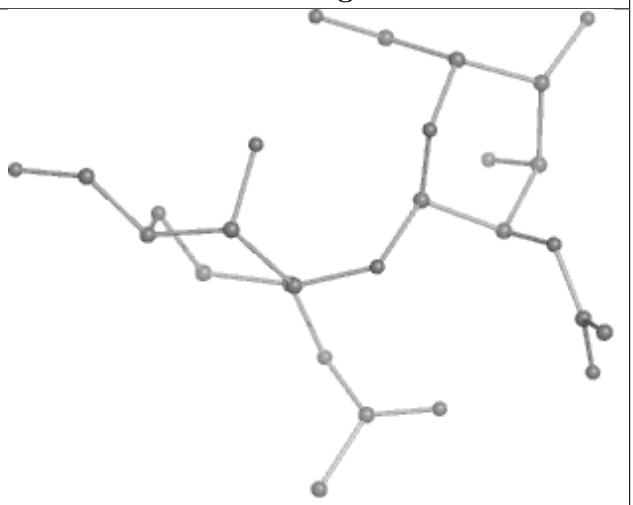
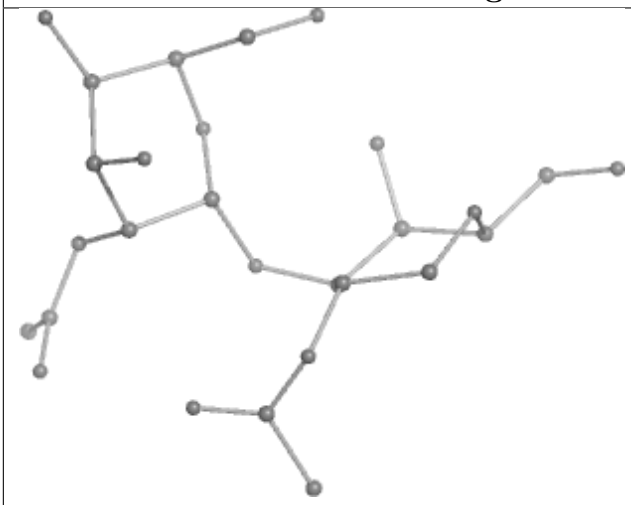


Rings

Oligosaccharide Chain 3A



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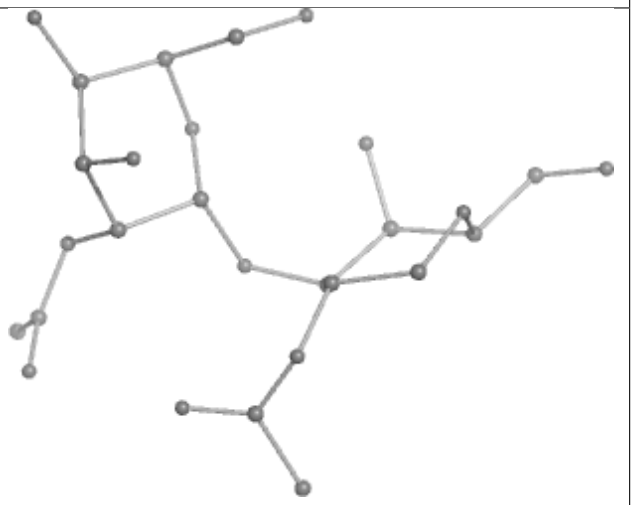

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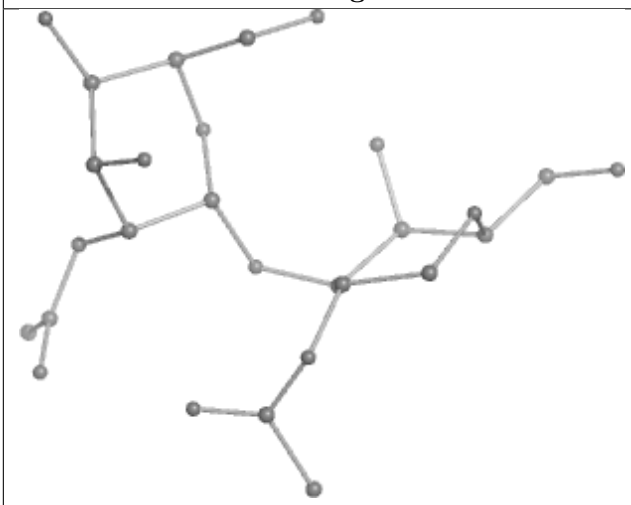

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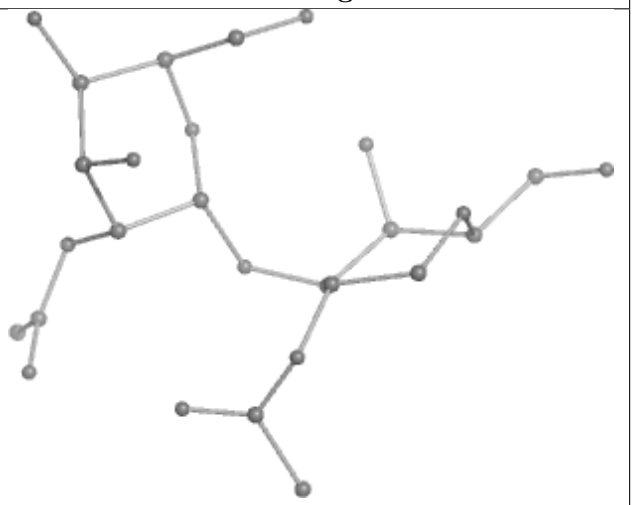
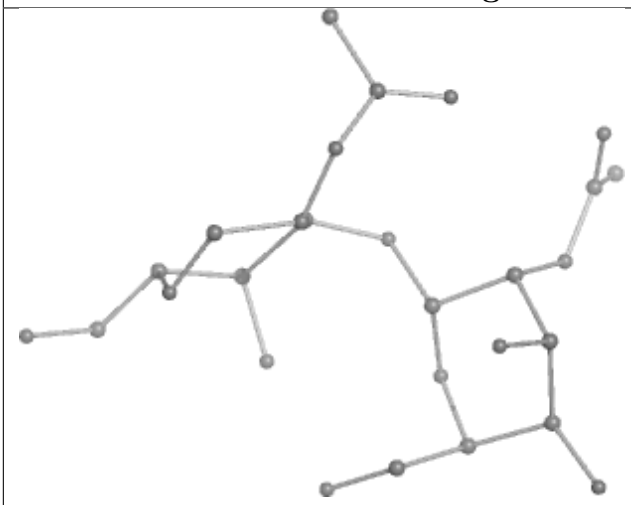


Rings

Oligosaccharide Chain BB



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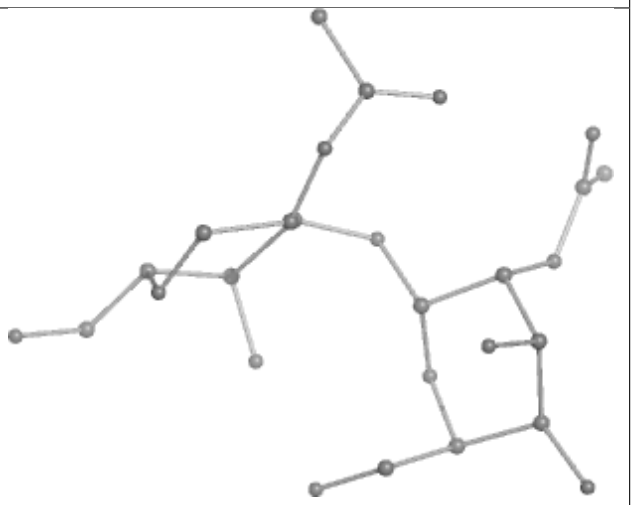
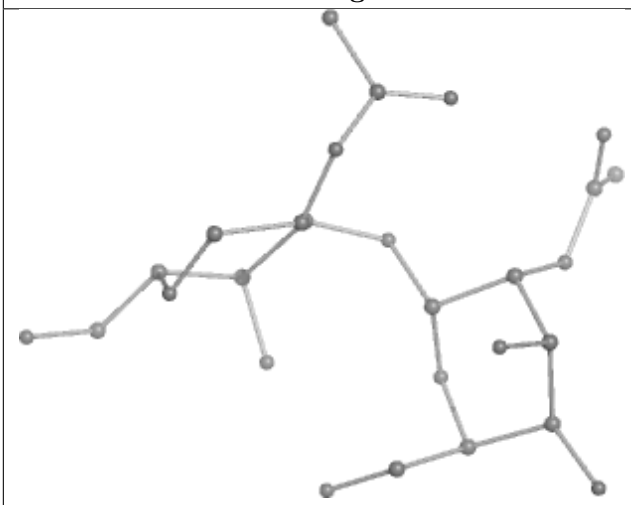


Bond angles



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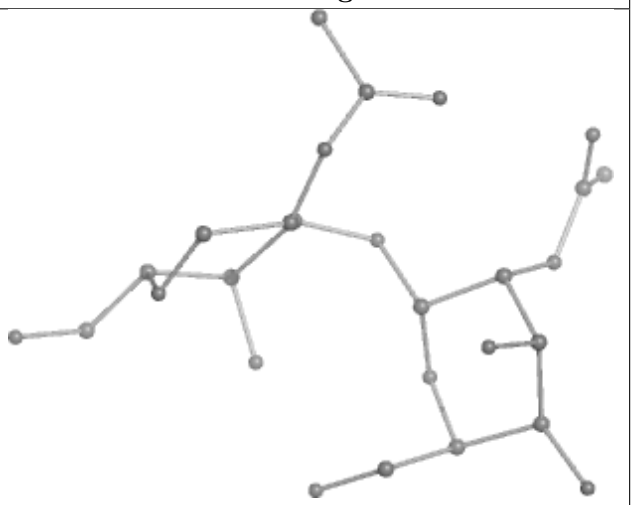
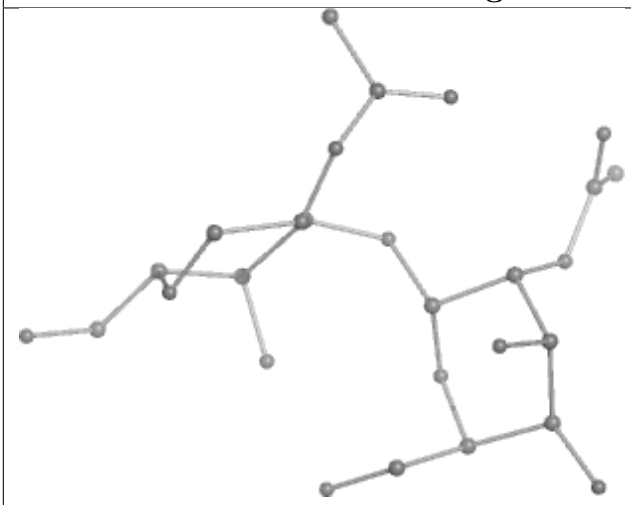


Rings

Oligosaccharide Chain JB



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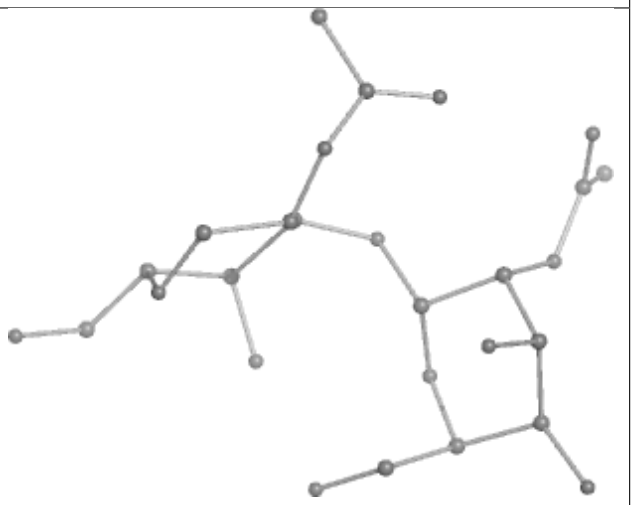
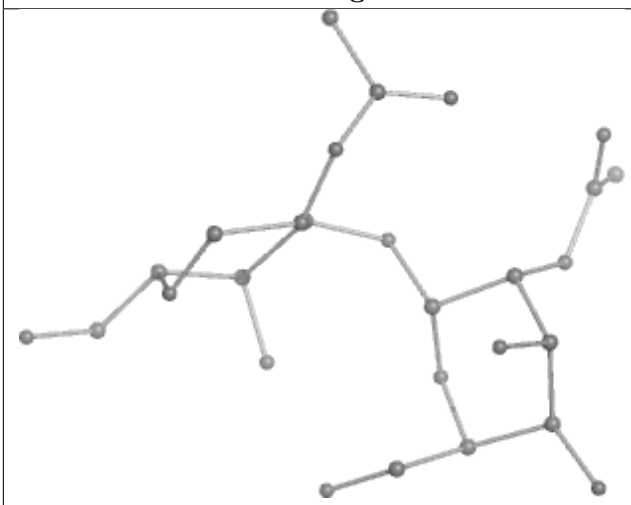
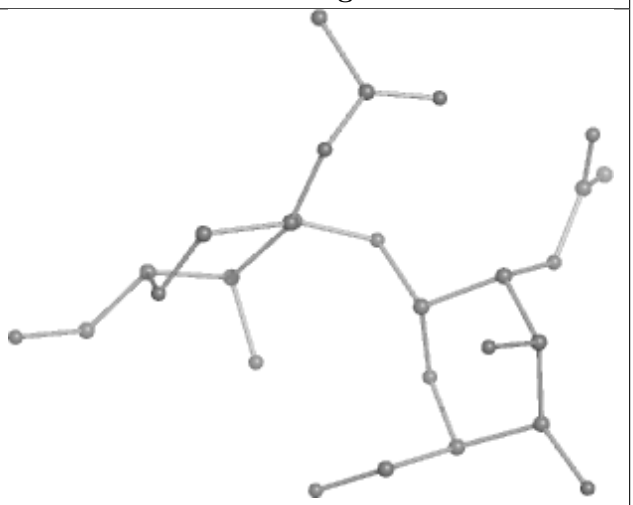


Bond angles

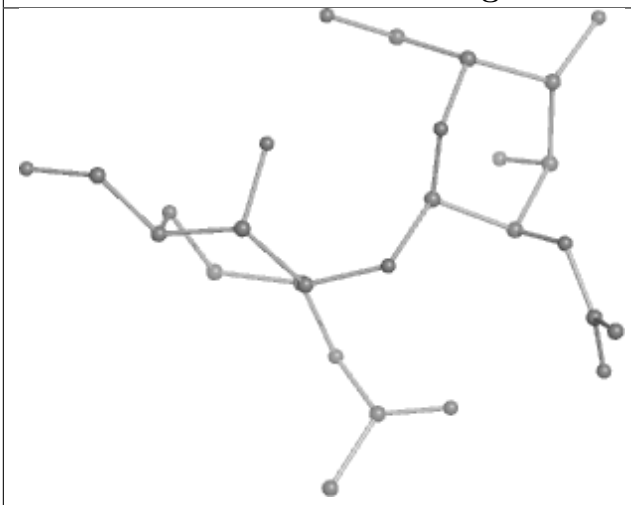


Torsions



Rings

Oligosaccharide Chain RB



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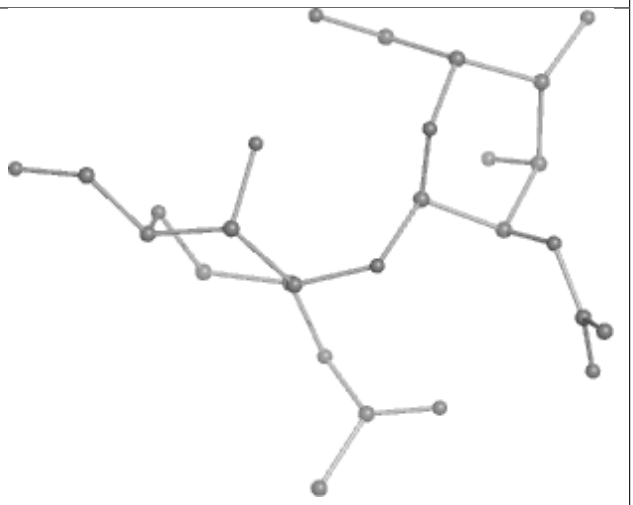
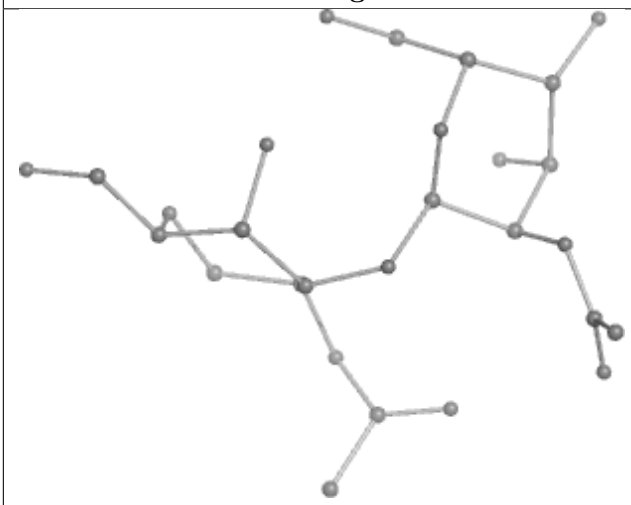
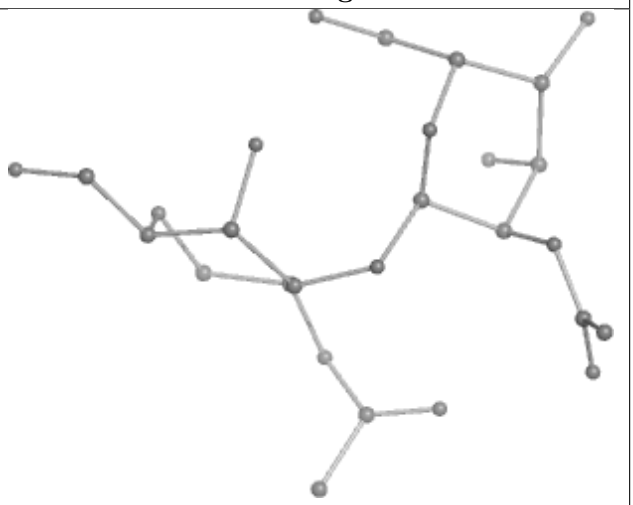


Bond angles

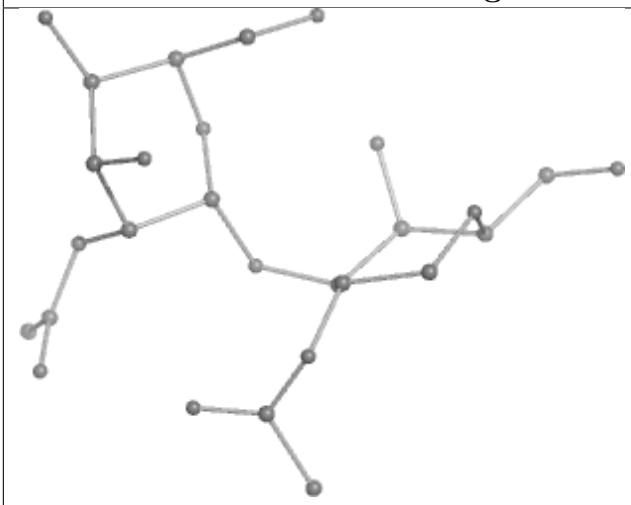


Torsions



Rings

Oligosaccharide Chain ZB



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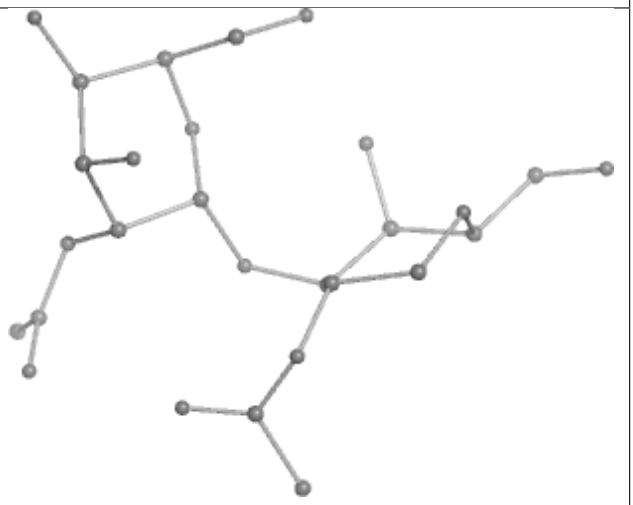
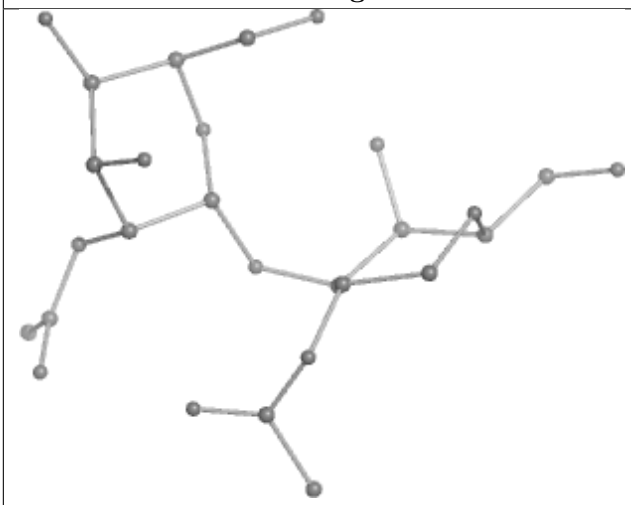


Bond angles



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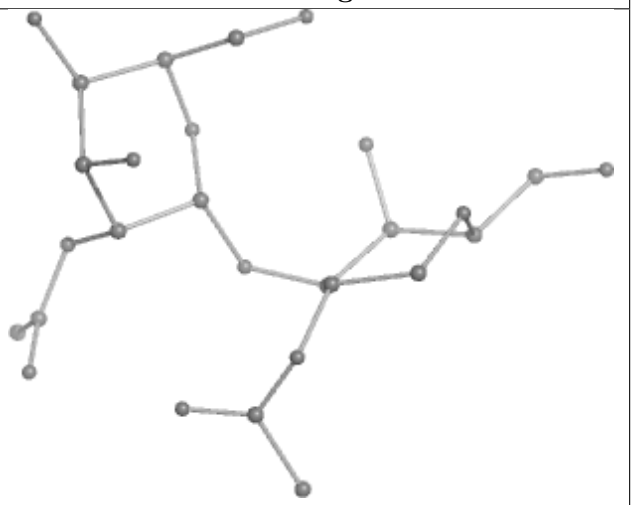
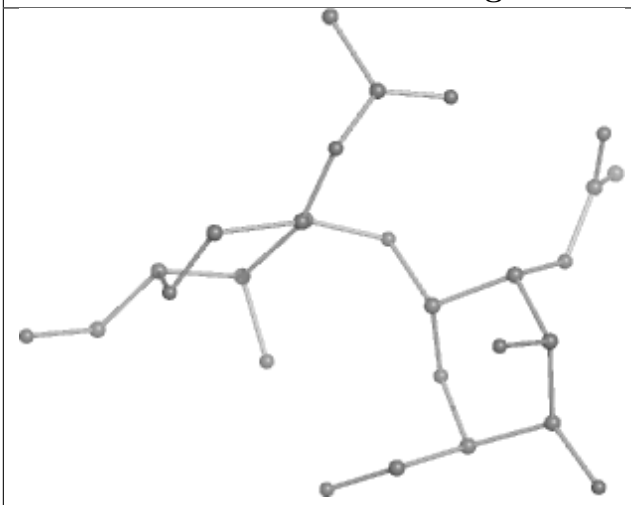
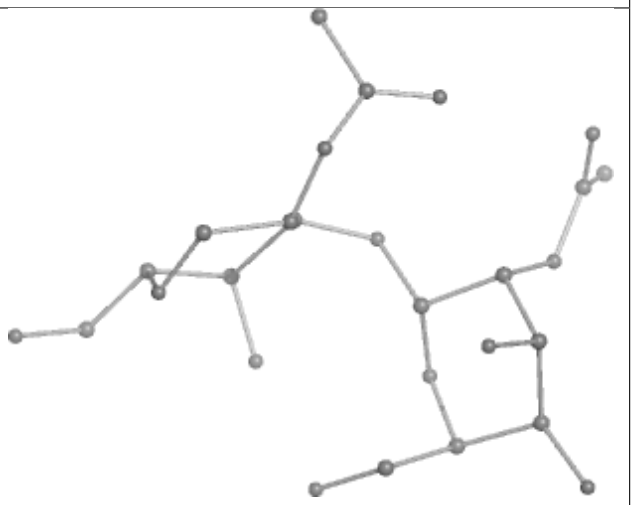


Rings

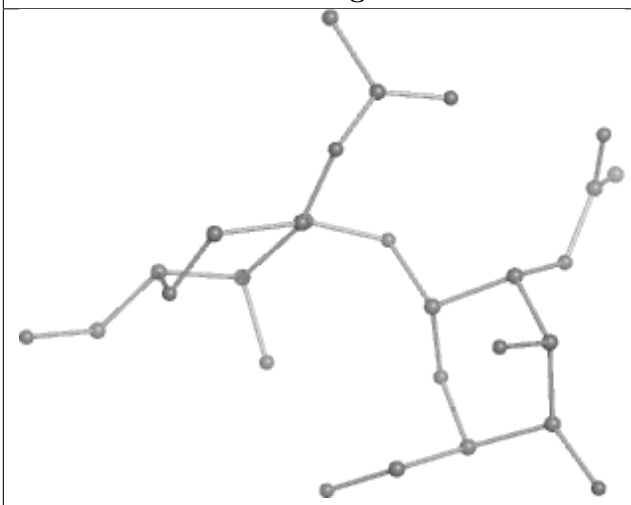
Oligosaccharide Chain hB



Bond lengths



Bond angles



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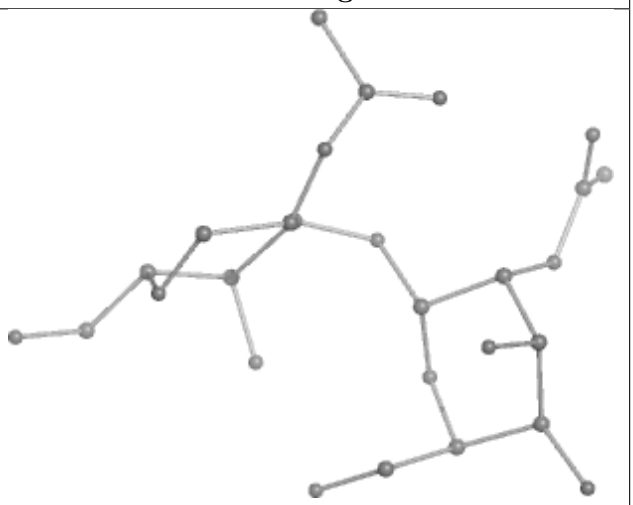
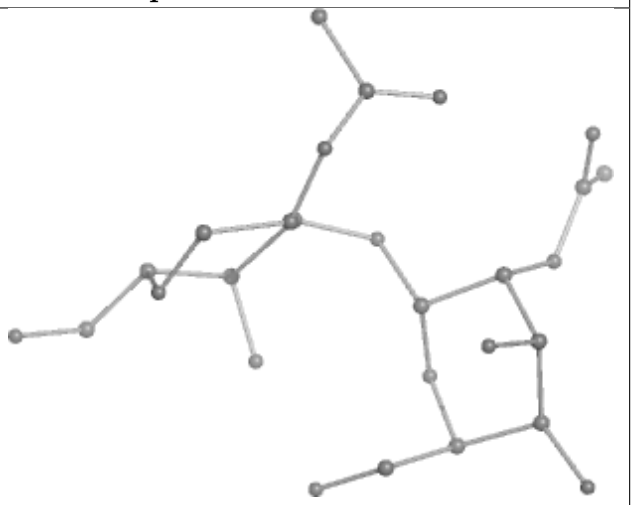


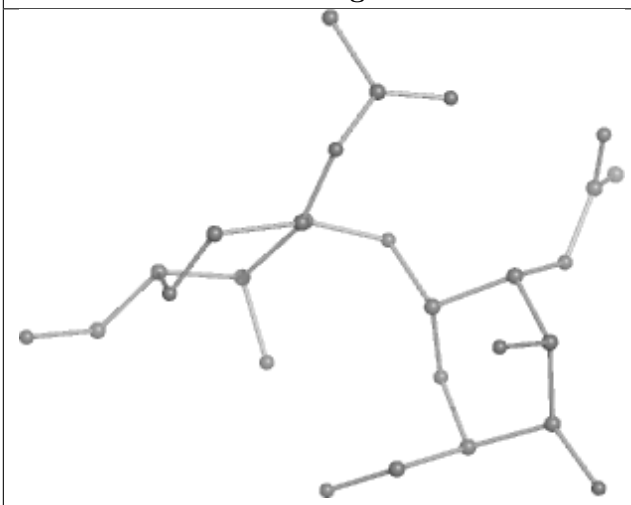
Rings

Oligosaccharide Chain pB

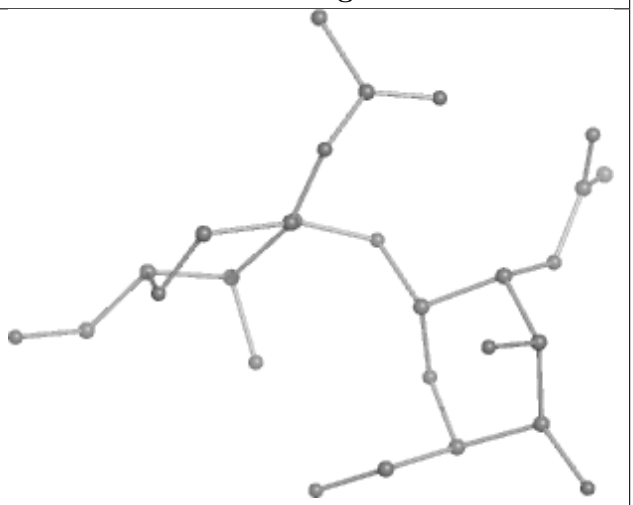
Bond lengths



Bond angles

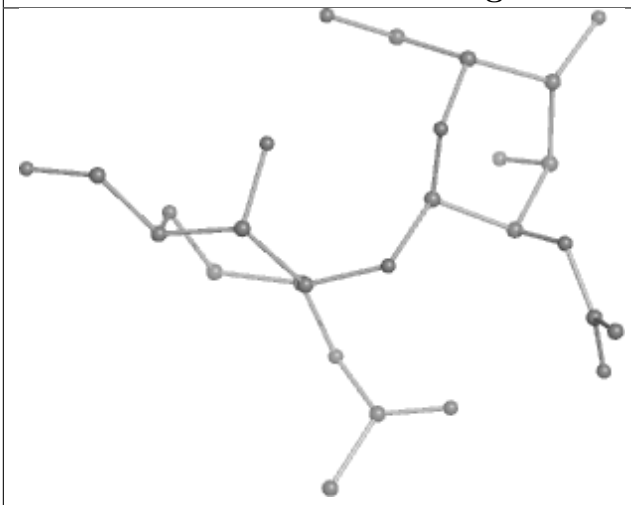


Torsions

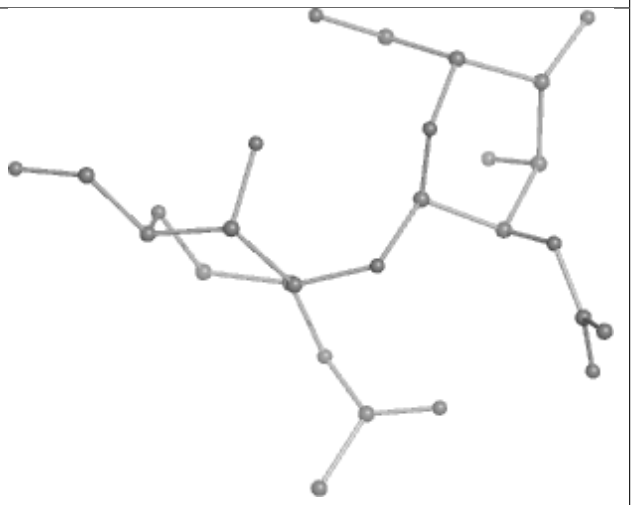


Rings

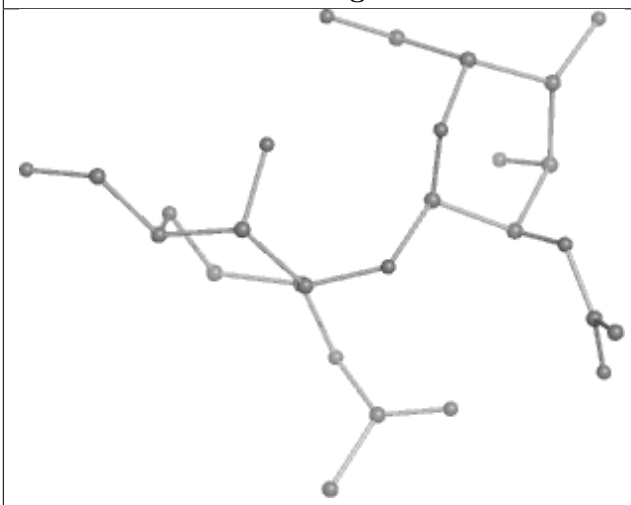
Oligosaccharide Chain xB



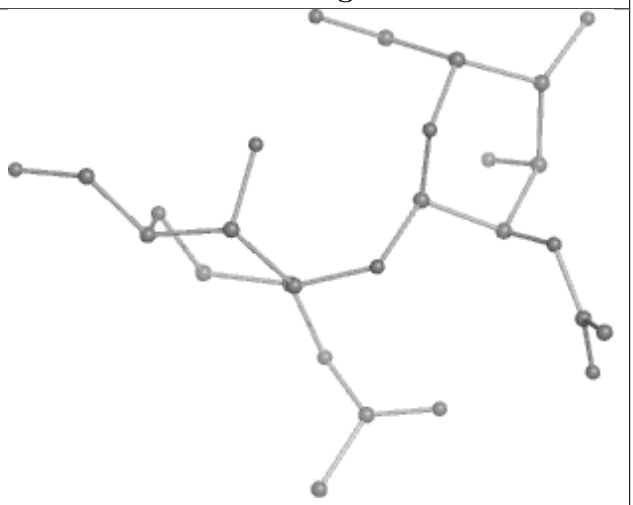
Bond lengths



Bond angles

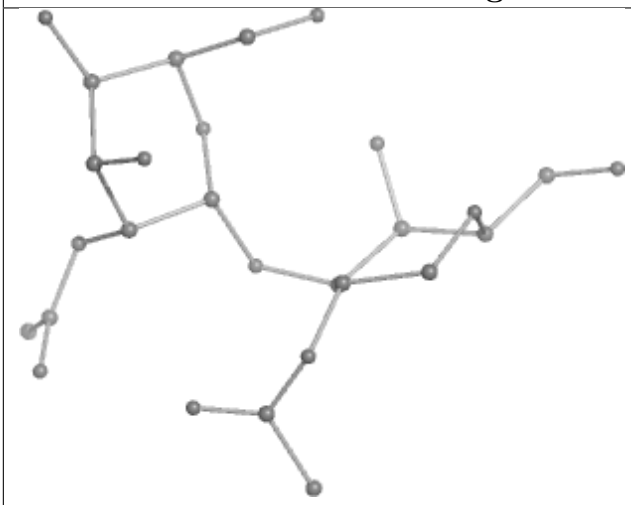


Torsions

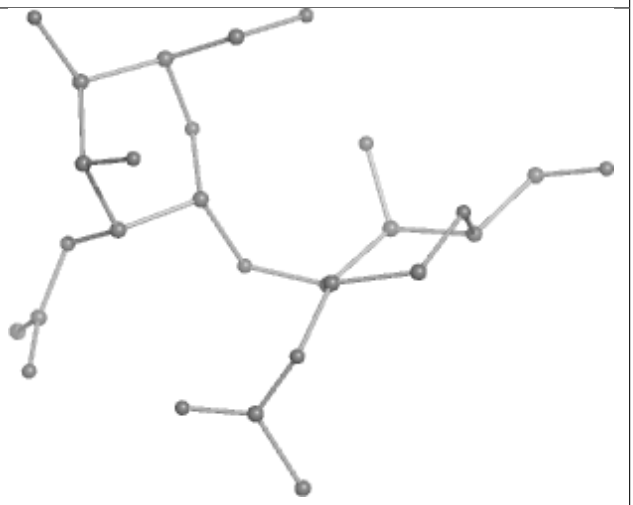


Rings

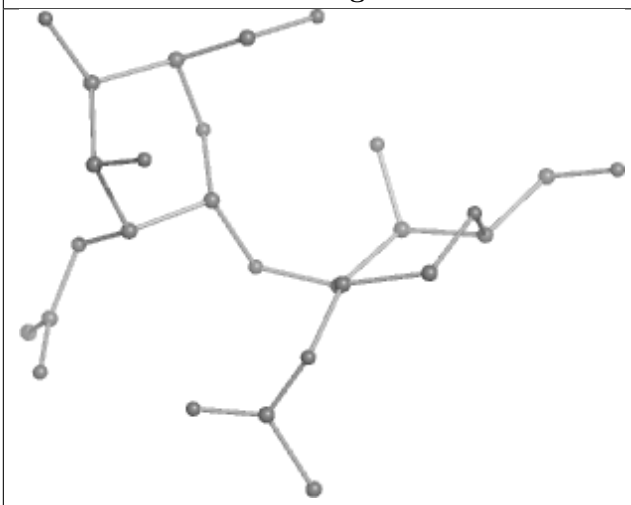
Oligosaccharide Chain 5B



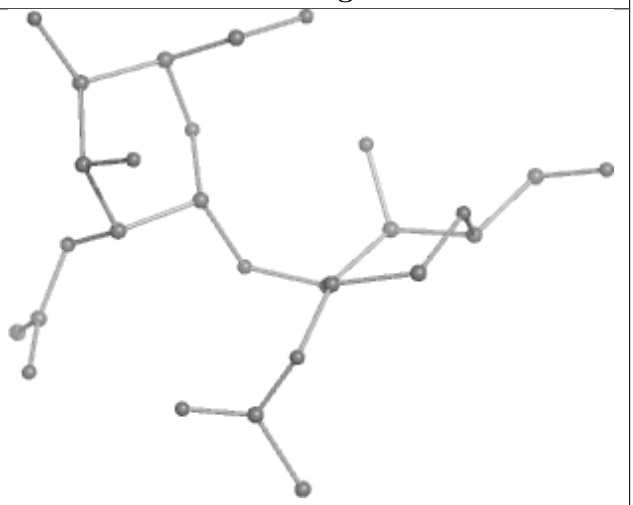
Bond lengths



Bond angles

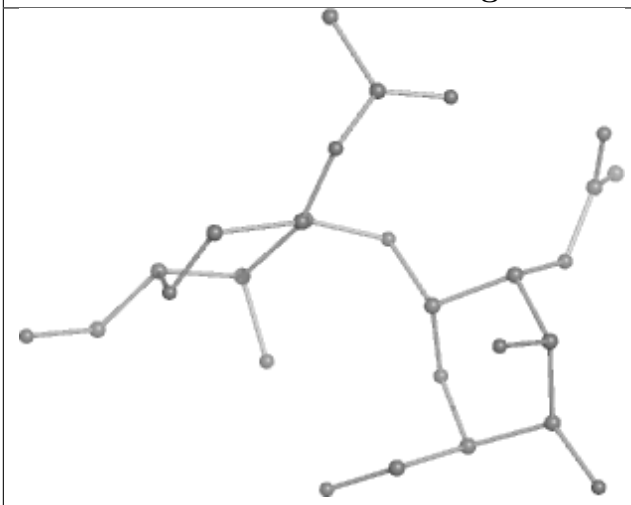


Torsions



Rings

Oligosaccharide Chain DC



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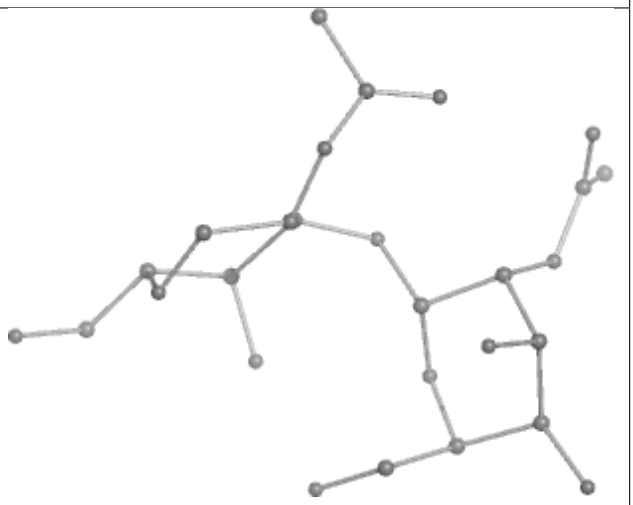

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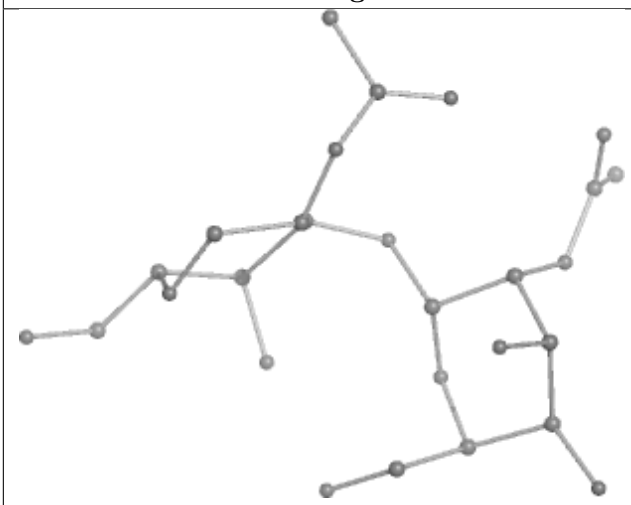

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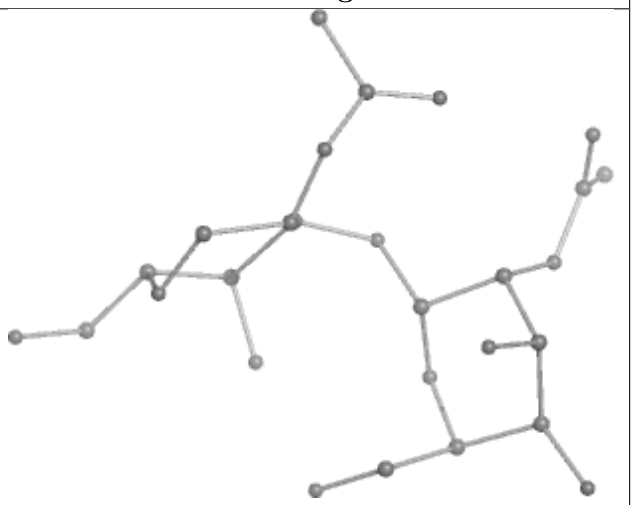
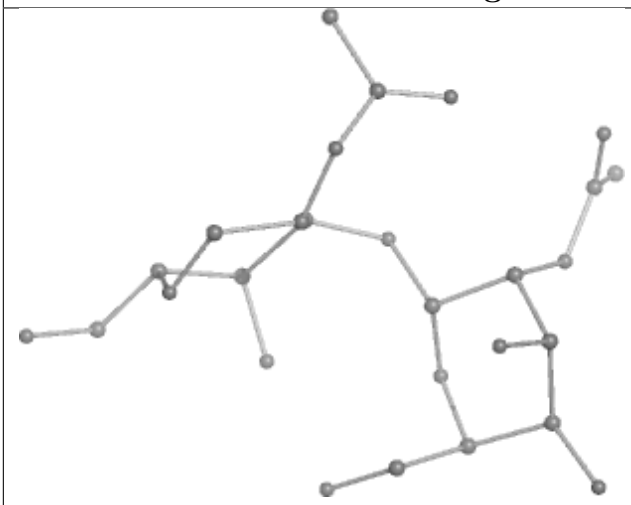
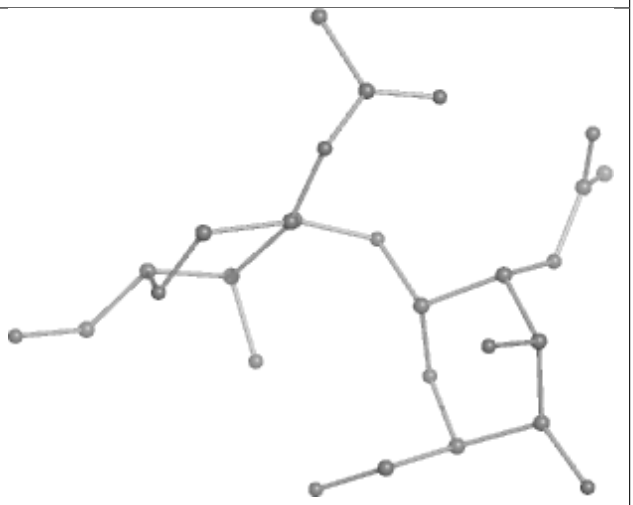


Rings

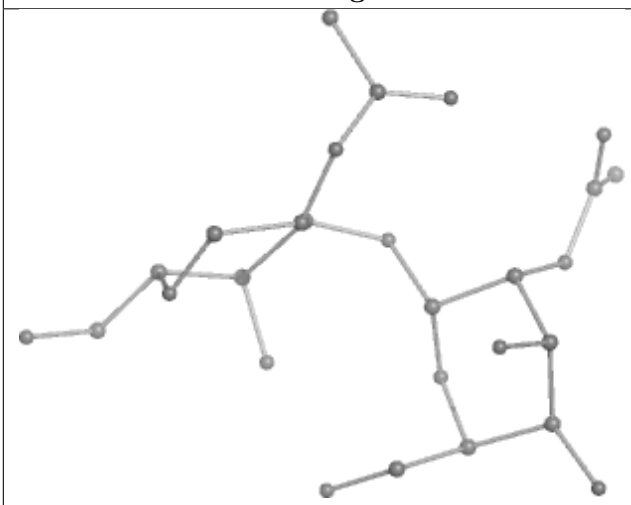
Oligosaccharide Chain LC



Bond lengths



Bond angles



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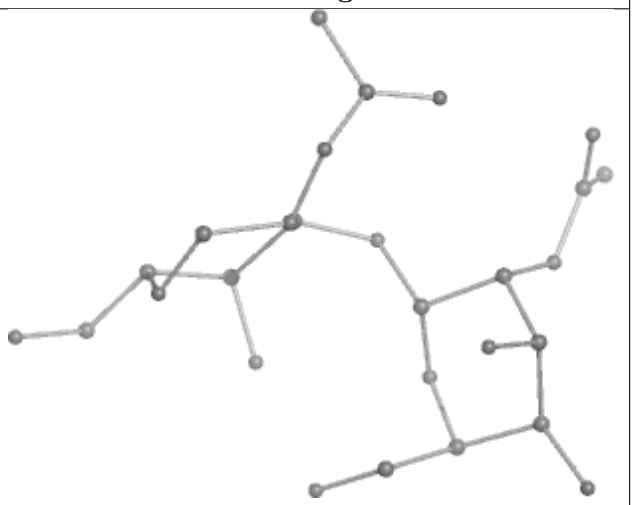
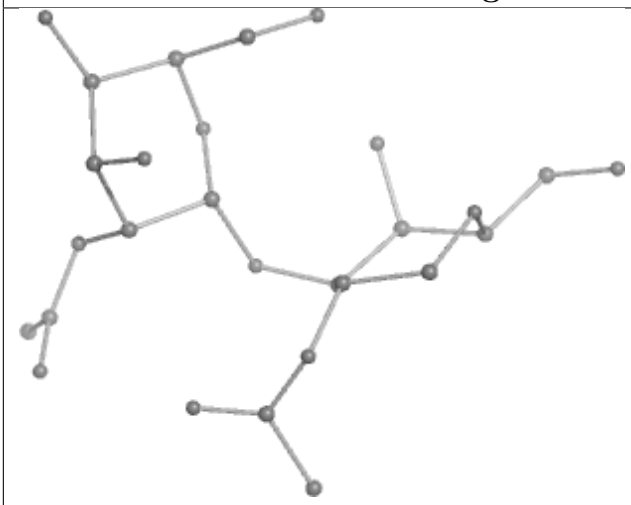


Rings

Oligosaccharide Chain TC



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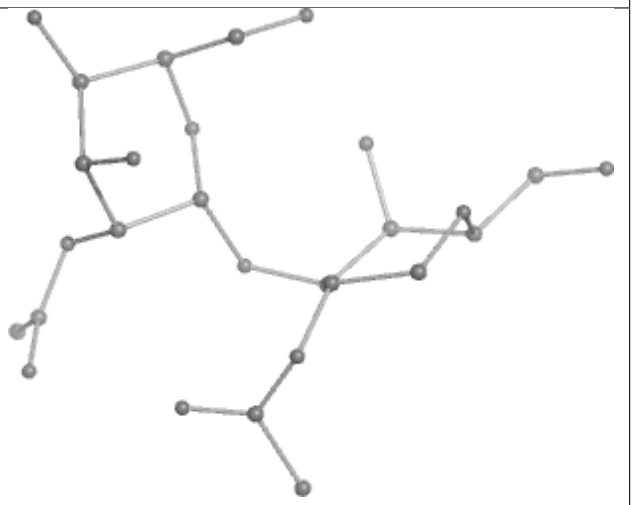
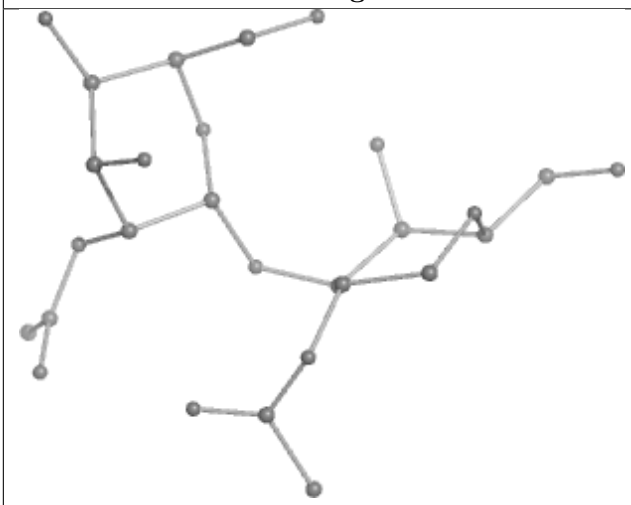


Bond angles



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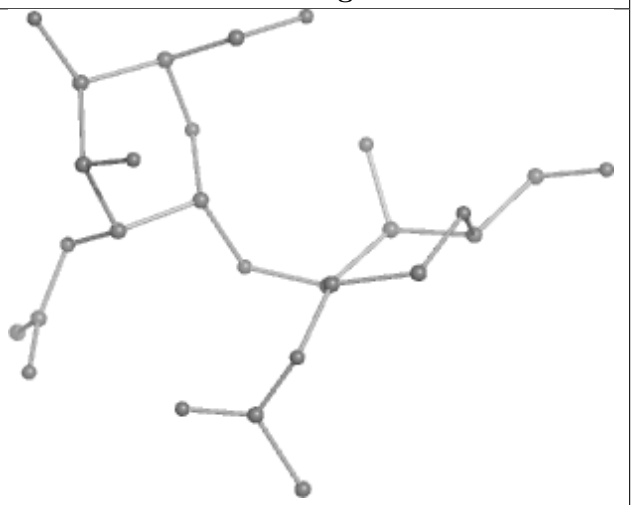
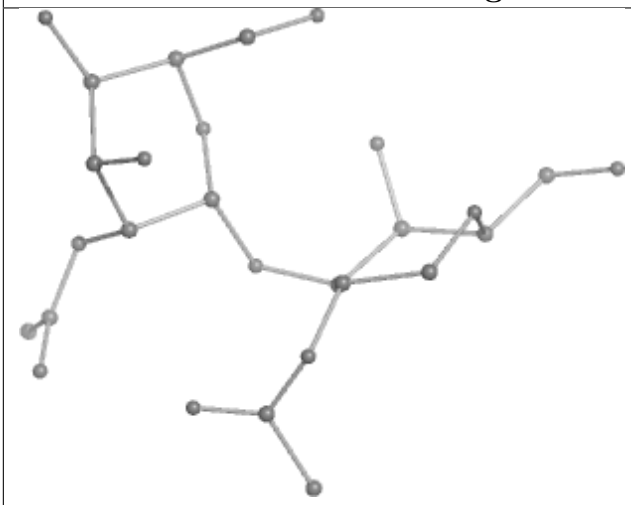
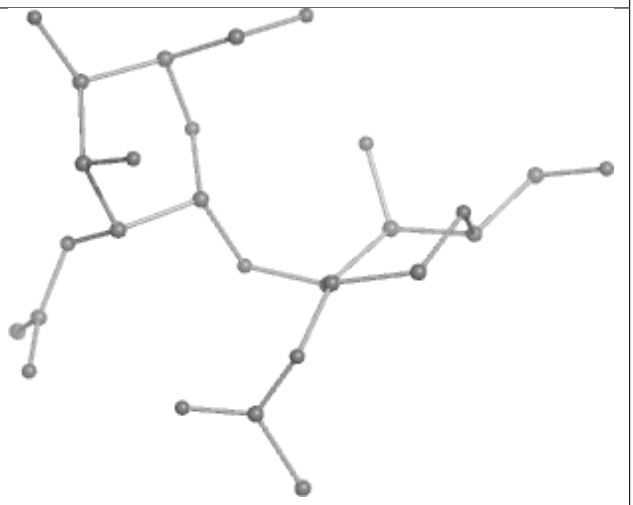


Rings

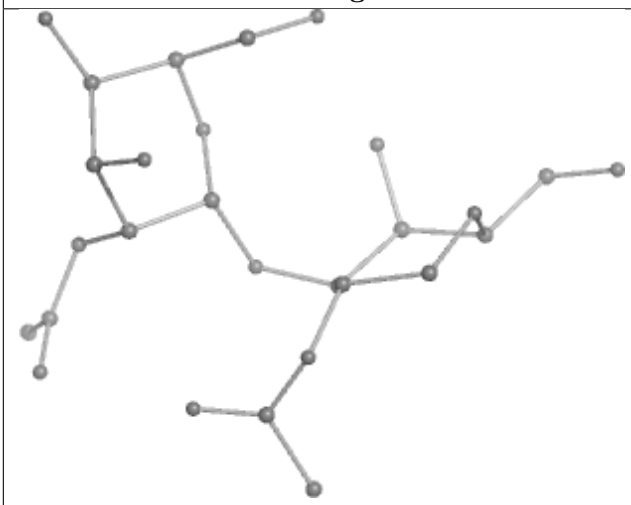
Oligosaccharide Chain bC



Bond lengths



Bond angles



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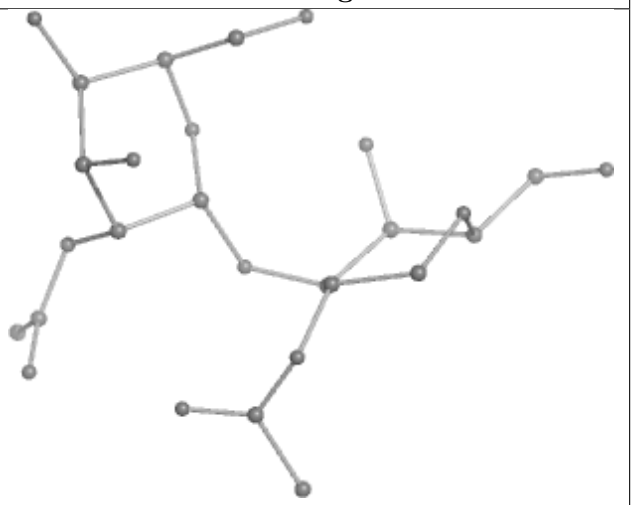
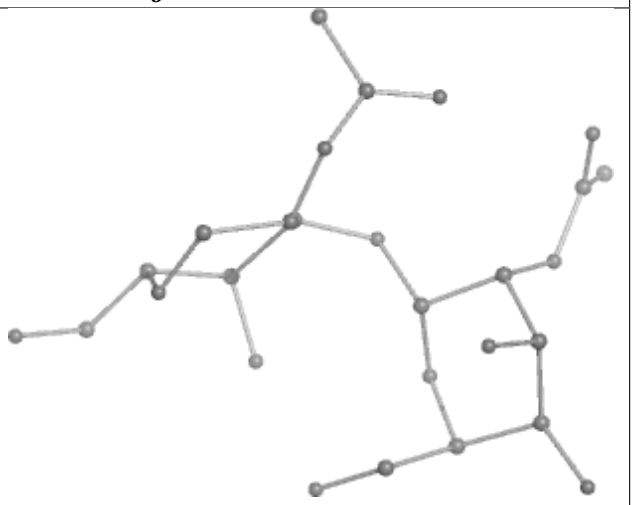


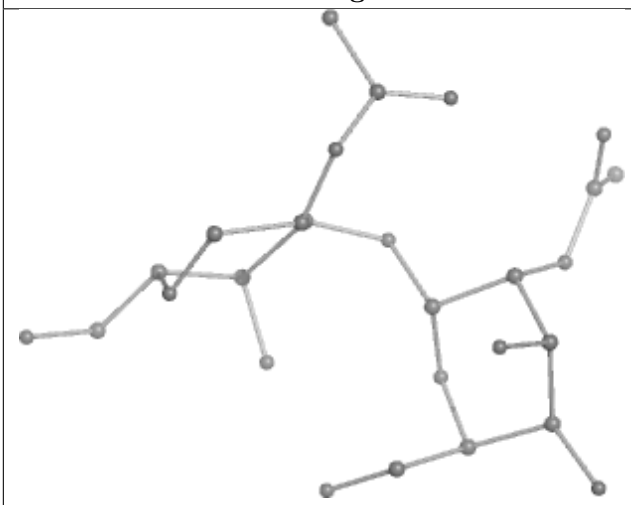
Rings

Oligosaccharide Chain jC

Bond lengths



Bond angles



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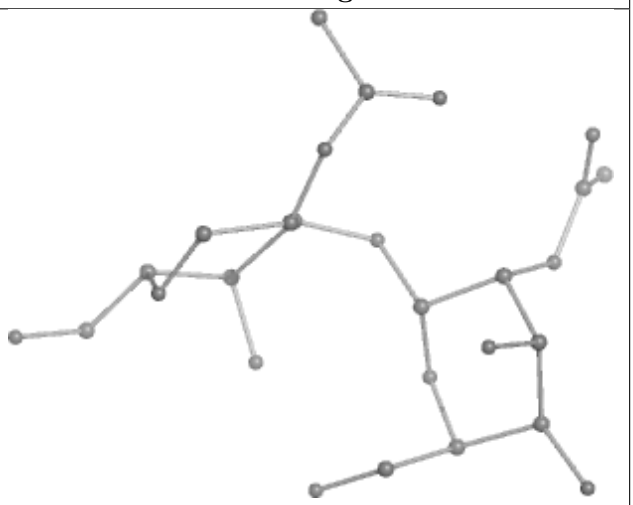
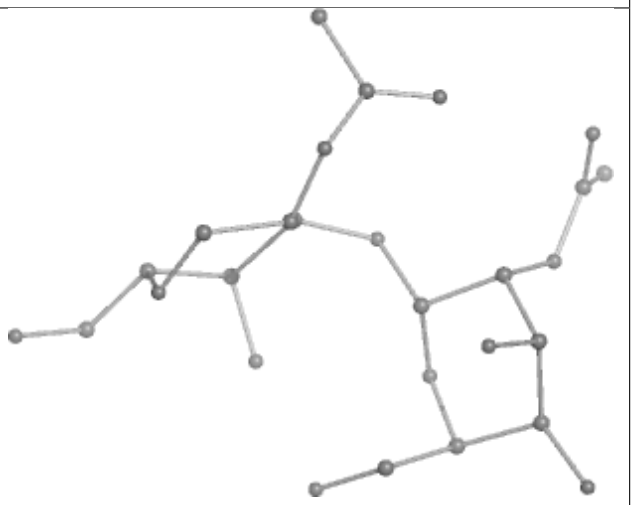


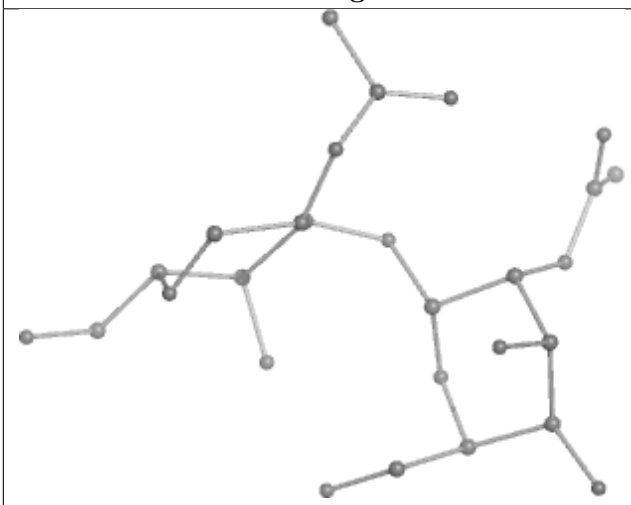
Rings

Oligosaccharide Chain rC

Bond lengths



Bond angles



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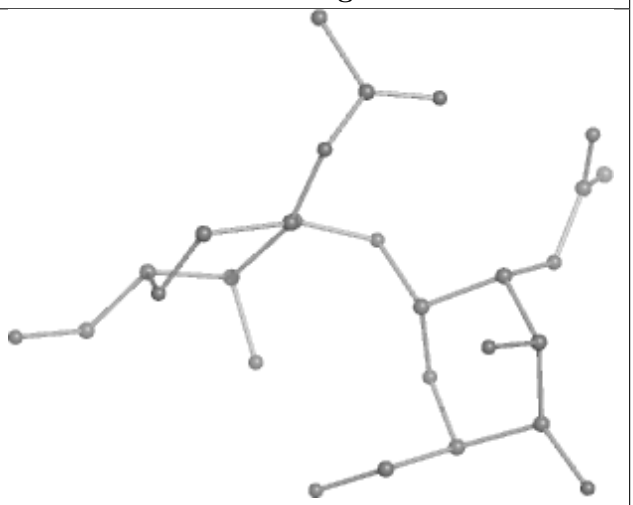
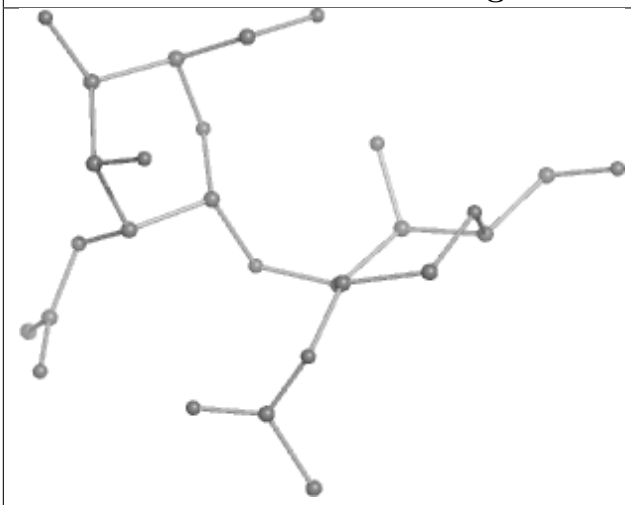
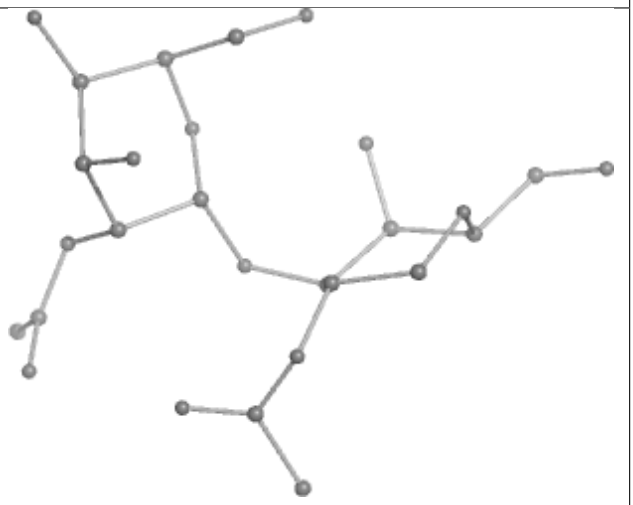


Rings

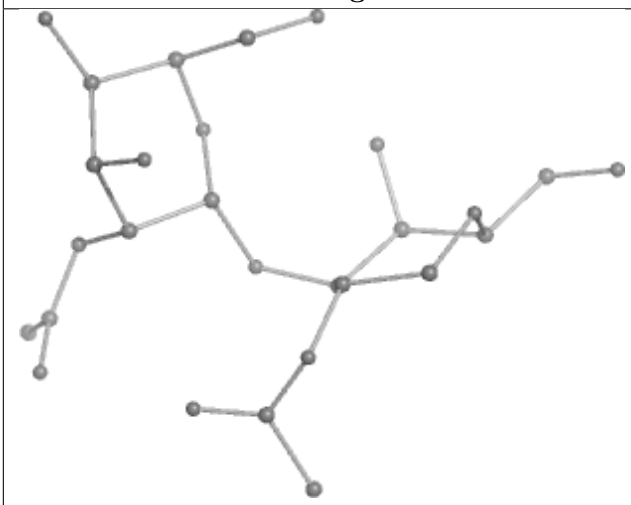
Oligosaccharide Chain zC



Bond lengths



Bond angles



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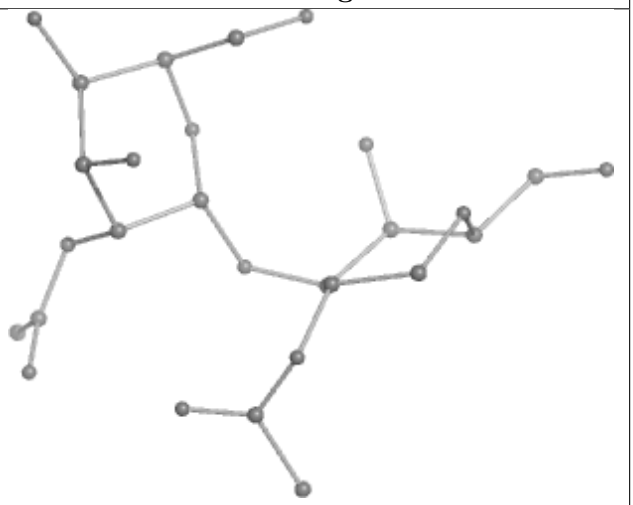
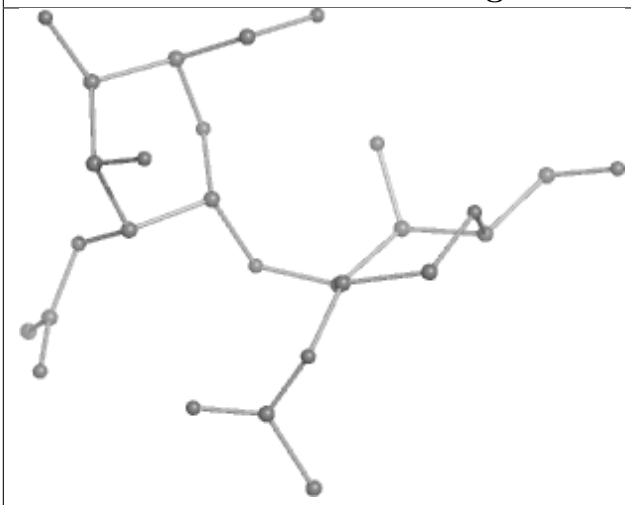


Rings

Oligosaccharide Chain 7C



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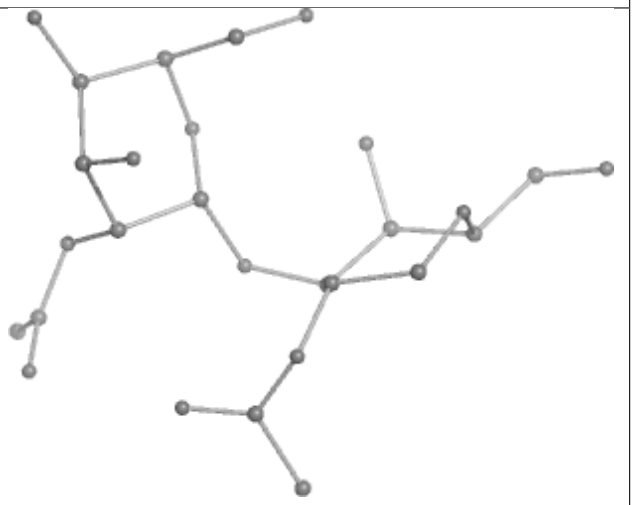

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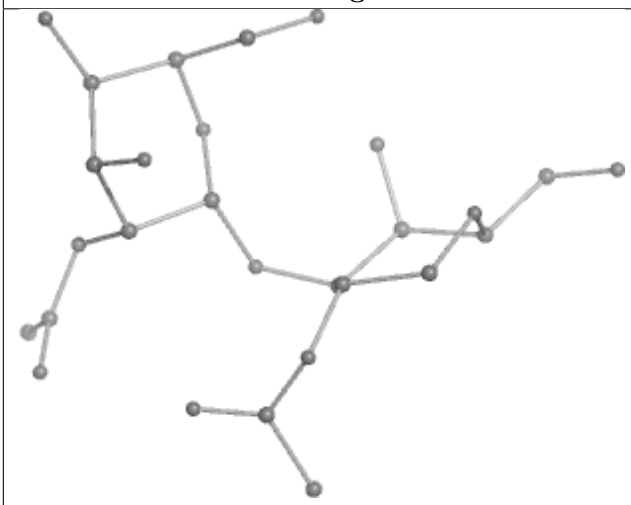

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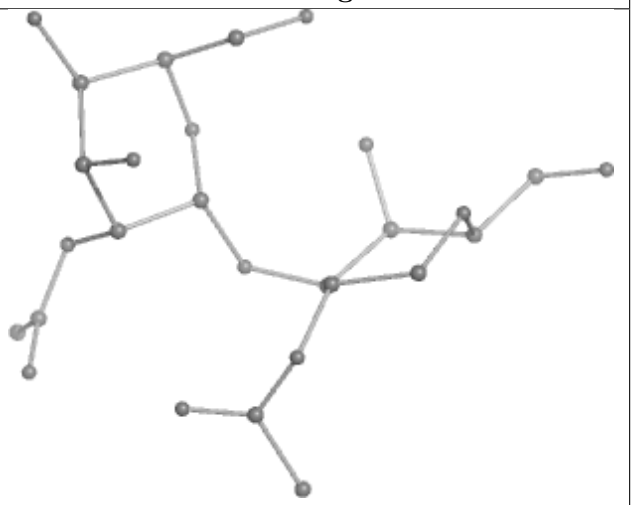
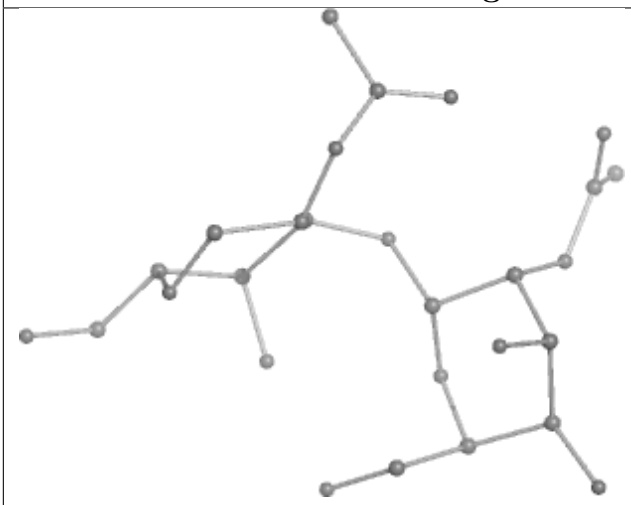


Rings

Oligosaccharide Chain FD



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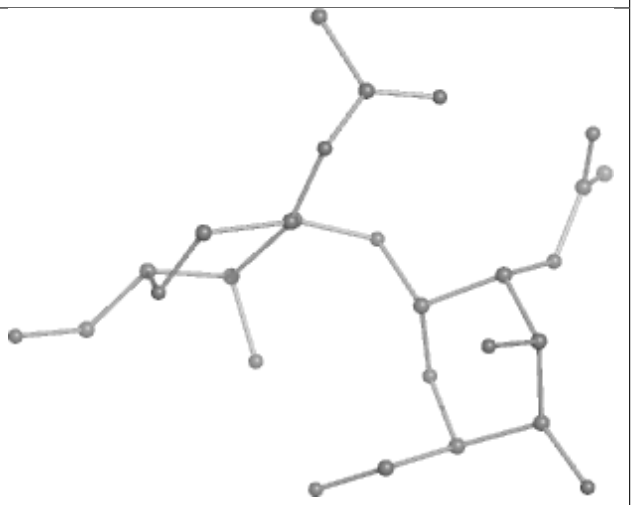
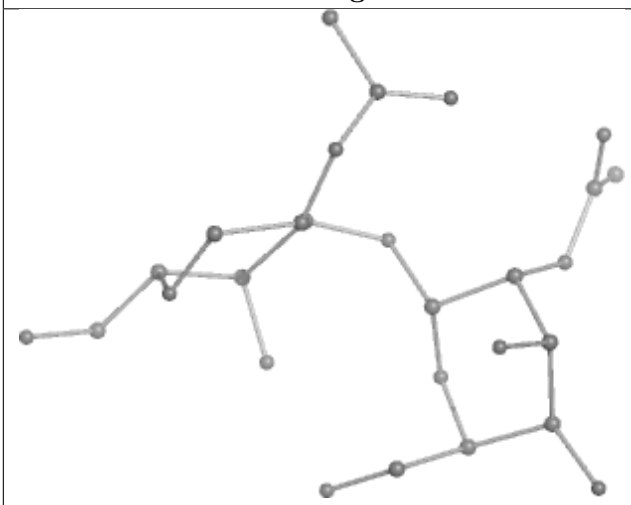
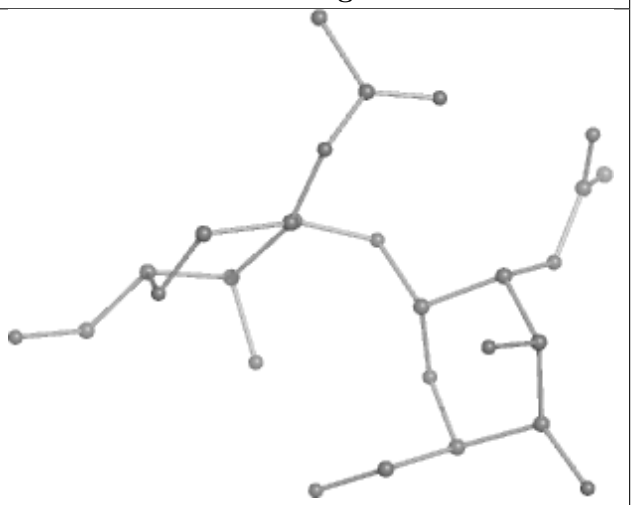


Bond angles

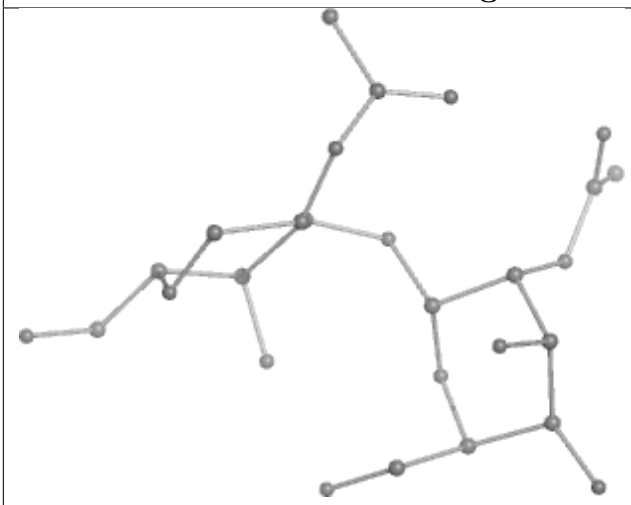


Torsions

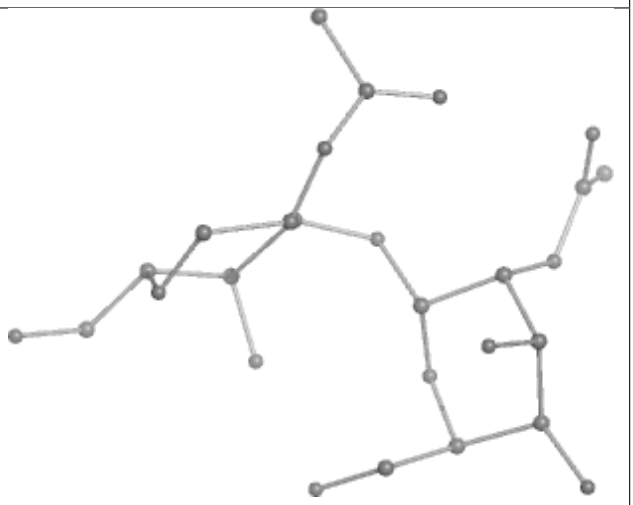


Rings

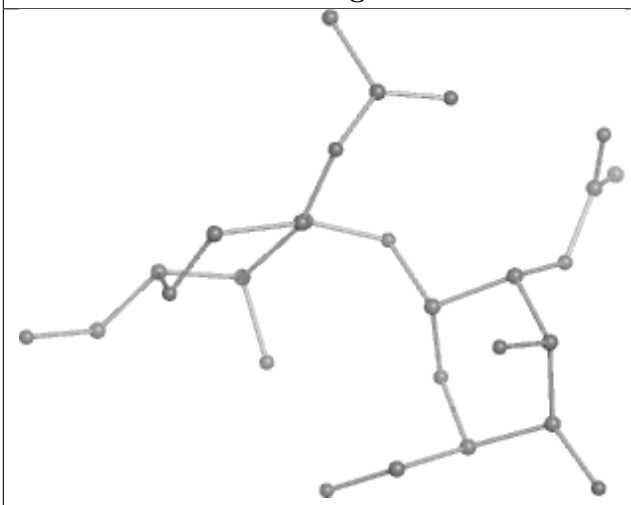
Oligosaccharide Chain ND



Bond lengths



Bond angles



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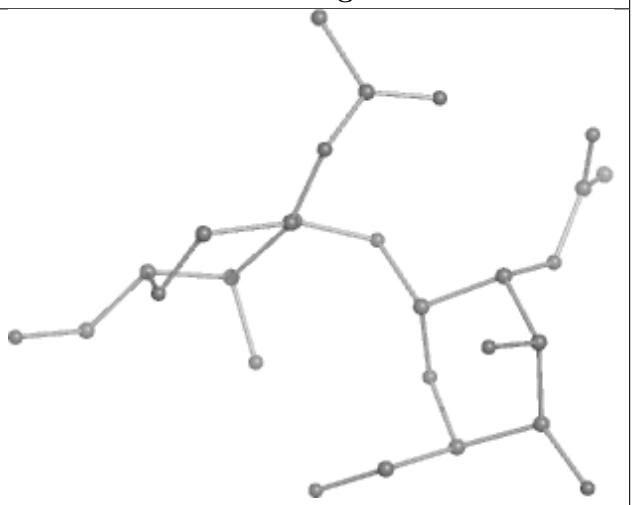
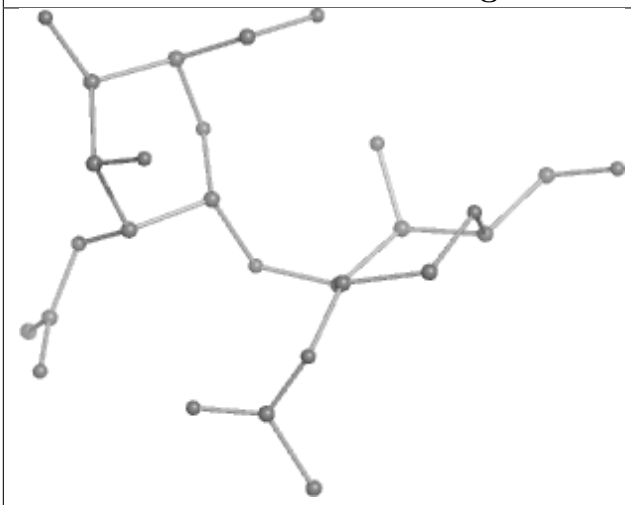
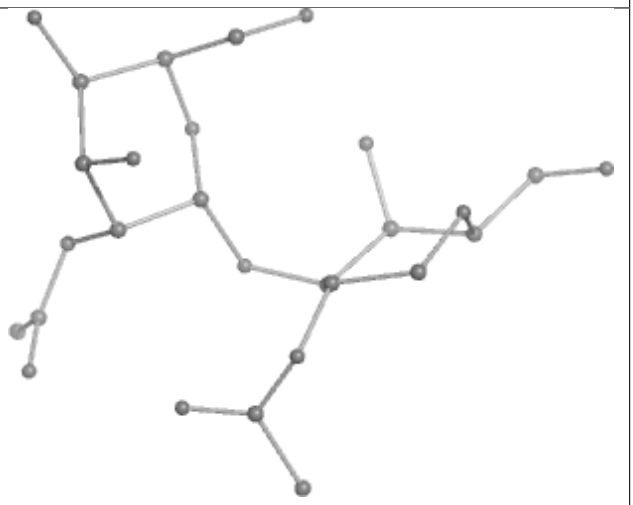


Rings

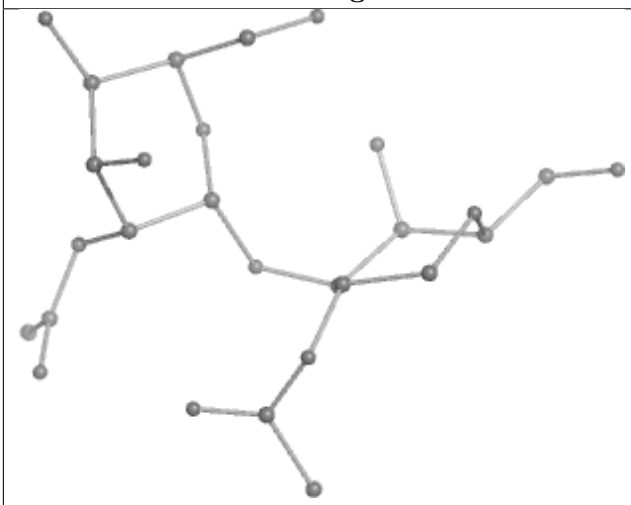
Oligosaccharide Chain VD



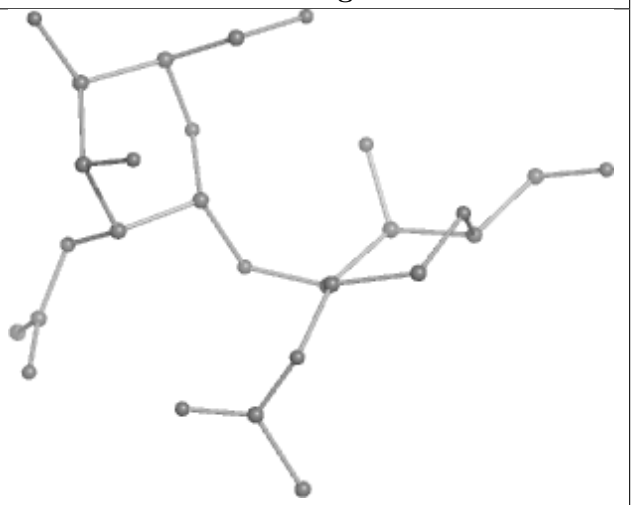
Bond lengths



Bond angles

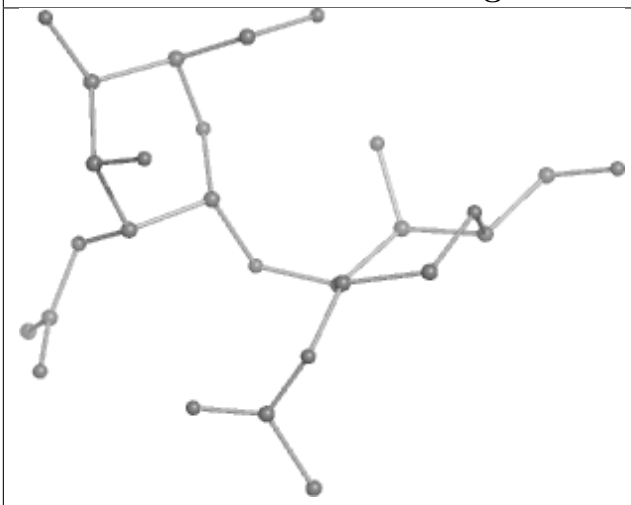


Torsions

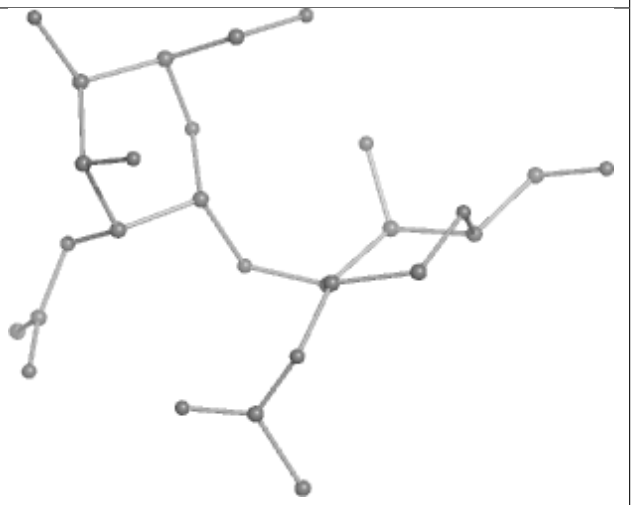


Rings

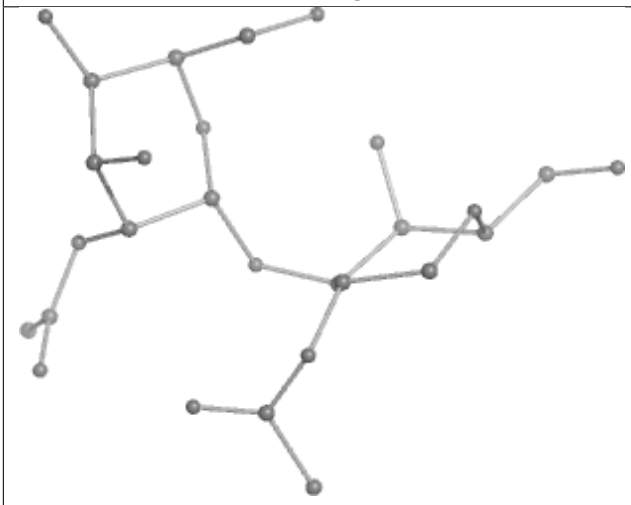
Oligosaccharide Chain dD



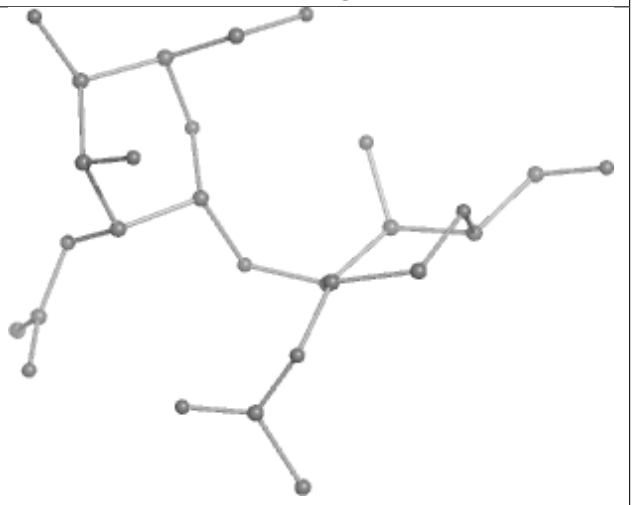
Bond lengths



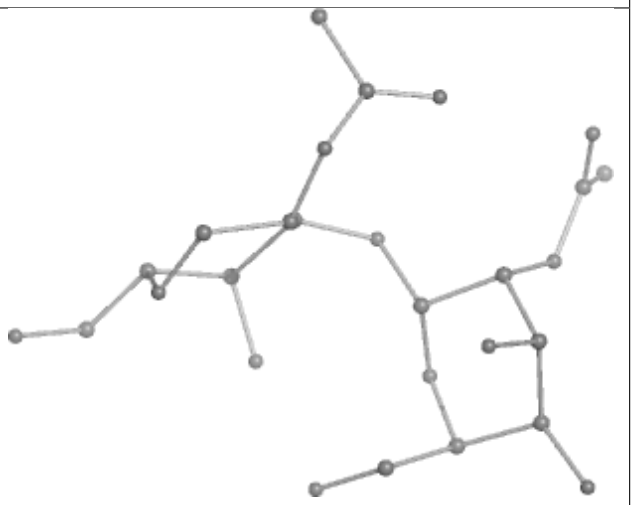
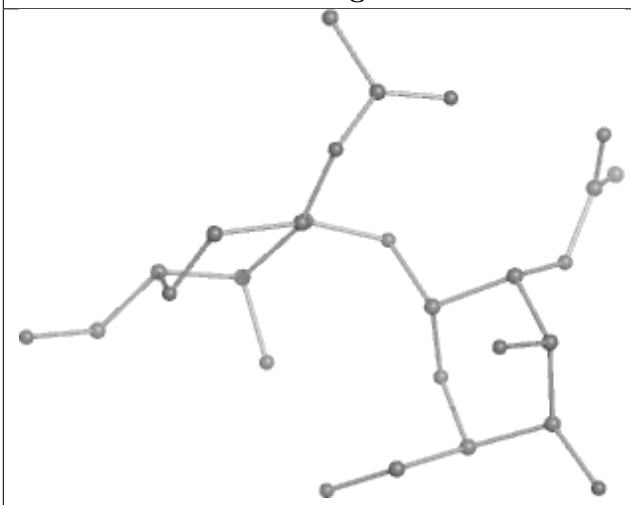
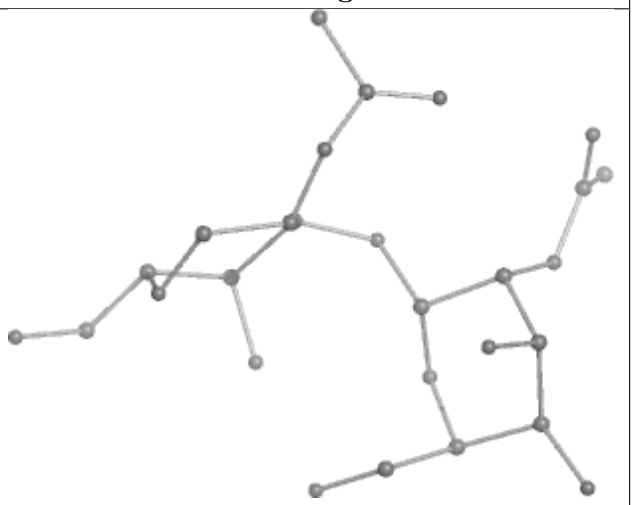
Bond angles



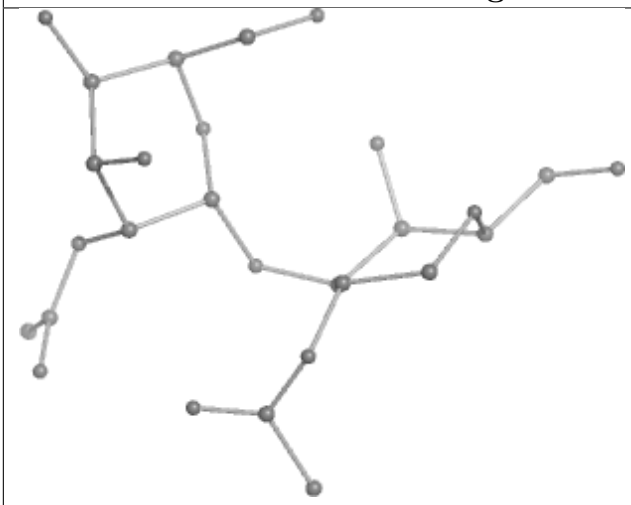
Torsions



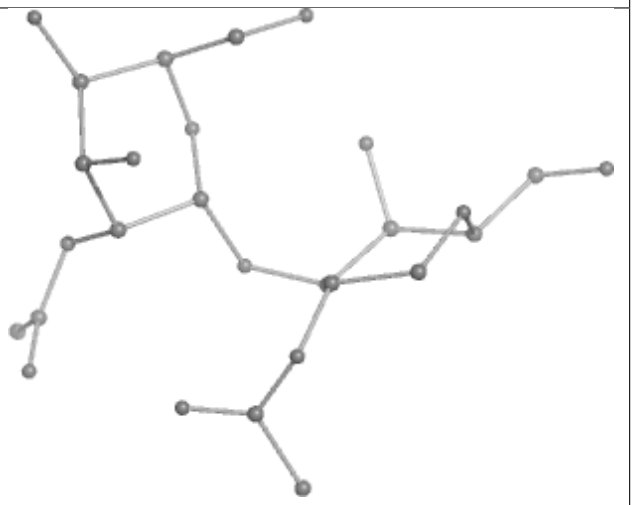
Rings

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

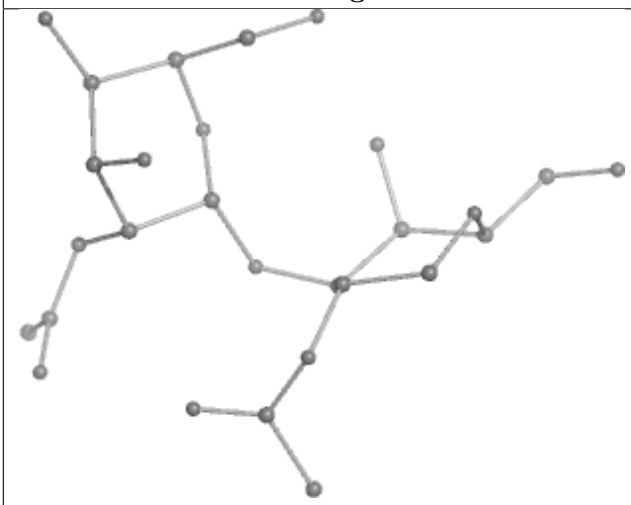
Oligosaccharide Chain tD



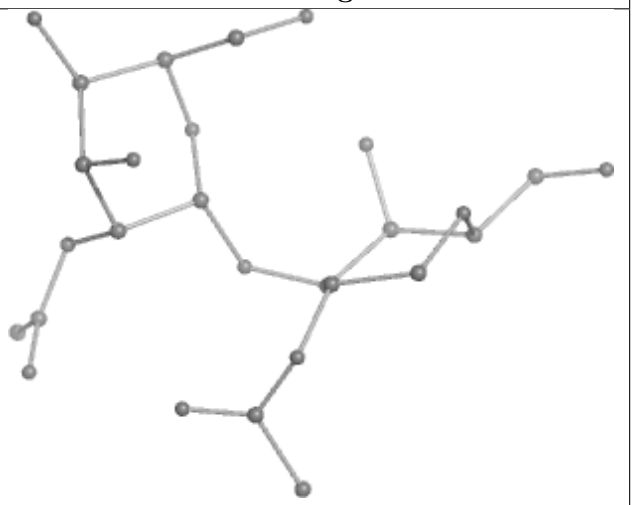
Bond lengths



Bond angles

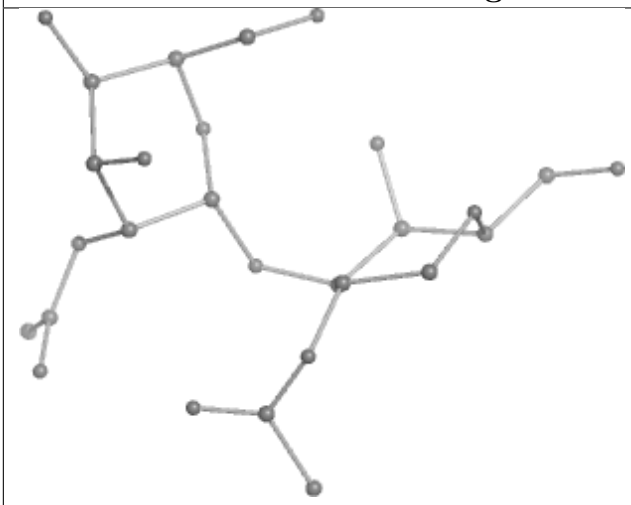


Torsions

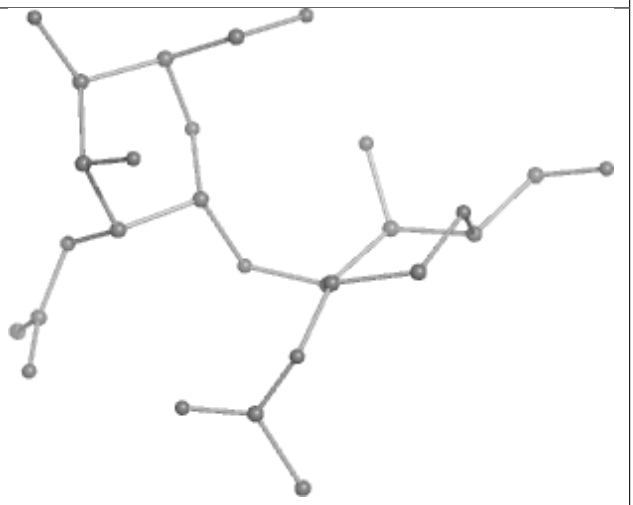


Rings

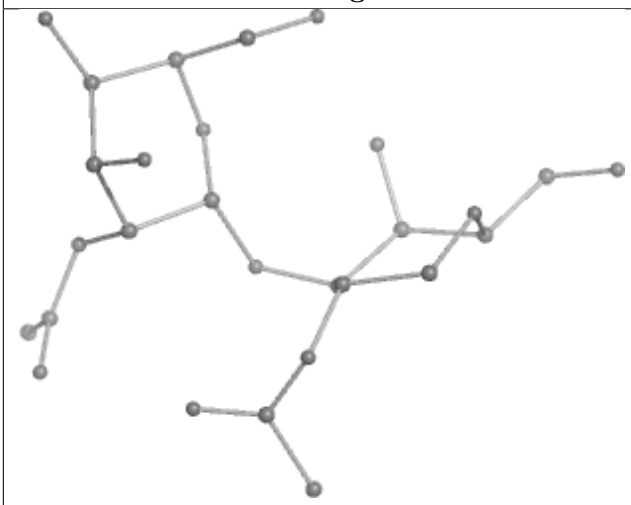
Oligosaccharide Chain 1D



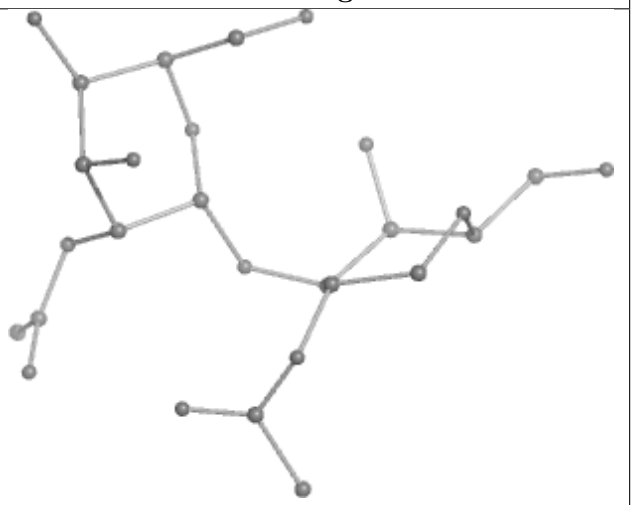
Bond lengths



Bond angles

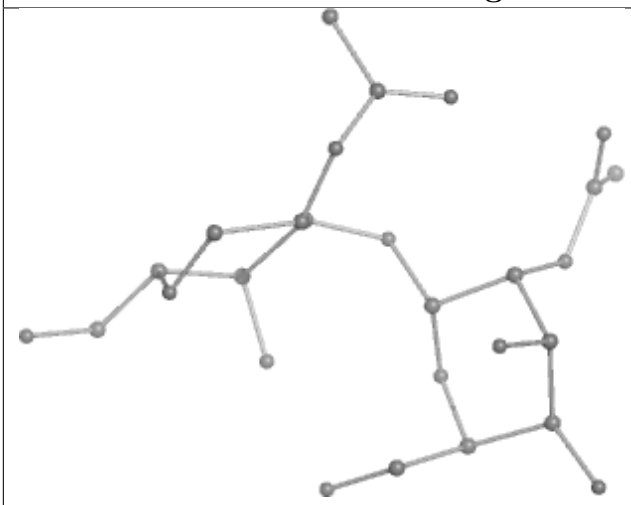


Torsions



Rings

Oligosaccharide Chain 9D



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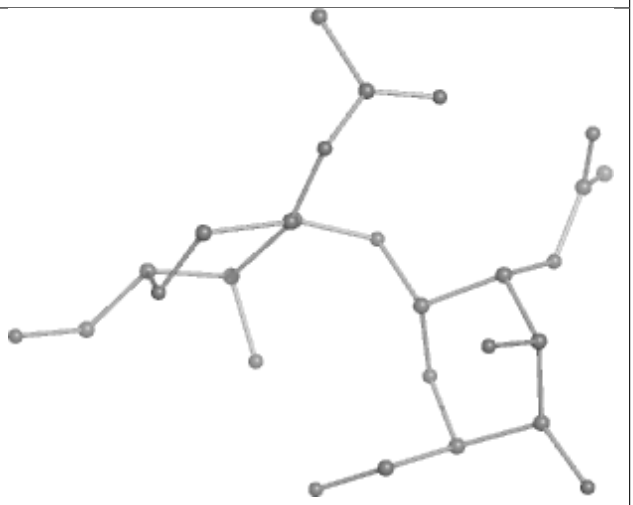
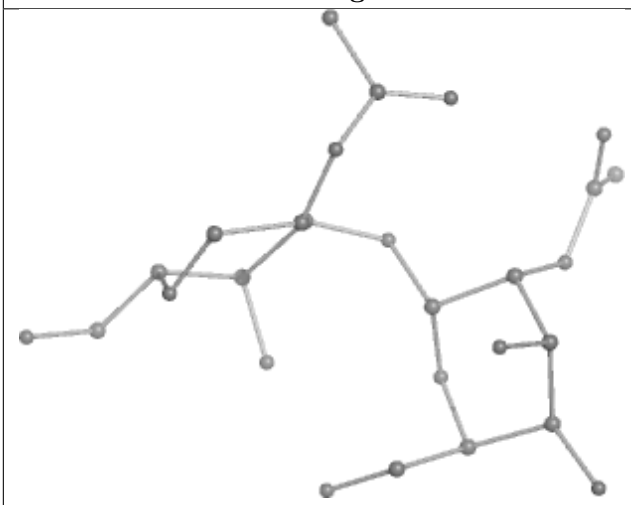


Bond angles



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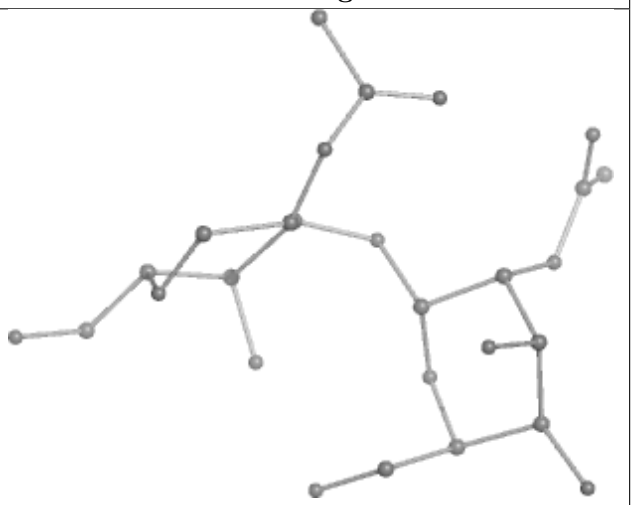
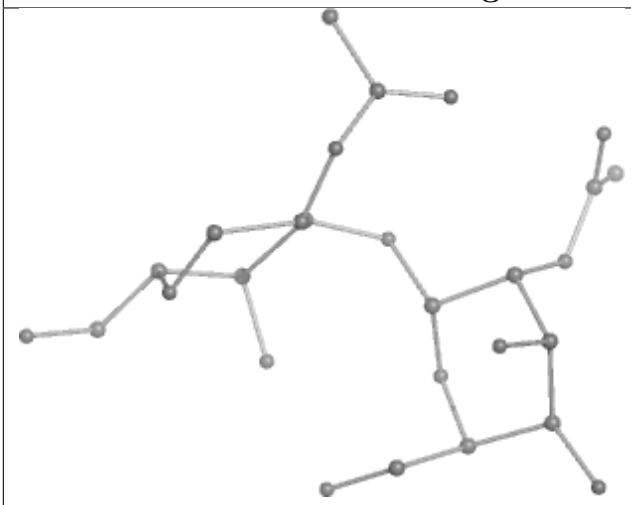
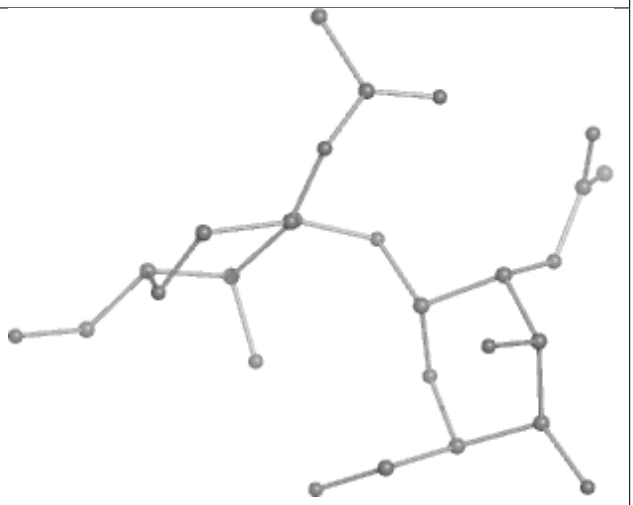


Rings

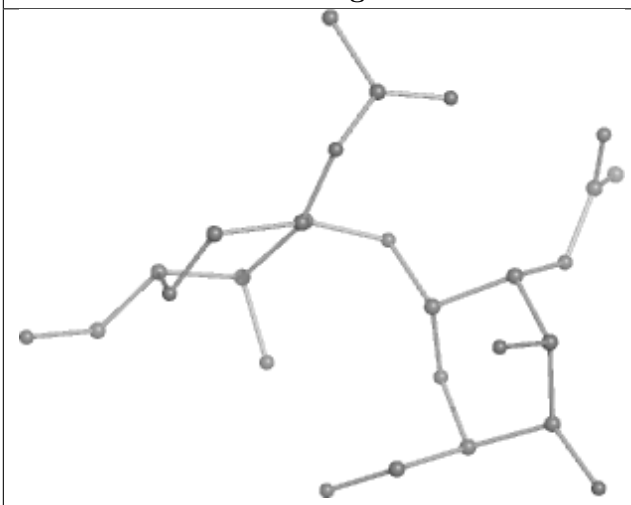
Oligosaccharide Chain HE



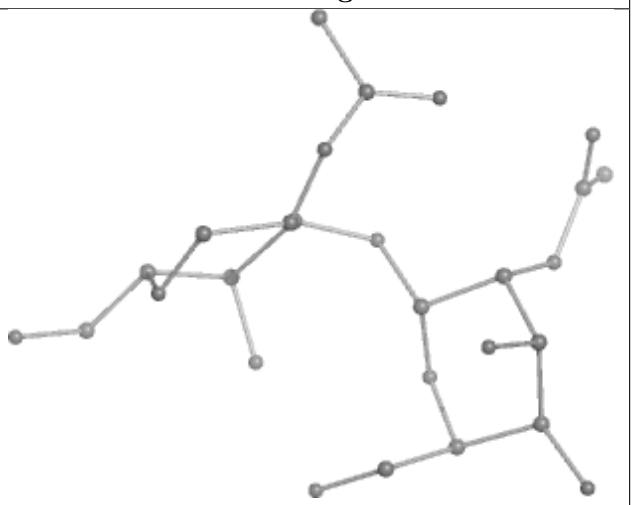
Bond lengths



Bond angles

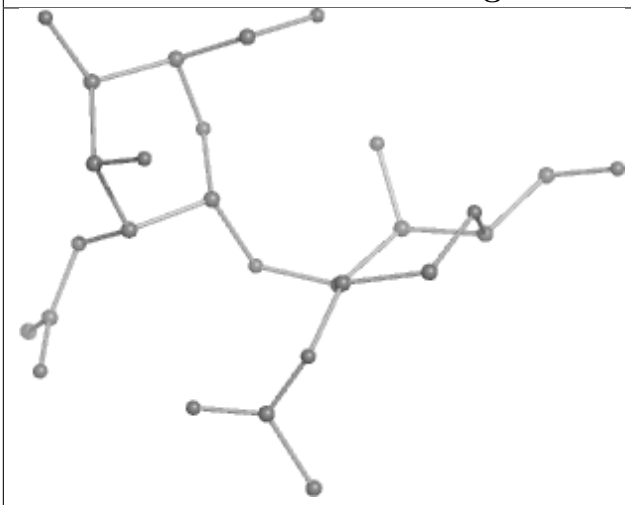


Torsions

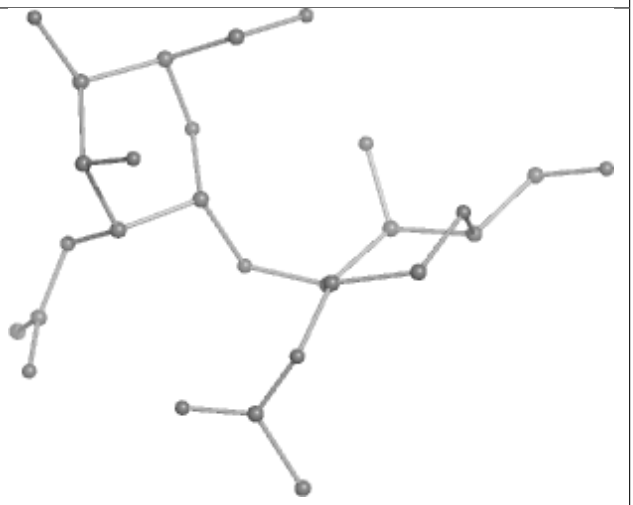


Rings

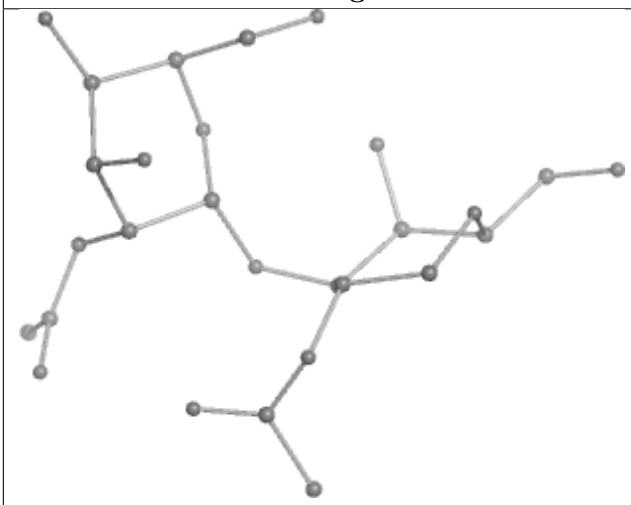
Oligosaccharide Chain PE



Bond lengths



Bond angles



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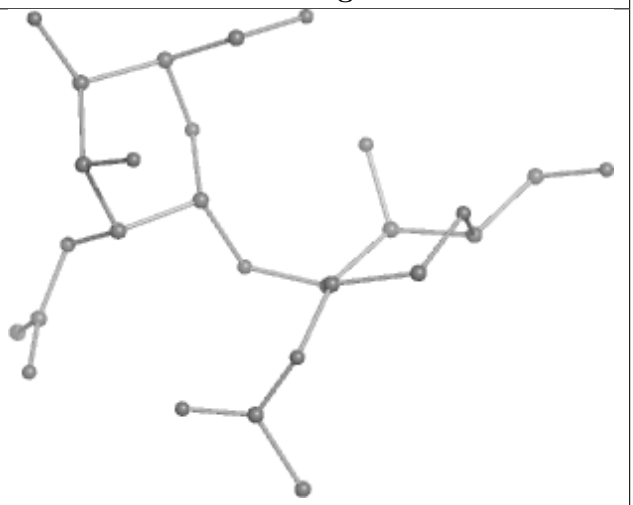
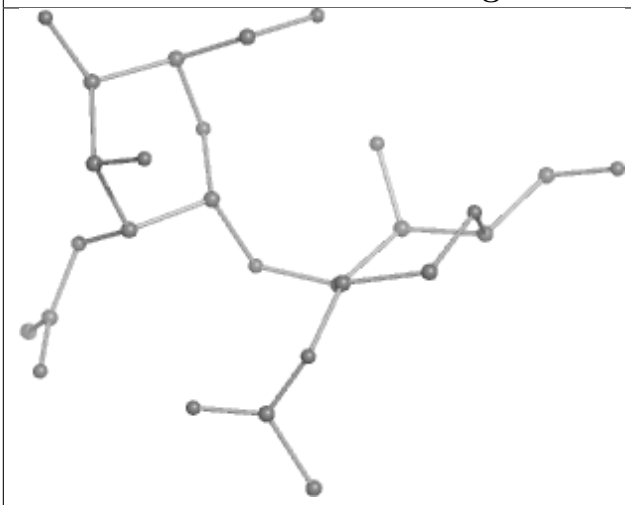
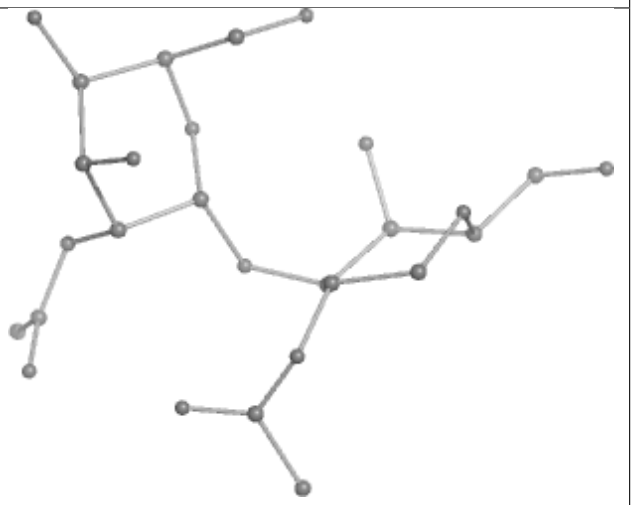


Rings

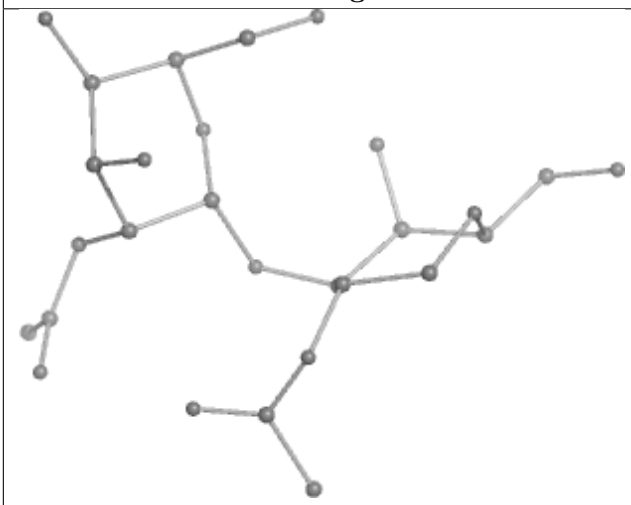
Oligosaccharide Chain XE



Bond lengths



Bond angles



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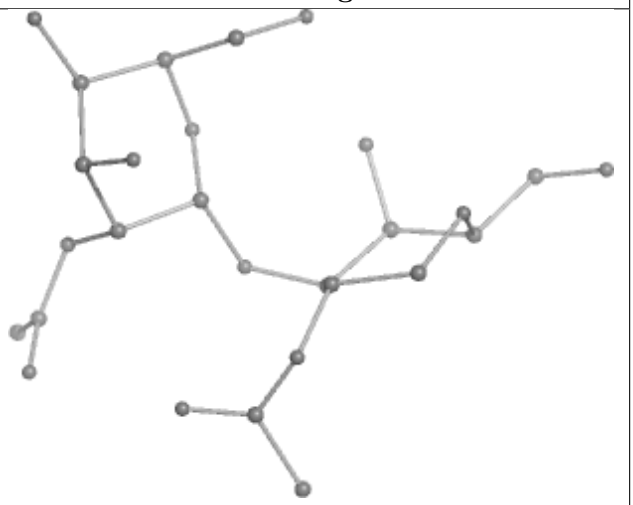
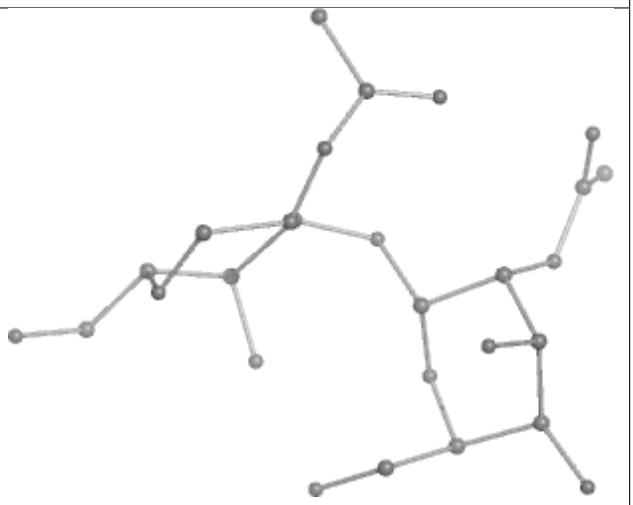


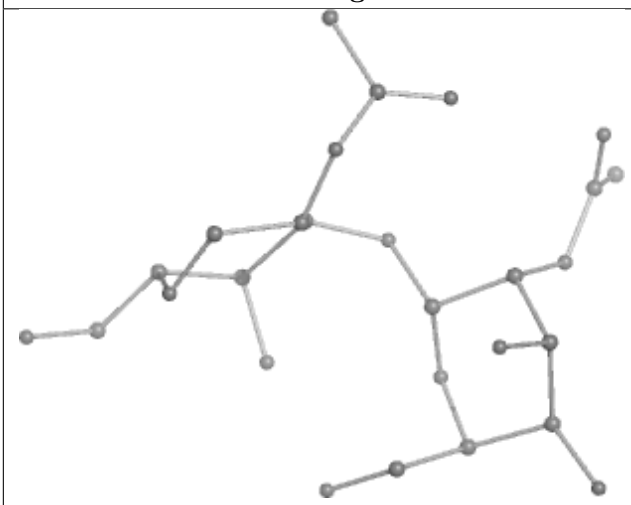
Rings

Oligosaccharide Chain fE

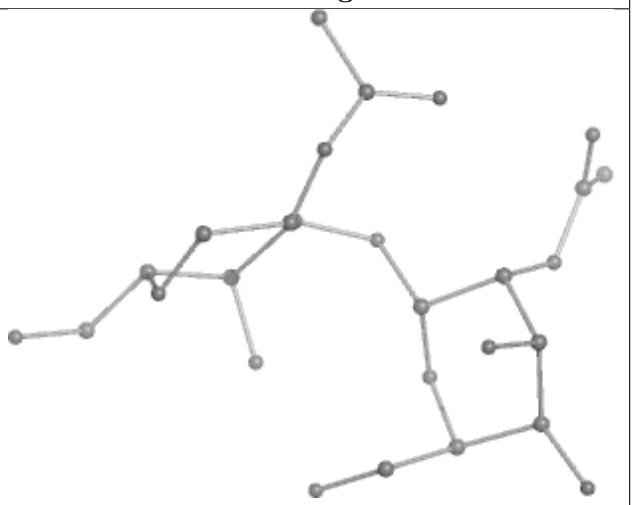
Bond lengths



Bond angles



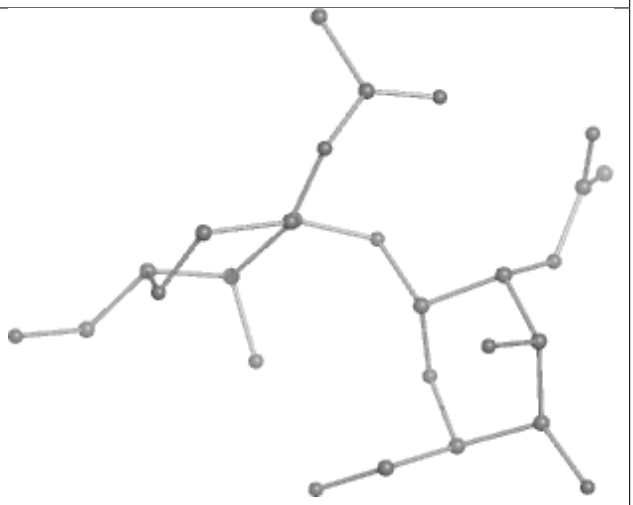
Torsions



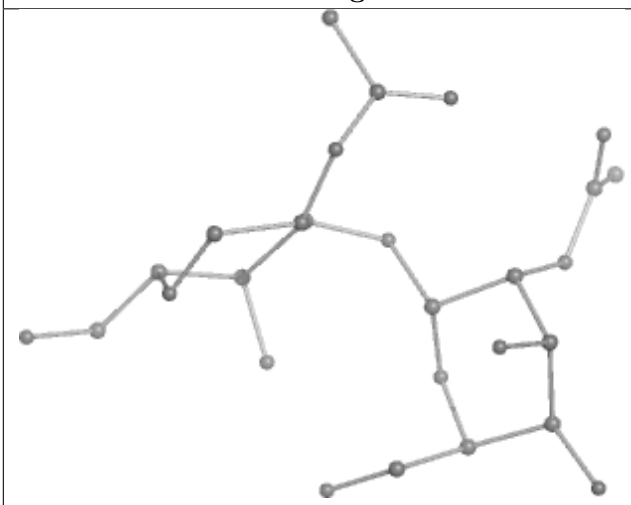
Rings

Oligosaccharide Chain nE

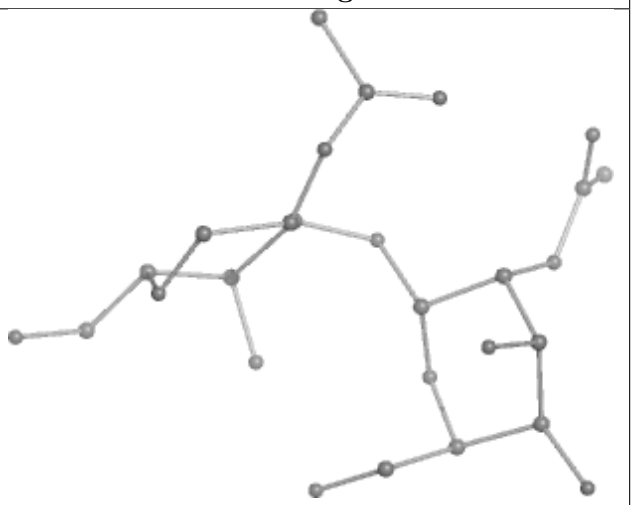
Bond lengths



Bond angles

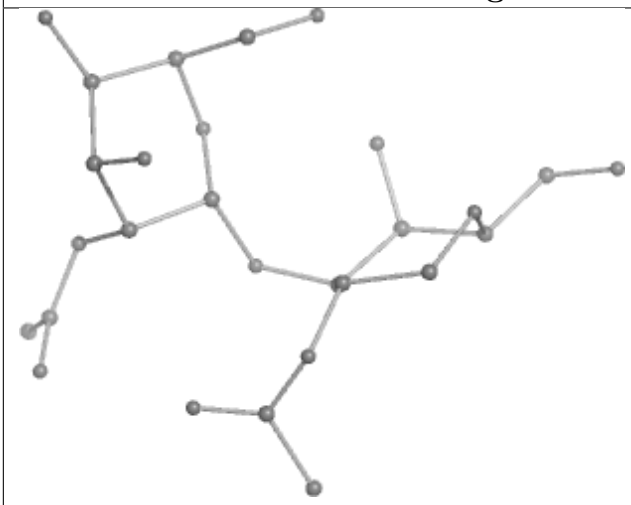


Torsions

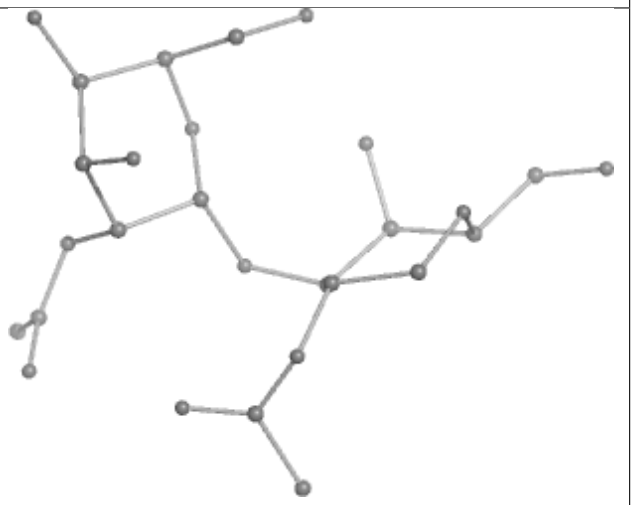


Rings

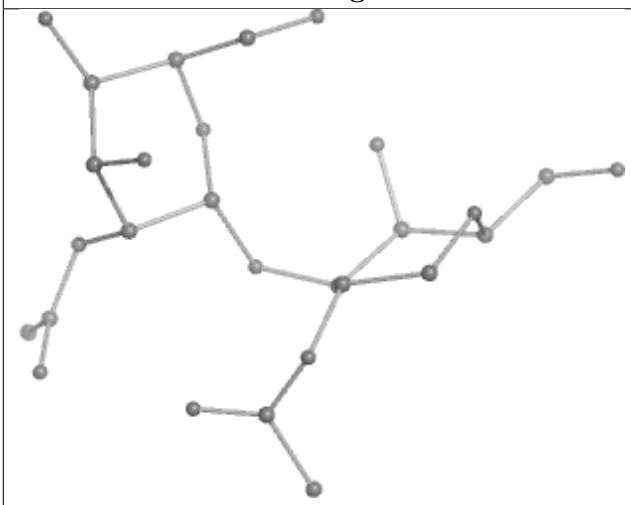
Oligosaccharide Chain vE



Bond lengths



Bond angles



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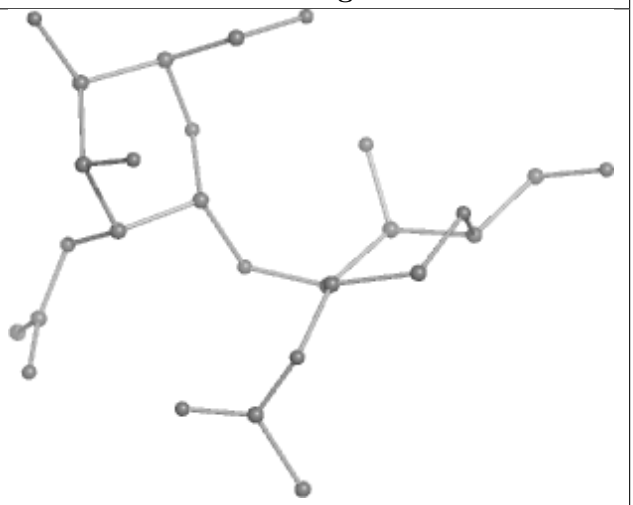
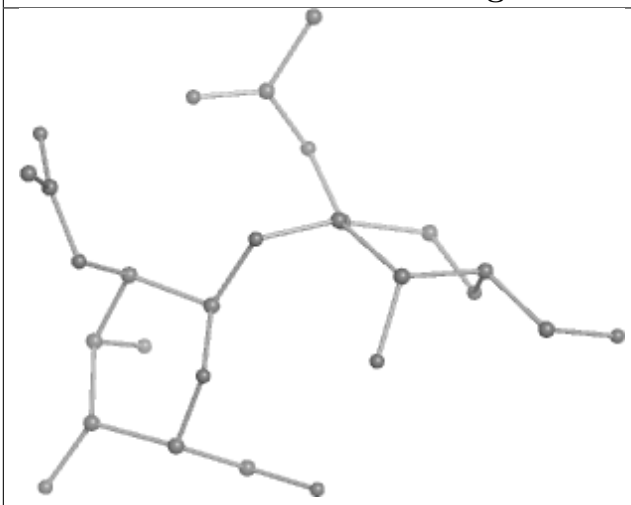


Rings

Oligosaccharide Chain 3E



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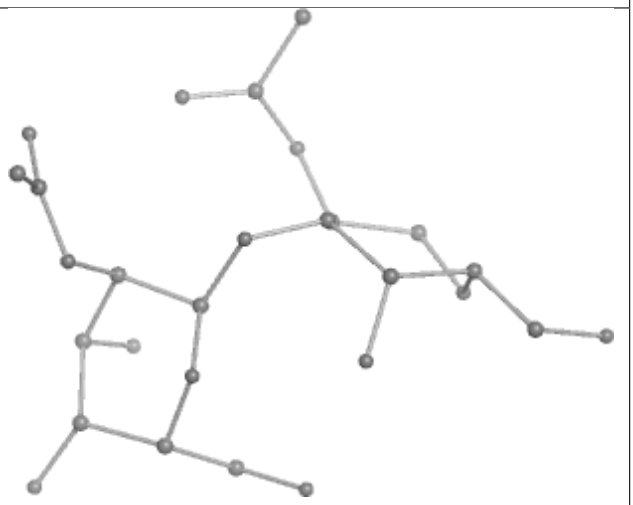

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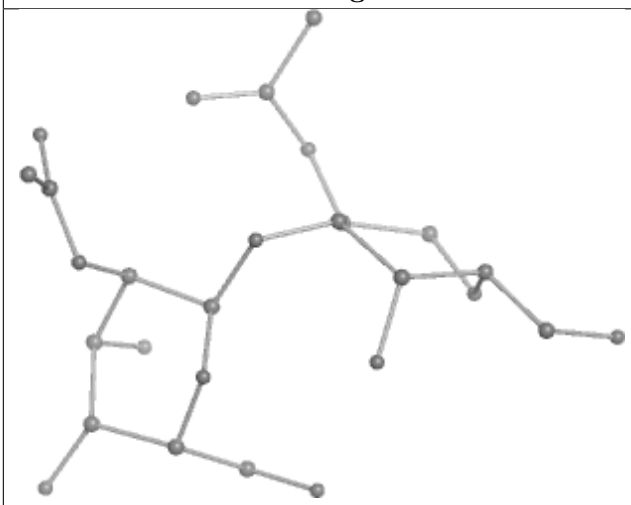

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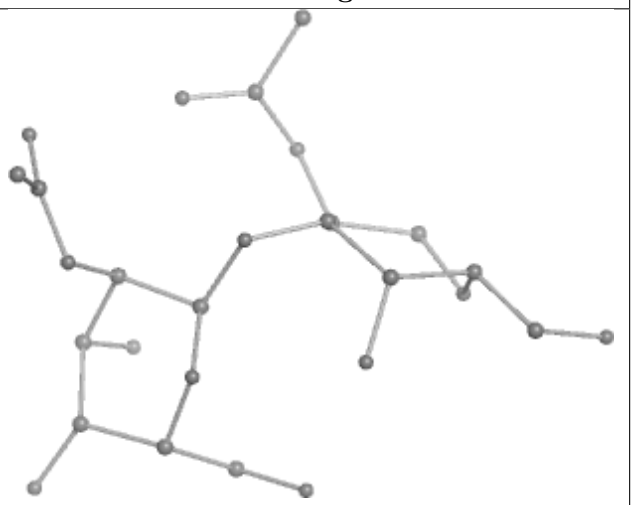
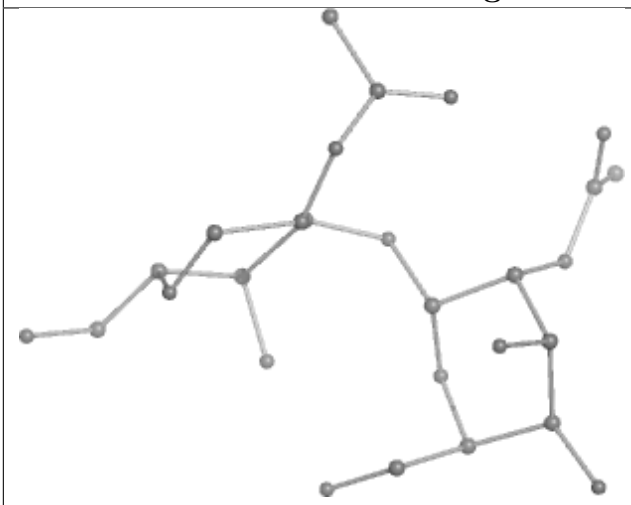
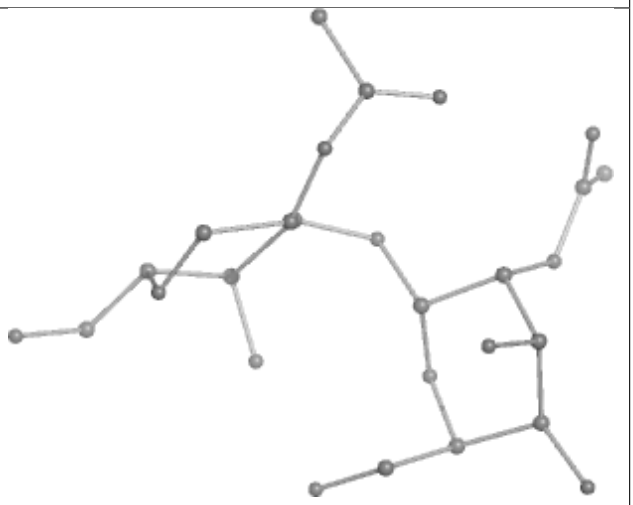


Rings

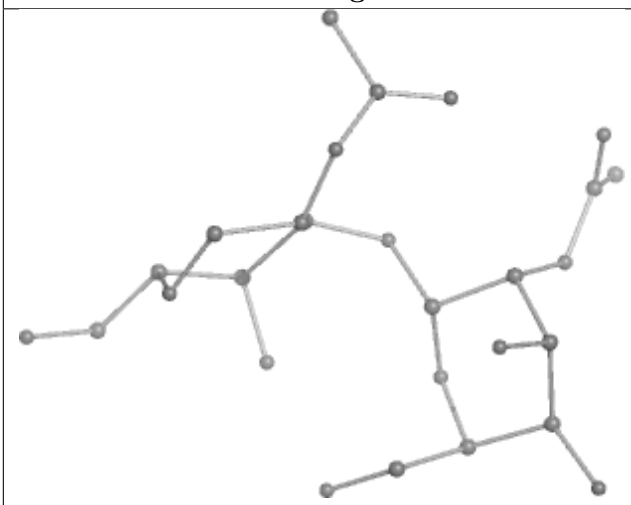
Oligosaccharide Chain BF



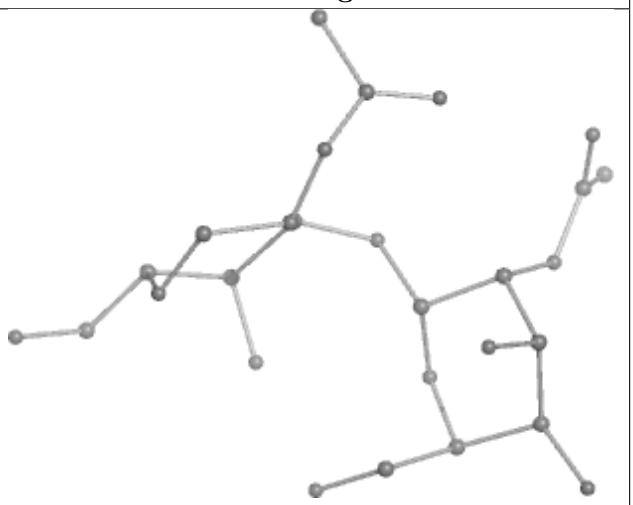
Bond lengths



Bond angles

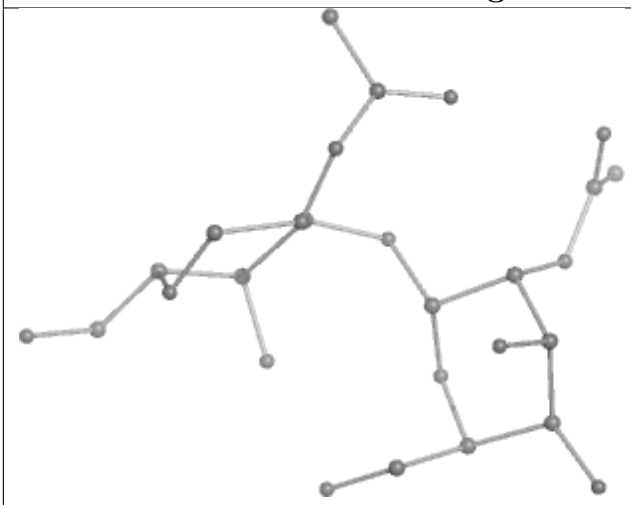


Torsions



Rings

Oligosaccharide Chain JF



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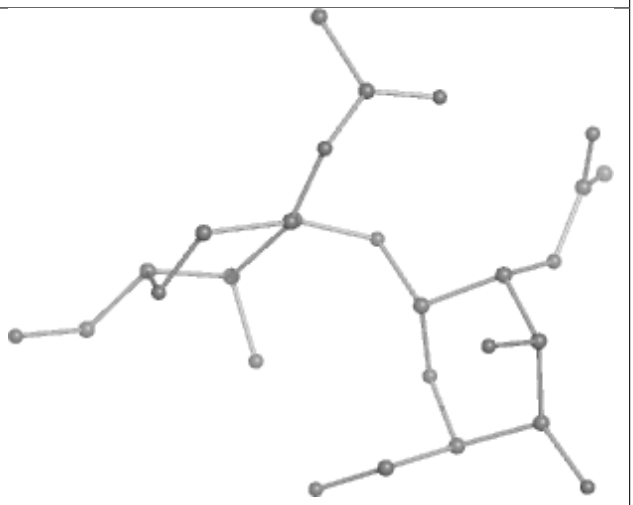
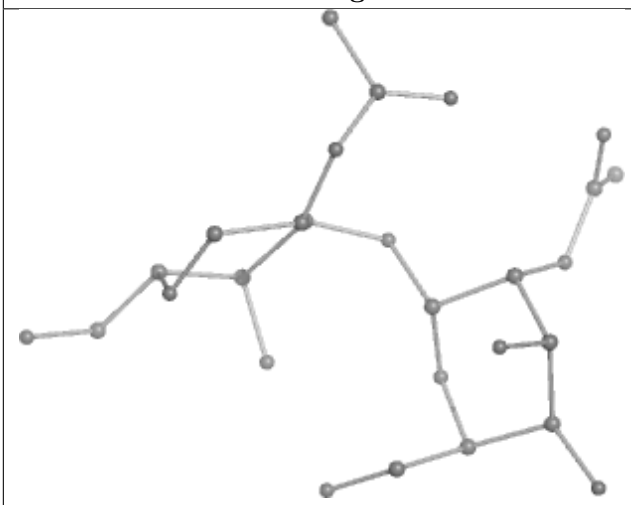


Bond angles



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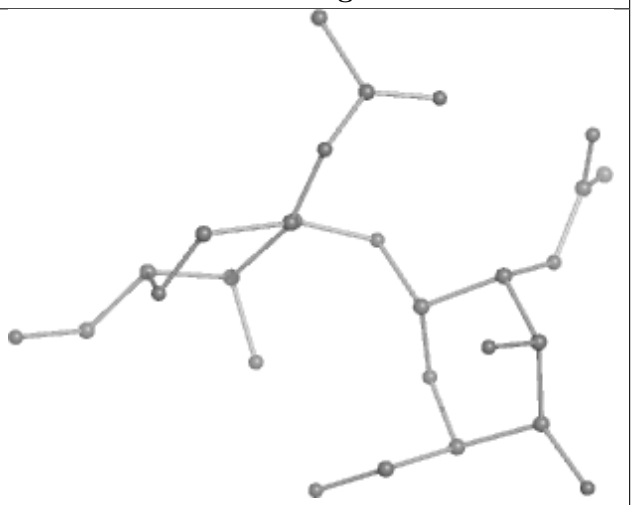
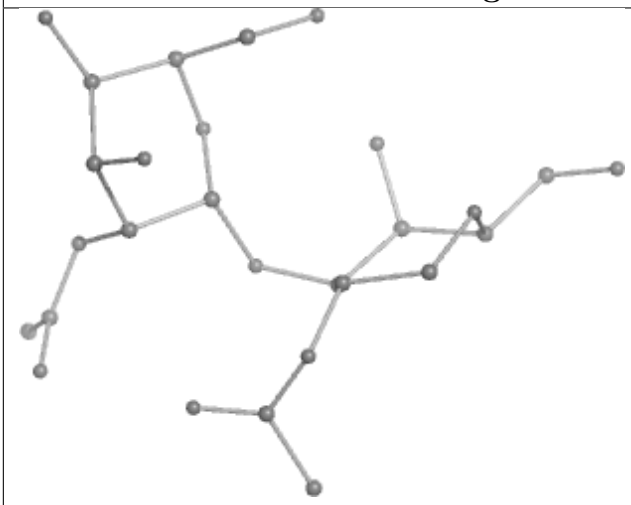


Rings

Oligosaccharide Chain RF



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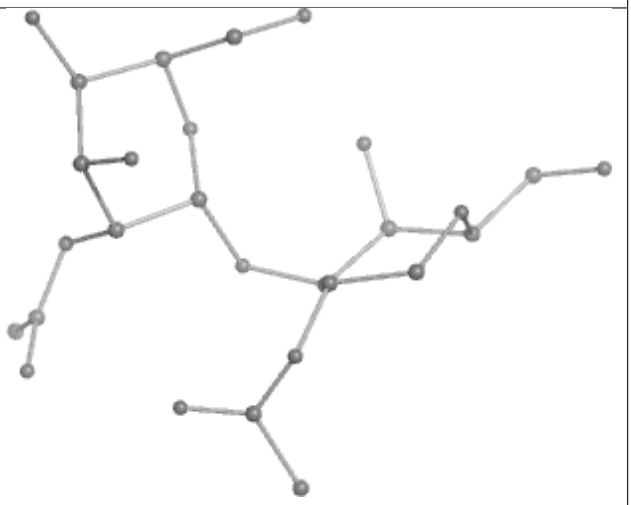
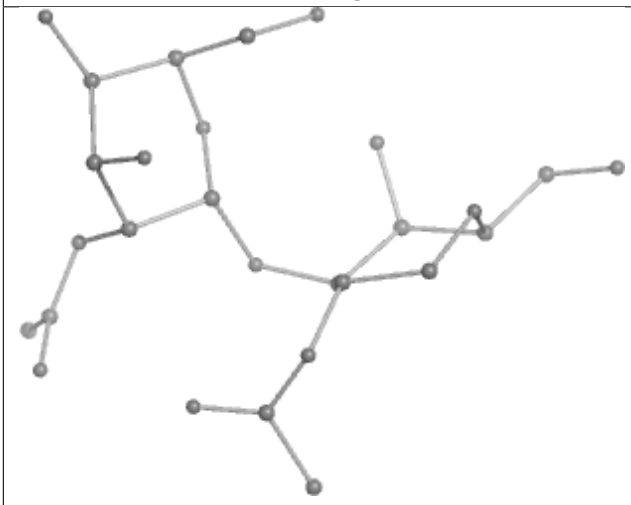


Bond angles



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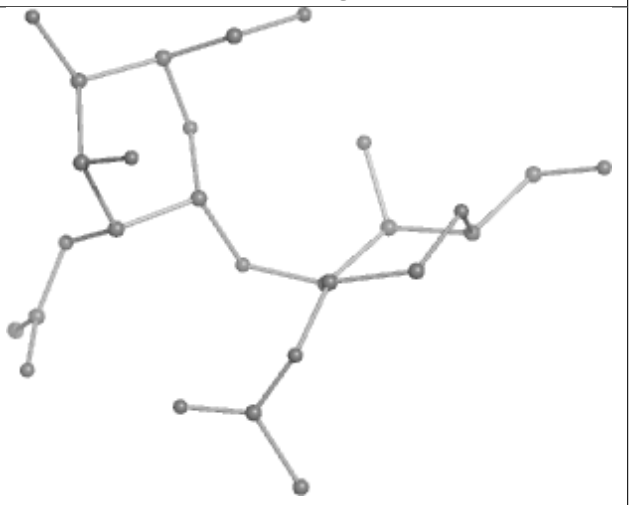
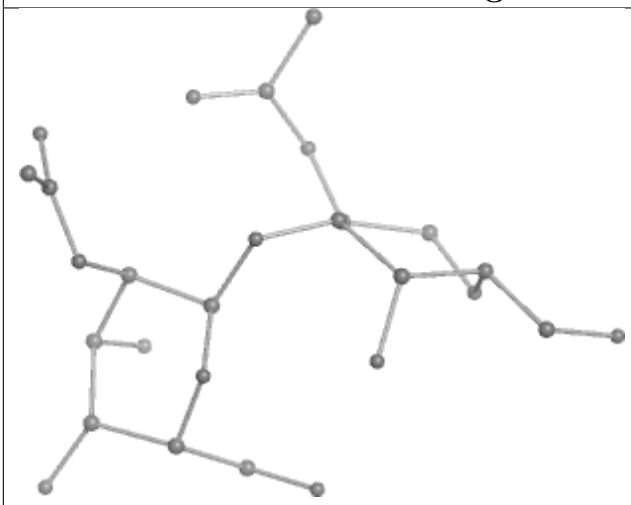


Rings

Oligosaccharide Chain ZF



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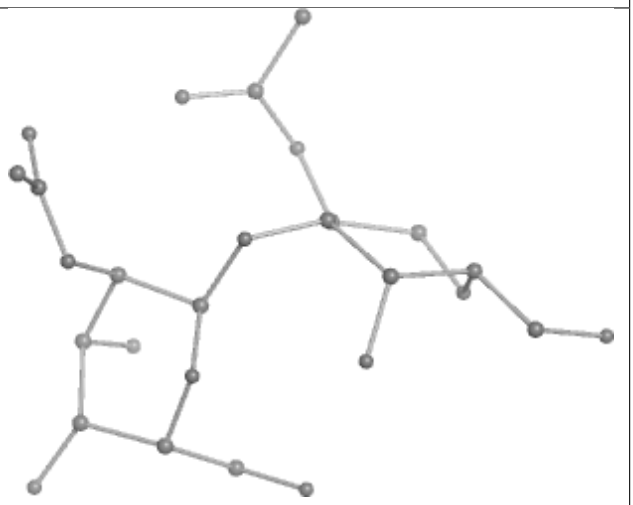
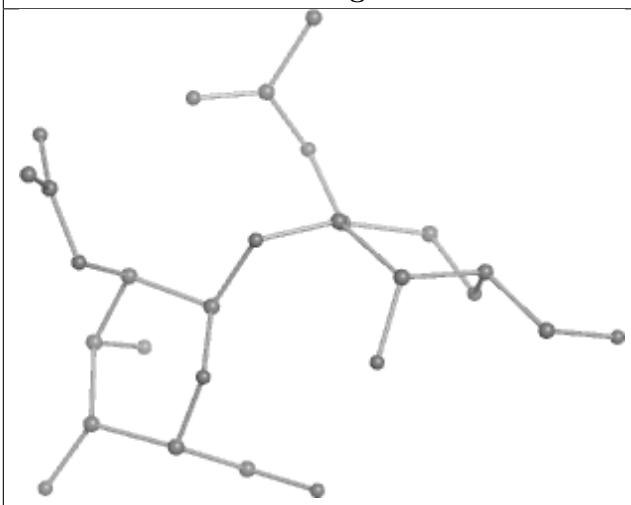


Bond angles



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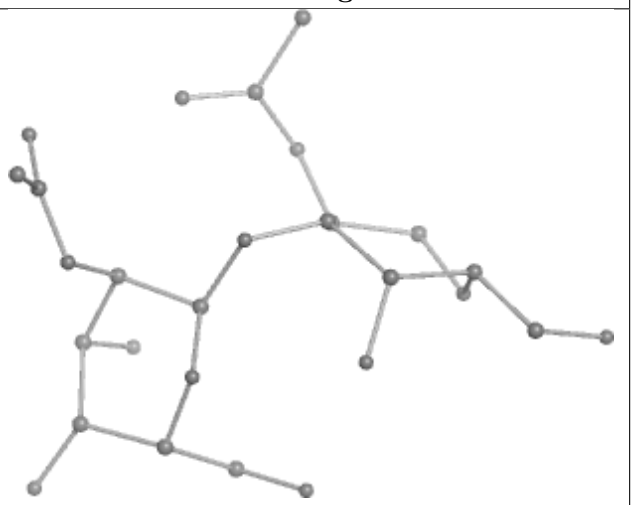
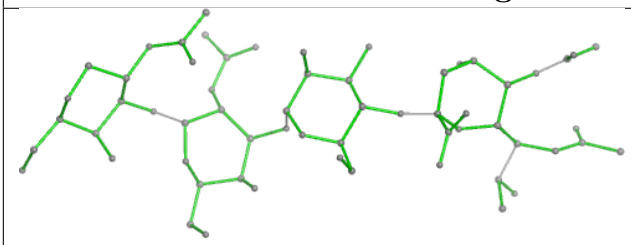
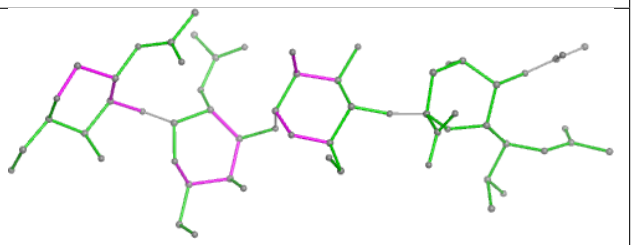


Rings

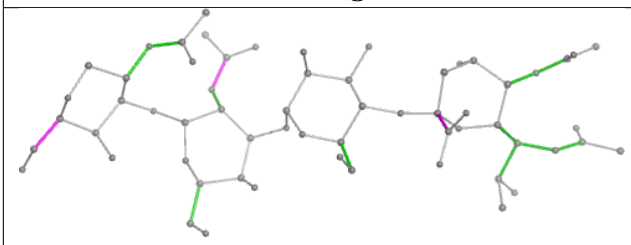
Oligosaccharide Chain w



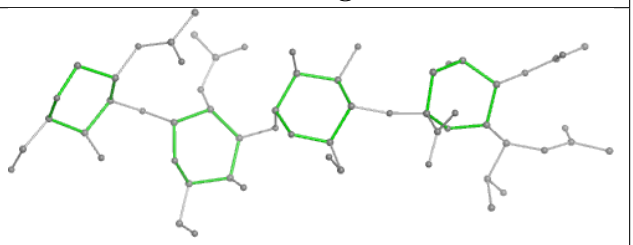
Bond lengths



Bond angles

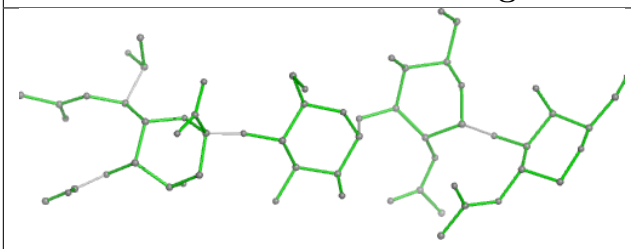


Torsions

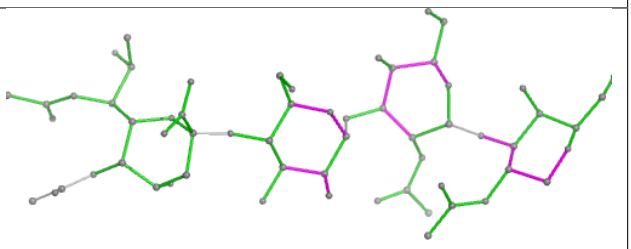


Rings

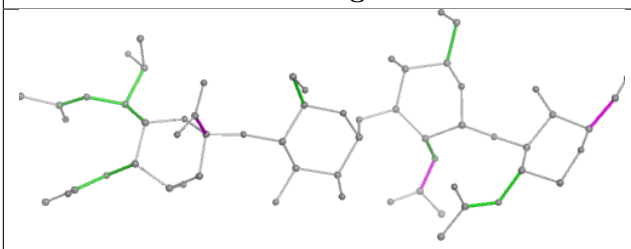
Oligosaccharide Chain 4



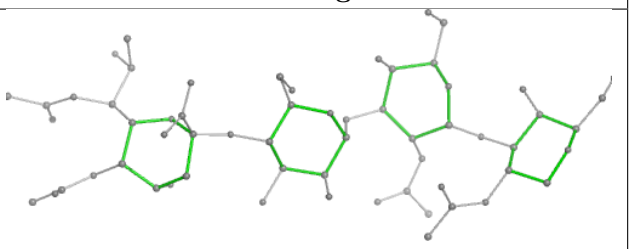
Bond lengths



Bond angles

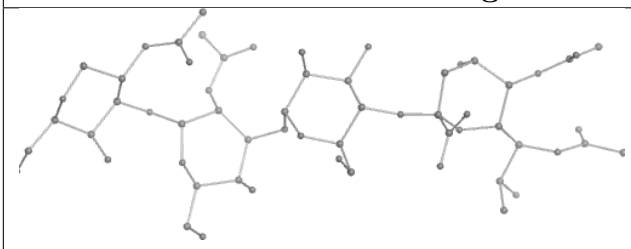


Torsions

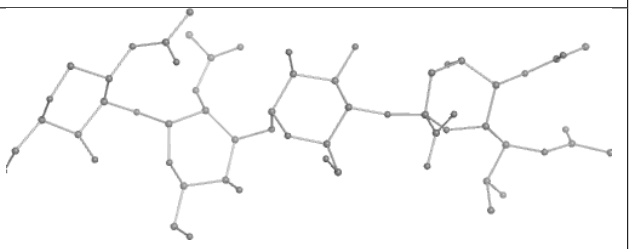


Rings

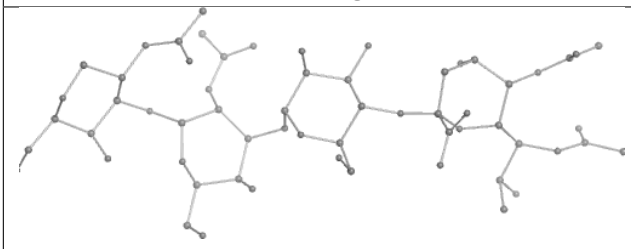
Oligosaccharide Chain CA



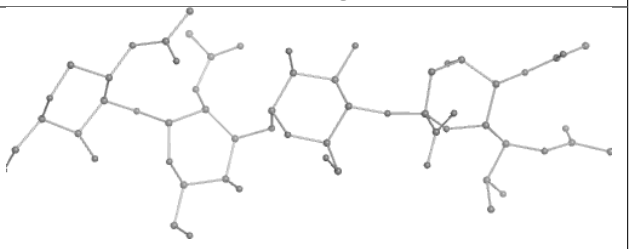
Bond lengths



Bond angles

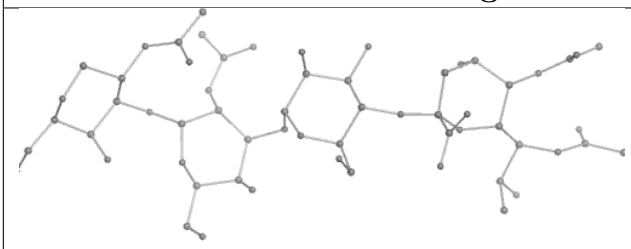


Torsions



Rings

Oligosaccharide Chain KA



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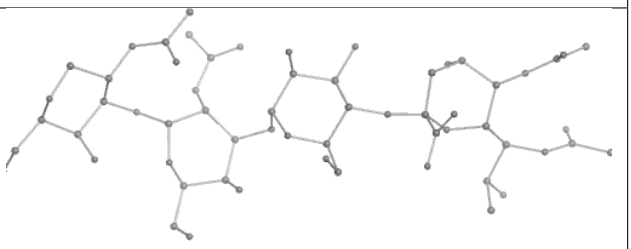
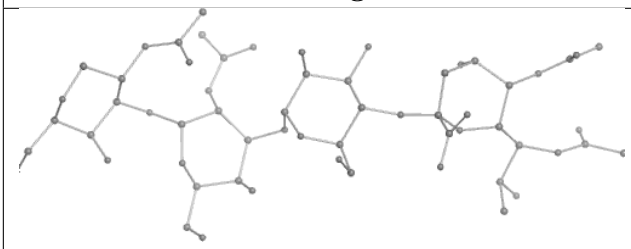


Bond angles



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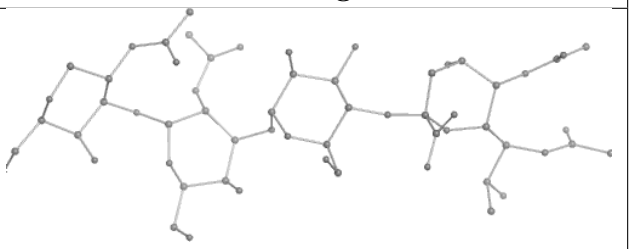
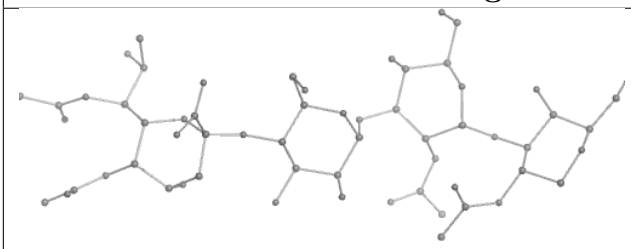
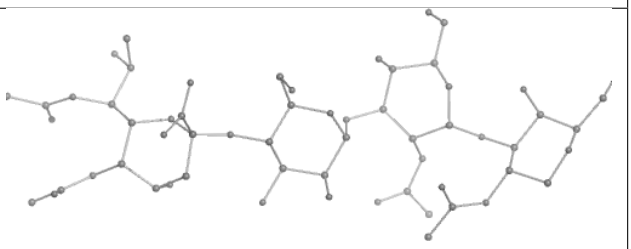


Rings

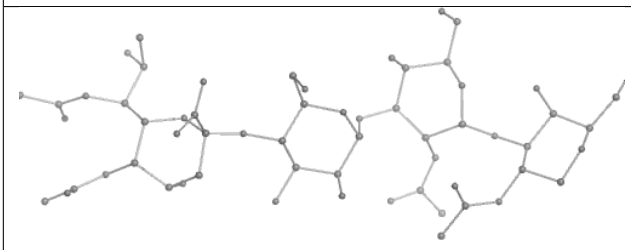
Oligosaccharide Chain SA



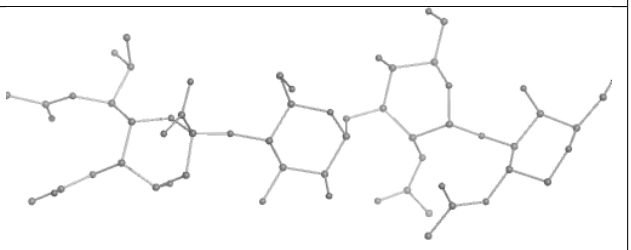
Bond lengths



Bond angles

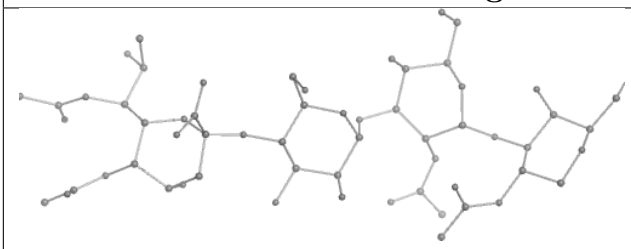


Torsions



Rings

Oligosaccharide Chain aA



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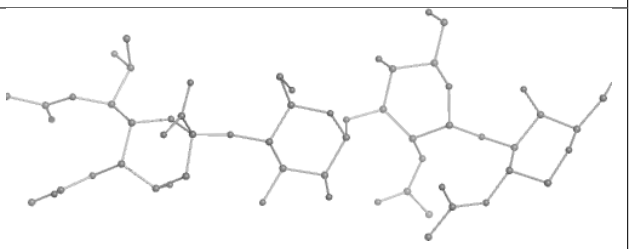
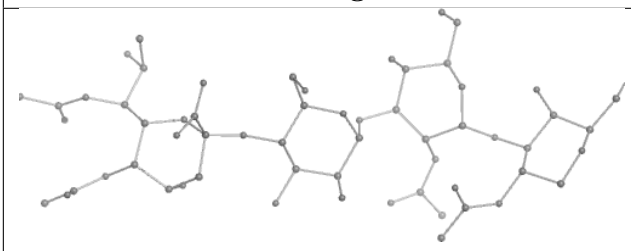
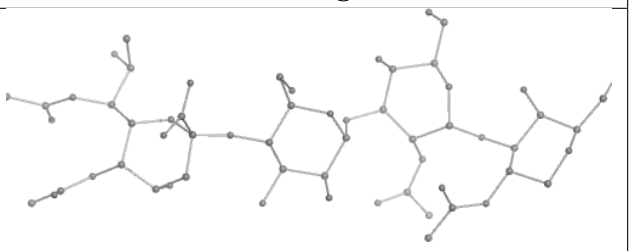


Bond angles

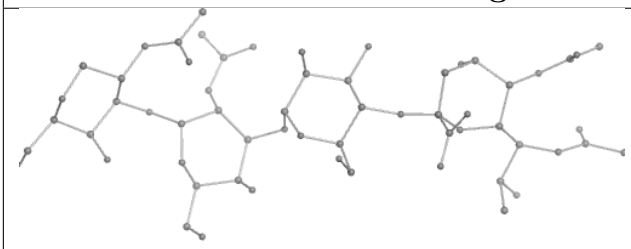


Torsions

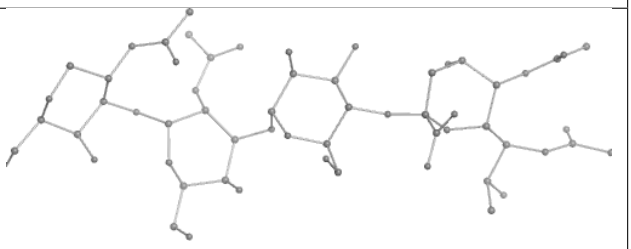


Rings

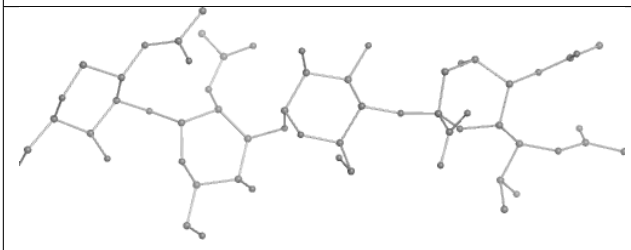
Oligosaccharide Chain iA



Bond lengths



Bond angles



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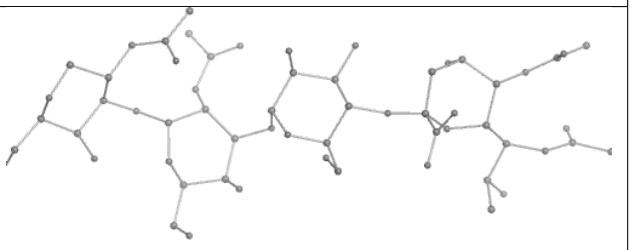
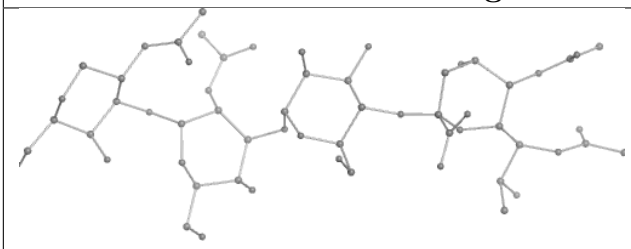
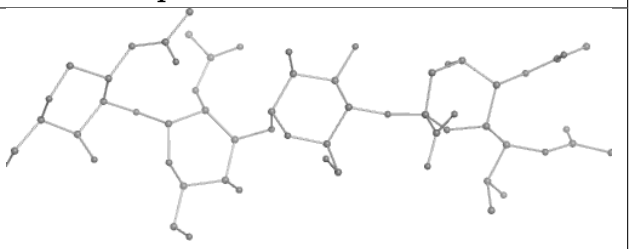


Rings

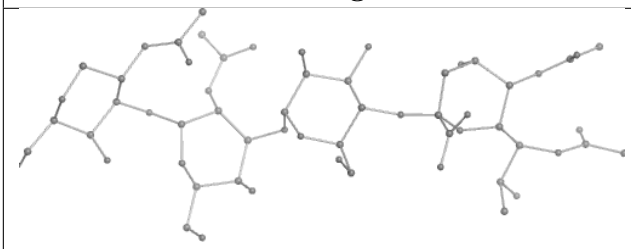
Oligosaccharide Chain qA



Bond lengths



Bond angles



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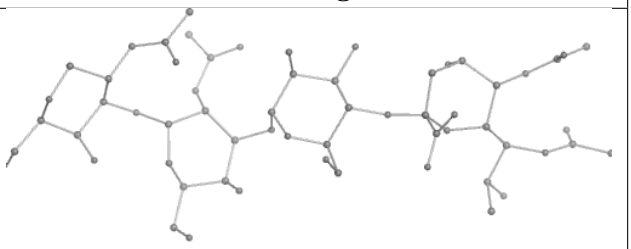
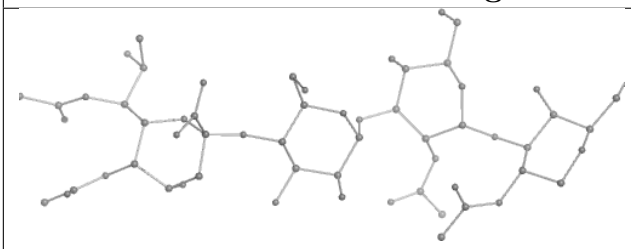


Rings

Oligosaccharide Chain yA



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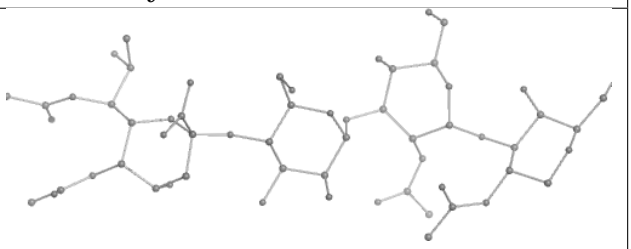
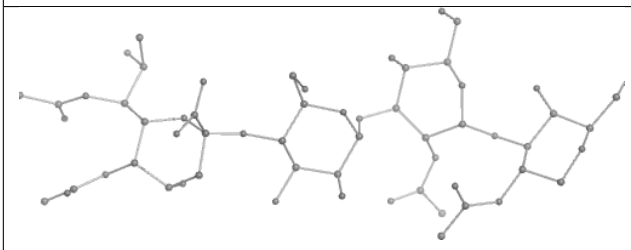
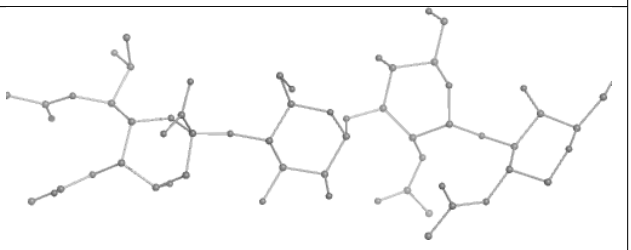


Bond angles

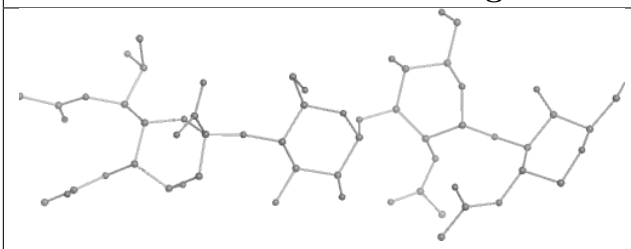


Torsions

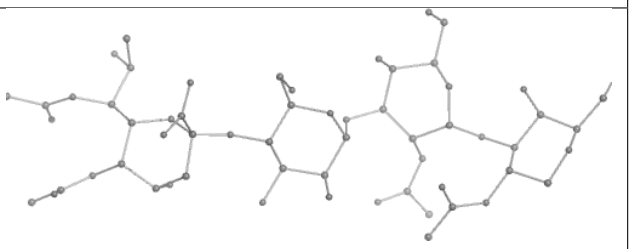


Rings

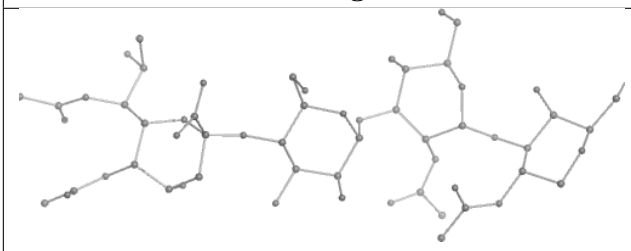
Oligosaccharide Chain 6A



Bond lengths



Bond angles



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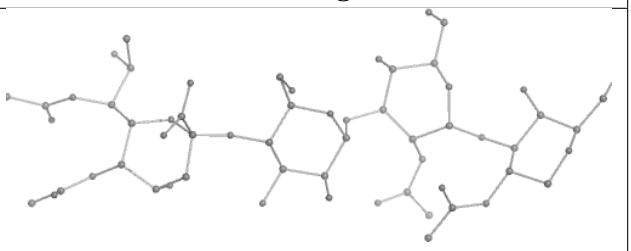
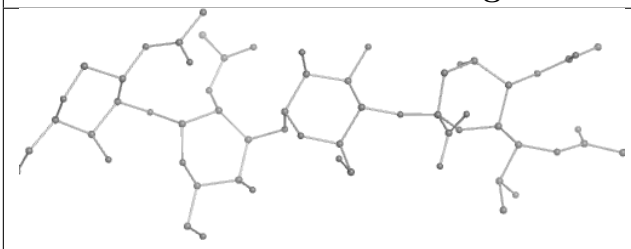
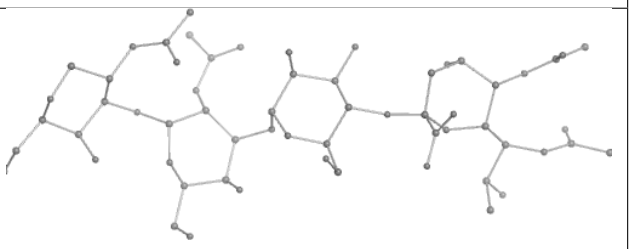


Rings

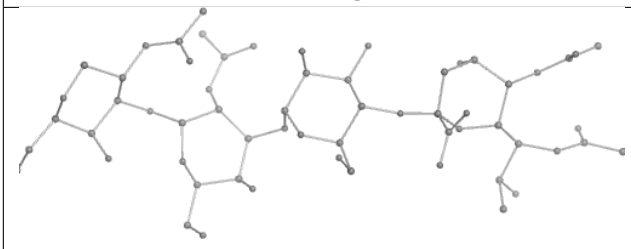
Oligosaccharide Chain EB



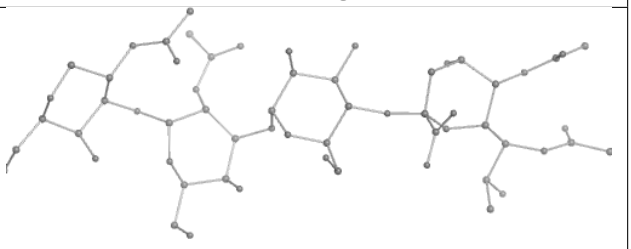
Bond lengths



Bond angles

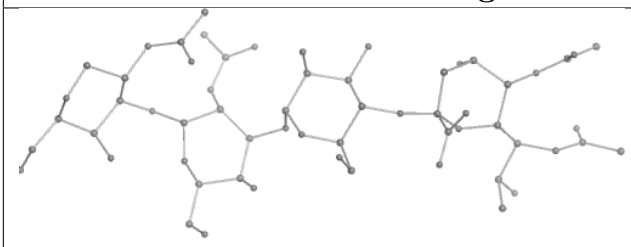


Torsions

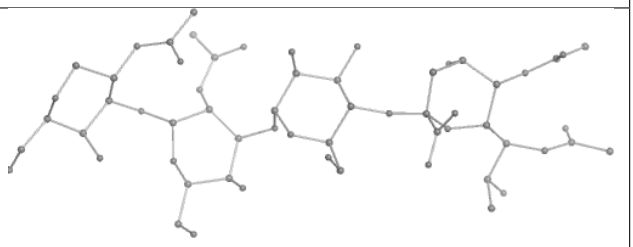


Rings

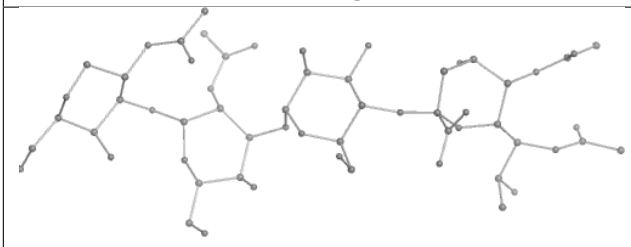
Oligosaccharide Chain MB



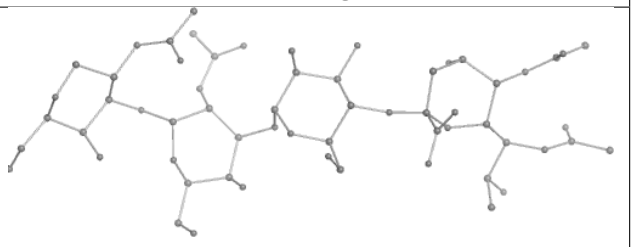
Bond lengths



Bond angles

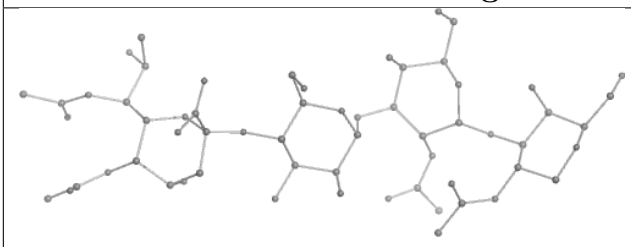


Torsions

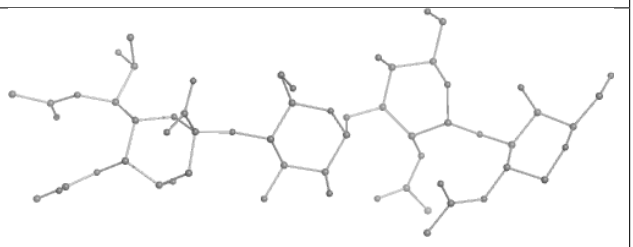


Rings

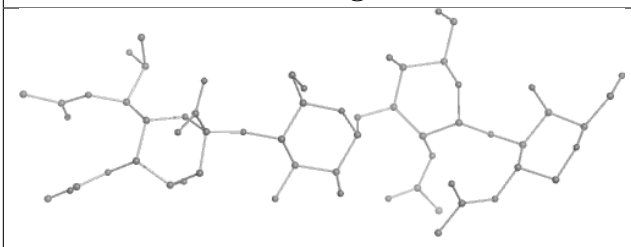
Oligosaccharide Chain UB



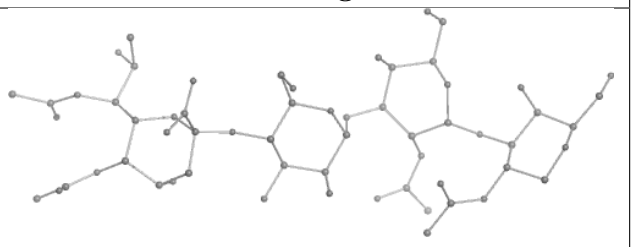
Bond lengths



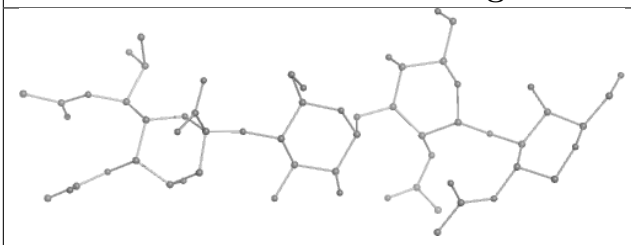
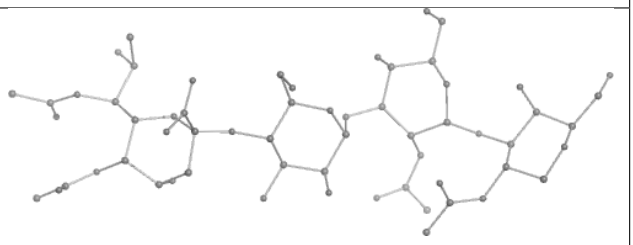
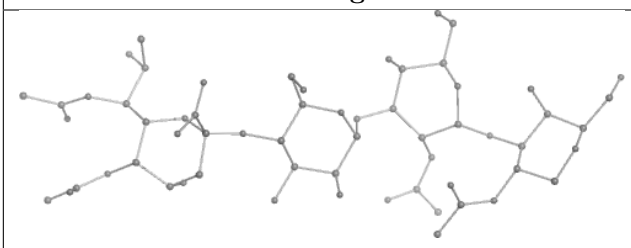
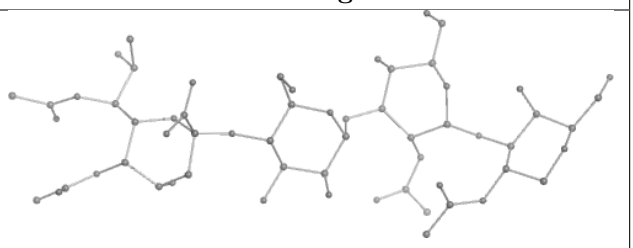
Bond angles

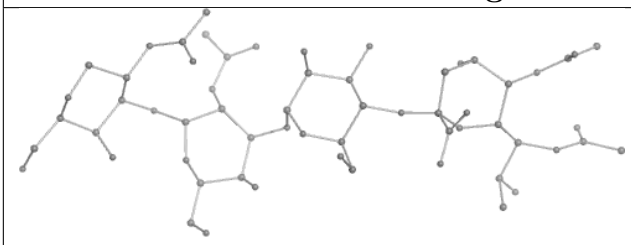
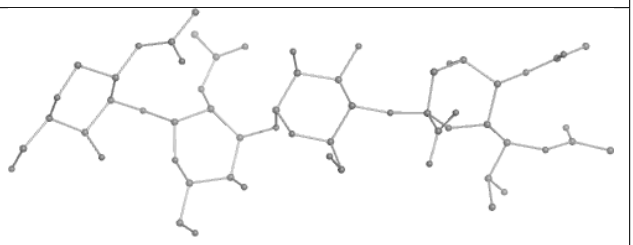
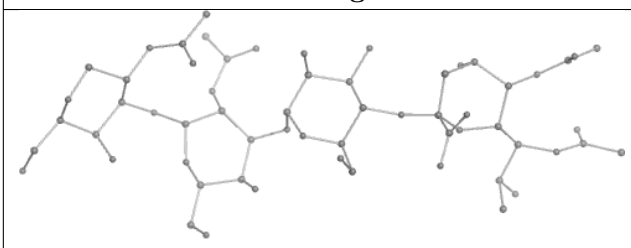
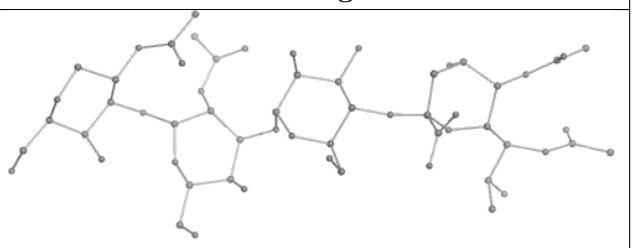


Torsions

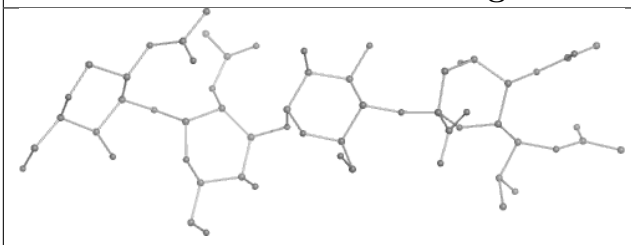


Rings

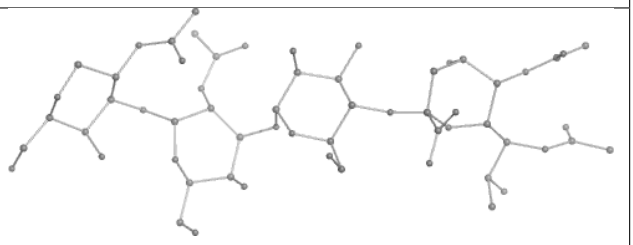
Oligosaccharide Chain cB	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

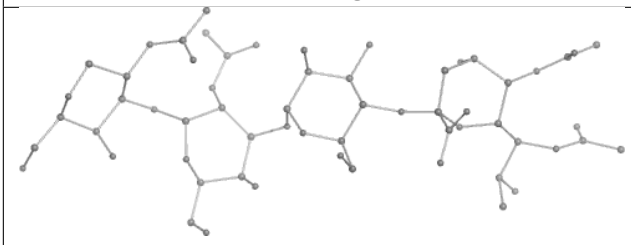
Oligosaccharide Chain sB



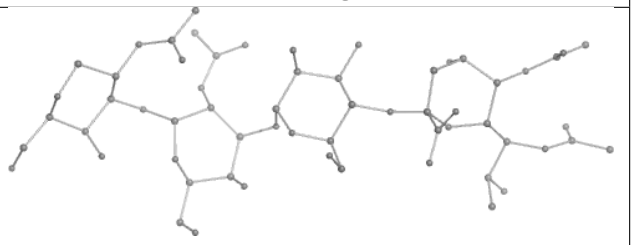
Bond lengths



Bond angles

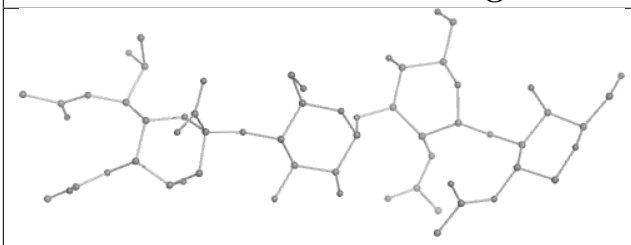


Torsions

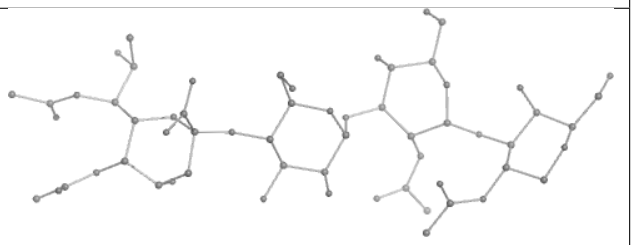


Rings

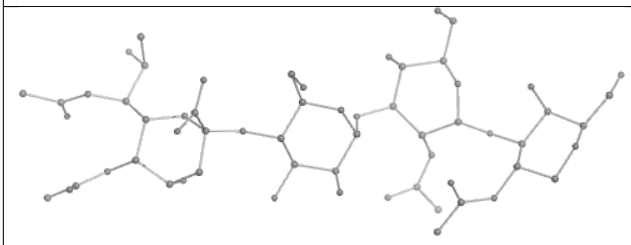
Oligosaccharide Chain 0B



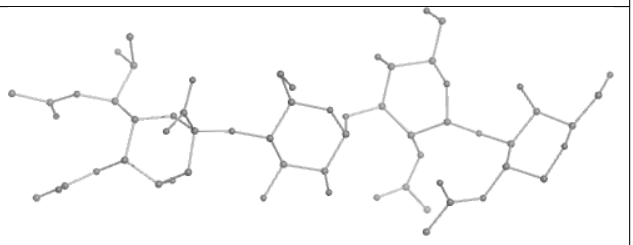
Bond lengths



Bond angles

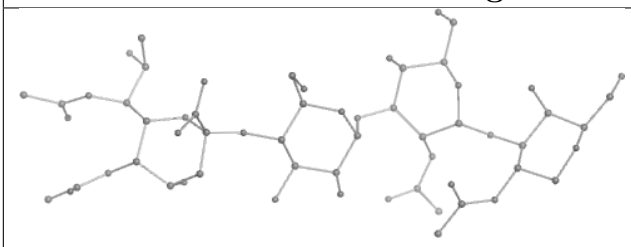


Torsions

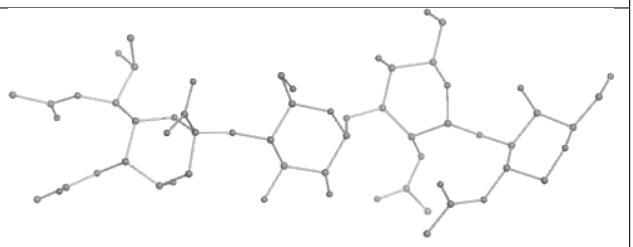


Rings

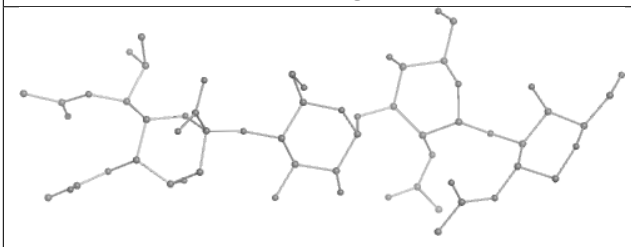
Oligosaccharide Chain 8B



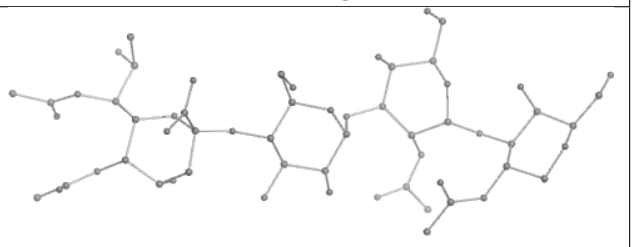
Bond lengths



Bond angles

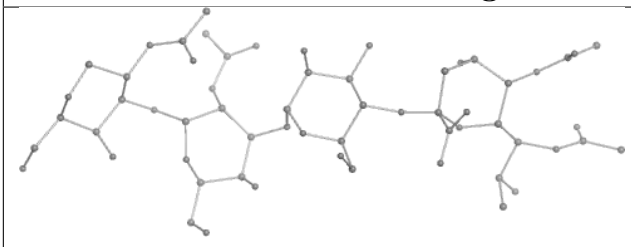


Torsions



Rings

Oligosaccharide Chain GC



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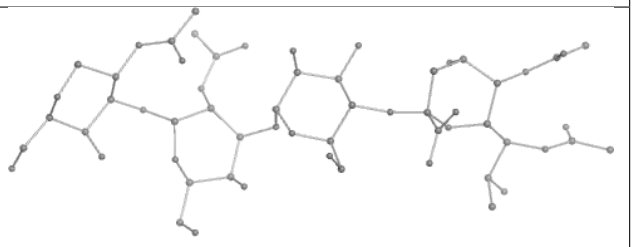
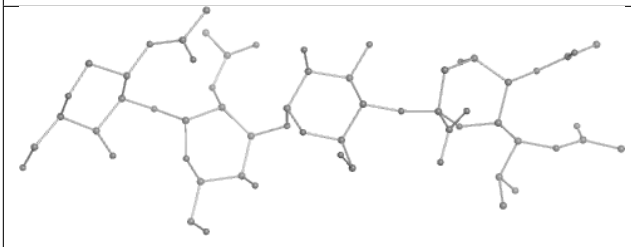


Bond angles



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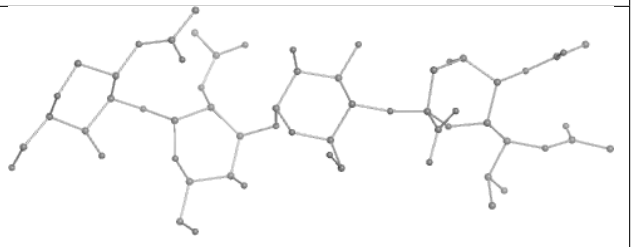
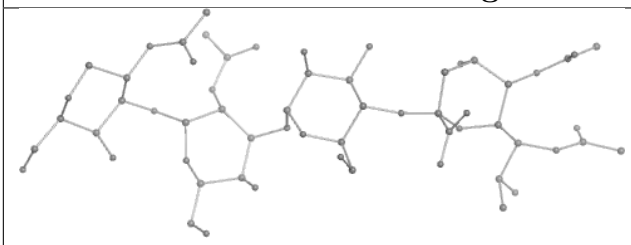


Rings

Oligosaccharide Chain OC



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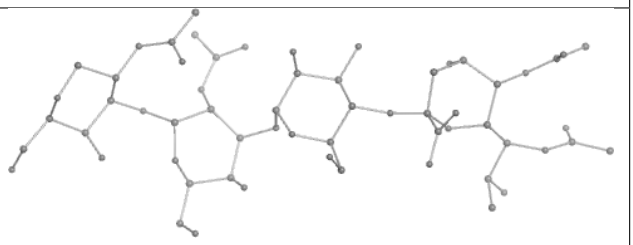
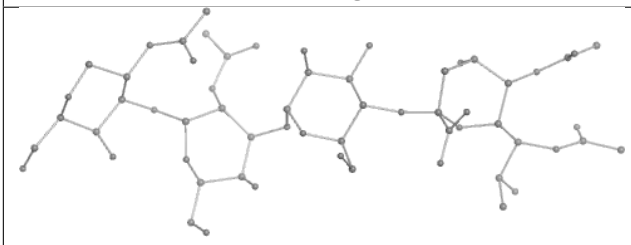


Bond angles



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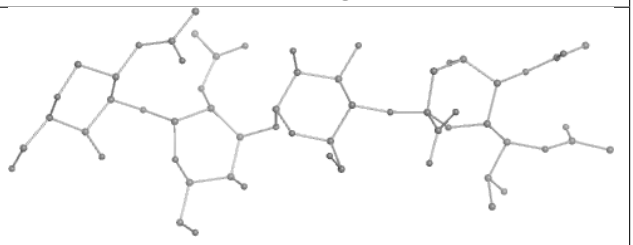
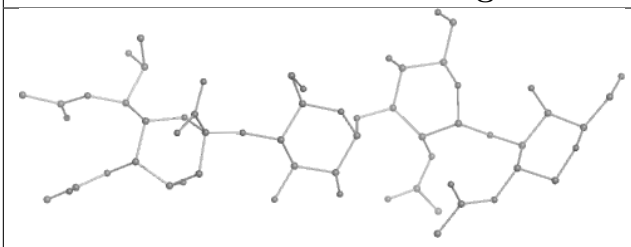


Rings

Oligosaccharide Chain WC



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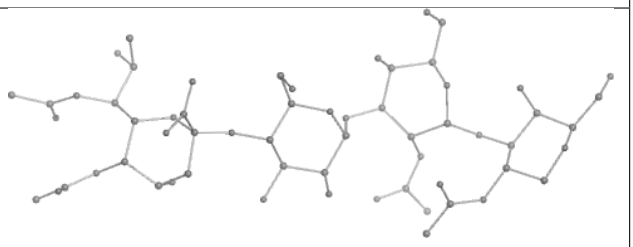
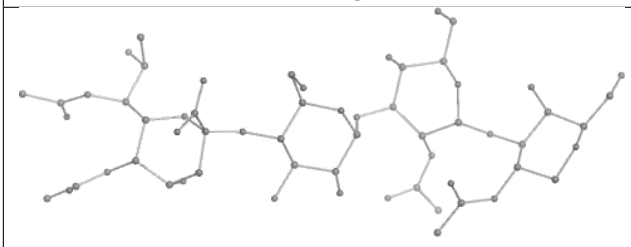


Bond angles



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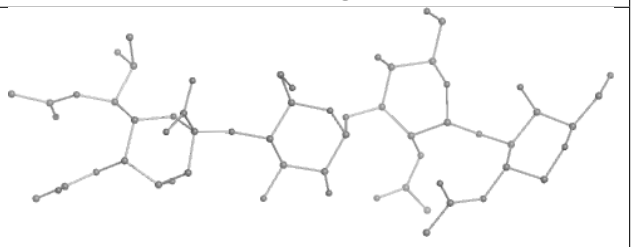
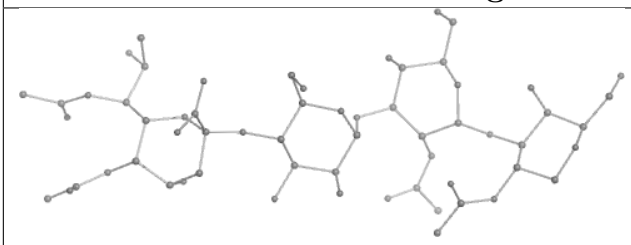


Rings

Oligosaccharide Chain eC



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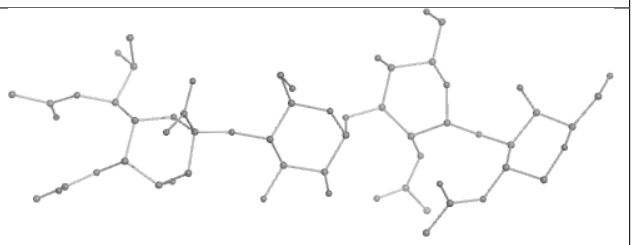
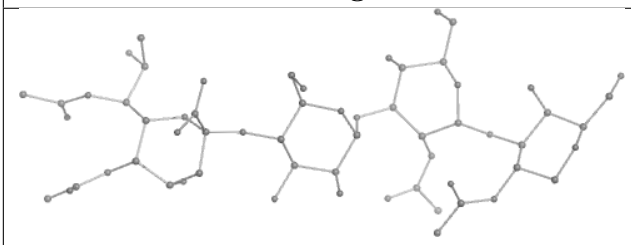


Bond angles



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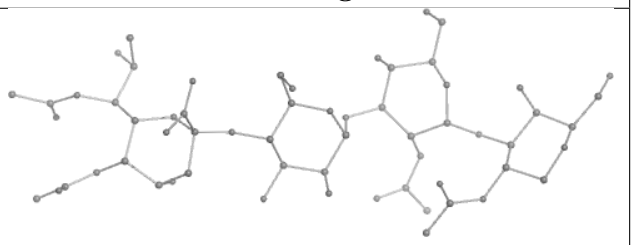
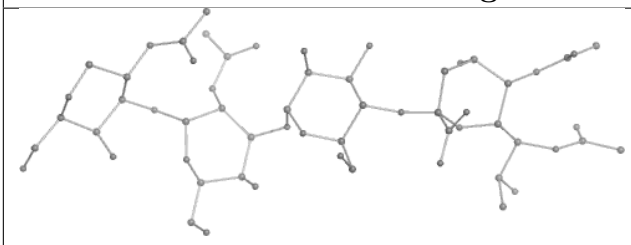


Rings

Oligosaccharide Chain mC



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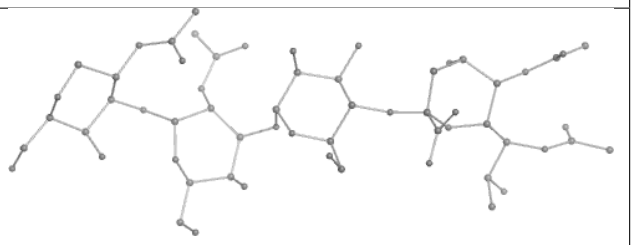

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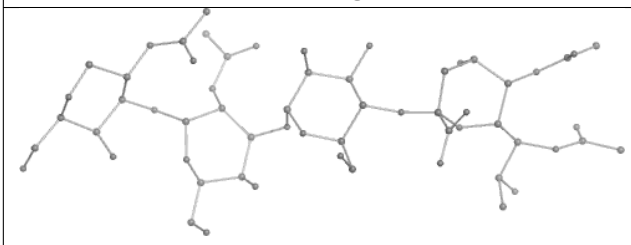

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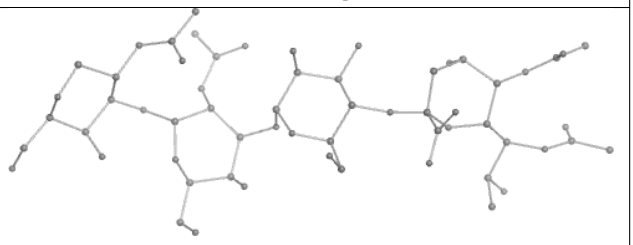
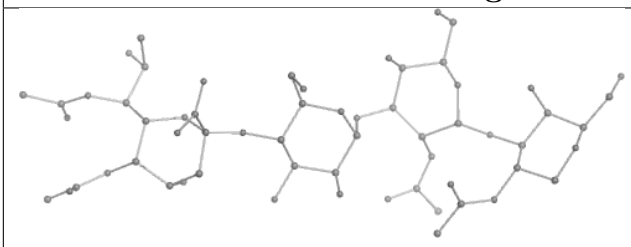


Rings

Oligosaccharide Chain uC



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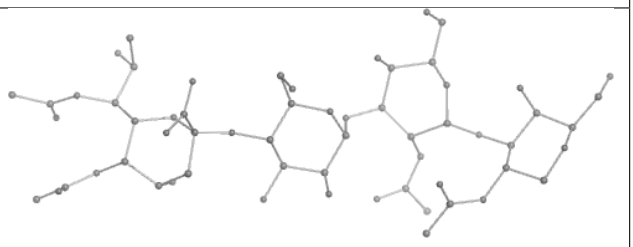
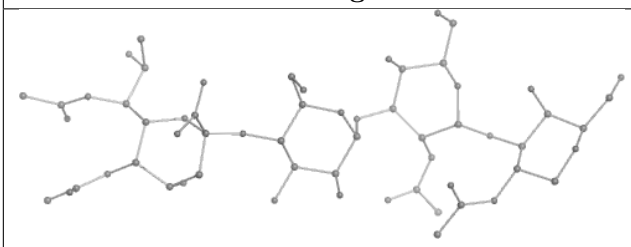


Bond angles



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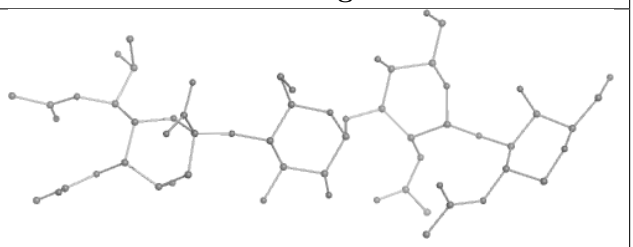
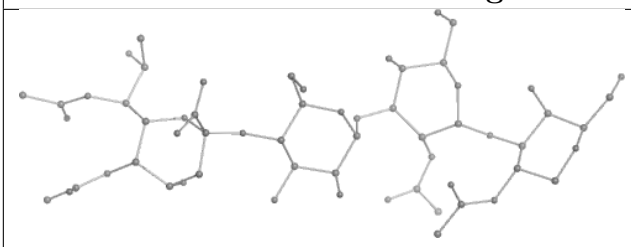


Rings

Oligosaccharide Chain 2C



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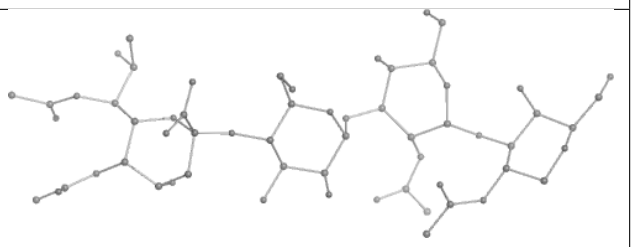
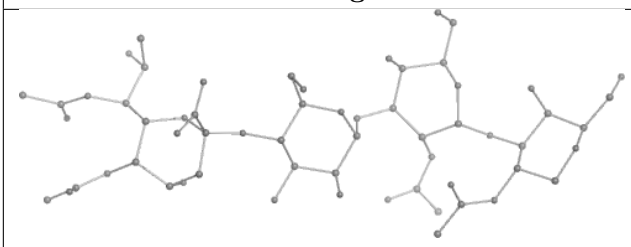


Bond angles



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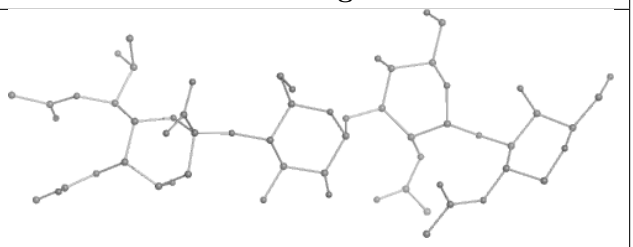
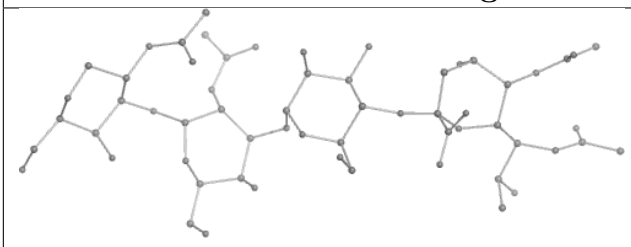


Rings

Oligosaccharide Chain AD



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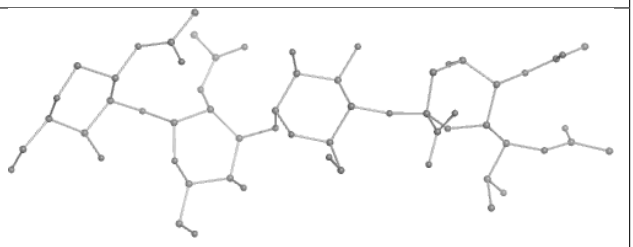
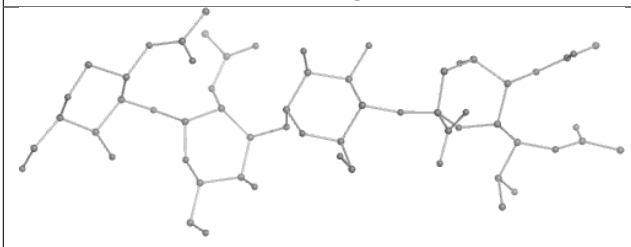


Bond angles



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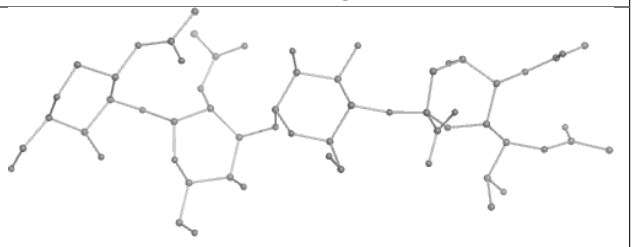
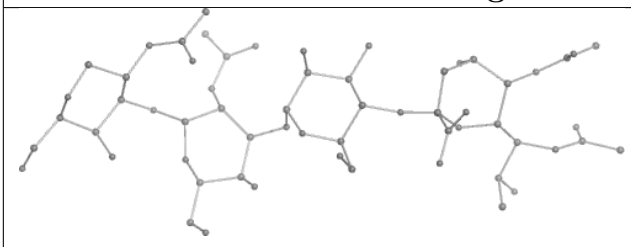


Rings

Oligosaccharide Chain ID



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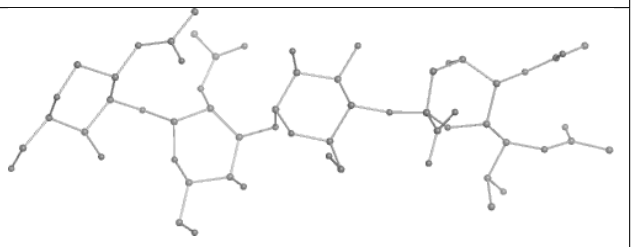

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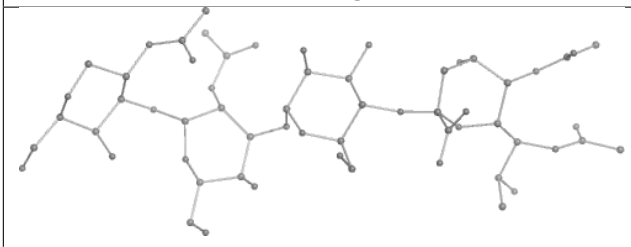

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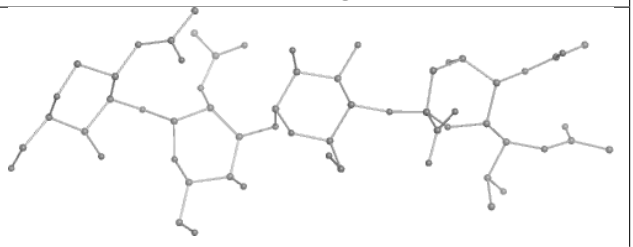
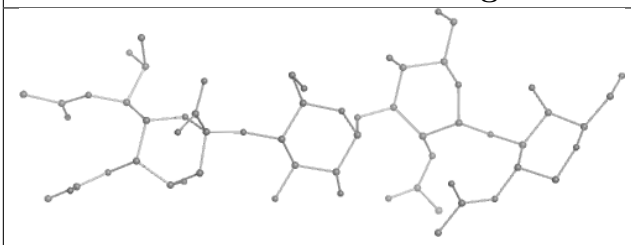


Rings

Oligosaccharide Chain QD



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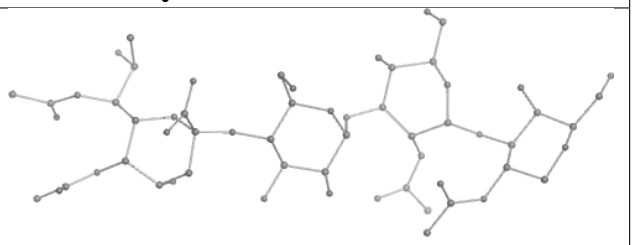

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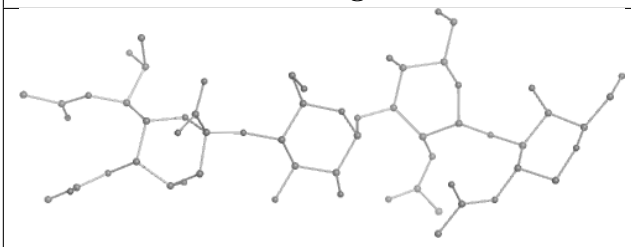

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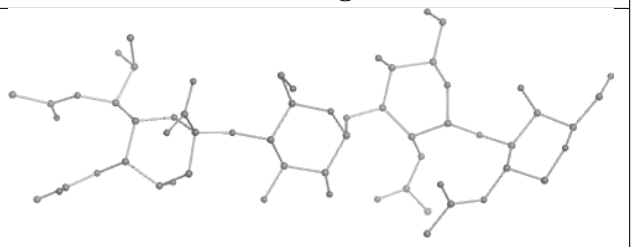
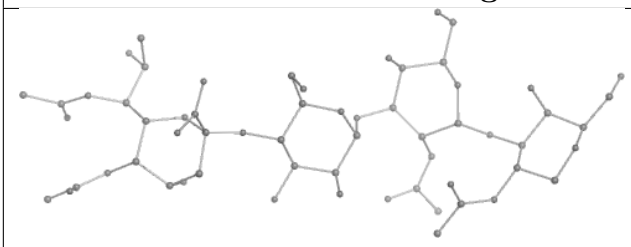


Rings

Oligosaccharide Chain YD



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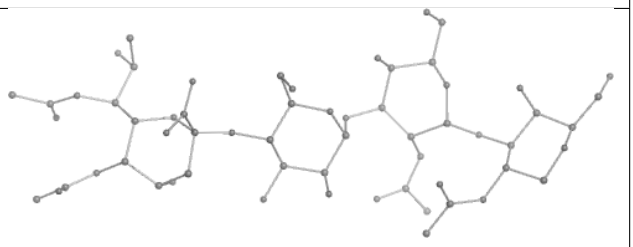
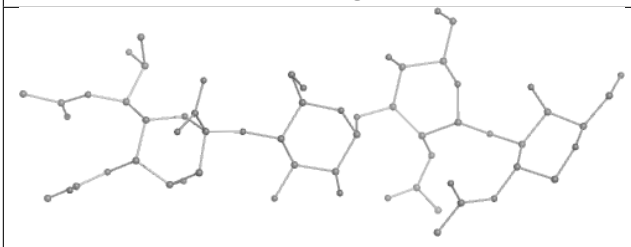
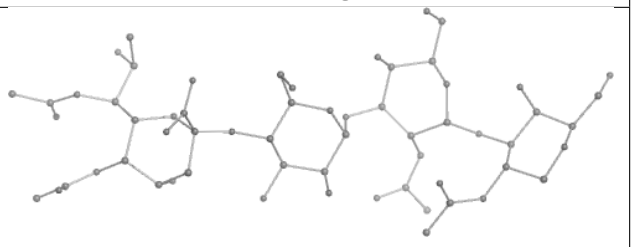


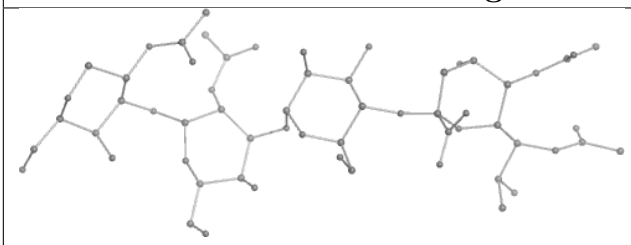
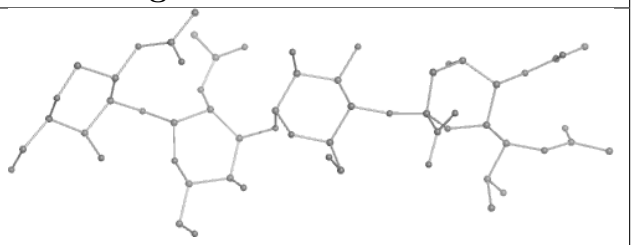
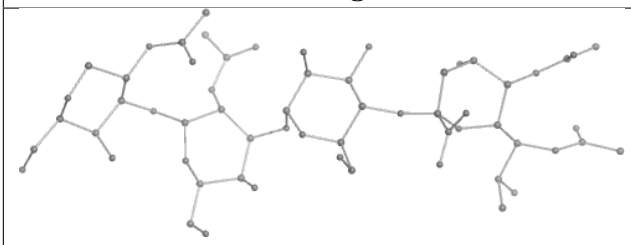
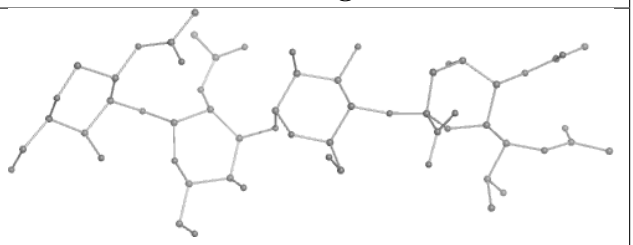
Bond angles

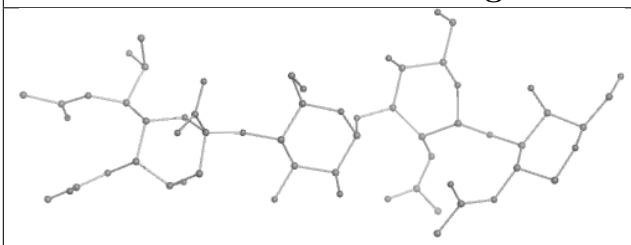
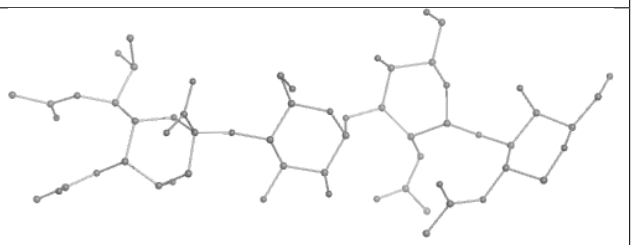
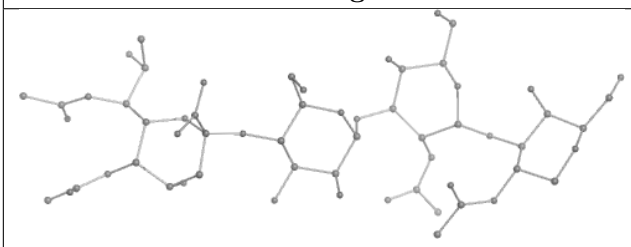
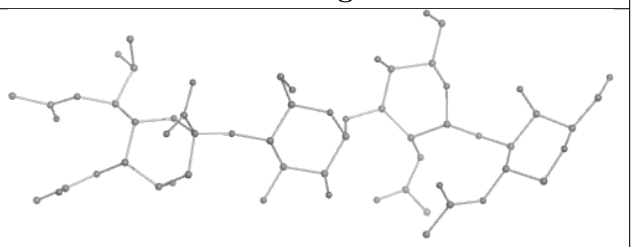


Torsions

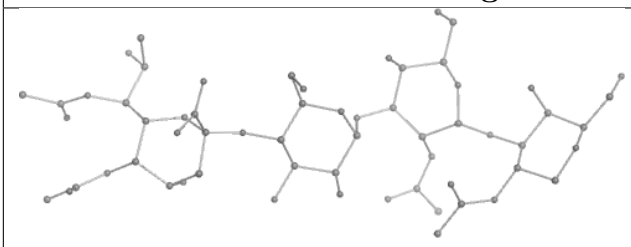


Rings

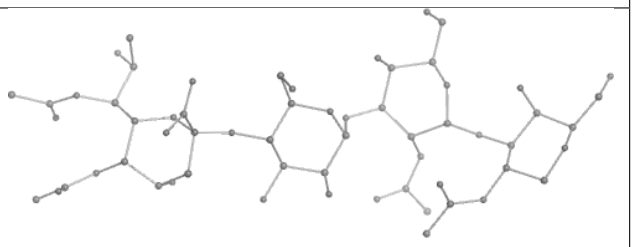
Oligosaccharide Chain gD	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

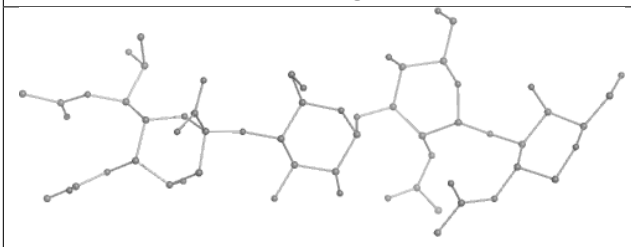
Oligosaccharide Chain wD



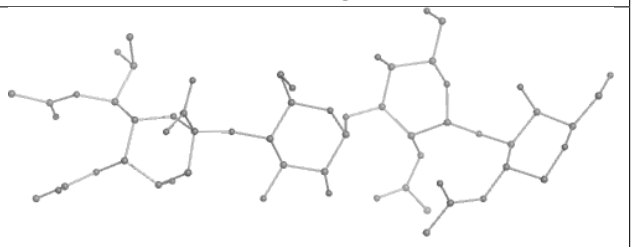
Bond lengths



Bond angles

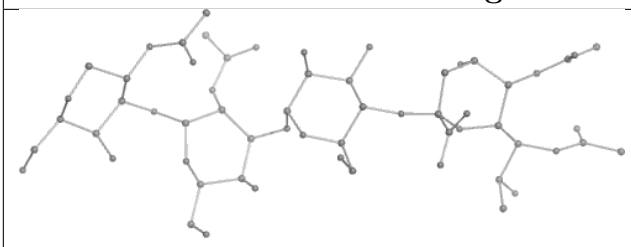


Torsions



Rings

Oligosaccharide Chain 4D



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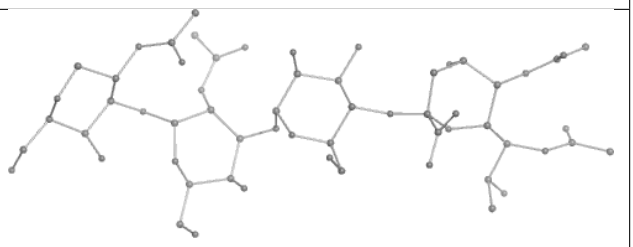
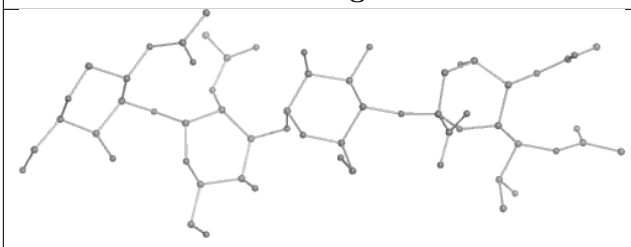


Bond angles



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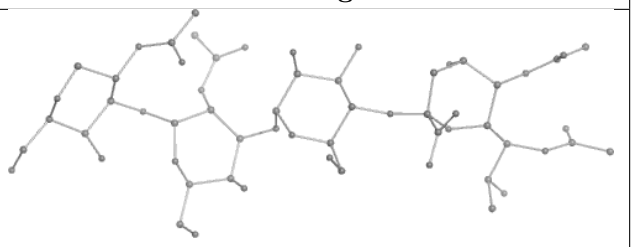
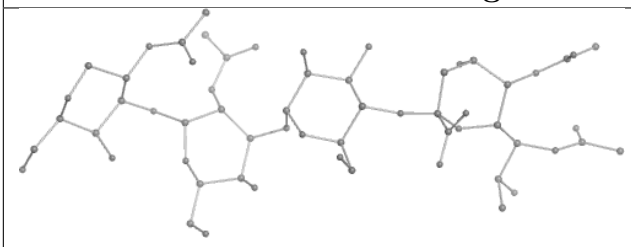
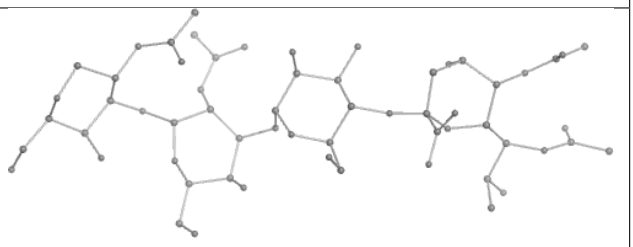
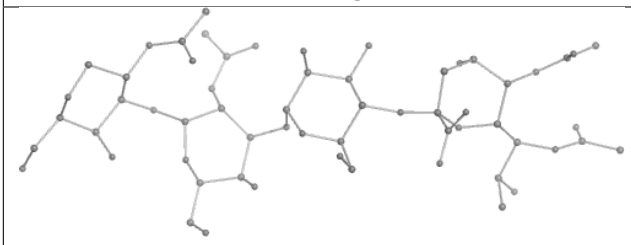
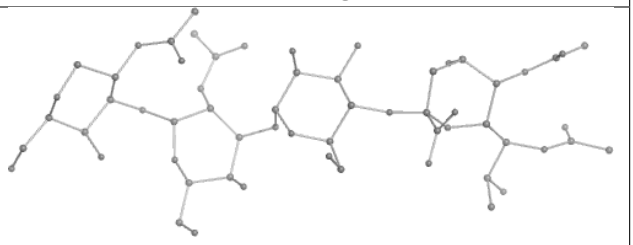
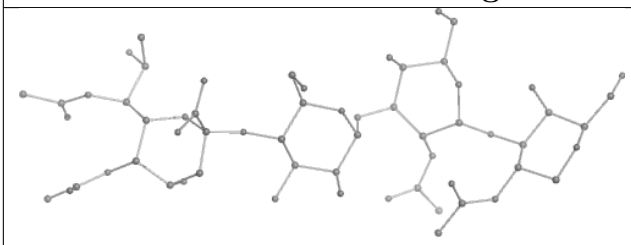
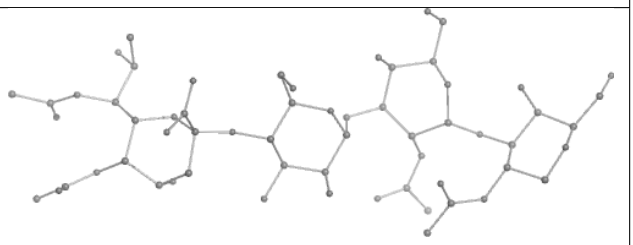
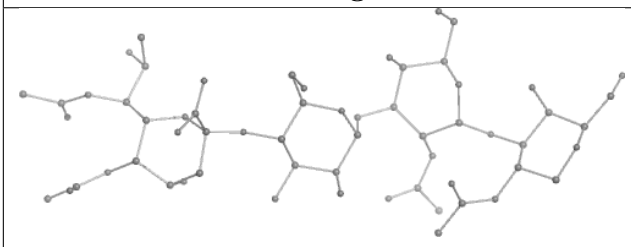
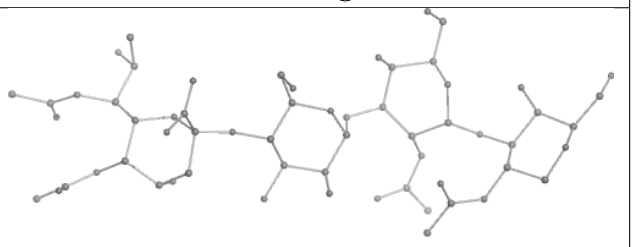
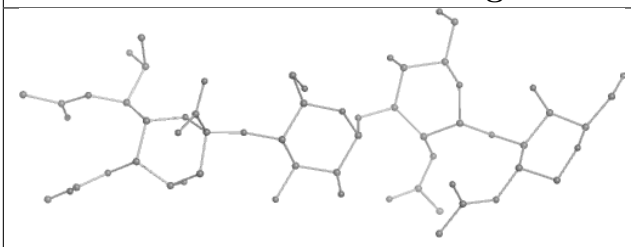


Rings

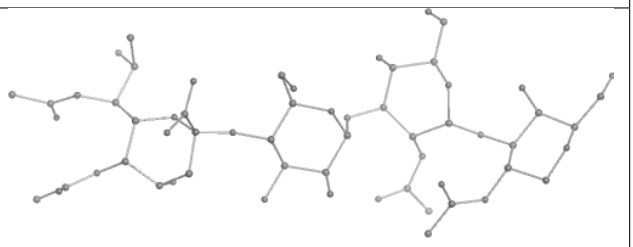
Oligosaccharide Chain CE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

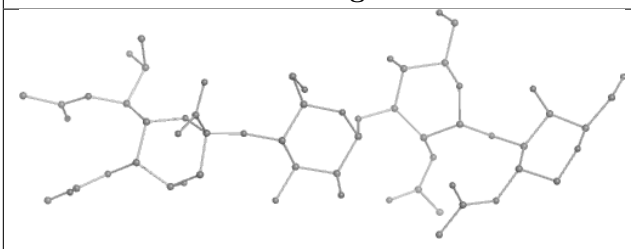
Oligosaccharide Chain SE



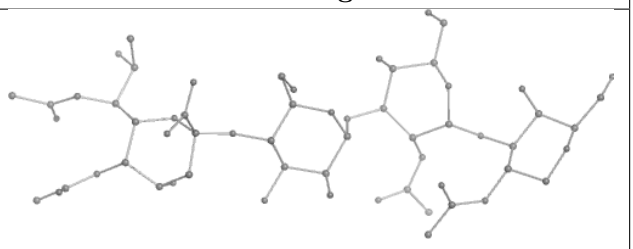
Bond lengths



Bond angles

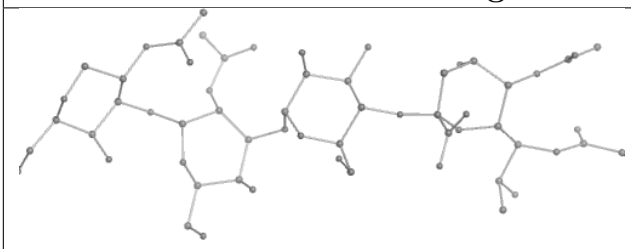


Torsions

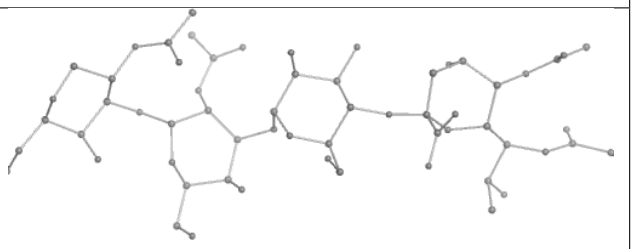


Rings

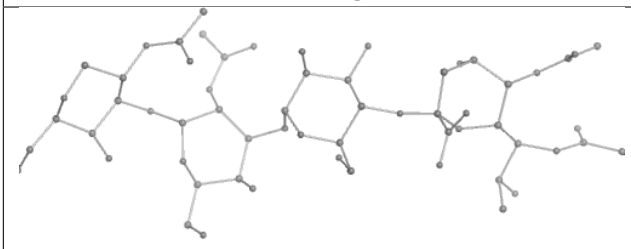
Oligosaccharide Chain aE



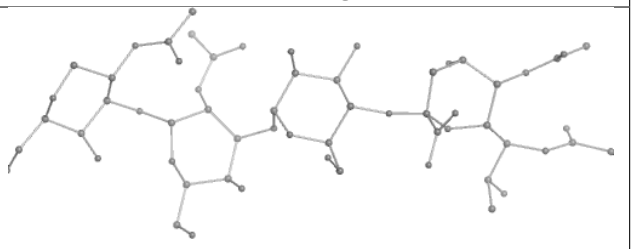
Bond lengths



Bond angles

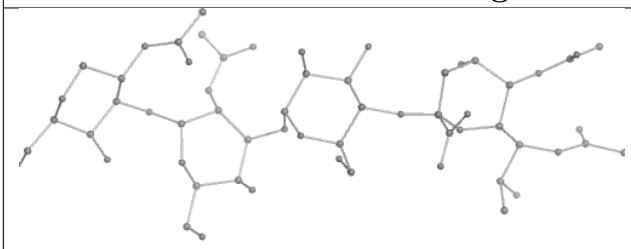


Torsions

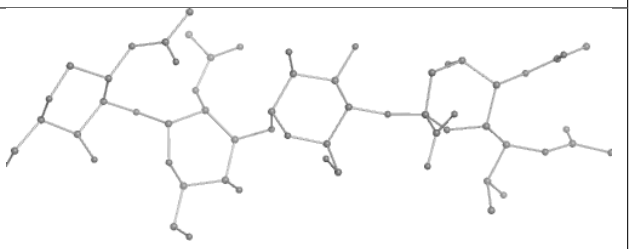


Rings

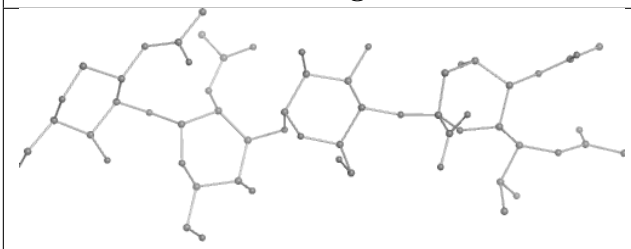
Oligosaccharide Chain iE



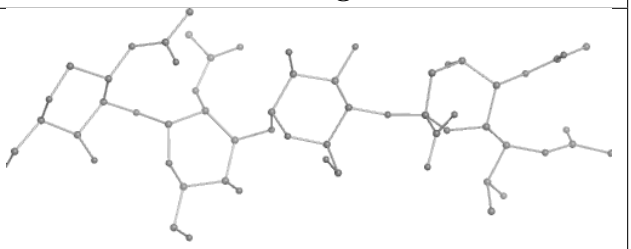
Bond lengths



Bond angles

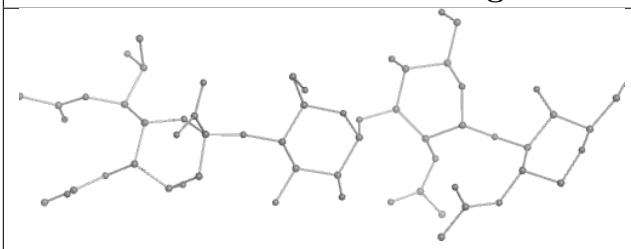


Torsions

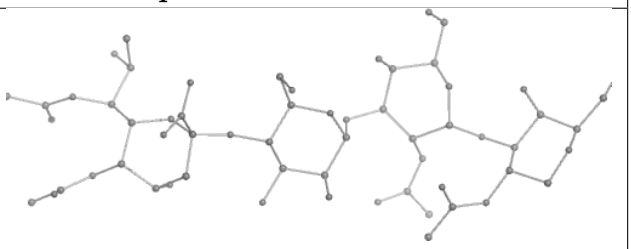


Rings

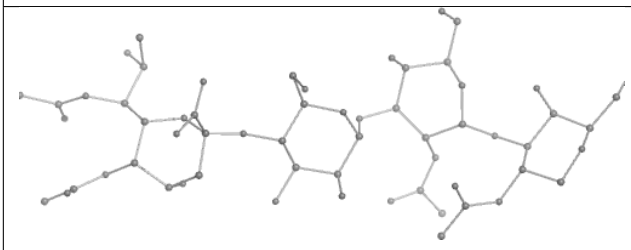
Oligosaccharide Chain qE



Bond lengths



Bond angles



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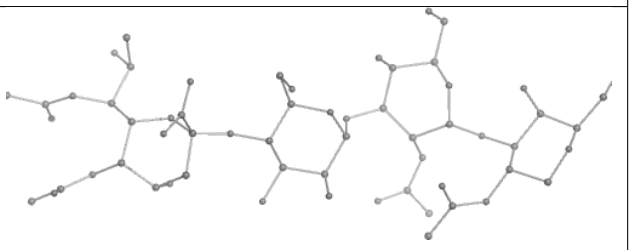
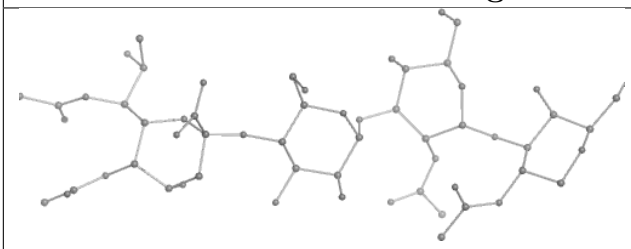
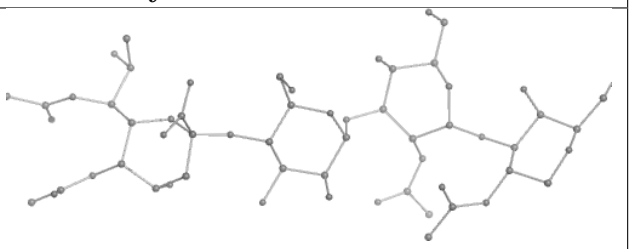


Rings

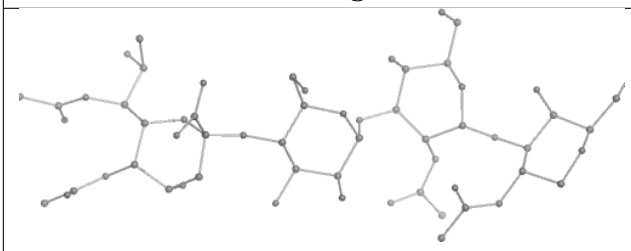
Oligosaccharide Chain yE



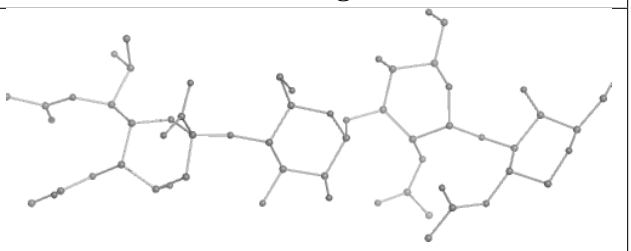
Bond lengths



Bond angles

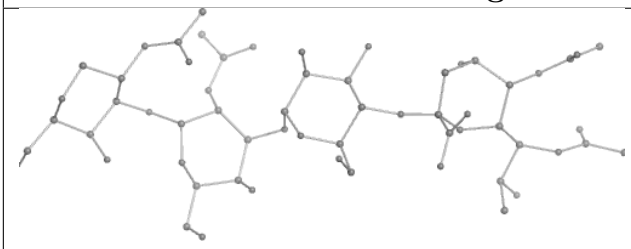


Torsions

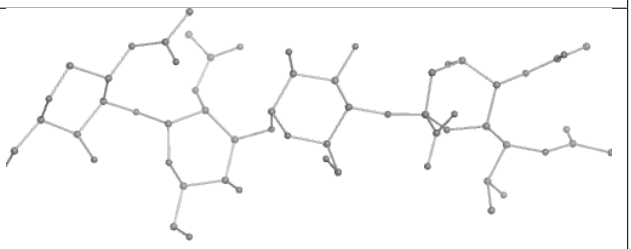


Rings

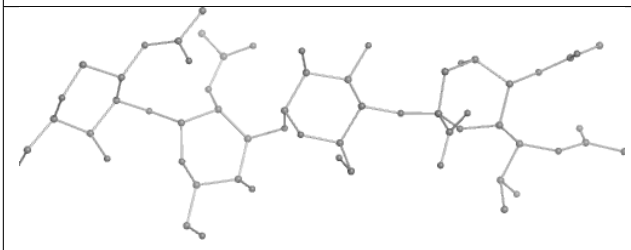
Oligosaccharide Chain 6E



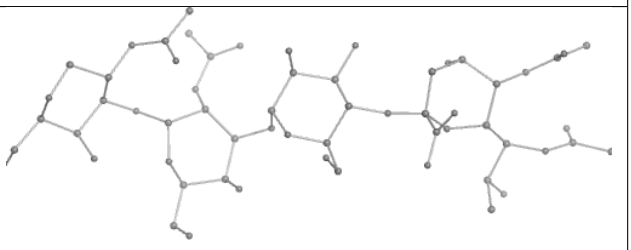
Bond lengths



Bond angles

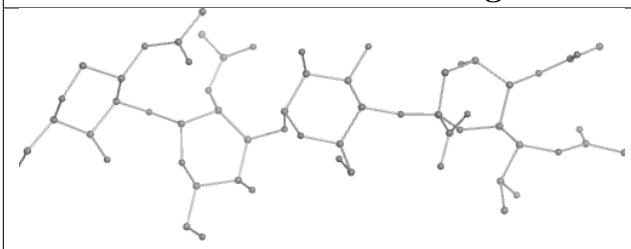


Torsions

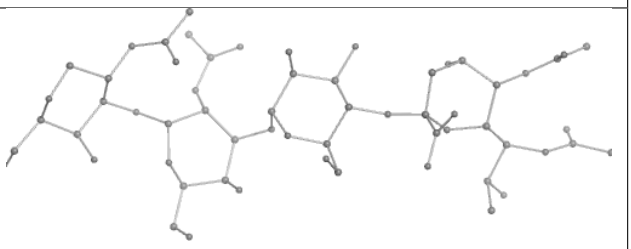


Rings

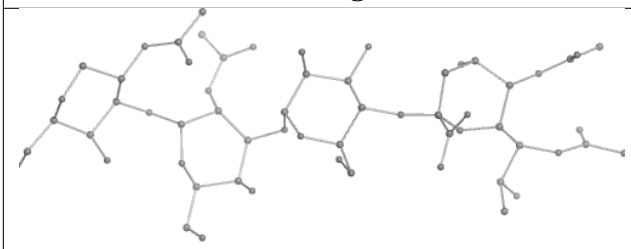
Oligosaccharide Chain EF



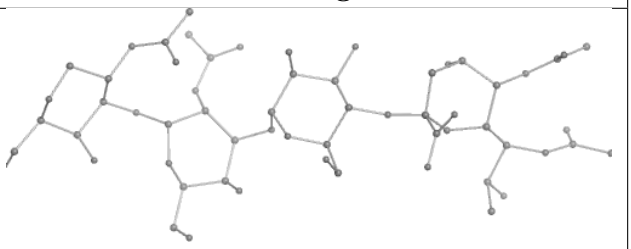
Bond lengths



Bond angles

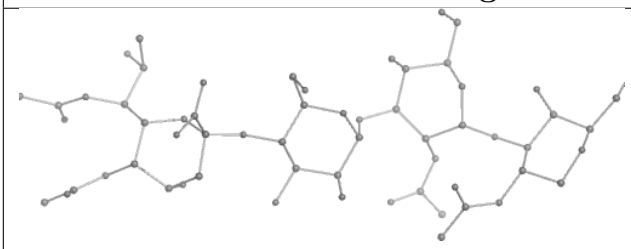


Torsions

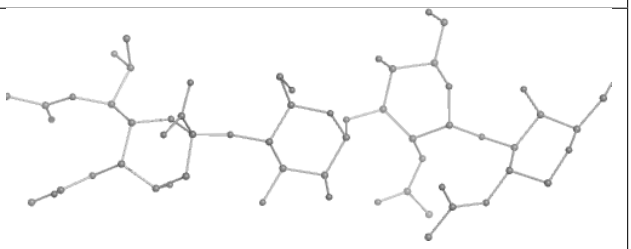


Rings

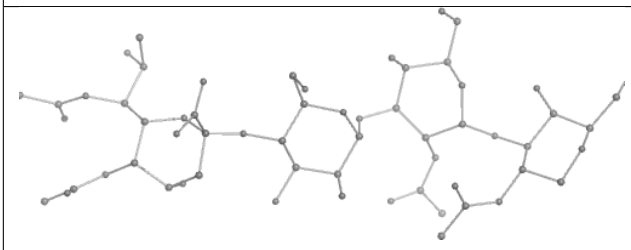
Oligosaccharide Chain MF



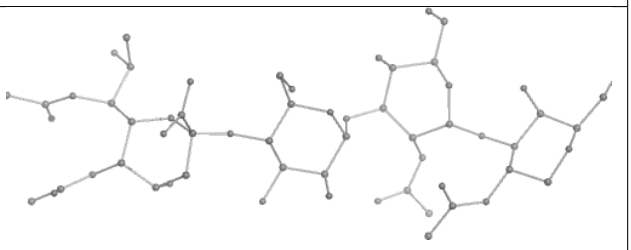
Bond lengths



Bond angles

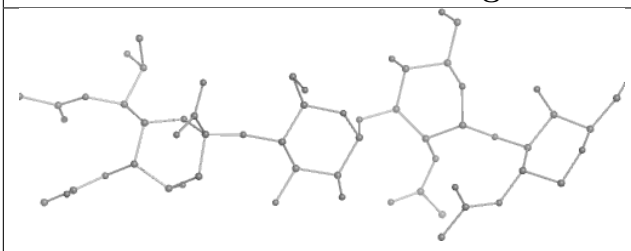


Torsions

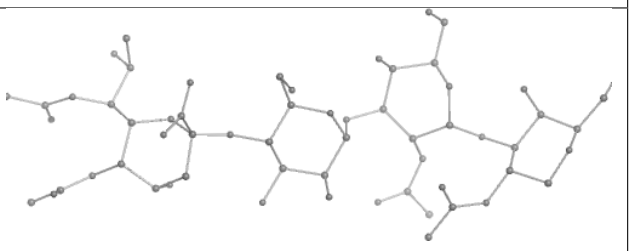


Rings

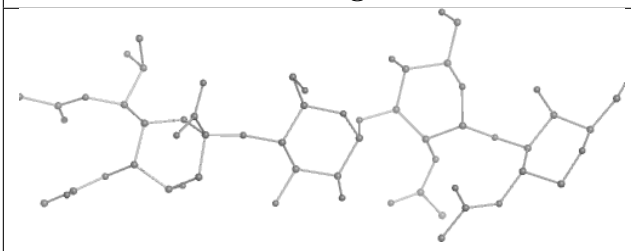
Oligosaccharide Chain UF



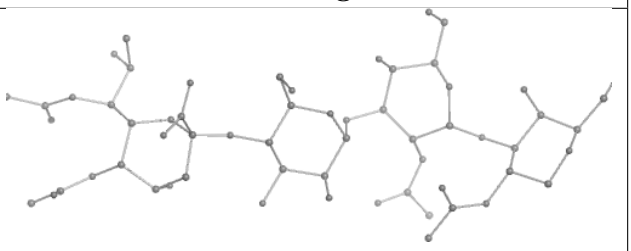
Bond lengths



Bond angles

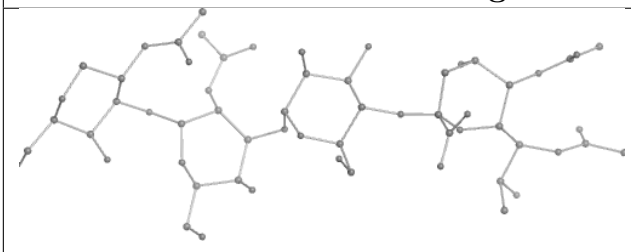


Torsions

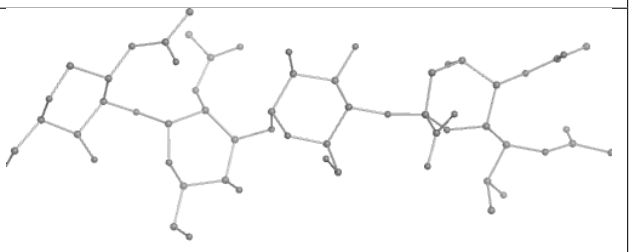


Rings

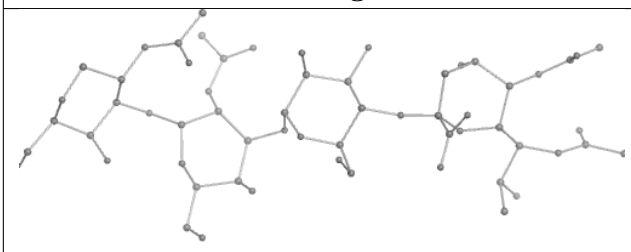
Oligosaccharide Chain cF



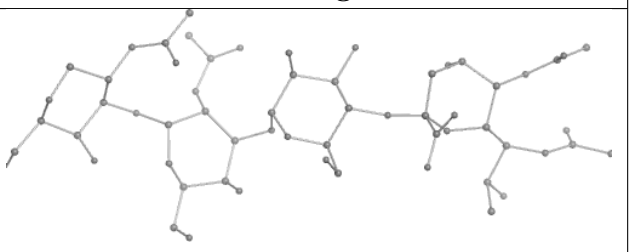
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

90 ligands 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	$\#\|Z\|>2$
5	A2G	i	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
5	A2G	M	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	c	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	s	202	1	14,14,15	0.46	0	17,19,21	1.11	1 (5%)
4	MAN	b	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
4	MAN	Z	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	S	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
5	A2G	L	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	p	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	K	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
5	A2G	I	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
5	A2G	C	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
5	A2G	J	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	H	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.82	4 (26%)
4	MAN	I	201	-	11,11,12	0.77	0	15,15,17	2.84	4 (26%)
5	A2G	T	202	1	14,14,15	0.45	0	17,19,21	1.12	1 (5%)
5	A2G	D	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	k	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	V	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
4	MAN	F	201	-	11,11,12	0.79	0	15,15,17	2.83	4 (26%)
5	A2G	b	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
5	A2G	Z	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	S	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	Q	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
4	MAN	K	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	d	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
5	A2G	A	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
4	MAN	N	201	-	11,11,12	0.77	0	15,15,17	2.83	4 (26%)
4	MAN	O	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
4	MAN	o	201	-	11,11,12	0.77	0	15,15,17	2.83	4 (26%)
4	MAN	G	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	f	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	e	201	-	11,11,12	0.78	0	15,15,17	2.84	4 (26%)
4	MAN	g	201	-	11,11,12	0.78	0	15,15,17	2.84	4 (26%)
5	A2G	Y	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	D	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	r	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
5	A2G	k	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	U	201	-	11,11,12	0.79	0	15,15,17	2.83	4 (26%)
5	A2G	R	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
5	A2G	W	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	Q	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	n	202	1	14,14,15	0.43	0	17,19,21	1.12	1 (5%)
4	MAN	d	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	E	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	A	201	-	11,11,12	0.80	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	c	202	1	14,14,15	0.43	0	17,19,21	1.11	1 (5%)
5	A2G	j	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
5	A2G	O	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
5	A2G	g	202	1	14,14,15	0.45	0	17,19,21	1.12	1 (5%)
4	MAN	Y	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	h	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	R	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
4	MAN	i	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
4	MAN	q	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	a	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
5	A2G	o	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	L	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
4	MAN	M	201	-	11,11,12	0.77	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	l	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	s	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	B	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	X	201	-	11,11,12	0.79	0	15,15,17	2.83	4 (26%)
5	A2G	m	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	T	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
4	MAN	h	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	F	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
5	A2G	U	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	W	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
4	MAN	J	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	f	201	-	11,11,12	0.78	1 (9%)	15,15,17	2.83	4 (26%)
4	MAN	a	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
5	A2G	N	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	r	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.84	4 (26%)
4	MAN	E	201	-	11,11,12	0.80	1 (9%)	15,15,17	2.83	4 (26%)
4	MAN	V	201	-	11,11,12	0.78	0	15,15,17	2.83	4 (26%)
4	MAN	l	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	G	202	1	14,14,15	0.43	0	17,19,21	1.11	1 (5%)
5	A2G	e	202	1	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
4	MAN	B	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.84	4 (26%)
5	A2G	P	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	C	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	p	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	m	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
5	A2G	X	202	1	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
4	MAN	n	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)
4	MAN	j	201	-	11,11,12	0.79	0	15,15,17	2.83	4 (26%)
5	A2G	q	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
5	A2G	H	202	1	14,14,15	0.44	0	17,19,21	1.11	1 (5%)
4	MAN	P	201	-	11,11,12	0.79	1 (9%)	15,15,17	2.83	4 (26%)

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
5	A2G	i	202	1	-	2/6/23/26	0/1/1/1
5	A2G	M	202	1	-	2/6/23/26	0/1/1/1
4	MAN	c	201	-	-	1/2/19/22	0/1/1/1
5	A2G	s	202	1	-	2/6/23/26	0/1/1/1
4	MAN	b	201	-	-	1/2/19/22	0/1/1/1
4	MAN	Z	201	-	-	1/2/19/22	0/1/1/1
5	A2G	S	202	1	-	2/6/23/26	0/1/1/1
5	A2G	L	202	1	-	2/6/23/26	0/1/1/1
4	MAN	p	201	-	-	1/2/19/22	0/1/1/1
5	A2G	K	202	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A2G	I	202	1	-	2/6/23/26	0/1/1/1
5	A2G	C	202	1	-	2/6/23/26	0/1/1/1
5	A2G	J	202	1	-	2/6/23/26	0/1/1/1
4	MAN	H	201	-	-	1/2/19/22	0/1/1/1
4	MAN	I	201	-	-	1/2/19/22	0/1/1/1
5	A2G	T	202	1	-	2/6/23/26	0/1/1/1
5	A2G	D	202	1	-	2/6/23/26	0/1/1/1
4	MAN	k	201	-	-	1/2/19/22	0/1/1/1
5	A2G	V	202	1	-	2/6/23/26	0/1/1/1
4	MAN	F	201	-	-	1/2/19/22	0/1/1/1
5	A2G	b	202	1	-	2/6/23/26	0/1/1/1
5	A2G	Z	202	1	-	2/6/23/26	0/1/1/1
4	MAN	S	201	-	-	1/2/19/22	0/1/1/1
5	A2G	Q	202	1	-	2/6/23/26	0/1/1/1
4	MAN	K	201	-	-	1/2/19/22	0/1/1/1
5	A2G	d	202	1	-	2/6/23/26	0/1/1/1
5	A2G	A	202	1	-	2/6/23/26	0/1/1/1
4	MAN	N	201	-	-	1/2/19/22	0/1/1/1
4	MAN	O	201	-	-	1/2/19/22	0/1/1/1
4	MAN	o	201	-	-	1/2/19/22	0/1/1/1
4	MAN	G	201	-	-	1/2/19/22	0/1/1/1
5	A2G	f	202	1	-	2/6/23/26	0/1/1/1
4	MAN	e	201	-	-	1/2/19/22	0/1/1/1
4	MAN	g	201	-	-	1/2/19/22	0/1/1/1
5	A2G	Y	202	1	-	2/6/23/26	0/1/1/1
4	MAN	D	201	-	-	1/2/19/22	0/1/1/1
5	A2G	r	202	1	-	2/6/23/26	0/1/1/1
5	A2G	k	202	1	-	2/6/23/26	0/1/1/1
4	MAN	U	201	-	-	1/2/19/22	0/1/1/1
5	A2G	R	202	1	-	2/6/23/26	0/1/1/1
5	A2G	W	202	1	-	2/6/23/26	0/1/1/1
4	MAN	Q	201	-	-	1/2/19/22	0/1/1/1
5	A2G	n	202	1	-	2/6/23/26	0/1/1/1
4	MAN	d	201	-	-	1/2/19/22	0/1/1/1
5	A2G	E	202	1	-	2/6/23/26	0/1/1/1
4	MAN	A	201	-	-	1/2/19/22	0/1/1/1
5	A2G	c	202	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A2G	j	202	1	-	2/6/23/26	0/1/1/1
5	A2G	O	202	1	-	2/6/23/26	0/1/1/1
5	A2G	g	202	1	-	2/6/23/26	0/1/1/1
4	MAN	Y	201	-	-	1/2/19/22	0/1/1/1
5	A2G	h	202	1	-	2/6/23/26	0/1/1/1
4	MAN	R	201	-	-	1/2/19/22	0/1/1/1
4	MAN	i	201	-	-	1/2/19/22	0/1/1/1
4	MAN	q	201	-	-	1/2/19/22	0/1/1/1
5	A2G	a	202	1	-	2/6/23/26	0/1/1/1
5	A2G	o	202	1	-	2/6/23/26	0/1/1/1
4	MAN	L	201	-	-	1/2/19/22	0/1/1/1
4	MAN	M	201	-	-	1/2/19/22	0/1/1/1
5	A2G	l	202	1	-	2/6/23/26	0/1/1/1
4	MAN	s	201	-	-	1/2/19/22	0/1/1/1
5	A2G	B	202	1	-	2/6/23/26	0/1/1/1
4	MAN	X	201	-	-	1/2/19/22	0/1/1/1
5	A2G	m	202	1	-	2/6/23/26	0/1/1/1
4	MAN	T	201	-	-	1/2/19/22	0/1/1/1
4	MAN	h	201	-	-	1/2/19/22	0/1/1/1
5	A2G	F	202	1	-	2/6/23/26	0/1/1/1
5	A2G	U	202	1	-	2/6/23/26	0/1/1/1
4	MAN	W	201	-	-	1/2/19/22	0/1/1/1
4	MAN	J	201	-	-	1/2/19/22	0/1/1/1
4	MAN	f	201	-	-	1/2/19/22	0/1/1/1
4	MAN	a	201	-	-	1/2/19/22	0/1/1/1
5	A2G	N	202	1	-	2/6/23/26	0/1/1/1
4	MAN	r	201	-	-	1/2/19/22	0/1/1/1
4	MAN	E	201	-	-	1/2/19/22	0/1/1/1
4	MAN	V	201	-	-	1/2/19/22	0/1/1/1
4	MAN	l	201	-	-	1/2/19/22	0/1/1/1
5	A2G	G	202	1	-	2/6/23/26	0/1/1/1
5	A2G	e	202	1	-	2/6/23/26	0/1/1/1
4	MAN	B	201	-	-	1/2/19/22	0/1/1/1
5	A2G	P	202	1	-	2/6/23/26	0/1/1/1
4	MAN	C	201	-	-	1/2/19/22	0/1/1/1
5	A2G	p	202	1	-	2/6/23/26	0/1/1/1
4	MAN	m	201	-	-	1/2/19/22	0/1/1/1
5	A2G	X	202	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	n	201	-	-	1/2/19/22	0/1/1/1
4	MAN	j	201	-	-	1/2/19/22	0/1/1/1
5	A2G	q	202	1	-	2/6/23/26	0/1/1/1
5	A2G	H	202	1	-	2/6/23/26	0/1/1/1
4	MAN	P	201	-	-	1/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	201	MAN	O2-C2	-2.04	1.39	1.43
4	L	201	MAN	O2-C2	-2.04	1.39	1.43
4	H	201	MAN	O2-C2	-2.04	1.39	1.43
4	A	201	MAN	O2-C2	-2.03	1.39	1.43
4	n	201	MAN	O2-C2	-2.02	1.39	1.43
4	c	201	MAN	O2-C2	-2.02	1.39	1.43
4	C	201	MAN	O2-C2	-2.02	1.39	1.43
4	P	201	MAN	O2-C2	-2.02	1.39	1.43
4	m	201	MAN	O2-C2	-2.02	1.39	1.43
4	h	201	MAN	O2-C2	-2.01	1.39	1.43
4	i	201	MAN	O2-C2	-2.01	1.39	1.43
4	K	201	MAN	O2-C2	-2.01	1.39	1.43
4	T	201	MAN	O2-C2	-2.01	1.39	1.43
4	l	201	MAN	O2-C2	-2.01	1.39	1.43
4	q	201	MAN	O2-C2	-2.01	1.39	1.43
4	r	201	MAN	O2-C2	-2.01	1.39	1.43
4	G	201	MAN	O2-C2	-2.01	1.39	1.43
4	f	201	MAN	O2-C2	-2.01	1.39	1.43
4	Z	201	MAN	O2-C2	-2.00	1.39	1.43
4	d	201	MAN	O2-C2	-2.00	1.39	1.43
4	B	201	MAN	O2-C2	-2.00	1.39	1.43
4	M	201	MAN	O2-C2	-2.00	1.39	1.43

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	201	MAN	C1-O5-C5	6.24	120.64	112.19
4	r	201	MAN	C1-O5-C5	6.23	120.64	112.19
4	X	201	MAN	C1-O5-C5	6.22	120.62	112.19
4	I	201	MAN	C1-O5-C5	6.22	120.62	112.19
4	N	201	MAN	C1-O5-C5	6.22	120.62	112.19
4	L	201	MAN	C1-O5-C5	6.22	120.62	112.19
4	e	201	MAN	C1-O5-C5	6.22	120.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	201	MAN	C1-O5-C5	6.22	120.61	112.19
4	A	201	MAN	C1-O5-C5	6.21	120.61	112.19
4	g	201	MAN	C1-O5-C5	6.21	120.61	112.19
4	s	201	MAN	C1-O5-C5	6.21	120.61	112.19
4	T	201	MAN	C1-O5-C5	6.21	120.61	112.19
4	U	201	MAN	C1-O5-C5	6.20	120.60	112.19
4	j	201	MAN	C1-O5-C5	6.20	120.60	112.19
4	C	201	MAN	C1-O5-C5	6.20	120.60	112.19
4	d	201	MAN	C1-O5-C5	6.20	120.59	112.19
4	Z	201	MAN	C1-O5-C5	6.20	120.59	112.19
4	k	201	MAN	C1-O5-C5	6.20	120.59	112.19
4	O	201	MAN	C1-O5-C5	6.20	120.59	112.19
4	l	201	MAN	C1-O5-C5	6.20	120.59	112.19
4	n	201	MAN	C1-O5-C5	6.20	120.59	112.19
4	Q	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	V	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	o	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	B	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	M	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	c	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	f	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	D	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	h	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	P	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	a	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	S	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	G	201	MAN	C1-O5-C5	6.19	120.58	112.19
4	b	201	MAN	C1-O5-C5	6.19	120.57	112.19
4	F	201	MAN	C1-O5-C5	6.18	120.57	112.19
4	J	201	MAN	C1-O5-C5	6.18	120.57	112.19
4	q	201	MAN	C1-O5-C5	6.18	120.57	112.19
4	W	201	MAN	C1-O5-C5	6.18	120.57	112.19
4	R	201	MAN	C1-O5-C5	6.18	120.56	112.19
4	i	201	MAN	C1-O5-C5	6.18	120.56	112.19
4	p	201	MAN	C1-O5-C5	6.17	120.55	112.19
4	K	201	MAN	C1-O5-C5	6.17	120.55	112.19
4	m	201	MAN	C1-O5-C5	6.16	120.53	112.19
4	H	201	MAN	C1-O5-C5	6.15	120.53	112.19
4	B	201	MAN	O2-C2-C1	-5.78	97.33	109.15
4	b	201	MAN	O2-C2-C1	-5.78	97.34	109.15
4	D	201	MAN	O2-C2-C1	-5.77	97.34	109.15
4	M	201	MAN	O2-C2-C1	-5.77	97.34	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	g	201	MAN	O2-C2-C1	-5.77	97.34	109.15
4	O	201	MAN	O2-C2-C1	-5.77	97.35	109.15
4	U	201	MAN	O2-C2-C1	-5.77	97.35	109.15
4	Z	201	MAN	O2-C2-C1	-5.77	97.35	109.15
4	r	201	MAN	O2-C2-C1	-5.77	97.35	109.15
4	h	201	MAN	O2-C2-C1	-5.77	97.35	109.15
4	R	201	MAN	O2-C2-C1	-5.77	97.36	109.15
4	Q	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	n	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	p	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	K	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	s	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	V	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	J	201	MAN	O2-C2-C1	-5.76	97.36	109.15
4	e	201	MAN	O2-C2-C1	-5.76	97.37	109.15
4	L	201	MAN	O2-C2-C1	-5.76	97.37	109.15
4	I	201	MAN	O2-C2-C1	-5.76	97.37	109.15
4	k	201	MAN	O2-C2-C1	-5.76	97.37	109.15
4	d	201	MAN	O2-C2-C1	-5.76	97.37	109.15
4	i	201	MAN	O2-C2-C1	-5.76	97.38	109.15
4	N	201	MAN	O2-C2-C1	-5.75	97.38	109.15
4	q	201	MAN	O2-C2-C1	-5.75	97.38	109.15
4	X	201	MAN	O2-C2-C1	-5.75	97.38	109.15
4	f	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	F	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	H	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	E	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	m	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	o	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	c	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	G	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	a	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	S	201	MAN	O2-C2-C1	-5.75	97.39	109.15
4	A	201	MAN	O2-C2-C1	-5.75	97.40	109.15
4	j	201	MAN	O2-C2-C1	-5.74	97.40	109.15
4	C	201	MAN	O2-C2-C1	-5.74	97.40	109.15
4	P	201	MAN	O2-C2-C1	-5.74	97.40	109.15
4	T	201	MAN	O2-C2-C1	-5.74	97.40	109.15
4	Y	201	MAN	O2-C2-C1	-5.74	97.41	109.15
4	l	201	MAN	O2-C2-C1	-5.74	97.42	109.15
4	W	201	MAN	O2-C2-C1	-5.73	97.43	109.15
4	h	201	MAN	C1-C2-C3	4.94	115.74	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	201	MAN	C1-C2-C3	4.93	115.73	109.67
4	o	201	MAN	C1-C2-C3	4.93	115.72	109.67
4	N	201	MAN	C1-C2-C3	4.93	115.72	109.67
4	c	201	MAN	C1-C2-C3	4.93	115.72	109.67
4	I	201	MAN	C1-C2-C3	4.93	115.72	109.67
4	Y	201	MAN	C1-C2-C3	4.92	115.72	109.67
4	k	201	MAN	C1-C2-C3	4.92	115.72	109.67
4	a	201	MAN	C1-C2-C3	4.91	115.71	109.67
4	J	201	MAN	C1-C2-C3	4.91	115.71	109.67
4	Q	201	MAN	C1-C2-C3	4.91	115.71	109.67
4	j	201	MAN	C1-C2-C3	4.91	115.71	109.67
4	p	201	MAN	C1-C2-C3	4.91	115.70	109.67
4	C	201	MAN	C1-C2-C3	4.91	115.70	109.67
4	K	201	MAN	C1-C2-C3	4.91	115.70	109.67
4	g	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	G	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	V	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	F	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	T	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	W	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	X	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	s	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	i	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	d	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	S	201	MAN	C1-C2-C3	4.90	115.69	109.67
4	e	201	MAN	C1-C2-C3	4.90	115.68	109.67
4	E	201	MAN	C1-C2-C3	4.89	115.68	109.67
4	D	201	MAN	C1-C2-C3	4.89	115.68	109.67
4	B	201	MAN	C1-C2-C3	4.89	115.68	109.67
4	Z	201	MAN	C1-C2-C3	4.89	115.67	109.67
4	O	201	MAN	C1-C2-C3	4.89	115.67	109.67
4	U	201	MAN	C1-C2-C3	4.89	115.67	109.67
4	q	201	MAN	C1-C2-C3	4.89	115.67	109.67
4	R	201	MAN	C1-C2-C3	4.88	115.67	109.67
4	L	201	MAN	C1-C2-C3	4.88	115.66	109.67
4	b	201	MAN	C1-C2-C3	4.88	115.66	109.67
4	H	201	MAN	C1-C2-C3	4.88	115.66	109.67
4	m	201	MAN	O5-C1-C2	4.88	118.30	110.77
4	A	201	MAN	C1-C2-C3	4.88	115.66	109.67
4	l	201	MAN	C1-C2-C3	4.88	115.66	109.67
4	P	201	MAN	C1-C2-C3	4.87	115.66	109.67
4	n	201	MAN	C1-C2-C3	4.87	115.65	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	r	201	MAN	C1-C2-C3	4.87	115.65	109.67
4	m	201	MAN	C1-C2-C3	4.86	115.65	109.67
4	q	201	MAN	O5-C1-C2	4.86	118.28	110.77
4	f	201	MAN	C1-C2-C3	4.86	115.64	109.67
4	R	201	MAN	O5-C1-C2	4.85	118.26	110.77
4	B	201	MAN	O5-C1-C2	4.85	118.26	110.77
4	p	201	MAN	O5-C1-C2	4.85	118.26	110.77
4	b	201	MAN	O5-C1-C2	4.85	118.26	110.77
4	f	201	MAN	O5-C1-C2	4.85	118.25	110.77
4	l	201	MAN	O5-C1-C2	4.85	118.25	110.77
4	F	201	MAN	O5-C1-C2	4.85	118.25	110.77
4	H	201	MAN	O5-C1-C2	4.84	118.25	110.77
4	O	201	MAN	O5-C1-C2	4.84	118.25	110.77
4	S	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	U	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	i	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	n	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	L	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	P	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	e	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	o	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	A	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	V	201	MAN	O5-C1-C2	4.84	118.24	110.77
4	T	201	MAN	O5-C1-C2	4.84	118.23	110.77
4	d	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	G	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	k	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	I	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	r	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	K	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	J	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	Q	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	a	201	MAN	O5-C1-C2	4.83	118.23	110.77
4	D	201	MAN	O5-C1-C2	4.83	118.22	110.77
4	j	201	MAN	O5-C1-C2	4.83	118.22	110.77
4	Z	201	MAN	O5-C1-C2	4.83	118.22	110.77
4	c	201	MAN	O5-C1-C2	4.83	118.22	110.77
4	X	201	MAN	O5-C1-C2	4.83	118.22	110.77
4	W	201	MAN	O5-C1-C2	4.83	118.22	110.77
4	g	201	MAN	O5-C1-C2	4.82	118.21	110.77
4	s	201	MAN	O5-C1-C2	4.82	118.21	110.77
4	C	201	MAN	O5-C1-C2	4.81	118.20	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	201	MAN	O5-C1-C2	4.81	118.20	110.77
4	M	201	MAN	O5-C1-C2	4.81	118.20	110.77
4	h	201	MAN	O5-C1-C2	4.81	118.19	110.77
4	N	201	MAN	O5-C1-C2	4.80	118.18	110.77
4	E	201	MAN	O5-C1-C2	4.80	118.18	110.77
5	S	202	A2G	O5-C1-C2	-4.37	104.38	111.29
5	Q	202	A2G	O5-C1-C2	-4.37	104.39	111.29
5	R	202	A2G	O5-C1-C2	-4.37	104.39	111.29
5	a	202	A2G	O5-C1-C2	-4.36	104.40	111.29
5	A	202	A2G	O5-C1-C2	-4.36	104.40	111.29
5	T	202	A2G	O5-C1-C2	-4.36	104.40	111.29
5	V	202	A2G	O5-C1-C2	-4.36	104.41	111.29
5	e	202	A2G	O5-C1-C2	-4.36	104.41	111.29
5	g	202	A2G	O5-C1-C2	-4.36	104.41	111.29
5	l	202	A2G	O5-C1-C2	-4.36	104.41	111.29
5	o	202	A2G	O5-C1-C2	-4.35	104.42	111.29
5	O	202	A2G	O5-C1-C2	-4.35	104.42	111.29
5	n	202	A2G	O5-C1-C2	-4.35	104.42	111.29
5	j	202	A2G	O5-C1-C2	-4.35	104.42	111.29
5	q	202	A2G	O5-C1-C2	-4.35	104.42	111.29
5	W	202	A2G	O5-C1-C2	-4.35	104.43	111.29
5	f	202	A2G	O5-C1-C2	-4.34	104.43	111.29
5	d	202	A2G	O5-C1-C2	-4.34	104.43	111.29
5	M	202	A2G	O5-C1-C2	-4.34	104.43	111.29
5	N	202	A2G	O5-C1-C2	-4.34	104.43	111.29
5	m	202	A2G	O5-C1-C2	-4.34	104.43	111.29
5	U	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	p	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	E	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	P	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	G	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	Z	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	D	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	i	202	A2G	O5-C1-C2	-4.34	104.44	111.29
5	c	202	A2G	O5-C1-C2	-4.33	104.44	111.29
5	J	202	A2G	O5-C1-C2	-4.33	104.44	111.29
5	C	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	H	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	B	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	K	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	X	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	Y	202	A2G	O5-C1-C2	-4.33	104.45	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	h	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	s	202	A2G	O5-C1-C2	-4.33	104.45	111.29
5	F	202	A2G	O5-C1-C2	-4.33	104.46	111.29
5	L	202	A2G	O5-C1-C2	-4.33	104.46	111.29
5	k	202	A2G	O5-C1-C2	-4.33	104.46	111.29
5	I	202	A2G	O5-C1-C2	-4.32	104.46	111.29
5	b	202	A2G	O5-C1-C2	-4.32	104.46	111.29
5	r	202	A2G	O5-C1-C2	-4.32	104.46	111.29

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	d	202	A2G	O7-C7-N2-C2
5	d	202	A2G	C8-C7-N2-C2
5	A	202	A2G	O7-C7-N2-C2
5	A	202	A2G	C8-C7-N2-C2
5	B	202	A2G	O7-C7-N2-C2
5	B	202	A2G	C8-C7-N2-C2
5	C	202	A2G	O7-C7-N2-C2
5	C	202	A2G	C8-C7-N2-C2
5	D	202	A2G	O7-C7-N2-C2
5	D	202	A2G	C8-C7-N2-C2
5	E	202	A2G	O7-C7-N2-C2
5	E	202	A2G	C8-C7-N2-C2
5	F	202	A2G	O7-C7-N2-C2
5	F	202	A2G	C8-C7-N2-C2
5	G	202	A2G	O7-C7-N2-C2
5	G	202	A2G	C8-C7-N2-C2
5	H	202	A2G	O7-C7-N2-C2
5	H	202	A2G	C8-C7-N2-C2
5	I	202	A2G	O7-C7-N2-C2
5	I	202	A2G	C8-C7-N2-C2
5	J	202	A2G	O7-C7-N2-C2
5	J	202	A2G	C8-C7-N2-C2
5	K	202	A2G	O7-C7-N2-C2
5	K	202	A2G	C8-C7-N2-C2
5	L	202	A2G	O7-C7-N2-C2
5	L	202	A2G	C8-C7-N2-C2
5	M	202	A2G	O7-C7-N2-C2
5	M	202	A2G	C8-C7-N2-C2
5	N	202	A2G	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	N	202	A2G	C8-C7-N2-C2
5	O	202	A2G	O7-C7-N2-C2
5	O	202	A2G	C8-C7-N2-C2
5	P	202	A2G	O7-C7-N2-C2
5	P	202	A2G	C8-C7-N2-C2
5	Q	202	A2G	O7-C7-N2-C2
5	Q	202	A2G	C8-C7-N2-C2
5	R	202	A2G	O7-C7-N2-C2
5	R	202	A2G	C8-C7-N2-C2
5	S	202	A2G	O7-C7-N2-C2
5	S	202	A2G	C8-C7-N2-C2
5	T	202	A2G	O7-C7-N2-C2
5	T	202	A2G	C8-C7-N2-C2
5	U	202	A2G	O7-C7-N2-C2
5	U	202	A2G	C8-C7-N2-C2
5	V	202	A2G	O7-C7-N2-C2
5	V	202	A2G	C8-C7-N2-C2
5	W	202	A2G	O7-C7-N2-C2
5	W	202	A2G	C8-C7-N2-C2
5	X	202	A2G	O7-C7-N2-C2
5	X	202	A2G	C8-C7-N2-C2
5	Y	202	A2G	O7-C7-N2-C2
5	Y	202	A2G	C8-C7-N2-C2
5	Z	202	A2G	O7-C7-N2-C2
5	Z	202	A2G	C8-C7-N2-C2
5	a	202	A2G	O7-C7-N2-C2
5	a	202	A2G	C8-C7-N2-C2
5	b	202	A2G	O7-C7-N2-C2
5	b	202	A2G	C8-C7-N2-C2
5	c	202	A2G	O7-C7-N2-C2
5	c	202	A2G	C8-C7-N2-C2
5	e	202	A2G	O7-C7-N2-C2
5	e	202	A2G	C8-C7-N2-C2
5	f	202	A2G	O7-C7-N2-C2
5	f	202	A2G	C8-C7-N2-C2
5	g	202	A2G	O7-C7-N2-C2
5	g	202	A2G	C8-C7-N2-C2
5	h	202	A2G	O7-C7-N2-C2
5	h	202	A2G	C8-C7-N2-C2
5	i	202	A2G	O7-C7-N2-C2
5	i	202	A2G	C8-C7-N2-C2
5	j	202	A2G	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	j	202	A2G	C8-C7-N2-C2
5	k	202	A2G	O7-C7-N2-C2
5	k	202	A2G	C8-C7-N2-C2
5	l	202	A2G	O7-C7-N2-C2
5	l	202	A2G	C8-C7-N2-C2
5	m	202	A2G	O7-C7-N2-C2
5	m	202	A2G	C8-C7-N2-C2
5	n	202	A2G	O7-C7-N2-C2
5	n	202	A2G	C8-C7-N2-C2
5	o	202	A2G	O7-C7-N2-C2
5	o	202	A2G	C8-C7-N2-C2
5	p	202	A2G	O7-C7-N2-C2
5	p	202	A2G	C8-C7-N2-C2
5	q	202	A2G	O7-C7-N2-C2
5	q	202	A2G	C8-C7-N2-C2
5	r	202	A2G	O7-C7-N2-C2
5	r	202	A2G	C8-C7-N2-C2
5	s	202	A2G	O7-C7-N2-C2
5	s	202	A2G	C8-C7-N2-C2
4	A	201	MAN	C4-C5-C6-O6
4	K	201	MAN	C4-C5-C6-O6
4	k	201	MAN	C4-C5-C6-O6
4	J	201	MAN	C4-C5-C6-O6
4	M	201	MAN	C4-C5-C6-O6
4	O	201	MAN	C4-C5-C6-O6
4	T	201	MAN	C4-C5-C6-O6
4	a	201	MAN	C4-C5-C6-O6
4	I	201	MAN	C4-C5-C6-O6
4	d	201	MAN	C4-C5-C6-O6
4	B	201	MAN	C4-C5-C6-O6
4	C	201	MAN	C4-C5-C6-O6
4	D	201	MAN	C4-C5-C6-O6
4	E	201	MAN	C4-C5-C6-O6
4	F	201	MAN	C4-C5-C6-O6
4	G	201	MAN	C4-C5-C6-O6
4	H	201	MAN	C4-C5-C6-O6
4	L	201	MAN	C4-C5-C6-O6
4	N	201	MAN	C4-C5-C6-O6
4	P	201	MAN	C4-C5-C6-O6
4	Q	201	MAN	C4-C5-C6-O6
4	R	201	MAN	C4-C5-C6-O6
4	S	201	MAN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	U	201	MAN	C4-C5-C6-O6
4	V	201	MAN	C4-C5-C6-O6
4	W	201	MAN	C4-C5-C6-O6
4	X	201	MAN	C4-C5-C6-O6
4	Y	201	MAN	C4-C5-C6-O6
4	Z	201	MAN	C4-C5-C6-O6
4	b	201	MAN	C4-C5-C6-O6
4	c	201	MAN	C4-C5-C6-O6
4	e	201	MAN	C4-C5-C6-O6
4	f	201	MAN	C4-C5-C6-O6
4	g	201	MAN	C4-C5-C6-O6
4	h	201	MAN	C4-C5-C6-O6
4	i	201	MAN	C4-C5-C6-O6
4	j	201	MAN	C4-C5-C6-O6
4	l	201	MAN	C4-C5-C6-O6
4	m	201	MAN	C4-C5-C6-O6
4	n	201	MAN	C4-C5-C6-O6
4	o	201	MAN	C4-C5-C6-O6
4	p	201	MAN	C4-C5-C6-O6
4	q	201	MAN	C4-C5-C6-O6
4	r	201	MAN	C4-C5-C6-O6
4	s	201	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

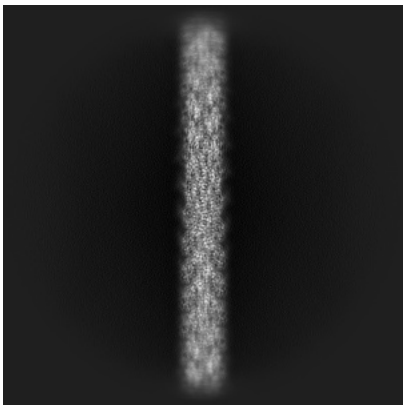
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18588. These allow visual inspection of the internal detail of the map and identification of artifacts.

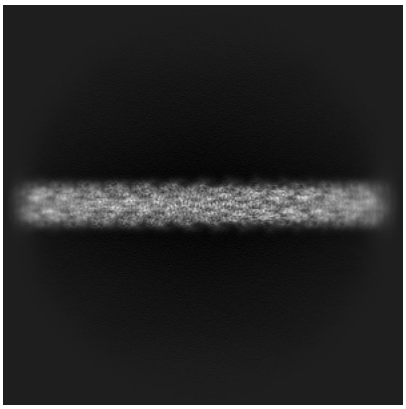
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

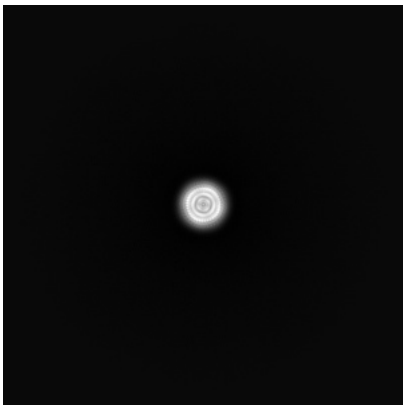
6.1.1 Primary map



X

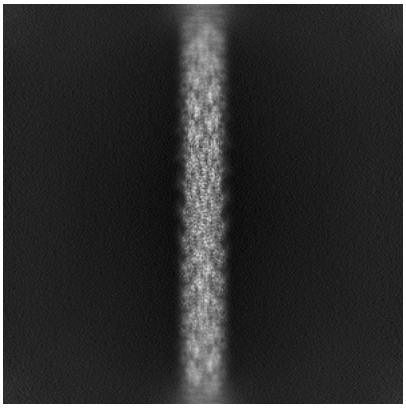


Y

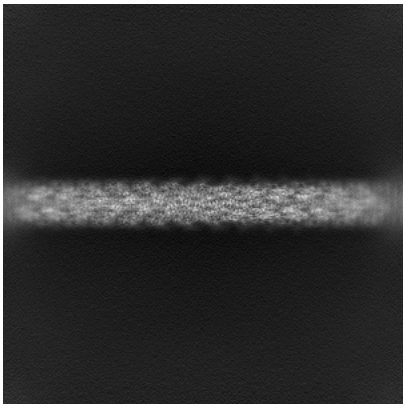


Z

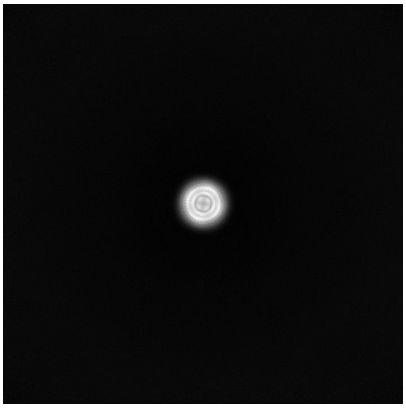
6.1.2 Raw map



X



Y

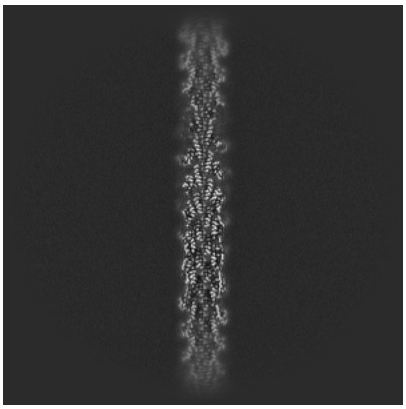


Z

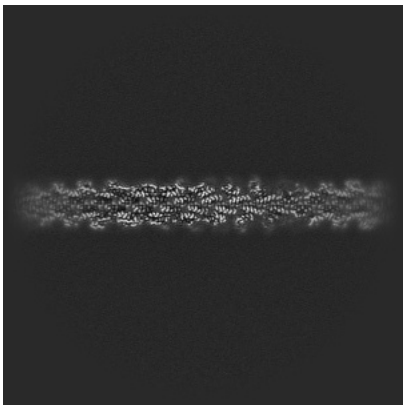
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

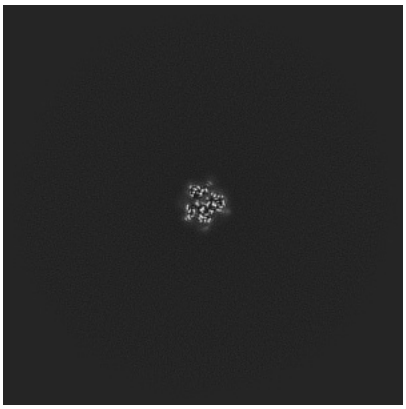
6.2.1 Primary map



X Index: 256

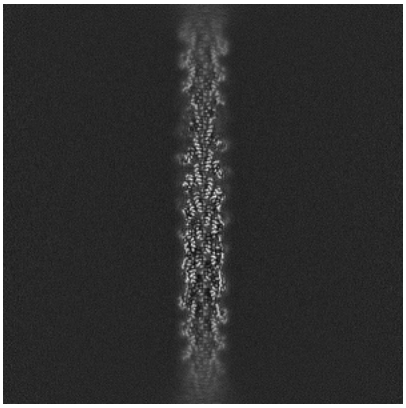


Y Index: 256

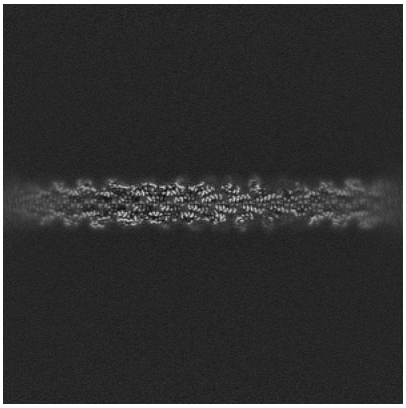


Z Index: 256

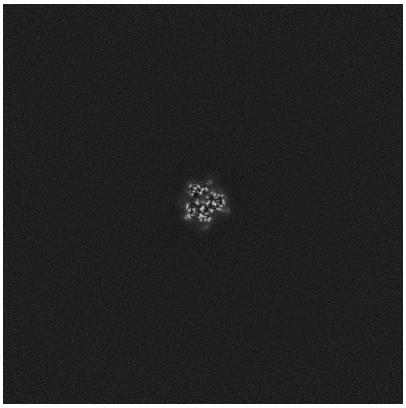
6.2.2 Raw map



X Index: 256



Y Index: 256

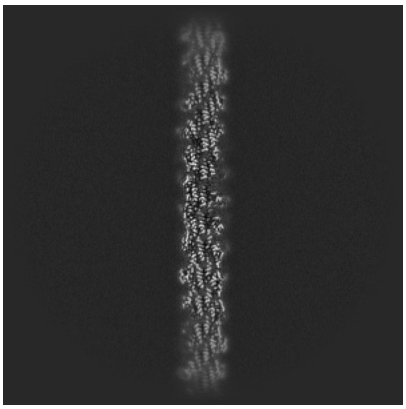


Z Index: 256

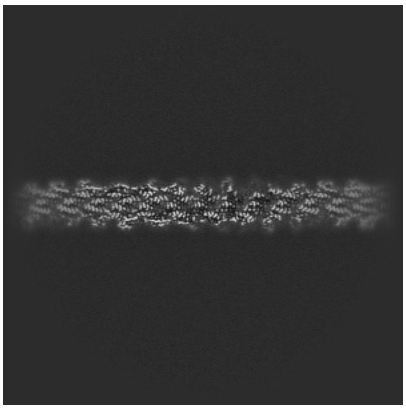
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

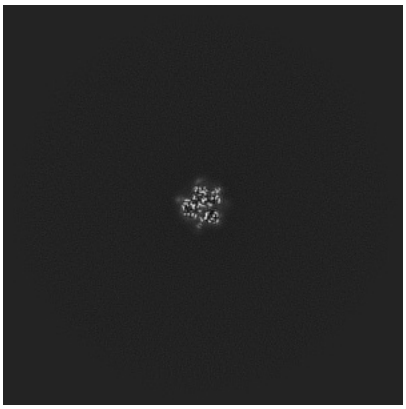
6.3.1 Primary map



X Index: 262

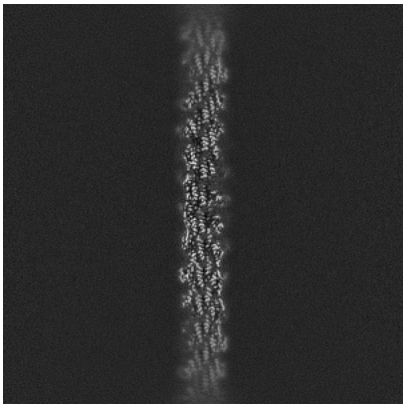


Y Index: 252

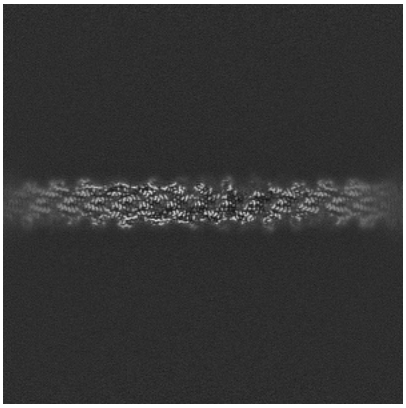


Z Index: 273

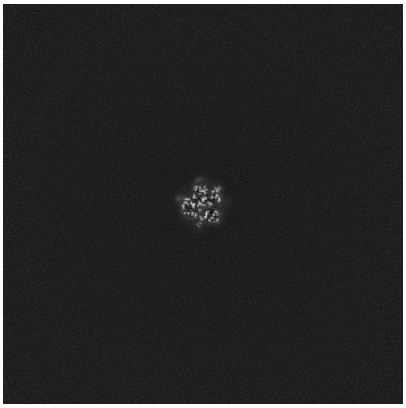
6.3.2 Raw map



X Index: 262



Y Index: 252

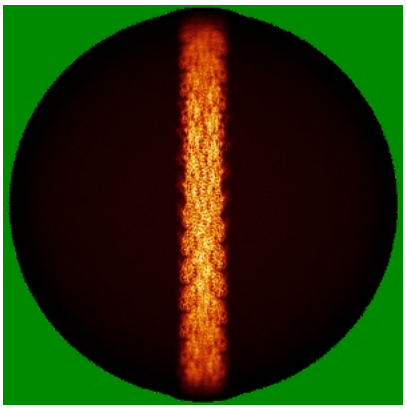


Z Index: 273

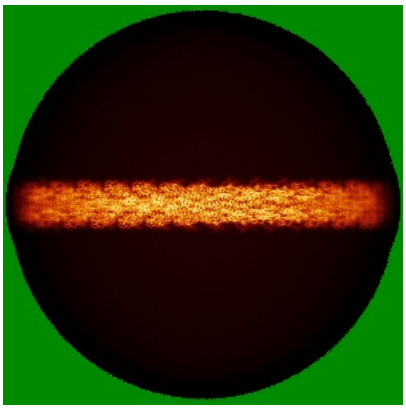
The images above show the largest variance slices of the map in three orthogonal directions.

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

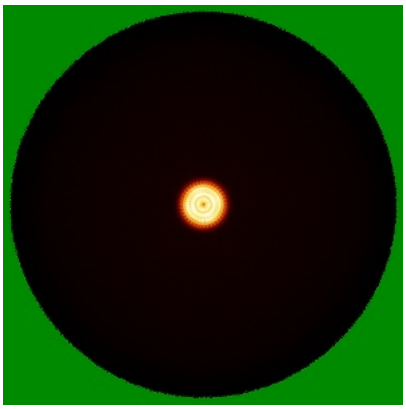
6.4.1 Primary map



X

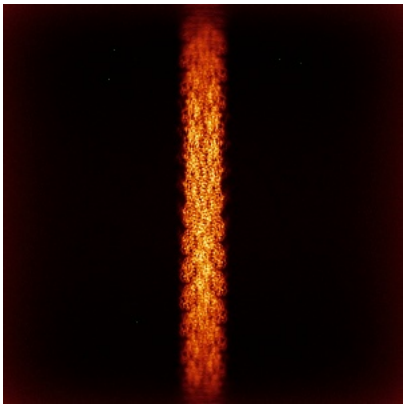


Y

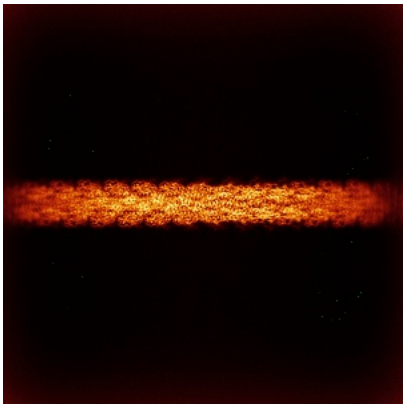


Z

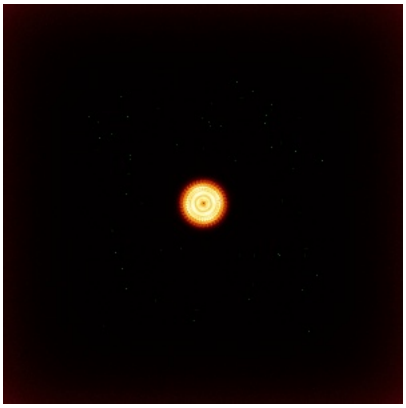
6.4.2 Raw map



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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

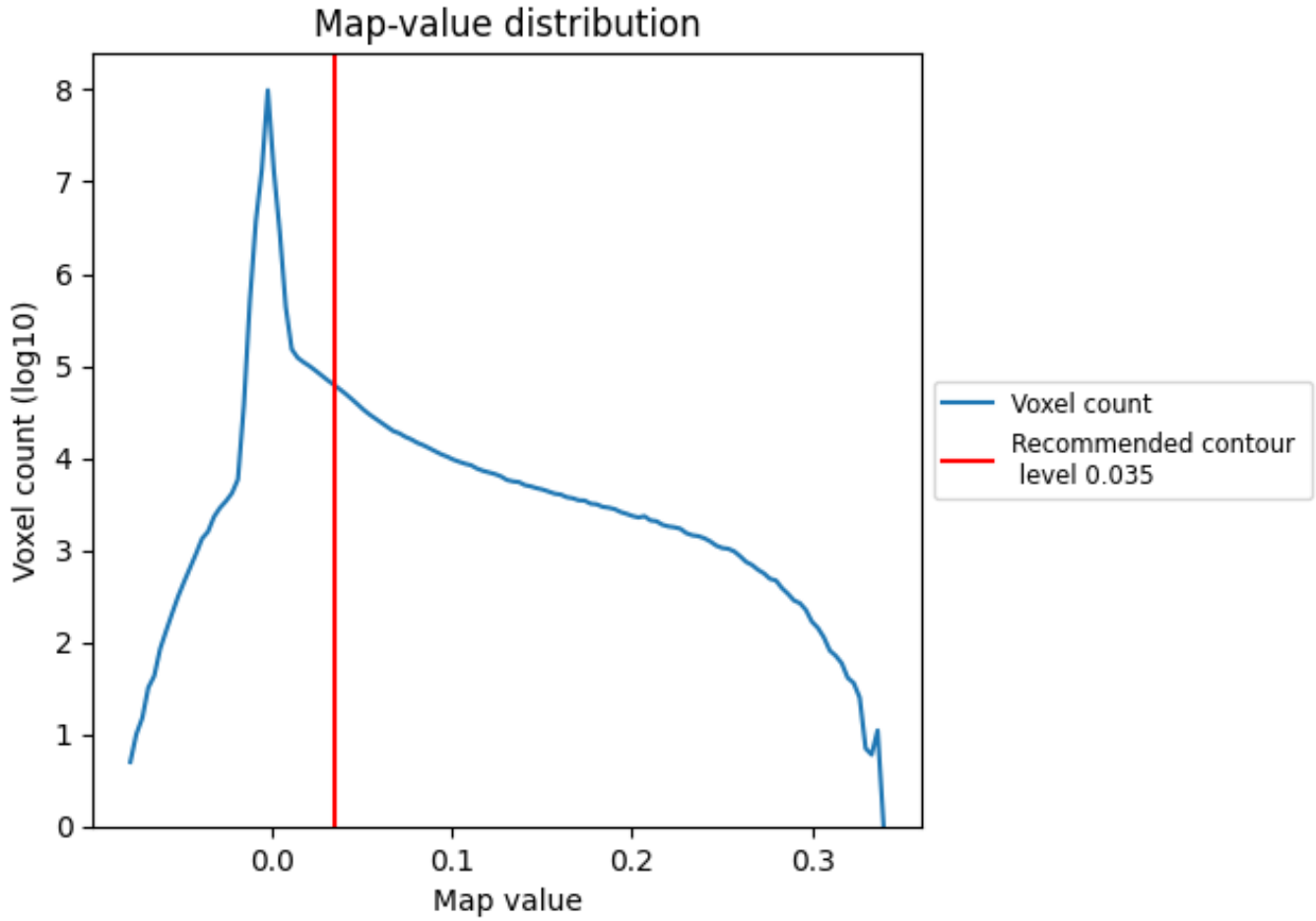
6.6 Mask visualisation (i)

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

7 Map analysis

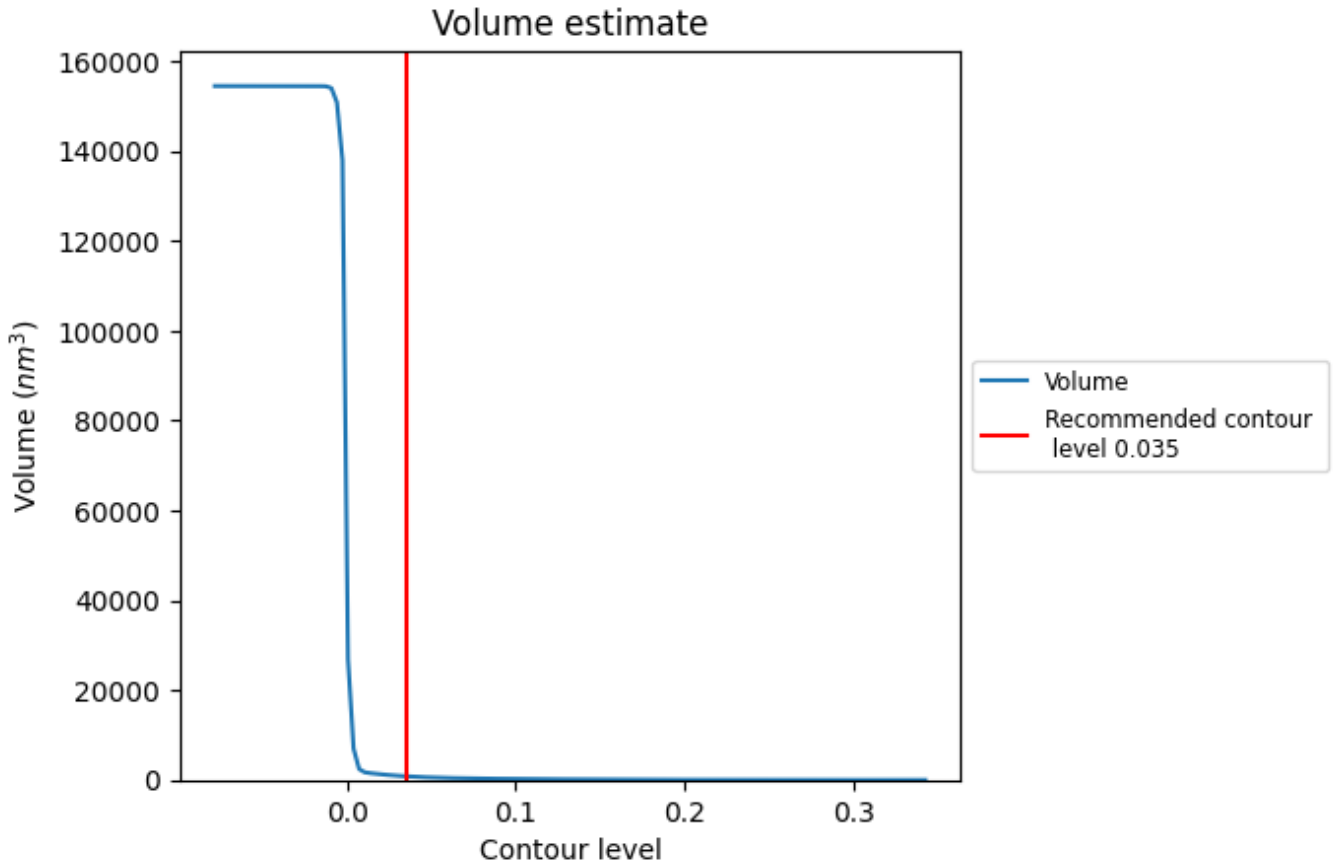
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

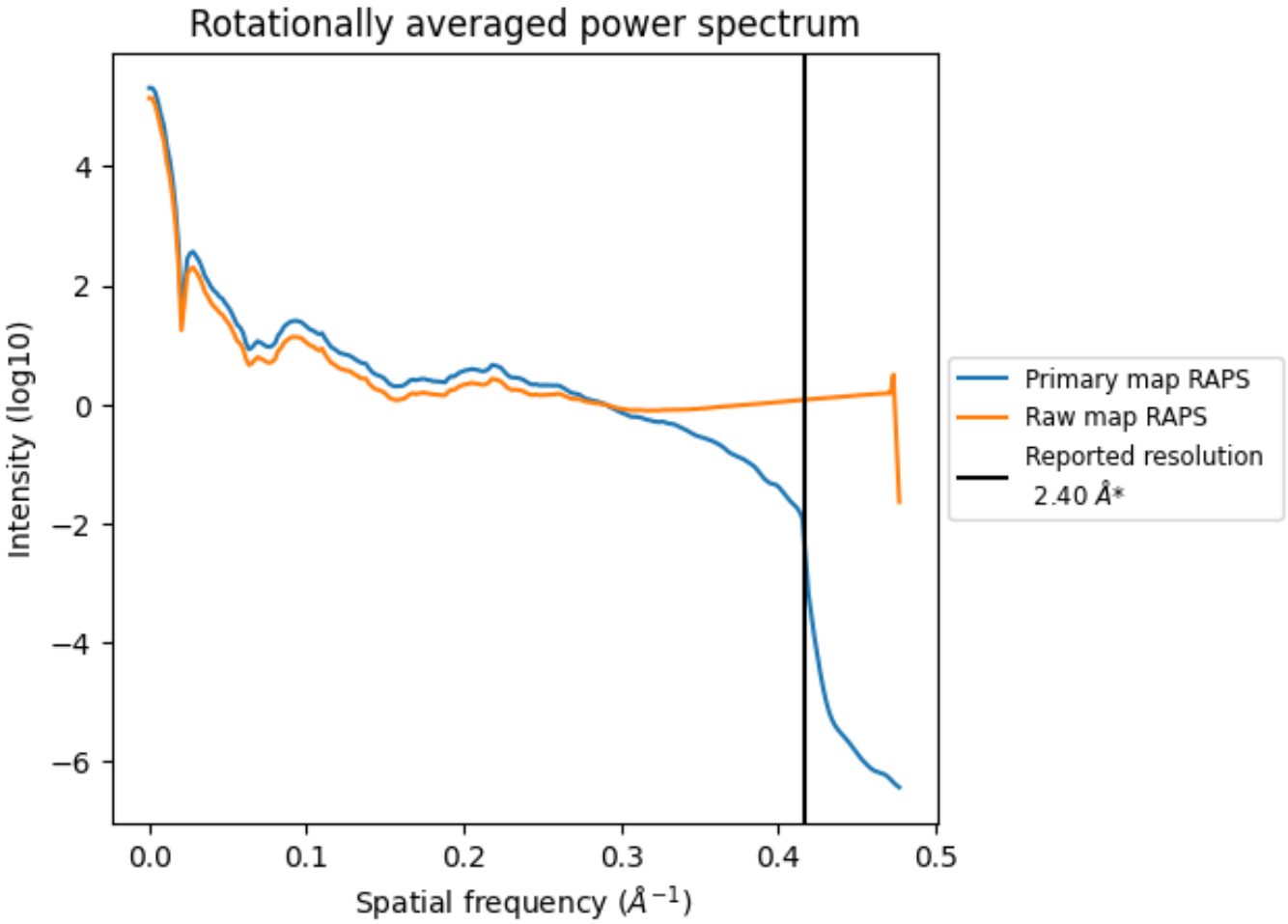
7.2 Volume estimate



The volume at the recommended contour level is 814 nm^3; this corresponds to an approximate mass of 735 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)

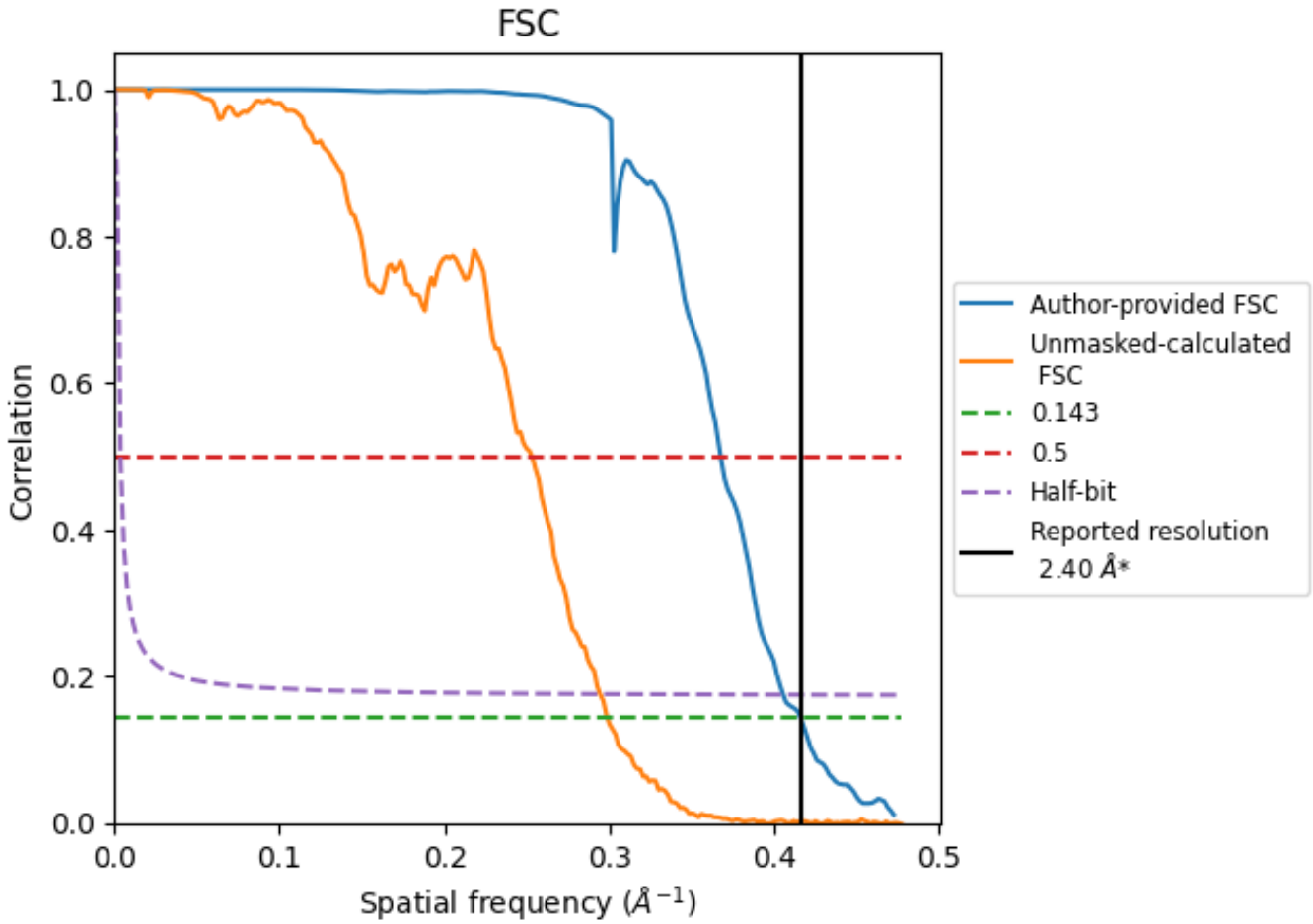


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

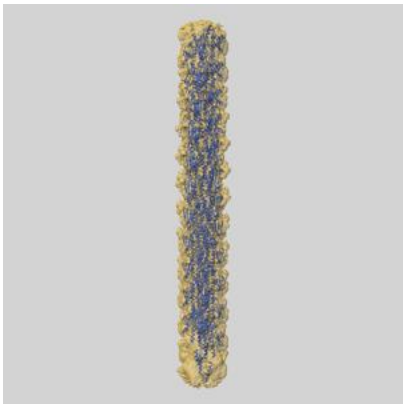
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.72	2.47
Unmasked-calculated*	3.35	3.95	3.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.4 by more than 10 %

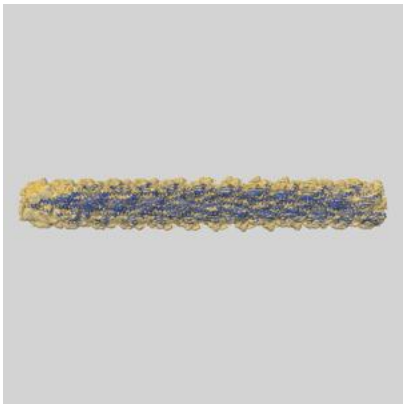
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18588 and PDB model 8QQD. Per-residue inclusion information can be found in section 3 on page 22.

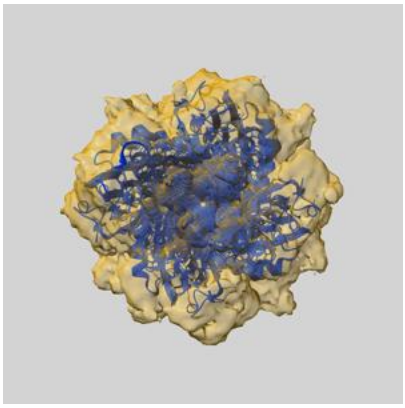
9.1 Map-model overlay



X



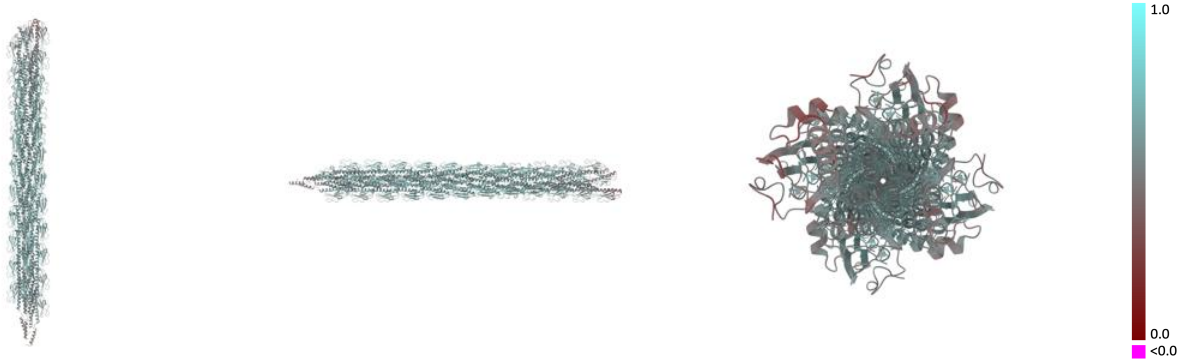
Y



Z

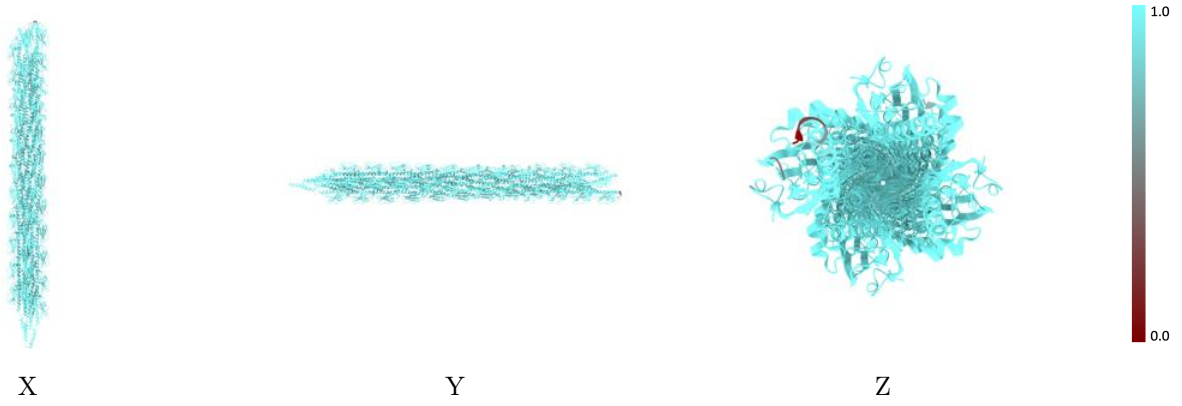
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



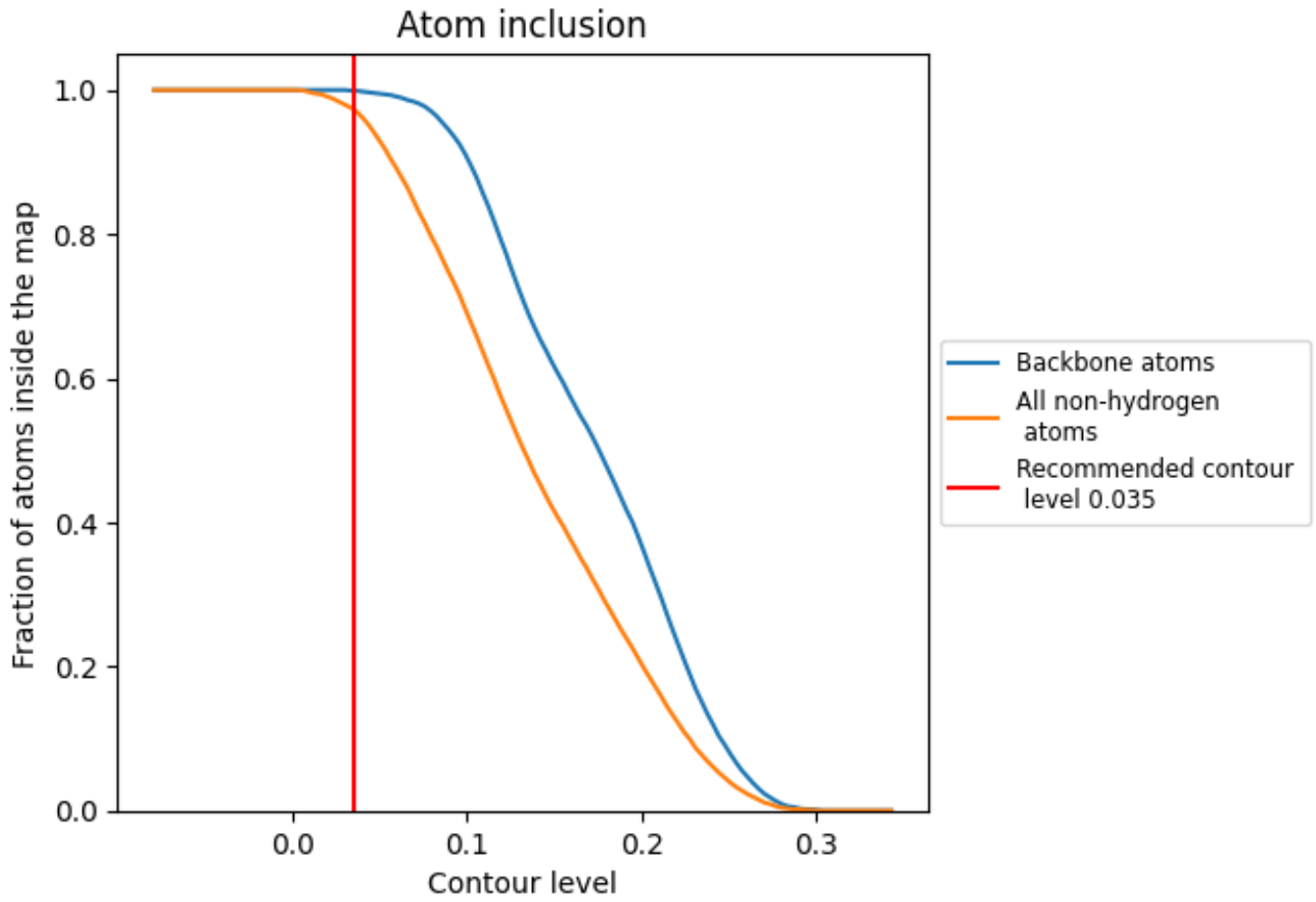
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9740	0.5460
0B	0.7870	0.3890
1	0.0710	0.1110
1D	0.9290	0.3150
2C	0.8200	0.3660
3A	0.9290	0.2970
3E	0.9640	0.3240
4	0.4430	0.3030
4D	0.7870	0.3610
5B	0.9640	0.3160
6A	0.7870	0.3640
6E	0.7870	0.3620
7C	0.9640	0.3470
8B	0.7700	0.3810
9	0.4640	0.1570
9D	0.9290	0.3240
A	0.9310	0.4440
AD	0.8200	0.3940
B	0.9810	0.4730
BB	0.8930	0.3170
BF	0.9290	0.2970
C	0.9860	0.4960
CA	0.6890	0.2930
CE	0.8030	0.3530
D	0.9890	0.5150
DC	0.9290	0.2990
E	0.9890	0.5280
EB	0.8030	0.3680
EF	0.7870	0.3760
F	0.9880	0.5380
FD	0.9640	0.3350
G	0.9890	0.5460
GC	0.7700	0.3700
H	0.9910	0.5560
HA	0.7140	0.2020

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Chain	Atom inclusion	Q-score
HE	0.9290	0.3180
I	0.9910	0.5590
ID	0.8030	0.4040
J	0.9910	0.5650
JB	0.9640	0.3370
JF	0.9640	0.3000
K	0.9890	0.5700
KA	0.7210	0.3170
KE	0.8030	0.3620
L	0.9910	0.5750
LC	0.9640	0.3450
M	0.9880	0.5760
MB	0.8030	0.3460
MF	0.7870	0.3940
N	0.9870	0.5790
ND	0.9640	0.3190
O	0.9880	0.5820
OC	0.8030	0.3760
P	0.9880	0.5850
PA	0.7860	0.2500
PE	0.9640	0.3440
Q	0.9870	0.5860
QD	0.7870	0.3860
R	0.9880	0.5850
RB	0.9290	0.3330
RF	0.9290	0.3210
S	0.9890	0.5890
SA	0.7210	0.3510
SE	0.8030	0.3660
T	0.9890	0.5910
TC	0.9290	0.3410
U	0.9870	0.5920
UB	0.7870	0.3610
UF	0.7870	0.3780
V	0.9890	0.5910
VD	0.9640	0.3150
W	0.9890	0.5920
WC	0.8030	0.3940
X	0.9920	0.5930
XA	0.9290	0.2460
XE	0.8930	0.3210
Y	0.9920	0.5930

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Chain	Atom inclusion	Q-score
YD	0.8030	0.3880
Z	0.9880	0.5900
ZB	0.9290	0.3360
ZF	0.9290	0.3350
a	0.9890	0.5890
aA	0.7540	0.3440
aE	0.8030	0.3580
b	0.9890	0.5900
bC	0.9640	0.3370
c	0.9920	0.5890
cB	0.7870	0.3650
cF	0.7870	0.3620
d	0.9920	0.5900
dD	0.9640	0.3260
e	0.9890	0.5870
eC	0.8030	0.4030
f	0.9880	0.5870
fA	0.9290	0.3010
fE	0.9290	0.3170
g	0.9880	0.5860
gD	0.8030	0.3730
h	0.9890	0.5830
hB	0.9640	0.3480
i	0.9910	0.5830
iA	0.7700	0.3580
iE	0.8030	0.3700
j	0.9930	0.5810
jC	0.9640	0.3270
k	0.9940	0.5780
kB	0.8200	0.3680
l	0.9930	0.5720
lD	0.9640	0.3560
m	0.9930	0.5710
mC	0.8030	0.3870
n	0.9920	0.5630
nA	0.9290	0.3090
nE	0.8930	0.3030
o	0.9930	0.5550
oD	0.8030	0.3580
p	0.9930	0.5440
pB	0.9640	0.3410
q	0.9920	0.5390

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Chain	Atom inclusion	Q-score
qA	0.7700	0.3700
qE	0.8030	0.3670
r	0.9910	0.5270
rC	0.9640	0.3390
s	0.9760	0.5170
sB	0.8200	0.3800
t	0.9640	0.3390
tD	0.9290	0.3270
uC	0.8030	0.3680
vA	0.9290	0.2860
vE	0.9640	0.3180
w	0.7870	0.3810
wD	0.8030	0.3600
xB	0.9640	0.3190
yA	0.7870	0.3480
yE	0.8030	0.3620
zC	0.9640	0.3410