Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 01:35 PM JST

PDB ID	:	9JKF
EMDB ID	:	EMD-61553
Title	:	Asymmetric structure of cleaved HIV-1 Tri FPPR envelope glycoprotein trimer in amphipol-lipid nanodiscs (Tri FPPR.1)
Authors	:	Qi, Y.; Zhang, S.; Sodroski, J.; Mao, Y.
Deposited on	:	2024-09-16
Resolution	:	3.40 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:

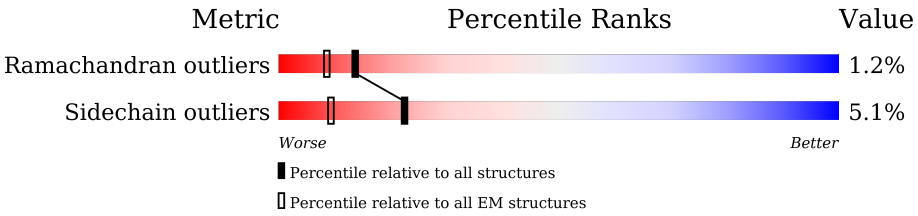
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	722	62% 34%
1	B	722	19% 79%
1	C	722	62% 34%
1	D	722	22% 77%
1	E	722	62% 34%
1	F	722	19% 80%
2	0	3	67% 100%
2	3	3	67% 33%
2	5	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	7	3	33% 100%
2	AA	3	67% 33%
2	BA	3	33% 67% 33%
2	EA	3	100%
2	G	3	100%
2	IA	3	100%
2	J	3	33% 33% 67%
2	K	3	33% 100%
2	L	3	67% 33%
2	M	3	33% 67%
2	P	3	100%
2	Q	3	33% 67% 33%
2	R	3	33% 67% 33%
2	V	3	67% 33%
2	Z	3	33% 67%
2	a	3	100%
2	c	3	67% 33%
2	g	3	33% 100%
2	h	3	67% 33%
2	m	3	100%
2	o	3	100%
2	q	3	67% 33%
2	r	3	33% 100%
2	s	3	100%
2	w	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	z	3	33% 67%
3	4	2	50% 50% 50%
3	6	2	100%
3	H	2	50% 100%
3	HA	2	100% 100%
3	I	2	50% 100%
3	KA	2	50% 100%
3	LA	2	50% 50%
3	MA	2	50% 50%
3	N	2	50% 50% 50%
3	U	2	100%
3	b	2	50% 100%
3	e	2	50% 100%
3	f	2	50% 100%
3	k	2	50% 100%
3	l	2	50% 50% 50%
3	n	2	100%
4	O	3	33% 100%
5	S	6	67% 33%
6	T	5	40% 20% 80%
7	1	5	20% 80%
7	W	5	80% 20%
7	i	5	40% 60%
7	j	5	20% 80% 20%
8	DA	7	14% 14% 86%

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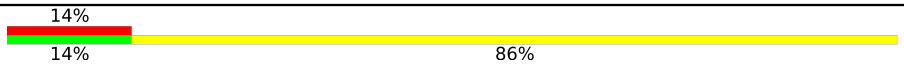
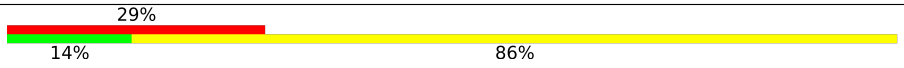
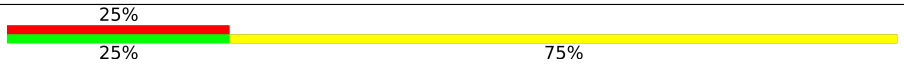
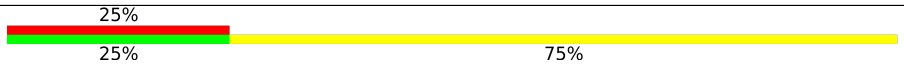
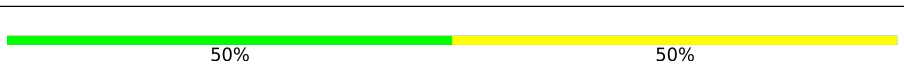
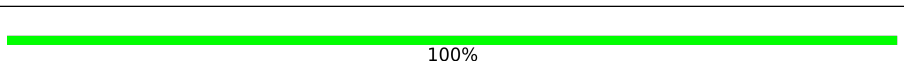
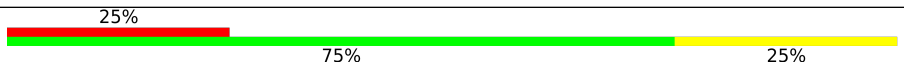
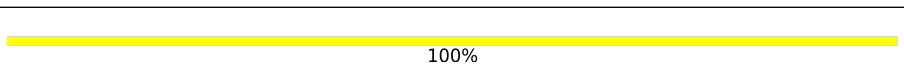
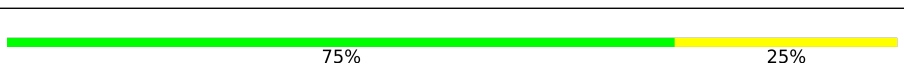
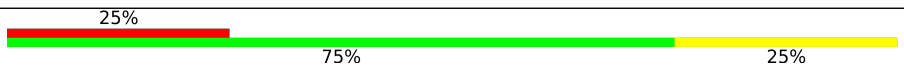
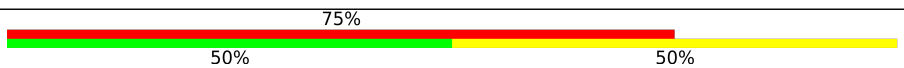
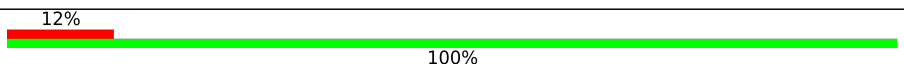
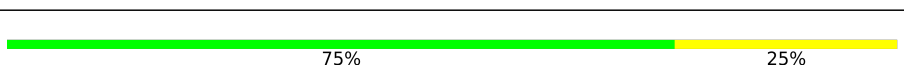
Mol	Chain	Length	Quality of chain
8	X	7	
8	u	7	
9	2	4	
9	9	4	
9	CA	4	
9	FA	4	
9	GA	4	
9	Y	4	
9	v	4	
10	JA	4	
10	d	4	
10	y	4	
11	p	8	
12	t	4	
12	x	4	
13	8	6	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 18127 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	150	Total	C	N	O	S	0	0
			1206	765	208	226	7		
1	C	476	Total	C	N	O	S	0	0
			3760	2350	667	717	26		
1	D	167	Total	C	N	O	S	0	0
			1379	891	232	249	7		
1	E	473	Total	C	N	O	S	0	0
			3731	2333	660	712	26		
1	A	474	Total	C	N	O	S	0	0
			3740	2338	661	715	26		
1	F	144	Total	C	N	O	S	0	0
			1159	735	200	217	7		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP G1JZH9
B	3	ARG	-	expression tag	UNP G1JZH9
B	4	VAL	-	expression tag	UNP G1JZH9
B	5	LYS	-	expression tag	UNP G1JZH9
B	6	GLU	-	expression tag	UNP G1JZH9
B	7	LYS	-	expression tag	UNP G1JZH9
B	8	TYR	-	expression tag	UNP G1JZH9
B	9	GLN	-	expression tag	UNP G1JZH9
B	10	HIS	-	expression tag	UNP G1JZH9
B	11	LEU	-	expression tag	UNP G1JZH9
B	12	TRP	-	expression tag	UNP G1JZH9
B	13	ARG	-	expression tag	UNP G1JZH9
B	14	TRP	-	expression tag	UNP G1JZH9
B	15	GLY	-	expression tag	UNP G1JZH9
B	16	TRP	-	expression tag	UNP G1JZH9
B	17	ARG	-	expression tag	UNP G1JZH9
B	18	TRP	-	expression tag	UNP G1JZH9
B	19	GLY	-	expression tag	UNP G1JZH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	THR	-	expression tag	UNP G1JZH9
B	32	THR	VAL	conflict	UNP G1JZH9
B	34	LYS	ASN	conflict	UNP G1JZH9
B	115	GLU	GLN	conflict	UNP G1JZH9
B	532	VAL	ALA	conflict	UNP G1JZH9
B	535	MET	ILE	conflict	UNP G1JZH9
B	543	GLN	LEU	conflict	UNP G1JZH9
B	567	LYS	GLN	conflict	UNP G1JZH9
B	582	THR	ALA	conflict	UNP G1JZH9
B	715	GLY	-	expression tag	UNP G1JZH9
B	716	GLY	-	expression tag	UNP G1JZH9
B	717	GLY	-	expression tag	UNP G1JZH9
B	718	HIS	-	expression tag	UNP G1JZH9
B	719	HIS	-	expression tag	UNP G1JZH9
B	720	HIS	-	expression tag	UNP G1JZH9
B	721	HIS	-	expression tag	UNP G1JZH9
B	722	HIS	-	expression tag	UNP G1JZH9
B	723	HIS	-	expression tag	UNP G1JZH9
C	1	MET	-	initiating methionine	UNP G1JZH9
C	2	ARG	-	expression tag	UNP G1JZH9
C	3	VAL	-	expression tag	UNP G1JZH9
C	4	LYS	-	expression tag	UNP G1JZH9
C	5	GLU	-	expression tag	UNP G1JZH9
C	6	LYS	-	expression tag	UNP G1JZH9
C	7	TYR	-	expression tag	UNP G1JZH9
C	8	GLN	-	expression tag	UNP G1JZH9
C	9	HIS	-	expression tag	UNP G1JZH9
C	10	LEU	-	expression tag	UNP G1JZH9
C	11	TRP	-	expression tag	UNP G1JZH9
C	12	ARG	-	expression tag	UNP G1JZH9
C	13	TRP	-	expression tag	UNP G1JZH9
C	14	GLY	-	expression tag	UNP G1JZH9
C	15	TRP	-	expression tag	UNP G1JZH9
C	16	ARG	-	expression tag	UNP G1JZH9
C	17	TRP	-	expression tag	UNP G1JZH9
C	18	GLY	-	expression tag	UNP G1JZH9
C	19	THR	-	expression tag	UNP G1JZH9
C	31	THR	VAL	conflict	UNP G1JZH9
C	33	LYS	ASN	conflict	UNP G1JZH9
C	114	GLU	GLN	conflict	UNP G1JZH9
C	533	VAL	ALA	conflict	UNP G1JZH9
C	536	MET	ILE	conflict	UNP G1JZH9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	544	GLN	LEU	conflict	UNP G1JZH9
C	568	LYS	GLN	conflict	UNP G1JZH9
C	583	THR	ALA	conflict	UNP G1JZH9
C	716	GLY	-	expression tag	UNP G1JZH9
C	717	GLY	-	expression tag	UNP G1JZH9
C	718	GLY	-	expression tag	UNP G1JZH9
C	719	HIS	-	expression tag	UNP G1JZH9
C	720	HIS	-	expression tag	UNP G1JZH9
C	721	HIS	-	expression tag	UNP G1JZH9
C	722	HIS	-	expression tag	UNP G1JZH9
C	723	HIS	-	expression tag	UNP G1JZH9
C	724	HIS	-	expression tag	UNP G1JZH9
D	2	MET	-	initiating methionine	UNP G1JZH9
D	3	ARG	-	expression tag	UNP G1JZH9
D	4	VAL	-	expression tag	UNP G1JZH9
D	5	LYS	-	expression tag	UNP G1JZH9
D	6	GLU	-	expression tag	UNP G1JZH9
D	7	LYS	-	expression tag	UNP G1JZH9
D	8	TYR	-	expression tag	UNP G1JZH9
D	9	GLN	-	expression tag	UNP G1JZH9
D	10	HIS	-	expression tag	UNP G1JZH9
D	11	LEU	-	expression tag	UNP G1JZH9
D	12	TRP	-	expression tag	UNP G1JZH9
D	13	ARG	-	expression tag	UNP G1JZH9
D	14	TRP	-	expression tag	UNP G1JZH9
D	15	GLY	-	expression tag	UNP G1JZH9
D	16	TRP	-	expression tag	UNP G1JZH9
D	17	ARG	-	expression tag	UNP G1JZH9
D	18	TRP	-	expression tag	UNP G1JZH9
D	19	GLY	-	expression tag	UNP G1JZH9
D	20	THR	-	expression tag	UNP G1JZH9
D	32	THR	VAL	conflict	UNP G1JZH9
D	34	LYS	ASN	conflict	UNP G1JZH9
D	115	GLU	GLN	conflict	UNP G1JZH9
D	532	VAL	ALA	conflict	UNP G1JZH9
D	535	MET	ILE	conflict	UNP G1JZH9
D	543	GLN	LEU	conflict	UNP G1JZH9
D	567	LYS	GLN	conflict	UNP G1JZH9
D	582	THR	ALA	conflict	UNP G1JZH9
D	715	GLY	-	expression tag	UNP G1JZH9
D	716	GLY	-	expression tag	UNP G1JZH9
D	717	GLY	-	expression tag	UNP G1JZH9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	718	HIS	-	expression tag	UNP G1JZH9
D	719	HIS	-	expression tag	UNP G1JZH9
D	720	HIS	-	expression tag	UNP G1JZH9
D	721	HIS	-	expression tag	UNP G1JZH9
D	722	HIS	-	expression tag	UNP G1JZH9
D	723	HIS	-	expression tag	UNP G1JZH9
E	1	MET	-	initiating methionine	UNP G1JZH9
E	2	ARG	-	expression tag	UNP G1JZH9
E	3	VAL	-	expression tag	UNP G1JZH9
E	4	LYS	-	expression tag	UNP G1JZH9
E	5	GLU	-	expression tag	UNP G1JZH9
E	6	LYS	-	expression tag	UNP G1JZH9
E	7	TYR	-	expression tag	UNP G1JZH9
E	8	GLN	-	expression tag	UNP G1JZH9
E	9	HIS	-	expression tag	UNP G1JZH9
E	10	LEU	-	expression tag	UNP G1JZH9
E	11	TRP	-	expression tag	UNP G1JZH9
E	12	ARG	-	expression tag	UNP G1JZH9
E	13	TRP	-	expression tag	UNP G1JZH9
E	14	GLY	-	expression tag	UNP G1JZH9
E	15	TRP	-	expression tag	UNP G1JZH9
E	16	ARG	-	expression tag	UNP G1JZH9
E	17	TRP	-	expression tag	UNP G1JZH9
E	18	GLY	-	expression tag	UNP G1JZH9
E	19	THR	-	expression tag	UNP G1JZH9
E	31	THR	VAL	conflict	UNP G1JZH9
E	33	LYS	ASN	conflict	UNP G1JZH9
E	114	GLU	GLN	conflict	UNP G1JZH9
E	533	VAL	ALA	conflict	UNP G1JZH9
E	536	MET	ILE	conflict	UNP G1JZH9
E	544	GLN	LEU	conflict	UNP G1JZH9
E	568	LYS	GLN	conflict	UNP G1JZH9
E	583	THR	ALA	conflict	UNP G1JZH9
E	716	GLY	-	expression tag	UNP G1JZH9
E	717	GLY	-	expression tag	UNP G1JZH9
E	718	GLY	-	expression tag	UNP G1JZH9
E	719	HIS	-	expression tag	UNP G1JZH9
E	720	HIS	-	expression tag	UNP G1JZH9
E	721	HIS	-	expression tag	UNP G1JZH9
E	722	HIS	-	expression tag	UNP G1JZH9
E	723	HIS	-	expression tag	UNP G1JZH9
E	724	HIS	-	expression tag	UNP G1JZH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP G1JZH9
A	2	ARG	-	expression tag	UNP G1JZH9
A	3	VAL	-	expression tag	UNP G1JZH9
A	4	LYS	-	expression tag	UNP G1JZH9
A	5	GLU	-	expression tag	UNP G1JZH9
A	6	LYS	-	expression tag	UNP G1JZH9
A	7	TYR	-	expression tag	UNP G1JZH9
A	8	GLN	-	expression tag	UNP G1JZH9
A	9	HIS	-	expression tag	UNP G1JZH9
A	10	LEU	-	expression tag	UNP G1JZH9
A	11	TRP	-	expression tag	UNP G1JZH9
A	12	ARG	-	expression tag	UNP G1JZH9
A	13	TRP	-	expression tag	UNP G1JZH9
A	14	GLY	-	expression tag	UNP G1JZH9
A	15	TRP	-	expression tag	UNP G1JZH9
A	16	ARG	-	expression tag	UNP G1JZH9
A	17	TRP	-	expression tag	UNP G1JZH9
A	18	GLY	-	expression tag	UNP G1JZH9
A	19	THR	-	expression tag	UNP G1JZH9
A	31	THR	VAL	conflict	UNP G1JZH9
A	33	LYS	ASN	conflict	UNP G1JZH9
A	114	GLU	GLN	conflict	UNP G1JZH9
A	533	VAL	ALA	conflict	UNP G1JZH9
A	536	MET	ILE	conflict	UNP G1JZH9
A	544	GLN	LEU	conflict	UNP G1JZH9
A	568	LYS	GLN	conflict	UNP G1JZH9
A	583	THR	ALA	conflict	UNP G1JZH9
A	716	GLY	-	expression tag	UNP G1JZH9
A	717	GLY	-	expression tag	UNP G1JZH9
A	718	GLY	-	expression tag	UNP G1JZH9
A	719	HIS	-	expression tag	UNP G1JZH9
A	720	HIS	-	expression tag	UNP G1JZH9
A	721	HIS	-	expression tag	UNP G1JZH9
A	722	HIS	-	expression tag	UNP G1JZH9
A	723	HIS	-	expression tag	UNP G1JZH9
A	724	HIS	-	expression tag	UNP G1JZH9
F	2	MET	-	initiating methionine	UNP G1JZH9
F	3	ARG	-	expression tag	UNP G1JZH9
F	4	VAL	-	expression tag	UNP G1JZH9
F	5	LYS	-	expression tag	UNP G1JZH9
F	6	GLU	-	expression tag	UNP G1JZH9
F	7	LYS	-	expression tag	UNP G1JZH9

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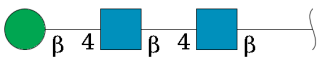
Chain	Residue	Modelled	Actual	Comment	Reference
F	8	TYR	-	expression tag	UNP G1JZH9
F	9	GLN	-	expression tag	UNP G1JZH9
F	10	HIS	-	expression tag	UNP G1JZH9
F	11	LEU	-	expression tag	UNP G1JZH9
F	12	TRP	-	expression tag	UNP G1JZH9
F	13	ARG	-	expression tag	UNP G1JZH9
F	14	TRP	-	expression tag	UNP G1JZH9
F	15	GLY	-	expression tag	UNP G1JZH9
F	16	TRP	-	expression tag	UNP G1JZH9
F	17	ARG	-	expression tag	UNP G1JZH9
F	18	TRP	-	expression tag	UNP G1JZH9
F	19	GLY	-	expression tag	UNP G1JZH9
F	20	THR	-	expression tag	UNP G1JZH9
F	32	THR	VAL	conflict	UNP G1JZH9
F	34	LYS	ASN	conflict	UNP G1JZH9
F	115	GLU	GLN	conflict	UNP G1JZH9
F	532	VAL	ALA	conflict	UNP G1JZH9
F	535	MET	ILE	conflict	UNP G1JZH9
F	543	GLN	LEU	conflict	UNP G1JZH9
F	567	LYS	GLN	conflict	UNP G1JZH9
F	582	THR	ALA	conflict	UNP G1JZH9
F	715	GLY	-	expression tag	UNP G1JZH9
F	716	GLY	-	expression tag	UNP G1JZH9
F	717	GLY	-	expression tag	UNP G1JZH9
F	718	HIS	-	expression tag	UNP G1JZH9
F	719	HIS	-	expression tag	UNP G1JZH9
F	720	HIS	-	expression tag	UNP G1JZH9
F	721	HIS	-	expression tag	UNP G1JZH9
F	722	HIS	-	expression tag	UNP G1JZH9
F	723	HIS	-	expression tag	UNP G1JZH9

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



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

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		
2	P	3	Total	C	N	O	0	0
			39	22	2	15		
2	Q	3	Total	C	N	O	0	0
			39	22	2	15		
2	R	3	Total	C	N	O	0	0
			39	22	2	15		
2	V	3	Total	C	N	O	0	0
			39	22	2	15		
2	Z	3	Total	C	N	O	0	0
			39	22	2	15		
2	a	3	Total	C	N	O	0	0
			39	22	2	15		
2	c	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	3	Total	C	N	O	0	0
			39	22	2	15		
2	h	3	Total	C	N	O	0	0
			39	22	2	15		
2	m	3	Total	C	N	O	0	0
			39	22	2	15		
2	o	3	Total	C	N	O	0	0
			39	22	2	15		
2	q	3	Total	C	N	O	0	0
			39	22	2	15		
2	r	3	Total	C	N	O	0	0
			39	22	2	15		
2	s	3	Total	C	N	O	0	0
			39	22	2	15		
2	w	3	Total	C	N	O	0	0
			39	22	2	15		
2	z	3	Total	C	N	O	0	0
			39	22	2	15		
2	0	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	3	Total	C	N	O	0	0
			39	22	2	15		
2	5	3	Total	C	N	O	0	0
			39	22	2	15		
2	7	3	Total	C	N	O	0	0
			39	22	2	15		
2	AA	3	Total	C	N	O	0	0
			39	22	2	15		
2	BA	3	Total	C	N	O	0	0
			39	22	2	15		
2	EA	3	Total	C	N	O	0	0
			39	22	2	15		
2	IA	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		

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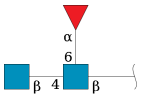
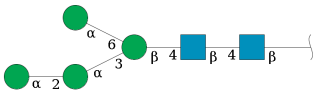
Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	2	Total	C	N	O	0	0
			28	16	2	10		
3	6	2	Total	C	N	O	0	0
			28	16	2	10		
3	HA	2	Total	C	N	O	0	0
			28	16	2	10		
3	KA	2	Total	C	N	O	0	0
			28	16	2	10		
3	LA	2	Total	C	N	O	0	0
			28	16	2	10		
3	MA	2	Total	C	N	O	0	0
			28	16	2	10		

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



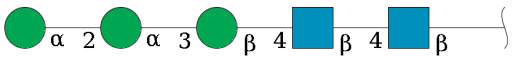
Mol	Chain	Residues	Atoms				AltConf	Trace
4	O	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



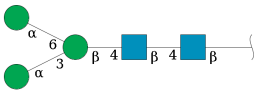
Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	6	Total	C	N	O	0	0
			72	40	2	30		

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



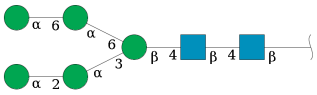
Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	W	5	Total	C	N	O	0	0
			61	34	2	25		
7	i	5	Total	C	N	O	0	0
			61	34	2	25		
7	j	5	Total	C	N	O	0	0
			61	34	2	25		
7	1	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

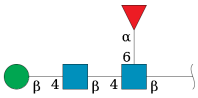


Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	7	Total	C	N	O	0	0
			83	46	2	35		
8	u	7	Total	C	N	O	0	0
			83	46	2	35		
8	DA	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

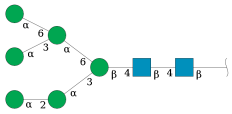
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Y	4	Total	C	N	O	0	0
			50	28	2	20		
9	v	4	Total	C	N	O	0	0
			50	28	2	20		
9	2	4	Total	C	N	O	0	0
			50	28	2	20		
9	9	4	Total	C	N	O	0	0
			50	28	2	20		
9	CA	4	Total	C	N	O	0	0
			50	28	2	20		
9	FA	4	Total	C	N	O	0	0
			50	28	2	20		
9	GA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



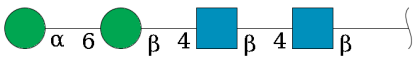
Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	4	Total	C	N	O	0	0
			49	28	2	19		
10	y	4	Total	C	N	O	0	0
			49	28	2	19		
10	JA	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



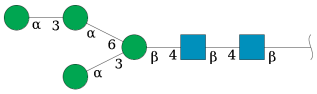
Mol	Chain	Residues	Atoms				AltConf	Trace
11	p	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



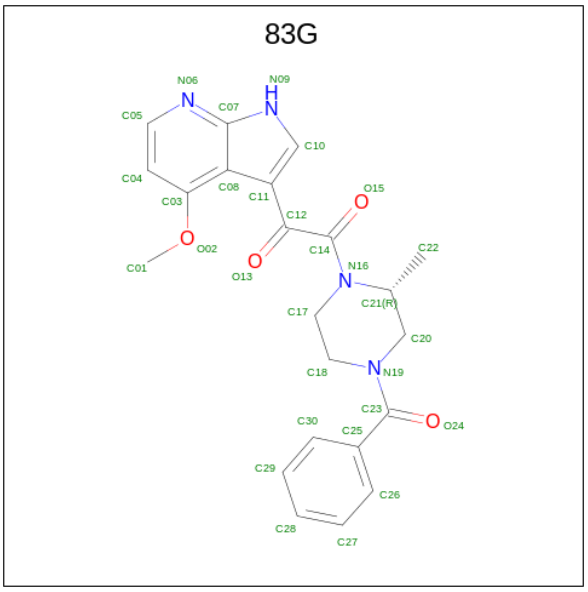
Mol	Chain	Residues	Atoms				AltConf	Trace
12	t	4	Total	C	N	O	0	0
			50	28	2	20		
12	x	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



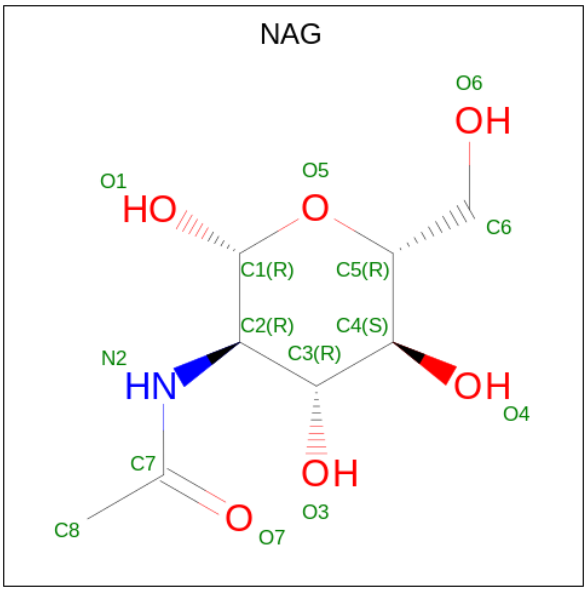
Mol	Chain	Residues	Atoms				AltConf	Trace
13	8	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 14 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (three-letter code: 83G) (formula: $C_{22}H_{22}N_4O_4$).



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	N	O	0
			30	22	4	4	
14	E	1	Total	C	N	O	0
			30	22	4	4	
14	A	1	Total	C	N	O	0
			30	22	4	4	

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

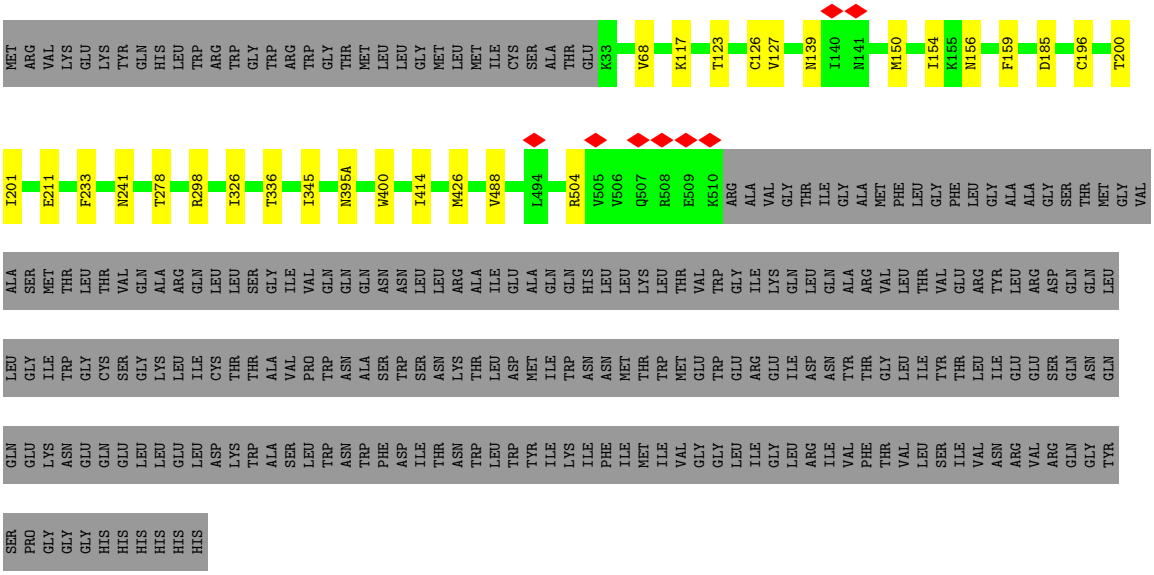
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Envelope glycoprotein gp160

Chain B:

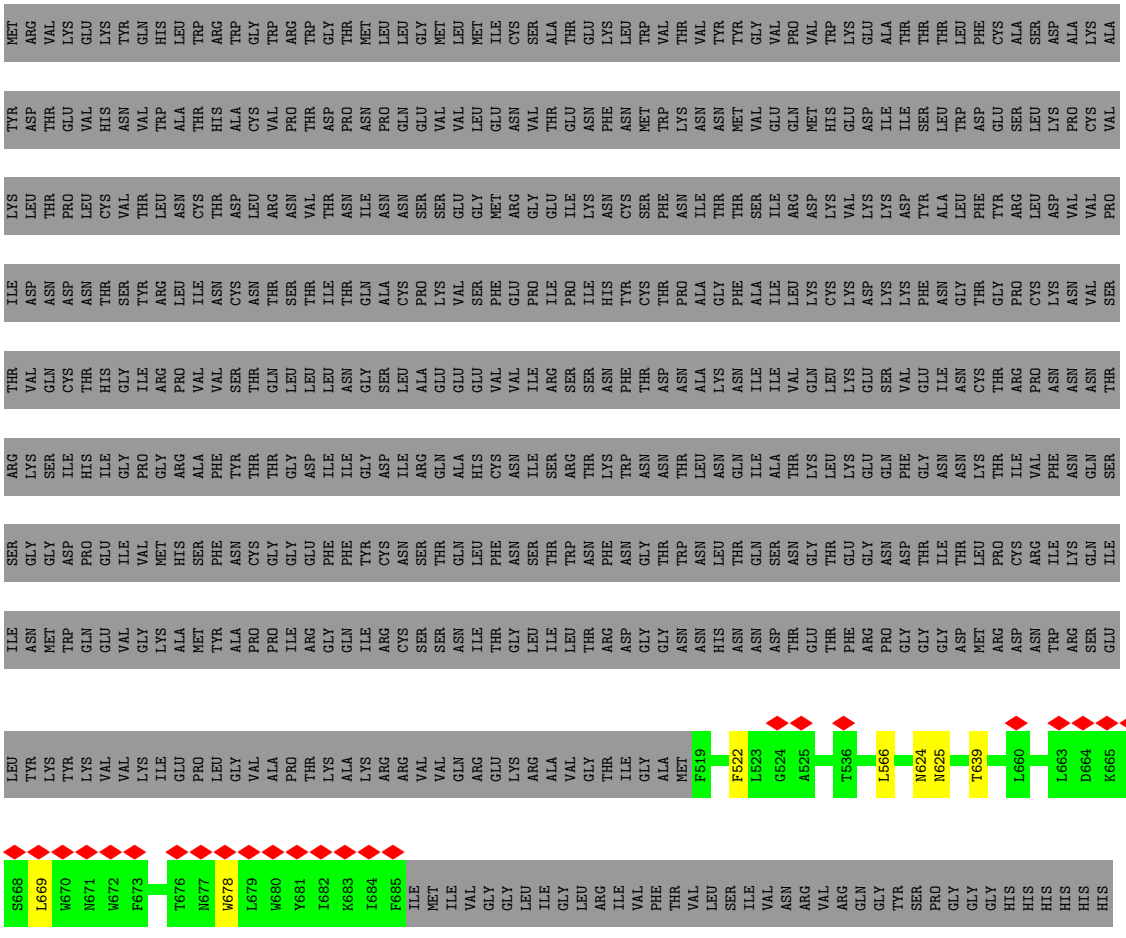
• Molecule 1: Envelope glycoprotein gp160

Chain C:



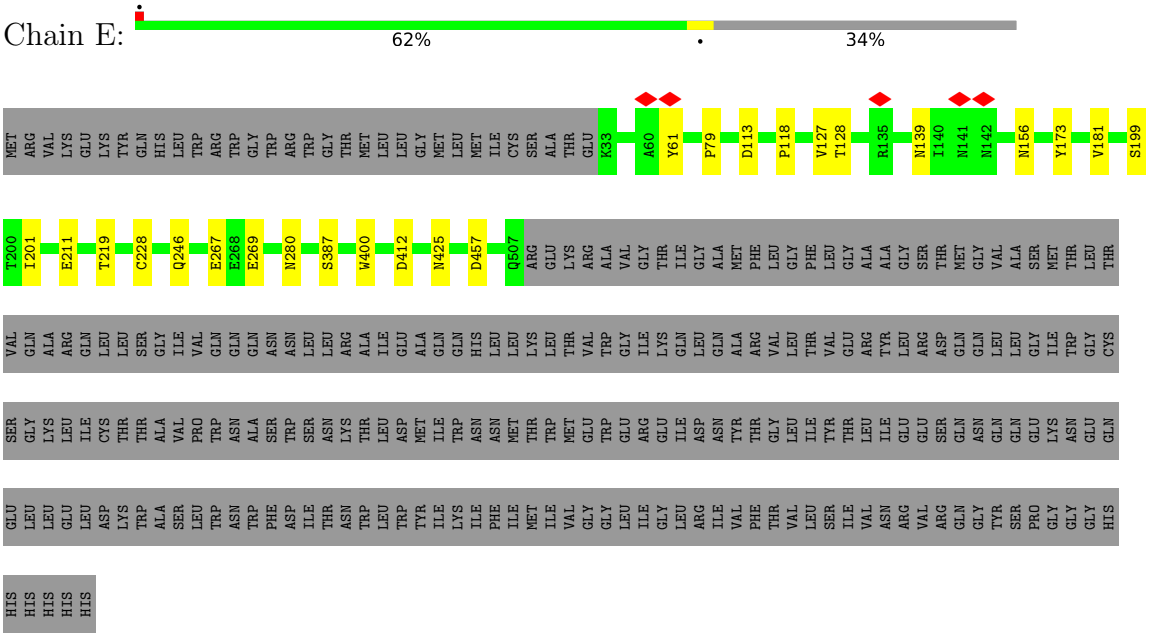
• Molecule 1: Envelope glycoprotein gp160

Chain D:



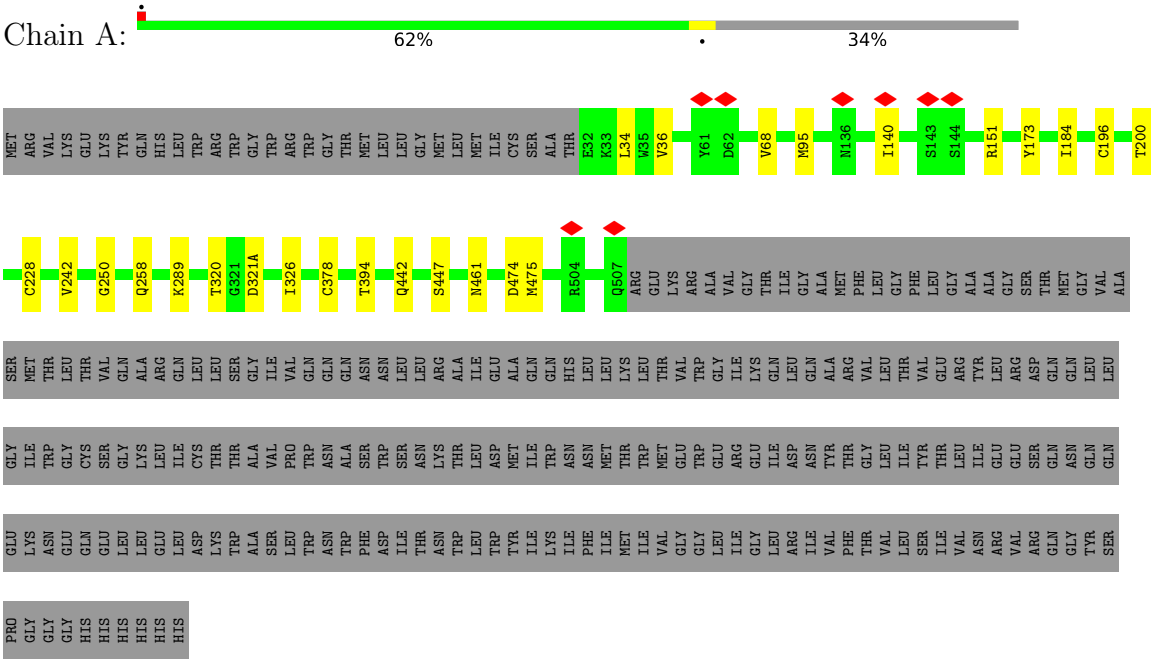
• Molecule 1: Envelope glycoprotein gp160

Chain E:



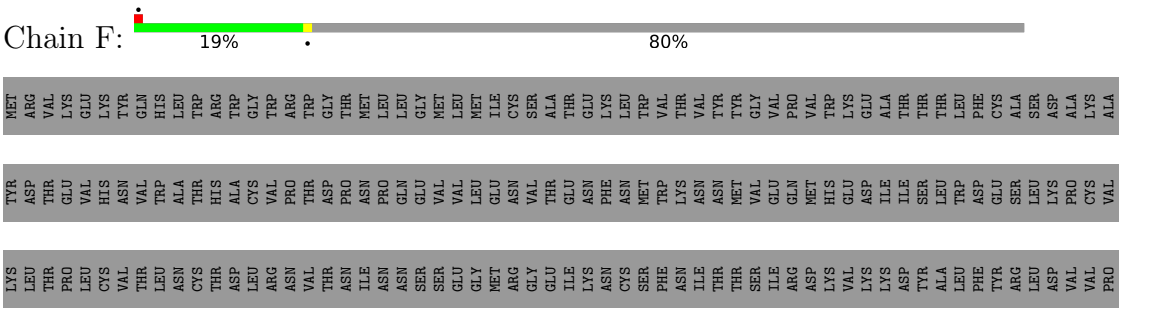
• Molecule 1: Envelope glycoprotein gp160

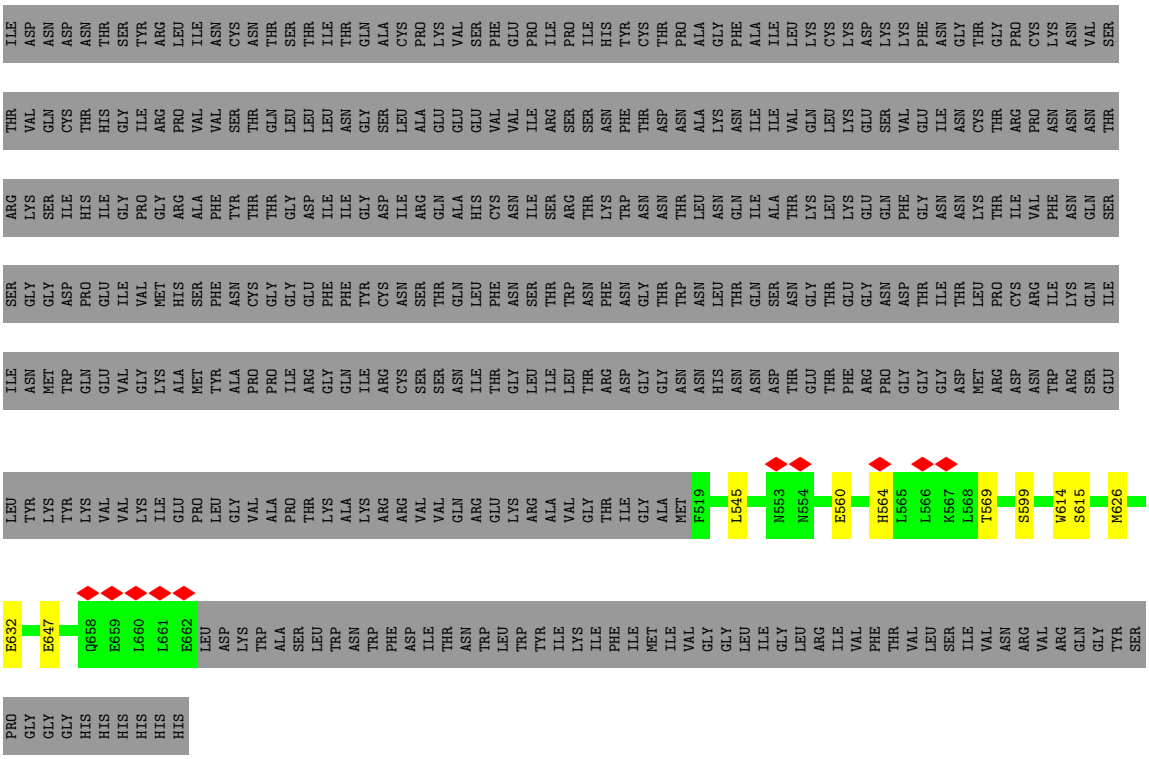
Chain A:



• Molecule 1: Envelope glycoprotein gp160

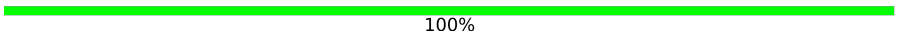
Chain F:





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

Chain G:

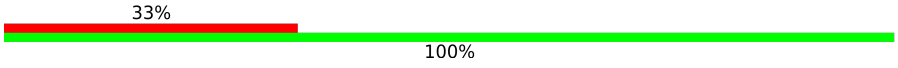


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain K:

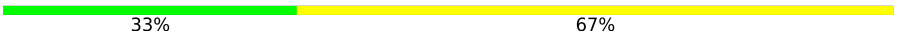


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

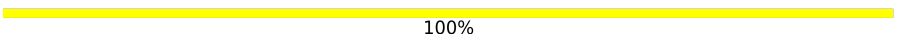
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain P:



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

Chain Q:

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

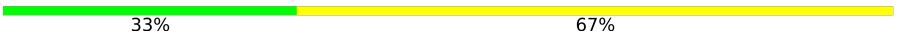
Chain R:

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

Chain V:

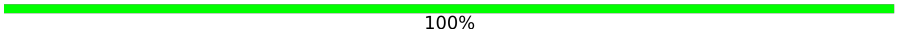
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain a:

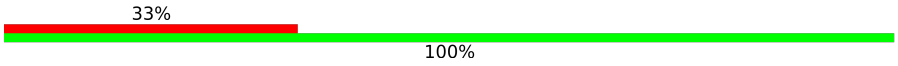


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

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

Chain g:

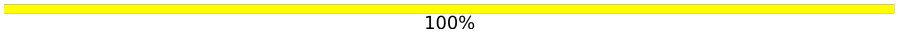


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

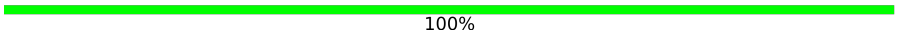
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



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

Chain o:

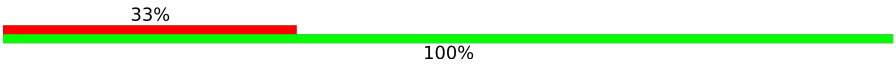


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

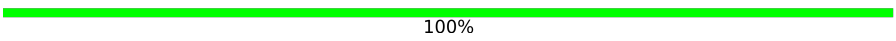
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



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

Chain s:

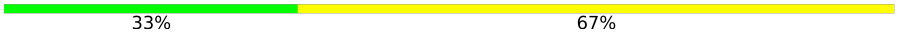


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

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

Chain z:



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

Chain 0:

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

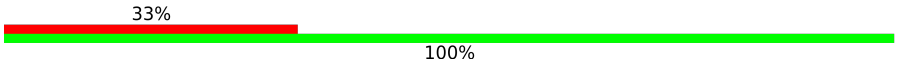
Chain 3:

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

Chain 5:

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

Chain 7:



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

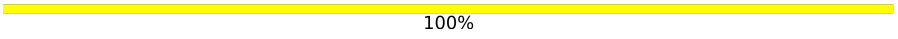
Chain AA:

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

Chain BA:

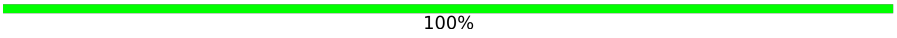
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:



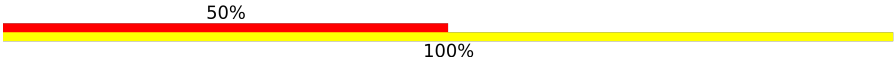
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:



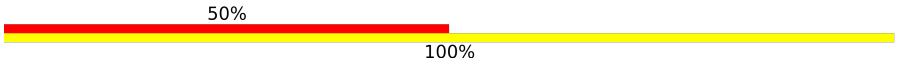
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:

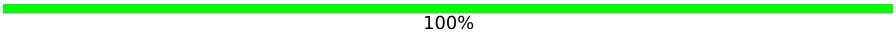


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

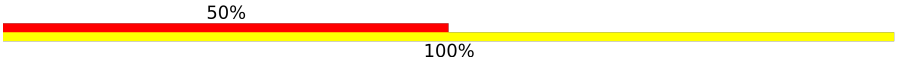
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



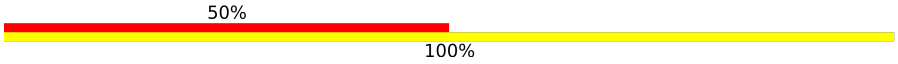
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



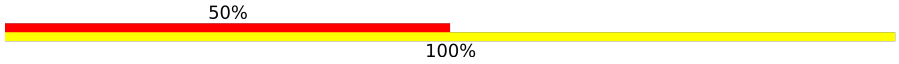
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



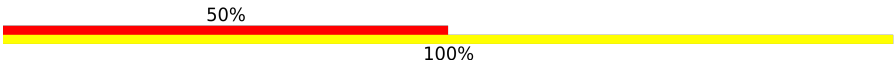
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



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

Chain k:

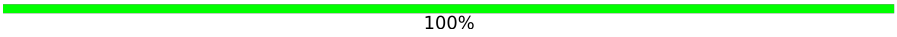


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

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

Chain n:

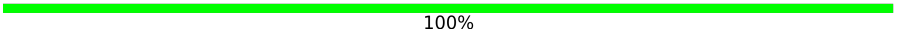


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

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

Chain 6:

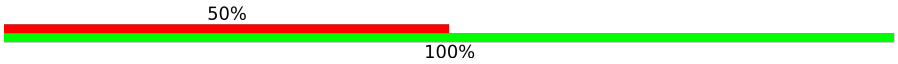


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:

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

Chain KA:



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

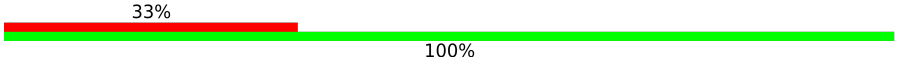
Chain LA:

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

Chain MA:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

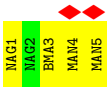


• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain T:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

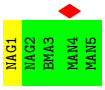
Chain W:

• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



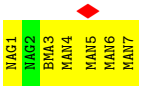
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-

D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

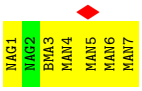


• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:

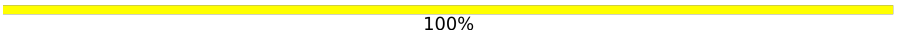


• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:

• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9: 

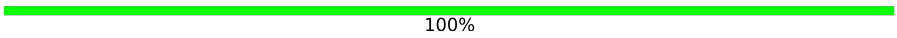
• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA: 

• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA: 

• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA: 

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

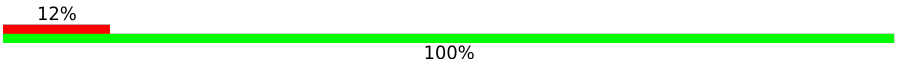
Chain y: 

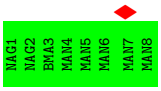
• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:

• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:





• Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

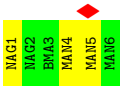
Chain t:

• Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

• Molecule 13: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.7	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.65, 1.65, 1.65	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 83G, NAG, MAN, BMA

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	0.62	0/3819	0.60	0/5191
1	B	0.62	0/1227	0.58	0/1665
1	C	0.63	0/3839	0.63	0/5216
1	D	0.62	0/1412	0.59	0/1921
1	E	0.62	0/3810	0.61	0/5179
1	F	0.63	0/1179	0.60	0/1599
All	All	0.62	0/15286	0.61	0/20771

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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	472/722 (65%)	436 (92%)	32 (7%)	4 (1%)	16	44
1	B	148/722 (20%)	134 (90%)	11 (7%)	3 (2%)	6	25
1	C	474/722 (66%)	436 (92%)	34 (7%)	4 (1%)	16	44
1	D	165/722 (23%)	140 (85%)	21 (13%)	4 (2%)	5	23
1	E	471/722 (65%)	423 (90%)	41 (9%)	7 (2%)	8	30
1	F	142/722 (20%)	132 (93%)	9 (6%)	1 (1%)	19	47
All	All	1872/4332 (43%)	1701 (91%)	148 (8%)	23 (1%)	14	35

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	127	VAL
1	A	250	GLY
1	B	568	LEU
1	B	636	ASP
1	C	139	ASN
1	D	566	LEU
1	D	624	ASN
1	D	625	ASN
1	E	412	ASP
1	A	474	ASP
1	C	395(A)	ASN
1	E	156	ASN
1	A	228	CYS
1	C	126	CYS
1	C	414	ILE
1	E	269	GLU
1	A	258	GLN
1	B	539	VAL
1	D	639	THR
1	E	387	SER
1	F	615	SER
1	E	118	PRO
1	E	79	PRO

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	426/639 (67%)	405 (95%)	21 (5%)	21 48
1	B	130/639 (20%)	119 (92%)	11 (8%)	8 29
1	C	428/639 (67%)	404 (94%)	24 (6%)	17 43
1	D	147/639 (23%)	144 (98%)	3 (2%)	50 70
1	E	425/639 (66%)	408 (96%)	17 (4%)	27 52
1	F	125/639 (20%)	116 (93%)	9 (7%)	12 37
All	All	1681/3834 (44%)	1596 (95%)	85 (5%)	22 46

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	523	LEU
1	B	529	THR
1	B	539	VAL
1	B	540	GLN
1	B	624	ASN
1	B	628	TRP
1	B	639	THR
1	B	643	TYR
1	B	654	GLU
1	B	660	LEU
1	B	663	LEU
1	C	68	VAL
1	C	117	LYS
1	C	123	THR
1	C	127	VAL
1	C	150	MET
1	C	154	ILE
1	C	156	ASN
1	C	159	PHE
1	C	185	ASP
1	C	196	CYS
1	C	200	THR
1	C	201	ILE
1	C	211	GLU
1	C	233	PHE
1	C	241	ASN
1	C	278	THR

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Mol	Chain	Res	Type
1	C	298	ARG
1	C	326	ILE
1	C	336	THR
1	C	345	ILE
1	C	400	TRP
1	C	426	MET
1	C	488	VAL
1	C	504	ARG
1	D	522	PHE
1	D	669	LEU
1	D	678	TRP
1	E	61	TYR
1	E	113	ASP
1	E	128	THR
1	E	139	ASN
1	E	173	TYR
1	E	181	VAL
1	E	199	SER
1	E	201	ILE
1	E	211	GLU
1	E	219	THR
1	E	228	CYS
1	E	246	GLN
1	E	267	GLU
1	E	280	ASN
1	E	400	TRP
1	E	425	ASN
1	E	457	ASP
1	A	34	LEU
1	A	36	VAL
1	A	68	VAL
1	A	95	MET
1	A	140	ILE
1	A	151	ARG
1	A	173	TYR
1	A	184	ILE
1	A	196	CYS
1	A	200	THR
1	A	242	VAL
1	A	289	LYS
1	A	320	THR
1	A	321(A)	ASP

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Mol	Chain	Res	Type
1	A	326	ILE
1	A	378	CYS
1	A	394	THR
1	A	442	GLN
1	A	447	SER
1	A	461	ASN
1	A	475	MET
1	F	545	LEU
1	F	560	GLU
1	F	564	HIS
1	F	569	THR
1	F	599	SER
1	F	614	TRP
1	F	626	MET
1	F	632	GLU
1	F	647	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	624	ASN
1	C	67	ASN
1	C	72	HIS
1	C	94	ASN
1	C	105	HIS
1	C	249	HIS
1	C	395(A)	ASN
1	C	464	ASN
1	C	478	ASN
1	D	671	ASN
1	E	195	ASN
1	E	363	GLN
1	E	374	HIS
1	E	428	GLN
1	E	463	ASN
1	A	99	ASN
1	A	395(A)	ASN
1	F	624	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

236 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	0	1	1,2	14,14,15	0.48	0	17,19,21	0.50	0
2	NAG	0	2	2	14,14,15	0.30	0	17,19,21	0.41	0
2	BMA	0	3	2	11,11,12	0.51	0	15,15,17	0.83	0
7	NAG	1	1	7,1	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
7	NAG	1	2	7	14,14,15	0.35	0	17,19,21	1.02	1 (5%)
7	BMA	1	3	7	11,11,12	0.27	0	15,15,17	0.70	1 (6%)
7	MAN	1	4	7	11,11,12	0.27	0	15,15,17	0.72	1 (6%)
7	MAN	1	5	7	11,11,12	0.30	0	15,15,17	0.54	0
9	NAG	2	1	1,9	14,14,15	0.46	0	17,19,21	0.52	0
9	NAG	2	2	9	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
9	BMA	2	3	9	11,11,12	1.11	0	15,15,17	1.18	2 (13%)
9	MAN	2	4	9	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
2	NAG	3	1	1,2	14,14,15	0.34	0	17,19,21	0.62	0
2	NAG	3	2	2	14,14,15	0.33	0	17,19,21	1.11	2 (11%)
2	BMA	3	3	2	11,11,12	0.24	0	15,15,17	0.58	0
3	NAG	4	1	3,1	14,14,15	0.28	0	17,19,21	0.85	1 (5%)
3	NAG	4	2	3	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	5	1	1,2	14,14,15	0.27	0	17,19,21	0.60	0
2	NAG	5	2	2	14,14,15	0.35	0	17,19,21	1.64	4 (23%)
2	BMA	5	3	2	11,11,12	0.21	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	6	1	3,1	14,14,15	0.38	0	17,19,21	0.50	0
3	NAG	6	2	3	14,14,15	0.29	0	17,19,21	0.59	0
2	NAG	7	1	1,2	14,14,15	0.35	0	17,19,21	0.39	0
2	NAG	7	2	2	14,14,15	0.20	0	17,19,21	0.49	0
2	BMA	7	3	2	11,11,12	0.61	0	15,15,17	0.72	0
13	NAG	8	1	13,1	14,14,15	1.06	1 (7%)	17,19,21	2.88	4 (23%)
13	NAG	8	2	13	14,14,15	0.27	0	17,19,21	0.88	0
13	BMA	8	3	13	11,11,12	0.29	0	15,15,17	0.61	0
13	MAN	8	4	13	11,11,12	1.02	0	15,15,17	1.46	2 (13%)
13	MAN	8	5	13	11,11,12	0.76	0	15,15,17	1.03	2 (13%)
13	MAN	8	6	13	11,11,12	0.20	0	15,15,17	0.68	0
9	NAG	9	1	1,9	14,14,15	0.61	1 (7%)	17,19,21	0.69	0
9	NAG	9	2	9	14,14,15	0.20	0	17,19,21	0.84	0
9	BMA	9	3	9	11,11,12	1.25	1 (9%)	15,15,17	1.83	3 (20%)
9	MAN	9	4	9	11,11,12	0.70	0	15,15,17	0.98	1 (6%)
2	NAG	AA	1	1,2	14,14,15	0.37	0	17,19,21	0.61	0
2	NAG	AA	2	2	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
2	BMA	AA	3	2	11,11,12	0.27	0	15,15,17	0.56	0
2	NAG	BA	1	1,2	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	BA	2	2	14,14,15	0.26	0	17,19,21	0.86	1 (5%)
2	BMA	BA	3	2	11,11,12	0.23	0	15,15,17	0.60	0
9	NAG	CA	1	1,9	14,14,15	0.30	0	17,19,21	0.48	0
9	NAG	CA	2	9	14,14,15	0.20	0	17,19,21	0.72	0
9	BMA	CA	3	9	11,11,12	0.93	1 (9%)	15,15,17	0.87	0
9	MAN	CA	4	9	11,11,12	0.75	1 (9%)	15,15,17	1.39	2 (13%)
8	NAG	DA	1	8,1	14,14,15	0.71	1 (7%)	17,19,21	0.79	0
8	NAG	DA	2	8	14,14,15	0.19	0	17,19,21	0.41	0
8	BMA	DA	3	8	11,11,12	0.92	1 (9%)	15,15,17	1.19	2 (13%)
8	MAN	DA	4	8	11,11,12	1.39	2 (18%)	15,15,17	1.90	2 (13%)
8	MAN	DA	5	8	11,11,12	0.85	1 (9%)	15,15,17	1.09	2 (13%)
8	MAN	DA	6	8	11,11,12	0.58	0	15,15,17	1.24	2 (13%)
8	MAN	DA	7	8	11,11,12	0.72	1 (9%)	15,15,17	1.11	2 (13%)
2	NAG	EA	1	1,2	14,14,15	0.39	0	17,19,21	0.85	2 (11%)
2	NAG	EA	2	2	14,14,15	0.49	0	17,19,21	0.80	1 (5%)
2	BMA	EA	3	2	11,11,12	0.61	0	15,15,17	1.30	2 (13%)
9	NAG	FA	1	1,9	14,14,15	0.26	0	17,19,21	1.03	2 (11%)
9	NAG	FA	2	9	14,14,15	0.33	0	17,19,21	1.64	4 (23%)
9	BMA	FA	3	9	11,11,12	0.20	0	15,15,17	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	FA	4	9	11,11,12	0.23	0	15,15,17	0.56	0
2	NAG	G	1	1,2	14,14,15	0.34	0	17,19,21	0.55	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.63	0
2	BMA	G	3	2	11,11,12	0.24	0	15,15,17	0.61	0
9	NAG	GA	1	1,9	14,14,15	0.38	0	17,19,21	0.46	0
9	NAG	GA	2	9	14,14,15	0.38	0	17,19,21	0.58	0
9	BMA	GA	3	9	11,11,12	0.26	0	15,15,17	0.57	0
9	MAN	GA	4	9	11,11,12	0.29	0	15,15,17	0.56	0
3	NAG	H	1	3,1	14,14,15	0.34	0	17,19,21	0.92	1 (5%)
3	NAG	H	2	3	14,14,15	0.44	0	17,19,21	2.40	4 (23%)
3	NAG	HA	1	3,1	14,14,15	0.32	0	17,19,21	0.60	0
3	NAG	HA	2	3	14,14,15	0.33	0	17,19,21	0.77	0
3	NAG	I	1	3,1	14,14,15	0.32	0	17,19,21	1.06	1 (5%)
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	0.92	2 (11%)
2	NAG	IA	1	1,2	14,14,15	0.30	0	17,19,21	0.80	0
2	NAG	IA	2	2	14,14,15	0.31	0	17,19,21	0.52	0
2	BMA	IA	3	2	11,11,12	0.20	0	15,15,17	0.59	0
2	NAG	J	1	1,2	14,14,15	0.30	0	17,19,21	1.23	2 (11%)
2	NAG	J	2	2	14,14,15	0.27	0	17,19,21	0.65	0
2	BMA	J	3	2	11,11,12	0.59	0	15,15,17	2.46	2 (13%)
10	NAG	JA	1	10,1	14,14,15	1.06	1 (7%)	17,19,21	2.19	4 (23%)
10	NAG	JA	2	10	14,14,15	0.30	0	17,19,21	0.58	0
10	BMA	JA	3	10	11,11,12	0.20	0	15,15,17	0.68	0
10	FUC	JA	4	10	10,10,11	0.25	0	14,14,16	0.54	0
2	NAG	K	1	1,2	14,14,15	0.30	0	17,19,21	0.53	0
2	NAG	K	2	2	14,14,15	0.33	0	17,19,21	0.65	0
2	BMA	K	3	2	11,11,12	0.23	0	15,15,17	0.65	0
3	NAG	KA	1	3,1	14,14,15	0.34	0	17,19,21	0.56	0
3	NAG	KA	2	3	14,14,15	0.27	0	17,19,21	0.73	0
2	NAG	L	1	1,2	14,14,15	0.30	0	17,19,21	0.86	1 (5%)
2	NAG	L	2	2	14,14,15	0.29	0	17,19,21	0.66	0
2	BMA	L	3	2	11,11,12	0.70	0	15,15,17	0.82	0
3	NAG	LA	1	3,1	14,14,15	0.29	0	17,19,21	0.65	0
3	NAG	LA	2	3	14,14,15	0.40	0	17,19,21	2.38	3 (17%)
2	NAG	M	1	1,2	14,14,15	0.43	0	17,19,21	0.53	0
2	NAG	M	2	2	14,14,15	0.41	0	17,19,21	0.82	1 (5%)
2	BMA	M	3	2	11,11,12	1.11	0	15,15,17	1.20	2 (13%)
3	NAG	MA	1	3,1	14,14,15	0.33	0	17,19,21	1.17	1 (5%)
3	NAG	MA	2	3	14,14,15	0.32	0	17,19,21	0.62	0
3	NAG	N	1	3,1	14,14,15	0.38	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	N	2	3	14,14,15	0.34	0	17,19,21	1.19	1 (5%)
4	NAG	O	1	4,1	14,14,15	0.31	0	17,19,21	0.71	0
4	NAG	O	2	4	14,14,15	0.29	0	17,19,21	0.54	0
4	FUC	O	3	4	10,10,11	0.25	0	14,14,16	0.53	0
2	NAG	P	1	1,2	14,14,15	0.48	0	17,19,21	1.48	4 (23%)
2	NAG	P	2	2	14,14,15	0.38	0	17,19,21	0.98	1 (5%)
2	BMA	P	3	2	11,11,12	0.33	0	15,15,17	1.88	3 (20%)
2	NAG	Q	1	1,2	14,14,15	0.54	0	17,19,21	0.71	0
2	NAG	Q	2	2	14,14,15	0.20	0	17,19,21	0.83	0
2	BMA	Q	3	2	11,11,12	1.23	1 (9%)	15,15,17	1.86	3 (20%)
2	NAG	R	1	1,2	14,14,15	0.32	0	17,19,21	0.93	1 (5%)
2	NAG	R	2	2	14,14,15	0.28	0	17,19,21	0.59	0
2	BMA	R	3	2	11,11,12	0.23	0	15,15,17	0.62	0
5	NAG	S	1	5,1	14,14,15	1.19	1 (7%)	17,19,21	3.30	6 (35%)
5	NAG	S	2	5	14,14,15	0.28	0	17,19,21	1.15	2 (11%)
5	BMA	S	3	5	11,11,12	0.25	0	15,15,17	0.74	0
5	MAN	S	4	5	11,11,12	0.17	0	15,15,17	0.70	0
5	MAN	S	5	5	11,11,12	0.21	0	15,15,17	0.57	0
5	MAN	S	6	5	11,11,12	0.22	0	15,15,17	0.65	0
6	NAG	T	1	6,1	14,14,15	0.60	1 (7%)	17,19,21	0.69	0
6	NAG	T	2	6	14,14,15	0.23	0	17,19,21	0.83	0
6	BMA	T	3	6	11,11,12	1.23	1 (9%)	15,15,17	1.84	3 (20%)
6	MAN	T	4	6	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
6	MAN	T	5	6	11,11,12	0.89	1 (9%)	15,15,17	1.12	1 (6%)
3	NAG	U	1	3,1	14,14,15	0.30	0	17,19,21	0.51	0
3	NAG	U	2	3	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	V	1	1,2	14,14,15	0.34	0	17,19,21	0.70	0
2	NAG	V	2	2	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
2	BMA	V	3	2	11,11,12	0.22	0	15,15,17	0.61	0
7	NAG	W	1	7,1	14,14,15	0.37	0	17,19,21	0.49	0
7	NAG	W	2	7	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
7	BMA	W	3	7	11,11,12	0.26	0	15,15,17	0.62	0
7	MAN	W	4	7	11,11,12	0.29	0	15,15,17	0.55	0
7	MAN	W	5	7	11,11,12	0.32	0	15,15,17	0.57	0
8	NAG	X	1	8,1	14,14,15	0.73	1 (7%)	17,19,21	0.78	0
8	NAG	X	2	8	14,14,15	0.18	0	17,19,21	0.36	0
8	BMA	X	3	8	11,11,12	0.95	1 (9%)	15,15,17	1.20	1 (6%)
8	MAN	X	4	8	11,11,12	1.38	2 (18%)	15,15,17	1.85	2 (13%)
8	MAN	X	5	8	11,11,12	0.87	1 (9%)	15,15,17	1.08	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	X	6	8	11,11,12	0.60	0	15,15,17	1.23	2 (13%)
8	MAN	X	7	8	11,11,12	0.73	1 (9%)	15,15,17	1.13	2 (13%)
9	NAG	Y	1	1,9	14,14,15	0.39	0	17,19,21	0.83	2 (11%)
9	NAG	Y	2	9	14,14,15	0.38	0	17,19,21	0.62	0
9	BMA	Y	3	9	11,11,12	0.26	0	15,15,17	0.55	0
9	MAN	Y	4	9	11,11,12	0.30	0	15,15,17	0.56	0
2	NAG	Z	1	1,2	14,14,15	0.34	0	17,19,21	1.07	1 (5%)
2	NAG	Z	2	2	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
2	BMA	Z	3	2	11,11,12	0.23	0	15,15,17	0.64	0
2	NAG	a	1	1,2	14,14,15	0.36	0	17,19,21	0.67	0
2	NAG	a	2	2	14,14,15	0.26	0	17,19,21	0.81	0
2	BMA	a	3	2	11,11,12	0.22	0	15,15,17	0.60	0
3	NAG	b	1	3,1	14,14,15	0.36	0	17,19,21	1.14	1 (5%)
3	NAG	b	2	3	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
2	NAG	c	1	1,2	14,14,15	0.31	0	17,19,21	0.45	0
2	NAG	c	2	2	14,14,15	0.28	0	17,19,21	0.47	0
2	BMA	c	3	2	11,11,12	0.96	1 (9%)	15,15,17	1.22	2 (13%)
10	NAG	d	1	10,1	14,14,15	1.07	1 (7%)	17,19,21	2.20	4 (23%)
10	NAG	d	2	10	14,14,15	0.34	0	17,19,21	0.58	0
10	BMA	d	3	10	11,11,12	0.23	0	15,15,17	0.67	0
10	FUC	d	4	10	10,10,11	0.26	0	14,14,16	0.53	0
3	NAG	e	1	3,1	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
3	NAG	e	2	3	14,14,15	0.41	0	17,19,21	2.39	4 (23%)
3	NAG	f	1	3,1	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
3	NAG	f	2	3	14,14,15	0.42	0	17,19,21	2.40	4 (23%)
2	NAG	g	1	1,2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	g	2	2	14,14,15	0.28	0	17,19,21	0.57	0
2	BMA	g	3	2	11,11,12	0.25	0	15,15,17	0.64	0
2	NAG	h	1	1,2	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	h	2	2	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
2	BMA	h	3	2	11,11,12	0.22	0	15,15,17	0.57	0
7	NAG	i	1	7,1	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
7	NAG	i	2	7	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
7	BMA	i	3	7	11,11,12	0.28	0	15,15,17	0.65	0
7	MAN	i	4	7	11,11,12	0.41	0	15,15,17	1.34	3 (20%)
7	MAN	i	5	7	11,11,12	0.31	0	15,15,17	0.54	0
7	NAG	j	1	7,1	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
7	NAG	j	2	7	14,14,15	0.30	0	17,19,21	0.63	0
7	BMA	j	3	7	11,11,12	0.24	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	j	4	7	11,11,12	0.21	0	15,15,17	0.58	0
7	MAN	j	5	7	11,11,12	0.23	0	15,15,17	0.61	0
3	NAG	k	1	3,1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
3	NAG	k	2	3	14,14,15	0.29	0	17,19,21	0.76	1 (5%)
3	NAG	l	1	3,1	14,14,15	0.36	0	17,19,21	1.54	2 (11%)
3	NAG	l	2	3	14,14,15	0.30	0	17,19,21	0.67	0
2	NAG	m	1	1,2	14,14,15	0.89	1 (7%)	17,19,21	0.72	0
2	NAG	m	2	2	14,14,15	0.38	0	17,19,21	0.95	2 (11%)
2	BMA	m	3	2	11,11,12	0.49	0	15,15,17	0.96	1 (6%)
3	NAG	n	1	3,1	14,14,15	0.40	0	17,19,21	0.64	0
3	NAG	n	2	3	14,14,15	0.38	0	17,19,21	0.72	0
2	NAG	o	1	1,2	14,14,15	0.26	0	17,19,21	0.80	0
2	NAG	o	2	2	14,14,15	0.30	0	17,19,21	0.65	0
2	BMA	o	3	2	11,11,12	0.21	0	15,15,17	0.60	0
11	NAG	p	1	11,1	14,14,15	0.39	0	17,19,21	0.56	0
11	NAG	p	2	11	14,14,15	0.40	0	17,19,21	0.47	0
11	BMA	p	3	11	11,11,12	0.33	0	15,15,17	0.53	0
11	MAN	p	4	11	11,11,12	0.31	0	15,15,17	0.51	0
11	MAN	p	5	11	11,11,12	0.28	0	15,15,17	0.59	0
11	MAN	p	6	11	11,11,12	0.30	0	15,15,17	0.73	0
11	MAN	p	7	11	11,11,12	0.27	0	15,15,17	0.56	0
11	MAN	p	8	11	11,11,12	0.25	0	15,15,17	0.54	0
2	NAG	q	1	1,2	14,14,15	0.59	0	17,19,21	0.69	0
2	NAG	q	2	2	14,14,15	0.23	0	17,19,21	0.81	0
2	BMA	q	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.83	3 (20%)
2	NAG	r	1	1,2	14,14,15	0.31	0	17,19,21	0.58	0
2	NAG	r	2	2	14,14,15	0.25	0	17,19,21	0.74	0
2	BMA	r	3	2	11,11,12	0.22	0	15,15,17	0.63	0
2	NAG	s	1	1,2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	s	2	2	14,14,15	0.32	0	17,19,21	0.56	0
2	BMA	s	3	2	11,11,12	0.22	0	15,15,17	0.59	0
12	NAG	t	1	12,1	14,14,15	0.29	0	17,19,21	0.41	0
12	NAG	t	2	12	14,14,15	0.32	0	17,19,21	0.70	0
12	BMA	t	3	12	11,11,12	0.24	0	15,15,17	0.72	0
12	MAN	t	4	12	11,11,12	0.20	0	15,15,17	0.83	1 (6%)
8	NAG	u	1	8,1	14,14,15	0.74	1 (7%)	17,19,21	0.77	0
8	NAG	u	2	8	14,14,15	0.19	0	17,19,21	0.37	0
8	BMA	u	3	8	11,11,12	0.95	1 (9%)	15,15,17	1.18	1 (6%)
8	MAN	u	4	8	11,11,12	1.40	2 (18%)	15,15,17	1.87	2 (13%)
8	MAN	u	5	8	11,11,12	0.87	1 (9%)	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	u	6	8	11,11,12	0.59	0	15,15,17	1.25	2 (13%)
8	MAN	u	7	8	11,11,12	0.74	1 (9%)	15,15,17	1.12	2 (13%)
9	NAG	v	1	1,9	14,14,15	0.36	0	17,19,21	0.85	2 (11%)
9	NAG	v	2	9	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
9	BMA	v	3	9	11,11,12	1.07	1 (9%)	15,15,17	1.03	1 (6%)
9	MAN	v	4	9	11,11,12	0.75	0	15,15,17	1.28	2 (13%)
2	NAG	w	1	1,2	14,14,15	0.27	0	17,19,21	0.92	1 (5%)
2	NAG	w	2	2	14,14,15	0.32	0	17,19,21	0.62	0
2	BMA	w	3	2	11,11,12	0.22	0	15,15,17	0.60	0
12	NAG	x	1	12,1	14,14,15	0.27	0	17,19,21	0.60	0
12	NAG	x	2	12	14,14,15	0.26	0	17,19,21	0.96	1 (5%)
12	BMA	x	3	12	11,11,12	0.24	0	15,15,17	0.60	0
12	MAN	x	4	12	11,11,12	0.22	0	15,15,17	0.64	0
10	NAG	y	1	10,1	14,14,15	0.37	0	17,19,21	1.23	3 (17%)
10	NAG	y	2	10	14,14,15	0.39	0	17,19,21	1.09	1 (5%)
10	BMA	y	3	10	11,11,12	0.22	0	15,15,17	0.65	0
10	FUC	y	4	10	10,10,11	0.25	0	14,14,16	0.68	0
2	NAG	z	1	1,2	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
2	NAG	z	2	2	14,14,15	0.25	0	17,19,21	0.82	1 (5%)
2	BMA	z	3	2	11,11,12	0.22	0	15,15,17	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	0	2	2	-	0/6/23/26	0/1/1/1
2	BMA	0	3	2	-	2/2/19/22	0/1/1/1
7	NAG	1	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	1	2	7	-	4/6/23/26	0/1/1/1
7	BMA	1	3	7	-	2/2/19/22	0/1/1/1
7	MAN	1	4	7	-	0/2/19/22	0/1/1/1
7	MAN	1	5	7	-	0/2/19/22	0/1/1/1
9	NAG	2	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	2	2	9	-	2/6/23/26	0/1/1/1
9	BMA	2	3	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	2	4	9	-	0/2/19/22	0/1/1/1
2	NAG	3	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	3	2	2	-	3/6/23/26	0/1/1/1
2	BMA	3	3	2	-	1/2/19/22	0/1/1/1
3	NAG	4	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	4	2	3	-	0/6/23/26	0/1/1/1
2	NAG	5	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	5	2	2	-	3/6/23/26	0/1/1/1
2	BMA	5	3	2	-	0/2/19/22	0/1/1/1
3	NAG	6	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	6	2	3	-	2/6/23/26	0/1/1/1
2	NAG	7	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	7	2	2	-	1/6/23/26	0/1/1/1
2	BMA	7	3	2	-	0/2/19/22	0/1/1/1
13	NAG	8	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	8	2	13	-	5/6/23/26	0/1/1/1
13	BMA	8	3	13	-	2/2/19/22	0/1/1/1
13	MAN	8	4	13	-	1/2/19/22	0/1/1/1
13	MAN	8	5	13	-	0/2/19/22	0/1/1/1
13	MAN	8	6	13	-	0/2/19/22	0/1/1/1
9	NAG	9	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	9	2	9	-	3/6/23/26	0/1/1/1
9	BMA	9	3	9	-	1/2/19/22	0/1/1/1
9	MAN	9	4	9	-	0/2/19/22	0/1/1/1
2	NAG	AA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	1/6/23/26	0/1/1/1
2	BMA	AA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	BA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	4/6/23/26	0/1/1/1
2	BMA	BA	3	2	-	0/2/19/22	0/1/1/1
9	NAG	CA	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	CA	2	9	-	3/6/23/26	0/1/1/1
9	BMA	CA	3	9	-	0/2/19/22	0/1/1/1
9	MAN	CA	4	9	-	2/2/19/22	0/1/1/1
8	NAG	DA	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	DA	2	8	-	0/6/23/26	0/1/1/1
8	BMA	DA	3	8	-	2/2/19/22	0/1/1/1
8	MAN	DA	4	8	-	0/2/19/22	0/1/1/1
8	MAN	DA	5	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	DA	6	8	-	0/2/19/22	0/1/1/1
8	MAN	DA	7	8	-	0/2/19/22	0/1/1/1
2	NAG	EA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	EA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	EA	3	2	-	0/2/19/22	0/1/1/1
9	NAG	FA	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	FA	2	9	-	3/6/23/26	0/1/1/1
9	BMA	FA	3	9	-	0/2/19/22	0/1/1/1
9	MAN	FA	4	9	-	1/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
9	NAG	GA	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	GA	2	9	-	0/6/23/26	0/1/1/1
9	BMA	GA	3	9	-	1/2/19/22	0/1/1/1
9	MAN	GA	4	9	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	HA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	HA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
2	NAG	IA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	IA	3	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
10	NAG	JA	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	JA	2	10	-	0/6/23/26	0/1/1/1
10	BMA	JA	3	10	-	0/2/19/22	0/1/1/1
10	FUC	JA	4	10	-	-	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
3	NAG	KA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	KA	2	3	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
3	NAG	LA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	LA	2	3	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	BMA	M	3	2	-	1/2/19/22	0/1/1/1
3	NAG	MA	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	MA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	FUC	O	3	4	-	-	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	BMA	P	3	2	-	1/2/19/22	0/1/1/1
2	NAG	Q	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	1/2/19/22	0/1/1/1
2	NAG	R	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	BMA	R	3	2	-	0/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	3/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	MAN	S	4	5	-	0/2/19/22	0/1/1/1
5	MAN	S	5	5	-	1/2/19/22	0/1/1/1
5	MAN	S	6	5	-	0/2/19/22	0/1/1/1
6	NAG	T	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	T	2	6	-	3/6/23/26	0/1/1/1
6	BMA	T	3	6	-	1/2/19/22	0/1/1/1
6	MAN	T	4	6	-	0/2/19/22	0/1/1/1
6	MAN	T	5	6	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	4/6/23/26	0/1/1/1
2	BMA	V	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	W	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	1/6/23/26	0/1/1/1
7	BMA	W	3	7	-	1/2/19/22	0/1/1/1
7	MAN	W	4	7	-	0/2/19/22	0/1/1/1
7	MAN	W	5	7	-	0/2/19/22	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	0/2/19/22	0/1/1/1
8	MAN	X	5	8	-	0/2/19/22	0/1/1/1
8	MAN	X	6	8	-	0/2/19/22	0/1/1/1
8	MAN	X	7	8	-	0/2/19/22	0/1/1/1
9	NAG	Y	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	0/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	0/2/19/22	0/1/1/1
2	NAG	a	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	3/6/23/26	0/1/1/1
2	BMA	a	3	2	-	0/2/19/22	0/1/1/1
3	NAG	b	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	1/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	2/6/23/26	0/1/1/1
2	BMA	c	3	2	-	2/2/19/22	0/1/1/1
10	NAG	d	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	FUC	d	4	10	-	-	0/1/1/1
3	NAG	e	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	0/6/23/26	0/1/1/1
2	NAG	g	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	1/6/23/26	0/1/1/1
2	BMA	g	3	2	-	1/2/19/22	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	h	2	2	-	3/6/23/26	0/1/1/1
2	BMA	h	3	2	-	0/2/19/22	0/1/1/1
7	NAG	i	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	i	2	7	-	4/6/23/26	0/1/1/1
7	BMA	i	3	7	-	2/2/19/22	0/1/1/1
7	MAN	i	4	7	-	0/2/19/22	0/1/1/1
7	MAN	i	5	7	-	0/2/19/22	0/1/1/1
7	NAG	j	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
7	MAN	j	4	7	-	1/2/19/22	0/1/1/1
7	MAN	j	5	7	-	0/2/19/22	0/1/1/1
3	NAG	k	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	k	2	3	-	0/6/23/26	0/1/1/1
3	NAG	l	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
2	NAG	m	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	1/6/23/26	0/1/1/1
2	BMA	m	3	2	-	0/2/19/22	0/1/1/1
3	NAG	n	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	3/6/23/26	0/1/1/1
2	NAG	o	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	BMA	o	3	2	-	0/2/19/22	0/1/1/1
11	NAG	p	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	p	2	11	-	0/6/23/26	0/1/1/1
11	BMA	p	3	11	-	0/2/19/22	0/1/1/1
11	MAN	p	4	11	-	0/2/19/22	0/1/1/1
11	MAN	p	5	11	-	0/2/19/22	0/1/1/1
11	MAN	p	6	11	-	1/2/19/22	0/1/1/1
11	MAN	p	7	11	-	0/2/19/22	0/1/1/1
11	MAN	p	8	11	-	0/2/19/22	0/1/1/1
2	NAG	q	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	q	2	2	-	3/6/23/26	0/1/1/1
2	BMA	q	3	2	-	1/2/19/22	0/1/1/1
2	NAG	r	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	r	2	2	-	3/6/23/26	0/1/1/1
2	BMA	r	3	2	-	0/2/19/22	0/1/1/1
2	NAG	s	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	s	2	2	-	0/6/23/26	0/1/1/1
2	BMA	s	3	2	-	0/2/19/22	0/1/1/1
12	NAG	t	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	t	2	12	-	2/6/23/26	0/1/1/1
12	BMA	t	3	12	-	2/2/19/22	0/1/1/1
12	MAN	t	4	12	-	0/2/19/22	0/1/1/1
8	NAG	u	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	u	2	8	-	0/6/23/26	0/1/1/1
8	BMA	u	3	8	-	2/2/19/22	0/1/1/1
8	MAN	u	4	8	-	0/2/19/22	0/1/1/1
8	MAN	u	5	8	-	0/2/19/22	0/1/1/1
8	MAN	u	6	8	-	0/2/19/22	0/1/1/1
8	MAN	u	7	8	-	0/2/19/22	0/1/1/1
9	NAG	v	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	2/6/23/26	0/1/1/1
9	BMA	v	3	9	-	0/2/19/22	0/1/1/1
9	MAN	v	4	9	-	0/2/19/22	0/1/1/1
2	NAG	w	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	w	2	2	-	0/6/23/26	0/1/1/1
2	BMA	w	3	2	-	0/2/19/22	0/1/1/1
12	NAG	x	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	x	2	12	-	3/6/23/26	0/1/1/1
12	BMA	x	3	12	-	2/2/19/22	0/1/1/1
12	MAN	x	4	12	-	1/2/19/22	0/1/1/1
10	NAG	y	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	y	3	10	-	0/2/19/22	0/1/1/1
10	FUC	y	4	10	-	-	0/1/1/1
2	NAG	z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	z	2	2	-	4/6/23/26	0/1/1/1
2	BMA	z	3	2	-	0/2/19/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	1	NAG	C1-C2	3.84	1.58	1.52
10	d	1	NAG	C1-C2	3.75	1.57	1.52
10	JA	1	NAG	C1-C2	3.72	1.57	1.52
13	8	1	NAG	C1-C2	3.50	1.57	1.52
8	DA	4	MAN	C1-C2	3.38	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	4	MAN	C1-C2	3.34	1.59	1.52
8	u	4	MAN	C1-C2	3.32	1.59	1.52
6	T	3	BMA	O5-C5	3.28	1.50	1.43
2	q	3	BMA	O5-C5	3.27	1.50	1.43
9	9	3	BMA	O5-C5	3.26	1.50	1.43
2	Q	3	BMA	O5-C5	3.22	1.50	1.43
2	m	1	NAG	O5-C1	-3.21	1.38	1.43
9	v	3	BMA	C1-C2	3.04	1.59	1.52
8	u	4	MAN	O5-C1	2.64	1.47	1.43
8	u	1	NAG	O5-C1	-2.62	1.39	1.43
8	X	1	NAG	O5-C1	-2.59	1.39	1.43
8	X	4	MAN	O5-C1	2.59	1.47	1.43
8	DA	4	MAN	O5-C1	2.58	1.47	1.43
8	DA	1	NAG	O5-C1	-2.51	1.39	1.43
9	CA	3	BMA	O5-C1	-2.39	1.39	1.43
8	X	5	MAN	C1-C2	2.27	1.57	1.52
9	CA	4	MAN	C1-C2	2.22	1.57	1.52
8	u	5	MAN	C1-C2	2.18	1.57	1.52
8	u	3	BMA	C4-C3	2.15	1.57	1.52
8	X	3	BMA	C4-C3	2.12	1.57	1.52
8	DA	3	BMA	C4-C3	2.11	1.57	1.52
6	T	5	MAN	O5-C1	-2.10	1.40	1.43
9	9	1	NAG	O5-C1	-2.10	1.40	1.43
6	T	1	NAG	O5-C1	-2.08	1.40	1.43
8	DA	5	MAN	C1-C2	2.04	1.56	1.52
2	c	3	BMA	C1-C2	2.03	1.56	1.52
8	X	7	MAN	C1-C2	2.02	1.56	1.52
8	u	7	MAN	C1-C2	2.01	1.56	1.52
8	DA	7	MAN	C1-C2	2.00	1.56	1.52

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	1	NAG	C1-O5-C5	9.87	125.56	112.19
13	8	1	NAG	O5-C1-C2	-8.84	97.34	111.29
2	J	3	BMA	O2-C2-C3	8.51	127.18	110.14
3	H	2	NAG	O5-C5-C6	8.46	120.47	107.20
3	f	2	NAG	O5-C5-C6	8.45	120.45	107.20
3	e	2	NAG	O5-C5-C6	8.44	120.43	107.20
3	LA	2	NAG	O5-C5-C6	8.41	120.39	107.20
10	d	1	NAG	O5-C1-C2	-7.33	99.72	111.29
10	JA	1	NAG	O5-C1-C2	-7.30	99.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	1	NAG	O5-C1-C2	-6.51	101.01	111.29
8	DA	4	MAN	C1-O5-C5	6.01	120.34	112.19
8	u	4	MAN	C1-O5-C5	5.88	120.16	112.19
8	X	4	MAN	C1-O5-C5	5.81	120.06	112.19
2	P	3	BMA	C1-O5-C5	5.11	119.12	112.19
13	8	1	NAG	C2-N2-C7	-4.63	116.31	122.90
13	8	1	NAG	C1-O5-C5	4.63	118.46	112.19
2	Q	3	BMA	C1-O5-C5	4.61	118.44	112.19
6	T	3	BMA	C1-O5-C5	4.54	118.34	112.19
9	9	3	BMA	C1-O5-C5	4.50	118.28	112.19
2	q	3	BMA	C1-O5-C5	4.49	118.28	112.19
9	FA	2	NAG	C1-O5-C5	4.44	118.21	112.19
2	5	2	NAG	C1-O5-C5	4.43	118.20	112.19
3	l	1	NAG	C2-N2-C7	4.39	129.16	122.90
13	8	4	MAN	C1-O5-C5	4.11	117.76	112.19
9	CA	4	MAN	C1-O5-C5	3.96	117.55	112.19
9	v	4	MAN	C1-O5-C5	3.94	117.53	112.19
8	u	6	MAN	C1-O5-C5	3.80	117.34	112.19
7	1	2	NAG	C2-N2-C7	3.76	128.26	122.90
2	Q	3	BMA	O3-C3-C2	3.74	117.16	109.99
8	X	6	MAN	C1-O5-C5	3.73	117.25	112.19
3	N	2	NAG	C1-O5-C5	3.73	117.25	112.19
8	DA	6	MAN	C1-O5-C5	3.72	117.24	112.19
6	T	3	BMA	O3-C3-C2	3.71	117.11	109.99
9	9	3	BMA	O3-C3-C2	3.69	117.06	109.99
2	q	3	BMA	O3-C3-C2	3.67	117.03	109.99
3	b	2	NAG	C1-O5-C5	3.62	117.10	112.19
7	i	2	NAG	C2-N2-C7	3.60	128.02	122.90
6	T	5	MAN	O2-C2-C3	-3.54	103.04	110.14
10	y	2	NAG	C1-O5-C5	3.53	116.98	112.19
2	J	1	NAG	C2-N2-C7	3.49	127.87	122.90
13	8	1	NAG	C3-C4-C5	-3.46	104.06	110.24
2	P	3	BMA	C1-C2-C3	3.43	113.88	109.67
10	d	1	NAG	C3-C4-C5	-3.27	104.40	110.24
5	S	1	NAG	C2-N2-C7	-3.26	118.25	122.90
2	P	1	NAG	O5-C1-C2	3.17	116.29	111.29
10	JA	1	NAG	C3-C4-C5	-3.17	104.59	110.24
2	P	1	NAG	O4-C4-C5	3.15	117.12	109.30
13	8	4	MAN	O3-C3-C2	3.10	115.94	109.99
2	Z	1	NAG	C2-N2-C7	3.06	127.26	122.90
5	S	1	NAG	O5-C5-C6	-3.02	102.47	107.20
2	P	2	NAG	C1-O5-C5	3.02	116.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	1	NAG	C1-C2-N2	3.00	115.61	110.49
8	DA	4	MAN	C1-C2-C3	2.98	113.32	109.67
7	i	4	MAN	O2-C2-C3	2.97	116.08	110.14
8	X	7	MAN	C1-O5-C5	2.97	116.21	112.19
8	u	4	MAN	C1-C2-C3	2.95	113.30	109.67
8	u	7	MAN	C1-O5-C5	2.94	116.18	112.19
9	FA	2	NAG	O5-C5-C6	2.93	111.79	107.20
8	DA	7	MAN	C1-O5-C5	2.88	116.10	112.19
2	P	1	NAG	C4-C3-C2	-2.88	106.80	111.02
5	S	2	NAG	C2-N2-C7	2.88	127.00	122.90
7	i	4	MAN	C1-O5-C5	2.86	116.06	112.19
2	M	3	BMA	O3-C3-C4	2.86	116.95	110.35
9	2	4	MAN	C1-O5-C5	2.84	116.04	112.19
13	8	5	MAN	C1-O5-C5	2.84	116.04	112.19
8	u	5	MAN	C1-O5-C5	2.82	116.02	112.19
8	X	4	MAN	C1-C2-C3	2.81	113.12	109.67
9	2	3	BMA	O3-C3-C4	2.81	116.85	110.35
3	f	2	NAG	C4-C3-C2	2.80	115.12	111.02
8	X	5	MAN	C1-O5-C5	2.78	115.96	112.19
3	e	2	NAG	C4-C3-C2	2.77	115.08	111.02
3	MA	1	NAG	C2-N2-C7	2.77	126.85	122.90
2	5	2	NAG	O5-C5-C6	2.76	111.53	107.20
3	H	2	NAG	C4-C3-C2	2.76	115.06	111.02
8	DA	5	MAN	C1-O5-C5	2.74	115.90	112.19
3	LA	2	NAG	C4-C3-C2	2.72	115.01	111.02
5	S	1	NAG	O4-C4-C3	-2.72	104.06	110.35
2	EA	3	BMA	O2-C2-C3	-2.70	104.73	110.14
2	R	1	NAG	C2-N2-C7	2.68	126.72	122.90
5	S	2	NAG	C1-C2-N2	-2.66	105.94	110.49
7	j	1	NAG	C1-O5-C5	2.66	115.80	112.19
3	f	1	NAG	C1-O5-C5	2.65	115.78	112.19
3	k	1	NAG	C1-C2-N2	-2.63	105.99	110.49
12	t	4	MAN	O5-C5-C6	2.62	111.32	107.20
2	5	2	NAG	O5-C1-C2	2.62	115.42	111.29
3	e	1	NAG	C1-O5-C5	2.59	115.70	112.19
2	q	3	BMA	C3-C4-C5	-2.57	105.66	110.24
8	X	3	BMA	C1-C2-C3	-2.56	106.52	109.67
9	9	3	BMA	C3-C4-C5	-2.56	105.68	110.24
3	b	1	NAG	O4-C4-C5	2.55	115.63	109.30
2	Q	3	BMA	C3-C4-C5	-2.54	105.71	110.24
9	FA	2	NAG	C3-C4-C5	2.53	114.75	110.24
8	u	3	BMA	C1-C2-C3	-2.53	106.56	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C1-O5-C5	2.52	115.61	112.19
3	f	2	NAG	O3-C3-C4	2.52	116.18	110.35
10	d	1	NAG	C1-O5-C5	2.51	115.59	112.19
6	T	3	BMA	C3-C4-C5	-2.50	105.77	110.24
3	LA	2	NAG	O3-C3-C4	2.50	116.12	110.35
3	H	2	NAG	O3-C3-C4	2.49	116.11	110.35
9	FA	1	NAG	C1-O5-C5	2.49	115.57	112.19
2	m	3	BMA	C1-O5-C5	2.49	115.56	112.19
5	S	1	NAG	C4-C3-C2	2.49	114.66	111.02
2	c	3	BMA	C1-C2-C3	-2.48	106.62	109.67
2	m	2	NAG	C3-C4-C5	2.48	114.66	110.24
3	e	2	NAG	O3-C3-C4	2.46	116.04	110.35
2	5	2	NAG	C3-C4-C5	2.46	114.62	110.24
10	JA	1	NAG	C1-O5-C5	2.45	115.52	112.19
9	9	4	MAN	O2-C2-C3	-2.45	105.23	110.14
2	J	1	NAG	C1-C2-N2	2.44	114.66	110.49
2	P	3	BMA	C3-C4-C5	2.44	114.59	110.24
8	DA	3	BMA	C1-C2-C3	-2.44	106.67	109.67
2	3	2	NAG	O5-C1-C2	-2.43	107.44	111.29
2	P	1	NAG	O5-C5-C4	-2.42	104.94	110.83
10	y	1	NAG	C1-O5-C5	2.42	115.47	112.19
9	FA	2	NAG	O5-C1-C2	2.42	115.11	111.29
2	c	3	BMA	O2-C2-C3	-2.41	105.31	110.14
6	T	4	MAN	O2-C2-C3	-2.40	105.34	110.14
9	v	3	BMA	O2-C2-C3	-2.36	105.41	110.14
2	J	3	BMA	C2-C3-C4	2.36	114.97	110.89
2	EA	3	BMA	C2-C3-C4	2.34	114.94	110.89
8	u	6	MAN	O2-C2-C3	-2.33	105.46	110.14
2	AA	2	NAG	C2-N2-C7	2.33	126.22	122.90
8	DA	6	MAN	O2-C2-C3	-2.33	105.47	110.14
9	CA	4	MAN	O2-C2-C3	-2.33	105.48	110.14
3	4	1	NAG	C2-N2-C7	2.32	126.20	122.90
2	M	3	BMA	C1-O5-C5	2.32	115.33	112.19
2	h	2	NAG	C2-N2-C7	2.31	126.19	122.90
7	i	1	NAG	C2-N2-C7	2.30	126.19	122.90
7	W	2	NAG	C2-N2-C7	2.30	126.18	122.90
8	X	7	MAN	O2-C2-C3	-2.29	105.54	110.14
8	DA	7	MAN	O2-C2-C3	-2.27	105.58	110.14
2	V	2	NAG	C1-O5-C5	2.26	115.25	112.19
8	X	6	MAN	O2-C2-C3	-2.26	105.61	110.14
2	z	2	NAG	C1-O5-C5	2.25	115.24	112.19
9	FA	1	NAG	C2-N2-C7	2.24	126.09	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	4	MAN	O2-C2-C3	-2.22	105.68	110.14
2	w	1	NAG	C2-N2-C7	2.22	126.07	122.90
2	L	1	NAG	O5-C1-C2	-2.22	107.79	111.29
9	2	3	BMA	C1-O5-C5	2.21	115.19	112.19
8	u	7	MAN	O2-C2-C3	-2.21	105.70	110.14
7	1	1	NAG	C2-N2-C7	2.21	126.05	122.90
8	u	5	MAN	O2-C2-C3	-2.21	105.71	110.14
2	3	2	NAG	C4-C3-C2	-2.20	107.80	111.02
3	I	1	NAG	O4-C4-C5	2.19	114.74	109.30
8	DA	5	MAN	O2-C2-C3	-2.19	105.76	110.14
9	Y	1	NAG	O4-C4-C5	-2.16	103.93	109.30
8	X	5	MAN	O2-C2-C3	-2.16	105.81	110.14
9	v	1	NAG	O4-C4-C5	-2.16	103.94	109.30
10	y	1	NAG	C2-N2-C7	2.16	125.97	122.90
2	EA	1	NAG	O4-C4-C5	-2.15	103.95	109.30
7	1	3	BMA	C1-O5-C5	2.15	115.11	112.19
7	i	4	MAN	O5-C1-C2	2.15	114.09	110.77
9	v	4	MAN	O2-C2-C3	-2.15	105.83	110.14
3	k	2	NAG	O5-C5-C6	2.14	110.56	107.20
3	I	2	NAG	C1-O5-C5	2.14	115.09	112.19
2	z	1	NAG	C1-O5-C5	2.13	115.08	112.19
13	8	5	MAN	O2-C2-C3	-2.12	105.89	110.14
2	Z	2	NAG	C2-N2-C7	2.11	125.91	122.90
12	x	2	NAG	C2-N2-C7	2.11	125.91	122.90
3	f	2	NAG	O4-C4-C5	2.11	114.54	109.30
2	BA	2	NAG	C2-N2-C7	2.09	125.89	122.90
7	1	4	MAN	C1-O5-C5	2.08	115.02	112.19
10	JA	1	NAG	C4-C3-C2	-2.08	107.97	111.02
9	v	1	NAG	O4-C4-C3	2.08	115.16	110.35
2	EA	1	NAG	O4-C4-C3	2.07	115.14	110.35
2	M	2	NAG	O4-C4-C3	2.07	115.14	110.35
9	Y	1	NAG	O4-C4-C3	2.06	115.11	110.35
2	EA	2	NAG	C1-O5-C5	2.06	114.98	112.19
9	v	2	NAG	C1-O5-C5	2.06	114.98	112.19
2	m	2	NAG	O4-C4-C5	-2.06	104.19	109.30
3	H	2	NAG	O4-C4-C5	2.05	114.38	109.30
3	e	2	NAG	O4-C4-C5	2.04	114.37	109.30
8	DA	3	BMA	C1-O5-C5	2.04	114.95	112.19
10	y	1	NAG	O4-C4-C5	2.04	114.35	109.30
3	I	2	NAG	C1-C2-N2	2.03	113.95	110.49
10	d	1	NAG	C4-C3-C2	-2.03	108.05	111.02
9	2	2	NAG	O4-C4-C3	2.01	114.99	110.35

There are no chirality outliers.

All (261) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	R	1	NAG	C8-C7-N2-C2
2	R	1	NAG	O7-C7-N2-C2
2	V	2	NAG	C3-C2-N2-C7
2	V	2	NAG	O7-C7-N2-C2
2	Z	2	NAG	O7-C7-N2-C2
2	a	2	NAG	O7-C7-N2-C2
2	g	1	NAG	C8-C7-N2-C2
2	g	1	NAG	O7-C7-N2-C2
2	h	2	NAG	C8-C7-N2-C2
2	h	2	NAG	O7-C7-N2-C2
2	o	1	NAG	C8-C7-N2-C2
2	o	1	NAG	O7-C7-N2-C2
2	r	2	NAG	C8-C7-N2-C2
2	r	2	NAG	O7-C7-N2-C2
2	z	1	NAG	C8-C7-N2-C2
2	z	1	NAG	O7-C7-N2-C2
2	z	2	NAG	C3-C2-N2-C7
2	z	2	NAG	O7-C7-N2-C2
2	3	2	NAG	C8-C7-N2-C2
2	3	2	NAG	O7-C7-N2-C2
2	5	2	NAG	C8-C7-N2-C2
2	5	2	NAG	O7-C7-N2-C2
2	BA	2	NAG	C8-C7-N2-C2
2	BA	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	k	1	NAG	C8-C7-N2-C2
3	k	1	NAG	O7-C7-N2-C2
3	n	2	NAG	C1-C2-N2-C7
3	n	2	NAG	C8-C7-N2-C2
3	n	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	4	1	NAG	C8-C7-N2-C2
3	4	1	NAG	O7-C7-N2-C2
3	6	2	NAG	C8-C7-N2-C2
3	6	2	NAG	O7-C7-N2-C2
3	HA	1	NAG	C8-C7-N2-C2
3	HA	1	NAG	O7-C7-N2-C2
3	HA	2	NAG	C8-C7-N2-C2
3	HA	2	NAG	O7-C7-N2-C2
3	MA	1	NAG	O7-C7-N2-C2
5	S	2	NAG	C3-C2-N2-C7
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
7	i	2	NAG	C3-C2-N2-C7
7	i	2	NAG	C8-C7-N2-C2
7	i	2	NAG	O7-C7-N2-C2
7	j	2	NAG	C8-C7-N2-C2
7	j	2	NAG	O7-C7-N2-C2
7	1	2	NAG	C3-C2-N2-C7
7	1	2	NAG	O7-C7-N2-C2
10	y	1	NAG	C1-C2-N2-C7
10	y	1	NAG	C8-C7-N2-C2
10	y	1	NAG	O7-C7-N2-C2
12	x	2	NAG	O7-C7-N2-C2
13	8	2	NAG	C3-C2-N2-C7
2	K	1	NAG	C8-C7-N2-C2
2	V	2	NAG	C8-C7-N2-C2
2	Z	2	NAG	C8-C7-N2-C2
2	a	2	NAG	C8-C7-N2-C2
2	w	1	NAG	C8-C7-N2-C2
2	w	1	NAG	O7-C7-N2-C2
2	z	2	NAG	C8-C7-N2-C2
3	MA	1	NAG	C8-C7-N2-C2
7	1	2	NAG	C8-C7-N2-C2
9	FA	2	NAG	C8-C7-N2-C2
9	FA	2	NAG	O7-C7-N2-C2
12	x	2	NAG	C8-C7-N2-C2
13	8	2	NAG	C8-C7-N2-C2
13	8	2	NAG	O7-C7-N2-C2
2	0	3	BMA	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
9	2	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	CA	4	MAN	O5-C5-C6-O6
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	l	1	NAG	C8-C7-N2-C2
3	l	1	NAG	O7-C7-N2-C2
3	MA	2	NAG	C8-C7-N2-C2
9	FA	1	NAG	C8-C7-N2-C2
9	FA	1	NAG	O7-C7-N2-C2
12	t	2	NAG	C8-C7-N2-C2
8	X	3	BMA	O5-C5-C6-O6
8	u	3	BMA	O5-C5-C6-O6
8	DA	3	BMA	O5-C5-C6-O6
12	t	3	BMA	O5-C5-C6-O6
2	0	3	BMA	C4-C5-C6-O6
13	8	2	NAG	O5-C5-C6-O6
2	c	3	BMA	C4-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	q	2	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
9	2	2	NAG	O5-C5-C6-O6
9	9	2	NAG	O5-C5-C6-O6
2	c	3	BMA	O5-C5-C6-O6
2	V	1	NAG	C8-C7-N2-C2
2	5	1	NAG	C8-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	e	1	NAG	C8-C7-N2-C2
3	f	1	NAG	C8-C7-N2-C2
3	MA	2	NAG	O7-C7-N2-C2
7	j	1	NAG	C8-C7-N2-C2
12	x	3	BMA	O5-C5-C6-O6
2	J	1	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	h	2	NAG	C1-C2-N2-C7
2	L	3	BMA	O5-C5-C6-O6
9	CA	4	MAN	C4-C5-C6-O6
12	t	3	BMA	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
9	2	1	NAG	O5-C5-C6-O6
2	EA	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	T	2	NAG	C4-C5-C6-O6
9	v	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	q	2	NAG	C4-C5-C6-O6
8	X	3	BMA	C4-C5-C6-O6
8	u	3	BMA	C4-C5-C6-O6
8	DA	3	BMA	C4-C5-C6-O6
9	2	2	NAG	C4-C5-C6-O6
9	9	2	NAG	C4-C5-C6-O6
12	x	3	BMA	C4-C5-C6-O6
2	R	2	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	h	1	NAG	C8-C7-N2-C2
2	o	2	NAG	C8-C7-N2-C2
2	5	1	NAG	O7-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
3	f	1	NAG	O7-C7-N2-C2
3	l	2	NAG	C8-C7-N2-C2
7	j	1	NAG	O7-C7-N2-C2
9	GA	1	NAG	C8-C7-N2-C2
9	GA	1	NAG	O7-C7-N2-C2
12	t	2	NAG	O7-C7-N2-C2
12	x	1	NAG	C8-C7-N2-C2
13	8	1	NAG	C8-C7-N2-C2
2	c	1	NAG	O5-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
7	i	3	BMA	O5-C5-C6-O6
2	r	2	NAG	C1-C2-N2-C7
3	l	1	NAG	C1-C2-N2-C7
3	MA	1	NAG	C1-C2-N2-C7
9	FA	1	NAG	C1-C2-N2-C7
12	x	2	NAG	C1-C2-N2-C7
9	CA	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O7-C7-N2-C2
12	x	1	NAG	O7-C7-N2-C2
2	o	1	NAG	O5-C5-C6-O6
2	EA	2	NAG	O5-C5-C6-O6
9	v	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	i	3	BMA	C4-C5-C6-O6
2	m	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O7-C7-N2-C2
2	h	1	NAG	O7-C7-N2-C2
2	o	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
13	8	1	NAG	O7-C7-N2-C2
2	o	1	NAG	C1-C2-N2-C7
3	4	1	NAG	C1-C2-N2-C7
2	P	2	NAG	C8-C7-N2-C2
2	IA	1	NAG	C8-C7-N2-C2
7	1	3	BMA	O5-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
12	x	4	MAN	O5-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	BA	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
7	1	3	BMA	C4-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C4-C5-C6-O6
2	z	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C1-C2-N2-C7
2	K	2	NAG	O5-C5-C6-O6
2	3	3	BMA	O5-C5-C6-O6
9	GA	3	BMA	O5-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
9	2	3	BMA	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	1	2	NAG	O5-C5-C6-O6
2	P	3	BMA	O5-C5-C6-O6
2	g	3	BMA	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
2	3	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O7-C7-N2-C2
2	BA	1	NAG	C8-C7-N2-C2
7	j	4	MAN	O5-C5-C6-O6
9	FA	4	MAN	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
2	5	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
9	FA	2	NAG	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
2	q	3	BMA	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
6	T	3	BMA	O5-C5-C6-O6
9	9	3	BMA	O5-C5-C6-O6
5	S	5	MAN	O5-C5-C6-O6
2	Z	2	NAG	C3-C2-N2-C7
2	a	2	NAG	C3-C2-N2-C7
2	w	1	NAG	C3-C2-N2-C7
2	IA	1	NAG	O7-C7-N2-C2
3	LA	1	NAG	C8-C7-N2-C2
13	8	2	NAG	C4-C5-C6-O6
9	CA	2	NAG	C4-C5-C6-O6
13	8	3	BMA	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
2	BA	1	NAG	O7-C7-N2-C2
3	LA	1	NAG	O7-C7-N2-C2
3	b	1	NAG	C4-C5-C6-O6
13	8	4	MAN	O5-C5-C6-O6
13	8	3	BMA	O5-C5-C6-O6
9	CA	1	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C3-C2-N2-C7
2	Q	2	NAG	C3-C2-N2-C7
2	R	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C3-C2-N2-C7
2	q	1	NAG	C3-C2-N2-C7
2	q	2	NAG	C3-C2-N2-C7
2	AA	2	NAG	C3-C2-N2-C7
2	BA	2	NAG	C3-C2-N2-C7
6	T	1	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
7	W	2	NAG	C3-C2-N2-C7
7	i	1	NAG	C3-C2-N2-C7
7	1	1	NAG	C3-C2-N2-C7
9	9	1	NAG	C3-C2-N2-C7
9	9	2	NAG	C3-C2-N2-C7
9	CA	2	NAG	C3-C2-N2-C7
2	o	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C1-C2-N2-C7

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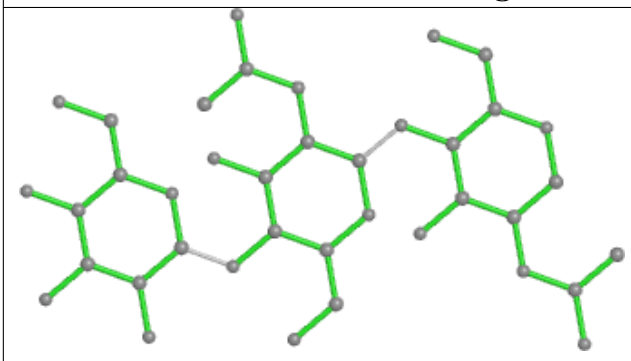
Mol	Chain	Res	Type	Atoms
7	W	1	NAG	O5-C5-C6-O6
2	s	1	NAG	C8-C7-N2-C2
9	CA	1	NAG	O5-C5-C6-O6
7	j	1	NAG	C1-C2-N2-C7
10	y	2	NAG	C4-C5-C6-O6
11	p	6	MAN	O5-C5-C6-O6
2	0	1	NAG	O5-C5-C6-O6
2	0	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C3-C2-N2-C7
2	7	2	NAG	O5-C5-C6-O6
2	s	1	NAG	O7-C7-N2-C2

There are no ring outliers.

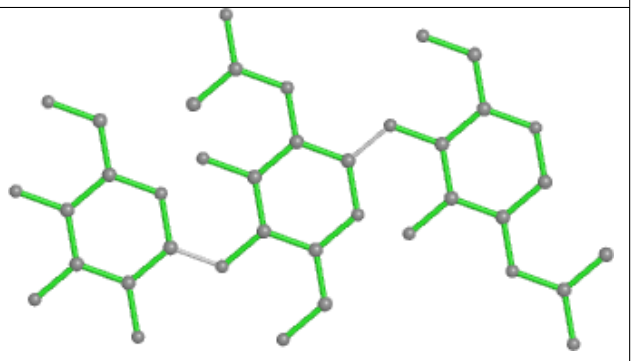
No monomer is involved in short contacts.

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

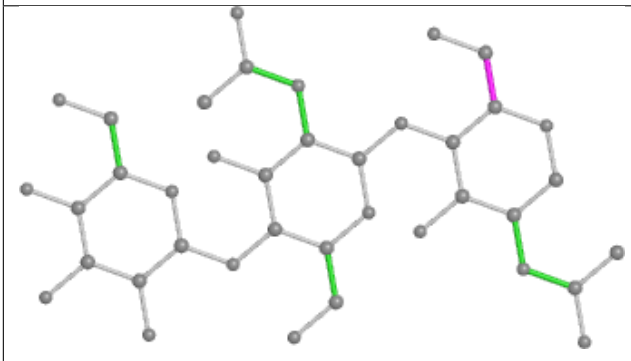
Oligosaccharide Chain G



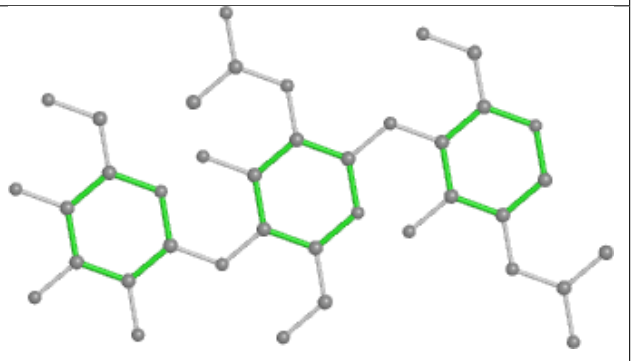
Bond lengths



Bond angles

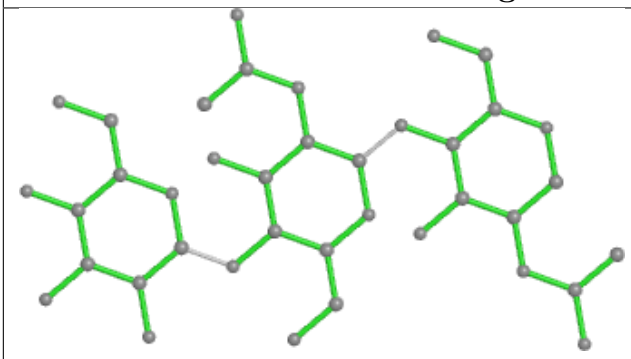


Torsions

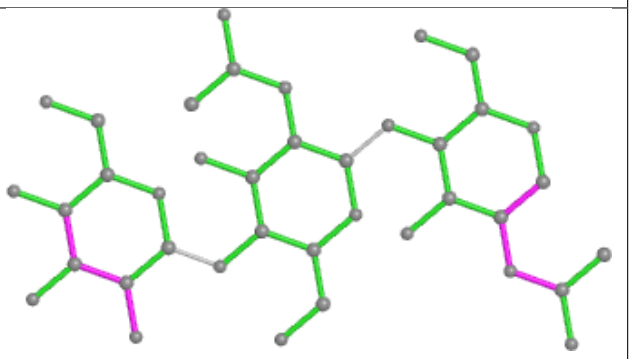


Rings

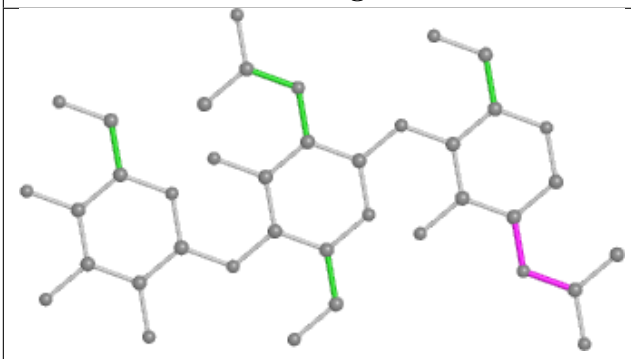
Oligosaccharide Chain J



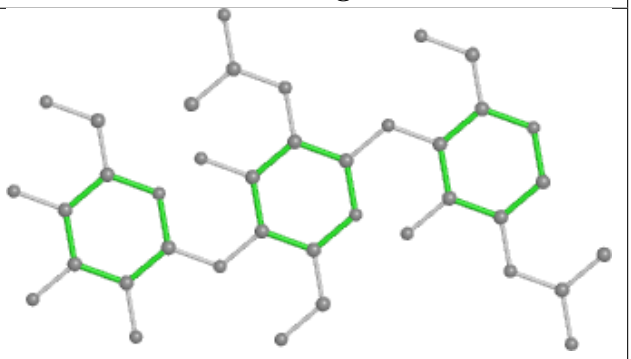
Bond lengths



Bond angles

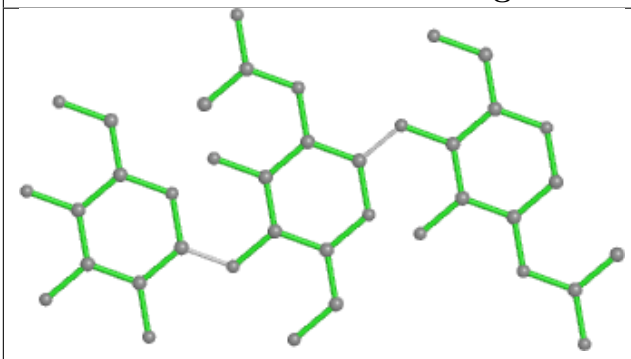


Torsions

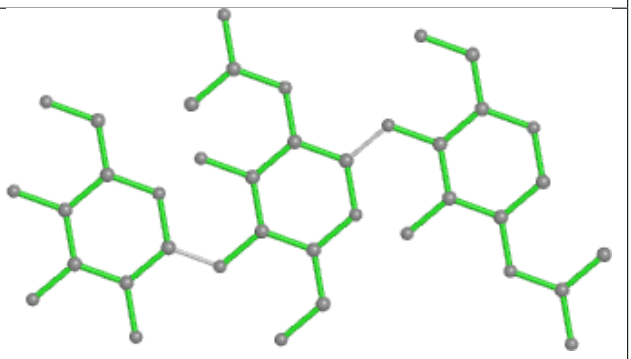


Rings

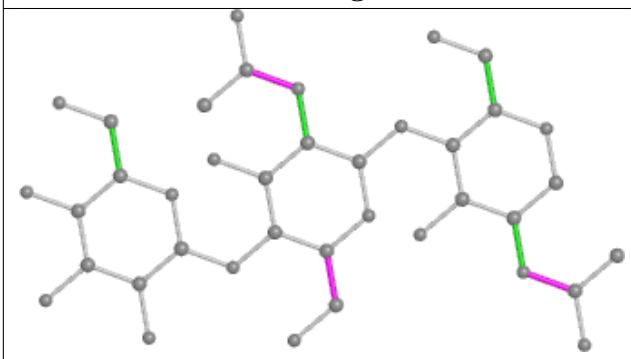
Oligosaccharide Chain K



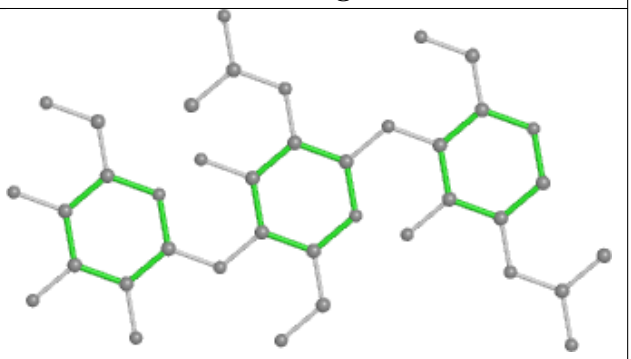
Bond lengths



Bond angles

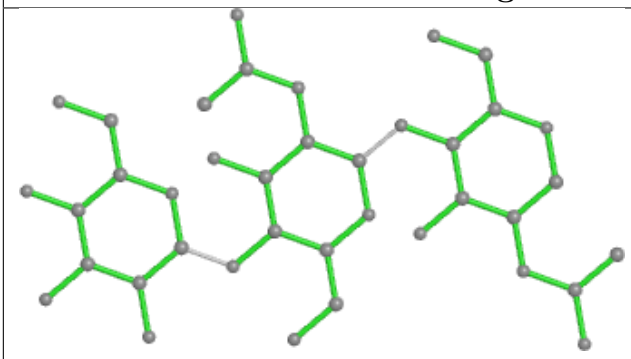


Torsions

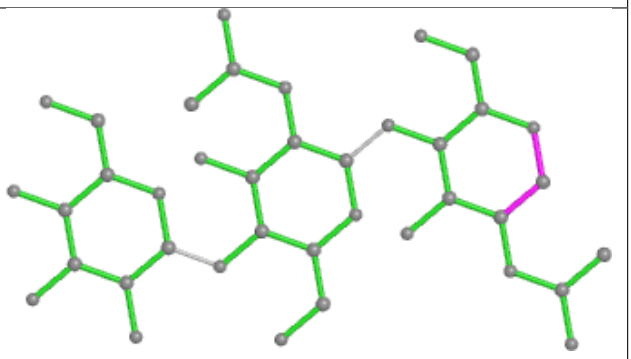


Rings

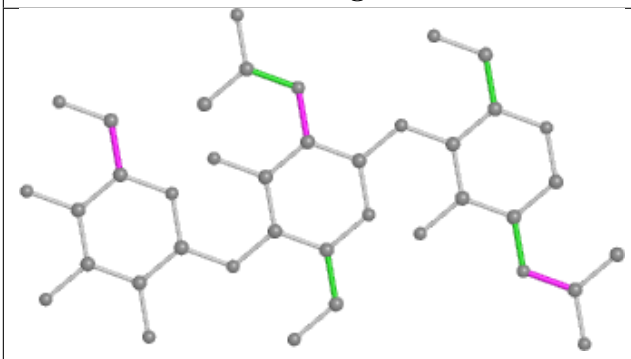
Oligosaccharide Chain L



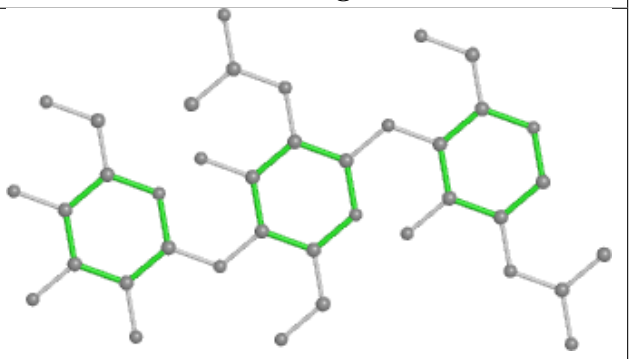
Bond lengths



Bond angles

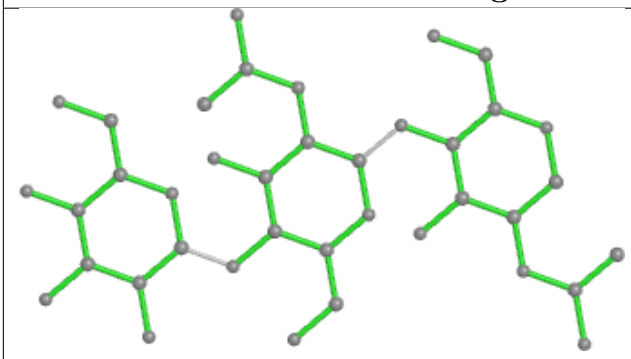


Torsions

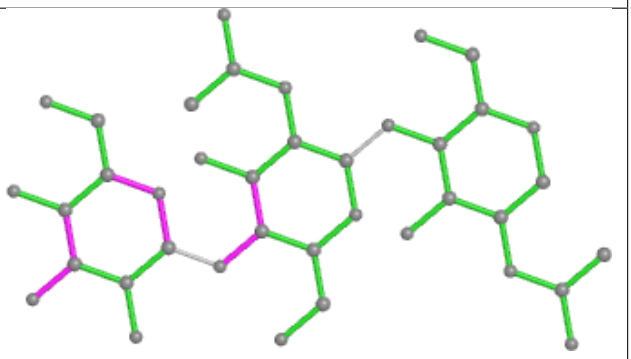


Rings

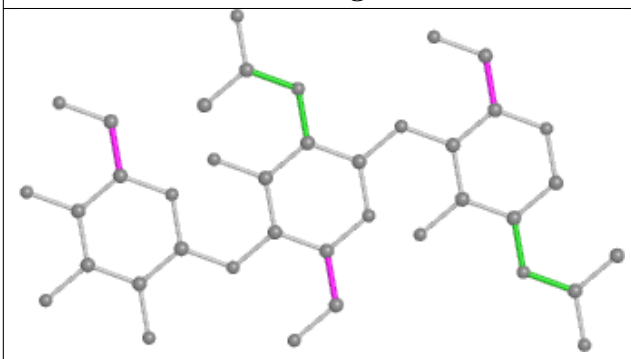
Oligosaccharide Chain M



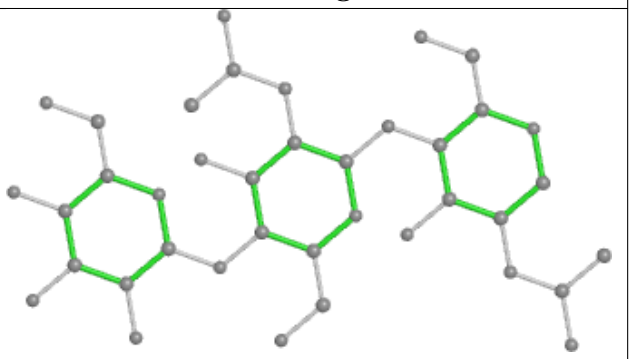
Bond lengths



Bond angles

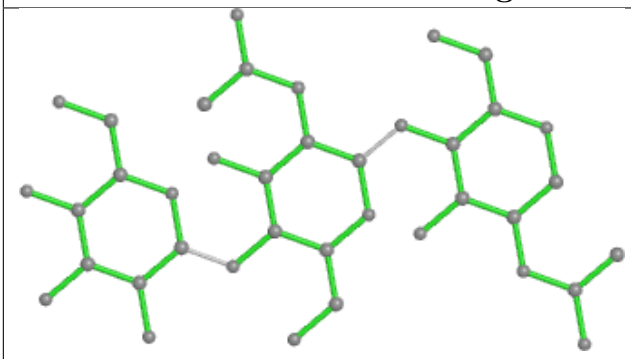


Torsions

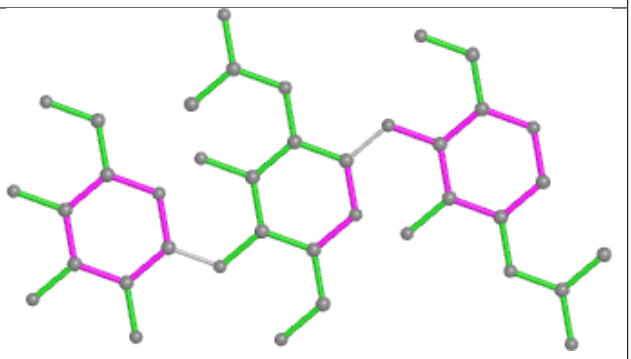


Rings

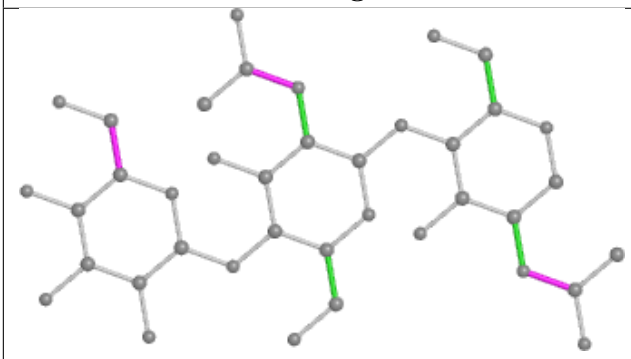
Oligosaccharide Chain P



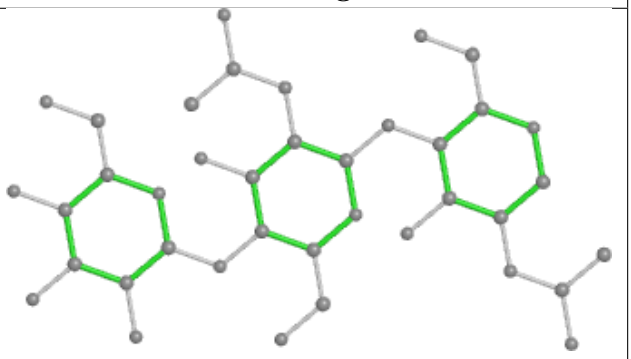
Bond lengths



Bond angles

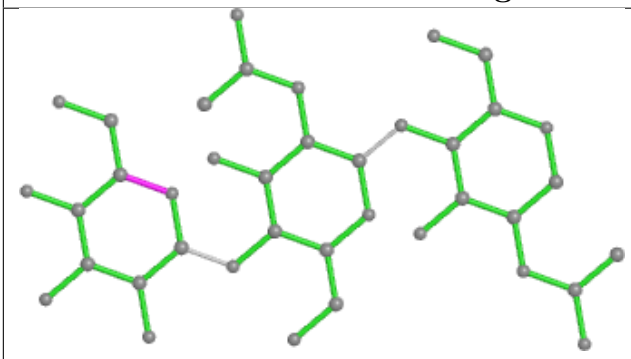


Torsions

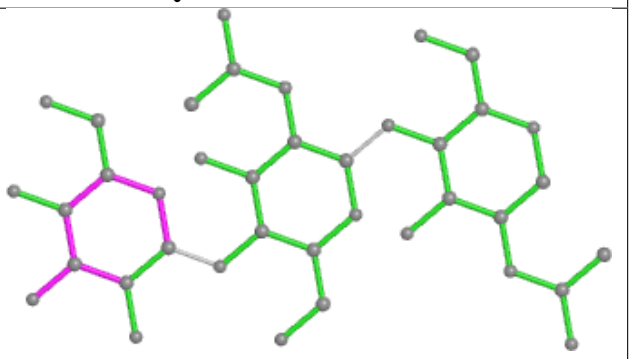


Rings

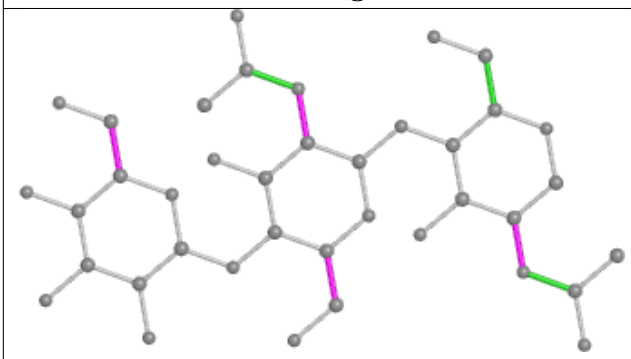
Oligosaccharide Chain Q



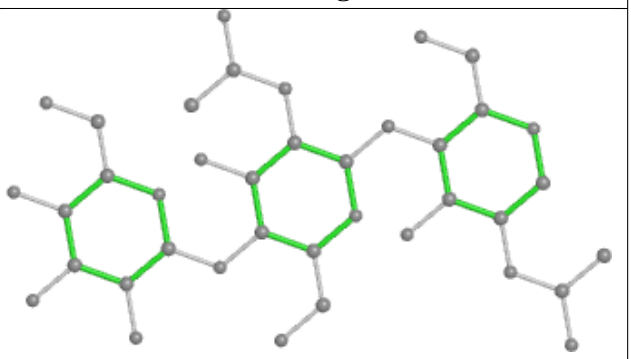
Bond lengths



Bond angles

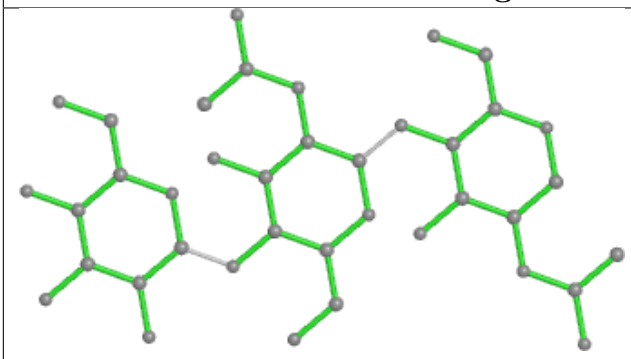


Torsions

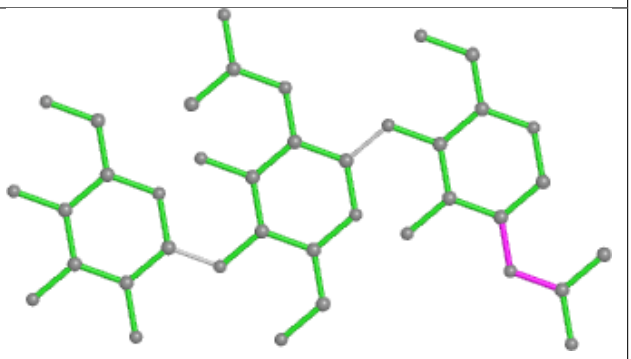


Rings

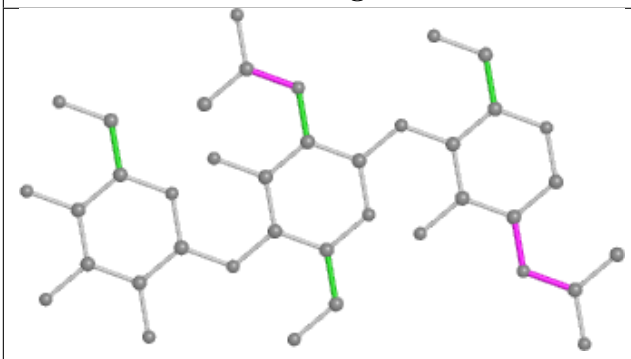
Oligosaccharide Chain R



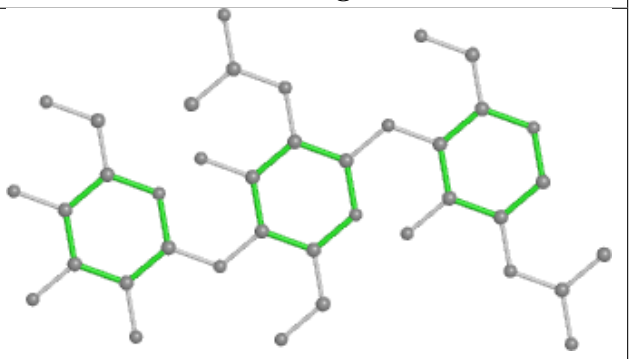
Bond lengths



Bond angles

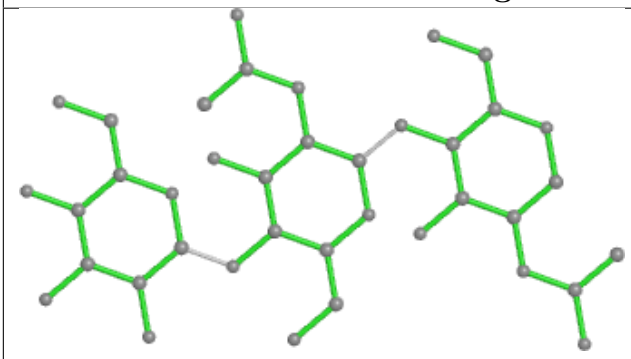


Torsions

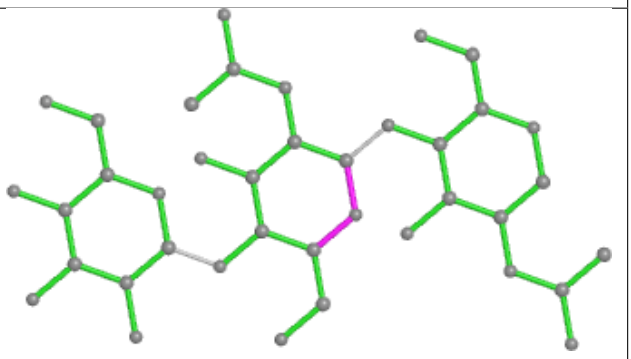


Rings

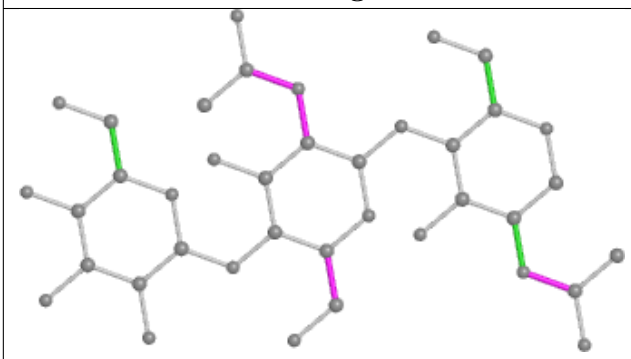
Oligosaccharide Chain V



Bond lengths



Bond angles



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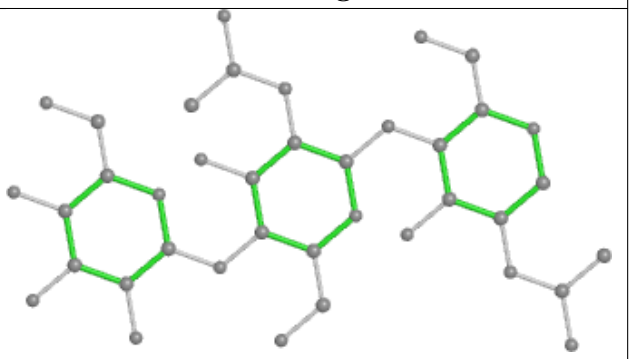
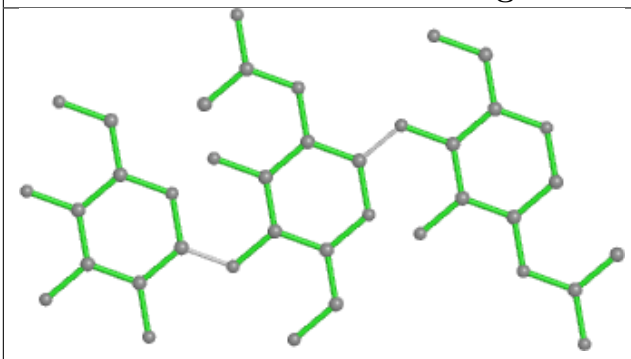
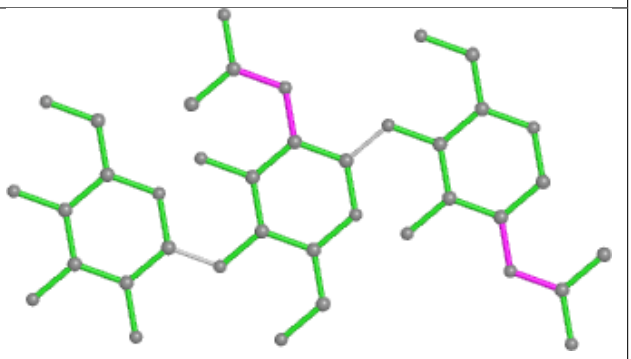


Rings

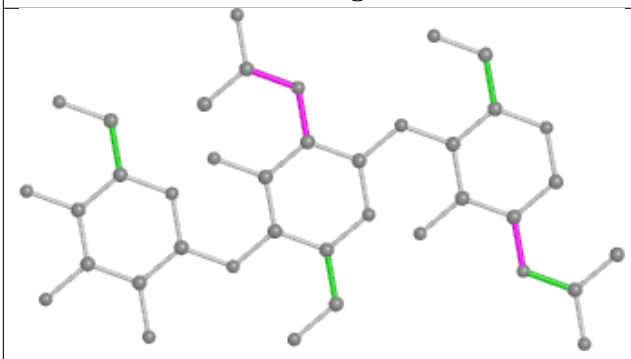
Oligosaccharide Chain Z



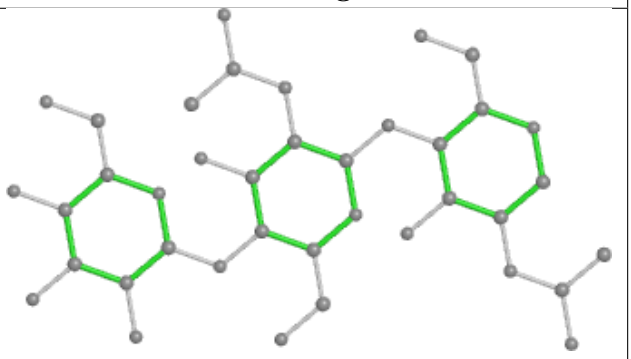
Bond lengths



Bond angles

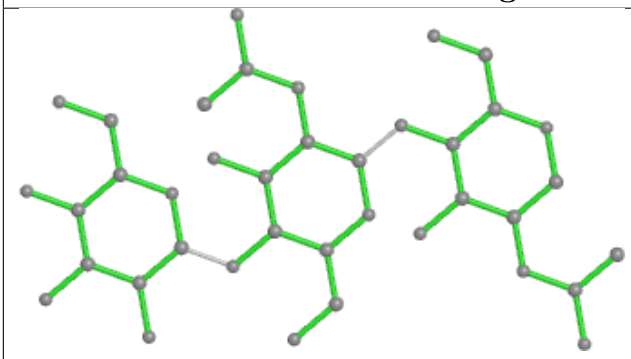


Torsions

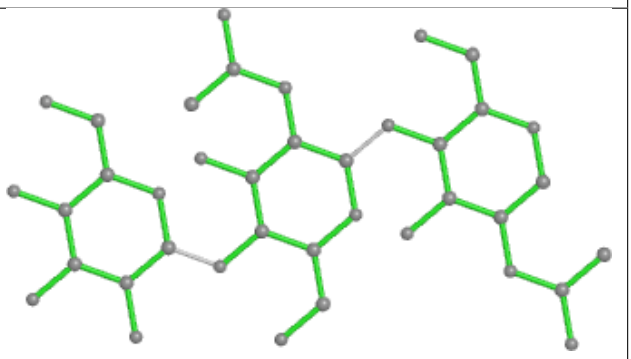


Rings

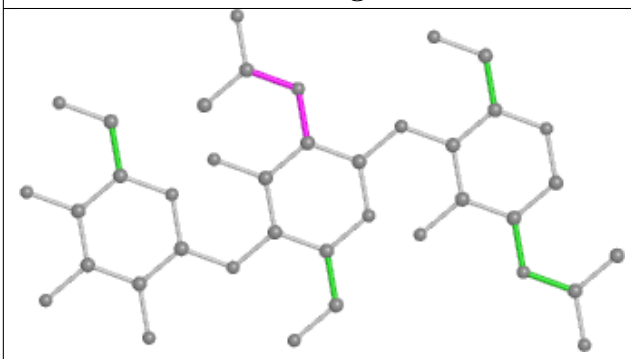
Oligosaccharide Chain a



Bond lengths



Bond angles



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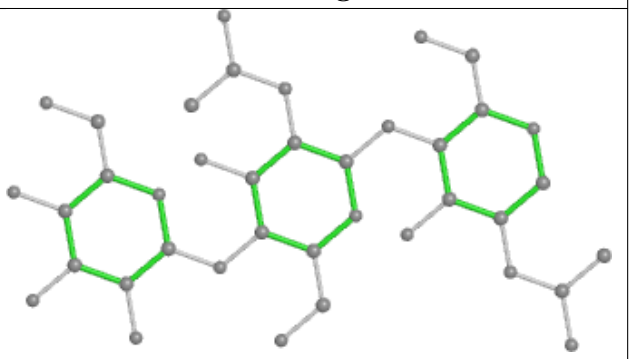
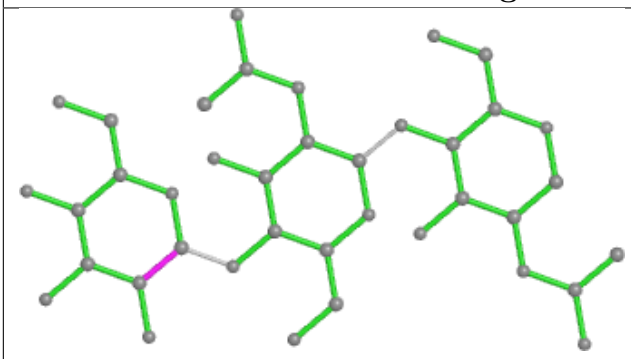
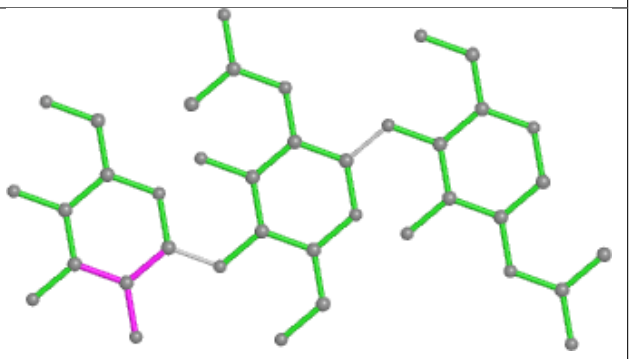


Rings

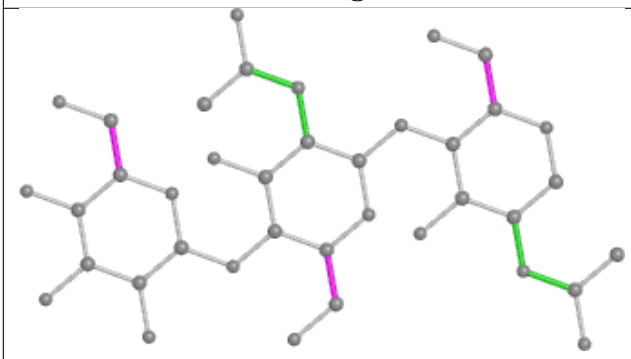
Oligosaccharide Chain c



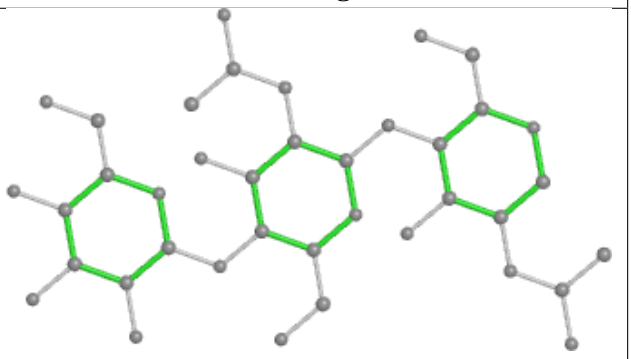
Bond lengths



Bond angles

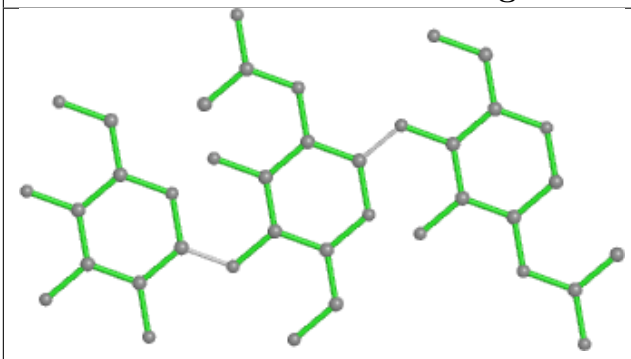


Torsions



Rings

Oligosaccharide Chain g



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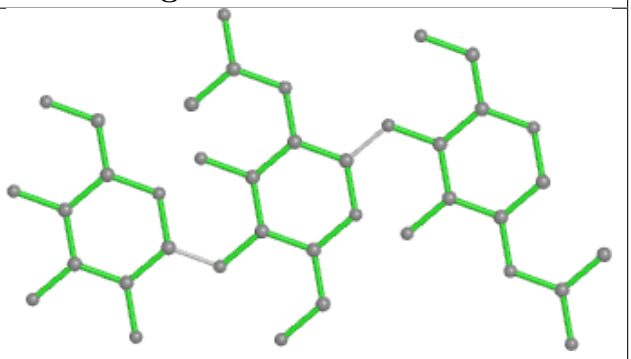

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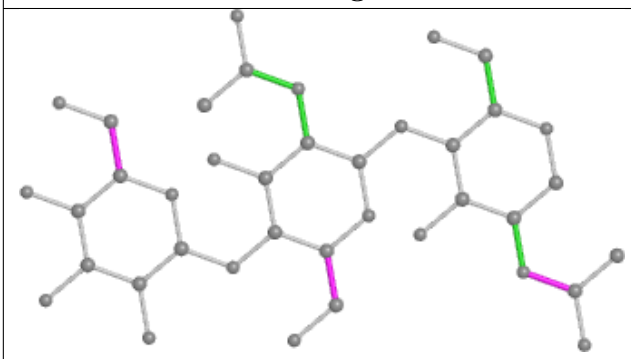

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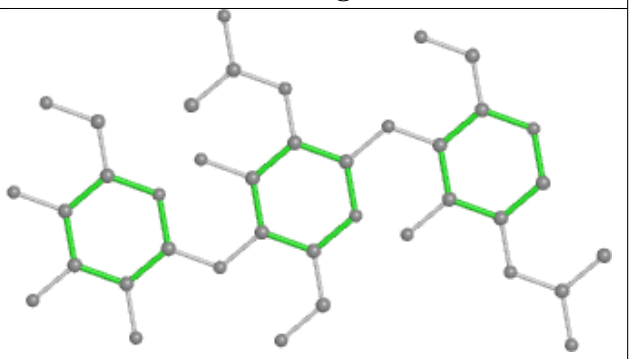
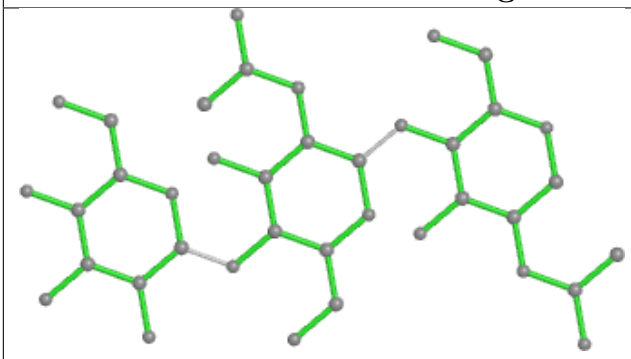


Rings

Oligosaccharide Chain h



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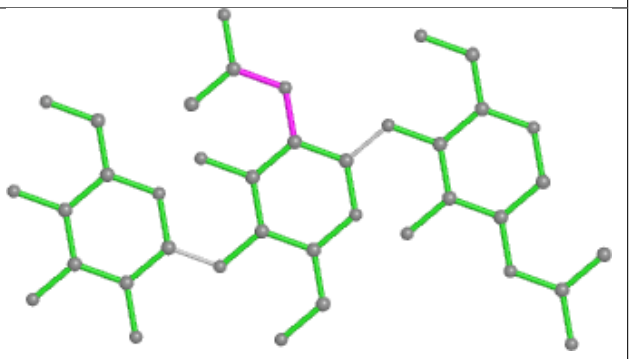

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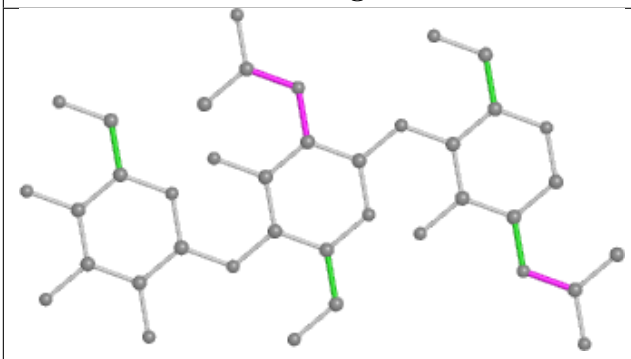

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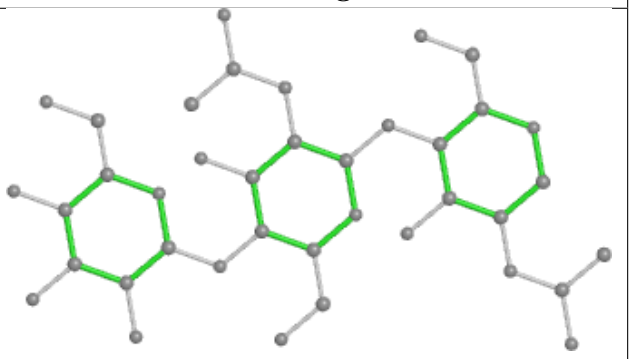
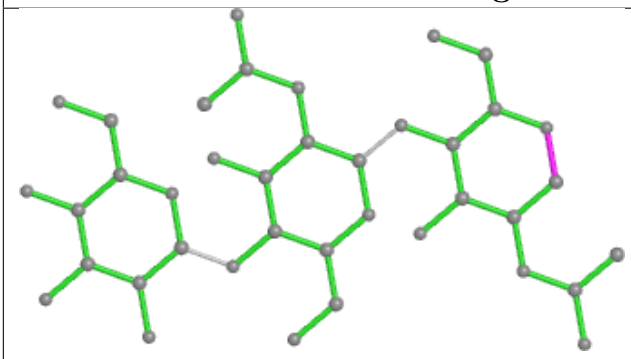


Rings

Oligosaccharide Chain m



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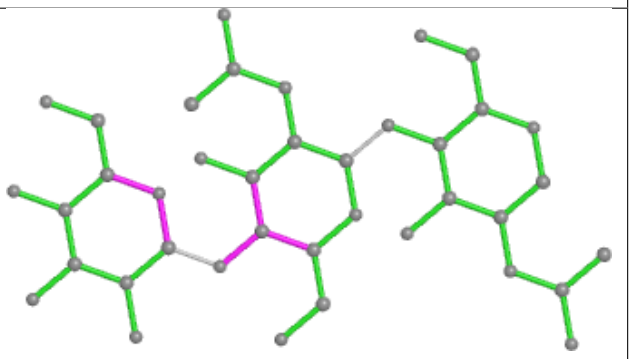
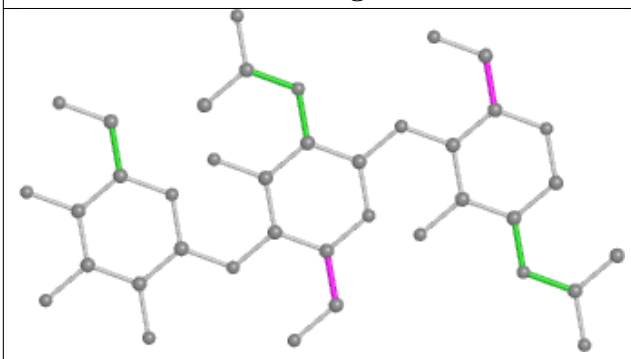


Bond angles



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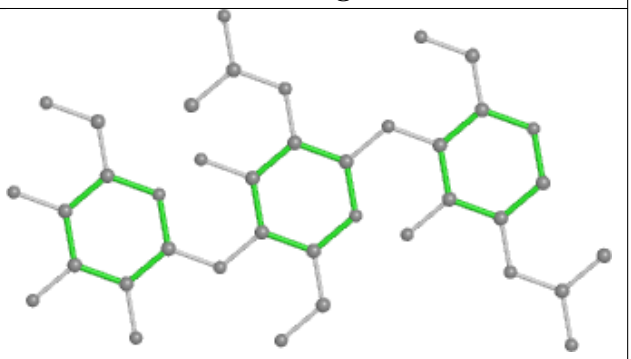
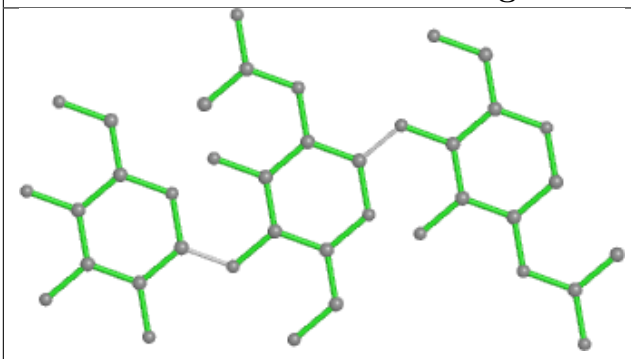


Rings

Oligosaccharide Chain o



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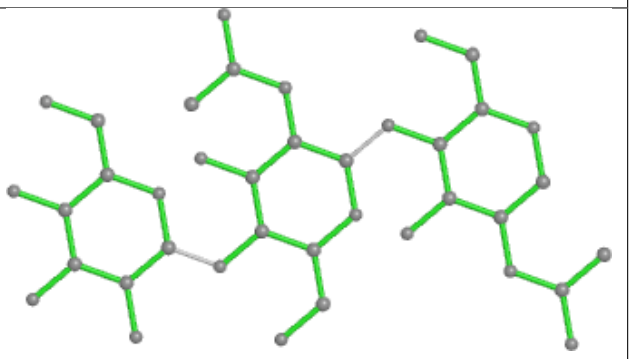

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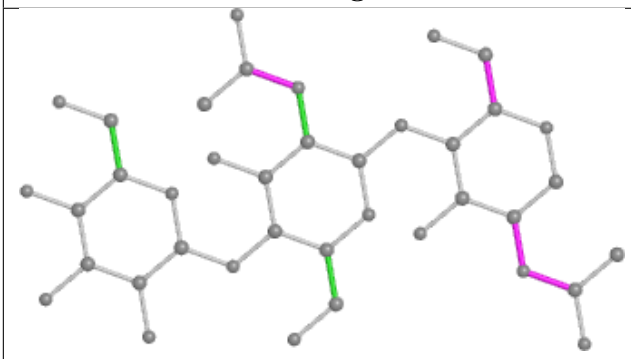

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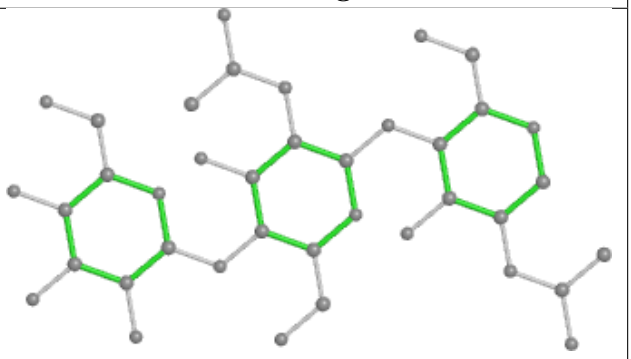
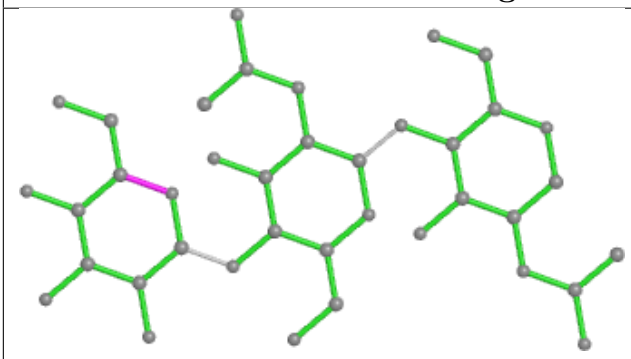


Rings

Oligosaccharide Chain q



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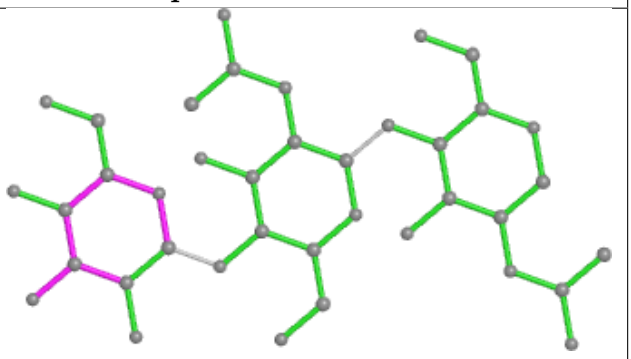

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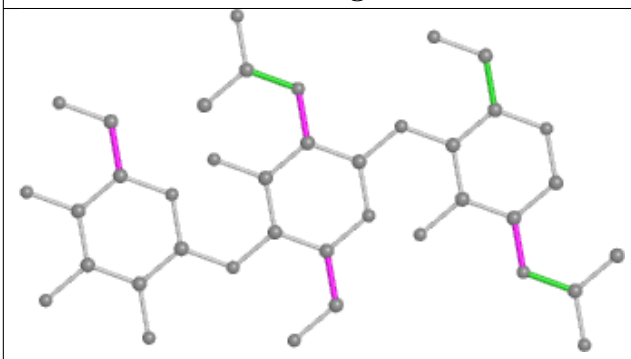

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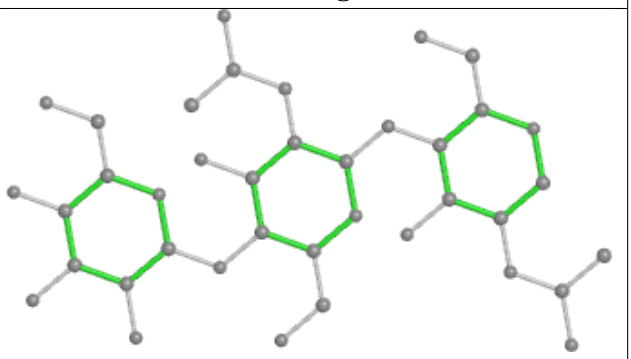
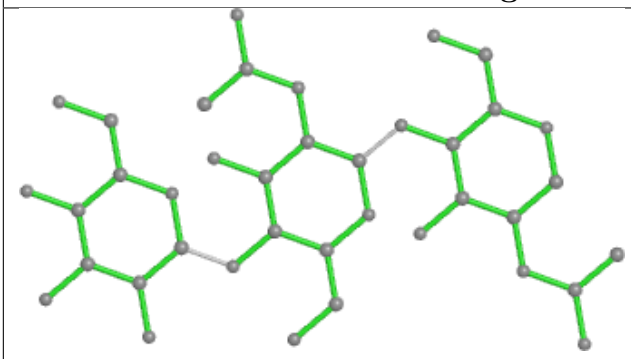


Rings

Oligosaccharide Chain r



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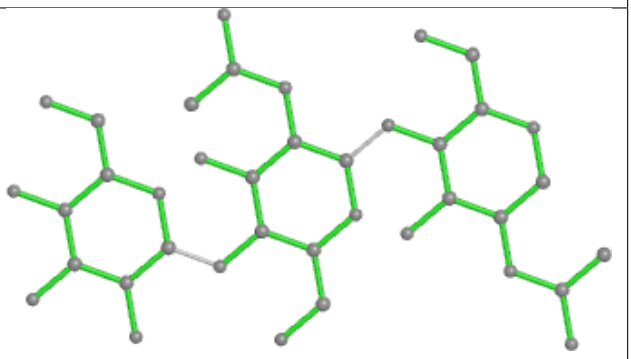
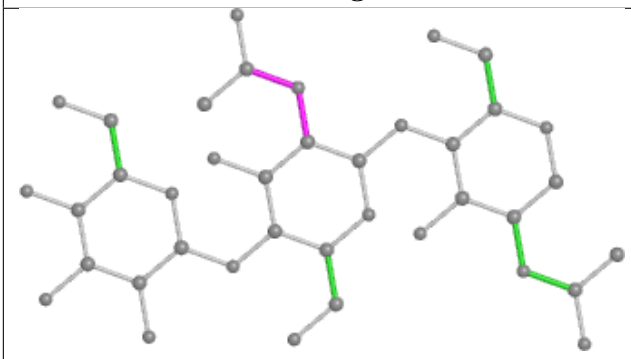


Bond angles



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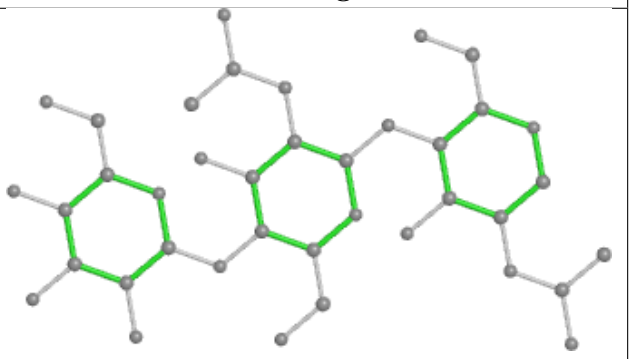
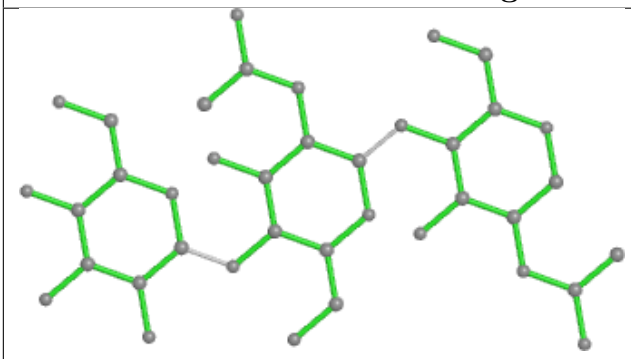


Rings

Oligosaccharide Chain s



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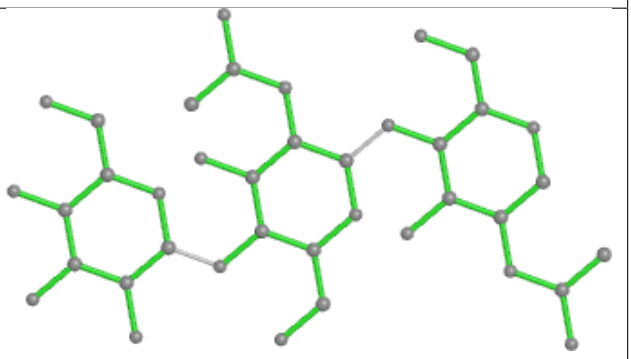
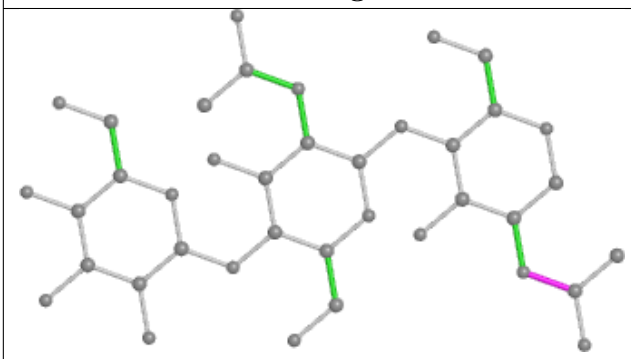


Bond angles



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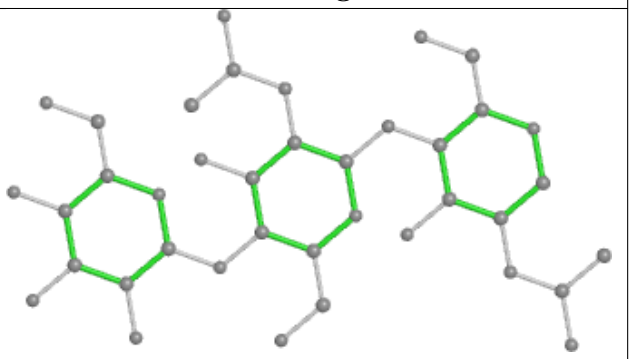
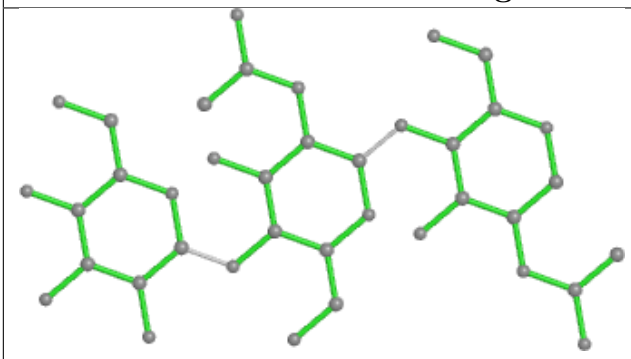


Rings

Oligosaccharide Chain w



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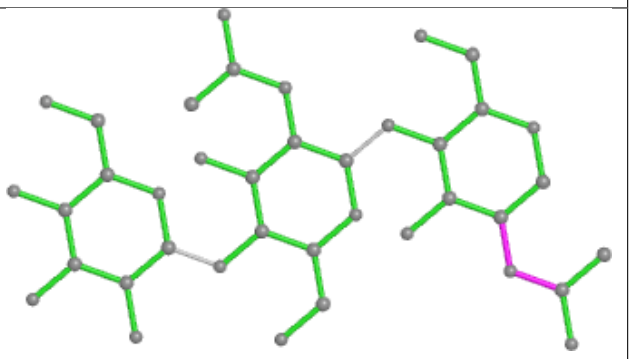

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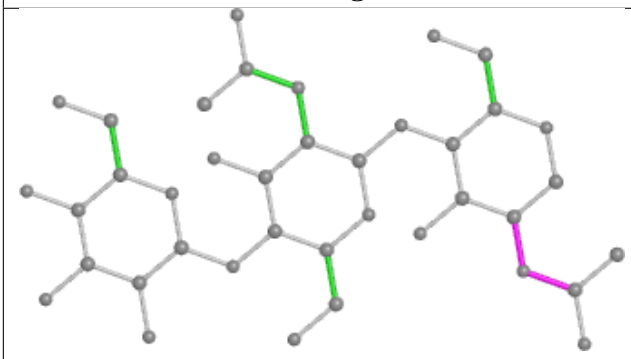

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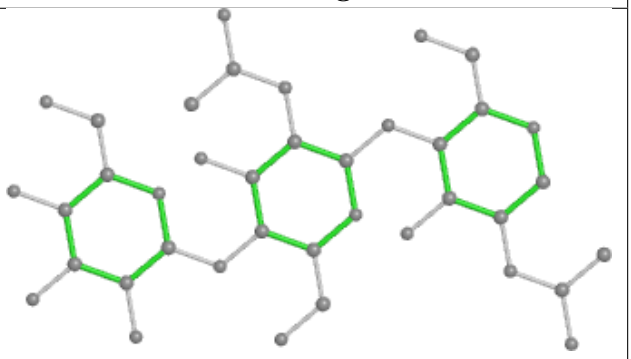
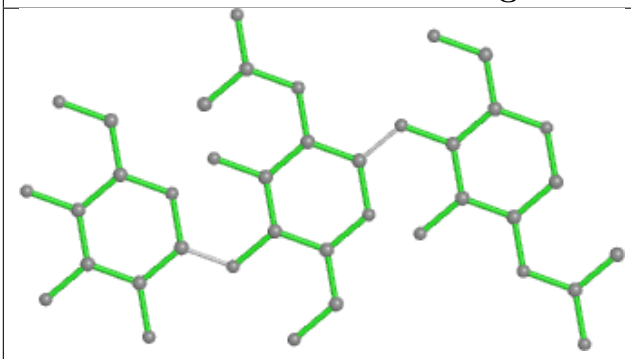


Rings

Oligosaccharide Chain z



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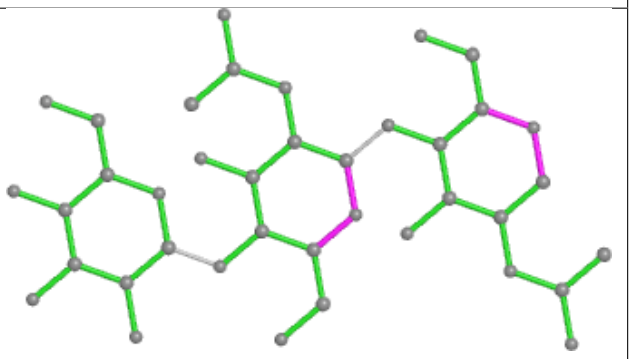
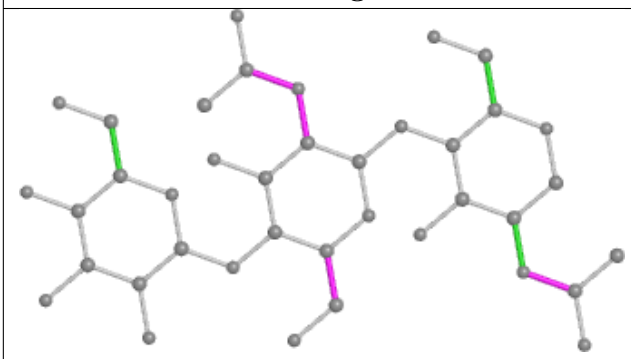


Bond angles



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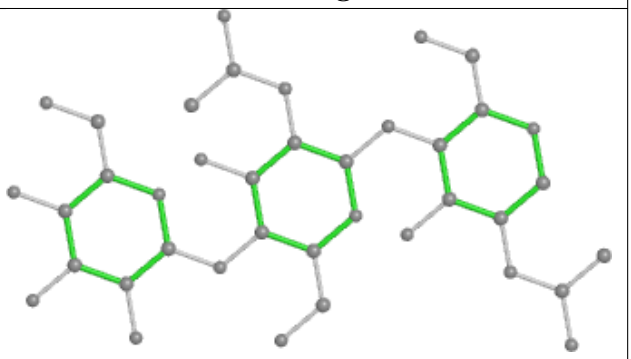
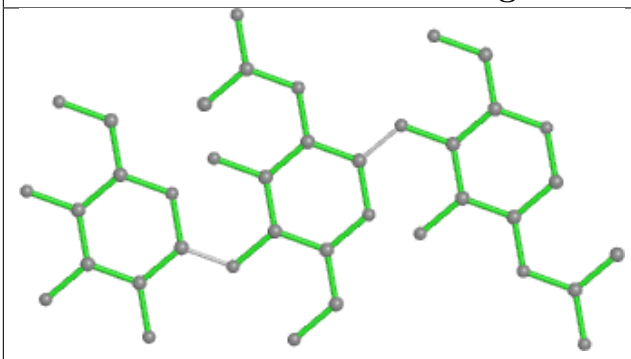


Rings

Oligosaccharide Chain 0



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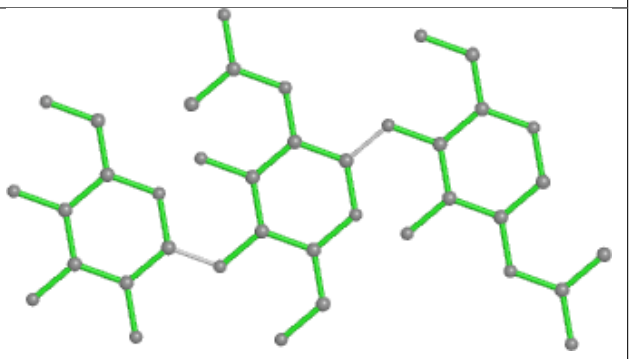
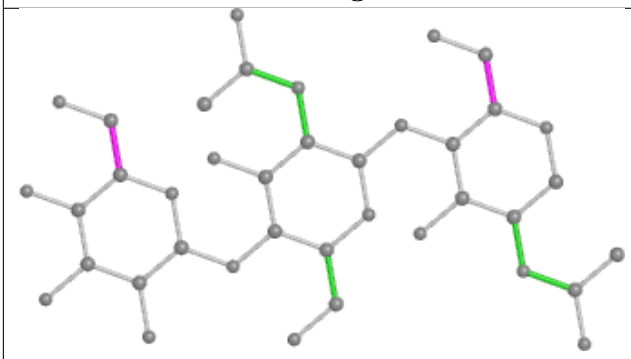


Bond angles



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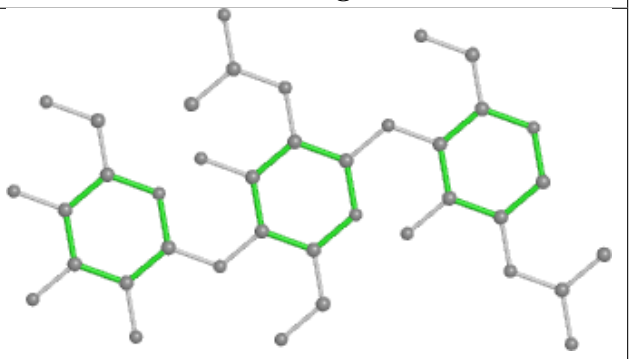
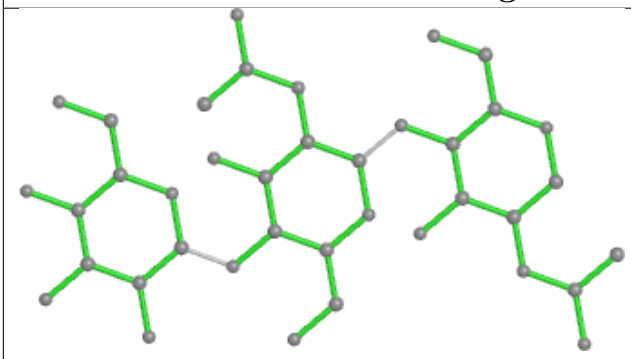


Rings

Oligosaccharide Chain 3



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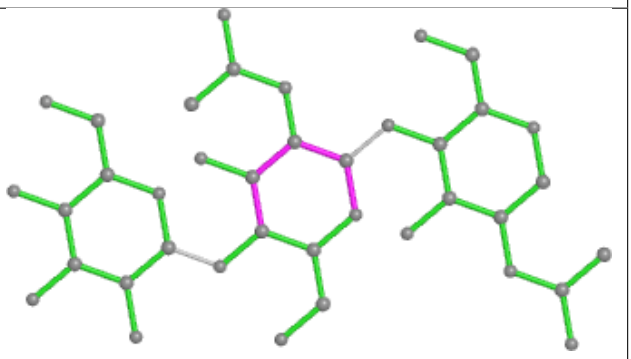
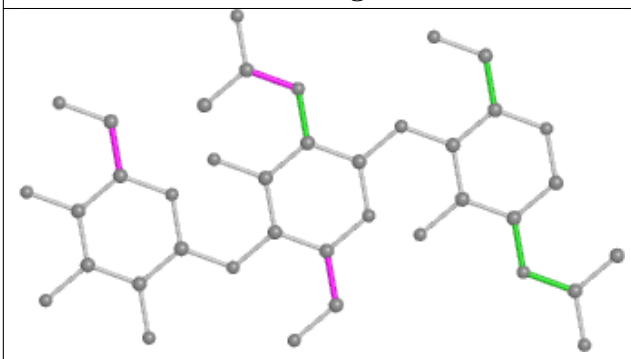


Bond angles



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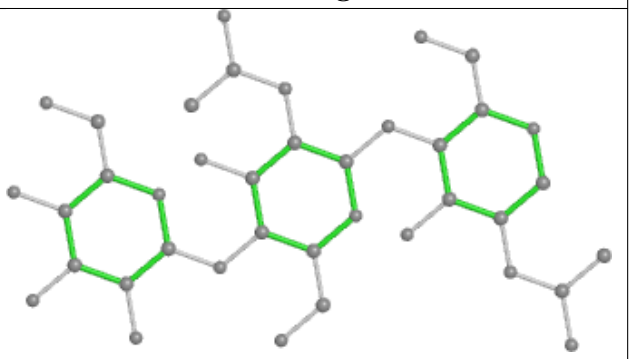
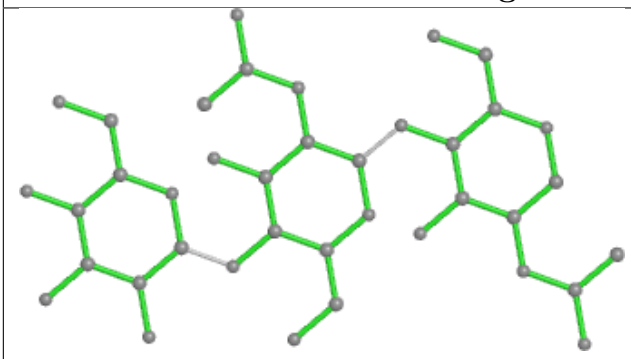


Rings

Oligosaccharide Chain 5



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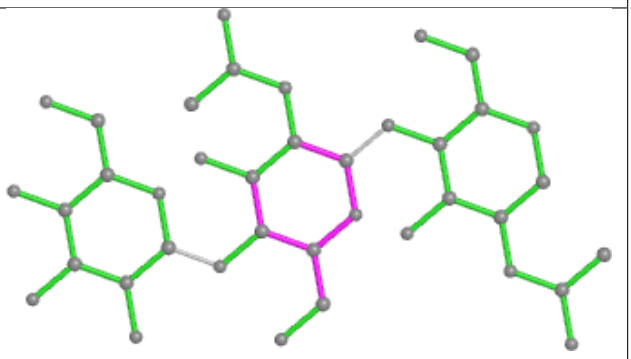
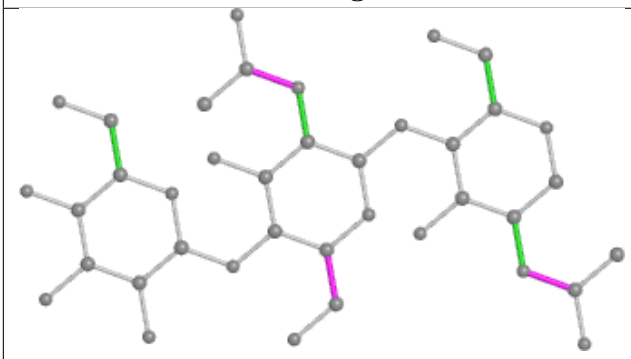


Bond angles



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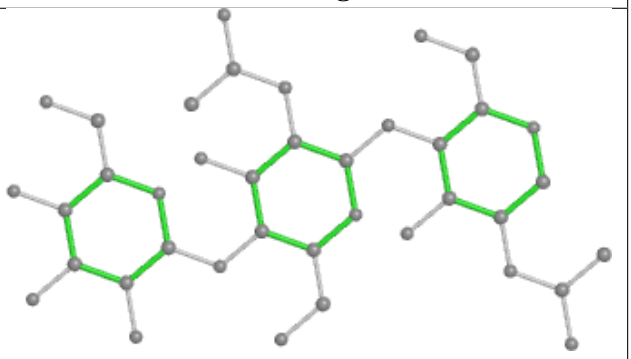
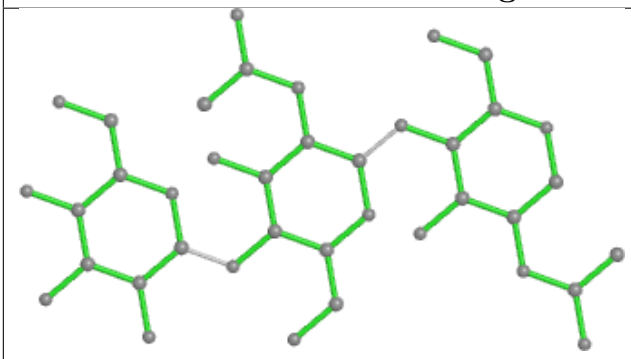
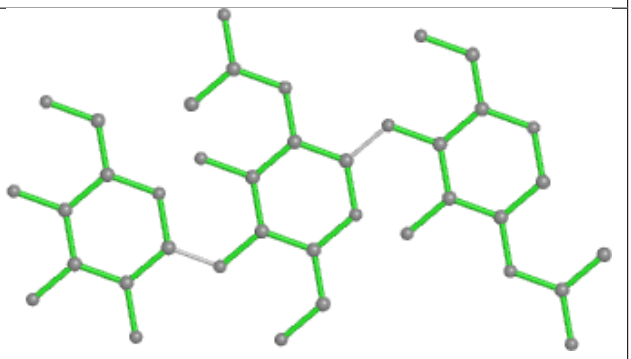


Rings

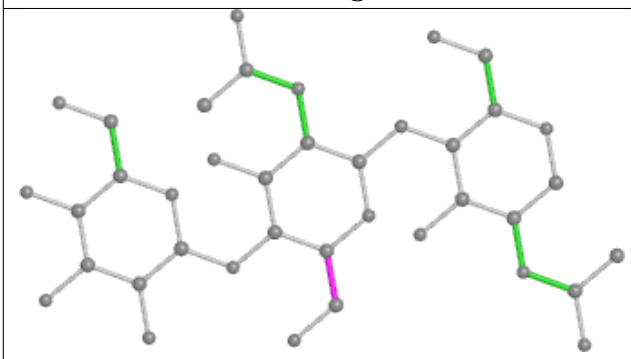
Oligosaccharide Chain 7



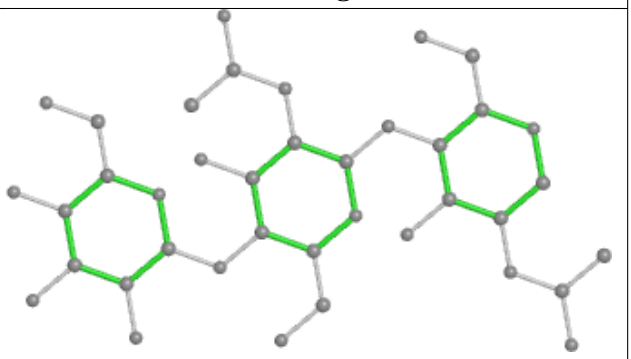
Bond lengths



Bond angles

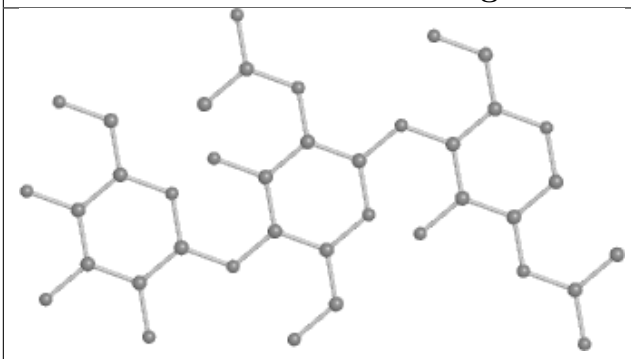


Torsions

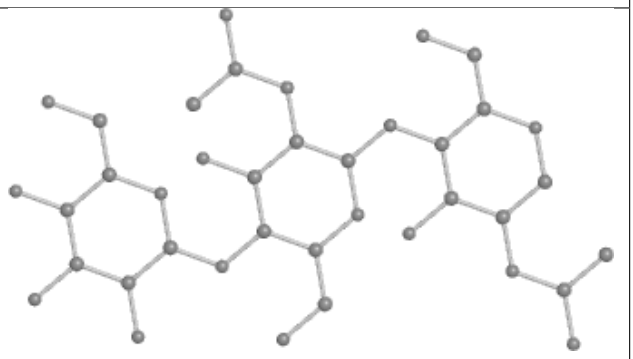


Rings

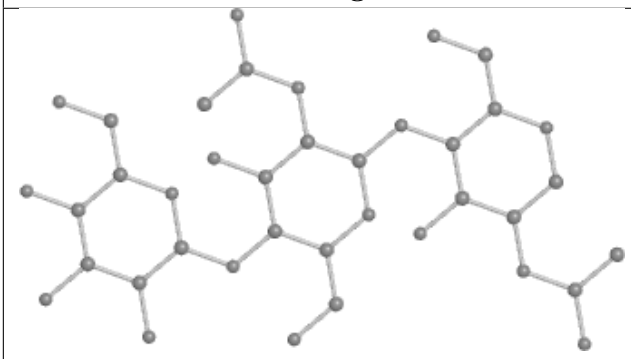
Oligosaccharide Chain AA



Bond lengths



Bond angles



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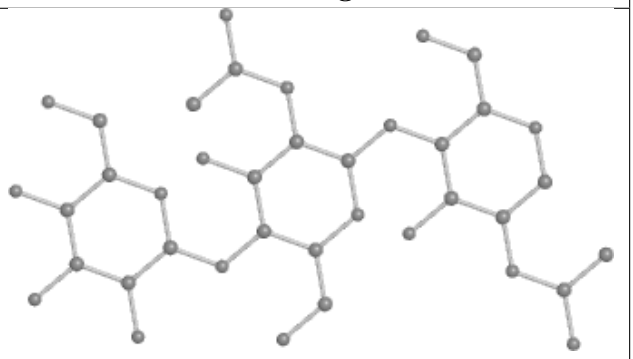
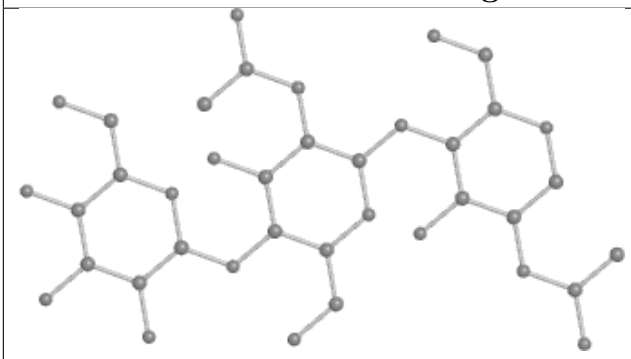


Rings

Oligosaccharide Chain BA



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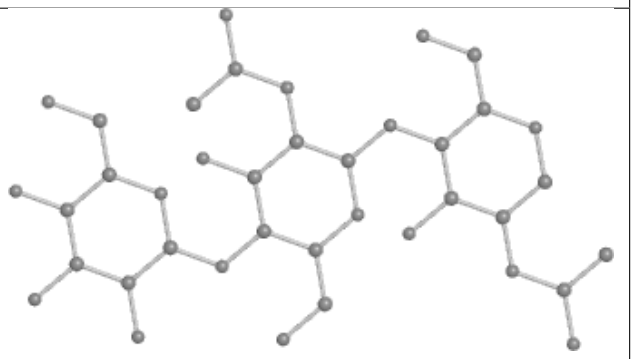
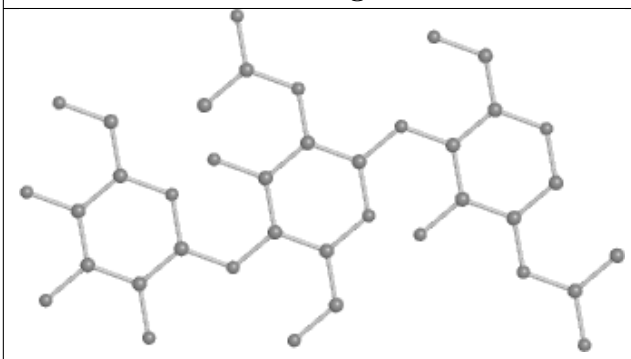


Bond angles



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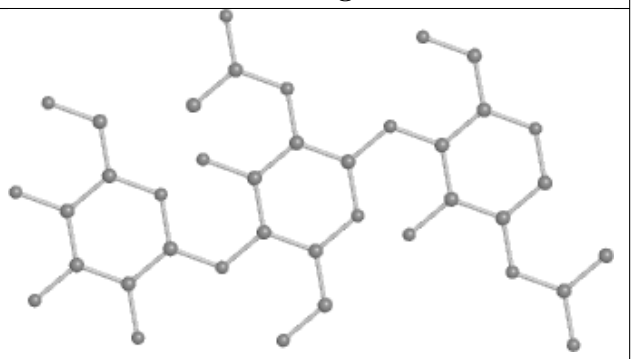
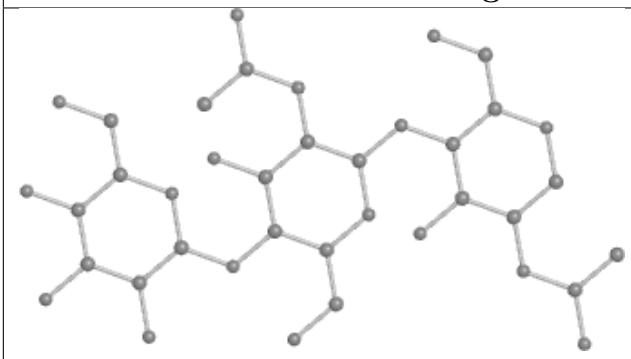


Rings

Oligosaccharide Chain EA



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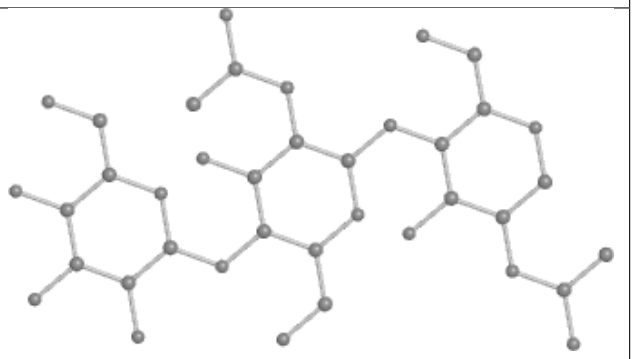
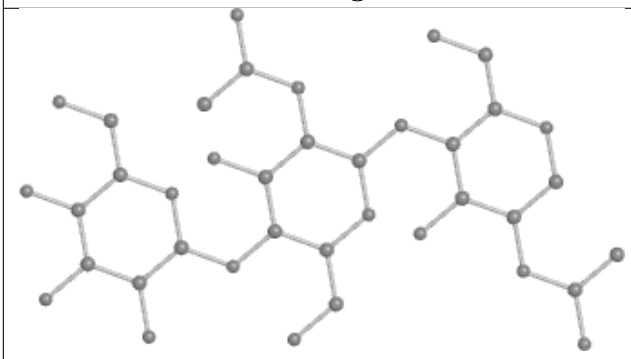


Bond angles



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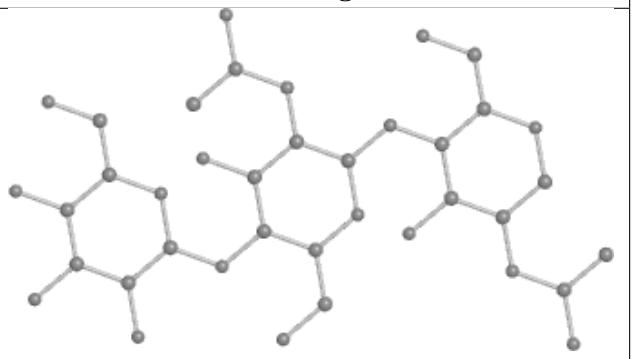
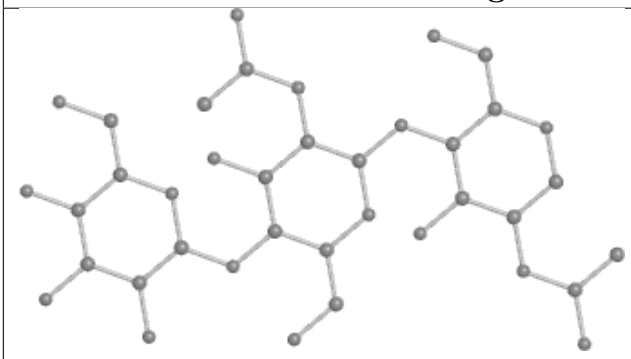
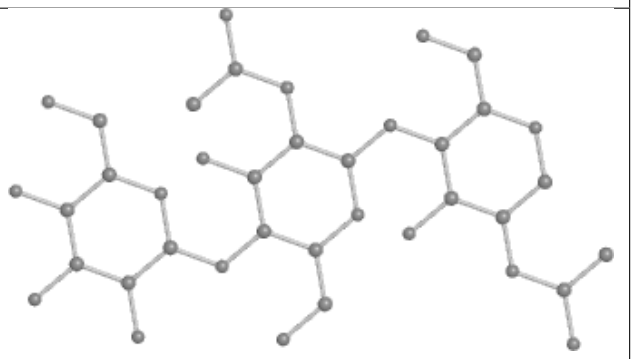


Rings

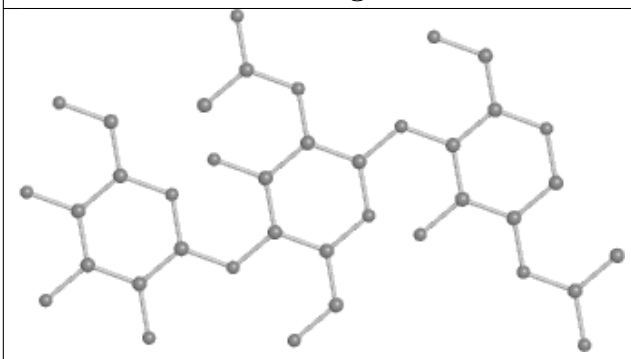
Oligosaccharide Chain IA



Bond lengths



Bond angles



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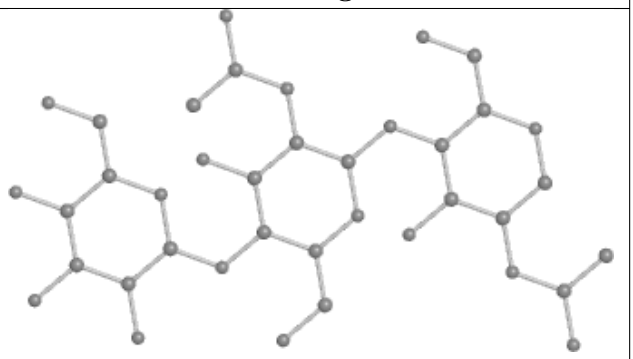
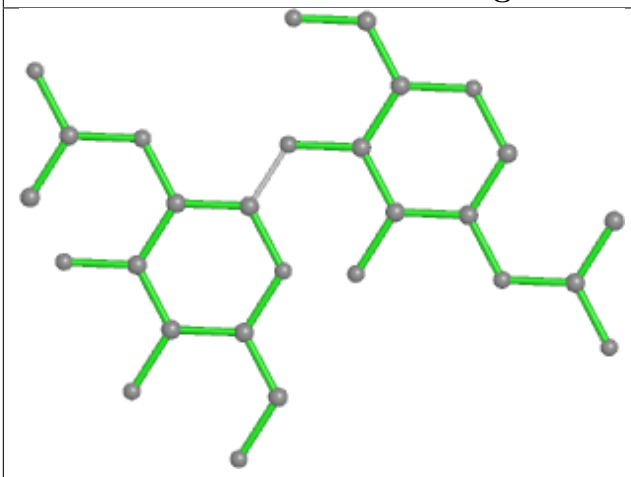


Rings

Oligosaccharide Chain H



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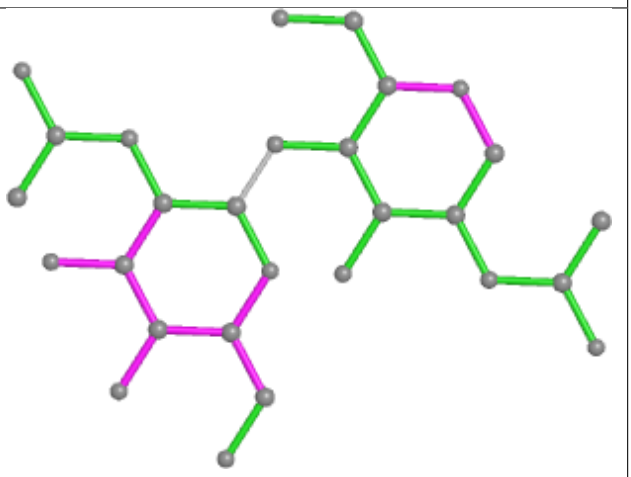
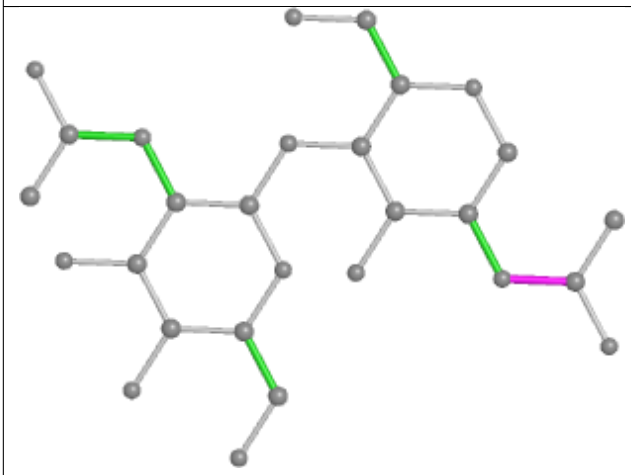


Bond angles



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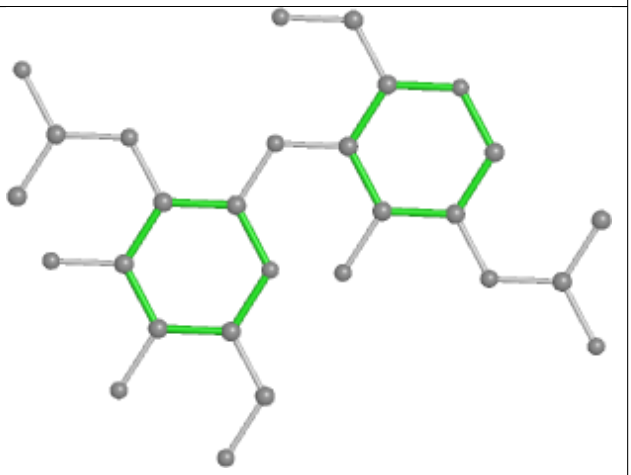
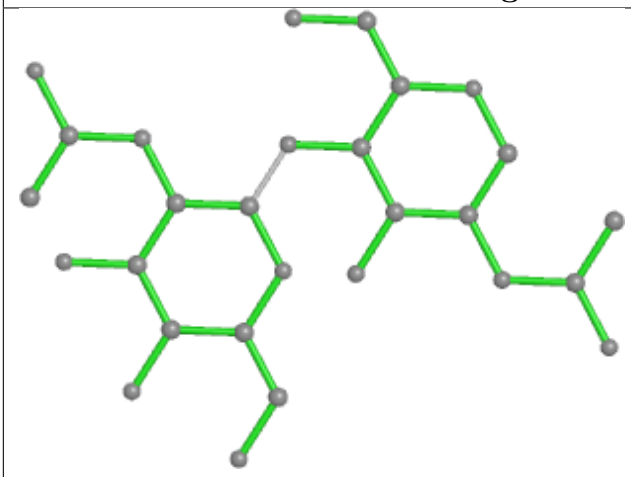


Rings

Oligosaccharide Chain I



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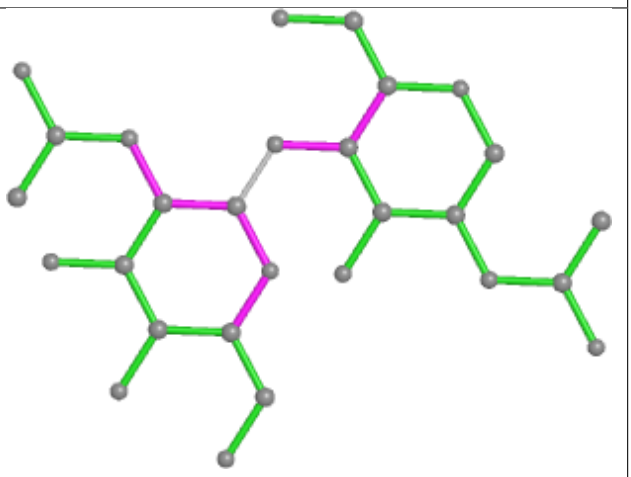
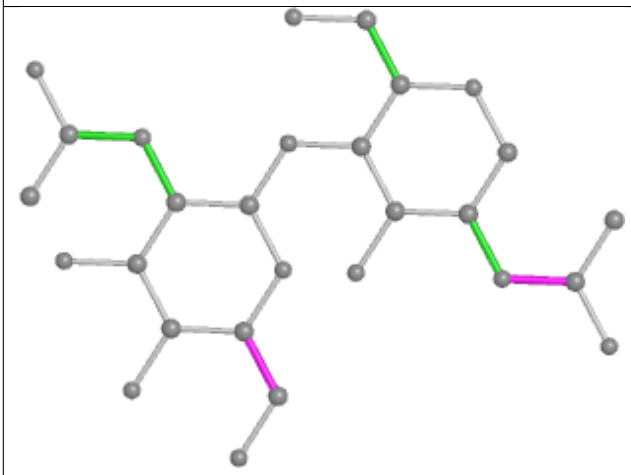


Bond angles



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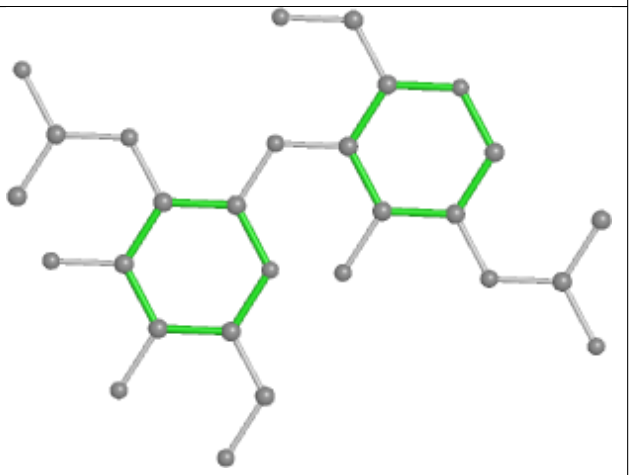
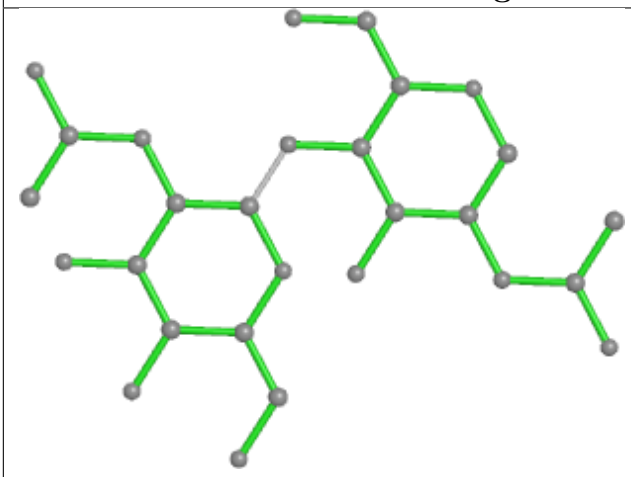


Rings

Oligosaccharide Chain N



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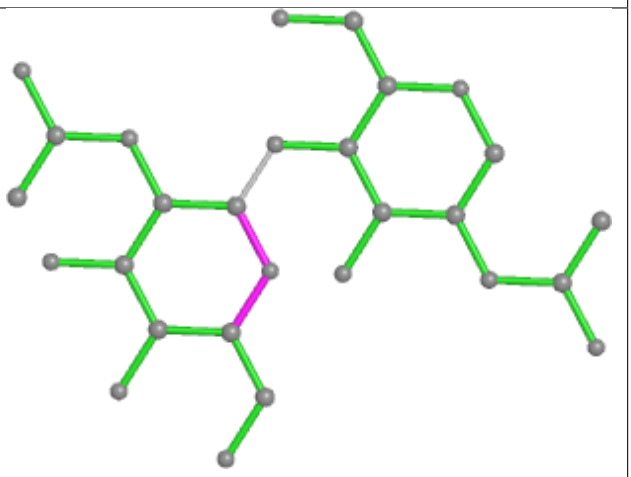
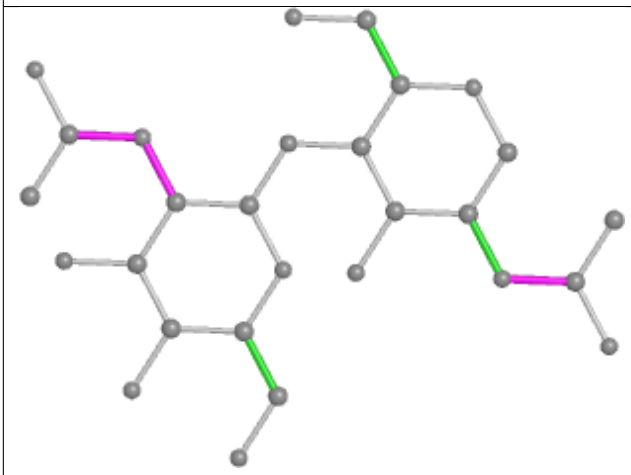


Bond angles



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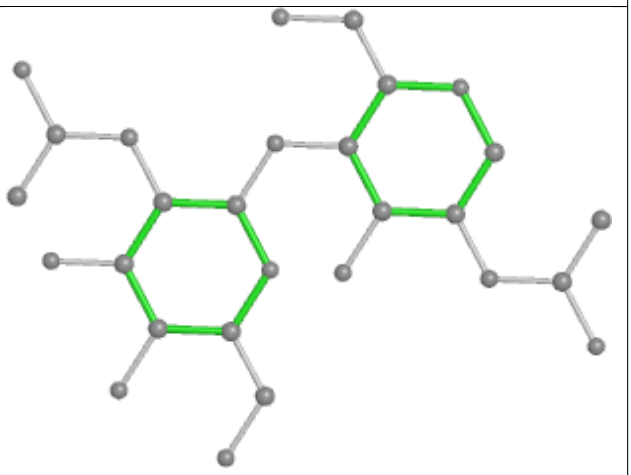
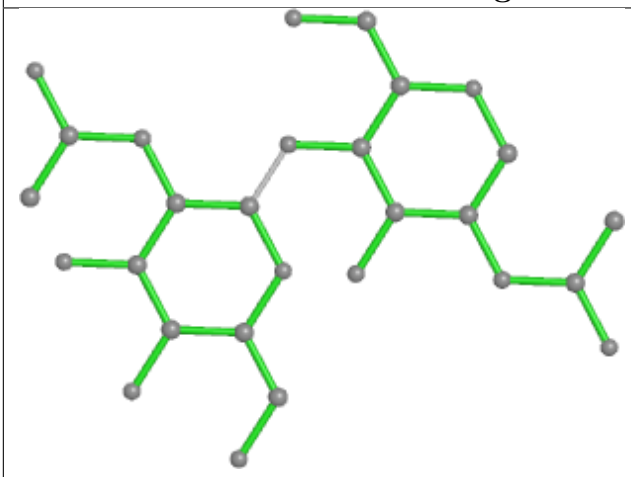
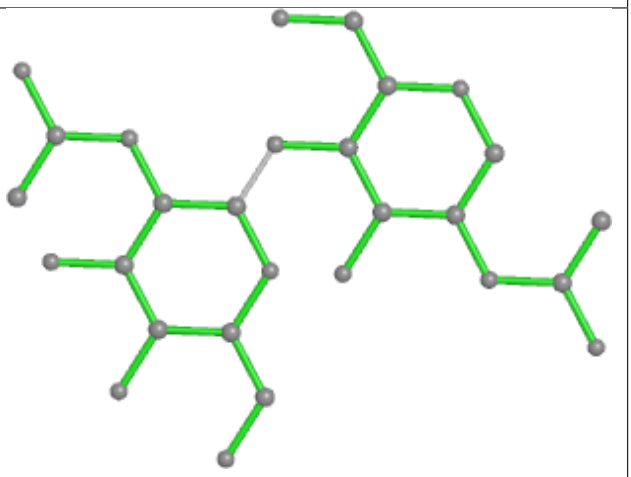


Rings

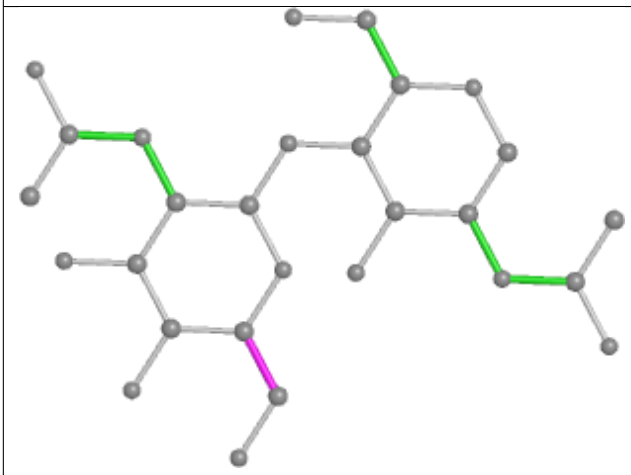
Oligosaccharide Chain U



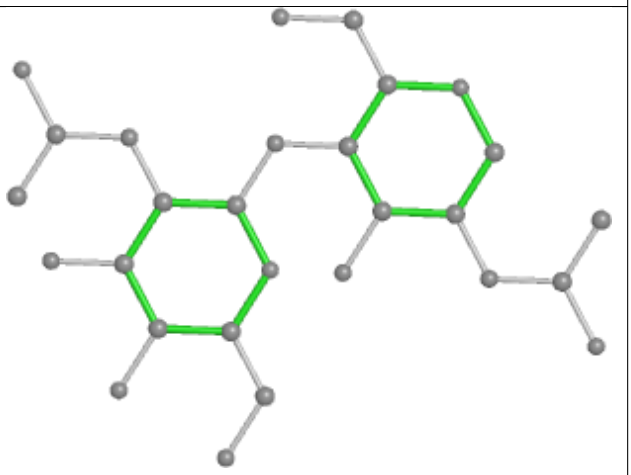
Bond lengths



Bond angles



Torsions



Rings

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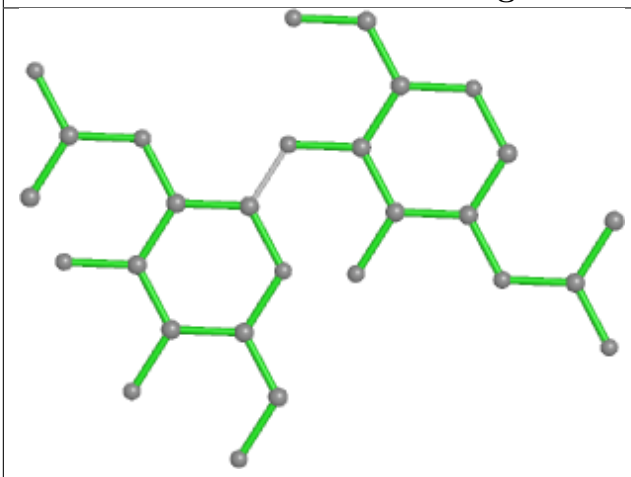

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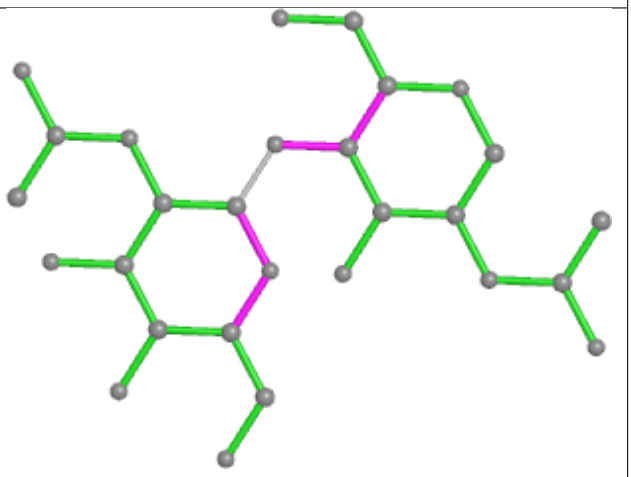
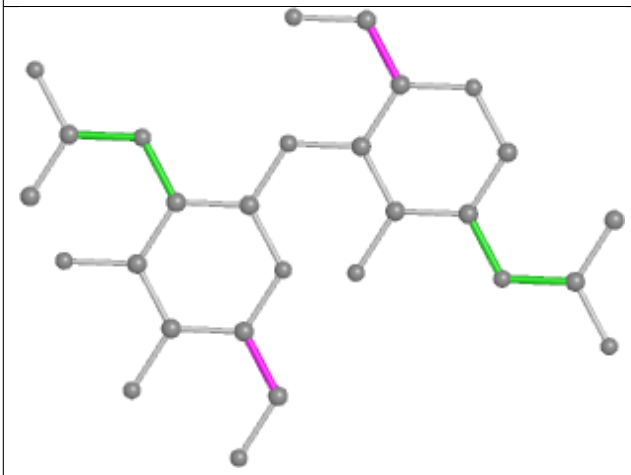


Bond angles



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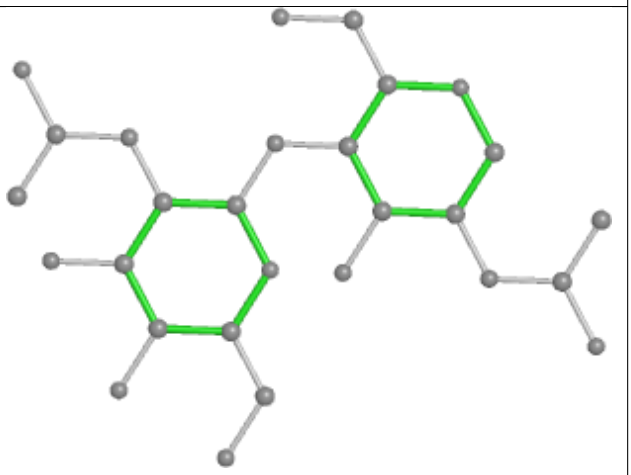
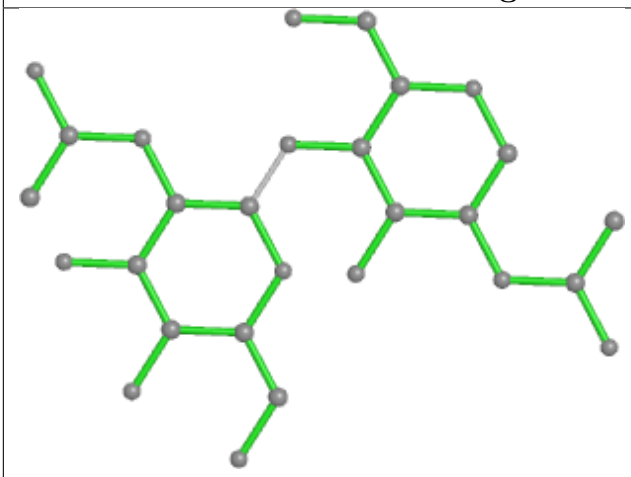


Rings

Oligosaccharide Chain e



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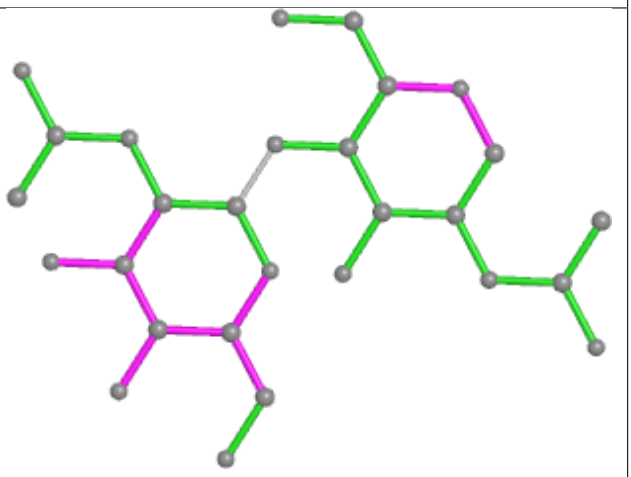
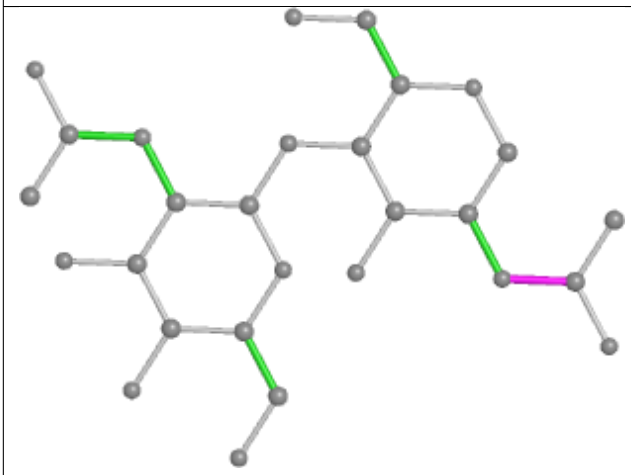


Bond angles



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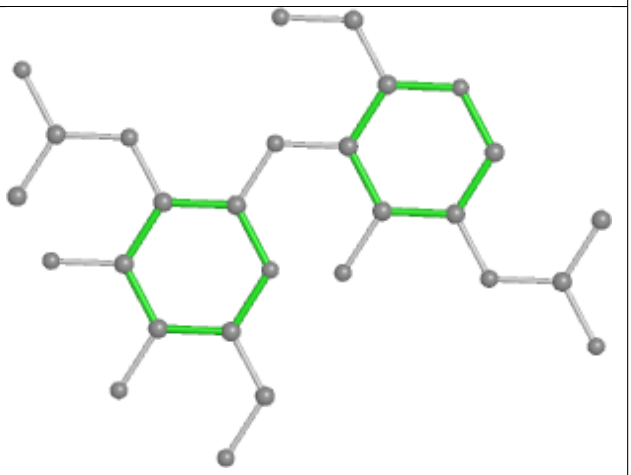
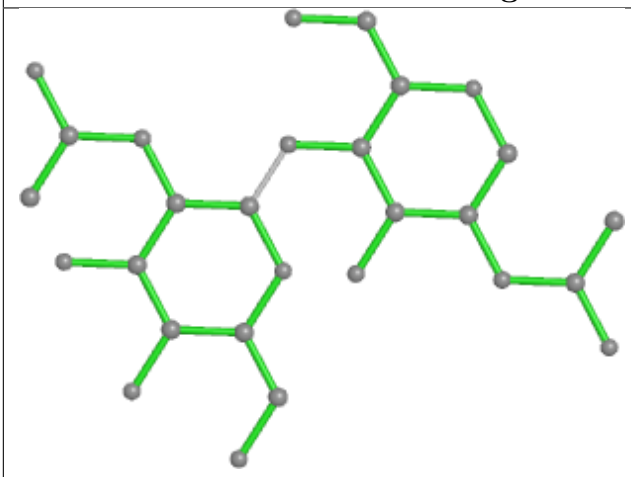


Rings

Oligosaccharide Chain f



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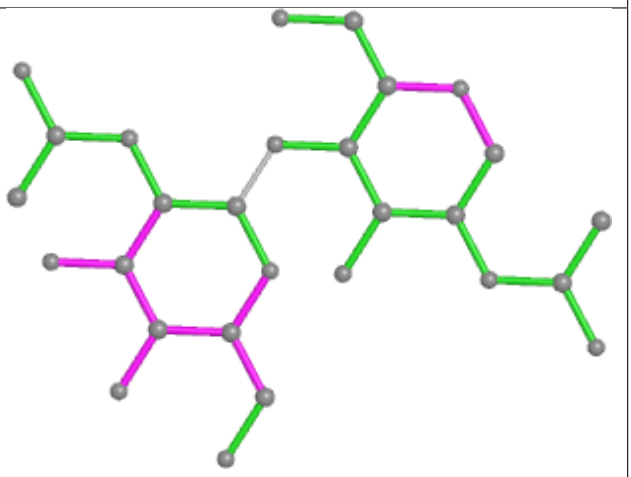
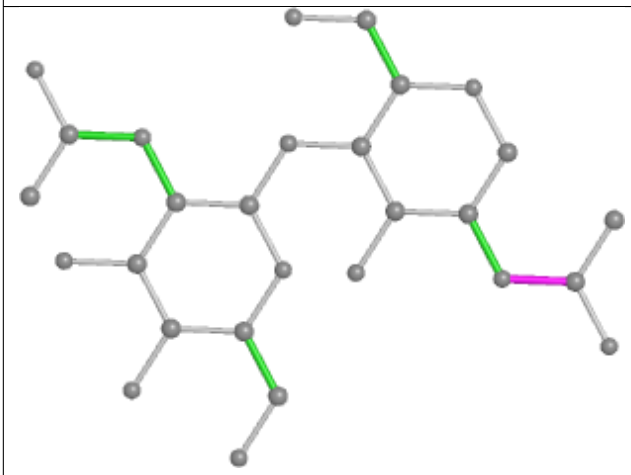


Bond angles



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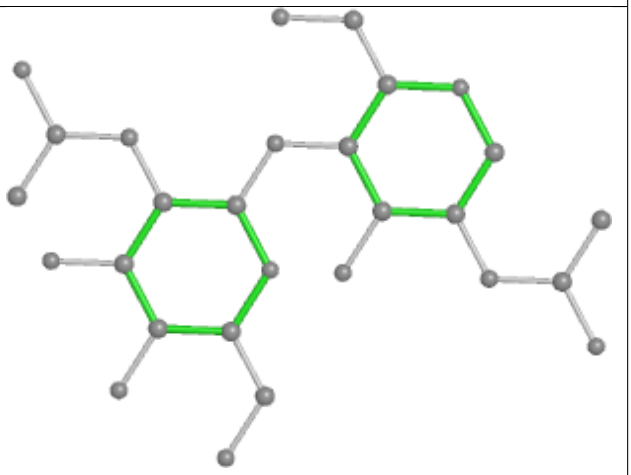
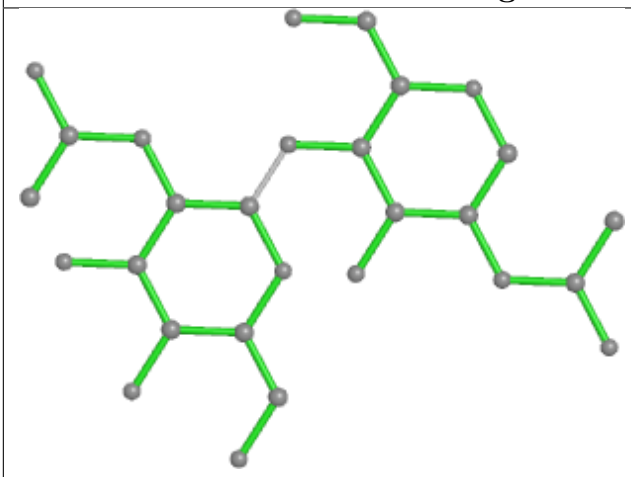
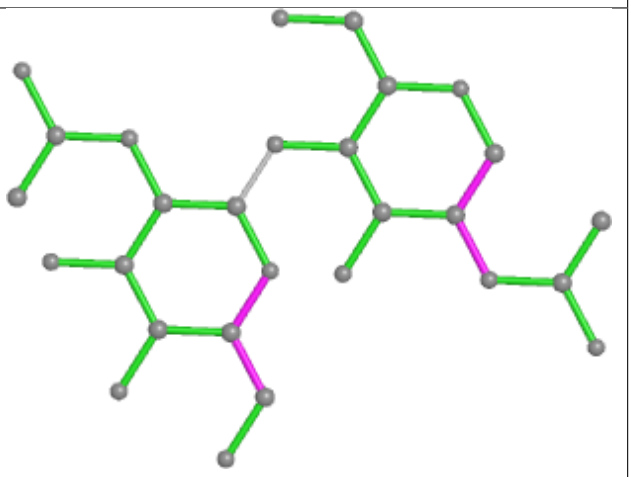


Rings

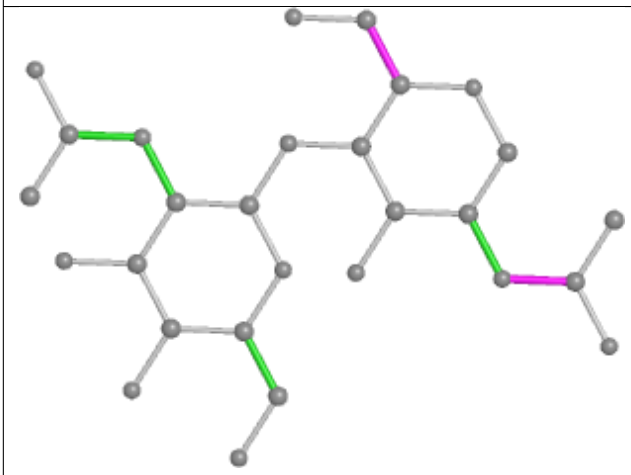
Oligosaccharide Chain k



Bond lengths



Bond angles



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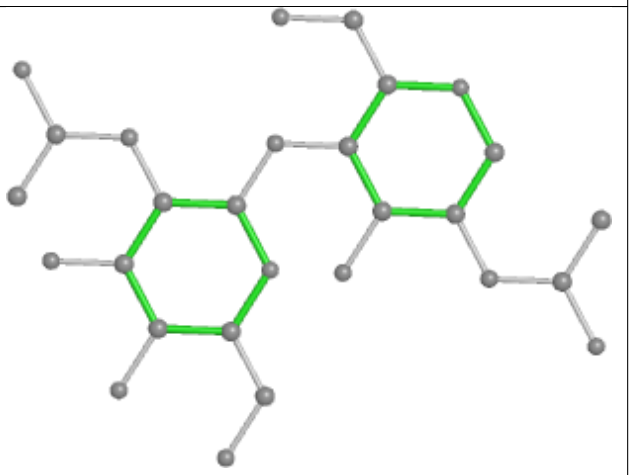
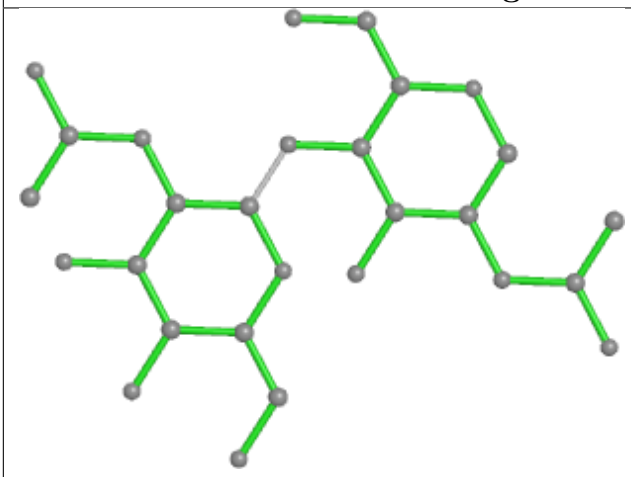
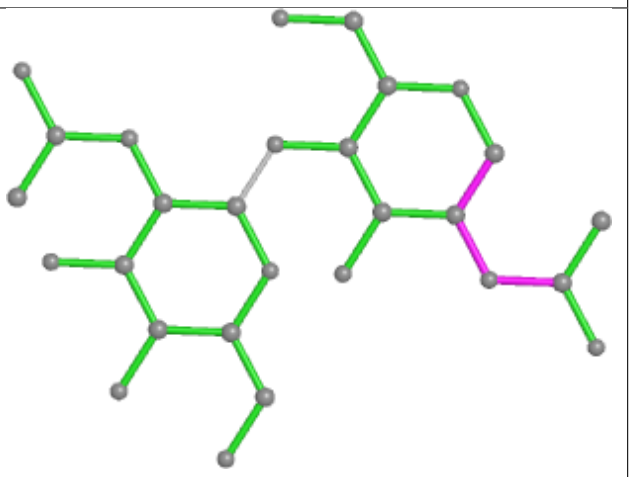


Rings

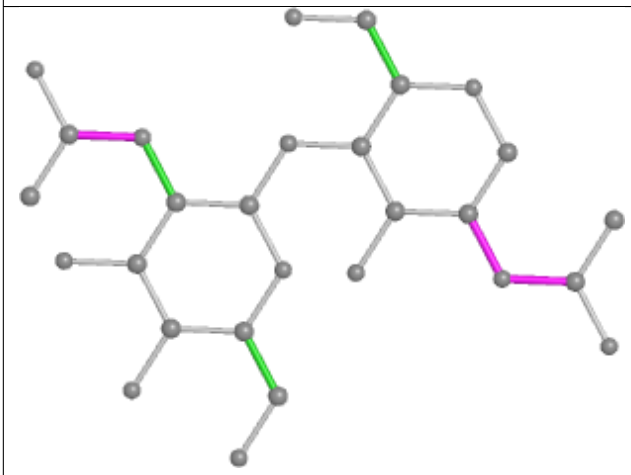
Oligosaccharide Chain l



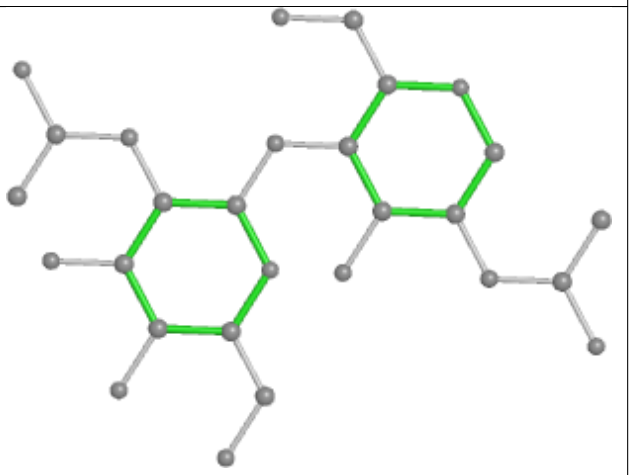
Bond lengths



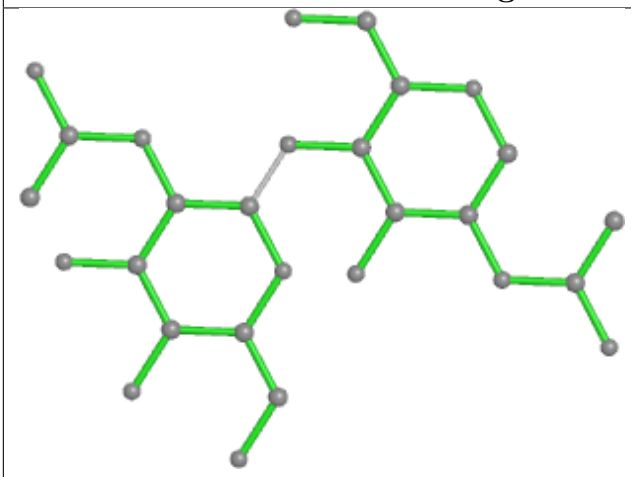
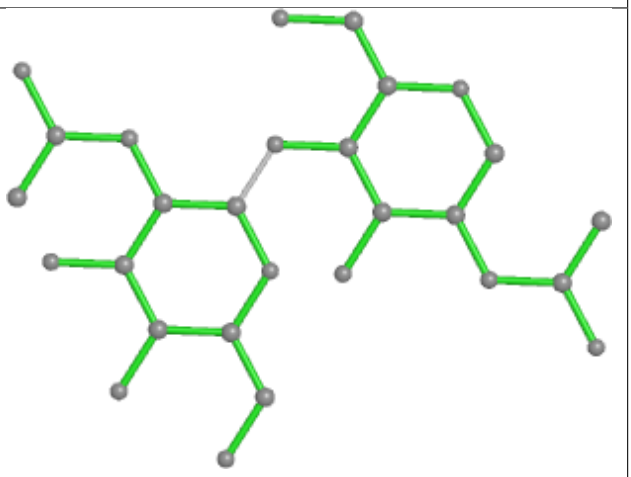
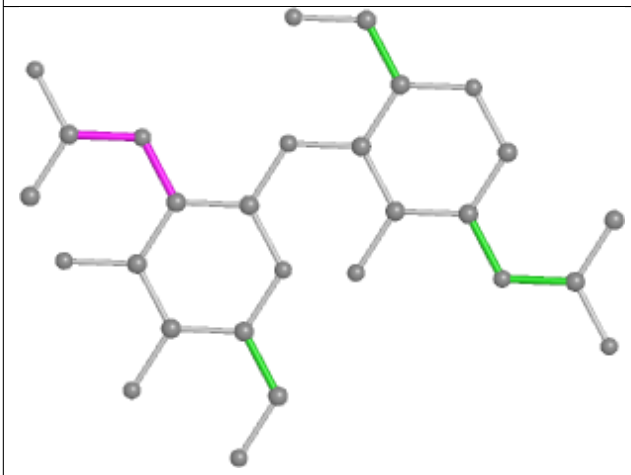
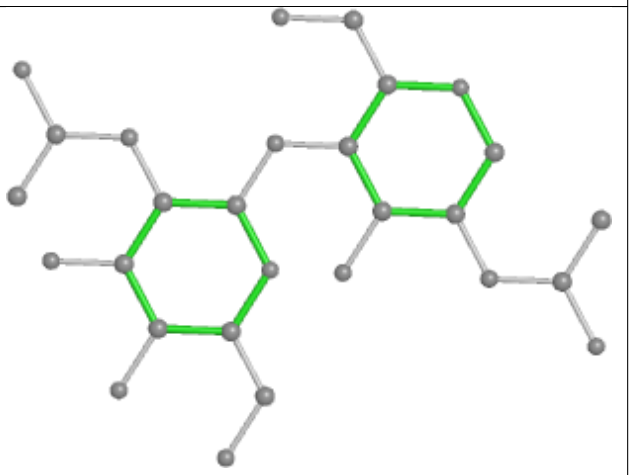
Bond angles



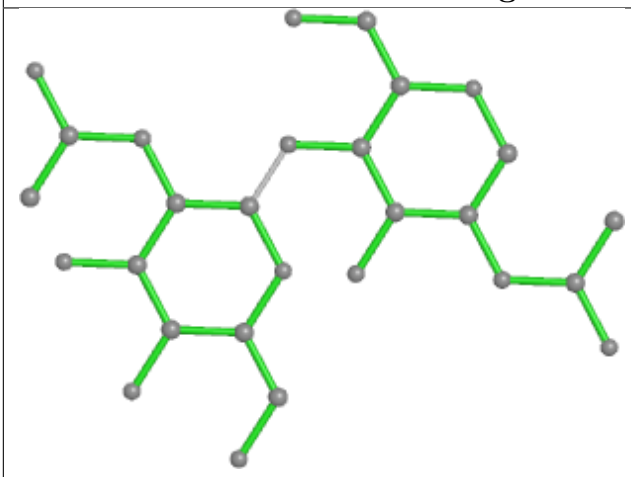
Torsions



Rings

Oligosaccharide Chain n	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 4



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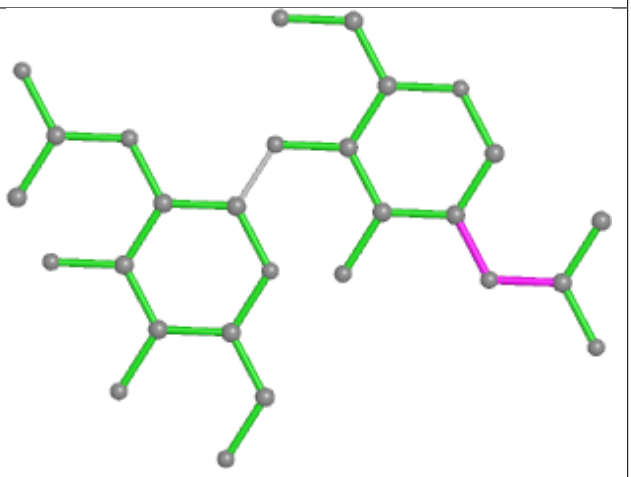
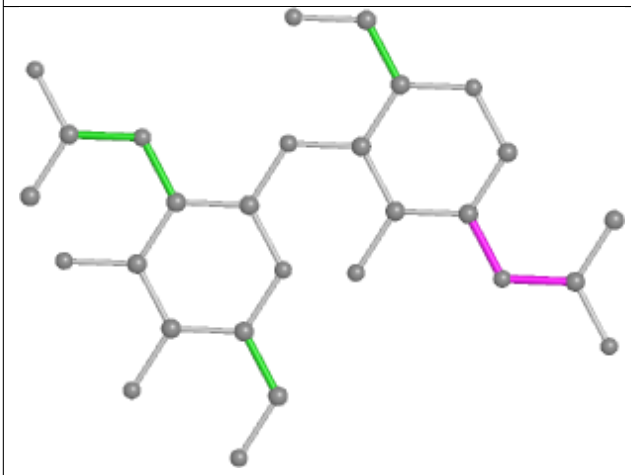
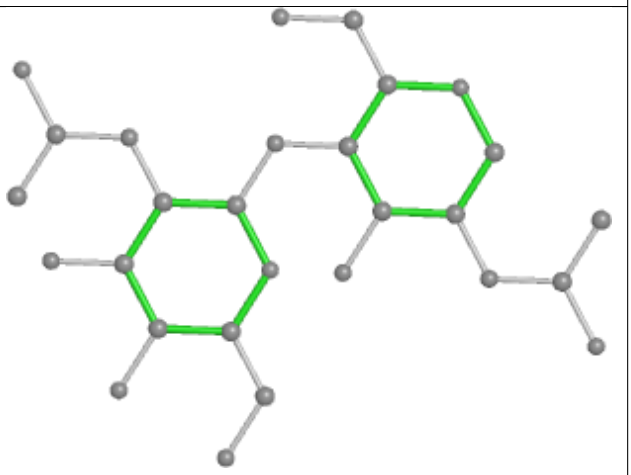


Bond angles

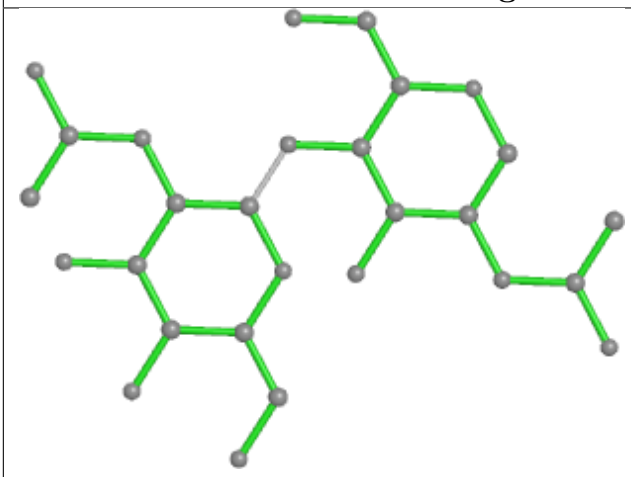


Torsions



Rings

Oligosaccharide Chain 6



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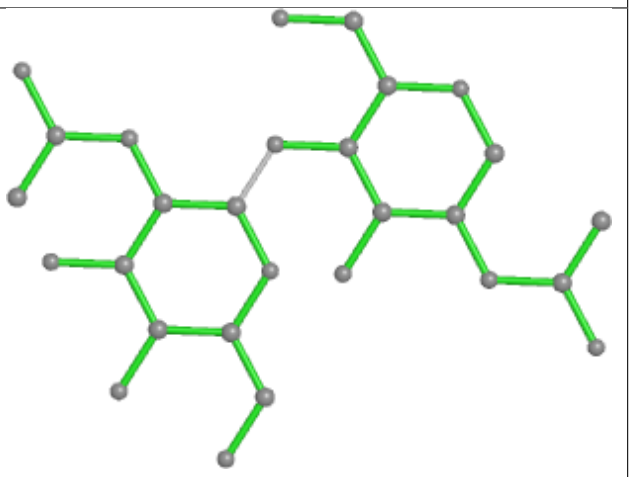
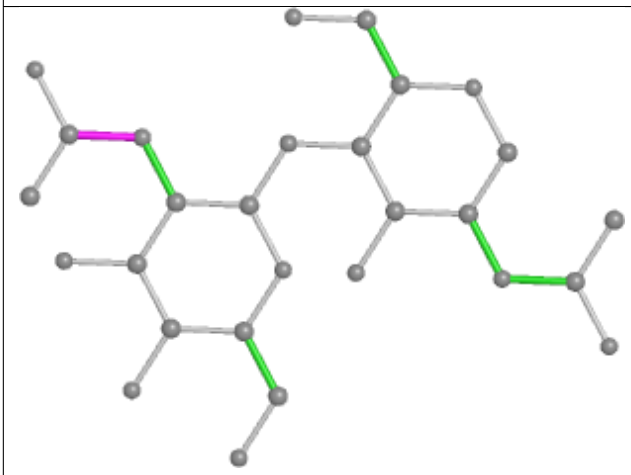


Bond angles



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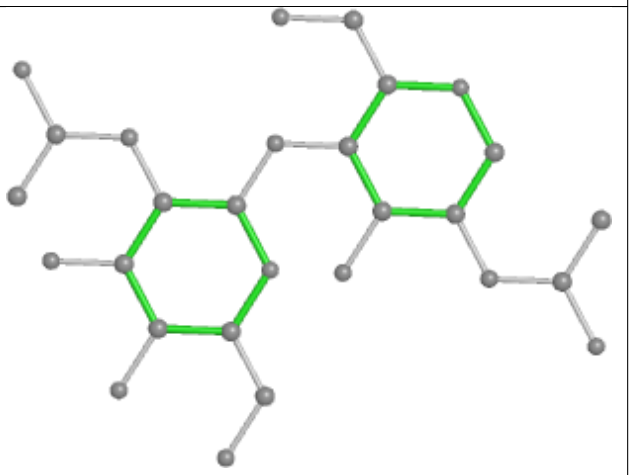
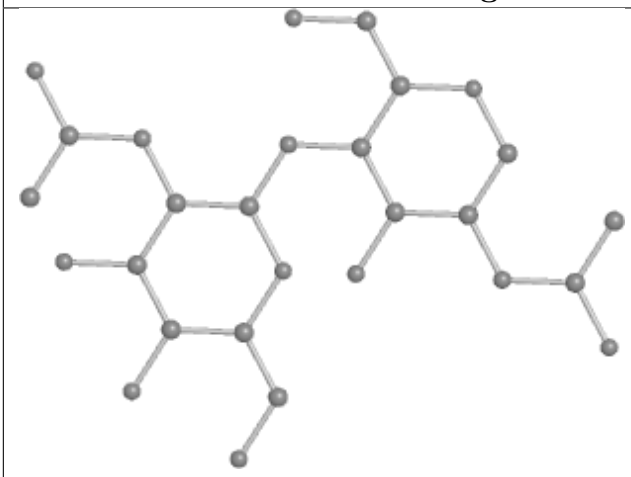


Rings

Oligosaccharide Chain HA



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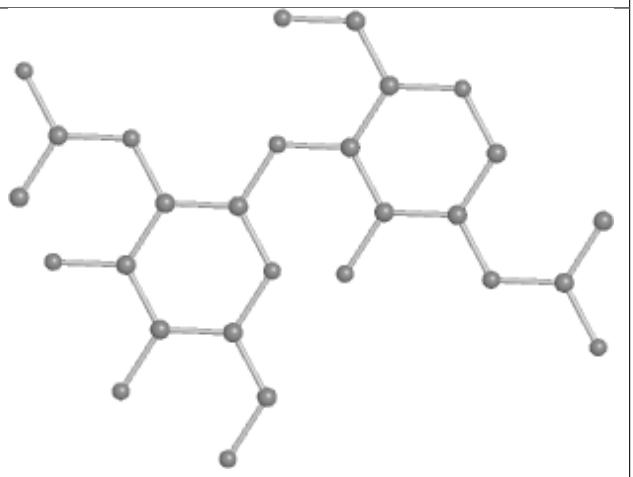
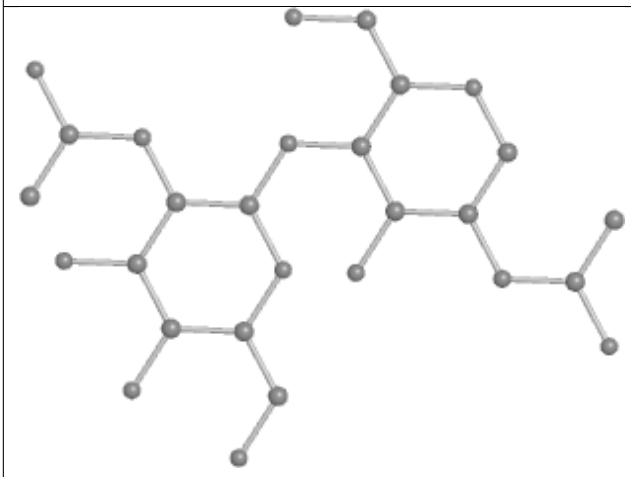


Bond angles



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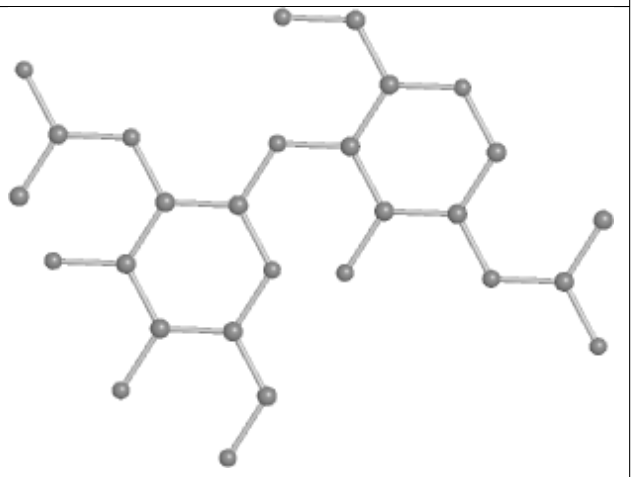
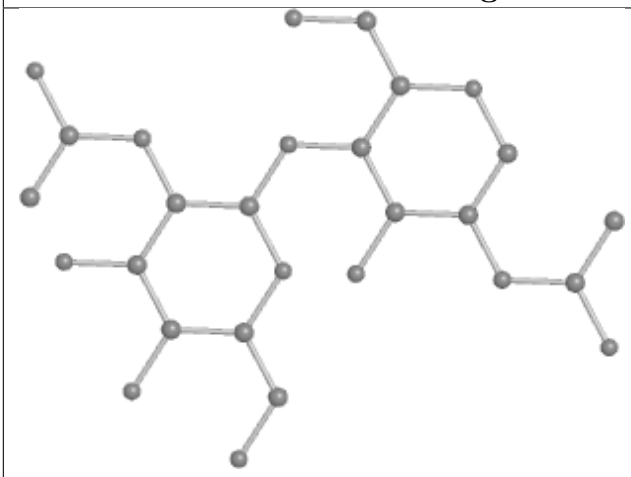


Rings

Oligosaccharide Chain KA



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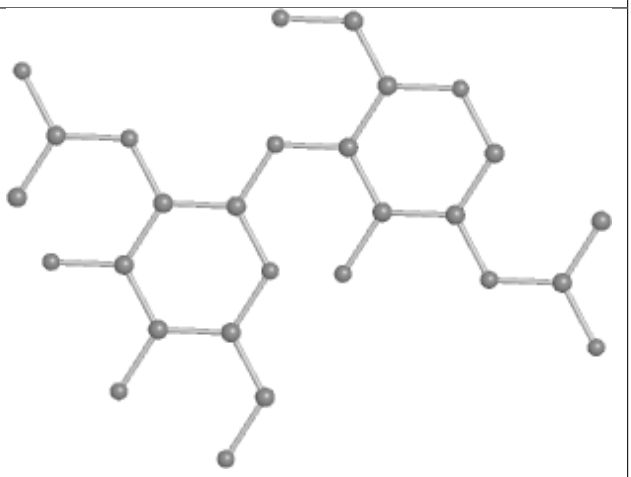
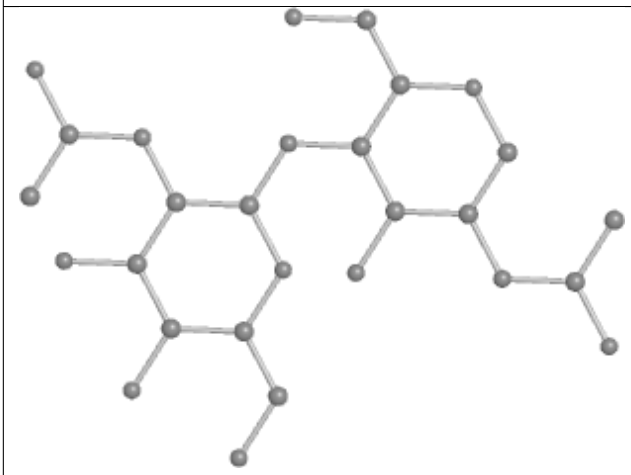


Bond angles



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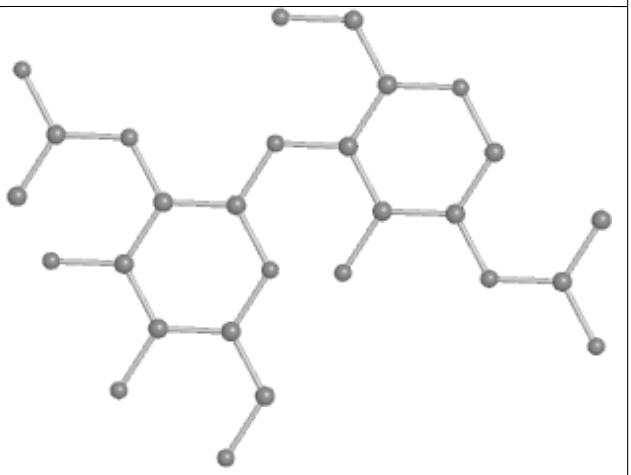
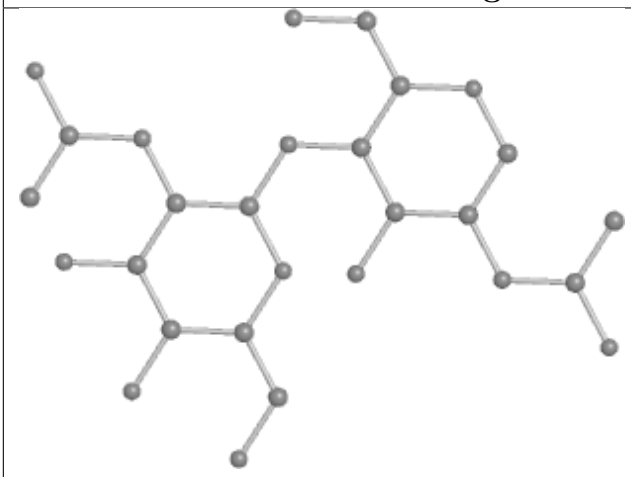


Rings

Oligosaccharide Chain LA



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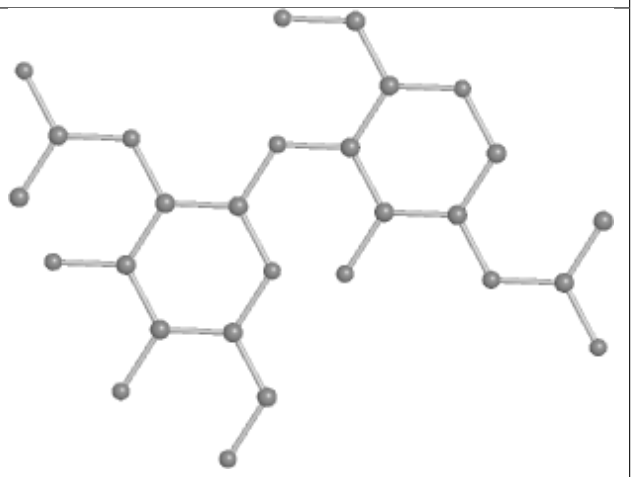

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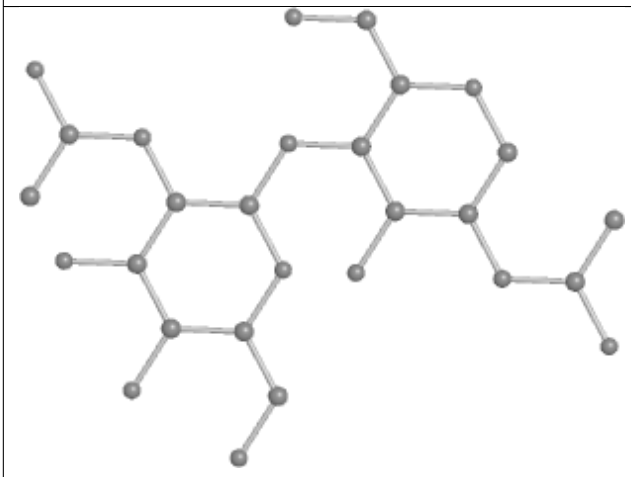

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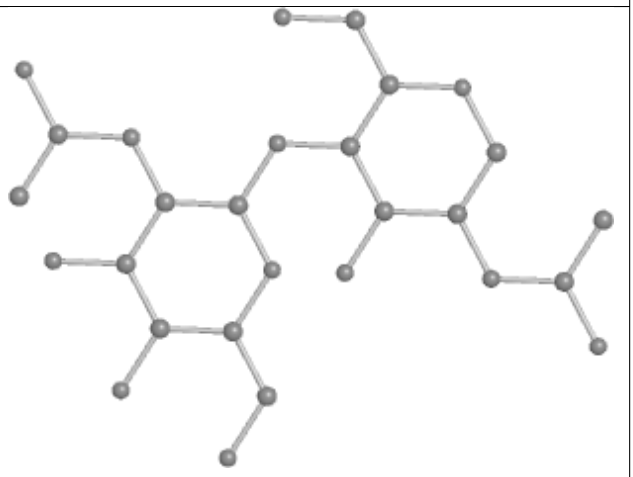
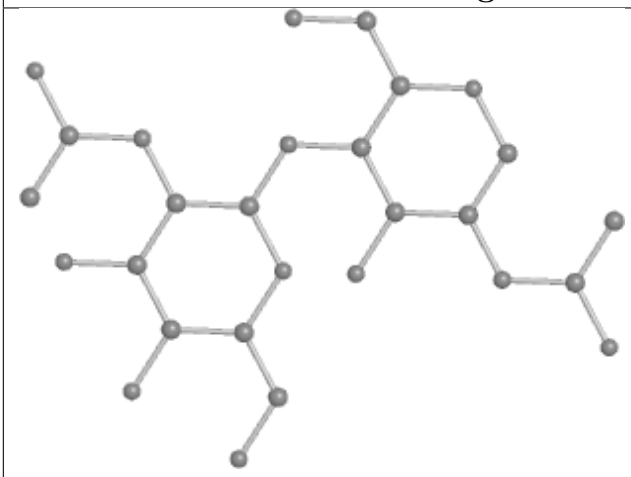


Rings

Oligosaccharide Chain MA



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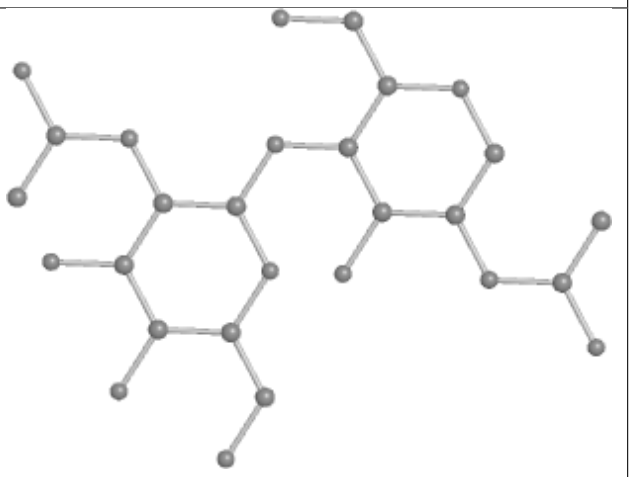
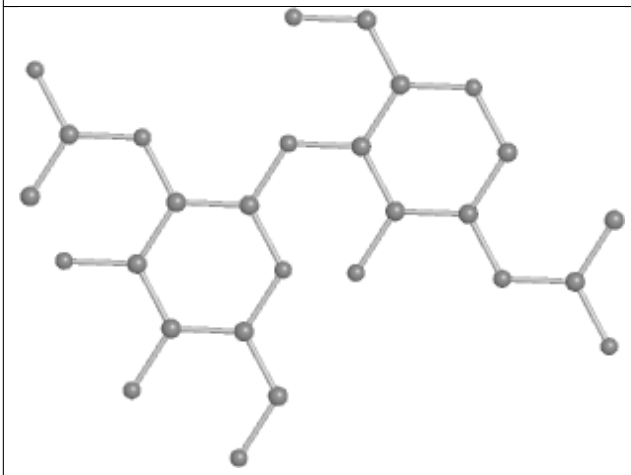


Bond angles



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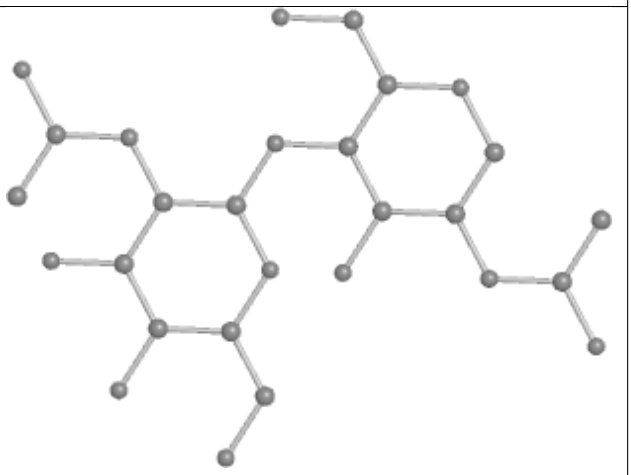
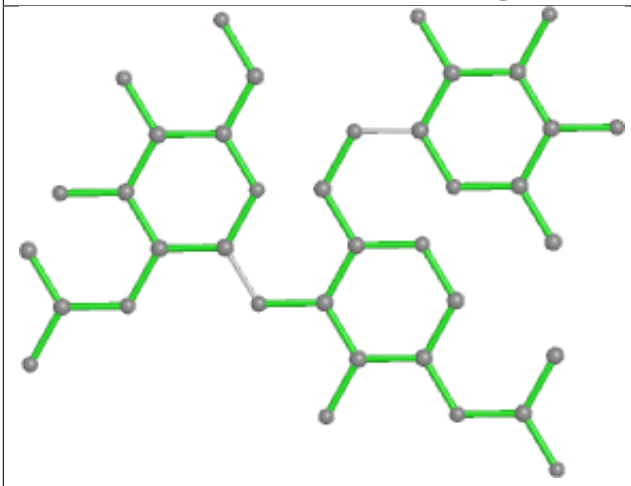


Rings

Oligosaccharide Chain O



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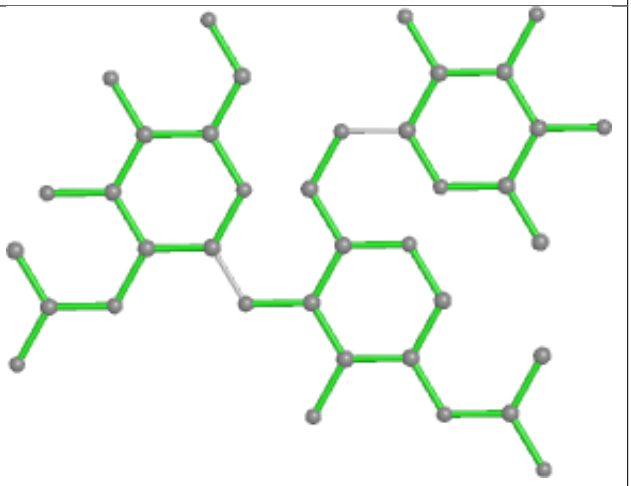
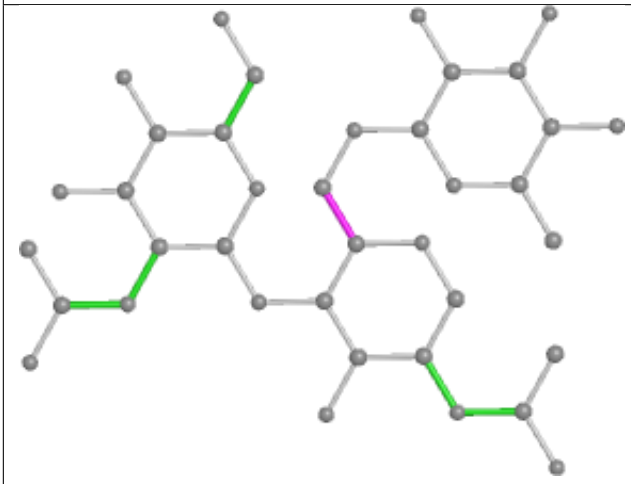


Bond angles



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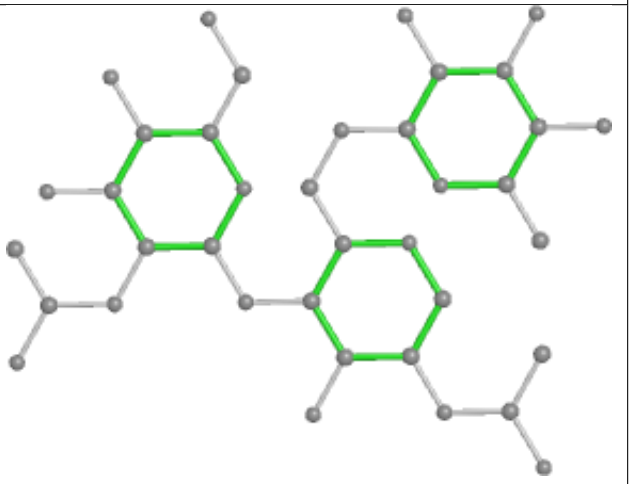
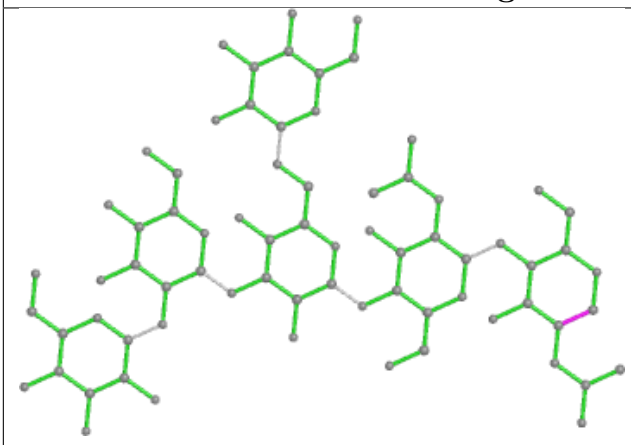
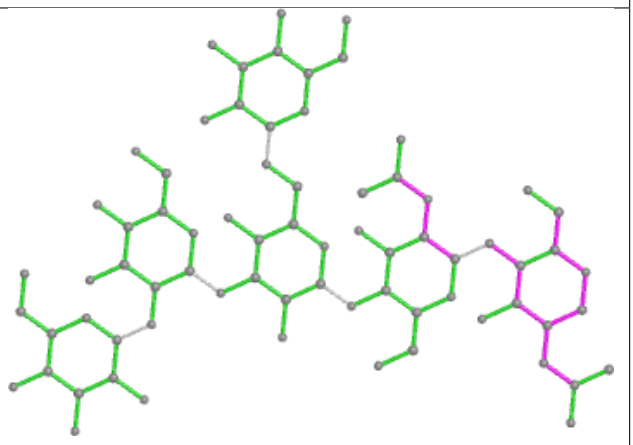


Rings

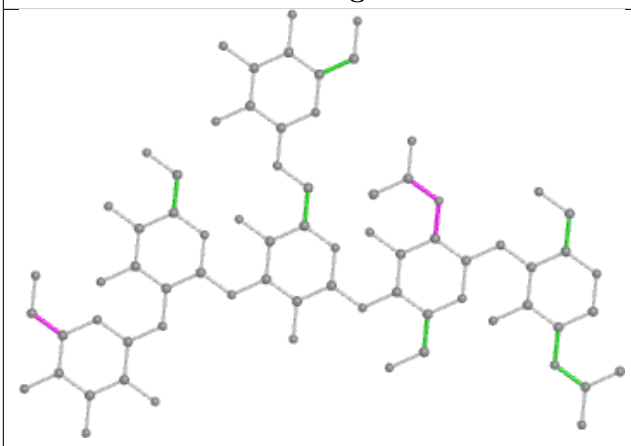
Oligosaccharide Chain S



Bond lengths



Bond angles



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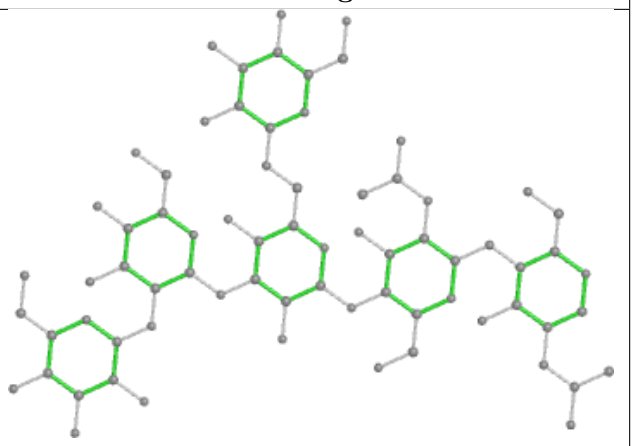
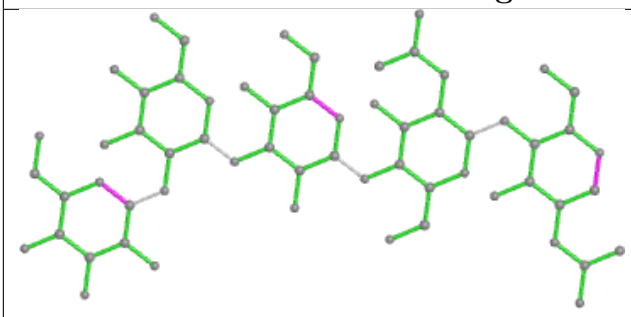
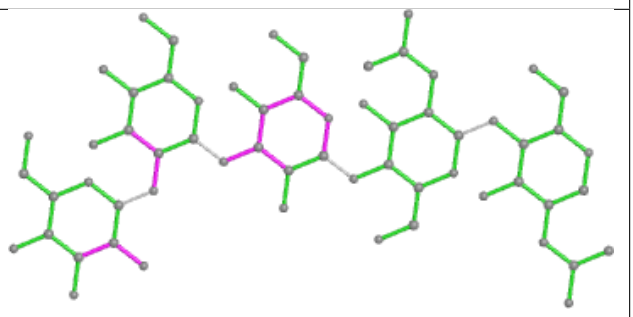


Rings

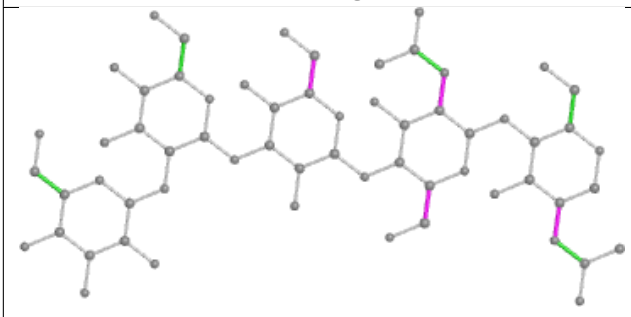
Oligosaccharide Chain T



Bond lengths



Bond angles



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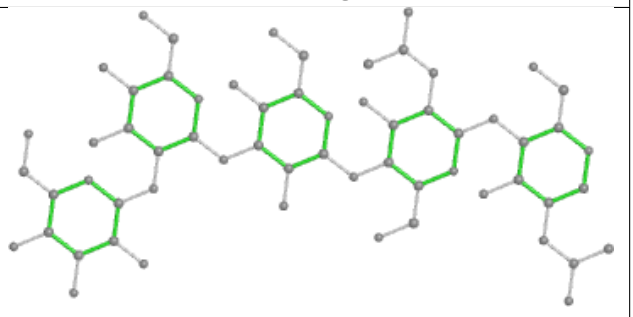
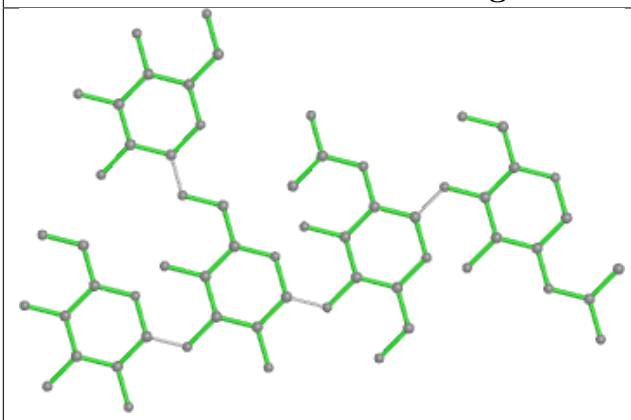


Rings

Oligosaccharide Chain W



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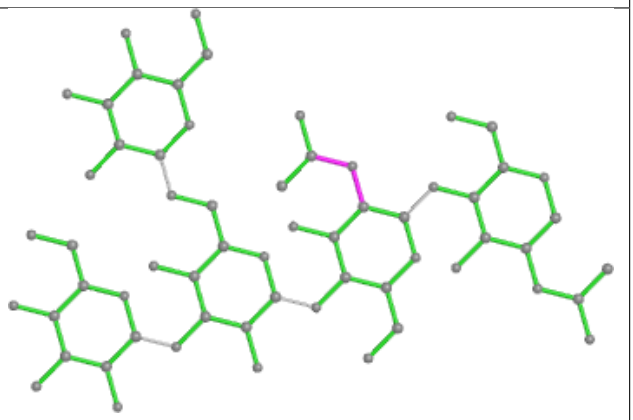
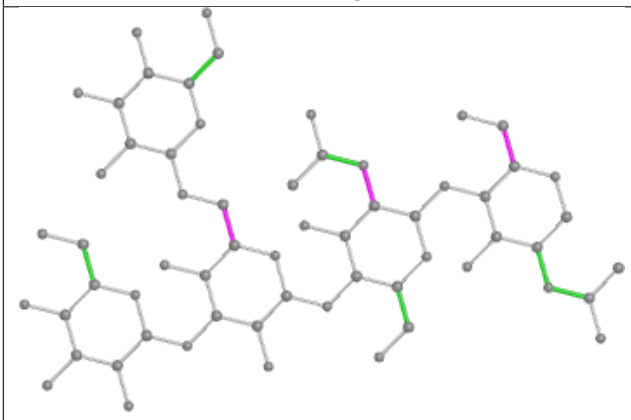


Bond angles



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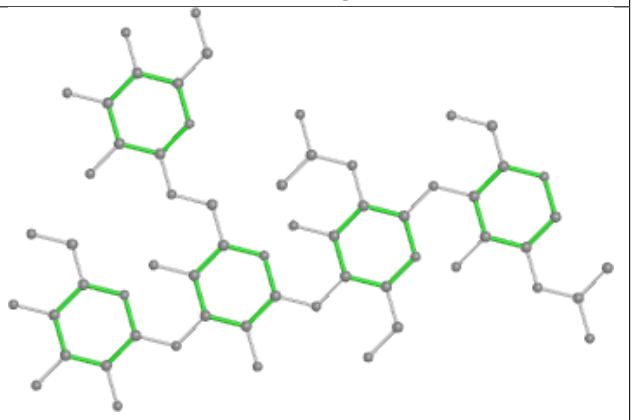
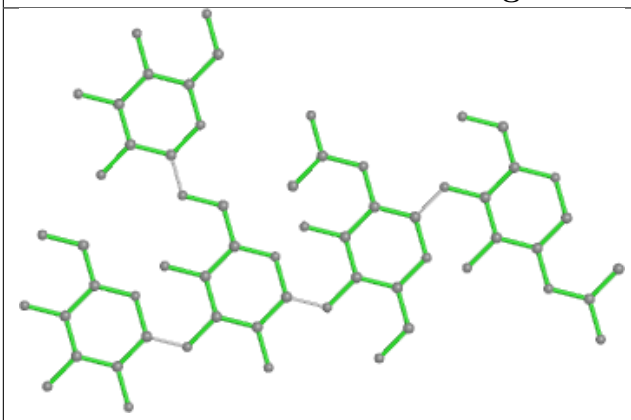


Rings

Oligosaccharide Chain i



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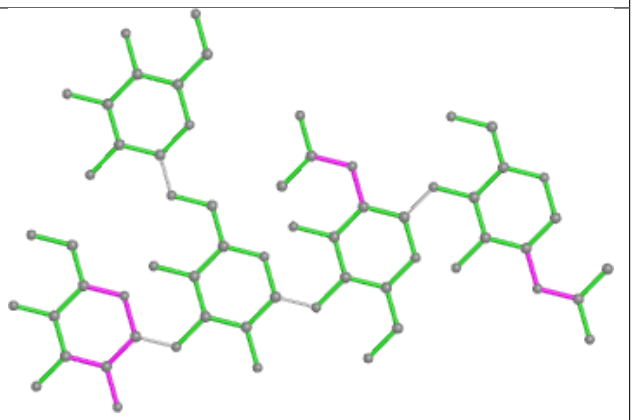
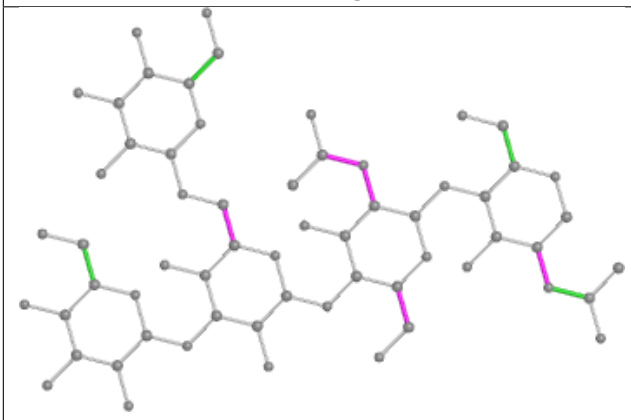


Bond angles



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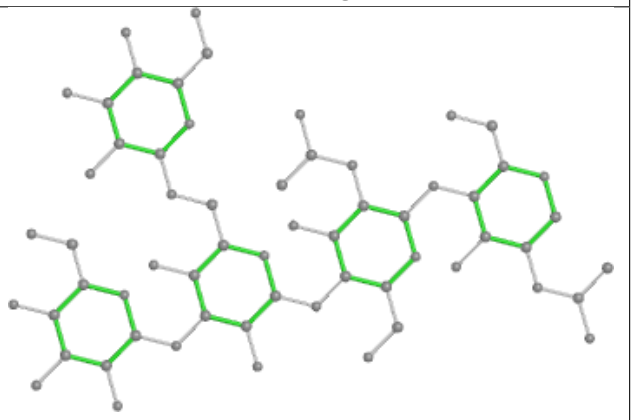
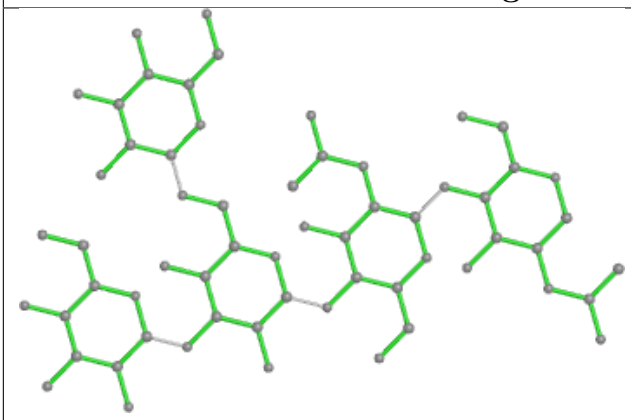


Rings

Oligosaccharide Chain j



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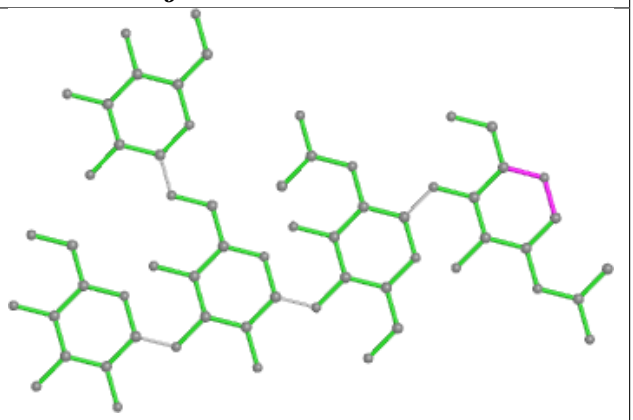
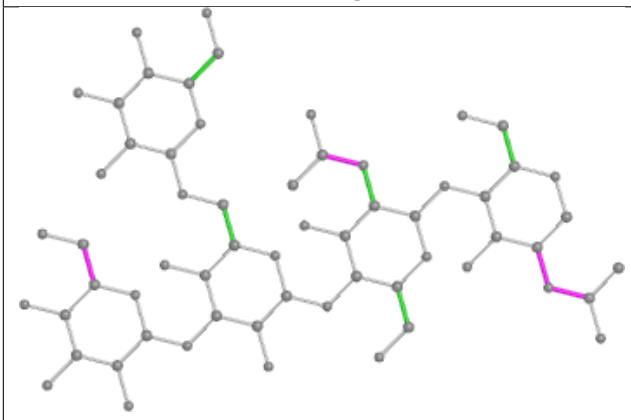


Bond angles



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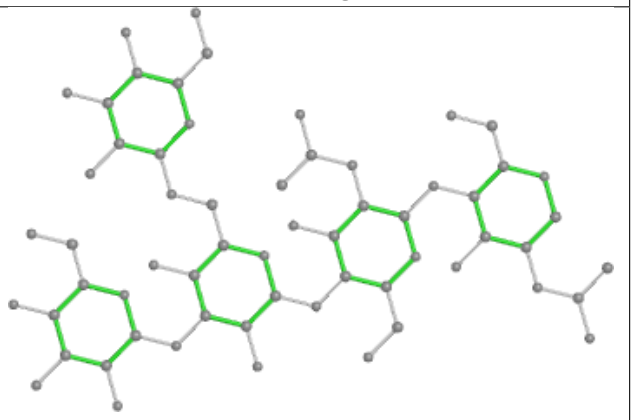
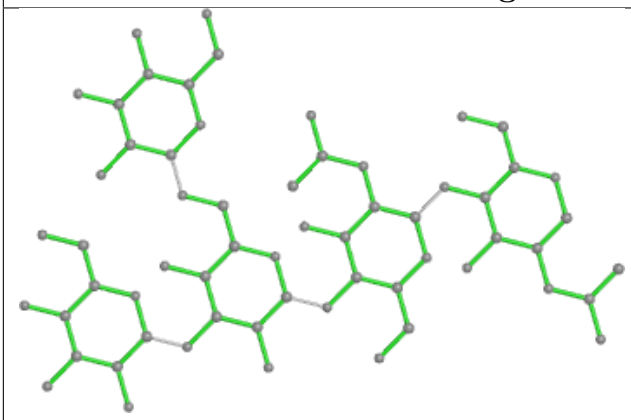
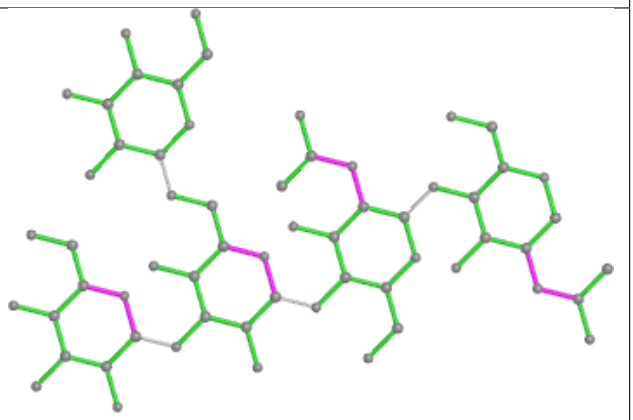


Rings

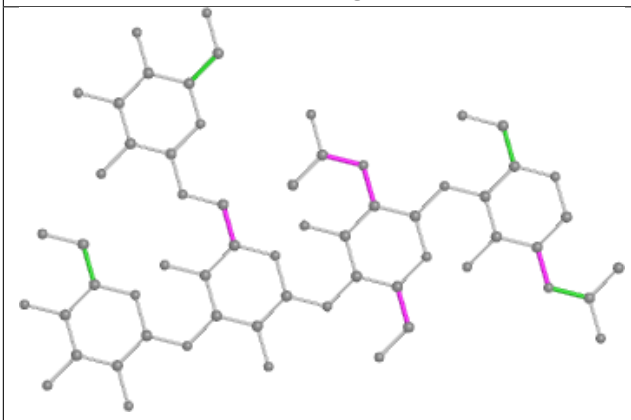
Oligosaccharide Chain 1



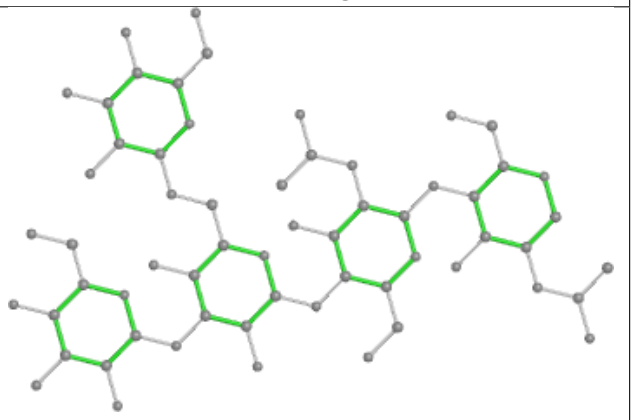
Bond lengths



Bond angles

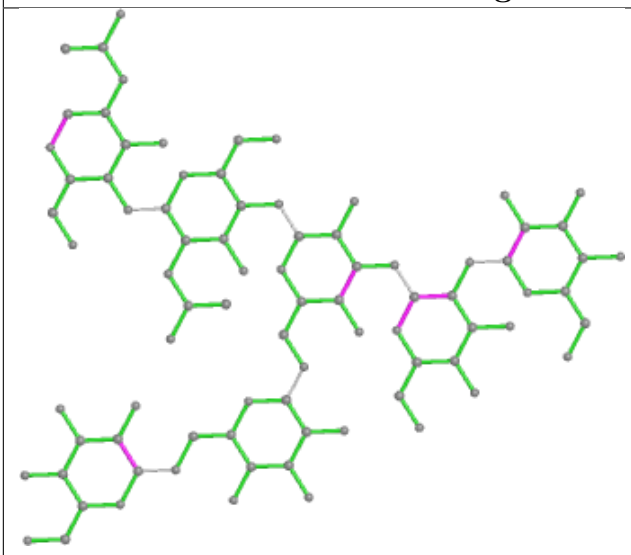


Torsions



Rings

Oligosaccharide Chain X



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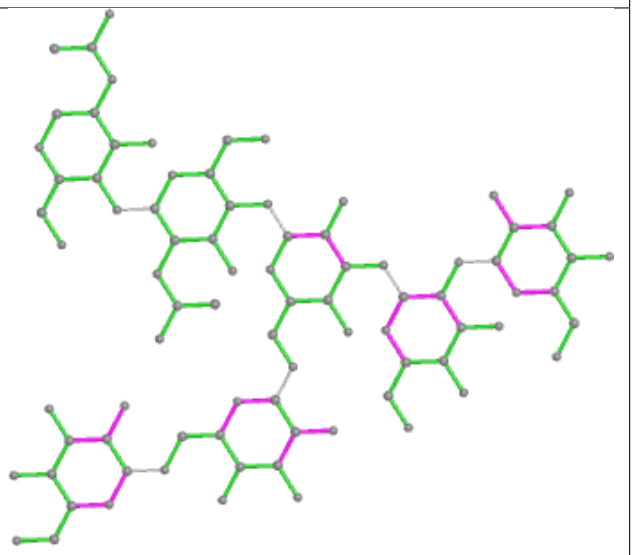
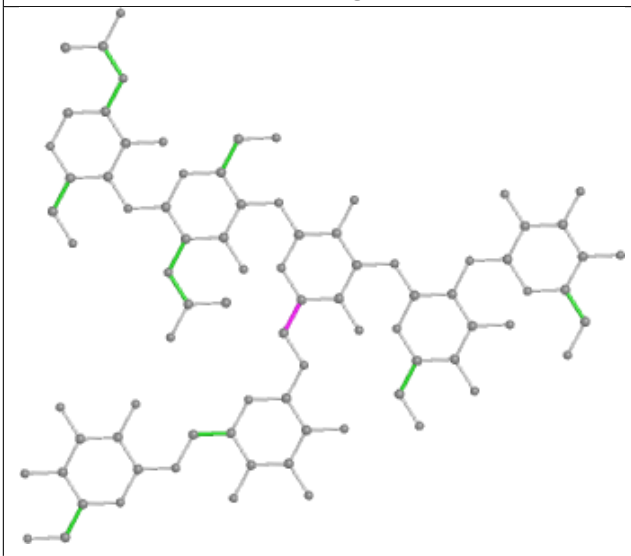


Bond angles



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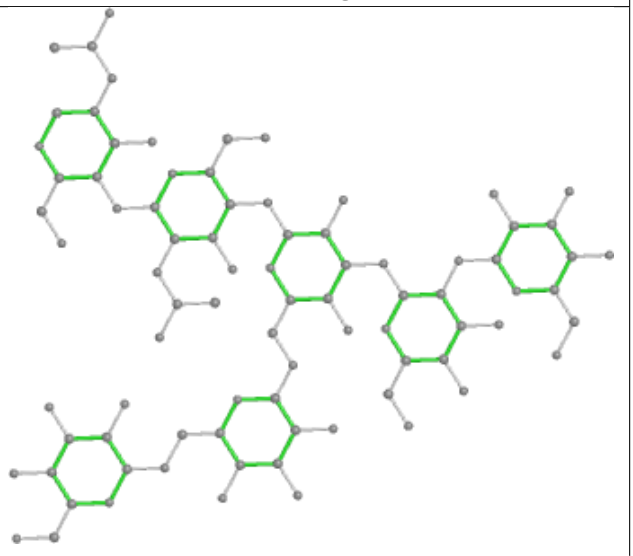
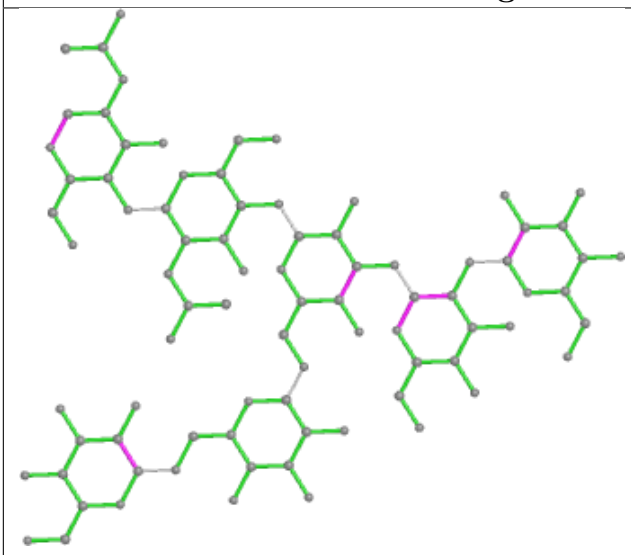


Rings

Oligosaccharide Chain u



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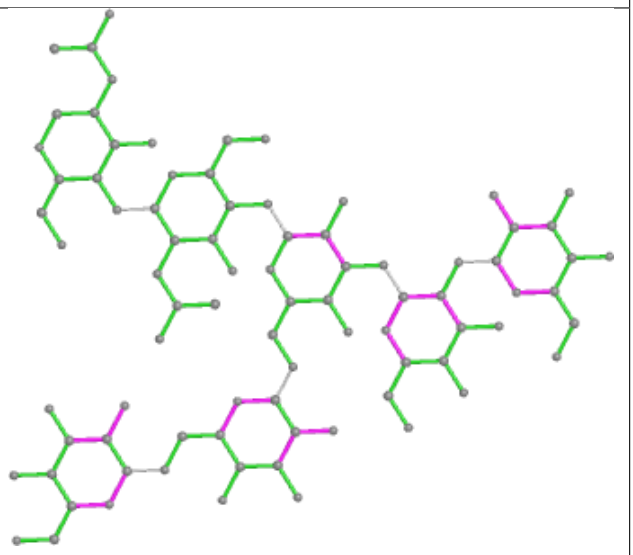
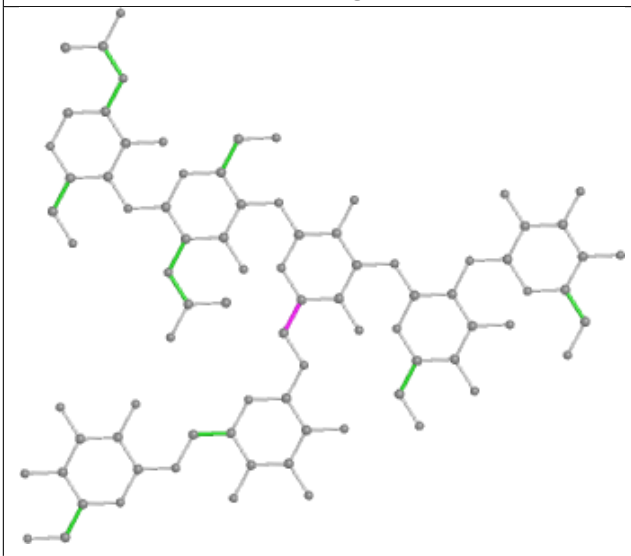


Bond angles



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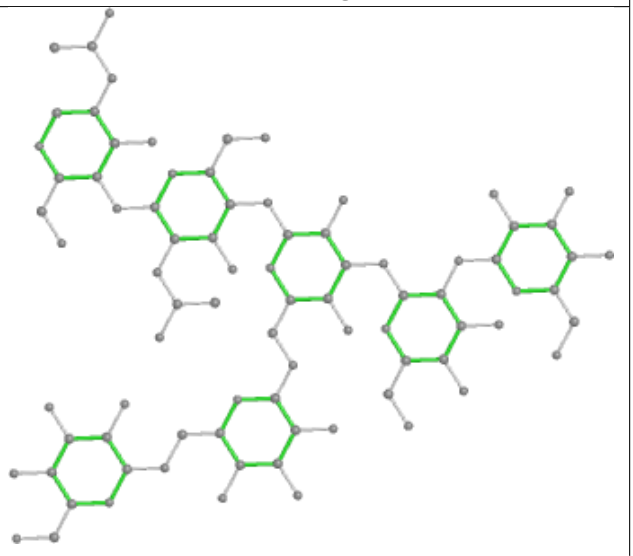
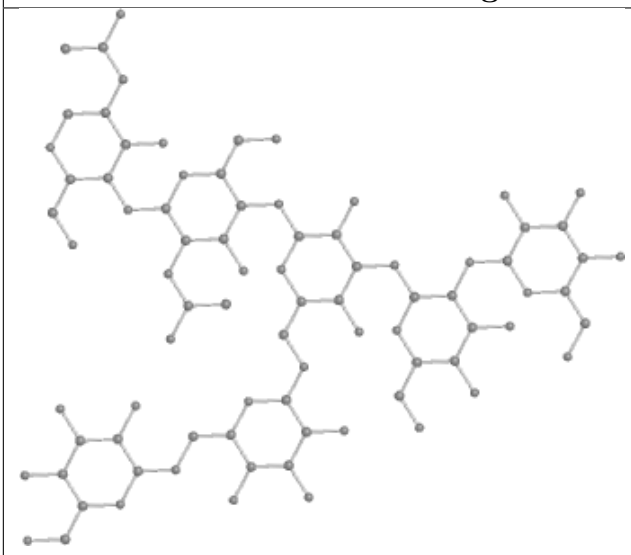


Rings

Oligosaccharide Chain DA



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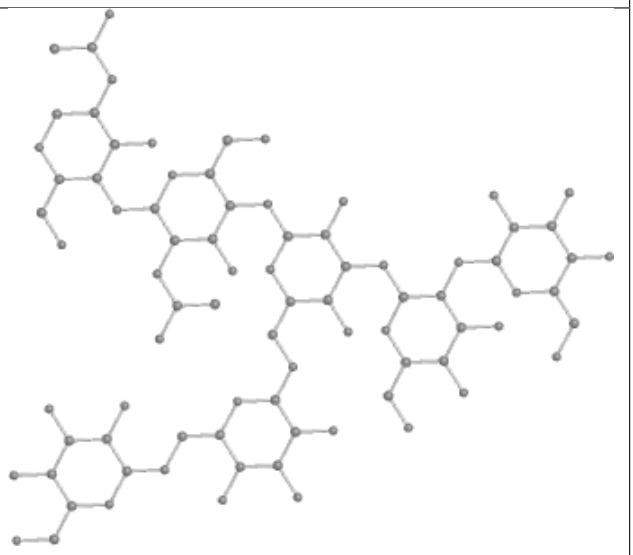
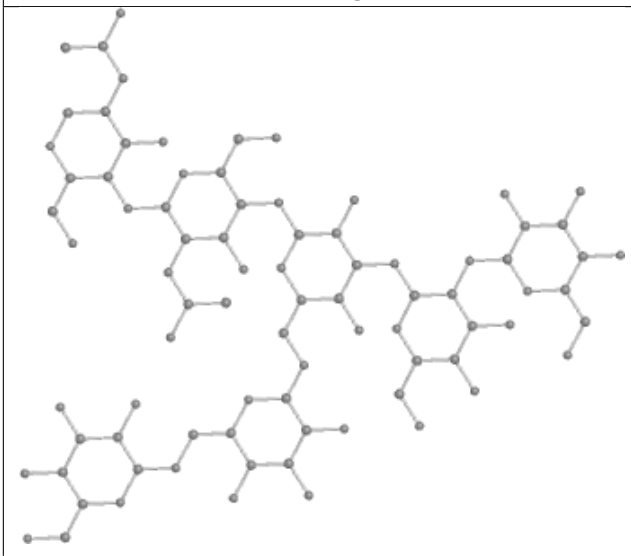
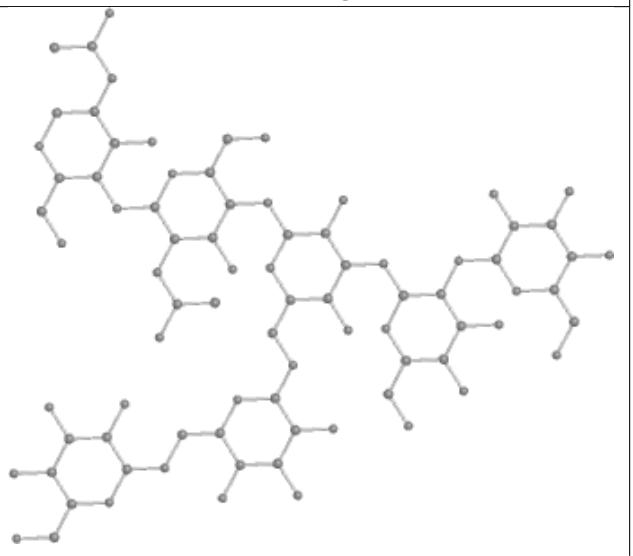


Bond angles

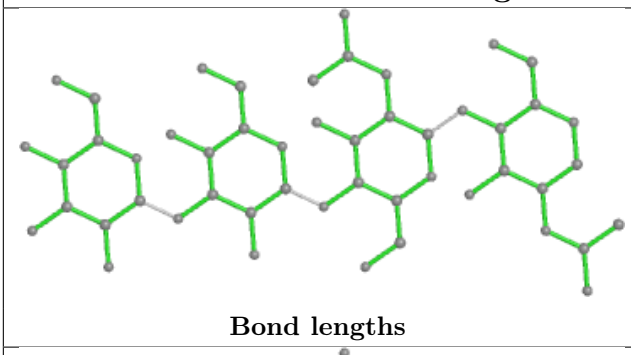


Torsions



Rings

Oligosaccharide Chain Y



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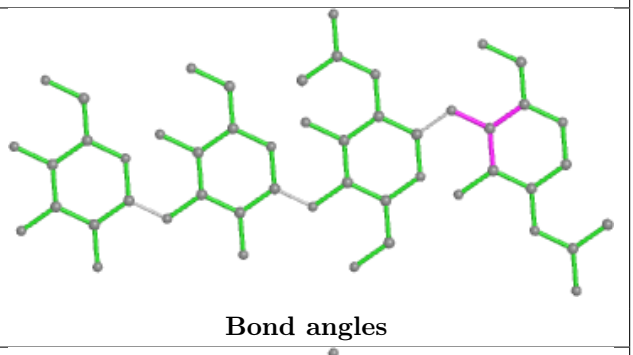
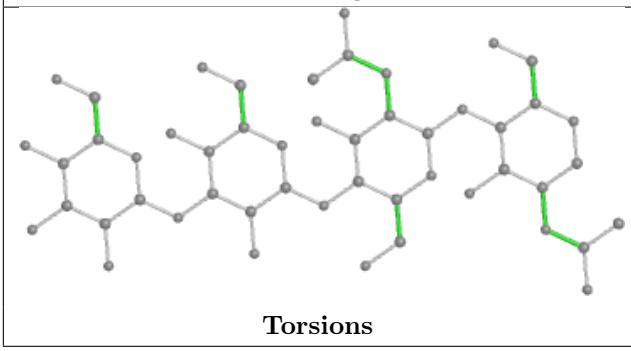


Bond angles



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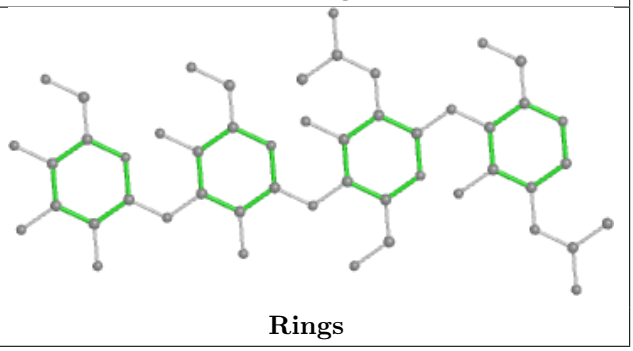
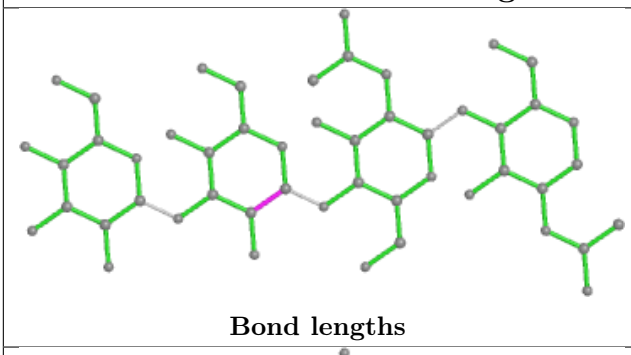


Rings

Oligosaccharide Chain v



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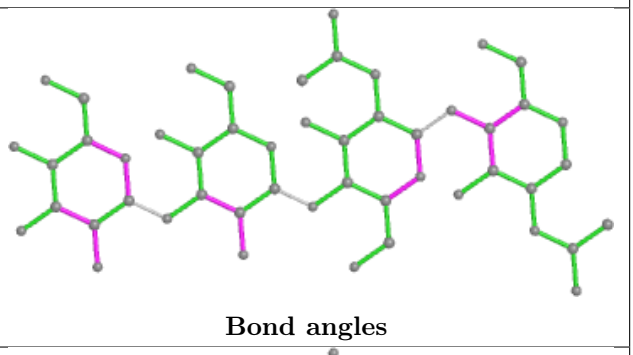
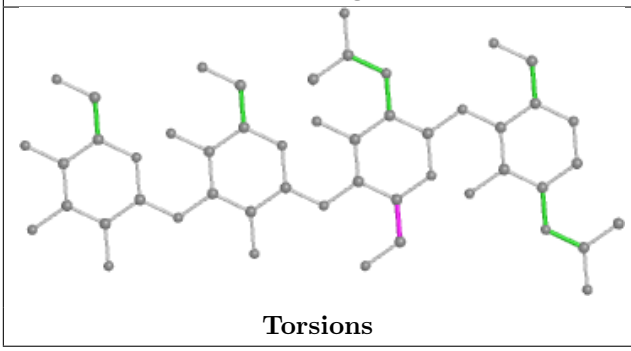


Bond angles



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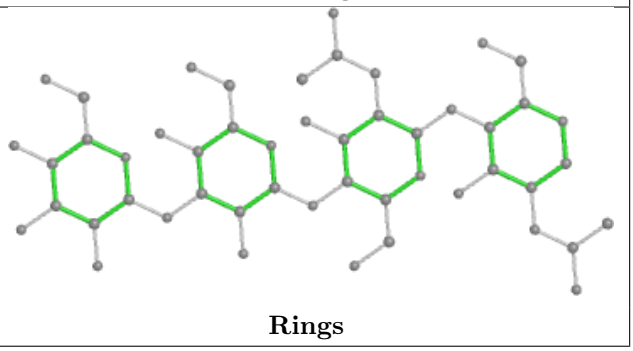
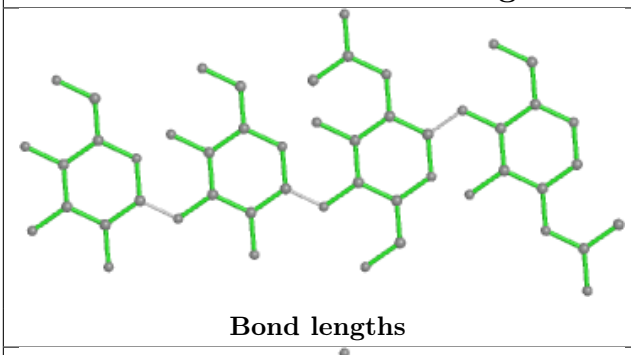


Rings

Oligosaccharide Chain 2



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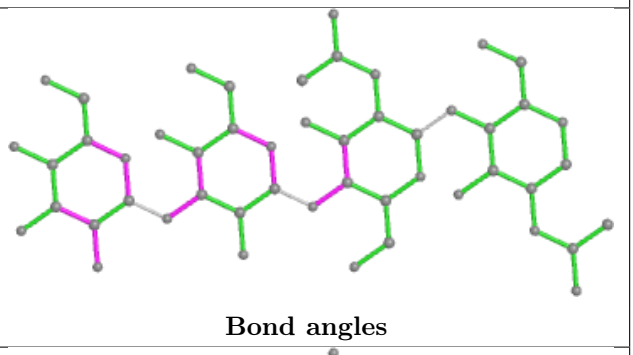
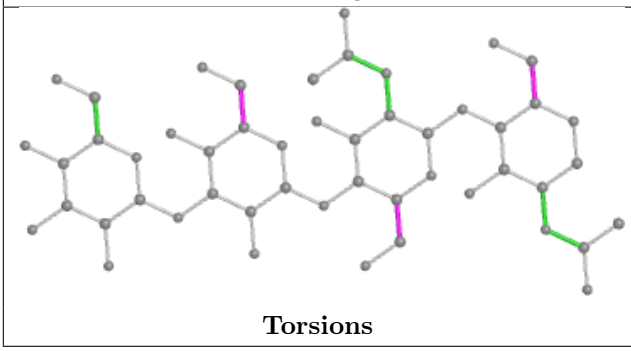


Bond angles



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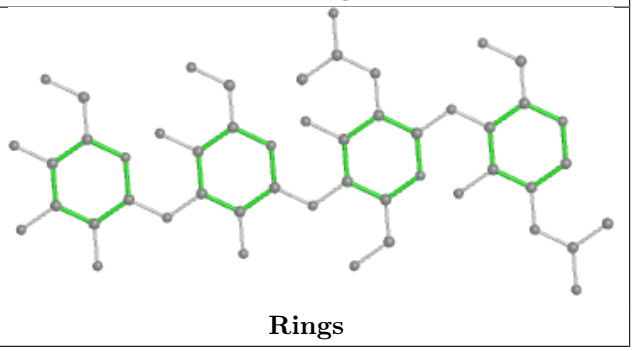
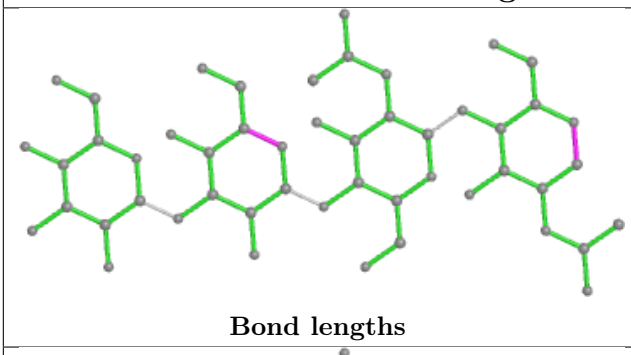


Rings

Oligosaccharide Chain 9



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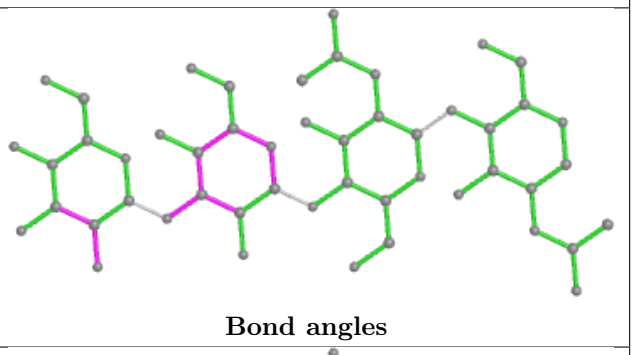

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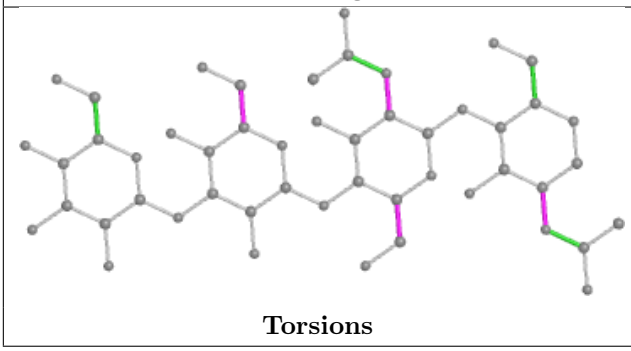

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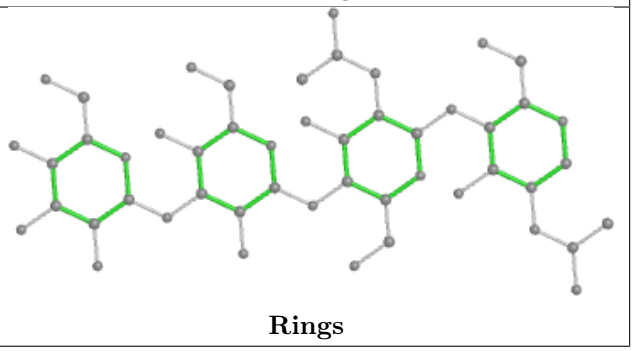
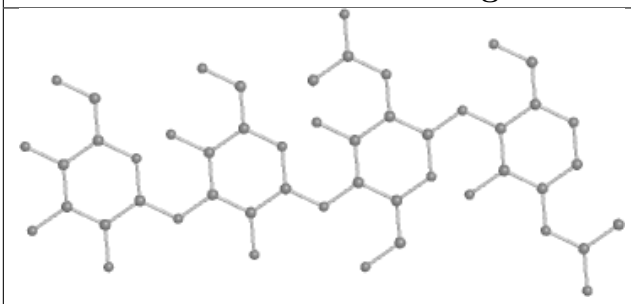
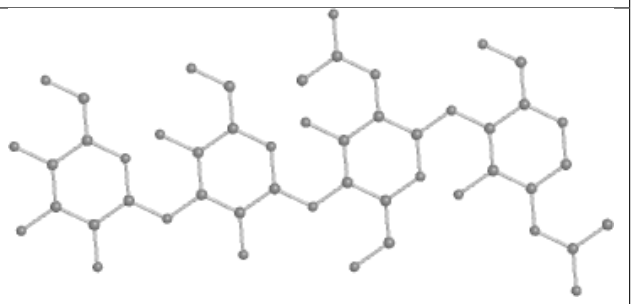


Rings

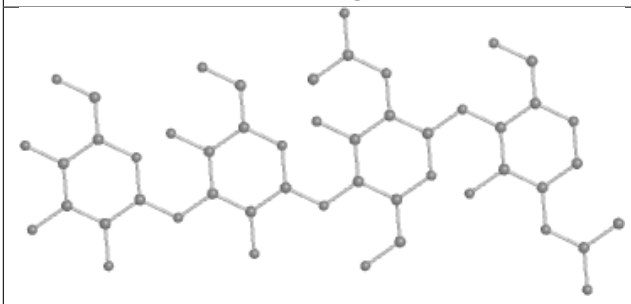
Oligosaccharide Chain CA



Bond lengths



Bond angles



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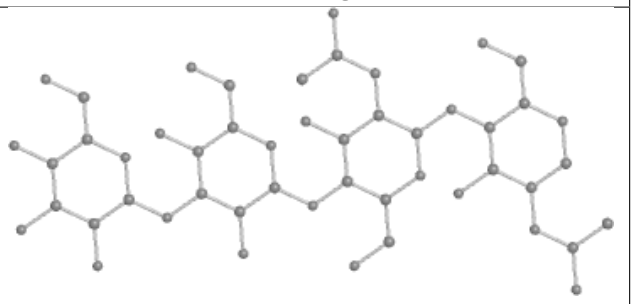
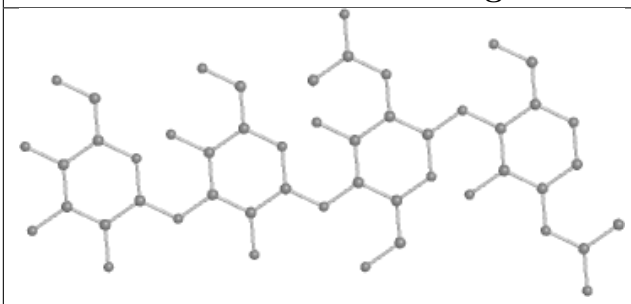


Rings

Oligosaccharide Chain FA



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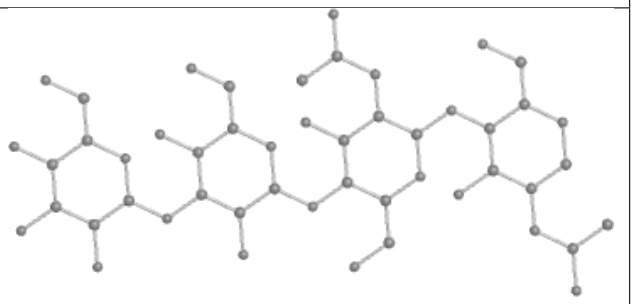
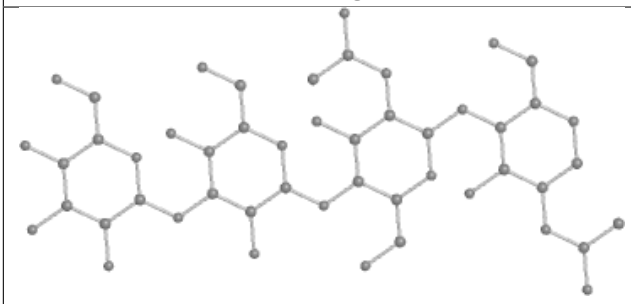
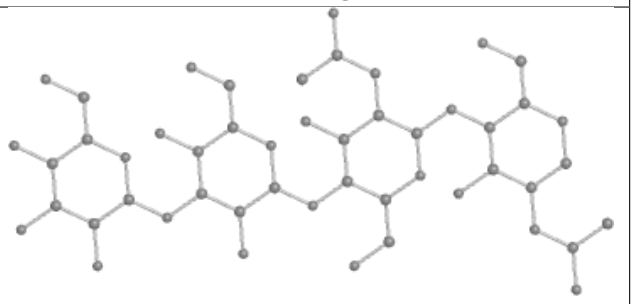


Bond angles

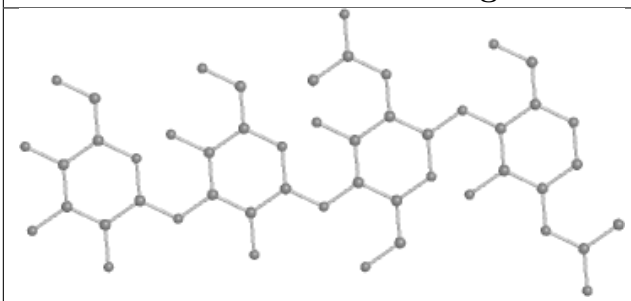


Torsions



Rings

Oligosaccharide Chain GA



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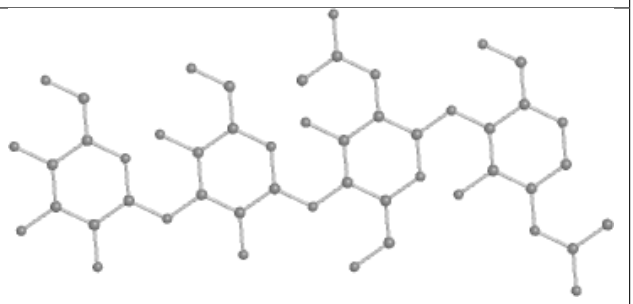
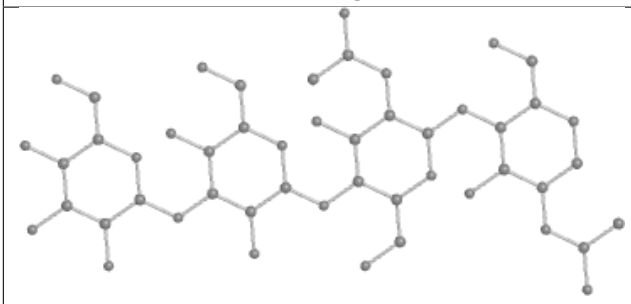


Bond angles



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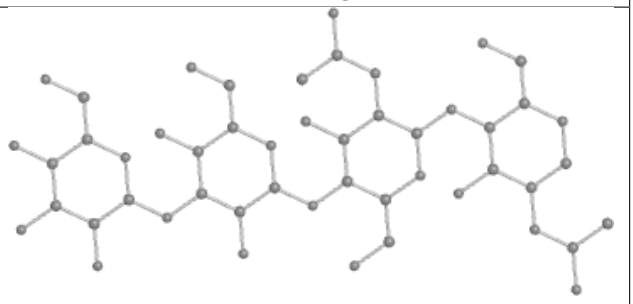
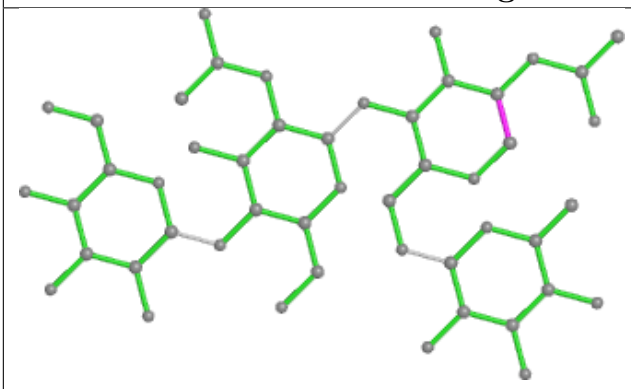


Rings

Oligosaccharide Chain d



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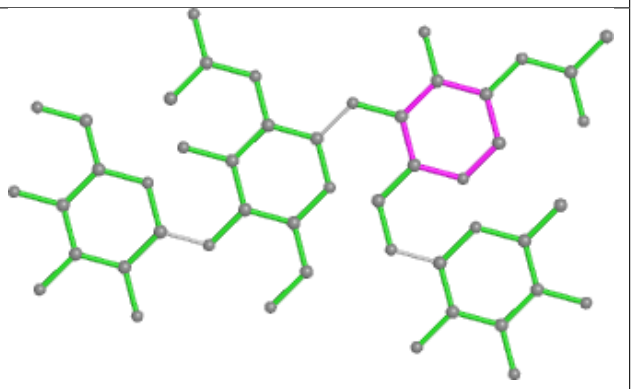
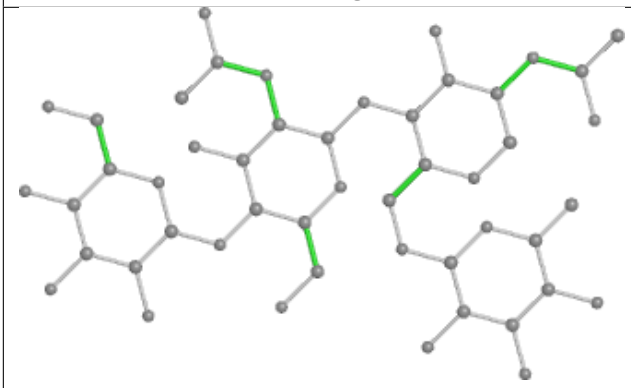


Bond angles



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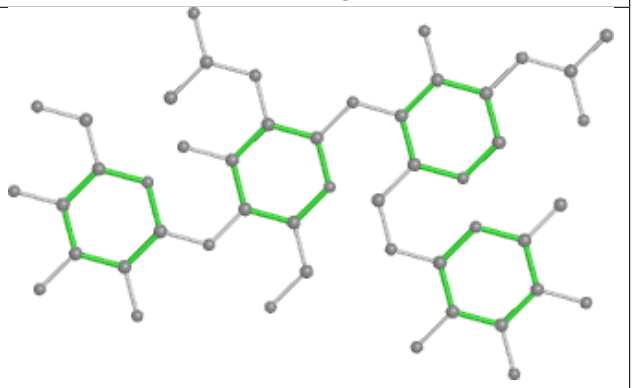
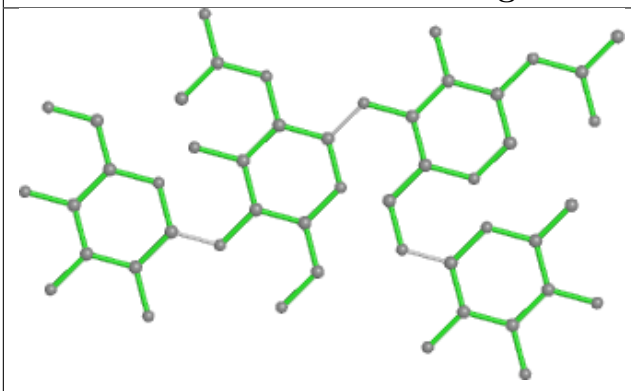
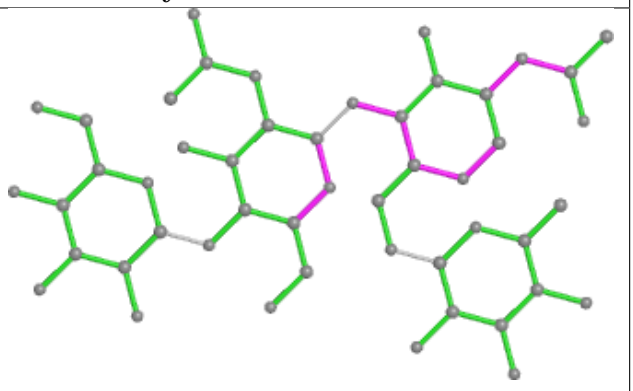


Rings

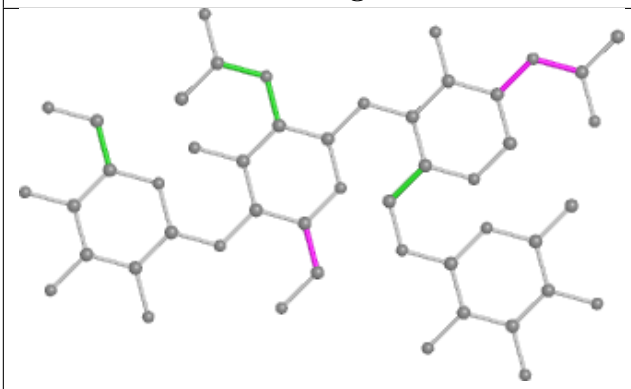
Oligosaccharide Chain y



Bond lengths



Bond angles



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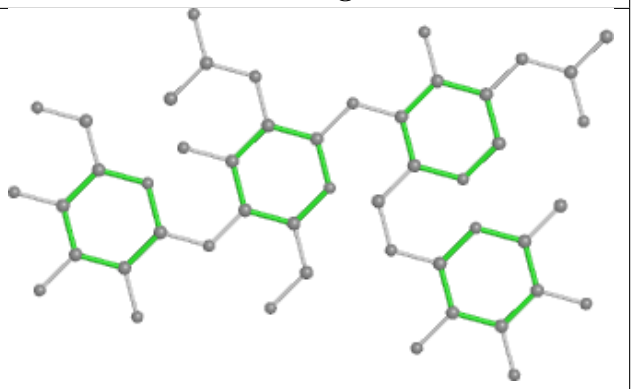
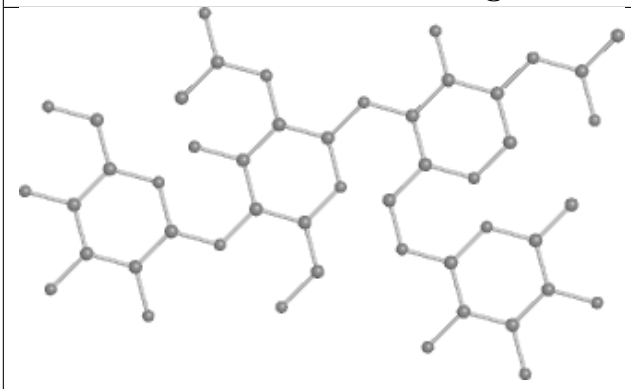
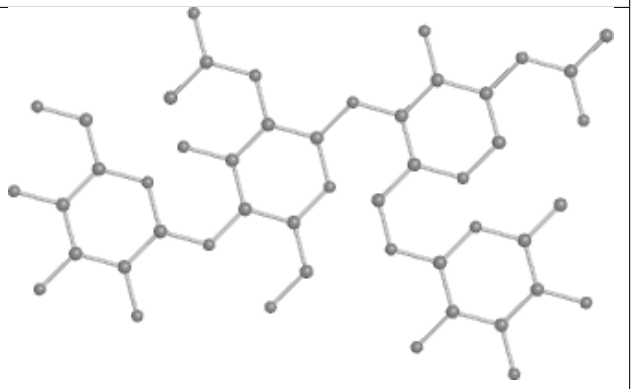


Rings

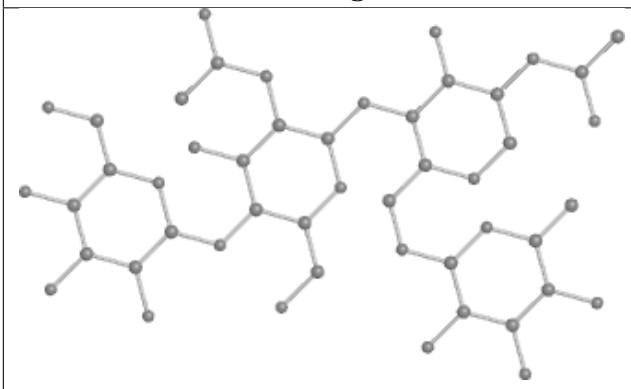
Oligosaccharide Chain JA



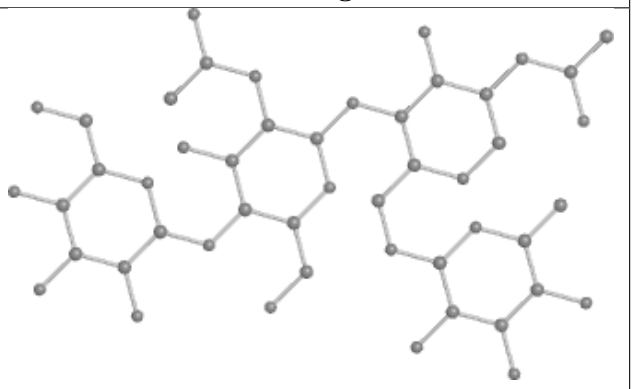
Bond lengths



Bond angles

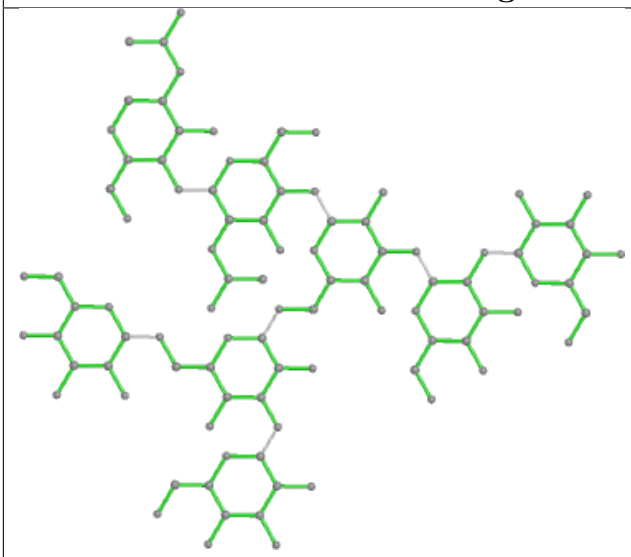


Torsions

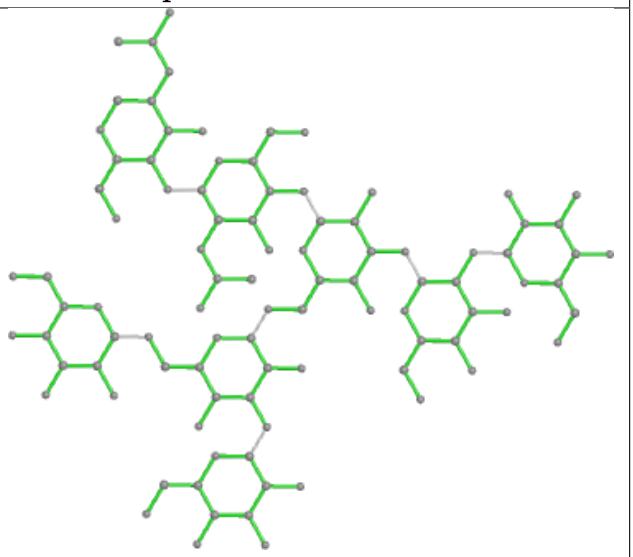


Rings

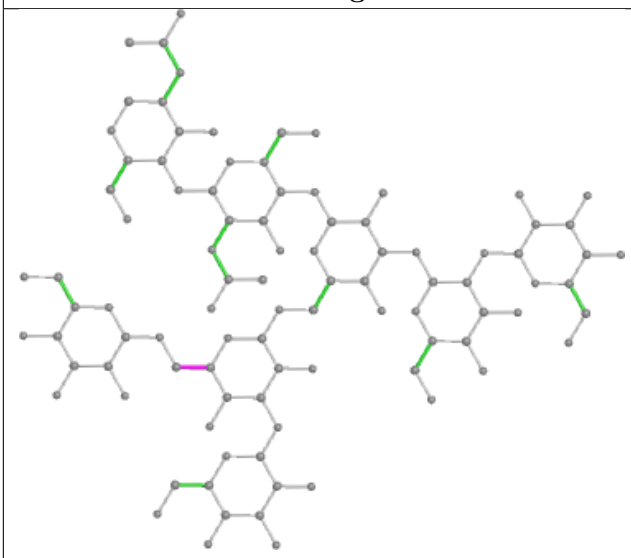
Oligosaccharide Chain p



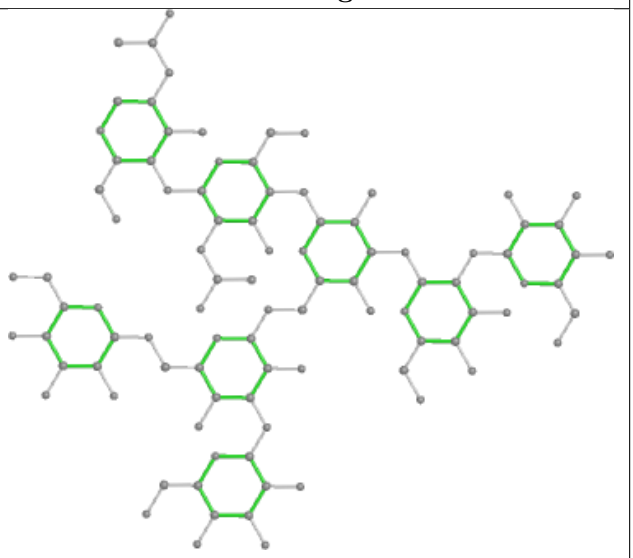
Bond lengths



Bond angles

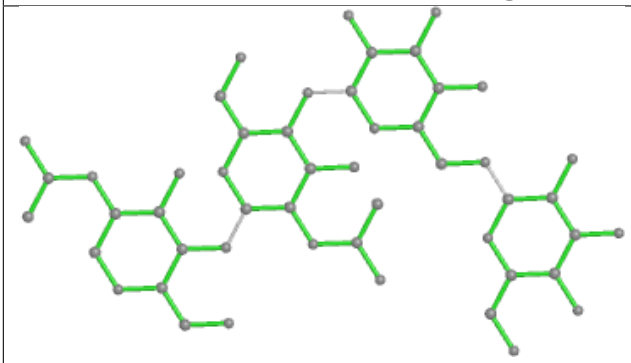


Torsions

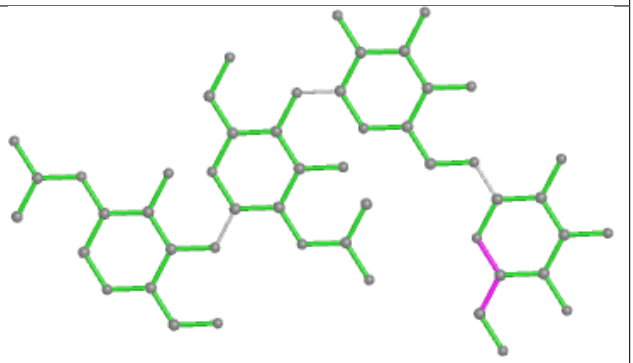


Rings

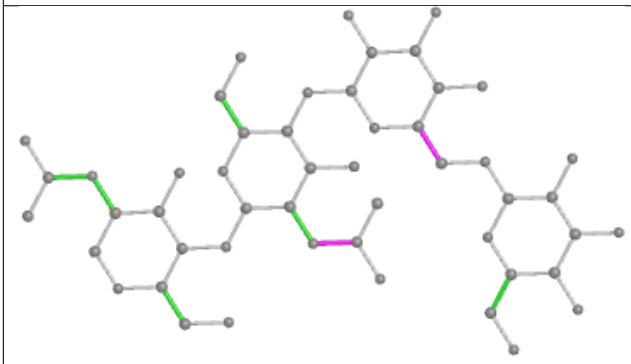
Oligosaccharide Chain t



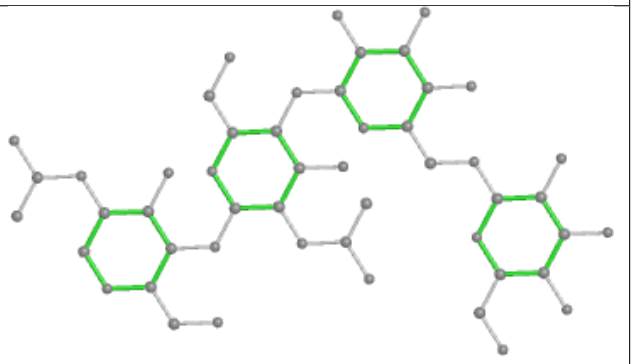
Bond lengths



Bond angles

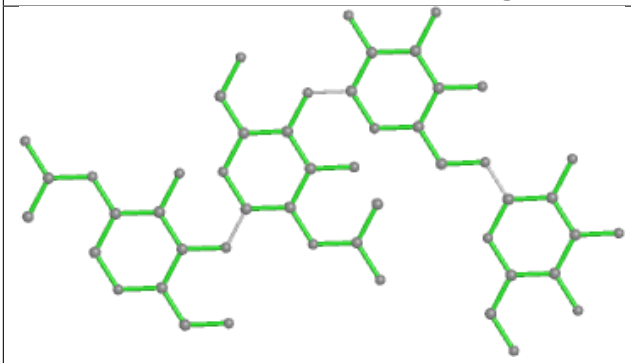


Torsions

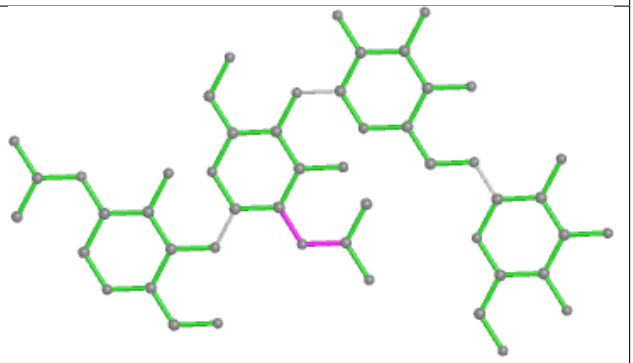


Rings

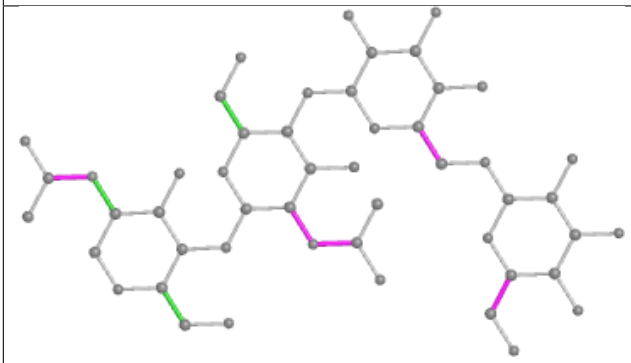
Oligosaccharide Chain x



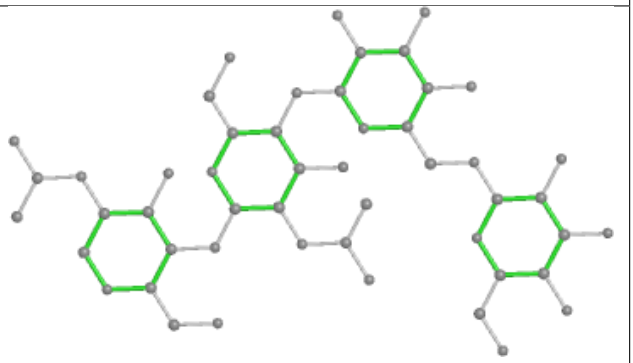
Bond lengths



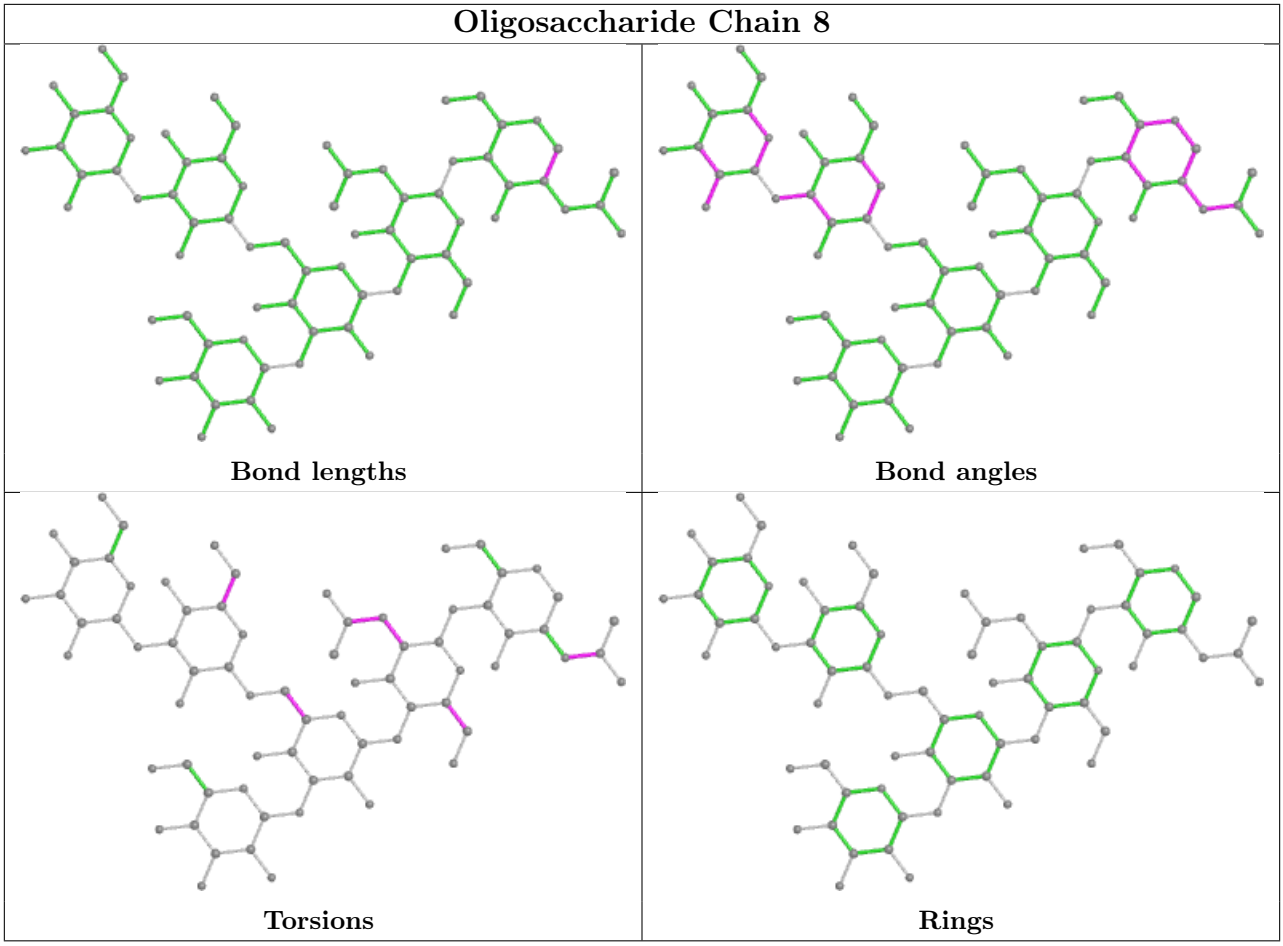
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
15	NAG	E	802	1	14,14,15	0.42	0	17,19,21	0.82	0
15	NAG	C	803	1	14,14,15	0.32	0	17,19,21	0.70	0
14	83G	A	801	-	32,33,33	0.90	3 (9%)	38,47,47	0.98	3 (7%)
14	83G	E	801	-	32,33,33	0.93	4 (12%)	38,47,47	1.23	3 (7%)
15	NAG	A	802	1	14,14,15	0.36	0	17,19,21	0.52	0
15	NAG	C	802	1	14,14,15	0.23	0	17,19,21	0.99	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	83G	C	801	-	32,33,33	0.90	2 (6%)	38,47,47	1.06	3 (7%)

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
15	NAG	E	802	1	-	0/6/23/26	0/1/1/1
15	NAG	C	803	1	-	2/6/23/26	0/1/1/1
14	83G	A	801	-	-	9/18/35/35	0/4/4/4
14	83G	E	801	-	-	4/18/35/35	0/4/4/4
15	NAG	A	802	1	-	0/6/23/26	0/1/1/1
15	NAG	C	802	1	-	5/6/23/26	0/1/1/1
14	83G	C	801	-	-	5/18/35/35	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	801	83G	C11-C12	-2.89	1.43	1.49
14	C	801	83G	C11-C12	-2.86	1.43	1.49
14	E	801	83G	C11-C12	-2.79	1.43	1.49
14	E	801	83G	C11-C08	2.29	1.45	1.42
14	E	801	83G	C14-C12	-2.26	1.50	1.53
14	C	801	83G	C11-C08	2.25	1.45	1.42
14	A	801	83G	C11-C08	2.14	1.44	1.42
14	E	801	83G	C07-N06	-2.07	1.34	1.37
14	A	801	83G	C07-N06	-2.01	1.34	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	E	801	83G	C11-C12-C14	3.85	124.14	118.61
14	C	801	83G	C11-C12-C14	2.99	122.90	118.61
14	A	801	83G	C11-C12-C14	2.79	122.61	118.61
14	C	801	83G	O02-C03-C08	2.47	119.52	115.89
14	C	801	83G	C11-C08-C07	-2.40	105.62	107.54
14	E	801	83G	O02-C03-C08	2.34	119.33	115.89
14	E	801	83G	C11-C08-C07	-2.32	105.69	107.54
15	C	802	NAG	C2-N2-C7	2.10	125.89	122.90
14	A	801	83G	C12-C14-N16	2.09	121.06	118.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	801	83G	C11-C08-C07	-2.06	105.90	107.54
15	C	802	NAG	C4-C3-C2	-2.01	108.07	111.02

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	801	83G	O15-C14-N16-C17
14	A	801	83G	O15-C14-N16-C17
14	A	801	83G	C08-C03-O02-C01
15	C	803	NAG	C8-C7-N2-C2
15	C	803	NAG	O7-C7-N2-C2
15	C	802	NAG	C8-C7-N2-C2
14	A	801	83G	C04-C03-O02-C01
15	C	802	NAG	O5-C5-C6-O6
15	C	802	NAG	O7-C7-N2-C2
14	E	801	83G	C08-C03-O02-C01
14	A	801	83G	C25-C23-N19-C20
14	A	801	83G	O24-C23-N19-C20
15	C	802	NAG	C4-C5-C6-O6
14	E	801	83G	O15-C14-N16-C17
14	C	801	83G	C12-C14-N16-C17
14	E	801	83G	C04-C03-O02-C01
15	C	802	NAG	C3-C2-N2-C7
14	A	801	83G	C12-C14-N16-C17
14	C	801	83G	O13-C12-C14-O15
14	A	801	83G	O13-C12-C14-O15
14	A	801	83G	C11-C12-C14-O15
14	C	801	83G	O24-C23-N19-C20
14	C	801	83G	C12-C14-N16-C21
14	E	801	83G	C12-C14-N16-C21
14	A	801	83G	C12-C14-N16-C21

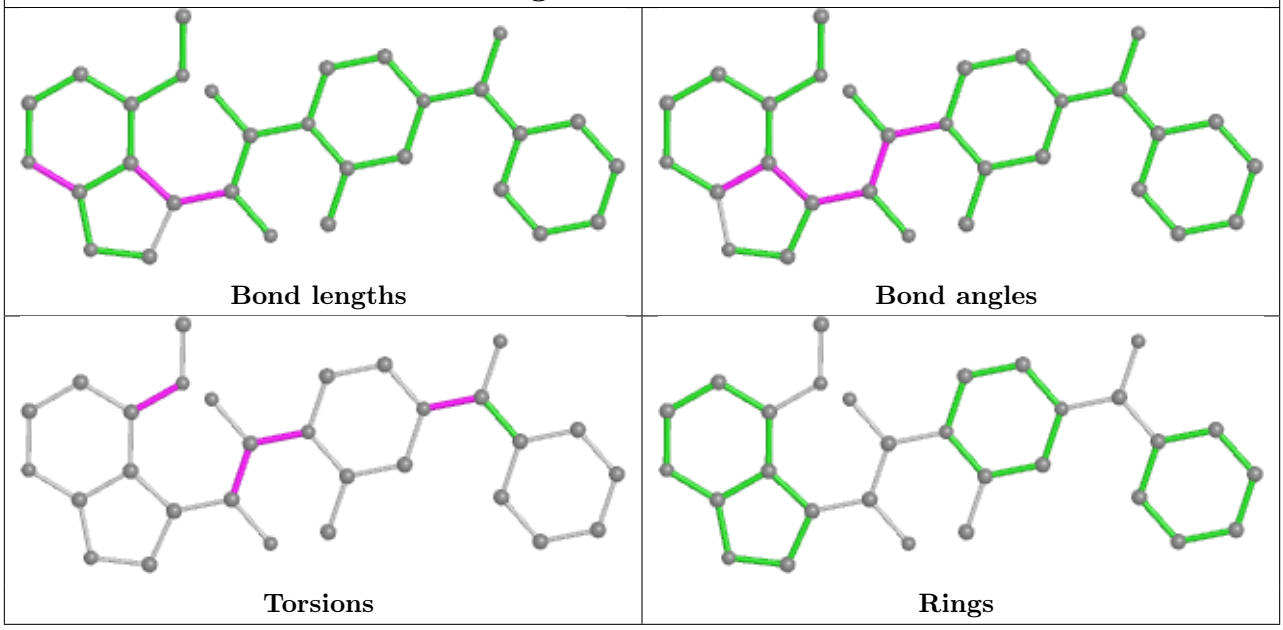
There are no ring outliers.

No monomer is involved in short contacts.

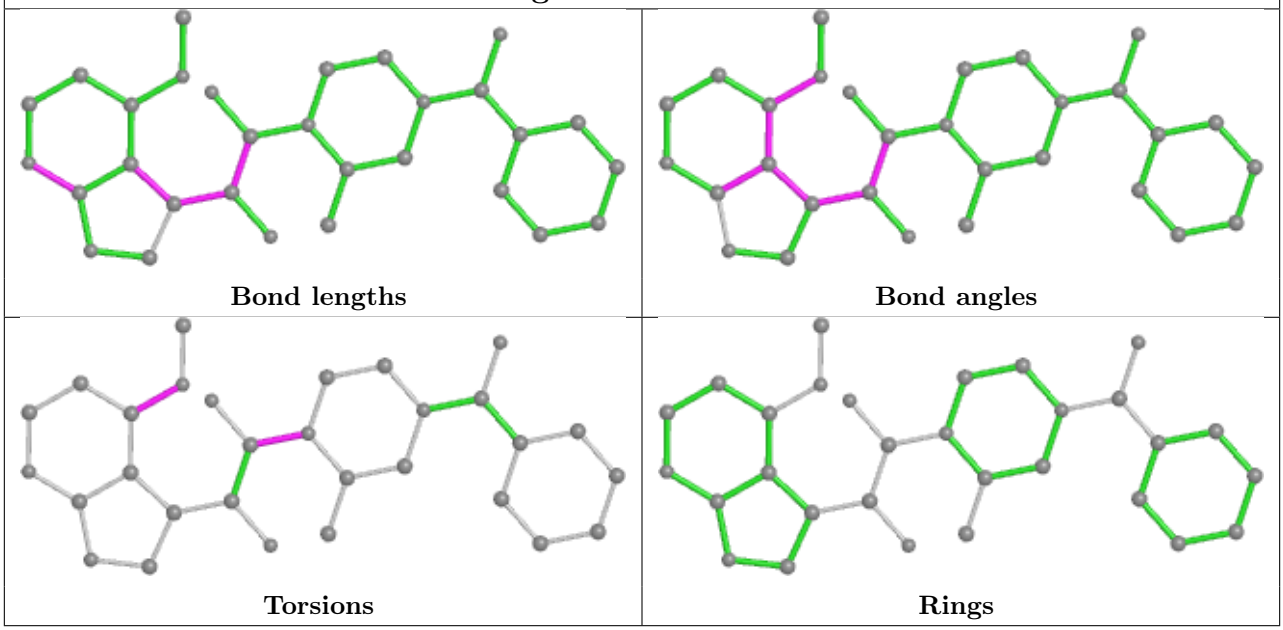
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

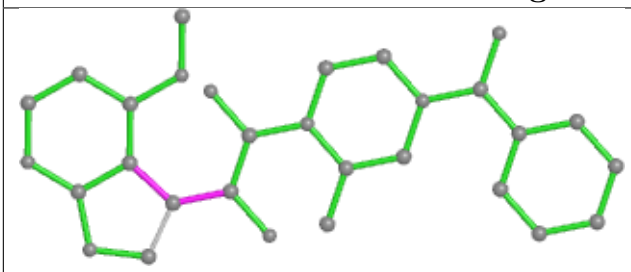
Ligand 83G A 801



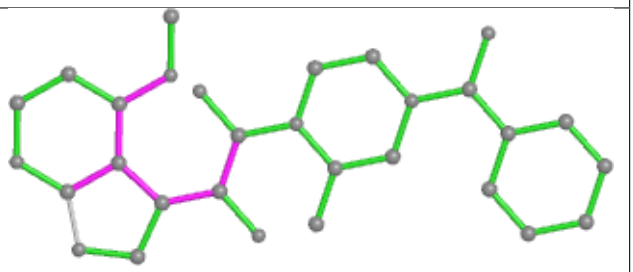
Ligand 83G E 801



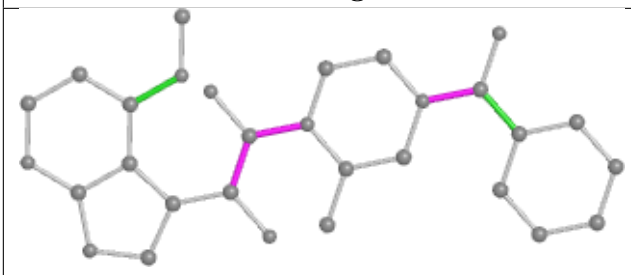
Ligand 83G C 801



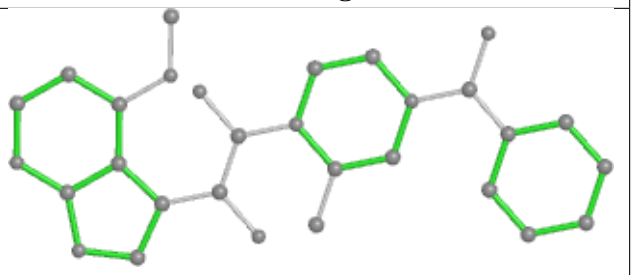
Bond lengths



Bond angles



Torsions



Rings

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.

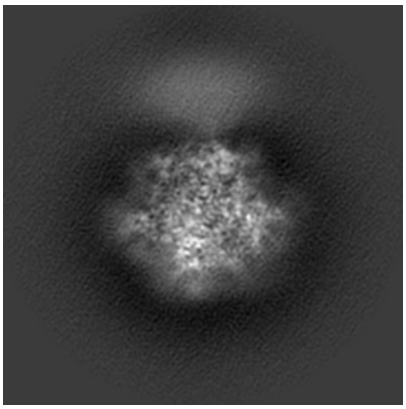
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61553. These allow visual inspection of the internal detail of the map and identification of artifacts.

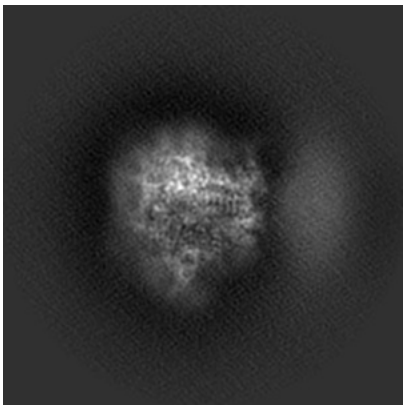
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

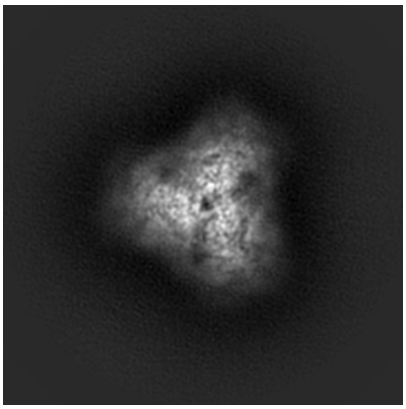
6.1.1 Primary map



X

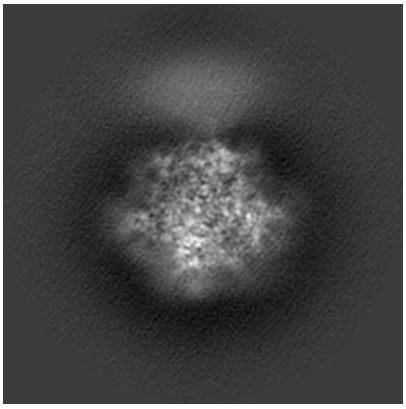


Y

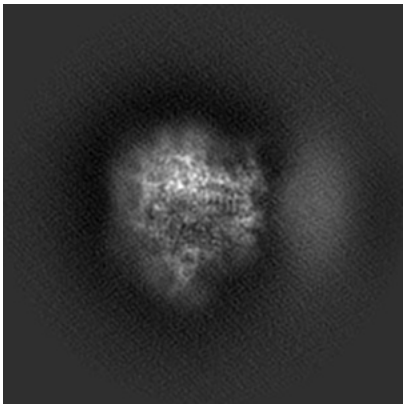


Z

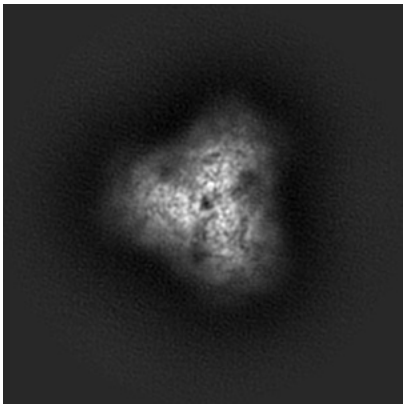
6.1.2 Raw map



X



Y

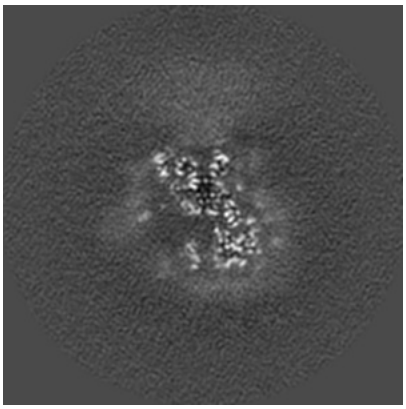


Z

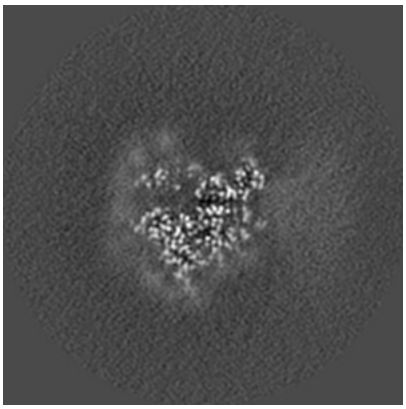
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

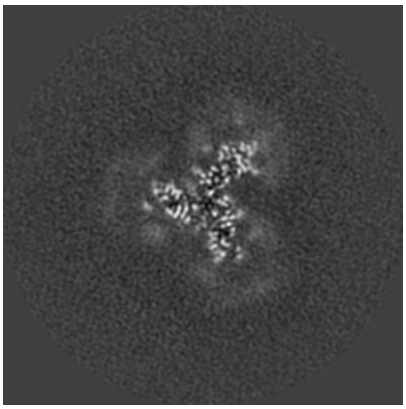
6.2.1 Primary map



X Index: 90

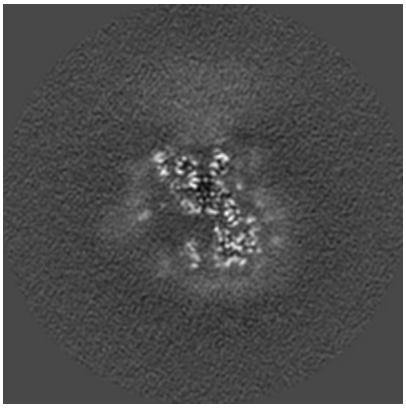


Y Index: 90

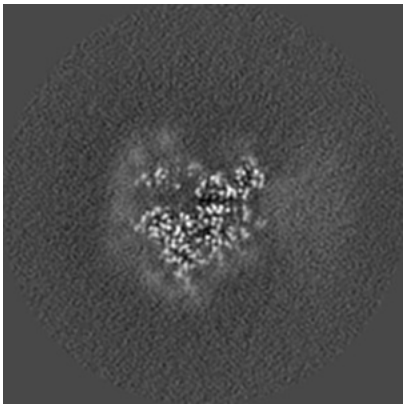


Z Index: 90

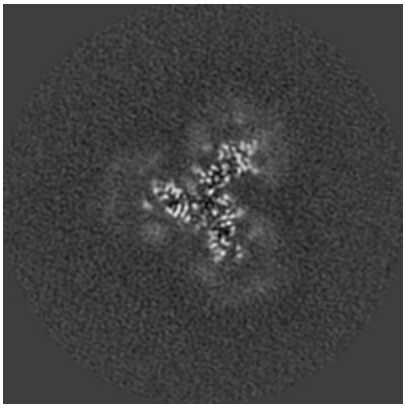
6.2.2 Raw map



X Index: 90



Y Index: 90

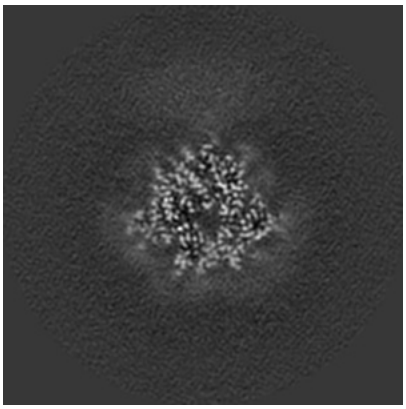


Z Index: 90

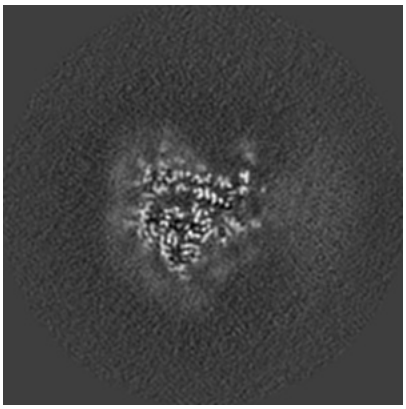
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

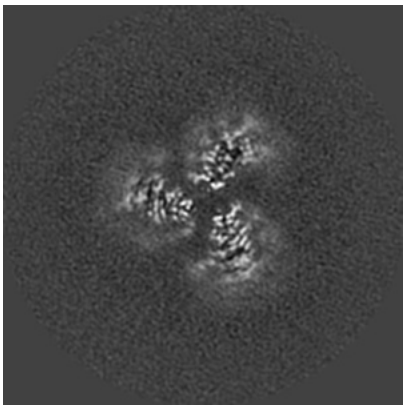
6.3.1 Primary map



X Index: 99

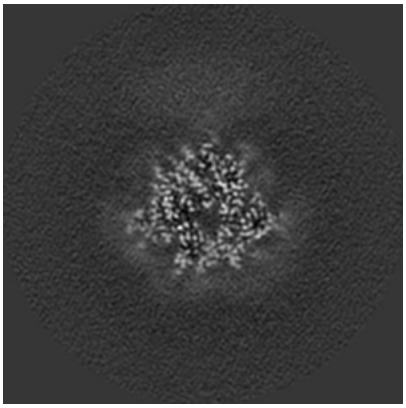


Y Index: 87

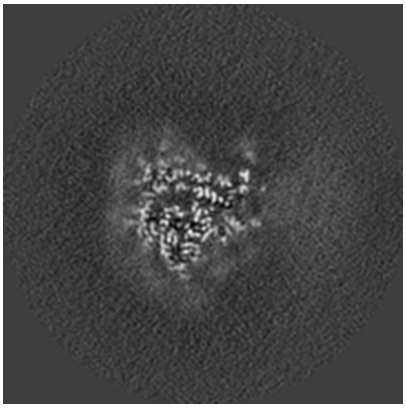


Z Index: 83

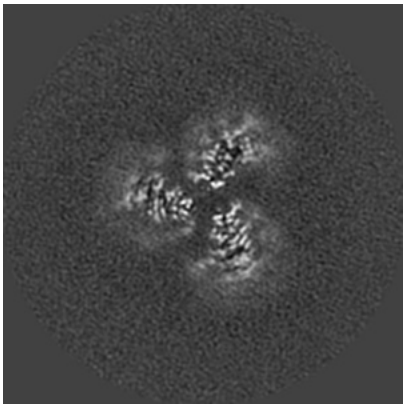
6.3.2 Raw map



X Index: 99



Y Index: 87

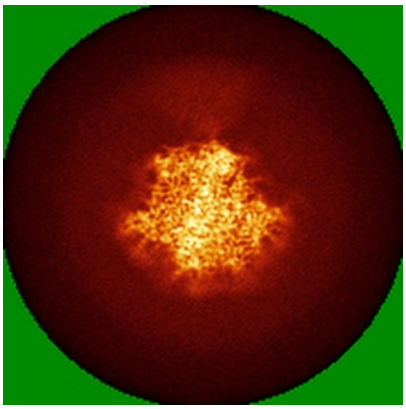


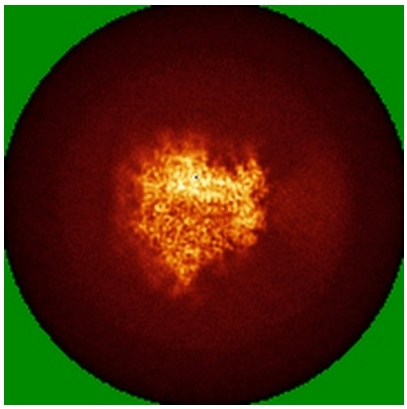
Z Index: 83

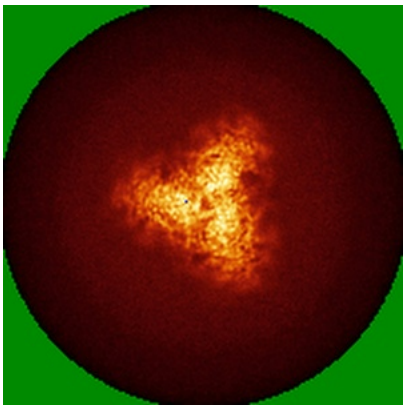
The images above show the largest variance slices of the map in three orthogonal directions.

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

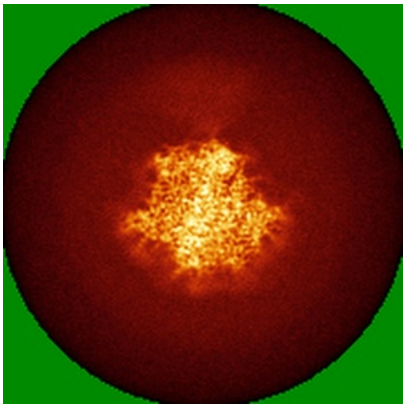
6.4.1 Primary map

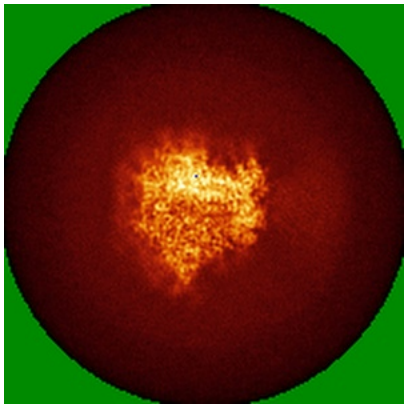

X

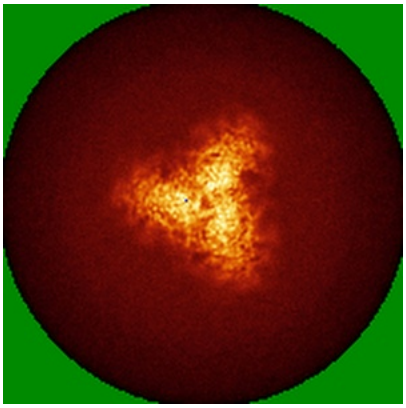

Y


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 0.02. 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.

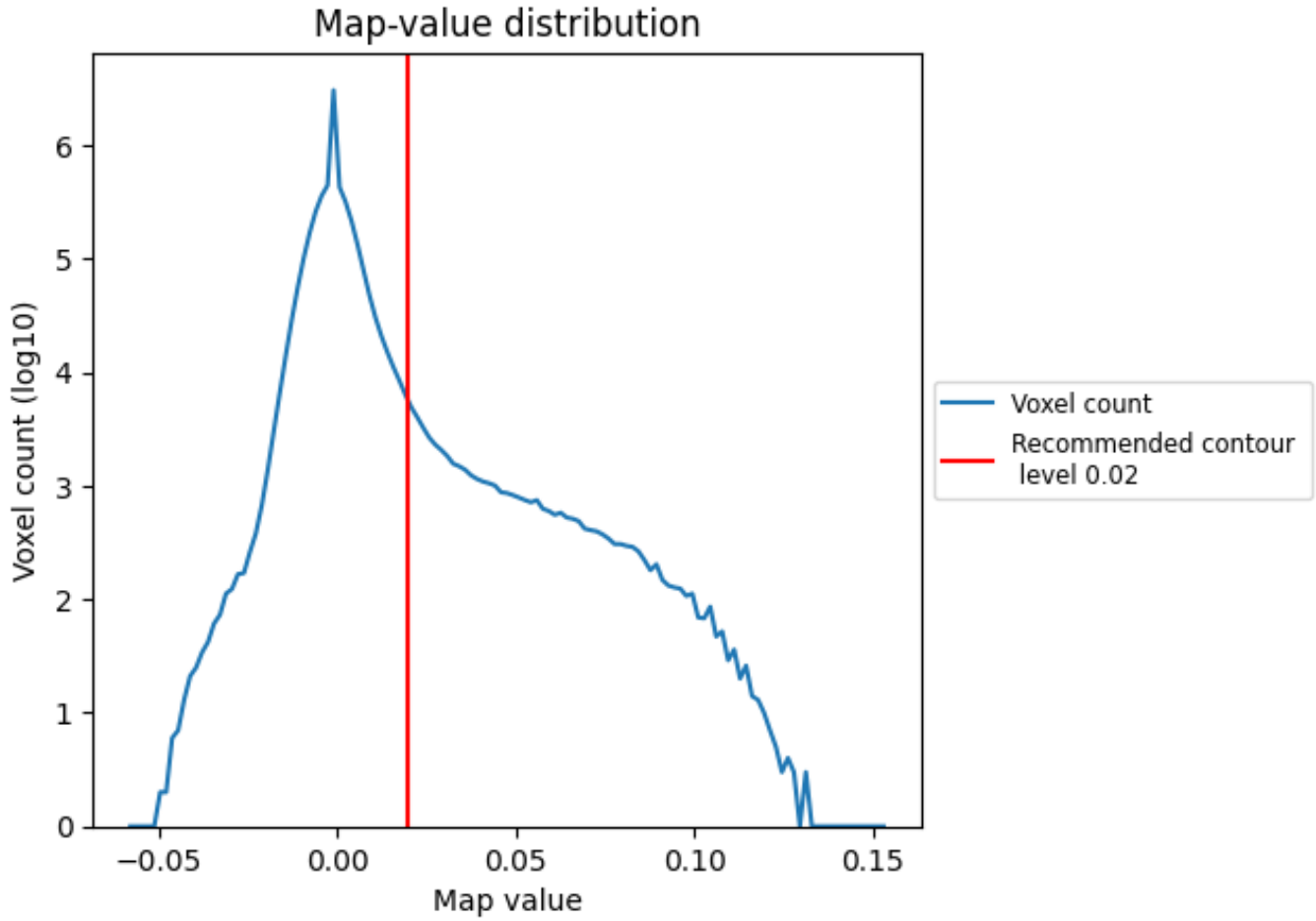
6.6 Mask visualisation (i)

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

7 Map analysis

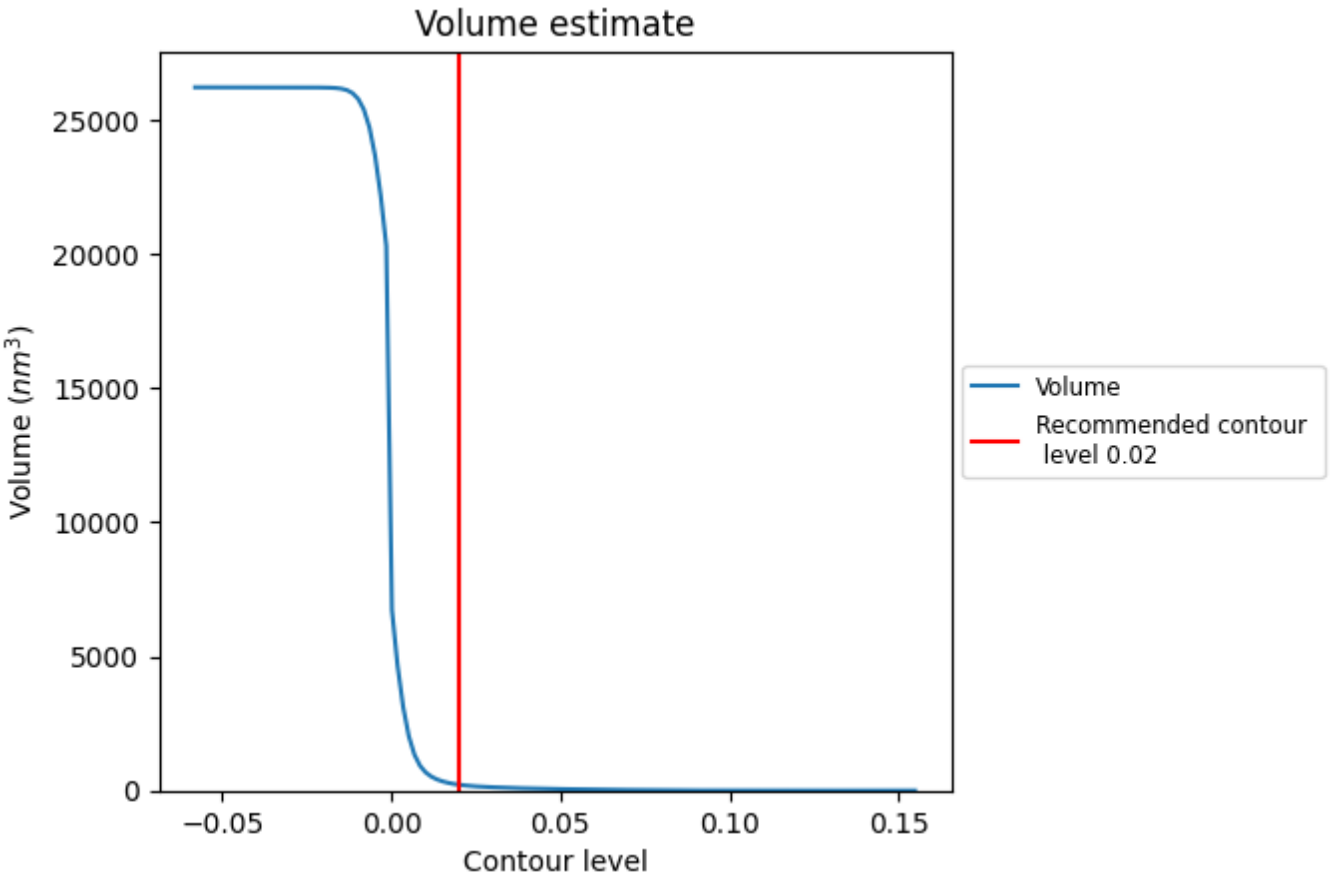
This section contains the results of statistical analysis of the map.

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.

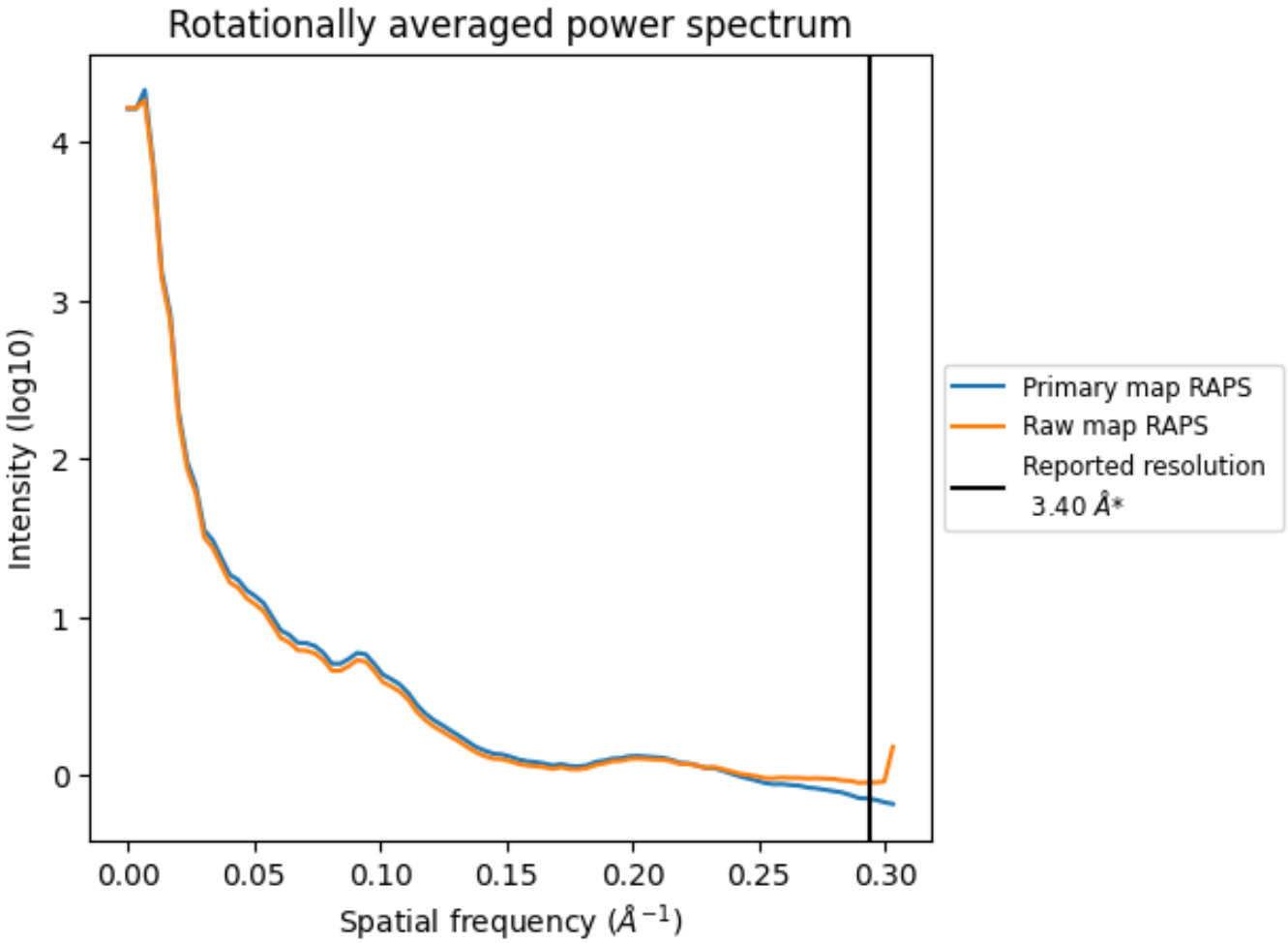
7.2 Volume estimate



The volume at the recommended contour level is 218 nm^3; this corresponds to an approximate mass of 197 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)

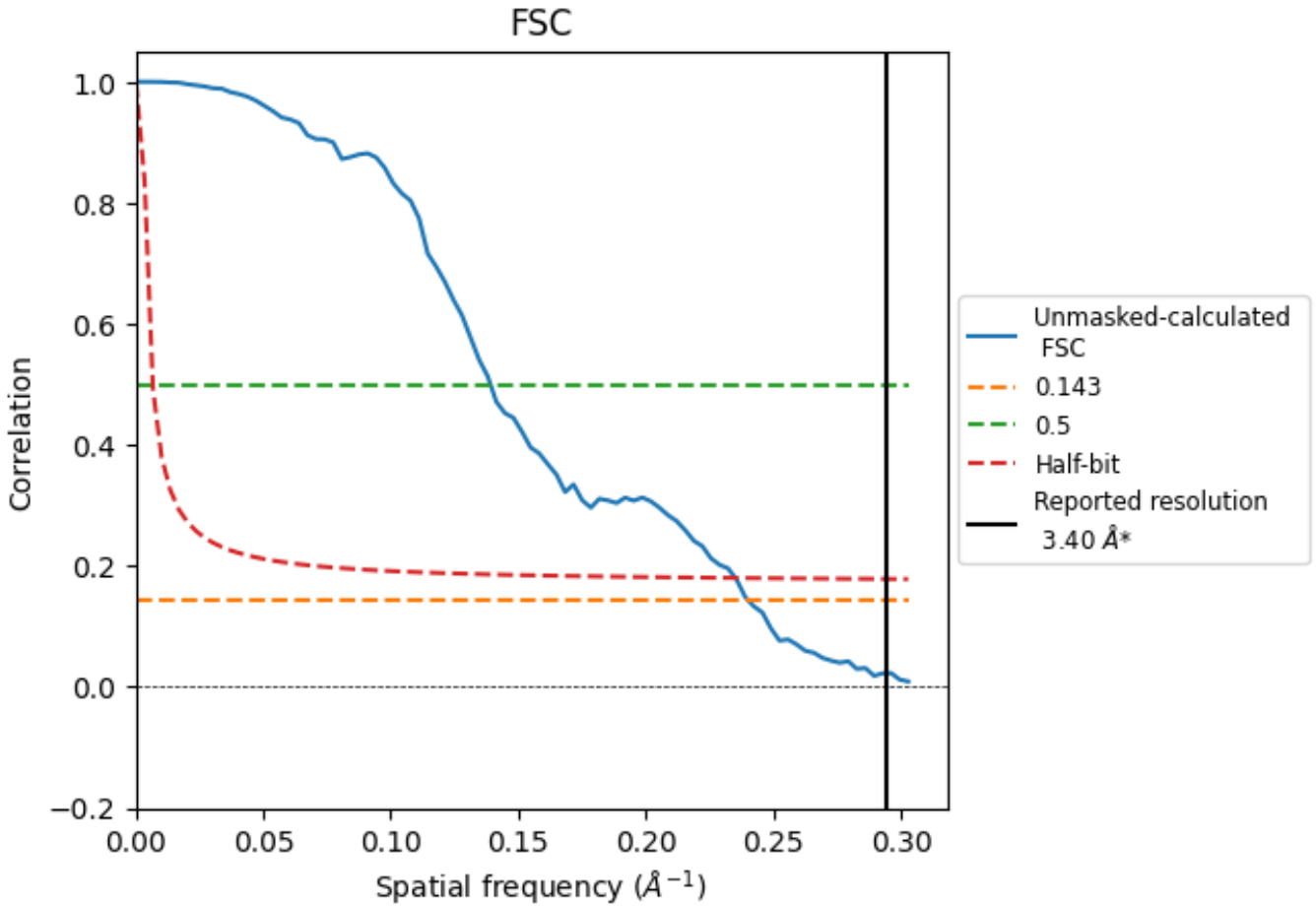


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

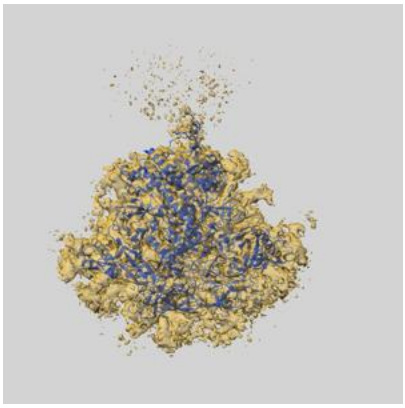
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.19	4.25

*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 4.16 differs from the reported value 3.4 by more than 10 %

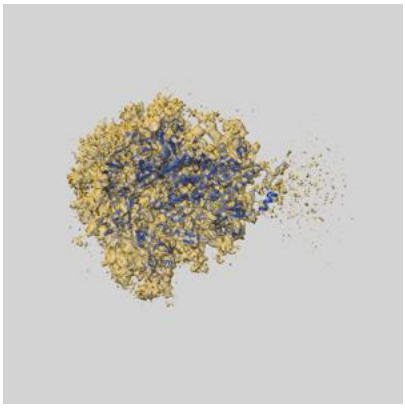
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61553 and PDB model 9JKF. Per-residue inclusion information can be found in section 3 on page 20.

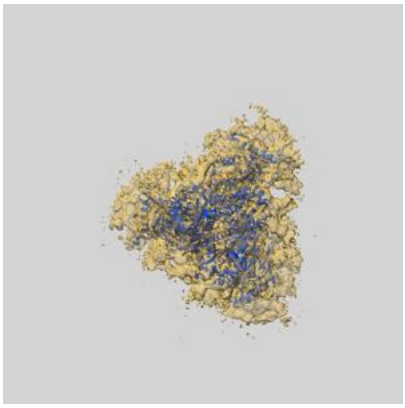
9.1 Map-model overlay



X



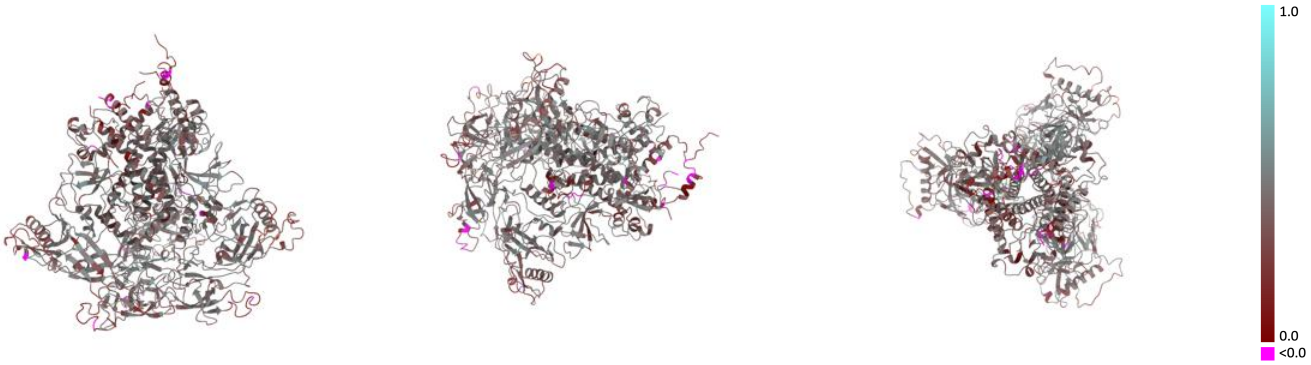
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

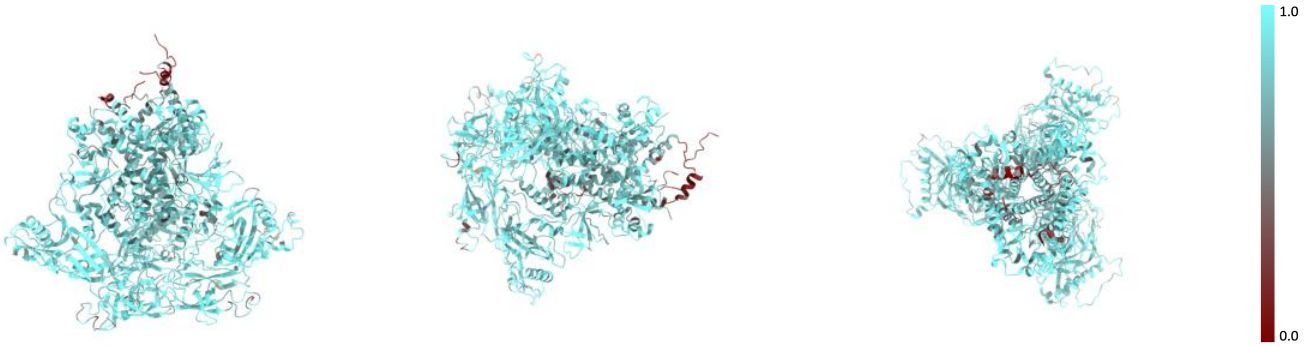
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

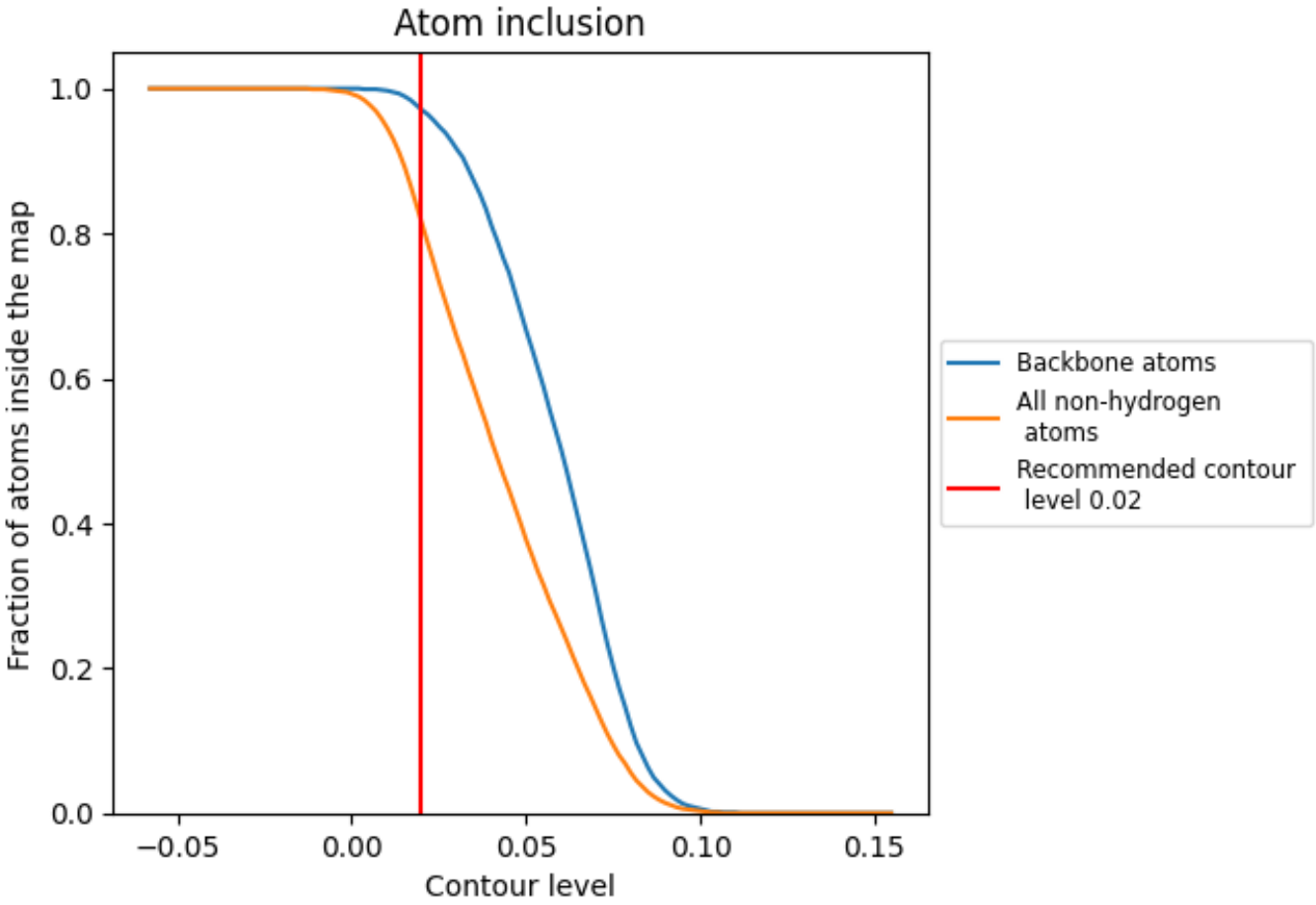
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.3570
0	0.4620	0.2100
1	0.8690	0.3050
2	0.7800	0.2670
3	0.6920	0.2430
4	0.5360	0.2180
5	0.7180	0.2470
6	0.6070	0.2570
7	0.5900	0.1820
8	0.5970	0.0960
9	0.6400	0.1700
A	0.8620	0.3870
AA	0.7440	0.2750
B	0.7910	0.3640
BA	0.7180	0.2590
C	0.8610	0.3860
CA	0.7200	0.2120
D	0.7150	0.3210
DA	0.7110	0.2430
E	0.8710	0.4060
EA	0.8210	0.2720
F	0.7950	0.3710
FA	0.8200	0.3060
G	0.7440	0.3230
GA	0.8600	0.3080
H	0.3930	0.2310
HA	0.2860	0.0490
I	0.2500	0.1420
IA	0.8970	0.2410
J	0.5130	0.2240
JA	0.8370	0.3060
K	0.5380	0.2470
KA	0.5710	0.3230
L	0.6920	0.1620
LA	0.6430	0.2780

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Chain	Atom inclusion	Q-score
M	0.8210	0.1780
MA	0.8210	0.3450
N	0.5000	0.0840
O	0.5260	0.1550
P	0.7440	0.2810
Q	0.5900	0.2110
R	0.5640	0.1910
S	0.8330	0.3200
T	0.5740	0.1630
U	0.8210	0.2970
V	0.8210	0.2630
W	0.7540	0.2650
X	0.6870	0.1770
Y	0.7400	0.2590
Z	0.9230	0.2280
a	0.8460	0.2750
b	0.5000	0.1810
c	0.7690	0.3600
d	0.6730	0.2070
e	0.5000	0.2670
f	0.4290	0.0920
g	0.5900	0.2000
h	0.7950	0.3530
i	0.7210	0.2390
j	0.7870	0.2070
k	0.5710	0.1360
l	0.5710	0.1750
m	0.7440	0.2110
n	0.7500	0.3090
o	0.7690	0.1750
p	0.7450	0.2380
q	0.8970	0.3020
r	0.6670	0.3180
s	0.8460	0.3520
t	0.7800	0.2250
u	0.7110	0.1390
v	0.7400	0.0900
w	0.8460	0.3270
x	0.7600	0.1940
y	0.4080	0.1680
z	0.8210	0.2870