wwPDB EM Validation Summary Report

Nov 9, 2024 – 11:30 AM EST

PDB ID	:	5SZS
EMDB ID	:	EMD-8331
Title	:	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy
Authors	:	Walls, A.C.; Tortorici, M.A.; Frenz, B.; Snijder, J.; Li, W.; Rey, F.A.; DiMaio, F.; Bosch, B.J.; Veesler, D.
Deposited on	:	2016-08-15
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

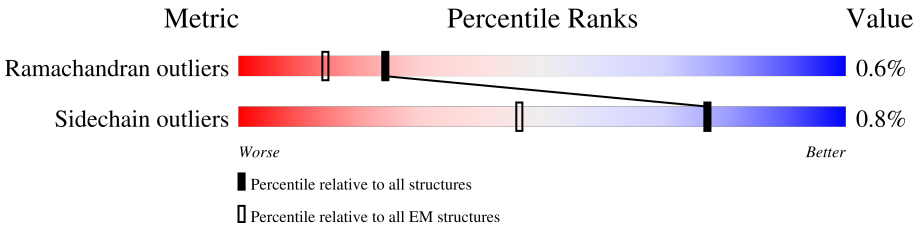
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	1325	5% 86% • 11%
1	B	1325	5% 86% • 11%
1	C	1325	5% 86% • 11%
2	D	6	17% 100%
2	Y	6	17% 100%
2	t	6	17% 100%
3	2	2	50% 100%
3	5	2	100% 100%
3	6	2	50% 100%

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Mol	Chain	Length	Quality of chain
3	7	2	50% 100%
3	8	2	50% 100%
3	9	2	100% 100%
3	CA	2	100%
3	E	2	50% 100%
3	G	2	50% 100%
3	I	2	100% 100%
3	J	2	50% 100%
3	M	2	100% 100%
3	P	2	100% 100%
3	Q	2	50% 100%
3	R	2	50% 100%
3	S	2	50% 100%
3	T	2	100% 100%
3	W	2	100%
3	Z	2	100%
3	b	2	50% 100%
3	d	2	100% 100%
3	e	2	50% 100%
3	h	2	50% 100%
3	k	2	100% 100%
3	l	2	50% 100%
3	m	2	50% 100%
3	n	2	50% 100%
3	o	2	100% 100%

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Mol	Chain	Length	Quality of chain
3	r	2	100%
3	u	2	50% 100%
3	w	2	50% 100%
3	y	2	100% 100%
3	z	2	50% 100%
4	AA	4	75% 100%
4	F	4	50% 100%
4	U	4	75% 100%
4	a	4	50% 100%
4	p	4	75% 100%
4	v	4	50% 100%
5	H	4	50% 100%
5	c	4	50% 100%
5	x	4	50% 100%
6	0	8	38% 100%
6	K	8	38% 100%
6	f	8	38% 100%
7	1	3	67% 100%
7	4	3	67% 100%
7	DA	3	67% 100%
7	L	3	67% 100%
7	O	3	67% 100%
7	X	3	67% 100%
7	g	3	67% 100%
7	j	3	67% 100%

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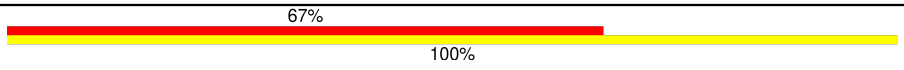
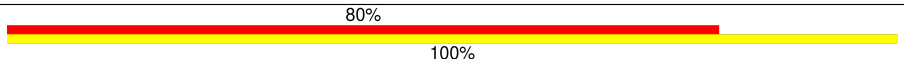
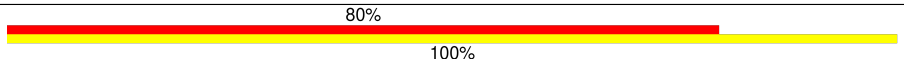
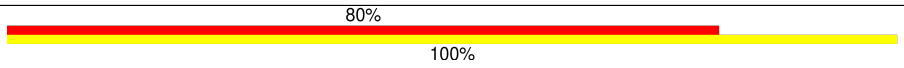
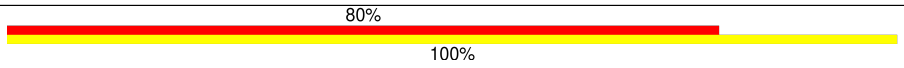
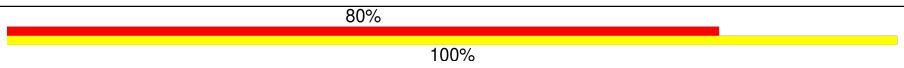
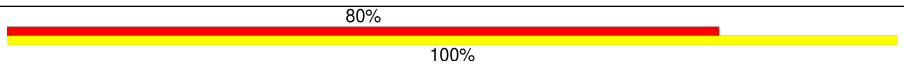
Mol	Chain	Length	Quality of chain
7	s	3	
8	3	5	
8	BA	5	
8	N	5	
8	V	5	
8	i	5	
8	q	5	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 30306 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		
1	B	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		
1	C	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	LEU	-	expression tag	UNP Q6Q1S2
A	1293	ILE	-	expression tag	UNP Q6Q1S2
A	1294	LYS	-	expression tag	UNP Q6Q1S2
A	1295	ARG	-	expression tag	UNP Q6Q1S2
A	1296	MET	-	expression tag	UNP Q6Q1S2
A	1297	LYS	-	expression tag	UNP Q6Q1S2
A	1298	GLN	-	expression tag	UNP Q6Q1S2
A	1299	ILE	-	expression tag	UNP Q6Q1S2
A	1300	GLU	-	expression tag	UNP Q6Q1S2
A	1301	ASP	-	expression tag	UNP Q6Q1S2
A	1302	LYS	-	expression tag	UNP Q6Q1S2
A	1303	ILE	-	expression tag	UNP Q6Q1S2
A	1304	GLU	-	expression tag	UNP Q6Q1S2
A	1305	GLU	-	expression tag	UNP Q6Q1S2
A	1306	ILE	-	expression tag	UNP Q6Q1S2
A	1307	GLU	-	expression tag	UNP Q6Q1S2
A	1308	SER	-	expression tag	UNP Q6Q1S2
A	1309	LYS	-	expression tag	UNP Q6Q1S2
A	1310	GLN	-	expression tag	UNP Q6Q1S2
A	1311	LYS	-	expression tag	UNP Q6Q1S2
A	1312	LYS	-	expression tag	UNP Q6Q1S2
A	1313	ILE	-	expression tag	UNP Q6Q1S2
A	1314	GLU	-	expression tag	UNP Q6Q1S2
A	1315	ASN	-	expression tag	UNP Q6Q1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1316	GLU	-	expression tag	UNP Q6Q1S2
A	1317	ILE	-	expression tag	UNP Q6Q1S2
A	1318	ALA	-	expression tag	UNP Q6Q1S2
A	1319	ARG	-	expression tag	UNP Q6Q1S2
A	1320	ILE	-	expression tag	UNP Q6Q1S2
A	1321	LYS	-	expression tag	UNP Q6Q1S2
A	1322	LYS	-	expression tag	UNP Q6Q1S2
A	1323	ILE	-	expression tag	UNP Q6Q1S2
A	1324	LYS	-	expression tag	UNP Q6Q1S2
A	1325	LEU	-	expression tag	UNP Q6Q1S2
A	1326	VAL	-	expression tag	UNP Q6Q1S2
A	1327	PRO	-	expression tag	UNP Q6Q1S2
A	1328	ARG	-	expression tag	UNP Q6Q1S2
A	1329	GLY	-	expression tag	UNP Q6Q1S2
A	1330	SER	-	expression tag	UNP Q6Q1S2
A	1331	LEU	-	expression tag	UNP Q6Q1S2
A	1332	GLU	-	expression tag	UNP Q6Q1S2
A	1333	TRP	-	expression tag	UNP Q6Q1S2
A	1334	SER	-	expression tag	UNP Q6Q1S2
A	1335	HIS	-	expression tag	UNP Q6Q1S2
A	1336	PRO	-	expression tag	UNP Q6Q1S2
A	1337	GLN	-	expression tag	UNP Q6Q1S2
A	1338	PHE	-	expression tag	UNP Q6Q1S2
A	1339	GLU	-	expression tag	UNP Q6Q1S2
A	1340	LYS	-	expression tag	UNP Q6Q1S2
B	1292	LEU	-	expression tag	UNP Q6Q1S2
B	1293	ILE	-	expression tag	UNP Q6Q1S2
B	1294	LYS	-	expression tag	UNP Q6Q1S2
B	1295	ARG	-	expression tag	UNP Q6Q1S2
B	1296	MET	-	expression tag	UNP Q6Q1S2
B	1297	LYS	-	expression tag	UNP Q6Q1S2
B	1298	GLN	-	expression tag	UNP Q6Q1S2
B	1299	ILE	-	expression tag	UNP Q6Q1S2
B	1300	GLU	-	expression tag	UNP Q6Q1S2
B	1301	ASP	-	expression tag	UNP Q6Q1S2
B	1302	LYS	-	expression tag	UNP Q6Q1S2
B	1303	ILE	-	expression tag	UNP Q6Q1S2
B	1304	GLU	-	expression tag	UNP Q6Q1S2
B	1305	GLU	-	expression tag	UNP Q6Q1S2
B	1306	ILE	-	expression tag	UNP Q6Q1S2
B	1307	GLU	-	expression tag	UNP Q6Q1S2
B	1308	SER	-	expression tag	UNP Q6Q1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1309	LYS	-	expression tag	UNP Q6Q1S2
B	1310	GLN	-	expression tag	UNP Q6Q1S2
B	1311	LYS	-	expression tag	UNP Q6Q1S2
B	1312	LYS	-	expression tag	UNP Q6Q1S2
B	1313	ILE	-	expression tag	UNP Q6Q1S2
B	1314	GLU	-	expression tag	UNP Q6Q1S2
B	1315	ASN	-	expression tag	UNP Q6Q1S2
B	1316	GLU	-	expression tag	UNP Q6Q1S2
B	1317	ILE	-	expression tag	UNP Q6Q1S2
B	1318	ALA	-	expression tag	UNP Q6Q1S2
B	1319	ARG	-	expression tag	UNP Q6Q1S2
B	1320	ILE	-	expression tag	UNP Q6Q1S2
B	1321	LYS	-	expression tag	UNP Q6Q1S2
B	1322	LYS	-	expression tag	UNP Q6Q1S2
B	1323	ILE	-	expression tag	UNP Q6Q1S2
B	1324	LYS	-	expression tag	UNP Q6Q1S2
B	1325	LEU	-	expression tag	UNP Q6Q1S2
B	1326	VAL	-	expression tag	UNP Q6Q1S2
B	1327	PRO	-	expression tag	UNP Q6Q1S2
B	1328	ARG	-	expression tag	UNP Q6Q1S2
B	1329	GLY	-	expression tag	UNP Q6Q1S2
B	1330	SER	-	expression tag	UNP Q6Q1S2
B	1331	LEU	-	expression tag	UNP Q6Q1S2
B	1332	GLU	-	expression tag	UNP Q6Q1S2
B	1333	TRP	-	expression tag	UNP Q6Q1S2
B	1334	SER	-	expression tag	UNP Q6Q1S2
B	1335	HIS	-	expression tag	UNP Q6Q1S2
B	1336	PRO	-	expression tag	UNP Q6Q1S2
B	1337	GLN	-	expression tag	UNP Q6Q1S2
B	1338	PHE	-	expression tag	UNP Q6Q1S2
B	1339	GLU	-	expression tag	UNP Q6Q1S2
B	1340	LYS	-	expression tag	UNP Q6Q1S2
C	1292	LEU	-	expression tag	UNP Q6Q1S2
C	1293	ILE	-	expression tag	UNP Q6Q1S2
C	1294	LYS	-	expression tag	UNP Q6Q1S2
C	1295	ARG	-	expression tag	UNP Q6Q1S2
C	1296	MET	-	expression tag	UNP Q6Q1S2
C	1297	LYS	-	expression tag	UNP Q6Q1S2
C	1298	GLN	-	expression tag	UNP Q6Q1S2
C	1299	ILE	-	expression tag	UNP Q6Q1S2
C	1300	GLU	-	expression tag	UNP Q6Q1S2
C	1301	ASP	-	expression tag	UNP Q6Q1S2

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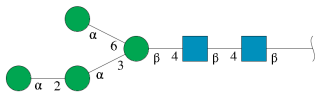
Chain	Residue	Modelled	Actual	Comment	Reference
C	1302	LYS	-	expression tag	UNP Q6Q1S2
C	1303	ILE	-	expression tag	UNP Q6Q1S2
C	1304	GLU	-	expression tag	UNP Q6Q1S2
C	1305	GLU	-	expression tag	UNP Q6Q1S2
C	1306	ILE	-	expression tag	UNP Q6Q1S2
C	1307	GLU	-	expression tag	UNP Q6Q1S2
C	1308	SER	-	expression tag	UNP Q6Q1S2
C	1309	LYS	-	expression tag	UNP Q6Q1S2
C	1310	GLN	-	expression tag	UNP Q6Q1S2
C	1311	LYS	-	expression tag	UNP Q6Q1S2
C	1312	LYS	-	expression tag	UNP Q6Q1S2
C	1313	ILE	-	expression tag	UNP Q6Q1S2
C	1314	GLU	-	expression tag	UNP Q6Q1S2
C	1315	ASN	-	expression tag	UNP Q6Q1S2
C	1316	GLU	-	expression tag	UNP Q6Q1S2
C	1317	ILE	-	expression tag	UNP Q6Q1S2
C	1318	ALA	-	expression tag	UNP Q6Q1S2
C	1319	ARG	-	expression tag	UNP Q6Q1S2
C	1320	ILE	-	expression tag	UNP Q6Q1S2
C	1321	LYS	-	expression tag	UNP Q6Q1S2
C	1322	LYS	-	expression tag	UNP Q6Q1S2
C	1323	ILE	-	expression tag	UNP Q6Q1S2
C	1324	LYS	-	expression tag	UNP Q6Q1S2
C	1325	LEU	-	expression tag	UNP Q6Q1S2
C	1326	VAL	-	expression tag	UNP Q6Q1S2
C	1327	PRO	-	expression tag	UNP Q6Q1S2
C	1328	ARG	-	expression tag	UNP Q6Q1S2
C	1329	GLY	-	expression tag	UNP Q6Q1S2
C	1330	SER	-	expression tag	UNP Q6Q1S2
C	1331	LEU	-	expression tag	UNP Q6Q1S2
C	1332	GLU	-	expression tag	UNP Q6Q1S2
C	1333	TRP	-	expression tag	UNP Q6Q1S2
C	1334	SER	-	expression tag	UNP Q6Q1S2
C	1335	HIS	-	expression tag	UNP Q6Q1S2
C	1336	PRO	-	expression tag	UNP Q6Q1S2
C	1337	GLN	-	expression tag	UNP Q6Q1S2
C	1338	PHE	-	expression tag	UNP Q6Q1S2
C	1339	GLU	-	expression tag	UNP Q6Q1S2
C	1340	LYS	-	expression tag	UNP Q6Q1S2

- Molecule 2 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
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	Y	6	Total	C	N	O	0	0
			72	40	2	30		
2	t	6	Total	C	N	O	0	0
			72	40	2	30		

- 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	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	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	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	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	h	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	m	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	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	r	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	w	2	Total	C	N	O	0	0
			28	16	2	10		
3	y	2	Total	C	N	O	0	0
			28	16	2	10		
3	z	2	Total	C	N	O	0	0
			28	16	2	10		
3	2	2	Total	C	N	O	0	0
			28	16	2	10		
3	5	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	7	2	Total	C	N	O	0	0
			28	16	2	10		
3	8	2	Total	C	N	O	0	0
			28	16	2	10		
3	9	2	Total	C	N	O	0	0
			28	16	2	10		
3	CA	2	Total	C	N	O	0	0
			28	16	2	10		

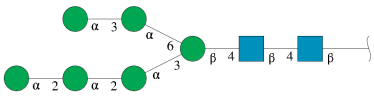
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	4	Total	C	N	O	0	0
			50	28	2	20		
4	U	4	Total	C	N	O	0	0
			50	28	2	20		
4	a	4	Total	C	N	O	0	0
			50	28	2	20		
4	p	4	Total	C	N	O	0	0
			50	28	2	20		
4	v	4	Total	C	N	O	0	0
			50	28	2	20		
4	AA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 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.

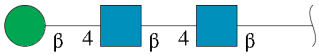
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	4	Total	C	N	O	0	0
			50	28	2	20		
5	c	4	Total	C	N	O	0	0
			50	28	2	20		
5	x	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



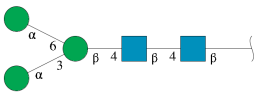
Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	8	Total	C	N	O	0	0
			94	52	2	40		
6	f	8	Total	C	N	O	0	0
			94	52	2	40		
6	0	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 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.



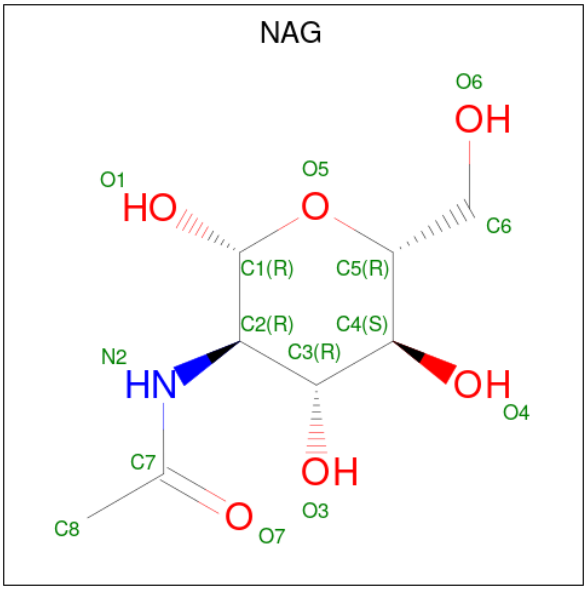
Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	3	Total	C	N	O	0	0
			39	22	2	15		
7	O	3	Total	C	N	O	0	0
			39	22	2	15		
7	X	3	Total	C	N	O	0	0
			39	22	2	15		
7	g	3	Total	C	N	O	0	0
			39	22	2	15		
7	j	3	Total	C	N	O	0	0
			39	22	2	15		
7	s	3	Total	C	N	O	0	0
			39	22	2	15		
7	1	3	Total	C	N	O	0	0
			39	22	2	15		
7	4	3	Total	C	N	O	0	0
			39	22	2	15		
7	DA	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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
8	N	5	Total C N O 61 34 2 25	0	0
8	V	5	Total C N O 61 34 2 25	0	0
8	i	5	Total C N O 61 34 2 25	0	0
8	q	5	Total C N O 61 34 2 25	0	0
8	3	5	Total C N O 61 34 2 25	0	0
8	BA	5	Total C N O 61 34 2 25	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

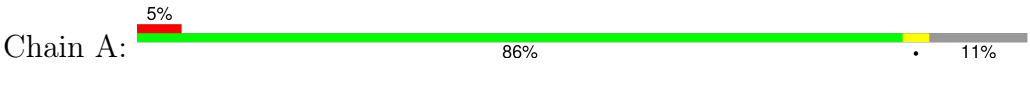
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O 14 8 1 5	0
9	A	1	Total C N O 14 8 1 5	0
9	A	1	Total C N O 14 8 1 5	0
9	A	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	B	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0
9	C	1	Total C N O 14 8 1 5	0

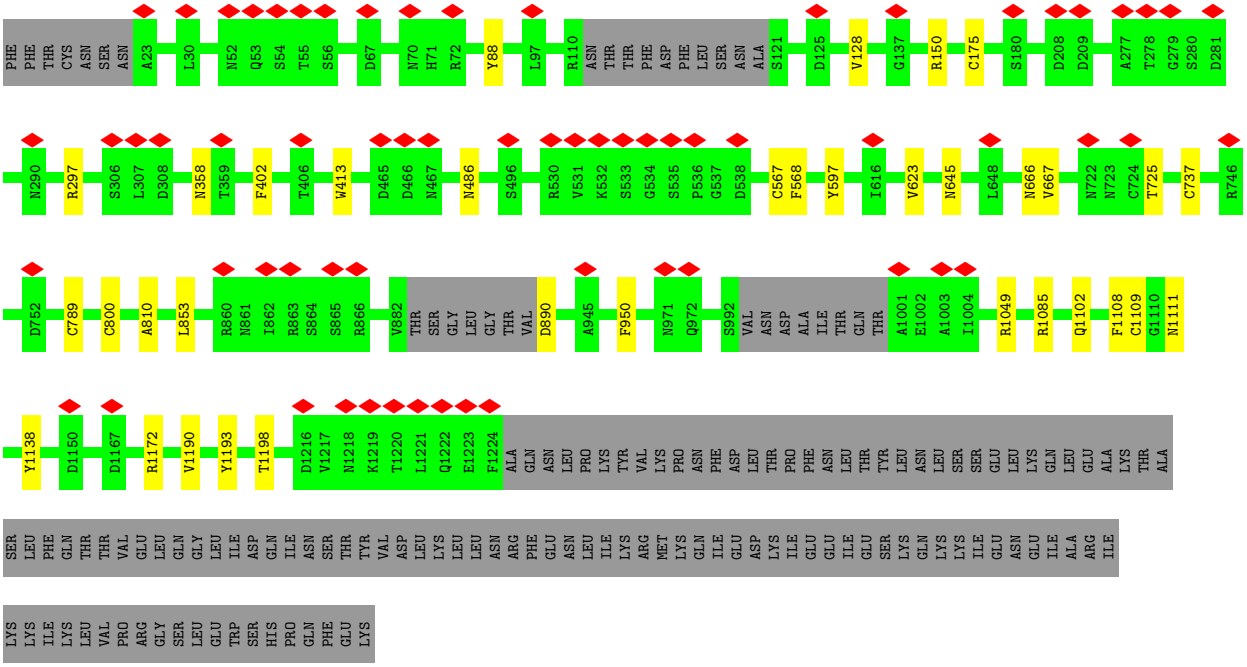
3 Residue-property plots (i)

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: Spike glycoprotein

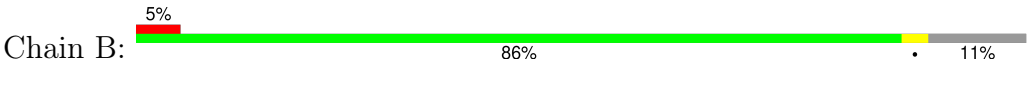
Chain A:

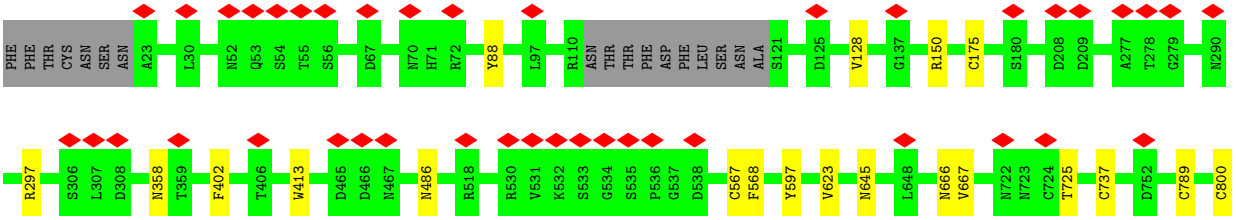


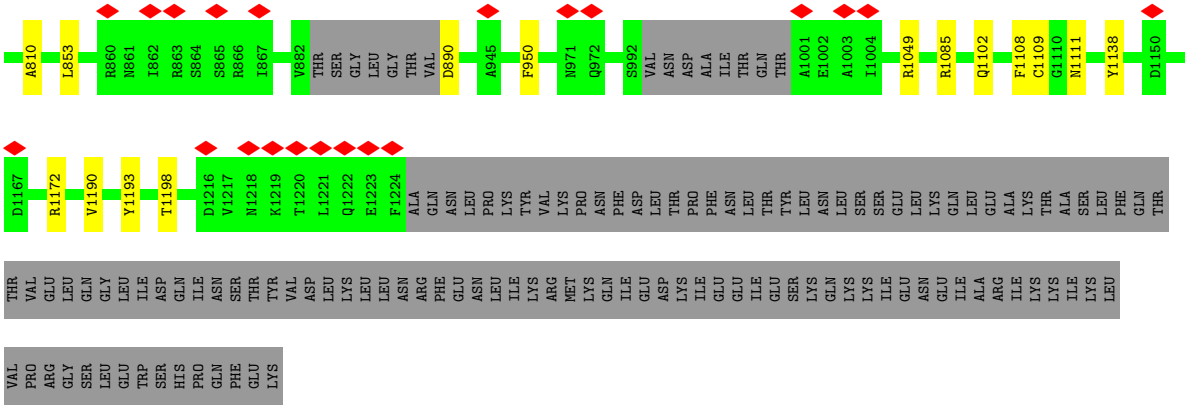


• Molecule 1: Spike glycoprotein

Chain B:

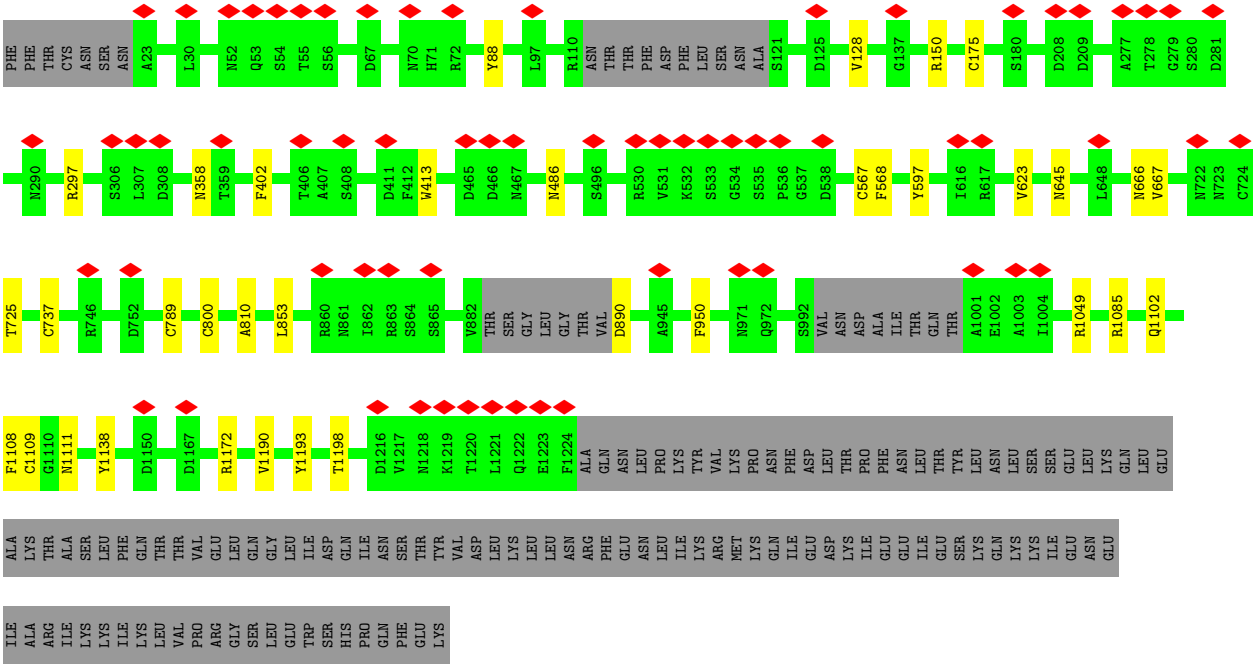






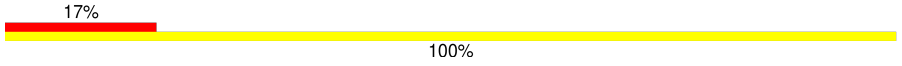
• Molecule 1: Spike glycoprotein

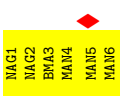
Chain C:



• Molecule 2: 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

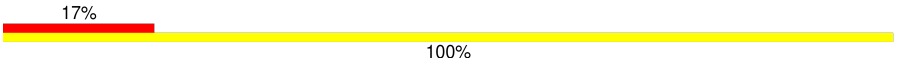
Chain D:





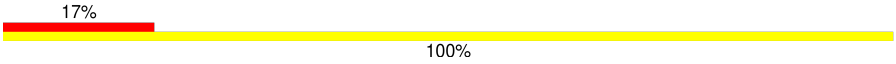
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



• Molecule 2: 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 t:

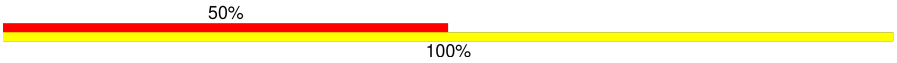


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain G:

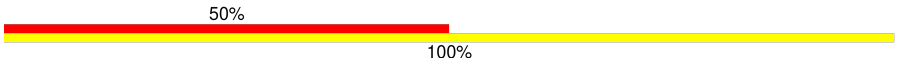


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



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

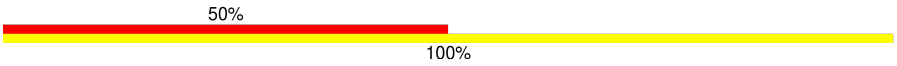
Chain M:

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

Chain P:

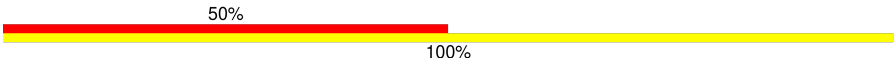
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



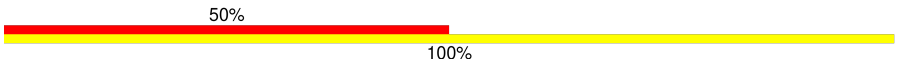
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain S:

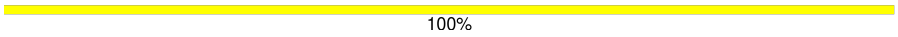


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

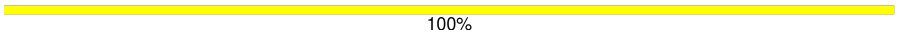
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



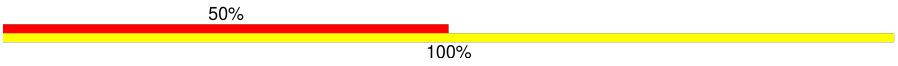
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain b:

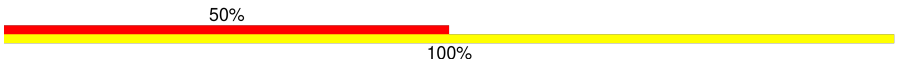


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

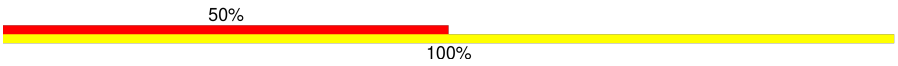
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain h:

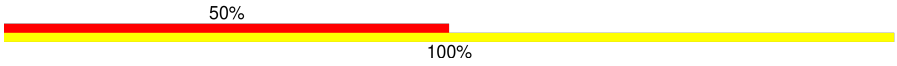


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

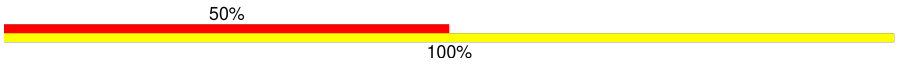
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



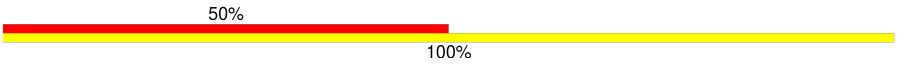
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



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

Chain n:

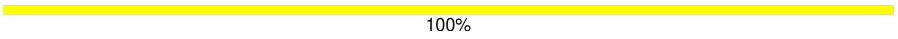


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

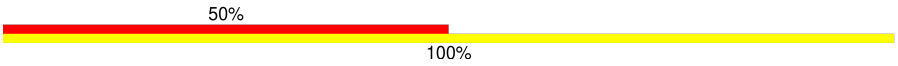
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



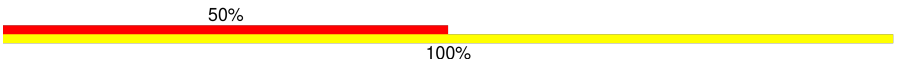
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



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

Chain w:

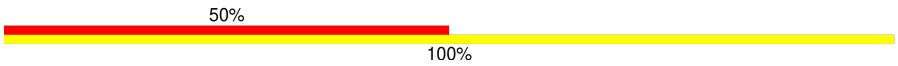


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:

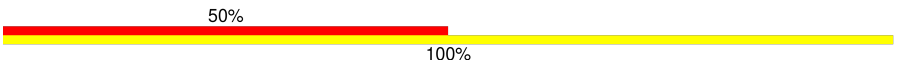
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



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

Chain 2:

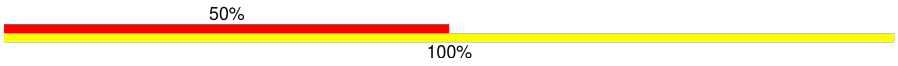


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:

• 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 7:

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

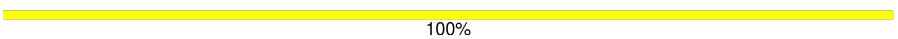
Chain 8:

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

Chain 9:

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

Chain CA:

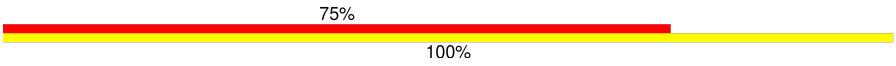


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

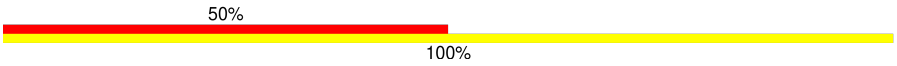
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 4: 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 a:

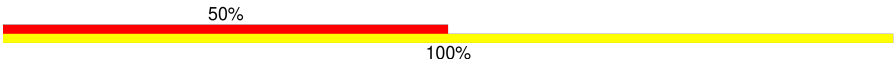


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

• Molecule 4: 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:

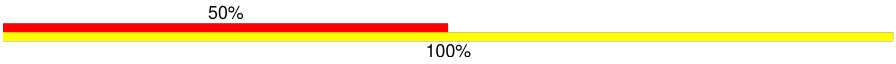


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:

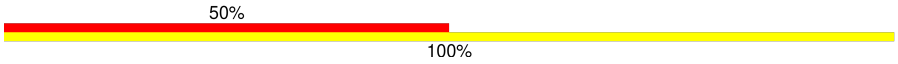
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



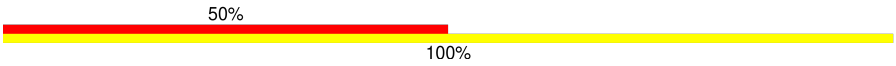
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 5: 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:

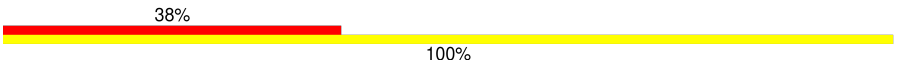


• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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

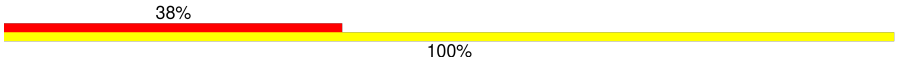
Chain f:



• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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-glucopyranos
e

Chain 0:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

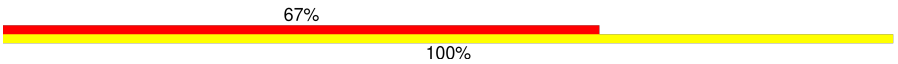
Chain L:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain O:

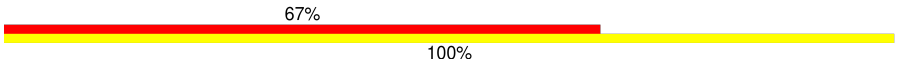
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain X:



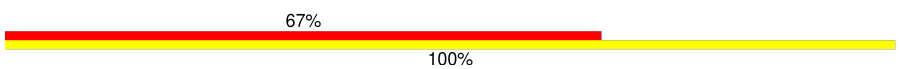
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain g:



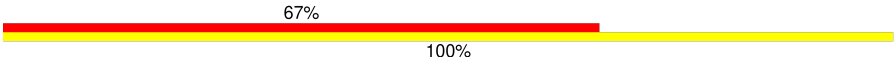
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain j:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:

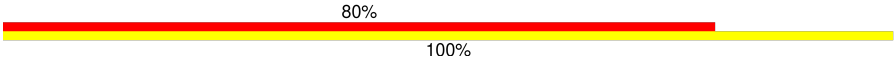
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 8: 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-glucopyra

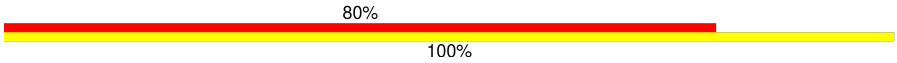
nose

Chain V:



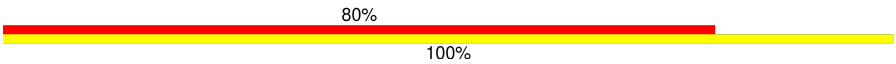
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain i:



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

Chain q:



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

Chain 3:

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

Chain BA:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	79667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
1	B	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
1	C	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
All	All	0.95	30/28035 (0.1%)	0.82	36/38241 (0.1%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	737	CYS	CB-SG	-8.38	1.68	1.82
1	C	737	CYS	CB-SG	-8.37	1.68	1.82
1	B	737	CYS	CB-SG	-8.34	1.68	1.82
1	C	800	CYS	CB-SG	-7.71	1.69	1.82
1	A	800	CYS	CB-SG	-7.70	1.69	1.82

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	C	297	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	297	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	C	1172	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	B	1172	ARG	NE-CZ-NH2	-8.53	116.04	120.30

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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1169/1325 (88%)	1095 (94%)	67 (6%)	7 (1%)	22	50
1	B	1169/1325 (88%)	1096 (94%)	66 (6%)	7 (1%)	22	50
1	C	1169/1325 (88%)	1095 (94%)	67 (6%)	7 (1%)	22	50
All	All	3507/3975 (88%)	3286 (94%)	200 (6%)	21 (1%)	24	50

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	667	VAL
1	A	853	LEU
1	B	667	VAL
1	B	853	LEU
1	C	667	VAL

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	1031/1169 (88%)	1023 (99%)	8 (1%)	79	87
1	B	1031/1169 (88%)	1023 (99%)	8 (1%)	79	87
1	C	1031/1169 (88%)	1023 (99%)	8 (1%)	79	87
All	All	3093/3507 (88%)	3069 (99%)	24 (1%)	77	87

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1111	ASN
1	C	358	ASN
1	C	175	CYS
1	C	402	PHE
1	A	1111	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	ASN
1	B	660	ASN
1	C	660	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

201 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	$\#\|Z\| > 2$
6	NAG	0	1	1,6	14,14,15	2.69	3 (21%)	17,19,21	3.96	6 (35%)
6	NAG	0	2	6	14,14,15	2.81	4 (28%)	17,19,21	3.54	5 (29%)
6	BMA	0	3	6	11,11,12	1.84	2 (18%)	15,15,17	5.50	6 (40%)
6	MAN	0	4	6	11,11,12	1.69	2 (18%)	15,15,17	8.19	6 (40%)
6	MAN	0	5	6	11,11,12	1.69	3 (27%)	15,15,17	4.22	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	0	6	6	11,11,12	1.97	3 (27%)	15,15,17	2.47	1 (6%)
6	MAN	0	7	6	11,11,12	1.93	4 (36%)	15,15,17	5.07	6 (40%)
6	MAN	0	8	6	11,11,12	2.57	6 (54%)	15,15,17	3.75	6 (40%)
7	NAG	1	1	1,7	14,14,15	3.23	4 (28%)	17,19,21	5.61	6 (35%)
7	NAG	1	2	7	14,14,15	2.96	4 (28%)	17,19,21	2.72	7 (41%)
7	BMA	1	3	7	11,11,12	2.06	5 (45%)	15,15,17	3.60	5 (33%)
3	NAG	2	1	1,3	14,14,15	2.80	3 (21%)	17,19,21	4.13	6 (35%)
3	NAG	2	2	3	14,14,15	2.81	3 (21%)	17,19,21	2.10	3 (17%)
8	NAG	3	1	1,8	14,14,15	2.62	3 (21%)	17,19,21	3.21	6 (35%)
8	NAG	3	2	8	14,14,15	2.79	3 (21%)	17,19,21	6.10	7 (41%)
8	BMA	3	3	8	11,11,12	1.86	3 (27%)	15,15,17	2.98	5 (33%)
8	MAN	3	4	8	11,11,12	2.08	5 (45%)	15,15,17	2.73	6 (40%)
8	MAN	3	5	8	11,11,12	1.96	4 (36%)	15,15,17	3.02	5 (33%)
7	NAG	4	1	1,7	14,14,15	2.85	3 (21%)	17,19,21	3.06	5 (29%)
7	NAG	4	2	7	14,14,15	2.91	4 (28%)	17,19,21	4.01	8 (47%)
7	BMA	4	3	7	11,11,12	1.95	3 (27%)	15,15,17	3.81	5 (33%)
3	NAG	5	1	1,3	14,14,15	2.77	3 (21%)	17,19,21	3.46	5 (29%)
3	NAG	5	2	3	14,14,15	2.78	4 (28%)	17,19,21	2.60	6 (35%)
3	NAG	6	1	1,3	14,14,15	2.77	4 (28%)	17,19,21	4.60	7 (41%)
3	NAG	6	2	3	14,14,15	2.79	2 (14%)	17,19,21	2.88	3 (17%)
3	NAG	7	1	1,3	14,14,15	2.68	3 (21%)	17,19,21	3.79	6 (35%)
3	NAG	7	2	3	14,14,15	2.92	3 (21%)	17,19,21	3.64	4 (23%)
3	NAG	8	1	1,3	14,14,15	2.77	3 (21%)	17,19,21	3.83	4 (23%)
3	NAG	8	2	3	14,14,15	2.68	4 (28%)	17,19,21	2.26	2 (11%)
3	NAG	9	1	1,3	14,14,15	2.73	3 (21%)	17,19,21	4.09	3 (17%)
3	NAG	9	2	3	14,14,15	2.90	3 (21%)	17,19,21	3.23	4 (23%)
4	NAG	AA	1	1,4	14,14,15	2.63	3 (21%)	17,19,21	5.21	5 (29%)
4	NAG	AA	2	4	14,14,15	2.86	3 (21%)	17,19,21	3.32	6 (35%)
4	BMA	AA	3	4	11,11,12	1.82	1 (9%)	15,15,17	4.26	4 (26%)
4	MAN	AA	4	4	11,11,12	2.00	3 (27%)	15,15,17	3.43	6 (40%)
8	NAG	BA	1	1,8	14,14,15	2.69	3 (21%)	17,19,21	4.18	7 (41%)
8	NAG	BA	2	8	14,14,15	2.75	4 (28%)	17,19,21	5.47	8 (47%)
8	BMA	BA	3	8	11,11,12	1.85	3 (27%)	15,15,17	4.41	6 (40%)
8	MAN	BA	4	8	11,11,12	2.06	4 (36%)	15,15,17	2.91	5 (33%)
8	MAN	BA	5	8	11,11,12	2.02	4 (36%)	15,15,17	3.74	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	CA	1	1,3	14,14,15	2.86	4 (28%)	17,19,21	5.69	7 (41%)
3	NAG	CA	2	3	14,14,15	2.90	2 (14%)	17,19,21	1.63	3 (17%)
2	NAG	D	1	1,2	14,14,15	2.66	3 (21%)	17,19,21	3.24	5 (29%)
2	NAG	D	2	2	14,14,15	2.81	4 (28%)	17,19,21	5.15	8 (47%)
2	BMA	D	3	2	11,11,12	1.98	4 (36%)	15,15,17	3.11	5 (33%)
2	MAN	D	4	2	11,11,12	1.93	4 (36%)	15,15,17	4.11	5 (33%)
2	MAN	D	5	2	11,11,12	2.66	6 (54%)	15,15,17	2.54	6 (40%)
2	MAN	D	6	2	11,11,12	2.58	6 (54%)	15,15,17	3.27	5 (33%)
7	NAG	DA	1	1,7	14,14,15	2.73	3 (21%)	17,19,21	4.54	6 (35%)
7	NAG	DA	2	7	14,14,15	2.81	3 (21%)	17,19,21	5.78	9 (52%)
7	BMA	DA	3	7	11,11,12	2.03	3 (27%)	15,15,17	3.22	5 (33%)
3	NAG	E	1	1,3	14,14,15	2.88	3 (21%)	17,19,21	3.89	7 (41%)
3	NAG	E	2	3	14,14,15	3.20	6 (42%)	17,19,21	3.74	6 (35%)
4	NAG	F	1	1,4	14,14,15	2.73	3 (21%)	17,19,21	5.68	6 (35%)
4	NAG	F	2	4	14,14,15	2.74	3 (21%)	17,19,21	7.16	6 (35%)
4	BMA	F	3	4	11,11,12	1.84	3 (27%)	15,15,17	2.78	4 (26%)
4	MAN	F	4	4	11,11,12	2.01	3 (27%)	15,15,17	3.46	5 (33%)
3	NAG	G	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	2.43	5 (29%)
3	NAG	G	2	3	14,14,15	2.81	3 (21%)	17,19,21	4.44	4 (23%)
5	NAG	H	1	1,5	14,14,15	2.70	3 (21%)	17,19,21	2.90	5 (29%)
5	NAG	H	2	5	14,14,15	2.95	3 (21%)	17,19,21	4.86	8 (47%)
5	BMA	H	3	5	11,11,12	1.88	3 (27%)	15,15,17	3.45	4 (26%)
5	MAN	H	4	5	11,11,12	1.91	3 (27%)	15,15,17	3.41	5 (33%)
3	NAG	I	1	1,3	14,14,15	2.73	3 (21%)	17,19,21	4.44	6 (35%)
3	NAG	I	2	3	14,14,15	2.90	4 (28%)	17,19,21	2.11	3 (17%)
3	NAG	J	1	1,3	14,14,15	2.58	3 (21%)	17,19,21	5.00	6 (35%)
3	NAG	J	2	3	14,14,15	2.68	3 (21%)	17,19,21	2.10	4 (23%)
6	NAG	K	1	1,6	14,14,15	2.69	3 (21%)	17,19,21	3.96	6 (35%)
6	NAG	K	2	6	14,14,15	2.82	4 (28%)	17,19,21	3.54	5 (29%)
6	BMA	K	3	6	11,11,12	1.84	2 (18%)	15,15,17	5.49	6 (40%)
6	MAN	K	4	6	11,11,12	1.70	2 (18%)	15,15,17	8.19	6 (40%)
6	MAN	K	5	6	11,11,12	1.70	3 (27%)	15,15,17	4.22	5 (33%)
6	MAN	K	6	6	11,11,12	1.96	3 (27%)	15,15,17	2.47	1 (6%)
6	MAN	K	7	6	11,11,12	1.93	4 (36%)	15,15,17	5.07	6 (40%)
6	MAN	K	8	6	11,11,12	2.57	6 (54%)	15,15,17	3.74	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	L	1	1,7	14,14,15	3.23	4 (28%)	17,19,21	5.61	6 (35%)
7	NAG	L	2	7	14,14,15	2.97	4 (28%)	17,19,21	2.73	7 (41%)
7	BMA	L	3	7	11,11,12	2.07	5 (45%)	15,15,17	3.60	5 (33%)
3	NAG	M	1	1,3	14,14,15	2.79	3 (21%)	17,19,21	4.14	6 (35%)
3	NAG	M	2	3	14,14,15	2.82	3 (21%)	17,19,21	2.09	3 (17%)
8	NAG	N	1	1,8	14,14,15	2.62	3 (21%)	17,19,21	3.21	6 (35%)
8	NAG	N	2	8	14,14,15	2.79	3 (21%)	17,19,21	6.11	7 (41%)
8	BMA	N	3	8	11,11,12	1.87	3 (27%)	15,15,17	2.98	5 (33%)
8	MAN	N	4	8	11,11,12	2.07	5 (45%)	15,15,17	2.73	6 (40%)
8	MAN	N	5	8	11,11,12	1.96	4 (36%)	15,15,17	3.02	5 (33%)
7	NAG	O	1	1,7	14,14,15	2.86	3 (21%)	17,19,21	3.06	5 (29%)
7	NAG	O	2	7	14,14,15	2.91	4 (28%)	17,19,21	4.01	8 (47%)
7	BMA	O	3	7	11,11,12	1.95	3 (27%)	15,15,17	3.81	5 (33%)
3	NAG	P	1	1,3	14,14,15	2.78	3 (21%)	17,19,21	3.47	5 (29%)
3	NAG	P	2	3	14,14,15	2.78	4 (28%)	17,19,21	2.60	6 (35%)
3	NAG	Q	1	1,3	14,14,15	2.77	4 (28%)	17,19,21	4.60	7 (41%)
3	NAG	Q	2	3	14,14,15	2.79	2 (14%)	17,19,21	2.88	3 (17%)
3	NAG	R	1	1,3	14,14,15	2.67	3 (21%)	17,19,21	3.79	6 (35%)
3	NAG	R	2	3	14,14,15	2.93	3 (21%)	17,19,21	3.64	4 (23%)
3	NAG	S	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	3.83	4 (23%)
3	NAG	S	2	3	14,14,15	2.68	4 (28%)	17,19,21	2.27	2 (11%)
3	NAG	T	1	1,3	14,14,15	2.72	3 (21%)	17,19,21	4.09	3 (17%)
3	NAG	T	2	3	14,14,15	2.89	3 (21%)	17,19,21	3.23	4 (23%)
4	NAG	U	1	1,4	14,14,15	2.64	3 (21%)	17,19,21	5.21	5 (29%)
4	NAG	U	2	4	14,14,15	2.86	3 (21%)	17,19,21	3.32	6 (35%)
4	BMA	U	3	4	11,11,12	1.82	2 (18%)	15,15,17	4.26	4 (26%)
4	MAN	U	4	4	11,11,12	2.01	3 (27%)	15,15,17	3.43	6 (40%)
8	NAG	V	1	1,8	14,14,15	2.69	3 (21%)	17,19,21	4.18	7 (41%)
8	NAG	V	2	8	14,14,15	2.75	4 (28%)	17,19,21	5.47	8 (47%)
8	BMA	V	3	8	11,11,12	1.85	2 (18%)	15,15,17	4.41	6 (40%)
8	MAN	V	4	8	11,11,12	2.05	4 (36%)	15,15,17	2.91	5 (33%)
8	MAN	V	5	8	11,11,12	2.02	4 (36%)	15,15,17	3.74	4 (26%)
3	NAG	W	1	1,3	14,14,15	2.87	4 (28%)	17,19,21	5.69	7 (41%)
3	NAG	W	2	3	14,14,15	2.90	2 (14%)	17,19,21	1.63	3 (17%)
7	NAG	X	1	1,7	14,14,15	2.73	3 (21%)	17,19,21	4.54	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	X	2	7	14,14,15	2.81	3 (21%)	17,19,21	5.78	9 (52%)
7	BMA	X	3	7	11,11,12	2.04	3 (27%)	15,15,17	3.22	5 (33%)
2	NAG	Y	1	1,2	14,14,15	2.67	3 (21%)	17,19,21	3.24	5 (29%)
2	NAG	Y	2	2	14,14,15	2.81	4 (28%)	17,19,21	5.15	8 (47%)
2	BMA	Y	3	2	11,11,12	1.99	4 (36%)	15,15,17	3.11	5 (33%)
2	MAN	Y	4	2	11,11,12	1.93	4 (36%)	15,15,17	4.11	5 (33%)
2	MAN	Y	5	2	11,11,12	2.65	6 (54%)	15,15,17	2.54	6 (40%)
2	MAN	Y	6	2	11,11,12	2.58	6 (54%)	15,15,17	3.27	5 (33%)
3	NAG	Z	1	1,3	14,14,15	2.88	3 (21%)	17,19,21	3.90	7 (41%)
3	NAG	Z	2	3	14,14,15	3.20	6 (42%)	17,19,21	3.74	6 (35%)
4	NAG	a	1	1,4	14,14,15	2.73	3 (21%)	17,19,21	5.68	6 (35%)
4	NAG	a	2	4	14,14,15	2.74	3 (21%)	17,19,21	7.16	6 (35%)
4	BMA	a	3	4	11,11,12	1.84	3 (27%)	15,15,17	2.78	4 (26%)
4	MAN	a	4	4	11,11,12	2.00	3 (27%)	15,15,17	3.46	5 (33%)
3	NAG	b	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	2.43	5 (29%)
3	NAG	b	2	3	14,14,15	2.80	3 (21%)	17,19,21	4.44	4 (23%)
5	NAG	c	1	1,5	14,14,15	2.70	3 (21%)	17,19,21	2.90	5 (29%)
5	NAG	c	2	5	14,14,15	2.94	3 (21%)	17,19,21	4.85	8 (47%)
5	BMA	c	3	5	11,11,12	1.87	3 (27%)	15,15,17	3.45	4 (26%)
5	MAN	c	4	5	11,11,12	1.92	3 (27%)	15,15,17	3.41	5 (33%)
3	NAG	d	1	1,3	14,14,15	2.73	3 (21%)	17,19,21	4.44	6 (35%)
3	NAG	d	2	3	14,14,15	2.90	4 (28%)	17,19,21	2.10	3 (17%)
3	NAG	e	1	1,3	14,14,15	2.58	3 (21%)	17,19,21	5.00	6 (35%)
3	NAG	e	2	3	14,14,15	2.68	3 (21%)	17,19,21	2.10	4 (23%)
6	NAG	f	1	1,6	14,14,15	2.69	3 (21%)	17,19,21	3.96	6 (35%)
6	NAG	f	2	6	14,14,15	2.82	4 (28%)	17,19,21	3.54	5 (29%)
6	BMA	f	3	6	11,11,12	1.83	2 (18%)	15,15,17	5.49	6 (40%)
6	MAN	f	4	6	11,11,12	1.70	2 (18%)	15,15,17	8.19	6 (40%)
6	MAN	f	5	6	11,11,12	1.70	3 (27%)	15,15,17	4.22	5 (33%)
6	MAN	f	6	6	11,11,12	1.96	3 (27%)	15,15,17	2.47	1 (6%)
6	MAN	f	7	6	11,11,12	1.92	4 (36%)	15,15,17	5.08	6 (40%)
6	MAN	f	8	6	11,11,12	2.57	6 (54%)	15,15,17	3.74	6 (40%)
7	NAG	g	1	1,7	14,14,15	3.22	4 (28%)	17,19,21	5.61	6 (35%)
7	NAG	g	2	7	14,14,15	2.98	4 (28%)	17,19,21	2.73	7 (41%)
7	BMA	g	3	7	11,11,12	2.07	5 (45%)	15,15,17	3.60	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	h	1	1,3	14,14,15	2.79	3 (21%)	17,19,21	4.13	6 (35%)
3	NAG	h	2	3	14,14,15	2.81	3 (21%)	17,19,21	2.09	3 (17%)
8	NAG	i	1	1,8	14,14,15	2.61	3 (21%)	17,19,21	3.21	6 (35%)
8	NAG	i	2	8	14,14,15	2.79	3 (21%)	17,19,21	6.11	7 (41%)
8	BMA	i	3	8	11,11,12	1.86	3 (27%)	15,15,17	2.98	5 (33%)
8	MAN	i	4	8	11,11,12	2.08	5 (45%)	15,15,17	2.73	6 (40%)
8	MAN	i	5	8	11,11,12	1.96	4 (36%)	15,15,17	3.02	5 (33%)
7	NAG	j	1	1,7	14,14,15	2.85	3 (21%)	17,19,21	3.06	5 (29%)
7	NAG	j	2	7	14,14,15	2.91	4 (28%)	17,19,21	4.01	8 (47%)
7	BMA	j	3	7	11,11,12	1.95	3 (27%)	15,15,17	3.80	5 (33%)
3	NAG	k	1	1,3	14,14,15	2.77	3 (21%)	17,19,21	3.47	5 (29%)
3	NAG	k	2	3	14,14,15	2.78	4 (28%)	17,19,21	2.60	6 (35%)
3	NAG	l	1	1,3	14,14,15	2.77	4 (28%)	17,19,21	4.60	7 (41%)
3	NAG	l	2	3	14,14,15	2.79	2 (14%)	17,19,21	2.88	3 (17%)
3	NAG	m	1	1,3	14,14,15	2.68	3 (21%)	17,19,21	3.79	6 (35%)
3	NAG	m	2	3	14,14,15	2.93	3 (21%)	17,19,21	3.64	4 (23%)
3	NAG	n	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	3.83	4 (23%)
3	NAG	n	2	3	14,14,15	2.68	4 (28%)	17,19,21	2.27	2 (11%)
3	NAG	o	1	1,3	14,14,15	2.73	3 (21%)	17,19,21	4.09	3 (17%)
3	NAG	o	2	3	14,14,15	2.89	4 (28%)	17,19,21	3.23	4 (23%)
4	NAG	p	1	1,4	14,14,15	2.64	3 (21%)	17,19,21	5.22	5 (29%)
4	NAG	p	2	4	14,14,15	2.87	3 (21%)	17,19,21	3.32	6 (35%)
4	BMA	p	3	4	11,11,12	1.82	1 (9%)	15,15,17	4.26	4 (26%)
4	MAN	p	4	4	11,11,12	2.00	3 (27%)	15,15,17	3.43	6 (40%)
8	NAG	q	1	1,8	14,14,15	2.68	3 (21%)	17,19,21	4.18	7 (41%)
8	NAG	q	2	8	14,14,15	2.74	4 (28%)	17,19,21	5.47	8 (47%)
8	BMA	q	3	8	11,11,12	1.85	3 (27%)	15,15,17	4.41	6 (40%)
8	MAN	q	4	8	11,11,12	2.05	4 (36%)	15,15,17	2.91	5 (33%)
8	MAN	q	5	8	11,11,12	2.03	4 (36%)	15,15,17	3.74	4 (26%)
3	NAG	r	1	1,3	14,14,15	2.88	4 (28%)	17,19,21	5.69	7 (41%)
3	NAG	r	2	3	14,14,15	2.89	2 (14%)	17,19,21	1.63	3 (17%)
7	NAG	s	1	1,7	14,14,15	2.72	3 (21%)	17,19,21	4.55	6 (35%)
7	NAG	s	2	7	14,14,15	2.82	3 (21%)	17,19,21	5.78	9 (52%)
7	BMA	s	3	7	11,11,12	2.04	3 (27%)	15,15,17	3.23	5 (33%)
2	NAG	t	1	1,2	14,14,15	2.67	3 (21%)	17,19,21	3.24	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	t	2	2	14,14,15	2.81	4 (28%)	17,19,21	5.15	8 (47%)
2	BMA	t	3	2	11,11,12	1.99	4 (36%)	15,15,17	3.10	5 (33%)
2	MAN	t	4	2	11,11,12	1.94	4 (36%)	15,15,17	4.12	5 (33%)
2	MAN	t	5	2	11,11,12	2.66	6 (54%)	15,15,17	2.53	6 (40%)
2	MAN	t	6	2	11,11,12	2.57	6 (54%)	15,15,17	3.27	5 (33%)
3	NAG	u	1	1,3	14,14,15	2.87	3 (21%)	17,19,21	3.90	7 (41%)
3	NAG	u	2	3	14,14,15	3.20	6 (42%)	17,19,21	3.74	6 (35%)
4	NAG	v	1	1,4	14,14,15	2.73	3 (21%)	17,19,21	5.68	6 (35%)
4	NAG	v	2	4	14,14,15	2.74	3 (21%)	17,19,21	7.16	6 (35%)
4	BMA	v	3	4	11,11,12	1.84	3 (27%)	15,15,17	2.78	4 (26%)
4	MAN	v	4	4	11,11,12	2.01	3 (27%)	15,15,17	3.46	5 (33%)
3	NAG	w	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	2.43	5 (29%)
3	NAG	w	2	3	14,14,15	2.81	3 (21%)	17,19,21	4.44	4 (23%)
5	NAG	x	1	1,5	14,14,15	2.71	3 (21%)	17,19,21	2.90	5 (29%)
5	NAG	x	2	5	14,14,15	2.94	3 (21%)	17,19,21	4.86	8 (47%)
5	BMA	x	3	5	11,11,12	1.87	3 (27%)	15,15,17	3.45	4 (26%)
5	MAN	x	4	5	11,11,12	1.91	3 (27%)	15,15,17	3.41	5 (33%)
3	NAG	y	1	1,3	14,14,15	2.73	3 (21%)	17,19,21	4.44	6 (35%)
3	NAG	y	2	3	14,14,15	2.90	4 (28%)	17,19,21	2.11	3 (17%)
3	NAG	z	1	1,3	14,14,15	2.59	3 (21%)	17,19,21	5.00	6 (35%)
3	NAG	z	2	3	14,14,15	2.68	3 (21%)	17,19,21	2.10	4 (23%)

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
6	NAG	0	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	0	2	6	-	2/6/23/26	0/1/1/1
6	BMA	0	3	6	-	2/2/19/22	0/1/1/1
6	MAN	0	4	6	-	0/2/19/22	0/1/1/1
6	MAN	0	5	6	-	0/2/19/22	0/1/1/1
6	MAN	0	6	6	-	0/2/19/22	0/1/1/1
6	MAN	0	7	6	-	1/2/19/22	0/1/1/1
6	MAN	0	8	6	-	1/2/19/22	0/1/1/1
7	NAG	1	1	1,7	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	DA	3	7	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1
6	MAN	K	6	6	-	0/2/19/22	0/1/1/1
6	MAN	K	7	6	-	1/2/19/22	0/1/1/1
6	MAN	K	8	6	-	1/2/19/22	0/1/1/1
7	NAG	L	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
8	NAG	N	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	N	2	8	-	1/6/23/26	0/1/1/1
8	BMA	N	3	8	-	2/2/19/22	0/1/1/1
8	MAN	N	4	8	-	0/2/19/22	0/1/1/1
8	MAN	N	5	8	-	1/2/19/22	0/1/1/1
7	NAG	O	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	1/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	1/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	BMA	U	3	4	-	1/2/19/22	0/1/1/1
4	MAN	U	4	4	-	0/2/19/22	0/1/1/1
8	NAG	V	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	BMA	V	3	8	-	2/2/19/22	0/1/1/1
8	MAN	V	4	8	-	0/2/19/22	0/1/1/1
8	MAN	V	5	8	-	1/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	1/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	1/2/19/22	0/1/1/1
2	MAN	Y	4	2	-	1/2/19/22	0/1/1/1
2	MAN	Y	5	2	-	1/2/19/22	0/1/1/1
2	MAN	Y	6	2	-	1/2/19/22	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	a	2	4	-	1/6/23/26	0/1/1/1
4	BMA	a	3	4	-	1/2/19/22	0/1/1/1
4	MAN	a	4	4	-	0/2/19/22	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	1/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	-	0/2/19/22	0/1/1/1

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

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

The worst 5 of 685 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	8.80	1.58	1.43
3	u	2	NAG	O5-C1	8.79	1.58	1.43
3	Z	2	NAG	O5-C1	8.79	1.58	1.43
7	1	1	NAG	O5-C1	8.54	1.58	1.43
7	L	1	NAG	O5-C1	8.52	1.58	1.43

The worst 5 of 1074 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	0	4	MAN	O3-C3-C2	20.43	151.74	110.05
6	f	4	MAN	O3-C3-C2	20.42	151.73	110.05
6	K	4	MAN	O3-C3-C2	20.41	151.70	110.05
4	v	1	NAG	C1-C2-N2	20.35	142.51	110.43
4	F	1	NAG	C1-C2-N2	20.35	142.50	110.43

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

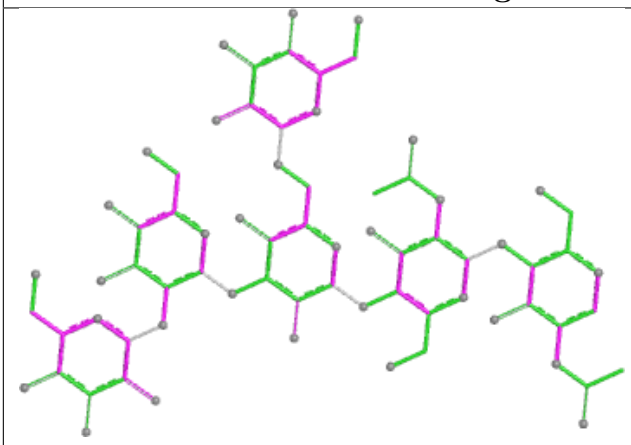
Mol	Chain	Res	Type	Atoms
3	W	1	NAG	C1-C2-N2-C7
3	r	1	NAG	C1-C2-N2-C7
3	CA	1	NAG	C1-C2-N2-C7
5	H	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6

There are no ring outliers.

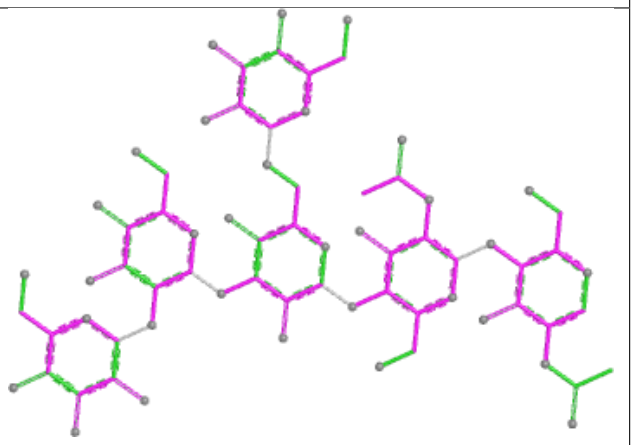
No monomer is involved in short contacts.

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

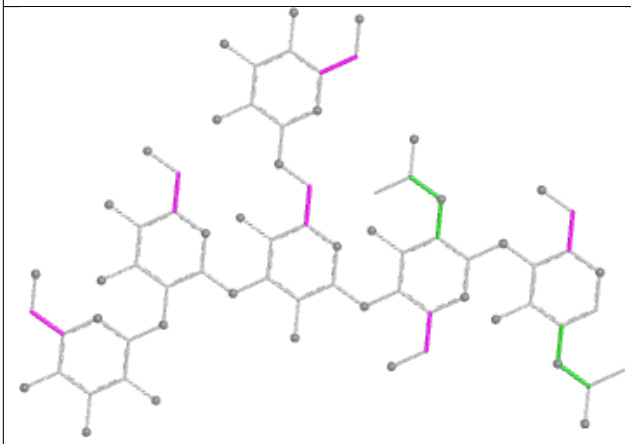
Oligosaccharide Chain D



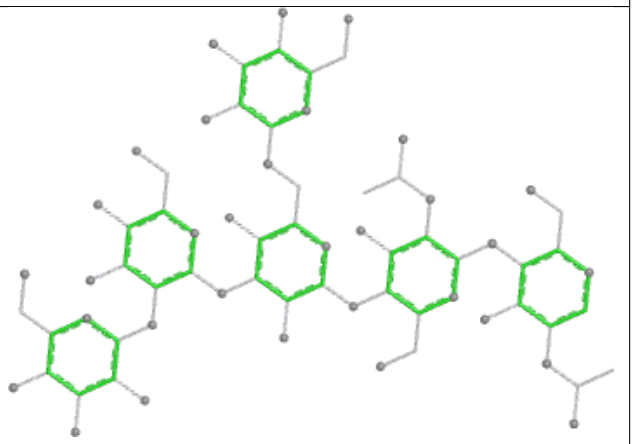
Bond lengths



Bond angles

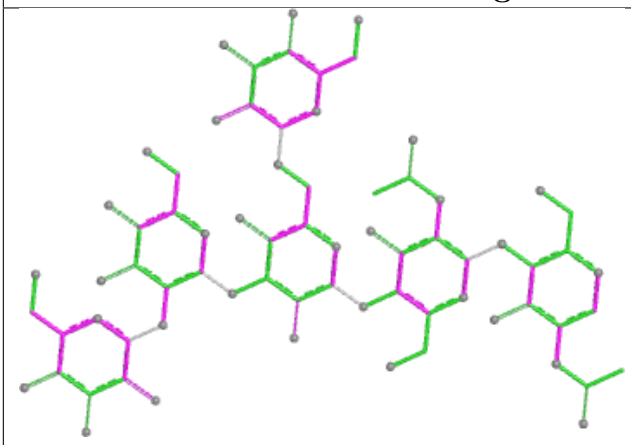


Torsions

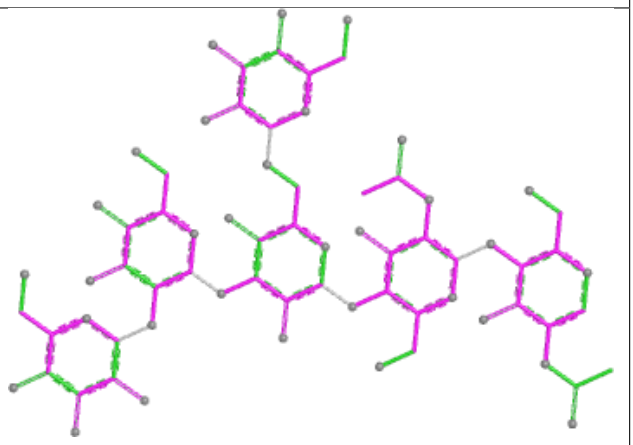


Rings

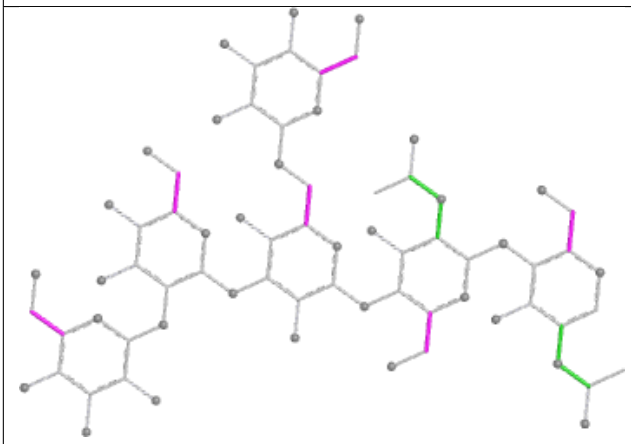
Oligosaccharide Chain Y



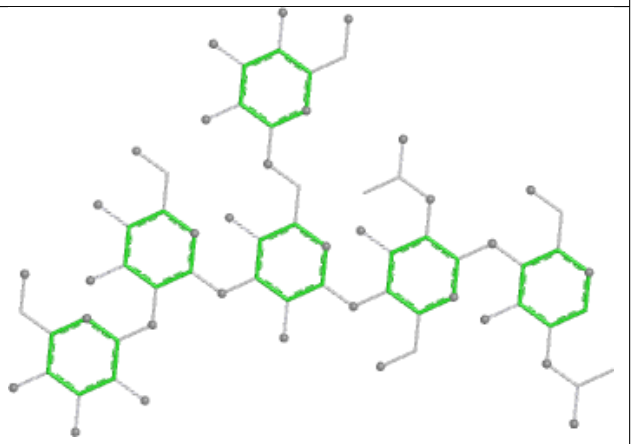
Bond lengths



Bond angles

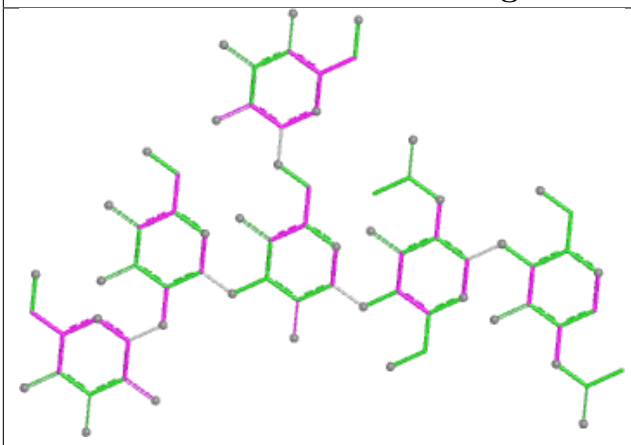


Torsions

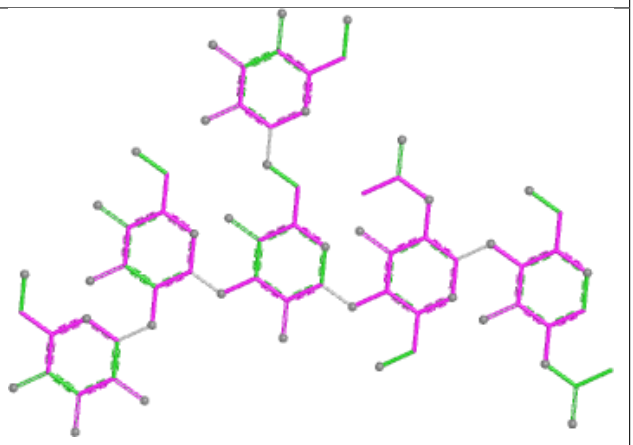


Rings

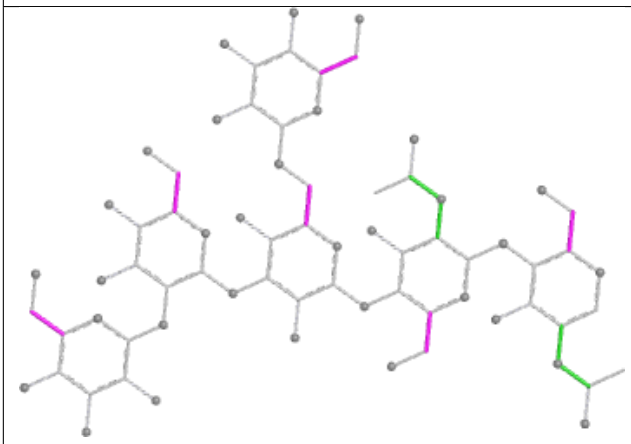
Oligosaccharide Chain t



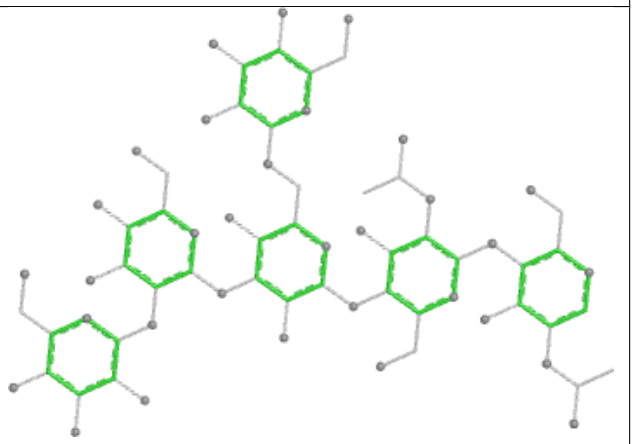
Bond lengths



Bond angles

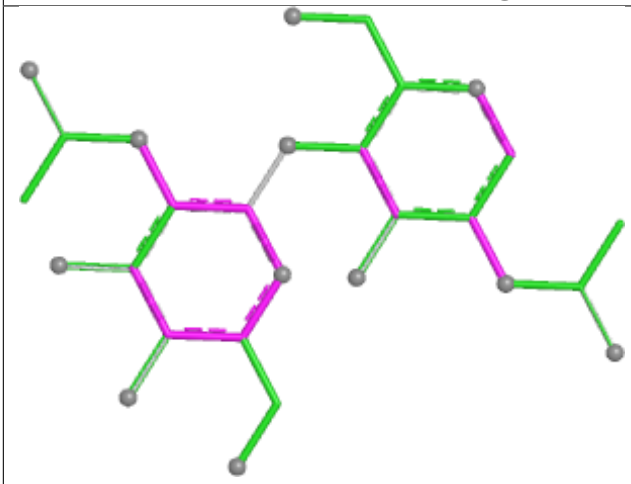


Torsions

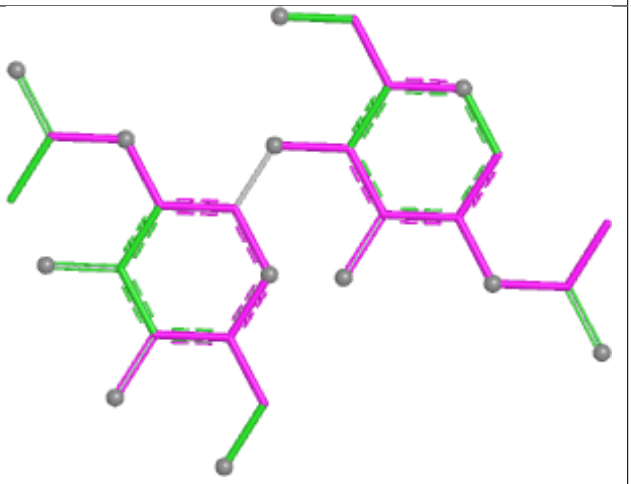


Rings

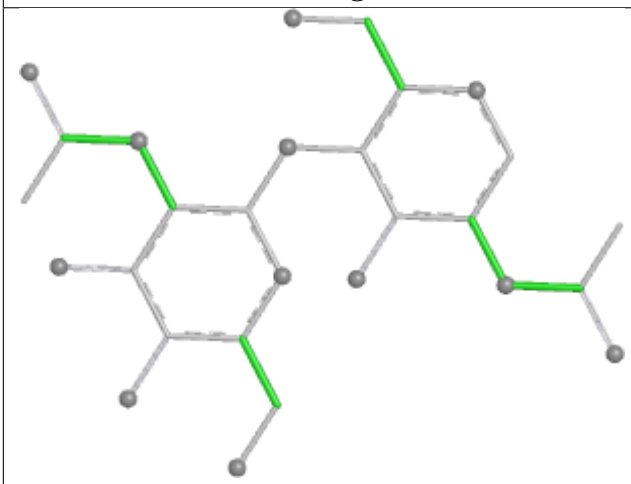
Oligosaccharide Chain E



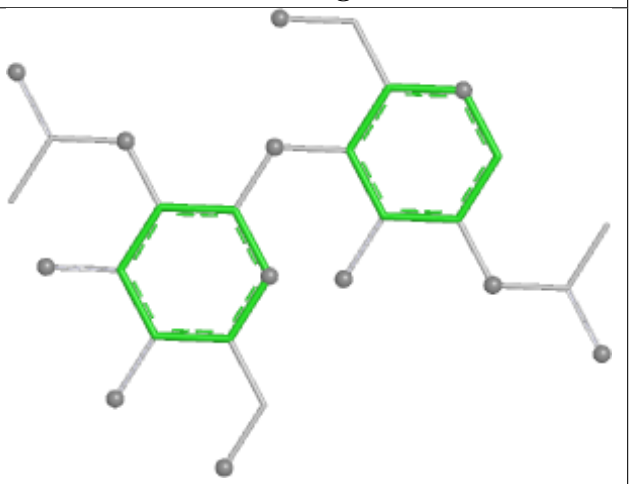
Bond lengths



Bond angles

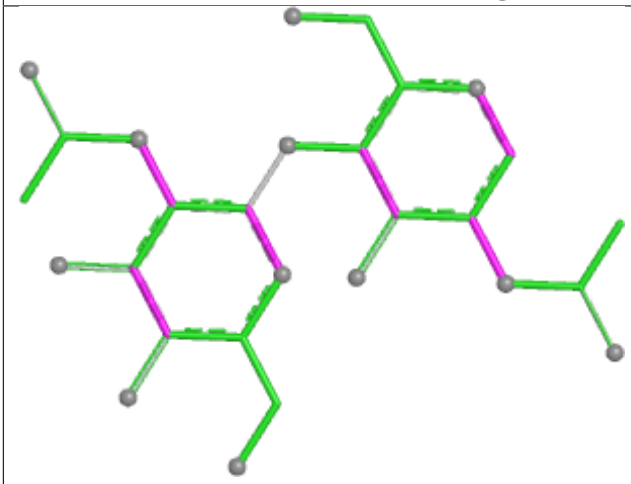


Torsions



Rings

Oligosaccharide Chain G



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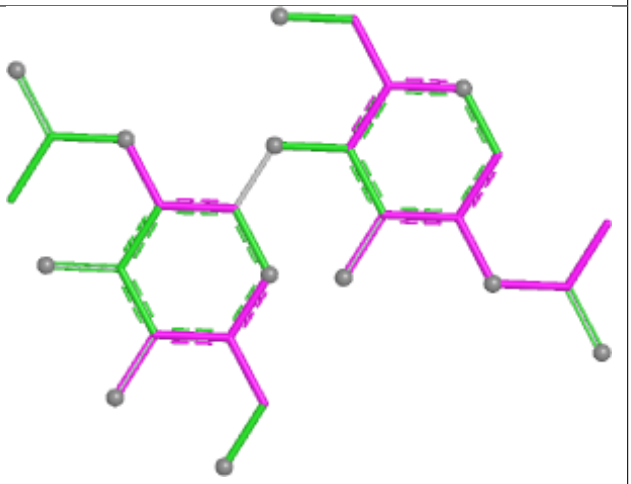
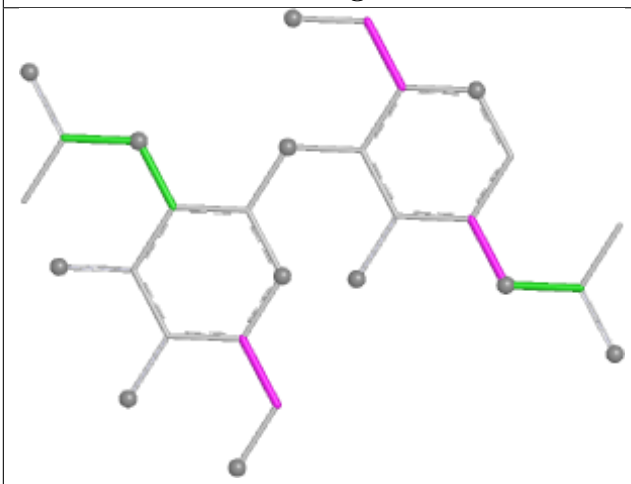


Bond angles



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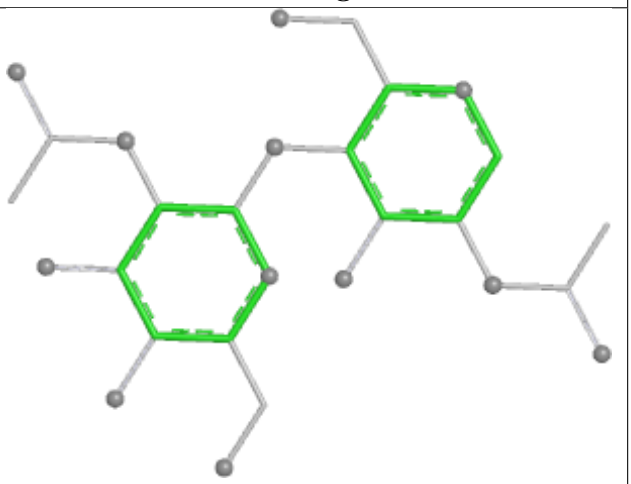
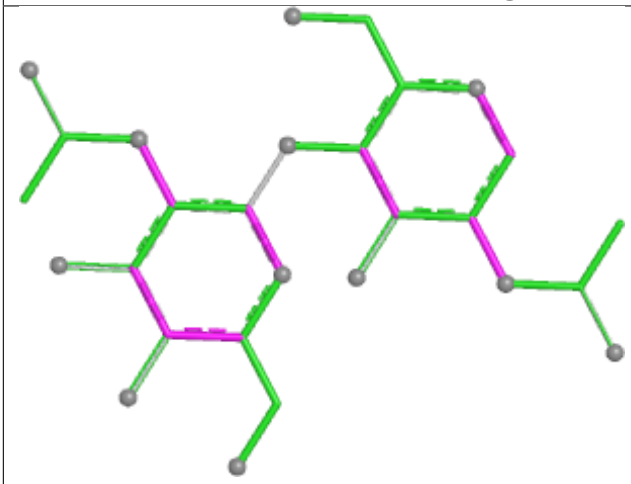


Rings

Oligosaccharide Chain I



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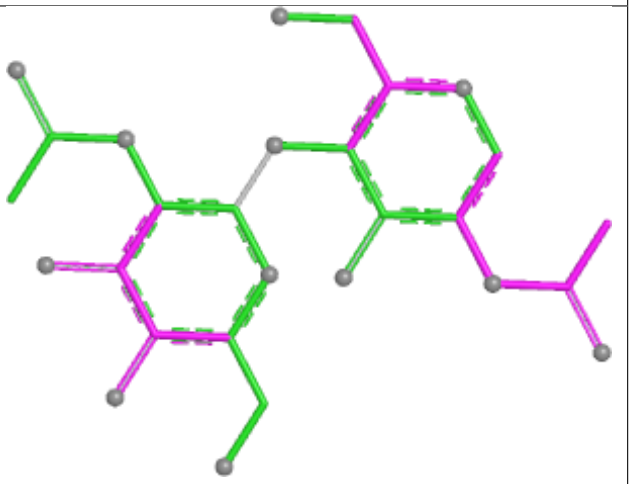
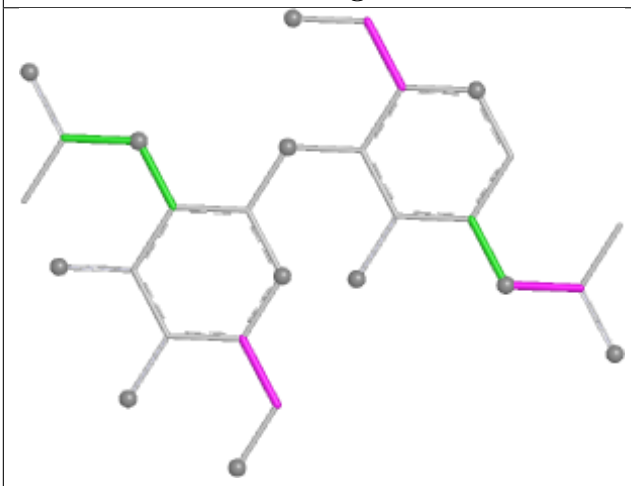
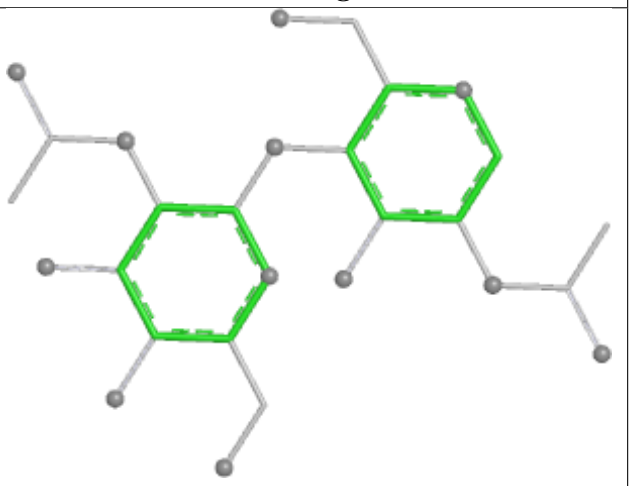


Bond angles

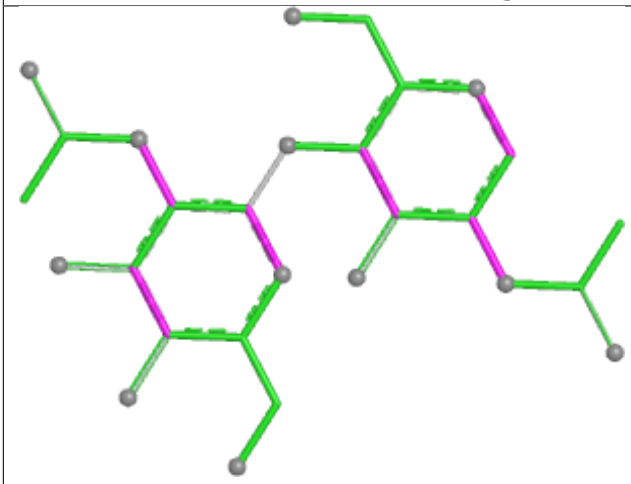


Torsions



Rings

Oligosaccharide Chain J



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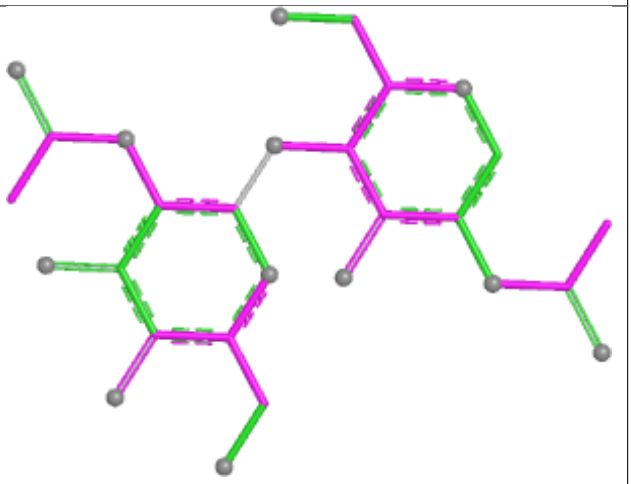
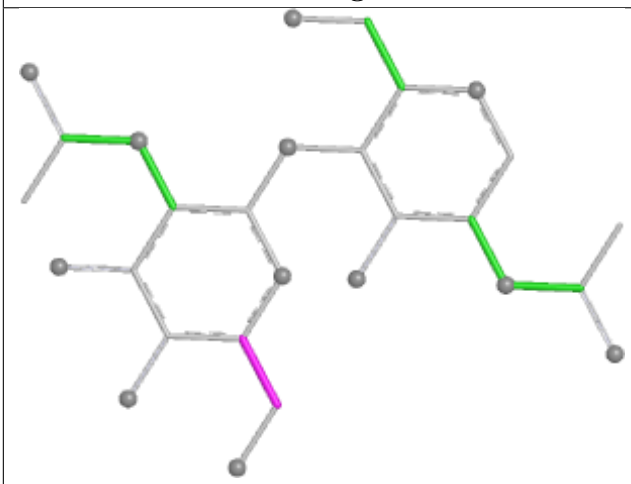
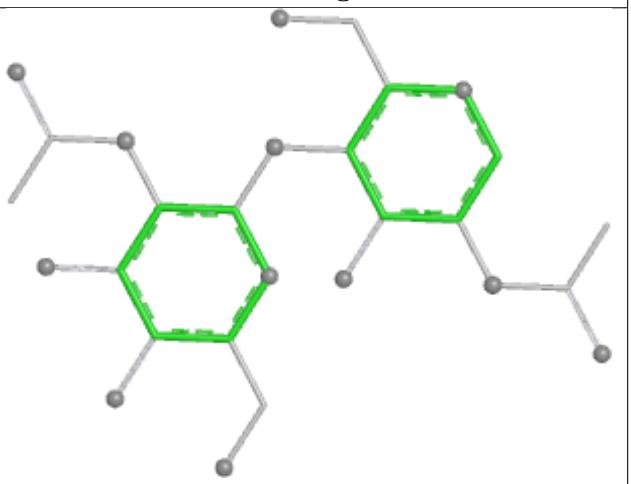


Bond angles

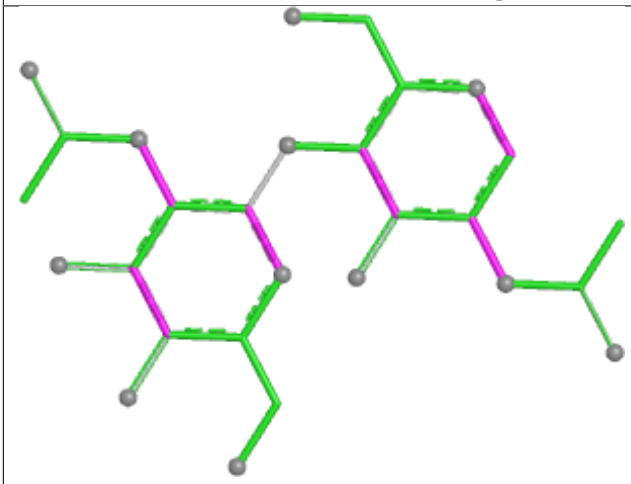


Torsions



Rings

Oligosaccharide Chain M



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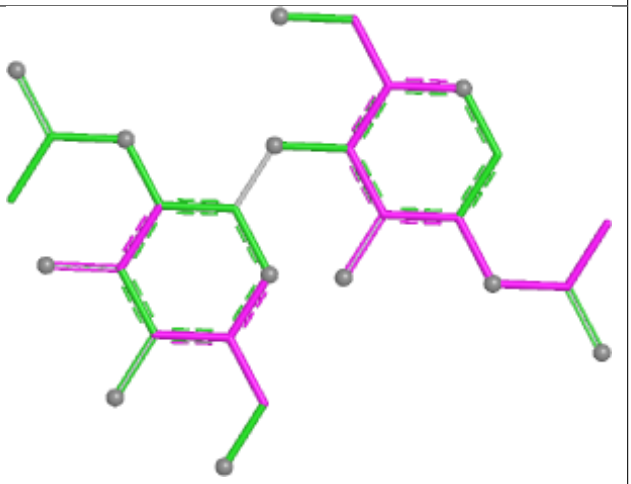
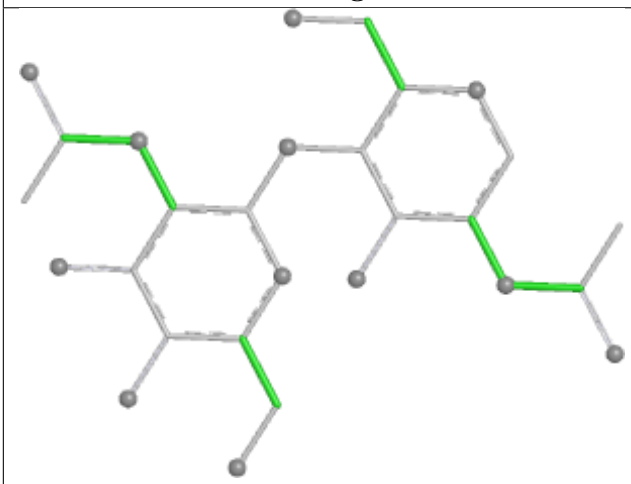
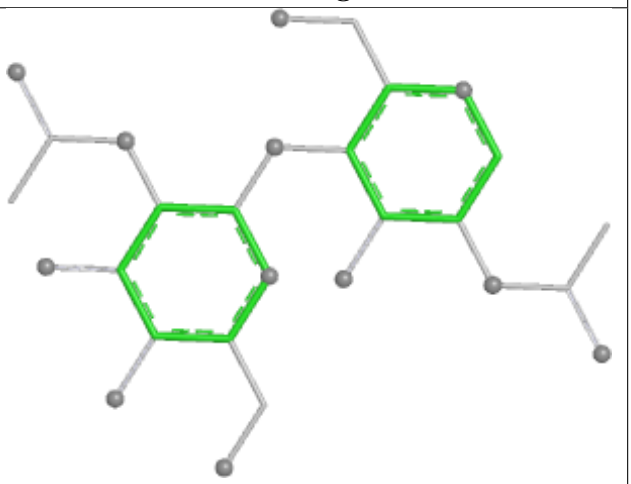


Bond angles

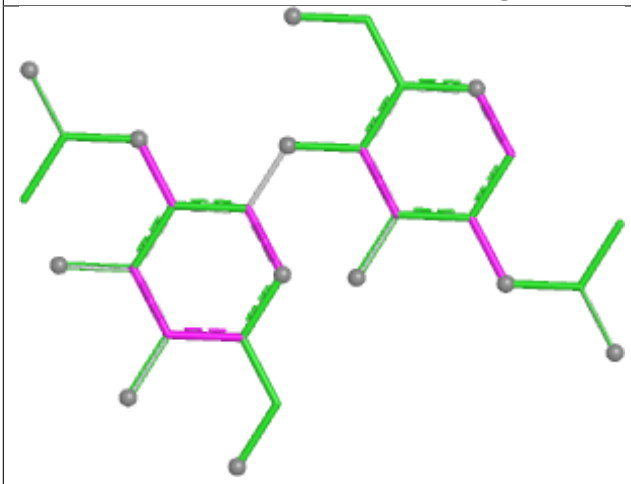


Torsions

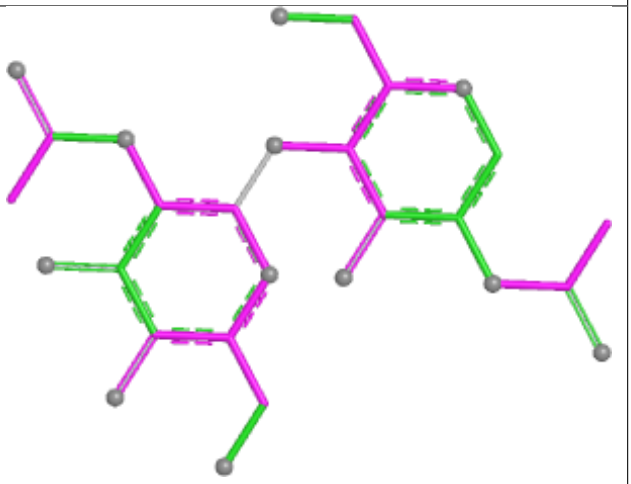


Rings

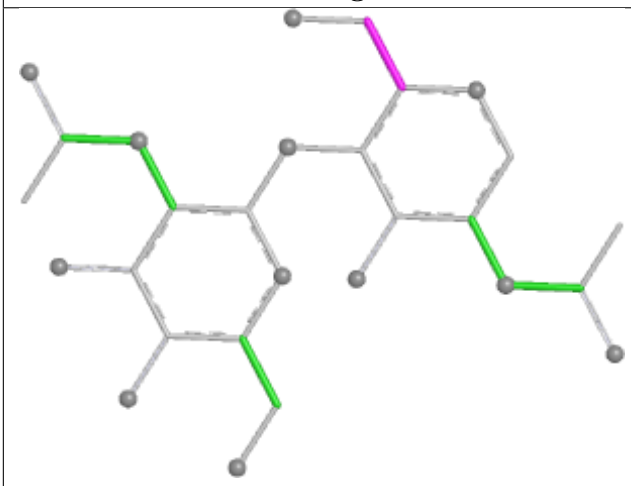
Oligosaccharide Chain P



Bond lengths



Bond angles



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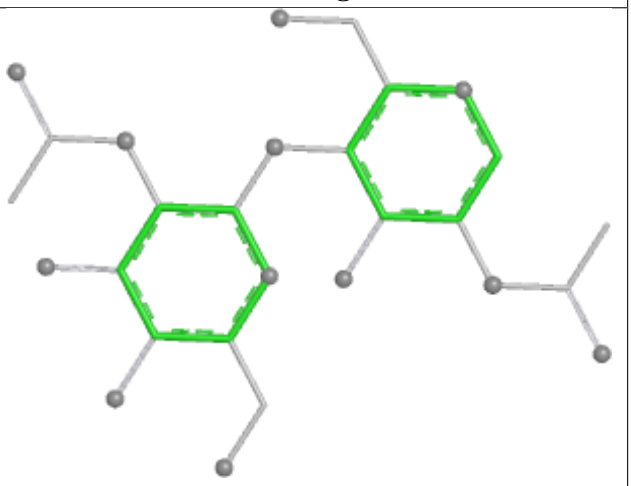
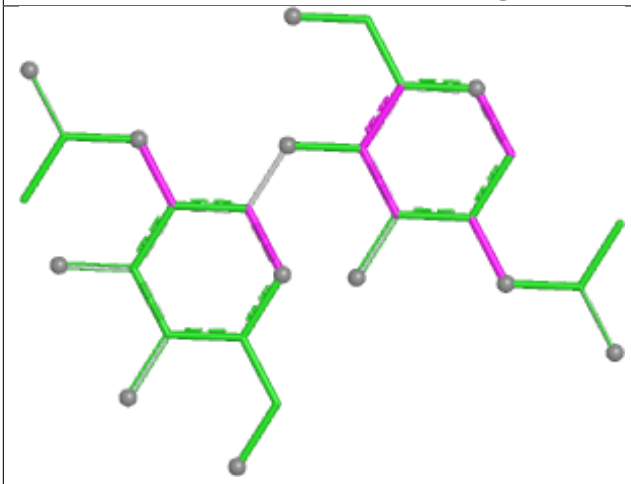
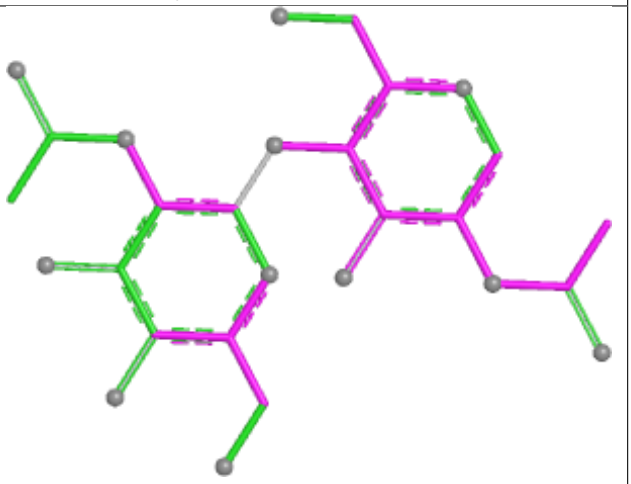


Rings

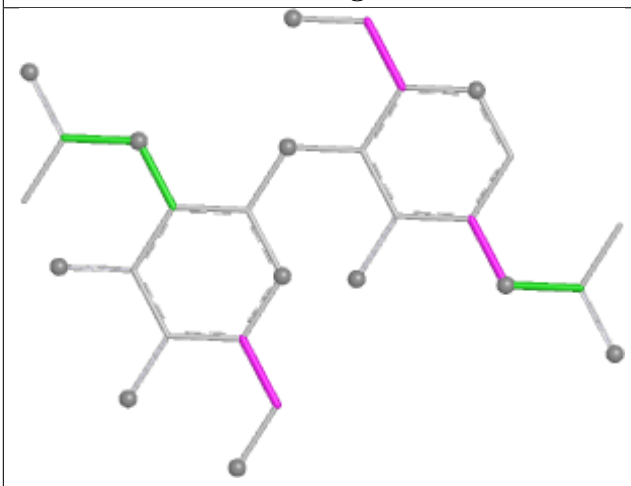
Oligosaccharide Chain Q



Bond lengths



Bond angles



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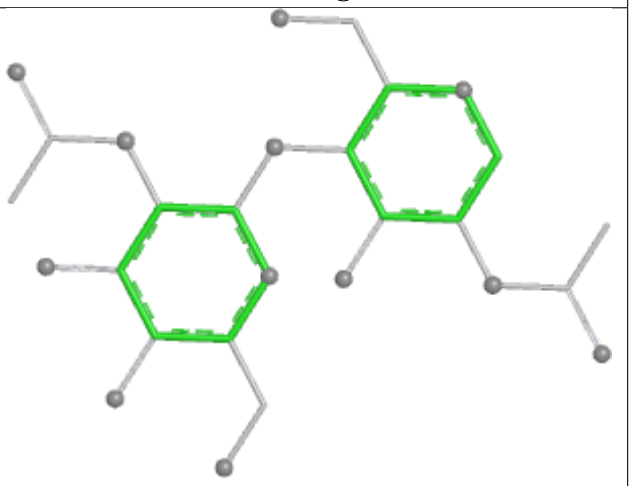
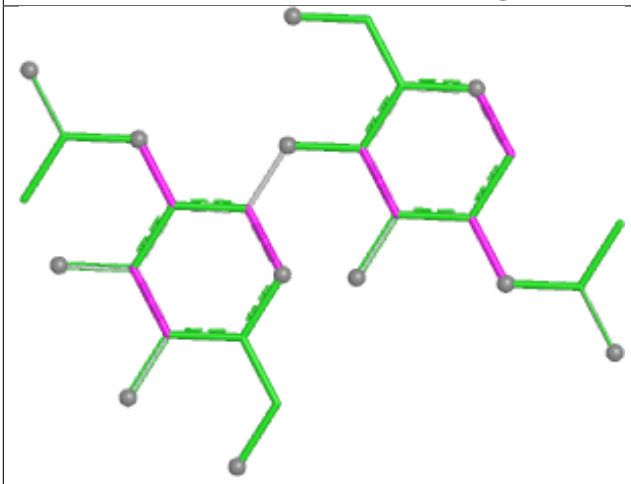


Rings

Oligosaccharide Chain R



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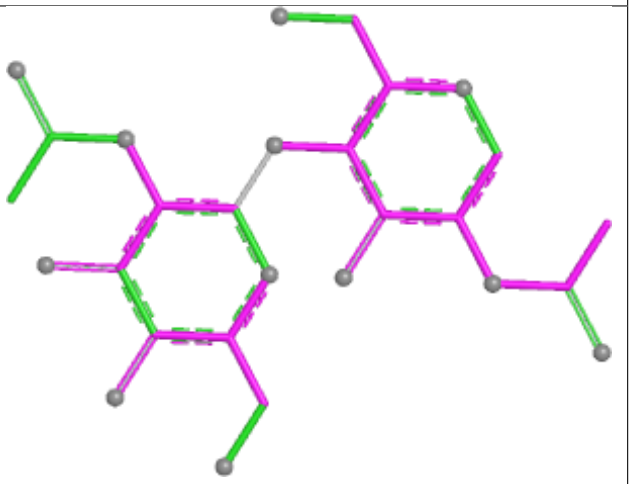
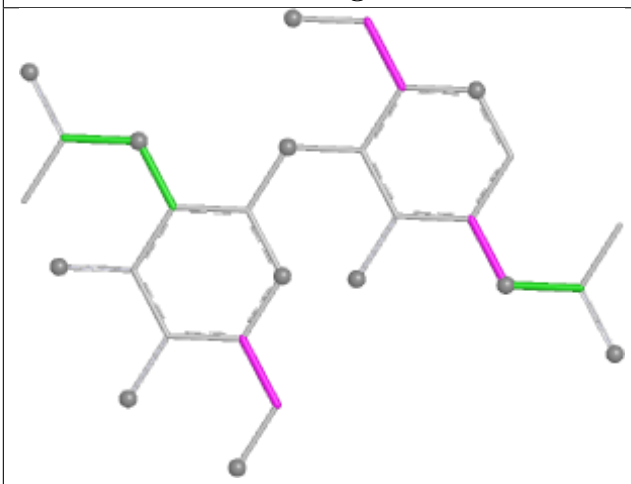
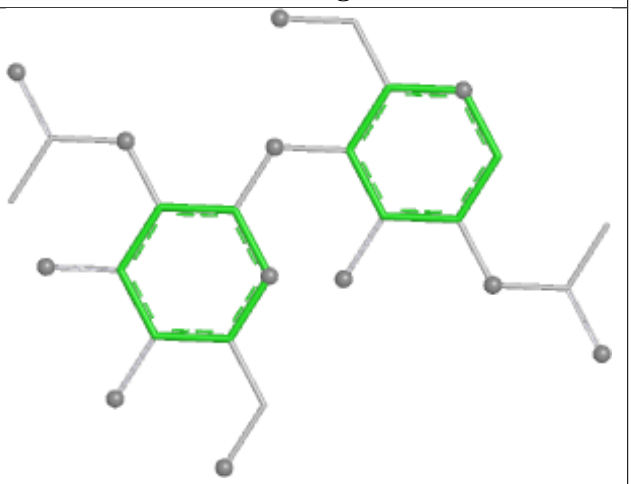


Bond angles

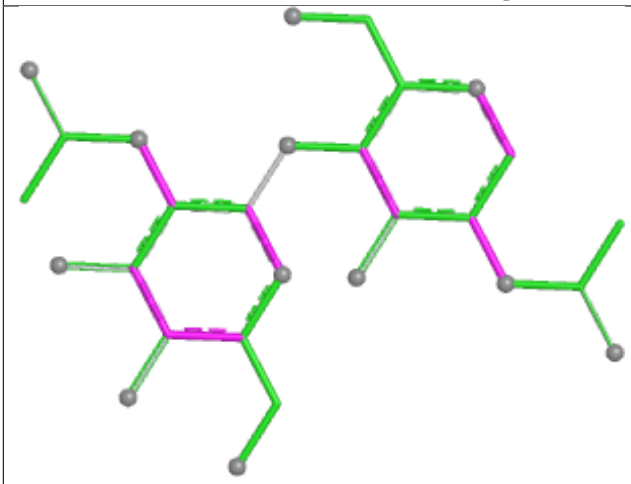


Torsions



Rings

Oligosaccharide Chain S



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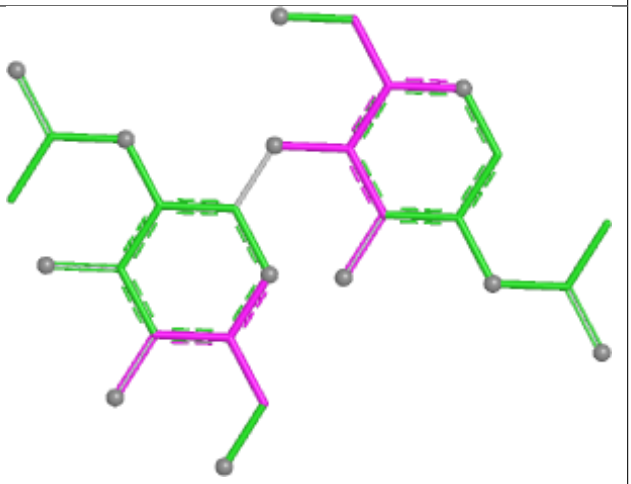
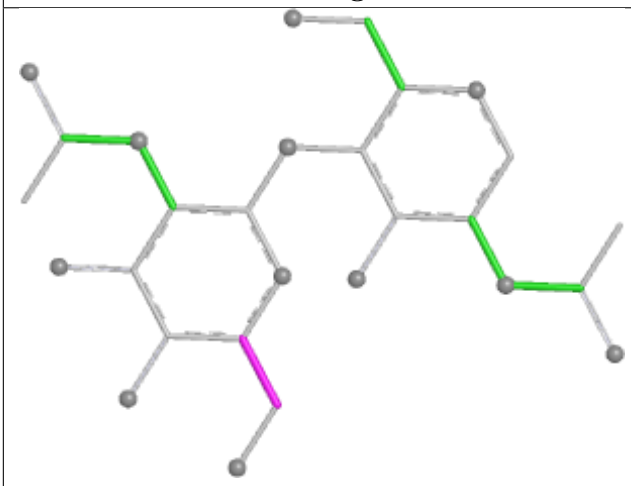


Bond angles



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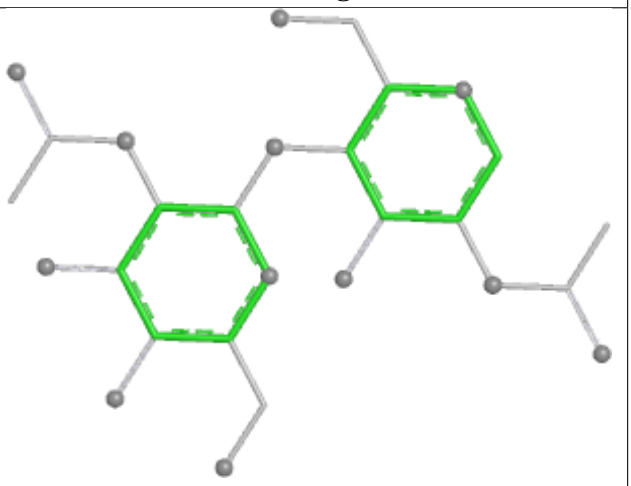
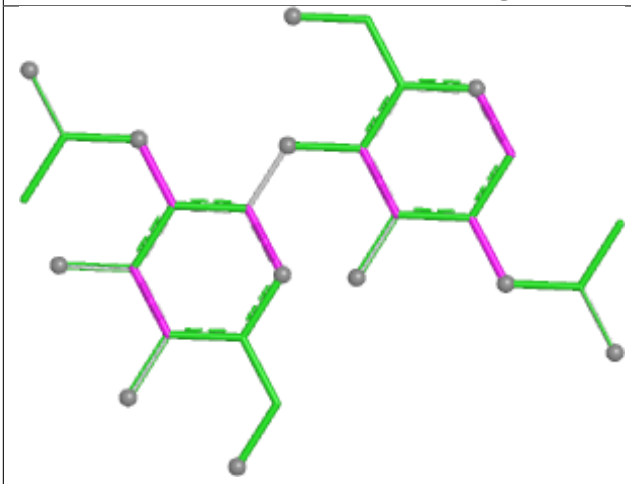


Rings

Oligosaccharide Chain T



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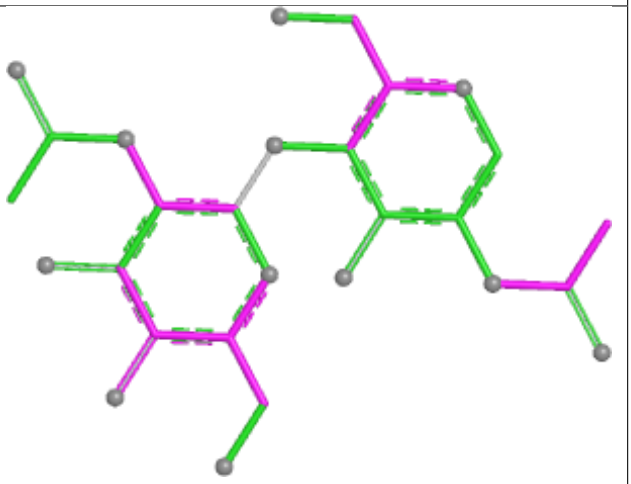
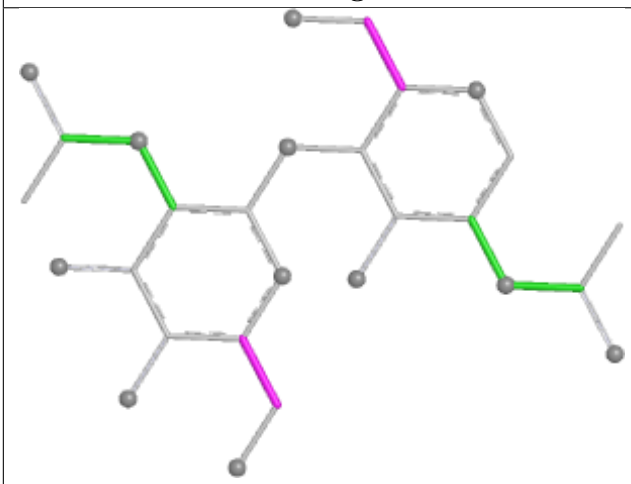
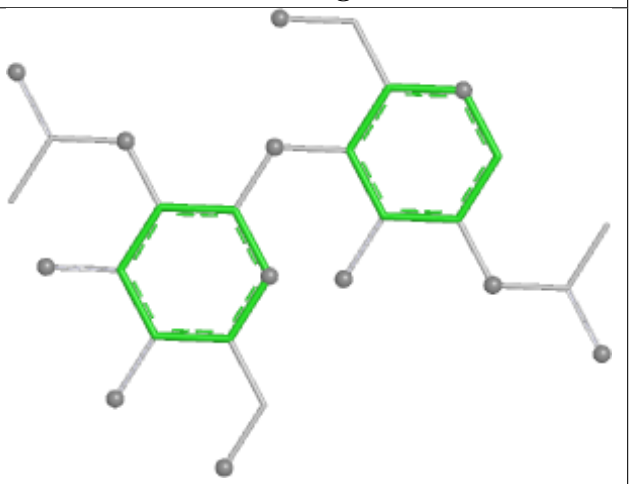


Bond angles

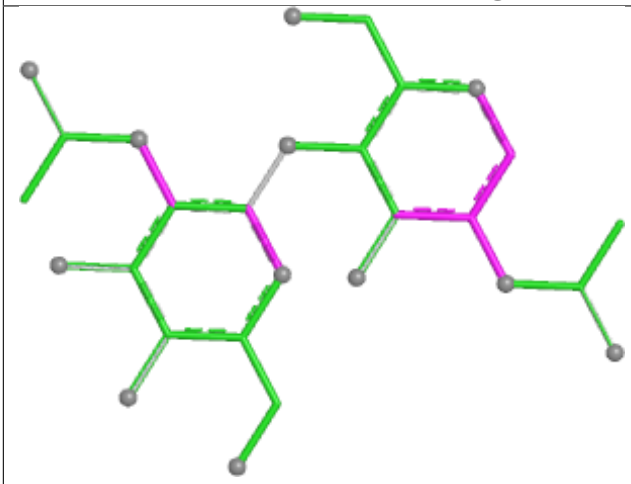


Torsions



Rings

Oligosaccharide Chain W



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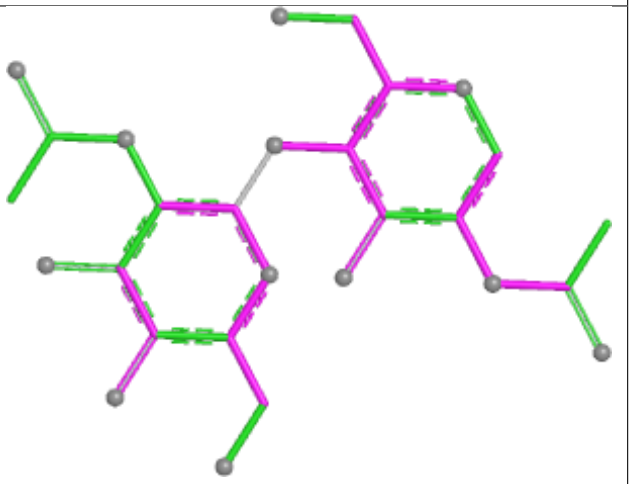
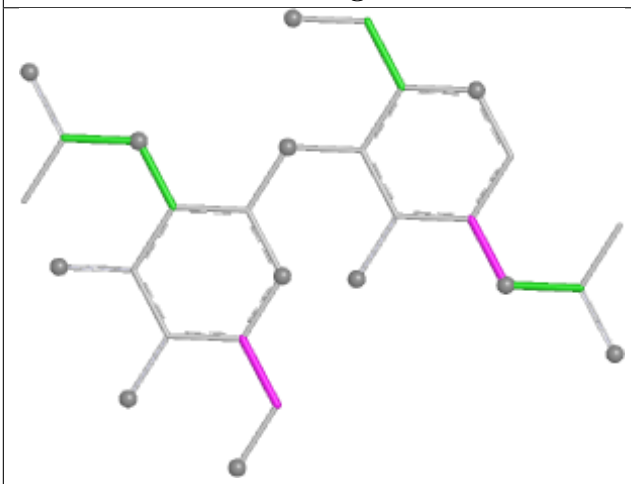


Bond angles



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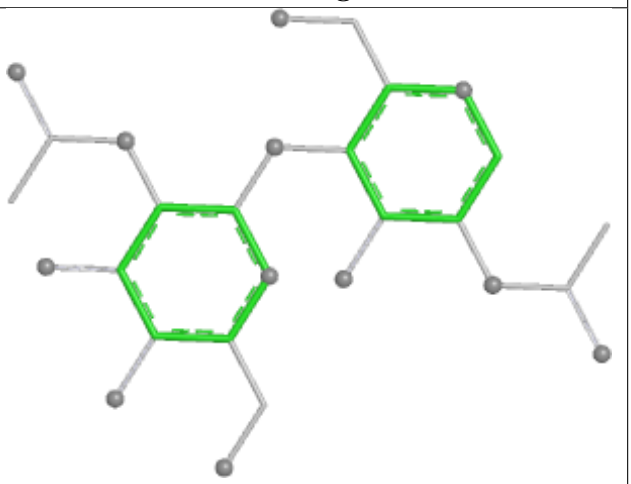
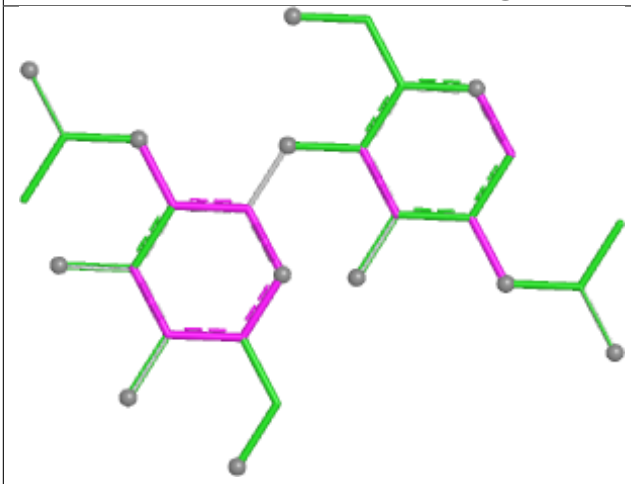


Rings

Oligosaccharide Chain Z



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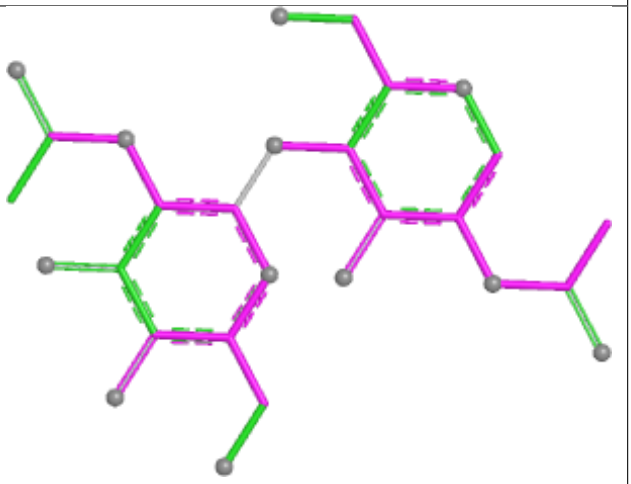
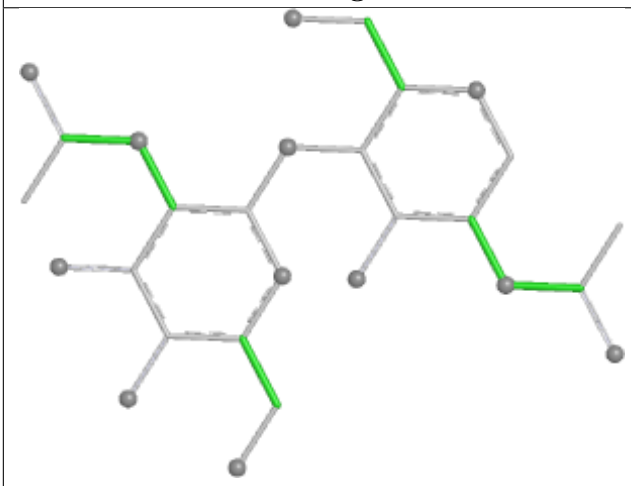
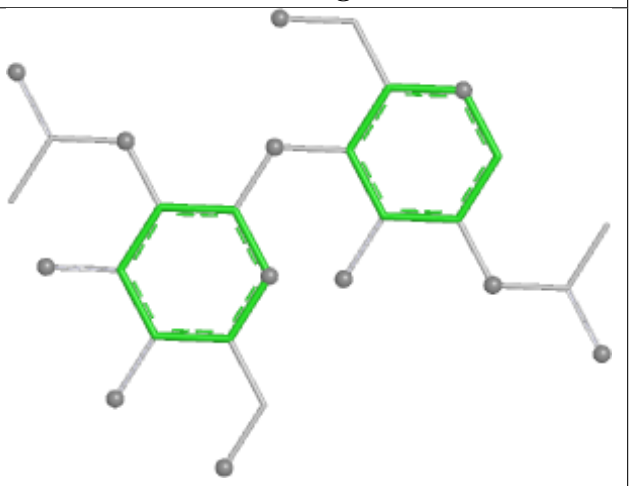


Bond angles

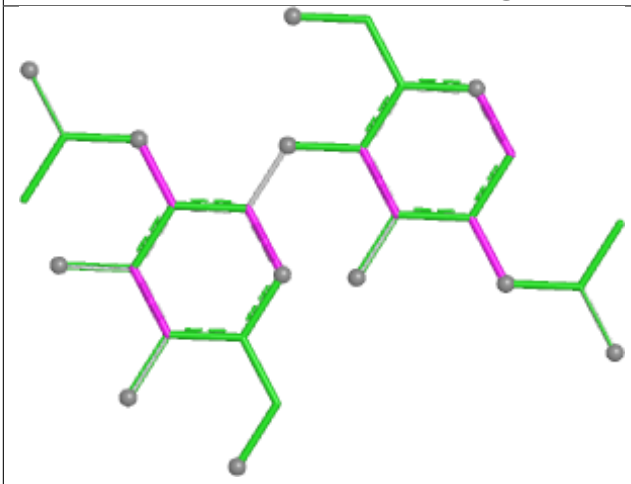


Torsions



Rings

Oligosaccharide Chain b



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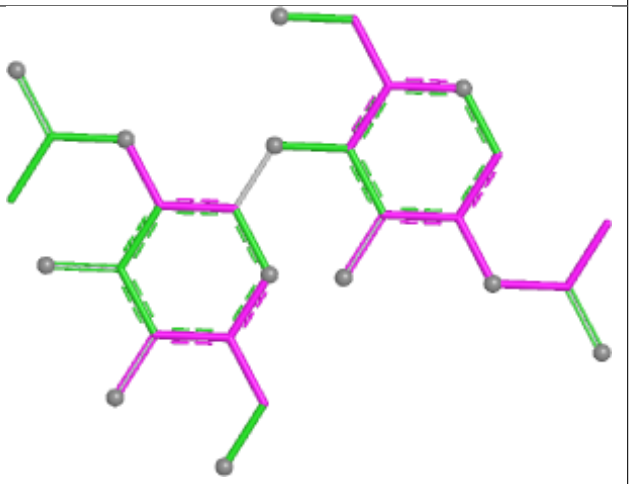
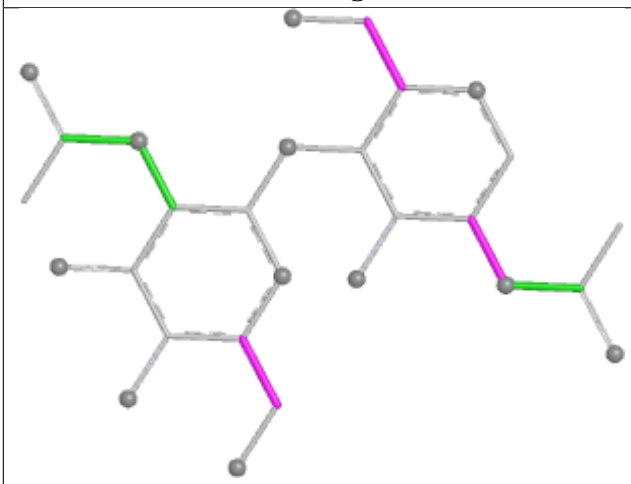
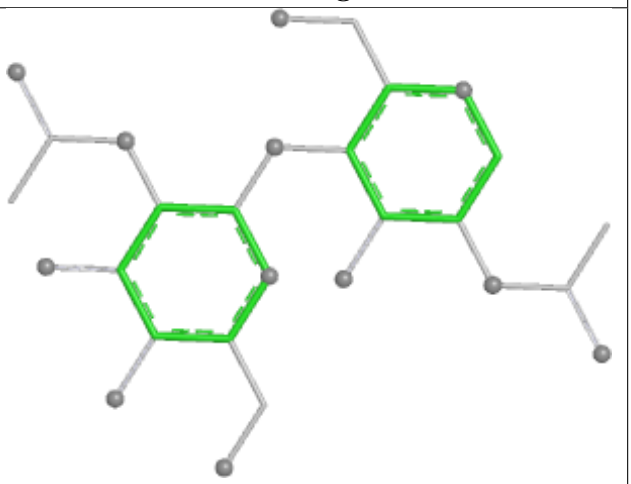


Bond angles

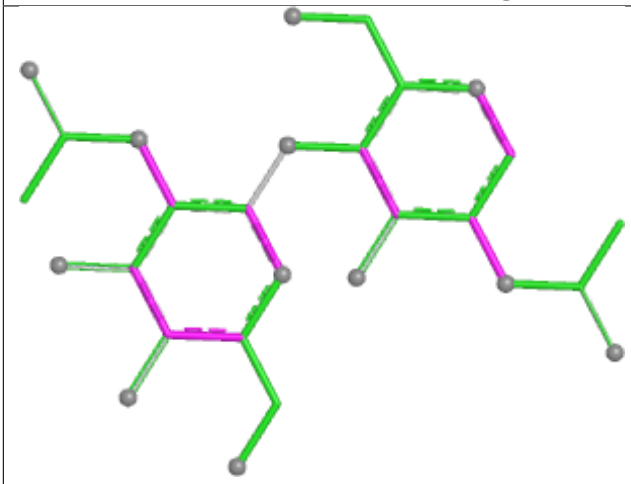


Torsions



Rings

Oligosaccharide Chain d



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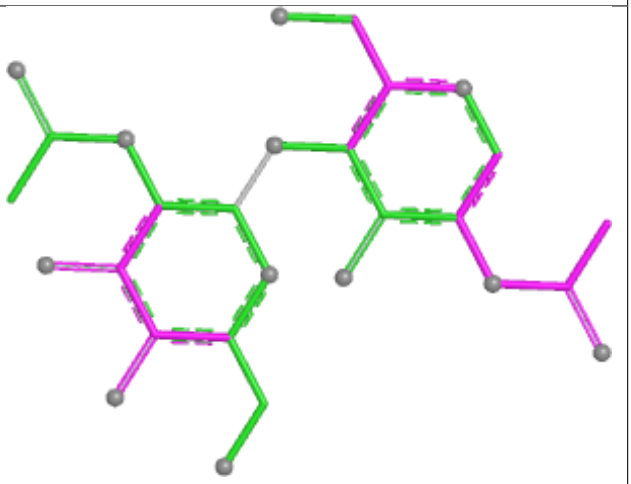
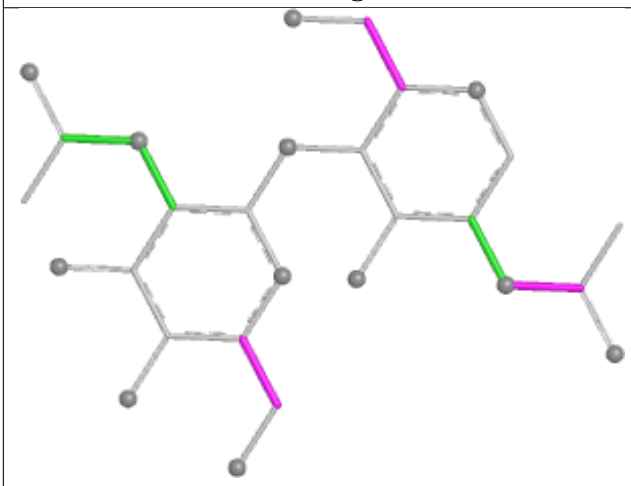
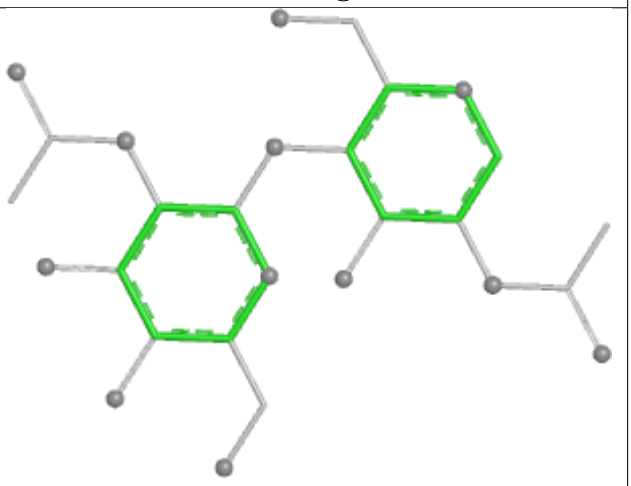


Bond angles

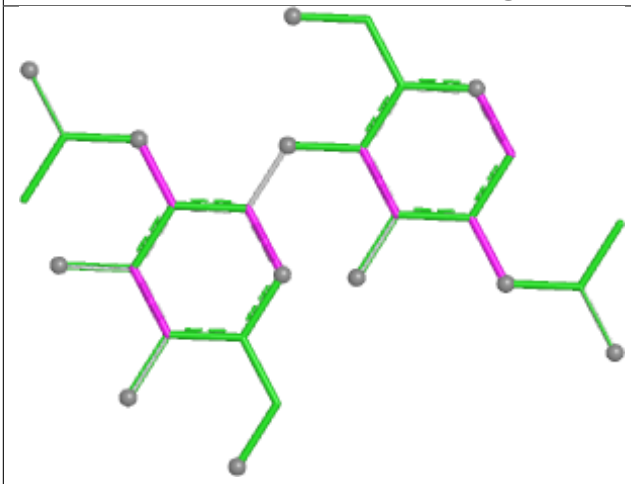


Torsions

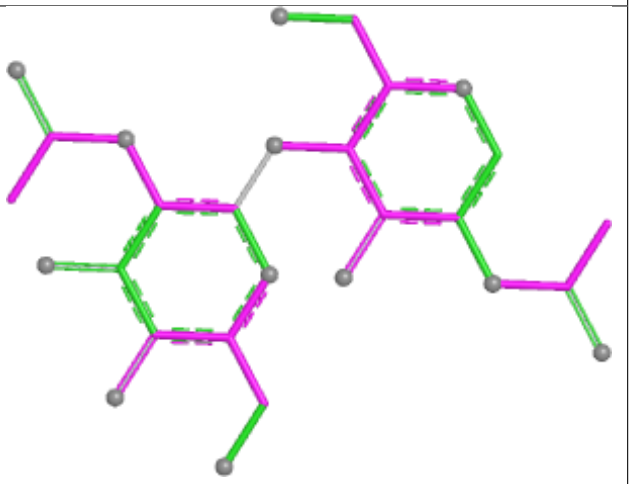


Rings

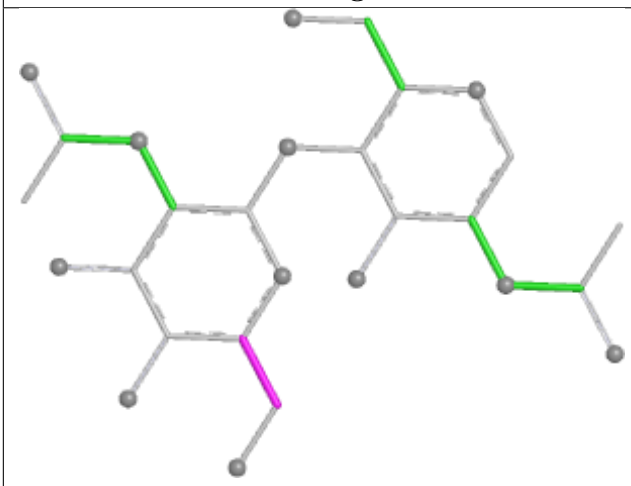
Oligosaccharide Chain e



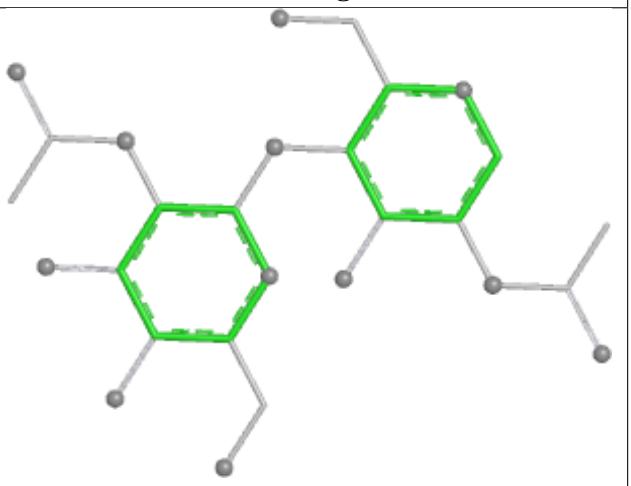
Bond lengths



Bond angles

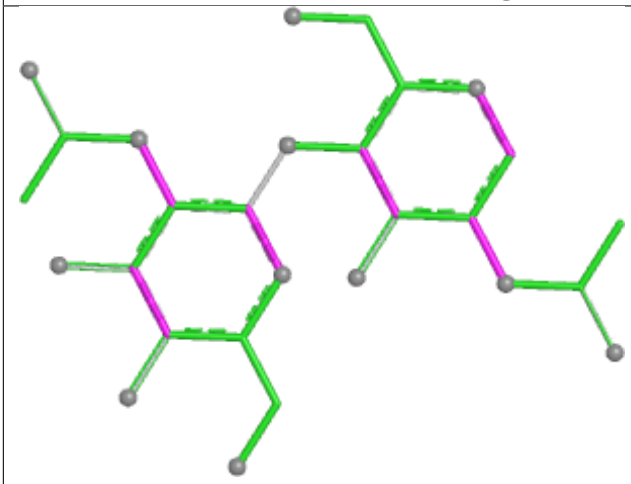


Torsions

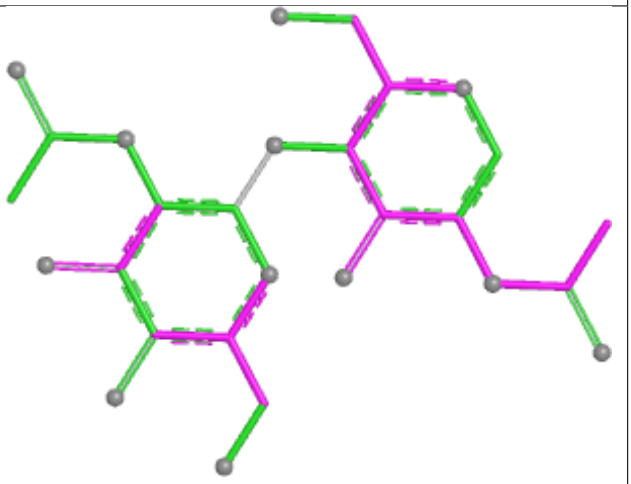


Rings

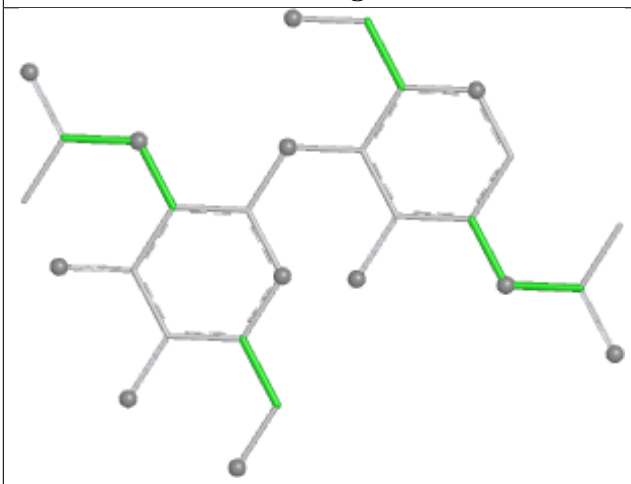
Oligosaccharide Chain h



Bond lengths



Bond angles



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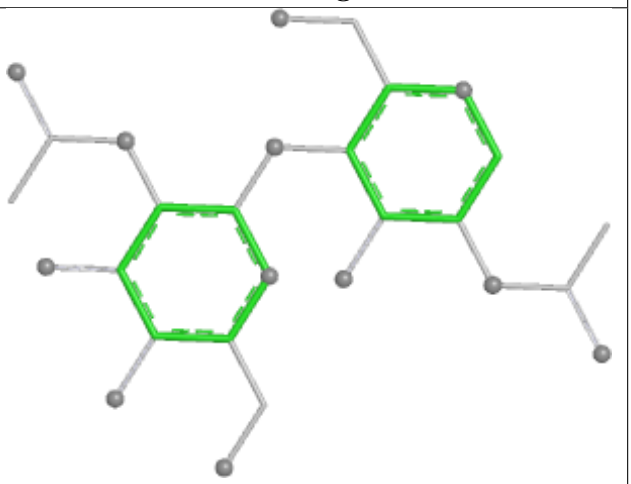
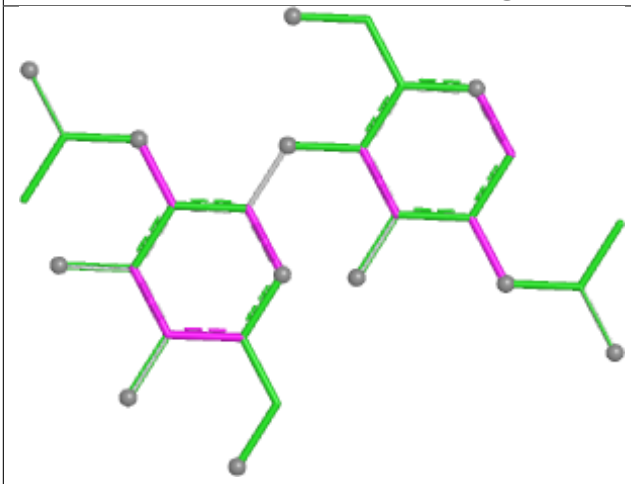


Rings

Oligosaccharide Chain k



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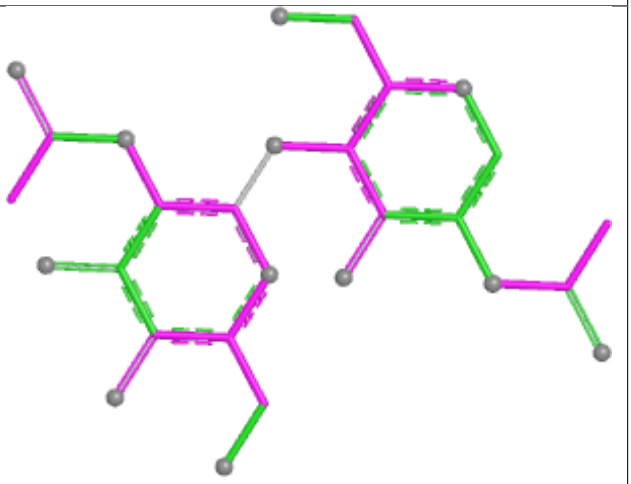
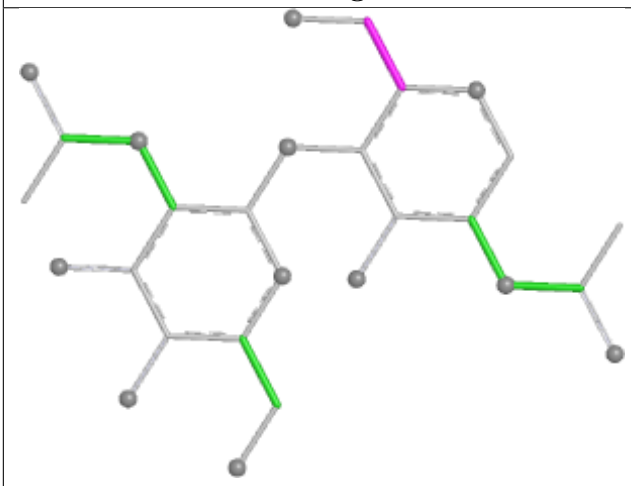


Bond angles



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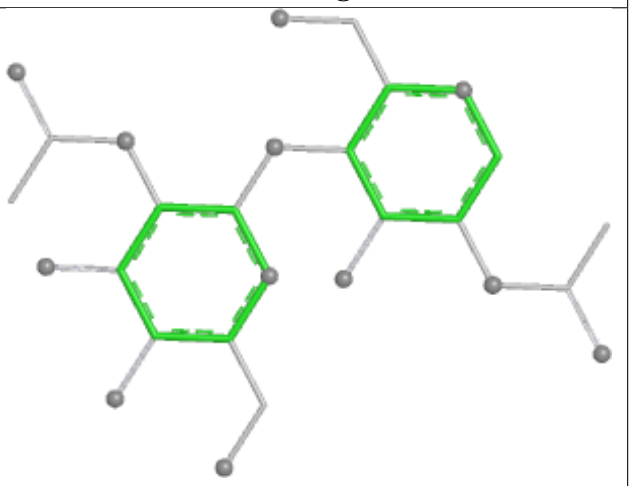
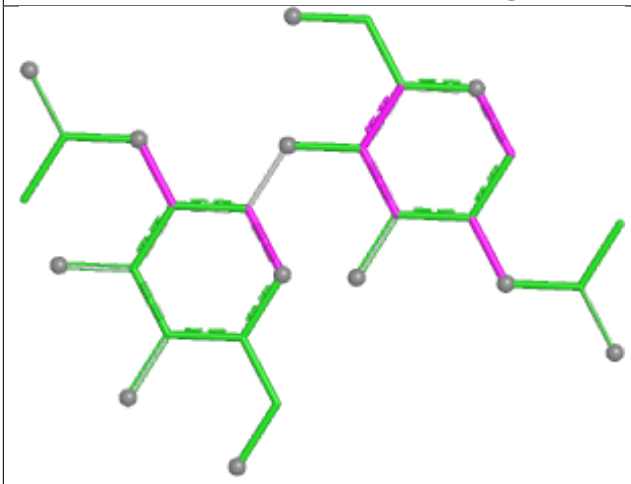


Rings

Oligosaccharide Chain l



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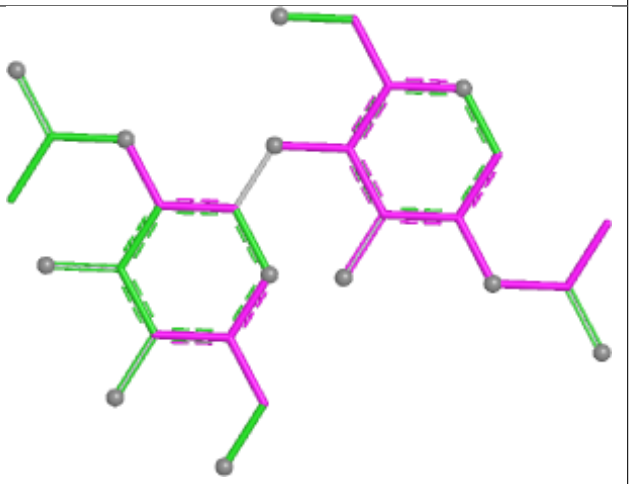

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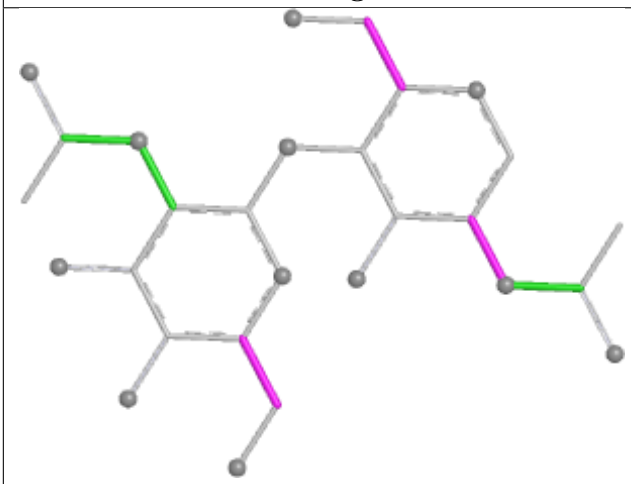

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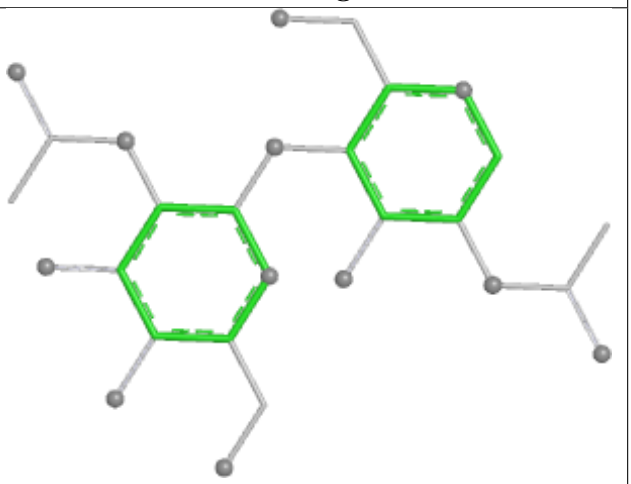
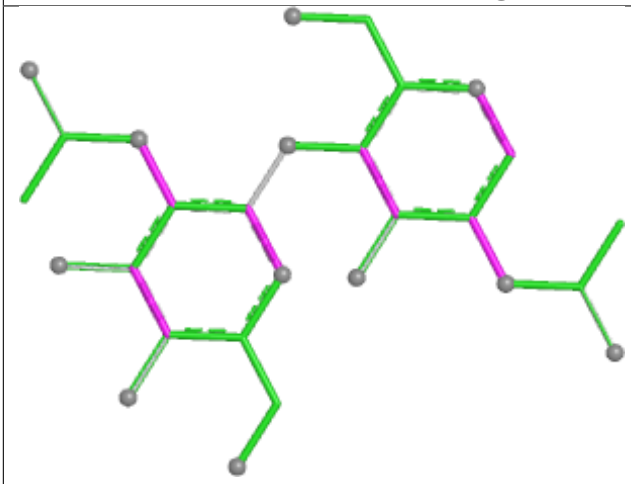


Rings

Oligosaccharide Chain m



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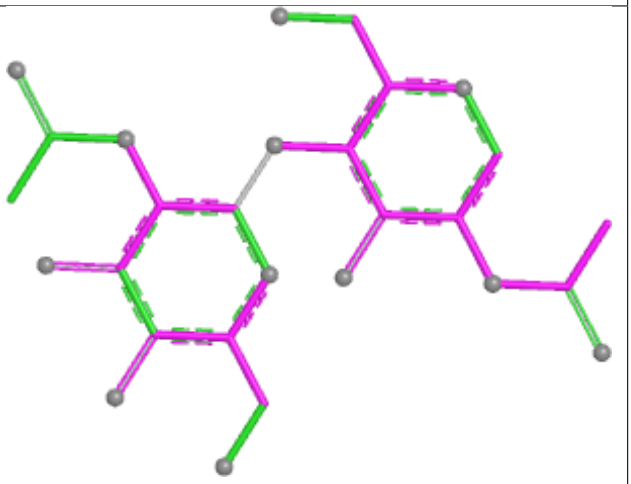

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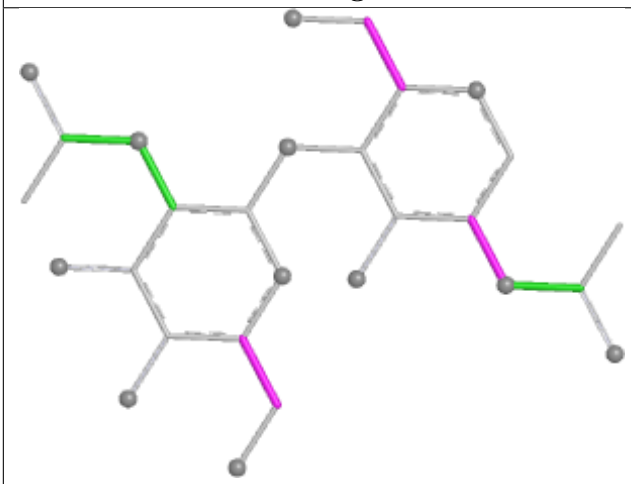

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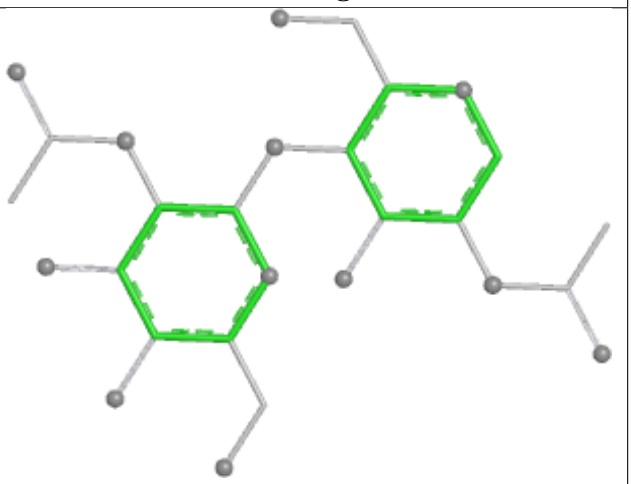
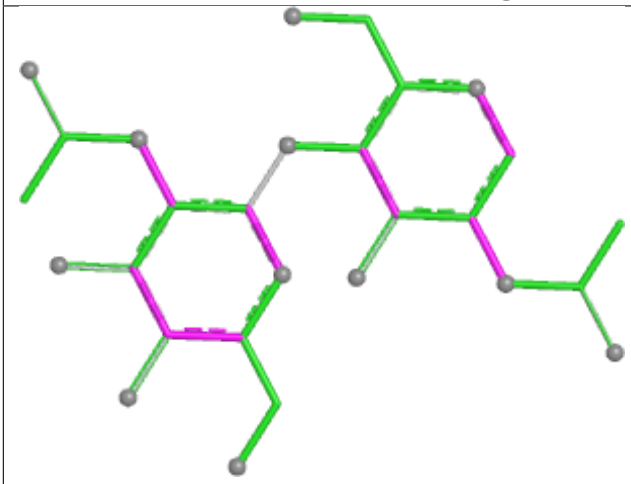


Rings

Oligosaccharide Chain n



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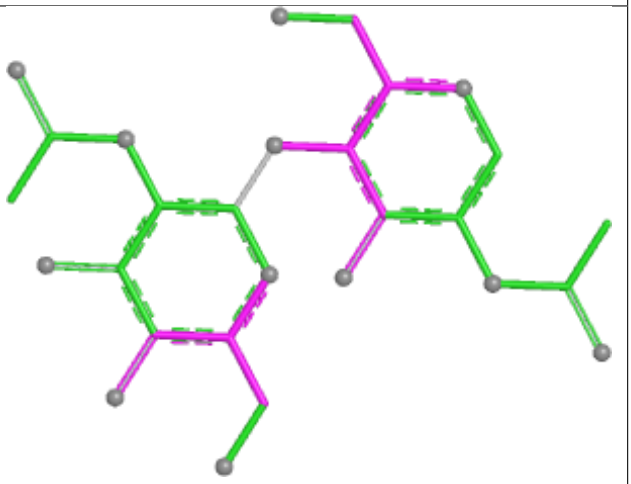
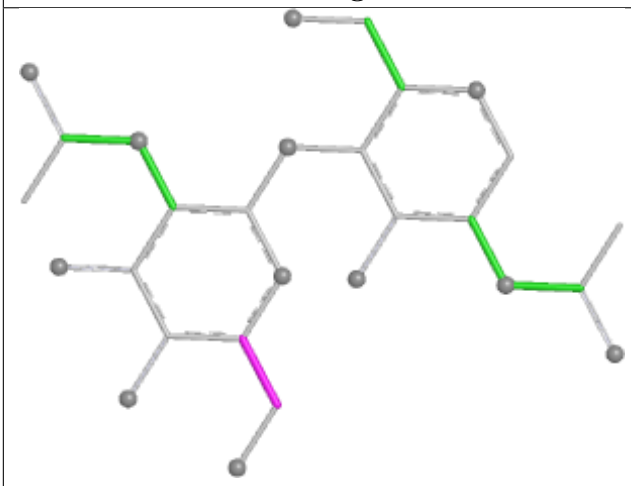


Bond angles



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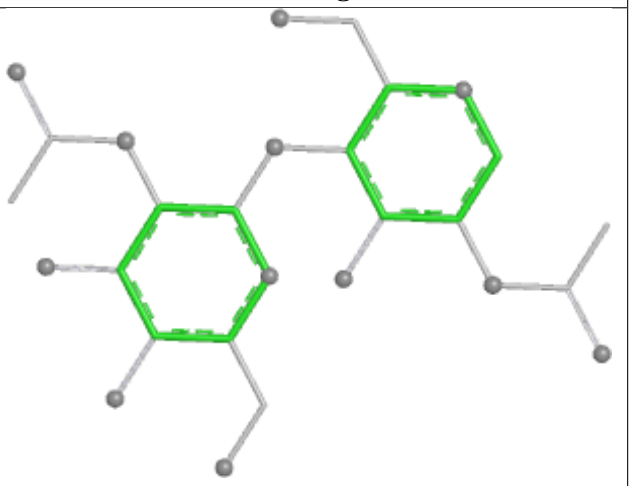
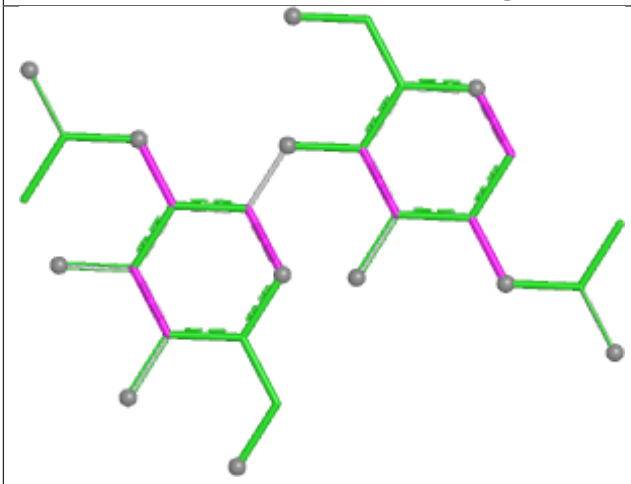


Rings

Oligosaccharide Chain o



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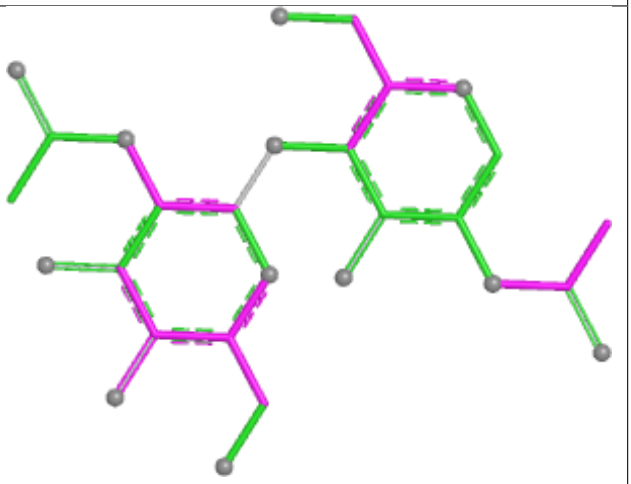
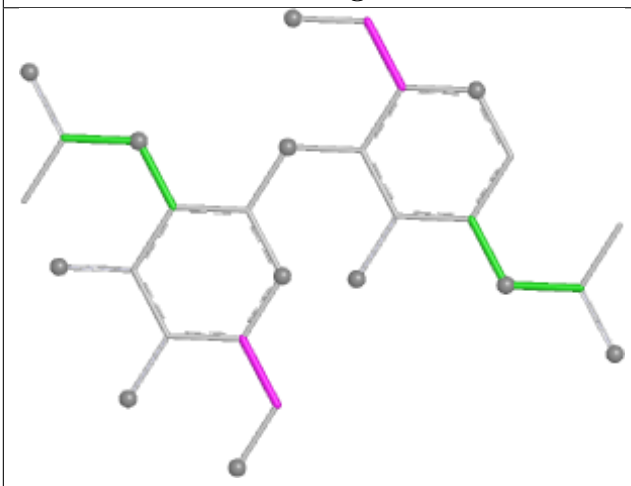


Bond angles



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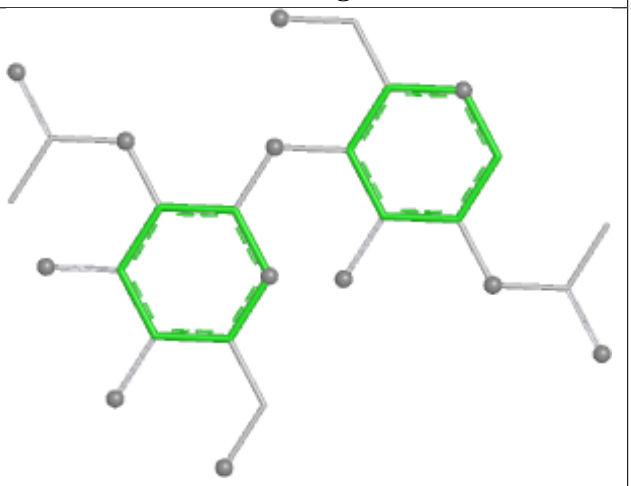
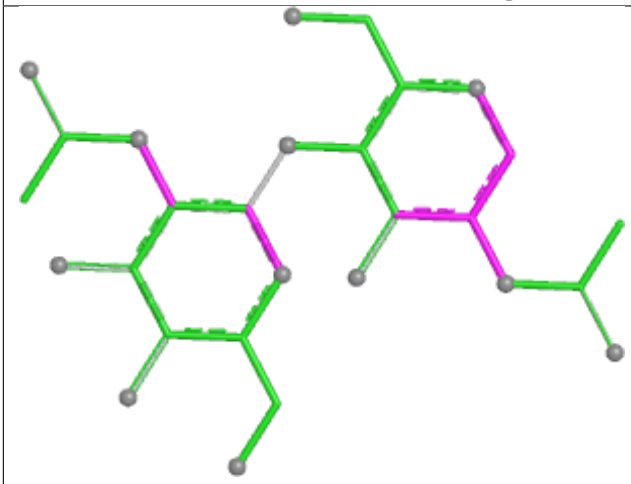


Rings

Oligosaccharide Chain r



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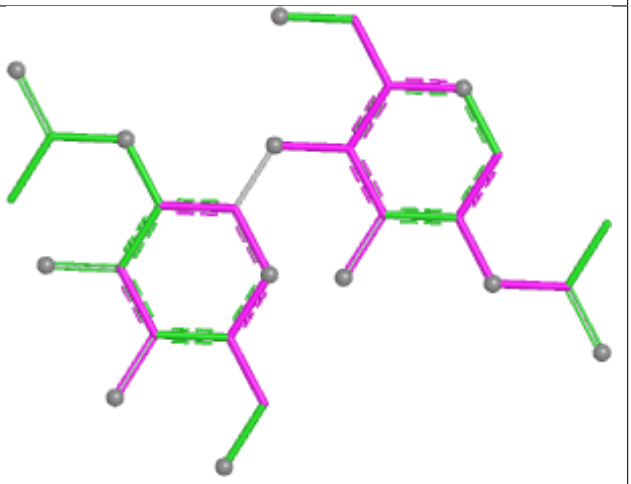
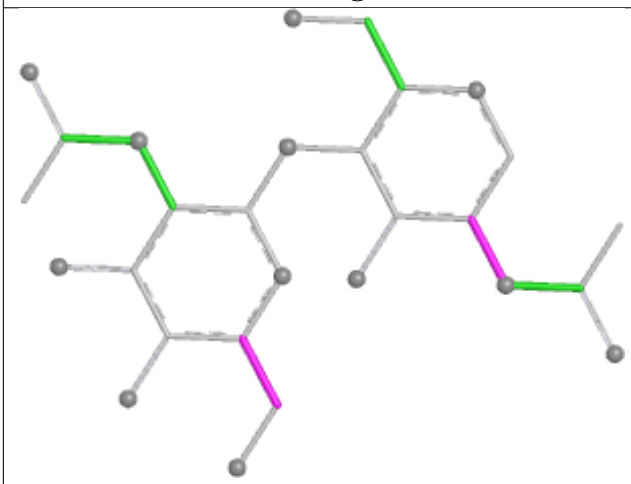


Bond angles



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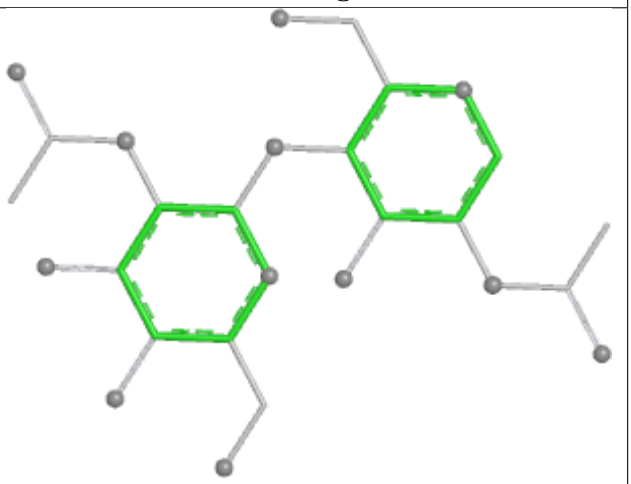
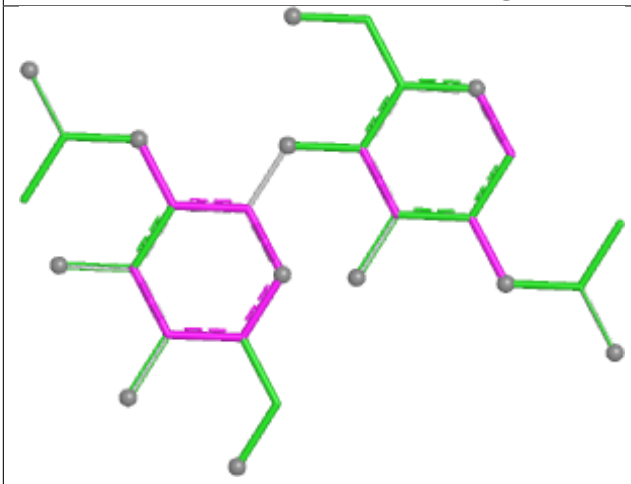


Rings

Oligosaccharide Chain u



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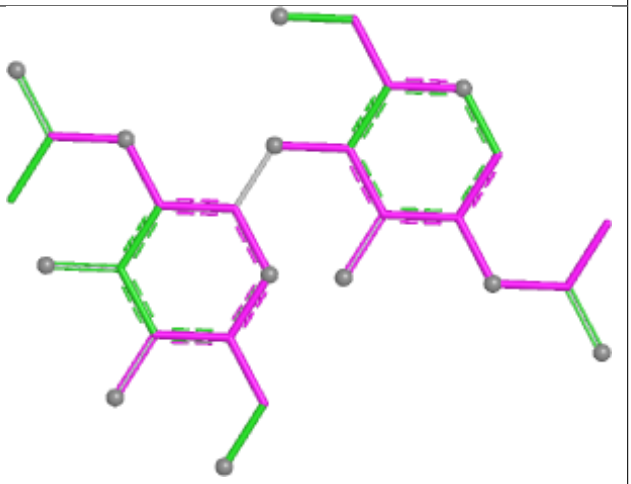
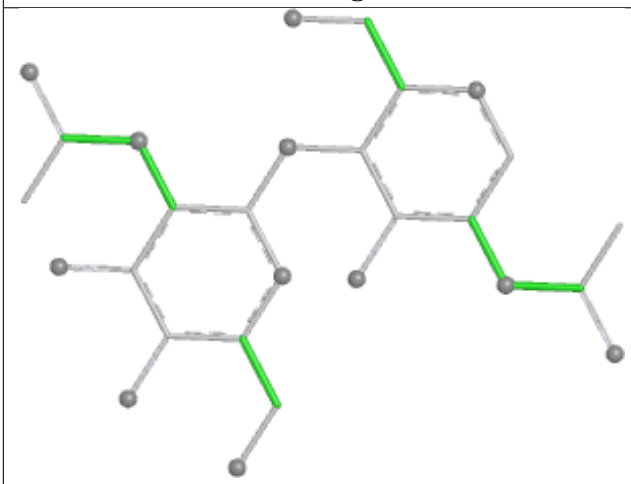


Bond angles



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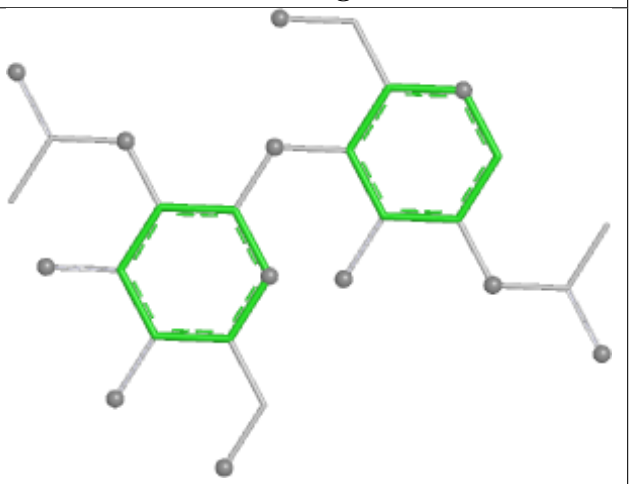
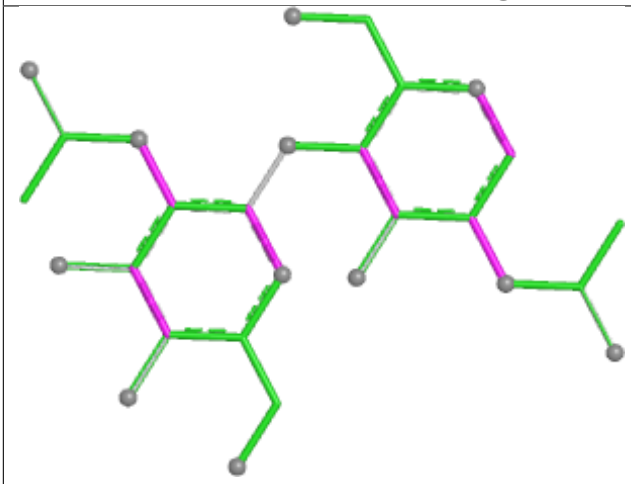


Rings

Oligosaccharide Chain w



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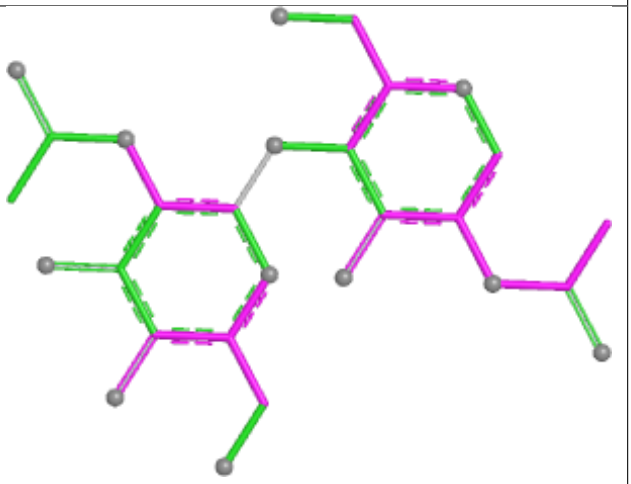
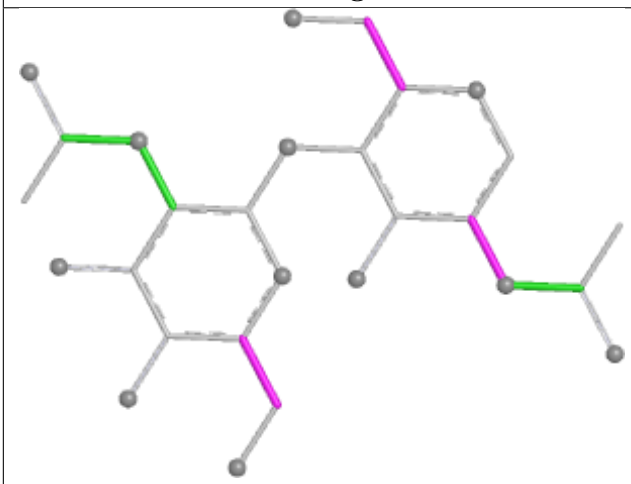


Bond angles



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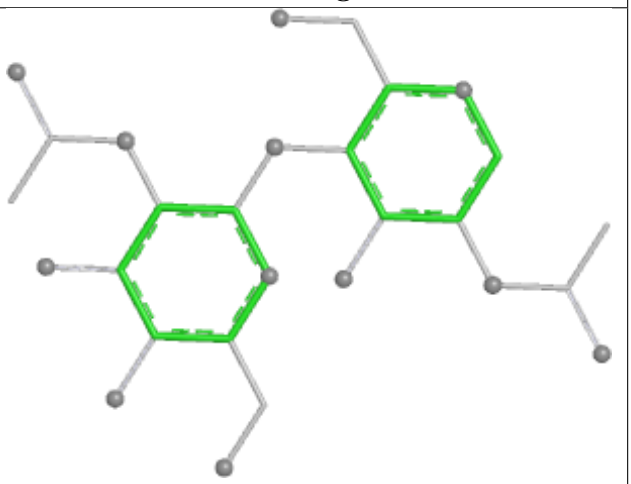
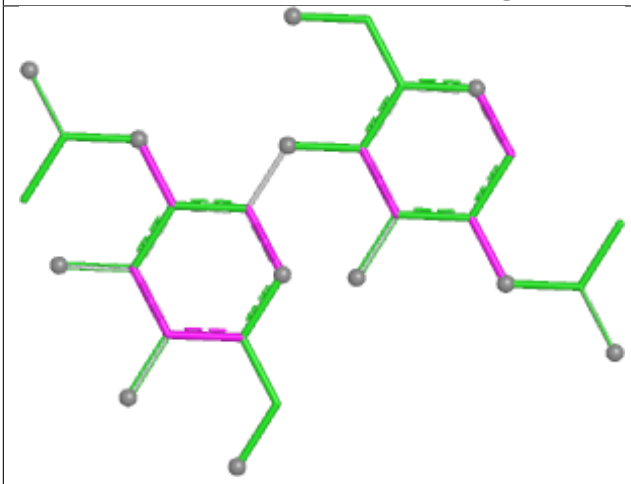


Rings

Oligosaccharide Chain y



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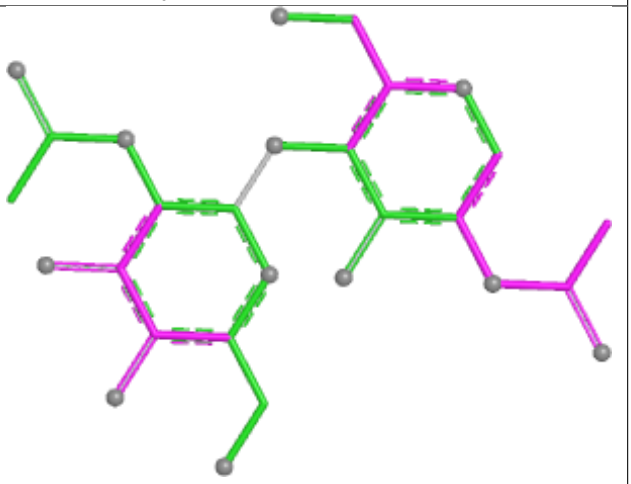
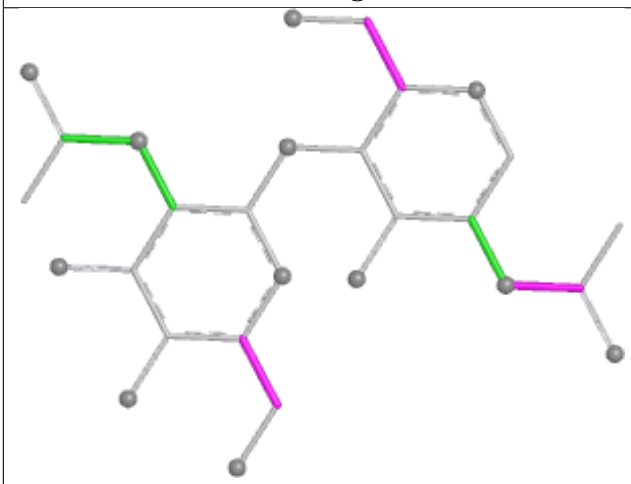


Bond angles



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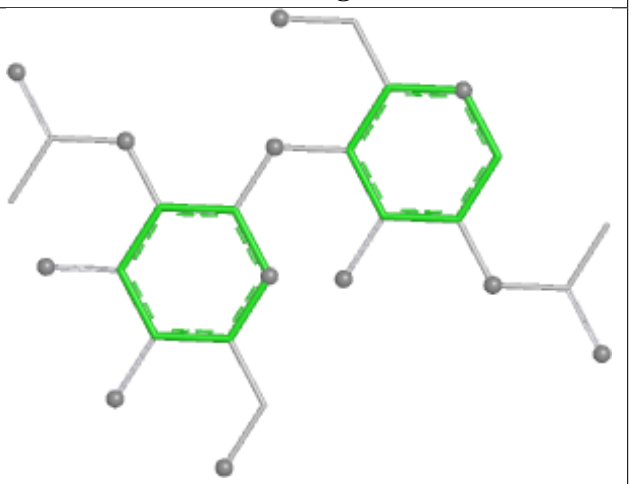
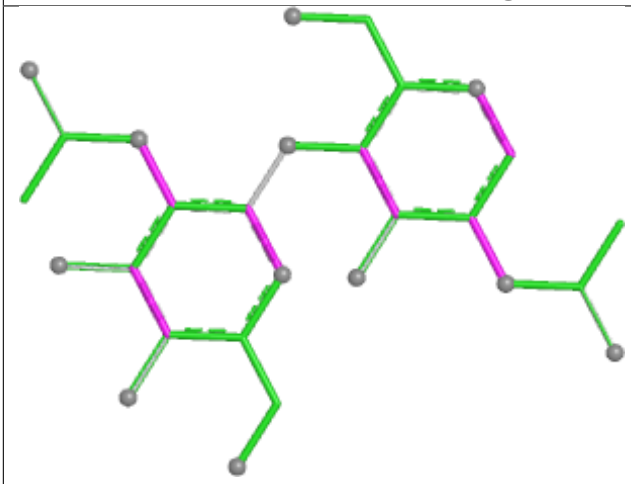


Rings

Oligosaccharide Chain z



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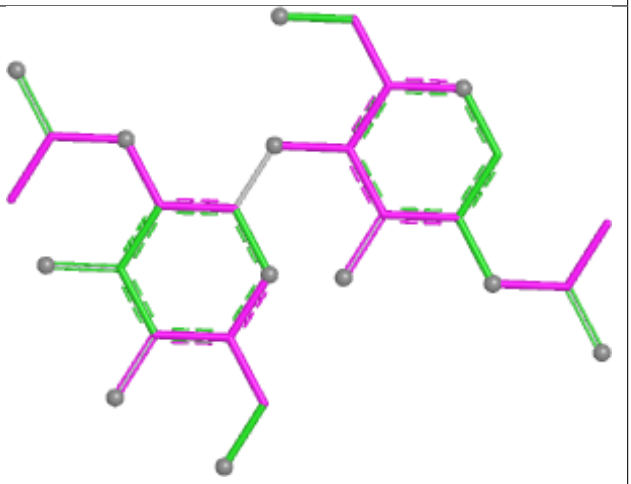
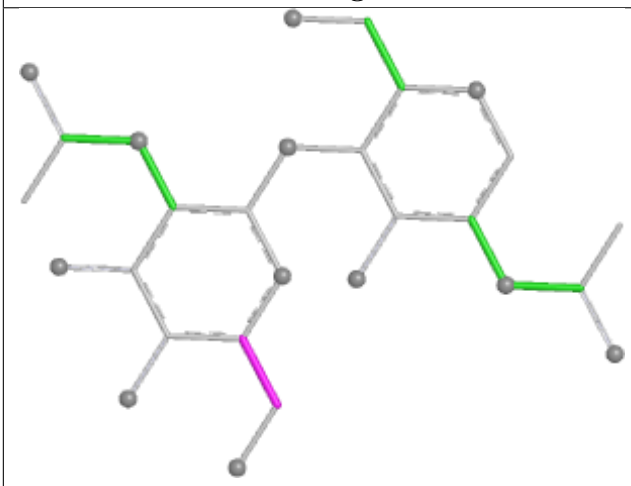


Bond angles



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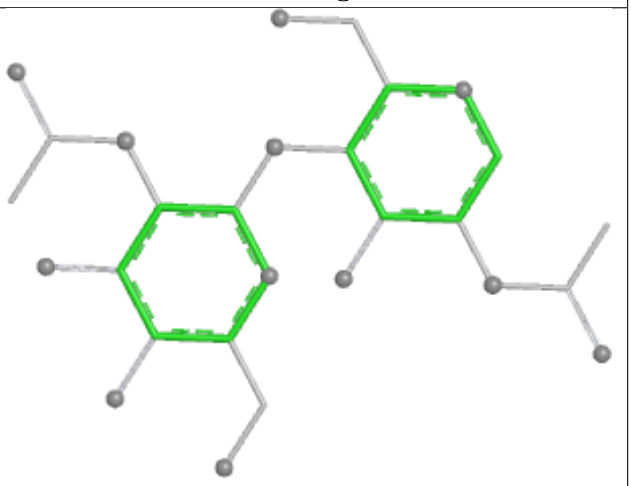
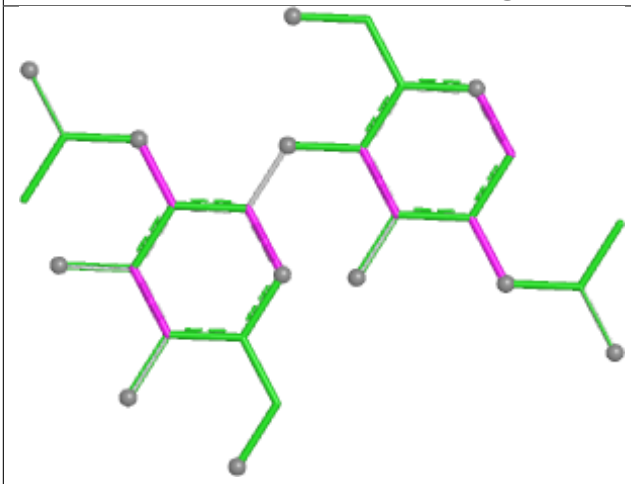


Rings

Oligosaccharide Chain 2



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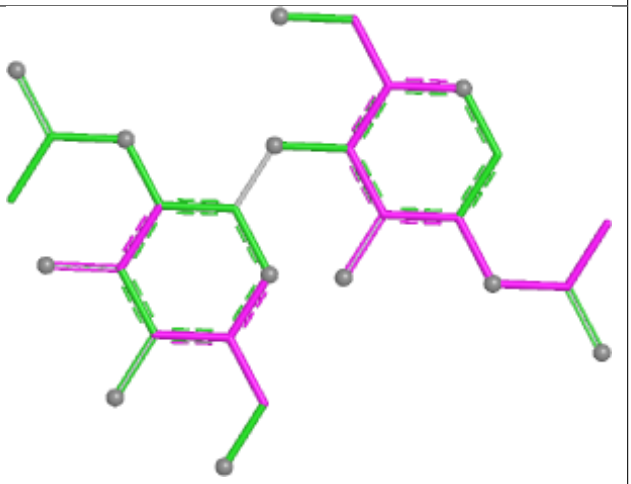

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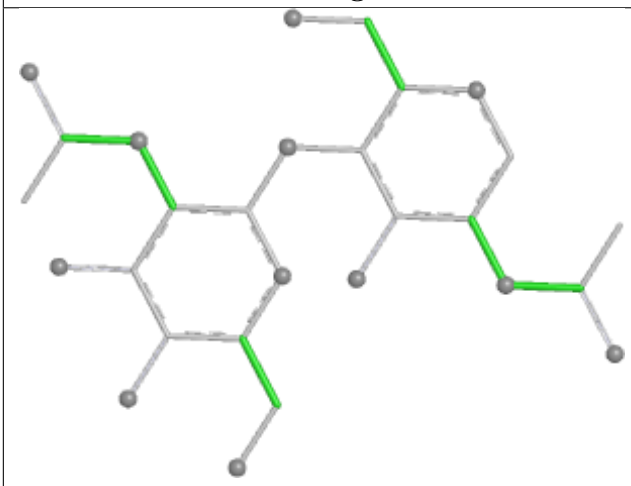

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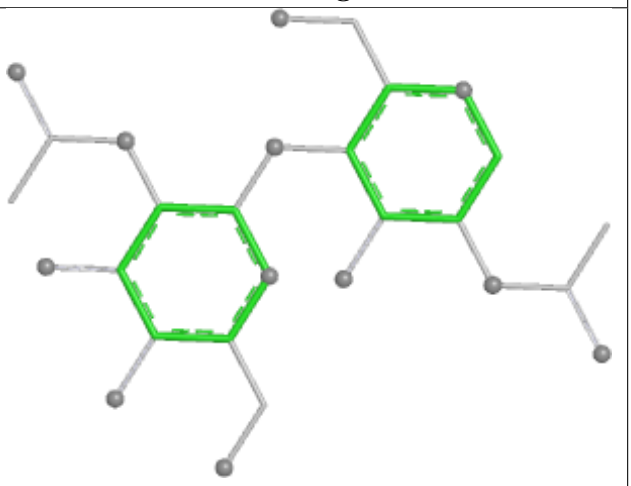
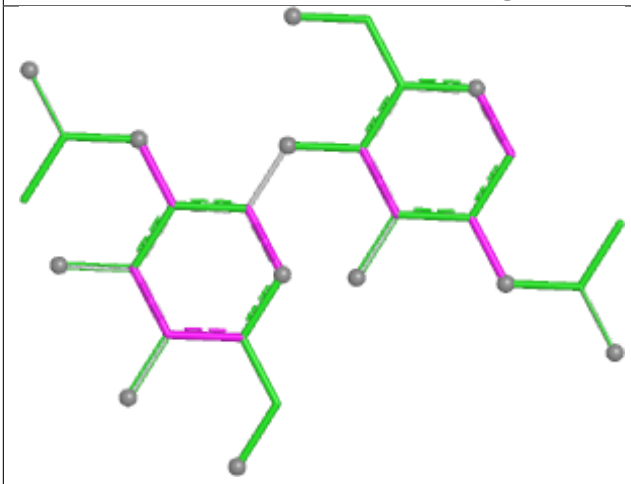


Rings

Oligosaccharide Chain 5



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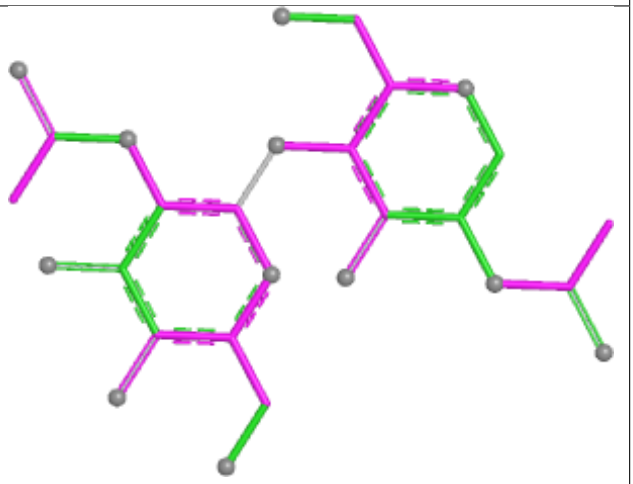
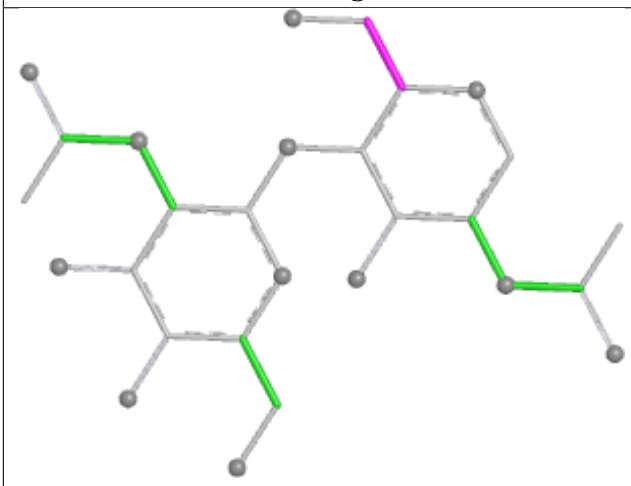


Bond angles



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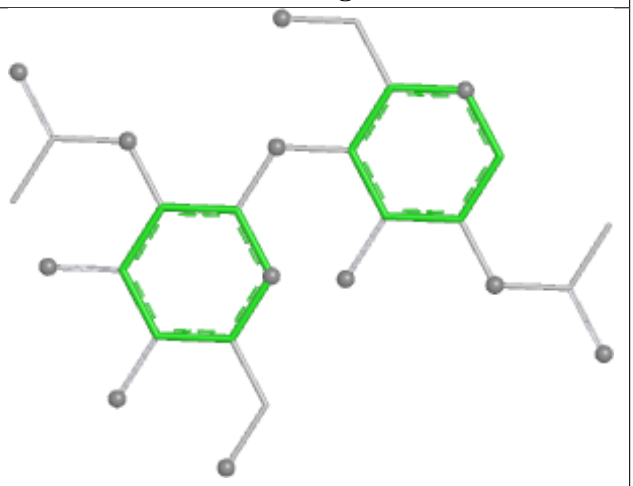
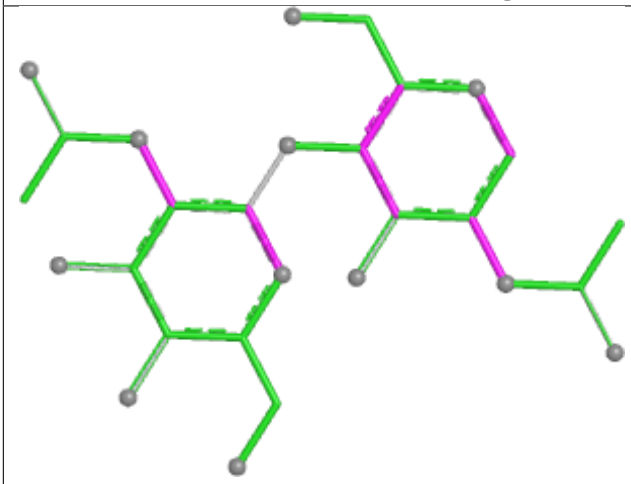


Rings

Oligosaccharide Chain 6



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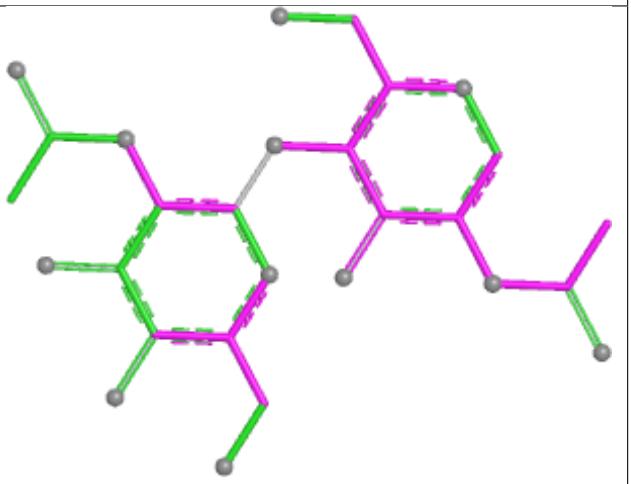
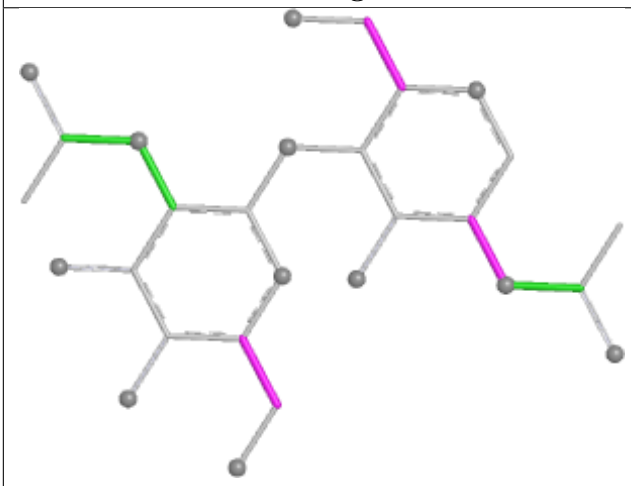


Bond angles



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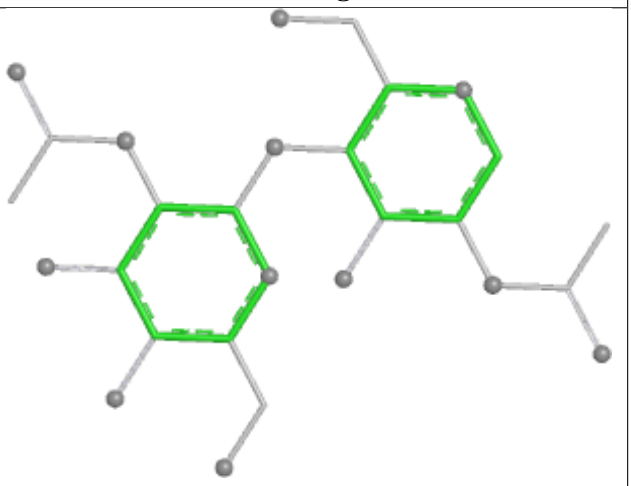
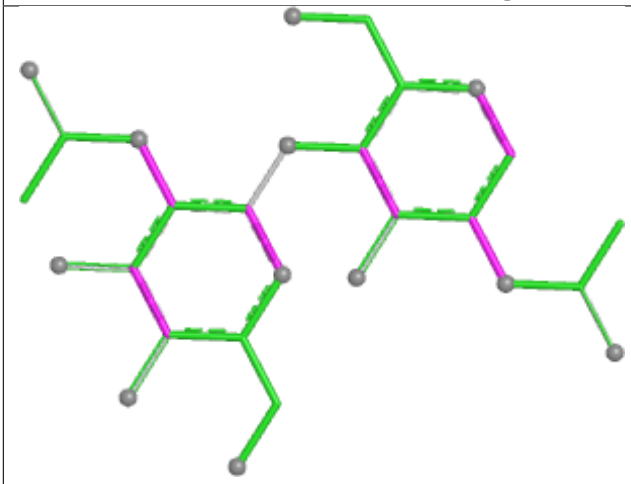
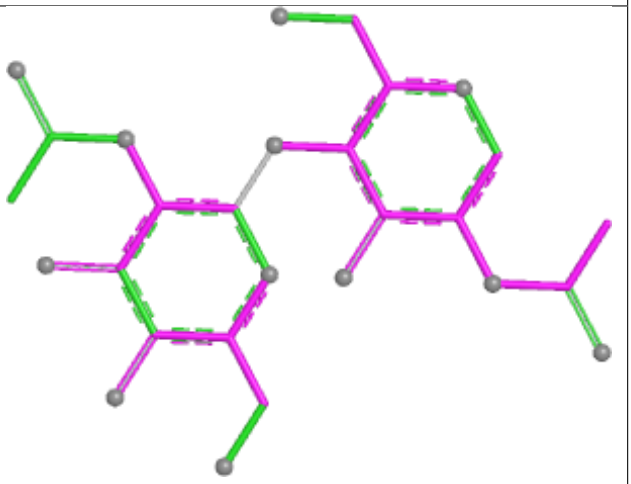


Rings

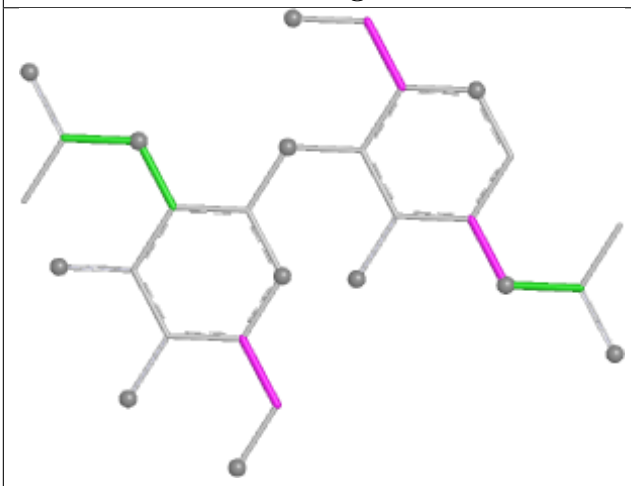
Oligosaccharide Chain 7



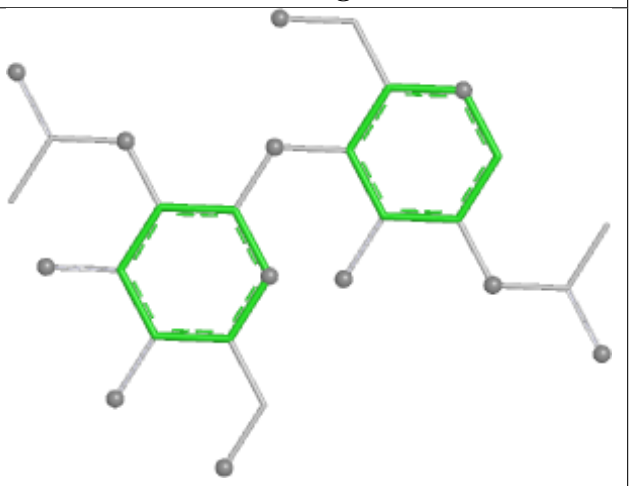
Bond lengths



Bond angles

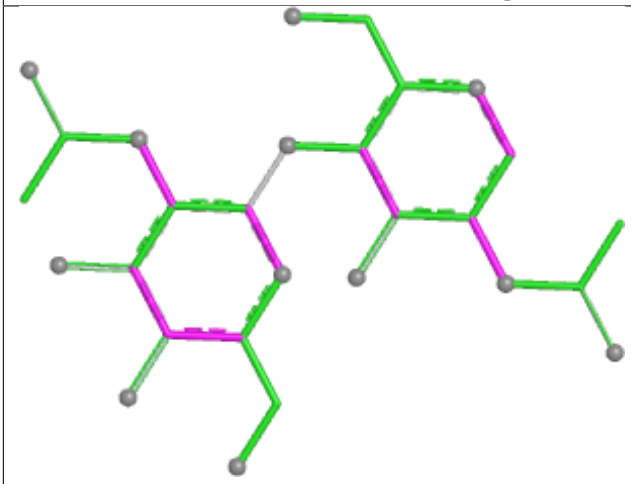


Torsions



Rings

Oligosaccharide Chain 8



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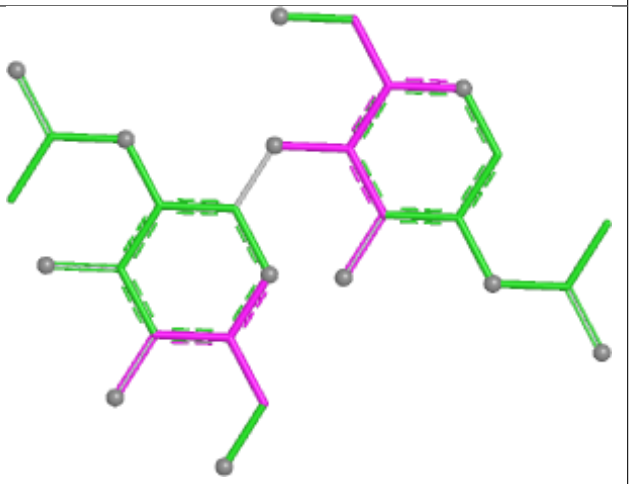
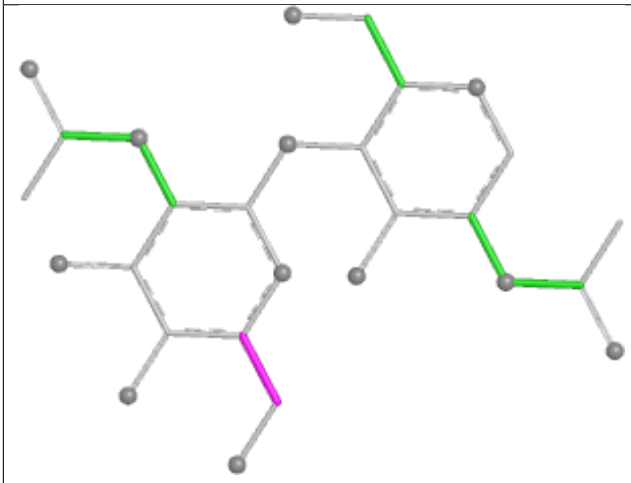


Bond angles



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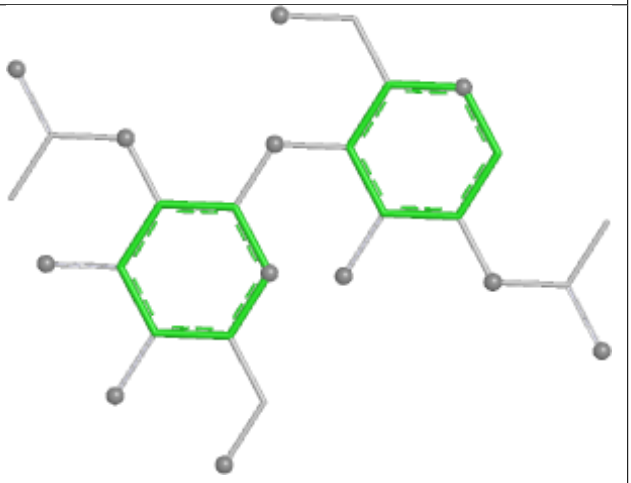
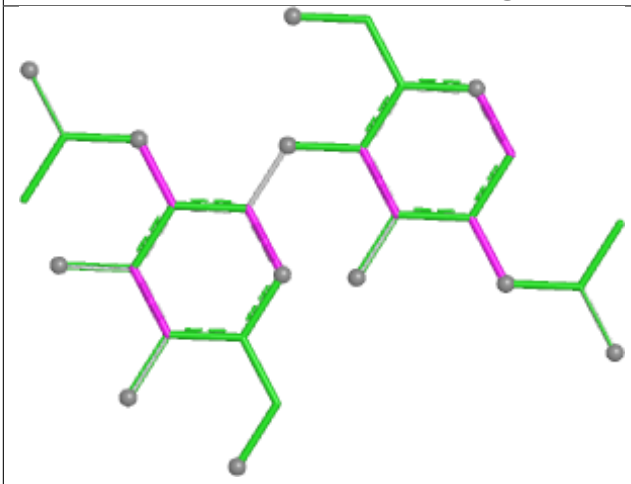


Rings

Oligosaccharide Chain 9



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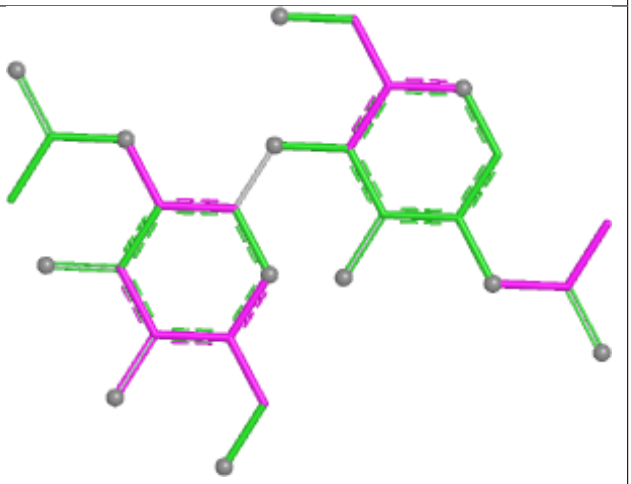
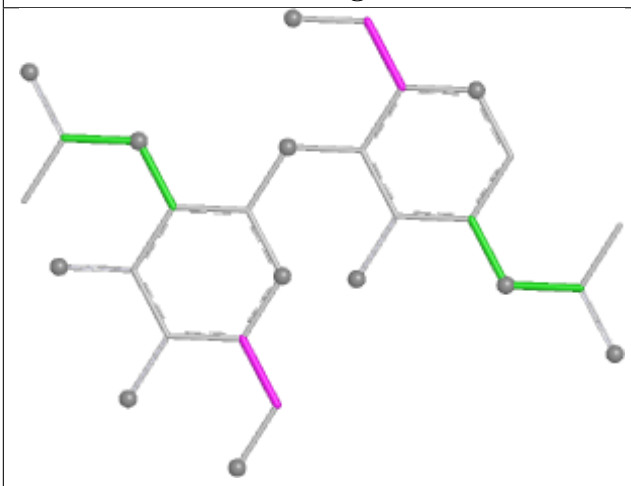
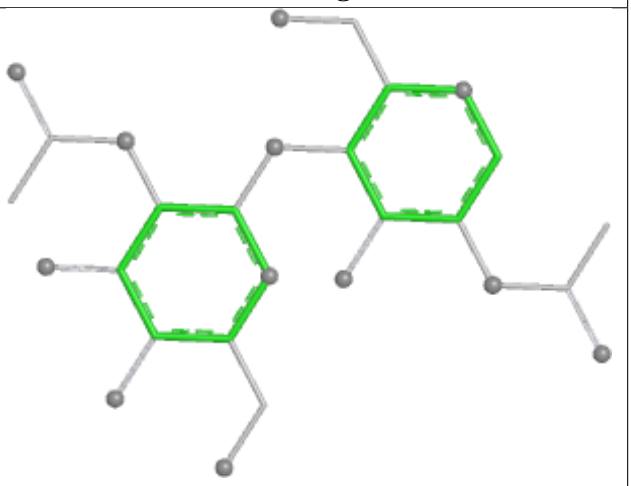


Bond angles

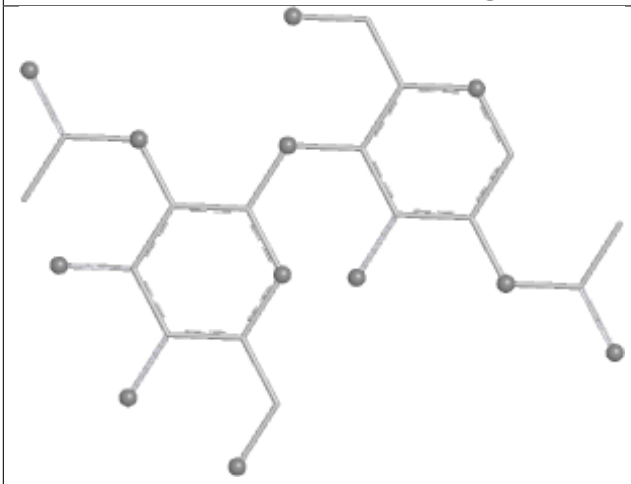


Torsions

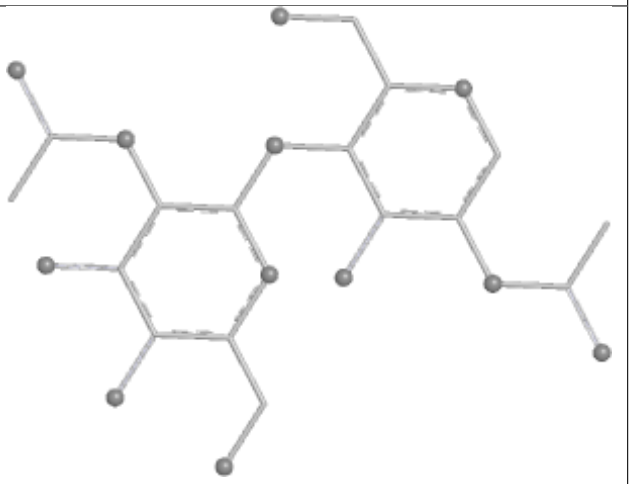


Rings

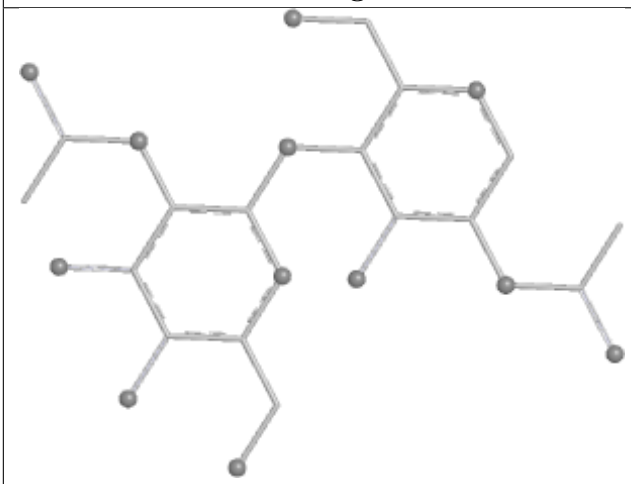
Oligosaccharide Chain CA



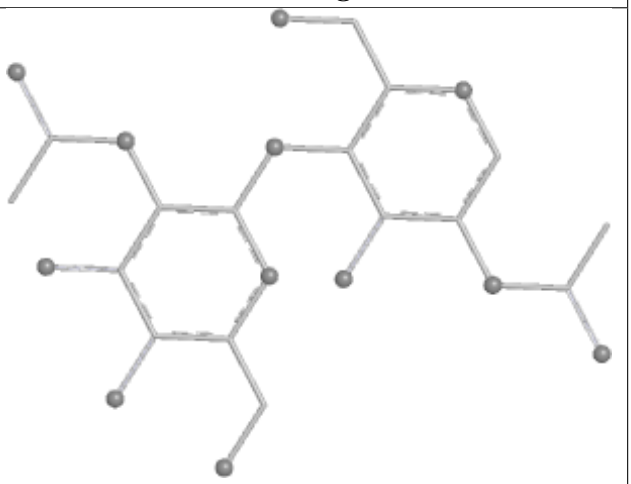
Bond lengths



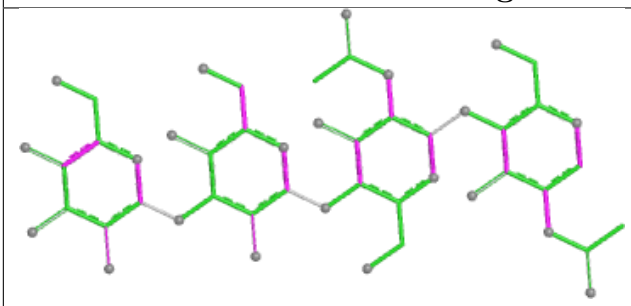
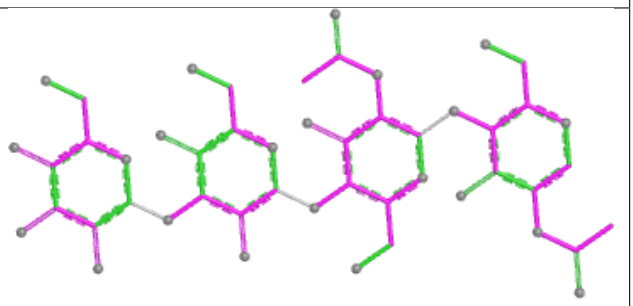
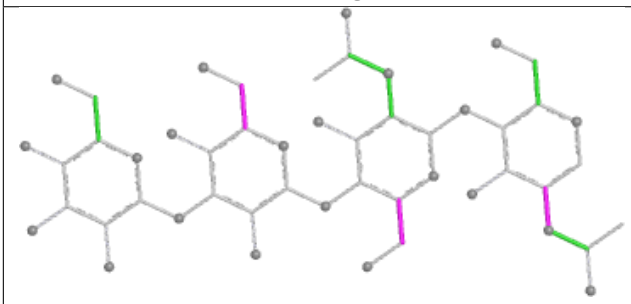
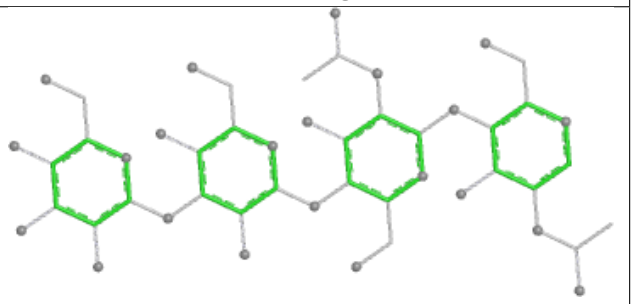
Bond angles

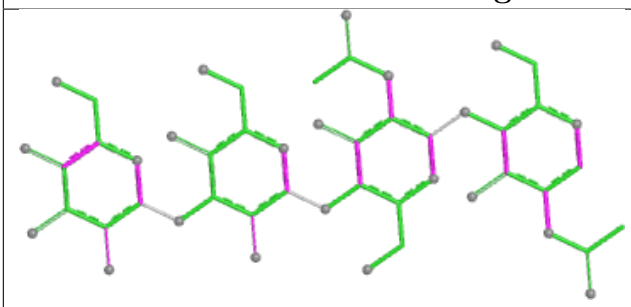
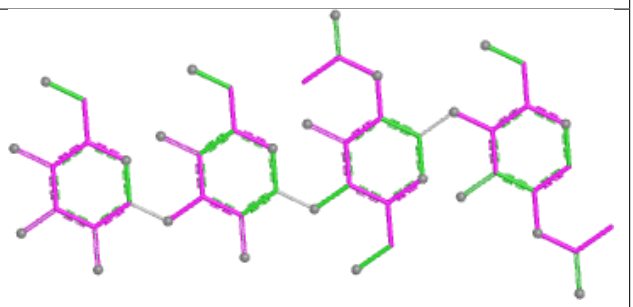
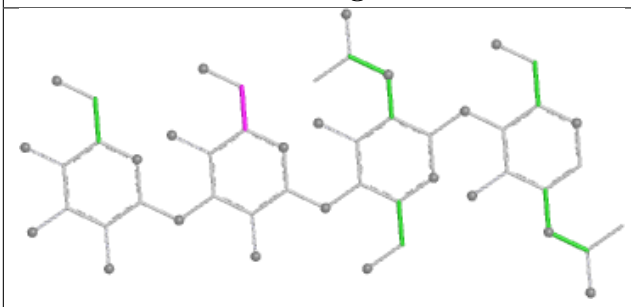
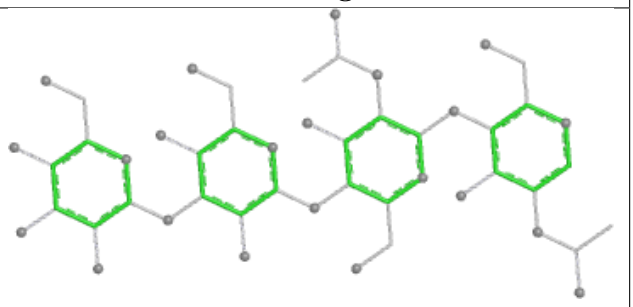


Torsions

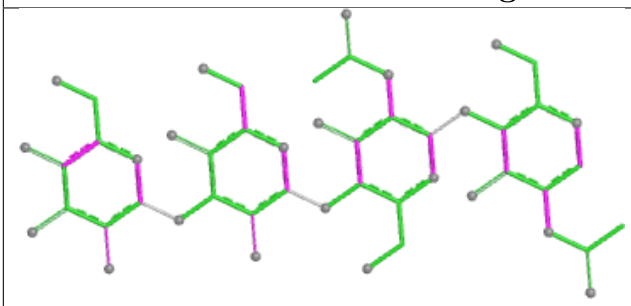


Rings

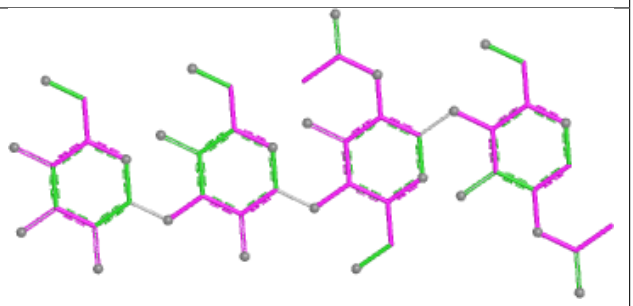
Oligosaccharide Chain F	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain U	
	
Bond lengths	Bond angles
	
Torsions	Rings

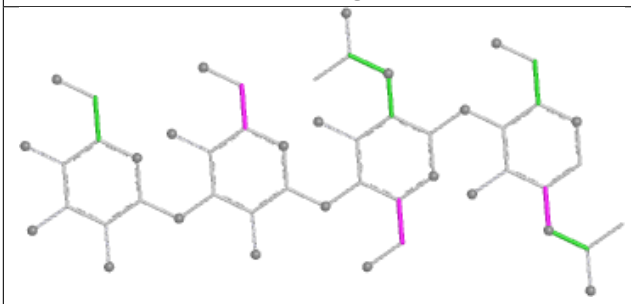
Oligosaccharide Chain a



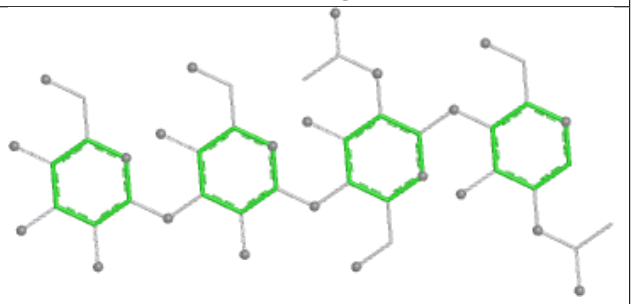
Bond lengths



Bond angles

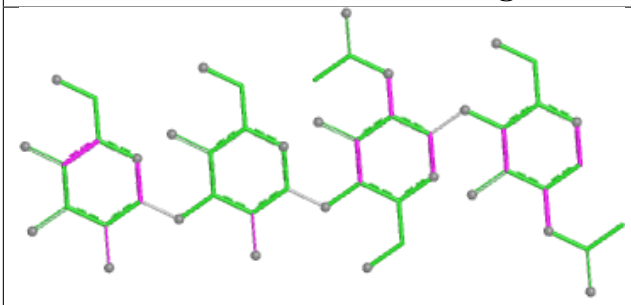


Torsions



Rings

Oligosaccharide Chain p



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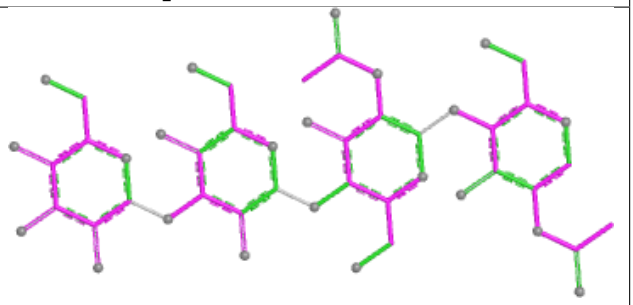
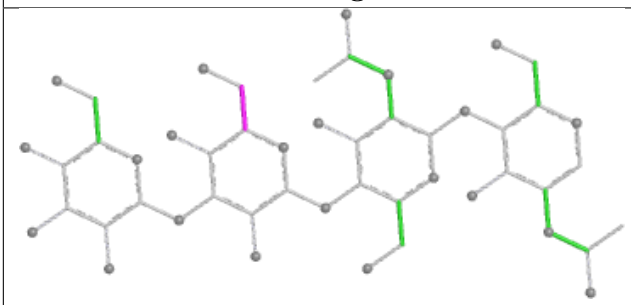
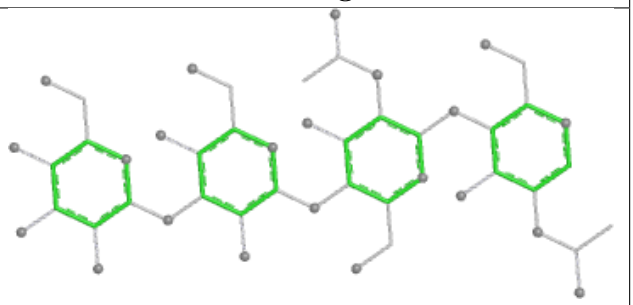


Bond angles

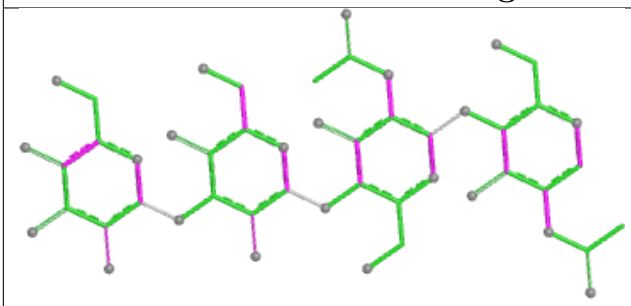


Torsions



Rings

Oligosaccharide Chain v



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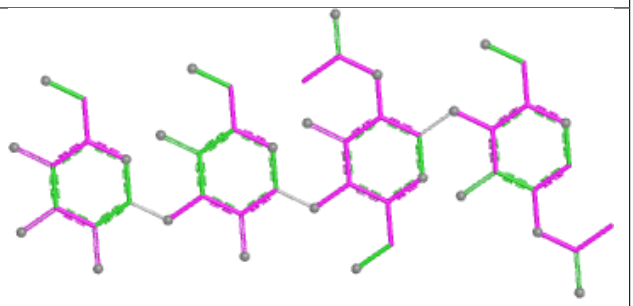
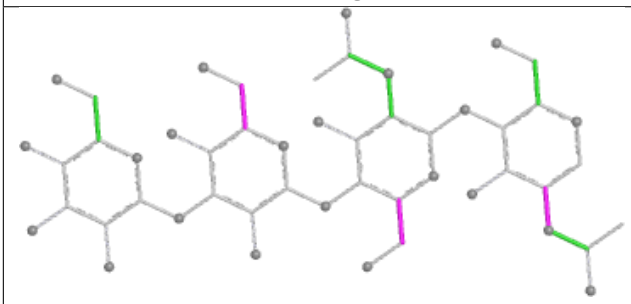
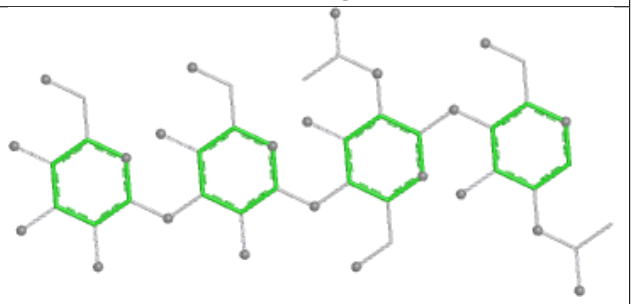


Bond angles

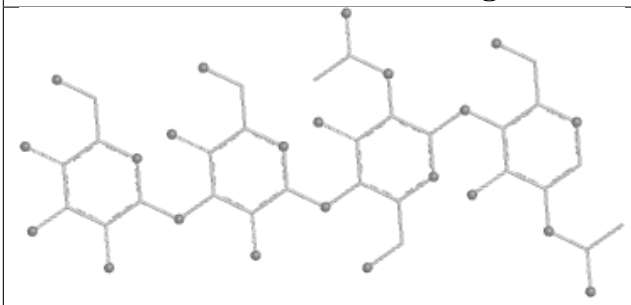


Torsions

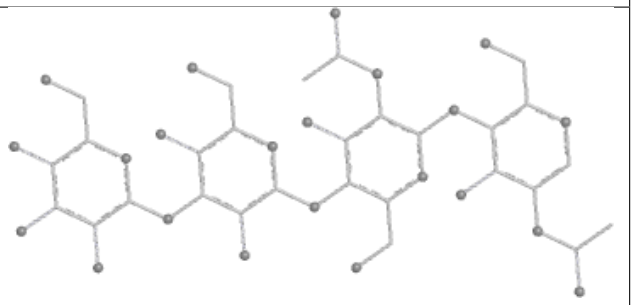


Rings

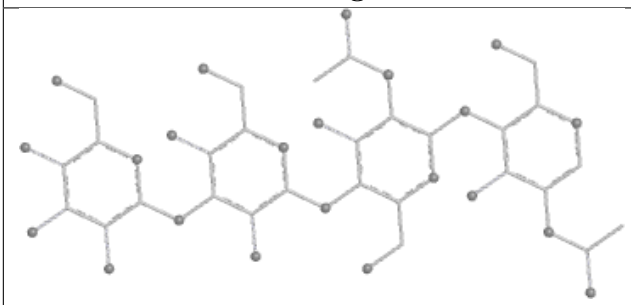
Oligosaccharide Chain AA



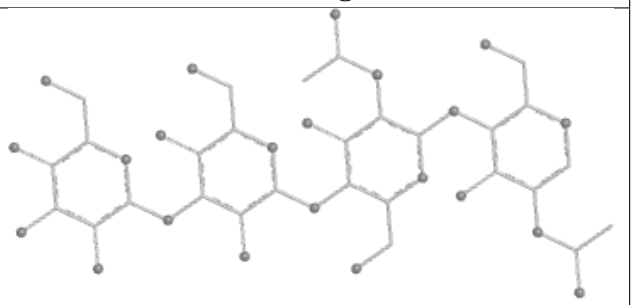
Bond lengths



Bond angles

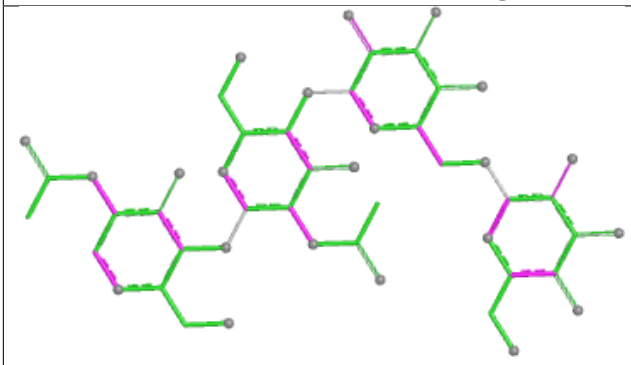


Torsions



Rings

Oligosaccharide Chain H



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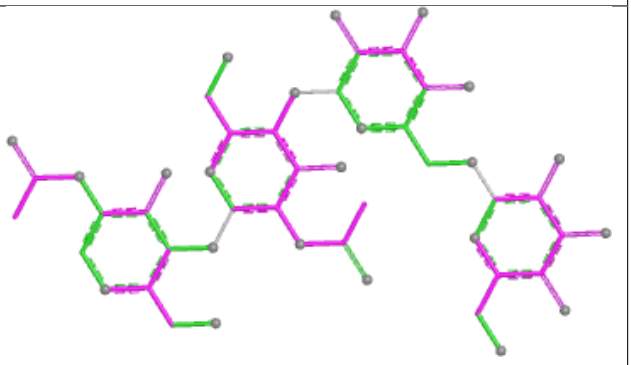
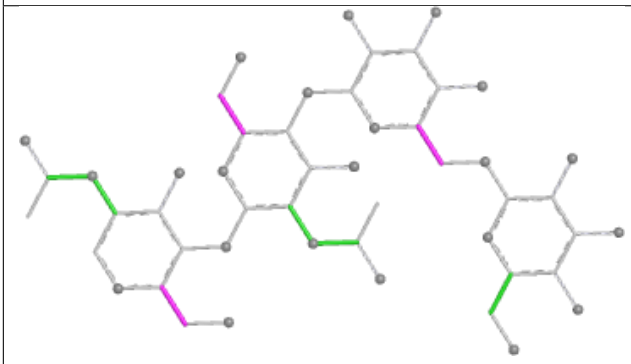
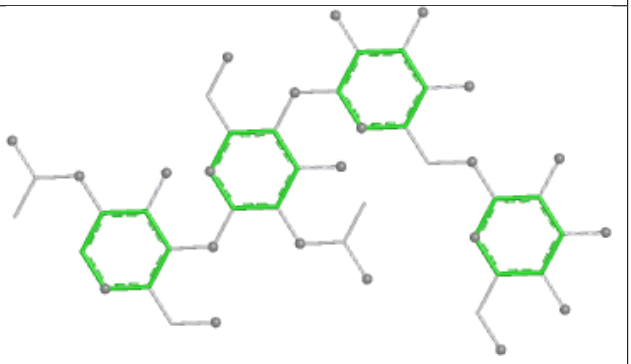


Bond angles

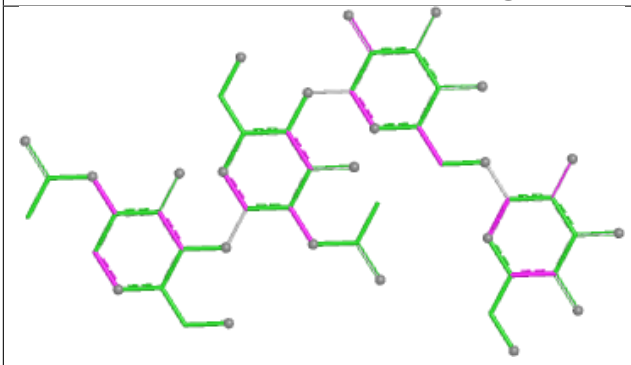


Torsions



Rings

Oligosaccharide Chain c



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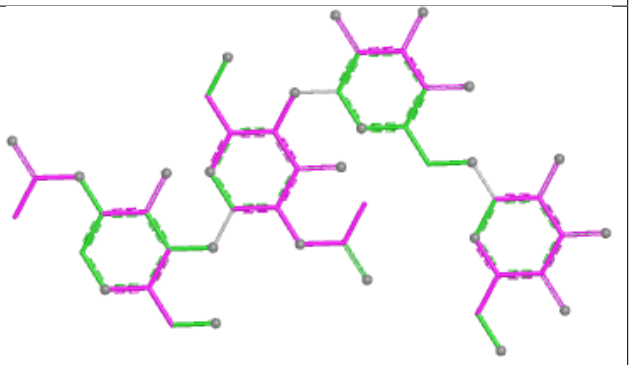
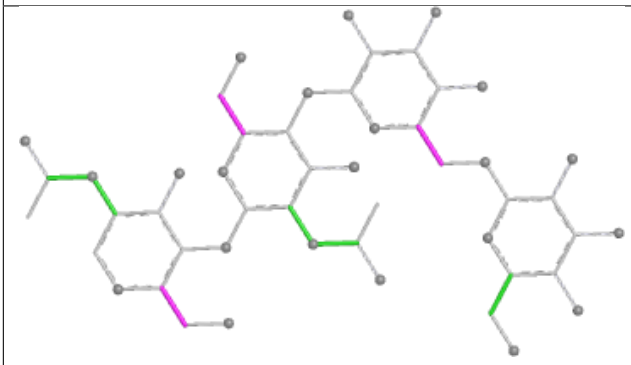
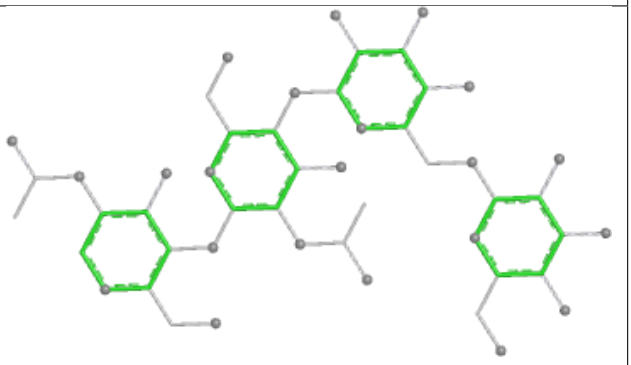


Bond angles

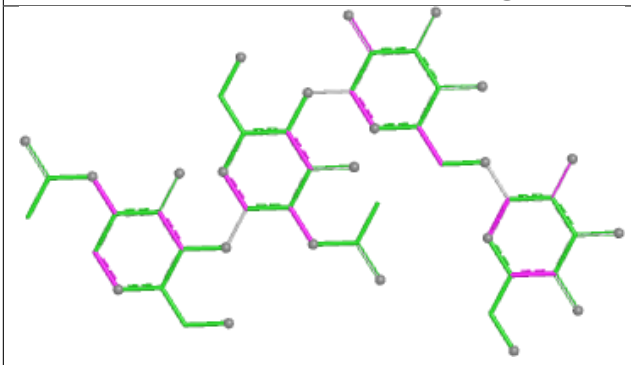


Torsions



Rings

Oligosaccharide Chain x



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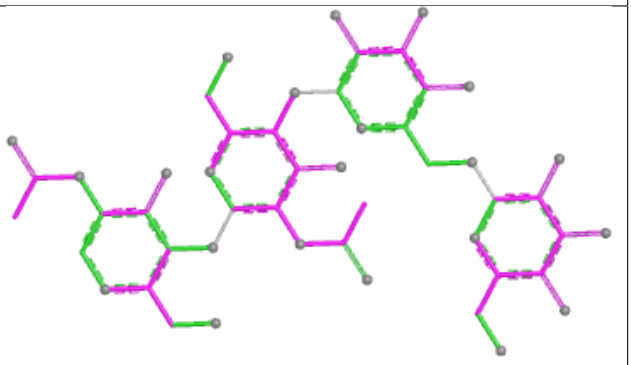
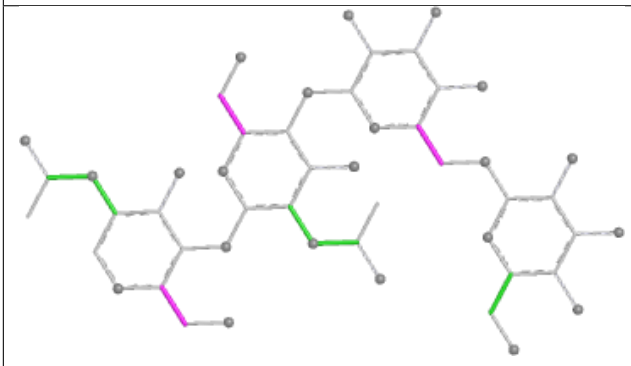
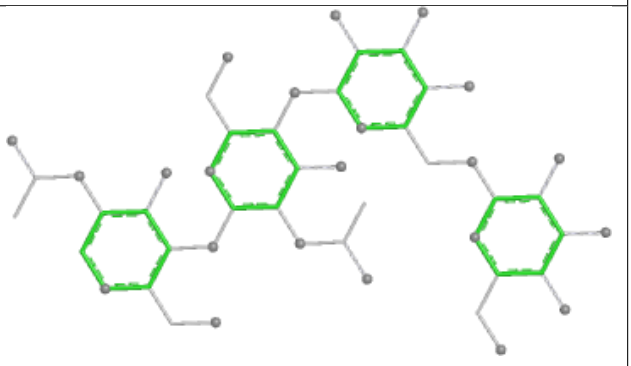


Bond angles

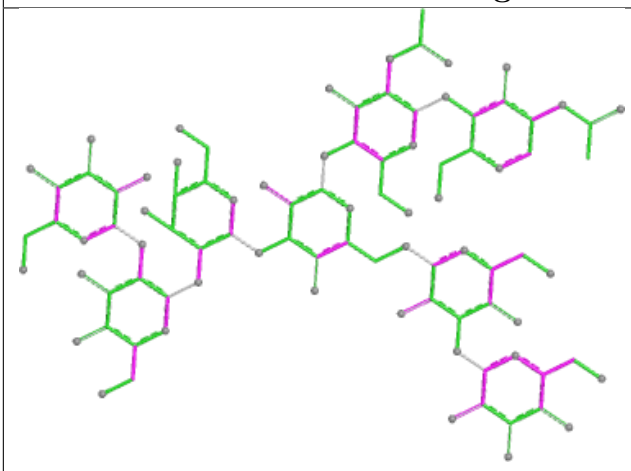


Torsions

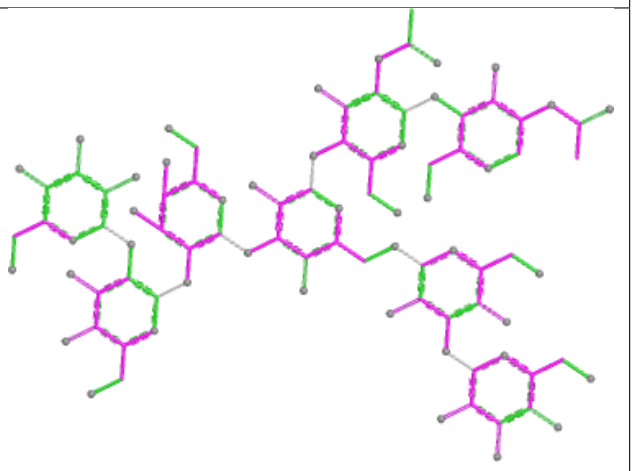


Rings

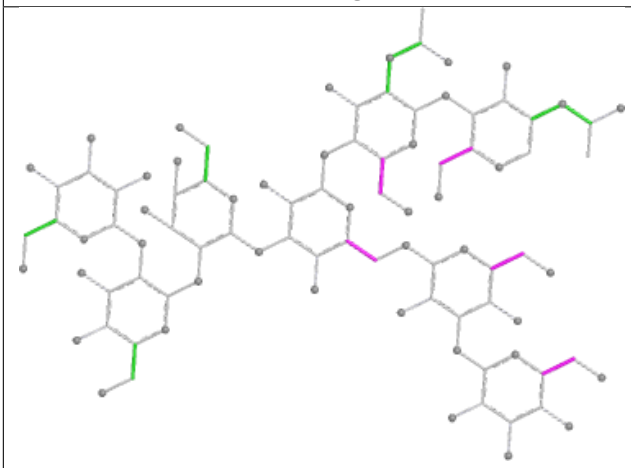
Oligosaccharide Chain K



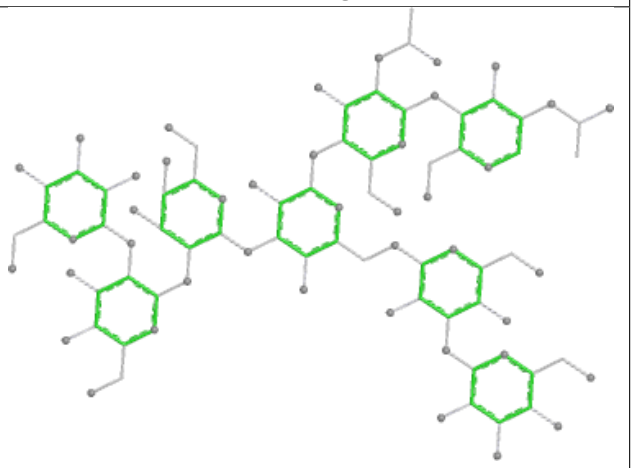
Bond lengths



Bond angles

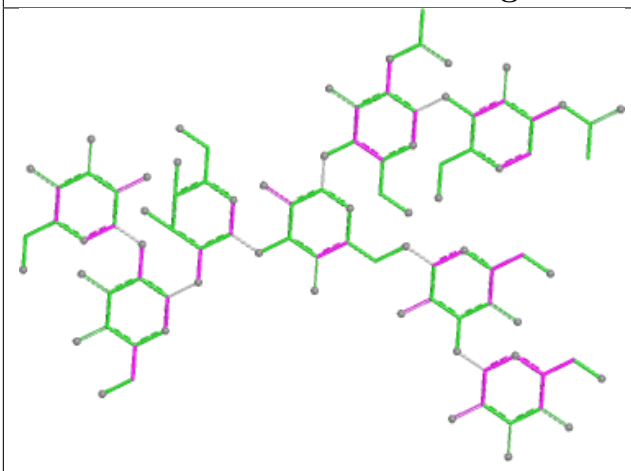


Torsions

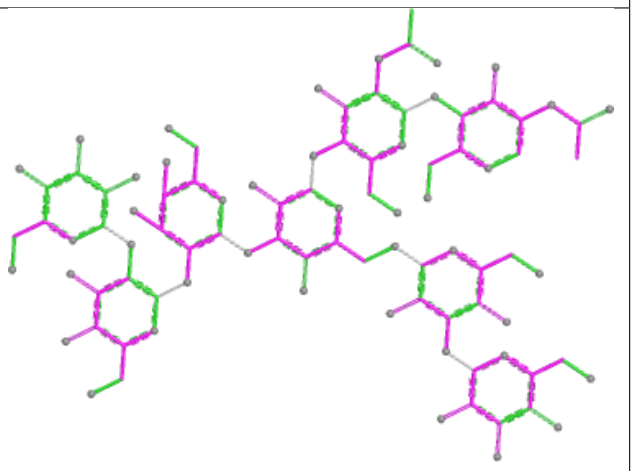


Rings

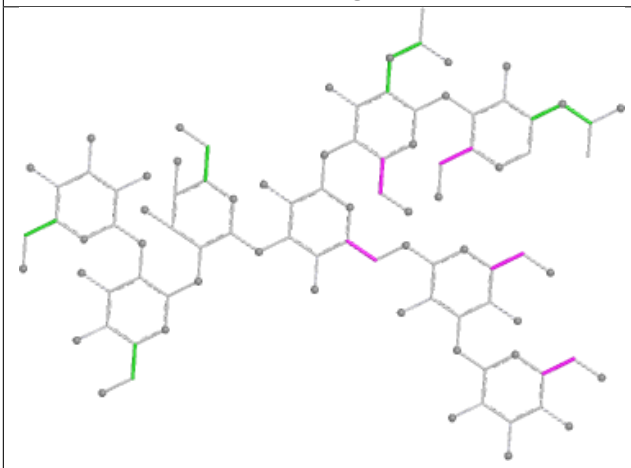
Oligosaccharide Chain f



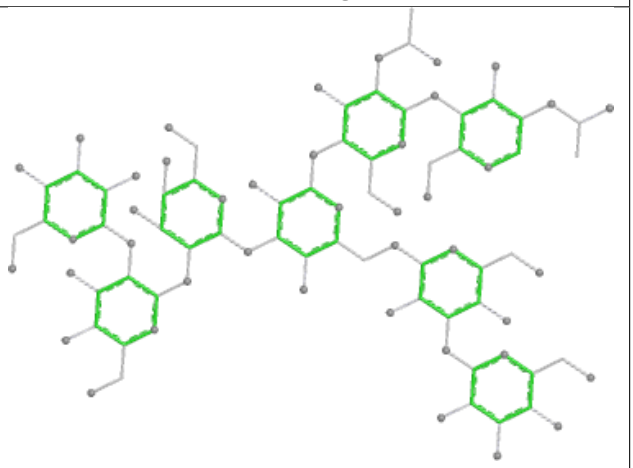
Bond lengths



Bond angles

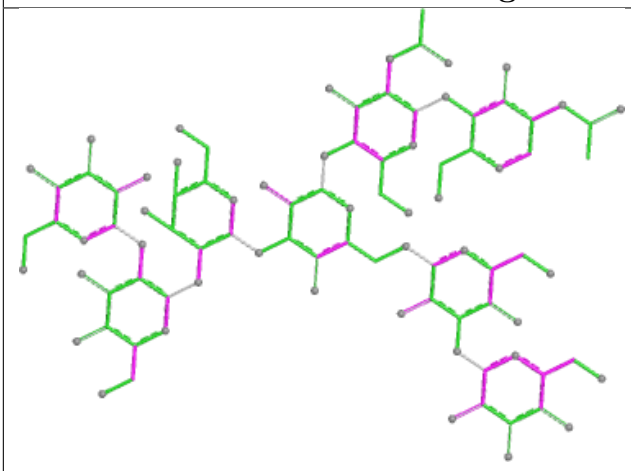


Torsions

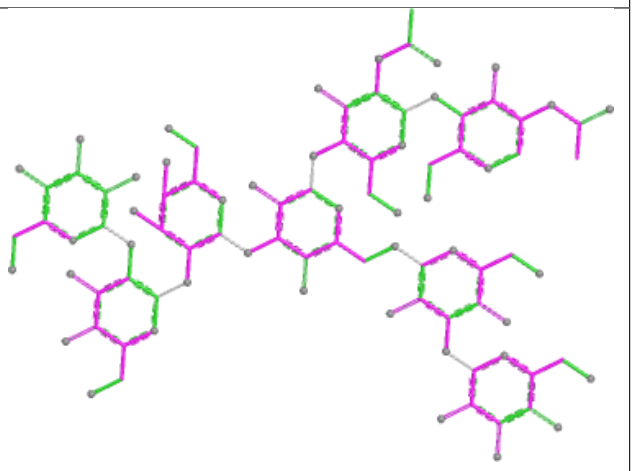


Rings

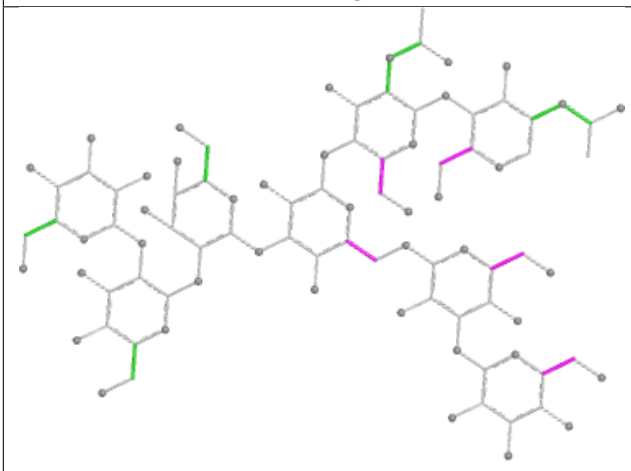
Oligosaccharide Chain 0



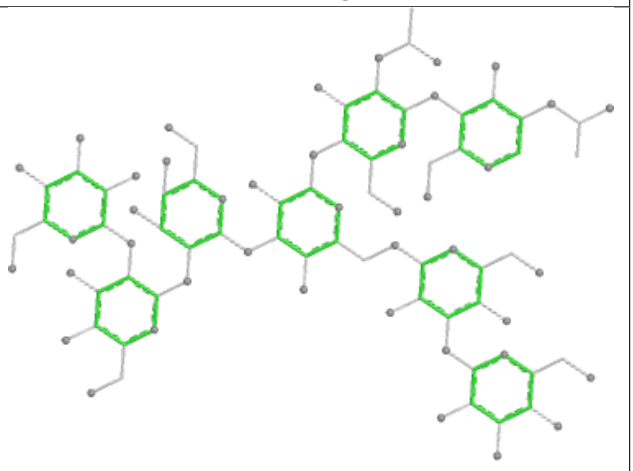
Bond lengths



Bond angles

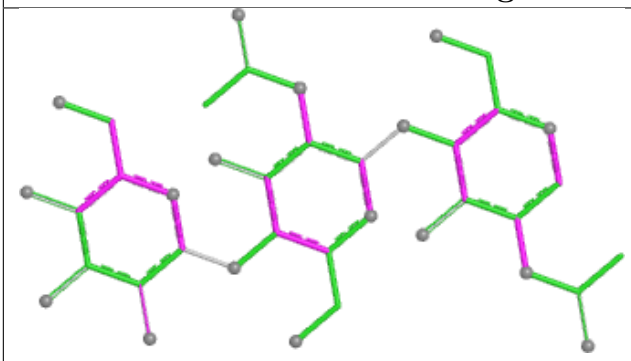


Torsions



Rings

Oligosaccharide Chain L



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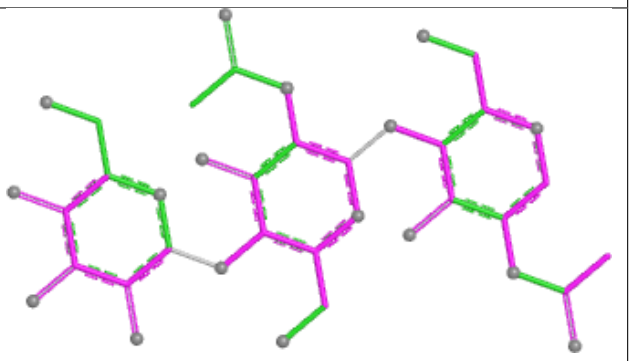
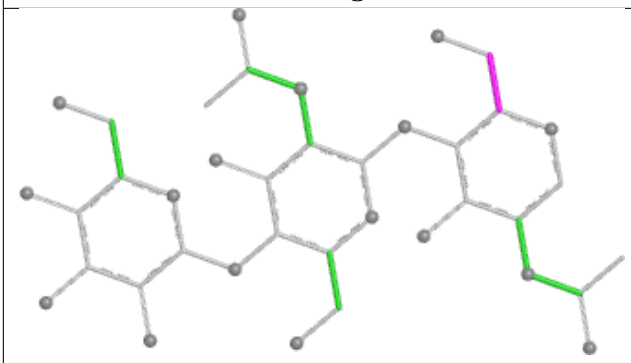


Bond angles



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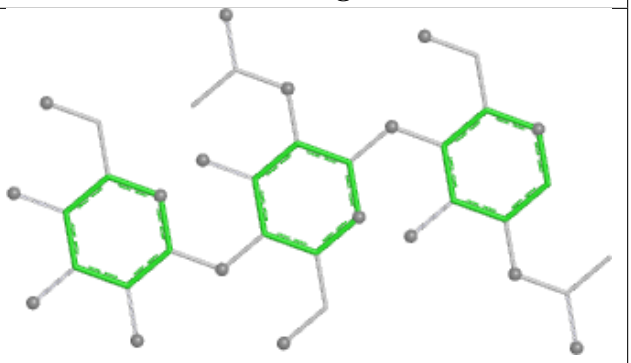
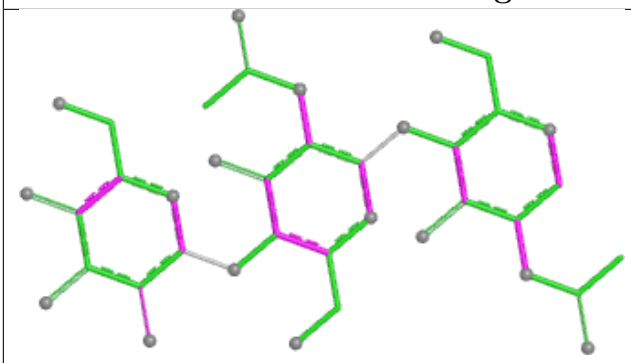


Rings

Oligosaccharide Chain O



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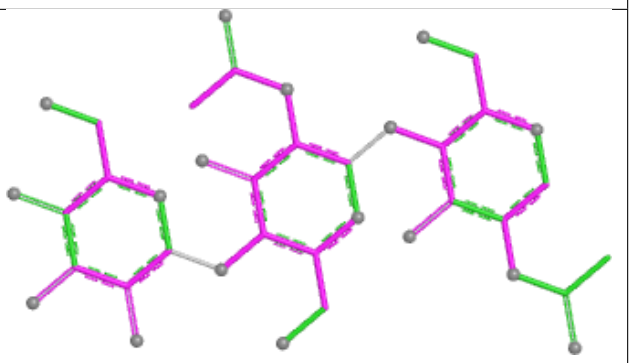
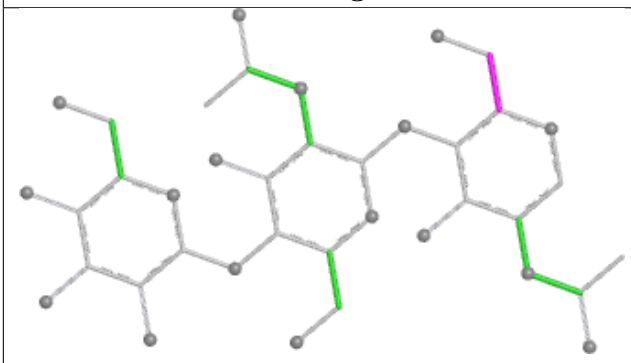


Bond angles



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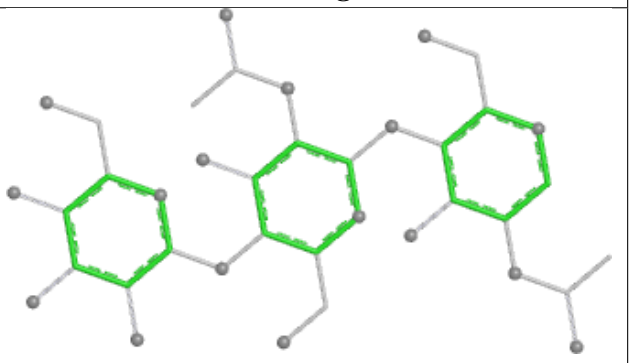
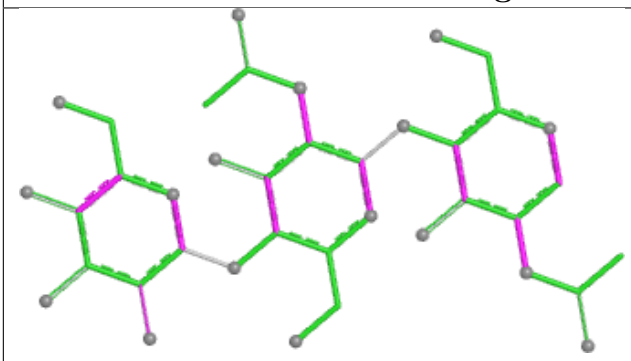


Rings

Oligosaccharide Chain X



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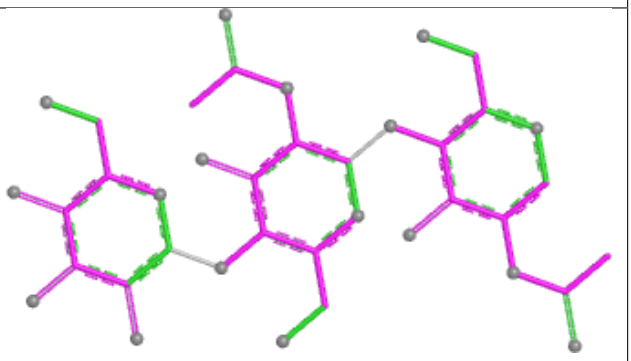
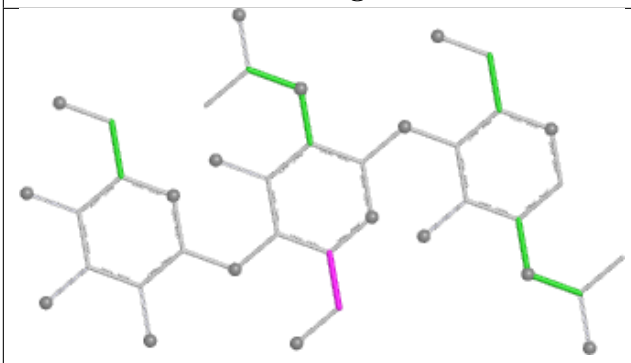


Bond angles



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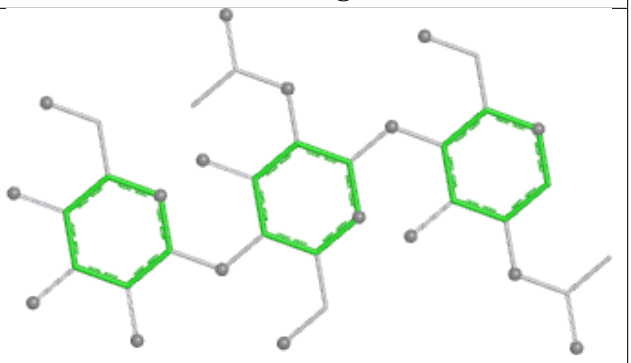
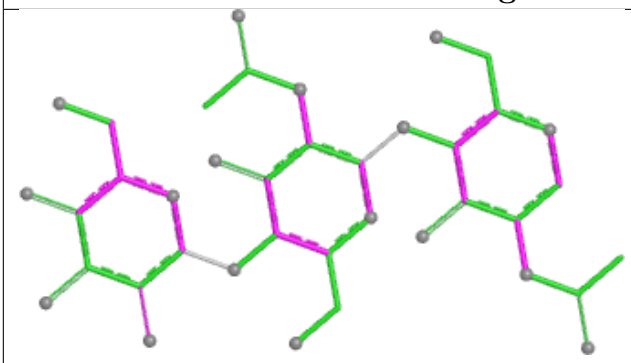


Rings

Oligosaccharide Chain g



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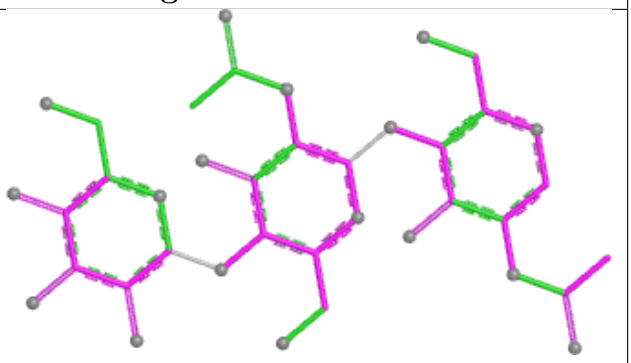
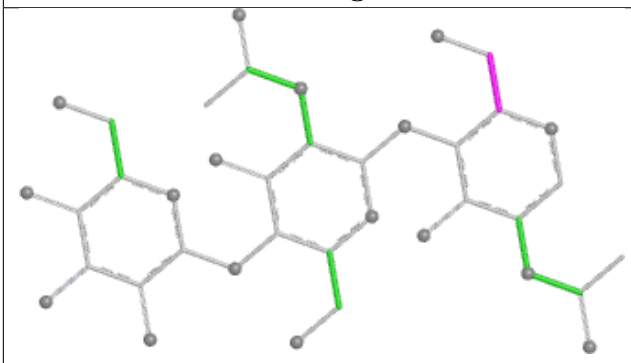


Bond angles



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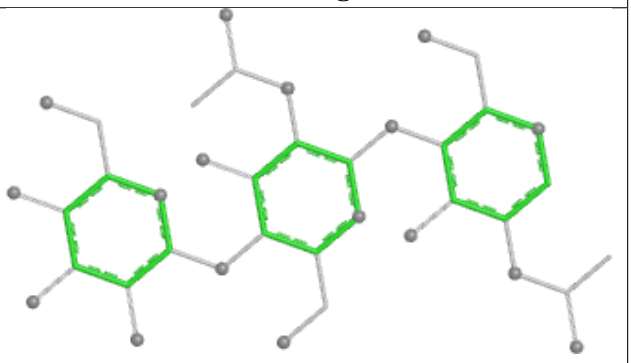
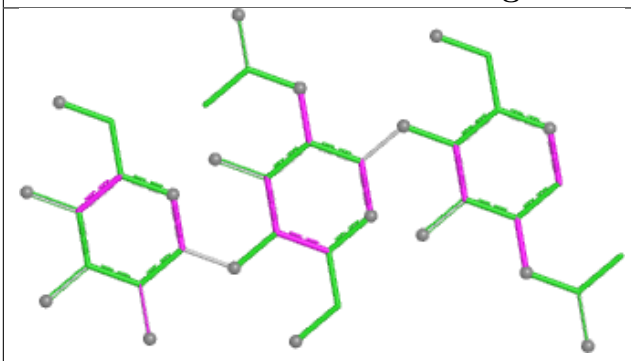


Rings

Oligosaccharide Chain j



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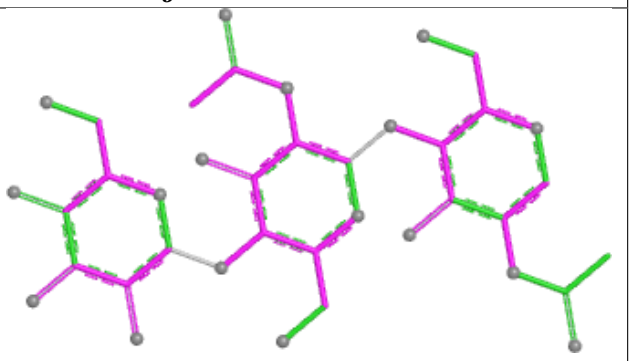
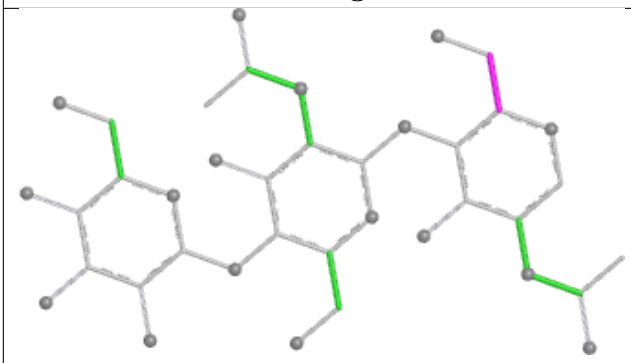


Bond angles



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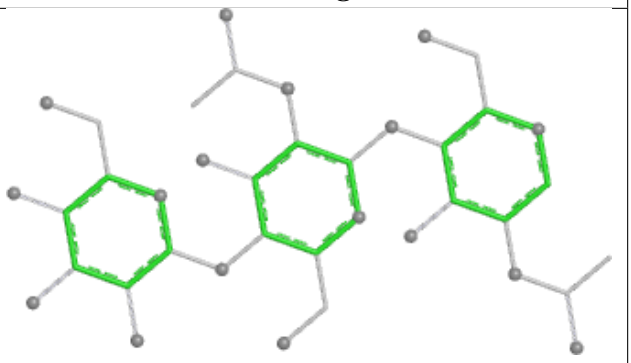
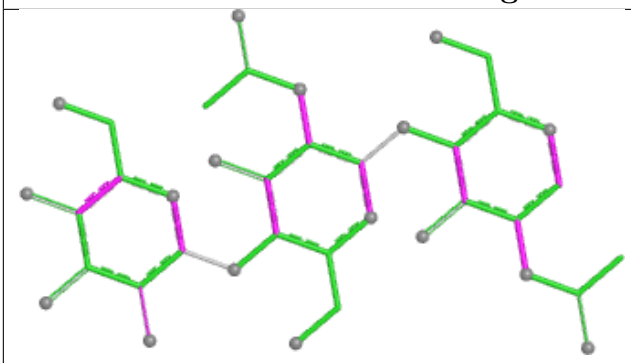


Rings

Oligosaccharide Chain s



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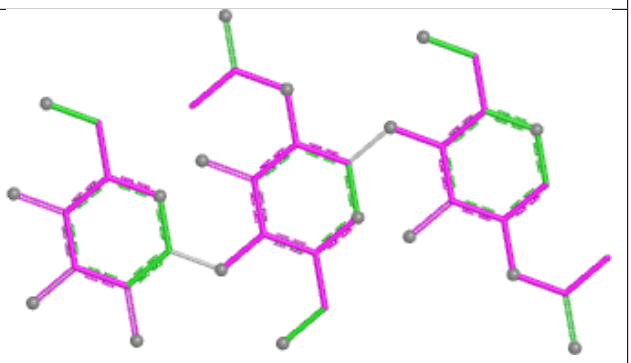
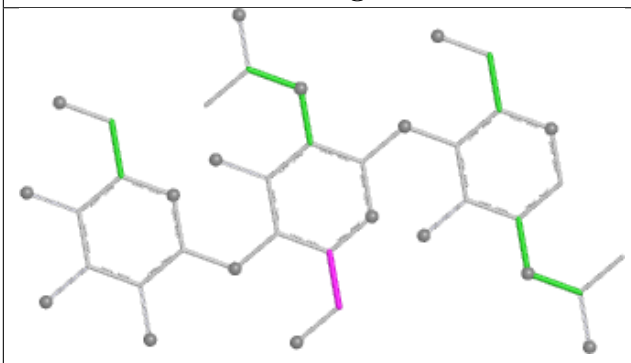


Bond angles



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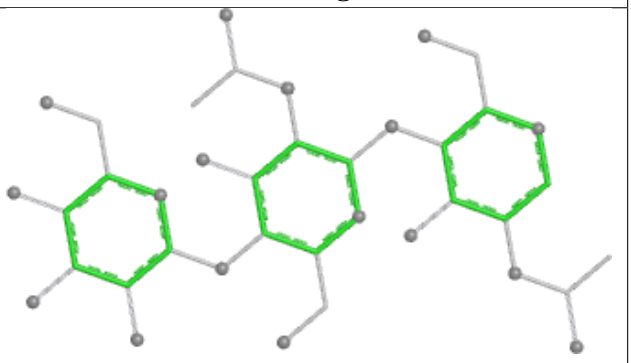
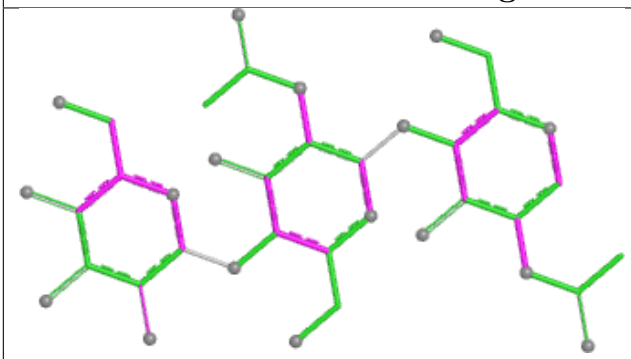


Rings

Oligosaccharide Chain 1



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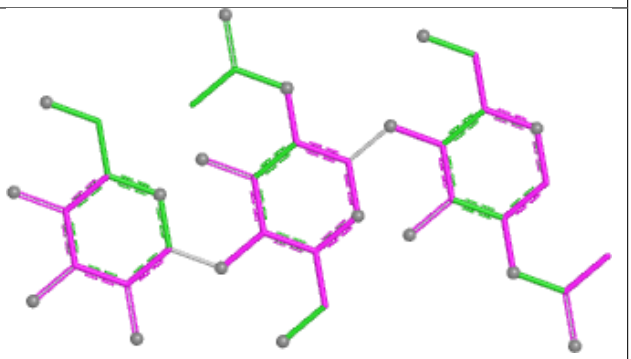
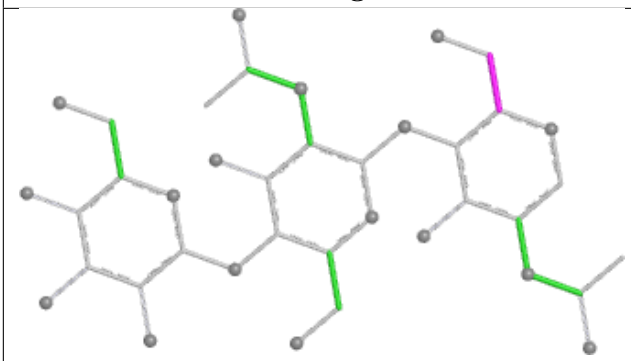


Bond angles



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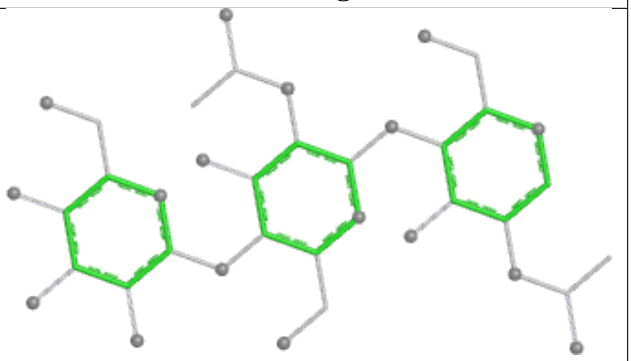
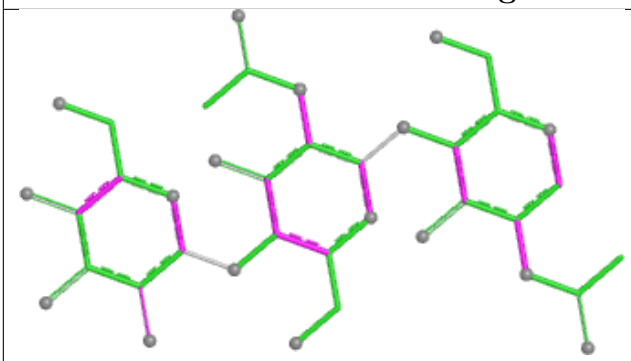


Rings

Oligosaccharide Chain 4



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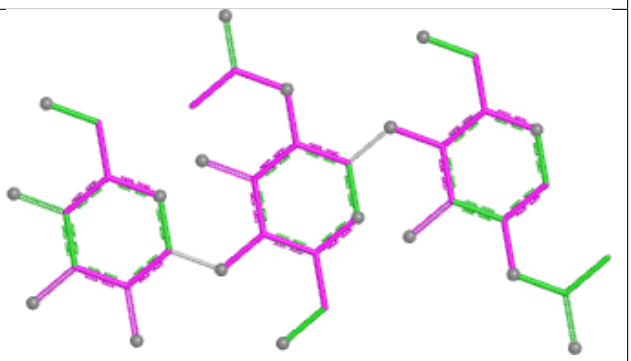
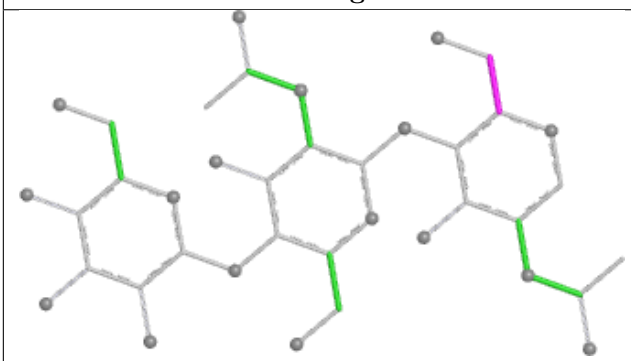


Bond angles



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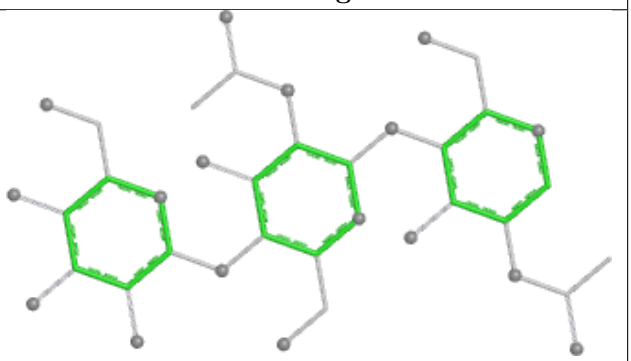
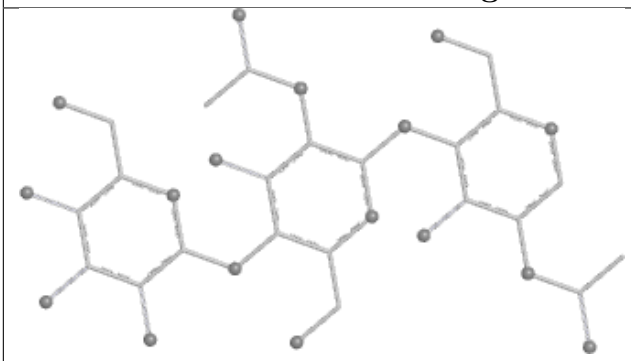


Rings

Oligosaccharide Chain DA



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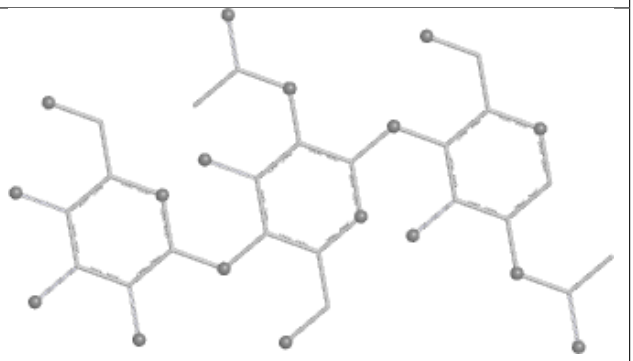
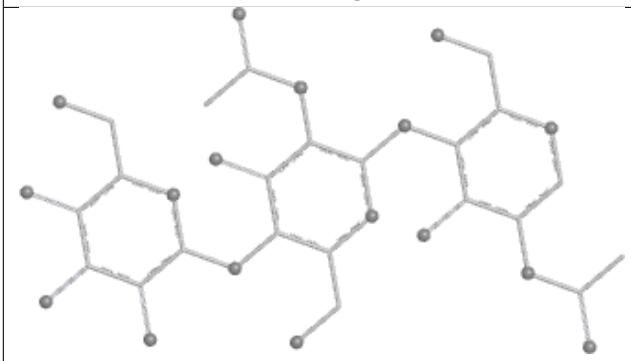


Bond angles



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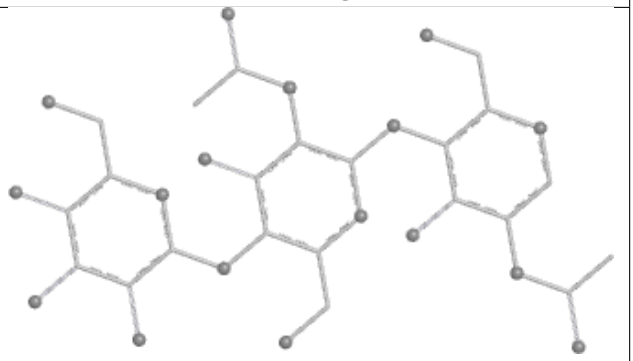
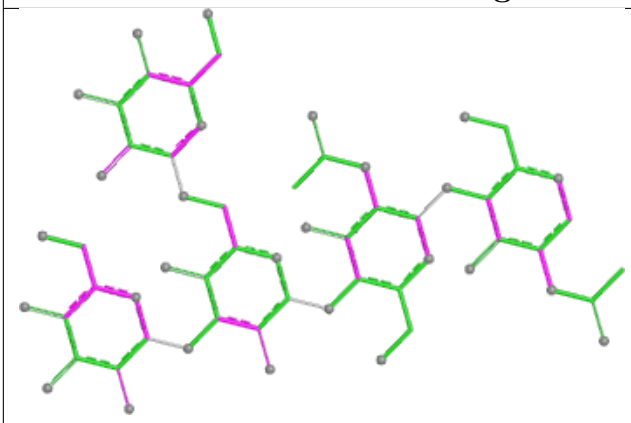


Rings

Oligosaccharide Chain N



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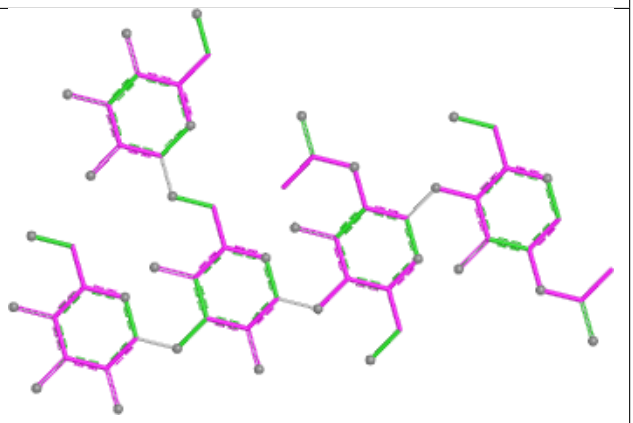
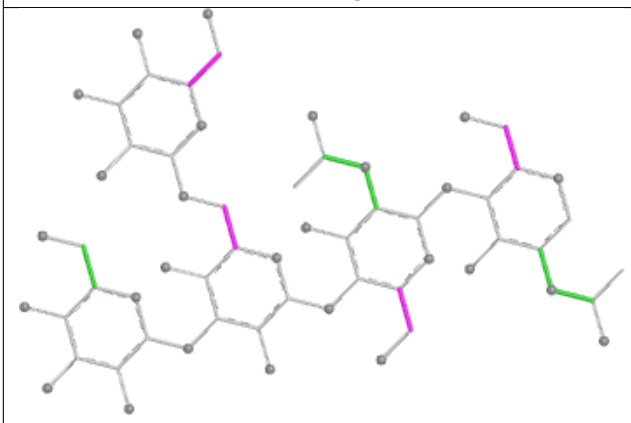


Bond angles



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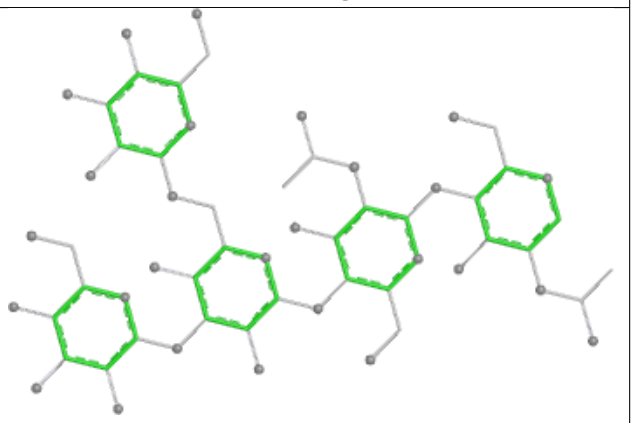
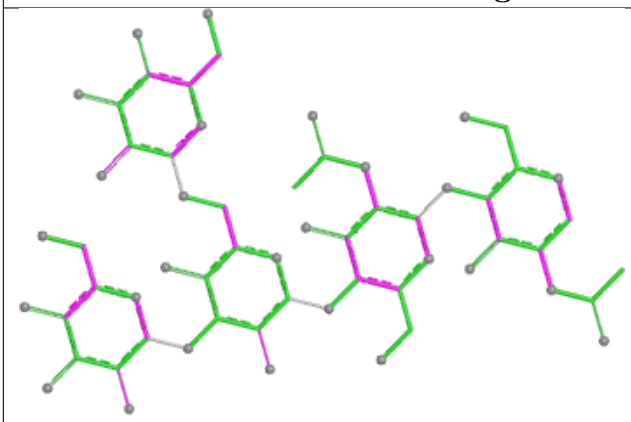


Rings

Oligosaccharide Chain V



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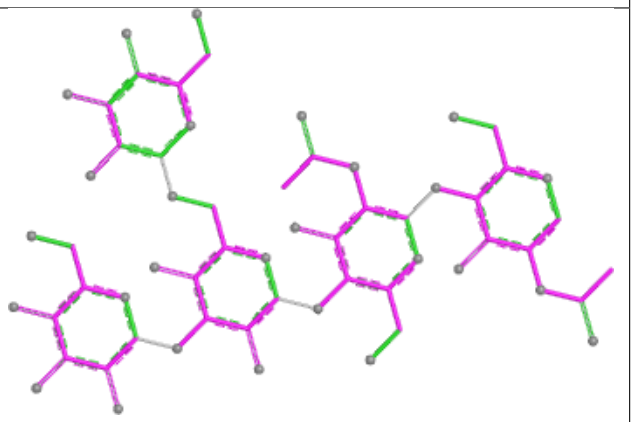
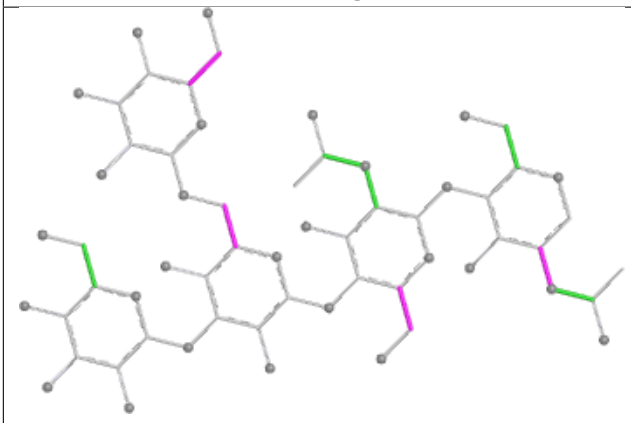
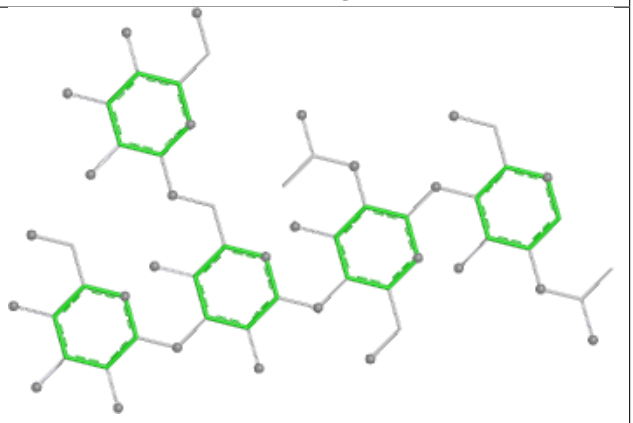


Bond angles

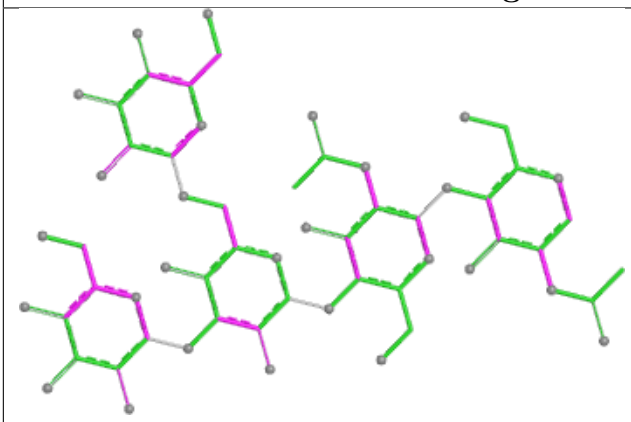


Torsions

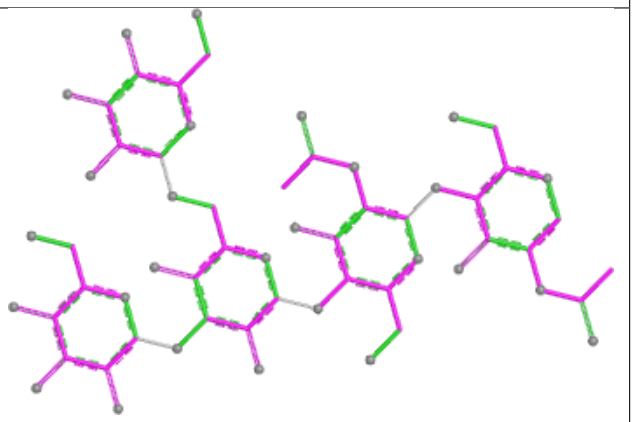


Rings

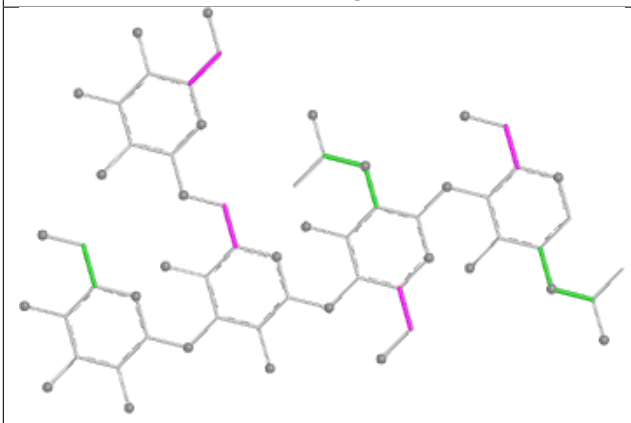
Oligosaccharide Chain i



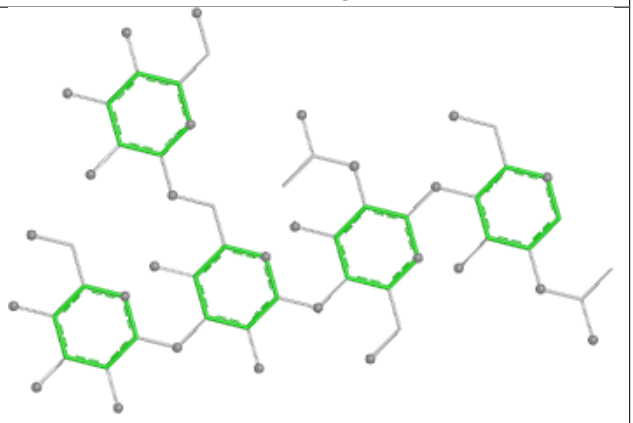
Bond lengths



Bond angles

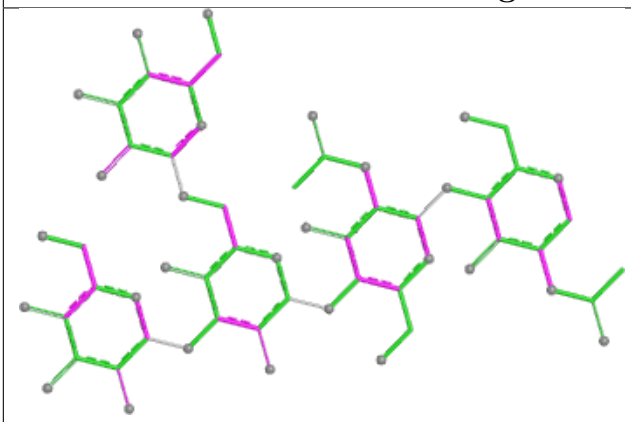


Torsions

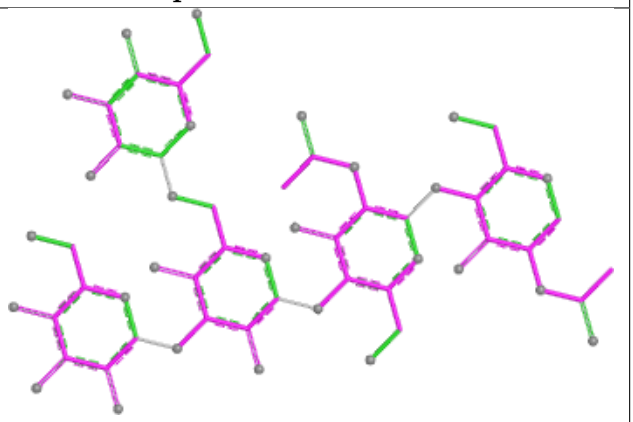


Rings

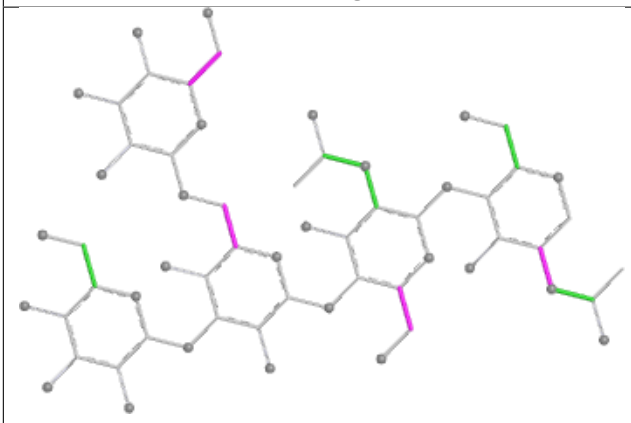
Oligosaccharide Chain q



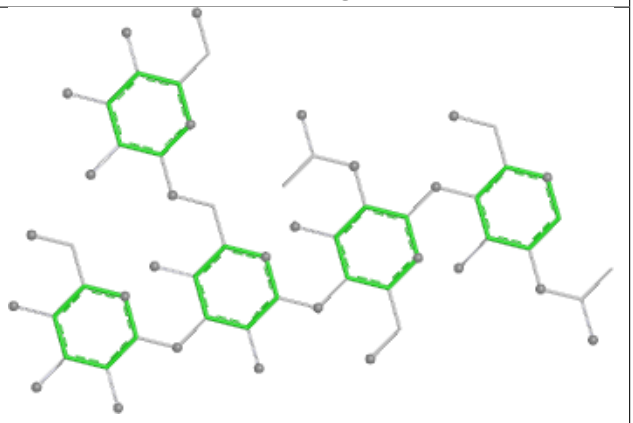
Bond lengths



Bond angles

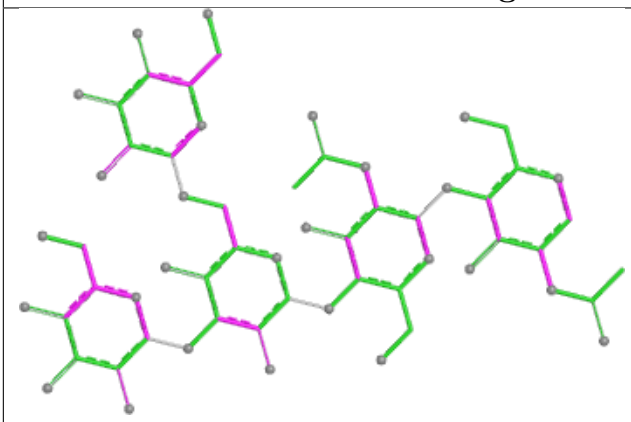


Torsions

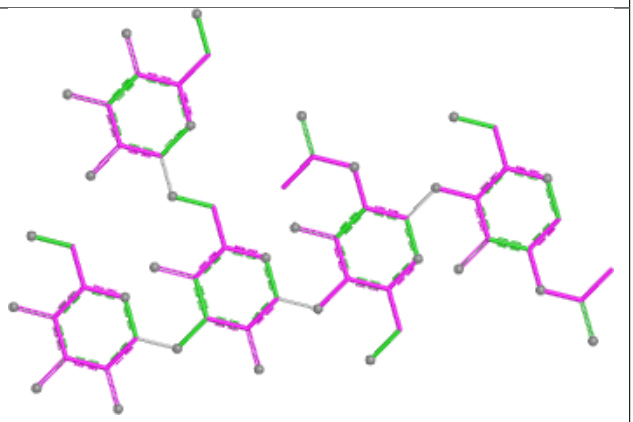


Rings

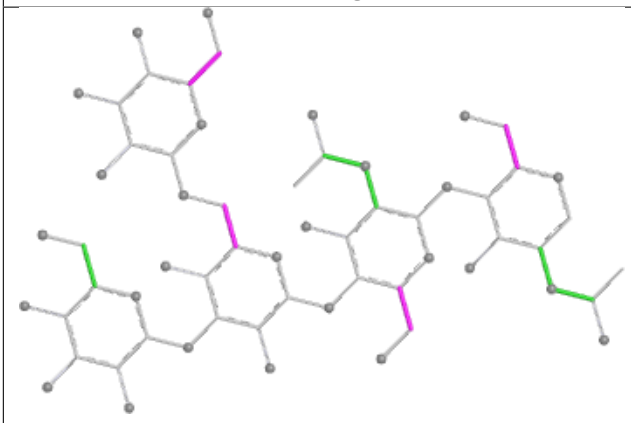
Oligosaccharide Chain 3



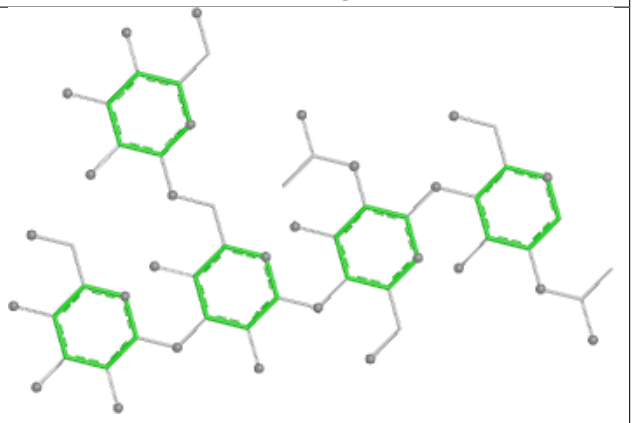
Bond lengths



Bond angles

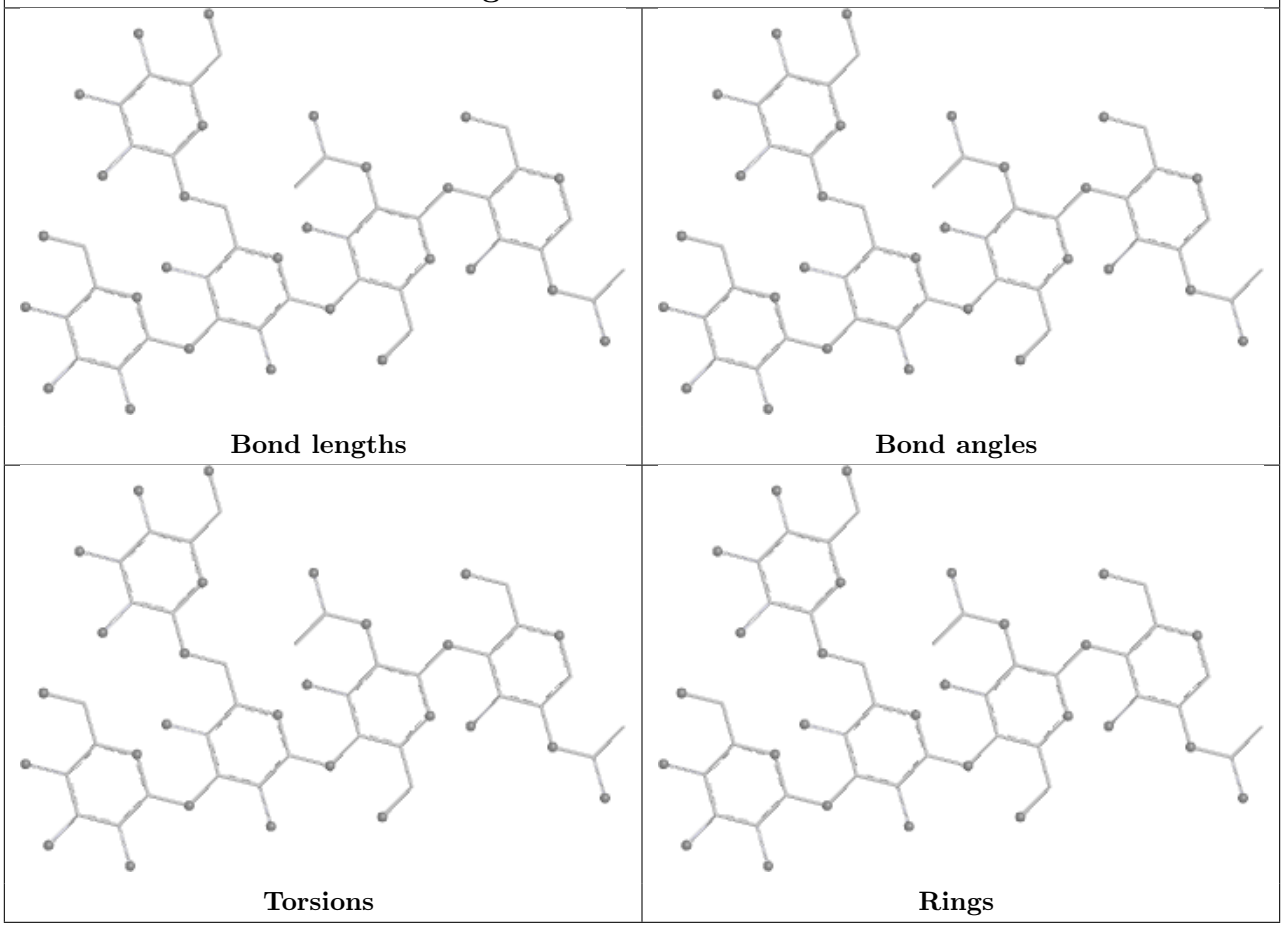


Torsions



Rings

Oligosaccharide Chain BA



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
9	NAG	A	1440	1	14,14,15	3.55	6 (42%)	17,19,21	3.47	8 (47%)
9	NAG	B	1440	1	14,14,15	3.56	6 (42%)	17,19,21	3.46	8 (47%)
9	NAG	C	1474	1	14,14,15	2.78	3 (21%)	17,19,21	3.02	4 (23%)
9	NAG	B	1401	1	14,14,15	2.82	4 (28%)	17,19,21	2.00	3 (17%)
9	NAG	C	1440	1	14,14,15	3.55	6 (42%)	17,19,21	3.47	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	A	1402	1	14,14,15	2.70	4 (28%)	17,19,21	3.68	6 (35%)
9	NAG	B	1403	1	14,14,15	2.63	3 (21%)	17,19,21	4.06	6 (35%)
9	NAG	B	1402	1	14,14,15	2.70	4 (28%)	17,19,21	3.68	6 (35%)
9	NAG	C	1402	1	14,14,15	2.69	4 (28%)	17,19,21	3.68	6 (35%)
9	NAG	C	1401	1	14,14,15	2.82	4 (28%)	17,19,21	2.00	4 (23%)
9	NAG	A	1439	1	14,14,15	2.45	3 (21%)	17,19,21	3.31	3 (17%)
9	NAG	B	1439	1	14,14,15	2.45	3 (21%)	17,19,21	3.31	3 (17%)
9	NAG	A	1403	1	14,14,15	2.62	3 (21%)	17,19,21	4.06	6 (35%)
9	NAG	C	1441	1	14,14,15	2.99	4 (28%)	17,19,21	4.50	4 (23%)
9	NAG	C	1403	1	14,14,15	2.62	3 (21%)	17,19,21	4.06	6 (35%)
9	NAG	A	1474	1	14,14,15	2.79	3 (21%)	17,19,21	3.01	4 (23%)
9	NAG	A	1441	1	14,14,15	3.00	4 (28%)	17,19,21	4.50	4 (23%)
9	NAG	C	1439	1	14,14,15	2.46	3 (21%)	17,19,21	3.31	3 (17%)
9	NAG	B	1474	1	14,14,15	2.78	3 (21%)	17,19,21	3.01	4 (23%)
9	NAG	B	1441	1	14,14,15	3.00	4 (28%)	17,19,21	4.49	4 (23%)
9	NAG	A	1401	1	14,14,15	2.82	4 (28%)	17,19,21	2.00	3 (17%)

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
9	NAG	A	1440	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1440	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1474	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1440	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1439	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1439	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1441	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1474	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1441	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1439	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1474	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1441	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1401	1	-	0/6/23/26	0/1/1/1

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1440	NAG	O5-C1	8.55	1.58	1.43
9	A	1440	NAG	O5-C1	8.55	1.58	1.43
9	B	1440	NAG	O5-C1	8.54	1.58	1.43
9	A	1441	NAG	O5-C1	7.68	1.56	1.43
9	C	1441	NAG	O5-C1	7.67	1.56	1.43

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1403	NAG	O5-C5-C6	-14.07	80.28	107.66
9	A	1403	NAG	O5-C5-C6	-14.06	80.29	107.66
9	C	1403	NAG	O5-C5-C6	-14.06	80.31	107.66
9	A	1402	NAG	O5-C5-C6	-11.42	85.44	107.66
9	C	1402	NAG	O5-C5-C6	-11.42	85.44	107.66

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1441	NAG	C1-C2-N2-C7
9	B	1441	NAG	C1-C2-N2-C7
9	C	1441	NAG	C1-C2-N2-C7
9	C	1439	NAG	O5-C5-C6-O6
9	A	1439	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

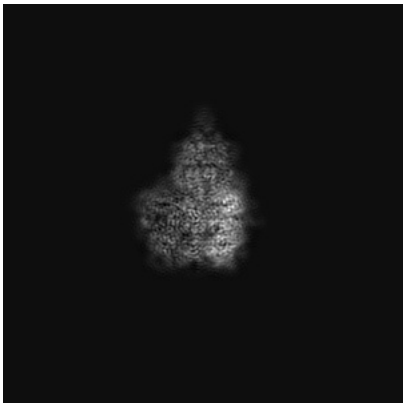
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8331. These allow visual inspection of the internal detail of the map and identification of artifacts.

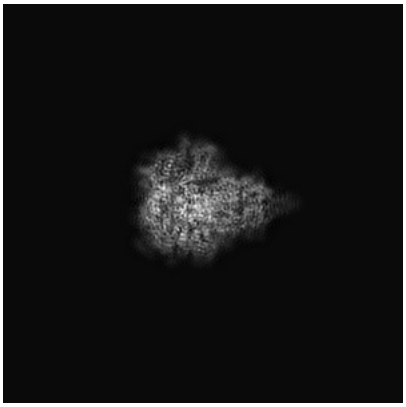
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

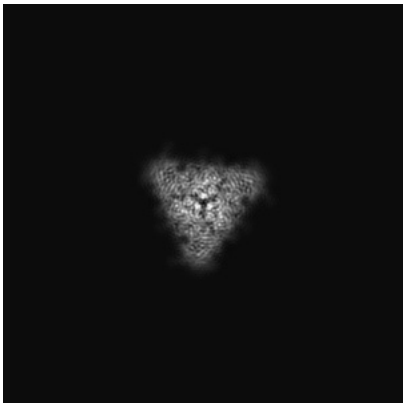
6.1.1 Primary map



X



Y

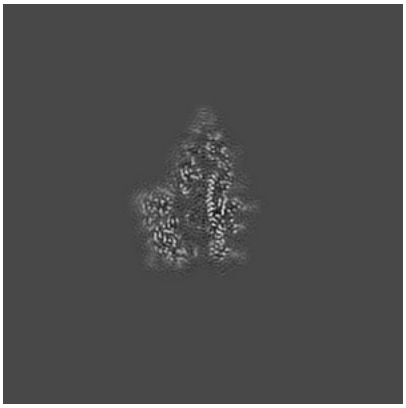


Z

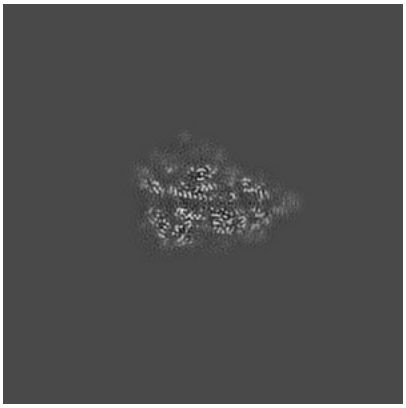
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 160



Y Index: 160

Z Index: 160

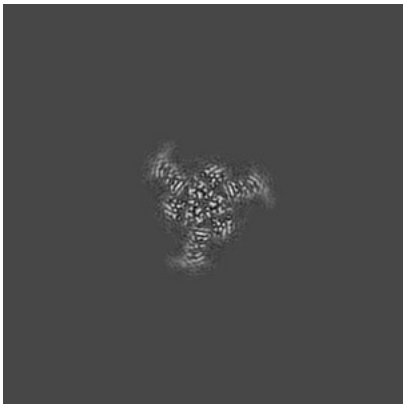
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 165

Y Index: 168

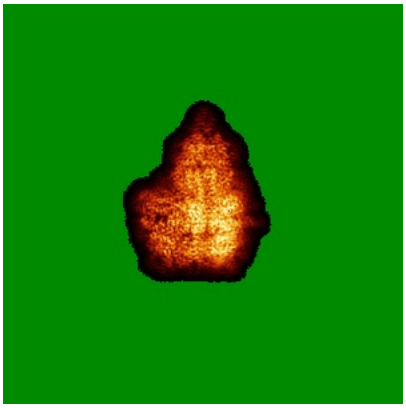


Z Index: 145

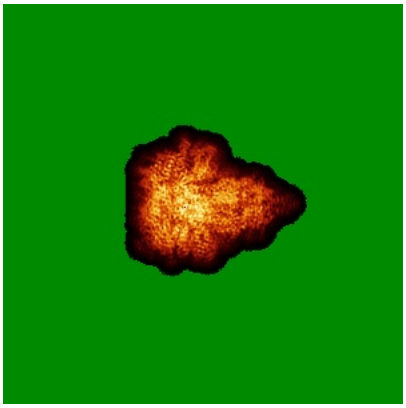
The images above show the largest variance slices of the map in three orthogonal directions.

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

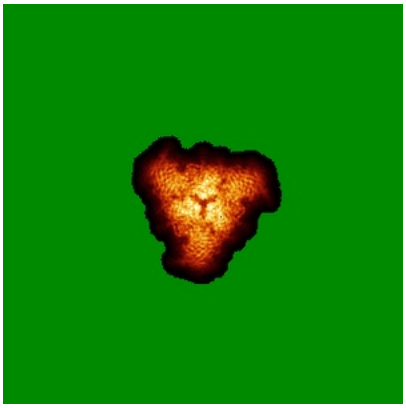
6.4.1 Primary map



X



Y



Z

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

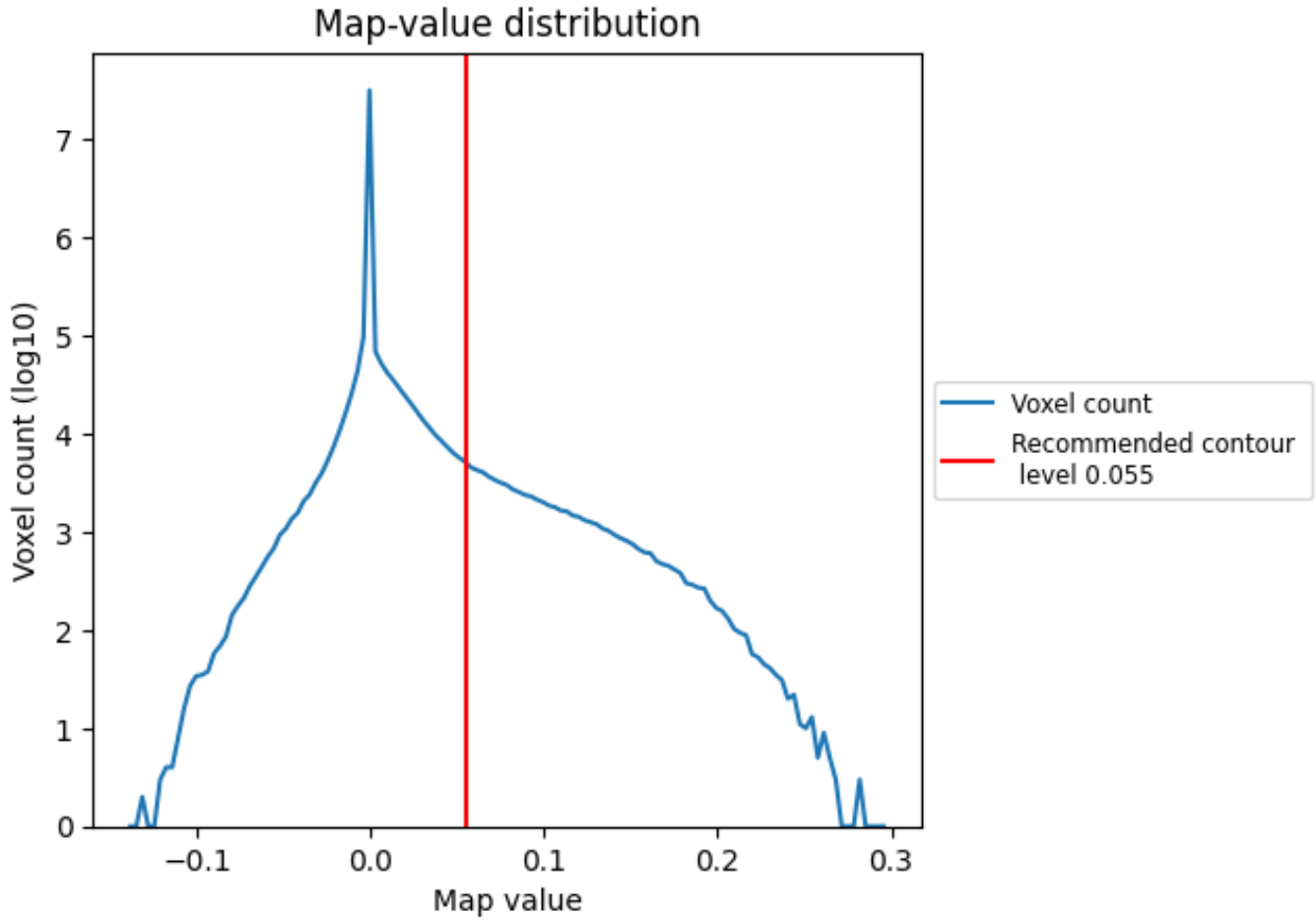
6.6 Mask visualisation (i)

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

7 Map analysis

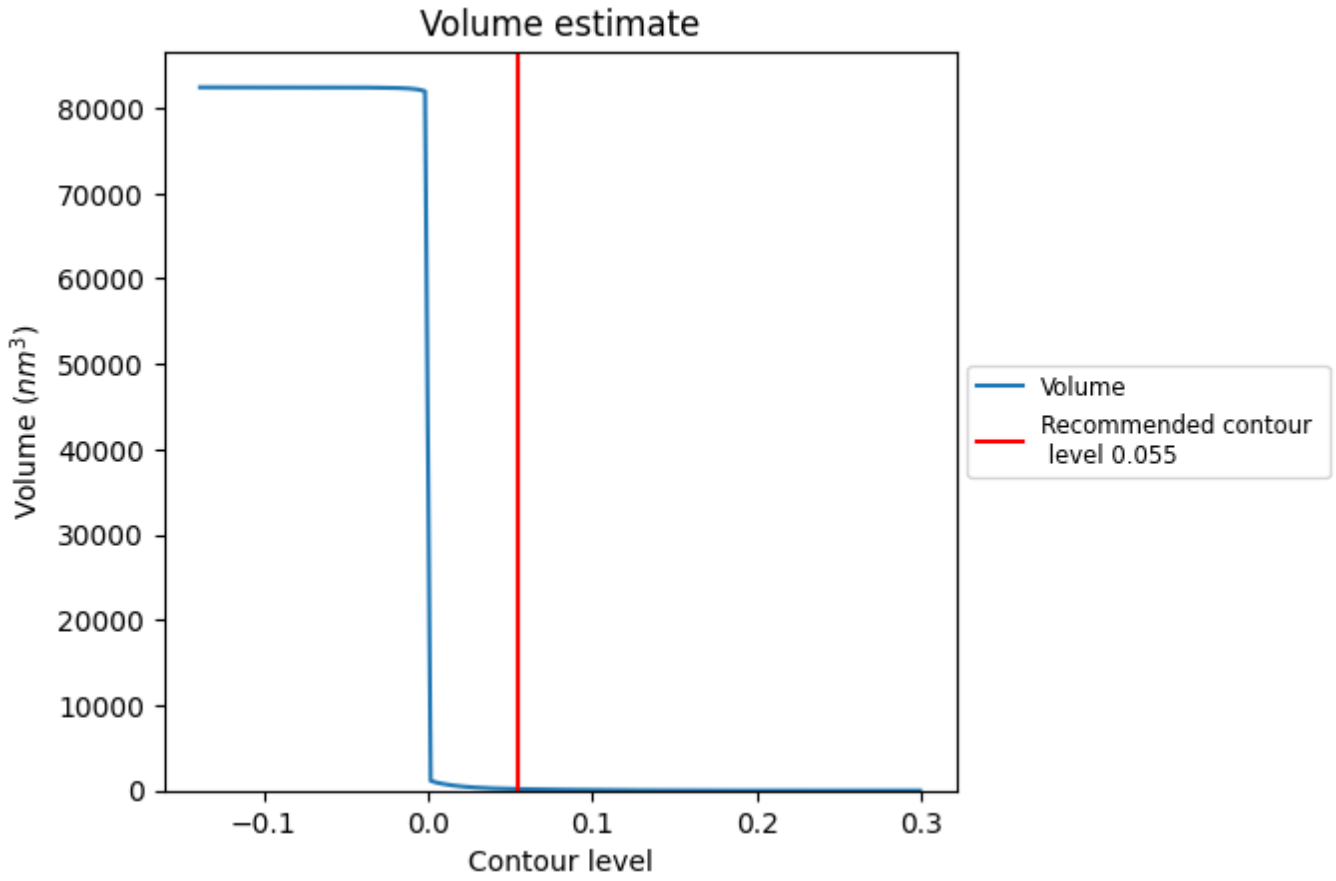
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

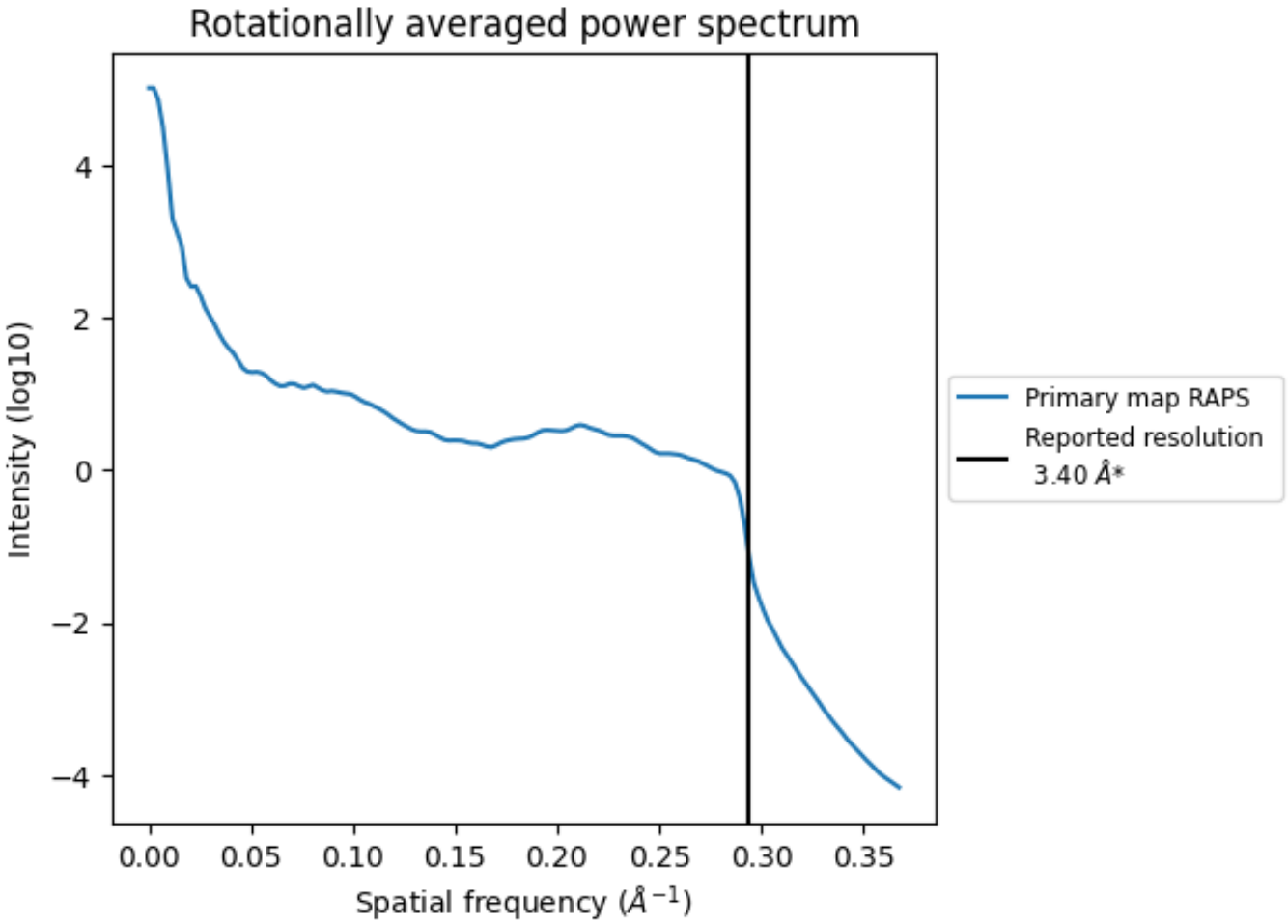
7.2 Volume estimate (i)



The volume at the recommended contour level is 177 nm^3; this corresponds to an approximate mass of 160 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}

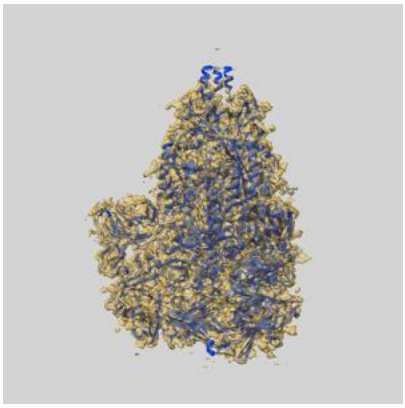
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

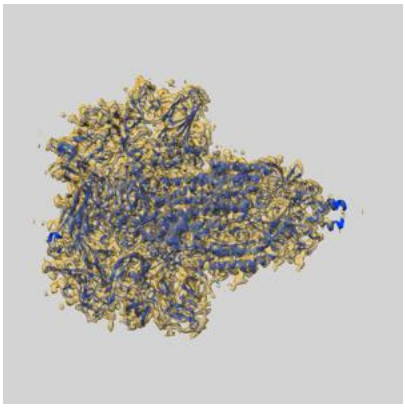
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8331 and PDB model 5SZS. Per-residue inclusion information can be found in section 3 on page 16.

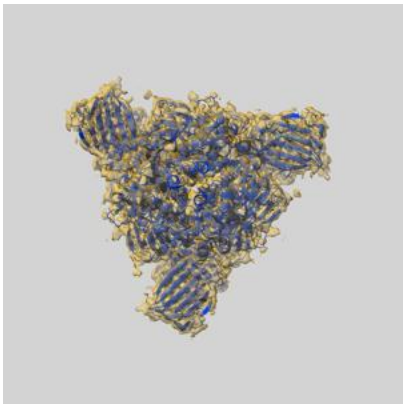
9.1 Map-model overlay



X



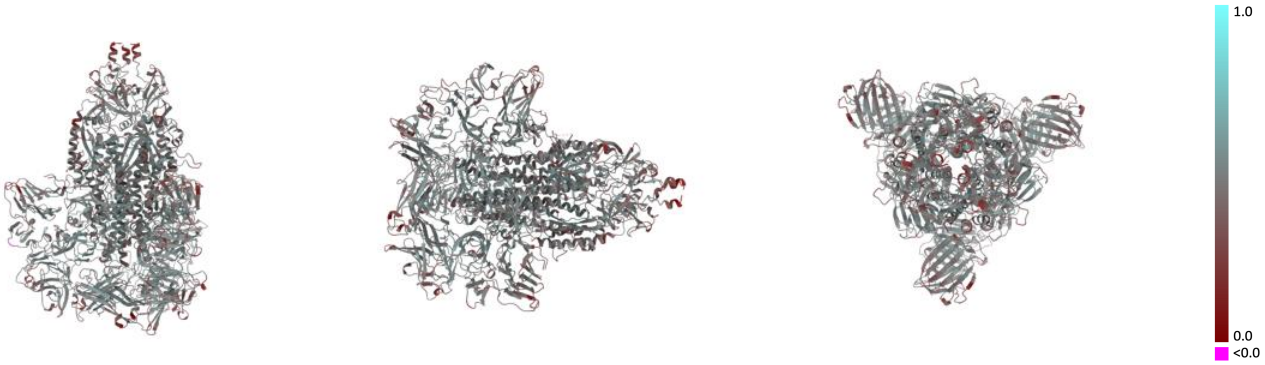
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

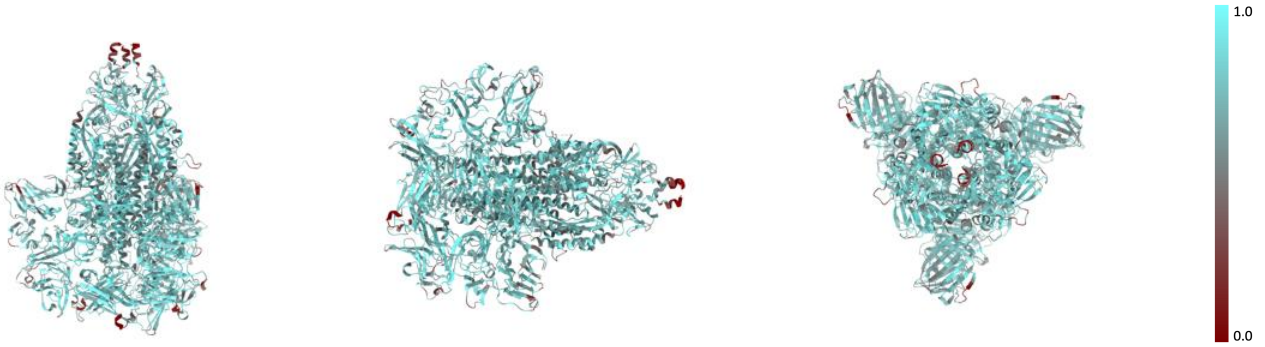
9.2 Q-score mapped to coordinate model (i)



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.

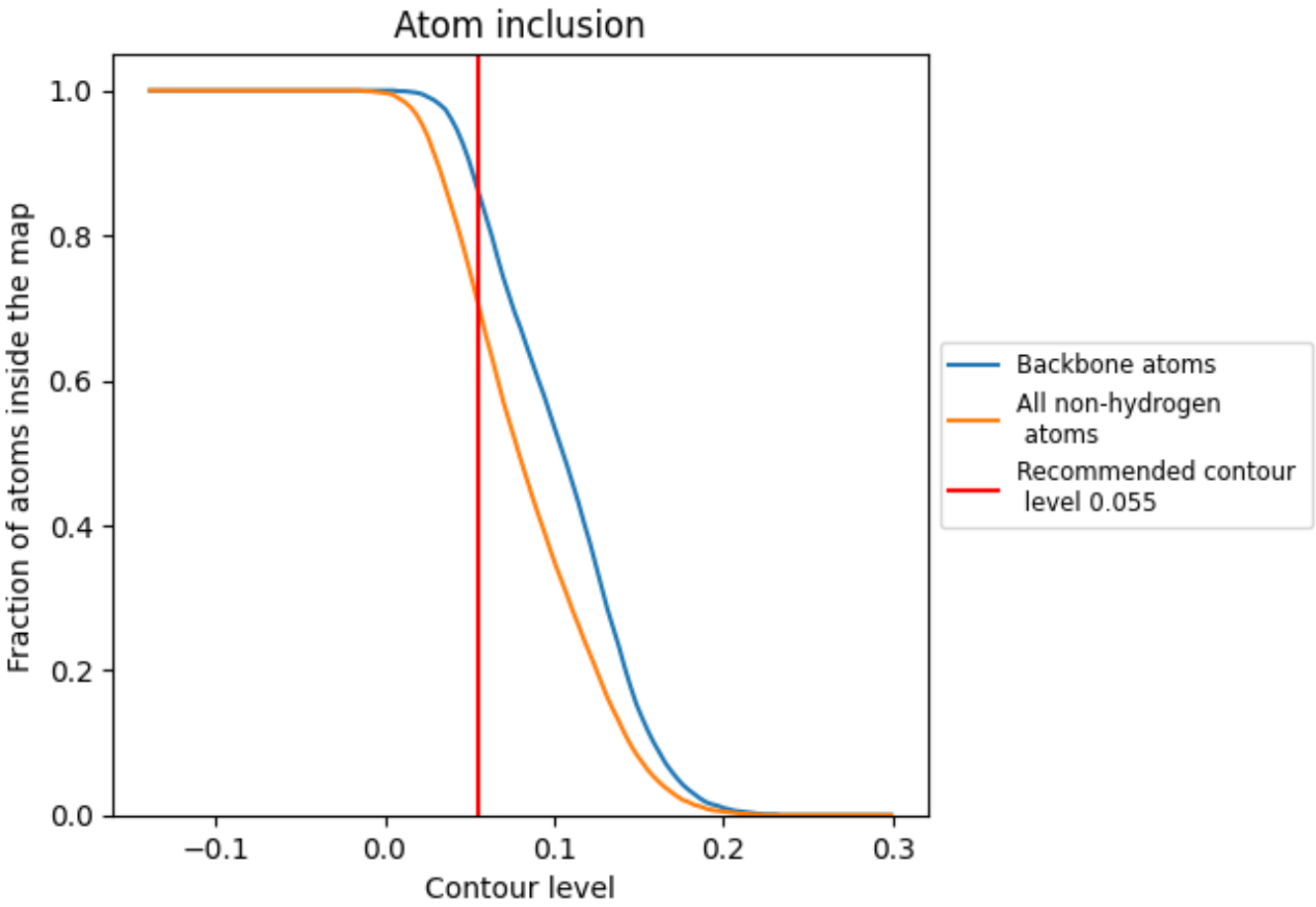
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.4500
0	0.4890	0.4000
1	0.2820	0.2840
2	0.2140	0.3660
3	0.1800	0.2190
4	0.2560	0.3880
5	0.1070	0.2770
6	0.2860	0.1090
7	0.2860	0.2640
8	0.2500	0.3100
9	0.1790	0.1990
A	0.7440	0.4630
AA	0.2400	0.2810
B	0.7440	0.4620
BA	0.2300	0.2980
C	0.7450	0.4630
CA	0.5000	0.4620
D	0.5140	0.3610
DA	0.2820	0.3110
E	0.5000	0.3390
F	0.3400	0.3400
G	0.2860	0.3100
H	0.3600	0.3390
I	0.0360	0.1950
J	0.2860	0.3410
K	0.4890	0.4060
L	0.2820	0.2780
M	0.1790	0.3610
N	0.1800	0.2230
O	0.2560	0.3910
P	0.1430	0.2880
Q	0.2500	0.1180
R	0.2860	0.2760
S	0.2500	0.3170
T	0.1790	0.2120

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Chain	Atom inclusion	Q-score
U	0.2800	0.2650
V	0.2460	0.2990
W	0.5000	0.4490
X	0.3080	0.3330
Y	0.5280	0.3640
Z	0.5000	0.3260
a	0.3400	0.3360
b	0.2500	0.3020
c	0.3400	0.3480
d	0.0360	0.1820
e	0.2860	0.2960
f	0.5110	0.4040
g	0.2820	0.2750
h	0.2140	0.3580
i	0.1640	0.2280
j	0.2560	0.3800
k	0.1070	0.2850
l	0.2140	0.1100
m	0.2500	0.2590
n	0.2500	0.3110
o	0.1790	0.1950
p	0.2800	0.2680
q	0.2300	0.3000
r	0.5000	0.4250
s	0.2820	0.3290
t	0.5560	0.3710
u	0.4640	0.3480
v	0.3400	0.3410
w	0.2500	0.3140
x	0.3800	0.3510
y	0.0360	0.1720
z	0.2860	0.3160