wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 06:52 PM EDT

PDB ID	:	4O5I
Title	:	Crystal structure of broadly neutralizing antibody F045-092 in complex with A/Victoria/361/2011 (H3N2) influenza hemagglutinin
Authors	:	Lee, P.S.; Wilson, I.A.
Deposited on	:	2013-12-19
Resolution	:	6.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

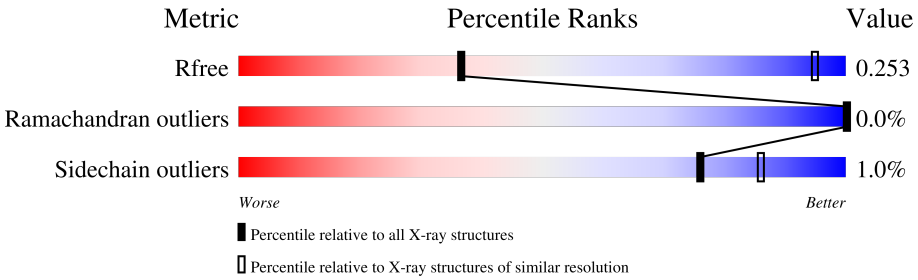
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Mol	Chain	Length	Quality of chain
1	A	323	97%
1	C	323	97%
1	E	323	97%
1	G	323	97%
1	I	323	97%
1	K	323	97%
2	B	176	98%
2	D	176	98%

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Mol	Chain	Length	Quality of chain
2	F	176	98%
2	H	176	98%
2	J	176	98%
2	L	176	98%
3	M	240	93% 6%
3	O	240	93% 6%
3	Q	240	92% 6%
3	S	240	93% 6%
3	U	240	92% 6%
3	W	240	93% 6%
4	N	216	97%
4	P	216	98%
4	R	216	98%
4	T	216	98%
4	V	216	97%
4	X	216	96%
5	0	3	100%
5	3	3	33% 67%
5	5	3	100%
5	6	3	100%
5	Y	3	33% 67%
5	i	3	67% 33%
5	j	3	100%
5	l	3	33% 67%
5	p	3	100%

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Mol	Chain	Length	Quality of chain
5	t	3	67% 33%
5	u	3	100%
5	y	3	100%
5	z	3	67% 33%
6	1	2	100%
6	2	2	100%
6	4	2	50% 50%
6	Z	2	50% 50%
6	a	2	50% 50%
6	c	2	50% 50%
6	d	2	100%
6	f	2	50% 50%
6	o	2	100%
6	q	2	50% 50%
6	r	2	50% 50%
6	s	2	50% 50%
6	v	2	100%
6	w	2	50% 50%
6	x	2	50% 50%
7	b	5	40% 60%
7	h	5	40% 60%
7	k	5	60% 40%
7	n	5	20% 80%
8	e	4	50% 50%
8	g	4	75% 25%

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Mol	Chain	Length	Quality of chain
8	m	4	50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 44305 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	C	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	E	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	G	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	I	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	K	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP R9U684
A	8	ASP	-	expression tag	UNP R9U684
A	9	PRO	-	expression tag	UNP R9U684
A	10	GLY	-	expression tag	UNP R9U684
C	7	ALA	-	expression tag	UNP R9U684
C	8	ASP	-	expression tag	UNP R9U684
C	9	PRO	-	expression tag	UNP R9U684
C	10	GLY	-	expression tag	UNP R9U684
E	7	ALA	-	expression tag	UNP R9U684
E	8	ASP	-	expression tag	UNP R9U684
E	9	PRO	-	expression tag	UNP R9U684
E	10	GLY	-	expression tag	UNP R9U684
G	7	ALA	-	expression tag	UNP R9U684
G	8	ASP	-	expression tag	UNP R9U684
G	9	PRO	-	expression tag	UNP R9U684
G	10	GLY	-	expression tag	UNP R9U684
I	7	ALA	-	expression tag	UNP R9U684

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Chain	Residue	Modelled	Actual	Comment	Reference
I	8	ASP	-	expression tag	UNP R9U684
I	9	PRO	-	expression tag	UNP R9U684
I	10	GLY	-	expression tag	UNP R9U684
K	7	ALA	-	expression tag	UNP R9U684
K	8	ASP	-	expression tag	UNP R9U684
K	9	PRO	-	expression tag	UNP R9U684
K	10	GLY	-	expression tag	UNP R9U684

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	D	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	F	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	H	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	J	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	L	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			

- Molecule 3 is a protein called Fab F045-092 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	O	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	Q	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	S	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	U	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	W	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	217	HIS	-	expression tag	UNP S6C4S0
M	218	HIS	-	expression tag	UNP S6C4S0
M	219	HIS	-	expression tag	UNP S6C4S0
M	220	HIS	-	expression tag	UNP S6C4S0
M	221	HIS	-	expression tag	UNP S6C4S0
M	222	HIS	-	expression tag	UNP S6C4S0
O	217	HIS	-	expression tag	UNP S6C4S0
O	218	HIS	-	expression tag	UNP S6C4S0
O	219	HIS	-	expression tag	UNP S6C4S0
O	220	HIS	-	expression tag	UNP S6C4S0
O	221	HIS	-	expression tag	UNP S6C4S0
O	222	HIS	-	expression tag	UNP S6C4S0
Q	217	HIS	-	expression tag	UNP S6C4S0
Q	218	HIS	-	expression tag	UNP S6C4S0
Q	219	HIS	-	expression tag	UNP S6C4S0
Q	220	HIS	-	expression tag	UNP S6C4S0
Q	221	HIS	-	expression tag	UNP S6C4S0
Q	222	HIS	-	expression tag	UNP S6C4S0
S	217	HIS	-	expression tag	UNP S6C4S0
S	218	HIS	-	expression tag	UNP S6C4S0
S	219	HIS	-	expression tag	UNP S6C4S0
S	220	HIS	-	expression tag	UNP S6C4S0
S	221	HIS	-	expression tag	UNP S6C4S0
S	222	HIS	-	expression tag	UNP S6C4S0
U	217	HIS	-	expression tag	UNP S6C4S0
U	218	HIS	-	expression tag	UNP S6C4S0
U	219	HIS	-	expression tag	UNP S6C4S0
U	220	HIS	-	expression tag	UNP S6C4S0
U	221	HIS	-	expression tag	UNP S6C4S0
U	222	HIS	-	expression tag	UNP S6C4S0
W	217	HIS	-	expression tag	UNP S6C4S0
W	218	HIS	-	expression tag	UNP S6C4S0
W	219	HIS	-	expression tag	UNP S6C4S0
W	220	HIS	-	expression tag	UNP S6C4S0
W	221	HIS	-	expression tag	UNP S6C4S0
W	222	HIS	-	expression tag	UNP S6C4S0

- Molecule 4 is a protein called Fab F045-092 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	P	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

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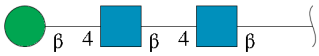
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	T	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	V	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	X	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

- Molecule 5 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.

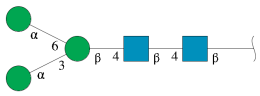


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	i	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	l	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	p	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	t	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	u	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	z	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	0	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	3	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	5	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	6	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	o	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	r	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	s	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	v	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	w	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	x	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	1	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	2	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	4	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

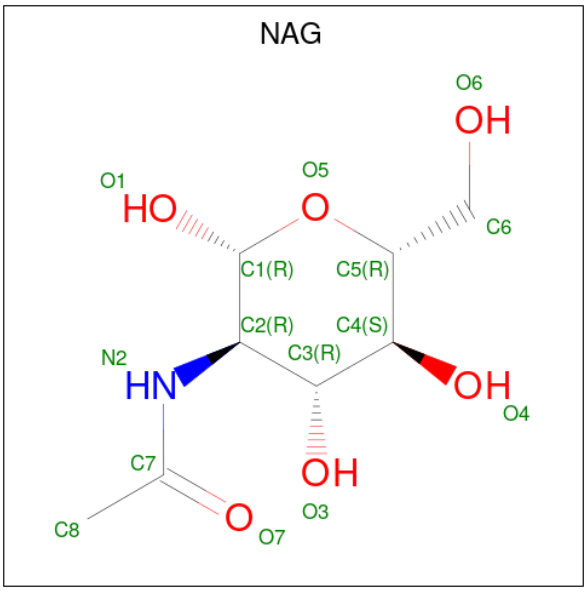


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	b	5	Total C N O 61 34 2 25	0	0	0
7	h	5	Total C N O 61 34 2 25	0	0	0
7	k	5	Total C N O 61 34 2 25	0	0	0
7	n	5	Total C N O 61 34 2 25	0	0	0

- Molecule 8 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	ZeroOcc	AltConf	Trace
8	e	4	Total C N O 50 28 2 20	0	0	0
8	g	4	Total C N O 50 28 2 20	0	0	0
8	m	4	Total C N O 50 28 2 20	0	0	0

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



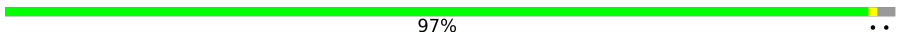
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	D	1	Total C N O 14 8 1 5	0	0
9	E	1	Total C N O 14 8 1 5	0	0
9	F	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	H	1	Total C N O 14 8 1 5	0	0
9	I	1	Total C N O 14 8 1 5	0	0
9	J	1	Total C N O 14 8 1 5	0	0
9	K	1	Total C N O 14 8 1 5	0	0
9	L	1	Total C N O 14 8 1 5	0	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. 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. 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.

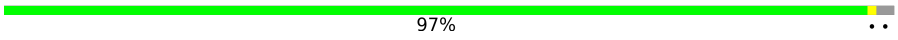
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



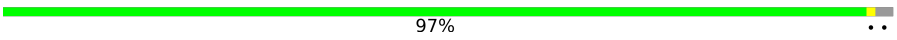
- Molecule 1: Hemagglutinin HA1 chain

Chain C:



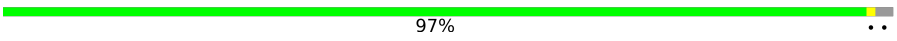
- Molecule 1: Hemagglutinin HA1 chain

Chain E:



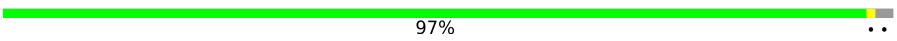
- Molecule 1: Hemagglutinin HA1 chain

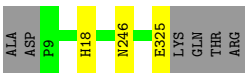
Chain G:



- Molecule 1: Hemagglutinin HA1 chain

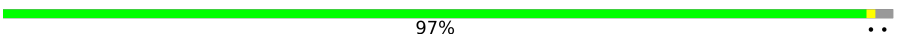
Chain I:





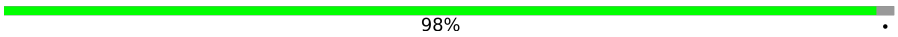
- Molecule 1: Hemagglutinin HA1 chain

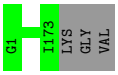
Chain K:



• Molecule 2: Hemagglutinin HA2 chain

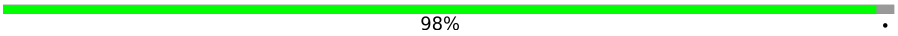
Chain B:

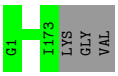




• Molecule 2: Hemagglutinin HA2 chain

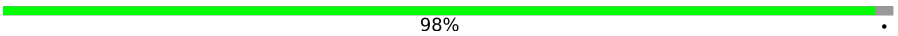
Chain D:

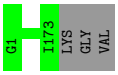




• Molecule 2: Hemagglutinin HA2 chain

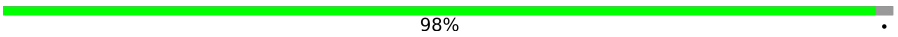
Chain F:

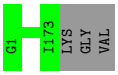




• Molecule 2: Hemagglutinin HA2 chain

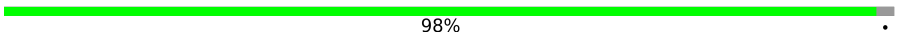
Chain H:

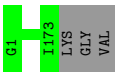




• Molecule 2: Hemagglutinin HA2 chain

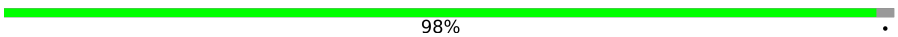
Chain J:

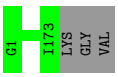




• Molecule 2: Hemagglutinin HA2 chain

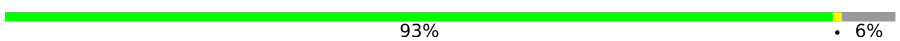
Chain L:

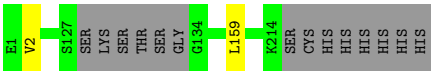




• Molecule 3: Fab F045-092 heavy chain

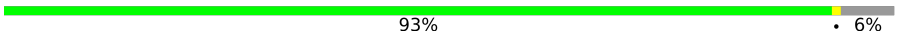
Chain M:

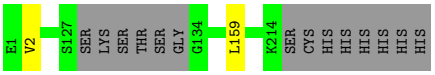




• Molecule 3: Fab F045-092 heavy chain

Chain O:



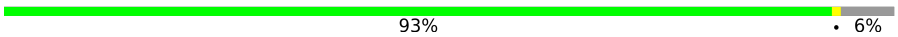


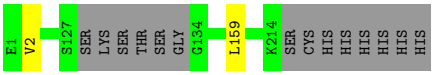
• Molecule 3: Fab F045-092 heavy chain

Chain Q:

• Molecule 3: Fab F045-092 heavy chain

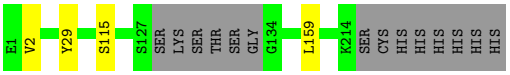
Chain S:





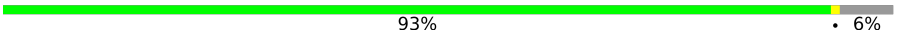
• Molecule 3: Fab F045-092 heavy chain

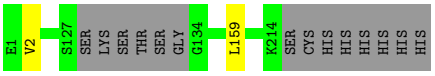
Chain U:



• Molecule 3: Fab F045-092 heavy chain

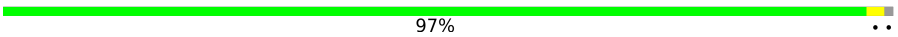
Chain W:

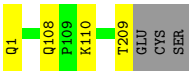




• Molecule 4: Fab F045-092 light chain

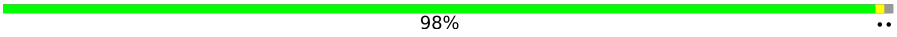
Chain N:

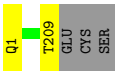




• Molecule 4: Fab F045-092 light chain

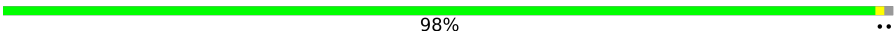
Chain P:

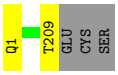




• Molecule 4: Fab F045-092 light chain

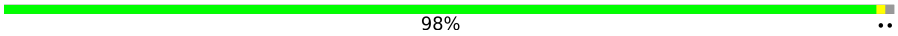
Chain R:

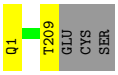




• Molecule 4: Fab F045-092 light chain

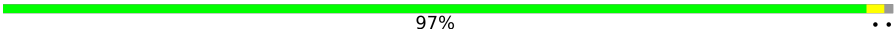
Chain T:

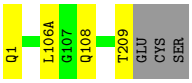




• Molecule 4: Fab F045-092 light chain

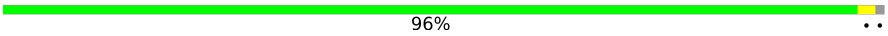
Chain V:

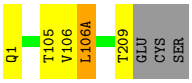




• Molecule 4: Fab F045-092 light chain

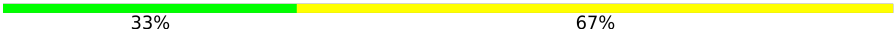
Chain X:





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

Chain Y:

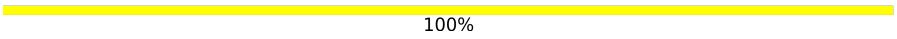


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

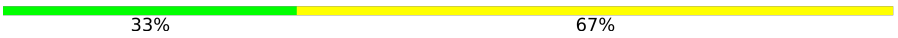
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



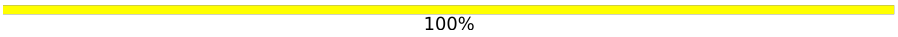
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



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

Chain p:

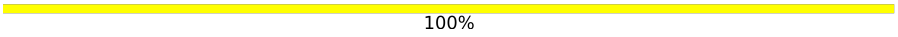


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

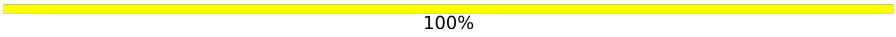
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



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

Chain y:

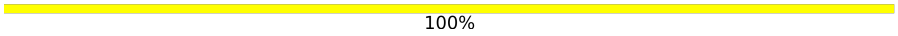


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:

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

Chain 0:

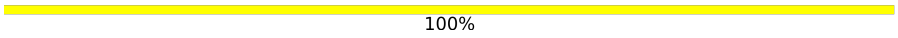


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:

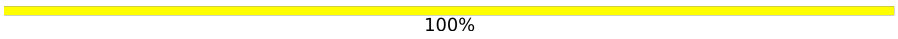
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



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

Chain 6:



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

Chain Z:

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

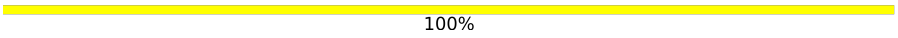
Chain a:

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

Chain c:

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

Chain d:

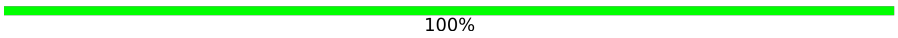


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

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

Chain o:



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

Chain q:

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

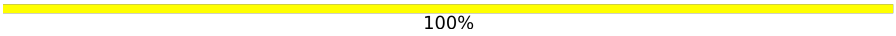
Chain r:

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

Chain s:

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

Chain v:



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

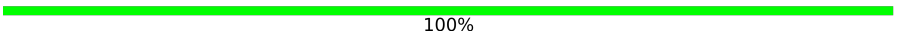
Chain w:

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

Chain x:

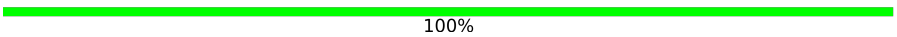
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:



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

Chain 2:

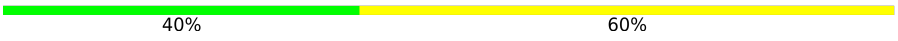


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

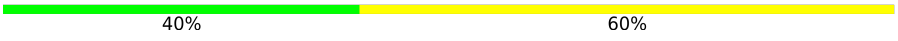
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



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

Chain h:



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

Chain k:

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

Chain n:

• Molecule 8: 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 e:

• Molecule 8: 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 g:

• Molecule 8: 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 m:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	318.12Å 187.17Å 353.64Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	49.00 – 6.50 49.00 – 6.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.00-6.50) 89.1 (49.00-6.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.201 , 0.248 0.210 , 0.253	Depositor DCC
R_{free} test set	1926 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	209.5	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 205.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.038 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.039 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.297 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.289 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.047 for -h,-k,l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	44305	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/2532	0.59	0/3443
1	C	0.34	0/2532	0.57	0/3443
1	E	0.35	0/2532	0.58	0/3443
1	G	0.31	0/2532	0.57	0/3443
1	I	0.31	0/2532	0.57	0/3443
1	K	0.31	0/2532	0.58	0/3443
2	B	0.31	0/1420	0.57	0/1906
2	D	0.31	0/1420	0.55	0/1906
2	F	0.30	0/1420	0.55	0/1906
2	H	0.29	0/1420	0.54	0/1906
2	J	0.30	0/1420	0.54	0/1906
2	L	0.30	0/1420	0.54	0/1906
3	M	0.33	0/1740	0.63	0/2373
3	O	0.34	0/1740	0.64	0/2373
3	Q	0.33	0/1740	0.64	1/2373 (0.0%)
3	S	0.32	0/1740	0.64	0/2373
3	U	0.33	0/1740	0.66	1/2373 (0.0%)
3	W	0.31	0/1740	0.62	0/2373
4	N	0.34	0/1604	0.60	0/2190
4	P	0.30	0/1604	0.59	0/2190
4	R	0.30	0/1604	0.59	0/2190
4	T	0.30	0/1604	0.59	0/2190
4	V	0.31	0/1604	0.60	1/2190 (0.0%)
4	X	0.31	0/1604	0.65	3/2190 (0.1%)
All	All	0.32	0/43776	0.59	6/59472 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	105	THR	C-N-CA	6.21	137.22	121.70
4	V	106(A)	LEU	CA-CB-CG	5.87	128.80	115.30
4	X	106(A)	LEU	CA-CB-CG	5.73	128.47	115.30
4	X	105	THR	CA-C-N	5.50	129.29	117.20
3	U	29	TYR	CB-CG-CD1	-5.37	117.78	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	C	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	E	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	G	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	I	315/323 (98%)	306 (97%)	9 (3%)	0	100	100
1	K	315/323 (98%)	306 (97%)	9 (3%)	0	100	100
2	B	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
2	D	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
2	F	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	H	171/176 (97%)	164 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	L	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
3	M	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	O	222/240 (92%)	216 (97%)	6 (3%)	0	100	100
3	Q	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	S	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	U	222/240 (92%)	219 (99%)	3 (1%)	0	100	100
3	W	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
4	N	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	P	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
4	R	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	T	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	V	211/216 (98%)	208 (99%)	3 (1%)	0	100	100
4	X	211/216 (98%)	205 (97%)	5 (2%)	1 (0%)	29	69
All	All	5514/5730 (96%)	5369 (97%)	144 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	106	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 X-ray entries followed by that with respect to entries of similar resolution.

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	280/285 (98%)	277 (99%)	3 (1%)	73	84
1	C	280/285 (98%)	277 (99%)	3 (1%)	73	84
1	E	280/285 (98%)	277 (99%)	3 (1%)	73	84
1	G	280/285 (98%)	277 (99%)	3 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	280/285 (98%)	277 (99%)	3 (1%)	73	84
1	K	280/285 (98%)	277 (99%)	3 (1%)	73	84
2	B	146/148 (99%)	146 (100%)	0	100	100
2	D	146/148 (99%)	146 (100%)	0	100	100
2	F	146/148 (99%)	146 (100%)	0	100	100
2	H	146/148 (99%)	146 (100%)	0	100	100
2	J	146/148 (99%)	146 (100%)	0	100	100
2	L	146/148 (99%)	146 (100%)	0	100	100
3	M	188/201 (94%)	186 (99%)	2 (1%)	73	84
3	O	188/201 (94%)	186 (99%)	2 (1%)	73	84
3	Q	188/201 (94%)	184 (98%)	4 (2%)	53	72
3	S	188/201 (94%)	186 (99%)	2 (1%)	73	84
3	U	188/201 (94%)	185 (98%)	3 (2%)	62	79
3	W	188/201 (94%)	186 (99%)	2 (1%)	73	84
4	N	178/181 (98%)	174 (98%)	4 (2%)	52	71
4	P	178/181 (98%)	176 (99%)	2 (1%)	73	84
4	R	178/181 (98%)	176 (99%)	2 (1%)	73	84
4	T	178/181 (98%)	176 (99%)	2 (1%)	73	84
4	V	178/181 (98%)	175 (98%)	3 (2%)	60	78
4	X	178/181 (98%)	175 (98%)	3 (2%)	60	78
All	All	4752/4890 (97%)	4703 (99%)	49 (1%)	76	86

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	2	VAL
3	S	159	LEU
3	Q	113	SER
4	R	1	GLN
4	T	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	108	GLN
3	O	204	ASN
3	O	34	ASN
3	Q	34	ASN
1	E	216	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)

101 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	$\#\|Z\| > 2$
5	NAG	0	1	5,1	14,14,15	0.56	0	17,19,21	1.36	3 (17%)
5	NAG	0	2	5	14,14,15	0.56	0	17,19,21	1.01	2 (11%)
5	BMA	0	3	5	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
6	NAG	1	1	6,1	14,14,15	0.58	0	17,19,21	0.85	0
6	NAG	1	2	6	14,14,15	0.53	0	17,19,21	0.86	0
6	NAG	2	1	6,1	14,14,15	0.56	0	17,19,21	0.76	0
6	NAG	2	2	6	14,14,15	0.55	0	17,19,21	0.73	0
5	NAG	3	1	5,1	14,14,15	0.66	0	17,19,21	1.03	1 (5%)
5	NAG	3	2	5	14,14,15	0.54	0	17,19,21	0.73	0
5	BMA	3	3	5	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
6	NAG	4	1	6,1	14,14,15	0.55	0	17,19,21	0.79	0
6	NAG	4	2	6	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
5	NAG	5	1	5,1	14,14,15	0.46	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	5	2	5	14,14,15	0.49	0	17,19,21	0.88	1 (5%)
5	BMA	5	3	5	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
5	NAG	6	1	5,1	14,14,15	1.35	2 (14%)	17,19,21	1.94	4 (23%)
5	NAG	6	2	5	14,14,15	0.60	0	17,19,21	1.08	1 (5%)
5	BMA	6	3	5	11,11,12	0.52	0	15,15,17	1.09	1 (6%)
5	NAG	Y	1	5,1	14,14,15	0.64	0	17,19,21	0.93	1 (5%)
5	NAG	Y	2	5	14,14,15	0.60	0	17,19,21	1.46	1 (5%)
5	BMA	Y	3	5	11,11,12	0.63	0	15,15,17	0.80	0
6	NAG	Z	1	6,1	14,14,15	0.52	0	17,19,21	0.90	2 (11%)
6	NAG	Z	2	6	14,14,15	0.56	0	17,19,21	0.86	0
6	NAG	a	1	6,1	14,14,15	0.63	0	17,19,21	0.86	2 (11%)
6	NAG	a	2	6	14,14,15	0.53	0	17,19,21	0.80	0
7	NAG	b	1	7,1	14,14,15	0.51	0	17,19,21	0.84	0
7	NAG	b	2	7	14,14,15	0.57	0	17,19,21	0.96	2 (11%)
7	BMA	b	3	7	11,11,12	0.60	0	15,15,17	1.22	3 (20%)
7	MAN	b	4	7	11,11,12	0.62	0	15,15,17	0.85	0
7	MAN	b	5	7	11,11,12	0.63	0	15,15,17	1.65	3 (20%)
6	NAG	c	1	6,1	14,14,15	0.50	0	17,19,21	0.78	0
6	NAG	c	2	6	14,14,15	0.50	0	17,19,21	0.83	1 (5%)
6	NAG	d	1	6,1	14,14,15	0.47	0	17,19,21	1.25	1 (5%)
6	NAG	d	2	6	14,14,15	0.58	0	17,19,21	0.86	1 (5%)
8	NAG	e	1	8,1	14,14,15	0.61	0	17,19,21	0.95	2 (11%)
8	NAG	e	2	8	14,14,15	0.62	0	17,19,21	0.74	0
8	BMA	e	3	8	11,11,12	0.64	0	15,15,17	0.94	1 (6%)
8	MAN	e	4	8	11,11,12	0.61	0	15,15,17	0.86	0
6	NAG	f	1	6,1	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
6	NAG	f	2	6	14,14,15	0.56	0	17,19,21	0.66	0
8	NAG	g	1	8,1	14,14,15	0.60	0	17,19,21	0.74	0
8	NAG	g	2	8	14,14,15	0.52	0	17,19,21	0.69	0
8	BMA	g	3	8	11,11,12	0.59	0	15,15,17	1.10	1 (6%)
8	MAN	g	4	8	11,11,12	0.63	0	15,15,17	0.68	0
7	NAG	h	1	7,1	14,14,15	0.56	0	17,19,21	0.80	0
7	NAG	h	2	7	14,14,15	0.56	0	17,19,21	0.90	2 (11%)
7	BMA	h	3	7	11,11,12	0.68	0	15,15,17	1.09	1 (6%)
7	MAN	h	4	7	11,11,12	0.57	0	15,15,17	1.03	1 (6%)
7	MAN	h	5	7	11,11,12	0.67	0	15,15,17	0.79	0
5	NAG	i	1	5,1	14,14,15	0.52	0	17,19,21	0.79	0
5	NAG	i	2	5	14,14,15	0.51	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	i	3	5	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
5	NAG	j	1	5,1	14,14,15	0.46	0	17,19,21	1.26	1 (5%)
5	NAG	j	2	5	14,14,15	0.56	0	17,19,21	0.97	1 (5%)
5	BMA	j	3	5	11,11,12	0.61	0	15,15,17	1.10	2 (13%)
7	NAG	k	1	7,1	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
7	NAG	k	2	7	14,14,15	0.59	0	17,19,21	0.74	0
7	BMA	k	3	7	11,11,12	0.60	0	15,15,17	0.87	0
7	MAN	k	4	7	11,11,12	0.60	0	15,15,17	0.79	0
7	MAN	k	5	7	11,11,12	0.71	0	15,15,17	0.96	1 (6%)
5	NAG	l	1	5,1	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
5	NAG	l	2	5	14,14,15	0.58	0	17,19,21	0.82	1 (5%)
5	BMA	l	3	5	11,11,12	0.68	0	15,15,17	0.70	0
8	NAG	m	1	8,1	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
8	NAG	m	2	8	14,14,15	0.51	0	17,19,21	0.86	0
8	BMA	m	3	8	11,11,12	0.56	0	15,15,17	1.30	2 (13%)
8	MAN	m	4	8	11,11,12	0.59	0	15,15,17	0.77	0
7	NAG	n	1	7,1	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
7	NAG	n	2	7	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
7	BMA	n	3	7	11,11,12	0.55	0	15,15,17	0.93	0
7	MAN	n	4	7	11,11,12	0.57	0	15,15,17	1.01	1 (6%)
7	MAN	n	5	7	11,11,12	0.52	0	15,15,17	1.59	2 (13%)
6	NAG	o	1	6,1	14,14,15	0.51	0	17,19,21	0.66	0
6	NAG	o	2	6	14,14,15	0.54	0	17,19,21	0.67	0
5	NAG	p	1	5,1	14,14,15	0.47	0	17,19,21	1.27	1 (5%)
5	NAG	p	2	5	14,14,15	0.57	0	17,19,21	0.98	1 (5%)
5	BMA	p	3	5	11,11,12	0.63	0	15,15,17	1.10	2 (13%)
6	NAG	q	1	6,1	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
6	NAG	q	2	6	14,14,15	0.54	0	17,19,21	0.76	0
6	NAG	r	1	6,1	14,14,15	0.48	0	17,19,21	0.76	0
6	NAG	r	2	6	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
6	NAG	s	1	6,1	14,14,15	0.50	0	17,19,21	0.76	0
6	NAG	s	2	6	14,14,15	0.58	0	17,19,21	1.05	1 (5%)
5	NAG	t	1	5,1	14,14,15	0.45	0	17,19,21	0.58	0
5	NAG	t	2	5	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
5	BMA	t	3	5	11,11,12	0.61	0	15,15,17	0.82	0
5	NAG	u	1	5,1	14,14,15	0.49	0	17,19,21	1.46	3 (17%)
5	NAG	u	2	5	14,14,15	0.55	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	u	3	5	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
6	NAG	v	1	6,1	14,14,15	0.54	0	17,19,21	0.87	1 (5%)
6	NAG	v	2	6	14,14,15	0.50	0	17,19,21	0.91	1 (5%)
6	NAG	w	1	6,1	14,14,15	0.68	0	17,19,21	0.97	0
6	NAG	w	2	6	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
6	NAG	x	1	6,1	14,14,15	0.55	0	17,19,21	0.68	1 (5%)
6	NAG	x	2	6	14,14,15	0.49	0	17,19,21	0.76	0
5	NAG	y	1	5,1	14,14,15	0.48	0	17,19,21	0.74	1 (5%)
5	NAG	y	2	5	14,14,15	0.59	0	17,19,21	0.90	2 (11%)
5	BMA	y	3	5	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
5	NAG	z	1	5,1	14,14,15	0.49	0	17,19,21	0.63	0
5	NAG	z	2	5	14,14,15	0.55	0	17,19,21	0.83	1 (5%)
5	BMA	z	3	5	11,11,12	0.67	0	15,15,17	0.81	0

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	y	2	5	-	2/6/23/26	0/1/1/1
5	BMA	y	3	5	-	0/2/19/22	0/1/1/1
5	NAG	z	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	z	2	5	-	0/6/23/26	0/1/1/1
5	BMA	z	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	1	NAG	O5-C1	-2.75	1.39	1.43
5	6	1	NAG	C2-N2	-2.65	1.41	1.46

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	1	NAG	C1-C2-N2	-5.61	100.90	110.49
5	Y	2	NAG	C1-O5-C5	5.05	119.03	112.19
7	n	5	MAN	C1-O5-C5	3.97	117.58	112.19
7	n	5	MAN	O5-C5-C6	3.94	113.38	107.20
5	p	1	NAG	O5-C5-C6	3.75	113.08	107.20

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	p	1	NAG	C8-C7-N2-C2
5	p	1	NAG	O7-C7-N2-C2
5	t	1	NAG	O7-C7-N2-C2
5	u	1	NAG	O7-C7-N2-C2
5	z	1	NAG	C8-C7-N2-C2

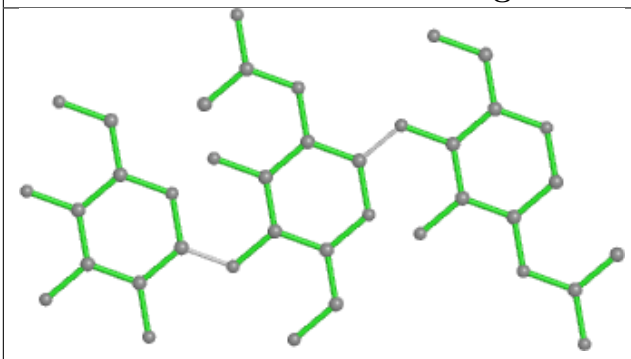
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	n	5	MAN	C1-C2-C3-C4-C5-O5

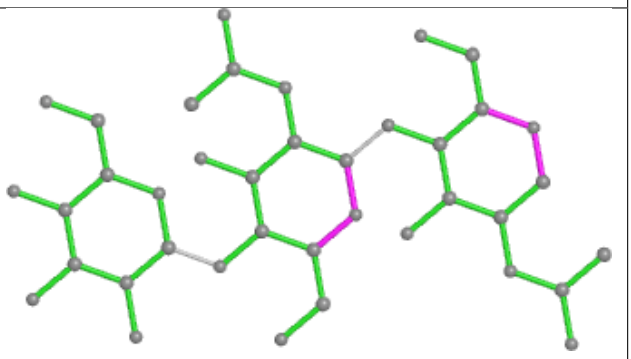
No monomer is involved in short contacts.

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

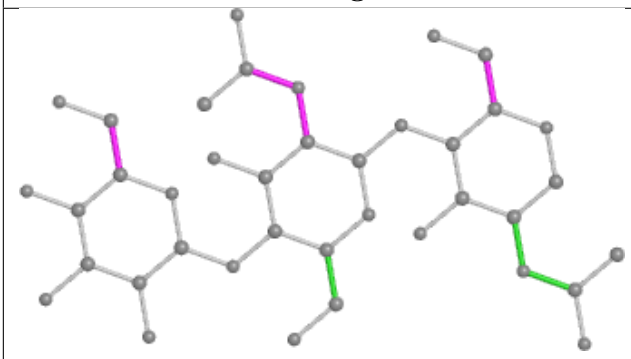
Oligosaccharide Chain Y



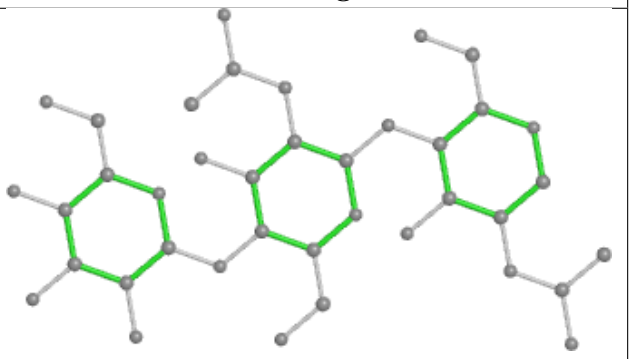
Bond lengths



Bond angles

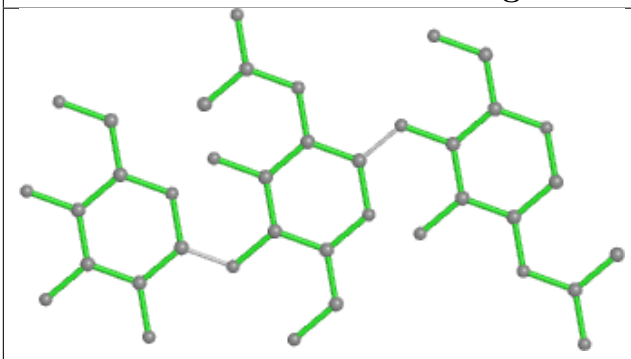


Torsions

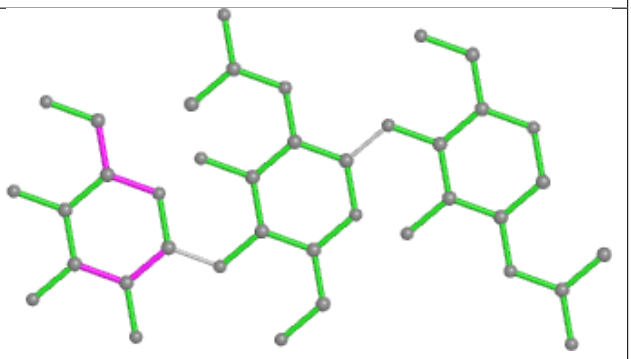


Rings

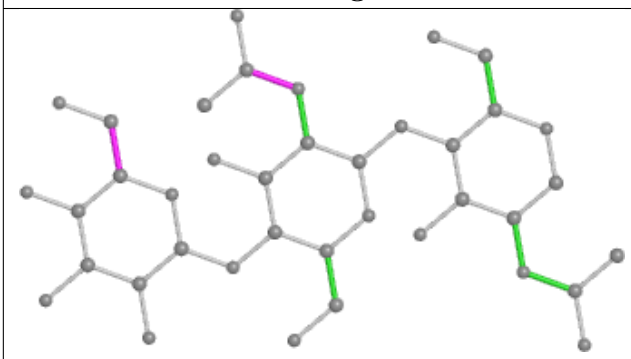
Oligosaccharide Chain i



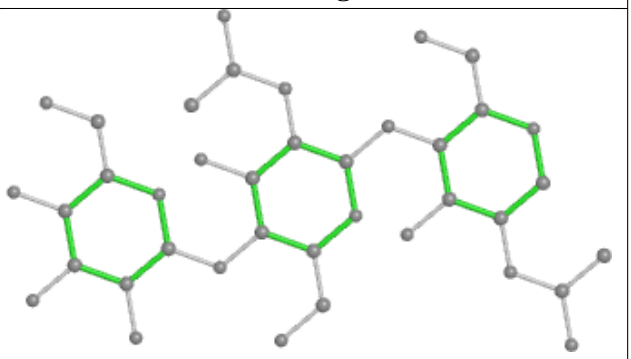
Bond lengths



Bond angles

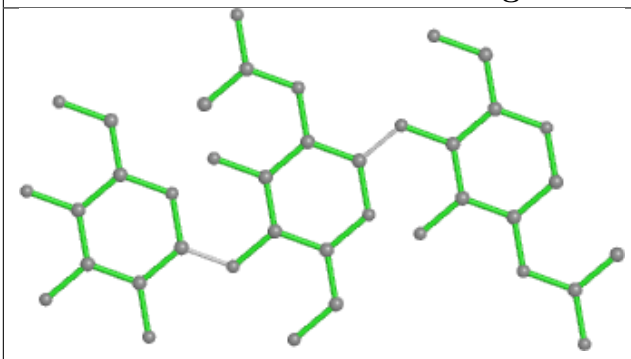


Torsions

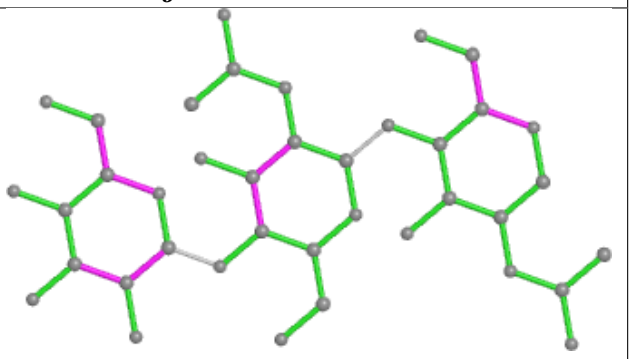


Rings

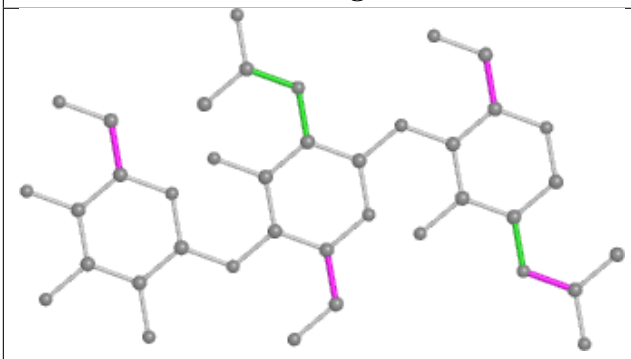
Oligosaccharide Chain j



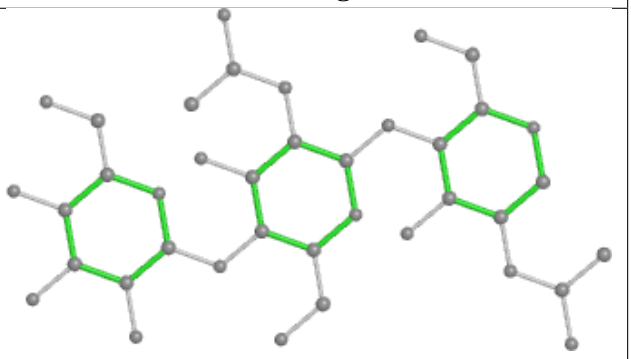
Bond lengths



Bond angles

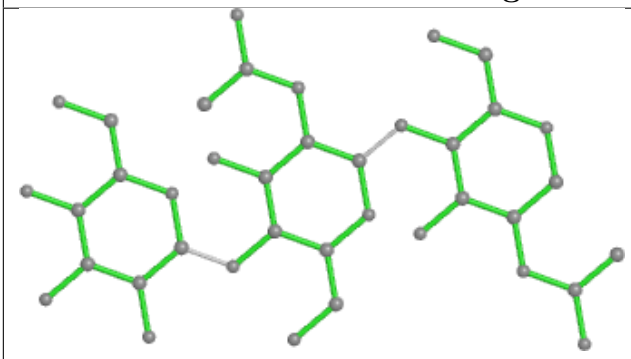


Torsions

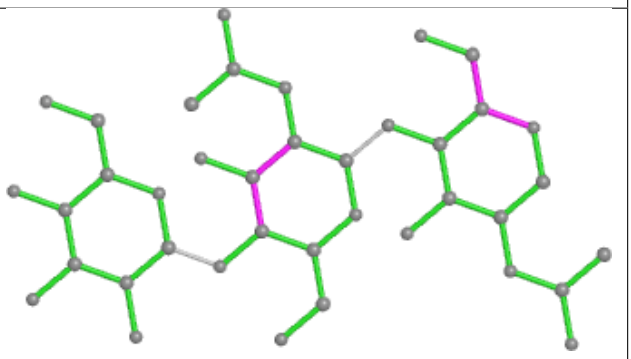


Rings

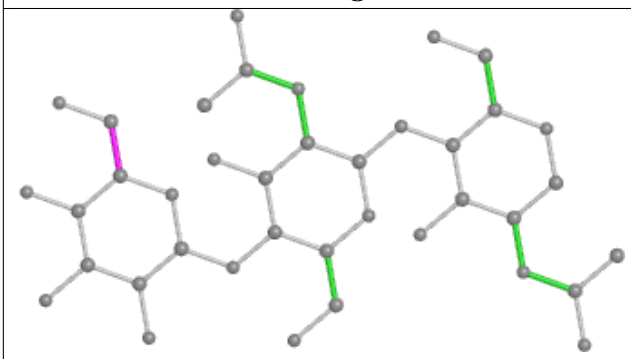
Oligosaccharide Chain l



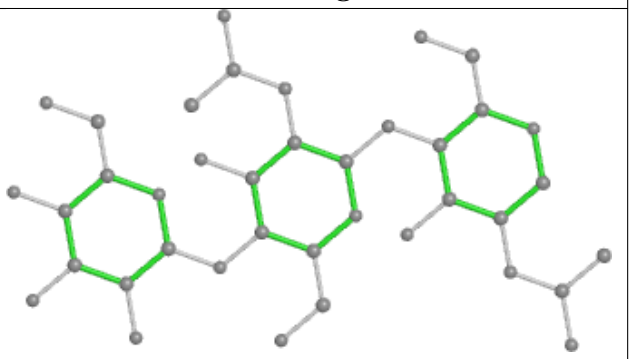
Bond lengths



Bond angles

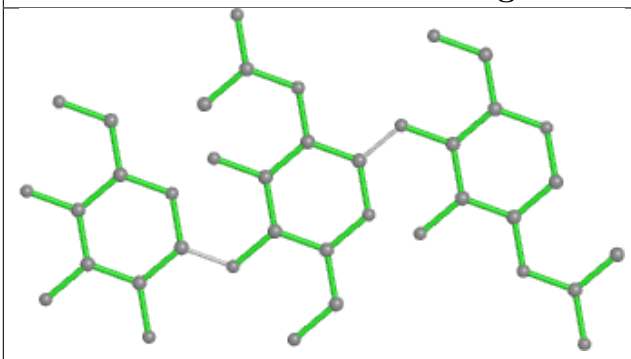


Torsions

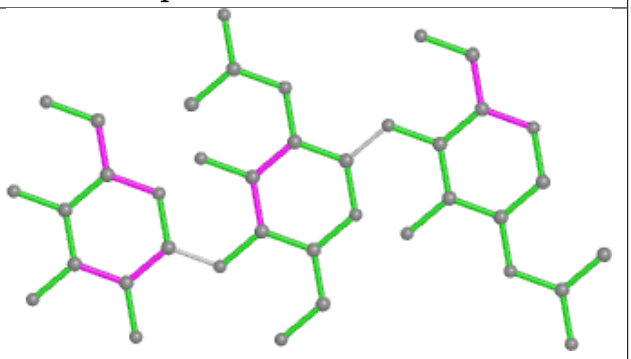


Rings

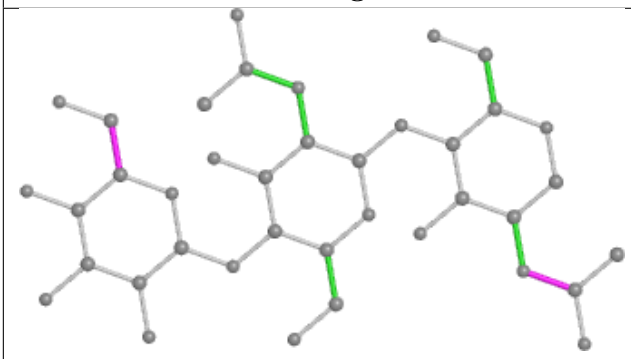
Oligosaccharide Chain p



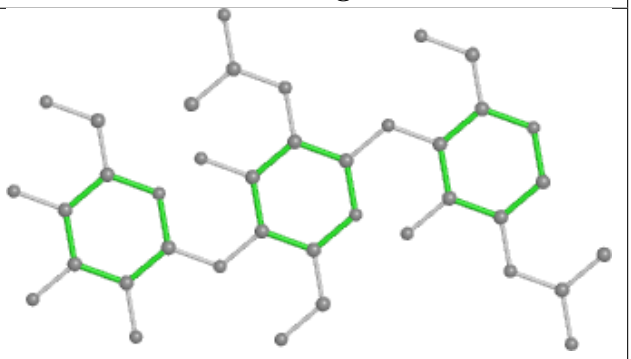
Bond lengths



Bond angles

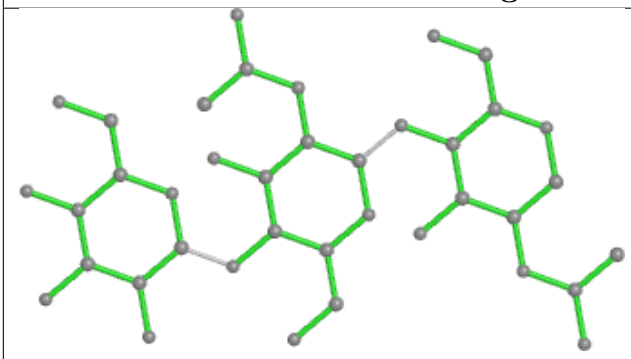


Torsions

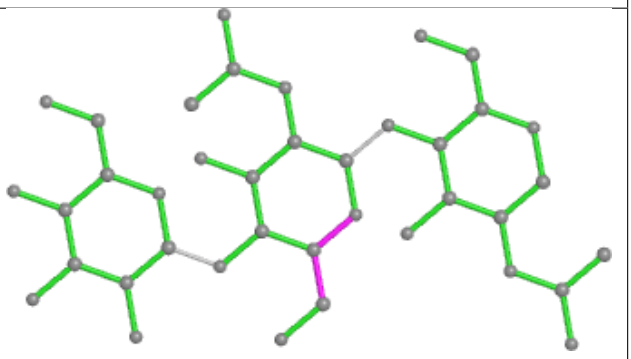


Rings

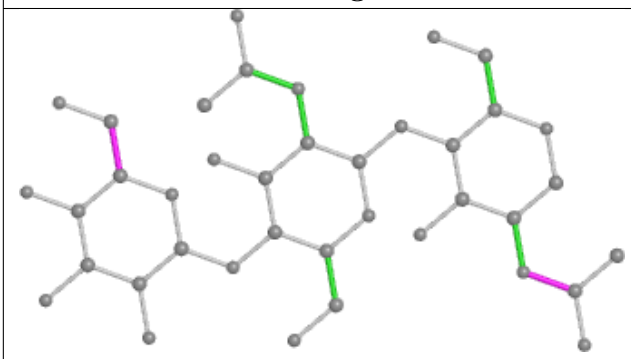
Oligosaccharide Chain t



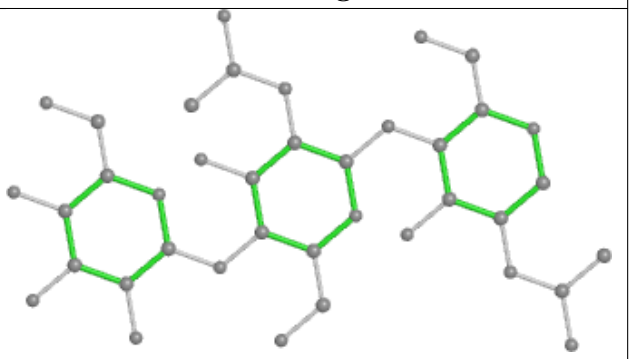
Bond lengths



Bond angles

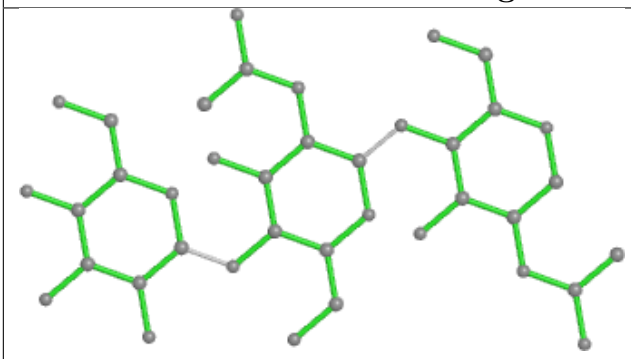


Torsions

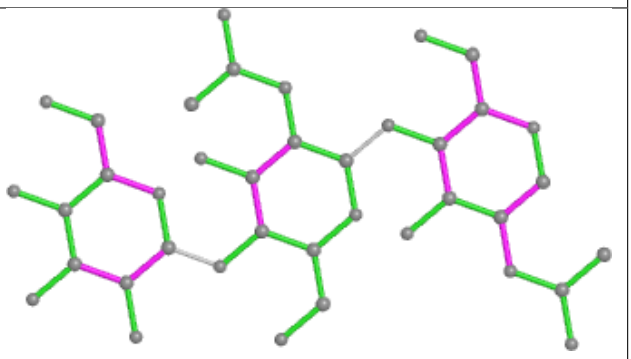


Rings

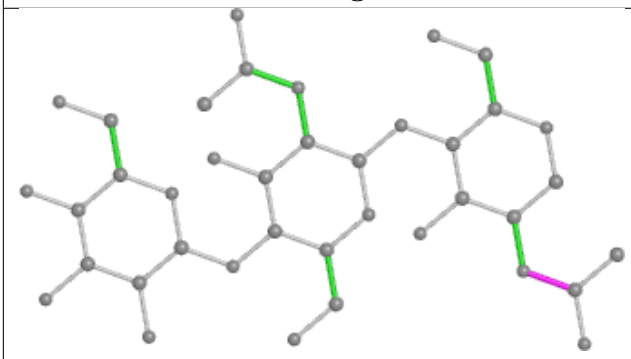
Oligosaccharide Chain u



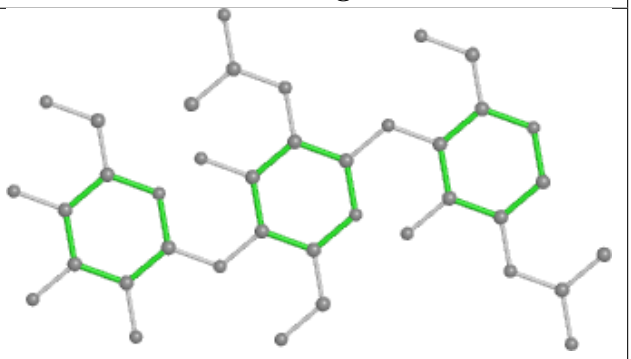
Bond lengths



Bond angles

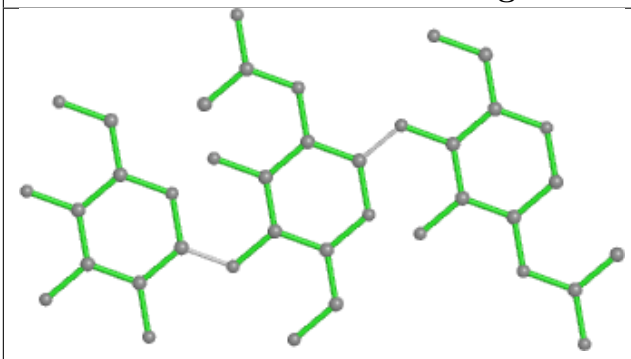


Torsions

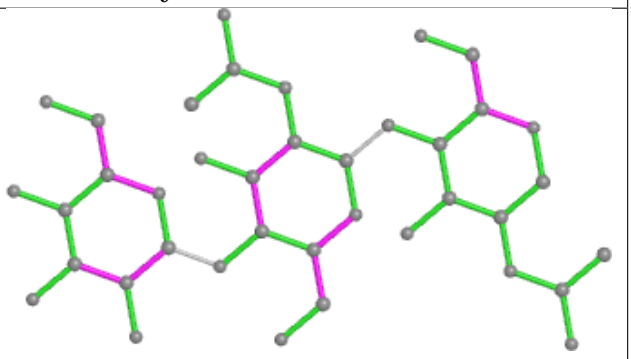


Rings

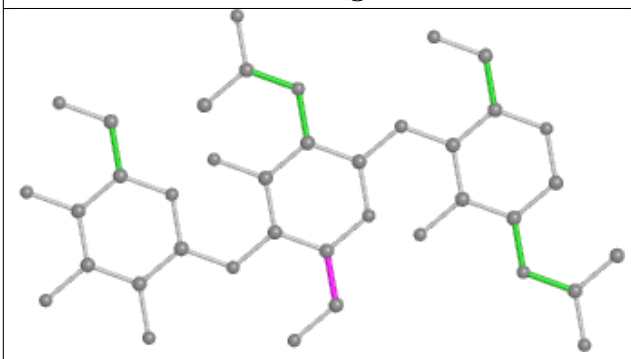
Oligosaccharide Chain y



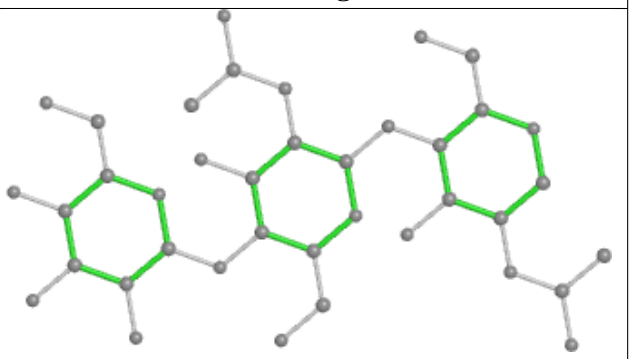
Bond lengths



Bond angles

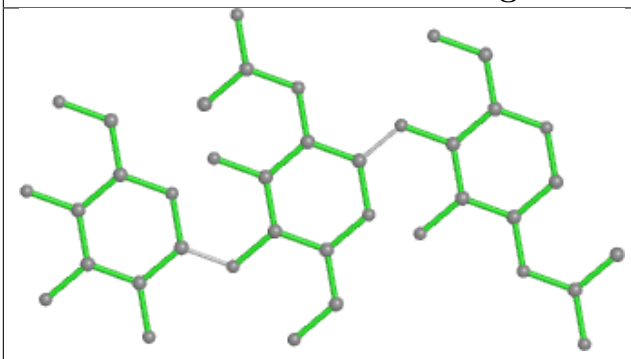


Torsions



Rings

Oligosaccharide Chain z



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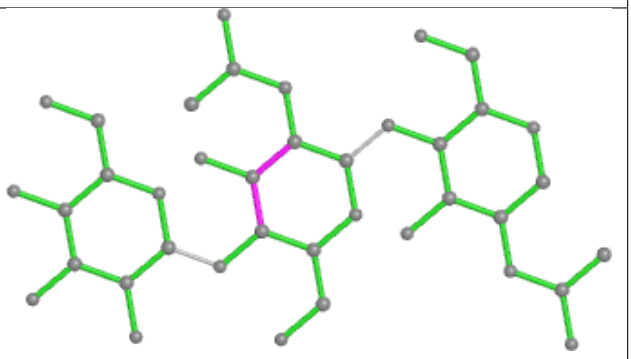

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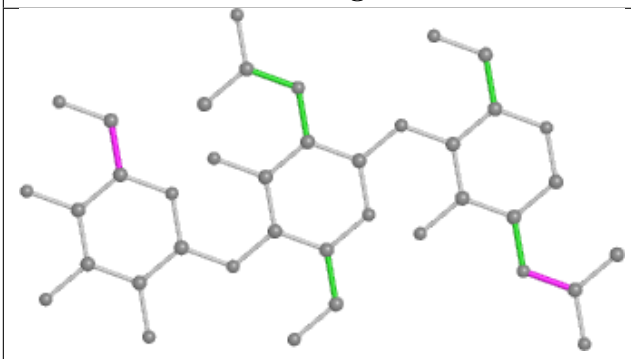

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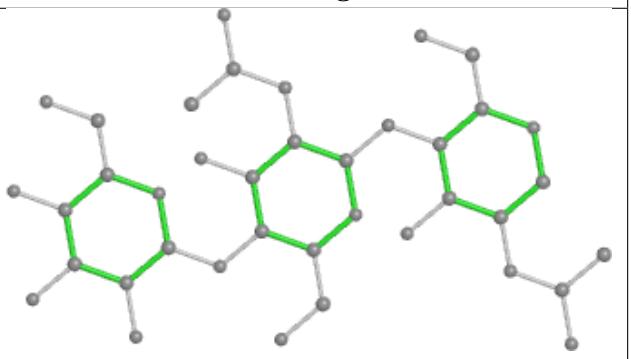
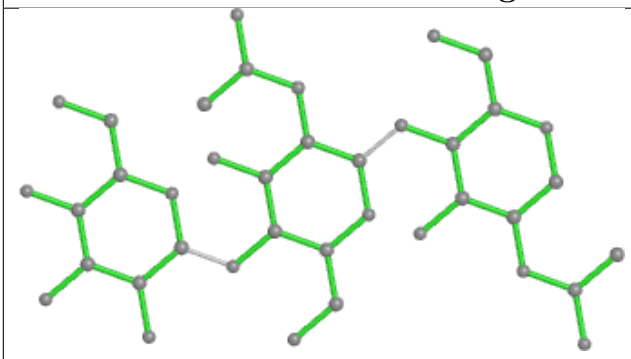


Rings

Oligosaccharide Chain 0



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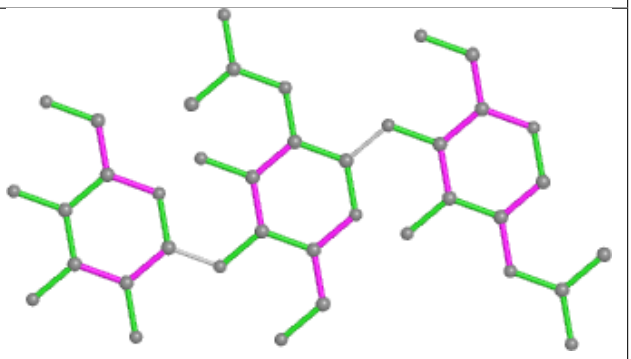
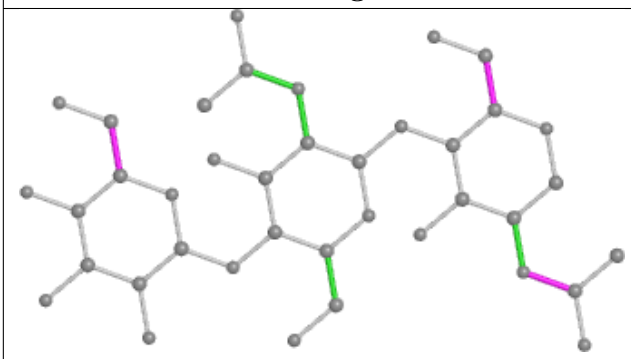
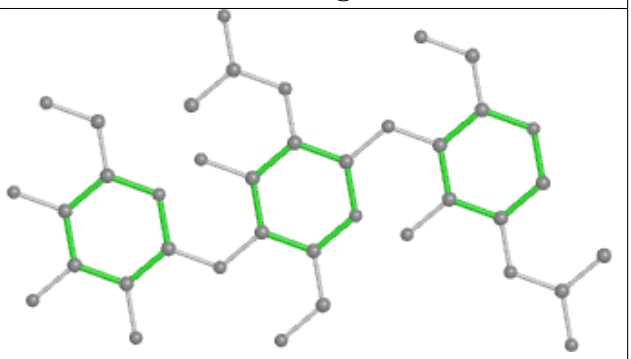


Bond angles

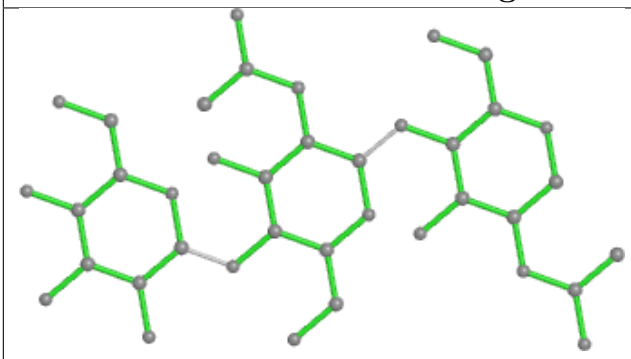


Torsions



Rings

Oligosaccharide Chain 3



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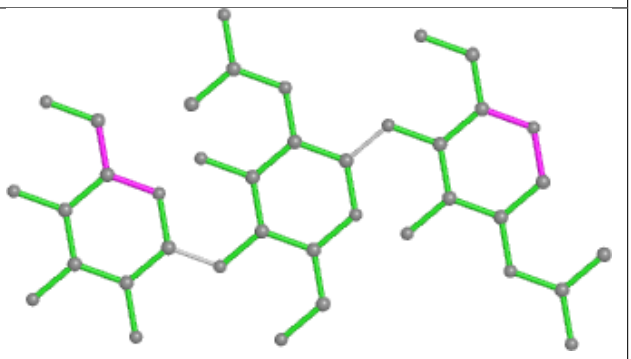

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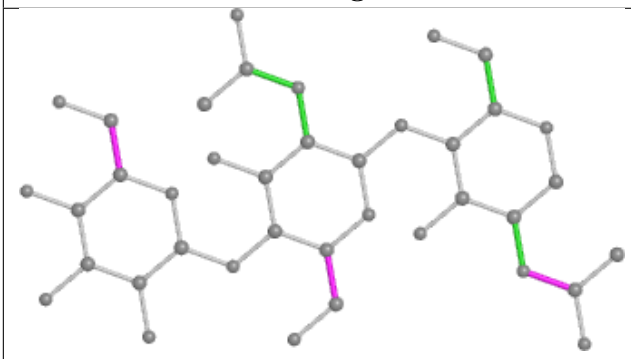

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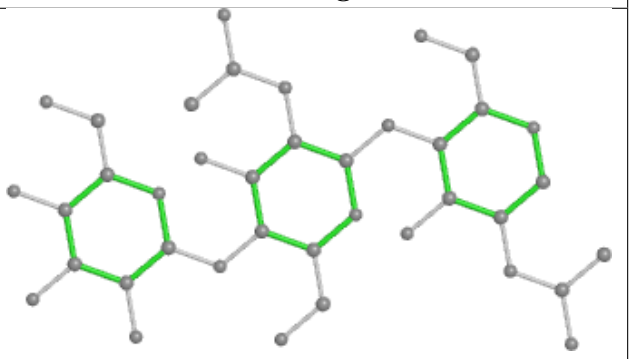
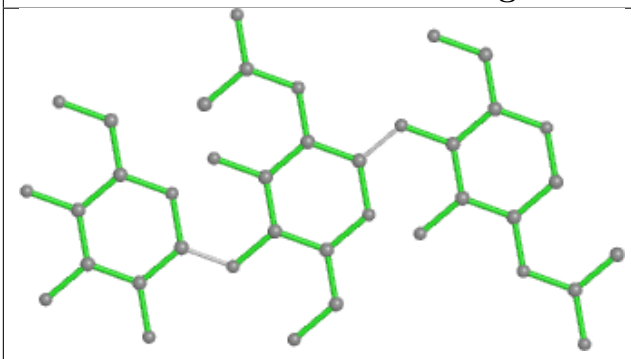


Rings

Oligosaccharide Chain 5



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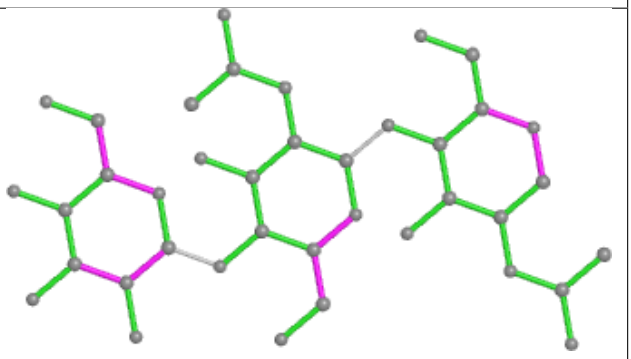
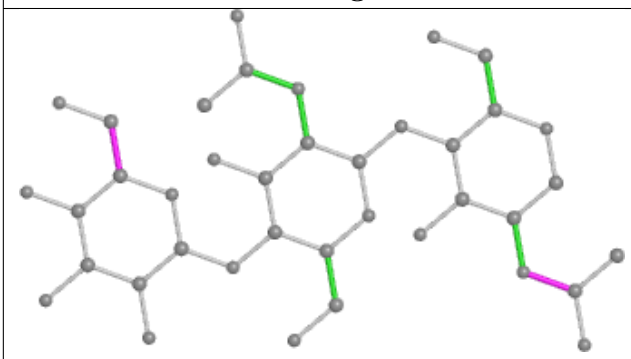
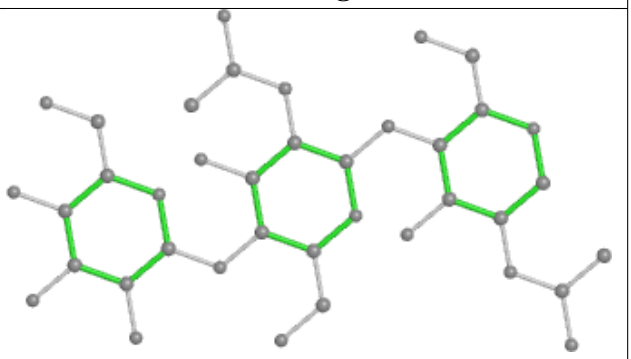


Bond angles

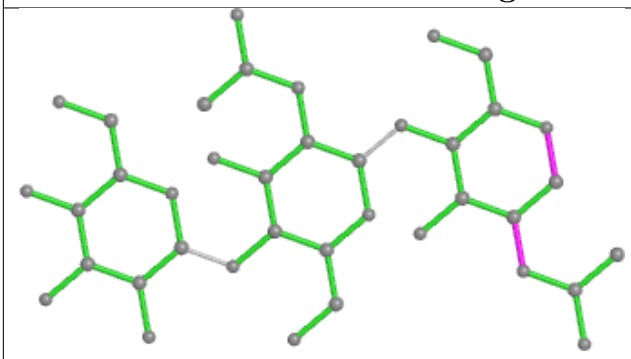


Torsions



Rings

Oligosaccharide Chain 6



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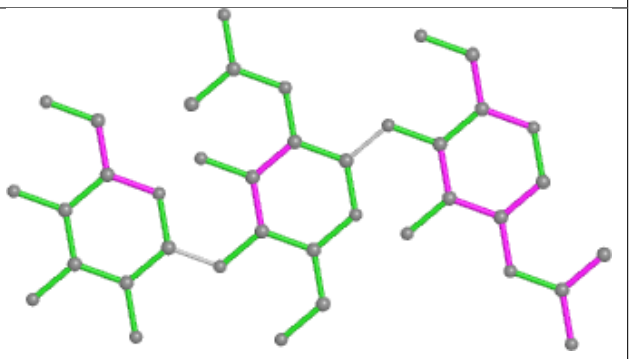
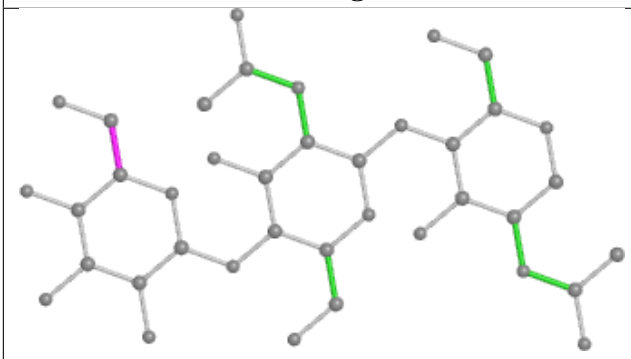
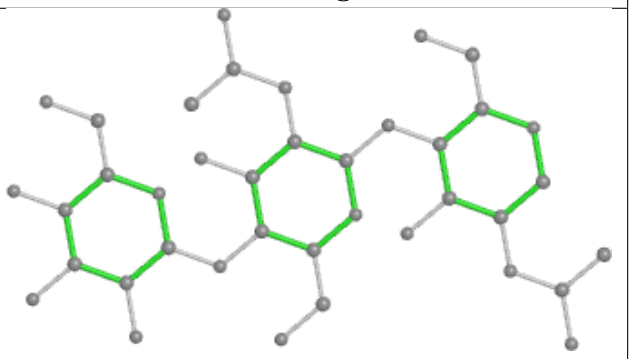


Bond angles

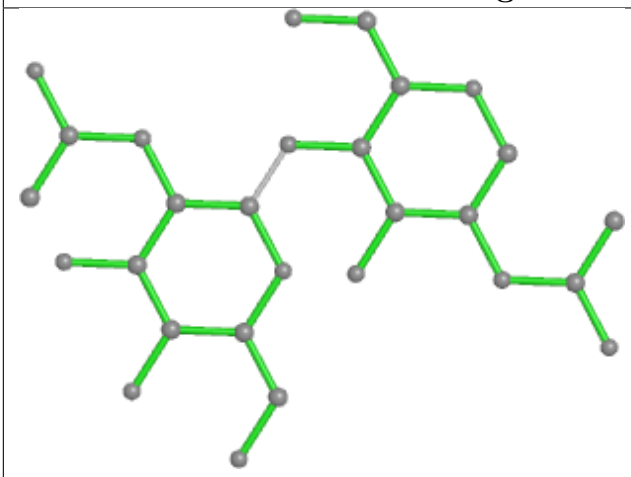


Torsions



Rings

Oligosaccharide Chain Z



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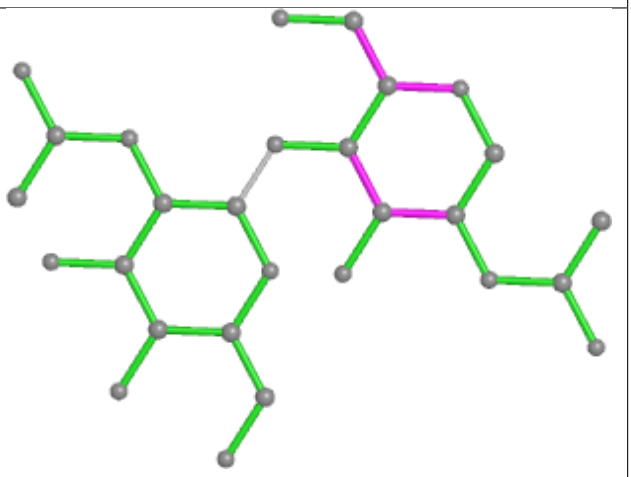
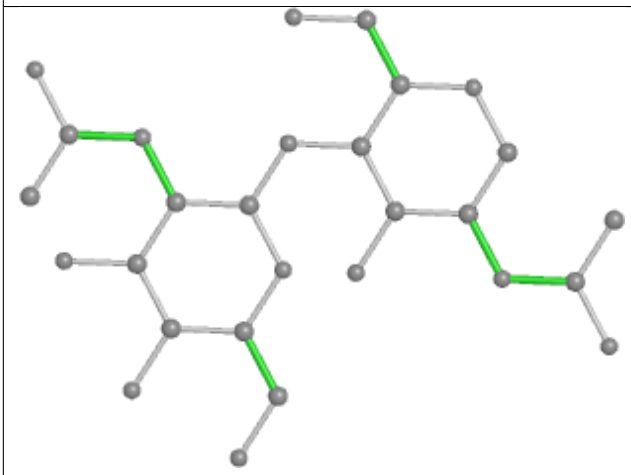


Bond angles



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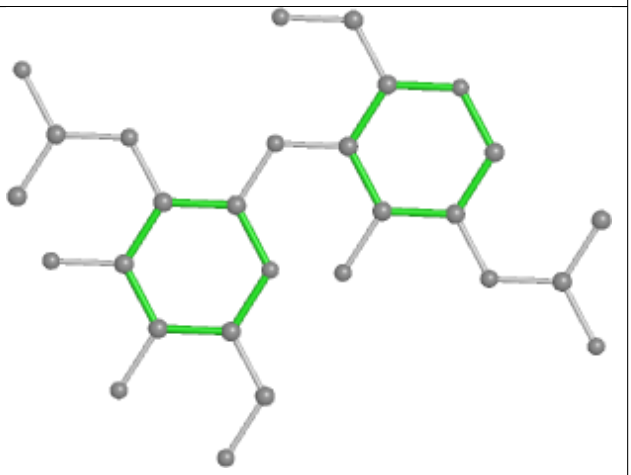
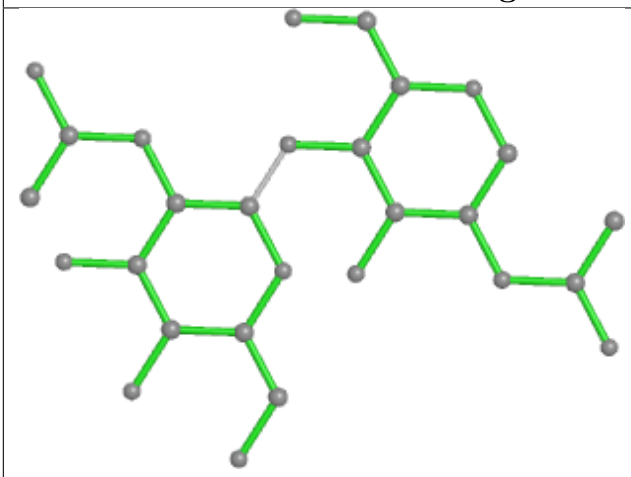


Rings

Oligosaccharide Chain a



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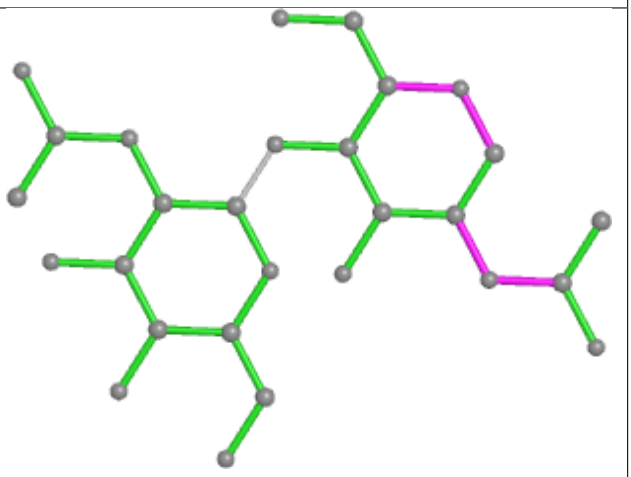
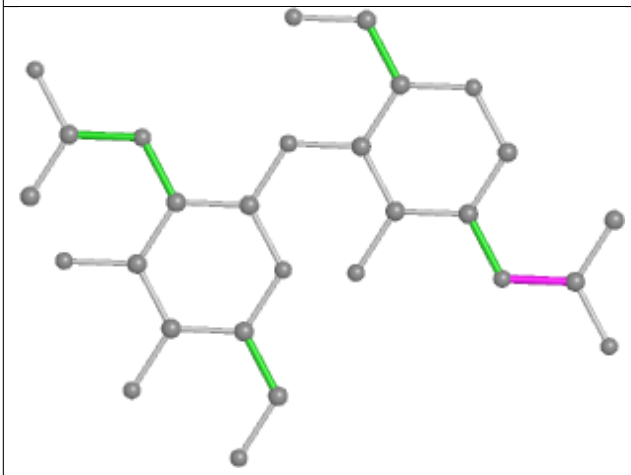


Bond angles



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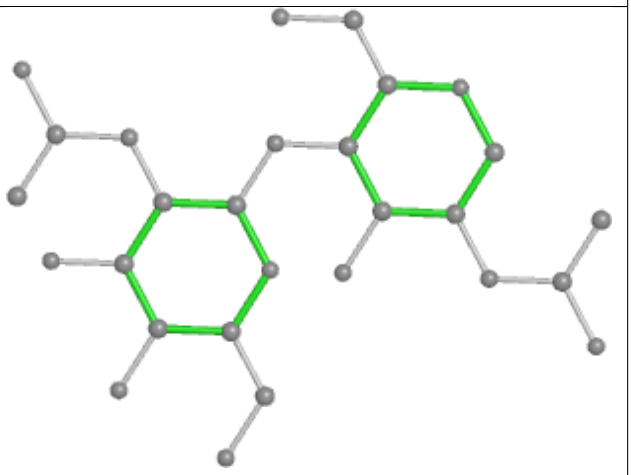
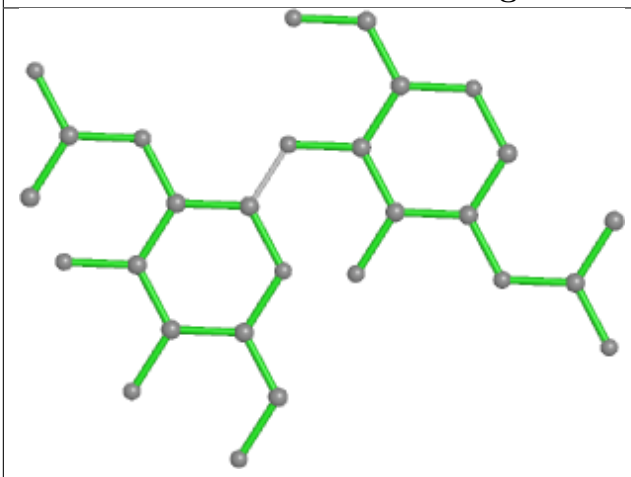


Rings

Oligosaccharide Chain c



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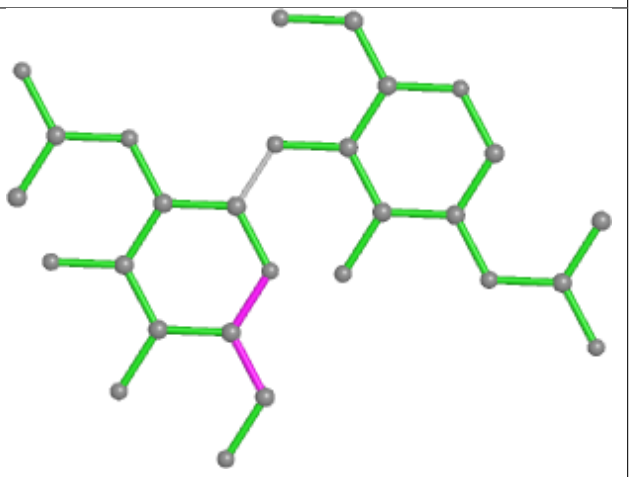
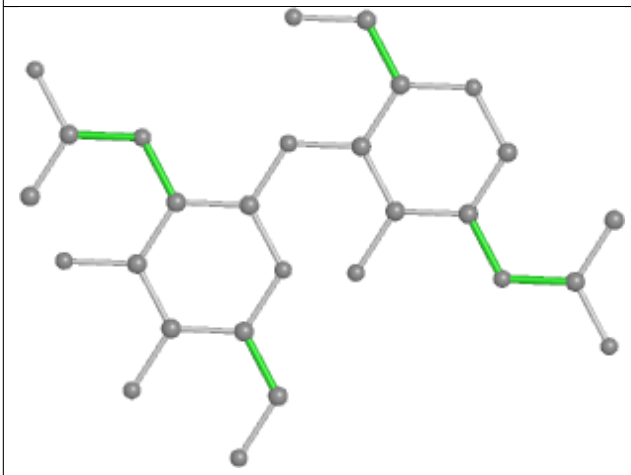
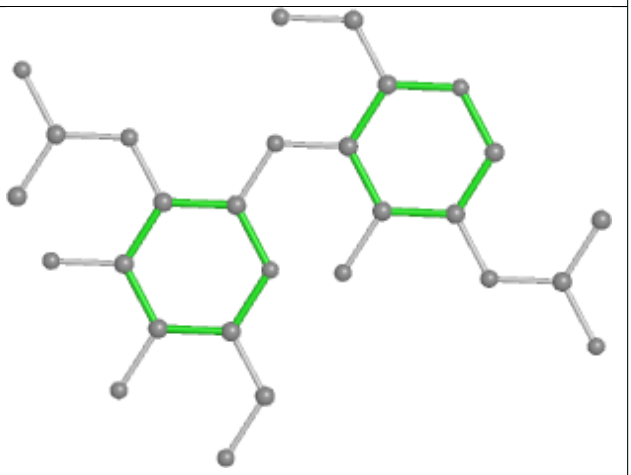


Bond angles

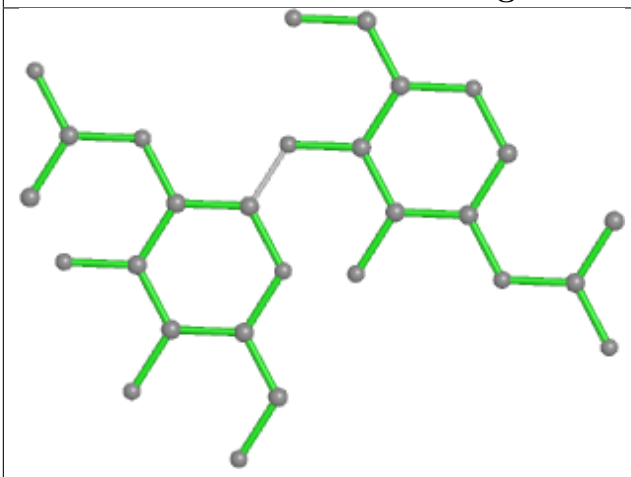


Torsions



Rings

Oligosaccharide Chain d



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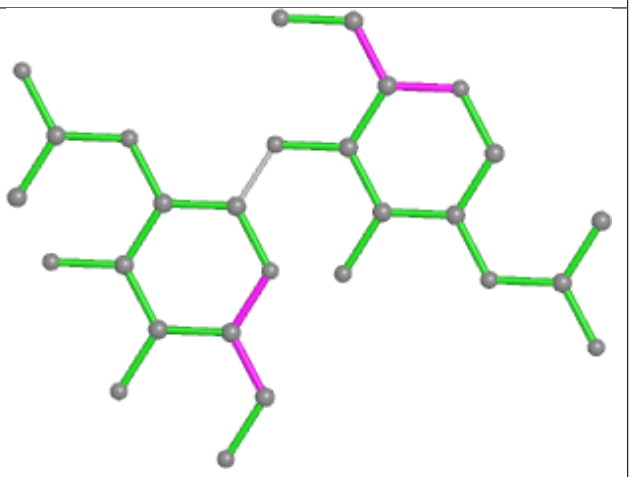

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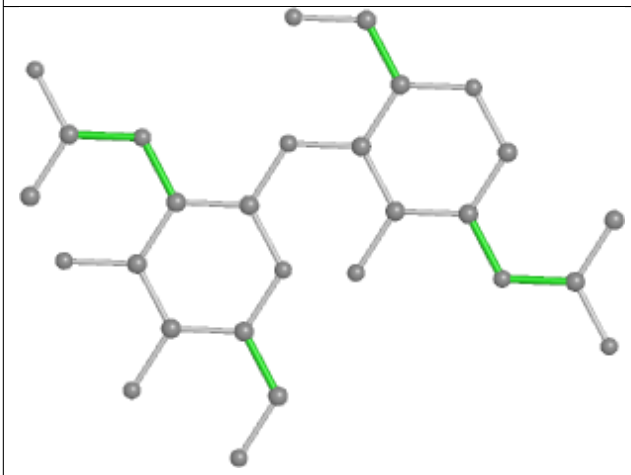

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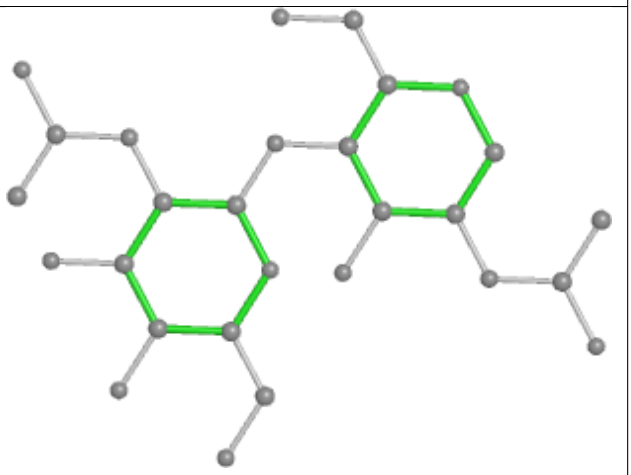
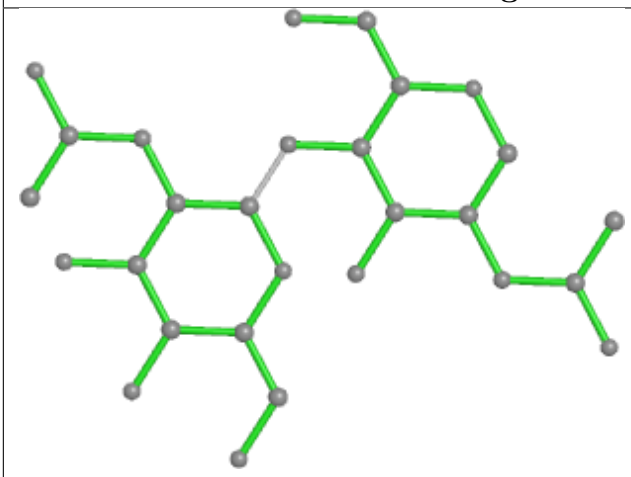


Rings

Oligosaccharide Chain f



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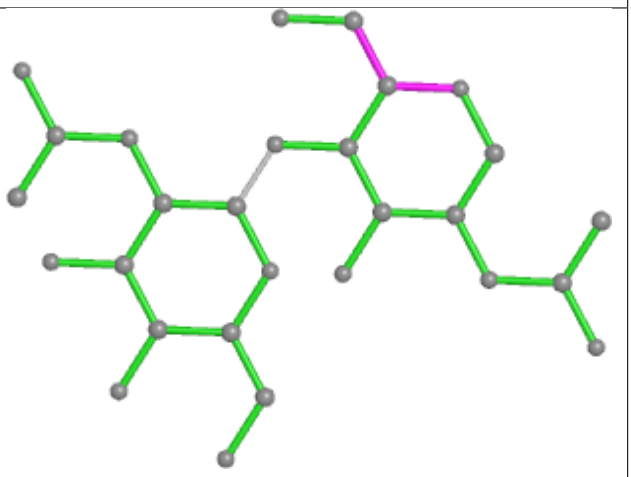
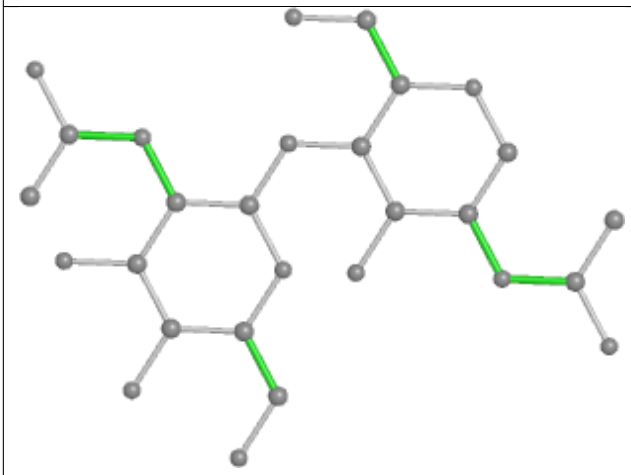
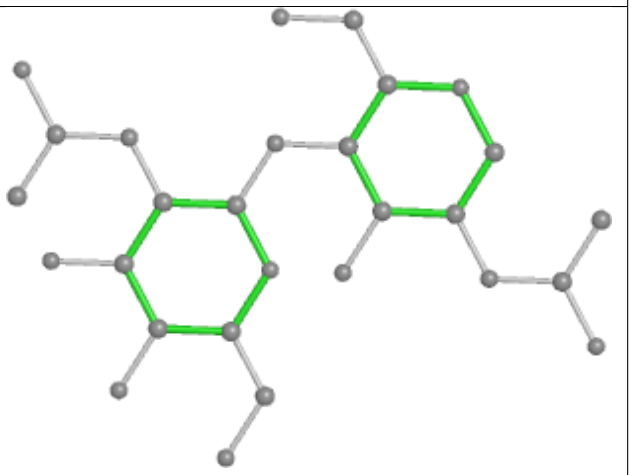


Bond angles

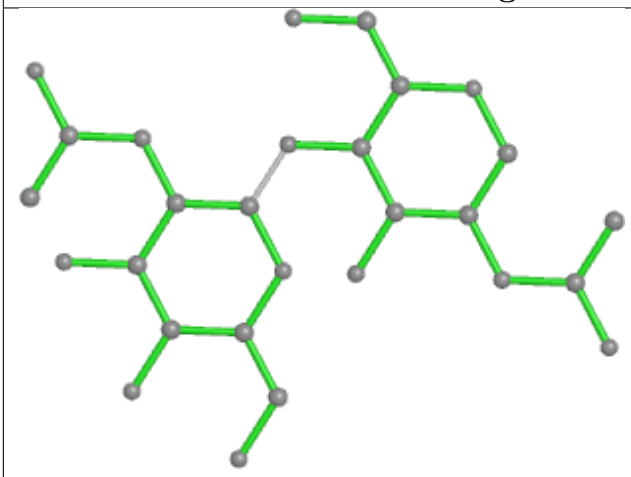


Torsions



Rings

Oligosaccharide Chain o



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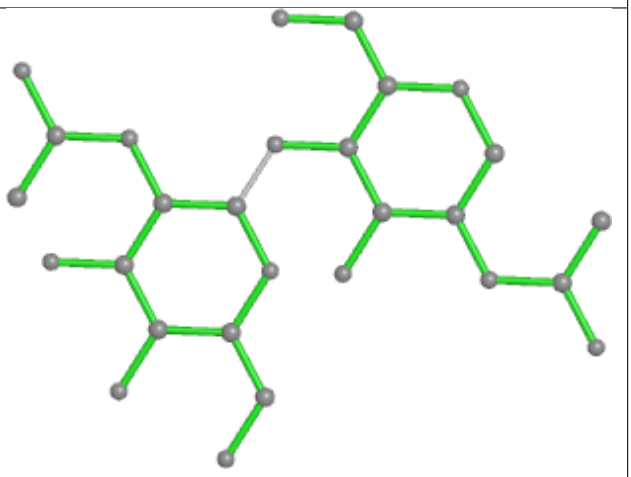
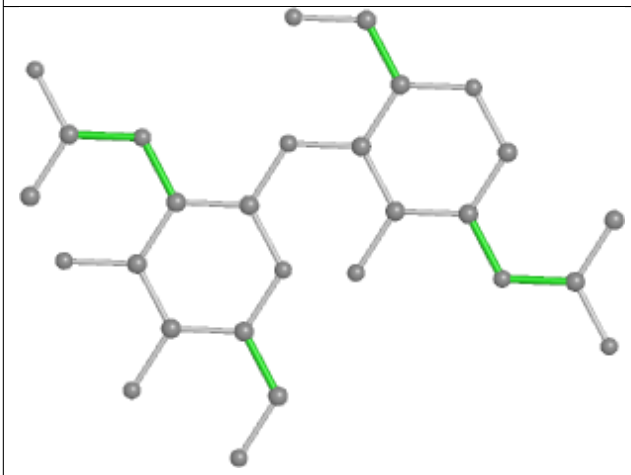


Bond angles



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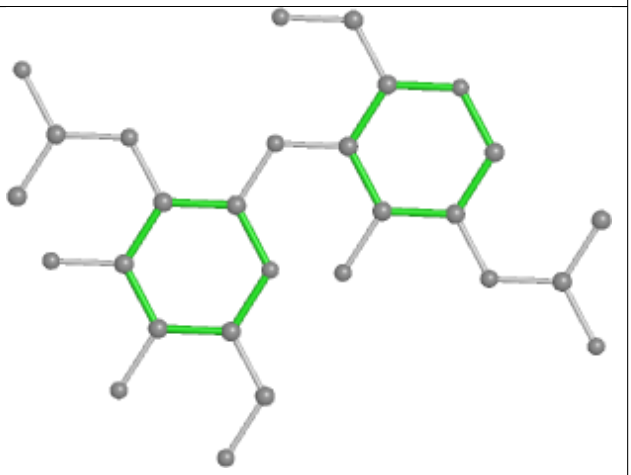
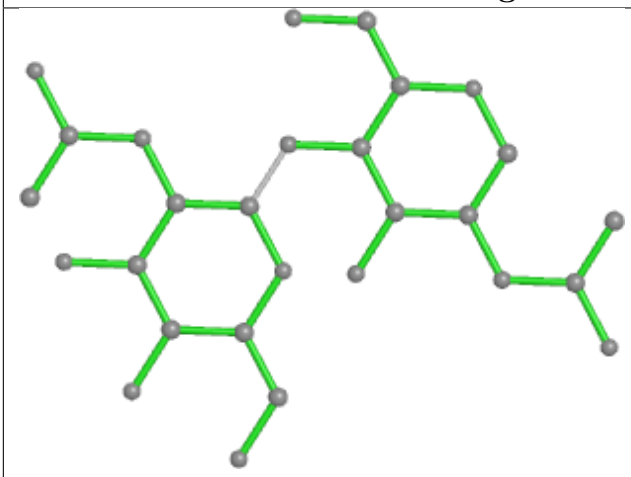


Rings

Oligosaccharide Chain q



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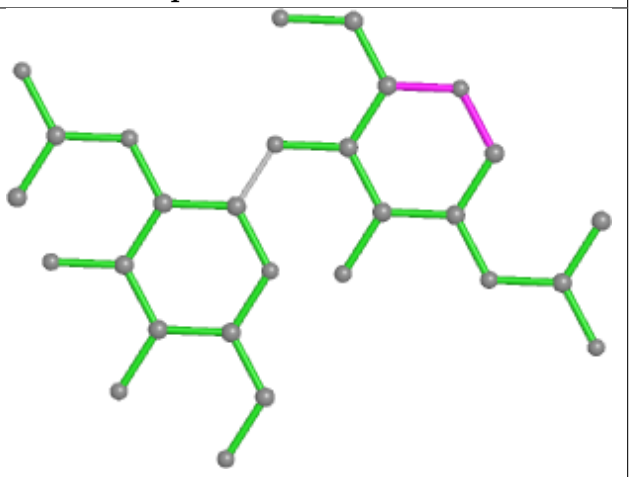
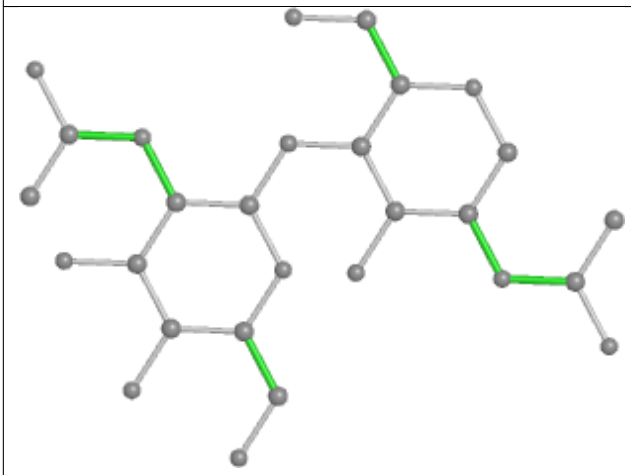


Bond angles



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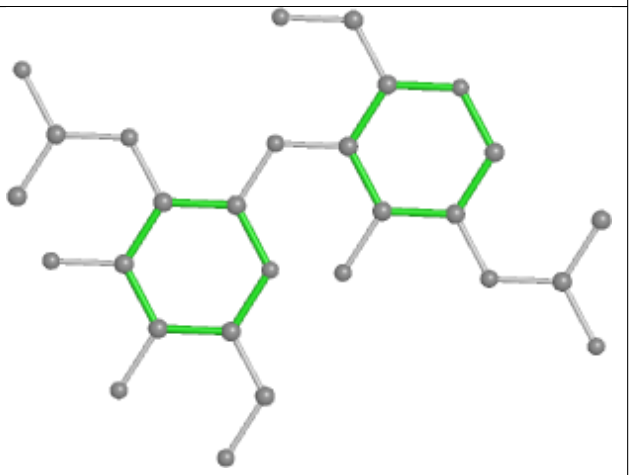
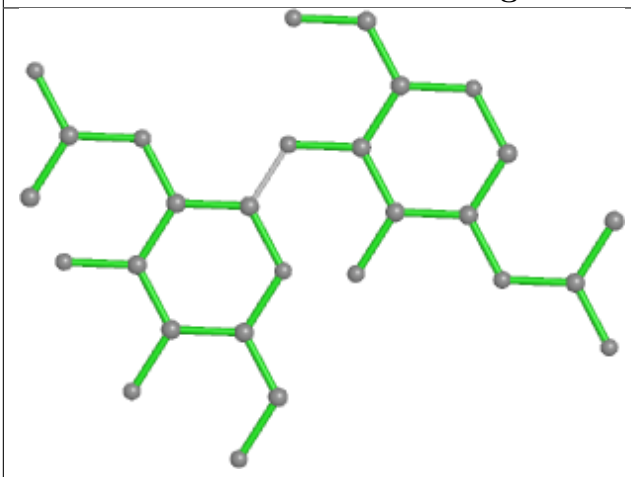
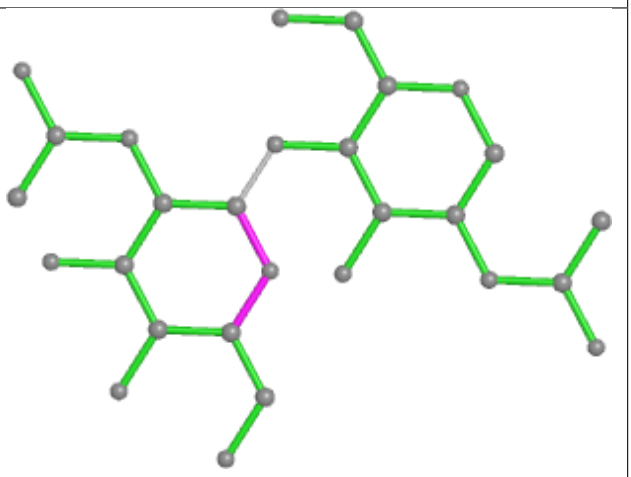


Rings

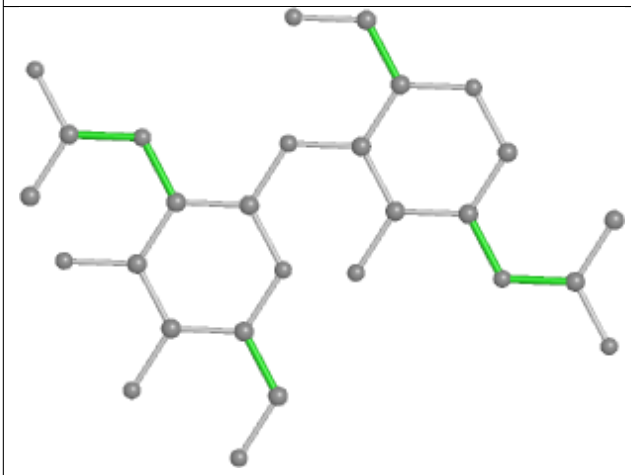
Oligosaccharide Chain r



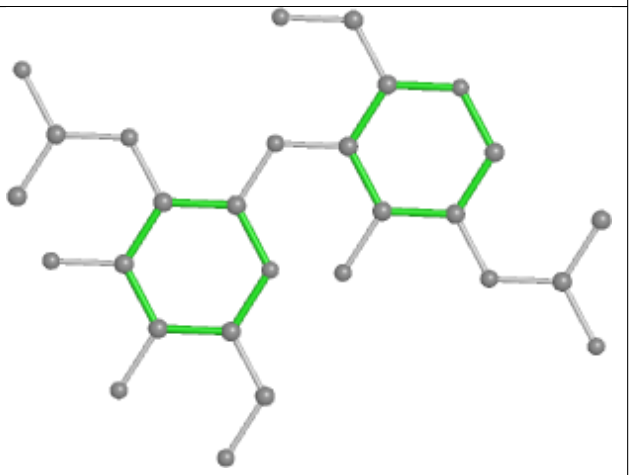
Bond lengths



Bond angles

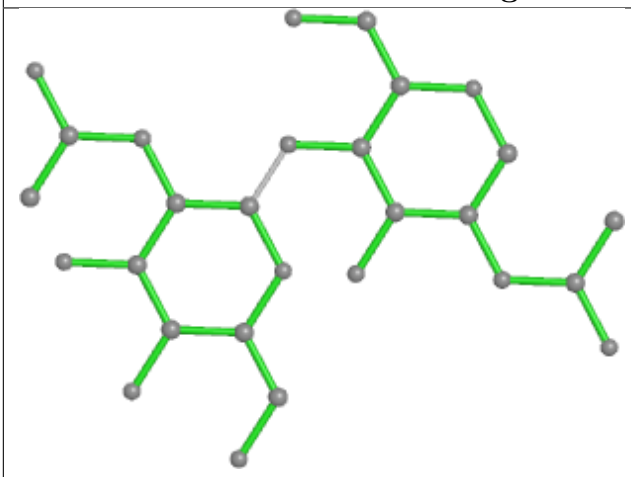


Torsions

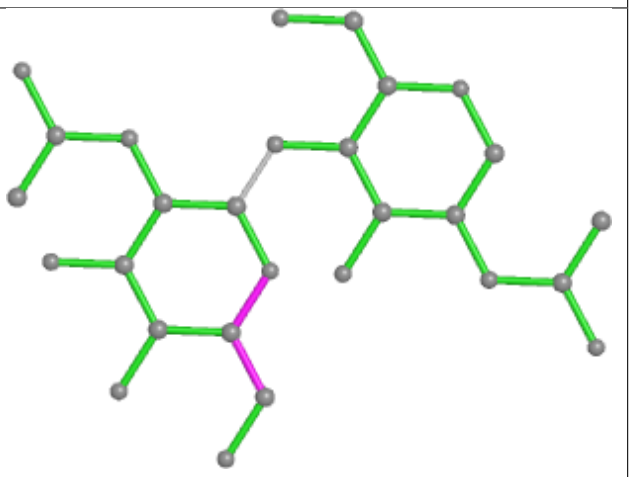


Rings

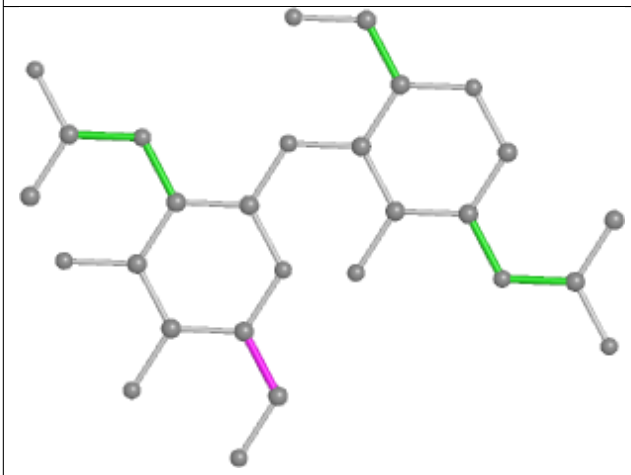
Oligosaccharide Chain s



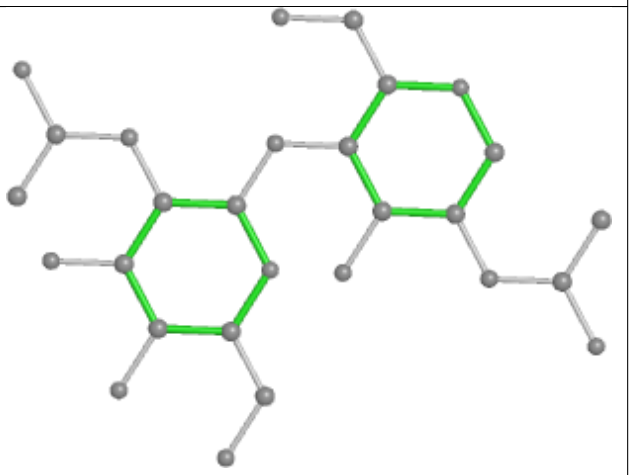
Bond lengths



Bond angles

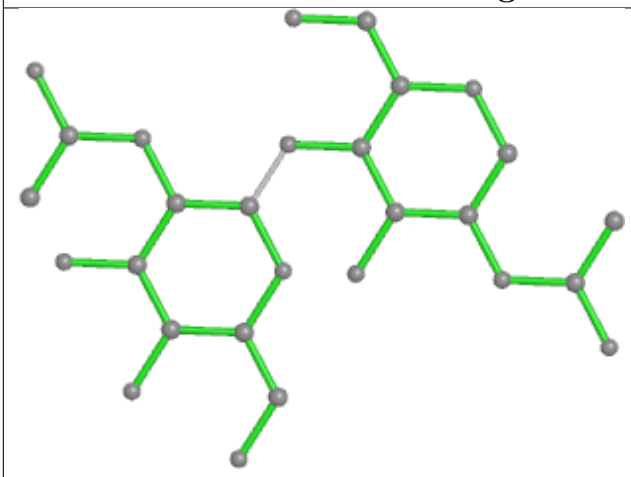


Torsions



Rings

Oligosaccharide Chain v



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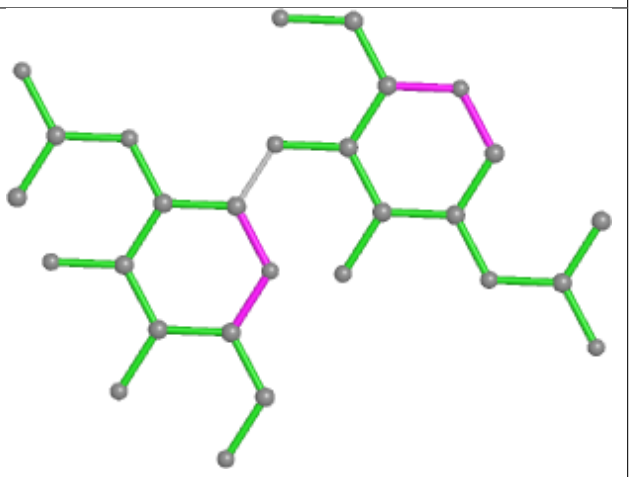
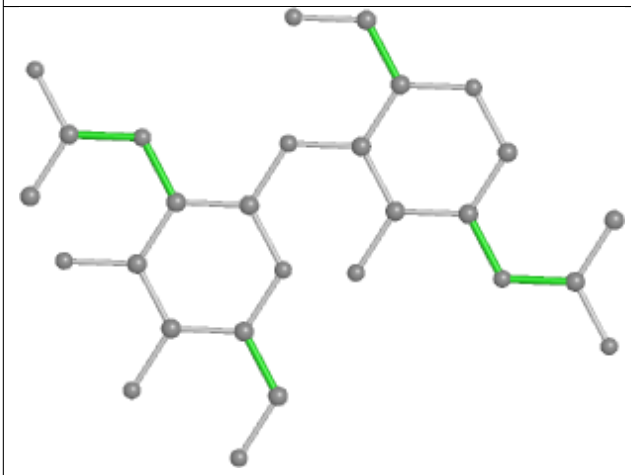


Bond angles



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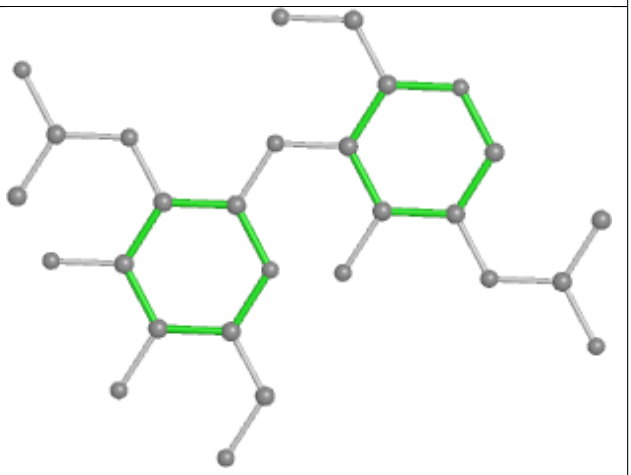
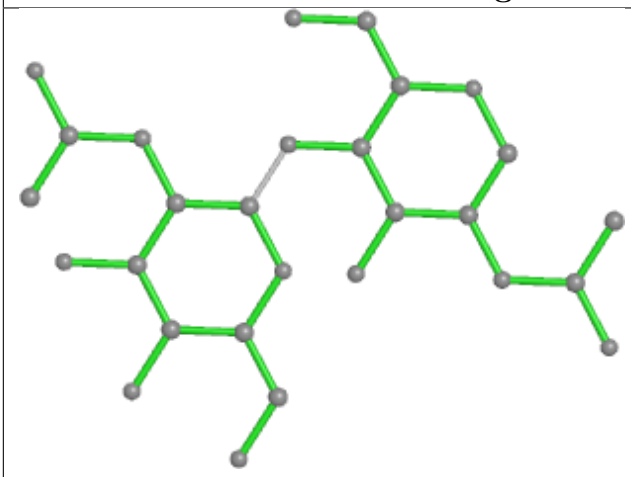


Rings

Oligosaccharide Chain w



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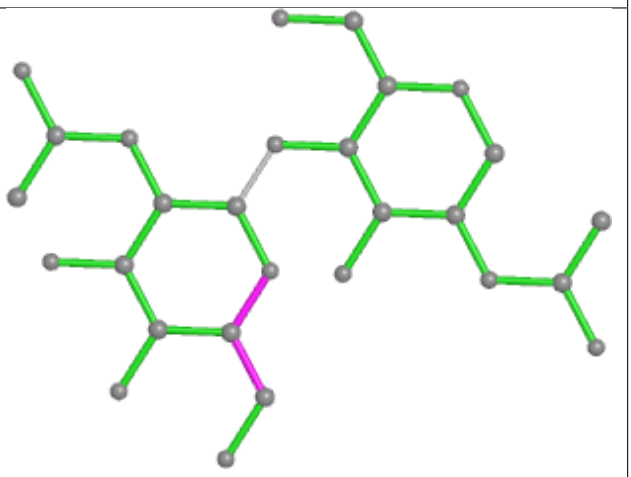
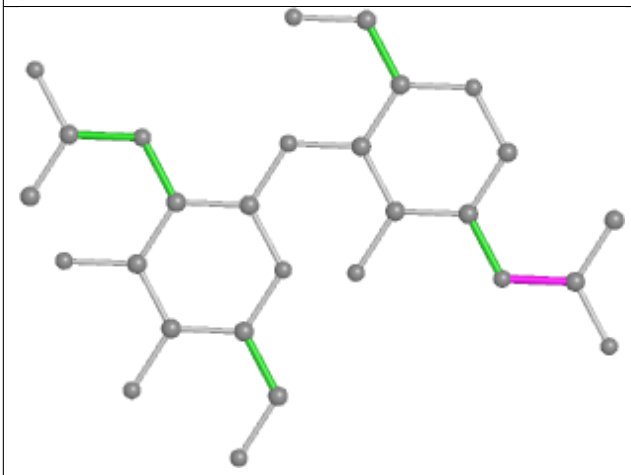
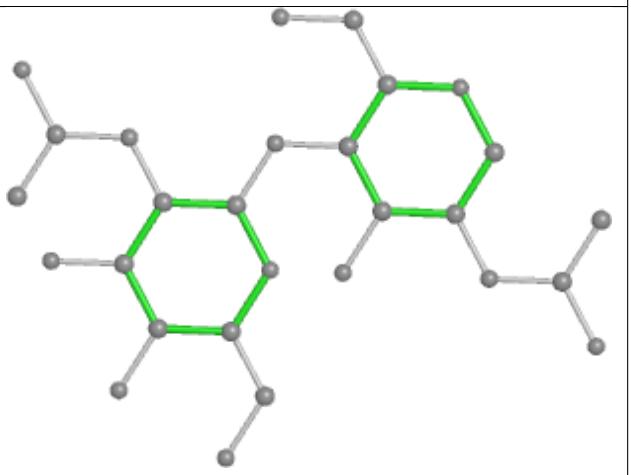


Bond angles

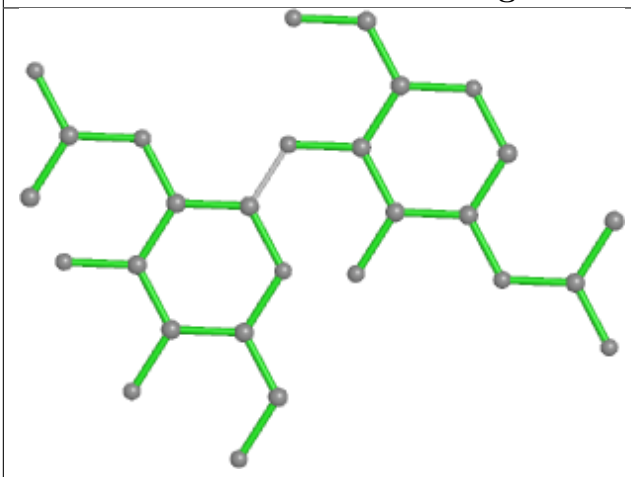


Torsions



Rings

Oligosaccharide Chain x



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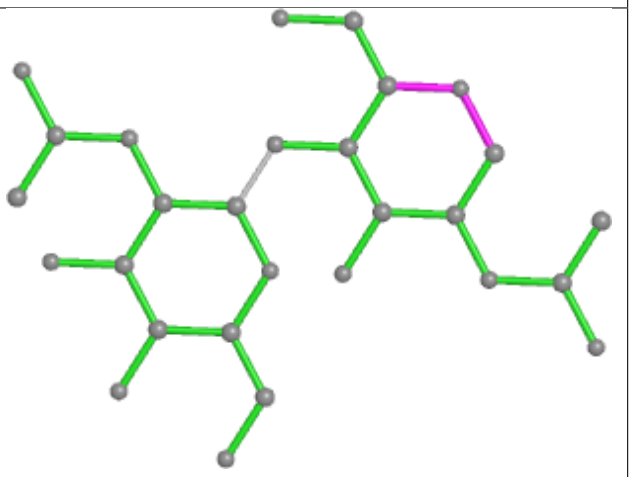
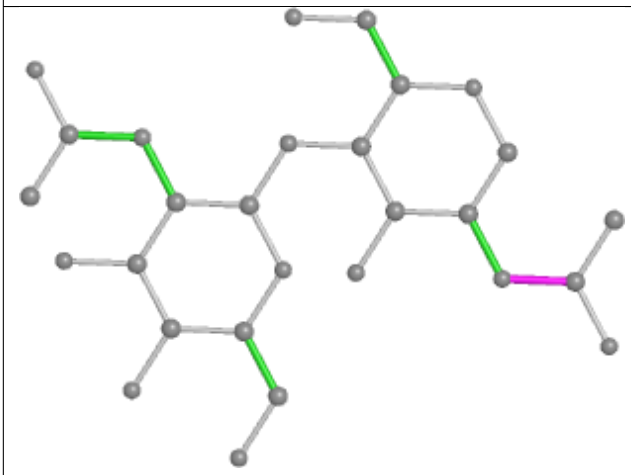


Bond angles



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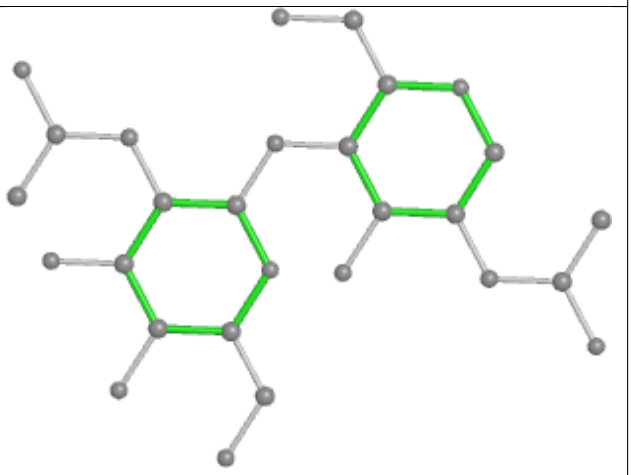
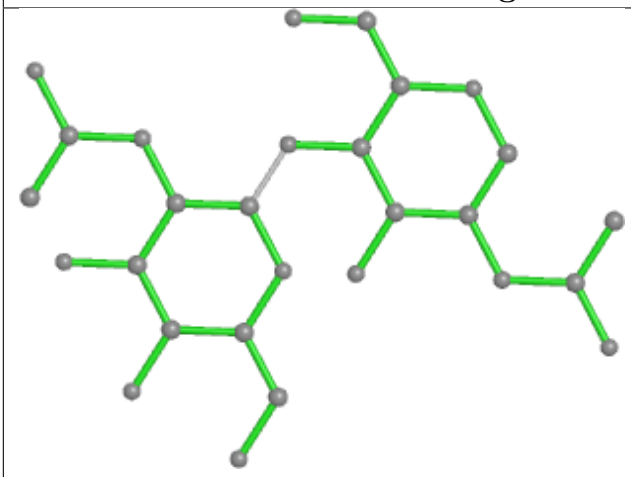
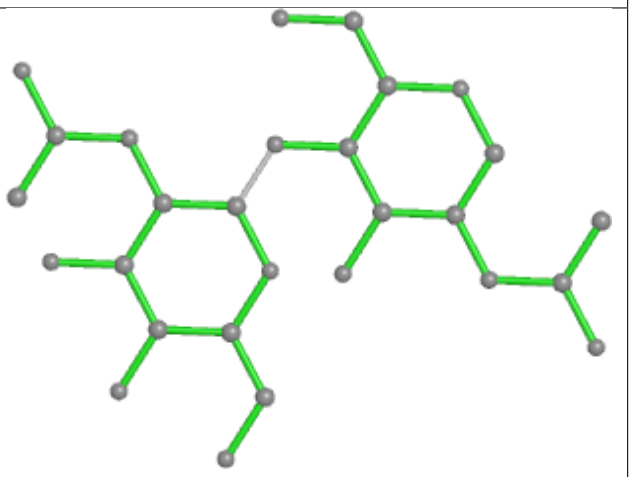


Rings

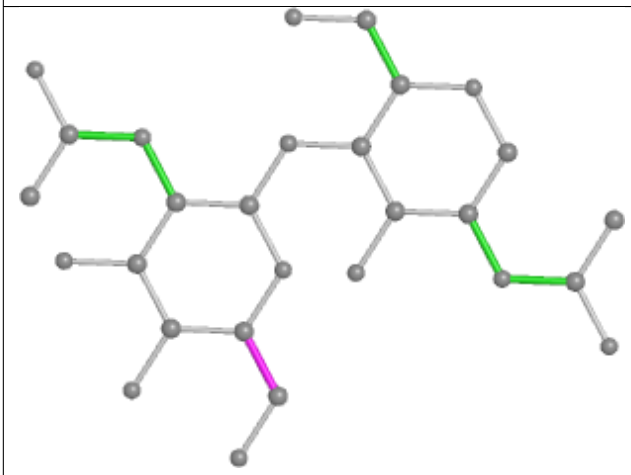
Oligosaccharide Chain 1



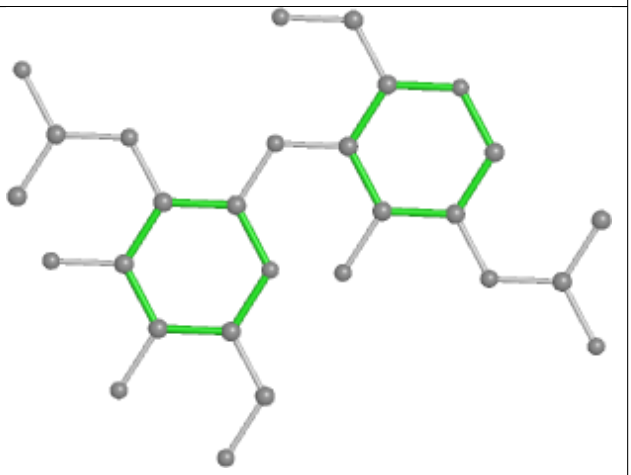
Bond lengths



Bond angles

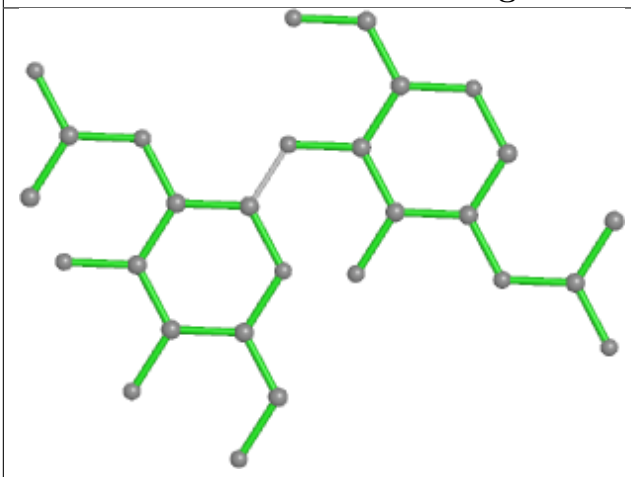


Torsions

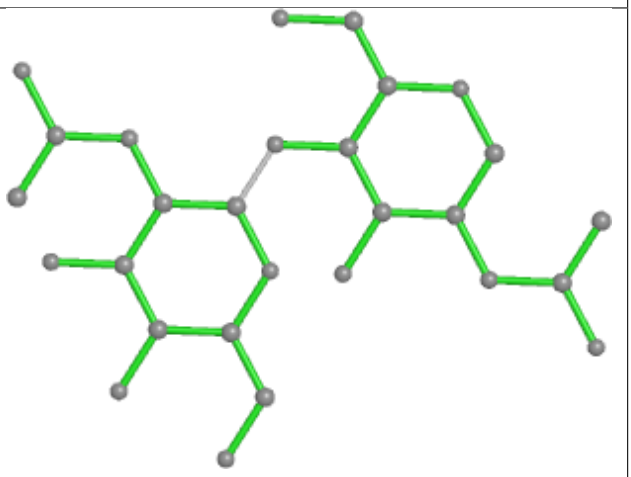


Rings

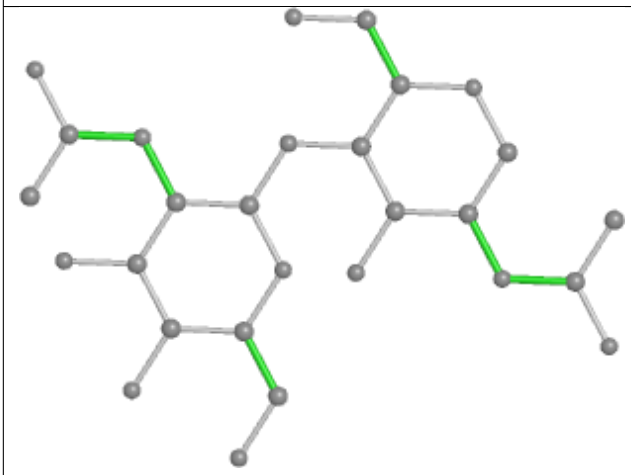
Oligosaccharide Chain 2



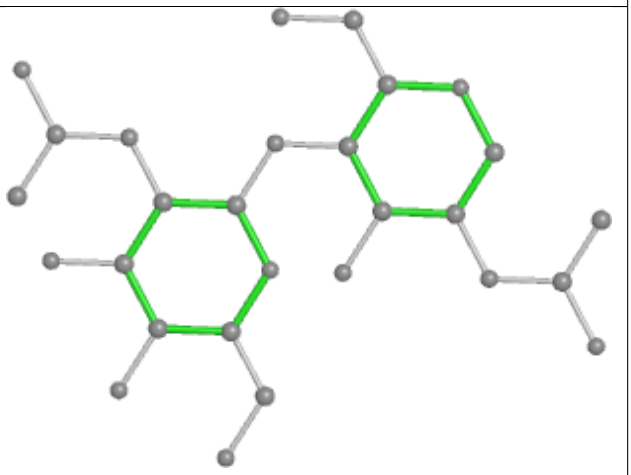
Bond lengths



Bond angles

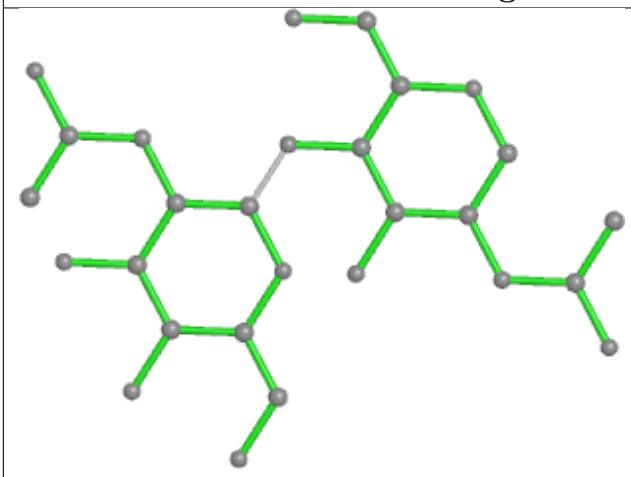


Torsions

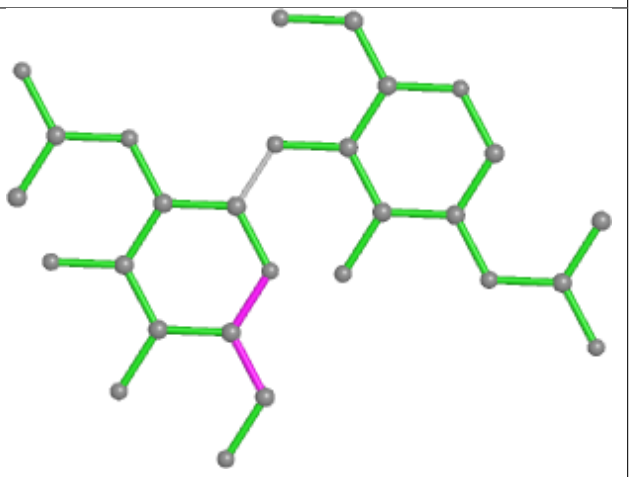


Rings

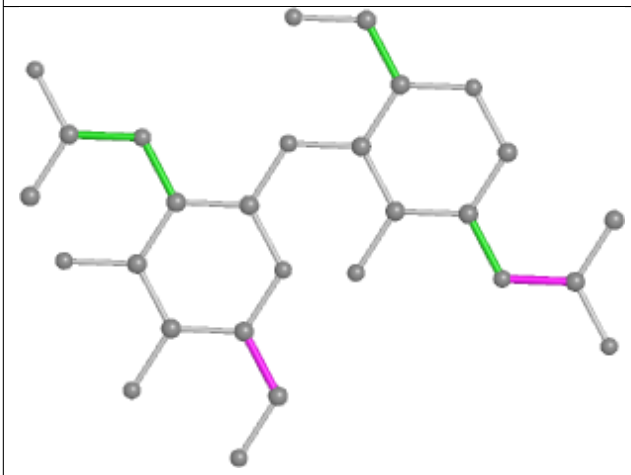
Oligosaccharide Chain 4



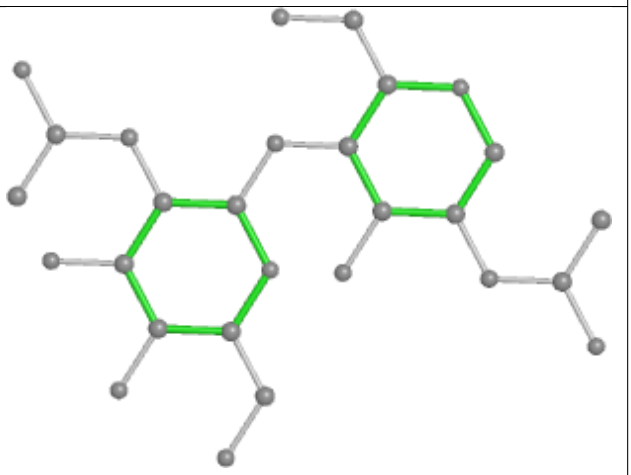
Bond lengths



Bond angles

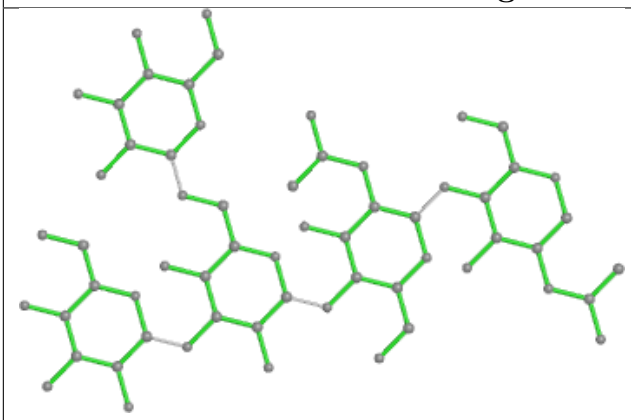


Torsions



Rings

Oligosaccharide Chain b



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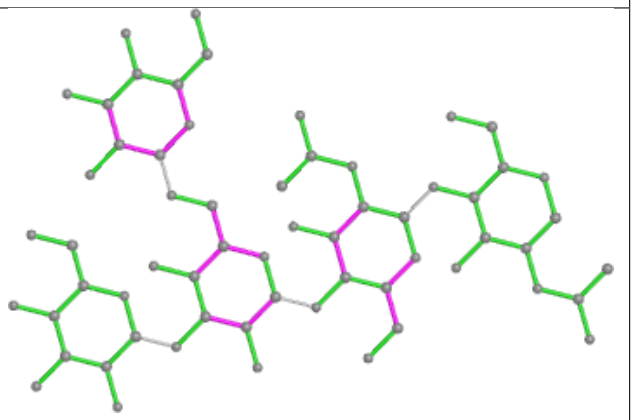
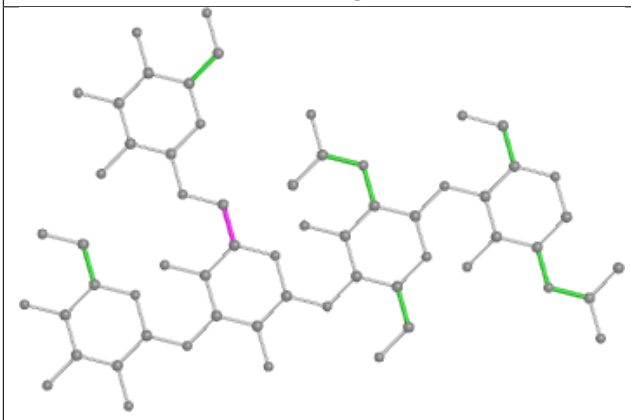
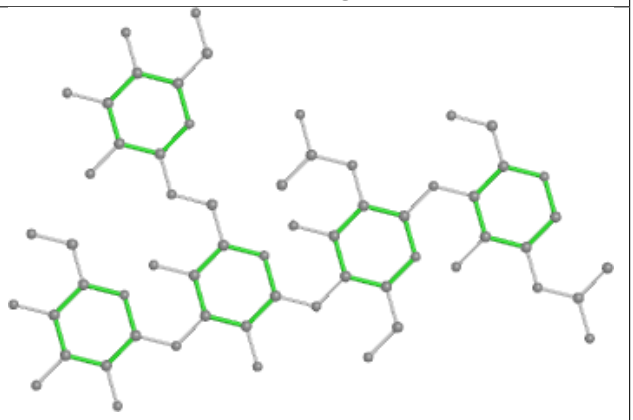


Bond angles

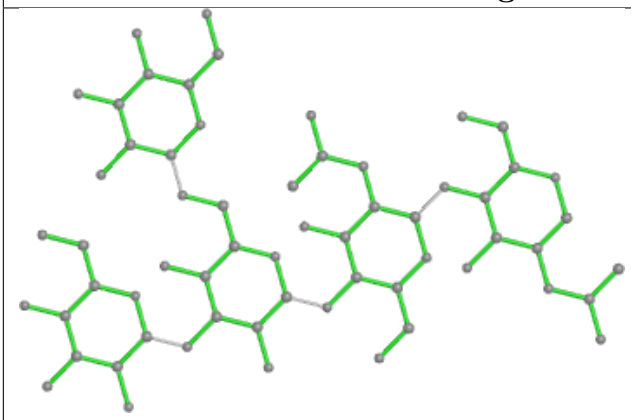


Torsions

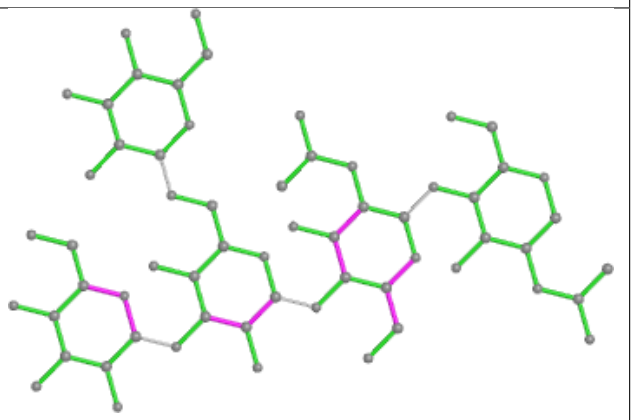


Rings

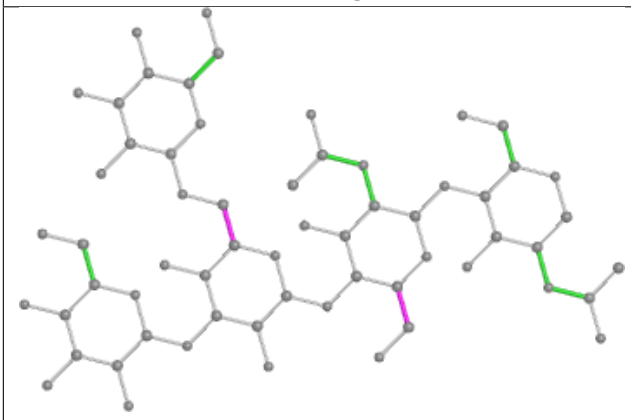
Oligosaccharide Chain h



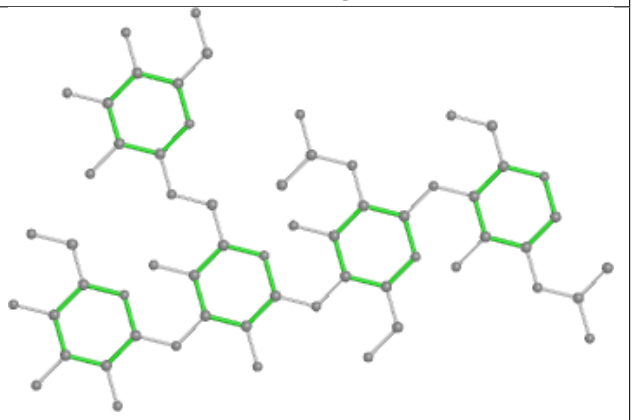
Bond lengths



Bond angles

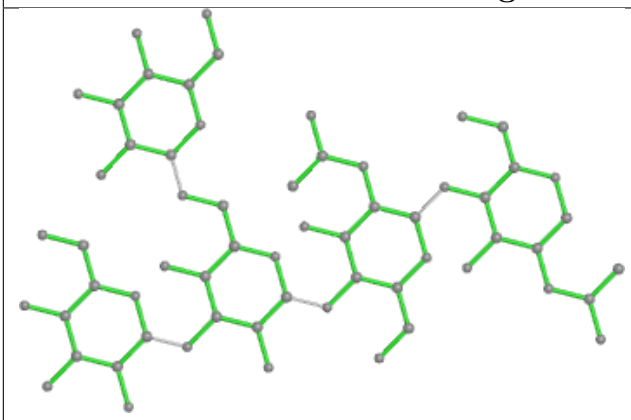


Torsions

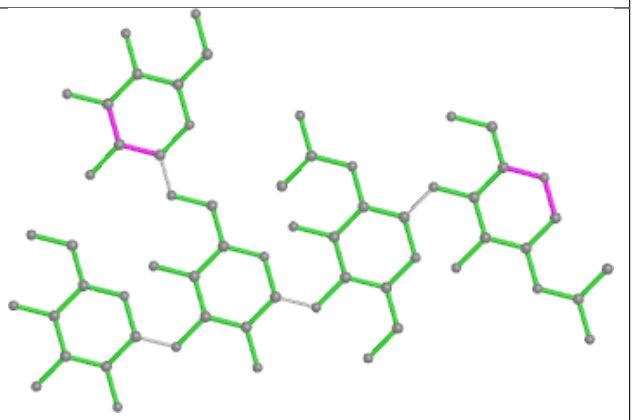


Rings

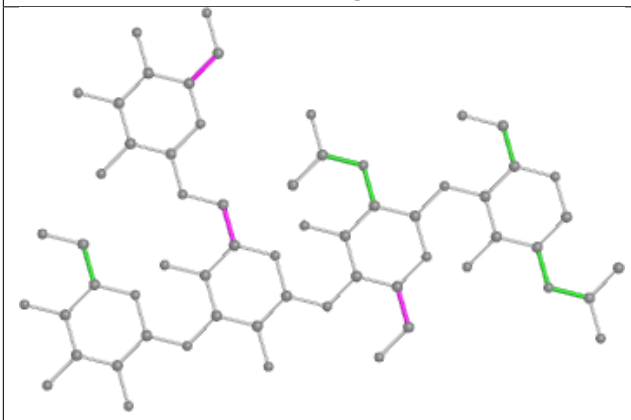
Oligosaccharide Chain k



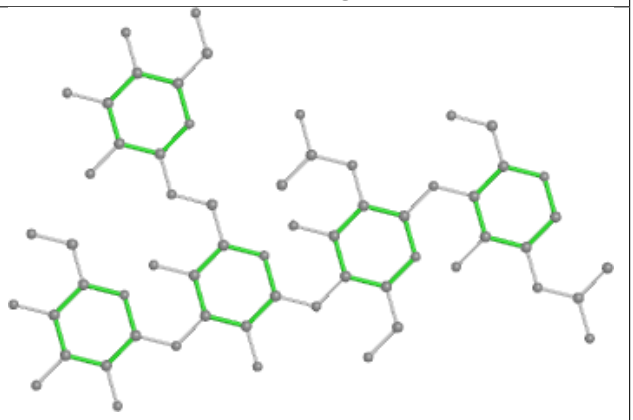
Bond lengths



Bond angles

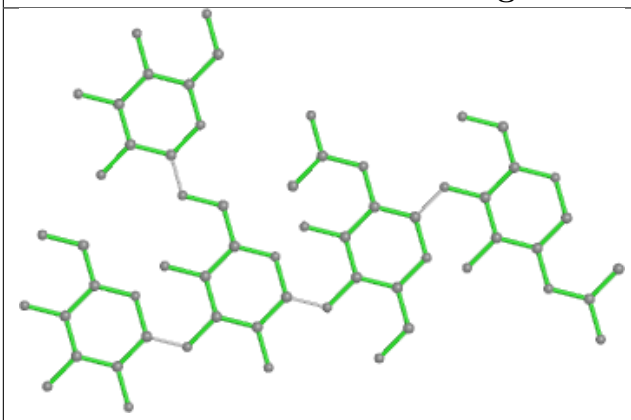


Torsions

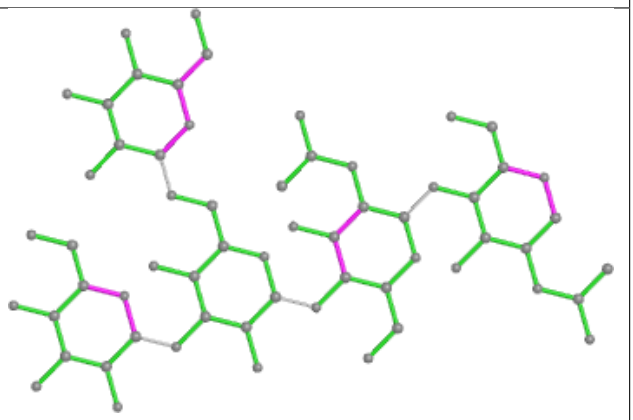


Rings

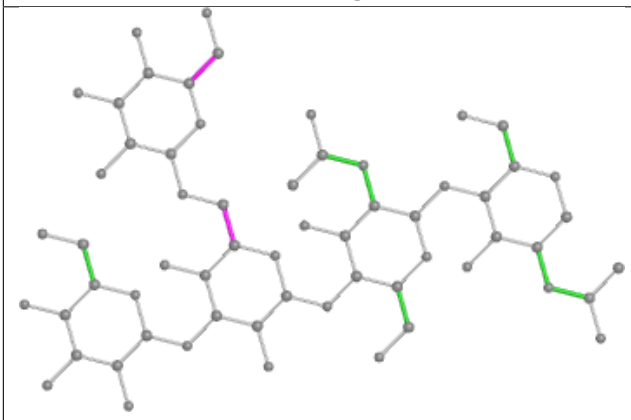
Oligosaccharide Chain n



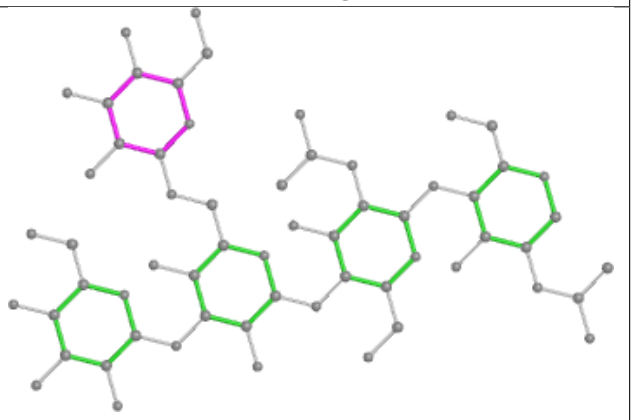
Bond lengths



Bond angles

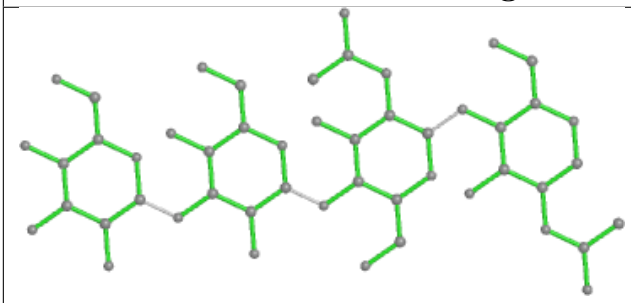


Torsions



Rings

Oligosaccharide Chain e



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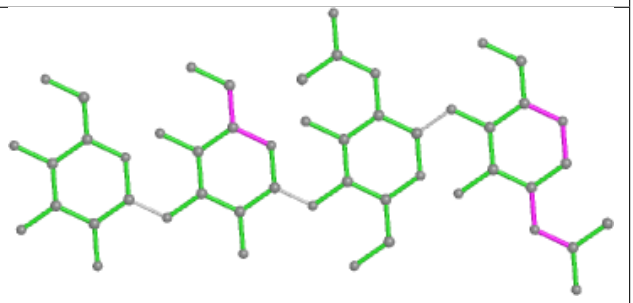
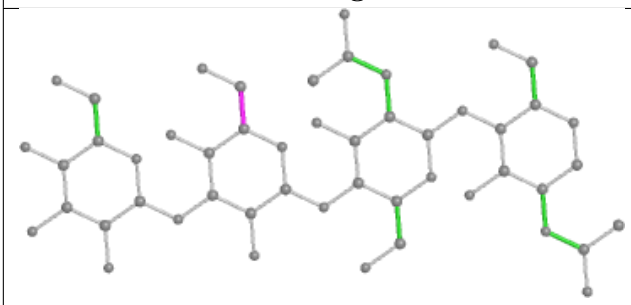
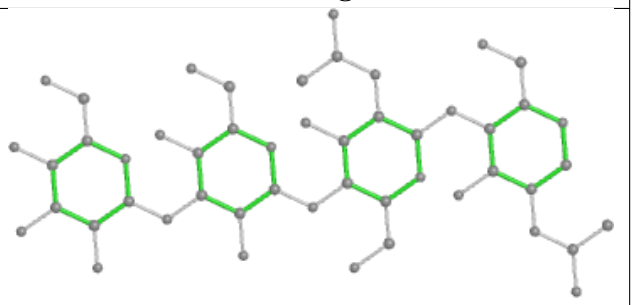


Bond angles

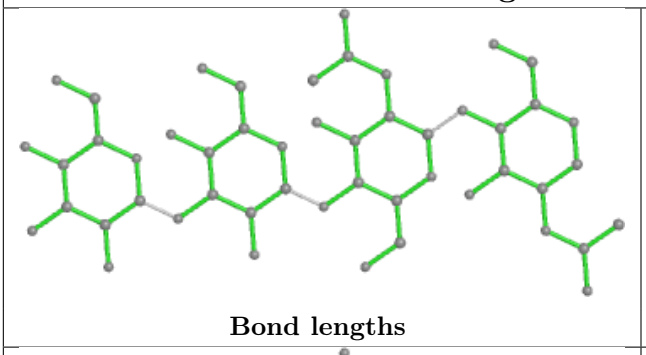


Torsions

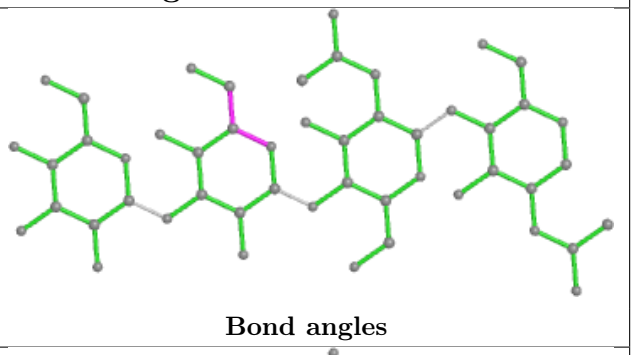


Rings

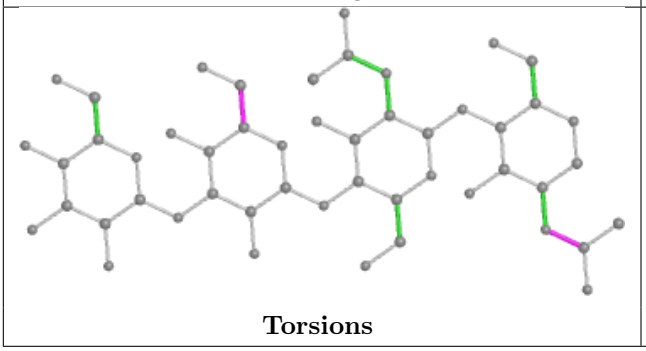
Oligosaccharide Chain g



Bond lengths



Bond angles



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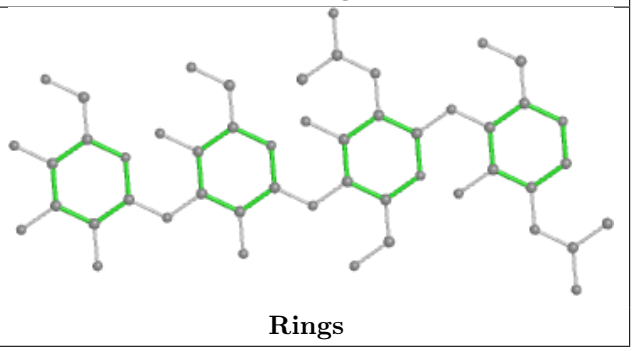
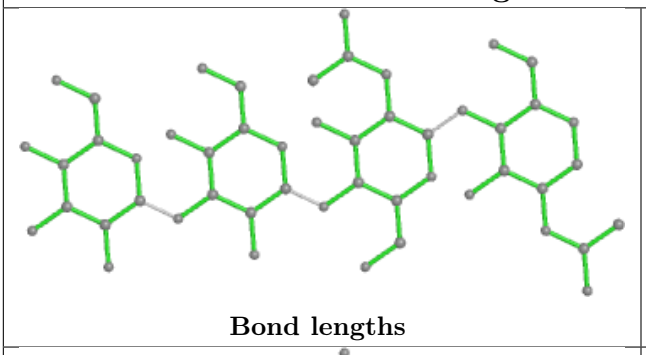
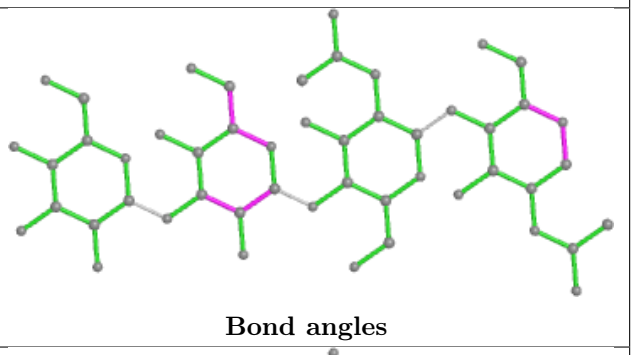


Rings

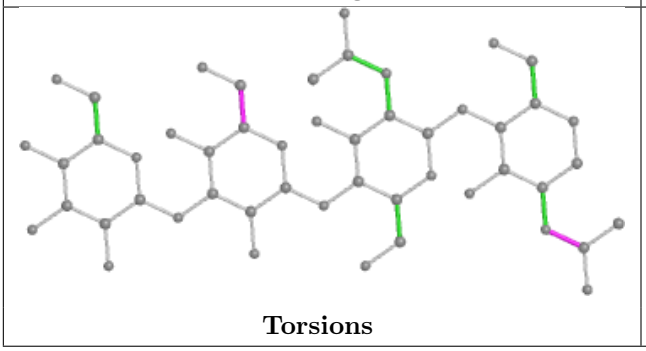
Oligosaccharide Chain m



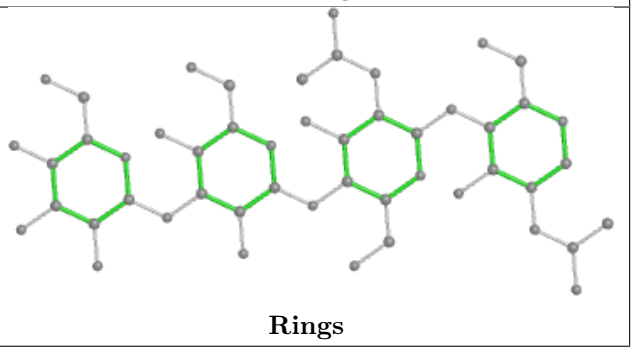
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

12 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	I	413	1	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
9	NAG	B	201	2	14,14,15	0.50	0	17,19,21	0.99	1 (5%)
9	NAG	G	411	1	14,14,15	0.51	0	17,19,21	0.81	1 (5%)
9	NAG	H	201	2	14,14,15	0.47	0	17,19,21	0.84	1 (5%)
9	NAG	K	413	1	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
9	NAG	J	201	2	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
9	NAG	F	201	2	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
9	NAG	D	201	2	14,14,15	0.54	0	17,19,21	0.78	0
9	NAG	G	403	1	14,14,15	0.47	0	17,19,21	0.74	1 (5%)
9	NAG	L	201	2	14,14,15	0.51	0	17,19,21	0.88	1 (5%)
9	NAG	C	419	1	14,14,15	0.48	0	17,19,21	0.86	1 (5%)
9	NAG	E	420	1	14,14,15	0.51	0	17,19,21	1.09	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	I	413	1	-	0/6/23/26	0/1/1/1
9	NAG	B	201	2	-	2/6/23/26	0/1/1/1
9	NAG	G	411	1	-	0/6/23/26	0/1/1/1
9	NAG	H	201	2	-	4/6/23/26	0/1/1/1
9	NAG	K	413	1	-	0/6/23/26	0/1/1/1
9	NAG	J	201	2	-	3/6/23/26	0/1/1/1
9	NAG	F	201	2	-	2/6/23/26	0/1/1/1
9	NAG	D	201	2	-	0/6/23/26	0/1/1/1
9	NAG	G	403	1	-	2/6/23/26	0/1/1/1
9	NAG	L	201	2	-	0/6/23/26	0/1/1/1
9	NAG	C	419	1	-	0/6/23/26	0/1/1/1
9	NAG	E	420	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	420	NAG	O5-C5-C6	2.94	111.81	107.20
9	B	201	NAG	C1-O5-C5	2.91	116.14	112.19
9	L	201	NAG	O5-C5-C6	2.41	110.99	107.20
9	K	413	NAG	O5-C5-C6	2.31	110.82	107.20
9	H	201	NAG	O5-C5-C6	2.29	110.80	107.20

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	403	NAG	C8-C7-N2-C2
9	G	403	NAG	O7-C7-N2-C2
9	H	201	NAG	C8-C7-N2-C2
9	B	201	NAG	C8-C7-N2-C2
9	H	201	NAG	O7-C7-N2-C2

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

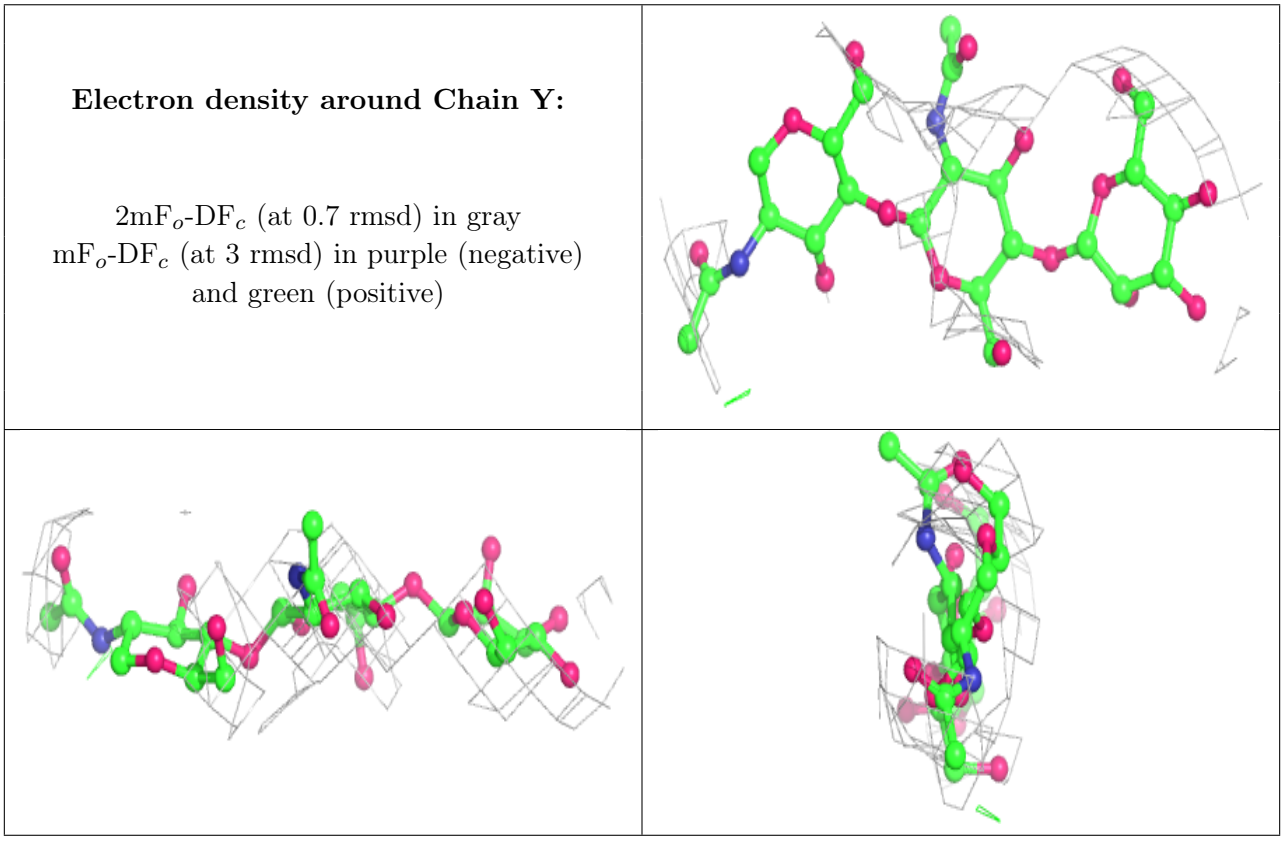
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

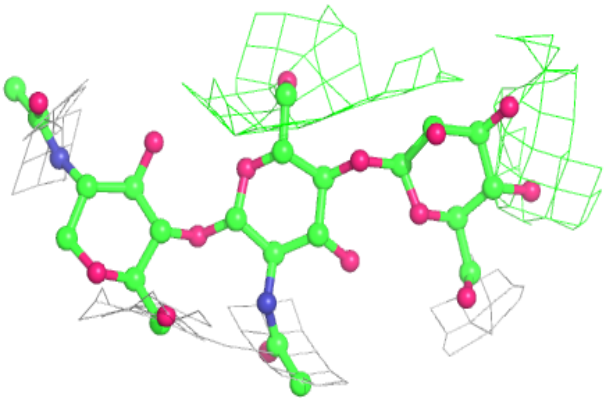
Unable to reproduce the depositors R factor - this section is therefore empty.

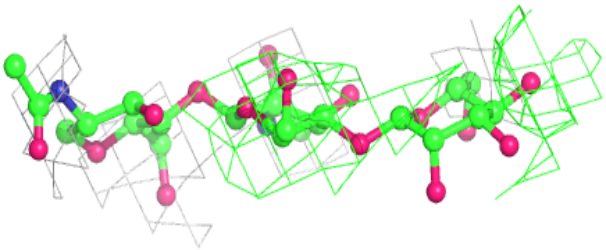
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

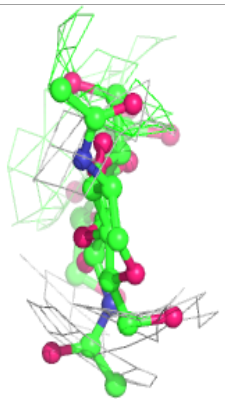


Electron density around Chain i:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

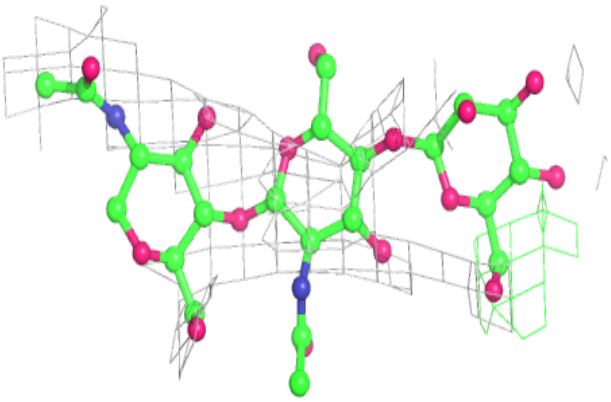


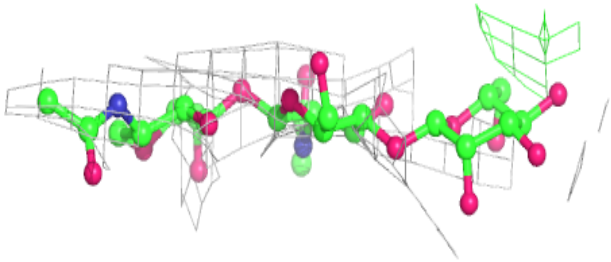


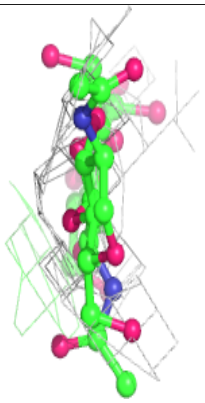


Electron density around Chain j:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

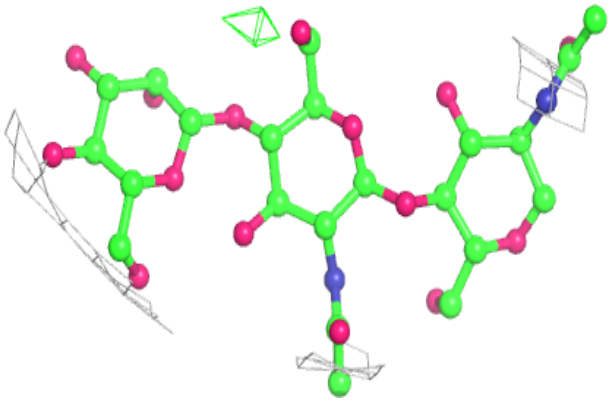


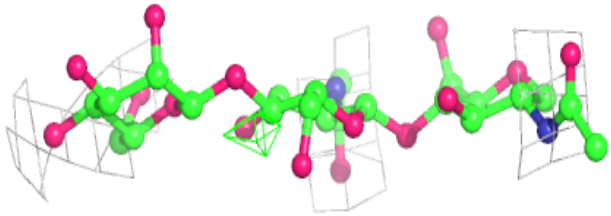


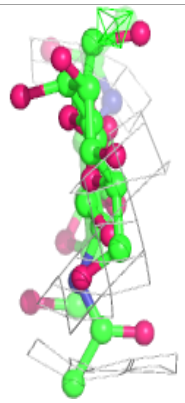


Electron density around Chain l:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

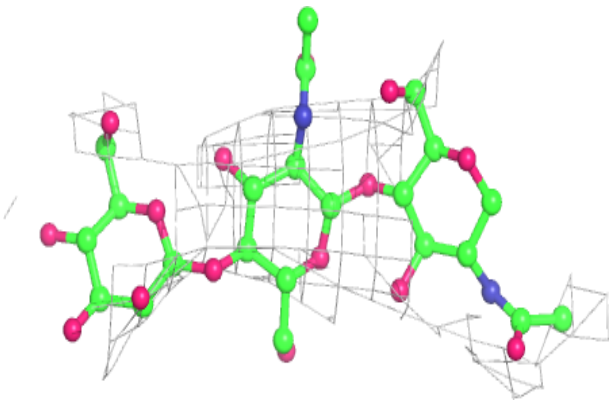


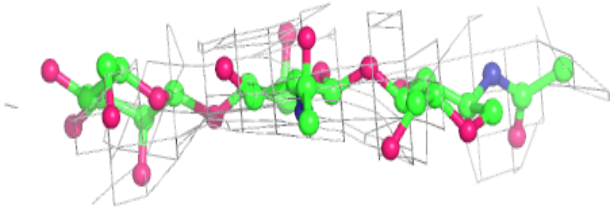


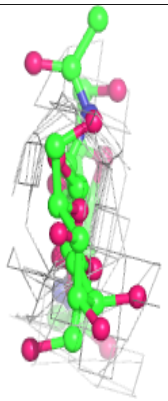


Electron density around Chain p:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

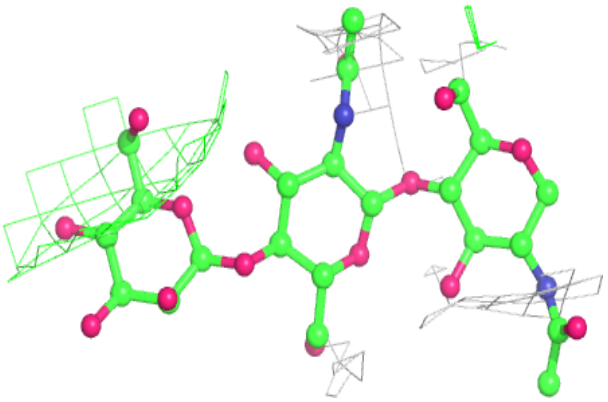


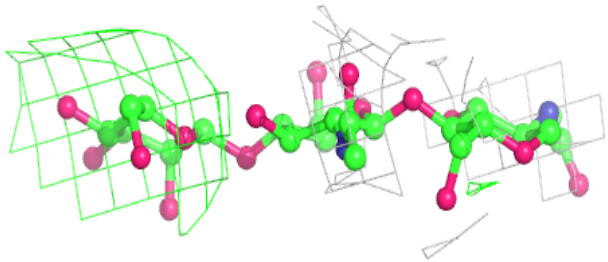


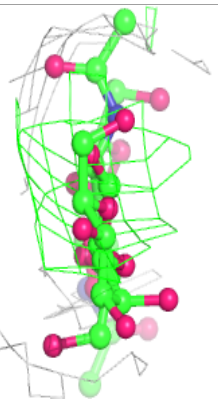


Electron density around Chain t:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

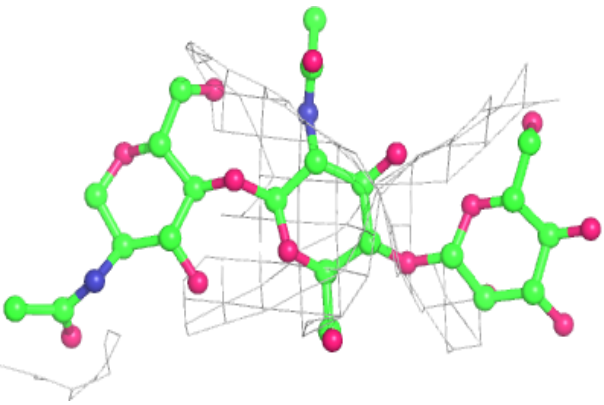


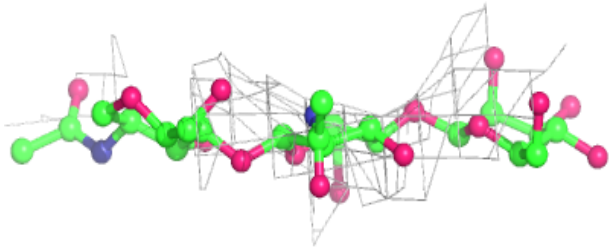


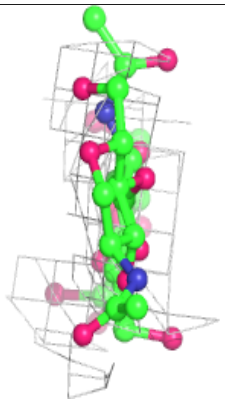


Electron density around Chain u:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

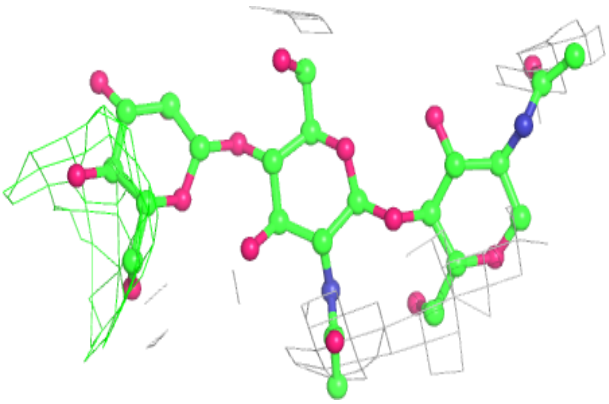


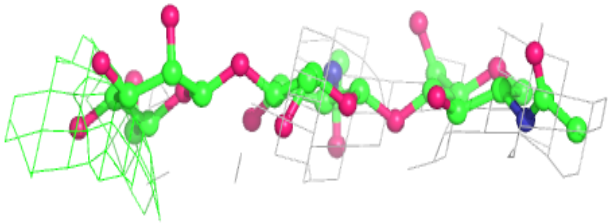


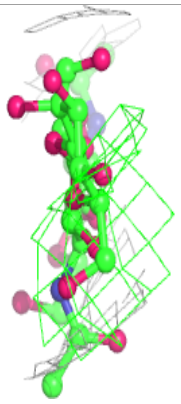


Electron density around Chain y:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

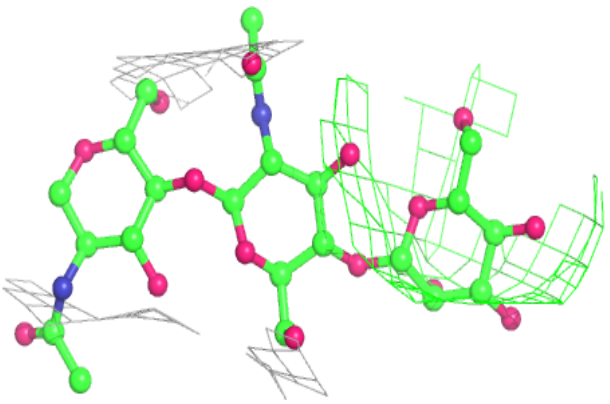


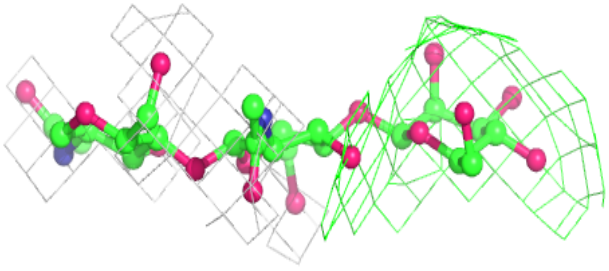


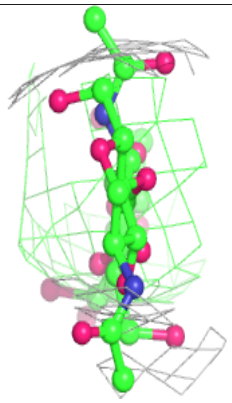


Electron density around Chain z:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

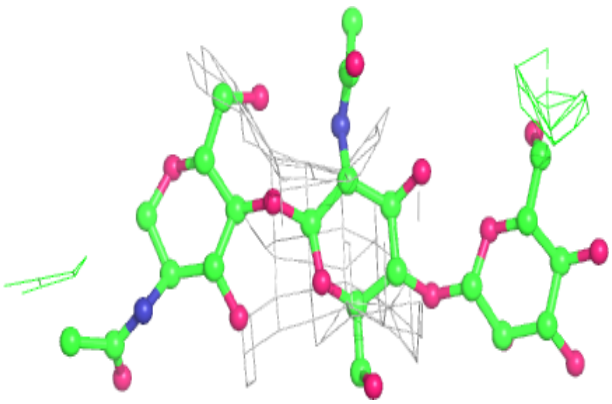


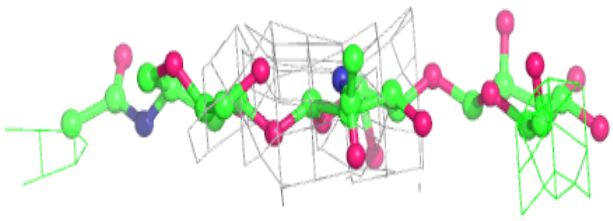


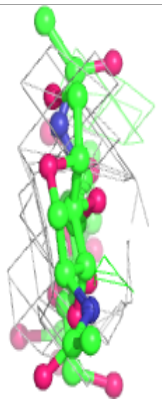


Electron density around Chain 0:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

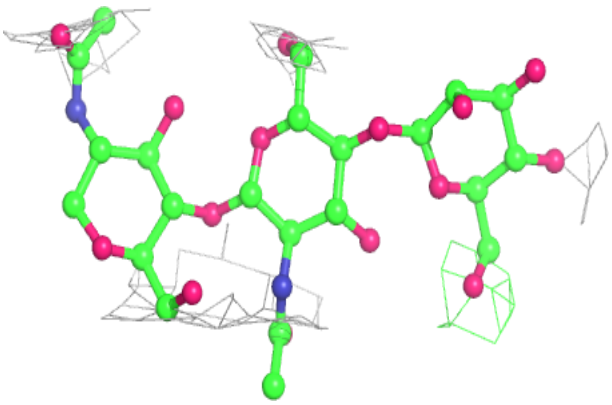


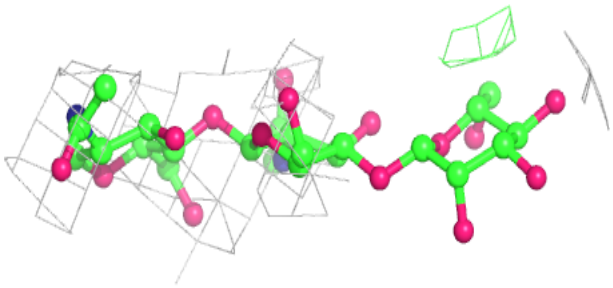


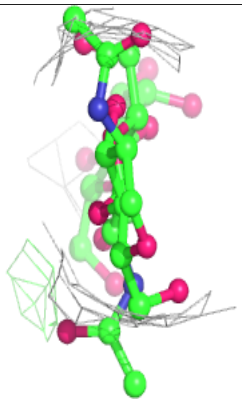


Electron density around Chain 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

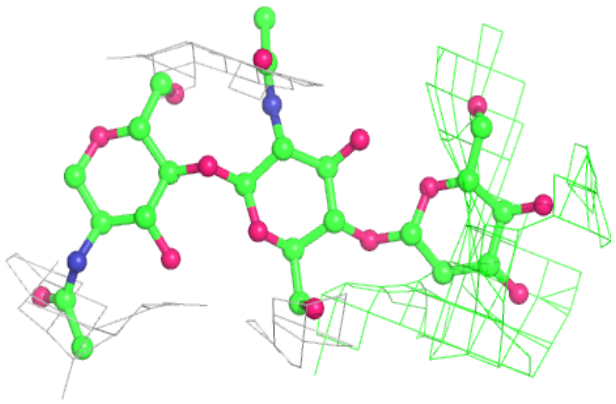


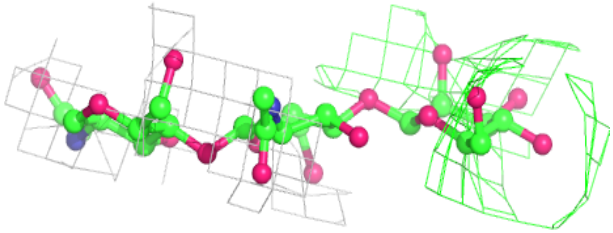


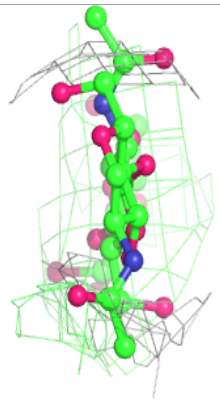


Electron density around Chain 5:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

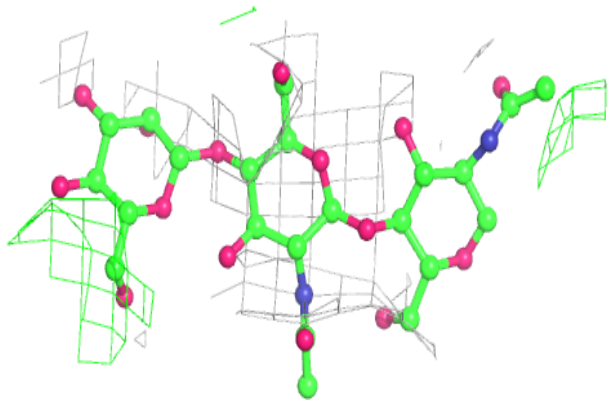


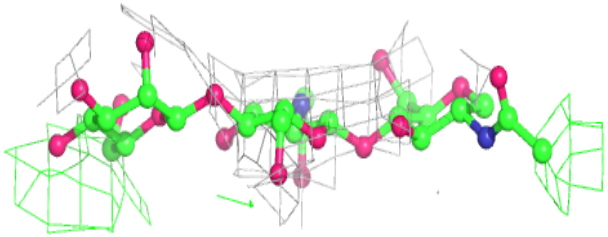


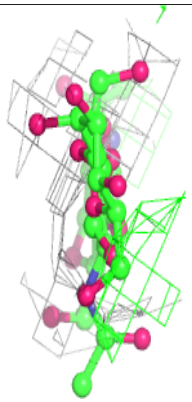


Electron density around Chain 6:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

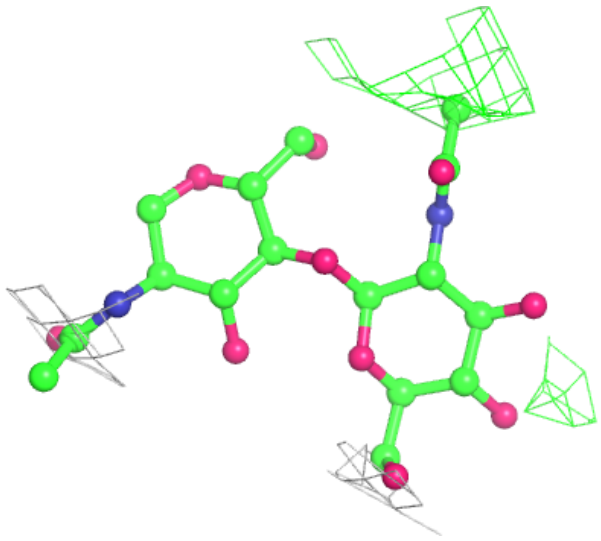


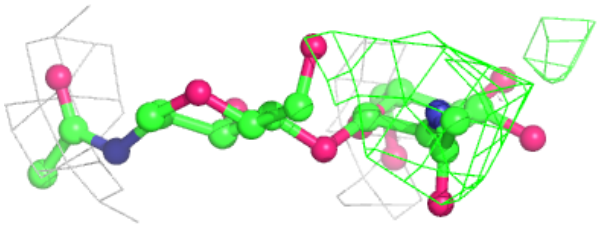


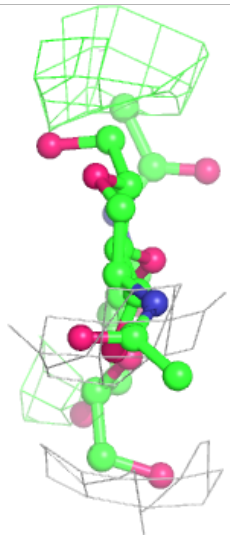


Electron density around Chain Z:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

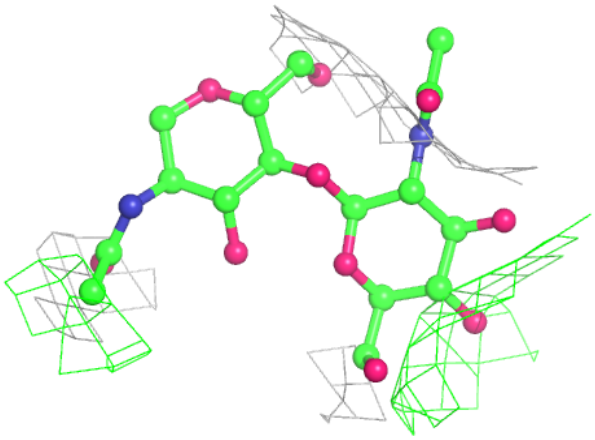


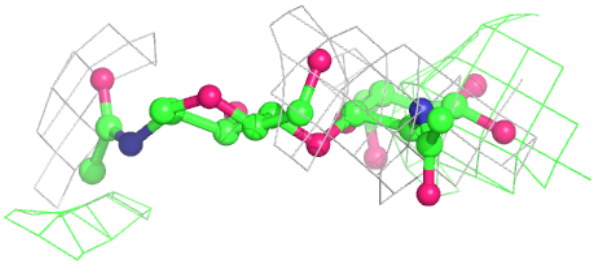


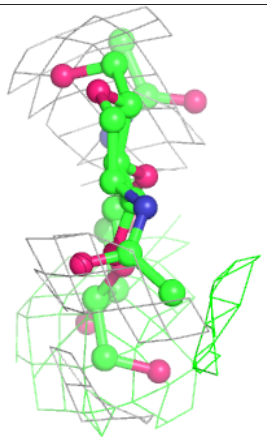


Electron density around Chain a:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

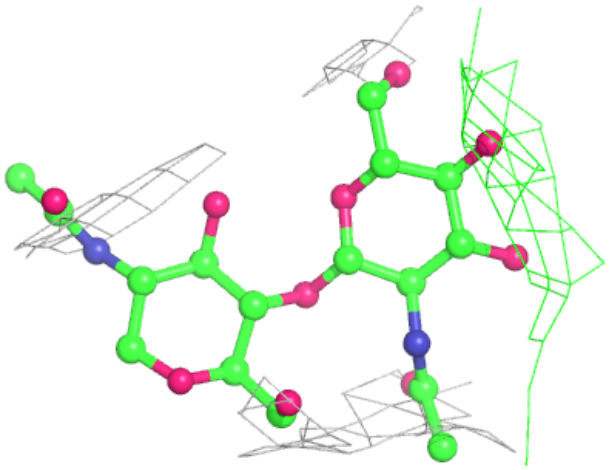


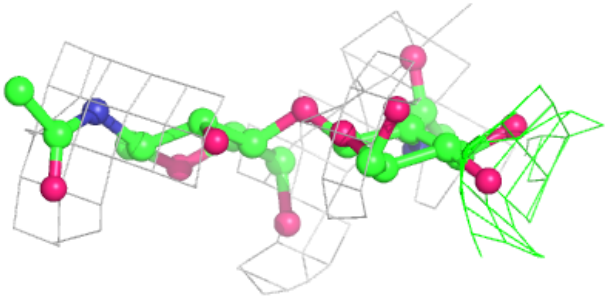


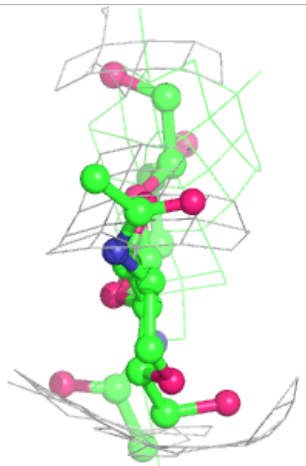


Electron density around Chain c:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

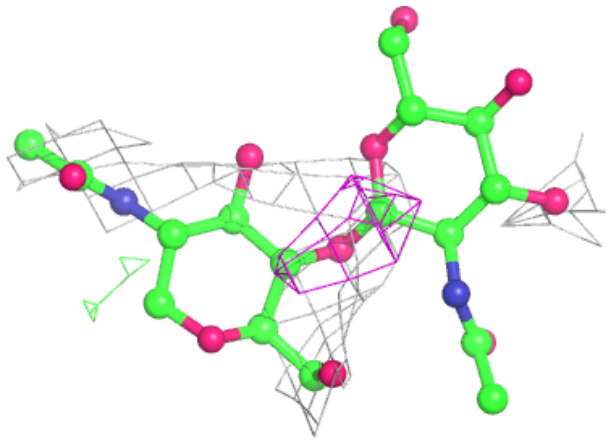


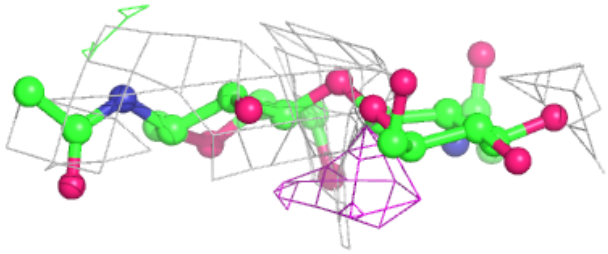


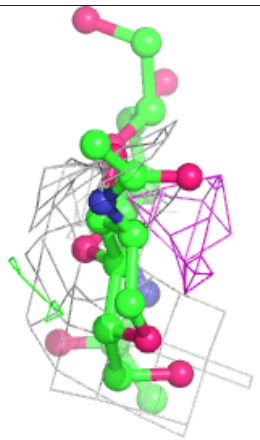


Electron density around Chain d:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

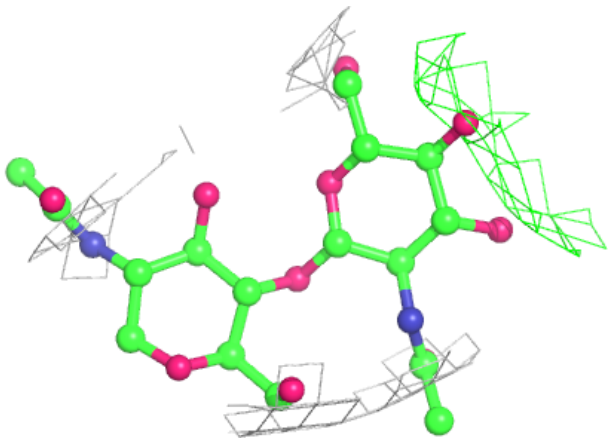


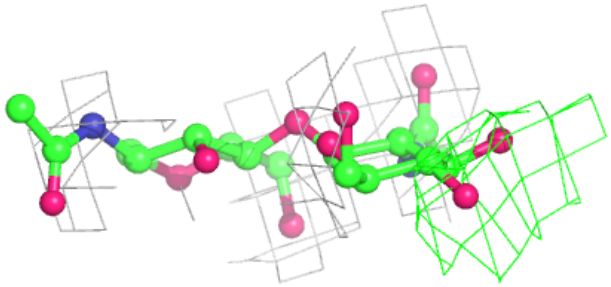


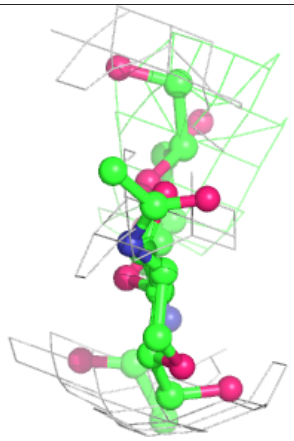


Electron density around Chain f:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

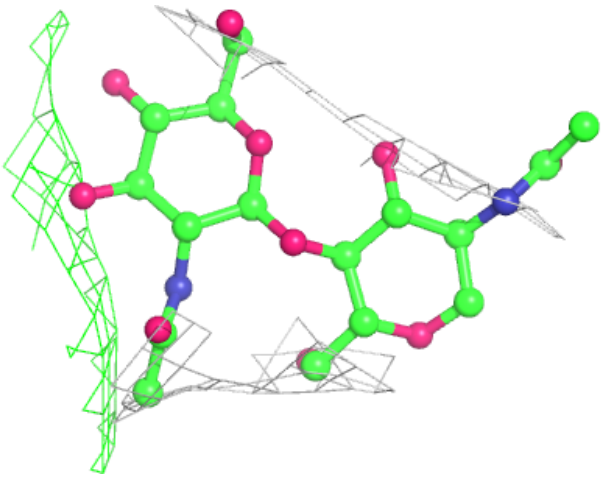


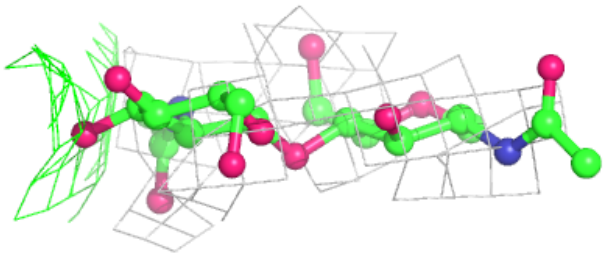


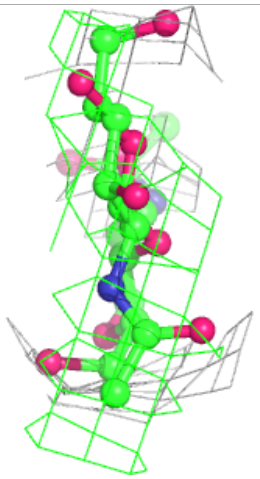


Electron density around Chain o:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

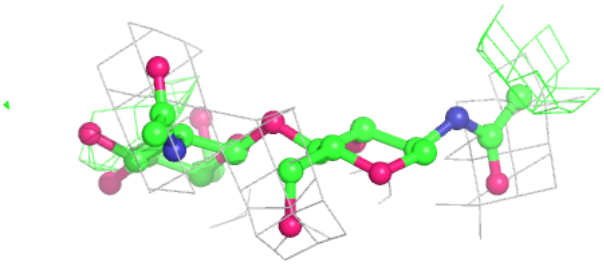


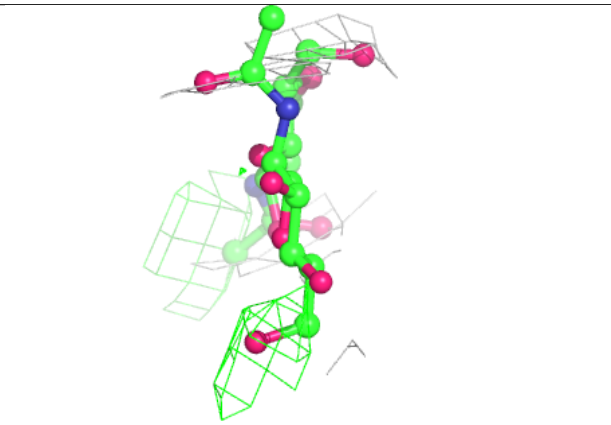




Electron density around Chain q:

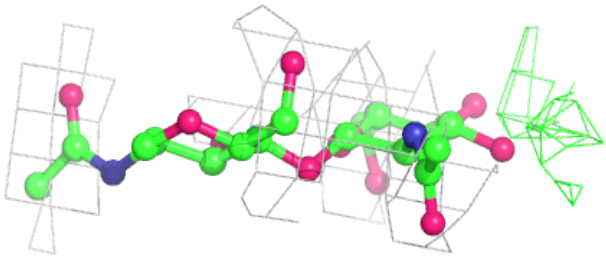
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

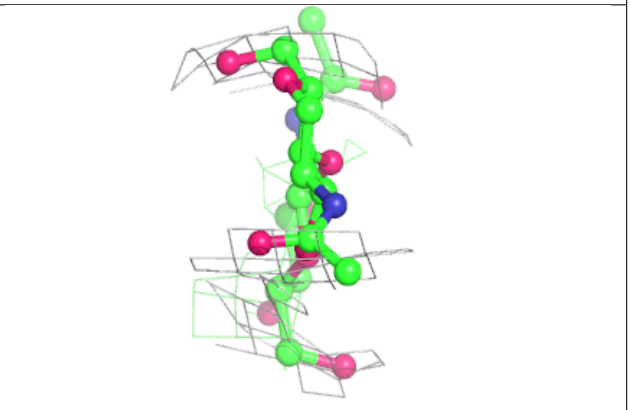




Electron density around Chain r:

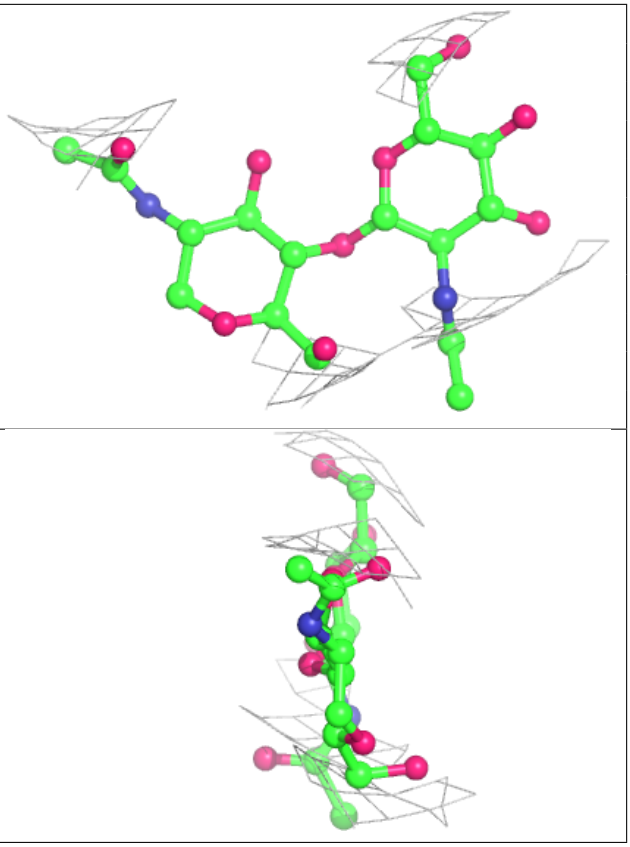
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





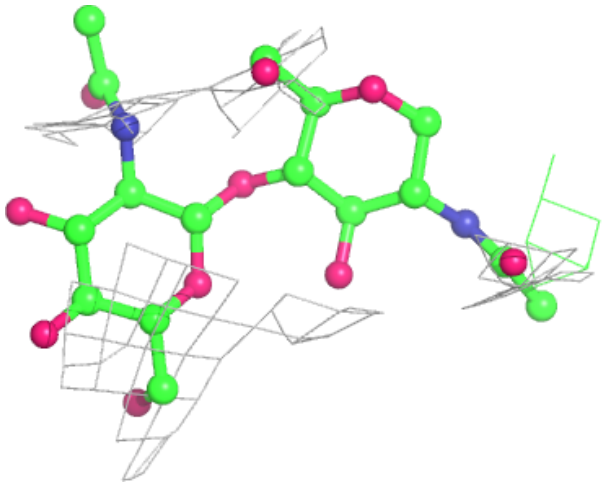
Electron density around Chain s:

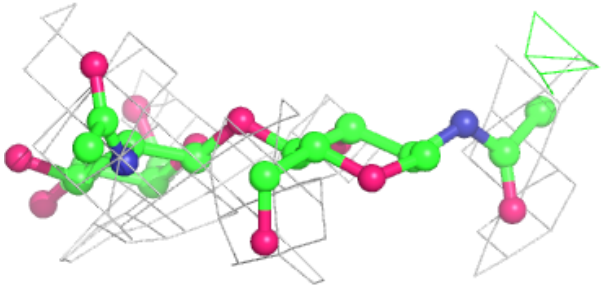
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

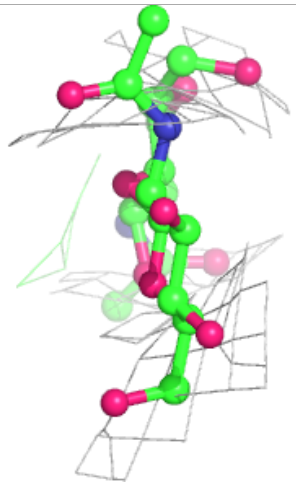


Electron density around Chain v:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

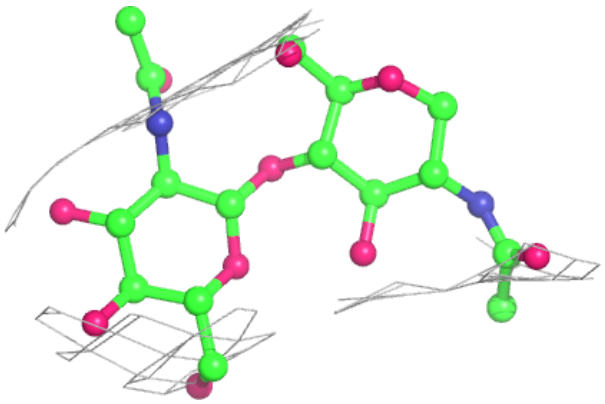


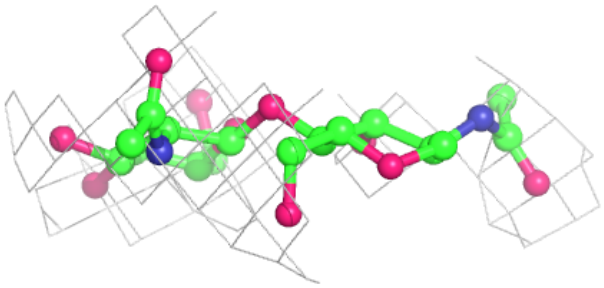


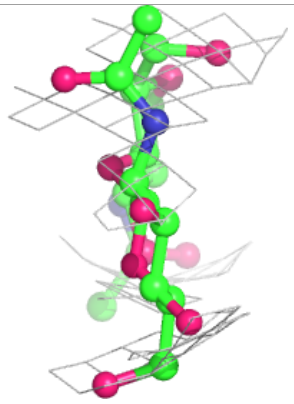


Electron density around Chain w:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

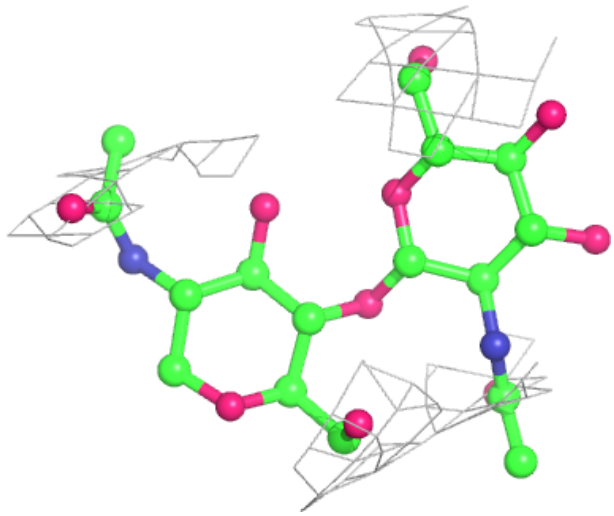


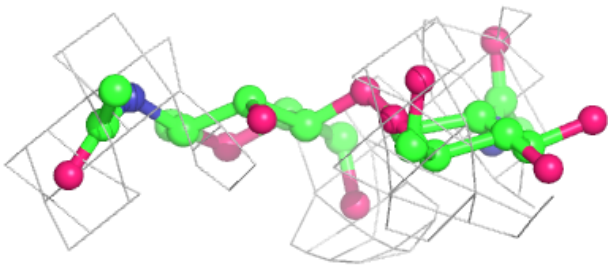


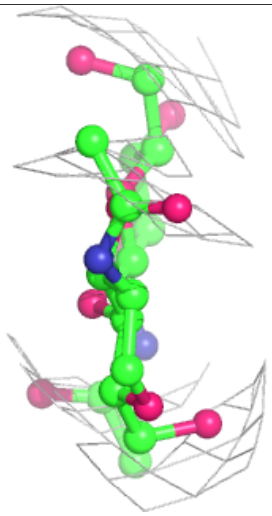


Electron density around Chain x:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

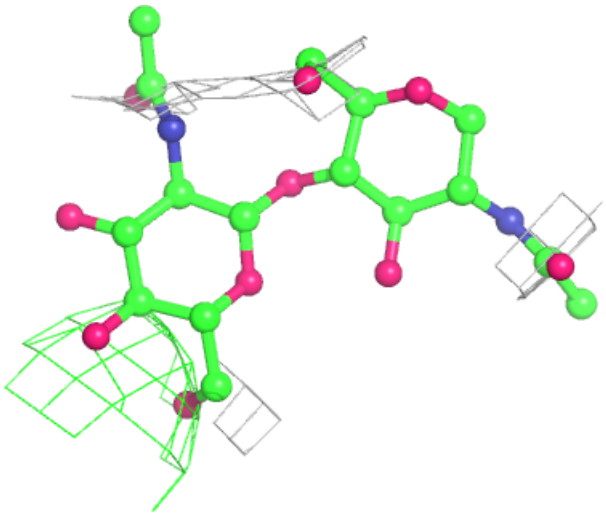


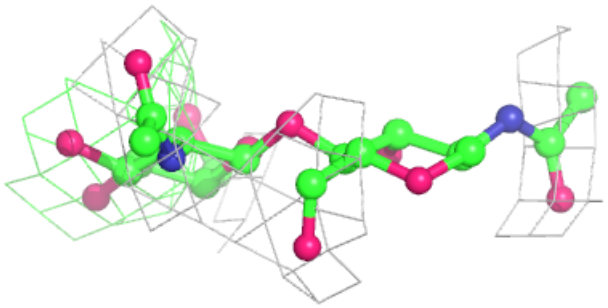


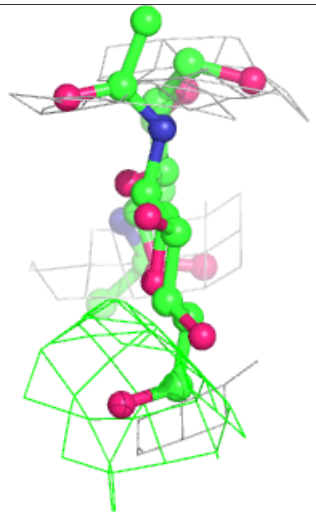


Electron density around Chain 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

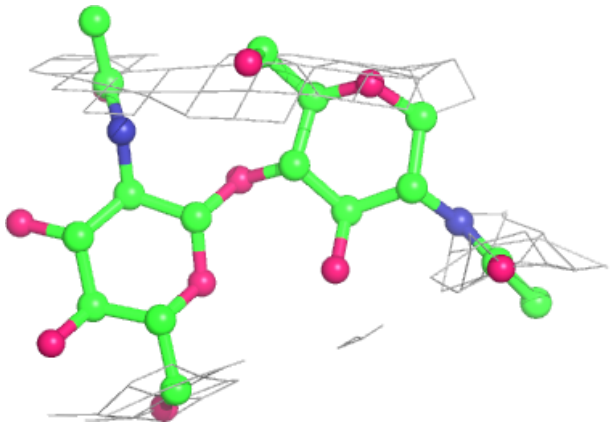


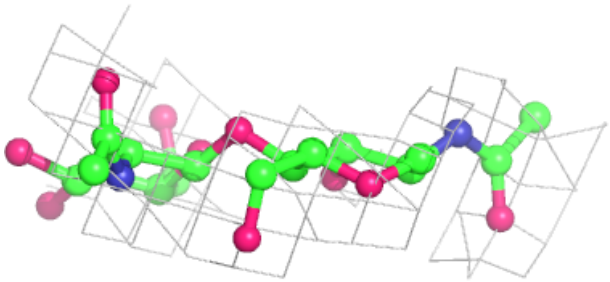


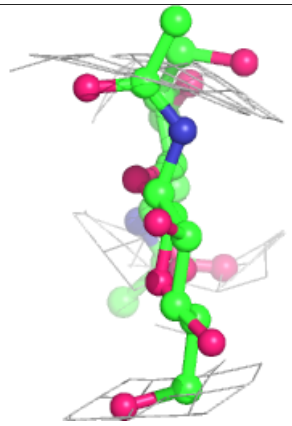


Electron density around Chain 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

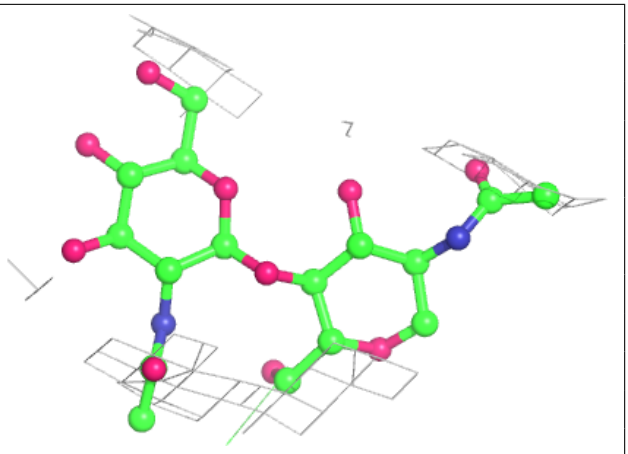


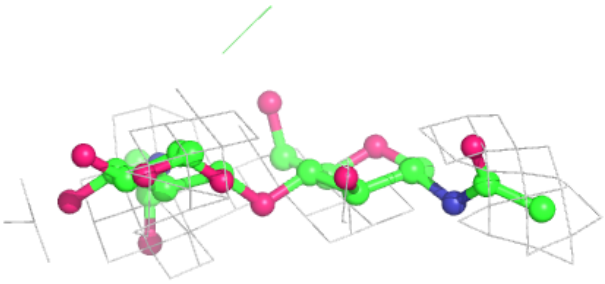


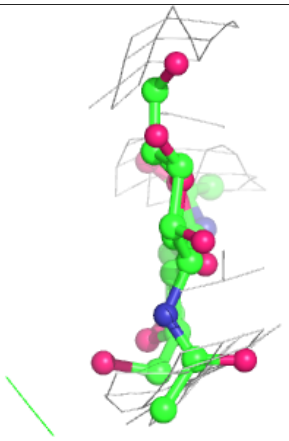


Electron density around Chain 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

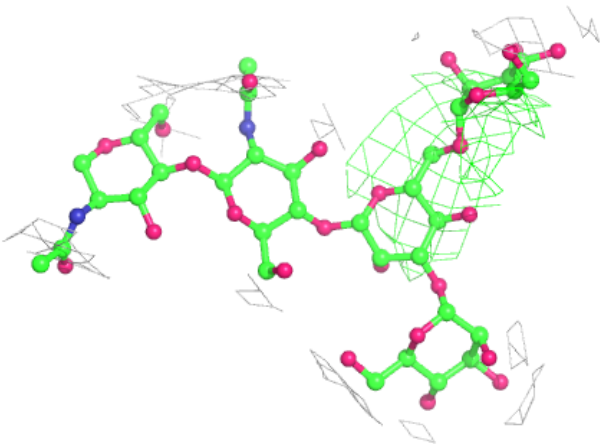


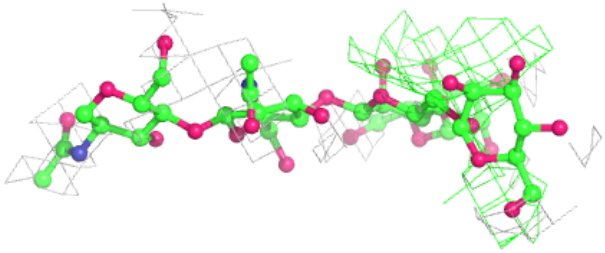


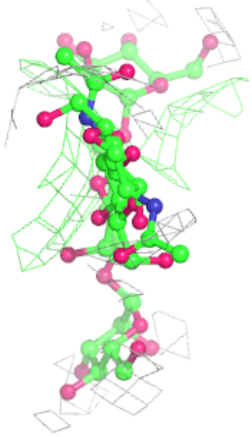


Electron density around Chain b:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

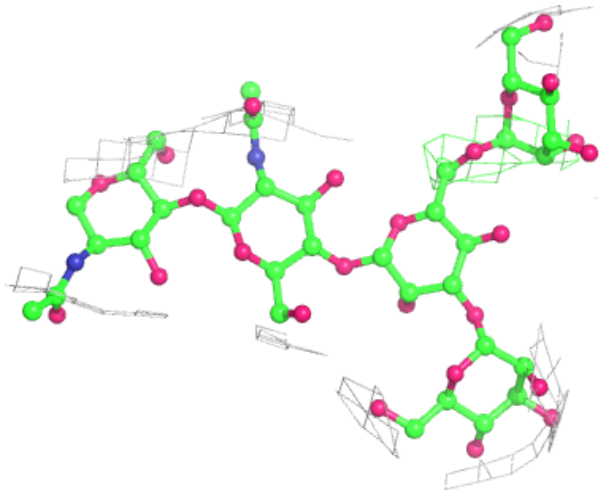


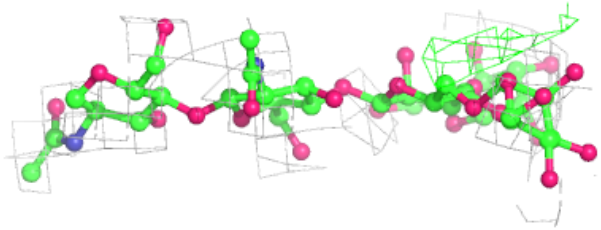


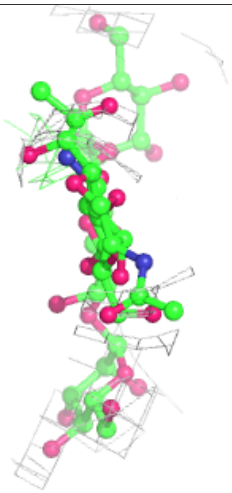


Electron density around Chain h:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

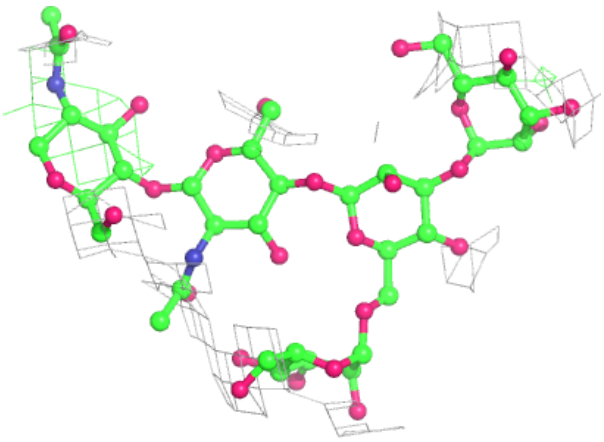


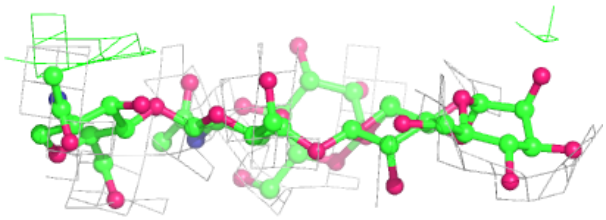


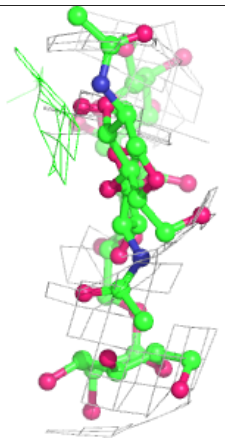


Electron density around Chain k:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

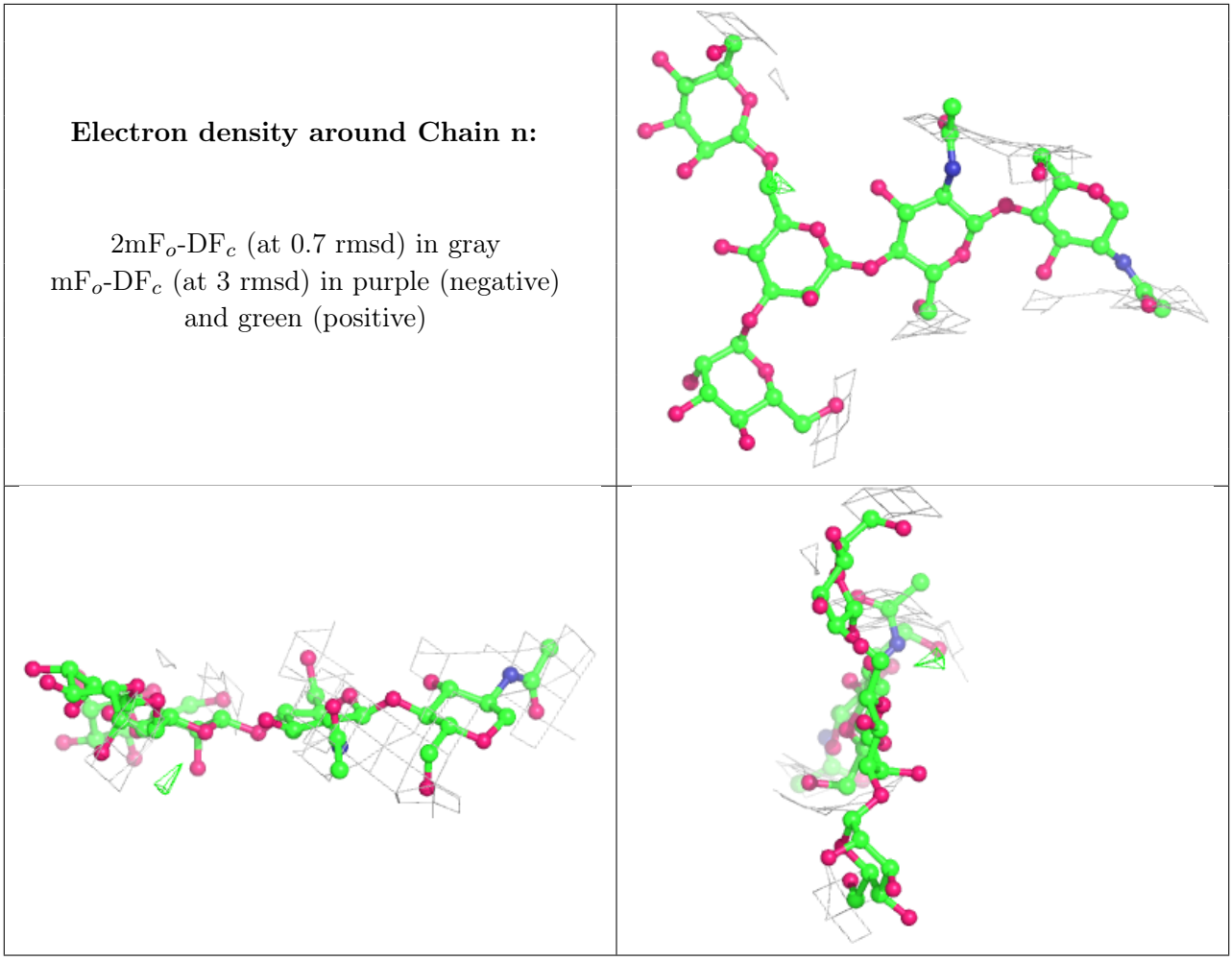






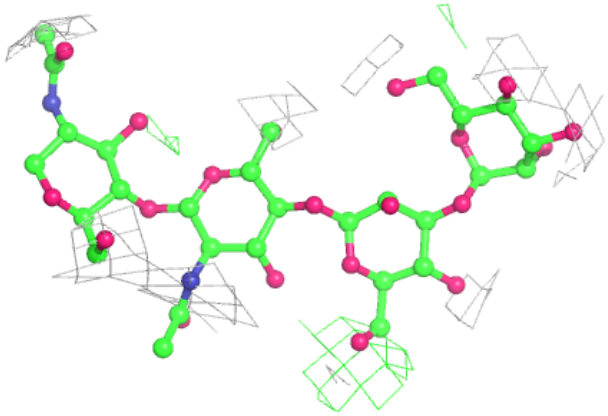
Electron density around Chain n:

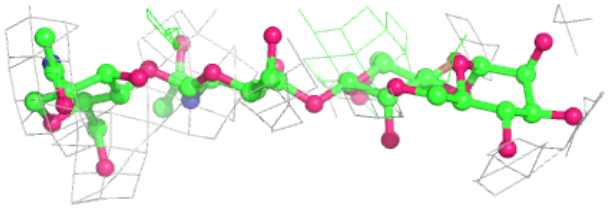
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

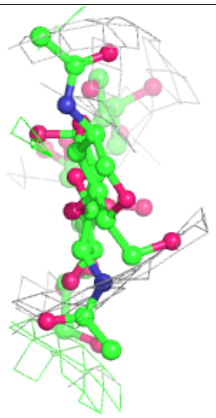


Electron density around Chain e:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

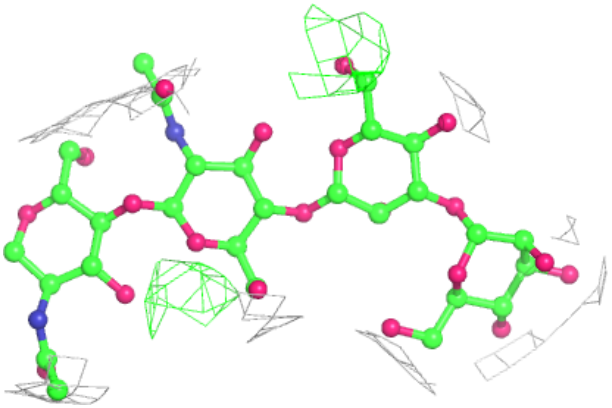


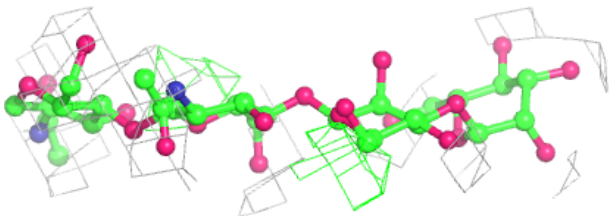


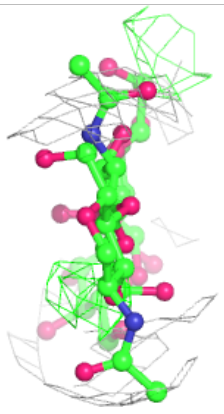


Electron density around Chain g:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

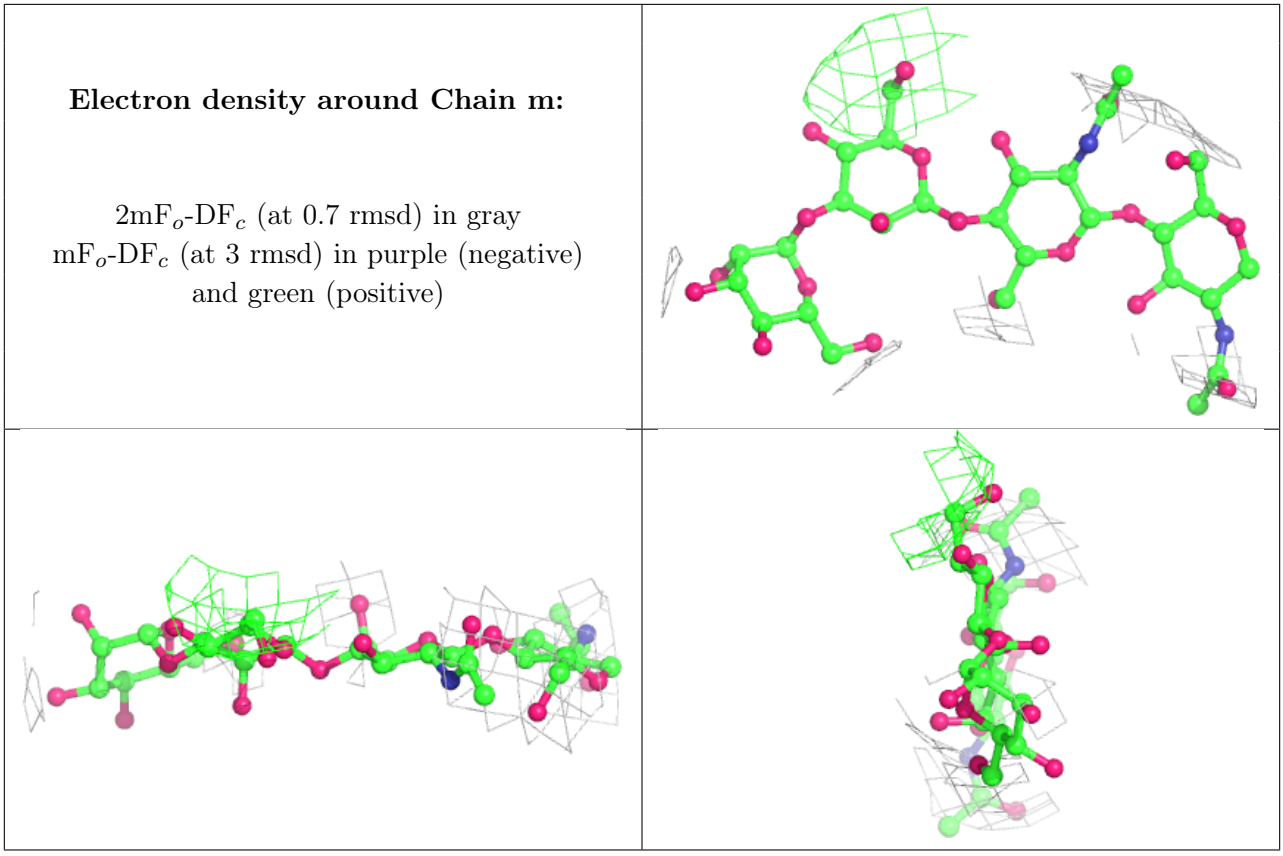






Electron density around Chain m:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.