Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2023 – 03:42 AM EDT

PDB ID	:	1BOS
Title	:	SHIGA-LIKE TOXIN COMPLEXED WITH ITS RECEPTOR
Authors	:	Ling, H.; Boodhoo, A.; Hazes, B.; Cummings, M.D.; Armstrong, G.D.; Brunton, J.L.; Read, R.J.
Deposited on	:	1998-01-13
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

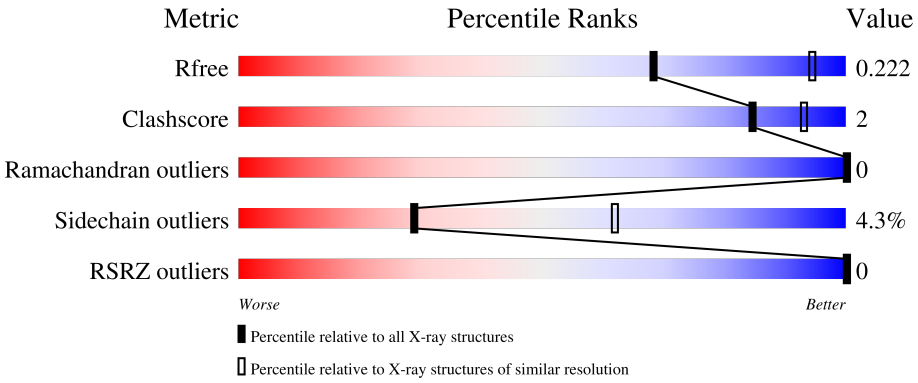
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	69	90% 9% •
1	B	69	90% 9% •
1	C	69	87% 10% •
1	D	69	91% 6% ••
1	E	69	90% 7% •

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Mol	Chain	Length	Quality of chain
1	F	69	88% 9%
1	G	69	90% 7%
1	H	69	87% 10%
1	I	69	90% 9%
1	J	69	88% 10%
1	K	69	90% 7%
1	L	69	91% 7%
1	M	69	91% 6%
1	N	69	88% 10%
1	O	69	87% 9%
1	P	69	90% 9%
1	Q	69	93% 6%
1	R	69	90% 9%
1	S	69	90% 7%
1	T	69	90% 9%
2	0	3	67% 33%
2	2	3	100%
2	4	3	100%
2	5	3	100%
2	7	3	100%
2	8	3	100%
2	9	3	33% 67%
2	AA	3	33% 33% 33%
2	BA	3	100%
2	CA	3	100%

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Mol	Chain	Length	Quality of chain
2	EA	3	67% 33%
2	FA	3	100%
2	U	3	100%
2	W	3	33% 33% 33%
2	X	3	100%
2	a	3	100%
2	c	3	100%
2	e	3	67% 33%
2	f	3	100%
2	g	3	100%
2	h	3	100%
2	i	3	100%
2	j	3	33% 67%
2	k	3	67% 33%
2	m	3	67% 33%
2	o	3	67% 33%
2	p	3	100%
2	r	3	67% 33%
2	s	3	100%
2	t	3	67% 33%
2	v	3	100%
2	x	3	100%
2	z	3	67% 33%
3	1	2	100%
3	3	2	100%

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Mol	Chain	Length	Quality of chain
3	6	2	100%
3	DA	2	50% 50%
3	GA	2	100%
3	V	2	50% 50%
3	Y	2	50% 50%
3	Z	2	50% 50%
3	b	2	50% 50%
3	d	2	50% 50%
3	l	2	100%
3	n	2	100%
3	q	2	100%
3	u	2	100%
3	w	2	100%
3	y	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GAL	C	1370	-	-	-	X
4	GAL	E	1570	-	-	-	X
4	GAL	G	2270	-	-	-	X
4	GAL	J	2570	-	-	-	X
4	GAL	K	3170	-	-	-	X
4	GAL	N	3470	-	-	-	X
4	GAL	R	4370	-	-	-	X
4	GAL	T	4570	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12767 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 SHIGA-LIKE TOXIN I B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	F	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	G	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	H	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	I	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	J	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	K	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	L	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	M	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	N	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	O	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	P	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

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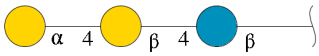
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	R	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	S	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	T	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	U	3	Total	C	O	0	0	0
			34	18	16			
2	W	3	Total	C	O	0	0	0
			34	18	16			
2	X	3	Total	C	O	0	0	0
			34	18	16			
2	a	3	Total	C	O	0	0	0
			34	18	16			
2	c	3	Total	C	O	0	0	0
			34	18	16			
2	e	3	Total	C	O	0	0	0
			34	18	16			
2	f	3	Total	C	O	0	0	0
			34	18	16			
2	g	3	Total	C	O	11	0	0
			34	18	16			
2	h	3	Total	C	O	0	0	0
			34	18	16			
2	i	3	Total	C	O	11	0	0
			34	18	16			
2	j	3	Total	C	O	0	0	0
			34	18	16			
2	k	3	Total	C	O	0	0	0
			34	18	16			
2	m	3	Total	C	O	0	0	0
			34	18	16			

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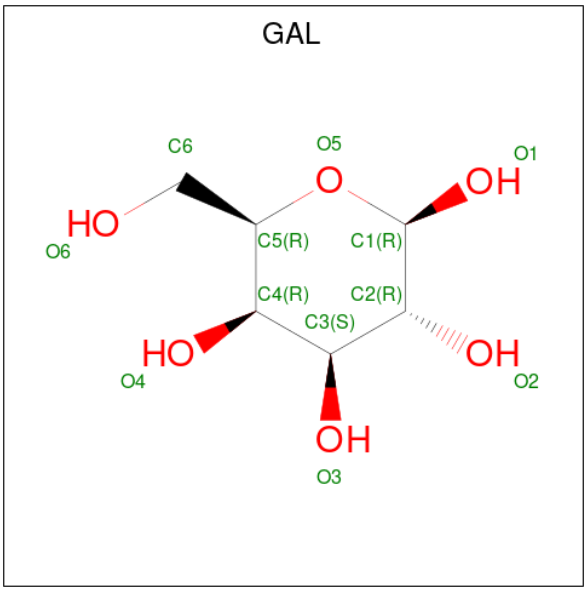
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	o	3	Total C O 34 18 16	0	0	0
2	p	3	Total C O 34 18 16	0	0	0
2	r	3	Total C O 34 18 16	0	0	0
2	s	3	Total C O 34 18 16	0	0	0
2	t	3	Total C O 34 18 16	0	0	0
2	v	3	Total C O 34 18 16	0	0	0
2	x	3	Total C O 34 18 16	0	0	0
2	z	3	Total C O 34 18 16	0	0	0
2	0	3	Total C O 34 18 16	0	0	0
2	2	3	Total C O 34 18 16	0	0	0
2	4	3	Total C O 34 18 16	0	0	0
2	5	3	Total C O 34 18 16	0	0	0
2	7	3	Total C O 34 18 16	0	0	0
2	8	3	Total C O 34 18 16	8	0	0
2	9	3	Total C O 34 18 16	0	0	0
2	AA	3	Total C O 34 18 16	0	0	0
2	BA	3	Total C O 34 18 16	4	0	0
2	CA	3	Total C O 34 18 16	0	0	0
2	EA	3	Total C O 34 18 16	0	0	0
2	FA	3	Total C O 34 18 16	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-beta-D-galactopyrano se.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	V	2	Total C O 23 12 11	0	0	0
3	Y	2	Total C O 23 12 11	0	0	0
3	Z	2	Total C O 23 12 11	0	0	0
3	b	2	Total C O 23 12 11	0	0	0
3	d	2	Total C O 23 12 11	0	0	0
3	l	2	Total C O 23 12 11	0	0	0
3	n	2	Total C O 23 12 11	0	0	0
3	q	2	Total C O 23 12 11	0	0	0
3	u	2	Total C O 23 12 11	0	0	0
3	w	2	Total C O 23 12 11	0	0	0
3	y	2	Total C O 23 12 11	0	0	0
3	1	2	Total C O 23 12 11	0	0	0
3	3	2	Total C O 23 12 11	0	0	0
3	6	2	Total C O 23 12 11	0	0	0
3	DA	2	Total C O 23 12 11	0	0	0
3	GA	2	Total C O 23 12 11	0	0	0

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 12 6 6	0	0
4	E	1	Total C O 12 6 6	0	0
4	G	1	Total C O 12 6 6	0	0
4	I	1	Total C O 12 6 6	0	0
4	J	1	Total C O 12 6 6	0	0
4	K	1	Total C O 12 6 6	0	0
4	L	1	Total C O 12 6 6	0	0
4	N	1	Total C O 12 6 6	0	0
4	P	1	Total C O 12 6 6	0	0
4	R	1	Total C O 12 6 6	0	0
4	T	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0

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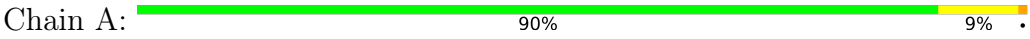
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	27	Total O 27 27	0	0
5	C	19	Total O 19 19	0	0
5	D	16	Total O 16 16	0	0
5	E	18	Total O 18 18	0	0
5	F	15	Total O 15 15	0	0
5	G	21	Total O 21 21	0	0
5	H	17	Total O 17 17	0	0
5	I	17	Total O 17 17	0	0
5	J	15	Total O 15 15	0	0
5	K	21	Total O 21 21	0	0
5	L	23	Total O 23 23	0	0
5	M	24	Total O 24 24	0	0
5	N	14	Total O 14 14	0	0
5	O	23	Total O 23 23	0	0
5	P	17	Total O 17 17	0	0
5	Q	13	Total O 13 13	0	0
5	R	10	Total O 10 10	0	0
5	S	11	Total O 11 11	0	0
5	T	12	Total O 12 12	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

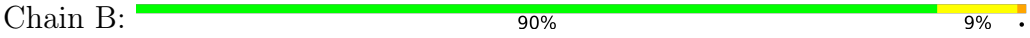
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain A:



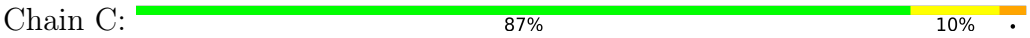
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain B:



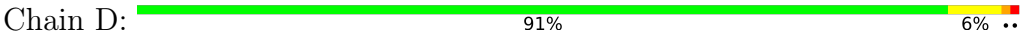
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

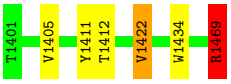
Chain C:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

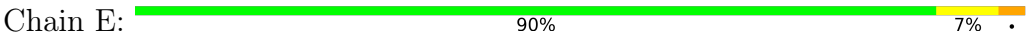
Chain D:





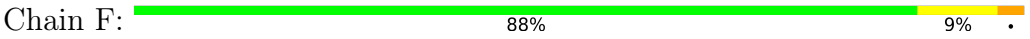
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain E:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain F:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

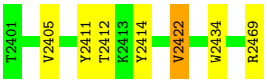
Chain G:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain H:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain I:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

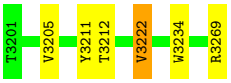
Chain J:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain K:

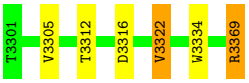
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain L:



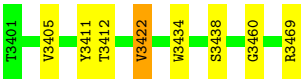
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain M:



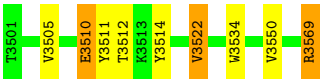
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain N:



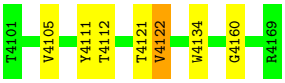
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain O:



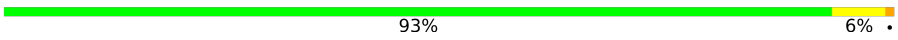
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

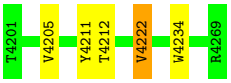
Chain P:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain Q:



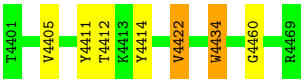


• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain R:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain S:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

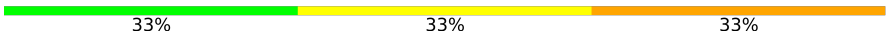
Chain T:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain U:

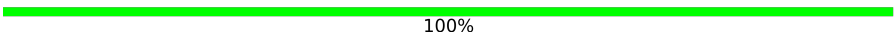
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain W:



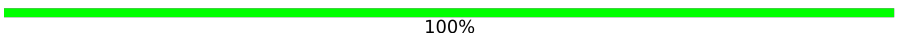
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain X:



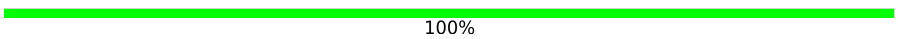
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain a:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain c:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

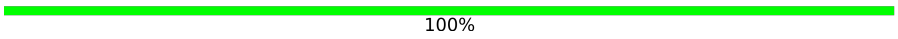
Chain e:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain f:

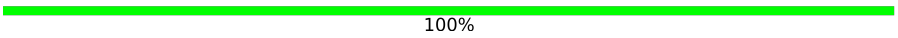
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain g:



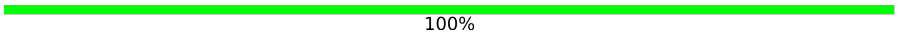
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain h:



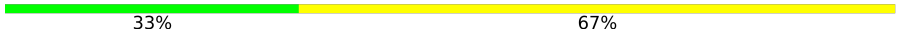
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain i:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain j:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain k:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

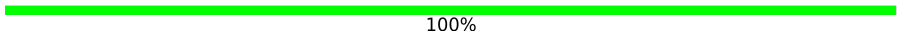
Chain m:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain o:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain p:

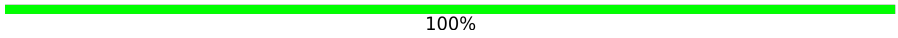


• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain r:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain s:

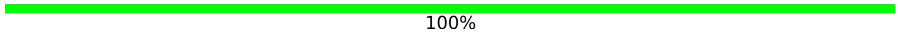


• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain t:

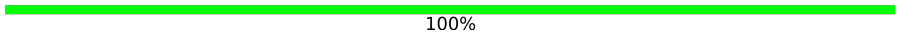
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain v:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain x:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain z: 

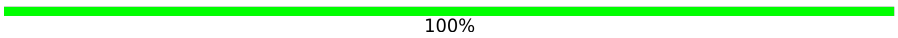
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain 0: 

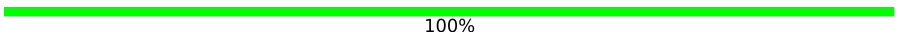
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain 2: 

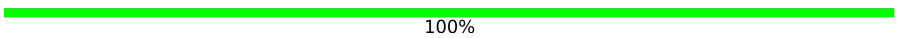
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain 4: 

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain 5: 

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

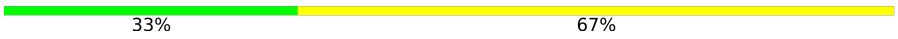
Chain 7: 

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain 8:

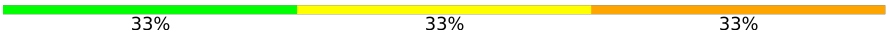
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain 9:



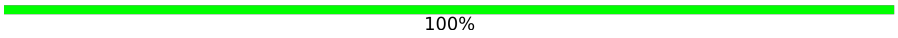
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain AA:



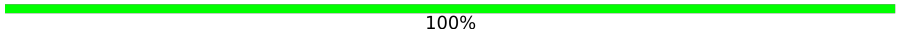
• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain BA:



• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain CA:

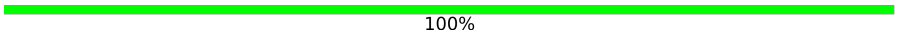


• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain EA:

• Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain FA:



• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain V:

• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain Y:

• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain Z:

• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain b:

• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

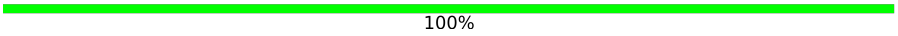
Chain d:

• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain l:

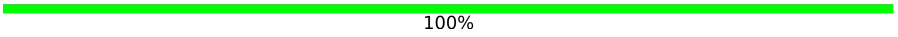
• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain n:



• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain q:

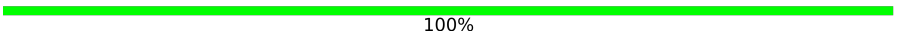


• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain u:

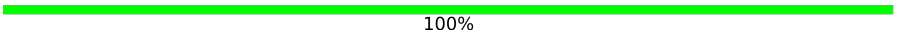
• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain w:



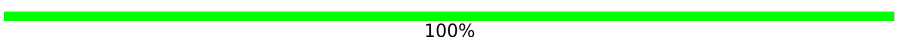
• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain y:



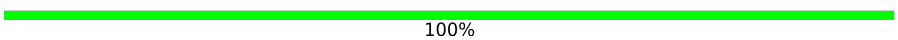
• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain 1:



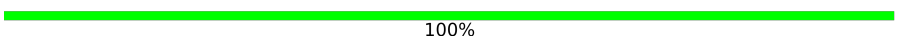
• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain 3:



• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain 6:

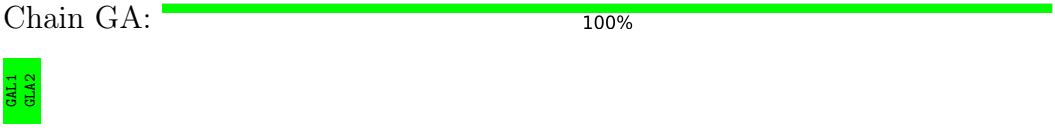


• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain DA:

• Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain GA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.50Å 97.70Å 164.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.80 21.05 – 2.75	Depositor EDS
% Data completeness (in resolution range)	81.6 (21.00-2.80) 77.6 (21.05-2.75)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 2.75Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.170 , 0.226 0.169 , 0.222	Depositor DCC
R_{free} test set	2091 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12767	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: BGC, GLA, GAL

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	0.85	0/549	1.42	4/742 (0.5%)
1	B	0.85	0/549	1.40	5/742 (0.7%)
1	C	0.88	1/549 (0.2%)	1.44	6/742 (0.8%)
1	D	0.86	0/549	1.33	4/742 (0.5%)
1	E	0.90	0/549	1.35	4/742 (0.5%)
1	F	0.96	1/549 (0.2%)	1.41	7/742 (0.9%)
1	G	0.84	0/549	1.35	5/742 (0.7%)
1	H	0.95	1/549 (0.2%)	1.43	7/742 (0.9%)
1	I	0.88	0/549	1.35	5/742 (0.7%)
1	J	0.76	0/549	1.34	4/742 (0.5%)
1	K	0.85	0/549	1.49	5/742 (0.7%)
1	L	0.84	0/549	1.44	5/742 (0.7%)
1	M	0.86	0/549	1.34	3/742 (0.4%)
1	N	0.88	0/549	1.39	4/742 (0.5%)
1	O	0.88	1/549 (0.2%)	1.46	10/742 (1.3%)
1	P	0.86	0/549	1.33	4/742 (0.5%)
1	Q	0.80	0/549	1.34	3/742 (0.4%)
1	R	0.86	0/549	1.30	4/742 (0.5%)
1	S	0.88	0/549	1.32	5/742 (0.7%)
1	T	0.88	1/549 (0.2%)	1.37	5/742 (0.7%)
All	All	0.87	5/10980 (0.0%)	1.38	99/14840 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	4510	GLU	CG-CD	6.03	1.60	1.51
1	O	3510	GLU	CG-CD	5.75	1.60	1.51
1	C	1369	ARG	CZ-NH1	5.41	1.40	1.33
1	F	2169	ARG	NE-CZ	5.20	1.39	1.33
1	H	2369	ARG	NE-CZ	5.04	1.39	1.33

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	3169	ARG	NE-CZ-NH1	16.70	128.65	120.30
1	L	3269	ARG	NE-CZ-NH2	-13.63	113.49	120.30
1	K	3169	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	T	4569	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	G	2269	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	1169	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	F	2169	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	L	3269	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	1269	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	N	3411	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	C	1369	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	H	2369	ARG	CA-CB-CG	8.10	131.22	113.40
1	I	2469	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	O	3569	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	I	2411	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	H	2334	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	C	1334	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	P	4134	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	C	1333	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	T	4569	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	1234	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	R	4311	TYR	CB-CG-CD2	-7.21	116.68	121.00
1	B	1234	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	C	1333	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	Q	4234	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	P	4134	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	B	1269	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	O	3514	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	F	2169	ARG	CG-CD-NE	7.01	126.52	111.80
1	H	2334	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	F	2134	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	N	3434	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	F	2134	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	C	1334	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	T	4534	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	D	1434	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	J	2511	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	O	3511	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	Q	4234	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	S	4434	TRP	CD1-CG-CD2	6.61	111.59	106.30
1	R	4334	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	D	1434	TRP	CD1-CG-CD2	6.48	111.48	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	4414	TYR	CB-CG-CD1	-6.44	117.13	121.00
1	L	3234	TRP	CE2-CD2-CG	-6.43	102.15	107.30
1	A	1134	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	O	3534	TRP	CE2-CD2-CG	-6.39	102.18	107.30
1	O	3534	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	E	1534	TRP	CE2-CD2-CG	-6.37	102.20	107.30
1	J	2569	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	T	4534	TRP	CD1-CG-CD2	6.33	111.37	106.30
1	E	1511	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	L	3211	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	E	1534	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	J	2534	TRP	CD1-CG-CD2	6.18	111.25	106.30
1	S	4434	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	O	3550	VAL	CG1-CB-CG2	-6.04	101.24	110.90
1	M	3334	TRP	CD1-CG-CD2	6.02	111.11	106.30
1	N	3434	TRP	CD1-CG-CD2	6.00	111.10	106.30
1	L	3234	TRP	CD1-CG-CD2	5.93	111.05	106.30
1	G	2234	TRP	CE2-CD2-CG	-5.93	102.56	107.30
1	F	2169	ARG	CD-NE-CZ	5.90	131.86	123.60
1	H	2311	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	K	3134	TRP	CD1-CG-CD2	5.87	111.00	106.30
1	I	2434	TRP	CE2-CD2-CG	-5.87	102.61	107.30
1	S	4411	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	M	3369	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	P	4111	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	1134	TRP	CD1-CG-CD2	5.83	110.96	106.30
1	Q	4211	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	I	2414	TYR	CB-CG-CD1	-5.79	117.52	121.00
1	M	3334	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	O	3510	GLU	CA-CB-CG	5.74	126.03	113.40
1	K	3134	TRP	CE2-CD2-CG	-5.73	102.72	107.30
1	N	3469	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	J	2534	TRP	CE2-CD2-CG	-5.63	102.80	107.30
1	A	1111	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	G	2211	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	D	1411	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	R	4334	TRP	NE1-CE2-CD2	5.51	112.81	107.30
1	H	2333	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	H	2334	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	T	4510	GLU	CA-CB-CG	5.45	125.40	113.40
1	O	3510	GLU	N-CA-CB	-5.41	100.86	110.60
1	O	3569	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	3111	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	R	4334	TRP	CD1-CG-CD2	5.34	110.57	106.30
1	E	1569	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	1369	ARG	CG-CD-NE	-5.31	100.64	111.80
1	B	1211	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	D	1469	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	2269	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	G	2234	TRP	CD1-CG-CD2	5.18	110.44	106.30
1	P	4134	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	F	2169	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	I	2434	TRP	CD1-CG-CD2	5.13	110.41	106.30
1	F	2111	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	H	2326	ASP	CB-CG-OD1	5.12	122.91	118.30
1	O	3569	ARG	CB-CA-C	-5.10	100.20	110.40
1	S	4434	TRP	CG-CD1-NE1	-5.00	105.09	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	540	0	524	2	0
1	B	540	0	524	2	0
1	C	540	0	524	5	0
1	D	540	0	524	2	0
1	E	540	0	524	1	0
1	F	540	0	524	2	0
1	G	540	0	524	5	0
1	H	540	0	524	1	0
1	I	540	0	524	1	0
1	J	540	0	524	3	0
1	K	540	0	524	3	0
1	L	540	0	524	1	0
1	M	540	0	524	2	0
1	N	540	0	524	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	540	0	524	2	0
1	P	540	0	524	4	0
1	Q	540	0	524	1	0
1	R	540	0	524	3	0
1	S	540	0	524	3	0
1	T	540	0	524	2	0
2	0	34	0	30	0	0
2	2	34	0	30	0	0
2	4	34	0	30	0	0
2	5	34	0	30	0	0
2	7	34	0	30	0	0
2	8	34	0	30	0	0
2	9	34	0	30	1	0
2	AA	34	0	30	1	0
2	BA	34	0	30	0	0
2	CA	34	0	30	0	0
2	EA	34	0	30	1	0
2	FA	34	0	30	0	0
2	U	34	0	30	0	0
2	W	34	0	30	1	0
2	X	34	0	30	0	0
2	a	34	0	30	0	0
2	c	34	0	30	0	0
2	e	34	0	30	0	0
2	f	34	0	30	0	0
2	g	34	0	30	0	0
2	h	34	0	30	0	0
2	i	34	0	30	0	0
2	j	34	0	30	0	0
2	k	34	0	30	0	0
2	m	34	0	30	0	0
2	o	34	0	30	0	0
2	p	34	0	30	0	0
2	r	34	0	30	0	0
2	s	34	0	30	0	0
2	t	34	0	30	0	0
2	v	34	0	30	0	0
2	x	34	0	30	0	0
2	z	34	0	30	0	0
3	1	23	0	21	0	0
3	3	23	0	21	0	0
3	6	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DA	23	0	21	1	0
3	GA	23	0	21	0	0
3	V	23	0	21	0	0
3	Y	23	0	21	0	0
3	Z	23	0	21	0	0
3	b	23	0	21	0	0
3	d	23	0	21	0	0
3	l	23	0	21	0	0
3	n	23	0	21	0	0
3	q	23	0	21	0	0
3	u	23	0	21	0	0
3	w	23	0	21	0	0
3	y	23	0	21	0	0
4	C	12	0	12	1	0
4	E	12	0	12	0	0
4	G	12	0	12	2	0
4	I	12	0	12	0	0
4	J	12	0	12	0	0
4	K	12	0	12	0	0
4	L	12	0	12	0	0
4	N	12	0	12	2	0
4	P	12	0	12	3	0
4	R	12	0	12	2	0
4	T	12	0	12	1	0
5	A	12	0	0	0	0
5	B	27	0	0	1	0
5	C	19	0	0	0	0
5	D	16	0	0	0	0
5	E	18	0	0	0	0
5	F	15	0	0	2	0
5	G	21	0	0	0	0
5	H	17	0	0	0	0
5	I	17	0	0	0	0
5	J	15	0	0	2	0
5	K	21	0	0	2	0
5	L	23	0	0	0	0
5	M	24	0	0	2	0
5	N	14	0	0	0	0
5	O	23	0	0	0	0
5	P	17	0	0	0	0
5	Q	13	0	0	0	0
5	R	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	11	0	0	0	0
5	T	12	0	0	0	0
All	All	12767	0	11938	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:4360:GLY:HA2	4:R:4370:GAL:H61	1.62	0.81
1:G:2269:ARG:HH11	1:G:2269:ARG:HG2	1.44	0.80
1:P:4112:THR:HG22	1:P:4122:VAL:HG23	1.73	0.71
1:K:3112:THR:HG22	1:K:3122:VAL:HG23	1.75	0.69
1:I:2412:THR:HG22	1:I:2422:VAL:HG23	1.74	0.68
1:D:1412:THR:HG22	1:D:1422:VAL:HG23	1.76	0.67
1:P:4160:GLY:HA2	4:P:4170:GAL:H61	1.77	0.67
1:M:3312:THR:HG22	1:M:3322:VAL:HG23	1.77	0.66
1:C:1312:THR:HG22	1:C:1322:VAL:HG23	1.78	0.66
1:T:4512:THR:HG22	1:T:4522:VAL:HG23	1.76	0.65
1:A:1112:THR:HG22	1:A:1122:VAL:HG23	1.78	0.65
1:J:2512:THR:HG22	1:J:2522:VAL:HG23	1.78	0.65
1:N:3412:THR:HG22	1:N:3422:VAL:HG23	1.79	0.65
1:F:2112:THR:HG22	1:F:2122:VAL:HG23	1.79	0.64
1:S:4412:THR:HG22	1:S:4422:VAL:HG23	1.79	0.64
1:H:2312:THR:HG22	1:H:2322:VAL:HG23	1.80	0.64
1:O:3512:THR:HG22	1:O:3522:VAL:HG23	1.80	0.63
1:R:4312:THR:HG22	1:R:4322:VAL:HG23	1.80	0.63
1:L:3212:THR:HG22	1:L:3222:VAL:HG23	1.81	0.63
1:Q:4212:THR:HG22	1:Q:4222:VAL:HG23	1.81	0.62
1:K:3169:ARG:HD2	5:K:5224:HOH:O	1.98	0.62
1:E:1512:THR:HG22	1:E:1522:VAL:HG23	1.80	0.62
1:B:1212:THR:HG22	1:B:1222:VAL:HG23	1.82	0.61
1:R:4360:GLY:HA2	4:R:4370:GAL:C6	2.30	0.61
1:J:2537:GLN:HB2	5:J:5179:HOH:O	2.01	0.60
1:G:2212:THR:HG22	1:G:2222:VAL:HG23	1.81	0.60
1:N:3460:GLY:HA2	4:N:3470:GAL:H61	1.83	0.59
1:P:4160:GLY:HA2	4:P:4170:GAL:C6	2.33	0.57
1:S:4460:GLY:HA2	2:EA:3:GLA:O6	2.09	0.53
1:M:3316:ASP:HB3	5:M:5319:HOH:O	2.09	0.52
1:N:3460:GLY:HA2	4:N:3470:GAL:C6	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:4121:THR:HG1	4:P:4170:GAL:HO4	1.60	0.47
1:T:4560:GLY:HA2	4:T:4570:GAL:H61	1.97	0.47
5:M:5314:HOH:O	1:N:3438:SER:HB3	2.15	0.47
2:9:2:GAL:O3	2:9:3:GLA:H5	2.16	0.46
1:J:2501:THR:HG21	5:J:5104:HOH:O	2.15	0.44
1:S:4434:TRP:CE3	3:DA:1:GAL:H3	2.52	0.44
1:O:3569:ARG:HE	1:O:3569:ARG:HB3	1.72	0.44
1:G:2269:ARG:HG2	1:G:2269:ARG:NH1	2.20	0.44
1:C:1308:LYS:HE2	5:F:5232:HOH:O	2.18	0.43
1:A:1160:GLY:HA2	2:W:3:GLA:O6	2.18	0.43
1:C:1360:GLY:HA2	4:C:1370:GAL:H61	1.99	0.43
1:B:1237:GLN:HB2	5:B:5126:HOH:O	2.19	0.43
1:C:1306:THR:HG21	1:F:2159:ASN:HB2	2.01	0.43
1:D:1469:ARG:HH11	1:D:1469:ARG:HG3	1.82	0.43
2:AA:2:GAL:O3	2:AA:3:GLA:H5	2.18	0.43
1:C:1308:LYS:CE	5:F:5232:HOH:O	2.67	0.43
1:G:2260:GLY:HA2	4:G:2270:GAL:C6	2.50	0.42
1:G:2260:GLY:HA2	4:G:2270:GAL:H61	2.01	0.41
1:K:3119:THR:HG21	5:K:5192:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	B	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	C	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	D	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	E	67/69 (97%)	65 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
1	G	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
1	H	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	I	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	J	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	K	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	L	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	M	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	N	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	O	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	P	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	Q	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	R	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	S	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	T	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
All	All	1340/1380 (97%)	1302 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	61/61 (100%)	59 (97%)	2 (3%)	38	72
1	B	61/61 (100%)	59 (97%)	2 (3%)	38	72
1	C	61/61 (100%)	58 (95%)	3 (5%)	25	57
1	D	61/61 (100%)	58 (95%)	3 (5%)	25	57
1	E	61/61 (100%)	57 (93%)	4 (7%)	16	44
1	F	61/61 (100%)	57 (93%)	4 (7%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	61/61 (100%)	58 (95%)	3 (5%)	25 57
1	H	61/61 (100%)	57 (93%)	4 (7%)	16 44
1	I	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	J	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	K	61/61 (100%)	58 (95%)	3 (5%)	25 57
1	L	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	M	61/61 (100%)	58 (95%)	3 (5%)	25 57
1	N	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	O	61/61 (100%)	58 (95%)	3 (5%)	25 57
1	P	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	Q	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	R	61/61 (100%)	58 (95%)	3 (5%)	25 57
1	S	61/61 (100%)	59 (97%)	2 (3%)	38 72
1	T	61/61 (100%)	59 (97%)	2 (3%)	38 72
All	All	1220/1220 (100%)	1167 (96%)	53 (4%)	29 62

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1105	VAL
1	A	1122	VAL
1	B	1205	VAL
1	B	1222	VAL
1	C	1305	VAL
1	C	1322	VAL
1	C	1369	ARG
1	D	1405	VAL
1	D	1422	VAL
1	D	1469	ARG
1	E	1505	VAL
1	E	1510	GLU
1	E	1522	VAL
1	E	1569	ARG
1	F	2105	VAL
1	F	2110	GLU
1	F	2122	VAL
1	F	2169	ARG

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Mol	Chain	Res	Type
1	G	2205	VAL
1	G	2222	VAL
1	G	2269	ARG
1	H	2305	VAL
1	H	2310	GLU
1	H	2322	VAL
1	H	2369	ARG
1	I	2405	VAL
1	I	2422	VAL
1	J	2505	VAL
1	J	2522	VAL
1	K	3105	VAL
1	K	3122	VAL
1	K	3169	ARG
1	L	3205	VAL
1	L	3222	VAL
1	M	3305	VAL
1	M	3322	VAL
1	M	3369	ARG
1	N	3405	VAL
1	N	3422	VAL
1	O	3505	VAL
1	O	3510	GLU
1	O	3522	VAL
1	P	4105	VAL
1	P	4122	VAL
1	Q	4205	VAL
1	Q	4222	VAL
1	R	4305	VAL
1	R	4322	VAL
1	R	4369	ARG
1	S	4405	VAL
1	S	4422	VAL
1	T	4505	VAL
1	T	4522	VAL

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

5.3.3 RNA

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)

131 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGC	0	1	2	12,12,12	0.52	0	17,17,17	0.39	0
2	GAL	0	2	2	11,11,12	0.61	0	15,15,17	0.86	1 (6%)
2	GLA	0	3	2	11,11,12	0.40	0	15,15,17	0.71	0
3	GAL	1	1	3	12,12,12	0.47	0	17,17,17	0.45	0
3	GLA	1	2	3	11,11,12	0.69	0	15,15,17	0.67	0
2	BGC	2	1	2	12,12,12	0.52	0	17,17,17	0.39	0
2	GAL	2	2	2	11,11,12	0.51	0	15,15,17	0.80	0
2	GLA	2	3	2	11,11,12	0.58	0	15,15,17	0.63	0
3	GAL	3	1	3	12,12,12	0.46	0	17,17,17	0.65	0
3	GLA	3	2	3	11,11,12	0.56	0	15,15,17	0.52	0
2	BGC	4	1	2	12,12,12	0.40	0	17,17,17	0.60	0
2	GAL	4	2	2	11,11,12	0.63	0	15,15,17	0.80	0
2	GLA	4	3	2	11,11,12	0.36	0	15,15,17	0.77	0
2	BGC	5	1	2	12,12,12	0.44	0	17,17,17	0.40	0
2	GAL	5	2	2	11,11,12	0.65	0	15,15,17	0.76	0
2	GLA	5	3	2	11,11,12	0.43	0	15,15,17	0.62	0
3	GAL	6	1	3	12,12,12	0.41	0	17,17,17	0.47	0
3	GLA	6	2	3	11,11,12	0.64	0	15,15,17	0.58	0
2	BGC	7	1	2	12,12,12	0.39	0	17,17,17	0.54	0
2	GAL	7	2	2	11,11,12	0.66	0	15,15,17	0.59	0
2	GLA	7	3	2	11,11,12	0.47	0	15,15,17	0.67	0
2	BGC	8	1	2	12,12,12	0.44	0	17,17,17	0.34	0
2	GAL	8	2	2	11,11,12	0.66	0	15,15,17	0.55	0
2	GLA	8	3	2	11,11,12	0.65	0	15,15,17	0.76	0
2	BGC	9	1	2	12,12,12	0.38	0	17,17,17	0.59	0
2	GAL	9	2	2	11,11,12	0.63	0	15,15,17	0.48	0
2	GLA	9	3	2	11,11,12	0.71	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	AA	1	2	12,12,12	0.43	0	17,17,17	0.51	0
2	GAL	AA	2	2	11,11,12	0.61	0	15,15,17	0.59	0
2	GLA	AA	3	2	11,11,12	0.51	0	15,15,17	0.85	1 (6%)
2	BGC	BA	1	2	12,12,12	0.66	0	17,17,17	0.46	0
2	GAL	BA	2	2	11,11,12	0.50	0	15,15,17	0.43	0
2	GLA	BA	3	2	11,11,12	0.75	0	15,15,17	0.55	0
2	BGC	CA	1	2	12,12,12	0.40	0	17,17,17	0.40	0
2	GAL	CA	2	2	11,11,12	0.66	0	15,15,17	0.43	0
2	GLA	CA	3	2	11,11,12	0.45	0	15,15,17	0.70	0
3	GAL	DA	1	3	12,12,12	0.45	0	17,17,17	0.41	0
3	GLA	DA	2	3	11,11,12	0.55	0	15,15,17	0.64	0
2	BGC	EA	1	2	12,12,12	0.35	0	17,17,17	0.42	0
2	GAL	EA	2	2	11,11,12	0.52	0	15,15,17	0.60	0
2	GLA	EA	3	2	11,11,12	0.48	0	15,15,17	0.81	1 (6%)
2	BGC	FA	1	2	12,12,12	0.30	0	17,17,17	0.37	0
2	GAL	FA	2	2	11,11,12	0.49	0	15,15,17	0.47	0
2	GLA	FA	3	2	11,11,12	0.40	0	15,15,17	0.70	0
3	GAL	GA	1	3	12,12,12	0.47	0	17,17,17	0.50	0
3	GLA	GA	2	3	11,11,12	0.63	0	15,15,17	0.73	0
2	BGC	U	1	2	12,12,12	0.41	0	17,17,17	0.32	0
2	GAL	U	2	2	11,11,12	0.46	0	15,15,17	0.63	0
2	GLA	U	3	2	11,11,12	0.44	0	15,15,17	0.74	0
3	GAL	V	1	3	12,12,12	0.36	0	17,17,17	0.58	0
3	GLA	V	2	3	11,11,12	0.48	0	15,15,17	0.96	1 (6%)
2	BGC	W	1	2	12,12,12	0.57	0	17,17,17	0.63	0
2	GAL	W	2	2	11,11,12	0.71	0	15,15,17	0.81	1 (6%)
2	GLA	W	3	2	11,11,12	0.40	0	15,15,17	0.73	1 (6%)
2	BGC	X	1	2	12,12,12	0.38	0	17,17,17	0.53	0
2	GAL	X	2	2	11,11,12	0.55	0	15,15,17	0.61	0
2	GLA	X	3	2	11,11,12	0.48	0	15,15,17	0.62	0
3	GAL	Y	1	3	12,12,12	0.36	0	17,17,17	0.45	0
3	GLA	Y	2	3	11,11,12	0.46	0	15,15,17	0.88	1 (6%)
3	GAL	Z	1	3	12,12,12	0.48	0	17,17,17	0.46	0
3	GLA	Z	2	3	11,11,12	0.48	0	15,15,17	0.79	1 (6%)
2	BGC	a	1	2	12,12,12	0.42	0	17,17,17	0.48	0
2	GAL	a	2	2	11,11,12	0.56	0	15,15,17	0.52	0
2	GLA	a	3	2	11,11,12	0.49	0	15,15,17	0.68	0
3	GAL	b	1	3	12,12,12	0.63	0	17,17,17	0.59	0
3	GLA	b	2	3	11,11,12	0.66	0	15,15,17	0.92	1 (6%)
2	BGC	c	1	2	12,12,12	0.38	0	17,17,17	0.56	0
2	GAL	c	2	2	11,11,12	0.55	0	15,15,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLA	c	3	2	11,11,12	0.43	0	15,15,17	0.59	0
3	GAL	d	1	3	12,12,12	0.82	0	17,17,17	0.96	0
3	GLA	d	2	3	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
2	BGC	e	1	2	12,12,12	0.49	0	17,17,17	0.51	0
2	GAL	e	2	2	11,11,12	0.47	0	15,15,17	0.59	0
2	GLA	e	3	2	11,11,12	0.61	0	15,15,17	0.95	1 (6%)
2	BGC	f	1	2	12,12,12	0.40	0	17,17,17	0.52	0
2	GAL	f	2	2	11,11,12	0.48	0	15,15,17	0.41	0
2	GLA	f	3	2	11,11,12	0.52	0	15,15,17	0.60	0
2	BGC	g	1	2	12,12,12	0.31	0	17,17,17	0.35	0
2	GAL	g	2	2	11,11,12	0.56	0	15,15,17	0.69	0
2	GLA	g	3	2	11,11,12	0.47	0	15,15,17	0.73	0
2	BGC	h	1	2	12,12,12	0.60	0	17,17,17	0.59	0
2	GAL	h	2	2	11,11,12	0.59	0	15,15,17	0.76	0
2	GLA	h	3	2	11,11,12	0.63	0	15,15,17	0.86	0
2	BGC	i	1	2	12,12,12	0.39	0	17,17,17	0.37	0
2	GAL	i	2	2	11,11,12	0.50	0	15,15,17	0.41	0
2	GLA	i	3	2	11,11,12	0.47	0	15,15,17	0.56	0
2	BGC	j	1	2	12,12,12	0.26	0	17,17,17	0.56	0
2	GAL	j	2	2	11,11,12	0.49	0	15,15,17	0.76	1 (6%)
2	GLA	j	3	2	11,11,12	0.36	0	15,15,17	1.23	2 (13%)
2	BGC	k	1	2	12,12,12	0.29	0	17,17,17	0.46	0
2	GAL	k	2	2	11,11,12	0.37	0	15,15,17	0.54	0
2	GLA	k	3	2	11,11,12	0.56	0	15,15,17	0.86	1 (6%)
3	GAL	l	1	3	12,12,12	0.36	0	17,17,17	0.43	0
3	GLA	l	2	3	11,11,12	0.58	0	15,15,17	0.57	0
2	BGC	m	1	2	12,12,12	0.62	0	17,17,17	0.46	0
2	GAL	m	2	2	11,11,12	0.65	0	15,15,17	0.47	0
2	GLA	m	3	2	11,11,12	0.48	0	15,15,17	0.82	1 (6%)
3	GAL	n	1	3	12,12,12	0.39	0	17,17,17	0.42	0
3	GLA	n	2	3	11,11,12	0.63	0	15,15,17	0.68	0
2	BGC	o	1	2	12,12,12	0.51	0	17,17,17	0.92	1 (5%)
2	GAL	o	2	2	11,11,12	0.55	0	15,15,17	0.70	0
2	GLA	o	3	2	11,11,12	0.44	0	15,15,17	0.66	0
2	BGC	p	1	2	12,12,12	0.56	0	17,17,17	0.58	0
2	GAL	p	2	2	11,11,12	0.65	0	15,15,17	0.63	0
2	GLA	p	3	2	11,11,12	0.49	0	15,15,17	0.71	0
3	GAL	q	1	3	12,12,12	0.53	0	17,17,17	0.80	0
3	GLA	q	2	3	11,11,12	0.70	0	15,15,17	0.75	0
2	BGC	r	1	2	12,12,12	0.45	0	17,17,17	0.36	0
2	GAL	r	2	2	11,11,12	0.48	0	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLA	r	3	2	11,11,12	0.49	0	15,15,17	0.97	2 (13%)
2	BGC	s	1	2	12,12,12	0.34	0	17,17,17	0.37	0
2	GAL	s	2	2	11,11,12	0.45	0	15,15,17	0.60	0
2	GLA	s	3	2	11,11,12	0.64	0	15,15,17	0.48	0
2	BGC	t	1	2	12,12,12	0.40	0	17,17,17	0.48	0
2	GAL	t	2	2	11,11,12	0.53	0	15,15,17	0.66	0
2	GLA	t	3	2	11,11,12	0.37	0	15,15,17	0.78	1 (6%)
3	GAL	u	1	3	12,12,12	0.48	0	17,17,17	0.43	0
3	GLA	u	2	3	11,11,12	0.52	0	15,15,17	0.47	0
2	BGC	v	1	2	12,12,12	0.40	0	17,17,17	0.50	0
2	GAL	v	2	2	11,11,12	0.54	0	15,15,17	0.56	0
2	GLA	v	3	2	11,11,12	0.41	0	15,15,17	0.61	0
3	GAL	w	1	3	12,12,12	0.52	0	17,17,17	0.53	0
3	GLA	w	2	3	11,11,12	0.49	0	15,15,17	0.68	0
2	BGC	x	1	2	12,12,12	0.39	0	17,17,17	0.36	0
2	GAL	x	2	2	11,11,12	0.48	0	15,15,17	0.68	0
2	GLA	x	3	2	11,11,12	0.48	0	15,15,17	0.64	0
3	GAL	y	1	3	12,12,12	0.25	0	17,17,17	0.57	0
3	GLA	y	2	3	11,11,12	0.49	0	15,15,17	0.75	0
2	BGC	z	1	2	12,12,12	0.48	0	17,17,17	0.69	0
2	GAL	z	2	2	11,11,12	0.55	0	15,15,17	0.57	0
2	GLA	z	3	2	11,11,12	0.61	0	15,15,17	1.08	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	0	1	2	-	2/2/22/22	0/1/1/1
2	GAL	0	2	2	-	0/2/19/22	0/1/1/1
2	GLA	0	3	2	-	0/2/19/22	0/1/1/1
3	GAL	1	1	3	-	1/2/22/22	0/1/1/1
3	GLA	1	2	3	-	0/2/19/22	0/1/1/1
2	BGC	2	1	2	-	0/2/22/22	0/1/1/1
2	GAL	2	2	2	-	0/2/19/22	0/1/1/1
2	GLA	2	3	2	-	0/2/19/22	0/1/1/1
3	GAL	3	1	3	-	0/2/22/22	0/1/1/1
3	GLA	3	2	3	-	2/2/19/22	0/1/1/1
2	BGC	4	1	2	-	1/2/22/22	0/1/1/1
2	GAL	4	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	4	3	2	-	1/2/19/22	0/1/1/1
2	BGC	5	1	2	-	0/2/22/22	0/1/1/1
2	GAL	5	2	2	-	0/2/19/22	0/1/1/1
2	GLA	5	3	2	-	0/2/19/22	0/1/1/1
3	GAL	6	1	3	-	0/2/22/22	0/1/1/1
3	GLA	6	2	3	-	2/2/19/22	0/1/1/1
2	BGC	7	1	2	-	0/2/22/22	0/1/1/1
2	GAL	7	2	2	-	0/2/19/22	0/1/1/1
2	GLA	7	3	2	-	0/2/19/22	0/1/1/1
2	BGC	8	1	2	-	0/2/22/22	0/1/1/1
2	GAL	8	2	2	-	1/2/19/22	0/1/1/1
2	GLA	8	3	2	-	0/2/19/22	0/1/1/1
2	BGC	9	1	2	-	0/2/22/22	0/1/1/1
2	GAL	9	2	2	-	0/2/19/22	0/1/1/1
2	GLA	9	3	2	-	1/2/19/22	0/1/1/1
2	BGC	AA	1	2	-	0/2/22/22	0/1/1/1
2	GAL	AA	2	2	-	0/2/19/22	0/1/1/1
2	GLA	AA	3	2	-	0/2/19/22	0/1/1/1
2	BGC	BA	1	2	-	0/2/22/22	0/1/1/1
2	GAL	BA	2	2	-	0/2/19/22	0/1/1/1
2	GLA	BA	3	2	-	2/2/19/22	0/1/1/1
2	BGC	CA	1	2	-	0/2/22/22	0/1/1/1
2	GAL	CA	2	2	-	0/2/19/22	0/1/1/1
2	GLA	CA	3	2	-	0/2/19/22	0/1/1/1
3	GAL	DA	1	3	-	0/2/22/22	0/1/1/1
3	GLA	DA	2	3	-	2/2/19/22	0/1/1/1
2	BGC	EA	1	2	-	2/2/22/22	0/1/1/1
2	GAL	EA	2	2	-	0/2/19/22	0/1/1/1
2	GLA	EA	3	2	-	0/2/19/22	0/1/1/1
2	BGC	FA	1	2	-	0/2/22/22	0/1/1/1
2	GAL	FA	2	2	-	0/2/19/22	0/1/1/1
2	GLA	FA	3	2	-	0/2/19/22	0/1/1/1
3	GAL	GA	1	3	-	0/2/22/22	0/1/1/1
3	GLA	GA	2	3	-	2/2/19/22	0/1/1/1
2	BGC	U	1	2	-	0/2/22/22	0/1/1/1
2	GAL	U	2	2	-	0/2/19/22	0/1/1/1
2	GLA	U	3	2	-	0/2/19/22	0/1/1/1
3	GAL	V	1	3	-	0/2/22/22	0/1/1/1
3	GLA	V	2	3	-	0/2/19/22	0/1/1/1
2	BGC	W	1	2	-	0/2/22/22	0/1/1/1
2	GAL	W	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	W	3	2	-	0/2/19/22	0/1/1/1
2	BGC	X	1	2	-	0/2/22/22	0/1/1/1
2	GAL	X	2	2	-	0/2/19/22	0/1/1/1
2	GLA	X	3	2	-	1/2/19/22	0/1/1/1
3	GAL	Y	1	3	-	0/2/22/22	0/1/1/1
3	GLA	Y	2	3	-	2/2/19/22	0/1/1/1
3	GAL	Z	1	3	-	0/2/22/22	0/1/1/1
3	GLA	Z	2	3	-	1/2/19/22	0/1/1/1
2	BGC	a	1	2	-	0/2/22/22	0/1/1/1
2	GAL	a	2	2	-	0/2/19/22	0/1/1/1
2	GLA	a	3	2	-	0/2/19/22	0/1/1/1
3	GAL	b	1	3	-	1/2/22/22	0/1/1/1
3	GLA	b	2	3	-	1/2/19/22	0/1/1/1
2	BGC	c	1	2	-	0/2/22/22	0/1/1/1
2	GAL	c	2	2	-	0/2/19/22	0/1/1/1
2	GLA	c	3	2	-	0/2/19/22	0/1/1/1
3	GAL	d	1	3	-	0/2/22/22	0/1/1/1
3	GLA	d	2	3	-	0/2/19/22	0/1/1/1
2	BGC	e	1	2	-	0/2/22/22	0/1/1/1
2	GAL	e	2	2	-	0/2/19/22	0/1/1/1
2	GLA	e	3	2	-	1/2/19/22	0/1/1/1
2	BGC	f	1	2	-	0/2/22/22	0/1/1/1
2	GAL	f	2	2	-	0/2/19/22	0/1/1/1
2	GLA	f	3	2	-	0/2/19/22	0/1/1/1
2	BGC	g	1	2	-	0/2/22/22	0/1/1/1
2	GAL	g	2	2	-	0/2/19/22	0/1/1/1
2	GLA	g	3	2	-	2/2/19/22	0/1/1/1
2	BGC	h	1	2	-	0/2/22/22	0/1/1/1
2	GAL	h	2	2	-	0/2/19/22	0/1/1/1
2	GLA	h	3	2	-	0/2/19/22	0/1/1/1
2	BGC	i	1	2	-	0/2/22/22	0/1/1/1
2	GAL	i	2	2	-	0/2/19/22	0/1/1/1
2	GLA	i	3	2	-	0/2/19/22	0/1/1/1
2	BGC	j	1	2	-	0/2/22/22	0/1/1/1
2	GAL	j	2	2	-	0/2/19/22	0/1/1/1
2	GLA	j	3	2	-	1/2/19/22	0/1/1/1
2	BGC	k	1	2	-	0/2/22/22	0/1/1/1
2	GAL	k	2	2	-	0/2/19/22	0/1/1/1
2	GLA	k	3	2	-	0/2/19/22	0/1/1/1
3	GAL	l	1	3	-	0/2/22/22	0/1/1/1
3	GLA	l	2	3	-	2/2/19/22	0/1/1/1
2	BGC	m	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	m	2	2	-	0/2/19/22	0/1/1/1
2	GLA	m	3	2	-	0/2/19/22	0/1/1/1
3	GAL	n	1	3	-	0/2/22/22	0/1/1/1
3	GLA	n	2	3	-	2/2/19/22	0/1/1/1
2	BGC	o	1	2	-	2/2/22/22	0/1/1/1
2	GAL	o	2	2	-	0/2/19/22	0/1/1/1
2	GLA	o	3	2	-	1/2/19/22	0/1/1/1
2	BGC	p	1	2	-	0/2/22/22	0/1/1/1
2	GAL	p	2	2	-	0/2/19/22	0/1/1/1
2	GLA	p	3	2	-	0/2/19/22	0/1/1/1
3	GAL	q	1	3	-	0/2/22/22	0/1/1/1
3	GLA	q	2	3	-	0/2/19/22	0/1/1/1
2	BGC	r	1	2	-	0/2/22/22	0/1/1/1
2	GAL	r	2	2	-	0/2/19/22	0/1/1/1
2	GLA	r	3	2	-	0/2/19/22	0/1/1/1
2	BGC	s	1	2	-	0/2/22/22	0/1/1/1
2	GAL	s	2	2	-	0/2/19/22	0/1/1/1
2	GLA	s	3	2	-	0/2/19/22	0/1/1/1
2	BGC	t	1	2	-	0/2/22/22	0/1/1/1
2	GAL	t	2	2	-	0/2/19/22	0/1/1/1
2	GLA	t	3	2	-	0/2/19/22	0/1/1/1
3	GAL	u	1	3	-	0/2/22/22	0/1/1/1
3	GLA	u	2	3	-	2/2/19/22	0/1/1/1
2	BGC	v	1	2	-	0/2/22/22	0/1/1/1
2	GAL	v	2	2	-	0/2/19/22	0/1/1/1
2	GLA	v	3	2	-	0/2/19/22	0/1/1/1
3	GAL	w	1	3	-	0/2/22/22	0/1/1/1
3	GLA	w	2	3	-	0/2/19/22	0/1/1/1
2	BGC	x	1	2	-	0/2/22/22	0/1/1/1
2	GAL	x	2	2	-	0/2/19/22	0/1/1/1
2	GLA	x	3	2	-	0/2/19/22	0/1/1/1
3	GAL	y	1	3	-	0/2/22/22	0/1/1/1
3	GLA	y	2	3	-	0/2/19/22	0/1/1/1
2	BGC	z	1	2	-	2/2/22/22	0/1/1/1
2	GAL	z	2	2	-	0/2/19/22	0/1/1/1
2	GLA	z	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	3	GLA	C1-O5-C5	3.32	116.69	112.19
3	b	2	GLA	C1-O5-C5	2.86	116.07	112.19
3	V	2	GLA	C1-C2-C3	2.85	113.17	109.67
2	z	3	GLA	C1-O5-C5	2.76	115.92	112.19
2	j	3	GLA	C1-C2-C3	2.75	113.05	109.67
2	e	3	GLA	C1-C2-C3	2.69	112.97	109.67
3	d	2	GLA	C1-C2-C3	2.68	112.96	109.67
2	AA	3	GLA	C1-O5-C5	2.47	115.54	112.19
2	o	1	BGC	C4-C3-C2	2.32	114.88	110.82
2	0	2	GAL	C3-C4-C5	-2.27	106.19	110.24
2	EA	3	GLA	C1-C2-C3	2.23	112.41	109.67
2	r	3	GLA	C1-O5-C5	2.17	115.14	112.19
2	t	3	GLA	C1-O5-C5	2.16	115.12	112.19
2	W	2	GAL	C1-C2-C3	2.14	112.30	109.67
3	Z	2	GLA	C1-C2-C3	2.13	112.29	109.67
2	m	3	GLA	C1-O5-C5	2.13	115.08	112.19
2	j	2	GAL	C1-C2-C3	2.09	112.23	109.67
2	r	3	GLA	C1-C2-C3	2.03	112.16	109.67
2	W	3	GLA	C1-O5-C5	2.03	114.94	112.19
2	k	3	GLA	C1-C2-C3	2.02	112.15	109.67
3	Y	2	GLA	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	GA	2	GLA	O5-C5-C6-O6
3	GA	2	GLA	C4-C5-C6-O6
2	g	3	GLA	O5-C5-C6-O6
2	z	1	BGC	O5-C5-C6-O6
2	g	3	GLA	C4-C5-C6-O6
2	BA	3	GLA	C4-C5-C6-O6
2	BA	3	GLA	O5-C5-C6-O6
2	EA	1	BGC	O5-C5-C6-O6
3	DA	2	GLA	O5-C5-C6-O6
3	n	2	GLA	O5-C5-C6-O6
2	o	3	GLA	O5-C5-C6-O6
3	DA	2	GLA	C4-C5-C6-O6
3	Y	2	GLA	O5-C5-C6-O6
3	n	2	GLA	C4-C5-C6-O6
3	Y	2	GLA	C4-C5-C6-O6
3	6	2	GLA	C4-C5-C6-O6
2	EA	1	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Z	2	GLA	O5-C5-C6-O6
3	u	2	GLA	C4-C5-C6-O6
3	u	2	GLA	O5-C5-C6-O6
3	6	2	GLA	O5-C5-C6-O6
2	o	1	BGC	C4-C5-C6-O6
3	l	2	GLA	C4-C5-C6-O6
2	o	1	BGC	O5-C5-C6-O6
3	b	2	GLA	O5-C5-C6-O6
2	W	2	GAL	C4-C5-C6-O6
2	4	3	GLA	O5-C5-C6-O6
2	z	3	GLA	O5-C5-C6-O6
2	e	3	GLA	O5-C5-C6-O6
3	3	2	GLA	C4-C5-C6-O6
2	9	3	GLA	O5-C5-C6-O6
2	j	3	GLA	O5-C5-C6-O6
2	z	1	BGC	C4-C5-C6-O6
2	4	1	BGC	O5-C5-C6-O6
3	l	2	GLA	O5-C5-C6-O6
3	3	2	GLA	O5-C5-C6-O6
2	W	2	GAL	O5-C5-C6-O6
2	0	1	BGC	C4-C5-C6-O6
2	8	2	GAL	C4-C5-C6-O6
3	b	1	GAL	C4-C5-C6-O6
3	1	1	GAL	O5-C5-C6-O6
2	0	1	BGC	O5-C5-C6-O6
2	X	3	GLA	C4-C5-C6-O6
2	4	2	GAL	C4-C5-C6-O6

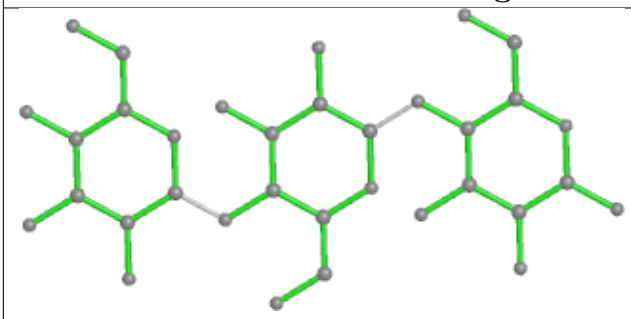
There are no ring outliers.

7 monomers are involved in 5 short contacts:

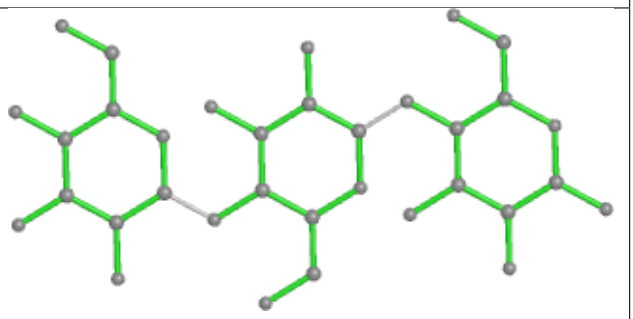
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	3	GLA	1	0
2	EA	3	GLA	1	0
2	9	3	GLA	1	0
2	AA	3	GLA	1	0
2	9	2	GAL	1	0
3	DA	1	GAL	1	0
2	AA	2	GAL	1	0

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

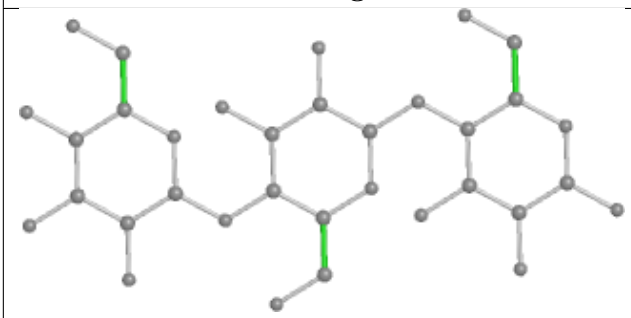
Oligosaccharide Chain U



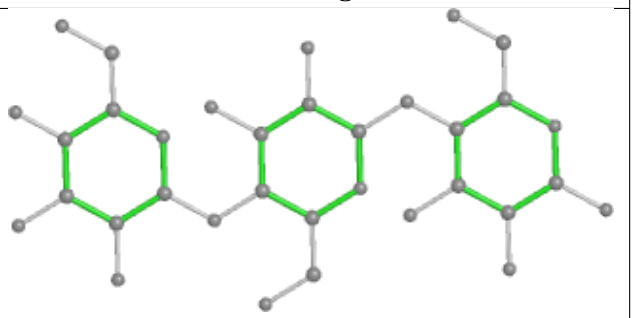
Bond lengths



Bond angles

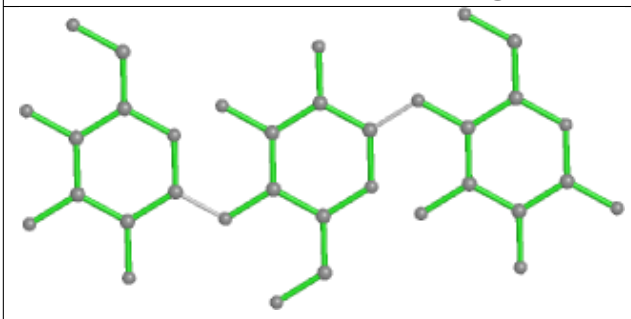


Torsions

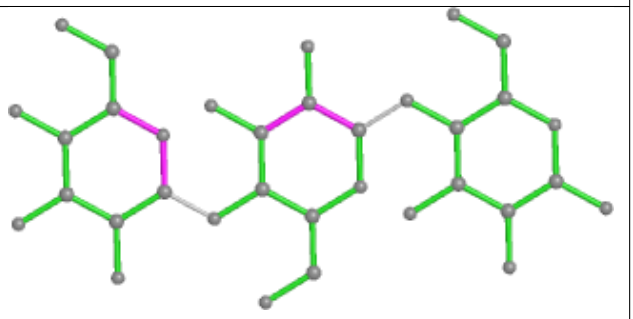


Rings

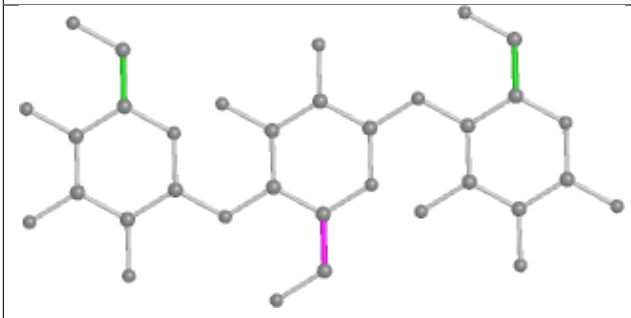
Oligosaccharide Chain W



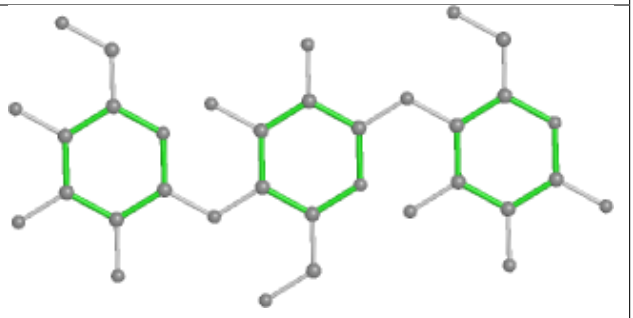
Bond lengths



Bond angles

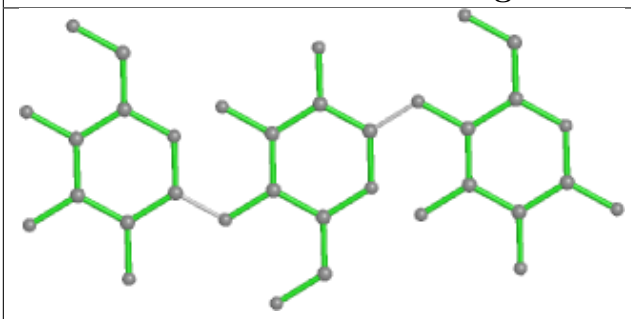


Torsions

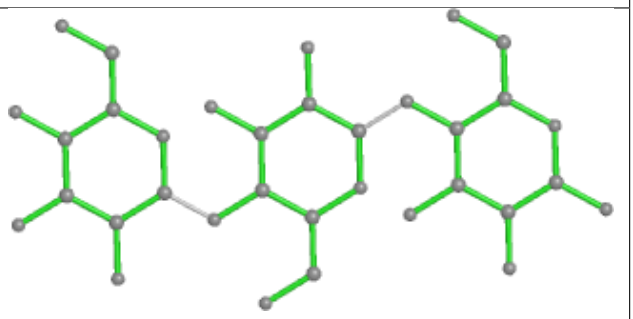


Rings

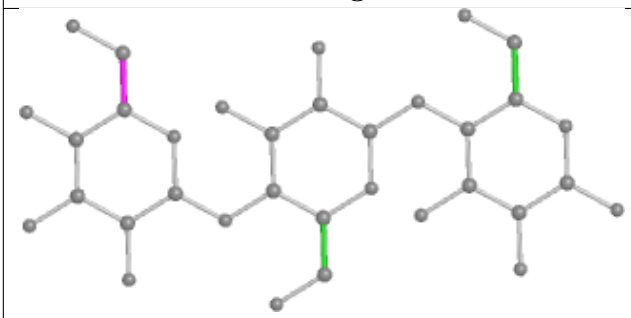
Oligosaccharide Chain X



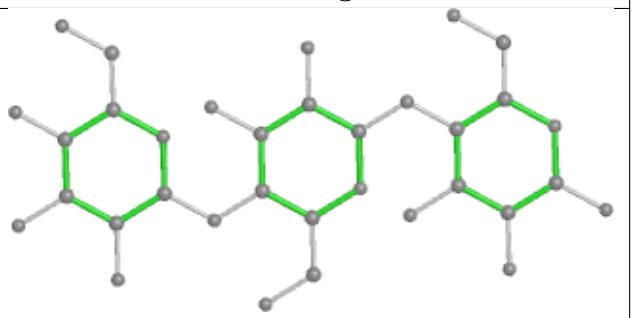
Bond lengths



Bond angles

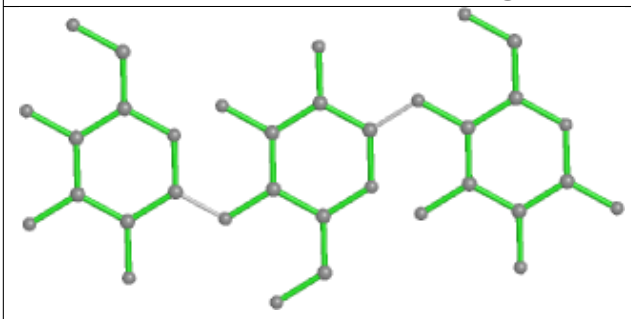


Torsions

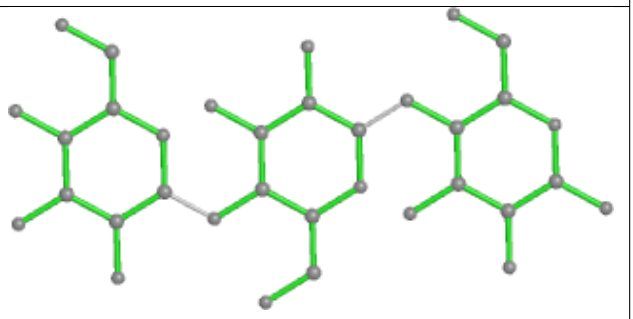


Rings

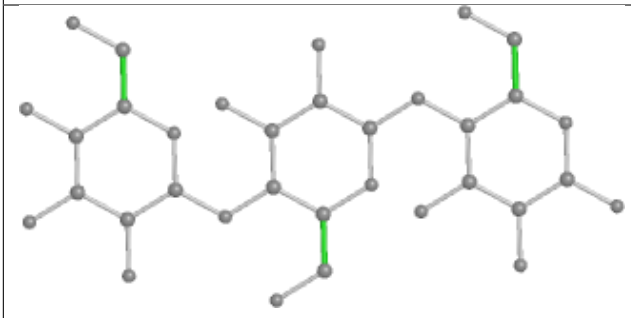
Oligosaccharide Chain a



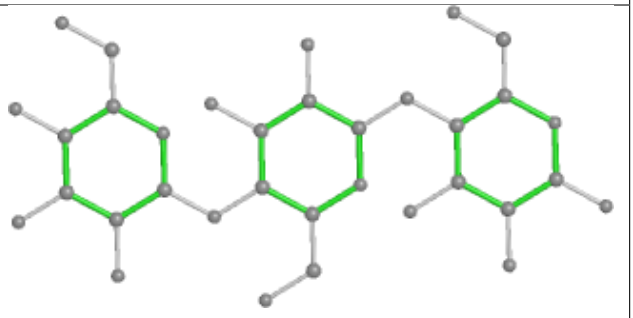
Bond lengths



Bond angles

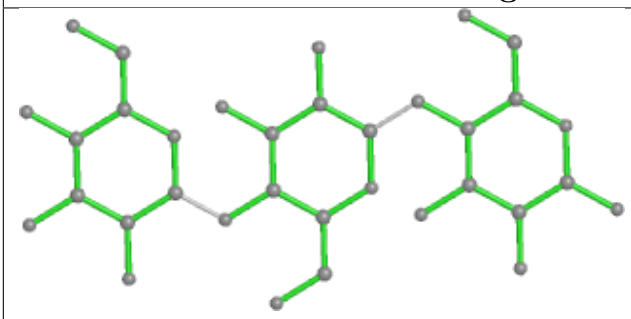


Torsions

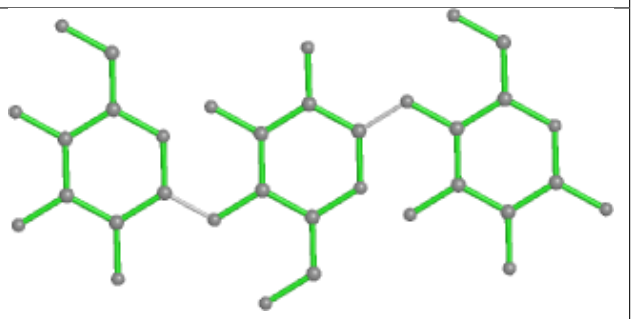


Rings

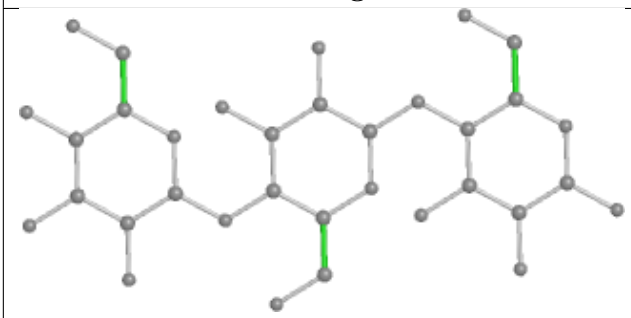
Oligosaccharide Chain c



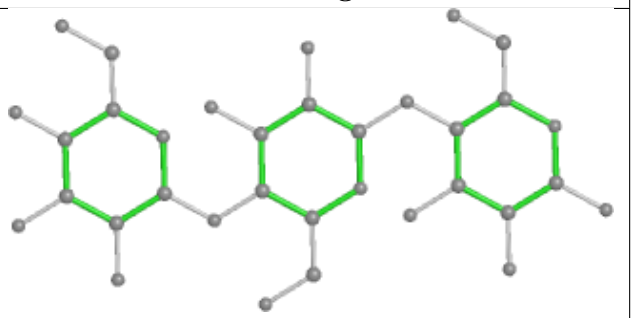
Bond lengths



Bond angles

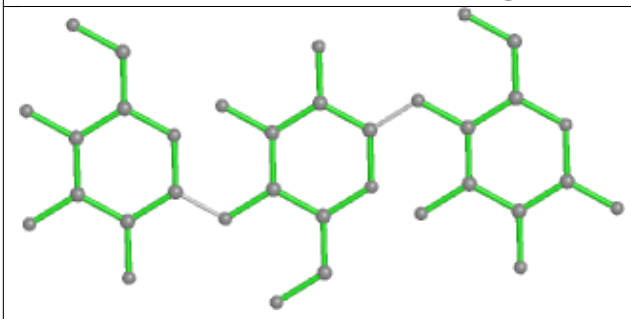


Torsions

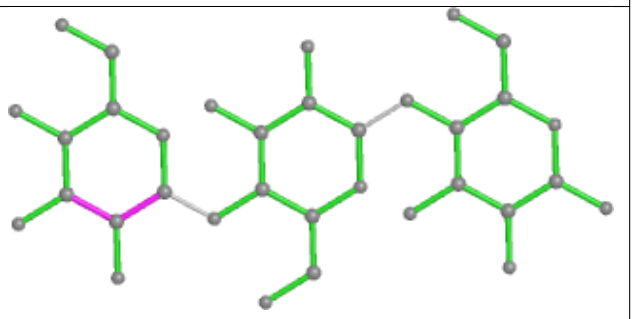


Rings

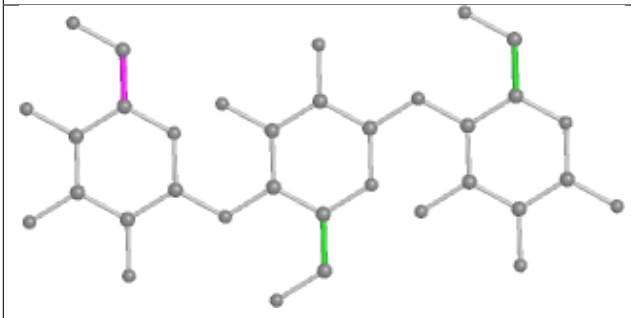
Oligosaccharide Chain e



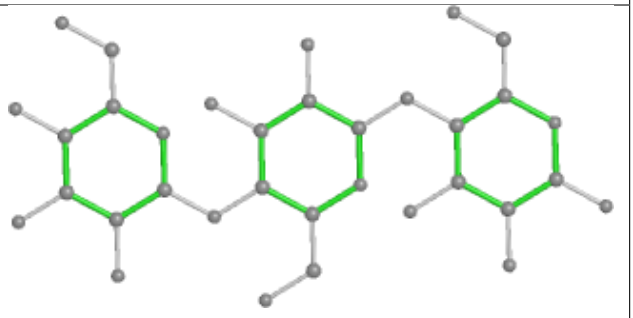
Bond lengths



Bond angles

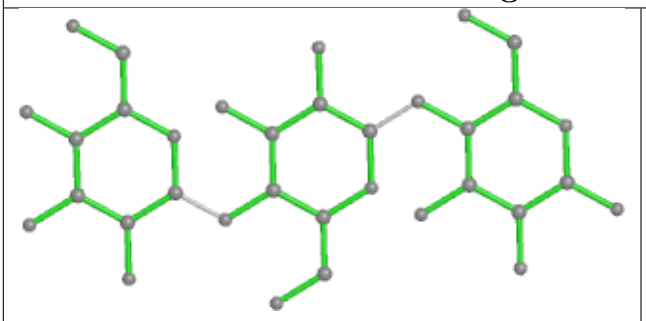


Torsions

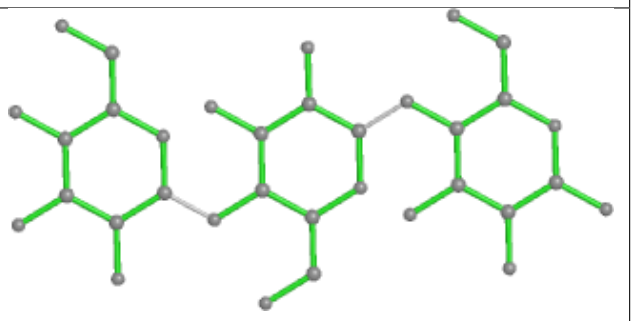


Rings

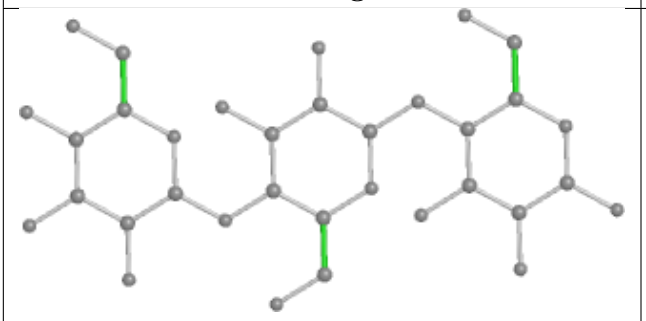
Oligosaccharide Chain f



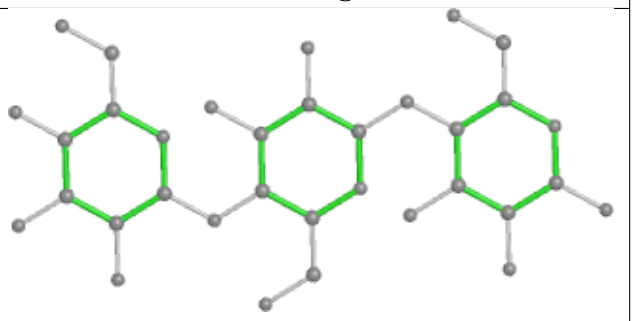
Bond lengths



Bond angles

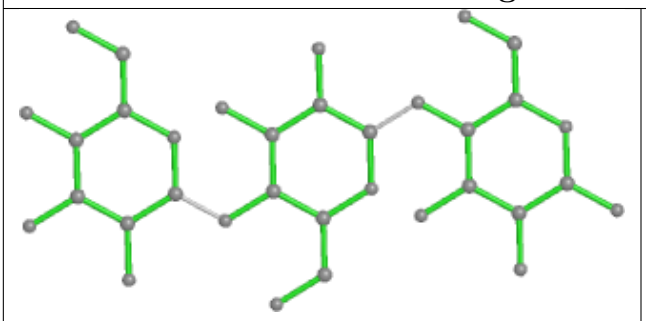


Torsions

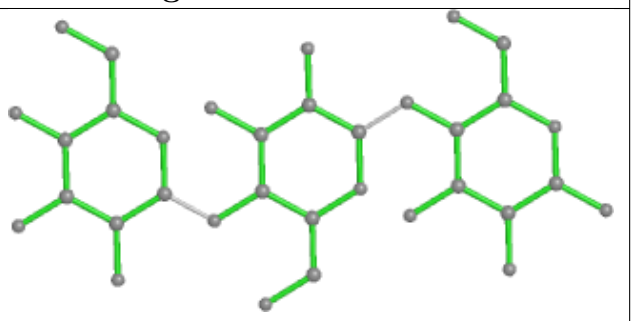


Rings

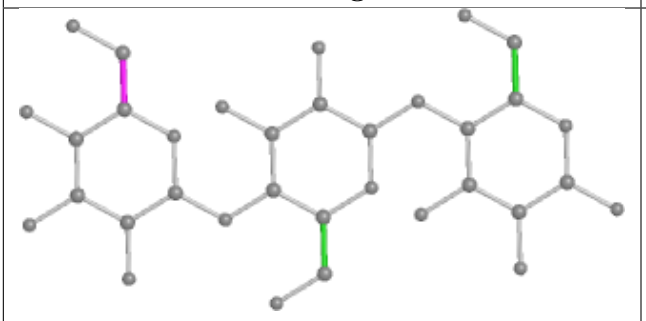
Oligosaccharide Chain g



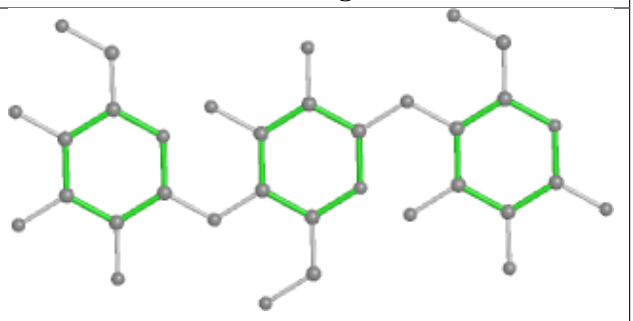
Bond lengths



Bond angles

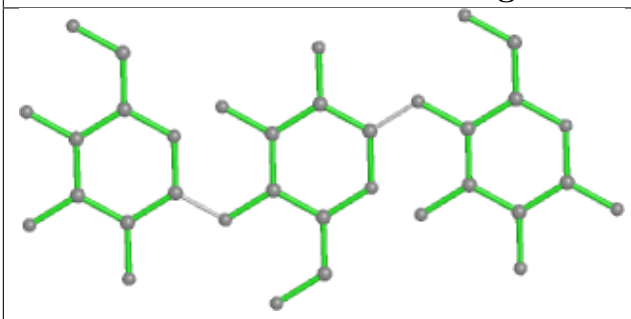


Torsions

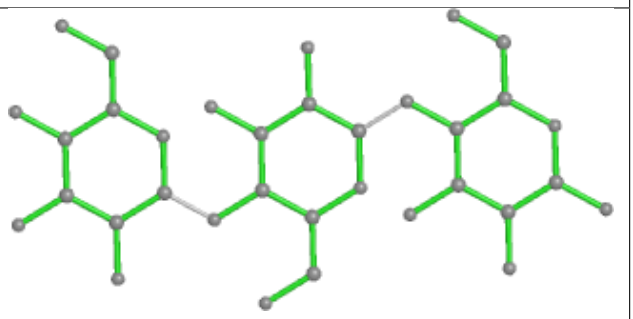


Rings

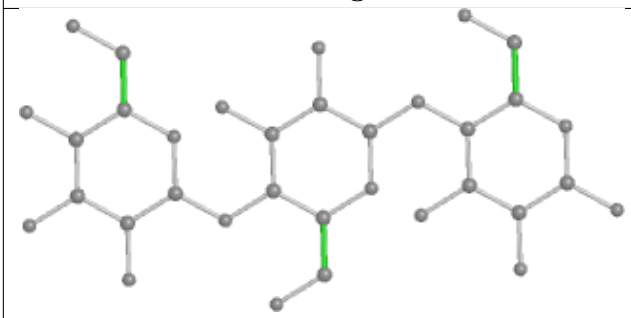
Oligosaccharide Chain h



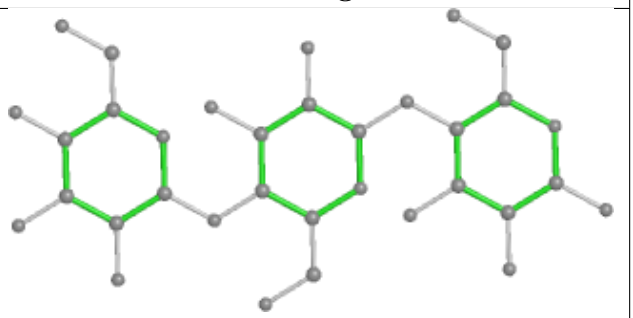
Bond lengths



Bond angles

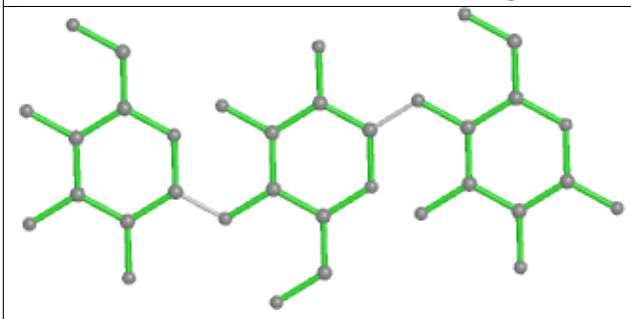


Torsions

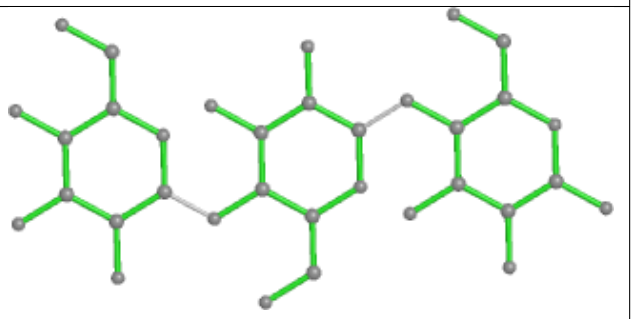


Rings

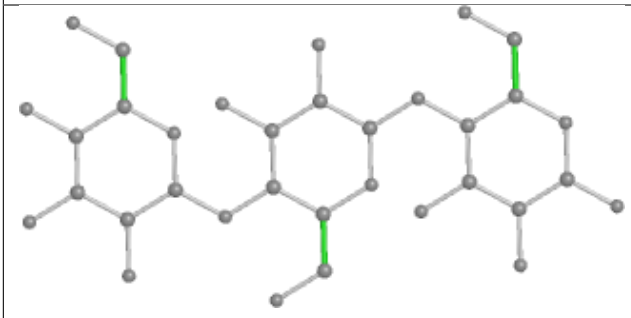
Oligosaccharide Chain i



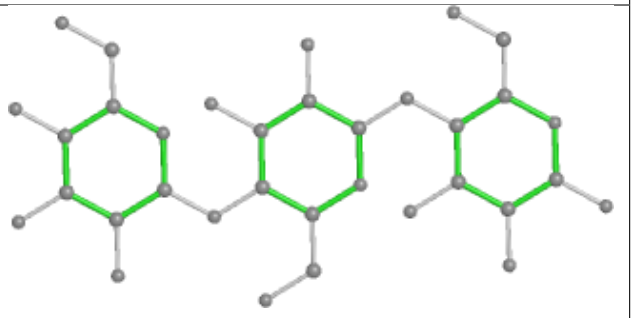
Bond lengths



Bond angles

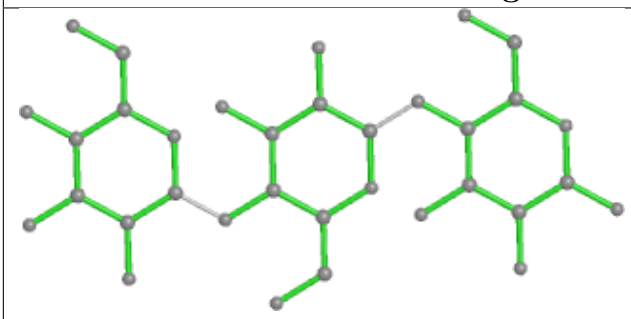


Torsions

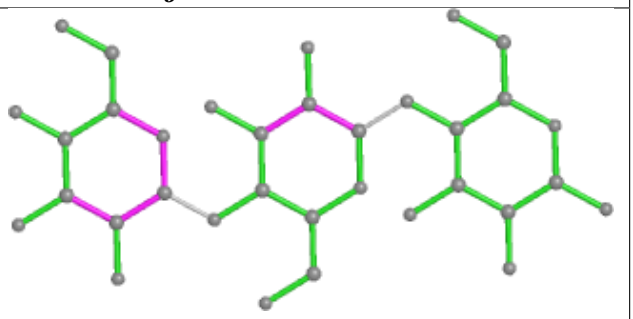


Rings

Oligosaccharide Chain j



Bond lengths



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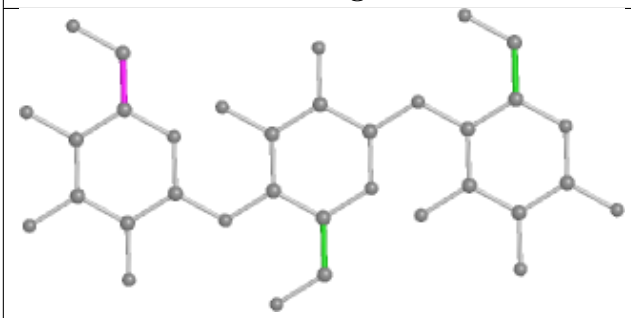
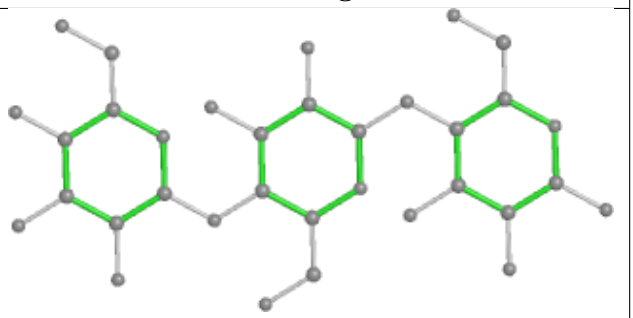
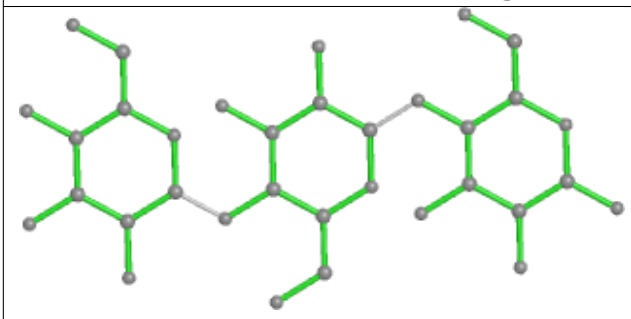


Torsions



Rings

Oligosaccharide Chain k



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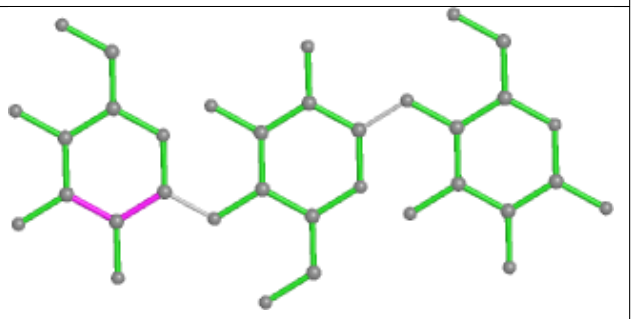

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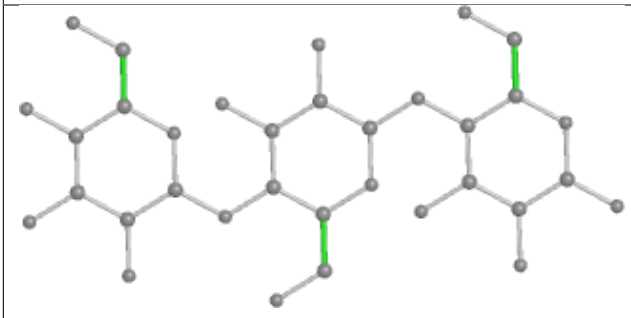

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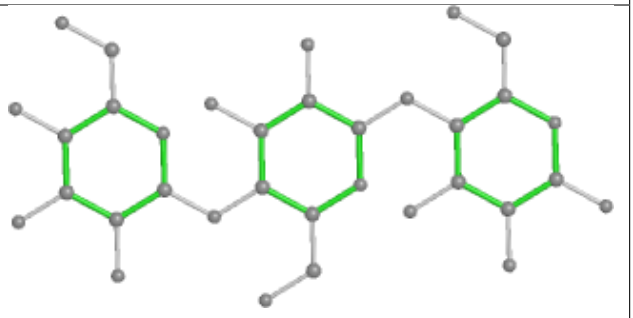
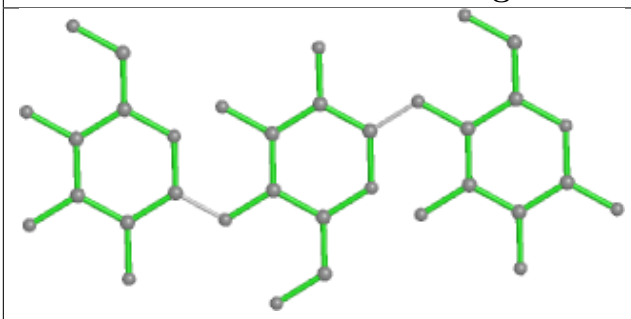


Rings

Oligosaccharide Chain m



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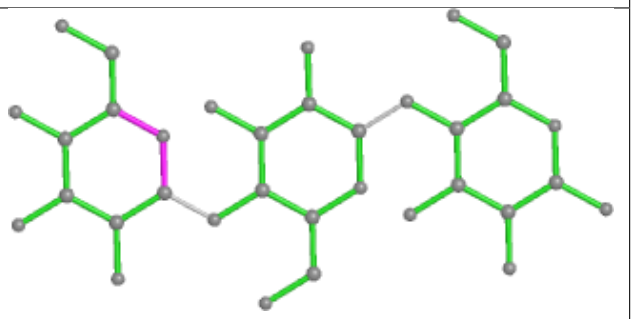

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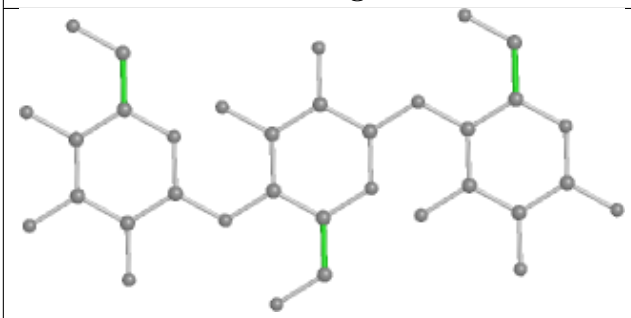

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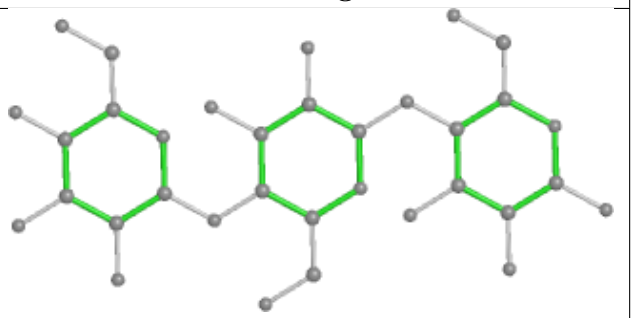
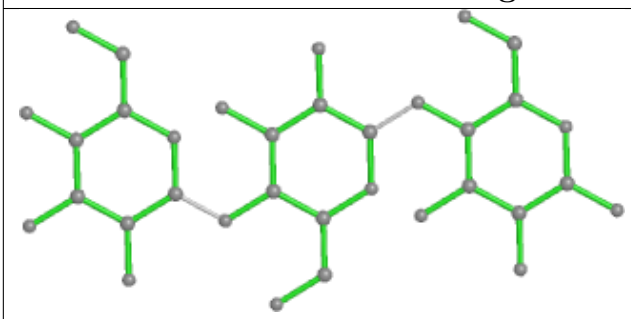


Rings

Oligosaccharide Chain o



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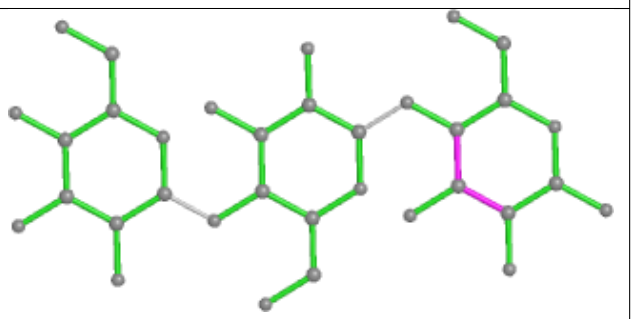

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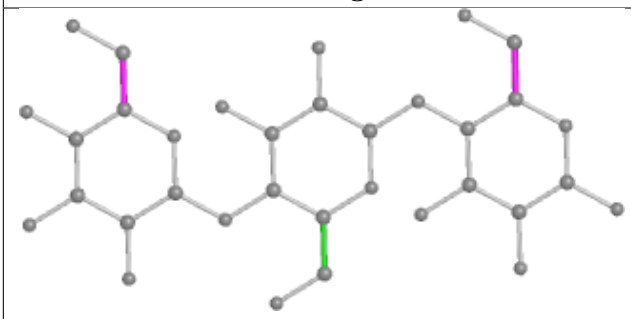

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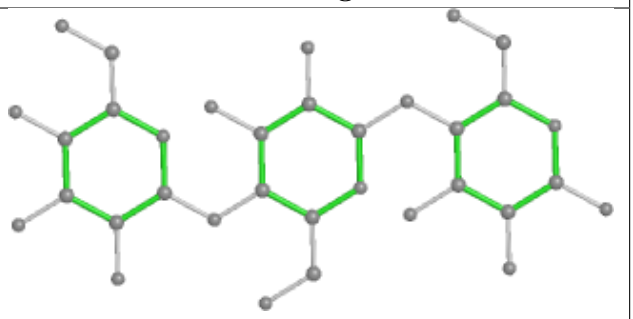
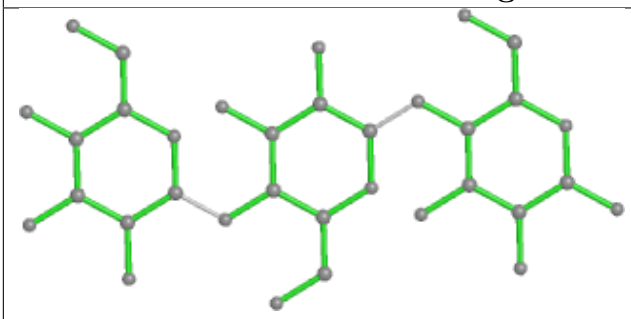


Rings

Oligosaccharide Chain p



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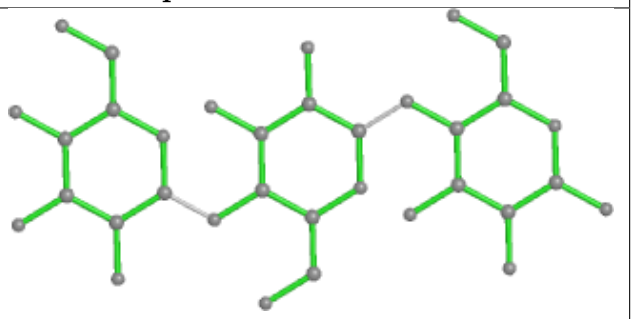
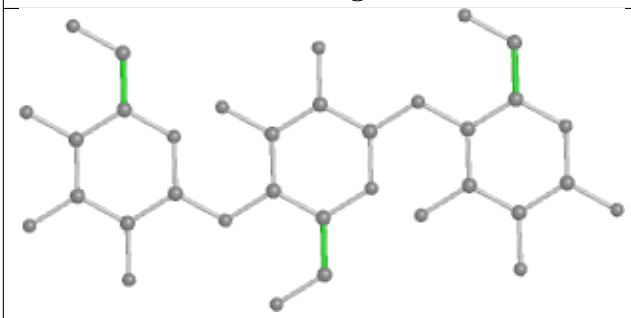


Bond angles



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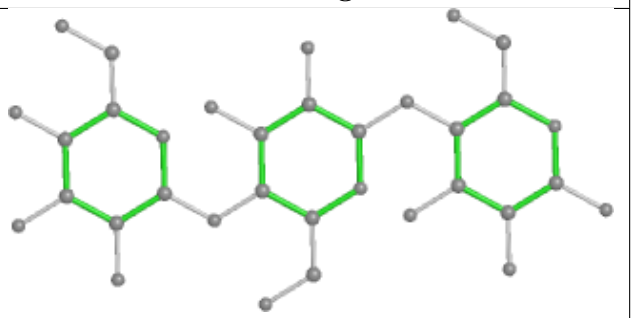
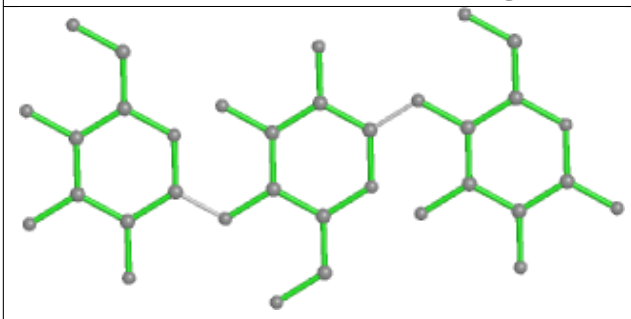


Rings

Oligosaccharide Chain r



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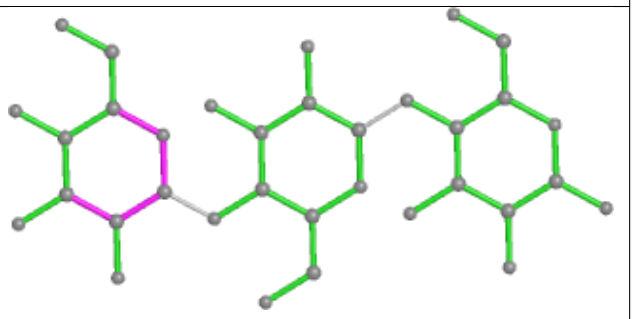

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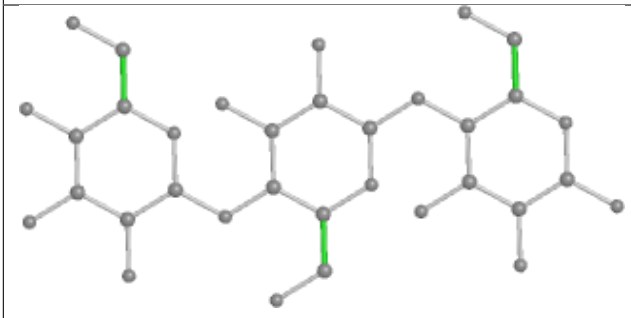

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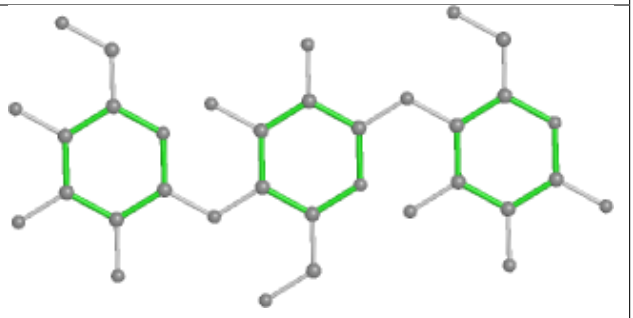
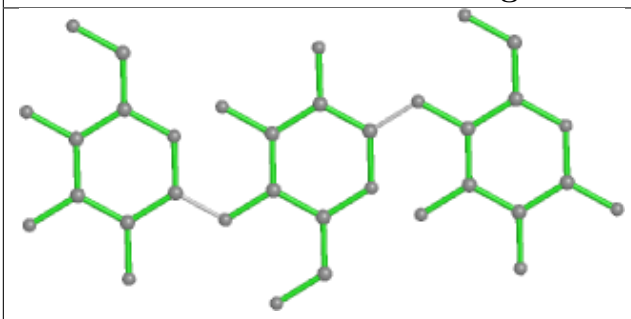


Rings

Oligosaccharide Chain s



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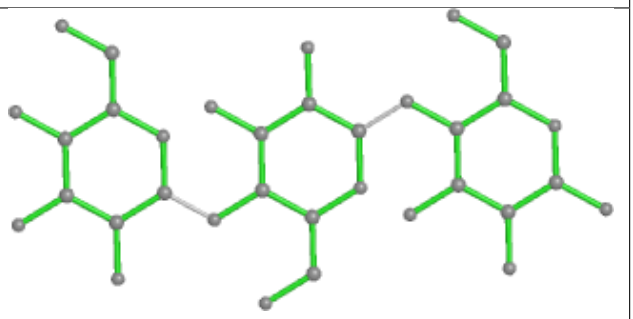
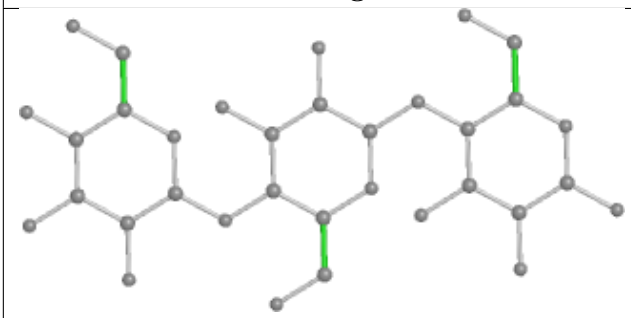


Bond angles



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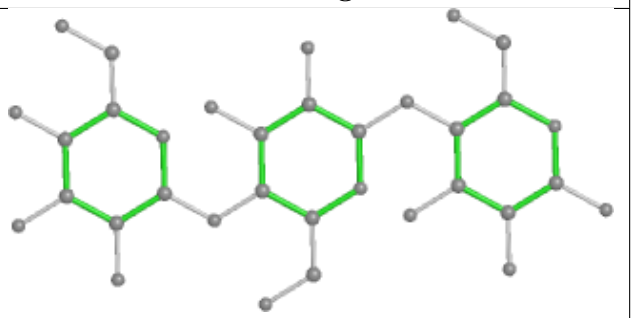
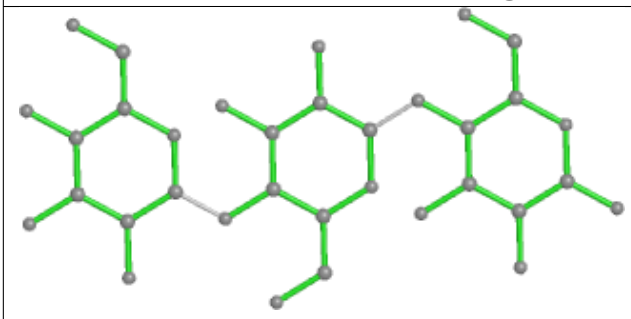


Rings

Oligosaccharide Chain t



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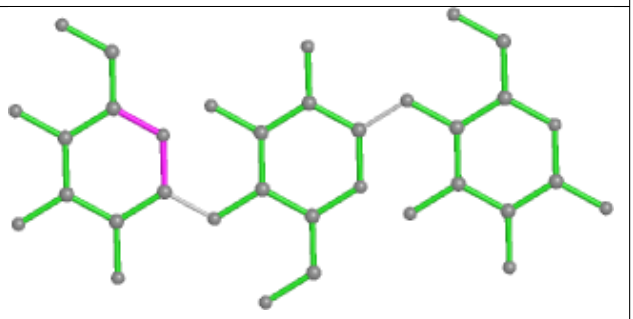

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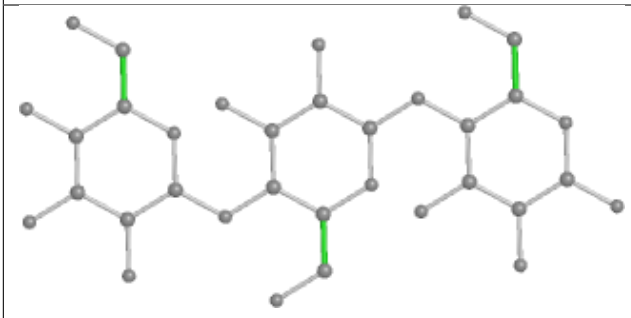

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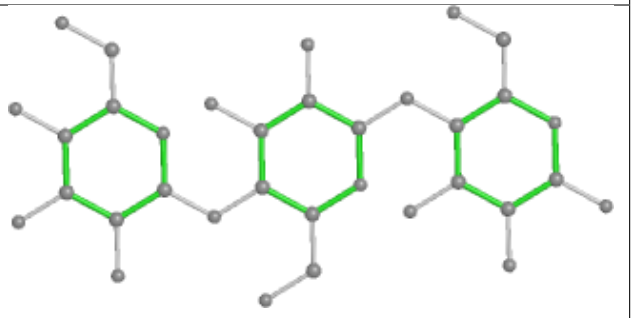
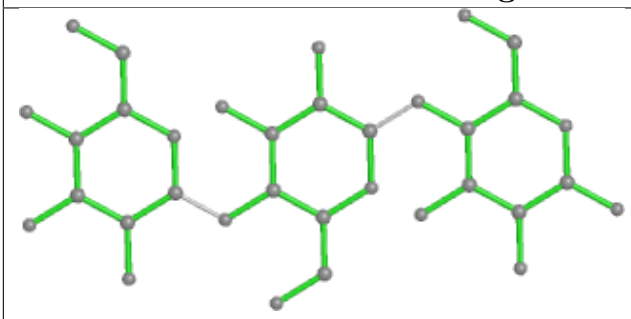


Rings

Oligosaccharide Chain v



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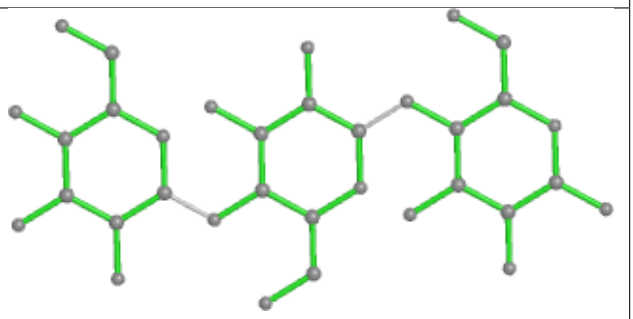
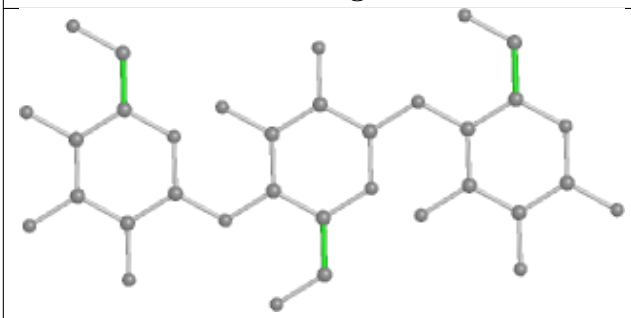


Bond angles



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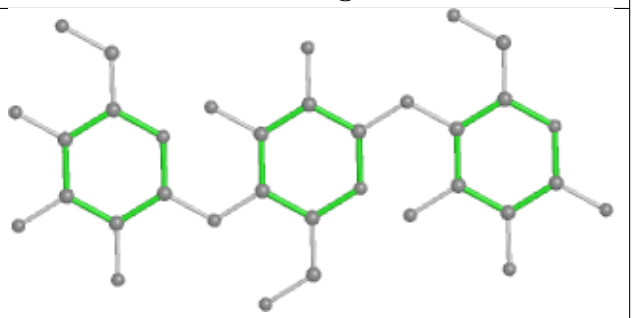
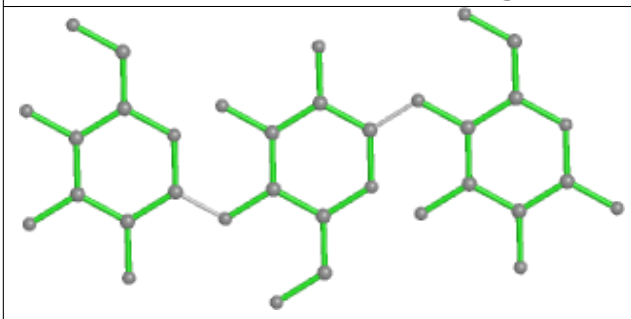


Rings

Oligosaccharide Chain x



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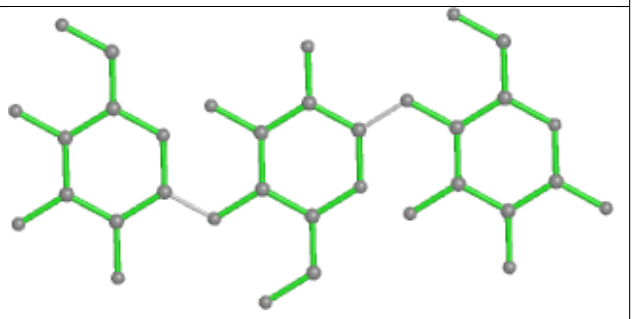
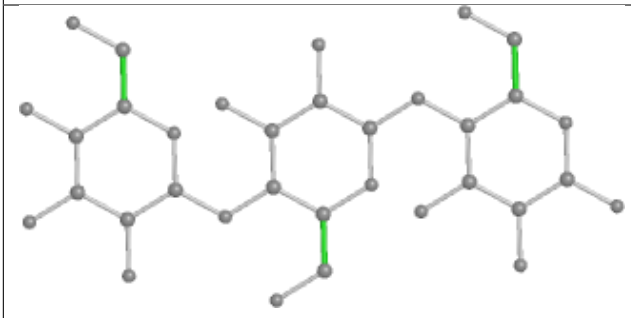
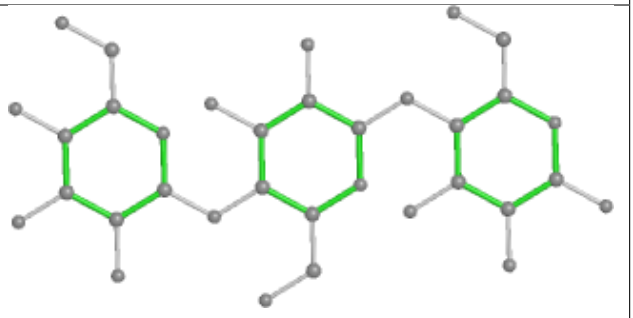


Bond angles

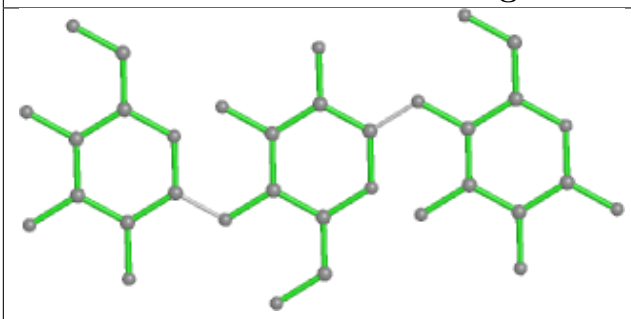


Torsions



Rings

Oligosaccharide Chain z



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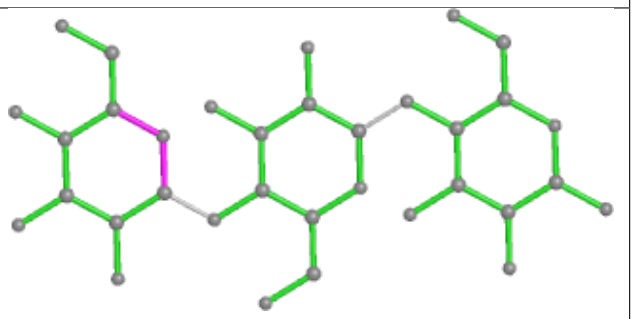
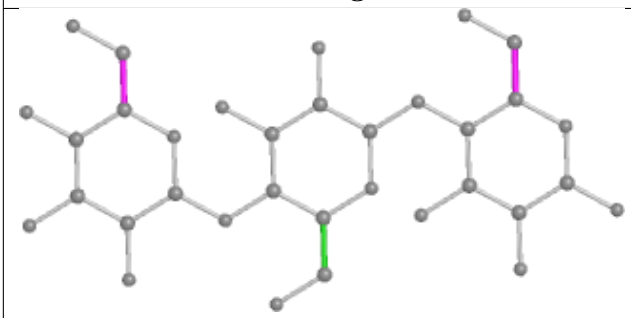


Bond angles



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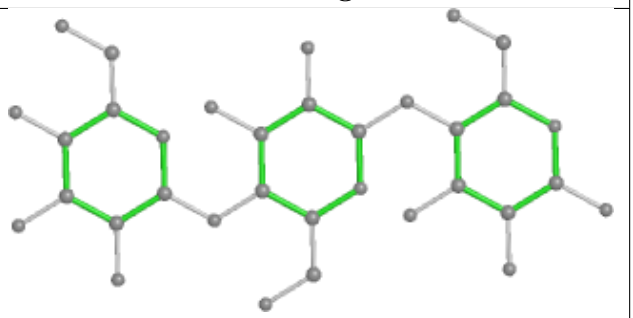
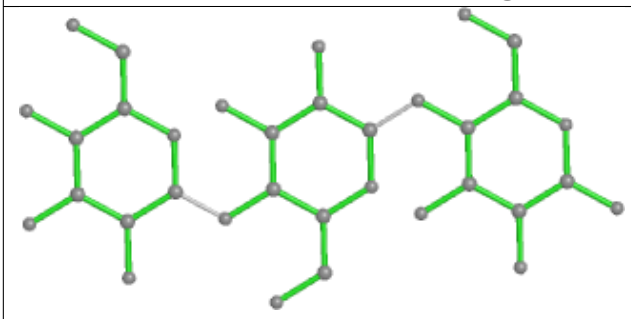


Rings

Oligosaccharide Chain 0



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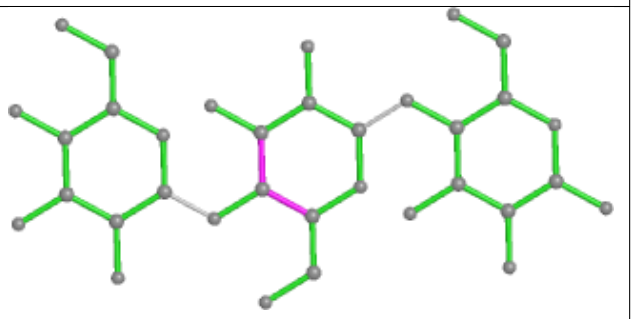
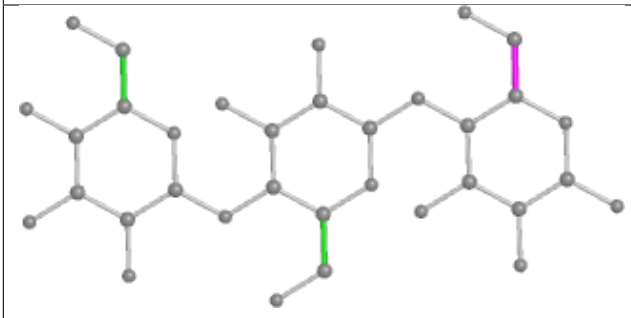


Bond angles



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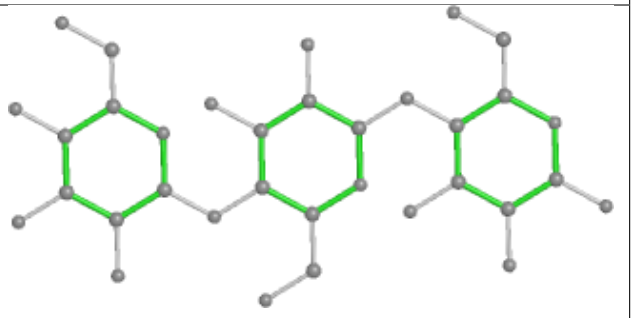
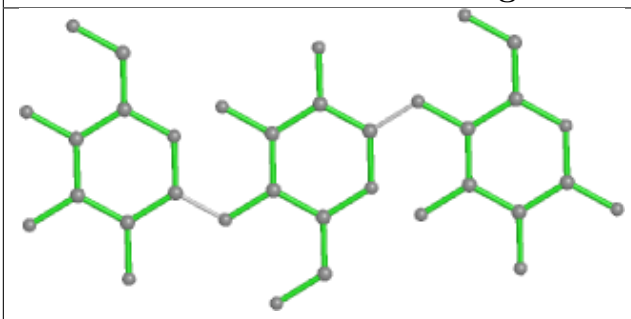


Rings

Oligosaccharide Chain 2



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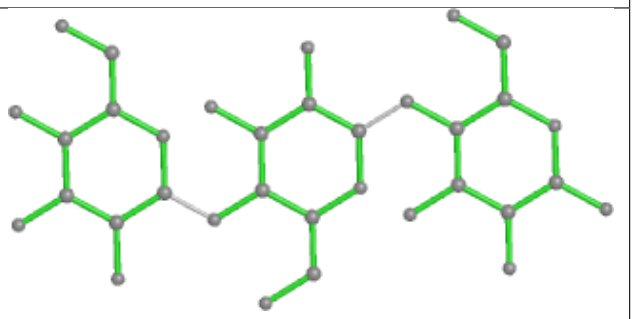
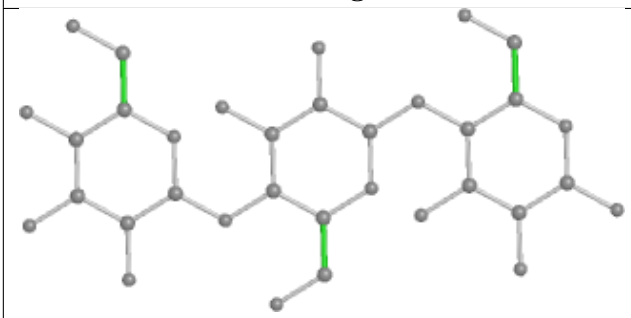


Bond angles



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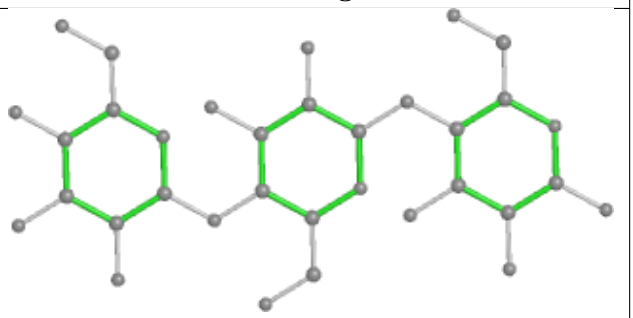
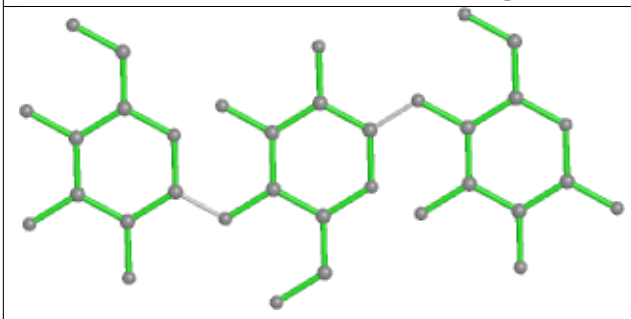
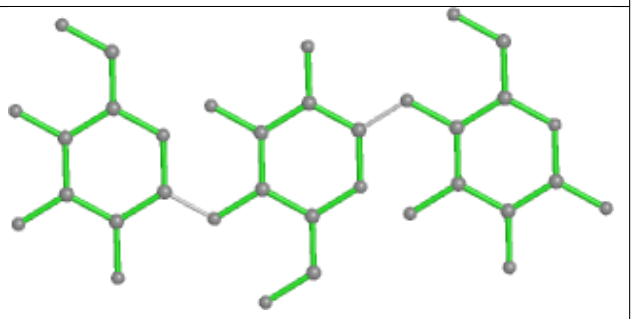


Rings

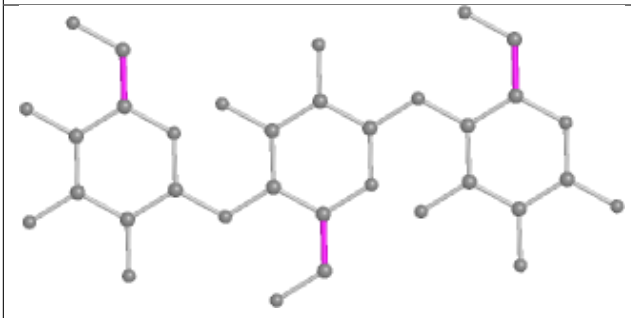
Oligosaccharide Chain 4



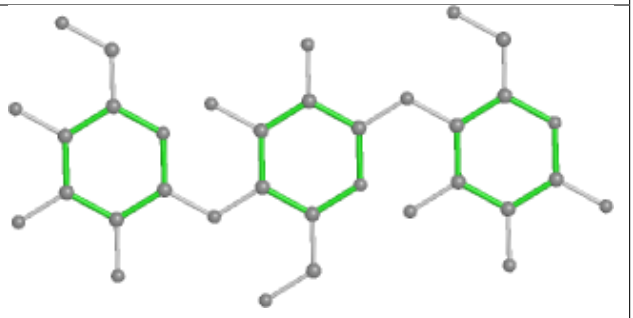
Bond lengths



Bond angles

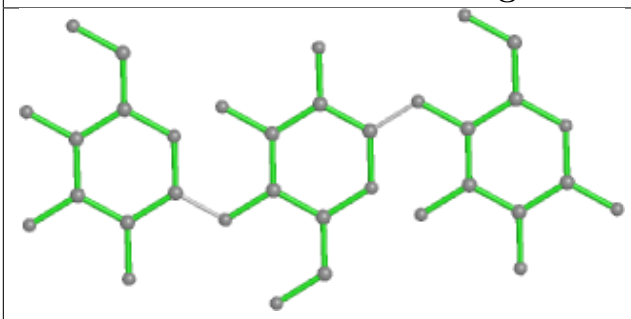


Torsions

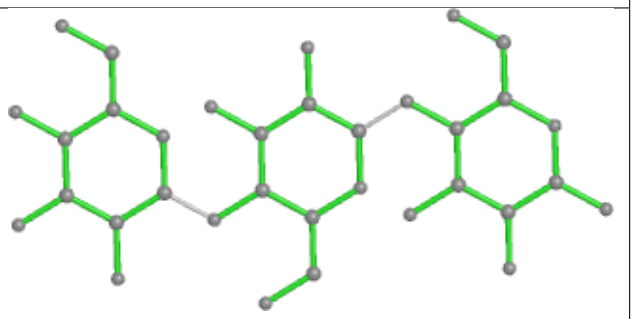


Rings

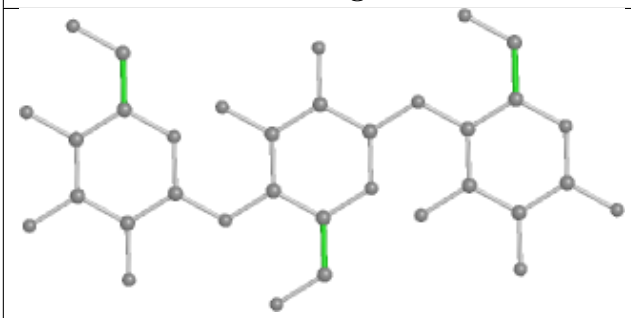
Oligosaccharide Chain 5



Bond lengths



Bond angles



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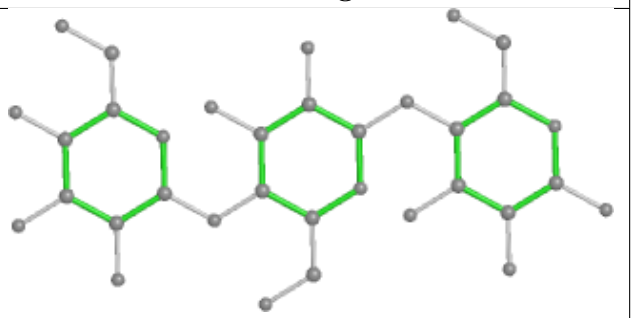
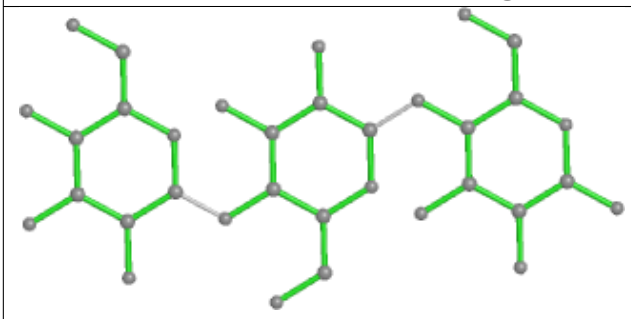
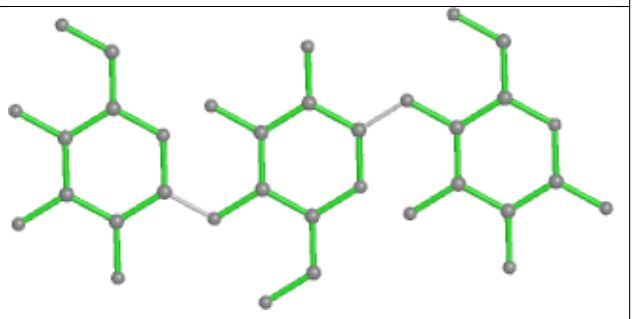


Rings

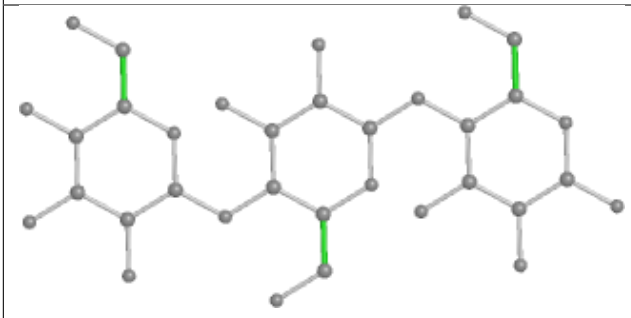
Oligosaccharide Chain 7



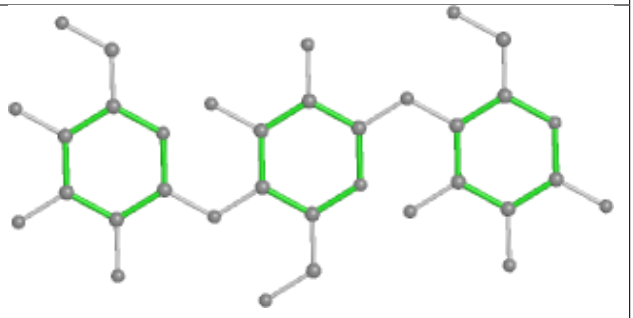
Bond lengths



Bond angles

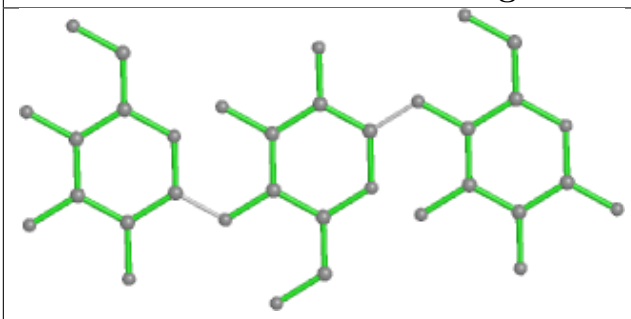


Torsions



Rings

Oligosaccharide Chain 8



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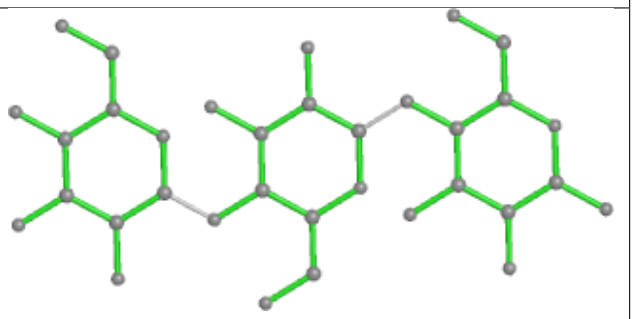

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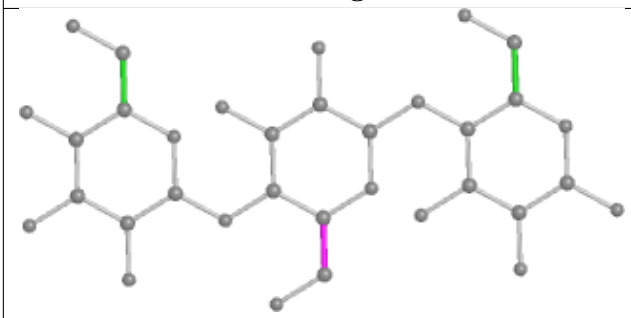

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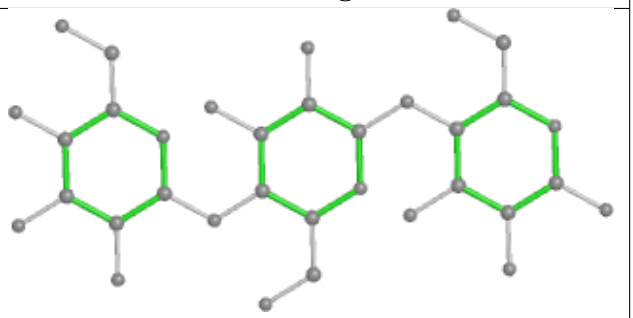
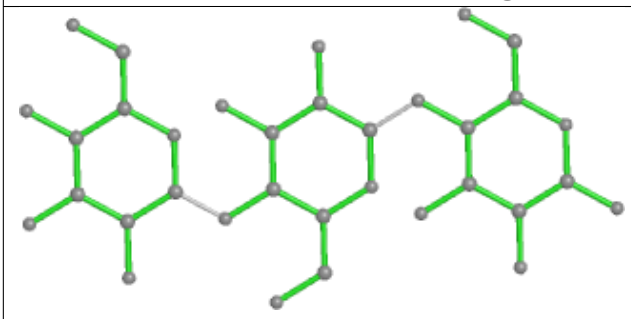


Rings

Oligosaccharide Chain 9



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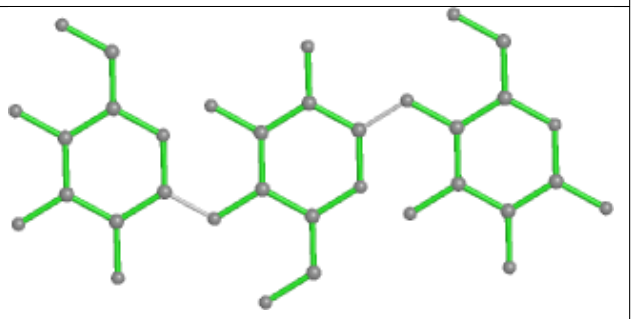
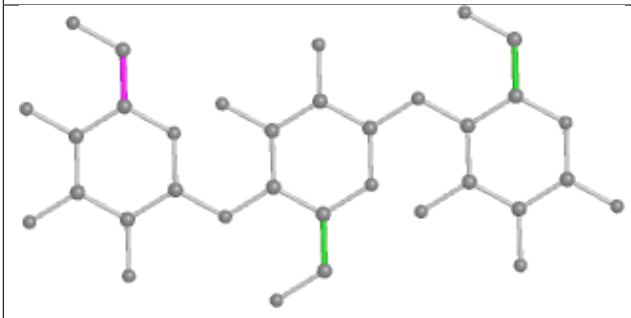


Bond angles



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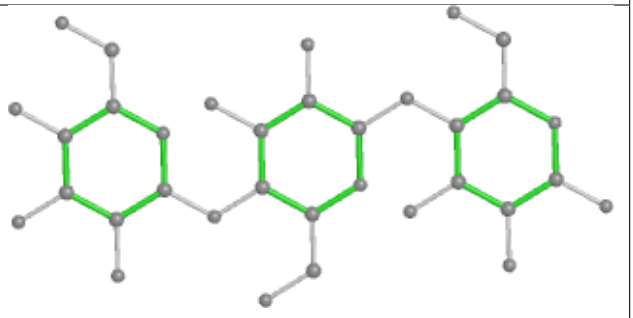
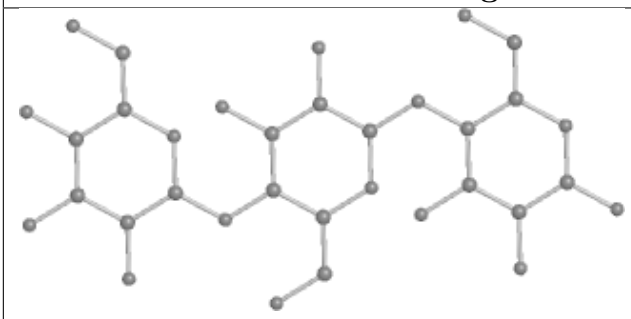


Rings

Oligosaccharide Chain AA



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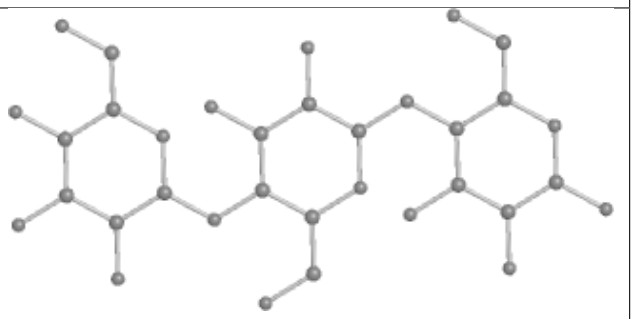
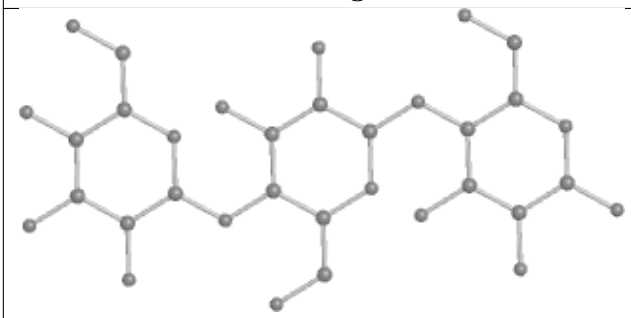


Bond angles



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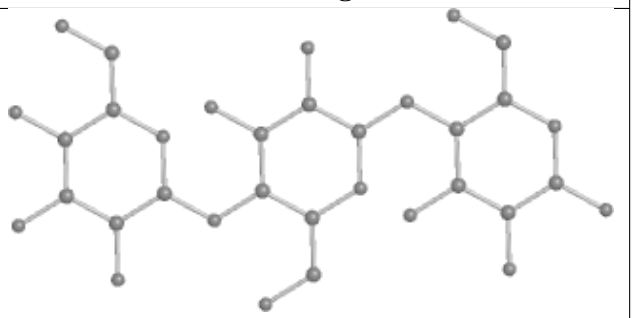
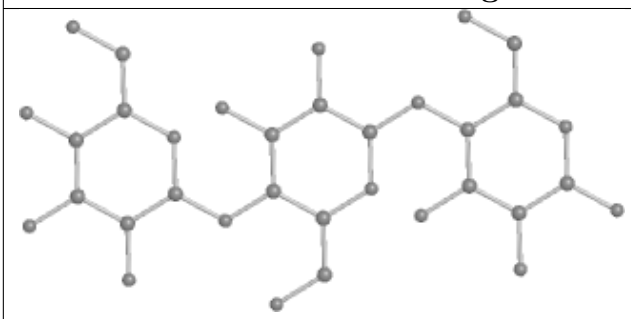


Rings

Oligosaccharide Chain BA



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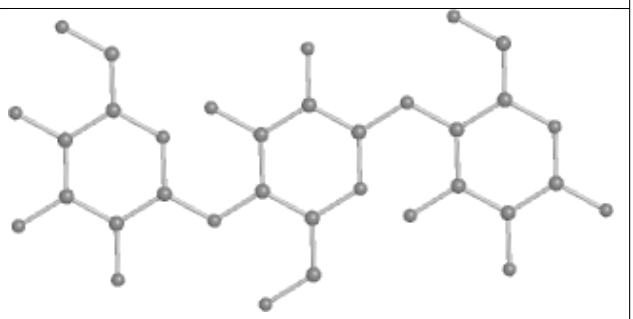
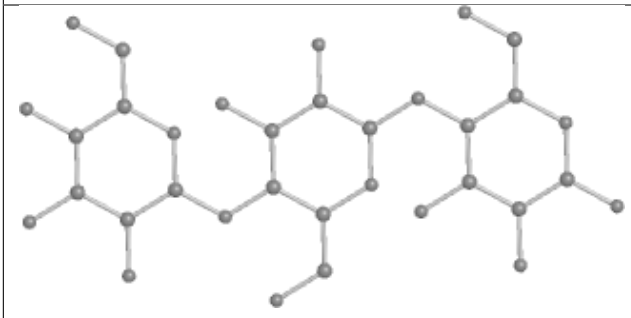


Bond angles



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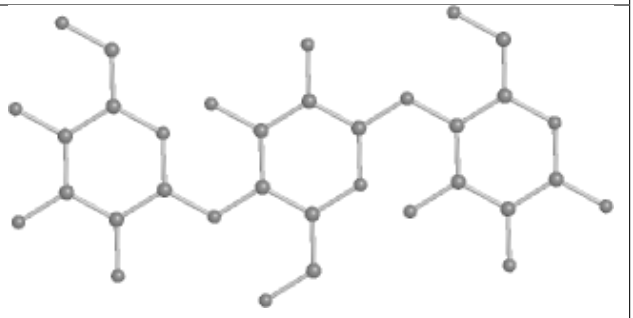
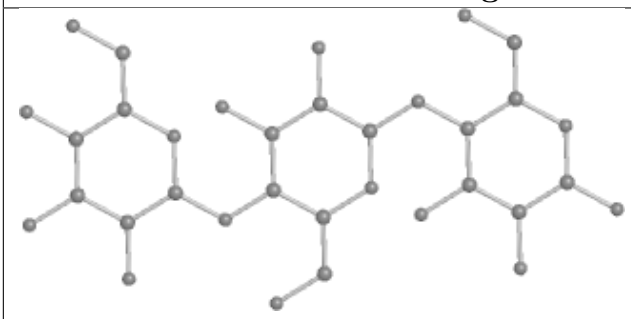


Rings

Oligosaccharide Chain CA



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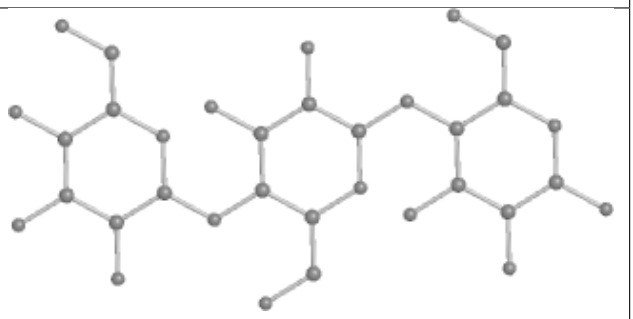
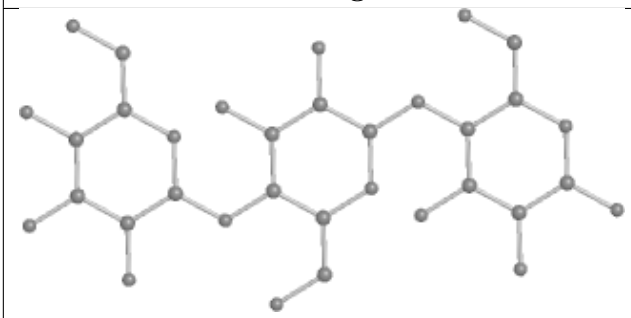
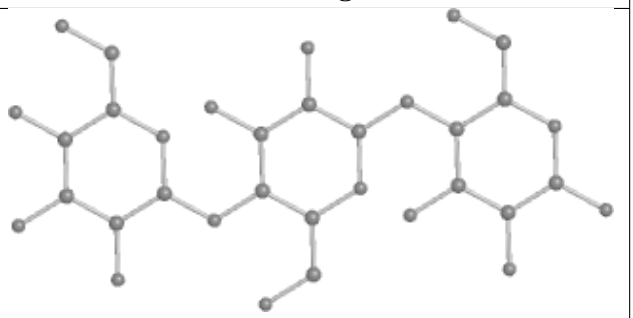


Bond angles

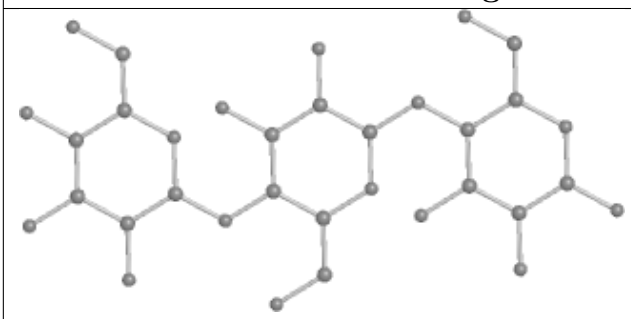


Torsions



Rings

Oligosaccharide Chain EA



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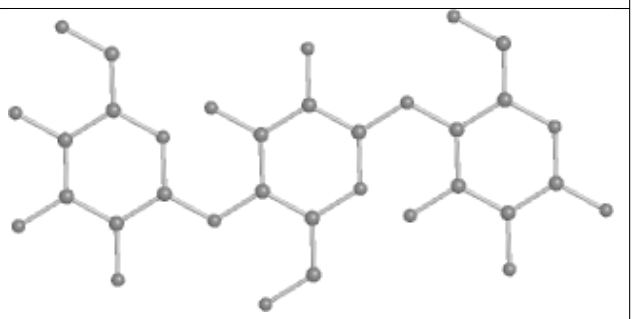
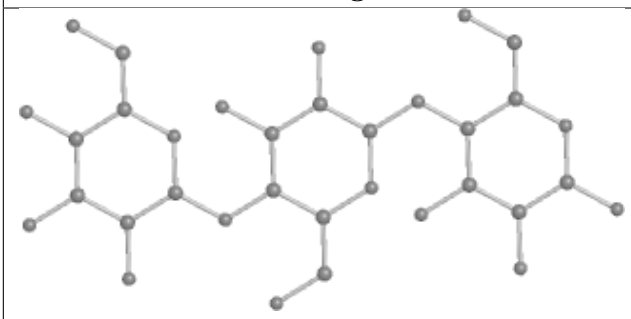


Bond angles



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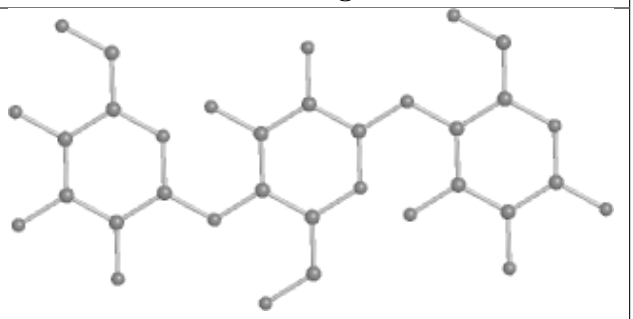
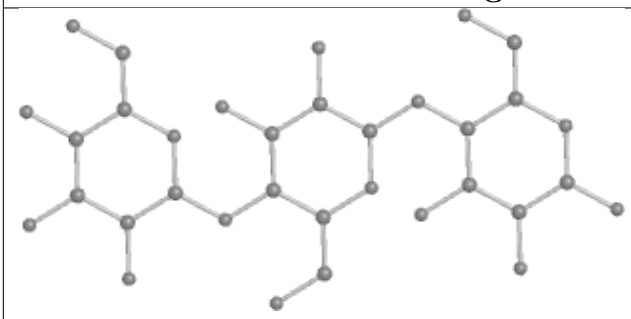


Rings

Oligosaccharide Chain FA



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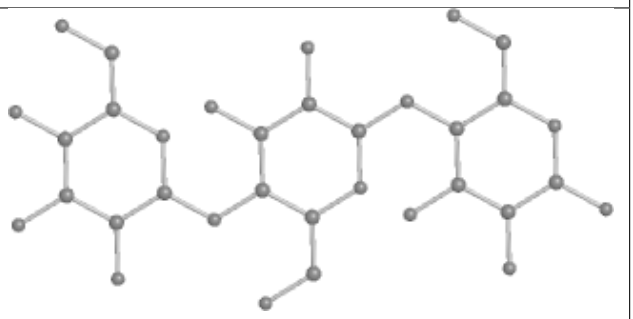
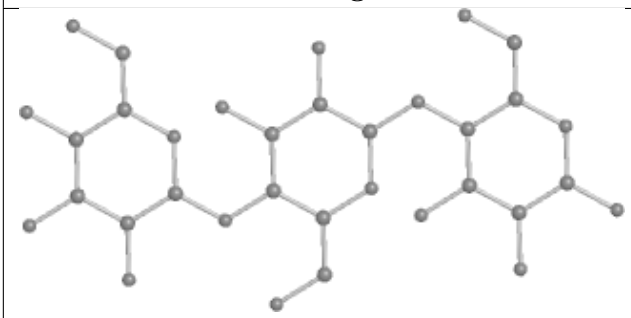
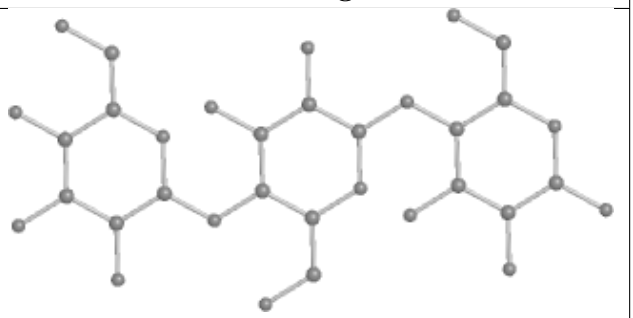


Bond angles

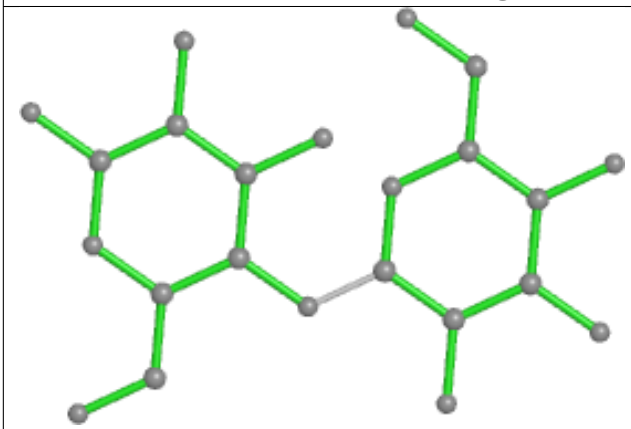


Torsions



Rings

Oligosaccharide Chain V



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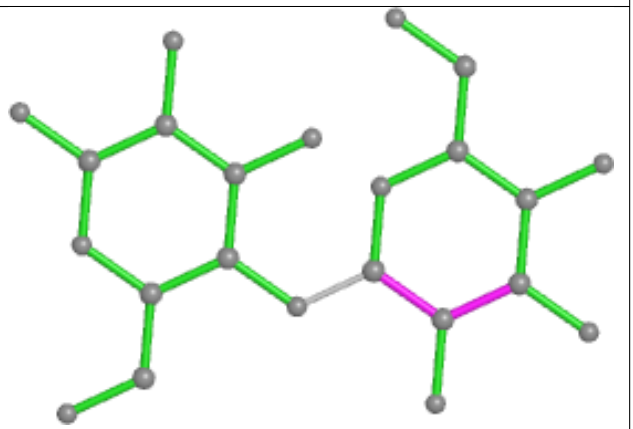
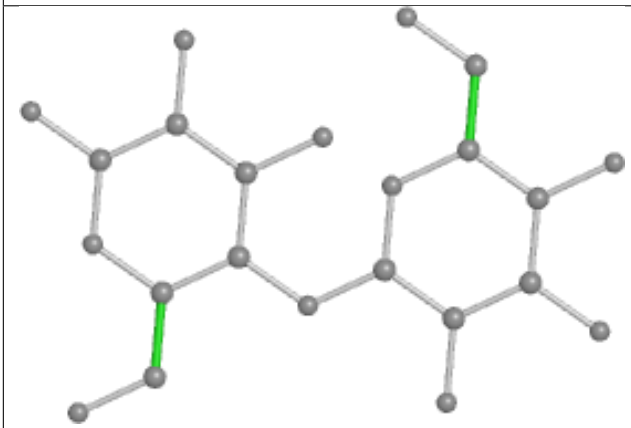
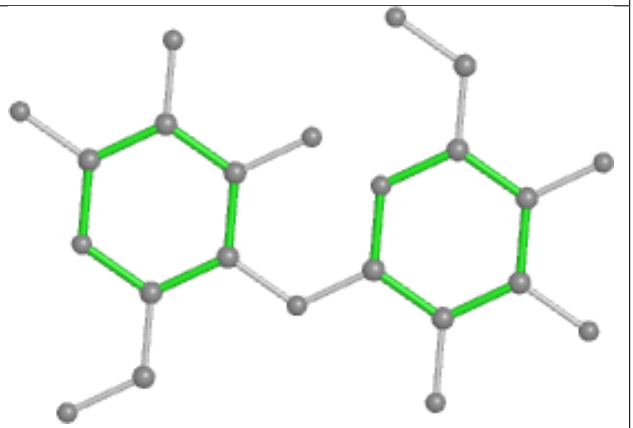


Bond angles

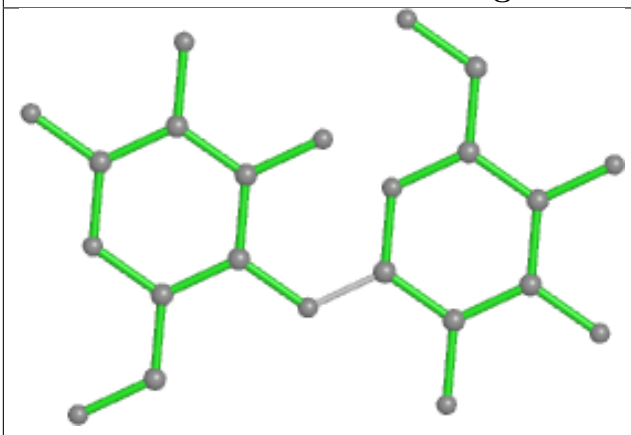


Torsions



Rings

Oligosaccharide Chain Y



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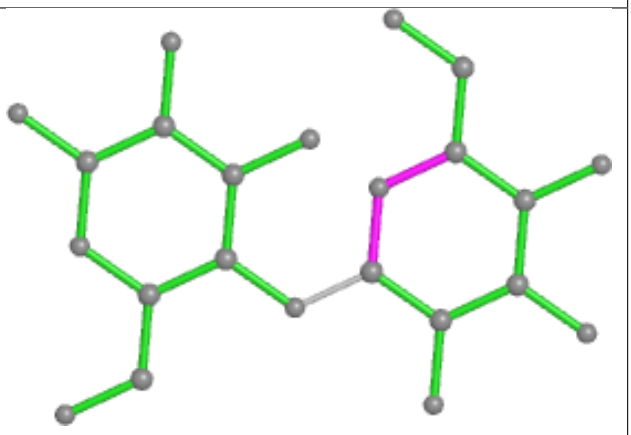
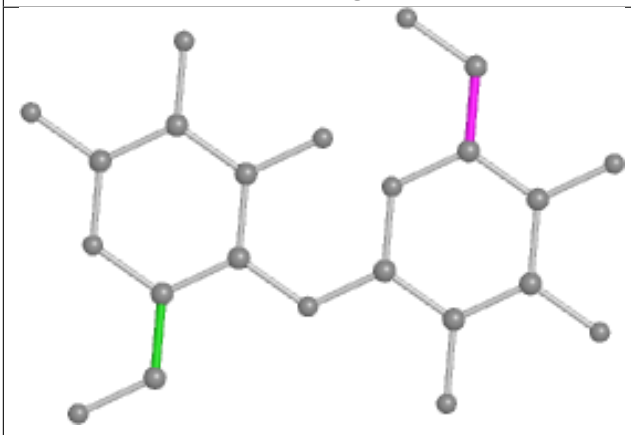
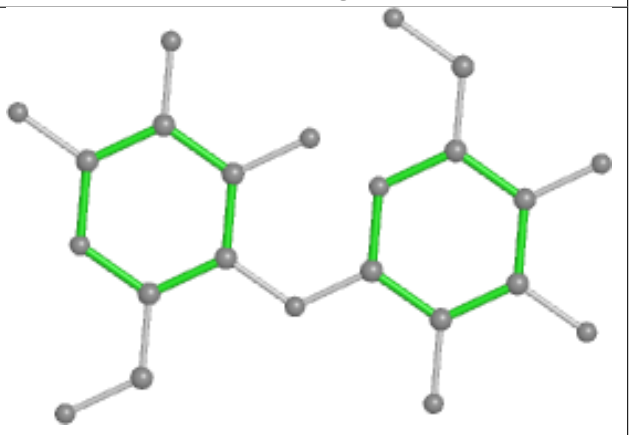


Bond angles

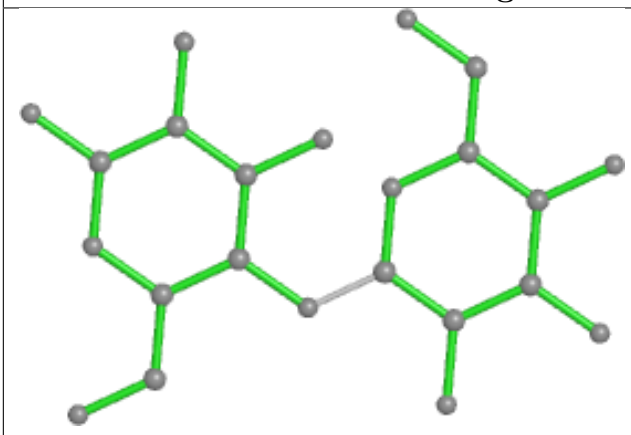


Torsions



Rings

Oligosaccharide Chain Z



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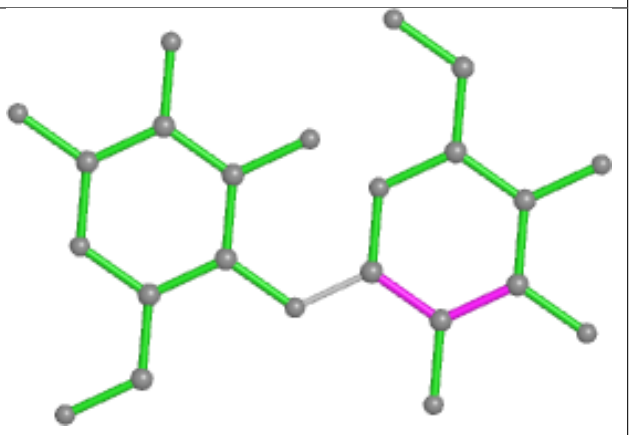
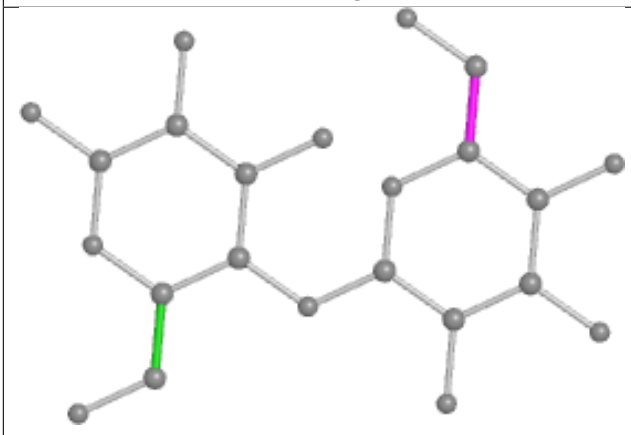
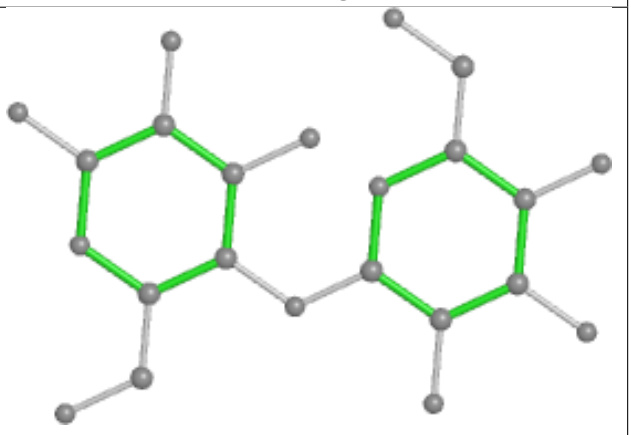


Bond angles

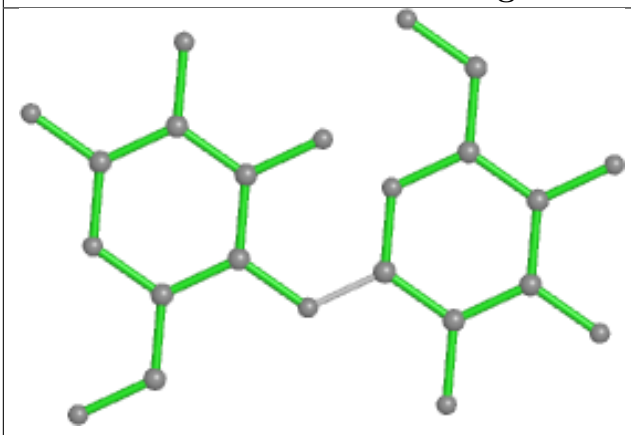


Torsions



Rings

Oligosaccharide Chain b



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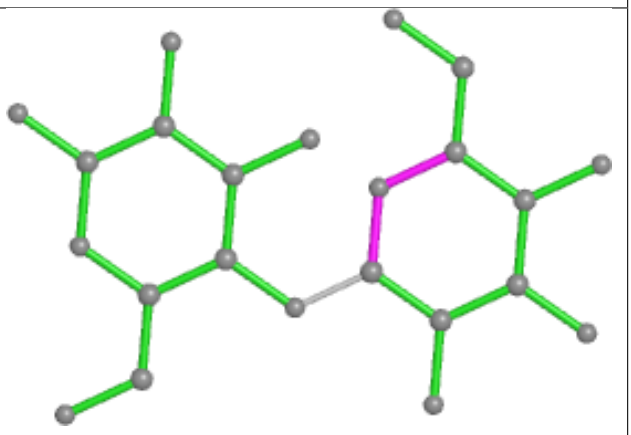
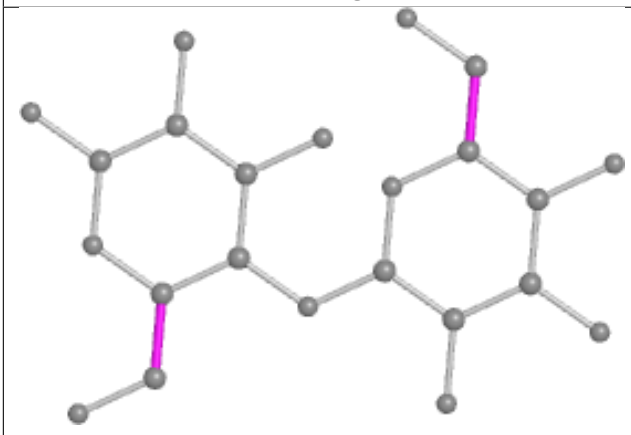
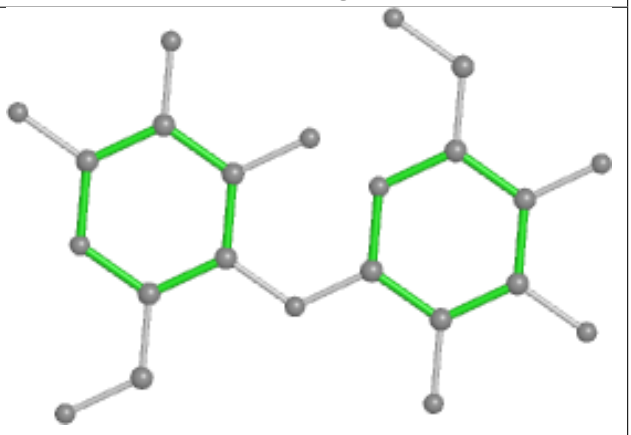


Bond angles

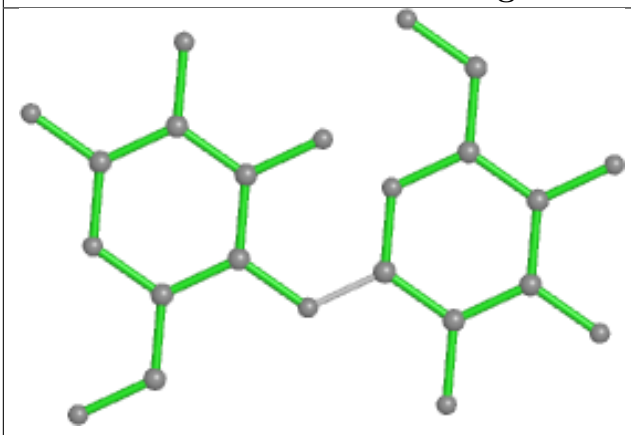


Torsions

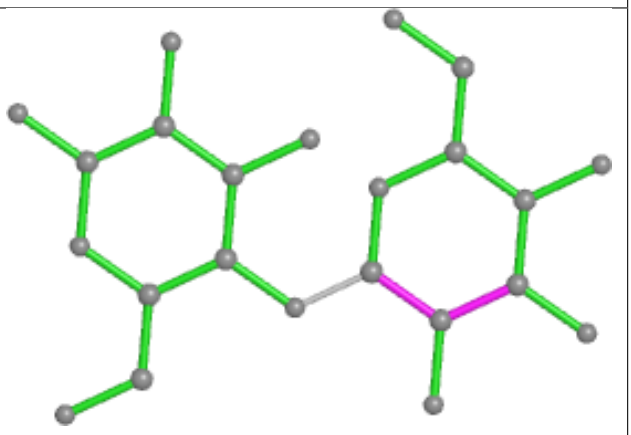


Rings

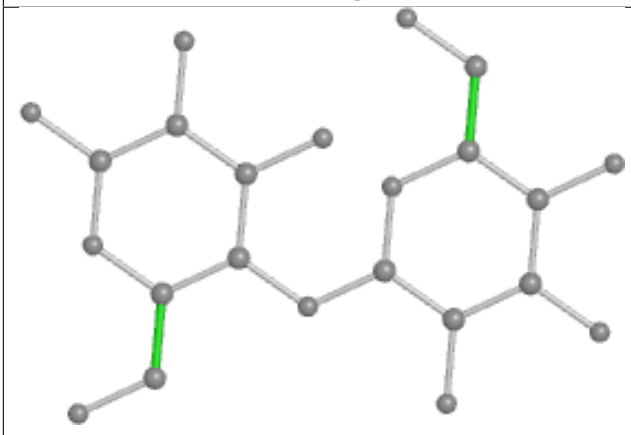
Oligosaccharide Chain d



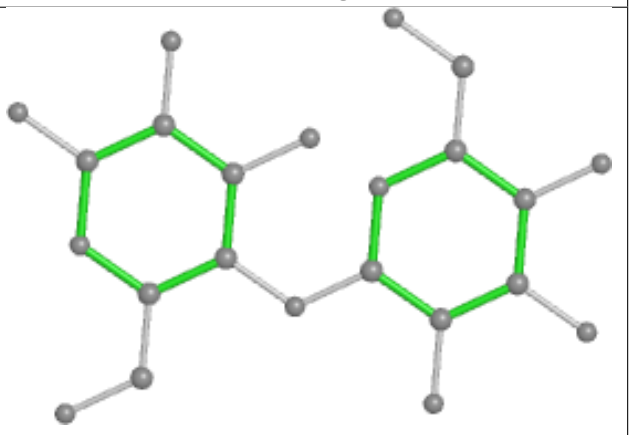
Bond lengths



Bond angles

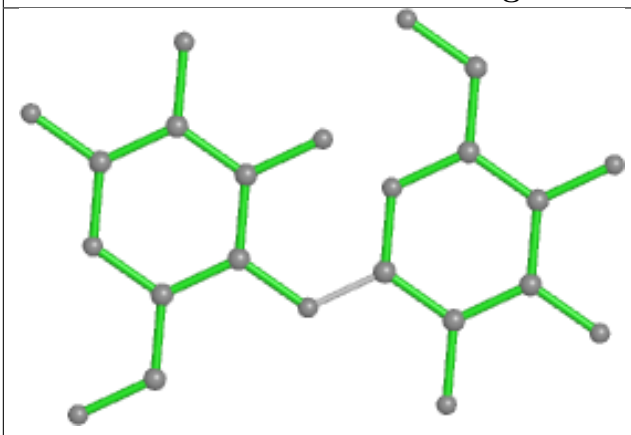


Torsions

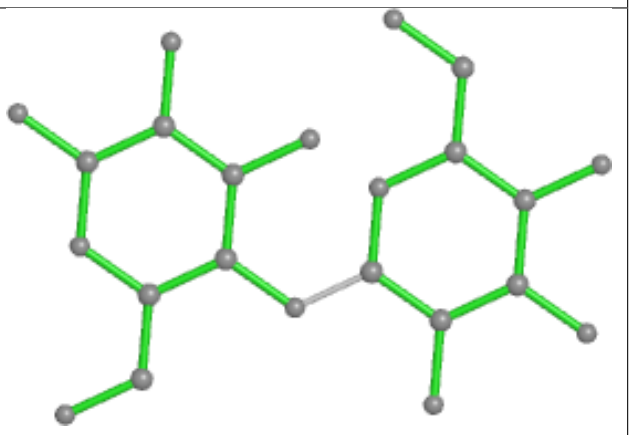


Rings

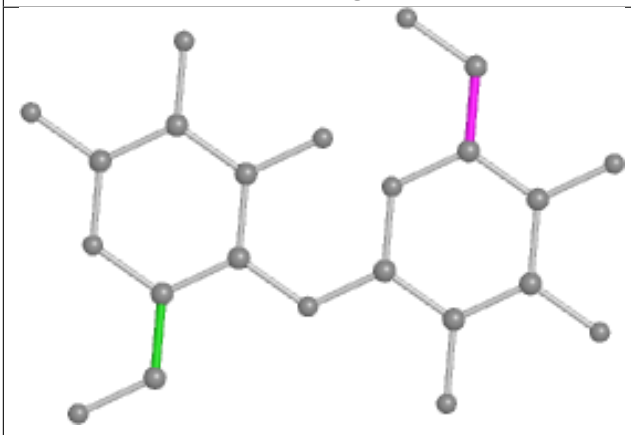
Oligosaccharide Chain l



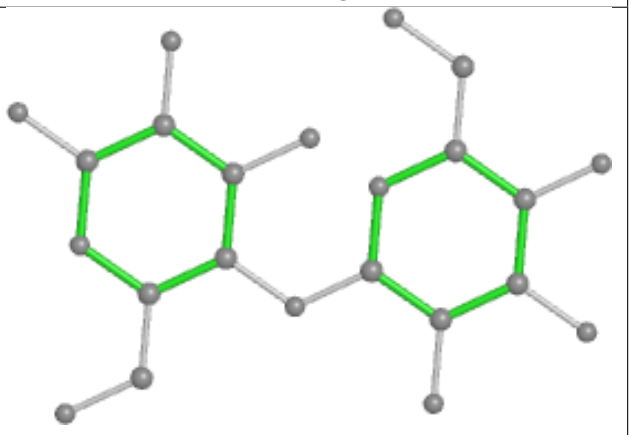
Bond lengths



Bond angles

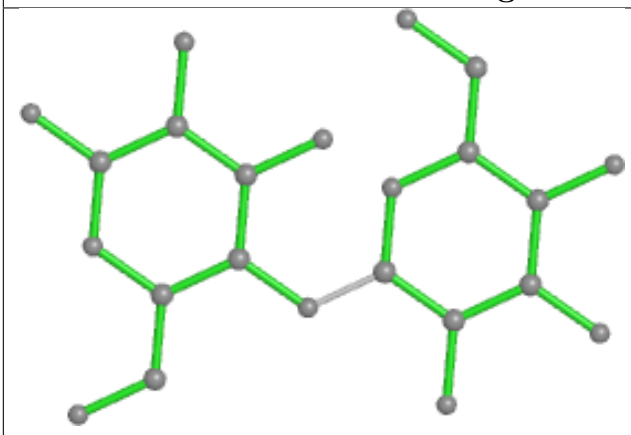


Torsions

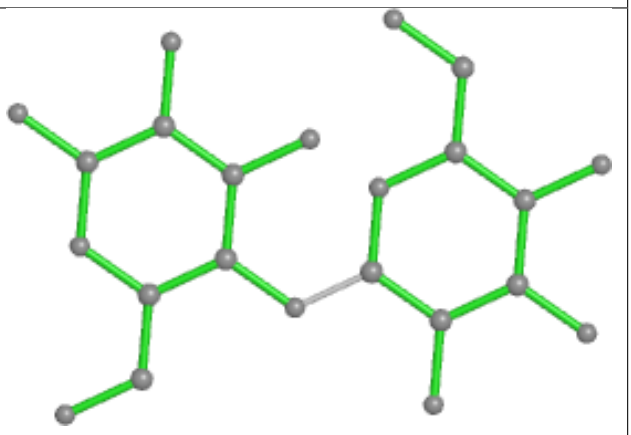


Rings

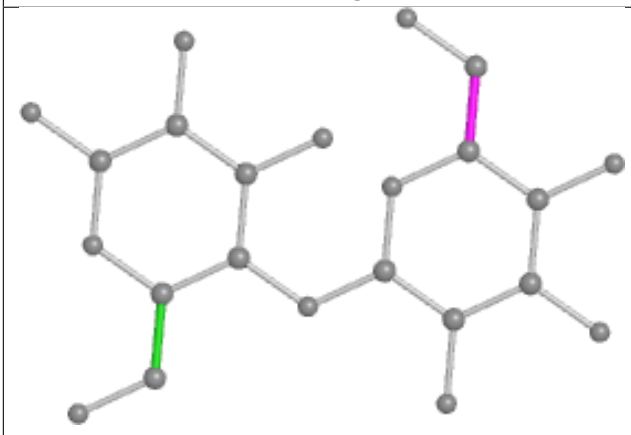
Oligosaccharide Chain n



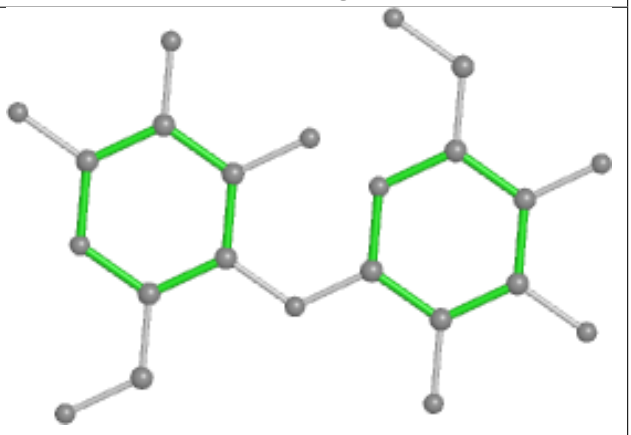
Bond lengths



Bond angles

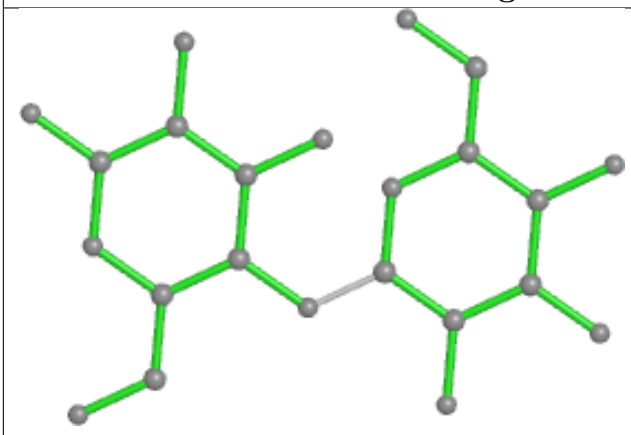


Torsions

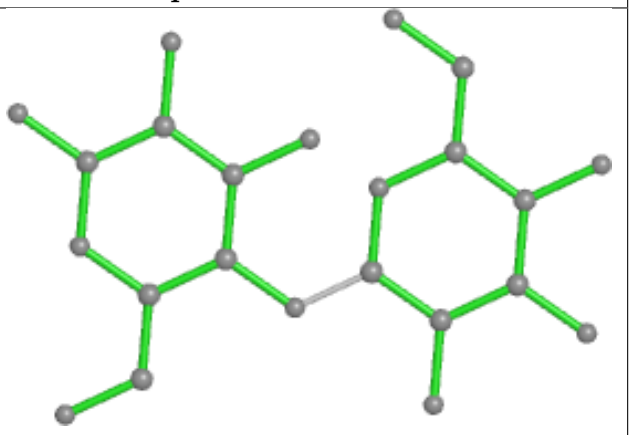


Rings

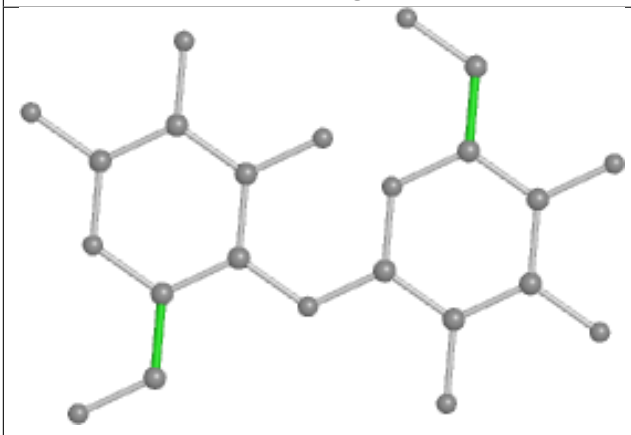
Oligosaccharide Chain q



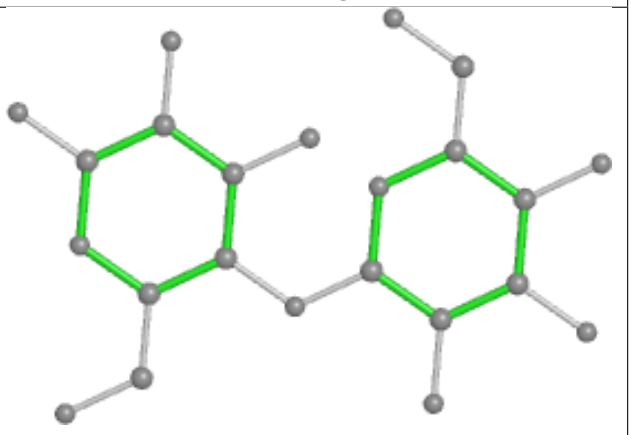
Bond lengths



Bond angles

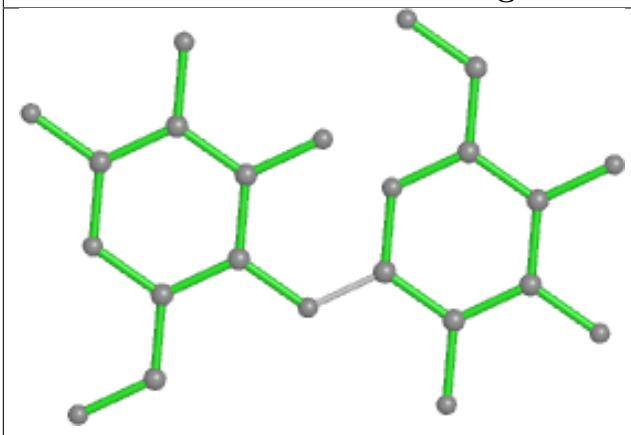


Torsions

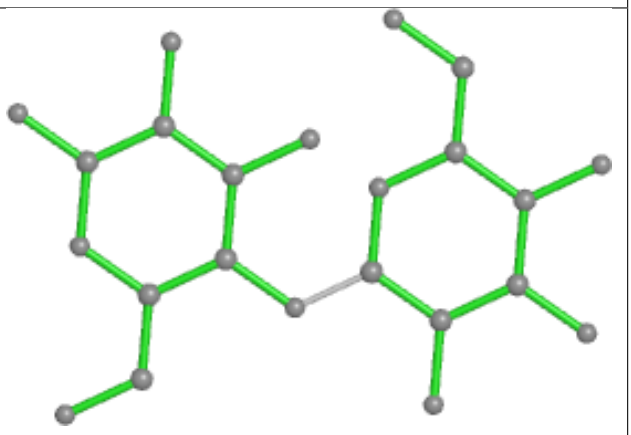


Rings

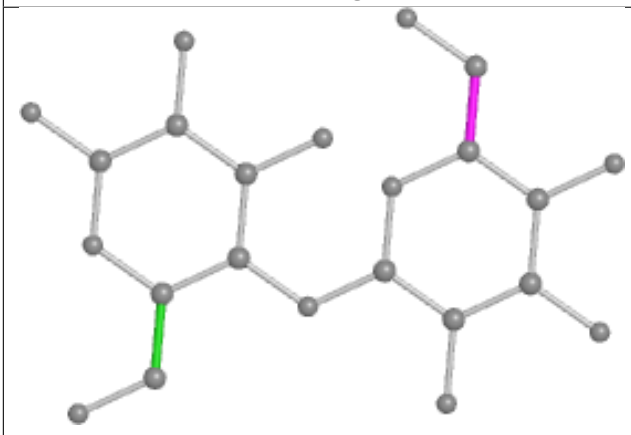
Oligosaccharide Chain u



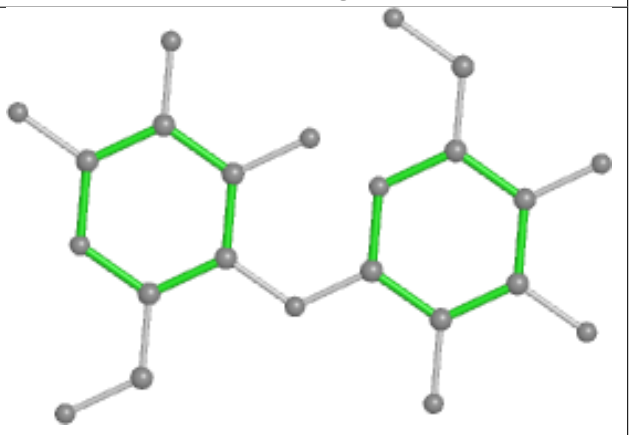
Bond lengths



Bond angles

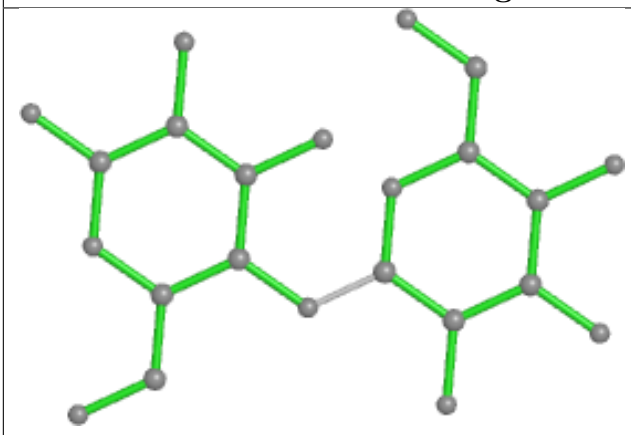


Torsions

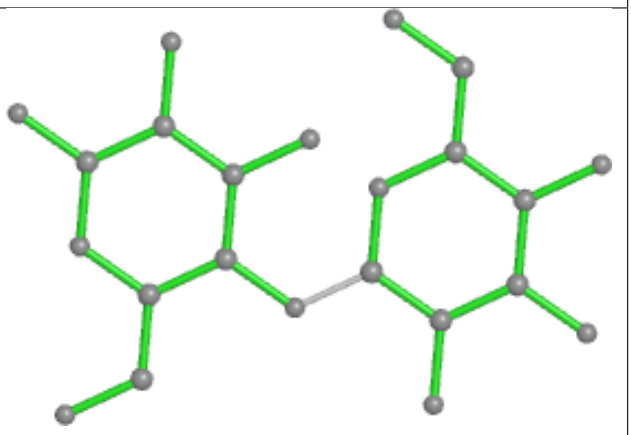


Rings

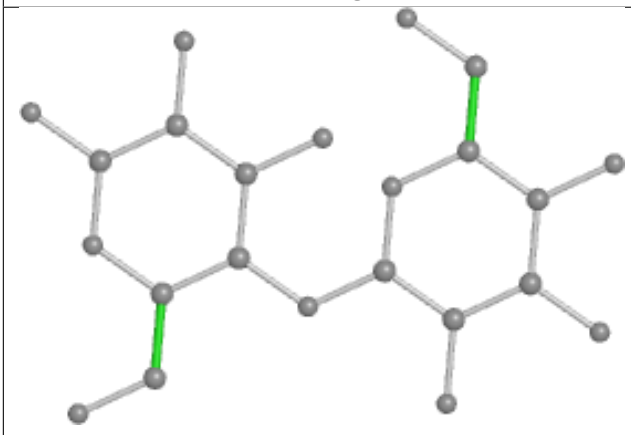
Oligosaccharide Chain w



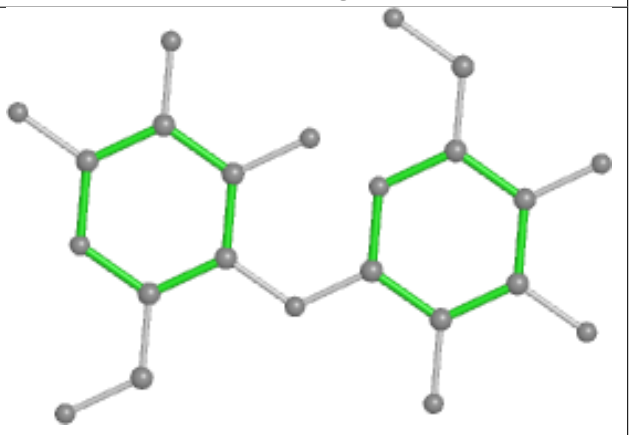
Bond lengths



Bond angles

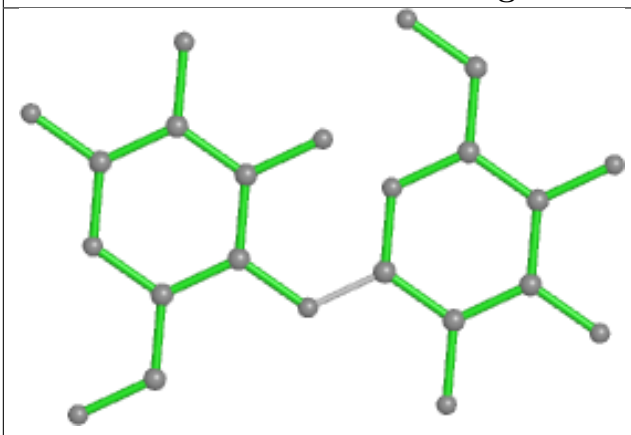


Torsions

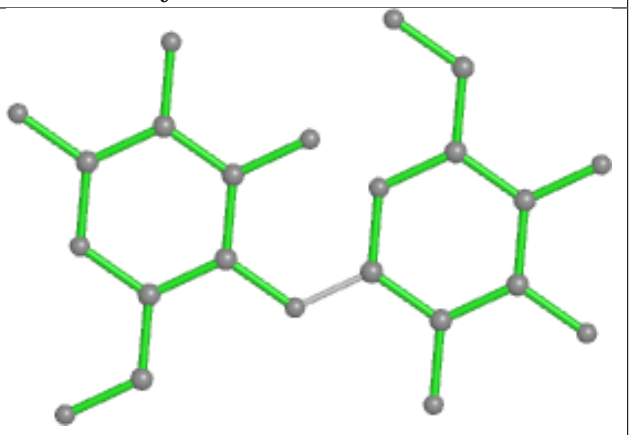


Rings

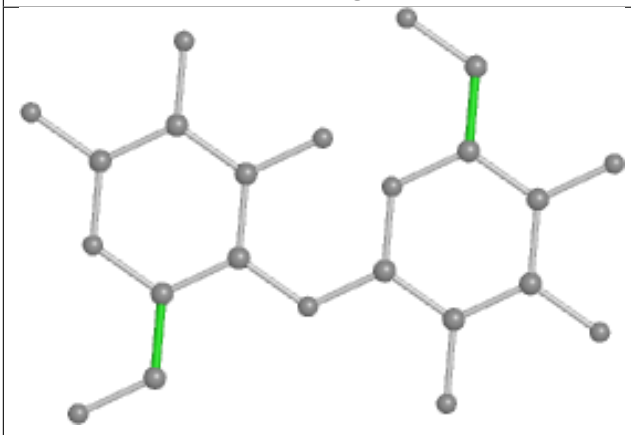
Oligosaccharide Chain y



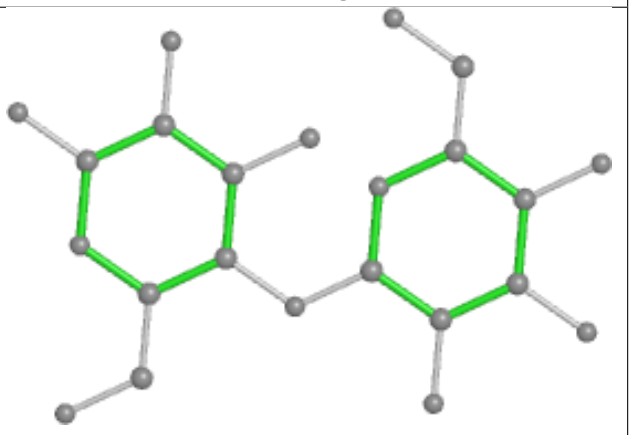
Bond lengths



Bond angles

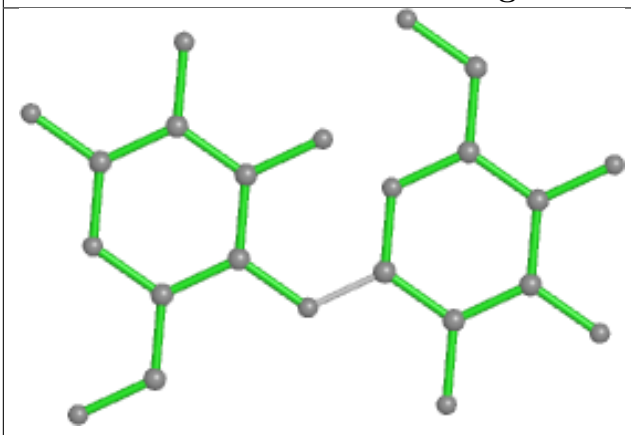


Torsions

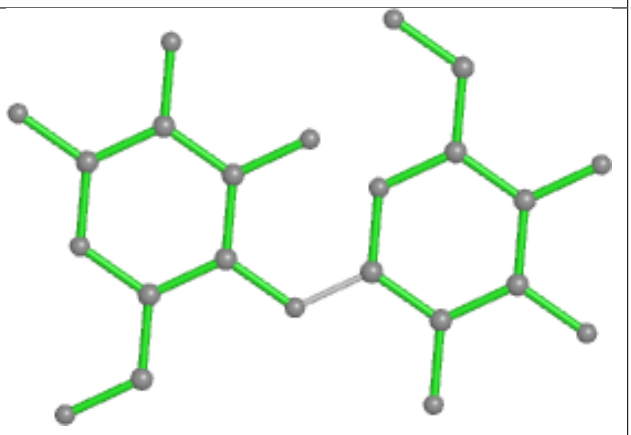


Rings

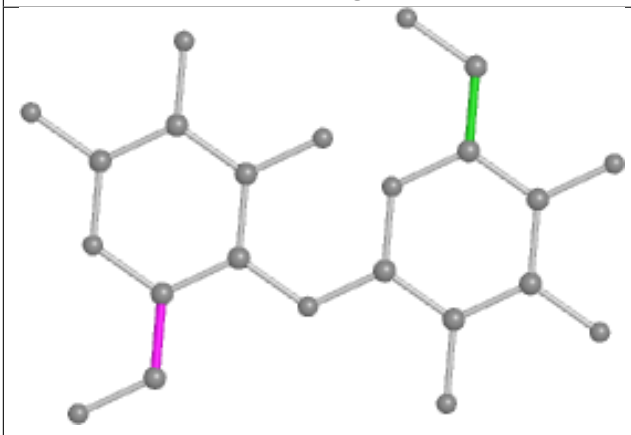
Oligosaccharide Chain 1



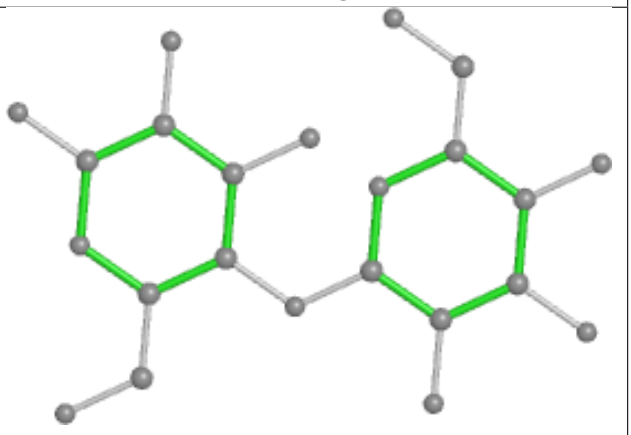
Bond lengths



Bond angles

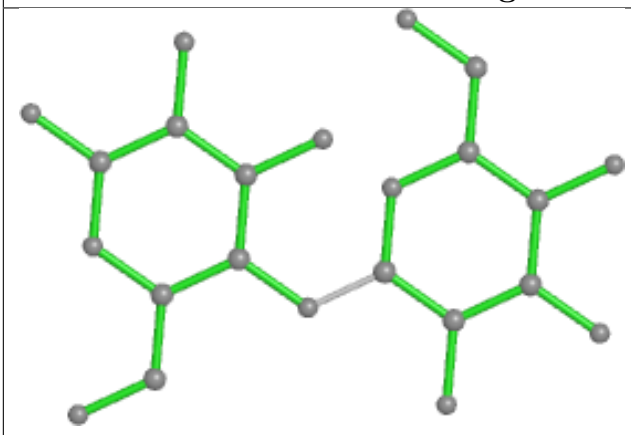


Torsions

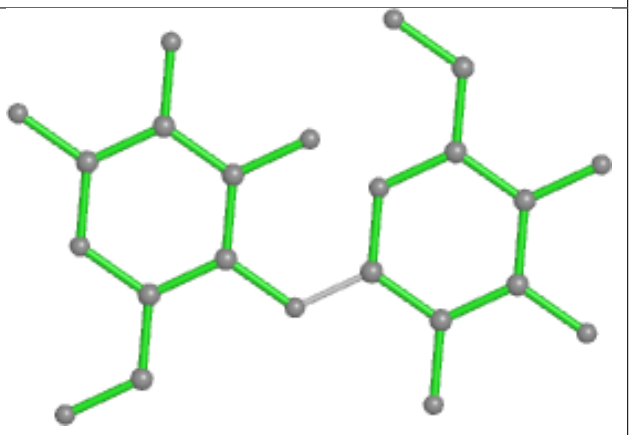


Rings

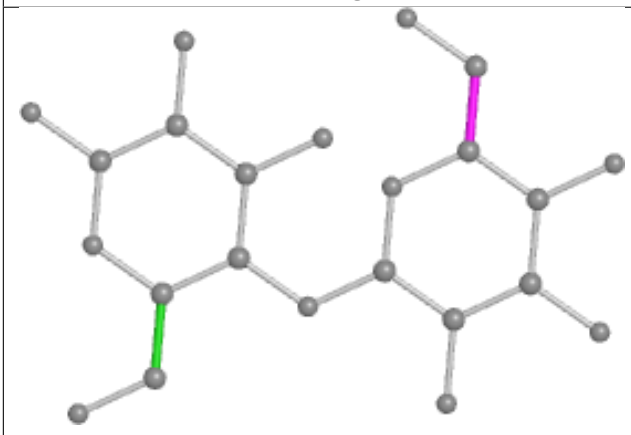
Oligosaccharide Chain 3



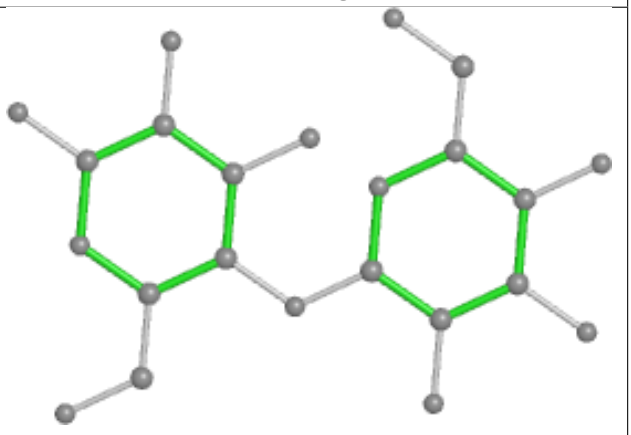
Bond lengths



Bond angles

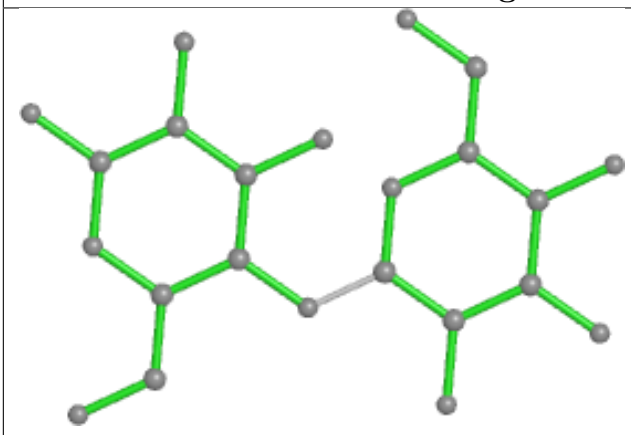


Torsions

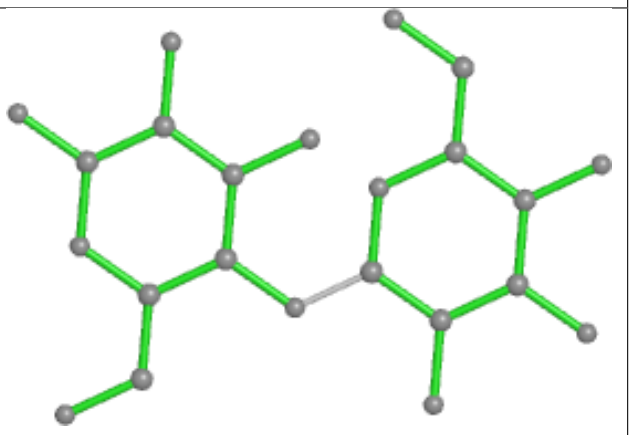


Rings

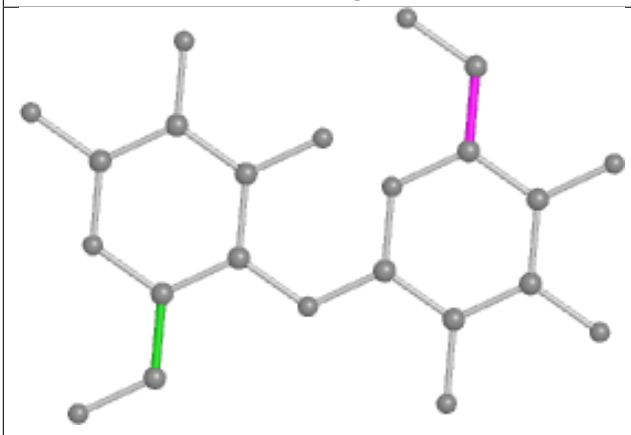
Oligosaccharide Chain 6



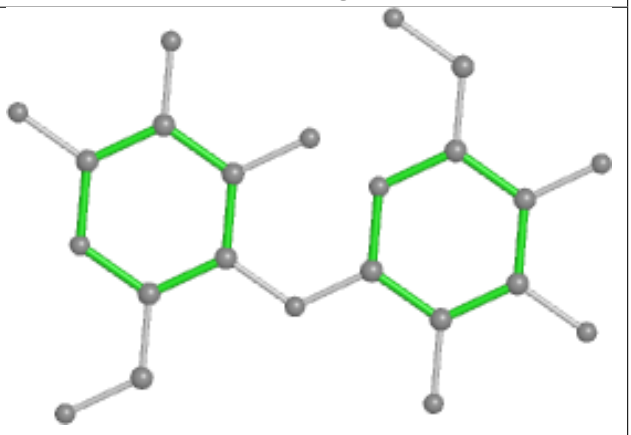
Bond lengths



Bond angles

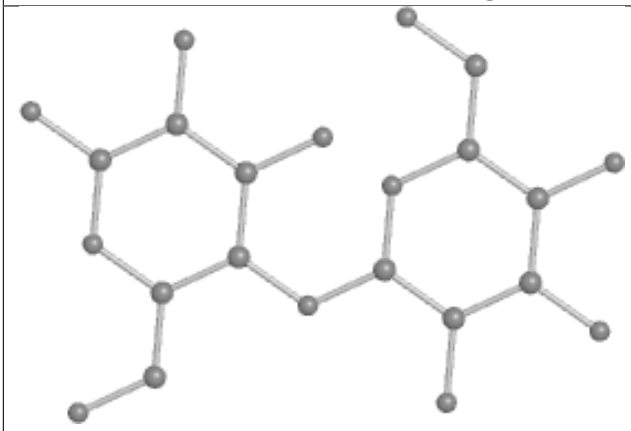


Torsions

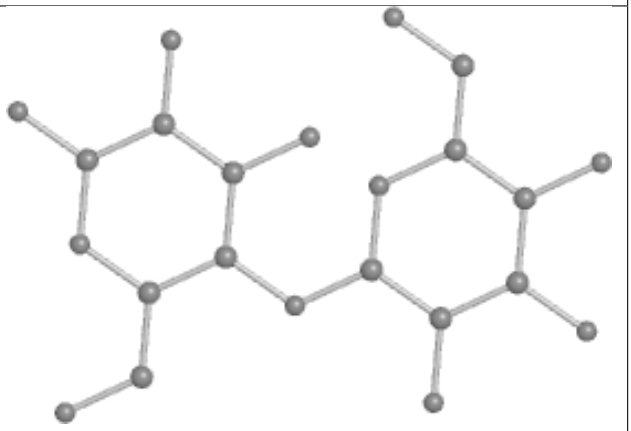


Rings

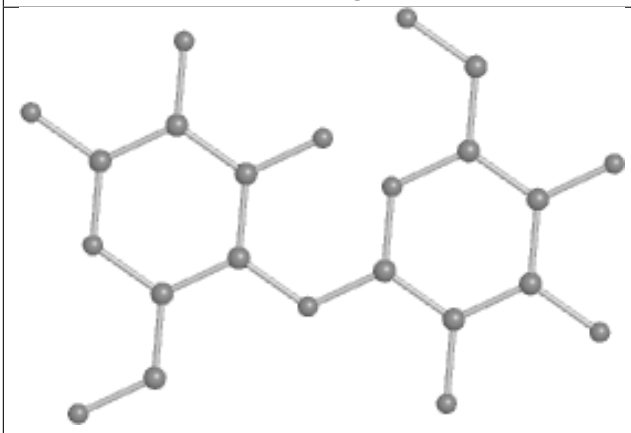
Oligosaccharide Chain DA



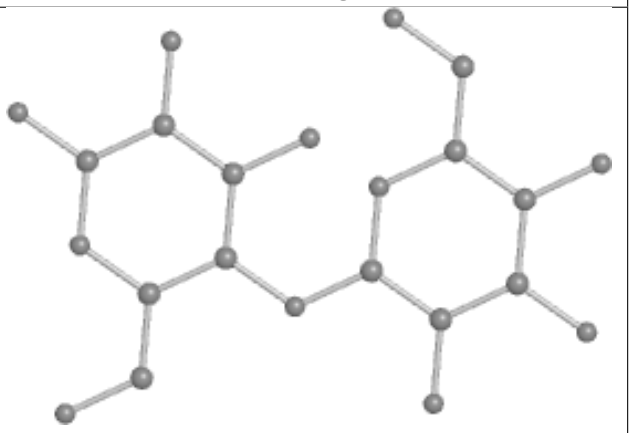
Bond lengths



Bond angles

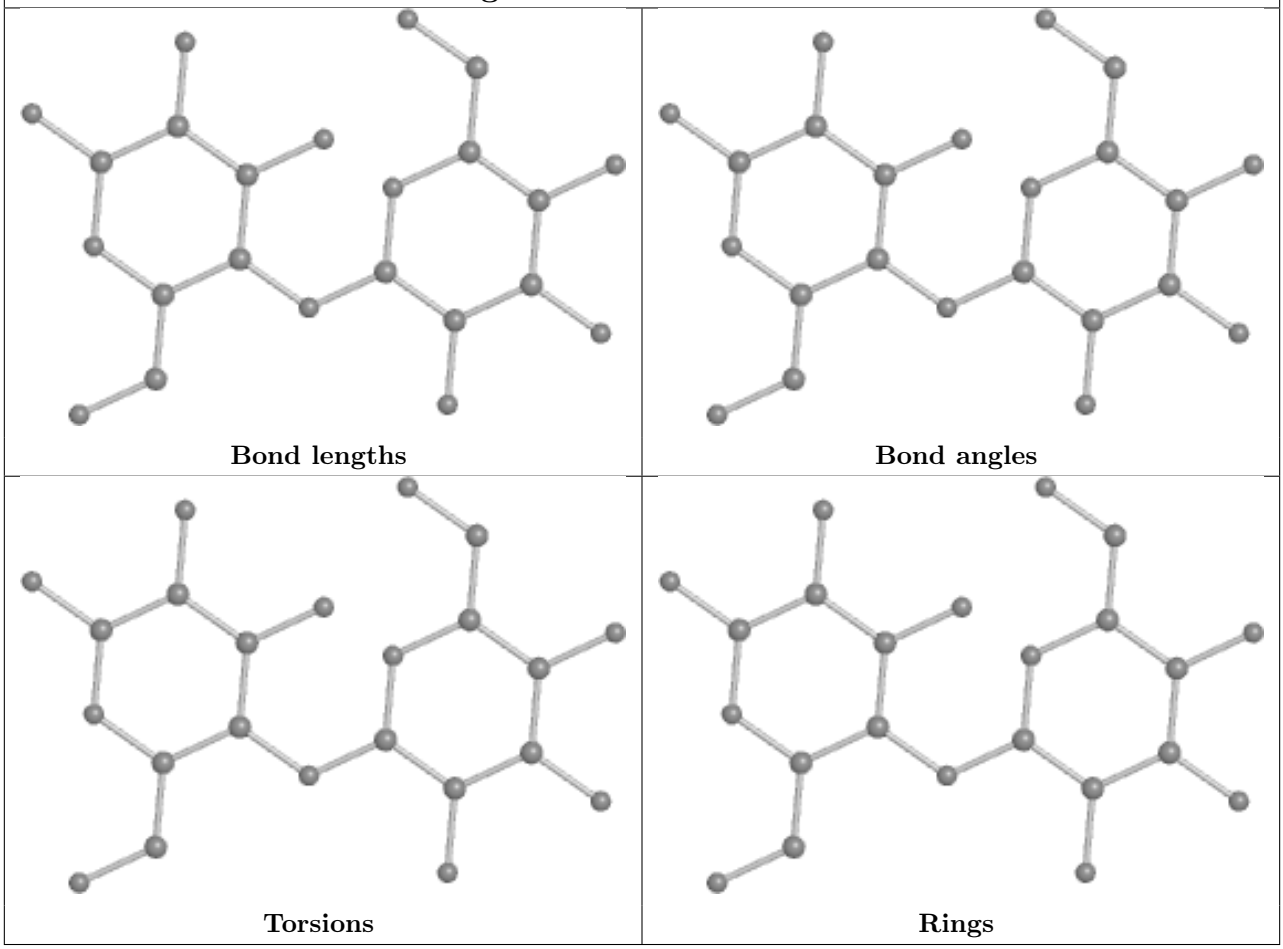


Torsions



Rings

Oligosaccharide Chain GA



5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
4	GAL	L	3270	-	12,12,12	0.43	0	17,17,17	0.40	0
4	GAL	P	4170	-	12,12,12	0.41	0	17,17,17	0.77	1 (5%)
4	GAL	N	3470	-	12,12,12	0.46	0	17,17,17	0.38	0
4	GAL	I	2470	-	12,12,12	0.44	0	17,17,17	0.49	0
4	GAL	G	2270	-	12,12,12	0.49	0	17,17,17	0.51	0
4	GAL	C	1370	-	12,12,12	0.48	0	17,17,17	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GAL	E	1570	-	12,12,12	0.43	0	17,17,17	0.42	0
4	GAL	J	2570	-	12,12,12	0.44	0	17,17,17	0.44	0
4	GAL	R	4370	-	12,12,12	0.46	0	17,17,17	0.53	0
4	GAL	K	3170	-	12,12,12	0.41	0	17,17,17	0.48	0
4	GAL	T	4570	-	12,12,12	0.61	0	17,17,17	0.63	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
4	GAL	L	3270	-	-	0/2/22/22	0/1/1/1
4	GAL	P	4170	-	-	1/2/22/22	0/1/1/1
4	GAL	N	3470	-	-	2/2/22/22	0/1/1/1
4	GAL	I	2470	-	-	1/2/22/22	0/1/1/1
4	GAL	G	2270	-	-	1/2/22/22	0/1/1/1
4	GAL	C	1370	-	-	2/2/22/22	0/1/1/1
4	GAL	E	1570	-	-	1/2/22/22	0/1/1/1
4	GAL	J	2570	-	-	2/2/22/22	0/1/1/1
4	GAL	R	4370	-	-	2/2/22/22	0/1/1/1
4	GAL	K	3170	-	-	1/2/22/22	0/1/1/1
4	GAL	T	4570	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	4170	GAL	C3-C4-C5	2.43	114.57	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	3470	GAL	O5-C5-C6-O6
4	J	2570	GAL	O5-C5-C6-O6
4	R	4370	GAL	O5-C5-C6-O6
4	C	1370	GAL	O5-C5-C6-O6
4	K	3170	GAL	O5-C5-C6-O6
4	I	2470	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	J	2570	GAL	C4-C5-C6-O6
4	N	3470	GAL	C4-C5-C6-O6
4	E	1570	GAL	O5-C5-C6-O6
4	T	4570	GAL	O5-C5-C6-O6
4	G	2270	GAL	O5-C5-C6-O6
4	P	4170	GAL	O5-C5-C6-O6
4	R	4370	GAL	C4-C5-C6-O6
4	C	1370	GAL	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	4170	GAL	3	0
4	N	3470	GAL	2	0
4	G	2270	GAL	2	0
4	C	1370	GAL	1	0
4	R	4370	GAL	2	0
4	T	4570	GAL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	69/69 (100%)	-0.72	0	100	100	8, 17, 30, 34	0
1	B	69/69 (100%)	-0.73	0	100	100	8, 17, 28, 36	0
1	C	69/69 (100%)	-0.69	0	100	100	7, 16, 29, 36	0
1	D	69/69 (100%)	-0.72	0	100	100	5, 16, 29, 34	0
1	E	69/69 (100%)	-0.70	0	100	100	8, 19, 31, 39	0
1	F	69/69 (100%)	-0.73	0	100	100	7, 15, 26, 40	0
1	G	69/69 (100%)	-0.83	0	100	100	4, 14, 26, 34	0
1	H	69/69 (100%)	-0.81	0	100	100	4, 14, 23, 34	0
1	I	69/69 (100%)	-0.67	0	100	100	7, 17, 30, 42	0
1	J	69/69 (100%)	-0.58	0	100	100	7, 22, 33, 42	0
1	K	69/69 (100%)	-0.69	0	100	100	7, 18, 30, 34	0
1	L	69/69 (100%)	-0.79	0	100	100	7, 15, 26, 34	0
1	M	69/69 (100%)	-0.78	0	100	100	5, 13, 24, 32	0
1	N	69/69 (100%)	-0.75	0	100	100	6, 16, 28, 36	0
1	O	69/69 (100%)	-0.73	0	100	100	5, 15, 27, 41	0
1	P	69/69 (100%)	-0.67	0	100	100	8, 19, 30, 40	0
1	Q	69/69 (100%)	-0.68	0	100	100	11, 18, 29, 43	0
1	R	69/69 (100%)	-0.53	0	100	100	11, 25, 38, 44	0
1	S	69/69 (100%)	-0.59	0	100	100	12, 25, 34, 45	0
1	T	69/69 (100%)	-0.58	0	100	100	12, 25, 37, 47	0
All	All	1380/1380 (100%)	-0.70	0	100	100	4, 18, 32, 47	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	g	1	12/12	0.59	0.21	36,41,42,42	11
2	BGC	x	1	12/12	0.80	0.23	33,47,49,52	0
2	BGC	U	1	12/12	0.81	0.26	37,50,54,56	0
2	BGC	2	1	12/12	0.81	0.30	44,51,54,55	0
2	BGC	r	1	12/12	0.82	0.31	51,55,61,62	0
2	BGC	s	1	12/12	0.84	0.31	47,67,73,74	0
3	GAL	Z	1	12/12	0.84	0.36	60,67,69,73	0
2	BGC	i	1	12/12	0.85	0.26	43,48,48,48	11
2	BGC	BA	1	12/12	0.85	0.23	46,58,61,62	4
2	BGC	h	1	12/12	0.85	0.29	36,49,53,53	0
2	BGC	AA	1	12/12	0.86	0.22	47,55,59,61	0
2	BGC	W	1	12/12	0.88	0.22	22,30,39,45	0
2	BGC	FA	1	12/12	0.88	0.32	49,56,61,62	0
2	BGC	X	1	12/12	0.88	0.20	28,39,43,46	0
3	GLA	Z	2	11/12	0.88	0.36	72,74,77,78	0
2	BGC	v	1	12/12	0.89	0.22	29,41,45,49	0
2	BGC	m	1	12/12	0.89	0.24	27,39,43,44	0
2	BGC	0	1	12/12	0.89	0.20	40,49,54,54	0
2	BGC	p	1	12/12	0.89	0.23	36,42,47,51	0
2	BGC	8	1	12/12	0.89	0.16	35,40,40,41	8
3	GAL	u	1	12/12	0.89	0.21	28,37,41,44	0
2	BGC	f	1	12/12	0.90	0.19	38,42,44,44	0
2	GAL	t	2	11/12	0.90	0.16	30,32,38,39	0
2	GAL	FA	2	11/12	0.90	0.14	38,41,45,47	0
2	BGC	5	1	12/12	0.91	0.24	36,46,49,53	0
2	GAL	s	2	11/12	0.91	0.19	25,33,41,45	0
2	BGC	t	1	12/12	0.91	0.24	40,51,53,55	0
2	BGC	e	1	12/12	0.91	0.16	20,25,32,33	0
2	BGC	CA	1	12/12	0.91	0.28	40,52,56,59	0
2	GAL	i	2	11/12	0.91	0.16	27,37,40,40	0
2	BGC	j	1	12/12	0.91	0.20	28,31,36,38	0
2	GAL	r	2	11/12	0.91	0.17	27,35,40,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	k	1	12/12	0.91	0.17	26,38,40,43	0
3	GAL	d	1	12/12	0.91	0.18	23,28,30,34	0
2	GAL	2	2	11/12	0.91	0.19	27,31,34,36	0
3	GLA	6	2	11/12	0.91	0.17	18,21,26,27	0
2	GAL	AA	2	11/12	0.92	0.16	30,41,44,44	0
2	GAL	8	2	11/12	0.92	0.17	22,28,33,33	0
2	BGC	7	1	12/12	0.93	0.16	31,39,43,45	0
2	GAL	EA	2	11/12	0.93	0.13	26,30,34,34	0
2	GLA	W	3	11/12	0.93	0.16	4,12,17,25	0
2	GAL	g	2	11/12	0.93	0.14	25,26,31,35	0
3	GAL	V	1	12/12	0.93	0.17	29,32,35,38	0
2	GAL	o	2	11/12	0.93	0.15	21,29,33,38	0
2	BGC	4	1	12/12	0.93	0.16	25,31,36,42	0
3	GAL	b	1	12/12	0.93	0.17	22,26,30,35	0
2	GLA	AA	3	11/12	0.93	0.16	21,28,30,31	0
3	GAL	n	1	12/12	0.93	0.14	18,28,31,32	0
3	GAL	q	1	12/12	0.93	0.15	18,23,26,27	0
2	BGC	c	1	12/12	0.93	0.16	29,36,38,40	0
3	GAL	3	1	12/12	0.93	0.19	25,31,38,42	0
2	GAL	BA	2	11/12	0.93	0.16	32,34,39,39	0
3	GAL	DA	1	12/12	0.93	0.19	29,32,35,36	0
2	GLA	5	3	11/12	0.94	0.14	13,20,24,28	0
2	GLA	t	3	11/12	0.94	0.13	14,16,25,28	0
2	GLA	FA	3	11/12	0.94	0.13	28,30,33,36	0
2	GLA	p	3	11/12	0.94	0.13	10,12,17,18	0
2	GAL	v	2	11/12	0.94	0.12	17,21,24,25	0
2	GAL	h	2	11/12	0.94	0.12	14,21,29,30	0
2	BGC	z	1	12/12	0.94	0.15	2,8,12,15	0
2	BGC	a	1	12/12	0.94	0.21	31,36,43,43	0
2	BGC	o	1	12/12	0.94	0.16	14,23,29,29	0
2	GLA	e	3	11/12	0.94	0.11	5,9,13,15	0
2	GAL	U	2	11/12	0.94	0.12	21,29,34,34	0
3	GAL	w	1	12/12	0.94	0.18	20,27,31,33	0
3	GAL	1	1	12/12	0.94	0.20	22,27,37,42	0
2	BGC	EA	1	12/12	0.94	0.17	19,26,38,44	0
3	GAL	6	1	12/12	0.94	0.21	25,31,38,38	0
2	GAL	p	2	11/12	0.94	0.17	21,27,37,40	0
2	GLA	EA	3	11/12	0.94	0.14	14,25,30,31	0
3	GLA	GA	2	11/12	0.94	0.17	19,22,24,25	0
2	GLA	a	3	11/12	0.95	0.12	2,10,15,20	0
2	GLA	o	3	11/12	0.95	0.12	8,14,17,21	0
2	GAL	7	2	11/12	0.95	0.13	15,20,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	W	2	11/12	0.95	0.14	8,13,22,23	0
3	GLA	V	2	11/12	0.95	0.14	11,23,28,29	0
2	GLA	i	3	11/12	0.95	0.14	20,22,27,27	0
2	BGC	9	1	12/12	0.95	0.18	19,28,32,38	0
2	GAL	9	2	11/12	0.95	0.14	2,5,9,11	0
2	GAL	c	2	11/12	0.95	0.12	18,22,28,35	0
3	GLA	d	2	11/12	0.95	0.16	14,20,26,27	0
3	GAL	l	1	12/12	0.95	0.17	23,26,32,34	0
2	GLA	g	3	11/12	0.95	0.16	14,22,23,24	0
2	GAL	k	2	11/12	0.95	0.13	8,15,20,20	0
3	GLA	q	2	11/12	0.95	0.17	15,21,25,29	0
2	GAL	0	2	11/12	0.95	0.14	25,29,34,36	0
3	GLA	u	2	11/12	0.95	0.14	7,18,25,26	0
2	GLA	0	3	11/12	0.95	0.14	10,16,23,26	0
3	GLA	w	2	11/12	0.95	0.16	7,18,19,21	0
3	GAL	y	1	12/12	0.95	0.16	20,24,29,29	0
3	GLA	y	2	11/12	0.95	0.15	5,15,22,22	0
2	GLA	U	3	11/12	0.95	0.13	8,15,20,20	0
3	GLA	1	2	11/12	0.95	0.17	23,24,27,28	0
2	GAL	CA	2	11/12	0.95	0.12	27,33,37,37	0
2	GLA	CA	3	11/12	0.95	0.13	26,29,31,31	0
2	GAL	m	2	11/12	0.95	0.10	10,20,23,23	0
2	GLA	s	3	11/12	0.95	0.20	19,29,30,31	0
3	GLA	DA	2	11/12	0.95	0.14	18,22,29,30	0
3	GAL	GA	1	12/12	0.95	0.14	21,27,32,34	0
2	GAL	a	2	11/12	0.95	0.13	15,19,26,27	0
2	GLA	2	3	11/12	0.96	0.12	6,10,14,16	0
2	GLA	c	3	11/12	0.96	0.11	9,11,14,14	0
3	GLA	l	2	11/12	0.96	0.12	14,16,20,22	0
2	GLA	BA	3	11/12	0.96	0.14	19,22,29,30	0
3	GLA	n	2	11/12	0.96	0.12	14,17,21,25	0
2	GAL	4	2	11/12	0.96	0.15	14,24,32,36	0
2	GLA	m	3	11/12	0.96	0.13	7,10,16,20	0
2	GLA	v	3	11/12	0.96	0.09	5,10,16,16	0
2	GLA	r	3	11/12	0.96	0.12	21,25,27,30	0
2	GAL	x	2	11/12	0.96	0.12	17,22,25,25	0
2	GLA	7	3	11/12	0.96	0.13	13,15,18,22	0
2	GAL	f	2	11/12	0.96	0.12	21,27,34,34	0
2	GAL	z	2	11/12	0.96	0.11	5,8,10,12	0
2	GLA	8	3	11/12	0.96	0.17	15,25,28,32	0
2	GLA	j	3	11/12	0.96	0.13	17,19,21,27	0
2	GLA	f	3	11/12	0.96	0.11	16,20,24,24	0

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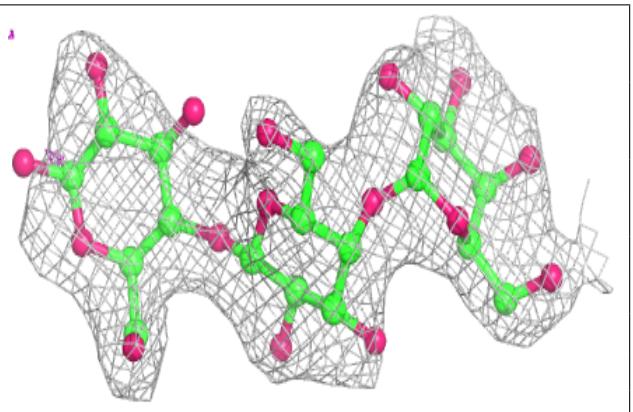
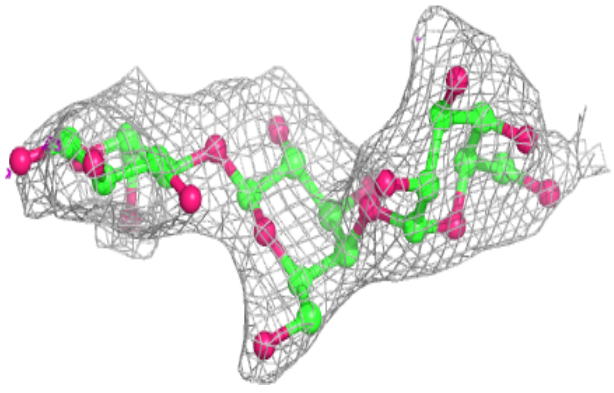
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLA	3	2	11/12	0.96	0.15	24,27,28,29	0
3	GAL	Y	1	12/12	0.96	0.16	22,28,29,31	0
2	GLA	9	3	11/12	0.96	0.11	2,9,13,17	0
2	GLA	X	3	11/12	0.96	0.12	9,12,16,19	0
2	GLA	k	3	11/12	0.96	0.12	2,9,12,14	0
3	GLA	b	2	11/12	0.96	0.15	17,19,22,30	0
2	GAL	X	2	11/12	0.96	0.09	10,20,23,25	0
2	GLA	4	3	11/12	0.97	0.11	20,22,30,35	0
2	GLA	h	3	11/12	0.97	0.11	4,7,14,15	0
2	GAL	5	2	11/12	0.97	0.15	15,26,28,30	0
3	GLA	Y	2	11/12	0.97	0.15	15,18,20,22	0
2	GLA	z	3	11/12	0.97	0.10	2,3,15,18	0
2	GAL	j	2	11/12	0.97	0.13	18,25,29,30	0
2	GLA	x	3	11/12	0.97	0.10	9,14,18,22	0
2	GAL	e	2	11/12	0.97	0.11	10,14,18,18	0

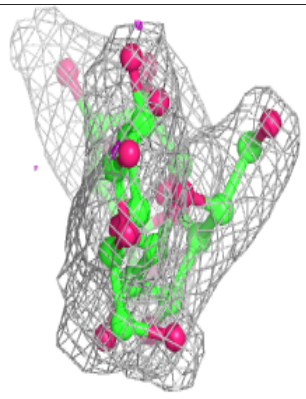
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

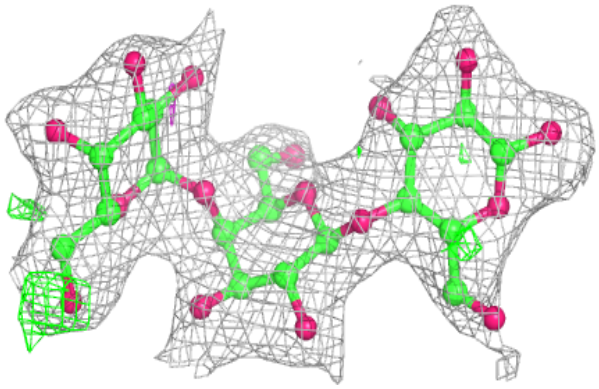


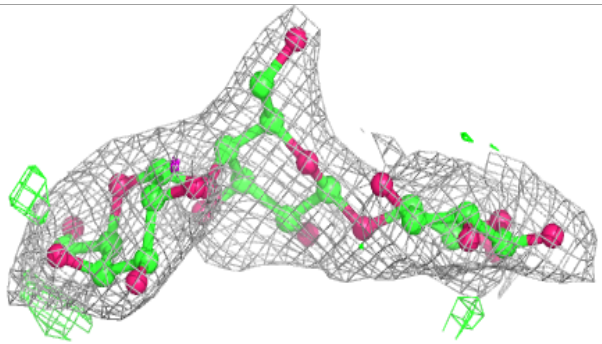


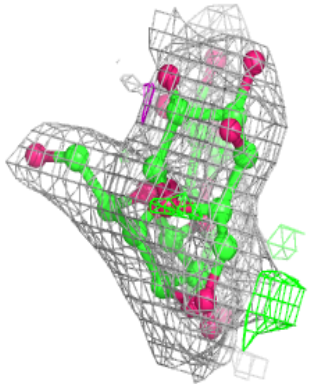


Electron density around Chain W:

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

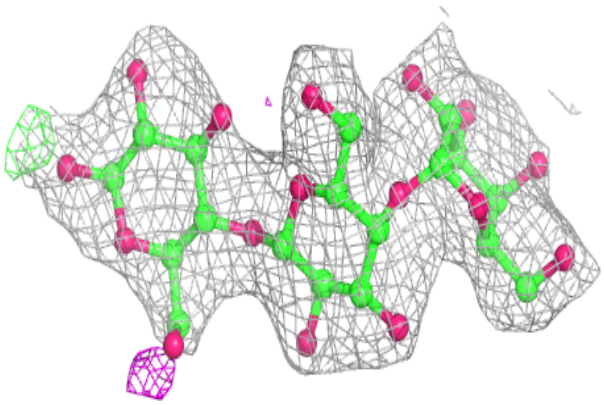


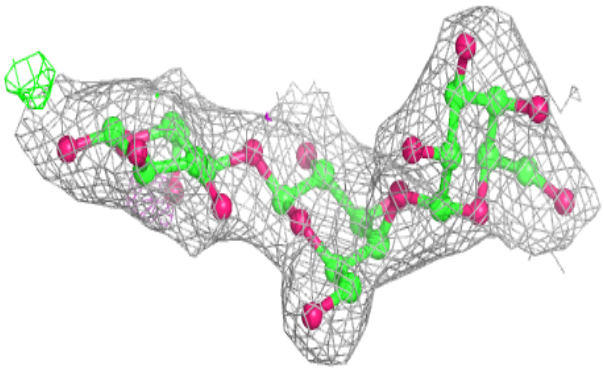


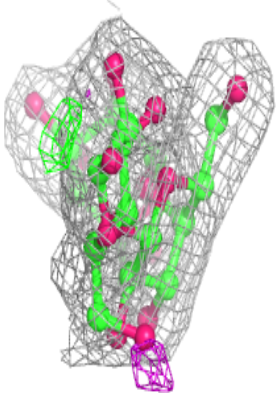


Electron density around Chain X:

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

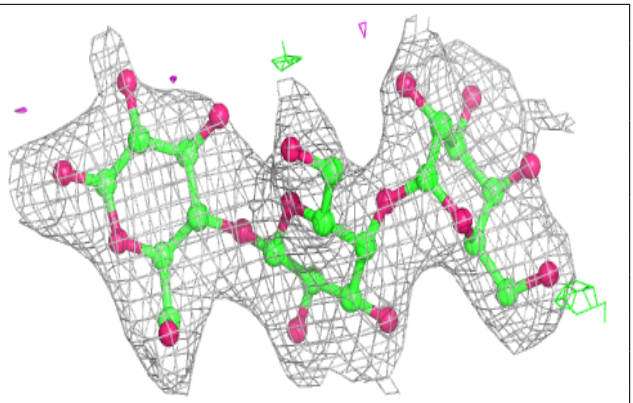


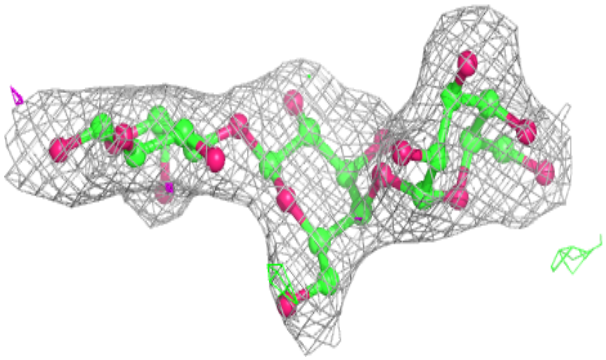


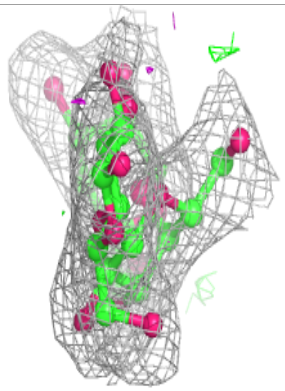


Electron density around Chain a:

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

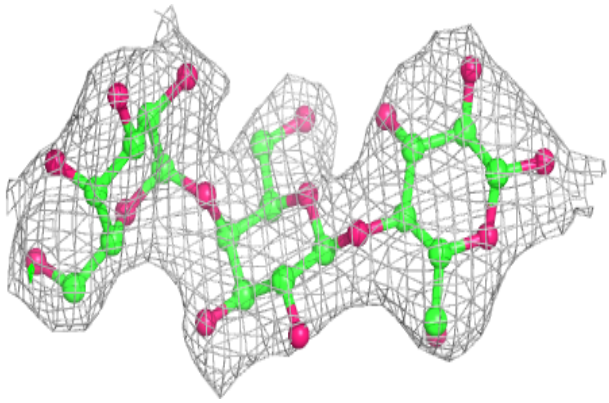


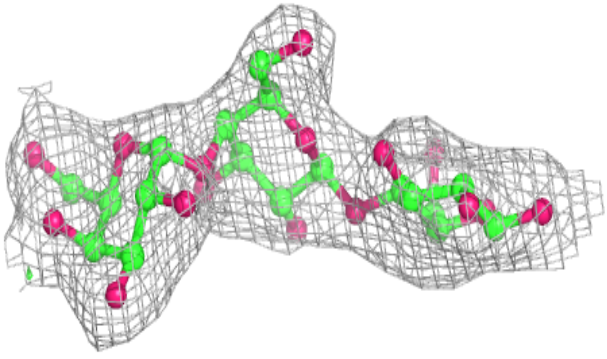


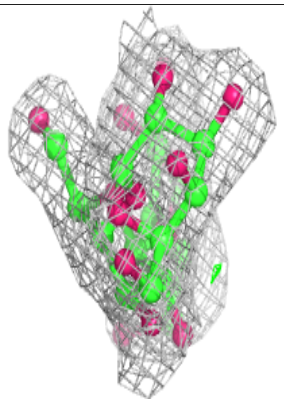


Electron density around Chain c:

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

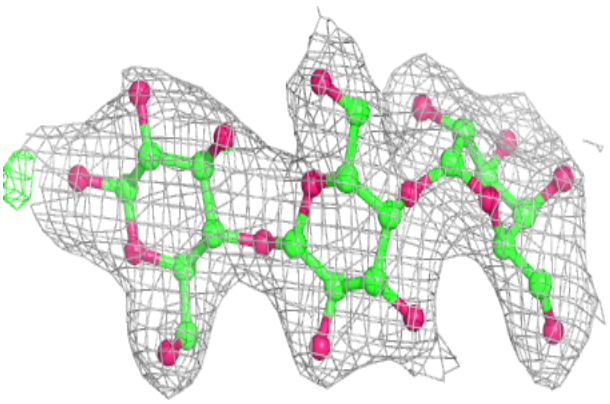


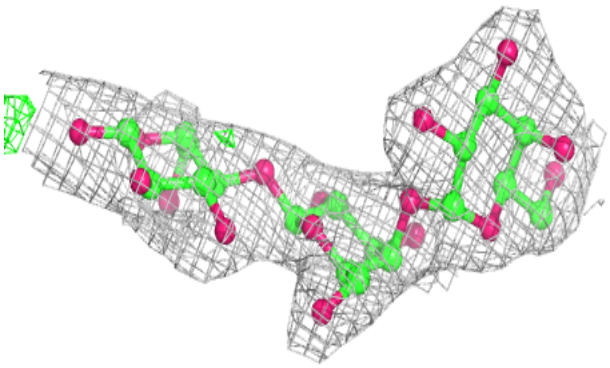


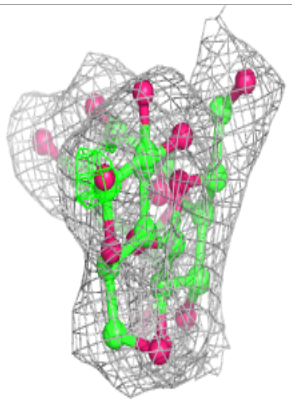


Electron density around Chain e:

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

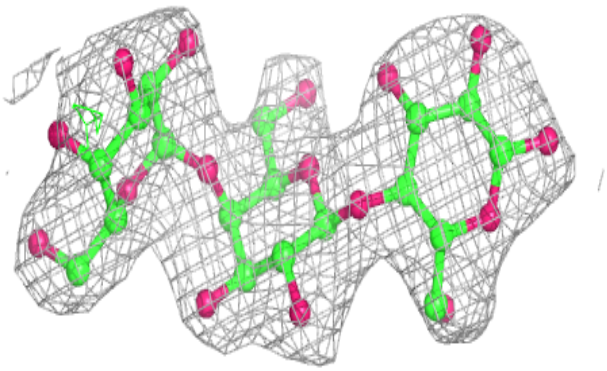


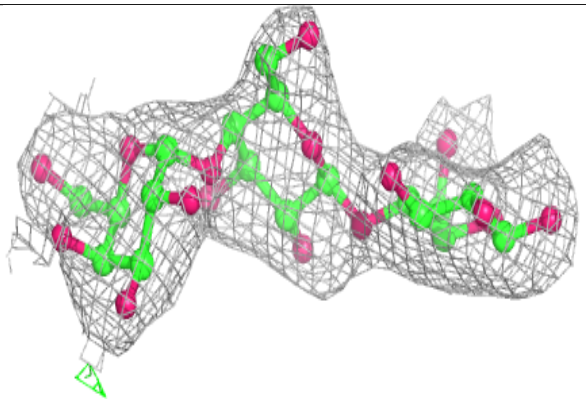


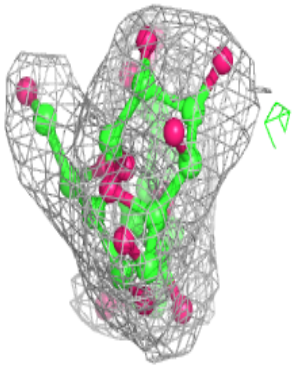


Electron density around Chain f:

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

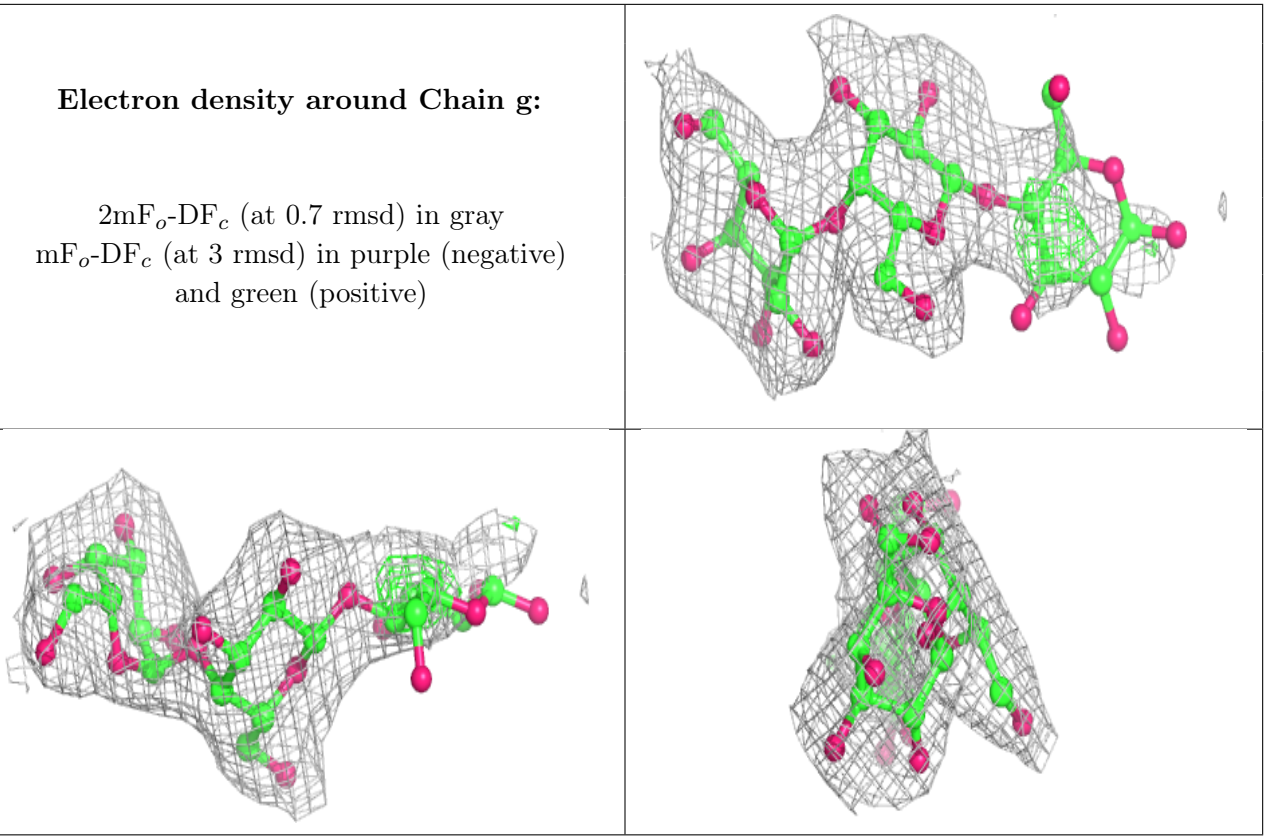






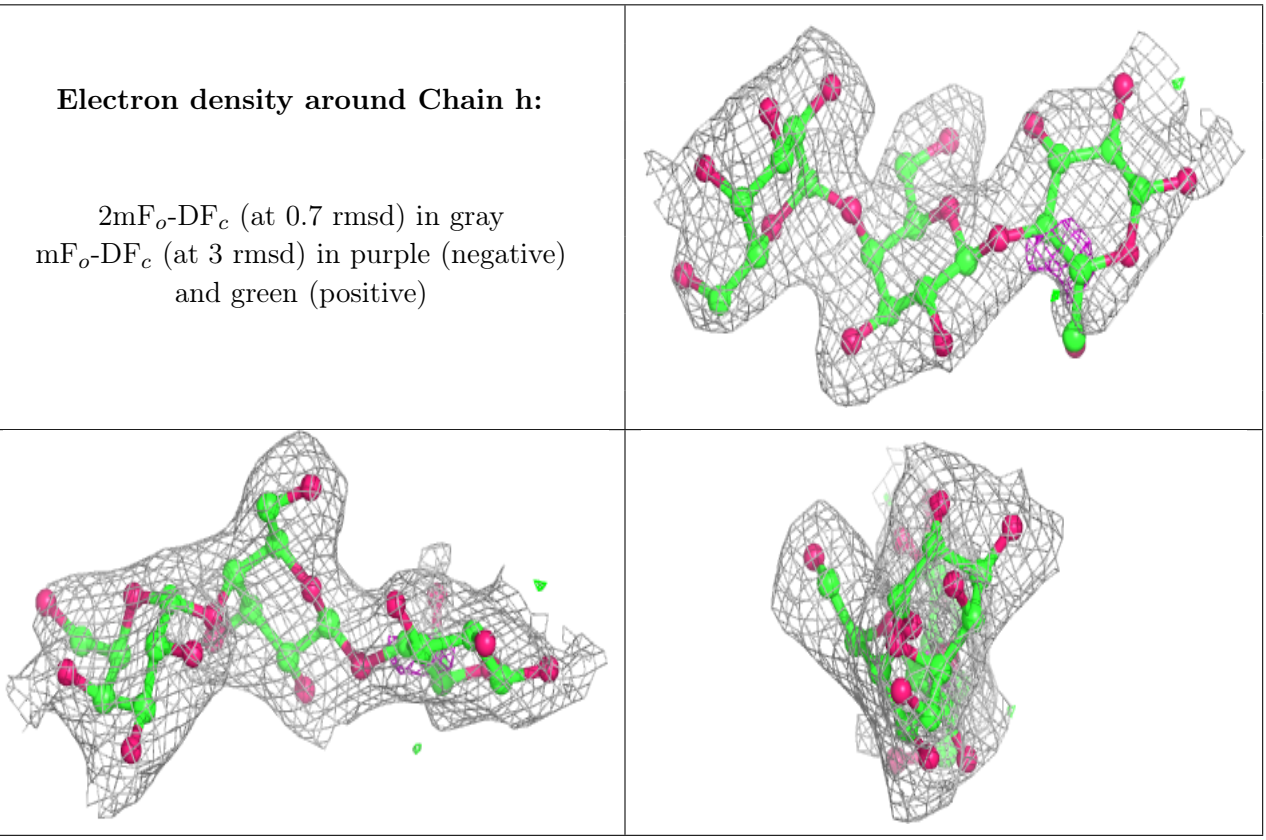
Electron density around Chain g:

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



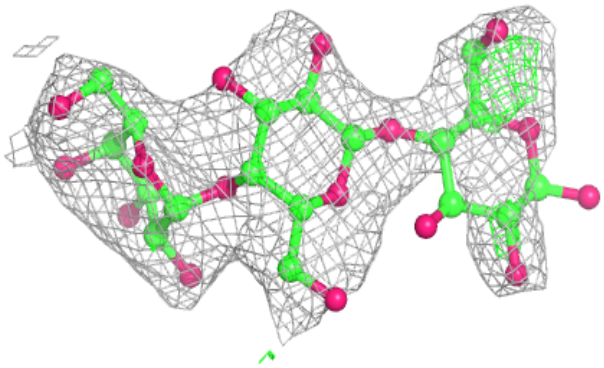
Electron density around Chain h:

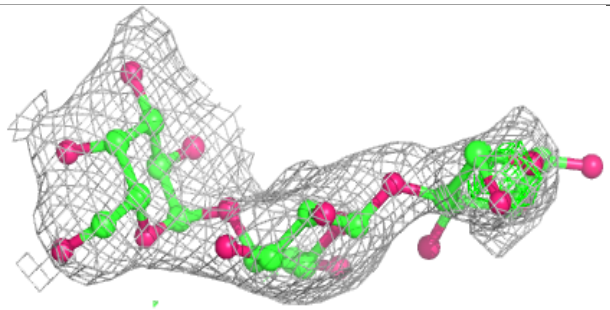
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

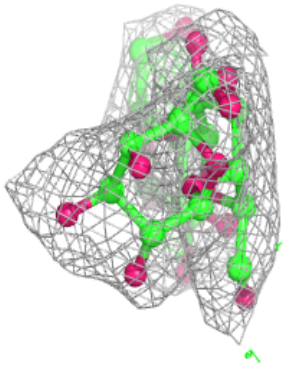


Electron density around Chain i:

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

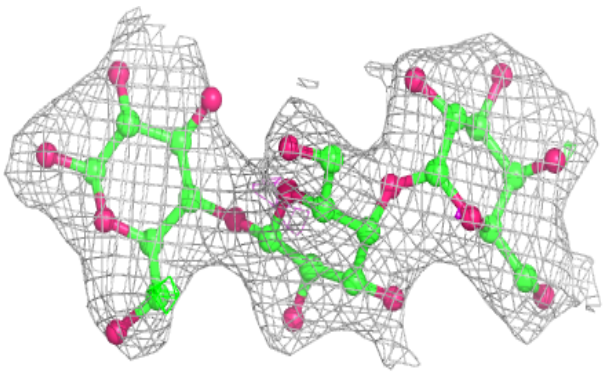


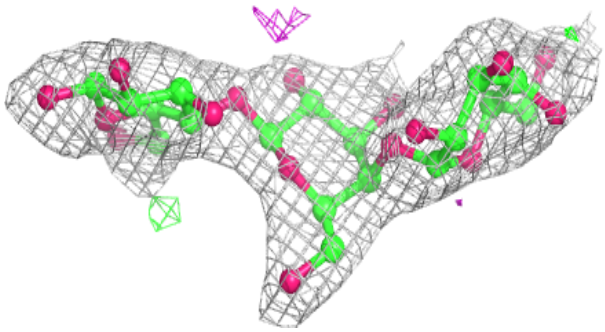


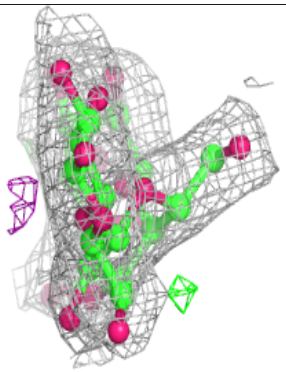


Electron density around Chain j:

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

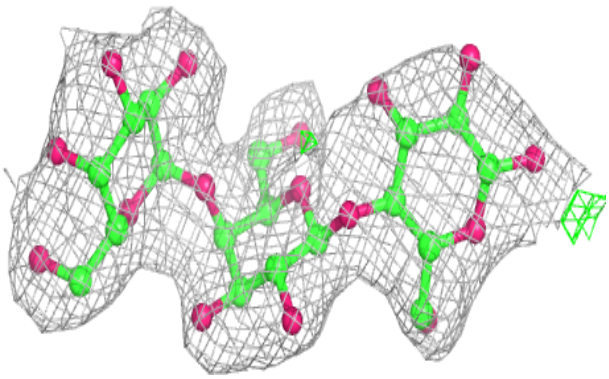


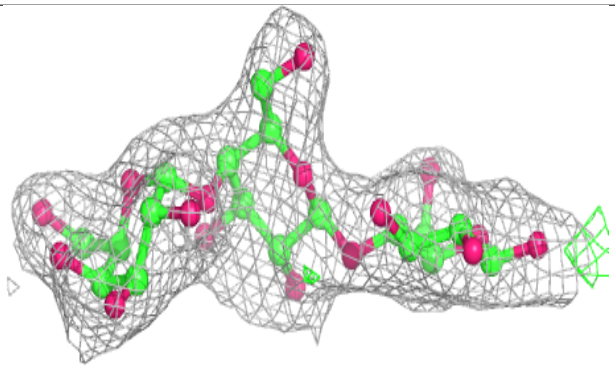


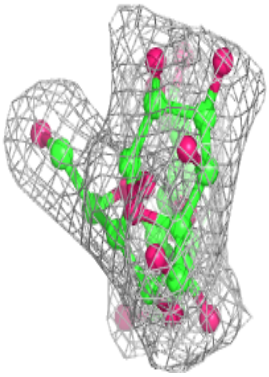


Electron density around Chain k:

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

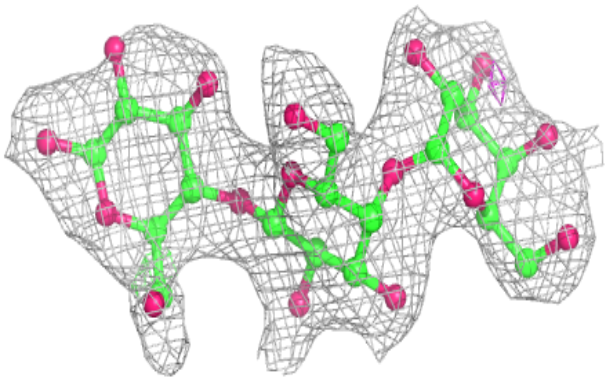


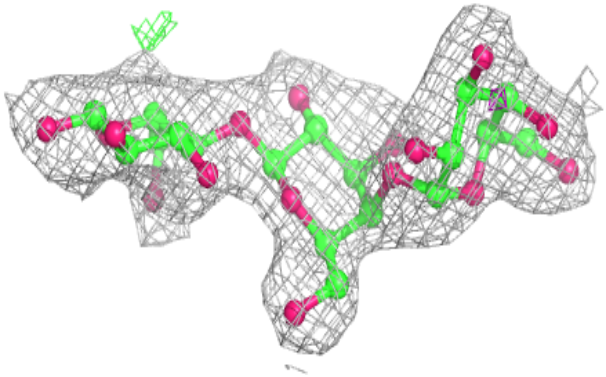


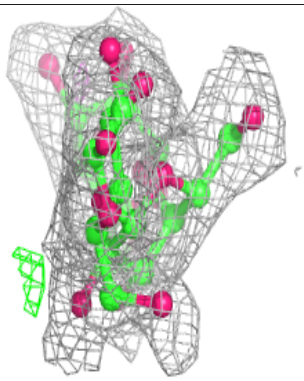


Electron density around Chain m:

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

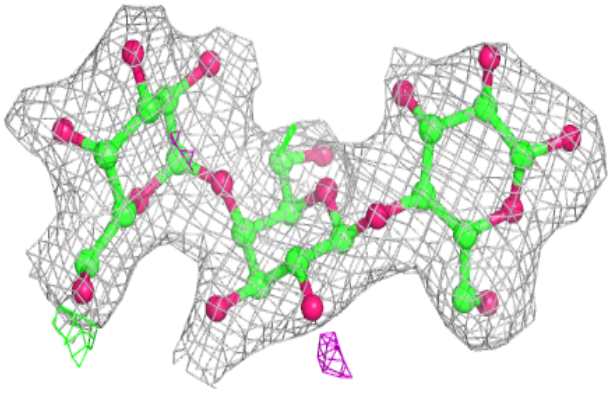


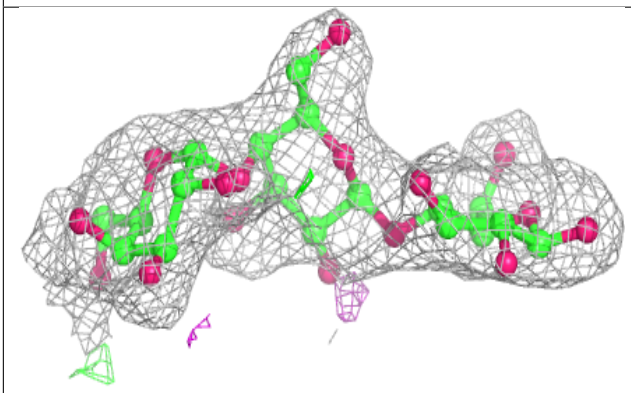


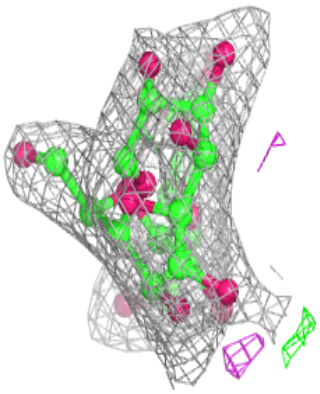


Electron density around Chain o:

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

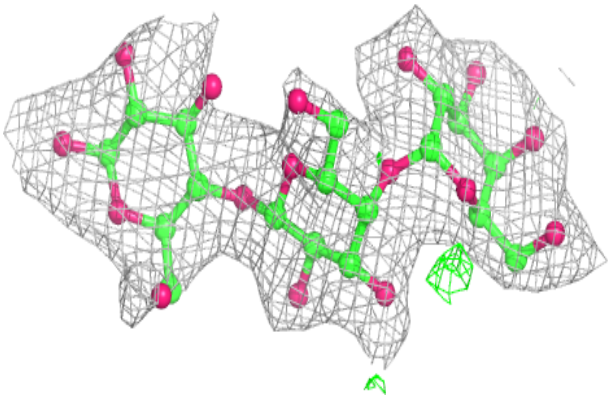


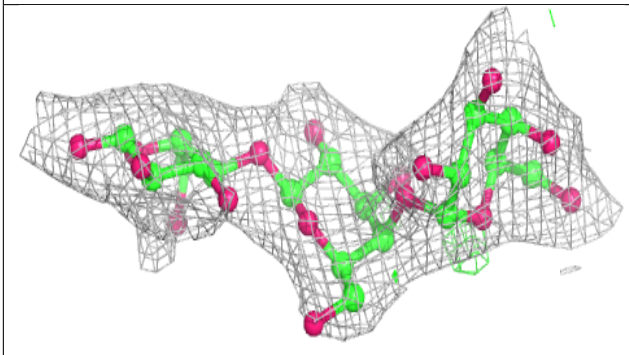


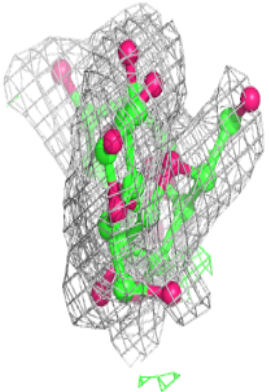


Electron density around Chain p:

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

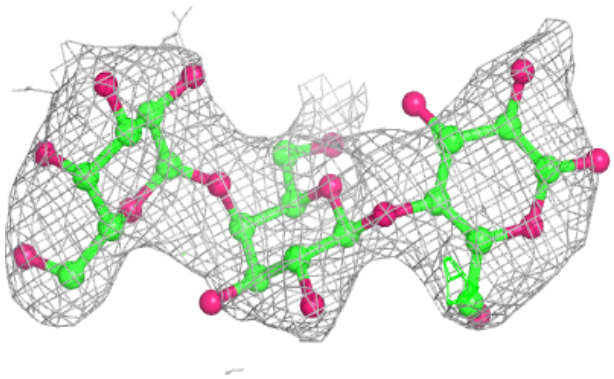


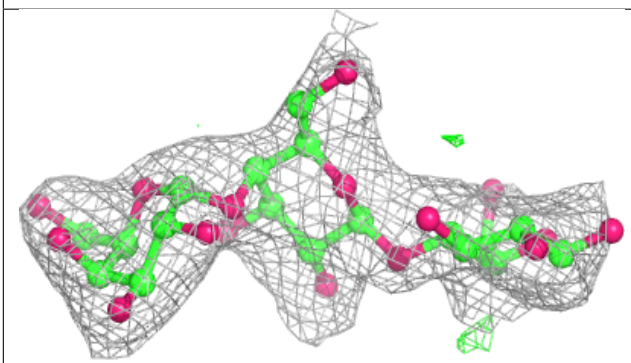


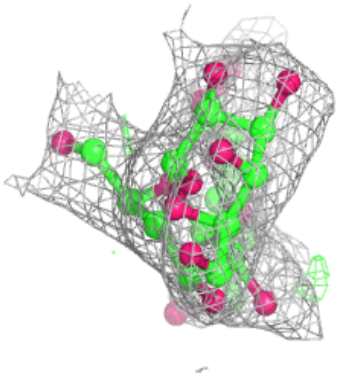


Electron density around Chain r:

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

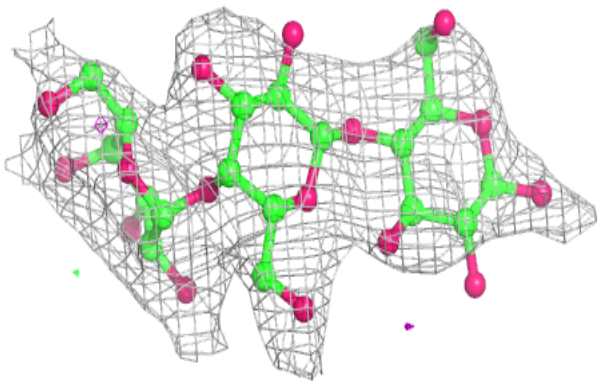


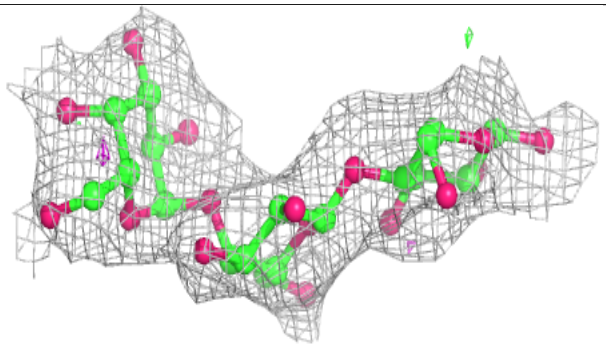


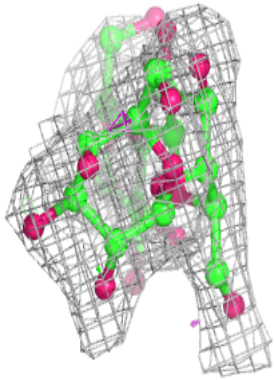


Electron density around Chain s:

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

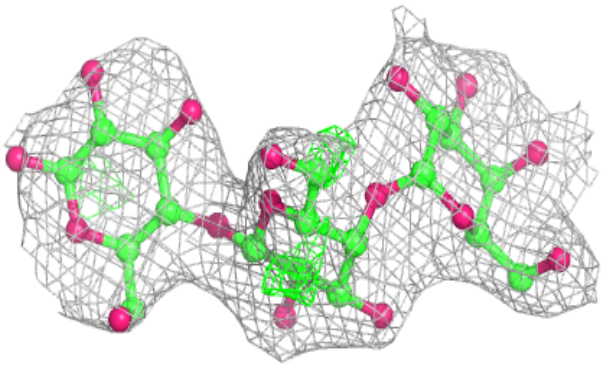


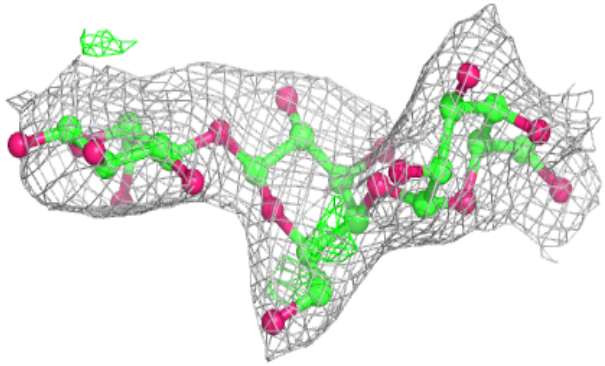




Electron density around Chain t:

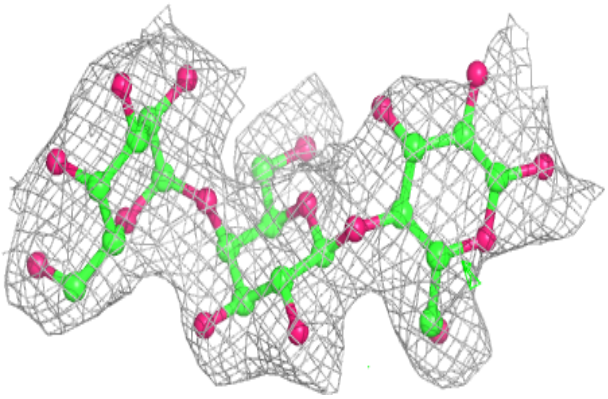
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

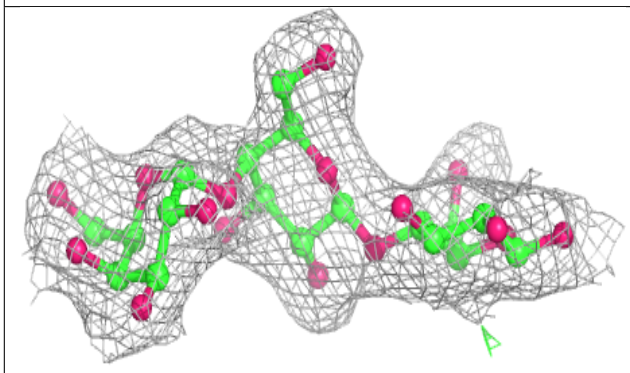


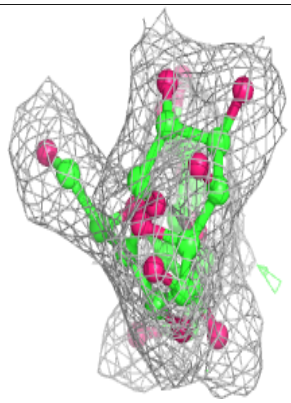


Electron density around Chain v:

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

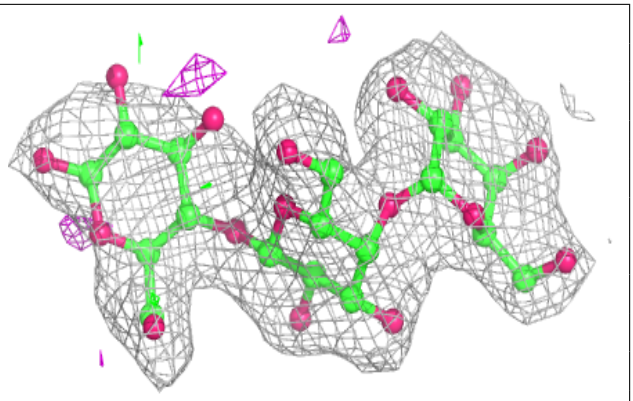


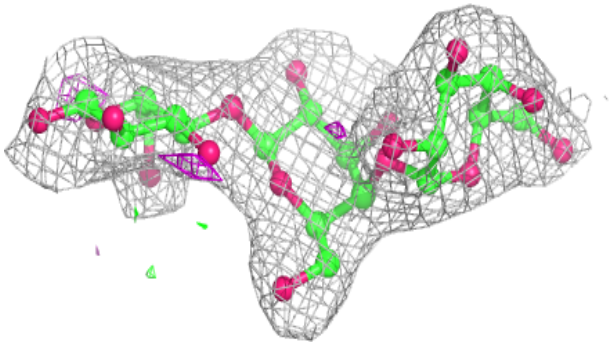


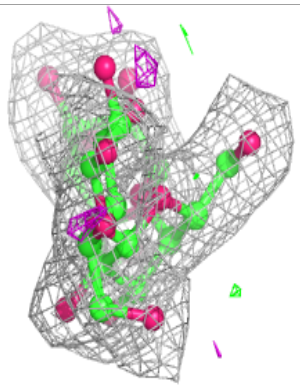


Electron density around Chain x:

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

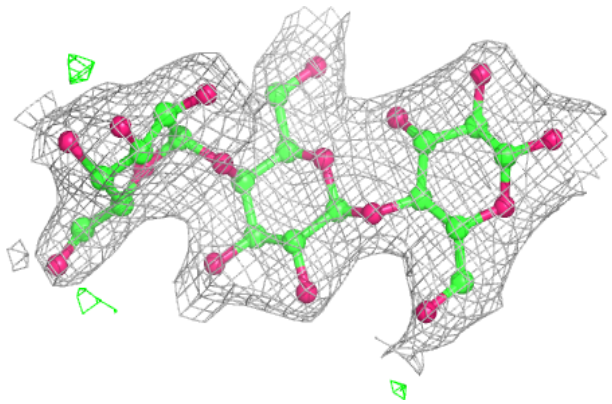


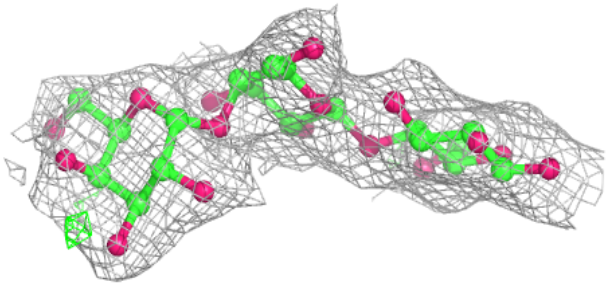


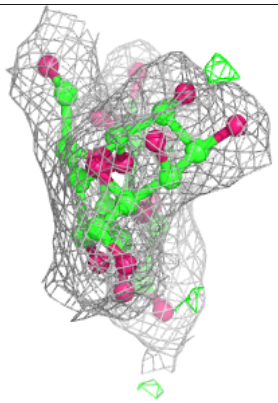


Electron density around Chain z:

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

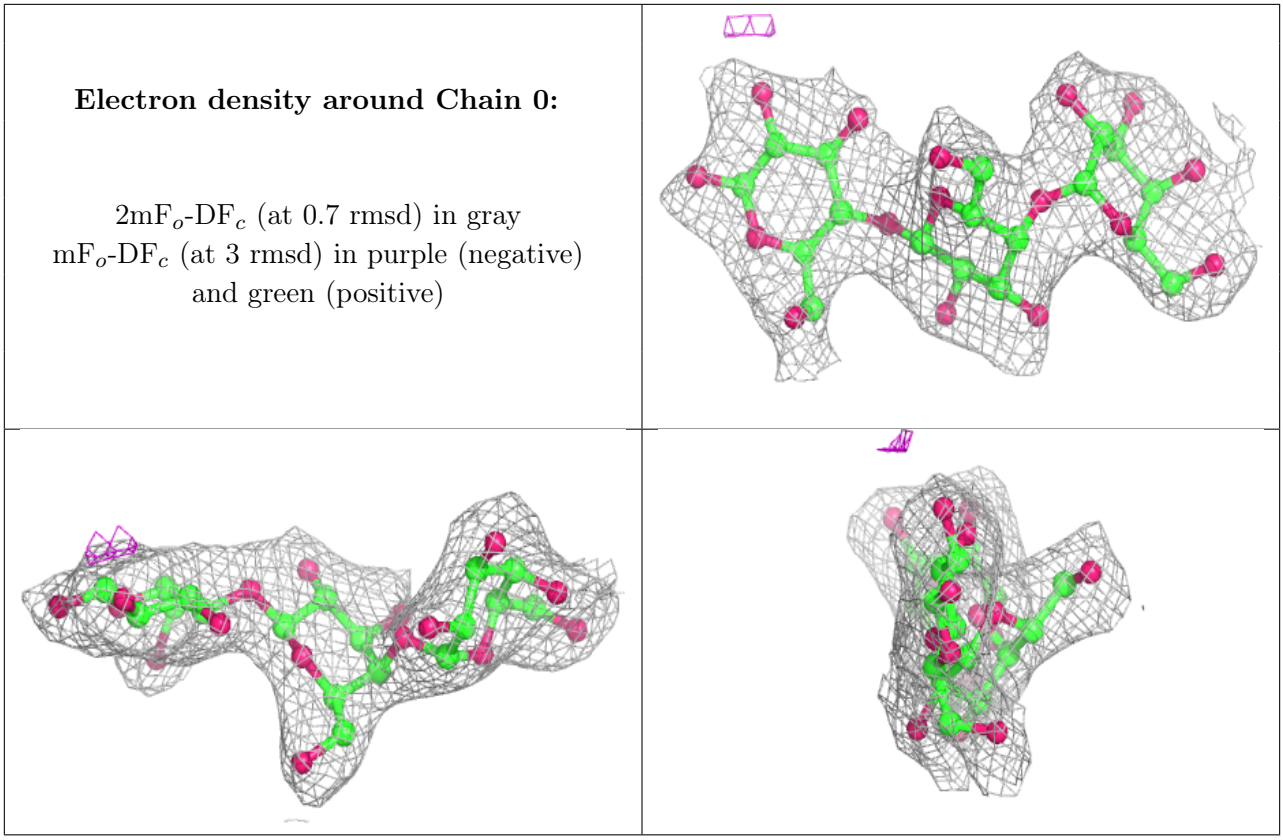






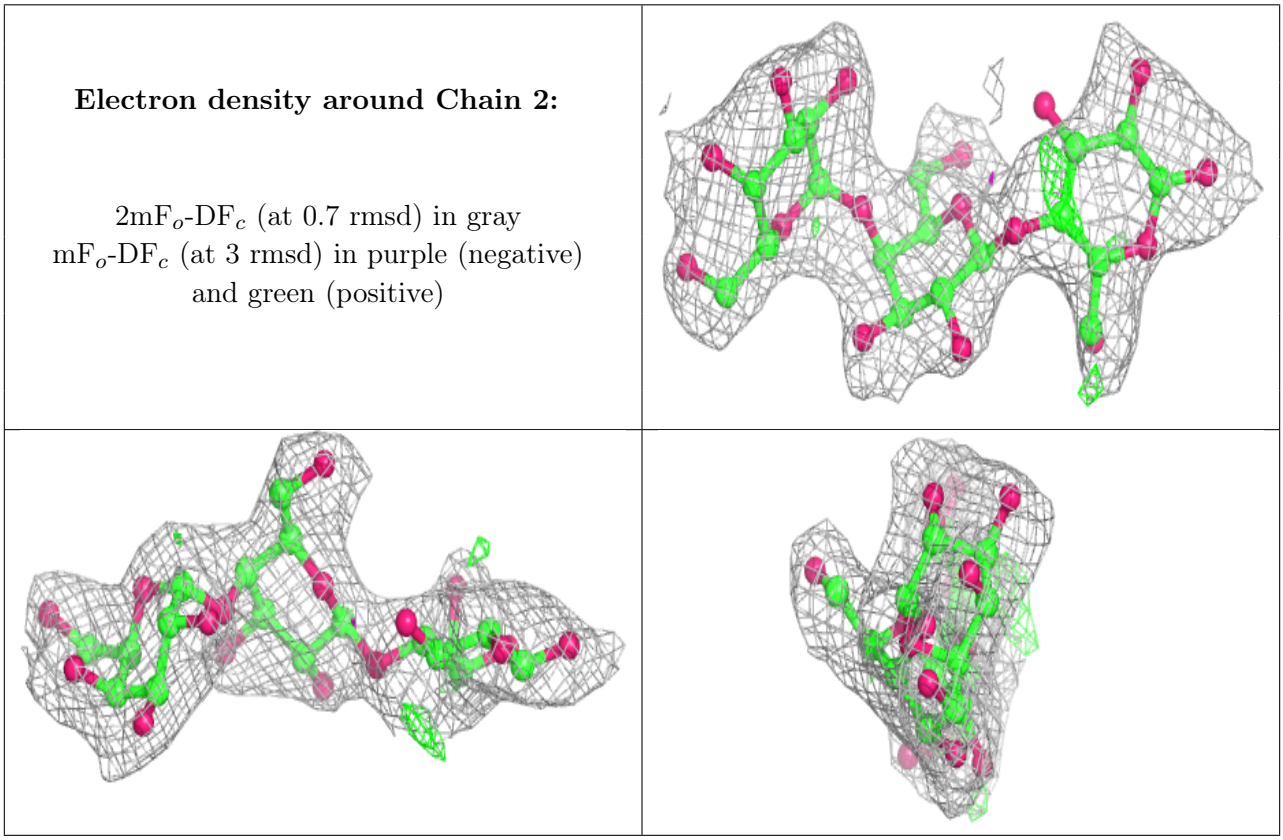
Electron density around Chain 0:

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



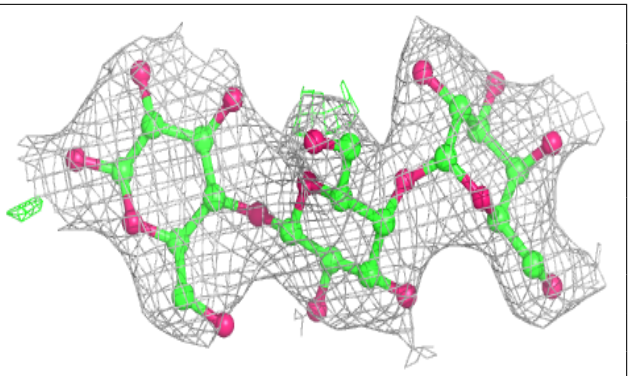
Electron density around Chain 2:

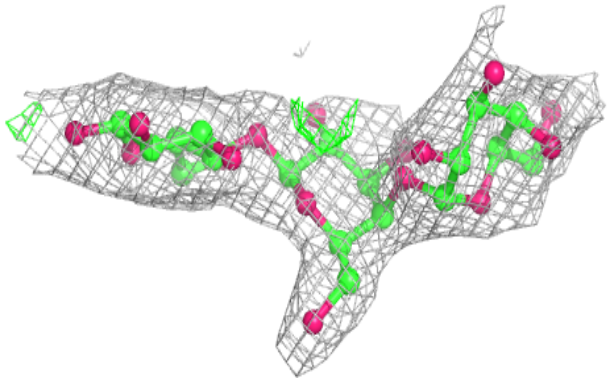
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

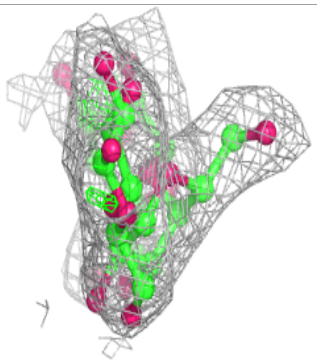


Electron density around Chain 4:

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

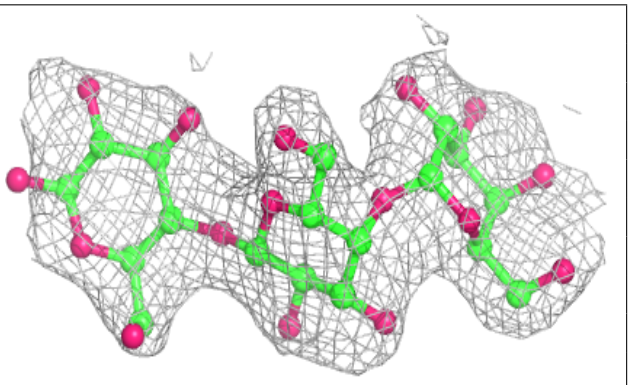


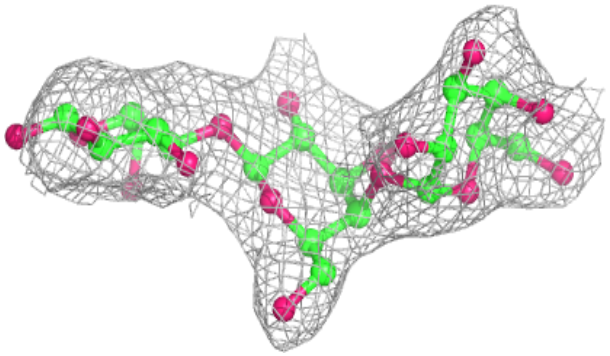


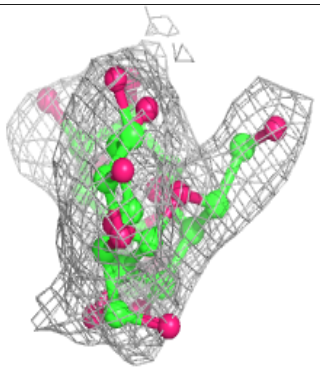


Electron density around Chain 5:

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

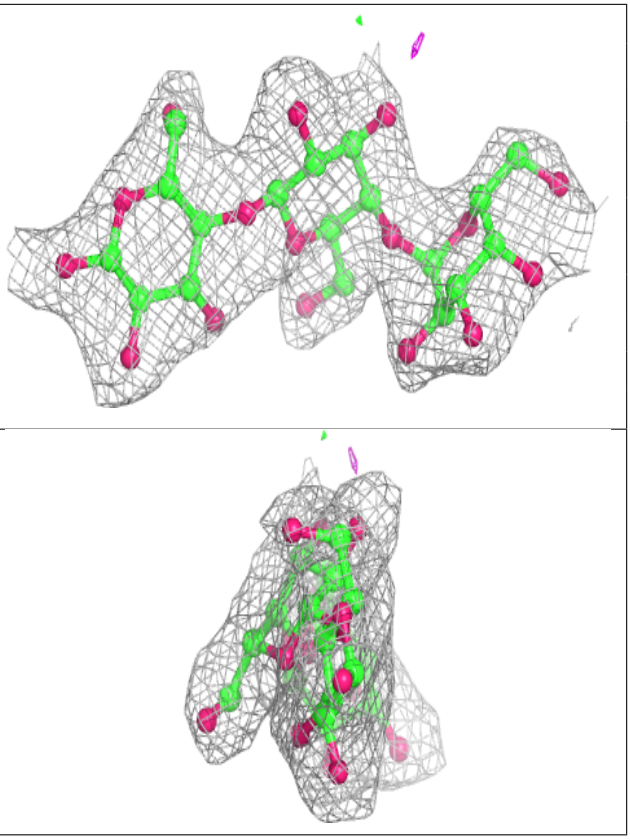






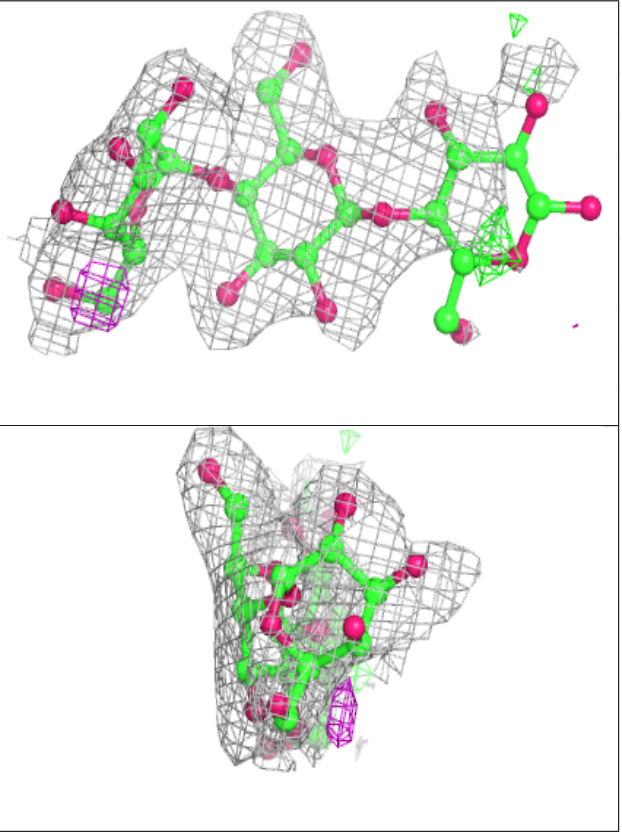
Electron density around Chain 7:

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



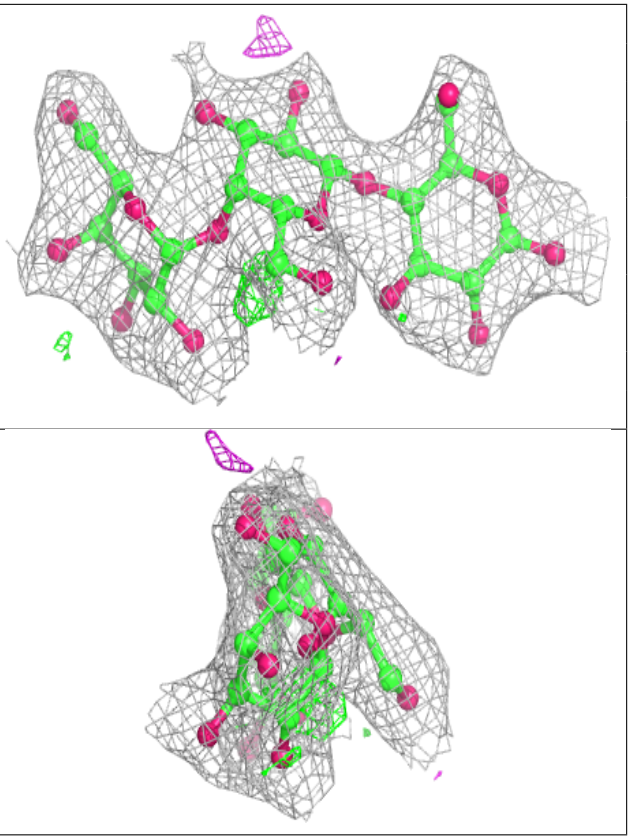
Electron density around Chain 8:

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



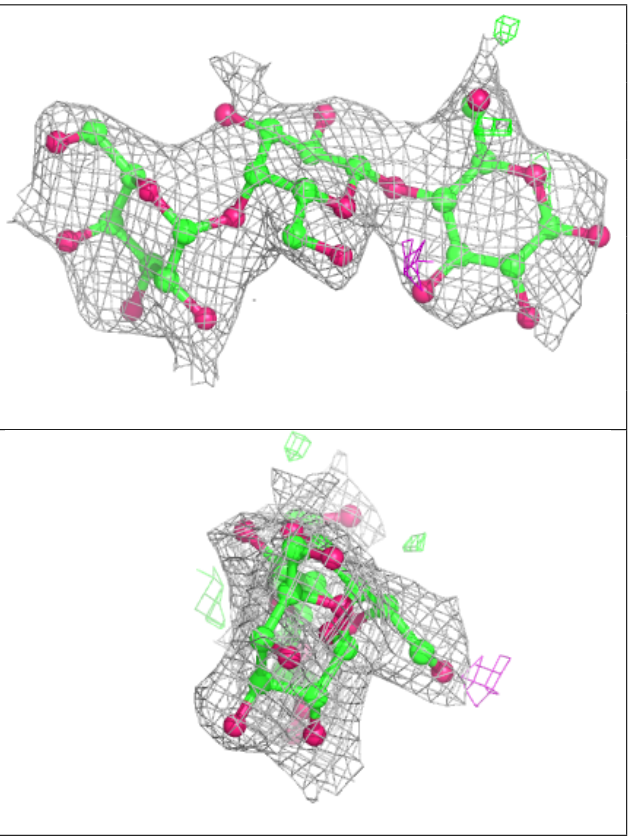
Electron density around Chain 9:

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



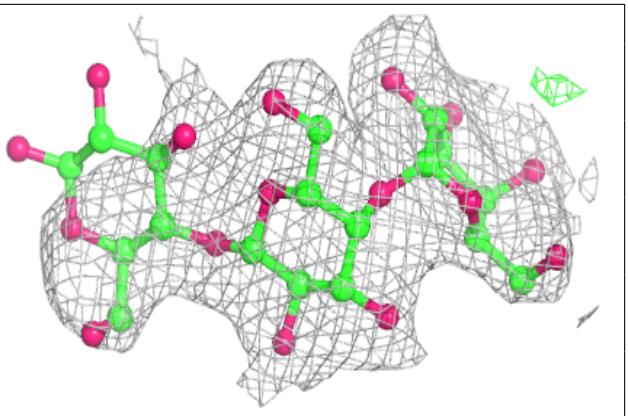
Electron density around Chain AA:

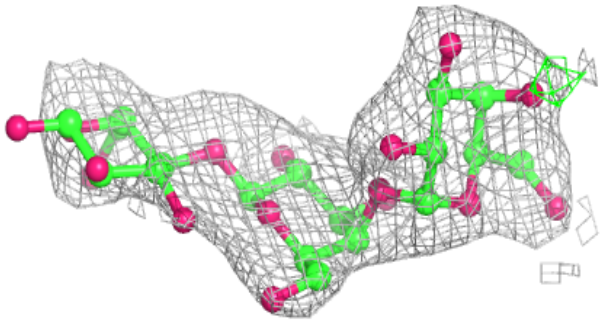
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

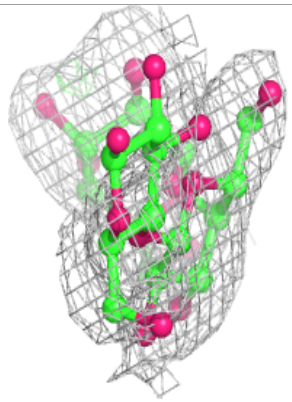


Electron density around Chain BA:

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

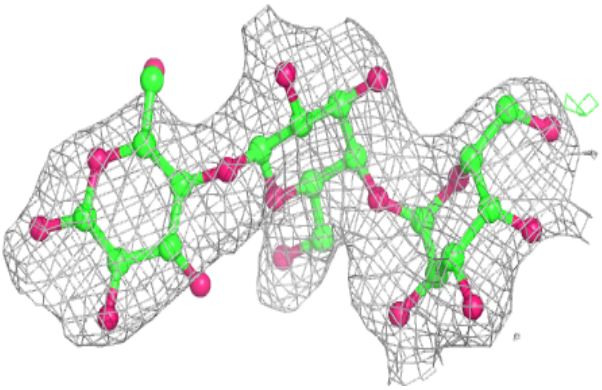


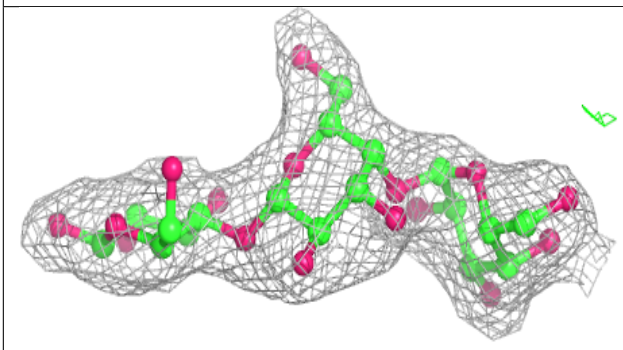


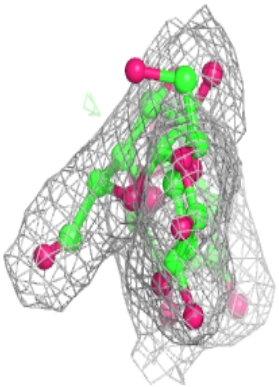


Electron density around Chain CA:

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

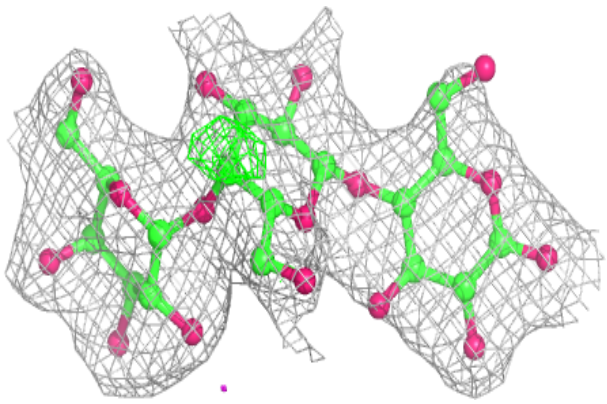


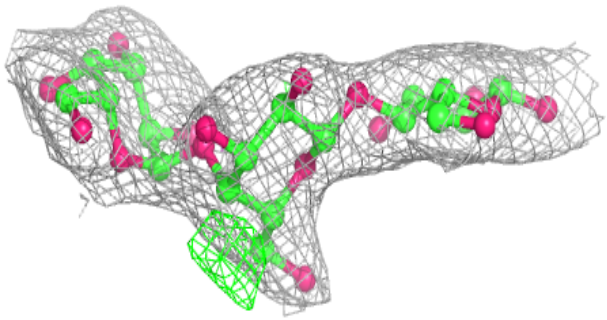


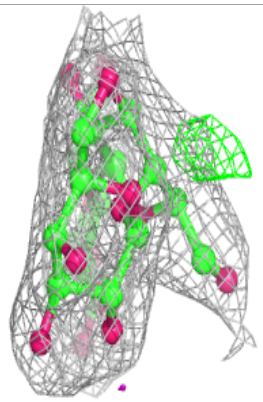


Electron density around Chain EA:

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

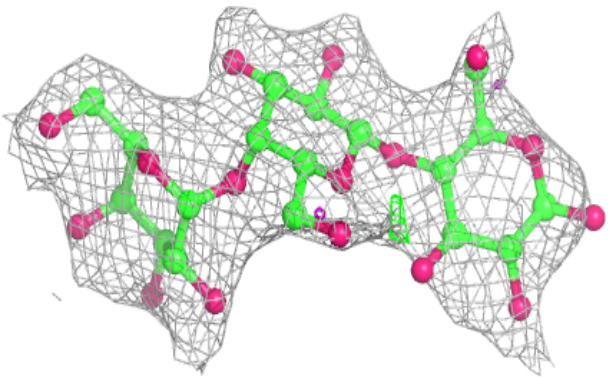


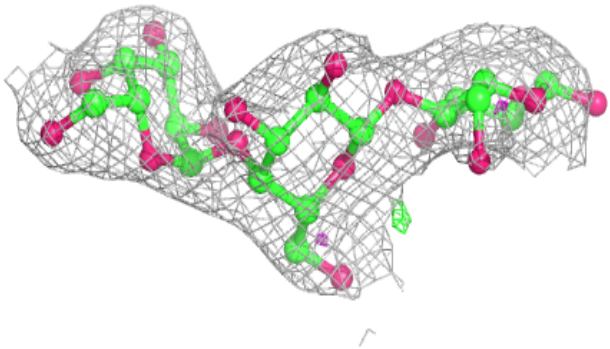


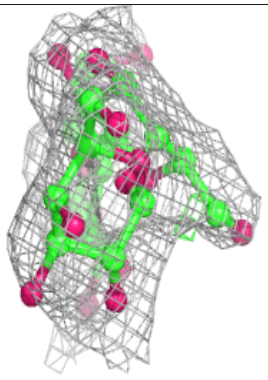


Electron density around Chain FA:

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

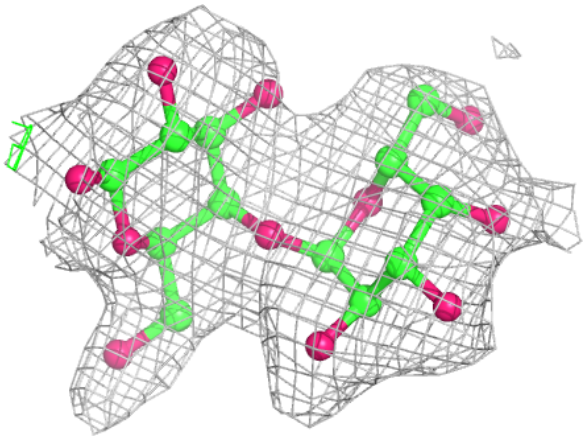


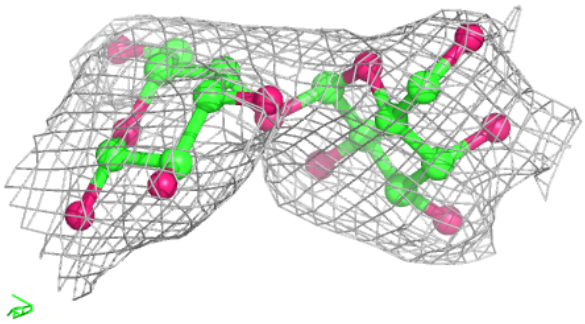


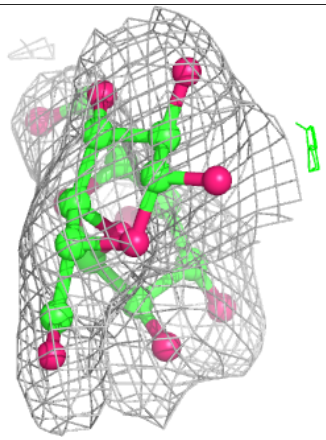


Electron density around Chain V:

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

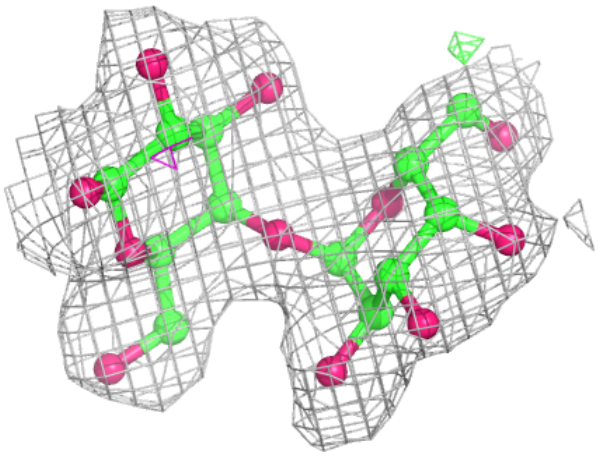


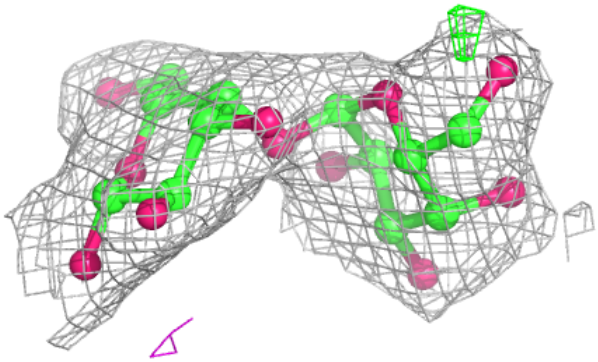


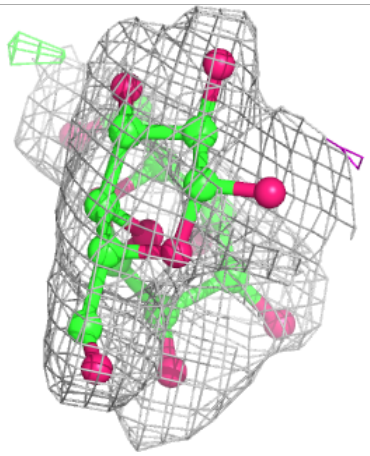


Electron density around Chain Y:

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

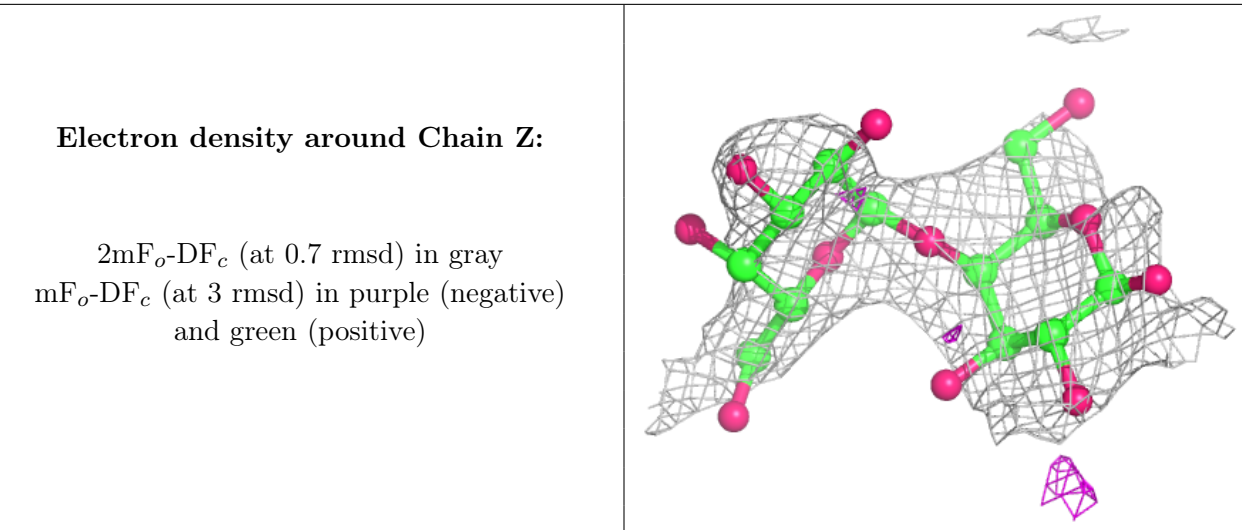


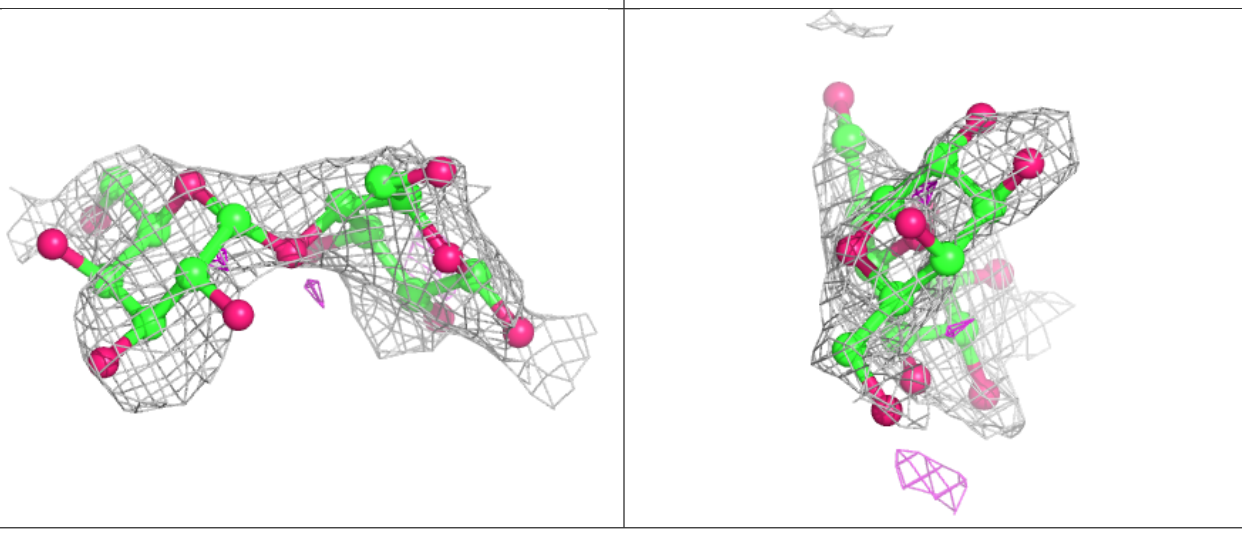




Electron density around Chain Z:

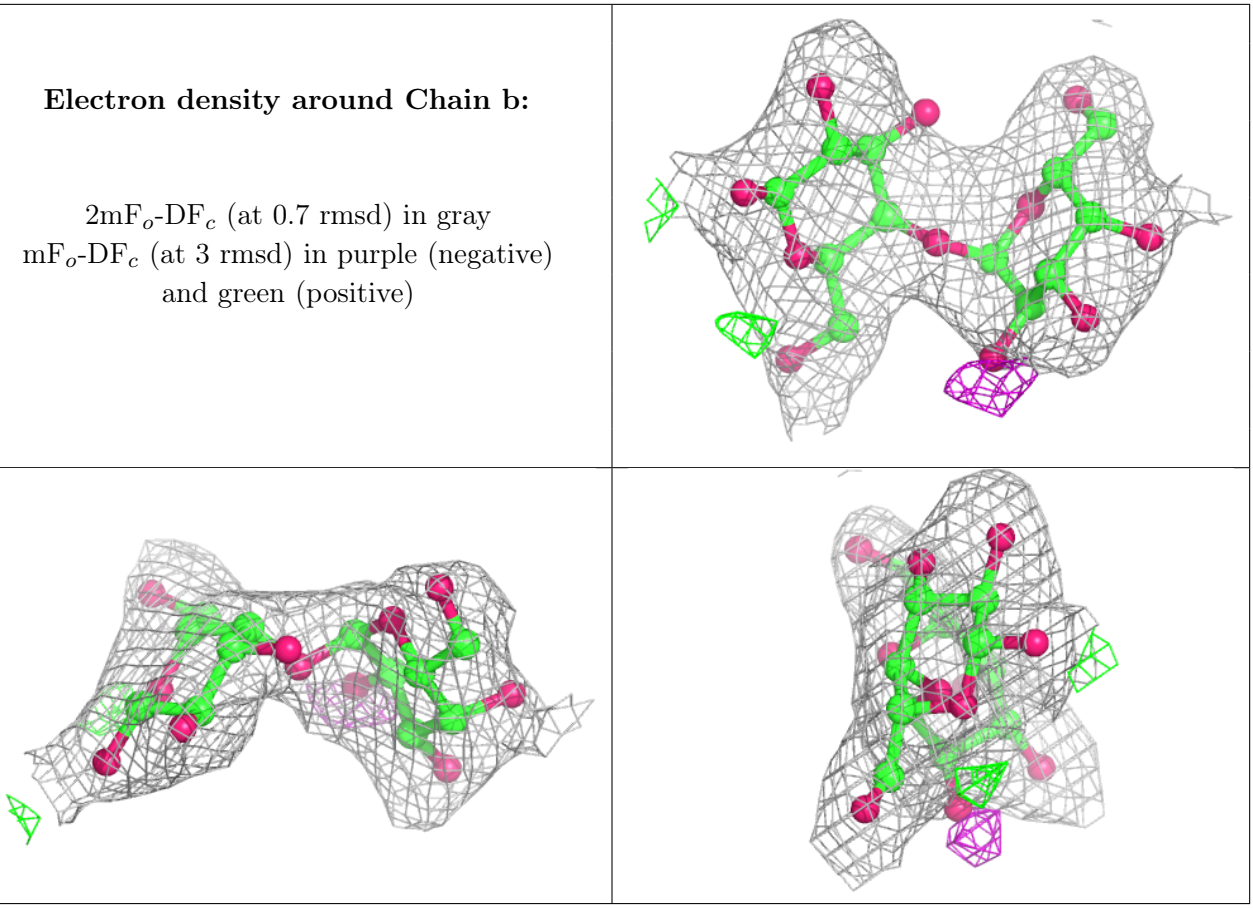
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





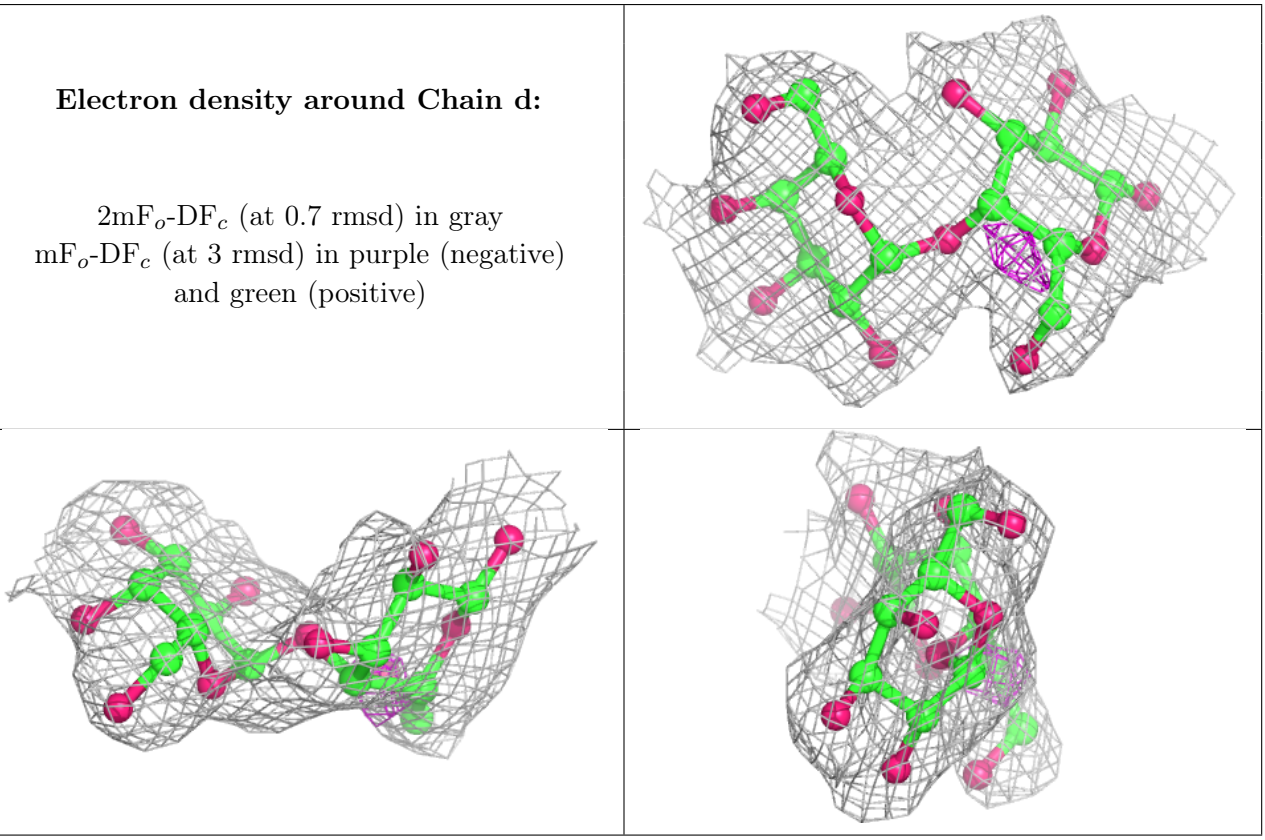
Electron density around Chain b:

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



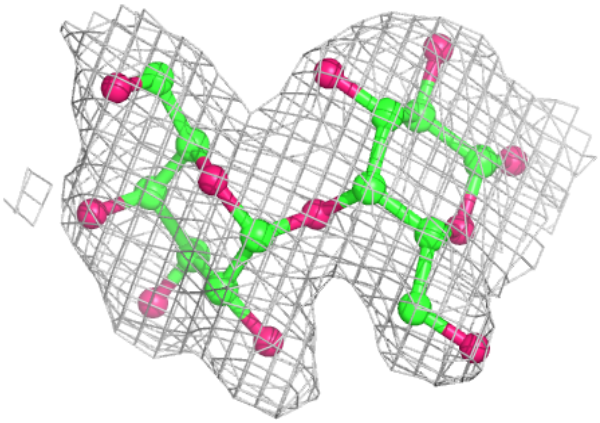
Electron density around Chain d:

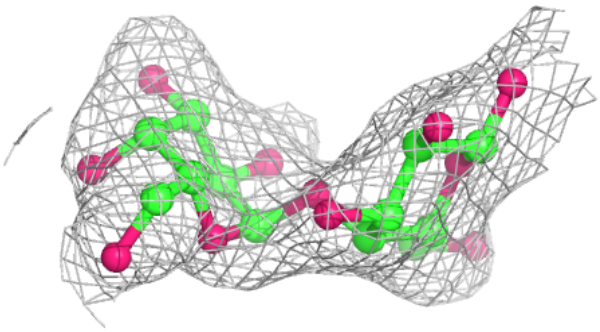
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

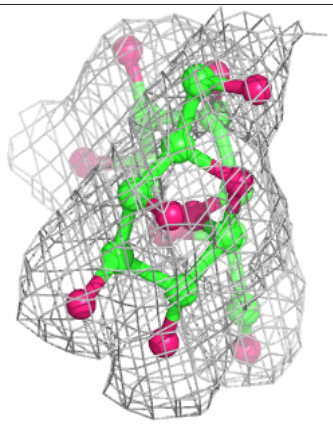


Electron density around Chain l:

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

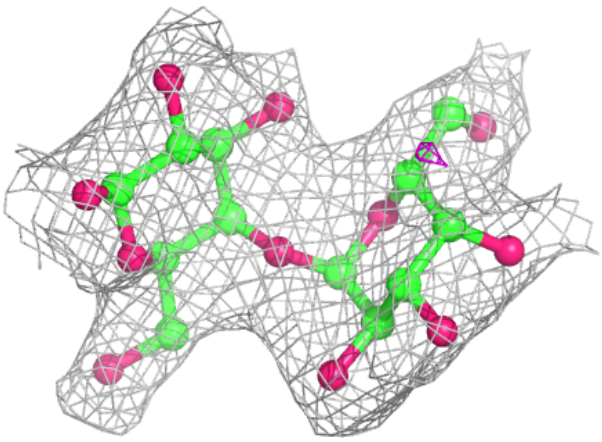


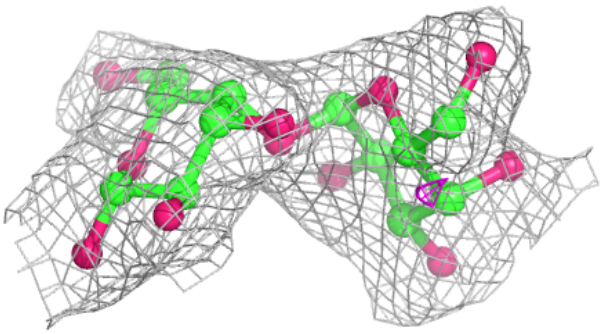


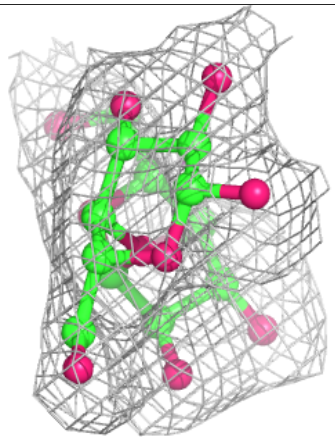


Electron density around Chain n:

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

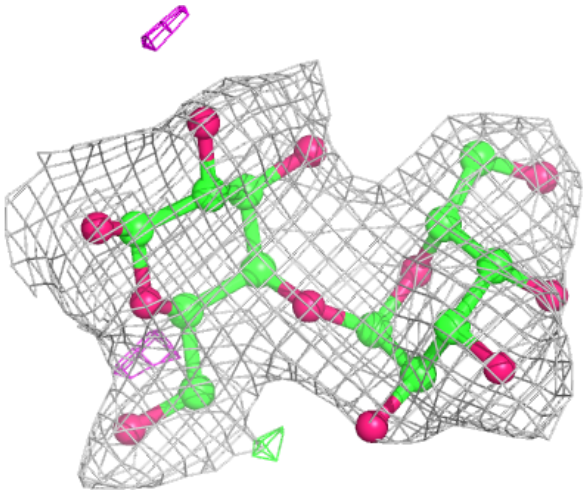


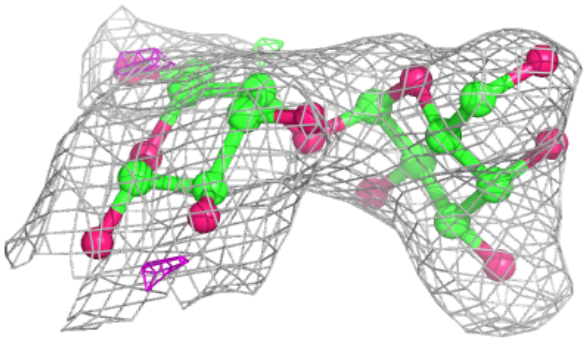


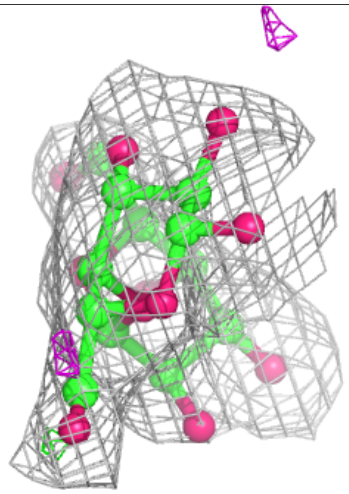


Electron density around Chain q:

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

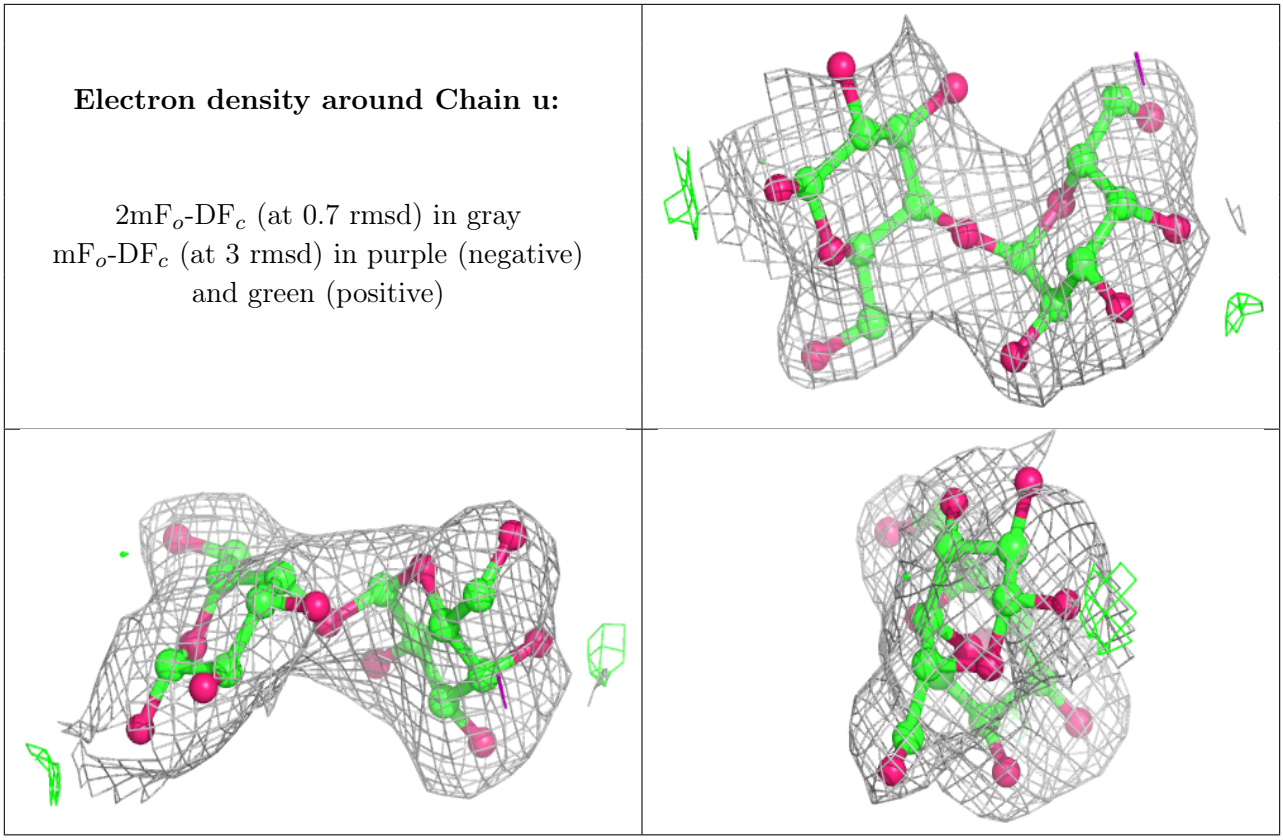






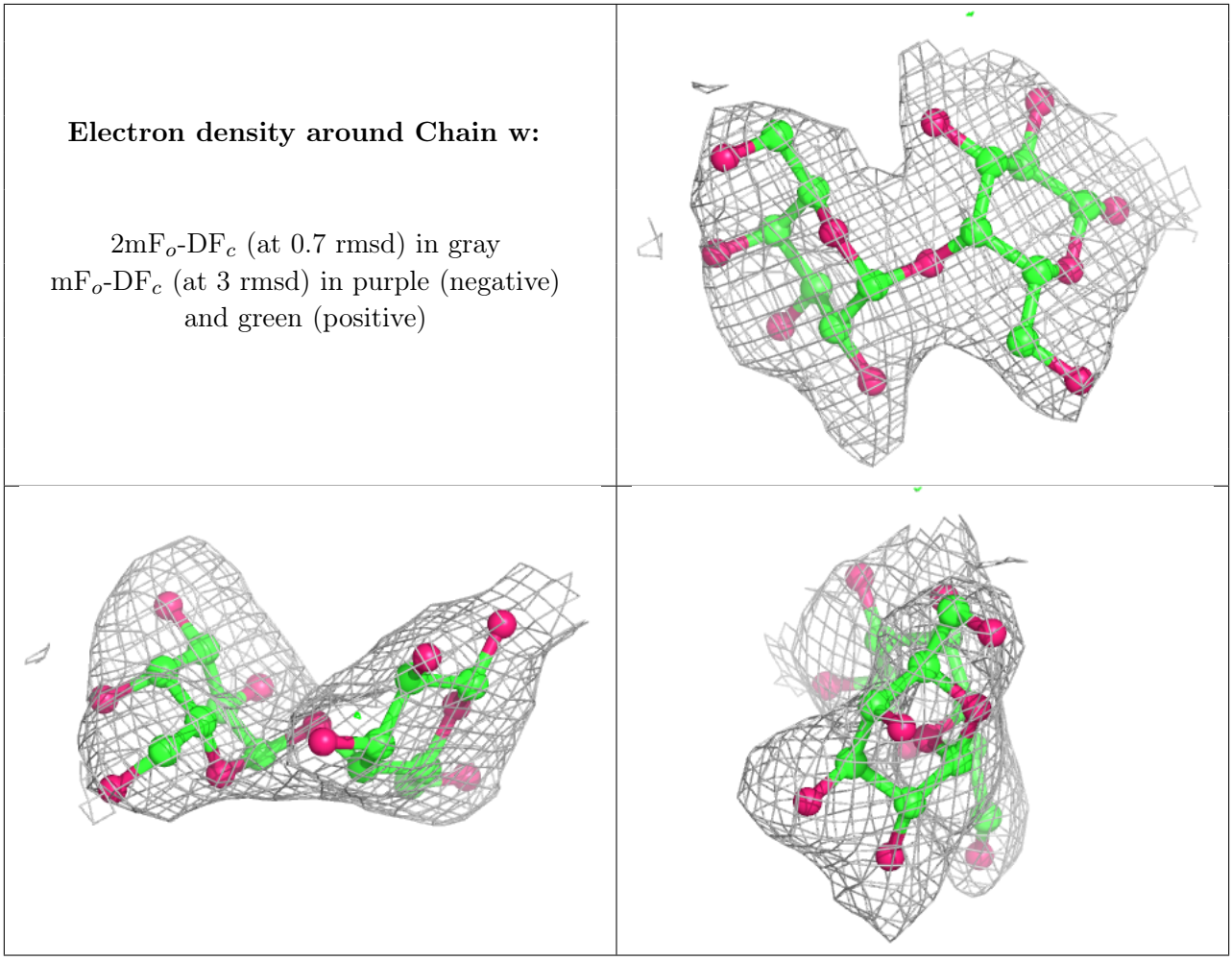
Electron density around Chain u:

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



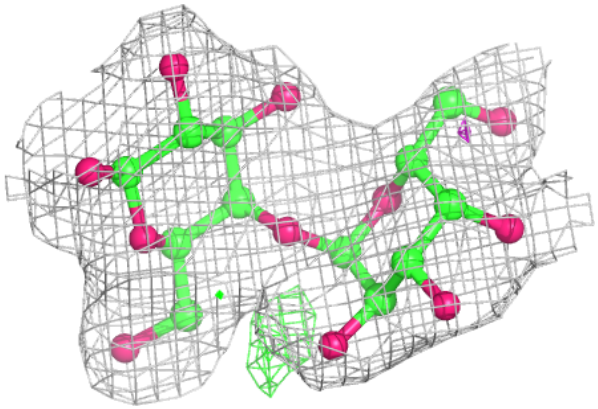
Electron density around Chain w:

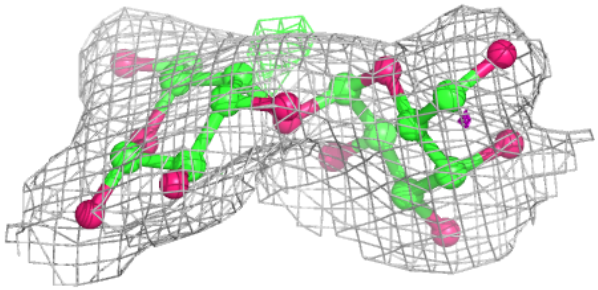
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

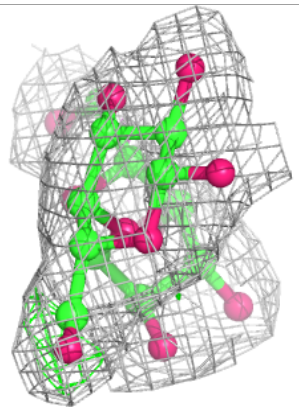


Electron density around Chain y:

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

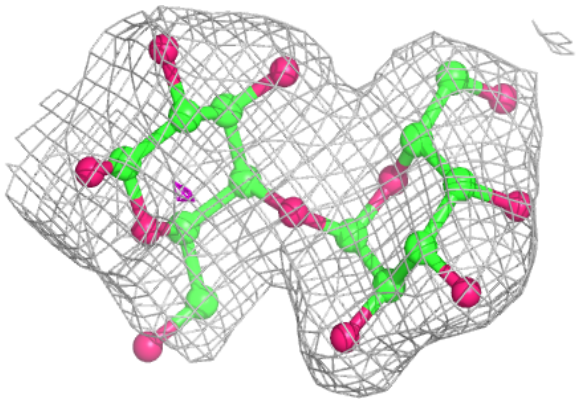


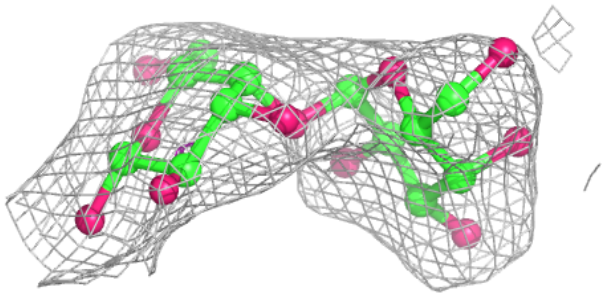


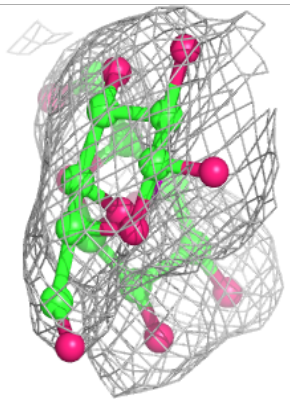


Electron density around Chain 1:

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

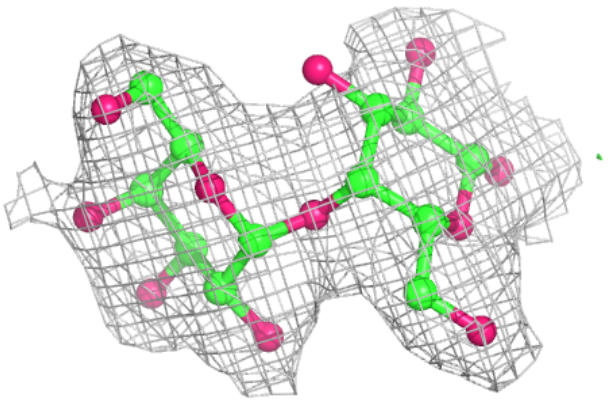


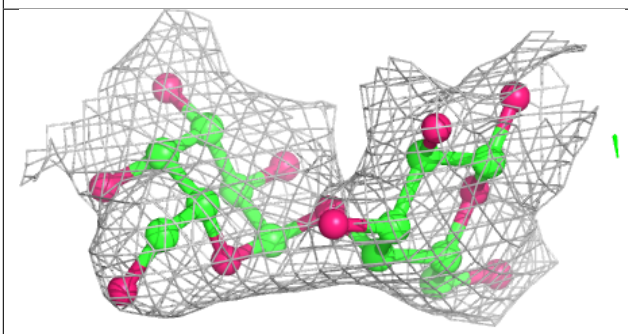


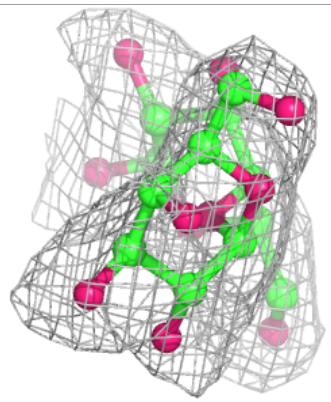


Electron density around Chain 3:

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

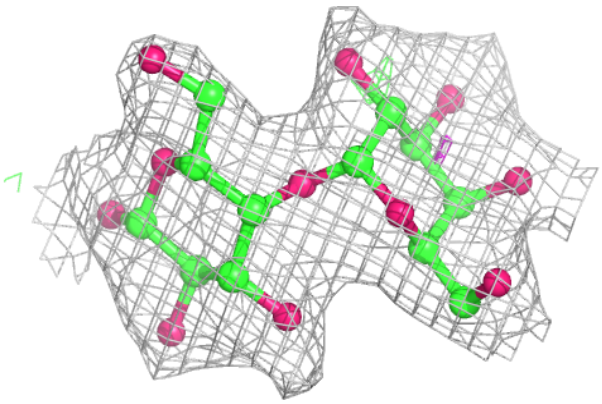


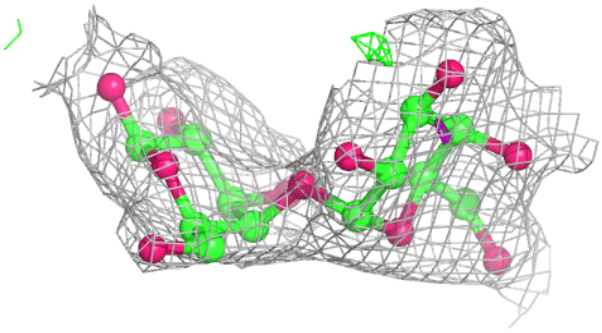


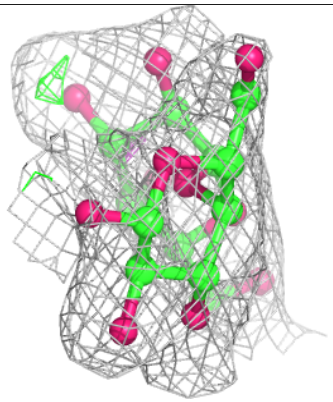


Electron density around Chain 6:

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

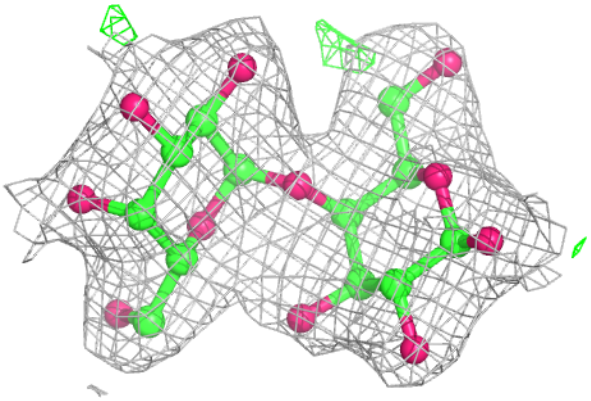


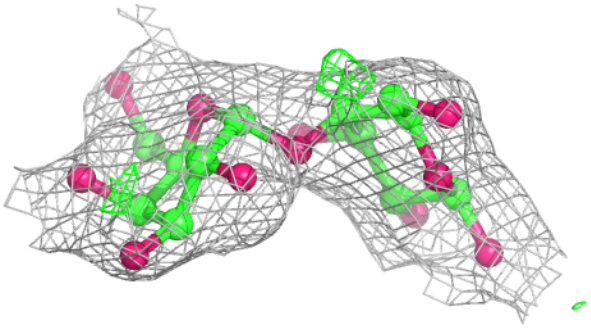


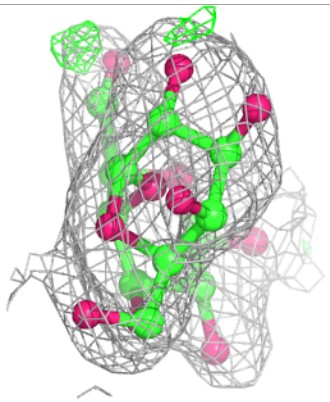


Electron density around Chain DA:

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

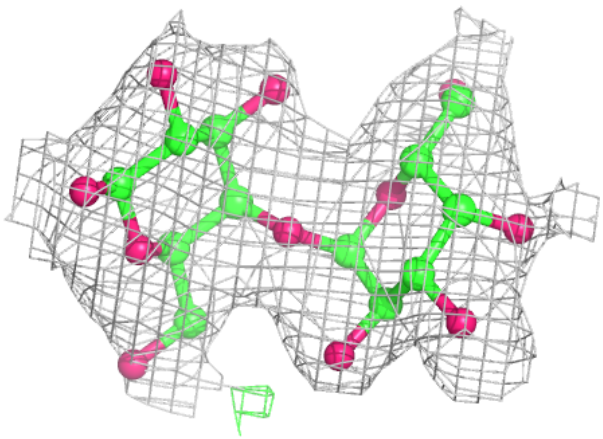


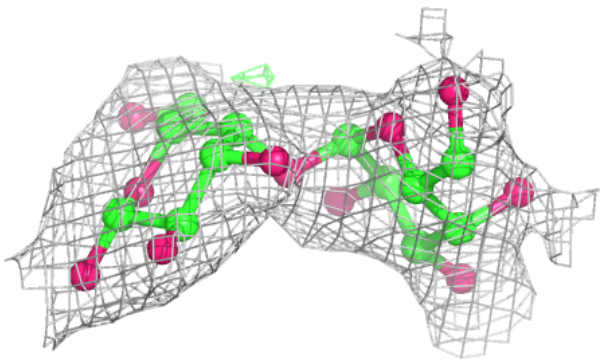


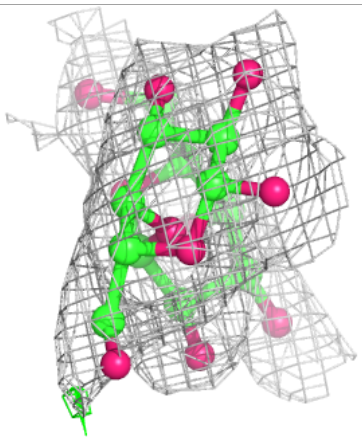


Electron density around Chain GA:

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







6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GAL	N	3470	12/12	0.63	0.58	81,85,86,87	0
4	GAL	T	4570	12/12	0.63	0.42	65,74,76,77	0
4	GAL	C	1370	12/12	0.72	0.54	67,74,77,77	0
4	GAL	R	4370	12/12	0.72	0.52	81,88,90,91	0
4	GAL	E	1570	12/12	0.72	0.45	85,88,90,90	0
4	GAL	K	3170	12/12	0.76	0.51	72,84,87,87	0
4	GAL	J	2570	12/12	0.76	0.58	84,89,91,91	0
4	GAL	P	4170	12/12	0.79	0.37	68,81,83,83	0
4	GAL	G	2270	12/12	0.80	0.42	79,88,90,93	0
4	GAL	L	3270	12/12	0.81	0.37	55,65,68,71	0
4	GAL	I	2470	12/12	0.83	0.44	79,81,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.