



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 02:53 PM BST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

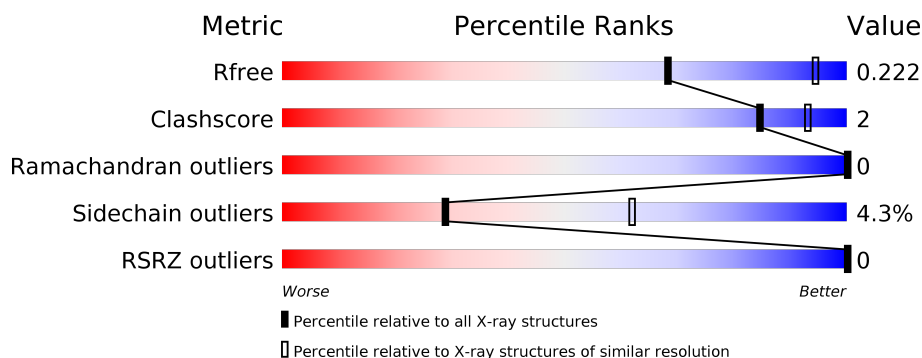
# 1 Overall quality at a glance

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.



















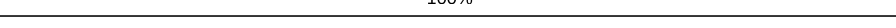
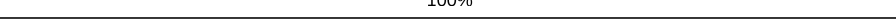
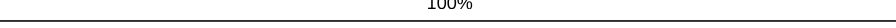
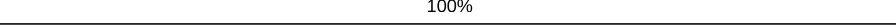
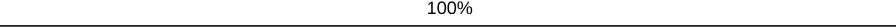

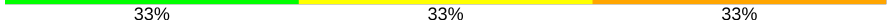
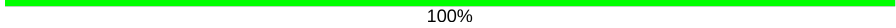
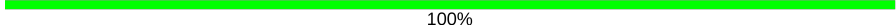
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	69	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	C	69	<div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	D	69	<div> <div>91%</div> <div>6%</div> <div>..</div> </div>
1	E	69	<div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	F	69	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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%
2	EA	3	 67% 33%

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Mol	Chain	Length	Quality of chain
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%
3	6	2	100%

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

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

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.

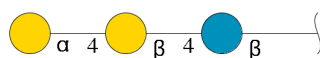
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
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	0	0	0
			34	18	16			
2	p	3	Total	C	O	0	0	0
			34	18	16			
2	r	3	Total	C	O	0	0	0
			34	18	16			
2	s	3	Total	C	O	0	0	0
			34	18	16			
2	t	3	Total	C	O	0	0	0
			34	18	16			
2	v	3	Total	C	O	0	0	0
			34	18	16			
2	x	3	Total	C	O	0	0	0
			34	18	16			
2	z	3	Total	C	O	0	0	0
			34	18	16			
2	0	3	Total	C	O	0	0	0
			34	18	16			
2	2	3	Total	C	O	0	0	0
			34	18	16			
2	4	3	Total	C	O	0	0	0
			34	18	16			
2	5	3	Total	C	O	0	0	0
			34	18	16			
2	7	3	Total	C	O	0	0	0
			34	18	16			
2	8	3	Total	C	O	8	0	0
			34	18	16			
2	9	3	Total	C	O	0	0	0
			34	18	16			
2	AA	3	Total	C	O	0	0	0
			34	18	16			
2	BA	3	Total	C	O	4	0	0
			34	18	16			
2	CA	3	Total	C	O	0	0	0
			34	18	16			
2	EA	3	Total	C	O	0	0	0
			34	18	16			
2	FA	3	Total	C	O	0	0	0
			34	18	16			

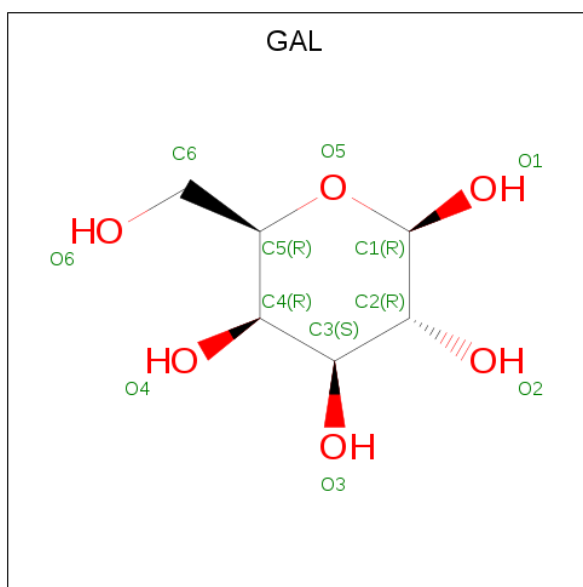
- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose.





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

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 5 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	27	Total 27	O 27	0	0
5	C	19	Total 19	O 19	0	0
5	D	16	Total 16	O 16	0	0
5	E	18	Total 18	O 18	0	0
5	F	15	Total 15	O 15	0	0
5	G	21	Total 21	O 21	0	0
5	H	17	Total 17	O 17	0	0
5	I	17	Total 17	O 17	0	0
5	J	15	Total 15	O 15	0	0
5	K	21	Total 21	O 21	0	0
5	L	23	Total 23	O 23	0	0
5	M	24	Total 24	O 24	0	0
5	N	14	Total 14	O 14	0	0
5	O	23	Total 23	O 23	0	0
5	P	17	Total 17	O 17	0	0
5	Q	13	Total 13	O 13	0	0
5	R	10	Total 10	O 10	0	0
5	S	11	Total 11	O 11	0	0
5	T	12	Total 12	O 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: 




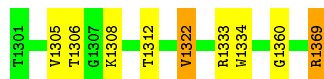
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

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: 90% 7% ..



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain H: 87% 10% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain I: 90% 9% .



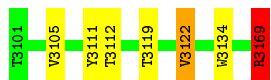
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain J: 88% 10% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain K: 90% 7% ..



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain L: 91% 7% .



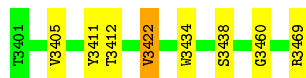
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain M: 91% 6% .



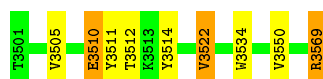
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain N: 88% 10% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain O: 87% 9% .



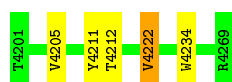
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain P: 90% 9% .



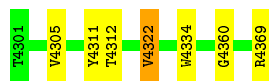
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain Q: 93% 6% .



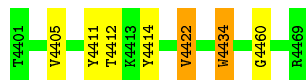
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain R: 90% 9% .



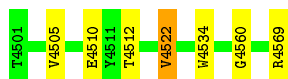
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain S: 90% 7% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain T: 90% 9% .



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

Chain U:  100%



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

Chain W:  33% 33% 33%



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

Chain X:  100%



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

Chain a:  100%



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

Chain c:  100%



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

Chain e:  67% 33%



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

Chain f:  100%

BGC1  
GAL2  
GLA3

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

Chain g:  100%

BGC1  
GAL2  
GLA3

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

Chain h:  100%

BGC1  
GAL2  
GLA3

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

Chain i:  100%

BGC1  
GAL2  
GLA3

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

Chain j:  33% 67%

BGC1  
GAL2  
GLA3

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

Chain k:  67% 33%

BGC1  
GAL2  
GLA3

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

Chain m:  67% 33%

BGC1  
GAL2  
GLA3



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

Chain o:  67% 33%

BGC1  
GAL2  
GLA3

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

Chain p:  100%

BGC1  
GAL2  
GLA3

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

Chain r:  67% 33%

BGC1  
GAL2  
GLA3

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

Chain s:  100%

BGC1  
GAL2  
GLA3

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

Chain t:  67% 33%

BGC1  
GAL2  
GLA3

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

Chain v:  100%

BGC1  
GAL2  
GLA3

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

Chain x:  100%



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

Chain z: 67% 33%



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

Chain 0: 67% 33%



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

Chain 2: 100%



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

Chain 4: 100%



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

Chain 5: 100%



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

Chain 7: 100%



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

Chain 8:  100%

BUC1  
GAL2  
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranos e

Chain 9:  33% 67%

BUC1  
GAL2  
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranos e

Chain AA:  33% 33% 33%

BUC1  
GAL2  
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranos e

Chain BA:  100%

BUC1  
GAL2  
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranos e

Chain CA:  100%

BUC1  
GAL2  
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranos e

Chain EA:  67% 33%

BUC1  
GAL2  
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranos e

Chain FA:  100%

BUC1  
GAL2  
GLA3

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



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



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



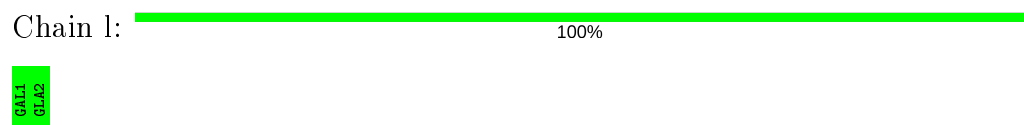
- Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



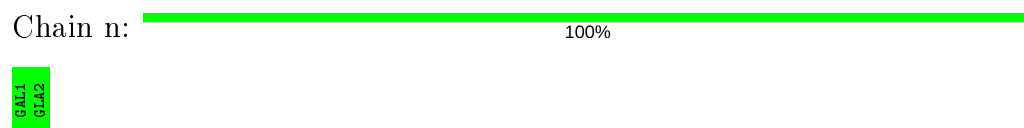
- Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



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



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



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





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

Chain u: 100%



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

Chain w: 100%



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

Chain y: 100%



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

Chain 1: 100%



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

Chain 3: 100%



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

Chain 6: 100%



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

Chain DA: 50% 50%



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

Chain GA:

100%

GA1  
GA2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.50 Å 97.70 Å 164.20 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.90 (at 2.75 Å)	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 <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: GLA, BGC, 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



The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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:HG2	1:G:2269:ARG:HH11	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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2322	VAL
1	K	3105	VAL
1	R	4369	ARG
1	H	2369	ARG
1	I	2422	VAL

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

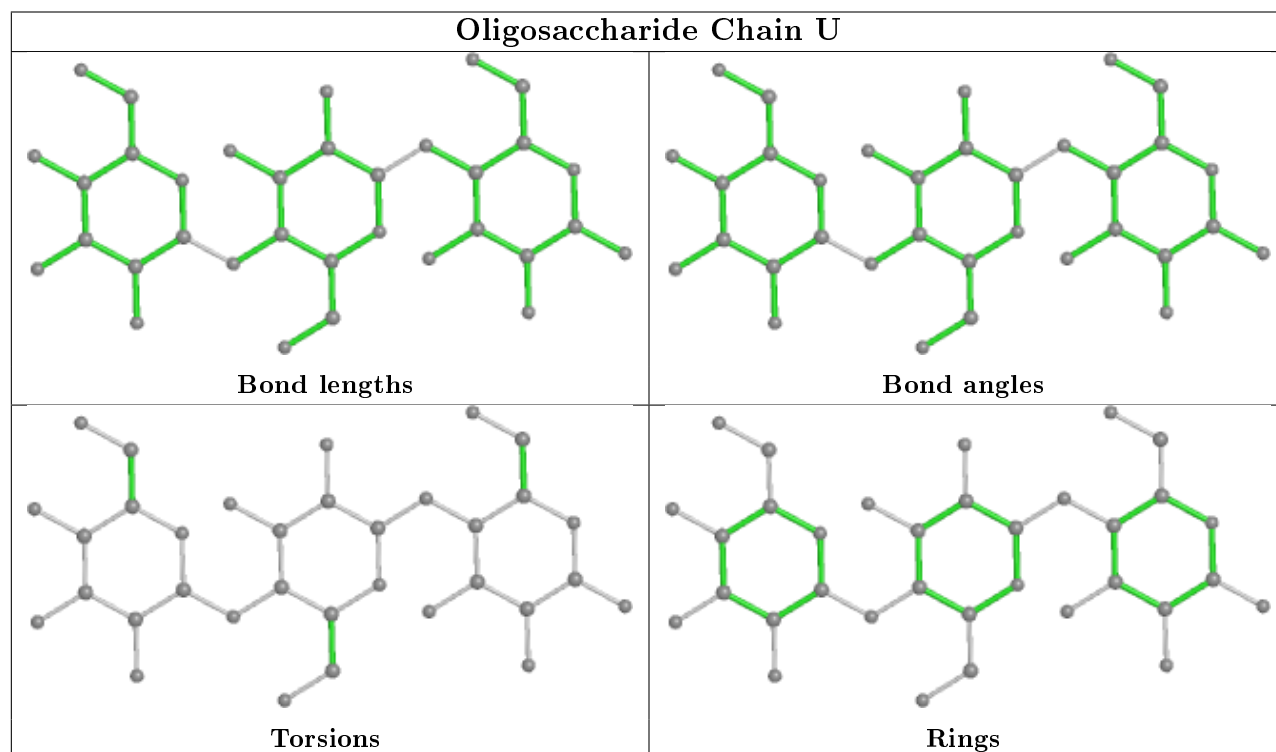
Mol	Chain	Res	Type	Atoms
3	GA	2	GLA	O5-C5-C6-O6
3	GA	2	GLA	C4-C5-C6-O6
2	g	3	GLA	O5-C5-C6-O6
2	z	1	BGC	O5-C5-C6-O6
2	g	3	GLA	C4-C5-C6-O6

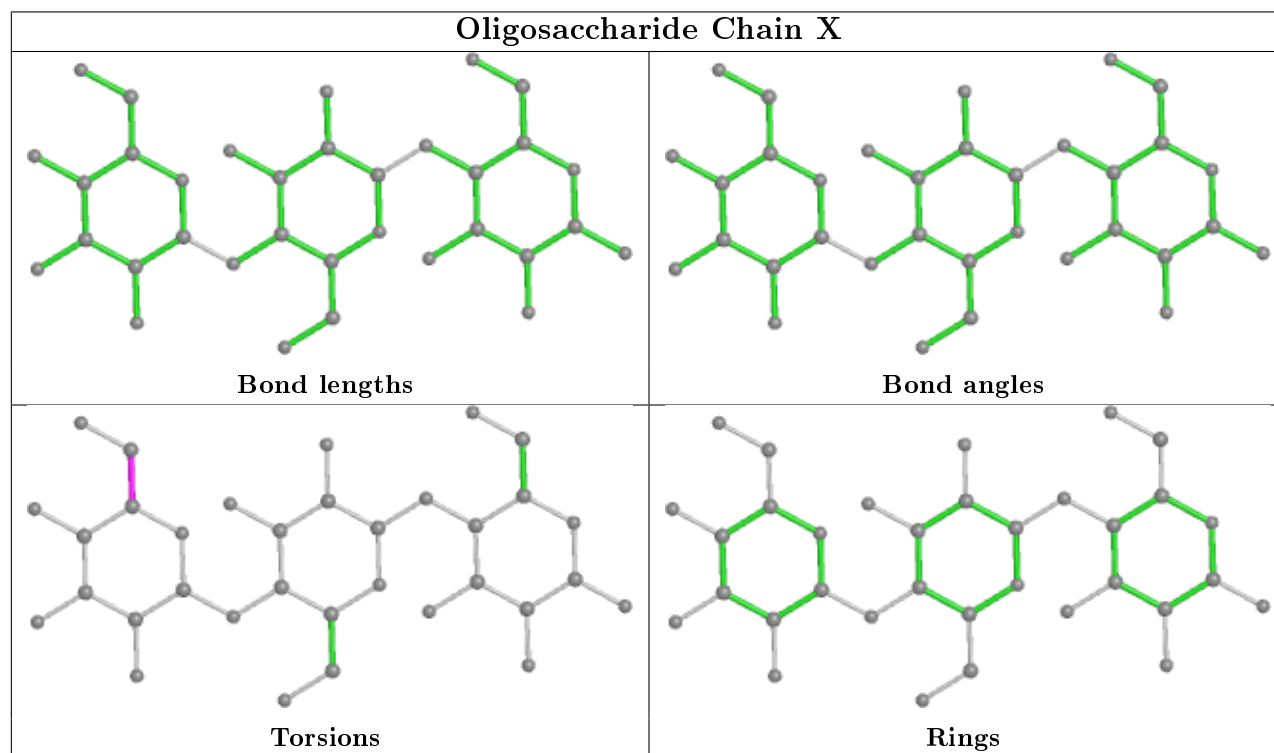
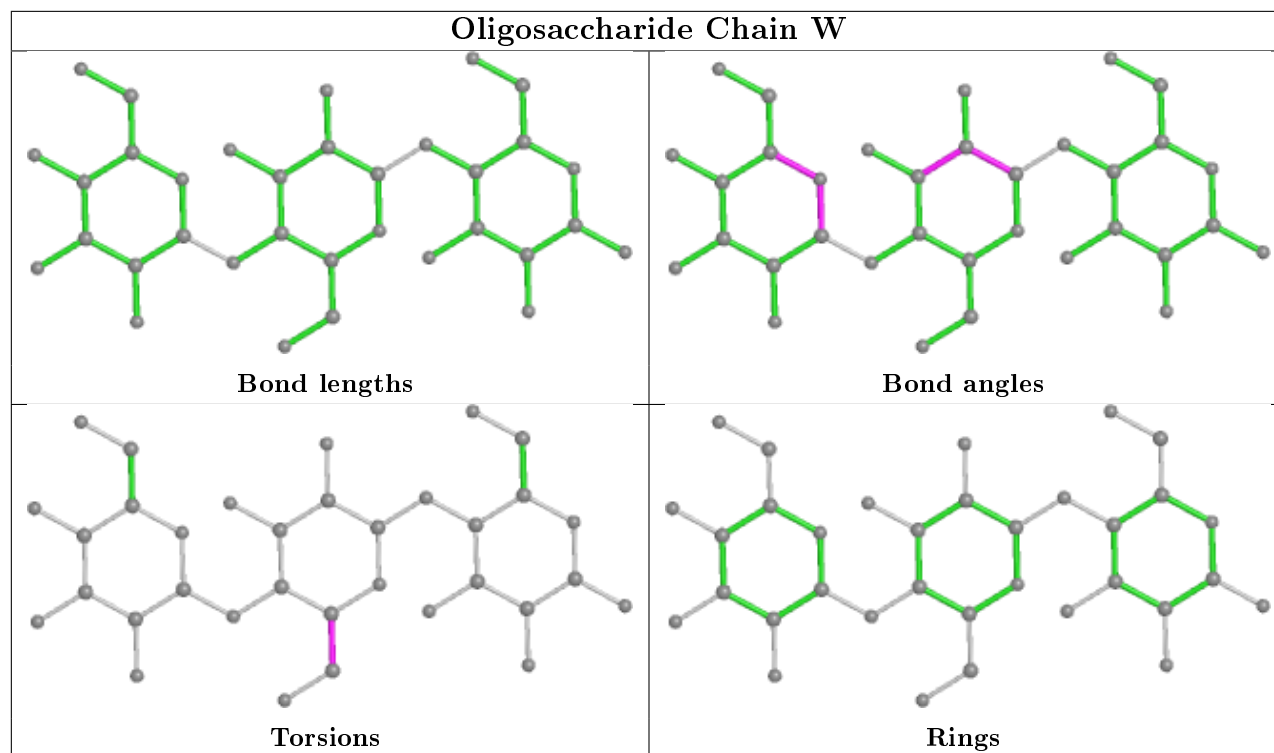
There are no ring outliers.

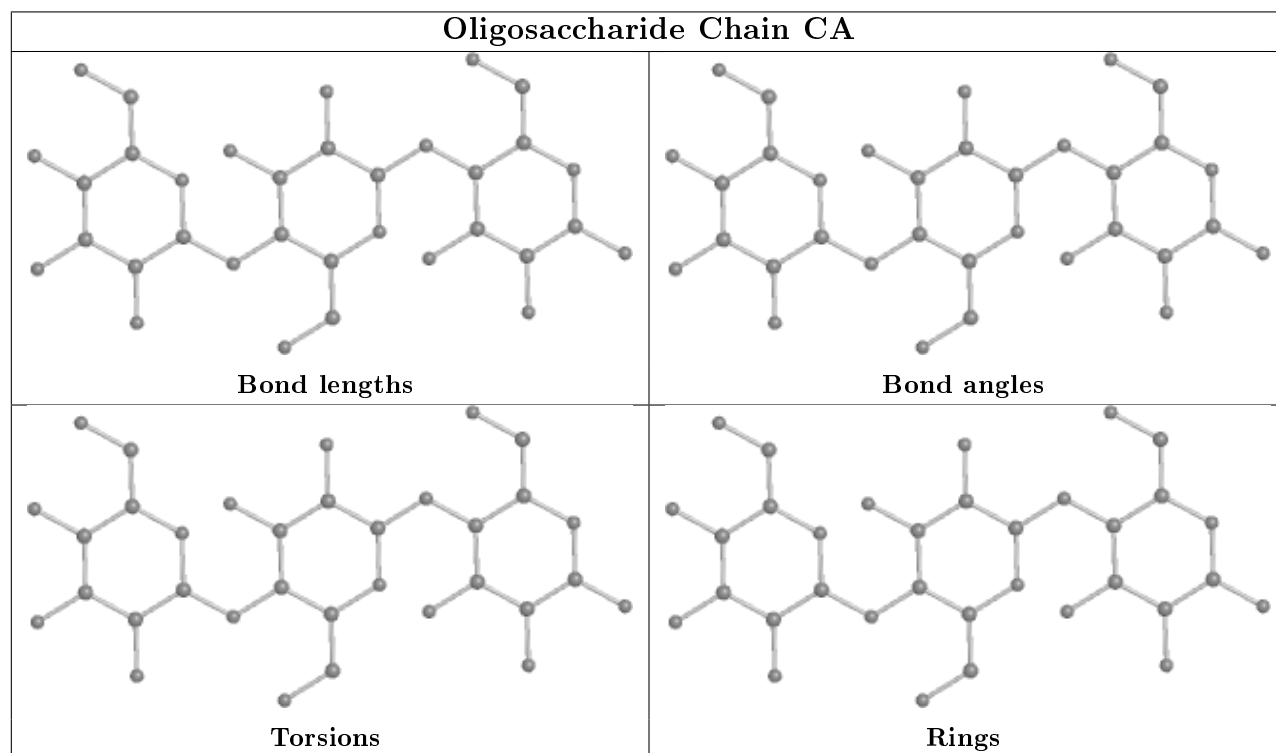
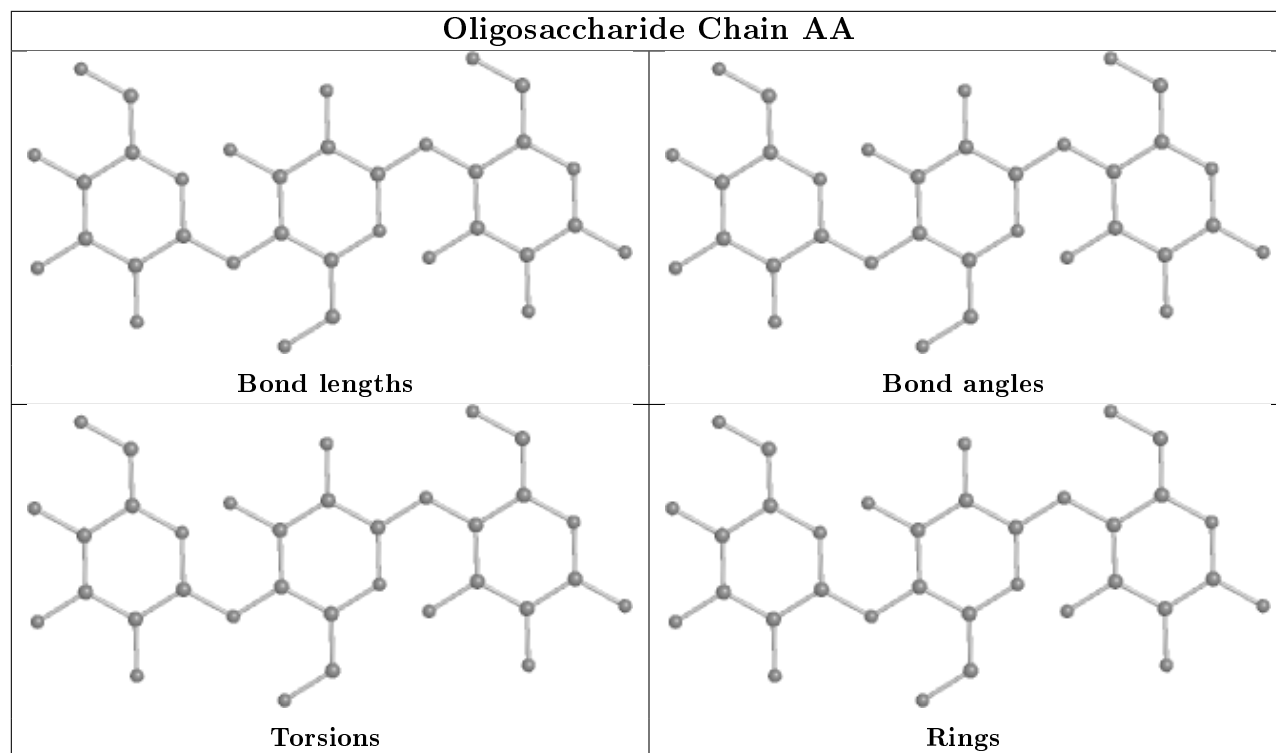
7 monomers are involved in 5 short contacts:

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

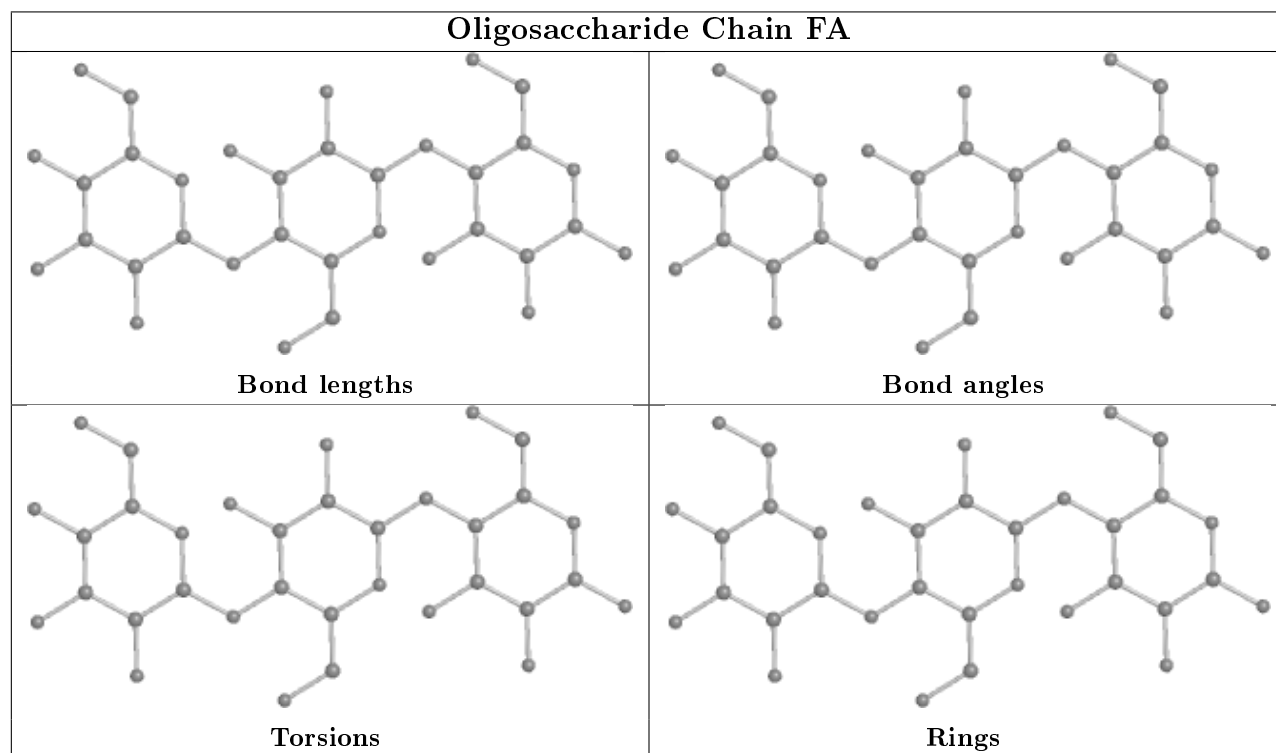
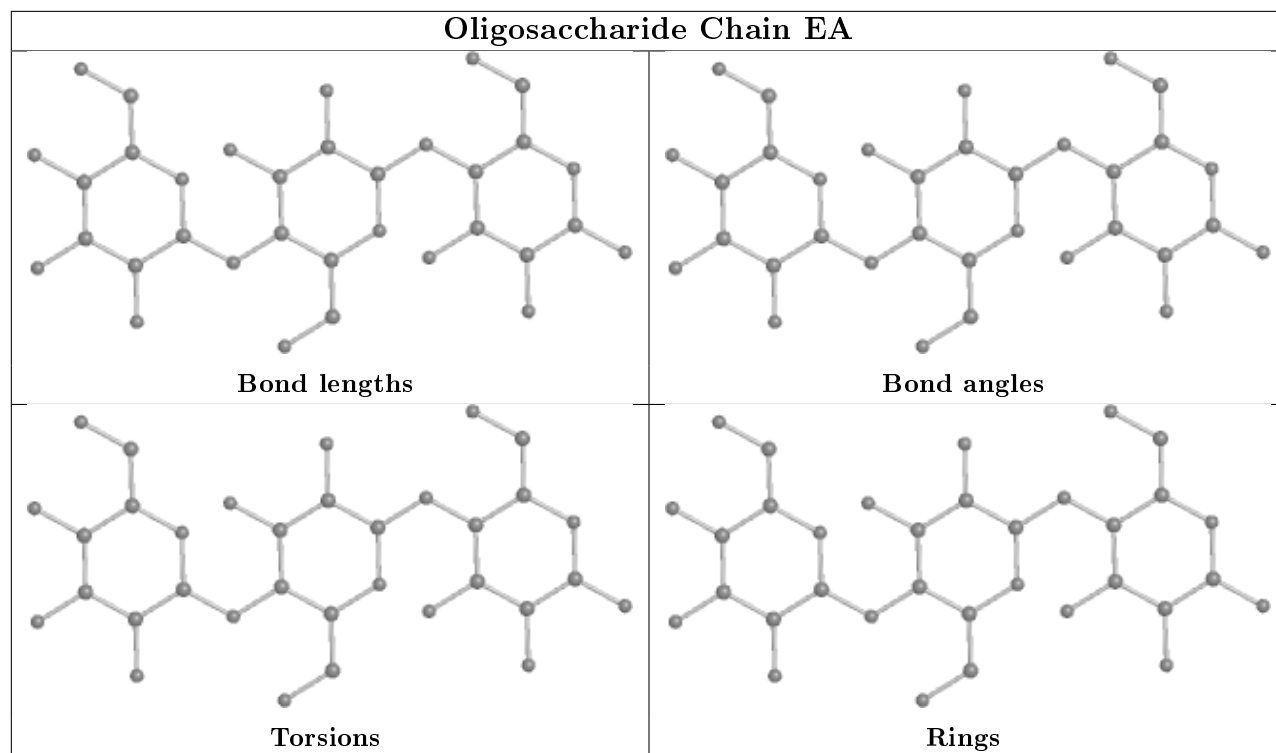
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

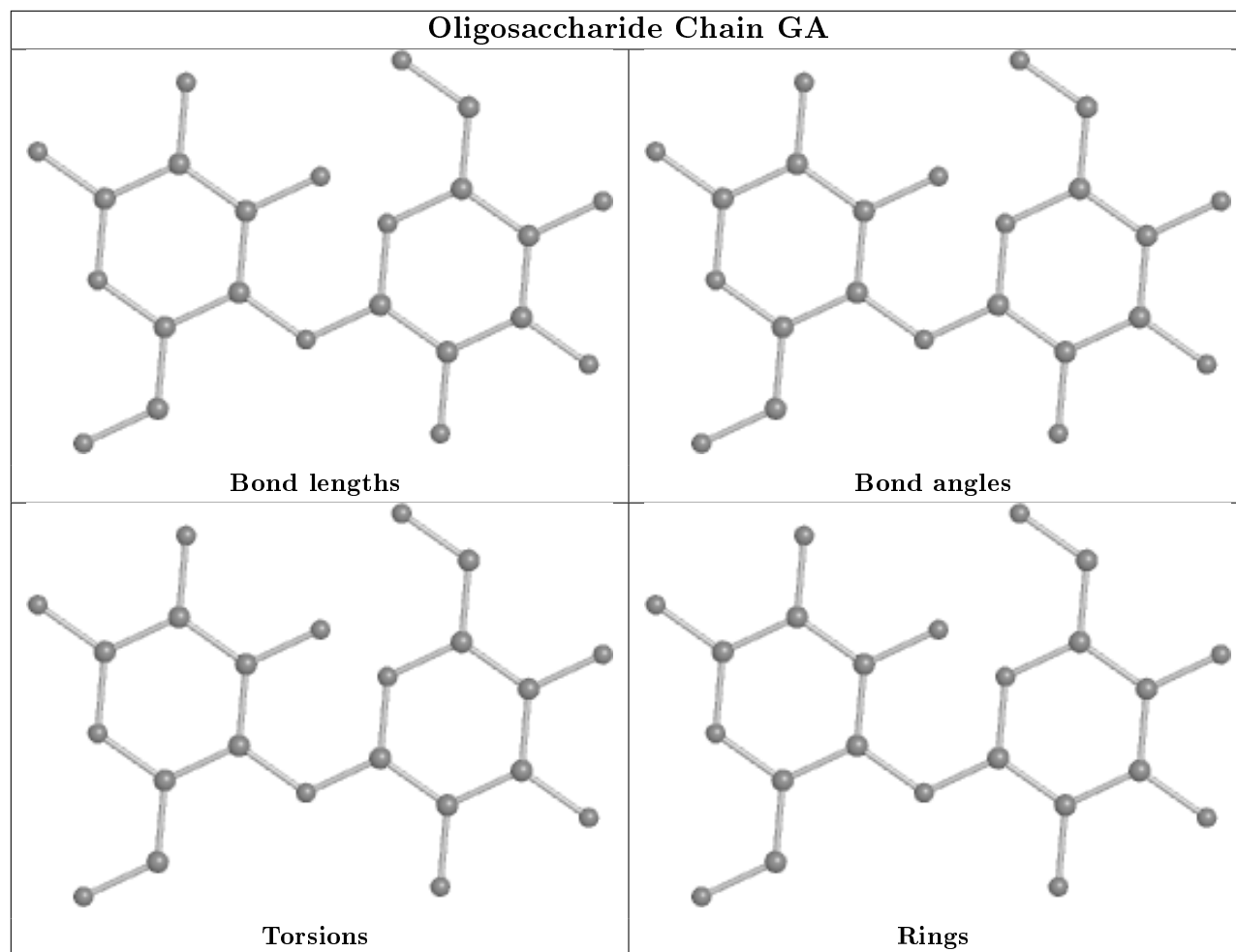


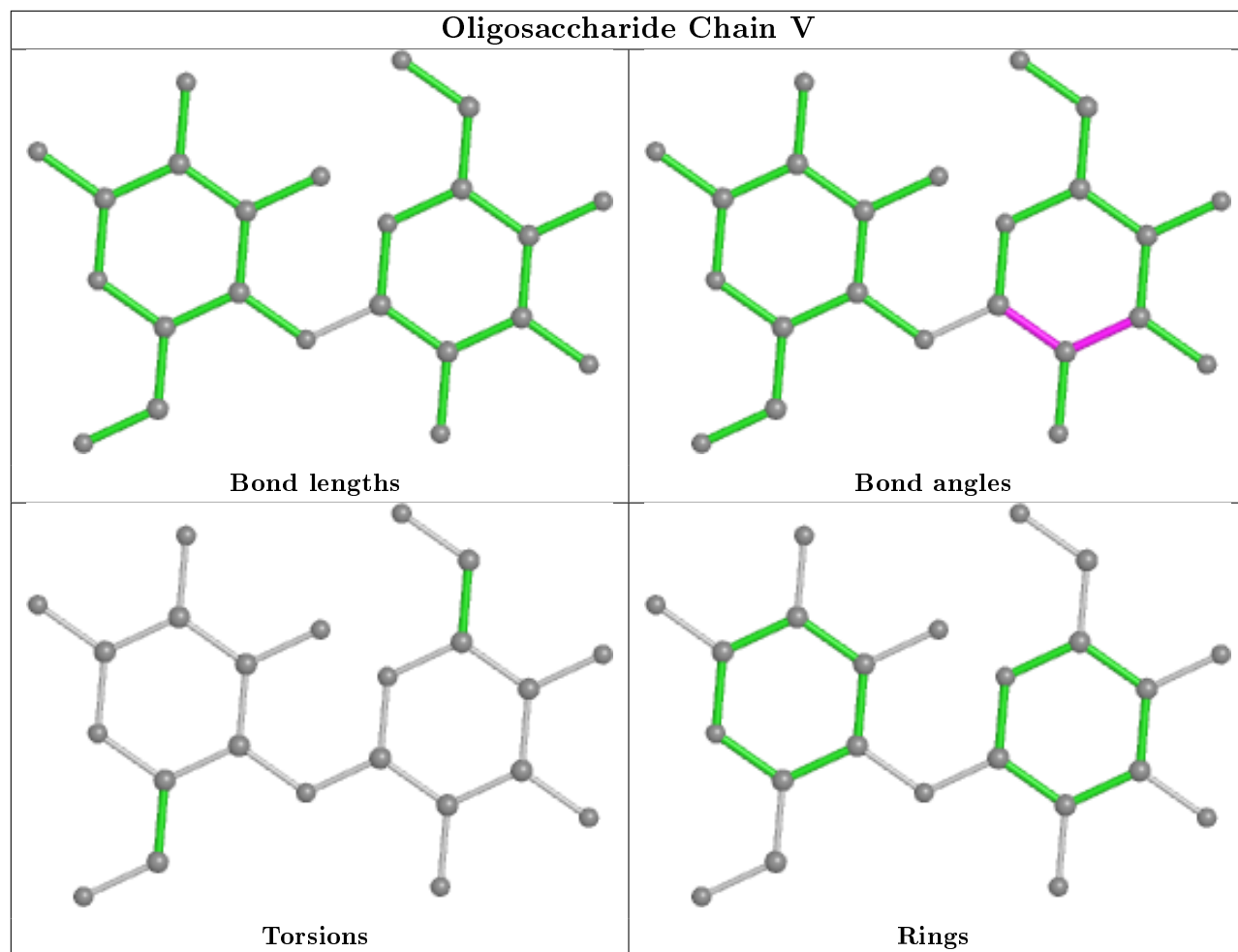


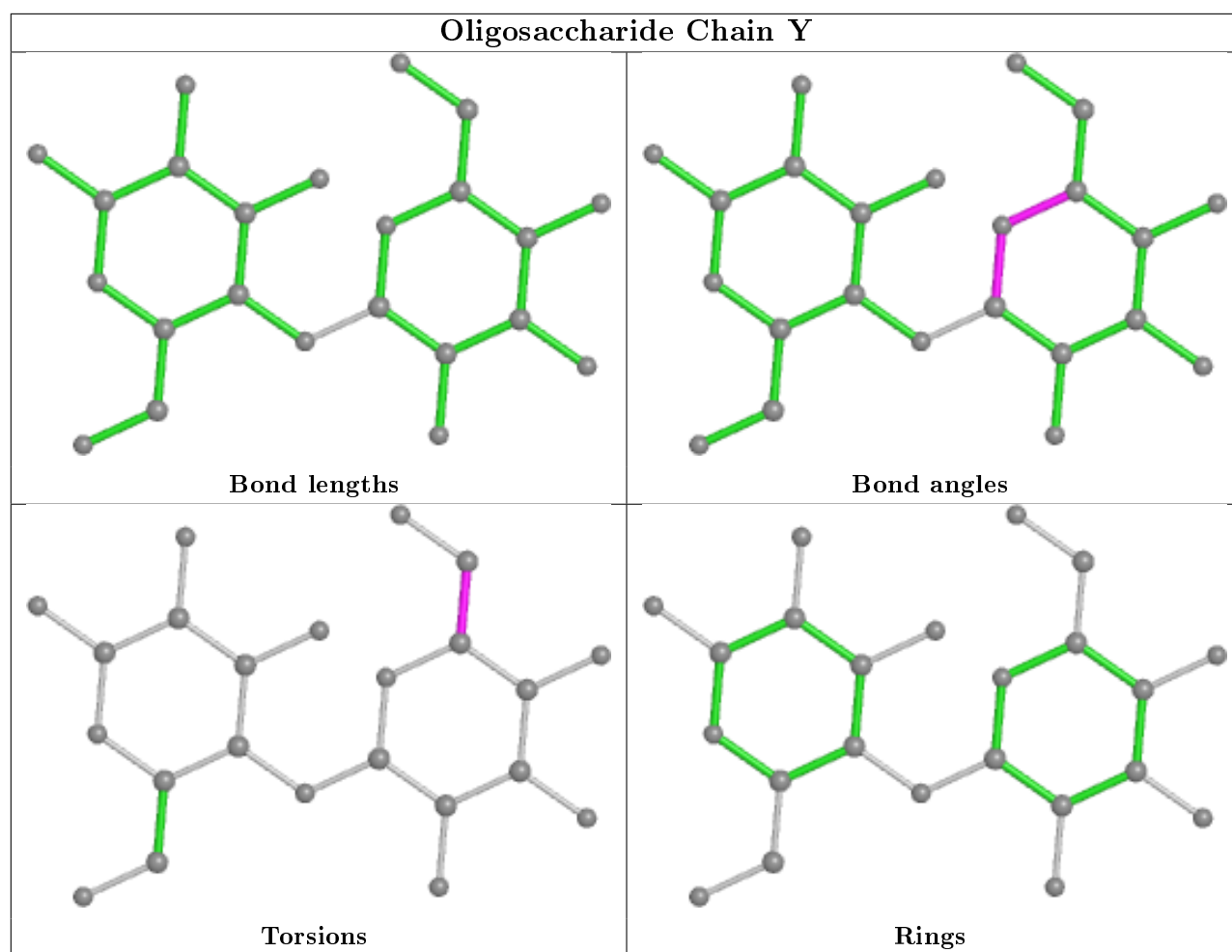


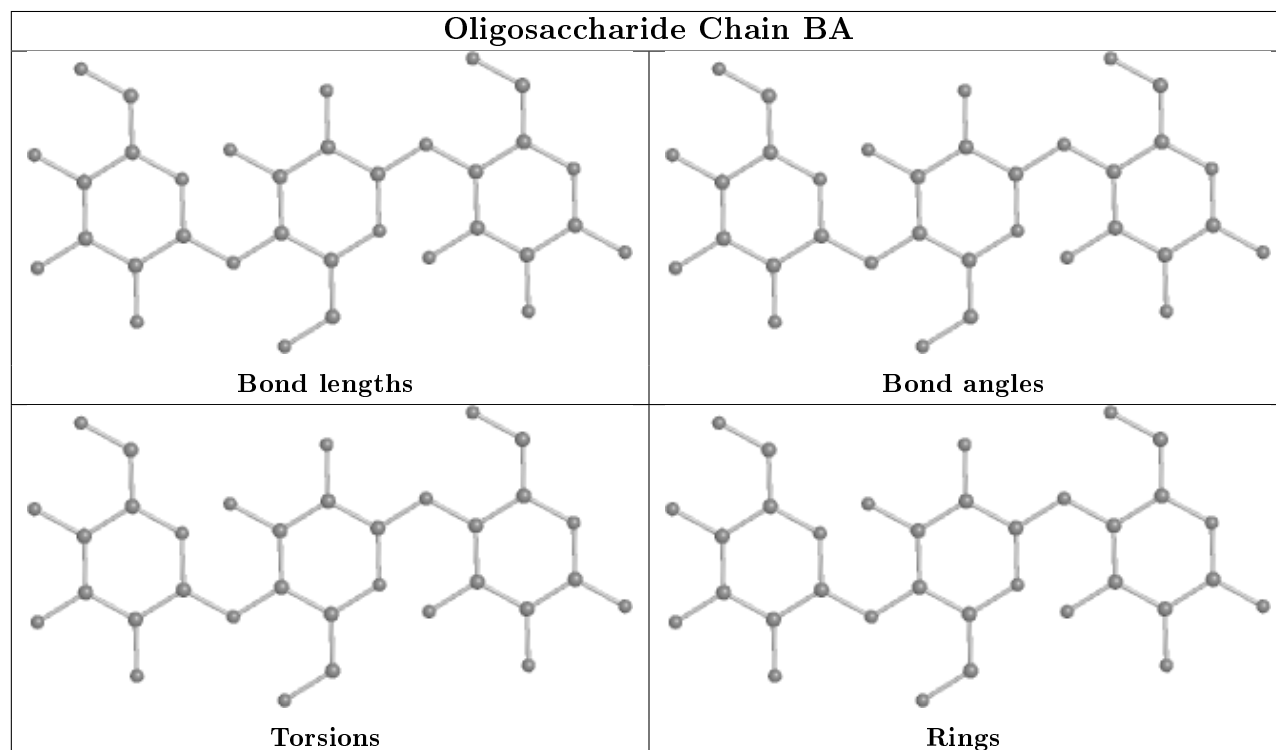
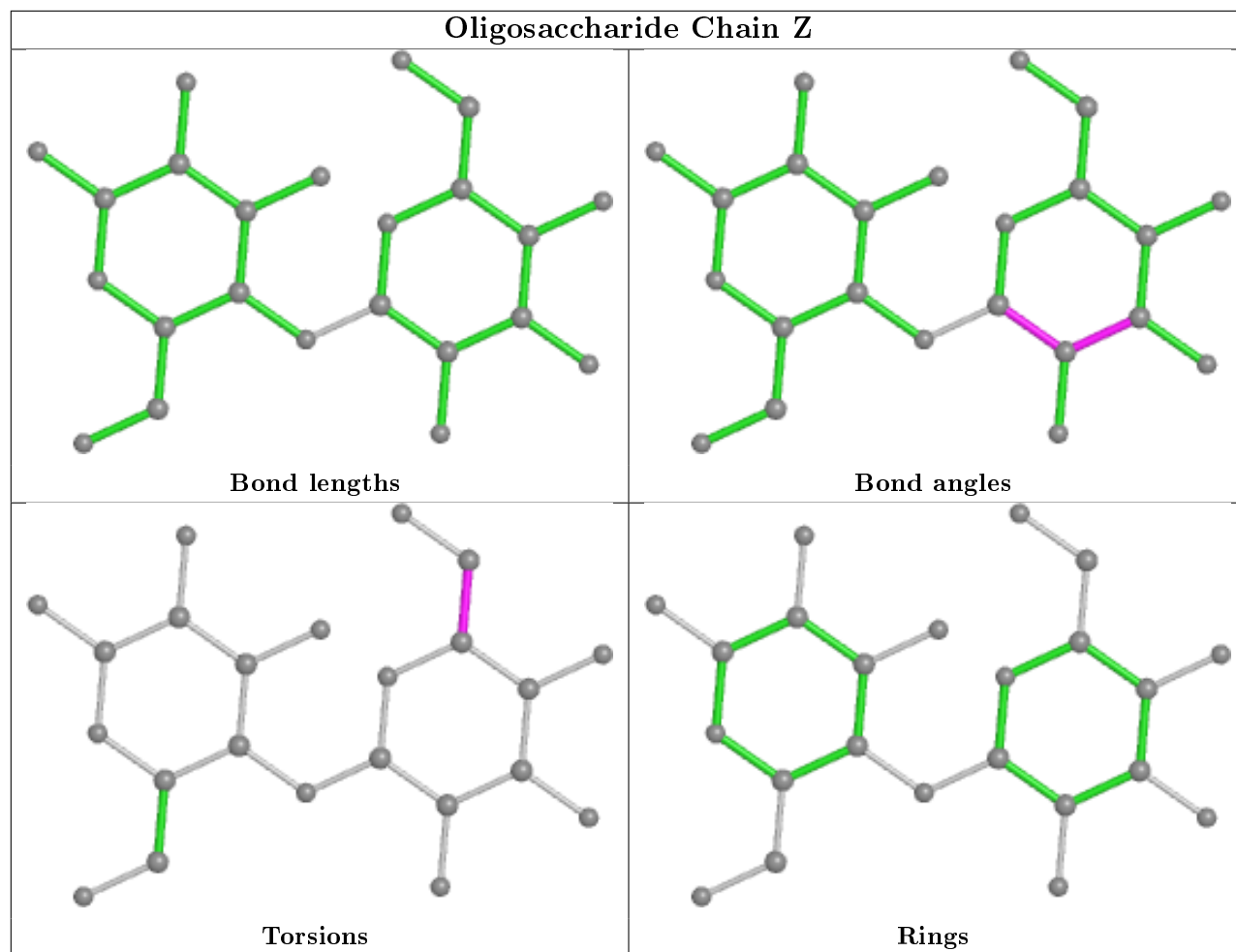


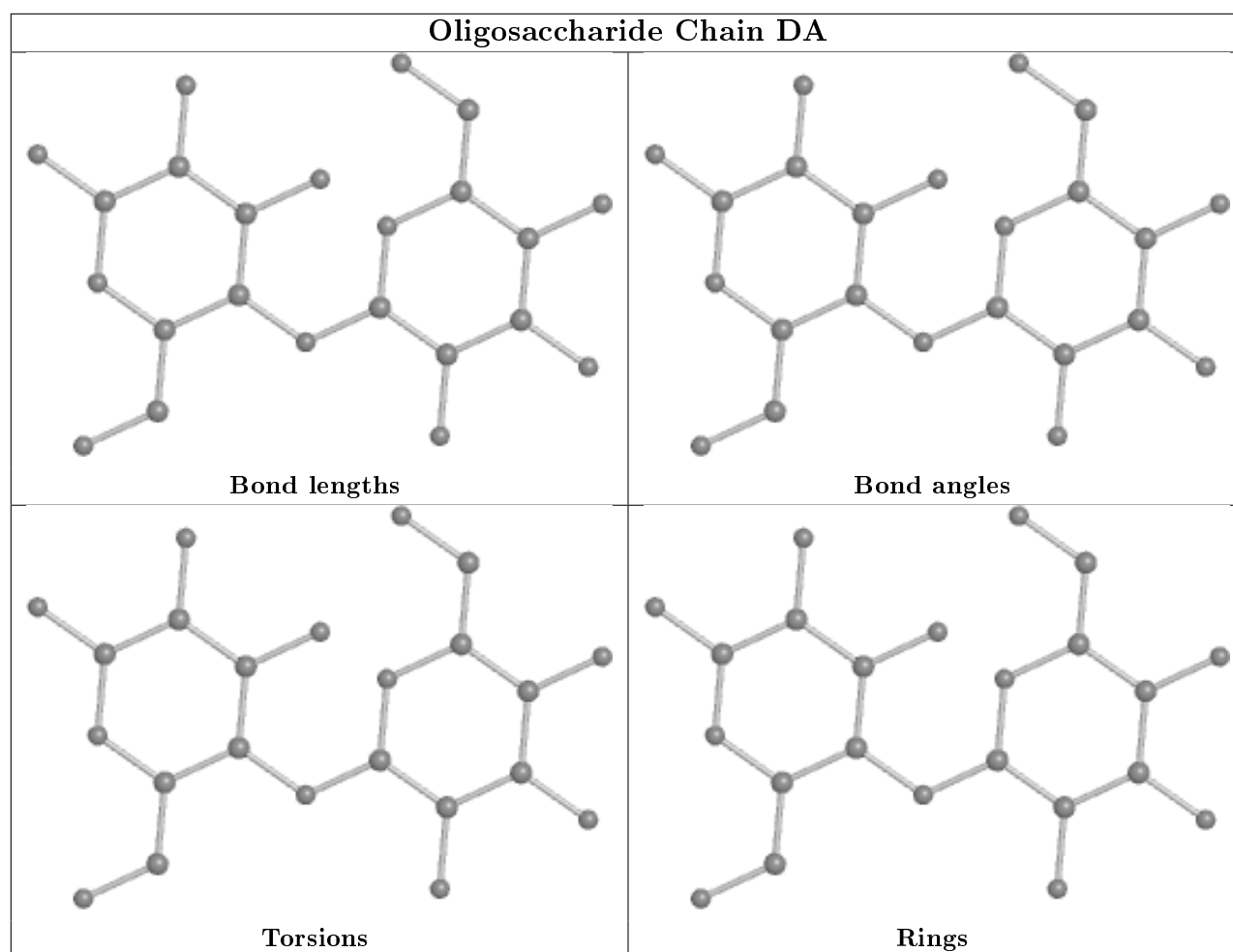












## 5.6 Ligand geometry [i](#)

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	K	3170	-	12,12,12	0.41	0	17,17,17	0.48	0
4	GAL	N	3470	-	12,12,12	0.46	0	17,17,17	0.38	0
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	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
4	GAL	I	2470	-	12,12,12	0.44	0	17,17,17	0.49	0
4	GAL	R	4370	-	12,12,12	0.46	0	17,17,17	0.53	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	K	3170	-	-	1/2/22/22	0/1/1/1
4	GAL	N	3470	-	-	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	L	3270	-	-	0/2/22/22	0/1/1/1
4	GAL	P	4170	-	-	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	I	2470	-	-	1/2/22/22	0/1/1/1
4	GAL	R	4370	-	-	2/2/22/22	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(°)	Ideal(°)
4	P	4170	GAL	C3-C4-C5	2.43	114.57	110.24

There are no chirality outliers.

5 of 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

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	3470	GAL	2	0
4	P	4170	GAL	3	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<sup>th</sup> 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 <sup>2</sup> )	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, 29, 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 ⓘ

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

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	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
3	GAL	Z	1	12/12	0.84	0.36	60,67,69,73	0
2	BGC	s	1	12/12	0.84	0.31	47,67,73,74	0
2	BGC	h	1	12/12	0.85	0.29	36,49,53,53	0
2	BGC	BA	1	12/12	0.85	0.23	46,58,61,62	4
2	BGC	i	1	12/12	0.85	0.26	43,48,48,48	11
2	BGC	AA	1	12/12	0.86	0.22	47,55,59,61	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
2	BGC	W	1	12/12	0.88	0.22	22,30,39,45	0
3	GLA	Z	2	11/12	0.88	0.36	72,74,77,78	0
2	BGC	0	1	12/12	0.89	0.20	40,49,54,54	0
2	BGC	8	1	12/12	0.89	0.16	35,40,40,41	8
2	BGC	m	1	12/12	0.89	0.24	27,39,43,44	0
2	BGC	v	1	12/12	0.89	0.22	29,41,45,49	0
2	BGC	p	1	12/12	0.89	0.23	36,42,47,51	0
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	FA	2	11/12	0.90	0.14	38,41,45,47	0
2	GAL	t	2	11/12	0.90	0.16	30,32,38,39	0
2	BGC	5	1	12/12	0.91	0.24	36,46,49,53	0
2	BGC	j	1	12/12	0.91	0.20	28,31,36,38	0
3	GAL	d	1	12/12	0.91	0.18	23,28,30,34	0
2	BGC	k	1	12/12	0.91	0.17	26,38,40,43	0
2	GAL	i	2	11/12	0.91	0.16	27,37,40,40	0
2	BGC	CA	1	12/12	0.91	0.28	40,52,56,59	0
2	GAL	2	2	11/12	0.91	0.19	27,31,34,36	0
2	GAL	s	2	11/12	0.91	0.19	25,33,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GAL	r	2	11/12	0.91	0.17	27,35,40,44	0
2	BGC	t	1	12/12	0.91	0.24	40,51,53,55	0
3	GLA	6	2	11/12	0.91	0.17	18,21,26,27	0
2	BGC	e	1	12/12	0.91	0.16	20,25,32,33	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	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
2	GAL	BA	2	11/12	0.93	0.16	32,34,39,39	0
2	GLA	AA	3	11/12	0.93	0.16	21,28,30,31	0
3	GAL	V	1	12/12	0.93	0.17	29,32,35,38	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
3	GAL	DA	1	12/12	0.93	0.19	29,32,35,36	0
2	GAL	g	2	11/12	0.93	0.14	25,26,31,35	0
2	GLA	W	3	11/12	0.93	0.16	4,12,17,25	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	BGC	7	1	12/12	0.93	0.16	31,39,43,45	0
3	GAL	b	1	12/12	0.93	0.17	22,26,30,35	0
2	GAL	EA	2	11/12	0.93	0.13	26,30,34,34	0
2	GLA	t	3	11/12	0.94	0.13	14,16,25,28	0
2	BGC	z	1	12/12	0.94	0.15	2,8,12,15	0
3	GLA	GA	2	11/12	0.94	0.17	19,22,24,25	0
2	GAL	h	2	11/12	0.94	0.12	14,21,29,30	0
2	GLA	5	3	11/12	0.94	0.14	13,20,24,28	0
2	BGC	EA	1	12/12	0.94	0.17	19,26,38,44	0
2	GLA	FA	3	11/12	0.94	0.13	28,30,33,36	0
2	GAL	v	2	11/12	0.94	0.12	17,21,24,25	0
2	GLA	p	3	11/12	0.94	0.13	10,12,17,18	0
2	GLA	e	3	11/12	0.94	0.11	5,9,13,15	0
3	GAL	w	1	12/12	0.94	0.18	20,27,31,33	0
2	GAL	U	2	11/12	0.94	0.12	21,29,34,34	0
3	GAL	1	1	12/12	0.94	0.20	22,27,37,42	0
3	GAL	6	1	12/12	0.94	0.21	25,31,38,38	0
2	BGC	o	1	12/12	0.94	0.16	14,23,29,29	0
2	GLA	EA	3	11/12	0.94	0.14	14,25,30,31	0
2	BGC	a	1	12/12	0.94	0.21	31,36,43,43	0
2	GAL	p	2	11/12	0.94	0.17	21,27,37,40	0
2	GAL	7	2	11/12	0.95	0.13	15,20,28,29	0
3	GLA	1	2	11/12	0.95	0.17	23,24,27,28	0
2	GAL	9	2	11/12	0.95	0.14	2,5,9,11	0

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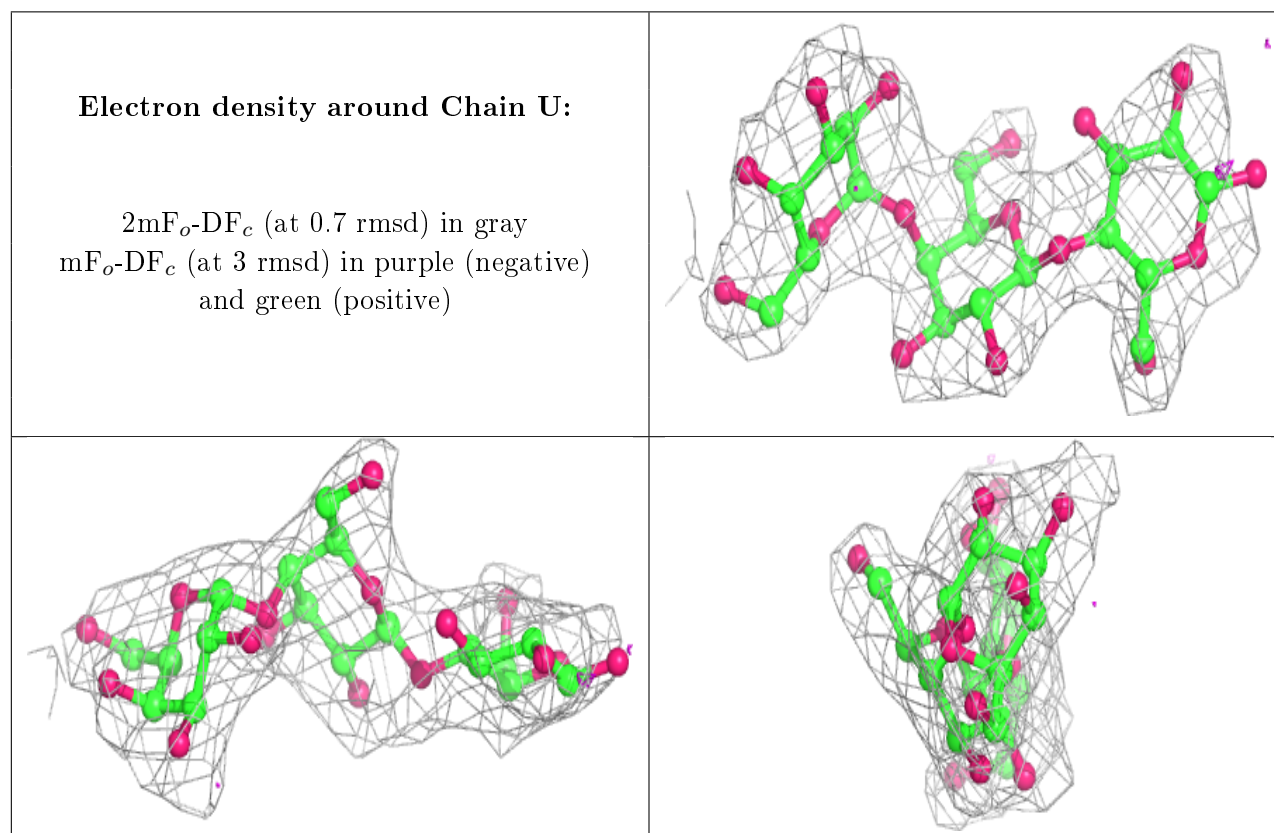
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GAL	m	2	11/12	0.95	0.10	10,20,23,23	0
3	GLA	V	2	11/12	0.95	0.14	11,23,28,29	0
2	BGC	9	1	12/12	0.95	0.18	19,28,32,38	0
2	GAL	k	2	11/12	0.95	0.13	8,15,20,20	0
2	GLA	g	3	11/12	0.95	0.16	14,22,23,24	0
2	GLA	0	3	11/12	0.95	0.14	10,16,23,26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

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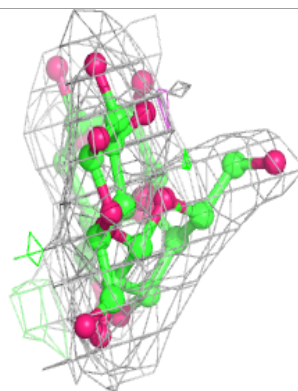
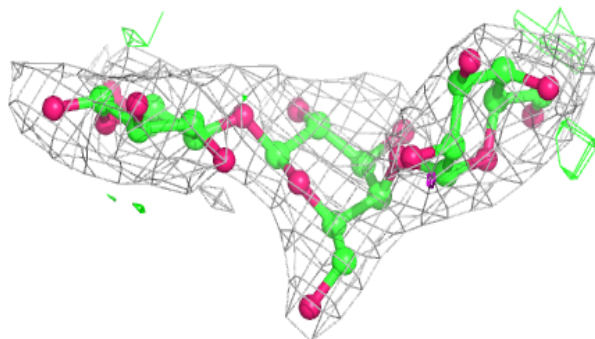
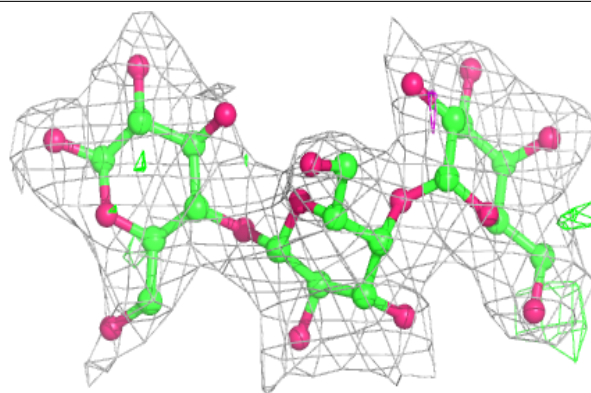
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLA	b	2	11/12	0.96	0.15	17,19,22,30	0
2	GLA	c	3	11/12	0.96	0.11	9,11,14,14	0
2	GLA	f	3	11/12	0.96	0.11	16,20,24,24	0
2	GLA	k	3	11/12	0.96	0.12	2,9,12,14	0
3	GLA	l	2	11/12	0.96	0.12	14,16,20,22	0
2	GLA	r	3	11/12	0.96	0.12	21,25,27,30	0
2	GLA	2	3	11/12	0.96	0.12	6,10,14,16	0
2	GAL	5	2	11/12	0.97	0.15	15,26,28,30	0
2	GAL	j	2	11/12	0.97	0.13	18,25,29,30	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
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	e	2	11/12	0.97	0.11	10,14,18,18	0
2	GLA	x	3	11/12	0.97	0.10	9,14,18,22	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.

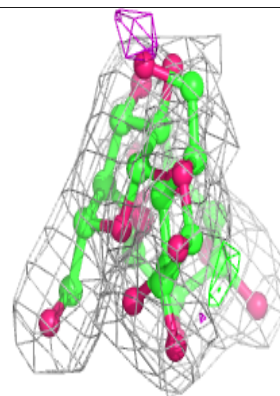
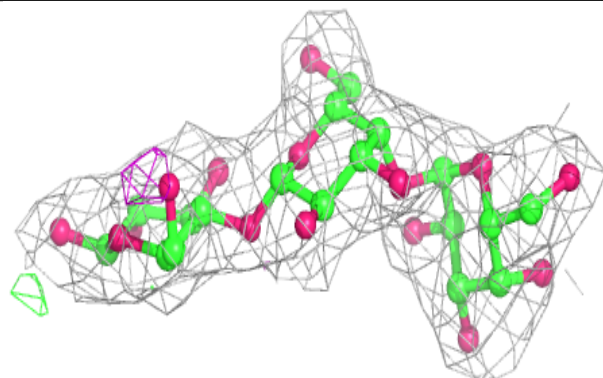
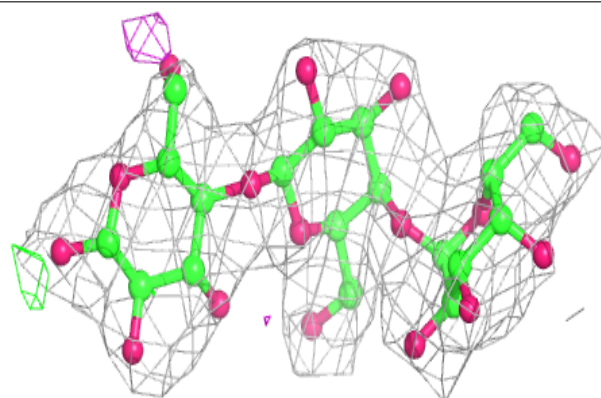


**Electron density around Chain W:**

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

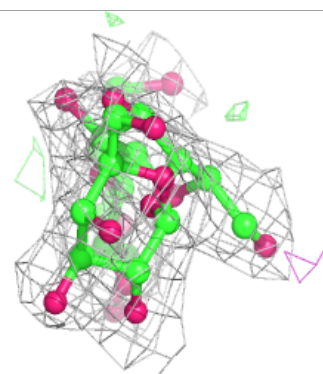
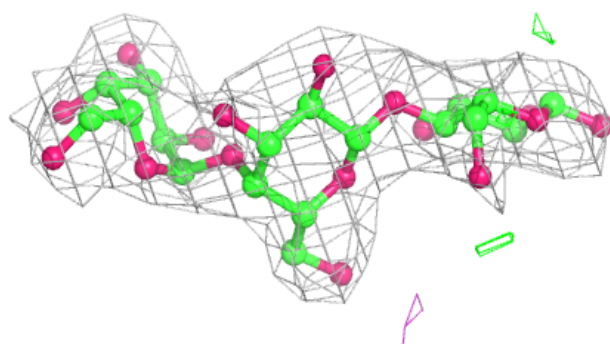
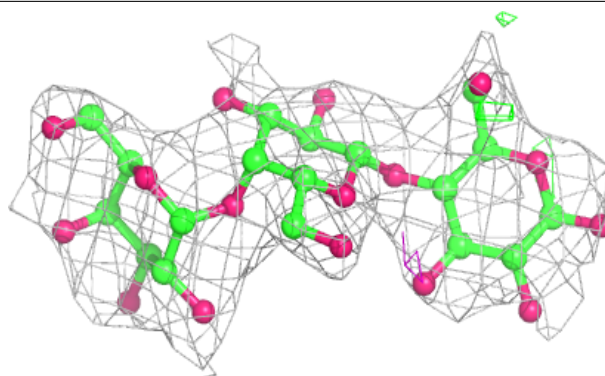
**Electron density around Chain X:**

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

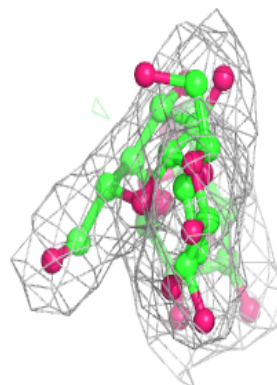
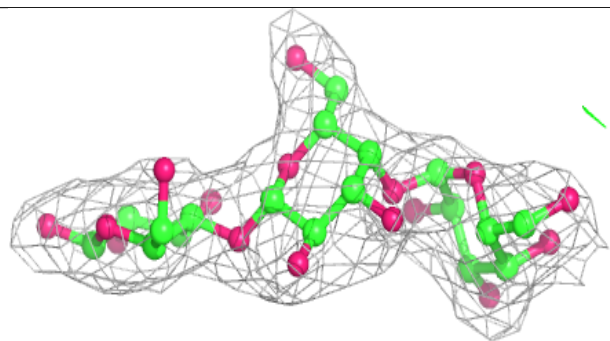
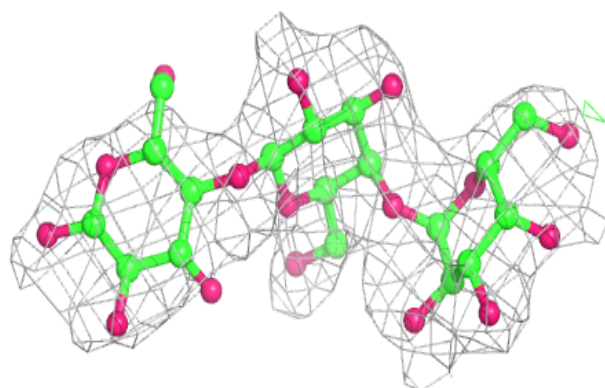


**Electron density around Chain AA:**

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

**Electron density around Chain CA:**

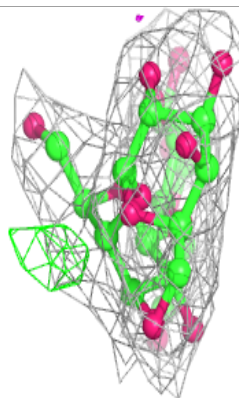
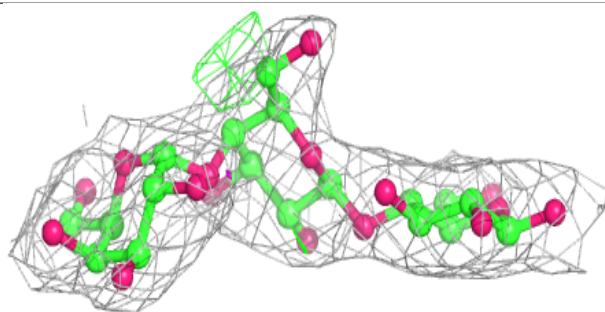
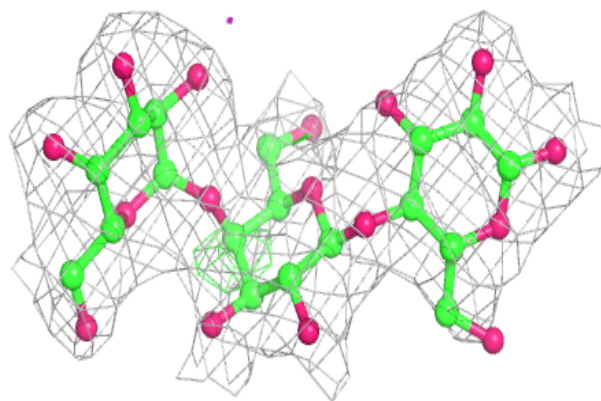
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



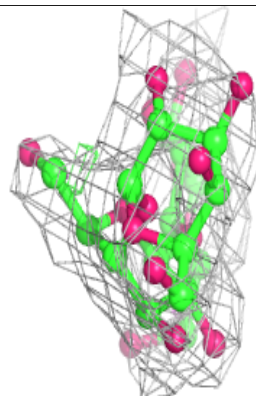
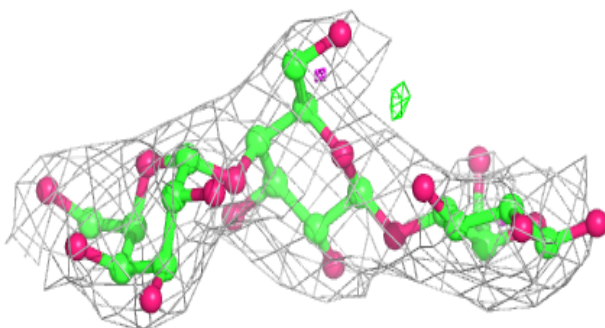
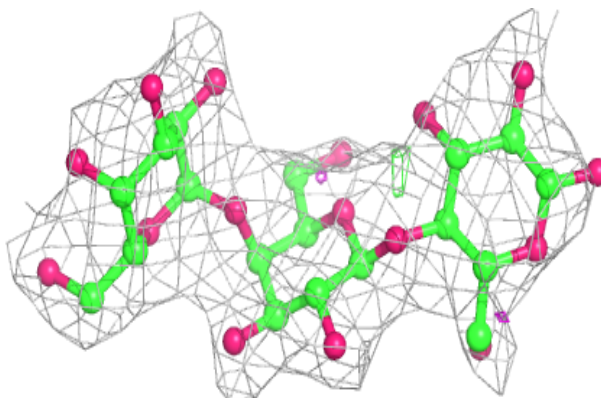


**Electron density around Chain EA:**

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

**Electron density around Chain FA:**

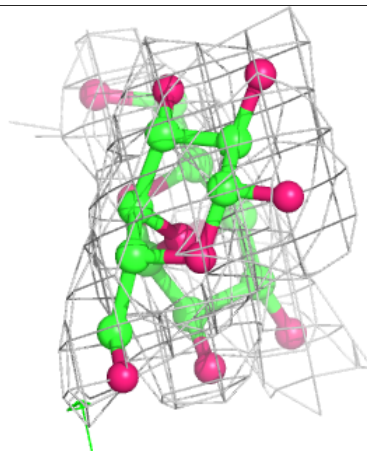
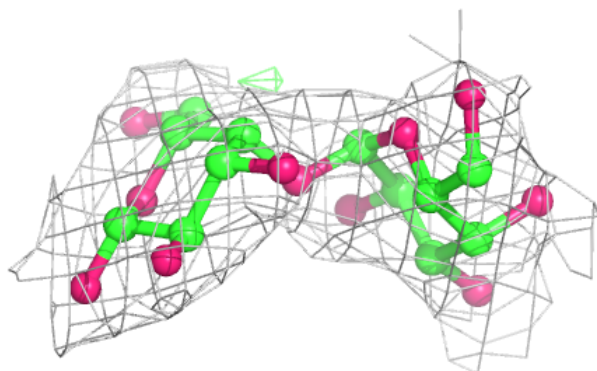
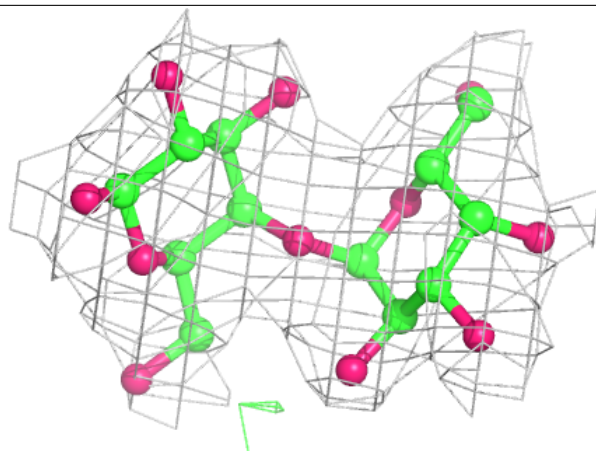
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





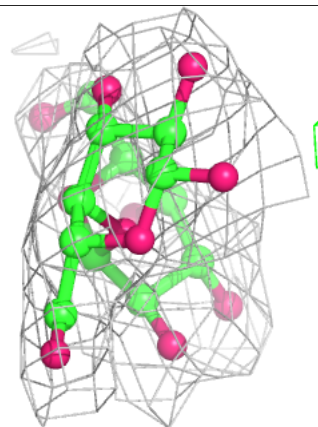
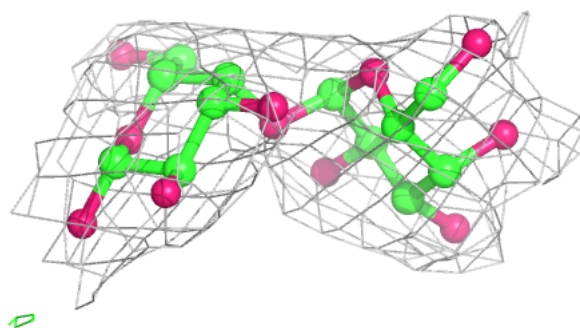
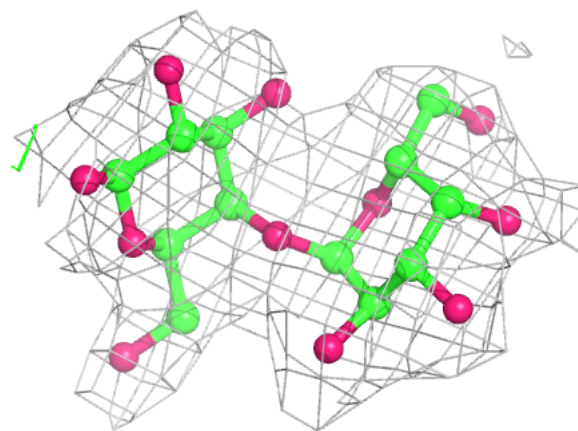
**Electron density around Chain GA:**

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



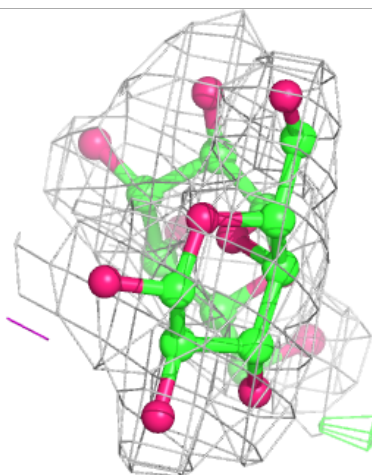
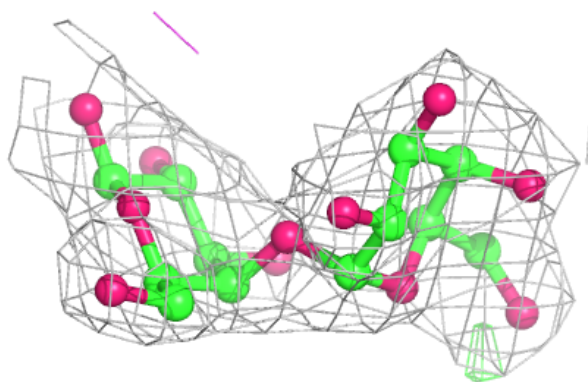
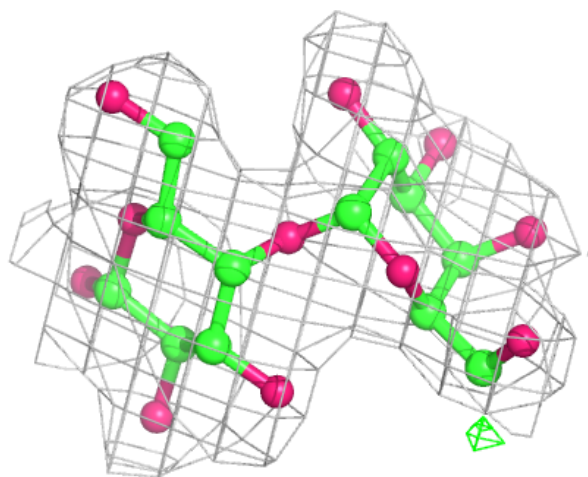
**Electron density around Chain V:**

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



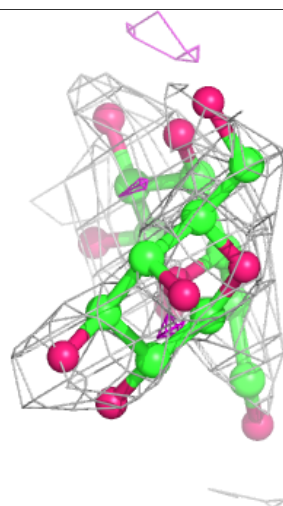
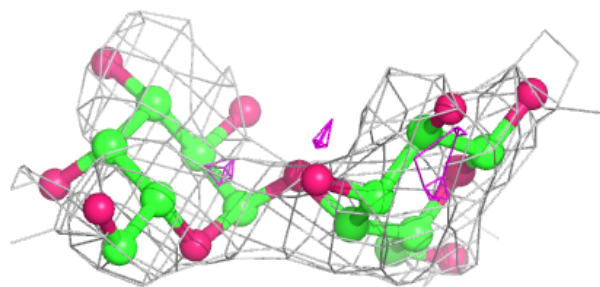
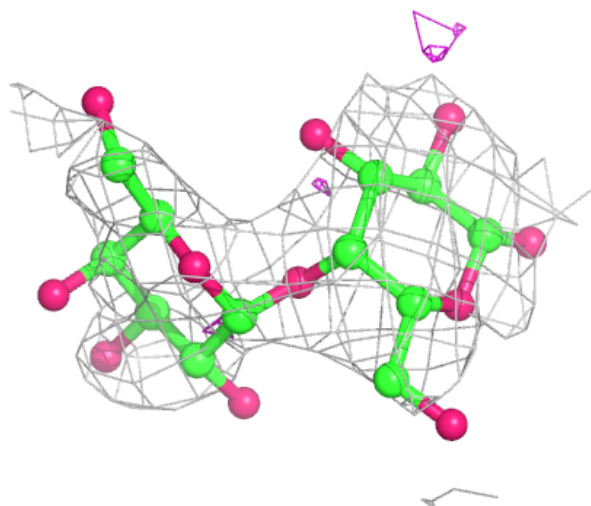
**Electron density around Chain Y:**

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



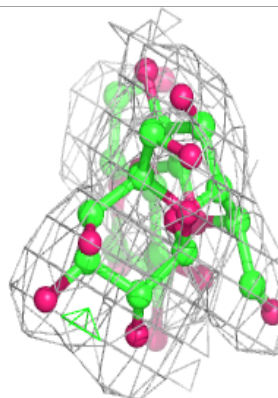
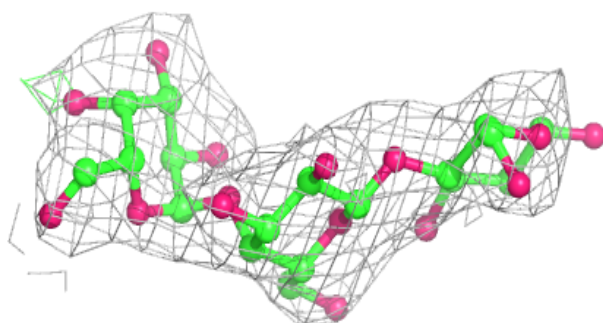
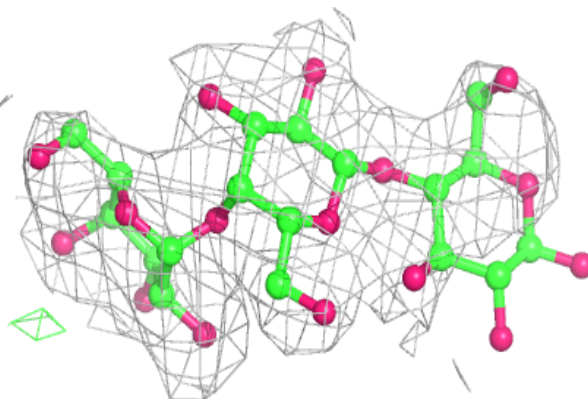
**Electron density around Chain Z:**

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

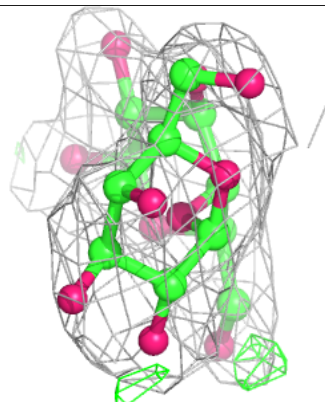
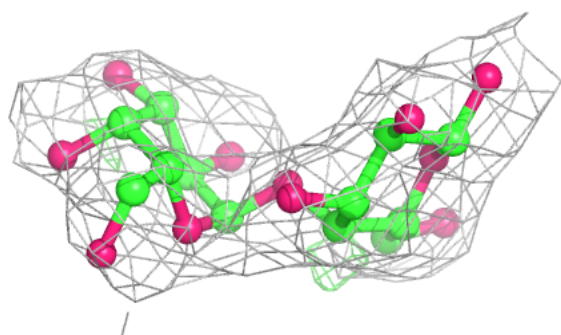
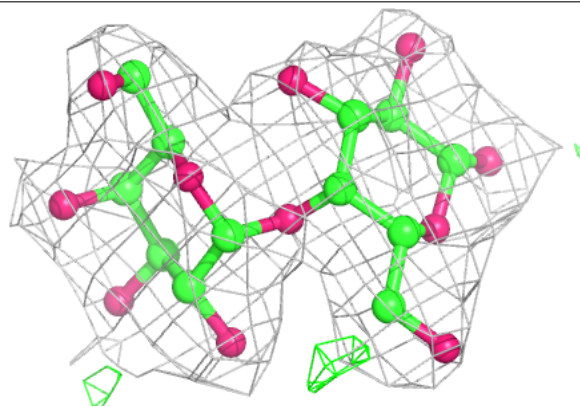


**Electron density around Chain BA:**

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

**Electron density around Chain DA:**

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



## 6.4 Ligands

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<sup>th</sup> 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( $\text{\AA}^2$ )	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	J	2570	12/12	0.76	0.58	84,89,91,91	0
4	GAL	K	3170	12/12	0.76	0.51	72,84,87,87	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

There are no such residues in this entry.