



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 1BOS / pdb_00001bos
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

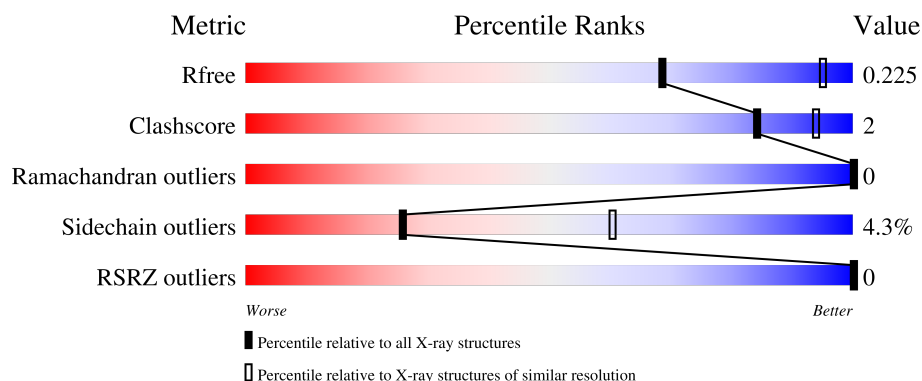
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

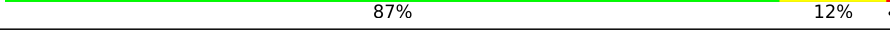
The reported resolution of this entry is 2.80 Å.

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.



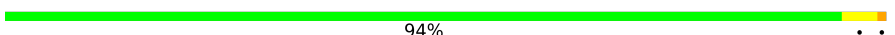
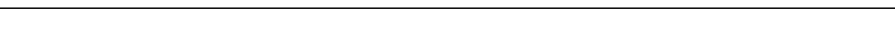
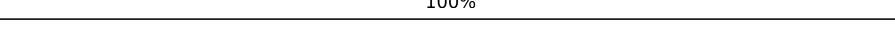
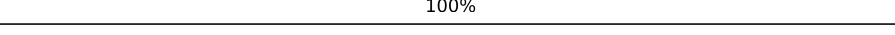
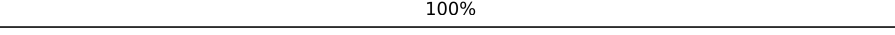
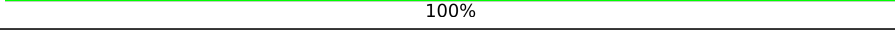
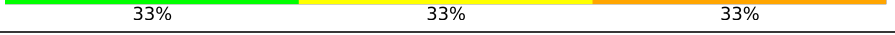
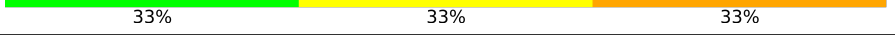
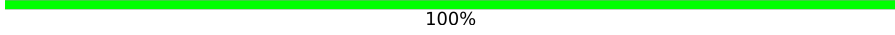
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	
1	B	69	
1	C	69	
1	D	69	
1	E	69	

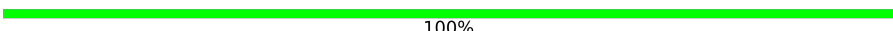
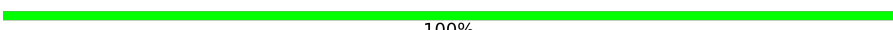
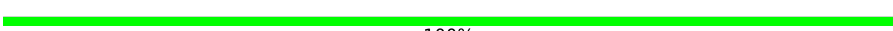
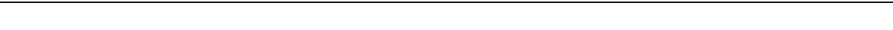
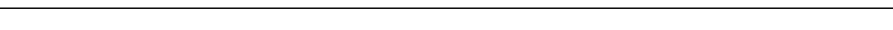
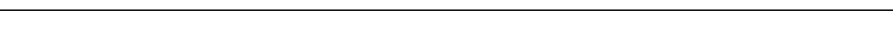
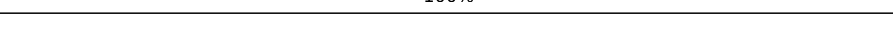
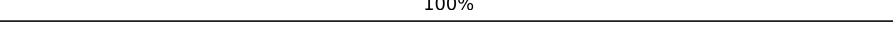
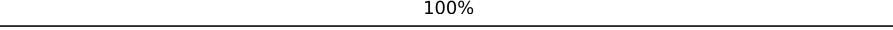
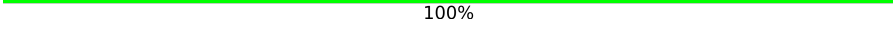
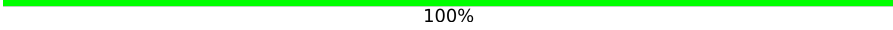
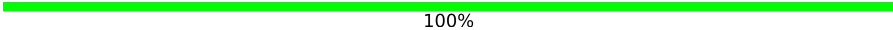
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Mol	Chain	Length	Quality of chain
1	F	69	 84%10%6%
1	G	69	 87%10%.
1	H	69	 87%10%.
1	I	69	 94%. .
1	J	69	 88%10%.
1	K	69	 84%13%..
1	L	69	 90%9%.
1	M	69	 87%12%.
1	N	69	 88%10%.
1	O	69	 90%6%.
1	P	69	 86%12%.
1	Q	69	 90%9%.
1	R	69	 90%9%.
1	S	69	 81%17%.
1	T	69	 88%10%.
2	0	3	 67%33%
2	2	3	 100%
2	4	3	 67%33%
2	5	3	 100%
2	7	3	 100%
2	8	3	 100%
2	9	3	 33%33%33%
2	AA	3	 33%33%33%
2	BA	3	 100%
2	CA	3	 100%

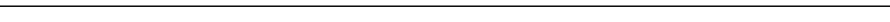
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Mol	Chain	Length	Quality of chain
2	EA	3	 67% 33%
2	FA	3	 100%
2	U	3	 100%
2	W	3	 67% 33%
2	X	3	 100%
2	a	3	 100%
2	c	3	 100%
2	e	3	 67% 33%
2	f	3	 100%
2	g	3	 100%
2	h	3	 67% 33%
2	i	3	 33% 67%
2	j	3	 33% 67%
2	k	3	 100%
2	m	3	 67% 33%
2	o	3	 67% 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	 100%
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%

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.

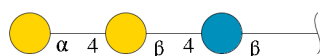
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
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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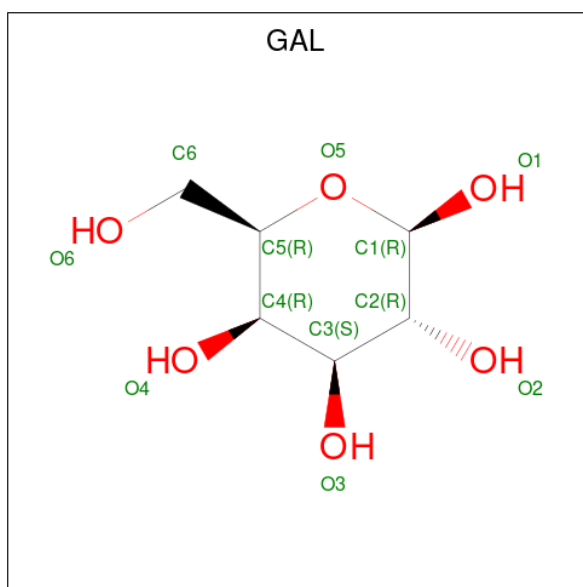
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	o	3	Total	C	O	0	0	0
			34	18	16			
2	p	3	Total	C	O	0	0	0
			34	18	16			
2	r	3	Total	C	O	0	0	0
			34	18	16			
2	s	3	Total	C	O	0	0	0
			34	18	16			
2	t	3	Total	C	O	0	0	0
			34	18	16			
2	v	3	Total	C	O	0	0	0
			34	18	16			
2	x	3	Total	C	O	0	0	0
			34	18	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 (CCD ID: GAL) (formula: C₆H₁₂O₆).



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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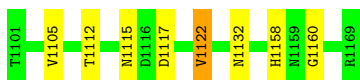
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	27	Total 27	O 27	0	0
5	C	19	Total 19	O 19	0	0
5	D	16	Total 16	O 16	0	0
5	E	18	Total 18	O 18	0	0
5	F	15	Total 15	O 15	0	0
5	G	21	Total 21	O 21	0	0
5	H	17	Total 17	O 17	0	0
5	I	17	Total 17	O 17	0	0
5	J	15	Total 15	O 15	0	0
5	K	21	Total 21	O 21	0	0
5	L	23	Total 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.

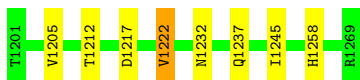
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain A: 



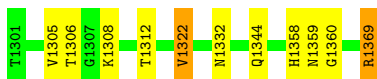
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

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: 



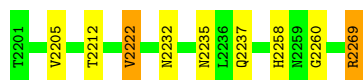
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain F: 



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain G: 87% 10% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain H: 87% 10% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain I: 94% 10% .



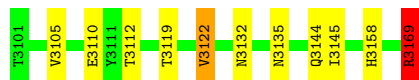
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain J: 88% 10% .



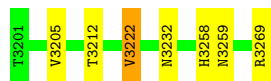
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain K: 84% 13% ..



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain L: 90% 9% .



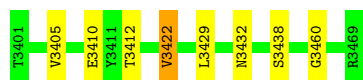
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain M: 87% 12% .



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain N: 88% 10%



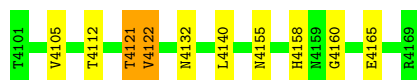
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain O: 90% 6%



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain P: 86% 12%



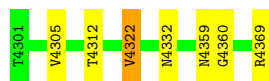
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain Q: 90% 9%



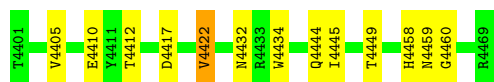
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain R: 90% 9%



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain S: 81% 17%



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain T: 88% 10%



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

Chain U: 100%



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

Chain W: 67% 33%



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

Chain X: 100%



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

Chain a: 100%



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

Chain c: 100%



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

Chain e: 67% 33%



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

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:  67% 33%

BGC1
GAL2
GLA3

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

Chain i:  33% 67%

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:  100%

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



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



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



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



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



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



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

Chain 8:  100%



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

Chain 9:  33% 33% 33%



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

Chain AA:  33% 33% 33%



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

Chain BA:  100%



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

Chain CA:  100%



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

Chain EA:  67% 33%



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

Chain FA:  100%



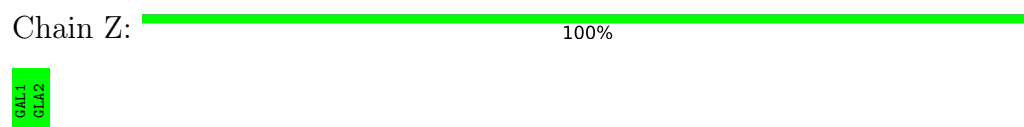
- Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



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



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



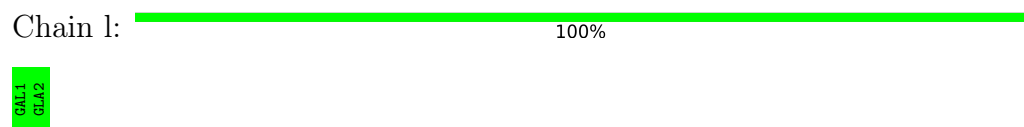
- Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



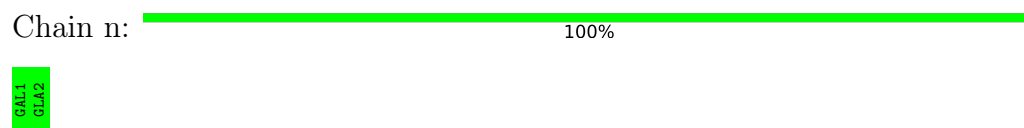
- Molecule 3: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



- 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, α , β , γ	127.50Å 97.70Å 164.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.80 21.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.6 (21.00-2.80) 80.7 (21.00-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.75Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.170 , 0.226 0.171 , 0.225	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)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GAL, GLA, BGC

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	1.08	0/549	1.66	4/742 (0.5%)
1	B	1.03	0/549	1.54	4/742 (0.5%)
1	C	1.08	2/549 (0.4%)	1.65	5/742 (0.7%)
1	D	1.06	1/549 (0.2%)	1.58	5/742 (0.7%)
1	E	1.06	1/549 (0.2%)	1.59	4/742 (0.5%)
1	F	1.16	2/549 (0.4%)	1.64	7/742 (0.9%)
1	G	1.05	1/549 (0.2%)	1.53	4/742 (0.5%)
1	H	1.13	1/549 (0.2%)	1.64	5/742 (0.7%)
1	I	1.05	0/549	1.49	1/742 (0.1%)
1	J	0.94	1/549 (0.2%)	1.51	3/742 (0.4%)
1	K	1.02	0/549	1.64	7/742 (0.9%)
1	L	1.00	1/549 (0.2%)	1.57	3/742 (0.4%)
1	M	1.09	0/549	1.58	4/742 (0.5%)
1	N	1.07	1/549 (0.2%)	1.55	3/742 (0.4%)
1	O	1.05	0/549	1.60	5/742 (0.7%)
1	P	1.08	1/549 (0.2%)	1.54	5/742 (0.7%)
1	Q	0.98	0/549	1.57	5/742 (0.7%)
1	R	1.05	0/549	1.51	3/742 (0.4%)
1	S	1.07	1/549 (0.2%)	1.55	8/742 (1.1%)
1	T	1.01	0/549	1.52	4/742 (0.5%)
All	All	1.05	13/10980 (0.1%)	1.57	89/14840 (0.6%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	2169	ARG	NE-CZ	6.14	1.39	1.33
1	E	1558	HIS	CD2-NE2	-6.09	1.31	1.37
1	H	2369	ARG	NE-CZ	5.95	1.39	1.33
1	P	4165	GLU	CA-CB	-5.91	1.45	1.53
1	D	1458	HIS	CD2-NE2	-5.51	1.31	1.37
1	J	2558	HIS	CD2-NE2	-5.45	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1358	HIS	CD2-NE2	-5.30	1.32	1.37
1	S	4458	HIS	CD2-NE2	-5.29	1.32	1.37
1	N	3410	GLU	CA-CB	-5.26	1.45	1.53
1	C	1369	ARG	CZ-NH1	5.23	1.40	1.32
1	F	2158	HIS	CD2-NE2	-5.12	1.32	1.37
1	L	3258	HIS	CD2-NE2	-5.10	1.32	1.37
1	G	2258	HIS	CD2-NE2	-5.04	1.32	1.37

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1432	ASN	OD1-CG-ND2	-8.64	113.96	122.60
1	H	2369	ARG	CA-CB-CG	8.56	131.22	114.10
1	E	1535	ASN	OD1-CG-ND2	-8.46	114.14	122.60
1	R	4332	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	H	2332	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	C	1332	ASN	OD1-CG-ND2	-7.34	115.25	122.60
1	T	4532	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	K	3132	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	K	3169	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	M	3345	ILE	CA-C-O	-7.11	113.63	121.17
1	Q	4232	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	E	1532	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	F	2169	ARG	CG-CD-NE	6.60	126.52	112.00
1	G	2237	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	L	3269	ARG	NE-CZ-NH2	-6.35	113.49	119.20
1	S	4432	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	1115	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	I	2432	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	O	3510	GLU	N-CA-CB	-6.27	100.86	110.20
1	H	2358	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	N	3410	GLU	CB-CG-CD	-6.15	102.14	112.60
1	D	1417	ASP	CA-CB-CG	6.10	118.70	112.60
1	F	2132	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	P	4121	THR	CA-CB-OG1	-6.02	100.57	109.60
1	J	2532	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	O	3510	GLU	CA-CB-CG	5.97	126.03	114.10
1	R	4359	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	B	1217	ASP	CA-CB-CG	5.92	118.52	112.60
1	O	3532	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	B	1258	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	K	3144	GLN	OE1-CD-NE2	-5.79	116.81	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	4458	HIS	CB-CG-CD2	-5.76	123.72	131.20
1	H	2317	ASP	CA-CB-CG	5.72	118.32	112.60
1	L	3259	ASN	CA-CB-CG	-5.70	106.90	112.60
1	A	1117	ASP	CA-CB-CG	5.67	118.27	112.60
1	Q	4259	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	T	4510	GLU	CA-CB-CG	5.65	125.40	114.10
1	A	1158	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	H	2309	VAL	O-C-N	-5.59	116.23	122.66
1	Q	4258	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	G	2258	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	F	2158	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	G	2232	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	S	4445	ILE	CA-C-O	-5.53	115.20	120.95
1	B	1245	ILE	CA-C-O	-5.52	115.53	121.27
1	M	3358	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	P	4155	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	E	1558	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	J	2517	ASP	CA-CB-CG	5.41	118.01	112.60
1	L	3232	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	N	3432	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	T	4558	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	C	1344	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	B	1232	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	S	4444	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	S	4417	ASP	CA-CB-CG	5.34	117.94	112.60
1	F	2169	ARG	CD-NE-CZ	5.33	131.86	124.40
1	J	2558	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	K	3158	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	S	4459	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	M	3317	ASP	CA-CB-CG	5.26	117.86	112.60
1	Q	4217	ASP	CA-CB-CG	5.25	117.85	112.60
1	P	4140	LEU	O-C-N	-5.24	116.18	122.15
1	P	4158	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	O	3569	ARG	CB-CA-C	-5.21	100.20	110.10
1	D	1420	PHE	CA-CB-CG	5.19	118.99	113.80
1	S	4449	THR	CA-C-O	-5.18	114.79	120.43
1	C	1369	ARG	CG-CD-NE	-5.16	100.64	112.00
1	K	3110	GLU	N-CA-C	5.15	116.97	111.36
1	Q	4259	ASN	CA-CB-CG	-5.15	107.45	112.60
1	P	4132	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	F	2159	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	K	3145	ILE	CA-C-O	-5.14	115.70	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2235	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	F	2144	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	D	1422	VAL	N-CA-CB	-5.10	102.50	111.93
1	K	3135	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	E	1517	ASP	CA-CB-CG	5.08	117.68	112.60
1	N	3429	LEU	CA-C-O	-5.08	115.69	121.58
1	T	4517	ASP	CA-CB-CG	5.08	117.68	112.60
1	S	4410	GLU	CB-CG-CD	-5.07	103.97	112.60
1	C	1358	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	R	4332	ASN	CB-CG-ND2	5.06	123.98	116.40
1	F	2110	GLU	O-C-N	-5.03	115.69	122.23
1	C	1359	ASN	CA-CB-CG	-5.03	107.57	112.60
1	D	1458	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	M	3332	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	O	3555	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	1132	ASN	OD1-CG-ND2	-5.00	117.60	122.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4	0
1	E	540	0	524	1	0
1	F	540	0	524	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	540	0	524	4	0
1	O	540	0	524	2	0
1	P	540	0	524	5	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	2	0
2	f	34	0	30	0	0
2	g	34	0	30	0	0
2	h	34	0	30	1	0
2	i	34	0	30	1	0
2	j	34	0	30	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	56	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 (56) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:3460:GLY:HA2	4:N:3470:GAL:C6	2.42	0.49
1:T:4560:GLY:HA2	4:T:4570:GAL:H61	1.97	0.47
1:D:1460:GLY:HA2	2:e:3:GLA: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:D:1460:GLY:HA2	2:e:3:GLA:C6	2.47	0.45
1:P:4121:THR:HG1	4:P:4170:GAL:HO4	1.63	0.44
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:F:2130:PHE:CE1	2:j:2:GAL:H3	2.54	0.42
1:G:2260:GLY:HA2	4:G:2270:GAL:C6	2.50	0.42
2:i:2:GAL:O3	2:i:3:GLA:H5	2.19	0.41
1:G:2260:GLY:HA2	4:G:2270:GAL:H61	2.01	0.41
1:P:4121:THR:OG1	4:P:4170:GAL:O4	2.35	0.41
1:K:3119:THR:HG21	5:K:5192:HOH:O	2.22	0.40
1:F:2131:THR:HA	2:h:3:GLA:O6	2.21	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
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 ⓘ

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%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	C	61/61 (100%)	58 (95%)	3 (5%)	22	55
1	D	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	E	61/61 (100%)	57 (93%)	4 (7%)	15	43
1	F	61/61 (100%)	57 (93%)	4 (7%)	15	43
1	G	61/61 (100%)	58 (95%)	3 (5%)	22	55
1	H	61/61 (100%)	57 (93%)	4 (7%)	15	43
1	I	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	J	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	K	61/61 (100%)	58 (95%)	3 (5%)	22	55
1	L	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	M	61/61 (100%)	58 (95%)	3 (5%)	22	55
1	N	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	O	61/61 (100%)	58 (95%)	3 (5%)	22	55
1	P	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	Q	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	R	61/61 (100%)	58 (95%)	3 (5%)	22	55
1	S	61/61 (100%)	59 (97%)	2 (3%)	33	69
1	T	61/61 (100%)	59 (97%)	2 (3%)	33	69
All	All	1220/1220 (100%)	1168 (96%)	52 (4%)	26	60

All (52) 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	E	1505	VAL
1	E	1510	GLU

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Mol	Chain	Res	Type
1	E	1522	VAL
1	E	1569	ARG
1	F	2105	VAL
1	F	2110	GLU
1	F	2122	VAL
1	F	2169	ARG
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. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1137	GLN
1	B	1237	GLN
1	C	1337	GLN
1	D	1437	GLN
1	E	1537	GLN
1	F	2137	GLN
1	F	2158	HIS
1	G	2237	GLN
1	G	2258	HIS
1	H	2337	GLN
1	H	2344	GLN
1	J	2537	GLN
1	K	3137	GLN
1	K	3144	GLN
1	L	3237	GLN
1	M	3337	GLN
1	N	3437	GLN
1	O	3537	GLN
1	O	3558	HIS
1	P	4137	GLN
1	P	4158	HIS
1	Q	4237	GLN
1	R	4337	GLN
1	S	4437	GLN
1	T	4537	GLN

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	0.50	0	17,17,17	0.39	0
2	GAL	0	2	2	11,11,12	0.60	0	15,15,17	0.80	1 (6%)
2	GLA	0	3	2	11,11,12	0.40	0	15,15,17	0.69	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	0.67	0	15,15,17	0.63	0
2	BGC	2	1	2	12,12,12	0.51	0	17,17,17	0.39	0
2	GAL	2	2	2	11,11,12	0.49	0	15,15,17	0.75	0
2	GLA	2	3	2	11,11,12	0.57	0	15,15,17	0.60	0
3	GAL	3	1	3	12,12,12	0.45	0	17,17,17	0.65	0
3	GLA	3	2	3	11,11,12	0.55	0	15,15,17	0.50	0
2	BGC	4	1	2	12,12,12	0.39	0	17,17,17	0.61	0
2	GAL	4	2	2	11,11,12	0.61	0	15,15,17	0.73	0
2	GLA	4	3	2	11,11,12	0.35	0	15,15,17	0.75	1 (6%)
2	BGC	5	1	2	12,12,12	0.43	0	17,17,17	0.40	0
2	GAL	5	2	2	11,11,12	0.64	0	15,15,17	0.73	0
2	GLA	5	3	2	11,11,12	0.42	0	15,15,17	0.61	0
3	GAL	6	1	3	12,12,12	0.40	0	17,17,17	0.46	0
3	GLA	6	2	3	11,11,12	0.63	0	15,15,17	0.57	0
2	BGC	7	1	2	12,12,12	0.39	0	17,17,17	0.53	0
2	GAL	7	2	2	11,11,12	0.65	0	15,15,17	0.56	0
2	GLA	7	3	2	11,11,12	0.46	0	15,15,17	0.61	0
2	BGC	8	1	2	12,12,12	0.43	0	17,17,17	0.35	0
2	GAL	8	2	2	11,11,12	0.66	0	15,15,17	0.49	0
2	GLA	8	3	2	11,11,12	0.64	0	15,15,17	0.71	0
2	BGC	9	1	2	12,12,12	0.37	0	17,17,17	0.59	0
2	GAL	9	2	2	11,11,12	0.61	0	15,15,17	0.46	0
2	GLA	9	3	2	11,11,12	0.70	0	15,15,17	0.67	1 (6%)
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	0.56	0
2	GLA	AA	3	2	11,11,12	0.51	0	15,15,17	0.82	1 (6%)
2	BGC	BA	1	2	12,12,12	0.64	0	17,17,17	0.46	0
2	GAL	BA	2	2	11,11,12	0.49	0	15,15,17	0.39	0
2	GLA	BA	3	2	11,11,12	0.74	0	15,15,17	0.50	0
2	BGC	CA	1	2	12,12,12	0.39	0	17,17,17	0.40	0
2	GAL	CA	2	2	11,11,12	0.66	0	15,15,17	0.42	0
2	GLA	CA	3	2	11,11,12	0.44	0	15,15,17	0.67	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	0.54	0	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	EA	1	2	12,12,12	0.34	0	17,17,17	0.42	0
2	GAL	EA	2	2	11,11,12	0.51	0	15,15,17	0.57	0
2	GLA	EA	3	2	11,11,12	0.47	0	15,15,17	0.75	0
2	BGC	FA	1	2	12,12,12	0.29	0	17,17,17	0.37	0
2	GAL	FA	2	2	11,11,12	0.49	0	15,15,17	0.45	0
2	GLA	FA	3	2	11,11,12	0.40	0	15,15,17	0.69	0
3	GAL	GA	1	3	12,12,12	0.45	0	17,17,17	0.50	0
3	GLA	GA	2	3	11,11,12	0.61	0	15,15,17	0.69	0
2	BGC	U	1	2	12,12,12	0.40	0	17,17,17	0.32	0
2	GAL	U	2	2	11,11,12	0.45	0	15,15,17	0.61	0
2	GLA	U	3	2	11,11,12	0.43	0	15,15,17	0.69	0
3	GAL	V	1	3	12,12,12	0.35	0	17,17,17	0.57	0
3	GLA	V	2	3	11,11,12	0.47	0	15,15,17	0.88	1 (6%)
2	BGC	W	1	2	12,12,12	0.55	0	17,17,17	0.62	0
2	GAL	W	2	2	11,11,12	0.69	0	15,15,17	0.74	0
2	GLA	W	3	2	11,11,12	0.39	0	15,15,17	0.71	1 (6%)
2	BGC	X	1	2	12,12,12	0.37	0	17,17,17	0.53	0
2	GAL	X	2	2	11,11,12	0.55	0	15,15,17	0.59	0
2	GLA	X	3	2	11,11,12	0.48	0	15,15,17	0.58	0
3	GAL	Y	1	3	12,12,12	0.36	0	17,17,17	0.44	0
3	GLA	Y	2	3	11,11,12	0.45	0	15,15,17	0.82	1 (6%)
3	GAL	Z	1	3	12,12,12	0.47	0	17,17,17	0.46	0
3	GLA	Z	2	3	11,11,12	0.47	0	15,15,17	0.73	0
2	BGC	a	1	2	12,12,12	0.41	0	17,17,17	0.48	0
2	GAL	a	2	2	11,11,12	0.56	0	15,15,17	0.49	0
2	GLA	a	3	2	11,11,12	0.48	0	15,15,17	0.64	0
3	GAL	b	1	3	12,12,12	0.62	0	17,17,17	0.59	0
3	GLA	b	2	3	11,11,12	0.64	0	15,15,17	0.91	1 (6%)
2	BGC	c	1	2	12,12,12	0.37	0	17,17,17	0.56	0
2	GAL	c	2	2	11,11,12	0.53	0	15,15,17	0.61	0
2	GLA	c	3	2	11,11,12	0.42	0	15,15,17	0.57	0
3	GAL	d	1	3	12,12,12	0.81	0	17,17,17	0.95	0
3	GLA	d	2	3	11,11,12	0.70	0	15,15,17	0.80	1 (6%)
2	BGC	e	1	2	12,12,12	0.48	0	17,17,17	0.52	0
2	GAL	e	2	2	11,11,12	0.45	0	15,15,17	0.57	0
2	GLA	e	3	2	11,11,12	0.59	0	15,15,17	0.83	1 (6%)
2	BGC	f	1	2	12,12,12	0.39	0	17,17,17	0.52	0
2	GAL	f	2	2	11,11,12	0.47	0	15,15,17	0.39	0
2	GLA	f	3	2	11,11,12	0.53	0	15,15,17	0.59	0
2	BGC	g	1	2	12,12,12	0.30	0	17,17,17	0.35	0
2	GAL	g	2	2	11,11,12	0.55	0	15,15,17	0.62	0
2	GLA	g	3	2	11,11,12	0.47	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	h	1	2	12,12,12	0.58	0	17,17,17	0.58	0
2	GAL	h	2	2	11,11,12	0.58	0	15,15,17	0.73	0
2	GLA	h	3	2	11,11,12	0.61	0	15,15,17	0.84	0
2	BGC	i	1	2	12,12,12	0.38	0	17,17,17	0.37	0
2	GAL	i	2	2	11,11,12	0.49	0	15,15,17	0.37	0
2	GLA	i	3	2	11,11,12	0.45	0	15,15,17	0.56	0
2	BGC	j	1	2	12,12,12	0.25	0	17,17,17	0.55	0
2	GAL	j	2	2	11,11,12	0.48	0	15,15,17	0.69	0
2	GLA	j	3	2	11,11,12	0.35	0	15,15,17	1.15	2 (13%)
2	BGC	k	1	2	12,12,12	0.28	0	17,17,17	0.46	0
2	GAL	k	2	2	11,11,12	0.36	0	15,15,17	0.51	0
2	GLA	k	3	2	11,11,12	0.54	0	15,15,17	0.82	0
3	GAL	l	1	3	12,12,12	0.35	0	17,17,17	0.43	0
3	GLA	l	2	3	11,11,12	0.57	0	15,15,17	0.53	0
2	BGC	m	1	2	12,12,12	0.60	0	17,17,17	0.46	0
2	GAL	m	2	2	11,11,12	0.64	0	15,15,17	0.44	0
2	GLA	m	3	2	11,11,12	0.48	0	15,15,17	0.80	1 (6%)
3	GAL	n	1	3	12,12,12	0.38	0	17,17,17	0.42	0
3	GLA	n	2	3	11,11,12	0.63	0	15,15,17	0.66	0
2	BGC	o	1	2	12,12,12	0.49	0	17,17,17	0.91	1 (5%)
2	GAL	o	2	2	11,11,12	0.54	0	15,15,17	0.65	0
2	GLA	o	3	2	11,11,12	0.43	0	15,15,17	0.62	0
2	BGC	p	1	2	12,12,12	0.54	0	17,17,17	0.58	0
2	GAL	p	2	2	11,11,12	0.65	0	15,15,17	0.59	0
2	GLA	p	3	2	11,11,12	0.48	0	15,15,17	0.68	0
3	GAL	q	1	3	12,12,12	0.52	0	17,17,17	0.80	0
3	GLA	q	2	3	11,11,12	0.68	0	15,15,17	0.70	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	0.47	0	15,15,17	0.79	0
2	GLA	r	3	2	11,11,12	0.48	0	15,15,17	0.91	1 (6%)
2	BGC	s	1	2	12,12,12	0.33	0	17,17,17	0.37	0
2	GAL	s	2	2	11,11,12	0.44	0	15,15,17	0.58	0
2	GLA	s	3	2	11,11,12	0.63	0	15,15,17	0.45	0
2	BGC	t	1	2	12,12,12	0.39	0	17,17,17	0.48	0
2	GAL	t	2	2	11,11,12	0.51	0	15,15,17	0.62	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	0.47	0	17,17,17	0.43	0
3	GLA	u	2	3	11,11,12	0.51	0	15,15,17	0.43	0
2	BGC	v	1	2	12,12,12	0.39	0	17,17,17	0.50	0
2	GAL	v	2	2	11,11,12	0.53	0	15,15,17	0.54	0
2	GLA	v	3	2	11,11,12	0.40	0	15,15,17	0.60	0
3	GAL	w	1	3	12,12,12	0.51	0	17,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLA	w	2	3	11,11,12	0.48	0	15,15,17	0.63	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	0.49	0	15,15,17	0.65	0
2	GLA	x	3	2	11,11,12	0.46	0	15,15,17	0.61	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	0.73	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	0.54	0	15,15,17	0.55	0
2	GLA	z	3	2	11,11,12	0.59	0	15,15,17	1.01	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	3	GLA	C1-O5-C5	3.36	116.69	112.19
3	b	2	GLA	C1-O5-C5	2.90	116.07	112.19
2	z	3	GLA	C1-O5-C5	2.79	115.92	112.19
2	AA	3	GLA	C1-O5-C5	2.50	115.54	112.19
3	V	2	GLA	C1-C2-C3	2.42	113.17	109.64
2	j	3	GLA	C1-C2-C3	2.34	113.05	109.64
2	o	1	BGC	C4-C3-C2	2.31	114.88	110.83
2	e	3	GLA	C1-C2-C3	2.28	112.97	109.64
3	d	2	GLA	C1-C2-C3	2.28	112.96	109.64
2	0	2	GAL	C3-C4-C5	-2.23	106.19	110.23
2	r	3	GLA	C1-O5-C5	2.20	115.14	112.19
2	t	3	GLA	C1-O5-C5	2.19	115.12	112.19
2	m	3	GLA	C1-O5-C5	2.16	115.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	3	GLA	C1-O5-C5	2.05	114.94	112.19
3	Y	2	GLA	C1-O5-C5	2.03	114.91	112.19
2	4	3	GLA	C1-O5-C5	2.01	114.88	112.19
2	9	3	GLA	C1-O5-C5	2.01	114.88	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	g	3	GLA	C4-C5-C6-O6
2	BA	3	GLA	C4-C5-C6-O6
2	BA	3	GLA	O5-C5-C6-O6
2	z	1	BGC	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
3	DA	2	GLA	C4-C5-C6-O6
3	n	2	GLA	C4-C5-C6-O6
2	o	3	GLA	O5-C5-C6-O6
3	Y	2	GLA	O5-C5-C6-O6
3	Y	2	GLA	C4-C5-C6-O6
3	6	2	GLA	C4-C5-C6-O6
3	u	2	GLA	C4-C5-C6-O6
3	Z	2	GLA	O5-C5-C6-O6
2	EA	1	BGC	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

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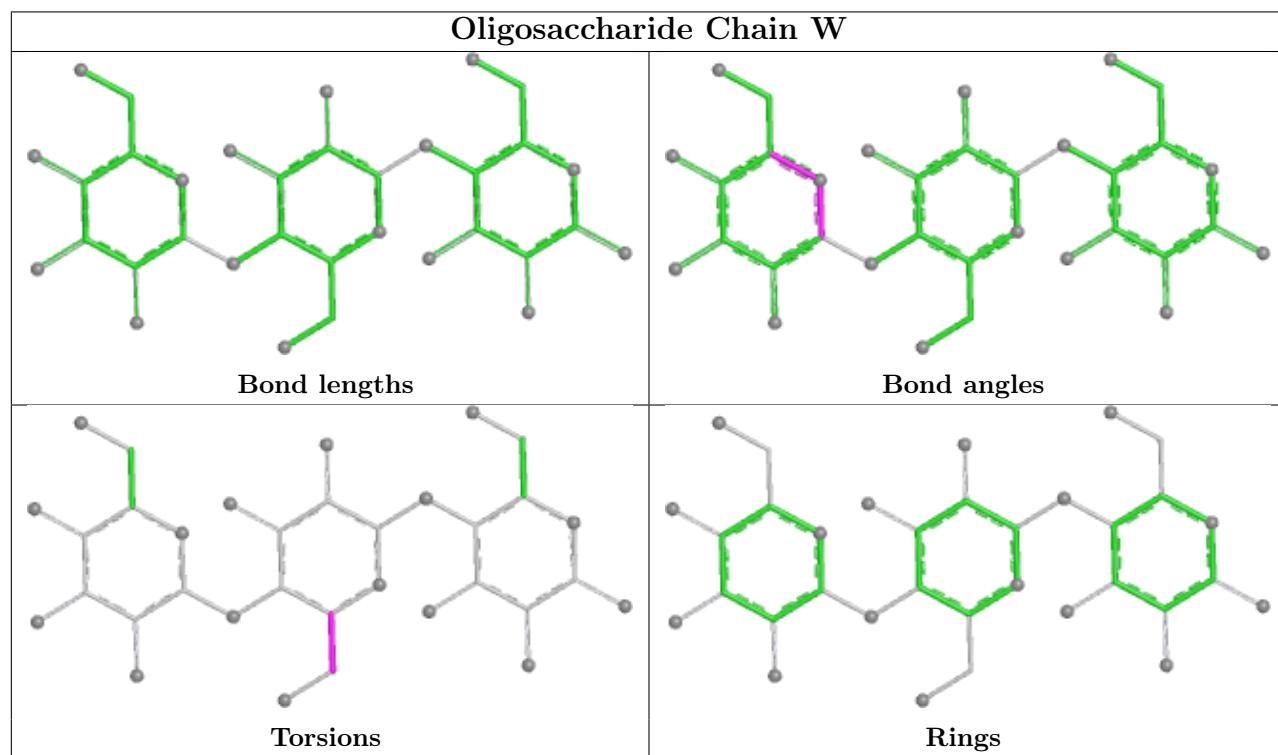
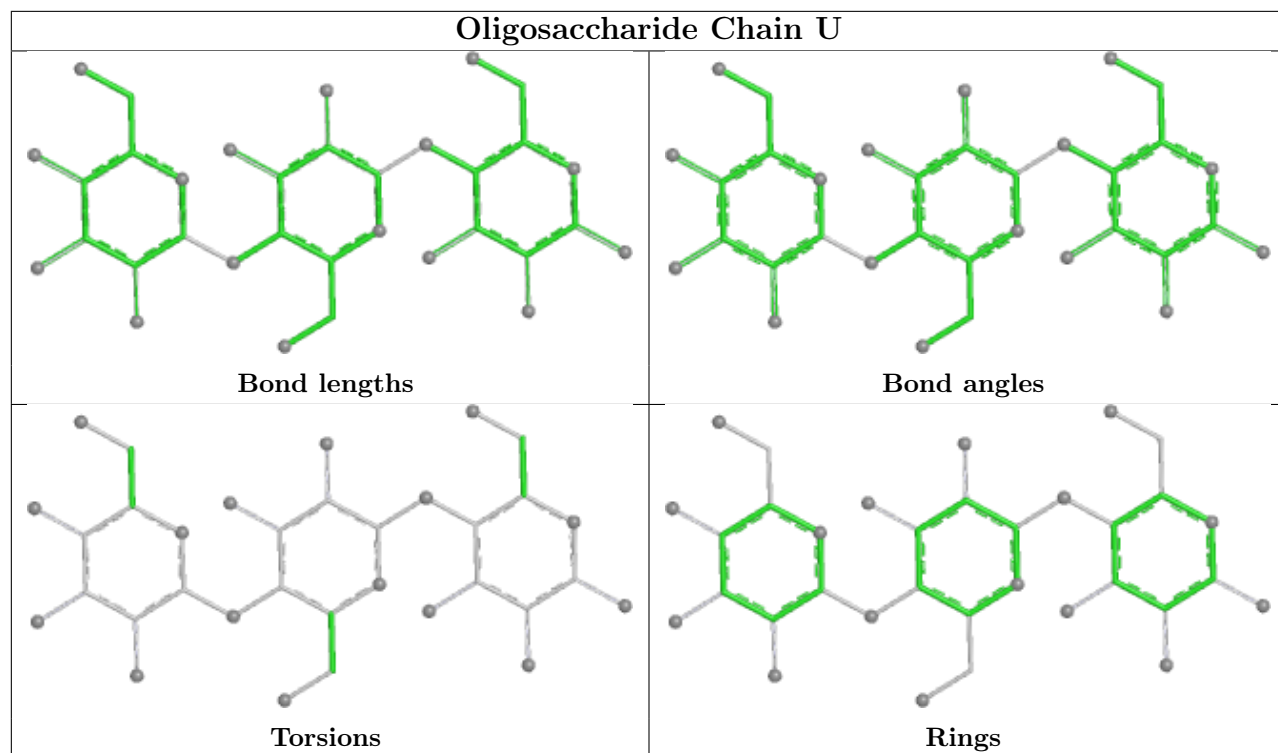
Mol	Chain	Res	Type	Atoms
2	4	1	BGC	O5-C5-C6-O6
3	1	2	GLA	O5-C5-C6-O6
3	3	2	GLA	O5-C5-C6-O6
2	W	2	GAL	O5-C5-C6-O6
2	0	1	BGC	C4-C5-C6-O6
2	8	2	GAL	C4-C5-C6-O6
3	b	1	GAL	C4-C5-C6-O6
3	1	1	GAL	O5-C5-C6-O6
2	0	1	BGC	O5-C5-C6-O6
2	X	3	GLA	C4-C5-C6-O6
2	4	2	GAL	C4-C5-C6-O6

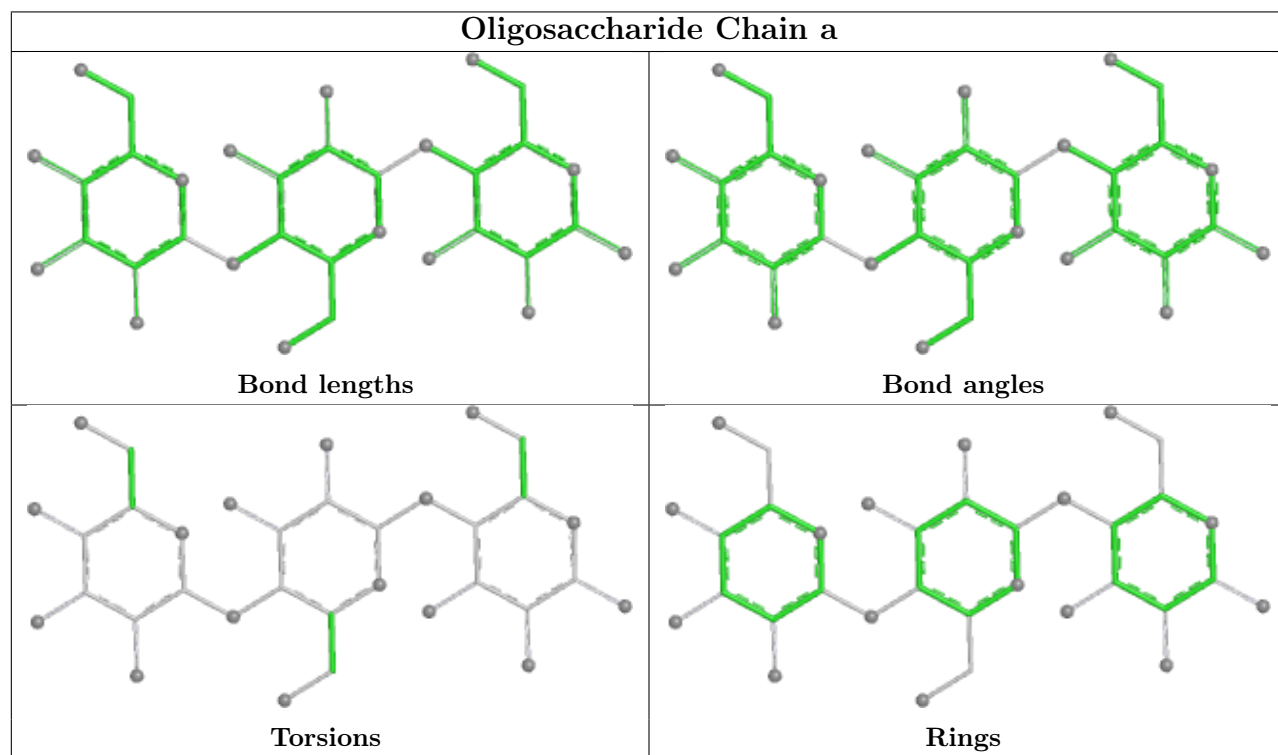
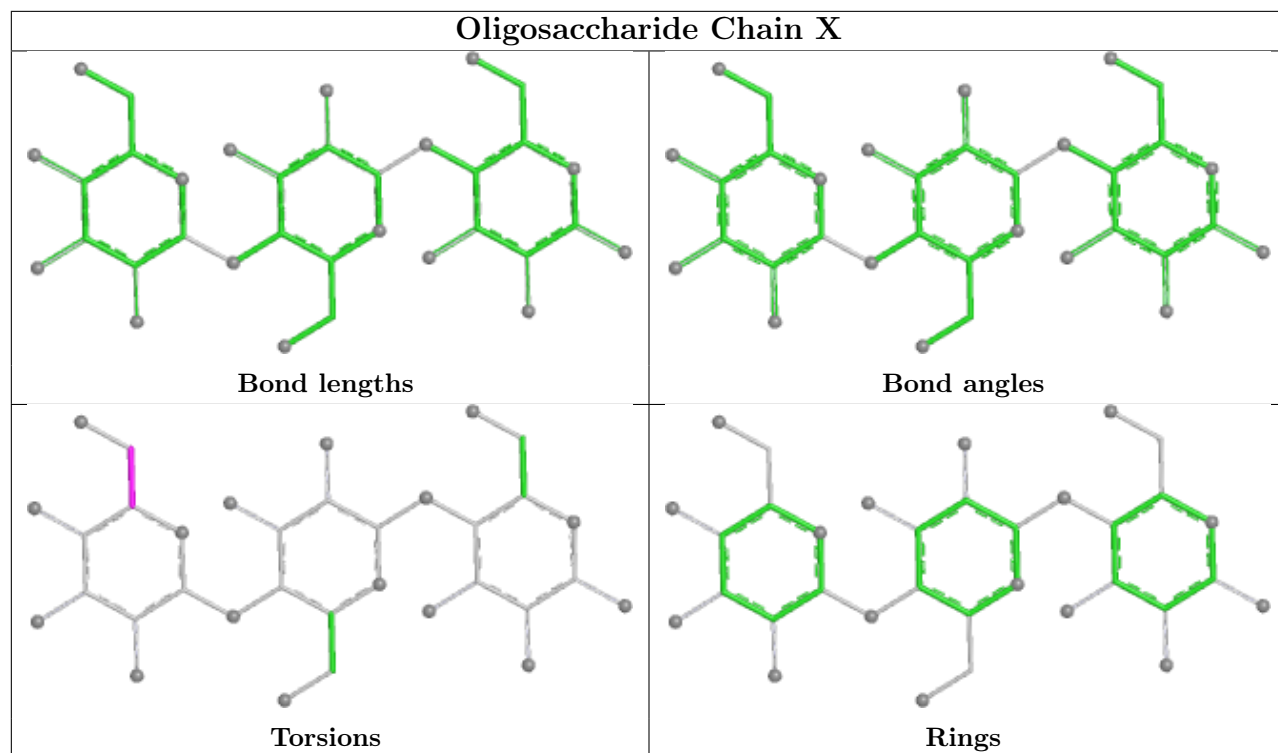
There are no ring outliers.

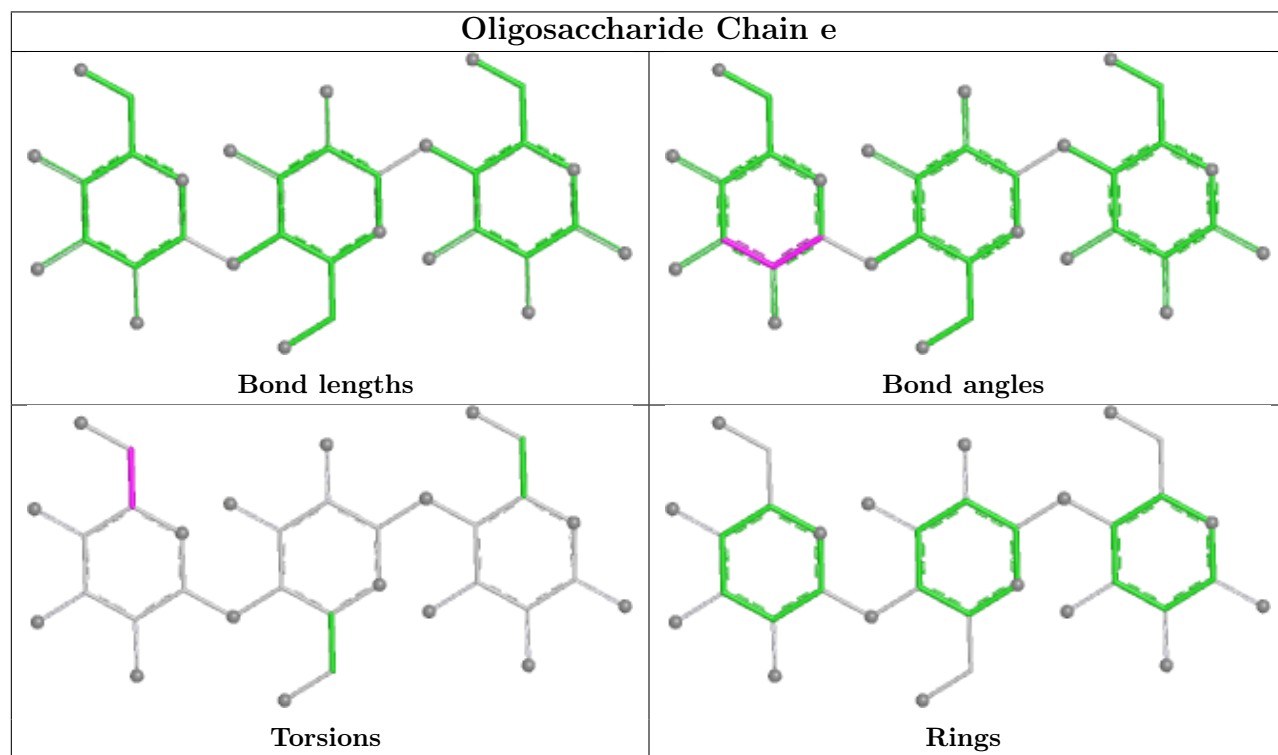
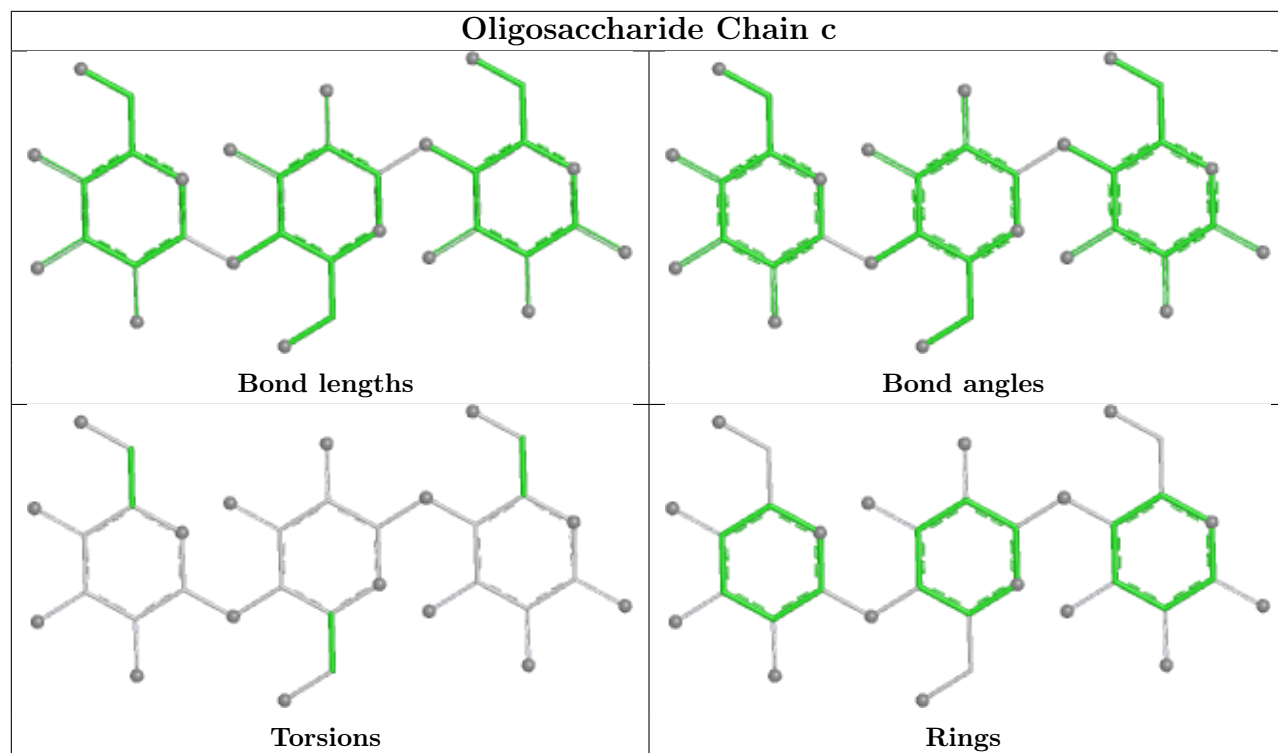
12 monomers are involved in 10 short contacts:

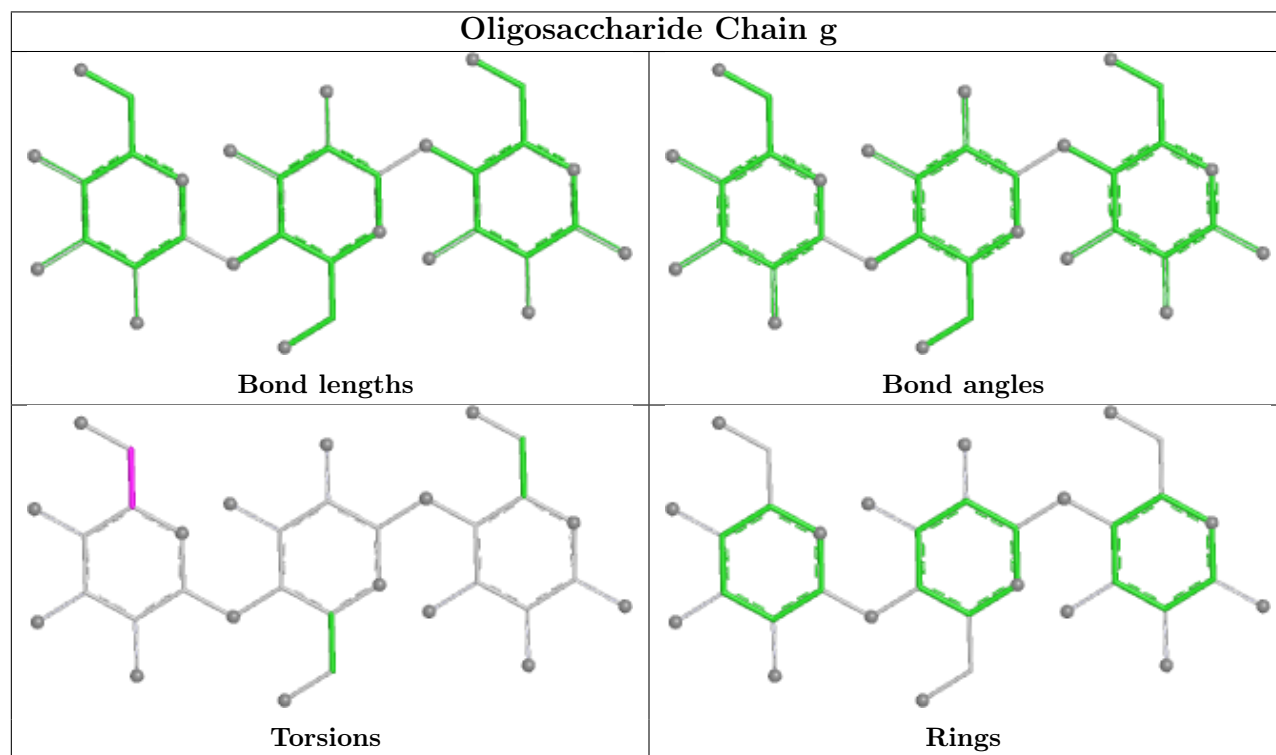
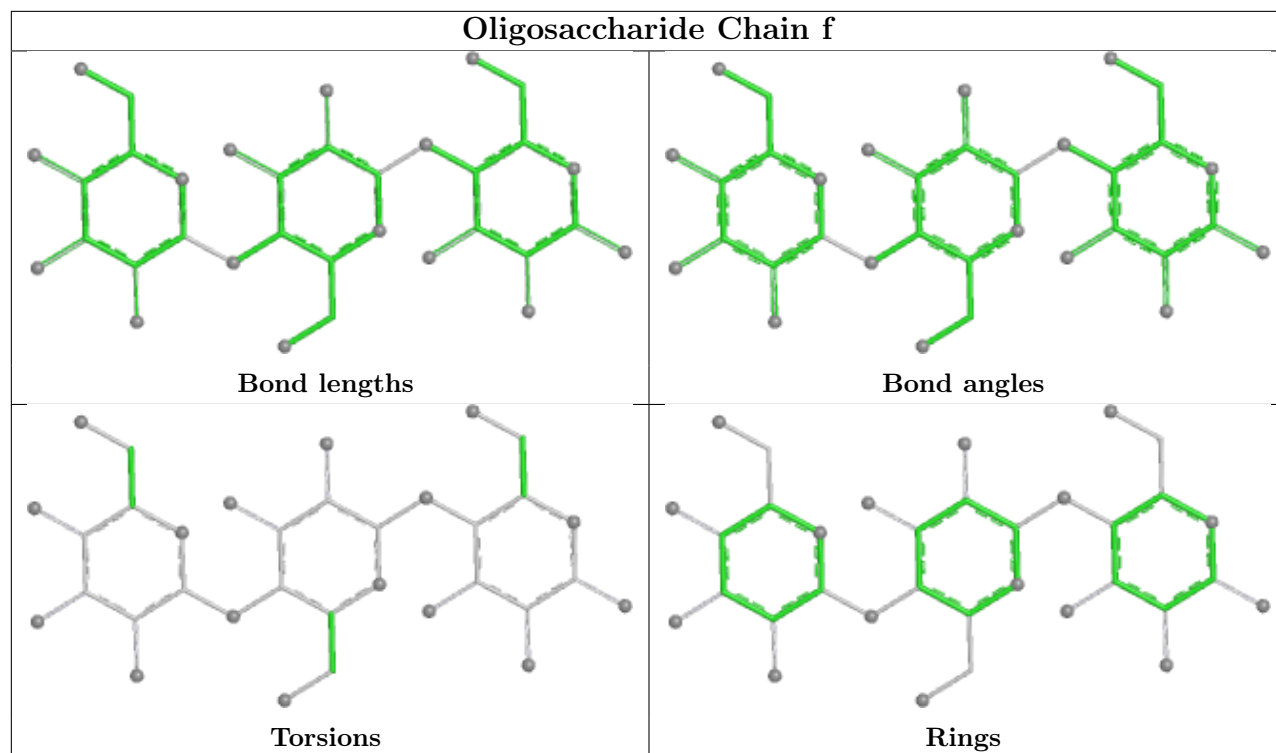
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	9	3	GLA	1	0
2	e	3	GLA	2	0
2	EA	3	GLA	1	0
2	AA	3	GLA	1	0
2	9	2	GAL	1	0
2	i	2	GAL	1	0
2	AA	2	GAL	1	0
2	i	3	GLA	1	0
3	DA	1	GAL	1	0
2	j	2	GAL	1	0
2	h	3	GLA	1	0
2	W	3	GLA	1	0

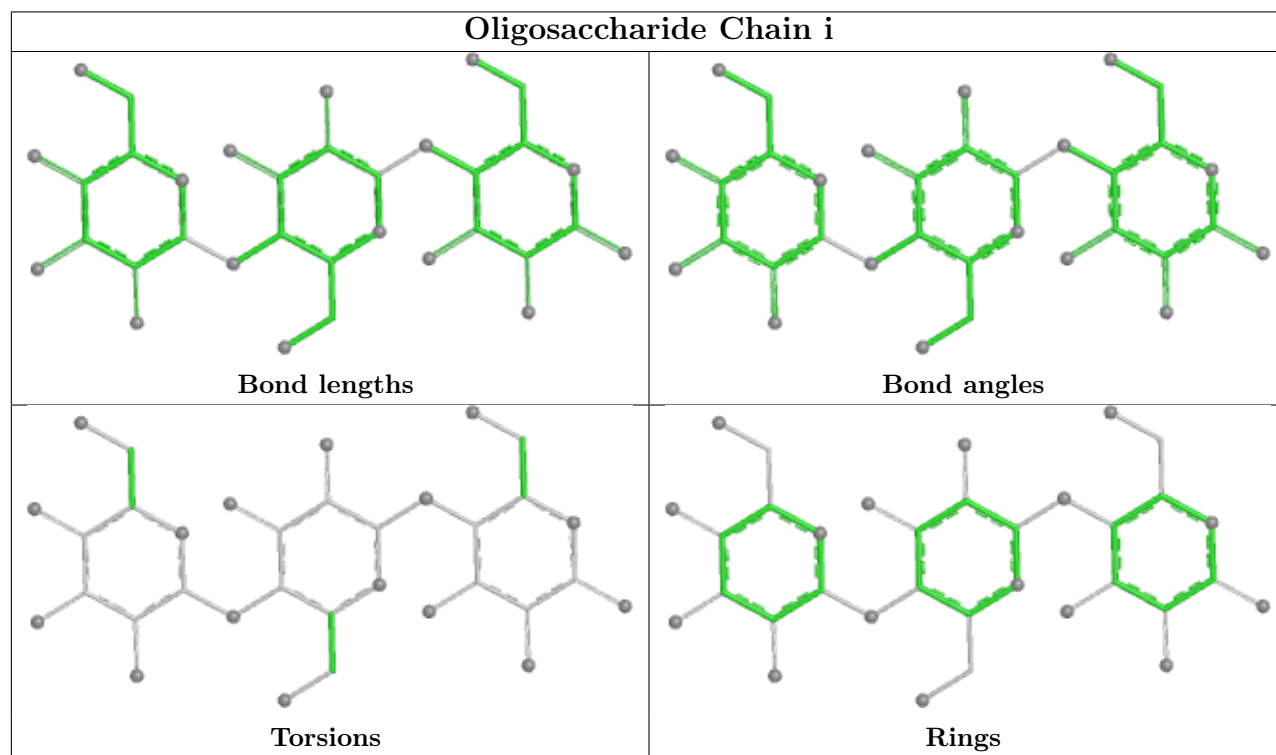
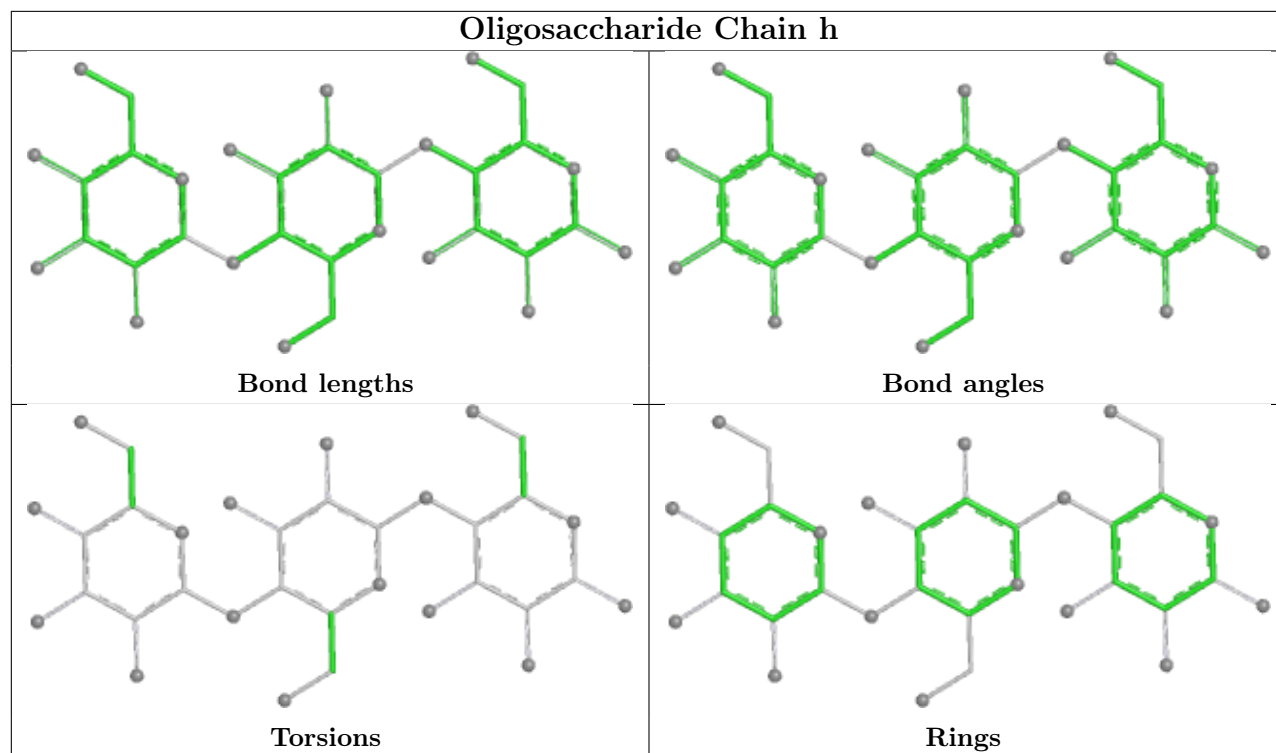
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

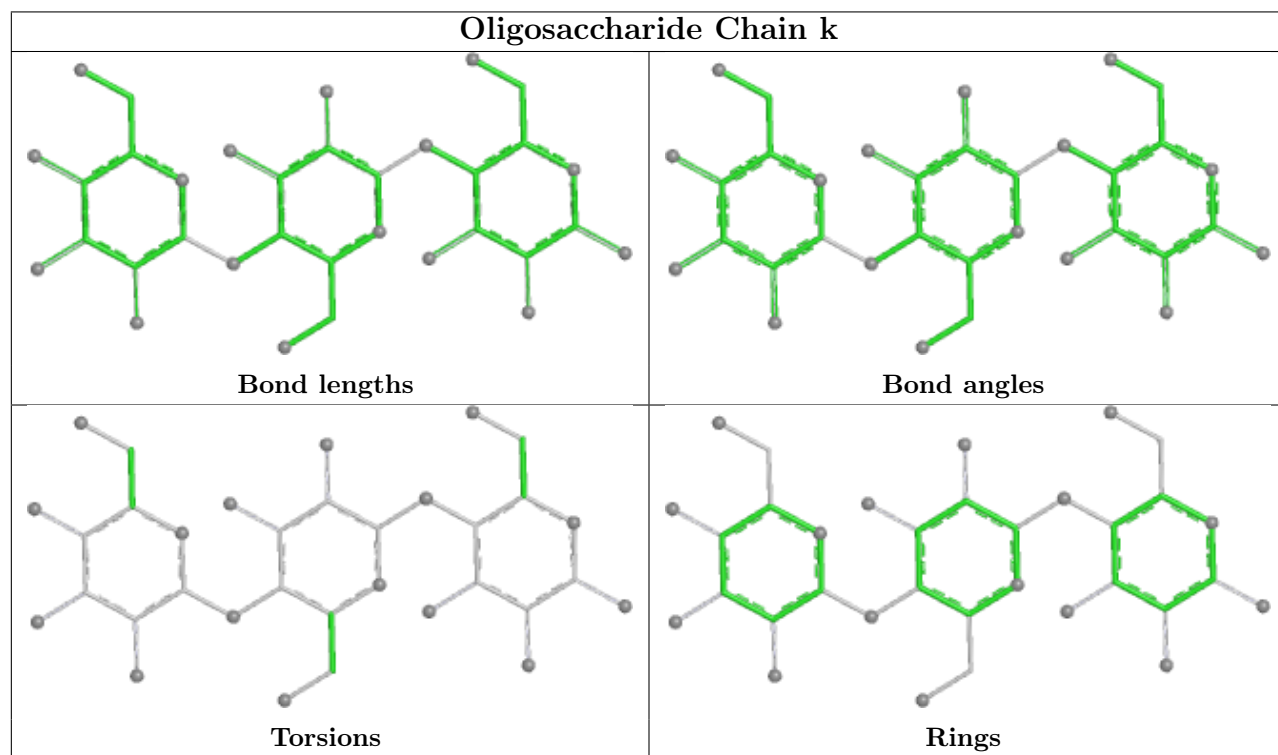
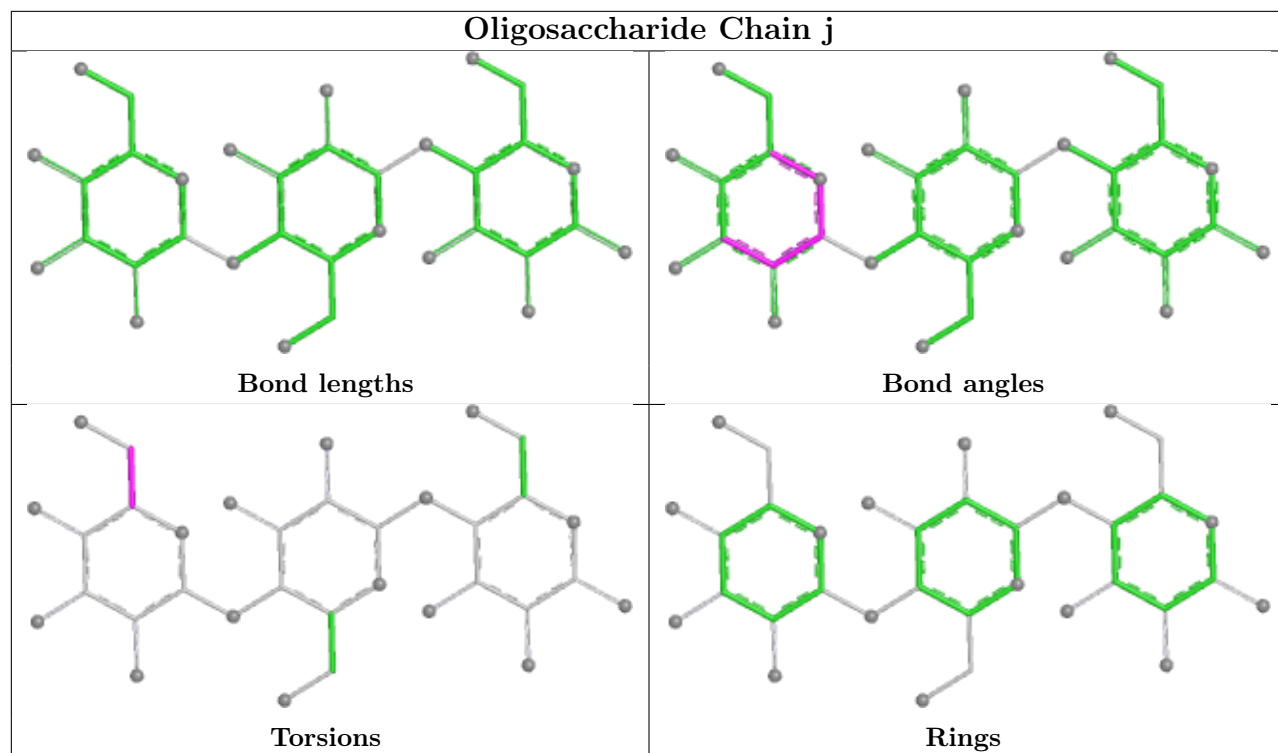


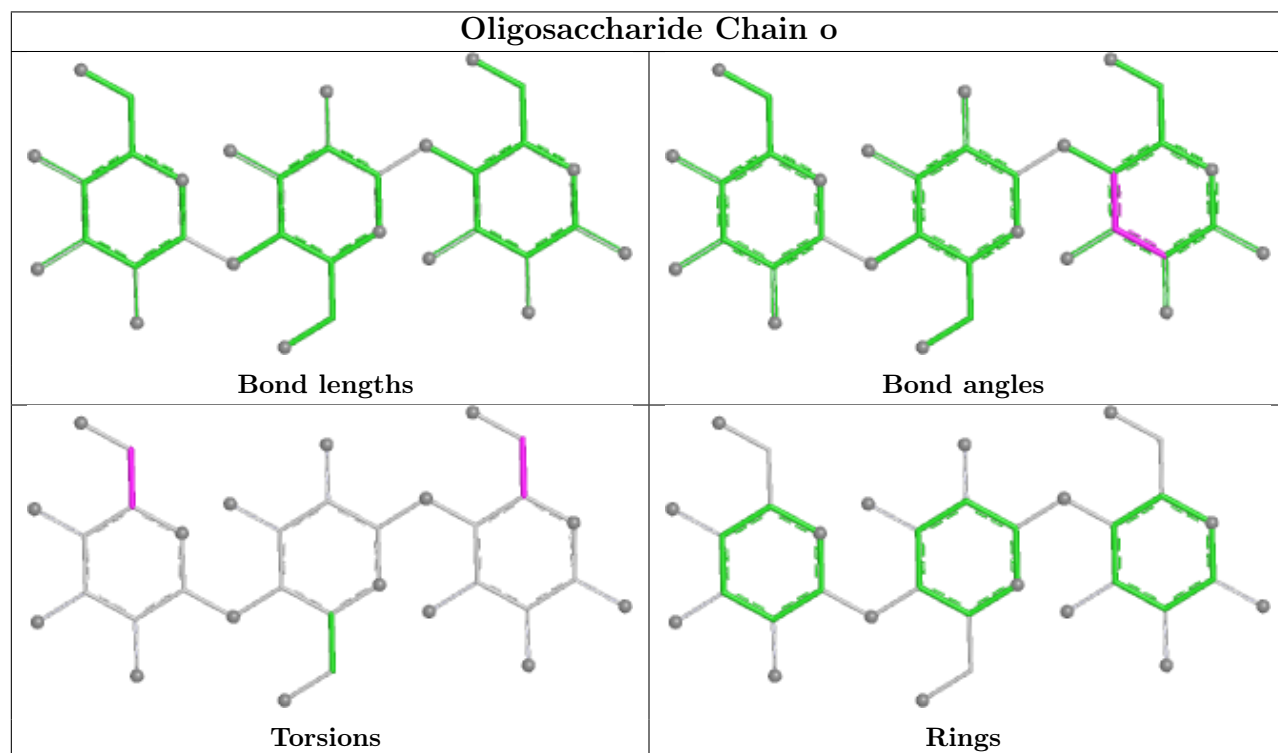
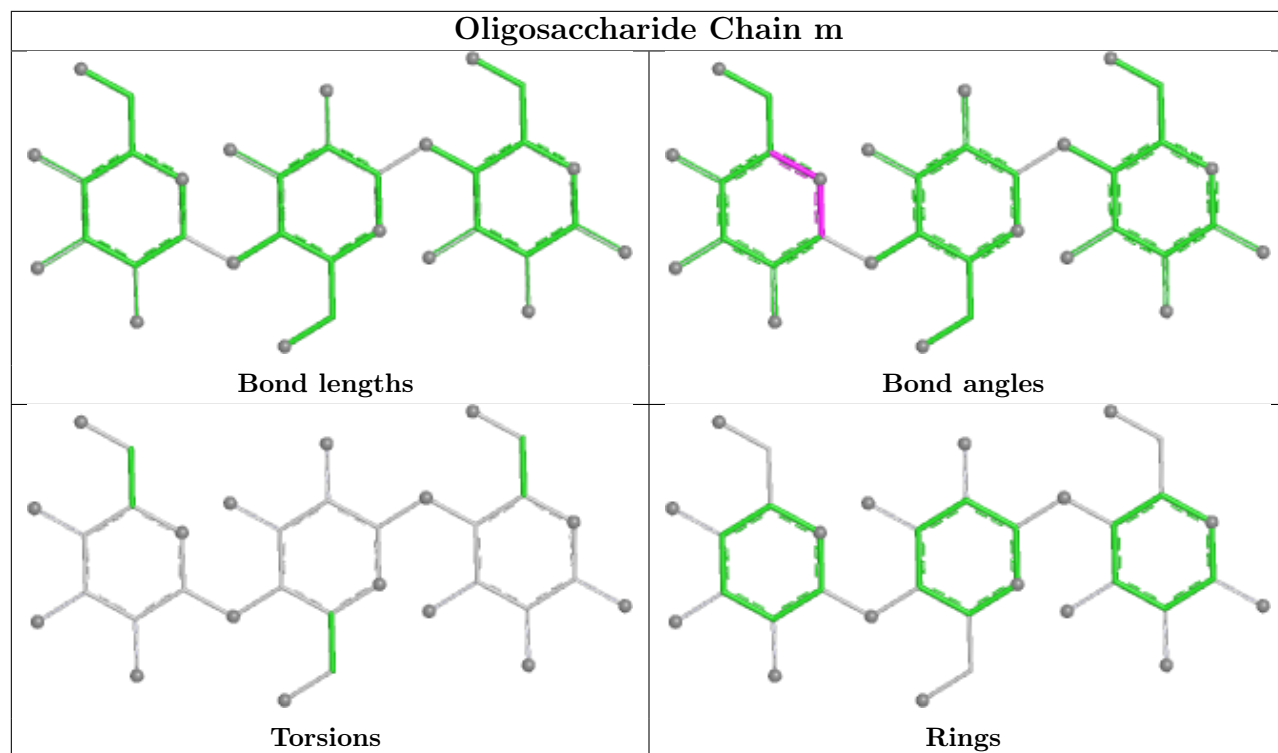


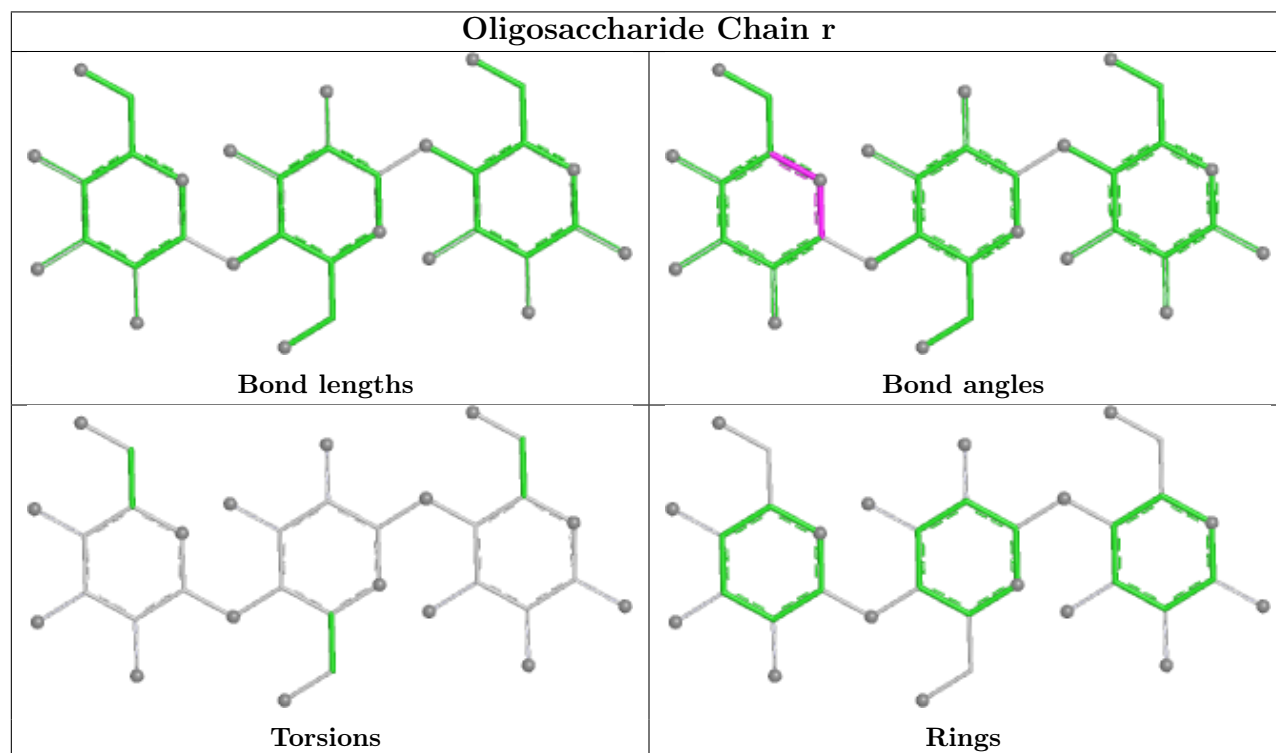
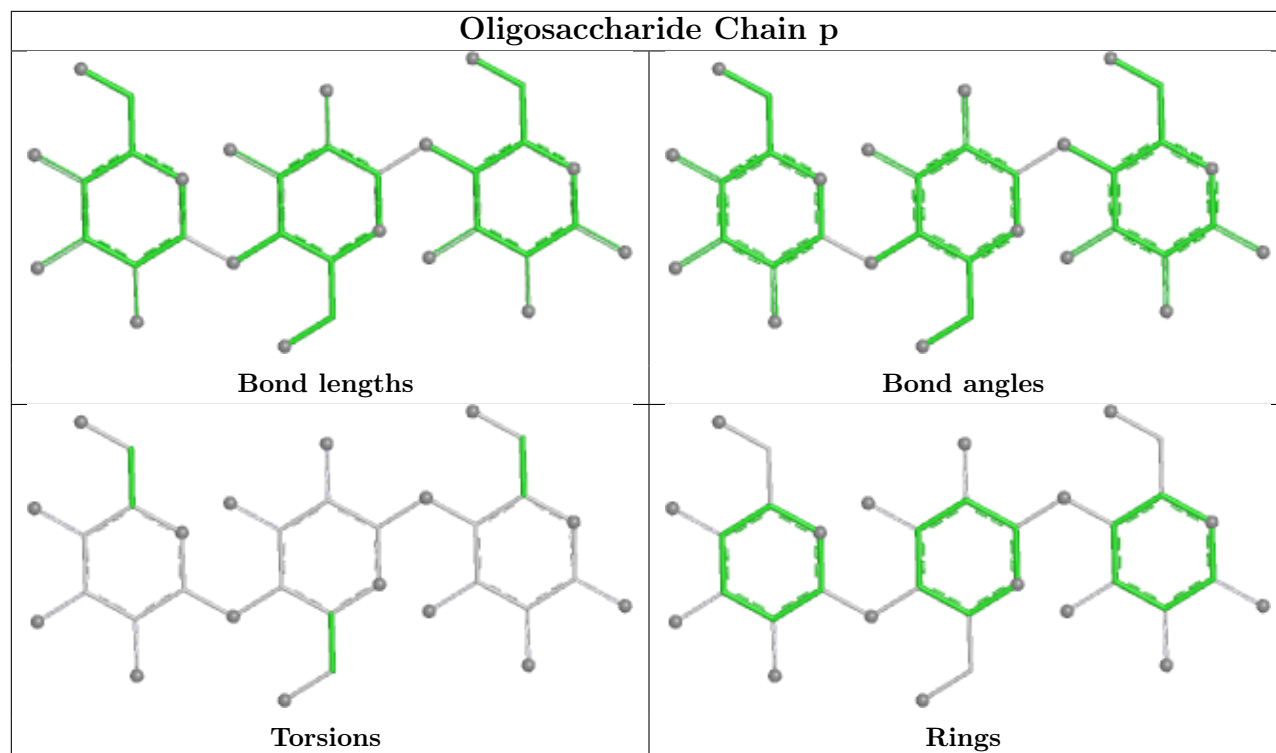


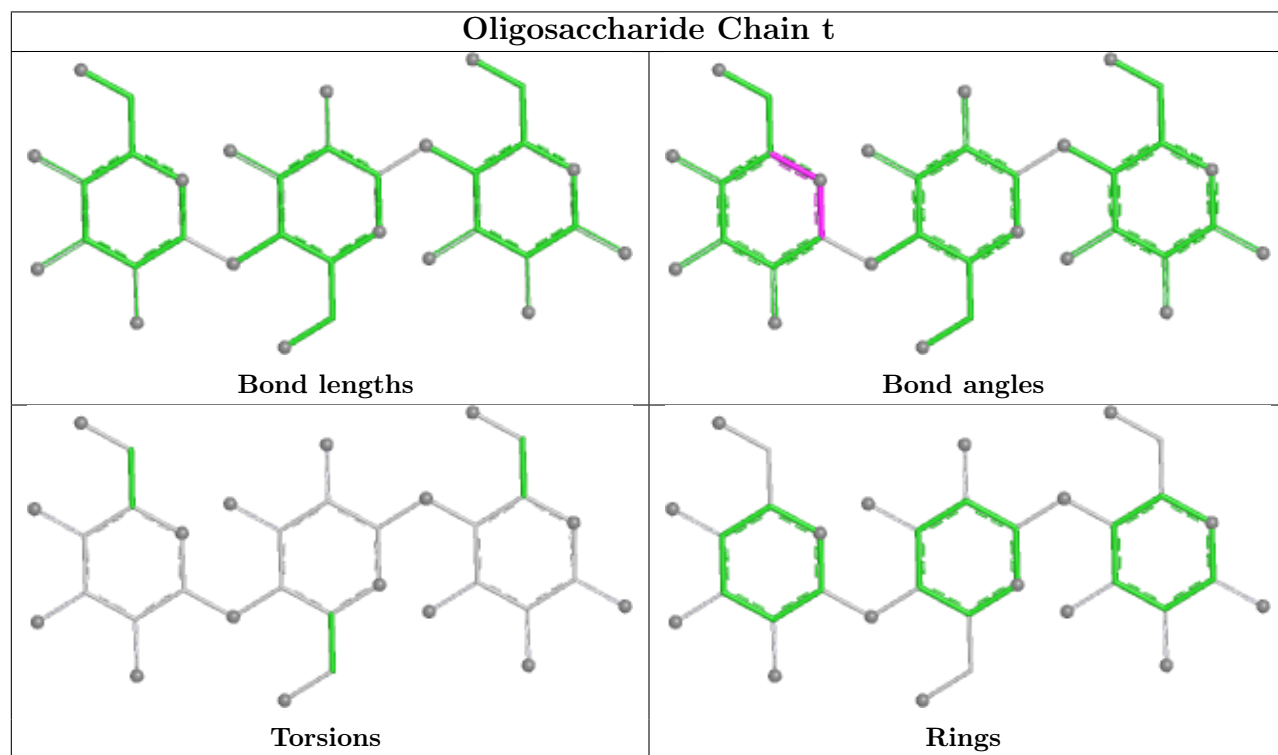
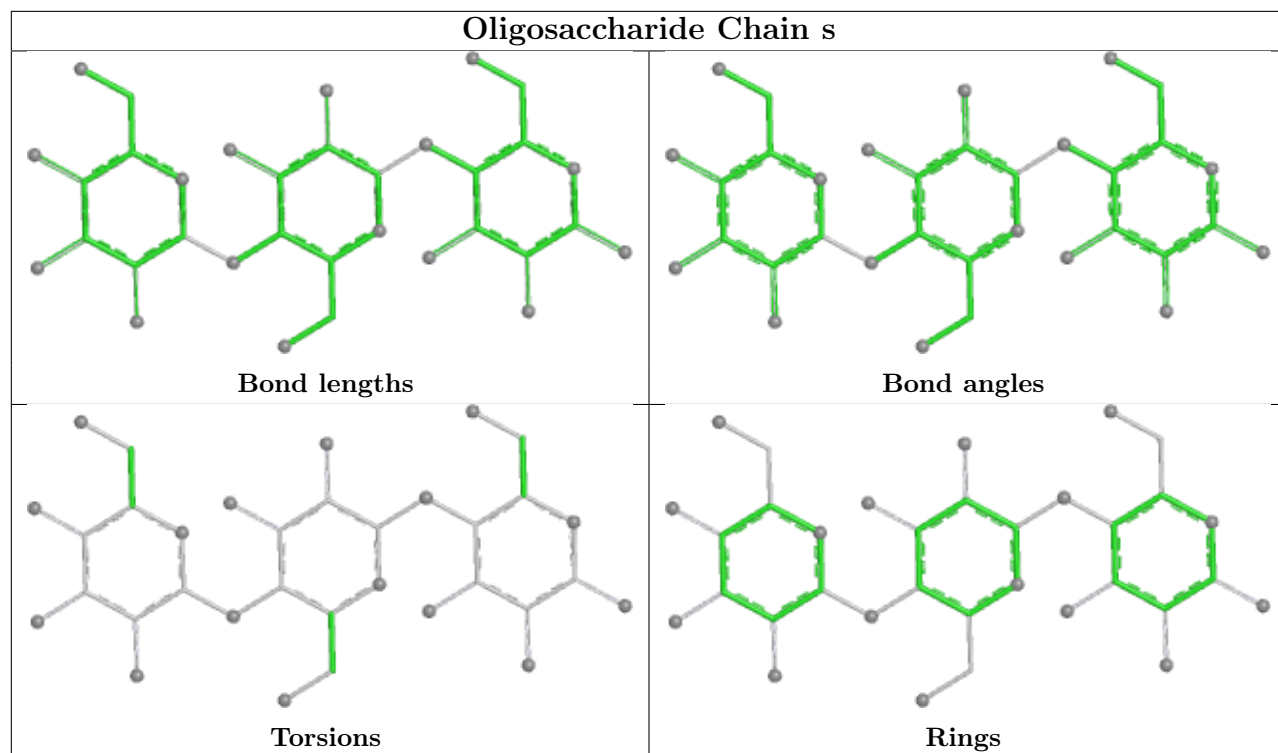


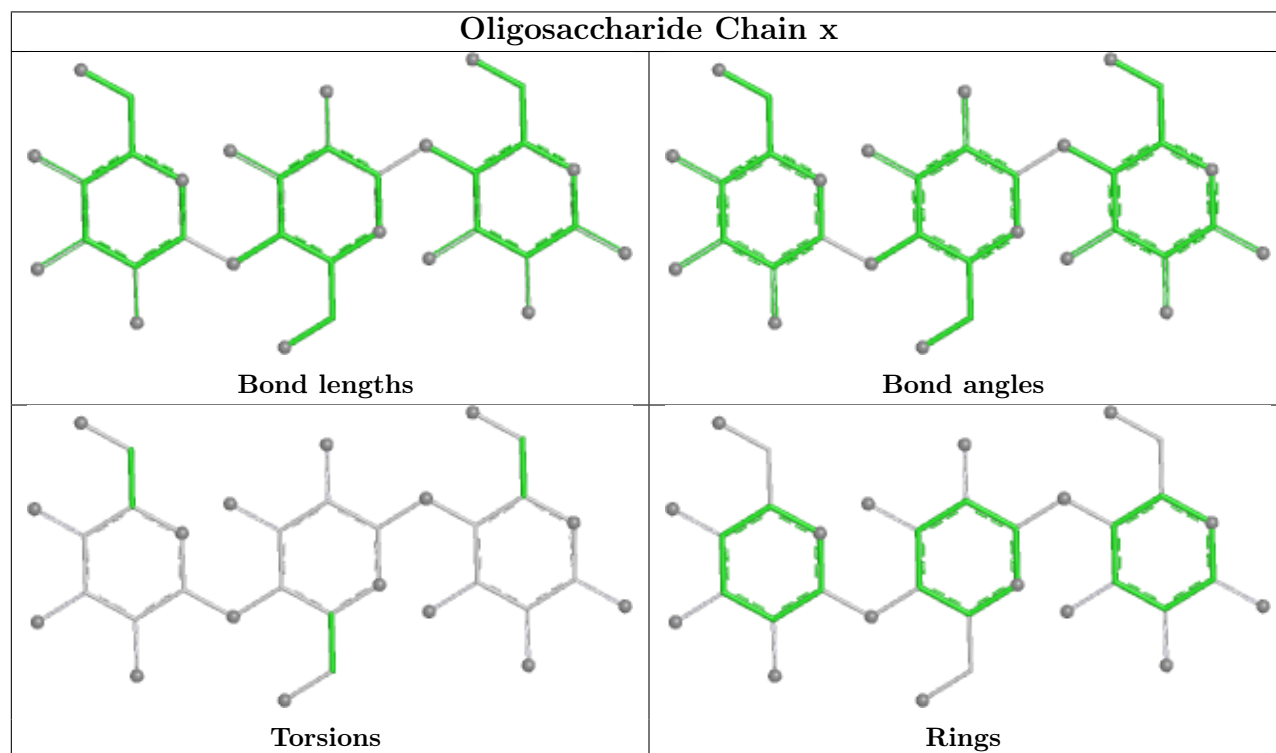
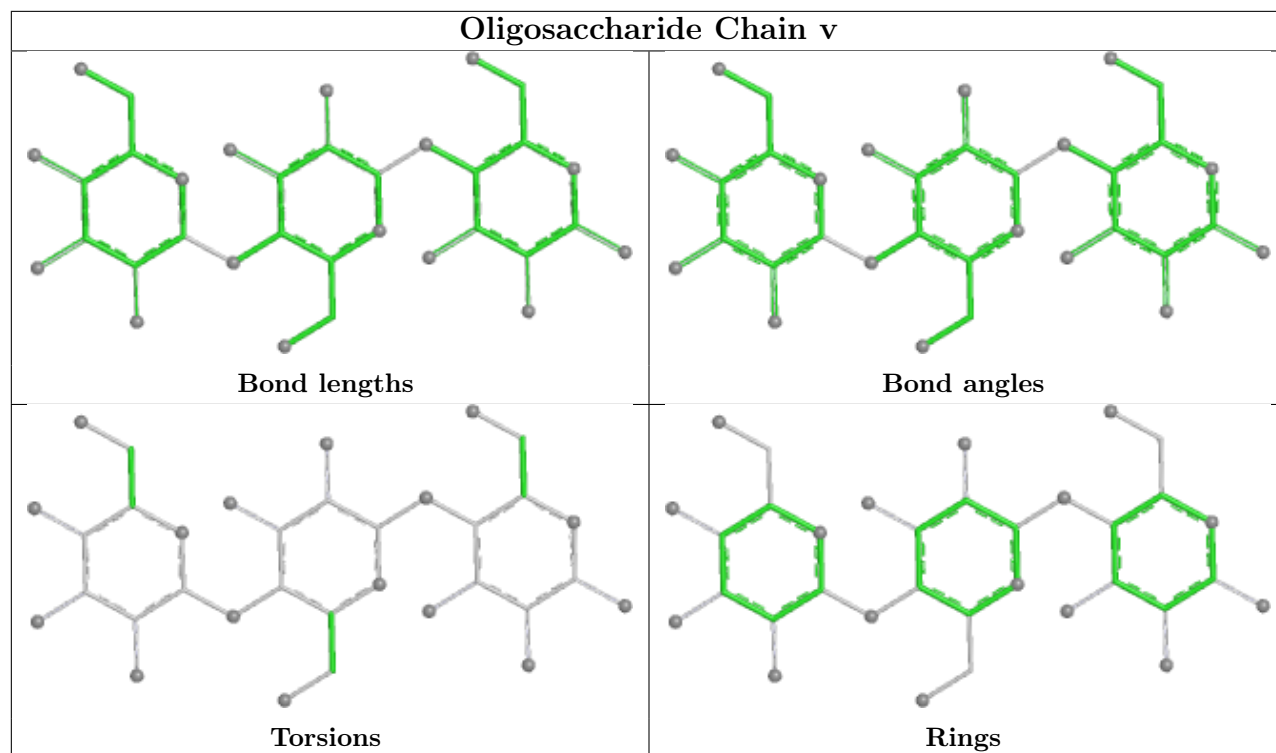


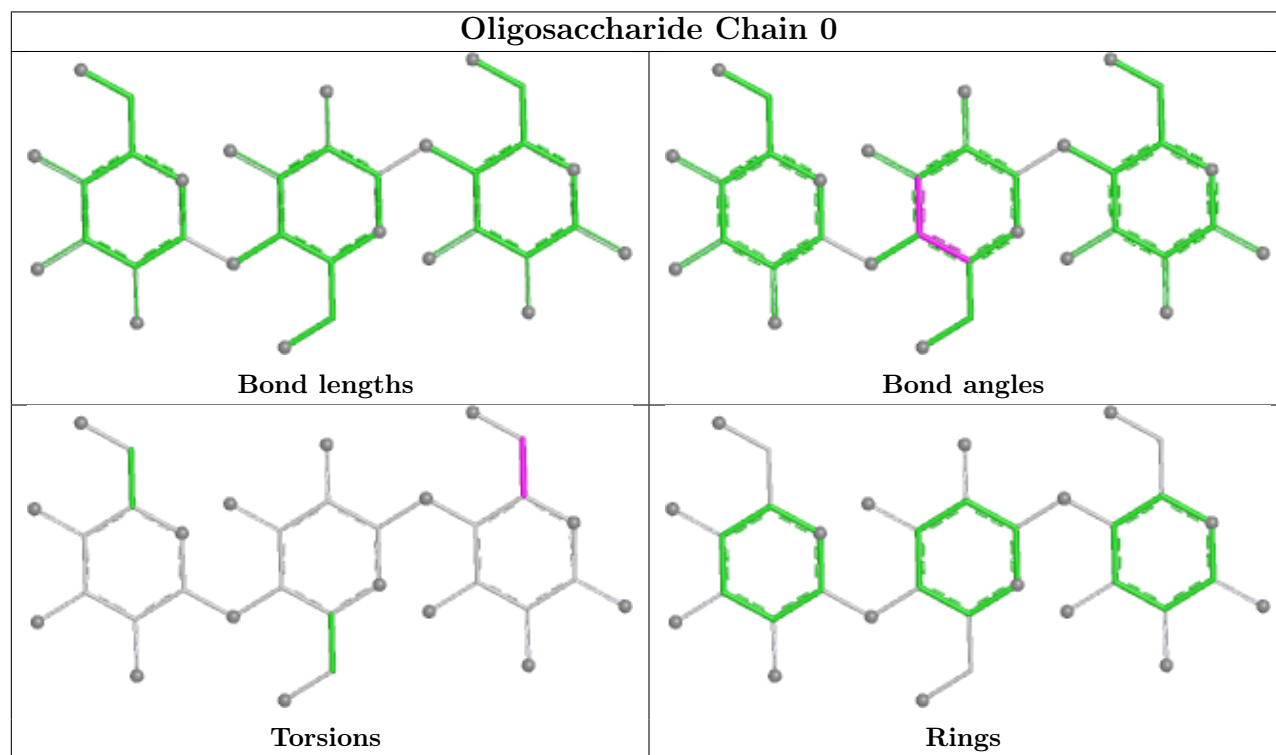
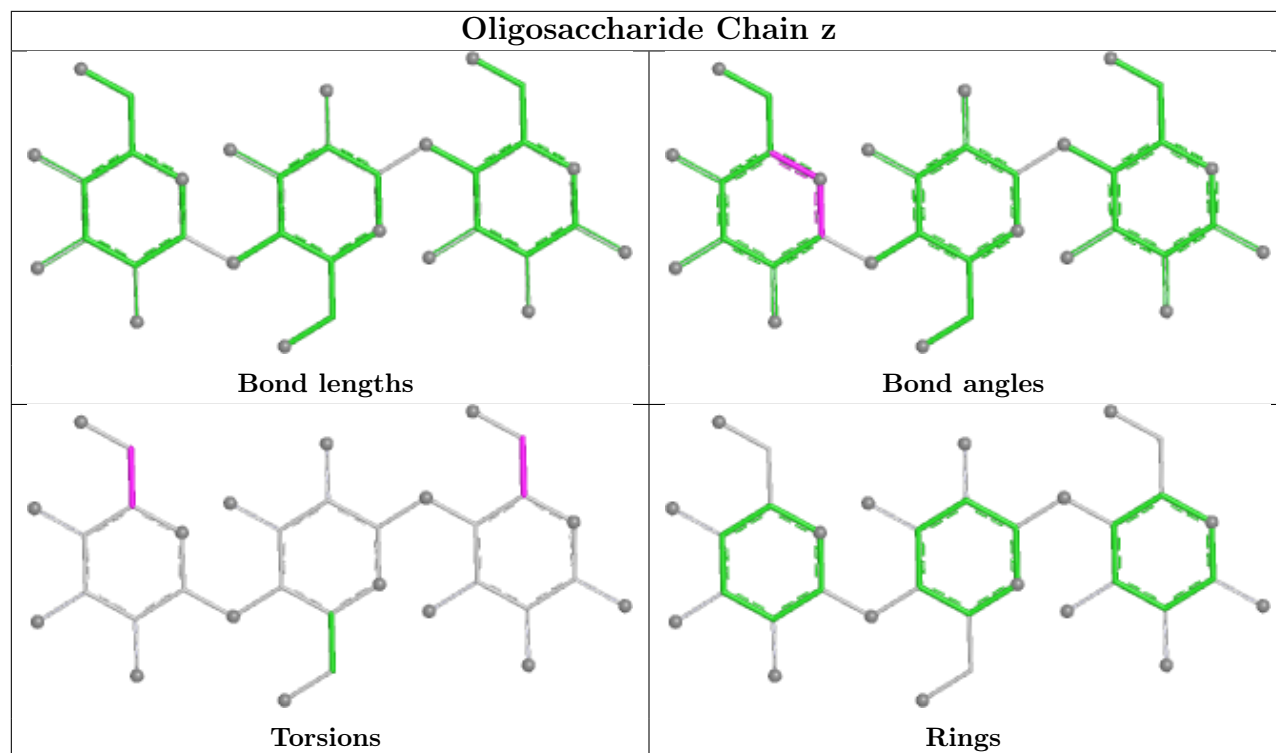


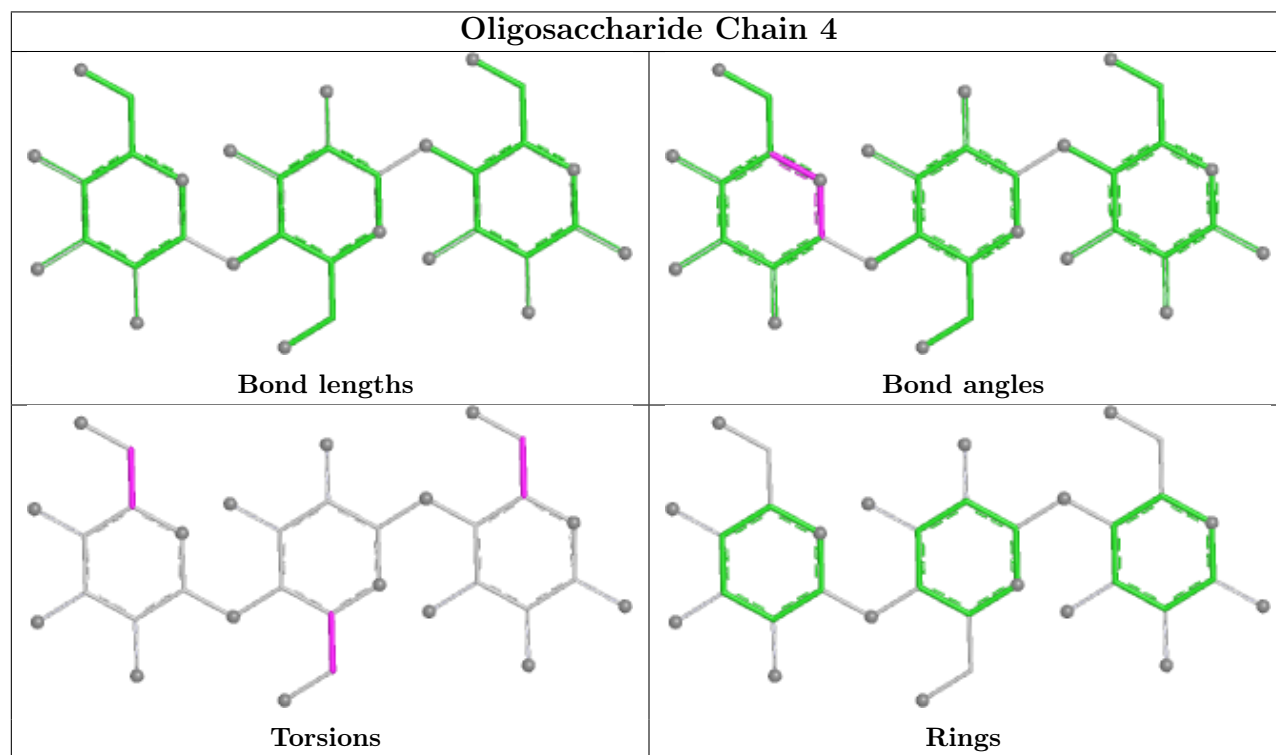
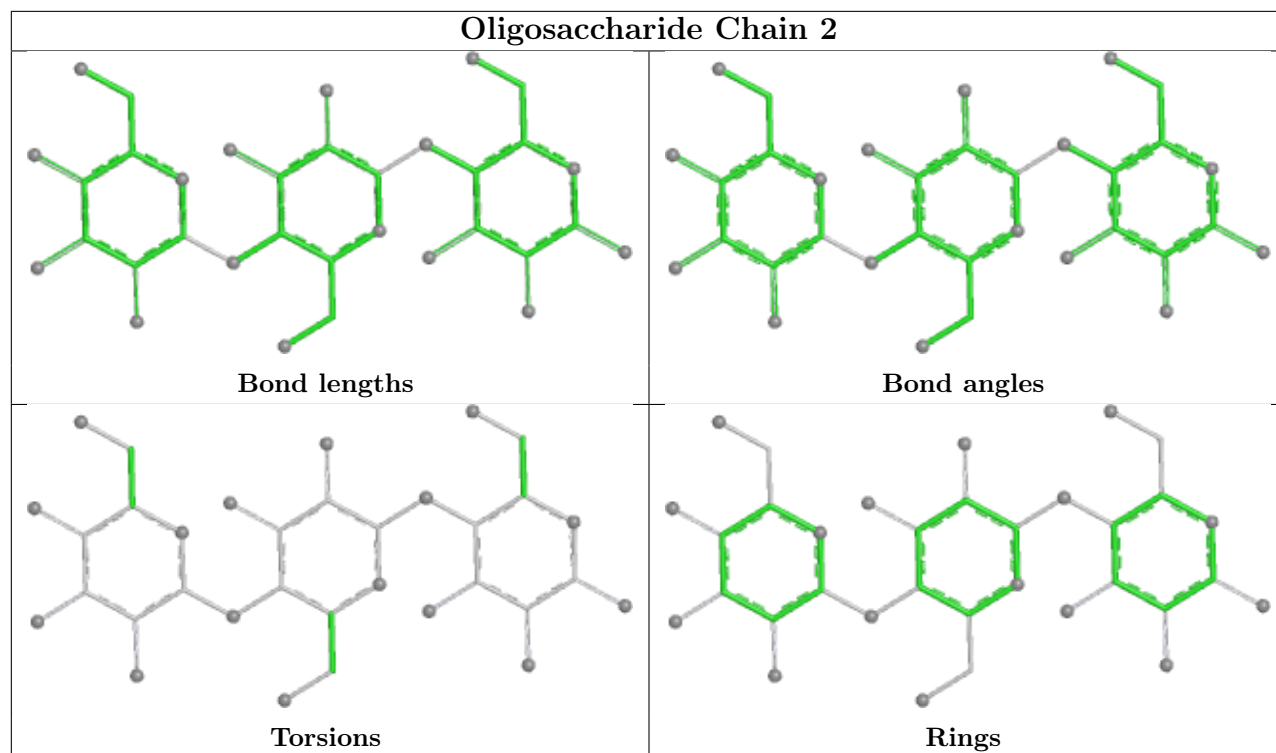




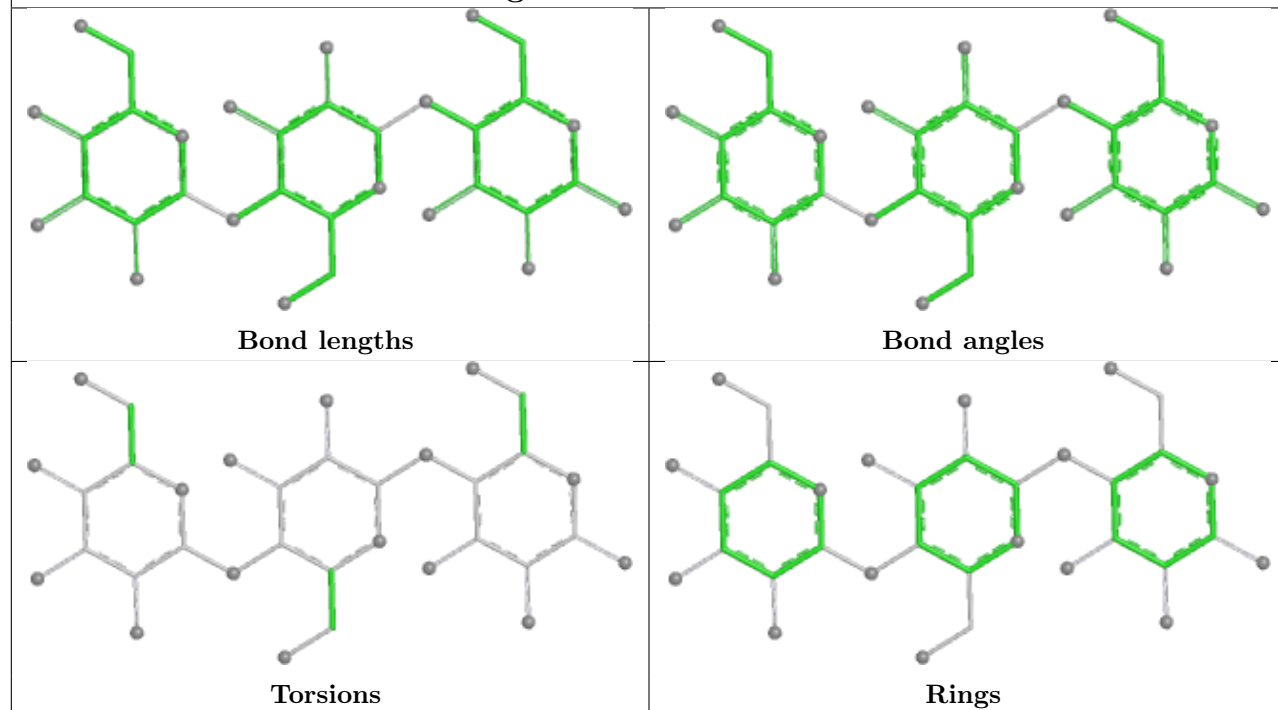




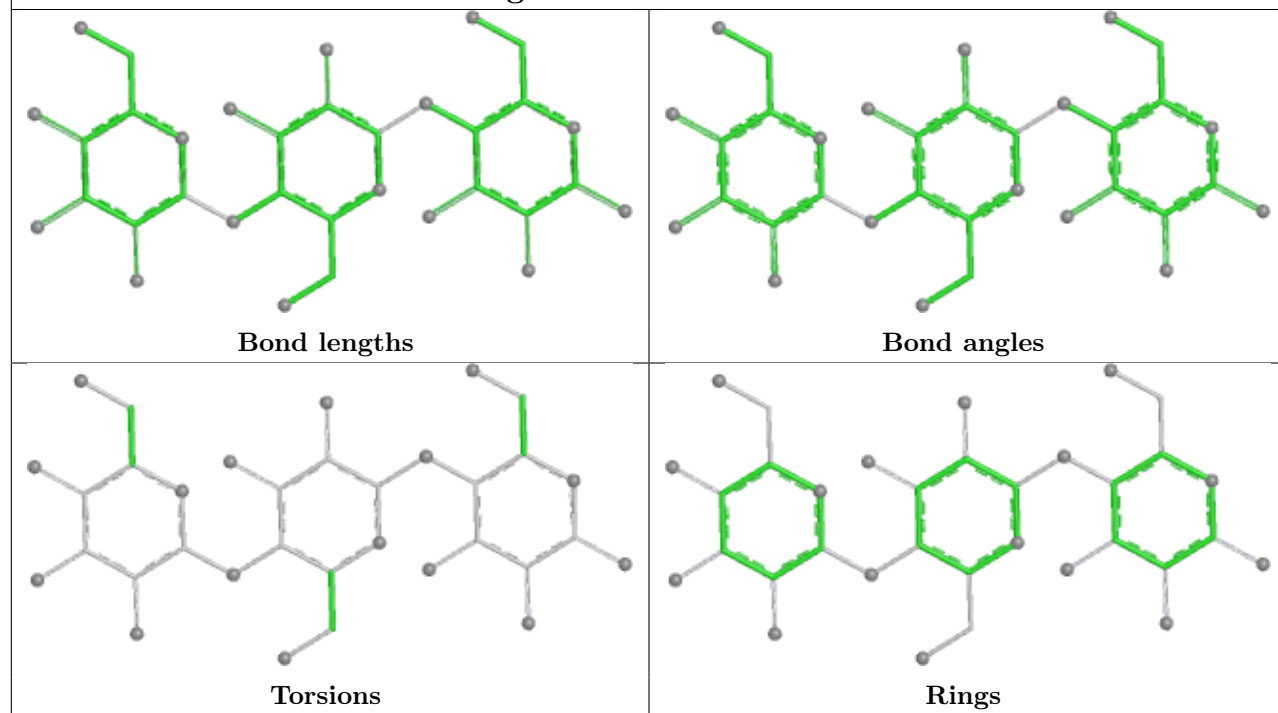


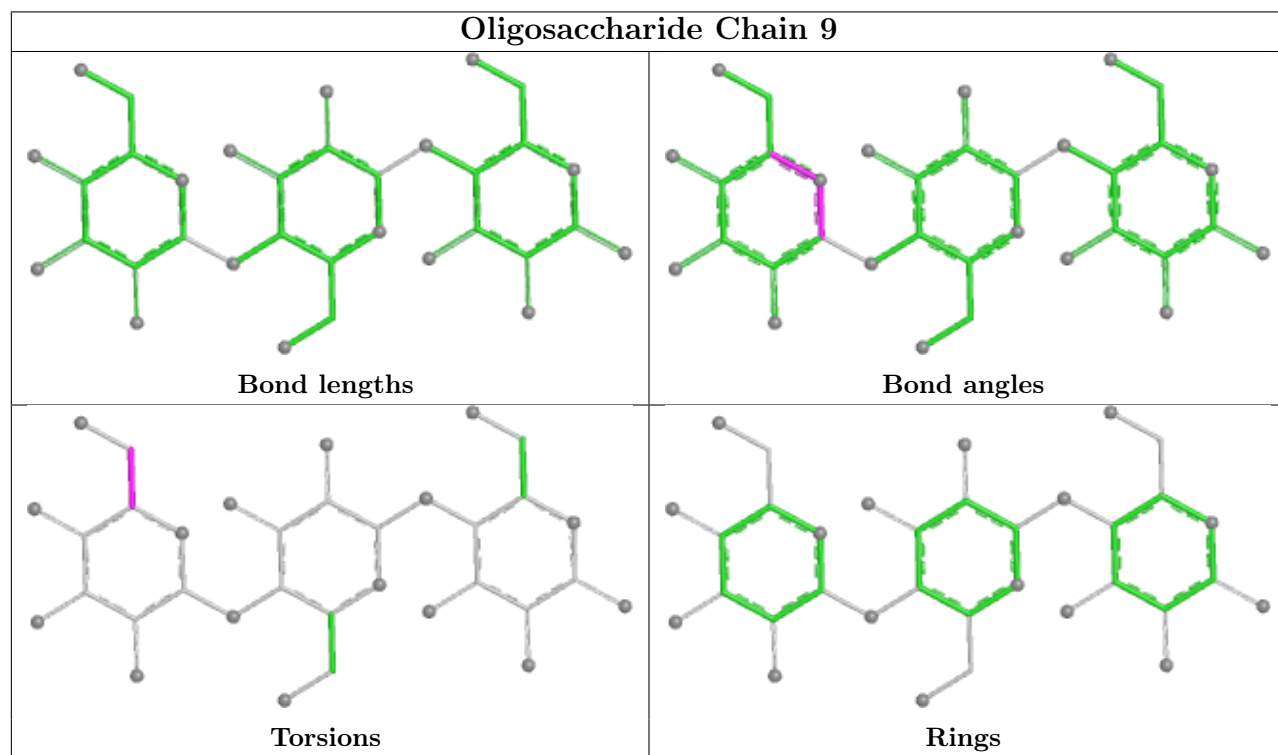
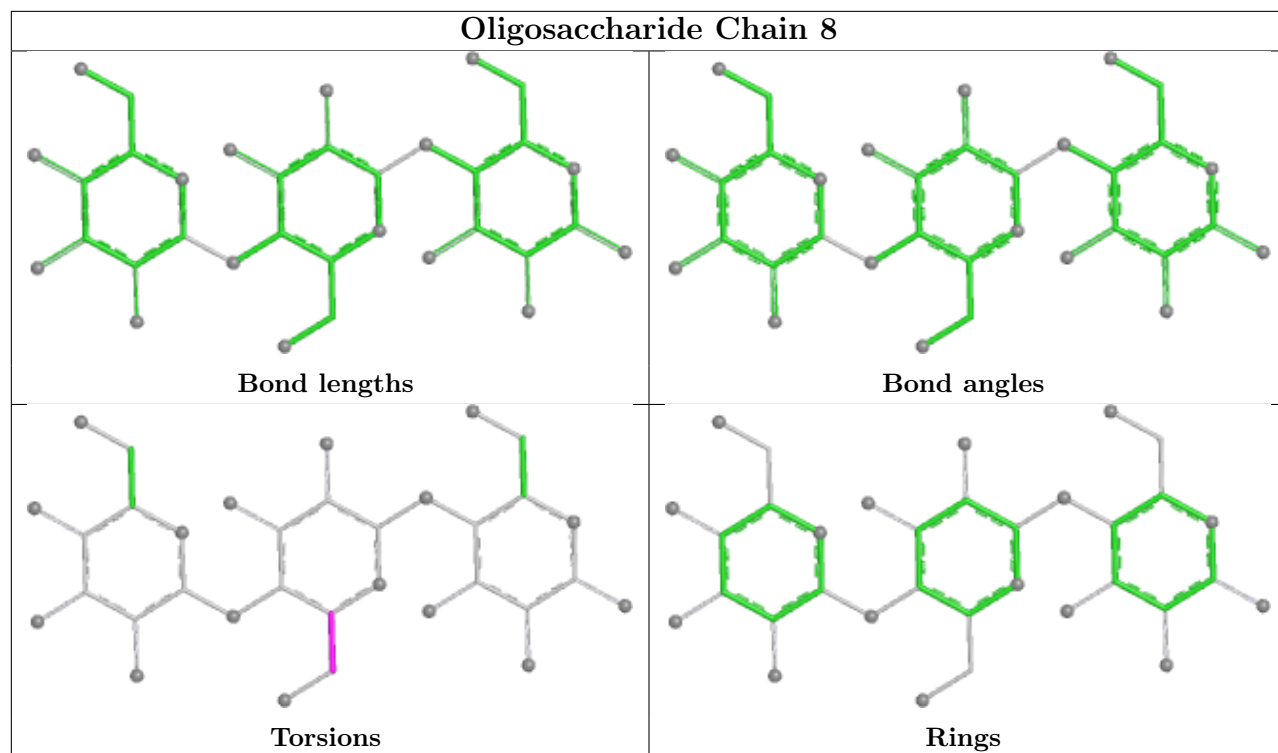


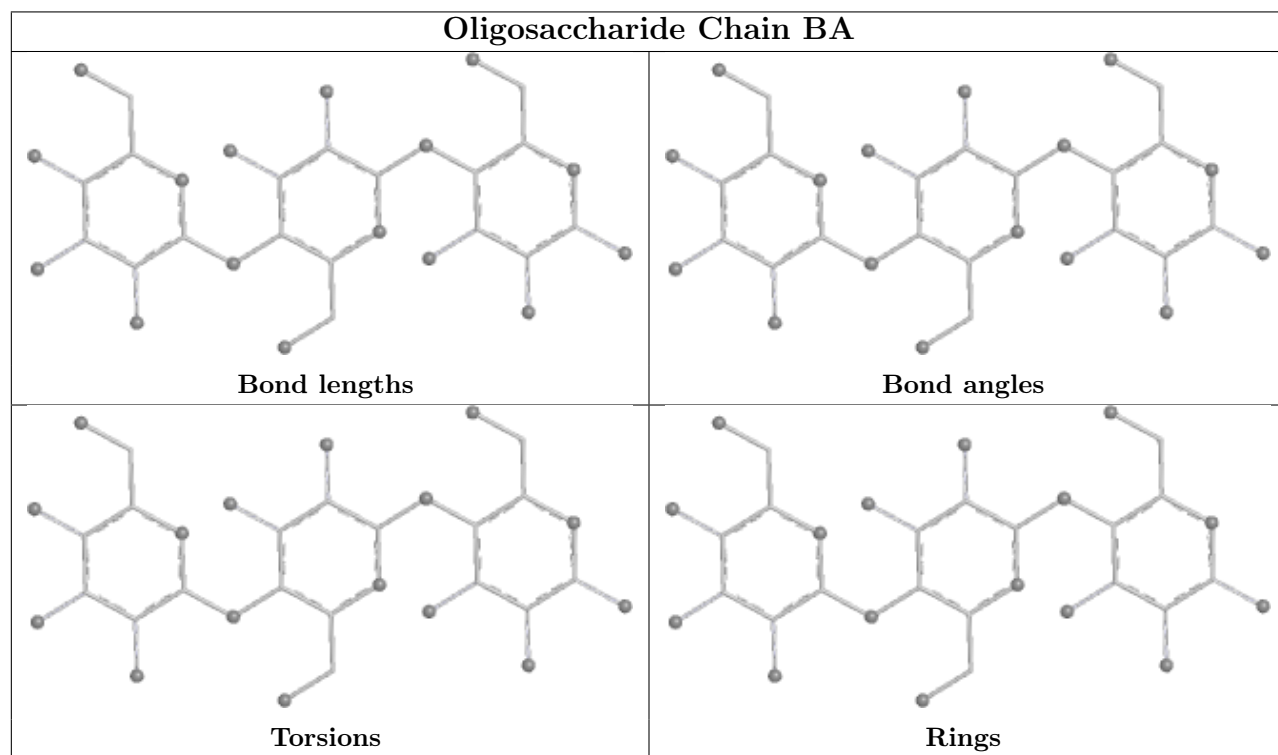
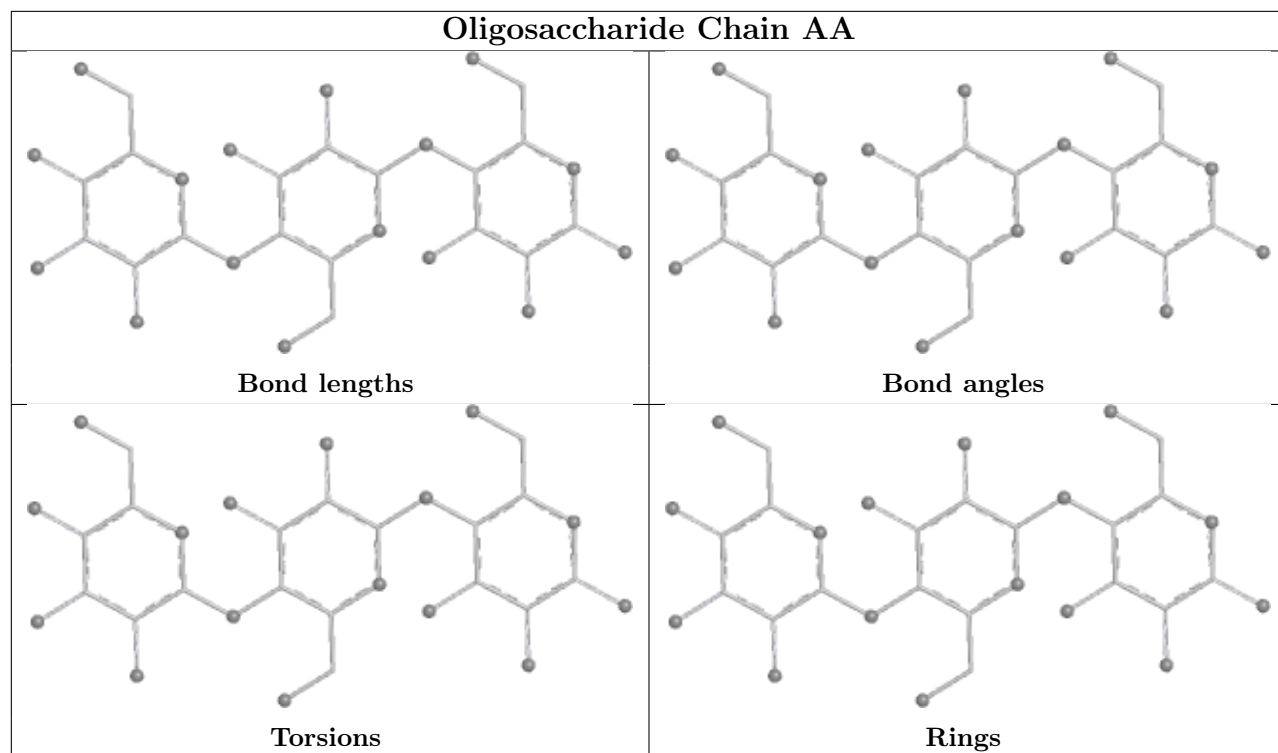
Oligosaccharide Chain 5

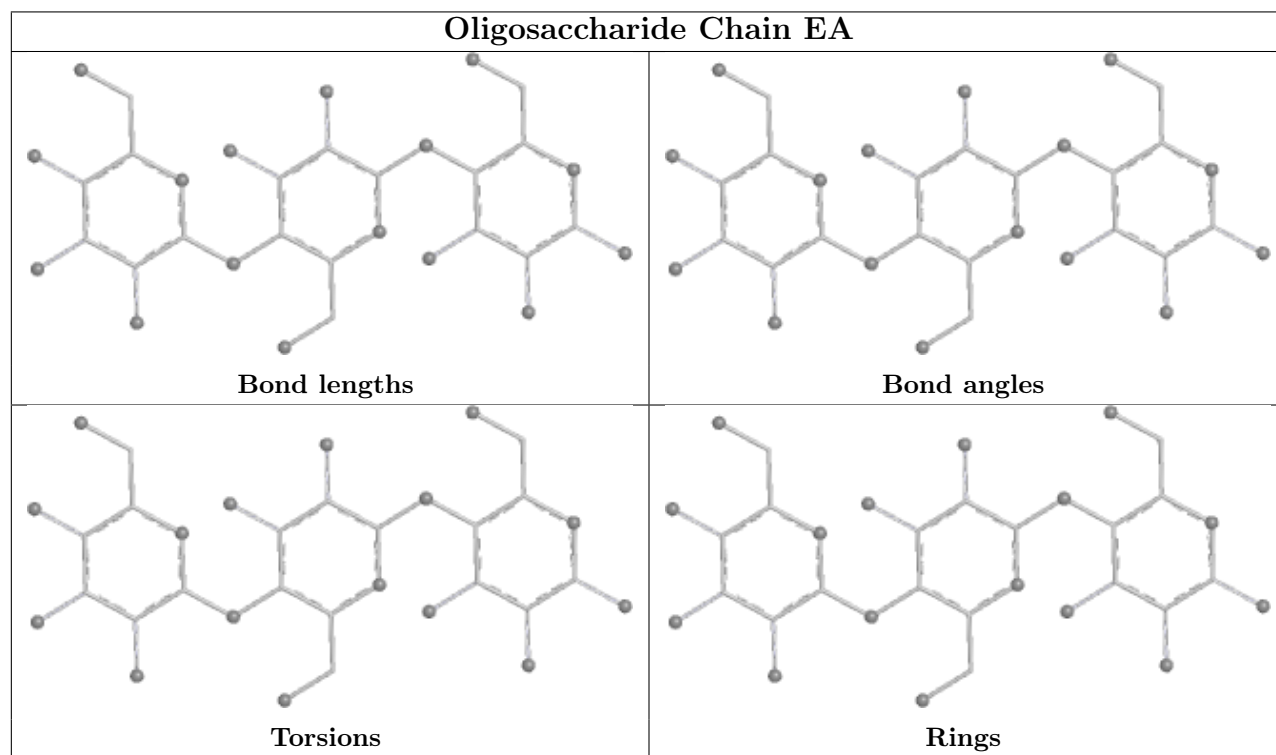
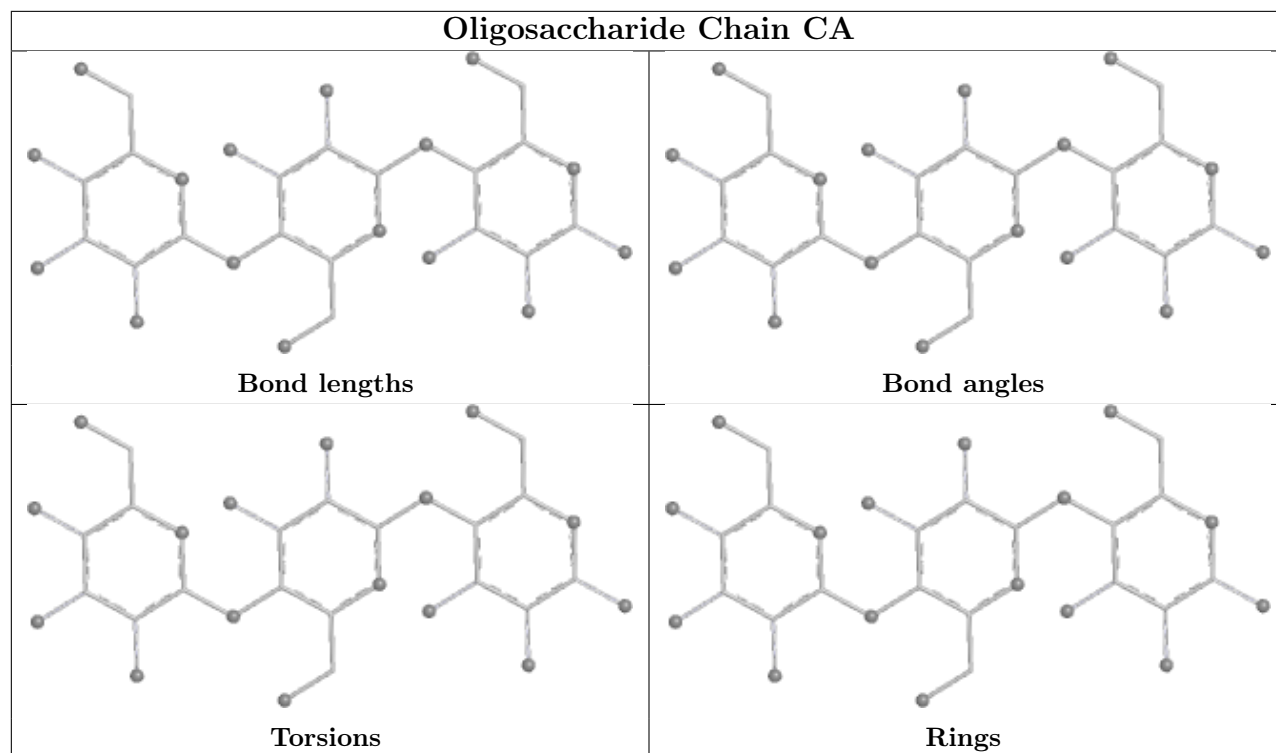


Oligosaccharide Chain 7

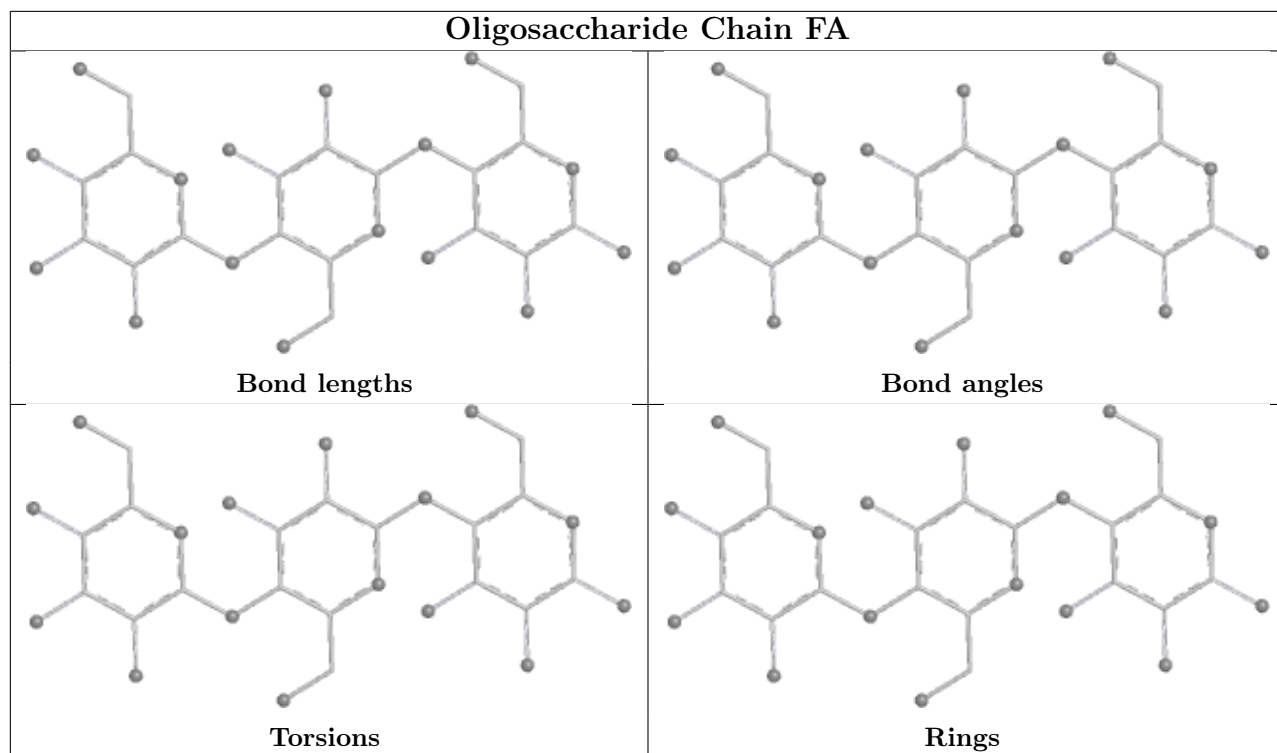




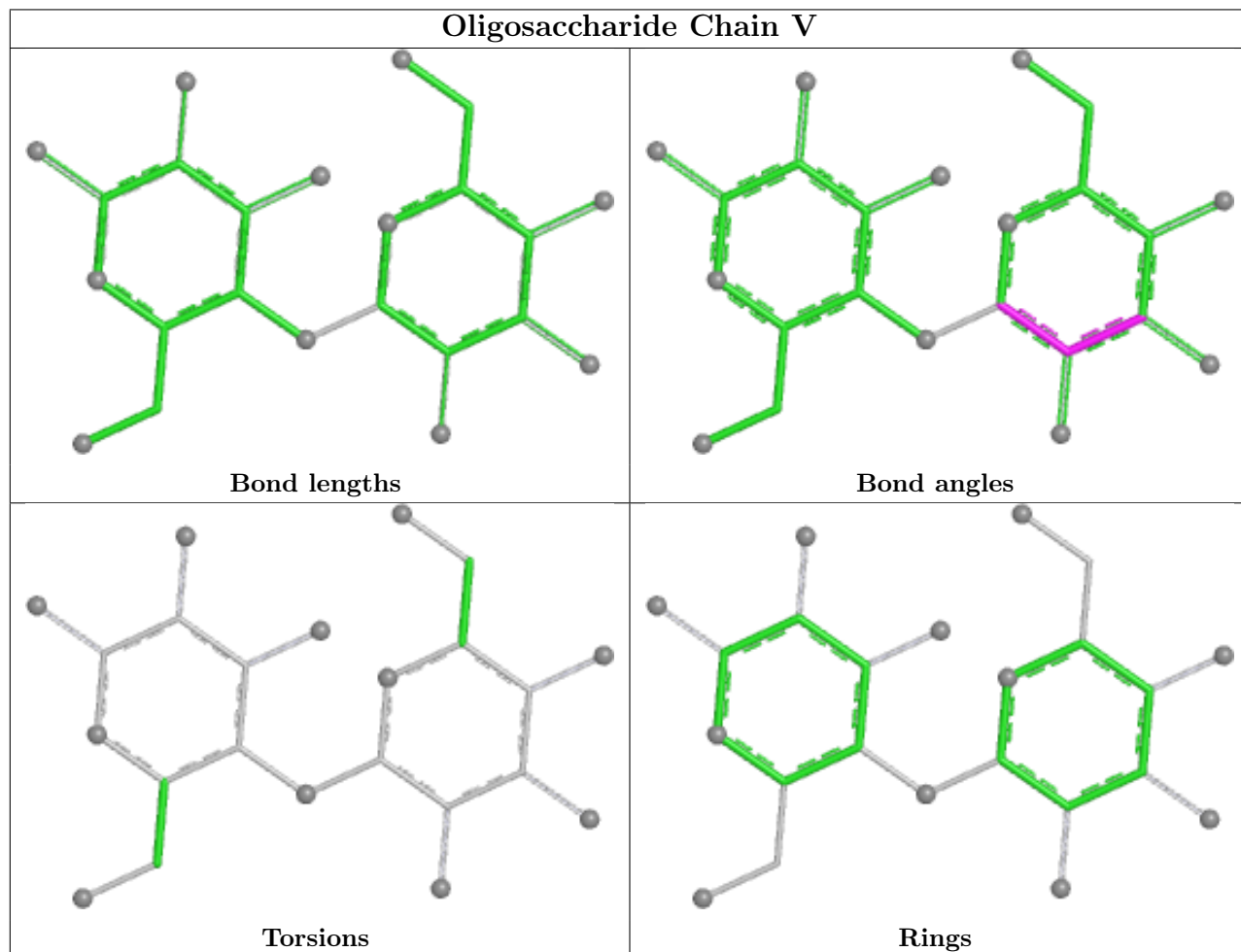


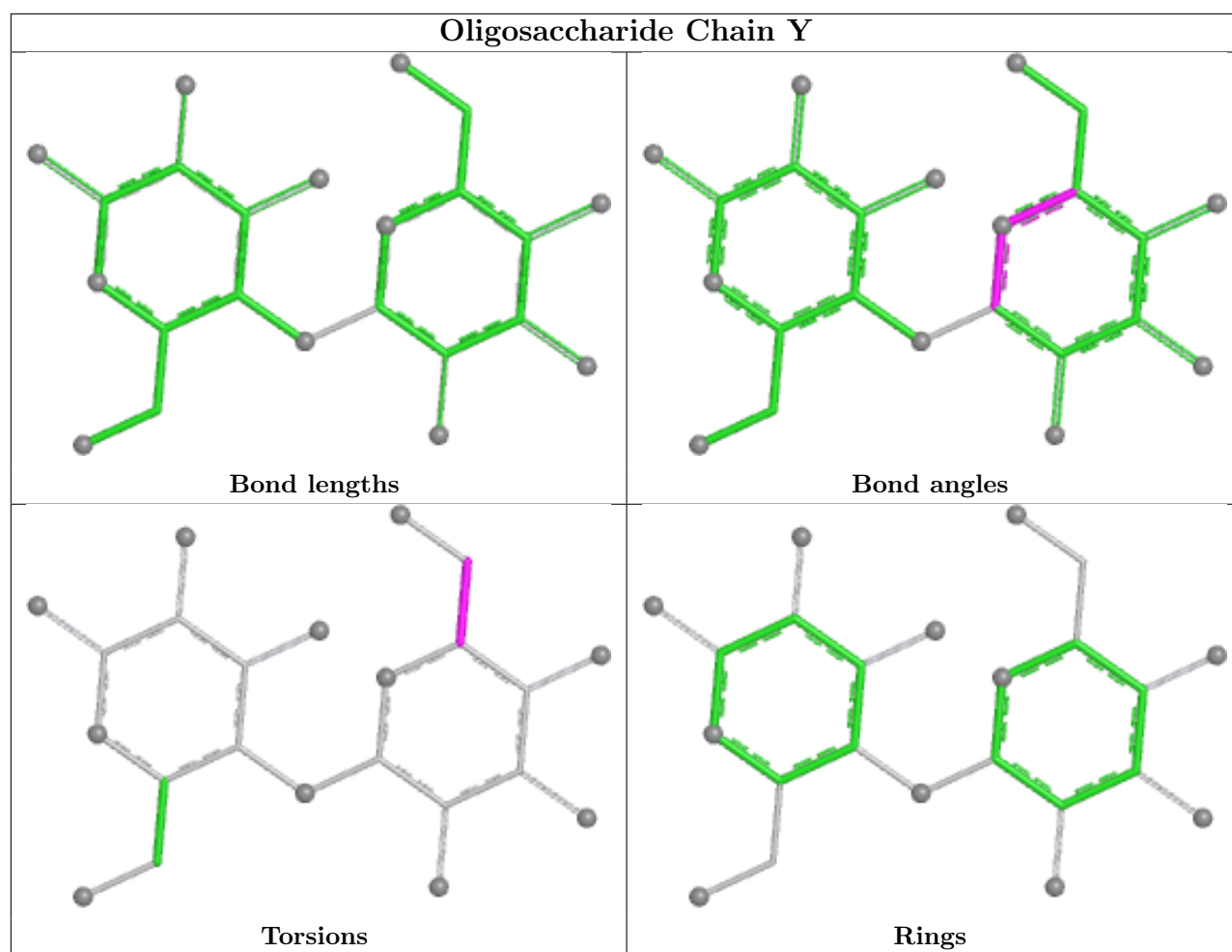


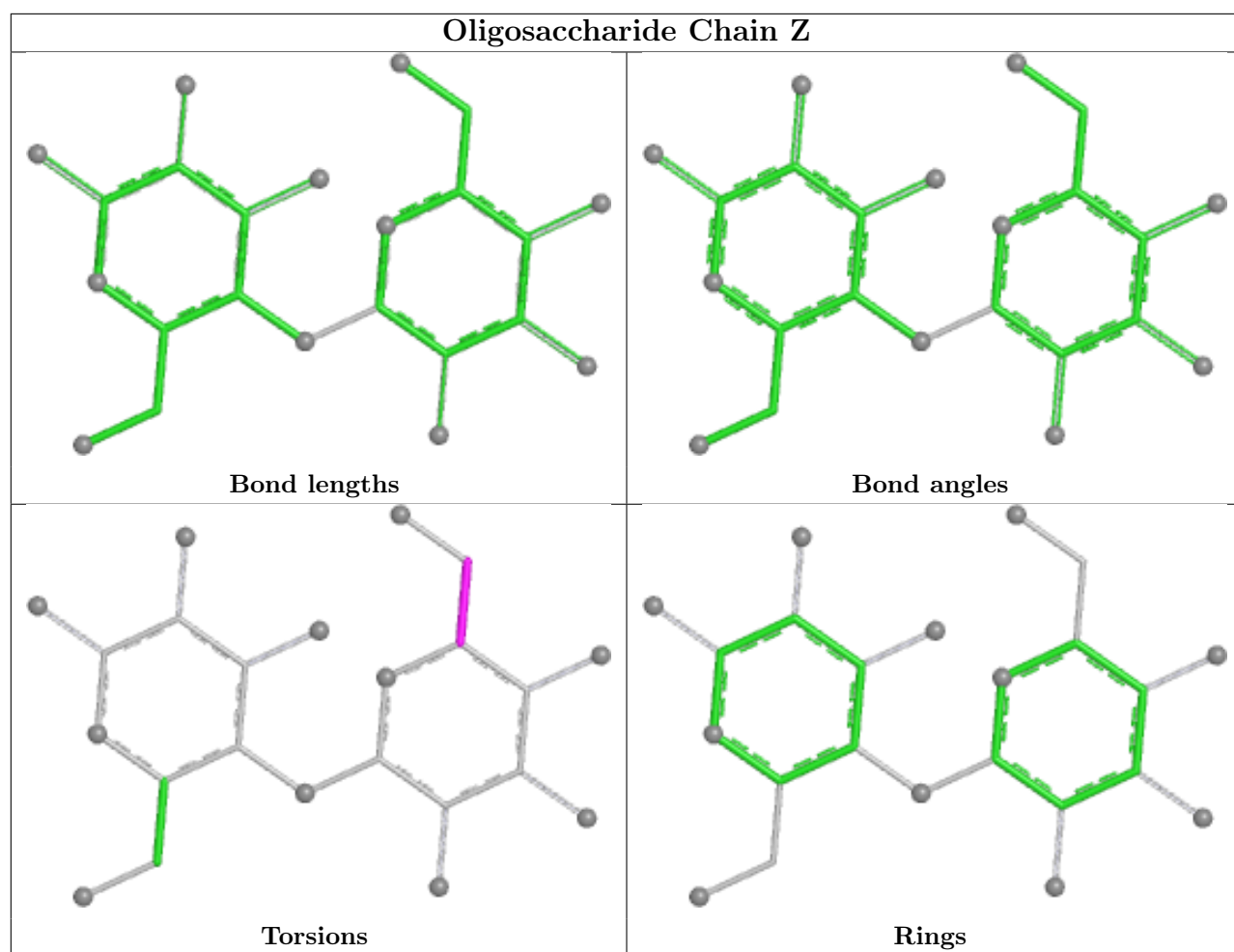
Oligosaccharide Chain FA

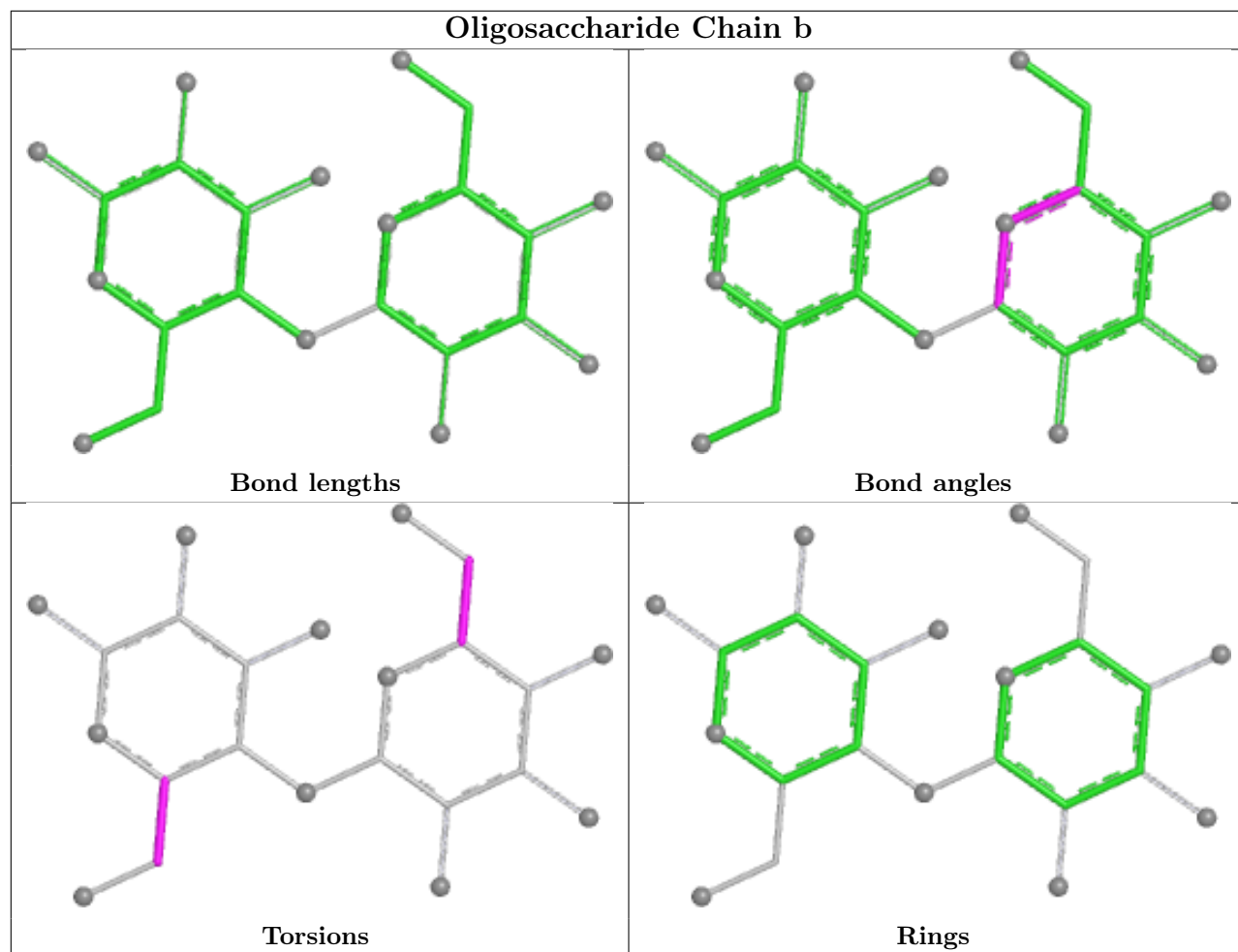


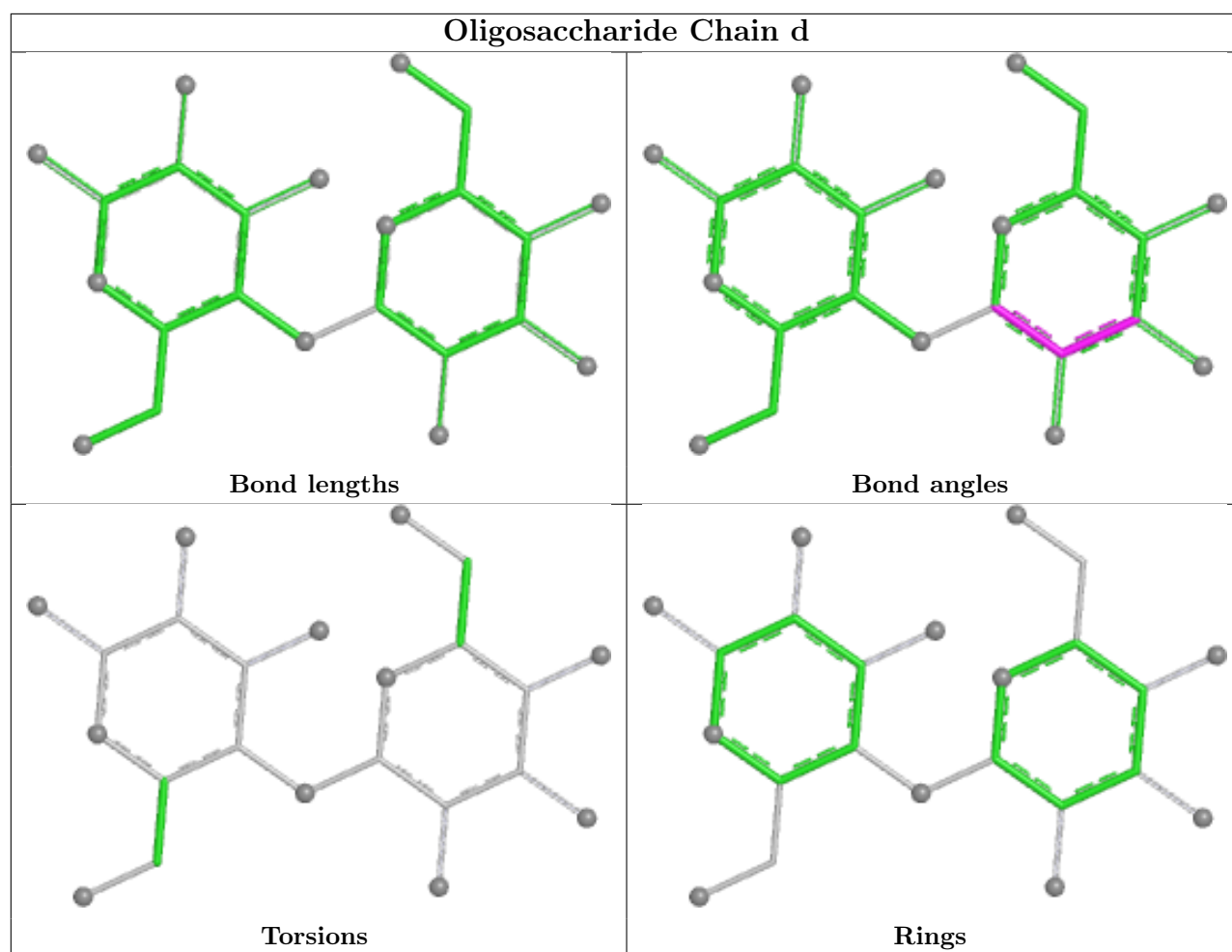
Oligosaccharide Chain V

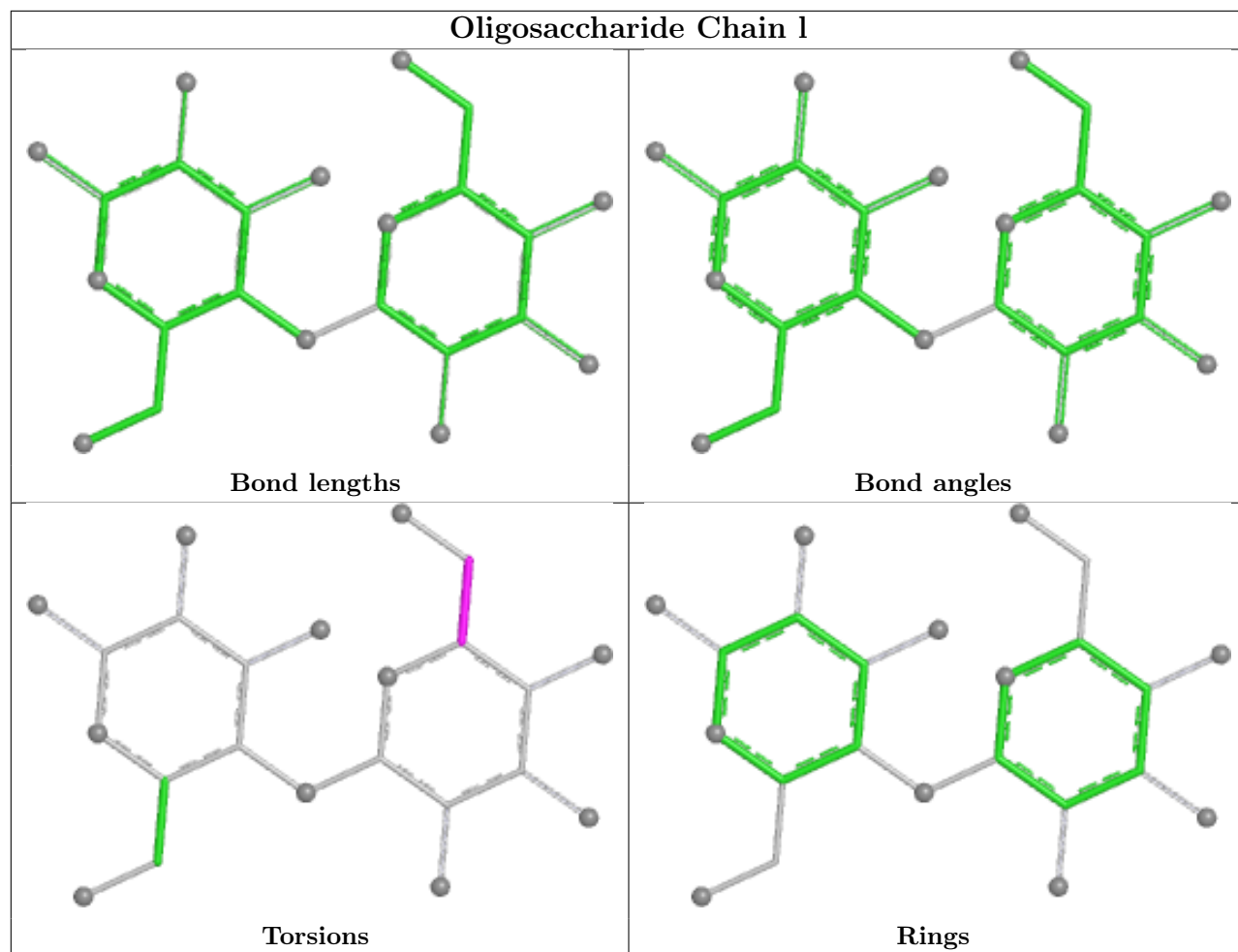


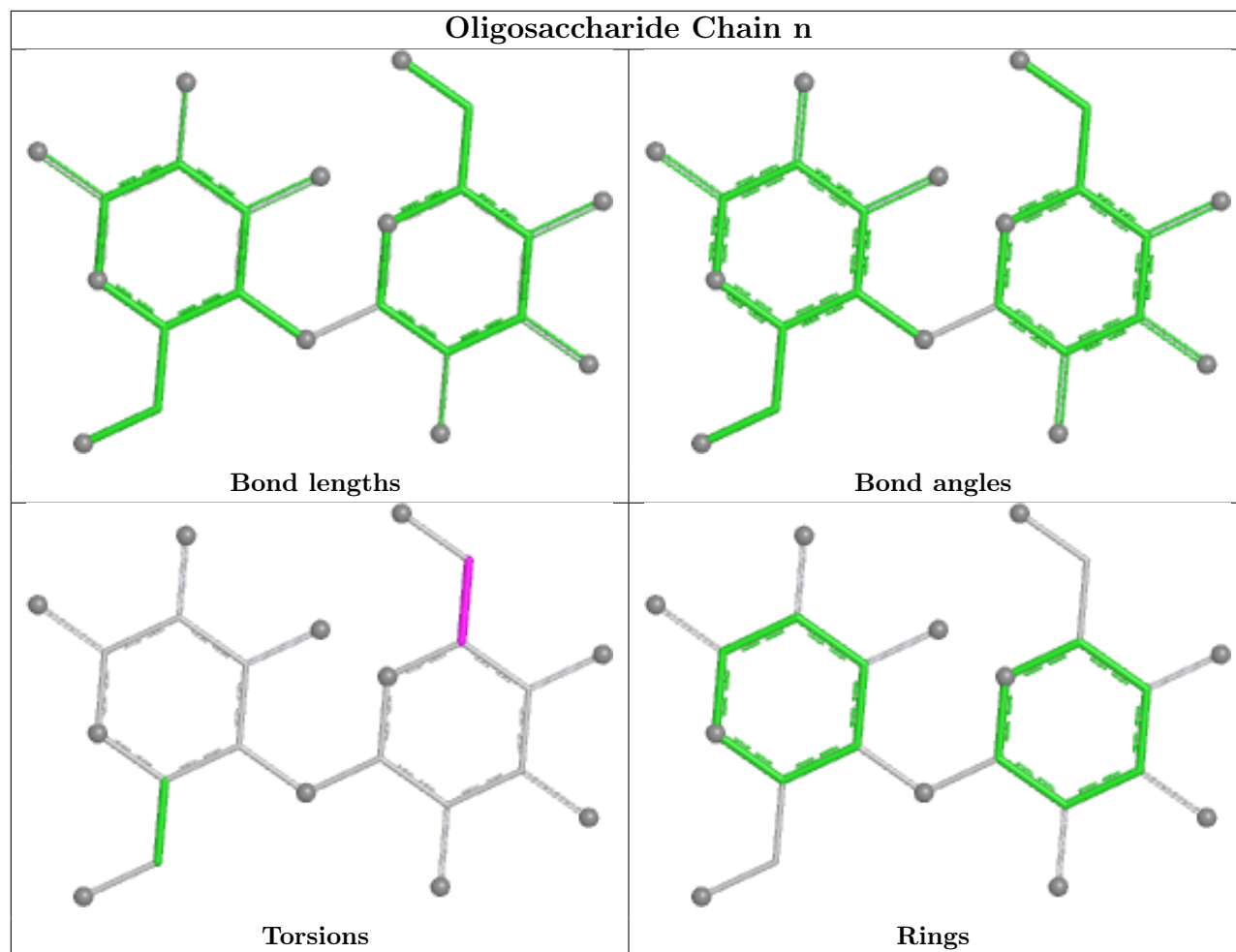


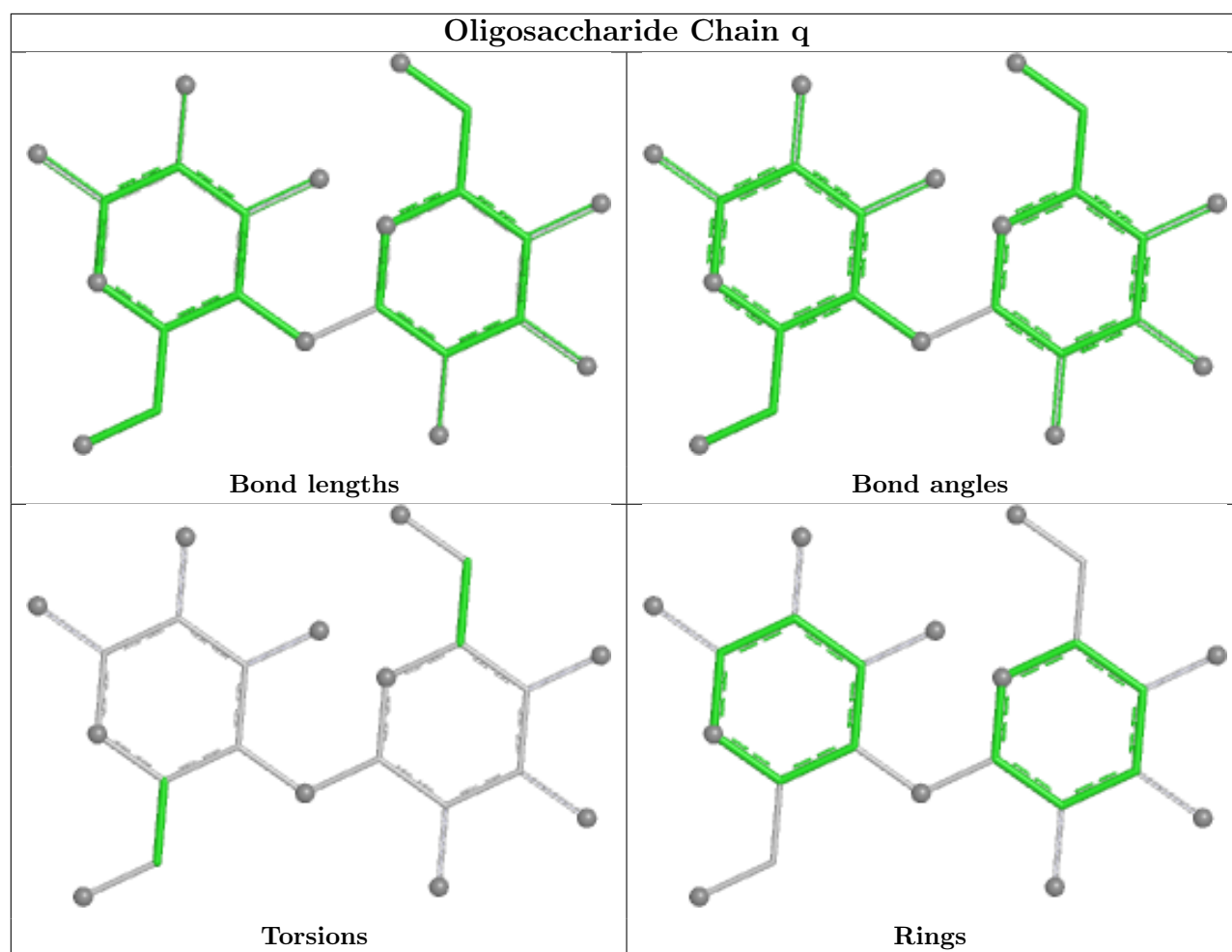


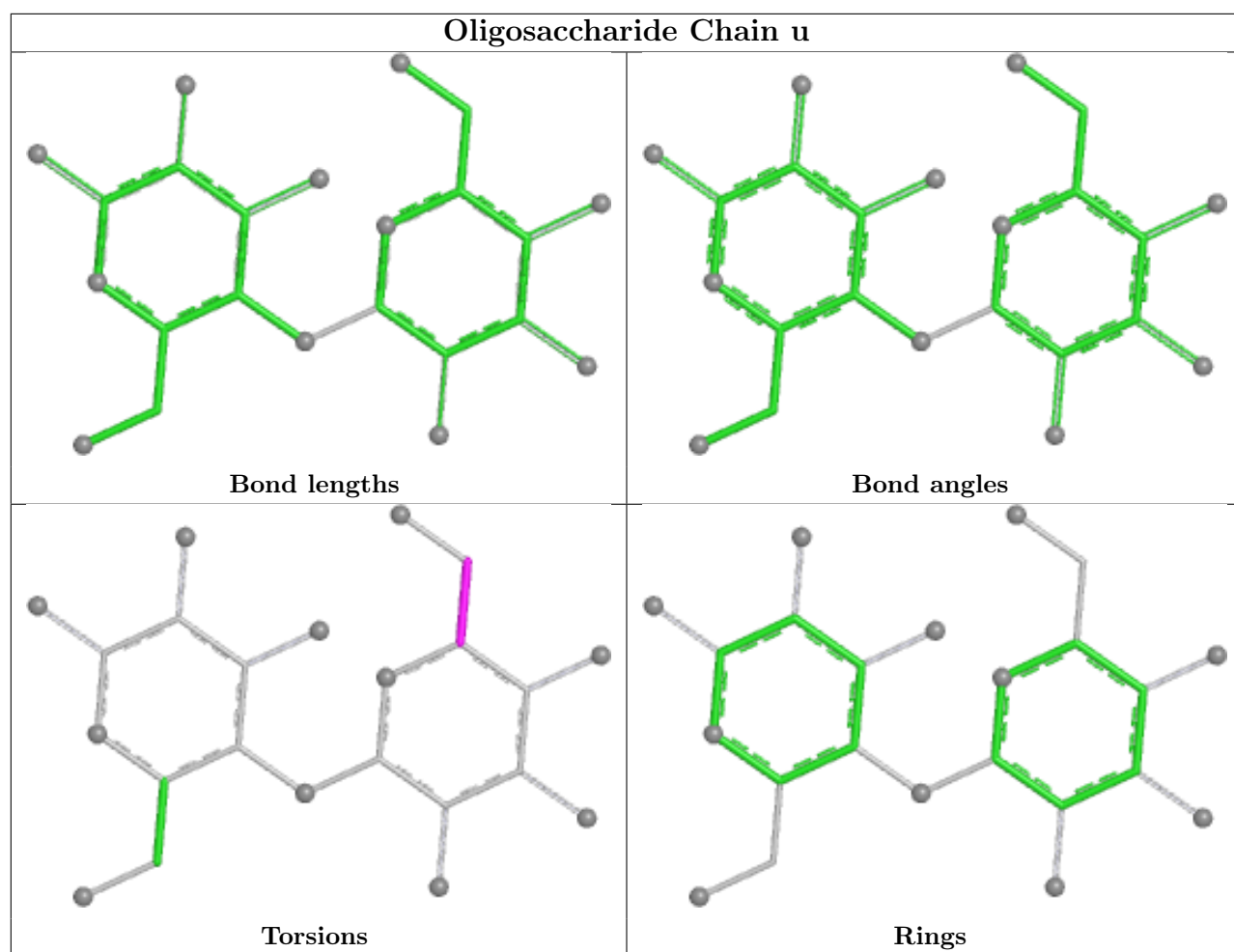


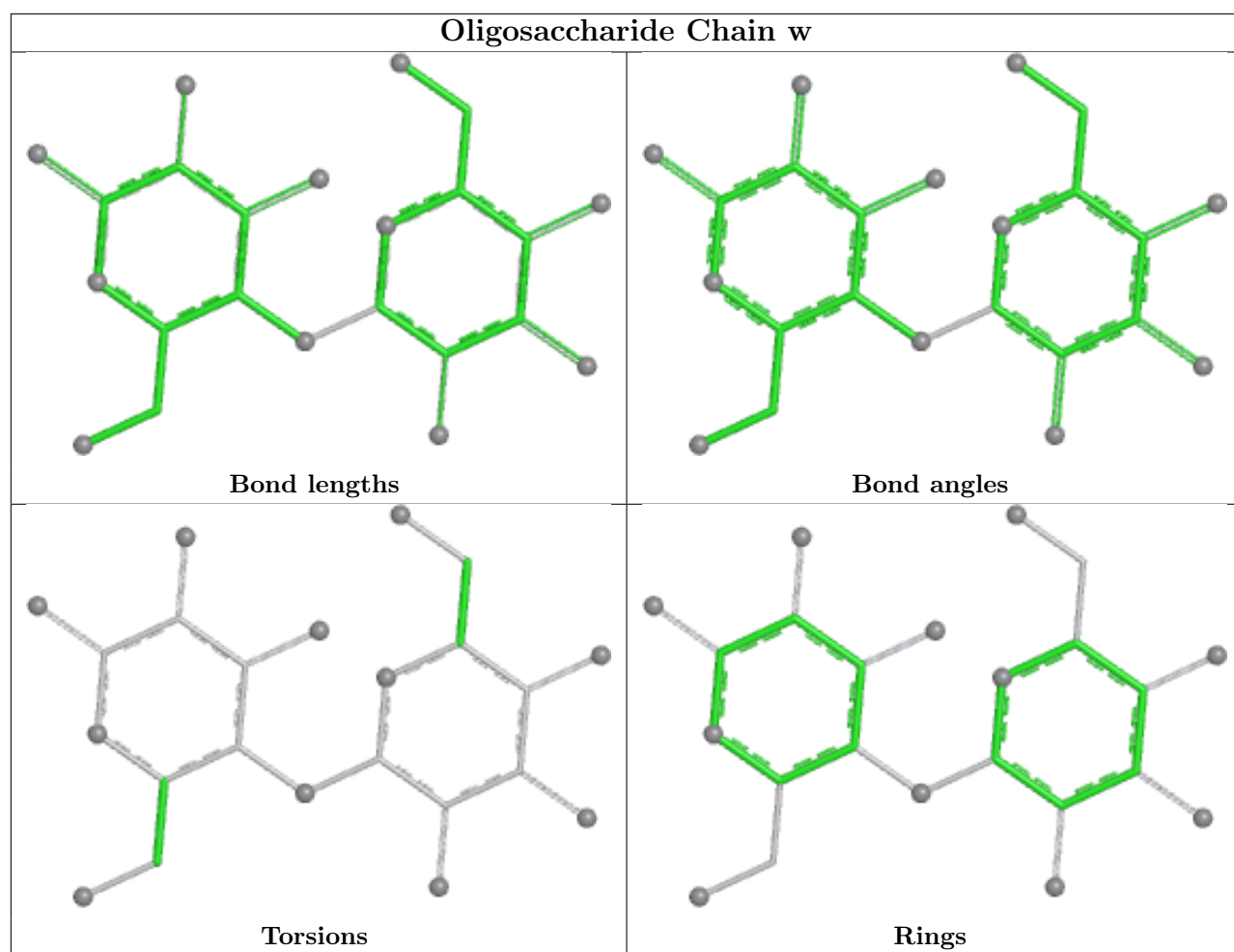


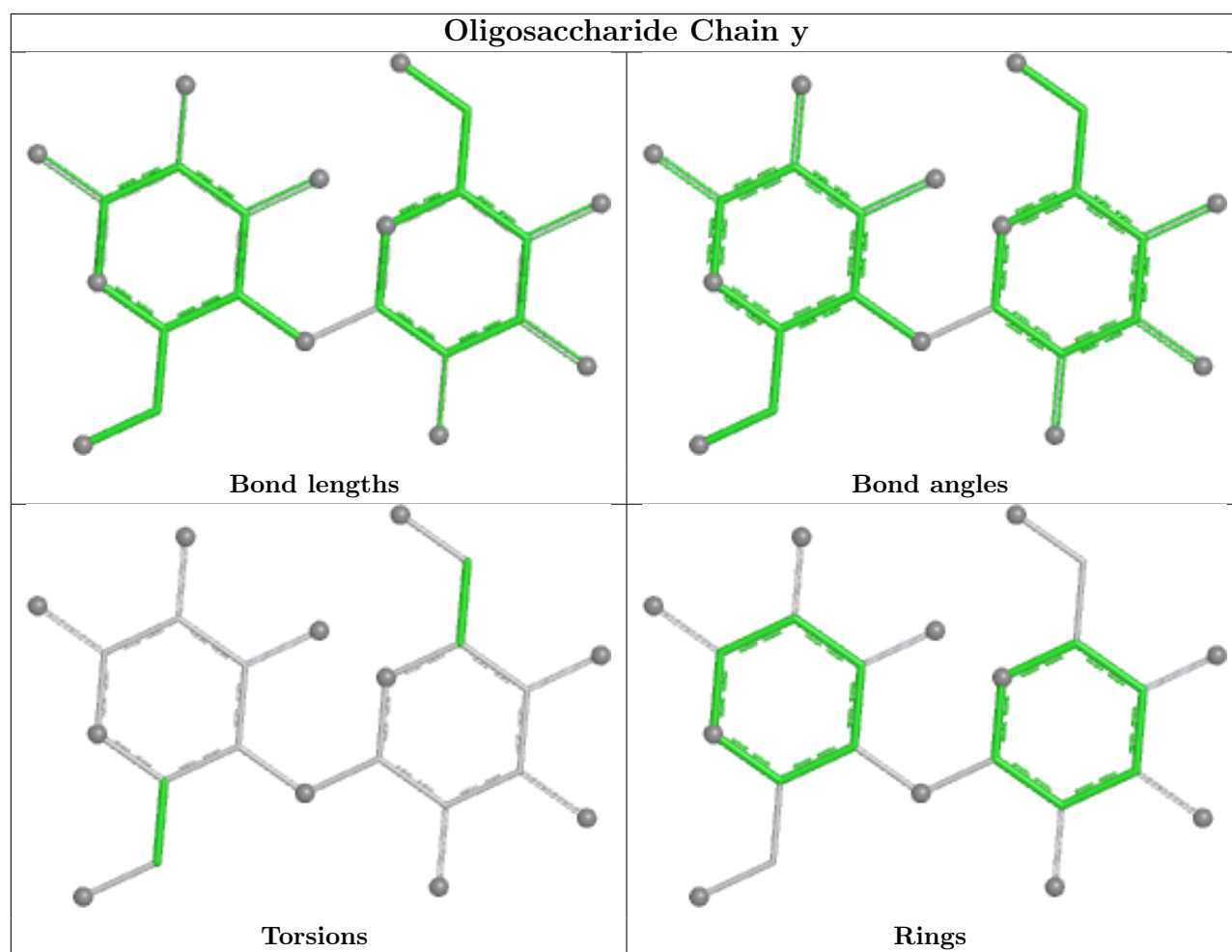


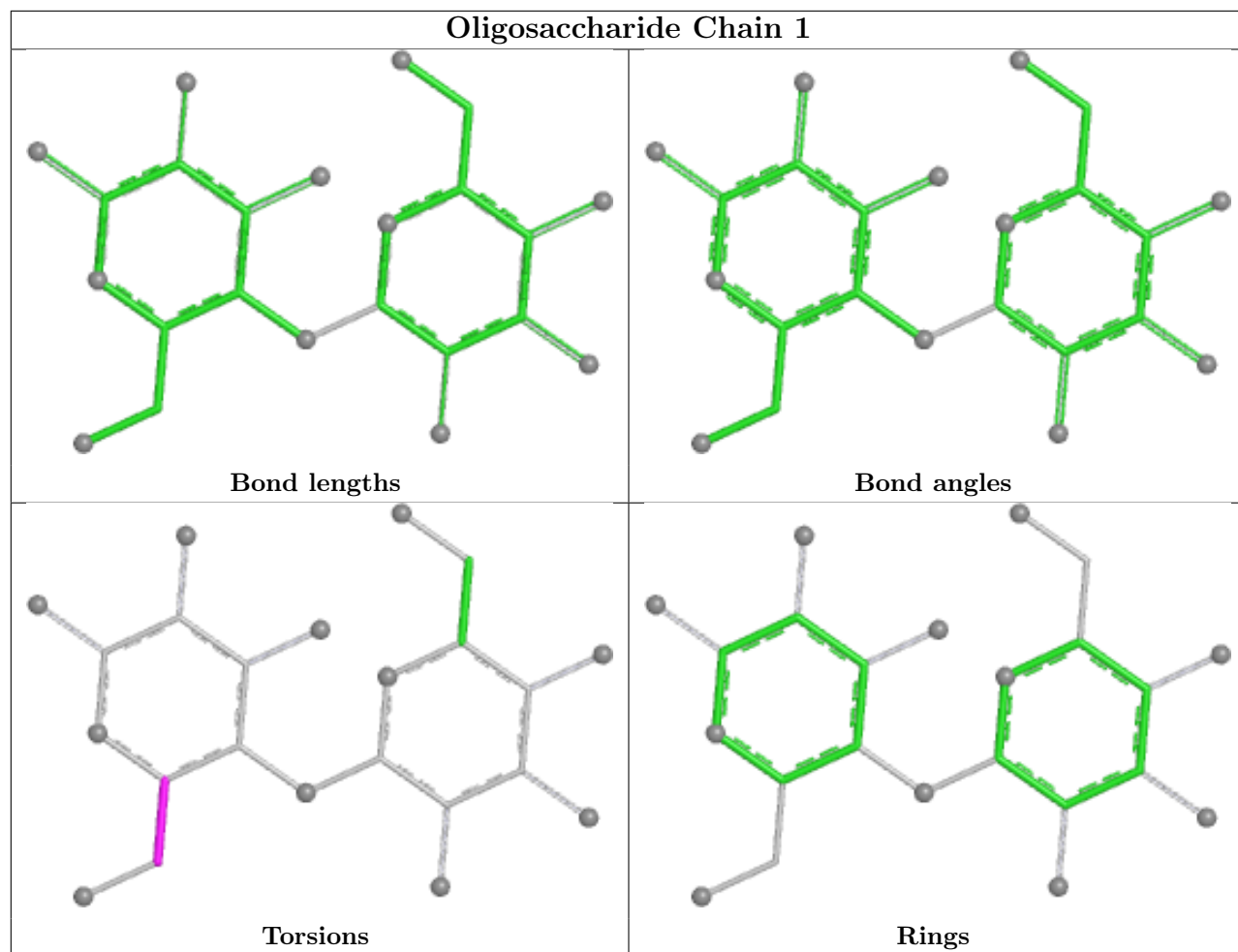


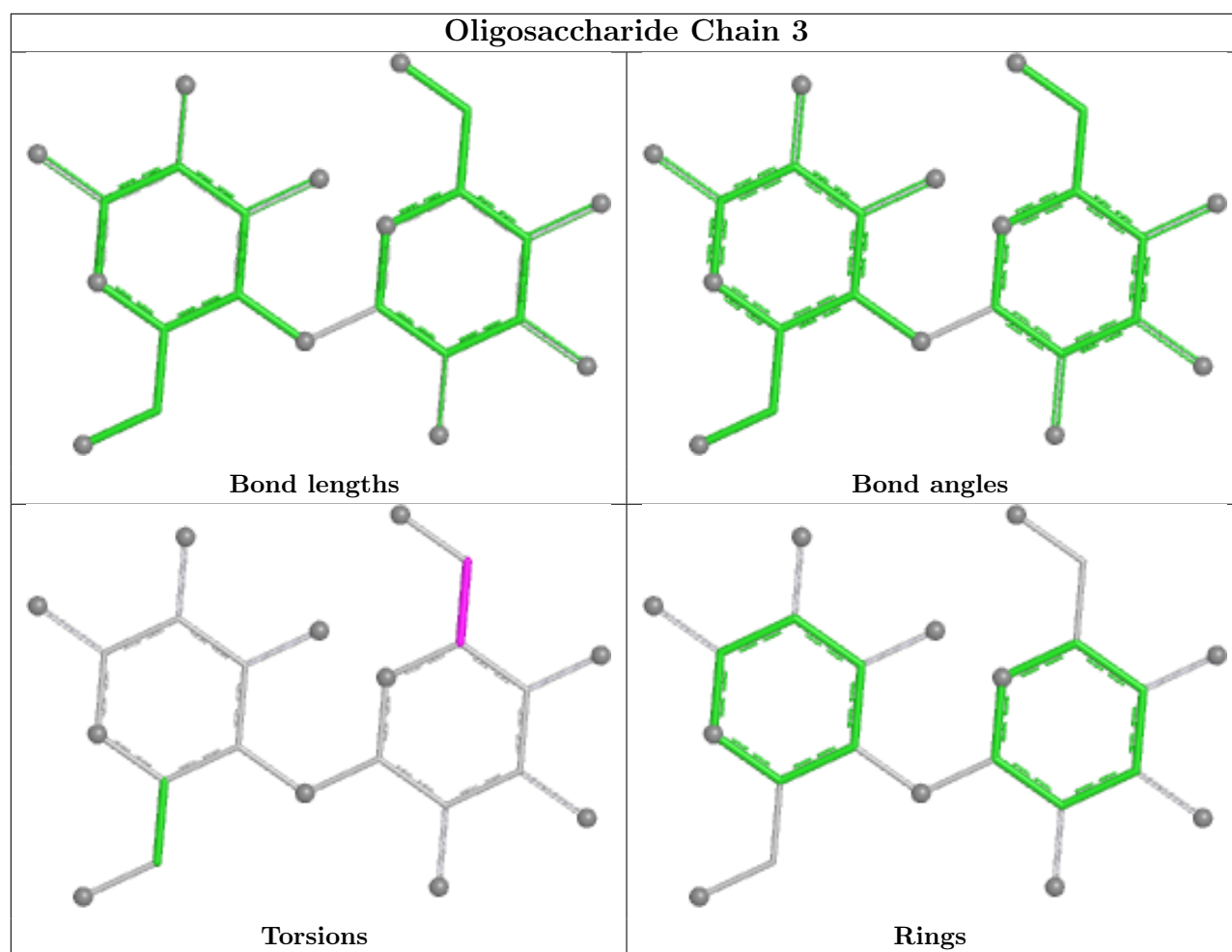


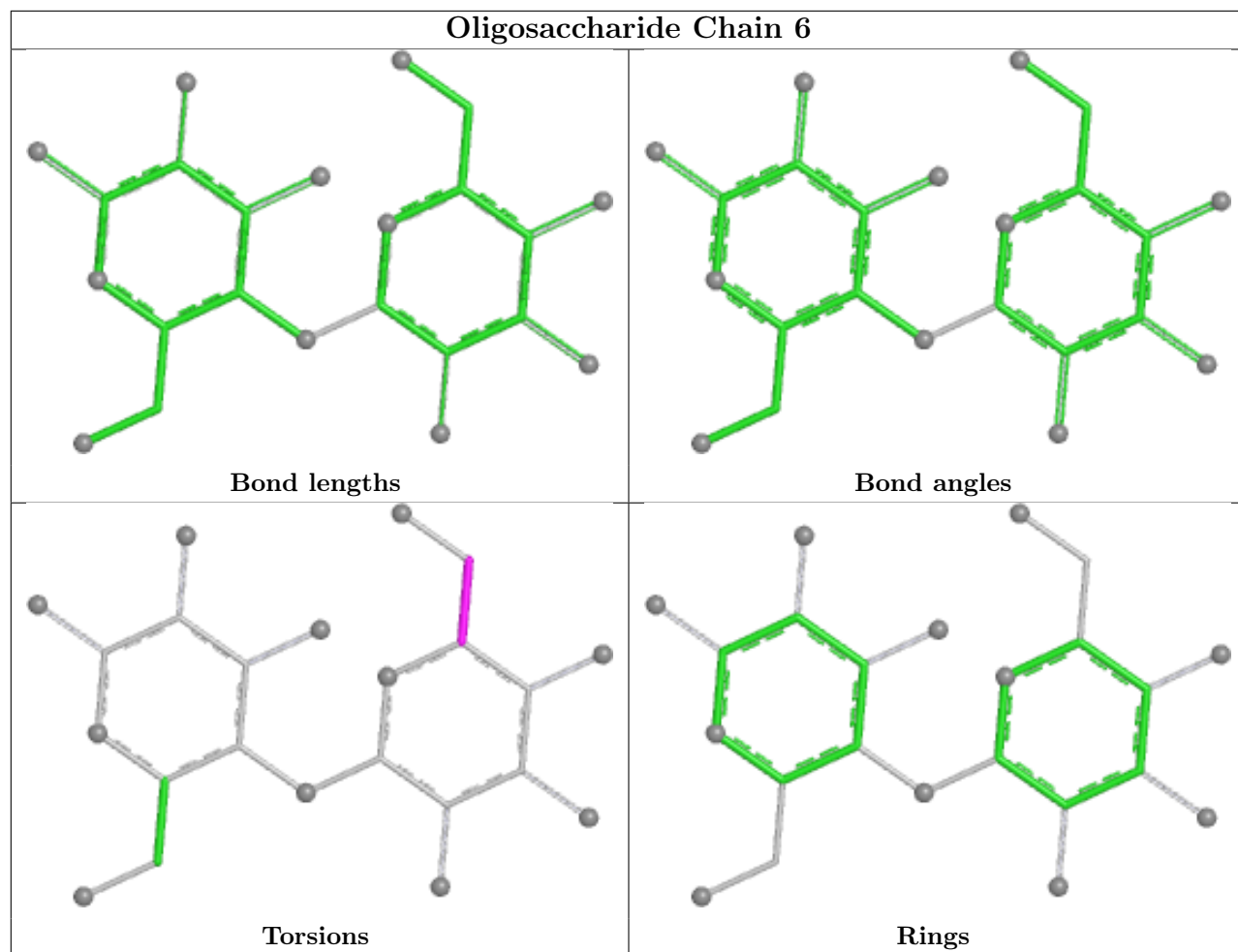




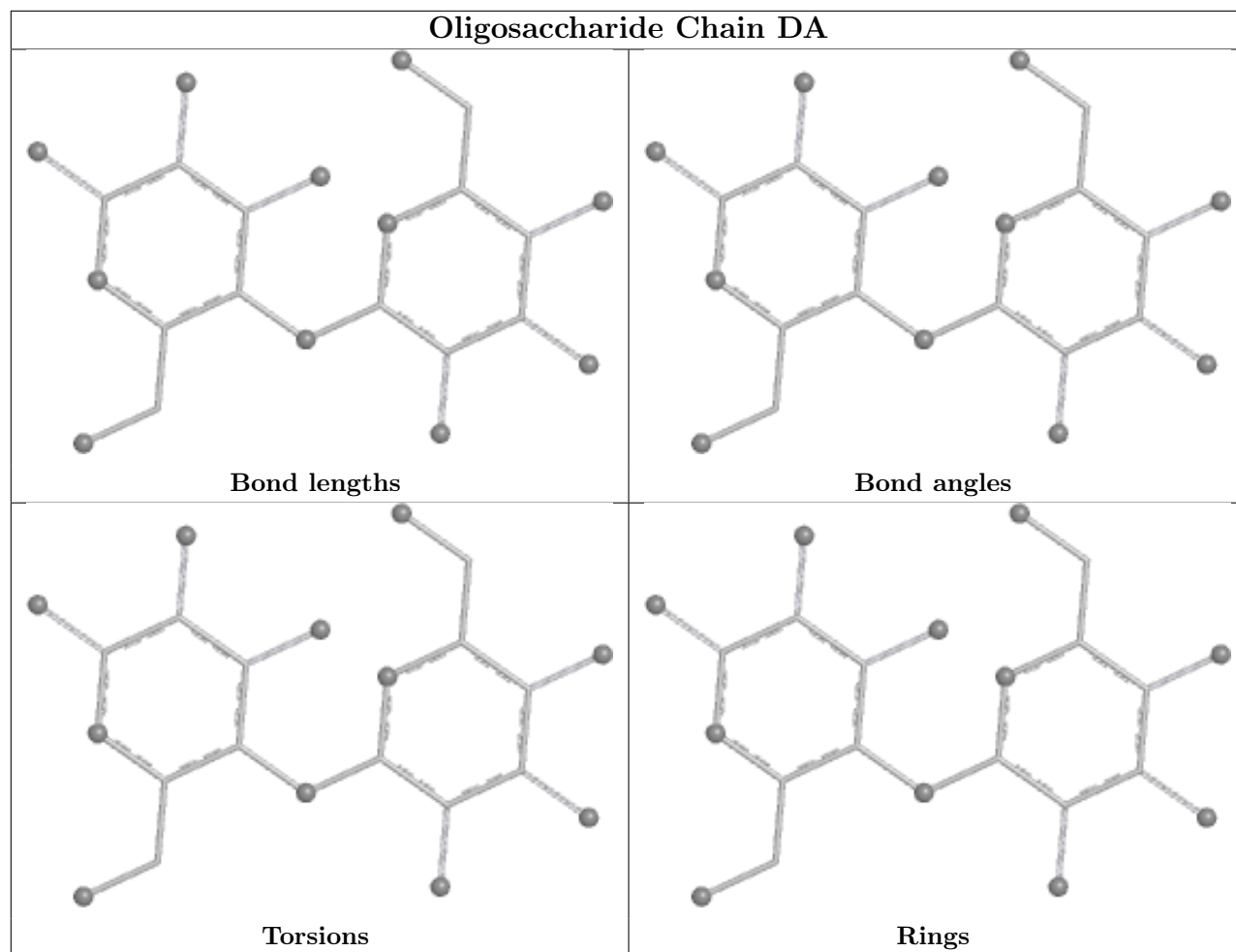


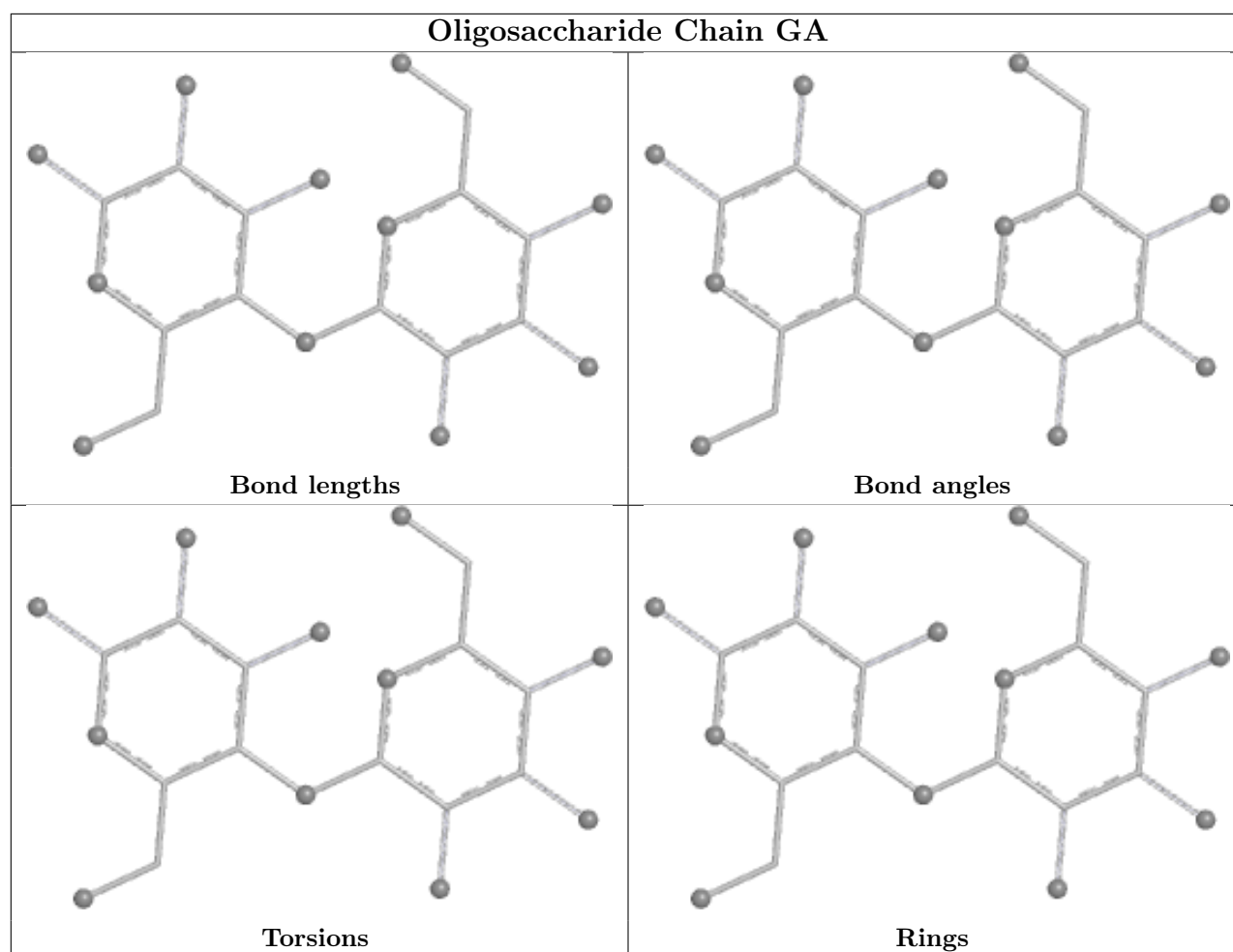






Oligosaccharide Chain DA





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	0.42	0	17,17,17	0.40	0
4	GAL	R	4370	-	12,12,12	0.45	0	17,17,17	0.53	0
4	GAL	I	2470	-	12,12,12	0.44	0	17,17,17	0.49	0
4	GAL	N	3470	-	12,12,12	0.46	0	17,17,17	0.37	0
4	GAL	P	4170	-	12,12,12	0.40	0	17,17,17	0.76	1 (5%)
4	GAL	T	4570	-	12,12,12	0.61	0	17,17,17	0.63	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	0.41	0
4	GAL	K	3170	-	12,12,12	0.41	0	17,17,17	0.48	0
4	GAL	G	2270	-	12,12,12	0.48	0	17,17,17	0.51	0
4	GAL	C	1370	-	12,12,12	0.48	0	17,17,17	0.43	0
4	GAL	J	2570	-	12,12,12	0.44	0	17,17,17	0.43	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	R	4370	-	-	2/2/22/22	0/1/1/1
4	GAL	I	2470	-	-	1/2/22/22	0/1/1/1
4	GAL	N	3470	-	-	2/2/22/22	0/1/1/1
4	GAL	P	4170	-	-	1/2/22/22	0/1/1/1
4	GAL	T	4570	-	-	1/2/22/22	0/1/1/1
4	GAL	E	1570	-	-	1/2/22/22	0/1/1/1
4	GAL	K	3170	-	-	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	J	2570	-	-	2/2/22/22	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	2.39	114.57	110.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2570	GAL	O5-C5-C6-O6
4	N	3470	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	T	4570	GAL	O5-C5-C6-O6
4	E	1570	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 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	4370	GAL	2	0
4	N	3470	GAL	2	0
4	P	4170	GAL	4	0
4	T	4570	GAL	1	0
4	G	2270	GAL	2	0
4	C	1370	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.47	0 100 100	8, 17, 30, 34	0
1	B	69/69 (100%)	-0.55	0 100 100	8, 17, 28, 36	0
1	C	69/69 (100%)	-0.58	0 100 100	7, 16, 29, 36	0
1	D	69/69 (100%)	-0.51	0 100 100	5, 16, 29, 34	0
1	E	69/69 (100%)	-0.45	0 100 100	8, 19, 31, 39	0
1	F	69/69 (100%)	-0.46	0 100 100	7, 15, 26, 40	0
1	G	69/69 (100%)	-0.64	0 100 100	4, 14, 26, 34	0
1	H	69/69 (100%)	-0.59	0 100 100	4, 14, 23, 34	0
1	I	69/69 (100%)	-0.45	0 100 100	7, 17, 30, 42	0
1	J	69/69 (100%)	-0.39	0 100 100	7, 22, 33, 42	0
1	K	69/69 (100%)	-0.50	0 100 100	7, 18, 30, 34	0
1	L	69/69 (100%)	-0.56	0 100 100	7, 15, 26, 34	0
1	M	69/69 (100%)	-0.66	0 100 100	5, 13, 24, 32	0
1	N	69/69 (100%)	-0.61	0 100 100	6, 16, 28, 36	0
1	O	69/69 (100%)	-0.56	0 100 100	5, 15, 27, 41	0
1	P	69/69 (100%)	-0.45	0 100 100	8, 19, 30, 40	0
1	Q	69/69 (100%)	-0.51	0 100 100	11, 18, 29, 43	0
1	R	69/69 (100%)	-0.18	0 100 100	11, 25, 38, 44	0
1	S	69/69 (100%)	-0.20	0 100 100	12, 25, 34, 45	0
1	T	69/69 (100%)	-0.25	0 100 100	12, 25, 37, 47	0
All	All	1380/1380 (100%)	-0.48	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, 95th 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
2	BGC	FA	1	12/12	0.78	0.12	49,56,61,62	0
2	BGC	U	1	12/12	0.79	0.12	37,50,54,56	0
2	BGC	X	1	12/12	0.80	0.14	28,39,43,46	0
3	GLA	Z	2	11/12	0.81	0.15	72,74,77,78	0
2	BGC	W	1	12/12	0.82	0.10	22,30,39,45	0
3	GAL	Z	1	12/12	0.84	0.13	60,67,69,73	0
2	BGC	EA	1	12/12	0.84	0.10	19,26,38,44	0
2	BGC	CA	1	12/12	0.85	0.10	40,52,56,59	0
3	GAL	DA	1	12/12	0.86	0.10	29,32,35,36	0
2	BGC	a	1	12/12	-	-	31,36,43,43	0
2	GAL	a	2	11/12	-	-	15,19,26,27	0
2	GLA	a	3	11/12	-	-	2,10,15,20	0
2	BGC	c	1	12/12	-	-	29,36,38,40	0
2	GAL	c	2	11/12	-	-	18,22,28,35	0
2	GLA	c	3	11/12	-	-	9,11,14,14	0
2	BGC	e	1	12/12	-	-	20,25,32,33	0
2	GAL	e	2	11/12	-	-	10,14,18,18	0
2	GLA	e	3	11/12	-	-	5,9,13,15	0
2	BGC	f	1	12/12	-	-	38,42,44,44	0
2	GAL	f	2	11/12	-	-	21,27,34,34	0
2	GLA	f	3	11/12	-	-	16,20,24,24	0
2	BGC	g	1	12/12	-	-	36,41,42,42	11
2	GAL	g	2	11/12	-	-	25,26,31,35	0
2	GLA	g	3	11/12	-	-	14,22,23,24	0
2	BGC	h	1	12/12	-	-	36,49,53,53	0
2	GAL	h	2	11/12	-	-	14,21,29,30	0
2	GLA	h	3	11/12	-	-	4,7,14,15	0
2	BGC	i	1	12/12	-	-	43,48,48,48	11
2	GAL	i	2	11/12	-	-	27,37,40,40	0
2	GLA	i	3	11/12	-	-	20,22,27,27	0
2	BGC	j	1	12/12	-	-	28,31,36,38	0
2	GAL	j	2	11/12	-	-	18,25,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLA	j	3	11/12	-	-	17,19,21,27	0
2	BGC	k	1	12/12	-	-	26,38,40,43	0
2	GAL	k	2	11/12	-	-	8,15,20,20	0
2	GLA	k	3	11/12	-	-	2,9,12,14	0
2	BGC	m	1	12/12	-	-	27,39,43,44	0
2	GAL	m	2	11/12	-	-	10,20,23,23	0
2	GLA	m	3	11/12	-	-	7,10,16,20	0
2	BGC	o	1	12/12	-	-	14,23,29,29	0
2	GAL	o	2	11/12	-	-	21,29,33,38	0
2	GLA	o	3	11/12	-	-	8,14,17,21	0
2	BGC	p	1	12/12	-	-	36,42,47,51	0
2	GAL	p	2	11/12	-	-	21,27,37,40	0
2	GLA	p	3	11/12	-	-	10,12,17,18	0
2	BGC	r	1	12/12	-	-	51,55,61,62	0
2	GAL	r	2	11/12	-	-	27,35,40,44	0
2	GLA	r	3	11/12	-	-	21,25,27,30	0
2	BGC	s	1	12/12	-	-	47,67,73,74	0
2	GAL	s	2	11/12	-	-	25,33,41,45	0
2	GLA	s	3	11/12	-	-	19,29,30,31	0
2	BGC	t	1	12/12	-	-	40,51,53,55	0
2	GAL	t	2	11/12	-	-	30,32,38,39	0
2	GLA	t	3	11/12	-	-	14,16,25,28	0
2	BGC	v	1	12/12	-	-	29,41,45,49	0
2	GAL	v	2	11/12	-	-	17,21,24,25	0
2	GLA	v	3	11/12	-	-	5,10,16,16	0
2	BGC	x	1	12/12	-	-	33,47,49,52	0
2	GAL	x	2	11/12	-	-	17,22,25,25	0
2	GLA	x	3	11/12	-	-	9,14,18,22	0
2	BGC	z	1	12/12	-	-	2,8,12,15	0
2	GAL	z	2	11/12	-	-	5,8,10,12	0
2	GLA	z	3	11/12	-	-	2,3,15,18	0
2	BGC	0	1	12/12	-	-	40,49,54,54	0
2	GAL	0	2	11/12	-	-	25,29,34,36	0
2	GLA	0	3	11/12	-	-	10,16,23,26	0
2	BGC	2	1	12/12	-	-	44,51,54,55	0
2	GAL	2	2	11/12	-	-	27,31,34,36	0
2	GLA	2	3	11/12	-	-	6,10,14,16	0
2	BGC	4	1	12/12	-	-	25,31,36,42	0
2	GAL	4	2	11/12	-	-	14,24,32,36	0
2	GLA	4	3	11/12	-	-	20,22,30,35	0
2	BGC	5	1	12/12	-	-	36,46,49,53	0
2	GAL	5	2	11/12	-	-	15,26,28,30	0

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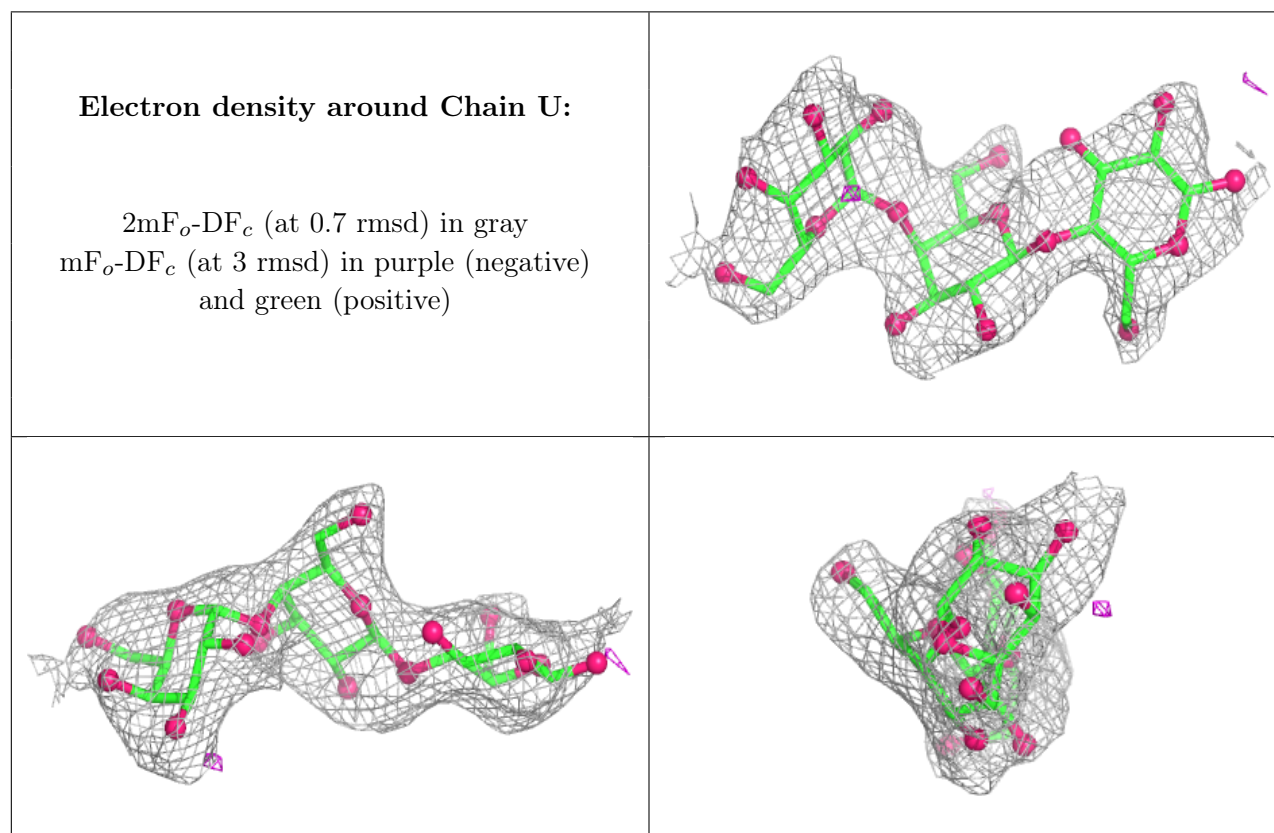
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLA	5	3	11/12	-	-	13,20,24,28	0
2	BGC	7	1	12/12	-	-	31,39,43,45	0
2	GAL	7	2	11/12	-	-	15,20,28,29	0
2	GLA	7	3	11/12	-	-	13,15,18,22	0
2	BGC	8	1	12/12	-	-	35,40,40,41	8
2	GAL	8	2	11/12	-	-	22,28,33,33	0
2	GLA	8	3	11/12	-	-	15,25,28,32	0
2	BGC	9	1	12/12	-	-	19,28,32,38	0
2	GAL	9	2	11/12	-	-	2,5,9,11	0
2	GLA	9	3	11/12	-	-	2,9,13,17	0
3	GAL	V	1	12/12	0.88	0.10	29,32,35,38	0
2	BGC	AA	1	12/12	0.89	0.09	47,55,59,61	0
2	GAL	U	2	11/12	0.90	0.10	21,29,34,34	0
2	BGC	BA	1	12/12	-	-	46,58,61,62	4
2	GAL	BA	2	11/12	-	-	32,34,39,39	0
2	GLA	BA	3	11/12	-	-	19,22,29,30	0
3	GLA	V	2	11/12	0.91	0.09	11,23,28,29	0
2	GAL	FA	2	11/12	0.92	0.08	38,41,45,47	0
2	GAL	AA	2	11/12	0.92	0.09	30,41,44,44	0
2	GAL	W	2	11/12	0.92	0.09	8,13,22,23	0
3	GAL	Y	1	12/12	0.93	0.07	22,28,29,31	0
2	GAL	CA	2	11/12	0.93	0.09	27,33,37,37	0
2	GAL	X	2	11/12	0.94	0.08	10,20,23,25	0
2	GLA	W	3	11/12	0.94	0.09	4,12,17,25	0
2	GLA	FA	3	11/12	0.94	0.08	28,30,33,36	0
2	GLA	X	3	11/12	0.95	0.08	9,12,16,19	0
2	GLA	AA	3	11/12	0.95	0.07	21,28,30,31	0
2	GLA	EA	3	11/12	0.95	0.06	14,25,30,31	0
2	GLA	U	3	11/12	0.95	0.07	8,15,20,20	0
3	GLA	Y	2	11/12	0.96	0.05	15,18,20,22	0
3	GLA	DA	2	11/12	0.96	0.06	18,22,29,30	0
3	GAL	b	1	12/12	-	-	22,26,30,35	0
3	GLA	b	2	11/12	-	-	17,19,22,30	0
3	GAL	d	1	12/12	-	-	23,28,30,34	0
3	GLA	d	2	11/12	-	-	14,20,26,27	0
3	GAL	l	1	12/12	-	-	23,26,32,34	0
3	GLA	l	2	11/12	-	-	14,16,20,22	0
3	GAL	n	1	12/12	-	-	18,28,31,32	0
3	GLA	n	2	11/12	-	-	14,17,21,25	0
3	GAL	q	1	12/12	-	-	18,23,26,27	0
3	GLA	q	2	11/12	-	-	15,21,25,29	0
3	GAL	u	1	12/12	-	-	28,37,41,44	0

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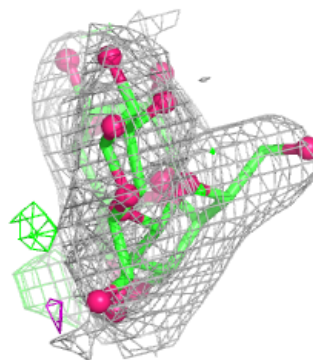
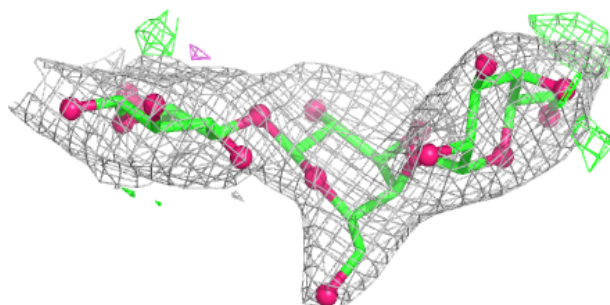
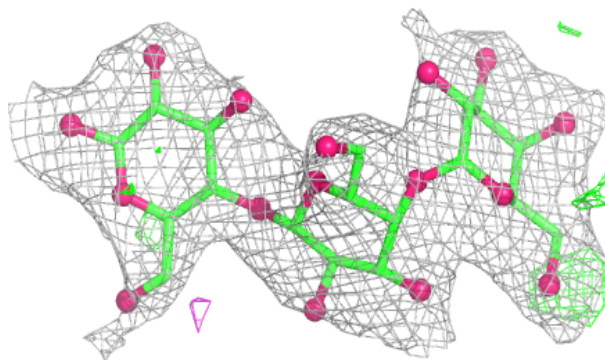
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLA	u	2	11/12	-	-	7,18,25,26	0
3	GAL	w	1	12/12	-	-	20,27,31,33	0
3	GLA	w	2	11/12	-	-	7,18,19,21	0
3	GAL	y	1	12/12	-	-	20,24,29,29	0
3	GLA	y	2	11/12	-	-	5,15,22,22	0
3	GAL	1	1	12/12	-	-	22,27,37,42	0
3	GLA	1	2	11/12	-	-	23,24,27,28	0
3	GAL	3	1	12/12	-	-	25,31,38,42	0
3	GLA	3	2	11/12	-	-	24,27,28,29	0
3	GAL	6	1	12/12	-	-	25,31,38,38	0
3	GLA	6	2	11/12	-	-	18,21,26,27	0
2	GLA	CA	3	11/12	0.97	0.06	26,29,31,31	0
2	GAL	EA	2	11/12	0.97	0.05	26,30,34,34	0
3	GAL	GA	1	12/12	-	-	21,27,32,34	0
3	GLA	GA	2	11/12	-	-	19,22,24,25	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.

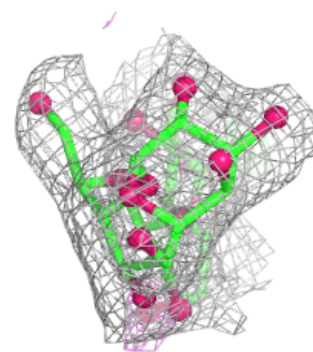
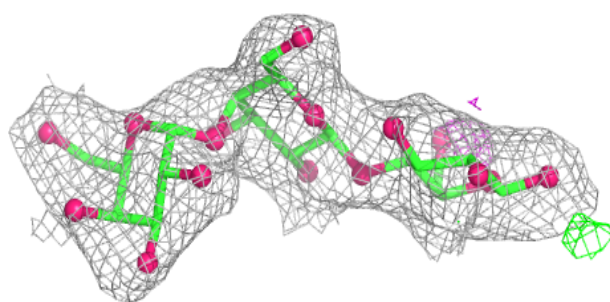
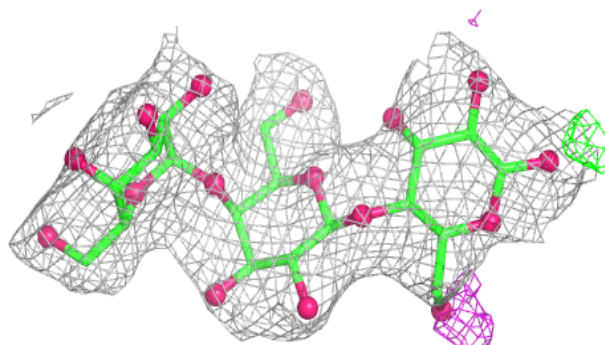


Electron density around Chain W:

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

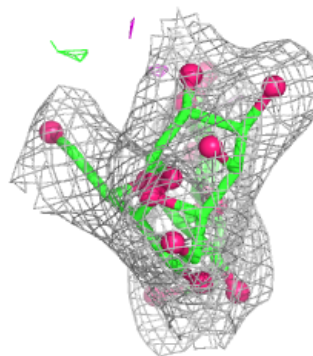
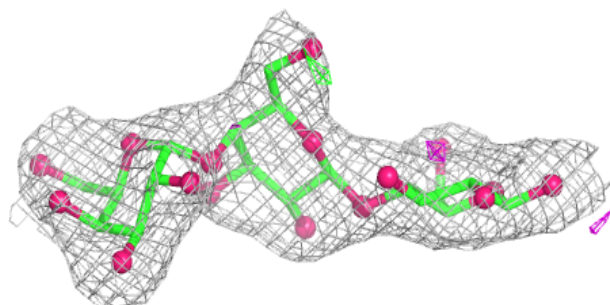
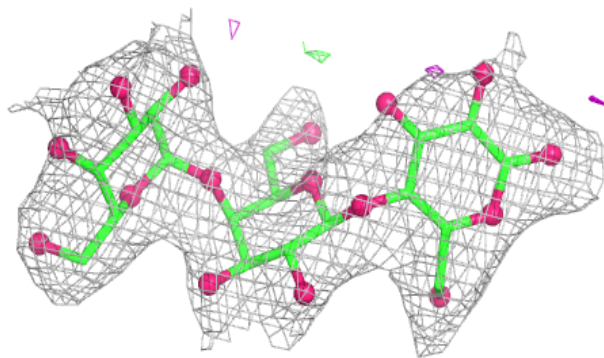
**Electron density around Chain X:**

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

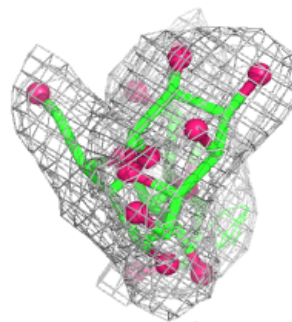
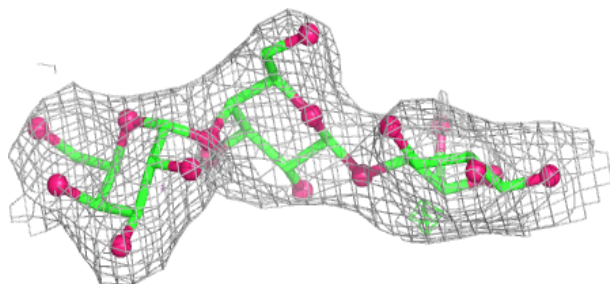
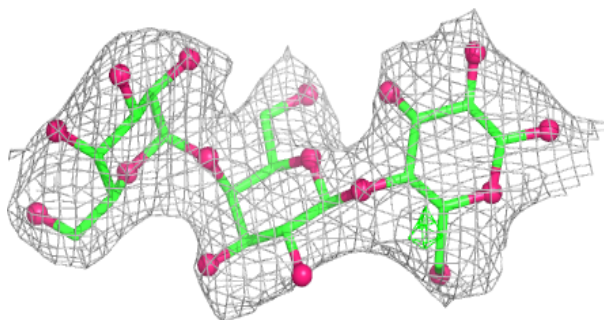


Electron density around Chain a:

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

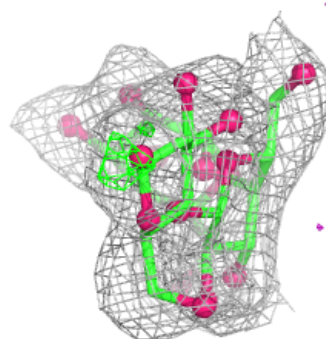
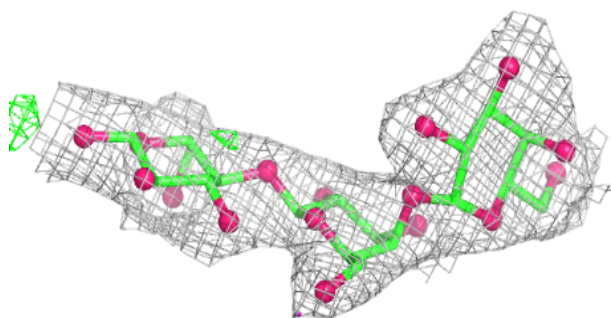
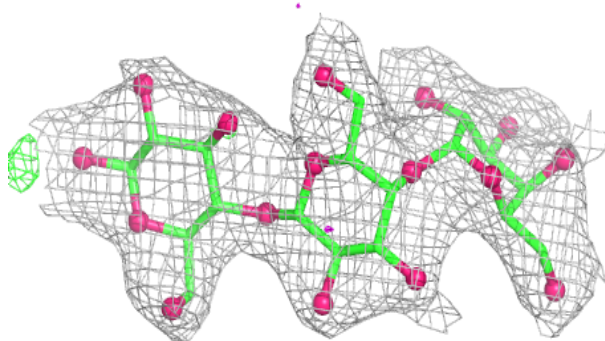
**Electron density around Chain c:**

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

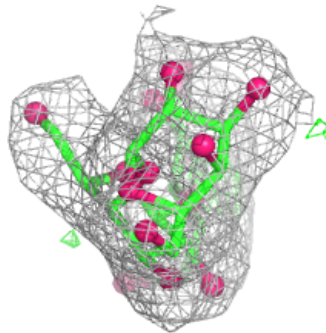
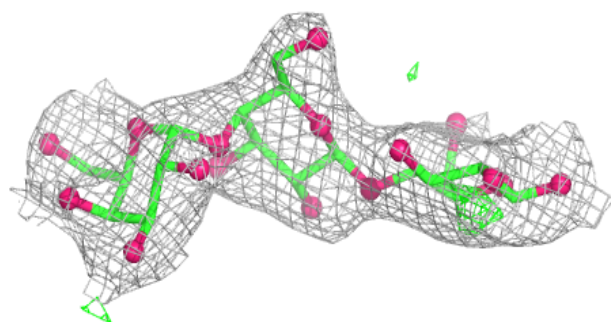
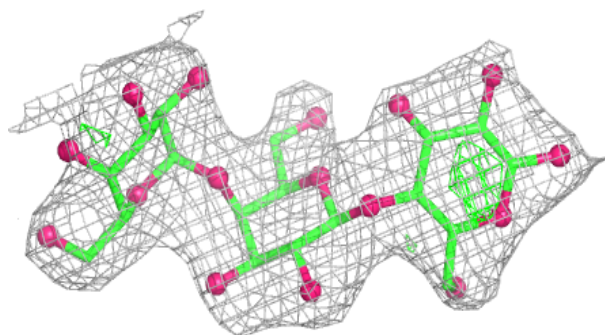


Electron density around Chain e:

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

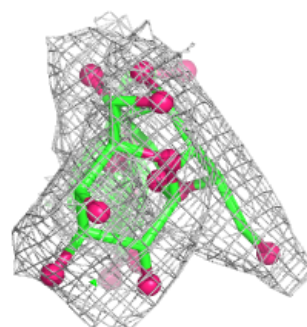
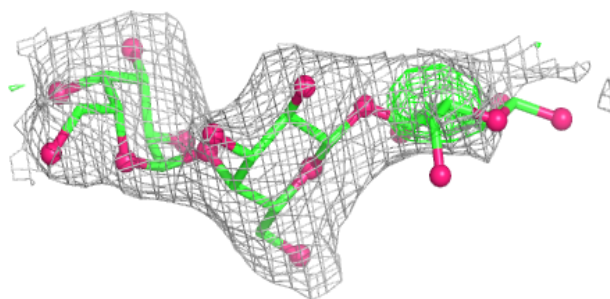
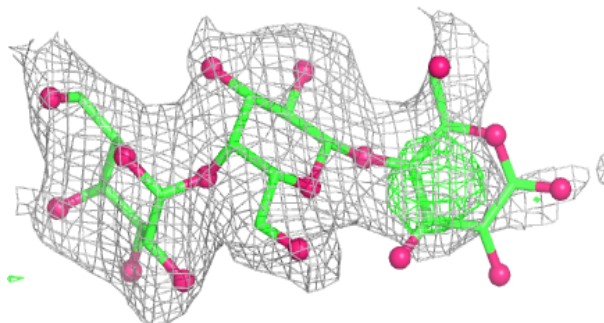
**Electron density around Chain f:**

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

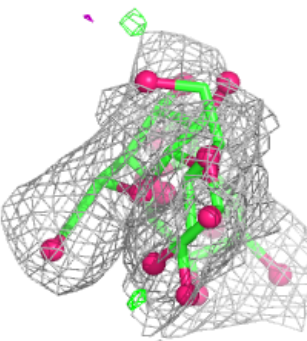
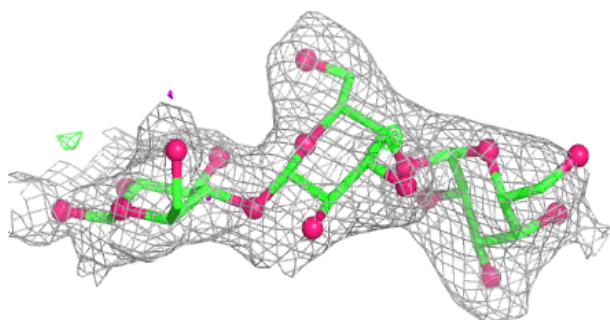
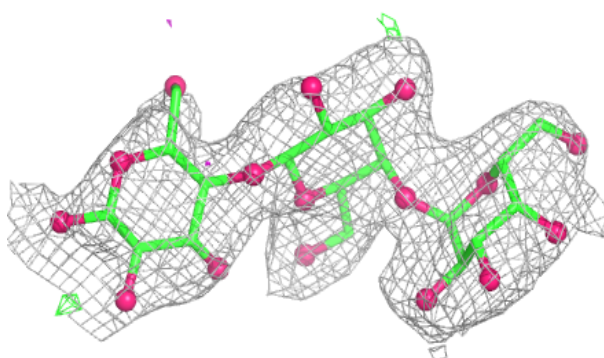


Electron density around Chain g:

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

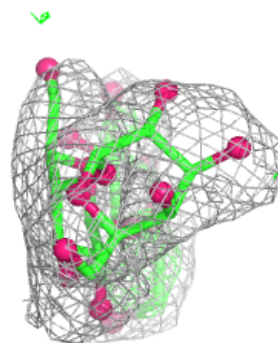
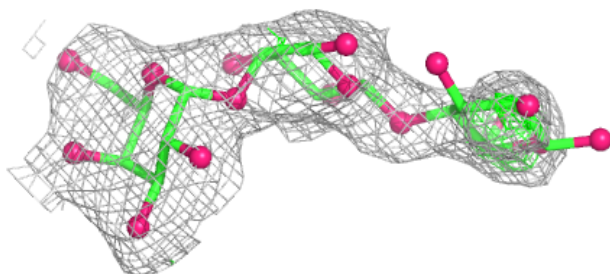
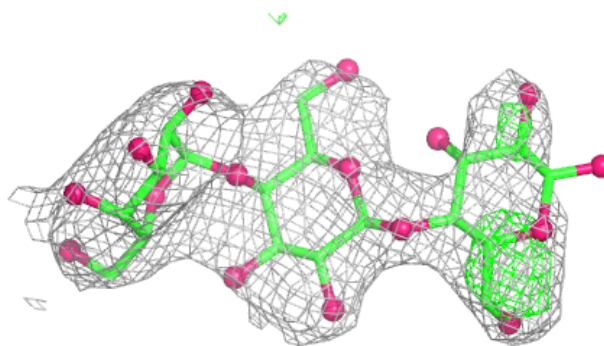
**Electron density around Chain h:**

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

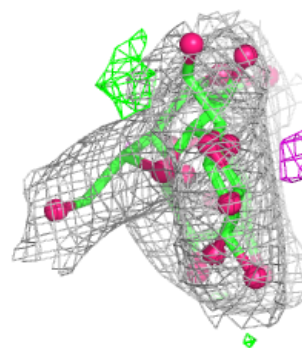
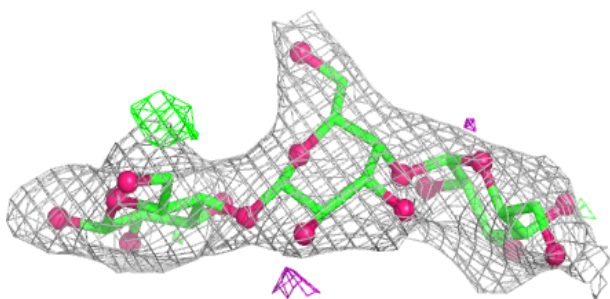
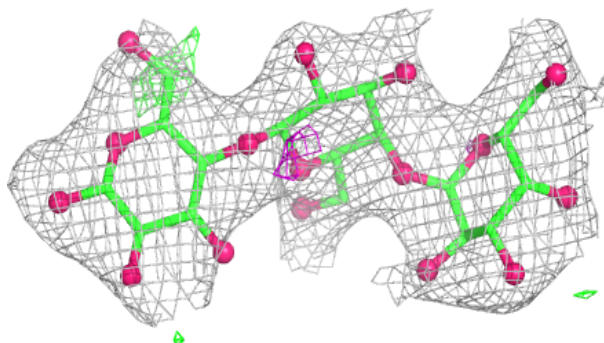


Electron density around Chain i:

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

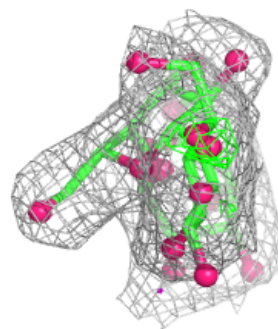
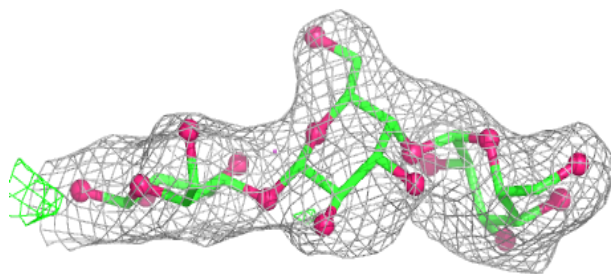
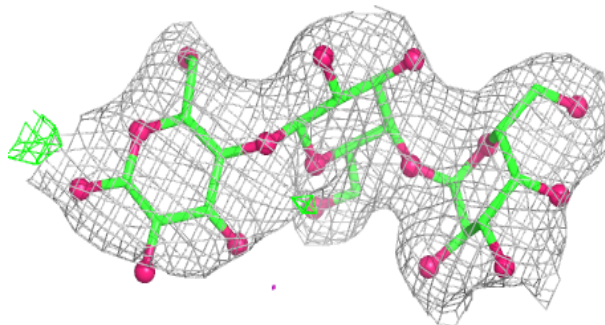
**Electron density around Chain j:**

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

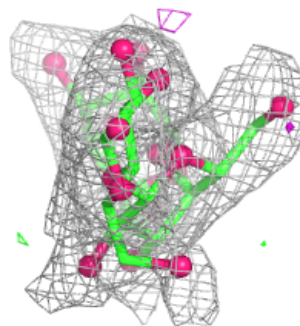
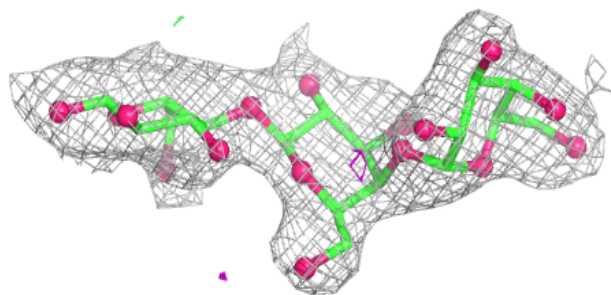
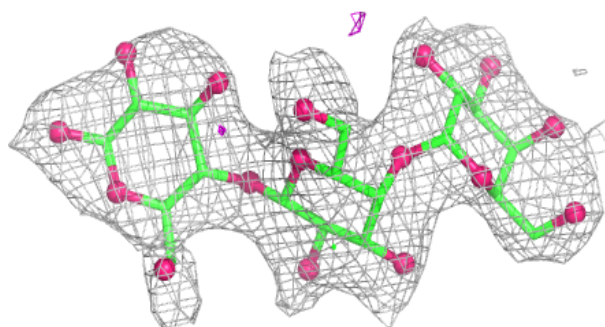


Electron density around Chain k:

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

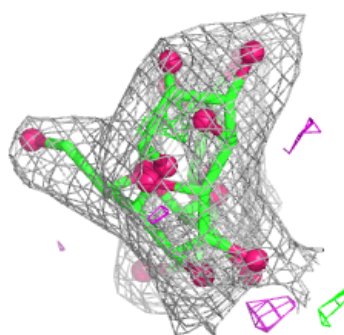
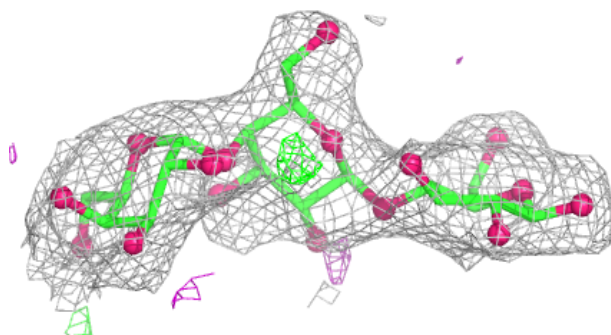
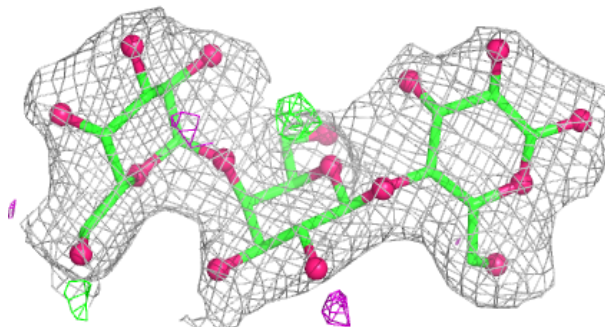
**Electron density around Chain m:**

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

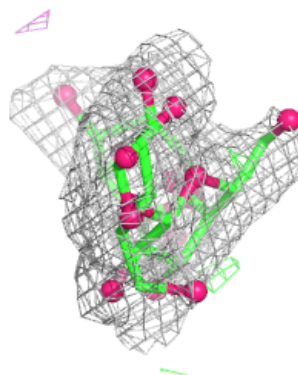
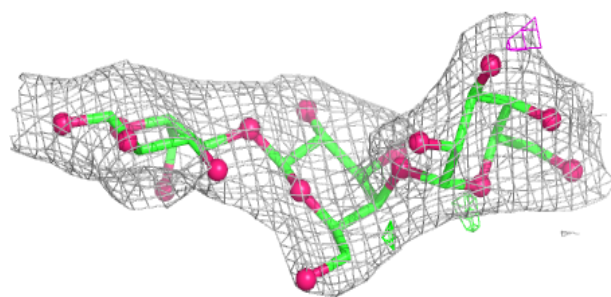
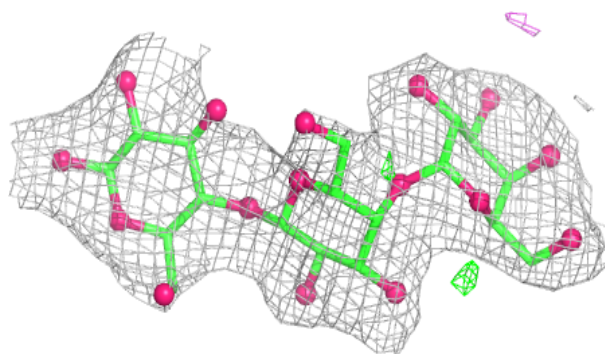


Electron density around Chain o:

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

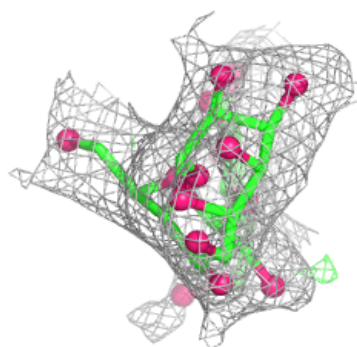
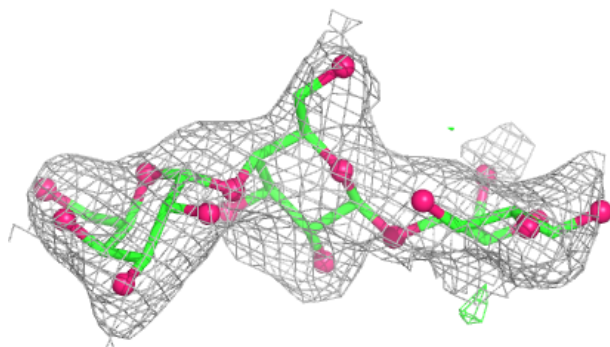
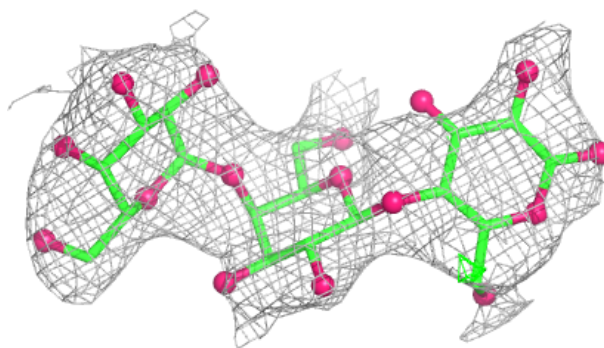
**Electron density around Chain p:**

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

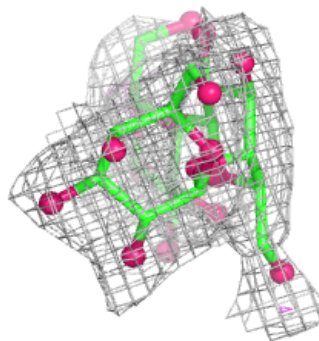
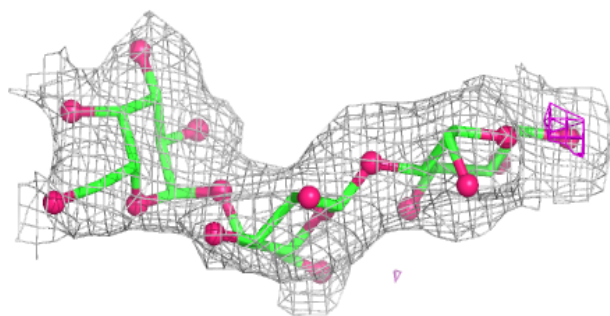
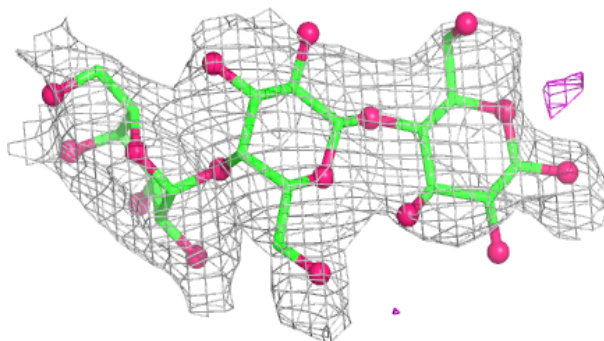


Electron density around Chain r:

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

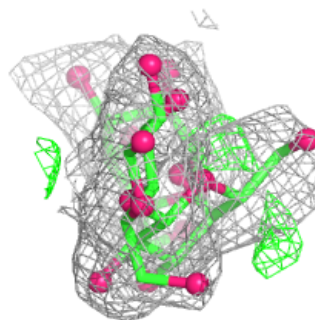
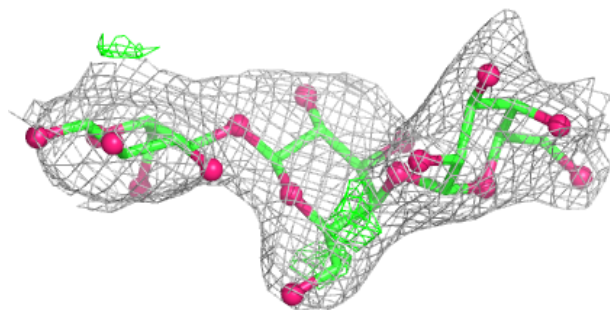
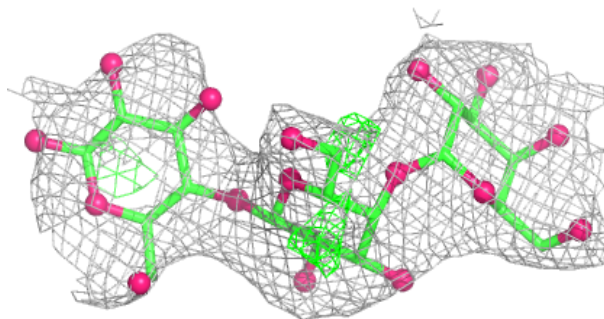
**Electron density around Chain s:**

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

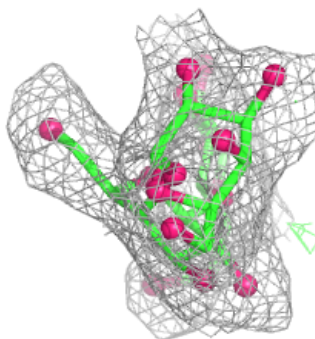
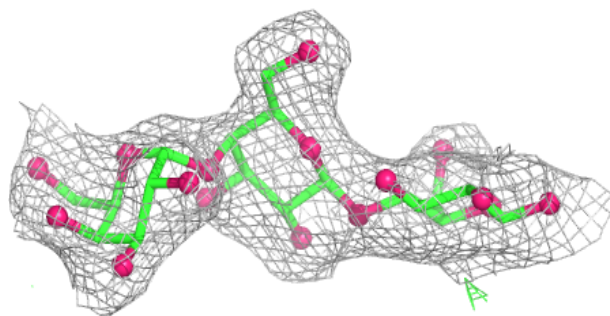
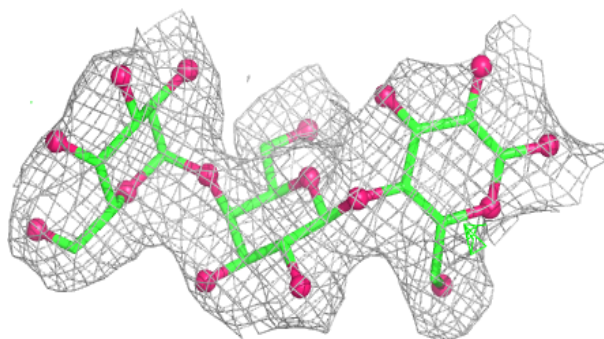


Electron density around Chain t:

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

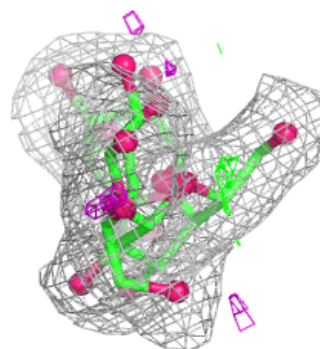
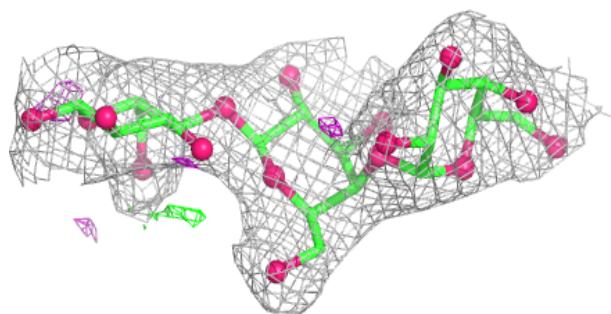
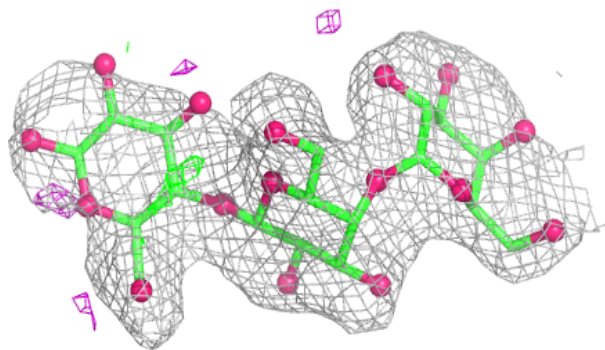
**Electron density around Chain v:**

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

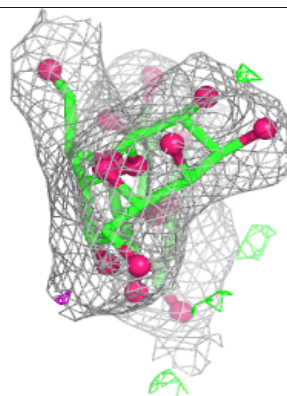
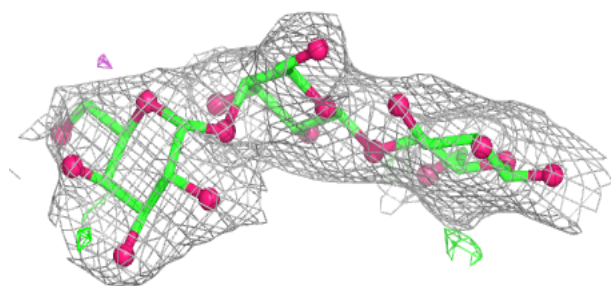
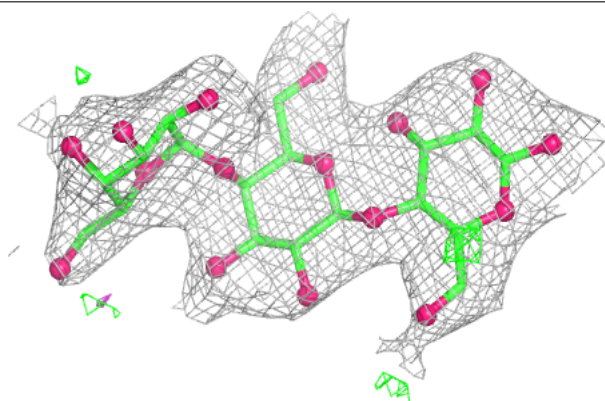


Electron density around Chain x:

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

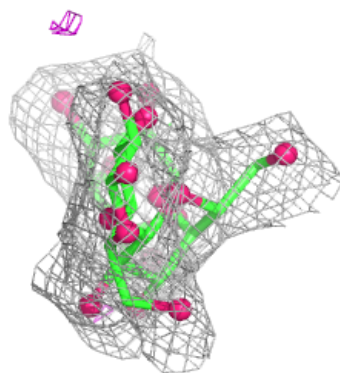
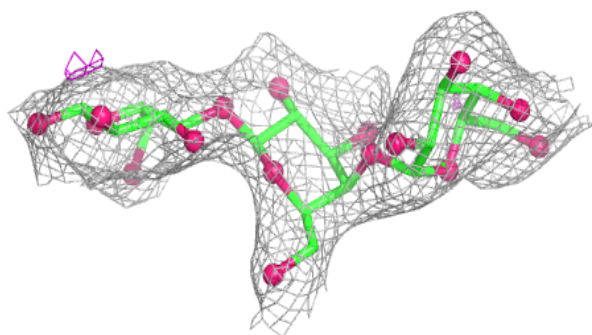
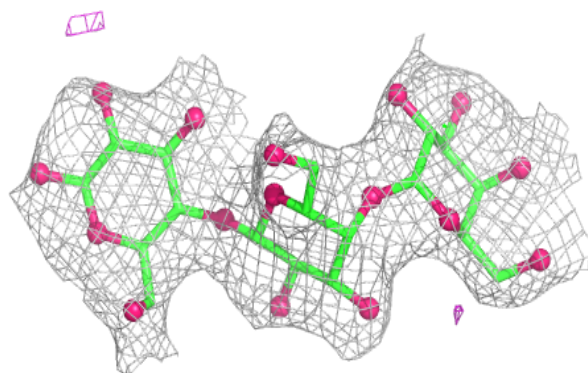
**Electron density around Chain z:**

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

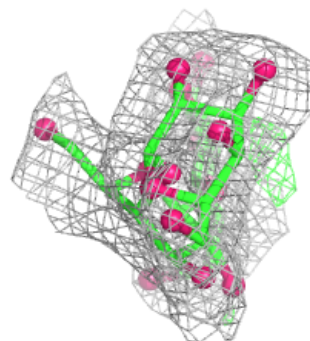
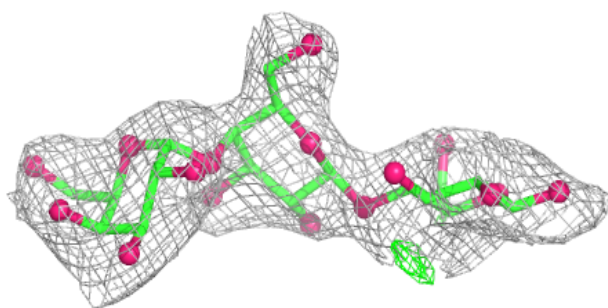
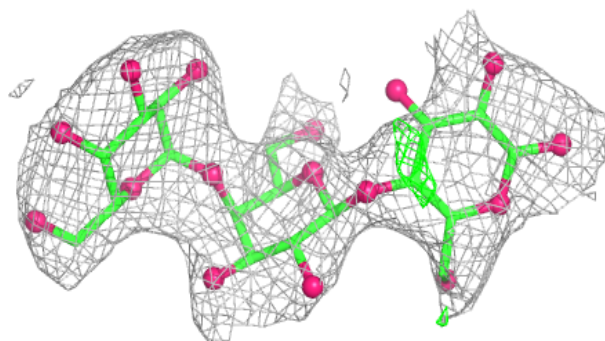


Electron density around Chain 0:

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

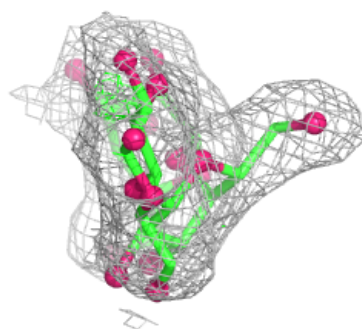
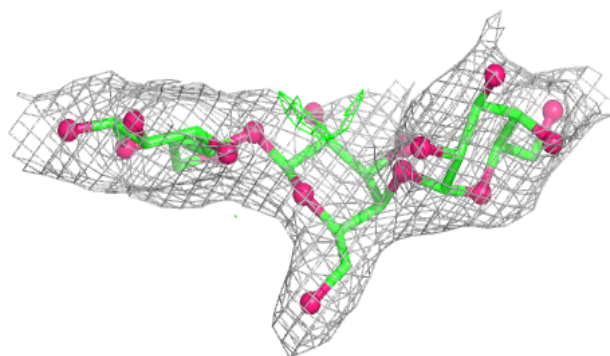
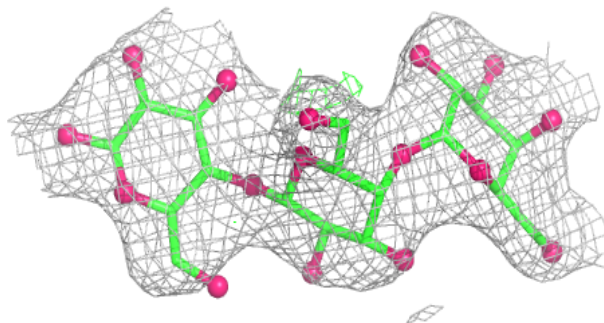
**Electron density around Chain 2:**

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

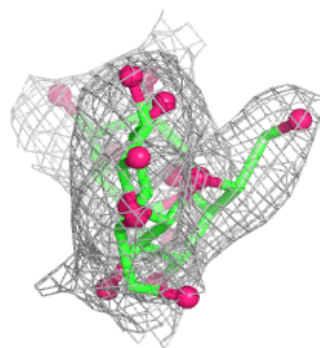
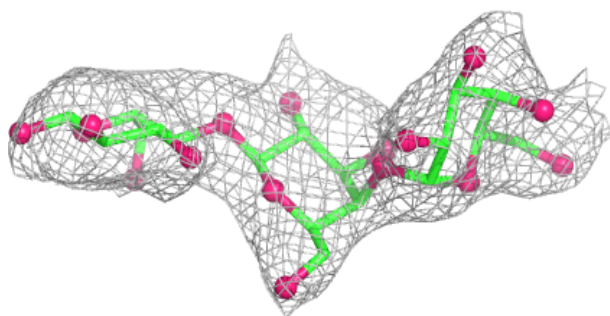
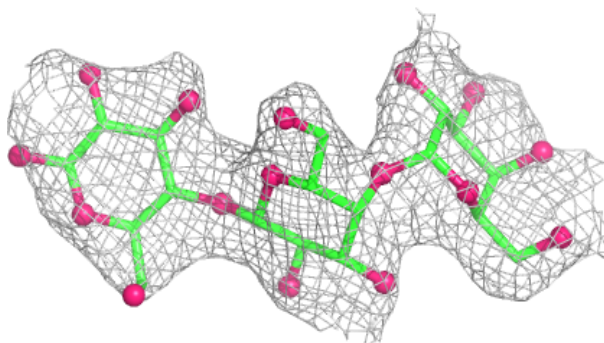


Electron density around Chain 4:

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

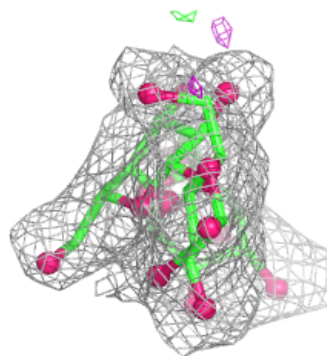
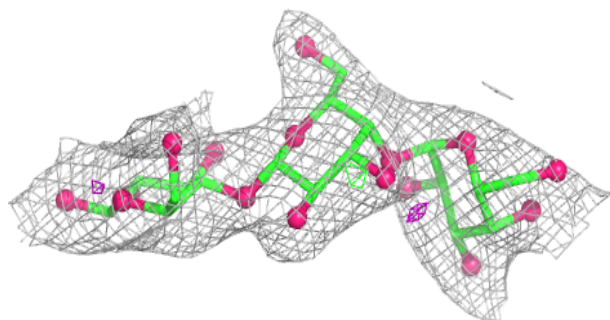
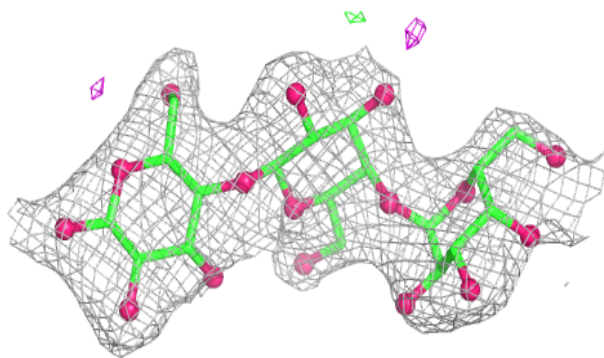
**Electron density around Chain 5:**

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

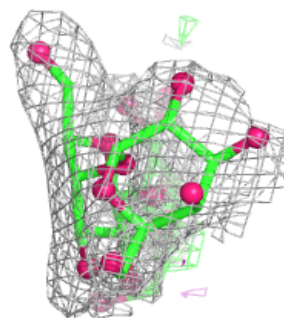
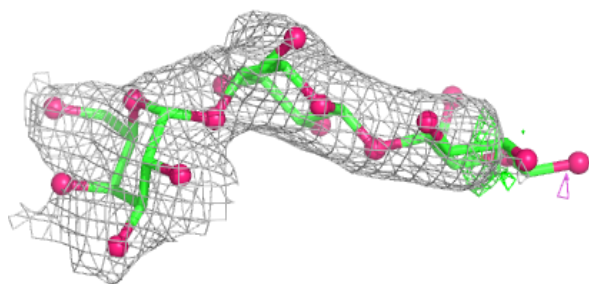
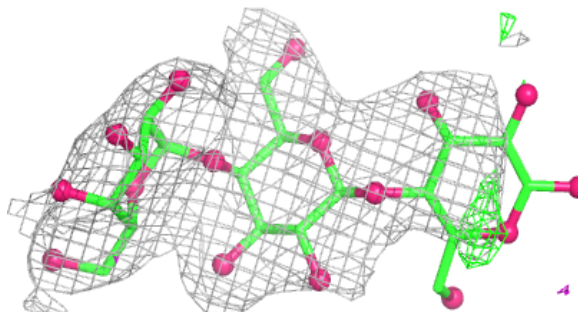


Electron density around Chain 7:

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

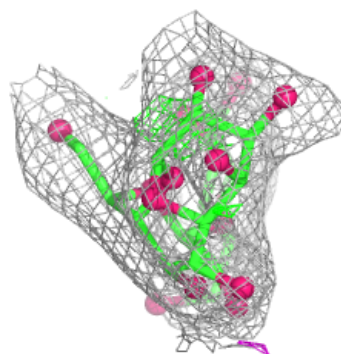
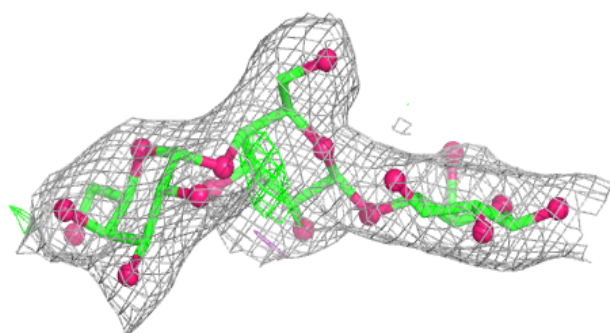
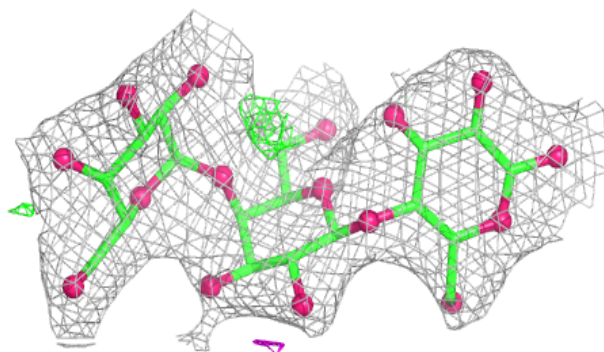
**Electron density around Chain 8:**

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

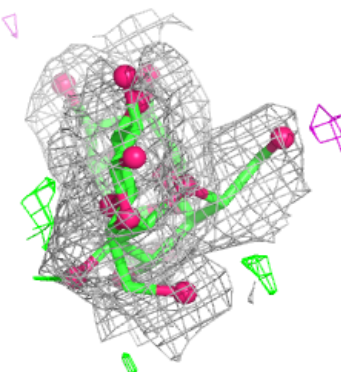
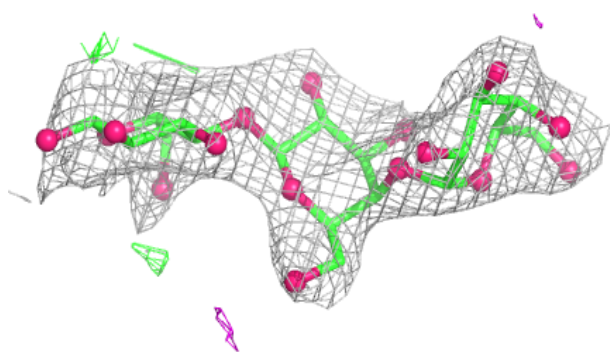
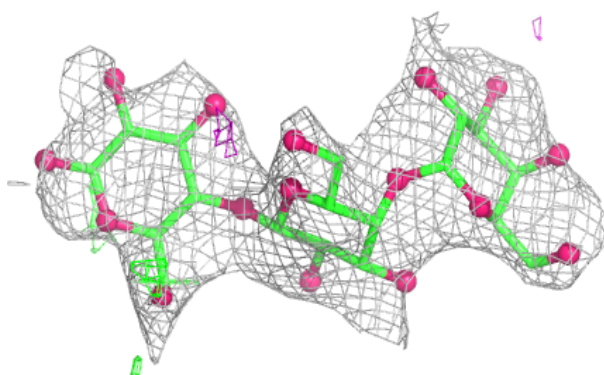


Electron density around Chain 9:

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

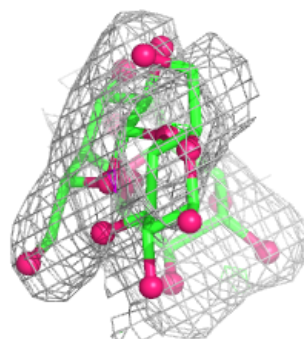
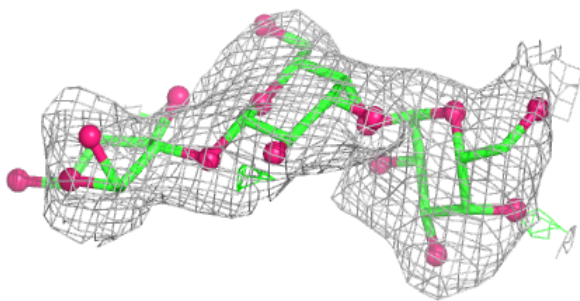
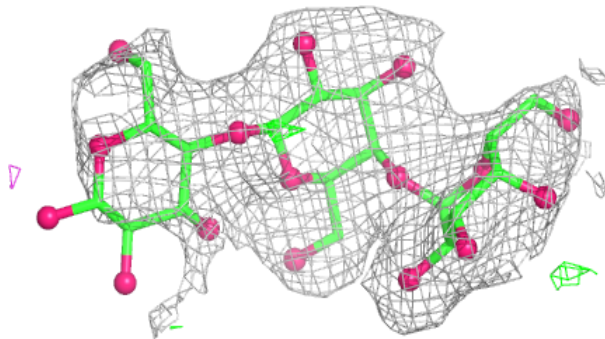
**Electron density around Chain AA:**

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

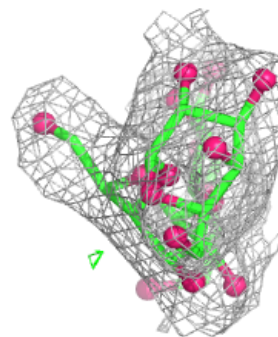
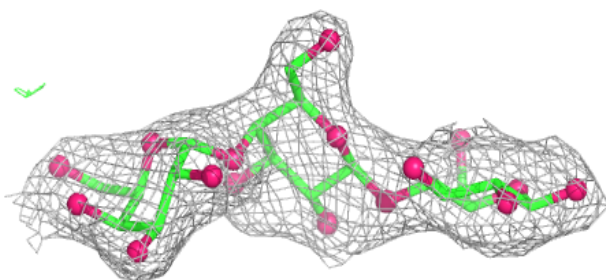
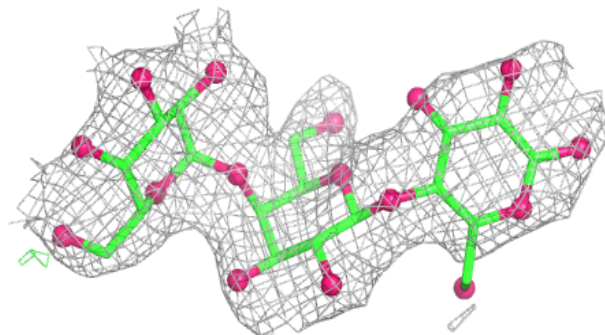


Electron density around Chain BA:

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

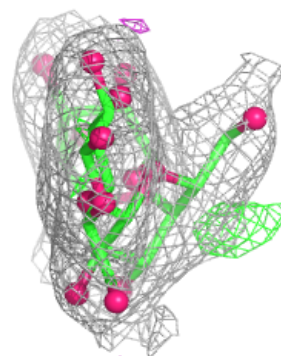
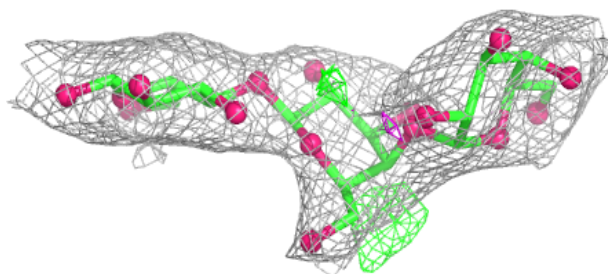
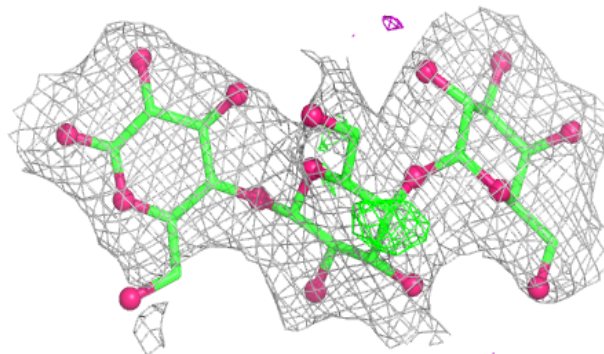
**Electron density around Chain CA:**

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

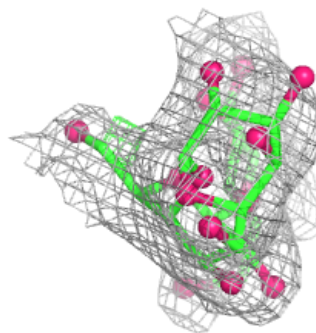
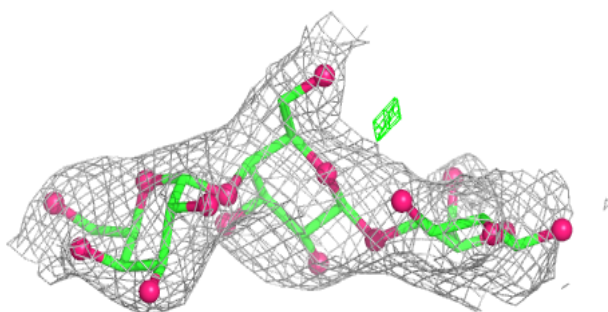
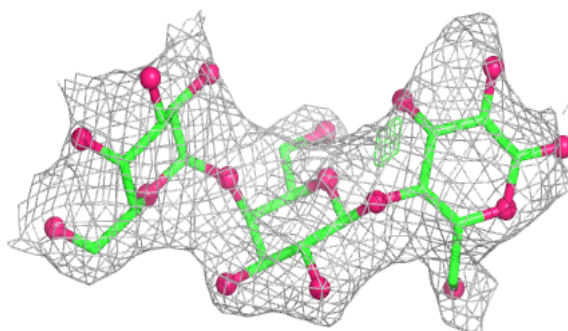


Electron density around Chain EA:

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

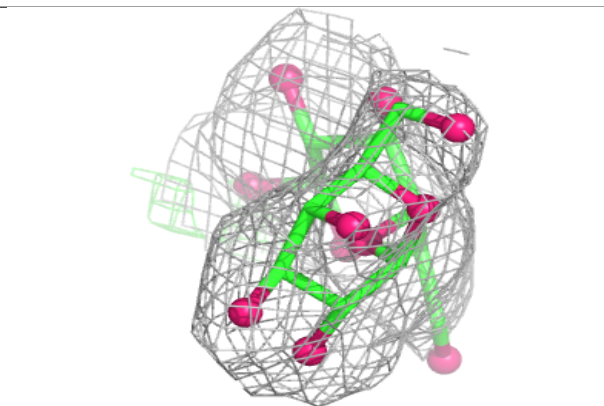
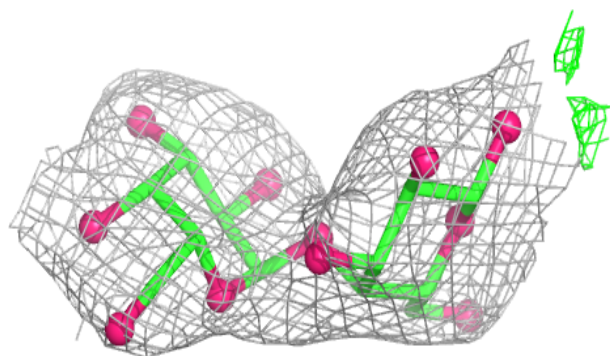
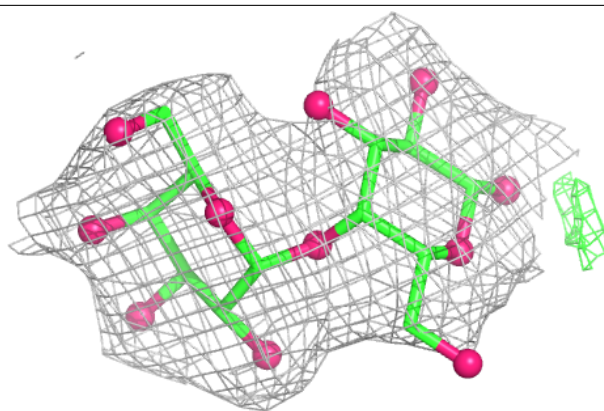
**Electron density around Chain FA:**

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

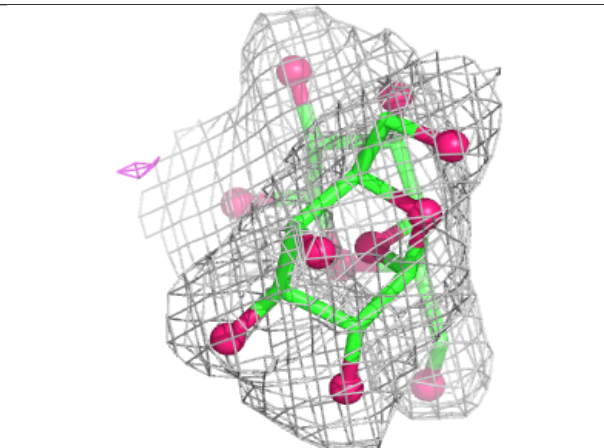
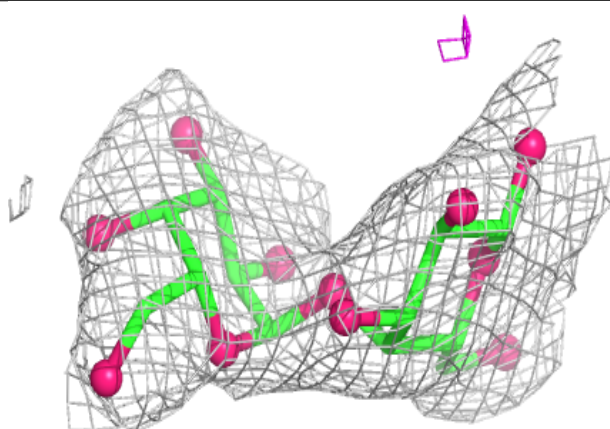
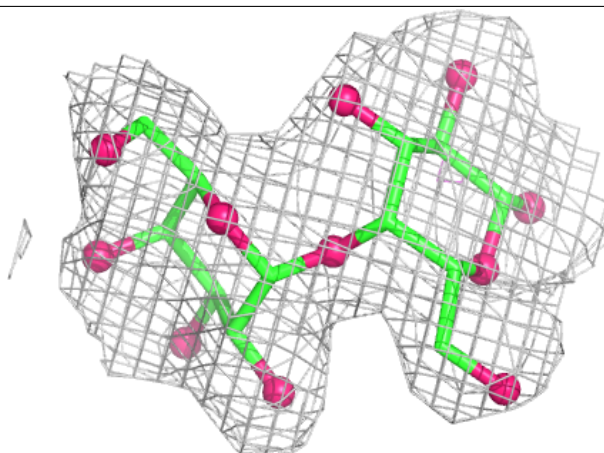


Electron density around Chain V:

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

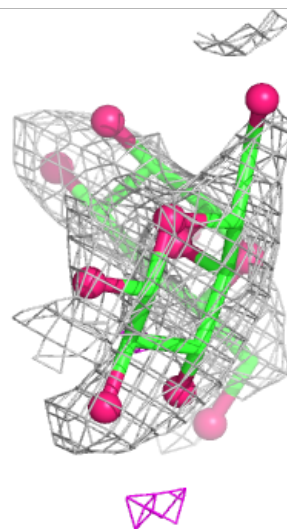
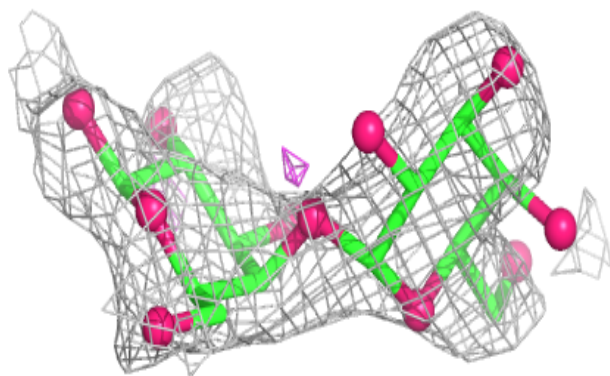
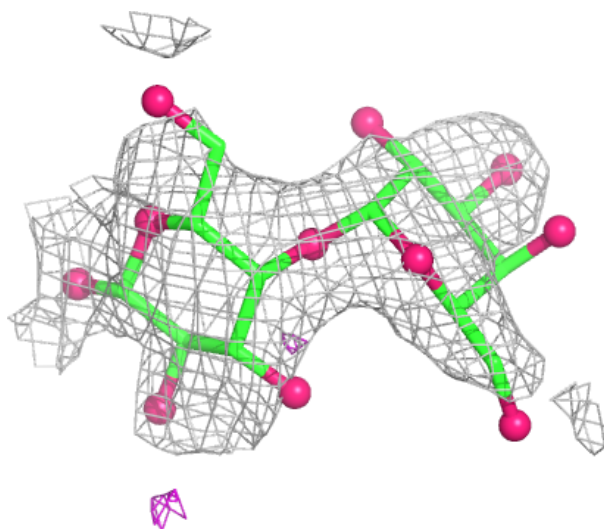
**Electron density around Chain Y:**

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



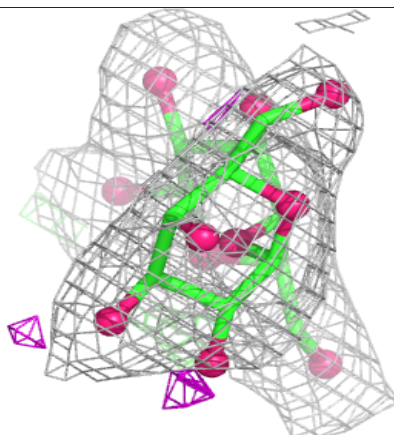
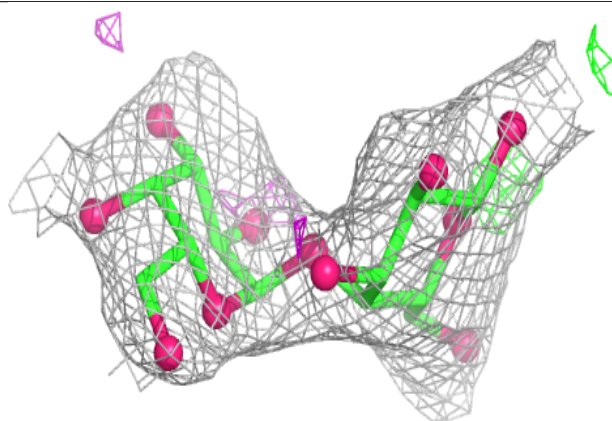
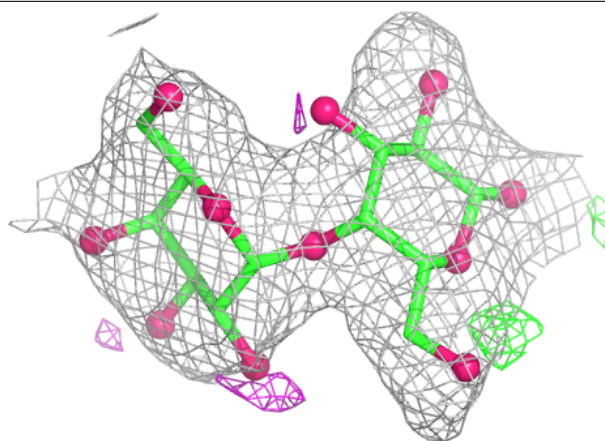
Electron density around Chain Z:

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

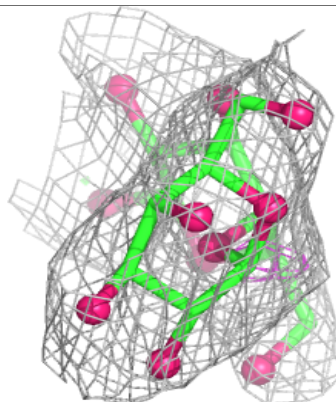
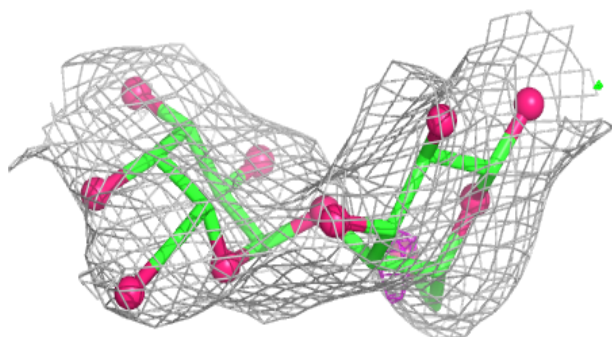
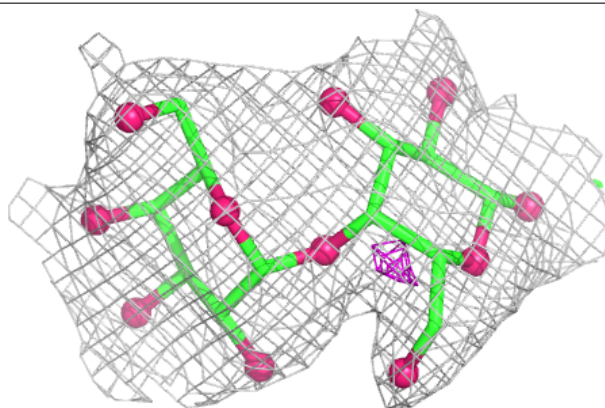


Electron density around Chain b:

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

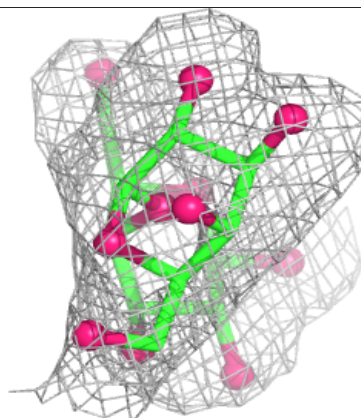
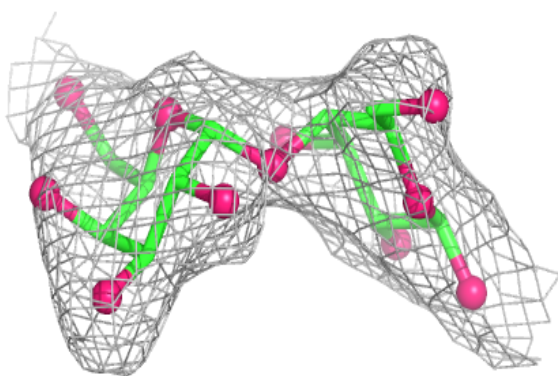
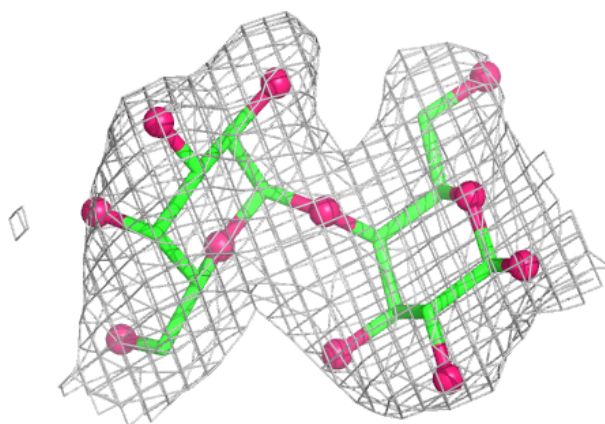
**Electron density around Chain d:**

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



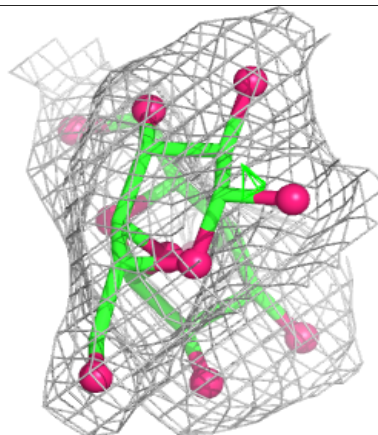
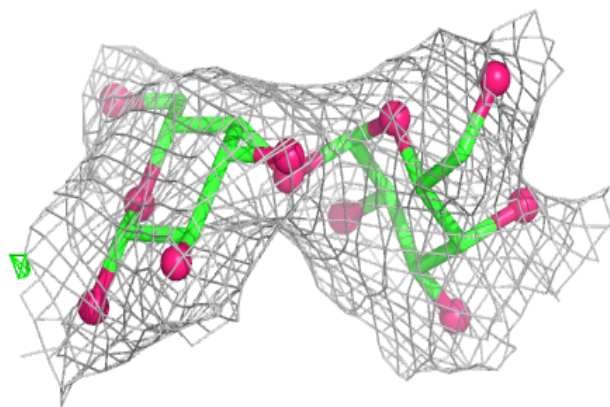
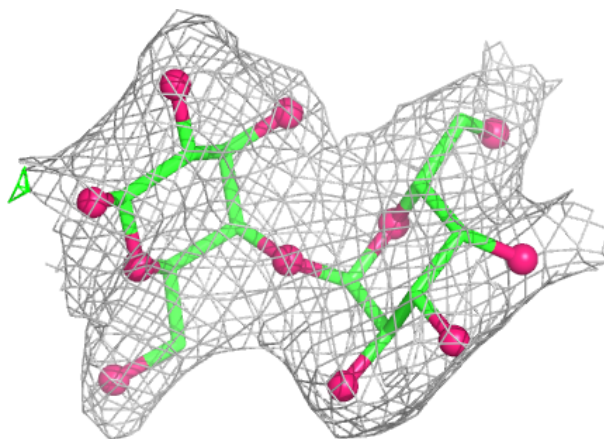
Electron density around Chain 1:

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



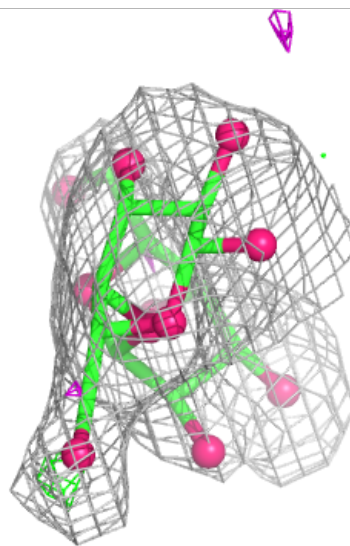
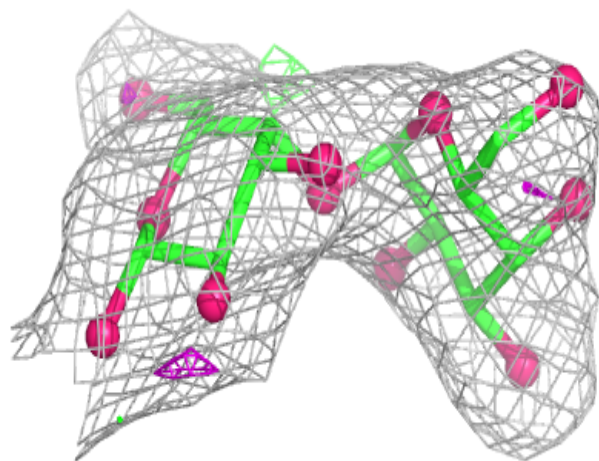
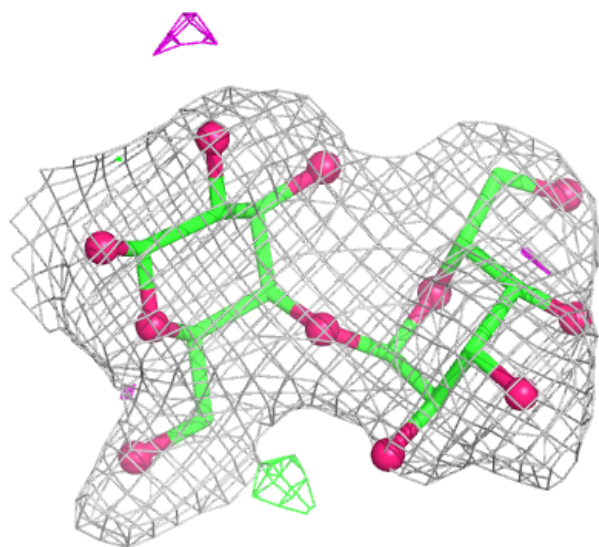
Electron density around Chain n:

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



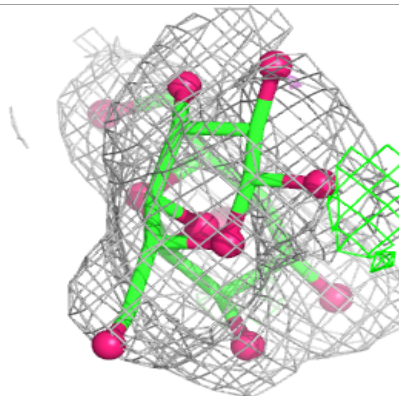
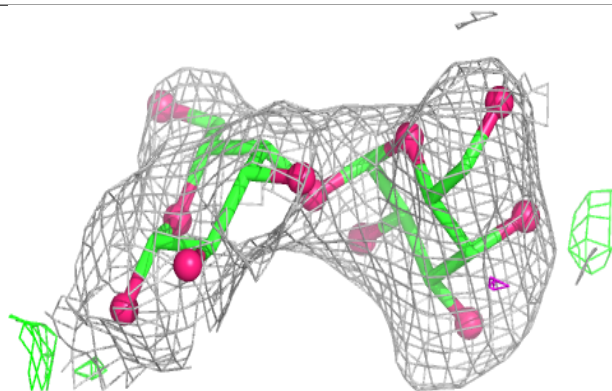
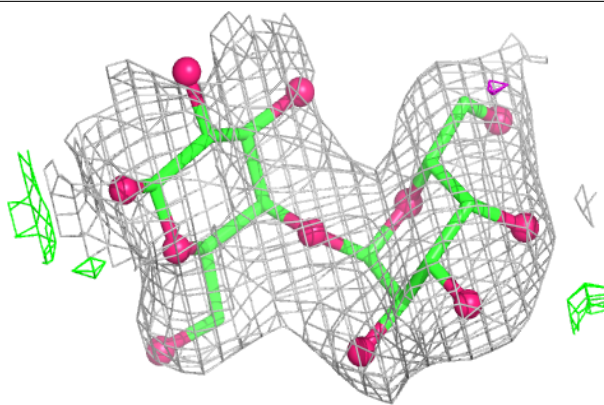
Electron density around Chain q:

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



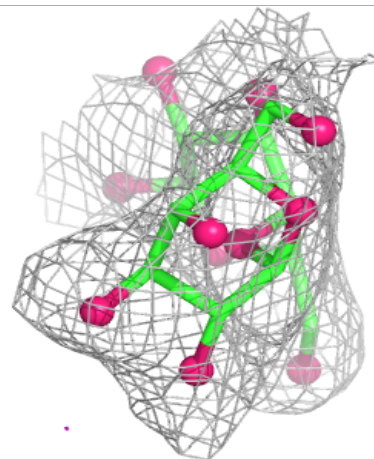
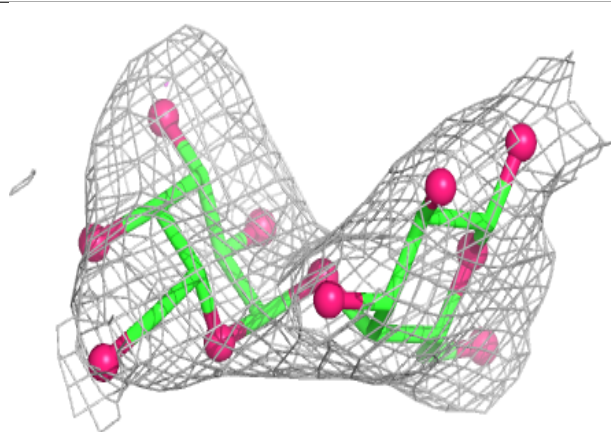
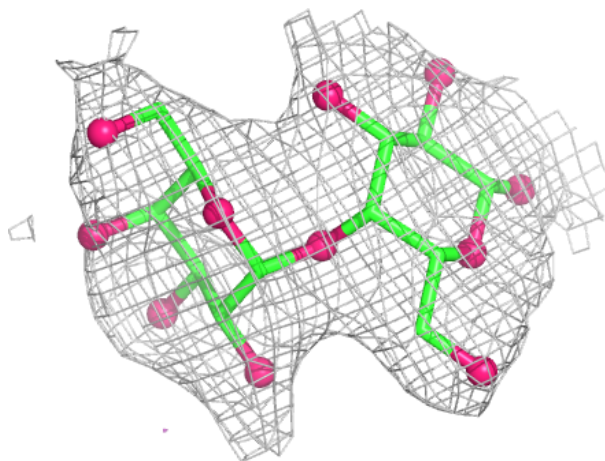
Electron density around Chain u:

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



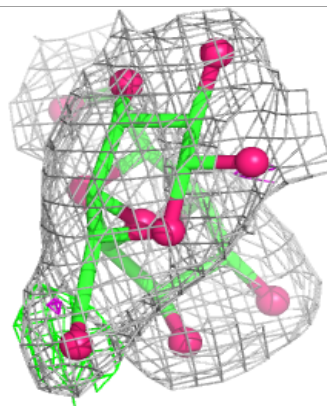
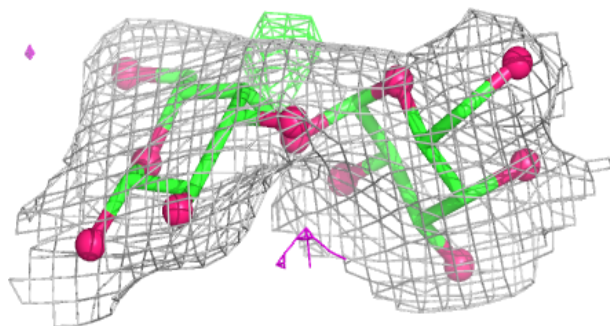
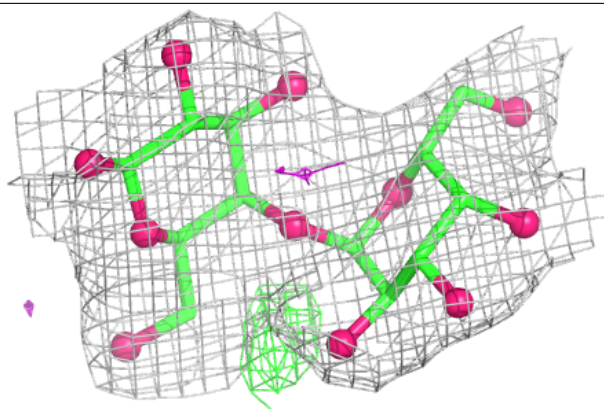
Electron density around Chain w:

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

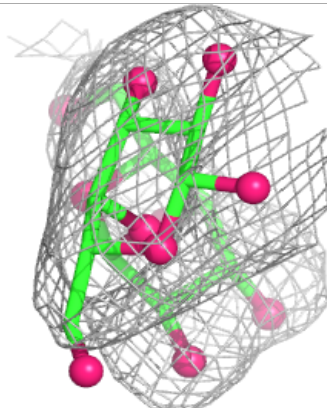
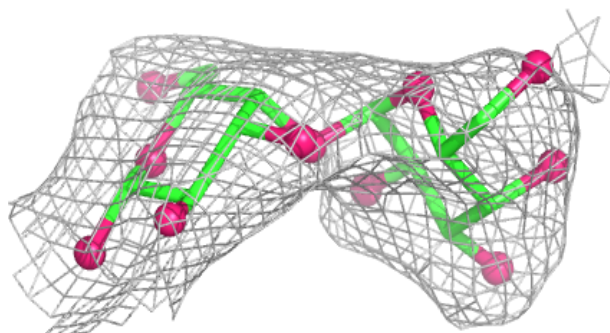
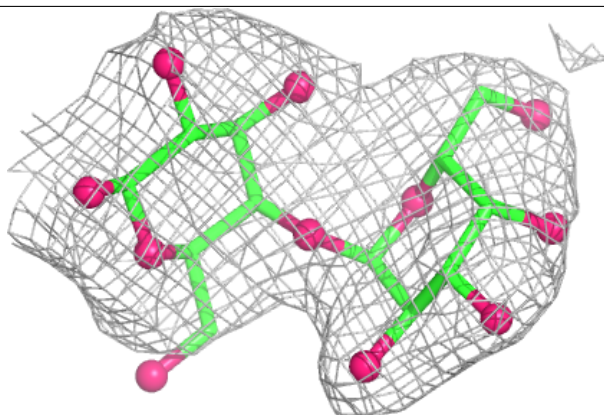


Electron density around Chain y:

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

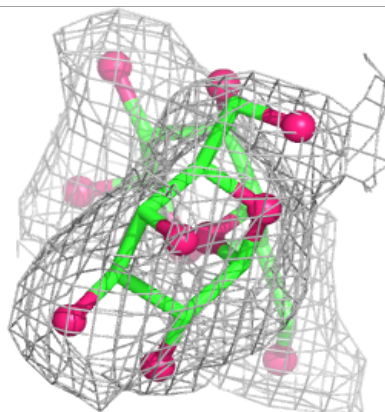
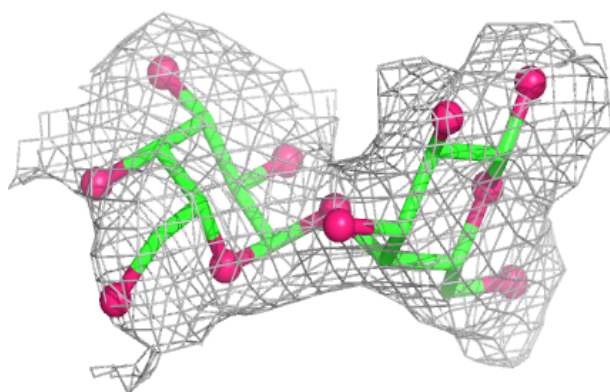
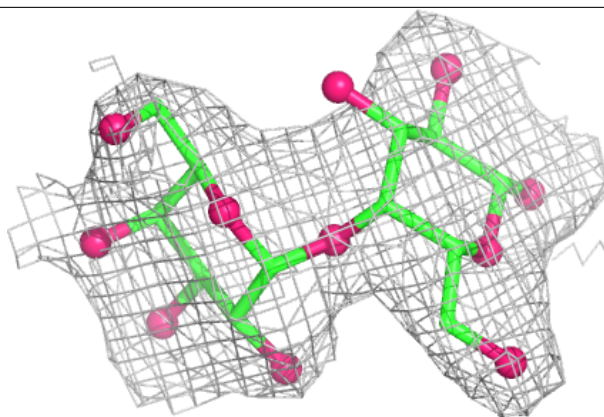
**Electron density around Chain 1:**

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

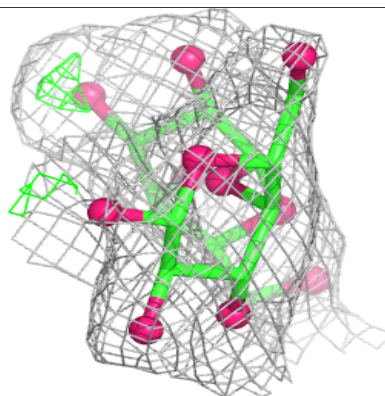
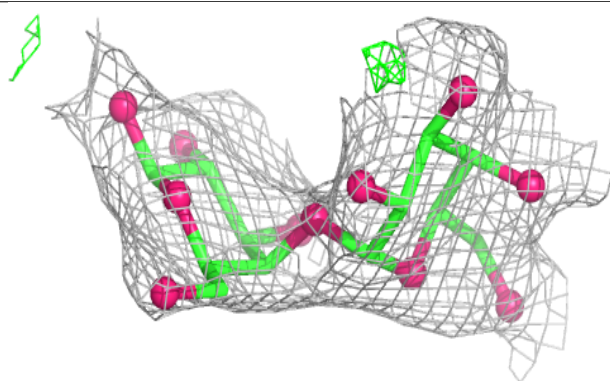
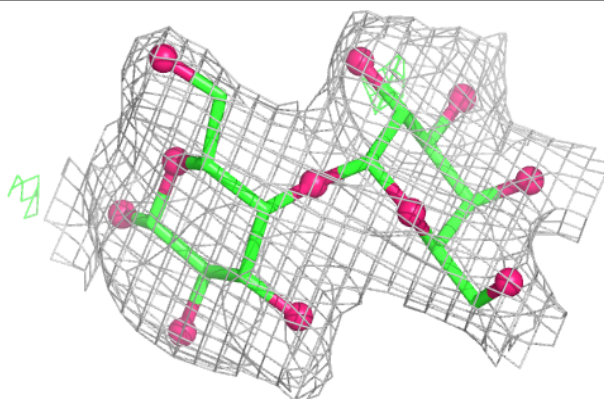


Electron density around Chain 3:

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

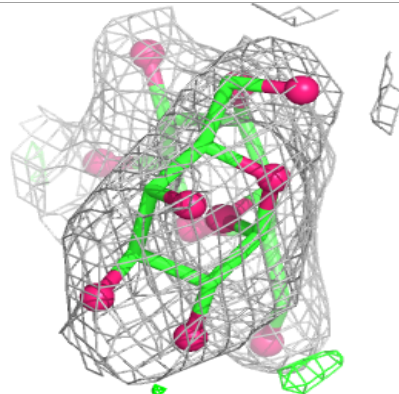
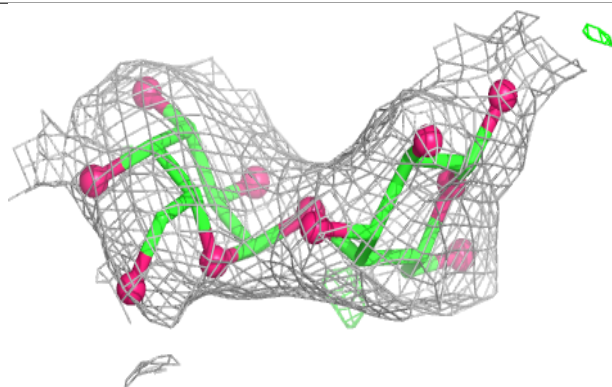
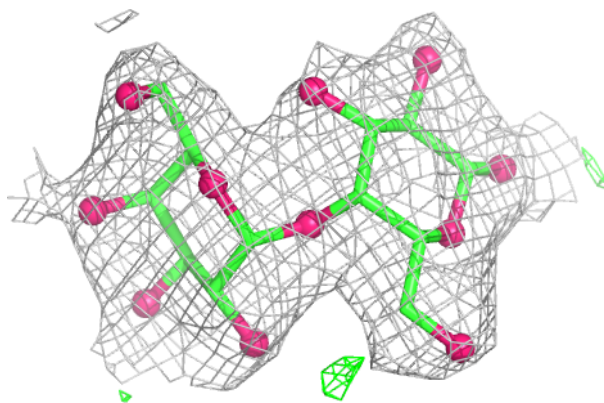
**Electron density around Chain 6:**

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

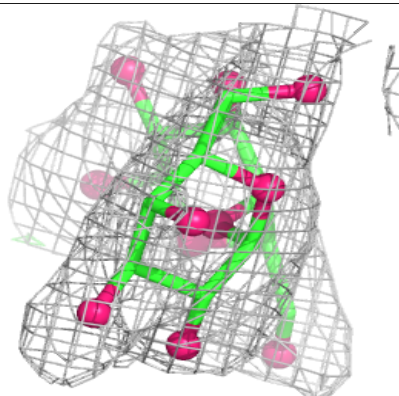
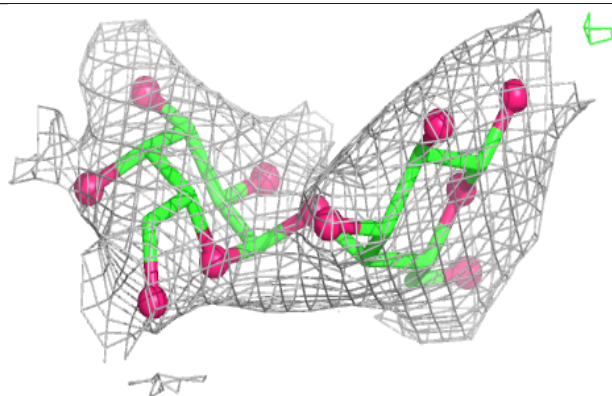
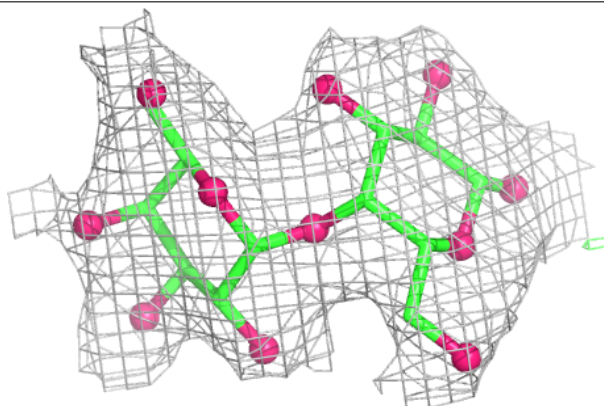


Electron density around Chain DA:

$2mF_o-DF_c$ (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, 95th 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	T	4570	12/12	0.61	0.23	65,74,76,77	0
4	GAL	N	3470	12/12	0.69	0.23	81,85,86,87	0
4	GAL	R	4370	12/12	0.71	0.18	81,88,90,91	0
4	GAL	J	2570	12/12	0.72	0.17	84,89,91,91	0
4	GAL	P	4170	12/12	0.72	0.18	68,81,83,83	0
4	GAL	E	1570	12/12	0.73	0.18	85,88,90,90	0
4	GAL	C	1370	12/12	0.75	0.19	67,74,77,77	0
4	GAL	G	2270	12/12	0.77	0.20	79,88,90,93	0
4	GAL	L	3270	12/12	0.79	0.20	55,65,68,71	0
4	GAL	K	3170	12/12	0.83	0.17	72,84,87,87	0
4	GAL	I	2470	12/12	0.83	0.17	79,81,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.