



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:50 PM UTC

PDB ID : 8VCQ / pdb_00008vcq
Title : Crystal structure of the oligomeric rMcL-1 in complex with raffinose
Authors : Hernandez-Santoyo, A.; Loera-Rubalcava, J.
Deposited on : 2023-12-14
Resolution : 2.09 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:

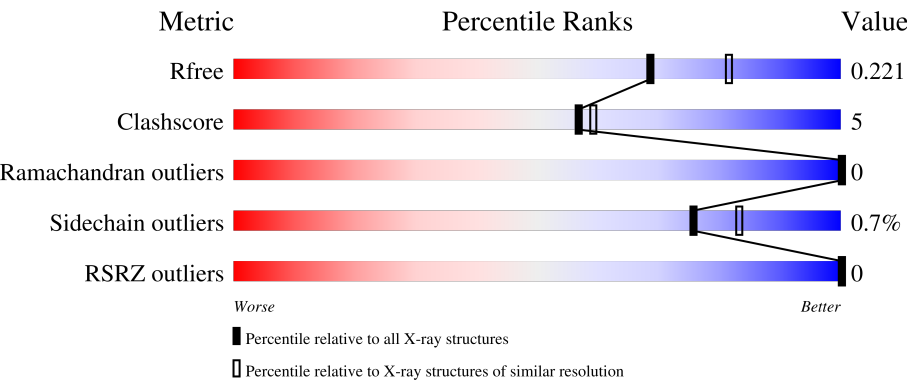
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.09 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.



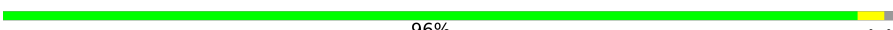
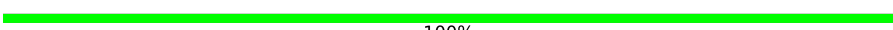
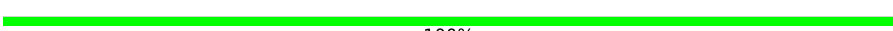
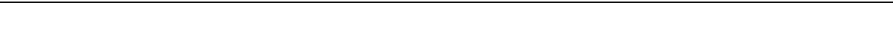
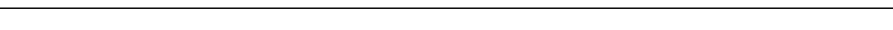
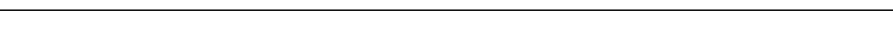
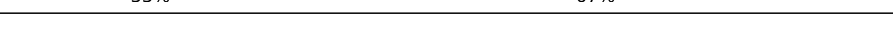
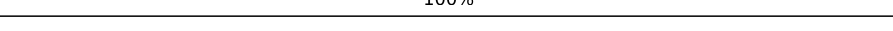
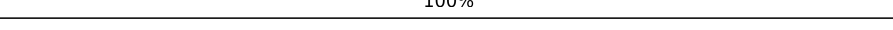
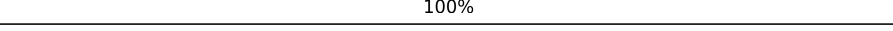
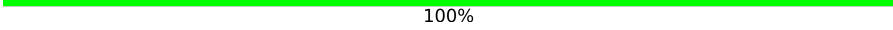
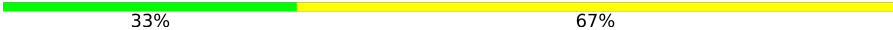
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	152	88%11%.
1	B	152	88%11%.
1	C	152	78%20%..
1	D	152	93%5%.
1	E	152	88%10%..

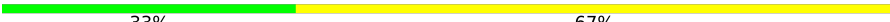
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Mol	Chain	Length	Quality of chain
1	F	152	 88% 11%
1	G	152	 88% 11%
1	H	152	 96%
2	I	3	 100%
2	L	3	 100%
2	M	3	 100%
2	N	3	 33% 67%
2	O	3	 100%
2	P	3	 67% 33%
2	Q	3	 100%
2	R	3	 100%
2	S	3	 33% 67%
2	T	3	 67% 33%
2	U	3	 33% 67%
2	V	3	 100%
2	W	3	 100%
2	X	3	 67% 33%
2	Y	3	 100%
2	Z	3	 33% 67%
2	a	3	 67% 33%
2	b	3	 33% 67%
2	c	3	 100%
2	d	3	 67% 33%
2	e	3	 33% 67%
2	f	3	 67% 33%

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Mol	Chain	Length	Quality of chain
2	g	3	 33%67%
2	h	3	 33%67%
2	i	3	 100%
2	j	3	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10897 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 Galactose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1198	765	216	213	4			
1	B	150	Total	C	N	O	S	0	0	0
			1201	767	216	213	5			
1	C	150	Total	C	N	O	S	0	0	0
			1198	765	216	213	4			
1	D	150	Total	C	N	O	S	0	0	0
			1201	767	216	213	5			
1	E	150	Total	C	N	O	S	0	0	0
			1201	767	216	213	5			
1	F	150	Total	C	N	O	S	0	0	0
			1201	767	216	213	5			
1	G	150	Total	C	N	O	S	0	0	0
			1198	765	216	213	4			
1	H	150	Total	C	N	O	S	0	0	0
			1201	767	216	213	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0P0E482
A	0	HIS	-	expression tag	UNP A0A0P0E482
A	107	ILE	VAL	variant	UNP A0A0P0E482
A	130	LYS	GLY	variant	UNP A0A0P0E482
A	141	ASP	ASN	variant	UNP A0A0P0E482
B	-1	GLY	-	expression tag	UNP A0A0P0E482
B	0	HIS	-	expression tag	UNP A0A0P0E482
B	107	ILE	VAL	variant	UNP A0A0P0E482
B	130	LYS	GLY	variant	UNP A0A0P0E482
B	141	ASP	ASN	variant	UNP A0A0P0E482
C	-1	GLY	-	expression tag	UNP A0A0P0E482
C	0	HIS	-	expression tag	UNP A0A0P0E482
C	107	ILE	VAL	variant	UNP A0A0P0E482

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Chain	Residue	Modelled	Actual	Comment	Reference
C	130	LYS	GLY	variant	UNP A0A0P0E482
C	141	ASP	ASN	variant	UNP A0A0P0E482
D	-1	GLY	-	expression tag	UNP A0A0P0E482
D	0	HIS	-	expression tag	UNP A0A0P0E482
D	107	ILE	VAL	variant	UNP A0A0P0E482
D	130	LYS	GLY	variant	UNP A0A0P0E482
D	141	ASP	ASN	variant	UNP A0A0P0E482
E	-1	GLY	-	expression tag	UNP A0A0P0E482
E	0	HIS	-	expression tag	UNP A0A0P0E482
E	107	ILE	VAL	variant	UNP A0A0P0E482
E	130	LYS	GLY	variant	UNP A0A0P0E482
E	141	ASP	ASN	variant	UNP A0A0P0E482
F	-1	GLY	-	expression tag	UNP A0A0P0E482
F	0	HIS	-	expression tag	UNP A0A0P0E482
F	107	ILE	VAL	variant	UNP A0A0P0E482
F	130	LYS	GLY	variant	UNP A0A0P0E482
F	141	ASP	ASN	variant	UNP A0A0P0E482
G	-1	GLY	-	expression tag	UNP A0A0P0E482
G	0	HIS	-	expression tag	UNP A0A0P0E482
G	107	ILE	VAL	variant	UNP A0A0P0E482
G	130	LYS	GLY	variant	UNP A0A0P0E482
G	141	ASP	ASN	variant	UNP A0A0P0E482
H	-1	GLY	-	expression tag	UNP A0A0P0E482
H	0	HIS	-	expression tag	UNP A0A0P0E482
H	107	ILE	VAL	variant	UNP A0A0P0E482
H	130	LYS	GLY	variant	UNP A0A0P0E482
H	141	ASP	ASN	variant	UNP A0A0P0E482

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranoside-(1-2)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	3	Total	C	O	0	0	0
			34	18	16			
2	L	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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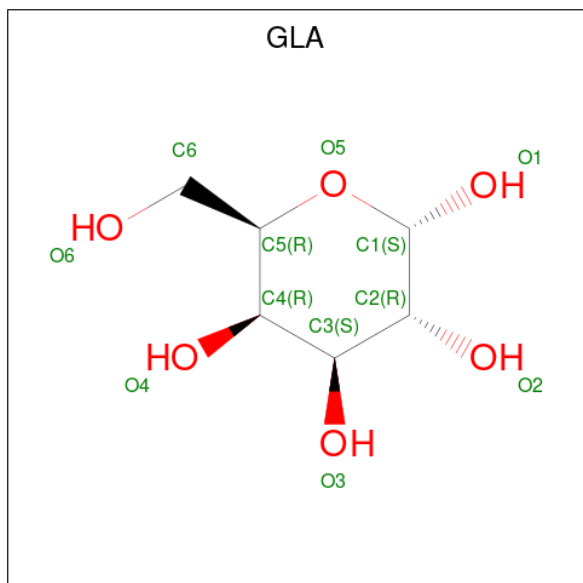
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	N	3	Total	C	O	0	0	0
			34	18	16			
2	O	3	Total	C	O	0	0	0
			34	18	16			
2	P	3	Total	C	O	0	0	0
			34	18	16			
2	Q	3	Total	C	O	0	0	0
			34	18	16			
2	R	3	Total	C	O	0	0	0
			34	18	16			
2	S	3	Total	C	O	0	0	0
			34	18	16			
2	T	3	Total	C	O	0	0	0
			34	18	16			
2	U	3	Total	C	O	0	0	0
			34	18	16			
2	V	3	Total	C	O	0	0	1
			23	12	11			
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	Y	3	Total	C	O	0	0	0
			34	18	16			
2	Z	3	Total	C	O	0	0	0
			34	18	16			
2	a	3	Total	C	O	0	0	0
			34	18	16			
2	b	3	Total	C	O	0	0	0
			34	18	16			
2	c	3	Total	C	O	0	0	0
			34	18	16			
2	d	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	0	0	1
			23	12	11			
2	h	3	Total	C	O	0	0	1
			23	12	11			

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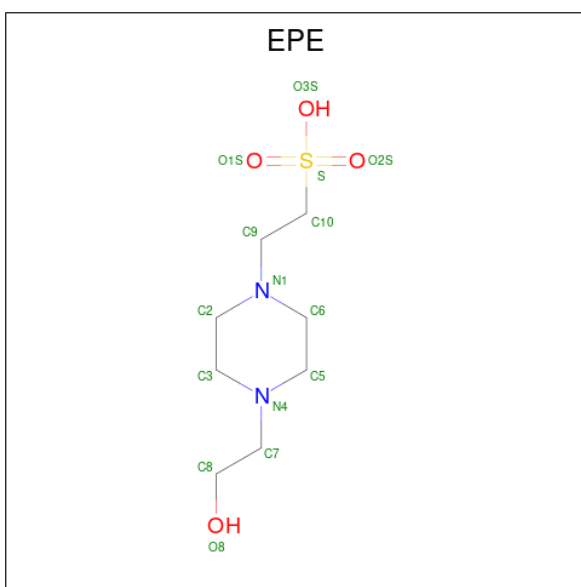
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	i	3	Total	C	O	0	0	0
			34	18	16			
2	j	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is alpha-D-galactopyranose (CCD ID: GLA) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



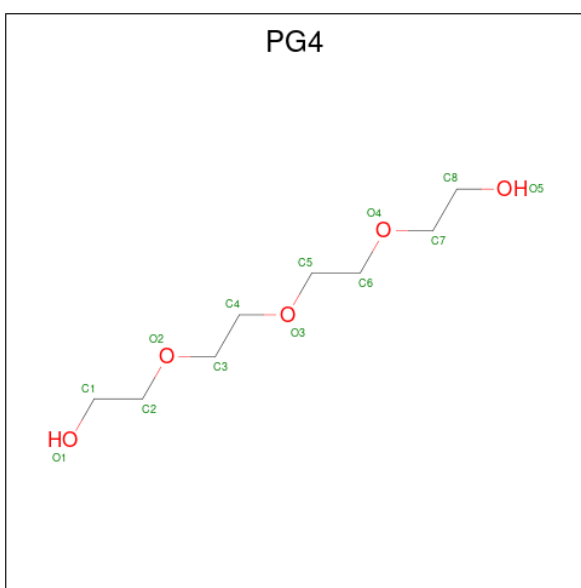
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

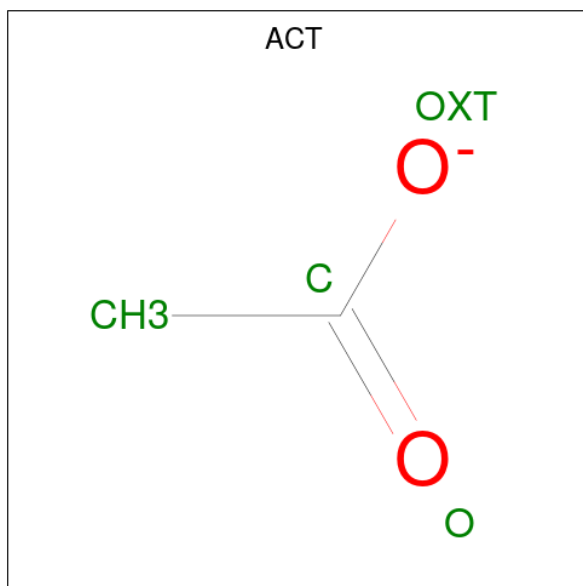


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		
5	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

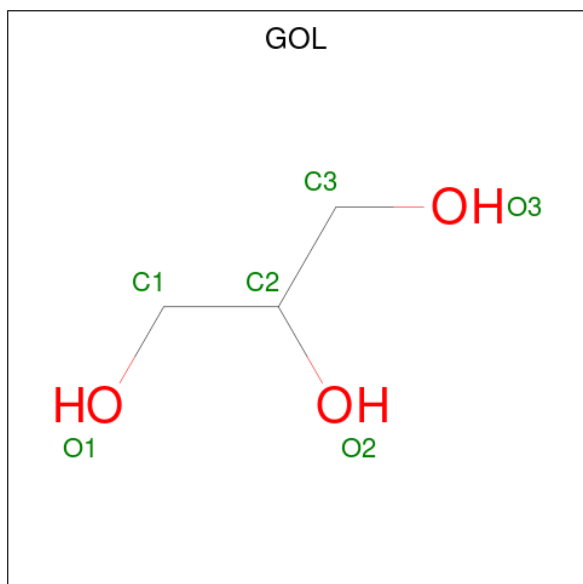
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	40	Total	O	0	0
			40	40		
9	B	68	Total	O	0	0
			68	68		
9	C	22	Total	O	0	0
			22	22		
9	D	50	Total	O	0	0
			50	50		
9	E	27	Total	O	0	0
			27	27		
9	F	45	Total	O	0	0
			45	45		
9	G	41	Total	O	0	0
			41	41		
9	H	63	Total	O	0	0
			63	63		

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: Galactose-binding lectin

Chain A: 



- Molecule 1: Galactose-binding lectin

Chain B: 

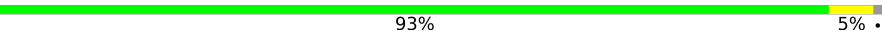


- Molecule 1: Galactose-binding lectin

Chain C: 



- Molecule 1: Galactose-binding lectin

Chain D: 



- Molecule 1: Galactose-binding lectin

Chain E: 



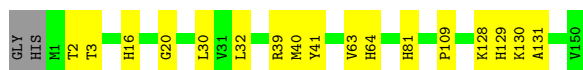
- Molecule 1: Galactose-binding lectin

Chain F: 



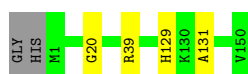
- Molecule 1: Galactose-binding lectin

Chain G: 88% 11%



- Molecule 1: Galactose-binding lectin

Chain H: 96%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain I: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain L: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain M: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain N: 33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain O:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain P:  67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain Q:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain R:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain S:  33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain T:  67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain U:  33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain V:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain W:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain X:  67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain Y:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain Z:  33% 67%

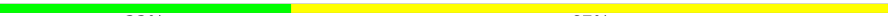


- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain a:  67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain b:  33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain c:  100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain d:  67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain e:  33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain f:  67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain g:  33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain h:  33% 67%



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain i:  100%

FRU1
GLC2
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain j:  100%

FRU1
GLC2
GLA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.52Å 77.93Å 156.28Å 90.00° 89.89° 90.00°	Depositor
Resolution (Å)	49.34 – 2.09 49.34 – 2.09	Depositor EDS
% Data completeness (in resolution range)	89.5 (49.34-2.09) 80.9 (49.34-2.09)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.202 , 0.236 (Not available) , 0.221	Depositor DCC
R_{free} test set	1777 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10897	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9049e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PG4, ACT, GLC, GLA, EPE, GOL, FRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1233	0.54	0/1663
1	B	0.18	0/1236	0.51	0/1666
1	C	0.32	0/1233	0.56	0/1663
1	D	0.25	0/1236	0.50	0/1666
1	E	0.31	0/1236	0.55	0/1666
1	F	0.21	0/1236	0.50	0/1666
1	G	0.18	0/1233	0.49	0/1663
1	H	0.15	0/1236	0.45	0/1666
All	All	0.24	0/9879	0.51	0/13319

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1198	0	1179	11	0
1	B	1201	0	1186	9	0
1	C	1198	0	1179	26	0
1	D	1201	0	1186	7	0
1	E	1201	0	1186	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1201	0	1186	16	0
1	G	1198	0	1179	10	0
1	H	1201	0	1186	3	0
2	I	34	0	30	0	0
2	L	34	0	30	0	0
2	M	34	0	30	0	0
2	N	34	0	30	1	0
2	O	34	0	30	0	0
2	P	34	0	30	0	0
2	Q	34	0	30	0	0
2	R	34	0	30	0	0
2	S	34	0	30	1	0
2	T	34	0	30	0	0
2	U	34	0	30	0	0
2	V	23	0	19	0	0
2	W	34	0	30	0	0
2	X	34	0	30	0	0
2	Y	34	0	30	0	0
2	Z	34	0	30	0	0
2	a	34	0	30	1	0
2	b	34	0	30	1	0
2	c	34	0	30	0	0
2	d	34	0	30	0	0
2	e	34	0	30	1	0
2	f	34	0	30	0	0
2	g	23	0	19	0	0
2	h	23	0	19	0	0
2	i	34	0	30	0	0
2	j	34	0	30	0	0
3	A	12	0	12	1	0
3	G	12	0	12	1	0
4	D	15	0	18	0	0
4	F	15	0	18	1	0
5	D	13	0	18	0	0
5	F	13	0	18	4	0
6	D	1	0	0	0	0
7	F	4	0	3	0	0
8	F	6	0	8	0	0
9	A	40	0	0	0	0
9	B	68	0	0	0	0
9	C	22	0	0	0	0
9	D	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	27	0	0	0	0
9	F	45	0	0	1	0
9	G	41	0	0	0	0
9	H	63	0	0	0	0
All	All	10897	0	10321	95	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 5.

All (95) 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:D:129:HIS:CE1	1:D:131:ALA:HB3	1.74	1.21
1:F:82:GLN:HE21	5:F:203:PG4:H12	1.14	1.04
1:C:29:ASN:ND2	1:C:77:LYS:HE3	1.76	1.00
1:D:129:HIS:HE1	1:D:131:ALA:HB3	1.19	0.98
1:F:83:ASP:OD1	5:F:203:PG4:H11	1.65	0.94
1:C:29:ASN:HD21	1:C:77:LYS:HE3	1.28	0.94
1:F:15:LEU:HD11	1:F:30:LEU:HB3	1.58	0.84
1:F:82:GLN:NE2	5:F:203:PG4:H12	1.97	0.74
1:F:82:GLN:HE21	5:F:203:PG4:C1	1.98	0.70
1:F:18:LYS:NZ	1:F:119:GLU:OE1	2.24	0.69
1:F:118:ASN:O	1:F:119:GLU:HB2	1.94	0.68
1:C:15:LEU:HG	1:C:30:LEU:HD12	1.78	0.64
1:C:27:ASP:HA	1:C:79:VAL:HG21	1.80	0.64
1:B:32:LEU:HD12	1:B:116:PRO:HG2	1.80	0.63
1:D:129:HIS:ND1	1:D:131:ALA:HB3	2.12	0.63
1:C:29:ASN:HD21	1:C:77:LYS:CE	2.07	0.62
1:A:129:HIS:CE1	1:A:131:ALA:HB3	2.34	0.62
1:F:129:HIS:ND1	4:F:201:EPE:H21	2.15	0.61
1:C:129:HIS:CE1	1:C:131:ALA:HB3	2.36	0.61
1:E:129:HIS:CE1	1:E:131:ALA:HB3	2.36	0.61
1:C:61:LYS:HE3	1:C:82:GLN:HG2	1.84	0.59
3:G:201:GLA:H62	2:N:3:GLA:O2	2.03	0.58
1:G:129:HIS:CE1	1:G:131:ALA:HB3	2.37	0.58
1:F:129:HIS:CE1	1:F:131:ALA:HB3	2.40	0.56
2:b:1:FRU:H61	2:b:2:GLC:H62	1.87	0.56
1:A:129:HIS:HE1	1:A:131:ALA:HB3	1.71	0.55
1:C:129:HIS:HE1	1:C:131:ALA:HB3	1.72	0.55
1:H:129:HIS:CE1	1:H:131:ALA:HB3	2.42	0.54
3:A:201:GLA:H62	2:S:3:GLA:O2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:HD21	1:C:124:MET:SD	2.49	0.53
1:D:149:TYR:O	1:D:150:VAL:HG13	2.09	0.52
1:C:11:SER:HB3	1:C:116:PRO:HD2	1.91	0.52
1:B:99:ILE:HG21	1:B:107:ILE:HD12	1.92	0.52
1:C:27:ASP:HA	1:C:79:VAL:CG2	2.40	0.52
1:E:78:LEU:HD21	1:E:124:MET:SD	2.51	0.51
1:G:30:LEU:HD11	1:G:63:VAL:HG22	1.93	0.51
1:G:129:HIS:HE1	1:G:131:ALA:HB3	1.75	0.51
1:E:2:THR:OG1	1:E:150:VAL:O	2.27	0.51
1:E:31:VAL:HG12	1:E:121:LEU:HD12	1.92	0.51
2:e:1:FRU:H62	2:e:2:GLC:H5	1.92	0.51
1:A:7:LYS:HE2	1:A:135:ILE:HD11	1.94	0.50
1:G:20:GLY:O	1:G:39:ARG:HD2	2.12	0.50
1:C:77:LYS:HD2	1:C:121:LEU:HD13	1.92	0.50
1:H:20:GLY:O	1:H:39:ARG:HD2	2.12	0.50
1:E:119:GLU:OE1	2:a:2:GLC:O4	2.31	0.48
1:E:129:HIS:HE1	1:E:131:ALA:HB3	1.77	0.48
1:A:140:LYS:HE2	1:A:140:LYS:HB3	1.50	0.48
1:E:117:PRO:O	1:E:120:THR:OG1	2.31	0.48
1:E:16:HIS:CE1	1:E:40:MET:HG2	2.49	0.48
1:F:129:HIS:HE1	1:F:131:ALA:HB3	1.79	0.48
1:B:7:LYS:HE2	1:B:135:ILE:HD11	1.96	0.47
1:B:78:LEU:HD21	1:B:124:MET:SD	2.54	0.47
1:C:41:TYR:CZ	1:C:139:PRO:HB3	2.50	0.47
1:B:37:HIS:CE1	1:B:39:ARG:HB2	2.49	0.47
1:C:31:VAL:HG12	1:C:121:LEU:HA	1.97	0.46
1:G:3:THR:CG2	1:G:41:TYR:HB3	2.45	0.46
1:B:20:GLY:O	1:B:39:ARG:HD2	2.16	0.46
1:C:31:VAL:HG12	1:C:121:LEU:HD23	1.97	0.46
1:F:118:ASN:O	1:F:119:GLU:CB	2.64	0.46
1:C:28:THR:O	1:C:79:VAL:HB	2.15	0.45
1:D:78:LEU:HD21	1:D:124:MET:SD	2.56	0.45
1:B:64:HIS:CD2	1:B:81:HIS:HB3	2.52	0.45
1:B:108:HIS:CD2	1:B:125:HIS:HB3	2.52	0.45
1:C:34:SER:H	1:C:118:ASN:HD21	1.64	0.44
1:F:78:LEU:HD21	1:F:124:MET:SD	2.57	0.44
1:E:7:LYS:HD3	1:E:135:ILE:HD11	1.99	0.44
1:D:20:GLY:O	1:D:39:ARG:HD2	2.18	0.44
1:F:20:GLY:O	1:F:39:ARG:HD2	2.17	0.44
1:A:47:VAL:HG13	1:C:82:GLN:HG3	2.00	0.44
1:C:32:LEU:CD1	1:C:109:PRO:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:HIS:CE1	1:G:40:MET:HG2	2.53	0.43
1:C:16:HIS:CD2	1:C:33:HIS:HB3	2.54	0.43
1:A:78:LEU:HD21	1:A:124:MET:SD	2.59	0.43
1:C:5:LEU:HD22	1:C:40:MET:SD	2.59	0.43
1:G:130:LYS:HA	1:G:130:LYS:HD2	1.90	0.43
1:G:64:HIS:CD2	1:G:81:HIS:HB3	2.54	0.43
1:H:129:HIS:HE1	1:H:131:ALA:HB3	1.82	0.42
1:A:128:LYS:HB3	1:A:128:LYS:HE2	1.80	0.42
1:B:16:HIS:CE1	1:B:40:MET:HG2	2.54	0.42
1:C:20:GLY:O	1:C:39:ARG:HD2	2.20	0.42
1:C:30:LEU:HD13	1:C:30:LEU:HA	1.83	0.42
1:A:20:GLY:O	1:A:39:ARG:HD2	2.20	0.41
1:A:5:LEU:HD22	1:A:40:MET:SD	2.60	0.41
1:C:29:ASN:HA	1:C:79:VAL:HG12	2.02	0.41
1:F:38:GLU:H	1:F:38:GLU:CD	2.27	0.41
1:A:64:HIS:CD2	1:A:81:HIS:HB3	2.56	0.41
1:G:128:LYS:HB3	1:G:128:LYS:HE2	1.75	0.41
1:E:69:LYS:HA	1:E:69:LYS:HD2	1.69	0.41
1:C:32:LEU:HD11	1:C:109:PRO:HB3	2.03	0.41
1:D:149:TYR:O	1:D:150:VAL:CG1	2.69	0.41
1:F:24:PRO:HB3	9:F:336:HOH:O	2.20	0.41
1:G:32:LEU:CD1	1:G:109:PRO:HB3	2.52	0.41
1:C:9:LYS:HD3	1:C:135:ILE:HG23	2.04	0.40
1:A:106:TYR:CE2	1:A:128:LYS:HG3	2.56	0.40
1:E:95:PHE:CE2	1:F:93:ASP:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/152 (97%)	144 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
1	C	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
1	D	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
1	E	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
1	F	148/152 (97%)	143 (97%)	5 (3%)	0	100	100
1	G	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
1	H	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
All	All	1184/1216 (97%)	1147 (97%)	37 (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	129/131 (98%)	128 (99%)	1 (1%)	73	81
1	B	130/131 (99%)	130 (100%)	0	100	100
1	C	129/131 (98%)	127 (98%)	2 (2%)	55	64
1	D	130/131 (99%)	130 (100%)	0	100	100
1	E	130/131 (99%)	128 (98%)	2 (2%)	57	65
1	F	130/131 (99%)	129 (99%)	1 (1%)	73	81
1	G	129/131 (98%)	128 (99%)	1 (1%)	73	81
1	H	130/131 (99%)	130 (100%)	0	100	100
All	All	1037/1048 (99%)	1030 (99%)	7 (1%)	76	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	VAL
1	C	3	THR

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Mol	Chain	Res	Type
1	C	30	LEU
1	E	69	LYS
1	E	150	VAL
1	F	22	SER
1	G	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	115	ASN
1	C	29	ASN
1	C	115	ASN
1	C	118	ASN
1	E	29	ASN
1	F	29	ASN
1	F	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

Of 78 monosaccharides modelled in this entry, 75 were used for Mogul analysis.

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	FRU	I	1	2	11,12,12	0.55	0	10,18,18	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	I	2	2	11,11,12	0.21	0	15,15,17	0.64	0
2	GLA	I	3	2	11,11,12	0.22	0	15,15,17	0.61	0
2	FRU	L	1	2	11,12,12	0.57	0	10,18,18	0.68	0
2	GLC	L	2	2	11,11,12	0.27	0	15,15,17	0.74	0
2	GLA	L	3	2	11,11,12	0.24	0	15,15,17	0.72	0
2	FRU	M	1	2	11,12,12	0.55	0	10,18,18	0.54	0
2	GLC	M	2	2	11,11,12	0.19	0	15,15,17	0.63	0
2	GLA	M	3	2	11,11,12	0.22	0	15,15,17	0.66	0
2	FRU	N	1	2	11,12,12	0.55	0	10,18,18	0.73	0
2	GLC	N	2	2	11,11,12	0.30	0	15,15,17	1.16	3 (20%)
2	GLA	N	3	2	11,11,12	0.18	0	15,15,17	0.61	0
2	FRU	O	1	2	11,12,12	0.60	0	10,18,18	0.68	0
2	GLC	O	2	2	11,11,12	0.21	0	15,15,17	0.70	0
2	GLA	O	3	2	11,11,12	0.24	0	15,15,17	0.67	0
2	FRU	P	1	2	11,12,12	0.53	0	10,18,18	0.70	0
2	GLC	P	2	2	11,11,12	0.21	0	15,15,17	0.97	1 (6%)
2	GLA	P	3	2	11,11,12	0.21	0	15,15,17	0.57	0
2	FRU	Q	1	2	11,12,12	0.49	0	10,18,18	0.89	0
2	GLC	Q	2	2	11,11,12	0.24	0	15,15,17	0.72	0
2	GLA	Q	3	2	11,11,12	0.21	0	15,15,17	0.46	0
2	FRU	R	1	2	11,12,12	0.56	0	10,18,18	0.59	0
2	GLC	R	2	2	11,11,12	0.23	0	15,15,17	0.67	0
2	GLA	R	3	2	11,11,12	0.26	0	15,15,17	0.66	0
2	FRU	S	1	2	11,12,12	0.51	0	10,18,18	0.89	0
2	GLC	S	2	2	11,11,12	0.27	0	15,15,17	1.72	5 (33%)
2	GLA	S	3	2	11,11,12	0.24	0	15,15,17	0.73	0
2	FRU	T	1	2	11,12,12	0.55	0	10,18,18	0.58	0
2	GLC	T	2	2	11,11,12	0.19	0	15,15,17	1.01	1 (6%)
2	GLA	T	3	2	11,11,12	0.22	0	15,15,17	0.64	0
2	FRU	U	1	2	11,12,12	0.54	0	10,18,18	0.73	0
2	GLC	U	2	2	11,11,12	0.41	0	15,15,17	1.37	2 (13%)
2	GLA	U	3	2	11,11,12	0.28	0	15,15,17	0.96	1 (6%)
2	GLC	V	2	2	11,11,12	0.35	0	15,15,17	0.89	0
2	GLA	V	3	2	11,11,12	0.19	0	15,15,17	0.60	0
2	FRU	W	1	2	11,12,12	0.53	0	10,18,18	0.60	0
2	GLC	W	2	2	11,11,12	0.29	0	15,15,17	0.75	0
2	GLA	W	3	2	11,11,12	0.21	0	15,15,17	0.63	0
2	FRU	X	1	2	11,12,12	0.61	0	10,18,18	0.64	0
2	GLC	X	2	2	11,11,12	0.21	0	15,15,17	0.56	0
2	GLA	X	3	2	11,11,12	0.20	0	15,15,17	0.75	1 (6%)
2	FRU	Y	1	2	11,12,12	0.58	0	10,18,18	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	Y	2	2	11,11,12	0.33	0	15,15,17	0.70	0
2	GLA	Y	3	2	11,11,12	0.25	0	15,15,17	0.44	0
2	FRU	Z	1	2	11,12,12	0.67	1 (9%)	10,18,18	0.80	0
2	GLC	Z	2	2	11,11,12	0.40	0	15,15,17	1.81	4 (26%)
2	GLA	Z	3	2	11,11,12	0.19	0	15,15,17	0.67	0
2	FRU	a	1	2	11,12,12	0.51	0	10,18,18	0.86	0
2	GLC	a	2	2	11,11,12	0.30	0	15,15,17	0.80	0
2	GLA	a	3	2	11,11,12	0.22	0	15,15,17	0.50	0
2	FRU	b	1	2	11,12,12	0.66	0	10,18,18	0.78	0
2	GLC	b	2	2	11,11,12	0.41	0	15,15,17	1.00	0
2	GLA	b	3	2	11,11,12	0.24	0	15,15,17	0.53	0
2	FRU	c	1	2	11,12,12	0.56	0	10,18,18	0.89	0
2	GLC	c	2	2	11,11,12	0.33	0	15,15,17	0.80	0
2	GLA	c	3	2	11,11,12	0.23	0	15,15,17	0.54	0
2	FRU	d	1	2	11,12,12	0.58	0	10,18,18	0.75	0
2	GLC	d	2	2	11,11,12	0.38	0	15,15,17	2.05	7 (46%)
2	GLA	d	3	2	11,11,12	0.21	0	15,15,17	0.52	0
2	FRU	e	1	2	11,12,12	0.57	0	10,18,18	0.56	0
2	GLC	e	2	2	11,11,12	0.31	0	15,15,17	0.88	0
2	GLA	e	3	2	11,11,12	0.21	0	15,15,17	0.59	0
2	FRU	f	1	2	11,12,12	0.57	0	10,18,18	0.48	0
2	GLC	f	2	2	11,11,12	0.35	0	15,15,17	1.34	2 (13%)
2	GLA	f	3	2	11,11,12	0.20	0	15,15,17	0.50	0
2	GLC	g	2	2	11,11,12	0.36	0	15,15,17	1.59	2 (13%)
2	GLA	g	3	2	11,11,12	0.44	0	15,15,17	1.48	2 (13%)
2	GLC	h	2	2	11,11,12	0.32	0	15,15,17	1.48	2 (13%)
2	GLA	h	3	2	11,11,12	0.44	0	15,15,17	1.49	2 (13%)
2	FRU	i	1	2	11,12,12	0.54	0	10,18,18	0.68	0
2	GLC	i	2	2	11,11,12	0.19	0	15,15,17	0.76	0
2	GLA	i	3	2	11,11,12	0.20	0	15,15,17	0.64	0
2	FRU	j	1	2	11,12,12	0.55	0	10,18,18	0.82	0
2	GLC	j	2	2	11,11,12	0.32	0	15,15,17	0.76	0
2	GLA	j	3	2	11,11,12	0.22	0	15,15,17	0.66	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
2	FRU	I	1	2	-	3/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	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	FRU	L	1	2	-	1/5/24/24	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1
2	GLA	L	3	2	-	0/2/19/22	0/1/1/1
2	FRU	M	1	2	-	3/5/24/24	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLA	M	3	2	-	0/2/19/22	0/1/1/1
2	FRU	N	1	2	-	3/5/24/24	0/1/1/1
2	GLC	N	2	2	-	0/2/19/22	0/1/1/1
2	GLA	N	3	2	-	0/2/19/22	0/1/1/1
2	FRU	O	1	2	-	2/5/24/24	0/1/1/1
2	GLC	O	2	2	-	2/2/19/22	0/1/1/1
2	GLA	O	3	2	-	0/2/19/22	0/1/1/1
2	FRU	P	1	2	-	5/5/24/24	0/1/1/1
2	GLC	P	2	2	-	0/2/19/22	0/1/1/1
2	GLA	P	3	2	-	0/2/19/22	0/1/1/1
2	FRU	Q	1	2	-	1/5/24/24	0/1/1/1
2	GLC	Q	2	2	-	0/2/19/22	0/1/1/1
2	GLA	Q	3	2	-	0/2/19/22	0/1/1/1
2	FRU	R	1	2	-	1/5/24/24	0/1/1/1
2	GLC	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	FRU	S	1	2	-	3/5/24/24	0/1/1/1
2	GLC	S	2	2	-	2/2/19/22	0/1/1/1
2	GLA	S	3	2	-	0/2/19/22	0/1/1/1
2	FRU	T	1	2	-	2/5/24/24	0/1/1/1
2	GLC	T	2	2	-	0/2/19/22	0/1/1/1
2	GLA	T	3	2	-	0/2/19/22	0/1/1/1
2	FRU	U	1	2	-	2/5/24/24	0/1/1/1
2	GLC	U	2	2	-	2/2/19/22	0/1/1/1
2	GLA	U	3	2	-	0/2/19/22	0/1/1/1
2	GLC	V	2	2	-	2/2/19/22	0/1/1/1
2	GLA	V	3	2	-	1/2/19/22	0/1/1/1
2	FRU	W	1	2	-	1/5/24/24	0/1/1/1
2	GLC	W	2	2	-	0/2/19/22	0/1/1/1
2	GLA	W	3	2	-	0/2/19/22	0/1/1/1
2	FRU	X	1	2	-	2/5/24/24	0/1/1/1
2	GLC	X	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	X	3	2	-	0/2/19/22	0/1/1/1
2	FRU	Y	1	2	-	3/5/24/24	0/1/1/1
2	GLC	Y	2	2	-	0/2/19/22	0/1/1/1
2	GLA	Y	3	2	-	0/2/19/22	0/1/1/1
2	FRU	Z	1	2	-	3/5/24/24	0/1/1/1
2	GLC	Z	2	2	-	0/2/19/22	0/1/1/1
2	GLA	Z	3	2	-	1/2/19/22	0/1/1/1
2	FRU	a	1	2	-	3/5/24/24	0/1/1/1
2	GLC	a	2	2	-	0/2/19/22	0/1/1/1
2	GLA	a	3	2	-	0/2/19/22	0/1/1/1
2	FRU	b	1	2	-	5/5/24/24	0/1/1/1
2	GLC	b	2	2	-	0/2/19/22	0/1/1/1
2	GLA	b	3	2	-	0/2/19/22	0/1/1/1
2	FRU	c	1	2	-	3/5/24/24	0/1/1/1
2	GLC	c	2	2	-	1/2/19/22	0/1/1/1
2	GLA	c	3	2	-	1/2/19/22	0/1/1/1
2	FRU	d	1	2	-	4/5/24/24	0/1/1/1
2	GLC	d	2	2	-	0/2/19/22	0/1/1/1
2	GLA	d	3	2	-	0/2/19/22	0/1/1/1
2	FRU	e	1	2	-	5/5/24/24	0/1/1/1
2	GLC	e	2	2	-	0/2/19/22	0/1/1/1
2	GLA	e	3	2	-	0/2/19/22	0/1/1/1
2	FRU	f	1	2	-	3/5/24/24	0/1/1/1
2	GLC	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	GLC	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	GLC	h	2	2	-	0/2/19/22	0/1/1/1
2	GLA	h	3	2	-	2/2/19/22	0/1/1/1
2	FRU	i	1	2	-	1/5/24/24	0/1/1/1
2	GLC	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	FRU	j	1	2	-	1/5/24/24	0/1/1/1
2	GLC	j	2	2	-	1/2/19/22	0/1/1/1
2	GLA	j	3	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	1	FRU	O2-C2	2.02	1.44	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	2	GLC	C1-O5-C5	4.46	118.16	112.19
2	h	2	GLC	C1-O5-C5	4.22	117.85	112.19
2	h	3	GLA	C3-C4-C5	3.75	117.04	110.23
2	S	2	GLC	C1-C2-C3	-3.63	104.36	109.64
2	g	3	GLA	C3-C4-C5	3.61	116.77	110.23
2	Z	2	GLC	C3-C4-C5	3.54	116.65	110.23
2	d	2	GLC	C3-C4-C5	3.35	116.31	110.23
2	d	2	GLC	C1-O5-C5	3.31	116.62	112.19
2	Z	2	GLC	C2-C3-C4	3.19	116.47	110.86
2	g	3	GLA	C2-C3-C4	3.09	116.29	110.86
2	d	2	GLC	C6-C5-C4	-3.06	105.50	113.02
2	g	2	GLC	C1-C2-C3	3.04	114.07	109.64
2	d	2	GLC	O6-C6-C5	-3.00	101.13	111.33
2	U	2	GLC	C1-C2-C3	2.86	113.81	109.64
2	f	2	GLC	C3-C4-C5	2.84	115.38	110.23
2	d	2	GLC	O5-C5-C6	-2.84	102.14	107.66
2	S	2	GLC	O5-C1-C2	-2.80	104.12	110.79
2	Z	2	GLC	C1-C2-C3	2.78	113.69	109.64
2	h	2	GLC	C1-C2-C3	2.66	113.51	109.64
2	U	2	GLC	C1-O5-C5	2.60	115.67	112.19
2	h	3	GLA	C2-C3-C4	2.60	115.43	110.86
2	N	2	GLC	C3-C4-C5	2.55	114.85	110.23
2	f	2	GLC	C2-C3-C4	2.51	115.28	110.86
2	d	2	GLC	O5-C1-C2	-2.47	104.89	110.79
2	S	2	GLC	C1-O5-C5	2.47	115.50	112.19
2	Z	2	GLC	O6-C6-C5	-2.31	103.48	111.33
2	X	3	GLA	C1-O5-C5	2.28	115.25	112.19
2	T	2	GLC	C1-C2-C3	-2.27	106.34	109.64
2	S	2	GLC	O5-C5-C4	2.25	116.30	110.83
2	U	3	GLA	C1-C2-C3	2.19	112.83	109.64
2	d	2	GLC	O5-C5-C4	2.19	116.15	110.83
2	S	2	GLC	C6-C5-C4	-2.19	107.65	113.02
2	P	2	GLC	C1-C2-C3	-2.08	106.61	109.64
2	N	2	GLC	O5-C1-C2	-2.01	105.99	110.79
2	N	2	GLC	C6-C5-C4	-2.00	108.11	113.02

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	FRU	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	M	1	FRU	O1-C1-C2-O2
2	N	1	FRU	O1-C1-C2-C3
2	N	1	FRU	O1-C1-C2-O2
2	N	1	FRU	O1-C1-C2-O5
2	P	1	FRU	O1-C1-C2-O2
2	Y	1	FRU	O1-C1-C2-C3
2	Y	1	FRU	O1-C1-C2-O2
2	Z	1	FRU	O1-C1-C2-C3
2	Z	1	FRU	O1-C1-C2-O2
2	a	1	FRU	O1-C1-C2-C3
2	a	1	FRU	O1-C1-C2-O2
2	a	1	FRU	O1-C1-C2-O5
2	b	1	FRU	O1-C1-C2-O2
2	c	1	FRU	O1-C1-C2-C3
2	c	1	FRU	O1-C1-C2-O2
2	c	1	FRU	O1-C1-C2-O5
2	e	1	FRU	O1-C1-C2-C3
2	e	1	FRU	O1-C1-C2-O2
2	e	1	FRU	O5-C5-C6-O6
2	f	1	FRU	O5-C5-C6-O6
2	g	3	GLA	O5-C5-C6-O6
2	P	1	FRU	C4-C5-C6-O6
2	b	1	FRU	C4-C5-C6-O6
2	f	1	FRU	C4-C5-C6-O6
2	h	3	GLA	O5-C5-C6-O6
2	h	3	GLA	C4-C5-C6-O6
2	U	2	GLC	C4-C5-C6-O6
2	g	3	GLA	C4-C5-C6-O6
2	e	1	FRU	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	Y	1	FRU	O1-C1-C2-O5
2	Z	1	FRU	O1-C1-C2-O5
2	e	1	FRU	O1-C1-C2-O5
2	P	1	FRU	O5-C5-C6-O6
2	b	1	FRU	O5-C5-C6-O6
2	U	2	GLC	O5-C5-C6-O6
2	I	1	FRU	O1-C1-C2-C3
2	P	1	FRU	O1-C1-C2-C3
2	O	2	GLC	C4-C5-C6-O6
2	S	2	GLC	O5-C5-C6-O6
2	I	1	FRU	O1-C1-C2-O5
2	O	1	FRU	O1-C1-C2-O5

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Mol	Chain	Res	Type	Atoms
2	P	1	FRU	O1-C1-C2-O5
2	T	1	FRU	O1-C1-C2-O5
2	X	1	FRU	O1-C1-C2-O5
2	V	2	GLC	C4-C5-C6-O6
2	Z	3	GLA	O5-C5-C6-O6
2	V	3	GLA	O5-C5-C6-O6
2	U	1	FRU	O5-C5-C6-O6
2	M	1	FRU	O1-C1-C2-C3
2	O	1	FRU	O1-C1-C2-C3
2	T	1	FRU	O1-C1-C2-C3
2	X	1	FRU	O1-C1-C2-C3
2	b	1	FRU	O1-C1-C2-C3
2	d	1	FRU	O1-C1-C2-C3
2	S	1	FRU	O5-C5-C6-O6
2	O	2	GLC	O5-C5-C6-O6
2	j	2	GLC	C4-C5-C6-O6
2	d	1	FRU	O1-C1-C2-O2
2	S	1	FRU	O1-C1-C2-C3
2	S	1	FRU	O1-C1-C2-O5
2	V	2	GLC	O5-C5-C6-O6
2	d	1	FRU	O5-C5-C6-O6
2	c	3	GLA	O5-C5-C6-O6
2	M	1	FRU	O1-C1-C2-O5
2	b	1	FRU	O1-C1-C2-O5
2	c	2	GLC	C4-C5-C6-O6
2	L	1	FRU	O1-C1-C2-C3
2	Q	1	FRU	O1-C1-C2-C3
2	i	1	FRU	O1-C1-C2-C3
2	d	1	FRU	C4-C5-C6-O6
2	R	1	FRU	O1-C1-C2-C3
2	U	1	FRU	O1-C1-C2-C3
2	W	1	FRU	O1-C1-C2-C3
2	f	1	FRU	O1-C1-C2-C3
2	j	1	FRU	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 5 short contacts:

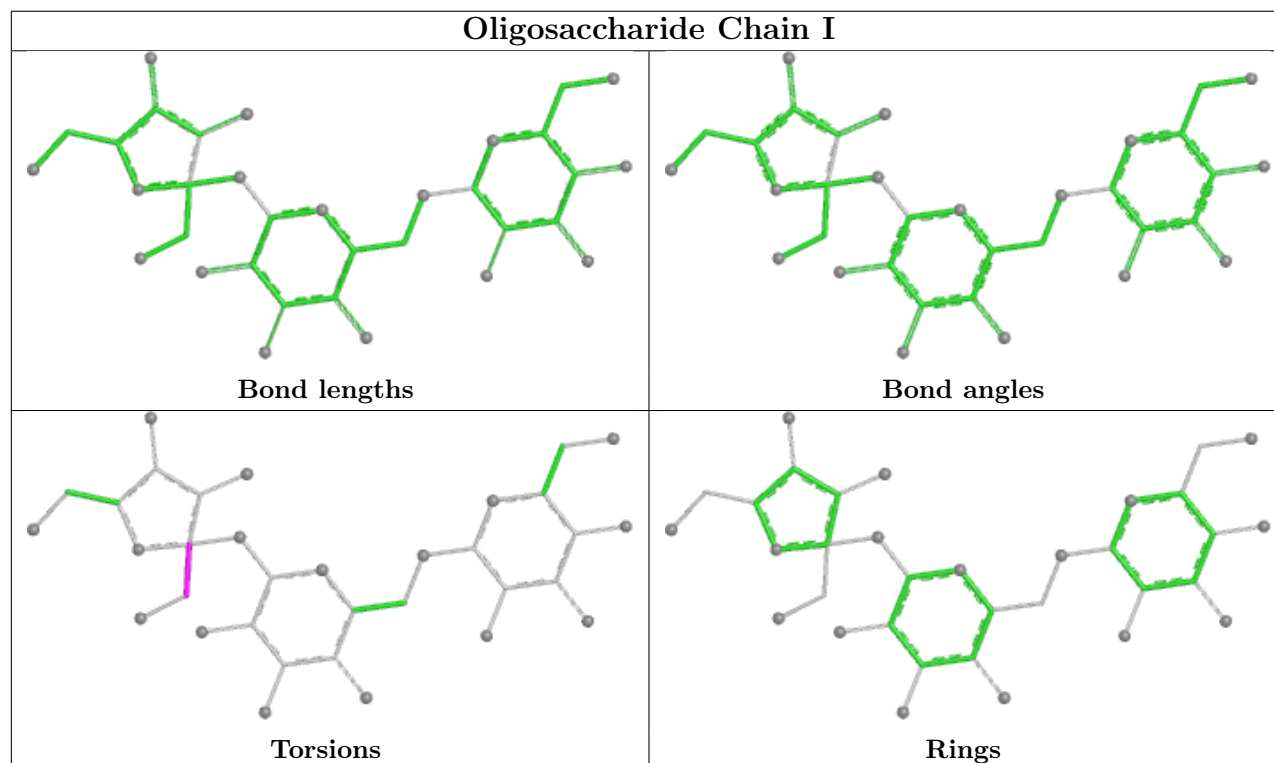
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	2	GLC	1	0
2	e	2	GLC	1	0
2	e	1	FRU	1	0

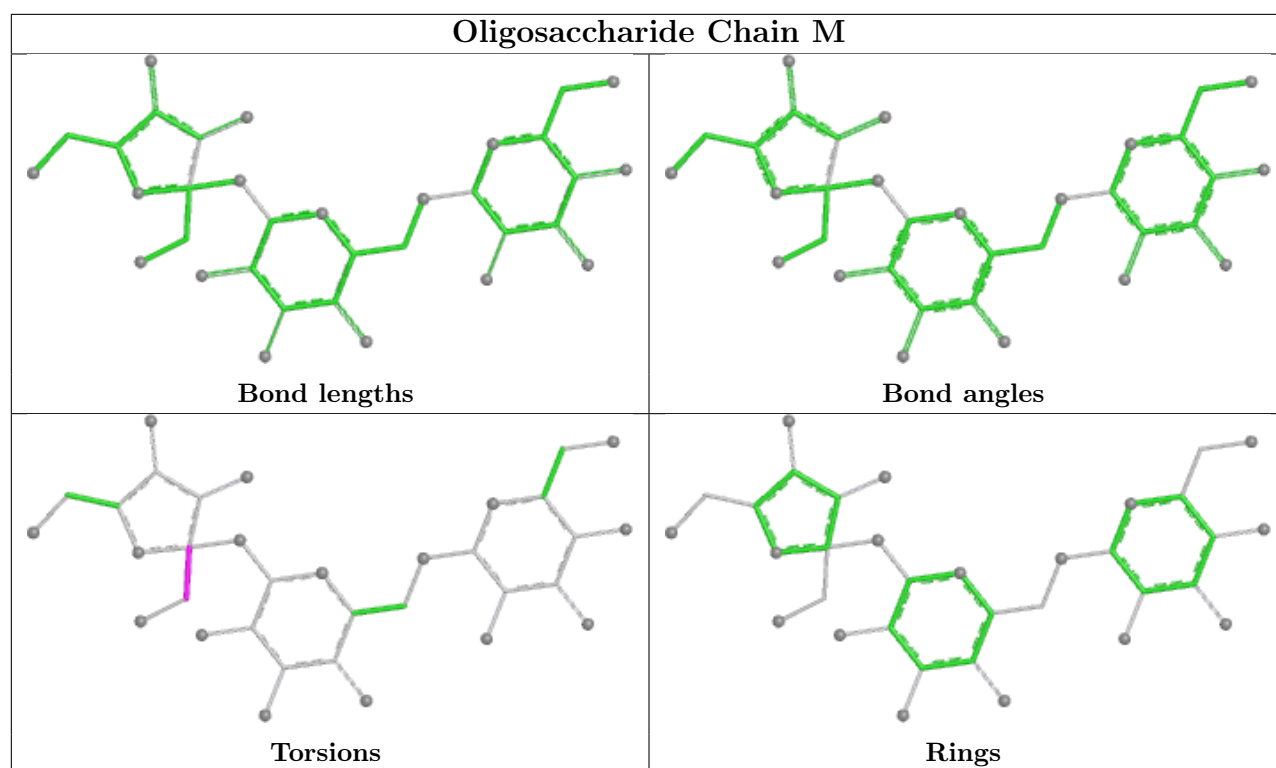
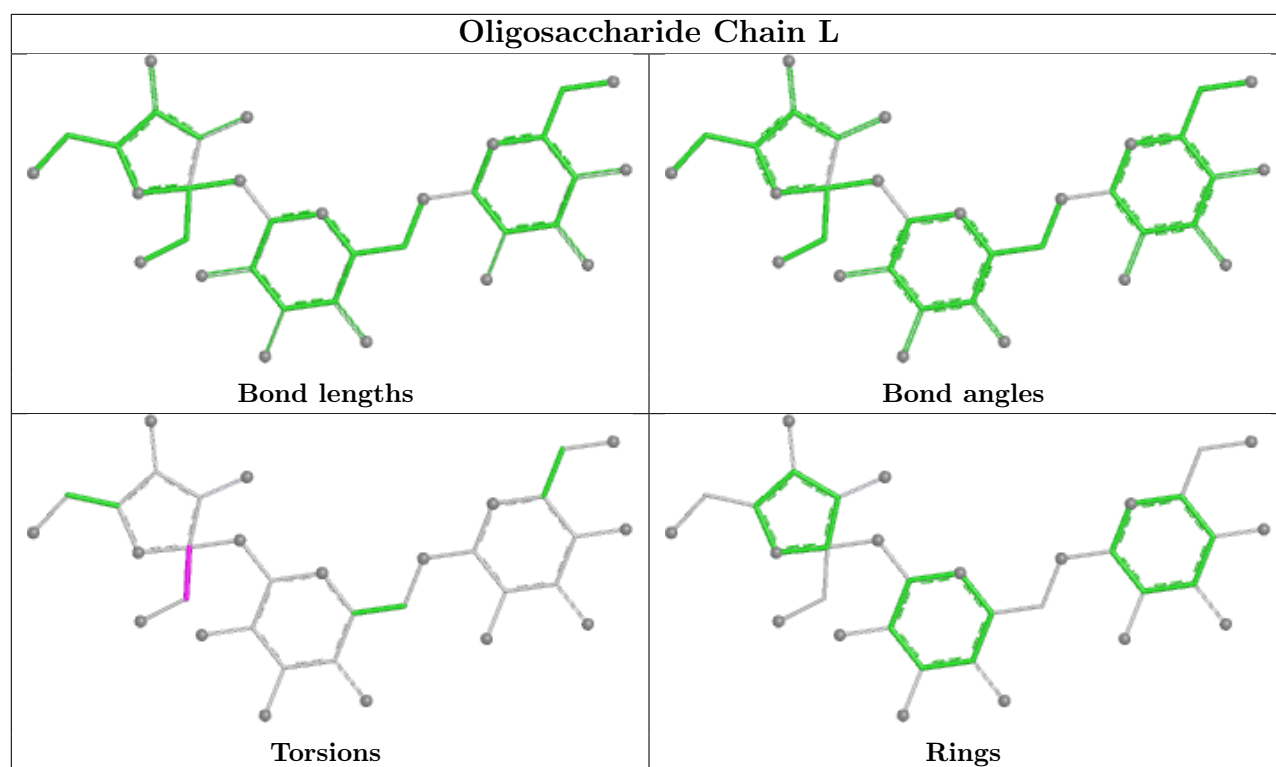
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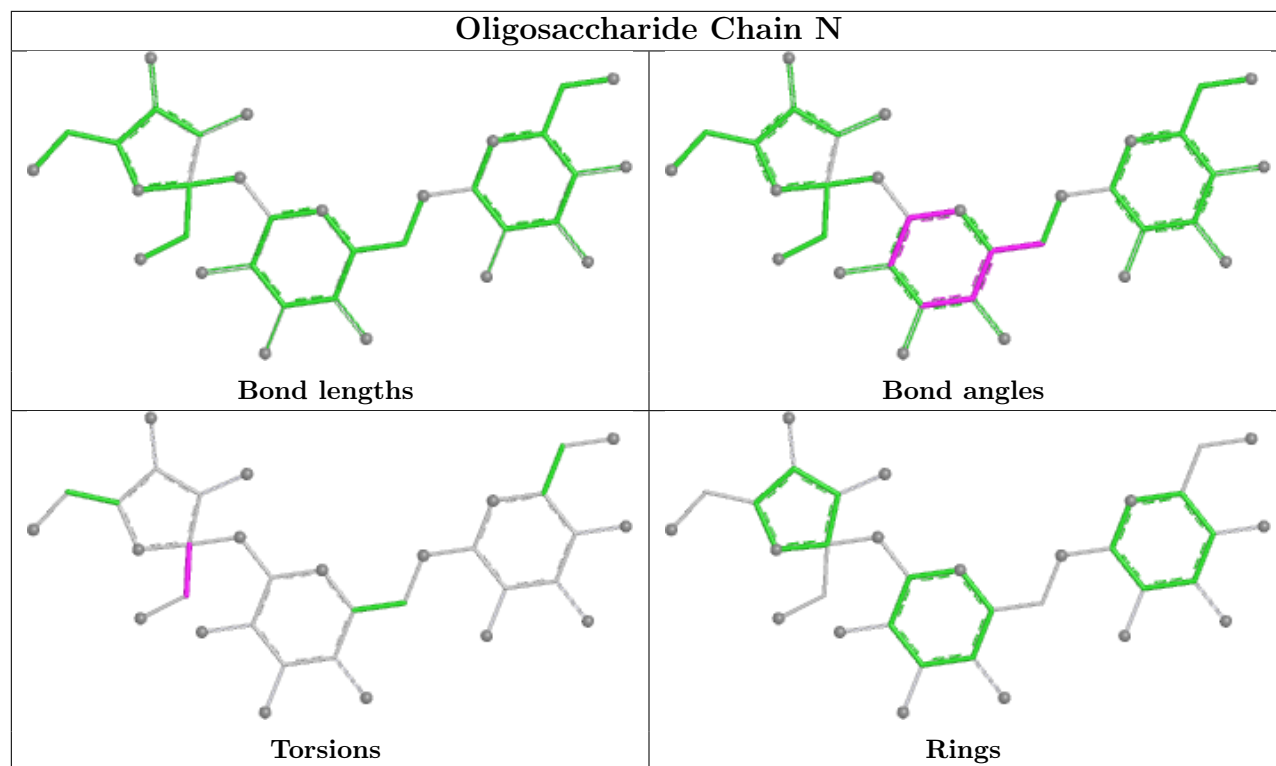
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	3	GLA	1	0
2	b	2	GLC	1	0
2	b	1	FRU	1	0
2	S	3	GLA	1	0

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

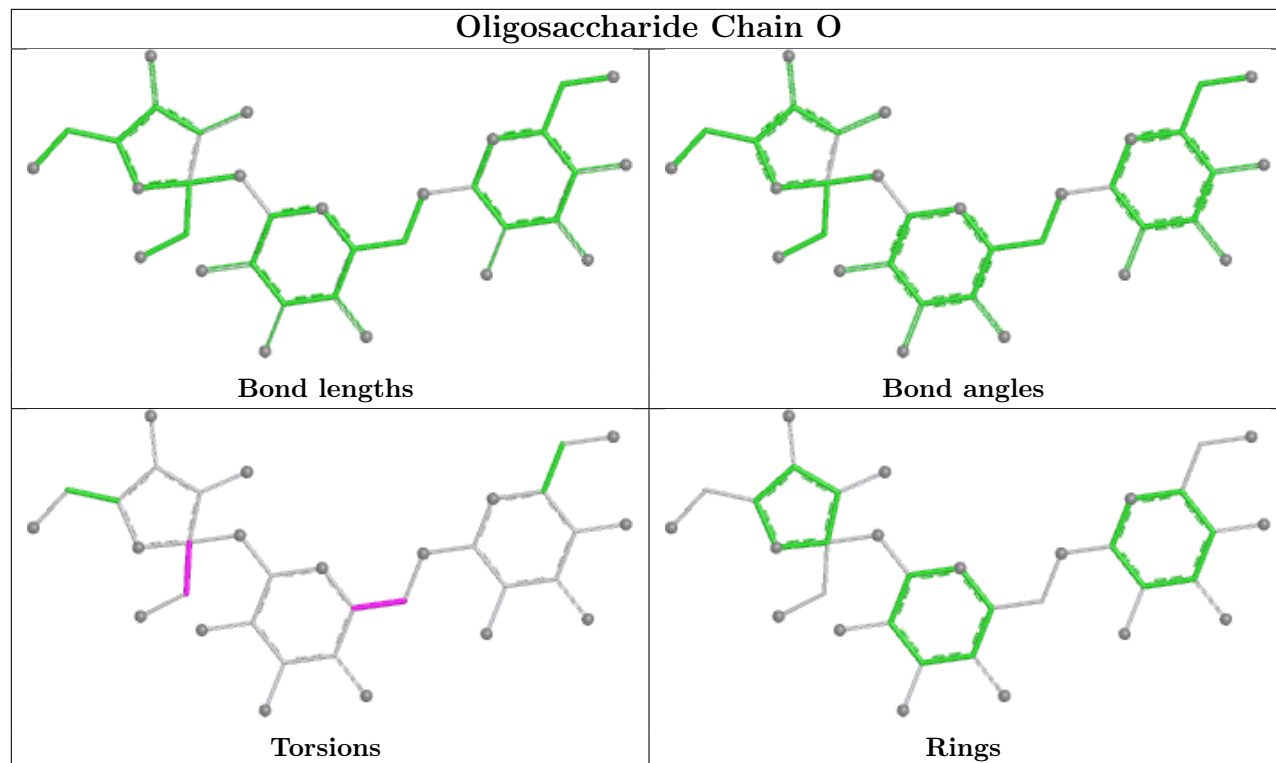




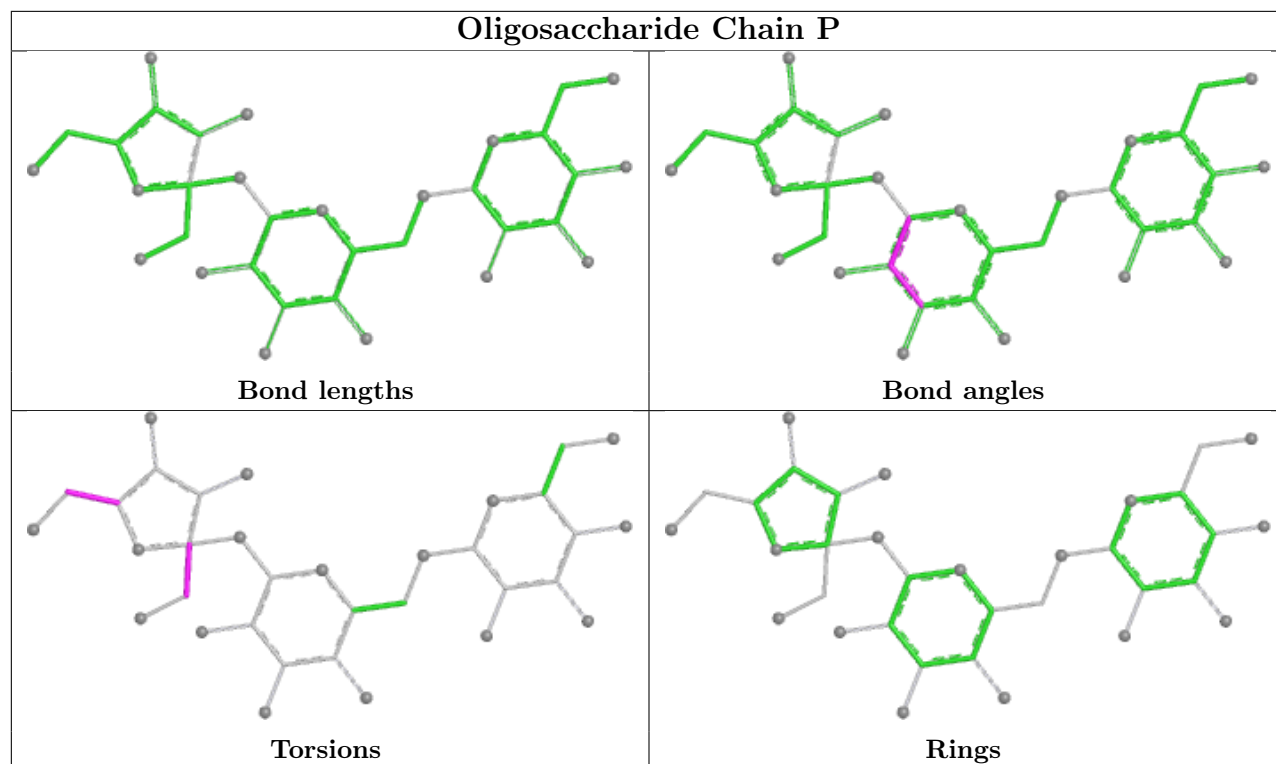
Oligosaccharide Chain N



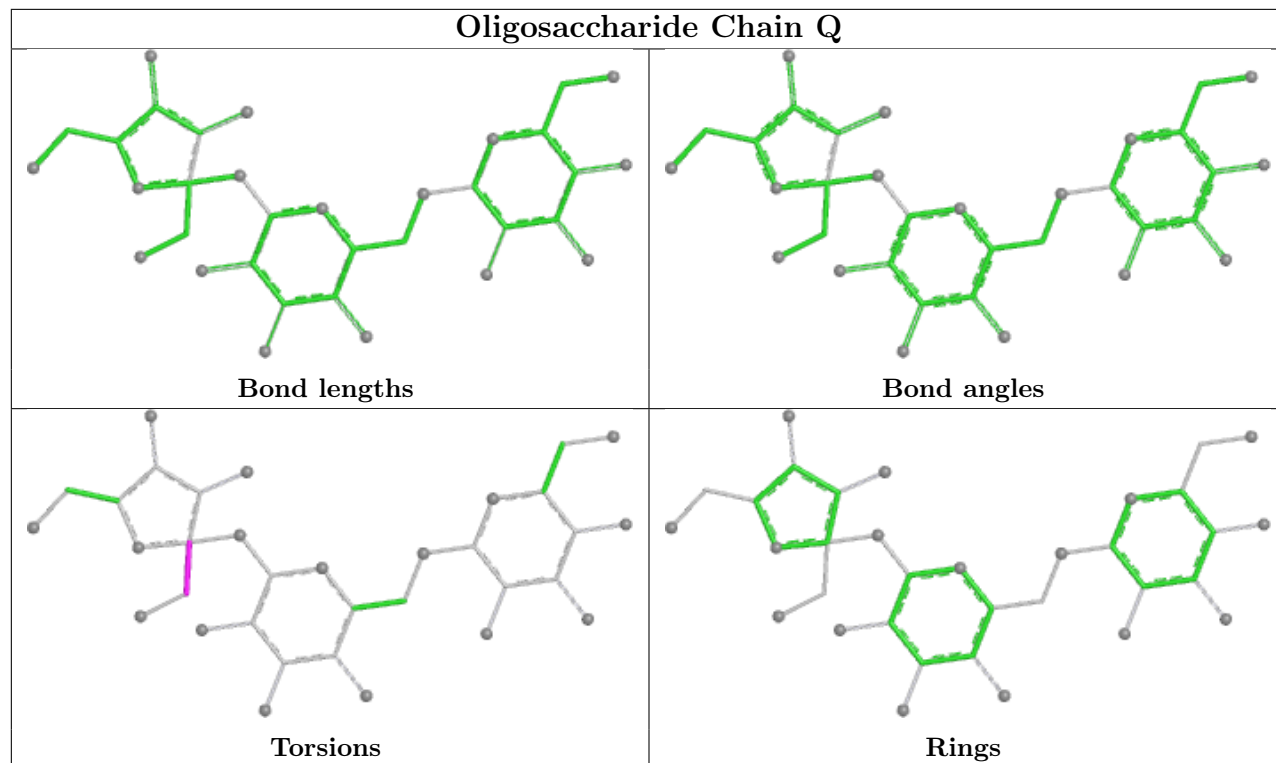
Oligosaccharide Chain O

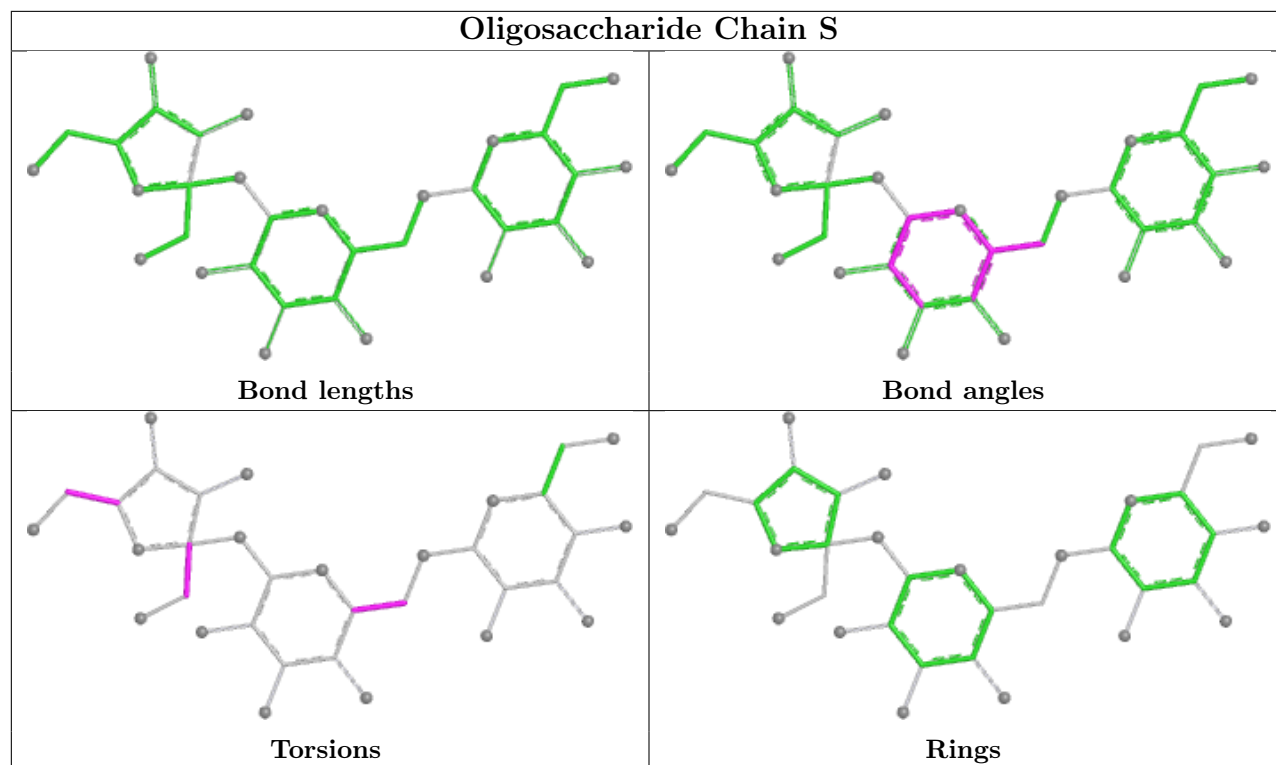
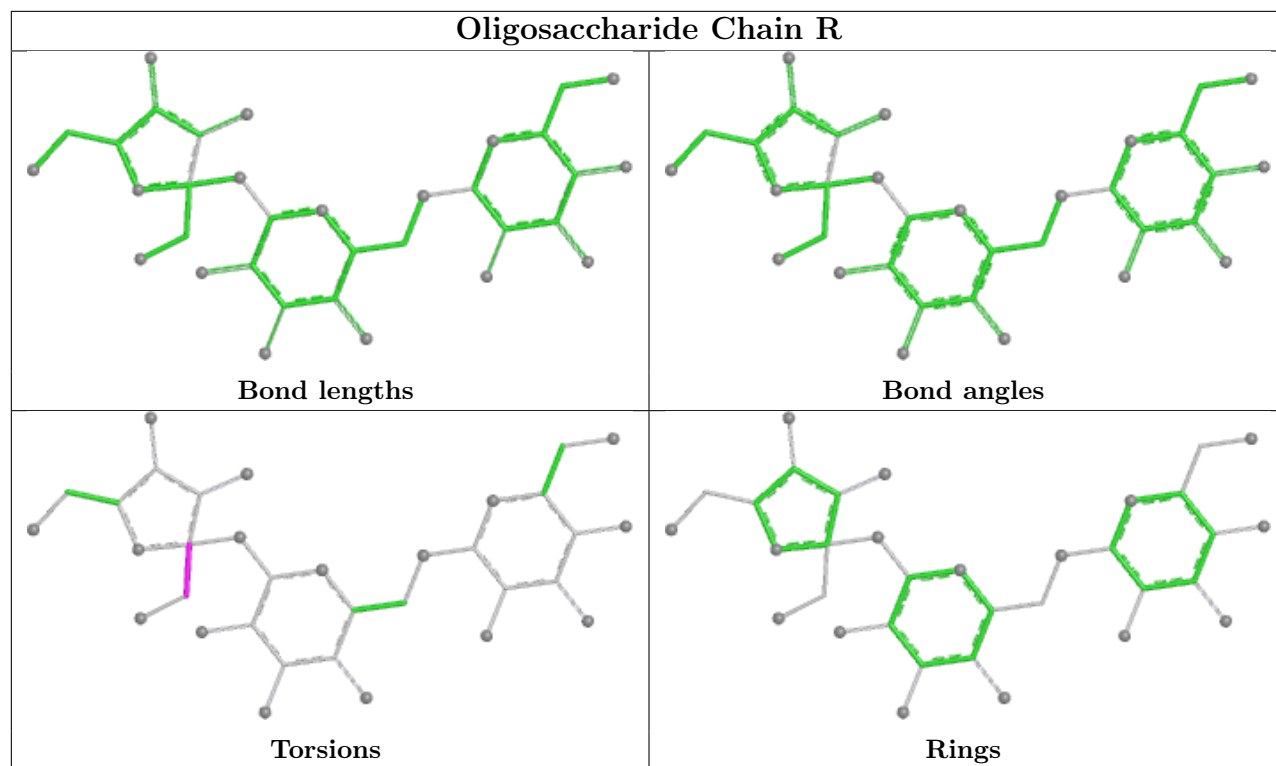


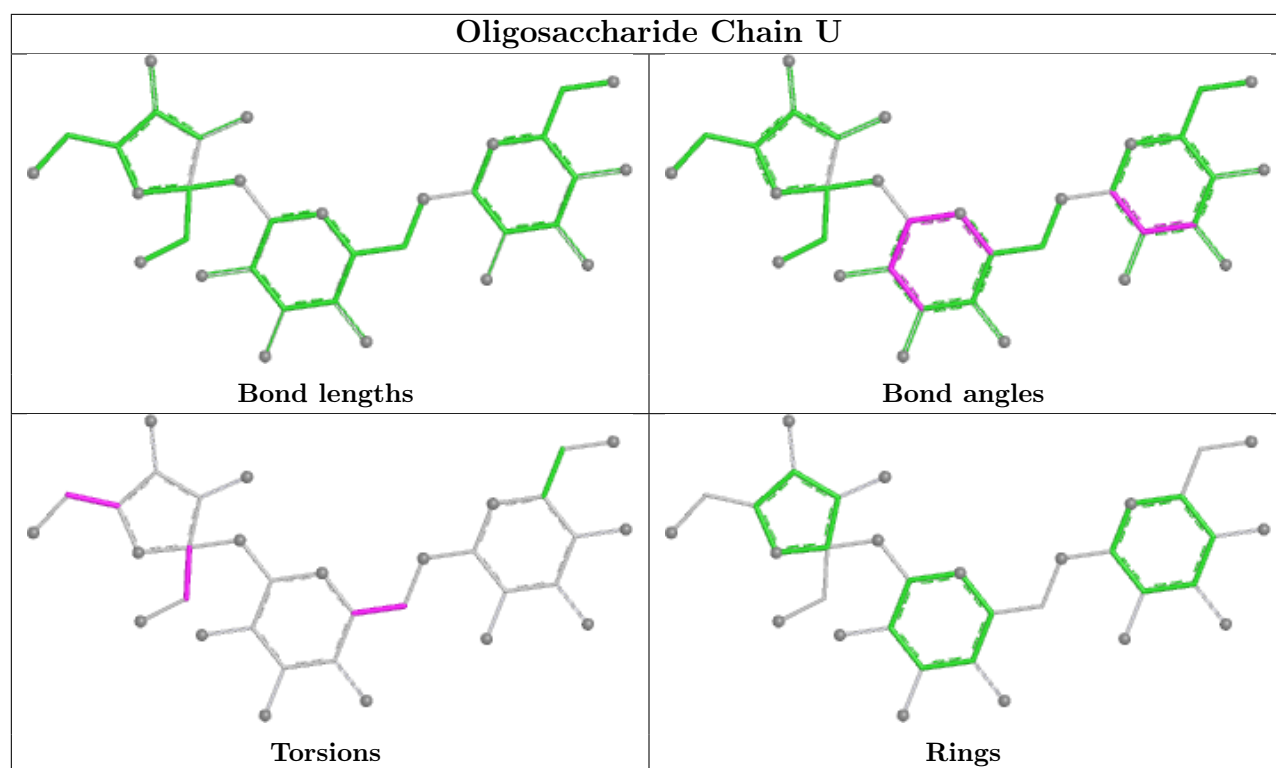
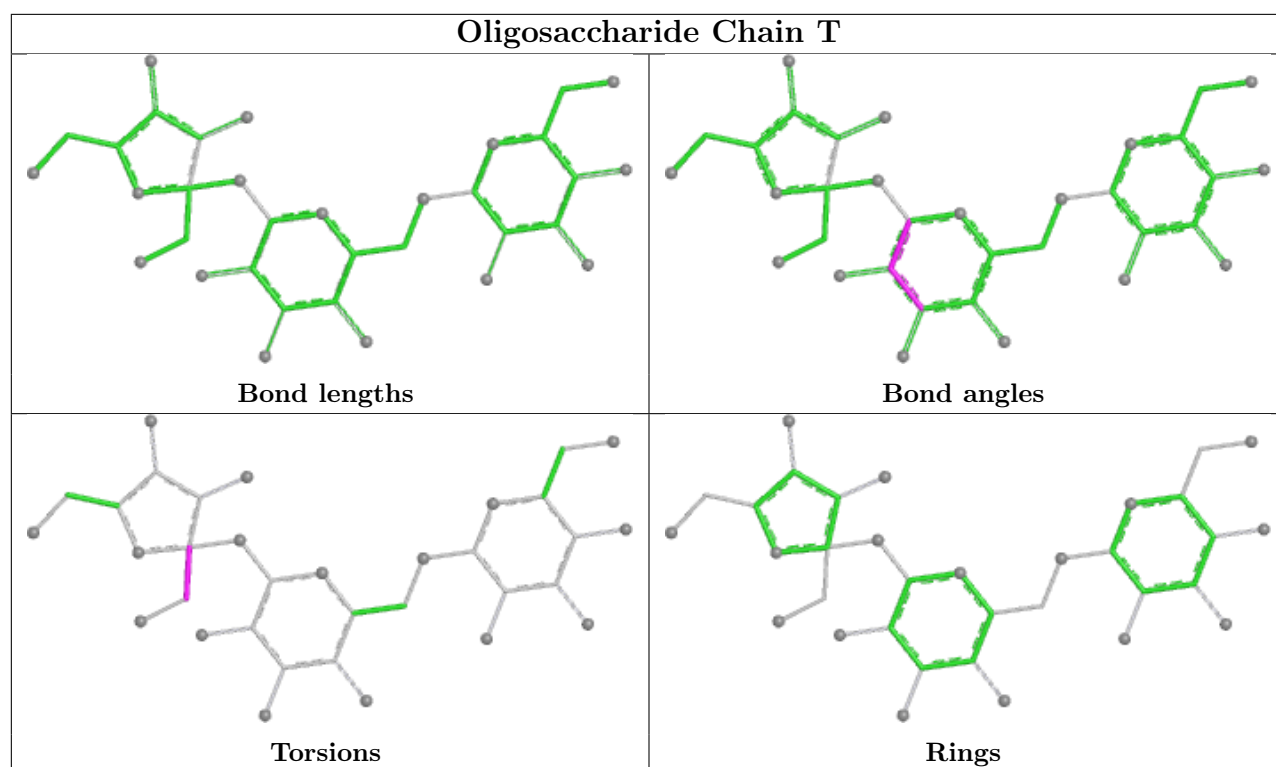
Oligosaccharide Chain P

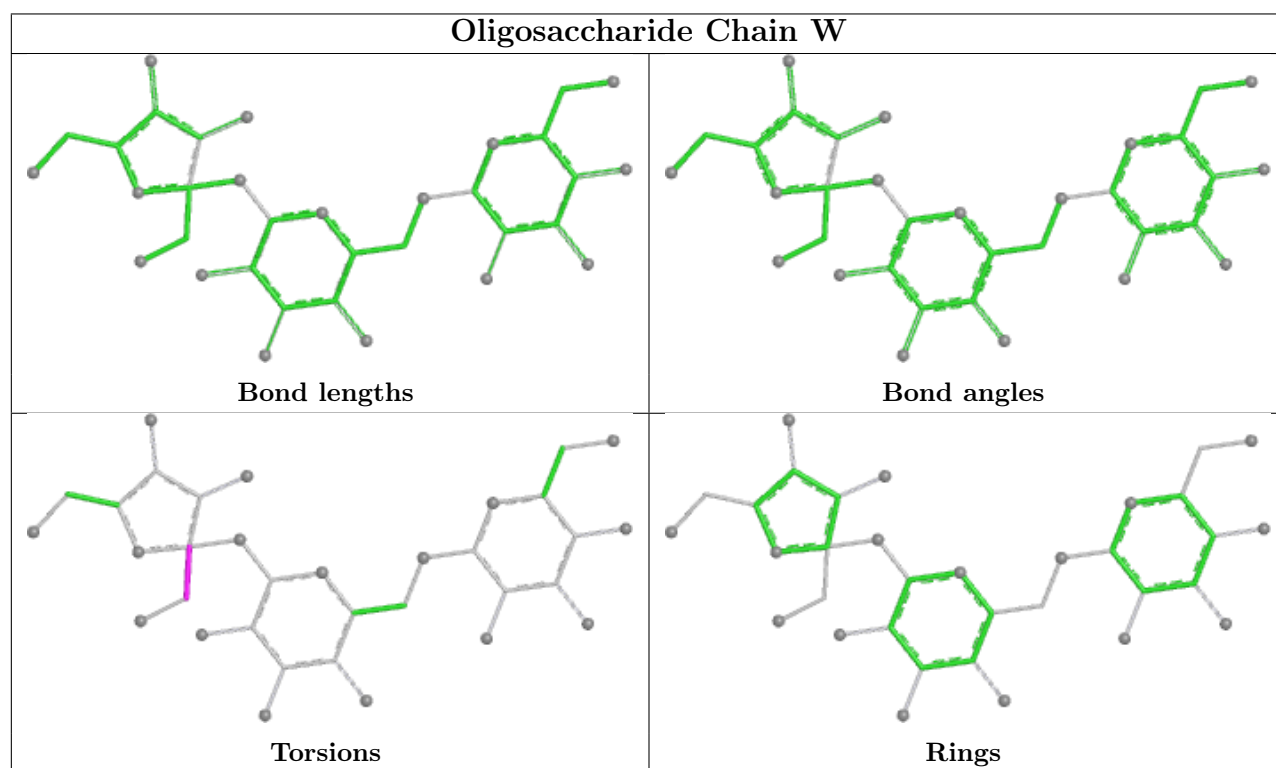
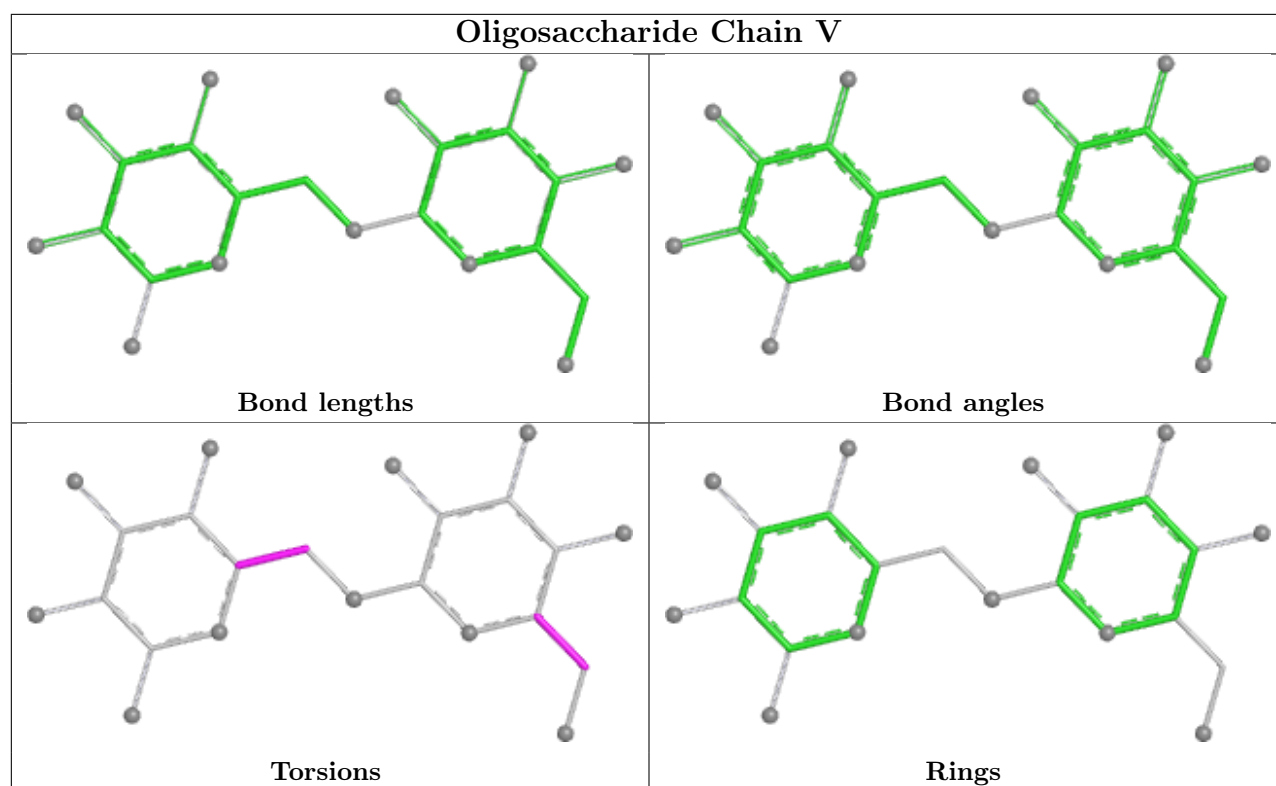


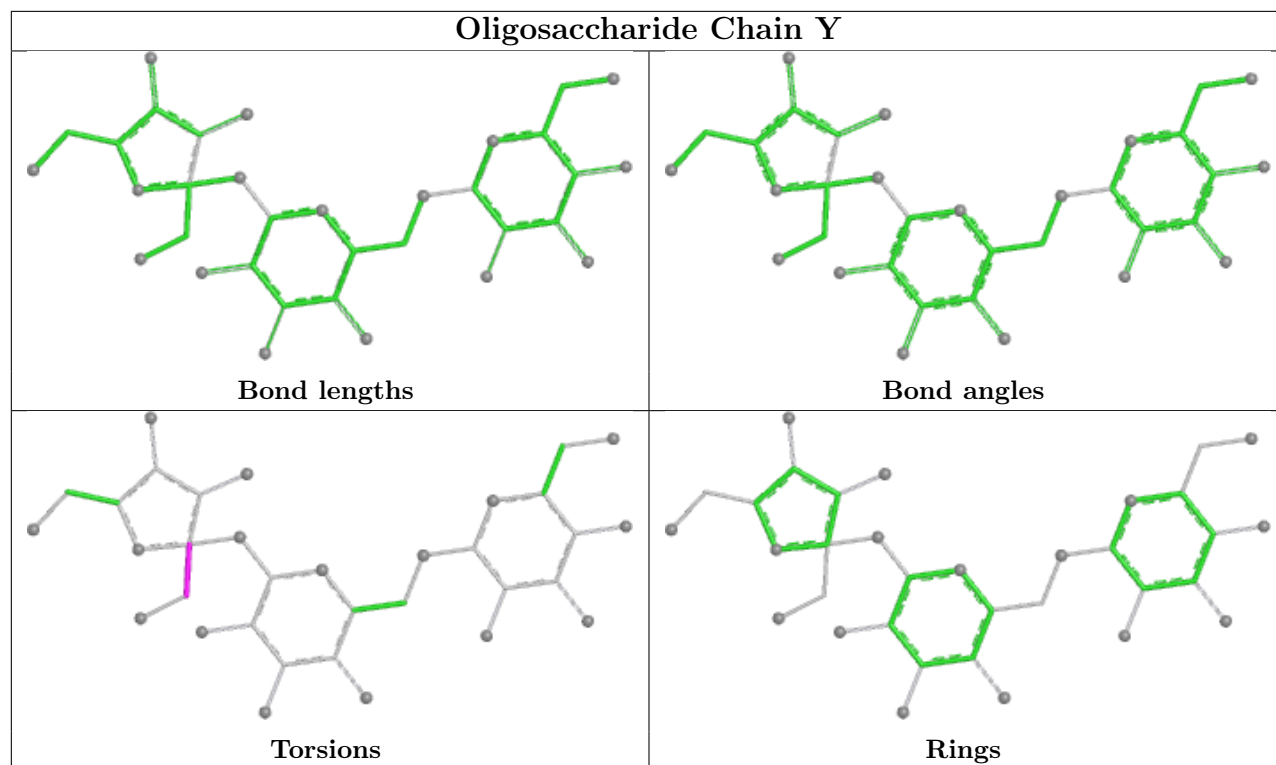
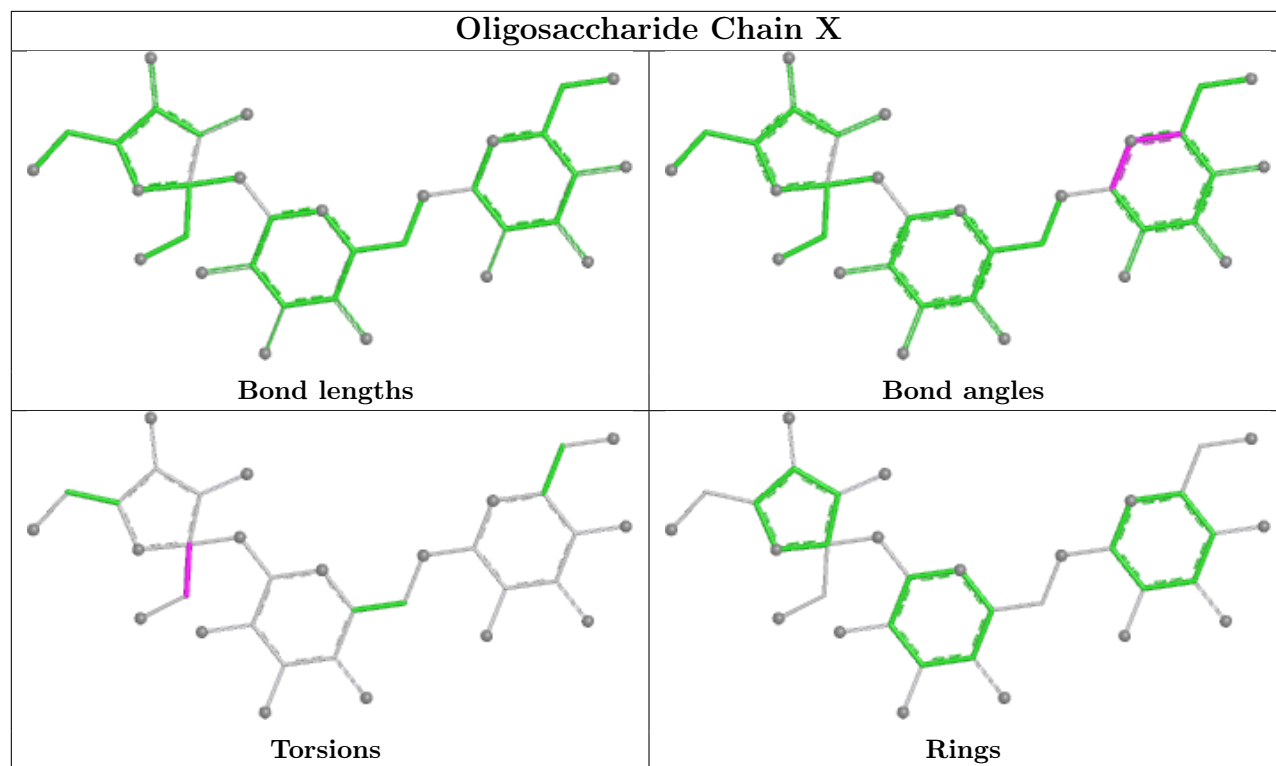
Oligosaccharide Chain Q

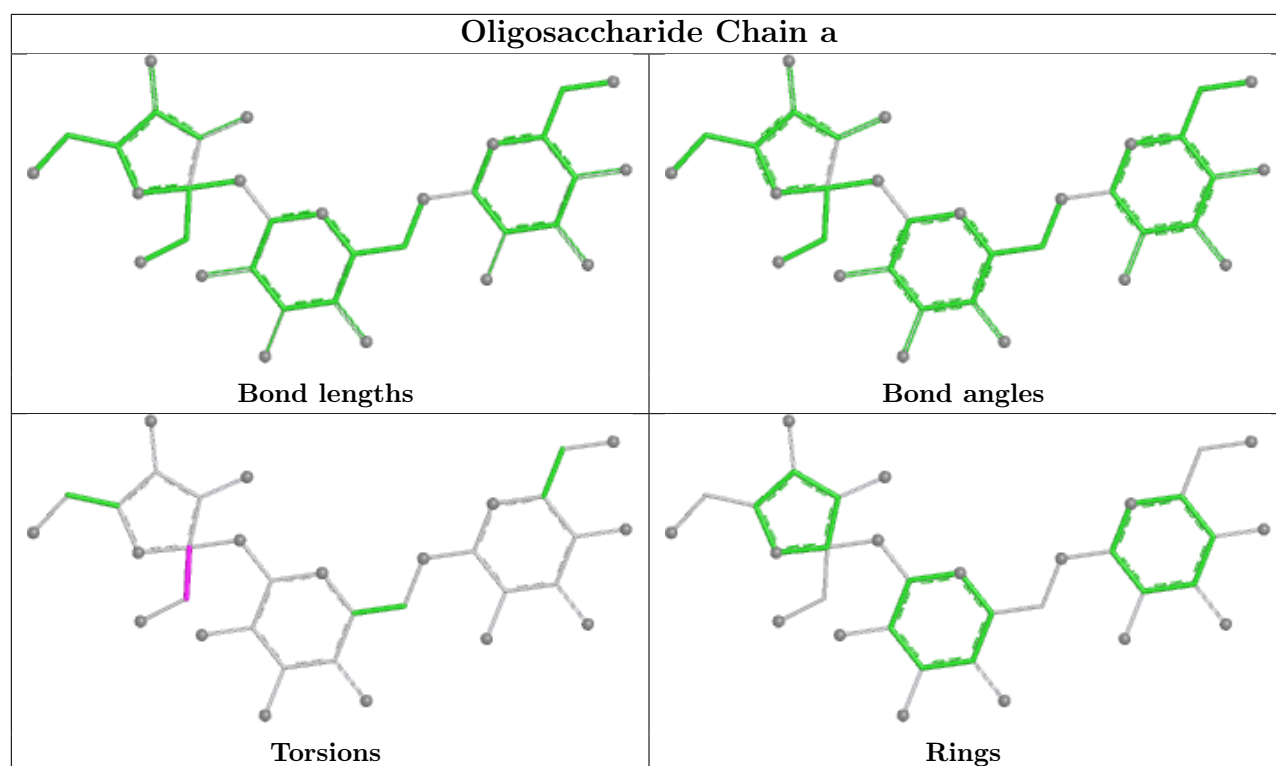
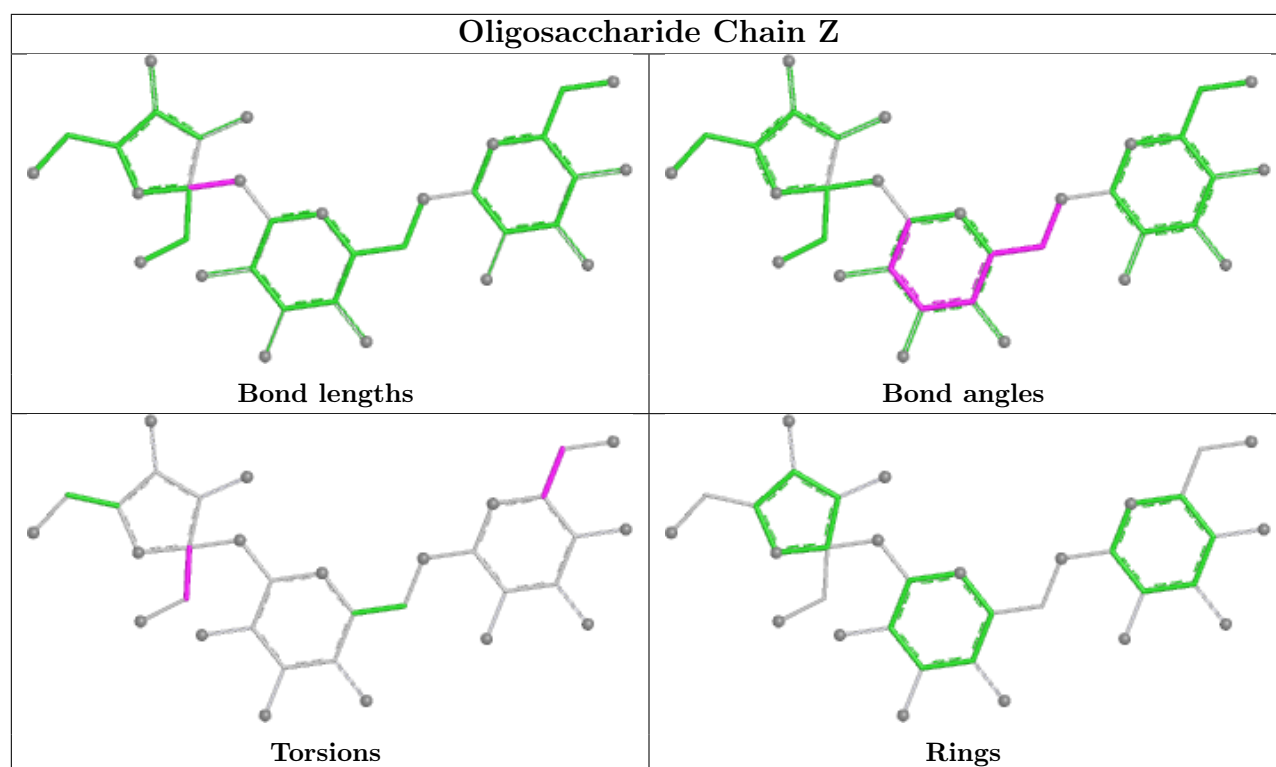


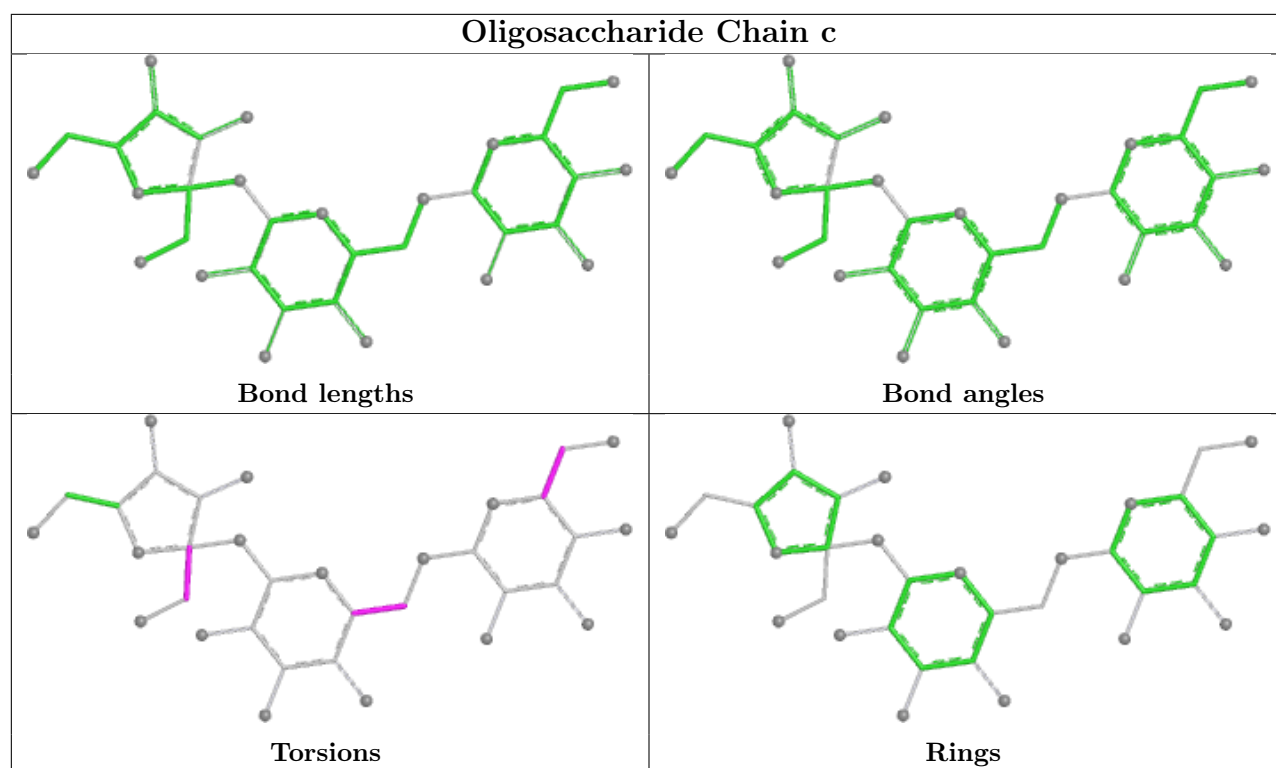
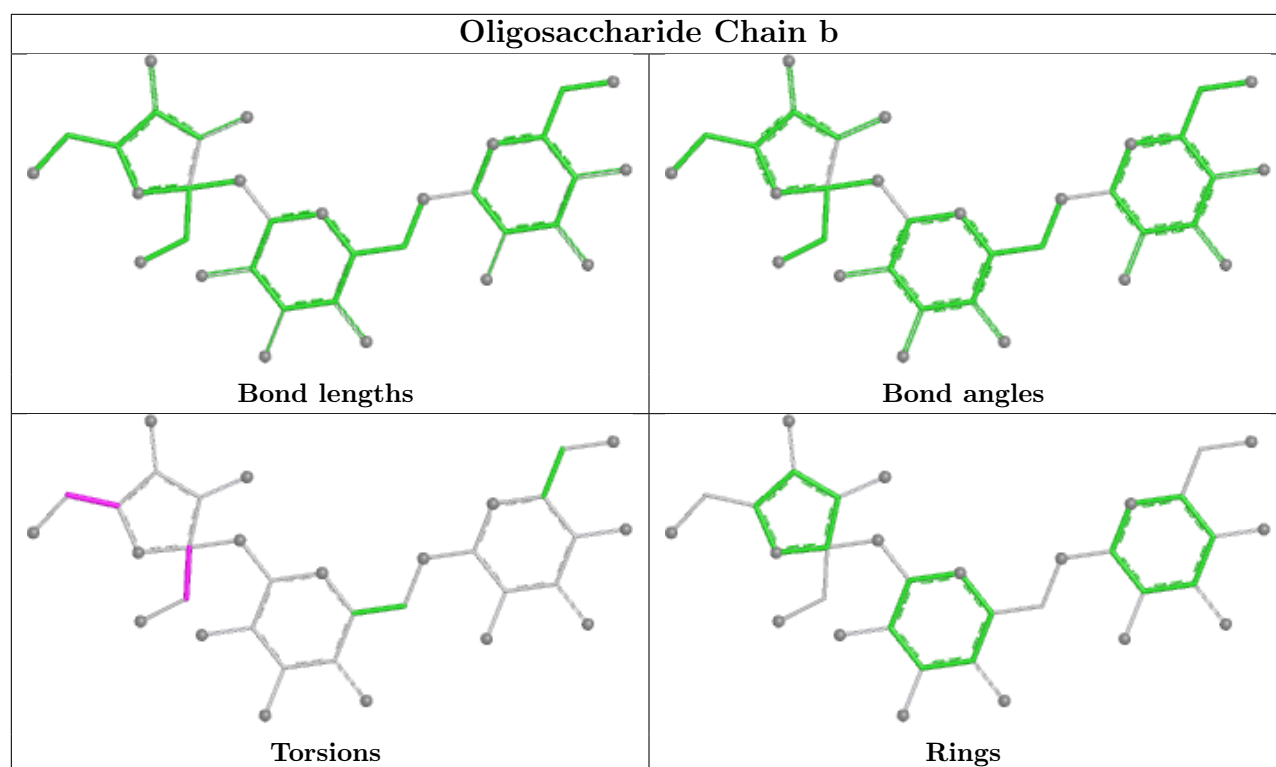


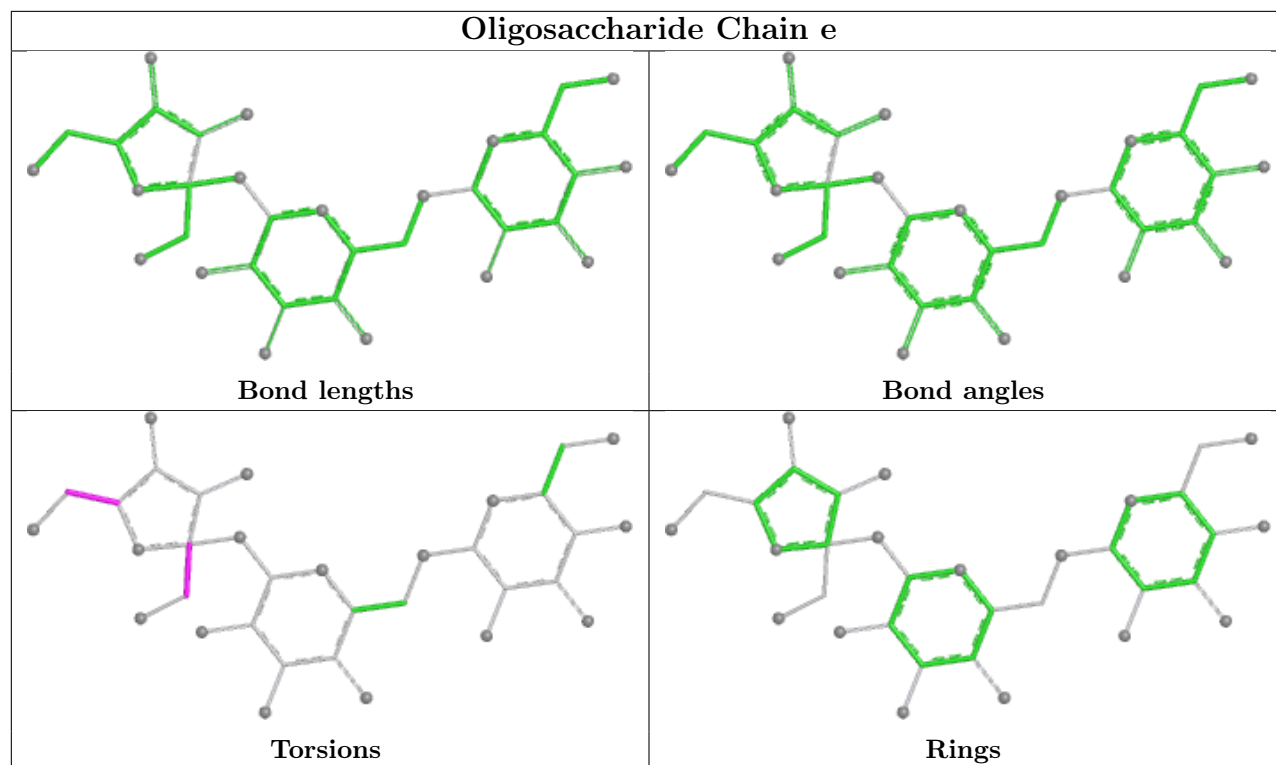
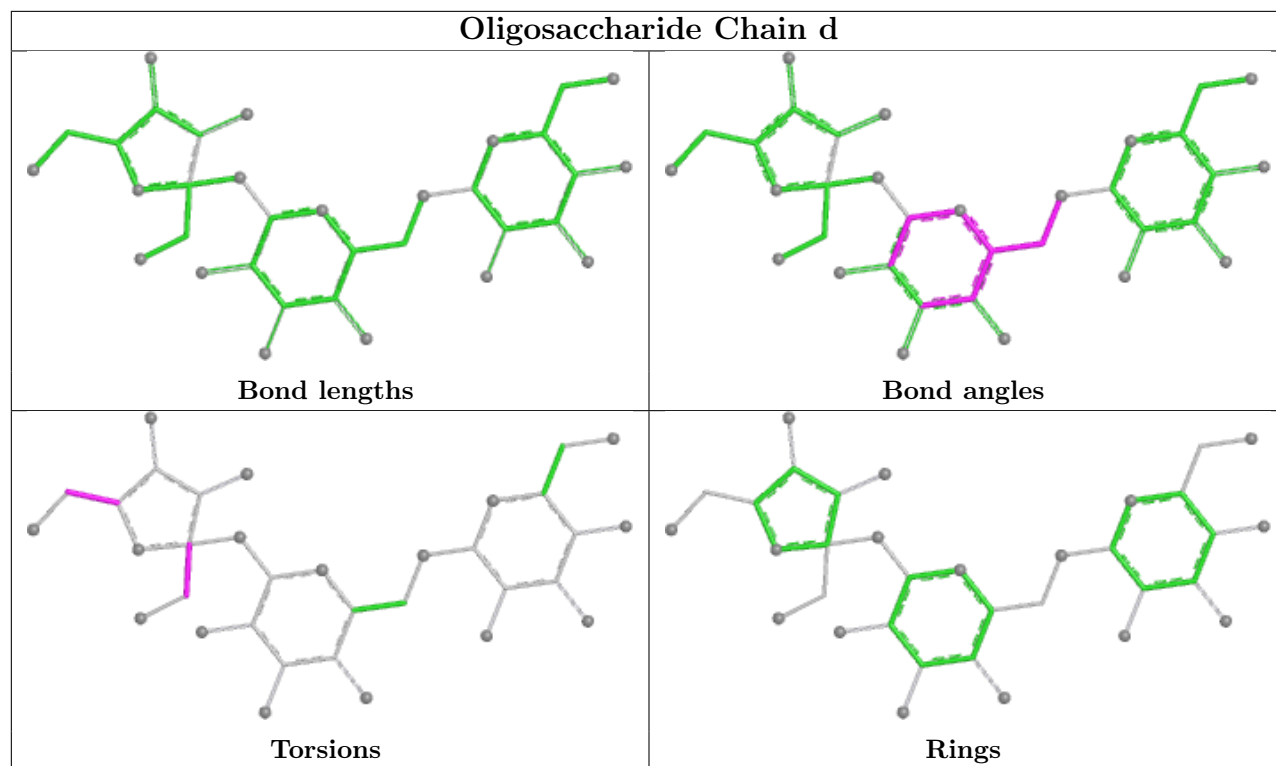


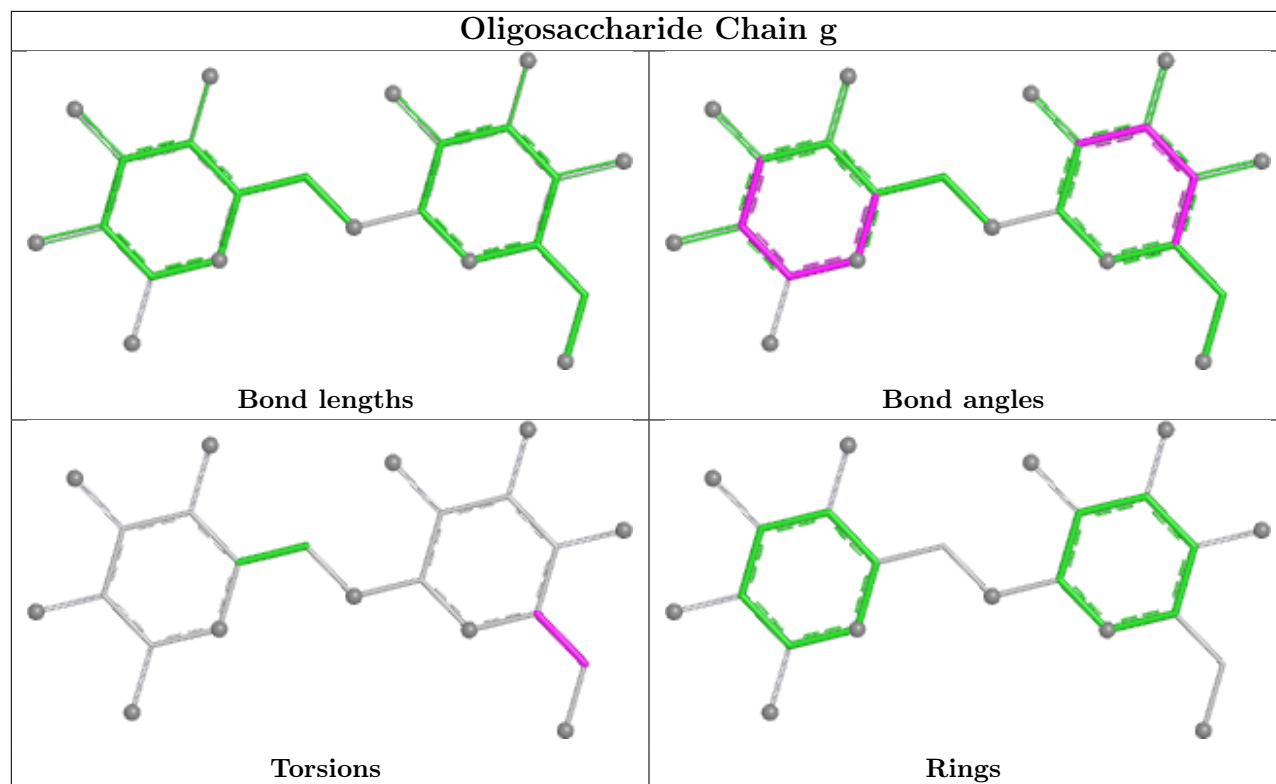
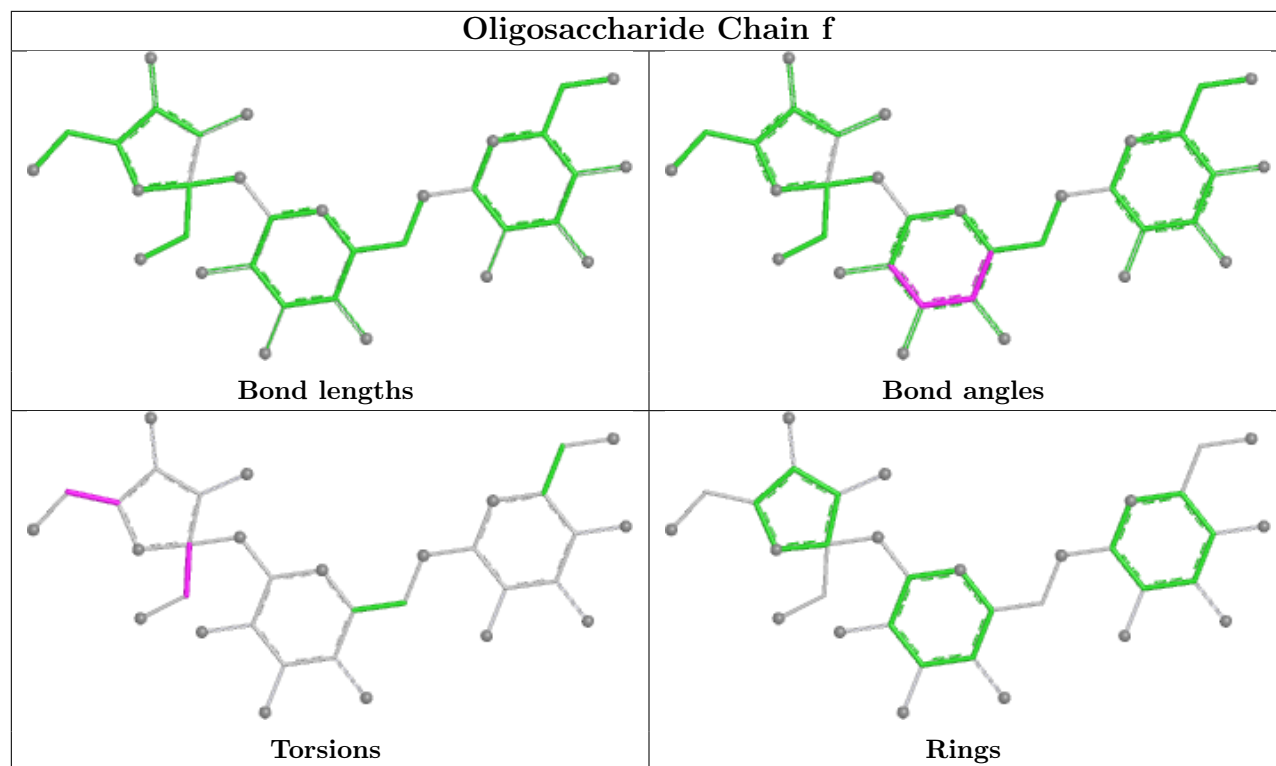


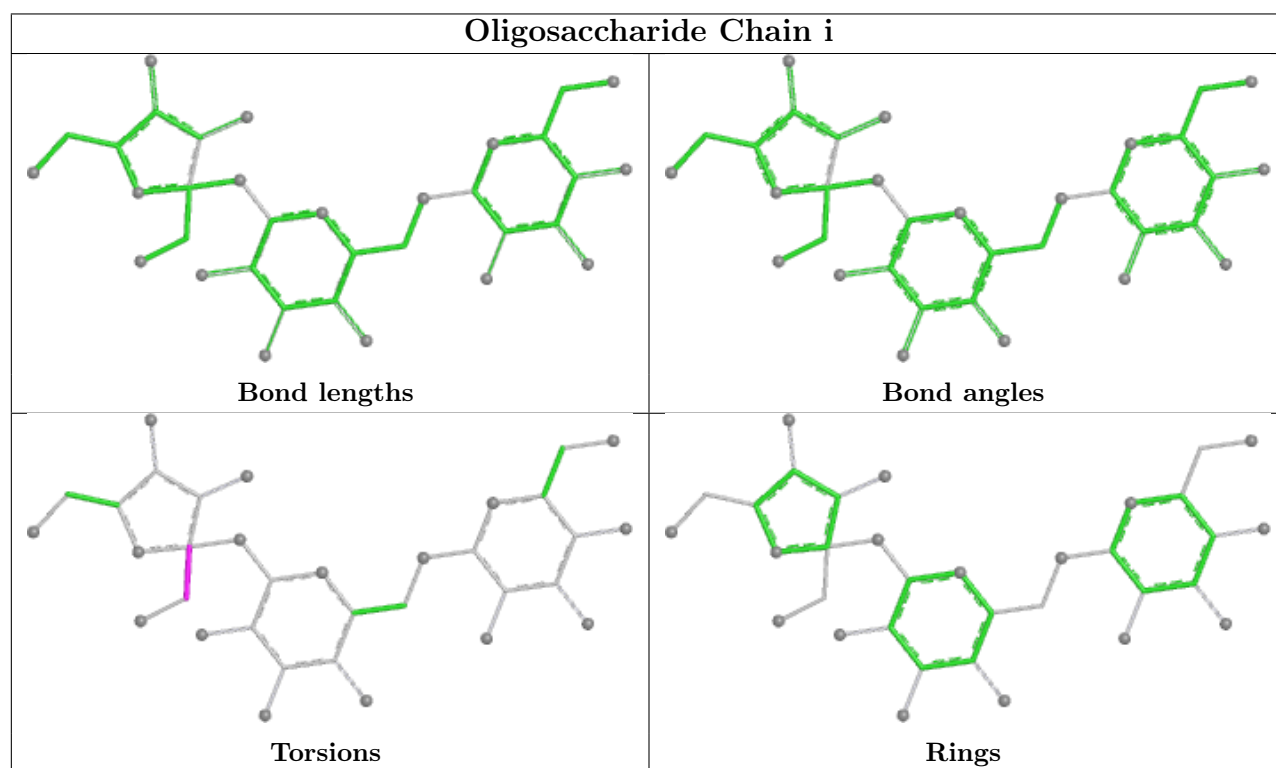
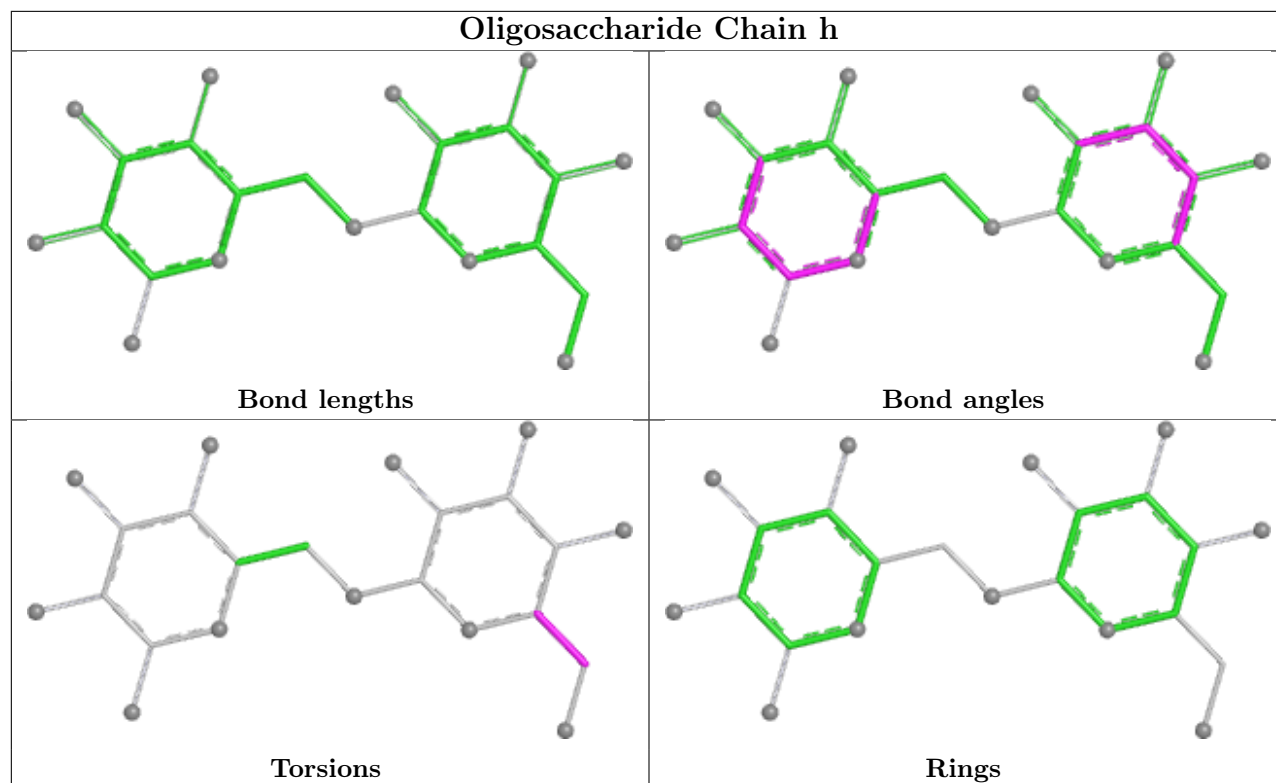


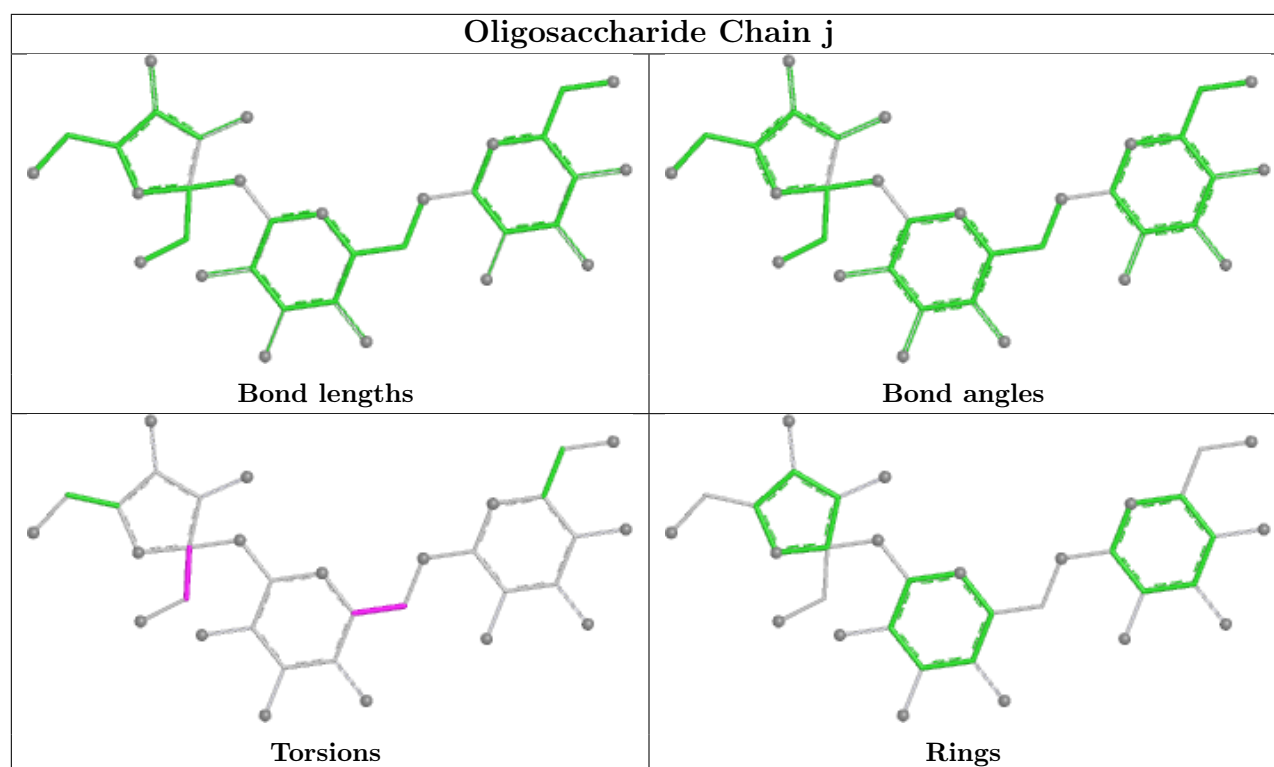












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
7	ACT	F	202	-	3,3,3	1.12	0	3,3,3	1.21	0
5	PG4	D	202	-	12,12,12	0.14	0	11,11,11	0.13	0
4	EPE	D	201	-	15,15,15	0.81	1 (6%)	19,20,20	0.63	0
5	PG4	F	203	-	12,12,12	0.14	0	11,11,11	0.13	0
4	EPE	F	201	-	15,15,15	0.85	1 (6%)	19,20,20	0.68	0
3	GLA	A	201	-	12,12,12	0.64	0	17,17,17	0.93	0
3	GLA	G	201	-	12,12,12	0.48	0	17,17,17	0.71	0
8	GOL	F	204	-	5,5,5	0.09	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	D	202	-	-	2/10/10/10	-
4	EPE	D	201	-	-	2/9/19/19	0/1/1/1
5	PG4	F	203	-	-	1/10/10/10	-
4	EPE	F	201	-	-	7/9/19/19	0/1/1/1
3	GLA	A	201	-	-	2/2/22/22	0/1/1/1
3	GLA	G	201	-	-	2/2/22/22	0/1/1/1
8	GOL	F	204	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	201	EPE	C10-S	2.45	1.81	1.77
4	D	201	EPE	C10-S	2.27	1.80	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

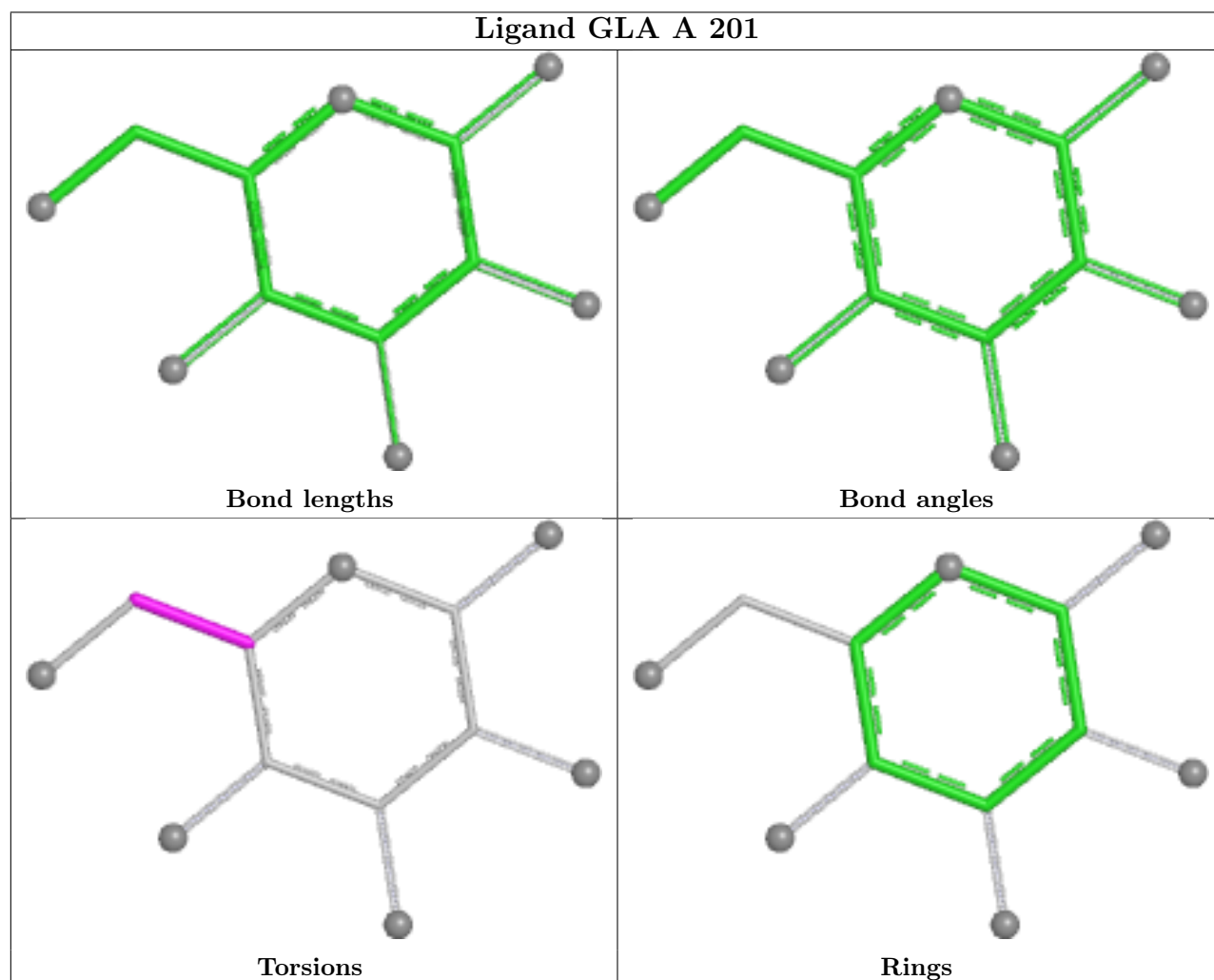
Mol	Chain	Res	Type	Atoms
4	D	201	EPE	C8-C7-N4-C3
4	F	201	EPE	C8-C7-N4-C5
4	F	201	EPE	S-C10-C9-N1
3	G	201	GLA	C4-C5-C6-O6
3	G	201	GLA	O5-C5-C6-O6
3	A	201	GLA	C4-C5-C6-O6
3	A	201	GLA	O5-C5-C6-O6
4	F	201	EPE	C10-C9-N1-C2
4	F	201	EPE	C10-C9-N1-C6
4	F	201	EPE	C9-C10-S-O3S
4	F	201	EPE	C9-C10-S-O1S
4	F	201	EPE	C9-C10-S-O2S
5	D	202	PG4	O2-C3-C4-O3
5	D	202	PG4	O3-C5-C6-O4
5	F	203	PG4	O3-C5-C6-O4
4	D	201	EPE	C8-C7-N4-C5

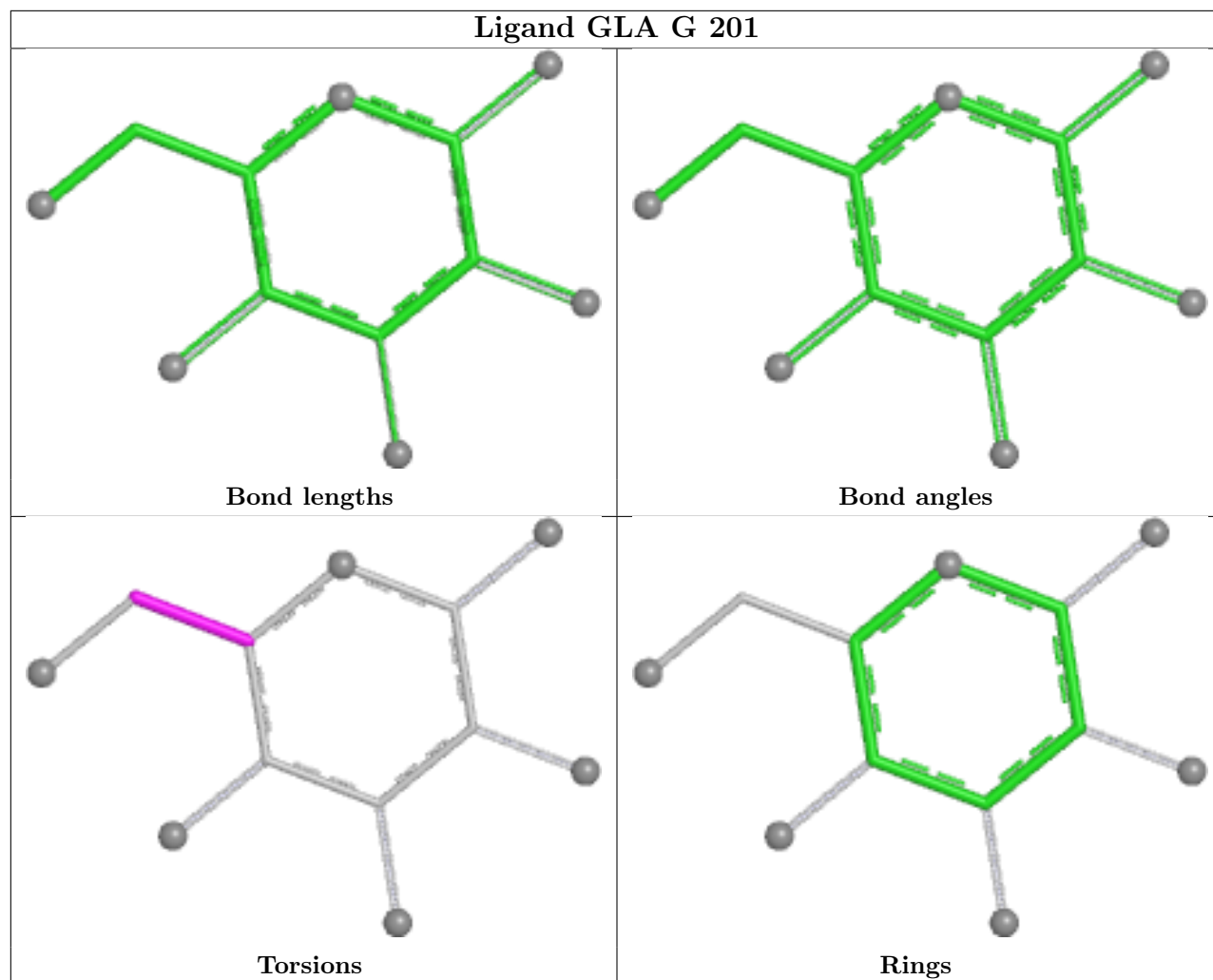
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	203	PG4	4	0
4	F	201	EPE	1	0
3	A	201	GLA	1	0
3	G	201	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	150/152 (98%)	-1.05	0 100 100	25, 37, 48, 58	0
1	B	150/152 (98%)	-1.13	0 100 100	25, 32, 42, 52	0
1	C	150/152 (98%)	-0.99	0 100 100	33, 44, 53, 63	0
1	D	150/152 (98%)	-1.08	0 100 100	26, 36, 48, 65	0
1	E	150/152 (98%)	-1.01	0 100 100	36, 44, 54, 63	0
1	F	150/152 (98%)	-1.15	0 100 100	25, 34, 44, 55	0
1	G	150/152 (98%)	-1.03	0 100 100	28, 39, 50, 58	0
1	H	150/152 (98%)	-1.13	0 100 100	25, 35, 43, 53	0
All	All	1200/1216 (98%)	-1.07	0 100 100	25, 38, 51, 65	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(Å ²)	Q<0.9
2	FRU	M	1	12/12	0.95	0.07	37,41,47,50	0
2	FRU	Z	1	12/12	0.95	0.05	55,64,67,73	0
2	GLC	T	2	11/12	0.96	0.06	31,33,37,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRU	V	1	1/12	0.96	0.06	76,76,76,76	0
2	FRU	Y	1	12/12	0.96	0.06	65,70,78,81	0
2	GLC	P	2	11/12	0.96	0.04	41,44,51,54	0
2	FRU	S	1	12/12	0.97	0.05	44,56,64,65	0
2	FRU	L	1	12/12	0.97	0.05	61,68,78,79	0
2	FRU	U	1	12/12	0.97	0.05	48,58,60,67	0
2	FRU	P	1	12/12	0.97	0.05	49,56,58,58	0
2	FRU	W	1	12/12	0.97	0.05	41,49,55,66	0
2	GLC	W	2	11/12	0.97	0.05	33,38,48,50	0
2	FRU	X	1	12/12	0.97	0.06	56,65,72,73	0
2	GLC	L	2	11/12	0.97	0.04	46,54,66,75	0
2	GLC	Y	2	11/12	0.97	0.04	53,65,68,74	0
2	FRU	Q	1	12/12	0.97	0.04	70,77,80,85	0
2	GLC	R	2	11/12	0.98	0.04	39,48,55,56	0
2	GLA	R	3	11/12	0.98	0.04	48,51,54,56	0
2	FRU	N	1	12/12	0.98	0.05	55,65,67,80	0
2	GLC	S	2	11/12	0.98	0.04	48,53,60,60	0
2	GLA	S	3	11/12	0.98	0.04	42,44,53,54	0
2	FRU	T	1	12/12	0.98	0.06	31,37,47,48	0
2	GLC	N	2	11/12	0.98	0.04	49,62,66,67	0
2	FRU	O	1	12/12	0.98	0.05	54,63,68,72	0
2	GLC	U	2	11/12	0.98	0.03	52,54,65,66	0
2	GLC	O	2	11/12	0.98	0.04	47,55,64,73	0
2	GLC	V	2	11/12	0.98	0.04	57,68,76,76	0
2	GLC	I	2	11/12	0.98	0.04	35,43,57,61	0
2	FRU	I	1	12/12	0.98	0.05	35,38,49,51	0
2	GLA	W	3	11/12	0.98	0.05	27,32,39,42	0
2	GLC	M	2	11/12	0.98	0.04	35,39,46,47	0
2	GLC	X	2	11/12	0.98	0.04	36,51,58,64	0
2	GLA	X	3	11/12	0.98	0.05	27,29,32,33	0
2	GLC	Q	2	11/12	0.98	0.04	52,62,72,75	0
2	GLA	Q	3	11/12	0.98	0.03	45,49,54,54	0
2	GLA	Y	3	11/12	0.98	0.04	43,45,50,51	0
2	FRU	R	1	12/12	0.98	0.04	44,51,55,55	0
2	GLC	Z	2	11/12	0.98	0.04	53,65,73,76	0
2	GLA	T	3	11/12	0.99	0.04	28,34,37,38	0
2	GLA	P	3	11/12	0.99	0.03	33,42,44,50	0
2	GLA	M	3	11/12	0.99	0.03	30,33,36,39	0
2	GLA	U	3	11/12	0.99	0.03	36,40,48,49	0
2	GLA	I	3	11/12	0.99	0.03	32,36,40,42	0
2	GLA	O	3	11/12	0.99	0.04	30,35,43,45	0
2	GLA	V	3	11/12	0.99	0.03	49,58,63,64	0

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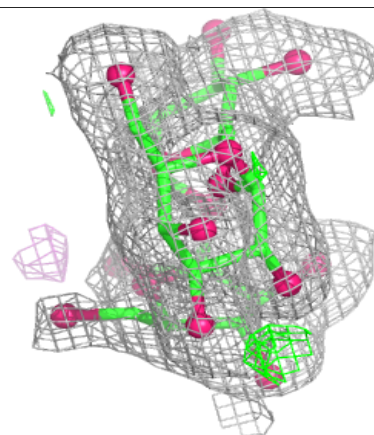
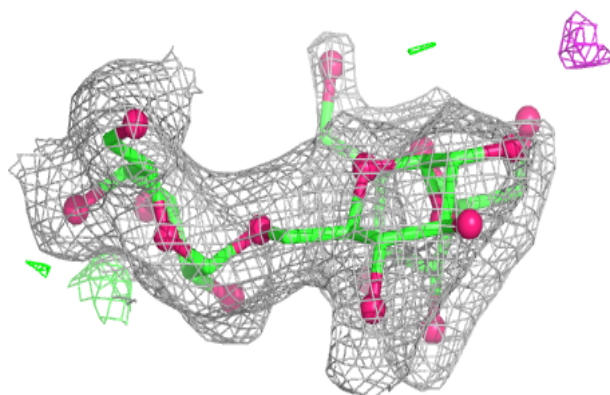
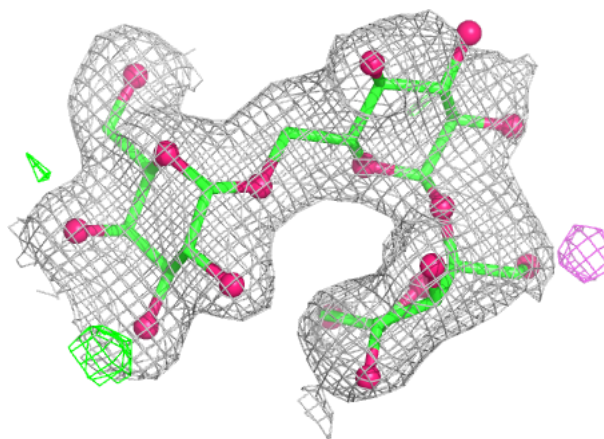
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLA	L	3	11/12	0.99	0.02	31,35,44,45	0
2	GLA	N	3	11/12	0.99	0.04	35,43,48,53	0
2	GLA	Z	3	11/12	0.99	0.04	45,53,55,57	0
2	FRU	a	1	12/12	-	-	52,72,78,80	0
2	GLC	a	2	11/12	-	-	59,67,76,78	0
2	GLA	a	3	11/12	-	-	43,47,51,51	0
2	FRU	b	1	12/12	-	-	54,62,67,72	0
2	GLC	b	2	11/12	-	-	47,52,62,66	0
2	GLA	b	3	11/12	-	-	37,44,46,46	0
2	FRU	c	1	12/12	-	-	58,64,69,70	0
2	GLC	c	2	11/12	-	-	51,59,67,70	0
2	GLA	c	3	11/12	-	-	46,56,59,60	0
2	FRU	d	1	12/12	-	-	47,57,59,61	0
2	GLC	d	2	11/12	-	-	45,55,56,66	0
2	GLA	d	3	11/12	-	-	30,36,40,42	0
2	FRU	e	1	12/12	-	-	44,51,59,65	0
2	GLC	e	2	11/12	-	-	42,58,64,65	0
2	GLA	e	3	11/12	-	-	32,36,38,39	0
2	FRU	f	1	12/12	-	-	52,61,69,74	0
2	GLC	f	2	11/12	-	-	45,57,67,71	0
2	GLA	f	3	11/12	-	-	29,33,41,45	0
2	FRU	g	1	1/12	-	-	63,63,63,63	0
2	GLC	g	2	11/12	-	-	60,62,68,68	0
2	GLA	g	3	11/12	-	-	51,55,62,64	0
2	FRU	h	1	1/12	-	-	60,60,60,60	0
2	GLC	h	2	11/12	-	-	53,57,68,72	0
2	GLA	h	3	11/12	-	-	44,51,59,60	0
2	FRU	i	1	12/12	-	-	62,73,77,82	0
2	GLC	i	2	11/12	-	-	48,54,62,66	0
2	GLA	i	3	11/12	-	-	45,49,53,53	0
2	FRU	j	1	12/12	-	-	57,70,73,73	0
2	GLC	j	2	11/12	-	-	43,55,70,75	0
2	GLA	j	3	11/12	-	-	30,37,41,44	0

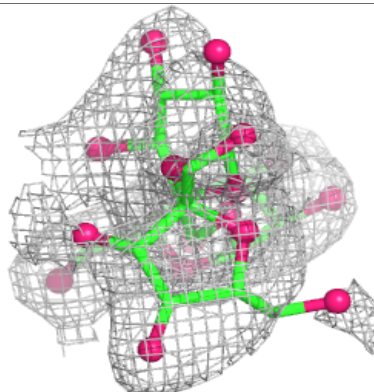
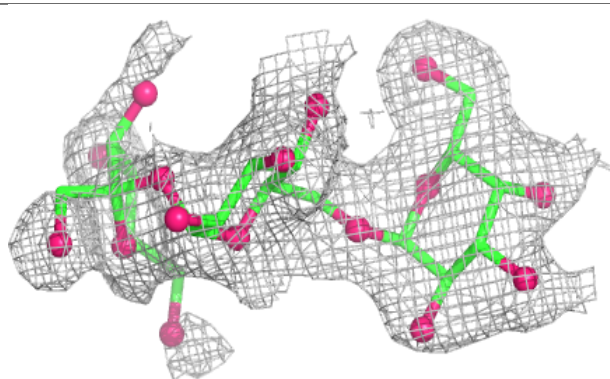
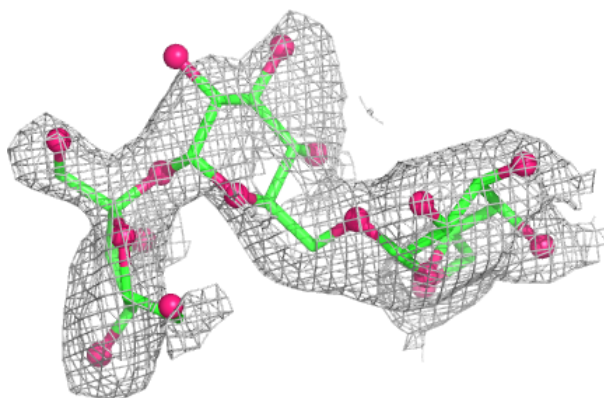
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

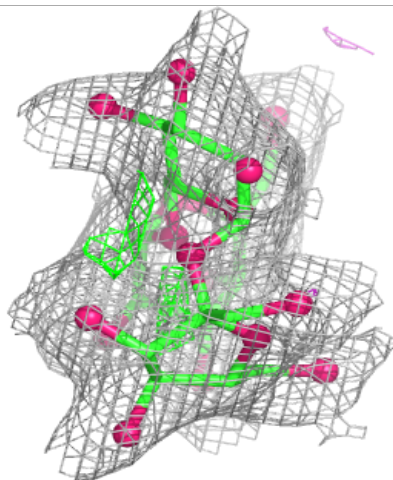
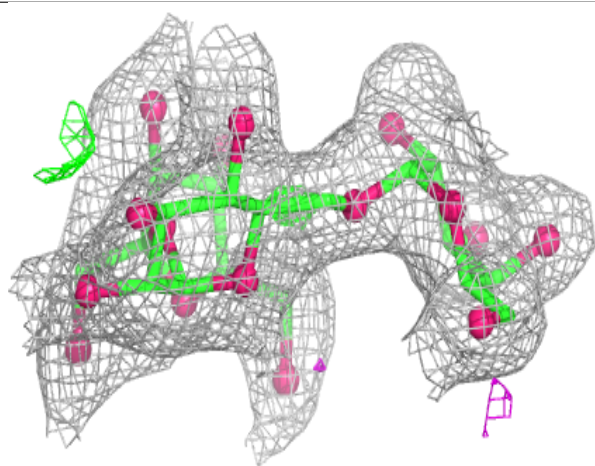
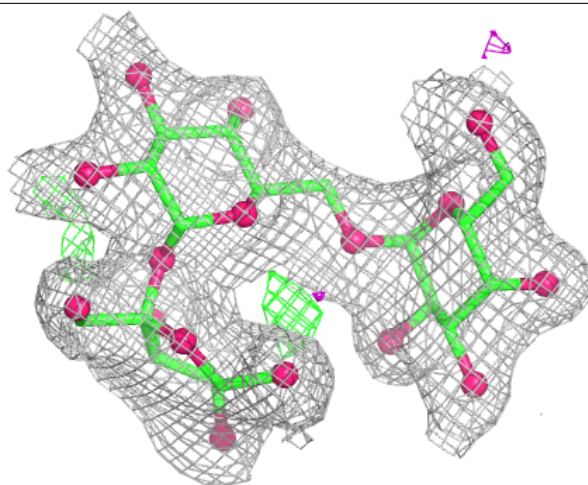
**Electron density around Chain L:**

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and green (positive)



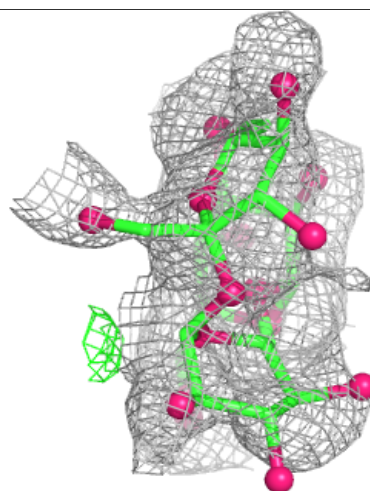
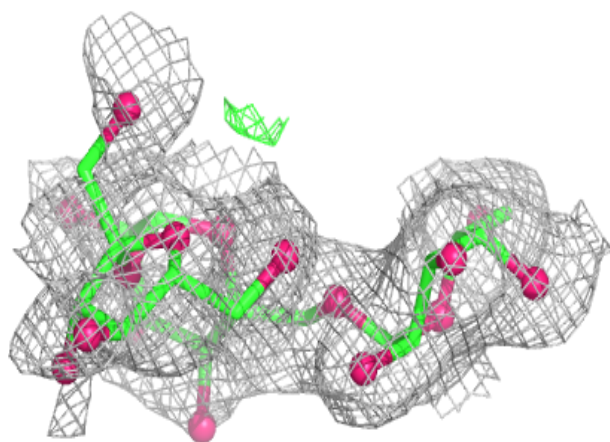
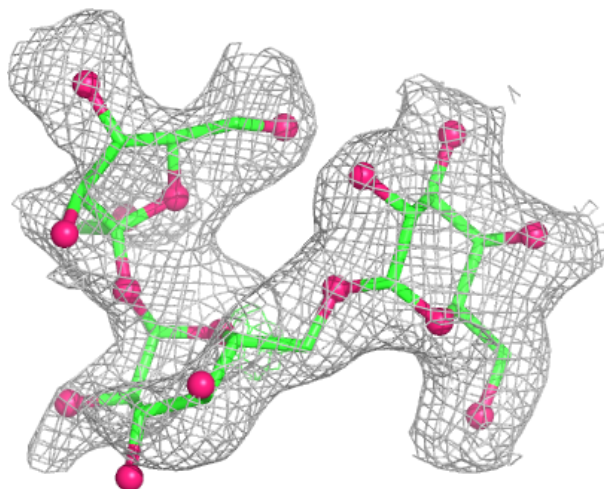
Electron density around Chain M:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



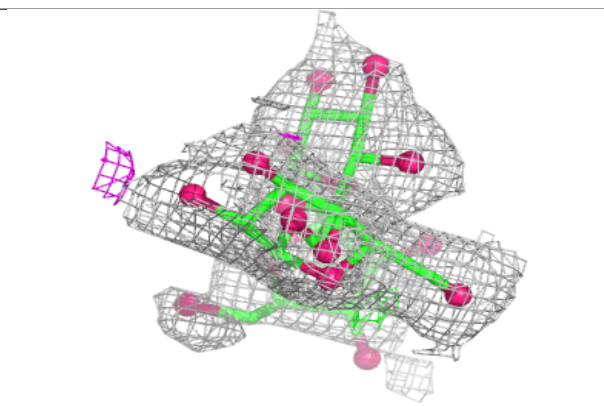
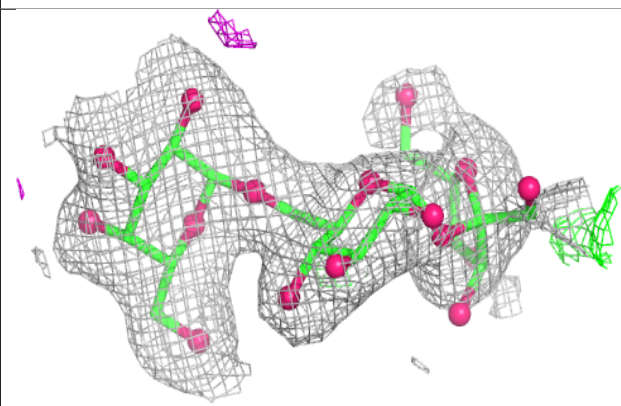
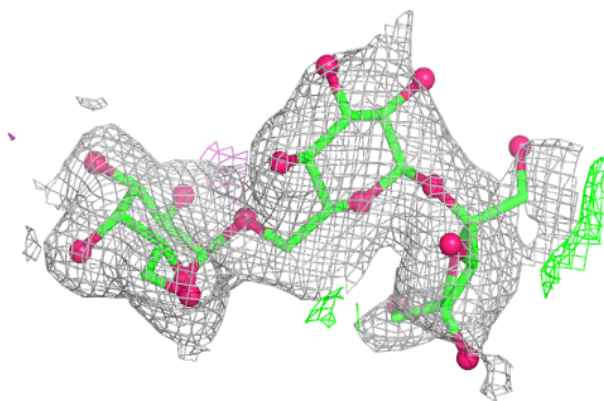
Electron density around Chain N:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

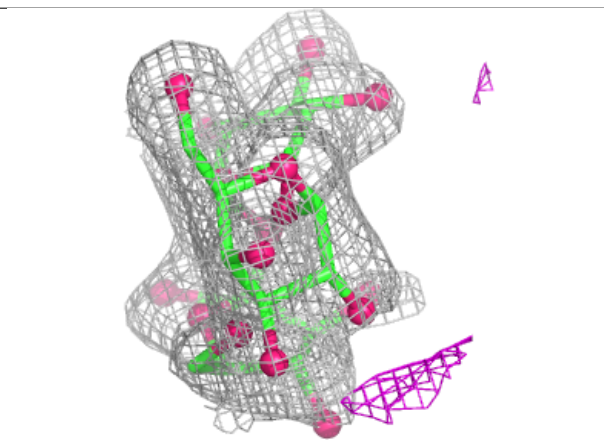
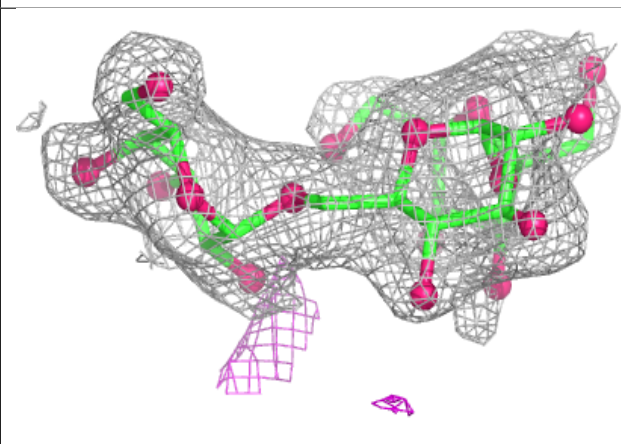
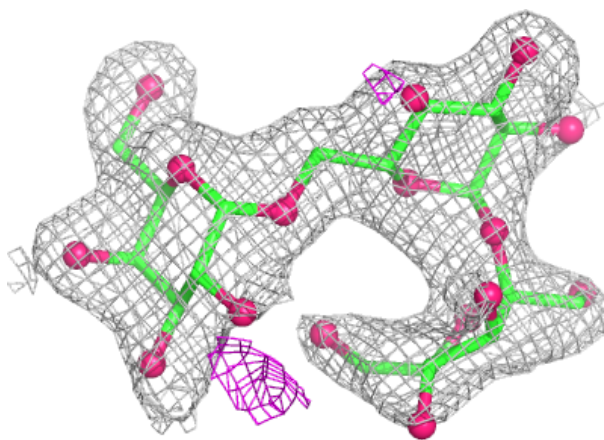


Electron density around Chain O:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

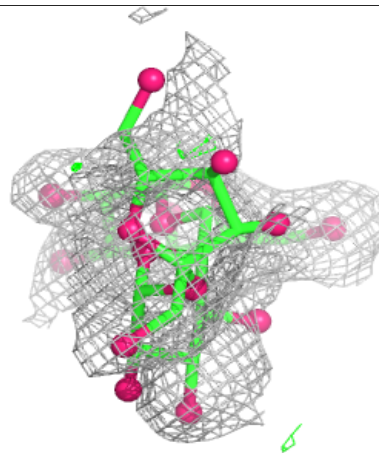
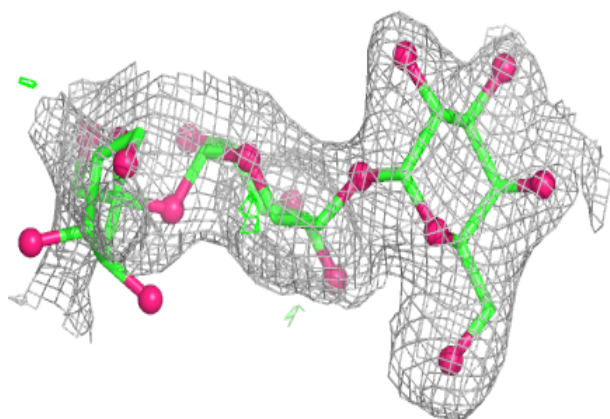
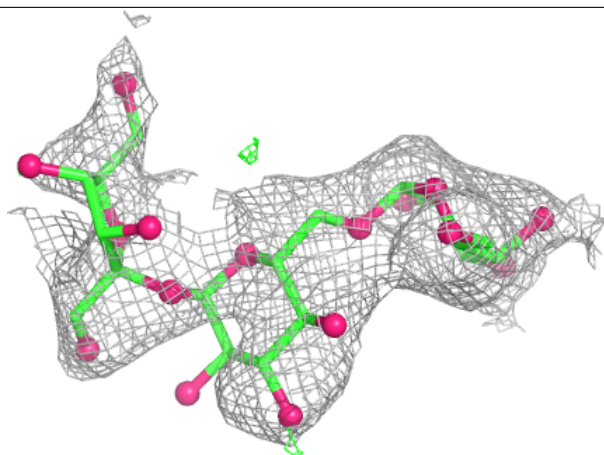
**Electron density around Chain P:**

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and green (positive)



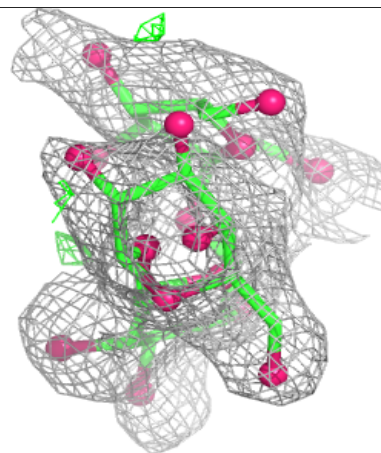
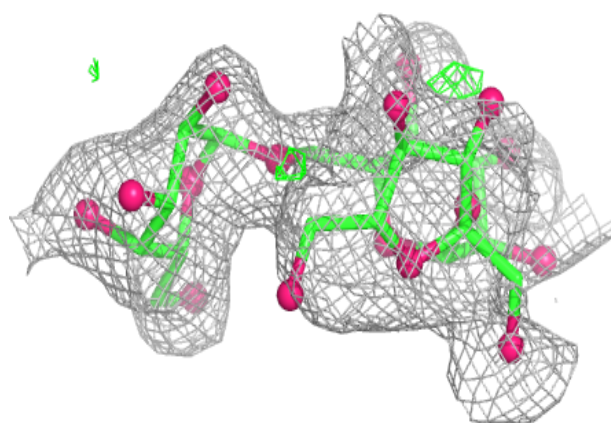
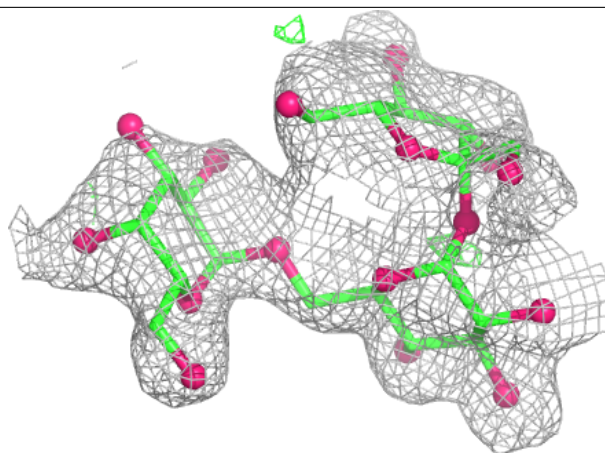
Electron density around Chain Q:

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



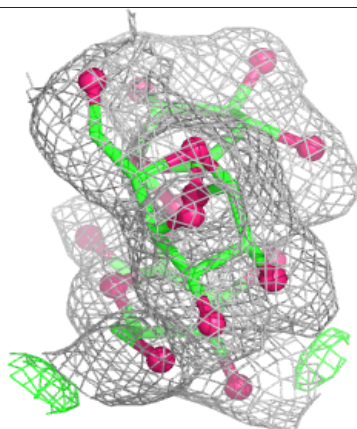
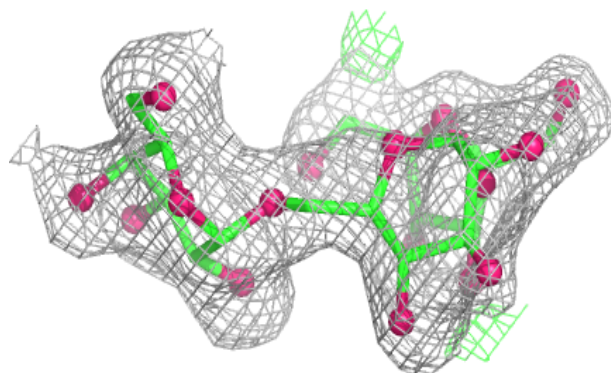
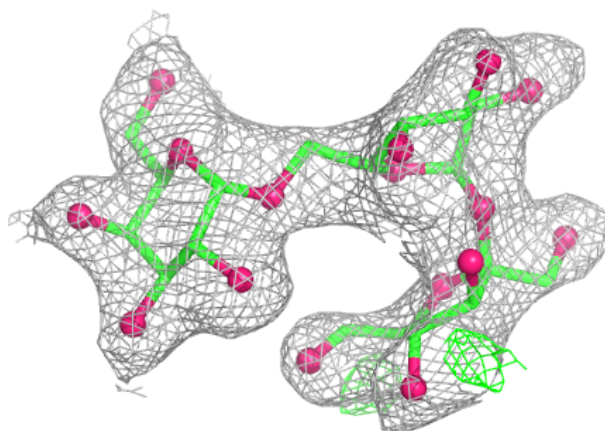
Electron density around Chain R:

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



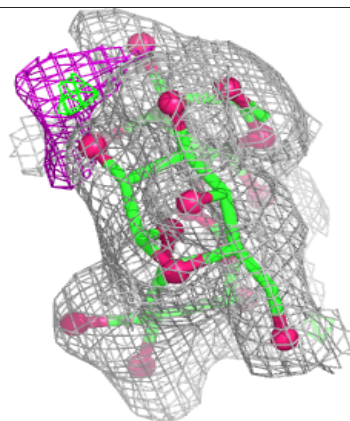
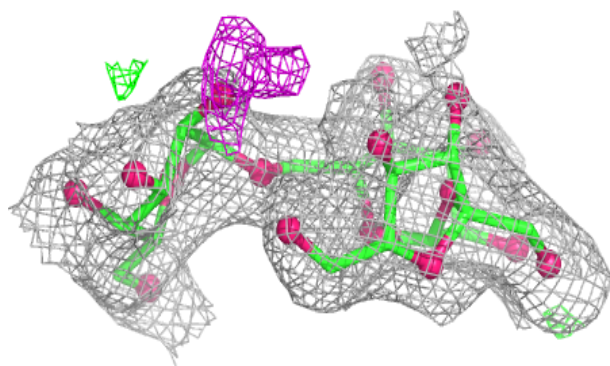
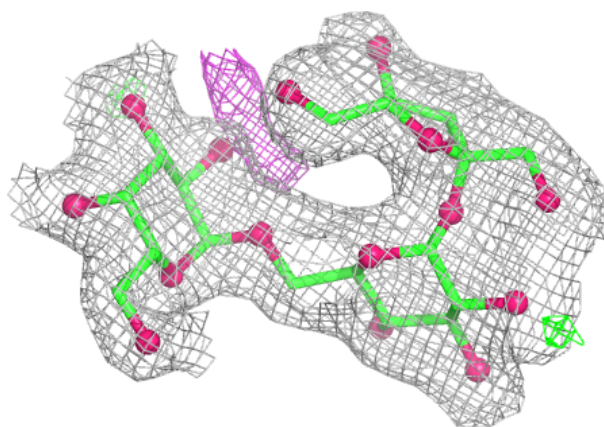
Electron density around Chain S:

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



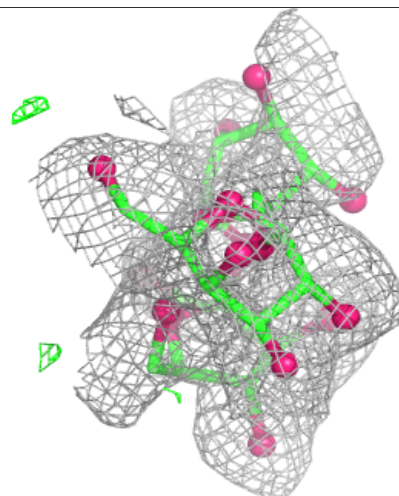
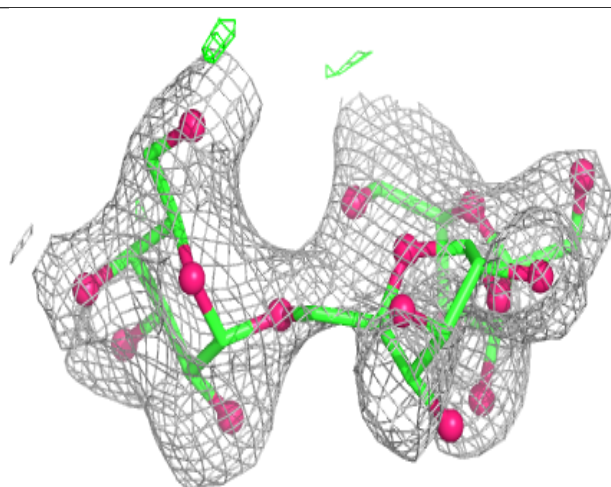
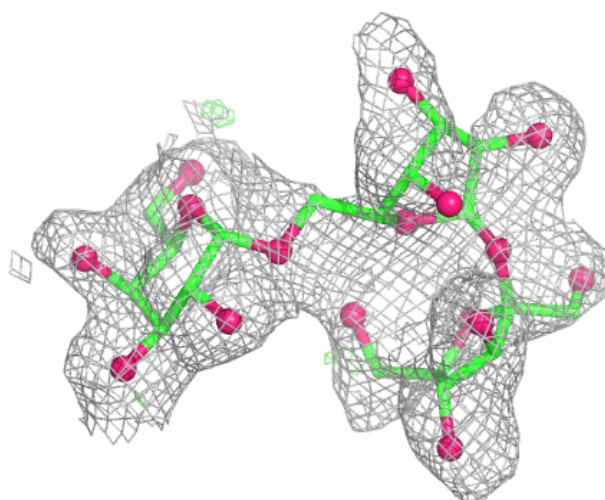
Electron density around Chain T:

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



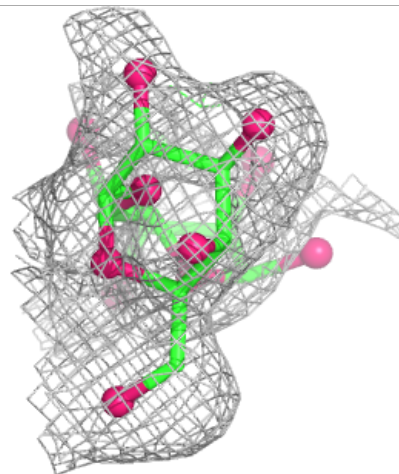
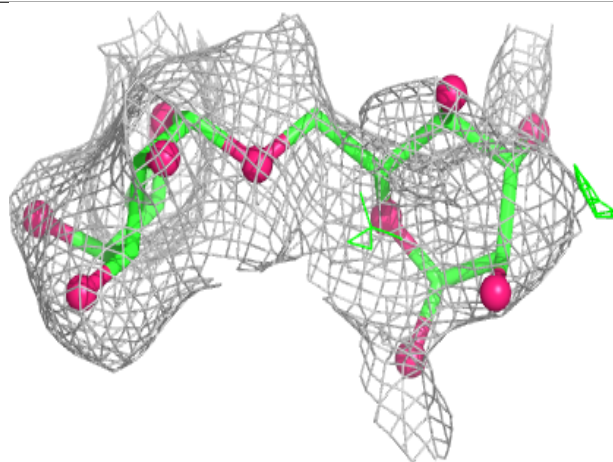
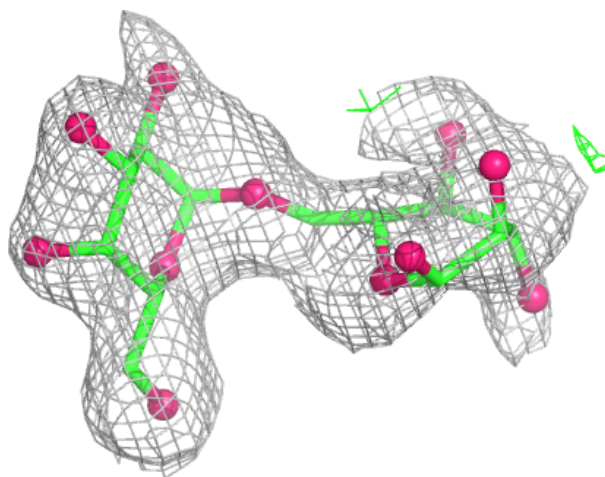
Electron density around Chain U:

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



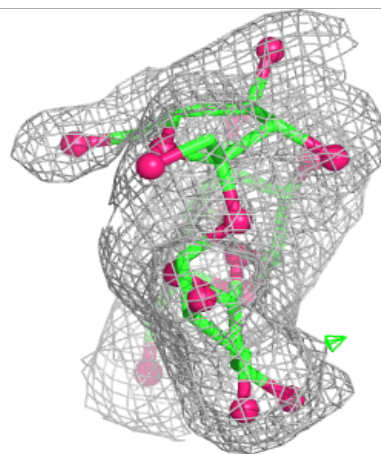
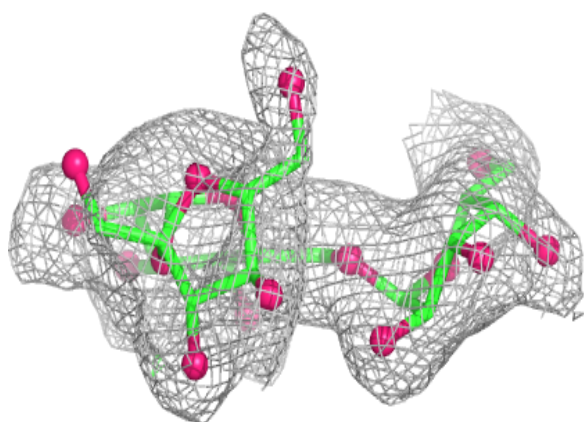
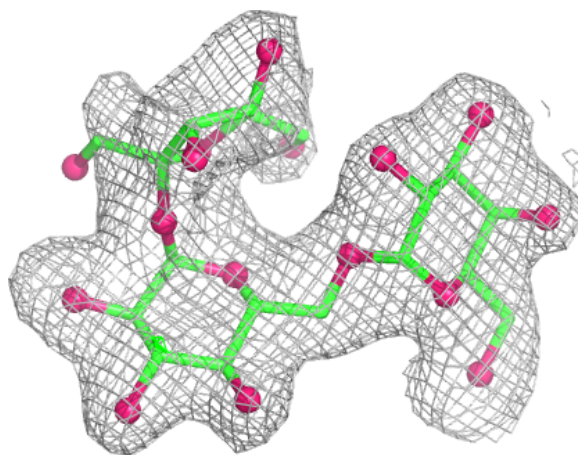
Electron density around Chain V:

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



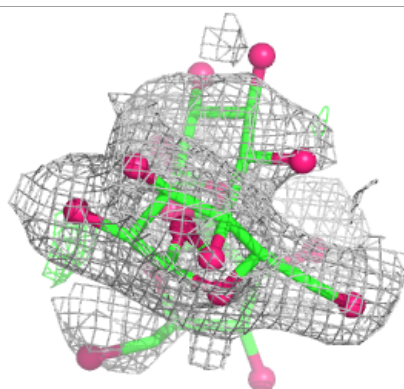
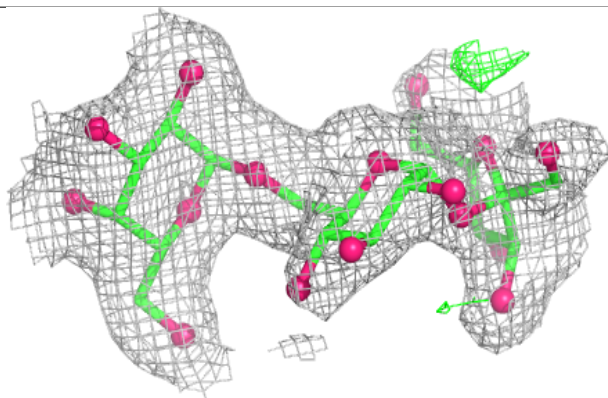
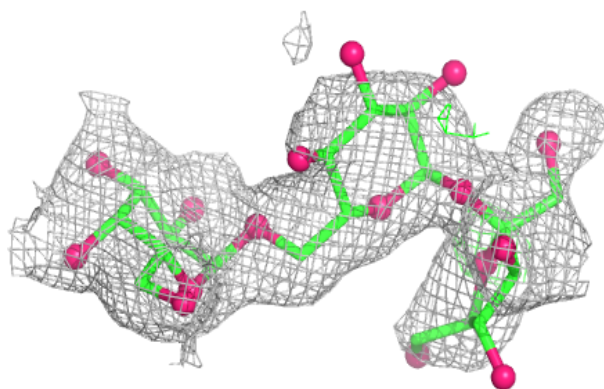
Electron density around Chain W:

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

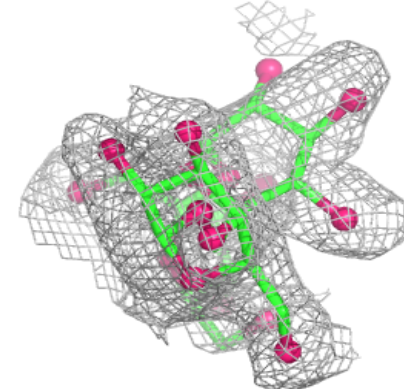
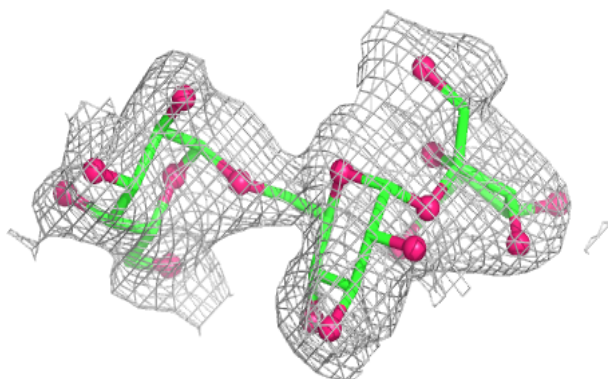
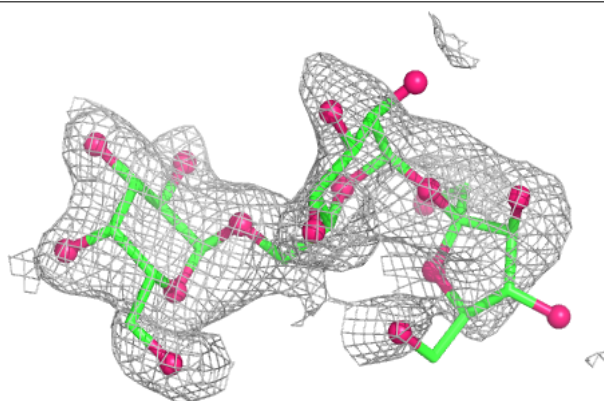


Electron density around Chain X:

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

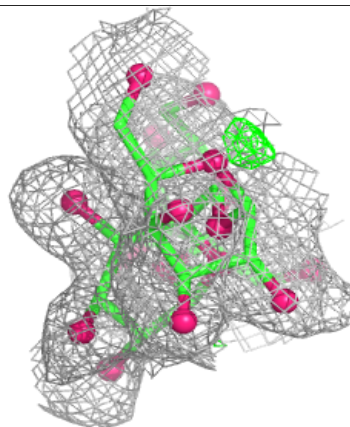
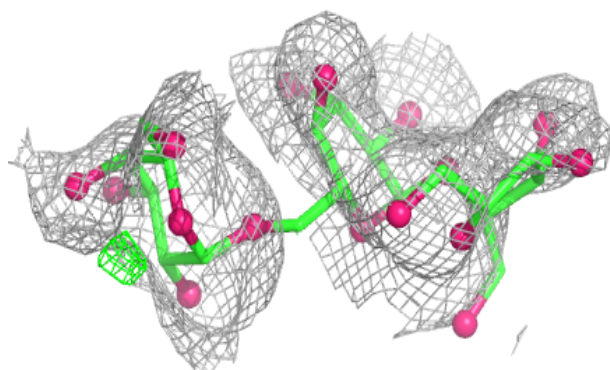
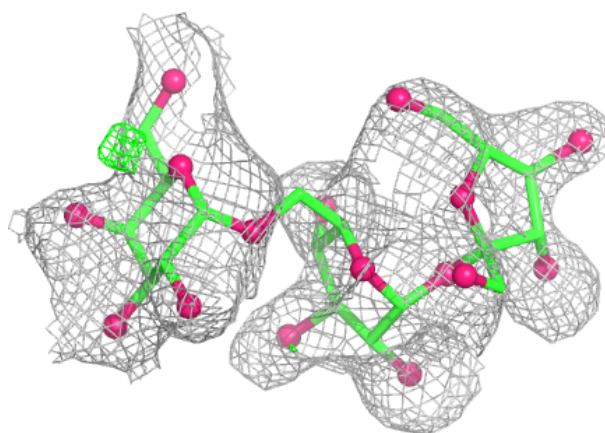
**Electron density around Chain Y:**

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

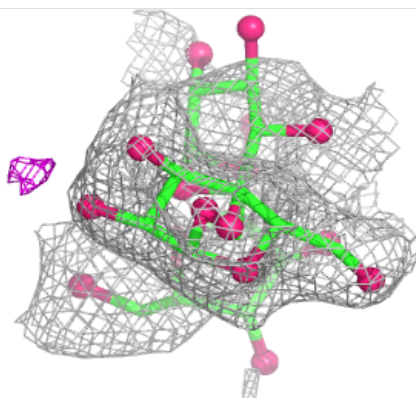
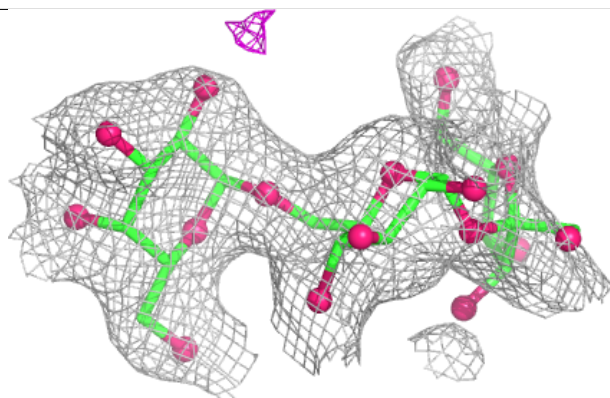
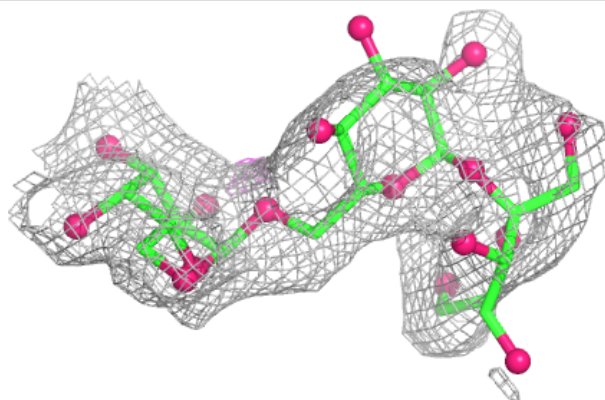


Electron density around Chain Z:

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

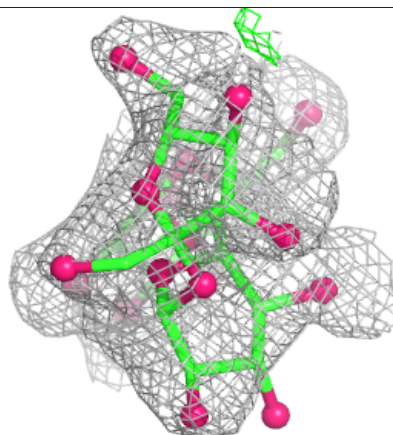
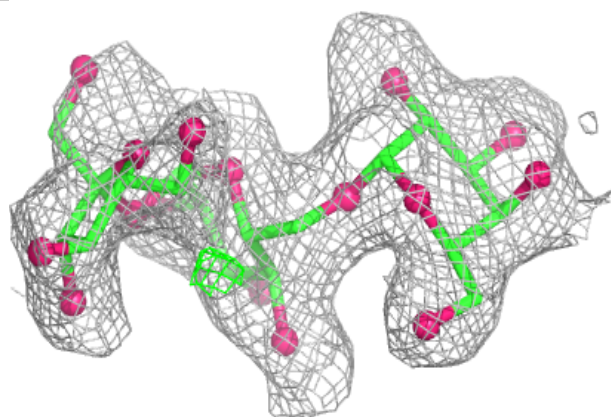
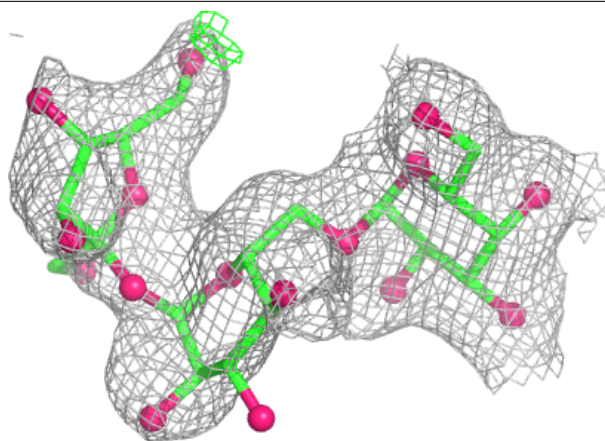
**Electron density around Chain a:**

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

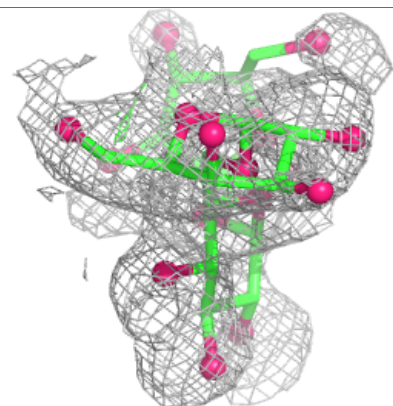
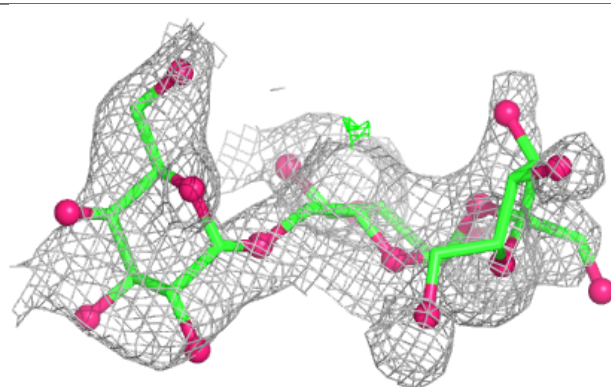
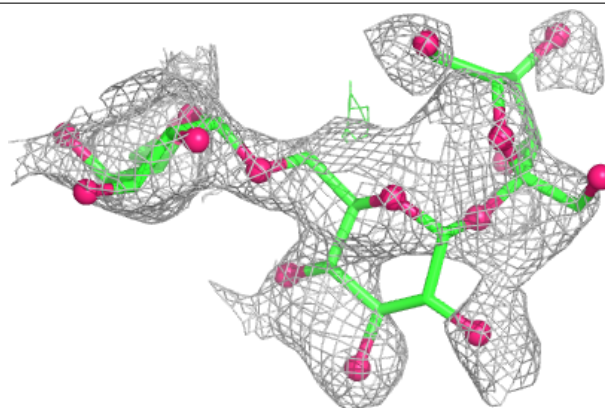


Electron density around Chain b:

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

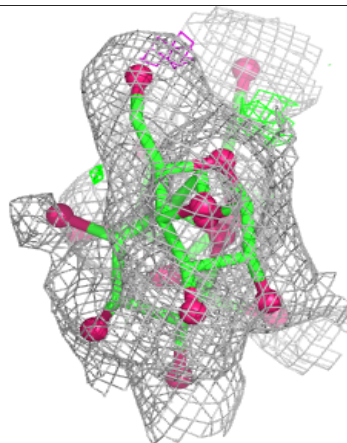
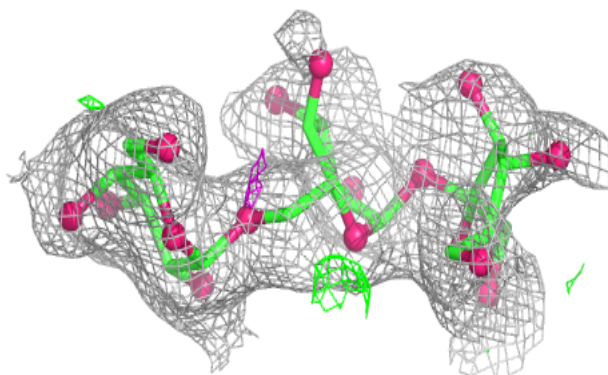
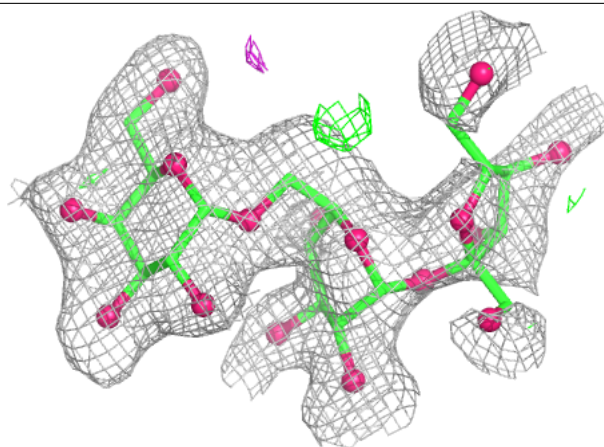
**Electron density around Chain c:**

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

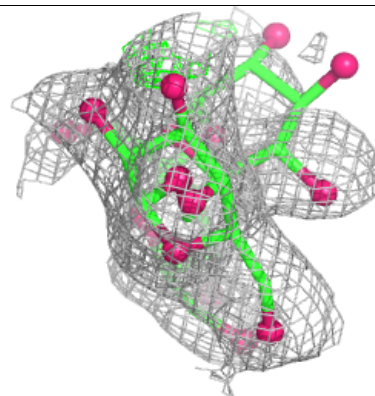
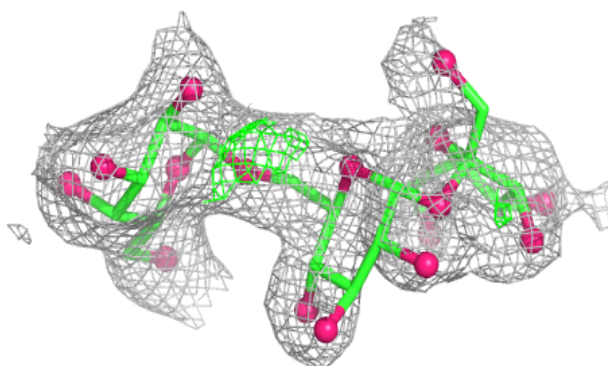
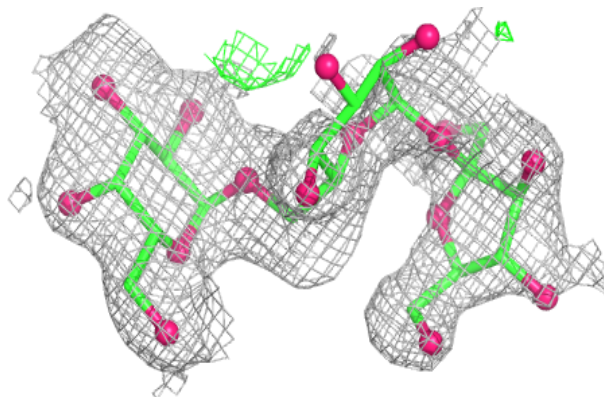


Electron density around Chain d:

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

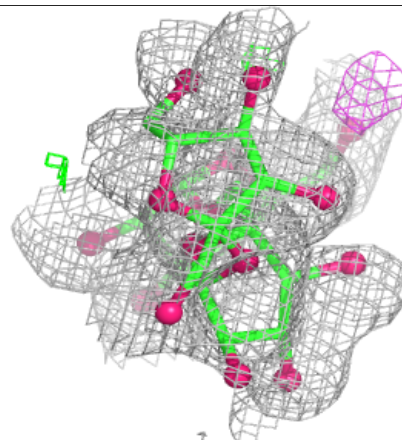
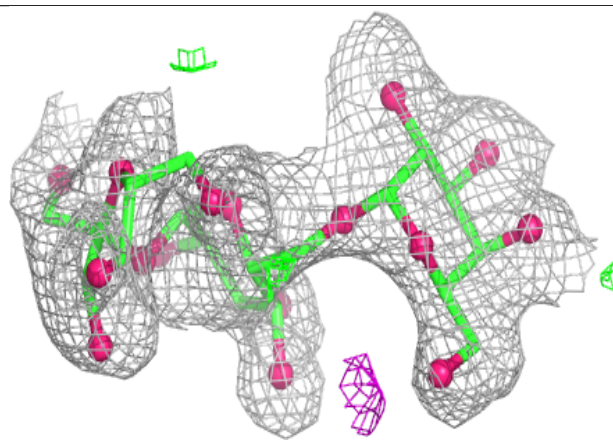
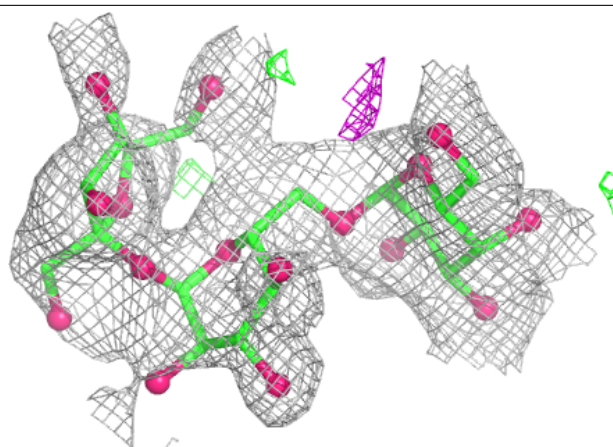
**Electron density around Chain e:**

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



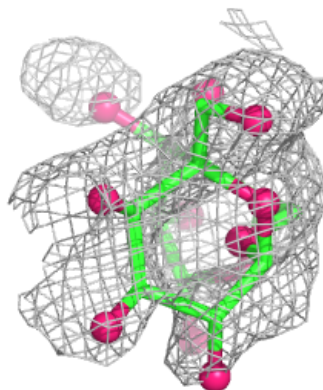
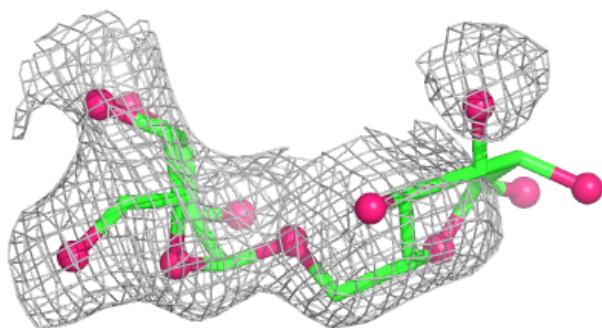
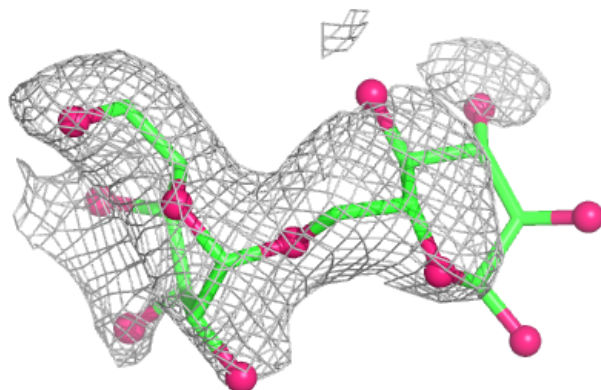
Electron density around Chain f:

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

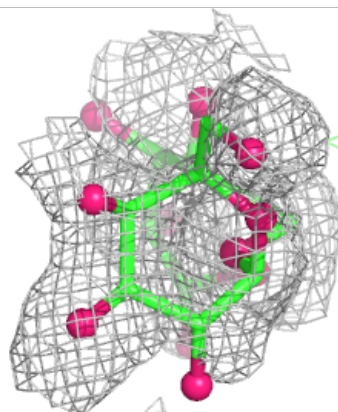
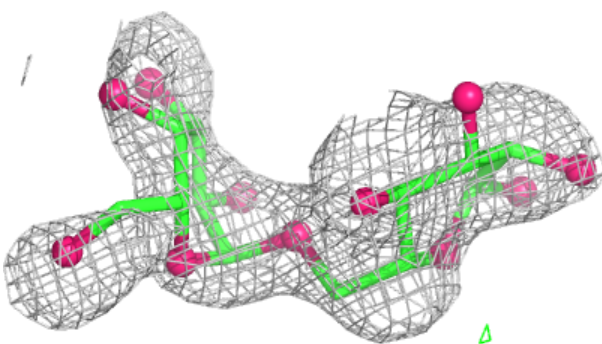
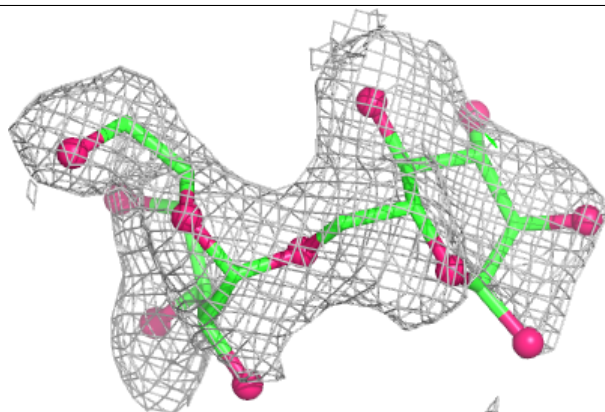


Electron density around Chain g:

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

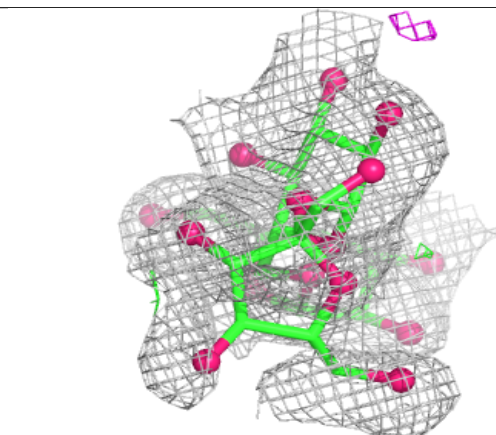
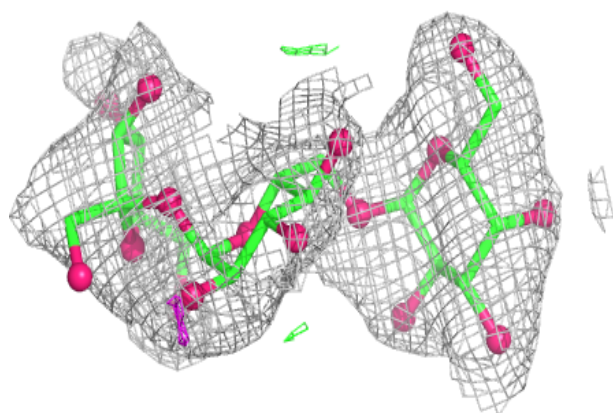
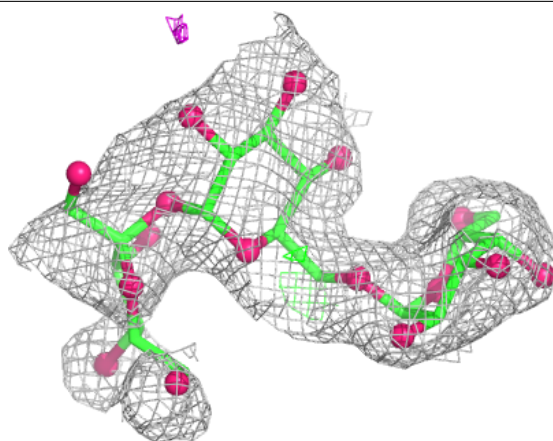
**Electron density around Chain h:**

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

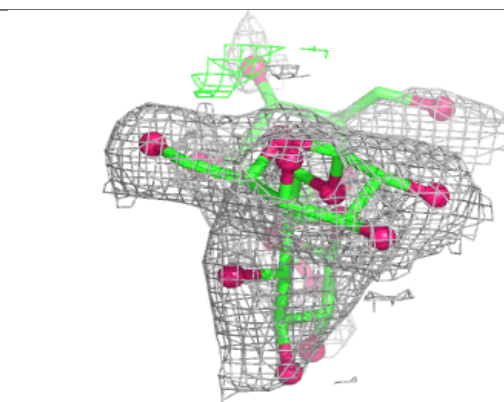
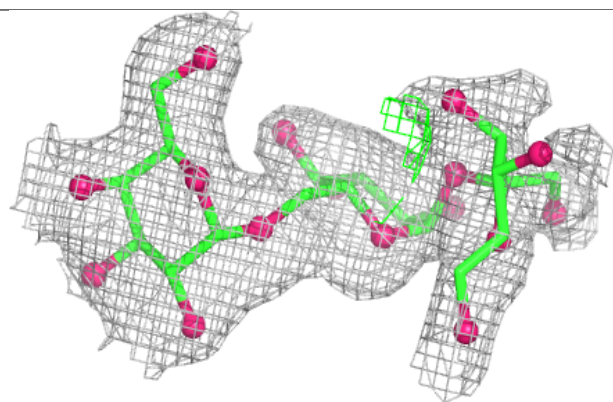
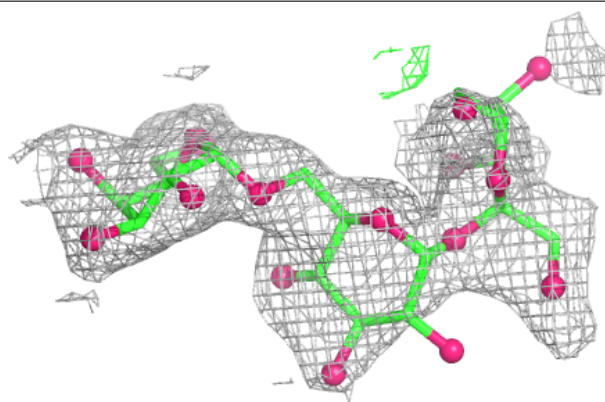


Electron density around Chain i:

$2mF_o - DF_c$ (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)



6.4 Ligands

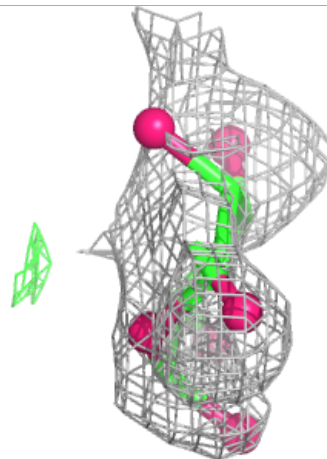
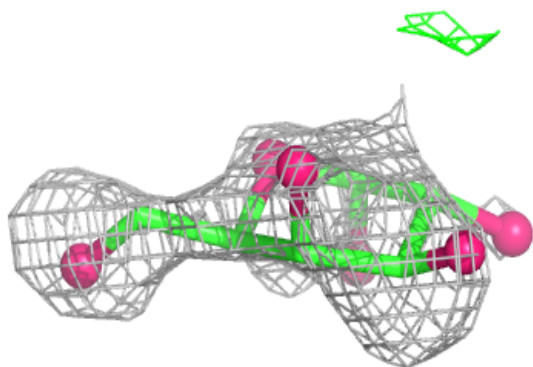
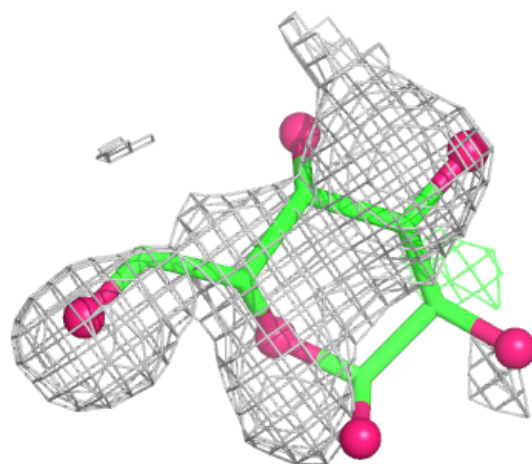
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	F	203	13/13	0.94	0.07	29,40,52,54	0
5	PG4	D	202	13/13	0.96	0.06	39,45,55,56	0
3	GLA	A	201	12/12	0.97	0.05	53,58,61,65	0
4	EPE	D	201	15/15	0.97	0.06	37,46,73,75	0
3	GLA	G	201	12/12	0.98	0.06	41,59,66,67	0
4	EPE	F	201	15/15	0.98	0.04	40,44,73,77	0
7	ACT	F	202	4/4	0.98	0.04	32,33,34,41	0
8	GOL	F	204	6/6	0.98	0.06	27,33,41,43	0
6	CA	D	203	1/1	0.99	0.04	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

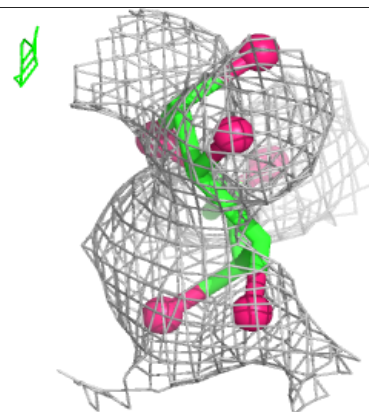
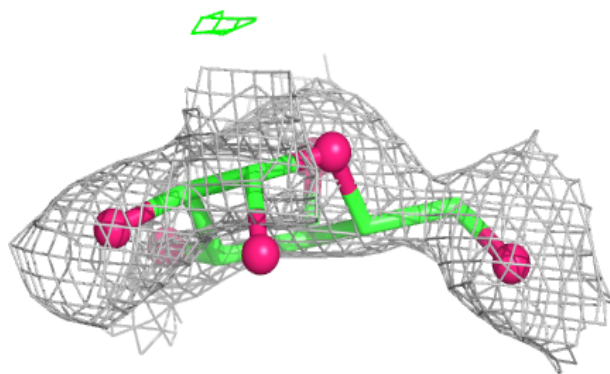
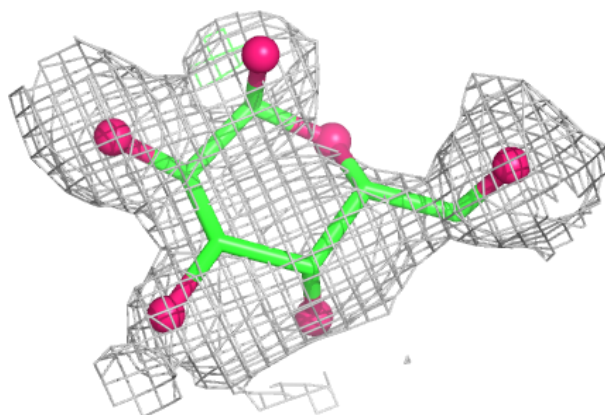
Electron density around GLA A 201:

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



Electron density around GLA G 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.