



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 5XRS / pdb_00005xrs
Title : Crystal structure of A/Minnesota/11/2010 (H3N2) influenza virus hemagglutinin in complex with LSTc
Authors : Zhang, H.; Wilson, I.A.
Deposited on : 2017-06-09
Resolution : 2.91 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

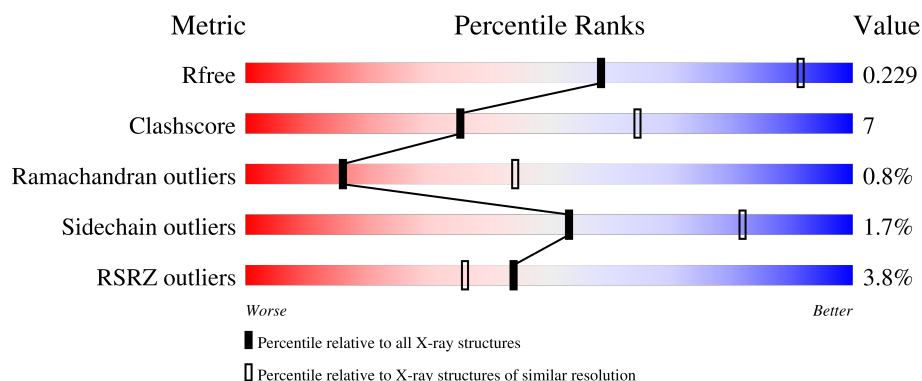
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	329	2% 84% 12% ..
1	C	329	2% 84% 12% ..
1	E	329	3% 88% 9% .
1	G	329	2% 81% 15% ..
2	B	174	0% 87% 10% ...

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Mol	Chain	Length	Quality of chain
2	D	174	
2	F	174	
2	H	174	
3	I	3	
4	J	4	
4	M	4	
5	K	4	
5	Q	4	
5	R	4	
5	W	4	
5	c	4	
6	L	6	
7	N	3	
7	b	3	
7	e	3	
8	O	5	
8	V	5	
8	g	5	
9	P	2	
10	S	7	
11	T	5	
11	X	5	
12	U	2	
12	Y	2	
12	Z	2	

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Mol	Chain	Length	Quality of chain
12	a	2	 50%50%
12	f	2	 50%50%
13	d	5	 20%20%60%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 16918 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

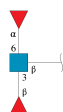
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			
1	C	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			
1	E	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			
1	G	321	Total	C	N	O	S	0	0	0
			2522	1580	441	488	13			

- Molecule 2 is a protein called Hemagglutinin.

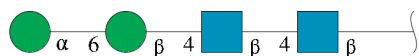
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			
2	D	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			
2	F	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			
2	H	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			34	20	1	13			

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



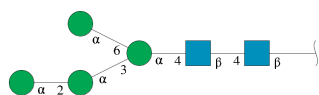
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



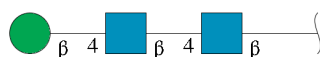
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	W	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	c	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



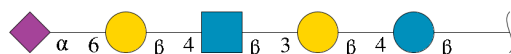
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



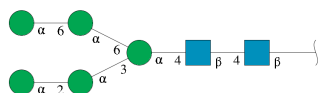
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	O	5	Total	C	N	O	0	0	0
			68	37	2	29			
8	V	5	Total	C	N	O	0	0	0
			68	37	2	29			
8	g	5	Total	C	N	O	0	0	0
			68	37	2	29			

- Molecule 9 is an oligosaccharide called beta-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



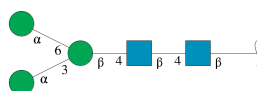
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



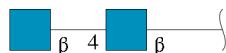
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	S	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	T	5	Total	C	N	O	0	0	0
			61	34	2	25			
11	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



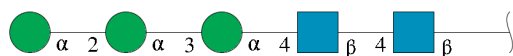
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
12	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

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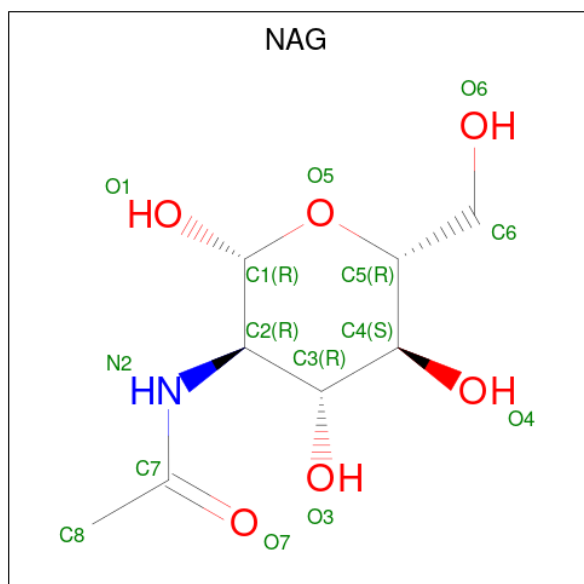
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
12	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
12	f	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	d	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



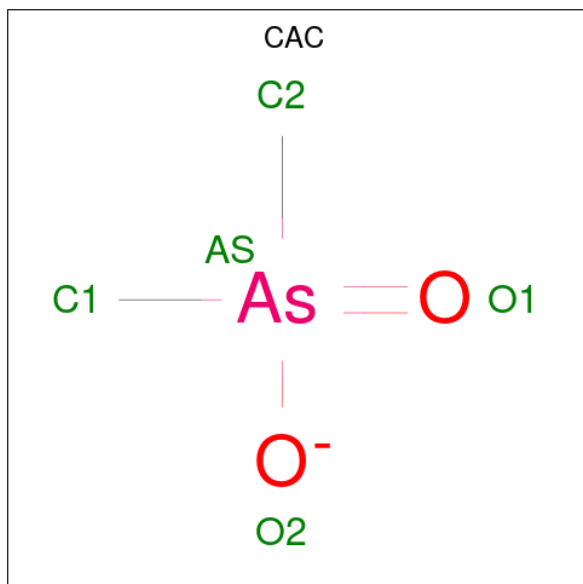
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	C	1	Total	C	N	O	0	0
			14	8	1	5		
14	D	1	Total	C	N	O	0	0
			14	8	1	5		
14	E	1	Total	C	N	O	0	0
			14	8	1	5		
14	F	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 15 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).

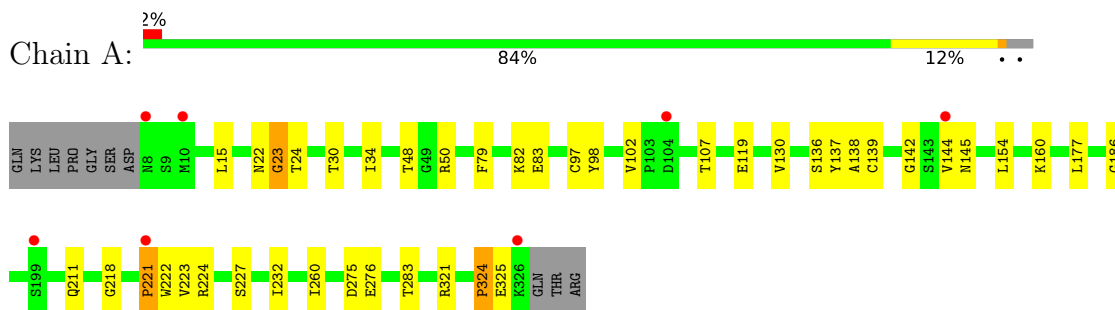


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	D	1	Total	As	C	O	0	0
			5	1	2	2		

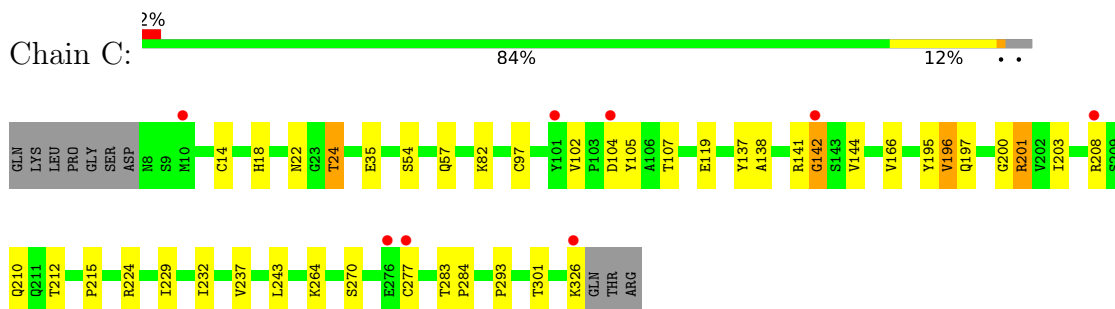
3 Residue-property plots [i](#)

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.

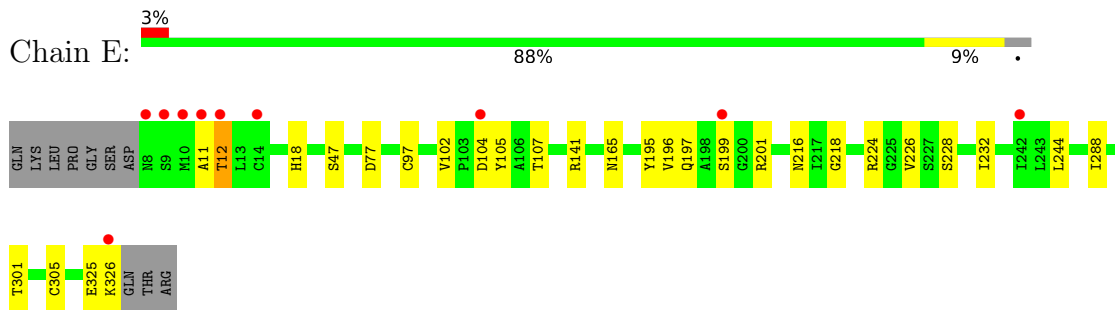
- Molecule 1: Hemagglutinin



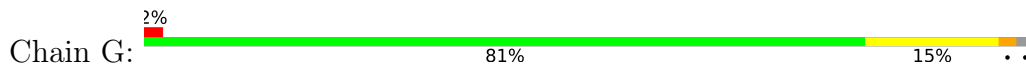
- Molecule 1: Hemagglutinin

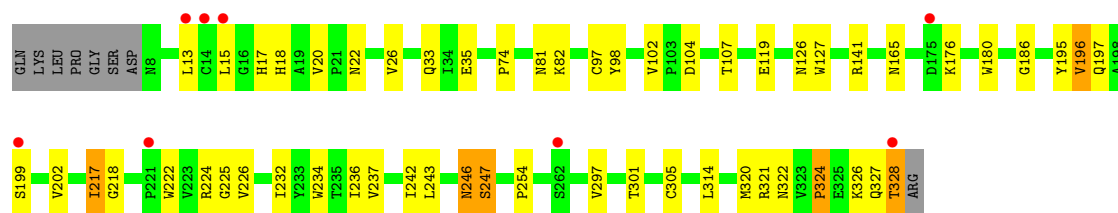


- Molecule 1: Hemagglutinin

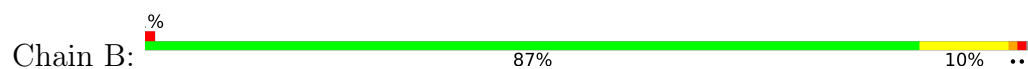


- Molecule 1: Hemagglutinin

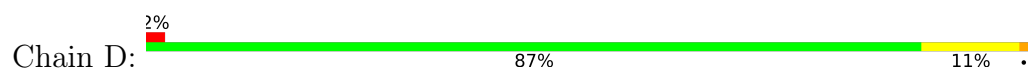




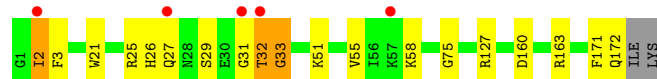
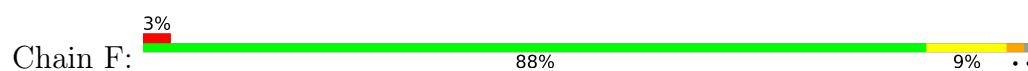
• Molecule 2: Hemagglutinin



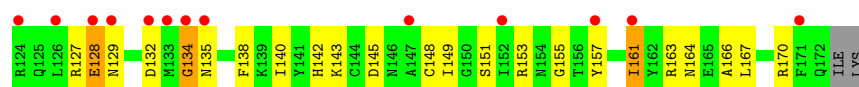
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



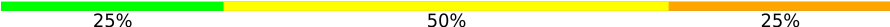
• Molecule 2: Hemagglutinin



• Molecule 3: beta-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

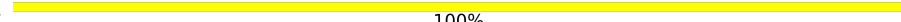


• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  25% 50% 25%



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

Chain M:  100%

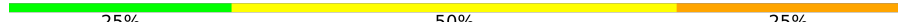


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  25% 50% 25%

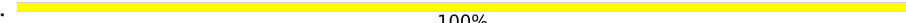


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  25% 25% 50%

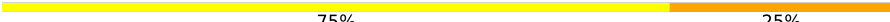


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

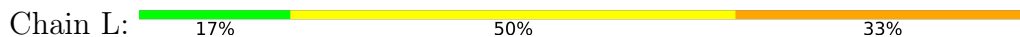


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  75% 25%



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



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



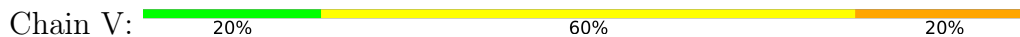
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



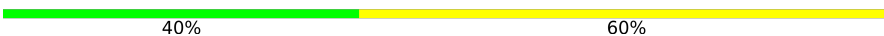
- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain g:  40% 60%

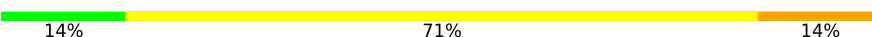
BGC1
GAL2
NAG3
GAL4
SIA5

- Molecule 9: beta-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

NAG1
FUC2

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  14% 71% 14%

NAG1
NAG2
MAN3
MAN4
MAN5
MAN6
MAN7

- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  40% 60%

NAG1
NAG2
MAN3
MAN4
MAN5

- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  60% 40%

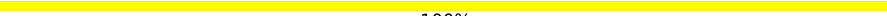
NAG1
NAG2
MAN3
MAN4
MAN5

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

NAG1
NAG2

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1
MAG2

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1
MAG2

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%

MAG1
MAG2

- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  50% 50%

MAG1
MAG2

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  20% 20% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	292.98Å 292.98Å 292.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.91 46.32 – 2.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.32-2.91) 100.0 (46.32-2.91)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.225 0.193 , 0.229	Depositor DCC
R_{free} test set	4471 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16918	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CAC, BMA, FUL, SIA, NAG, FUC, GAL, 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	0.17	0/2565	0.63	7/3492 (0.2%)
1	C	0.15	0/2565	0.52	7/3492 (0.2%)
1	E	0.15	0/2565	0.46	2/3492 (0.1%)
1	G	0.18	0/2581	0.49	5/3514 (0.1%)
2	B	0.21	0/1416	0.55	1/1902 (0.1%)
2	D	0.24	0/1416	0.46	0/1902
2	F	0.18	0/1416	0.69	3/1902 (0.2%)
2	H	0.22	0/1416	1.09	16/1902 (0.8%)
All	All	0.18	0/15940	0.61	41/21598 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	THR	CB-CA-C	-17.19	77.51	110.35
1	A	22	ASN	N-CA-C	16.98	139.38	111.37
2	H	58	LYS	N-CA-C	-16.15	86.92	108.24
2	F	32	THR	N-CA-C	13.12	139.54	113.29
2	H	57	LYS	CB-CA-C	12.36	135.01	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	38	LEU	Peptide
2	H	39	LYS	Peptide

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	2506	0	2420	31	0
1	C	2506	0	2421	24	0
1	E	2506	0	2422	22	0
1	G	2522	0	2439	51	0
2	B	1392	0	1323	17	0
2	D	1392	0	1323	25	0
2	F	1392	0	1324	20	1
2	H	1392	0	1325	63	0
3	I	34	0	31	2	0
4	J	50	0	43	1	0
4	M	50	0	43	0	0
5	K	50	0	43	1	0
5	Q	50	0	43	1	0
5	R	50	0	43	2	0
5	W	50	0	43	0	0
5	c	50	0	43	2	0
6	L	72	0	61	2	0
7	N	39	0	34	1	0
7	b	39	0	34	1	0
7	e	39	0	34	1	0
8	O	68	0	58	1	0
8	V	68	0	58	1	0
8	g	68	0	58	0	0
9	P	24	0	22	2	0
10	S	83	0	70	1	0
11	T	61	0	52	0	0
11	X	61	0	52	2	0
12	U	28	0	25	2	0
12	Y	28	0	25	3	0
12	Z	28	0	25	0	0
12	a	28	0	25	1	0
12	f	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	d	61	0	52	2	0
14	A	14	0	13	0	0
14	B	14	0	13	0	0
14	C	14	0	13	0	0
14	D	14	0	13	0	0
14	E	14	0	13	0	0
14	F	14	0	13	0	0
14	G	14	0	13	0	0
15	D	5	0	0	0	0
All	All	16918	0	16130	243	1

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 7.

The worst 5 of 243 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)
2:F:2:ILE:CD1	2:F:3:PHE:CE1	2.00	1.42
2:F:2:ILE:HD11	2:F:3:PHE:CE1	1.55	1.42
2:F:2:ILE:HD12	2:F:3:PHE:CD1	1.62	1.32
2:F:2:ILE:CD1	2:F:3:PHE:CD1	2.25	1.14
1:G:195:TYR:O	1:G:196:VAL:CG1	1.96	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ARG:NH1	2:F:32:THR:O[14_555]	1.88	0.32

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	317/329 (96%)	296 (93%)	19 (6%)	2 (1%)	21	51
1	C	317/329 (96%)	303 (96%)	13 (4%)	1 (0%)	36	65
1	E	317/329 (96%)	300 (95%)	15 (5%)	2 (1%)	21	51
1	G	319/329 (97%)	300 (94%)	16 (5%)	3 (1%)	14	41
2	B	170/174 (98%)	161 (95%)	8 (5%)	1 (1%)	21	51
2	D	170/174 (98%)	163 (96%)	7 (4%)	0	100	100
2	F	170/174 (98%)	160 (94%)	9 (5%)	1 (1%)	21	51
2	H	170/174 (98%)	140 (82%)	24 (14%)	6 (4%)	3	12
All	All	1950/2012 (97%)	1823 (94%)	111 (6%)	16 (1%)	16	44

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLY
2	B	58	LYS
1	E	196	VAL
2	H	39	LYS
2	H	57	LYS

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	284/293 (97%)	280 (99%)	4 (1%)	59	85
1	C	284/293 (97%)	276 (97%)	8 (3%)	38	72
1	E	284/293 (97%)	284 (100%)	0	100	100
1	G	286/293 (98%)	282 (99%)	4 (1%)	59	85
2	B	146/148 (99%)	142 (97%)	4 (3%)	39	73
2	D	146/148 (99%)	145 (99%)	1 (1%)	76	92
2	F	146/148 (99%)	144 (99%)	2 (1%)	59	85
2	H	146/148 (99%)	140 (96%)	6 (4%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1722/1764 (98%)	1693 (98%)	29 (2%)	53 82

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	210	GLN
2	H	128	GLU
2	F	2	ILE
2	H	45	ILE
2	D	2	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	42	GLN
2	H	12	ASN
2	H	129	ASN
2	H	28	ASN
1	G	158	ASN

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 ⓘ

95 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
3	NAG	I	1	1,3	14,14,15	0.27	0	17,19,21	1.14	2 (11%)
3	FUL	I	2	3	10,10,11	2.05	2 (20%)	14,14,16	3.04	7 (50%)
3	FUC	I	3	3	10,10,11	0.80	0	14,14,16	0.83	0
4	NAG	J	1	4,1	14,14,15	0.71	1 (7%)	17,19,21	0.69	0
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	0.66	0
4	BMA	J	3	4	11,11,12	0.79	1 (9%)	15,15,17	1.45	2 (13%)
4	MAN	J	4	4	11,11,12	0.85	1 (9%)	15,15,17	1.12	1 (6%)
5	NAG	K	1	5,1	14,14,15	0.58	0	17,19,21	0.86	0
5	NAG	K	2	5	14,14,15	0.22	0	17,19,21	0.79	0
5	BMA	K	3	5	11,11,12	0.41	0	15,15,17	0.87	0
5	MAN	K	4	5	11,11,12	0.69	1 (9%)	15,15,17	1.09	2 (13%)
6	NAG	L	1	1,6	14,14,15	0.22	0	17,19,21	0.59	0
6	NAG	L	2	6	14,14,15	0.35	0	17,19,21	0.54	0
6	MAN	L	3	6	11,11,12	0.94	1 (9%)	15,15,17	2.11	5 (33%)
6	MAN	L	4	6	11,11,12	1.94	3 (27%)	15,15,17	1.80	4 (26%)
6	MAN	L	5	6	11,11,12	1.17	2 (18%)	15,15,17	1.36	1 (6%)
6	MAN	L	6	6	11,11,12	1.50	3 (27%)	15,15,17	1.85	2 (13%)
4	NAG	M	1	4,1	14,14,15	0.22	0	17,19,21	0.90	1 (5%)
4	NAG	M	2	4	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
4	BMA	M	3	4	11,11,12	1.82	4 (36%)	15,15,17	1.41	3 (20%)
4	MAN	M	4	4	11,11,12	1.16	1 (9%)	15,15,17	1.24	3 (20%)
7	NAG	N	1	1,7	14,14,15	0.41	0	17,19,21	1.31	2 (11%)
7	NAG	N	2	7	14,14,15	0.31	0	17,19,21	0.64	0
7	BMA	N	3	7	11,11,12	1.17	2 (18%)	15,15,17	1.61	3 (20%)
8	BGC	O	1	8	12,12,12	1.76	4 (33%)	17,17,17	1.48	4 (23%)
8	GAL	O	2	8	11,11,12	0.63	0	15,15,17	0.78	0
8	NAG	O	3	8	14,14,15	0.36	0	17,19,21	0.43	0
8	GAL	O	4	8	11,11,12	0.41	0	15,15,17	0.92	1 (6%)
8	SIA	O	5	8	20,20,21	1.69	2 (10%)	21,28,31	1.83	5 (23%)
9	NAG	P	1	9,1	14,14,15	0.69	1 (7%)	17,19,21	0.54	0
9	FUL	P	2	9	10,10,11	1.99	3 (30%)	14,14,16	1.90	4 (28%)
5	NAG	Q	1	5,1	14,14,15	0.80	1 (7%)	17,19,21	0.81	0
5	NAG	Q	2	5	14,14,15	0.47	0	17,19,21	0.63	0
5	BMA	Q	3	5	11,11,12	1.04	0	15,15,17	1.04	2 (13%)
5	MAN	Q	4	5	11,11,12	0.98	0	15,15,17	0.91	2 (13%)
5	NAG	R	1	5,1	14,14,15	0.41	0	17,19,21	0.70	0
5	NAG	R	2	5	14,14,15	0.47	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	R	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.18	2 (13%)
5	MAN	R	4	5	11,11,12	1.00	1 (9%)	15,15,17	0.90	1 (6%)
10	NAG	S	1	10,1	14,14,15	0.25	0	17,19,21	0.53	0
10	NAG	S	2	10	14,14,15	0.23	0	17,19,21	0.52	0
10	MAN	S	3	10	11,11,12	0.97	0	15,15,17	1.69	2 (13%)
10	MAN	S	4	10	11,11,12	1.69	2 (18%)	15,15,17	1.61	3 (20%)
10	MAN	S	5	10	11,11,12	1.11	1 (9%)	15,15,17	2.09	5 (33%)
10	MAN	S	6	10	11,11,12	1.13	1 (9%)	15,15,17	1.29	2 (13%)
10	MAN	S	7	10	11,11,12	0.90	1 (9%)	15,15,17	1.41	2 (13%)
11	NAG	T	1	11,1	14,14,15	0.25	0	17,19,21	0.58	0
11	NAG	T	2	11	14,14,15	0.51	0	17,19,21	0.55	0
11	BMA	T	3	11	11,11,12	0.66	0	15,15,17	1.24	1 (6%)
11	MAN	T	4	11	11,11,12	0.96	0	15,15,17	1.25	2 (13%)
11	MAN	T	5	11	11,11,12	0.89	0	15,15,17	1.02	1 (6%)
12	NAG	U	1	12,1	14,14,15	0.32	0	17,19,21	1.41	2 (11%)
12	NAG	U	2	12	14,14,15	0.46	0	17,19,21	1.35	2 (11%)
8	BGC	V	1	8	12,12,12	1.39	2 (16%)	17,17,17	1.32	1 (5%)
8	GAL	V	2	8	11,11,12	0.83	0	15,15,17	0.88	1 (6%)
8	NAG	V	3	8	14,14,15	0.34	0	17,19,21	0.51	0
8	GAL	V	4	8	11,11,12	0.96	1 (9%)	15,15,17	1.07	1 (6%)
8	SIA	V	5	8	20,20,21	1.62	2 (10%)	21,28,31	1.57	2 (9%)
5	NAG	W	1	5,1	14,14,15	0.76	1 (7%)	17,19,21	0.65	0
5	NAG	W	2	5	14,14,15	1.57	2 (14%)	17,19,21	1.34	2 (11%)
5	BMA	W	3	5	11,11,12	0.70	0	15,15,17	1.13	1 (6%)
5	MAN	W	4	5	11,11,12	0.77	0	15,15,17	0.97	1 (6%)
11	NAG	X	1	11,1	14,14,15	0.61	0	17,19,21	0.98	2 (11%)
11	NAG	X	2	11	14,14,15	0.97	1 (7%)	17,19,21	1.43	1 (5%)
11	BMA	X	3	11	11,11,12	0.89	0	15,15,17	1.08	1 (6%)
11	MAN	X	4	11	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
11	MAN	X	5	11	11,11,12	1.43	2 (18%)	15,15,17	1.47	2 (13%)
12	NAG	Y	1	12,1	14,14,15	0.47	0	17,19,21	0.51	0
12	NAG	Y	2	12	14,14,15	0.44	0	17,19,21	0.67	0
12	NAG	Z	1	12,1	14,14,15	0.21	0	17,19,21	0.49	0
12	NAG	Z	2	12	14,14,15	0.34	0	17,19,21	0.43	0
12	NAG	a	1	12,1	14,14,15	0.50	0	17,19,21	1.65	3 (17%)
12	NAG	a	2	12	14,14,15	0.53	0	17,19,21	0.66	0
7	NAG	b	1	1,7	14,14,15	0.28	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	b	2	7	14,14,15	1.29	2 (14%)	17,19,21	1.27	3 (17%)
7	BMA	b	3	7	11,11,12	0.67	0	15,15,17	0.97	0
5	NAG	c	1	5,1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
5	NAG	c	2	5	14,14,15	0.32	0	17,19,21	2.36	1 (5%)
5	BMA	c	3	5	11,11,12	0.83	1 (9%)	15,15,17	0.90	0
5	MAN	c	4	5	11,11,12	0.99	1 (9%)	15,15,17	1.71	3 (20%)
13	NAG	d	1	13,1	14,14,15	0.52	0	17,19,21	0.60	0
13	NAG	d	2	13	14,14,15	0.46	0	17,19,21	0.57	0
13	MAN	d	3	13	11,11,12	1.71	3 (27%)	15,15,17	1.51	3 (20%)
13	MAN	d	4	13	11,11,12	1.97	2 (18%)	15,15,17	1.89	3 (20%)
13	MAN	d	5	13	11,11,12	1.07	1 (9%)	15,15,17	1.45	2 (13%)
7	NAG	e	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	1.11	1 (5%)
7	NAG	e	2	7	14,14,15	0.39	0	17,19,21	0.65	0
7	BMA	e	3	7	11,11,12	0.93	0	15,15,17	1.02	1 (6%)
12	NAG	f	1	12,1	14,14,15	1.33	2 (14%)	17,19,21	1.38	2 (11%)
12	NAG	f	2	12	14,14,15	0.36	0	17,19,21	0.50	0
8	BGC	g	1	8	12,12,12	1.59	3 (25%)	17,17,17	1.38	2 (11%)
8	GAL	g	2	8	11,11,12	0.57	0	15,15,17	1.03	1 (6%)
8	NAG	g	3	8	14,14,15	0.25	0	17,19,21	0.52	0
8	GAL	g	4	8	11,11,12	0.60	0	15,15,17	0.72	0
8	SIA	g	5	8	20,20,21	1.62	1 (5%)	21,28,31	1.51	2 (9%)

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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	FUL	I	2	3	-	-	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	K	4	5	-	1/2/19/22	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	MAN	L	3	6	-	1/2/19/22	1/1/1/1
6	MAN	L	4	6	-	1/2/19/22	0/1/1/1
6	MAN	L	5	6	-	2/2/19/22	0/1/1/1
6	MAN	L	6	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	2/2/19/22	0/1/1/1
7	NAG	N	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
8	BGC	O	1	8	-	2/2/22/22	0/1/1/1
8	GAL	O	2	8	-	2/2/19/22	0/1/1/1
8	NAG	O	3	8	-	0/6/23/26	0/1/1/1
8	GAL	O	4	8	-	0/2/19/22	0/1/1/1
8	SIA	O	5	8	-	2/18/34/38	0/1/1/1
9	NAG	P	1	9,1	-	0/6/23/26	0/1/1/1
9	FUL	P	2	9	-	-	0/1/1/1
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	2/2/19/22	0/1/1/1
10	NAG	S	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	MAN	S	3	10	-	2/2/19/22	0/1/1/1
10	MAN	S	4	10	-	2/2/19/22	1/1/1/1
10	MAN	S	5	10	-	0/2/19/22	0/1/1/1
10	MAN	S	6	10	-	0/2/19/22	1/1/1/1
10	MAN	S	7	10	-	2/2/19/22	1/1/1/1
11	NAG	T	1	11,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	T	2	11	-	0/6/23/26	0/1/1/1
11	BMA	T	3	11	-	2/2/19/22	0/1/1/1
11	MAN	T	4	11	-	1/2/19/22	1/1/1/1
11	MAN	T	5	11	-	2/2/19/22	1/1/1/1
12	NAG	U	1	12,1	-	5/6/23/26	0/1/1/1
12	NAG	U	2	12	-	6/6/23/26	0/1/1/1
8	BGC	V	1	8	-	2/2/22/22	0/1/1/1
8	GAL	V	2	8	-	2/2/19/22	0/1/1/1
8	NAG	V	3	8	-	0/6/23/26	0/1/1/1
8	GAL	V	4	8	-	2/2/19/22	0/1/1/1
8	SIA	V	5	8	-	4/18/34/38	0/1/1/1
5	NAG	W	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	1/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
5	MAN	W	4	5	-	2/2/19/22	1/1/1/1
11	NAG	X	1	11,1	-	3/6/23/26	0/1/1/1
11	NAG	X	2	11	-	0/6/23/26	0/1/1/1
11	BMA	X	3	11	-	2/2/19/22	0/1/1/1
11	MAN	X	4	11	-	0/2/19/22	0/1/1/1
11	MAN	X	5	11	-	0/2/19/22	0/1/1/1
12	NAG	Y	1	12,1	-	1/6/23/26	0/1/1/1
12	NAG	Y	2	12	-	3/6/23/26	0/1/1/1
12	NAG	Z	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	Z	2	12	-	0/6/23/26	0/1/1/1
12	NAG	a	1	12,1	-	4/6/23/26	0/1/1/1
12	NAG	a	2	12	-	2/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	4/6/23/26	0/1/1/1
7	BMA	b	3	7	-	1/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
5	MAN	c	4	5	-	1/2/19/22	0/1/1/1
13	NAG	d	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	d	2	13	-	4/6/23/26	0/1/1/1
13	MAN	d	3	13	-	2/2/19/22	0/1/1/1
13	MAN	d	4	13	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	d	5	13	-	2/2/19/22	0/1/1/1
7	NAG	e	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
12	NAG	f	1	12,1	-	5/6/23/26	0/1/1/1
12	NAG	f	2	12	-	0/6/23/26	0/1/1/1
8	BGC	g	1	8	-	2/2/22/22	0/1/1/1
8	GAL	g	2	8	-	0/2/19/22	0/1/1/1
8	NAG	g	3	8	-	2/6/23/26	0/1/1/1
8	GAL	g	4	8	-	2/2/19/22	0/1/1/1
8	SIA	g	5	8	-	2/18/34/38	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	5	SIA	C2-C1	5.82	1.59	1.52
8	V	5	SIA	C2-C1	5.74	1.59	1.52
8	g	5	SIA	C2-C1	5.69	1.59	1.52
3	I	2	FUL	O5-C1	5.17	1.52	1.43
9	P	2	FUL	O5-C1	4.83	1.51	1.43

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	2	NAG	C1-O5-C5	9.16	124.47	112.19
3	I	2	FUL	C1-C2-C3	6.07	118.49	109.64
10	S	5	MAN	C1-O5-C5	6.00	120.23	112.19
11	X	2	NAG	C1-O5-C5	5.66	119.77	112.19
13	d	4	MAN	C1-O5-C5	5.55	119.63	112.19

There are no chirality outliers.

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	O	5	SIA	C4-C5-N5-C10
8	O	5	SIA	O6-C6-C7-O7
8	g	5	SIA	O8-C8-C9-O9
10	S	1	NAG	O5-C5-C6-O6
11	X	3	BMA	C4-C5-C6-O6

5 of 7 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	S	7	MAN	C1-C2-C3-C4-C5-O5
6	L	3	MAN	C1-C2-C3-C4-C5-O5
10	S	4	MAN	C1-C2-C3-C4-C5-O5
11	T	5	MAN	C1-C2-C3-C4-C5-O5
5	W	4	MAN	C1-C2-C3-C4-C5-O5

34 monomers are involved in 26 short contacts:

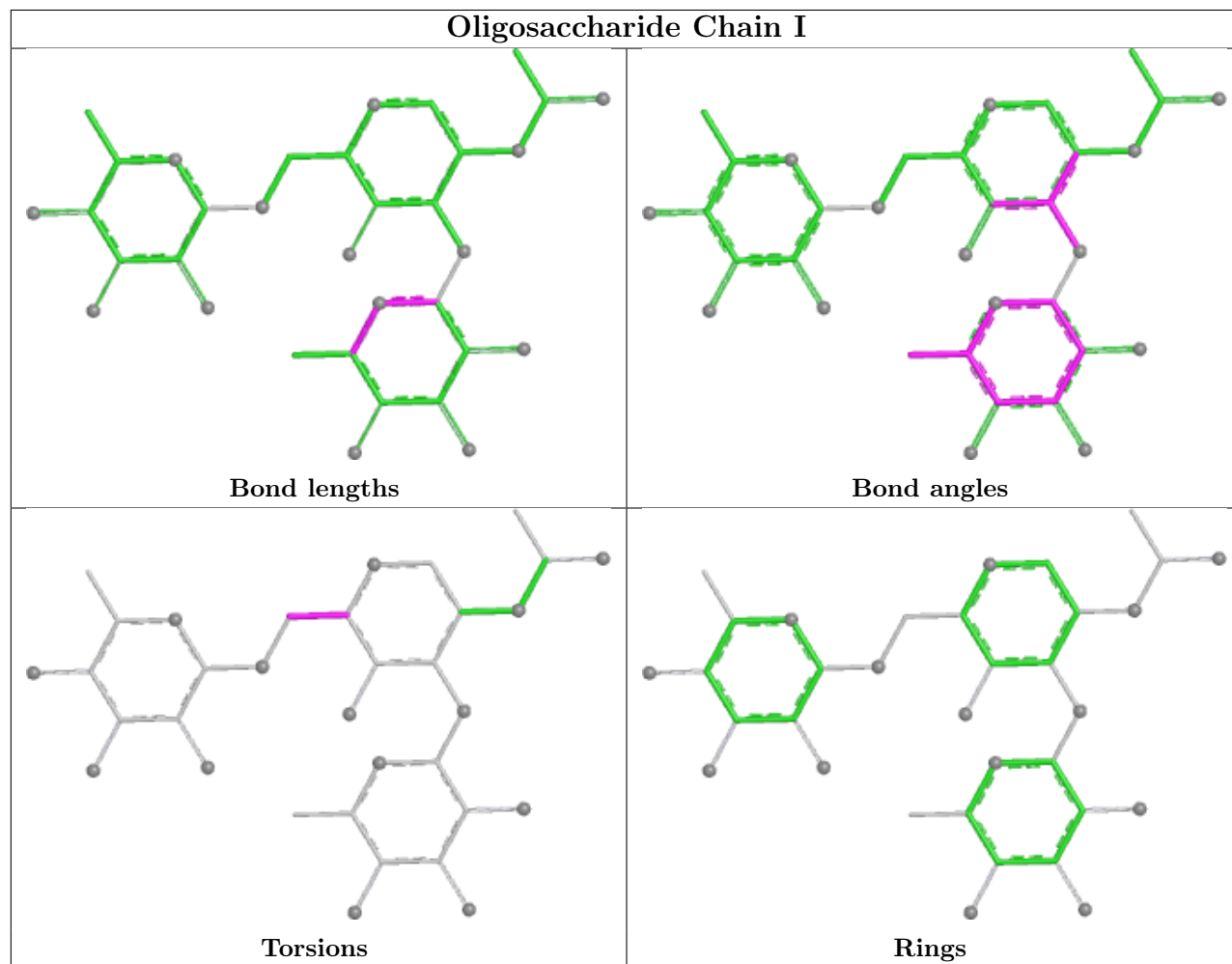
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	1	NAG	1	0
5	R	1	NAG	1	0
5	R	4	MAN	1	0
7	b	1	NAG	1	0
8	V	5	SIA	1	0
12	U	1	NAG	1	0
4	J	1	NAG	1	0
12	U	2	NAG	1	0
13	d	5	MAN	1	0
7	e	1	NAG	1	0
5	c	1	NAG	2	0
12	Y	2	NAG	2	0
3	I	1	NAG	1	0
6	L	6	MAN	1	0
11	X	2	NAG	1	0
13	d	4	MAN	1	0
6	L	3	MAN	1	0
5	Q	1	NAG	1	0
8	O	5	SIA	1	0
5	R	3	BMA	1	0
10	S	3	MAN	1	0
9	P	2	FUL	1	0
12	Y	1	NAG	1	0
13	d	3	MAN	1	0
7	N	1	NAG	1	0
3	I	2	FUL	1	0
11	X	1	NAG	1	0
10	S	2	NAG	1	0
13	d	2	NAG	1	0
7	b	2	NAG	1	0
6	L	1	NAG	1	0
5	K	1	NAG	1	0
12	a	1	NAG	1	0

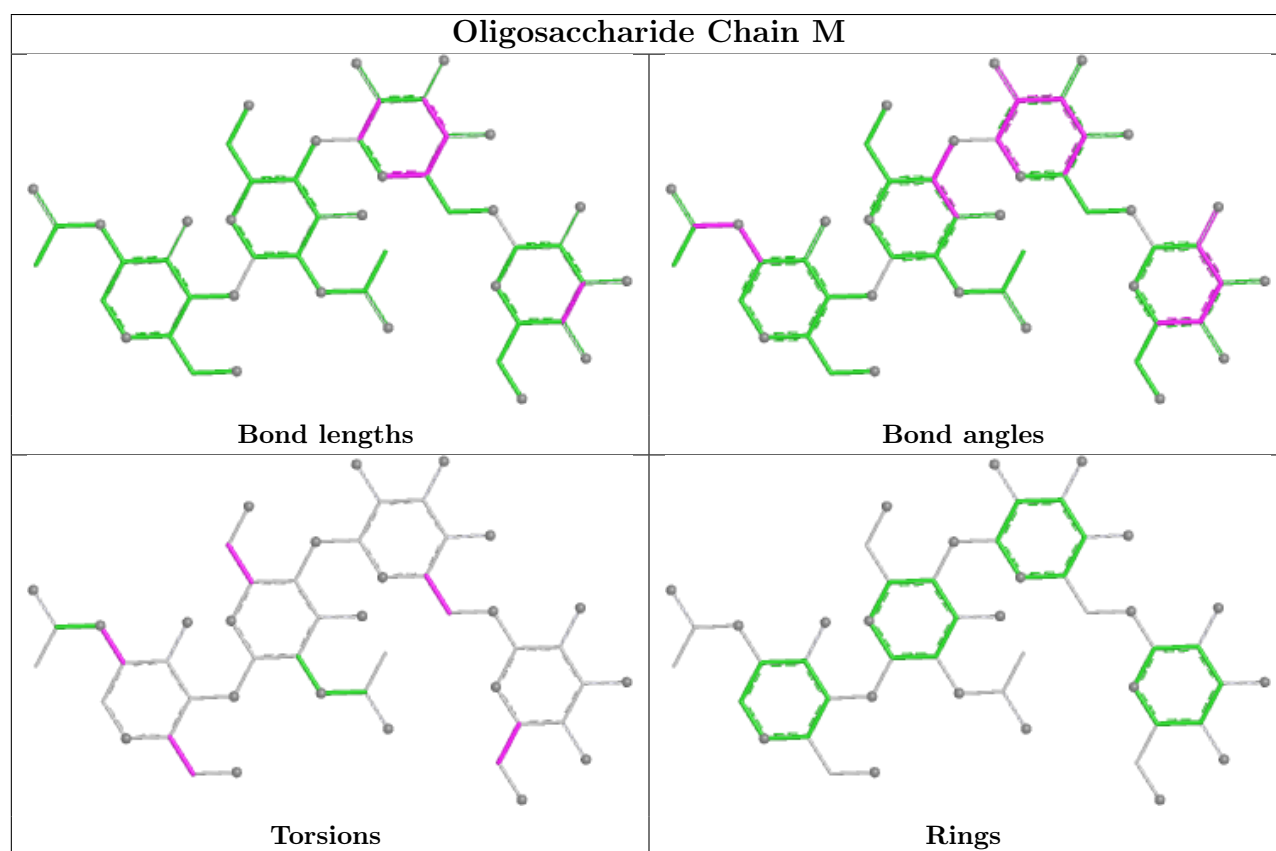
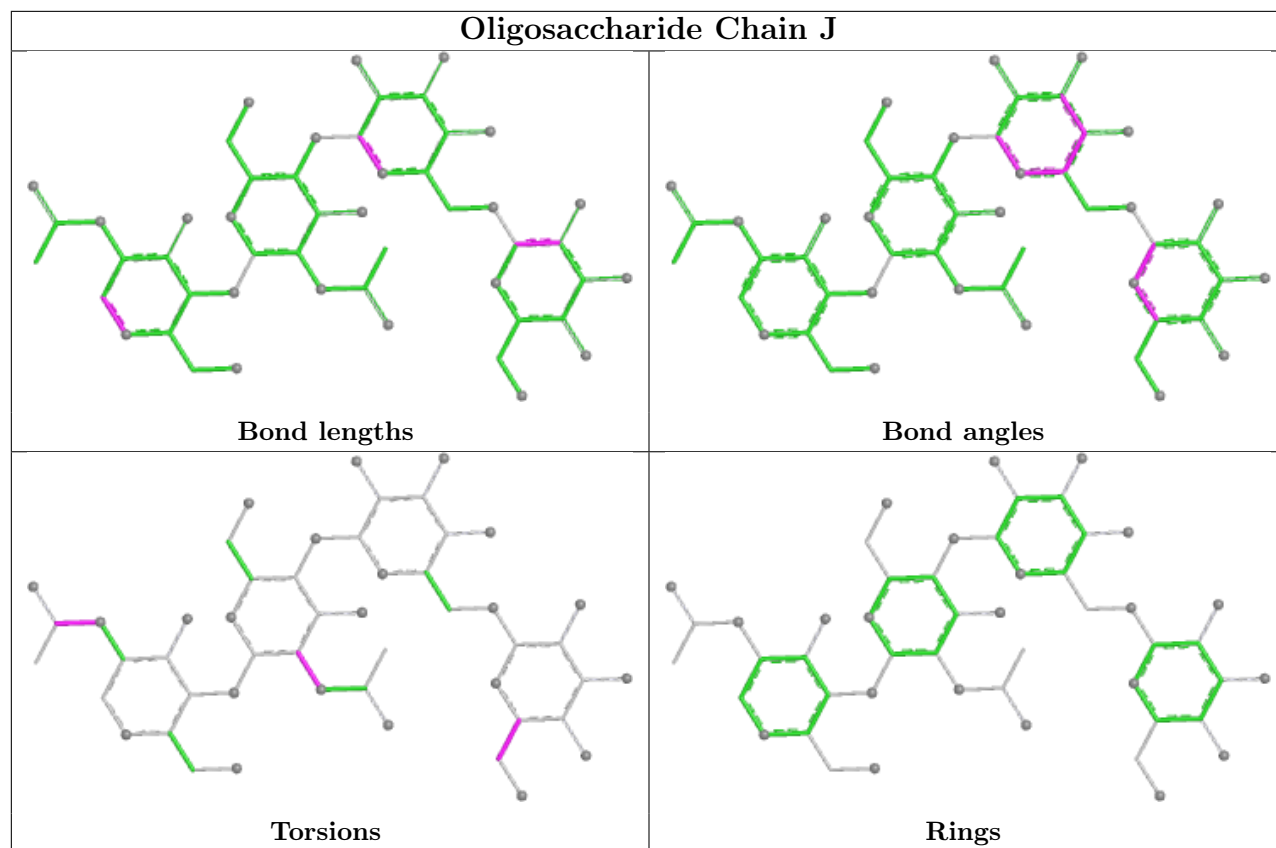
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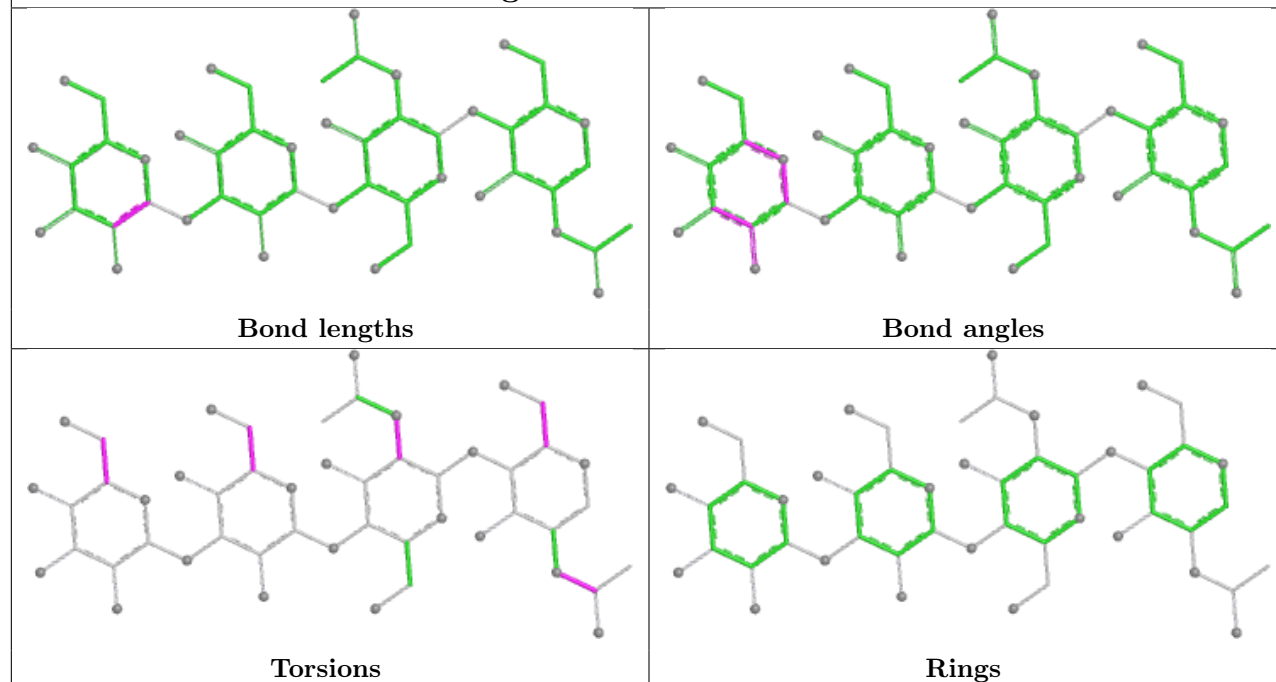
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	f	1	NAG	1	0

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

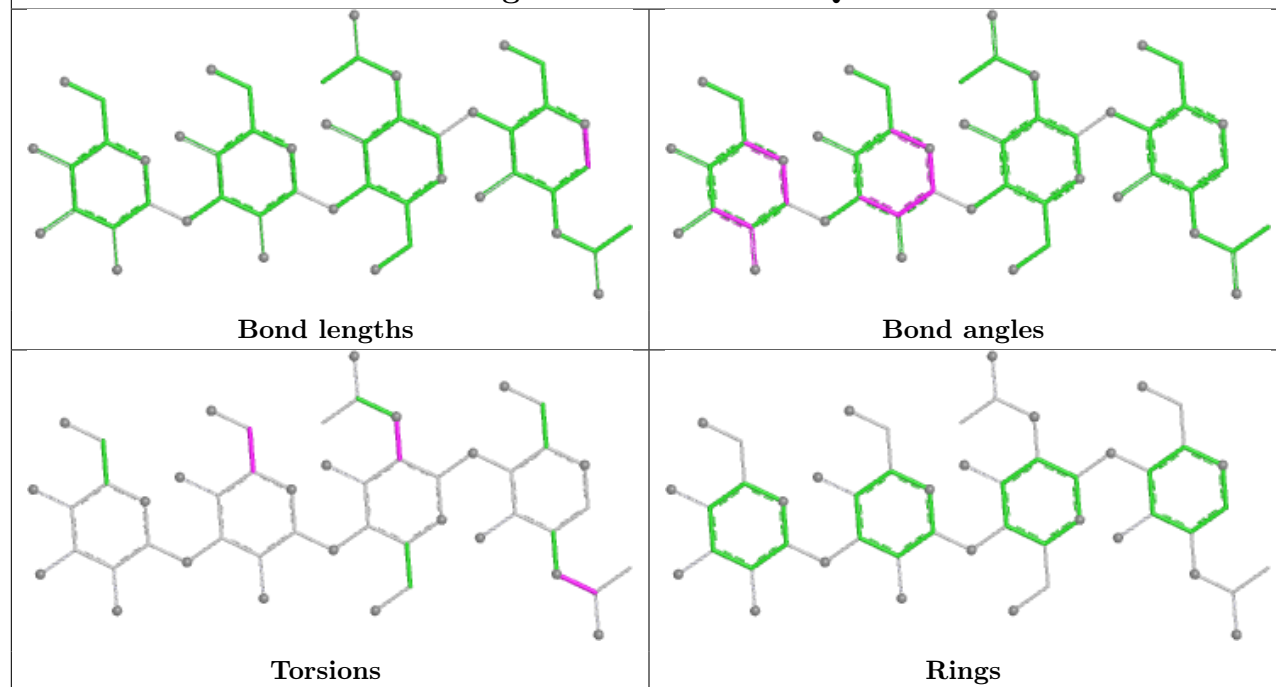


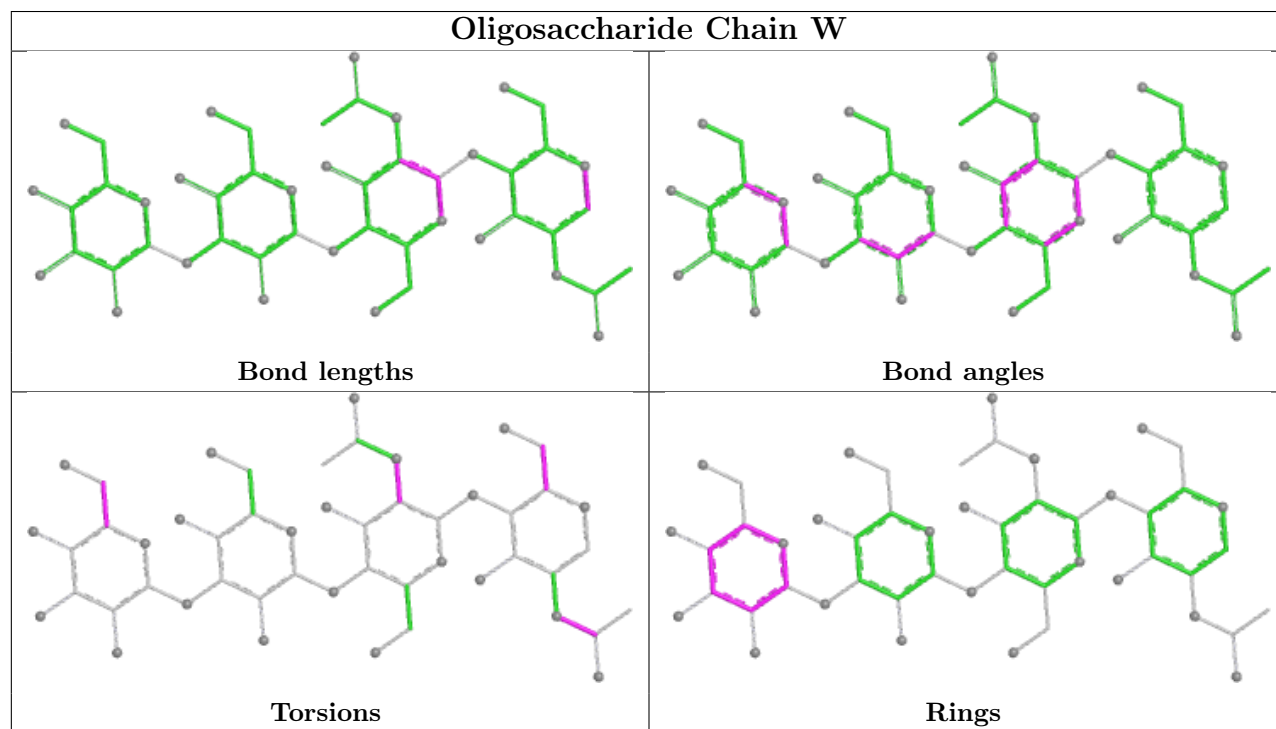
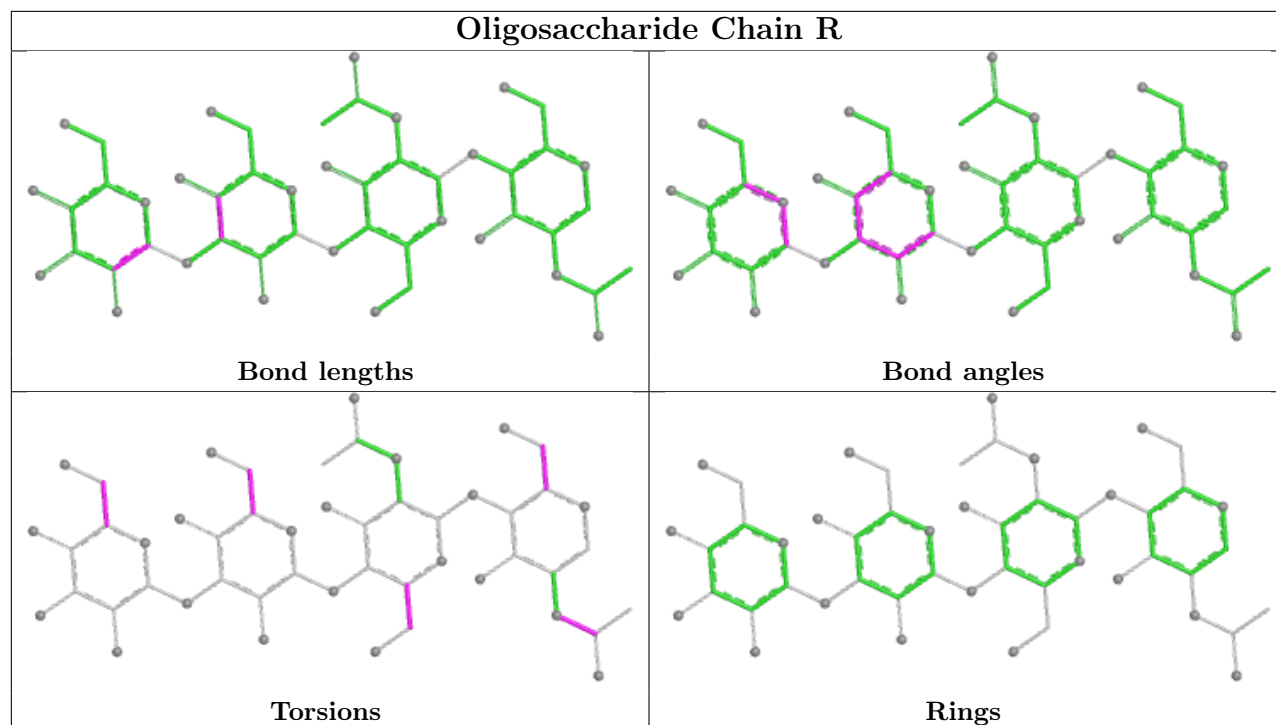


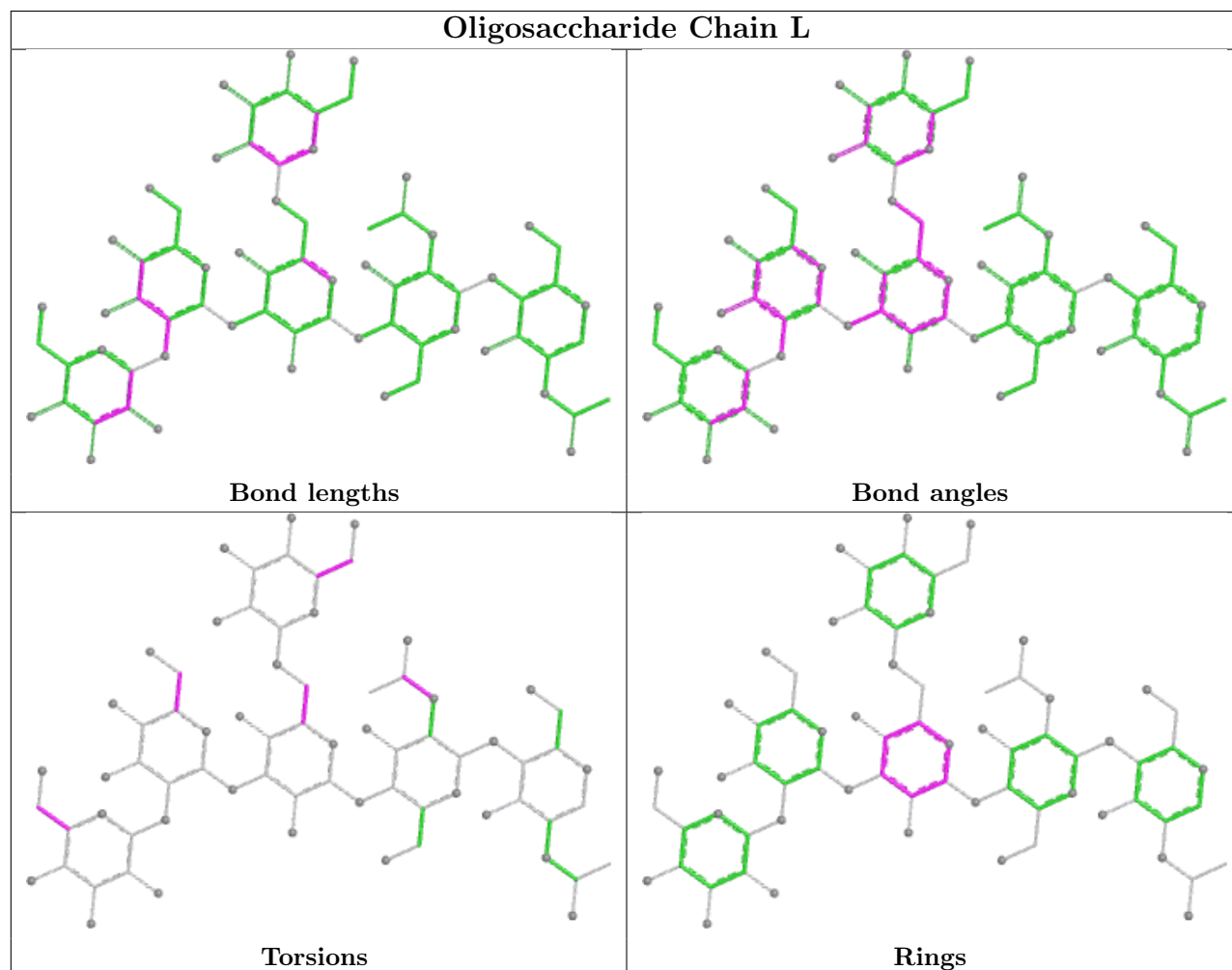
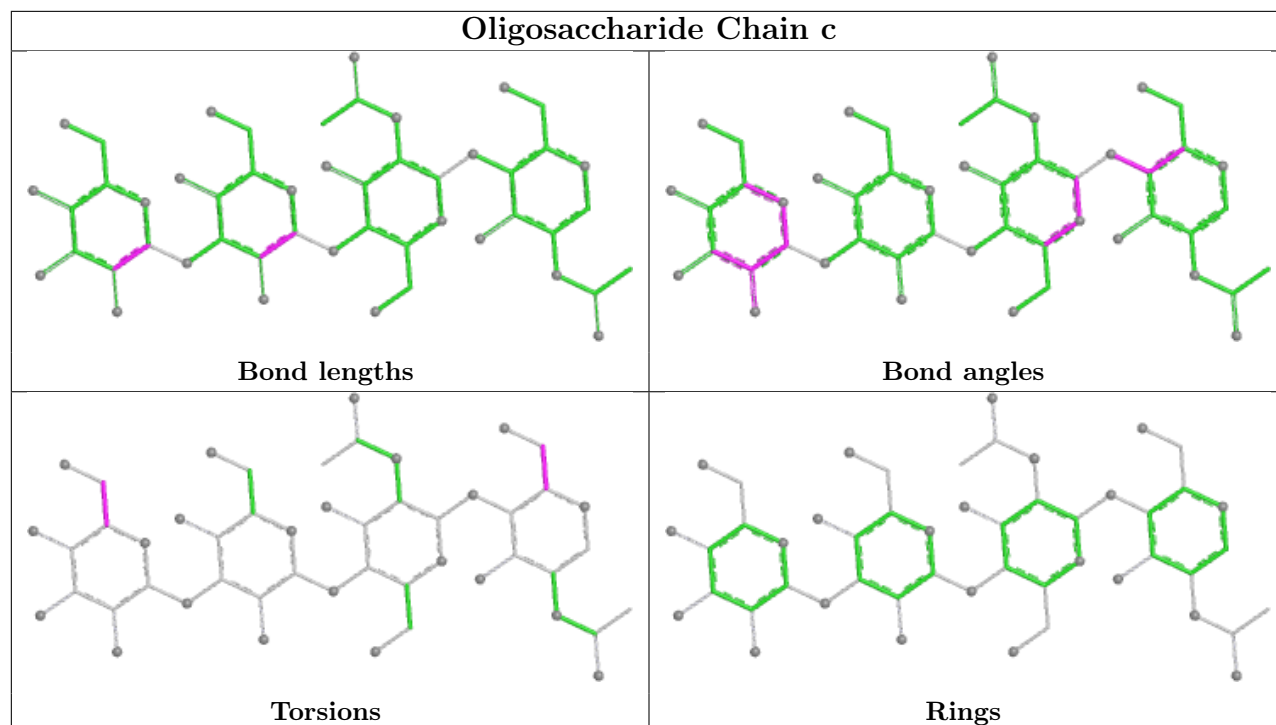
Oligosaccharide Chain K

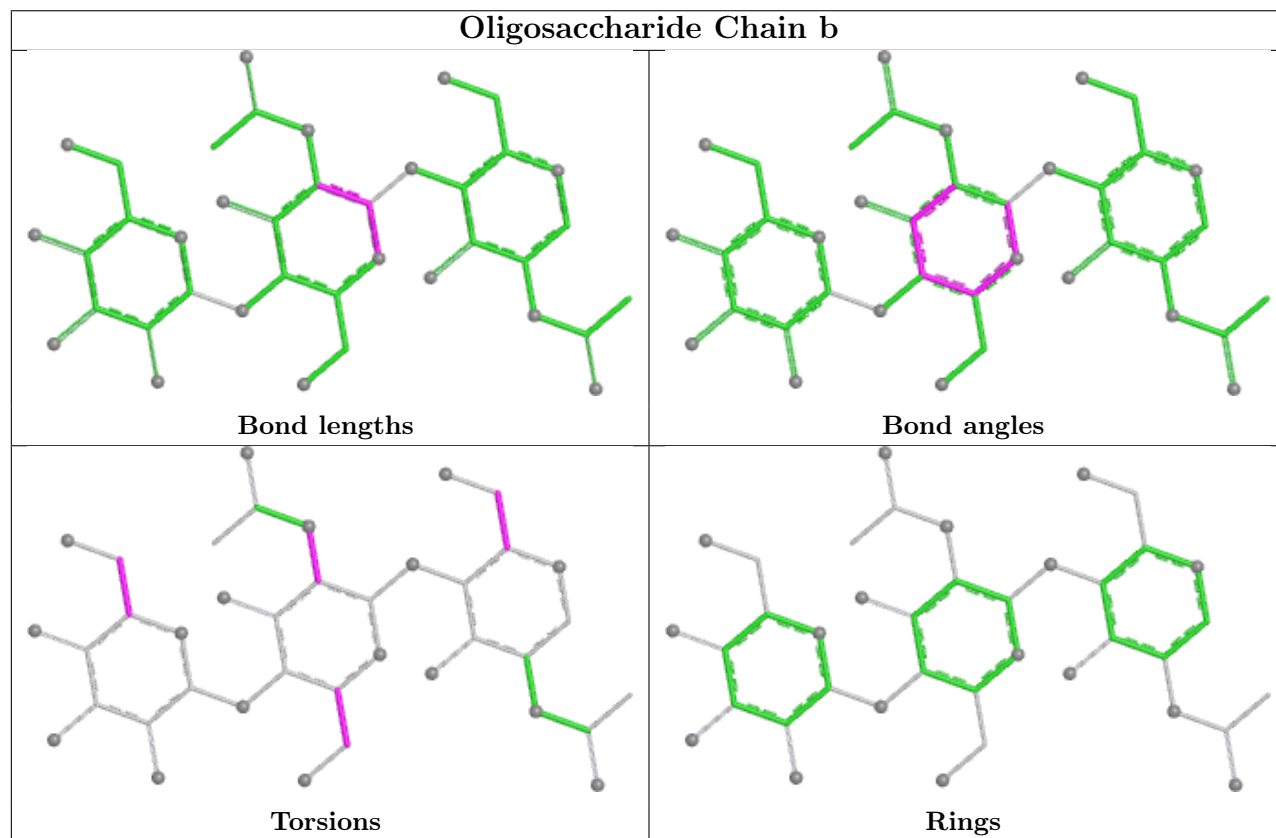
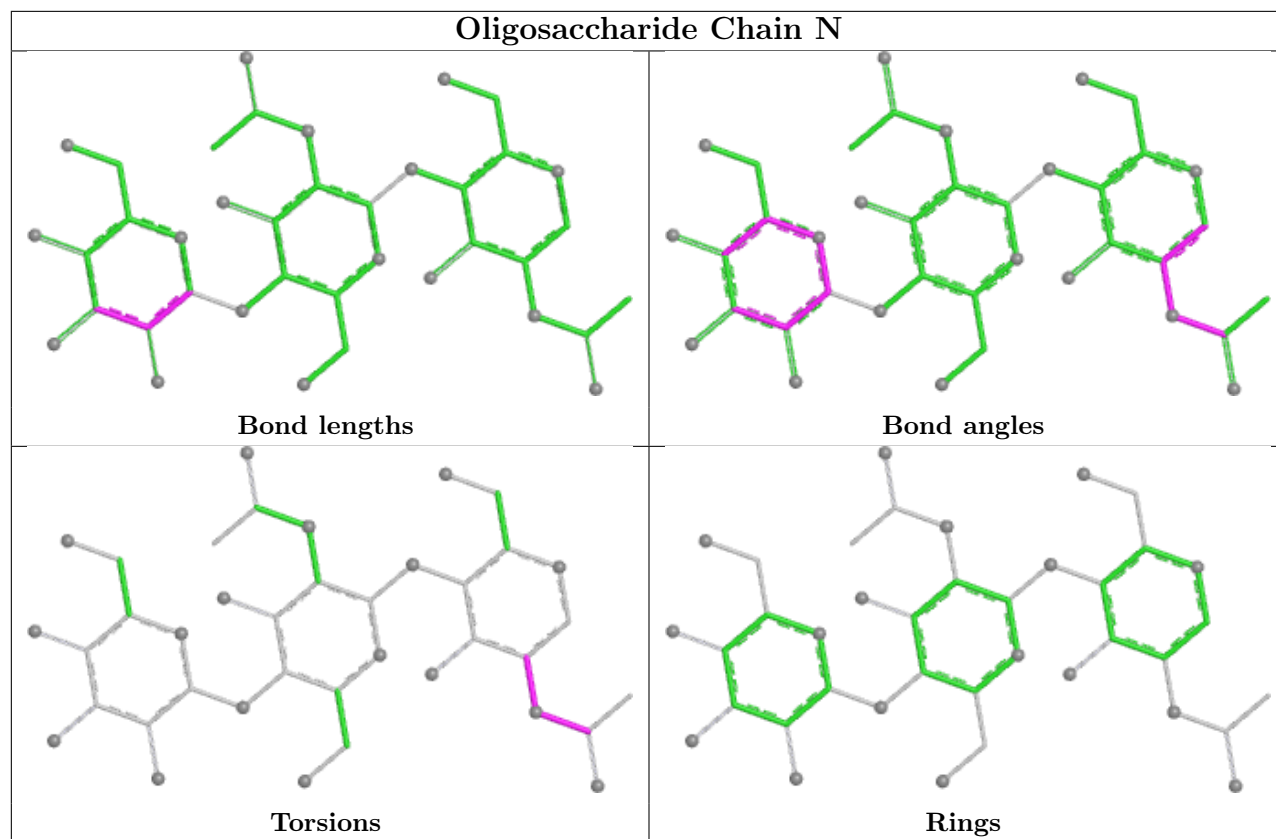


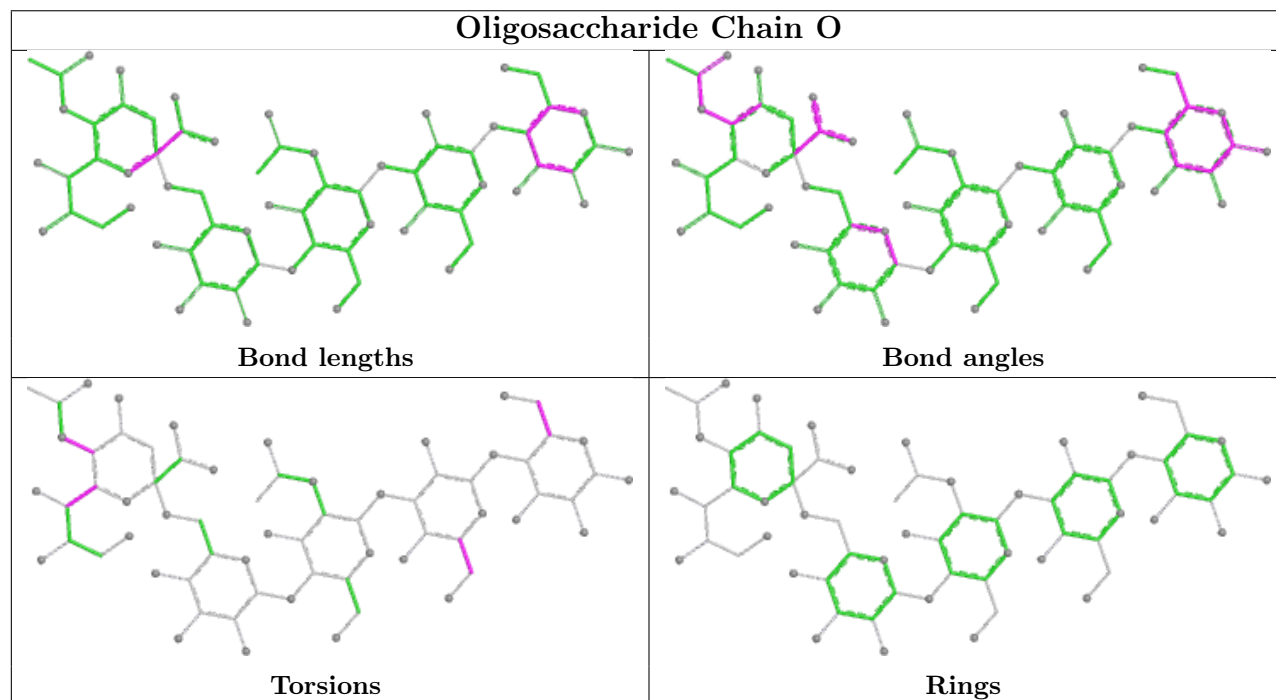
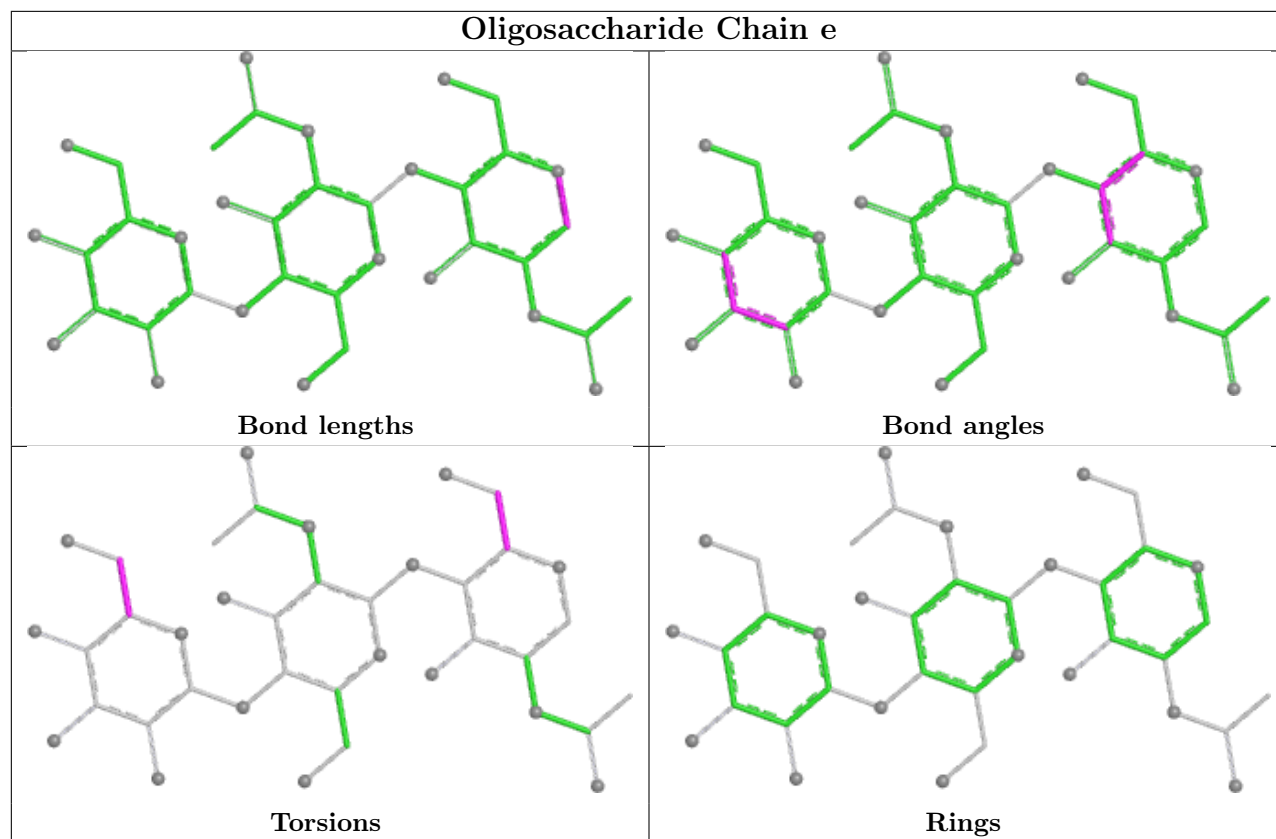
Oligosaccharide Chain Q



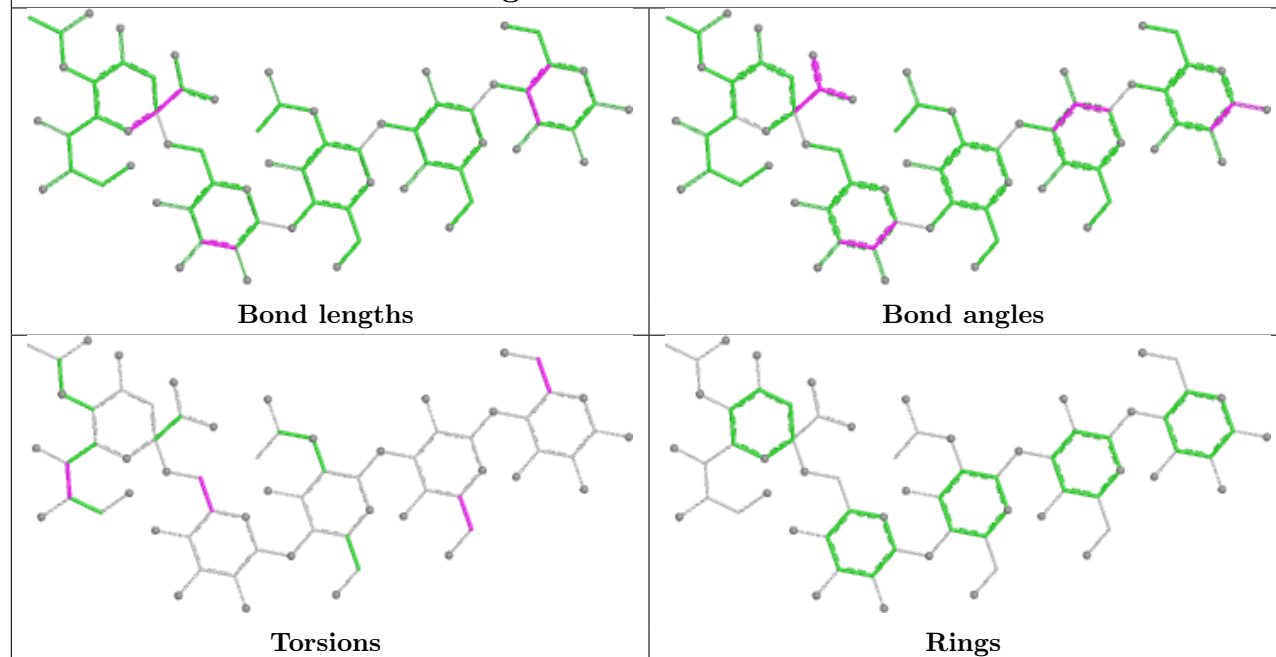




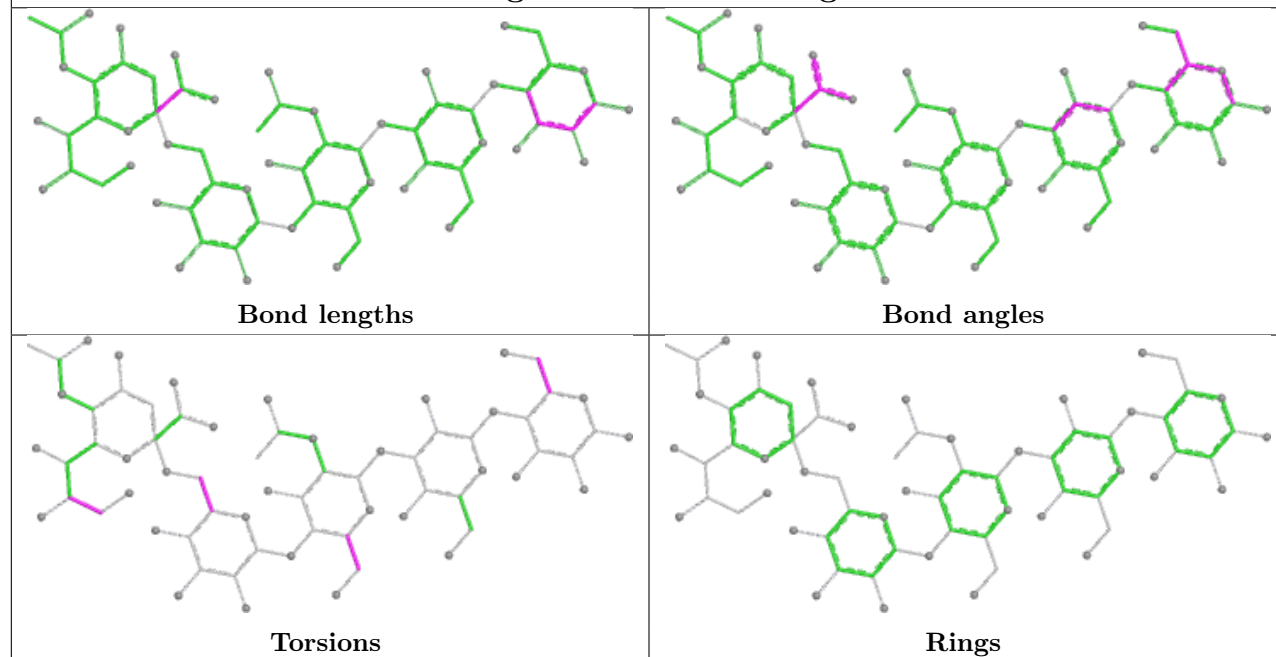


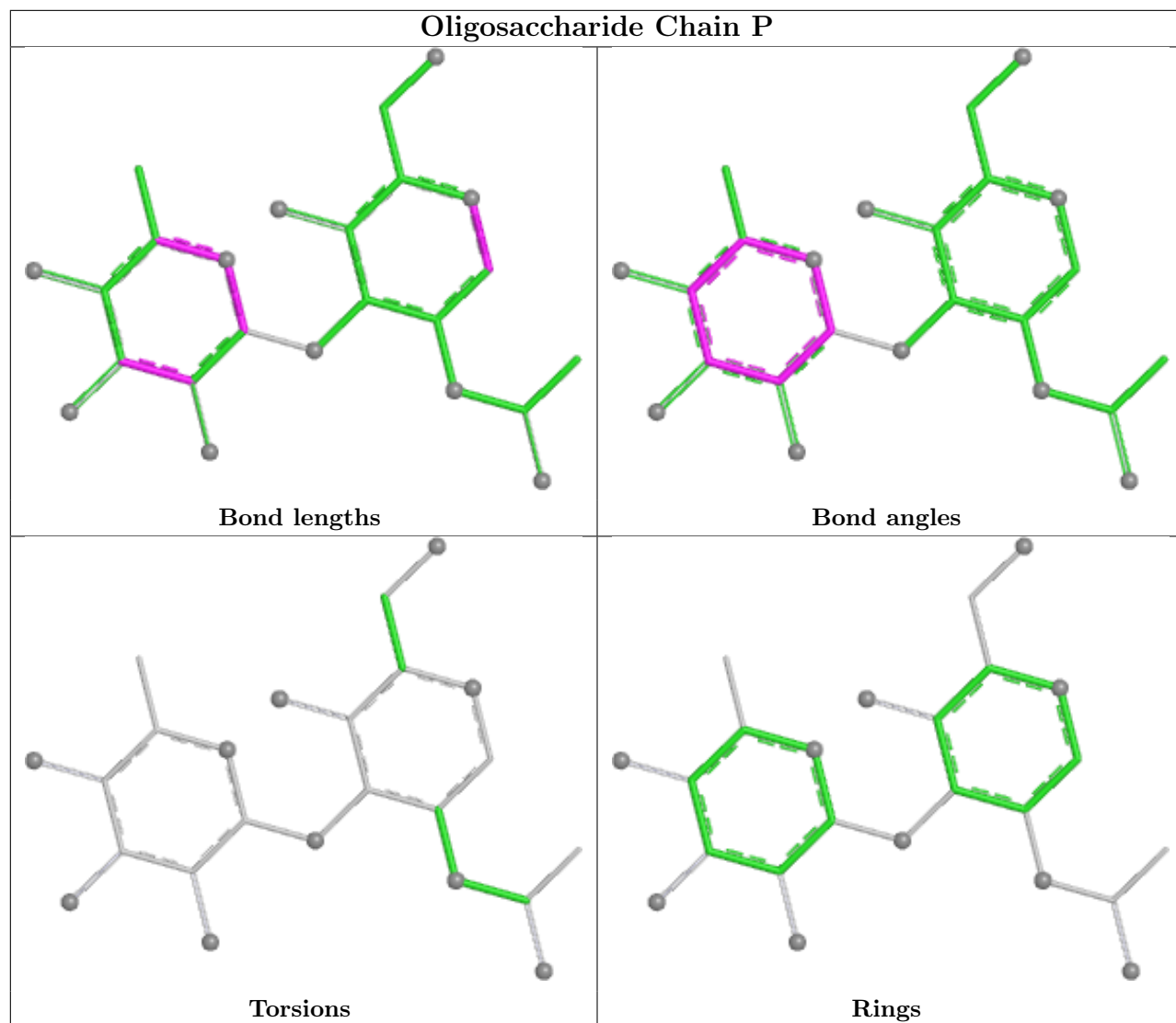


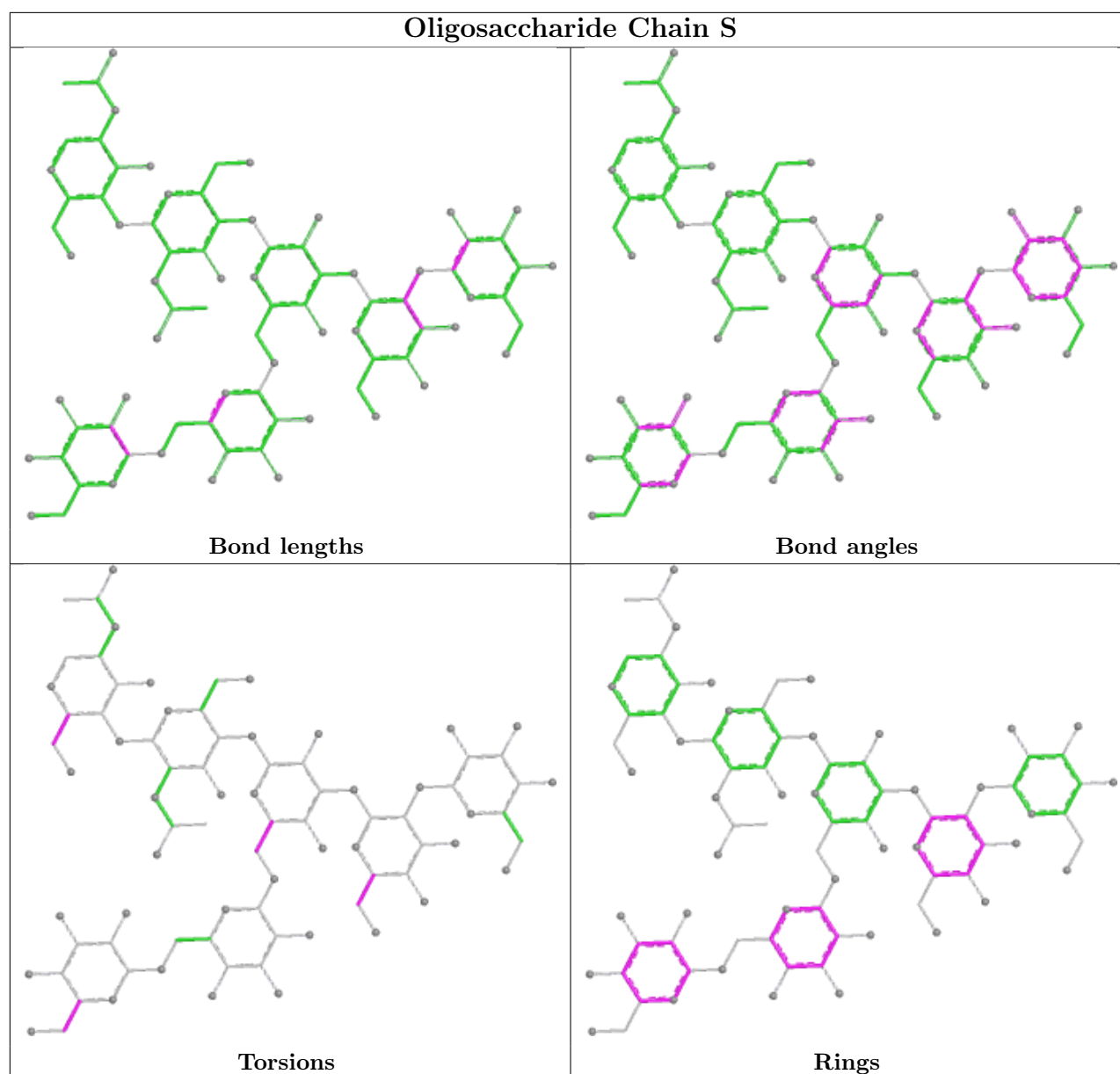
Oligosaccharide Chain V

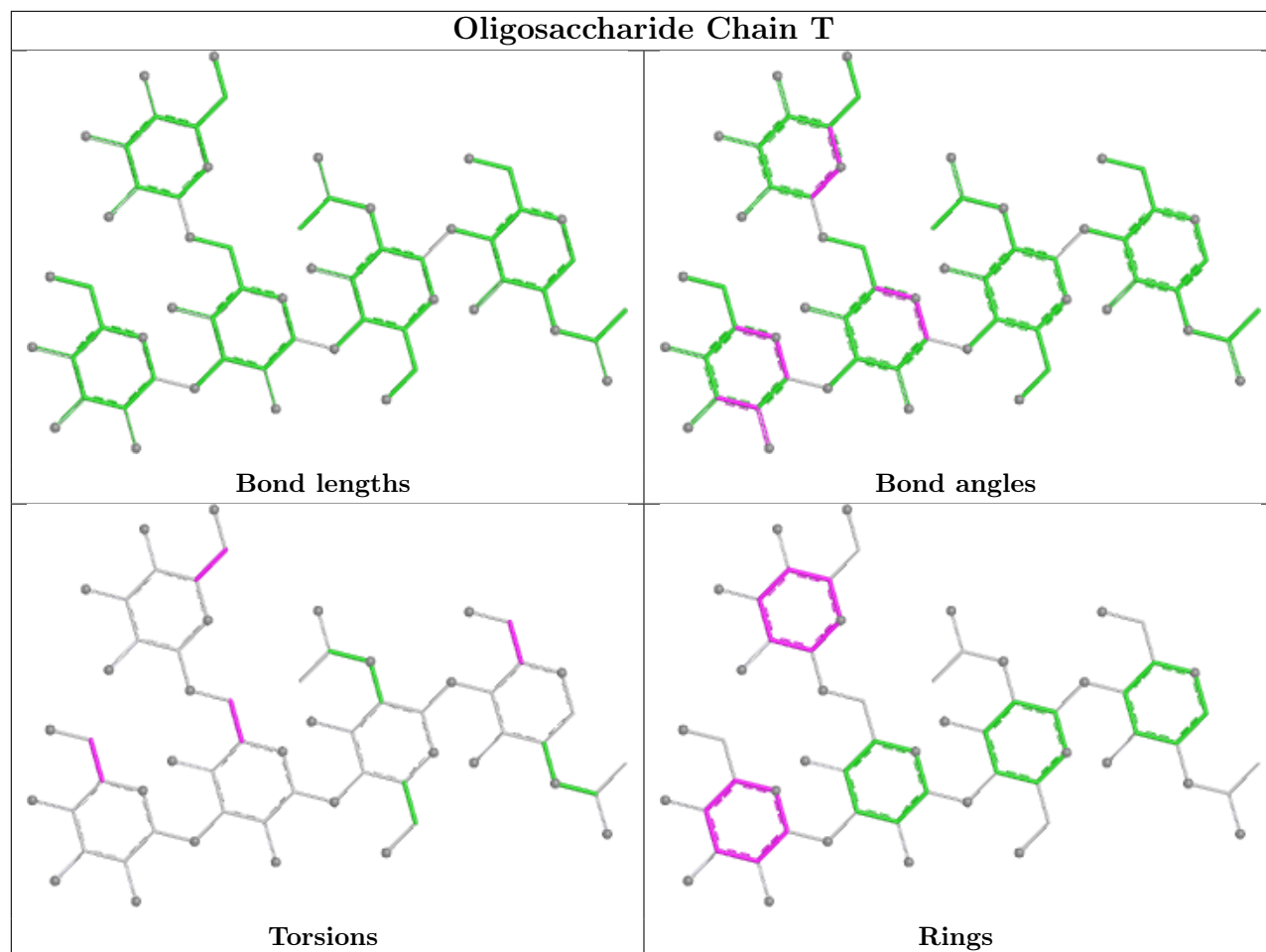


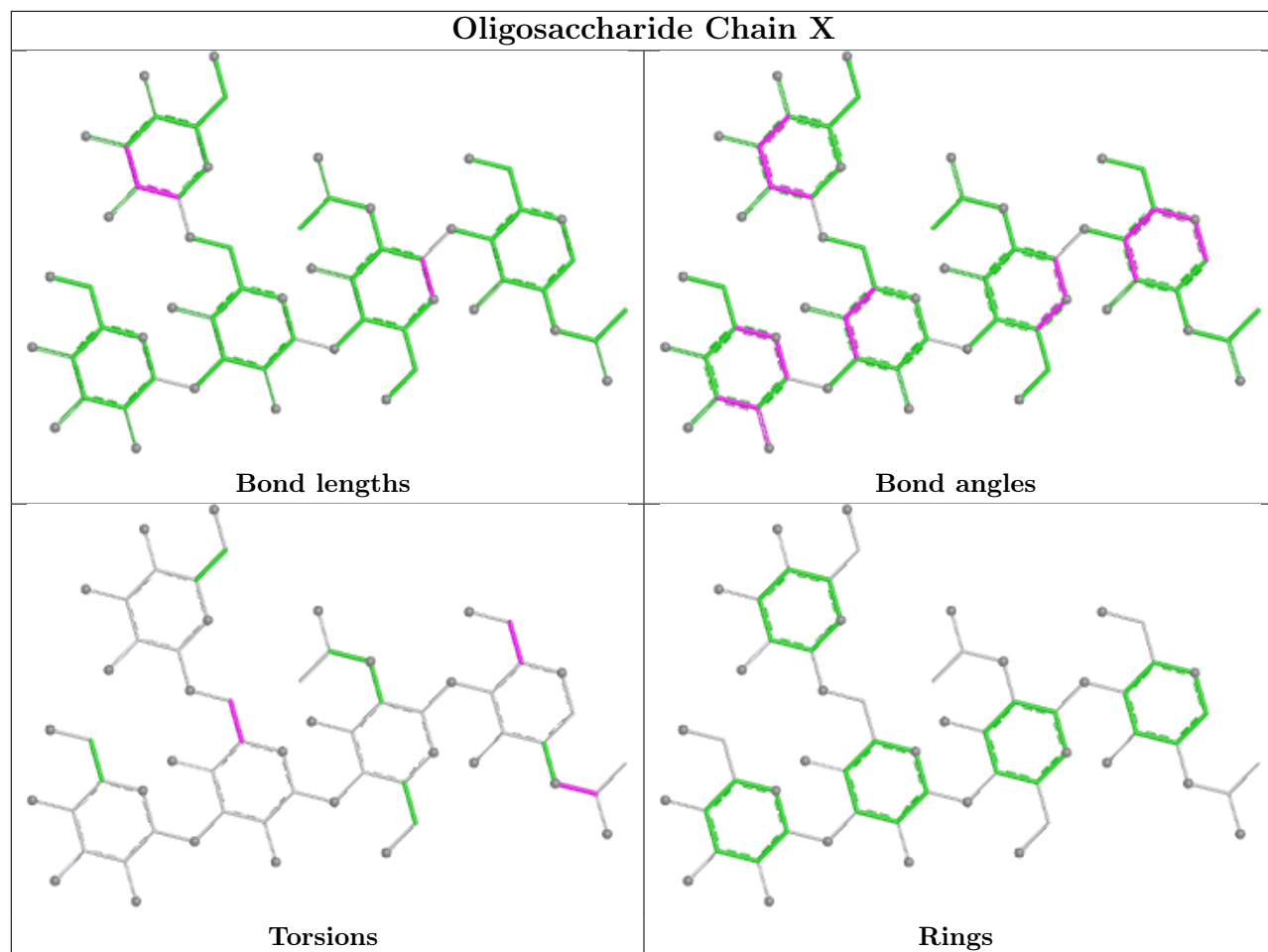
Oligosaccharide Chain g

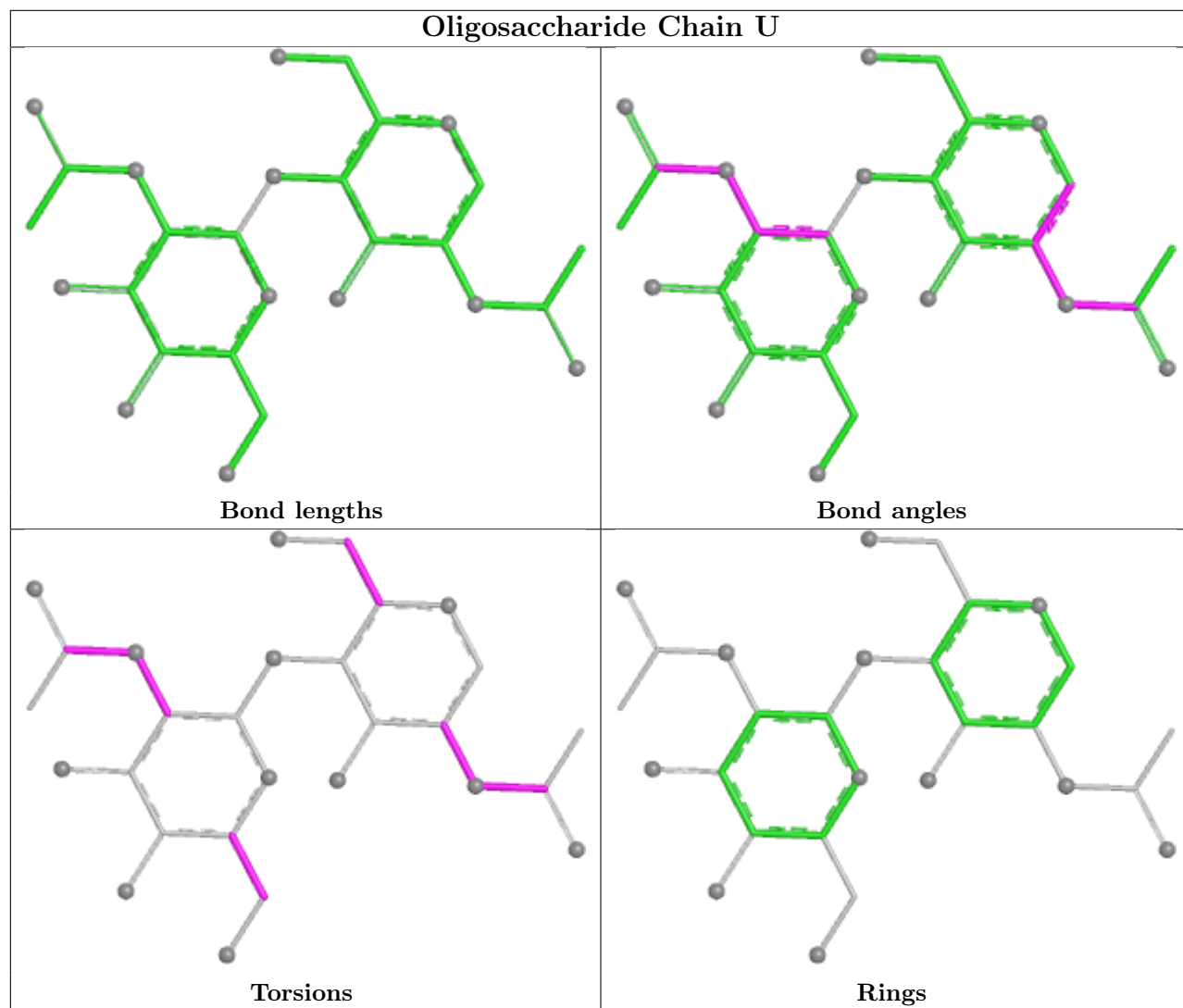


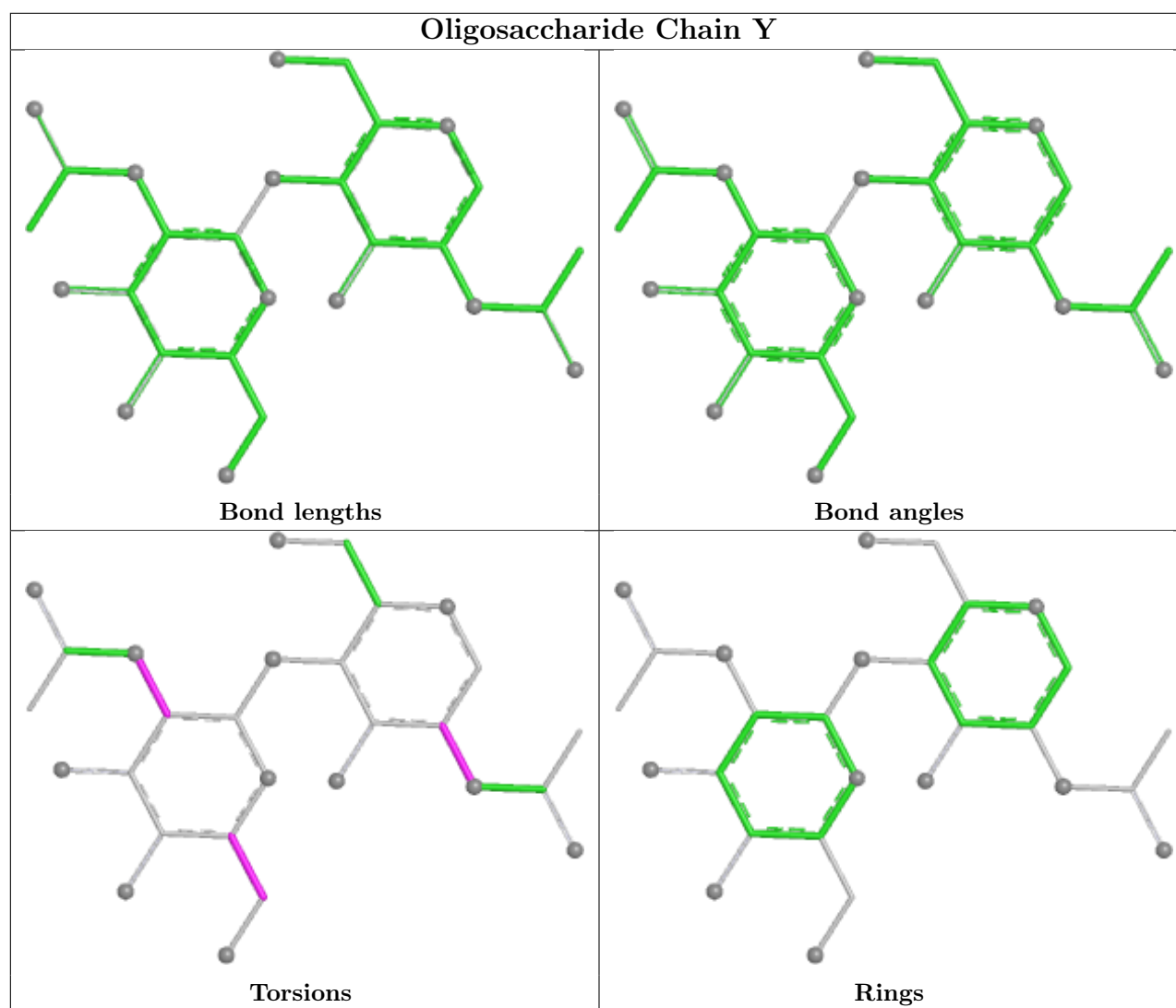


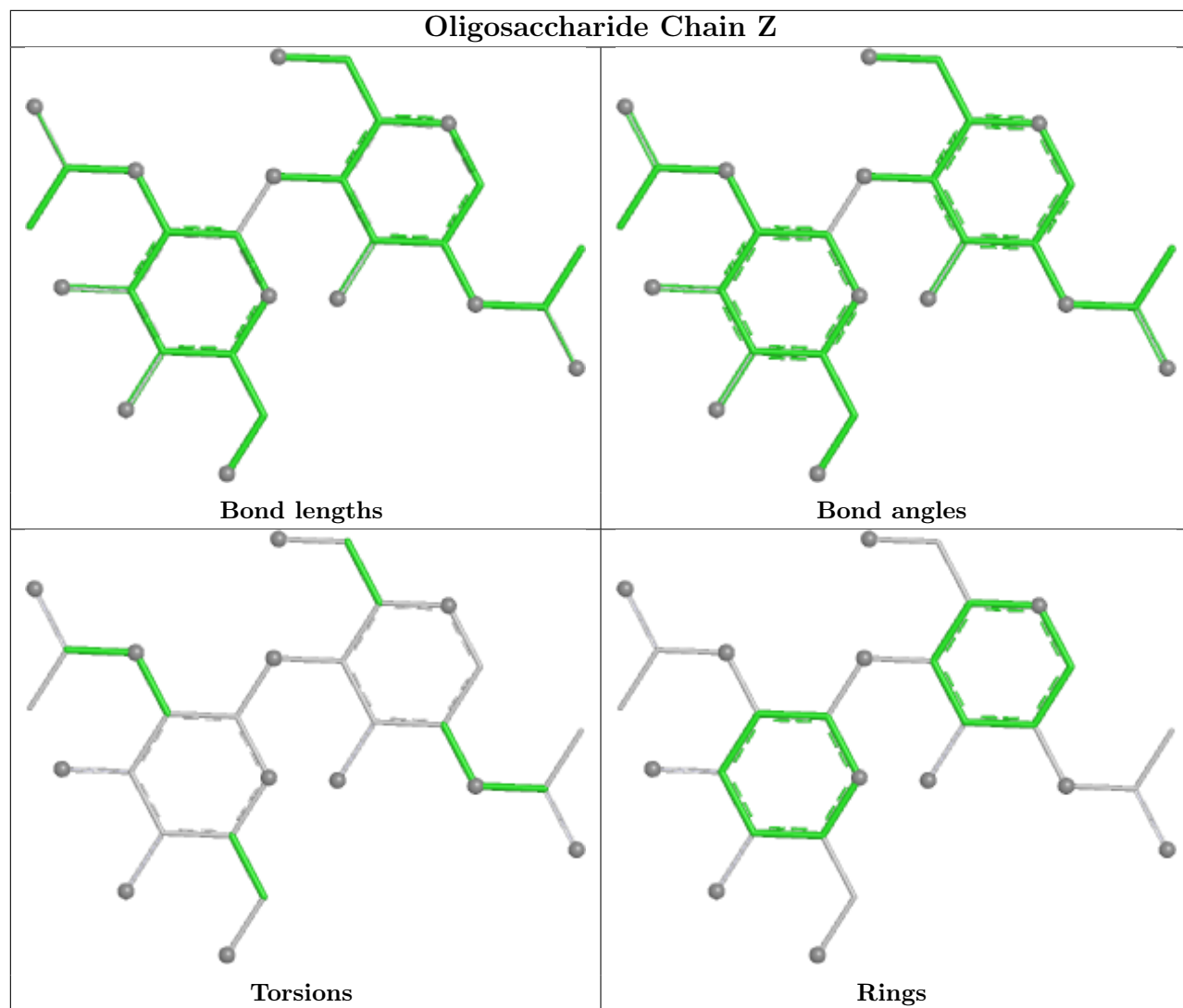


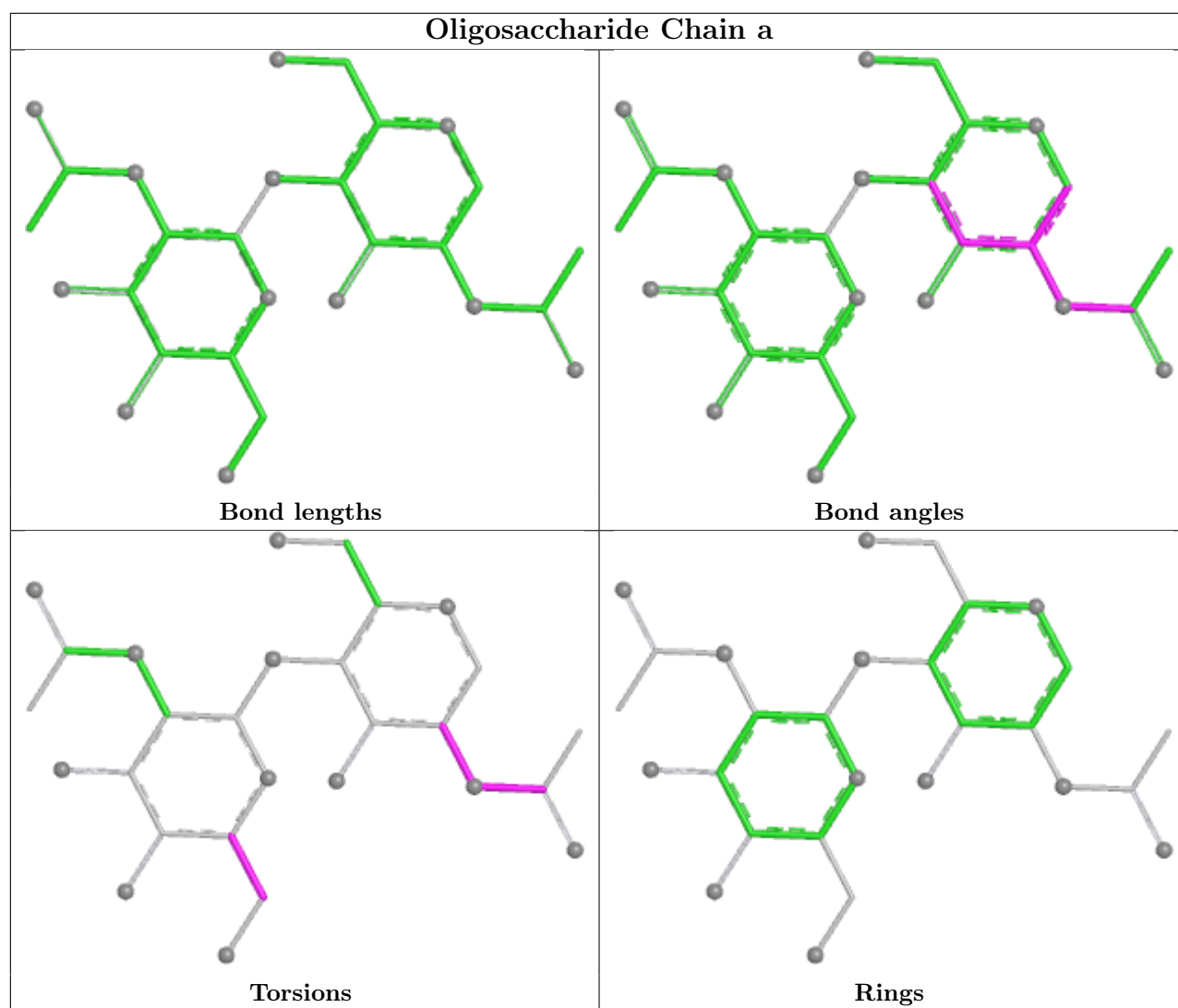


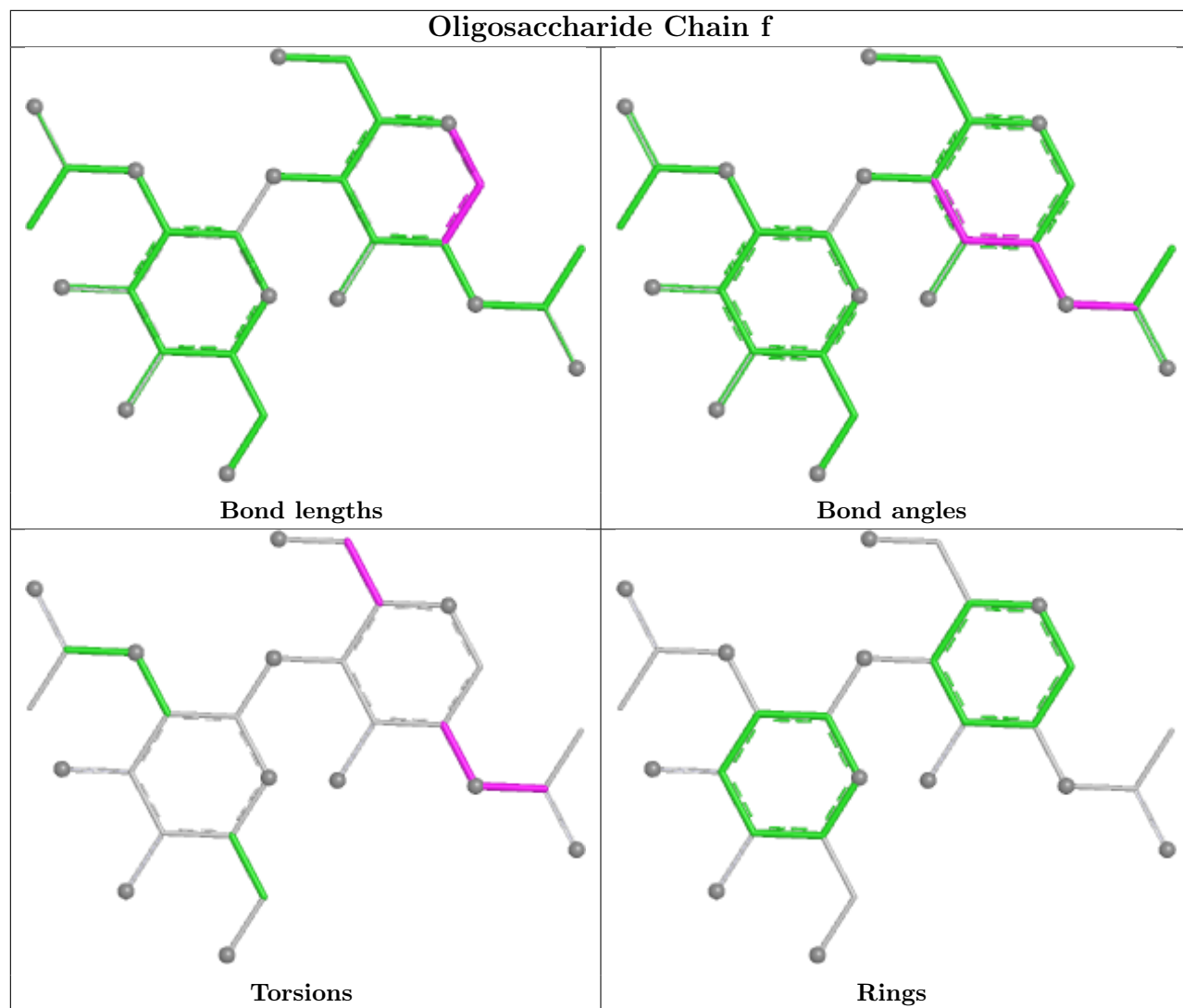


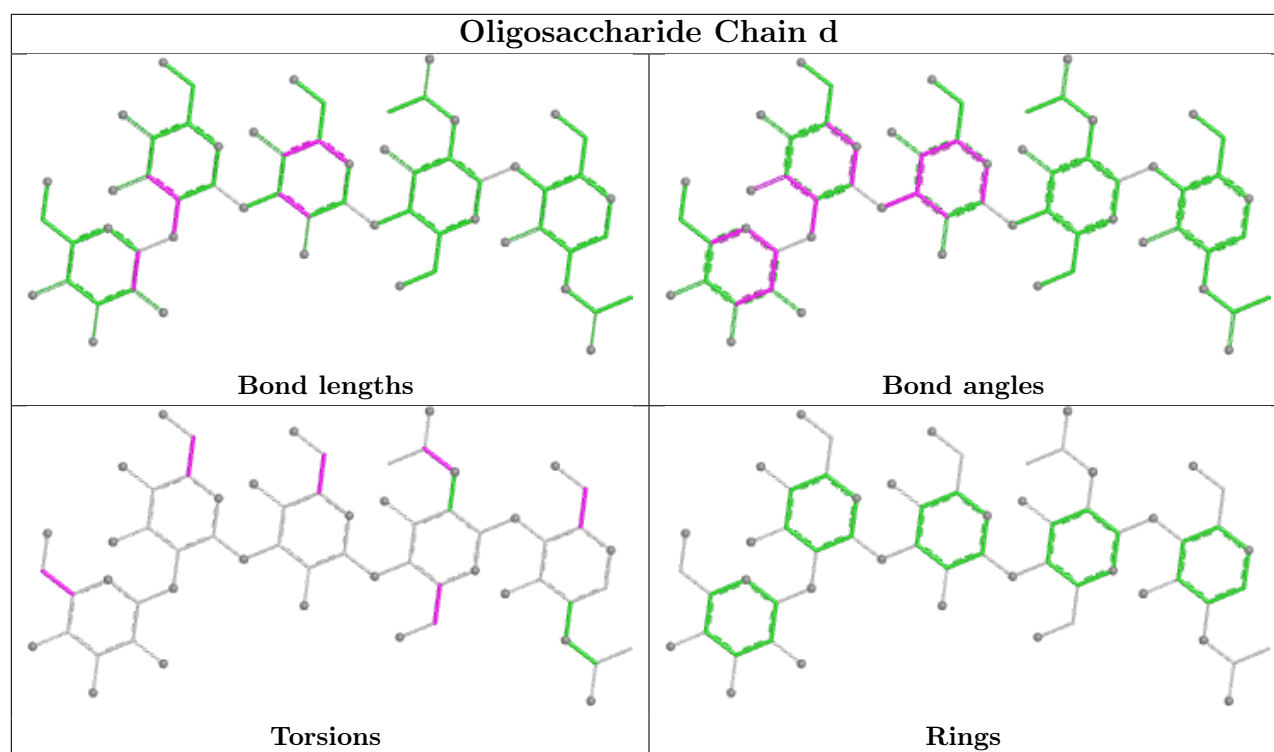












5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
14	NAG	C	523	1	14,14,15	0.25	0	17,19,21	1.07	1 (5%)
14	NAG	F	201	2	14,14,15	0.37	0	17,19,21	0.65	1 (5%)
14	NAG	E	414	1	14,14,15	0.38	0	17,19,21	0.53	0
14	NAG	D	202	2	14,14,15	1.09	1 (7%)	17,19,21	0.73	0
14	NAG	A	522	1	14,14,15	0.38	0	17,19,21	0.49	0
15	CAC	D	201	-	2,4,4	2.20	2 (100%)	4,6,6	1.57	1 (25%)
14	NAG	B	201	2	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
14	NAG	G	416	1	14,14,15	1.24	1 (7%)	17,19,21	1.49	1 (5%)

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
14	NAG	C	523	1	-	2/6/23/26	0/1/1/1
14	NAG	F	201	2	-	2/6/23/26	0/1/1/1
14	NAG	E	414	1	-	0/6/23/26	0/1/1/1
14	NAG	D	202	2	-	0/6/23/26	0/1/1/1
14	NAG	A	522	1	-	0/6/23/26	0/1/1/1
14	NAG	B	201	2	-	2/6/23/26	0/1/1/1
14	NAG	G	416	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	416	NAG	O5-C1	4.44	1.51	1.43
14	D	202	NAG	O5-C1	-3.38	1.38	1.43
15	D	201	CAC	AS-C1	2.34	1.95	1.90
15	D	201	CAC	AS-C2	2.04	1.95	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	416	NAG	C1-O5-C5	5.90	120.10	112.19
14	B	201	NAG	C1-O5-C5	4.43	118.13	112.19
14	C	523	NAG	C1-O5-C5	3.55	116.95	112.19
15	D	201	CAC	O1-AS-C1	-2.61	108.26	111.50
14	F	201	NAG	C1-O5-C5	2.07	114.97	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	416	NAG	O5-C5-C6-O6
14	B	201	NAG	O5-C5-C6-O6
14	C	523	NAG	O5-C5-C6-O6
14	B	201	NAG	C4-C5-C6-O6
14	G	416	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	319/329 (96%)	-0.33	7 (2%) 62 53	36, 63, 116, 177	0
1	C	319/329 (96%)	-0.22	8 (2%) 58 48	46, 76, 116, 186	0
1	E	319/329 (96%)	-0.36	10 (3%) 51 42	52, 74, 111, 178	0
1	G	321/329 (97%)	-0.01	8 (2%) 58 48	53, 92, 173, 245	0
2	B	172/174 (98%)	-0.40	2 (1%) 76 69	38, 60, 100, 139	0
2	D	172/174 (98%)	-0.33	4 (2%) 61 52	25, 76, 116, 163	0
2	F	172/174 (98%)	-0.29	5 (2%) 53 45	40, 71, 109, 160	0
2	H	172/174 (98%)	0.97	30 (17%) 4 3	50, 162, 227, 274	0
All	All	1966/2012 (97%)	-0.15	74 (3%) 44 36	25, 76, 174, 274	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	ILE	7.8
2	H	119	PHE	7.4
1	G	13	LEU	6.8
1	A	326	LYS	4.6
2	F	32	THR	4.5

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
11	MAN	T	5	11/12	0.08	0.18	150,179,184,186	0
5	BMA	W	3	11/12	0.23	0.13	196,199,202,203	0
6	MAN	L	4	11/12	0.33	0.10	170,179,185,190	0
4	MAN	M	4	11/12	0.33	0.13	142,159,173,180	0
5	BMA	Q	3	11/12	0.41	0.12	197,204,208,208	0
12	NAG	U	2	14/15	0.42	0.14	147,171,181,182	0
5	MAN	W	4	11/12	0.43	0.10	167,187,193,194	0
5	BMA	K	3	11/12	0.44	0.10	144,171,177,178	0
4	BMA	J	3	11/12	0.45	0.12	143,161,171,185	0
4	BMA	M	3	11/12	0.45	0.10	185,198,205,205	0
5	MAN	R	4	11/12	0.47	0.13	164,184,193,194	0
3	FUL	I	2	10/11	0.47	0.16	151,161,168,176	0
7	BMA	N	3	11/12	0.48	0.11	175,201,208,210	0
10	MAN	S	7	11/12	0.50	0.11	181,183,188,189	0
11	MAN	X	5	11/12	0.54	0.15	114,133,140,141	0
4	MAN	J	4	11/12	0.54	0.12	147,161,172,176	0
7	NAG	N	2	14/15	0.56	0.13	138,187,202,212	0
11	MAN	X	4	11/12	0.57	0.13	104,160,175,176	0
12	NAG	Y	2	14/15	0.57	0.11	178,182,187,189	0
11	BMA	T	3	11/12	0.58	0.10	172,186,187,189	0
5	MAN	Q	4	11/12	0.59	0.08	180,193,203,203	0
11	MAN	T	4	11/12	0.61	0.11	137,173,185,188	0
5	MAN	K	4	11/12	0.61	0.11	140,160,169,170	0
5	NAG	K	2	14/15	0.63	0.11	112,135,147,164	0
10	MAN	S	5	11/12	0.64	0.08	137,162,168,170	0
11	BMA	X	3	11/12	0.64	0.12	138,156,162,164	0
10	MAN	S	6	11/12	0.65	0.11	155,172,181,182	0
5	NAG	c	1	14/15	-	-	108,131,147,155	0
5	NAG	c	2	14/15	-	-	123,161,177,191	0
5	BMA	c	3	11/12	-	-	161,186,195,195	0
5	MAN	c	4	11/12	-	-	153,179,183,185	0
6	MAN	L	6	11/12	0.65	0.09	147,160,167,167	0
12	NAG	Z	2	14/15	0.65	0.12	156,192,207,214	0
12	NAG	Y	1	14/15	0.66	0.12	113,148,163,167	0
9	FUL	P	2	10/11	0.68	0.14	179,182,184,185	0
6	MAN	L	5	11/12	0.68	0.09	132,170,178,178	0
10	MAN	S	4	11/12	0.69	0.08	141,169,172,177	0
5	NAG	Q	2	14/15	0.71	0.12	129,175,188,197	0
9	NAG	P	1	14/15	0.72	0.13	136,162,179,196	0
4	NAG	M	2	14/15	0.72	0.14	112,171,187,198	0
7	NAG	b	1	14/15	-	-	144,171,190,199	0

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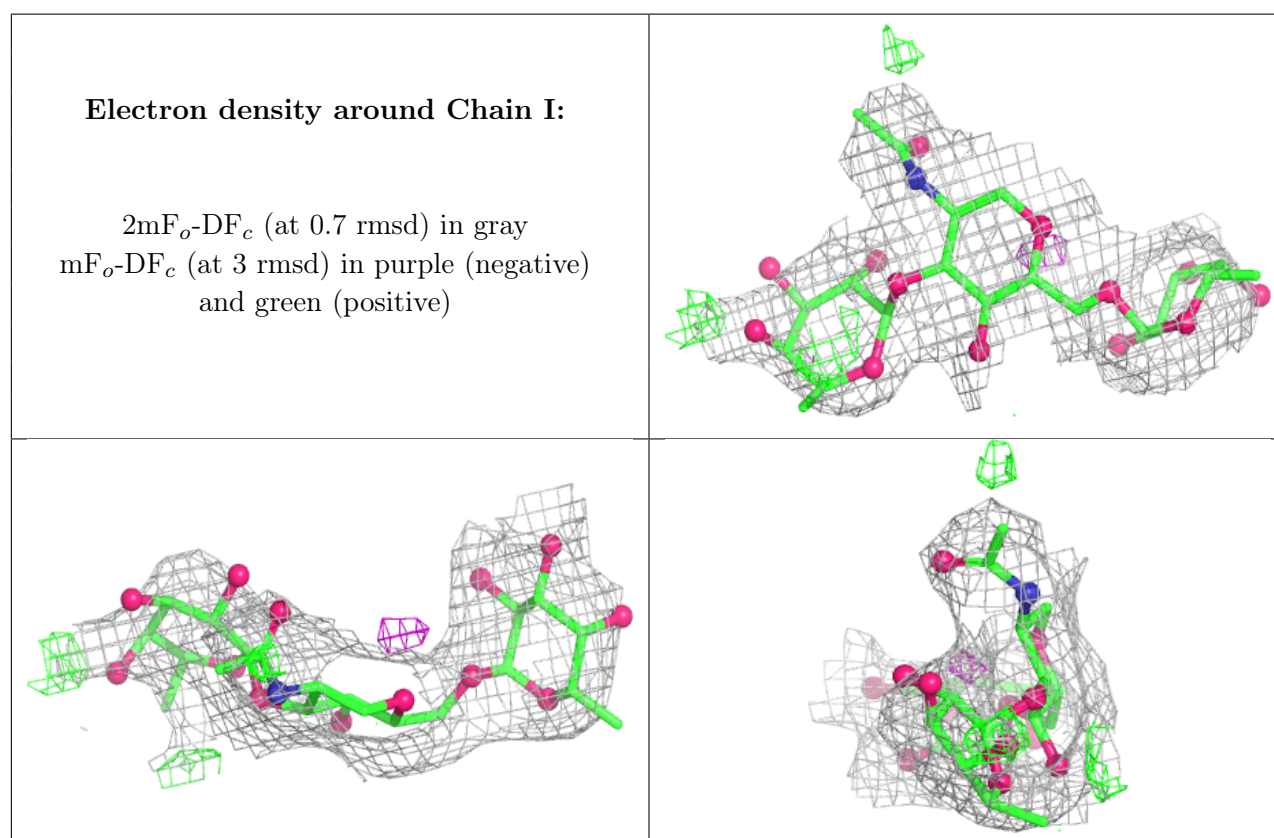
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	b	2	14/15	-	-	166,205,210,210	0
7	BMA	b	3	11/12	-	-	167,179,193,193	0
7	NAG	e	1	14/15	-	-	98,114,130,147	0
7	NAG	e	2	14/15	-	-	86,155,172,177	0
7	BMA	e	3	11/12	-	-	153,178,185,186	0
3	FUC	I	3	10/11	0.73	0.12	139,152,159,161	0
8	BGC	V	1	12/12	0.73	0.10	129,146,153,155	0
7	NAG	N	1	14/15	0.76	0.13	100,128,154,176	0
5	NAG	W	1	14/15	0.77	0.14	100,121,145,165	0
11	NAG	T	2	14/15	0.77	0.12	97,158,173,184	0
5	BMA	R	3	11/12	0.78	0.08	122,160,173,187	0
8	NAG	V	3	14/15	0.79	0.09	76,124,140,140	0
3	NAG	I	1	14/15	0.80	0.13	131,141,150,153	0
8	GAL	V	2	11/12	0.80	0.08	105,138,153,154	0
5	NAG	W	2	14/15	0.82	0.13	132,167,182,192	0
8	BGC	g	1	12/12	-	-	167,182,186,189	0
8	GAL	g	2	11/12	-	-	162,174,179,180	0
8	NAG	g	3	14/15	-	-	150,166,172,173	0
8	GAL	g	4	11/12	-	-	142,149,154,154	0
8	SIA	g	5	20/21	-	-	107,142,149,149	0
12	NAG	U	1	14/15	0.82	0.13	125,135,156,170	0
11	NAG	T	1	14/15	0.82	0.15	85,98,117,132	0
5	NAG	Q	1	14/15	0.83	0.11	82,95,125,148	0
4	NAG	M	1	14/15	0.83	0.11	78,98,119,147	0
8	BGC	O	1	12/12	0.83	0.08	101,129,142,144	0
5	NAG	R	2	14/15	0.83	0.11	102,126,149,158	0
6	NAG	L	2	14/15	0.83	0.13	98,113,136,138	0
11	NAG	X	2	14/15	0.84	0.13	77,107,124,128	0
6	MAN	L	3	11/12	0.85	0.07	153,158,164,175	0
8	GAL	V	4	11/12	0.85	0.08	113,124,135,139	0
10	MAN	S	3	11/12	0.85	0.10	101,135,153,160	0
4	NAG	J	1	14/15	0.86	0.11	66,77,101,114	0
12	NAG	Z	1	14/15	0.87	0.10	104,115,130,152	0
5	NAG	K	1	14/15	0.87	0.12	93,107,114,123	0
4	NAG	J	2	14/15	0.88	0.12	94,121,136,150	0
8	GAL	O	2	11/12	0.88	0.07	97,111,116,118	0
5	NAG	R	1	14/15	0.89	0.14	102,126,141,150	0
6	NAG	L	1	14/15	0.90	0.09	71,83,106,109	0
8	SIA	V	5	20/21	0.90	0.13	86,110,139,139	0
10	NAG	S	1	14/15	0.91	0.18	50,82,109,110	0
11	NAG	X	1	14/15	0.91	0.10	84,103,114,115	0
10	NAG	S	2	14/15	0.92	0.12	87,103,115,137	0

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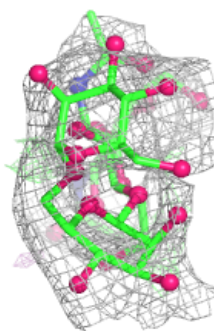
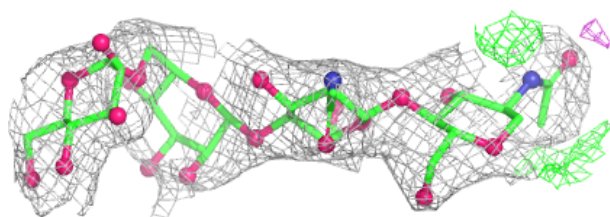
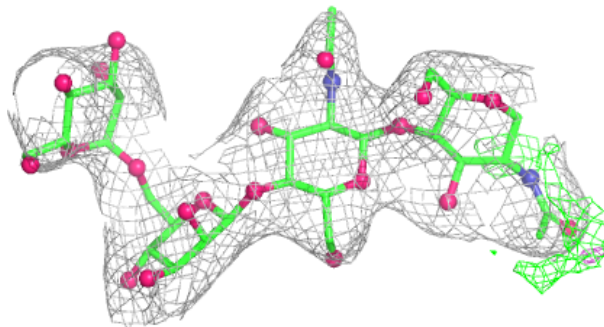
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	O	3	14/15	0.92	0.08	73,98,108,115	0
8	SIA	O	5	20/21	0.94	0.08	67,89,119,129	0
8	GAL	O	4	11/12	0.95	0.05	71,77,91,99	0
12	NAG	a	1	14/15	-	-	102,121,148,167	0
12	NAG	a	2	14/15	-	-	124,169,182,185	0
12	NAG	f	1	14/15	-	-	110,142,172,184	0
12	NAG	f	2	14/15	-	-	136,171,182,184	0
13	NAG	d	1	14/15	-	-	86,101,119,123	0
13	NAG	d	2	14/15	-	-	108,130,159,166	0
13	MAN	d	3	11/12	-	-	164,177,193,200	0
13	MAN	d	4	11/12	-	-	160,181,191,196	0
13	MAN	d	5	11/12	-	-	163,174,189,190	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.

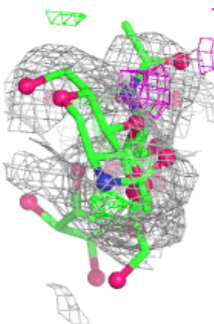
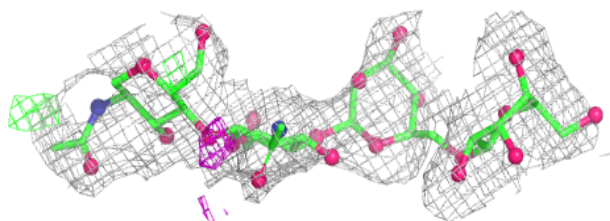
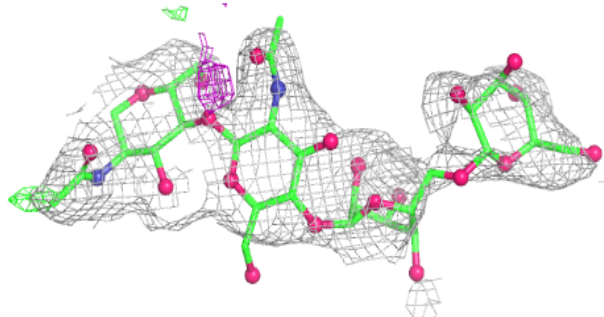


Electron density around Chain J:

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

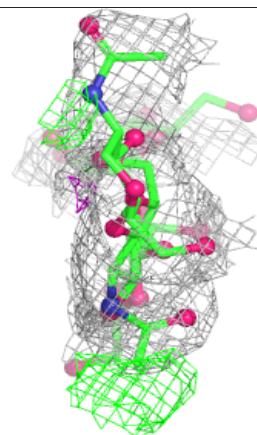
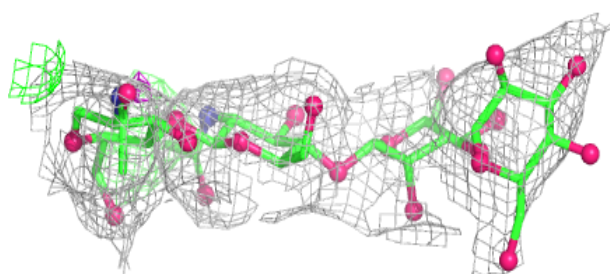
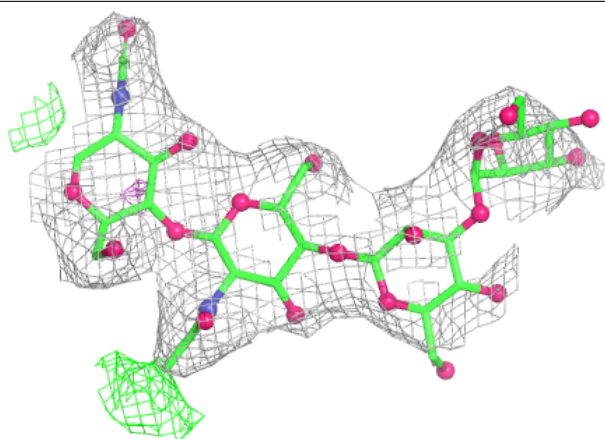
**Electron density around Chain M:**

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

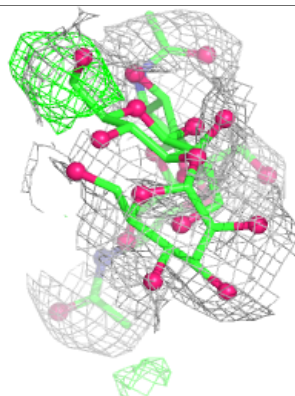
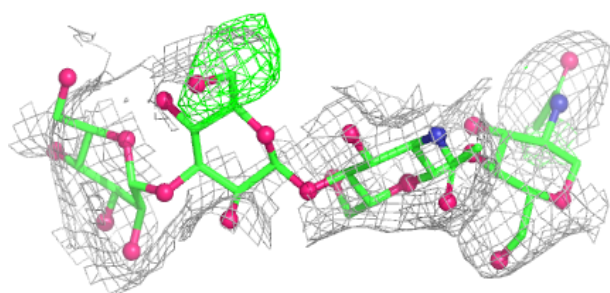
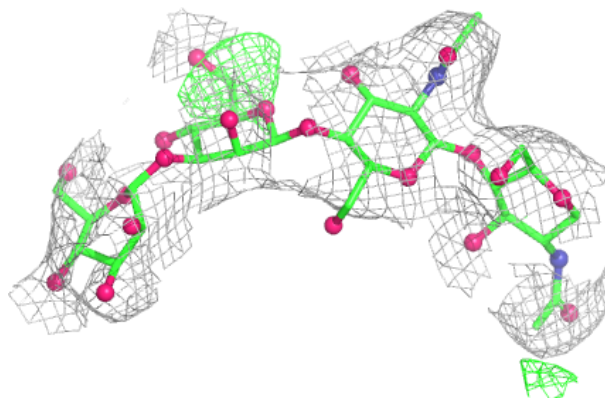


Electron density around Chain K:

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

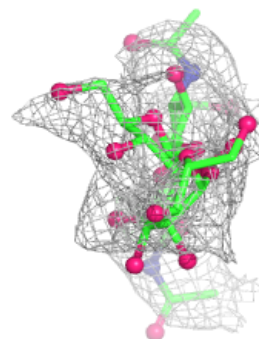
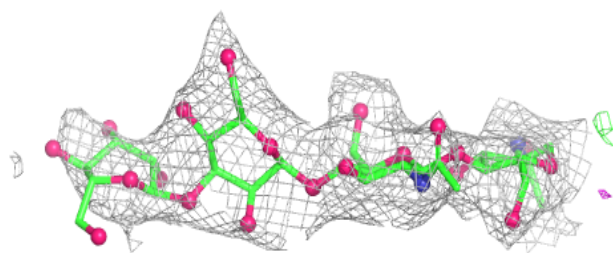
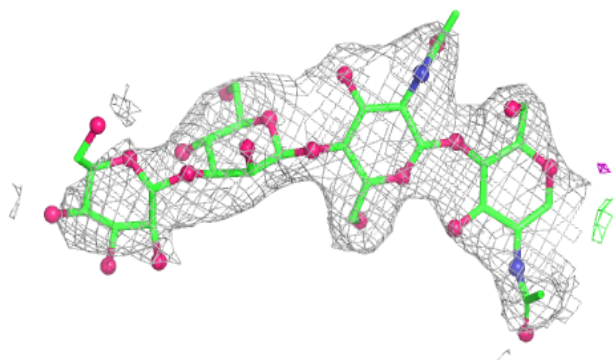
**Electron density around Chain Q:**

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

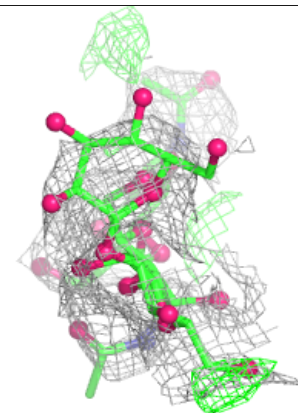
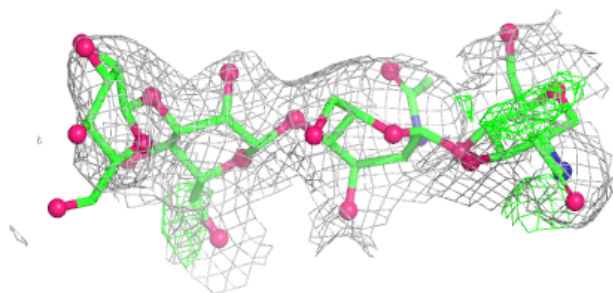
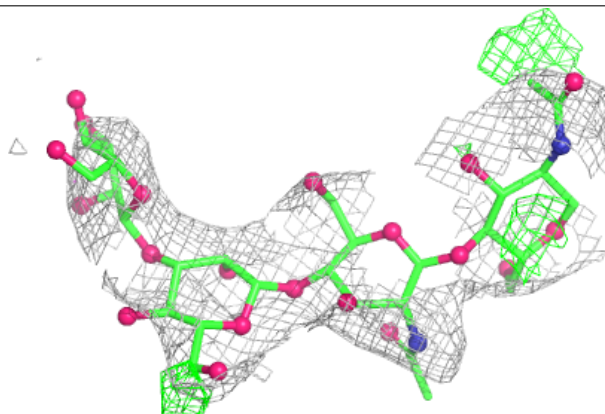


Electron density around Chain R:

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and green (positive)

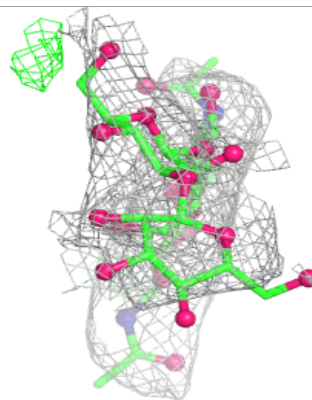
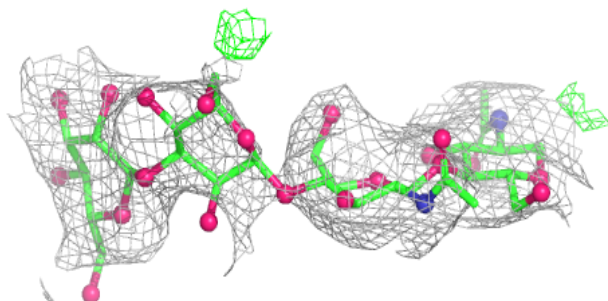
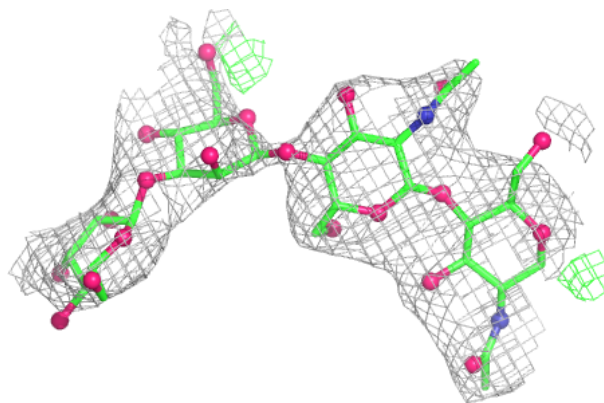
**Electron density around Chain W:**

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



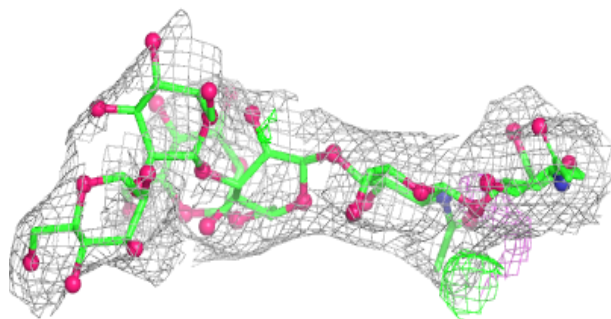
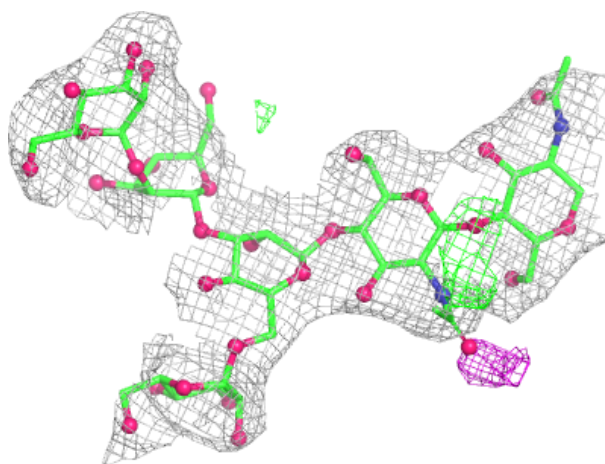
Electron density around Chain c:

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



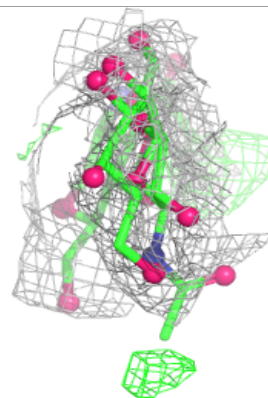
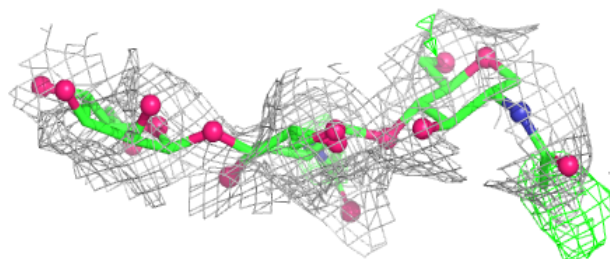
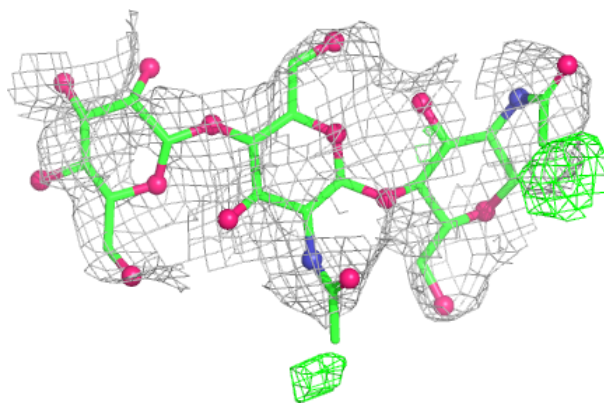
Electron density around Chain L:

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and green (positive)

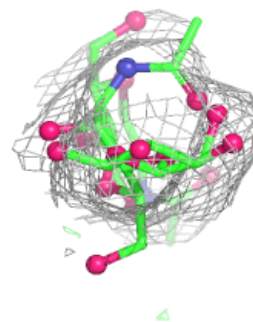
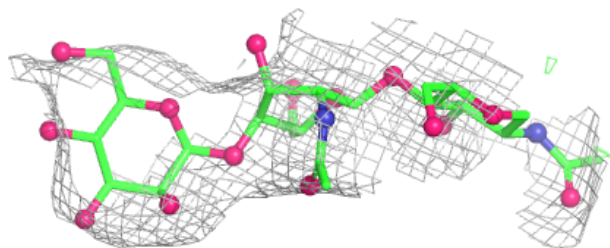
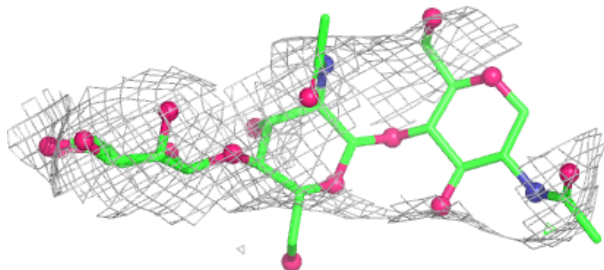


Electron density around Chain N:

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

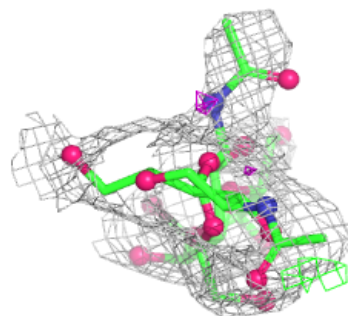
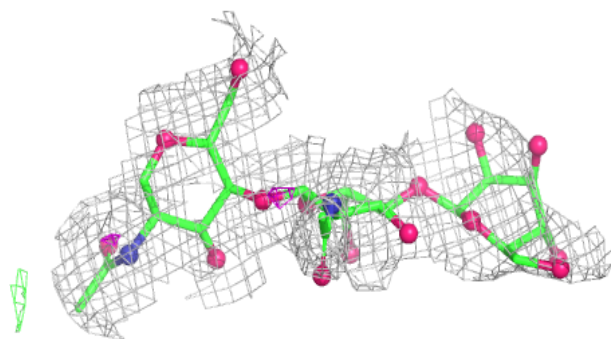
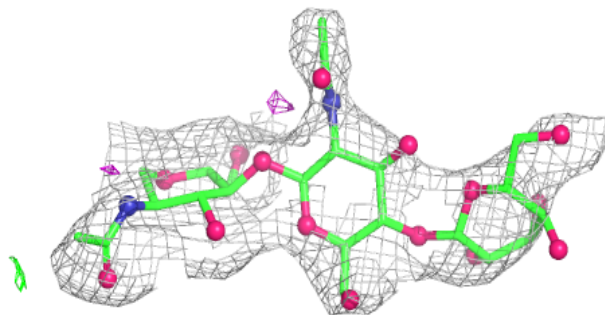
**Electron density around Chain b:**

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

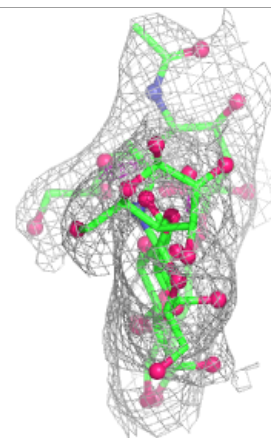
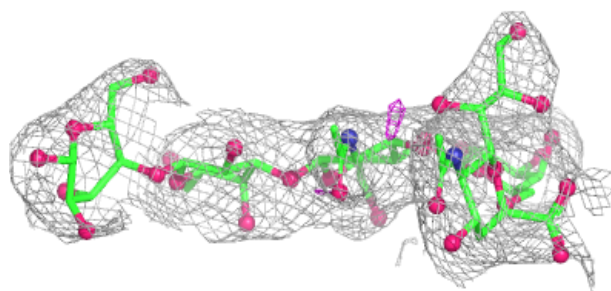
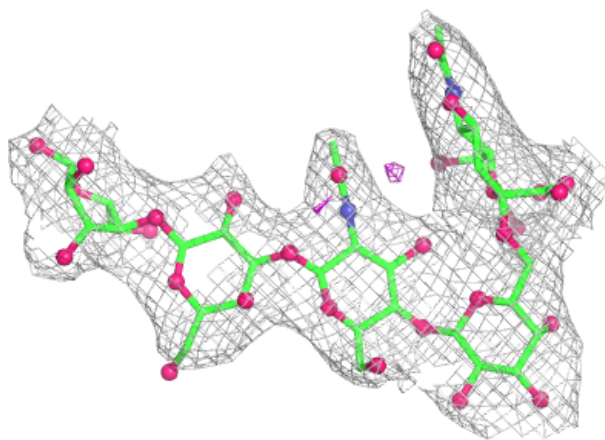


Electron density around Chain e:

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

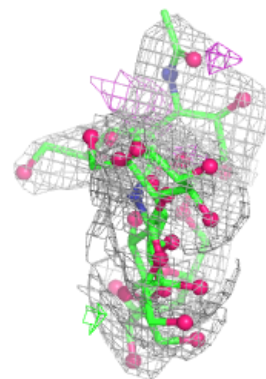
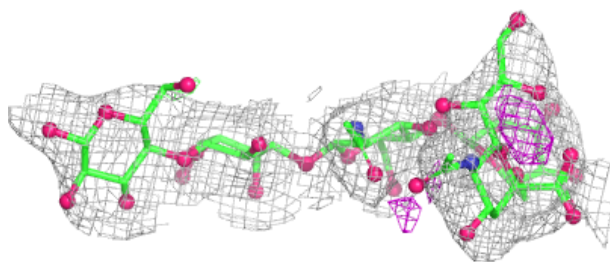
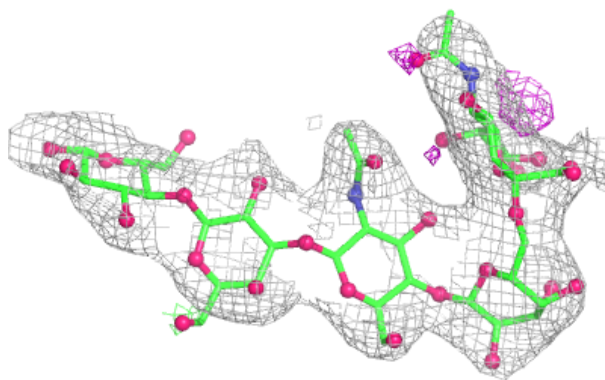
**Electron density around Chain O:**

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

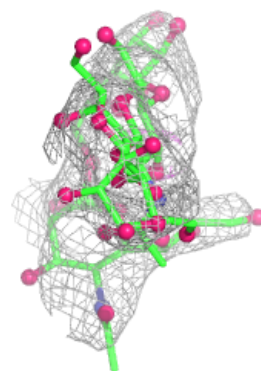
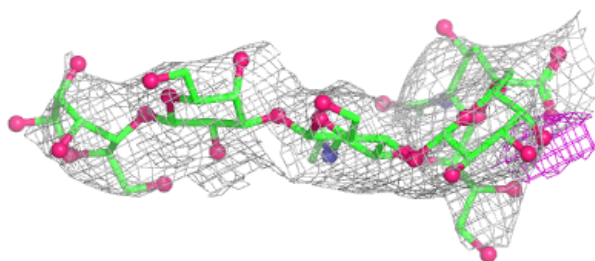
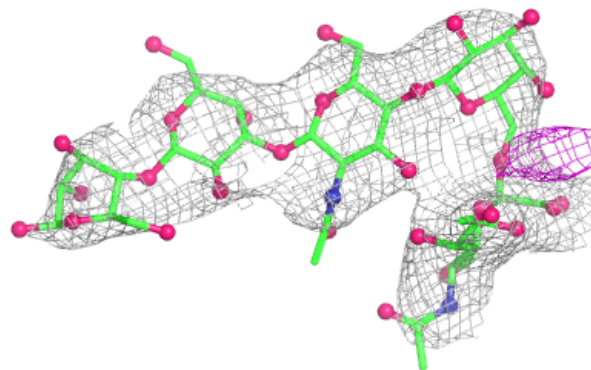


Electron density around Chain V:

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

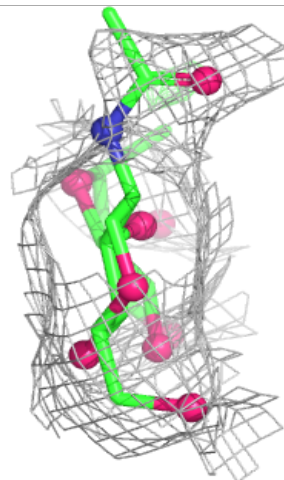
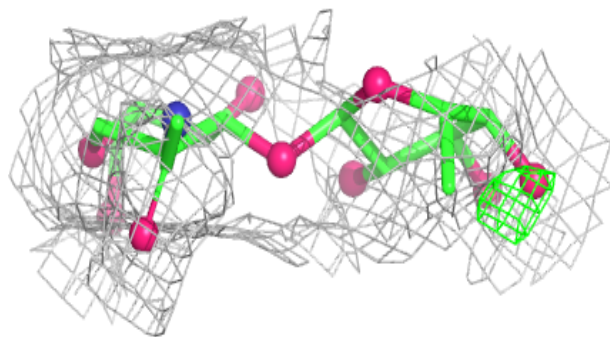
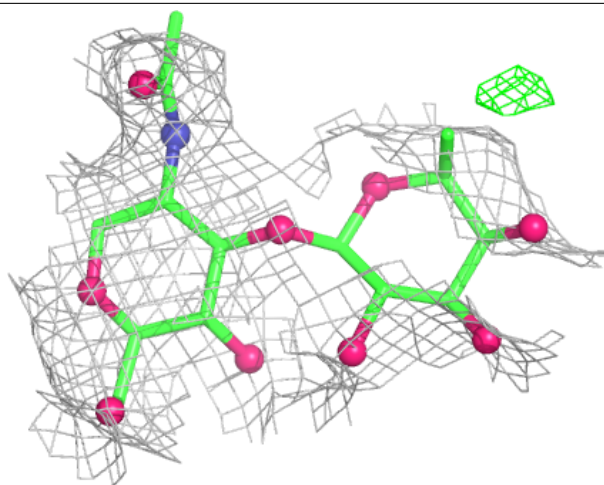
**Electron density around Chain g:**

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



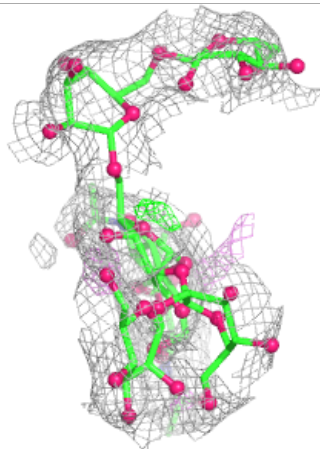
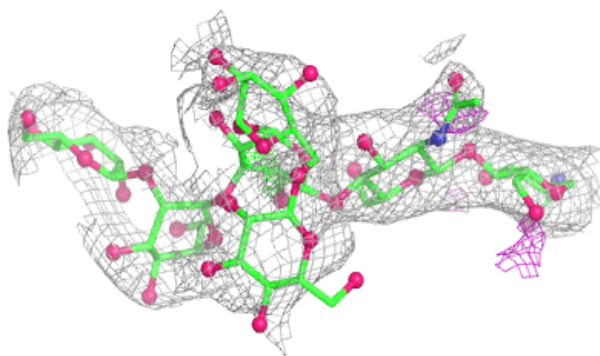
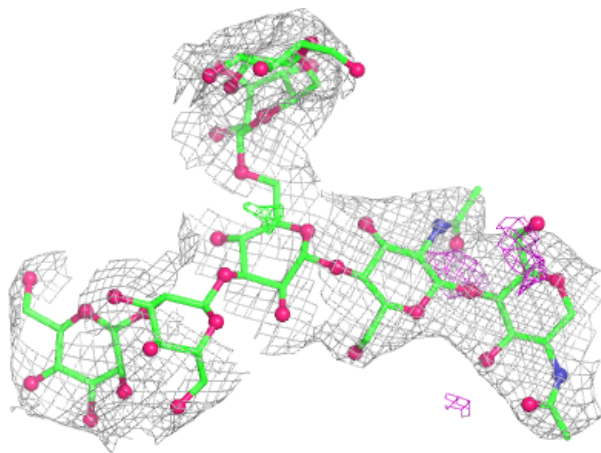
Electron density around Chain P:

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



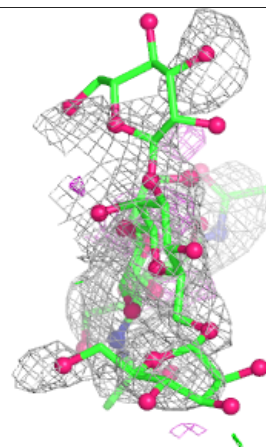
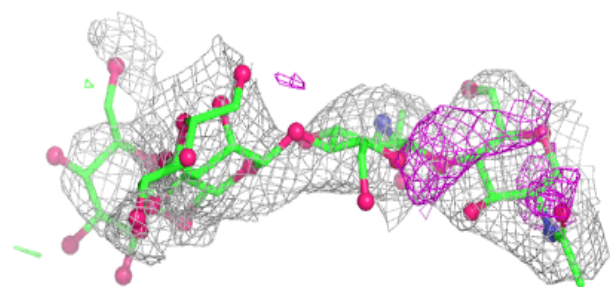
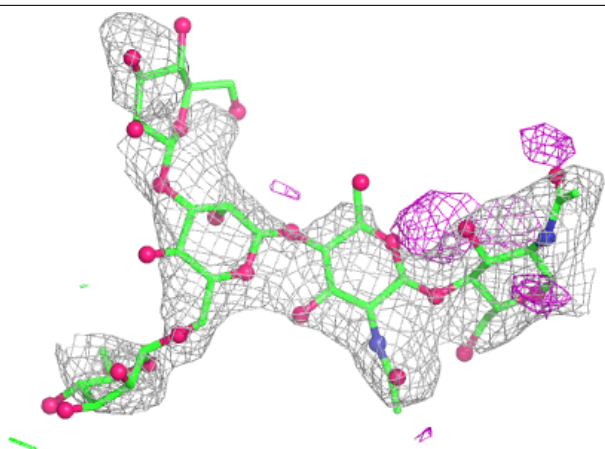
Electron density around Chain S:

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



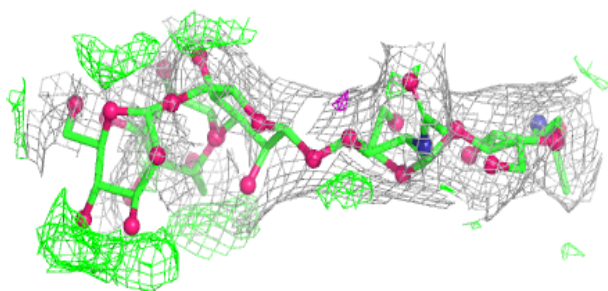
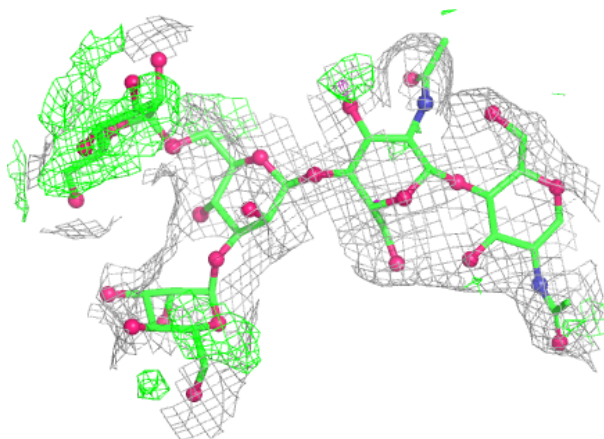
Electron density around Chain T:

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



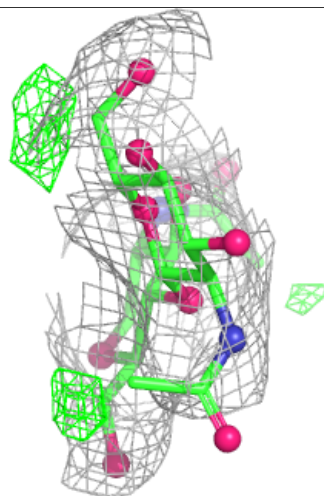
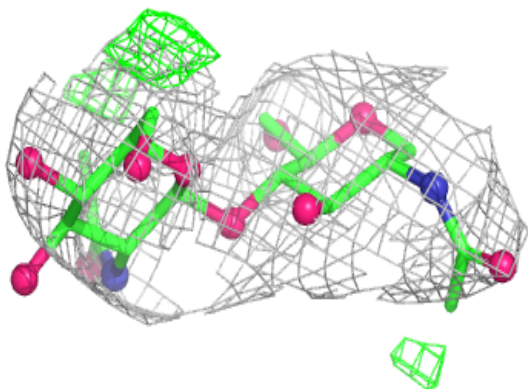
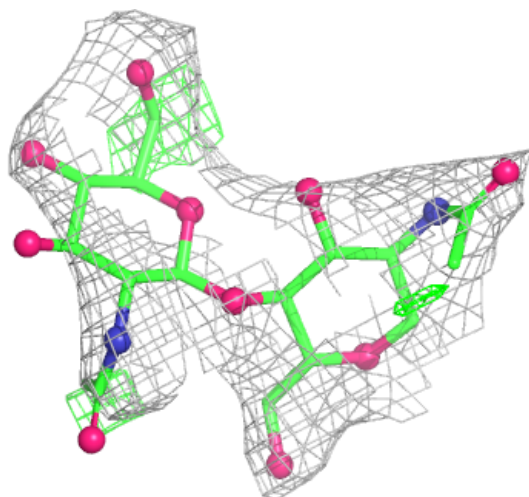
Electron density around Chain X:

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



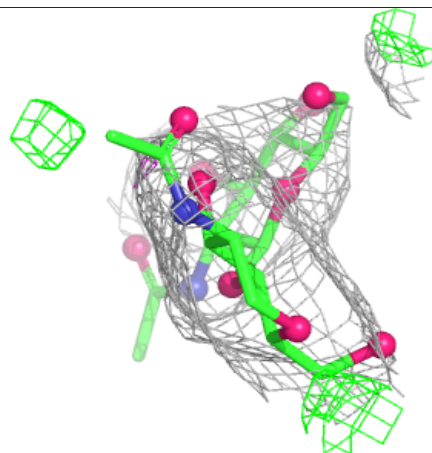
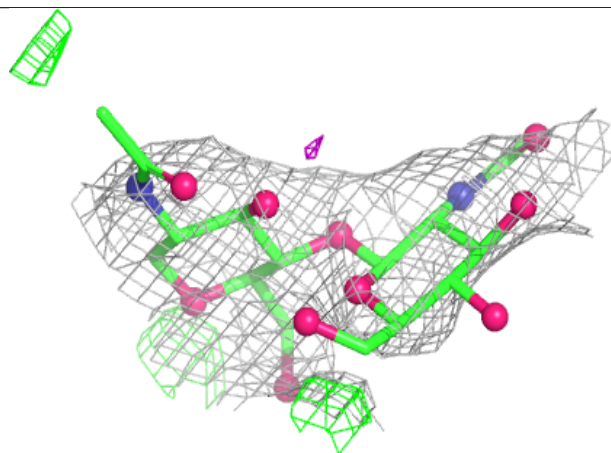
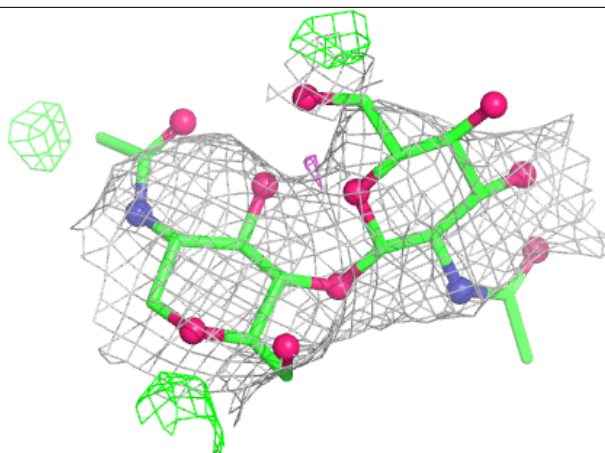
Electron density around Chain U:

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



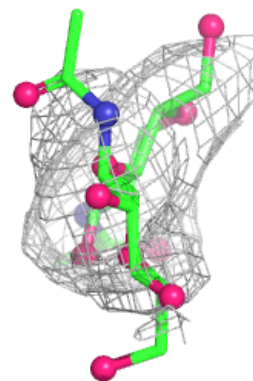
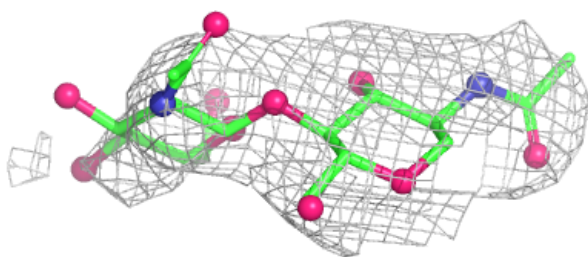
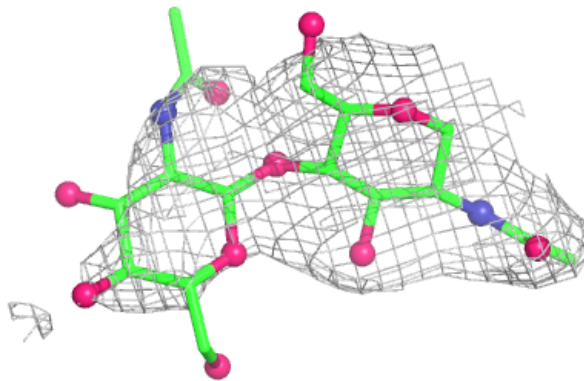
Electron density around Chain Y:

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



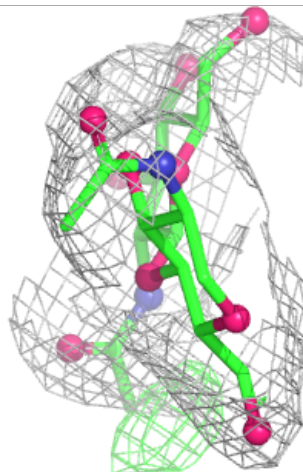
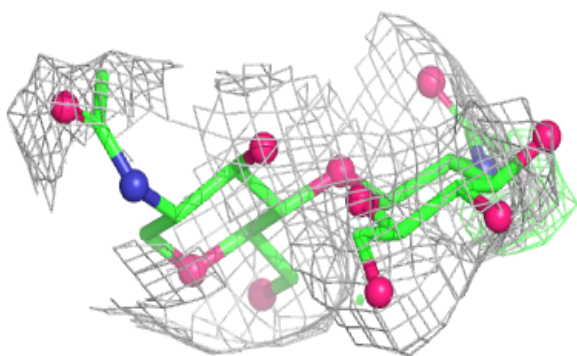
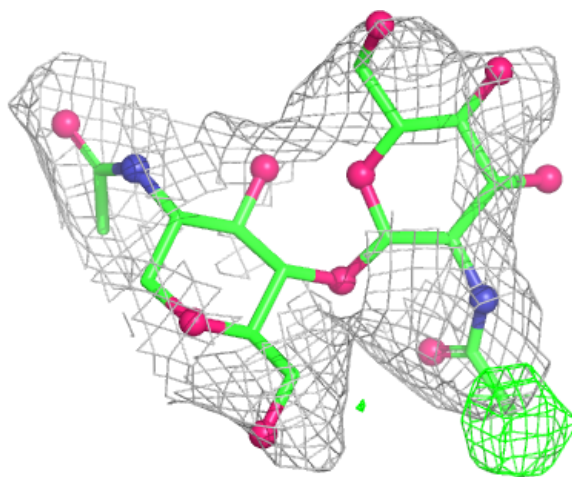
Electron density around Chain Z:

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



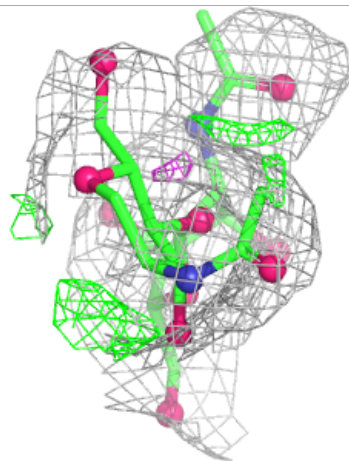
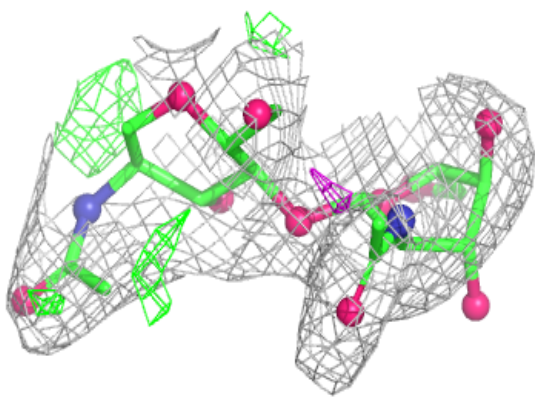
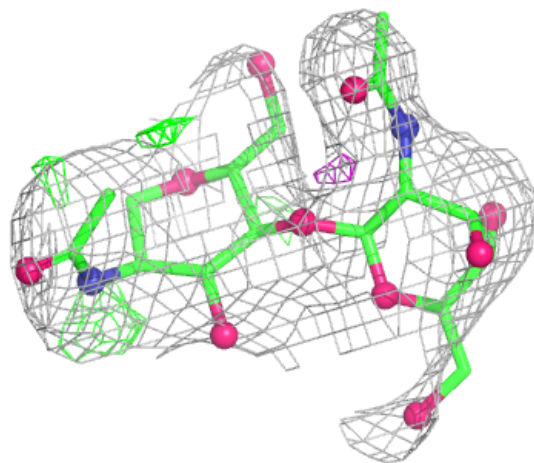
Electron density around Chain a:

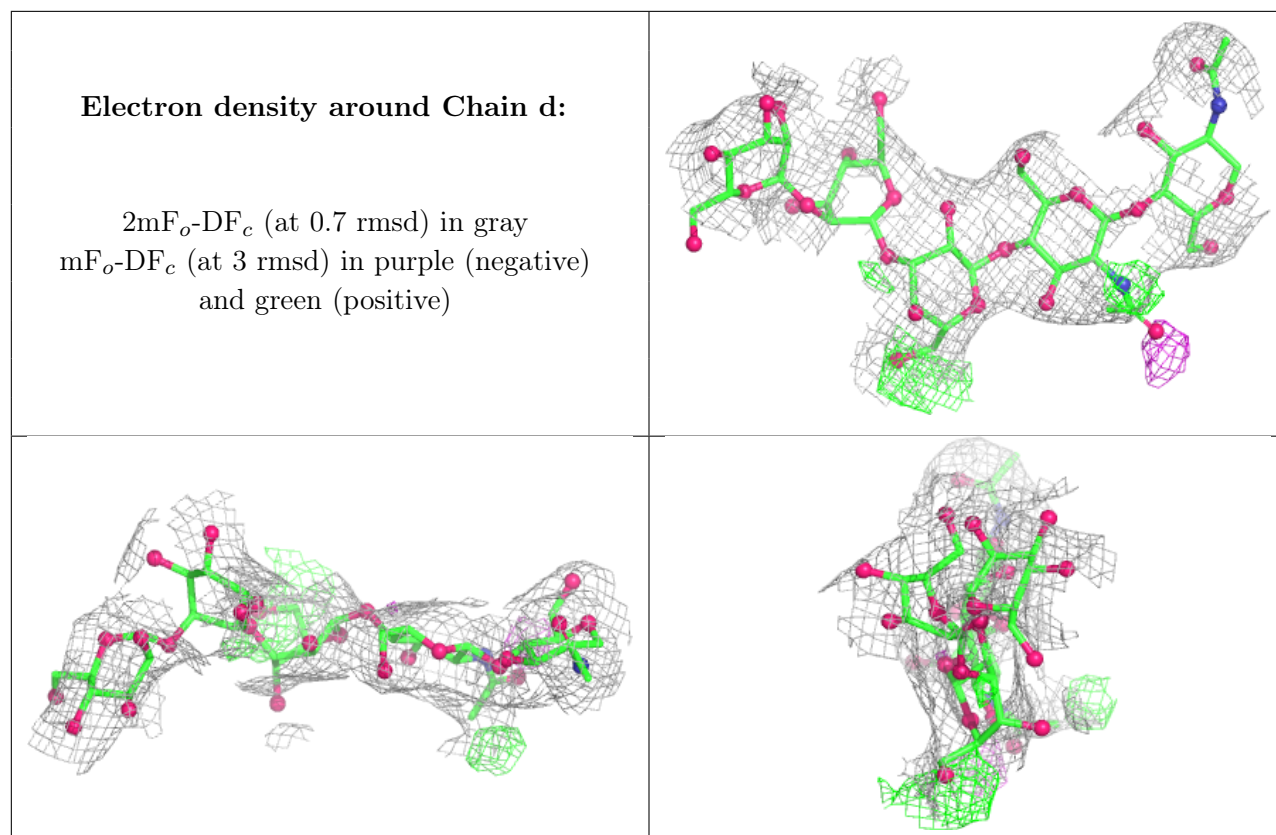
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain f:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
14	NAG	A	522	14/15	0.30	0.17	132,160,170,173	0
14	NAG	E	414	14/15	0.31	0.16	120,156,178,183	0
14	NAG	C	523	14/15	0.43	0.14	113,146,151,152	0
14	NAG	B	201	14/15	0.58	0.14	106,165,174,175	0
14	NAG	D	202	14/15	0.67	0.17	117,138,149,156	0
14	NAG	G	416	14/15	0.73	0.13	133,149,163,164	0
14	NAG	F	201	14/15	0.82	0.12	109,130,138,139	0
15	CAC	D	201	5/5	0.84	0.20	145,146,151,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.