



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2025 – 09:30 am GMT

PDB ID : 8S1Z  
Title : Crystal structure of glycosylated human primary amine oxidase AOC3  
Authors : Guedez, G.; Alix, M.; Salminen, T.A.  
Deposited on : 2024-02-16  
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

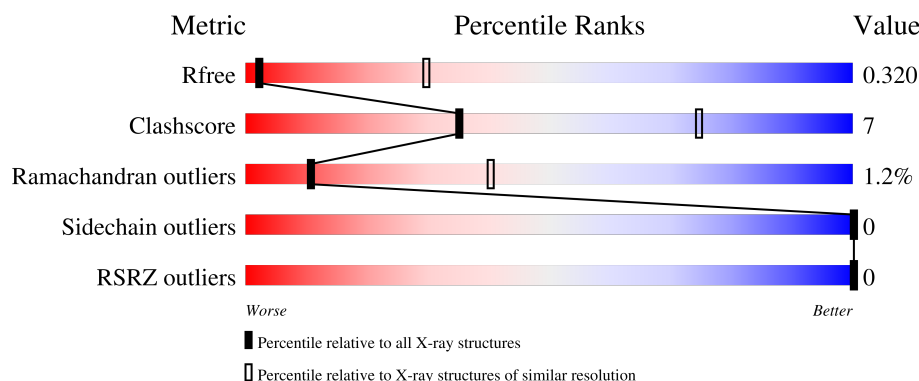
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





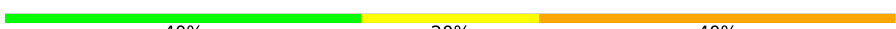
The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



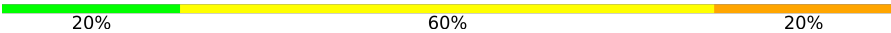
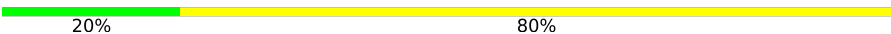
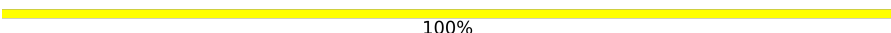


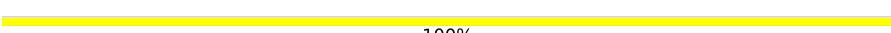
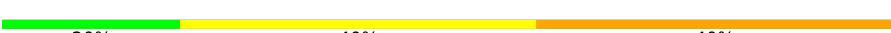







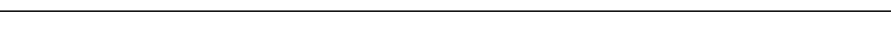
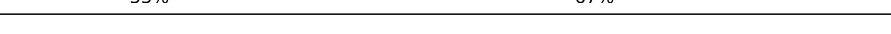


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1025 (3.98-3.62)
Clashscore	180529	1005 (3.96-3.64)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RSRZ outliers	164620	1025 (3.98-3.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	 81% 15% ..
1	B	737	 80% 17% ..
1	C	737	 79% 16% ..
1	D	737	 80% 16% ..
2	E	5	 40% 20% 40%

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Mol	Chain	Length	Quality of chain
3	F	5	
3	J	5	
3	O	5	
3	S	5	
4	G	2	
5	H	5	
5	M	5	
5	W	5	
6	I	2	
7	K	4	
8	L	2	
8	V	2	
9	N	6	
10	P	3	
10	U	3	
11	Q	4	
12	R	4	
13	T	6	

## 2 Entry composition [i](#)

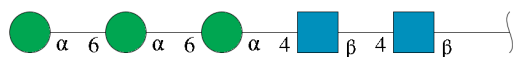
There are 16 unique types of molecules in this entry. The entry contains 23705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Membrane primary amine oxidase.

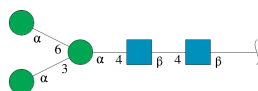
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5642	3619	976	1026	21			
1	B	723	Total	C	N	O	S	0	0	0
			5697	3654	985	1037	21			
1	C	713	Total	C	N	O	S	0	0	0
			5627	3611	973	1022	21			
1	D	723	Total	C	N	O	S	0	0	0
			5697	3654	985	1037	21			

- Molecule 2 is an oligosaccharide called 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
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is an oligosaccharide called 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
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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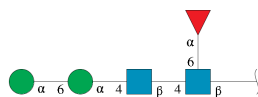
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			
5	M	5	Total	C	N	O	0	0	0
			60	34	2	24			
5	W	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called 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.



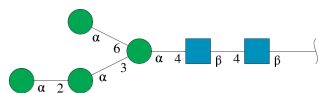
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



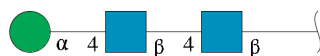
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	L	2	Total	C	N	O	0	0	0
			24	14	1	9			
8	V	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 9 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.



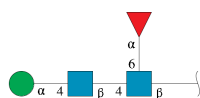
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 10 is an oligosaccharide called 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	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



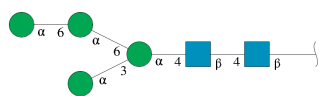
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Q	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 12 is an oligosaccharide called 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
12	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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	T	6	Total	C	N	O	0	0	0
			72	40	2	30			

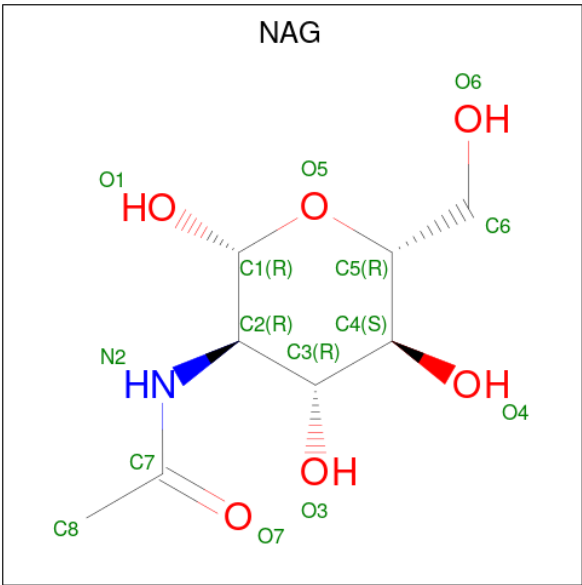
- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Ca	0	0
			2	2		
14	B	2	Total	Ca	0	0
			2	2		
14	C	2	Total	Ca	0	0
			2	2		
14	D	2	Total	Ca	0	0
			2	2		

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	B	1	Total	Cu	0	0
			1	1		
15	C	1	Total	Cu	0	0
			1	1		
15	D	1	Total	Cu	0	0
			1	1		

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

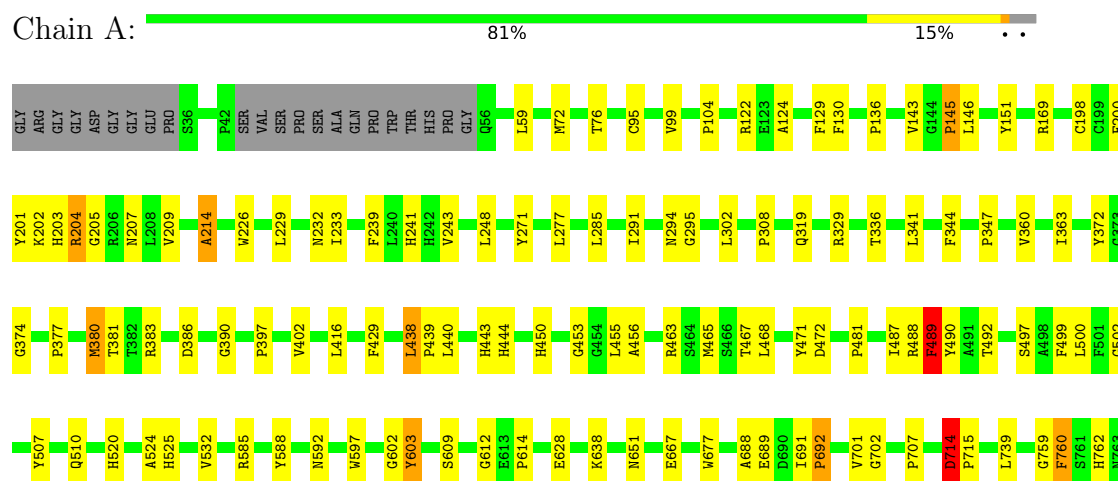


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	A	1	Total	C	N	O	0	0
			14	8	1	5		
16	B	1	Total	C	N	O	0	0
			14	8	1	5		
16	B	1	Total	C	N	O	0	0
			14	8	1	5		
16	D	1	Total	C	N	O	0	0
			14	8	1	5		
16	D	1	Total	C	N	O	0	0
			14	8	1	5		

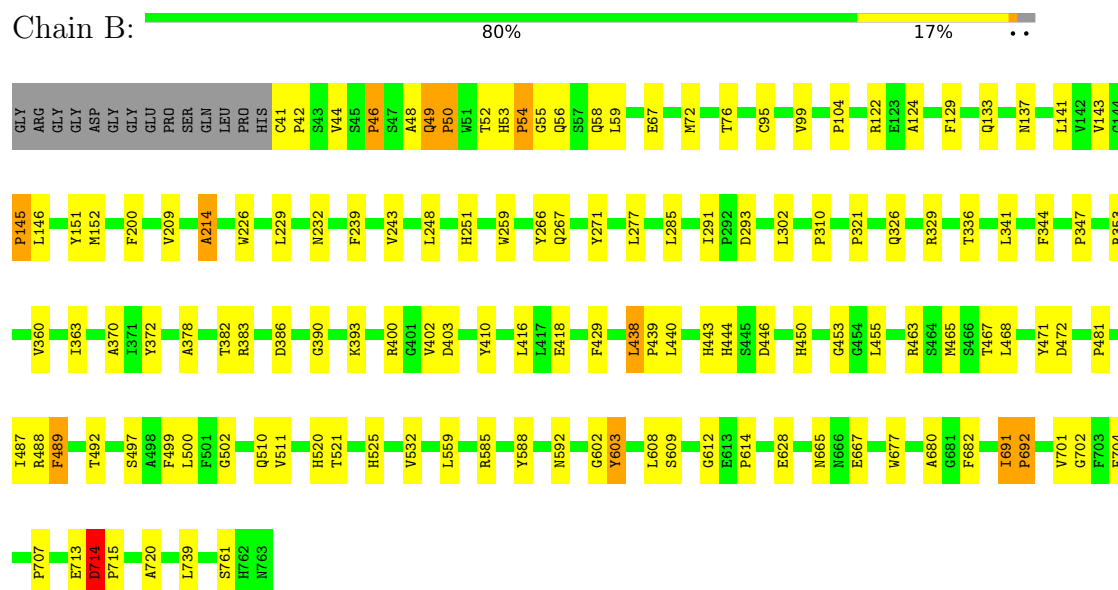
### 3 Residue-property plots

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: Membrane primary amine oxidase

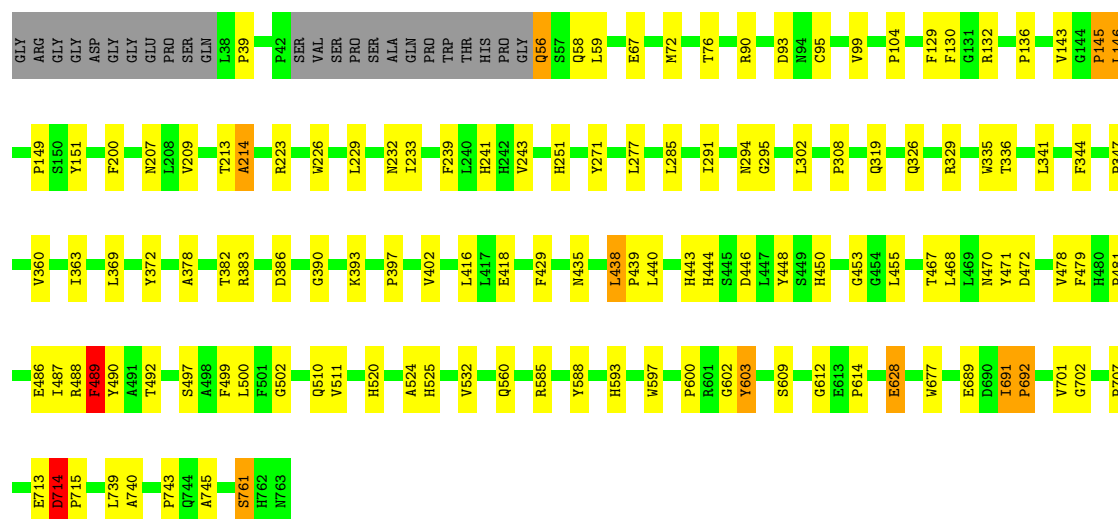


- Molecule 1: Membrane primary amine oxidase




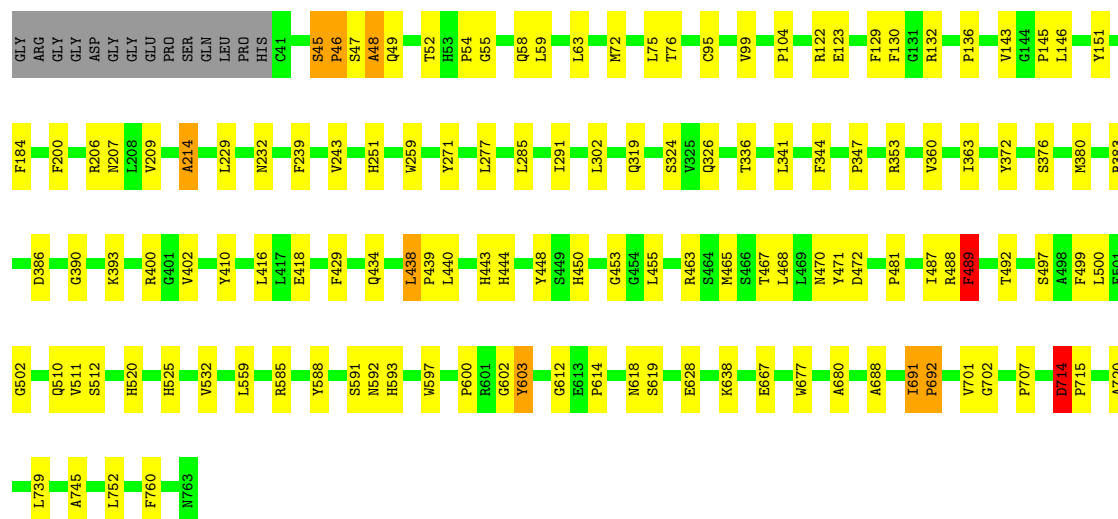
- Molecule 1: Membrane primary amine oxidase

Chain C:  79% 16% ..



- Molecule 1: Membrane primary amine oxidase

Chain D:  80% 16% ..

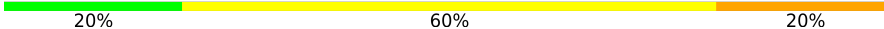


- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  40% 20% 40%



- Molecule 3: 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

Chain F:  20% 60% 20%

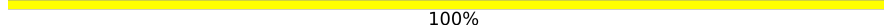


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  20% 80%

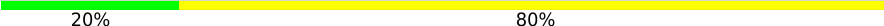


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 3: 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

Chain S:  20% 80%



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

Chain G:  50% 50%

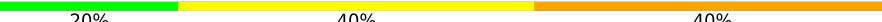


- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  20% 40% 40%



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  40% 60%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 7: 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 K:  50% 50%



- Molecule 8: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

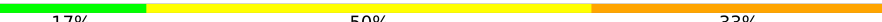


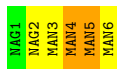
- Molecule 8: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%



- Molecule 9: 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

Chain N:  17% 50% 33%



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

Chain P:  67% 33%


MAG1  
MAG2  
MAN3

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

Chain U:  33% 67%

MAG1  
MAG2  
MAN3

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

Chain Q:  25% 25% 50%

MAG1  
MAG2  
MAN3  
FUC4

- Molecule 12: 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 R:  50% 50%

MAG1  
MAG2  
MAN3  
MAN4

- Molecule 13: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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 T:  50% 50%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.96Å 127.96Å 220.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.80 29.88 – 3.80	Depositor EDS
% Data completeness (in resolution range)	79.5 (29.88-3.80) 69.7 (29.88-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.11 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.286 , 0.320 0.286 , 0.320	Depositor DCC
$R_{free}$ test set	23039 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.207 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	23705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, FUC, NAG, CA, TPQ, MAN

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	0.38	3/5807 (0.1%)	1.05	12/7918 (0.2%)
1	B	0.37	2/5867 (0.0%)	1.10	14/8005 (0.2%)
1	C	0.38	5/5792 (0.1%)	1.21	14/7898 (0.2%)
1	D	0.34	1/5867 (0.0%)	0.86	11/8005 (0.1%)
All	All	0.37	11/23333 (0.0%)	1.06	51/31826 (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
1	A	0	6
1	B	0	4
1	C	0	5
1	D	0	5
All	All	0	20

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	MET	CB-CG	8.17	1.77	1.51
1	A	489	PHE	CE1-CZ	7.52	1.51	1.37
1	B	489	PHE	CG-CD1	7.40	1.49	1.38
1	C	489	PHE	CE2-CZ	-7.07	1.24	1.37
1	C	489	PHE	CE1-CZ	-7.02	1.24	1.37

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	PHE	CB-CG-CD2	-63.70	76.21	120.80
1	C	489	PHE	CB-CG-CD2	-61.78	77.55	120.80
1	C	489	PHE	CB-CG-CD1	56.43	160.30	120.80
1	A	489	PHE	CB-CG-CD2	-54.90	82.37	120.80
1	B	489	PHE	CB-CG-CD1	44.84	152.19	120.80

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	VAL	Peptide
1	A	145	PRO	Peptide
1	A	198	CYS	Peptide
1	A	204	ARG	Peptide
1	A	489	PHE	Sidechain

## 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	5642	0	5384	96	0
1	B	5697	0	5432	96	0
1	C	5627	0	5371	95	0
1	D	5697	0	5429	100	0
2	E	61	0	52	1	0
3	F	61	0	52	1	0
3	J	61	0	52	2	0
3	O	61	0	52	1	0
3	S	61	0	52	0	0
4	G	28	0	25	0	0
5	H	60	0	52	2	0
5	M	60	0	52	2	0
5	W	60	0	52	1	0
6	I	28	0	25	0	0
7	K	50	0	43	1	0
8	L	24	0	22	0	0
8	V	24	0	22	0	0
9	N	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	P	39	0	34	1	0
10	U	39	0	34	0	0
11	Q	49	0	43	1	0
12	R	50	0	43	0	0
13	T	72	0	61	2	0
14	A	2	0	0	0	0
14	B	2	0	0	0	0
14	C	2	0	0	0	0
14	D	2	0	0	0	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	D	1	0	0	0	0
16	A	14	0	13	0	0
16	B	28	0	26	0	0
16	D	28	0	26	1	0
All	All	23705	0	22510	336	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 7.

The worst 5 of 336 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:A:380:MET:CB	1:A:380:MET:CG	1.77	1.57
1:C:450:HIS:HB3	1:D:760:PHE:CE2	2.12	0.84
1:D:122:ARG:HG2	1:D:146:LEU:HD12	1.62	0.81
1:A:200:PHE:O	1:A:207:ASN:ND2	2.13	0.81
1:A:592:ASN:HD21	5:H:1:NAG:H83	1.47	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	710/737 (96%)	659 (93%)	45 (6%)	6 (1%)	16	49
1	B	720/737 (98%)	667 (93%)	42 (6%)	11 (2%)	8	37
1	C	708/737 (96%)	661 (93%)	40 (6%)	7 (1%)	13	44
1	D	720/737 (98%)	663 (92%)	47 (6%)	10 (1%)	9	37
All	All	2858/2948 (97%)	2650 (93%)	174 (6%)	34 (1%)	11	40

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	502	GLY
1	B	46	PRO
1	B	49	GLN
1	B	53	HIS

### 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	595/610 (98%)	595 (100%)	0	100	100
1	B	601/610 (98%)	601 (100%)	0	100	100
1	C	593/610 (97%)	593 (100%)	0	100	100
1	D	601/610 (98%)	601 (100%)	0	100	100
All	All	2390/2440 (98%)	2390 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN

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Mol	Chain	Res	Type
1	B	267	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TPQ	A	471	1	13,14,15	0.73	0	15,19,21	1.57	2 (13%)
1	TPQ	B	471	1	13,14,15	0.74	0	15,19,21	1.61	2 (13%)
1	TPQ	C	471	1	13,14,15	0.74	0	15,19,21	1.50	2 (13%)
1	TPQ	D	471	1	13,14,15	0.72	0	15,19,21	1.61	2 (13%)

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
1	TPQ	A	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	B	471	1	-	3/5/22/24	0/1/1/1
1	TPQ	C	471	1	-	3/5/22/24	0/1/1/1
1	TPQ	D	471	1	-	4/5/22/24	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	TPQ	C6-C1-C2	4.28	121.92	118.64
1	B	471	TPQ	C6-C1-C2	4.12	121.80	118.64
1	D	471	TPQ	C6-C1-C2	4.07	121.77	118.64
1	C	471	TPQ	C6-C1-C2	4.00	121.71	118.64
1	B	471	TPQ	CB-CA-C	-3.88	104.20	111.47

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	TPQ	N-CA-CB-C1
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	N-CA-CB-C1
1	B	471	TPQ	C-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

78 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	E	1	1,2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.68	0
2	MAN	E	3	2	11,11,12	1.31	1 (9%)	15,15,17	1.98	3 (20%)
2	MAN	E	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.13	0
2	MAN	E	5	2	11,11,12	1.55	1 (9%)	15,15,17	1.72	3 (20%)
3	NAG	F	1	1,3	14,14,15	0.64	1 (7%)	17,19,21	1.39	2 (11%)
3	NAG	F	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.62	0
3	MAN	F	3	3	11,11,12	1.43	2 (18%)	15,15,17	1.49	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	F	4	3	11,11,12	0.84	0	15,15,17	0.85	0
3	MAN	F	5	3	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.60	1 (7%)	17,19,21	0.90	0
4	NAG	G	2	4	14,14,15	0.45	0	17,19,21	0.46	0
5	NAG	H	1	1,5	14,14,15	0.30	0	17,19,21	0.59	0
5	NAG	H	2	5	14,14,15	0.74	1 (7%)	17,19,21	0.90	1 (5%)
5	MAN	H	3	5	11,11,12	0.85	0	15,15,17	1.19	2 (13%)
5	MAN	H	4	5	11,11,12	1.05	1 (9%)	15,15,17	1.61	3 (20%)
5	FUC	H	5	5	10,10,11	0.96	0	14,14,16	0.95	1 (7%)
6	NAG	I	1	1,6	14,14,15	1.06	2 (14%)	17,19,21	0.93	0
6	NAG	I	2	6	14,14,15	0.77	1 (7%)	17,19,21	0.61	0
3	NAG	J	1	3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.52	0
3	MAN	J	3	3	11,11,12	1.03	1 (9%)	15,15,17	2.59	3 (20%)
3	MAN	J	4	3	11,11,12	0.82	1 (9%)	15,15,17	1.05	1 (6%)
3	MAN	J	5	3	11,11,12	0.93	1 (9%)	15,15,17	1.32	2 (13%)
7	NAG	K	1	1,7	14,14,15	0.64	1 (7%)	17,19,21	0.55	0
7	NAG	K	2	7	14,14,15	0.58	1 (7%)	17,19,21	0.67	0
7	MAN	K	3	7	11,11,12	0.85	0	15,15,17	1.08	1 (6%)
7	MAN	K	4	7	11,11,12	1.08	1 (9%)	15,15,17	1.32	3 (20%)
8	NAG	L	1	1,8	14,14,15	0.57	1 (7%)	17,19,21	0.57	0
8	FUC	L	2	8	10,10,11	1.18	1 (10%)	14,14,16	1.44	2 (14%)
5	NAG	M	1	1,5	14,14,15	0.53	0	17,19,21	0.65	0
5	NAG	M	2	5	14,14,15	0.67	0	17,19,21	0.86	1 (5%)
5	MAN	M	3	5	11,11,12	1.06	1 (9%)	15,15,17	1.31	3 (20%)
5	MAN	M	4	5	11,11,12	1.16	1 (9%)	15,15,17	1.55	2 (13%)
5	FUC	M	5	5	10,10,11	0.84	0	14,14,16	0.76	0
9	NAG	N	1	9,1	14,14,15	0.49	0	17,19,21	0.44	0
9	NAG	N	2	9	14,14,15	0.54	0	17,19,21	0.87	1 (5%)
9	MAN	N	3	9	11,11,12	1.20	1 (9%)	15,15,17	1.40	3 (20%)
9	MAN	N	4	9	11,11,12	0.84	0	15,15,17	1.48	1 (6%)
9	MAN	N	5	9	11,11,12	1.21	3 (27%)	15,15,17	1.21	2 (13%)
9	MAN	N	6	9	11,11,12	0.78	0	15,15,17	1.12	2 (13%)
3	NAG	O	1	1,3	14,14,15	0.45	0	17,19,21	0.47	0
3	NAG	O	2	3	14,14,15	0.69	1 (7%)	17,19,21	0.63	0
3	MAN	O	3	3	11,11,12	1.47	2 (18%)	15,15,17	1.52	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	O	4	3	11,11,12	0.86	0	15,15,17	0.87	1 (6%)
3	MAN	O	5	3	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
10	NAG	P	1	10,1	14,14,15	0.57	0	17,19,21	0.83	1 (5%)
10	NAG	P	2	10	14,14,15	0.42	0	17,19,21	0.44	0
10	MAN	P	3	10	11,11,12	0.84	1 (9%)	15,15,17	0.88	1 (6%)
11	NAG	Q	1	1,11	14,14,15	0.70	1 (7%)	17,19,21	0.74	0
11	NAG	Q	2	11	14,14,15	0.55	0	17,19,21	0.70	0
11	MAN	Q	3	11	11,11,12	0.90	1 (9%)	15,15,17	0.98	1 (6%)
11	FUC	Q	4	11	10,10,11	1.08	1 (10%)	14,14,16	0.76	0
12	NAG	R	1	1,12	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
12	NAG	R	2	12	14,14,15	0.17	0	17,19,21	0.36	0
12	MAN	R	3	12	11,11,12	0.91	0	15,15,17	0.85	0
12	MAN	R	4	12	11,11,12	0.85	0	15,15,17	0.90	1 (6%)
3	NAG	S	1	3	14,14,15	0.69	1 (7%)	17,19,21	0.67	0
3	NAG	S	2	3	14,14,15	0.17	0	17,19,21	0.65	0
3	MAN	S	3	3	11,11,12	1.38	3 (27%)	15,15,17	2.27	6 (40%)
3	MAN	S	4	3	11,11,12	0.80	0	15,15,17	1.03	1 (6%)
3	MAN	S	5	3	11,11,12	0.97	1 (9%)	15,15,17	1.28	2 (13%)
13	NAG	T	1	13,1	14,14,15	0.37	0	17,19,21	0.42	0
13	NAG	T	2	13	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
13	MAN	T	3	13	11,11,12	0.69	0	15,15,17	1.08	2 (13%)
13	MAN	T	4	13	11,11,12	1.32	1 (9%)	15,15,17	1.61	2 (13%)
13	MAN	T	5	13	11,11,12	1.55	1 (9%)	15,15,17	1.79	3 (20%)
13	MAN	T	6	13	11,11,12	0.71	0	15,15,17	1.19	1 (6%)
10	NAG	U	1	10,1	14,14,15	0.45	0	17,19,21	0.48	0
10	NAG	U	2	10	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
10	MAN	U	3	10	11,11,12	0.86	1 (9%)	15,15,17	1.12	2 (13%)
8	NAG	V	1	1,8	14,14,15	0.62	0	17,19,21	0.47	0
8	FUC	V	2	8	10,10,11	0.93	0	14,14,16	1.22	2 (14%)
5	NAG	W	1	1,5	14,14,15	0.54	0	17,19,21	0.63	0
5	NAG	W	2	5	14,14,15	0.62	0	17,19,21	0.87	0
5	MAN	W	3	5	11,11,12	1.30	1 (9%)	15,15,17	1.54	3 (20%)
5	MAN	W	4	5	11,11,12	1.60	3 (27%)	15,15,17	1.92	4 (26%)
5	FUC	W	5	5	10,10,11	0.78	0	14,14,16	0.75	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	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	MAN	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	MAN	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	MAN	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	FUC	H	5	5	-	-	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
3	NAG	J	1	3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	MAN	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	1/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	MAN	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
8	NAG	L	1	1,8	-	4/6/23/26	0/1/1/1
8	FUC	L	2	8	-	-	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	MAN	M	3	5	-	2/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	FUC	M	5	5	-	-	0/1/1/1
9	NAG	N	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
9	MAN	N	3	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	N	4	9	-	2/2/19/22	0/1/1/1
9	MAN	N	5	9	-	0/2/19/22	0/1/1/1
9	MAN	N	6	9	-	2/2/19/22	1/1/1/1
3	NAG	O	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	MAN	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1
3	MAN	O	5	3	-	2/2/19/22	0/1/1/1
10	NAG	P	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	MAN	P	3	10	-	2/2/19/22	1/1/1/1
11	NAG	Q	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Q	2	11	-	1/6/23/26	0/1/1/1
11	MAN	Q	3	11	-	2/2/19/22	0/1/1/1
11	FUC	Q	4	11	-	-	0/1/1/1
12	NAG	R	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	R	2	12	-	2/6/23/26	0/1/1/1
12	MAN	R	3	12	-	1/2/19/22	0/1/1/1
12	MAN	R	4	12	-	1/2/19/22	0/1/1/1
3	NAG	S	1	3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	MAN	S	3	3	-	2/2/19/22	0/1/1/1
3	MAN	S	4	3	-	2/2/19/22	0/1/1/1
3	MAN	S	5	3	-	2/2/19/22	1/1/1/1
13	NAG	T	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	T	2	13	-	2/6/23/26	0/1/1/1
13	MAN	T	3	13	-	0/2/19/22	0/1/1/1
13	MAN	T	4	13	-	1/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	1/2/19/22	0/1/1/1
10	NAG	U	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	0/6/23/26	0/1/1/1
10	MAN	U	3	10	-	0/2/19/22	0/1/1/1
8	NAG	V	1	1,8	-	1/6/23/26	0/1/1/1
8	FUC	V	2	8	-	-	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	MAN	W	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	W	4	5	-	2/2/19/22	0/1/1/1
5	FUC	W	5	5	-	-	0/1/1/1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	5	MAN	C1-C2	4.46	1.62	1.52
2	E	5	MAN	C1-C2	4.38	1.62	1.52
2	E	3	MAN	C1-C2	3.83	1.60	1.52
5	W	4	MAN	C1-C2	3.58	1.60	1.52
5	W	3	MAN	C1-C2	3.31	1.59	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	3	MAN	C1-O5-C5	7.80	122.76	112.19
2	E	3	MAN	C1-O5-C5	6.15	120.53	112.19
3	S	3	MAN	C1-O5-C5	6.00	120.32	112.19
5	W	4	MAN	C1-O5-C5	5.49	119.64	112.19
3	J	3	MAN	C1-C2-C3	5.07	115.90	109.67

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C3-C2-N2-C7
4	G	2	NAG	O5-C5-C6-O6
3	O	3	MAN	C4-C5-C6-O6
10	P	3	MAN	O5-C5-C6-O6
3	F	3	MAN	C4-C5-C6-O6

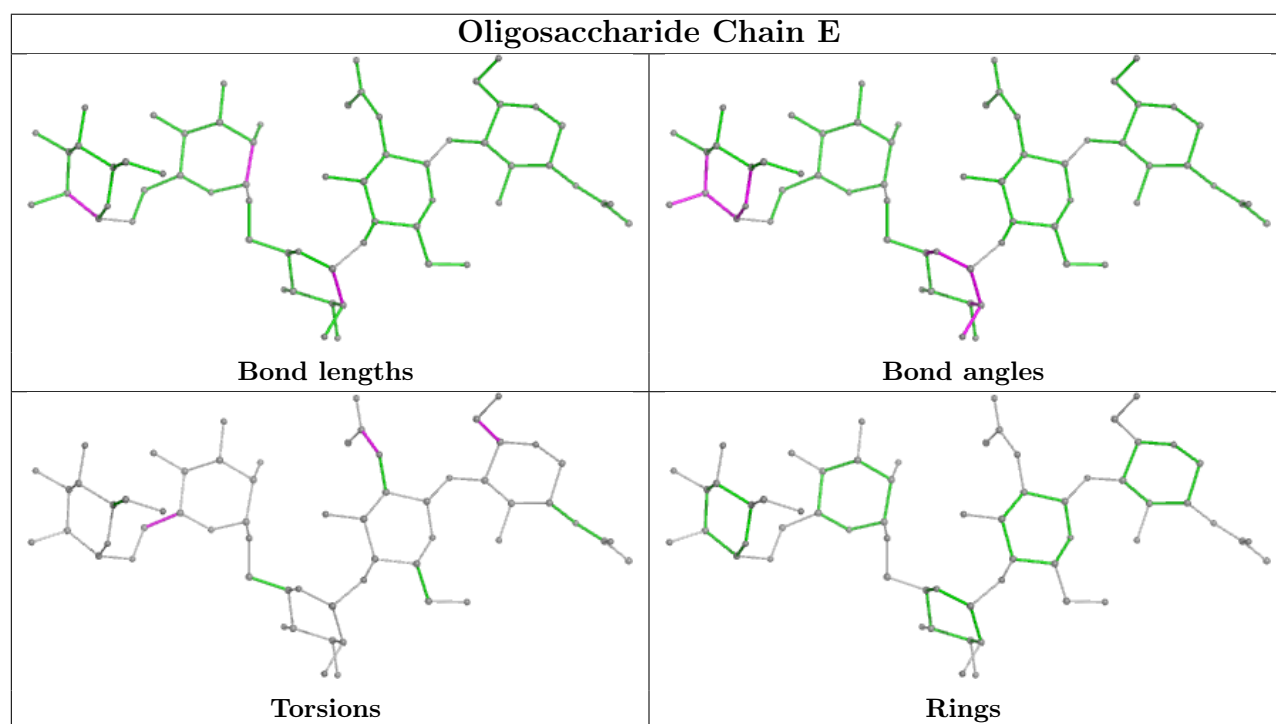
All (3) ring outliers are listed below:

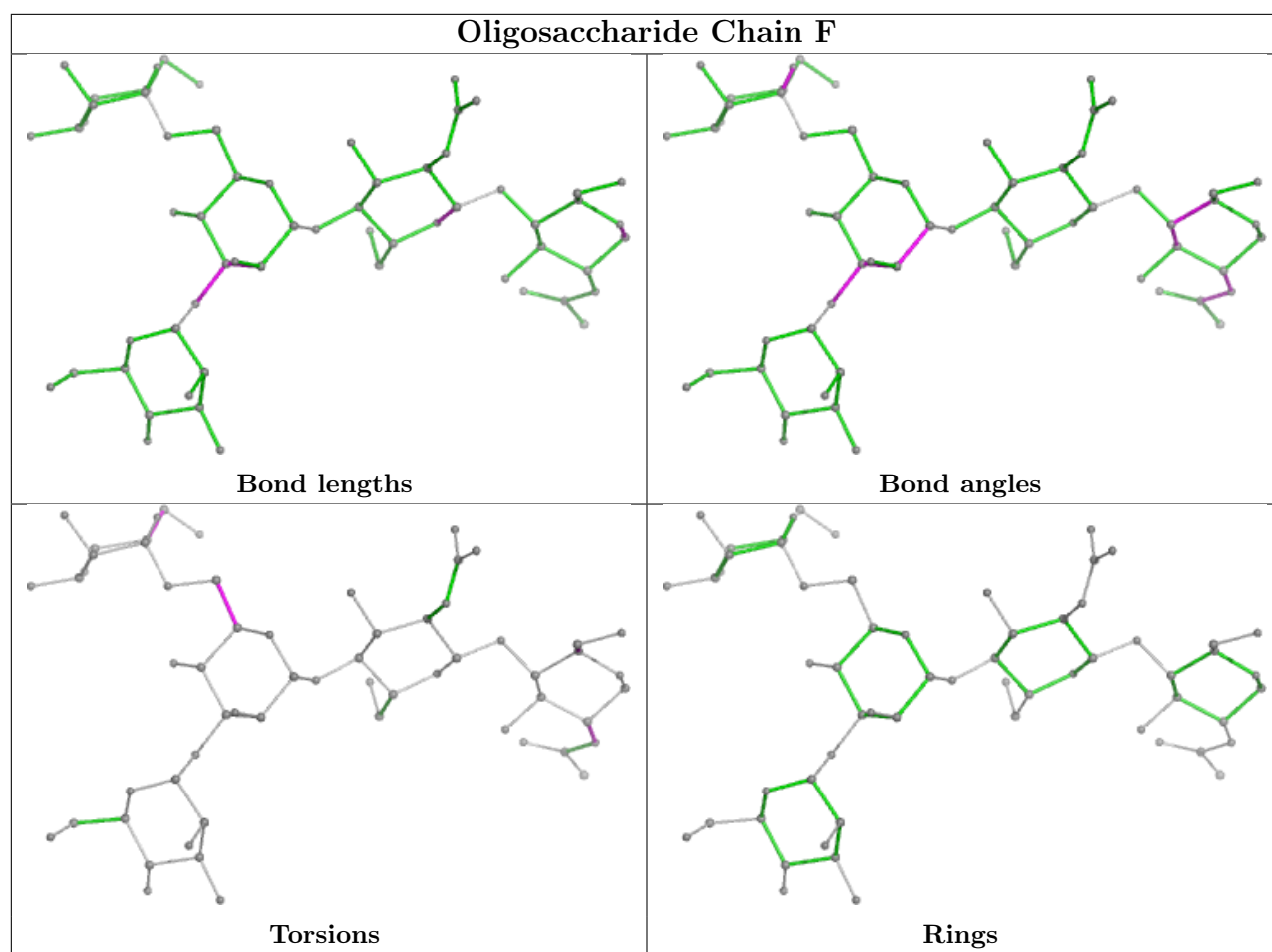
Mol	Chain	Res	Type	Atoms
10	P	3	MAN	C1-C2-C3-C4-C5-O5
3	S	5	MAN	C1-C2-C3-C4-C5-O5
9	N	6	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 16 short contacts:

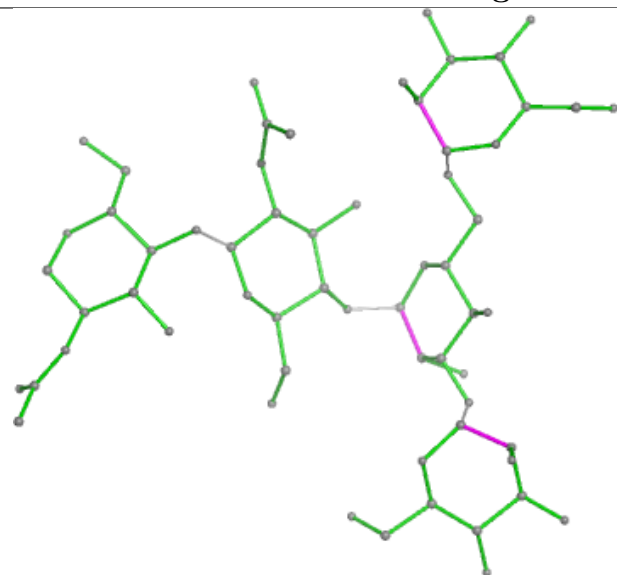
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	J	1	NAG	2	0
5	M	3	MAN	1	0
5	W	1	NAG	1	0
2	E	4	MAN	1	0
11	Q	4	FUC	1	0
13	T	1	NAG	1	0
5	M	4	MAN	1	0
2	E	5	MAN	1	0
9	N	4	MAN	1	0
10	P	1	NAG	1	0
3	O	1	NAG	1	0
11	Q	1	NAG	1	0
9	N	5	MAN	1	0
7	K	3	MAN	1	0
7	K	4	MAN	1	0
13	T	2	NAG	1	0
13	T	4	MAN	1	0
10	P	2	NAG	1	0
13	T	5	MAN	1	0
5	M	1	NAG	1	0
5	H	1	NAG	2	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.

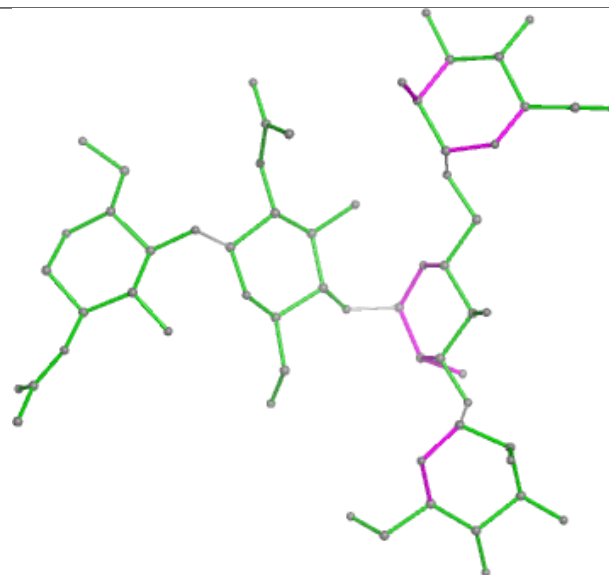




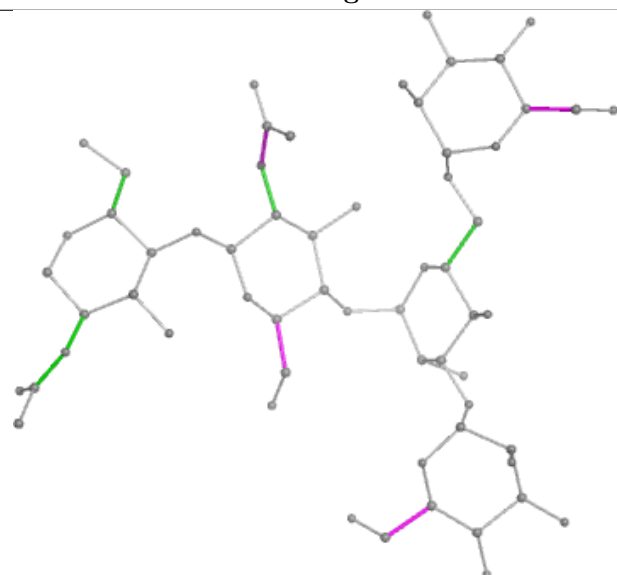
## Oligosaccharide Chain J



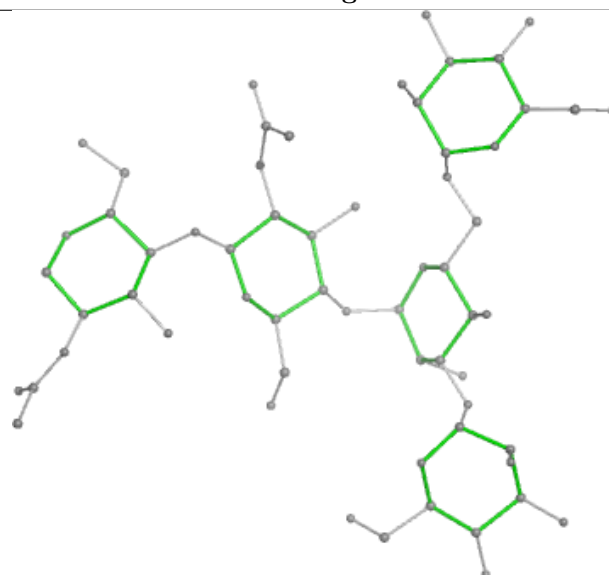
Bond lengths



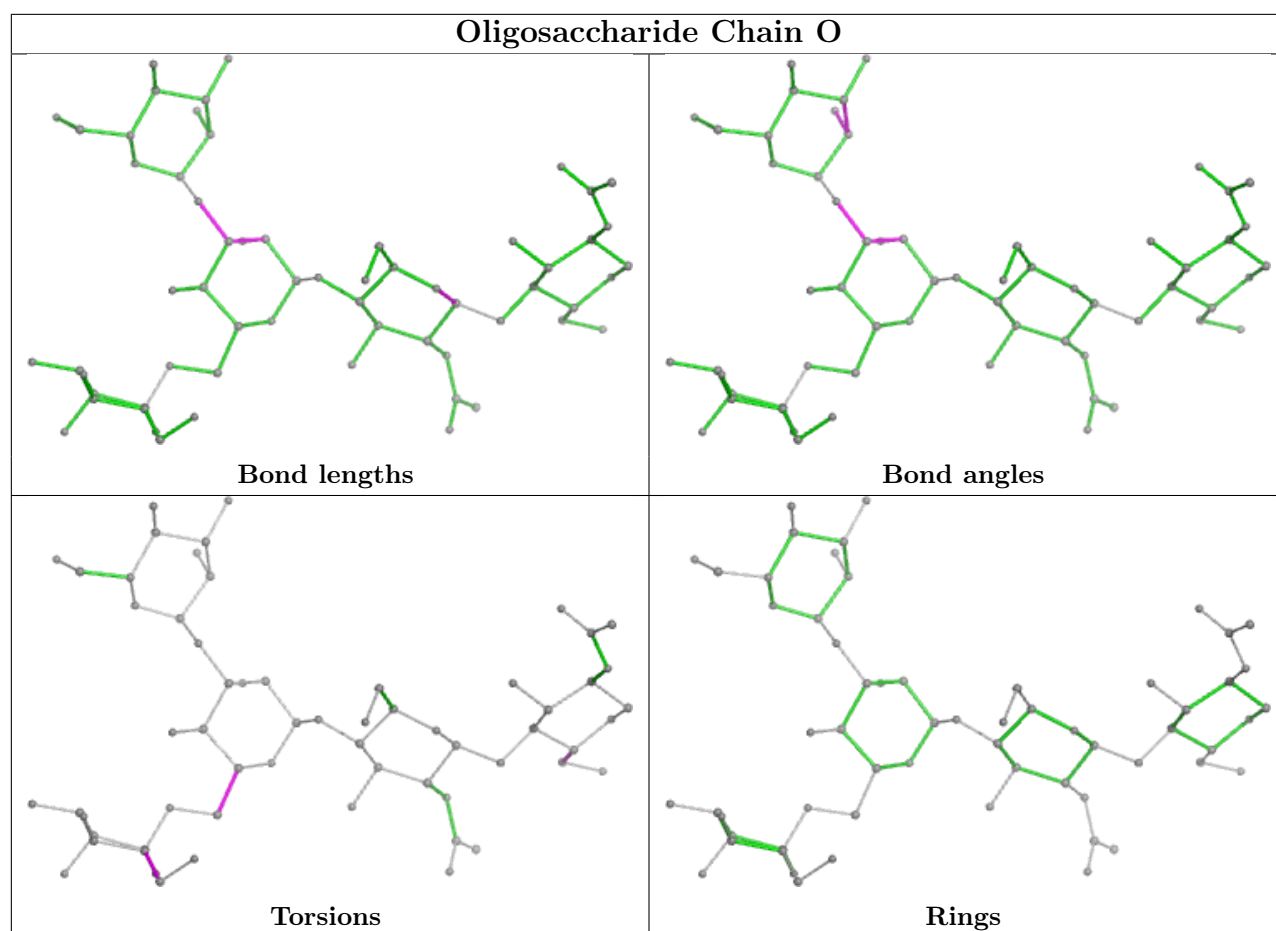
Bond angles

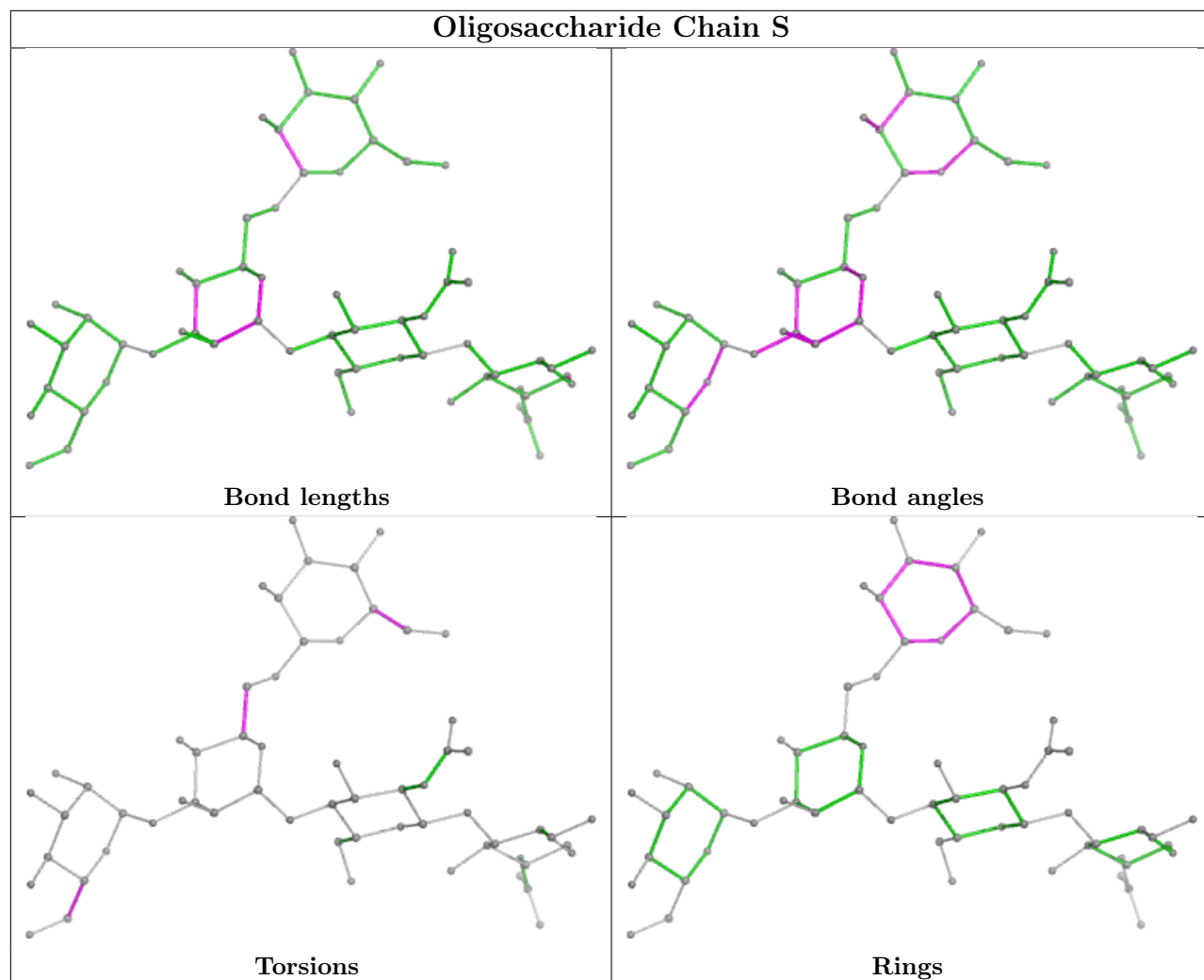


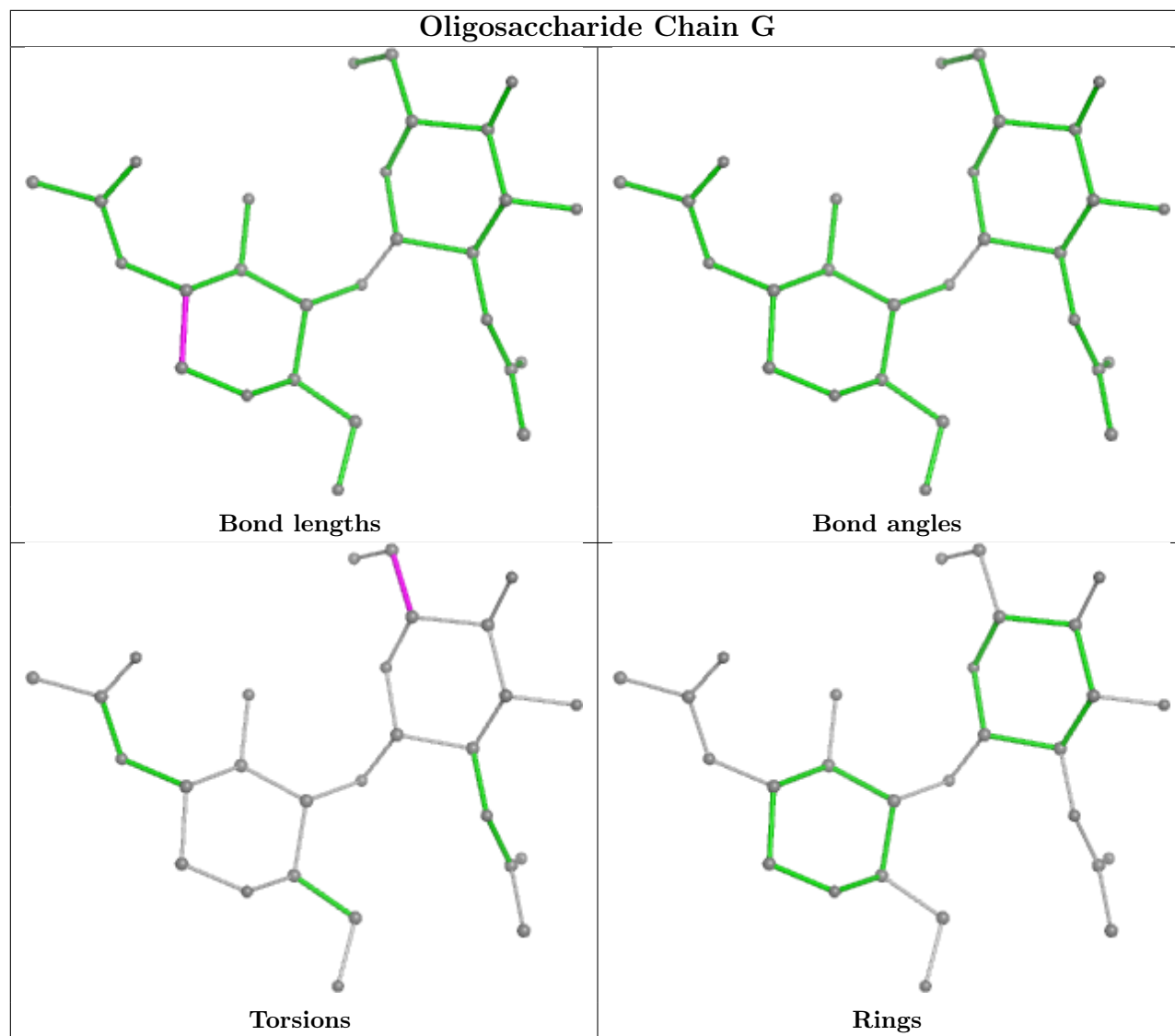
Torsions

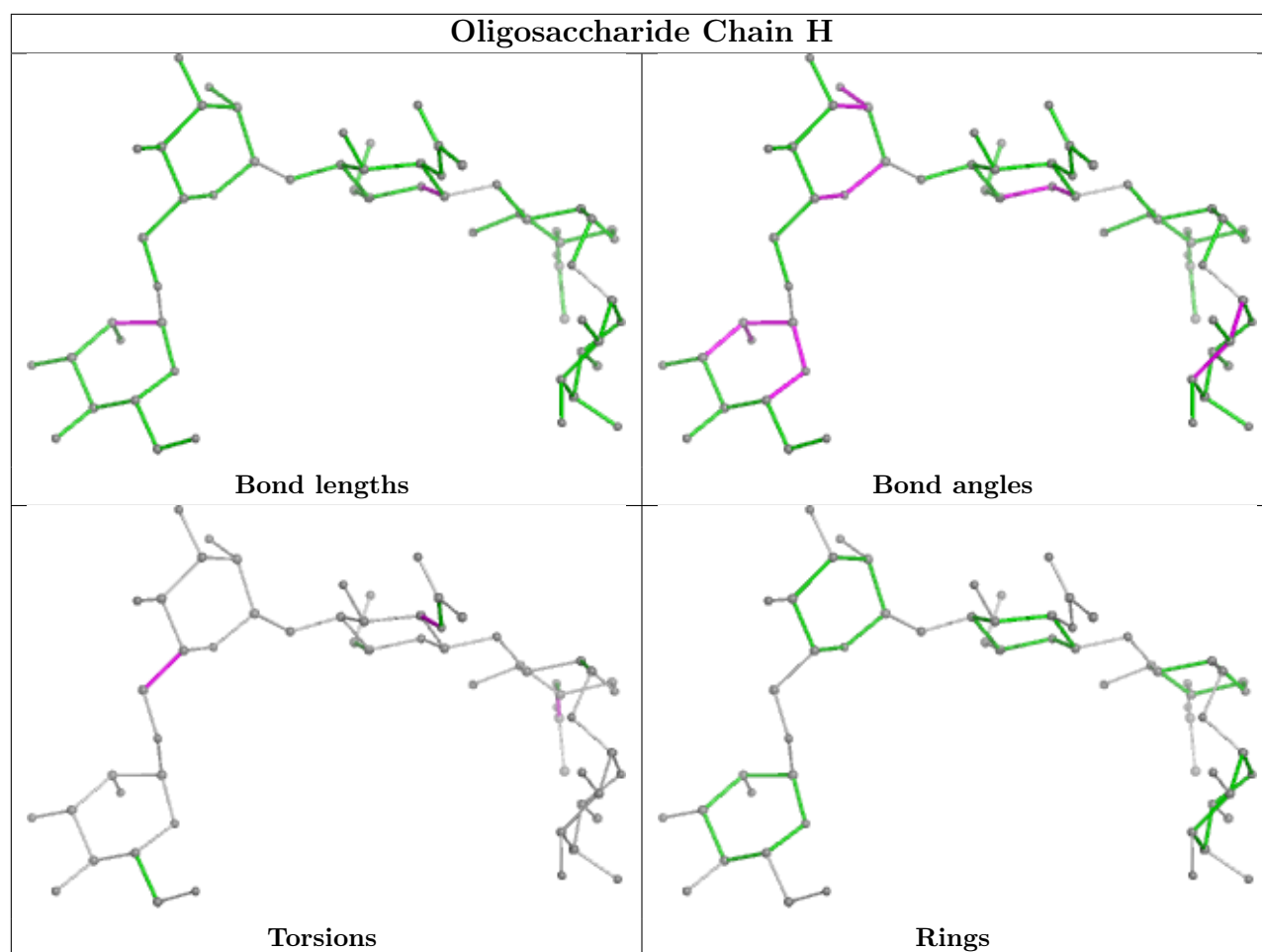


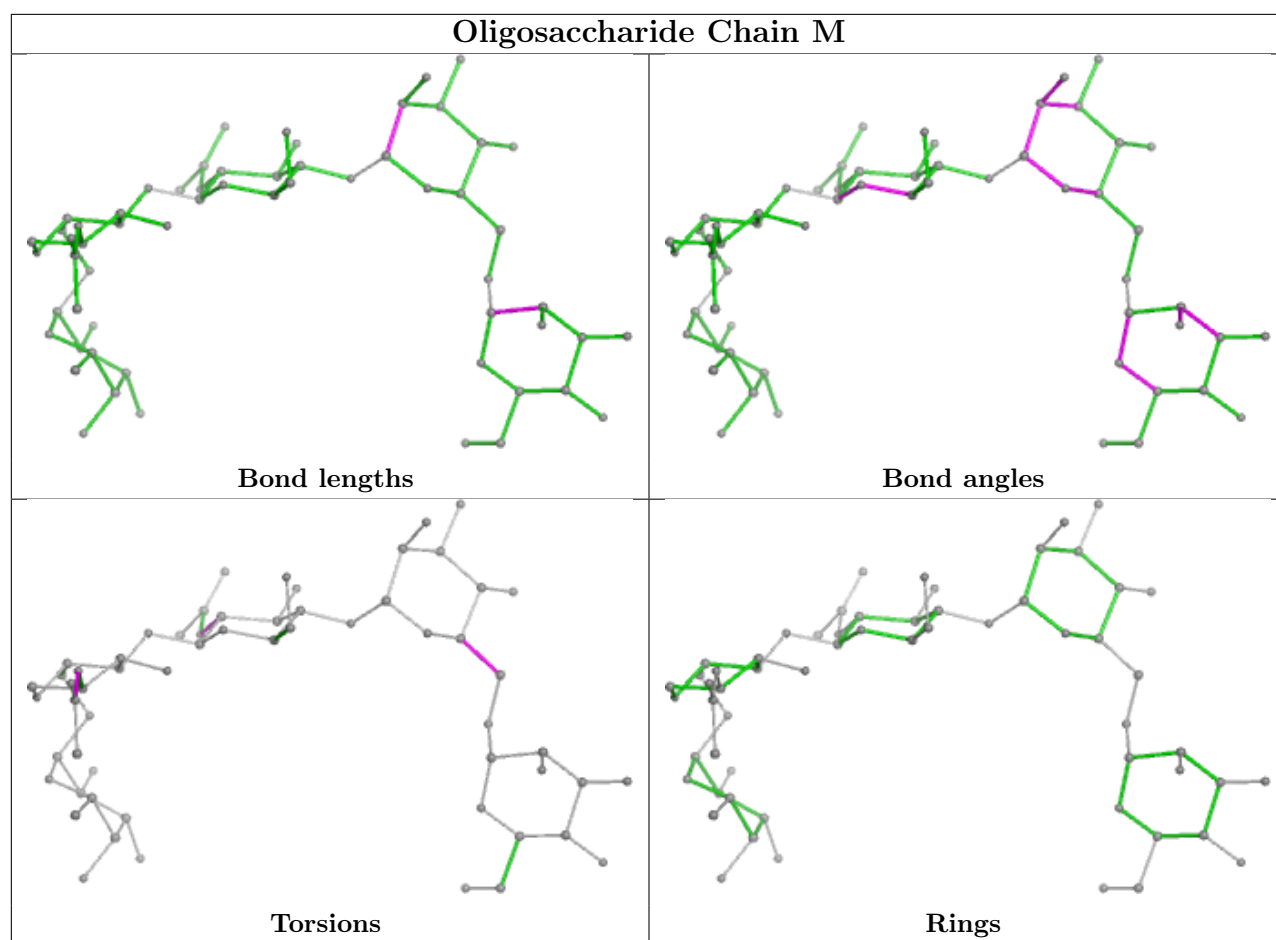
Rings

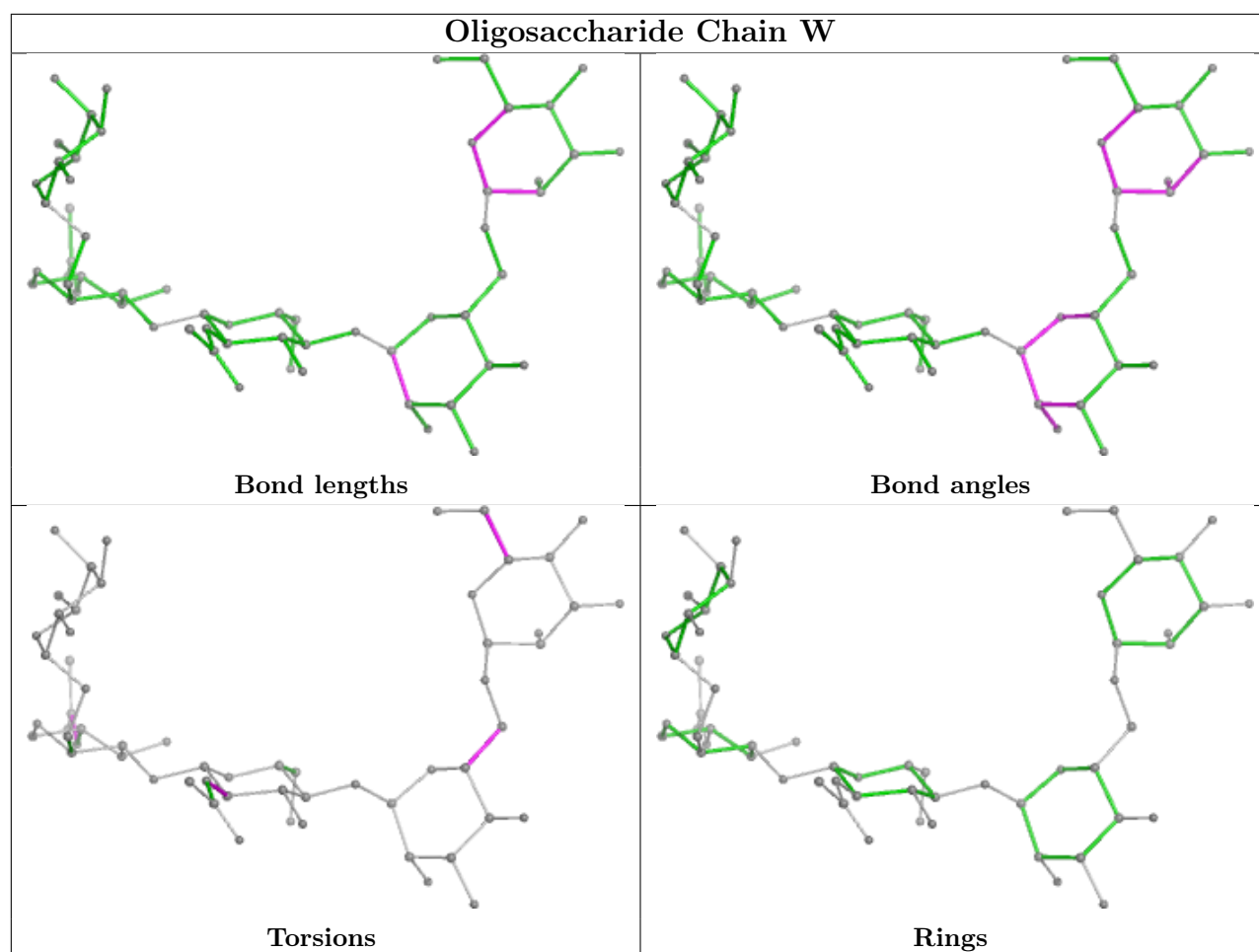


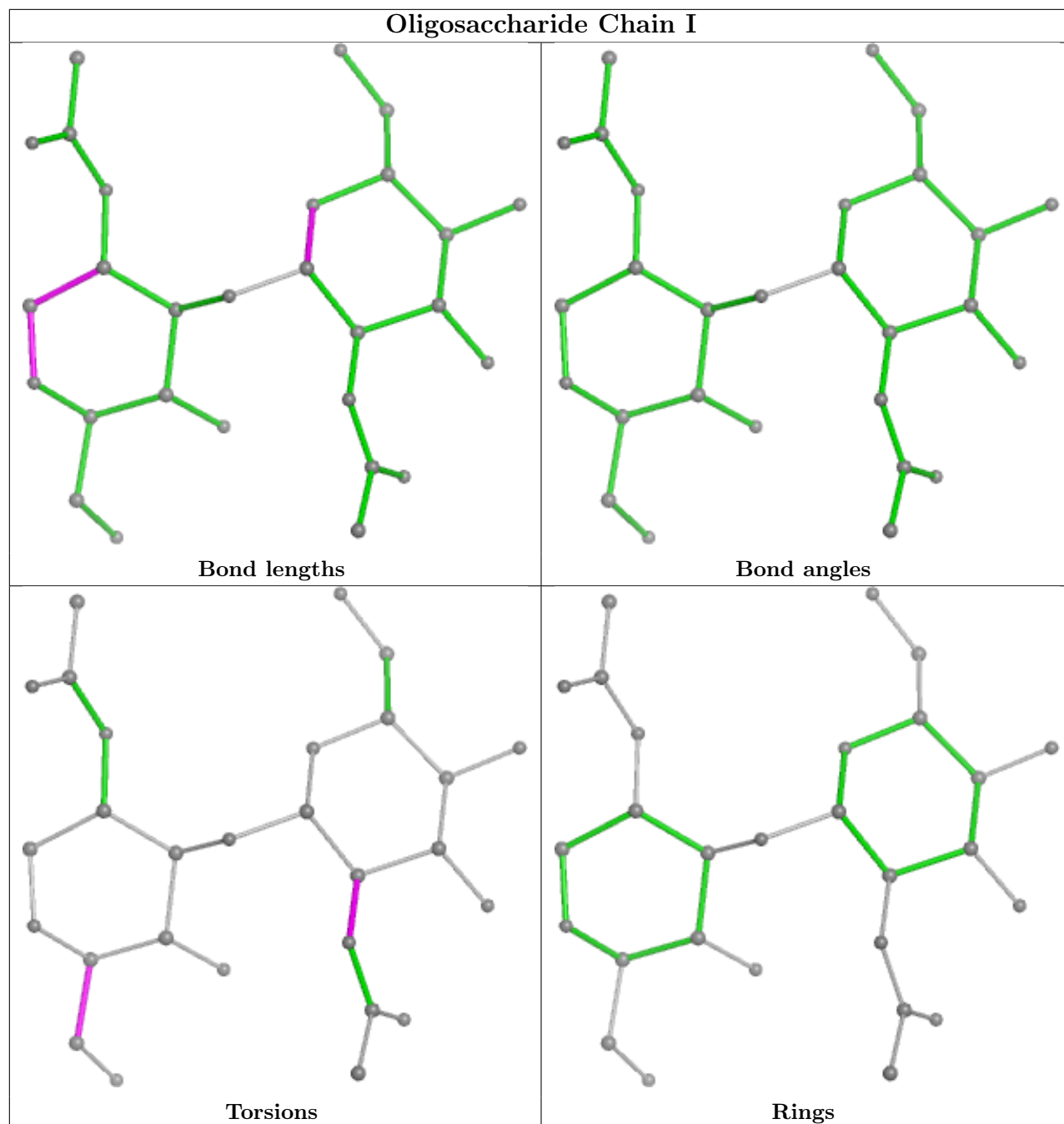




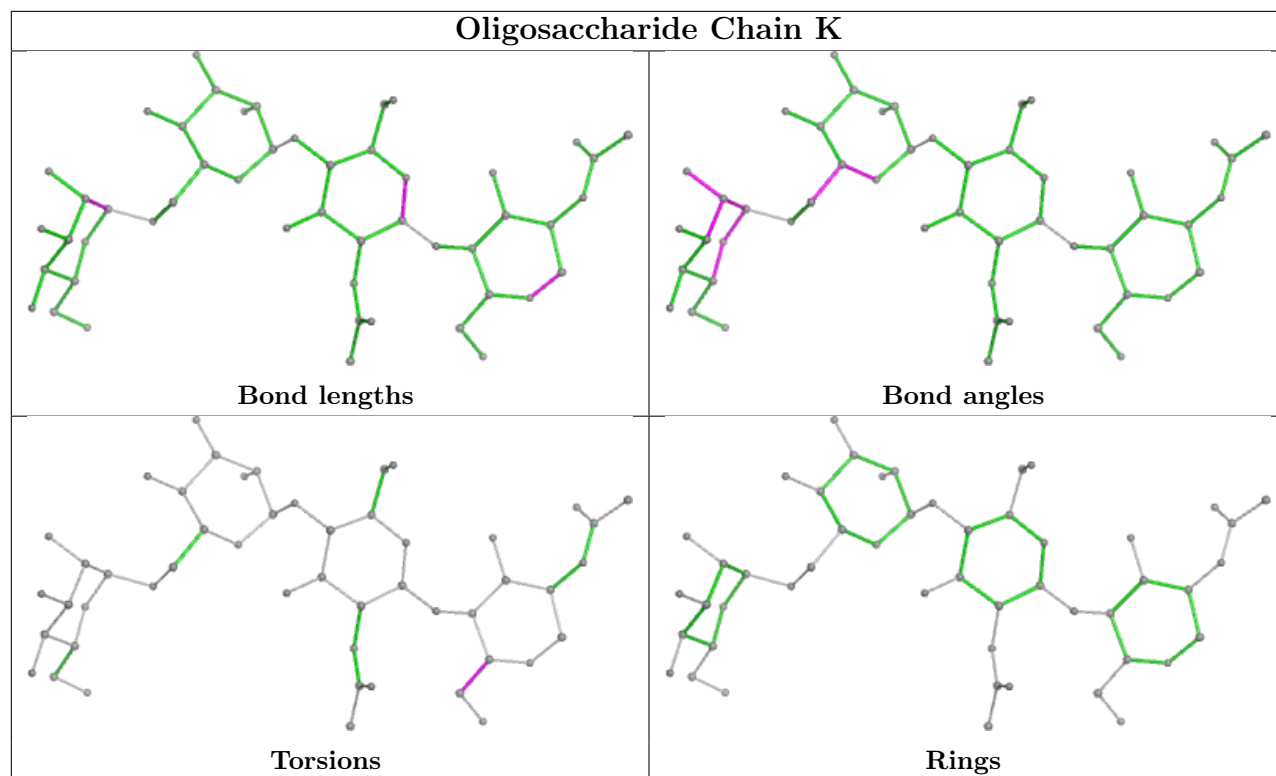




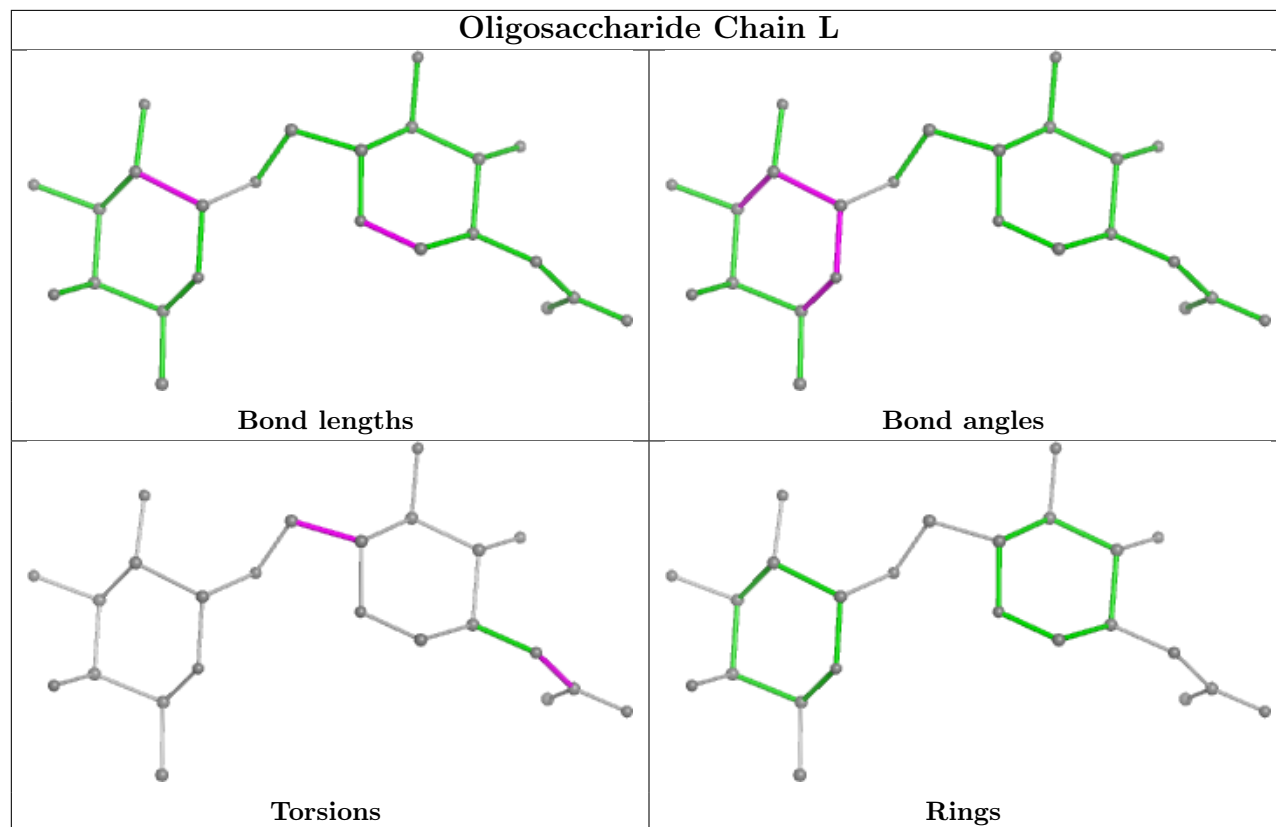


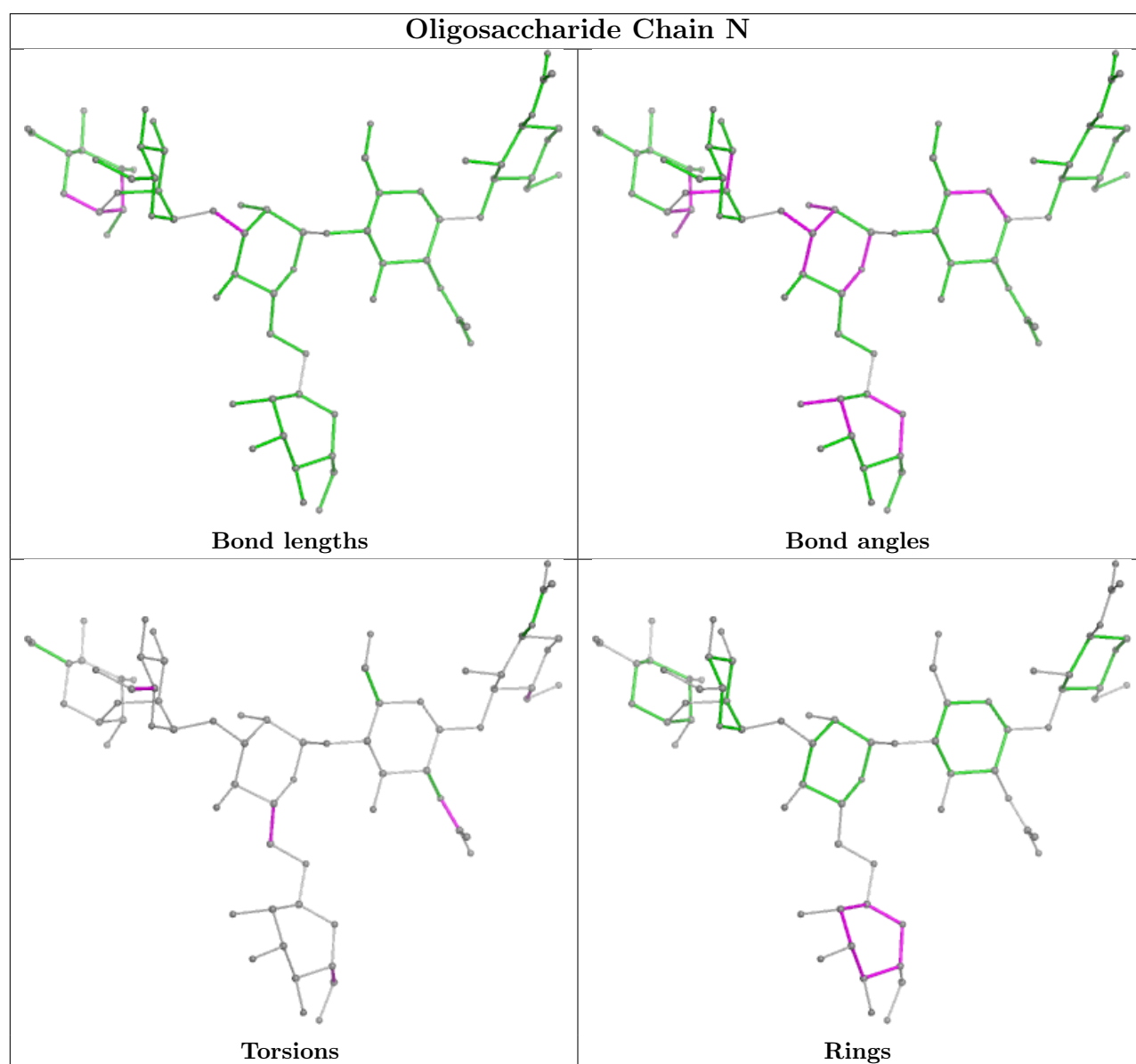
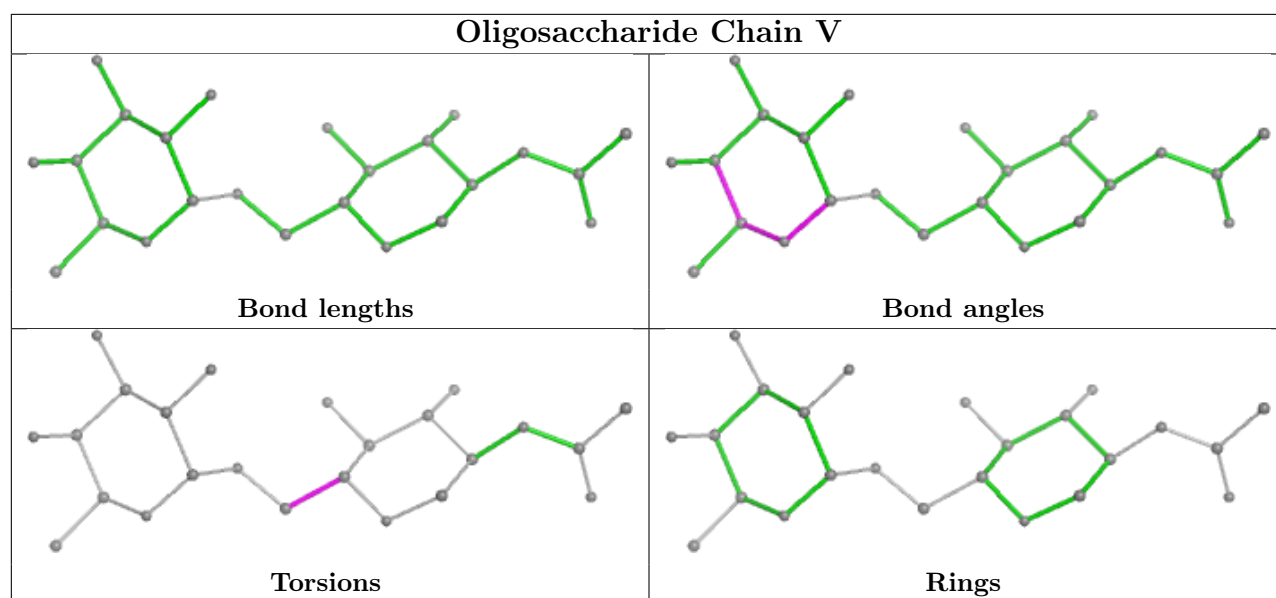


## Oligosaccharide Chain K

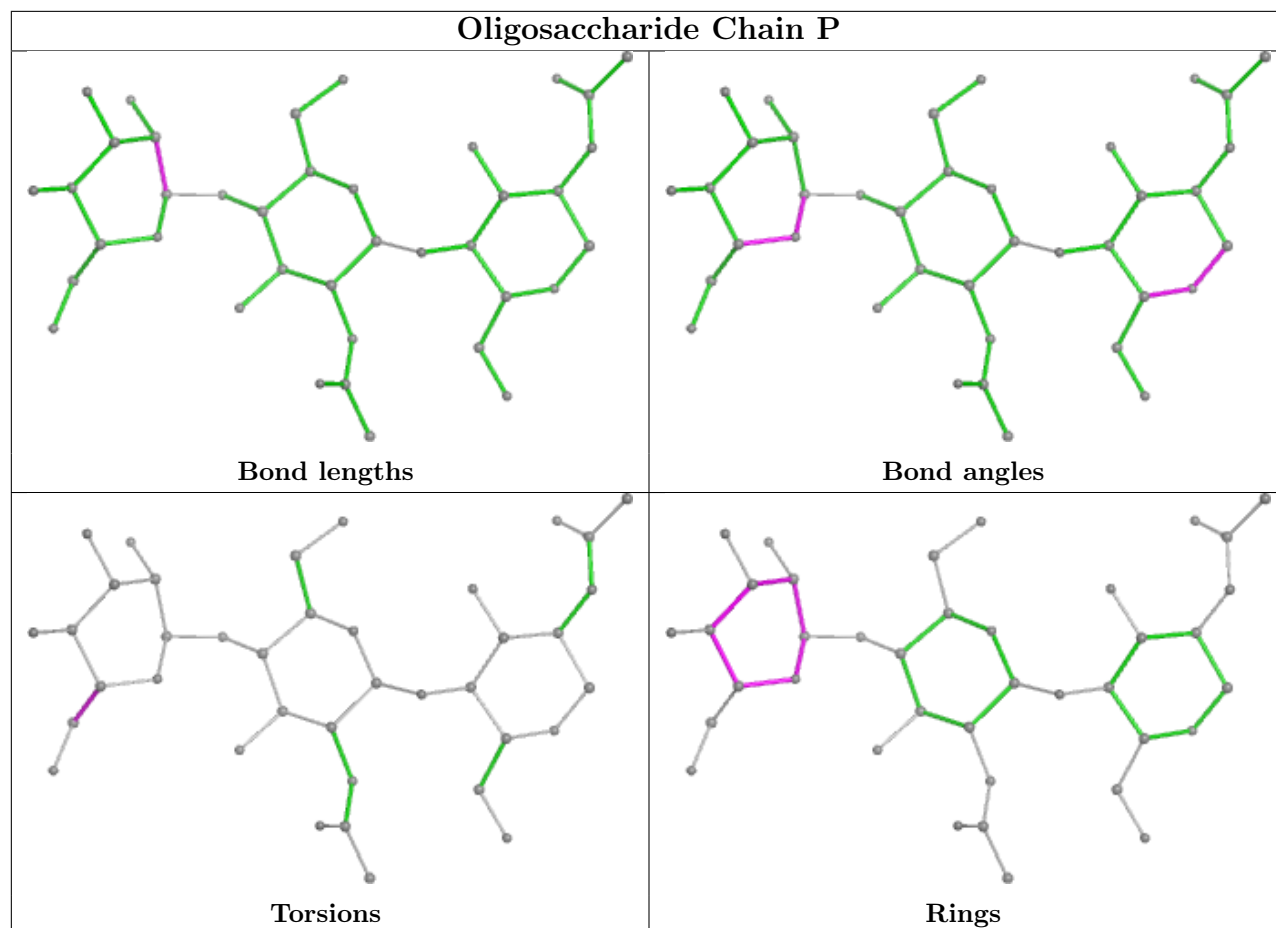


## Oligosaccharide Chain L

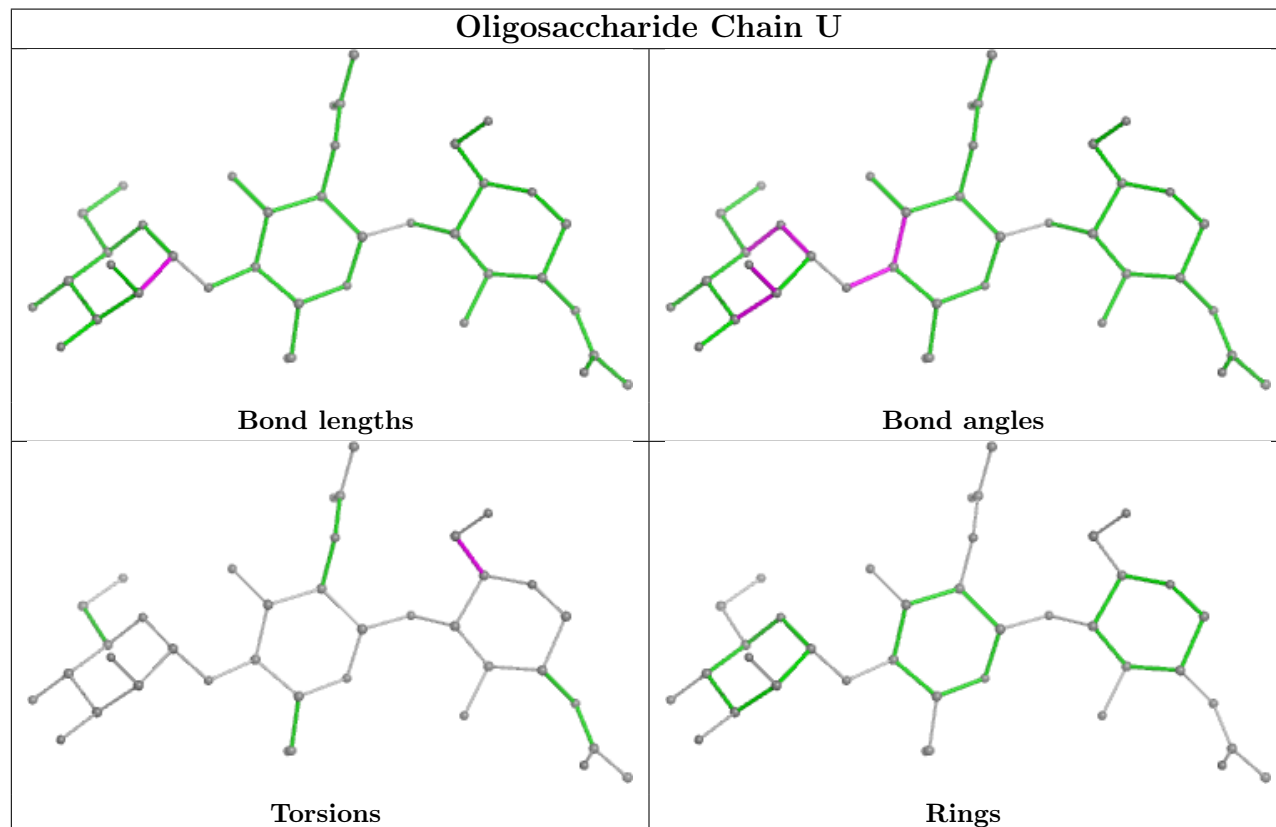


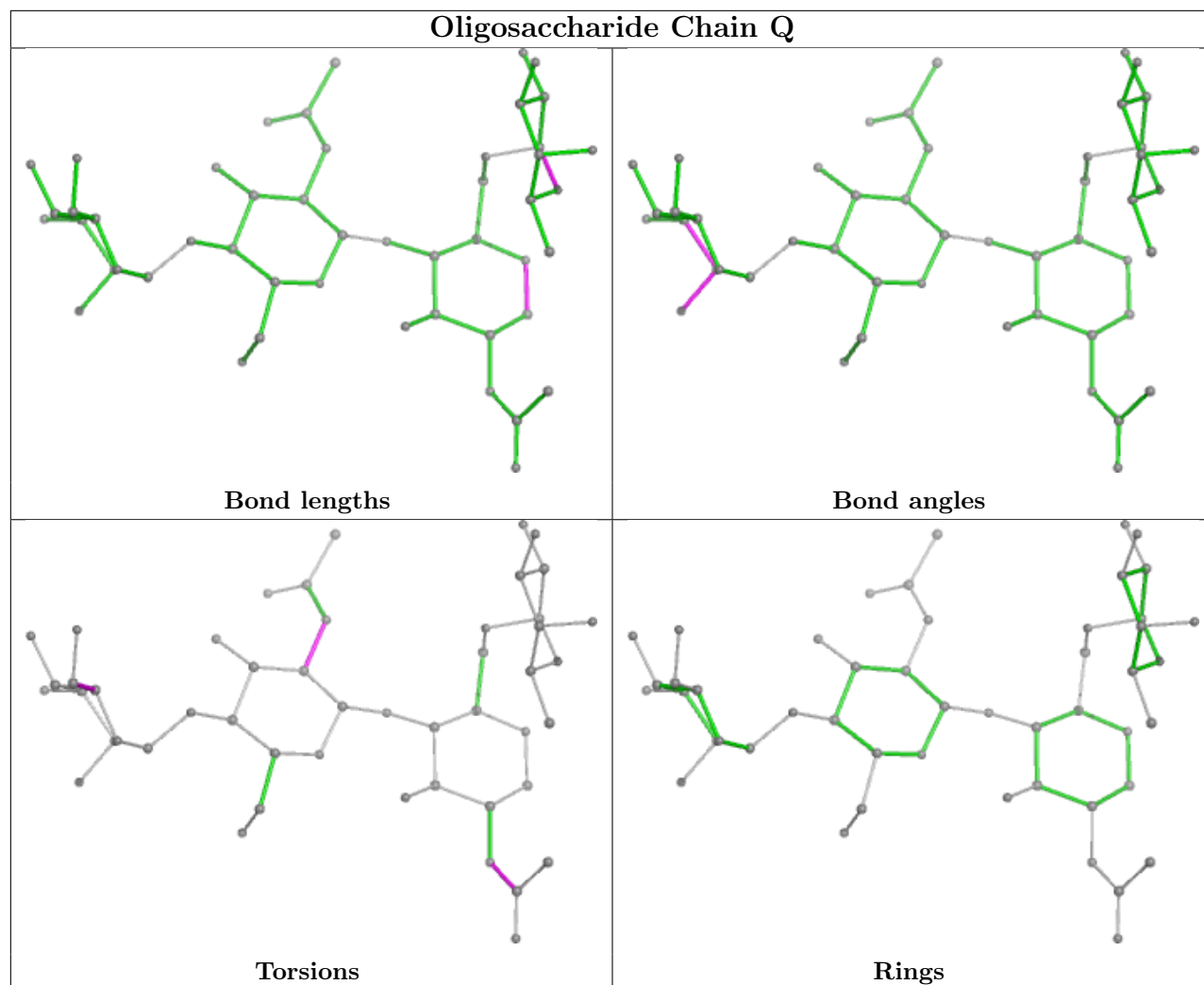


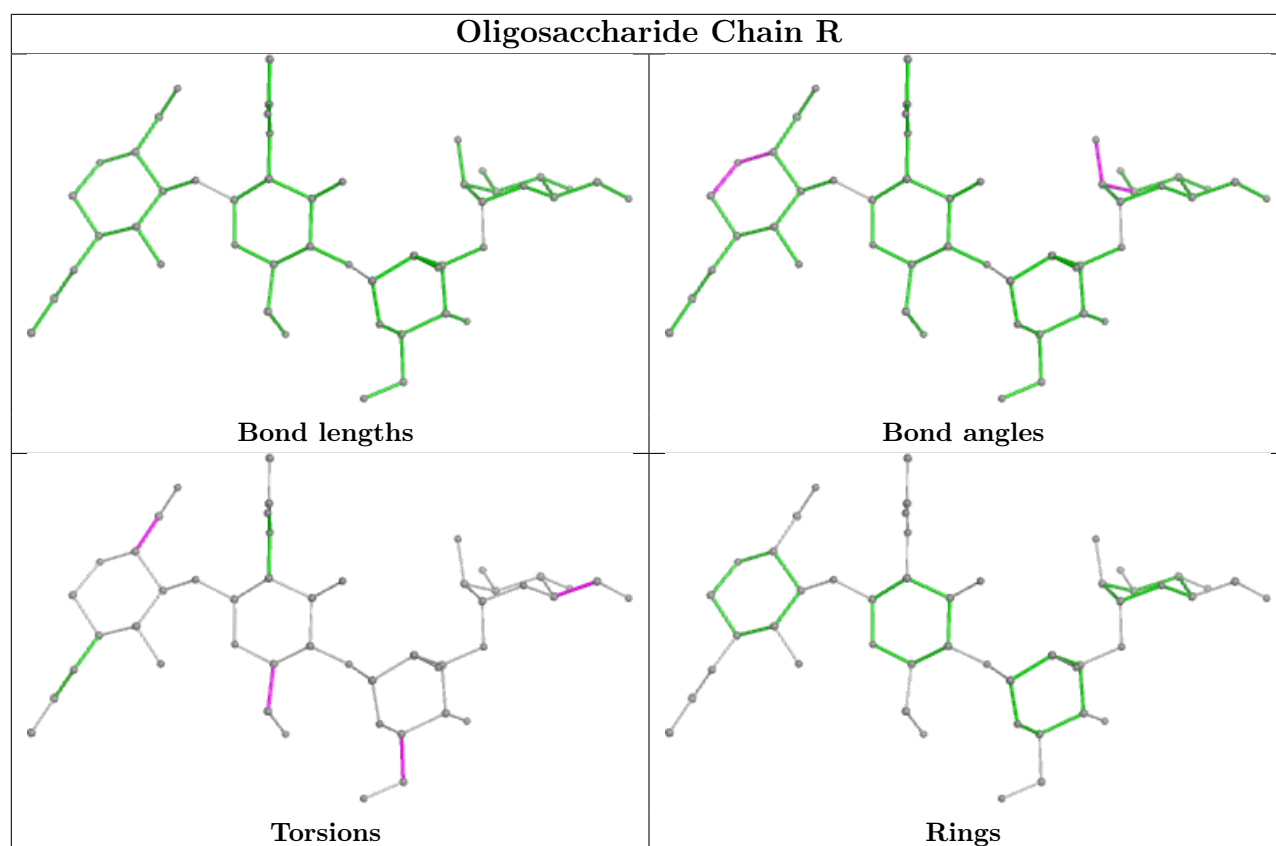
## Oligosaccharide Chain P

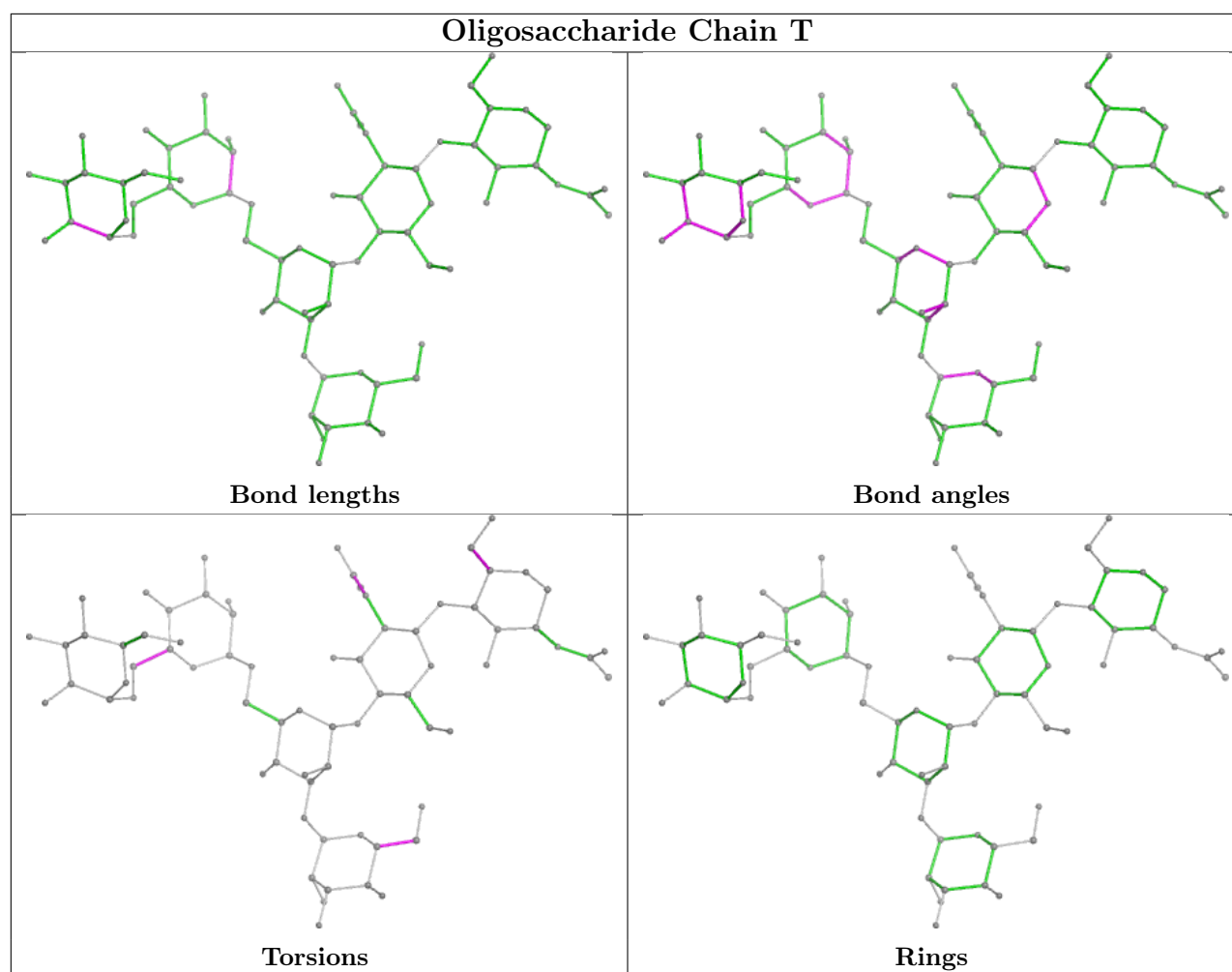


## Oligosaccharide Chain U









## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	$\# Z  > 2$
16	NAG	D	805	1	14,14,15	1.02	1 (7%)	17,19,21	0.89	1 (5%)
16	NAG	B	804	1	14,14,15	0.36	0	17,19,21	0.49	0
16	NAG	A	804	-	14,14,15	0.17	0	17,19,21	0.42	0
16	NAG	B	805	1	14,14,15	0.38	0	17,19,21	0.49	0
16	NAG	D	804	1	14,14,15	0.30	0	17,19,21	0.46	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
16	NAG	D	805	1	-	2/6/23/26	0/1/1/1
16	NAG	B	804	1	-	2/6/23/26	0/1/1/1
16	NAG	A	804	-	-	2/6/23/26	0/1/1/1
16	NAG	B	805	1	-	0/6/23/26	0/1/1/1
16	NAG	D	804	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	805	NAG	O5-C1	-3.36	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	805	NAG	C3-C4-C5	2.26	114.26	110.24

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	D	804	NAG	O5-C5-C6-O6
16	B	804	NAG	O5-C5-C6-O6
16	A	804	NAG	O5-C5-C6-O6
16	D	805	NAG	O5-C5-C6-O6
16	A	804	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	804	NAG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	714/737 (96%)	-1.51	0 100 100	103, 124, 141, 161	0
1	B	722/737 (97%)	-1.49	0 100 100	96, 125, 144, 174	0
1	C	712/737 (96%)	-1.51	0 100 100	105, 126, 144, 164	0
1	D	722/737 (97%)	-1.50	0 100 100	101, 126, 147, 191	0
All	All	2870/2948 (97%)	-1.50	0 100 100	96, 125, 144, 191	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	D	471	14/15	0.97	0.07	125,130,141,148	0
1	TPQ	C	471	14/15	0.98	0.04	126,131,141,146	0
1	TPQ	A	471	14/15	0.98	0.04	124,130,135,145	0
1	TPQ	B	471	14/15	0.99	0.06	121,126,133,146	0

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	MAN	T	6	11/12	0.91	0.04	191,215,219,220	0
12	MAN	R	4	11/12	0.93	0.03	195,204,211,212	0
3	MAN	J	5	11/12	0.93	0.04	177,192,196,202	0
3	NAG	S	2	14/15	0.94	0.03	160,183,189,189	0
10	MAN	P	3	11/12	0.94	0.03	146,176,187,189	0
3	MAN	J	4	11/12	0.94	0.04	208,219,226,227	0
3	MAN	J	3	11/12	0.94	0.03	201,208,216,224	0
5	MAN	H	4	11/12	0.95	0.04	118,165,183,184	0
5	FUC	H	5	10/11	0.95	0.06	149,161,164,165	0
5	MAN	M	3	11/12	0.95	0.04	182,198,207,208	0
5	MAN	W	3	11/12	0.95	0.03	174,184,191,192	0
9	MAN	N	6	11/12	0.95	0.04	194,213,220,223	0
10	NAG	P	2	14/15	0.95	0.03	156,187,191,192	0
3	MAN	F	3	11/12	0.95	0.04	188,192,195,198	0
10	MAN	U	3	11/12	0.95	0.04	168,175,180,180	0
11	NAG	Q	2	14/15	0.95	0.05	185,191,208,218	0
12	MAN	R	3	11/12	0.95	0.03	214,217,219,220	0
3	NAG	S	1	14/15	0.95	0.04	145,156,173,181	0
3	MAN	F	5	11/12	0.95	0.05	177,185,192,194	0
5	FUC	W	5	10/11	0.96	0.05	146,152,155,166	0
6	NAG	I	2	14/15	0.96	0.03	186,194,199,199	0
7	MAN	K	4	11/12	0.96	0.04	138,149,153,154	0
8	NAG	V	1	14/15	0.96	0.03	138,162,172,173	0
9	MAN	N	4	11/12	0.96	0.03	145,172,189,190	0
4	NAG	G	2	14/15	0.96	0.03	163,196,204,204	0
5	NAG	H	1	14/15	0.96	0.04	138,158,167,169	0
3	MAN	O	4	11/12	0.96	0.06	167,176,187,188	0
3	MAN	O	5	11/12	0.96	0.03	160,183,192,193	0
2	NAG	E	2	14/15	0.96	0.04	164,176,181,186	0
11	FUC	Q	4	10/11	0.96	0.10	156,172,177,180	0
12	NAG	R	2	14/15	0.96	0.02	188,206,210,214	0
5	MAN	M	4	11/12	0.96	0.05	154,177,198,202	0
5	NAG	W	2	14/15	0.96	0.03	161,180,191,195	0
13	MAN	T	4	11/12	0.96	0.03	185,206,218,234	0
13	MAN	T	5	11/12	0.96	0.03	202,213,218,220	0
3	NAG	O	2	14/15	0.96	0.04	147,164,172,178	0
5	NAG	M	1	14/15	0.97	0.04	119,160,173,185	0
3	MAN	F	4	11/12	0.97	0.04	158,162,174,179	0
10	NAG	P	1	14/15	0.97	0.03	141,169,180,184	0
2	MAN	E	5	11/12	0.97	0.04	207,219,223,223	0
5	FUC	M	5	10/11	0.97	0.06	145,151,156,157	0
10	NAG	U	2	14/15	0.97	0.03	142,152,167,172	0
5	NAG	W	1	14/15	0.97	0.03	126,149,164,177	0

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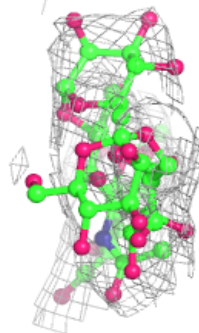
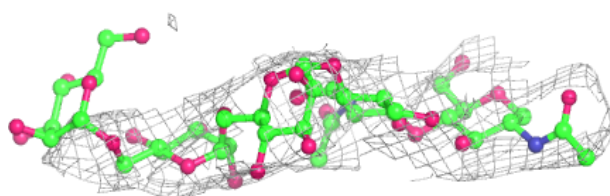
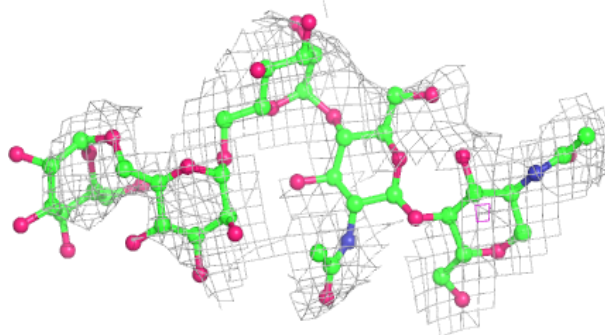
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	NAG	Q	1	14/15	0.97	0.04	137,166,181,185	0
3	MAN	S	3	11/12	0.97	0.02	174,183,191,191	0
3	NAG	O	1	14/15	0.97	0.04	125,148,157,161	0
5	MAN	W	4	11/12	0.97	0.03	143,166,178,181	0
3	NAG	J	1	14/15	0.97	0.04	134,147,160,167	0
5	NAG	H	2	14/15	0.97	0.04	138,171,174,174	0
3	NAG	J	2	14/15	0.97	0.04	173,187,198,203	0
8	NAG	L	1	14/15	0.97	0.03	153,165,172,173	0
2	MAN	E	3	11/12	0.97	0.03	183,191,201,207	0
9	MAN	N	5	11/12	0.98	0.03	157,164,171,175	0
3	MAN	S	4	11/12	0.98	0.04	162,192,201,212	0
3	MAN	S	5	11/12	0.98	0.02	166,181,185,190	0
5	NAG	M	2	14/15	0.98	0.03	169,192,207,208	0
6	NAG	I	1	14/15	0.98	0.03	143,181,188,192	0
4	NAG	G	1	14/15	0.98	0.02	136,158,184,185	0
7	NAG	K	2	14/15	0.98	0.03	146,162,172,174	0
7	MAN	K	3	11/12	0.98	0.03	156,168,174,174	0
3	NAG	F	2	14/15	0.98	0.03	166,175,181,190	0
11	MAN	Q	3	11/12	0.98	0.03	153,175,192,193	0
2	MAN	E	4	11/12	0.98	0.03	192,206,221,225	0
12	NAG	R	1	14/15	0.98	0.02	156,186,201,205	0
8	FUC	L	2	10/11	0.98	0.02	123,131,146,148	0
3	MAN	O	3	11/12	0.98	0.03	180,183,190,190	0
8	FUC	V	2	10/11	0.98	0.03	138,155,160,160	0
13	NAG	T	2	14/15	0.98	0.03	165,185,201,206	0
9	NAG	N	1	14/15	0.98	0.04	107,138,152,160	0
9	NAG	N	2	14/15	0.98	0.04	165,179,187,189	0
2	NAG	E	1	14/15	0.98	0.03	109,136,155,156	0
10	NAG	U	1	14/15	0.99	0.04	137,146,151,152	0
13	NAG	T	1	14/15	0.99	0.03	124,138,152,155	0
7	NAG	K	1	14/15	0.99	0.04	131,153,160,162	0
13	MAN	T	3	11/12	0.99	0.02	203,211,225,229	0
9	MAN	N	3	11/12	0.99	0.02	187,191,202,207	0
3	NAG	F	1	14/15	0.99	0.04	144,151,158,171	0
5	MAN	H	3	11/12	0.99	0.03	160,170,177,178	0

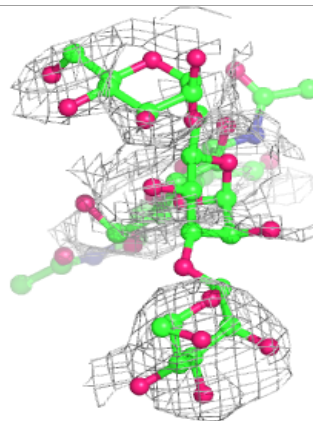
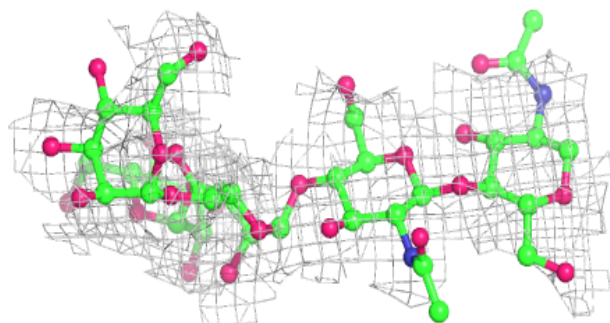
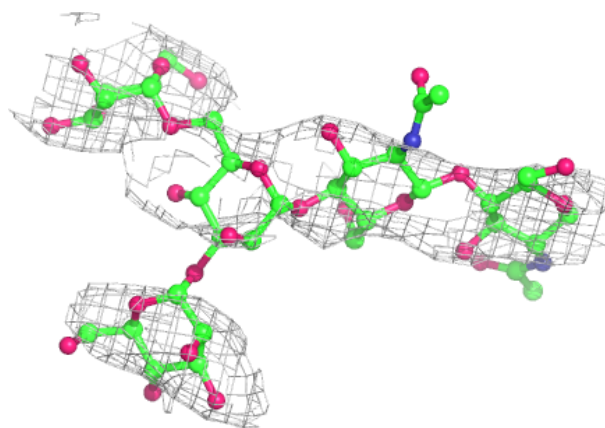
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

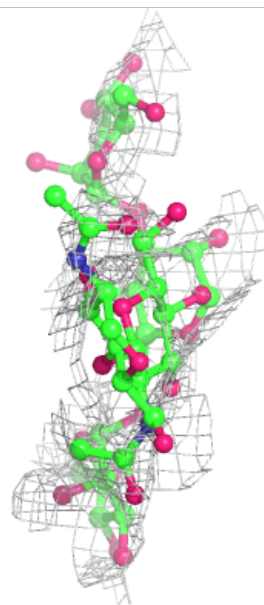
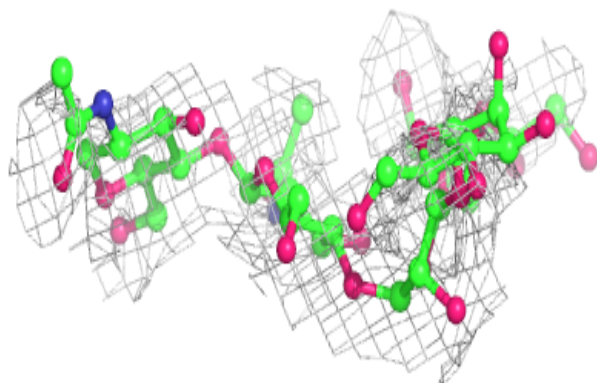
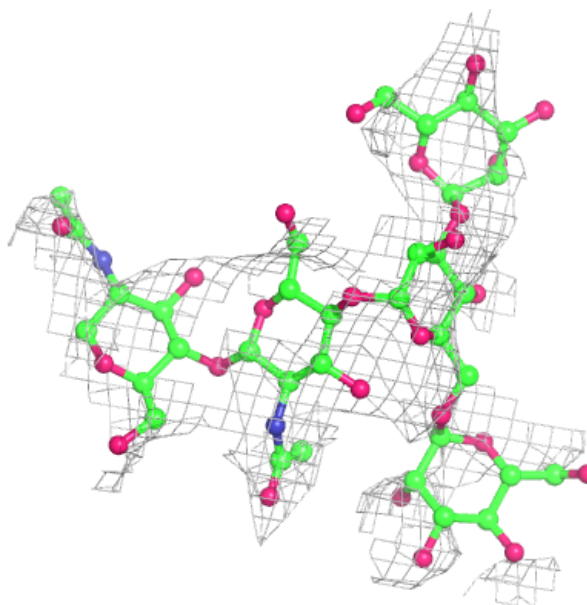
**Electron density around Chain F:**

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



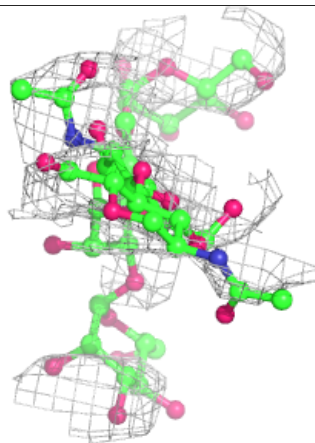
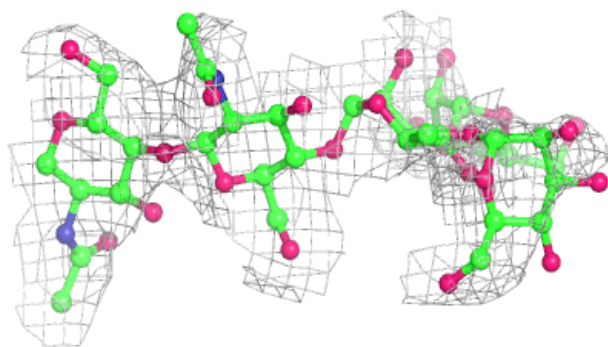
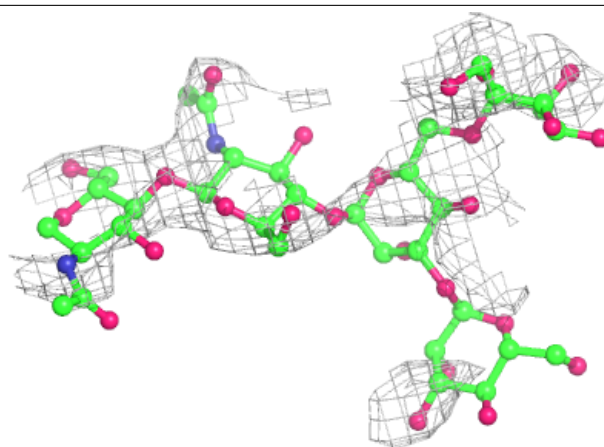
**Electron density around Chain J:**

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



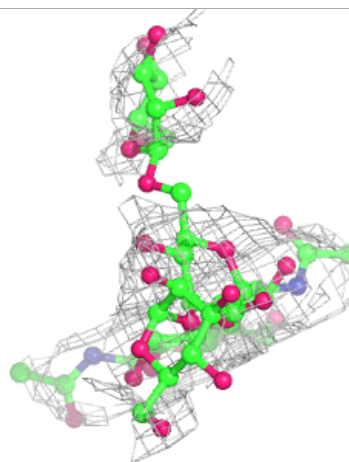
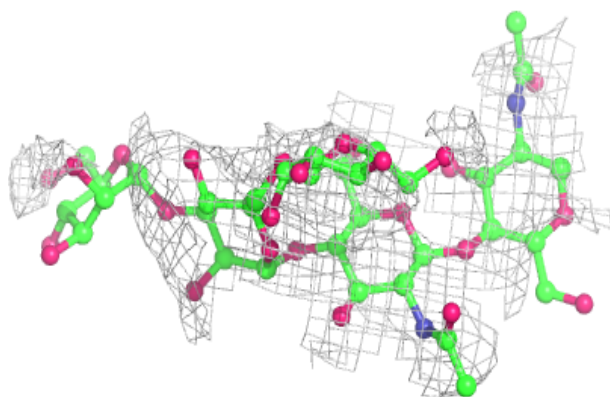
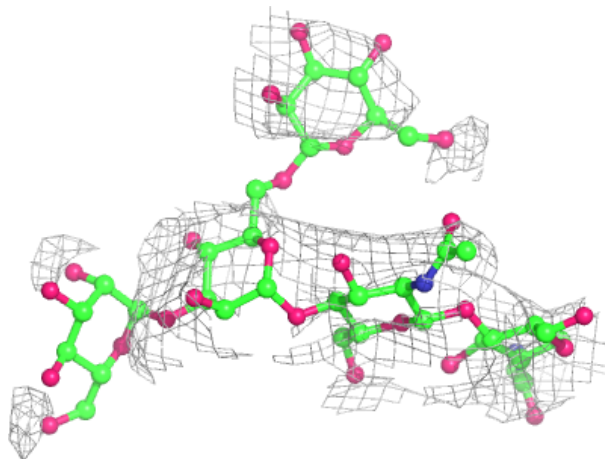
**Electron density around Chain O:**

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



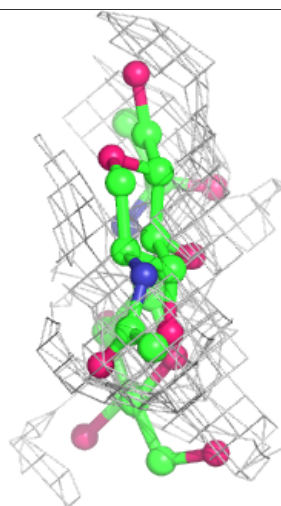
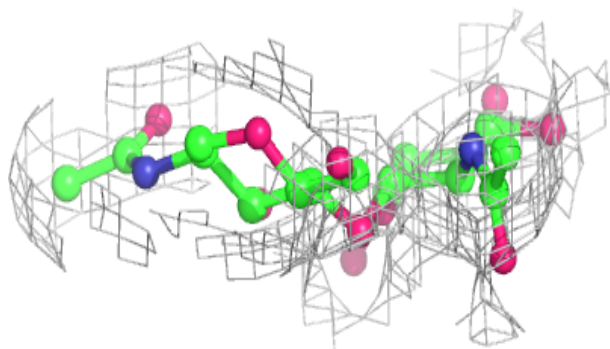
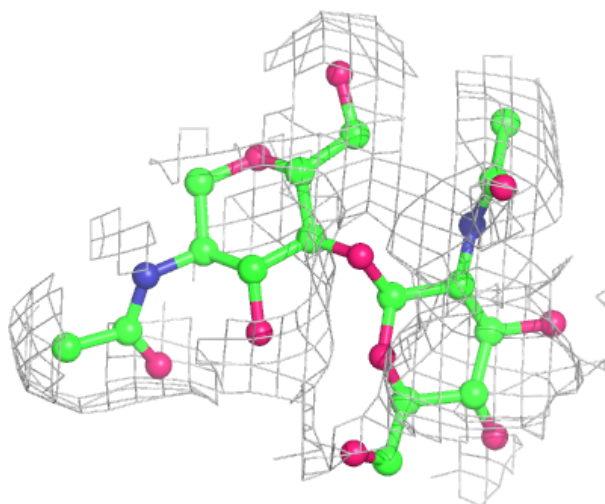
**Electron density around Chain S:**

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



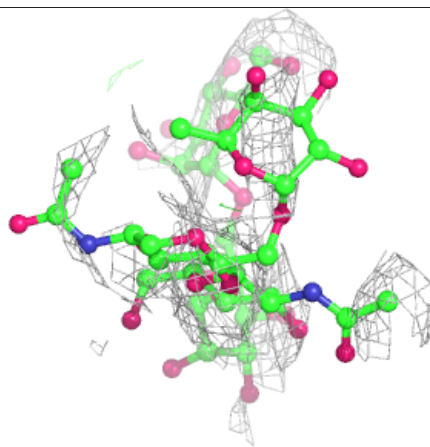
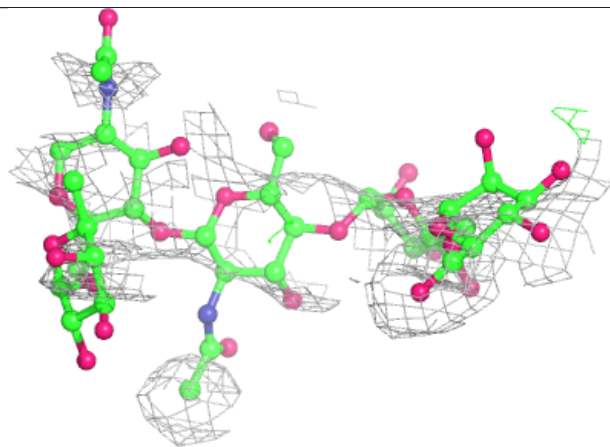
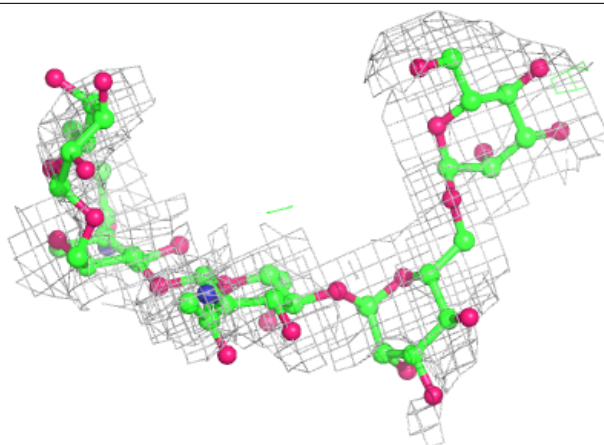
**Electron density around Chain G:**

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



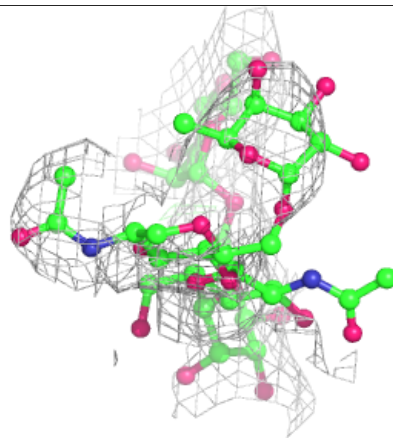
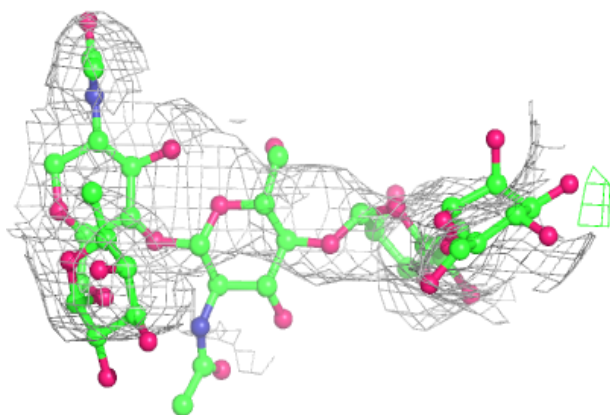
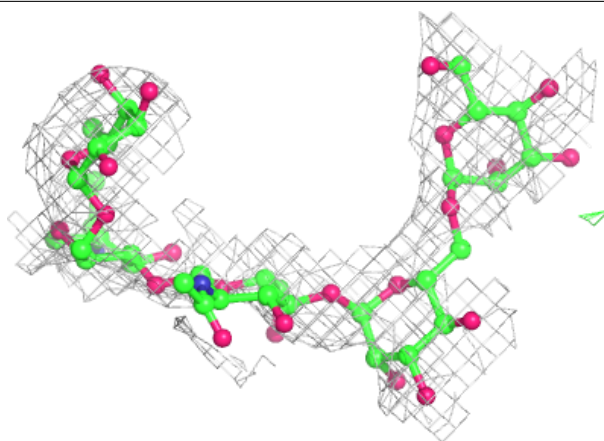
**Electron density around Chain H:**

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



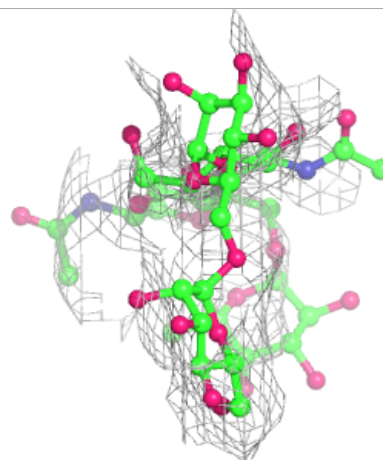
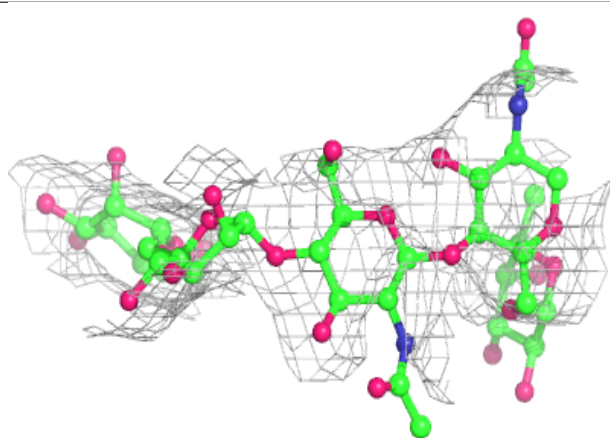
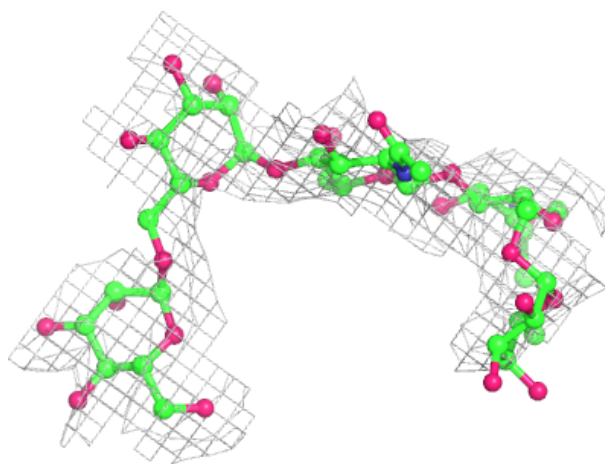
**Electron density around Chain M:**

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



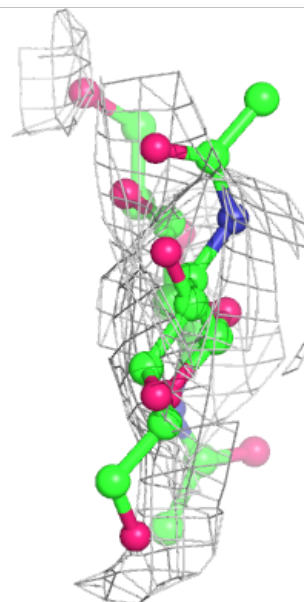
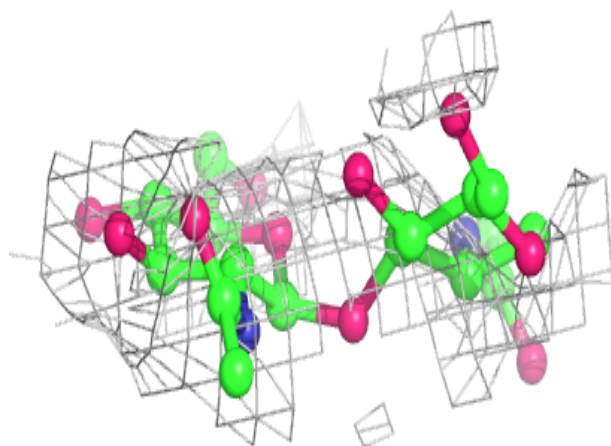
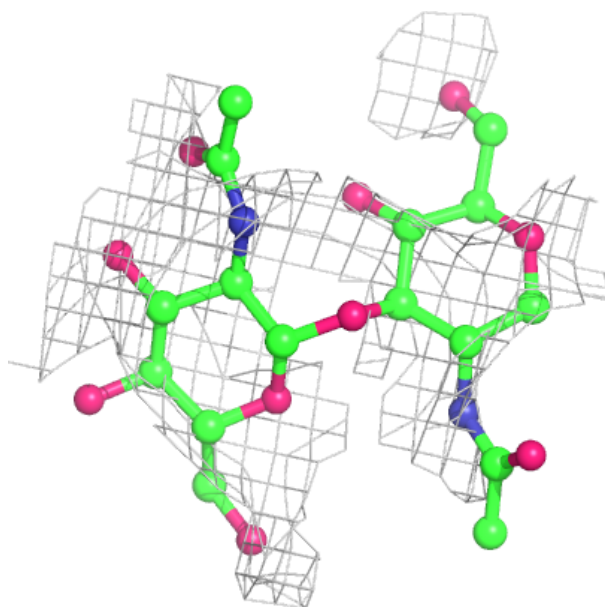
**Electron density around Chain W:**

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



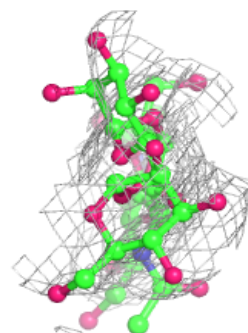
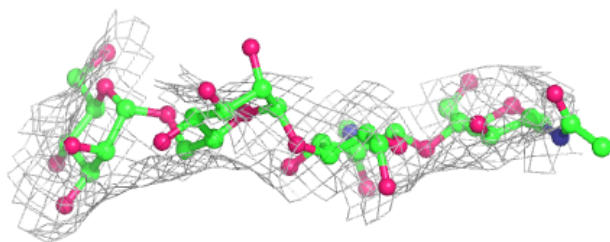
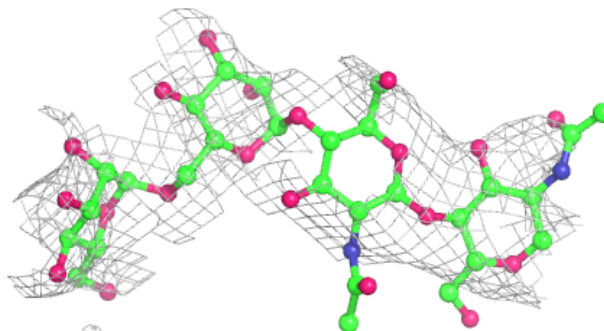
**Electron density around Chain I:**

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

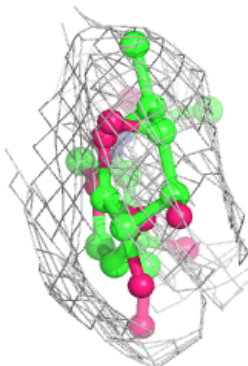
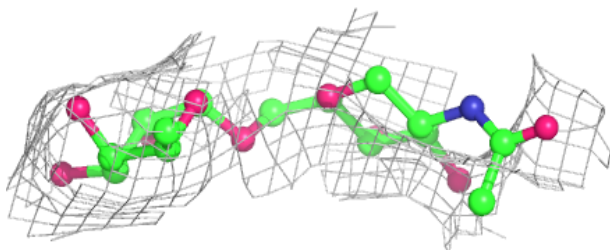
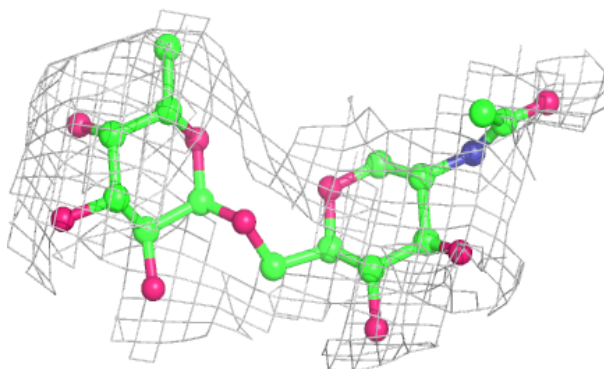


**Electron density around Chain K:**

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

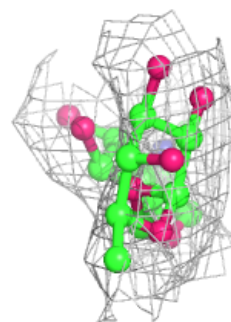
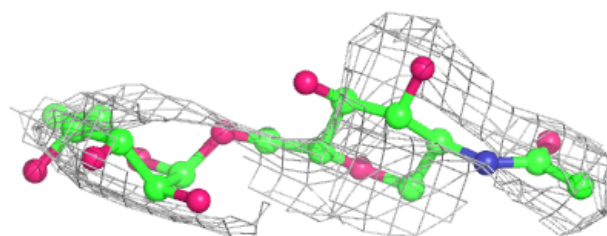
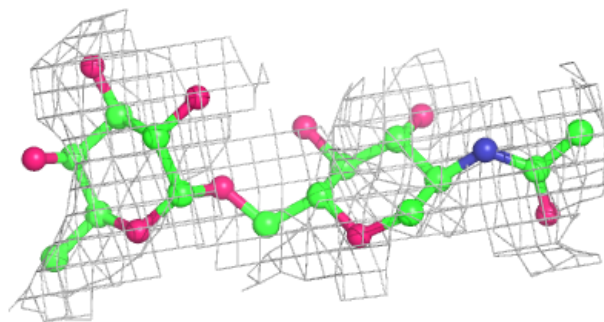
**Electron density around Chain L:**

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



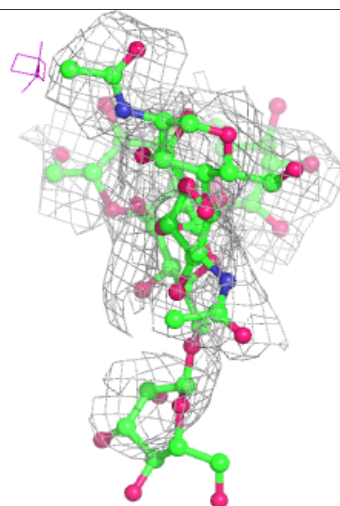
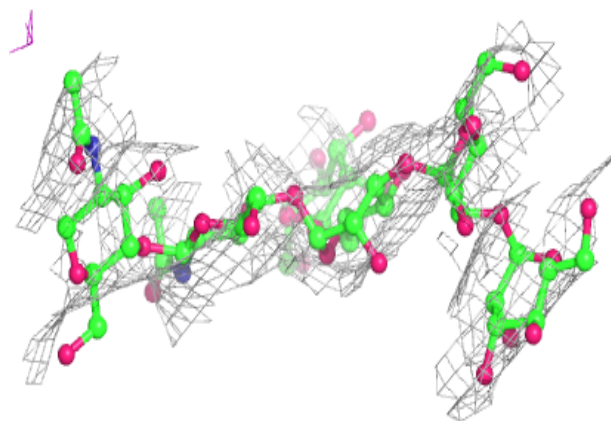
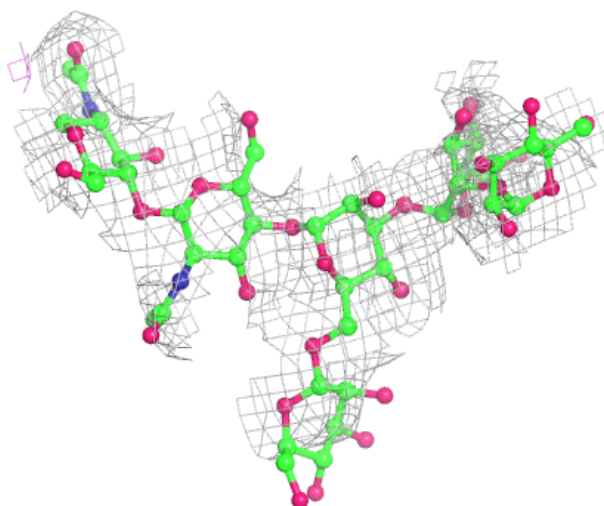
**Electron density around Chain V:**

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



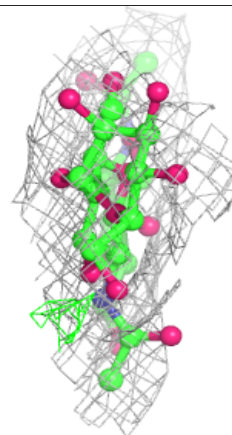
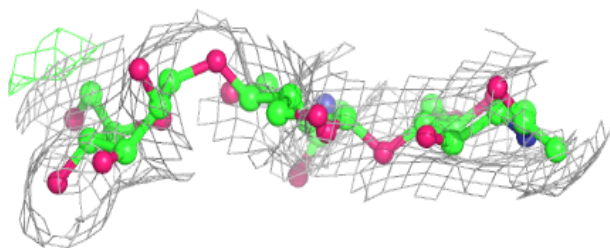
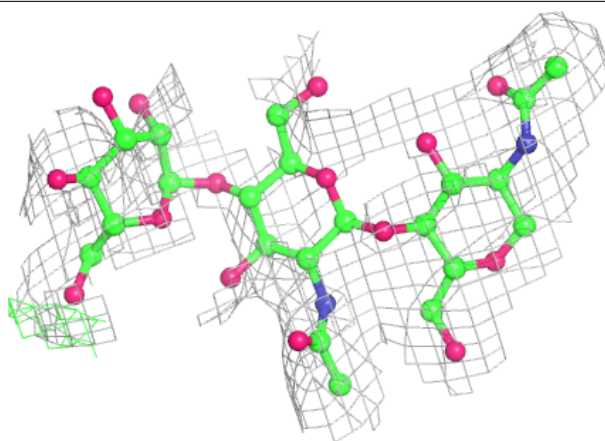
**Electron density around Chain N:**

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



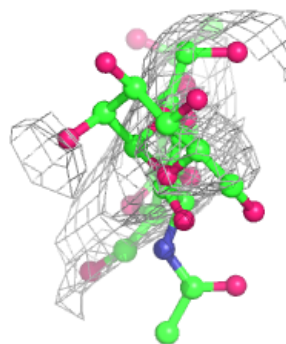
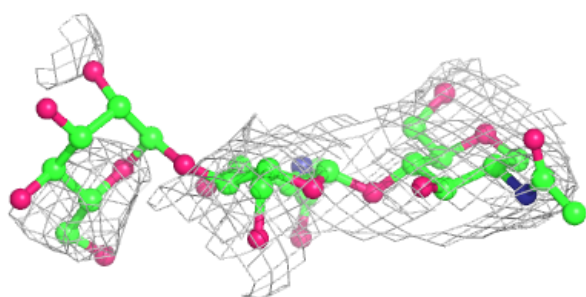
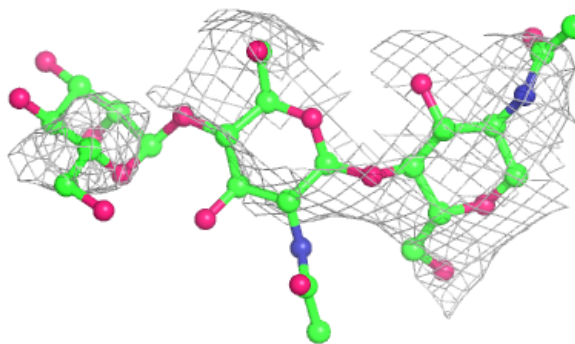
**Electron density around Chain P:**

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

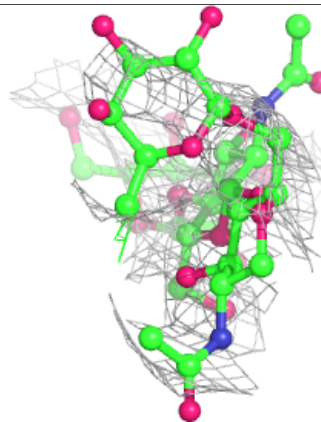
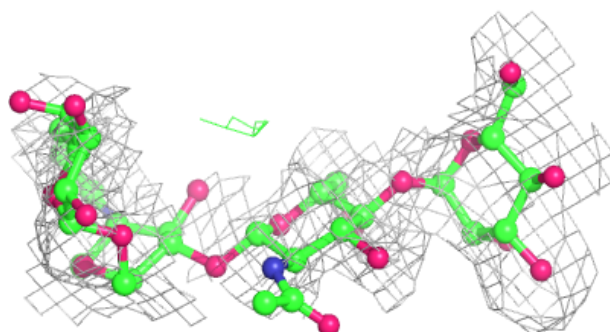
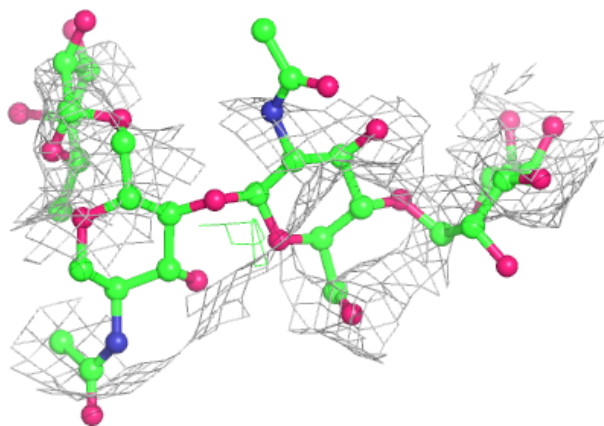


**Electron density around Chain U:**

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

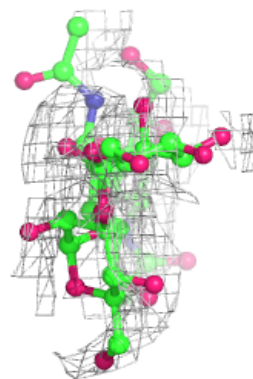
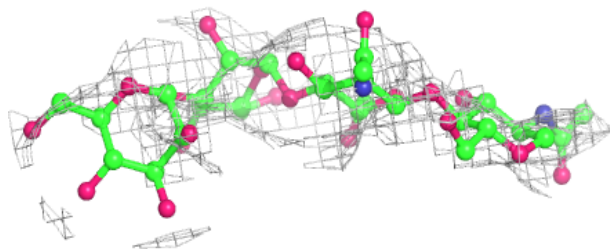
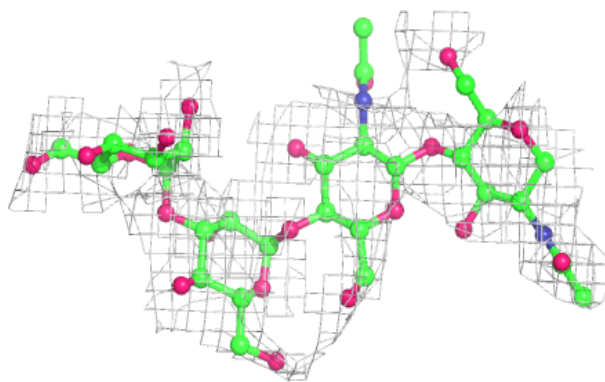
**Electron density around Chain Q:**

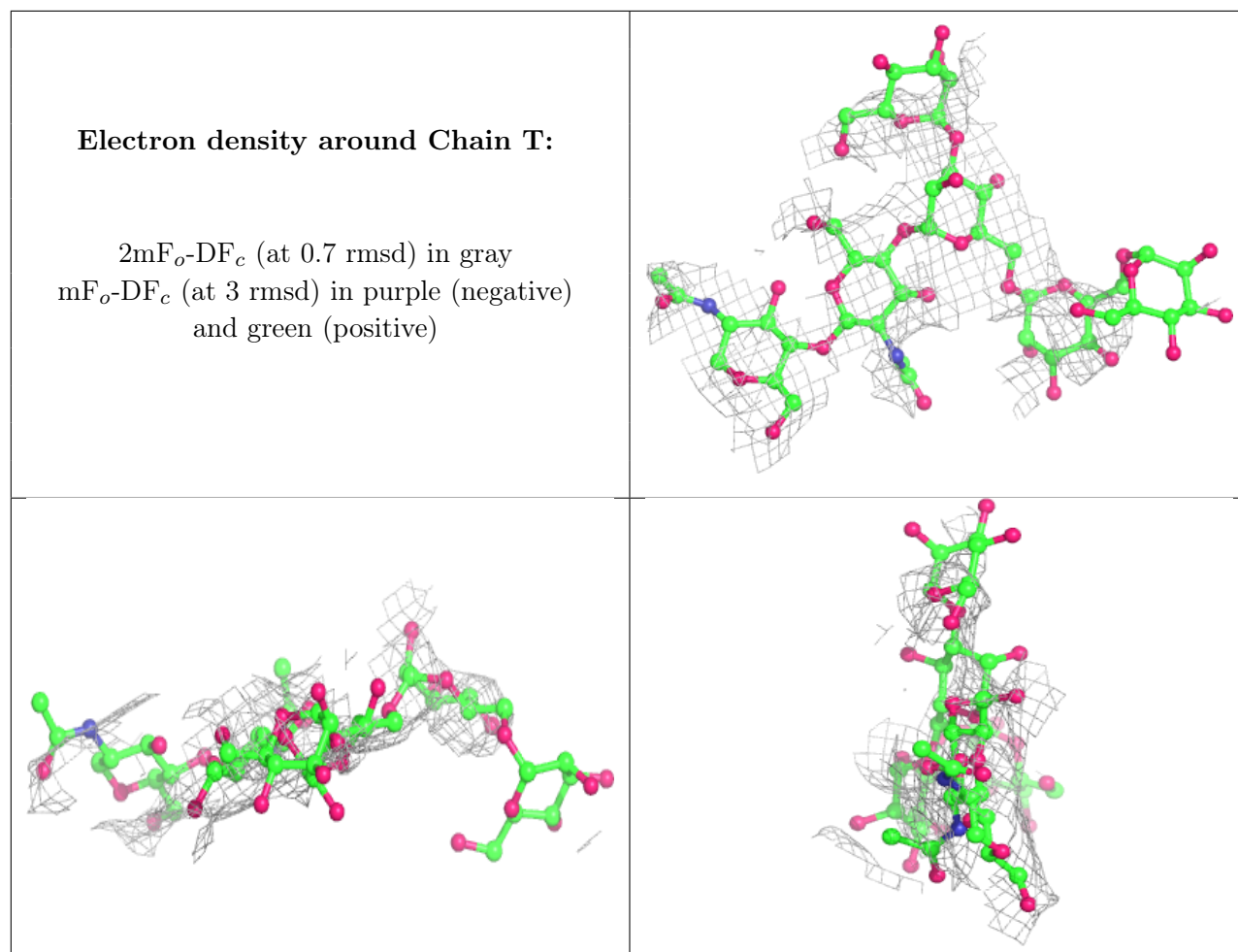
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
16	NAG	B	805	14/15	0.96	0.03	108,141,153,157	0
16	NAG	A	804	14/15	0.97	0.03	148,153,158,162	0
16	NAG	B	804	14/15	0.98	0.03	168,175,182,184	0
16	NAG	D	804	14/15	0.98	0.03	125,147,157,158	0
16	NAG	D	805	14/15	0.98	0.02	140,153,162,167	0
15	CU	D	803	1/1	0.99	0.02	126,126,126,126	0
14	CA	D	801	1/1	1.00	0.01	102,102,102,102	0
14	CA	D	802	1/1	1.00	0.02	113,113,113,113	0
15	CU	A	803	1/1	1.00	0.02	119,119,119,119	0
15	CU	B	803	1/1	1.00	0.02	112,112,112,112	0
15	CU	C	803	1/1	1.00	0.02	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	CA	A	801	1/1	1.00	0.02	118,118,118,118	0
14	CA	A	802	1/1	1.00	0.03	121,121,121,121	0
14	CA	B	801	1/1	1.00	0.02	104,104,104,104	0
14	CA	B	802	1/1	1.00	0.01	108,108,108,108	0
14	CA	C	801	1/1	1.00	0.01	101,101,101,101	0
14	CA	C	802	1/1	1.00	0.04	114,114,114,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.