



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2024 – 12:38 AM EDT

PDB ID : 4IIE  
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with calystegine B(2)  
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.  
Deposited on : 2012-12-20  
Resolution : 2.00 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:

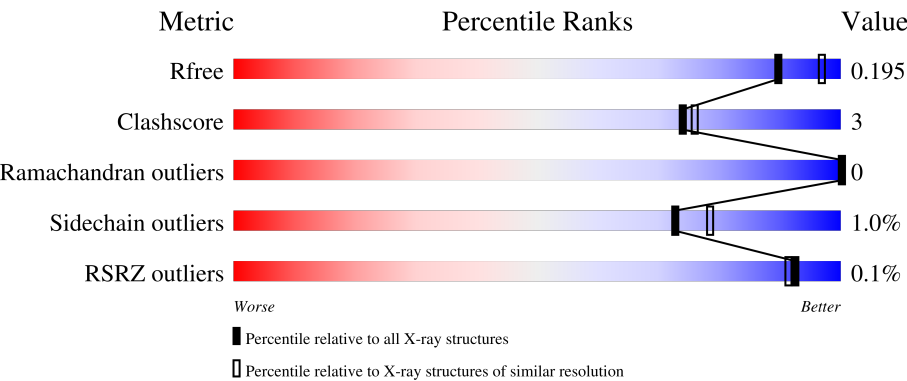
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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 <sub>free</sub>	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	841	<div><div></div><div>93%6%</div></div>
1	B	841	<div><div></div><div>90%8%</div></div>
2	C	4	<div><div></div><div>75%25%</div></div>
3	D	3	<div><div></div><div>33%67%</div></div>
3	G	3	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
3	L	3	 100%
3	N	3	 33% 67%
4	E	2	 100%
5	F	10	 100%
5	M	10	 100%
6	H	7	 86% 14%
6	O	7	 71% 29%
7	I	7	 100%
8	J	7	 100%
9	K	6	 83% 17%
10	P	8	 75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	MRD	A	940	-	-	X	-
14	CGB	A	943	-	-	X	-
14	CGB	B	952	-	-	X	-

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 15193 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 Beta-glucosidase 1.

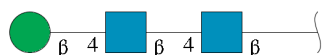
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6387	4031	1097	1241	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- Molecule 2 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
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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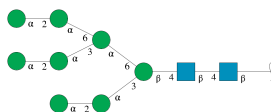
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



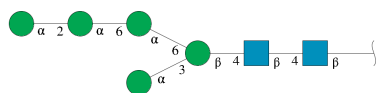
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.



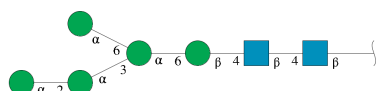
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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.



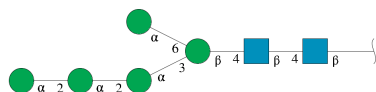
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



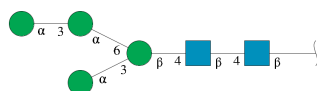
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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.



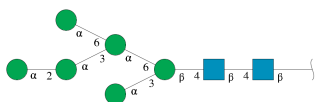
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



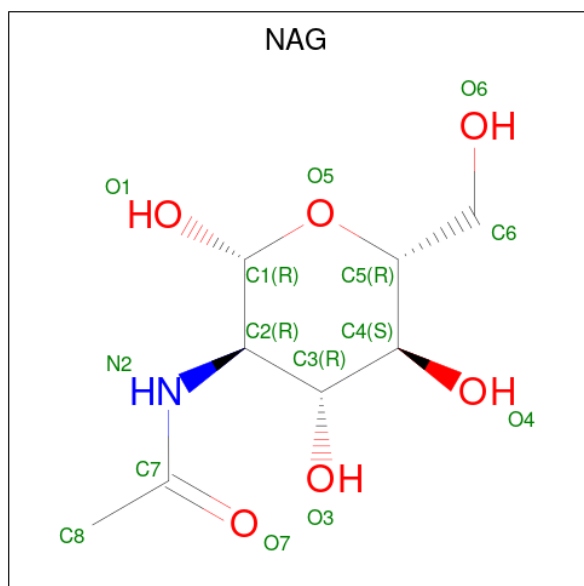
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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-(1-3)]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
10	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

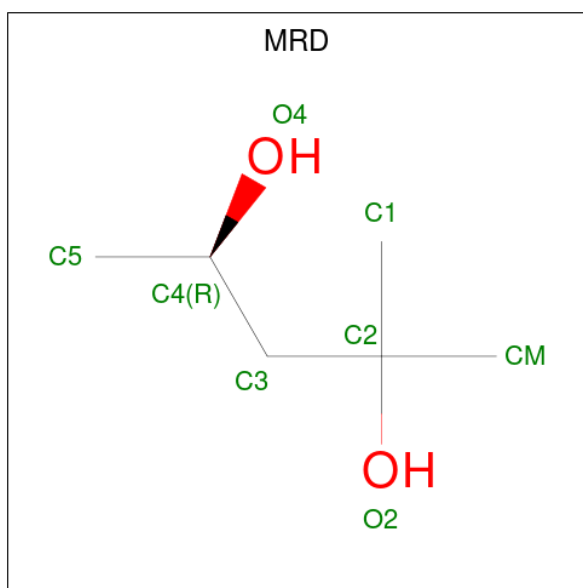
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 12 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:

C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



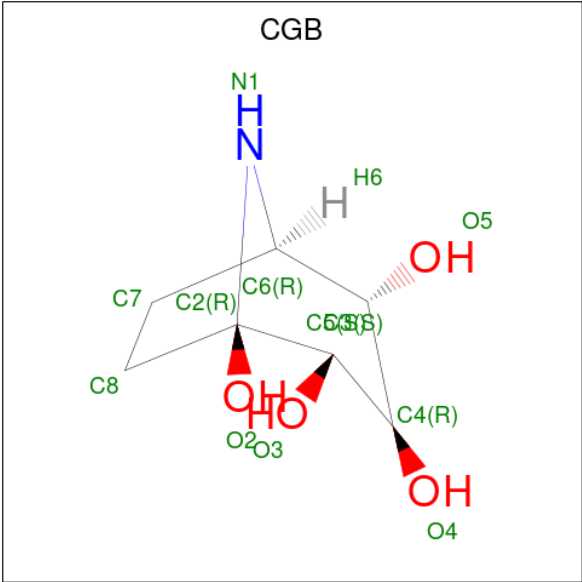
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			8	6	2		
12	A	1	Total	C	O	0	0
			8	6	2		
12	A	1	Total	C	O	0	0
			8	6	2		
12	B	1	Total	C	O	0	0
			8	6	2		
12	B	1	Total	C	O	0	0
			8	6	2		
12	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Na	0	0
			1	1		
13	B	1	Total	Na	0	0
			1	1		

- Molecule 14 is CALYSTEGINE B2 (three-letter code: CGB) (formula: C<sub>7</sub>H<sub>13</sub>NO<sub>4</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			12	7	1	4		
14	B	1	Total	C	N	O	0	0
			12	7	1	4		

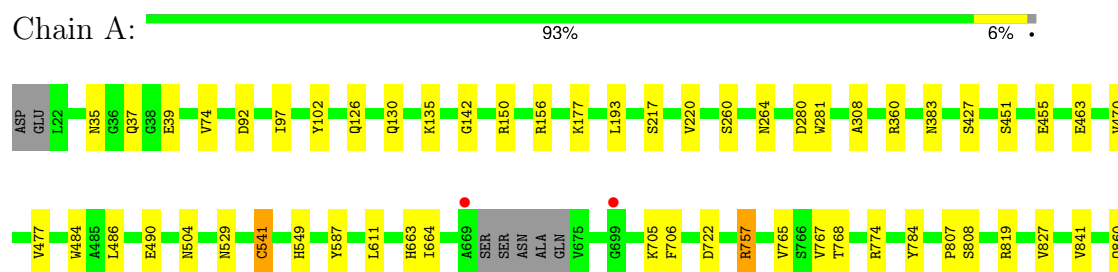
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	610	Total	O	0	0
			610	610		
15	B	713	Total	O	0	0
			713	713		

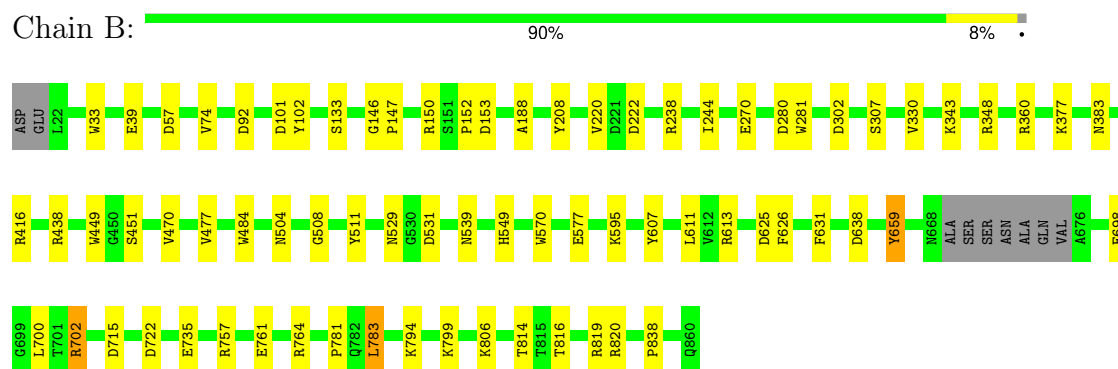
### 3 Residue-property plots

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.

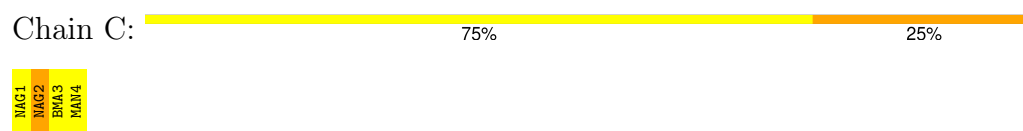
#### • Molecule 1: Beta-glucosidase 1



#### • Molecule 1: Beta-glucosidase 1



#### • Molecule 2: 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



#### • Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain G:  100%

MAG1  
MAG2  
BMA3

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

Chain L:  100%

MAG1  
MAG2  
BMA3

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

Chain N:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain E:  100%

MAG1  
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 F:  100%

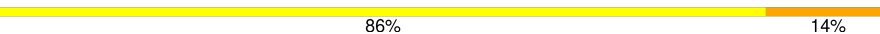
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 M:  100%

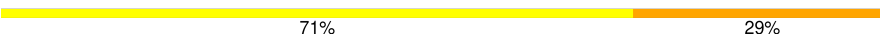
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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 H:  86% 14%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7
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- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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 O:  71% 29%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7
------	------	------	------	------	------	------

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 I:  100%


MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7
------	------	------	------	------	------	------

- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 J:  100%

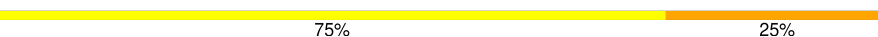
MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7
------	------	------	------	------	------	------

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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:  83% 17%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6
------	------	------	------	------	------

- 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-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  75% 25%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.13Å 122.15Å 222.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.00 39.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.07-2.00) 99.5 (39.07-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.149 , 0.193 0.151 , 0.195	Depositor DCC
$R_{free}$ test set	7597 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: MRD, BMA, CGB, MAN, NA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.21	6/6550 (0.1%)	1.02	10/8930 (0.1%)
1	B	1.32	9/6538 (0.1%)	1.08	25/8913 (0.3%)
All	All	1.27	15/13088 (0.1%)	1.05	35/17843 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLU	CD-OE2	5.76	1.31	1.25
1	B	270	GLU	CD-OE2	5.63	1.31	1.25
1	B	348	ARG	CZ-NH1	5.55	1.40	1.33
1	B	511	TYR	CG-CD2	5.45	1.46	1.39
1	B	761	GLU	CD-OE2	-5.43	1.19	1.25

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	B	348	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	348	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	B	702	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	438	ARG	NE-CZ-NH1	-7.52	116.54	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6387	0	6097	34	0
1	B	6375	0	6082	33	0
2	C	50	0	43	1	0
3	D	39	0	34	2	0
3	G	39	0	34	0	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	24	0	0
5	F	116	0	97	0	0
5	M	116	0	97	0	0
6	H	83	0	70	2	0
6	O	83	0	69	2	0
7	I	83	0	69	0	0
8	J	83	0	70	0	0
9	K	72	0	61	2	0
10	P	94	0	78	1	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	24	0	42	8	0
12	B	24	0	42	5	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
14	A	12	0	13	7	0
14	B	12	0	12	7	0
15	A	610	0	0	4	0
15	B	713	0	0	7	0
All	All	15193	0	13167	81	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 3.

The worst 5 of 81 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:92:ASP:OD2	14:A:943:CGB:H7C1	1.71	0.90
1:B:92:ASP:OD2	14:B:952:CGB:H7C1	1.75	0.86
1:A:280:ASP:OD1	14:A:943:CGB:H3	1.78	0.82
1:A:360:ARG:HH11	12:A:940:MRD:HMC3	1.44	0.82
1:A:819:ARG:HH12	1:A:860:GLN:C	1.82	0.82



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	830/841 (99%)	798 (96%)	32 (4%)	0	100	100
1	B	828/841 (98%)	803 (97%)	25 (3%)	0	100	100
All	All	1658/1682 (99%)	1601 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	671/677 (99%)	667 (99%)	4 (1%)	84	88
1	B	670/677 (99%)	661 (99%)	9 (1%)	65	71
All	All	1341/1354 (99%)	1328 (99%)	13 (1%)	73	78

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	302	ASP
1	B	377	LYS
1	B	757	ARG
1	B	700	LEU
1	B	735	GLU

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

### 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 ⓘ

80 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	C	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	1.57	4 (23%)
2	NAG	C	2	2	14,14,15	0.91	1 (7%)	17,19,21	2.02	5 (29%)
2	BMA	C	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.82	5 (33%)
2	MAN	C	4	2	11,11,12	0.96	0	15,15,17	2.42	6 (40%)
3	NAG	D	1	1,3	14,14,15	1.03	1 (7%)	17,19,21	1.44	3 (17%)
3	NAG	D	2	3	14,14,15	1.15	1 (7%)	17,19,21	1.34	2 (11%)
3	BMA	D	3	3	11,11,12	1.11	0	15,15,17	2.56	9 (60%)
4	NAG	E	1	1,4	14,14,15	0.99	0	17,19,21	1.68	4 (23%)
4	NAG	E	2	4	14,14,15	1.01	1 (7%)	17,19,21	2.40	5 (29%)
5	NAG	F	1	1,5	14,14,15	1.59	3 (21%)	17,19,21	1.67	4 (23%)
5	MAN	F	10	5	11,11,12	1.46	3 (27%)	15,15,17	2.28	5 (33%)
5	NAG	F	2	5	14,14,15	1.00	1 (7%)	17,19,21	0.96	0
5	BMA	F	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.15	1 (6%)
5	MAN	F	4	5	11,11,12	0.59	0	15,15,17	1.53	5 (33%)
5	MAN	F	5	5	11,11,12	1.22	1 (9%)	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	F	6	5	11,11,12	0.82	0	15,15,17	1.47	2 (13%)
5	MAN	F	7	5	11,11,12	1.00	1 (9%)	15,15,17	1.22	1 (6%)
5	MAN	F	8	5	11,11,12	1.11	1 (9%)	15,15,17	1.75	3 (20%)
5	MAN	F	9	5	11,11,12	1.06	1 (9%)	15,15,17	1.60	3 (20%)
3	NAG	G	1	1,3	14,14,15	0.95	0	17,19,21	1.37	1 (5%)
3	NAG	G	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.47	4 (23%)
3	BMA	G	3	3	11,11,12	1.01	1 (9%)	15,15,17	2.31	3 (20%)
6	NAG	H	1	6,1	14,14,15	0.91	0	17,19,21	1.54	4 (23%)
6	NAG	H	2	6	14,14,15	0.90	0	17,19,21	2.12	5 (29%)
6	BMA	H	3	6	11,11,12	0.91	0	15,15,17	1.15	1 (6%)
6	MAN	H	4	6	11,11,12	0.69	0	15,15,17	1.49	3 (20%)
6	MAN	H	5	6	11,11,12	1.35	2 (18%)	15,15,17	1.98	5 (33%)
6	MAN	H	6	6	11,11,12	1.17	1 (9%)	15,15,17	1.28	2 (13%)
6	MAN	H	7	6	11,11,12	0.84	1 (9%)	15,15,17	1.97	5 (33%)
7	NAG	I	1	7,1,13	14,14,15	1.13	0	17,19,21	1.64	3 (17%)
7	NAG	I	2	7	14,14,15	1.18	2 (14%)	17,19,21	1.48	3 (17%)
7	BMA	I	3	7	11,11,12	0.84	0	15,15,17	2.07	3 (20%)
7	MAN	I	4	7	11,11,12	1.16	1 (9%)	15,15,17	1.30	1 (6%)
7	MAN	I	5	7	11,11,12	1.33	1 (9%)	15,15,17	2.17	5 (33%)
7	MAN	I	6	7	11,11,12	0.82	0	15,15,17	1.75	5 (33%)
7	MAN	I	7	7	11,11,12	1.06	1 (9%)	15,15,17	2.36	7 (46%)
8	NAG	J	1	8,1	14,14,15	1.65	1 (7%)	17,19,21	1.46	5 (29%)
8	NAG	J	2	8	14,14,15	1.07	2 (14%)	17,19,21	1.54	2 (11%)
8	BMA	J	3	8	11,11,12	1.14	1 (9%)	15,15,17	2.06	6 (40%)
8	MAN	J	4	8	11,11,12	0.63	0	15,15,17	1.89	6 (40%)
8	MAN	J	5	8	11,11,12	1.06	1 (9%)	15,15,17	1.62	3 (20%)
8	MAN	J	6	8	11,11,12	0.95	0	15,15,17	1.54	2 (13%)
8	MAN	J	7	8	11,11,12	0.69	0	15,15,17	1.89	5 (33%)
9	NAG	K	1	1,9	14,14,15	1.17	1 (7%)	17,19,21	1.49	3 (17%)
9	NAG	K	2	9	14,14,15	1.21	2 (14%)	17,19,21	1.58	4 (23%)
9	BMA	K	3	9	11,11,12	0.75	0	15,15,17	1.64	3 (20%)
9	MAN	K	4	9	11,11,12	0.66	0	15,15,17	1.61	6 (40%)
9	MAN	K	5	9	11,11,12	0.69	0	15,15,17	1.37	3 (20%)
9	MAN	K	6	9	11,11,12	1.60	1 (9%)	15,15,17	2.28	5 (33%)
3	NAG	L	1	1,3	14,14,15	0.66	0	17,19,21	1.76	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	L	2	3	14,14,15	0.55	0	17,19,21	1.62	4 (23%)
3	BMA	L	3	3	11,11,12	0.83	0	15,15,17	1.74	5 (33%)
5	NAG	M	1	1,5	14,14,15	1.16	2 (14%)	17,19,21	1.92	5 (29%)
5	MAN	M	10	5	11,11,12	1.05	0	15,15,17	1.77	5 (33%)
5	NAG	M	2	5	14,14,15	1.38	3 (21%)	17,19,21	1.36	3 (17%)
5	BMA	M	3	5	11,11,12	1.06	1 (9%)	15,15,17	1.71	4 (26%)
5	MAN	M	4	5	11,11,12	0.79	0	15,15,17	1.73	5 (33%)
5	MAN	M	5	5	11,11,12	0.75	0	15,15,17	2.45	6 (40%)
5	MAN	M	6	5	11,11,12	0.74	0	15,15,17	1.30	2 (13%)
5	MAN	M	7	5	11,11,12	1.27	1 (9%)	15,15,17	2.27	2 (13%)
5	MAN	M	8	5	11,11,12	1.34	1 (9%)	15,15,17	1.94	4 (26%)
5	MAN	M	9	5	11,11,12	0.81	0	15,15,17	1.42	2 (13%)
3	NAG	N	1	1,3	14,14,15	0.61	0	17,19,21	1.31	2 (11%)
3	NAG	N	2	3	14,14,15	0.86	0	17,19,21	1.20	0
3	BMA	N	3	3	11,11,12	0.89	0	15,15,17	1.25	2 (13%)
6	NAG	O	1	6,1	14,14,15	1.10	2 (14%)	17,19,21	2.11	5 (29%)
6	NAG	O	2	6	14,14,15	1.08	0	17,19,21	1.81	6 (35%)
6	BMA	O	3	6	11,11,12	1.06	0	15,15,17	1.72	3 (20%)
6	MAN	O	4	6	11,11,12	1.03	1 (9%)	15,15,17	1.42	3 (20%)
6	MAN	O	5	6	11,11,12	1.21	1 (9%)	15,15,17	2.05	6 (40%)
6	MAN	O	6	6	11,11,12	0.78	0	15,15,17	1.62	3 (20%)
6	MAN	O	7	6	11,11,12	0.89	0	15,15,17	1.90	5 (33%)
10	NAG	P	1	10,1,13	14,14,15	1.23	1 (7%)	17,19,21	1.54	4 (23%)
10	NAG	P	2	10	14,14,15	0.77	0	17,19,21	1.46	3 (17%)
10	BMA	P	3	10	11,11,12	1.36	2 (18%)	15,15,17	4.18	9 (60%)
10	MAN	P	4	10	11,11,12	1.02	1 (9%)	15,15,17	1.72	4 (26%)
10	MAN	P	5	10	11,11,12	1.02	0	15,15,17	1.77	3 (20%)
10	MAN	P	6	10	11,11,12	0.64	0	15,15,17	2.58	6 (40%)
10	MAN	P	7	10	11,11,12	0.91	1 (9%)	15,15,17	1.61	1 (6%)
10	MAN	P	8	10	11,11,12	0.92	0	15,15,17	1.92	5 (33%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	2/2/19/22	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	2/2/19/22	0/1/1/1
6	MAN	H	6	6	-	2/2/19/22	0/1/1/1
6	MAN	H	7	6	-	2/2/19/22	0/1/1/1
7	NAG	I	1	7,1,13	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	2/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	2/2/19/22	0/1/1/1
7	MAN	I	7	7	-	1/2/19/22	0/1/1/1
8	NAG	J	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	J	6	8	-	2/2/19/22	0/1/1/1
8	MAN	J	7	8	-	0/2/19/22	0/1/1/1
9	NAG	K	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	MAN	K	4	9	-	0/2/19/22	0/1/1/1
9	MAN	K	5	9	-	1/2/19/22	0/1/1/1
9	MAN	K	6	9	-	1/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	M	10	5	-	0/2/19/22	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	0/2/19/22	0/1/1/1
5	MAN	M	9	5	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	BMA	N	3	3	-	1/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
6	MAN	O	6	6	-	0/2/19/22	0/1/1/1
6	MAN	O	7	6	-	2/2/19/22	0/1/1/1
10	NAG	P	1	10,1,13	-	1/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	2/2/19/22	0/1/1/1
10	MAN	P	4	10	-	1/2/19/22	0/1/1/1
10	MAN	P	5	10	-	0/2/19/22	0/1/1/1
10	MAN	P	6	10	-	2/2/19/22	0/1/1/1
10	MAN	P	7	10	-	2/2/19/22	0/1/1/1
10	MAN	P	8	10	-	2/2/19/22	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	C1-C2	4.94	1.59	1.52
9	K	6	MAN	C2-C3	4.07	1.58	1.52
5	F	1	NAG	C2-N2	3.91	1.52	1.46
10	P	1	NAG	C2-N2	3.12	1.51	1.46
10	P	3	BMA	C2-C3	3.07	1.57	1.52

The worst 5 of 303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	3	BMA	C1-O5-C5	9.95	125.53	112.19
10	P	3	BMA	C6-C5-C4	-8.02	93.32	113.02
4	E	2	NAG	C3-C4-C5	-6.95	97.63	110.23
3	G	3	BMA	C1-O5-C5	6.72	121.19	112.19
5	M	7	MAN	C1-O5-C5	6.55	120.96	112.19

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

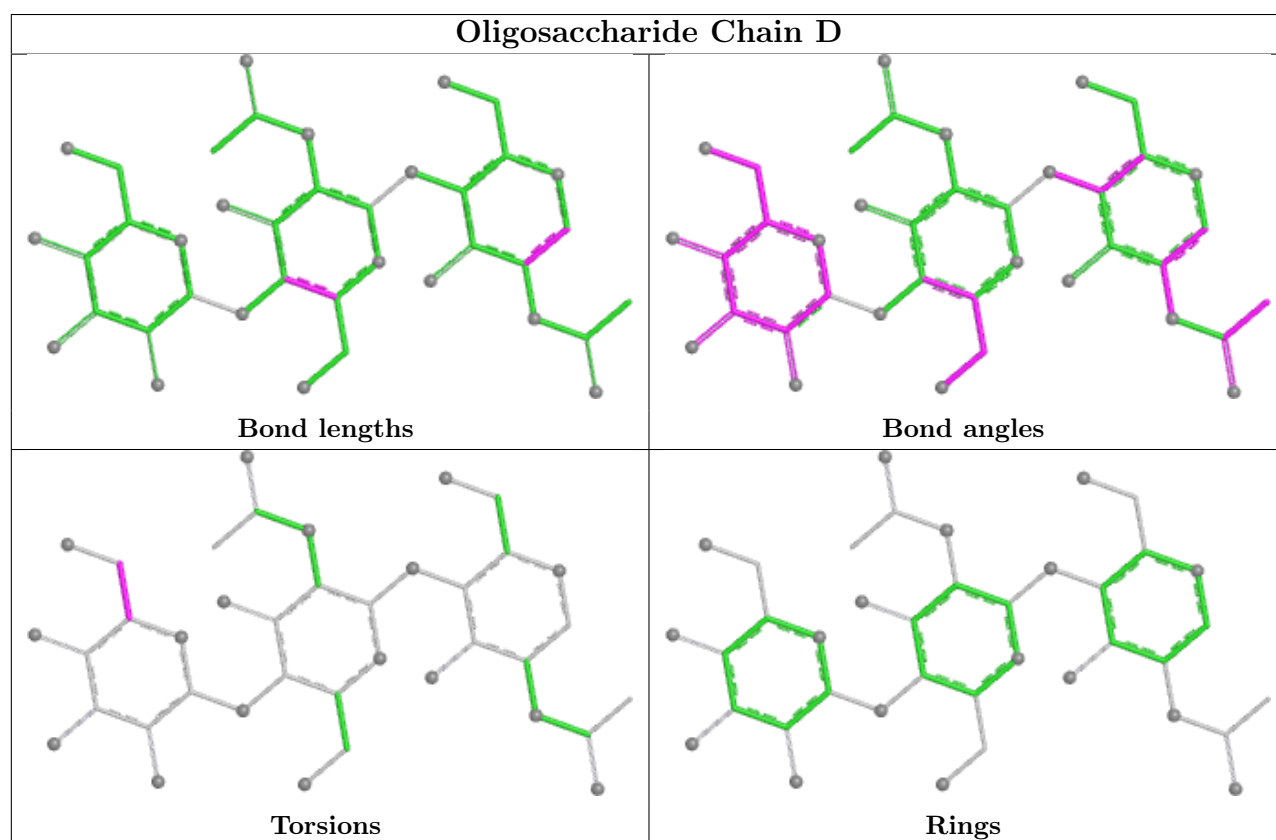
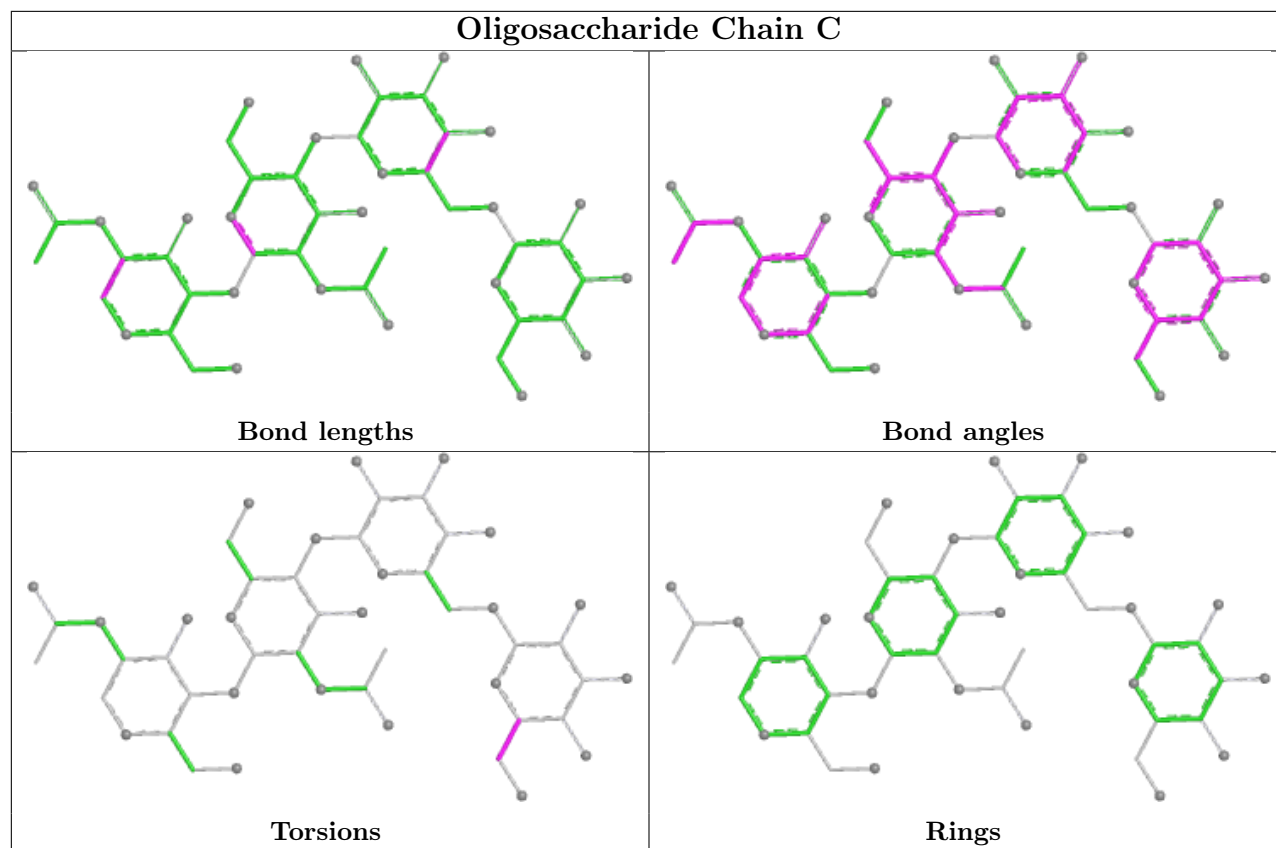
Mol	Chain	Res	Type	Atoms
7	I	6	MAN	C4-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
6	O	7	MAN	O5-C5-C6-O6
6	H	6	MAN	O5-C5-C6-O6

There are no ring outliers.

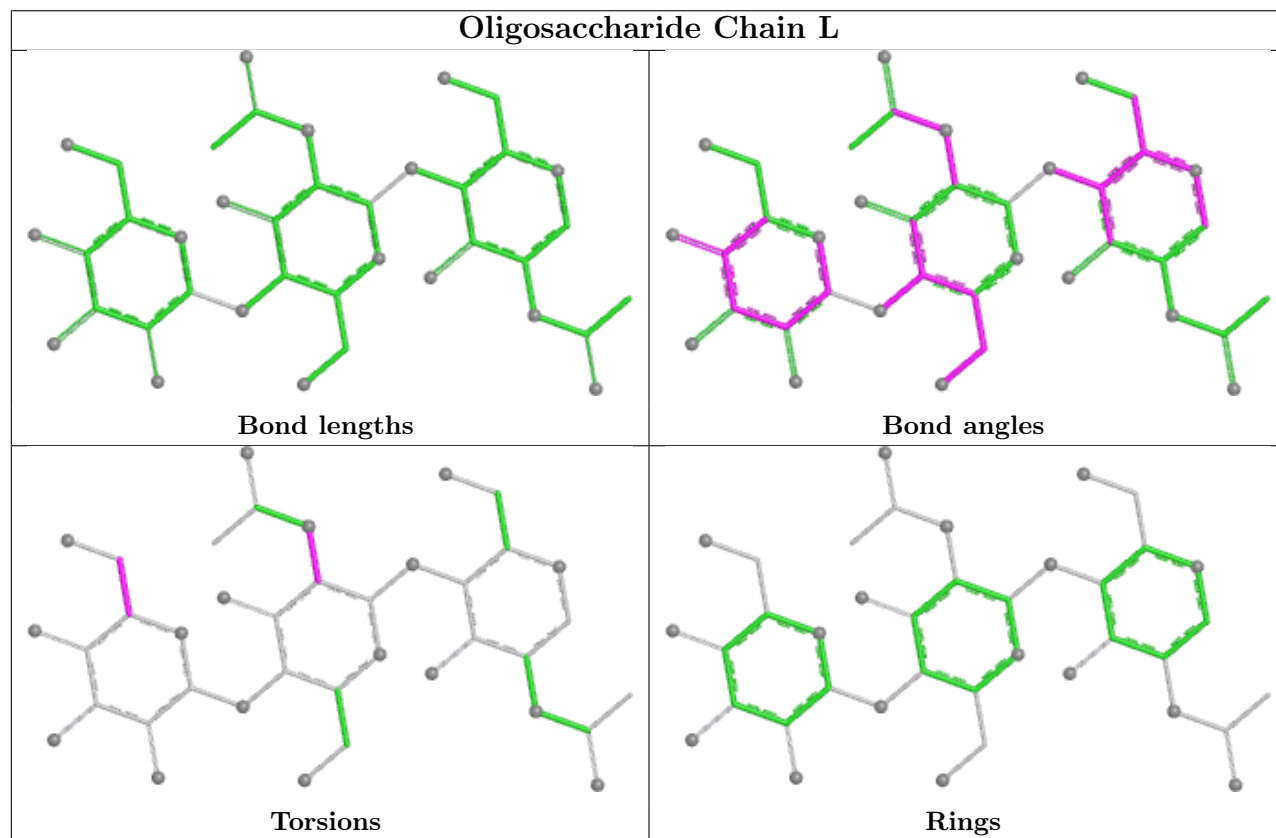
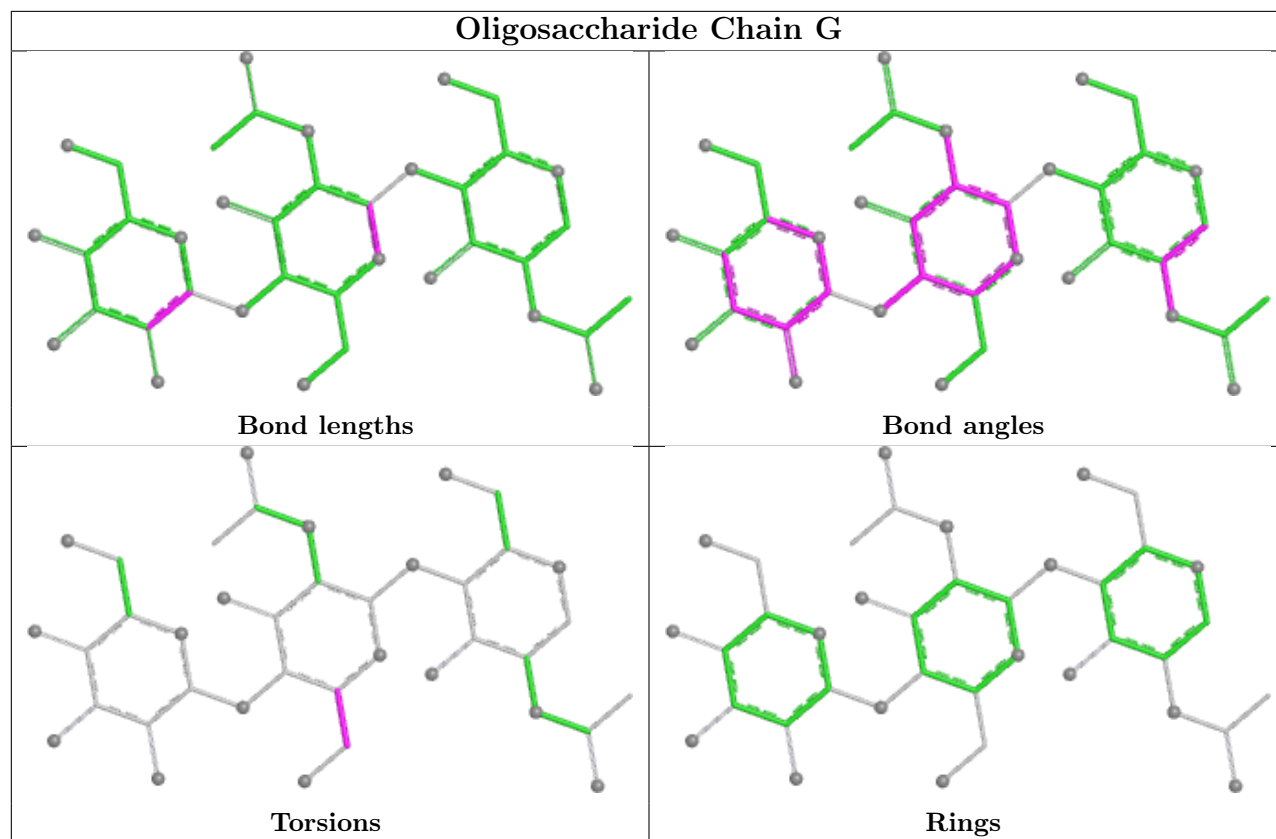
9 monomers are involved in 10 short contacts:

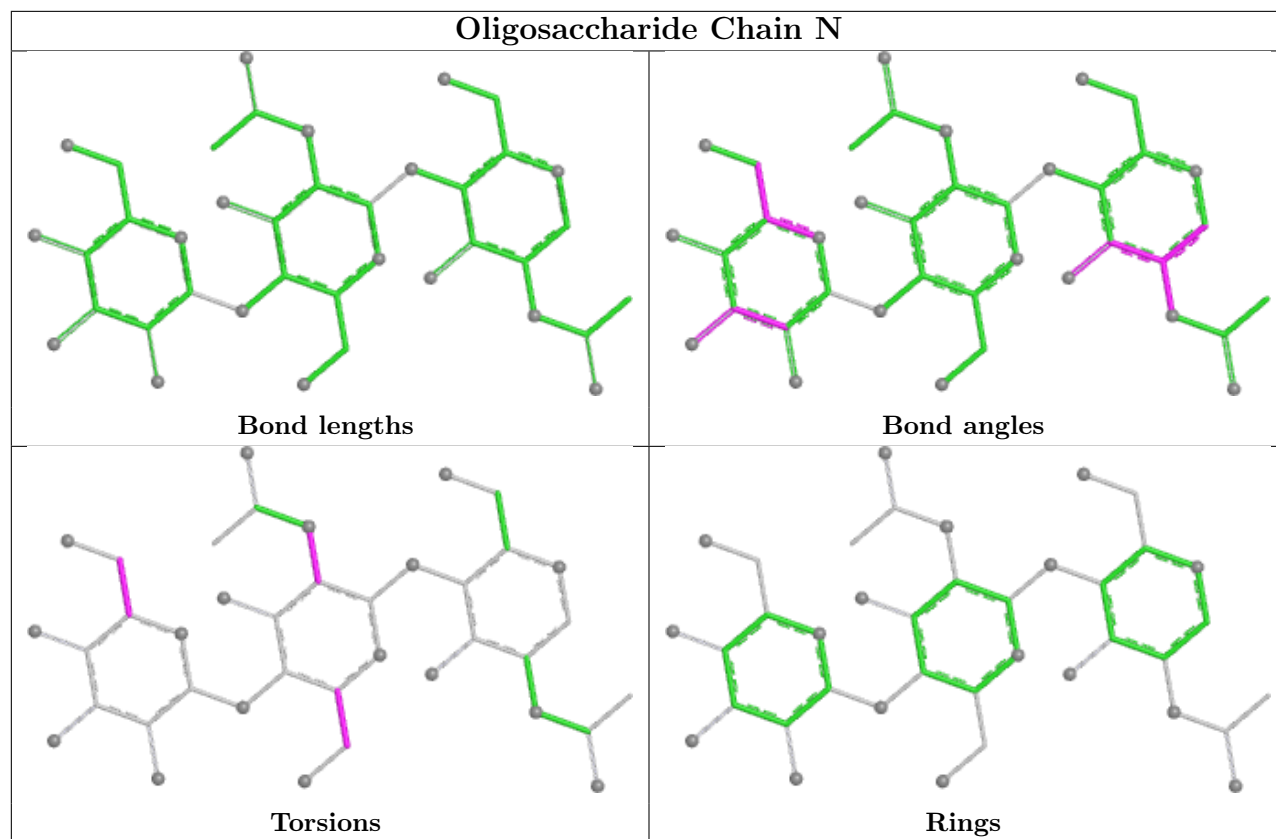
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3	BMA	2	0
3	D	2	NAG	1	0
6	O	3	BMA	2	0
10	P	4	MAN	1	0
6	O	4	MAN	1	0
2	C	2	NAG	1	0
3	D	3	BMA	1	0
10	P	3	BMA	1	0
9	K	1	NAG	2	0

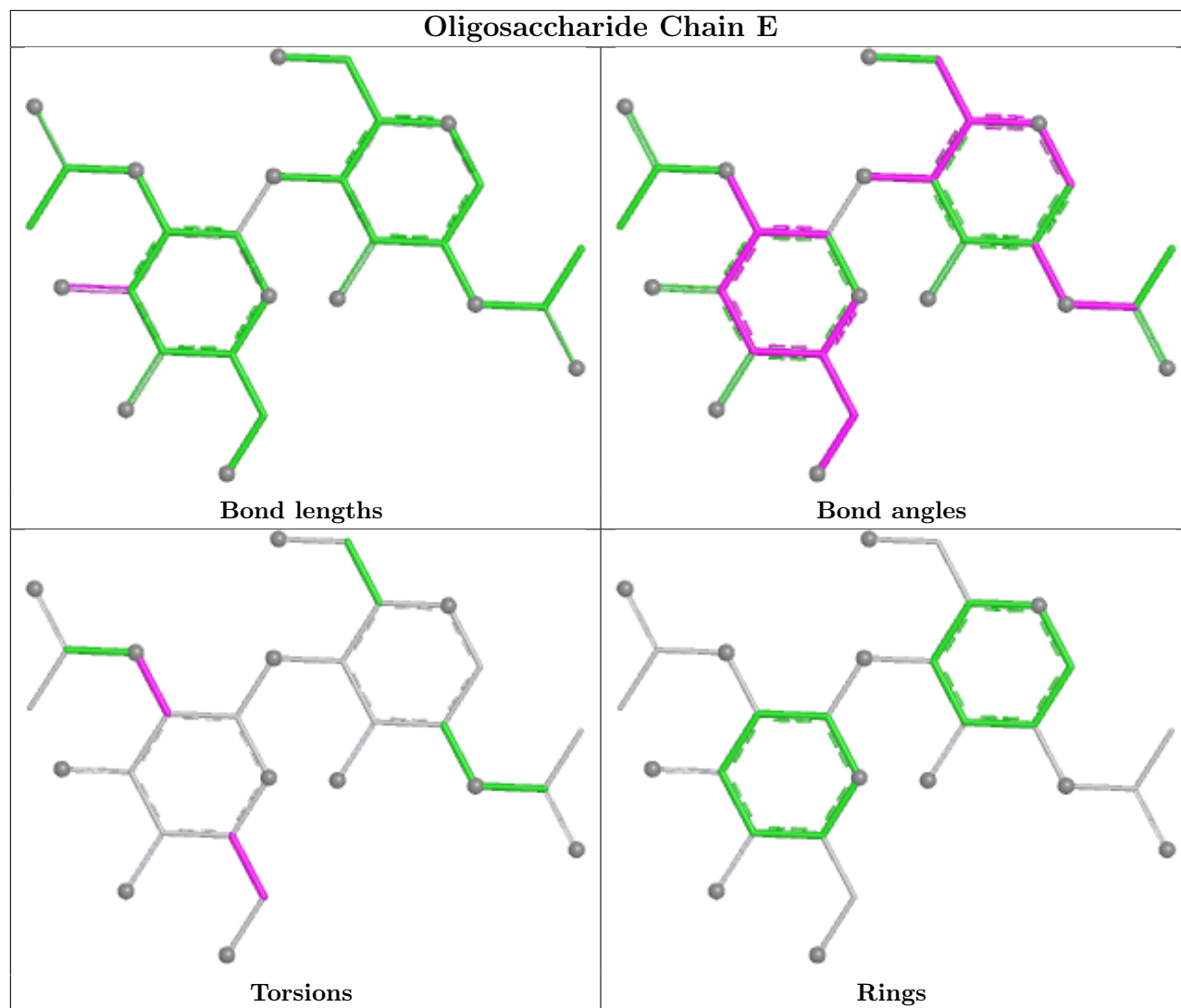
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

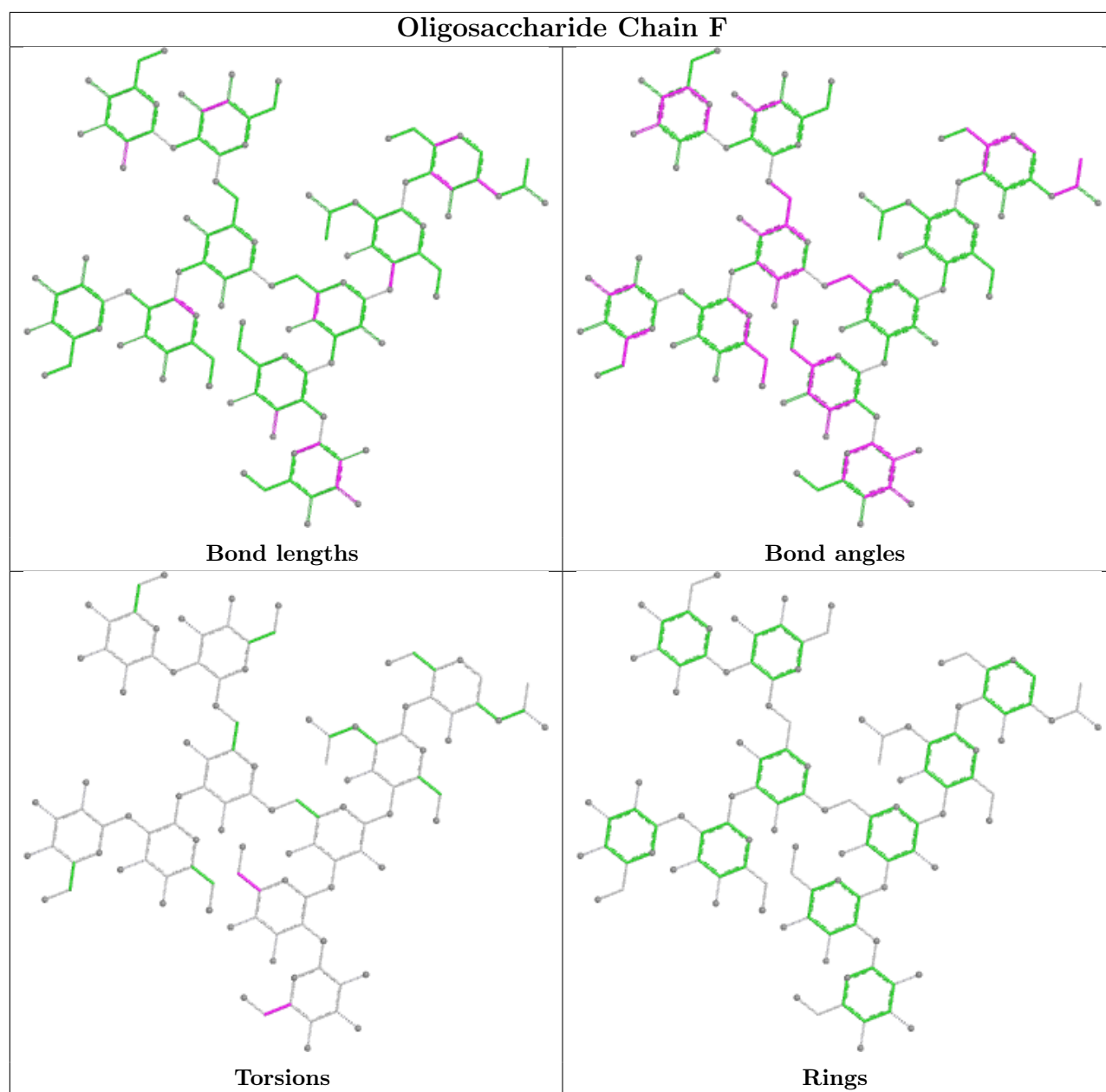


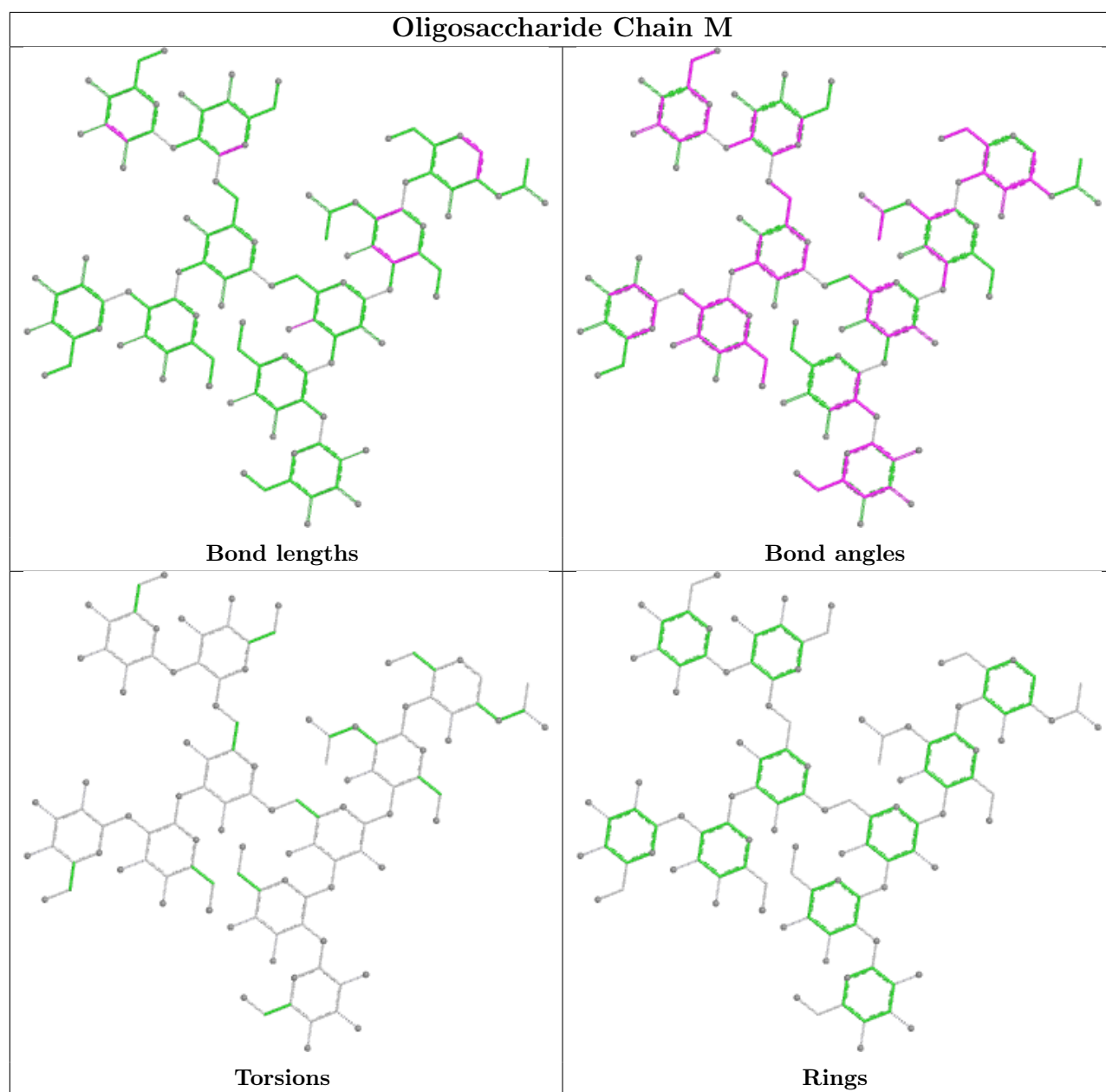


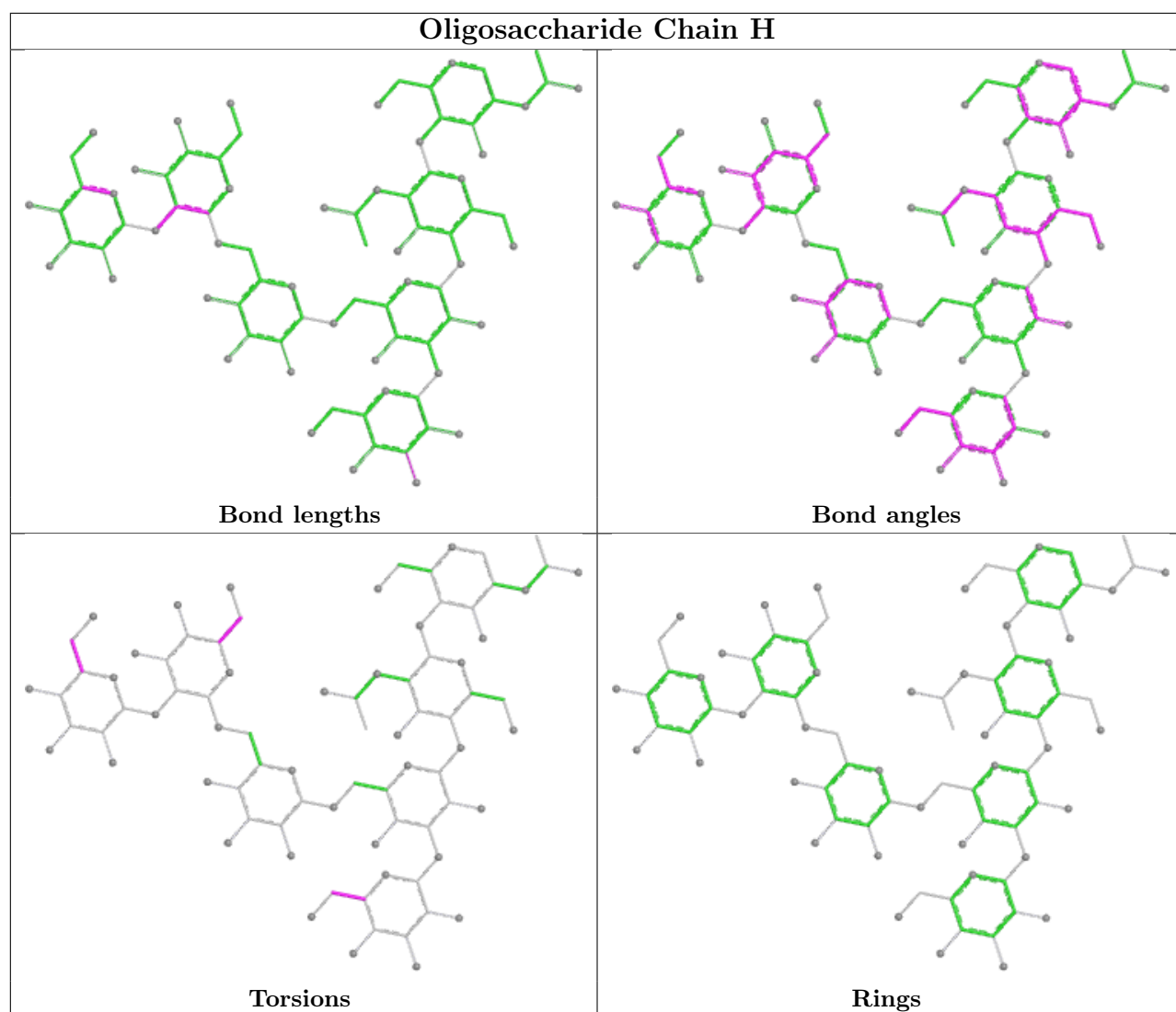


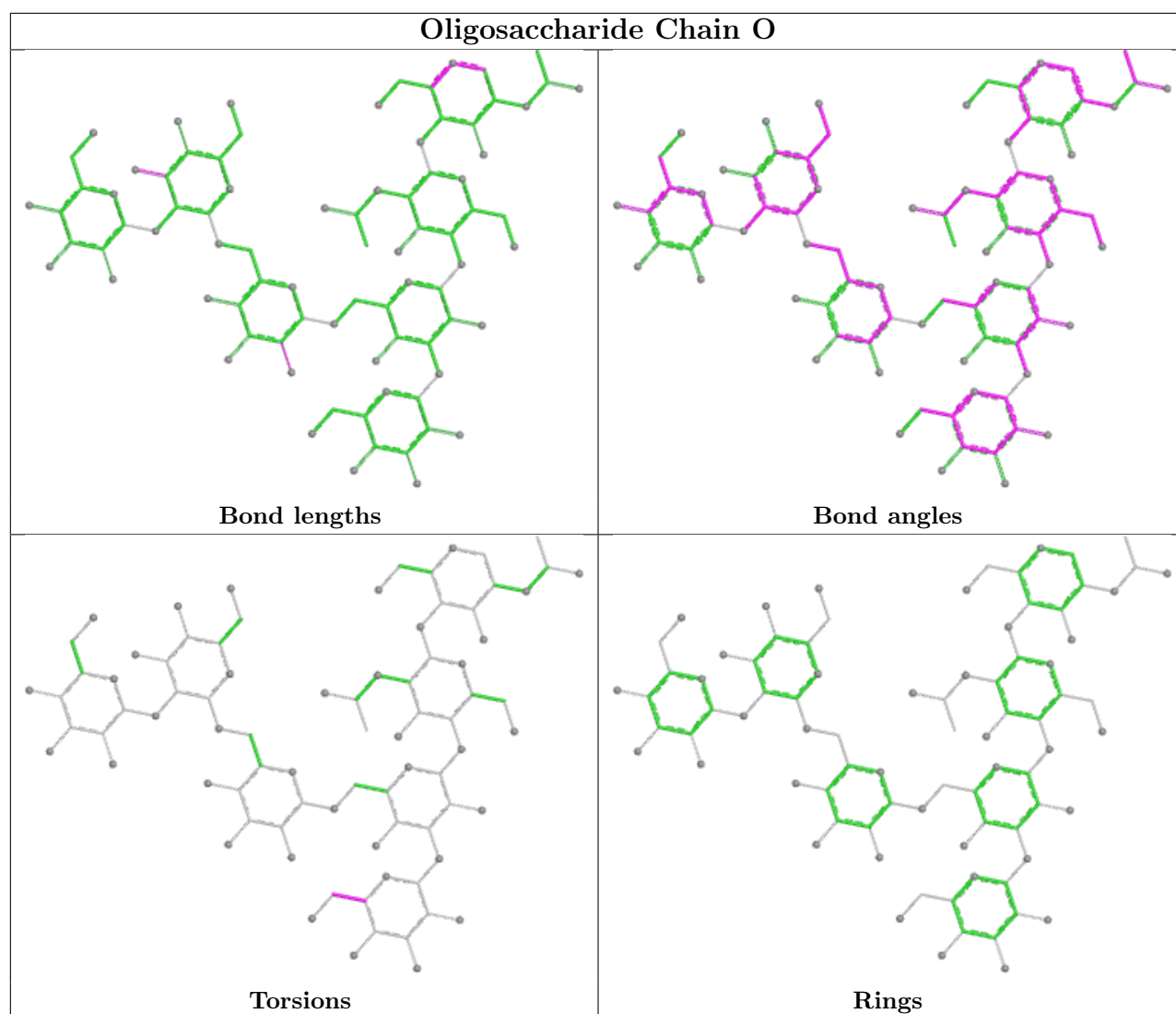


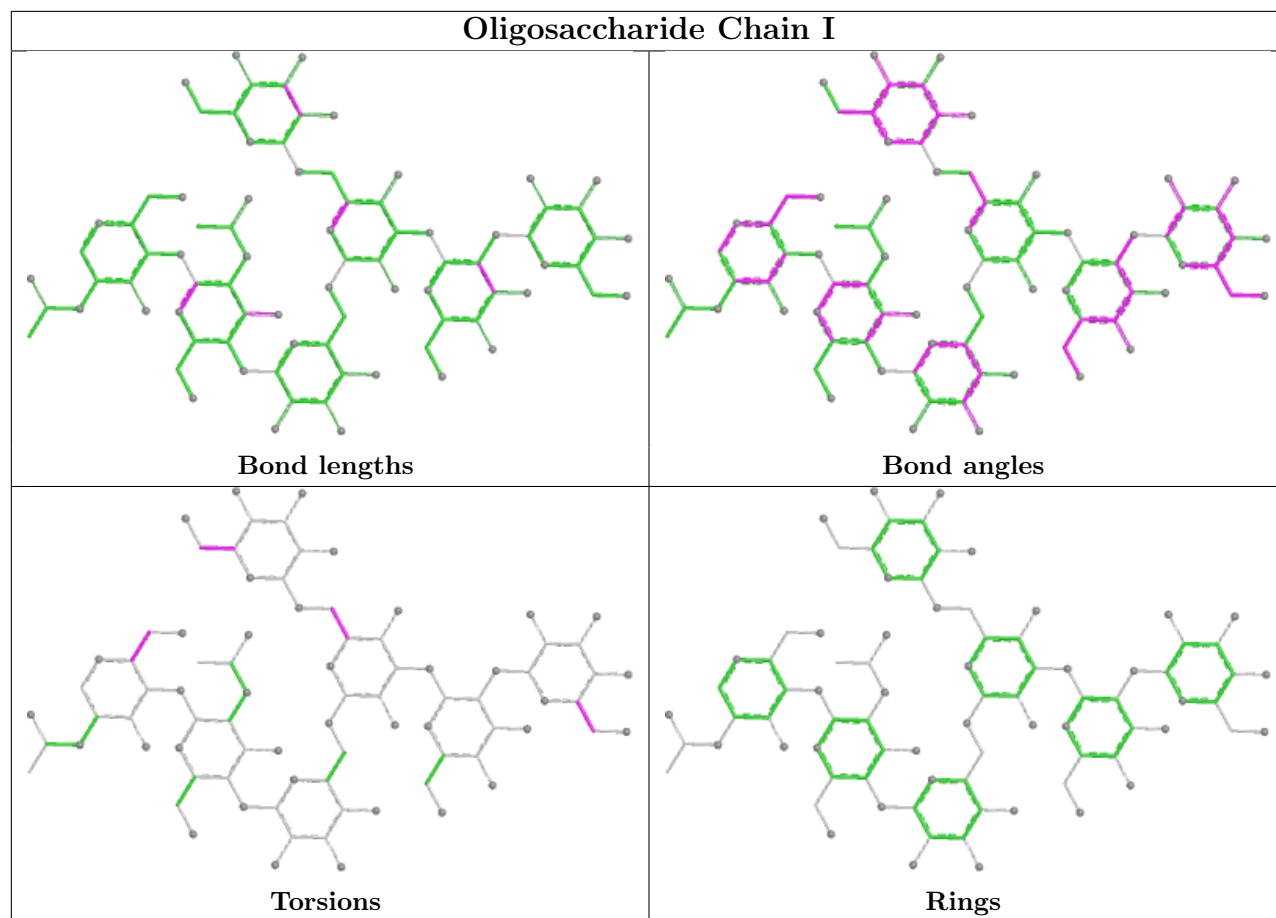




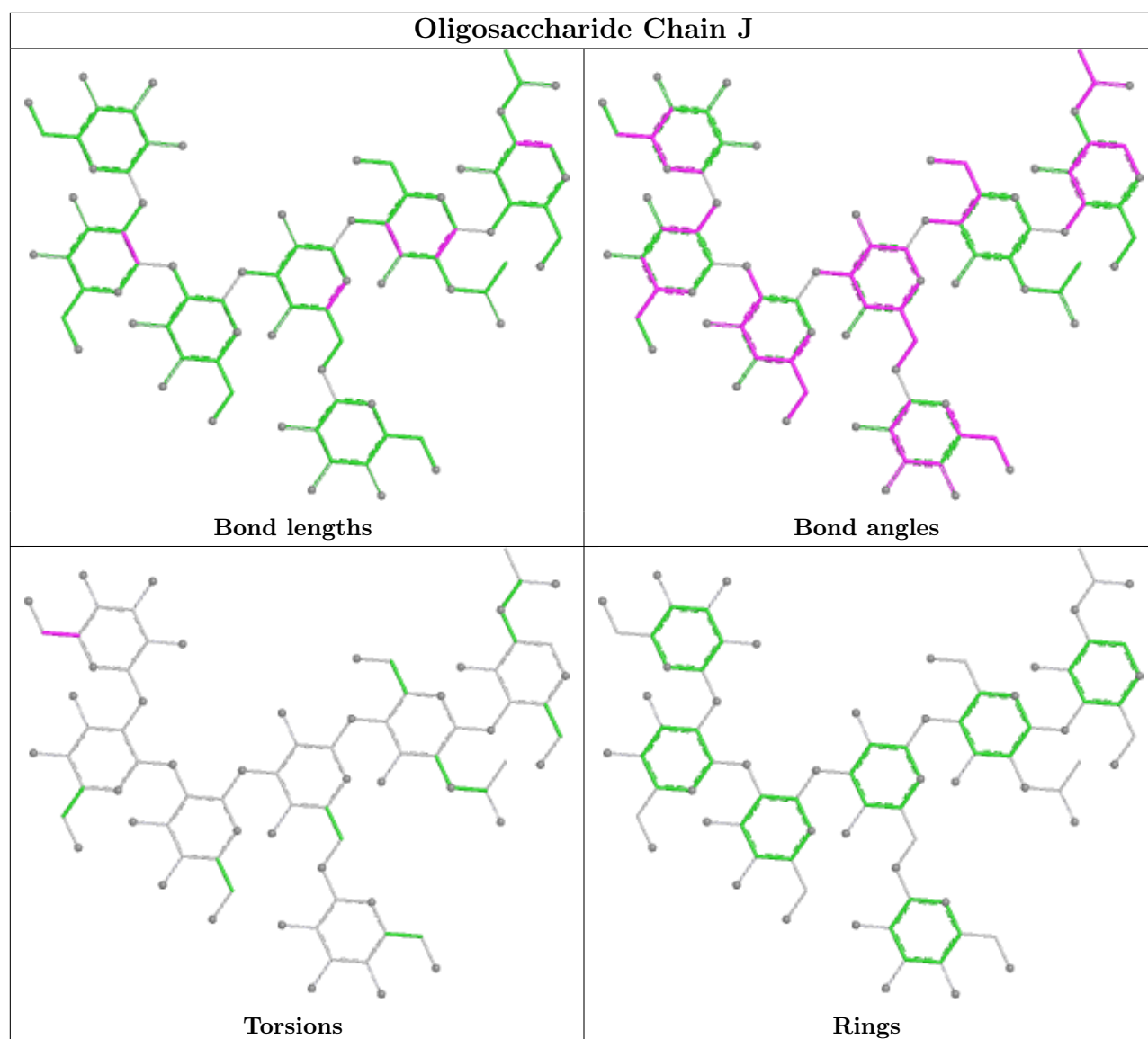


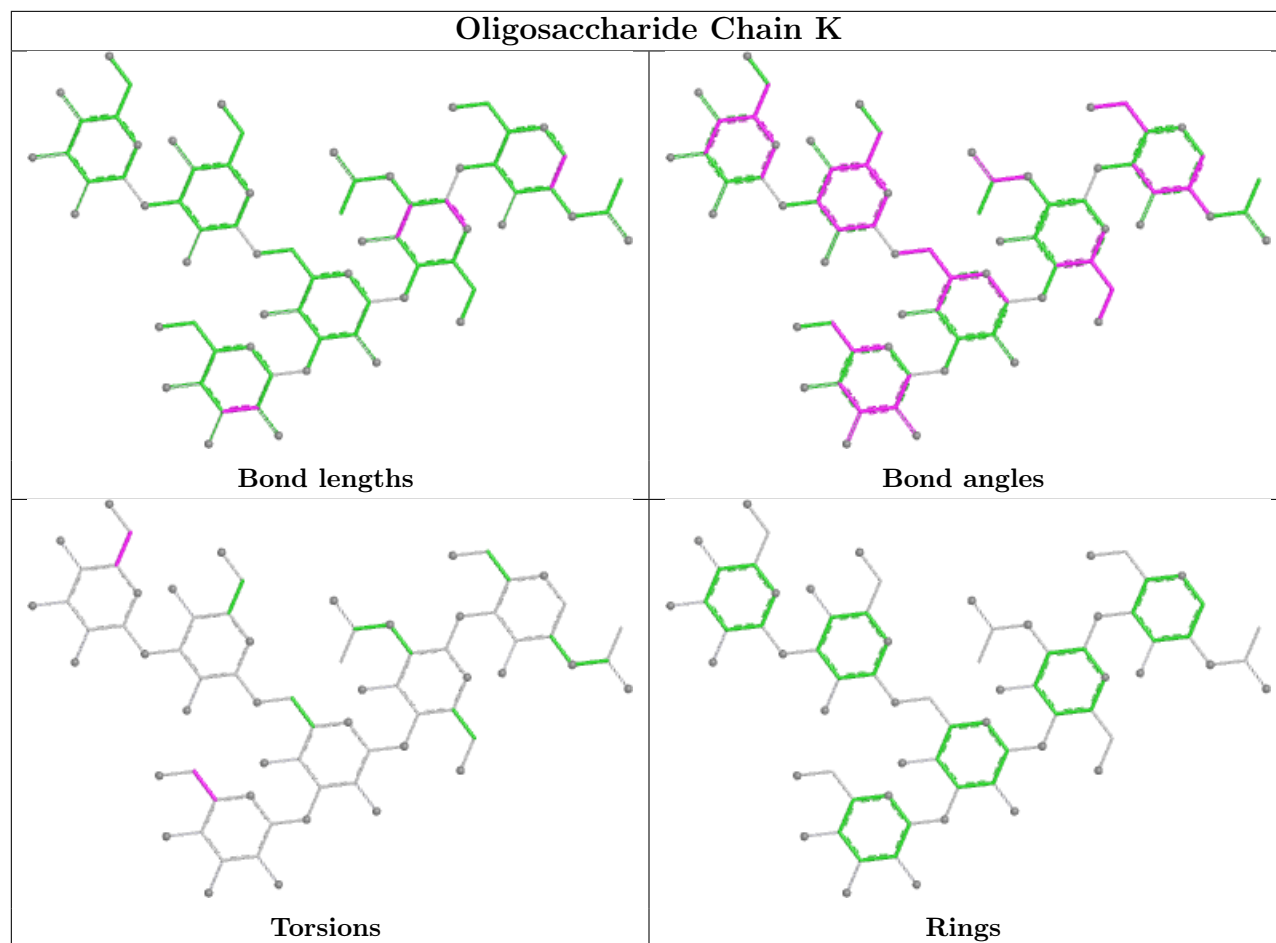


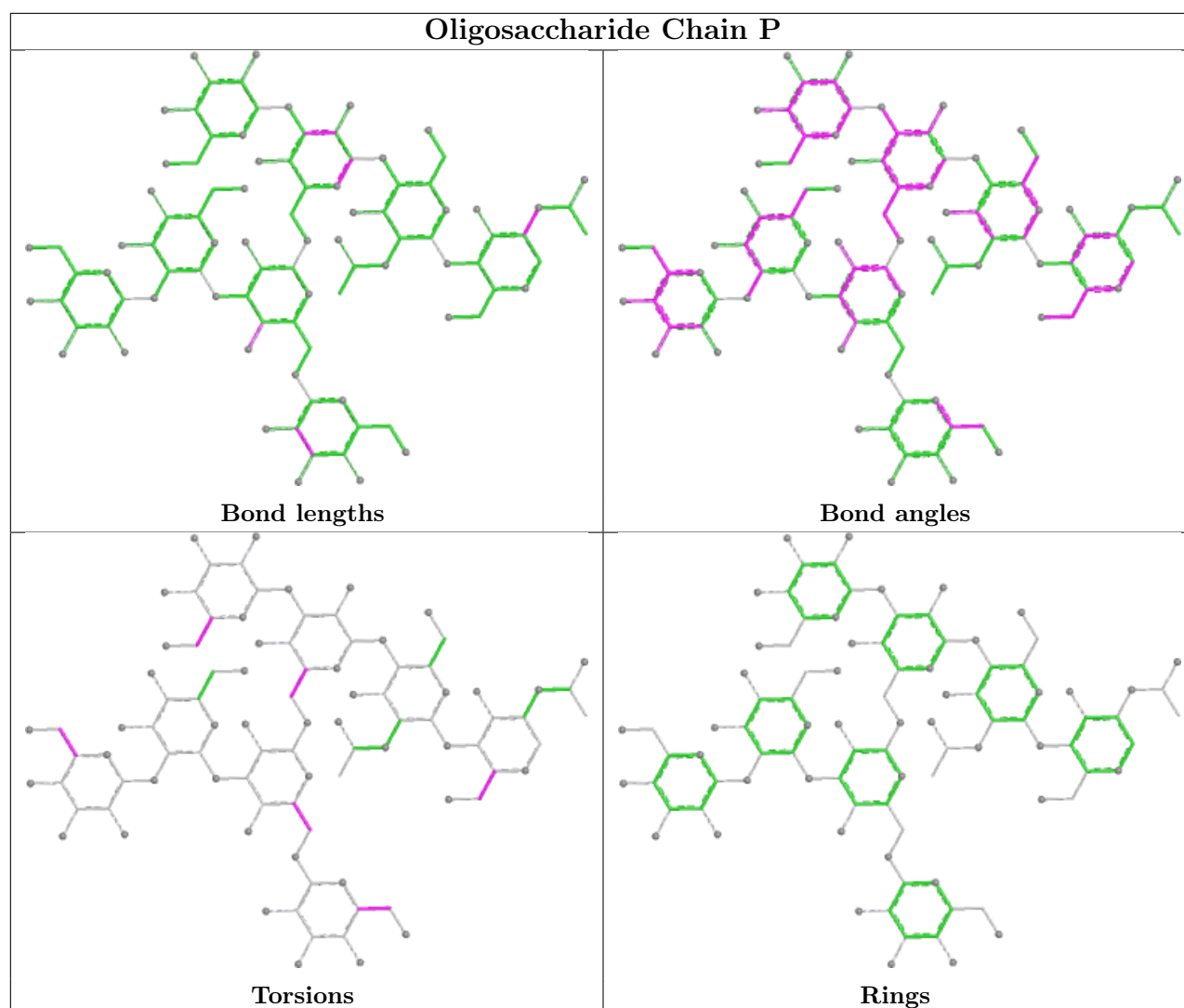












## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\# Z  > 2$
11	NAG	B	947	1	14,14,15	1.04	0	17,19,21	2.01	5 (29%)
14	CGB	B	952	-	11,13,13	2.70	4 (36%)	12,21,21	8.72	9 (75%)
11	NAG	B	946	1	14,14,15	1.04	0	17,19,21	1.88	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	A	905	1	14,14,15	0.97	1 (7%)	17,19,21	1.31	2 (11%)
12	MRD	A	941	-	7,7,7	1.20	1 (14%)	9,10,10	1.15	1 (11%)
14	CGB	A	943	-	11,13,13	2.33	3 (27%)	12,21,21	7.63	10 (83%)
12	MRD	B	950	-	7,7,7	1.02	1 (14%)	9,10,10	0.97	1 (11%)
12	MRD	A	940	-	7,7,7	1.47	2 (28%)	9,10,10	1.34	2 (22%)
11	NAG	A	938	1	14,14,15	0.80	1 (7%)	17,19,21	2.14	7 (41%)
12	MRD	B	949	-	7,7,7	1.01	0	9,10,10	1.57	2 (22%)
11	NAG	B	908	1	14,14,15	0.92	0	17,19,21	2.48	7 (41%)
12	MRD	B	948	-	7,7,7	1.60	1 (14%)	9,10,10	3.23	7 (77%)
12	MRD	A	939	-	7,7,7	1.29	0	9,10,10	0.60	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
11	NAG	B	947	1	-	2/6/23/26	0/1/1/1
14	CGB	B	952	-	-	-	0/3/2/2
11	NAG	B	946	1	-	0/6/23/26	0/1/1/1
11	NAG	A	905	1	-	0/6/23/26	0/1/1/1
12	MRD	A	941	-	-	0/5/5/5	-
14	CGB	A	943	-	-	-	0/3/2/2
12	MRD	B	950	-	-	0/5/5/5	-
12	MRD	A	940	-	-	3/5/5/5	-
11	NAG	A	938	1	-	0/6/23/26	0/1/1/1
12	MRD	B	949	-	-	4/5/5/5	-
11	NAG	B	908	1	-	6/6/23/26	0/1/1/1
12	MRD	B	948	-	-	0/5/5/5	-
12	MRD	A	939	-	-	0/5/5/5	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	952	CGB	C8-C2	-5.99	1.45	1.53
14	A	943	CGB	C8-C2	-5.96	1.45	1.53
14	B	952	CGB	C6-N1	4.18	1.51	1.47
12	B	948	MRD	C3-C2	3.00	1.62	1.54
14	B	952	CGB	O4-C4	-2.99	1.35	1.43

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	952	CGB	C7-C6-C5	-27.93	87.84	113.30
14	A	943	CGB	C7-C6-C5	-23.28	92.07	113.30
14	A	943	CGB	O4-C4-C5	7.16	127.25	110.38
14	B	952	CGB	O4-C4-C5	5.43	123.18	110.38
14	A	943	CGB	O3-C3-C2	5.24	123.14	109.92

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	908	NAG	C1-C2-N2-C7
12	B	949	MRD	C2-C3-C4-O4
12	B	949	MRD	C2-C3-C4-C5
11	B	908	NAG	C8-C7-N2-C2
11	B	908	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	952	CGB	7	0
14	A	943	CGB	7	0
12	B	950	MRD	3	0
12	A	940	MRD	6	0
12	B	949	MRD	1	0
12	B	948	MRD	1	0
12	A	939	MRD	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	834/841 (99%)	-0.81	2 (0%) 92 91	11, 20, 34, 63	0
1	B	832/841 (98%)	-1.00	0 100 100	9, 16, 28, 53	0
All	All	1666/1682 (99%)	-0.90	2 (0%) 92 91	9, 17, 31, 63	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	669	ALA	3.5
1	A	699	GLY	2.2

### 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, 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
10	MAN	P	8	11/12	0.66	0.18	58,71,82,84	0
9	MAN	K	6	11/12	0.69	0.18	57,62,68,68	0
7	MAN	I	7	11/12	0.76	0.15	50,54,60,73	0
3	BMA	G	3	11/12	0.76	0.15	46,60,73,77	0
10	MAN	P	7	11/12	0.76	0.16	47,56,66,68	0
3	BMA	L	3	11/12	0.76	0.13	55,65,76,80	0
6	MAN	H	7	11/12	0.77	0.14	54,60,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	O	7	11/12	0.77	0.14	62,71,74,79	0
7	MAN	I	6	11/12	0.78	0.17	54,58,62,66	0
2	MAN	C	4	11/12	0.78	0.12	45,52,65,71	0
9	MAN	K	5	11/12	0.78	0.16	68,74,76,85	0
3	BMA	D	3	11/12	0.79	0.11	42,48,57,62	0
10	MAN	P	6	11/12	0.80	0.14	49,52,56,61	0
9	MAN	K	4	11/12	0.81	0.13	56,66,70,70	0
10	BMA	P	3	11/12	0.83	0.15	37,41,54,60	0
2	BMA	C	3	11/12	0.84	0.11	36,44,48,53	0
7	BMA	I	3	11/12	0.85	0.13	30,41,52,63	0
3	NAG	G	2	14/15	0.85	0.14	42,50,61,69	0
3	BMA	N	3	11/12	0.86	0.11	43,52,60,62	0
8	MAN	J	7	11/12	0.89	0.09	27,31,36,38	0
10	MAN	P	4	11/12	0.90	0.11	31,34,43,48	0
5	MAN	M	10	11/12	0.90	0.09	30,37,41,42	0
5	MAN	F	10	11/12	0.91	0.10	39,40,50,51	0
9	BMA	K	3	11/12	0.91	0.08	40,44,54,60	0
10	NAG	P	2	14/15	0.92	0.09	26,30,37,39	0
7	MAN	I	4	11/12	0.92	0.09	24,30,38,45	0
6	MAN	H	4	11/12	0.92	0.08	27,30,40,43	0
8	MAN	J	6	11/12	0.93	0.09	26,30,35,42	0
5	MAN	F	5	11/12	0.93	0.07	23,30,33,42	0
7	MAN	I	5	11/12	0.93	0.08	28,34,44,44	0
10	MAN	P	5	11/12	0.93	0.09	28,35,42,47	0
6	NAG	H	2	14/15	0.93	0.07	20,26,32,40	0
4	NAG	E	2	14/15	0.93	0.07	30,33,48,53	0
8	MAN	J	5	11/12	0.93	0.08	28,34,42,49	0
7	NAG	I	2	14/15	0.94	0.07	23,27,36,42	0
3	NAG	N	2	14/15	0.94	0.09	31,33,46,48	0
3	NAG	D	2	14/15	0.94	0.07	25,29,34,37	0
6	BMA	O	3	11/12	0.94	0.07	23,27,34,46	0
6	MAN	O	4	11/12	0.94	0.07	25,27,37,39	0
5	MAN	F	6	11/12	0.94	0.07	33,38,43,44	0
8	MAN	J	4	11/12	0.94	0.06	27,32,39,43	0
7	NAG	I	1	14/15	0.95	0.06	21,23,25,26	0
5	MAN	F	9	11/12	0.95	0.06	27,31,34,36	0
6	MAN	H	5	11/12	0.95	0.07	21,24,34,41	0
2	NAG	C	2	14/15	0.95	0.07	24,32,43,48	0
9	NAG	K	2	14/15	0.95	0.07	20,27,31,35	0
3	NAG	G	1	14/15	0.95	0.07	25,29,36,38	0
6	NAG	H	1	14/15	0.95	0.07	20,22,41,47	0
3	NAG	L	2	14/15	0.95	0.07	19,26,41,45	0

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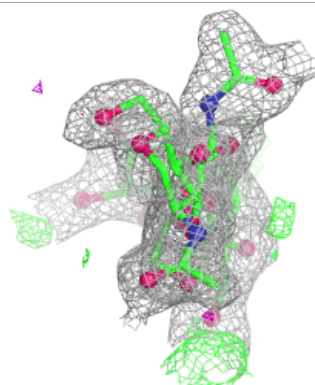
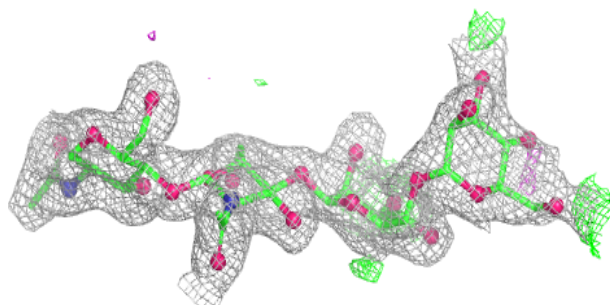
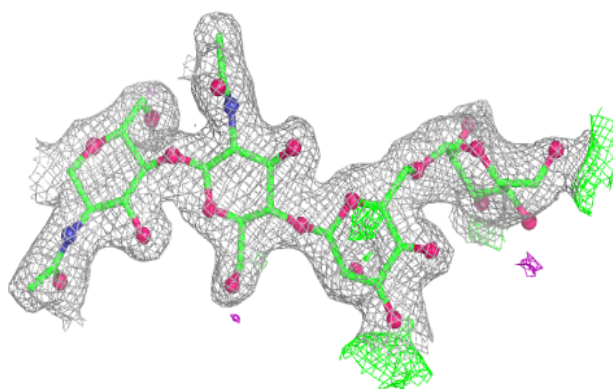
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	H	6	11/12	0.96	0.06	21,24,37,43	0
5	NAG	F	1	14/15	0.96	0.07	26,28,33,35	0
6	NAG	O	1	14/15	0.96	0.07	16,21,36,38	0
6	NAG	O	2	14/15	0.96	0.06	19,24,32,33	0
10	NAG	P	1	14/15	0.96	0.06	19,21,23,24	0
5	BMA	F	3	11/12	0.96	0.07	24,26,29,32	0
8	BMA	J	3	11/12	0.96	0.05	20,24,26,27	0
3	NAG	D	1	14/15	0.96	0.05	22,25,27,27	0
6	MAN	O	6	11/12	0.96	0.06	20,24,30,34	0
6	BMA	H	3	11/12	0.96	0.06	23,27,34,43	0
5	MAN	M	5	11/12	0.96	0.05	18,22,25,33	0
5	MAN	M	6	11/12	0.96	0.07	24,29,33,36	0
5	MAN	M	8	11/12	0.97	0.05	17,19,20,24	0
3	NAG	N	1	14/15	0.97	0.06	22,28,32,33	0
5	MAN	F	8	11/12	0.97	0.05	23,24,26,26	0
5	NAG	F	2	14/15	0.97	0.05	21,23,27,27	0
8	NAG	J	2	14/15	0.97	0.05	15,18,23,29	0
6	MAN	O	5	11/12	0.97	0.05	21,22,29,34	0
4	NAG	E	1	14/15	0.97	0.05	19,23,27,28	0
5	NAG	M	1	14/15	0.97	0.05	16,17,24,24	0
5	NAG	M	2	14/15	0.97	0.05	12,16,18,18	0
5	MAN	F	4	11/12	0.97	0.05	20,24,26,28	0
9	NAG	K	1	14/15	0.97	0.05	17,20,22,24	0
2	NAG	C	1	14/15	0.97	0.06	17,23,26,27	0
8	NAG	J	1	14/15	0.98	0.04	14,16,18,19	0
5	BMA	M	3	11/12	0.98	0.04	17,18,19,20	0
5	MAN	M	9	11/12	0.98	0.04	19,21,25,29	0
5	MAN	M	4	11/12	0.98	0.04	16,18,19,19	0
5	MAN	F	7	11/12	0.98	0.04	20,22,25,26	0
3	NAG	L	1	14/15	0.98	0.04	13,17,21,21	0
5	MAN	M	7	11/12	0.98	0.04	16,18,18,19	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.

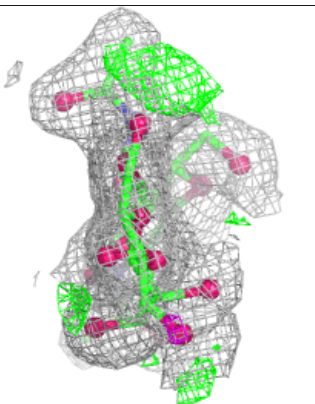
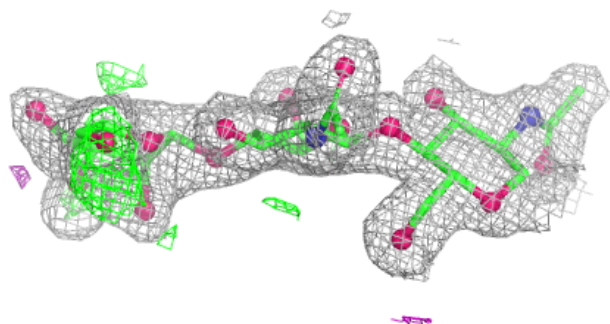
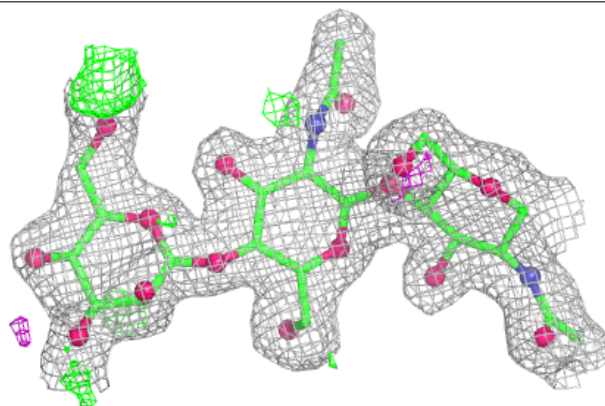


**Electron density around Chain C:**

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

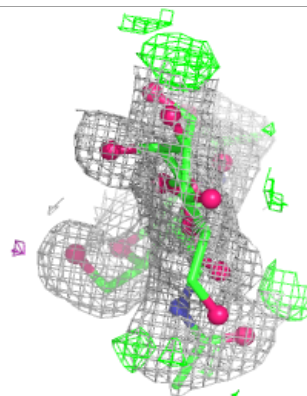
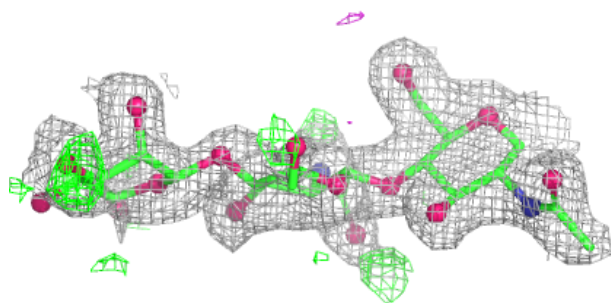
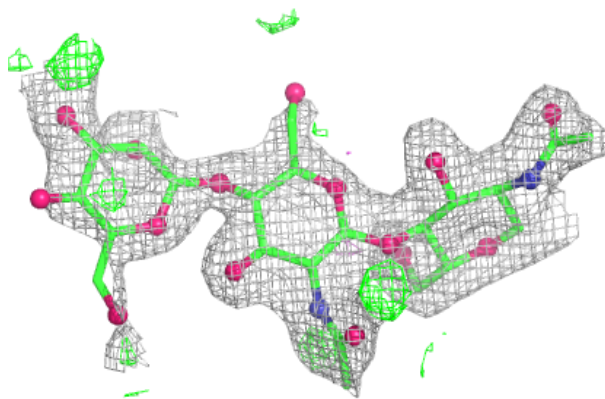
**Electron density around Chain D:**

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



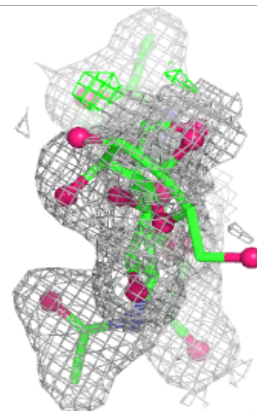
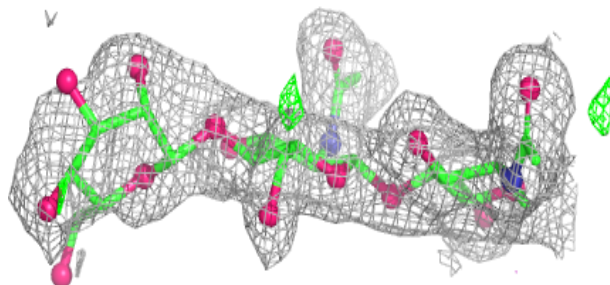
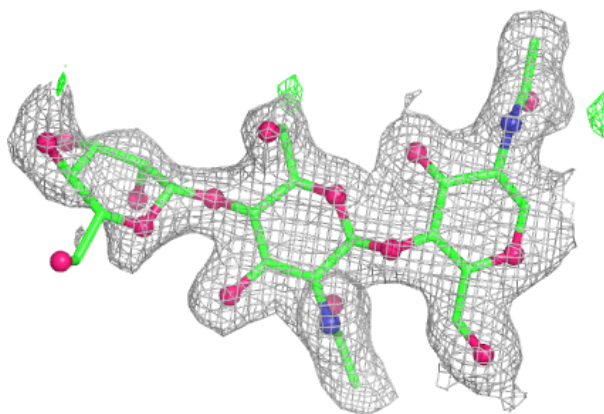
**Electron density around Chain G:**

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



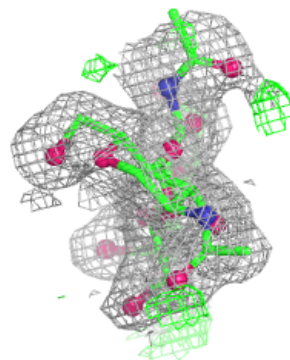
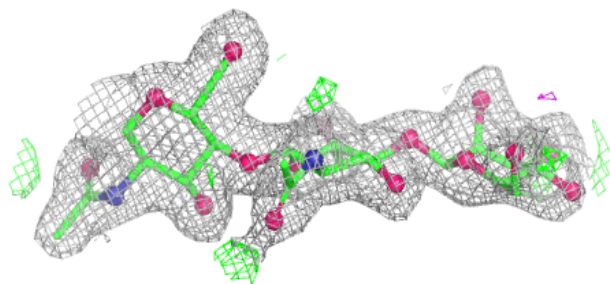
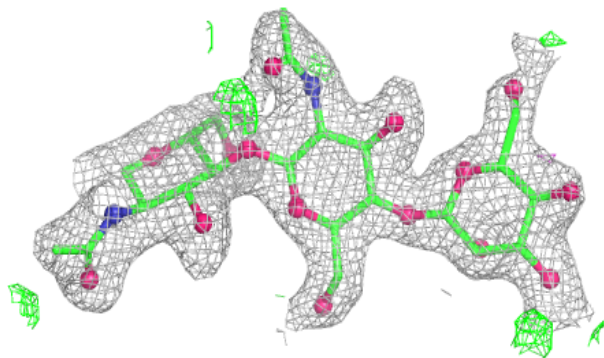
**Electron density around Chain L:**

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



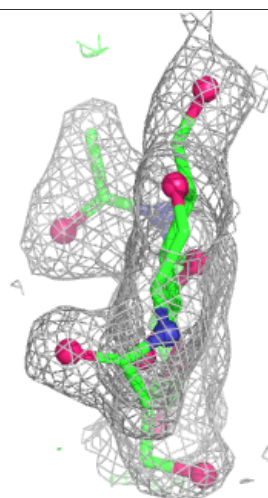
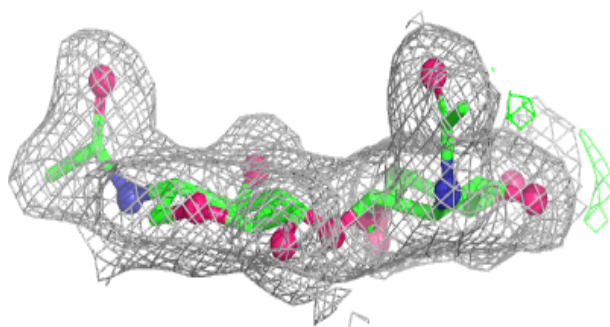
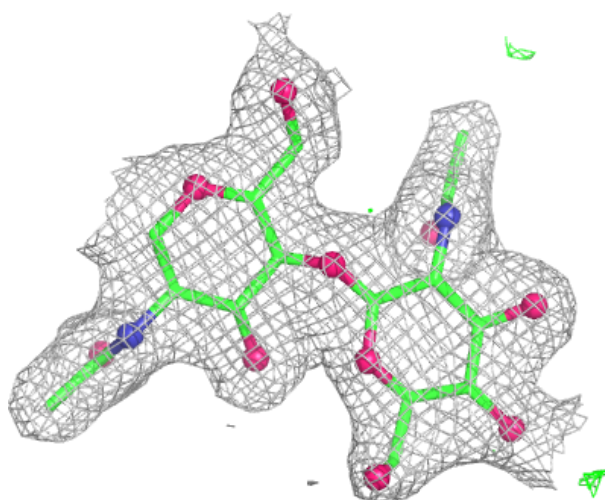
**Electron density around Chain N:**

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



**Electron density around Chain E:**

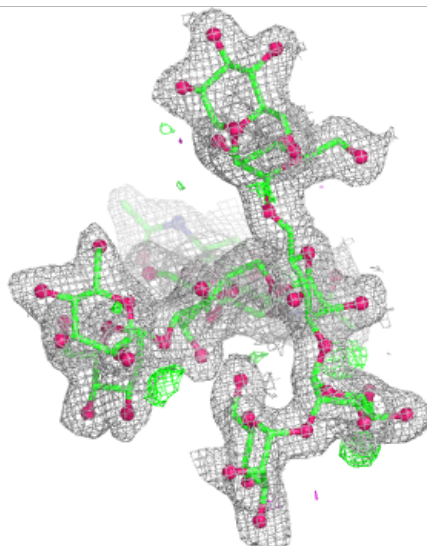
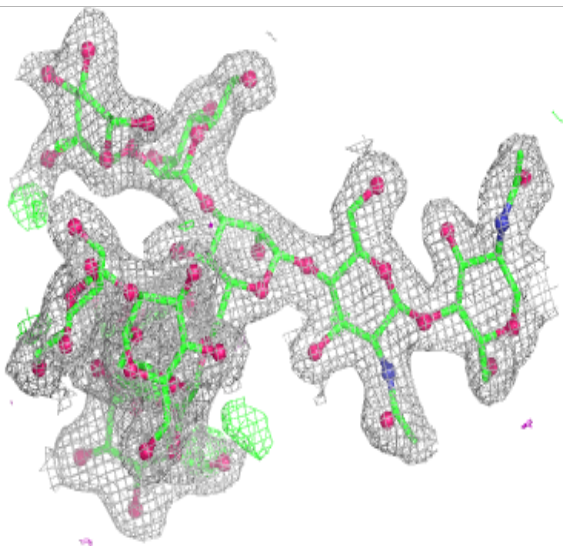
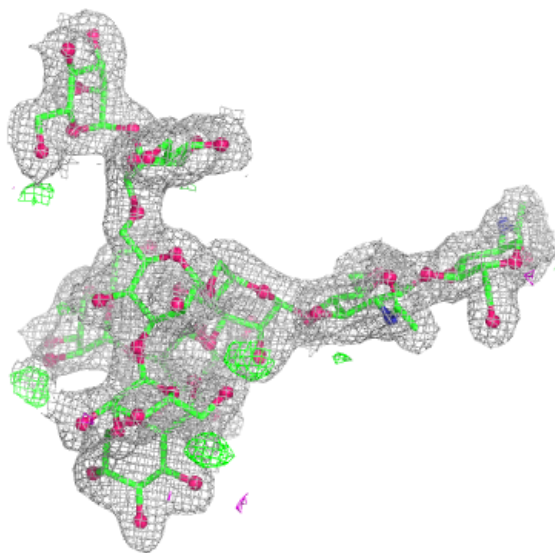
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





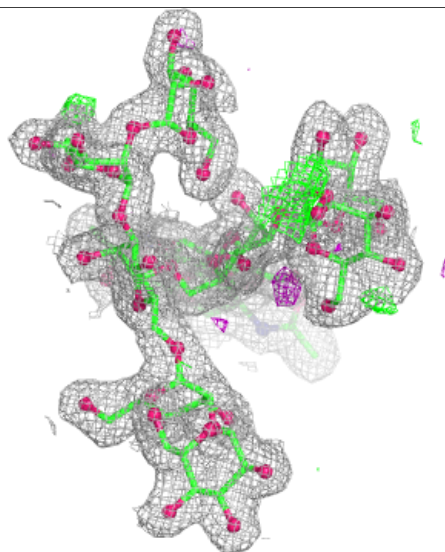
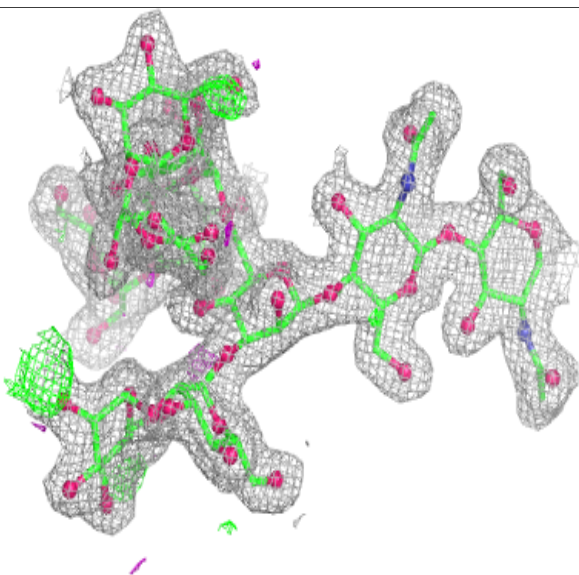
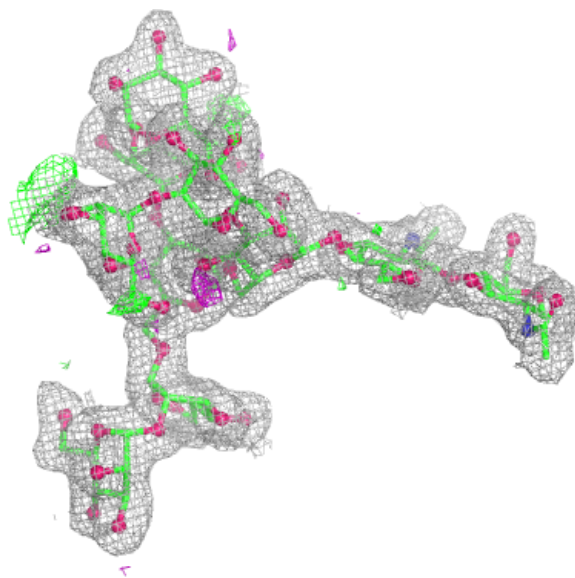
**Electron density around Chain F:**

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



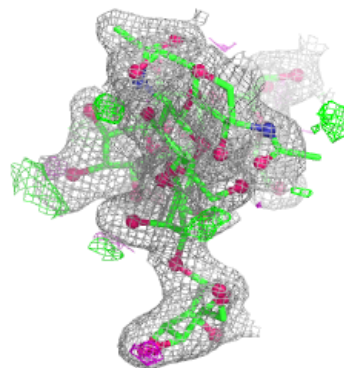
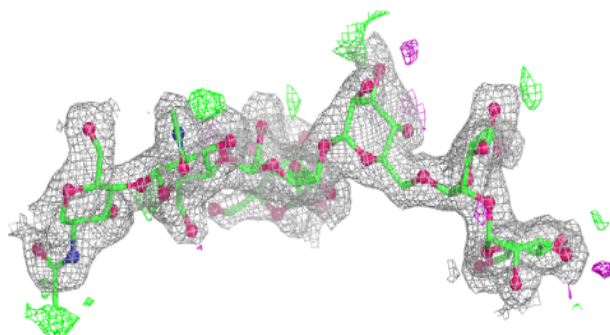
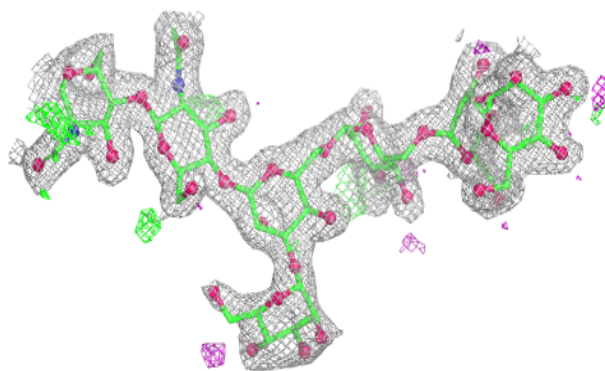
**Electron density around Chain M:**

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

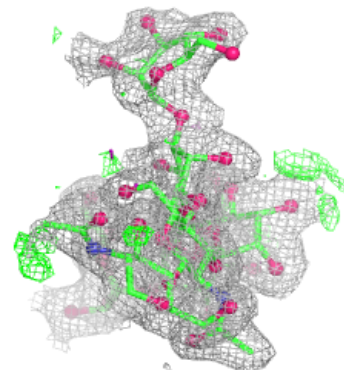
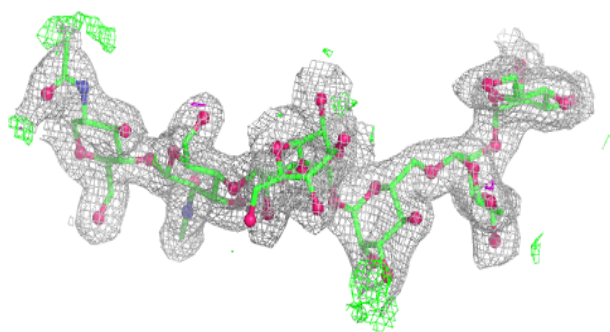
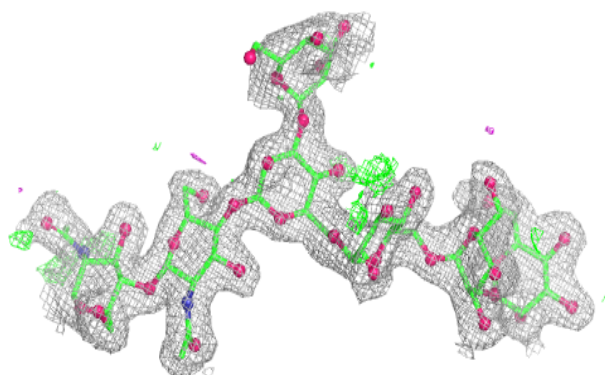


**Electron density around Chain H:**

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

**Electron density around Chain O:**

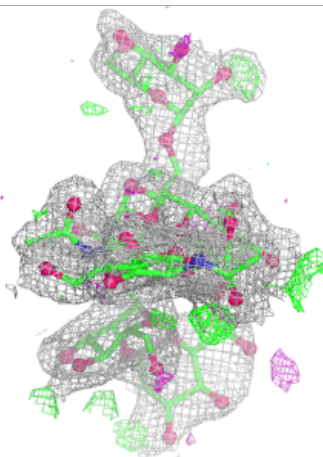
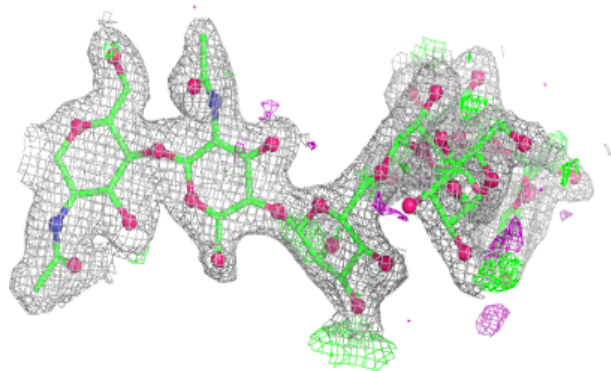
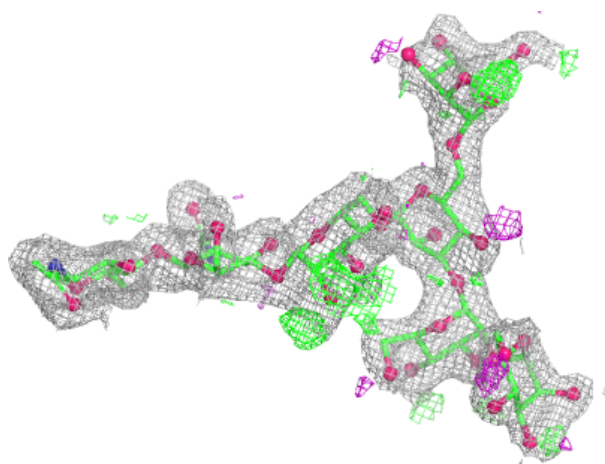
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





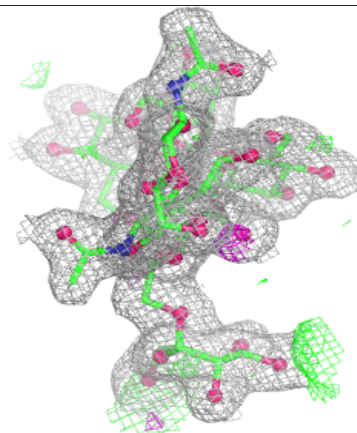
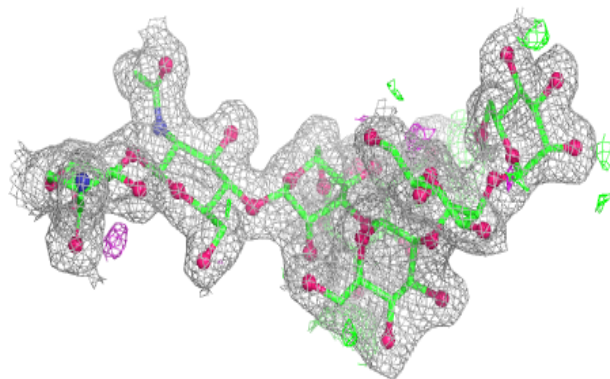
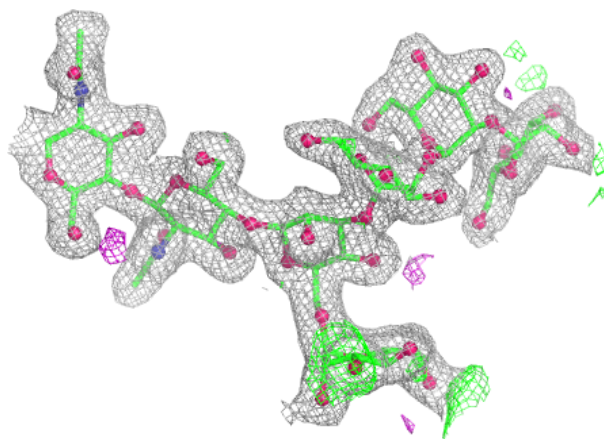
**Electron density around Chain I:**

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



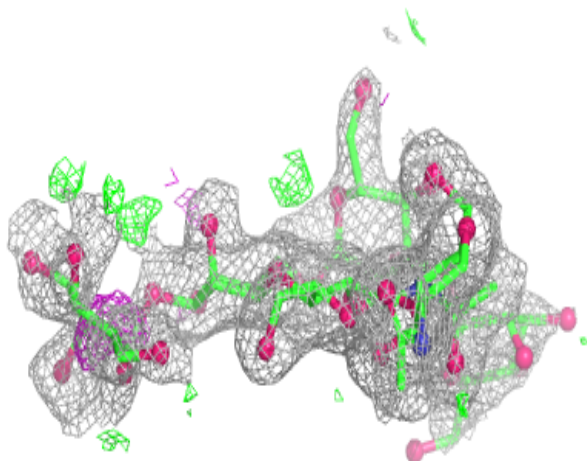
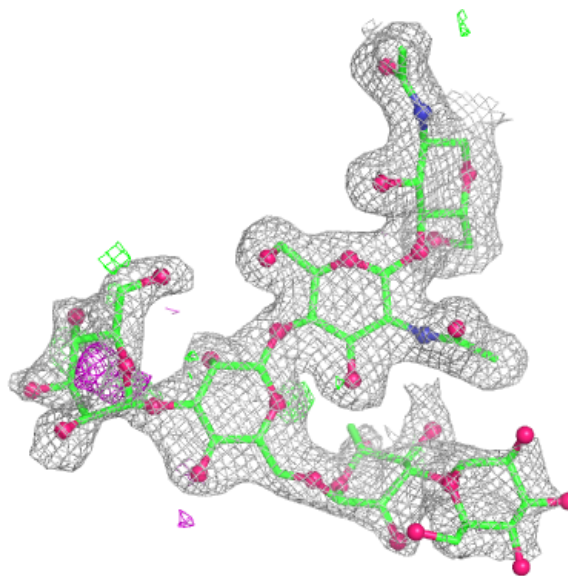
**Electron density around Chain J:**

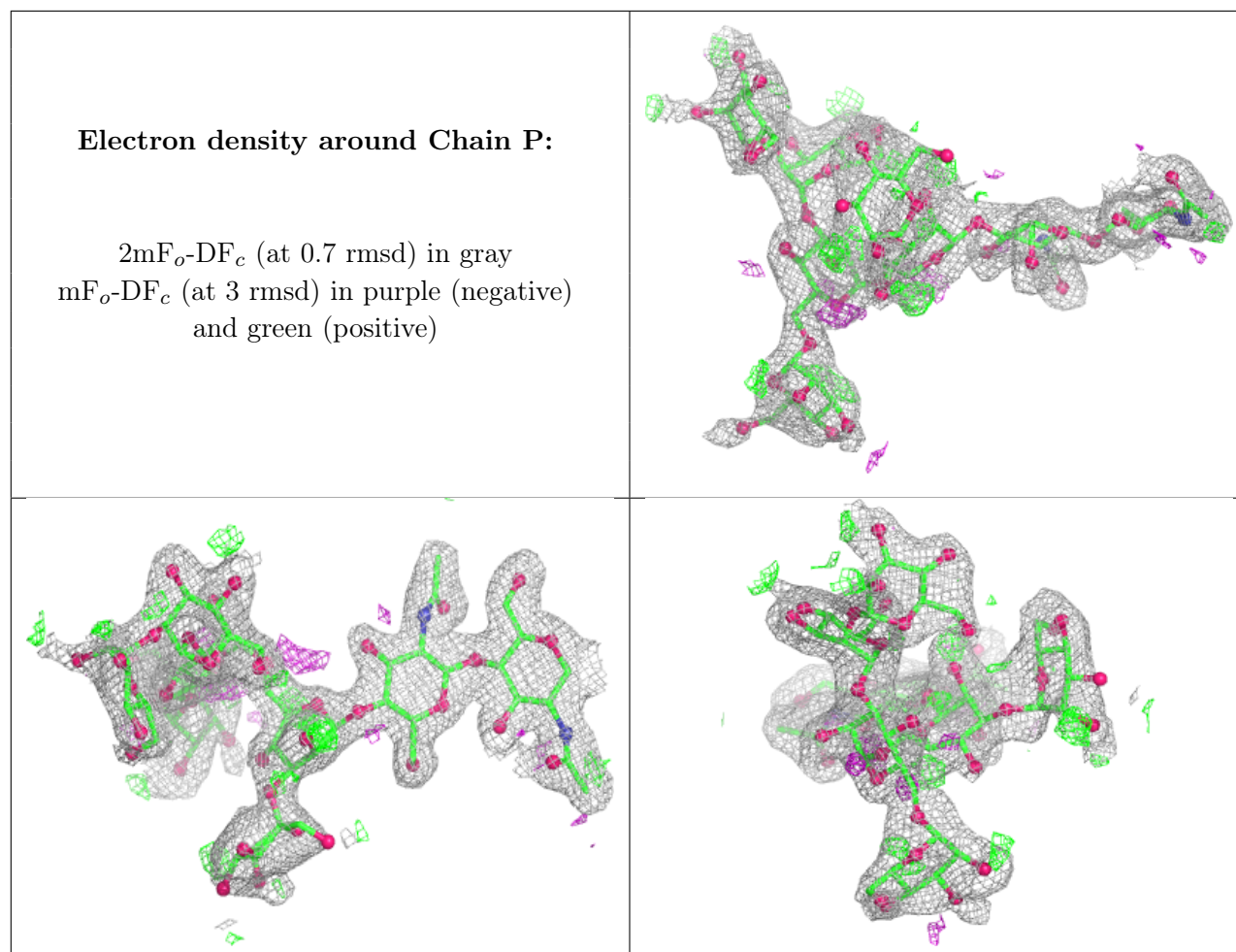
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain K:**

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





## 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( $\text{\AA}^2$ )	Q<0.9
11	NAG	B	908	14/15	0.74	0.15	43,53,59,63	0
11	NAG	A	905	14/15	0.80	0.13	51,58,69,75	0
12	MRD	A	941	8/8	0.82	0.18	34,40,45,47	0
12	MRD	A	940	8/8	0.85	0.14	21,29,41,43	0
11	NAG	B	946	14/15	0.85	0.11	38,50,53,55	0
12	MRD	B	948	8/8	0.85	0.17	31,44,52,53	0
12	MRD	B	949	8/8	0.88	0.11	21,28,35,39	0
12	MRD	B	950	8/8	0.91	0.12	33,43,45,48	0
13	NA	B	951	1/1	0.91	0.08	32,32,32,32	0
14	CGB	A	943	12/12	0.91	0.10	21,28,33,34	0
11	NAG	A	938	14/15	0.92	0.09	33,42,49,50	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	CGB	B	952	12/12	0.94	0.08	15,23,29,29	0
12	MRD	A	939	8/8	0.95	0.07	20,25,29,31	0
11	NAG	B	947	14/15	0.95	0.06	25,31,36,38	0
13	NA	A	942	1/1	0.95	0.06	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.