



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:06 AM BST

PDB ID : 6N08  
Title : Crystal structure of hemagglutinin from influenza virus A/Netherlands/209/1980 (H3N2)  
Authors : Dai, Y.N.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2018-11-06  
Resolution : 1.92 Å(reported)

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

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

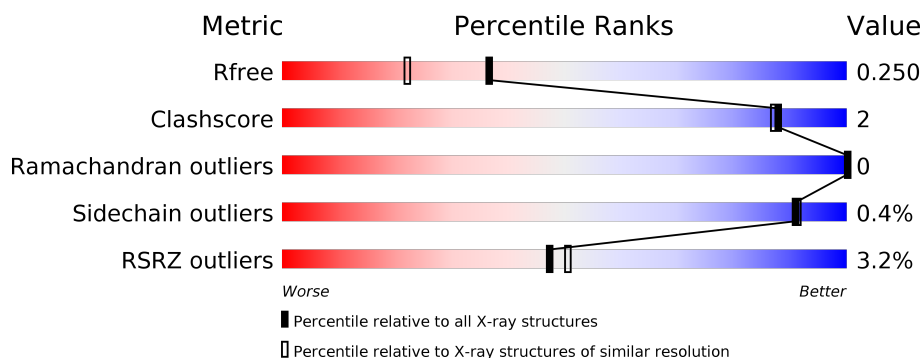
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	497	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	497	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>
1	C	497	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>.</div> <div>.</div> </div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>
2	G	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 50%50%
2	J	2	 100%
2	K	2	 100%
2	M	2	 50%50%
3	E	3	 67%33%
3	I	3	 100%
3	L	3	 67%33%
3	N	3	 100%

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
4	NAG	B	700	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	1	0
			3858	2406	682	752	18			
1	B	488	Total	C	N	O	S	0	1	0
			3858	2406	682	752	18			
1	C	488	Total	C	N	O	S	0	1	0
			3858	2406	682	752	18			

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



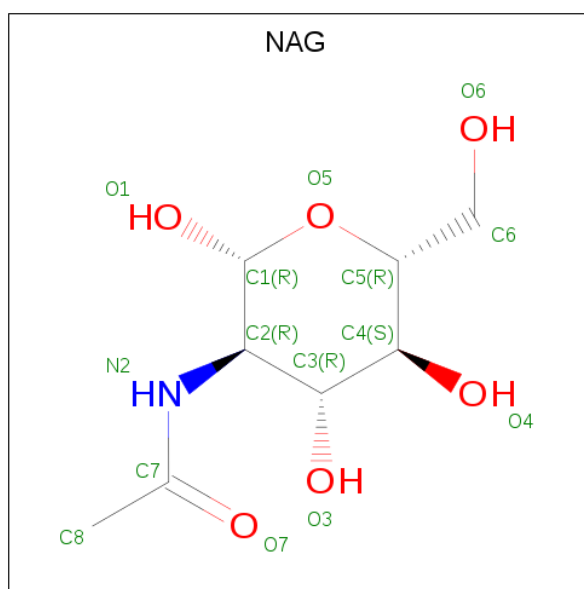
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	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			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

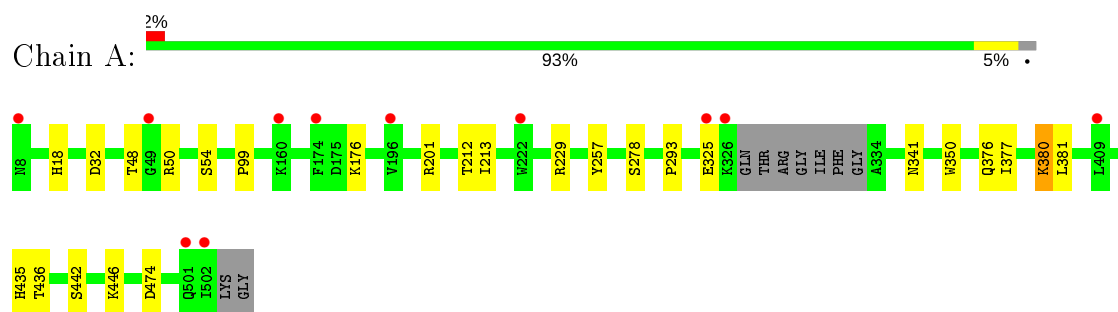
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	375	Total	O	0	0
			375	375		
5	B	297	Total	O	0	0
			297	297		
5	C	363	Total	O	0	0
			363	363		

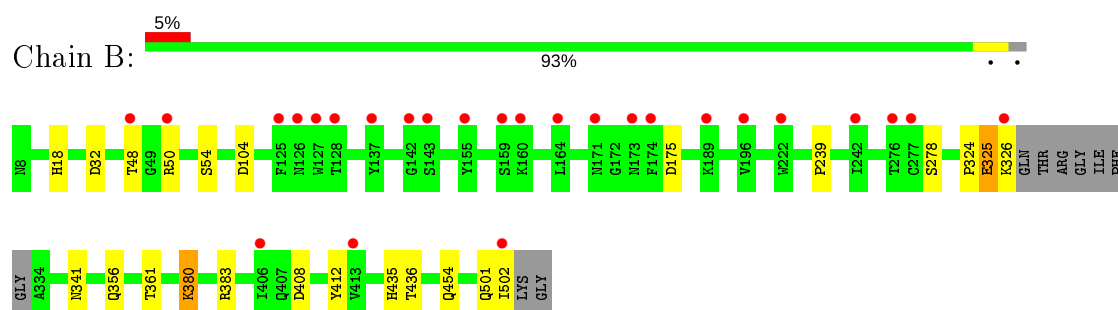
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

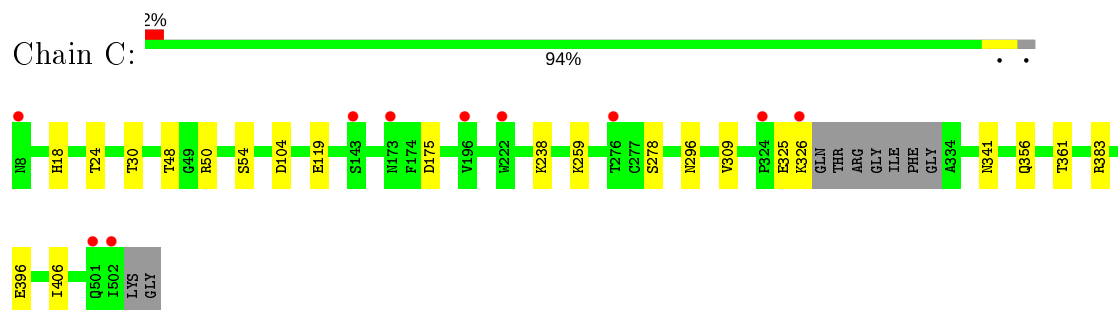
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



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



MAG1  
MAG2

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

Chain F:  100%

MAG1  
MAG2

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

Chain G:  50% 50%

MAG1  
MAG2

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

Chain H:  50% 50%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain M:  50% 50%

MAG1  
MAG2



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

Chain E:  67% 33%

UAG1  
UAG2  
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 I:  100%

UAG1  
UAG2  
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:  67% 33%

UAG1  
UAG2  
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:  100%

UAG1  
UAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.99Å 188.77Å 108.76Å 90.00° 109.82° 90.00°	Depositor
Resolution (Å)	46.34 – 1.92 46.34 – 1.92	Depositor EDS
% Data completeness (in resolution range)	89.7 (46.34-1.92) 89.7 (46.34-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.224 , 0.252 0.224 , 0.250	Depositor DCC
$R_{free}$ test set	12939 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: BMA, 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	0.77	3/3941 (0.1%)	0.74	4/5337 (0.1%)
1	B	0.68	3/3941 (0.1%)	0.71	4/5337 (0.1%)
1	C	0.72	1/3941 (0.0%)	0.72	2/5337 (0.0%)
All	All	0.72	7/11823 (0.1%)	0.73	10/16011 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	GLU	CB-CG	7.57	1.66	1.52
1	C	396	GLU	CB-CG	6.76	1.65	1.52
1	A	325	GLU	CB-CG	6.05	1.63	1.52
1	A	350	TRP	CE3-CZ3	5.67	1.48	1.38
1	B	325	GLU	CG-CD	5.53	1.60	1.51
1	B	412	TYR	CE1-CZ	5.10	1.45	1.38
1	A	325	GLU	CG-CD	5.04	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	LYS	CD-CE-NZ	-8.33	92.54	111.70
1	A	380	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	A	474	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	104	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	201	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	104	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	325	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	A	325	GLU	OE1-CD-OE2	-5.47	116.73	123.30
1	C	325	GLU	CG-CD-OE1	5.29	128.88	118.30
1	B	408	ASP	CB-CG-OD1	5.17	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3858	0	3724	14	0
1	B	3858	0	3725	19	0
1	C	3858	0	3724	17	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
3	E	39	0	34	0	0
3	I	39	0	34	0	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	A	42	0	39	1	0
4	B	14	0	13	0	0
4	C	28	0	26	1	0
5	A	375	0	0	0	0
5	B	297	0	0	0	0
5	C	363	0	0	0	0
All	All	13045	0	11562	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (46) 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:C:326:LYS:H	1:C:341:ASN:HD22	1.33	0.76
1:B:325:GLU:HA	1:B:341:ASN:HD22	1.51	0.75
1:C:356:GLN:HG2	1:C:361:THR:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:OD1	1:B:383:ARG:NH1	2.23	0.72
1:C:326:LYS:N	1:C:341:ASN:HD22	1.90	0.69
1:B:326:LYS:N	1:B:341:ASN:HD22	1.96	0.62
1:B:32:ASP:OD1	1:C:383:ARG:NH1	2.33	0.61
4:A:704:NAG:H3	4:A:704:NAG:H83	1.82	0.60
1:B:356:GLN:HG2	1:B:361:THR:HG22	1.83	0.59
1:A:380:LYS:HZ1	1:A:435:HIS:CE1	2.21	0.59
1:B:325:GLU:HA	1:B:341:ASN:ND2	2.19	0.58
1:B:326:LYS:H	1:B:341:ASN:HD22	1.49	0.58
1:B:380:LYS:HE2	1:B:436:THR:OG1	2.05	0.57
1:A:212:THR:C	1:A:213:ILE:HD12	2.26	0.55
1:B:325:GLU:CA	1:B:341:ASN:HD22	2.19	0.55
1:B:326:LYS:H	1:B:341:ASN:ND2	2.07	0.52
1:B:326:LYS:HG2	1:B:341:ASN:HB3	1.93	0.51
1:C:24:THR:HB	4:C:601:NAG:H81	1.94	0.49
1:A:48:THR:HG21	1:A:50:ARG:NH1	2.28	0.49
1:A:376:GLN:HG2	1:C:30:THR:HG23	1.94	0.49
1:C:175:ASP:OD1	1:C:238:LYS:HD2	2.14	0.48
1:C:54:SER:O	1:C:278:SER:HA	2.13	0.48
1:B:324:PRO:O	1:B:341:ASN:HB2	2.14	0.47
1:B:48:THR:HG21	1:B:50:ARG:NH1	2.29	0.47
1:C:48:THR:HG21	1:C:50:ARG:NH1	2.31	0.46
1:A:176:LYS:HD3	1:A:257:TYR:CD1	2.50	0.46
1:B:380:LYS:NZ	1:B:435:HIS:ND1	2.61	0.46
1:C:296[A]:ASN:ND2	1:C:309:VAL:O	2.48	0.46
1:A:442:SER:O	1:A:446:LYS:HG3	2.16	0.46
1:B:356:GLN:HG2	1:B:361:THR:CG2	2.46	0.45
1:B:54:SER:O	1:B:278:SER:HA	2.16	0.45
1:A:377:ILE:O	1:A:380:LYS:HB2	2.17	0.45
1:A:435:HIS:NE2	1:C:30:THR:OG1	2.47	0.44
1:A:380:LYS:HE2	1:A:436:THR:OG1	2.18	0.44
1:C:119:GLU:CD	1:C:259:LYS:HD2	2.38	0.44
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.99	0.44
1:C:356:GLN:HG2	1:C:361:THR:CG2	2.45	0.43
1:A:54:SER:HB2	1:A:278:SER:HB3	2.00	0.43
1:A:435:HIS:CE1	1:C:30:THR:HG1	2.37	0.43
1:B:54:SER:HB2	1:B:278:SER:HB3	1.99	0.43
1:C:238:LYS:HB3	1:C:238:LYS:HE3	1.74	0.42
1:B:175:ASP:OD1	1:B:239:PRO:HD3	2.20	0.41
1:C:406:ILE:HG23	1:C:406:ILE:HD12	1.77	0.41
1:A:293:PRO:HG3	1:A:381:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:OE2	1:C:259:LYS:HD2	2.20	0.41
1:B:501:GLN:O	1:B:502:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/497 (98%)	469 (97%)	16 (3%)	0	100	100
1	B	485/497 (98%)	468 (96%)	17 (4%)	0	100	100
1	C	485/497 (98%)	471 (97%)	14 (3%)	0	100	100
All	All	1455/1491 (98%)	1408 (97%)	47 (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	428/433 (99%)	426 (100%)	2 (0%)	88	89
1	B	428/433 (99%)	426 (100%)	2 (0%)	88	89
1	C	428/433 (99%)	427 (100%)	1 (0%)	93	94
All	All	1284/1299 (99%)	1279 (100%)	5 (0%)	91	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	341	ASN
1	B	18	HIS
1	B	454	GLN
1	C	18	HIS

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

Mol	Chain	Res	Type
1	B	341	ASN
1	C	341	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

26 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	D	1	1,2	14,14,15	0.95	1 (7%)	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	0.66	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	0.68	0
3	NAG	E	2	3	14,14,15	0.44	0	17,19,21	0.62	0
3	BMA	E	3	3	11,11,12	1.01	0	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	F	1	1,2	14,14,15	0.60	0	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	G	1	1,2	14,14,15	0.71	1 (7%)	17,19,21	0.52	0
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	0.61	0
2	NAG	H	1	1,2	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
2	NAG	H	2	2	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	I	1	1,3	14,14,15	1.05	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	I	2	3	14,14,15	0.18	0	17,19,21	0.98	2 (11%)
3	BMA	I	3	3	11,11,12	4.06	7 (63%)	15,15,17	2.82	9 (60%)
2	NAG	J	1	1,2	14,14,15	0.56	0	17,19,21	0.57	0
2	NAG	J	2	2	14,14,15	0.41	0	17,19,21	0.40	0
2	NAG	K	1	1,2	14,14,15	0.61	0	17,19,21	0.78	0
2	NAG	K	2	2	14,14,15	0.49	0	17,19,21	0.58	0
3	NAG	L	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	0.46	0
3	NAG	L	2	3	14,14,15	0.49	0	17,19,21	0.41	0
3	BMA	L	3	3	11,11,12	1.00	0	15,15,17	0.85	0
2	NAG	M	1	1,2	14,14,15	0.90	1 (7%)	17,19,21	0.51	0
2	NAG	M	2	2	14,14,15	0.39	0	17,19,21	0.42	0
3	NAG	N	1	1,3	14,14,15	0.58	0	17,19,21	0.90	1 (5%)
3	NAG	N	2	3	14,14,15	0.64	0	17,19,21	0.85	1 (5%)
3	BMA	N	3	3	11,11,12	2.79	4 (36%)	15,15,17	2.90	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	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	1/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	BMA	C4-C3	-7.65	1.32	1.52
3	N	3	BMA	C2-C3	-5.98	1.43	1.52
3	I	3	BMA	O2-C2	5.83	1.55	1.43
3	N	3	BMA	O5-C1	5.53	1.52	1.43
3	I	3	BMA	O3-C3	5.49	1.55	1.43
3	I	3	BMA	O6-C6	4.01	1.59	1.42
3	I	3	BMA	O5-C5	3.95	1.51	1.43
3	I	3	BMA	O4-C4	3.42	1.51	1.43
3	I	3	BMA	C4-C5	3.39	1.60	1.53
2	D	1	NAG	O5-C1	3.27	1.48	1.43
3	I	1	NAG	O5-C1	3.12	1.48	1.43
3	L	1	NAG	O5-C1	3.04	1.48	1.43
2	M	1	NAG	C1-C2	2.74	1.56	1.52
3	N	3	BMA	O5-C5	2.40	1.48	1.43
2	G	1	NAG	O5-C1	2.34	1.47	1.43
3	N	3	BMA	O3-C3	2.16	1.48	1.43
3	I	1	NAG	C1-C2	2.14	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	BMA	O2-C2-C3	-7.31	95.49	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	BMA	O3-C3-C4	-5.38	97.91	110.35
3	I	3	BMA	O2-C2-C3	-4.44	101.24	110.14
3	I	3	BMA	O5-C5-C4	-4.25	100.49	110.83
3	I	3	BMA	O4-C4-C3	-4.20	100.64	110.35
3	N	3	BMA	O5-C5-C4	-4.09	100.89	110.83
3	N	3	BMA	O4-C4-C3	-3.68	101.84	110.35
3	I	3	BMA	O3-C3-C4	-3.65	101.92	110.35
3	I	3	BMA	C2-C3-C4	-3.12	105.50	110.89
3	E	3	BMA	C1-O5-C5	3.03	116.30	112.19
3	N	3	BMA	O6-C6-C5	-2.96	101.14	111.29
3	N	2	NAG	C1-O5-C5	2.77	115.94	112.19
3	I	3	BMA	O3-C3-C2	2.76	115.28	109.99
3	I	3	BMA	C1-C2-C3	-2.62	106.44	109.67
3	I	3	BMA	O2-C2-C1	-2.59	103.85	109.15
2	H	1	NAG	C1-O5-C5	2.54	115.64	112.19
3	N	1	NAG	O4-C4-C5	-2.43	103.27	109.30
3	I	2	NAG	O4-C4-C3	-2.42	104.77	110.35
3	I	2	NAG	O4-C4-C5	-2.41	103.32	109.30
3	I	1	NAG	C2-N2-C7	2.40	126.32	122.90
3	I	3	BMA	O5-C1-C2	-2.31	107.20	110.77
2	D	2	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	BMA	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	N	3	BMA	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6

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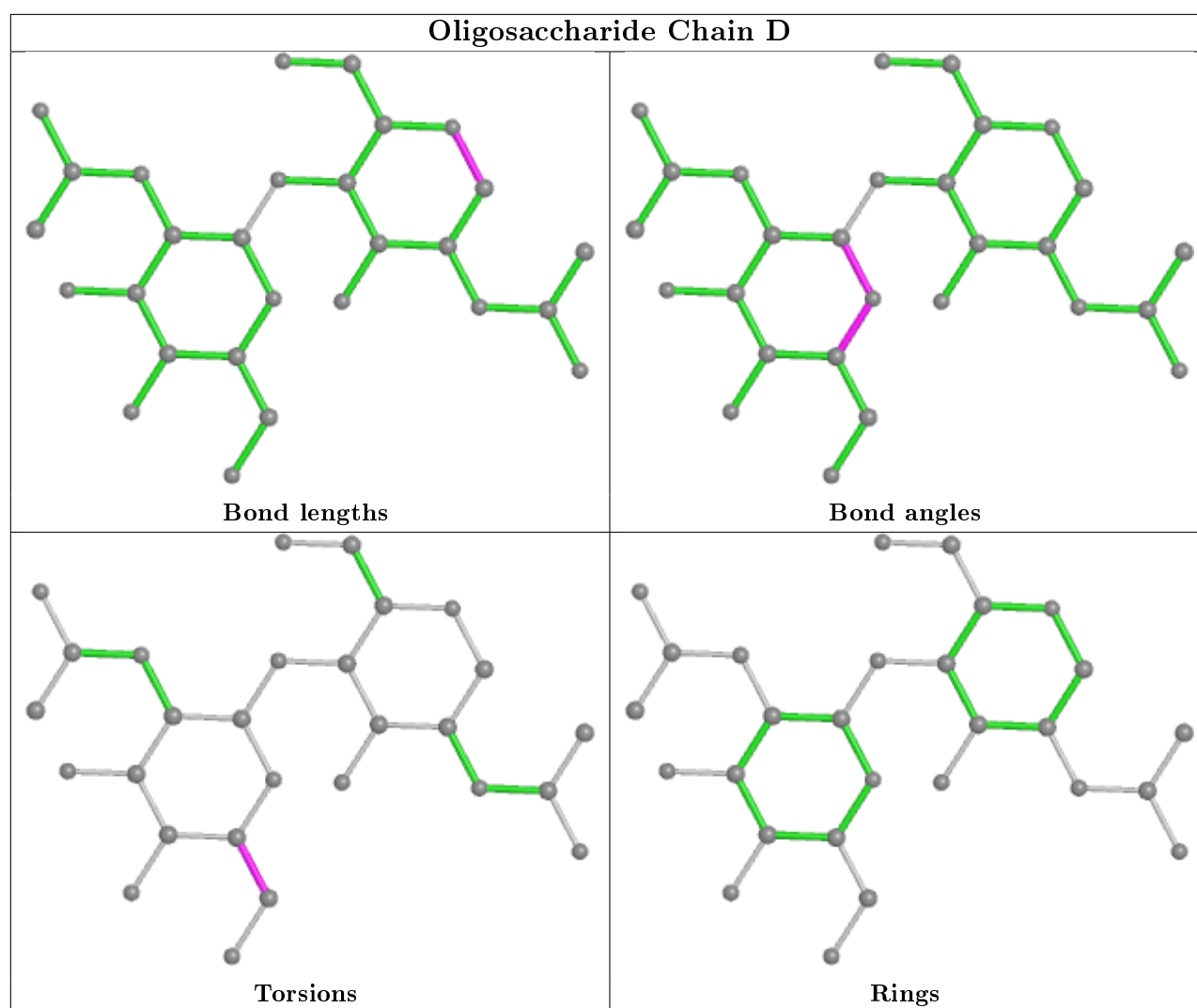
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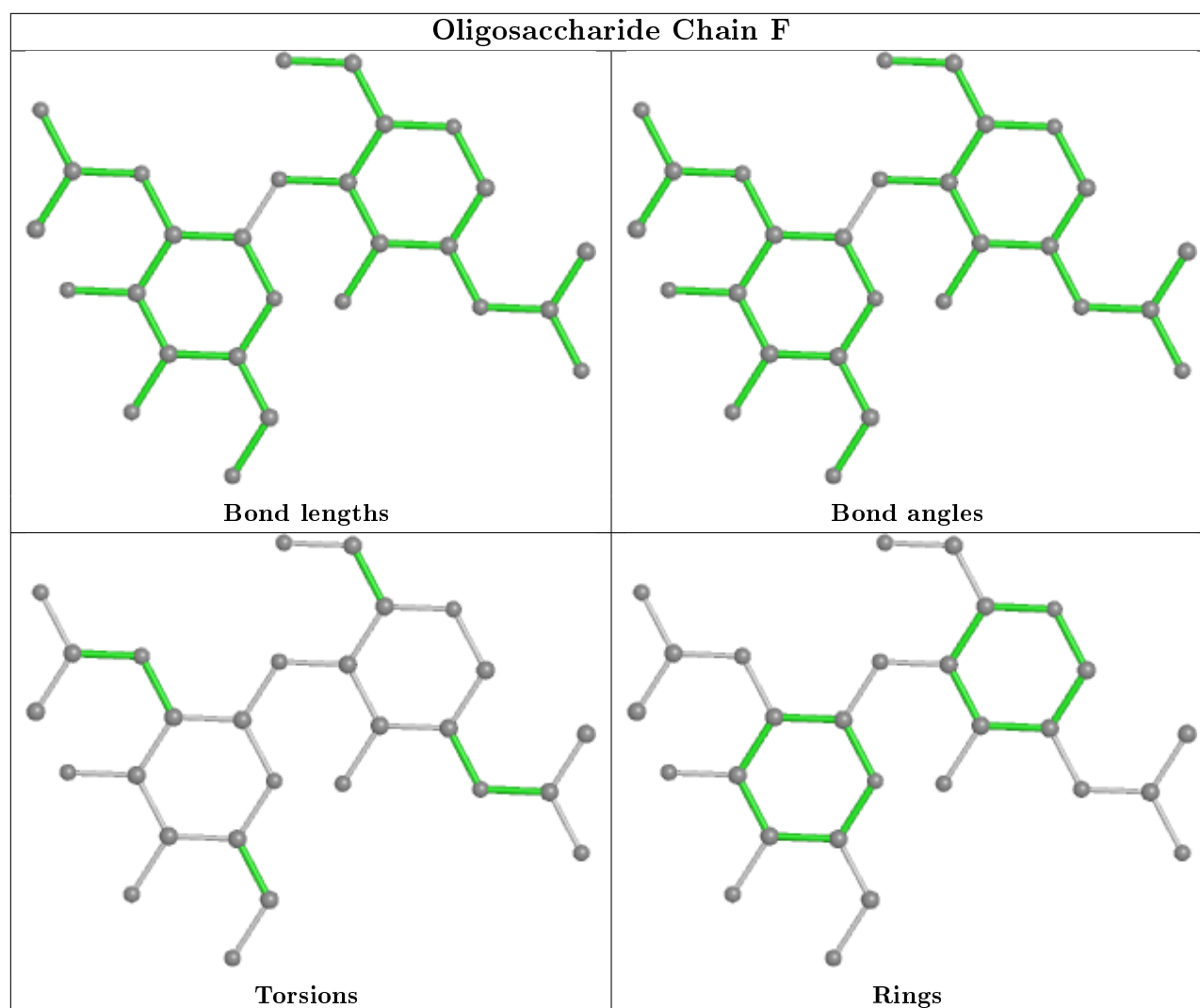
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6

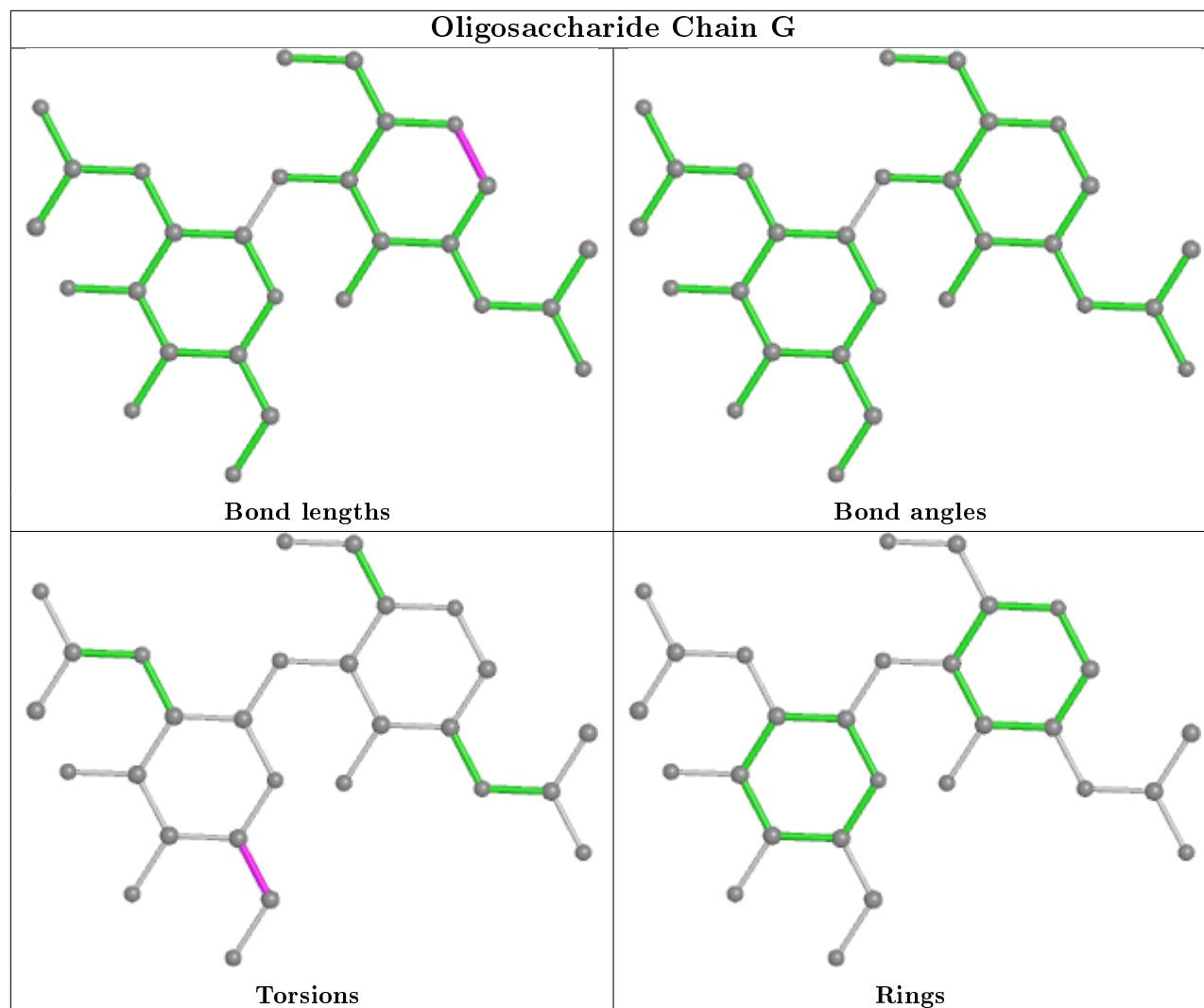
There are no ring outliers.

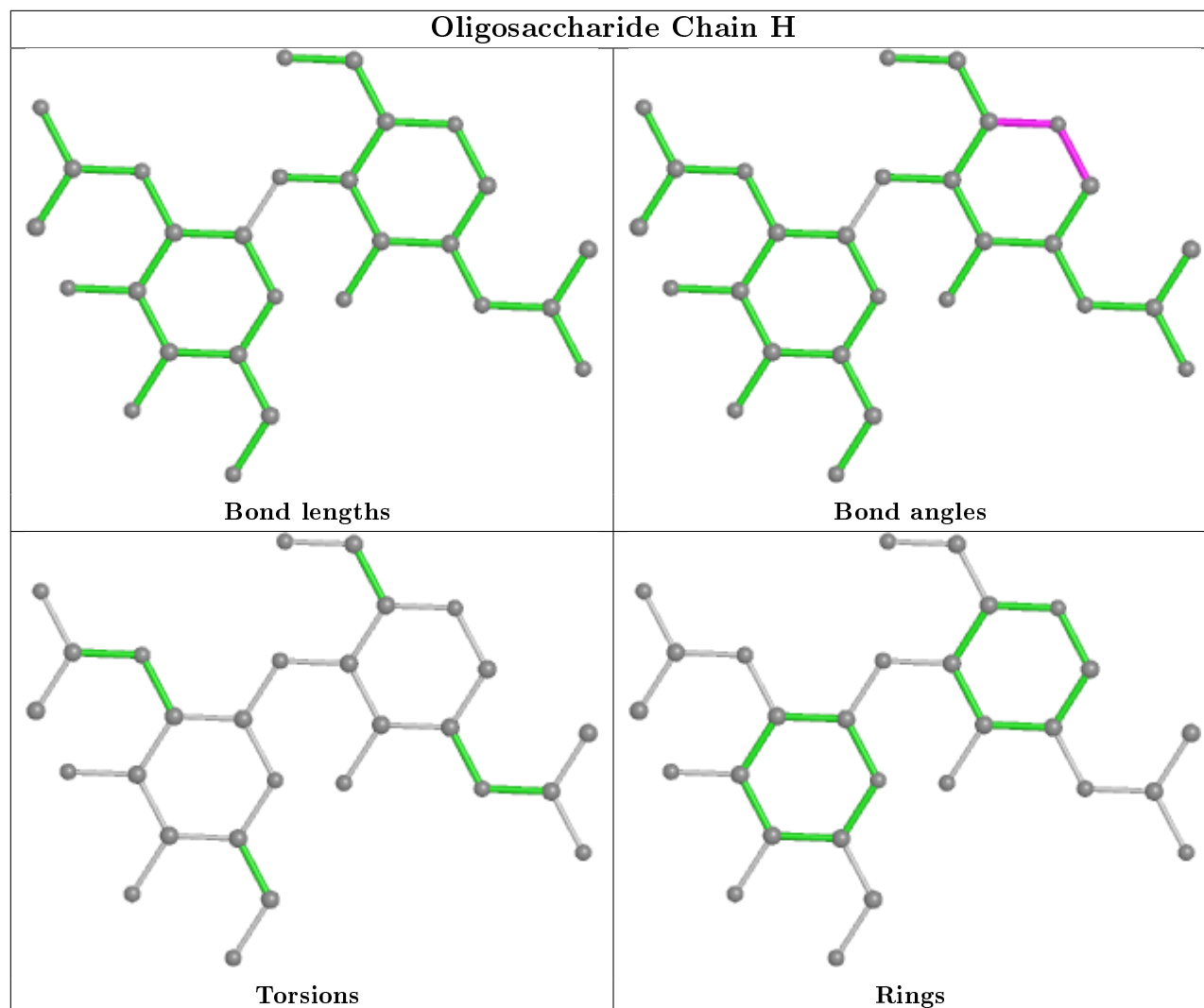
No monomer is involved in short contacts.

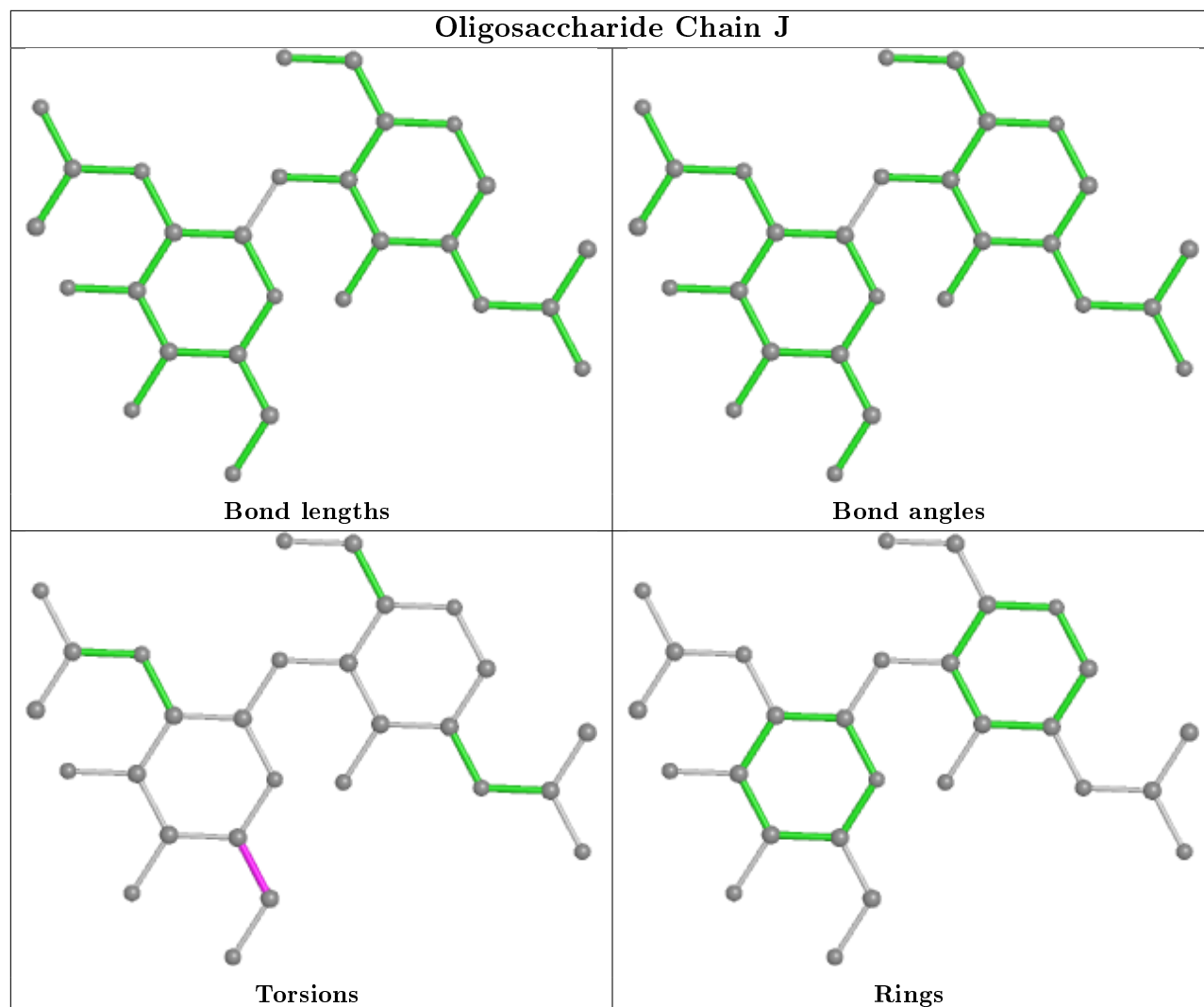
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

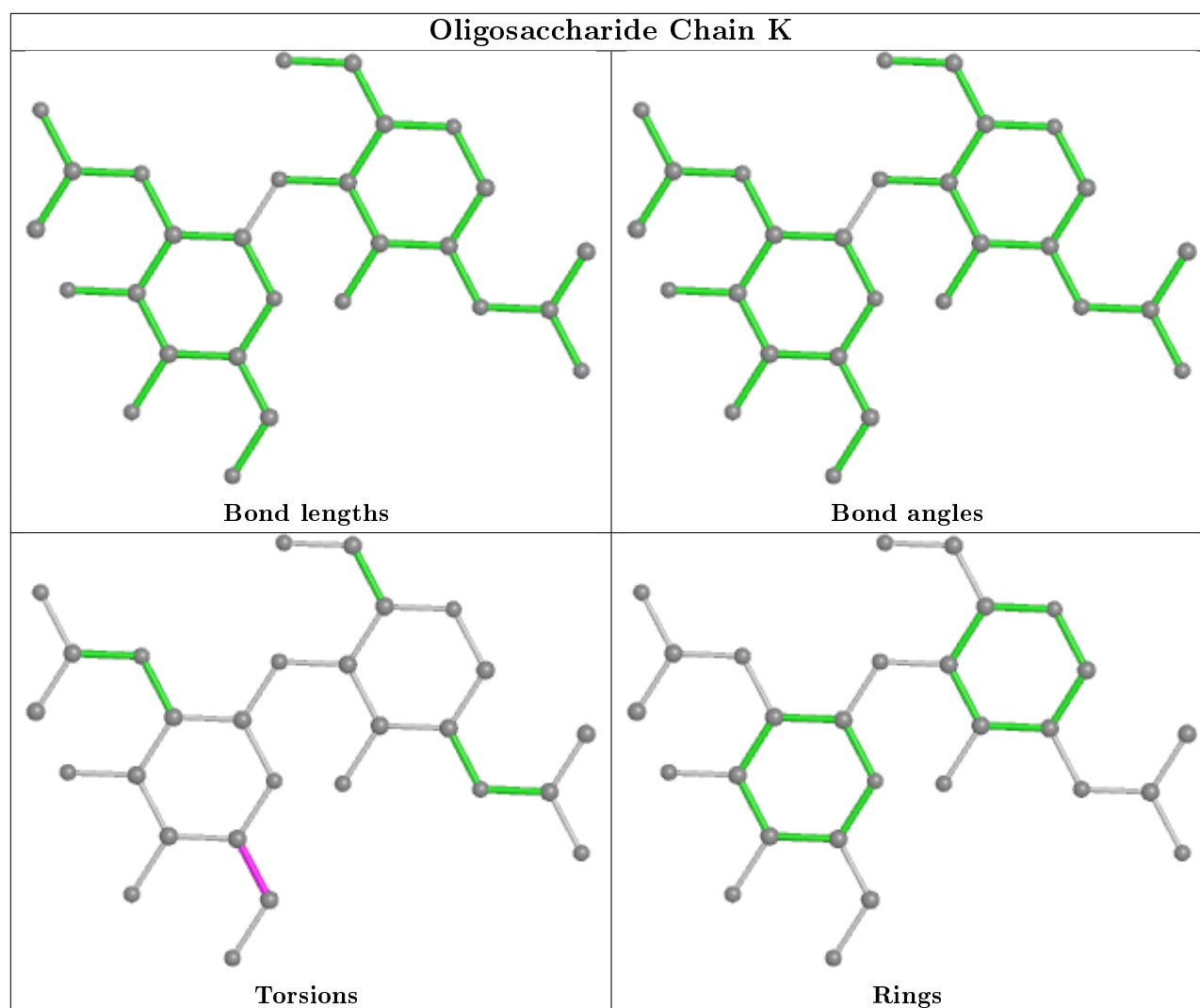




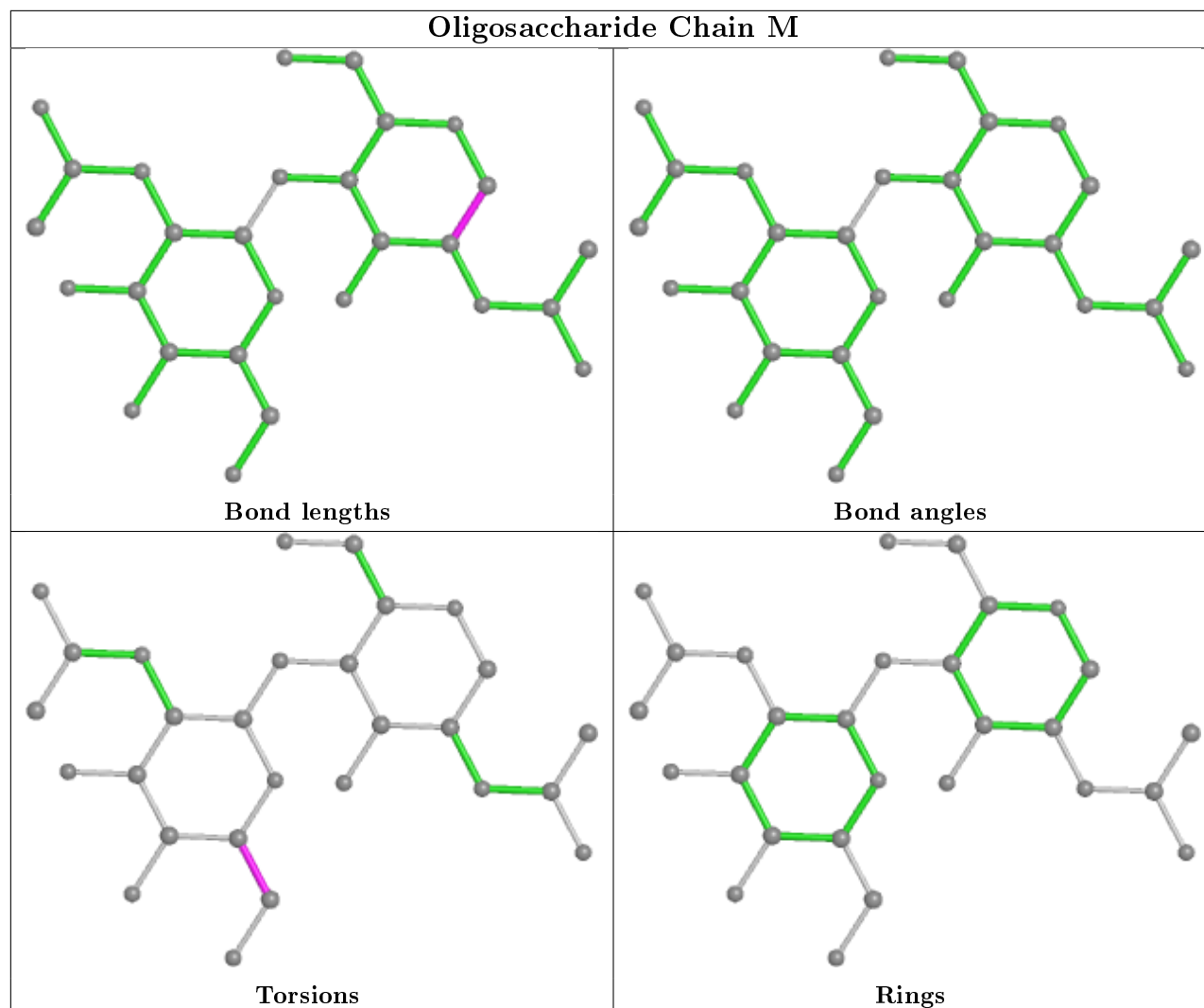


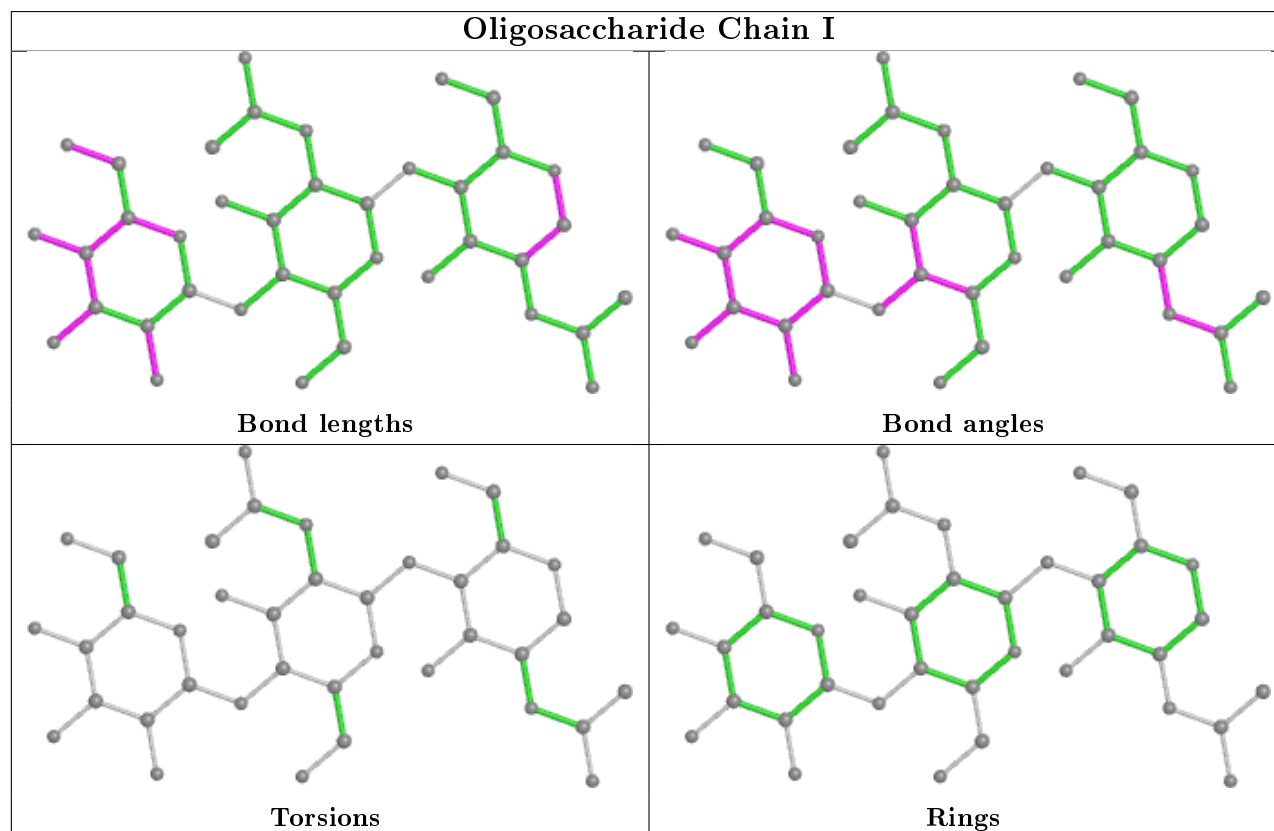
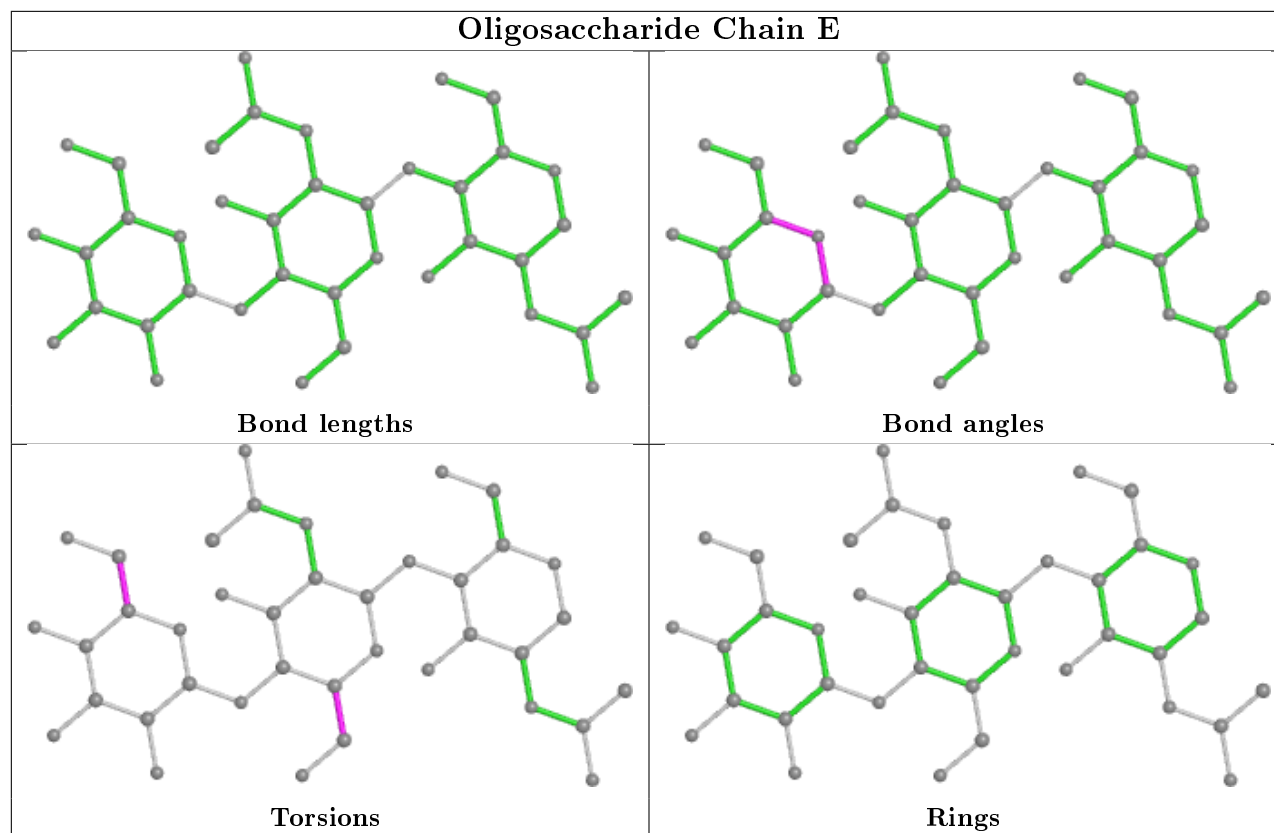


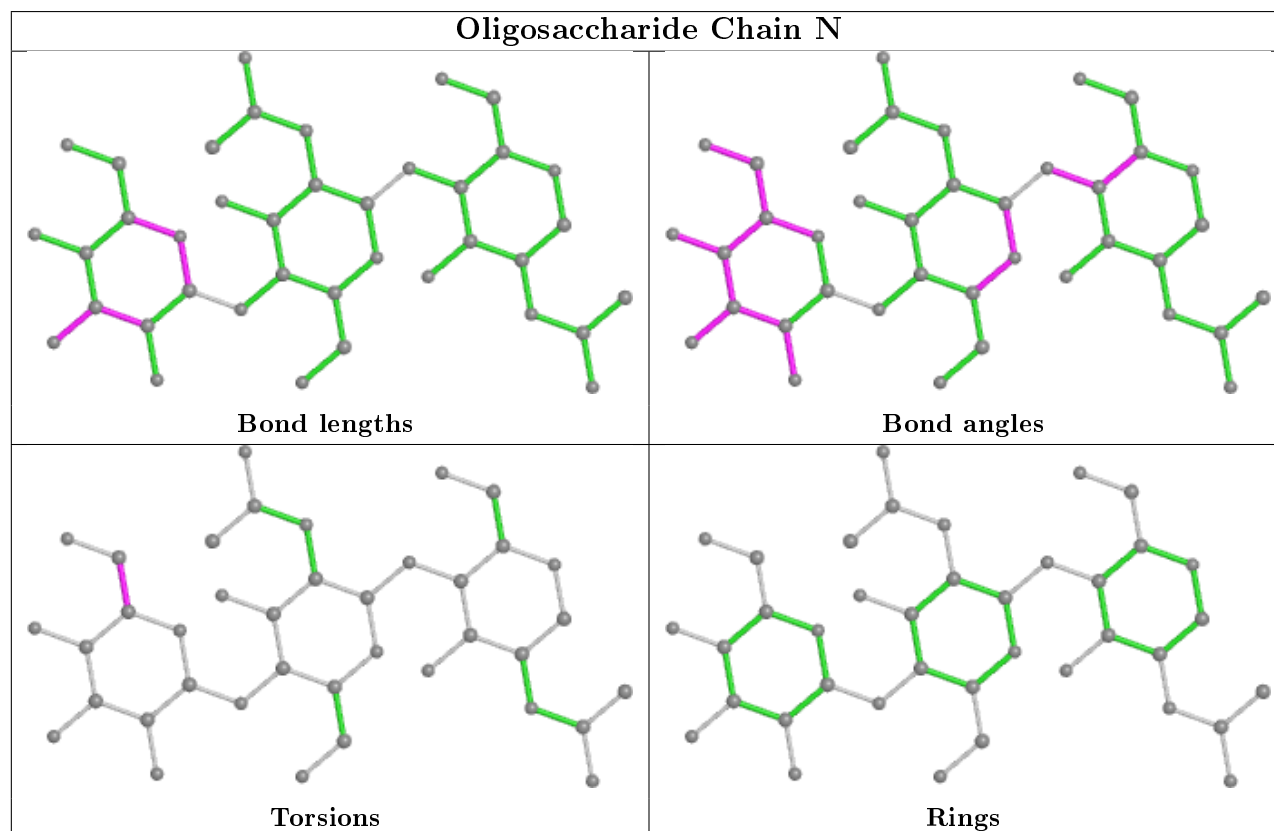
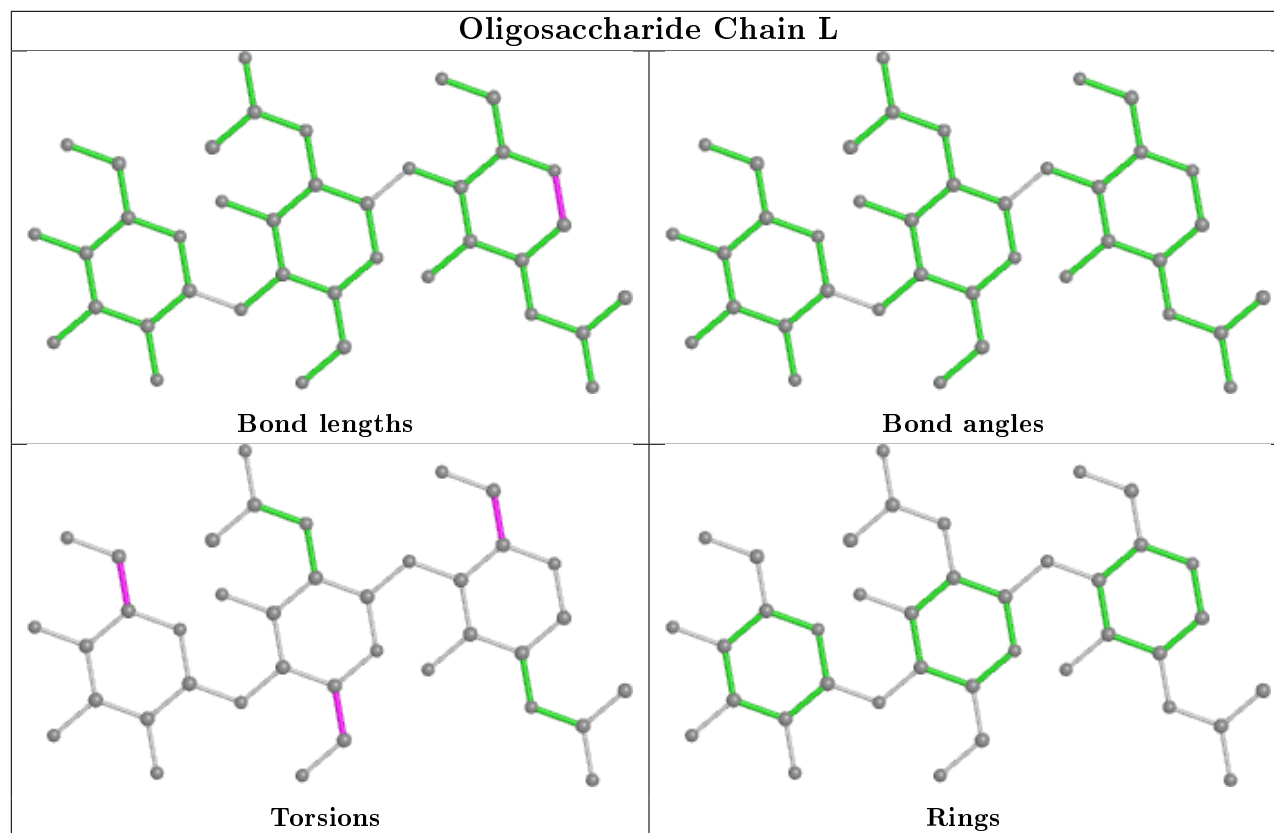












## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	703	1	14,14,15	0.62	0	17,19,21	1.02	1 (5%)
4	NAG	B	700	1	14,14,15	1.10	2 (14%)	17,19,21	0.57	0
4	NAG	C	601	1	14,14,15	1.08	2 (14%)	17,19,21	0.65	0
4	NAG	A	700	1	14,14,15	1.43	2 (14%)	17,19,21	0.79	0
4	NAG	C	604	1	14,14,15	0.67	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	A	704	1	14,14,15	0.63	0	17,19,21	1.44	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	703	1	-	0/6/23/26	0/1/1/1
4	NAG	B	700	1	-	0/6/23/26	0/1/1/1
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	700	1	-	2/6/23/26	0/1/1/1
4	NAG	C	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	NAG	O5-C1	3.75	1.49	1.43
4	A	700	NAG	C1-C2	3.48	1.57	1.52
4	C	601	NAG	C1-C2	3.29	1.57	1.52
4	B	700	NAG	C1-C2	3.25	1.57	1.52
4	B	700	NAG	O5-C1	2.18	1.47	1.43
4	C	601	NAG	O5-C1	2.06	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	NAG	C1-C2	2.01	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	NAG	C2-N2-C7	4.82	129.76	122.90
4	A	703	NAG	C1-O5-C5	3.56	117.02	112.19
4	C	604	NAG	C1-O5-C5	2.51	115.59	112.19
4	A	704	NAG	C1-C2-N2	2.31	114.44	110.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	700	NAG	C4-C5-C6-O6
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
4	A	700	NAG	O5-C5-C6-O6
4	A	704	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	1	0
4	A	704	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	488/497 (98%)	-0.11	11 (2%) 60 63	24, 41, 68, 86	0
1	B	488/497 (98%)	0.08	26 (5%) 26 29	26, 48, 75, 95	0
1	C	488/497 (98%)	-0.11	10 (2%) 65 68	22, 44, 68, 88	0
All	All	1464/1491 (98%)	-0.05	47 (3%) 47 50	22, 44, 71, 95	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	502	ILE	9.2
1	A	502	ILE	7.4
1	B	502	ILE	5.8
1	B	160	LYS	5.1
1	A	8	ASN	4.9
1	B	277	CYS	4.3
1	C	8	ASN	4.3
1	B	174	PHE	4.1
1	B	143	SER	4.0
1	B	222	TRP	3.9
1	B	155	TYR	3.9
1	B	196	VAL	3.8
1	B	189	LYS	3.8
1	C	326	LYS	3.8
1	A	174	PHE	3.5
1	B	326	LYS	3.5
1	A	222	TRP	3.4
1	B	142	GLY	3.2
1	A	326	LYS	3.1
1	A	325	GLU	3.1
1	B	48	THR	3.1
1	C	324	PRO	3.0
1	B	50	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	173	ASN	3.0
1	C	222	TRP	2.9
1	B	126	ASN	2.9
1	B	128	THR	2.6
1	C	143	SER	2.6
1	B	242	ILE	2.6
1	C	173	ASN	2.4
1	C	501	GLN	2.4
1	C	276	THR	2.3
1	B	137	TYR	2.3
1	A	501	GLN	2.2
1	B	276	THR	2.2
1	B	164	LEU	2.2
1	A	196	VAL	2.2
1	B	159	SER	2.1
1	A	409	LEU	2.1
1	A	160	LYS	2.1
1	A	49	GLY	2.1
1	C	196	VAL	2.1
1	B	171	ASN	2.1
1	B	125	PHE	2.0
1	B	127	TRP	2.0
1	B	413	VAL	2.0
1	B	406	ILE	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
3	BMA	I	3	11/12	0.67	0.26	72,79,84,86	0
2	NAG	J	2	14/15	0.69	0.32	78,86,94,95	0
3	BMA	E	3	11/12	0.79	0.27	79,81,89,89	0
2	NAG	M	2	14/15	0.82	0.28	81,86,94,95	0

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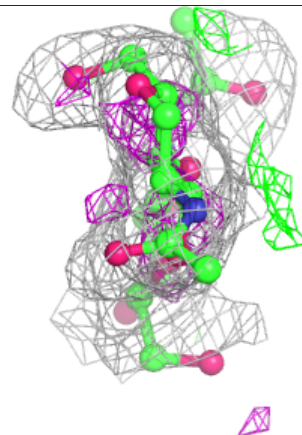
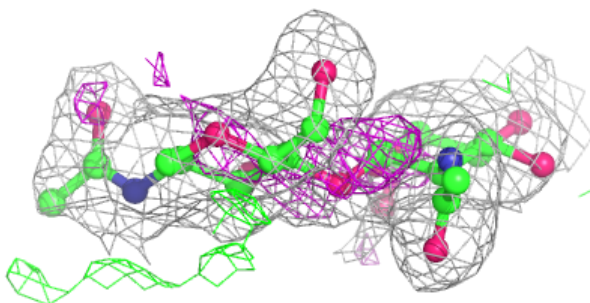
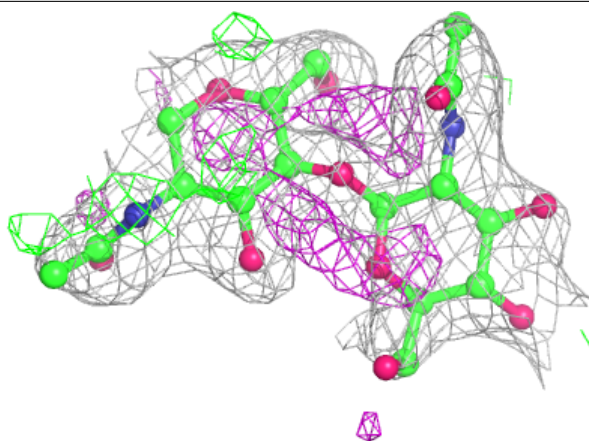
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	2	14/15	0.82	0.32	69,85,90,91	0
2	NAG	G	2	14/15	0.84	0.34	81,91,97,99	0
3	BMA	L	3	11/12	0.84	0.24	86,88,90,91	0
2	NAG	K	2	14/15	0.85	0.31	64,78,86,88	0
2	NAG	H	2	14/15	0.86	0.31	93,98,102,104	0
3	BMA	N	3	11/12	0.86	0.27	63,73,77,80	0
2	NAG	H	1	14/15	0.90	0.26	49,59,72,85	0
3	NAG	L	2	14/15	0.90	0.21	43,72,83,85	0
2	NAG	F	2	14/15	0.90	0.20	79,84,90,93	0
2	NAG	D	1	14/15	0.91	0.21	40,51,56,65	0
3	NAG	N	1	14/15	0.91	0.18	39,51,61,62	0
2	NAG	K	1	14/15	0.92	0.17	50,55,63,66	0
2	NAG	M	1	14/15	0.92	0.15	42,53,60,72	0
3	NAG	N	2	14/15	0.94	0.20	53,65,74,75	0
3	NAG	E	2	14/15	0.94	0.17	51,61,75,78	0
3	NAG	L	1	14/15	0.94	0.13	40,55,60,61	0
2	NAG	G	1	14/15	0.95	0.15	50,63,67,77	0
2	NAG	F	1	14/15	0.95	0.16	44,52,61,70	0
3	NAG	I	2	14/15	0.95	0.16	54,66,74,74	0
3	NAG	I	1	14/15	0.95	0.14	48,59,64,67	0
2	NAG	J	1	14/15	0.96	0.15	39,54,57,68	0
3	NAG	E	1	14/15	0.96	0.13	38,54,65,71	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.



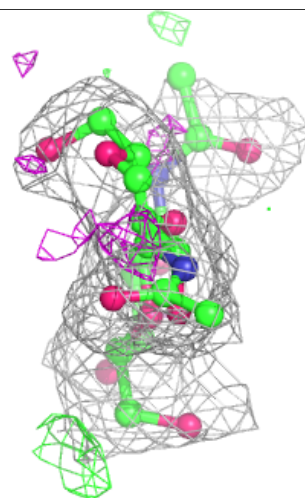
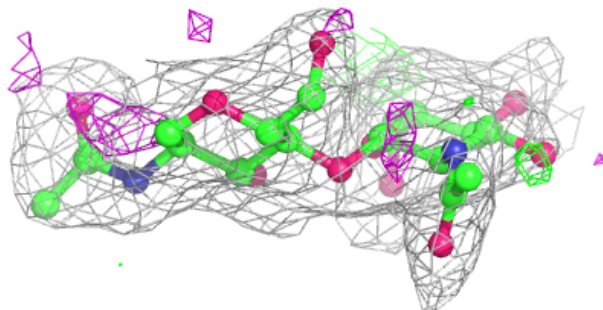
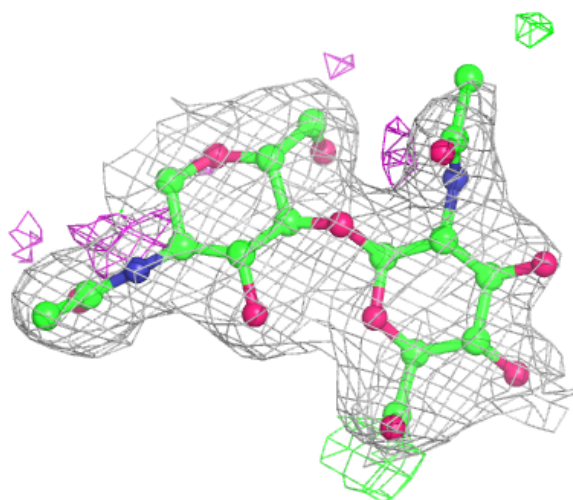
**Electron density around Chain D:**

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



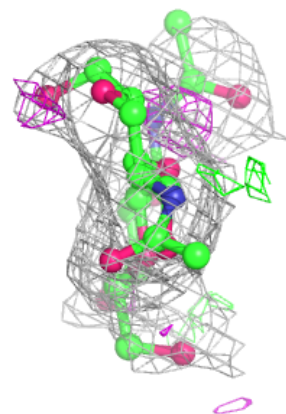
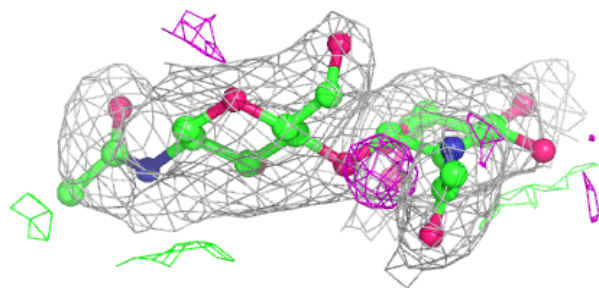
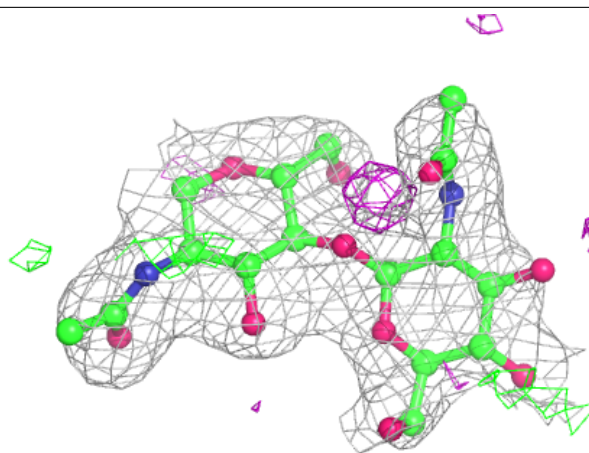
**Electron density around Chain F:**

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



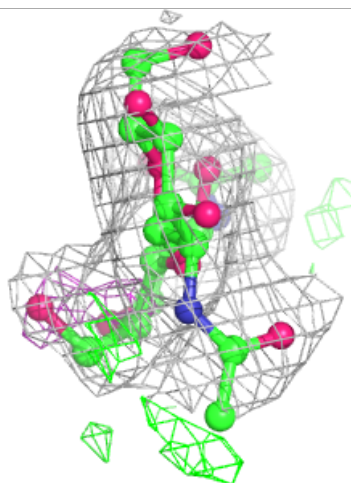
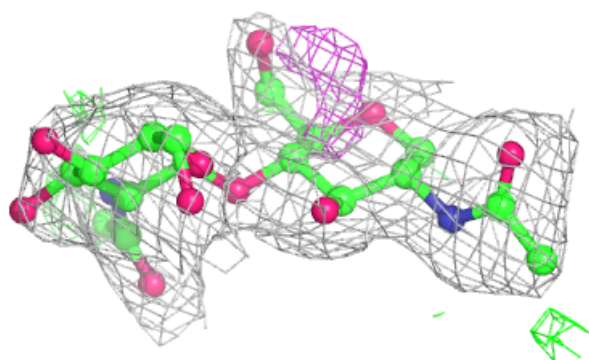
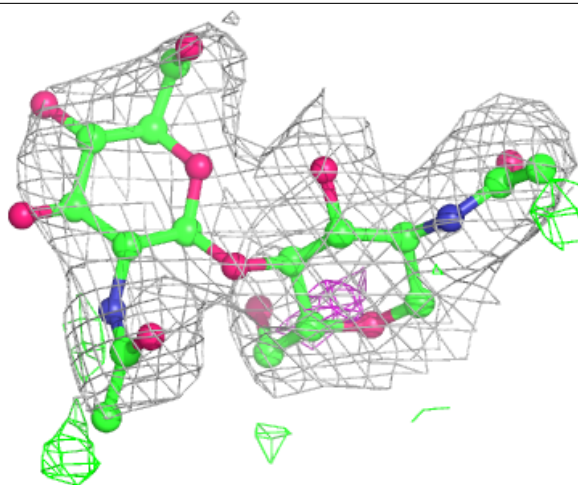
**Electron density around Chain G:**

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



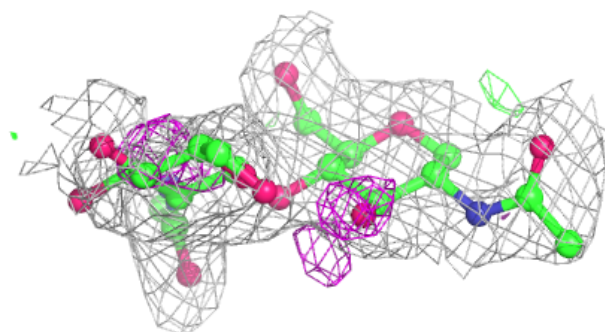
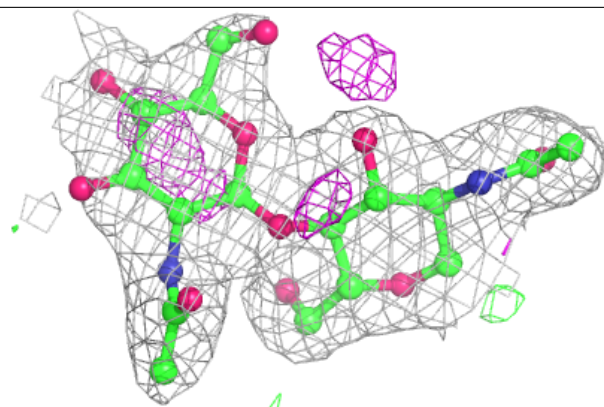
**Electron density around Chain H:**

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



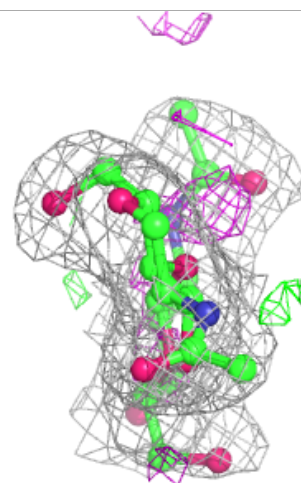
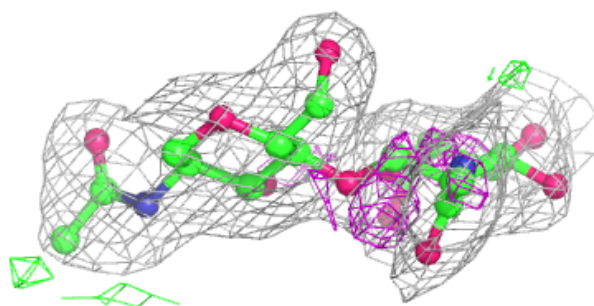
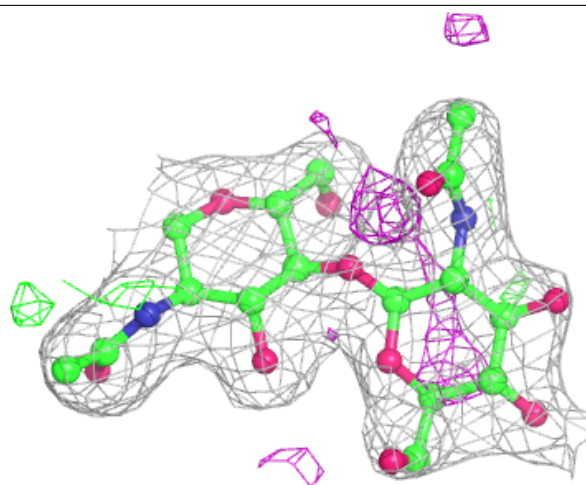
**Electron density around Chain J:**

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



**Electron density around Chain K:**

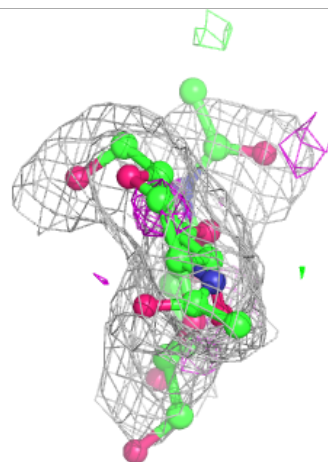
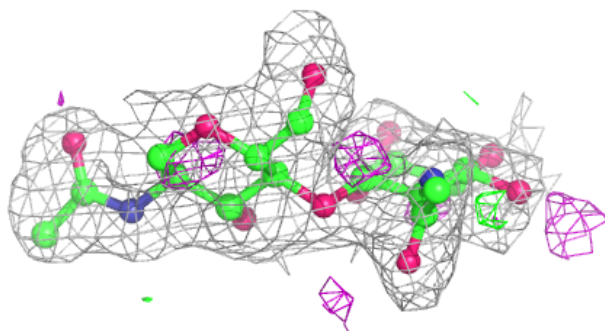
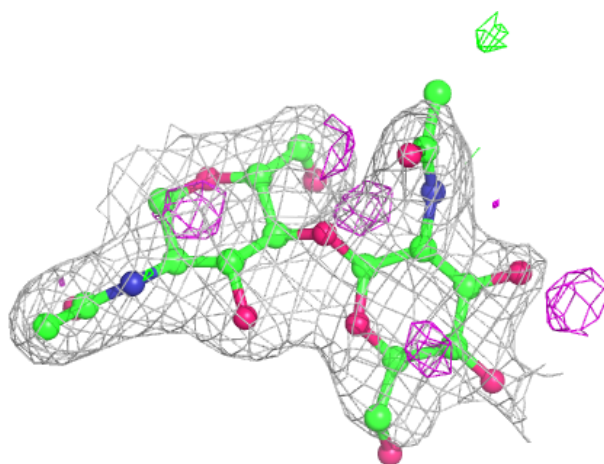
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





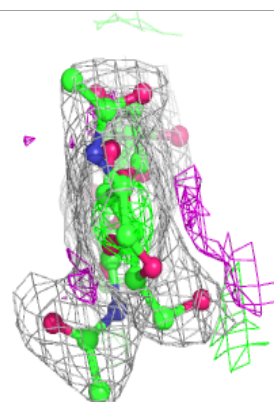
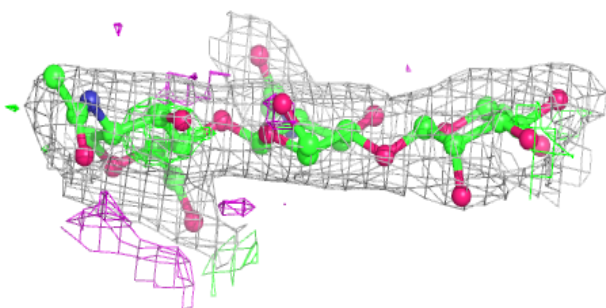
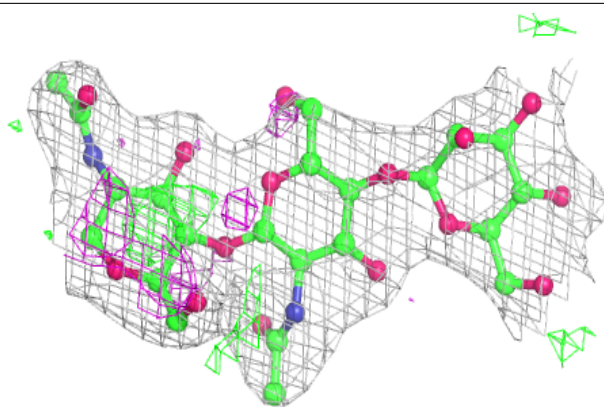
**Electron density around Chain M:**

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

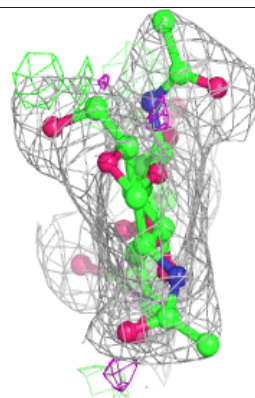
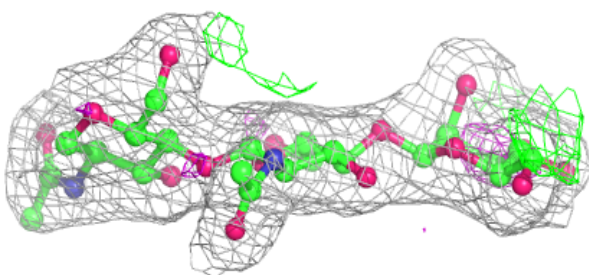
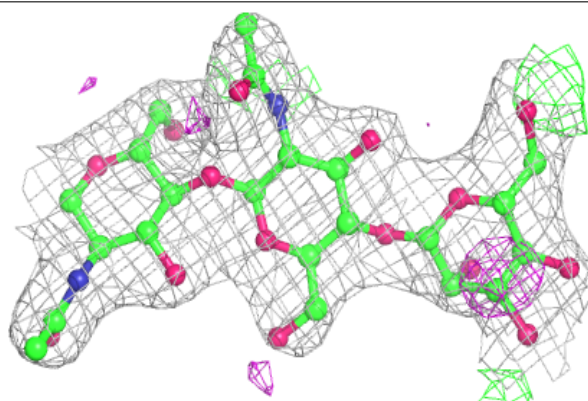


**Electron density around Chain E:**

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

**Electron density around Chain I:**

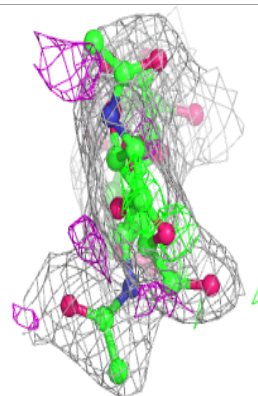
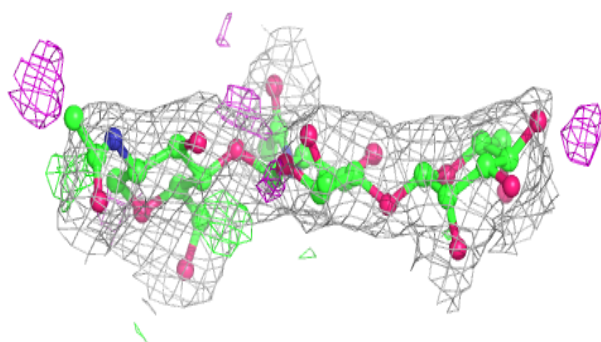
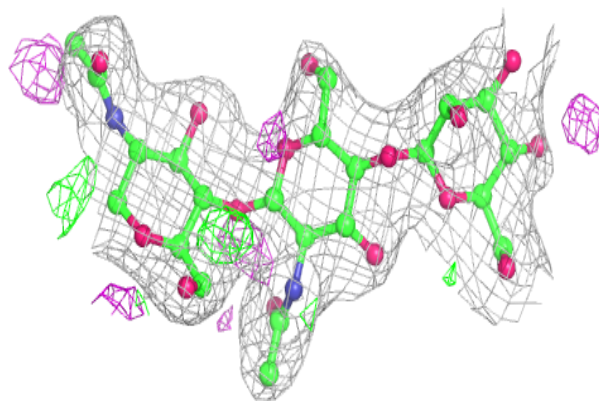
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



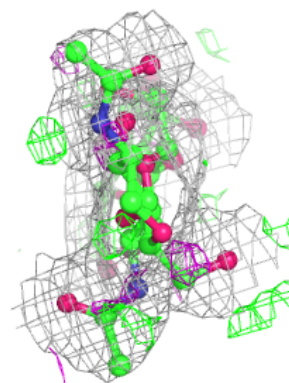
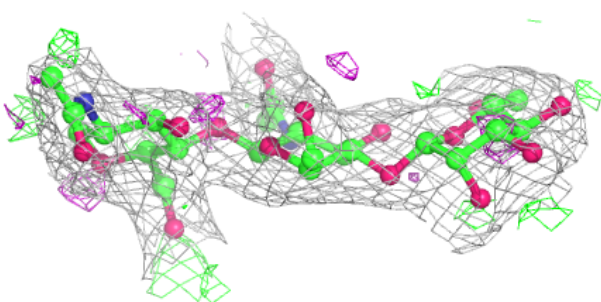
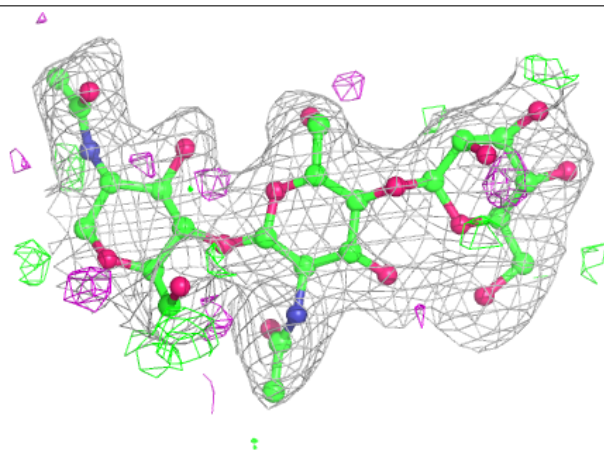


**Electron density around Chain L:**

$2mF_o-DF_c$  (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)



## 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
4	NAG	B	700	14/15	0.61	0.43	73,94,98,100	0
4	NAG	A	700	14/15	0.71	0.33	61,74,78,81	0
4	NAG	A	704	14/15	0.78	0.35	66,89,95,96	0
4	NAG	C	601	14/15	0.80	0.38	74,92,98,98	0
4	NAG	C	604	14/15	0.91	0.23	46,61,69,70	0
4	NAG	A	703	14/15	0.94	0.14	41,54,66,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.