



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:16 AM BST

PDB ID : 5CEZ  
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with an early putative precursor of the PGT121 family at 3.0 Angstrom  
Authors : Wilson, I.A.; Garces, F.  
Deposited on : 2015-07-08  
Resolution : 3.03 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.

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

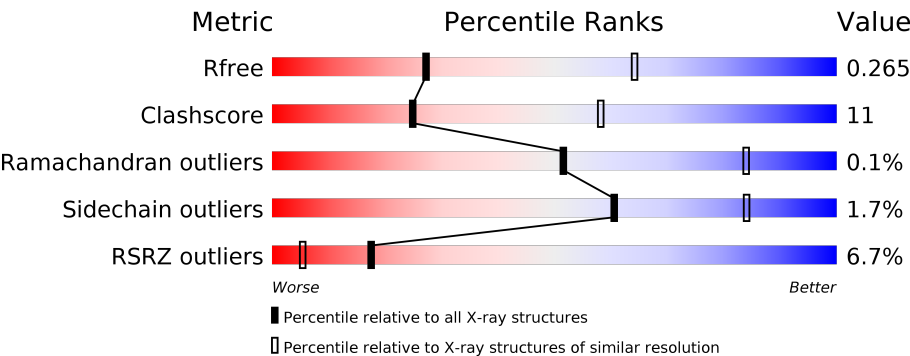
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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	G	480	<div><div>0%</div><div><div></div><div>73%</div><div>21%</div><div>6%</div></div></div>
2	B	153	<div><div>3%</div><div><div></div><div>75%</div><div>21%</div><div></div></div></div>
3	L	218	<div><div></div><div><div></div><div>78%</div><div>17%</div><div></div></div></div>
4	H	236	<div><div>2%</div><div><div></div><div>74%</div><div>22%</div><div></div></div></div>
5	D	240	<div><div>25%</div><div><div></div><div>86%</div><div>14%</div></div></div>
6	E	216	<div><div>12%</div><div><div></div><div>82%</div><div>16%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
7	A	7	
8	C	2	
8	F	2	
8	I	2	
8	J	2	
8	K	2	
8	M	2	
9	N	5	
10	O	4	
11	P	6	
12	Q	9	

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	MAN	Q	6	-	-	X	-
7	MAN	A	6	-	-	-	X
9	MAN	N	5	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 12135 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	452	Total	C	N	O	S	0	0	0
			3544	2224	625	668	27			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	insertion	UNP Q2N0S6
G	510	ARG	LYS	insertion	UNP Q2N0S6
G	512	ARG	-	insertion	UNP Q2N0S6
G	513	ARG	-	insertion	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	147	Total	C	N	O	S	0	0	0
			1171	740	205	220	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called 3H+109L Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1603	1007	276	315	5			

- Molecule 4 is a protein called 3H+109L Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	231	Total	C	N	O	S	0	0	0
			1744	1108	283	347	6			

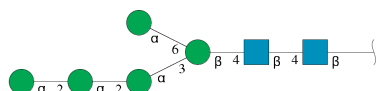
- Molecule 5 is a protein called 35022 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 6 is a protein called 35022 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 7 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
7	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



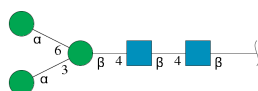
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



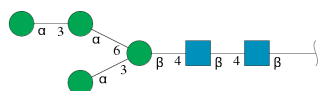
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



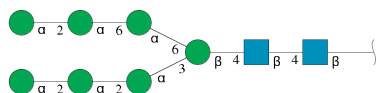
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 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.



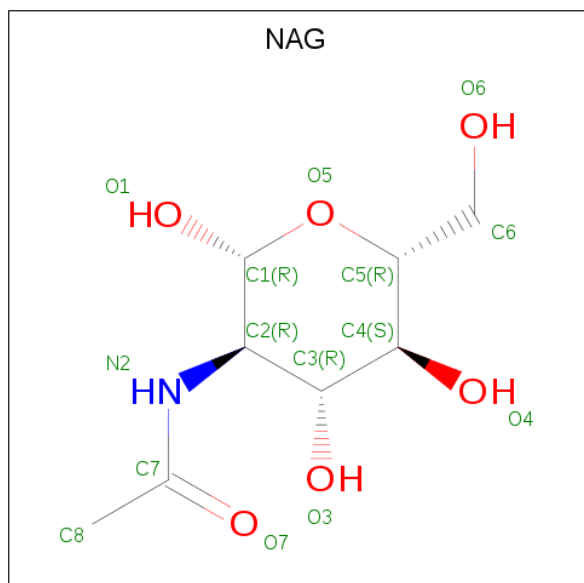
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	P	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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)]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
12	Q	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 13 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>).



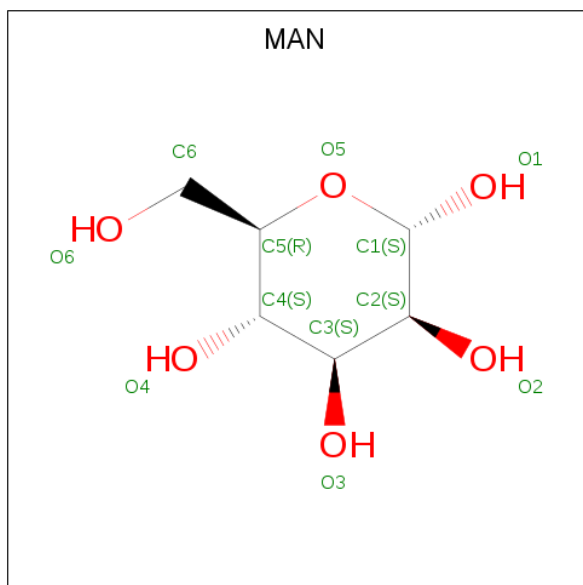
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



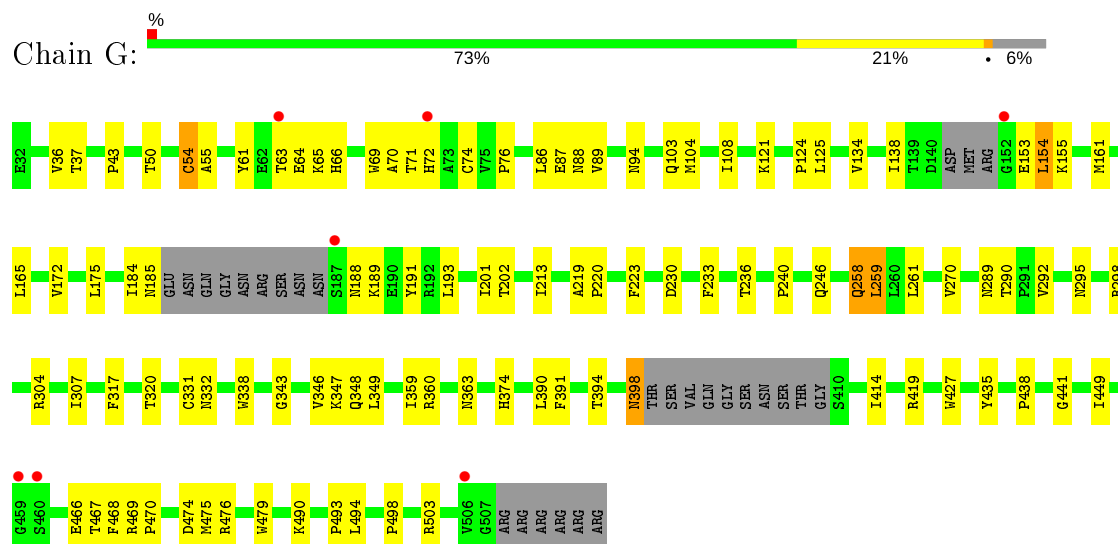
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	H	1	Total	C	O	0	0
			11	6	5		
14	D	1	Total	C	O	0	0
			11	6	5		



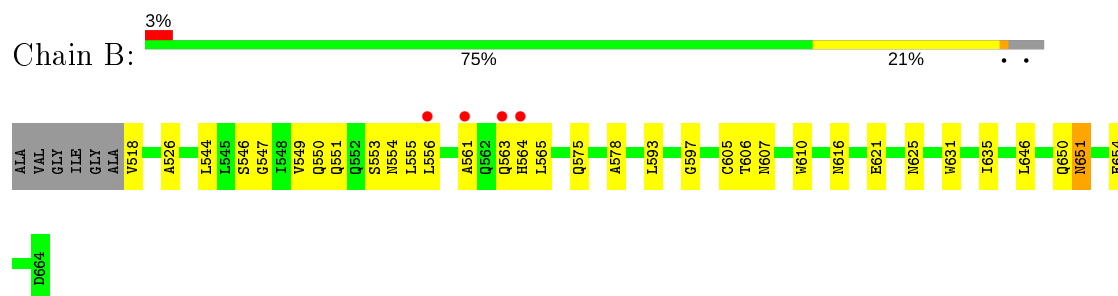
### 3 Residue-property plots [i](#)

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.

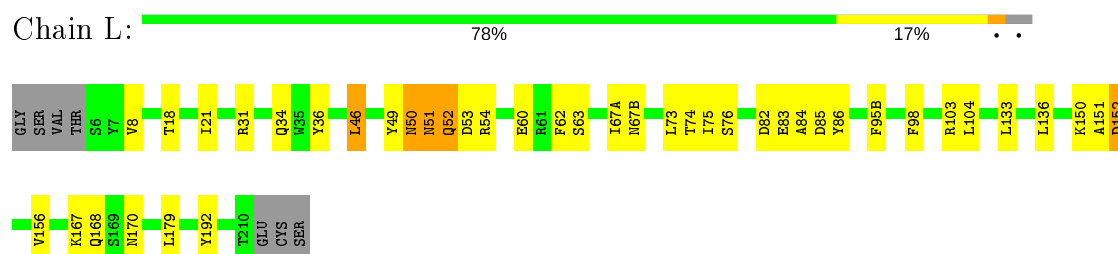
#### • Molecule 1: Envelope glycoprotein gp160



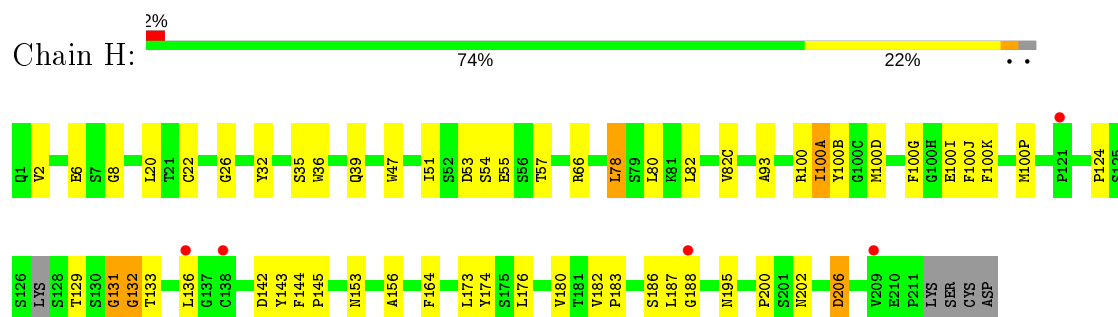
#### • Molecule 2: Envelope glycoprotein gp160



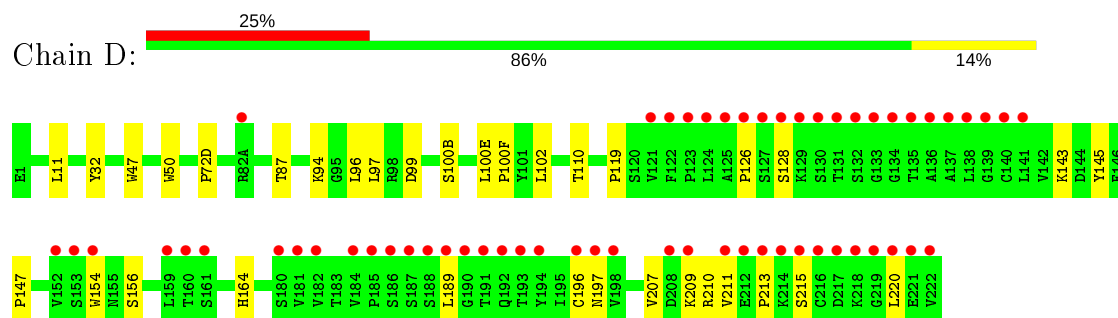
#### • Molecule 3: 3H+109L Fab Light Chain



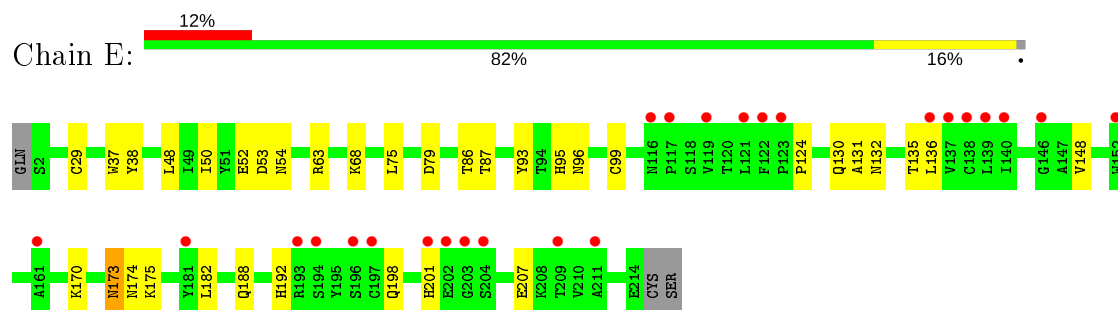
- Molecule 4: 3H+109L Fab Heavy Chain



- Molecule 5: 35022 Fab Heavy Chain



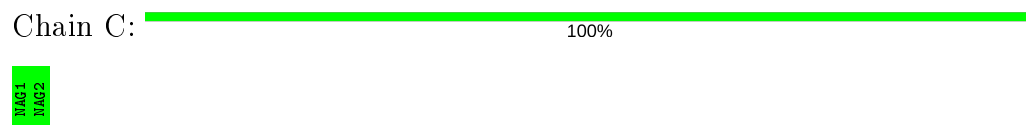
- Molecule 6: 35022 Fab Light Chain



- Molecule 7: 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



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

NAG1  
NAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

NAG1  
NAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

NAG1  
NAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1  
NAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

NAG1  
NAG2

- Molecule 9: 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 N:  40% 60%

NAG1  
NAG2  
BNA3  
MAN4  
MAN5

- Molecule 10: 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:  75% 25%



- Molecule 11: 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 P:  17% 33% 50%



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

Chain Q:  33% 56% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.98Å 127.98Å 316.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.49 – 3.03 44.97 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.49-3.03) 99.7 (44.97-3.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.233 , 0.266 0.233 , 0.265	Depositor DCC
$R_{free}$ test set	2811 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.6	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	G	0.26	0/3617	0.46	0/4911
2	B	0.24	0/1192	0.42	0/1618
3	L	0.25	0/1646	0.45	1/2247 (0.0%)
4	H	0.25	0/1787	0.45	0/2436
5	D	0.25	0/1860	0.45	0/2533
6	E	0.25	0/1659	0.47	0/2269
All	All	0.25	0/11761	0.45	1/16014 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	3
4	H	0	2
6	E	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	46	LEU	CA-CB-CG	5.67	128.33	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	131	GLY	Peptide
4	H	132	GLY	Peptide
3	L	150	LYS	Peptide
3	L	50	ASN	Peptide
3	L	52	GLN	Peptide

## 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	G	3544	0	3474	106	0
2	B	1171	0	1158	48	1
3	L	1603	0	1545	39	0
4	H	1744	0	1710	39	0
5	D	1813	0	1784	21	0
6	E	1615	0	1544	24	1
7	A	83	0	70	6	0
8	C	28	0	25	0	0
8	F	28	0	25	0	0
8	I	28	0	25	0	0
8	J	28	0	25	0	0
8	K	28	0	25	0	0
8	M	28	0	25	0	0
9	N	61	0	52	1	0
10	O	50	0	43	0	0
11	P	72	0	59	3	0
12	Q	105	0	85	17	0
13	B	42	0	38	1	0
13	G	42	0	39	0	0
14	D	11	0	10	0	0
14	H	11	0	10	4	0
All	All	12135	0	11771	257	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 257 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:G:259:LEU:HD13	1:G:449:ILE:CD1	1.74	1.16
1:G:259:LEU:CD1	1:G:449:ILE:HD12	1.75	1.14
1:G:65:LYS:HD2	2:B:563:GLN:NE2	1.65	1.11
1:G:259:LEU:HD13	1:G:449:ILE:HD12	1.31	1.06
1:G:71:THR:HG22	1:G:72:HIS:H	1.21	1.03

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:VAL:CG2	6:E:130:GLN:O[2_5115]	1.27	0.93

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	444/480 (92%)	423 (95%)	21 (5%)	0	100	100
2	B	145/153 (95%)	136 (94%)	9 (6%)	0	100	100
3	L	209/218 (96%)	201 (96%)	7 (3%)	1 (0%)	29	65
4	H	227/236 (96%)	222 (98%)	5 (2%)	0	100	100
5	D	238/240 (99%)	236 (99%)	2 (1%)	0	100	100
6	E	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
All	All	1474/1543 (96%)	1424 (97%)	49 (3%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	84	ALA



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	401/427 (94%)	394 (98%)	7 (2%)	60	84
2	B	127/129 (98%)	125 (98%)	2 (2%)	62	85
3	L	175/181 (97%)	171 (98%)	4 (2%)	50	78
4	H	200/205 (98%)	194 (97%)	6 (3%)	41	73
5	D	203/203 (100%)	202 (100%)	1 (0%)	88	95
6	E	186/189 (98%)	184 (99%)	2 (1%)	73	90
All	All	1292/1334 (97%)	1270 (98%)	22 (2%)	60	84

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	31	ARG
3	L	152	ASP
6	E	99	CYS
3	L	51	ASN
3	L	95(B)	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	127	GLN
3	L	170	ASN
6	E	95	HIS
2	B	607	ASN
5	D	197	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 ⓘ

43 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	$\# Z  > 2$
7	NAG	A	1	1,7	14,14,15	0.26	0	17,19,21	0.48	0
7	NAG	A	2	7	14,14,15	0.33	0	17,19,21	0.41	0
7	BMA	A	3	7	11,11,12	0.67	0	15,15,17	0.70	0
7	MAN	A	4	7	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
7	MAN	A	5	7	11,11,12	0.54	0	15,15,17	0.74	0
7	MAN	A	6	7	11,11,12	0.64	0	15,15,17	0.63	0
7	MAN	A	7	7	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
8	NAG	C	1	1,8	14,14,15	0.20	0	17,19,21	0.49	0
8	NAG	C	2	8	14,14,15	0.27	0	17,19,21	0.36	0
8	NAG	F	1	1,8	14,14,15	0.28	0	17,19,21	0.47	0
8	NAG	F	2	8	14,14,15	0.18	0	17,19,21	0.39	0
8	NAG	I	1	1,8	14,14,15	0.25	0	17,19,21	0.61	0
8	NAG	I	2	8	14,14,15	1.38	1 (7%)	17,19,21	0.40	0
8	NAG	J	1	1,8	14,14,15	0.17	0	17,19,21	0.42	0
8	NAG	J	2	8	14,14,15	2.63	3 (21%)	17,19,21	0.88	1 (5%)
8	NAG	K	1	1,8	14,14,15	0.23	0	17,19,21	0.37	0
8	NAG	K	2	8	14,14,15	0.20	0	17,19,21	0.42	0
8	NAG	M	1	1,8	14,14,15	0.23	0	17,19,21	0.38	0
8	NAG	M	2	8	14,14,15	0.23	0	17,19,21	0.44	0
9	NAG	N	1	1,9	14,14,15	0.26	0	17,19,21	0.36	0
9	NAG	N	2	9	14,14,15	0.21	0	17,19,21	0.37	0
9	BMA	N	3	9	11,11,12	0.60	0	15,15,17	0.79	0
9	MAN	N	4	9	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
9	MAN	N	5	9	11,11,12	0.70	0	15,15,17	1.11	2 (13%)
10	NAG	O	1	1,10	14,14,15	0.27	0	17,19,21	0.36	0
10	NAG	O	2	10	14,14,15	0.24	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	BMA	O	3	10	11,11,12	0.62	0	15,15,17	0.79	0
10	MAN	O	4	10	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
11	NAG	P	1	1,11	14,14,15	0.31	0	17,19,21	0.41	0
11	NAG	P	2	11	14,14,15	0.93	1 (7%)	17,19,21	1.28	1 (5%)
11	BMA	P	3	11	11,11,12	0.69	0	15,15,17	0.77	0
11	MAN	P	4	11	11,11,12	0.84	1 (9%)	15,15,17	1.32	4 (26%)
11	MAN	P	5	11	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
11	MAN	P	6	11	11,11,12	0.65	0	15,15,17	1.20	2 (13%)
12	NAG	Q	1	1,12	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
12	NAG	Q	2	12	14,14,15	0.38	0	17,19,21	0.96	0
12	BMA	Q	3	12	11,11,12	1.49	3 (27%)	15,15,17	4.27	4 (26%)
12	MAN	Q	4	12	11,11,12	0.23	0	15,15,17	0.75	0
12	MAN	Q	5	3,12	11,11,12	0.29	0	15,15,17	0.73	0
12	MAN	Q	6	12	11,11,12	0.36	0	15,15,17	0.69	0
12	MAN	Q	7	12	11,11,12	0.24	0	15,15,17	0.78	0
12	MAN	Q	8	12	11,11,12	0.28	0	15,15,17	0.80	0
12	MAN	Q	9	12	11,11,12	0.24	0	15,15,17	0.70	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
7	NAG	A	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	NAG	F	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
8	NAG	I	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	NAG	J	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	K	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	NAG	M	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
9	NAG	N	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
9	BMA	N	3	9	-	2/2/19/22	0/1/1/1
9	MAN	N	4	9	-	1/2/19/22	0/1/1/1
9	MAN	N	5	9	-	0/2/19/22	0/1/1/1
10	NAG	O	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
10	BMA	O	3	10	-	2/2/19/22	0/1/1/1
10	MAN	O	4	10	-	1/2/19/22	0/1/1/1
11	NAG	P	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	P	2	11	-	5/6/23/26	0/1/1/1
11	BMA	P	3	11	-	2/2/19/22	0/1/1/1
11	MAN	P	4	11	-	0/2/19/22	0/1/1/1
11	MAN	P	5	11	-	0/2/19/22	0/1/1/1
11	MAN	P	6	11	-	0/2/19/22	0/1/1/1
12	NAG	Q	1	1,12	-	3/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	1/6/23/26	0/1/1/1
12	BMA	Q	3	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	4	12	-	2/2/19/22	0/1/1/1
12	MAN	Q	5	3,12	-	2/2/19/22	0/1/1/1
12	MAN	Q	6	12	-	2/2/19/22	0/1/1/1
12	MAN	Q	7	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	8	12	-	2/2/19/22	0/1/1/1
12	MAN	Q	9	12	-	2/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	2	NAG	C1-C2	8.11	1.64	1.52
8	J	2	NAG	C2-N2	-5.08	1.37	1.46
8	I	2	NAG	C8-C7	-5.06	1.40	1.50
11	P	2	NAG	O6-C6	3.08	1.55	1.42
12	Q	3	BMA	O5-C1	2.66	1.48	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q	3	BMA	O3-C3-C2	-12.54	85.99	109.99
12	Q	3	BMA	O3-C3-C4	9.48	132.27	110.35
11	P	2	NAG	C2-N2-C7	4.40	129.17	122.90
12	Q	3	BMA	C1-O5-C5	2.91	116.14	112.19
11	P	4	MAN	C1-O5-C5	2.87	116.07	112.19

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

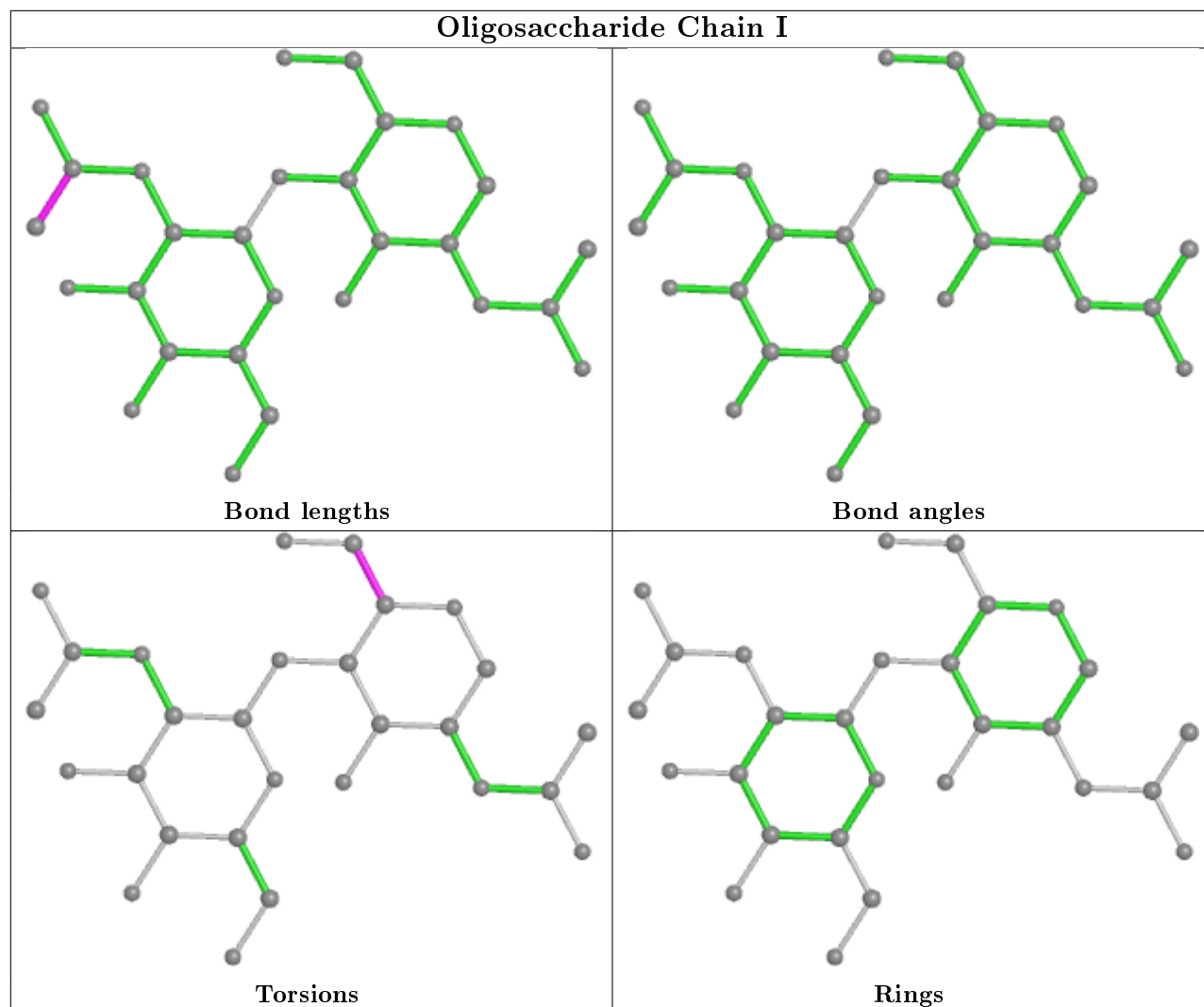
Mol	Chain	Res	Type	Atoms
12	Q	1	NAG	C3-C2-N2-C7
12	Q	1	NAG	C8-C7-N2-C2
12	Q	1	NAG	O7-C7-N2-C2
9	N	3	BMA	C4-C5-C6-O6
10	O	3	BMA	C4-C5-C6-O6

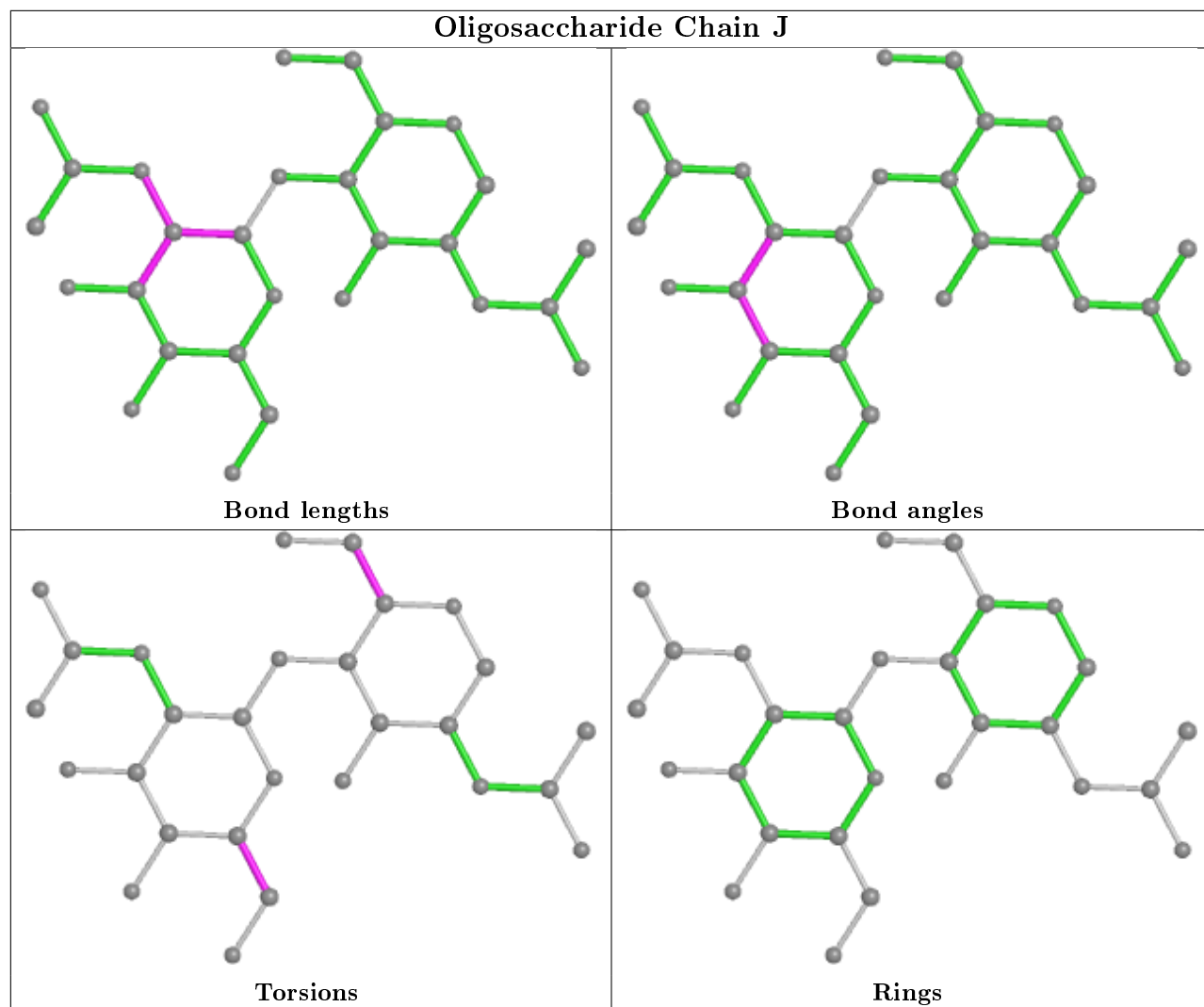
There are no ring outliers.

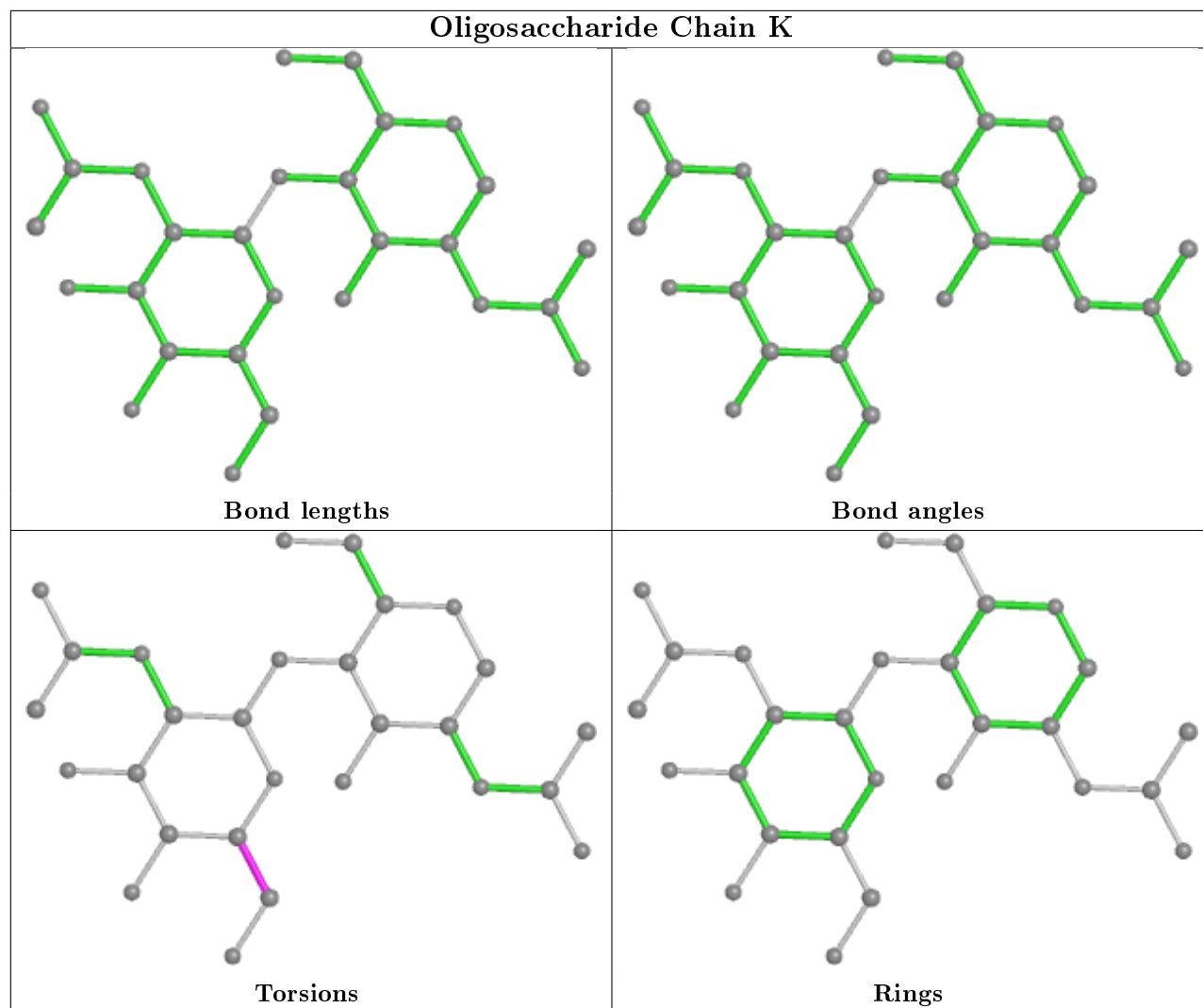
14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6	MAN	4	0
7	A	1	NAG	1	0
12	Q	7	MAN	4	0
12	Q	2	NAG	2	0
7	A	4	MAN	1	0
12	Q	1	NAG	4	0
11	P	3	BMA	1	0
12	Q	5	MAN	2	0
11	P	6	MAN	1	0
7	A	2	NAG	1	0
11	P	4	MAN	1	0
9	N	1	NAG	1	0
11	P	2	NAG	1	0
12	Q	6	MAN	6	0

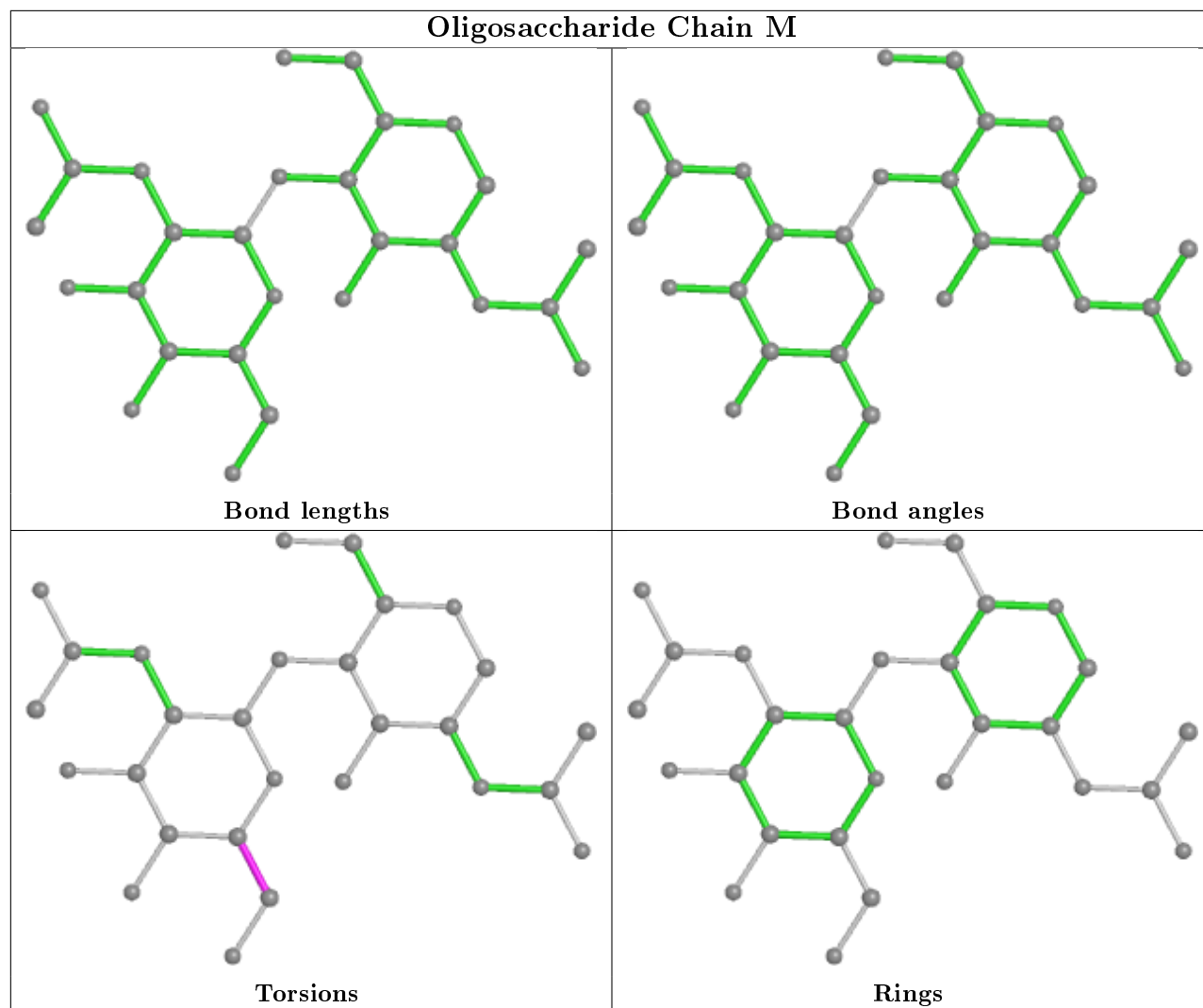
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

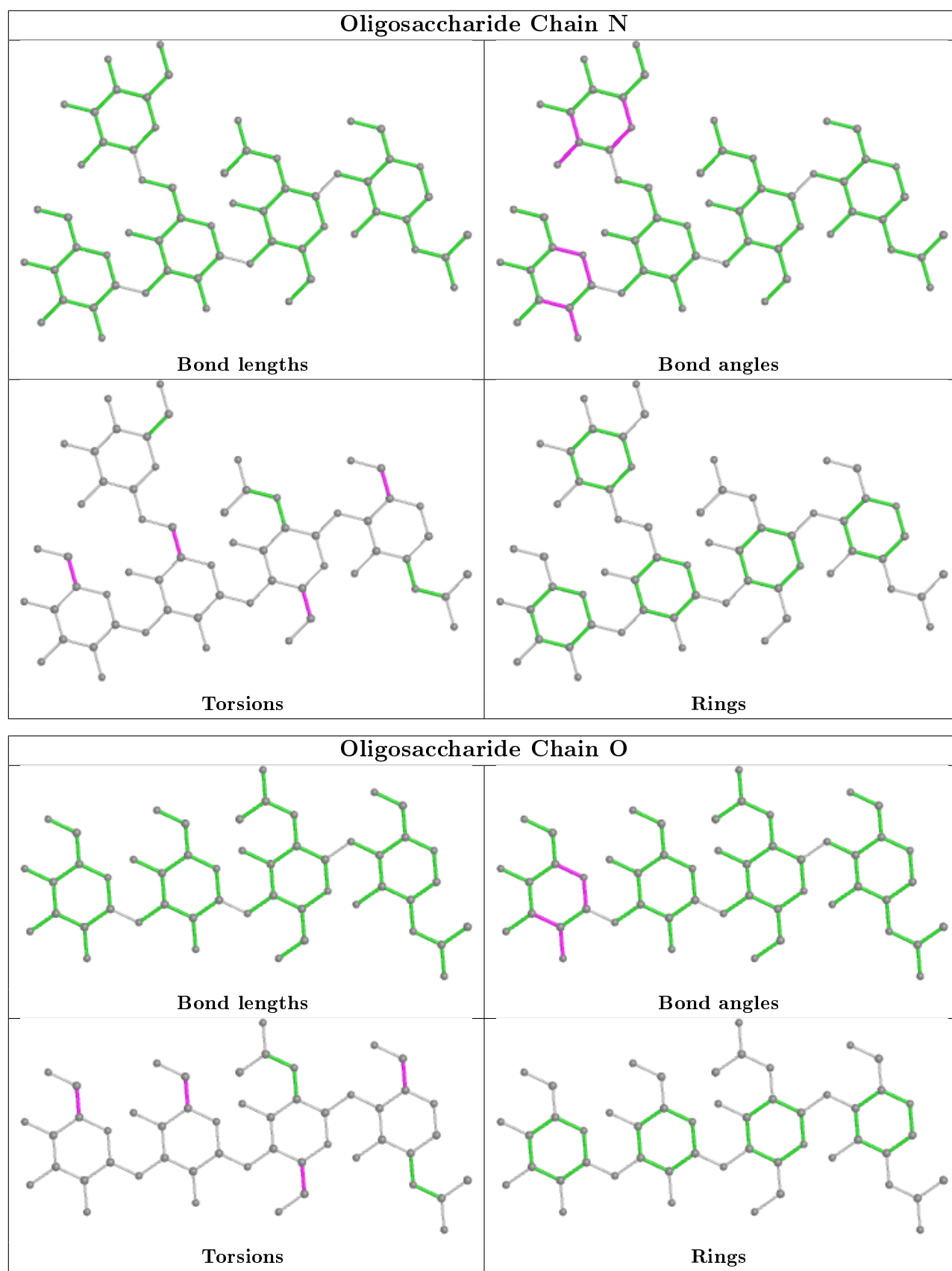


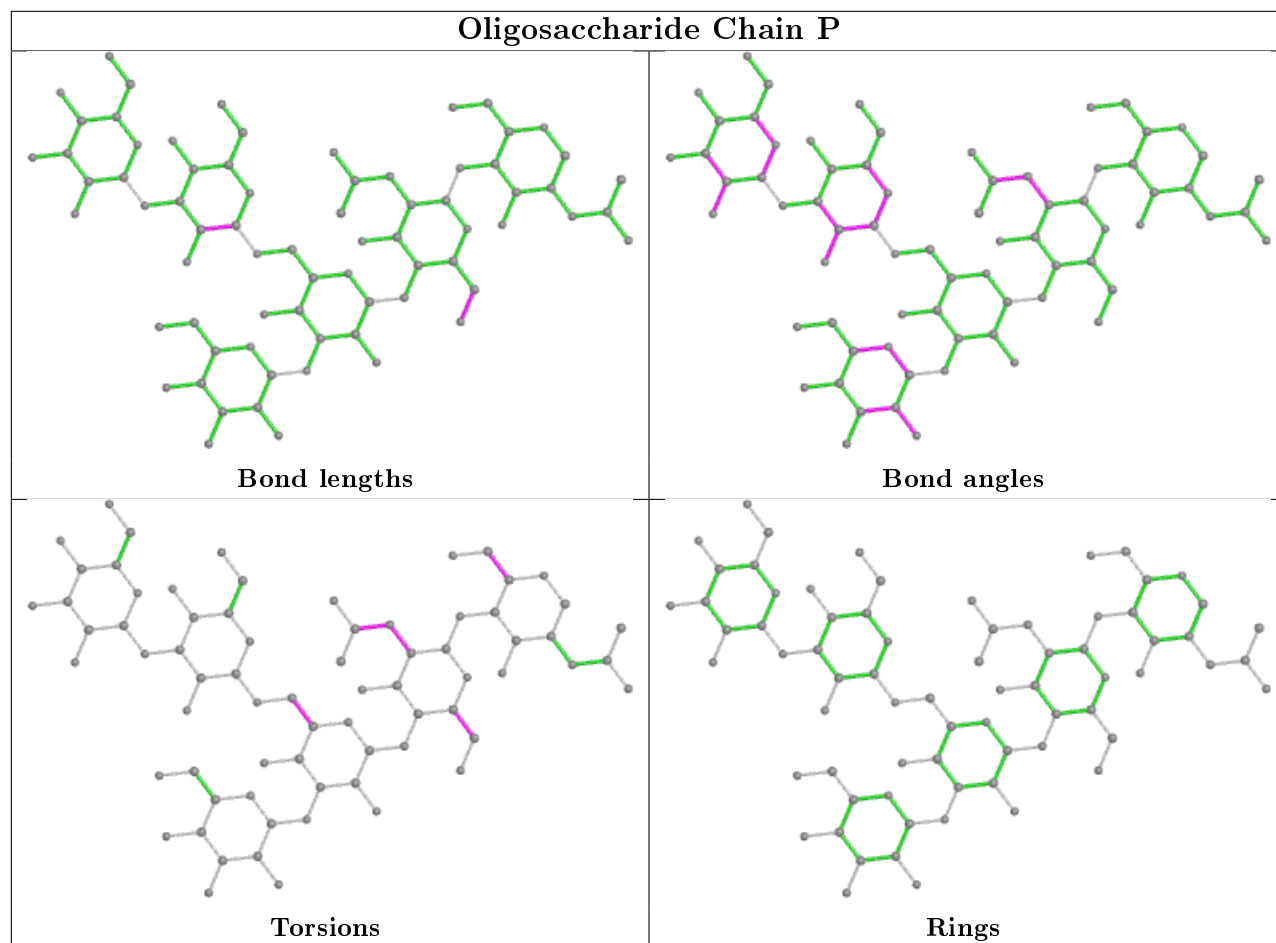


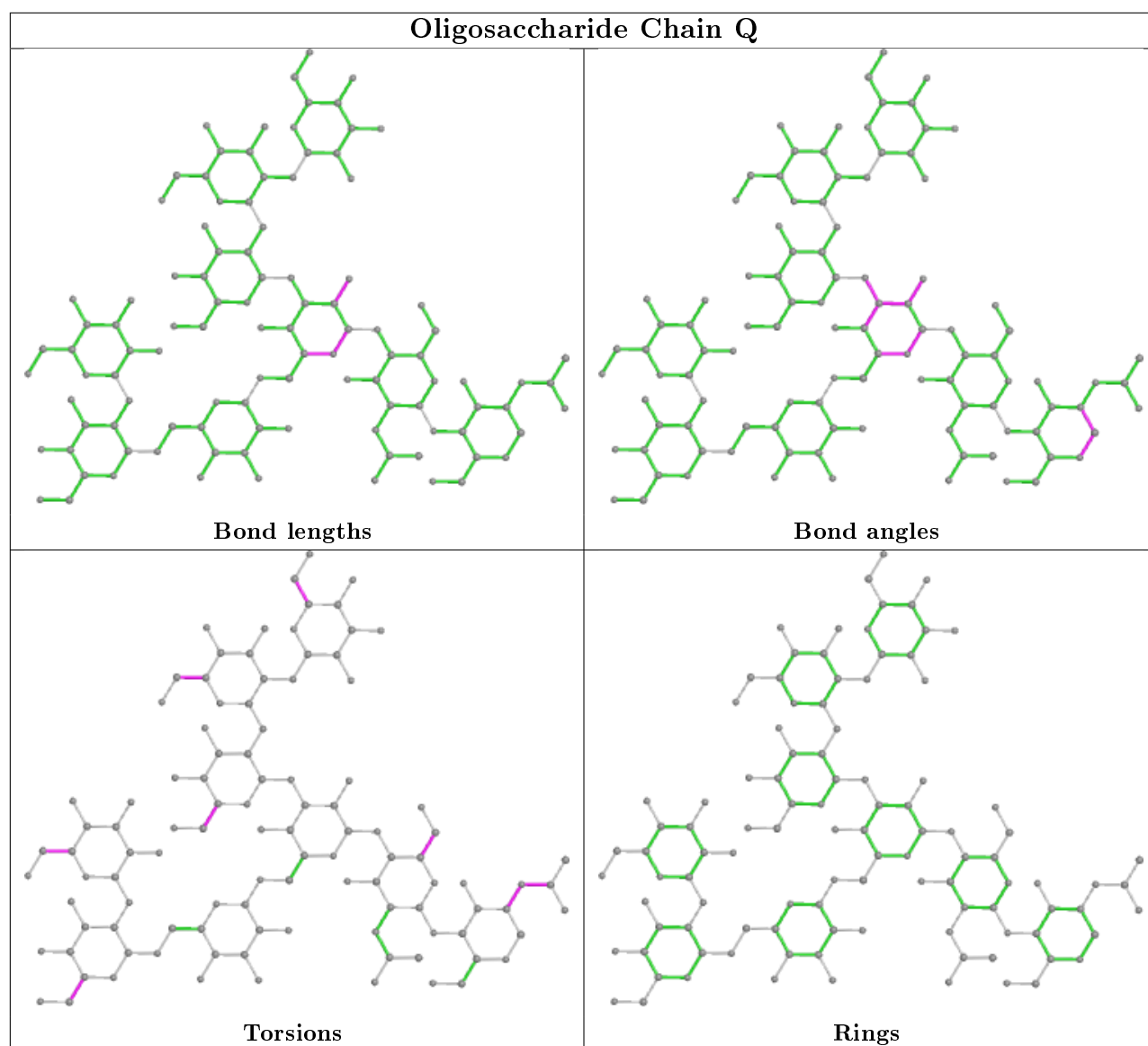












## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
13	NAG	G	611	1	14,14,15	0.18	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	B	702	2	14,14,15	2.02	2 (14%)	17,19,21	1.44	1 (5%)
13	NAG	G	616	1	14,14,15	0.21	0	17,19,21	0.36	0
13	NAG	B	701	2	14,14,15	2.67	3 (21%)	17,19,21	1.34	1 (5%)
14	MAN	H	301	-	11,11,12	0.26	0	15,15,17	0.67	0
13	NAG	G	610	1	14,14,15	0.17	0	17,19,21	0.41	0
14	MAN	D	301	-	11,11,12	0.65	0	15,15,17	1.11	2 (13%)
13	NAG	B	703	2	14,14,15	0.20	0	17,19,21	0.41	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
13	NAG	G	611	1	-	2/6/23/26	0/1/1/1
13	NAG	B	702	2	-	2/6/23/26	0/1/1/1
13	NAG	G	616	1	-	0/6/23/26	0/1/1/1
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1
14	MAN	H	301	-	-	0/2/19/22	0/1/1/1
13	NAG	G	610	1	-	2/6/23/26	0/1/1/1
14	MAN	D	301	-	-	0/2/19/22	0/1/1/1
13	NAG	B	703	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	701	NAG	O6-C6	-8.11	1.08	1.42
13	B	702	NAG	O5-C1	6.07	1.53	1.43
13	B	701	NAG	C1-C2	4.79	1.59	1.52
13	B	702	NAG	C1-C2	-4.51	1.45	1.52
13	B	701	NAG	O5-C1	3.23	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	702	NAG	C1-O5-C5	5.47	119.60	112.19
13	B	701	NAG	O5-C1-C2	-4.92	103.52	111.29
14	D	301	MAN	C1-O5-C5	2.53	115.62	112.19
14	D	301	MAN	O2-C2-C3	-2.32	105.50	110.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	611	NAG	C4-C5-C6-O6
13	B	702	NAG	C4-C5-C6-O6
13	G	610	NAG	C4-C5-C6-O6
13	B	703	NAG	C4-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	702	NAG	1	0
14	H	301	MAN	4	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	G	452/480 (94%)	0.01	7 (1%) 73 46	58, 95, 164, 244	0
2	B	147/153 (96%)	0.09	4 (2%) 54 26	61, 95, 200, 230	0
3	L	211/218 (96%)	-0.26	0 100 100	77, 113, 140, 169	0
4	H	231/236 (97%)	-0.06	5 (2%) 62 33	81, 118, 171, 189	0
5	D	240/240 (100%)	1.12	59 (24%) 0 0	71, 143, 294, 323	0
6	E	213/216 (98%)	0.54	25 (11%) 4 1	74, 145, 223, 240	0
All	All	1494/1543 (96%)	0.22	100 (6%) 17 5	58, 111, 217, 323	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	213	PRO	12.5
5	D	214	LYS	11.0
5	D	132	SER	10.5
5	D	215	SER	9.8
5	D	212	GLU	9.7

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

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

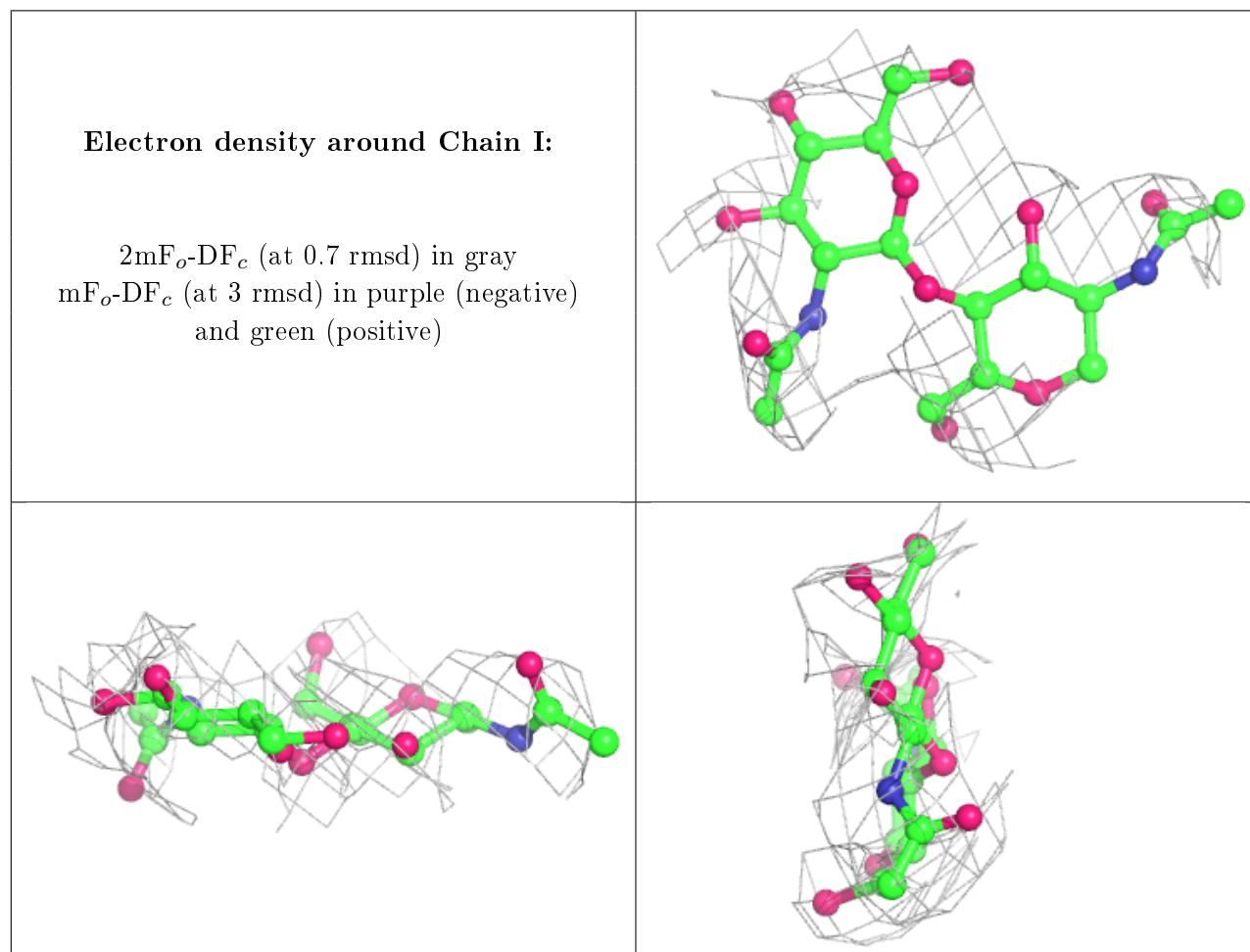
### 6.3 Carbohydrates [i](#)

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
9	BMA	N	3	11/12	0.61	0.24	229,237,248,259	0
7	MAN	A	6	11/12	0.68	0.48	223,233,240,249	0
7	MAN	A	7	11/12	0.69	0.32	173,200,215,218	0
10	MAN	O	4	11/12	0.73	0.38	191,222,229,231	0
9	MAN	N	4	11/12	0.73	0.23	195,215,230,234	0
9	MAN	N	5	11/12	0.74	0.61	251,264,271,276	0
10	BMA	O	3	11/12	0.75	0.28	188,209,222,228	0
7	MAN	A	5	11/12	0.78	0.21	171,199,222,235	0
8	NAG	J	2	14/15	0.81	0.27	143,184,189,202	0
11	MAN	P	4	11/12	0.81	0.17	119,129,145,159	0
8	NAG	I	2	14/15	0.82	0.26	129,176,187,190	0
8	NAG	M	2	14/15	0.82	0.39	157,175,191,195	0
7	BMA	A	3	11/12	0.83	0.14	176,187,196,202	0
8	NAG	C	1	14/15	0.85	0.23	118,152,170,174	0
8	NAG	C	2	14/15	0.87	0.23	163,176,183,206	0
8	NAG	J	1	14/15	0.88	0.25	132,143,176,177	0
8	NAG	M	1	14/15	0.88	0.28	136,156,163,166	0
12	MAN	Q	9	11/12	0.90	0.30	136,147,157,161	0
8	NAG	K	1	14/15	0.90	0.20	120,145,166,169	0
8	NAG	I	1	14/15	0.90	0.17	92,142,163,169	0
12	MAN	Q	7	11/12	0.90	0.12	119,124,135,140	0
7	MAN	A	4	11/12	0.90	0.16	173,199,206,215	0
9	NAG	N	2	14/15	0.90	0.25	154,200,221,233	0
8	NAG	F	2	14/15	0.91	0.16	137,156,165,178	0
10	NAG	O	2	14/15	0.91	0.14	135,146,175,197	0
11	BMA	P	3	11/12	0.91	0.23	78,87,127,130	0
8	NAG	K	2	14/15	0.91	0.17	134,170,177,179	0
12	NAG	Q	1	14/15	0.92	0.22	92,106,116,116	0
7	NAG	A	2	14/15	0.94	0.16	108,133,150,163	0
12	NAG	Q	2	14/15	0.94	0.15	79,100,119,122	0
11	MAN	P	5	11/12	0.94	0.23	125,148,163,164	0
11	MAN	P	6	11/12	0.94	0.18	74,92,101,105	0
12	BMA	Q	3	11/12	0.94	0.17	93,96,121,125	0
9	NAG	N	1	14/15	0.94	0.18	108,145,179,182	0
12	MAN	Q	5	11/12	0.95	0.16	88,98,116,118	0
12	MAN	Q	8	11/12	0.96	0.11	108,123,130,135	0
12	MAN	Q	4	11/12	0.96	0.14	73,78,107,108	0
11	NAG	P	2	14/15	0.96	0.22	60,84,92,97	0
11	NAG	P	1	14/15	0.96	0.21	65,79,91,93	0
7	NAG	A	1	14/15	0.96	0.23	77,92,110,113	0
10	NAG	O	1	14/15	0.96	0.19	86,118,135,138	0
12	MAN	Q	6	11/12	0.96	0.12	89,107,112,113	0
8	NAG	F	1	14/15	0.97	0.19	83,104,137,143	0

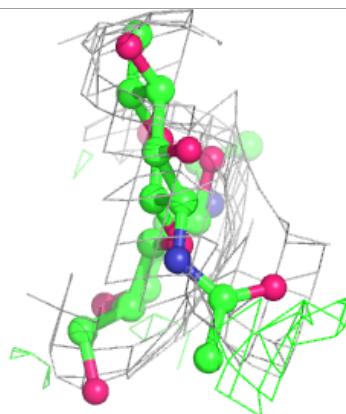
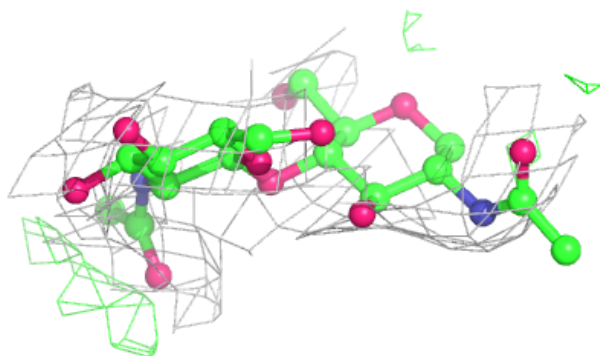
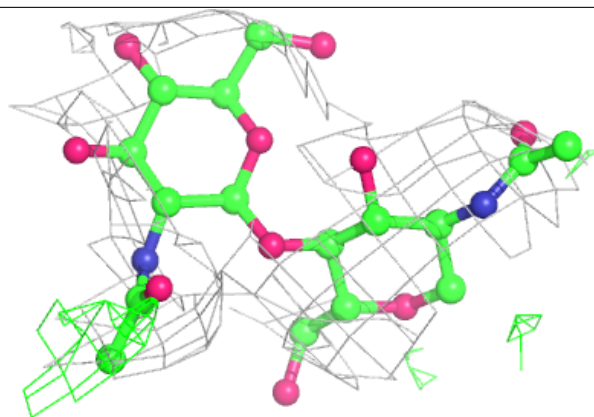


The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

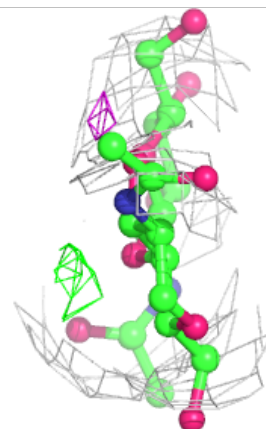
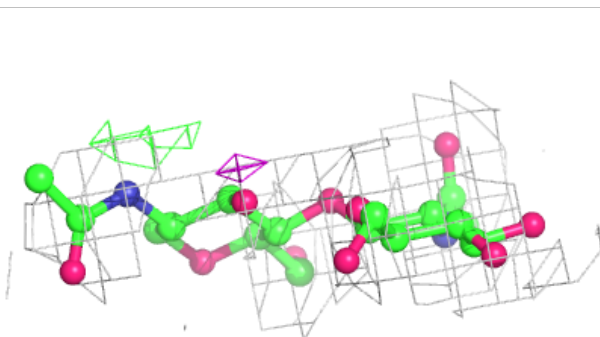
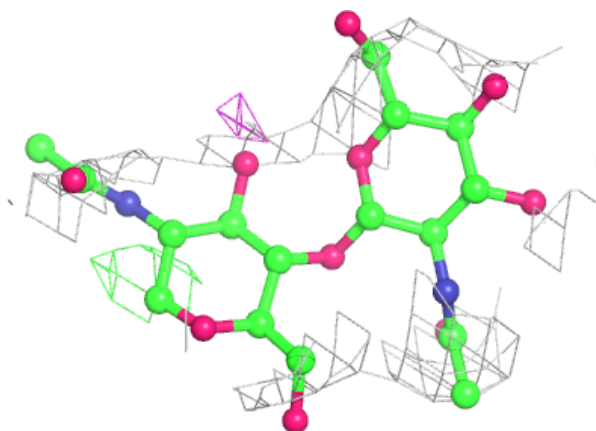


**Electron density around Chain J:**

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

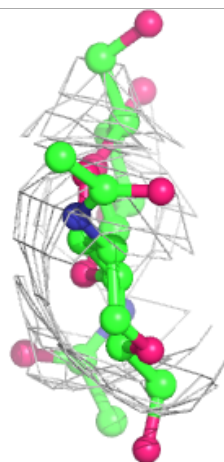
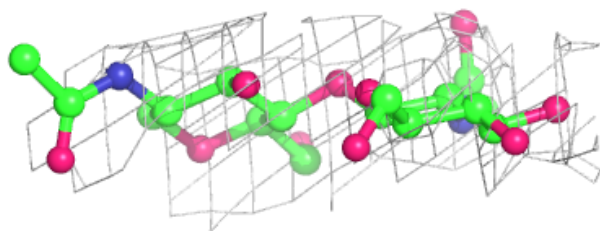
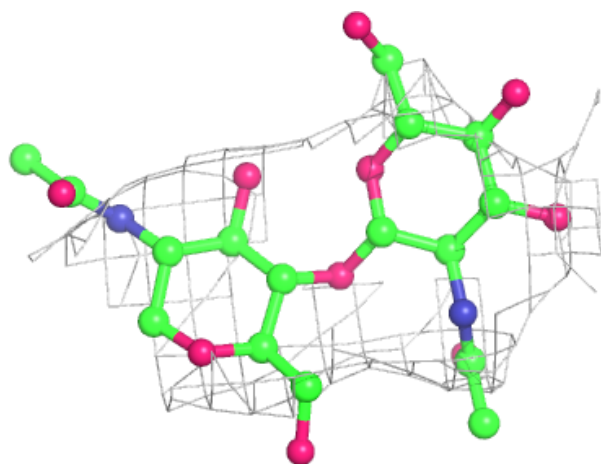
**Electron density around Chain K:**

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



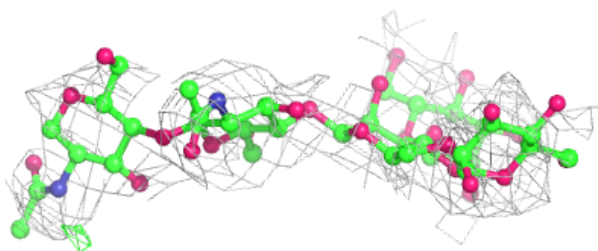
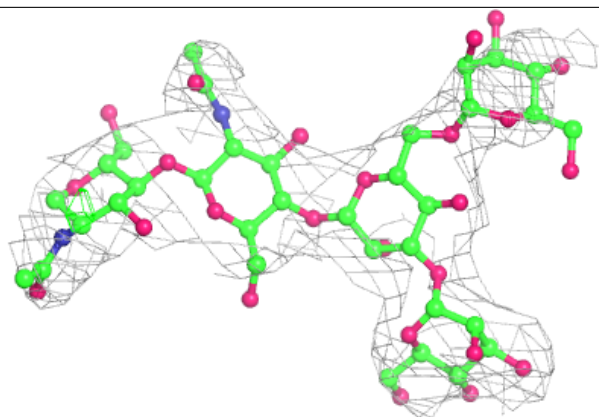
**Electron density around Chain M:**

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

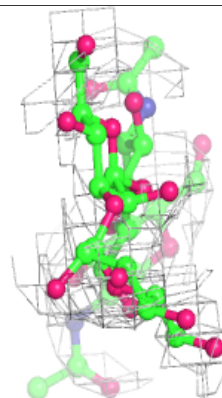
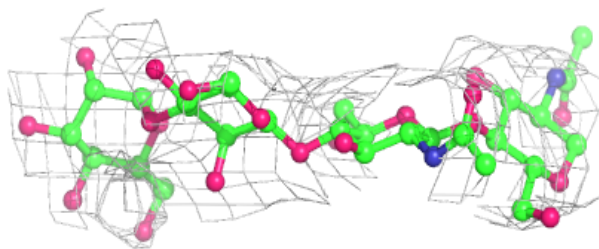
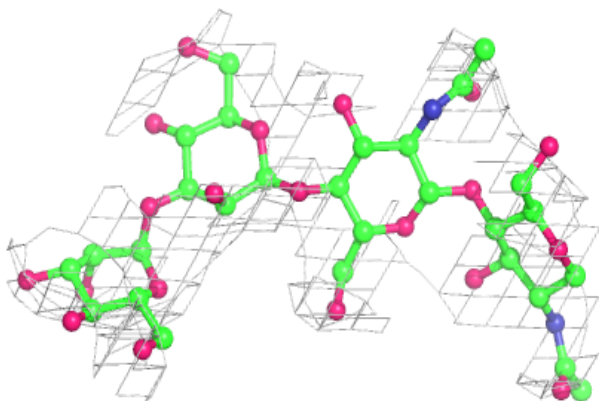


**Electron density around Chain N:**

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

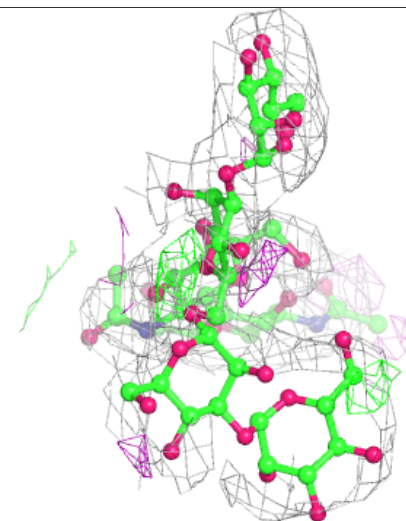
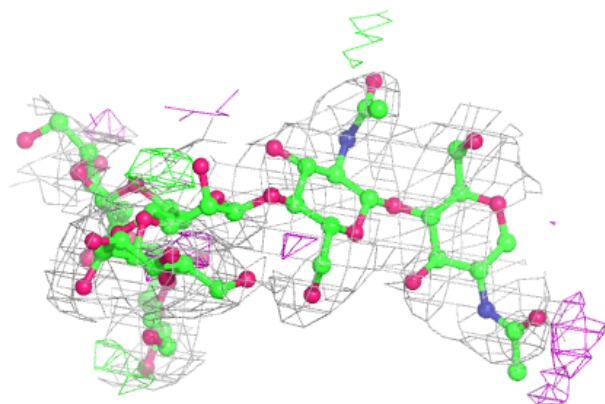
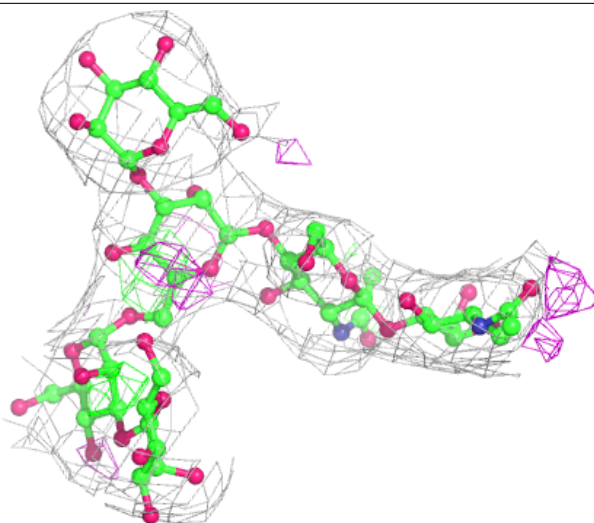
**Electron density around Chain O:**

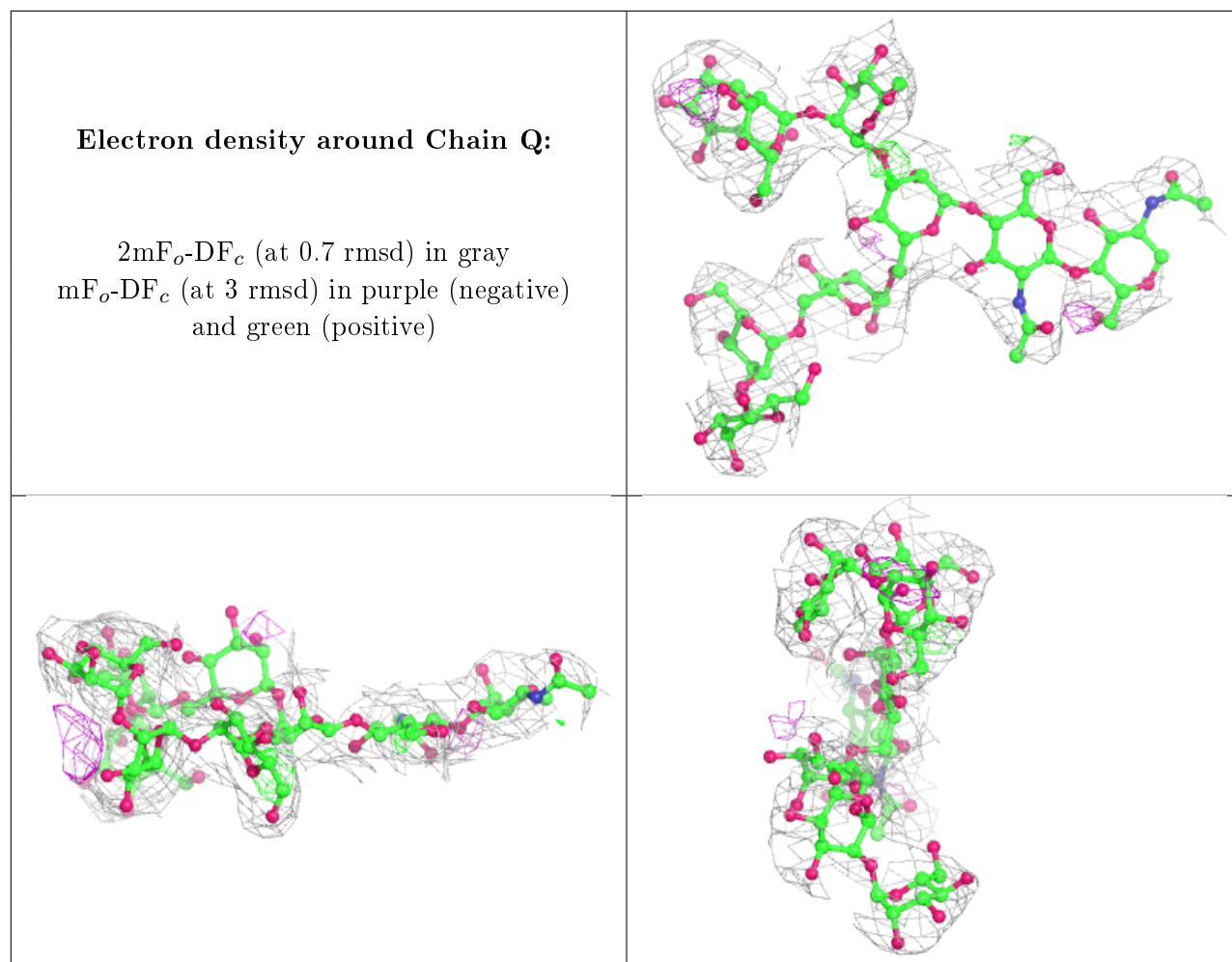
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain P:**

$2mF_o-DF_c$  (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
13	NAG	B	703	14/15	0.85	0.27	150,170,188,199	0
13	NAG	G	610	14/15	0.86	0.23	104,132,154,161	0
14	MAN	D	301	11/12	0.88	0.20	118,135,149,151	0
13	NAG	B	701	14/15	0.89	0.12	129,150,172,172	0
13	NAG	B	702	14/15	0.90	0.13	116,143,159,164	0
14	MAN	H	301	11/12	0.92	0.14	134,138,155,160	0
13	NAG	G	616	14/15	0.92	0.19	101,141,154,157	0
13	NAG	G	611	14/15	0.93	0.27	128,151,164,173	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.