



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:48 PM BST

PDB ID : 4R0A  
Title : Crystal structure of human TLR8 in complex with uridine mononucleoside  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2014-07-30  
Resolution : 1.90 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

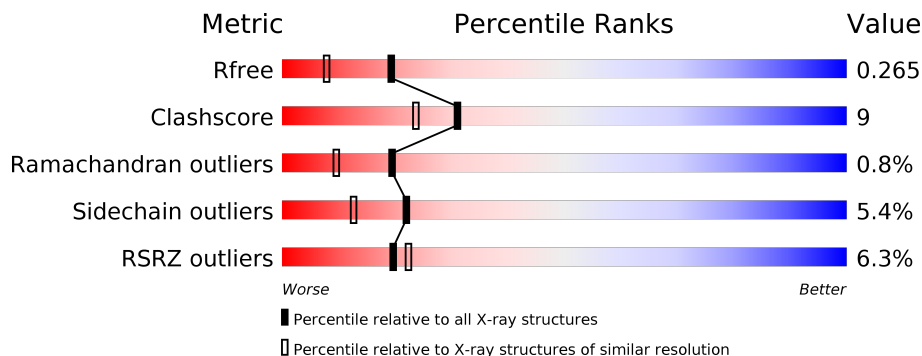
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	811	 6% 74% 16% •• 8%
2	B	5	 100%
3	C	2	 100%
4	D	3	 100%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6567 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	748	5994	3833	1020	1122	19	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97

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

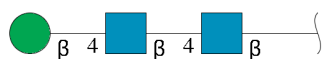
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	61	34	2	25	0	0	0

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



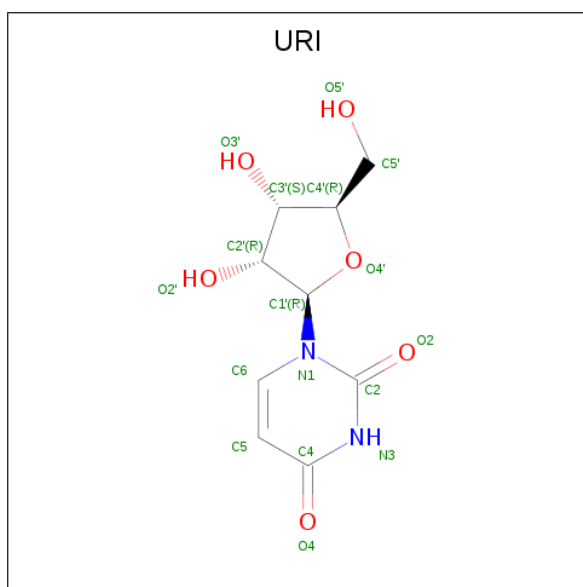
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	D	3	39	22	2	15	0	0	0

- Molecule 5 is URIDINE (three-letter code: URI) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	17	9	2	6	0	0

- Molecule 6 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
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0

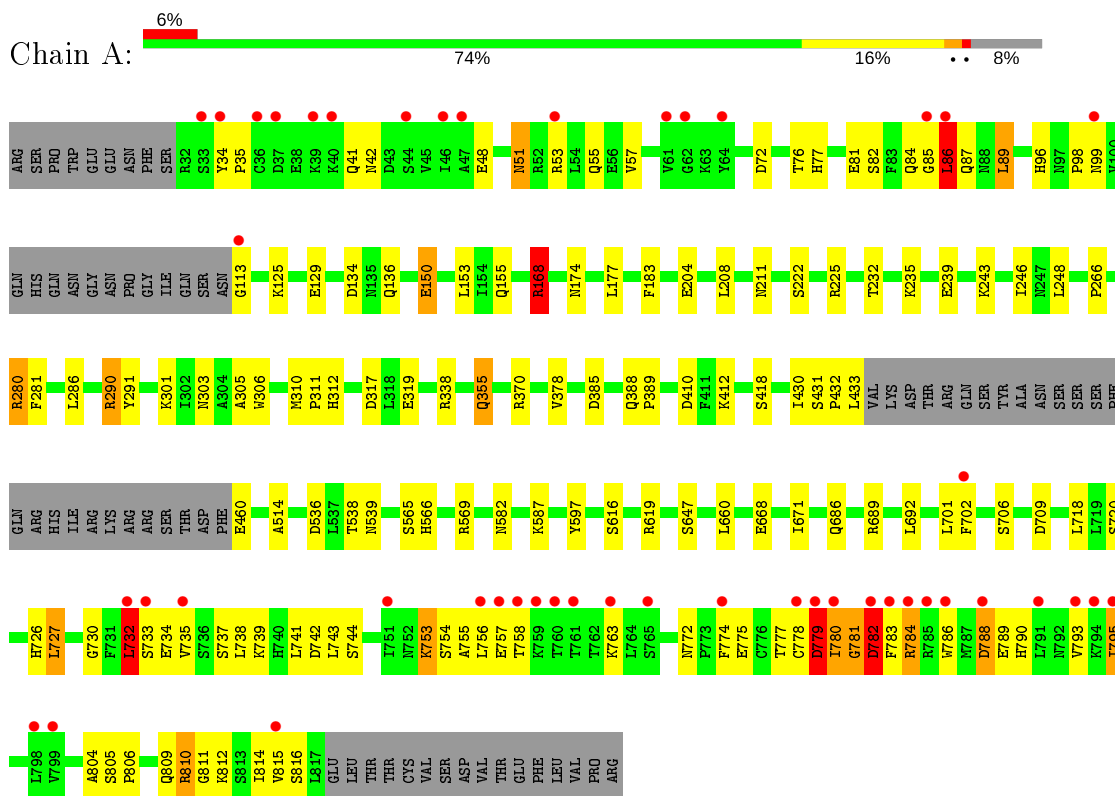
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	330	330	330	0	0

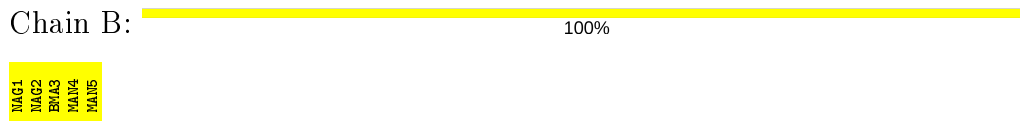
### 3 Residue-property plots [i](#)

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.

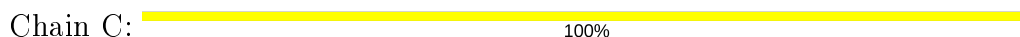
- Molecule 1: Toll-like receptor 8



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



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



MAG1  
MAG2

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

Chain D:

100%

MAG1  
MAG2  
BVA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.44Å 133.32Å 120.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 1.90 48.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.58-1.90) 98.3 (48.58-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.200 , 0.260 0.207 , 0.265	Depositor DCC
$R_{free}$ test set	3309 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, URI, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.67	0/6118	0.76	3/8300 (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
1	A	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	225	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	168	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	225	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	732	LEU	Peptide
1	A	779	ASP	Peptide
1	A	781	GLY	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5994	0	5946	112	3
2	B	61	0	52	0	0
3	C	28	0	25	0	0
4	D	39	0	34	0	0
5	A	17	0	12	0	0
6	A	98	0	91	4	0
7	A	330	0	0	5	0
All	All	6567	0	6160	113	3

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 9.

All (113) 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:753:LYS:HB3	1:A:782:ASP:HB2	1.24	1.17
1:A:780:ILE:N	1:A:781:GLY:HA2	1.83	0.93
1:A:779:ASP:HA	1:A:780:ILE:HG12	1.53	0.91
1:A:780:ILE:HB	1:A:781:GLY:C	1.92	0.89
1:A:732:LEU:HD22	1:A:754:SER:O	1.73	0.88
1:A:784:ARG:O	1:A:784:ARG:NE	2.09	0.86
1:A:779:ASP:HA	1:A:780:ILE:CG1	2.05	0.86
1:A:753:LYS:HB3	1:A:782:ASP:CB	2.06	0.85
1:A:460:GLU:OE1	7:A:1312:HOH:O	1.97	0.81
1:A:780:ILE:H	1:A:781:GLY:HA2	1.43	0.80
1:A:781:GLY:C	1:A:783:PHE:N	2.34	0.79
1:A:168:ARG:HH11	1:A:168:ARG:HG3	1.48	0.79
1:A:780:ILE:HB	1:A:781:GLY:O	1.85	0.76
1:A:732:LEU:HG	1:A:733:SER:N	2.04	0.72
1:A:780:ILE:H	1:A:781:GLY:CA	2.01	0.72
1:A:96:HIS:HD2	1:A:134:ASP:OD2	1.78	0.67
1:A:784:ARG:HH21	1:A:788:ASP:HB2	1.60	0.67
1:A:772:ASN:HB2	1:A:774:PHE:CE2	2.28	0.66
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.08	0.66
1:A:784:ARG:NH2	1:A:788:ASP:HB2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ILE:HB	1:A:781:GLY:CA	2.27	0.65
1:A:129:GLU:HG2	1:A:150:GLU:HB2	1.78	0.65
1:A:536:ASP:OD1	1:A:538:THR:HG23	1.97	0.65
1:A:809:GLN:O	1:A:811:GLY:N	2.30	0.64
1:A:780:ILE:N	1:A:781:GLY:CA	2.56	0.64
1:A:290:ARG:HD2	1:A:312:HIS:O	2.00	0.61
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.19	0.61
1:A:781:GLY:C	1:A:783:PHE:H	2.03	0.59
1:A:222:SER:OG	6:A:905:NAG:O7	2.09	0.59
1:A:48:GLU:HB3	7:A:1184:HOH:O	2.01	0.59
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.86	0.58
1:A:150:GLU:HG2	1:A:174:ASN:HB2	1.86	0.58
1:A:780:ILE:CB	1:A:781:GLY:CA	2.82	0.58
1:A:781:GLY:O	1:A:783:PHE:N	2.37	0.57
1:A:795:ILE:O	1:A:795:ILE:HG13	2.04	0.57
1:A:793:VAL:HG23	1:A:793:VAL:O	2.04	0.57
1:A:168:ARG:NH1	1:A:168:ARG:HG3	2.19	0.57
1:A:784:ARG:C	1:A:784:ARG:HE	2.04	0.57
1:A:134:ASP:HA	1:A:155:GLN:O	2.05	0.57
1:A:784:ARG:C	1:A:784:ARG:NE	2.58	0.57
1:A:772:ASN:HB2	1:A:774:PHE:HE2	1.71	0.56
1:A:789:GLU:HB3	1:A:790:HIS:CE1	2.41	0.55
1:A:660:LEU:CD2	1:A:686:GLN:HG3	2.37	0.55
1:A:790:HIS:O	1:A:793:VAL:HG22	2.06	0.55
1:A:732:LEU:CD2	1:A:754:SER:O	2.51	0.55
1:A:732:LEU:HD12	1:A:758:THR:HA	1.89	0.55
1:A:246:ILE:HD11	6:A:905:NAG:H82	1.90	0.54
6:A:913:NAG:H83	7:A:1222:HOH:O	2.06	0.54
1:A:809:GLN:O	1:A:812:LYS:N	2.37	0.54
1:A:81:GLU:O	1:A:84:GLN:HG2	2.07	0.54
1:A:804:ALA:O	1:A:805:SER:OG	2.24	0.54
1:A:779:ASP:HA	1:A:780:ILE:HG13	1.87	0.53
1:A:789:GLU:HB3	1:A:790:HIS:ND1	2.23	0.53
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.90	0.53
1:A:96:HIS:CD2	1:A:134:ASP:OD2	2.59	0.52
1:A:782:ASP:O	1:A:786:TRP:N	2.40	0.52
1:A:153:LEU:HB2	1:A:177:LEU:HD23	1.91	0.51
1:A:756:LEU:HD23	1:A:786:TRP:CZ3	2.46	0.51
1:A:34:TYR:CG	1:A:35:PRO:HA	2.46	0.51
1:A:211:ASN:O	1:A:232:THR:HA	2.11	0.50
1:A:668:GLU:HG2	1:A:692:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ILE:HD12	1:A:782:ASP:N	2.26	0.50
1:A:385:ASP:O	1:A:388:GLN:HG2	2.11	0.50
1:A:735:VAL:O	1:A:737:SER:N	2.44	0.50
1:A:310:MET:N	1:A:311:PRO:CD	2.75	0.49
1:A:720:SER:HA	1:A:744:SER:O	2.12	0.49
1:A:51:ASN:HA	1:A:72:ASP:O	2.13	0.48
1:A:34:TYR:CD1	1:A:35:PRO:HA	2.49	0.48
1:A:739:LYS:HG2	1:A:763:LYS:HB3	1.94	0.48
1:A:84:GLN:N	1:A:85:GLY:HA3	2.27	0.48
1:A:113:GLY:HA3	1:A:136:GLN:HB2	1.95	0.48
1:A:310:MET:N	1:A:311:PRO:HD3	2.28	0.48
1:A:781:GLY:O	1:A:784:ARG:N	2.48	0.47
1:A:775:GLU:HG2	1:A:777:THR:HG23	1.95	0.47
1:A:239:GLU:HG3	1:A:281:PHE:HB2	1.97	0.47
1:A:85:GLY:O	1:A:86:LEU:HB2	2.15	0.47
1:A:235:LYS:HE2	7:A:1301:HOH:O	2.14	0.47
1:A:730:GLY:C	1:A:732:LEU:HD23	2.36	0.47
1:A:753:LYS:HG2	1:A:782:ASP:CG	2.36	0.46
1:A:514:ALA:HA	1:A:539:ASN:O	2.16	0.46
1:A:303:ASN:HB3	1:A:306:TRP:CE2	2.51	0.46
1:A:778:CYS:O	1:A:780:ILE:HA	2.15	0.46
1:A:727:LEU:HD13	1:A:755:ALA:HB1	1.98	0.46
1:A:76:THR:HG22	1:A:98:PRO:HG3	1.98	0.45
1:A:741:LEU:HD21	1:A:743:LEU:HD11	1.99	0.44
1:A:410:ASP:OD1	1:A:412:LYS:HG2	2.17	0.44
1:A:431:SER:HB2	1:A:432:PRO:CD	2.47	0.44
1:A:317:ASP:OD1	1:A:319:GLU:HG3	2.17	0.44
1:A:388:GLN:N	1:A:389:PRO:CD	2.81	0.44
1:A:310:MET:O	1:A:310:MET:HG2	2.18	0.44
1:A:370:ARG:NH1	7:A:1107:HOH:O	2.51	0.43
1:A:587:LYS:NZ	6:A:917:NAG:O3	2.51	0.43
1:A:732:LEU:HD13	1:A:757:GLU:C	2.38	0.43
1:A:57:VAL:HG21	1:A:82:SER:HB3	2.01	0.43
1:A:565:SER:O	1:A:566:HIS:C	2.56	0.43
1:A:86:LEU:CB	1:A:89:LEU:HD22	2.49	0.43
1:A:732:LEU:HD22	1:A:755:ALA:C	2.39	0.42
1:A:753:LYS:HG2	1:A:782:ASP:OD1	2.19	0.42
1:A:57:VAL:HG23	1:A:57:VAL:O	2.20	0.42
1:A:780:ILE:CB	1:A:781:GLY:HA2	2.48	0.42
1:A:86:LEU:N	1:A:86:LEU:HD13	2.34	0.42
1:A:597:TYR:HB3	1:A:619:ARG:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:HIS:O	1:A:569:ARG:HG2	2.21	0.41
1:A:290:ARG:HB3	1:A:291:TYR:CD1	2.55	0.41
1:A:280:ARG:CZ	1:A:305:ALA:HB1	2.51	0.41
1:A:183:PHE:HB3	1:A:266:PRO:HG2	2.02	0.41
1:A:815:VAL:HG22	1:A:816:SER:N	2.36	0.41
1:A:177:LEU:HB2	1:A:208:LEU:HD23	2.03	0.40
1:A:616:SER:HA	1:A:647:SER:O	2.21	0.40
1:A:732:LEU:HD13	1:A:757:GLU:N	2.36	0.40
1:A:86:LEU:HB2	1:A:89:LEU:HD22	2.03	0.40
1:A:41:GLN:HA	1:A:42:ASN:HA	1.81	0.40
1:A:805:SER:HA	1:A:806:PRO:C	2.42	0.40

All (3) 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)
1:A:204:GLU:OE1	1:A:689:ARG:NH1[8_455]	1.88	0.32
1:A:338:ARG:NH2	1:A:709:ASP:OD1[8_455]	1.88	0.32
1:A:77:HIS:NE2	1:A:355:GLN:OE1[7_444]	2.18	0.02

## 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	742/811 (92%)	689 (93%)	47 (6%)	6 (1%)	<b>19</b>   <b>9</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	782	ASP
1	A	86	LEU
1	A	810	ARG

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Mol	Chain	Res	Type
1	A	53	ARG
1	A	378	VAL
1	A	780	ILE

### 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	685/755 (91%)	648 (95%)	37 (5%)	22 13

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	55	GLN
1	A	86	LEU
1	A	87	GLN
1	A	89	LEU
1	A	99	ASN
1	A	125	LYS
1	A	150	GLU
1	A	168	ARG
1	A	243	LYS
1	A	248	LEU
1	A	280	ARG
1	A	286	LEU
1	A	290	ARG
1	A	301	LYS
1	A	355	GLN
1	A	418	SER
1	A	430	ILE
1	A	433	LEU
1	A	582	ASN
1	A	671	ILE
1	A	701	LEU
1	A	702	PHE

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Mol	Chain	Res	Type
1	A	706	SER
1	A	726	HIS
1	A	727	LEU
1	A	732	LEU
1	A	734	GLU
1	A	738	LEU
1	A	753	LYS
1	A	779	ASP
1	A	782	ASP
1	A	784	ARG
1	A	788	ASP
1	A	795	ILE
1	A	810	ARG
1	A	814	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	87	GLN
1	A	96	HIS
1	A	174	ASN
1	A	184	ASN
1	A	531	HIS
1	A	539	ASN
1	A	752	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

10 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	B	1	1,2	14,14,15	0.77	0	17,19,21	1.63	3 (17%)
2	NAG	B	2	2	14,14,15	0.88	1 (7%)	17,19,21	1.83	3 (17%)
2	BMA	B	3	2	11,11,12	1.07	1 (9%)	15,15,17	2.05	4 (26%)
2	MAN	B	4	2	11,11,12	1.11	1 (9%)	15,15,17	1.05	1 (6%)
2	MAN	B	5	2	11,11,12	0.69	0	13,15,17	4.25	4 (30%)
3	NAG	C	1	1,3	14,14,15	1.02	1 (7%)	17,19,21	1.31	2 (11%)
3	NAG	C	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.38	3 (17%)
4	NAG	D	1	1,4	14,14,15	0.60	0	17,19,21	1.21	1 (5%)
4	NAG	D	2	4	14,14,15	0.90	0	17,19,21	1.51	3 (17%)
4	BMA	D	3	4	11,11,12	0.72	0	15,15,17	1.37	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/18/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	O5-C1	-2.60	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.28	1.40	1.43
3	C	1	NAG	O5-C5	-2.27	1.38	1.43
2	B	4	MAN	O5-C1	-2.09	1.40	1.43
3	C	2	NAG	O5-C1	-2.05	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	MAN	O1-C1-O5	-13.93	76.05	108.36
2	B	2	NAG	O5-C1-C2	-5.60	102.45	111.29
2	B	3	BMA	C1-C2-C3	5.28	116.16	109.67
2	B	5	MAN	O1-C1-C2	-4.32	90.37	111.42
4	D	1	NAG	C1-O5-C5	3.77	117.30	112.19
2	B	1	NAG	O6-C6-C5	-3.63	98.85	111.29
2	B	1	NAG	O5-C5-C6	3.32	112.40	107.20
2	B	3	BMA	O2-C2-C3	-3.12	103.89	110.14
2	B	1	NAG	O5-C1-C2	-2.98	106.58	111.29
3	C	1	NAG	O5-C1-C2	-2.82	106.84	111.29
3	C	1	NAG	C1-C2-N2	-2.80	105.70	110.49
4	D	3	BMA	C2-C3-C4	-2.80	106.05	110.89
2	B	2	NAG	O5-C5-C6	2.80	111.59	107.20
3	C	2	NAG	O6-C6-C5	-2.77	101.78	111.29
2	B	3	BMA	O4-C4-C5	2.71	116.03	109.30
3	C	2	NAG	C3-C4-C5	-2.58	105.64	110.24
2	B	5	MAN	O5-C5-C4	2.52	114.27	109.69
2	B	3	BMA	O4-C4-C3	-2.50	104.58	110.35
4	D	2	NAG	O7-C7-N2	2.41	126.38	121.95
4	D	3	BMA	C1-C2-C3	2.28	112.47	109.67
2	B	5	MAN	C2-C3-C4	-2.19	107.51	110.69
4	D	2	NAG	C4-C3-C2	-2.15	107.86	111.02
2	B	4	MAN	C1-O5-C5	2.13	115.08	112.19
2	B	2	NAG	C1-O5-C5	-2.12	109.31	112.19
4	D	2	NAG	O5-C1-C2	-2.02	108.10	111.29
3	C	2	NAG	O3-C3-C4	2.00	114.98	110.35

There are no chirality outliers.

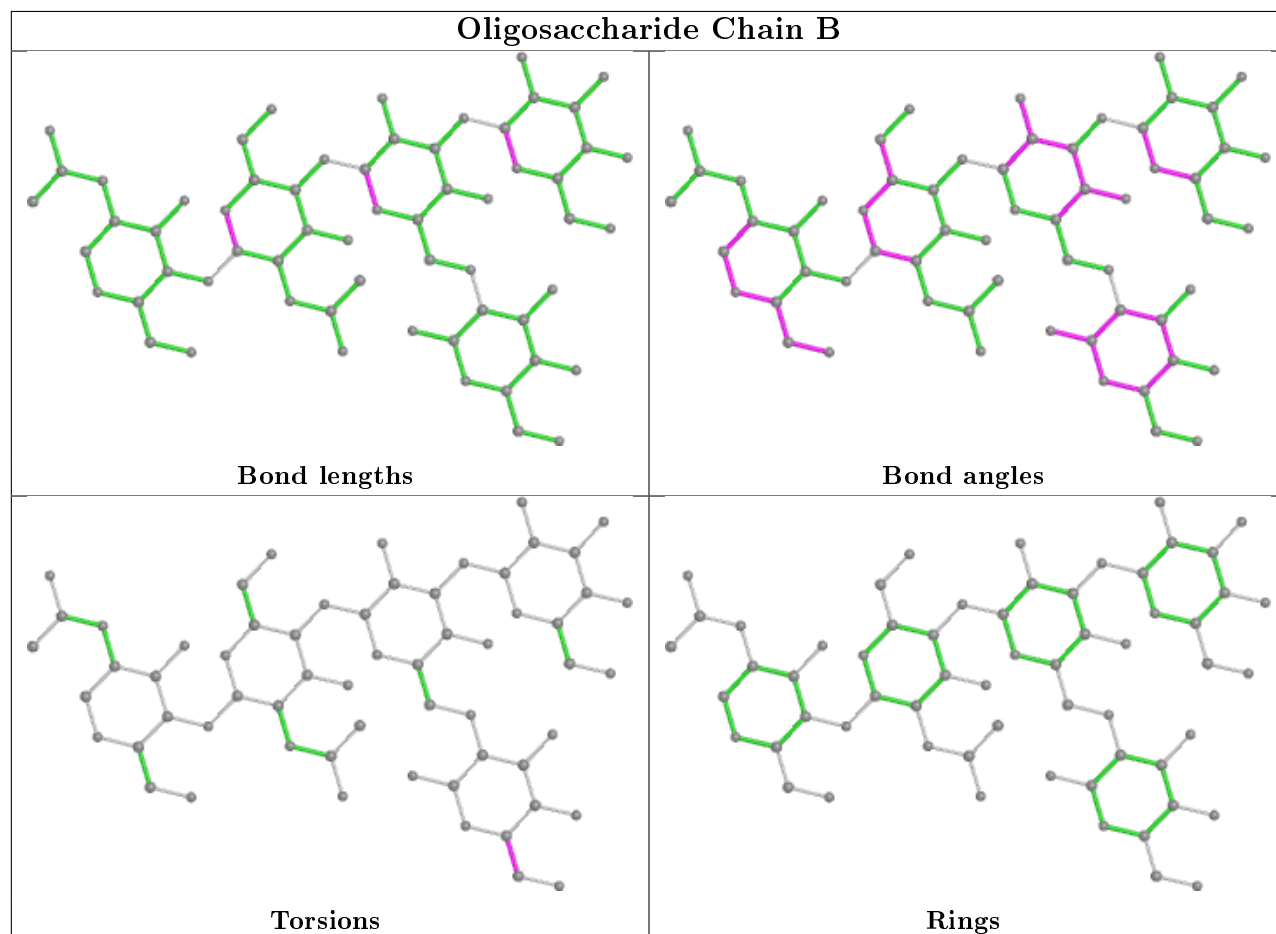
All (2) torsion outliers are listed below:

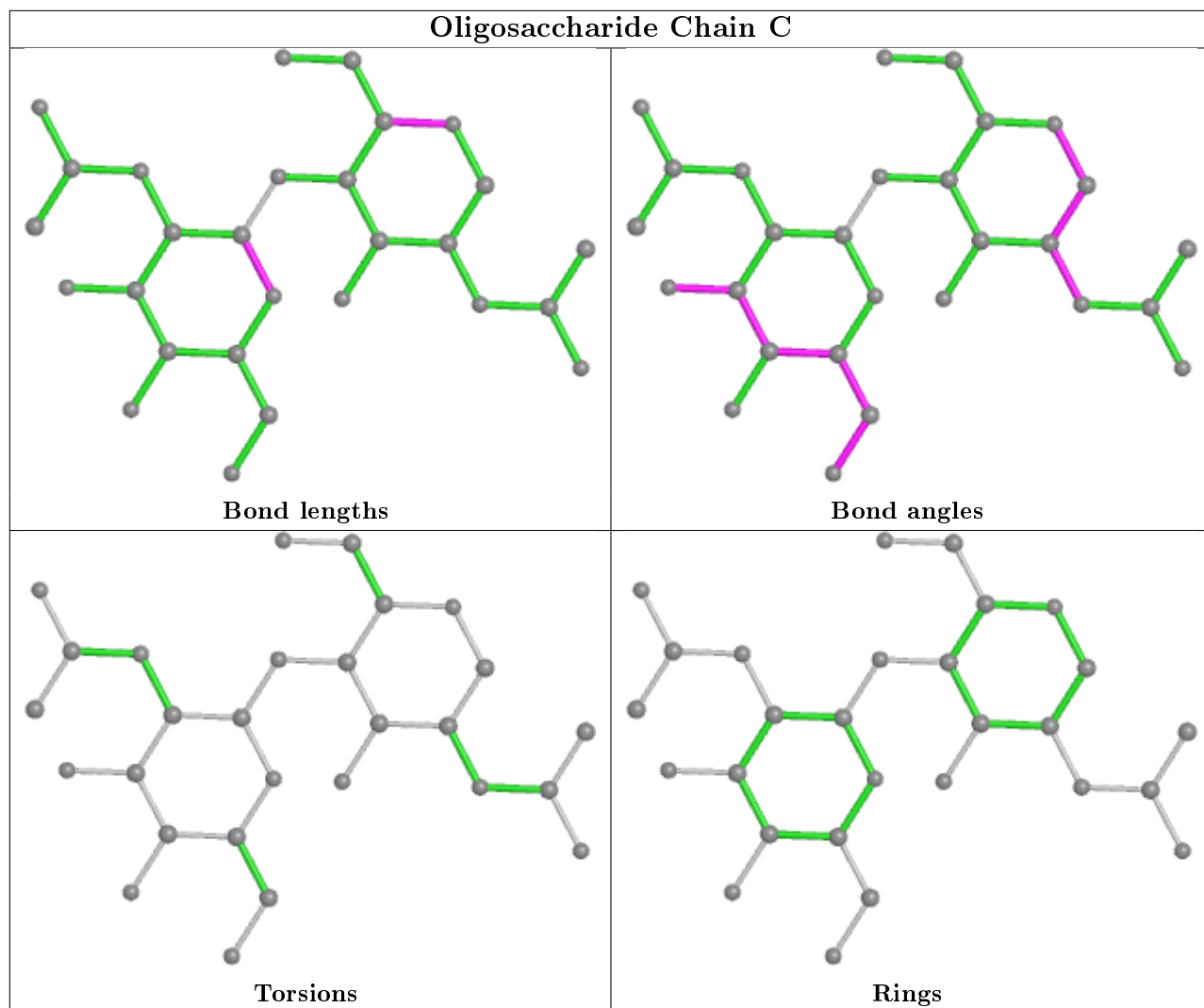
Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6

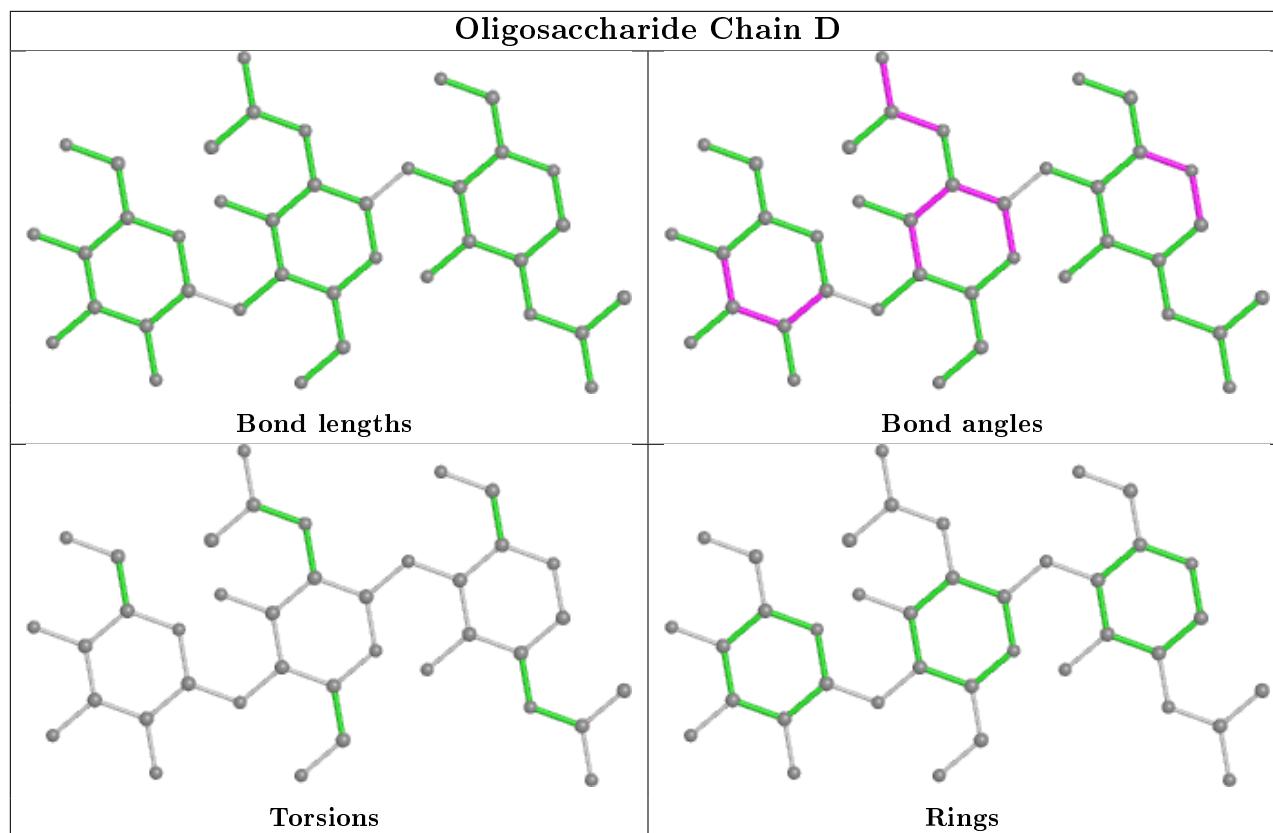
There are no ring outliers.

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 [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
6	NAG	A	904	1	14,14,15	1.02	1 (7%)	17,19,21	1.47	4 (23%)
6	NAG	A	903	1	14,14,15	0.67	0	17,19,21	1.16	2 (11%)
6	NAG	A	918	1	14,14,15	1.01	1 (7%)	17,19,21	1.77	3 (17%)
6	NAG	A	905	1	14,14,15	0.68	0	17,19,21	2.57	5 (29%)
6	NAG	A	902	1	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
5	URI	A	901	-	14,18,18	1.07	1 (7%)	14,26,26	1.21	1 (7%)
6	NAG	A	917	1	14,14,15	1.37	2 (14%)	17,19,21	1.95	4 (23%)
6	NAG	A	913	1	14,14,15	0.74	0	17,19,21	2.00	7 (41%)

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
6	NAG	A	904	1	-	0/6/23/26	0/1/1/1
6	NAG	A	903	1	-	2/6/23/26	0/1/1/1
6	NAG	A	918	1	-	2/6/23/26	0/1/1/1
6	NAG	A	905	1	-	0/6/23/26	0/1/1/1
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
5	URI	A	901	-	-	2/4/22/22	0/2/2/2
6	NAG	A	917	1	-	0/6/23/26	0/1/1/1
6	NAG	A	913	1	-	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)
5	A	901	URI	C4-N3	2.98	1.38	1.33
6	A	917	NAG	C2-N2	-2.91	1.41	1.46
6	A	904	NAG	O5-C1	-2.67	1.39	1.43
6	A	917	NAG	O5-C5	-2.61	1.38	1.43
6	A	918	NAG	O5-C1	-2.54	1.39	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	905	NAG	C1-O5-C5	8.80	124.11	112.19
6	A	917	NAG	C1-C2-N2	-5.97	100.28	110.49
6	A	918	NAG	O5-C1-C2	-5.18	103.11	111.29
5	A	901	URI	C5-C4-N3	-3.96	114.59	123.31
6	A	913	NAG	C4-C3-C2	-3.81	105.44	111.02
6	A	913	NAG	O5-C1-C2	-3.51	105.75	111.29
6	A	918	NAG	C1-C2-N2	-3.23	104.97	110.49
6	A	904	NAG	O5-C1-C2	-3.14	106.33	111.29
6	A	913	NAG	O7-C7-C8	-3.13	116.24	122.06
6	A	905	NAG	C4-C3-C2	-3.08	106.50	111.02
6	A	902	NAG	C1-O5-C5	2.89	116.11	112.19
6	A	913	NAG	O7-C7-N2	2.77	127.05	121.95
6	A	904	NAG	O5-C5-C4	-2.75	104.14	110.83
6	A	905	NAG	C2-N2-C7	-2.61	119.18	122.90
6	A	913	NAG	C1-C2-N2	2.54	114.83	110.49
6	A	917	NAG	O6-C6-C5	-2.36	103.20	111.29
6	A	904	NAG	O5-C5-C6	2.33	110.85	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	918	NAG	C8-C7-N2	-2.28	112.24	116.10
6	A	903	NAG	O5-C5-C6	2.20	110.66	107.20
6	A	913	NAG	O5-C5-C4	-2.20	105.47	110.83
6	A	917	NAG	C4-C3-C2	-2.17	107.84	111.02
6	A	913	NAG	C1-O5-C5	2.17	115.13	112.19
6	A	903	NAG	O5-C5-C4	-2.13	105.63	110.83
6	A	905	NAG	O5-C5-C6	2.13	110.54	107.20
6	A	917	NAG	C8-C7-N2	-2.13	112.50	116.10
6	A	905	NAG	C3-C4-C5	-2.06	106.56	110.24
6	A	904	NAG	C3-C4-C5	-2.03	106.62	110.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	URI	C2'-C1'-N1-C6
5	A	901	URI	O4'-C1'-N1-C6
6	A	903	NAG	O5-C5-C6-O6
6	A	903	NAG	C4-C5-C6-O6
6	A	918	NAG	O5-C5-C6-O6
6	A	918	NAG	C4-C5-C6-O6
6	A	913	NAG	C3-C2-N2-C7
6	A	913	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	905	NAG	2	0
6	A	917	NAG	1	0
6	A	913	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	748/811 (92%)	0.25	47 (6%) <span style="border: 1px solid red; padding: 2px;">20</span> <span style="border: 1px solid red; padding: 2px;">22</span>	20, 31, 76, 106	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	LEU	7.5
1	A	86	LEU	5.5
1	A	779	ASP	5.4
1	A	786	TRP	5.4
1	A	761	THR	4.9
1	A	815	VAL	4.4
1	A	799	VAL	4.2
1	A	780	ILE	4.1
1	A	778	CYS	4.0
1	A	702	PHE	3.9
1	A	34	TYR	3.9
1	A	732	LEU	3.8
1	A	760	THR	3.7
1	A	757	GLU	3.6
1	A	756	LEU	3.5
1	A	36	CYS	3.5
1	A	783	PHE	3.4
1	A	85	GLY	3.3
1	A	64	TYR	3.3
1	A	784	ARG	3.2
1	A	33	SER	3.1
1	A	113	GLY	3.0
1	A	774	PHE	3.0
1	A	785	ARG	2.9
1	A	61	VAL	2.9
1	A	794	LYS	2.9
1	A	735	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	782	ASP	2.9
1	A	46	ILE	2.8
1	A	62	GLY	2.7
1	A	40	LYS	2.7
1	A	759	LYS	2.7
1	A	53	ARG	2.7
1	A	44	SER	2.7
1	A	39	LYS	2.6
1	A	793	VAL	2.6
1	A	788	ASP	2.6
1	A	758	THR	2.5
1	A	751	ILE	2.5
1	A	47	ALA	2.3
1	A	99	ASN	2.2
1	A	37	ASP	2.1
1	A	763	LYS	2.1
1	A	733	SER	2.0
1	A	765	SER	2.0
1	A	795	ILE	2.0
1	A	798	LEU	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(Å <sup>2</sup> )	Q<0.9
2	MAN	B	4	11/12	0.84	0.16	35,47,52,53	0
2	MAN	B	5	11/12	0.88	0.14	56,61,74,74	0
4	BMA	D	3	11/12	0.90	0.10	34,39,50,52	0
3	NAG	C	2	14/15	0.93	0.10	32,38,44,49	0
2	BMA	B	3	11/12	0.94	0.09	29,37,49,50	0
2	NAG	B	2	14/15	0.96	0.09	22,24,32,33	0
2	NAG	B	1	14/15	0.96	0.10	19,21,24,28	0
4	NAG	D	2	14/15	0.96	0.10	23,26,32,39	0

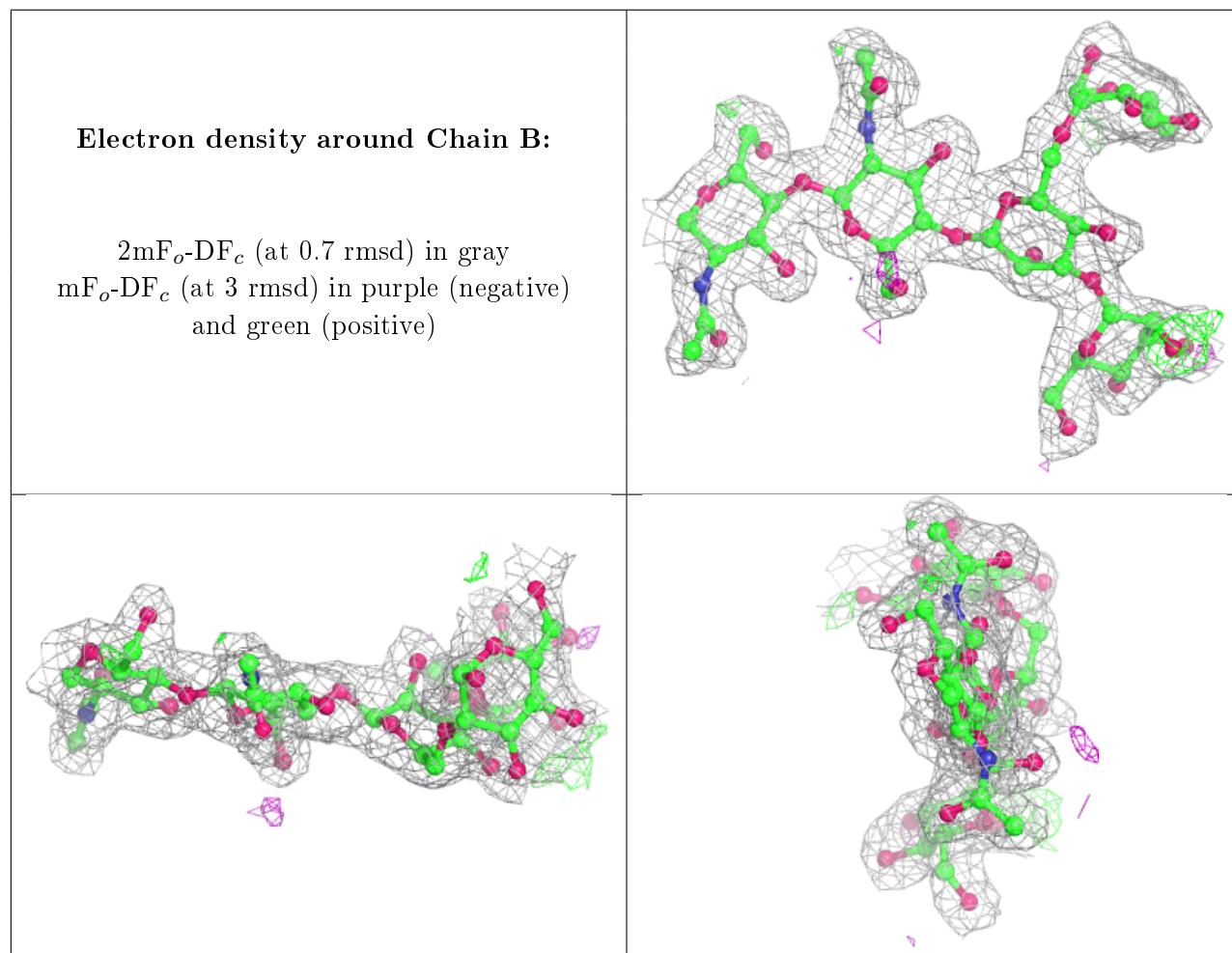
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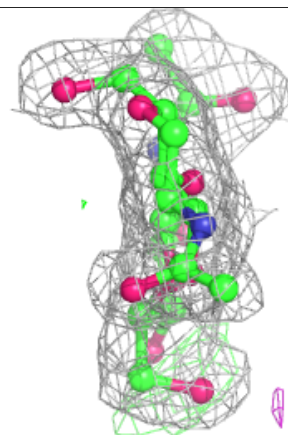
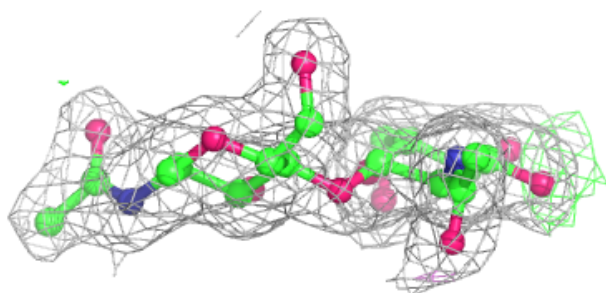
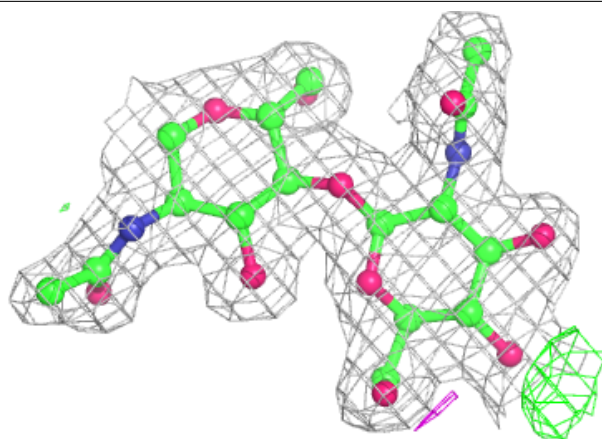
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	1	14/15	0.96	0.12	20,22,25,26	0
4	NAG	D	1	14/15	0.97	0.10	20,22,23,24	0

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.

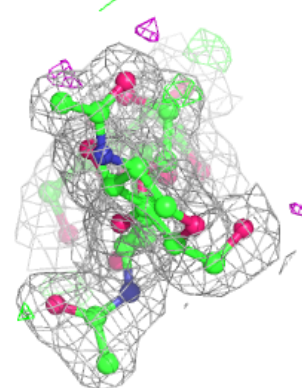
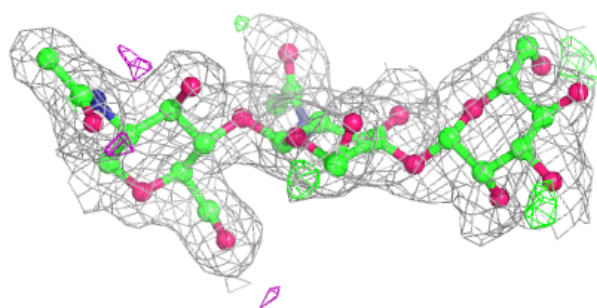
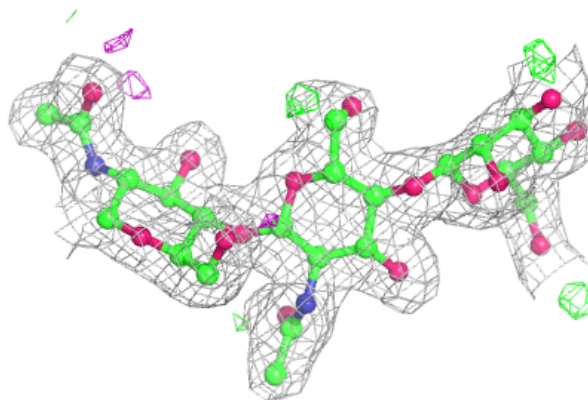


**Electron density around Chain C:**

$2mF_o-DF_c$  (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)



## 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
6	NAG	A	902	14/15	0.82	0.19	39,64,72,73	0
6	NAG	A	905	14/15	0.85	0.27	45,55,63,67	0
6	NAG	A	904	14/15	0.88	0.14	44,49,58,58	0
6	NAG	A	918	14/15	0.88	0.16	44,53,63,63	0
6	NAG	A	913	14/15	0.88	0.16	35,45,57,59	0
6	NAG	A	903	14/15	0.91	0.16	57,63,69,81	0
5	URI	A	901	17/17	0.96	0.11	21,25,35,37	0
6	NAG	A	917	14/15	0.97	0.09	21,23,28,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.