

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 08:00 am GMT

PDB ID	:	4UFL
Title	:	Mouse Galactocerebrosidase complexed with deoxy-galacto-noeurostegine
		DGN
Authors	:	Hill, C.H.; Viuff, A.H.; Spratley, S.J.; Salamone, S.; Christensen, S.H.; Read,
		R.J.; Moriarty, N.W.; Jensen, H.H.; Deane, J.E.
Deposited on		
Resolution	:	2.40  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

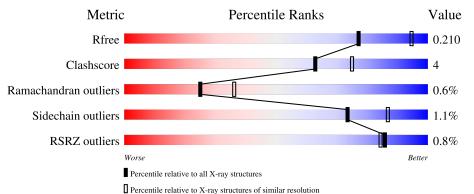
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	654	% 86% 11% •							
2	В	2	100%							
2	С	2	100%							
2	D	2	100%							



#### $4 \mathrm{UFL}$

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5594 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 GALACTOCEREBROSIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	641	Total 5260	C 3395	N 884	O 965	S 16	0	10	0

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	-	expression tag	UNP P54818
А	16	HIS	-	expression tag	UNP P54818
A	17	HIS	-	expression tag	UNP P54818
А	18	HIS	-	expression tag	UNP P54818
А	19	HIS	-	expression tag	UNP P54818
A	20	HIS	-	expression tag	UNP P54818
А	21	ILE	-	expression tag	UNP P54818
A	22	GLU	-	expression tag	UNP P54818
А	23	GLY	-	expression tag	UNP P54818
А	24	ARG	-	expression tag	UNP P54818
А	25	GLY	-	expression tag	UNP P54818
A	26	ALA	-	expression tag	UNP P54818

There are 12 discrepancies between the modelled and reference sequences:

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	В	2	Total 28			0	0	0
2	С	2	Total 28	C 16		0	0	0

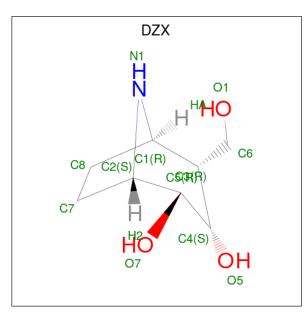
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	D	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 3 is DEOXY-GALACTO-NOEUROSTEGINE (three-letter code: DZX) (formula:  $C_8H_{15}NO_3$ ).



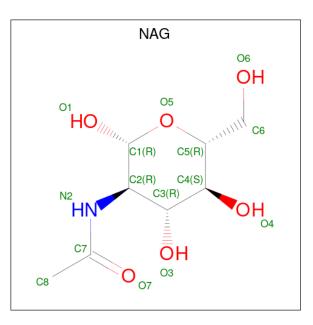
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 12	C 8	N 1	O 3	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	А	1	Total 1	Ca 1	0	0

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

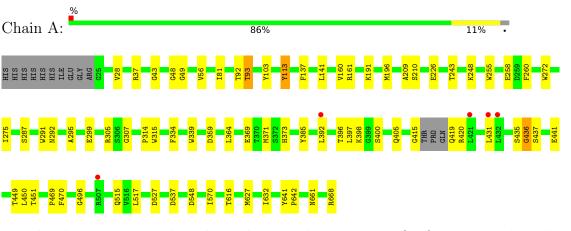
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	223	Total         O           223         223	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: GALACTOCEREBROSIDASE

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

Chain B:

100%

NAG1 NAG2

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

Ch	ain	$\mathbf{C}$ :
$\mathbf{O}\mathbf{\Pi}$	CULL	$\sim$ .

100%

#### NAG1 NAG2

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

Chain D:

100%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	248.53Å 248.53Å 77.65Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	73.04 - 2.40	Depositor
Resolution (A)	73.04 - 2.40	EDS
% Data completeness	97.9 (73.04-2.40)	Depositor
(in resolution range)	94.9 (73.04-2.40)	EDS
R <sub>merge</sub>	0.14	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 2.40 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.178 , $0.210$	Depositor
$R, R_{free}$	0.180 , $0.210$	DCC
$R_{free}$ test set	1785 reflections $(5.10%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 43.1	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5594	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: NAG, CA, DZX

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).

Mal	Mol Chain		lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.35	0/5424	0.60	2/7382~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	420	ARG	C-N-CA	6.04	136.80	121.70
1	А	420	ARG	N-CA-C	-5.50	96.16	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5260	0	5023	43	0
2	В	28	0	25	2	0
2	С	28	0	25	0	0
2	D	28	0	25	0	0
3	А	12	0	15	1	0
4	А	1	0	0	0	0
5	А	14	0	13	1	0
6	А	223	0	0	2	0
All	All	5594	0	5126	45	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 4.

The worst 5 of 45 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:435:SER:O	1:A:437:SER:N	2.05	0.89
1:A:196:MET:SD	6:A:2072:HOH:O	2.38	0.80
2:B:1:NAG:H62	2:B:2:NAG:HN2	1.56	0.69
1:A:299[A]:GLU:H	1:A:299[A]:GLU:CD	1.97	0.67
1:A:258:GLU:OE2	3:A:1001:DZX:N1	2.29	0.65

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	А	647/654~(99%)	620~(96%)	23~(4%)	4 (1%)	25 36	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	436	GLY
1	А	93	THR
1	А	260	PHE
1	А	400	SER

#### 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	$\operatorname{number}$	of	residues.
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	552/555~(100%)	546~(99%)	6 (1%)	73 87		

5 of 6 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	450	LEU
1	А	515	GLN
1	А	527	ASP
1	А	113	TYR
1	А	103	TYR

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

#### 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)

6 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			
10101	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	NAG	В	1	1,2	14,14,15	1.63	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	В	2	2	14,14,15	0.72	1 (7%)	17,19,21	0.65	1 (5%)
2	NAG	С	1	1,2	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	С	2	2	14,14,15	0.45	0	17,19,21	0.42	0



ſ	Mol	Type	Chain	Res	Link	Bo	Bond lengths		Bond angles		les
	WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	2	NAG	D	1	1,2	14,14,15	0.30	0	17,19,21	0.51	0
	2	NAG	D	2	2	14,14,15	0.20	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	В	2	2	-	2/6/23/26	0/1/1/1
2	NAG	С	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	$\mathbf{C}$	2	2	-	2/6/23/26	0/1/1/1
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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	1	NAG	O5-C1	-5.74	1.34	1.43
2	В	2	NAG	C1-C2	2.12	1.55	1.52

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1	NAG	C4-C3-C2	2.36	114.47	111.02
2	В	2	NAG	C1-O5-C5	2.18	115.15	112.19

All (2) bond angle outliers are listed below:

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	В	2	NAG	O5-C5-C6-O6
2	В	1	NAG	C8-C7-N2-C2
2	В	1	NAG	O7-C7-N2-C2

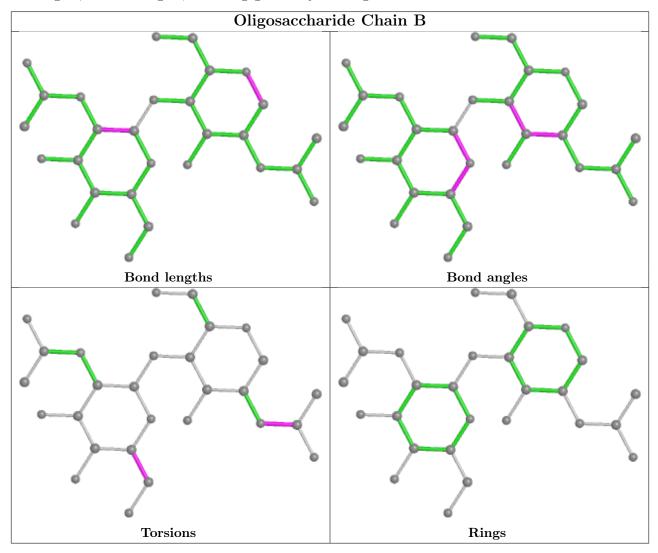
There are no ring outliers.

2 monomers are involved in 2 short contacts:



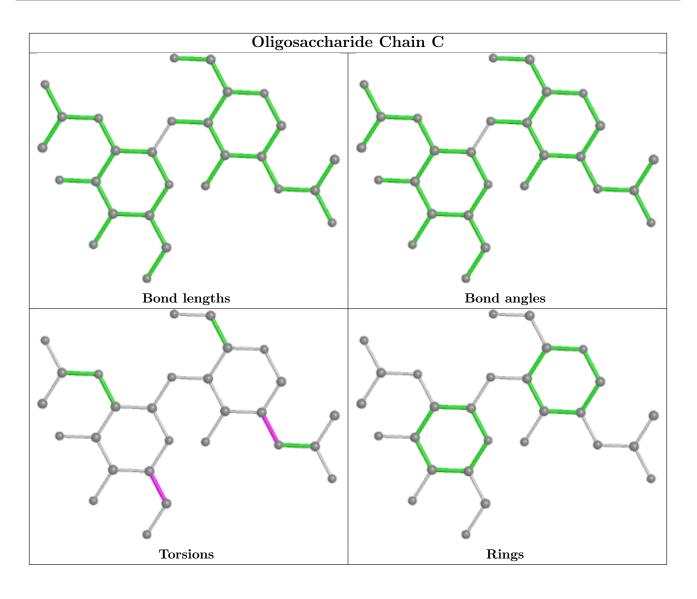
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2	NAG	2	0
2	В	1	NAG	2	0

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



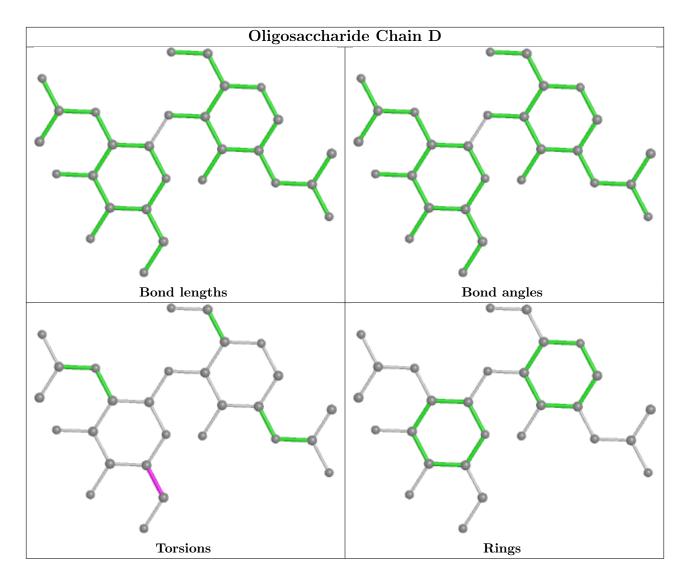












### 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Trune	Chain	Dec	Link	Bond lengths			Bond angles		
IVIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	NAG	А	1387	1	14,14,15	0.52	0	$17,\!19,\!21$	0.75	1 (5%)
3	DZX	А	1001	-	13,13,13	1.29	1 (7%)	14,19,19	1.55	2 (14%)



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
5	NAG	А	1387	1	-	2/6/23/26	0/1/1/1
3	DZX	А	1001	-	-	2/2/27/27	0/3/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	1001	DZX	C5-C4	3.01	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	1001	DZX	C5-C4-C3	3.62	116.95	110.74
5	А	1387	NAG	C1-O5-C5	2.65	115.79	112.19
3	А	1001	DZX	O7-C3-C4	-2.12	105.46	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1001	DZX	C4-C5-C6-O1
5	А	1387	NAG	O5-C5-C6-O6
5	А	1387	NAG	C4-C5-C6-O6
3	А	1001	DZX	C1-C5-C6-O1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	1387	NAG	1	0
3	А	1001	DZX	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 (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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	641/654~(98%)	-0.23	5 (0%) 86 84	24, 45, 80, 104	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	421	LEU	4.1
1	А	431	LEU	3.2
1	А	507	ARG	2.4
1	А	392	LEU	2.1
1	А	432	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,  $95^{th}$  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.

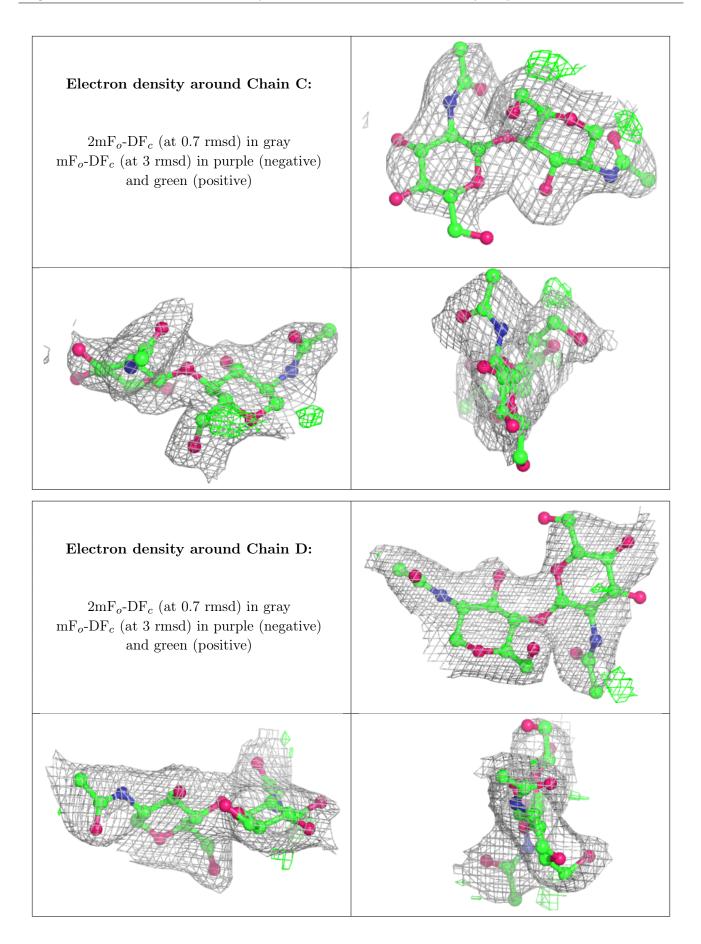
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	NAG	В	2	14/15	0.72	0.38	88,100,105,105	0
2	NAG	С	2	14/15	0.84	0.21	79,88,94,95	0
2	NAG	С	1	14/15	0.87	0.12	53,63,67,75	0
2	NAG	D	2	14/15	0.88	0.17	70,75,82,82	0
2	NAG	В	1	14/15	0.92	0.17	51,71,74,82	0
2	NAG	D	1	14/15	0.96	0.11	42,53,60,68	0



Electron density around Chain B:  $2mF_o$ -DF<sub>c</sub> (at 0.7 rmsd) in gray  $mF_o$ -DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

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.







### 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	NAG	А	1387	14/15	0.79	0.23	59,73,75,75	0
4	CA	А	1002	1/1	0.94	0.11	61,61,61,61	0
3	DZX	А	1001	12/12	0.97	0.16	26,33,45,46	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

