

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

Nov 22, 2023 – 05:42 PM JST

PDB ID : 7WH6

Title : The mutant crystal structure of b-1,4-Xylanase (XynAF1\_N179S)

Authors : Li, G.Q.; Zhang, R.F.

Deposited on : 2021-12-30

Resolution : 1.58 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
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: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 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) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

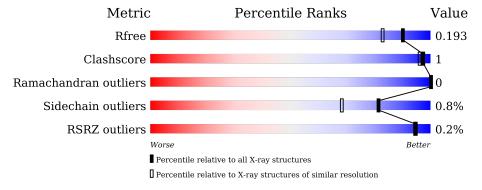
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.58 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	A	329		94%				
1	В	329		95%				
2	С	7	14%	86%				
3	D	5	20%	80%				



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

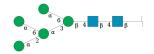
• Molecule 1 is a protein called Beta-xylanase.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	۸	319	Total	С	N	О	S	0	4	0
1	A	319	2443	1553	402	478	10	U	4	U
1	D	319	Total	С	N	О	S	0	7	0
1	D	319	2463	1563	406	484	10	0	(	U

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP A0A229WLM4
A	2	ALA	-	expression tag	UNP A0A229WLM4
A	3	GLU	-	expression tag	UNP A0A229WLM4
A	4	ALA	-	expression tag	UNP A0A229WLM4
A	179	SER	ASN	engineered mutation	UNP A0A229WLM4
В	1	GLU	-	expression tag	UNP A0A229WLM4
В	2	ALA	-	expression tag	UNP A0A229WLM4
В	3	GLU	-	expression tag	UNP A0A229WLM4
В	4	ALA	-	expression tag	UNP A0A229WLM4
В	179	SER	ASN	engineered mutation	UNP A0A229WLM4

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]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
2	С	7	Total 83	C 46	N 2	O 35	0	0	0

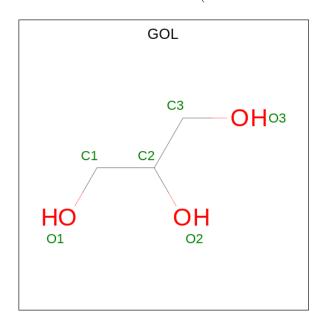


• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	5	Total 61	C 34		0	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0

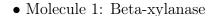
• Molecule 5 is water.

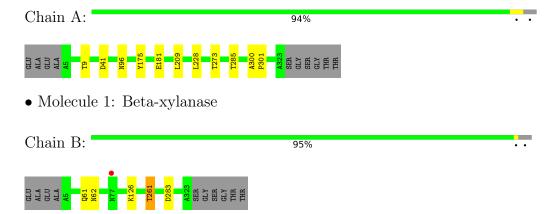
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	426	Total O 426 426	0	0
5	В	401	Total O 401 401	0	0



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

Chain C: 14% 86%

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





# 4 Data and refinement statistics (i)

Property	Value	Source		
Space group	P 1 21 1	Depositor		
Cell constants	55.30Å 119.14Å 60.83Å	Donositor		
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 102.28° 90.00°	Depositor		
Resolution (Å)	19.80 - 1.58	Depositor		
rtesolution (A)	19.79 - 1.58	EDS Depositor EDS Depositor Depositor Xtriage Depositor Depositor Depositor Depositor		
% Data completeness	99.2 (19.80-1.58)	Depositor		
(in resolution range)	99.3 (19.79-1.58)	EDS		
$R_{merge}$	0.12	Depositor		
$R_{sym}$	(Not available)	Depositor		
$< I/\sigma(I) > 1$	1.76 (at 1.58Å)	Xtriage		
Refinement program	REFMAC 5.8.0267	Depositor		
D D.	0.155 , 0.181	Depositor		
$R, R_{free}$	0.168 , 0.193	DCC		
$R_{free}$ test set	5147 reflections (4.93%)	wwPDB-VP		
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage		
Anisotropy	0.027	Xtriage		
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 45.3	EDS		
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage		
Estimated twinning fraction	No twinning to report.	Xtriage		
$F_o, F_c$ correlation	0.96	EDS		
Total number of atoms	5889	wwPDB-VP		
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP		

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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: MAN, NAG, BMA, GOL

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.72	0/2505	0.81	1/3422 (0.0%)	
1	В	0.69	0/2525	0.80	0/3449	
All	All	0.71	0/5030	0.81	1/6871 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	A	175	TYR	CB-CG-CD1	-5.03	117.98	121.00

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	A	2443	0	2340	5	0
1	В	2463	0	2354	3	0
2	С	83	0	70	0	0
3	D	61	0	52	0	0
4	A	6	0	8	0	0
4	В	6	0	8	0	0
5	A	426	0	0	1	0
5	В	401	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5889	0	4832	8	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 1.

All (8) 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:B:261:THR:HG21	5:B:996:HOH:O	2.05	0.57
1:A:9:THR:HG22	5:A:914:HOH:O	2.08	0.52
1:A:300:ALA:N	1:A:301:PRO:HD3	2.28	0.49
1:A:9:THR:HG23	1:A:41:ASP:HA	1.95	0.49
1:A:181:GLU:HA	1:A:209:LEU:HD23	1.99	0.45
1:B:61:GLN:O	1:B:62[A]:ASN:HB2	2.16	0.45
1:B:126:LYS:HE3	5:B:850:HOH:O	2.16	0.45
1:A:228:LEU:HB3	1:A:273:THR:HG21	2.02	0.41

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/329 (98%)	318 (99%)	3 (1%)	0	100	100
1	В	324/329 (98%)	319 (98%)	5 (2%)	0	100	100
All	All	$645/658 \; (98\%)$	637 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.



#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Rotameric Outliers		
1	A	255/257~(99%)	253 (99%)	2 (1%)	81	68
1	В	258/257 (100%)	256 (99%)	2 (1%)	81	68
All	All	513/514 (100%)	509 (99%)	4 (1%)	81	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	285	THR
1	В	261	THR
1	В	283	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	118	ASN
1	В	114	ASN
1	В	145	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)

12 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	Tuna	Chain	Res	Link	Вс	ond leng	$ ag{ths}$	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	NAG	С	1	1,2	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
2	NAG	С	2	2	14,14,15	0.73	0	17,19,21	1.16	2 (11%)
2	BMA	С	3	2	11,11,12	0.75	0	15,15,17	0.85	0
2	MAN	С	4	2	11,11,12	0.66	0	15,15,17	1.26	2 (13%)
2	MAN	С	5	2	11,11,12	0.50	0	15,15,17	1.33	2 (13%)
2	MAN	С	6	2	11,11,12	0.48	0	15,15,17	1.40	1 (6%)
2	MAN	С	7	2	11,11,12	1.17	1 (9%)	15,15,17	1.21	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.87	0	17,19,21	1.65	4 (23%)
3	NAG	D	2	3	14,14,15	0.77	0	17,19,21	0.92	0
3	BMA	D	3	3	11,11,12	0.88	0	15,15,17	1.21	1 (6%)
3	MAN	D	4	3	11,11,12	0.94	0	15,15,17	1.18	1 (6%)
3	MAN	D	5	3	11,11,12	0.88	0	15,15,17	1.15	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	С	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1
2	BMA	С	3	2	-	0/2/19/22	0/1/1/1
2	MAN	С	4	2	-	0/2/19/22	0/1/1/1
2	MAN	С	5	2	-	0/2/19/22	0/1/1/1
2	MAN	С	6	2	-	2/2/19/22	0/1/1/1
2	MAN	С	7	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	_	0/2/19/22	0/1/1/1



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	С	7	MAN	C2-C3	2.05	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	С	6	MAN	O5-C5-C6	4.50	114.25	107.20
3	D	1	NAG	O4-C4-C5	-3.61	100.34	109.30
2	С	1	NAG	O4-C4-C5	-3.42	100.81	109.30
2	С	5	MAN	C1-O5-C5	3.40	116.80	112.19
2	С	2	NAG	C1-O5-C5	3.28	116.64	112.19
3	D	4	MAN	O2-C2-C3	-2.74	104.66	110.14
2	С	7	MAN	O5-C1-C2	-2.66	106.67	110.77
3	D	3	BMA	C3-C4-C5	2.62	114.92	110.24
3	D	1	NAG	C2-N2-C7	2.52	126.49	122.90
2	С	4	MAN	C1-C2-C3	-2.44	106.67	109.67
3	D	5	MAN	O2-C2-C3	-2.40	105.34	110.14
2	С	1	NAG	O3-C3-C2	-2.26	104.78	109.47
2	С	2	NAG	O4-C4-C5	-2.26	103.69	109.30
2	С	5	MAN	O2-C2-C1	2.19	113.64	109.15
3	D	1	NAG	O7-C7-N2	-2.12	118.06	121.95
2	С	4	MAN	O3-C3-C2	-2.04	106.09	109.99
3	D	1	NAG	O3-C3-C4	2.00	114.98	110.35
3	D	5	MAN	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

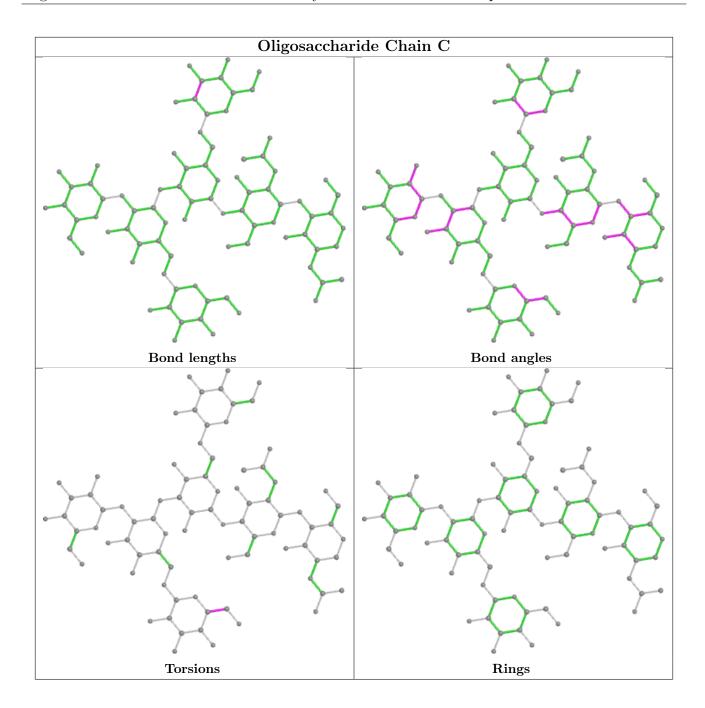
Mol	Chain	Res	Type	Atoms
2	С	6	MAN	O5-C5-C6-O6
2	С	6	MAN	C4-C5-C6-O6

There are no ring outliers.

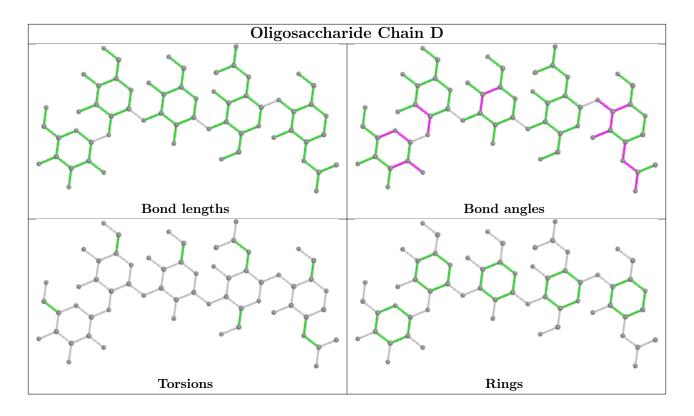
No monomer is involved in short contacts.

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)

#### 2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
4	GOL	A	601	-	5,5,5	0.25	0	5,5,5	0.48	0
4	GOL	В	601	-	5,5,5	0.18	0	5,5,5	0.46	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
4	GOL	A	601	-	-	2/4/4/4	-
4	GOL	В	601	-	-	0/4/4/4	-



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
4	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

# 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	<RSRZ $>$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	319/329 (96%)	-0.22	0 100 100	9, 14, 23, 34	0
1	В	319/329~(96%)	-0.21	1 (0%) 94 94	9, 14, 23, 35	0
All	All	638/658 (96%)	-0.21	1 (0%) 95 94	9, 14, 23, 35	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	77	ASN	2.1

#### 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MAN	С	7	11/12	0.68	0.28	32,34,39,40	0
2	MAN	С	6	11/12	0.81	0.32	38,41,48,49	0
3	MAN	D	4	11/12	0.90	0.17	22,24,29,33	0
3	MAN	D	5	11/12	0.90	0.13	20,22,24,26	0
3	BMA	D	3	11/12	0.93	0.13	18,19,24,31	0
3	NAG	D	1	14/15	0.94	0.08	16,18,21,23	0
3	NAG	D	2	14/15	0.94	0.12	17,20,24,25	0
2	MAN	С	5	11/12	0.94	0.12	20,23,26,28	0

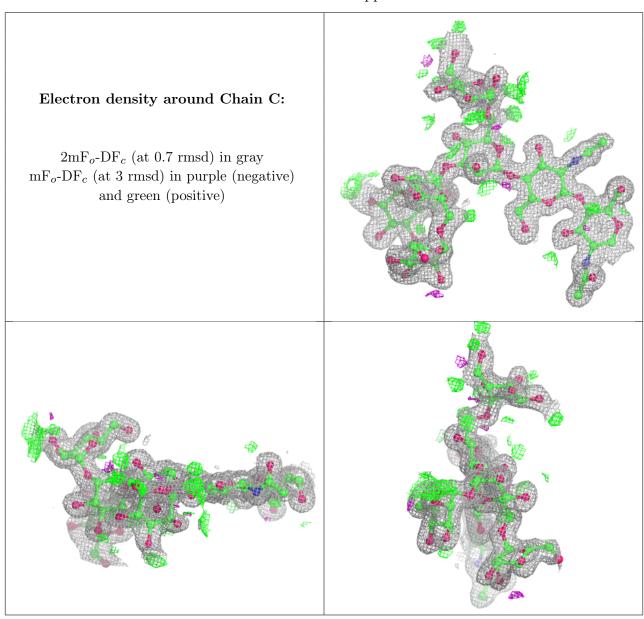
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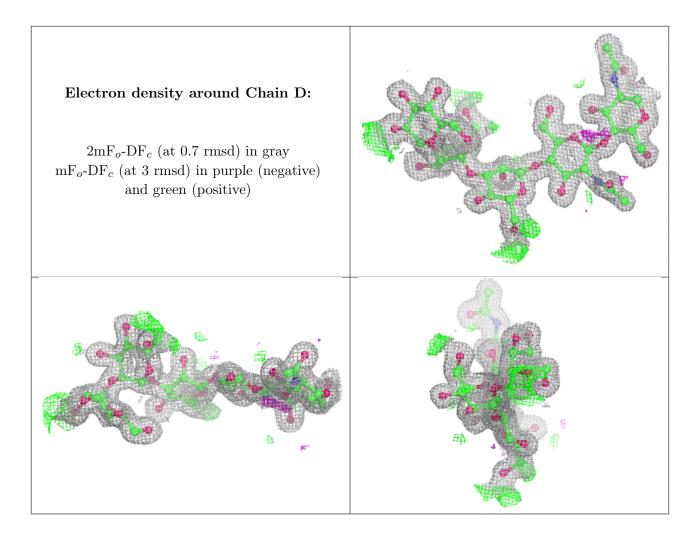
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BMA	С	3	11/12	0.94	0.13	16,17,21,27	0
2	MAN	С	4	11/12	0.94	0.20	21,23,26,30	0
2	NAG	С	1	14/15	0.95	0.08	15,17,22,23	0
2	NAG	С	2	14/15	0.96	0.10	16,17,22,22	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.







### 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	GOL	В	601	6/6	0.85	0.14	26,37,42,43	0
4	GOL	A	601	6/6	0.87	0.13	23,33,35,36	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

