

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

Feb 6, 2023 – 03:34 pm GMT

:	7R29
:	Crystal structure of TaCel5A E133Q Y200F variant with covalently linked
	cellotriose
:	Dutoit, R.
	2022-02-04
:	1.28 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:

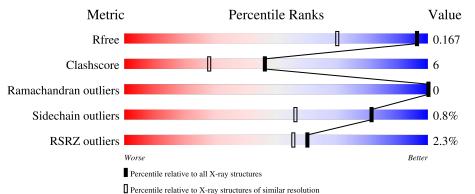
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

# 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 1.28 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	305	87%	13%		
1	В	305	% 91%	9%		
2	С	3	67%	33%		
2	D	3	67%	33%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	А	601	-	-	Х	-
3	GOL	А	603	-	-	Х	-
4	SO4	А	606	-	-	-	Х

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6027 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.

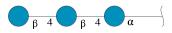
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	305	Total	С	Ν	0	S	0	25	0
	A	505	2500	1605	398	484	13	0	20	0
1	D	305	Total	С	Ν	0	S	0	22	0
	D	303	2476	1584	395	484	13	0		0

• Molecule 1 is a protein called EGI.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	GLN	GLU	engineered mutation	UNP Q8TG26
А	200	PHE	TYR	engineered mutation	UNP Q8TG26
В	133	GLN	GLU	engineered mutation	UNP Q8TG26
В	200	PHE	TYR	engineered mutation	UNP Q8TG26

• Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

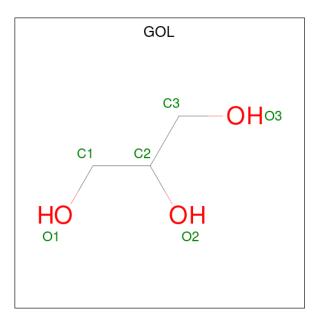


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	3	Total         C         O           44         24         20	0	1	0
2	D	3	Total         C         O           44         24         20	0	1	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

7R29

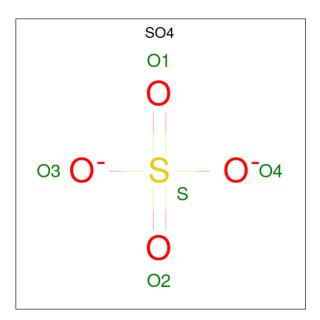




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	А	1	Total O	S	0	0
			5 4			
4	А	1	Total O	S	0	0
			5 4	1		
4	В	1	Total O	S	0	0
			5 4	1	Ŭ	
4	R	1	Total O	$\mathbf{S}$	0	0
	D	Ĩ	5 4	1		0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	430	Total         O           430         430	0	0
5	В	471	Total O 471 471	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.

Chain A:	87%	13%
A1 F7 F7 F7 F7 F1 F1 F1 F1 F1 F1 F1 F1 F1 F1	V89 R97 S105 F111 F114 F120 M123 M123 M124 F120 M124 T111	W174 N178 D202 S203 S203 T216 T216 T216 T221 T223
227 1254 1254 1254 1254 1254 1255 1255 1255		
• Molecule 1: EGI		
Chain B:	91%	9%
A1 W6 S18 S18 S18 N24 W24 W24 W24 W24 W24 W23 W53 W53 W53 W53 W53 W53 W53 W53	096 N131 N131 T175 T177 T177 T177 V179 N278 M273 M273 M274 W278	M286 1300 1300 1300 1300 1300 1300 1300 130
• Molecule 2: beta-D-glucop; e	yranose-(1-4)-beta-D-glucopyr	anose-(1-4)-alpha-D-glucopyranos
Chain C:	67%	33%
BGC3 BGC3 BGC3		
• Molecule 2: beta-D-glucop; e	yranose-(1-4)-beta-D-glucopyr	anose-(1-4)-alpha-D-glucopyranos
Chain D:	67%	33%
BGC2 BGC2 BGC3		

• Molecule 1: EGI



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	76.20Å $85.29$ Å $89.40$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.70 - 1.28	Depositor
Resolution (A)	47.96 - 1.28	EDS
% Data completeness	99.0 (44.70-1.28)	Depositor
(in resolution range)	99.0(47.96-1.28)	EDS
R <sub>merge</sub>	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.95 (at 1.28 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
$R, R_{free}$	0.151 , $0.169$	Depositor
II, IIfree	0.149 , $0.167$	DCC
$R_{free}$ test set	7443 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	14.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33 , $36.5$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6027	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.63% 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: BGC, GLC, GOL, SO4

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	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.49	0/2653	0.71	1/3619~(0.0%)	
1	В	0.51	0/2615	0.71	0/3566	
All	All	0.50	0/5268	0.71	1/7185~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	202	ASP	CB-CG-OD1	5.33	123.09	118.30

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	2500	0	2448	36	0
1	В	2476	0	2409	20	0
2	С	44	0	38	0	0
2	D	44	0	38	0	0
3	А	24	0	32	18	0
3	В	18	0	24	3	0
4	А	10	0	0	1	0
4	В	10	0	0	0	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 6.

The worst 5 of 63 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:69[B]:ASN:OD1	5:A:701:HOH:O	1.65	1.12
1:A:221:ARG:HE	3:A:601:GOL:H31	1.18	1.01
1:A:221:ARG:HH21	3:A:601:GOL:H11	1.33	0.92
1:B:35[B]:ASN:ND2	5:B:602:HOH:O	2.11	0.83
1:A:69[B]:ASN:ND2	5:A:706:HOH:O	2.20	0.75

The worst 5 of 7 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)
5:A:828:HOH:O	5:A:923:HOH:O[4_555]	1.47	0.73
5:A:791:HOH:O	5:A:793:HOH:O[3_545]	1.75	0.45
5:A:1050:HOH:O	5:B:979:HOH:O[4_456]	1.81	0.39
5:B:614:HOH:O	5:B:754:HOH:O[3_645]	1.85	0.35
5:B:663:HOH:O	5:B:905:HOH:O[4_556]	1.88	0.32

#### 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	331/305~(108%)	320~(97%)	11 (3%)	0	100 100



Chain Non-H H(model) H(added) Clashes Symm-Clashes Mol 5430 А 0 144 0 5 В 5 471 0 0 4  $\overline{7}$ All All 0 4989 63 6027

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	Chain	AnalysedFavouredAllowedOutliersPercent						
1	В	327/305~(107%)	317~(97%)	10 (3%)	0	100	100	
All	All	658/610~(108%)	637~(97%)	21 (3%)	0	100	100	

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There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Analysed Rotameric Outliers		Percentiles		
1	А	282/254~(111%)	279~(99%)	3(1%)	73 42		
1	В	278/254~(109%)	277 (100%)	1 (0%)	91 76		
All	All	560/508~(110%)	556~(99%)	4 (1%)	81 60		

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

Mol	Chain	Res	Type
1	А	131	ASN
1	А	171	THR
1	А	174	TRP
1	В	174	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	20	ASN
1	А	178	ASN
1	В	20	ASN
1	В	131	ASN
1	В	295	GLN

#### 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)

8 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).

Mal	Mol Type Chain		Chain Res Link		Bo	Bond lengths			Bond angles		
NIOI	Mol Type Chair	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	GLC	С	1	2	11,11,12	0.50	0	$15,\!15,\!17$	1.21	1 (6%)	
2	BGC	С	2	2	11,11,12	0.62	0	$15,\!15,\!17$	0.86	0	
2	BGC	С	3[A]	2	11,11,12	0.25	0	$15,\!15,\!17$	0.75	0	
2	BGC	С	3[B]	2	$11,\!11,\!12$	0.25	0	$15,\!15,\!17$	0.70	0	
2	GLC	D	1	2	11,11,12	0.54	0	$15,\!15,\!17$	1.37	1 (6%)	
2	BGC	D	2	2	11,11,12	0.41	0	$15,\!15,\!17$	0.63	0	
2	BGC	D	3[A]	2	11,11,12	0.26	0	$15,\!15,\!17$	0.69	0	
2	BGC	D	3[B]	2	11,11,12	0.25	0	$15,\!15,\!17$	0.76	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	GLC	С	1	2	-	0/2/19/22	0/1/1/1
2	BGC	С	2	2	-	0/2/19/22	0/1/1/1
2	BGC	С	3[A]	2	-	0/2/19/22	0/1/1/1
2	BGC	С	3[B]	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	D	3[A]	2	-	0/2/19/22	0/1/1/1
2	BGC	D	3[B]	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	1	GLC	C1-C2-C3	2.60	112.87	109.67
2	С	1	GLC	O4-C4-C5	-2.36	103.44	109.30

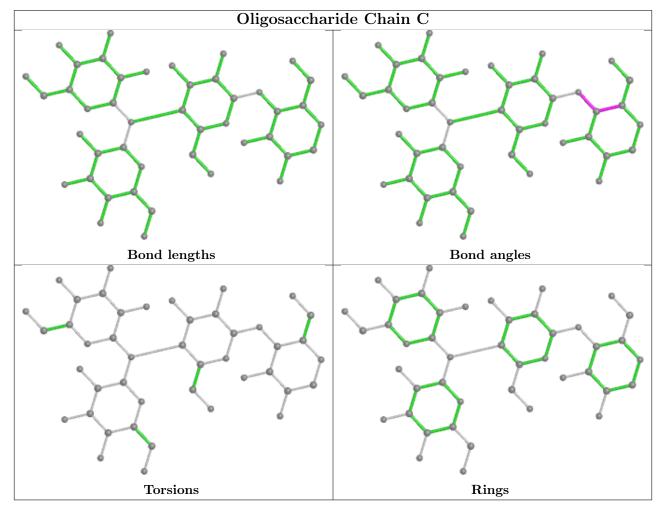
There are no chirality outliers.

There are no torsion outliers.

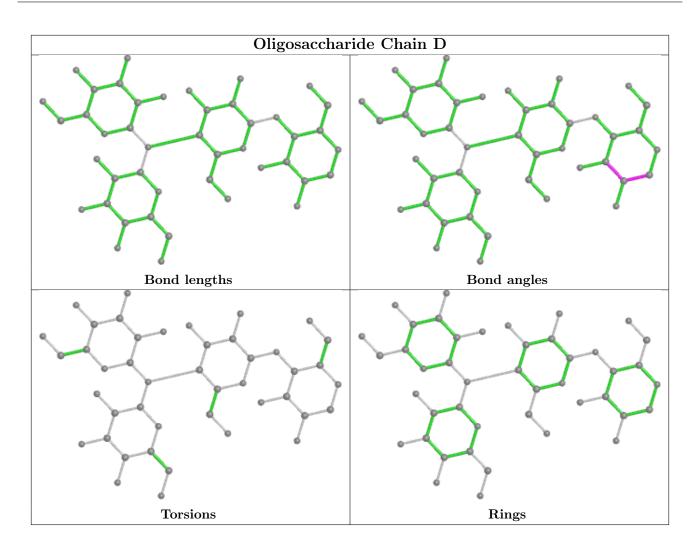
There are no ring outliers.

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)

11 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	Turne	Chain	un Res Li		Bond lengths			Bond angles		
	Type	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	GOL	В	502	-	$5,\!5,\!5$	1.08	0	$5,\!5,\!5$	0.87	0
4	SO4	В	504	-	4,4,4	0.14	0	$6,\!6,\!6$	0.30	0
3	GOL	А	604	-	$5,\!5,\!5$	1.03	0	$5,\!5,\!5$	0.92	0
3	GOL	А	603	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	1.28	0
4	SO4	А	606	-	4,4,4	0.16	0	$6,\!6,\!6$	0.12	0
4	SO4	А	605	-	4,4,4	0.15	0	$6,\!6,\!6$	0.12	0





Mal	Mol Type Chain	Res	Link	B	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	SO4	В	505	-	4,4,4	0.21	0	$6,\!6,\!6$	0.24	0
3	GOL	В	503	-	$5,\!5,\!5$	0.66	0	$5,\!5,\!5$	1.20	0
3	GOL	А	602	-	$5,\!5,\!5$	0.94	0	$5,\!5,\!5$	1.02	0
3	GOL	В	501	-	$5,\!5,\!5$	0.96	0	$5,\!5,\!5$	0.98	0
3	GOL	А	601	-	$5,\!5,\!5$	0.93	0	$5,\!5,\!5$	0.86	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
3	GOL	В	502	-	-	3/4/4/4	-
3	GOL	А	604	-	-	4/4/4/4	-
3	GOL	А	603	-	-	1/4/4/4	-
3	GOL	В	503	-	-	2/4/4/4	-
3	GOL	А	602	-	-	1/4/4/4	-
3	GOL	В	501	-	-	4/4/4/4	-
3	GOL	А	601	_	_	4/4/4/4	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	601	GOL	C1-C2-C3-O3
3	А	601	GOL	O2-C2-C3-O3
3	А	602	GOL	C1-C2-C3-O3
3	В	501	GOL	C1-C2-C3-O3
3	В	502	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	502	GOL	2	0
3	А	604	GOL	3	0
3	А	603	GOL	7	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	606	SO4	1	0
3	А	602	GOL	1	0
3	В	501	GOL	1	0
3	А	601	GOL	7	0

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### 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	305/305~(100%)	0.55	12 (3%) 39 34	11, 15, 25, 58	0
1	В	305/305~(100%)	0.46	2 (0%) 87 84	10, 14, 22, 49	0
All	All	610/610~(100%)	0.51	14 (2%) 60 56	10, 15, 24, 58	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1	ALA	3.7
1	В	1	ALA	3.3
1	А	302	THR	2.8
1	А	20	ASN	2.6
1	А	83[A]	GLN	2.6

### 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.

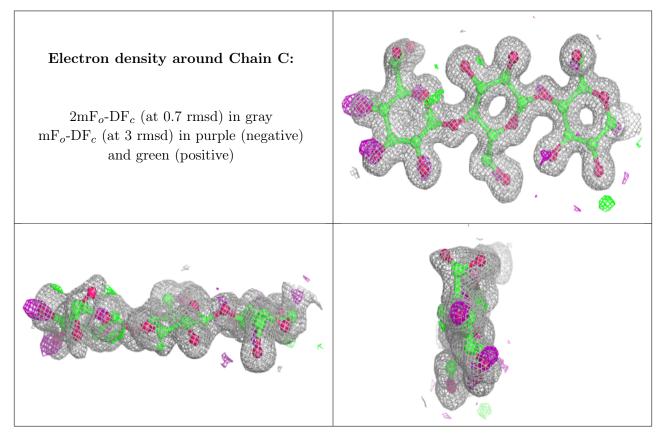
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	BGC	С	3[A]	11/12	0.91	0.11	$13,\!15,\!19,\!28$	11
2	BGC	С	3[B]	11/12	0.91	0.11	13,17,21,23	11
2	BGC	D	3[A]	11/12	0.91	0.12	13,14,20,24	11
2	BGC	D	3[B]	11/12	0.91	0.12	11,14,19,32	11
2	GLC	С	1	11/12	0.93	0.08	12,13,17,18	0



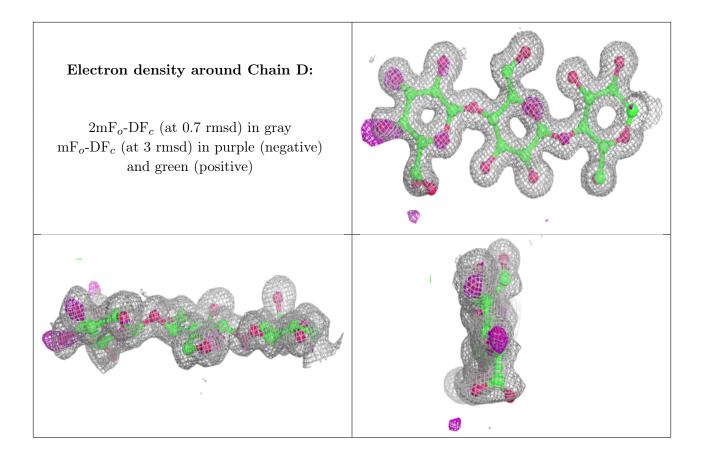
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	BGC	С	2	11/12	0.93	0.07	$12,\!14,\!16,\!18$	0
2	BGC	D	2	11/12	0.94	0.08	$11,\!13,\!15,\!16$	0
2	GLC	D	1	11/12	0.95	0.08	11,12,15,15	0

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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	А	606	5/5	0.51	0.41	21,24,48,48	5
3	GOL	В	503	6/6	0.64	0.22	31,34,43,44	6
3	GOL	А	603	6/6	0.65	0.38	14,24,31,33	6
3	GOL	В	501	6/6	0.67	0.16	40,44,46,49	0
3	GOL	В	502	6/6	0.70	0.24	$26,\!28,\!36,\!43$	6
3	GOL	А	602	6/6	0.80	0.17	30,38,42,44	6
3	GOL	А	604	6/6	0.81	0.24	14,23,40,49	6
3	GOL	А	601	6/6	0.84	0.26	13,29,36,48	6
4	SO4	А	605	5/5	0.89	0.23	36,42,42,43	5
4	SO4	В	505	5/5	0.90	0.14	20,30,39,42	5
4	SO4	В	504	5/5	0.94	0.12	21,21,28,33	5



### 6.5 Other polymers (i)

There are no such residues in this entry.

