



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:10 AM BST

PDB ID : 6J4H  
Title : Crystal Structure of maltotriose-complex of Pula-G680L mutant from *Klebsiella pneumoniae*  
Authors : Saka, N.; Iwamoto, H.; Takahashi, N.; Mizutani, K.; Mikami, B.  
Deposited on : 2019-01-09  
Resolution : 1.64 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

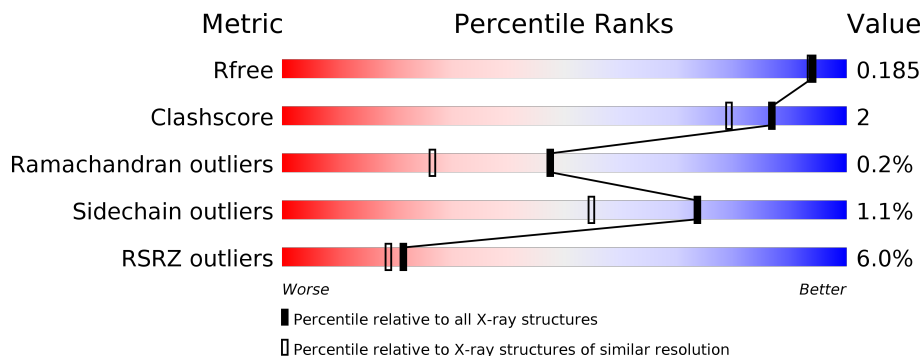
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	1053	 5% 82% 5% 13%
2	B	3	 100%
2	C	3	 67% 33%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8091 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 Pullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	917	7194	4476	1233	1461	24	0	21	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP W9BQ28
A	229	SER	ASN	see sequence details	UNP W9BQ28
A	680	LEU	GLY	engineered mutation	UNP W9BQ28

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	3	34	18	16	0	0	0
2	C	3	34	18	16	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- 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	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 12 6 6	0	1

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	801	Total O 801 801	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.94Å 60.10Å 133.96Å 90.00° 114.66° 90.00°	Depositor
Resolution (Å)	38.25 – 1.64 38.25 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.25-1.64) 99.8 (38.25-1.64)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 1.64Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.165 , 0.184 0.167 , 0.185	Depositor DCC
$R_{free}$ test set	6530 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtrriage
Anisotropy	0.858	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.8	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	0.97	EDS
Total number of atoms	8091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, GLC, MG

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	0.34	0/7335	0.55	0/9971

There are no bond length outliers.

There are no bond angle outliers.

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	7194	0	6887	30	0
2	B	34	0	30	0	0
2	C	34	0	30	1	0
3	A	2	0	0	0	0
4	A	24	0	32	0	0
5	A	2	0	0	0	0
6	A	801	0	0	3	0
All	All	8091	0	6979	30	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 2.

All (30) 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:1039:ALA:HB3	1:A:1043:SER:HB2	1.81	0.62
1:A:785[B]:ARG:NH2	6:A:1203:HOH:O	2.31	0.62
1:A:444:GLU:H	1:A:444:GLU:CD	2.04	0.61
1:A:675:ARG:HH21	1:A:832:LYS:NZ	2.01	0.59
1:A:199:ARG:HG2	1:A:222:LYS:HG2	1.86	0.58
1:A:977:ARG:HH11	1:A:1024:ASP:HB3	1.69	0.57
1:A:269:ASP:OD2	1:A:271:ILE:N	2.37	0.57
1:A:977:ARG:NH1	1:A:1024:ASP:HB3	2.24	0.52
1:A:675:ARG:HH21	1:A:832:LYS:HZ3	1.59	0.51
1:A:881:LEU:HD22	1:A:942:LEU:HD12	1.94	0.49
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.94	0.49
1:A:469:SER:HB2	6:A:1386:HOH:O	2.13	0.47
1:A:211:ASP:OD2	1:A:217:SER:OG	2.33	0.47
1:A:495:ILE:HA	1:A:524:VAL:HB	1.96	0.47
1:A:269:ASP:OD2	1:A:271:ILE:HG23	2.16	0.46
1:A:285:ASP:HA	1:A:289:ALA:HB2	2.00	0.44
1:A:262:VAL:HG12	1:A:264:ILE:HG13	1.99	0.43
1:A:834[B]:ASP:OD2	2:C:1:GLC:O2	2.33	0.43
1:A:680:LEU:HD13	1:A:708:TRP:HB2	2.00	0.43
1:A:311:TRP:CZ2	1:A:313:PRO:HG3	2.53	0.43
1:A:938:GLY:O	1:A:942:LEU:HD23	2.19	0.43
1:A:449:TYR:CZ	1:A:571:TYR:HB2	2.54	0.43
1:A:37:LEU:HA	1:A:37:LEU:HD12	1.84	0.42
1:A:490:ASP:N	1:A:490:ASP:OD2	2.52	0.42
1:A:592:LYS:HE2	1:A:672:ASP:OD2	2.19	0.42
1:A:411:MET:HE1	6:A:1258:HOH:O	2.19	0.42
1:A:875:ASP:OD2	1:A:879:SER:HB2	2.20	0.41
1:A:223:LEU:HB3	1:A:245:PHE:HB3	2.02	0.41
1:A:557:TRP:CD2	1:A:892:TYR:HA	2.56	0.40
1:A:1032:LEU:HD23	1:A:1037:GLN:HG2	2.03	0.40

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	934/1053 (89%)	918 (98%)	14 (2%)	2 (0%)	47 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	CYS
1	A	478	PRO

### 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	775/867 (89%)	767 (99%)	8 (1%)	76 59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	SER
1	A	374	TYR
1	A	423	LYS
1	A	478	PRO
1	A	482	LEU
1	A	562	PHE
1	A	710	SER
1	A	916	ARG

Some 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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	B	1	2	12,12,12	0.52	0	17,17,17	0.63	0
2	GLC	B	2	2	11,11,12	0.33	0	15,15,17	0.96	0
2	GLC	B	3	2	11,11,12	0.29	0	15,15,17	0.71	0
2	GLC	C	1	2	12,12,12	0.50	0	17,17,17	1.33	1 (5%)
2	GLC	C	2	2	11,11,12	0.31	0	15,15,17	0.91	0
2	GLC	C	3	2	11,11,12	0.26	0	15,15,17	0.74	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	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O5-C1-C2	-2.99	104.94	110.28

There are no chirality outliers.

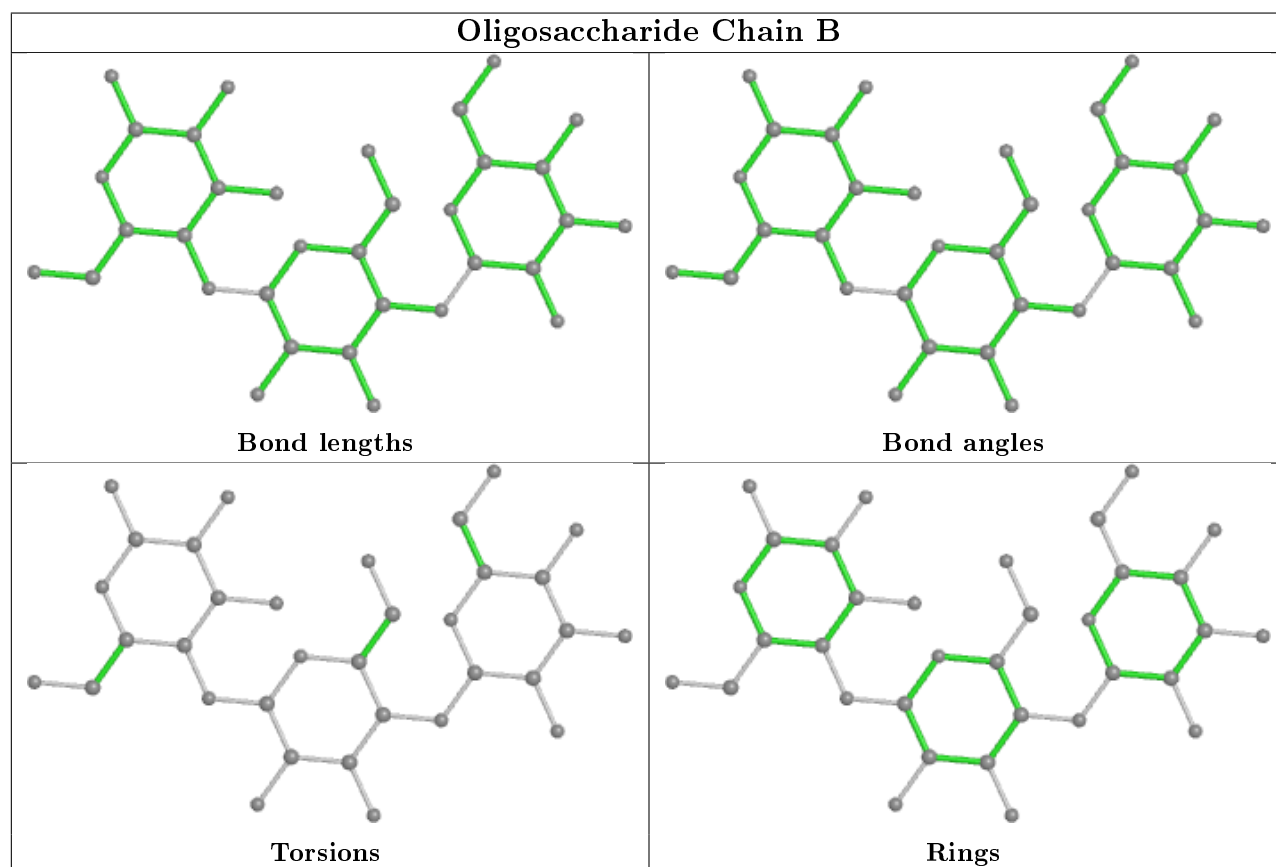
There are no torsion outliers.

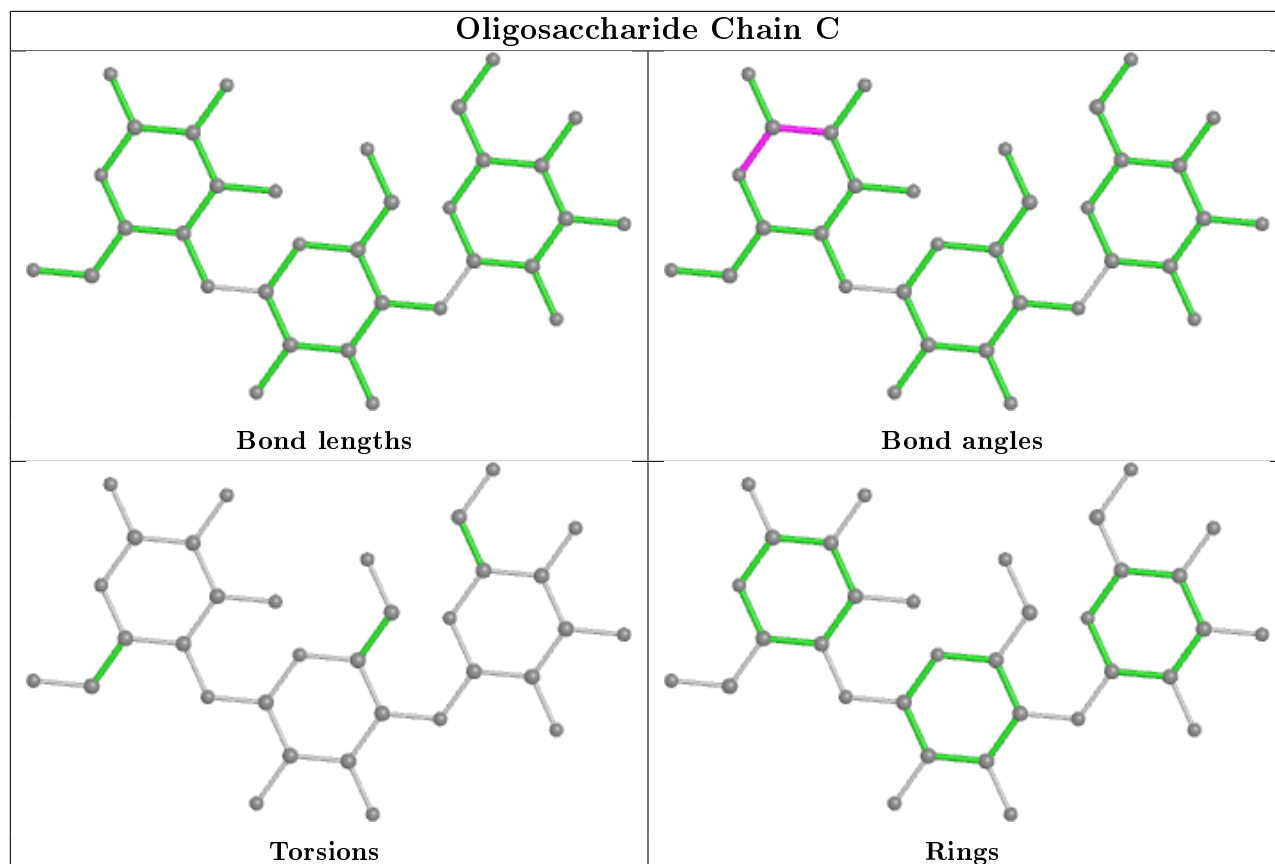
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GOL	A	1111[A]	-	5,5,5	0.35	0	5,5,5	0.31	0
4	GOL	A	1109	-	5,5,5	0.37	0	5,5,5	0.26	0
4	GOL	A	1111[B]	-	5,5,5	0.35	0	5,5,5	0.25	0
4	GOL	A	1110	-	5,5,5	0.34	0	5,5,5	0.27	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	1111[A]	-	-	0/4/4/4	-
4	GOL	A	1109	-	-	2/4/4/4	-
4	GOL	A	1111[B]	-	-	4/4/4/4	-
4	GOL	A	1110	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1109	GOL	O1-C1-C2-O2
4	A	1109	GOL	O1-C1-C2-C3
4	A	1111[B]	GOL	O1-C1-C2-C3
4	A	1111[B]	GOL	C1-C2-C3-O3
4	A	1111[B]	GOL	O2-C2-C3-O3
4	A	1110	GOL	O1-C1-C2-C3
4	A	1111[B]	GOL	O1-C1-C2-O2
4	A	1110	GOL	C1-C2-C3-O3
4	A	1110	GOL	O2-C2-C3-O3
4	A	1110	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

### 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	917/1053 (87%)	0.04	55 (5%) <span style="border: 1px solid red; padding: 2px;">21</span> <span style="border: 1px solid red; padding: 2px;">19</span>	14, 20, 52, 81	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ILE	8.6
1	A	37	LEU	7.0
1	A	270	GLY	6.9
1	A	216	PHE	6.8
1	A	214	GLY	6.7
1	A	217	SER	5.6
1	A	213	ASN	5.3
1	A	34	VAL	5.2
1	A	746	PHE	5.2
1	A	272	LEU	5.1
1	A	212	SER	4.8
1	A	215	GLU	4.8
1	A	35	VAL	4.6
1	A	249	ASP	4.2
1	A	1052	ALA	4.2
1	A	173	GLY	4.2
1	A	268	SER	4.2
1	A	269	ASP	4.1
1	A	303	ASP	4.1
1	A	209	ALA	4.1
1	A	196	PRO	3.9
1	A	210	ALA	3.8
1	A	32	ASP	3.8
1	A	711	ASN	3.8
1	A	223	LEU	3.6
1	A	33	VAL	3.5
1	A	874	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	197	ILE	3.4
1	A	230	GLN	3.4
1	A	211	ASP	3.4
1	A	250	ASP	3.4
1	A	36	ARG	3.4
1	A	710	SER	3.3
1	A	222	LYS	3.2
1	A	201	TYR	3.2
1	A	830	VAL	3.0
1	A	1072	GLU	2.8
1	A	198	VAL	2.8
1	A	220	TYR	2.8
1	A	267	GLU	2.6
1	A	234	MET	2.6
1	A	274	SER	2.6
1	A	426	ILE	2.5
1	A	221	VAL	2.4
1	A	603	VAL	2.3
1	A	863	LEU	2.3
1	A	227	THR	2.3
1	A	996	MET	2.3
1	A	1082	SER	2.2
1	A	873	ALA	2.1
1	A	202	TYR	2.1
1	A	829	TYR	2.1
1	A	408	GLY	2.1
1	A	266	ALA	2.0
1	A	476	LEU	2.0

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

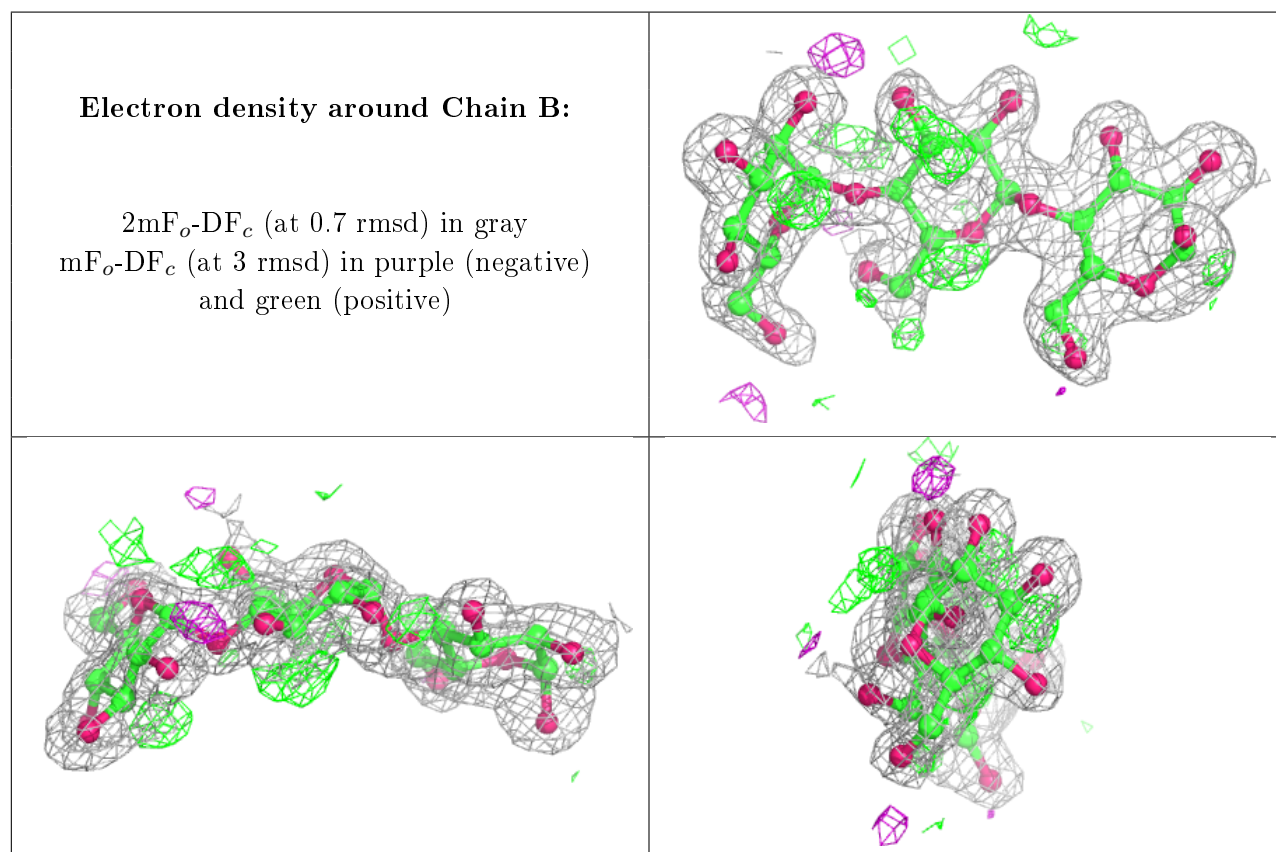
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

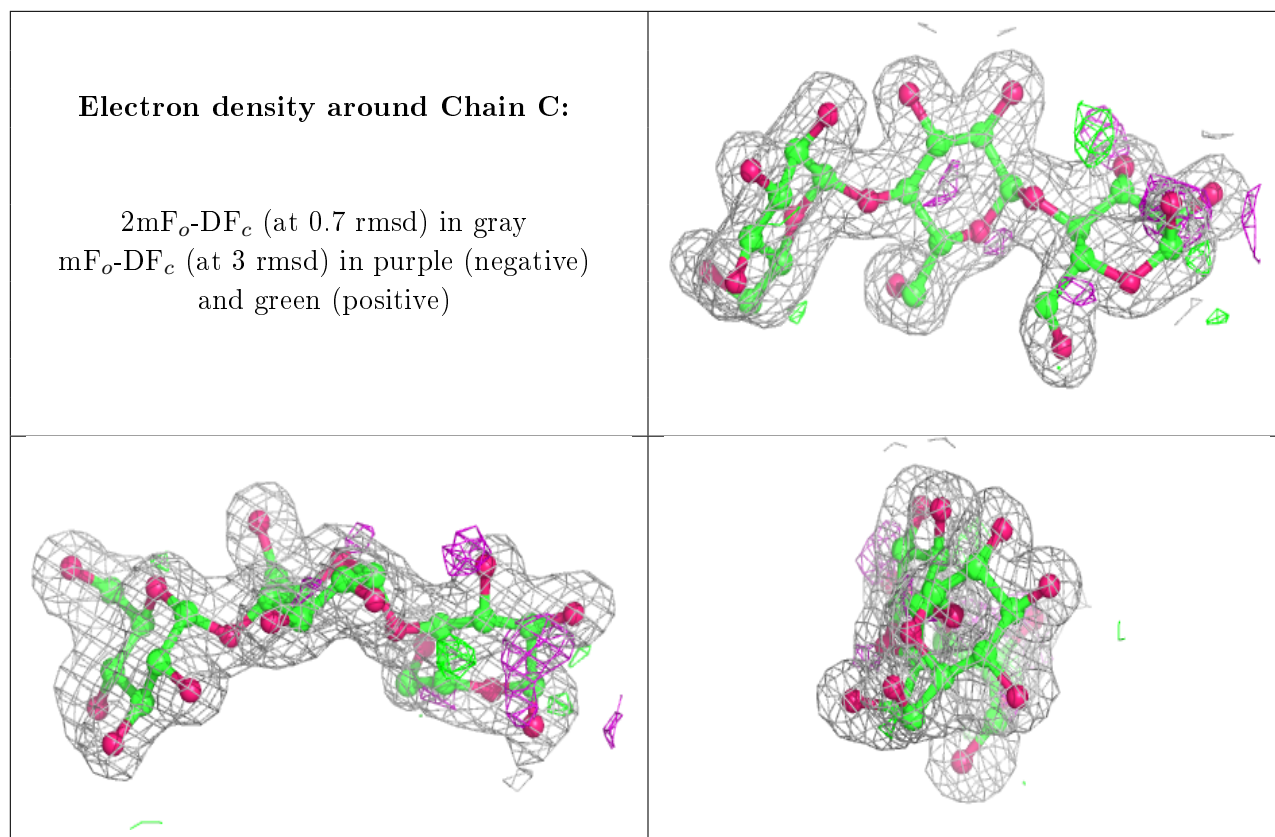
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	B	3	11/12	0.86	0.12	21,24,28,29	11
2	GLC	C	1	12/12	0.86	0.11	21,25,28,37	0
2	GLC	B	2	11/12	0.92	0.10	20,24,29,37	11
2	GLC	B	1	12/12	0.93	0.08	18,23,34,35	0
2	GLC	C	2	11/12	0.94	0.09	20,22,25,25	0
2	GLC	C	3	11/12	0.94	0.13	25,31,37,38	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<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
4	GOL	A	1111[A]	6/6	0.80	0.27	29,30,34,36	6
4	GOL	A	1111[B]	6/6	0.80	0.27	24,29,33,33	6
4	GOL	A	1109	6/6	0.83	0.44	26,35,38,46	6
4	GOL	A	1110	6/6	0.86	0.11	32,37,42,44	0
3	CA	A	1107	1/1	0.95	0.12	42,42,42,42	0
5	MG	A	1112	1/1	0.98	0.10	20,20,20,20	0
3	CA	A	1108	1/1	0.99	0.03	17,17,17,17	0
5	MG	A	1113	1/1	0.99	0.12	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.