



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 09:31 PM EDT

PDB ID : 2YIH  
Title : Structure of a Paenibacillus polymyxa Xyloglucanase from GH family 44 with Xyloglucan  
Authors : Ariza, A.; Eklof, J.M.; Spadiut, O.; Offen, W.A.; Roberts, S.M.; Besenmatter, W.; Friis, E.P.; Skjot, M.; Wilson, K.S.; Brumer, H.; Davies, G.  
Deposited on : 2011-05-13  
Resolution : 1.70 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

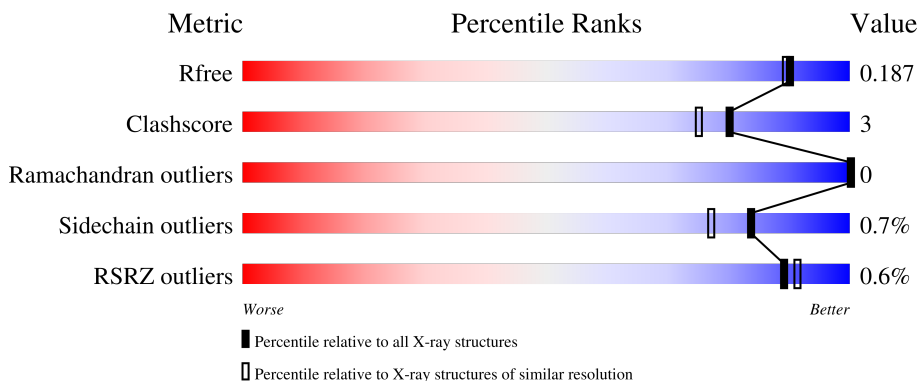
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	524	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>93%</span> <span>5% •</span> </div> </div>
2	B	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 50%, orange 17%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>33%</span> <span>50%</span> <span>17%</span> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4695 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.

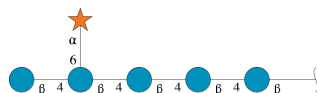
- Molecule 1 is a protein called CEL44C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	4050	2573	670	791	16	0	16	1

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	PHE	SER	conflict	UNP Q1A2D0
A	19	ASP	GLU	conflict	UNP Q1A2D0
A	68	HIS	GLN	engineered mutation	UNP Q1A2D0
A	92	VAL	THR	engineered mutation	UNP Q1A2D0
A	118	ALA	LYS	engineered mutation	UNP Q1A2D0
A	129	ALA	LYS	engineered mutation	UNP Q1A2D0
A	156	TYR	ARG	engineered mutation	UNP Q1A2D0
A	200	PRO	GLY	engineered mutation	UNP Q1A2D0
A	228	VAL	ILE	conflict	UNP Q1A2D0
A	272	VAL	ALA	conflict	UNP Q1A2D0
A	331	PHE	ASN	engineered mutation	UNP Q1A2D0
A	358	SER	GLU	engineered mutation	UNP Q1A2D0
A	473	ILE	SER	conflict	UNP Q1A2D0

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	6	65	35	30	0	0	0

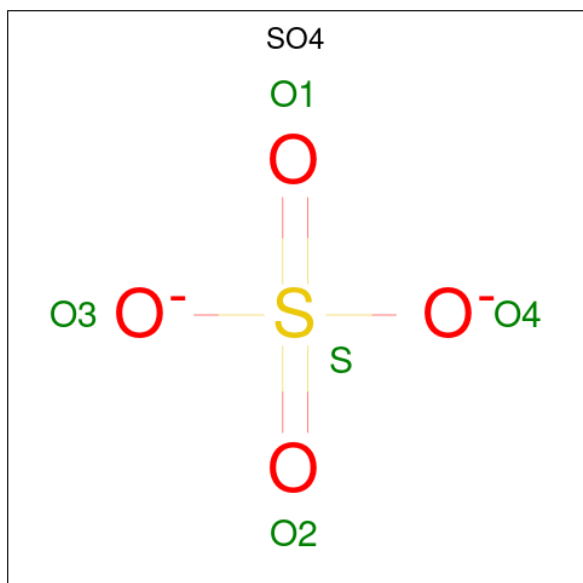
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

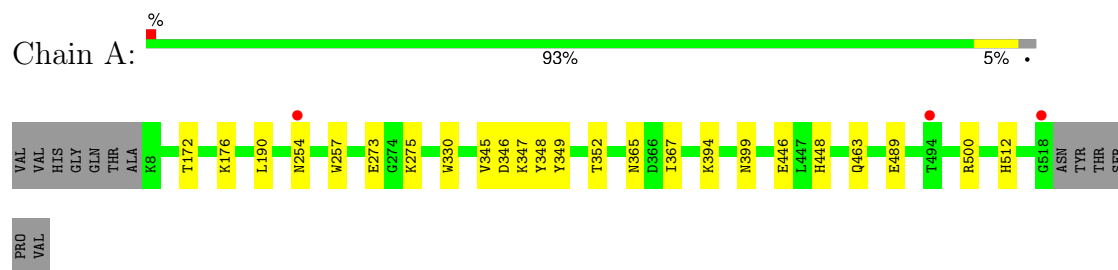
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	530	Total	O	0	2
			532	532		

### 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: CEL44C



- Molecule 2: beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.53Å 83.53Å 157.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.76 – 1.70 40.36 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (41.76-1.70) 88.1 (40.36-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0086	Depositor
R, $R_{free}$	0.157 , 0.184 0.156 , 0.187	Depositor DCC
$R_{free}$ test set	3131 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.075 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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: YYS, BGC, SO4, EDO, CA, CL

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	0.70	0/4201	0.66	0/5708

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	4050	0	3923	19	0
2	B	65	0	55	2	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
6	A	36	0	54	5	0
7	A	532	0	0	9	0
All	All	4695	0	4032	22	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 3.

The worst 5 of 22 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:346:ASP:OD2	7:A:2408:HOH:O	1.83	0.96
1:A:273[B]:GLU:HG2	7:A:2333:HOH:O	1.66	0.96
1:A:254:ASN:OD1	7:A:2324:HOH:O	1.96	0.82
6:A:1532:EDO:O2	7:A:2435:HOH:O	1.72	0.75
1:A:448:HIS:HD2	1:A:512:HIS:NE2	1.88	0.72

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	526/524 (100%)	510 (97%)	16 (3%)	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	Outliers	Percentiles	
1	A	440/437 (101%)	437 (99%)	3 (1%)	84	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	257	TRP

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Mol	Chain	Res	Type
1	A	349	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	ASN
1	A	448	HIS
1	A	298	ASN
1	A	343	GLN
1	A	365	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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	BGC	B	1	2	12,12,12	0.49	0	17,17,17	0.82	0
2	BGC	B	2	2	11,11,12	0.37	0	15,15,17	0.64	0
2	BGC	B	3	2	11,11,12	0.40	0	15,15,17	0.95	0
2	BGC	B	4	2	11,11,12	0.53	0	15,15,17	1.12	2 (13%)
2	BGC	B	5	2	11,11,12	0.41	0	15,15,17	0.97	1 (6%)
2	XYS	B	6	2	9,9,10	0.48	0	10,12,14	1.37	1 (10%)

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	BGC	B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	B	2	2	-	1/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	B	5	2	-	0/2/19/22	0/1/1/1
2	XYX	B	6	2	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	XYX	C4-C3-C2	-2.40	108.07	110.92
2	B	4	BGC	C3-C4-C5	-2.29	106.07	110.23
2	B	4	BGC	O4-C4-C5	2.09	114.48	109.32
2	B	5	BGC	C6-C5-C4	-2.04	108.01	113.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

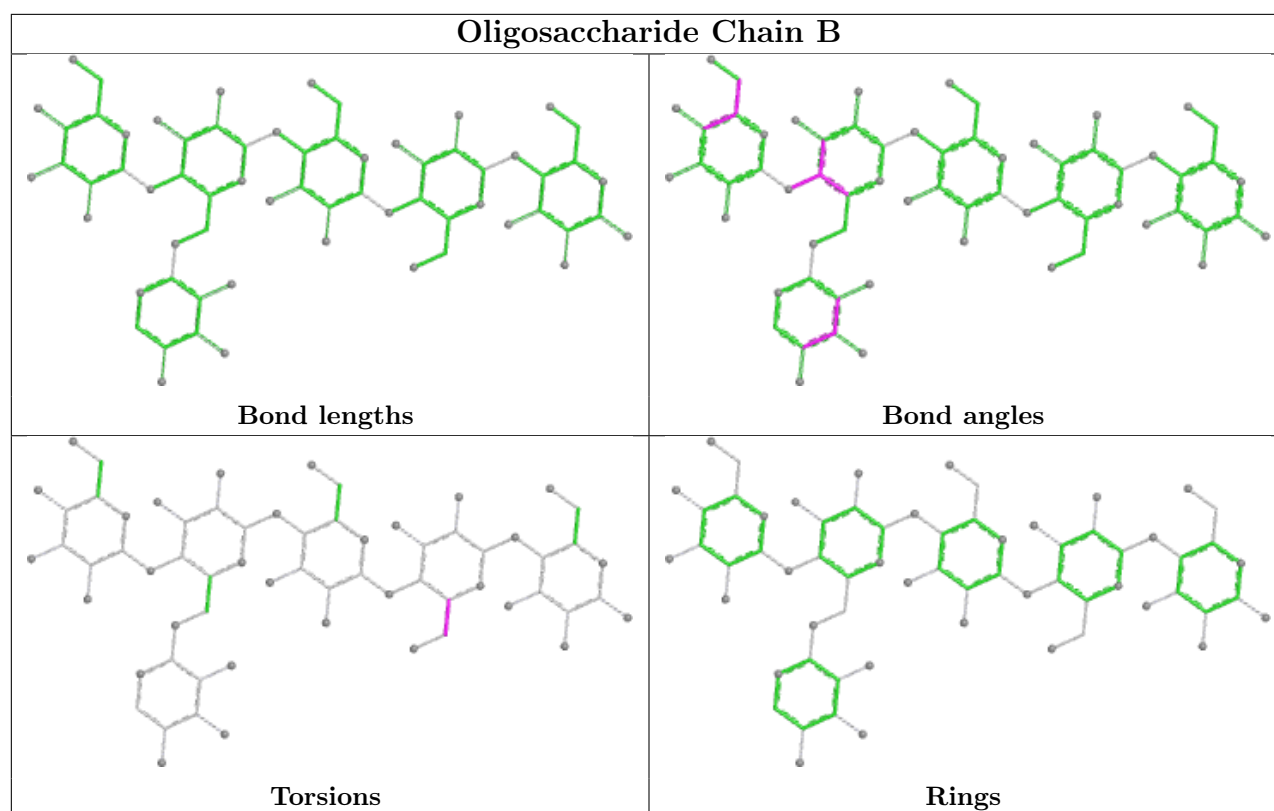
Mol	Chain	Res	Type	Atoms
2	B	2	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	BGC	1	0
2	B	1	BGC	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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
6	EDO	A	1528	-	3,3,3	0.44	0	2,2,2	0.48	0
6	EDO	A	1531	-	3,3,3	0.50	0	2,2,2	0.54	0
6	EDO	A	1524	-	3,3,3	0.43	0	2,2,2	0.60	0
5	SO4	A	1523	-	4,4,4	0.25	0	6,6,6	0.22	0
6	EDO	A	1526	-	3,3,3	0.50	0	2,2,2	0.18	0
6	EDO	A	1525	-	3,3,3	0.41	0	2,2,2	0.74	0
6	EDO	A	1527	-	3,3,3	0.34	0	2,2,2	0.58	0
6	EDO	A	1529	-	3,3,3	0.41	0	2,2,2	0.64	0
5	SO4	A	1522	-	4,4,4	0.21	0	6,6,6	0.34	0
6	EDO	A	1532	-	3,3,3	0.38	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	1530	-	3,3,3	0.59	0	2,2,2	0.32	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
6	EDO	A	1528	-	-	1/1/1/1	-
6	EDO	A	1531	-	-	1/1/1/1	-
6	EDO	A	1524	-	-	1/1/1/1	-
6	EDO	A	1529	-	-	0/1/1/1	-
6	EDO	A	1527	-	-	0/1/1/1	-
6	EDO	A	1526	-	-	1/1/1/1	-
6	EDO	A	1525	-	-	1/1/1/1	-
6	EDO	A	1532	-	-	1/1/1/1	-
6	EDO	A	1530	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1524	EDO	O1-C1-C2-O2
6	A	1531	EDO	O1-C1-C2-O2
6	A	1528	EDO	O1-C1-C2-O2
6	A	1532	EDO	O1-C1-C2-O2
6	A	1525	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1526	EDO	2	0
6	A	1527	EDO	1	0
6	A	1532	EDO	2	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<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	511/524 (97%)	-0.53	3 (0%) 89 91	7, 11, 22, 33	16 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	THR	3.1
1	A	254	ASN	2.9
1	A	518	GLY	2.1

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

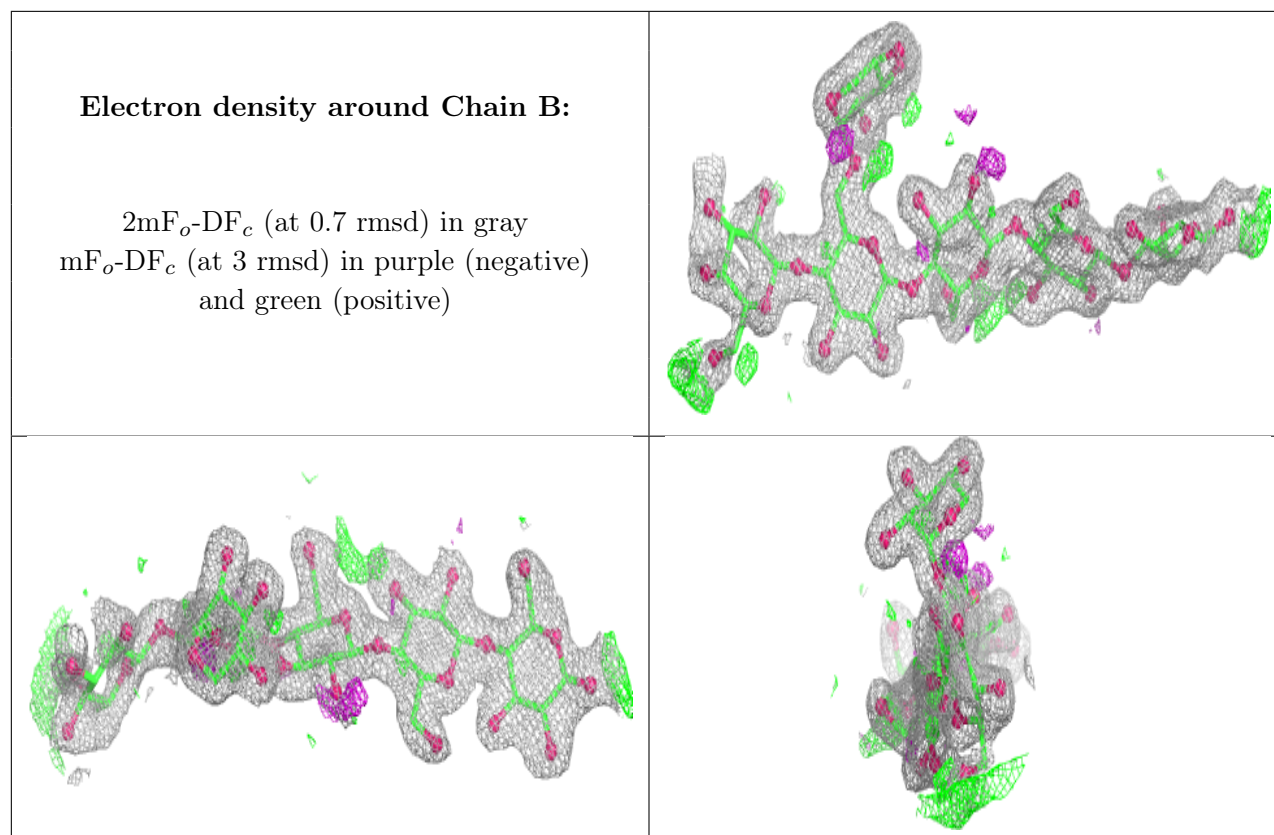
There are no non-standard protein/DNA/RNA residues in this entry.

### 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<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	BGC	B	5	11/12	0.82	0.17	19,20,22,22	11
2	BGC	B	2	11/12	0.90	0.13	28,29,32,40	0
2	BGC	B	1	12/12	0.91	0.15	33,38,41,44	0
2	BGC	B	4	11/12	0.92	0.11	22,23,26,26	0
2	BGC	B	3	11/12	0.92	0.12	24,26,28,28	0
2	XYS	B	6	9/10	0.94	0.10	23,25,27,27	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( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	1524	4/4	0.88	0.11	24,26,26,28	0
6	EDO	A	1528	4/4	0.89	0.17	23,23,23,24	4
6	EDO	A	1531	4/4	0.89	0.23	25,30,31,34	0
6	EDO	A	1527	4/4	0.91	0.10	30,34,34,38	0
6	EDO	A	1526	4/4	0.92	0.11	13,14,15,16	4
5	SO4	A	1523	5/5	0.93	0.19	20,22,24,24	5
6	EDO	A	1529	4/4	0.94	0.11	19,20,20,22	4
6	EDO	A	1530	4/4	0.95	0.08	14,15,15,16	0
5	SO4	A	1522	5/5	0.96	0.09	28,31,32,34	5
6	EDO	A	1525	4/4	0.98	0.07	17,18,18,18	0
6	EDO	A	1532	4/4	0.99	0.11	21,21,21,21	4
4	CL	A	1521	1/1	1.00	0.07	9,9,9,9	0
3	CA	A	1520	1/1	1.00	0.05	10,10,10,10	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.