



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:33 PM UTC

PDB ID : 1US2 / pdb_00001us2
Title : Xylanase10C (mutant E385A) from Cellvibrio japonicus in complex with xylopentaose
Authors : Pell, G.; Szabo, L.; Charnock, S.J.; Xie, H.; Gloster, T.M.; Davies, G.J.; Gilbert, H.J.
Deposited on : 2003-11-17
Resolution : 1.85 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

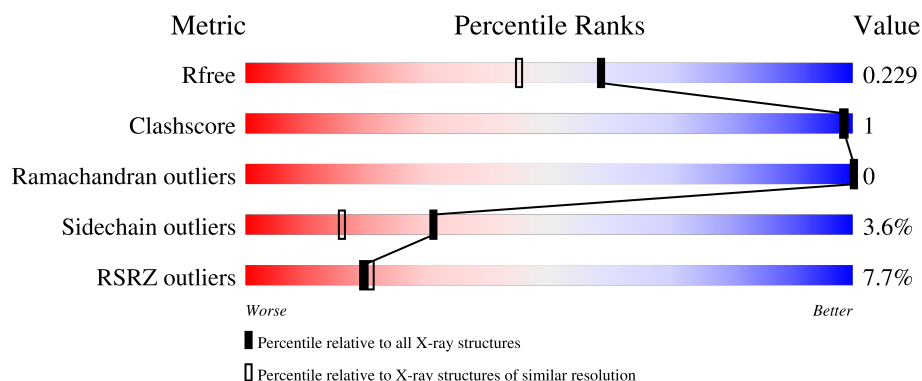
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 $\leq 5\%$. 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	530	7% 92% . .
2	B	4	100%
2	C	4	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4854 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 ENDO-BETA-1,4-XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	3947	2476	665	788	18	21	9	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	MET	-	expression tag	UNP Q59675
A	186	ALA	GLY	SEE REMARK 999	UNP Q59675
A	536	ALA	GLY	SEE REMARK 999	UNP Q59675
A	594	ALA	GLY	SEE REMARK 999	UNP Q59675
A	385	ALA	GLU	engineered mutation	UNP Q59675
A	607	GLU	-	expression tag	UNP Q59675
A	608	LEU	-	expression tag	UNP Q59675
A	609	HIS	-	expression tag	UNP Q59675
A	610	HIS	-	expression tag	UNP Q59675
A	611	HIS	-	expression tag	UNP Q59675
A	612	HIS	-	expression tag	UNP Q59675
A	613	HIS	-	expression tag	UNP Q59675
A	614	HIS	-	expression tag	UNP Q59675

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



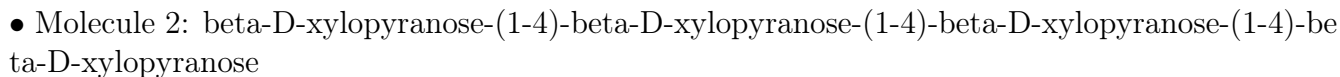
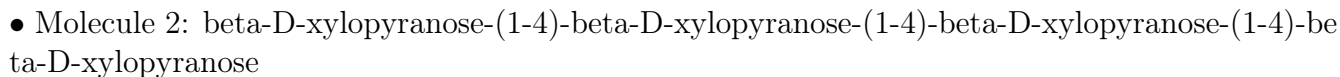
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	4	Total	C	O	0	0	0
			37	20	17			
2	C	4	Total	C	O	0	0	0
			37	20	17			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	833	Total 833	O 833	0	0

i

- Molecule 1: ENDO-BETA-1,4-XYLANASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.60Å 82.69Å 170.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.52 – 1.85 84.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (84.52-1.85) 97.6 (84.52-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.86 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.226 0.182 , 0.229	Depositor DCC
R_{free} test set	2682 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4854	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: XYP

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	0.96	0/4066	0.90	1/5540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	219	GLY	N-CA-C	5.07	119.85	111.59

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	3947	0	3763	4	0
2	B	37	0	0	0	0
2	C	37	0	0	0	0
3	A	833	0	0	0	0
All	All	4854	0	3763	4	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 (4) 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:566[B]:ARG:HG2	1:A:571:ASP:OD1	2.03	0.58
1:A:415:ARG:HA	1:A:418:GLN:HE21	1.72	0.54
1:A:174:GLU:HB3	1:A:214:ARG:HH11	1.83	0.43
1:A:479:ILE:HG22	1:A:483:MET:HE2	2.02	0.42

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	510/530 (96%)	490 (96%)	20 (4%)	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	429/438 (98%)	414 (96%)	15 (4%)	32	16

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG

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Mol	Chain	Res	Type
1	A	140	ARG
1	A	155	VAL
1	A	166	LEU
1	A	174	GLU
1	A	187	SER
1	A	189	GLU
1	A	196	LEU
1	A	214	ARG
1	A	232	ILE
1	A	239	LEU
1	A	303	MET
1	A	377	LEU
1	A	520	GLU
1	A	600	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	267	ASN
1	A	344	ASN
1	A	418	GLN
1	A	432	ASN
1	A	478	ASN
1	A	523	GLN
1	A	544	ASN
1	A	582	ASN
1	A	585	ASN
1	A	606	HIS

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 ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XYP	B	1	2	10,10,10	0.95	1 (10%)	14,14,14	1.07	2 (14%)
2	XYP	B	2	2	9,9,10	1.28	1 (11%)	10,12,14	1.08	0
2	XYP	B	3	2	9,9,10	0.98	1 (11%)	10,12,14	0.84	0
2	XYP	B	4	2	9,9,10	1.34	1 (11%)	10,12,14	0.92	1 (10%)
2	XYP	C	1	2	10,10,10	1.34	1 (10%)	14,14,14	0.68	0
2	XYP	C	2	2	9,9,10	1.29	1 (11%)	10,12,14	1.41	2 (20%)
2	XYP	C	3	2	9,9,10	1.33	1 (11%)	10,12,14	0.77	0
2	XYP	C	4	2	9,9,10	1.25	1 (11%)	10,12,14	0.93	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	XYP	B	1	2	-	-	0/1/1/1
2	XYP	B	2	2	-	-	0/1/1/1
2	XYP	B	3	2	-	-	0/1/1/1
2	XYP	B	4	2	-	-	0/1/1/1
2	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3	2	-	-	0/1/1/1
2	XYP	C	4	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	XYP	O5-C1	-3.90	1.36	1.43
2	C	3	XYP	O5-C1	-3.62	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	XYP	O5-C1	-3.57	1.36	1.43
2	C	2	XYP	O5-C1	-3.41	1.36	1.43
2	C	4	XYP	O5-C1	-3.36	1.36	1.43
2	B	2	XYP	O5-C1	-3.34	1.36	1.43
2	B	3	XYP	O5-C1	-2.69	1.37	1.43
2	B	1	XYP	O5-C1	-2.04	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	XYP	C1-C2-C3	2.35	113.06	109.64
2	B	1	XYP	O4-C4-C5	2.24	114.35	109.22
2	B	4	XYP	O2-C2-C3	-2.12	105.75	110.15
2	B	1	XYP	C5-C4-C3	-2.12	106.56	109.64
2	C	2	XYP	C4-C3-C2	2.01	113.31	110.92

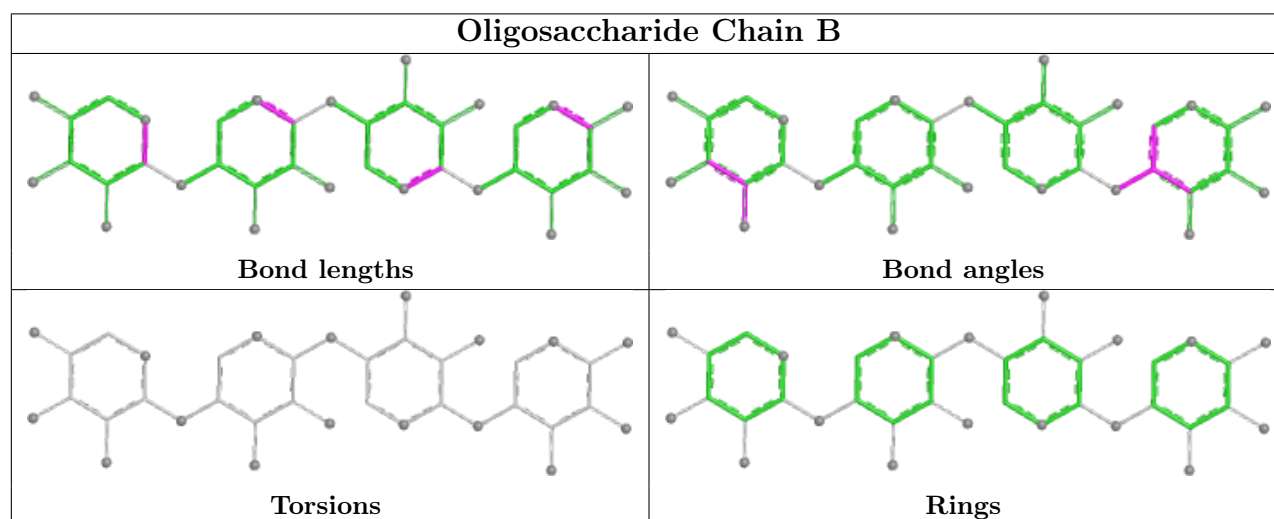
There are no chirality outliers.

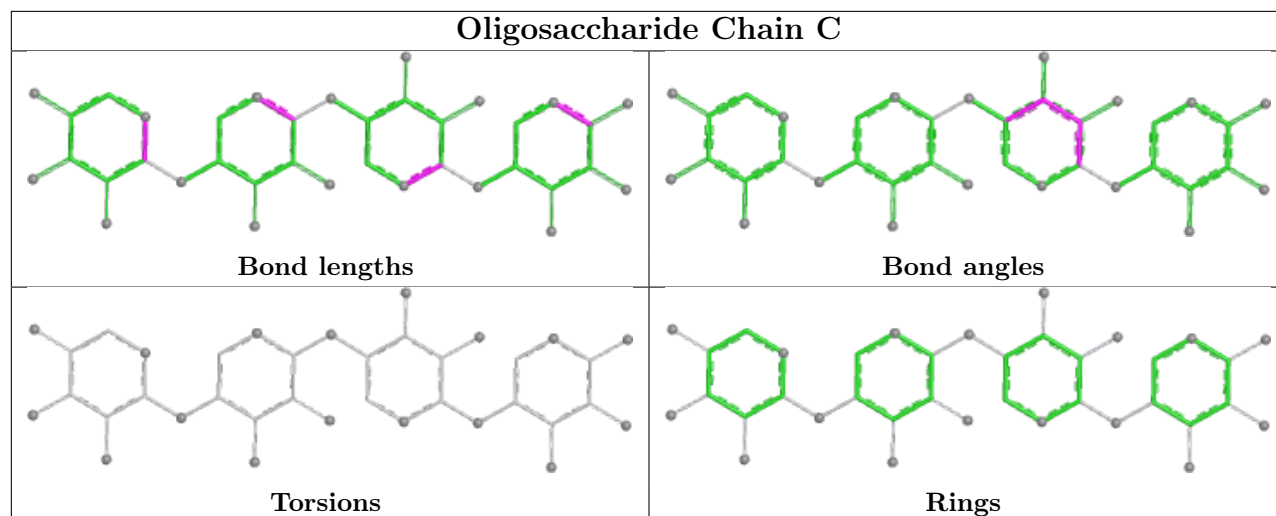
There are no torsion outliers.

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](#)

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	507/530 (95%)	-0.00	39 (7%)	19 20	3, 9, 20, 38	14 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	ALA	4.8
1	A	606	HIS	4.5
1	A	238	THR	4.5
1	A	202	ILE	4.5
1	A	207	ASP	4.3
1	A	153	VAL	4.1
1	A	209	PHE	3.9
1	A	184	LEU	3.5
1	A	203	ASP	3.5
1	A	147	ALA	3.1
1	A	120	ALA	3.1
1	A	95	ILE	3.0
1	A	199	THR	3.0
1	A	196	LEU	2.9
1	A	232	ILE	2.8
1	A	239	LEU	2.8
1	A	200	CYS	2.8
1	A	190	LEU	2.7
1	A	195	ASP	2.6
1	A	205	ASP	2.6
1	A	222	ALA	2.5
1	A	117	THR	2.5
1	A	166	LEU	2.4
1	A	243	ALA	2.4
1	A	187	SER	2.4
1	A	152	VAL	2.4
1	A	181	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	146	ASP	2.3
1	A	183	CYS	2.3
1	A	179	GLY	2.3
1	A	230	ILE	2.3
1	A	188	SER	2.2
1	A	206	ASP	2.2
1	A	157	ALA	2.1
1	A	161	ALA	2.1
1	A	201	THR	2.0
1	A	148	VAL	2.0
1	A	185	ALA	2.0
1	A	155	VAL	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](#)

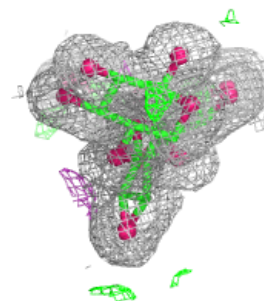
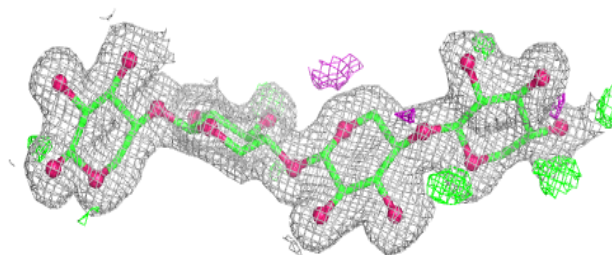
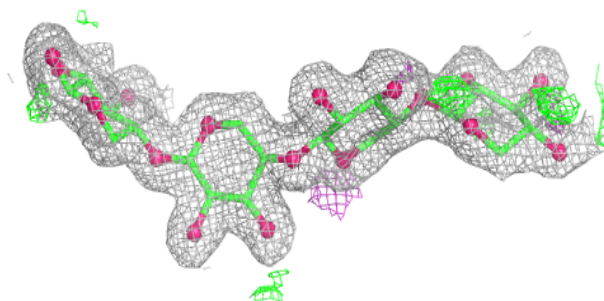
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XYP	C	1	10/10	0.68	0.16	56,60,61,62	0
2	XYP	C	4	9/10	0.69	0.16	61,62,63,64	0
2	XYP	C	2	9/10	0.86	0.13	50,52,53,54	0
2	XYP	C	3	9/10	0.87	0.10	54,55,57,59	0
2	XYP	B	4	9/10	0.88	0.12	23,26,28,29	0
2	XYP	B	3	9/10	0.95	0.07	16,18,21,22	0
2	XYP	B	1	10/10	0.98	0.04	8,9,11,11	0
2	XYP	B	2	9/10	0.98	0.04	10,12,13,14	0

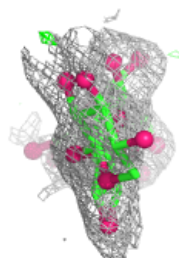
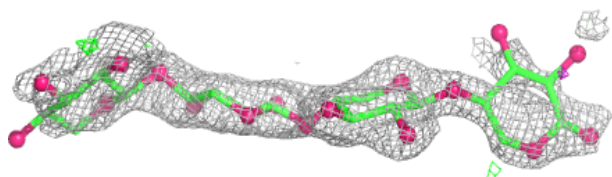
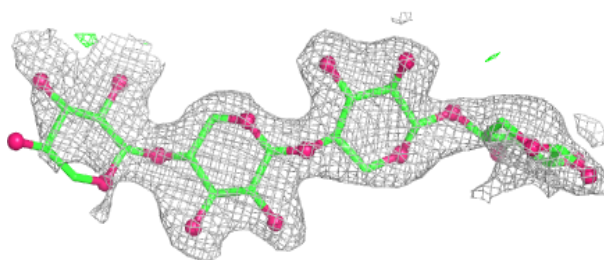
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain C:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.