

Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 12:34 PM EDT

PDB ID : 1B3Y

Title : XYLANASE FROM PENICILLIUM SIMPLICISSIMUM, COMPLEX WITH

XYLOTETRAOSE

Authors: Schmidt, A.; Kratky, C.

Deposited on : 1998-12-15

Resolution : 2.45 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.34

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

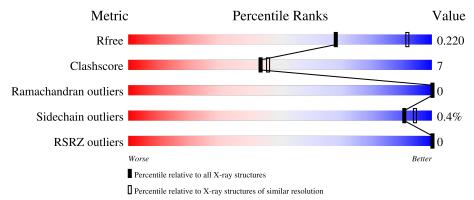
Validation Pipeline (wwPDB-VP) : 2.34

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 2.45 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	302	84%	15% •			
2	В	3	67%	33%			

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XYS	A	560	-	-	_	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2596 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 PROTEIN (XYLANASE).

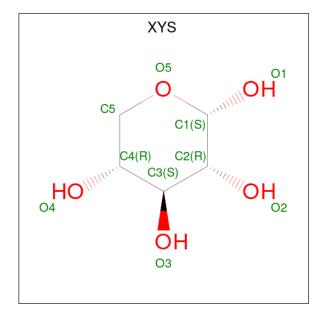
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	302	Total	С	N	О	S	0	1	0
1	A	302	2304	1458	396	445	5	0	1	

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	В	3	Total 28	C 15	O 13	0	0	0

• Molecule 3 is alpha-D-xylopyranose (three-letter code: XYS) (formula: C₅H₁₀O₅).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 10	C 5	O 5	0	0

• Molecule 4 is water.

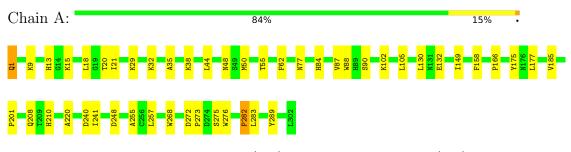
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	254	Total O 254 254	0	0



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 1: PROTEIN (XYLANASE)



• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain B: 67% 33%

XYP1 XYP2 XYP3



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	81.34Å 81.34Å 113.24Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	10.00 - 2.45	Depositor	
resolution (A)	14.95 - 2.45	EDS	
% Data completeness	99.6 (10.00-2.45)	Depositor	
(in resolution range)	99.7 (14.95-2.45)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.12	Depositor	
$< I/\sigma(I) > 1$	3.13 (at 2.45Å)	Xtriage	
Refinement program	X-PLOR 3.851	Depositor	
R, R_{free}	0.191 , 0.248	Depositor	
it, it free	0.172 , 0.220	DCC	
R_{free} test set	1633 reflections (10.03%)	wwPDB-VP	
Wilson B-factor (Å ²)	16.5	Xtriage	
Anisotropy	0.752	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 59.6	EDS	
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage	
F_o, F_c correlation	0.94	EDS	
Total number of atoms	2596	wwPDB-VP	
Average B, all atoms (Å ²)	11.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: XYP, XYS, PCA

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).

Mal	Chain	Bond	lengths	Bond angles		
Mol Chain		RMSZ $ \# Z > 5$		RMSZ	$SZ \mid \# Z > 5$	
1	A	0.36	0/2352	0.66	1/3199 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	18	LEU	N-CA-C	-5.64	95.76	111.00

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	2304	0	2262	29	0
2	В	28	0	0	2	0
3	A	10	0	10	5	0
4	A	254	0	0	3	0
All	All	2596	0	2272	31	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 7.

All (31) 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:175:TYR:HB3	1:A:208:GLN:OE1	1.94	0.68
1:A:177:LEU:HA	1:A:185:VAL:HG22	1.80	0.63
1:A:87:VAL:HB	1:A:130:LEU:HD23	1.83	0.61
1:A:32:LYS:HD3	1:A:289:TYR:HB2	1.84	0.60
1:A:241:ILE:HD13	1:A:248:ASP:HB3	1.83	0.59
1:A:240:ASP:HB2	1:A:282:PRO:HB2	1.89	0.55
1:A:158:PHE:HB3	1:A:201:PRO:HG2	1.90	0.54
1:A:210:HIS:HB2	3:A:560:XYS:O3	2.09	0.52
3:A:560:XYS:H51	4:A:541:HOH:O	2.09	0.52
1:A:9:LYS:O	1:A:13:HIS:HD2	1.93	0.52
1:A:276:TRP:HH2	3:A:560:XYS:H52	1.76	0.51
1:A:166:PRO:HG2	4:A:485:HOH:O	2.11	0.50
1:A:55:THR:O	1:A:62:PHE:HA	2.14	0.48
1:A:21:ILE:HG21	1:A:268:TRP:CE3	2.49	0.48
1:A:210:HIS:CD2	3:A:560:XYS:O3	2.67	0.48
3:A:560:XYS:O4	2:B:1:XYP:O1	2.30	0.48
1:A:38:LYS:HE3	1:A:77:ASN:OD1	2.15	0.47
1:A:88:TRP:CE2	1:A:90:SER:HB3	2.50	0.47
1:A:15:LYS:HE3	1:A:257:LEU:HA	1.97	0.46
1:A:220:ALA:HA	1:A:255:ALA:HB1	1.99	0.45
1:A:1:PCA:HG3	1:A:35:ALA:HB1	1.99	0.44
1:A:48:ASN:HB2	4:A:393:HOH:O	2.16	0.43
1:A:50:MET:HB2	1:A:84:HIS:O	2.18	0.43
1:A:29:LYS:HE3	1:A:29:LYS:HB2	1.88	0.43
1:A:102:LYS:HG3	1:A:149:ILE:HA	2.00	0.43
1:A:132:GLU:OE2	2:B:1:XYP:O1	2.36	0.43
1:A:272:ASP:N	1:A:273:PRO:HD2	2.35	0.42
1:A:20:THR:O	1:A:44:LEU:HA	2.20	0.41
1:A:102:LYS:HE3	1:A:149:ILE:O	2.21	0.41
1:A:105:LEU:HD12	1:A:105:LEU:HA	1.85	0.40
1:A:275:SER:HB2	1:A:283:LEU:CD1	2.52	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	$f d = f Favoured \mid Allowed$		Outliers	Percentiles	
1	A	301/302 (100%)	294 (98%)	7 (2%)	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.

Mo	l Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	243/242 (100%)	242 (100%)	1 (0%)	91 94		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type		
1	A	282	PRO		

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	142	ASN
1	A	251	ASN
1	A	296	ASN
1	A	300	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)

1 non-standard protein/DNA/RNA residue is 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
1	PCA	A	1	1	7,8,9	0.46	0	9,10,12	1.00	1 (11%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	A	1	PCA	CB-CA-C	-2.16	109.73	112.70

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
1	A	1	PCA	1	0

5.5 Carbohydrates (i)

3 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		
WIOI I	туре				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XYP	В	1	2	10,10,10	0.79	0	14,14,14	1.78	4 (28%)
2	XYP	В	2	2	9,9,10	0.96	1 (11%)	10,12,14	1.16	0
2	XYP	В	3	2	9,9,10	1.25	1 (11%)	10,12,14	0.85	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	В	1	2	-	-	0/1/1/1
2	XYP	В	2	2	-	-	0/1/1/1
2	XYP	В	3	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	В	3	XYP	C2-C3	2.66	1.56	1.52
2	В	2	XYP	C4-C3	2.09	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	1	XYP	C5-C4-C3	-3.96	104.80	109.67
2	В	1	XYP	C1-C2-C3	2.87	116.28	110.31
2	В	1	XYP	C4-C3-C2	-2.62	106.36	110.89
2	В	1	XYP	O5-C5-C4	-2.37	107.11	110.77

There are no chirality outliers.

There are no torsion outliers.

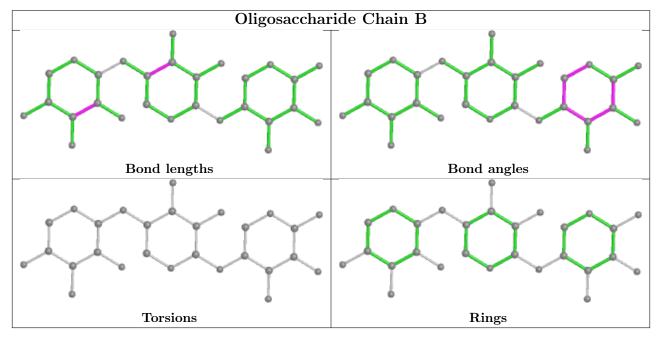
There are no ring outliers.

1 monomer is involved in 2 short contacts:

\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	XYP	2	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)

1 ligand is 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	Bo	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	XYS	A	560	-	10,10,10	1.33	1 (10%)	14,14,14	2.09	5 (35%)	

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	XYS	A	560	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	A	560	XYS	O4-C4	-2.45	1.38	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	560	XYS	C1-C2-C3	-4.14	101.72	110.31
3	A	560	XYS	O2-C2-C1	3.23	116.66	109.16
3	A	560	XYS	C5-C4-C3	2.75	113.05	109.67
3	A	560	XYS	O5-C5-C4	-2.58	106.79	110.77
3	A	560	XYS	O1-C1-C2	-2.54	101.87	109.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	560	XYS	5	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^{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	301/302 (99%)	-0.89	0 100 100	3, 9, 19, 31	1 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PCA	A	1	8/9	0.95	0.09	17,19,22,22	0

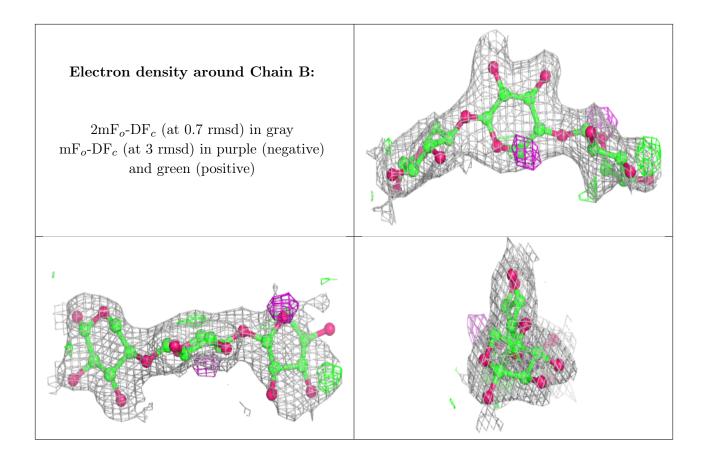
6.3 Carbohydrates (i)

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	XYP	В	3	9/10	0.74	0.32	42,44,54,56	0
2	XYP	В	2	9/10	0.84	0.14	20,22,27,34	0
2	XYP	В	1	10/10	0.95	0.13	14,22,25,27	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^{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
3	XYS	A	560	10/10	0.59	0.53	22,26,28,29	10

6.5 Other polymers (i)

There are no such residues in this entry.

