



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:43 PM BST

PDB ID : 3CUJ  
Title : Cellulomonas fimi Xylanase/Cellulase Cex (Cf Xyn10A) in complex with sulfur substituted beta-1,4 xylopentaose.  
Authors : Kuntz, D.A.; Saul, M.; Rose, D.R.  
Deposited on : 2008-04-16  
Resolution : 1.70 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	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

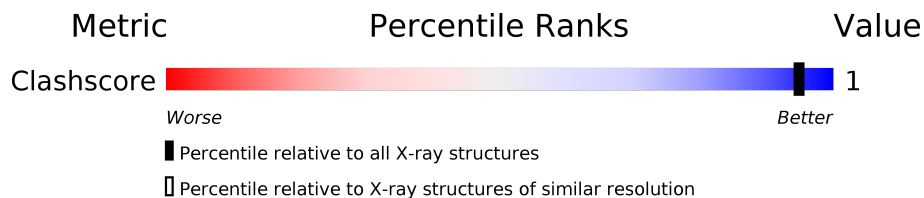
# 1 Overall quality at a glance

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))
Clashscore	141614	4695 (1.70-1.70)

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2857 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 Exo-beta-1,4-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	6	0
			2445	1537	425	472	11			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	O	S	0	0	0
			46	25	17	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	366	Total	O	0	0
			366	366		

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.37Å 85.37Å 78.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.76 – 1.70	Depositor
% Data completeness (in resolution range)	97.3 (18.76-1.70)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 1.70Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, $R_{free}$	0.158 , 0.170	Depositor
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.029	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2857	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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.

## 4 Model quality ⓘ

### 4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, TWY

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	0.66	0/2498	0.62	0/3386

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 4.2 Too-close contacts ⓘ

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	2445	0	2339	6	0
2	B	46	0	0	0	0
3	A	366	0	0	1	0
All	All	2857	0	2339	6	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 (6) 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:46[A]:MET:HE1	1:A:122:TRP:CH2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLY:HA2	3:A:385:HOH:O	2.07	0.54
1:A:84:TRP:CE2	1:A:86[A]:SER:HB2	2.48	0.49
1:A:191:LYS:HD2	1:A:191:LYS:HA	1.77	0.42
1:A:309[A]:MET:HG2	1:A:314[A]:ALA:HB3	2.03	0.41
1:A:46[A]:MET:CE	1:A:122:TRP:CH2	3.04	0.41

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 4.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 4.5 Carbohydrates [i](#)

5 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	TWY	B	1	2	9,10,10	1.81	3 (33%)	10,14,14	1.78	3 (30%)
2	TWY	B	2	2	8,9,10	1.04	1 (12%)	7,12,14	3.00	3 (42%)
2	TWY	B	3	2	8,9,10	1.31	2 (25%)	7,12,14	1.23	0
2	TWY	B	4	2	8,9,10	1.38	1 (12%)	7,12,14	2.21	3 (42%)
2	XYP	B	5	2	9,9,10	1.23	1 (11%)	10,12,14	1.09	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	TWY	B	1	2	-	-	0/1/1/1
2	TWY	B	2	2	-	-	0/1/1/1
2	TWY	B	3	2	-	-	0/1/1/1
2	TWY	B	4	2	-	-	0/1/1/1
2	XYP	B	5	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	TWY	C5-C4	3.04	1.54	1.52
2	B	1	TWY	C3-C4	2.97	1.56	1.53
2	B	1	TWY	O5-C1	2.82	1.47	1.43
2	B	1	TWY	C5-C4	2.74	1.54	1.52
2	B	2	TWY	C3-C4	2.54	1.55	1.53
2	B	5	XYP	O5-C1	2.42	1.47	1.42
2	B	3	TWY	C3-C4	2.07	1.55	1.53
2	B	3	TWY	O5-C5	2.00	1.46	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	TWY	C1-C2-C3	-4.66	103.94	109.67
2	B	2	TWY	C1-O5-C5	-4.35	104.83	111.52
2	B	2	TWY	C5-C4-C3	4.35	114.12	109.42
2	B	4	TWY	C1-C2-C3	-3.79	105.01	109.67
2	B	4	TWY	C1-O5-C5	-3.48	106.17	111.52
2	B	1	TWY	C5-C4-C3	3.43	113.12	109.42
2	B	1	TWY	O5-C1-C2	-2.81	105.25	109.43
2	B	4	TWY	C5-C4-C3	2.39	112.00	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	TWY	O3-C3-C4	2.01	113.19	108.82

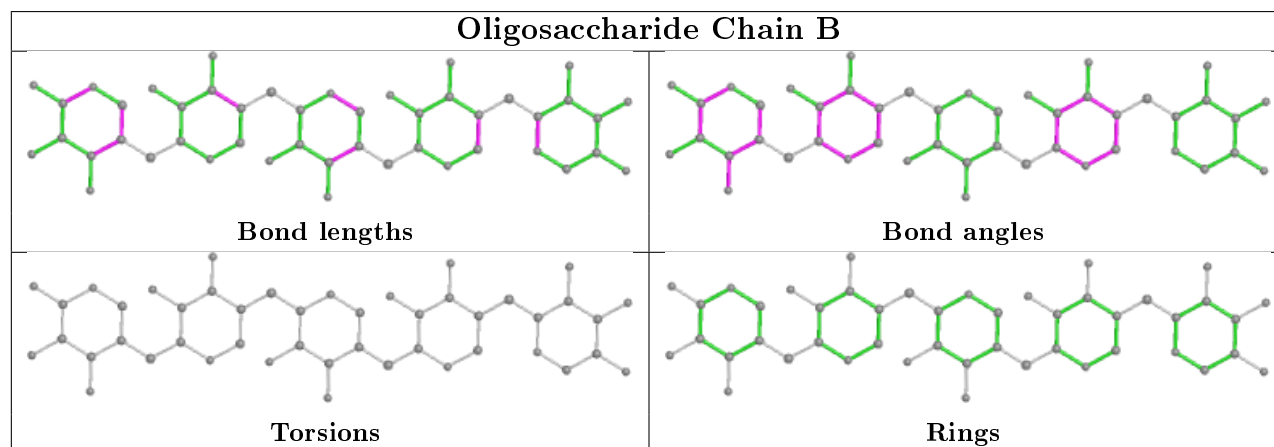
There are no chirality outliers.

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.



#### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.