

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:22 PM EDT

PDB ID : 6UB0

Title : Crystal structure of a GH128 (subgroup III) curdlan-specific exo-beta-1,3-g

lucanase from Blastomyces gilchristii (BgGH128_III) in complex with lami-

naribiose at -2 and -1 subsites

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Deposited on : 2019-09-11

Resolution : 1.75 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 (i)) were used in the production of this report:

 $\begin{array}{cccc} & Mol Probity & : & 4.02b\text{-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \\ & & \text{EDS} & : & \textbf{FAILED} \end{array}$

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)

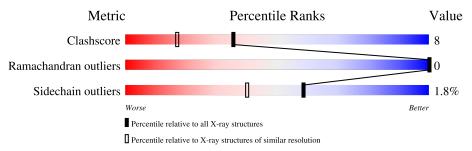
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.75 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	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain				
1	A	230	79%	21%			
2	В	2	100%				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1827 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 Glyco_hydro_cc domain-containing protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	230	Total 1756	C 1123	N 296	O 331	S 6	0	1	0

• Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	В	2	Total 23	C 12	O 11	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	48	Total O 48 48	0	0

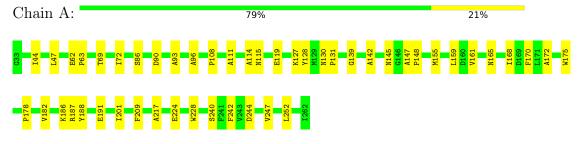


3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Glyco hydro cc domain-containing protein



• Molecule 2: beta-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain B:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	49.56Å 34.23Å 56.35Å	Depositor
a, b, c, α , β , γ	90.00° 104.88° 90.00°	Depositor
Resolution (Å)	32.11 - 1.75	Depositor
% Data completeness	99.0 (32.11-1.75)	Depositor
(in resolution range)	,	-
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.27 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.220 , 0.265	Depositor
Wilson B-factor (A^2)	26.2	Xtriage
Anisotropy	0.547	Xtriage
L-test for twinning ²	$ < L > = 0.45, < L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1827	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.10% 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: BGC, GLC

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	Bo	nd lengths	Bo	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.87	1/1808 (0.1%)	0.99	1/2458 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
1	A	178	PRO	CA-C	5.78	1.64	1.52

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	178	PRO	O-C-N	8.20	135.83	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ALA	Mainchain



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	1756	0	1659	28	0
2	В	23	0	21	0	0
3	A	48	0	0	1	0
All	All	1827	0	1680	28	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 8.

All (28) 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:69:THR:HG21	1:A:72:ILE:HD11	1.53	0.90	
1:A:69:THR:CG2	1:A:72:ILE:HD11	2.17	0.74	
1:A:119[A]:GLU:HA	1:A:161:VAL:HG11	1.74	0.69	
1:A:182:VAL:HG11	1:A:224:GLU:HG2	1.80	0.64	
1:A:119[B]:GLU:HA	1:A:161:VAL:HG11	1.81	0.62	
1:A:130:ASN:N	1:A:131:PRO:HD2	2.16	0.61	
1:A:111:ALA:O	1:A:115:ASN:HB2	2.04	0.58	
1:A:175:TRP:O	1:A:209:PHE:HA	2.05	0.57	
1:A:130:ASN:ND2	1:A:165:ASN:O	2.36	0.52	
1:A:187:ARG:NH1	1:A:191:GLU:OE1	2.37	0.50	
1:A:44:ILE:HG13	1:A:47:LEU:HD12	1.93	0.50	
1:A:127:LYS:HE3	1:A:128:TYR:CZ	2.46	0.50	
1:A:62:GLU:HB3	1:A:63:PRO:HD2	1.95	0.49	
1:A:142:ALA:HA	1:A:172:ALA:O	2.13	0.49	
1:A:108:PRO:HA	1:A:114:ALA:HB3	1.96	0.48	
1:A:168:ILE:HB	1:A:201:ILE:HD13	1.97	0.46	
1:A:86:SER:OG	1:A:90:ASP:OD2	2.26	0.46	
1:A:86:SER:HA	3:A:439:HOH:O	2.16	0.45	
1:A:155:MET:O	1:A:159:LEU:HG	2.17	0.45	
1:A:168:ILE:CG2	1:A:201:ILE:HD13	2.47	0.45	
1:A:119[B]:GLU:H	1:A:119[B]:GLU:HG2	1.37	0.44	
1:A:186:LYS:HE3	1:A:228:TRP:CG	2.53	0.44	
1:A:187:ARG:C	1:A:187:ARG:HD2	2.38	0.44	
1:A:139:GLY:HA3	1:A:170:PHE:CE1	2.53	0.44	

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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:247:VAL:HG22	1:A:252:LEU:HD23	1.99	0.43
1:A:147:ALA:O	1:A:148:PRO:C	2.57	0.42
1:A:145:ASN:HA	1:A:188:TYR:CE1	2.54	0.41
1:A:93:ALA:O	1:A:96:ALA:HB3	2.20	0.41

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	Percei	ntiles
1	A	229/230 (100%)	220 (96%)	9 (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	171/170 (101%)	168 (98%)	3 (2%)	59 40

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

Mol	Chain	Res	Type
1	A	240	SER
1	A	242	PHE

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Mol	Chain	Res	Type
1	A	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	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)

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

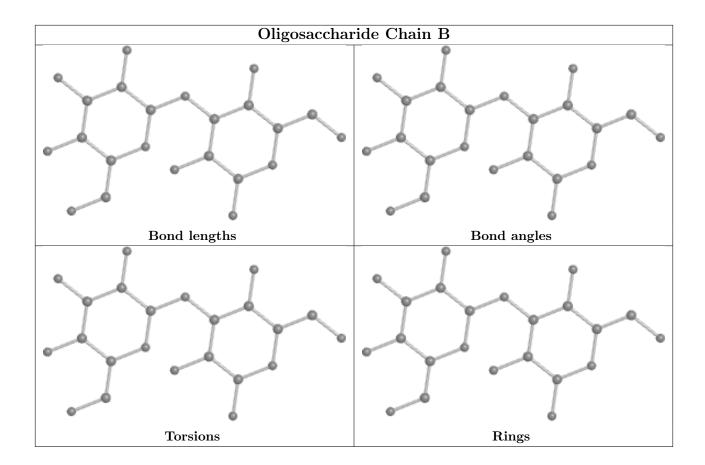
There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

