Additional file 1. Additional tables and figures

Title: Identification and molecular characterization of a psychrophilic GH1 βglucosidase from the subtropical soil microorganism *Exiguobacterium* sp. GXG2 Authors: Bangqiao Yin^{1*}, Hengsen Gu¹, Yue Xu¹, Bing Yan², Quanwen Li¹, Qian Ou¹, Bo Wu¹, Chen Guo^{3**}, and Chengjian Jiang^{1, 2***}

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Additional Tables

molpdf	DOPE score	GA341 score		
13346.14160	-58236.37891	1.00000		
13493.02832	-57447.93359	1.00000		
13395.54688	-57681.30078	1.00000		
	13346.14160 13493.02832	13346.14160 -58236.37891 13493.02832 -57447.93359		

Table S1 The results of homology modeling of BglG by multiple-template

$Table \ S2 \ The \ evaluation \ of \ and \ multi-template \ model \ of \ BglG$

Model	Ramachandran plot			G-factor			Errat	
	Core	Allow	Gener	Disall	Dihedrals	Covalent	Overall	
query.B99990001.pdb	91.1%	7.4%	1.2%	0.2%	0.00	-0.18	-0.07	64.396

Additional figure legends

Fig. S1 Functional screening of gene library. Hydrolyzing zones produced by *E.coli* strains harbored positive β -glucosidase genes on agar plates, containing ampicillin, esculin hydrate, and ferric ammonium citrate. A pGEMB0 clone was indicated by a black arrow.

Fig. S2 Agarose gel electrophoresis of *bglG* **gene.** Lane 1: 1kb DNA marker. Lane 2 and 3: *bglG* gene from pGEMB0.

Fig. S3 The ramachandran plot of BglG multi-template model.

Fig. S4 The PROSA evaluation of BglG multi-template model.

Fig. S5 Compare the changes in surrounding residues of active sites E163 and

E373 after mutant to glycine. (A) The distribution of all amino acid residues 4 Å away from E163 site in BglG. Four residues (Thr218, Phe167, Ile166 and Asn295) were formed hydrogen bonds with Glu163 (bond length of 2.7, 3.1, 3.1 and 3.2 Å) among 11 residues. (B) The distribution of all amino acid residues 4 Å away from A163 site in BglG. After mutate E163 to A163, the number of amino acid residues about 4.0 Å from A163 was significantly reduced to 7 and only leave 3 hydrogen bonds. (C) The distribution of all amino acid residues 4 Å away from E373 site in BglG. Glu373 was hydrogen bonded to Asn374, Asn295, Asn163 and Leu294 with bond length of 2.6 and 3.0, 3.3 and 3.4 Å, respectively. (D) The distribution of all amino acid residues 4 Å away from A373 site in BglG. After mutate E373 to A373, A373 forms only two hydrogen bonds with Asn374 and Leu294 (3.0 and 3.4 Å). Red dotted line represents hydrogen bond. The active site residues are showed as red for the C_a atoms, while the residues around active sites are showed as green sticks.



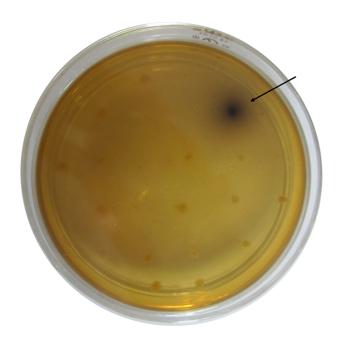
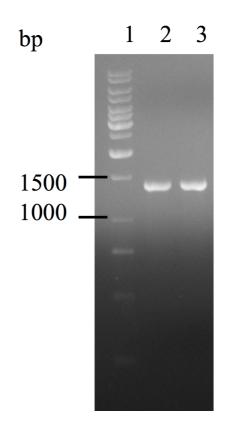


Fig. S2





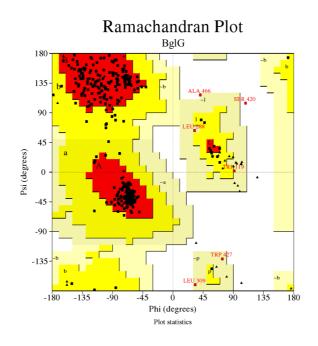


Fig. S4

