

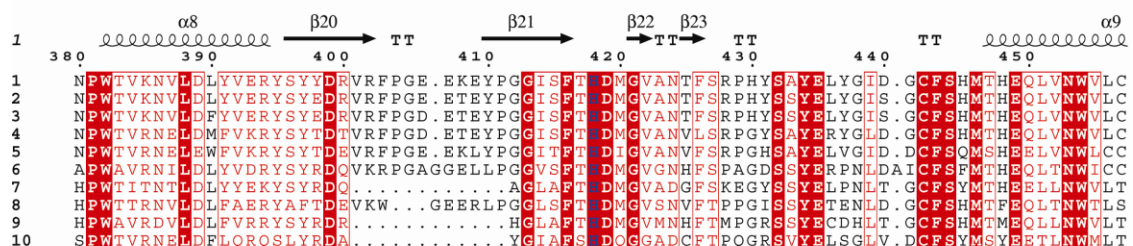
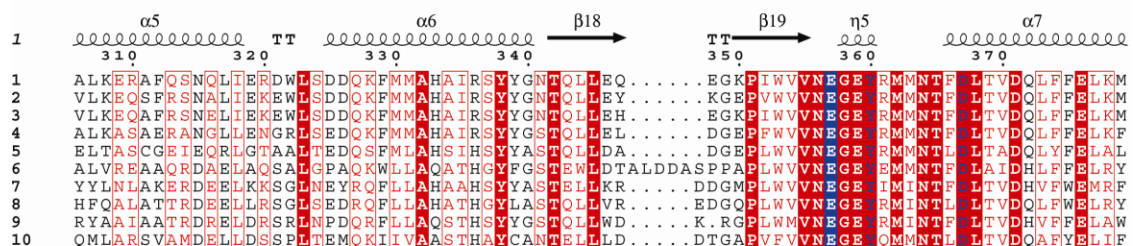
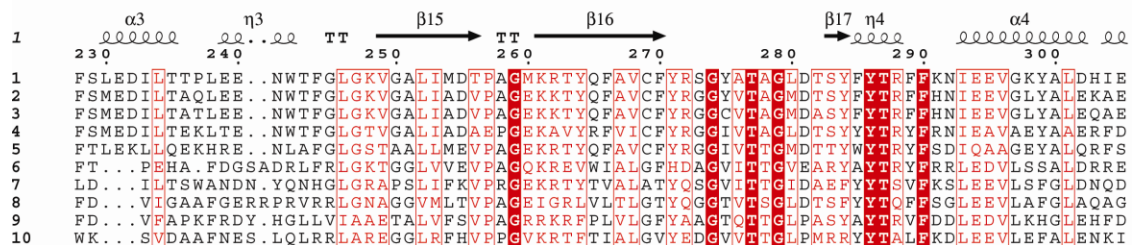
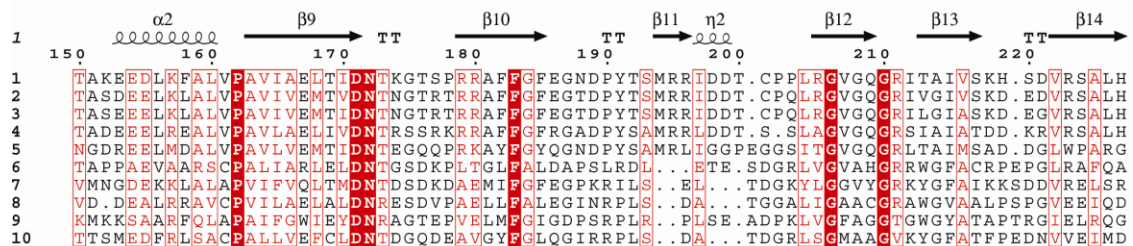
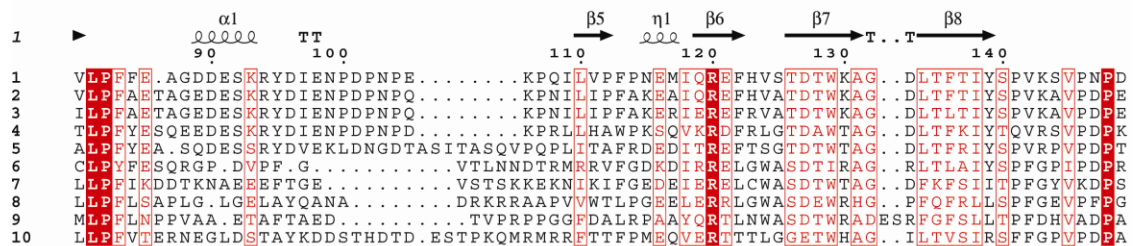
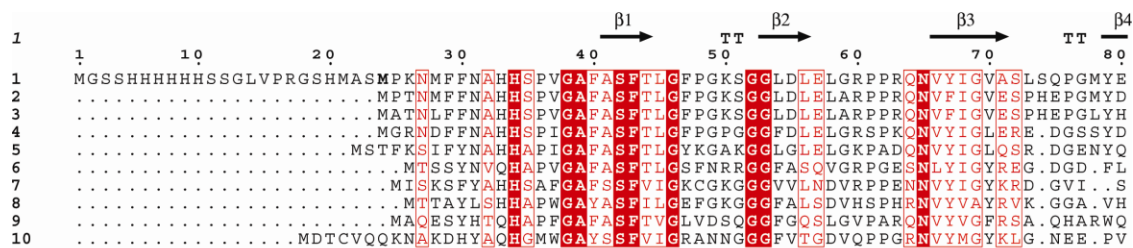
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Supporting information for article:

A novel β -xylosidase structure from *Geobacillus thermoglucosidasius*: the first crystal structure of a glycoside hydrolase family GH52 enzyme reveals unpredicted similarity with other glycoside hydrolase folds

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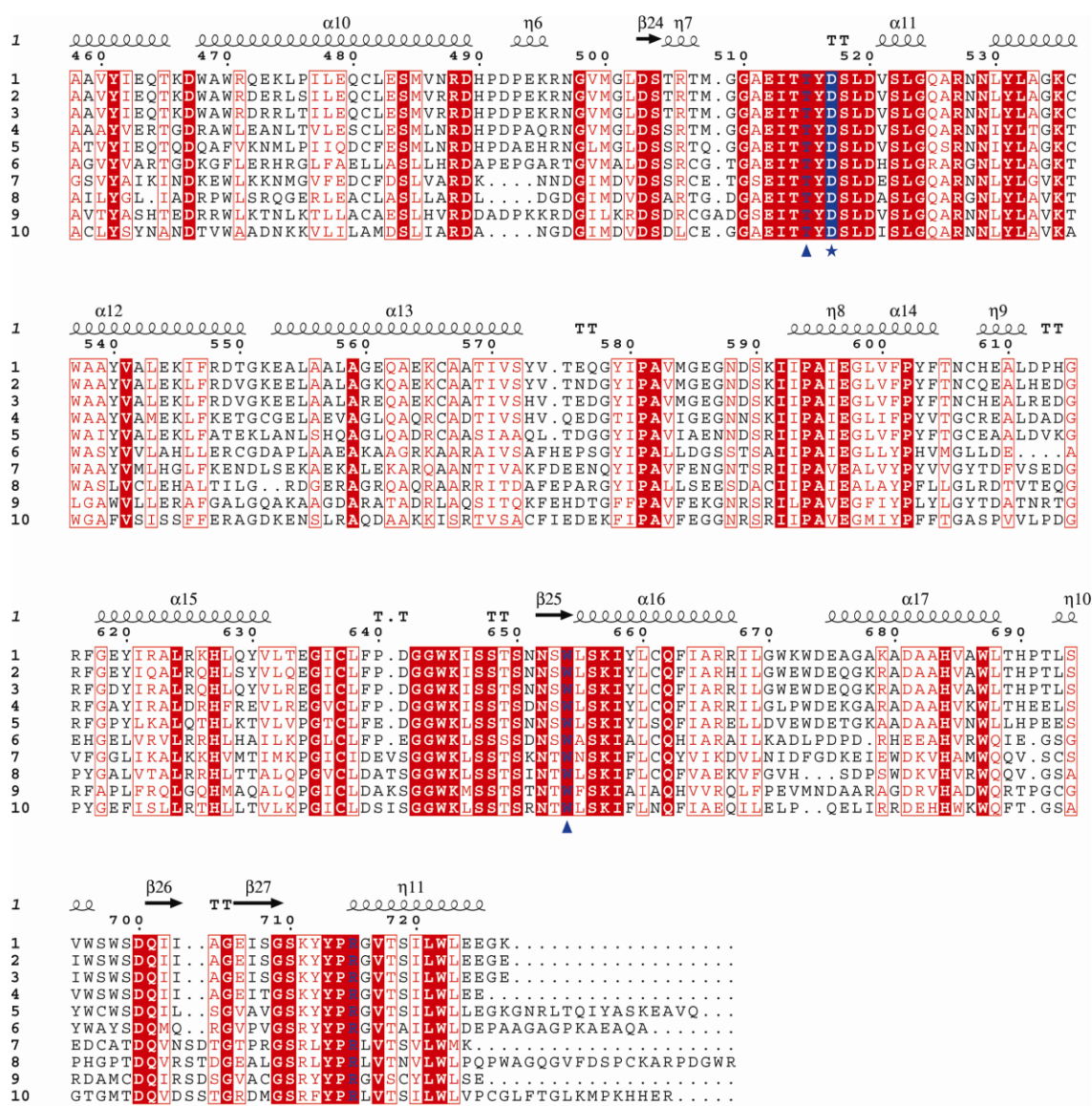


Table S1 Glycosidase hydrolase families classified in CAZy that contain at least one sequence with xylosidase (EC 3.2.1.37) activity: their mechanism of action, structure (with CATH classification where known), and a summary of the xylosidase structures deposited in the PDB.

GH family	Mechanism	Domain structure		Organism	PDB codes
1	Retaining	(α/β) ₈ barrel 3.20.20.80			
3	Retaining	(α/β) ₈ barrel 3.20.20.300	Rossmann 3.40.50.1700		
30	Retaining	(α/β) ₈ barrel 3.20.20.80	β -sandwich 2.60.40.1180		
39	Retaining	(α/β) ₈ barrel 3.20.20.80	β -sandwich 2.60.40.1500	<i>Caulobacter crescentus</i> CB15	4EKJ
				<i>Geobacillus stearothermophilus</i> T-6 NCIMB 40222	1W91, 2BFG, 2BS9
				<i>Thermoanaerobacterium</i> <i>saccharolyticum</i> B6A-RI	1PX8, 1UHV
43	Inverting	β -propellor 2.115.10.20	β -sandwich 2.60.120.200	<i>Bacillus halodurans</i> C-125	1YRZ
				<i>Bacillus subtilis</i> 168	1YIF
				<i>Clostridium acetobutylicum</i> ATCC 824	1Y7B, 1YI7, 3CPN, 3K1U
				<i>Geobacillus stearothermophilus</i> T-6 NCIMB 40222	2EXH, 2EXI, 2EXJ, 2EXK
				<i>Selenomonas ruminantium</i> GA192	3C2U
52*	Retaining	α/α_6 barrel	β -sandwich		4C1O, 4C1P
54	Retaining	β -sandwich 2.60.120.200	β -trefoil 2.80.10.50		
116	Retaining	unknown			
120*	Retaining	β -helix	β -sandwich	<i>Thermoanaerobacterium</i> <i>saccharolyticum</i> JW/SL-YS485	3VST, 3VSU, 3VSV

* these families contain only EC 3.2.1.37 xylosidase sequences.

Table S2 Structures identified as similar to *G.thermoglucoasidius*β-xylosidase by DaliLite V.3 (Holm & Rosenström, 2010) including only those structures that shared similarity across both domains.

PDB code	Description	Organism	Family	% Id	Z score	RMSD Å	L ali	Nres
1UG9	Glucodextranase	<i>Arthrobacter globiformis</i>	GH 15	8	25.9	4.7	379	1019
1LF6	Glucoamylase	<i>Thermoanaerobacterium thermosaccharolyticum</i>	GH 15	8	24.5	5.4	491	674
3W7S	Uncharacterized Protein Ygjk	<i>Escherichia coli K-12</i>	GH 63	13	24.4	5.1	525	760
1V7V	Chitobiose Phosphorylase	<i>Vibrio proteolyticus</i>	GH 94	9	21.0	4.3	512	779
3CIH	Putative Alpha-Rhamnosidase	<i>Bacteroides thetaiotaomicron</i>	GH 78	10	20.9	3.6	338	714
4J5T	Mannosyl-Oligosaccharide Glucosidase	<i>Saccharomyces cerevisiae</i>	GH 63	8	20.5	8.2	492	788
2CQS	Cellobiose Phosphorylase	<i>Cellvibrio gilvus</i>	GH 94	10	19.1	4.2	533	822
3RRS	Cellobiose Phosphorylase	<i>Cellulomonas uda</i>	GH 94	9	19.6	4.3	530	822
3QDE	Cellobiose Phosphorylase	<i>Clostridium thermocellum</i>	GH 94	11	19.4	4.3	524	811
1H54	Maltose Phosphorylase	<i>Lactobacillus brevis</i>	GH 65	8	17.3	5.5	504	754
3W5M	Putative Rhamnosidase	<i>Streptomyces avermitilis</i>	-	9	17.5	3.4	326	1030
2RDY	Bh0842 Protein	<i>Bacillus halodurans</i>	-	7	12.9	4.7	494	787
2WW2	Alpha-1,2-Mannosidase	<i>Bacteroides thetaiotaomicron</i>	GH 92	6	11.8	5.7	385	737
2XSG	Ccman5	<i>Cellulosimicrobium cellulans</i>	GH 92	7	10.3	4.9	376	765
2EAB	Alpha-Fucosidase	<i>Bifidobacterium bifidum</i>	GH 95	10	11.6	4.8	495	888

Z = Z-score (statistical significance) of the best domain-domain alignment (distance, in standard deviations, between the observed alignment RMSD and the mean RMSD for random pairs of the same length, with the same or fewer gaps).

RMSD = root-mean-square deviation of Cα atoms in rigid-body superimposition.

Lali = total number of structurally-equivalent residues.

%Id = percentage of sequence identity over equivalenced positions.