

**Structural characterization of β -xylosidase XynB2 from
Geobacillus stearothermophilus CECT43, a member of the glycoside hydrolase
family GH52**

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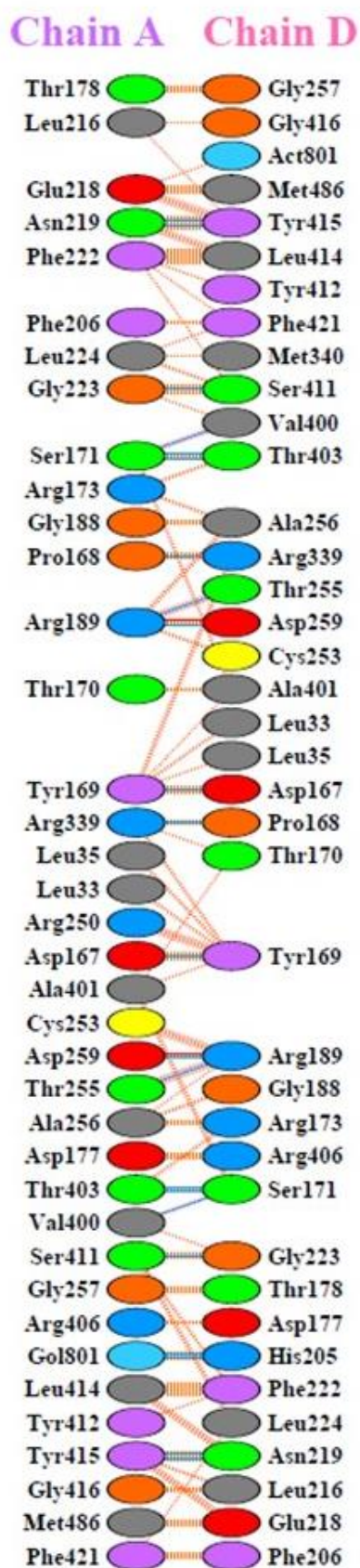


Figure S1. Contacts found in the Gst43XynB2 interface, calculated by PDBsum server. Salt bridges, hydrogen bonds and non-bonded contacts appear in red, blue and orange, respectively. Gol: glycerol. Act: acetate.

Gst43xynB2

1 10 20 30 40 50 TT β4

β1 β2 β3

Gst43xynB2 ... MPTNLFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESPHPEGLYH
GstT6XynB2 ... MATNLFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESPHPEGLYH
GthXynB2 MASMPKMMFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVASLSQPGMYE
Geost1A ... MPTNLFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESPHPEGLYH
Geost21 ... MPTNLFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESLHESGLYH
Geost22 ... MPTNLFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESPHPEGLYH
Aercav .MSTFKSIFYNAAHAPIGAFASTTIGYKGAKGGLGLELGPADQNVYIGLQSR.DGENYQ
PaeDG22 ... MGRNDDFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESLHESGLYH
Halhal .MFTPKNIFFNAHSPVGAFASTTIGFPGKSGGLDLELARPPRONVITGVESLHESGLYH
ThesacMISKSFYAAHSAFAGAFSTTIGKCGKGGGVVNDVRPPENNVITGVYKRD...GVVIS

* *

Gst43xynB2

60 70 80 90 100 TT β5 η1 β6 β7

Gst43xynB2 ILPFAETAG EDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
GstT6XynB2 ILPFAETAG EDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
GthXynB2 VLPFFEA.GDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
Geost1A ILPFAETAG EDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
Geost21 VLPFFEA.GDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
Geost22 ILPFAETAG EDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
Aercav ALPFFEA.SQDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
PaeDG22 TLPFFEA.SQDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
Halhal TLPFFEA.SQDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA
Thesac LLPFFEA.SQDESKRYDIENPDNPQ... KPNILIPFAKEETKREFCVAIDTWKA

* *

Gst43xynB2

110 120 130 140 150 160 TT β8 α1 β9 β10 TT

Gst43xynB2 GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
GstT6XynB2 GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
GthXynB2 GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
Geost1A GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
Geost21 GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
Geost22 GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
Aercav GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
PaeDG22 GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
Halhal GDLTFTIYSPVKAVDPDETAEELKLALVPAVIVEMTIDNTNGTRTARRAFFGFEGTDPY
Thesac GDFKFSITIPFGYVKDPSVMNGDEKKLALAPVIFVQLTMDNTDSDKDAEMIFGFEGPKRI

* *

Gst43xynB2

170 180 190 200 210 220 TT β11 η2 β12 β13 β14 α2 η3 TT

Gst43xynB2 TSMRRIDDT.CPQLRGVGGRIILGIA.SKDEGVRSAHFMSMEDILATLEEN.WTFGLGK
GstT6XynB2 TSMRRIDDT.CPQLRGVGGRIILGIA.SKDEGVRSAHFMSMEDILATLEEN.WTFGLGK
GthXynB2 TSMRRIDDT.CPQLRGVGGRIILGIA.SKDEGVRSAHFMSMEDILATLEEN.WTFGLGK
Geost1A TSMRRIDDT.CPQLRGVGGRIILGIA.SKDEGVRSAHFMSMEDILATLEEN.WTFGLGK
Geost21 TSMRRIDDT.CPQLRGVGGRIILGIA.SKDEGVRSAHFMSMEDILATLEEN.WTFGLGK
Geost22 TSMRRIDDT.CPQLRGVGGRIILGIA.SKDEGVRSAHFMSMEDILATLEEN.WTFGLGK
Aercav SAMRLIGGPEGGSITGVGGRIILGIA.SADDGLWPARGFTEKLLQEKHREN.LAFGLGS
PaeDG22 SAMRRIDDT.S.SLAGVGGRIILGIA.TDDKRVRSAHFMSMEDILATLEEN.WTFGLGK
Halhal SSMRKIDDT.S.SVAGVGGRIILGIA.SNDPSVKSALHFSMEDILATLEEN.WTFGLGK
Thesac LSELT...D.GKYLGGVYGRKYGFATIKSDVR...ELSRDLITLSWANDNYQNHGLGR

* *

Gst43xynB2

230 240 250 260 270 280 TT β15 β16 β17 η4 α3

Gst43xynB2 VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
GstT6XynB2 VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
GthXynB2 VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
Geost1A VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
Geost21 VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
Geost22 VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
Aercav TAALLMEVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
PaeDG22 VGALIVDVPAGEKKTYQFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
Halhal TGAIVVDVKPGEVKTIVRFVCFYRGCVTAGMDASYFYTRFFHNIIEVGLYALEQAEVLK
Thesac APSLIFKVPRGEKRTYTVATATYQSGVITIGIDAEFYFYSVFEKSLSEVLISFGLDNQDYIL

* *

Gst43xynB2

290 300 310 320 330 340 TT α4 α5 β18 β19 η5

Gst43xynB2 EQAFRSNE.LIEKEWLSDDQKFMMAHAIRSYGNTOLLE.HEGKPIWVVNEGEYRMNTFD
GstT6XynB2 EQAFRSNE.LIEKEWLSDDQKFMMAHAIRSYGNTOLLE.HEGKPIWVVNEGEYRMNTFD
GthXynB2 ERAFQSNQLIERDWLSDDQKFMMAHAIRSYGNTOLLE.QEGKPIWVVNEGEYRMNTFD
Geost1A EQAFRSNE.LIEKEWLSDDQKFMMAHAIRSYGNTOLLE.HEGKPIWVVNEGEYRMNTFD
Geost21 EQAFRSNE.LIEKEWLSDDQKFMMAHAIRSYGNTOLLE.HEGKPIWVVNEGEYRMNTFD
Geost22 EQAFRSNE.LIEKEWLSDDQKFMMAHAIRSYGNTOLLE.HEGKPIWVVNEGEYRMNTFD
Aercav ASCGEIEQRLGTAALTEDQS.FMLAHSIHSYASTOLL.DADGEPLWVVNEGEYRMNTFD
PaeDG22 ASAEERANGLENGLSEDQKFMMAHAIRSYGNTOLLE.LDGEPLWVVNEGEYRMNTFD
Halhal AKAAESDELVANSKLSDDQKFMMAHAIRSYGNTOLLE.HEGKPIWVVNEGEYRMNTFD
Thesac NLAKEERDELKKSGLNEVYRQFLLAHAHSYASTOLL.KRDLGMPLEWVVNEGEYRMNTFD

Gst43xynB2 α6 α7 β20 β21 β22 β23

350 360 370 380 390 400

Gst43xynB2 LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

GstT6XynB2 LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

GthXynB2 LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

Geost1A LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

Geost21 LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

Geost22 LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

Aercav LTADQLYFELALNPTWVRNELDWFKRYSYTDEVRFPGDETEYPGGISFTTHDMGVANTFSS

PaedG22 LTVDQLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

Halhal LTVDHLFFELKMNPTWKNVLDLYVERYSYEDRVRFPGDETEYPGGISFTTHDMGVANTFSS

Thesac LTVDHVFWEEMRFHPTWITNTLDLYYEKYSYRDQ.....AGLAFTHDMGVADGFS

Gst43xynB2 TT TT α8 α9 α10

410 420 430 440 450 460

Gst43xynB2 RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

GstT6XynB2 RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

GthXynB2 RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

Geost1A RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

Geost21 RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

Geost22 RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

Aercav RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

PaedG22 RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

Halhal RPHYSSYELYGITSGCFSHMTHEQLNWNVLCAAVYIEQTKDWAWRDRRLTILEOCLESMSVR

Thesac KEGYSSYELPNLTGCFSYMTHLELNWVLTGSVYAIKINDKEWLNKKNMGVFEDGFDLSLVJA

Gst43xynB2 η6 β24 η7 α11 α12

470 480 490 500 510 520

Gst43xynB2 RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

GstT6XynB2 RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

GthXynB2 RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

Geost1A RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

Geost21 RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

Geost22 RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

Aercav RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

PaedG22 RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

Halhal RDHPDPEKRRNGVMGLDSTRRTMGGAETITTYDSLDSVSLGOARNNLYLAGKCAWAAVVALEKLF

Thesac RDKN...NDGTHMDVDSRCETGSEITTYDSLDESLSGOARNNLYLAGKCAWAAVVALEKLF

Gst43xynB2 α13 TT η8 α14

530 540 550 560 570 580

Gst43xynB2 RDVKGKEELAAAREQAQEKCAATIVSHV.TEDGYIPAVMGECDNSKIIPAIIEGLVFPYFTN

GstT6XynB2 RDVKGKEELAAAREQAQEKCAATIVSHV.TEDGYIPAVMGECDNSKIIPAIIEGLVFPYFTN

GthXynB2 RDVKGKEELAAAREQAQEKCAATIVSHV.TEDGYIPAVMGECDNSKIIPAIIEGLVFPYFTN

Geost1A RDVKGKEELAAAREQAQEKCAATIVSHV.TEDGYIPAVMGECDNSKIIPAIIEGLVFPYFTN

Geost21 RDVKGKEELAAAREQAQEKCAATIVSHV.TEDGYIPAVMGECDNSKIIPAIIEGLVFPYFTN

Geost22 RDVKGKEELAAAREQAQEKCAATIVSHV.TEDGYIPAVMGECDNSKIIPAIIEGLVFPYFTN

Aercav ATEKLANLSHQAAGLQADRCDAASTIAAQL.TDGGYIPAVIAENNDNSRIIPAIIEGLVFPYFTG

PaedG22 KETGCELAEEVAGLQAQRCAADTVSHV.QEDGTIPAVIGEENNSKIIPAIIEGLVFPYFTG

Halhal AEEGLLEELSKAAGEQAERAAKTICGNV.TEGGYIPAVIGEENNSKIIPAIIEGLVFPYFTN

Thesac KENDLSEKAEKALEKARQAANTIVAKFDEENQYIPAVFENGNTSRIIPAVEALVVPYVVG

Gst43xynB2 η9 α15 T.T β25 α16

590 600 610 620 630 640

Gst43xynB2 CHEALREDGRFGDYIRALRQHLQYVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

GstT6XynB2 CHEALREDGRFGDYIRALRQHLQYVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

GthXynB2 CHEALREDGRFGDYIRALRQHLQYVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

Geost1A CHEALREDGRFGDYIRALRQHLQYVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

Geost21 CHEALREDGRFGDYIRALRQHLQYVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

Geost22 CHEALREDGRFGDYIRALRQHLQYVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

Aercav CEALADVKGRTCPYLKALQTHLKTIVLPCTCLFE.DGGWKTSSTSNNSWLSKIYLCQFIA

PaedG22 CREALDADGRFCAYIRALDRHFRFVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

Halhal CREALDRNGRFCAYIRALDRHFRFVLRGICLFF.DGGWKTSSTSNNSWLSKIYLCQFIA

Thesac YTDVFSSEDGVFGGLIKALKKHVMTIMKPGICIDEVS.DGGWKTSSTSNNTWNSTKIELCQYVI

Gst43xynB2 α17 η10 β26 β27 η11

650 660 670 680 690 700

Gst43xynB2 RRILGWEDWEQKGRADAAHVAVLTHPTLSIWSWSDQI..TAGEISGSKYYPRGVTSILWL

GstT6XynB2 RRILGWEDWEQKGRADAAHVAVLTHPTLSIWSWSDQI..TAGEISGSKYYPRGVTSILWL

GthXynB2 RRILGWEDWEQKGRADAAHVAVLTHPTLSIWSWSDQI..TAGEISGSKYYPRGVTSILWL

Geost1A RRILGWEDWEQKGRADAAHVAVLTHPTLSIWSWSDQI..TAGEISGSKYYPRGVTSILWL

Geost21 RRILGWEDWEQKGRADAAHVAVLTHPTLSIWSWSDQI..TAGEISGSKYYPRGVTSILWL

Geost22 RRILGWEDWEQKGRADAAHVAVLTHPTLSIWSWSDQI..TAGEISGSKYYPRGVTSILWL

Aercav RELLDVWEDETGAADAAHVAVLTHPTLSIWSWSDQI..LSGVAVGSKYYPRGVTSILWL

PaedG22 RRILGLPWDEKGAADAAHVAVLTHPTLSIWSWSDQI..TSGEIAGSKYYPRGVTSILWL

Halhal RHIIGLPWDEKGAADAAHVAVLTHPTLSIWSWSDQI..TSGEIAGSKYYPRGVTSILWL

Thesac KDVNLNIDFGDKETIWDKVHAMWQVSC.SEDCATDQVNSDTGTPRSRLYPRVTSVVLWM

Gst43xynB2 α18

710

Gst43xynB2 EEEHHHHHHH.....

GstT6XynB2 EEEHHHHHHH.....

GthXynB2 EEEHHHHHHH.....

Geost1A EEEHHHHHHH.....

Geost21 EEEHHHHHHH.....

Geost22 EEEHHHHHHH.....

Aercav LEGKGNRLTQIYASKEAVQ.....

PaedG22

Halhal EET.....

Thesac K.....

Figure S2. Sequence alignment of β -xylosidases of contrasted activity available at the CAZY database (http://www.cazy.org/GH52_characterized.html, accessed November, the 8th, 2023). Gst43XynB2, *Geobacillus stearothermophilus* CECT43, Genbank acc. No. WOK24302; GstT6XynB2, *Geobacillus stearothermophilus* T-6 NCIMB 40222, Uniprot Q09LZ0; GthXynB2, *Parageobacillus thermoglucosidasius* NBRC 107763 / TM242, Uniprot A0A067XG64; Geost1A, *Geobacillus stearothermophilus* 1A05583. Uniprot M1GNL7; Geost21, *Geobacillus stearothermophilus* 21, Uniprot P45702; Geost22, *Geobacillus stearothermophilus* 21, Genbank acc. No. KFL17027.1; Aercav, *Aeromonas caviae* ME-1, Uniprot Q9Z487; PaeDG22, *Paenibacillus* sp. DG-22, Uniprot B6C867; Halhal, *Halalkalibacterium halodurans* C-125, Uniprot Q9KB21; Thesac, *Thermoanaerobacterium saccharolyticum* strain DSM 8691, Uniprot I3VVB3. Residues conserved in the interface of Gst43XynB2 are marked with asterisks (*).

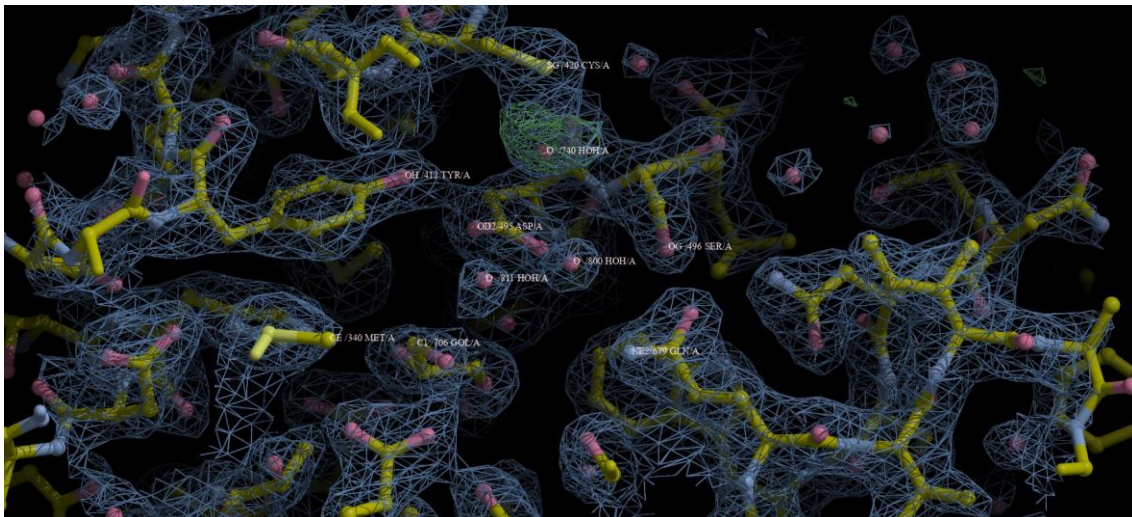
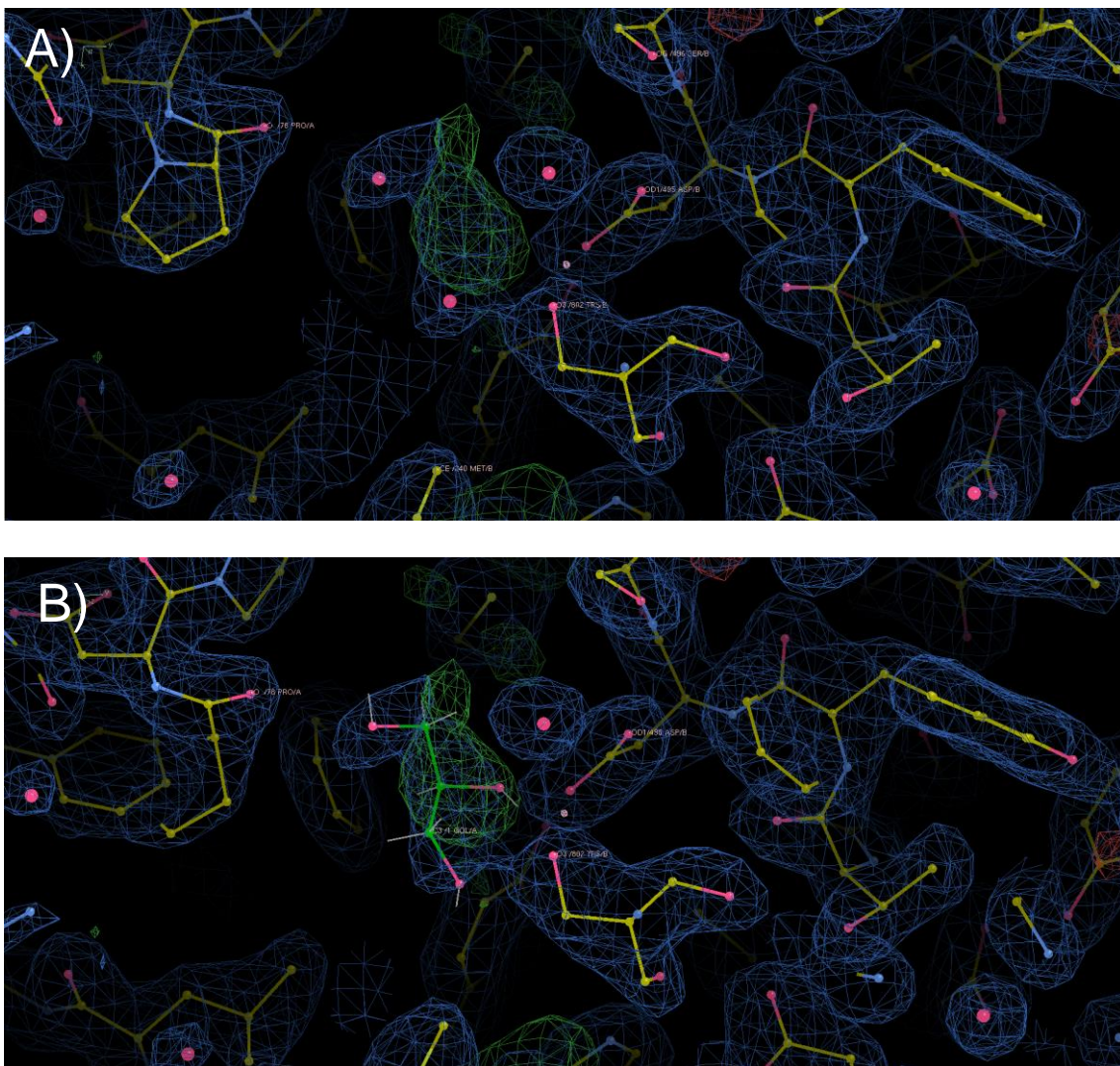


Figure S3. Electron densities in the Gst43XynB2 +1 site contoured at 1.09 σ . Modification of Cys420 by radiation damage is compatible with extra densities observed for this residue.



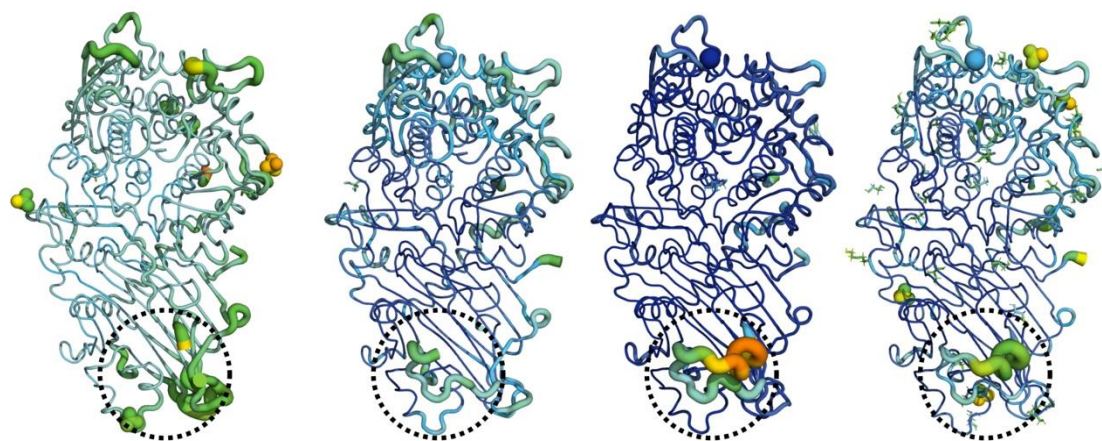


Figure S5. Representation in putty mode of the different *Geobacillus* XynB2 structures (from left to right, PDBs 4C1O, 4C1P, 4RHH and 8QME). The structures are coloured according to their B-factors. The position of the loop closing the catalytic centre (containing Pro100^{GthXynB2} / Pro78^{Gst43XynB2}) is highlighted.

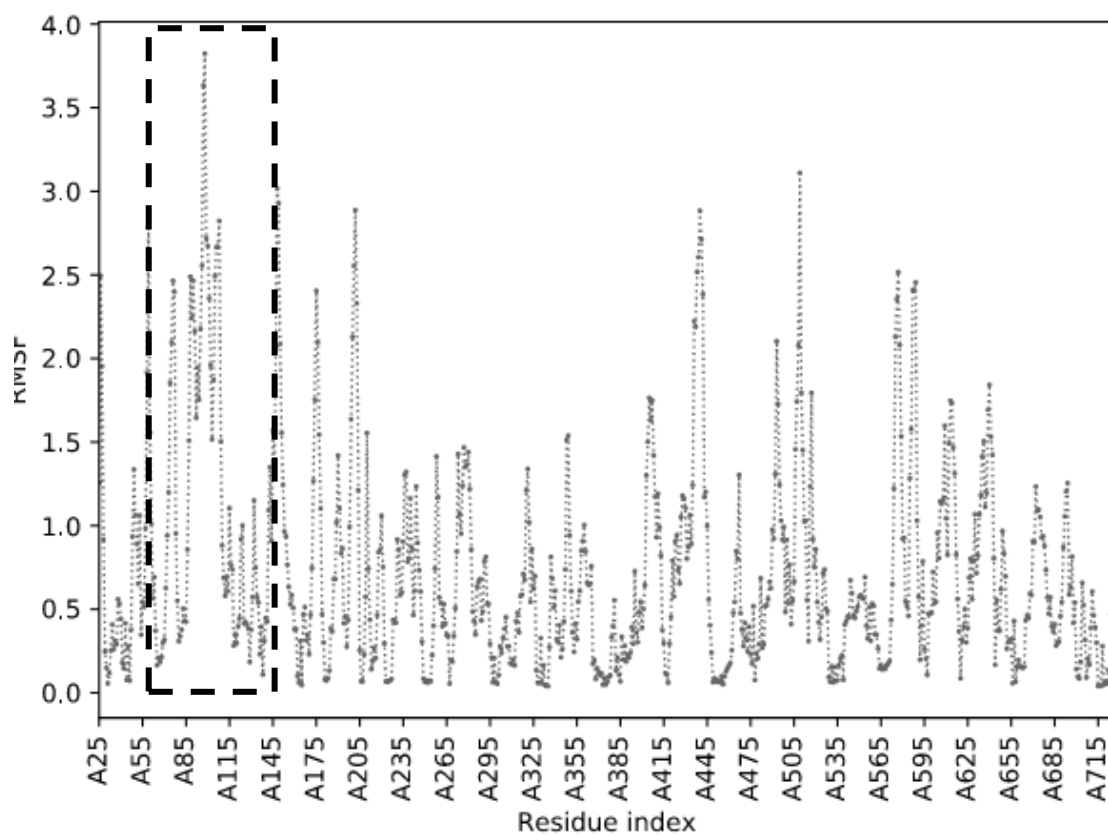


Figure S6. Fluctuation map obtained with the CABS-flex 2.0 server using the GthXynB2 structure as input (PDB 4C1O). The loop containing Pro100^{GthXynB2} (Pro78^{Gst43XynB2}) is highlighted.

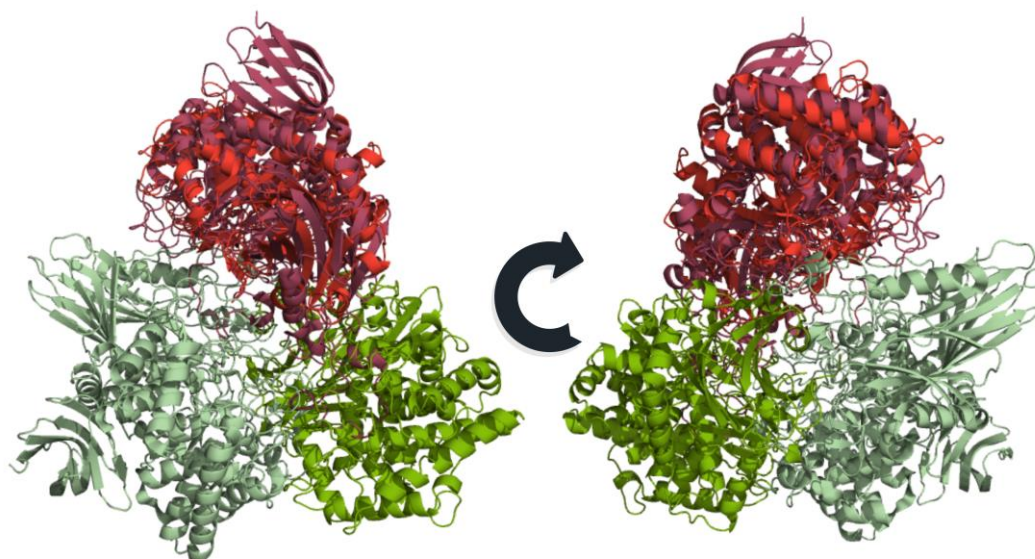


Figure S7. Different dimerization interfaces found in the GH52 and the GH116 families, using Gst43XynB2 (PDB 8QME) and ExoMA2 (PDB 8IC6) dimers as representatives. Both dimers were superposed using chain A (in red). As it is shown, the second protomer of each dimer (in different green colors) does not occupy the same position, being roughly rotated 100°.

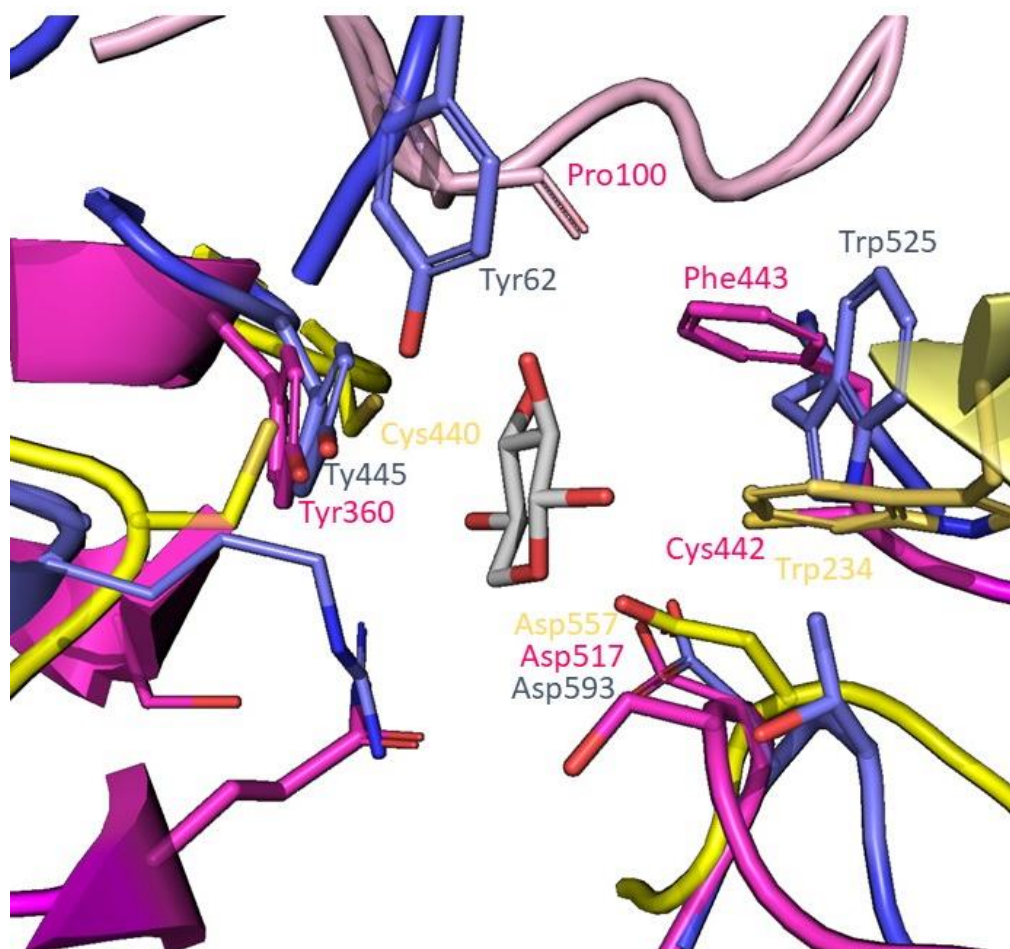


Figure S8. Superposition of the +1 binding site of GthXynB2 (PDB 4C1P, pink tones), TxGH116 (PDB 5BX5, blue tones) and ExoMA2 (PDB 8IC7, yellow tones). Xylose from PDB 4C1P, occupying the +1 site, is shown in white tones.



Figure S9. Common β -hairpin appearing in TxGH116 (PDB 5BX5, orange) and Gst43XynB2 (PDB 8QME, gray) which are totally displaced between the two structures (residues 480-504^{TxGH116}/373-395^{Gst43XynB2}).

	GthXyn	GthXynB	GstT6XynB2	Gst43XynB2
PDB ID	4C1P	4C1O	4RHH	8QME
Resolution (Å)	2.63	1.70	2.15	2.25
Ligand -1 subsite	xylobiose	Glycerol	Tris	Glycerol
	Glu357	Glu357	Gly335 ^{c,d}	Glu335^a
	Tyr360	Tyr360	Tyr338 ^c	Tyr338 ^c
	Met362	Met362	Met340 ^c	Met340 ^c
	Thr365	Thr365	Thr343	Thr343
	Asp367	Asp367	Asp345^a	Asp345^a
	Leu368	Leu368	Leu346 ^c	Leu346 ^c
	His418^a	His418^a	His396^a	His396^a
	Tyr434	Tyr434	Tyr412 ^c	Tyr412 ^c
	Met446	Met446	Met424	Met424
	Thr515^a	Thr515^a	Thr493^a	Thr493^a
	Tyr516 ^c	Tyr516	Tyr494 ^c	Tyr494 ^c
	Asp 517	Asp 517	Asp495^a	Asp495
	Trp654	Trp654	Trp632	Trp632
	Gln701	Gln701 ^c	Gln679	Gln679 ^c
	Ser710	Ser710	Ser688^a	Ser688 ^c
	Tyr713	Tyr713	Try691^a	Try691 ^c
	Arg715^a	Arg715^a	Arg693^a	Arg693^a
Ligand +1 subsite	xylobiose	Glycerol	None	None
Residues	Pro100^{a,b}	Pro100^{a,b}	Pro78*	Pro78 ^c
	Pro102 ^b	Pro102 ^b	Pro80 ^c	Pro80 ^c
	Tyr360^d	Tyr360	Tyr338 ^c	Tyr338 ^c
	Met362	Met362 ^c	Met340 ^c	Met340 ^c
	Tyr434	Tyr434	Tyr412 ^c	Tyr412 ^c
	Cys442	Cys442	Cys420 ^c	Cys420 ^c
	Phe443	Phe443	Phe421 ^c	Phe421 ^c
	Asp517	Asp517^a	Asp495 ^c	Asp495 ^c
	Ser518	Ser518	Ser496 ^c	Ser496 ^c
	Trp654 ^c	Trp654	Trp632 ^c	Trp632 ^c
	Gln701^a	Gln701^a	Gln679 ^c	Gln679 ^c
	Ser710	Ser710 ^c	Ser688 ^c	Ser688 ^c

Table S1. Correspondence of residues in the different *Geobacillus* XynB2 structures with any atom at less than 4Å from ligands found in binding subsites +1 and -1. ^aDirect polar contacts calculated by Pymol, also highlighted in bold. ^bResidues belonging to a second protomer. ^cCounterpart residues which do not appear or appear at more than 4Å from a ligand in the corresponding structure. ^dThis structure is a E335G active-site mutant.