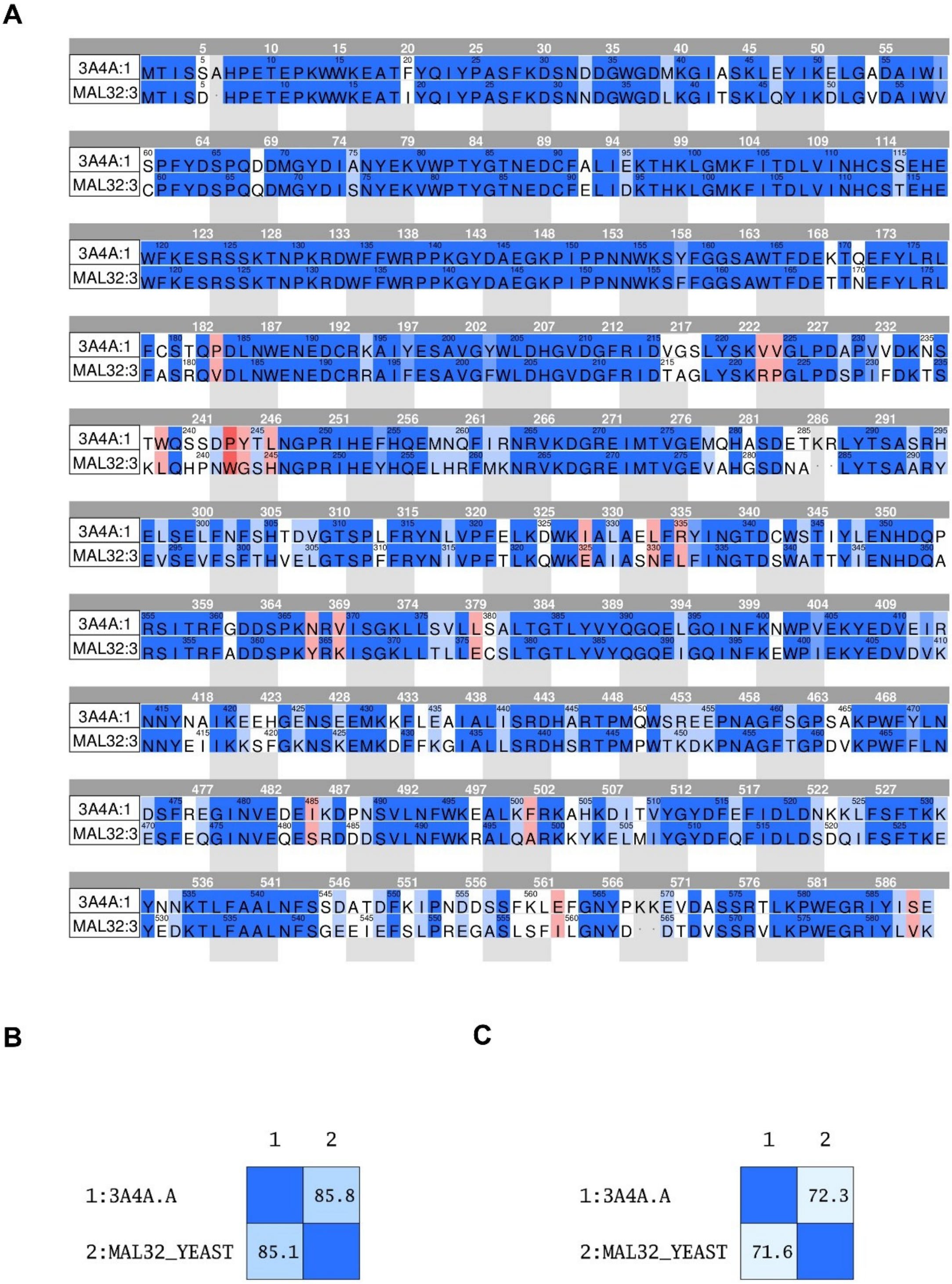
Supplementary information

Table S1. The structural template candidates for homology modeling of yeast α-glucosidase (YEAST_MAL32).

PDB ID	Chain ID	Title	Length (a.a.)	Identities	Ligand	Method	Resolution (Å)
3A47	A	Crystal structure of isomaltase from Saccharomyces cerevisiae	587	422/587 (72%)	Ca^{2+}	X-Ray	1.59
3A4A	**A**	**Crystal structure of isomaltase from Saccharomyces cerevisiae**	**587**	**422/587 (72%)**	**Ca^{2+} Alpha-D-Glucose**	**X-Ray**	**1.60**
3AJ7	A	Crystal	587	422/58	Ca^{2+}	X-ray	1.3

		structure of isomaltase from Saccharomyces cerevisiae		7 (72%)			
3AXH	A	Crystal structure of isomaltase in complex with isomaltose	587	421/587 (72%)	Ca^{2+} Alpha-D-Glucose	X-ray	1.8
3AXI	A	Crystal structure of isomaltase in complex with isomaltose	587	421/587 (72%)	Ca^{2+} Alpha-D-Glucose	X-ray	1.4



A

```
3A4A:1  MTISSAHPETEPKWWKEATFYQIYPASFKDSNDDGWGDMKGIASKLEYIKELGADAWI
MAL32:3 MTISD·HPETEPKWWKEATIYQIYPASFKDSNNDGWGDLKGITSKLQYIKDLGVDAIWV

3A4A:1  SPFYDSPQDDMGYDIANYEKVWPTYGTNEDCFALIEKTHKLGMKFITDLVINHCSSEHE
MAL32:3 CPFYDSPQQDMGYDISNYEKVWPTYGTNEDCFELIDKTHKLGMKFITDLVINHCSTEHE

3A4A:1  WFKESRSSKTNPKRDWFFWRPPKGYDAEGKPIPPNNWKSYFGGSAWTFDEKTQEFYLRL
MAL32:3 WFKESRSSKTNPKRDWFFWRPPKGYDAEGKPIPPNNWKSFFGGSAWTFDETTNEFYLRL

3A4A:1  FCSTQPDLNWENEDCRKAIYESAVGYWLDHGVDGFRIDVGSLYSKVVGLPDAPVVDKNS
MAL32:3 FASRQVDLNWENEDCRRAIFESAVGFWLDHGVDGFRIDTAGLYSKRPGLPDSPIFDKTS

3A4A:1  TWQSSDPYTLNGPRIHEFHQEMNQFIRNRVKDGREIMTVGEMQHASDETKRLYTSASRH
MAL32:3 KLQHPNWGSHNGPRIHEYHQELHRFMKNRVKDGREIMTVGEVAHGSDNA··LYTSAARY

3A4A:1  ELSELFNFSHTDVGTSPLFRYNLVPFELKDWKIALAELFRYINGTDCWSTIYLENHDQP
MAL32:3 EVSEVFSFTHVELGTSPFFRYNIVPFTLKQWKEAIASNFLFINGTDSWATTYIENHDQA

3A4A:1  RSITRFGDDSPKNRVISGKLLSVLLSALTGTLYVYQGQELGQINFKNWPVEKYEDVEIR
MAL32:3 RSITRFADDSPKYRKISGKLLTLLECSLTGTLYVYQGQEIGQINFKEWPIEKYEDVDVK

3A4A:1  NNYNAIKEEHGENSEEMKKFLEAIALISRDHARTPMQWSREEPNAGFSGPSAKPWFYLN
MAL32:3 NNYEIIKKSFGKNSKEMKDFFKGIALLSRDHSRTPMPWTKDKPNAGFTGPDVKPWFFLN

3A4A:1  DSFREGINVEDEIKDPNSVLNFWKEALKFRKAHKDITVYGYDFEFIDLDNKKLFSFTKK
MAL32:3 ESFEQGINVEQESRDDDSVLNFWKRALQARKKYKELMIYGYDFQFIDLDSDQIFSFTKE

3A4A:1  YNNKTLFAALNFSSDATDFKIPNDDSSFKLEFGNYPKKEVDASSRTLKPWEGRIYISE
MAL32:3 YEDKTLFAALNFSGEEIEFSLPREGASLSFILGNYD··DTDVSSRVLKPWEGRIYLVK
```

B

	1	2
1:3A4A.A		85.8
2:MAL32_YEAST	85.1	

C

	1	2
1:3A4A.A		72.3
2:MAL32_YEAST	71.6	

Figure S1. Sequence alignment between yeast α-glucosidase (mal32) and structural template (yeast isomaltase, PDB ID: 3A4A). (A) Sequence alignment colored by residue similarity (blue, similar; pink, dissimilar). (B) Sequence similarity. (C) Sequence identity.

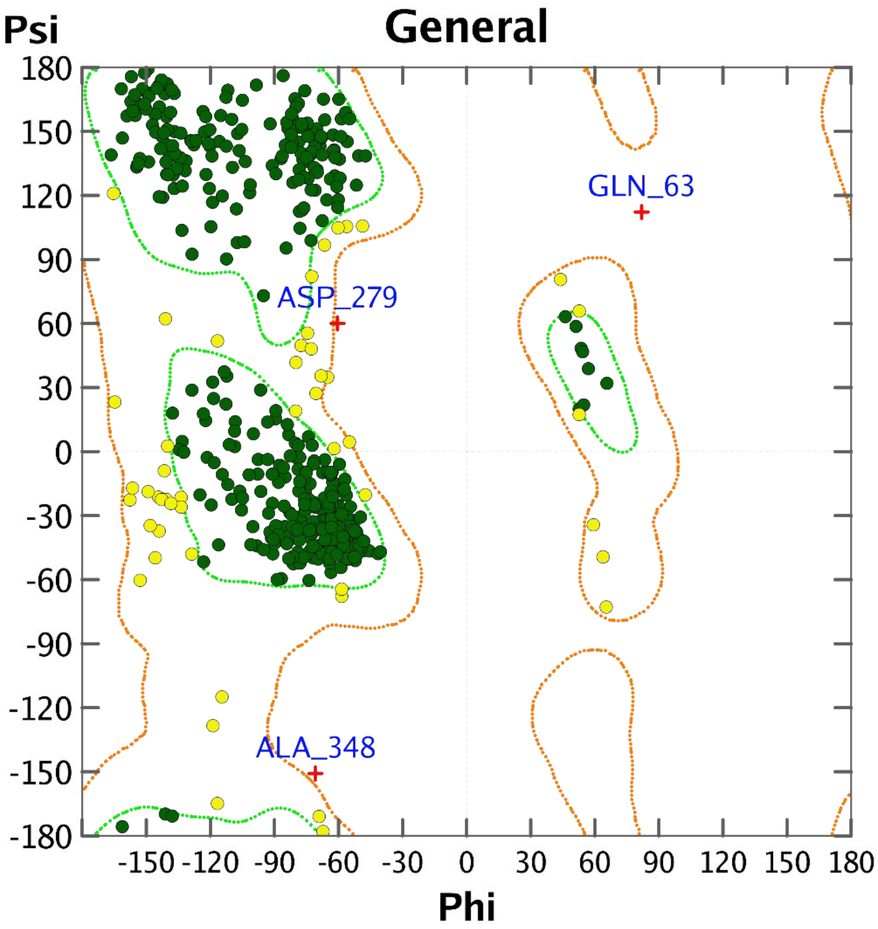


Figure S2. Phi-Psi plot (Ramachandran plot) of putative model of yeast α-glucosidase resulted from homology modeling and molecular dynamics simulation.