STRUCTURAL
BIOLOGY

Volume 78 (2022)

Supporting information for article:

Crystal structure of the domain-swapped dimeric maltodextrin-binding protein MalE from *Salmonella enterica*

Lulu Wang, Tingting Bu, Xue Bai, Shanru He, Jie Zhang, Liming Jin, Baoquan Liu, Yuesheng Dong, Nam-Chul Ha, Chunshan Quan, Ki Hyun Nam and Yongbin Xu

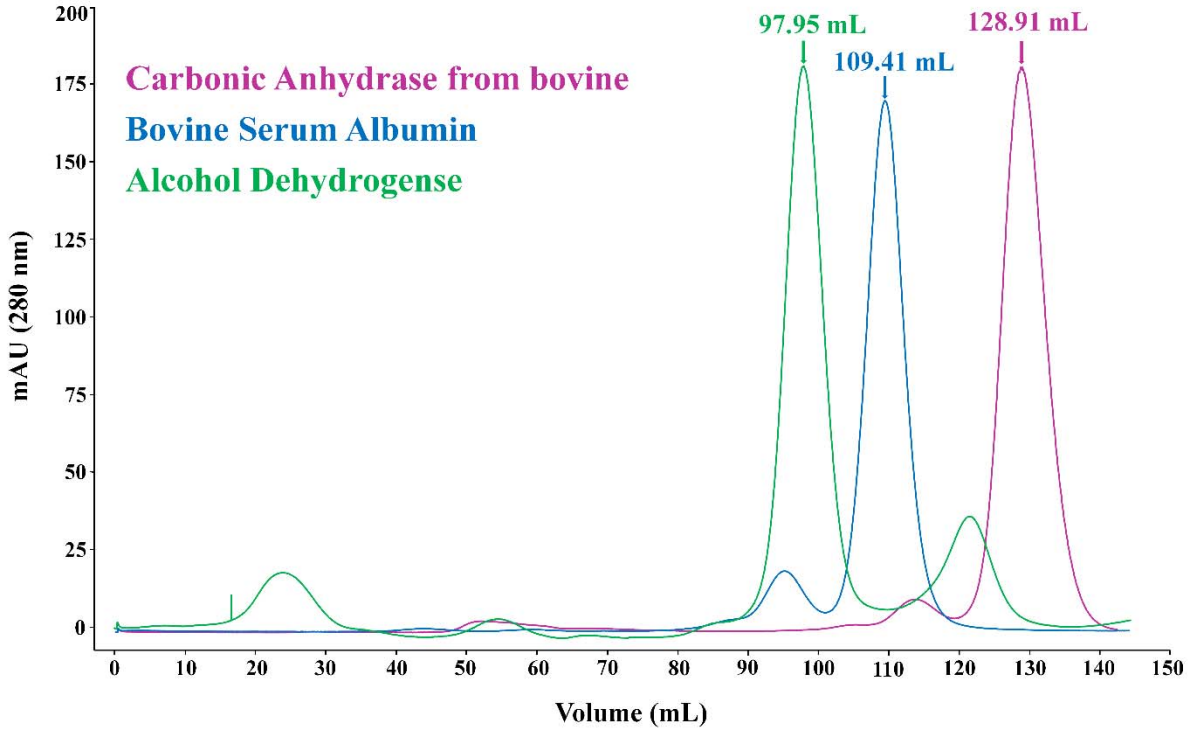


Figure S1 Size-exclusion chromatography of standard proteins. The carbonic anhydrase from bovine (30 kDa, colored in deep purple), bovine serum albumin (66 kDa, colored in blue), and alcohol dehydrogense (82 kDa, colored in green) were eluted at 128.91 mL, 109.41 mL and 97.95 mL, respectively.

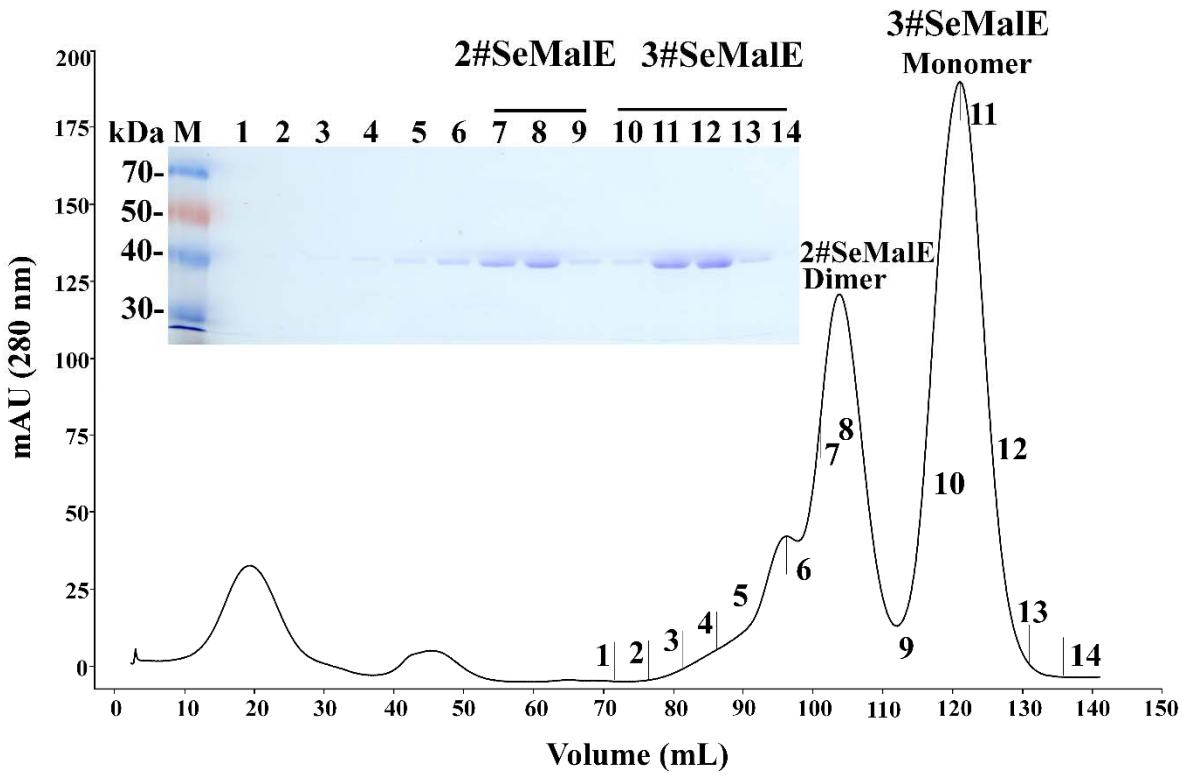


Figure S2 Size-exclusion chromatography of SeMalE in the later protein purification stage.The eluted peaks of the SeMalE protein are labeled 2#SeMalE (dimer), and 3#SeMalE (monomer).

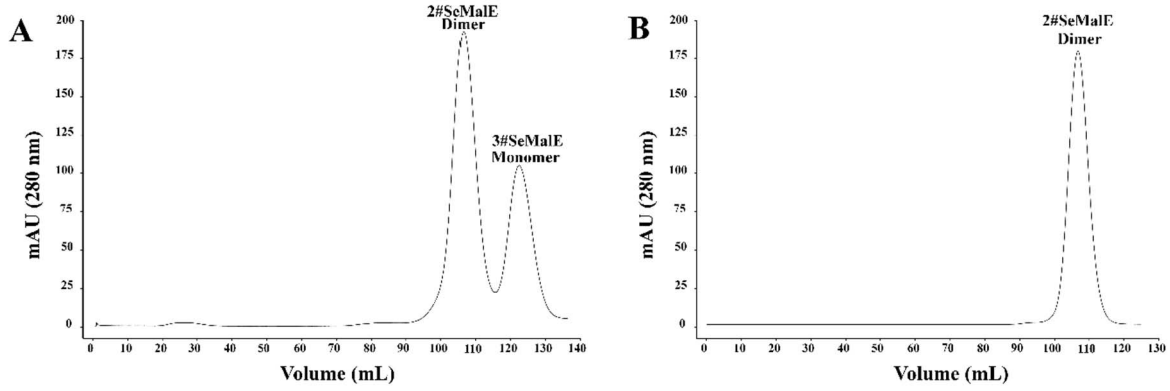


Figure S3 Size-exclusion chromatography of SeMalE. (A) Profile of size-exclusion chromatography of SeMalE after Ni-NTA purification. (B) Profile of size exclusion chromatography of SeMalE from dimeric fraction of SeMalE (red box in Figure S3A)

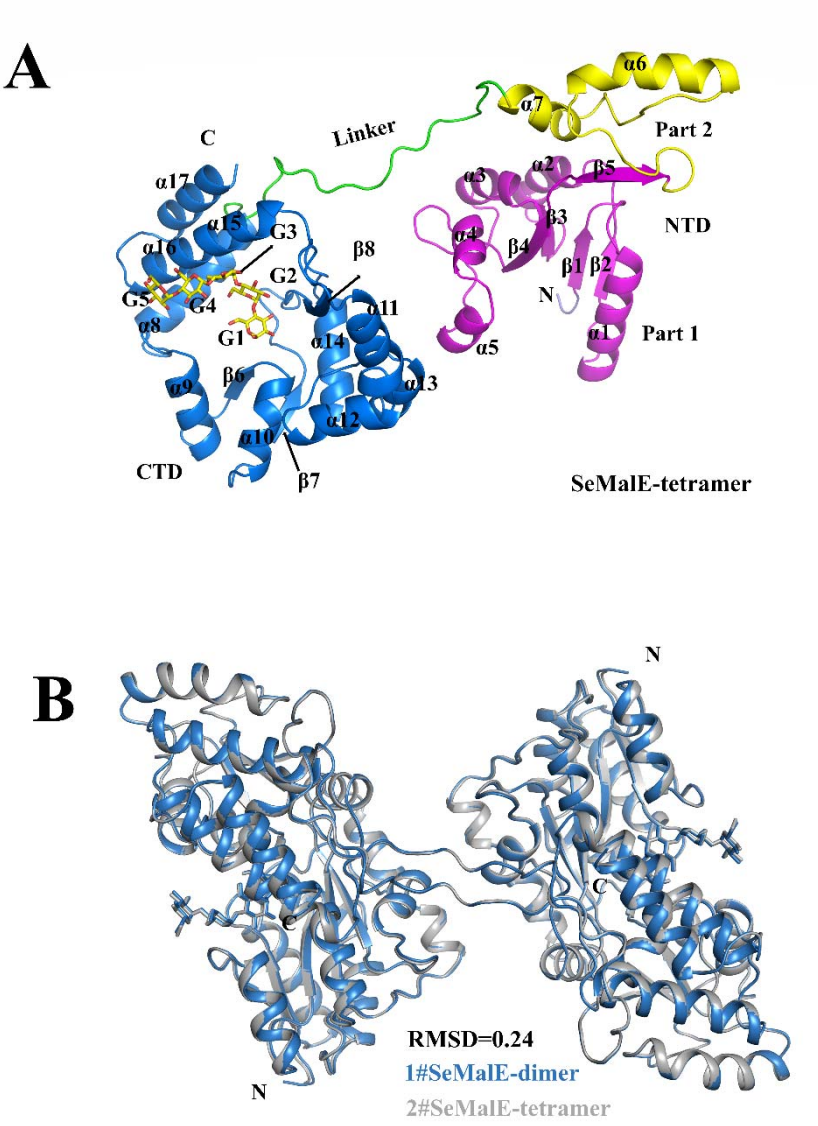


Figure S4 Overall folding of the SeMalE-tetramer molecule. (A) Overall folding of the SeMalE-tetramer molecule as viewed along the cartoon. The α-helices and β-strands are numbered, and the termini are labeled. Part 1 and part 2 of the NTD, linker, and CTD are colored magenta, yellow, green, and blue, respectively. The maltopentaose molecule is shown in the yellow stick model. (B) Comparison of the structures between the SeMalE-dimer and SeMalE-tetramer. The crystal structures of the SeMalE-dimer and SeMalE-tetramer are colored blue and gray.

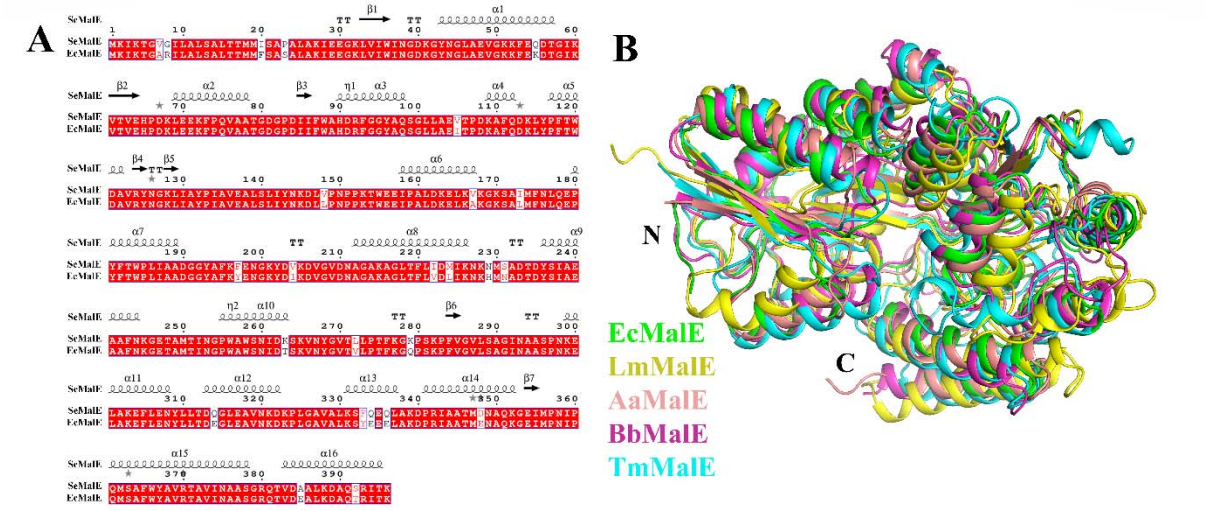


Figure S5 Structural and sequence analysis of SeMalE and its homologous proteins. (A) Sequence alignment of SeMalE and EcMalE. Conserved residues are shown as white letters on a red background, and similar residues are shown as red letters in blue boxes. The SeMalE secondary structure (PDB ID: 7FFW) is shown at the top of the panel. (B) Overall structural comparison of EcMalE, LmMalE, AaMalE, BbMalE and TmMalE, colored by green, yellow, pink, magenta, and cyan, respectively.

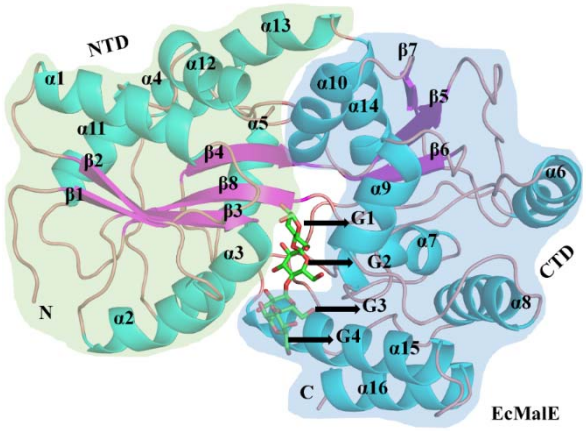
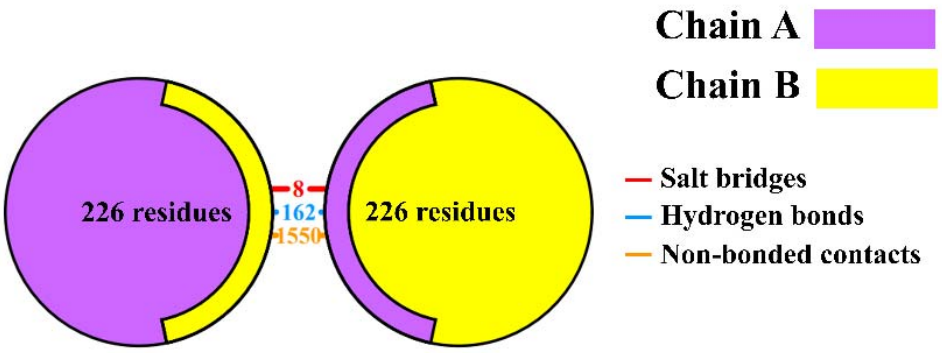


Figure S6 Overall folding of the EcMalE molecule (PDB ID: 4MBP) viewed along with the cartoon. The α-helices and β-strands are numbered, the termini are labeled, and the glucosyl rings of the substrates are numbered, and named G1, G2, G3, and G4, respectively.



Chain	No. of interface residues	interface area (Å²)	No. of salt bridges	No. of hydrogen bonds	No. of non-bonded contacts
A	226	11549	8	162	1550
B	226	11549	8	162	1550

Figure S7 Interaction between the two SeMalE molecules. The salt bridges, hydrogen bonds and nonbonded contacts between two SeMalE molecules are numbered and colored red, blue and orange, respectively.

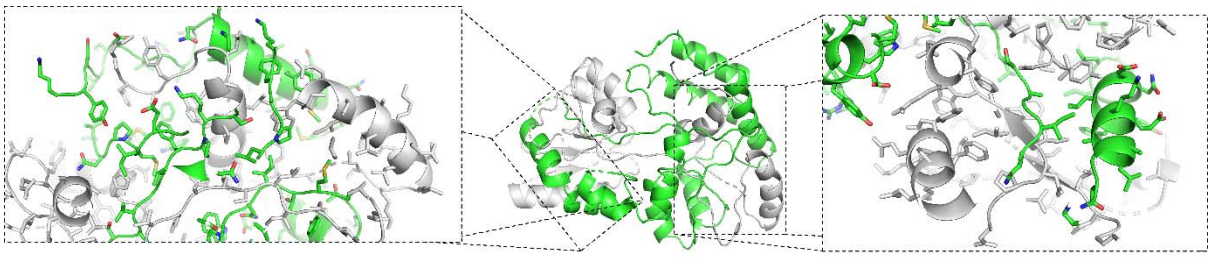


Figure S8 Highly intertwined SeMalE dimers. The A chain and B chain in SeMalE are colored green and gray, respectively.

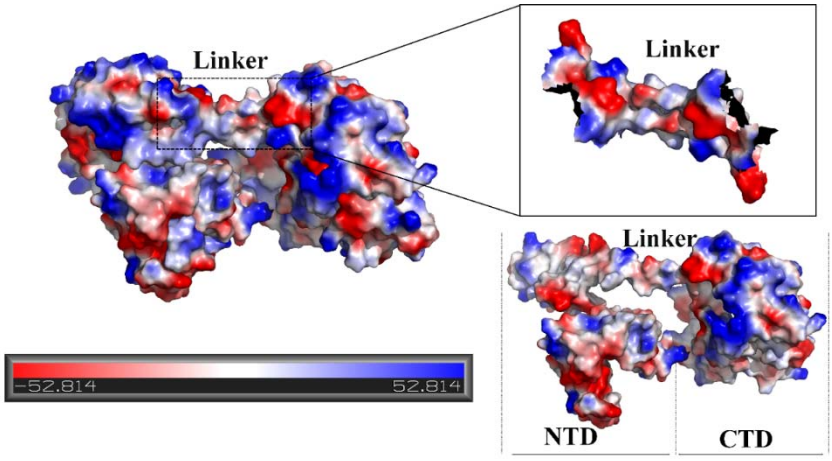


Figure S9 Charge complementarity analysis on the surface of domain-swapped SeMalE molecules. The charge complementarity analysis of the linkers of domain-swapped SeMalE molecules is shown in a black box on the upper right. The charge complementarity analysis of the monomer SeMalE molecule shown at the bottom right.

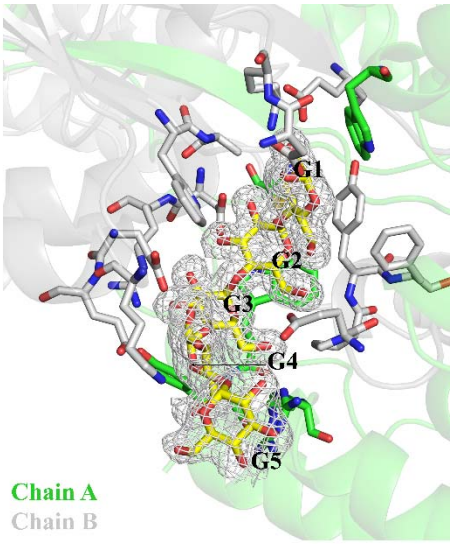


Figure S10 The electron density map of maltopentaose. The Fo-Fc electron density map of maltopentaose is shown as a gray mesh (contoured at 1.0 σ). The glucosyl rings of the substrates are numbered and named G1, G2, G3, G4, and G5.

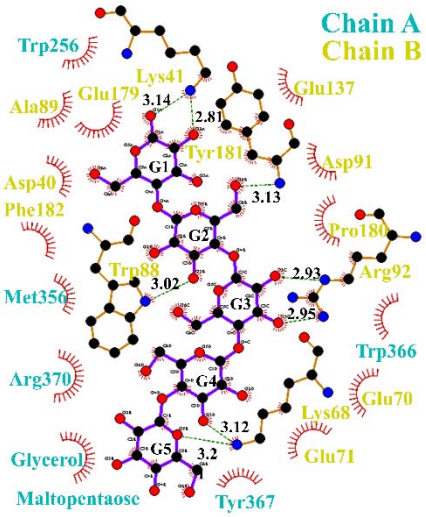


Figure S11 The maltopentaose molecule is recognized by SeMalE. Green dashed lines indicate hydrogen bonds or salt bridges. The residues from Chain A and Chain B were colored cyan and yellow.

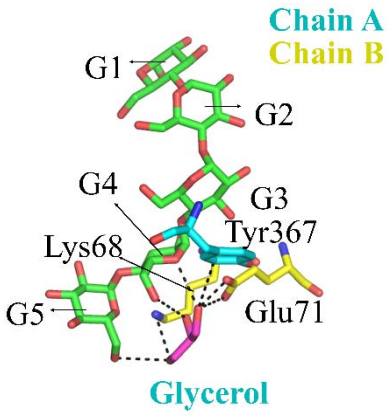


Figure S12 Interaction between the glycerol molecule and SeMalE. The glycerol molecule, maltopentaose molecule, residue from the A chain, and residues from the B chain are colored magenta, green, cyan, and yellow, respectively.

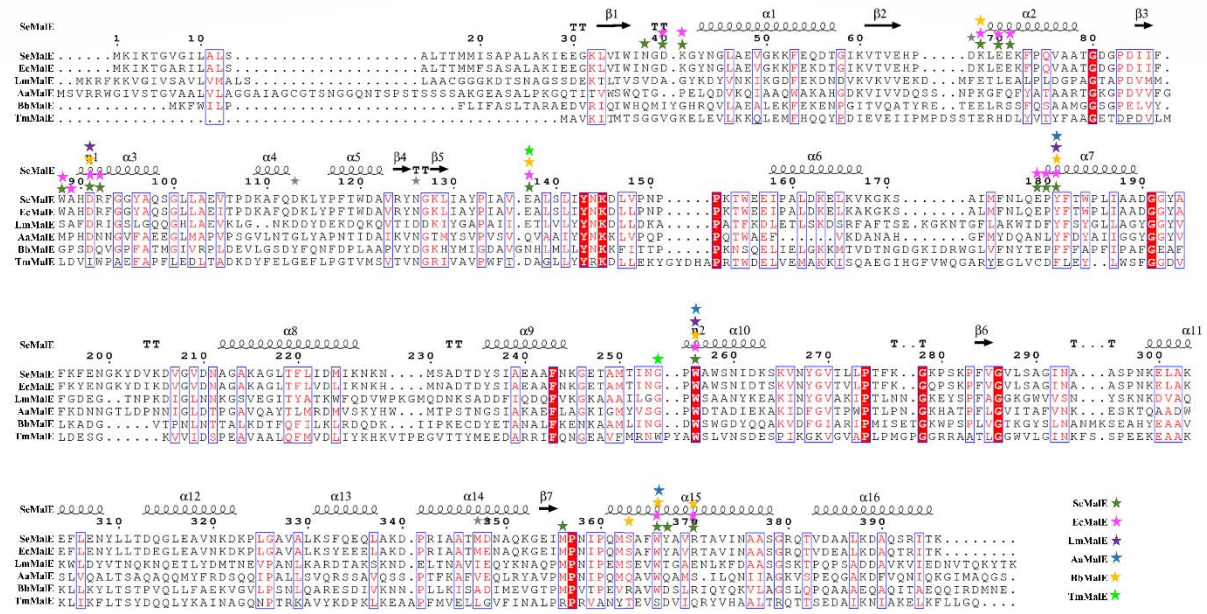


Figure S13 Sequence alignment of SeMalE and its homologous proteins. Homologous proteins including EcMalE (accession number: **4MBP_A**), LmMalE (**NP_465255**), AaMalE (**CAB65651**), BbMalE (**CAE79131**), and TmMalE (**6DTQ_A**). Conserved residues are shown as white letters on a red background, and similar residues are shown as red letters in blue boxes. The SeMalE secondary structure (PDB ID: 7FFW) is shown at the top of the panel. The residues responsible for substrate binding are marked with stars above the residues.

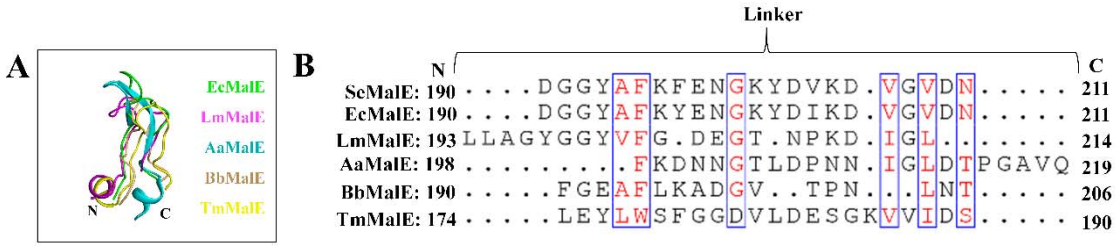


Figure S14 Structural and sequence analysis of the linkers from MalEs**.** (A) The overall structural comparison of linkers from MalEs. EcMalE, LmMalE, AaMalE, BbMalE and TmMalE are colored green, magenta, blue, brown, and yellow, respectively. (B) Sequence alignment of linkers from SeMalE and its homologous proteins. Homologous proteins included EcMalE (accession number: **4MBP_A**), LmMalE (**NP_465255**), aMalE (**CAB65651**), BbMalE (**CAE79131**), and TmMalE (**6DTQ_A**). Similar residues are shown as red letters in blue boxes.

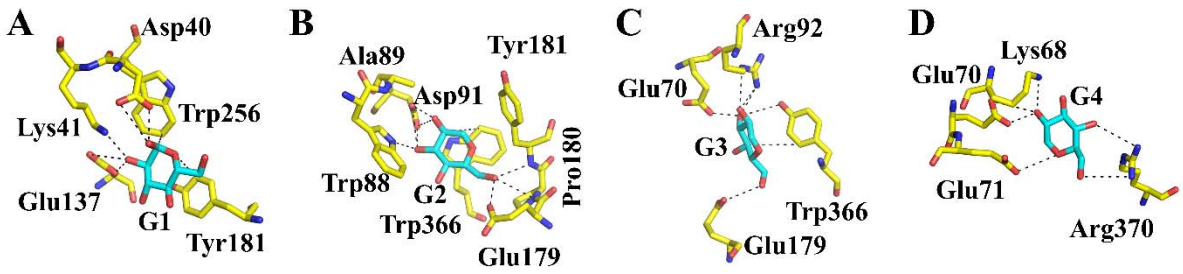


Figure S15 Substrate-binding sites of EcMalE. (A-D) Interaction between the glucose molecules (G1-G4) and amino acids of EcMalE. The dark dashed lines indicate hydrogen bonds or salt bridges between the glucose molecules and amino acids.