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[1]Both authors contributed equally to this work.

Supplementary Figures

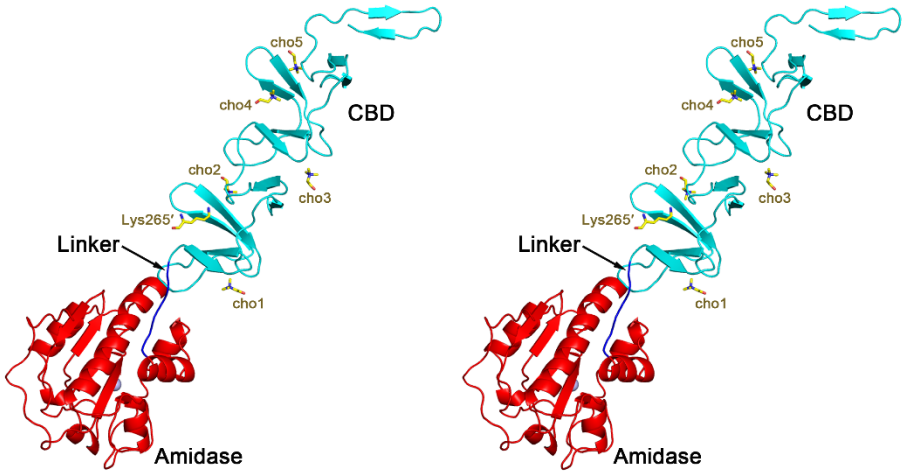

Figure S1. Stereo view of the full-length LytA. The N-terminal amidase domain, linker and C-terminal CBD are shown in red, blue and cyan, respectively. Five choline molecules and Lys265′ from the neighboring molecule are shown as yellow sticks.

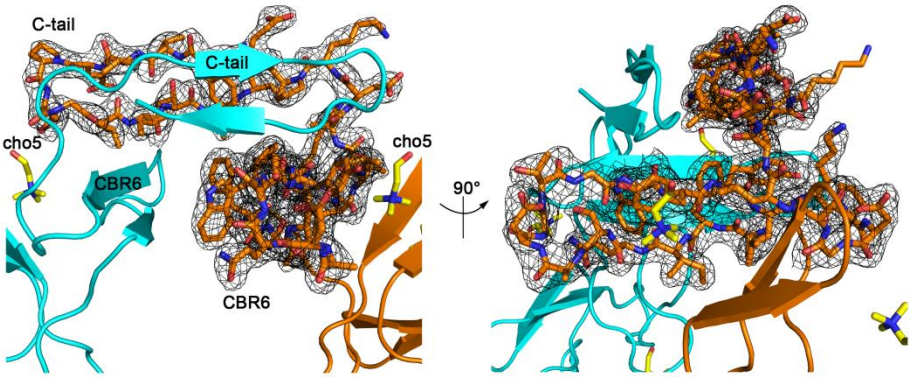

Figure S2. The electron density map of CBR6 and the C-terminal tail of one subunit at the dimeric interface. The omit electron density map (*2Fo-Fc*) is countered at 1.0 σ level. The two subunits are shown in cyan and orange, respectively.

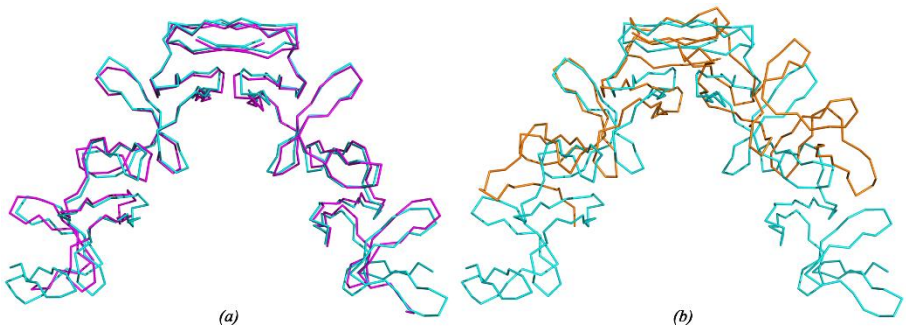

Figure S3. Structural superposition of LytA-CBD (cyan) against previously reported structures with PDB codes of (a) 1HCX (magenta) and (b) 1H8G (orange), respectively.

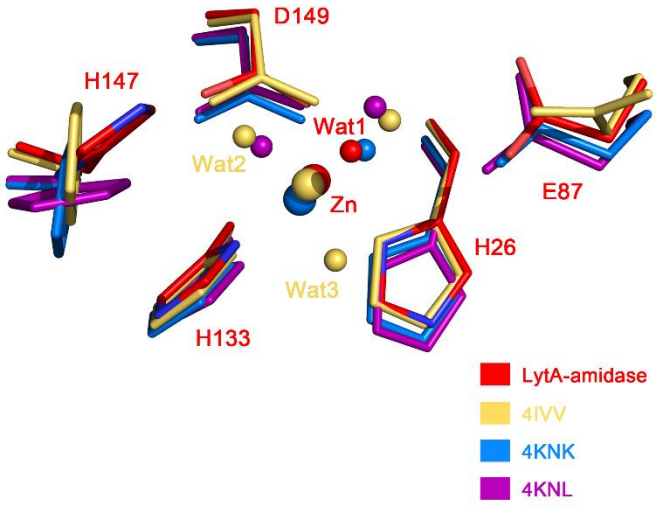

Figure S4. Comparison of the zinc coordination in different structures of amidase domains. The zinc coordinating residues and water molecules in our LytA-amidase, $LytA^{AMI}$ (PDB

code 4IVV), unliganded AmiA-cat (PDB code 4KNK), and liganded AmiA-cat (PDB code 4KNL) are shown in red, orange, blue and purple, respectively.

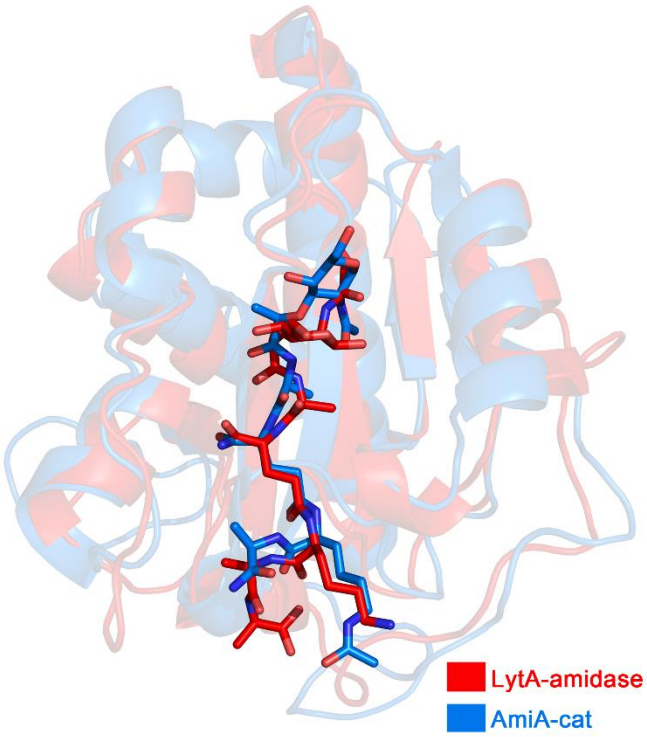

Figure S5. Superposition of the docked NAM-Pep5 in LytA active site against the substrate complexed to AmiA-cat (PDB code 4KNL). The substrates are shown as sticks, and colored in red and blue for LytA and AmiA-cat, respectively.

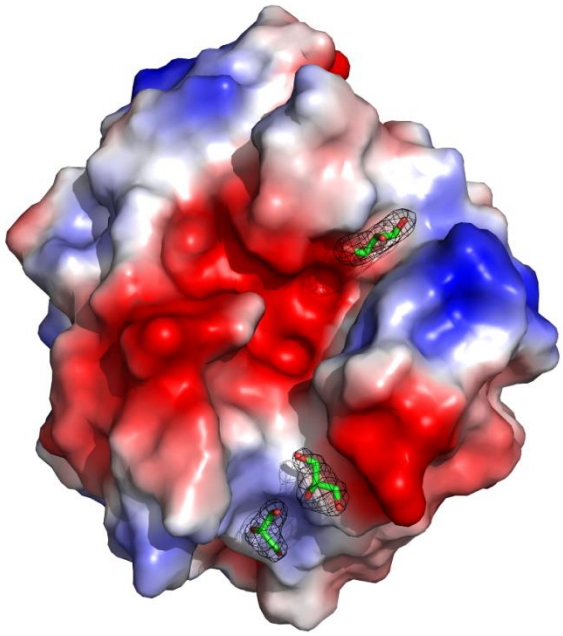

Figure S6. Three molecules of glycerol are found in the putative substrate-binding groove. The omit electron density map (*2Fo-Fc*) is countered at 1.0 σ level. The putative substrate-binding groove is displayed as an electrical potential diagram.

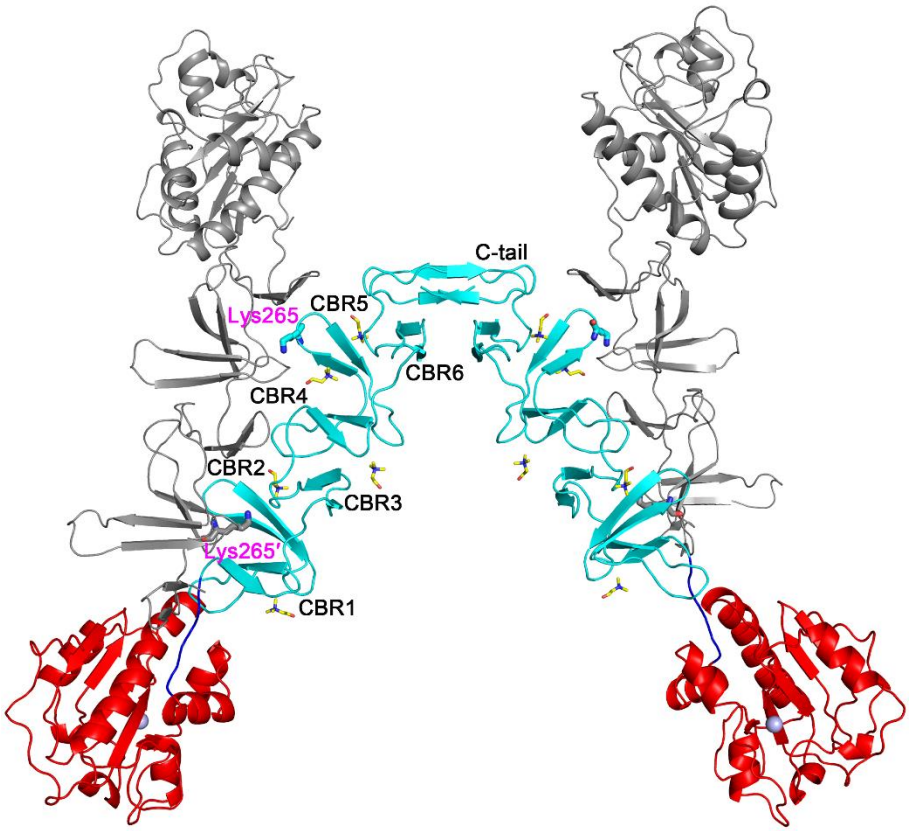

Figure S7. The CBS between CBR1 and CBR2 of each LytA subunit is occupied by Lys265′ (sticks) from neighboring molecules (gray) due to crystal packing.

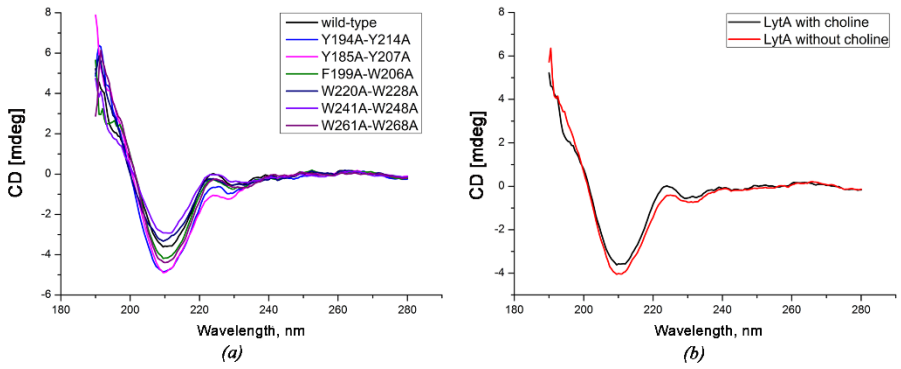

Figure S8. Circular dichroism spectra of (a) LytA CBS mutants and (b) LytA in the absence or in the presence of 10 mM choline.