Electronic Supplementary Material (ESI) for Molecular BioSystems

A single amino acid substitution affects the substrate specificity of the seryl-tRNA synthetase homologue

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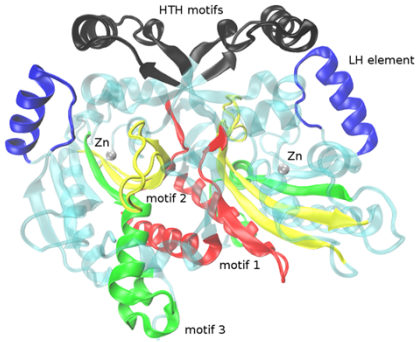

Fig. S1 Structure of Bj Gly:CP ligase 1. Class II signature motifs 1, 2 and 3 colored in red, yellow and green respectively, as well as loop-helix (LH) element colored in blue and helix-turn-helix (HTH) colored in black. Zn cations are shown in CPK representation as gray spheres.

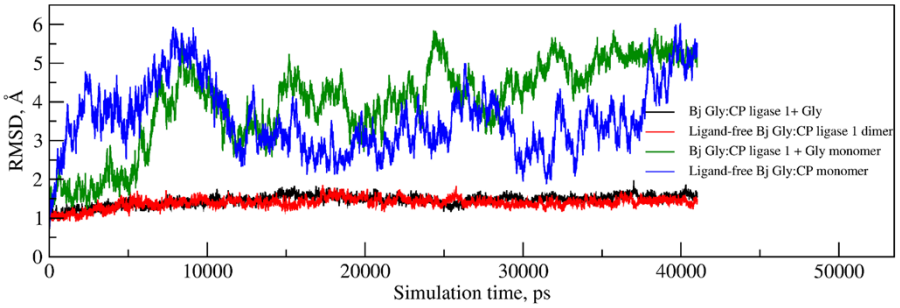

Fig. S2 The RMSD values for monomeric and dimeric Bj Gly:CP ligase 1, in ligand-free and substrates bound forms.

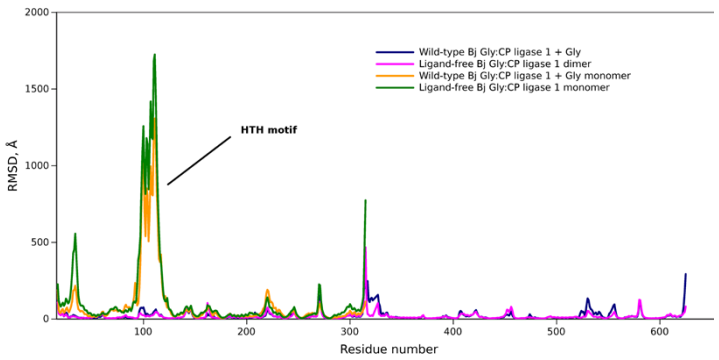

Fig. S3 B-factors calculated for monomeric (lines in green and orange) and dimeric (lines in blue and pink) enzyme, in ligand-free and substrates bound forms. Greatest differences are observed within the HTH motif comprising amino acid residues 94 to 121.

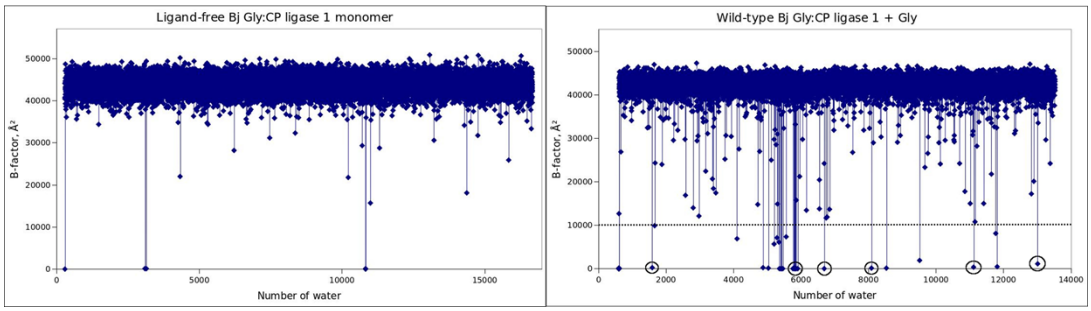

Fig. S4 B-factors calculated for water molecules for the Bj Gly:CP ligase 1 in monomeric (left) and dimeric (right) form. Black dotted line represents a threshold for analyzed structural waters. Rounded waters are placed at the dimerization interface.

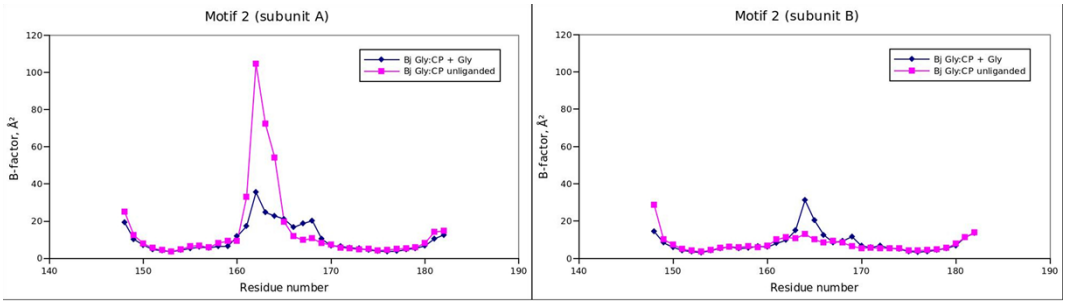

Fig. S5 B-factors calculated for amino acid residues of motif 2 in wild-type Bj Gly:CP ligase 1 with bound substrates (blue) and ligand-free Bj Gly:CP ligase 1 (pink).

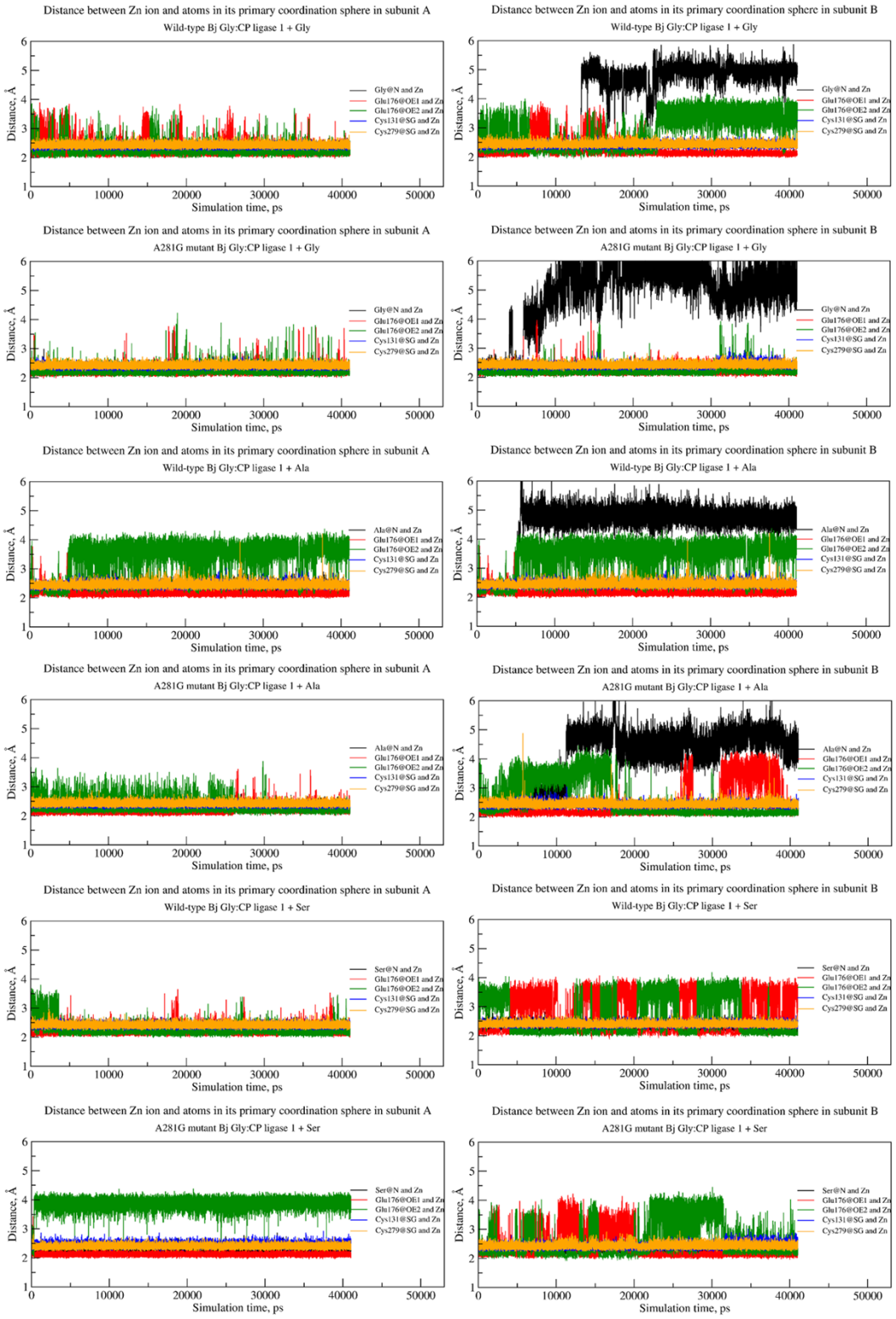

Fig. S6 Distance between zinc cation and atoms in its primary coordination sphere in the wild-type and A281G mutated Bj Gly:CP ligase 1 bound with both substrates, ATP and amino acids (Gly, Ala and Ser). Subunit A distances are shown on the left; subunit B distances are shown on the right.

Fig. S6 describes substrates (glycine, alanine and serine) positions in both active sites of the enzyme. In the subunit A, of all analysed structures, the amino acid substrates (Gly, Ala, Ser) were coordinated to the zinc ion during the whole simulations. In the subunit B of the wild-type enzyme, Gly was coordinated to Zn^{2+} during the first 12 ns of the simulation, while Ala remains coordinated to Zn^{2+} during the first 5 ns of the simulation. However, in subunit B of both, wt and mutated enzyme, Ser remains coordinated to Zn^{2+} during the whole simulation. In subunit B of the mutated (A281G) enzyme, glycine and alanine were coordinated to Zn^{2+} during the first 5 and 10 ns of the simulations, respectively.