

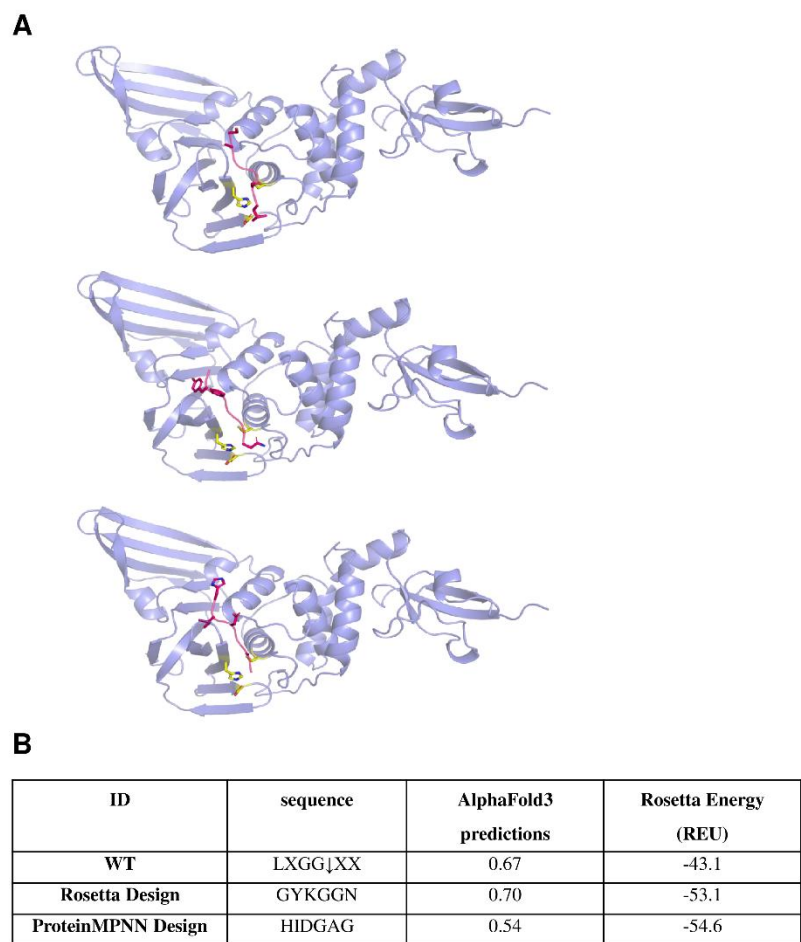


Figure S4. Structural models of PLpro (papain-like protease) and its peptide substrate. The catalytic triad was shown as yellow sticks. (A) WT peptide (shown as red linear strand, upper panel), Rosetta designed peptide (middle panel), ProteinMPNN designed peptide (lower panel). (B) The calculated binding capacity of PLpro peptide substrate.