Supplementary Figures

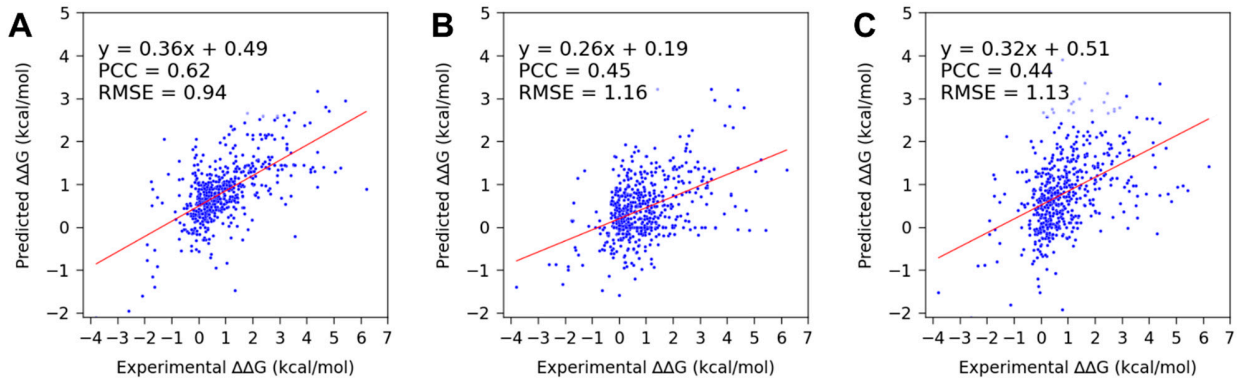


Figure S1. A plot of experimental vs. predicted binding free energy values and the fitted trend line for the complete (S596) protein mutation dataset. The predicted binding free energy was obtained using the following methods: (A) SAMPDI-3D, (B) mCSM-NA, and (C) PremPDI. The SAMPDI-3D and mCSM-NA predictions succeeded for all 596 data points in the dataset. However, PremPDI failed to predict the binding free energy change for twenty-three data points (approximately 4%).

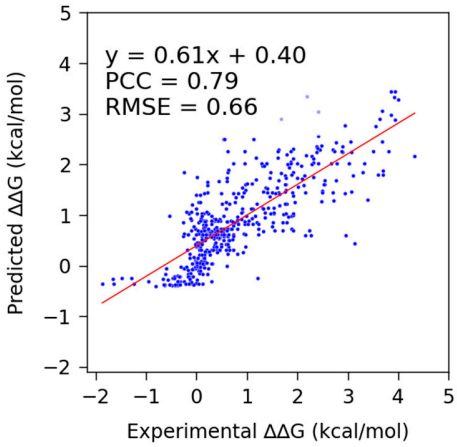


Figure S2. A plot of experimental vs. predicted binding free energy (using SAMPDI-3D) values and the fitted trend line for the complete (D502) DNA mutation dataset.