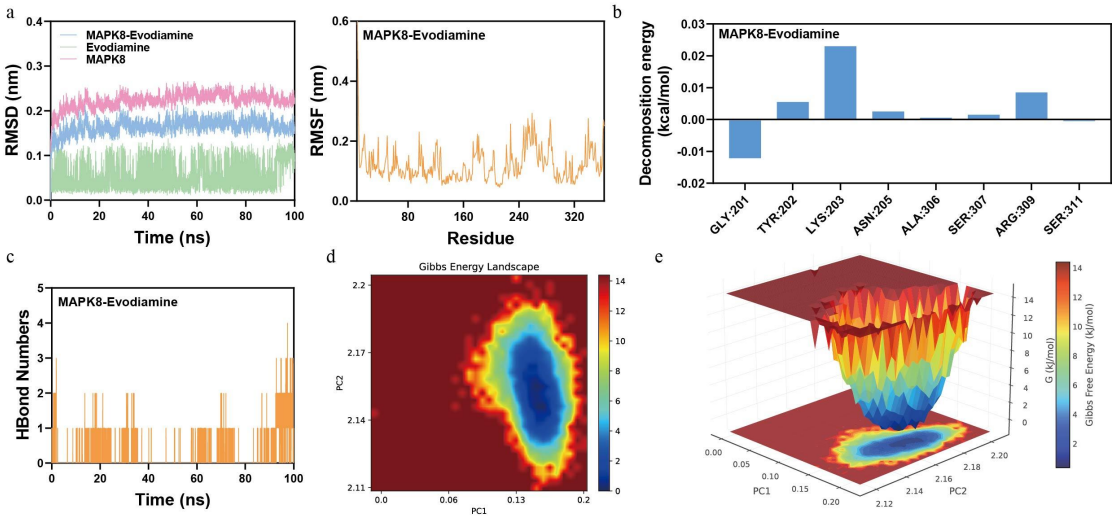


Supplementary Figure S5. Molecular dynamics simulation of the MAPK8-evodiamine complex over 100 ns.

(a) RMSD time series. (b) Per-residue binding free energy decomposition showing key binding residues. (c) Intermolecular hydrogen bond count profile. (d) Two-dimensional free energy landscape along PC1/PC2. (e) Three-dimensional FEL.