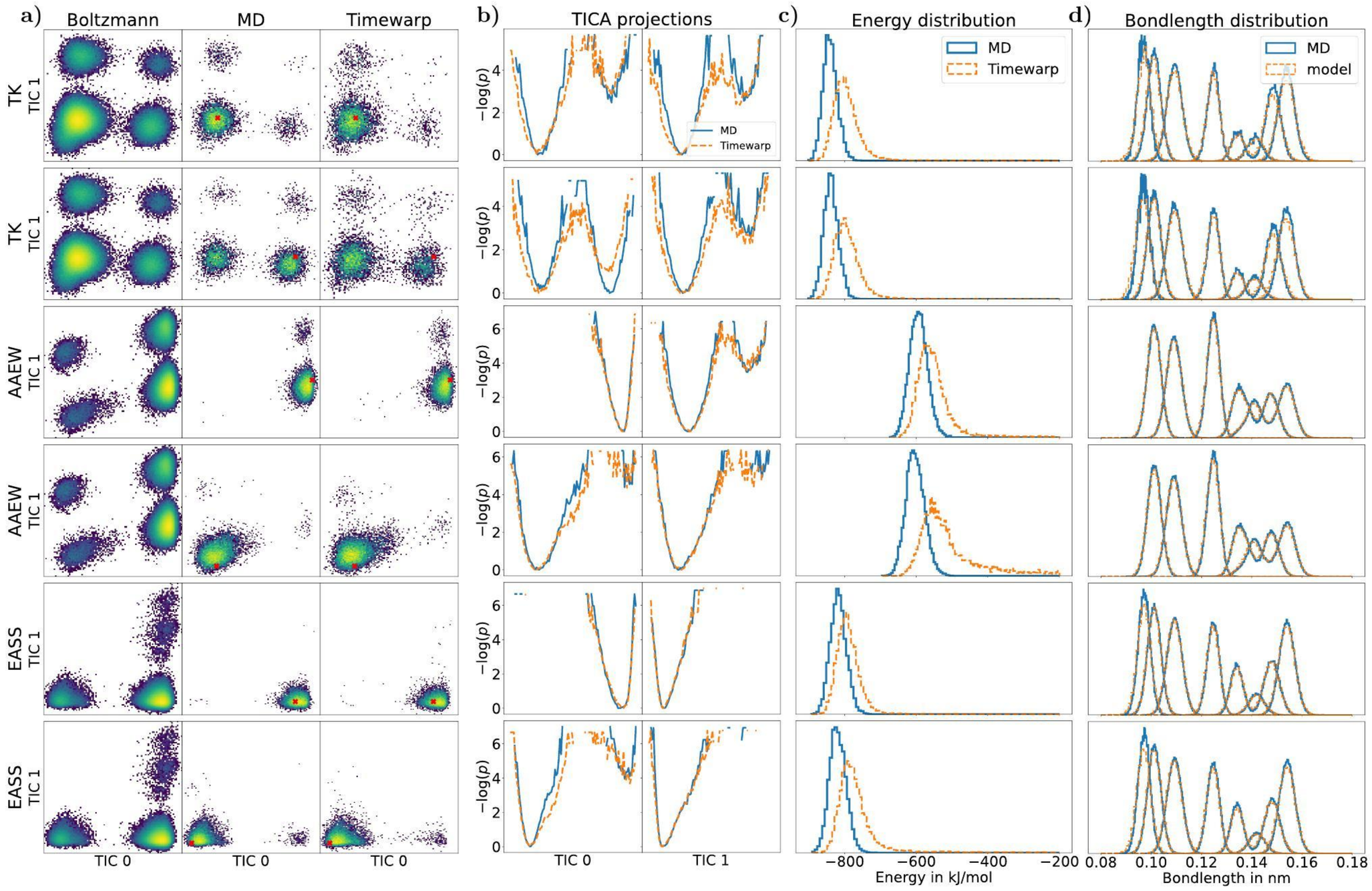

Figure 12. Comparing the conditional distribution of the Timewarp model $p_\theta(x(t+\tau)|x(t))$ with the conditional distribution generated with MD $\mu(x(t+\tau)|x(t))$. The rows correspond to the peptides TK, AAEW, EASS, respectively, where we show for each peptide two different conditioning states. (a) TICA plots. First column: samples from the Boltzmann distribution $\mu(x)$ generated with MD. Second column: samples from $\mu(x(t+\tau)|x(t))$ generated with MD. The conditioning state $x(t)$ is indicated with the red cross. Third column: samples from $p_\theta(x(t+\tau)|x(t))$ generated with the Timewarp conditional flow, without MH correction. The conditioning state $x(t)$ is indicated with the red cross. (b) Projection of the conditional distributions from (a) onto the first two TICA components. (c) Potential energy distributions of the conditional distributions. (d) Conditional bondlength distribution, which for these values of τ will be close to the equilibrium distribution. Each mode in the graph represents a different bond type, *e.g.*, C-H.