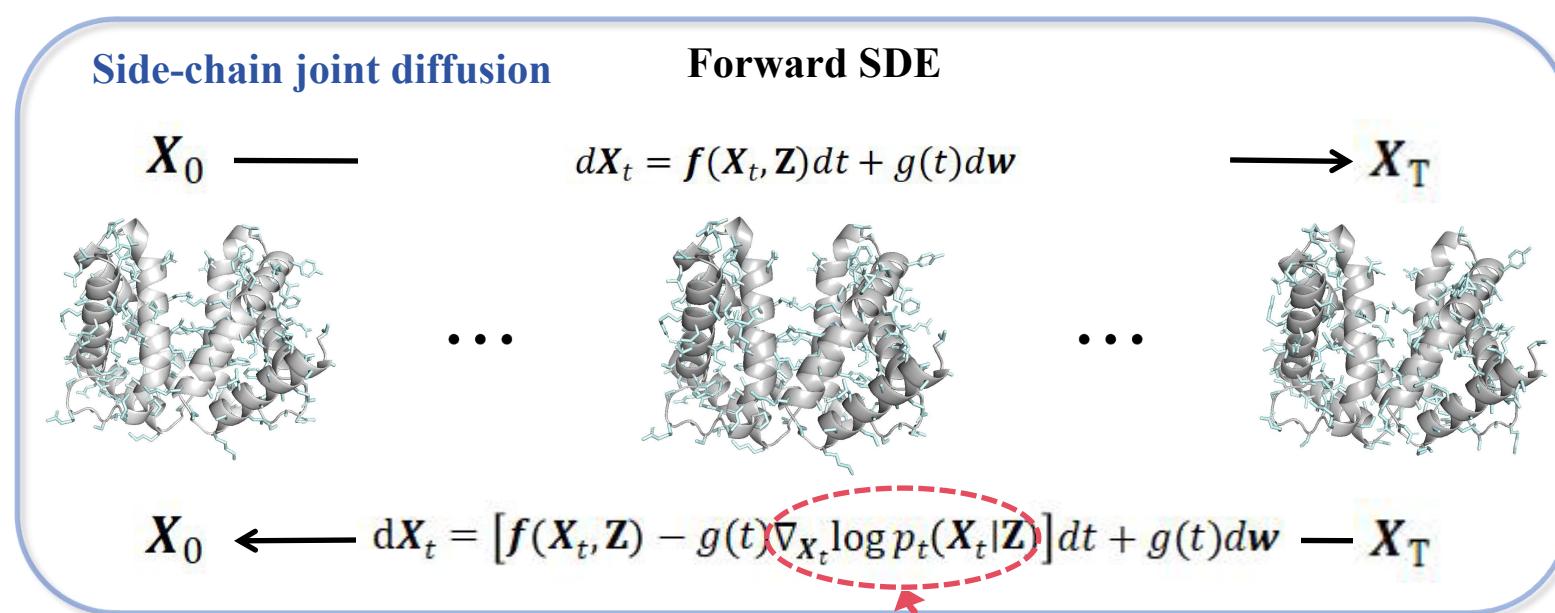
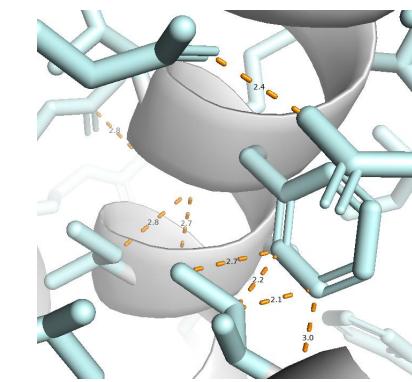
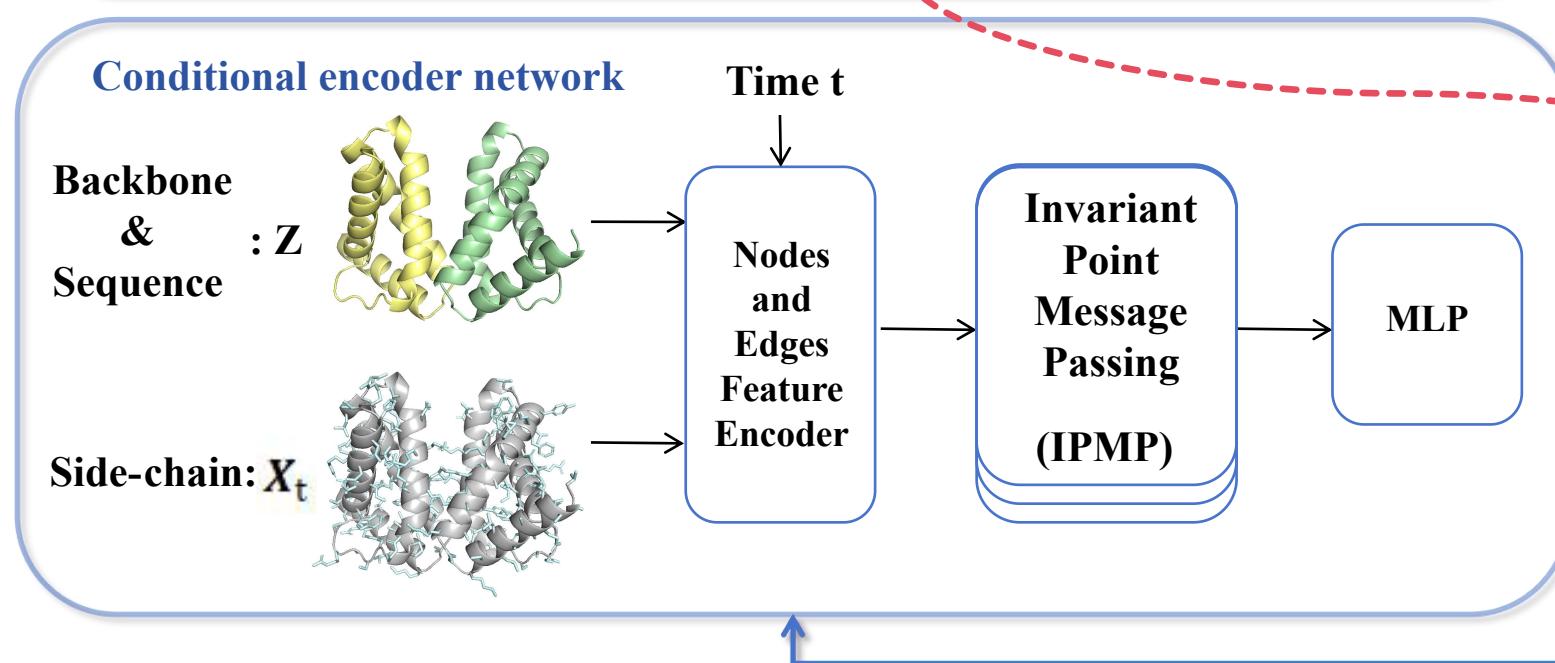


A**PakcPPI — Prox****PakcPPI — MSC**

Compute side-chain violations

Proximal optimization

$$\text{prox}_h(x) = \underset{\tilde{x}}{\operatorname{argmin}} \left\{ \lambda h(\tilde{x}) + \frac{1}{2} \|\tilde{x} - x\|^2 \right\}$$

**Score matching loss**

score function s_θ

noise score

$$\mathcal{L}_{\text{DSM}} = \mathbb{E} [\|s_\theta(x_t, z, t) - \nabla_{x_t} \log p_t(x_t|z)\|_2^2]$$

\mathcal{L}_{DSM}

B**PakcPPI — AP**