

Density [ $\text{g cm}^{-3}$ ]

$R^2$ : 0.930 [ 0.903, 0.953]  
MD: 0.036 [0.030, 0.041] kcal/mol  
RMSD: 0.056 [ 0.048, 0.064] kcal/mol

Experiment (ThermoML)

