

# Density [g cm<sup>-3</sup>]

R<sup>2</sup>: 0.977 [ 0.970, 0.983]  
MD: 0.011 [0.008, 0.014] kcal/mol  
RMSD: 0.024 [ 0.022, 0.026] kcal/mol

Experiment (ThermoML)

