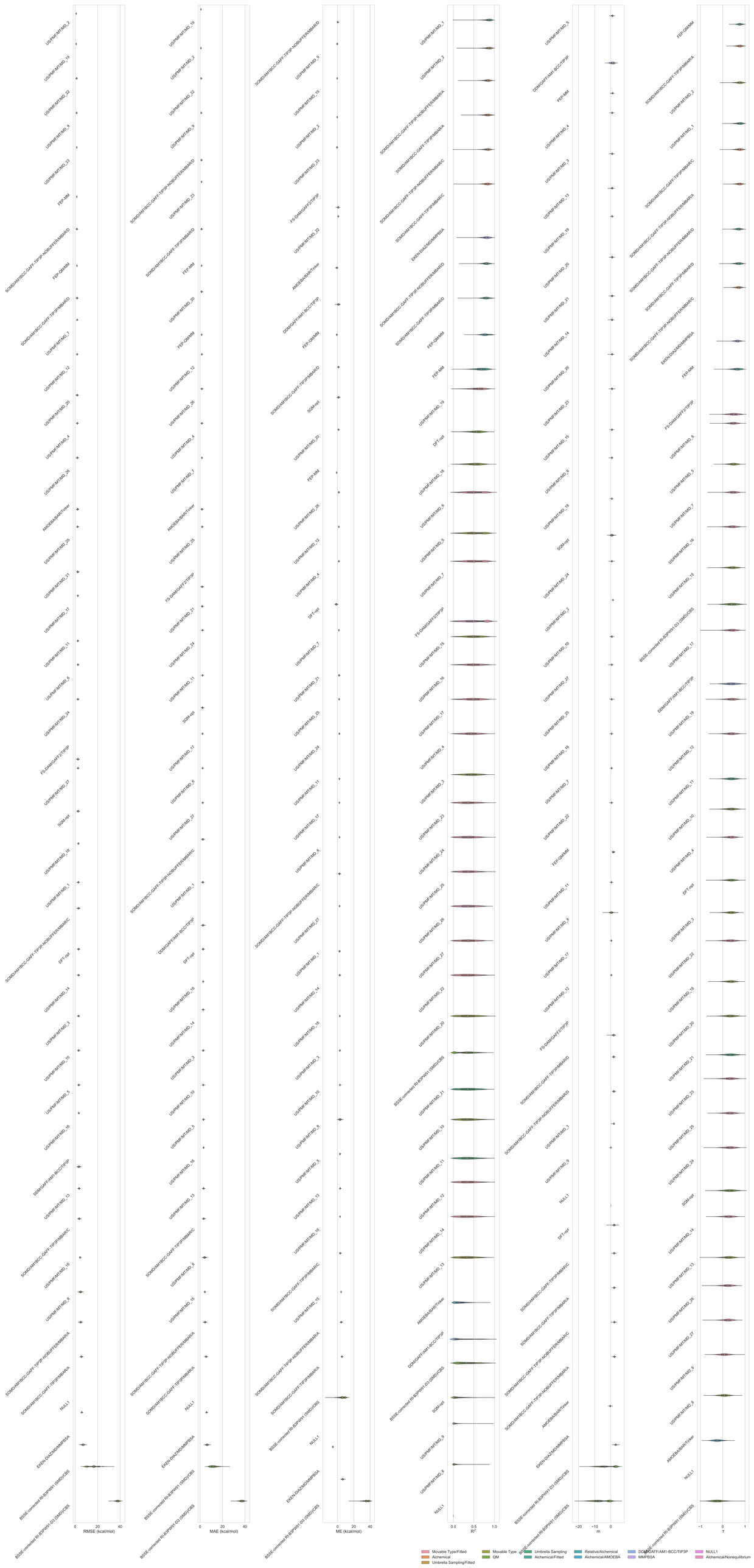
RMSE (kcal/mol)
MAE (kcal/mol)
ME (kcal/mol)
R²
m
τ
Movable Type/Fitted
Alchemical
Umbrella Sampling/Fitted
Movable Type
QM
Umbrella Sampling
Alchemical/Fitted
Relative/Alchemical
Alchemical/AMOEBA
DDM/GAFF/AM1-BCC/TIP3P
MMPBSA
NULL1
Alchemical/Nonequilibrium