l: 1 | mp: 2 | feat.: 128 params: 1.12e+05 | Test (n=800) Ε D 80 4.17/3.20 [kcal/mol] $1 - r^2$: 2.214E-04 0.62/0.31 [kcal/mol] $1 - r^2$: 4.374E-03 0.08/0.06 [eÅ] 60 -2000 $1 - r^2$: 6.974E-03 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -40-2600-2-6050 -2600-2400-2200-2000 -500 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 379.02/264.02 [kcal/mol] $1 - r^2$: 6.752E-03 6.62/2.90 [kcal/mol] $1 - r^2$: 1.005E+00 0.01/0.01 [e] 60 0.04 40 pred. [kcal/mol] pred. [kcal/mol] -50020 pred. [e] 0.02 -1000-1500-200.00 -40-2000-60 -0.02-250050 0.02 -2000-1000 0 -500 -0.020.00 0.04 ref. [kcal/mol] ref. [kcal/mol] ref. [e]