l: 2 | mp: 2 | feat.: 32 params: 1.31e+04 | Test (n=800) Ε D 80 2 7.60/5.36 [kcal/mol] $1 - r^2$: 6.717E-04 0.85/0.47 [kcal/mol] $1 - r^2$: 8.381E-03 0.11/0.09 [eÅ] 60 -2000 $1 - r^2$: 1.304E-02 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200pred. [*eÅ*] 20 0 0 -2400-20 -40-2600-2-60-280050 -2800-2600-2400-2200-2000 -500 1 0 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 0.01 380.64/265.40 [kcal/mol] $1 - r^2$: 6.660E-03 6.65/2.96 [kcal/mol] $1 - r^2$: 9.938E-01 0.01/0.01 [e] 60 0.00 40 pred. [kcal/mol] pred. [kcal/mol] -50020 pred. [e] -0.01-1000-0.02-1500-20-40-0.03-2000 -60 -2500-0.040 50 -0.02-2000-1000 0 -50-0.040.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]