l: 1 | mp: 4 | feat.: 32 params: 2.09e+04 | Test (n=800) Ε D 80 2 0.73/0.41 [kcal/mol] $1 - r^2$: 6.170E-03 5.78/4.31 [kcal/mol] 0.05/0.04 [eÅ] 60 $1 - r^2$: 4.108E-04 -2000 $1 - r^2$: 2.712E-03 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600-2-6050 -2600-2400-2200-2000 -50**-**2 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 0.0125 378.55/263.51 [kcal/mol] $1 - r^2$: 7.082E-03 0.**0**1/0.01 [*e*] 6.63/2.92 [kcal/mol] 60 $1 - r^2$: 1.000E+00 0.0100 bred -200 -1000 -1500 40 pred. [kcal/mol] 0.0075 20 pred. [e] 0.0050 0.0025 -200.0000 -40 -2000 -0.0025-60 -2500-0.0050-2000-10000 -500 50 -0.0050.000 0.005 0.010 ref. [kcal/mol] ref. [kcal/mol] ref. [e]