l: 1 | mp: 4 | feat.: 64 params: 7.04e+04 | Test (n=800) Ε D 80 2 4.42/3.35 [kcal/mol] $1 - r^2$: 2.483E-04 0.63/0.28 [kcal/mol] $1 - r^2$: 4.571E-03 0.08/0.06 [eÅ] 60 $1 - r^2$: 6.274E-03 -2000bred. [kcal/mol] -2500 -2400 40 1 ored. [kcal/mol] pred. [*eÅ*] 20 0 0 -20 -40 -2600 -2-6050 -2600-2400-2200-2000 -502 0 1 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 0.03 $0 = 378.43/263.35 \text{ [kcal/mol]} \\ 1 = r^2: 7.058E-03$ 6.62/2.88 [kcal/mol] 0.01/0.01 [e] 60 $1 - r^2$: 1.009E+00 0.02 bred -200 -1000 -1500 40 pred. [kcal/mol] 20 pred. [e] 0.01 0.00 -20-0.01-40-2000 -0.02-60 -250050 -2000-10000 -500 -0.020.00 0.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]