l: 0 | mp: 4 | feat.: 64 params: 3.94e+04 | Test (n=800) Ε D 80 2 6.51/4.08 [kcal/mol] $1 - r^2$: 5.421E-04 0.87/0.47 [kcal/mol] $1 - r^2$: 8.834E-03 0.06/0.05 [eÅ] 60 -2000 $1 - r^2$: 3.834E-03 40 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600-2-60 -280050 -2800-2600-2400-2200-2000 -50 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 0.010 $0 = 377.80/262.68 \text{ [kcal/mol]} \\ 1 = r^2: 6.835E-03$ 6.61/2.94 [kcal/mol] $1 - r^2$: 1.001E+00 0.01/0.01 [e]; 60 0.005 bred -200 -1000 -1500 40 pred. [kcal/mol] 20 0.000 -0.005-20-0.010-40-2000-0.015-60 -2500 -1000 0 50 -20000 -50 -0.010.00 0.01 ref. [kcal/mol] ref. [kcal/mol] ref. [e]