l: 2 | mp: 4 | feat.: 64 params: 1.03e+05 | Test (n=800) Ε D 80 6.07/4.11 [kcal/mol] $1 - r^2$: 3.242E-04 0.55/0.29 [kcal/mol] $1 - r^2$: 3.490E-03 0.07/0.05 [eÅ] 60 $1 - r^2$: 4.807E-03 -20001 40 ored. [kcal/mol] pred. [*eÅ*] 20 0 0 -20 -1-40-2600-2-6050 -2600-2400-2200-2000 -500 **-**2 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 $0 = 377.40/262.63 \text{ [kcal/mol]} \\ 1 = r^2: 6.974E-03$ 6.61/2.89 [kcal/mol] $1 - r^2$: 9.992E-01 0.00 0.01/0.01 [e] 60 bred -200 -1000 -1500 40 pred. [kcal/mol] -0.0120 pred. [e] -0.02-20-40-2000-0.03-60 -2500-1000 0 50 -0.03 -0.02 -0.01-20000 -50 0.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]