l: 2 | mp: 4 | feat.: 128 params: 3.70e+05 | Test (n=800) Ε D 80 2 8.43/6.58 [kcal/mol] $1 - r^2$: 2.346E-04 0.71/0.37 [kcal/mol] $1 - r^2$: 5.771E-03 0.05/0.04 [eÅ] 60 $1 - r^2$: 2.440E-03 -200040 1 pred. [kcal/mol] pred. [kcal/mol] pred. [*eÅ*] 20 -2200 0 0 -2400-20 -1-40-2600-2-6050 -2600-2400-2200-2000 -50 0 1 0 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 377.12/262.36 [kcal/mol] $1 - r^2$: 6.941E-03 6.64/2.93 [kcal/mol] 0.01/0.00 [e] 60 $1 - r^2$: 1.002E+00 0.01 bred -200 -1000 -1500 40 pred. [kcal/mol] 20 pred. [e] 0.00 -20-0.01-40-2000-60 -0.02-2500 -1000 50 -2000 0 -500 -0.02 -0.010.00 0.01 ref. [kcal/mol] ref. [kcal/mol] ref. [e]