l: 1 | mp: 2 | feat.: 32 params: 9.49e+03 | Test (n=800) Ε D 80 17.53/12.17 [kcal/mol] $1 - r^2$: 3.547E-03 1.08/0.60 [kcal/mol] $1 - r^2$: 1.345E-02 0.09/0.06 [eÅ] 60 -2000 $1 - r^2$: 7.702E-03 40 1 ored. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -2600 -40-60 -280050 -2750 -2500 -2250 -2000 -50 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 0.03 80 380.68/265.20 [kcal/mol] $1 - r^2$: 6.773E-03 6.67/2.99 [kcal/mol] $1 - r^2$: 9.972E-01 0.01/0.01 [] 60 0.02 40 ored. [kcal/mol] pred. [kcal/mol] -5000.01 20 pred. [*e*] 0.00 -1000 -0.01-1500-20-0.02-2000-40-0.03-60 -25000 50 0.00 -2000-1000 0 -50-0.020.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]