l: 0 | mp: 2 | feat.: 32 params: 5.97e+03 | Test (n=800) Ε D 80 17.92/13.17 [kcal/mol] $1 - r^2$: 4.113E-03 1.66/0.91 [kcal/mol] $1 - r^2$: 3.237E-02 0.12/0.09 [eÅ] 60 -2000 $1 - r^2$: 1.504E-02 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200pred. [*eÅ*] 20 0 0 -2400 -20 -2600 -40-2-60 -2800 50 -2750 -2500 -2250 -2000 -50 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 397.46/279.80 [kcal/mol] $1 - r^2$: 5.963E-03 6.64/3.06 [kcal/mol] 0.02 0.01/0.01 [e] · 60 $1 - r^2$: 9.981E-01 0.01 40 bred. [kcal/mol] -1000 -1500 pred. [kcal/mol] 0.00 20 pred. [e] -0.01-0.02-20-0.03-2000-40-0.04-60 -2500-100050 0.00 -20000 -50 0 -0.04-0.020.02 ref. [kcal/mol] ref. [kcal/mol] ref. [e]