l: 0 | mp: 2 | feat.: 64 params: 2.01e+04 | Test (n=800) Ε D 75 -8.47/6.21 [kcal/mol] $1 - r^2$: 9.222E-04 1.17/0.63 [kcal/mol] $1 - r^2$: 1.593E-02 0.11/0.08 [eÅ] -2000 $1 - r^2$: 1.243E-02 50 1 pred. [kcal/mol] pred. [kcal/mol] 25 -2200 pred. [*eÅ*] 0 0 -2400-1-25 -2600 -50**-**2 -2800**-**75 50 -2800-2600-2400-2200-2000 -50 **-**2 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 75 · 389.71/273.15 [kcal/mol] $1 - r^2$: 6.191E-03 0.04 6.64/2.99 [kcal/mol] 0.01/0**,**01 [e] $1 - r^2$: 9.965E-01 50 ored. [kcal/mol] 0.02 25 pred. [*e*] 0.00 -25-2000-50 -0.02-2500-75-100050 0.02 0.04 -20000 -500 -0.020.00 ref. [e] ref. [kcal/mol] ref. [kcal/mol]