l: 0 | mp: 5 | feat.: 64 params: 7.38e+04 | Test (n=2000) Ε D 0.8 -550 2.39/2.28 [kcal/mol] $1 - r^2$: 2.809E-05 0.93/0.37 [kcal/mol] $1 - r^2$: 1.914E-04 0.02/0.02 [eÅ] 750 0.6 $1 - r^2$: 3.175E-03 -600 -600 -650 -750 -750 500 0.4 ored. [kcal/mol] pred. [*eÅ*] 0.2 250 0.0 0 -0.2-250-0.4-800 -500-0.6-850 -750 -600 500 0.0 0.5 -800 -700 -500-0.50 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 0.3 34.18/28.94 [kcal/mol] $1 - r^2$: 1.798E-01 750 46.85/31.63 [kcal/mol] 0.02/0.02 [e] 200 $1 - r^2$: 9.953E-01 500 150 pred. [kcal/mol] pred. [kcal/mol] 0.2 250 pred. [e] 100 0.1 0 50 -250 0 -0.0 -500-50-750100 -500 500 0.1 0.2 0.3 0 200 0 0.0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]