l: 0 | mp: 4 | feat.: 128 params: 2.17e+05 | Test (n=2000) Ε D 0.8 -550 2.51/2.35 [kcal/mol] $1 - r^2$: 4.328E-05 2.01/0.27 [kcal/mol] $1 - r^2$: 9.104E-040.02/0.01 [eÅ] 750 0.6 $1 - r^2$: 1.728E-03 -600 pred. [Kcal/mol] -200 -220 -220 500 0.4 pred. [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 0.15 750 48.97/42.29 [kcal/mol] 46.79/31.66 [kcal/mol] 0.02/0.01 [e] 200 $1 - r^2$: 9.691E-01 $1 - r^2$: 1.798E-01 0.10 500 150 pred. [kcal/mol] ored. [kcal/mol] 0.05 100 250 pred. [e] 50 0.00 0 -0.050 -250 -50 -0.10-500-100-0.15-750 500 0.0 0.1 -1000 100 200 -5000 -0.1ref. [kcal/mol] ref. [kcal/mol] ref. [e]