l: 0 | mp: 2 | feat.: 32 params: 5.97e+03 | Test (n=800) Ε D 80 2 -22.33/17.03 [kcal/mol] $1 - r^2$: 6.398E-03 1.72/0.97 [kcal/mol] $1 - r^2$: 3.488E-02 0.18/0.14 [eÅ] 60 -2000 · $1 - r^2$: 3.252E-0 [kcal/mol -2400 -2400 -2600 -2600 40 pred. [kcal/mol] 20 pred. [eÅ] 0 0 -20 -40 -60-280050 -2750 -2500 -2250 -2000 -50 -10 ref. [kcal/mol] ref. [*e*Å] ref. [kcal/mol] E vs $E_{\rm ele}$ F Q 0.00 $0 = 395.46/278.46 \text{ [kcal/mol]} \\ 1 - r^2 : 6.068E-03$ 6.66/3.10 [kcal/mol] 0.02/0.02 [e] 60 -0.01 $1 - r^2$: 1.004E+00 40 pred. [kcal/mol] -0.0220 -0.03 -0.04-20 -0.05-40 -2000-0.06-60-2500-100050 -0.02-20000 -500 -0.06-0.040.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]