l: 2 | mp: 4 | feat.: 128 params: 3.70e+05 | Test (n=800) Ε D 80 2 5.67/3.36 [kcal/mol] $1 - r^2$: 1.922E-04 0.53/0.27 [kcal/mol] $1 - r^2$: 3.228E-03 0.12/0.09 [eÅ] 60 $1 - r^2$: 1.395E-02 -200040 1 pred. [kcal/mol] pred. [kcal/mol] -2200pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600**-**2 -60 -280050 -2800-2600-2400-2200-2000 -50 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 0.04 377.04/262.35 [kcal/mol] $1 - r^2$: 6.923E-03 6.57/2.86 [kcal/mol] 0.01/0.01 [e] 60 $1 - r^2$: 1.003E+00 0.03 kcal/mol -1000 -1500 40 pred. [kcal/mol] pred. [*e*] 0.02 20 0.01 -20 0.00 -40-2000-0.01-60 -2500-100050 0.02 0.04 -20000 -500 0.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]