l: 1 | mp: 4 | feat.: 128 params: 2.56e+05 | Test (n=800) Ε D 80 3.17/2.41 [kcal/mol] $1 - r^2$: 1.110E-040.54/0.26 [kcal/mol] $1 - r^2$: 3.346E-03 0.04/0.03 [eÅ] 60 $1 - r^2$: 1.623E-03 -2000bred. [kcal/mol] -2500 -2400 1 40 pred. [kcal/mol] 20 pred. [*eÅ*] 0 0 **-**20 -1-40-2600**-**2 -60 50 -2600-2400-2200-2000 -50 **-**2 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 377.58/262.82 [kcal/mol] $1 - r^2$: 6.981E-03 6.60/2.87 [kcal/mol] 0.01/0.00 [e] 0.00 60 $1 - r^2$: 1.005E+00 bred -200 -1000 -1500 40 pred. [kcal/mol] -0.0220 pred. [*e*] -0.04-20-0.06-40-2000-0.08-60 -2500 -1000 Ó 50 -0.075 - 0.050 - 0.025 0.000-20000 -50 ref. [kcal/mol] ref. [kcal/mol] ref. [e]