l: 1 | mp: 4 | feat.: 32 params: 2.09e+04 | Test (n=800) Ε D 80 10.03/7.85 [kcal/mol] $1 - r^2$: 1.227E-03 0.94/0.46 [kcal/mol] 0.06/0.05 [eÅ] 60 $1 - r^2$: 1.026E-02 -2000 $1 - r^2$: 3.341E-03 40 1 ored. [kcal/mol] pred. [kcal/mol] -2200pred. [*eÅ*] 20 0 0 -2400-20 -40-2600-2-60-280050 -2800-2600-2400-2200-2000 -50 **-**2 0 0 1 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} Q 80 $0 = 378.72/263.71 \text{ [kcal/mol]} \\ 1 = r^2: 6.996E-03$ 6.54/2.89 [kcal/mol] 0.01/0.01 [e] 60 $1 - r^2$: 1.002E+00 0.05 40 ored. [kcal/mol] pred. [kcal/mol] -50020 pred. [e] 0.00 -1000-1500-20-0.05-40-2000-60 -0.10-25000 50 -2000-10000 -50 -0.10 -0.050.00 0.05 ref. [kcal/mol] ref. [kcal/mol] ref. [e]