l: 1 | mp: 5 | feat.: 64 params: 1.35e+05 | Test (n=2000) Ε D 0.8 -550 1.72/1.62 [kcal/mol] $1 - r^2$: 5.194E-05 0.61/0.25 [kcal/mol] 0.02/0.01 [eÅ] 750 0.6 $1 - r^2$: 8.350E-05 $1 - r^2$: 2.573E-03 -600 -600 -650 -750 -750 500 0.4 ored. [kcal/mol] pred. [*eÅ*] 250 0.2 0.0 0 -0.2 -250-0.4-800 -500-0.6-850 -750500 0.0 0.5 -800 -700-600 -500-0.50 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 43.12/36.96 [kcal/mol] 46.93/31.65 [kcal/mol] 0.02/0.01 [e] 750 200 $1 - r^2$: 1.843E-01 $1 - r^2$: 9.926E-01 0.10 150 500 pred. [kcal/mol] pred. [kcal/mol] 100 pred. [e] 250 0.05 50 0 0.00 0 -250 -50-500-0.05-100**-750** 100 -100200 -5000 500 -0.050.00 0.05 0.10 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*]