l: 1 | mp: 4 | feat.: 64 params: 1.06e+05 | Test (n=2000) Ε D 0.8 2.26/2.03 [kcal/mol] $1 - r^2$: 1.323E-041.83/0.29 [kcal/mol] $1 - r^2$: 7.494E-04 -5500.02/0.01 [eÅ] 750 0.6 $1 - r^2$: 2.695E-03 -600 -600 -650 -750 -750 500 0.4 ored. [kcal/mol] pred. [*eÅ*] 0.2 250 0.0 0 -0.2-250-0.4-800 -500-0.6-850 -750-600 500 0.0 0.5 -700-500-0.5-8000 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 750 43.72/37.62 [kcal/mol] 46.80/31.65 [kcal/mol] 0.02/0.01 [e] 200 $1 - r^2$: 1.881E-01 $1 - r^2$: 9.811E-01 0.10 500 150 ored. [kcal/mol] ored. [kcal/mol] 250 100 pred. [e] 0.05 50 0 0.00 0 -250 -50-500 -0.05-100-750-100100 200 -5000 500 -0.05 0.00 0.05 0.10 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*]