l: 0 | mp: 5 | feat.: 128 params: 2.70e+05 | Test (n=2000) Ε D 0.8 1000 -550 0.70/0.61 [kcal/mol] 1.06/0.23 [kcal/mol] 0.02/0.01 [eÅ] 0.6 $1 - r^2$: 1.200E-05 $1 - r^2$: 2.492E-04 750 $1 - r^2$: 1.824E-03 -600 -600 -650 -750 -750 0.4 pred. [kcal/mol] 500 pred. [eÅ] 0.2 250 0.0 0 -0.2-250-0.4-500-800 -0.6-750-850 0.0 0.5 -800 -700-600-500500 1000 -0.50 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 0.15 1000 45.75/39.61 [kcal/mol] 47.13/31.70 [kcal/mol] 0.02/0.01 [e] 200 $1 - r^2$: 1.541E-01 $1 - r^2$: 9.742E-01 750 0.10 150 pred. [kcal/mol] pred. [kcal/mol] 500 100 0.05 pred. [e] 250 50 0 0.00 0 -250 -0.05-50-500-100-0.10-7500.1 -100100 200 -5000 500 1000 -0.10.0 0 ref. [e] ref. [kcal/mol] ref. [kcal/mol]