l: 0 | mp: 5 | feat.: 128 params: 2.70e+05 | Test (n=2000) Ε D 1000 0.8 -5500.35/0.27 [kcal/mol] 0.70/0.21 [kcal/mol] 0.02/0.01 [eÅ]750 0.6 $1 - r^2$: 7.025E-06 $1 - r^2$: 1.101E-04 $1 - r^2$: 1.810E-03 -600 -600 | Kcal/mol] | -750 | -750 0.4 pred. [kcal/mol] 500 pred. [eÅ] 0.2 250 0.0 0 -0.2-250-0.4-800 -500 -0.6-750-8500.0 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 0.100 1000 42.26/37.07 [kcal/mol] 47.02/31.63 [kcal/mol] 0.01/0.01 [e] 200 0.075 750 $1 - r^2$: 2.057E-01 $1 - r^2$: 9.811E-01 150 0.050 pred. [kcal/mol] pred. [kcal/mol] 500 100 0.025 pred. [e] 250 50 0.000 0 -0.025-250 -0.050-50-500-100-0.075-750-100100 200 -5000 500 1000 -0.050.00 0.05 0.10 0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]