l: 1 | mp: 4 | feat.: 128 params: 3.83e+05 | Test (n=2000) Ε D 1000 0.8 -550 1.49/1.33 [kcal/mol] $1 - r^2$: 7.412E-05 0.52/0.18 [kcal/mol] 0.01/0.01 [eÅ]750 0.6 $1 - r^2$: 6.080E-05 $1 - r^2$: 1.493E-03 -600 -600 -650 -750 -750 0.4 500 pred. [kcal/mol] pred. [*eÅ*] 0.2 250 0.0 0 -0.2 -250-0.4-800 -500-0.6-850 -750500 0.0 0.5 -800 -700-600-5001000 -0.50 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 1000 49.82/43.27 [kcal/mol] 47.00/31.66 [kcal/mol] 0.01/0.01 [e] 200 0.20 750 $1 - r^2$: 9.893E-01 $1 - r^2$: 1.895E-01 150 pred. [kcal/mol] 500 pred. [kcal/mol] 0.15 100 pred. [*e*] 250 0.10 50 0 0.05 0 -250 -50 0.00 -500-100-0.05-7500.1 0.2 -1000 100 200 -500 0 500 1000 0.0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]