l: 0 | mp: 4 | feat.: 64 params: 5.92e+04 | Test (n=2000) Ε D 0.8 -550 0.38/0.30 [kcal/mol] 0.90/0.32 [kcal/mol] 0.02/0.02 [eÅ] 750 0.6 $1 - r^2$: 1.851E-04 $1 - r^2$: 8.861E-06 $1 - r^2$: 3.743E-03 -600 -600 Fred -650 -750 -750 500 0.4 pred. [kcal/mol] pred. [*eÅ*] 250 0.2 0.0 0 -0.2-250-0.4-500-800 -0.6-750-850 500 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 35.93/29.61 [kcal/mol] 46.99/31.67 [kcal/mol] 0.3 750 0.02/0.02 [e] 200 $1 - r^2$: 1.729E-01 $1 - r^2$: 9.827E-01 500 150 ored. [kcal/mol] pred. [kcal/mol] 0.2 250 pred. [e] 100 0 0.1 50 -250 0 0.0 -500-50 -750-0.1100 0.1 0.2 0.3 200 -5000 500 -0.10.0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]