*l*: 1 | mp: 4 | feat.: 64 params: 1.06e+05 | Test (n=2000) Ε D 0.8 -550 2.33/2.26 [kcal/mol]  $1 - r^2$ : 5.158E-05 1.51/0.28 [kcal/mol]  $1 - r^2$ : 5.128E-04 0.02/0.01 [eÅ] 750 0.6  $1 - r^2$ : 2.660E-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 -750500 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 750 51.25/45.37 [kcal/mol] 46.84/31.66 [kcal/mol] 0.02/0.01 [e] 0.05 200  $1 - r^2$ : 1.865E-01  $1 - r^2$ : 9.650E-01 500 150 0.00 pred. [kcal/mol] ored. [kcal/mol] 100 250 pred. [*e*] -0.0550 0 -0.100 -250 -0.15-50 -500 -100-0.20-750500 -1000 100 200 -5000 -0.2-0.10.0 ref. [kcal/mol] ref. [kcal/mol] ref. [e]