*l*: 2 | mp: 4 | feat.: 128 params: 5.53e+05 | Test (n=2000) Ε D 0.8 -550 0.94/0.71 [kcal/mol] 0.51/0.17 [kcal/mol] 0.01/0.01 [eÅ]750 0.6  $1 - r^2$ : 7.464E-05  $1 - r^2$ : 5.901E-05  $1 - r^2$ : 1.517E-03 -600 pred (Kcal/mol) -650 -750 500 0.4 pred. [kcal/mol] pred. [eÅ] 250 0.2 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 42.69/36.87 [kcal/mol] 46.96/31.67 [kcal/mol] 0.01/0.01 [e] 750 200  $1 - r^2$ : 2.079E-01  $1 - r^2$ : 9.955E-01 0.10 500 150 ored. [kcal/mol] pred. [kcal/mol] 100 pred. [e] 250 0.05 50 0 0.00 0 -250 -50-500-0.05-100-750100 -100200 -5000 500 -0.050.00 0.05 0.10 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*]