*l*: 2 | mp: 4 | feat.: 32 params: 3.11e+04 | Test (n=800) Ε D 80 2 7.03/5.58 [kcal/mol]  $1 - r^2$ : 5.667E-04 0.66/0.36 [kcal/mol] 0.05/0.04 [eÅ] 60  $1 - r^2$ : 4.968E-03 -2000 $1 - r^2$ : 2.592E-03 40 1 pred. [kcal/mol] pred. [kcal/mol] -2200 pred. [*eÅ*] 20 0 0 -2400-20 -1-40-2600-2-60-280050 -2800-2600-2400-2200-2000 -500 1 0 2 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E<sub>ele</sub> F Q 80 378.38/263.39 [kcal/mol]  $1 - r^2$ : 7.159E-03 6.63/2.92 [kcal/mol]  $1 - r^2$ : 9.983E-01 0.020 0.01/0.01 [e] 60 0.015 40 pred. [kcal/mol] pred. [kcal/mol] -50020 pred. [e] 0.010 -10000.005 -1500-200.000 -40-2000-60 -0.005-25000 50 0.01 0.02 -2000-1000 0 -50 0.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]