l: 0 | mp: 4 | feat.: 128 params: 1.44e+05 | Test (n=800) Ε D 75 2 3.56/2.87 [kcal/mol] $1 - r^2$: 1.478E-04 0.80/0.38 [kcal/mol] 0.05/0.03 [*e*Å] $1 - r^2$: 7.273E-03 $1 - r^2$: 2.816E-03 -200050 1 pred. [kcal/mol] pred. [kcal/mol] 25 pred. [*eÅ*] -22000 0 -2400-1-25 -2600-50**-**2 **-**75 50 -2600-2400-2200-2000 -50 **-**2 0 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ Q 75 377.29/262.44 [kcal/mol] $1 - r^2$: 6.812E-03 6.72/2.95 [kcal/mol] 0.01/0.00 [e] 0.04 $1 - r^2$: 1.004E+00 50 kcal/mol -1000 -1500 ored. [kcal/mol] 0.02 25 pred. [e] 0.00 -25 -0.02-2000-50-0.04-2500**-**75 -100050 -20000 -500 -0.050-0.025 0.000 0.025 0.050 ref. [kcal/mol] ref. [kcal/mol] ref. [e]