l: 0 | mp: 4 | feat.: 64 params: 3.94e+04 | Test (n=800) Ε D 80 10.75/5.92 [kcal/mol] $1 - r^2$: 9.433E-04 0.88/0.46 [kcal/mol] $1 - r^2$: 9.030E-03 0.07/0.05 [eÅ] 60 -2000 $1 - r^2$: 4.261E-03 40 1 pred. [kcal/mol] pred. [kcal/mol] -220020 pred. [*eÅ*] 0 0 -2400-20-1-2600-40-60-2-280050 -2750 -2500 -2250 -2000 -50 0 1 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs E_{ele} F Q 80 377.15/262.29 [kcal/mol] $1 - r^2$: 6.808E-03 6.62/2.94 [kcal/mol] 0.01/0.01 [e] 60 0.00 $1 - r^2$: 9.995E-01 bred -200 -1000 -1500 40 -0.01pred. [kcal/mol] 20 -0.02-0.03-20-0.04-40-2000-0.05-60 -2500 -0.06-100050 -0.02-2000 0 -500 -0.06-0.040.00 ref. [kcal/mol] ref. [kcal/mol] ref. [e]