l: 2 | mp: 2 | feat.: 128 params: 1.51e+05 | Test (n=800) Ε D 80 2 -4.71/3.54 [kcal/mol] 0.56/0.29 [kcal/mol] $1 - r^2$: 3.657E-03 0.07/0.04 [eÅ] 60 $1 - r^2$: 2.827E-04 $1 - r^2$: 4.296E-03 -2000 1 . 40 pred. [kcal/mol] pred. [kcal/mol] pred. [*eÅ*] -220020 -0 -0 --2400-20 -40 -2600**-**2 -60 50 -2600-2400-2200-2000 -50 **-**2 -1 0 ref. [kcal/mol] ref. [kcal/mol] ref. [*e*Å] E vs $E_{\rm ele}$ F Q 0.04 80 $0 = 378.66/263.64 \text{ [kcal/mol]} \\ 1 = r^2: 6.775E-03$ 6.58/2.87 [kcal/mol] $1 - r^2$: 9.978E-01 0.01/0.00 [e] 0.03 60 -| Kcal/mol 0.02 40 pred. [kcal/mol] 0.01 20 pred. [*e*] 0.00 0 -0.01-20 -0.02-40-2000-0.03-60 · -2500-100050 0.02 -20000 -500 -0.020.00 0.04 ref. [kcal/mol] ref. [kcal/mol] ref. [e]