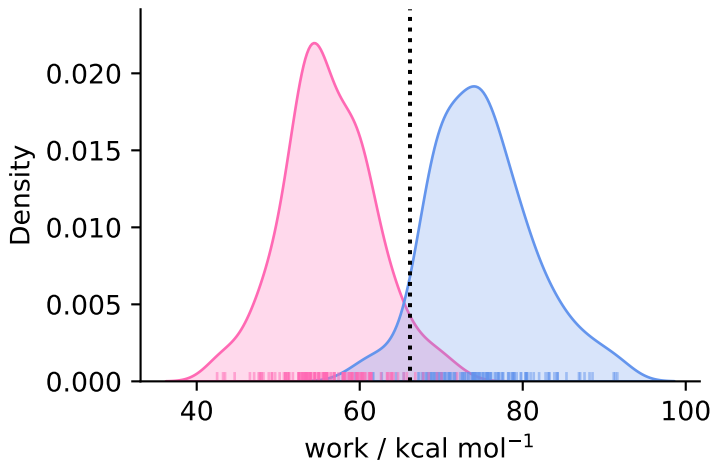RUN688

complex ($N = 133$)

solvent ($N = 90$)

direction
forward
reverse

work / kcal mol^{-1}