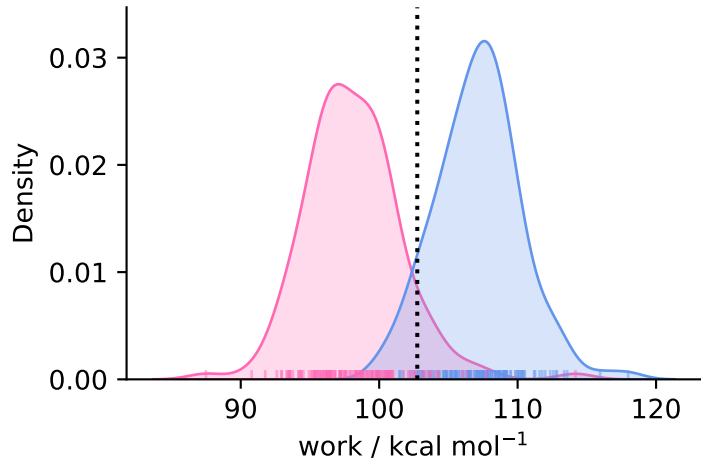RUN3832

complex ($N = 141$) solvent ($N = 160$)

direction
forward
reverse

work / kcal mol^{-1} work / kcal mol^{-1}