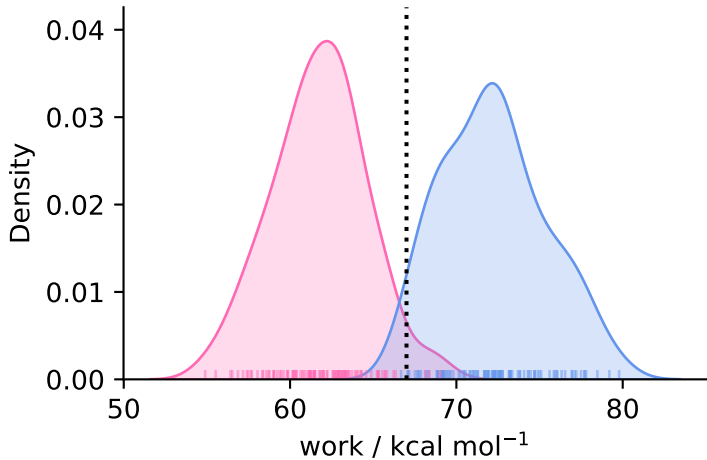RUN6884

complex ($N = 102$) solvent ($N = 80$)

Density

direction
forward
reverse

work / kcal mol^{-1}