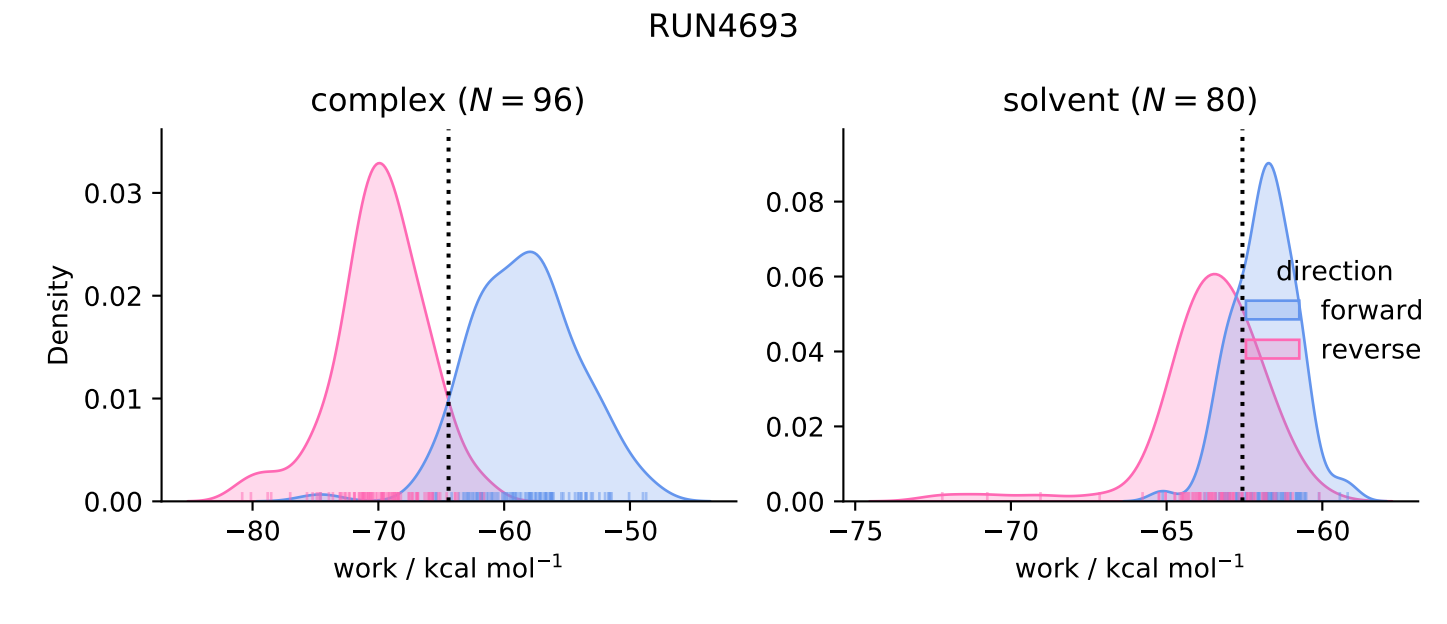
RUN4693
complex ($N = 96$)
solvent ($N = 80$)
Density
0.03
0.02
0.01
0.00
0.08
0.06
0.04
0.02
0.00
−80
−70
−60
−50
−75
−70
−65
−60
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse