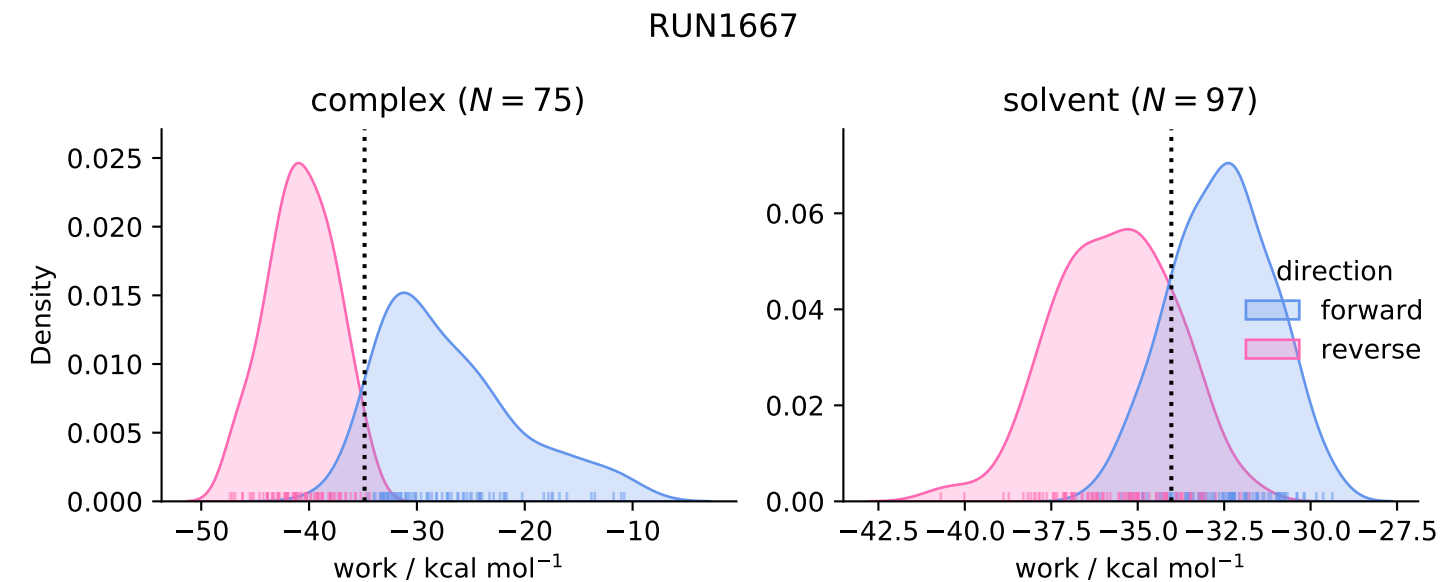
RUN1667
complex ($N = 75$)
solvent ($N = 97$)
Density
0.025
0.020
0.015
0.010
0.005
0.000
−50
−40
−30
−20
−10
work / kcal mol^{-1}
0.06
0.04
0.02
0.00
−42.5
−40.0
−37.5
−35.0
−32.5
−30.0
−27.5
work / kcal mol^{-1}
direction
forward
reverse