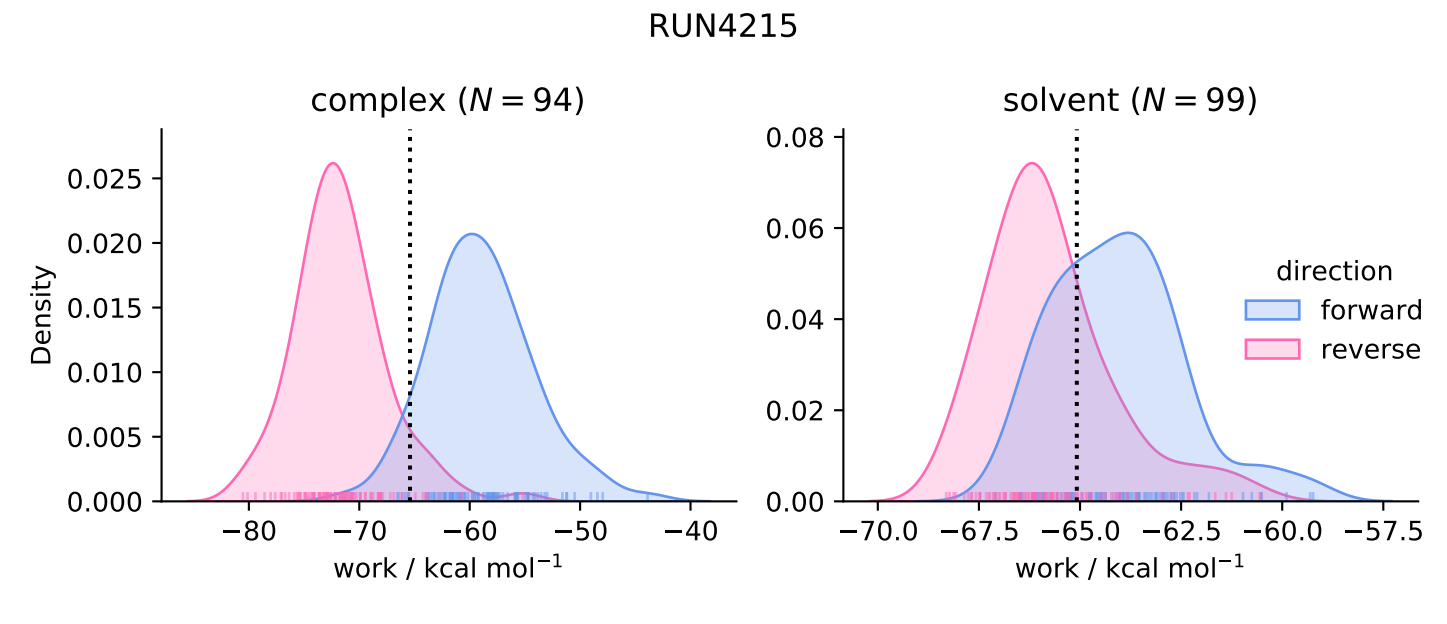
RUN4215
complex ($N = 94$)
solvent ($N = 99$)
Density
0.025
0.020
0.015
0.010
0.005
0.000
0.08
0.06
0.04
0.02
0.00
−80
−70
−60
−50
−40
−70.0
−67.5
−65.0
−62.5
−60.0
−57.5
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse