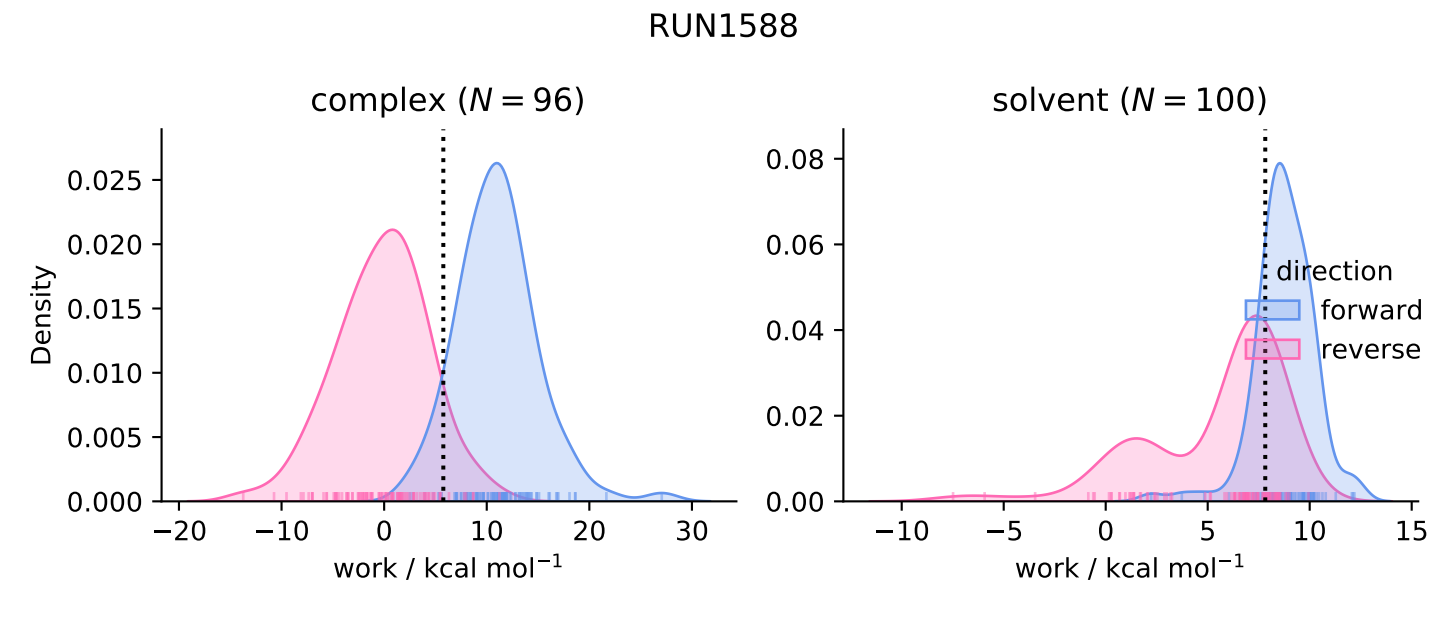
RUN1588
complex ($N = 96$)
solvent ($N = 100$)
Density
0.025
0.020
0.015
0.010
0.005
0.000
−20
−10
0
10
20
30
work / kcal mol^{-1}
0.08
0.06
0.04
0.02
0.00
−10
−5
0
5
10
15
work / kcal mol^{-1}
direction
forward
reverse