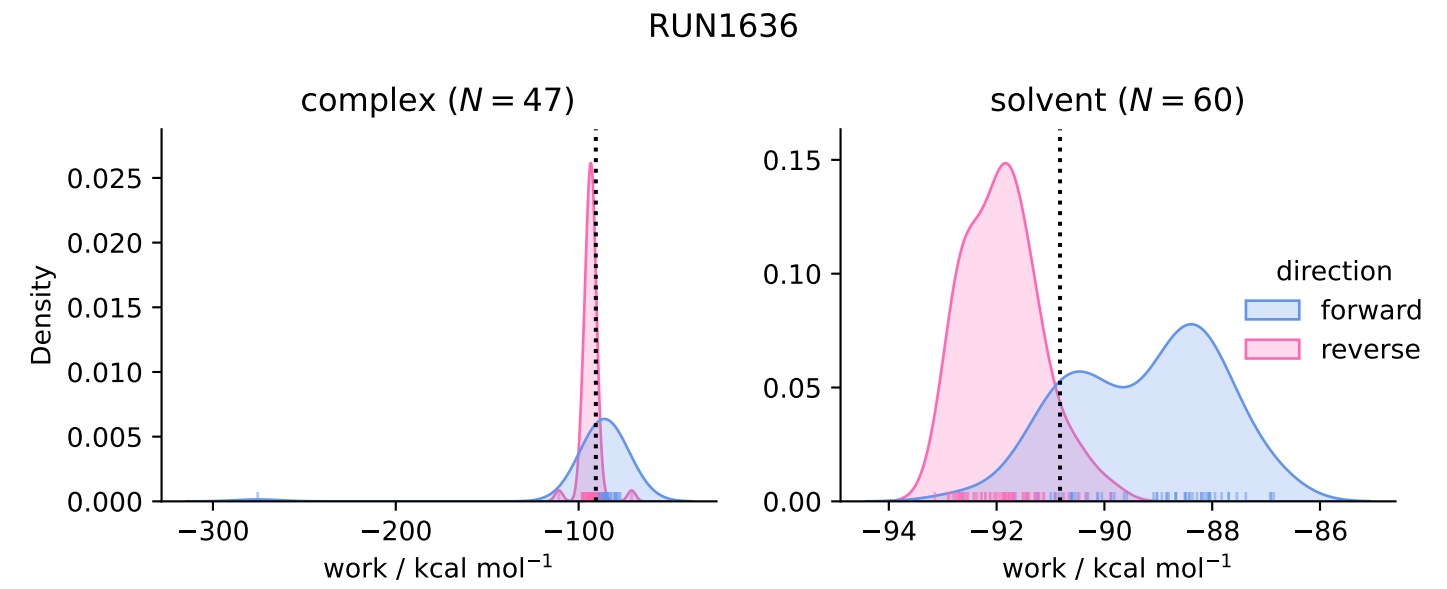
RUN1636
complex ($N = 47$)
solvent ($N = 60$)
Density
0.025
0.020
0.015
0.010
0.005
0.000
−300
−200
−100
work / kcal mol^{-1}
0.15
0.10
0.05
0.00
−94
−92
−90
−88
−86
work / kcal mol^{-1}
direction
forward
reverse