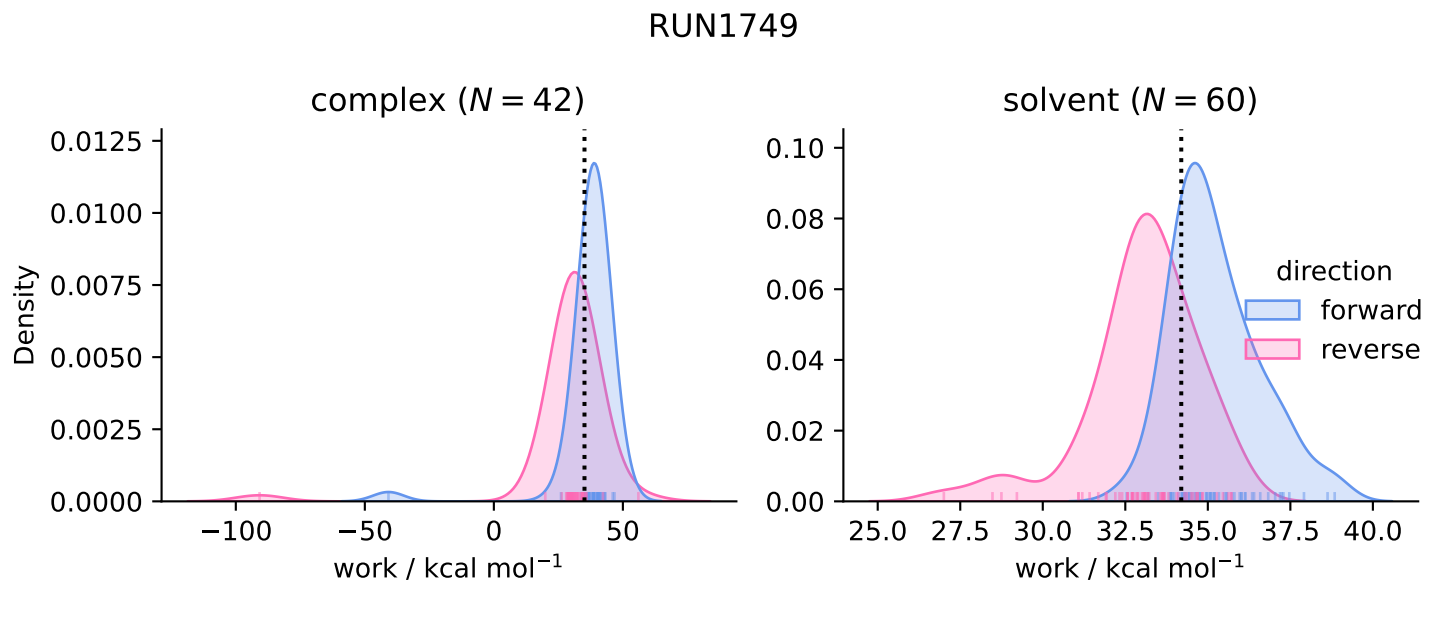
RUN1749
complex ($N = 42$)
solvent ($N = 60$)
Density
0.0125
0.0100
0.0075
0.0050
0.0025
0.0000
0.10
0.08
0.06
0.04
0.02
0.00
−100
−50
0
50
25.0
27.5
30.0
32.5
35.0
37.5
40.0
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse