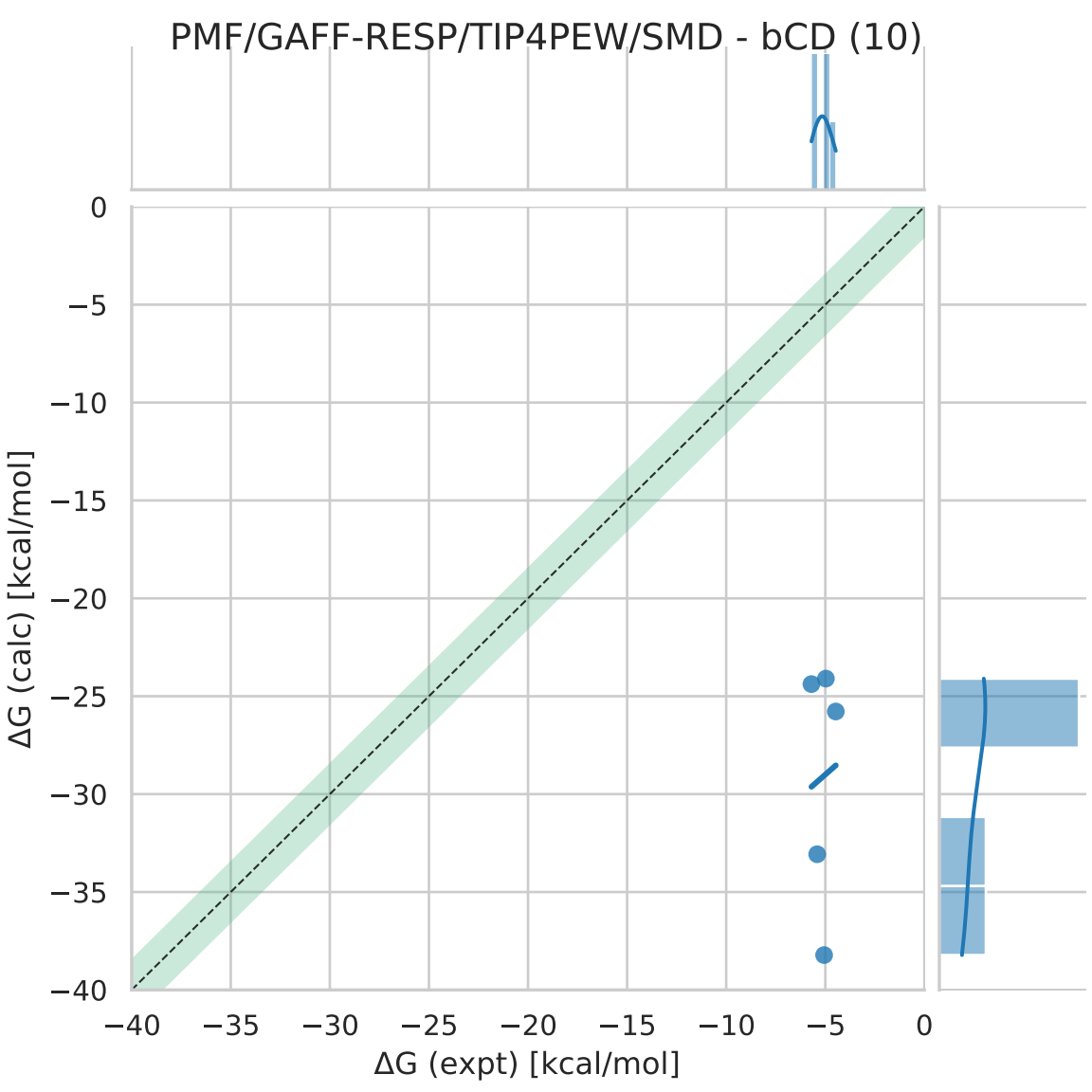
PMF/GAFF-RESP/TIP4PEW/SMD - bCD (10)
0
−5
−10
−15
−20
−25
−30
−35
−40
ΔG (calc) [kcal/mol]
−40
−35
−30
−25
−20
−15
−10
−5
0
ΔG (expt) [kcal/mol]