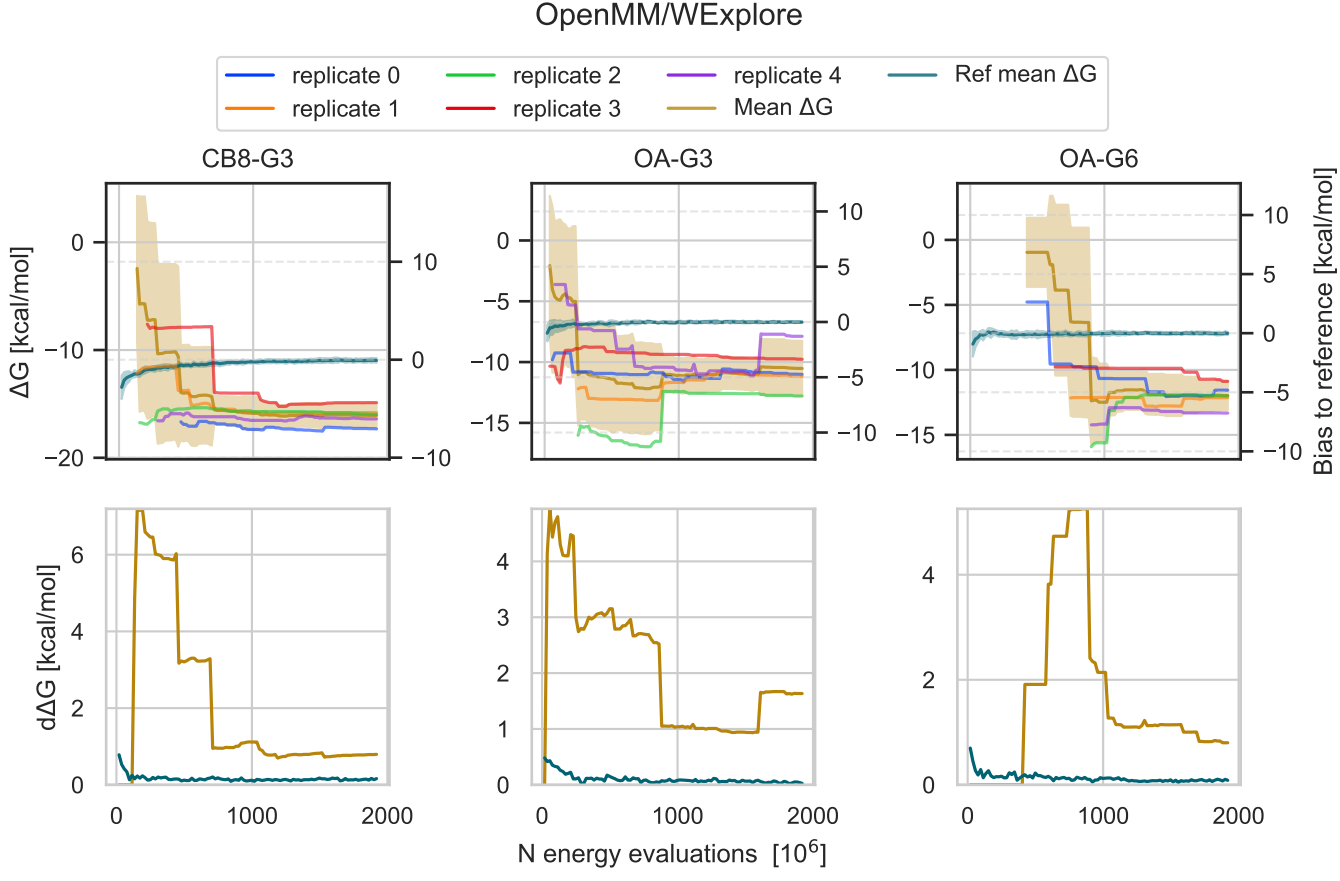
OpenMM/WExplore
replicate 0
replicate 1
replicate 2
replicate 3
replicate 4
Mean ΔG
Ref mean ΔG
CB8-G3
OA-G3
OA-G6
ΔG [kcal/mol]
Bias to reference [kcal/mol]
dΔG [kcal/mol]
N energy evaluations [10^6]