OA-G3 - SOMD/AM1BCC-GAFF-TIP3P/MBAR/C (5732g) 0 -5-10 OA-G3-0 OA-G3-4 OA-G3-1 Mean ΔG -15OA-G3-2 Ref mean ΔG Ref final ΔG OA-G3-3 -2020 40 60 80 100

∆G [kcal/mol]

Simulation percentage (N energy evaluations: 419,995,800)