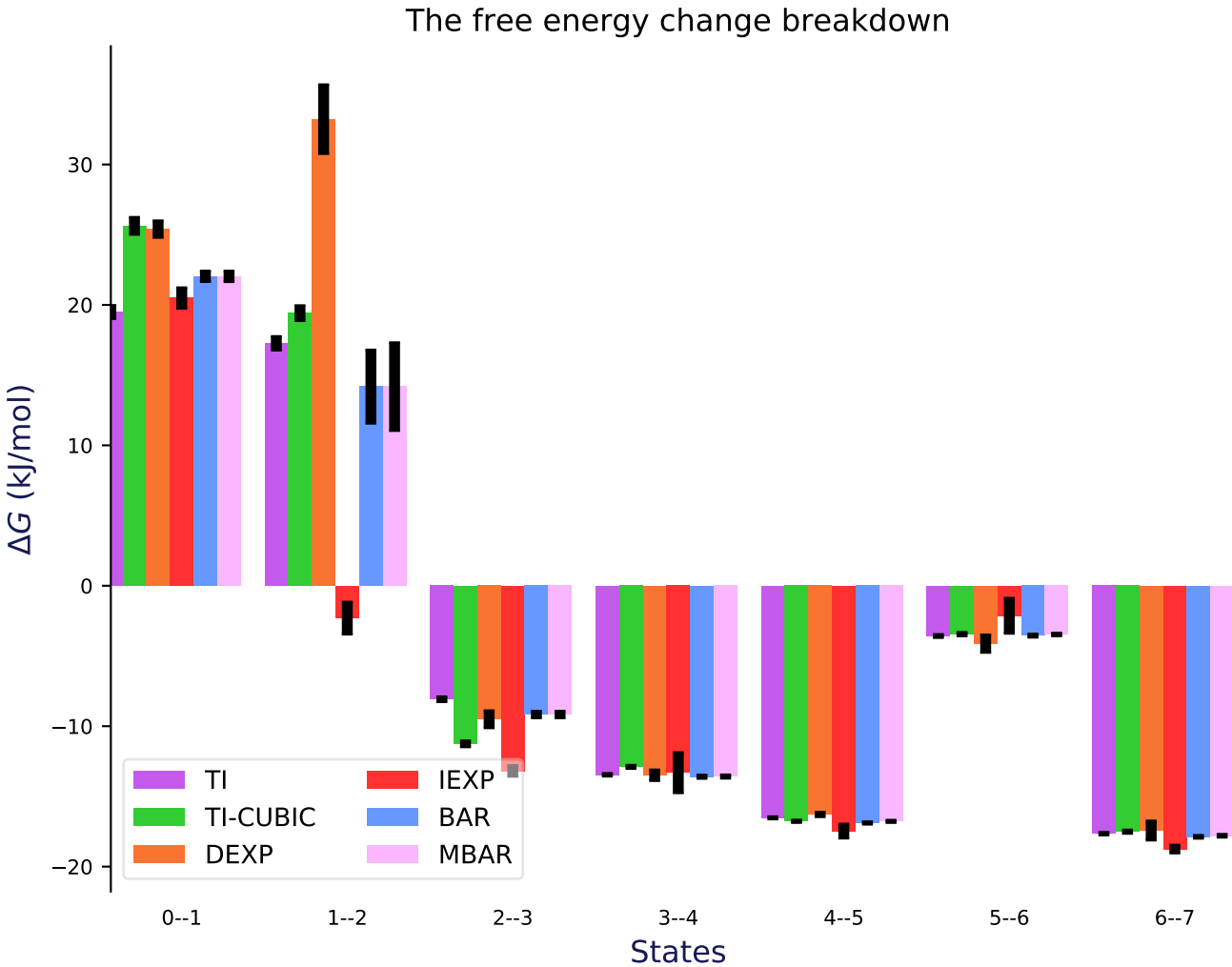
The free energy change breakdown
ΔG (kJ/mol)
30
20
10
0
−10
−20
TI
TI-CUBIC
DEXP
IEXP
BAR
MBAR
0--1
1--2
2--3
3--4
4--5
5--6
6--7
States