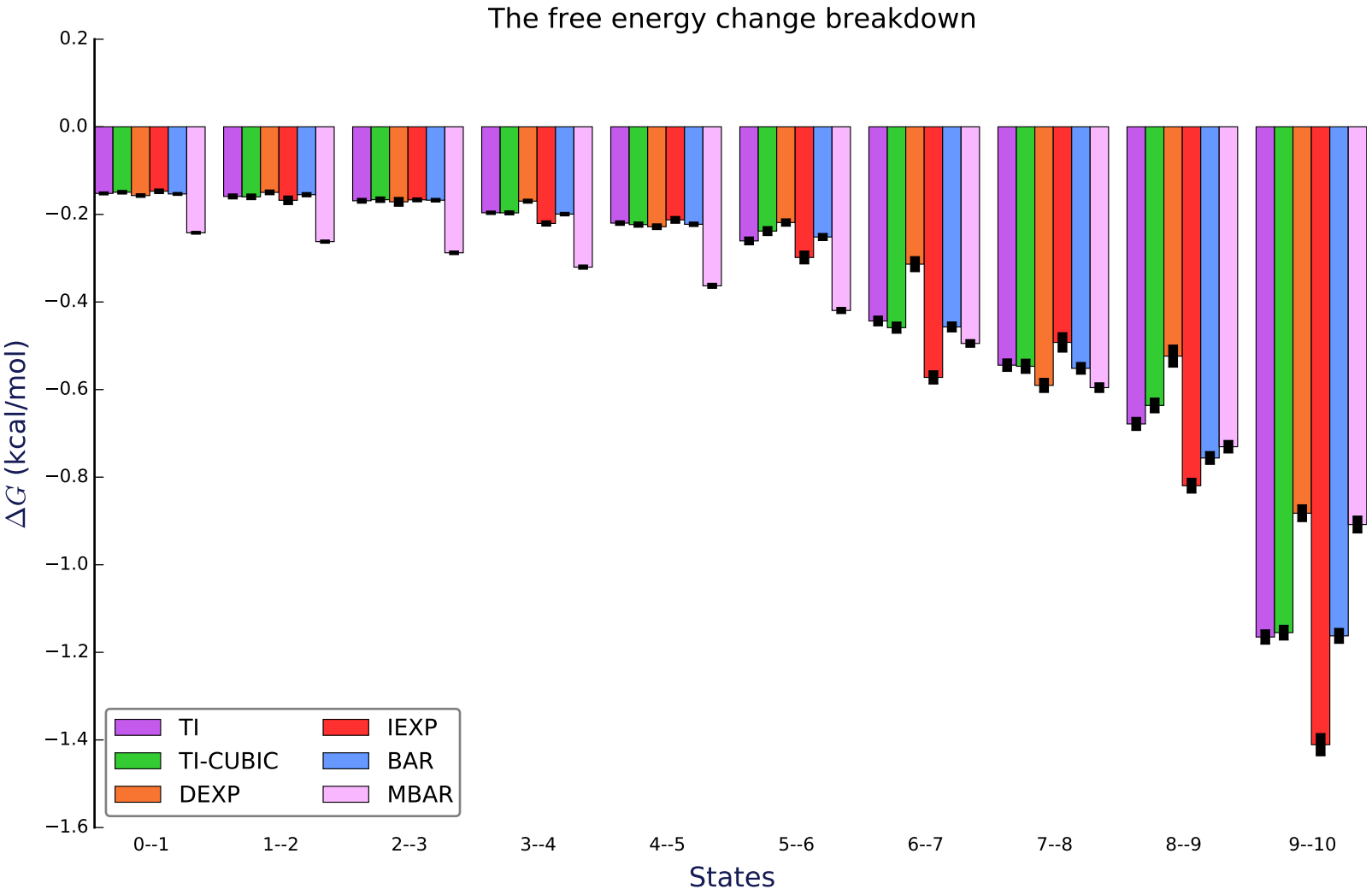
The free energy change breakdown
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
−1.4
−1.6
ΔG (kcal/mol)
TI
TI-CUBIC
DEXP
IEXP
BAR
MBAR
0--1
1--2
2--3
3--4
4--5
5--6
6--7
7--8
8--9
9--10
States