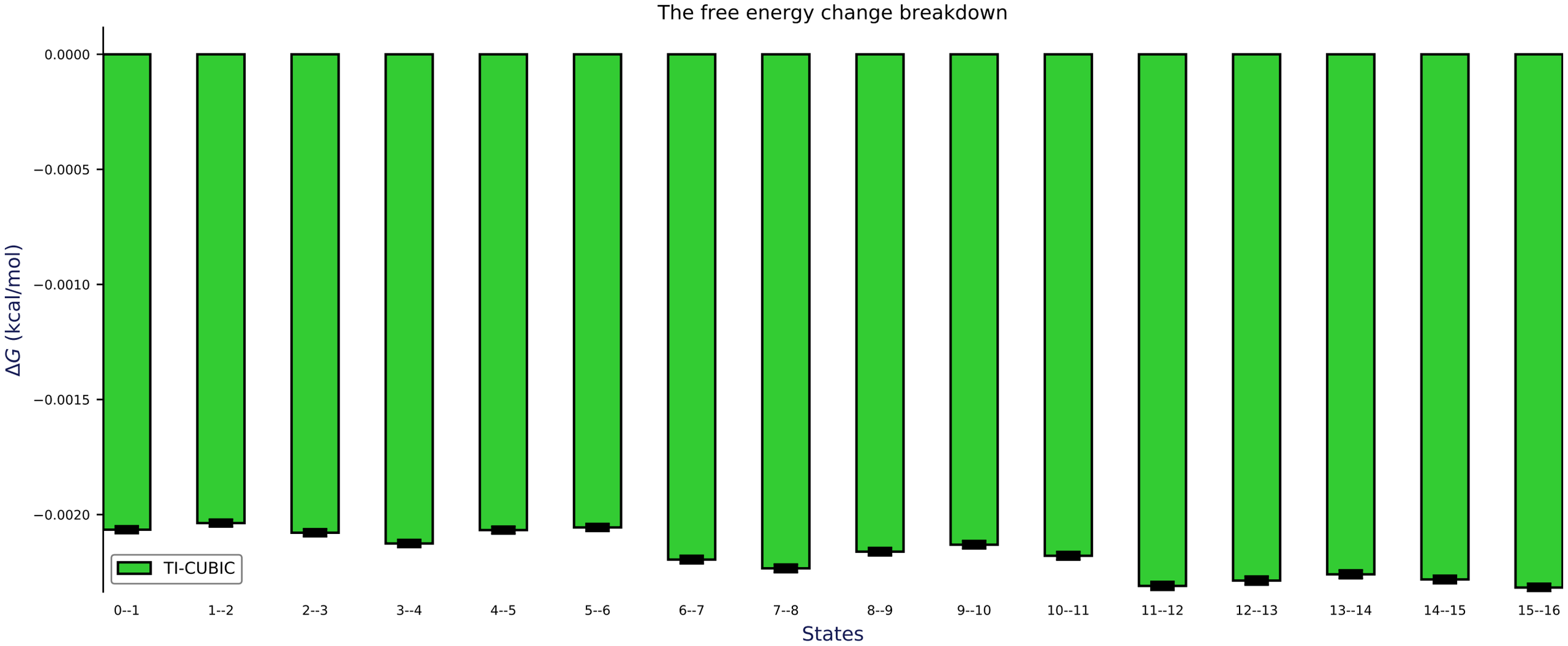
The free energy change breakdown
ΔG (kcal/mol)
0.0000
−0.0005
−0.0010
−0.0015
−0.0020
TI-CUBIC
0--1
1--2
2--3
3--4
4--5
5--6
6--7
7--8
8--9
9--10
10--11
11--12
12--13
13--14
14--15
15--16
States