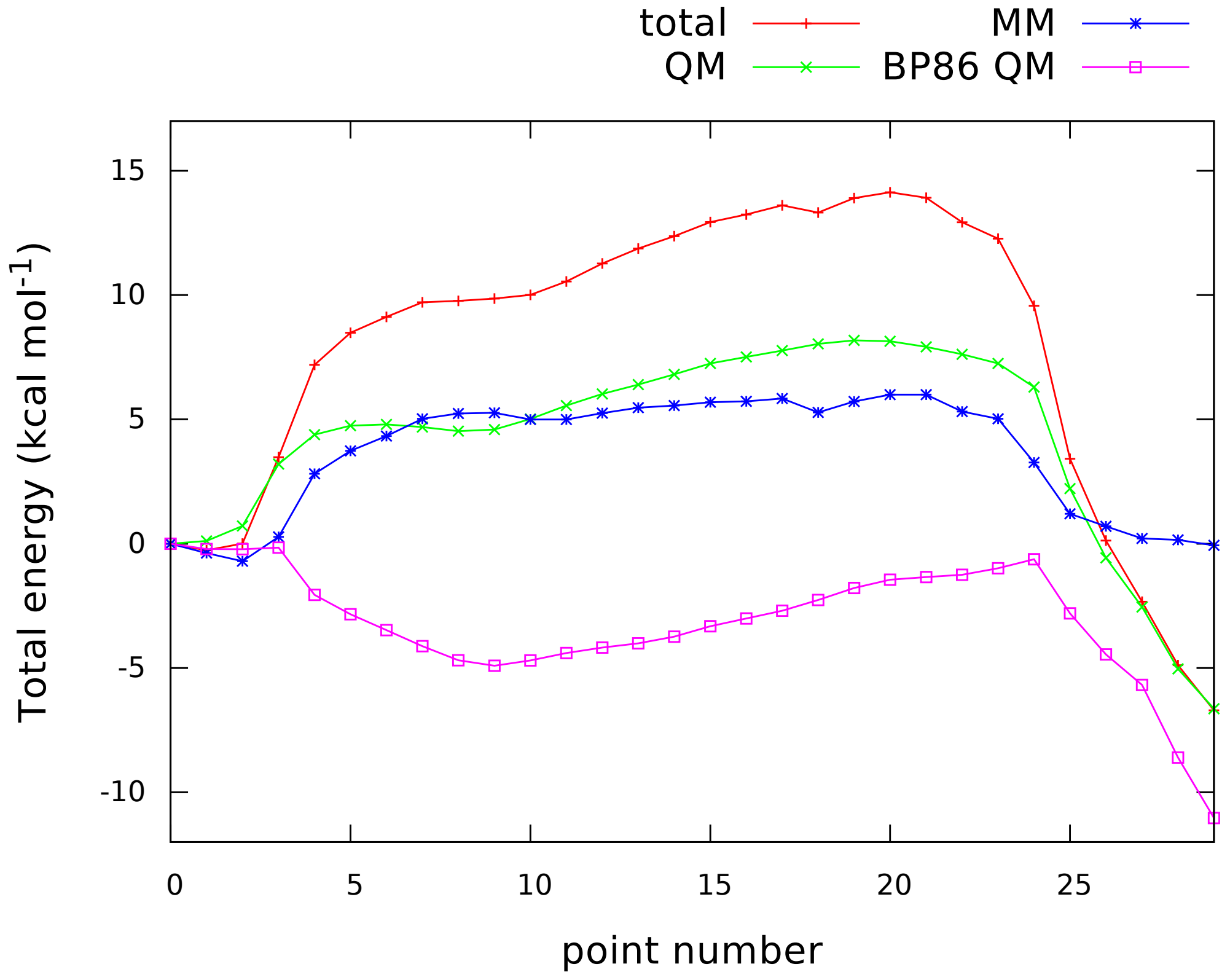
total
QM
MM
BP86 QM
Total energy (kcal mol-1)
point number
15
10
5
0
-5
-10
0
5
10
15
20
25