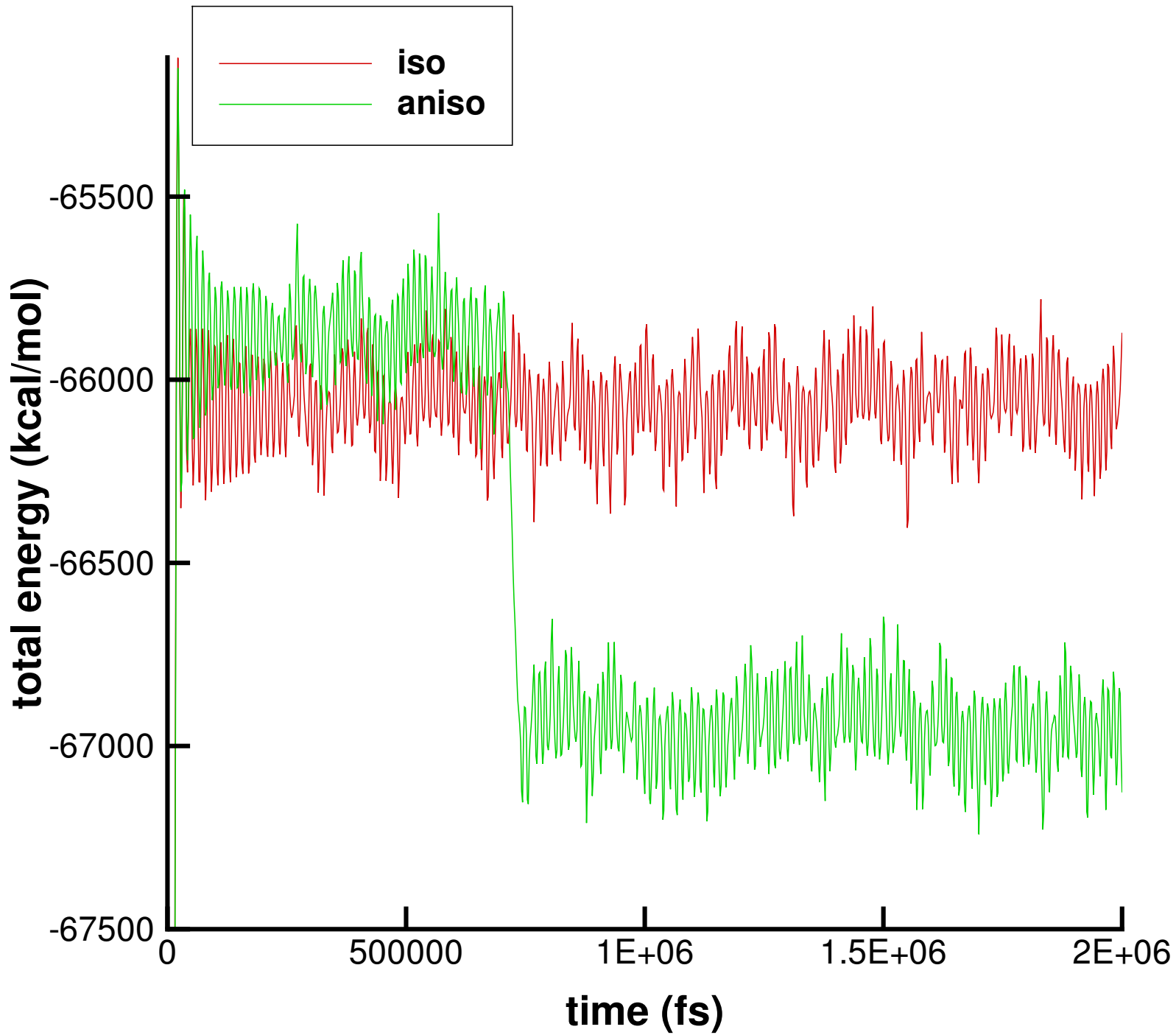
iso
aniso
-65500
-66000
-66500
-67000
-67500
total energy (kcal/mol)
0
500000
1E+06
1.5E+06
2E+06
time (fs)