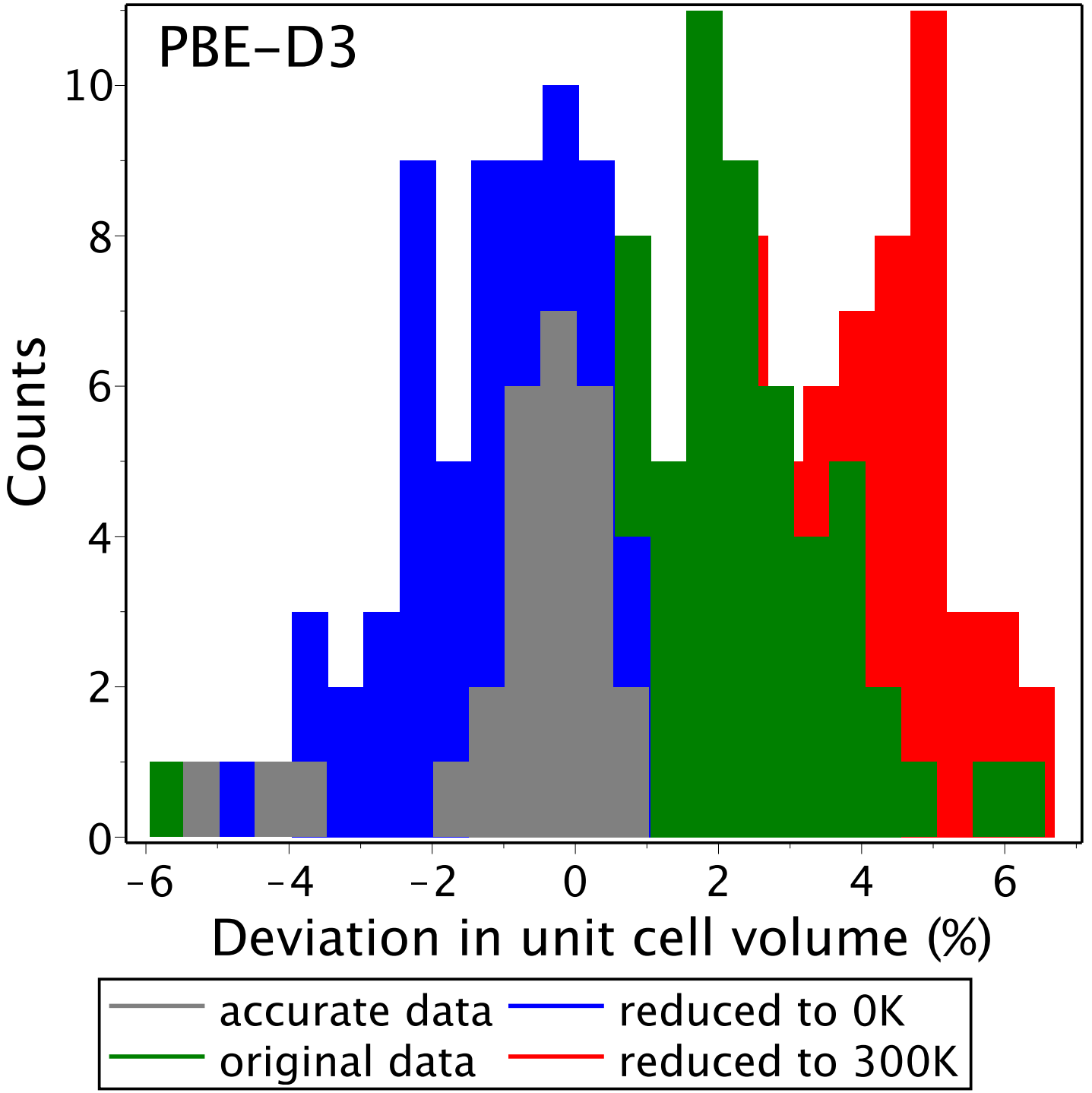
PBE-D3
Counts
0
2
4
6
8
10
-6
-4
-2
0
2
4
6
Deviation in unit cell volume (%)
accurate data
original data
reduced to 0K
reduced to 300K