Supplementary Information

Role of heme distortion on oxygen affinity in heme proteins: the protoglobin case

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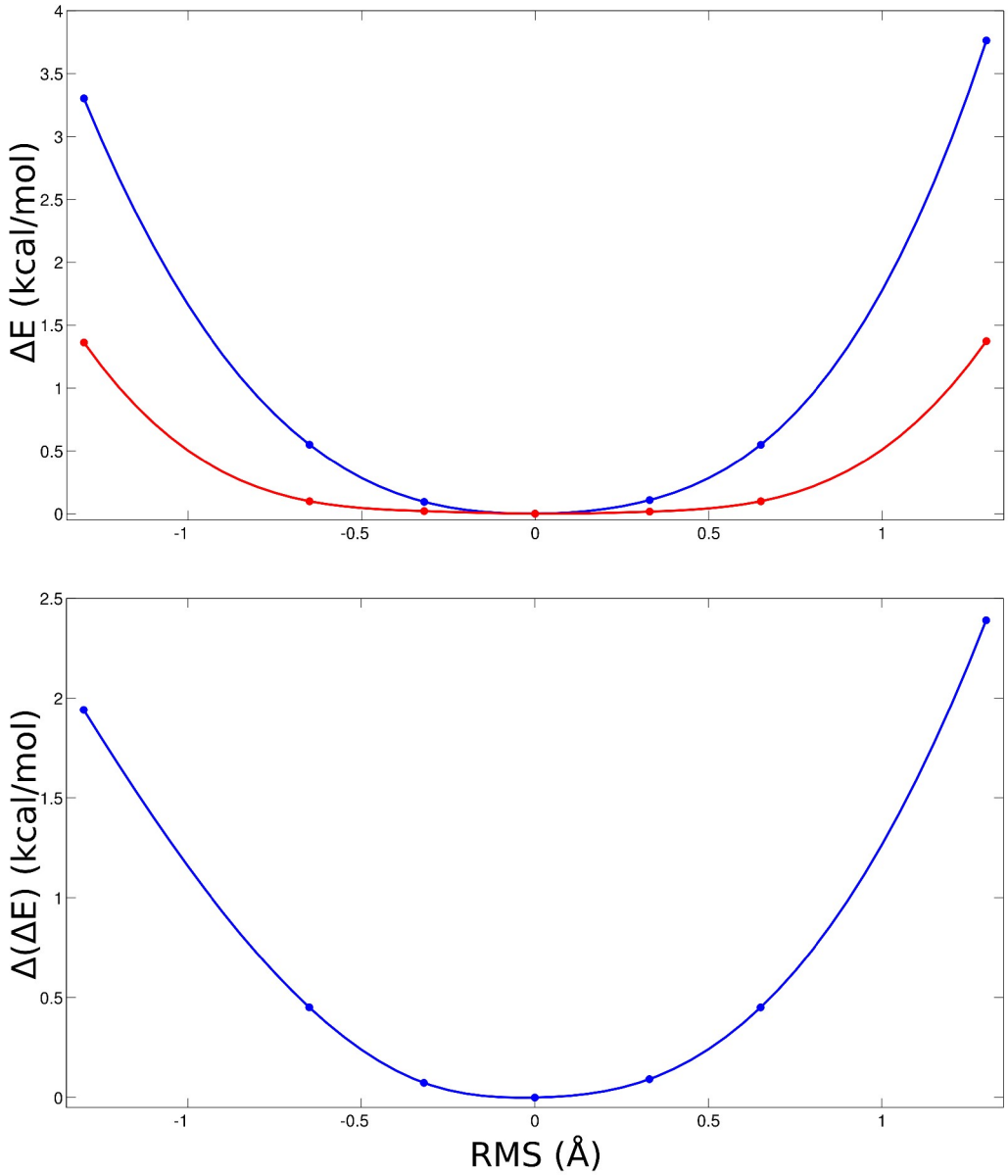


Figure S1. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***sad*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

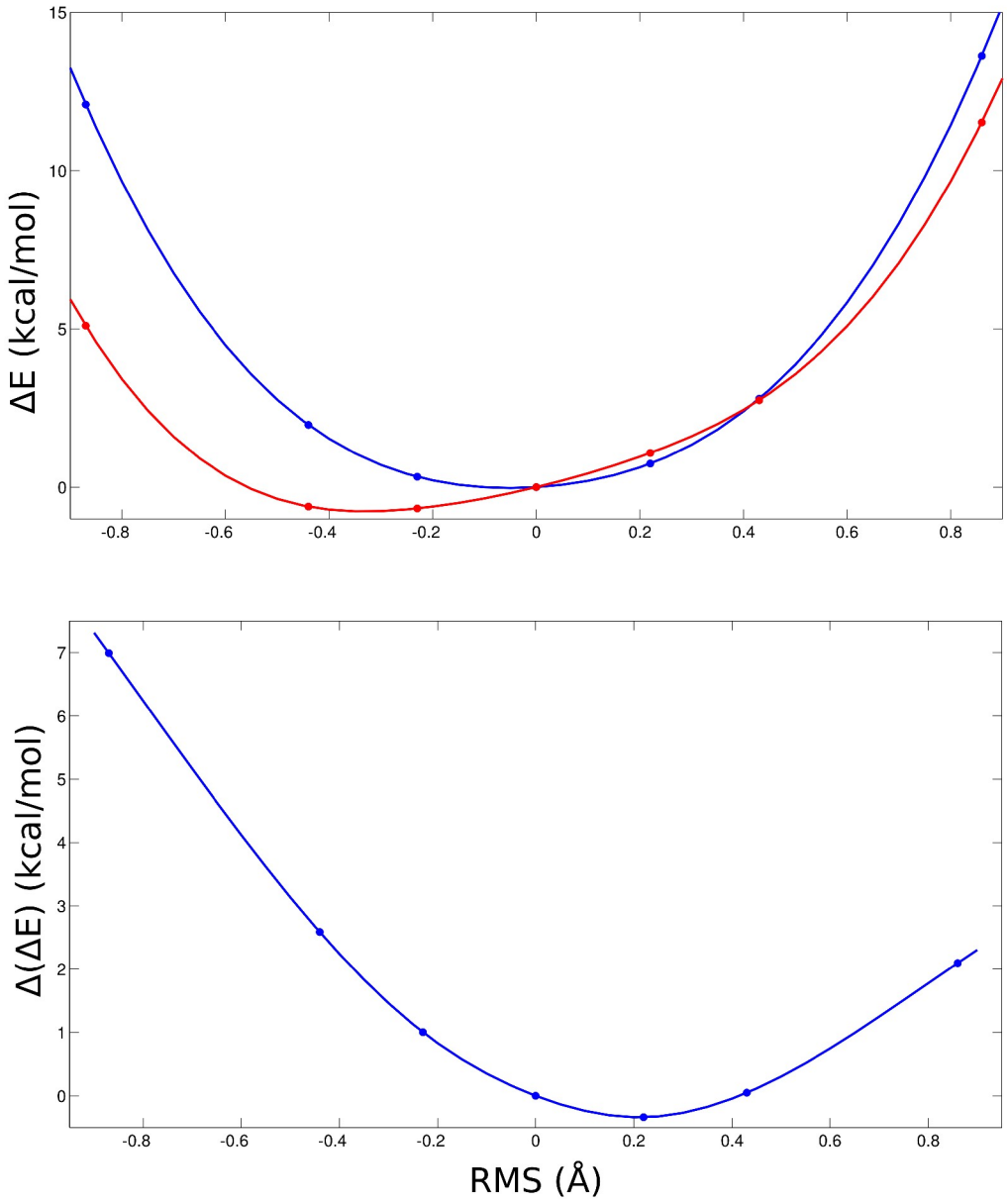


Figure S2. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***dom*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

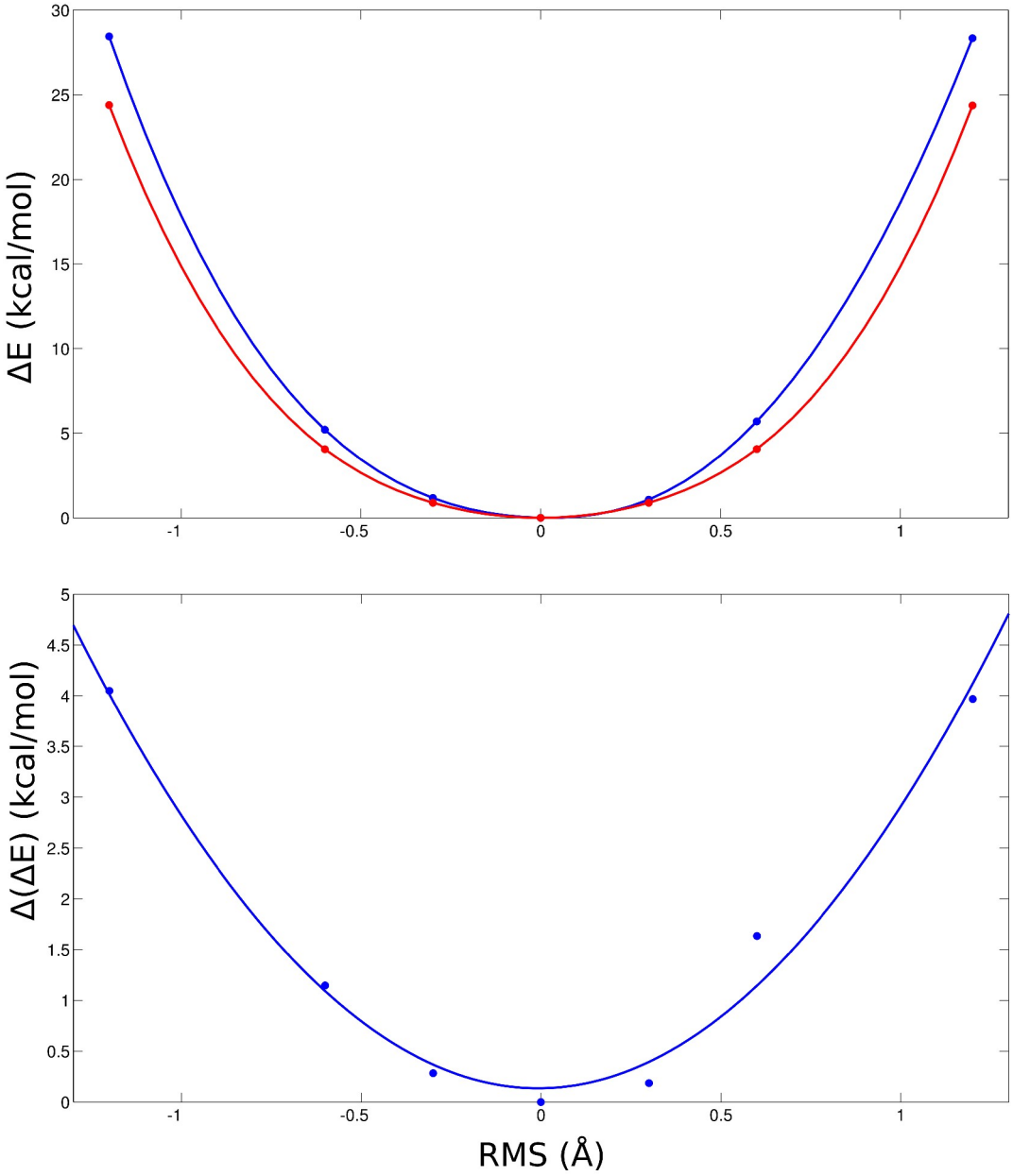
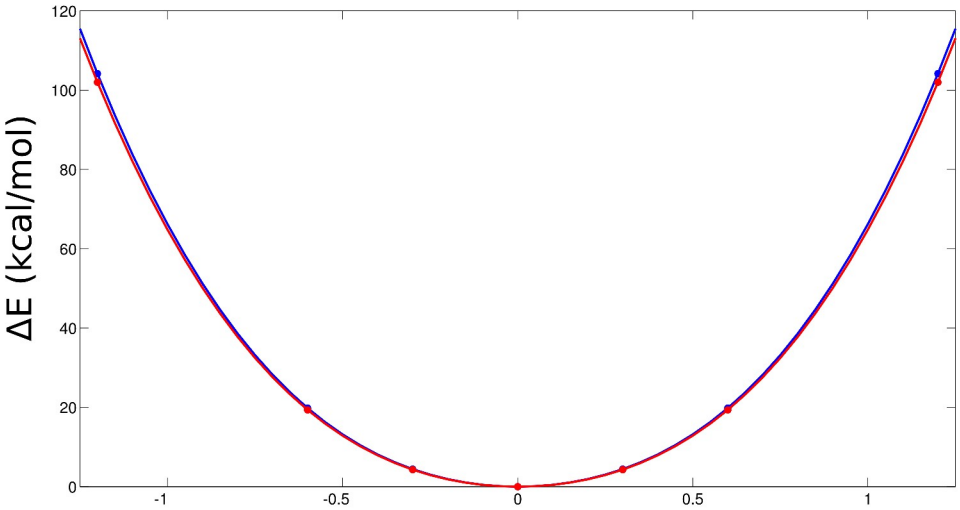


Figure S3. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***wax*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**


ΔE (kcal/mol)
120
100
80
60
40
20
0
-1
-0.5
0
0.5
1

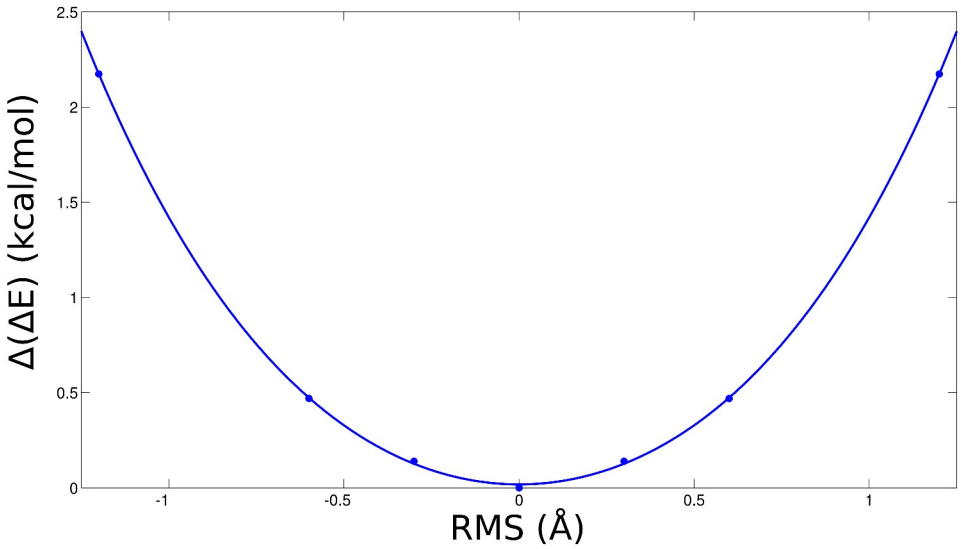

Δ(ΔE) (kcal/mol)
2.5
2
1.5
1
0.5
0
-1
-0.5
0
0.5
1
RMS (Å)

Figure S4. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***pro*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

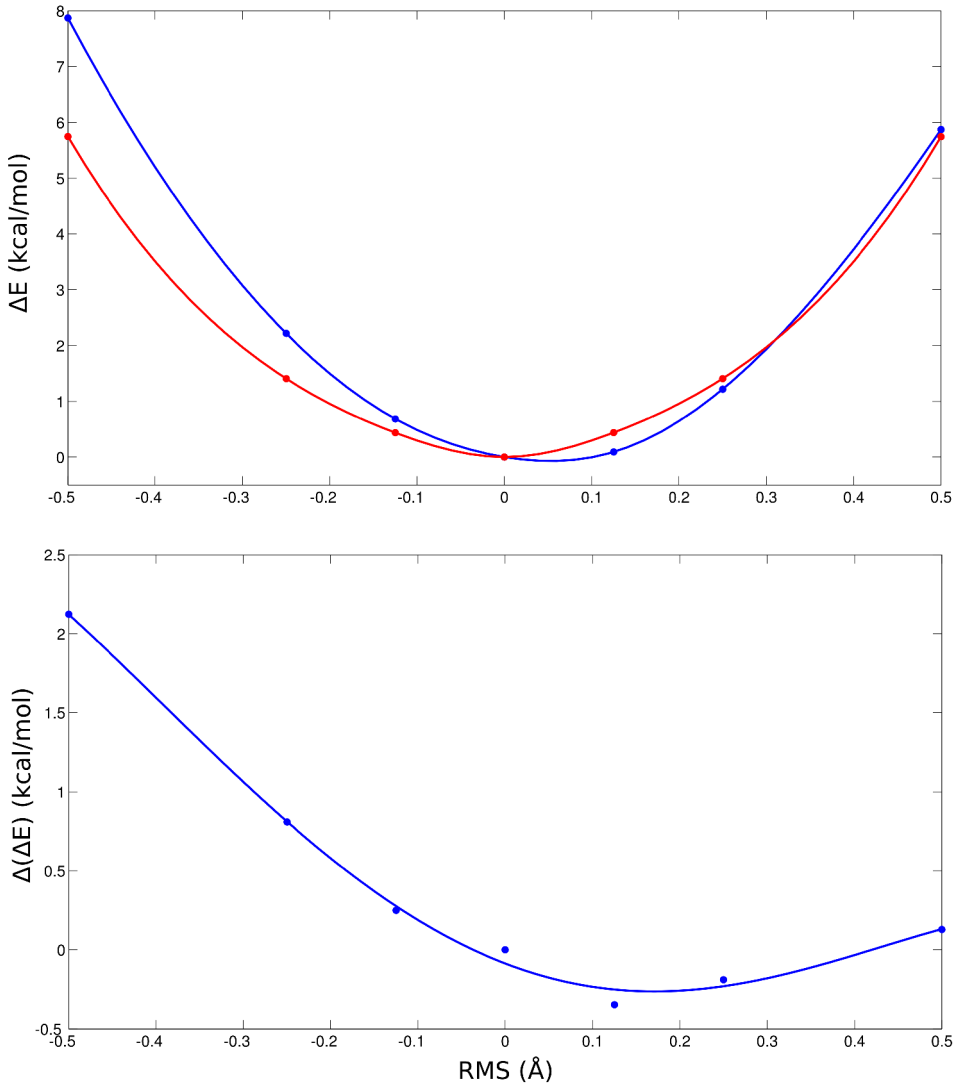

ΔE (kcal/mol)
8
7
6
5
4
3
2
1
0
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
Δ(ΔE) (kcal/mol)
2.5
2
1.5
1
0.5
0
-0.5
RMS (Å)

Figure S5. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***mst*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

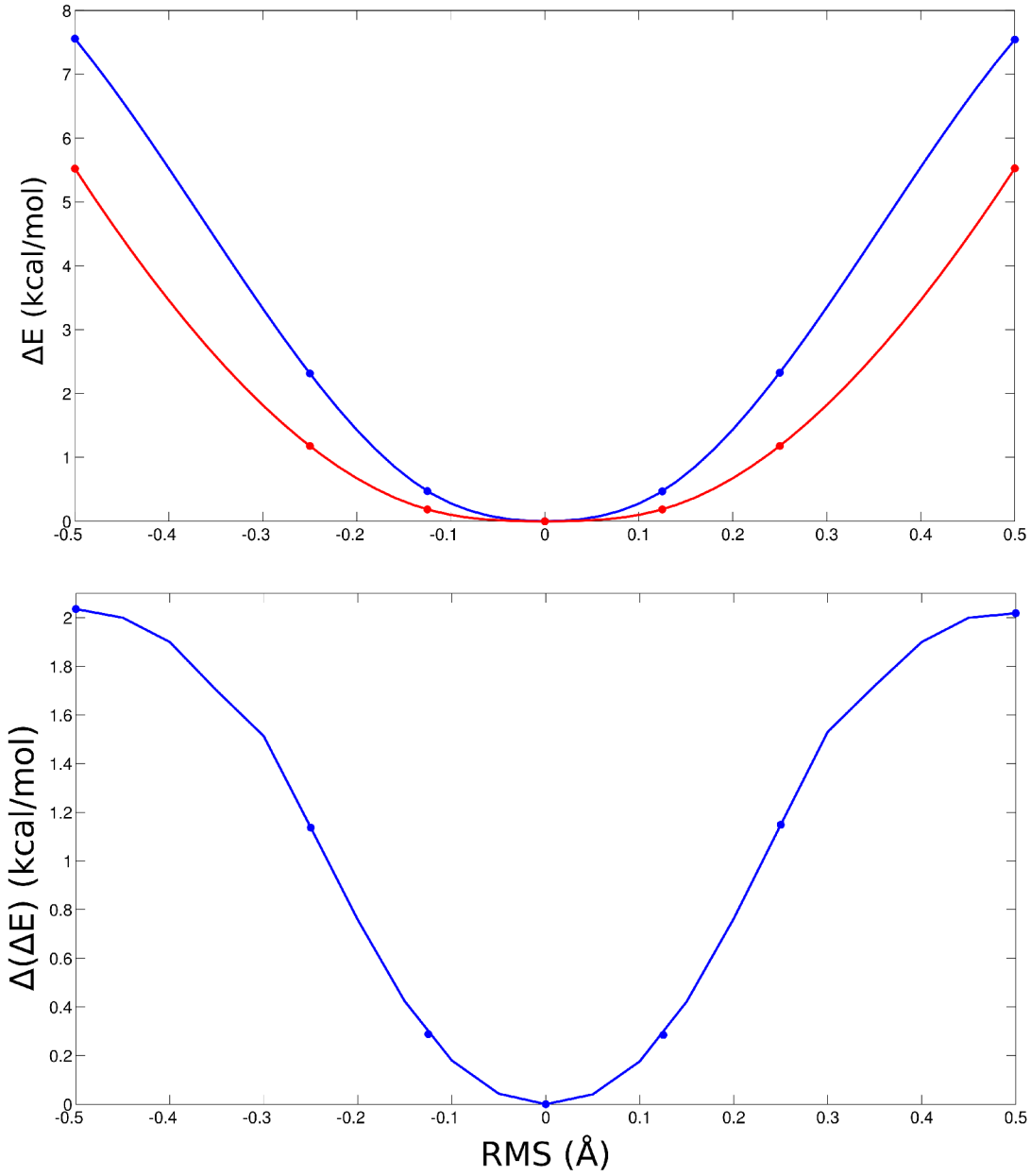


Figure S6. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***nst*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

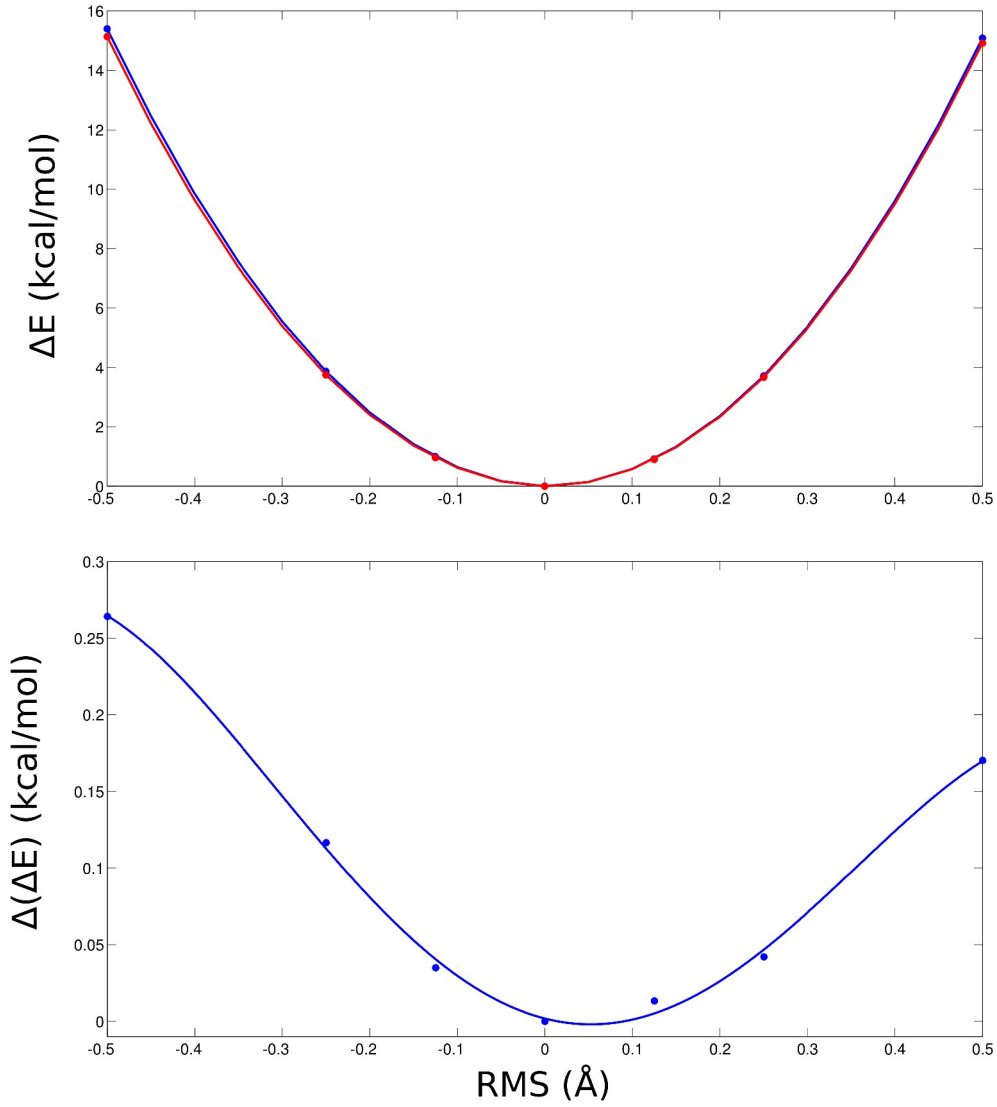

ΔE (kcal/mol)
16
14
12
10
8
6
4
2
0
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
Δ(ΔE) (kcal/mol)
0.3
0.25
0.2
0.15
0.1
0.05
0
RMS (Å)

Figure S7. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***trx*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

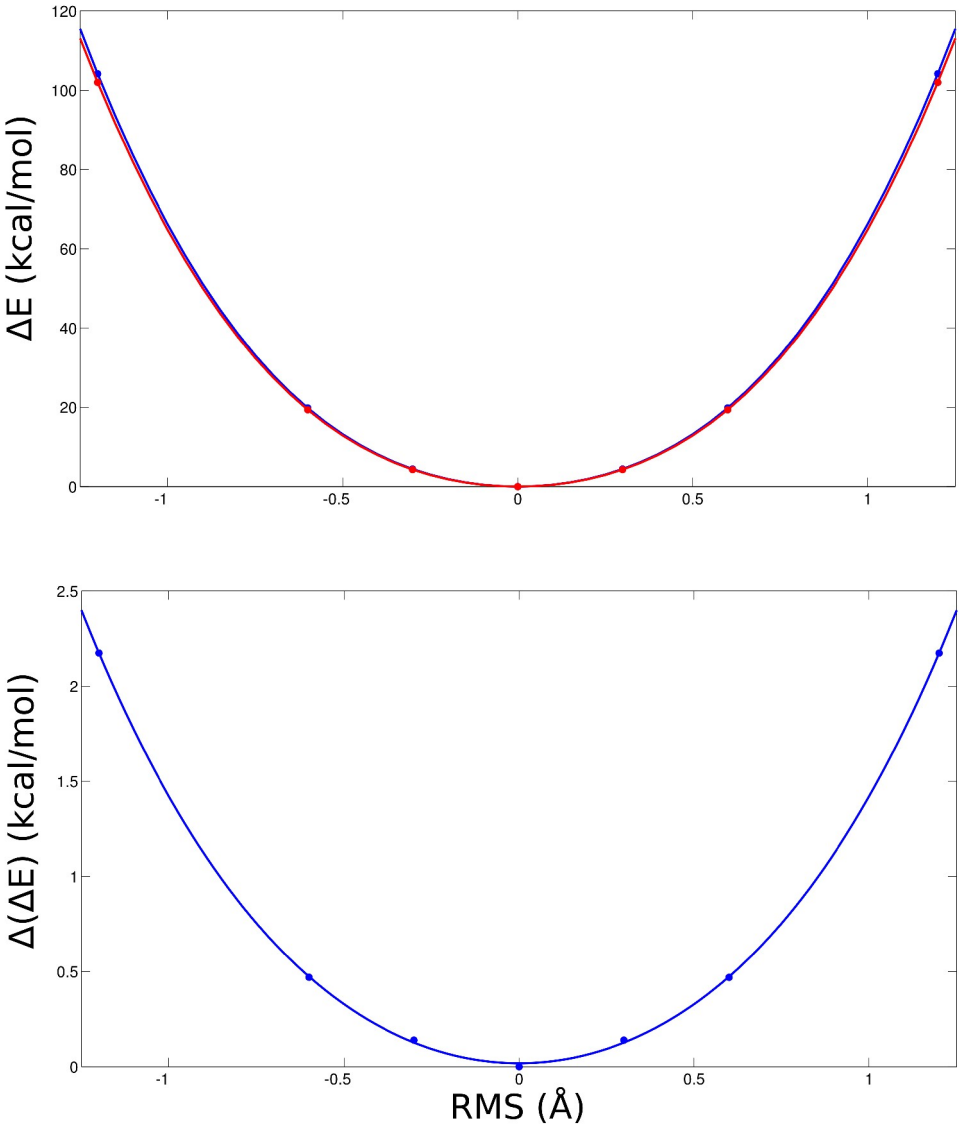

ΔE (kcal/mol)
120
100
80
60
40
20
0
-1
-0.5
0
0.5
1
Δ(ΔE) (kcal/mol)
2.5
2
1.5
1
0.5
0
-1
-0.5
0
0.5
1
RMS (Å)

Figure S8. ***Top*****. Energy profiles (kcal/mol) for the distortion of the heme following the** ***rot*** **mode in oxy (blue) and deoxy (red) states.** ***Bottom*****. Difference between the two distortion energy profiles.**

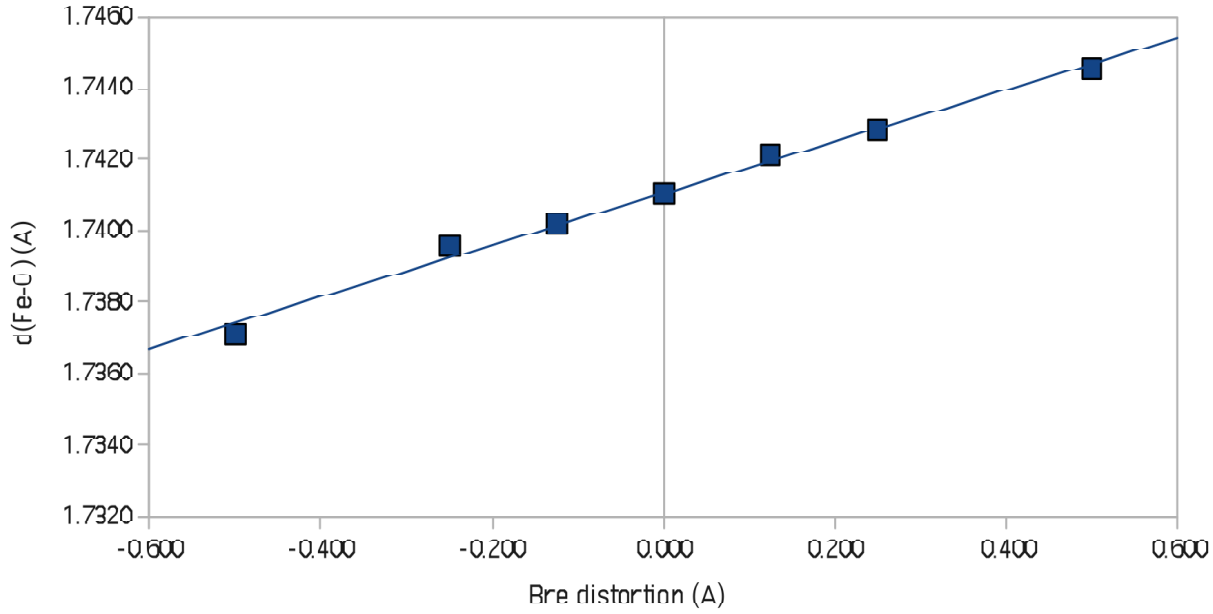


Figure S9. Effect of the *bre* mode in the d(Fe-O) distance.

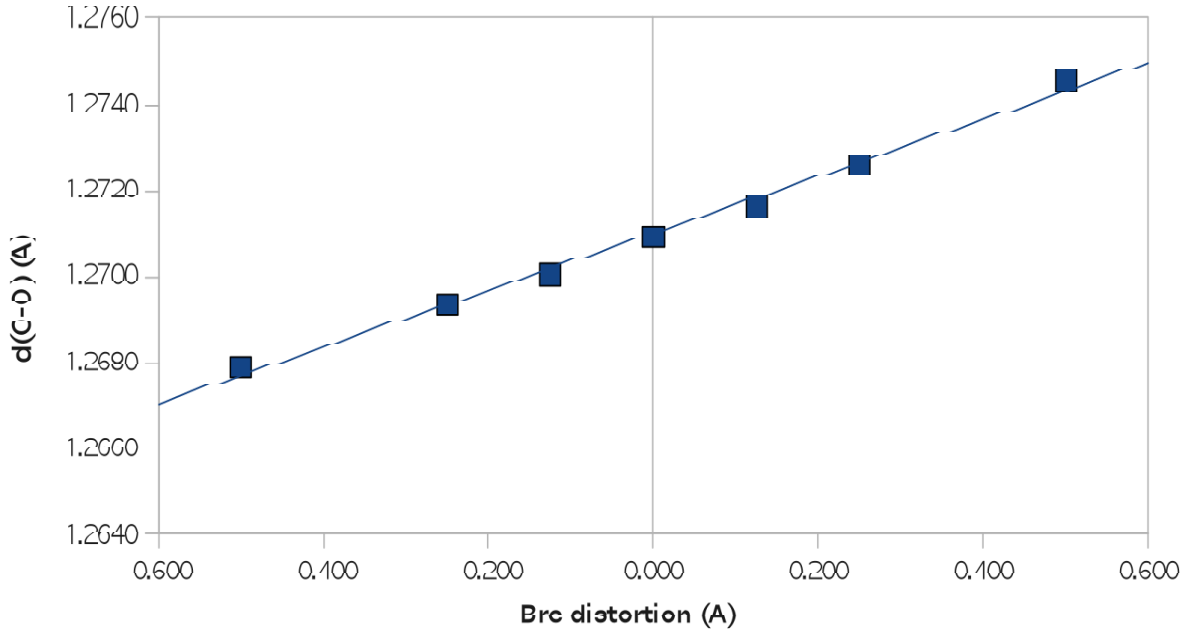


Figure S10. Effect of the *bre* mode in the d(O-O) distance.

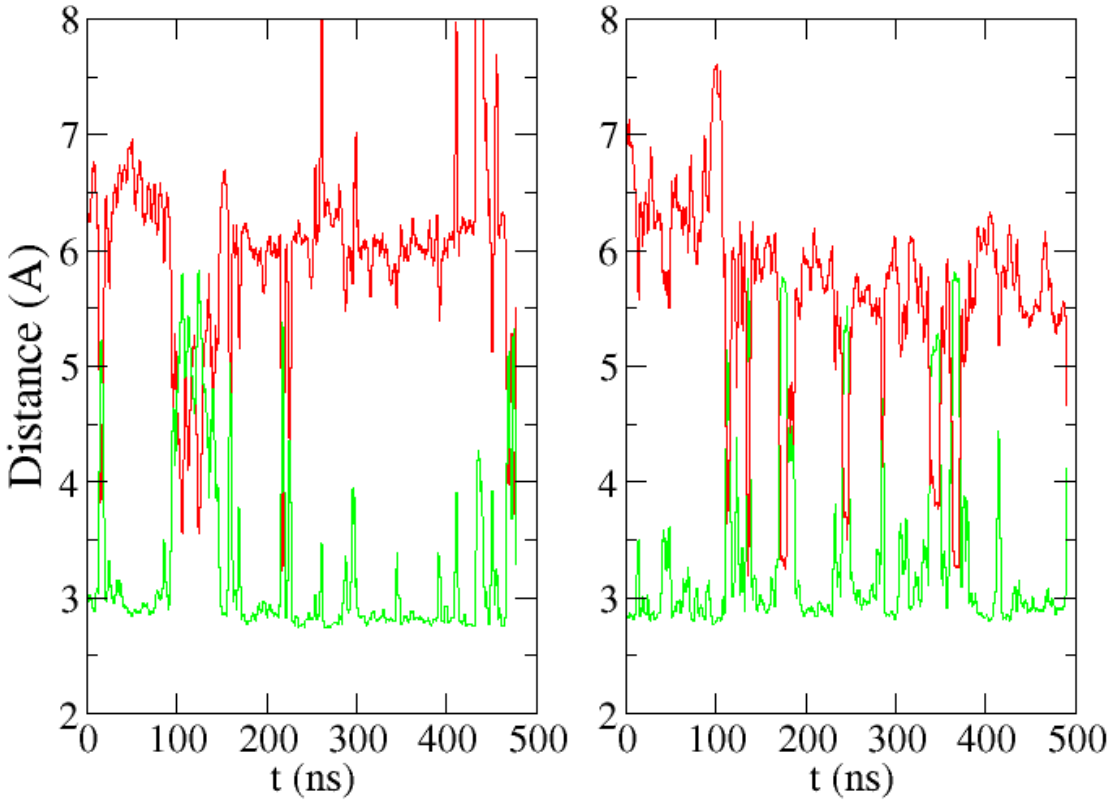


Figure S11. Time evolution of the distances between the hydroxyl group of TyrB10 and a) the heme-bound O2 (red) or the carbonyl oxygen of LeuE5 (green) along the trajectory sampled in a 500 ns molecular dynamics simulation of oxygenated Pgb. The left and right plots denote the evolution of the distances in the two subunits of the dimer.

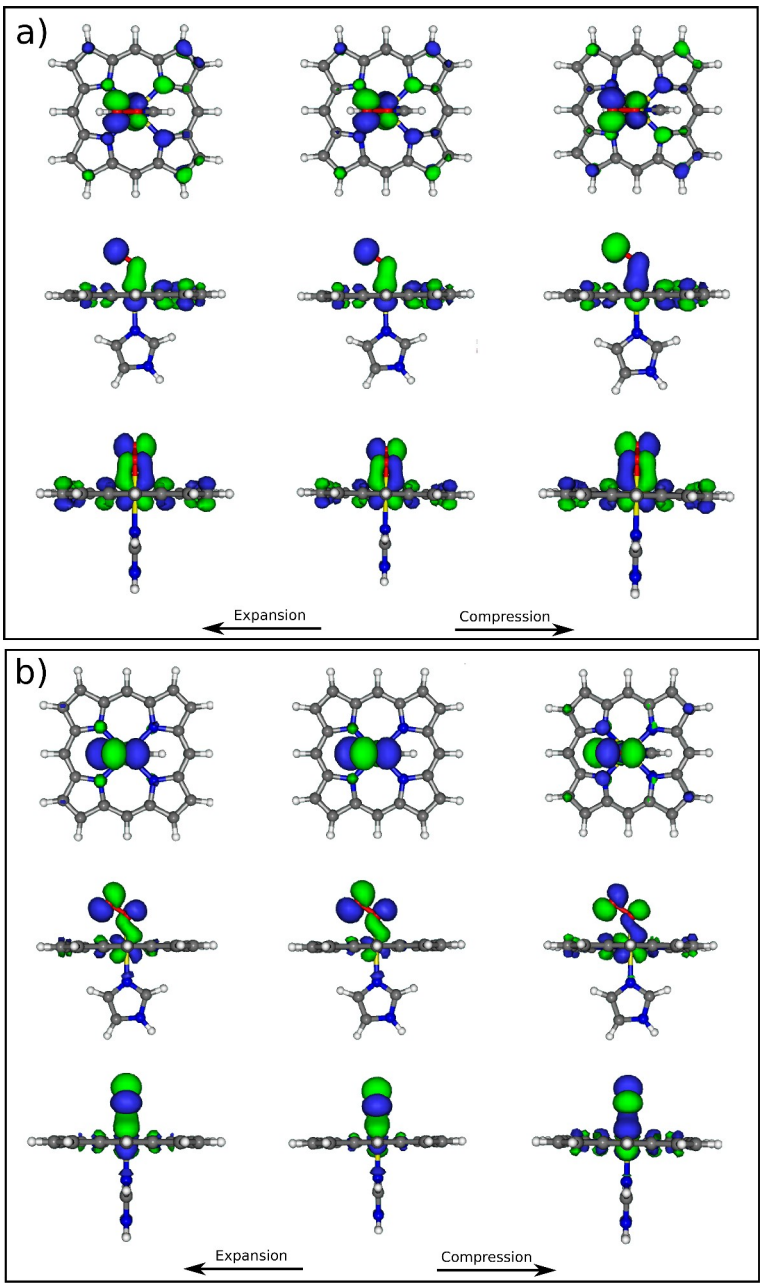


Figure S12. Side and upper views of selected NBO frontier orbitals showing the Fe-O_2 bonding orbitals