

Docking and electron transfer studies between rubredoxin and rubredoxin : oxygen oxidoreductase



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Abstract: The interaction and electron transfer (ET) between rubredoxin (Rd) and rubredoxin: oxygen oxidoreductase (ROO) from *Desulfovibrio gigas* is studied by molecular modelling techniques. Experimental kinetic assays using recombinant proteins show that the Rd reoxidation by ROO displays a bell-shaped dependence on ionic strength, suggesting a non-trivial electrostatic dependence of the interaction between these two proteins. Rigid docking studies reveal a prevalence for Rd to interact, in a very specific way, with the surface of the ROO dimer near its FMN cofactors. The optimization of the lowest energy complexes, using molecular dynamics simulation, shows a very tight interaction between the surface of the two proteins, with a high probability for Rd residues (but not the iron centre directly) to be in direct contact with the FMN cofactors of ROO. Both electrostatics and van der Waals interactions contribute to the final energy of the complex. In these complexes, the major contributions for complex formation are polar interactions between acidic residues of Rd and basic residues of ROO, plus substantial non-polar interactions between different groups. Important residues for this process are identified. ET estimates (using the Pathways model), in the optimized lowest energy complexes, suggest that these configurations are efficient for transferring electrons. The experimental bell-shaped dependence of kinetics on ionic strength is analysed in view of the molecular modelling results, and hypotheses for the molecular basis of this phenomenon are discussed.

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