

Structural insights into the electron/proton transfer pathways in the quinol:fumarate reductase from *Desulfovibrio gigas*

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Abstract

The membrane-embedded quinol:fumarate reductase (QFR), involved in the anaerobic respiration in anaerobic bacteria, catalyzes the reduction of fumarate to succinate by quinol in the anaerobic respiratory chain to produce utilized chemical energy. The electron/proton-transfer pathways in QFRs remain controversial. Here we cultured a large amount the anaerobic sulphate-reducing bacterium *Desulfovibrio gigas* (*D. gigas*) in anaerobic conditions. Subsequently, we purified, crystallized and determined the crystal structure of QFR at 3.6 Å resolution. The structure of the *D. gigas* QFR is a homo-dimer, each protomer consisting of two hydrophilic subunits, A and B, and one transmembrane subunit C, together with six redox cofactors including two *b*-hemes. One menaquinone molecule bound near heme *b_L* in the hydrophobic subunit C was observed. This location of the menaquinone-binding site differs from the menaquinol-binding cavity proposed previously for QFR from *Wolinella succinogenes* (*W. succinogenes*). The observed bound menaquinone might serve as an additional redox cofactor to mediate the proton-coupled electron transport across the membrane. Based on the comparisons with available QFR structures of *W. succinogenes* and *E. coli* and armed with these structural insights in *D. gigas* QFR, we propose electron/proton-transfer pathways in the quinol reduction of fumarate to succinate in the *D. gigas* QFR and emphasize some key residues in *D. gigas* QFR involved in the electron/proton-transfer pathways.

Keywords – quinol:fumarate reductase (QFR), electron/proton-transfer pathways, *Desulfovibrio gigas* (*D. gigas*), anaerobic respiration