**Crystal structures of the S64C mutant monomer and dimer from *desulfovibrio vulgaris* in the semiquinone state.** [a]Gabriella Bombieri, [a]Roberto Artali, [b]Davide Cavazzini, [c]Gianfranco Gilardi, [a]Nicoletta Marchini, [b]Gian Luigi Rossi [a]*Institute of Pharmaceutical Chemistry University of Milano,Italy,* [b]*Department of Biochemistry and Molecular Biology University of Parma.Italy* [c]*Department of Biological Sciences ,ImperialCollege,London.*
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Flavodoxins are small flavoproteins of 14-23 kDa having as cofactor flavin mononucleotide (FMN), found in many microorganisms, where they act as electron carriers at low oxidation-reduction potentials. FMN can accept two electrons and exist in the oxidized, semiquinone and hydroquinone states. Its interactions with the apoprotein modify the two one-electron redox potentials with positive shifts of the midpoint potential at pH 7of the oxidized/semiquinone couple and negative for the semiquinone/hydroquinone couple. As general trend for the structures of flavodoxins in different oxidation states[1],the reduction to the semiquinone state is accompanied by a movement of the peptide at a glicine residue allowing the formation of a hydrogen bond between the carbonyl oxygen of the glicine and the N(5)H of the reduced FMN. The monomer and dimer of S64C in the semireduced forms crystallize in the tetragonal system space group $P4_32_12$ a=b=50.49,c=137.03 Å (monomer) and $P4_12_12$ a=b=55.05,c=122.62 Å (dimer).The semireduced forms were obtained from the oxidized ones by reduction in aerobic conditions with sodium dithionite. Data sets were collected with syncrotrone radiation(ELECTRA beam line,Trieste,Italy).Structural changes were observed in both monomer and dimer forms with conformational changes at the 60-loop similar to those occurring in the S35C mutant[2] upon reduction to the semiquinone form.

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