Crystal Structures of *ox* and *sq* S64C Flavodoxin (*D. vulgaris*) Monomer and Dimer

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The crystal structures of the monomer and homodimer of S64C mutant from *D. vulgaris* in the oxidized and semiquinone states have been determined, at 1.80Å resolution with diffraction data at 100K, by molecular replacement using as starting model the wild type structure [1]. The interest for the new mutant S64C is due to the location of Cys64 in a key region for the interaction with the cofactor FMN and in a position favourable to the formation of homo- and heterodimers.

The structures of *ox* and *sq* S64C monomer crystallizes in the space group $P4_32_12$ and have the general fold of flavodoxin family. The pattern of hydrogen bonds between the protein and FMN is similar to that of the wild type. The main structural differences between the *ox* and *sq* monomer are in the loop-60, that is involved in a new hydrogen bond with the cofactor upon reduction [2]. The two forms of the dimeric S64C mutant crystallize in the space group $P4_12_12$ and the dimer link is due to Cys64, that makes the disulfide bridge with a simmetry related mate. These structural studies provide the seminal information towards a better understanding of the role of the protein moiety in tuning the redox potential and, therefore, the electron transfer.

[1] Artali R., Bombieri G., Cavazzini D., Meneghetti F., Gilardi G., Rossi G.L., Sadeghi S.J., *Acta Cryst. D*, 2002, **58**, 1787. [2] Watt W., Tulinski A., Swenson R.P., Watenpaugh K.D., *J. Mol. Biol*., 1991, **218**, 195.

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