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Flavodoxin from the Sulfate Reducing Bacterium *Desulfovibrio vulgaris*. Its Structure at 2.5 Å Resolution

K. D. WATENPAUGH, L. C. SIEKER, and L. H. JENSEN

Department of Biological Structure, University of Washington, Seattle, U.S.A.

and J. LE GALL and M. DUBOURDIEU

Department of Biochemistry, University of Georgia, Athens, U.S.A.

L. D. B., C. N. R. S., Marseille, France

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Protein structure, X-ray diffraction, Flavodoxin, *Desulfovibria vulgaris*

Crystals of oxidized *Desulfovibrio vulgaris* flavodoxin have been studied by X-ray diffraction techniques. The structure has been determined at 2.5 Å resolution. The molecule consists of a pleated sheet core with two sections of helix on each side of the sheet. The FMN group is distinguishable: it is mostly burried but 7- and 8-Methyl groups appear to be at the surface of the protein.

We report here the data obtained from a 2.5 Å resolution electron density map of *D. vulgaris* flavodoxin. The electron density map was relatively easy to interpret with only a few minor breaks in the main chain and no crossovers between neighboring molecules. The molecules of flavodoxin are approximately oblate spheroids of dimensions 25 Å × 40 Å × 40 Å, packed in the crystal lattice as shown in Fig. 1. There are large channels of solvent between molecules alternately parallel to the x-axis and the y-axis. The molecule essentially consists of a central portion of five sections of chain in a parallel pleated sheet configuration with two sections of helix on each side of the pleated sheet as shown in Fig. 1. Approximately 1/3 of the residues are involved in the pleated sheet, 1/3 in the helices and 1/3 in extended chain or other configurations.

Requests for reprints should be sento to K. D. WATENPAUGH, Department of Biological Structures, University of Washington, *Seattle*, U.S.A.

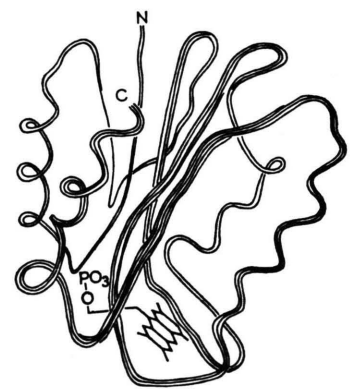

Fig. 1. The conformation of *D. vulgaris* flavodoxin peptidic chain including the position of FMN.

The sequence of this flavodoxin has not been completed yet and we cannot identify most residues with any degree of certainty. It does appear that none of the cysteine are involved in disulfide bridges or in binding to the FMN (flavin mononucleotide).

The FMN group is distinguishable from the protein. Fig. 2 shows the electron density through the plane of the flavin group. The position of the FMN in the

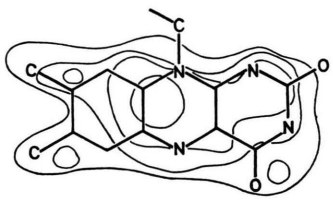

Fig. 2. Electron density through the plane of the isoalloxazine ring.

molecule is shown in Fig. 3. The phosphate position is at the largest peak in the Fourier map and is relatively buried in the protein as is the ribityl and most of the flavin. Only the methyl groups on the benzenoid ring of the flavin appear to be on the surface of the protein. Two of the three phosphate oxygens (excluding the oxygen bonded to C5′) are hydrogen bonded to atoms in the poly-peptide chain and the third oxygen to an atom in a residue. The two carbonyl oxygens on the pyrimidine ring of the

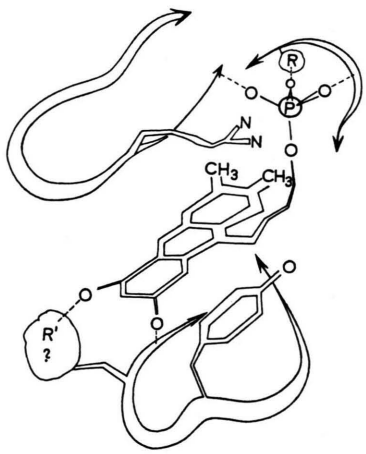

Fig. 3. Partial conformation of the protein around the FMN.

flavin are hydrogen bonded to the protein (one to the peptide chain and one to a residue). An aromatic group (probably tyrosine) is parallel to the plane of the flavin on one side of it. Another residue hydrogen bonded to atoms in the poly-peptide chain is roughly parallel to the flavin on the opposite side.