Comparison of the monomer structure of the FMN binding protein from *Desulfovibrio vulgaris* obtained by NMR and molecular dynamics simulation approaches

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Flavin mononucleotide (FMN)-binding proteins (FBPs) play an important role in the electron transport process in bacteria. In this work, the structures of the FBP from *Desulfovibrio vulgaris* (Miyazaki F) (*Dv*FBP) were compared between those obtained experimentally by nuclear magnetic resonance (NMR) spectroscopy and those derived from molecular dynamics simulations (MDSs). A high residue root of mean square deviation (*RMSD*) was observed in residues located at both sides of the wings (Gly22, Glu23, Asp24, Ala59, Arg60, Asp61, Glu62, Gly75, Arg76, Asn77, Gly78, and Pro79), whilst a low residue *RMSD* was found in residues located in a hollow of the structure (Asn12, Glu13, Gly14, Val15, Val16, Asn30, Thr31, Trp32, Asn33, Ser34, Gly69, Ser70, Arg71, and Lys72). Inter-planar angles between the Phe7 and Iso and between the Phe7 and Trp106 residues were remarkably different between the MDS- and NMR-derived *Dv*FBP structures. Distribution of the torsion angles around the covalent bonds in the aliphatic chain of FMN were similar in the MDS- and NMR-derived structures, except for those around the C1'-C2' and C5'-O5' bonds. Hydrogen bond formation between IsoO2 and the Gly49 or Gly50 peptide NH was formed in both the NMR- and MDS-derived structures. Overall, the MDS-derived structures were found to be considerably different from the NMR-derived ones, which must be considered when the photoinduced electron transfer in flavoproteins is analysed with MDS-derived structures.