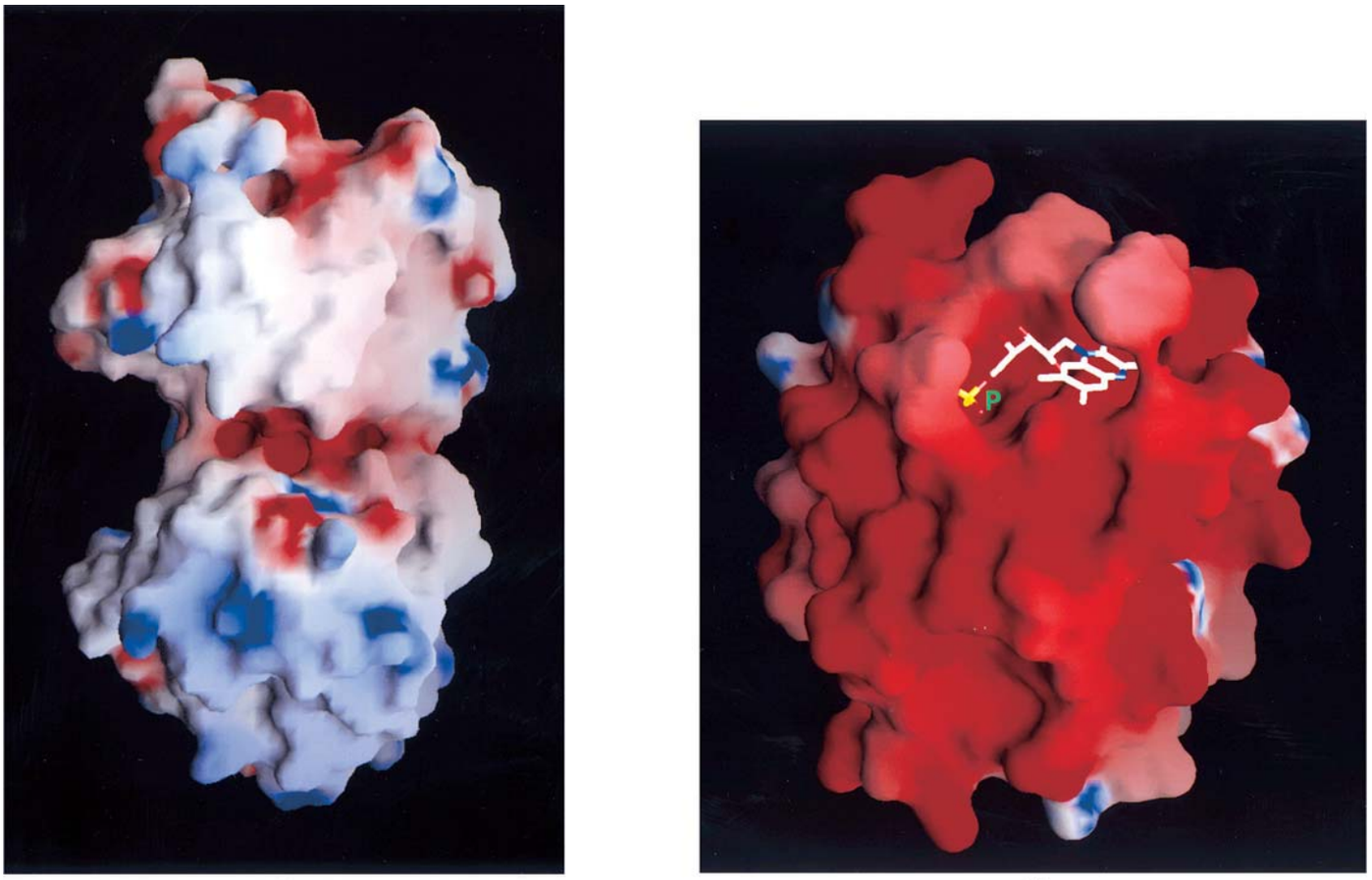

Fig. 23.2.5.3. Electrostatic surface potential of (*a*) the phosphate-binding protein and (*b*) flavodoxin. The molecular surface electrostatic potentials, calculated and displayed using *GRASP* (Nicholls *et al.*, 1991), are $-10\,kT$ (red), neutral (white) and $+10\,kT$ (blue) [see Ledvina *et al.* (1996) for more details]. (*a*) Wild-type phosphate-binding protein based on the X-ray structure of the open cleft, unliganded form (Ledvina *et al.*, 1996). The phosphate-binding site is located in the cleft (with negative surface potential) in the middle of the molecule and between the two domains. (*b*) Flavodoxin with bound flavin mononucleotide (FMN). The phosphoryl group (P) of the FMN is bound in a pocket with intense negatively charge surface potential. The surface potential was calculated without the bound flavin mononucleotide using the structure from the Protein Data Bank (PDB code: 2fox).

bonding interactions with only uncharged polar residues for anion binding and electrostatic balance, a non-complementary surface potential is not a barrier to binding. This conclusion is supported by very recent fast kinetic studies of binding of phosphate to PBP and the effect of ionic strength on binding (Ledvina *et al.*, 1998).

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references