Figure 39.This domain contains a slightly distorted tetrahedral [Fe(Cys)4] site that has a high homology to D. gigas desulforedoxin (Dx).364b This site, which is often referred to as "center I", was initially proposed to mediate intradomain electron transfer between a 2Fe-SOR redox partner and its SOR active center, but no evidence supporting this claim has been produced so far. In fact, the Fe- Fe distance is about 25 A, too large to allow catalytically significant intramolecular electron transfer. Instead, Emerson et al. have shown that the disruption of center I has no effect on the in vitro or in vivo activity of the D. vulgaris 2Fe-SOR.367b Additionally, the T. pallidum 1Fe-SOR, which can be viewed as a "naturally mutated" 2Fe-SOR that lost center I, retains its efficient in vitro and in vivo SOR activity.386b The ~15 residues loop connecting the two domains in the 2Fe-SORs or between the short 310 helix and the catalytic domain contains the mostly conserved (E)(K)HxP-motif.The change in conformation upon oxidation/reduction is expected to also occur in 2Fe-SORs, and indeed Fourier transform infrared (FTIR) studies suggest that the glutamate binds the Fe3+ center in the SORs from D. baarsii and T. pallidum and that this process is coupled to the change in the Fe redoxstate.385b Unfortunately, no crystallographic data have so far supported the binding of the glutamate ligand to the center in 2Fe-SORs, probably due to the difficulty of maintaining these enzymes in the Fe3+ state, in part due to X-ray-induced photoreduction of the protein during structural data collection.71b,389a,390 7.3.3.(A) Superimposition of 1Fe-SOR (blue) and 2Fe-SOR (red) monomers (PDB codes: 1DO6 and 1DFX); (B) structural conservation of amino acid residues in the monomer of 1Fe-SOR, mapped over P. furiosus structure and made using ConSurf;398,420 and (C) ribbon diagram of the same monomer in B (PDB code: 1DO6).While the SOR reduces superoxide to hydrogen peroxide, P450 binds O2 and catalyzes its two-electron reduction and double protonation to cleave the O-O bond, yielding 1 equiv of water and an enzyme intermediate known as Compound I (see section 7.5).The structure of the reduced center was determined after incubation of P. furiosus SOR crystals with sodium dithionite, showing the typical [Fe(His)4Cys] configuration (PDB code: 1DDK71b), albeit with low Fe occupancy at two of its subunits (~20%).Redox-Linked Structural Changes in the SOR Active Center.Structural conservation in SORs.7.3.2.