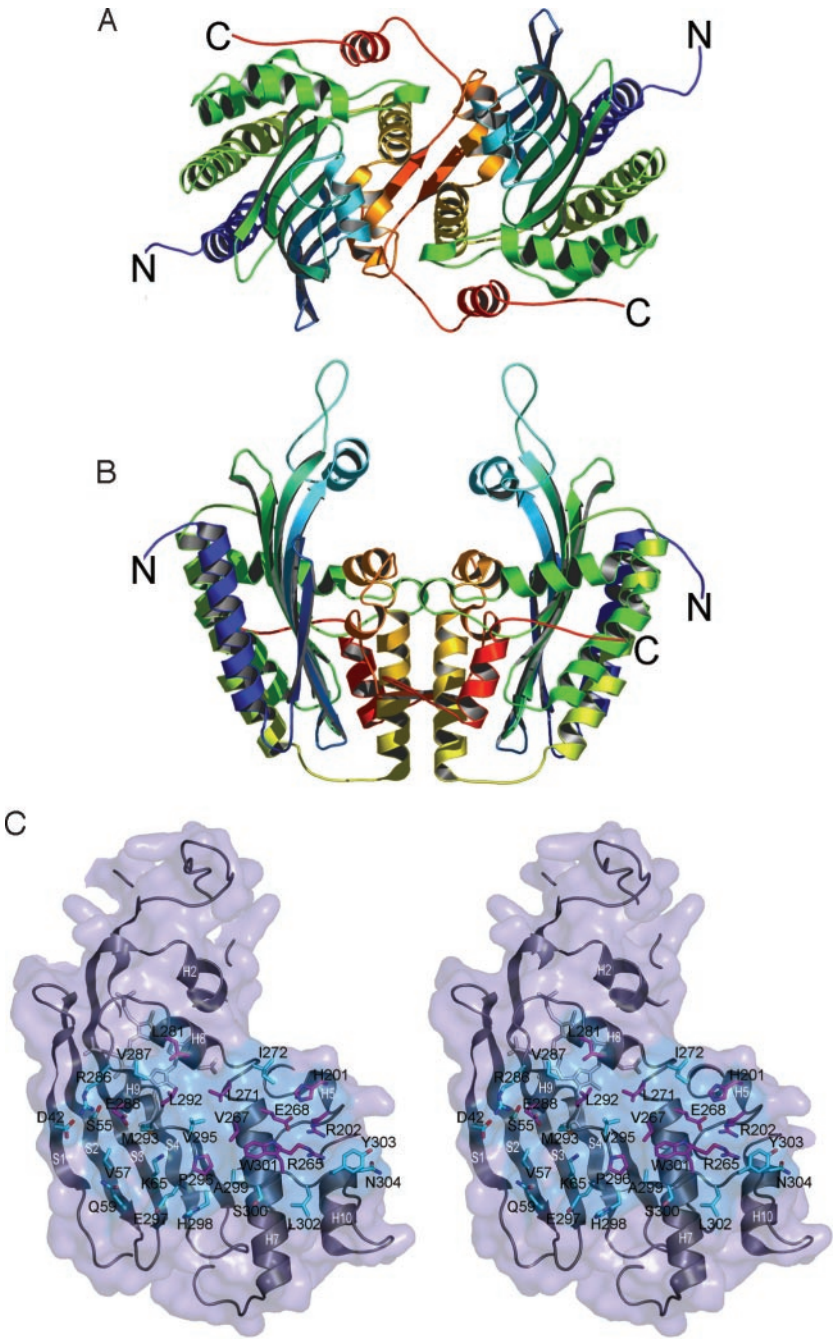

FIG. 4. **The odCPO/Hem13p dimer.** *A* and *B*, ribbon diagrams of the top view, looking along the non-crystallographic 2-fold axis (form I structure), and the side view, looking along the 2-fold axis vertical, respectively. *C*, stereo view of residues at the dimer interface. Residues that lose surface area upon dimer formation (*blue squares* in Fig. 3*B*) are shown explicitly and colored *magenta* if invariant. A modeled substrate molecule (*white*) indicates proximity of the dimer interface to the active-site cavity.

Arg^{8}–Ala^{41}, Gly^{51}–Lys^{91}, Asp^{107}–Lys^{191}, and Gly^{207}–Arg^{265}.

The anomalous scattering of sulfur atoms was used in the classic structure determination of crambin (29). Since then, sulfur anomalous scattering has contributed to a number of structure determinations (30), although only a few of the new structures have resulted from sulfur anomalous scattering data collected on a rotating anode source rather than at a synchrotron (31–34). The primary limitation of this approach is the small anomalous signal obtained from sulfur with conventional copper anode targets. In view of this, it has been suggested that use of a chromium anode, which more than doubles the f'' of sulfur, might allow a general approach to crystal structure determination without the need to prepare heavy atom derivatives, modified protein, or synchrotron radiation (22). To the best of our knowledge, this is the first report of a new protein structure determined using sulfur anomalous scattering data collected on a chromium target rotating anode generator. Our experience shows that this approach can work well for a 30-kDa protein that contains eight ordered sulfur atoms and diffracts to 2.5-Å resolution on a rotating anode source.

The structures of form I and II crystals, both of which contain the full-length protein, were subsequently determined using molecular replacement starting with the form C structure. These models were refined at resolutions of 2.0 Å (form I) and 2.4 Å (form II). The R factors/R_{free} values are 20.7/25.4% (form I) and 20.8/28.2% (form II), and the other statistics also indicate that the models have been refined appropriately (Table I).

Structure Description—The crystallographic refinements resulted in models for the form I and II structures that start from the first ordered residue (Pro^{4} (form I) and Ala^{3} (form II)) and extend to the C terminus. odCPO/Hem13p forms a seven-stranded antiparallel β-sheet that is relatively flat and is covered on both sides by helices (Fig. 3). This structure is essentially identical in all of the crystal forms. Consequently, the form C structure will not be discussed further because, al-