



**Experiment title: A twinned monoclinic crystal form of human peroxiredoxin 5 with eight molecules in the asymmetric unit**

**Experiment number:**  
30.01.138

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## **Abstract**

The monoclinic crystal form of human peroxiredoxin 5 with eight molecules in the asymmetric unit is obtained in exactly the same conditions as the tetragonal form with one molecule in the asymmetric unit, except that the latter was shortly cryo-soaked with halide for derivatization. We observe a merohedral twinning, rather unusual in the monoclinic system and only possible with particular unit-cell dimensions. After detwinning the native and one mercury derivative, the structure was solved by the SIR method with the help of the non crystallographic symmetry. The packing of the monoclinic and tetragonal forms are compared with a special attention to the role of bromide ions in the change of space group after crystallization. The availability of nine (8 monoclinic + 1 tetragonal) independent

molecules allows an analysis of the mobility. The two Cys residues implicated in the peroxide reduction mechanism are located in rigid regions but are covered by mobile loops.