

	Experiment title: Metal-free hydrogenase	Experiment number: LS1918
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Report:

1. Metal-free hydrogenase from *Methanopyrus kandleri*

The hydrogenase from *M. kandleri* crystallize in a monoclinic crystal form and diffract to around 3.0 Å. It was possible to crystallize a selenomethionine labelled protein and to measure the crystals at the wavelengths 0.9791 Å, 0.97923 Å and 0.915 Å. 360° per wavelength was collected. The peak data set resulted in an R_{sym} value of 6.6% (40.8%), in a completeness of 96.5% (87.2%) and in a multiplicity of 2.6 (2.4) within a resolution range 2.8 Å– 50 Å (2.8-2.87). The corresponding values were 7.0% (39.6%), 98.4% (96.6%) and 2.9 (2.7) for the inflection data set (3.2 Å - 50 Å) and 6.0% (31.3%), 81.1% (80.5%) and 2.3 (2.2) for the remote data set (3.5 Å - 30.0 Å). Because of the severe radiation damage the resolution of the data sets had significantly decreased. Most selenomethionines positions could be detected by using the program SnB. After intensive use of the program SHARP and standard phase improvement procedures a polypeptide model for the metal-free hydrogenase could be built. However, the quality of the model has to be improved by collecting new data because of the low resolution (2.8 Å) and the high temperature factor of the structure.

2. Metal-free hydrogenase from *Methanobacter marburgensis*

The crystals of metal-free hydrogenase from *M. marburgensis* normally showed a merohedral twinning. But we found a few very small crystals which were not twinned. Data to a resolution of 3 Å could be collected. The R_{sym} value was 8% and the completeness 84.4%.