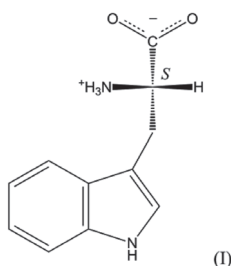


**MS42-03** Finally: The crystal structure of L-tryptophan  
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Due to their obvious interest as the building units of proteins and their role in many metabolic processes, amino acids were among the first chiral compounds to be investigated with X-ray diffraction methods. Prior to the present investigation, crystal structures were known for the enantiomeric form of 18 out of the 20 standard amino acids, with L-tryptophan (L-Trp) and L-lysine still missing. A disorder-free structure in space group *P1* has now been established for L-Trp (I).



Key features are the hydrogen-bond pattern not previously observed in crystal structures of amino acids and the occurrence of no less than **16** molecules in the asymmetric unit. In the crystal structure of DL-Trp [1], with  $Z' = 1$ , aromatic side chains form characteristic hydrophobic layers with  $>N-H \cdots C(\pi)$  interactions. Part of the complexity of (I) is the result of the way the stacking arrangement of DL-Trp is mimicked by letting molecules in two different conformations play the roles of the L- and D-enantiomers in the crystal structure of the racemate. Extended pseudosymmetry gives rise to very unusual systematic absences in the diffraction pattern.

[1] Hübschle, C. B., Messerschmidt, M. & Luger, P. (2004). *Cryst. Res. Technol.* **39**, 274-278.

**Keywords: amino acids; hydrogen-bond patterns; pseudosymmetry**

**MS42-04** Crystallization of bacterioferritin from *Blastochloris viridis*. Weixiao Y. Wahlgren<sup>a</sup>, Hadil Omran<sup>a</sup>, David von Stetten<sup>b</sup>, Antoine Royant<sup>b,c</sup>, Sjoerd van der Post<sup>d</sup> and Gergely Katona<sup>a</sup>, <sup>a</sup> Department of Chemistry and Molecular Biology, University of Gothenburg, SE-40530 Göteborg, Sweden, <sup>b</sup> European Synchrotron Radiation Facility, 41 rue Jules Horowitz, 38027 Grenoble Cedex 1, France, <sup>c</sup> Institut de Biologie Structurale Jean-Pierre Ebel, CNRS CEA Université Joseph Fourier, 41 rue Jules Horowitz, 38027 Grenoble Cedex, France, <sup>d</sup> Proteomics Core Facility, University of Gothenburg, Medicinaregatan 7, SE-413 90 Göteborg, Sweden  
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Iron has been proved to be essential for cell growth and evolution of most organisms, therefore disorder in iron metabolism leads to harmful consequences. Bacterioferritins and their closely related eukaryotic relatives play a key role in storing irons in an accessible form and protect the cell from oxidative damage. They self-assemble to form a hollow protein shell which contains the mineralized iron core. In order to convert the toxic ferrous to the insoluble ferric form of iron, bacterioferritins use molecular oxygen to perform the oxidation. How this process is catalyzed at the ferroxidase di-iron active site is still a matter of debate. Other intriguing process is the import of iron and phosphate ions into the cavity for which several pores were suggested to play a role. Here we report high resolution structures (1.58-1.80 Å) of a bacterioferritin from the purple bacterium *Blastochloris viridis* in different active site conformations upon different soaking treatments. In the absence of genomic information the amino acid sequence has been determined by the combination of nucleotide sequencing and *de novo* sequencing using tandem mass spectrometry. Upon Fe(II) and urea treatment the ferroxidase site undergoes reorganization as seen in bacterioferritin from *Escherichia coli* and *Pseudomonas aeruginosa*. When soaking with Fe(II) only, a closely bound small molecular ligand is observed close to Fe<sub>1</sub> and the coordination of Glu94 to Fe<sub>2</sub> changes from bidentate to monodentate. Density functional theory calculations indicate that the bound ligand is most likely a water or hydroxide molecule representing a product complex. The sequence and structure of the pore regions and different pore sizes between different species have also been examined. The structure of this new bacterioferritin form puts a number of mechanistic issues into a new perspective, and provides insight into the function of this remarkable enzyme.

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**Keywords: bacterioferritin; ferroxidase center; heme; iron storage; specific iron channel**