Crystal structure of a 6.5 MDa bacterial microcompartment shell

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Many bacteria contain self-assembling organelles composed entirely of protein. These bacterial microcompartments consist of an enzymatic core encapsulated by a selectively permeable protein shell. The best known example is the carboxysome for CO₂ fixation, and there are a number of microcompartments that are involved in degradation of various organic compounds. The shell sequesters enzymatic reactions from the cytosol to prevent undesired side reactions and protect the cell from toxic intermediates. There is a wealth of structural information for single building blocks but the principles of shell assembly have remained elusive. We present the X-ray crystal structure of an intact shell from *Haliangium ochraceum* at a resolution of 3.5 Å, revealing the basic principles of bacterial microcompartment shell construction. Half of the particle with icosahedral symmetry is found in the asymmetric part of the C222₁ unit cell with dimensions of 394x638x642 Å. The interactions we see in the crystal structure are mediated by highly conserved and are likely to apply to all functionally diverse organelles and can inform the design and engineering of shells with new functionalities.

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