Using Surface-Bound Rubidium Ions for Protein Phasing

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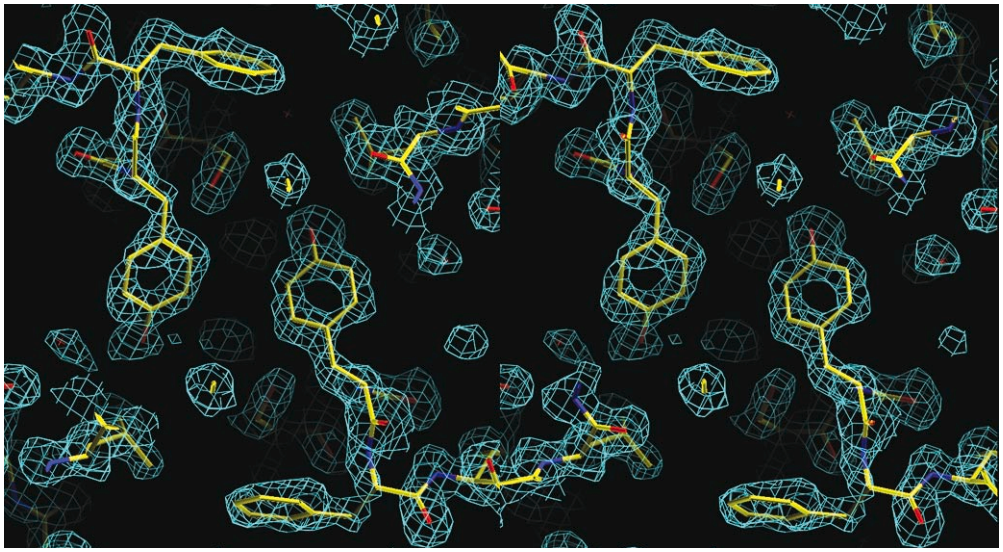

FIG. 1. Stereo view of representative part of the electron-density map obtained with experimental phases calculated with the program SHARP and solvent flattening procedure as implemented in SHARP at the 1 σ level.

Abstract

Rubidium is a monovalent metal that can be used as a counter ion in protein solutions. We used x-ray anomalous scattering from rubidium ions bound to protein surface for phasing of crystal structure of hsp60 apical domain from *Thermus thermophilus*. Multiple-wavelength anomalous dispersion (MAD) data were collected at SBC (Sector 19-ID) from the crystal obtained from solutions with 0.2 M rubidium salt. One molecule of protein of 147 amino acids binds one well-ordered and one poorly ordered rubidium atom. Phases calculated with the program SHARP were sufficient for automatic tracing and side-chain assignment by the program ARP/wARP. Our data show that bound rubidium ions can be used to determine protein structures and to study interaction of monovalent metal ions with proteins and other macromolecules.

Acknowledgments

We wish to thank all members of the Structural Biology Center (SBC) at Argonne National Laboratory for their help in conducting experiments and for fruitful discussions.

This research was supported by the U.S. Department of Energy, Office of Biological and Environmental Research, under Contract No. W-31-109-ENG-38.