Crystal structure of the *E. coli* YrdC protein

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Introduction

As part of a structural genomics pilot project, the crystal structure of the *E. coli* YrdC protein was determined at 2.0 Å resolution. The analysis reveals that the protein folds into a compact α/β structure with a new fold. Comparisons of the YrdC structure with those in the Protein Data Bank (PDB) database indicate no structural similarity to any other protein.

Methods and Materials

Diffraction data to a maximum resolution of 1.96 Å were collected at 100 K on the 19-ID beamline of the Structural Biology Center at the Advanced Photon Source, Argonne, IL, using a 3 x 3 mosaic CCD detector. Data were integrated and merged in the HKL 2000 suite to a maximum resolution of 2 Å. Multiwavelength Anomalous Diffraction (MAD) data were collected at three wavelengths on a single Se-Met YrdC crystal.

Results and Discussion

The structure of YrdC was determined by the MAD method. Two Se sites were determined in each of the two molecules per asymmetric unit, and MAD phases were calculated with CNS-solve. Solvent flipping and Noncrystallographic Symmetry (NCS) density averaging significantly improved the initial map, showing a clear chain trace in most regions except for the first three residues and six residues at the C terminus. The structural model was built using program O and refined using positional, simulated annealing, and temperature factor refinements with program CNS. The free R-factor was monitored by setting aside 10% of the reflection as a test set. Along with two YrdC molecules, 386 water molecules and two phosphate ions were built into the electron density map. The Ramachandran plot calculated with the program PROCHECK shows that 100% of the nonglycine and nonproline residues in the final model lie in the most-favored and additional allowed regions. The final R-work and R-free are 20.2% and 21.3%, respectively, for reflections in the resolution range between 25.0 and 2.0 Å (bulk solvent correction). The rms deviations from standard bond lengths and angles are 0.009 Å and 1.5°, respectively [1].

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Reference

[1] M. Teplova, V. Tereshko, R. Sanishvili, A. Joachimiak, W. F. Anderson, and M. Egli, Publication in preparation (2000).