

# High-Resolution Data Collection at the 17-ID Undulator Beamline at the APS

K. J. Kim, J. Chrzas, L. Keefe, W. Lavender, K. McCarthy, J. Rios, J. Fait,\* A. J. Howard

*Illinois Institute of Technology, Chicago, IL, U.S.A.*

*\*Current Address: Southeast Regional Collaborative Access Team, University of Georgia, Advanced Photon Source, Argonne, IL, U.S.A.*

## Introduction

Third-generation synchrotron x-ray sources are playing an increasing role in macromolecular crystallography. In addition to providing the capability of performing multiwavelength experiments for initial phasing, third-generation sources offer brilliant x-ray beams that often enable collection of data to higher resolution than can be obtained elsewhere. Higher resolution data collection gives better electron density maps, and these in turn provide a more detailed understanding of molecular structure and function. We report high-resolution data collection from four crystalline proteins at 17-ID undulator beamline at the APS and a comparison with published structures derived from non-APS data.

## Materials and Methods

Four commercially available proteins—bovine insulin, chicken citrate synthase, hen egg-white lysozyme, and horse myoglobin—were crystallized for this study. Bovine insulin cubic crystals have been formed from a solution of 0.4 M sodium potassium tartrate, 30% PEG3000. Chicken citrate synthase tetragonal crystals were grown from 1.1 M sodium citrate pH 6.0, and monoclinic crystals from the same well solution with 10 mM acetyl-CoA in the drop. Hen lysozyme tetragonal crystals were grown from 50 mM sodium acetate pH 4.72, 8.25% NaCl, 24% Ethylene glycol. Monoclinic hen lysozyme crystals were grown from 0.1 M sodium acetate pH 4.5, 2 % sodium nitrate. Horse myoglobin crystals were grown from 3.3 M sodium sulfate. X-ray data have been collected from cooled crystals at the 17-ID beamline of the Advanced Photon Source. All data were processed using X-GEN.

## Results

Each of these proteins crystallized in the same space group and with unit cell parameters nearly identical to those found in the published crystal structures; this indicates that the crystals were approximately isomorphous with those studied previously. Bovine insulin cubic crystals diffracted to 1.45 Å, whereas the published structure is based on 1.9 Å data. Chicken citrate synthase tetragonal crystals diffracted to 2.3 Å instead of 2.8 Å,<sup>2</sup> and monoclinic crystals to 1.24 Å instead of 1.6 Å.<sup>3</sup> Hen tetragonal lysozyme crystals diffracted to 1.0 Å instead of 1.33 Å,<sup>4</sup> and monoclinic crystals diffracted to 1.1 Å instead of 1.6 Å. Horse myoglobin monoclinic crystals diffracted to 1.1 Å instead of 1.4 Å.<sup>5</sup> Refinements of these structures at or near these resolution limits are planned.

## Discussion

High-resolution structures are always of interest to protein crystallographers. Several chemical and packing factors determine the resolution limit of a structure. The characteristics of the x-ray source and the detection method employed influence the resolution limit as well, and in obtaining data to higher resolution on these structures we are exploiting a variety of characteristics of the APS storage ring and IMCA-CAT's undulator facilities. Thus, the highly parallel character of 17-ID's beams provides for clear separation of spots and low backgrounds, both of which improve data quality near the limit of resolution, and the reliability and linearity of IMCA-CAT's charge-coupled device detector systems maintain the accuracy of the data.

## Acknowledgments

Data were collected at beamline 17-ID in the facilities of the Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT) at the Advanced Photon Source. These facilities are supported by the companies of the Industrial Macromolecular Crystallography Association through a contract with Illinois Institute of Technology (IIT), executed through IIT's Center for Synchrotron Radiation Research and Instrumentation. Use of the Advanced Photon Source is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

## References

- <sup>1</sup> O. Gursky, J. Badger, Y. Li, and D.L. Caspar, *Biophys. J.* **63**, 1210-1220 (1992).
- <sup>2</sup> D.I. Liao, M. Karpusas, and S.J. Remington, *Biochem.* **30**, 6031-6036 (1991).
- <sup>3</sup> K.C. Usher, S.J. Remington, D.P. Martin, and D.G. Drueckhammer, *Biochem.* **33**, 7753-7759 (1994).
- <sup>4</sup> M.C. Vaney, S. Maignan, M. RiesKautt, and A. Ducruix, *Acta Crystallogr. D Biol. Crystallogr.* **52**, 505-517 (1996).
- <sup>5</sup> K. Chu, J. Vojtechovsky, B.H. McMahon, R.M. Sweet, J. Berendzen, and I. Schlichting, *Nature* **403**, 921-923 (2000).