

Common conventions for interchange and archiving of three-dimensional electron microscopy information in structural biology

J. Bernard Heymann^{a,b}, Mónica Chagoyen^c, David M. Belnap^{a,*}

^a *Laboratory of Structural Biology Research, National Institute of Arthritis, Musculoskeletal and Skin Diseases, National Institutes of Health, Bethesda, MD 20892, USA*

^b *Division of Biology, Caltech, 1200 East California Blvd, Pasadena, CA 91125, USA*

^c *Centro Nacional de Biotecnología—CSIC, Campus Universidad Autónoma, 28049 Madrid, Spain*

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Abstract

Three-dimensional electron microscopy (3DEM) has made significant contributions to structural biology. To accomplish this feat, many image-processing software packages were developed by various laboratories. The independent development of methods naturally implied the adoption of dissimilar conventions—penalizing users who want to take advantage of the wealth of algorithms from different packages. In addition, a public repository of 3DEM research results, the EM Data Bank, is now established. In an era where information exchange is important, standardizing conventions is a necessity. The 3DEM field requires a consistent set of conventions. We propose a set of common conventions named the “3DEM Image Conventions.” They are designed as a standardized approach to image interpretation and presentation. In this regard, the conventions serve as a first step on which to build data-exchange solutions among existing software packages and as a vehicle for homogenous data representation in data archives, such as the EM Data Bank.

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1. Introduction

Biological electron microscopy spans the size range from molecular to cellular structures, providing an important tool to understand the cell and its molecular components. The use of computer image processing techniques greatly enhanced the information gleaned from electron micrographs. Not only were improve-

ments made to the two-dimensional (2D)¹ results obtained from the microscope, image processing made it possible to reconstruct structures in three dimensions.

Three-dimensional electron microscopy (3DEM) has had its greatest usefulness in understanding structures of macromolecular complexes. The structures of several protein complexes were solved to near-atomic resolution by 2D crystallography or helical reconstruction. Images

* Corresponding author. Present address: Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602, USA. Fax: +1 801 422 0153.

E-mail address: David_Belnap@byu.edu (D.M. Belnap).

¹ *Abbreviations used:* 2D, two-dimensional; 3D, three-dimensional; 3DEM, three-dimensional electron microscopy; CIF, crystallographic information file; EM, electron microscopy; EMDB, EM Data Bank; STAR, Self-Defining Text Archiving and Retrieval; XML, Extensible Markup Language.

of randomly oriented particles (“single-particle” images) have led to many reconstructions at resolutions from ~ 40 Å to better than 10 Å. Electron tomography has provided detailed 3D insight into viral and cellular structures approaching a resolution of 40–50 Å. In some cases, dynamic processes have been imaged by 3DEM, including a progression of states showing macromolecular metamorphoses.

With such a powerful tool and wealth of information produced, many and diverse techniques arose to process electron micrographs and reconstruct 2D or 3D maps of the specimens. These techniques were implemented in many software packages. The original packages appeared in the 1960s and 1970s, beginning with the work of DeRosier and Klug (1968).² The original packages benefited from exchanges of code that still form the backbone of several today. Over the years other packages were developed—often derivatives of the original ones. Many of the conventions adopted in the software packages have similar origins. However, even small differences contributed to confusion about the exact meaning of parameters used in image processing and led to multiple conventions throughout the 3DEM field; and now the interchange of information between packages is a serious productivity restraint. Users are typically limited to one package—because the transfer of parameters between packages is non-trivial and time-consuming. Furthermore, the complexity due to convention differences hampers the automation of large-scale processing.

A significant development in the 3DEM field is the establishment of a public database for electron microscopy data named the Electron Microscopy Data Bank (EMDB) (<http://www.ebi.ac.uk/msd>; Editorial, 2003; Fuller, 2003; Henrick et al., 2003; Tagari et al., 2002). This effort was initiated in Europe by the BioImage project (Carazo et al., 1999) and completed by the Integrated Information for Macromolecular Structure (IIMS) project. It is currently part of the European Bioinformatics Institute. Such a public forum requires a single set of common conventions to be able to serve the community in a self-consistent manner.

Here we propose common conventions, which we call the “3DEM Image Conventions,” as well as a set of recommendations for those involved in the task of encoding information for 3DEM digital images. The 3DEM Image Conventions include basic definitions and a common nomenclature relevant to the representation and interpretation of 3DEM data.

The standard conventions are based on four principles:

- *Generality.* The conventions must be applicable across the field with no exceptions.
- *Commonality.* We selected the most widely used or easiest understandable convention in most cases.
- *Clarity.* The most unambiguous statement of a convention is in mathematical form. Otherwise, we attempt to state the convention as clearly as possible.
- *Fairness.* The conventions may not be based on those of any specific software package, but rather evolve within a public forum, such as the EMDB.

Several of the conventions were proposed previously (Heymann, 2001).

The purposes of this document are threefold:

- To propose an open standard set of conventions for the 3DEM field. Some foreseen uses of this open standard are data exchange between software packages and data archiving in the EMDB. The conventions will be publicly available as a set of formal descriptions and specifications.
- To provide a technical recommendation for use in developing a broader consensus on what is required to ensure ‘image data’ interoperability among software packages in the 3DEM field and data exchange among the wider structural biology community (encompassing other structural data, such as atomic models).
- To recommend that the 3DEM community adopt a common parameter-file format for data exchange and archiving, and that all software packages read and write this parameter file.

Our recommendation *does not*:

- Specify a particular design or an implementation of an image-file format or a parameter-file format.
- Compare or list the conventions of current software packages.
- Provide direction on converting parameters from one package to another or on how to extract data from parameter files or data archives. It is our assumption that the responsibility for implementation of the conventions lies with the developers of the various software packages who will write routines to read and write the common parameter file.
- Require software developers to change their internal conventions.
- Provide any tools or data to allow conformance testing.

2. The 3DEM Image Conventions

All of the conventions below relate to digital images and the parameters required to process their content in

² For a summary of the history of 3DEM software and a description of 3DEM software packages available in the mid-1990s, please see Carragher and Smith (1996) and other articles in the same issue of *J. Struct. Biol.* (116 (1), January/February 1996).

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