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There is a pressing need for the archival and curation of raw X-ray diffraction data. However, the relatively large size of these datasets has presented challenges for storage in a single worldwide repository. This problem can be avoided by using a federated approach, where each institution or university utilizes its institutional repository. Institutional repositories are relatively stable and adequately funded, ensuring persistence. Here we describe a simple repository solution utilizing Fedora open source database software, and data annotation and deposition tools that can be deployed at any site cheaply and easily. Datasets and associated metadata from federated repositories are given a unique and persistent handle, providing a simple mechanism for search and retrieval via web interfaces. We call this initiative 'The Australian Repositories for Diffraction Images (TARDIS)' and have created a website (http://www.tardis.edu.au) where the deposition tools can be downloaded freely. The site will also function as a central portal allowing searching and browsing across all registered Australian repositories. In addition to ensuring that valuable data is not lost, the provision of raw data has several uses for the crystallographic community. Most importantly, structure determination can only be truly repeated or verified when the raw data is available. In addition, the availability of raw data is extremely useful for the development of improved methods of image analysis and data processing.

Keywords: raw data, databases, validation

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Virus particle explorer: An X-ray and electron microscopy database for icosahedral virus structures

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Three-dimensional crystal structures of 96 different virus capsids, from 27 families and 42 different genera of viruses, have been solved to near-atomic resolution and deposited in the Protein Data Bank. The enormous amount of information contained in these structures is difficult to access, even for scientists trained in structural biology. Virus Particle Explorer (VIPER) is a web-based (http://viperdb.scripps.edu/) catalogue of structural information that describes the icosahedral virus particles. In addition to high-resolution crystal structures, VIPER now includes virus structures obtained by cryo-electron microscopy (EM) techniques. The VIPER database is a powerful resource for virologists, microbiologists, crystallographers and EM researchers. This presentation will describe the novel features of VIPER, using several examples to show the power of this resource for research and educational purposes.

Keywords: virus structure,, protein-protein interactions, virus assembly

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Metal and small molecule agent environment in macromolecules

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Over 90% of X-ray protein structures deposited in the Protein Data Bank contain ordered small molecules, such as enzyme substrates, cofactors or ions. These ligands can be divided into two groups: molecules that are relevant to protein function, and non-physiological agents introduced during sample preparation (purification, crystallization or cryocooling). Our analysis shows that the structural and chemical quality of small molecule models in protein structures does not correlate with structure resolution. In particular, the analysis of metal-protein interaction distances, coordination numbers, B-factors (displacement parameters), and occupancies of metal binding sites in protein structures determined by X-ray crystallography and deposited in the PDB shows many unusual values and unexpected correlations. Our analysis of cation B-factors versus average B-factors of atoms in the cation environment reveals substantial numbers of structures contain either an incorrect metal ion assignment or an unusual coordination pattern. While validation of polypeptide models is a routine part of protein structure refinement, small molecule models within a protein structure are usually not validated and require new approach to validation process.

Keywords: macromolecular crystallography, macromolecular complex, structural genomics

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On atomic displacement parameters and coordinates in protein structures

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Macromolecular models refined against X-ray diffraction data are typically described by a set of atomic coordinates and atomic displacement parameters (ADPs). During the refinement process, coordinates and ADPs are usually considered independent of each other. However, as can be demonstrated here, up to 50% of the total ADP variation in macromolecular structures may be successfully predicted solely based on the atomic coordinates and just three additional parameters per structure. This finding may have serious implications in macromolecular structure refinement, particularly at low resolution, as well as in structure validation.

Keywords: macromolecular structure refinement, atomic displacement parameter, structure validation