Poster Presentation

The New wwPDB Deposition and Annotation System

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In anticipation of continued growth in the number, size and complexity of the structures that are being studied and deposited in the PDB and EMDB, the Worldwide Protein Data Bank (wwPDB) has developed a new system for deposition and annotation of structural data. The new wwPDB Deposition & Annotation (D&A) system offers a single entry point for depositors from around the world to deposit X-ray, NMR, 3DEM data, receive detailed validation feedback, and preview annotations, all prior to submission. The system will assign not only PDB identifiers upon submission, but also EMDB and BMRB identifiers for 3DEM and NMR data, respectively. Furthermore, the new system is used at all wwPDB processing sites around the globe. After deposition, wwPDB annotators use the system for sequence annotation, ligand annotation, additional structure analysis and validation, and review. Validation functionality implements recommendations from the wwPDB X-ray Validation Task Force and produces a structure validation report for depositor review and submission to scientific journals. Depositors will have the option to use the new system or one of the legacy deposition tools (ADIT, AutoDep) through the end of 2014. At that time, the legacy tools will stop accepting new entries, and will only be available for a limited period of time to complete in-progress deposition sessions. An important feature of the new deposition system is its ability to accept and produce data in PDBx/mmCIF format, which has no limitations in the size or complexity of structures that can be represented. The PDBx/mmCIF Working Group, consisting of software developers from CCP4, Global Phasing Ltd., Phenix, and the wwPDB, have adapted structure determination software packages to produce PDBx/mmCIF format files suitable for deposition. The new wwPDB deposition and annotation will produce more consistent and higher quality archive entries, and will improve the efficiency and throughput of deposition and annotation. The modular design of the system will facilitate incorporating new functionalities and support for hybrid and other methods in the future. wwPDB members are RCSB PDB (supported by NSF, NIH, and DOE), PDBe (EMBL-EBI, Wellcome Trust, BBSRC, NIGMS, and EU), PDBj (NBDC-JST) and BMRB (NLM).

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