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Deposition and Annotation at the RCSB PDB. K. Burkhardt, S. Dutta, Z. Feng, L.-C. Fernandez, V. Guranovic, S. Jain, R. Oughtred, I. Persikova, S. Richman, B. Schneider, H. Yang, J. Yang, J. Westbrook, C. Zardecki, H.M. Berman, Research Collaboratory for Structural Bioinformatics, Protein Data Bank, Rutgers Univ., Piscataway, NJ.

The RCSB Protein Data Bank has developed a variety of tools to facilitate data deposition and validation by the authors of structures. PDB_EXTRACT automatically extracts deposition information from the output files produced by many X-ray crystallographic applications and creates an mmCIF file that can be uploaded into ADIT. ADIT and the Validation Server generate validation reports on coordinate and structure factor files. Ligand Depot is used for ligand identification.

In addition to these tools, annotators use other RCSB-developed and commercially available software and resources for data processing. BLAST, PubMed, and ChemDraw are used to check sequences, citations, and ligands. All structures are visualized using RasMol. The annotator reviews the PDB file and reports; results are sent to the author along with any questions. Once approved by the author, the file is ready for release. The RCSB Citation Tracker and Citation Tool are used to search and extract citation information from PubMed to track structure publication.

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