ANNOUNCEMENT

Re: Letter to the Editor Regarding Deposition of 3D Structural Studies of Biological Macromolecules

Joel L. Sussman* and Geoffrey J. Barton†

*Protein Data Bank, Biology Department, Brookhaven National Laboratory, Upton, New York 11973; and †Macromolecular Structure Group, EMBL Outstation, European Bioinformatics Institute, Genome Campus, Hinxton, Cambridge, United Kingdom

Received March 24, 1998

We are pleased to announce the inauguration of a new deposition site for 3D structural studies of biological macromolecules. Authors using the Web-based tool AutoDep can submit data either to the European Bioinformatics Institute (EBI), UK, or to the Protein Data Bank (PDB) at Brookhaven National Laboratory (BNL), USA. The additional site is expected to facilitate significantly the submission procedure, especially for European researchers.

AutoDep is a Web-based tool originally designed at PDB for automatic submission of macromolecular data into the PDB. Extensive collaboration between EBI and PDB has produced significant changes to the original system allowing for the seamless operation of multiple deposition sites. This includes EBI specifications for standards and protocols to be used in making the code portable and generally more robust.

AutoDep is accessible from the following URLs: BNL-PDB, http://www.pdb.bnl.gov; EBI-MSD, http://autodep.ebi.ac.uk.

Those wishing to submit data using the electronic version of the Deposition Form must continue to deposit directly to BNL using e-mail or FTP.

The submission procedure will be identical, and equivalent, at both sites, but PDB ID codes will be issued by BNL. Data submitted at EBI will be forwarded automatically to PDB after depositors have reviewed the AutoDep-generated entry and diagnostics. Final preparation for archiving and release will be done by PDB staff. We encourage depositors to submit not only the structural results, but also their experimental data, i.e., for crystallographers, X-ray structure factors, and NMR spectroscopists, constraints lists and statisti-

cal data describing the calculated NMR conformers and constraints.

Important notes:

- (i) Submissions can be completed only at the site at which they were started.
- (ii) The option "Based on a previous submission" may be used to simplify submissions by using an earlier AutoDep session as a template. However, depositors will only have access to their earlier submissions at the site where those submissions were originally made.
- (iii) Existing PDB entries may be used as templates by choosing the option "Based on an existing PDB entry." The full set of entries will be available at either site, irrespective of where the original deposition was made.
- (iv) The date of submission for data deposited at EBI will be the corresponding U.S. eastern time of the date when submission is completed at EBI.
- (v) EBI staff will offer assistance (via e-mail: pdbhelp@ ebi.ac.uk) up to the point of submission. Once BNL has issued an ID code, correspondence should be directed to BNL (via e-mail: pdbhelp@pdb.bnl.gov).

Please note that authors should continue to deposit crystal structures of nucleic acids to the Nucleic Acid Database (NDB) at Rutgers, State University of New Jersey, USA, at URL http://ndbserver.rutgers.edu:80/NDB/deposition/index.html.

Experimental data related to NMR studies will also be transferred electronically to the BioMagResBank (BMRB) at the University of Wisconsin-Madison, USA, for further processing and inclusion into the database (http://www.bmrb.wisc.edu) as well.