world wide Protein Data Bank Advisory Committee (wwPDBAC) Report of November 21st 2004 Meeting Washington, D.C.

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wwPDBAC Mission Statement

To help ensure that the Protein Data Bank is maintained for the public good as a secure, single, global archive for experimental structural biology data that is freely accessible in perpetuity.

Meeting Summary

The <u>world wide Protein Data Bank Advisory Committee</u> (wwPDBAC) to the leadership of the <u>Research Collaboratory for Structural Bioinformatics</u> (RCSB), the <u>Macromolecular Structure Database</u> (MSD), and Protein Data Bank Japan (PDBj) met in Washington, D.C. on November 21st 2004. The agenda included

- (1) Overview of wwPDB;
- (2) wwPDB Member Presentations;
- (3) Roles and Responsibilities of the wwPDBAC; and
- (4) Long Term Issues.

The Committee considered various issues and provides the following unanimous commentary and recommendations:

PDB File Format

Commentary:

The flat file PDB format, adopted officially in 1996, has outlived is usefulness, and now represents an impediment to progress in structural biology, particularly for studies of large macromolecular complexes.

Recommendations:

- Preserve a facile means of access to the contents of the PBB via the 1996 flat file PDB format for the foreseeable future.
- Actively promote all future depositions and access to the PDB via PDB Exchange and PDBML format files.
- Provide a detailed timeline for execution of this transition and issue brief progress reports at an appropriate frequency to the wwPDBAC and funding agency representatives.

PDB Entry Remediation

Commentary:

There is a critical, scientific need for distribution of jointly remediated PDB entries, while retaining archival access to original PDB entries.

Recommendations:

- Preserve archival access to all original PDB entries.
- Perform a pilot study to establish a plan plus the resource requirements and timelines for reconciliation of PDB entries remediated at the RCSB and the MSD.
- Following appropriate consultation, execute the plan and issue brief progress reports at an appropriate frequency to the wwPDBAC and funding agency representatives.
- Establish and maintain archival access to annual versions of the PDB, beginning on December 31st 2004.
- Provide access to the remediated PDB as soon as possible, and no later than December 31st 2005.
- Maintain a facile pathway for additional necessary changes to PDB entries (e.g., corrections in protein primary structure, etc.).

Scope of the PDB

Commentary:

There is a critical, scientific need for inclusion of all experimental structural biology data from X-ray crystallography, NMR spectroscopy, and electron microscopy in the PDB. Recommendations:

- Perform a pilot study to establish a plan plus the resource requirements and timelines for inclusion of electron microscopy volume data in the PDB.
- Following appropriate consultation, execute the plan and issue brief progress reports at an appropriate frequency to the wwPDBAC and funding agency representatives.
- Formalize the approach taken by the MSD and the RCSB to inclusion of structural biology data from electron microscopy as a means of promoting inclusion of information coming from other experimental methodologies (e.g., small angle X-ray scattering, electron tomography, etc.).

Exclusion of Macromolecular Models with NO Direct Basis in Experiment

Commentary:

Macromolecular models without direct basis in experiment have no place in the PDB, which is an archive of structural biological data from experimental sources.

Recommendations:

- Preserve archival access to macromolecular models previously deposited into the PDB, with a clearly visible statement that these models are without direct basis in experiment.
- Purge or appropriately identify existing PDB records containing macromolecular models with no direct basis in experiment.
- Decline subsequent PDB depositions of macromolecular models without direct basis in experiment.

Dispute Resolution

Commentary:

Although the wwPDBAC fully expects the RCSB, the MSD, and PDBj to reach all significant decisions by consensus, the committee recognizes that a forum for dispute resolution may be required in future.

Recommendation:

The RCSB, the MSD, and PDBj shall utilize the wwPDBAC to resolve disputes as needed.

Global PDB Decision/Policy Making and Interactions

Commentary:

Global decision/policy making and some interactions with external parties are beyond the purview of the RCSB, the MSD, and PDBj acting as individual institutions.

Recommendations:

 The RCSB, the MSD, and PDBj shall utilize the wwPDBAC to mandate global decisions pertaining to the PDB.

- The wwPDBAC shall issue policy statements, etc. pertaining to such global decisions as necessary.
- The wwPDBAC shall actively participate in interactions with external parties as appropriate.

wwPDBAC Advocacy

Commentary:

The wwPDBAC is uniquely positioned to act as an advocate for PDB funding, and to serve as an interlocutor among the RCSB, the MSD, and PDBj and between the PDB and various community stakeholders.

Recommendations:

- The wwPDBAC shall work with the RCSB, the MSD, and PDBj plus current and prospective Funding Agencies to maximize financial support for the PDB.
- The RCSB, the MSD, and PDBj shall keep the wwPDBAC informed of relevant changes and issues to ensure timely support by the wwPDBAC.
- Each of the RCSB, the MSD, and PDBj shall appoint representatives to their own advisory committees drawn from those of the other two wwPDB member organizations.

Communications

Commentary:

Securing long term, stable funding for the collective enterprise is critical for its continued well being and growth. Communications must document that the RCSB, the MSD, and PDBj are (a) providing important structural database services to their host communities (i.e., USA, EU, and Japan), (b) serving as full partners in the wwPDB, and (c) playing essential roles in ensuring the maintenance of a secure, single, global archive for experimental structural biology data that is freely accessible in perpetuity.

Recommendations:

- Appropriate literature with which to influence opinion leaders and funding decision makers should be generated for wwPDB.
- The wwPDB website should serve as a resource in its own right by enabling access to the "best of" selection of data mining tools and other resources from the RCSB, the MSD, and PDBj.

wwPDBAC Membership and Meeting Logistics

Commentary:

The PDB user community will be best served by a wwPDBAC with continuity, full participation, and orderly turnover of its membership.

Recommendations:

- Each of the RCSB, the MSD, and PDBj shall develop appropriate plans to ensure continuity, full participation, and orderly turnover of wwPDBAC membership.
- Each of the stakeholder representative organizations (IUCr and ICMRBS, at present) shall develop appropriate plans to ensure continuity, full participation, and orderly turnover of wwPDBAC membership.
- The RCSB, the MSD, and PDBj shall develop appropriate plans to include wwPDBAC representation from the biological electron microscopy community.
- The RCSB, the MSD, and PDBj shall convene annual face-to-face meetings of the wwPDBAC and at least one telephonic meeting in the interim.