world wide Protein Data Bank Advisory Committee (wwPDBAC) Report of November 6th 2009 Meeting Osaka University, Osaka, Japan

Chair: Stephen K. Burley (RCSB-PDB)

PDB Site Representatives: Michael G. Rossmann (RCSB-PDB), Andreas Engel (PDBe-EBI), Randy J. Read (PDBe-EBI), Ichio Shimada (BMRB), Masatsune Kainosho (BMRB), Masahiro Shirakawa (PDBj), Soichi Wakatsuki (PDBj), and Kei Yura (PDBj)

Ex Officio Community Stakeholder Representatives: Edward N. Baker (IUCr), R. Andrew Byrd (ICMRBS), and Wah Chiu (Macromolecular EM, excused)

wwPDB Members: Helen M. Berman (RCSB-PDB), Martha Quesada (RCSB-PDB), Gerard J. Kleywegt (PDBe-EBI), John Markley (BMRB), and Haruki Nakamura (PDBj)

wwPDB Associate Members: Manju Bansal (India), Zihe Rao (China)

Funding Agency Representatives: Peter McCartney (NSF, absent)

Observer: Matthew Day (Nature Publishing Group)

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wwPDBAC Mission Statement

To help ensure that the Protein Data Bank is maintained for the public good as a secure, singular 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-PDB), the <u>BioMagResBank</u> (BMRB), the <u>Protein Data Bank Europe</u> (PDBe-EBI), and the <u>Protein Data Bank Japan</u> (PDBj) met at the Institute for Protein Research in Osaka, Japan on November 6^{th} 2009.

The agenda included

- (1) Responses to 2007/2008 wwPDBAC Meeting Recommendations;
- (2) Overview of Recent Progress;
- (3) Common Deposition and Annotation Tool;
- (4) Report from the NMR Validation Task Force;
- (5) Report from the X-ray Validation Task Force;

- (6) Report on EM Deposition Process;
- (7) Report on SAXS/SANS Inclusion in the PDB;
- (8) Report on Complex Chemistry in the PDB;
- (9) Discussion of Policy Issues/New Ventures; and
- (10) Other Matter

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

Responses to 2007/2008 wwPDBAC Meeting Recommendations

• The wwPDB shall establish augmented validation procedures for X-ray and NMR.

<u>wwPDB Response:</u> In progress. X-ray task force has produced a draft report. NMR task force established.

• The wwPDB shall establish recommendations for additional data deposition and release requirements:

wwPDB Response: Policy document updated.

• The wwPDB shall work with the SAXS/SANS community to evaluate the desirability/feasibility of incorporating small-angle scattering data/analyses into the PDB.

wwPDB Response: In Progress. Initial report completed.

• The wwPDB shall redefine the purview of the PDB.

wwPDB Response: Completed. Proposal presented for approval at this meeting.

• The wwPDB shall establish the feasibility of chemical shift inclusion in the PDB.

wwPDB Response: In progress. Implementation plan developed.

• The wwPDB shall establish a mechanism to provide for long term funding of wwPDB activities.

wwPDB Response: In progress. wwPDB Foundation established as a legal entity.

• The wwPDB shall establish an EM Task Force.

wwPDB Response: Completed. Initial EMDB AC Meeting held March 2009.

• The wwPDB shall broaden the membership of the wwPDB to include India and China.

<u>wwPDB Response:</u> Completed. Associate Members from India and China present at this meeting.

Overview of Recent Progress

Commentary:

The four wwPDB member organizations are working well together. The Committee continues to be impressed by the ever increasing level of cohesion and the quality of wwPDB activities. Of particular significance was successful resolution of funding renewal activities by all four member organizations, providing, for the first time, a modicum of funding stability until mid-2011. At PDBe-EBI, the funding renewal process yielded an increase in support, which the Committee interprets as an important affirmation of the mission of this wwPDB site and the wwPDB in its

entirety. The wwPDB continues to achieve significant visibility with joint publications and presentations/exhibit booths at international conferences and professional society meetings. Finally, the Committee was impressed by the evident maturation of the wwPDB leaders into a team of equals and the speed with which Kleywegt has become fully effective as director of PDBe-EBI.

Common Deposition and Annotation Tool

Commentary:

Quesada provided a detailed summary of the genesis, scope, and implementation of the much-needed Common Deposition and Annotation Tool. This process began in 2007. A PDB Contents Guide 3.2 was issued on September 15 2008, clarifying all data formats and data deposition procedures to create a more uniform archive. Implementation of this new standard occurred on November 15 2008, after the requisite 60-day comment period. All files in the archive now conform to this new standard. In early 2010, the annotation module will be put into service, with the goal of completing the entire project before the end of 2011.

The ultimate project deliverables are as follows:

- An interactive/informative deposition interface that supports faster processing and adds value in terms of input validation and annotation.
- An improved system for annotators that will increase throughput, be easier to maintain, augment existing quality control procedures, and expand functionality.
- A higher quality archive for end users.

Report from the NMR Validation Task Force

Commentary:

Markley described formation of the NMR Validation Task Force, and gave a brief account of the outcomes of their first meeting in Paris. In addition, Markley provided an overview of recent progress on implementation of the necessary tools for chemical shift deposition to the PDB, which is nearing completion. A report on progress towards developing the Small Molecule Structure Deposition (SMSDep) tool for deposition of small peptide and nucleic acid structures was also presented.

Recommendations:

- The wwPDB should ensure that the NMR Validation Task Force completes their deliberations and publishes a "white paper" describing their analyses and proposing adoption of validation metrics as soon as possible. Proposed Deadline: mid-2010.
- The wwPDB should work with the appropriate journal editors to encourage formal scrutiny of PDB-generated NMR structure validation reports during the refereeing process. Ideally, the relevant journals would adopt enhanced X-ray and NMR validation requirements simultaneously. If this is not possible, implementation of the X-ray validation requirements should not be delayed.
- The wwPDB should monitor the level of SMSDep utilization to determine what level of ongoing support for such depositions is warranted.

Report from the X-ray Validation Task Force

Commentary:

A draft report from the X-ray Validation Task Force was delivered by Read. Both global and local validation metrics were presented and discussed in some detail. The Committee unanimously supports wwPDB adoption of these metrics and looks forward to implementation of the validation software pipeline by Dr. Gore (PDBe-EBI) and incorporation of these tools into the new Common Deposition and Annotation system (described above).

Recommendations:

- The wwPDB should ensure that the X-ray Validation Task Force publishes a "white paper" describing their analyses and proposing adoption of global and local validation metrics as soon as possible. Proposed Deadline: mid-2010.
- The wwPDB should work with the appropriate journal editors to encourage formal scrutiny

PDB-generated X-ray structure validation reports during the refereeing process.

Report on Macromolecular EM Deposition Progress

Commentary:

Kleywegt provided an overview of recent progress on implementation of the necessary tools for one-stop shop deposition of EM coordinates and experimental electron density envelopes to the PDB, which is nearing completion. A compelling case for development and adoption of uniform EM validation system analogous to the output of the X-ray Validation Task Force was made by Rossmann and Engel.

Recommendations:

- The wwPDB should establish an EM Validation Task Force to develop validation metrics and publish a "white paper" describing the outcome of their deliberations as soon as possible. Proposed Deadline: Q4 2010.
- The wwPDB should work with the appropriate journal editors to encourage formal scrutiny of PDB-generated EM structure validation reports during the refereeing process.
- The wwPDB should ensure that their EM related activities are coordinated with those planned by INSTRUCT to avoid duplication of effort, etc.

Report on SAXS/SANS Inclusion in the PDB

Commentary:

Kleywegt made the case for inclusion of SAXS/SANS entries in the PDB and presented a detailed summary of proposed requirements for such depositions.

Recommendations:

- The wwPDB should establish a SAXS/SANS Task Force to provide advice on the following:
 - -Which SAXS/SANS models should be included in the PDB
 - -Requirements for deposition
 - -Validation standards
- Possible members of the task force include Jill Trewhella, Dmitri Svergun, Andrej Sali, John Tainer, and Mamoru Sato.
- The wwPDB should ensure that the task force publishes a "white paper" describing the outcome of their deliberations as soon as possible. Proposed Deadline: Q1 2011.
- The wwPDB should work with the appropriate journal editors to encourage formal scrutiny of PDB-generated SAXS/SANS structure validation reports during the refereeing process.

Report on Complex Chemistry in the PDB

<u>Commentary:</u>

Kleywegt presented a detailed summary of recently completed efforts to ensure consistency within the archive for exotic oligopeptide structures (i.e., peptide antibiotics and other natural products) and small molecule inhibitors (both natural products and man-made compounds), many of which occur in complexes with their target proteins. The benefits of this exercise to

PDB users are as follows: (i) to reflect correctly the genetic origins of the exotic oligopeptides and (ii) to facilitate comparisons among different ligand structures and across different target proteins. The Committee commends the team for undertaking this challenging task, and looks forward to its completion.

Policy Issues/New Ventures

Commentary:

Berman described Proposed Requirements for PDB Depositions, challenges posed by the current PDB Format, and formation of the wwPDB Foundation.

Proposed Requirements for PDB Depositions: Clarification of the requirements for inclusion in the PDB is urgently needed. The wwPDB leadership proposed the following inclusion criteria:

- Polypeptide Structures
 - -Gene products
 - -Naturally-occurring peptides that are non-ribosomal in origin
 - -Peptidic repeat units of larger polymers
 - -Synthetic peptides of at least 24 residues (smaller biologically relevant oligopeptides are also acceptable)
- Polynucleotide Structures
 - -Of four or more residues
- Polysaccharide Structures
 - -Of four or more residues

The Committee unanimously endorses the proposed requirements and looks forward to their announcement/implementation in early 2010.

PDB Format: As is well known to all who have watched the evolution of computer file formats over the past 30 years, the current PDB file format (i.e., limited to 80 column records, <62 polymeric chains, <100,000 atoms, ...) represents a serious impediment for successful evolution of the archive as deposited structures grow ever larger and more complex. The Committee strongly endorses wwPDB plans to work with community stakeholders to develop a new PDB format to overcome these challenges. Implementation should be effected no later than Q4 2010, following the requisite 60 day comment period.

wwPDB Foundation: Berman described formation of the wwPDB Foundation as a US tax exempt 501 (c) (3) corporation, which is intended to serve as a fund-raising vehicle to provide support for wwPDB activities. The Committee strongly supports this development and looks forward to helping the wwPDB leadership with fund raising.

Other Matter

Commentary:

Berman and Dr. Matt Day (Nature Publishing Group, NPG) presented a loose concept for a joint PDB-NPG structural biology journal. A lively discussion followed.

Various sentiments/concerns emerged, some of which are recounted below.

- The PDB should not be in the publishing business.
- The PDB already is in the publishing business. Every PDB entry is tagged with a citable DOI or Digital Object Identifier.

- There appears to be a need for a new structural biology journal that captures some of the many unpublished PDB depositions that are of particular biological interest and brings them to the attention of the biological community.
- The PDB brand could be debased by involvement with a commercial publisher. If the PDB wants to be part of a journal it should only do so with the IUCr. A PDB-NPG journal would constitute an affront to the IUCr and, in turn, the crystallographic community.
- Earlier attempts by the PDB to team up with the IUCr to establish a journal were not successful.
- A commercial arrangement is not an appropriate way for the wwPDB Foundation to raise money.
- The PDB could be construed as having a conflict of interest if publication in such a journal was in anyway seen to be tied to deposition.
- This sounds like an interesting idea, but only if the Nature brand appears together with the PDB brand.
- ullet More market research needs to be done, particularly in the light of the perceived lack of success of *Acta Crystallographic Section F* and the *Journal of Structural and Functional Genomics*.

The Committee looks forward to further discussion of a revised concept backed up with the results of market research.