# world wide Protein Data Bank Advisory Committee (wwPDBAC) Report of October 1<sup>st</sup> 2010 Meeting Rutgers University, New Brunswick, NJ

Chair: Stephen K. Burley (RCSB-PDB)

**PDB Site Representatives:** Michael G. Rossmann (RCSB-PDB), Andreas Engel (PDBe-EBI, absent), Randy J. Read (PDBe-EBI), Masatsune Kainosho (BMRB), Guy Montelione (BMRB), Genji Kurisu (PDBj), and Soichi Wakatsuki (PDBj)

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

**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), Jianpeng Ding (China)

**Funding Agency Representatives:** Peter McCartney (NSF, absent), Ward Smith (NIGMS-NIH), Roland Hirsch (DOE)

**Observers:** Philip Bourne (RCSB-PDB), John Westbrook (RCSB-PDB)

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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 world wide Protein Data Bank Advisory Committee (wwPDBAC) to the leadership of the Research Collaboratory for Structural Bioinformatics (RCSB-PDB), the BioMagResBank (BMRB), the Protein Data Bank Europe (PDBe-EBI), and the Protein Data Bank Japan (PDB) met at Rutgers University in New Brunswick, NJ on October 1<sup>st</sup> 2010.

The agenda included

- (1) Responses to 2009 wwPDB AC Recommendations;
- (2) Overview and State of the PDB;
- (3) Common Deposition and Annotation Tool;
- (4) X-ray Specific Activities;
- (5) Report from the X-ray Validation Task Force;
- (6) NMR Specific Activities;
- (7) EM Specific Activities;
- (8) SAXS/SANS Specific Activities;
- (9) PDBj Funding;
- (10) BMRB Funding; and
- (11) Discussion of Policy Issues/New Ventures

# Responses to 2009 wwPDBAC Meeting 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.

<u>wwPDB Response:</u> Report/"white paper" complete. Formal submission for publication expected Q4 2010.

• The wwPDB should work with appropriate journal editors to encourage formal scrutiny of PDB-generated X-ray structure validation reports during the refereeing process.

<u>wwPDB Response</u>: Journals notified. IUCr journal policies revised to conform to wwPDB recommendations. Discussion with remaining journals in progress.

• 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.

<u>wwPDB Response:</u> Final meeting of the NMR task force planned for January 2011. Report/"white paper" completion expected Q2 2011.

• 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.

<u>wwPDB Response:</u> EM task force established. First meeting held at Rutgers in September 2010. Report/"white paper" completion expected in 2011.

• The wwPDB should work with the appropriate journal editors to encourage formal scrutiny of PDB-generated EM structure validation reports during the refereeing process.

wwPDB Response: Process to be initiated once report/"white paper" is complete.

• The wwPDB should ensure that their EM related activities are coordinated with those planned by INSTRUCT to avoid duplication of effort, etc.

<u>wwPDB Response:</u> Engel (PDBe-EBI) assumed responsibility for ensuring adequate communication between the wwPDB and INSTRUCT efforts.

• 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

<u>wwPDB Response:</u> First SAXS/SANS task force meeting planned for Q2 2011. Report/"white paper" completion expected Q1 2012.

• The wwPDB should monitor the level of SMSDep utilization to determine what level of ongoing support for such depositions is warranted.

wwPDB Response: In progress.

# Overview

Commentary:

The four wwPDB member organizations continue to work well together. The Committee is impressed by the ever increasing level of cohesion and the quality of wwPDB activities. Current funding of all four member organizations is adequate, although longer term funding of two members is uncertain. During the past year, considerable progress has been made on the all important Common Deposition and Annotation Tool. The wwPDB continues to achieve significant visibility with joint publications and presentations/exhibit booths at international conferences and professional society meetings. Effective interactions with the editors of scientific journals are beginning to bear fruit in terms of both primary data submission and structure validation. The wwPDB Foundation was formally established and fundraising to support a wwPDB 40<sup>th</sup> anniversary scientific meeting in late 2011 is underway.

# **PDB Metrics**

In aggregate, 8,300 (8,850\*) depositions were processed between January 1<sup>st</sup> and December 31<sup>st</sup> 2009 with a two-week average turnaround (\* 2010 projection).

The breakdown of depositions by discipline in calendar 2009 was as follows:

X-ray Crystallography:	7640	(92%)
Solution State NMR Spectroscopy:	592	(~7%)
Electron Microscopy:	51	(<1%)
Other:	17	(<1%)

The breakdown of depositions processed by each wwPDB site in calendar 2009 was as follows:

RCSB-PDB:	5,069	(61%)
PDBj:	2,173	(26%)
PDBe-EBI:	1,058	(13%)

### **Common Deposition and Annotation Tool**

#### Commentary:

A description of progress by wwPDB collaborators towards establishing common, global deposition/annotation tools was presented by Quesada. The Committee was pleased to learn that the project's 2010 goals are well in hand and that substantial completion in 2011 is likely.

Once the new functionalities of the Common Tool are adopted across the wwPDB, the Committee recommends that rigorous estimates of speed and throughput be made, with the goal of understanding how best to balance load among the various deposition sites. It will also be important to model the longer term impact of various deposition growth scenarios to plan for future contingencies, including the possibility that one or more of RCSB-PDB, BMRB, PDBe-EBI, and PDBj ceases operations.

### X-ray Specific Activities

# Commentary:

Kleywegt reported considerable progress on remediation of the archive, including work on Biological Assemblies, construction of a Peptide Reference Dictionary, correction of Residual B-factors, and remediation/curation of entries with complex peptide bond chemistry. A new PDB Working Format (PWF) was proposed to address the many shortcomings of the existing PDB file format, dating from the 1970s. The Committee strongly supports adoption of this new format and the wwPDB plan for its phased implementation, beginning as soon as possible with key software developers.

#### **Report from the X-ray Validation Task Force**

#### Commentary:

Read presented the final report from the X-ray Validation Task force, which was enthusiastically received by the Committee. Immediate submission for formal publication was encouraged in the strongest possible terms. Domain experts on the Committee look forward to reviewing reports from the NMR and EM Validation Task Forces, which should build on the excellent foundation provided by the X-ray team.

#### NMR Specific Activities

#### Commentary:

Markley reported release of value-added data files and new software. Chemical shifts combined with restraints and atomic coordinates are now available from the BMRB FTP site. Validation software is now run by BMRB and PDBe-EBI on all NMR structure depositions. Implementation of Mandatory Chemical Shift Deposition is expected in December 2010. Utility monitoring of SMSDep, a non-wwPDB tool supported by BMRB, is underway. The final meeting of the NMR Validation Task Force is planned for January 2011. Completion of the NMR report/"white paper" is anticipated in Q2 2011, with submission for formal publication shortly thereafter.

# **EM Specific Activities**

### Commentary:

Berman 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. The EM Validation Task Force met in late September 2010 at Rutgers, where two discussion groups (respectively focused on Maps and Models) made excellent progress. Completion of the EM report/"white paper" is anticipated in 2011, with submission for formal publication shortly thereafter.

# **SAXS/SANS Specific Activities**

### Commentary:

Kleywegt presented proposed requirements for inclusion of SAXS/SANS-derived structural models in the PDB archive, which were endorsed by the Committee. He further outlined the membership of the SAXS/SANS Task Force (Trewhella, Svergun, Sali, Sato, and Tainer) and the charge to the group when it meets in Q2 2011. Completion of the SAXS/SANS report/"white paper" is anticipated in Q1 2012, with submission for formal publication shortly thereafter.

# PDBj Funding

### Commentary:

Nakamura summarized recent developments aimed at formation of a National Database Center for Biosciences, which would provide long term financial and infrastructure support for vital biological data resources in Japan. The impact of these ongoing activities on PDBj funding remains unclear at present.

Any reduction in or interruption of PDBj funding would be extremely deleterious to the PDB archive and wwPDB activities, and by extension to the global scientific community.

PDBj currently processes more than 25% of all PDB depositions worldwide. In addition, PDBj plays an essential role in many wwPDB collaborative projects, the most important of which is the Common Deposition and Annotation Tool.

With guidance from Nakamura and Wakatsuki, the leadership of RCSB-PDB, BMRB, and PDBe-EBI and the Committee will provide coordinated letters of support directed at appropriate Japanese government departments.

# BMRB Funding

#### Commentary:

Markley explained that the US National Library of Medicine recently announced that it will no longer support BMRB beyond August 2014. He further elaborated that between October 2011 and August 2014, BMRB will undergo a 30% reduction in funding.

Any interruption of BMRB funding would be extremely deleterious to the PDB archive and wwPDB activities, and by extension to the global NMR community.

BMRB currently provides value added processing of chemical shifts, restraints, etc. for all NMR structure depositions to the PDB archive, which account for ~7% of all structure depositions worldwide. In addition, BMRB contributes in various wwPDB collaborative projects, the most important of which is the Common Deposition and Annotation Tool.

With guidance from Markley, the leadership of RCSB-PDB, PDBe-EBI, and PDBj and the Committee will provide coordinated letters of support directed at appropriate US funding agencies.

# Policy Issues/New Ventures

<u>Commentary</u>: The wwPDB leadership reviewed plans for B-value remediation and adoption of a new PDB file format. Additional topics discussed included funding of PDBj and BMRB, required journal submission of wwPDB structure validation reports, wwPDB Foundation activities, and the NPG-PDB journal market research survey.

<u>B-Value Remediation</u>: Correction of the estimated 7,000 depositions that currently report only residual values is essential and urgently required to maintain the integrity of the PDB archive.

The Committee unanimously endorses wwPDB plans to furnish entries annotated as containing residual B-value content, and their commitment to provide a service for users to download modified entries with full isotropic B-values.

<u>PDB File Format</u>: Introduction of a new PDB file format is essential for successful evolution of the PDB archive as deposited structures grow ever larger and more complex.

The Committee strongly endorses the proposed PDB working format (PWF) and the staged plan for its instantiation with community stakeholders in 2011 and full implementation in 2012, following the requisite 60 day comment period.

<u>PDBj</u> Funding: Any interruption or loss of PDBj funding would be extremely deleterious to the PDB archive and the wwPDB.

The Committee will coordinate with wwPDB leaders to provide letters of support to appropriate Japanese funding agencies.

<u>BMRB Funding</u>: Any interruption or loss of BMRB funding would be extremely deleterious to the PDB archive and the wwPDB.

The Committee will coordinate with wwPDB leaders to provide letters of support to appropriate US funding agencies.

<u>Required Journal Submission wwPDB Structure Validation Reports</u>: Adoption of more thorough procedures for evaluation of structure quality at the time of manuscript evaluation is broadly supported by structural biologists worldwide. The logistics for providing the requisite validation reports are already in place at wwPDB member sites.

The Committee will coordinate with wwPDB leaders and advisors to RCSB-PDB, PDBe-EBI, PDBj, and BMRB to circulate a petition among expert structural biologists and super users of the PDB archive calling on journal editors to require submission of a wwPDB structure validation report.

<u>wwPDB Foundation Activities</u>: The necessary formalities for establishing the wwPDB Foundation as a US tax exempt 501 (c) (3) corporation have been completed. The foundation board of directors, consisting of Berman (wwPDB Foundation President), Burley (Chair), Kleywegt, Nakamura, and Markley, has begun development of a comprehensive fund raising plan. The initial focus of the fund raising effort will be the PDB 40<sup>th</sup> anniversary scientific conference, which will be held at Cold Spring Harbor Laboratory in October 2011.

The Committee strongly supports this development and looks forward to helping the wwPDB leadership with fund raising.

<u>NPG-PDB Journal Survey</u>: The outcome of initial Nature Publishing Group (NPG) market research efforts aimed at understanding the potential impact of a joint NPG-PDB structural biology journal was presented in detail. Following lively discussion, further market research was recommended.

Although the results of the initial NPG survey were viewed as being largely encouraging, the Committee remains concerned with a number of questions enumerated below.

- What scientific need(s) would the proposed journal address?
- What value would accrue from publication of some or all of the ~6,000 currently unpublished structures?
- What progress has wwPDB made with NPG re branding?

- Would the proposed journal be the best vehicle for wwPDB member organizations to exploit the coming revolution in 3-D enabled smart phones and tablet devices?
- Does the proposed journal offer sufficient benefit *versus* the risks inherent in abandoning the current wwPDB understanding that provides for full cooperation and coordination on Data In and healthy competition on Data Out?

• Does the proposed journal represent the most efficient means of raising funds to support wwPDB activities?

The Committee looks forward to discussion of further market research data and outstanding issues.