



General Programmatic Terms and Conditions (PTC) for the Protein Data Bank Management by the Research Collaboratory for Structural Biology Cooperative Agreements (NSF 08-507)

1. **Key Personnel:** Except for the principal Investigators(s) (PIs) or co-PIs identified in this award, requests to make any changes in personnel, organizations and/or partnerships specifically named in the proposal, that have been approved as part of this award, shall be submitted in writing to the cognizant NSF Program Official for approval prior to any changes taking effect. Changes to PIs/co-PIs must be submitted through FastLane for Grants Officer approval.
2. **Program/Project Description:** The overall purpose of the award is to provide for the continued development, operation, and management of an electronic database of three-dimensional structural information concerning biological macromolecules currently known as the “Protein Data Bank (PDB)” and also termed “Macromolecular Structure Database (MSD)”. The Protein Data Bank serves as the primary, authoritative international repository for experimentally determined macromolecular structural data. The PDB is a vital resource enabling structure-informed research and education in a wide variety of fields in biology and allied disciplines. Under this award, the project will maintain a reliable, fully documented physical archive that is fully transportable and that provides for preservation of the full spectrum of PDB records including legacy data, depositor submissions and associated information, and records associated with the annotation process and with the transactions and activities that are part of the maintenance and evolution of the resource.

A commitment to the continued success and development of this critical resource is shared by a group of Federal agencies that have formed a partnership for support of the Protein Data Bank, which is documented in a Memorandum of Understanding (MOU) signed by representatives of each of the participating agencies in January 2009. Signatories to this MOU in addition to the Foundation are the Department of Energy, National Institute of General Medical Sciences, National Library of Medicine, National Cancer Institute, National Institute of Diabetes and Digestive and Kidney Diseases, and National Institute of Neurological Disorders and Stroke for Coordinated Funding and Management of the Protein Data Bank. Hereinafter, those Federal Agencies that are signatories to this MOU and current and active contributors to support of the Protein Data Bank are referred to as the Participating Agencies.

3. **Project Governance:** The Awardee will ensure that an effective governing structure is in place throughout the award period to support all critical or significant project activities. Among the governing components will be the:
- a. Leadership Team (LT). The Leadership Team includes the Principal Investigator, Deputy Director and Associate Director. The LT will institute appropriate policies, programs, and procedures to ensure the successful and reliable operation of a modern, internet-accessible electronic database that provides for open, user-friendly, immediate, uninterrupted access for the broadest possible spectrum of investigators, students, educators, and the general public.
 - b. Principal Investigator (PI). The PI will be responsible for overall project management, including staffing, operation, and self-assessment of the Protein Data Bank. The PI will cooperate and coordinate with the cognizant NSF Program Official by: providing notifications in advance of all Advisory Committee (AC) meetings; contributing to the assessment of scientific progress and administration against targeted goals for each participant; and participating in NSF-initiated reviews conducted via telephone or site visit, on an as needed-basis during the course of the project.
 - c. Deputy Director (DD). The DD is responsible for oversight of all key projects and functions as managerial back up to the PI
 - d. Advisory Committee (AC). The AC represents the user community in providing advice and feedback to PDB management on all aspects of planning and operation. The AC will operate under the provisions of a written charter. The charter will describe the role of the AC in advising PDB management, including the right of approval for changes in policies and practices that directly impact the user community. Such policies and practices include, but are not limited to, data exchange formats and dictionaries, user interfaces, 'hold' policies (if any), and orderly procedures for implementing changes in policies and practices. The composition of the AC should be consistent with the PDB policy on diversity and reflect the full range of scientists, educators, and others that utilize and benefit from the PDB. Appropriate representation of the public and private sector is expected, as is the inclusion of members with relevant technical expertise in computer science and database/informatics technologies. The overall composition of AC membership and any changes to the charter will be evaluated as part of the annual report process. The AC is expected to meet at least once each calendar year and to prepare a written report describing its discussions, including any specific conclusions or recommendations with respect to changes in management and policies of the PDB. This report shall be provided to all senior PDB management personnel within 30 days of the date of the AC meeting. They, in turn, will prepare a timely written response. The Director will include both the AC report and PDB management's response as part of the annual report and these materials will be evaluated as part of the annual review process. In

addition, the Director will include a copy of the AC charter with the first annual report for NSF review and provide any subsequent revisions as appropriate.

4. **Reporting Requirements:** The Awardee will submit all ad hoc and regular reports as designated by the cognizant NSF Program Official with content, format, and submission timeline established by the NSF cognizant Program Official. The Awardee will submit all regular reports to NSF via FastLane using the appropriate reporting category; for any type of report not specifically mentioned in FastLane, the Awardee will use the “Interim reporting” function to submit reports.

Annual reports will include the following content:

- a. Summary of progress as measured against goals established through a defined project management timeline including the following:
 - i) Final report on progress toward goals in the previous calendar year.
 - ii) Status report on progress toward goals in the current calendar year and plans for achieving goals in the remaining portion of the calendar year.
- b. Tabulation for the current calendar year and, separately, for the previous calendar year of the total number of entries in the database and number of new entries added, including breakdown of entries by type, source, status, availability, and, if known, by geographical region (e.g. US, Canada, European Community, Japan, etc) for the submitting investigator/institution.
- c. Usage (access) data for the primary and mirror sites and a report on any downtime or access delays due to site traffic or other factors for the current calendar year and the previous calendar year.
- d. Average processing time for new entries processed during the current and previous calendar year at the project site(s) (i.e. at the Rutgers site and/or subawardee sites). Similar data for other processing sites (e.g. PDBj/Osaka University, MSD/EBI) should be presented separately, if available.
- e. Status of collaborations (including other databases, user’s groups, centers, etc), subcontractors and mirror sites. Roles, if any, of subcontractors and other collaborators in project goals as identified in the timeline(s).
- f. A copy of the current calendar year Advisory Committee (AC) report and the response to this report by the PDB senior management.
- g. A copy of the AC written charter will be submitted with the first annual report. Subsequent annual reports will include an updated copy if revisions have been made.
- h. Summary of efforts to broaden the impact of the project in the research, education/training, and lay communities including outreach efforts directed

- at each of these communities. Summary of efforts to integrate research and education and provide for integrating diversity into project activities.
- i. Detailed budgets and budget explanations for the upcoming project year (currently the project year is the same as the calendar year). A justification for any major changes being proposed must be included. A separate budget and budget explanation must be included for each subcontract/subaward in accordance with NSF policies.
 - j. An estimate of carryover funds, if any, and an explanation of the reasons for carryover (if more than 10% of the year's project budget) and plans for how these funds will be spent.
 - k. Biosketch information for any key personnel added to the project since the last approved annual report and narrative text summarizing the anticipated role for each such individual added to the project.
 - l. Updated current and pending support information for key personnel (NSF Form 1239).

The Awardee shall also submit Special Reports as may be reasonably requested by the Foundation. The PI is required to inform the NSF Program Official and designated representatives of the Participating Agencies of any notable progress, unexpected results, or major problems as they occur. These contacts can be made via email.

5. **Ongoing Management and Oversight:** The Awardee will ensure full commitment and cooperation among the governing structure components, and all project staff during all ongoing NSF project management and oversight activities. The Awardee will ensure availability of all key institutional partners during any desk or on-site review as well as timely access to all project documentation.

The Director will be responsible for providing both the AC report and PDB management's response as part of the annual report and these materials will be evaluated as part of the annual review process.

Maintain the name of the database as "The Protein Data Bank (PDB)" until such time as the NSF and the Participating Agencies approve a new name. In the event that a successor is named to operate the PDB, NSF and the Participating Agencies intend to allow use of the name by the successor. At their option, NSF and the Participating Agencies may require the use of a specific address (such as a "Uniform Resource Locator") for online access to the database. The Awardee will be responsible for payment of fees normally associated with securing the right to use such an address. In the event that responsibility for operation of the PDB is transferred to another entity, the Awardee will transfer its ownership of the address to the successor upon request from NSF and the Participating Agencies. The successor and not the Awardee will be responsible for payment of any costs associated with the transfer and for all fees for use of the address subsequent to transfer.

Maintain the content of the PDB database, associated software, and archival materials in a form that is readily transportable and fully operational by others and provide on request a current copy of the database, of all software and documentation necessary to operate the database, and all physical archive materials in the event that NSF and the Participating Agencies elect to transfer responsibility for operation of the PDB to another entity on expiration or termination of this agreement. To this end, the PDB system (both software and processes providing data processing, distribution, query, and archiving functions) must be developed and documented such that it can be installed, run and maintained by others using the same hardware and operating software as those that are in use by the current PDB management. In the event of transfer of responsibility for PDB, the negotiation of licenses and payment of fees for use of any commercial software necessary for operation of the database will be the responsibility of the successor(s); however, the Awardee agrees that it will not make use of second-source software necessary for operation of the PDB unless 1) it has reason to believe a similar license to use the software is generally available to other institutions, or 2) the software use license between the Awardee and the second source specifically includes a provision that the software will be available on similar terms to a successor who has been awarded responsibility for operation of the PDB. Any license with such provision must be submitted to NSF and the Participating Agencies for approval within 30 days of receipt of documentation. Satisfactory adherence to these expectations for transportability will be assessed regularly as part of the annual report process and may also be subject to a portability trial(s) to be held at the discretion of NSF and the Participating Agencies. Costs for any such trial will be born by NSF and the Participating Agencies via supplement to the award and conducted with adequate advance notice and designed to minimize any impact on PDB operations.

In order to evaluate progress and assess long term goals, the NSF will conduct a site/reverse site visit approximately 24 months after the start of the award, and as often thereafter as necessary. The results of such review(s) will be among the factors used to determine the continuation of support.

6. **Diversity Policy:** The Awardee will develop a diversity policy that guides all hiring, outreach and committee membership decisions. The policy should define goals for broadening opportunities and enabling the participation of all citizens (women and men, underrepresented minorities, persons with disabilities) and prescribe procedures for achievement and assessment. The policy will be delivered to the cognizant Program Officer for review and approval prior to the first annual project report. NSF will reference this policy in its approval of annual reports or requests for personnel actions.
7. **Intellectual Property:** An Awardee-to-Subawardee agreement on intellectual property including publication and patent rights must be negotiated. This Intellectual Property agreement shall be in place between the primary awardee,

subawardee(s) and any other institutional participants in the project within 60 days, and a copy of the signed and dated intellectual property agreement shall be provided to the cognizant program official within 30 days thereafter (or ninety days from the date of approval of this award).

8. **Information Technology Systems Security:** Security for all information technology (IT) systems employed in the performance of this award, including equipment and information, is the awardee's responsibility. Within a time mutually agreed upon by the awardee and the cognizant NSF Program Official, the awardee shall provide a written Summary of the policies, procedures, and practices employed by the awardee's organization as part of the organization's IT security program, in place or planned, to protect research and education activities in support of the award.

The Summary shall describe the information security program appropriate for the project including, but not limited to: roles and responsibilities, risk assessment, technical safeguards, administrative safeguards, physical safeguards, policies and procedures, awareness and training, and notification procedures in the event of a cyber-security breach. The Summary shall include the institution's evaluation criteria that will measure the successful implementation of the IT Security Program. In addition, the Summary shall address appropriate security measures required of all subawardees, subcontractors, researchers and others who will have access to the systems employed in support of this award.