# Beginner's Guide to the PDBbind Database (v.2016)

The PDBbind database provides a comprehensive collection of experimentally measured binding affinity data for the biomolecular complexes in the Protein Data Bank (PDB). This type of knowledge is the much needed basis for many computational and statistical studies on molecular recognition. PDBbind was first released to the public in May 2004. Over 3,200 users from over 70 countries have already registered to use this database. The PDBbind database is now updated annually to keep up with the growth of PDB. The current release is **version 2016**.

## What information does PDBbind provide?

- **Binding affinity data:** Originally, PDBbind only considered the complexes formed between proteins and small-molecule ligands. Other types of biomolecular complexes in PDB have been covered by PDBbind as well since 2008. This release contains binding data ($K_d$, $K_i$ & $IC_{50}$ values) for protein-ligand (13,308), protein-protein (1,976), protein-nucleic acid (777), and nucleic acid-ligand (118) complexes. All binding data are curated by ourselves from over 29,000 original references rather than copied from other data sources.

- **Processed structural files for download:** PDBbind also provides processed "clean" structural files for most of the protein-ligand complexes in this release. In brief, the biological unit of each complex is split into a protein molecule (in PDB format) and a ligand molecule (in Mol2 and SDF format). Atom/bond types on the ligand molecule are assigned as appropriate and examined manually. These structural files can be readily utilized by most molecular modeling software, which are wrapped in a data package for download.

- **Web-based display and analysis tools:** The user can access PDBbind through a web-based portal at http://www.pdbbind-cn.org/. Registration is free for academic as well as industrial users. On the PDBbind-CN web site, basic information of each complex is summarized on a single page. Text-based and structure-based search among the contents of PDBbind is also enabled. This web site actually provides structural information for all valid protein-ligand complexes in the Protein Data Bank, not limited to those with known binding data.

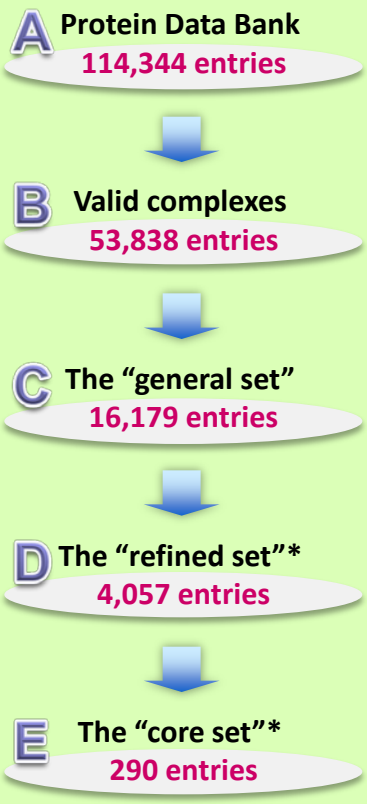
### Statistics of the PDBbind Database

| Version* | Entries in PDB | Complexes considered | Complexes with binding data | | |
|---|---|---|---|---|---|
| | | | General Set | Refined Set | Core Set |
| 2004 | 28,991 | 6,847 | 2,276 | 1,091 | 231 |
| ... | ... | ... | ... | ... | ... |
| 2012 | 78,235 | 34,180 | 9,308 | 2,897 | 201 |
| 2013 | 87,085 | 38,918 | 10,776 | 2,959 | 195 |
| 2014 | 96,952 | 44,569 | 12,995 | 3,446 | 195 |
| 2015 | 105,183 | 48,821 | 14,260 | 3,706 | 195 |
| 2016 | 114,344 | 53,838 | 16,179 | 4,057 | 290 |

*: Information of some earlier versions (v.2005 – v.2011) are not included in this table due to space limit.

## Basic Structure of the PDBbind data set

PDBbind is compiled through a stepwise process. It has a hierarchical structure as follows.




* Only complexed formed by proteins and small-molecule ligands are considered in this data set.

(A) The PDBbind v.2016 is based on the contents of PDB officially released at the first week of 2016, which contained totally **114,344** experimentally determined structures. Theoretical models are not considered.

(B) The entire PDB was screened by a set of computer programs to identify four major categories of molecular complexes, including protein-small ligand, nucleic acid-small ligand, protein-nucleic acid and protein-protein complexes. This step identified a total of **53,838** entries as valid complexes.

(C) The primary reference of each complex was examined to collect experimentally determined binding affinity data ($K_d$, $K_i$ and $IC_{50}$) of the given complex. Binding data for **16,179** complexes were collected in this way. They are the main body of the PDBbind database, which is referred to as the "**general set**".

(D) As an additional feature, a "**refined set**" was compiled to select the protein-ligand complexes with better quality out of the general set. A number of filters regarding binding data, crystal structures, as well as the nature of the complexes were applied in selection (see ref.2 below for details). The refined set in this release consists of **4,057** protein-ligand complexes.

(E) A "**core set**" was further provided as a high-quality benchmark for evaluating various docking/scoring methods. The core set included in this release was selected through a new procedure. In brief, it was selected through a systematic, non-redundant sampling of the refined set. The refined set was clustered by protein sequence similarity using a cutoff of 90%. Then, five complexes were selected as representatives for each cluster with emphasis on the diversity in structures and binding data. The core set in this release consists of a total of **290** protein-ligand complexes in **58** clusters. It has been applied to our Comparative Assessment of Scoring Functions (CASF) project (CASF-2016), which will be described in details in our up-coming publication.

## References and Notes

The PDBbind database was originally developed by Prof. Shaomeng Wang's group at the University of Michigan. It is currently maintained by Prof. Renxiao Wang's group at the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences under a mutual agreement. To cite the PDBbind database, please refer to the following references:

(1) Liu, Z.H. et al. *Bioinformatics*, **2015**, *31*, 405-412.
(2) Yan, L.; et al. *J. Chem. Inf. Model.*, **2014**, *54*, 1700-1716.
(3) Cheng, T. J.; et al. *J. Chem. Inf. Model.*, **2009**, *49*, 1079-1093.
(4) Wang, R. X.; et al. *J. Med. Chem.* **2005**, *48*, 4111-4119; *J. Med. Chem.* **2004**, *47*, 2977-2980.