



# Macromolecular Xtallography Raw Data Repository **MX-RDR**

M. Gilski, P. Poniatowska, A. Rynkiewicz

Dept Crystallography, A Mickiewicz Univ & Center for Biocrystallographic Research, Pol Acad Sci, Poznan, Poland

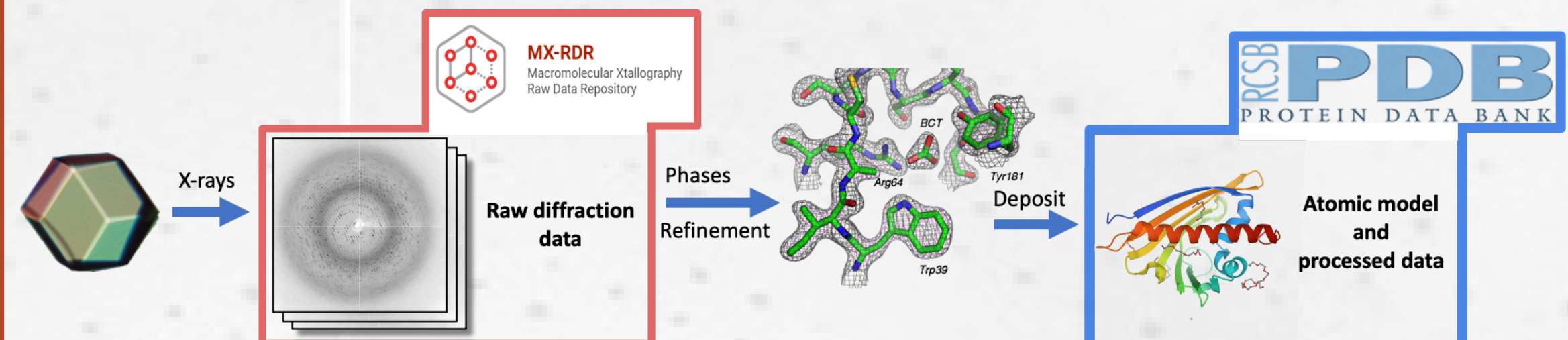
## What is **MX-RDR**?

The Macromolecular Xtallography Raw Data Repository (MX-RDR) was developed as a part of an EU funded project, coordinated by ICM UW, which aimed to create three open access discipline dedicated raw data repositories.

The MX-RDR repository, which is accessible via the web portal at <https://mxrdr.icm.edu.pl>, was designed to archive and provide access to raw diffraction data collected for macromolecular crystals. It includes tools for creating datasets of crystallographic metadata by combining information extracted directly from diffraction images and obtained from a PDB deposit and/or user input. Each data set is characterized by rich metadata, both to facilitate their management and long-term curation, and to allow effective scientific reuse. The resource can be searched using various criteria and all data are available for unrestricted access and download.

## What is the place of **MX-RDR** in crystallography data flow?

Typical X-Ray Crystallography data flow consists of getting diffraction patterns from protein crystals, then building electron density maps, which determine atomic models. Those atomic models are stored inside the Protein Data Bank. Our project comes way earlier, on the first step of this data flow - getting diffraction patterns, which explains a simple diagram below.



## MX-RDR key features

### Persistent identifiers

All data sets receive a persistent and unique DOI (Digital Object Identifier) that makes it easy to find and cite data.

### Versioning

Possibility of placing the next, corrected or supplemented version of the data set.

### Embargo

Possibility to set a period during which research data will not be made available to the public.

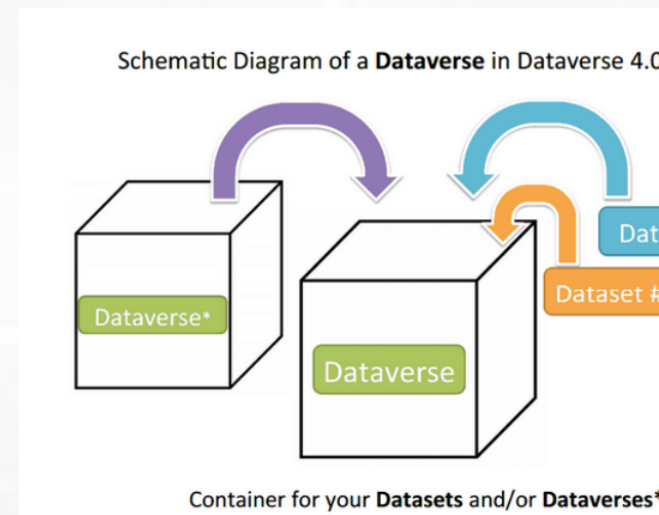
### API

(Application Programming Interface). Ability to prepare scripts that use internal API functions.

## Data inside **MX-RDR**

### can be stored as part of a dataverse

A dataverse is a container for datasets (research data, code, documentation, and metadata) and other dataverses, which can be setup for individual researchers, departments, journals and organizations. Dataverses are like folders on your computer - they allow to store and search data with ease.

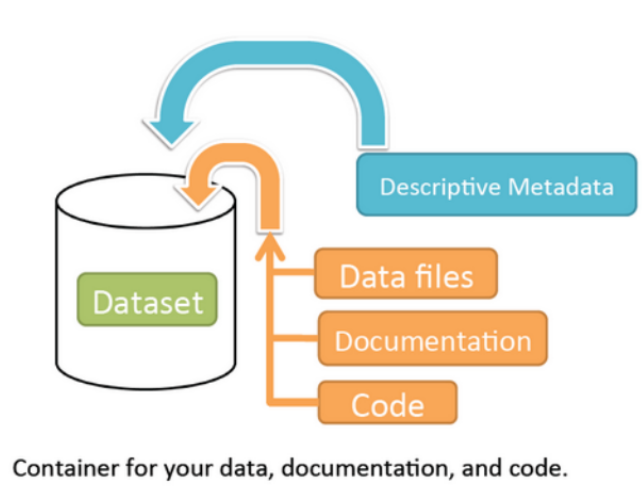


## What is a dataset

### and what could be stored inside it?

A dataset in Dataverse is a container for your data, documentation, code, and the metadata describing this Dataset. To put it in simple terms: one dataset is a single project with all additional information about it.

Schematic Diagram of a Dataset in Dataverse 4.0



## How can I store data inside **MX-RDR**?

### Do I need deep IT knowledge?

Absolutely not! **MX-RDR** was made to help You, not to make Your life harder. First of all, if Your metadata is stored in:

- XDS file,
- .cif file,
- .cbf file

then You can skip filling it on the site. Just provide a proper file and metadata will be filled automatically, as in example below:

.cif (PDBx/mmCIF) file importer

Unit Cell Parameters

Import if the field is empty

Overwrite existing metadata

Unit Cell Parameters (Unchecking the field will close this section respective metadata.)

a [Å]: 202.839

b [Å]: 202.839

c [Å]: 202.839

α [°]: 90.00

β [°]: 90.00

γ [°]: 90.00

If Your structure has been already accepted to Protein Data Bank, then first of all congratulations! On our site we allow to import metadata from PDB too, just follow example below:

.cif (PDBx/mmCIF) file importer

The importer collects data from .cif (PDBx/mmCIF) file, which could be uploaded by the user or downloaded automatically from... using the given PDB Id code. Either providing the structure symbol or uploading the file is mandatory. In case these two are provided only the uploaded file will be processed.

PDB Id code

.cif (PDBx/mmCIF) file

Select File

We know that this poster is probably not enough to explain everything great about our project. There are a lot of things to cover, like API, searching for data, possible data formats and many more. But fear no more, there is friendly (and really long) manual for **MX-RDR**. Furthermore, in case of any problems or doubts, contact our friendly support or visit <https://mxrdr.icm.edu.pl>



## MX-RDR dataverse