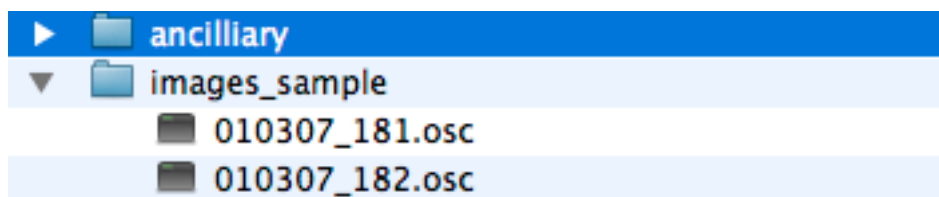


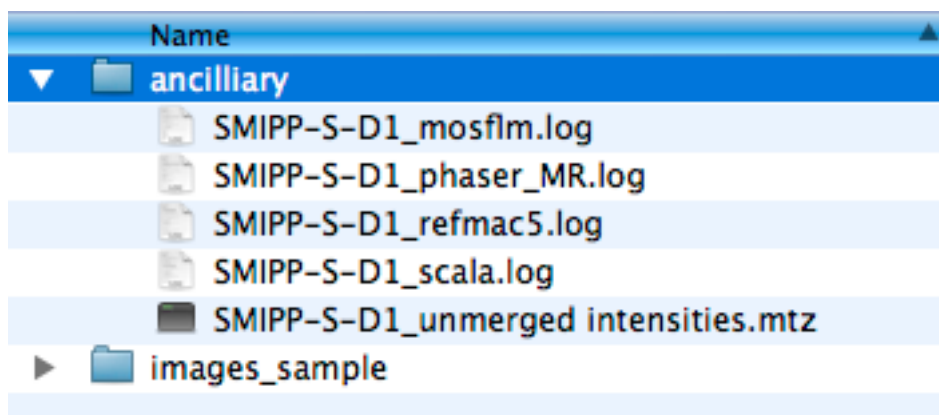
## TARDIS Data Deposition Guide

### Organise Data for Submission

There are two types of Datasets able to be published, raw and ancillary. Each set of raw diffraction images (img/osc/adsc etc..) should be in its own directory. Ancillary files are for log files, processed files, and anything else to be included with the published experiment.



*'images\_sample' – a directory containing raw diffraction images*



*'ancillary' – a directory containing all other types of files to be included*

### Annotating Data

Download the TARDIS Data Packager program and run it. The initial screen gives users the ability to describe the overall experiment (a collection of datasets). Also important is the "Destination for Data" field. Choose an empty directory for the annotated data to be output to.

The screenshot shows the 'TARDIS Data Packager' application window. The 'Experiment' tab is selected in the left sidebar. The main area contains the following fields and buttons:

- Experiment**
  - Title: My Experiment
  - Destination for Data: /Users/steve/Desktop/deposition/Datasets/MEXP (with a 'Browse..' button)
  - Authors (Use , to separate): Androulakis S, Buckle A
  - Abstract: Here is an example line of text..
- PDB ID**: MEXP (with 'Add' and 'Remove' buttons)
- Citation URL**: http://examplepublication.org/MEXP (with 'Add' and 'Remove' buttons)
- Institution Name**: Monash University

On the left sidebar, there are buttons for 'New Raw Dataset', 'New Ancillary Dataset', 'Remove Selected', 'Package Dataset', and 'Show Result Console'. At the bottom left is the 'TARDIS Data Packager' logo.

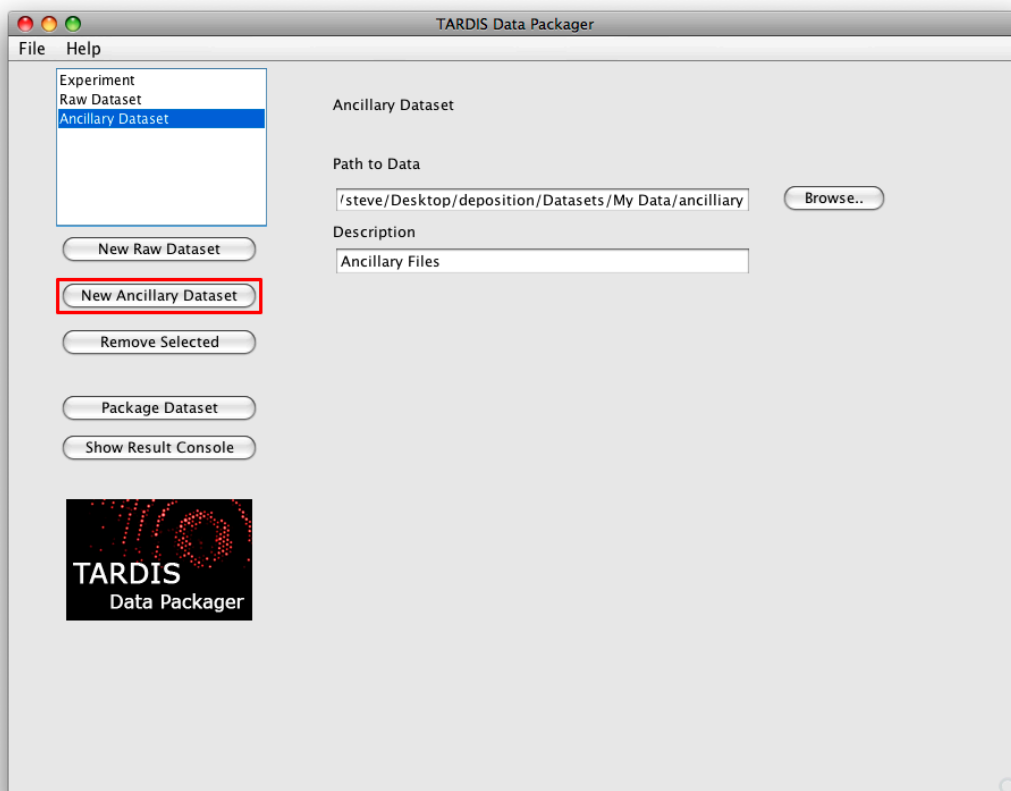
Click 'New Raw Dataset' to locate and annotate a set of diffraction images.

The screenshot shows the 'TARDIS Data Packager' application window with the 'Raw Dataset' tab selected. The 'New Raw Dataset' button in the left sidebar is highlighted with a red rectangle. The main area contains the following fields and buttons:

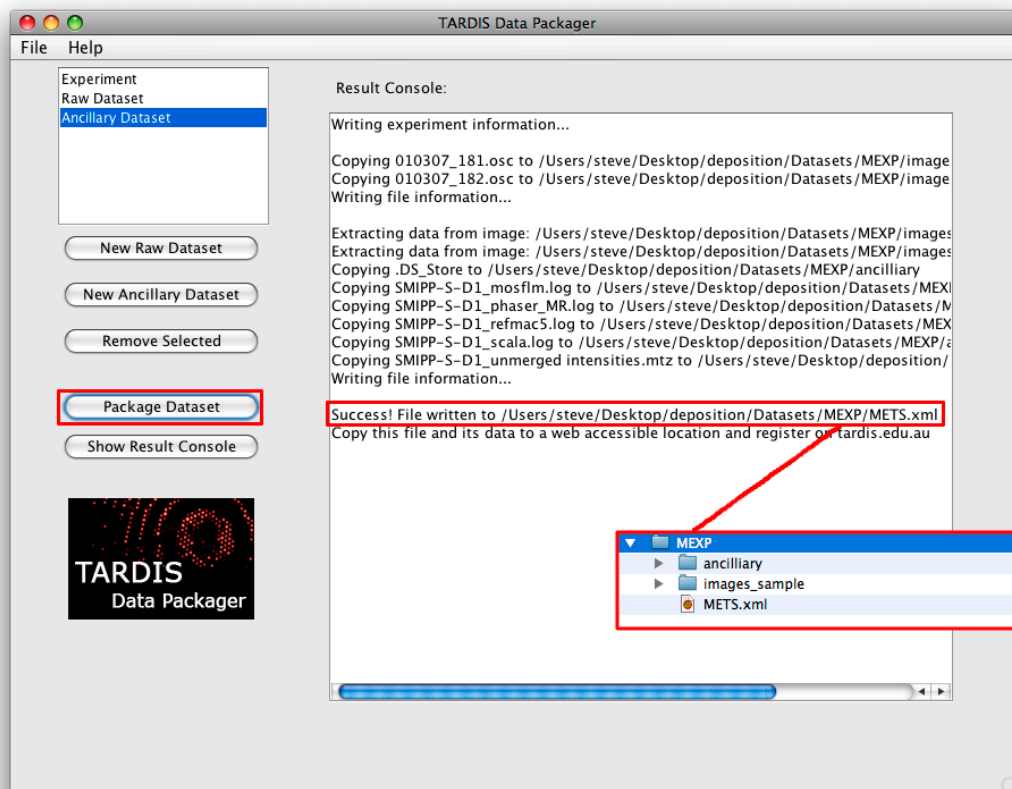
- Raw Dataset**
  - Path to Data: e/Desktop/deposition/Datasets/My Data/images\_sample (with a 'Browse..' button)
  - Description: Inhouse
  - Resolution Limit: 1.6
  - Diffraction Type: Rotating Anode
  - X-Ray Source: RIGAKU RAXIS IV
  - Crystal Name: PlyB
  - Mosaic Spread (optional):
  - Chi Angle (optional):

The left sidebar and logo are the same as in the previous screenshot.

Click 'New Ancillary Dataset' to choose the path to extra files, and describe the set.



Click 'Package Dataset' to begin the annotation and organisation process. Metadata is automatically extracted from raw diffraction images, files are copied to their destination and an annotation file 'METS.XML' is created.

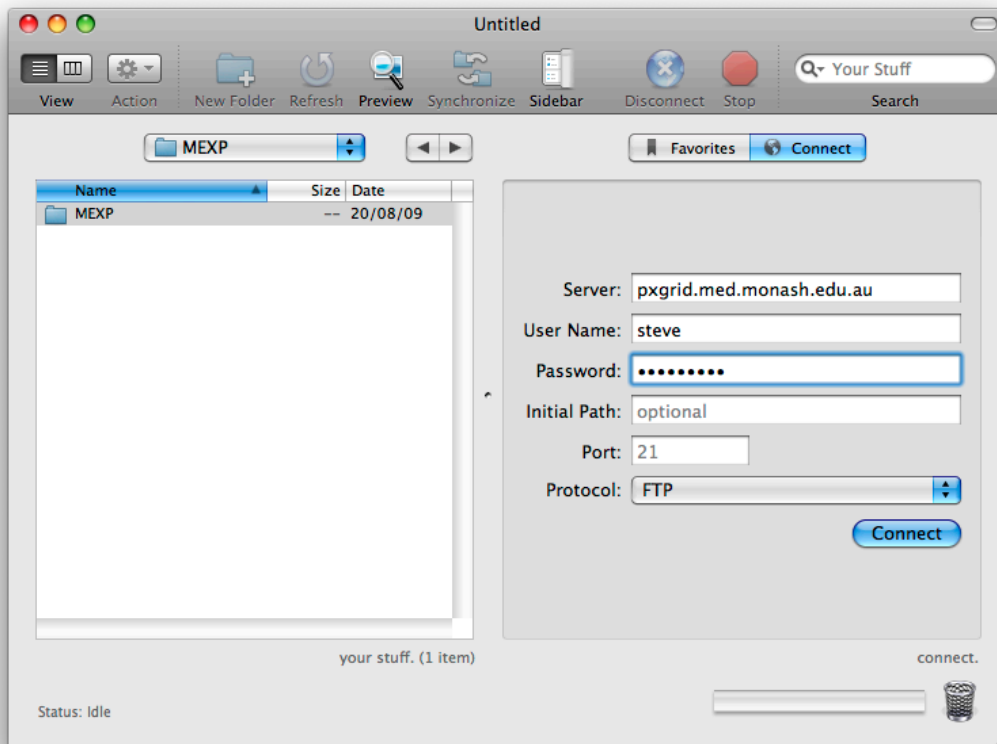


Files are copied along with the annotation file (METS.XML) to the destination path chosen in the experiment section. All of these files should be copied to a publicly web-accessible location, so a URL can be created and submitted to TARDIS.

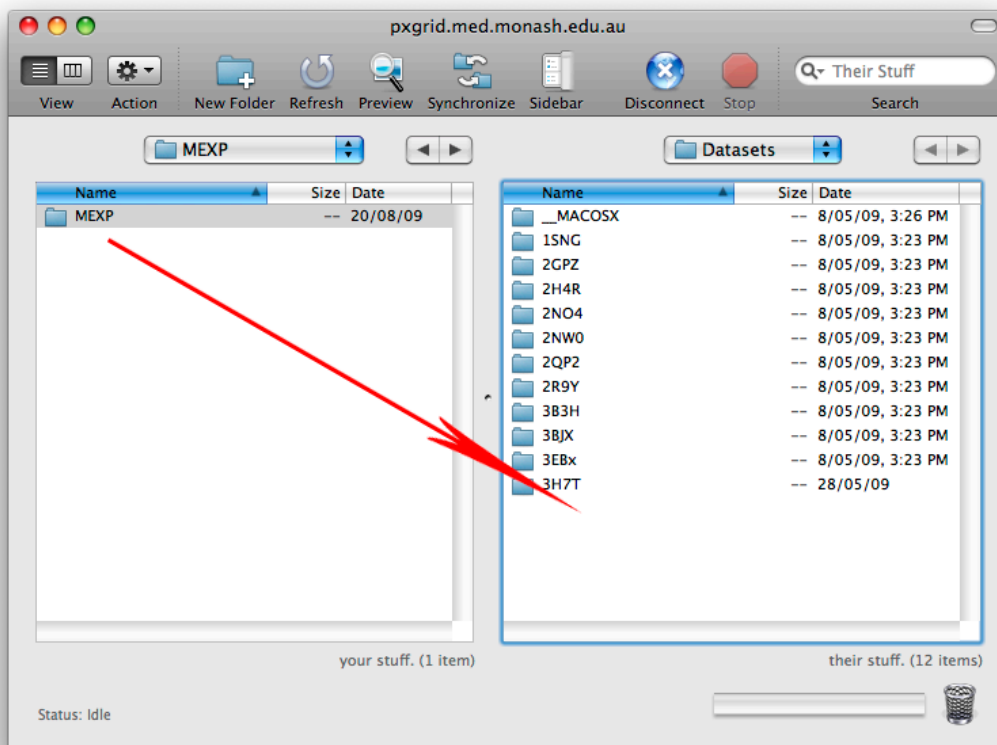
### Copying Data To A Public Location

**The copying of files to a web server can vary widely and a system administrator should be contacted for assistance. For example purposes, this section outlines how one might copy files via FTP to their web server.**

Open an FTP client (Transmit for the Mac is pictured here) and connect to the web server that will store the files.

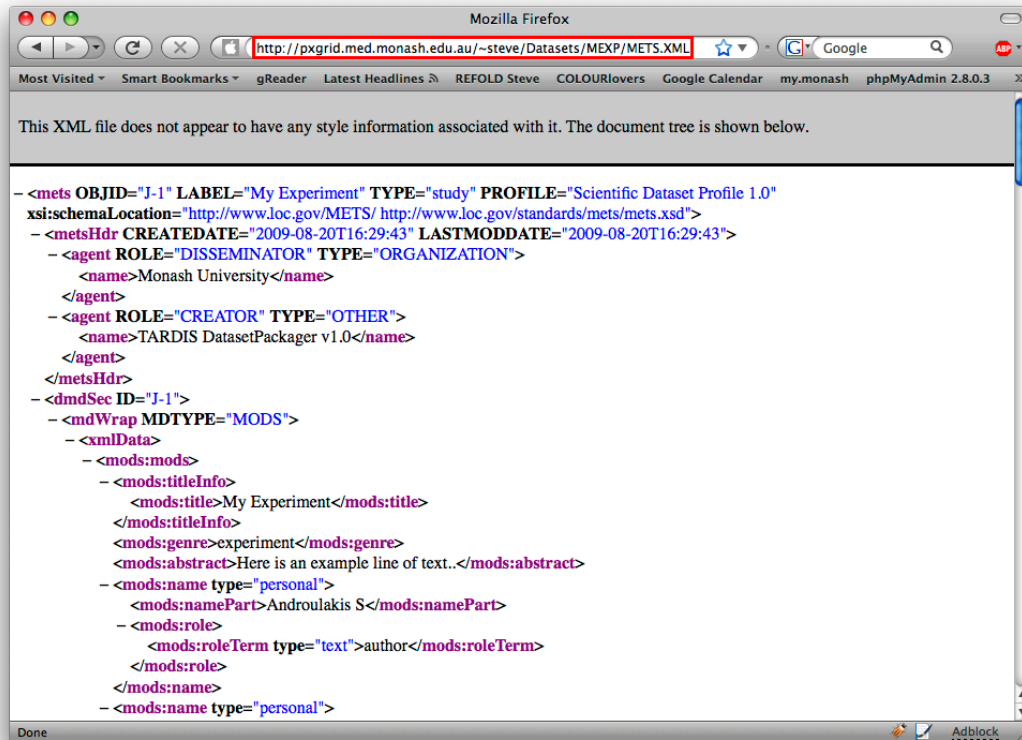


Copy the entire directory holding the datasets and the METS.XML file across to the server.



## Register Data on TARDIS

Once on a web server, the data should be accessible via URL. To verify this, a good test would be to try and access the METS.XML file in a browser. A successful display of METS.XML in Firefox is shown below.



This URL will provide as the basis for experiment registration. Log in to TARDIS and click 'Data' then 'New Experiment'. Paste the full URL to METS.XML in the 'METS XML url' field. A password can be entered to protect the experiment from the public view. Optionally, FTP details can be entered for easy downloading of full datasets.

**TARDIS** v2 Beta  
33 Datasets from 16 Structures, 7331 Files, 106.0 GB Data Indexed, 3.2 GB Avg. Dataset Size  
Welcome, steve [Log Out]

FEDERATED DIFFRACTION IMAGE PUBLICATION REPOSITORY  
(Androulakis et al (2008) Acta Cryst. D) [PubMed]

HOMENEWSABOUTDATASCHMAPARTNERS

## Register Experiment

Note: FTP details of the download location of the experiment are optional, but recommended. Experiment Registration/Editing/Reingestion may take a few minutes to process.

METS XML url:

Private Password:

Ftp location:

Ftp port:

Ftp username:

Ftp password:

Experiment ingestion into TARDIS' local cache can take minutes. A successful registration is shown below.

**TARDIS** v2 Beta  
33 Datasets from 16 Structures, 7331 Files, 106.0 GB Data Indexed, 3.2 GB Avg. Dataset Size  
Welcome, steve [Log Out]

FEDERATED DIFFRACTION IMAGE PUBLICATION REPOSITORY  
(Androulakis et al (2008) Acta Cryst. D) [PubMed]

HOMENEWSABOUTDATASCHMAPARTNERS

Experiment successfully registered. Experiment must be approved by an administrator before being made public.

Note: Data needs to be approved by an administrator before attaining a persistent handle or showing in the public experiment index.