XChem training: Directory structure

May 2022

Working directory

You will have a proposal number starting with lb, e.g.:

- lb13385

- **For each target/screen you will have a visit number, e.g.:**
  - lb13385**-1**

- **You will end up with visits assigned to both:**
  - Lab34: labxchem
  - The beamline: I04-1

- **Your first labxchem visit will be the working directory for the duration of the project**
  - Other lab visits will be created to trigger lab access
  - Other beamline visits will be created for data collection

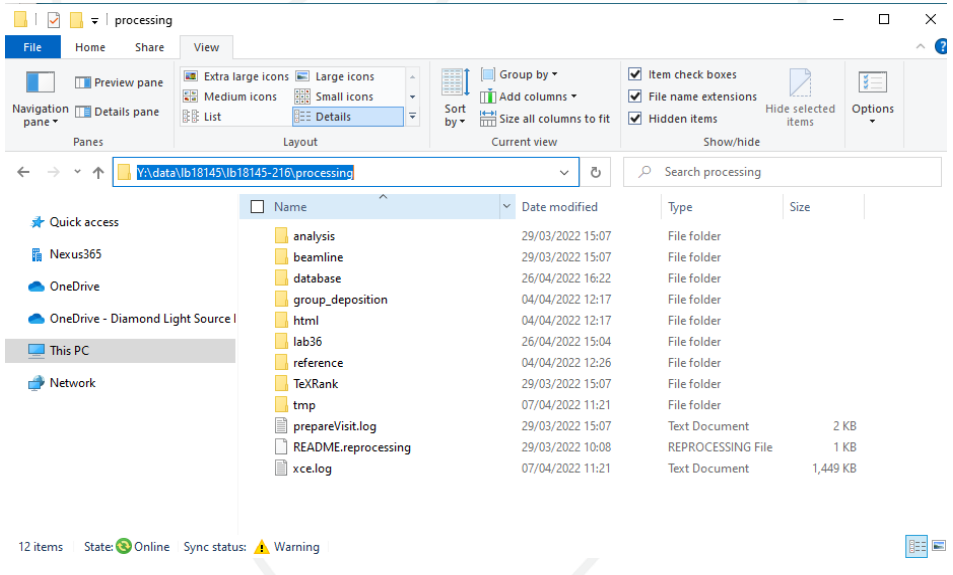
Useful linux commands

- Setup useful commands **(do this first)**:
  - cd /dls/labxchem/data/proposal/visit/processing/
  - source /dls/science/groups/i04-1/software/XChem/xchempaths.sh
- xchempaths.sh will set paths for these commands:
  - tserver - to launch a windows remote desktop from linux
  - xce - to launch XChemExplorer
  - csv2ispyb - to automatically load the data collection information in iSPyB
  - preparevisit - to create the subfolders needed for XChem
    - **It needs to be run under the 'processing' folder**
  - Cluster commands (listed below)
- Checking the status of the cluster:
  - Type: "qstat" **or "**watch qstat"
    - r = job running
    - S = job suspended (cluster is busy – it will run eventually)
    - Anything with an E (eg Eqw) is an error - bad
- Deleting jobs on the cluster:
  - qdel jobID

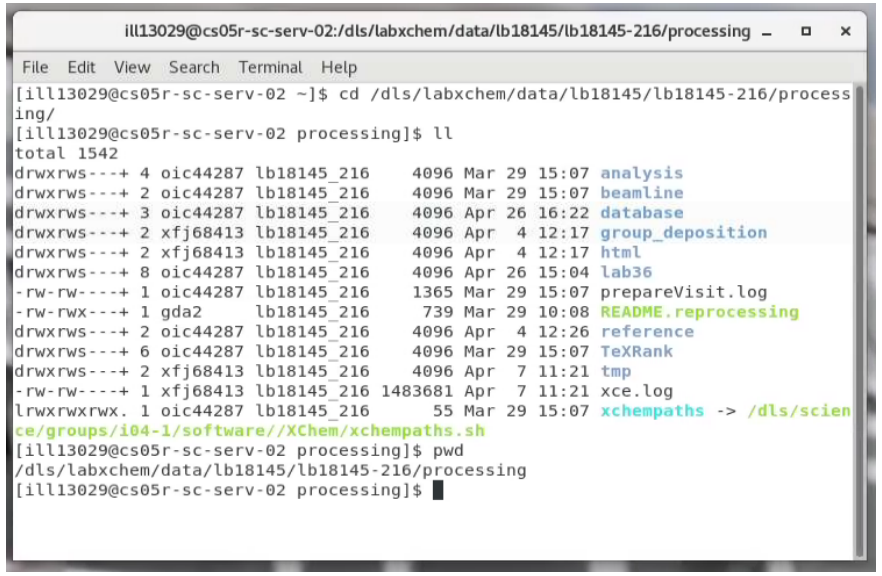
Linux and windows

- **From linux, the location is accessed via:**
  - /dls/labxchem/data/proposal/visit/processing/
- **You (or your local contact) will create your subfolders in visit-1 by running:**
  - cd /dls/labxchem/data/proposal/visit/processing/
  - preparevisit
- **From windows (lab PCs mainly), you will have access to your visit -1 working directory via:**
  - Y:\data\proposal\visit\processing\

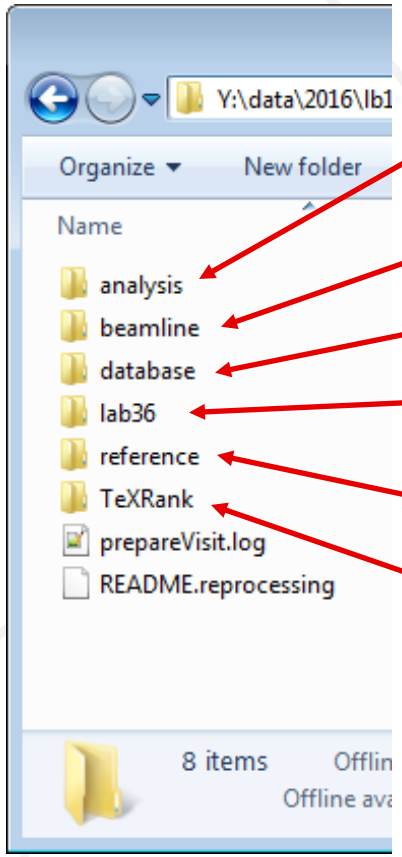
Windows world:
Y:\data\lb18145\lb18145-216\processing



Linux world:
/dls/labxchem/data/2016/lb13385-70/processing

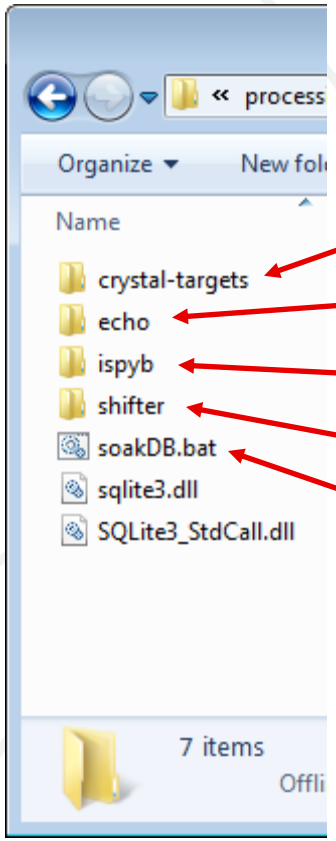


Working directory structure



- **Data collection results and pandda analysis**
- ~~*Links to beamline visit directories*~~ *(obsolete)*
- **The datafile (and backups)**
- **Directory for lab work (soakDB, echo, shifter)**
- **pdb of a good reference model**
- ~~*TeXRank executable and location for crystal image files*~~ *(obsolete)*

Lab 36 directory structure:



- Crystal target lists output from TeXRank
- csv files for echo soaking
- csv files for upload to ispyb
- csv files for the shifter
- soakDB launcher