XChemDirectory Structure& Linux commands

2024

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**

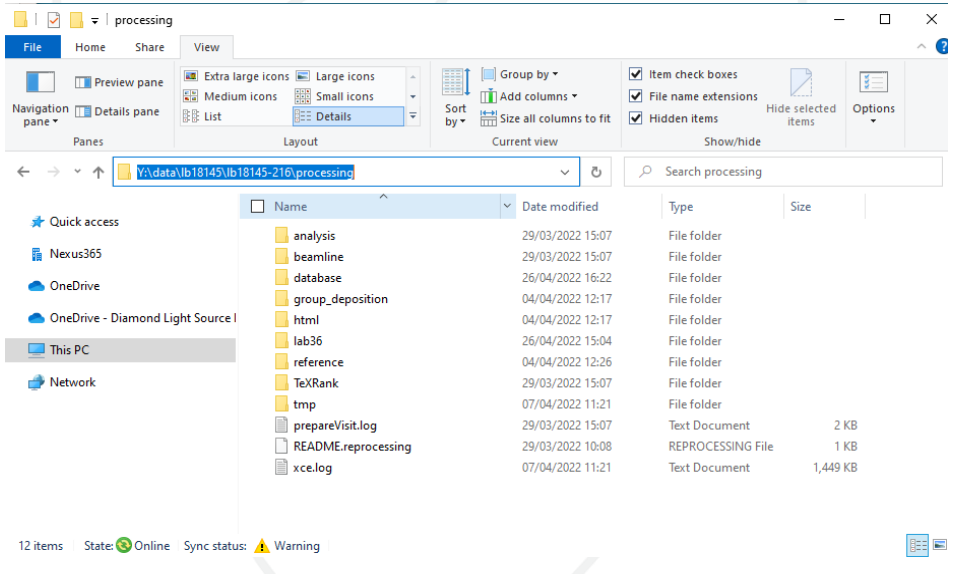
- **You will end up with visits assigned to both:**
  - Lab34: labxchem
  - The beamline: I04-1

- **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

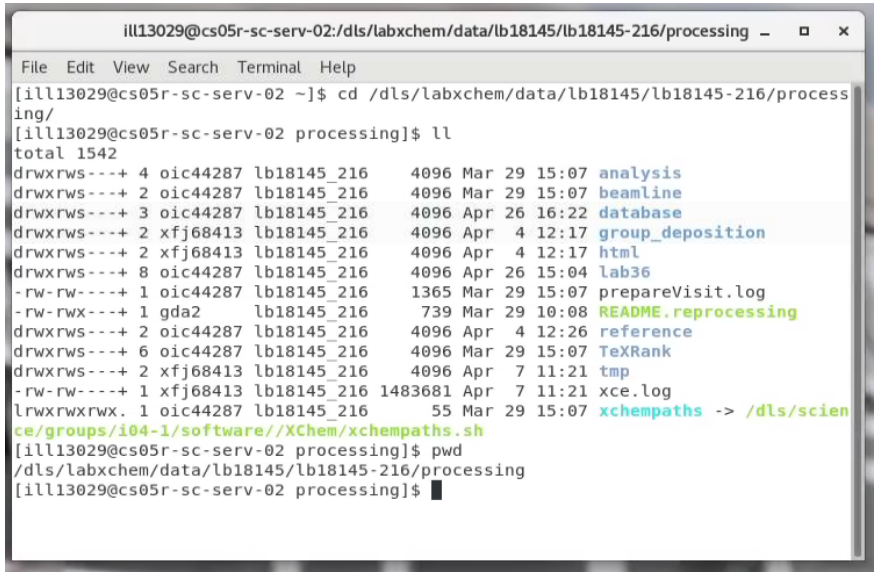
Linux and windows

- **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\

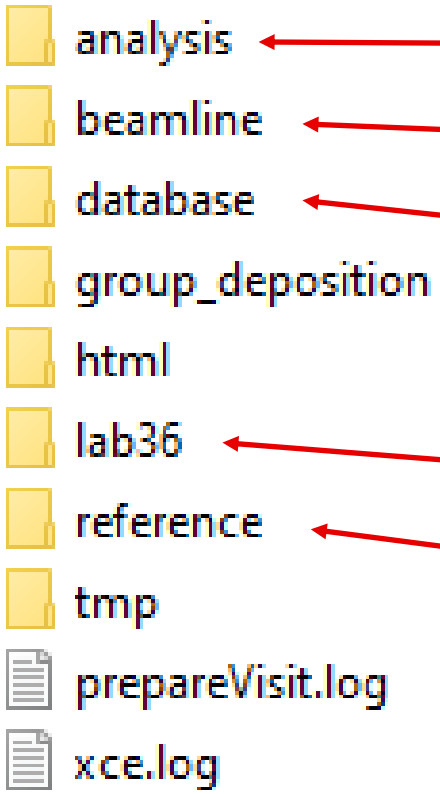
Windows world:
Y:\data\lb18145\lb18145-216\processing



Linux world:
/dls/labxchem/data/lb18145/lb18145-216/processing

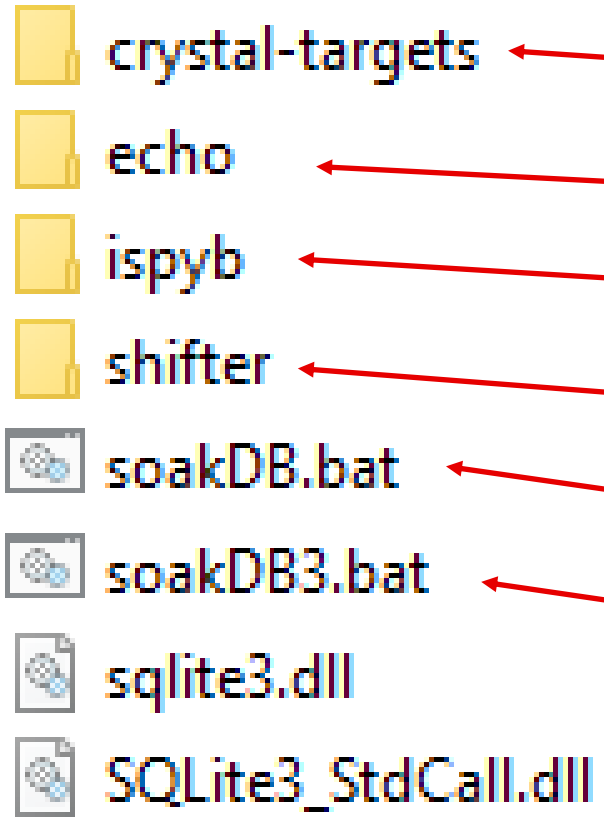


Working directory structure



- **Data collection results and pandda analysis**
- Links to beamline visit directories ***(obsolete – do not use)***
- **SQlite datafile (and backups)**
- **Files for PDB deposition**
- **Directory for lab work (soakDB, echo, shifter)**
- **pdb of a good reference model**

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**
- OldsoakDB launcher (***obsolete – do not use***)
- **Current soakDB launcher (use this one!)**

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:
  - preparevisit - to create the subfolders needed for XChem
  - tserver - to launch a windows remote desktop from linux
  - xce - to launch XChemExplorer
    - **Needs to be run under the 'processing' folder**
  - csv2ispyb - to automatically load the data collection information in iSPyB
- Checking the status of jobs on the cluster (type into terminal):
  - *"ssh wilson"* – connect to the Wilson Cluster
  - *"sacct"* – display jobs
  - *"scancel **<jobid>**"* – cancel a job
  - "*watch sq.sh -u **<yourfedid>*** -nf" – watch jobs