easypipe Documentation

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CONTENTS

You can also grab a hardcopy of the easYPipe documentation in PDF

CHAPTER

ONE

GETTING STARTED (LINUX)

1.1 Check your python version

First, open a terminal.

easYPipe needs at least Python 3.6.

You may already have Python installed – you can check which version by doing:

```
$ python --version
```

If the version is < 3.0, do:

```
$ python3 --version
```

If that fails or Python 3 version is <3.6, install a version of Python >= 3.6 using the package manager of your distribution. For example for Ubuntu 18.04:

Installing add-apt-repository (if add-apt-repository command not found):

```
$ su
# apt update
# install software-properties-common
```

Then:

```
$ su
# add-apt-repository ppa:deadsnakes/ppa
# apt update
# apt-get install python3.7
```

If you encounter difficulties, see supported versions for this repository … maybe it's time to upgrade your operating system !!

If you've updated you Python version from 3.5 to 3.6, you can change default Python 3 to Python 3.6:

```
# update-alternatives --install /usr/bin/python3 python3 /usr/bin/python3.5 1
# update-alternatives --install /usr/bin/python3 python3 /usr/bin/python3.6 2
```

Check that Python 3 has been correctly installed:

```
$ python3 --version
Python 3.6
```

To swap between versions of Python, run the following:

```
# update-alternatives --config python3
```

1.2 Check if pip is installed

pip is a package management tool for Python.

Check if pip3 is installed:

```
$ which pip3
```

If that fails, install pip3 using the package manager of your distribution. For example for Ubuntu:

```
$ su
# apt-get install python3-pip
```

Check if pip3 is linked to Python >= 3.6:

```
$ pip3 --version
pip 21.0.1 from /home/username/.local/lib/python3.6/site-packages/pip (python 3.6)
```

If it's not the case, you can try:

```
$ wget https://bootstrap.pypa.io/get-pip.py
$ su
# python3 get-pip.py
then check:
$ pip3 --version
```

1.3 Software requirements

easYPipe is a pipeline that requires other software.

1.3.1 Phenix

You need Phenix[1] installed and to modify PHENIX_PATH value in config.py file accordingly.

Example for PHENIX_PATH in config.py:

```
PHENIX_PATH = "/usr/local/phenix-1.18.2-3874/"
```

[1] https://www.phenix-online.org/

1.3.2 Open Babel

Open Babel[2] is a chemical toolbox needed for ligands.

Example for BABEL_PATH in config.py:

```
BABEL_PATH =  "/usr/local/OPENBABEL/openbabel-2-4-1/build/bin/"
```

Important

paths to these software have to be modified in config.py file accordingly to your installation (see next step)

1.4 Download and install easypipe package

Download the zip archive that should look like easypipe-1.4.8.tar.gz.

Go where is the archive and unzip:

```
$ tar -xvzf easypipe-1.4.8.tar.gz
```

Go to folder easypipe-1.4.8:

```
$ cd easypipe-1.4.8
```

Modify (open in a text editor) **config.py** file (in easypipe-1.4.8 folder), in particular 'Software used by modules' part since nothing will work without links to *software*.

Warning

config.py file modifications have to be done before installation !! If you want to modify it afterwards, just launch installation again.

Then install:

```
$ su
# python setup.py install # if your default python version is >=3.6
or
# python3 setup.py install # if your python3 version is >=3.6
or
# python3.6 setup.py install # if your python3 version is linked to python3.5
```

If you've updated you Python version from 3.5 to 3.6, you may encountered some dependecies and conflict problems. Read carefully the error messages. These commands can help you:

```
$ su
# apt-get install libffi-dev

# pip3 uninstall PyNaCl
# pip3 install PyNaCl
```

(continues on next page)

[2] http://openbabel.org/wiki/Main_Page

(continued from previous page)

```
# pip3 install setuptools_rust

# cd /usr/lib/python3/dist-packages
# sudo ln -s apt_pkg.cpython-{35m,36m}-x86_64-linux-gnu.so
```

1.5 Check easypipe installation

You can test if installation is successfull doing:

```
$ easypipe.py -h
```

If you get no error but the help message, easypipe installation is successfull.

If you've updated you Python version from 3.5 to 3.6, you may encountered the following error:

```
$ PermissionError: [Errno 13] Permission denied: '/usr/local/lib/python3.6/dist-packages/
↪easypipe-1.4.8-py3.6.egg/EGG-INFO/requires.txt'
```

In this case, this command should help:

```
$ cd /usr/local/lib/python3.6/dist-packages/easypipe-1.4.8-py3.6.egg/EGG-INFO/
$ su
# chmod a+r requires.txt
```

In the way, if you have 3.8 Python version (in Ubuntu 20.04 for example), you may encountered the following error:

```
$ PermissionError: [Errno 13] Permission denied: '/usr/local/lib/python3.8/dist-packages/
↪easypipe-1.4.8-py3.8.egg/EGG-INFO/requires.txt'
```

In this case, this command should help:

```
$ cd /usr/local/lib/python3.8/dist-packages/easypipe-1.4.8-py3.8.egg/EGG-INFO/
$ su
# chmod a+r requires.txt
```

1.6 Uninstall easypipe package

To uninstall easypipe package properly, do:

```
$ su
# pip3 uninstall easypipe
or
# python3 -m pip uninstall easypipe
or
# python3.6 -m pip uninstall easypipe
```

If you have such an error message: "Can't uninstall 'easypipe'. No files were found to uninstall.", try again after changing working directory (not in easypipe package directory), it should work.

Note

‘pip3 freeze’ lists the names of all python packages installed.

1.7 References

CHAPTER

TWO

GETTING STARTED (WINDOWS)

2.1 Check your python version

First, open a Command Prompt.

Note

To open Command Prompt, simply type 'cmd' in the search box of the Windows taskar.

easYPipe needs at least Python 3.6.

You may already have Python installed – you can check which version by doing:

```
C:\> python --version
or
C:\> py -V
```

If Python version is <3.6, install the latest Python 3 version. Download the latest python version Python downloads site. You can follow instructions here. But what you need is simply:

```
- Run the installer. You can do so by double-clicking python-<version>.exe in your Downloads folder.
- !!!! Check the box next to "Add Python <version> to PATH." It's at the bottom of the window.
- Install Now (customize installation not compulsory).
- Click Disable path length limit. This ensures that Python (and other apps) to use paths more than 260 characters in length.
```

Check that Python 3 has been correctly installed:

```
C:\> python --version
Python 3.9

or

C:\> py -V
Python 3.9
```

2.2 Software requirements

easYPipe is a pipeline that requires other software.

2.2.1 Phenix

You need Phenix[1] installed and to modify PHENIX_PATH value in config.py file accordingly.

Example for PHENIX_PATH in config.py:

```
PHENIX_PATH = r"C:\Users\myname\Phenix\phenix-installer-1.19.1-4122-intel-windows-x86_64"
```

2.2.2 Open Babel

Open Babel[2] is a chemical toolbox needed for ligands.

Install Open Babel GUI for Windows.

Example for BABEL_PATH in config.py:

```
BABEL_PATH = r"C:\Program Files\OpenBabel-3.1.1"
```

2.2.3 Advices

Important

paths to these software have to be modified in config.py file accordingly to your installation (see next step)

Tip

it might be wise to use LibreOffice[3] as many csv spreadsheets are generated by easYPipe and Excel does not handle the official csv format (i.e. comma-separated values) well for non-English speaking versions

2.3 Download and install easypipe package

Download the zip archive that should look like easypipe-1.4.8.tar.gz.

Go where is the archive and unzip:

```
C:\> tar -xvzf easypipe-1.4.8.tar.gz
```

Go to folder easypipe-1.4.8:

```
C:\> cd easypipe-1.4.8
```

[1] https://www.phenix-online.org/

[2] http://openbabel.org/wiki/Main_Page

[3] https://www.libreoffice.org/

Modify (open with a text editor like Notepad) **config.py** file (in easypipe-1.4.8 folder), in particular 'Software used by modules' part since nothing will work without links to *software*.

Warning

config.py file modifications have to be done before installation !! If you want to modify it afterwards, just launch installation again. Use a basic text editor and not a word processing software !

Then install:

```
C:\> python setup.py install
or
C:\> py setup.py install
```

2.4 Check easypipe installation

You can test if installation is successfull doing:

```
$ easypipe.py -h
```

If you get no error but the help message, easypipe installation is successfull.

Depending on your python version, you may encountered some dependecies and conflict problems. Read carefully the error messages.

In case of the following error:

```
$ cffi>=1.4.3 distribution was not found and is required by PyNaCl
```

This command should help:

```
$ py -m pip install cffi
```

2.5 Uninstall easypipe package

To uninstall easypipe package properly, do:

```
C:\>  pip uninstall easypipe
```

Note

'py -m pip freeze' lists the names of all python packages installed.

2.6 References

CHAPTER

THREE

EASYGET

easYGet comes with *easYPipe*.

easYGet makes it possible to download all at once the mx 'PROCESSED_DATA' from a synchrotron for a given beamline (several dates possible) and a given acronym.

Downloaded processed datasets are organized by dataset folders, ready to launch easypipe.

For the moment, only works for data from Grenoble ESRF and Barcelone ALBA synchrotrons.

3.1 easYGet usage

easyget.py [-h] [-s {ESRF}] [-l LOGIN] [[-m MX] [-b BEAMLINE] [-d DATES [DATES …]] [-p PROTEIN] [-g GROUP]

optional arguments	description
-h, –help	show this help message and exit
-s {ESRF}, –synchrotron {ESRF,ALBA}	which synchrotron? (default = ERSF)
-l LOGIN, –login LOGIN	synchrotron login (your personal SMIS login)
-m MX, –mx MX	name of mx proposal synchrotron login (Example: 'mx—-')
-b BEAMLINE, –beamline BEAMLINE	name of the beamline
-d DATES [DATES …], –dates DATES [DATES …]	date of the run (format AAAAMMJJ) or list of dates for the same run (format AAAAMMJJ AAAAMMJJ)
-p PROTEIN, –protein PROTEIN	protein acronym or space if no acronym (manual collections)
-g GROUP, –group GROUP	group added via MxCube3 as a supplementary folder level before acronym

Information can be provided either in command line or in interactive mode in a terminal, or mix.

For example, you can simply run:

```
$ easyget.py
```

or:

```
$ easyget.py --login anna2502 --mx mx1000
```

or:

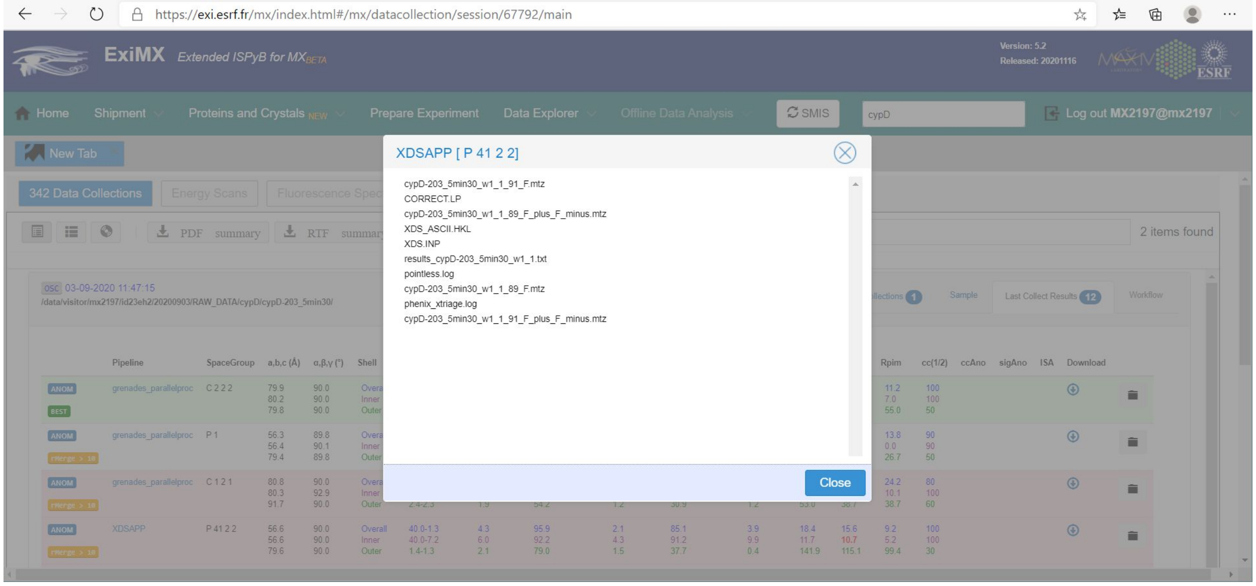
```
$ easyget.py --login anna2502 --mx mx1000 --protein myprot --beamline id30a1 --dates␣
↪20210131 20210201
```

other commands are possible …

> **Note**
>
> test also the day after each date given (useful for 24h experiments …)

3.2 What does it do ?

Processed data @ESRF: for each crystal collected, several proccesses can succeed and for each a zip is available for download

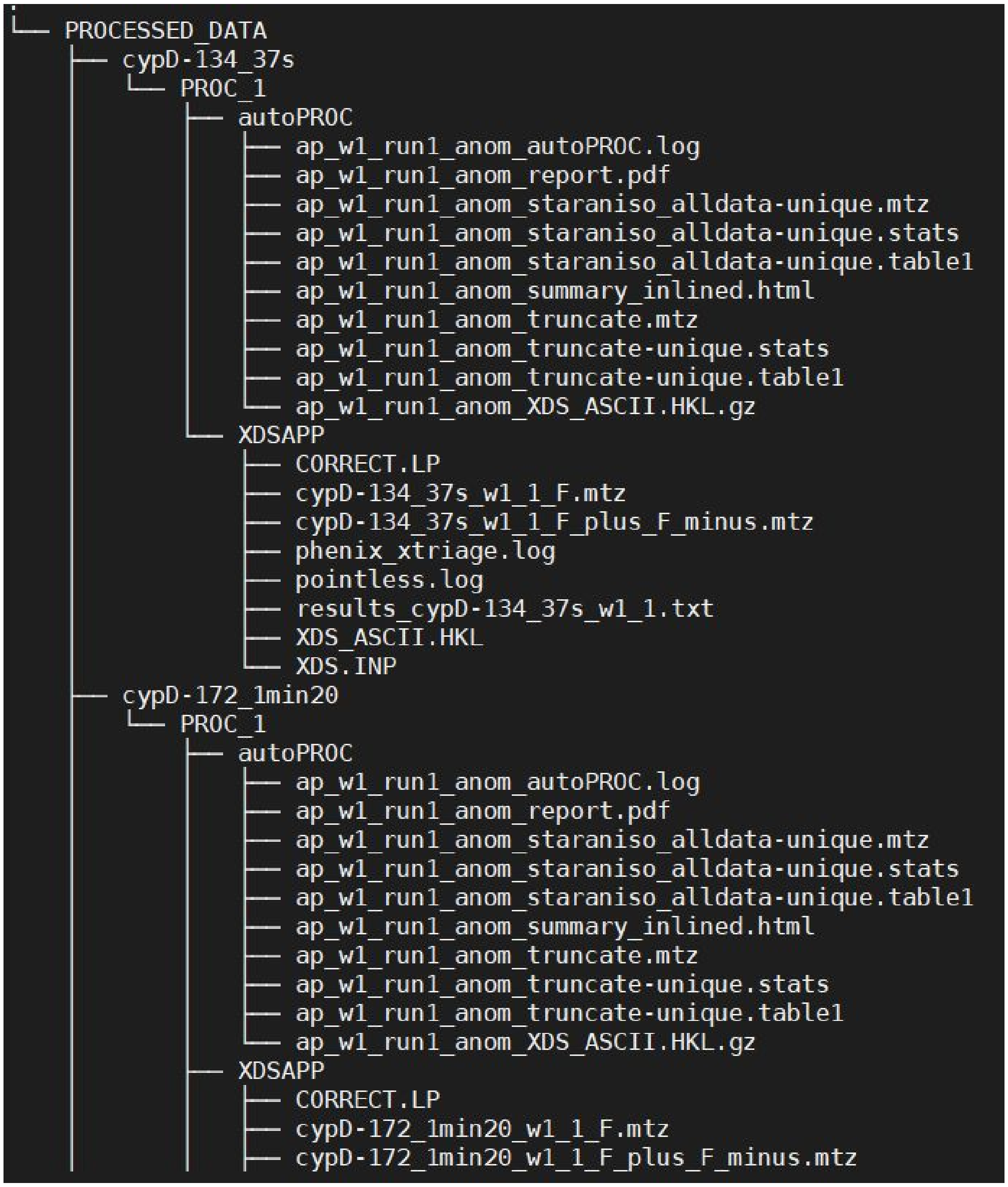


XDSAPP [P 41 2 2]

cypD-203_5min30_w1_1_91_F.mtz
CORRECT.LP
cypD-203_5min30_w1_1_89_F_plus_F_minus.mtz
XDS_ASCII.HKL
XDS.INP
results_cypD-203_5min30_w1_1.txt
pointless.log
cypD-203_5min30_w1_1_89_F.mtz
phenix_xtriage.log
cypD-203_5min30_w1_1_91_F_plus_F_minus.mtz

All these processed data are copied this way by easYGet:

- **dataset folder for each dataset**
  - PROC_1, PROC_2, … if run 1, run 2 …
  - process sub-folder, with processed data for each process



```
└── PROCESSED_DATA
    ├── cypD-134_37s
    │   └── PROC_1
    │       ├── autoPROC
    │       │   ├── ap_w1_run1_anom_autoPROC.log
    │       │   ├── ap_w1_run1_anom_report.pdf
    │       │   ├── ap_w1_run1_anom_staraniso_alldata-unique.mtz
    │       │   ├── ap_w1_run1_anom_staraniso_alldata-unique.stats
    │       │   ├── ap_w1_run1_anom_staraniso_alldata-unique.table1
    │       │   ├── ap_w1_run1_anom_summary_inlined.html
    │       │   ├── ap_w1_run1_anom_truncate.mtz
    │       │   ├── ap_w1_run1_anom_truncate-unique.stats
    │       │   ├── ap_w1_run1_anom_truncate-unique.table1
    │       │   └── ap_w1_run1_anom_XDS_ASCII.HKL.gz
    │       └── XDSAPP
    │           ├── CORRECT.LP
    │           ├── cypD-134_37s_w1_1_F.mtz
    │           ├── cypD-134_37s_w1_1_F_plus_F_minus.mtz
    │           ├── phenix_xtriage.log
    │           ├── pointless.log
    │           ├── results_cypD-134_37s_w1_1.txt
    │           ├── XDS_ASCII.HKL
    │           └── XDS.INP
    ├── cypD-172_1min20
    │   └── PROC_1
    │       ├── autoPROC
    │       │   ├── ap_w1_run1_anom_autoPROC.log
    │       │   ├── ap_w1_run1_anom_report.pdf
    │       │   ├── ap_w1_run1_anom_staraniso_alldata-unique.mtz
    │       │   ├── ap_w1_run1_anom_staraniso_alldata-unique.stats
    │       │   ├── ap_w1_run1_anom_staraniso_alldata-unique.table1
    │       │   ├── ap_w1_run1_anom_summary_inlined.html
    │       │   ├── ap_w1_run1_anom_truncate.mtz
    │       │   ├── ap_w1_run1_anom_truncate-unique.stats
    │       │   ├── ap_w1_run1_anom_truncate-unique.table1
    │       │   └── ap_w1_run1_anom_XDS_ASCII.HKL.gz
    │       ├── XDSAPP
    │       │   ├── CORRECT.LP
    │       │   ├── cypD-172_1min20_w1_1_F.mtz
    │       │   ├── cypD-172_1min20_w1_1_F_plus_F_minus.mtz
```

CHAPTER

FOUR

EASYPIPE

easYPipe is a pipeline for the automatization of ligand and fragment X-Ray crystallographic screening.

easYPipe sequentially runs phenix.ligand_pipeline[1] on several datasets of a protein that has been screened with different ligands.

When ligand smiles are given, ligand can be placed automatically in each corresponding structure.

Results are gathered and organized in a 'RESULTS' directory, which facilitates future visualization, refinement and deposition. Corresponding relevant information is summarized in a csv file.

easYPipe is specially adapted for ligand or fragment screening in structure-based drug design projects.

See also

easYGet that comes with easYPipe, for an automated download of processed data from synchrotron.

4.1 easYPipe usage

easypipe.py [-h] data {prep,reindex,ligands,launch,pandda} …

arguments	description
data	folder with datasets in subfolders (mandatory)
-h, –help	show this help message and exit

Example:

```
$ easypipe.py PROCESSED_DATA -h
```

[1] https://www.phenix-online.org/documentation/reference/ligand_pipeline.html

subcommands	description
prep	prepare data: listing of mtz to treat with information
reindex	try to reindex mtz according to the space group of reference file
ligands	generate ligands files before launching with ligand search
launch	launch all the "phenix.ligand-pipeline" (after the preparation steps)
summary	compile the results of all the 'launch' execution in a single csv file
auto	run main easYPipe steps (prep, reindex, launch, summary) in automatic mode, but without ligand search
pandda	copy results from easypipe to a 'PANDDA' folder, as data ready to launch PanDDA

Example:

```
$ easypipe.py PROCESSED_DATA prep
```

You can have a look to the *quickstart guide*.

For a better experience, also read instructions for each subcommands.

4.1.1 References

CHAPTER

FIVE

EASYPIPE QUICKSTART GUIDE

5.1 1. Retrieve and organize your processed data

Note

You can retrieve your processed data from synchrotron using *easYGet*.

Processed data should be in datasets folders, all grouped in a folder. More information on how to organize your data *here*.

5.2 2. Prepare the data with 'prep'

The first step is intended to list mtz to be treated:

```
$ easypipe.py PROCESSED_DATA prep
```

where here 'PROCESSED_DATA' is the folder with your datasets.

Warning

For Windows users, $ is the Linux prompt that corresponds to C:> in Windows command prompt, and should not be written

Now, you can have a look at /easypipe/1a_prep/mtz_to_treat_ALL.csv file that lists mtz found in your processed data with information like resolution, completeness or space group.

For more details on this step see *here*.

5.3 3. Reindex if necessary with ‘reindex’

If you see that some mtz should be in higher symmetry space group (in /easypipe/1a_prep/mtz_to_treat_ALL.csv file), then you can try to reindex.

Run:

```
$ easypipe.py PROCESSED_DATA reindex P41212
equivalent to:
$ easypipe.py PROCESSED_DATA reindex 92
```

For more details on this step see *here*.

5.4 4. Add ligands with ‘ligands’

This step is necessary if you want Phenix to try to find and place ligands, or if you want to automatically generate the CIF and PDB of your ligands.

First, you have to fill in the fields <ligand name> and <ligand smiles> of /1c_ligands/ligands_for_datasets.csv file.

Then, run:

```
$ easypipe.py PROCESSED_DATA ligands easYPipe/1c_ligands/ligands_for_datasets_OK.csv
```

where here ligands_for_datasets_OK.csv is the name of your filled ligand csv file.

For more details on this step see *here*.

5.5 5. Process the data with ‘launch’

Now you can run Phenix on your processed mtz.

5.5.1 Mode

Default mode, is ‘fast’ mode. This mode uses rigid body refinement and can be run to get a first result rapidly.

Example:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder
```

where my_ref_folder gather fasta file and pdb files for replacement, and cif file if there is a ligand in the model.

Warning

pdb files should include the row starting with ‘CRYST1’ containing information on space group

Now, have a look at your *results* in the corresponding ‘RESULTS’ csv file.

If some processes failed, they probably need longer calculations. You can try ‘full’ mode:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full
```

In case your protein changes its space group, with ligand for example, you can ask not to fix space group. As a result, all mtz could be treated even with 'bad' space group. The duration for this will be much longer. But you can only do it for some using simulation mode first (see above):

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode allsg
```

5.5.2 Ligand search

If you want LigandFit to place ligands, you first have to run 'ligand' subcommand (*see above*).

Then just add '–lig' option:

```
$  easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig
```

The default cutoff for LigandFit to place a ligand is 0.7, but you can change it if you see that it is too high, with '–cclig' option:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --cclig 0.6
```

If several ligands are supposed to fix, you can ask for LigandFit to place more than one ligand, with '–nblig' option:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --cclig 0.6 --nblig 5
```

5.5.3 Datasets to treat

Default behavior is to run phenix.ligand_pipeline on the mtz of best completeness for each dataset, you can start with it.

If there are failures in the treatment of 'best completeness' mtz, you can try to treat a higher number of mtz for each dataset.

You can first start by running on mtz from autoPROC process which is generally a good compromise between resolution and completeness:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --autoproc
```

Or you can run on the two first mtz of best completeness for each dataset:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --best 2
```

or more . . . :

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --best 5
```

or on the whole processed mtz files:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --whole
```

If only some datasets are problematic, you can run in simulation mode first, modify the corresponding 'launch' csv file in /easYPipe/2_launch/ (replace 'yes' by 'no' in the 'to treat' column, for those not to process), then run again:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --whole --simulate
then, after modification of the 'launch' csv file:
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --whole
```

Then, only selected mtz will be treated, reducing the duration of the treatment.

For more details on this step see *here*.

5.6 6. Compile results in a summary file

If you have run several times the 'launch' subcommand, you will have several 'RESULT' csv files in the RESULTS folder, that you probably wish to compile and clean.

The *'summary'* subcommand is automatically run at the end of each 'launch' subcommand.

If you have done several 'launch' with different space group for example, you will have to run manually the *'summary'* subcommand.

Then a global SUMMARY file will be created, that compiles all SUMMARY files present in RESULTS folders.

Then run:

```
$ easypipe.py PROCESSED_DATA summary
```

5.7 7. Automatic mode

This mode allows to run main easYPipe steps (prep, reindex, launch, summary) without any intervention. It could be a good starting point before running more 'launch' commands or ligand search.

Example:

```
$ easypipe.py PROCESSED_DATA auto my_ref_folder --best 2 --mode full
```

Note

Ligand search is not supported at this time in this mode.

For more details on this mode see *here*.

CHAPTER

SIX

EASYPIPE ‘PREP’

Important

This step is a first mandatory step for the preparation of the data.

6.1 Usage

easypipe.py data prep [-h]

Example:

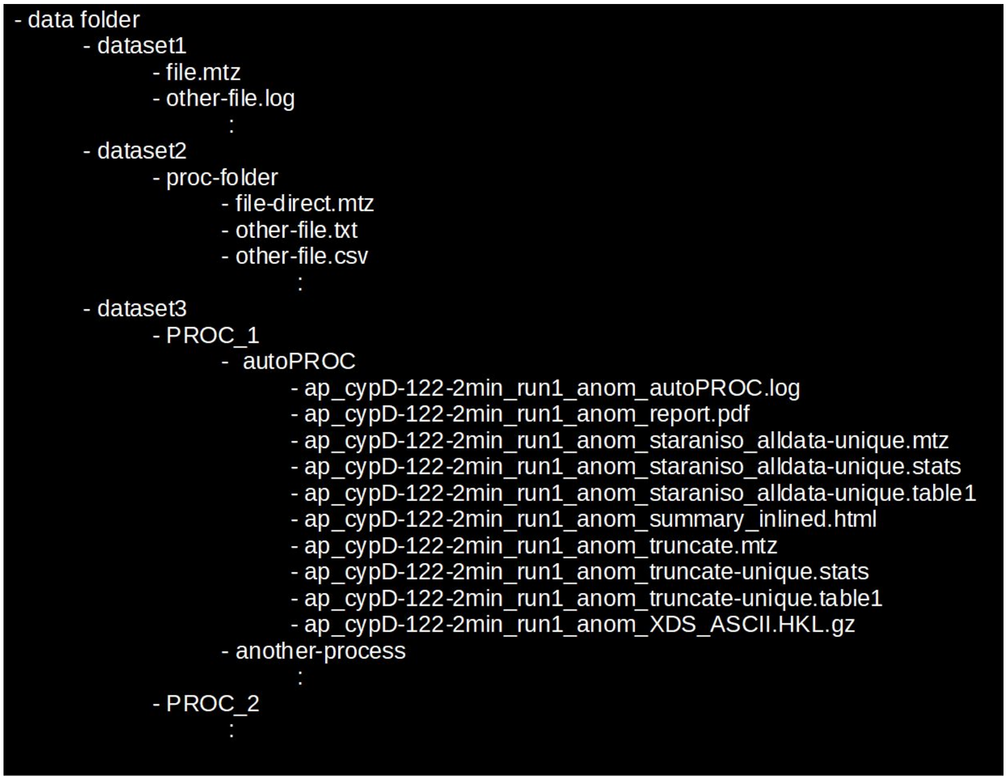
```
$ easypipe.py PROCESSED_DATA prep
```

6.2 How the data should be organized ?

The data folder (whatever it’s name) must contain only datasets folders.

Within each dataset folder, the processed data can be organized in several ways:

- a mtz file directly in dataset folder
- a mtz file in a sub-folder, or in a sub-sub-folder … of dataset folder
- several processes are possible for a dataset, better if they are in different sub-folders, but not mandatory
- if several mtz files are present in the same sub-folder, only the ones fitting the templates (from EDNA processes) will be treated, or if none fits only the first mtz file will be considered



```
- data folder
        - dataset1
                - file.mtz
                - other-file.log
                         :
        - dataset2
                - proc-folder
                        - file-direct.mtz
                        - other-file.txt
                        - other-file.csv
                                 :
        - dataset3
                - PROC_1
                        -  autoPROC
                                - ap_cypD-122-2min_run1_anom_autoPROC.log
                                - ap_cypD-122-2min_run1_anom_report.pdf
                                - ap_cypD-122-2min_run1_anom_staraniso_alldata-unique.mtz
                                - ap_cypD-122-2min_run1_anom_staraniso_alldata-unique.stats
                                - ap_cypD-122-2min_run1_anom_staraniso_alldata-unique.table1
                                - ap_cypD-122-2min_run1_anom_summary_inlined.html
                                - ap_cypD-122-2min_run1_anom_truncate.mtz
                                - ap_cypD-122-2min_run1_anom_truncate-unique.stats
                                - ap_cypD-122-2min_run1_anom_truncate-unique.table1
                                - ap_cypD-122-2min_run1_anom_XDS_ASCII.HKL.gz
                        - another-process
                                 :
                - PROC_2
                         :
```

Note

Data downloaded with *easYGet* are directly in the right tree organization.

6.3 What does it do ?

In an 'easYPipe' folder created at the place where it is executed, 'prep' copies each processed data mtz in a sub-folder of the dataset in this way:

- creation of an 'easYPipe' treatment directory where it is run
- creation of a subdirectory '0_processed_datasets' where all the datasets folder are created
- creation of a 'data' folder in each dataset folder and copy in this folder of processed mtz and log files
- if there are several mtz in a folder, search for 'EDNA' treatment template and selects the right mtz files

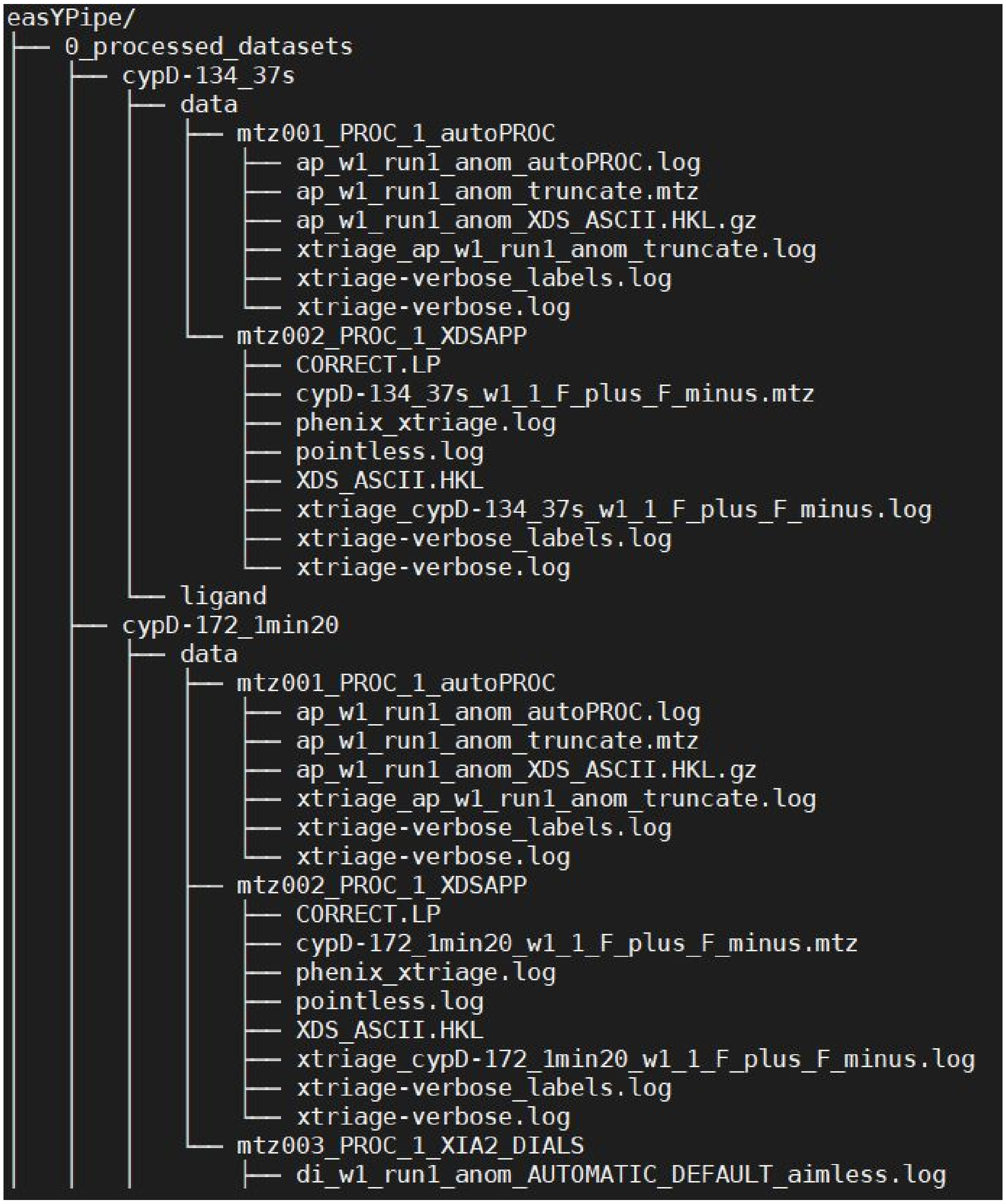
Note

if you add a process for a dataset after a first 'prep', you can launch 'prep' sub-command again, this process will be added to the processes already copied

Then:

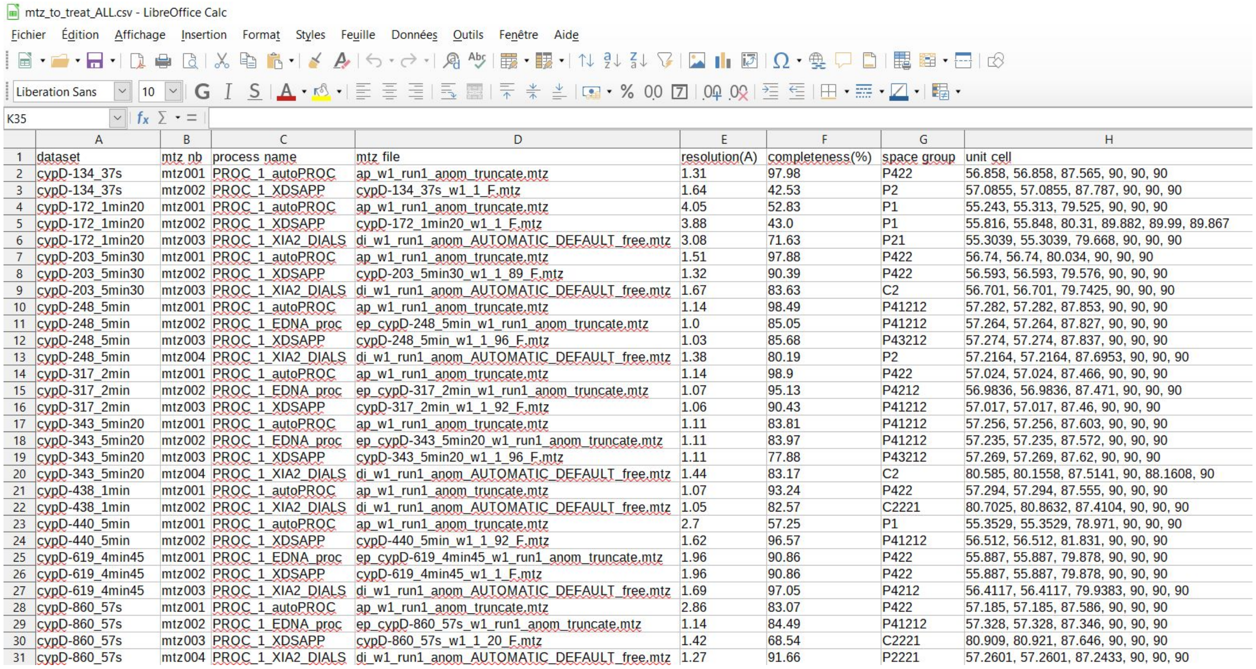
- launch of xtriage[1] for each mtz to get resolution, completeness, space group and cell parameters

[1] https://www.phenix-online.org/documentation/reference/xtriage.html



```
easYPipe/
├── 0_processed_datasets
│   ├── cypD-134_37s
│   │   ├── data
│   │   │   ├── mtz001_PROC_1_autoPROC
│   │   │   │   ├── ap_w1_run1_anom_autoPROC.log
│   │   │   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   │   │   ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
│   │   │   │   ├── xtriage_ap_w1_run1_anom_truncate.log
│   │   │   │   ├── xtriage-verbose_labels.log
│   │   │   │   └── xtriage-verbose.log
│   │   │   └── mtz002_PROC_1_XDSAPP
│   │   │       ├── CORRECT.LP
│   │   │       ├── cypD-134_37s_w1_1_F_plus_F_minus.mtz
│   │   │       ├── phenix_xtriage.log
│   │   │       ├── pointless.log
│   │   │       ├── XDS_ASCII.HKL
│   │   │       ├── xtriage_cypD-134_37s_w1_1_F_plus_F_minus.log
│   │   │       ├── xtriage-verbose_labels.log
│   │   │       └── xtriage-verbose.log
│   │   └── ligand
│   ├── cypD-172_1min20
│   │   ├── data
│   │   │   ├── mtz001_PROC_1_autoPROC
│   │   │   │   ├── ap_w1_run1_anom_autoPROC.log
│   │   │   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   │   │   ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
│   │   │   │   ├── xtriage_ap_w1_run1_anom_truncate.log
│   │   │   │   ├── xtriage-verbose_labels.log
│   │   │   │   └── xtriage-verbose.log
│   │   │   ├── mtz002_PROC_1_XDSAPP
│   │   │   │   ├── CORRECT.LP
│   │   │   │   ├── cypD-172_1min20_w1_1_F_plus_F_minus.mtz
│   │   │   │   ├── phenix_xtriage.log
│   │   │   │   ├── pointless.log
│   │   │   │   ├── XDS_ASCII.HKL
│   │   │   │   ├── xtriage_cypD-172_1min20_w1_1_F_plus_F_minus.log
│   │   │   │   ├── xtriage-verbose_labels.log
│   │   │   │   └── xtriage-verbose.log
│   │   │   └── mtz003_PROC_1_XIA2_DIALS
│   │   │       ├── di_w1_run1_anom_AUTOMATIC_DEFAULT_aimless.log
```

- information on mtz files to be treated written in '/easypipe/1a_prep/mtz_to_treat_ALL.csv' file


mtz_to_treat_ALL.csv - LibreOffice Calc
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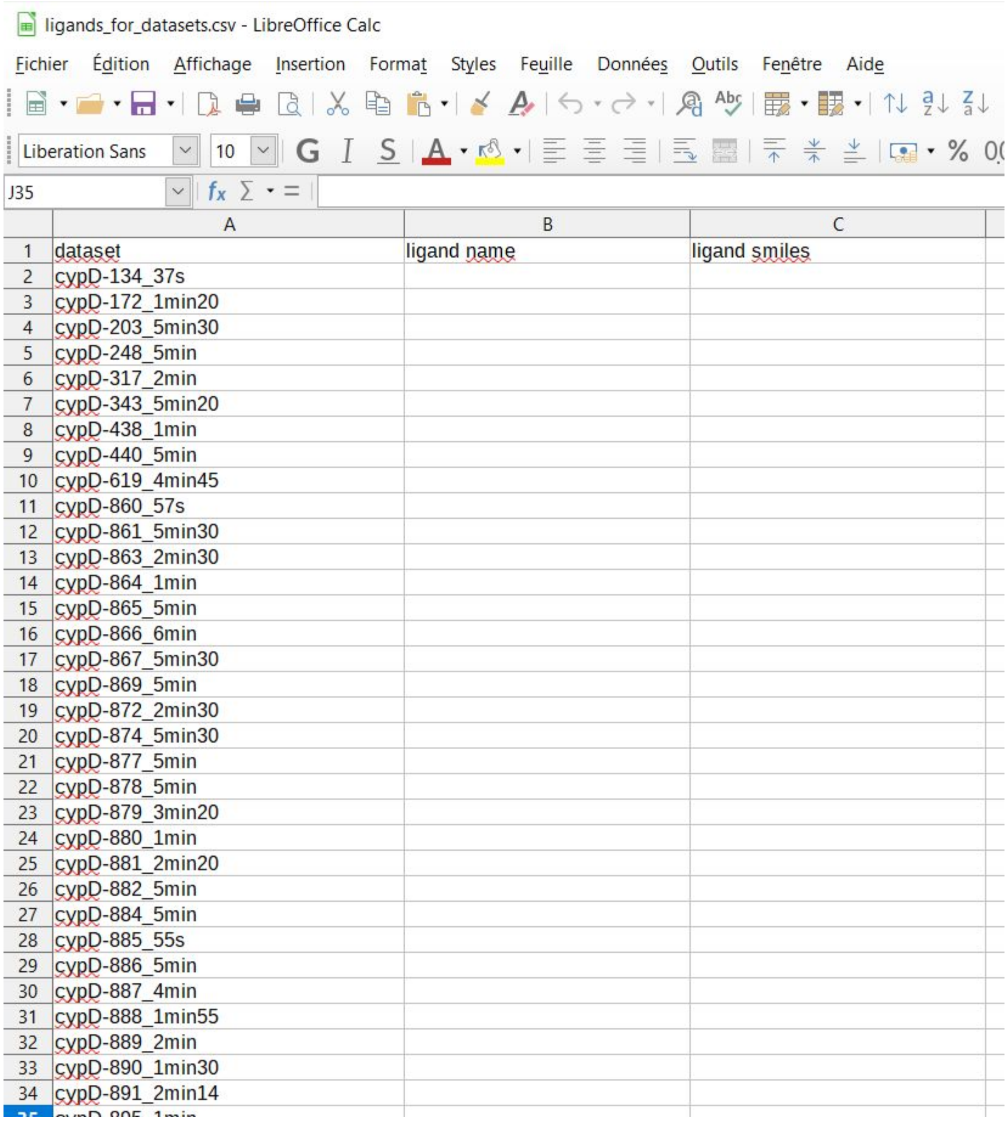
	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.31	97.98	P422	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F.mtz	1.64	42.53	P2	57.0855, 57.0855, 87.787, 90, 90, 90
4	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	4.05	52.83	P1	55.243, 55.313, 79.525, 90, 90, 90
5	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F.mtz	3.88	43.0	P1	55.816, 55.848, 80.31, 89.882, 89.99, 89.867
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	3.08	71.63	P21	55.3039, 55.3039, 79.668, 90, 90, 90
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.51	97.88	P422	56.74, 56.74, 80.034, 90, 90, 90
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F.mtz	1.32	90.39	P422	56.593, 56.593, 79.576, 90, 90, 90
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.67	83.63	C2	56.701, 56.701, 79.7425, 90, 90, 90
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
11	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41212	57.264, 57.264, 87.827, 90, 90, 90
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F.mtz	1.03	85.68	P43212	57.274, 57.274, 87.837, 90, 90, 90
13	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.38	80.19	P2	57.2164, 57.2164, 87.6953, 90, 90, 90
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.9	P422	57.024, 57.024, 87.466, 90, 90, 90
15	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate.mtz	1.07	95.13	P4212	56.9836, 56.9836, 87.471, 90, 90, 90
16	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F.mtz	1.06	90.43	P41212	57.017, 57.017, 87.46, 90, 90, 90
17	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90
18	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F.mtz	1.11	77.88	P43212	57.269, 57.269, 87.62, 90, 90, 90
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.44	83.17	C2	80.585, 80.1558, 87.5141, 90, 88.1608, 90
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.07	93.24	P422	57.294, 57.294, 87.555, 90, 90, 90
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.05	82.57	C2221	80.7025, 80.8632, 87.4104, 90, 90, 90
23	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.7	57.25	P1	55.3529, 55.3529, 78.971, 90, 90, 90
24	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41212	56.512, 56.512, 81.831, 90, 90, 90
25	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate.mtz	1.96	90.86	P422	55.887, 55.887, 79.878, 90, 90, 90
26	cypD-619_4min45	mtz002	PROC_1_XDSAPP	cypD-619_4min45_w1_1_F.mtz	1.96	90.86	P422	55.887, 55.887, 79.878, 90, 90, 90
27	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.69	97.05	P4212	56.4117, 56.4117, 79.9383, 90, 90, 90
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.86	83.07	P422	57.185, 57.185, 87.586, 90, 90, 90
29	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90
30	cypD-860_57s	mtz003	PROC_1_XDSAPP	cypD-860_57s_w1_1_20_F.mtz	1.42	68.54	C2221	80.909, 80.921, 87.646, 90, 90, 90
31	cypD-860_57s	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.27	91.66	P2221	57.2601, 57.2601, 87.2433, 90, 90, 90

-creation of a csv file '/easypipe/1c_ligands/ligands_for_datasets.csv' for future ligand generation with eLBOW[2]

[2] https://www.phenix-online.org/documentation/reference/elbow.html


ligands_for_datasets.csv - LibreOffice Calc
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	A	B	C
1	dataset	ligand name	ligand smiles
2	cypD-134_37s		
3	cypD-172_1min20		
4	cypD-203_5min30		
5	cypD-248_5min		
6	cypD-317_2min		
7	cypD-343_5min20		
8	cypD-438_1min		
9	cypD-440_5min		
10	cypD-619_4min45		
11	cypD-860_57s		
12	cypD-861_5min30		
13	cypD-863_2min30		
14	cypD-864_1min		
15	cypD-865_5min		
16	cypD-866_6min		
17	cypD-867_5min30		
18	cypD-869_5min		
19	cypD-872_2min30		
20	cypD-874_5min30		
21	cypD-877_5min		
22	cypD-878_5min		
23	cypD-879_3min20		
24	cypD-880_1min		
25	cypD-881_2min20		
26	cypD-882_5min		
27	cypD-884_5min		
28	cypD-885_55s		
29	cypD-886_5min		
30	cypD-887_4min		
31	cypD-888_1min55		
32	cypD-889_2min		
33	cypD-890_1min30		
34	cypD-891_2min14		
35	cypD-895_1min		

You have to fill 'ligand name' and 'ligand smiles' fields before running *'easYPipe ligands subcommand'*.

Caution

Save the modified csv file somewhere else or with another name if you don't want to overwrite it in case you launch 'prep' sub-command again . . .

You can also run *'easYPipe reindex subcommand'* if some mtz should be in higher symmetry space group.

If you are not interested in ligand placement or reindexation, you can directly run *'easYPipe launch subcommand'*.

6.4 References

CHAPTER

SEVEN

EASYPIPE ‘REINDEX’

This optional step is useful when several mtz should be in higher symmetry space group.

The program try to reindex according to the space group of the reference mtz.

Example: P422 can be re-indexed to P41212.

7.1 Usage

easypipe.py data reindex [-h] ref_mtz

arguments	description
-h, –help	show this help message and exit
sg_ref	space group of reference for reindexing (name or number)
-s, –simulate	only simulate, generate a csv file listing for each process if mtz file will be reindexed or not. Give the possibility to modify the csv file to choose not to launch some reindexation, before launching again without simulation mode.

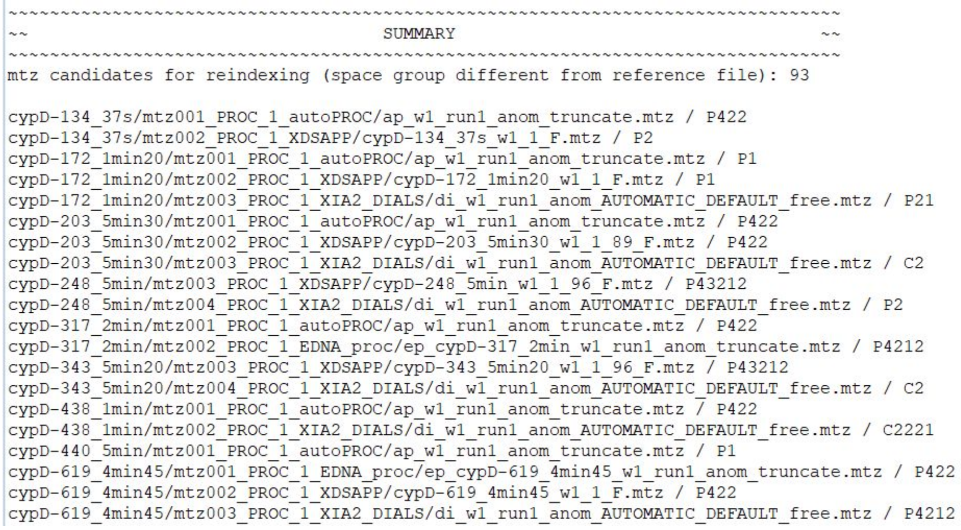
Example:

```
$ easypipe.py PROCESSED_DATA reindex P41212
equivalent to:
$ easypipe.py PROCESSED_DATA reindex 92
```

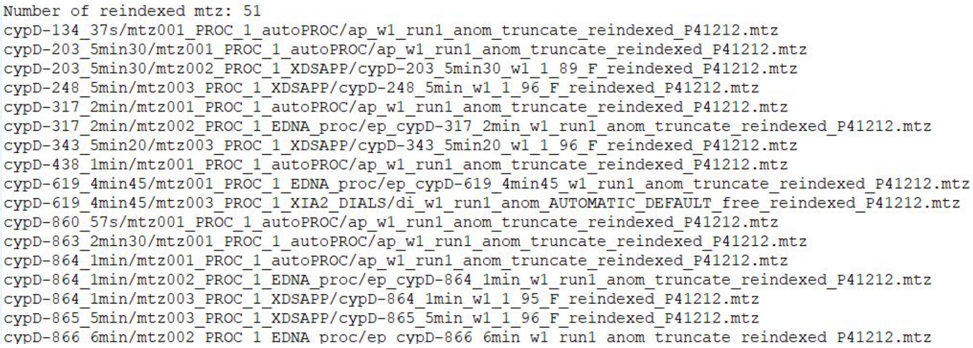
7.2 What does it do ?

- try to reindex mtz file with reflection_file_converter[1] if space group is different from reference space group

[1] https://phenix-online.org/documentation/reference/reflection_file_tools.html



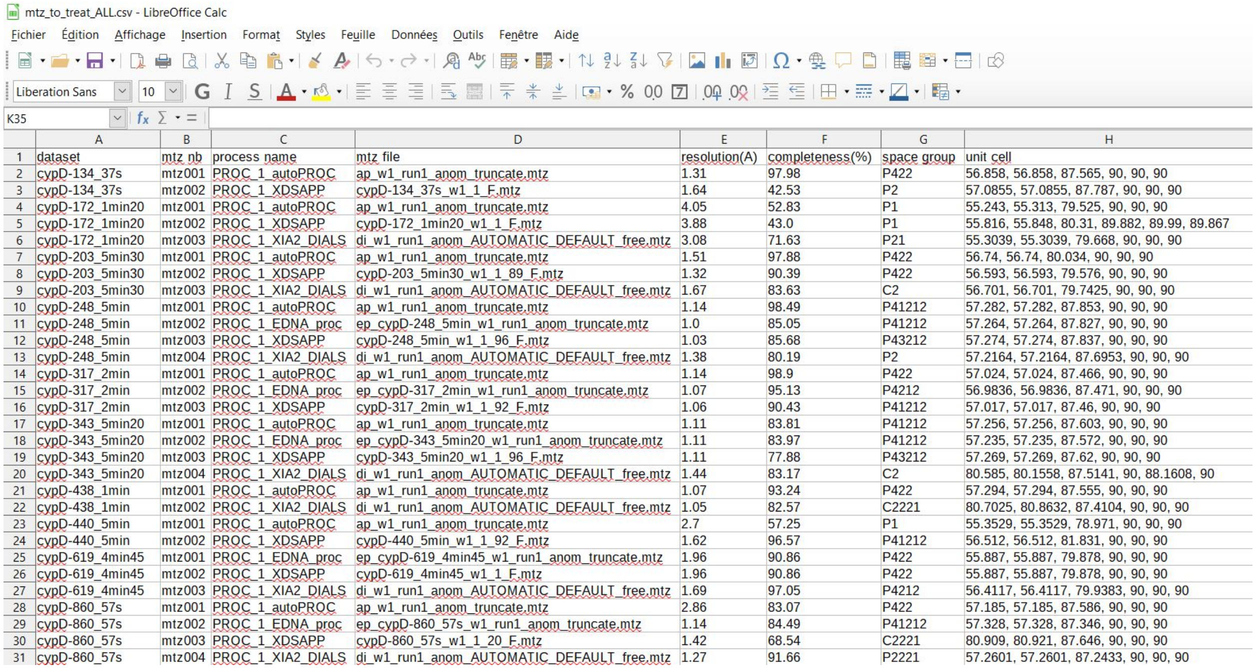
```
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
~~                                   SUMMARY                                  ~~
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
mtz candidates for reindexing (space group different from reference file): 93

cypD-134_37s/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-134_37s/mtz002_PROC_1_XDSAPP/cypD-134_37s_w1_1_F.mtz / P2
cypD-172_1min20/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P1
cypD-172_1min20/mtz002_PROC_1_XDSAPP/cypD-172_1min20_w1_1_F.mtz / P1
cypD-172_1min20/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / P21
cypD-203_5min30/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-203_5min30/mtz002_PROC_1_XDSAPP/cypD-203_5min30_w1_1_89_F.mtz / P422
cypD-203_5min30/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / C2
cypD-248_5min/mtz003_PROC_1_XDSAPP/cypD-248_5min_w1_1_96_F.mtz / P43212
cypD-248_5min/mtz004_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / P2
cypD-317_2min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-317_2min/mtz002_PROC_1_EDNA_proc/ep_cypD-317_2min_w1_run1_anom_truncate.mtz / P4212
cypD-343_5min20/mtz003_PROC_1_XDSAPP/cypD-343_5min20_w1_1_96_F.mtz / P43212
cypD-343_5min20/mtz004_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / C2
cypD-438_1min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-438_1min/mtz002_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / C2221
cypD-440_5min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P1
cypD-619_4min45/mtz001_PROC_1_EDNA_proc/ep_cypD-619_4min45_w1_run1_anom_truncate.mtz / P422
cypD-619_4min45/mtz002_PROC_1_XDSAPP/cypD-619_4min45_w1_1_F.mtz / P422
cypD-619_4min45/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / P4212
```



```
Number of reindexed mtz: 51
cypD-134_37s/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-203_5min30/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-203_5min30/mtz002_PROC_1_XDSAPP/cypD-203_5min30_w1_1_89_F_reindexed_P41212.mtz
cypD-248_5min/mtz003_PROC_1_XDSAPP/cypD-248_5min_w1_1_96_F_reindexed_P41212.mtz
cypD-317_2min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-317_2min/mtz002_PROC_1_EDNA_proc/ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-343_5min20/mtz003_PROC_1_XDSAPP/cypD-343_5min20_w1_1_96_F_reindexed_P41212.mtz
cypD-438_1min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-619_4min45/mtz001_PROC_1_EDNA_proc/ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-619_4min45/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz
cypD-860_57s/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-863_2min30/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-864_1min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-864_1min/mtz002_PROC_1_EDNA_proc/ep_cypD-864_1min_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-864_1min/mtz003_PROC_1_XDSAPP/cypD-864_1min_w1_1_95_F_reindexed_P41212.mtz
cypD-865_5min/mtz003_PROC_1_XDSAPP/cypD-865_5min_w1_1_96_F_reindexed_P41212.mtz
cypD-866_6min/mtz002_PROC_1_EDNA_proc/ep_cypD-866_6min_w1_run1_anom_truncate_reindexed_P41212.mtz
```

- launch xtriage[2] for each successfully reindexed mtz to get resolution, completeness, space group and cell parameters
- write a new 'mtz_to_treat_ALL_reindexed.csv' in '/easypipe/1b_reindex…' folder, with reindexed mtz files information

[2] https://www.phenix-online.org/documentation/reference/xtriage.html


mtz_to_treat_ALL.csv - LibreOffice Calc
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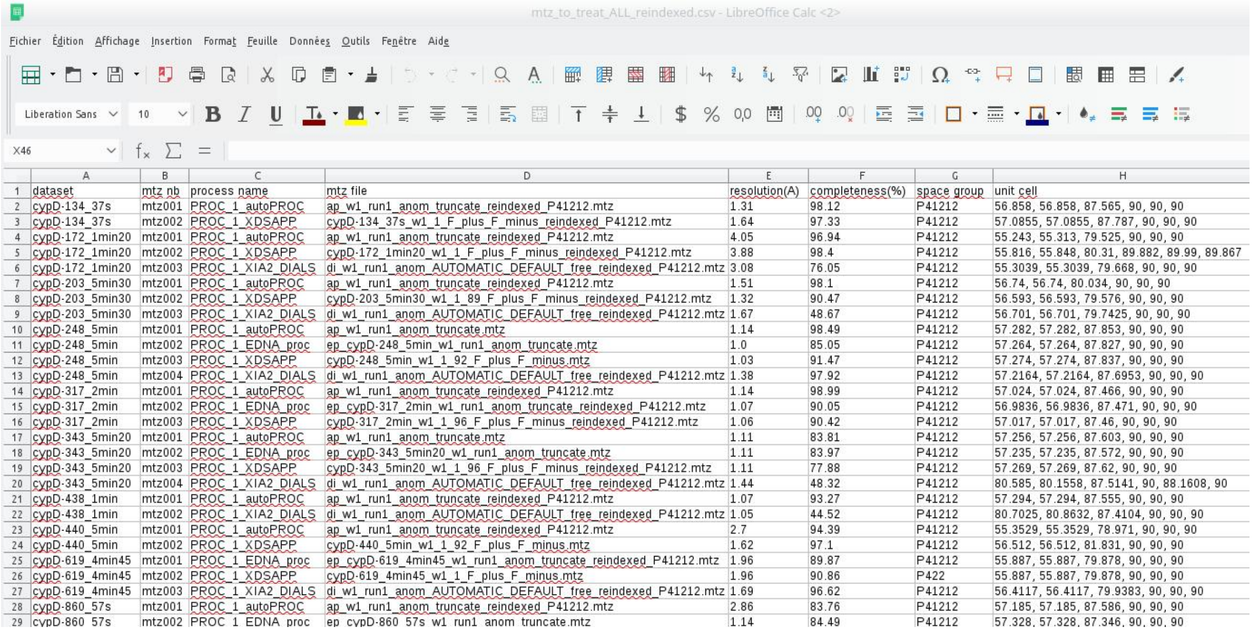
	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.31	97.98	P422	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F.mtz	1.64	42.53	P2	57.0855, 57.0855, 87.787, 90, 90, 90
4	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	4.05	52.83	P1	55.243, 55.313, 79.525, 90, 90, 90
5	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F.mtz	3.88	43.0	P1	55.816, 55.848, 80.31, 89.882, 89.99, 89.867
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	3.08	71.63	P21	55.3039, 55.3039, 79.668, 90, 90, 90
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.51	97.88	P422	56.74, 56.74, 80.034, 90, 90, 90
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F.mtz	1.32	90.39	P422	56.593, 56.593, 79.576, 90, 90, 90
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.67	83.63	C2	56.701, 56.701, 79.7425, 90, 90, 90
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
11	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41212	57.264, 57.264, 87.827, 90, 90, 90
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F.mtz	1.03	85.68	P43212	57.274, 57.274, 87.837, 90, 90, 90
13	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.38	80.19	P2	57.2164, 57.2164, 87.6953, 90, 90, 90
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.9	P422	57.024, 57.024, 87.466, 90, 90, 90
15	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate.mtz	1.07	95.13	P4212	56.9836, 56.9836, 87.471, 90, 90, 90
16	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F.mtz	1.06	90.43	P41212	57.017, 57.017, 87.46, 90, 90, 90
17	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90
18	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F.mtz	1.11	77.88	P43212	57.269, 57.269, 87.62, 90, 90, 90
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.44	83.17	C2	80.585, 80.1558, 87.5141, 90, 88.1608, 90
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.07	93.24	P422	57.294, 57.294, 87.555, 90, 90, 90
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.05	82.57	C2221	80.7025, 80.8632, 87.4104, 90, 90, 90
23	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.7	57.25	P1	55.3529, 55.3529, 78.971, 90, 90, 90
24	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41212	56.512, 56.512, 81.831, 90, 90, 90
25	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate.mtz	1.96	90.86	P422	55.887, 55.887, 79.878, 90, 90, 90
26	cypD-619_4min45	mtz002	PROC_1_XDSAPP	cypD-619_4min45_w1_1_F.mtz	1.96	90.86	P422	55.887, 55.887, 79.878, 90, 90, 90
27	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.69	97.05	P4212	56.4117, 56.4117, 79.9383, 90, 90, 90
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.86	83.07	P422	57.185, 57.185, 87.586, 90, 90, 90
29	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90
30	cypD-860_57s	mtz003	PROC_1_XDSAPP	cypD-860_57s_w1_1_20_F.mtz	1.42	68.54	C2221	80.909, 80.921, 87.646, 90, 90, 90
31	cypD-860_57s	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.27	91.66	P2221	57.2601, 57.2601, 87.2433, 90, 90, 90

becomes:


mtz_to_treat_ALL_reindexed.csv - LibreOffice Calc <2>
Fichier Édition Affichage Insertion Format Feuille Données Outils Fenêtre Aide
Liberation Sans
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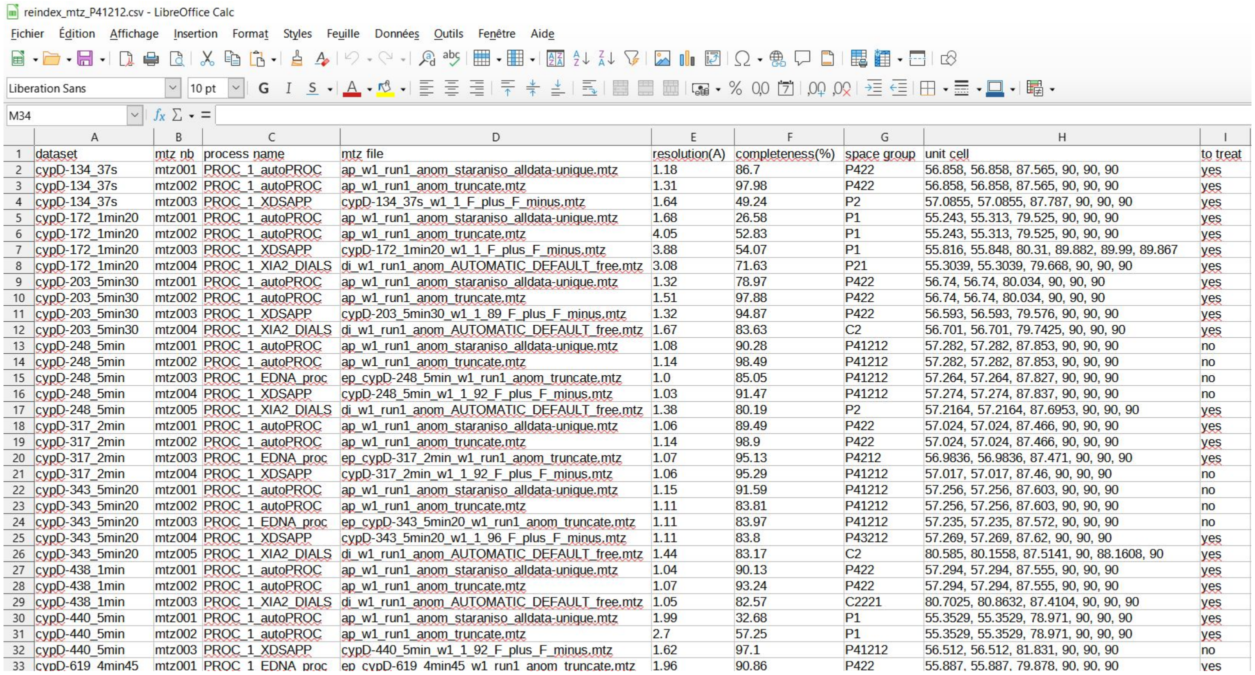
X46

	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12	P41212	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F_plus_F_minus_reindexed_P41212.mtz	1.64	97.33	P41212	57.0855, 57.0855, 87.787, 90, 90, 90
4	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	4.05	96.94	P41212	55.243, 55.313, 79.525, 90, 90, 90
5	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F_plus_F_minus_reindexed_P41212.mtz	3.88	98.4	P41212	55.816, 55.848, 80.31, 89.882, 89.99, 89.867
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	3.08	76.05	P41212	55.3039, 55.3039, 79.668, 90, 90, 90
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1	P41212	56.74, 56.74, 80.034, 90, 90, 90
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_plus_F_minus_reindexed_P41212.mtz	1.32	90.47	P41212	56.593, 56.593, 79.576, 90, 90, 90
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.67	48.67	P41212	56.701, 56.701, 79.7425, 90, 90, 90
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
11	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41212	57.264, 57.264, 87.827, 90, 90, 90
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_92_F_plus_F_minus.mtz	1.03	91.47	P41212	57.274, 57.274, 87.837, 90, 90, 90
13	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.38	97.92	P41212	57.2164, 57.2164, 87.6953, 90, 90, 90
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99	P41212	57.024, 57.024, 87.466, 90, 90, 90
15	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	90.05	P41212	56.9836, 56.9836, 87.471, 90, 90, 90
16	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.06	90.42	P41212	57.017, 57.017, 87.46, 90, 90, 90
17	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90
18	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.11	77.88	P41212	57.269, 57.269, 87.62, 90, 90, 90
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.44	48.32	P41212	80.585, 80.1558, 87.5141, 90, 88.1608, 90
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27	P41212	57.294, 57.294, 87.555, 90, 90, 90
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.05	44.52	P41212	80.7025, 80.8632, 87.4104, 90, 90, 90
23	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.7	94.39	P41212	55.3529, 55.3529, 78.971, 90, 90, 90
24	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62	97.1	P41212	56.512, 56.512, 81.831, 90, 90, 90
25	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	89.87	P41212	55.887, 55.887, 79.878, 90, 90, 90
26	cypD-619_4min45	mtz002	PROC_1_XDSAPP	cypD-619_4min45_w1_1_F_plus_F_minus.mtz	1.96	90.86	P422	55.887, 55.887, 79.878, 90, 90, 90
27	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	96.62	P41212	56.4117, 56.4117, 79.9383, 90, 90, 90
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86	83.76	P41212	57.185, 57.185, 87.586, 90, 90, 90
29	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90

where P422, P4212 processed data have been successfully reindexed to P41212 space group.

7.3 Reindex simulation mode

Simulation mode allows to generate the csv file “reindex_mtz_<sg_ref>.csv” listing processes to be reindexed, but whithout launching reindexation. Then, you can modify the ‘to treat’ column to turn ‘yes’ to ‘no’ for some processes you don’t want to reindex .



	A	B	C	D	E	F	G	H	I
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell	to treat
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.18	86.7	P422	56.858, 56.858, 87.565, 90, 90, 90	yes
3	cypD-134_37s	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.31	97.98	P422	56.858, 56.858, 87.565, 90, 90, 90	yes
4	cypD-134_37s	mtz003	PROC_1_XDSAPP	cypD-134_37s_w1_1_F_plus_F_minus.mtz	1.64	49.24	P2	57.0855, 57.0855, 87.787, 90, 90, 90	yes
5	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.68	26.58	P1	55.243, 55.313, 79.525, 90, 90, 90	yes
6	cypD-172_1min20	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	4.05	52.83	P1	55.243, 55.313, 79.525, 90, 90, 90	yes
7	cypD-172_1min20	mtz003	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F_plus_F_minus.mtz	3.88	54.07	P1	55.816, 55.848, 80.31, 89.882, 89.99, 89.867	yes
8	cypD-172_1min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	3.08	71.63	P21	55.3039, 55.3039, 79.668, 90, 90, 90	yes
9	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.32	78.97	P422	56.74, 56.74, 80.034, 90, 90, 90	yes
10	cypD-203_5min30	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.51	97.88	P422	56.74, 56.74, 80.034, 90, 90, 90	yes
11	cypD-203_5min30	mtz003	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_plus_F_minus.mtz	1.32	94.87	P422	56.593, 56.593, 79.576, 90, 90, 90	yes
12	cypD-203_5min30	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.67	83.63	C2	56.701, 56.701, 79.7425, 90, 90, 90	yes
13	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.08	90.28	P41212	57.282, 57.282, 87.853, 90, 90, 90	no
14	cypD-248_5min	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90	no
15	cypD-248_5min	mtz003	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41212	57.264, 57.264, 87.827, 90, 90, 90	no
16	cypD-248_5min	mtz004	PROC_1_XDSAPP	cypD-248_5min_w1_1_92_F_plus_F_minus.mtz	1.03	91.47	P41212	57.274, 57.274, 87.837, 90, 90, 90	no
17	cypD-248_5min	mtz005	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.38	80.19	P2	57.2164, 57.2164, 87.6953, 90, 90, 90	yes
18	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.06	89.49	P422	57.024, 57.024, 87.466, 90, 90, 90	yes
19	cypD-317_2min	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.9	P422	57.024, 57.024, 87.466, 90, 90, 90	yes
20	cypD-317_2min	mtz003	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate.mtz	1.07	95.13	P4212	56.9836, 56.9836, 87.471, 90, 90, 90	yes
21	cypD-317_2min	mtz004	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F_plus_F_minus.mtz	1.06	95.29	P41212	57.017, 57.017, 87.46, 90, 90, 90	no
22	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.15	91.59	P41212	57.256, 57.256, 87.603, 90, 90, 90	no
23	cypD-343_5min20	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90	no
24	cypD-343_5min20	mtz003	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90	no
25	cypD-343_5min20	mtz004	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_plus_F_minus.mtz	1.11	83.8	P43212	57.269, 57.269, 87.62, 90, 90, 90	yes
26	cypD-343_5min20	mtz005	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.44	83.17	C2	80.585, 80.1558, 87.5141, 90, 88.1608, 90	yes
27	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.04	90.13	P422	57.294, 57.294, 87.555, 90, 90, 90	yes
28	cypD-438_1min	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.07	93.24	P422	57.294, 57.294, 87.555, 90, 90, 90	yes
29	cypD-438_1min	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.05	82.57	C2221	80.7025, 80.8632, 87.4104, 90, 90, 90	yes
30	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_staraniso_alldata-unique.mtz	1.99	32.68	P1	55.3529, 55.3529, 78.971, 90, 90, 90	yes
31	cypD-440_5min	mtz002	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.7	57.25	P1	55.3529, 55.3529, 78.971, 90, 90, 90	yes
32	cypD-440_5min	mtz003	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62	97.1	P41212	56.512, 56.512, 81.831, 90, 90, 90	no
33	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate.mtz	1.96	90.86	P422	55.887, 55.887, 79.878, 90, 90, 90	yes

Example:

```
$ easypipe.py PROCESSED_DATA reindex P41212 --simulate
```

Warning

If you run again ‘prep’ step for any reason like adding new datasets, you will have to run again this ‘reindex’ step. Even if they don’t need to be reindexed, you have to run ‘reindex’ step to have the right reindexed csv file including these new datasets. For this, launch reindex again with simulate option to re-generate the csv file with new processes to treat, then launch again reindex.

7.4 References

CHAPTER

EIGHT

EASYPIPE ‘LIGANDS’

This step is mandatory if you want Phenix to search ligand, else it is optional.

‘ligands’ subcommand generates pdb and cif from smiles with eLBOW[2] .

Important

First, template csv file generated with ‘prep’ subcommand’ have to be completed with ligands names and smiles.

8.1 Usage

easypipe.py data ligands [-h] ligands_csv

arguments	description
-h, –help	show this help message and exit
ligands_csv	ligands_for_datasets.csv file from ‘prep’ with ligands names and smiles completed (mandatory)

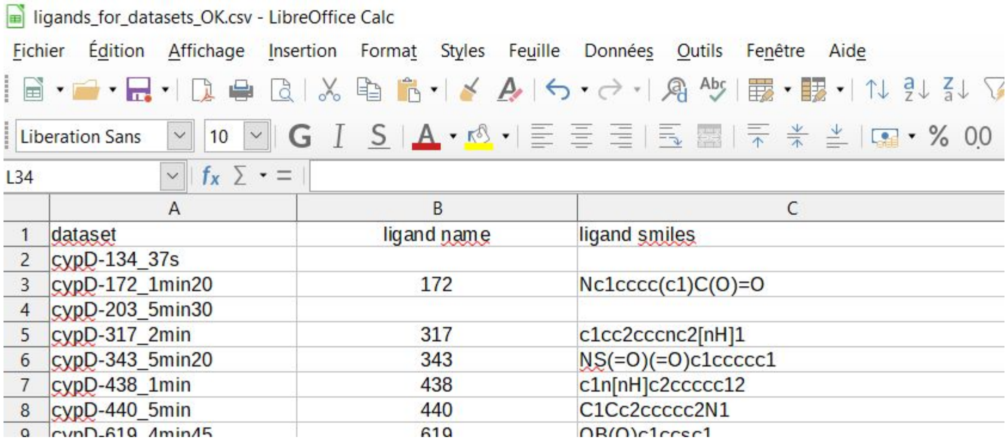
Example:

```
$ easypipe.py PROCESSED_DATA ligands easYPipe/1c_ligands/ligands_for_datasets_OK.csv
```

8.2 What does it do ?

- First, you have to fill in the fields ‘ligand name’ and ‘ligand smiles’ of /1c_ligands/ligands_for_datasets.csv csv file, then save the csv file somewhere else or with another name if you don’t want to overwrite it in case you run ‘prep’ subcommand again . . .

[2] https://www.phenix-online.org/documentation/reference/elbow.html



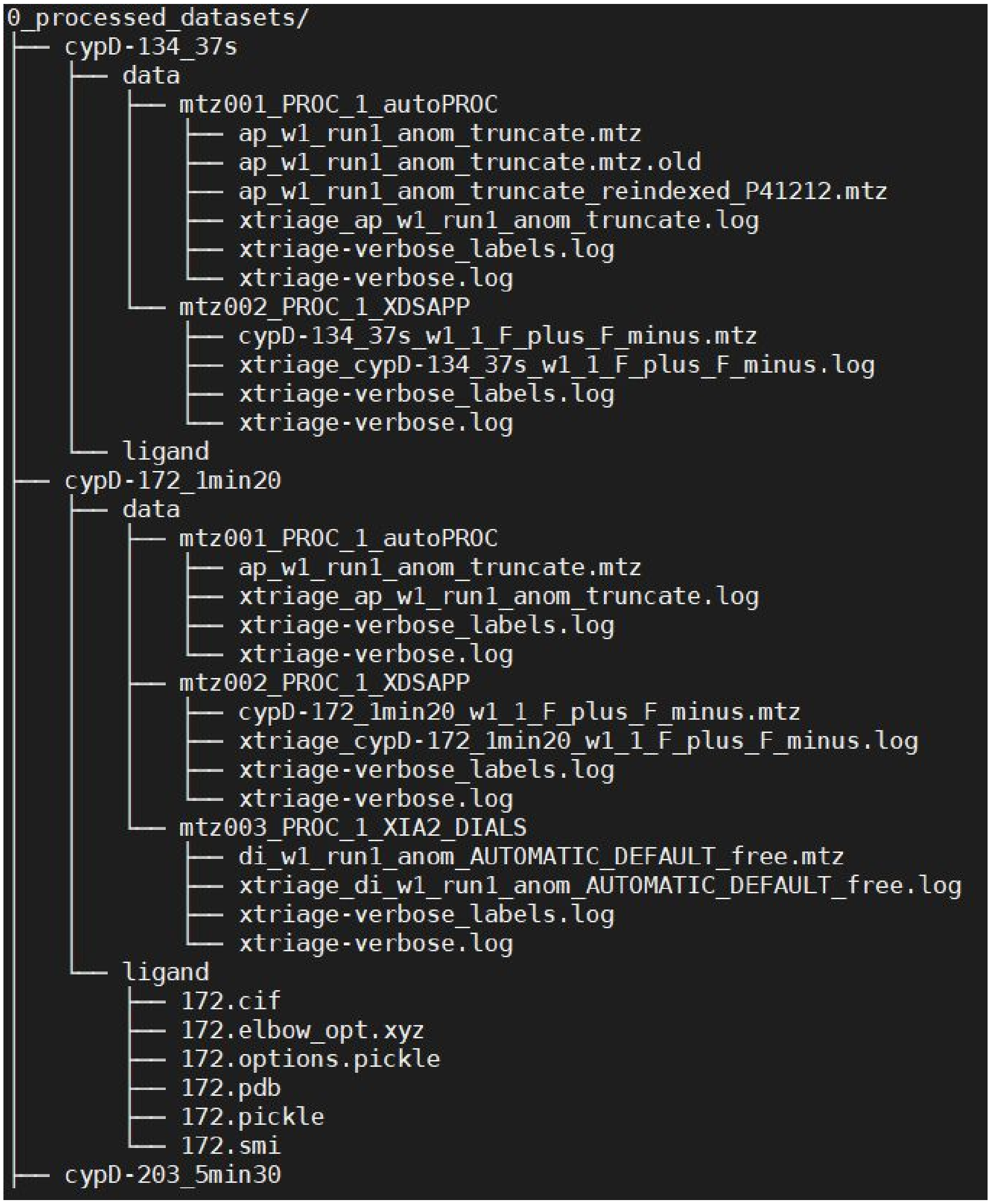
ligands_for_datasets_OK.csv - LibreOffice Calc

L34

	A	B	C
1	dataset	ligand name	ligand smiles
2	cypD-134_37s		
3	cypD-172_1min20	172	Nc1cccc(c1)C(O)=O
4	cypD-203_5min30		
5	cypD-317_2min	317	c1cc2cccnc2[nH]1
6	cypD-343_5min20	343	NS(=O)(=O)c1ccccc1
7	cypD-438_1min	438	c1n[nH]c2ccccc12
8	cypD-440_5min	440	C1Cc2ccccc2N1
9	cypD-619_4min45	619	OB(O)c1ccsc1

- 'ligands' subcommand generates pdb and cif of each ligand in a subfolder of the folder /1c_ligands/ligands and copies them in corresponding processed dataset folder (0_processed_datasets/'dataset name'), in a 'ligand' folder. It first creates a smiles file accordingly to the ligands_csv input, canonizes it thanks to Open Babel[1] and converts it with eLBOW[Page 33, 2] to pdb and cif.

[1] http://openbabel.org/wiki/Main_Page



```
0_processed_datasets/
├── cypD-134_37s
│   ├── data
│   │   ├── mtz001_PROC_1_autoPROC
│   │   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   │   ├── ap_w1_run1_anom_truncate.mtz.old
│   │   │   ├── ap_w1_run1_anom_truncate_reindexed_P41212.mtz
│   │   │   ├── xtriage_ap_w1_run1_anom_truncate.log
│   │   │   ├── xtriage-verbose_labels.log
│   │   │   └── xtriage-verbose.log
│   │   └── mtz002_PROC_1_XDSAPP
│   │       ├── cypD-134_37s_w1_1_F_plus_F_minus.mtz
│   │       ├── xtriage_cypD-134_37s_w1_1_F_plus_F_minus.log
│   │       ├── xtriage-verbose_labels.log
│   │       └── xtriage-verbose.log
│   └── ligand
├── cypD-172_1min20
│   ├── data
│   │   ├── mtz001_PROC_1_autoPROC
│   │   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   │   ├── xtriage_ap_w1_run1_anom_truncate.log
│   │   │   ├── xtriage-verbose_labels.log
│   │   │   └── xtriage-verbose.log
│   │   ├── mtz002_PROC_1_XDSAPP
│   │   │   ├── cypD-172_1min20_w1_1_F_plus_F_minus.mtz
│   │   │   ├── xtriage_cypD-172_1min20_w1_1_F_plus_F_minus.log
│   │   │   ├── xtriage-verbose_labels.log
│   │   │   └── xtriage-verbose.log
│   │   └── mtz003_PROC_1_XIA2_DIALS
│   │       ├── di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz
│   │       ├── xtriage_di_w1_run1_anom_AUTOMATIC_DEFAULT_free.log
│   │       ├── xtriage-verbose_labels.log
│   │       └── xtriage-verbose.log
│   └── ligand
│       ├── 172.cif
│       ├── 172.elbow_opt.xyz
│       ├── 172.options.pickle
│       ├── 172.pdb
│       ├── 172.pickle
│       └── 172.smi
├── cypD-203_5min30
```

Important

If eLBOW[Page 33, 2] fails to generate pdb and cif from smiles, you can copy your own cif in ligand sub-folder of the corresponding dataset, eLBOW[Page 33, 2] will generate pdb from this cif.

8.3 References

CHAPTER

NINE

EASYPIPE ‘LAUNCH’

‘launch’ subcommand runs phenix.ligand_pipeline[1] on all the mtz (several processed data, several datasets) according to options and information in ‘mtz_to_treat_ALL.csv’ file.

9.1 Usage

easypipe.py data launch [-h] [-m {fast,full,allsg}] [-l] [-n NUMBER] [-c NUMBER] [-b NUMBER | -a] [-s] [-t TEMPLATE] ref

arguments	description
ref	folder with fasta file and pdb file for replacement, and cif(s) if ligand(s) in the model

Warning

reference pdb files should include the row starting with ‘CRYST1’ containing information on space group

[1] https://www.phenix-online.org/documentation/reference/ligand_pipeline.html

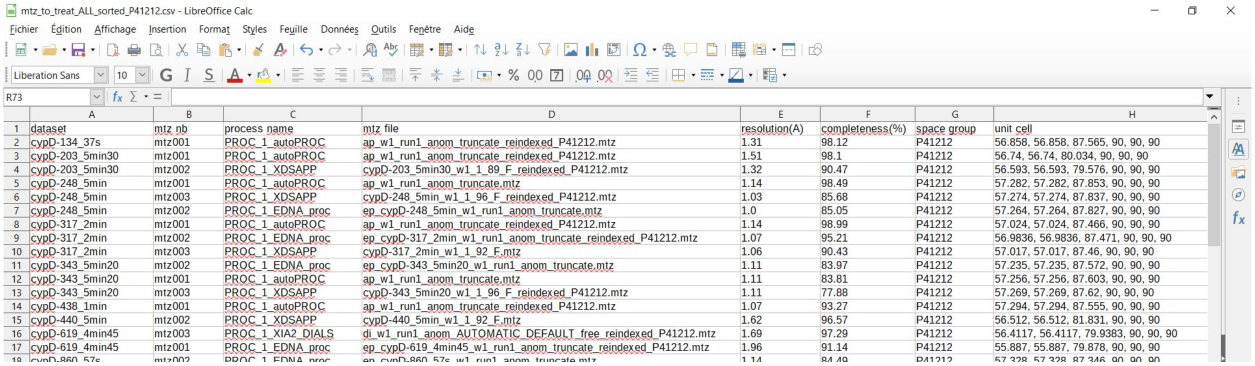
optional arguments	description
-h, –help	show this help message and exit
-m {fast,full,allsg}, –mode {fast,full,allsg}	running mode: fast, full, or allsg (default = fast)
-l, –lig	for ligand search and placement
-n NUMBER, –nblig NUMBER	number of ligand copies to be searched (default = 1, max 9 for the moment).
-c NUMBER, –cclig NUMBER	minimum CC to consider a ligand placement correct (default = 0.7). Ligands with at least this CC will be incorporated into the current model for refinement.
-b NUMBER, –best NUMBER	launch only for mtz with best completeness, NUMBER indicates how many mtz to treat (default 1), ex: –best 2
-a, –autoproc	launch only for mtz from autoPROC, or if none launch for mtz with best completeness
-w, –whole	launch for the whole mtz processes
-s, –simulate	only simulate, generate a csv file according to the future launch options. Give the possibility to modify the csv file to choose not to launch certain treatments, before launching again without simulation mode.
-t TEMPLATE, –template TEMPLATE	optional template name for log files and result folders, in case re-launching with different reference pdb of the same space group (else will be treated in existing folder and not launched again since it already exists).

Example:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --best 2 --cclig 0.6
equivalent to:
$ easypipe.py PROCESSED_DATA launch my_ref_folder -m full -l -b 2 -c 0.6
```

9.2 What does it do ?

9.2.1 1. Sort mtz files according to space group in reference pdb, and decreasing completeness



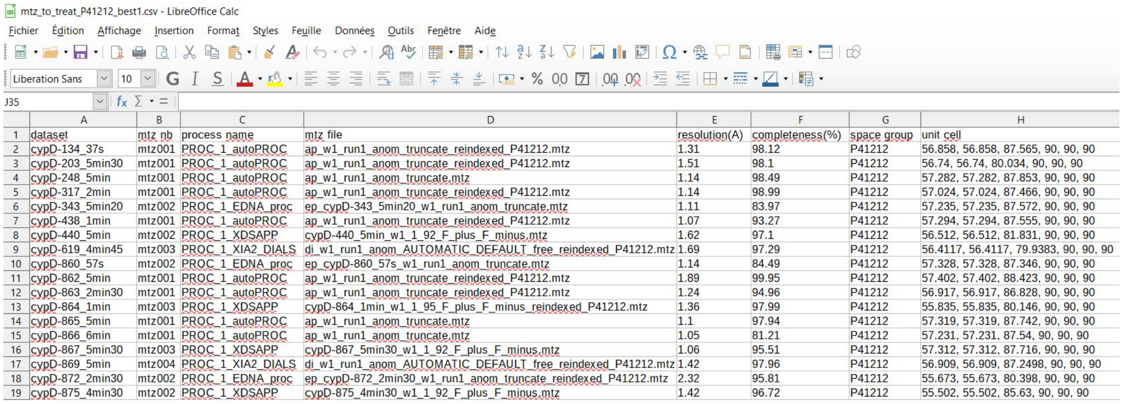
	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12	P41212	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1	P41212	56.74, 56.74, 80.034, 90, 90, 90
4	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_reindexed_P41212.mtz	1.32	90.47	P41212	56.593, 56.593, 79.576, 90, 90, 90
5	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
6	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F_reindexed_P41212.mtz	1.03	85.68	P41212	57.274, 57.274, 87.837, 90, 90, 90
7	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41212	57.264, 57.264, 87.827, 90, 90, 90
8	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99	P41212	57.024, 57.024, 87.466, 90, 90, 90
9	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	95.21	P41212	56.9836, 56.9836, 87.471, 90, 90, 90
10	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F.mtz	1.06	90.43	P41212	57.017, 57.017, 87.46, 90, 90, 90
11	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
12	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90
13	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_reindexed_P41212.mtz	1.11	77.88	P41212	57.269, 57.269, 87.62, 90, 90, 90
14	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27	P41212	57.294, 57.294, 87.555, 90, 90, 90
15	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41212	56.512, 56.512, 81.831, 90, 90, 90
16	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	97.29	P41212	56.4117, 56.4117, 79.9383, 90, 90, 90
17	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	91.14	P41212	55.887, 55.887, 79.878, 90, 90, 90
18	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90

If there are datasets without any mtz to treat according to space group, these datasets are listed in another csv file (“datasets_without_mtz_<sg_ref>.csv”).

9.2.2 2. List mtz files according to option ‘best’, ‘autoproc’ or ‘whole’

- Option example: --best 1 (default)

List only mtz with best completeness for each dataset.


mtz_to_treat_P41212_best1.csv - LibreOffice Calc
Fichier Édition Affichage Insertion Format Styles Feuille Données Outils Fenêtre Aide
Liberation Sans
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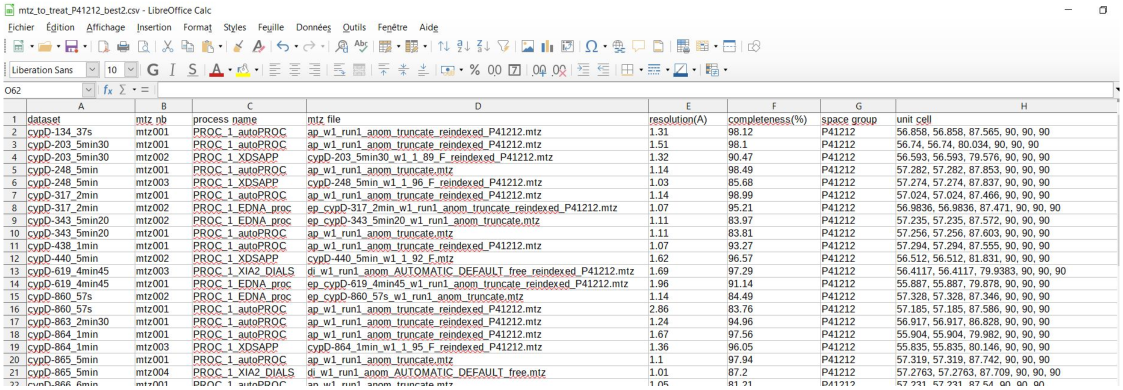
	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12	P41212	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1	P41212	56.74, 56.74, 80.034, 90, 90, 90
4	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
5	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99	P41212	57.024, 57.024, 87.466, 90, 90, 90
6	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
7	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27	P41212	57.294, 57.294, 87.555, 90, 90, 90
8	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62	97.1	P41212	56.512, 56.512, 81.831, 90, 90, 90
9	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	97.29	P41212	56.4117, 56.4117, 79.9383, 90, 90, 90
10	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90
11	cypD-862_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.89	99.95	P41212	57.402, 57.402, 88.423, 90, 90, 90
12	cypD-863_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.24	94.96	P41212	56.917, 56.917, 86.828, 90, 90, 90
13	cypD-864_1min	mtz003	PROC_1_XDSAPP	cypD-864_1min_w1_1_95_F_plus_F_minus_reindexed_P41212.mtz	1.36	97.99	P41212	55.835, 55.835, 80.146, 90, 90, 90
14	cypD-865_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.1	97.94	P41212	57.319, 57.319, 87.742, 90, 90, 90
15	cypD-866_6min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05	81.21	P41212	57.231, 57.231, 87.54, 90, 90, 90
16	cypD-867_5min30	mtz003	PROC_1_XDSAPP	cypD-867_5min30_w1_1_92_F_plus_F_minus.mtz	1.06	95.51	P41212	57.312, 57.312, 87.716, 90, 90, 90
17	cypD-869_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.42	97.96	P41212	56.909, 56.909, 87.2498, 90, 90, 90
18	cypD-872_2min30	mtz002	PROC_1_EDNA_proc	ep_cypD-872_2min30_w1_run1_anom_truncate_reindexed_P41212.mtz	2.32	95.81	P41212	55.673, 55.673, 80.398, 90, 90, 90
19	cypD-875_4min30	mtz002	PROC_1_XDSAPP	cypD-875_4min30_w1_1_92_F_plus_F_minus.mtz	1.42	96.72	P41212	55.502, 55.502, 85.63, 90, 90, 90

- Option example: --best 2

List only 2 first mtz, when exist, with best completeness, for each dataset.


mtz_to_treat_P41212_best2.csv - LibreOffice Calc
Fichier Édition Affichage Insertion Format Styles Feuille Données Outils Fenêtre Aide
Liberation Sans
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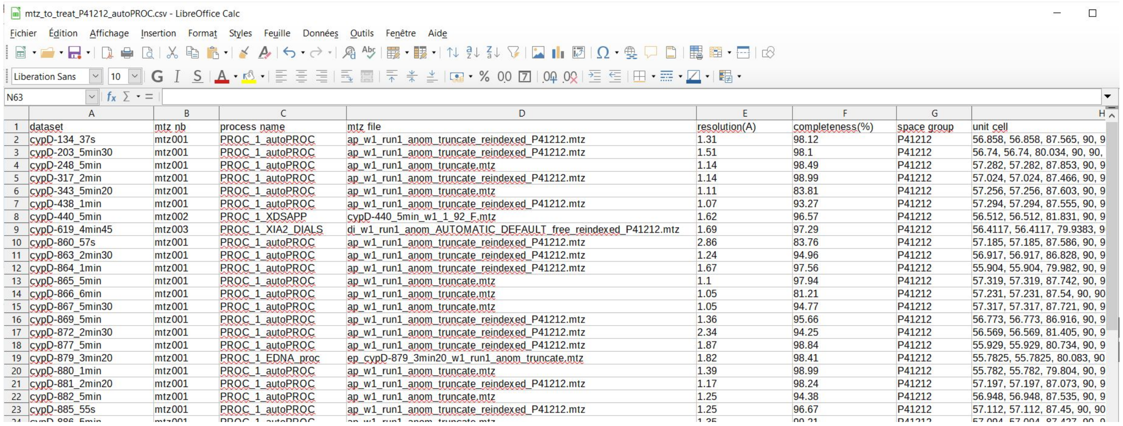
O62

	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12	P41212	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1	P41212	56.74, 56.74, 80.034, 90, 90, 90
4	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_reindexed_P41212.mtz	1.32	90.47	P41212	56.593, 56.593, 79.576, 90, 90, 90
5	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
6	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F_reindexed_P41212.mtz	1.03	85.68	P41212	57.274, 57.274, 87.837, 90, 90, 90
7	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99	P41212	57.024, 57.024, 87.466, 90, 90, 90
8	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	95.21	P41212	56.9836, 56.9836, 87.471, 90, 90, 90
9	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
10	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90
11	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27	P41212	57.294, 57.294, 87.555, 90, 90, 90
12	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41212	56.512, 56.512, 81.831, 90, 90, 90
13	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	97.29	P41212	56.4117, 56.4117, 79.9383, 90, 90, 90
14	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	91.14	P41212	55.887, 55.887, 79.878, 90, 90, 90
15	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90
16	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86	83.76	P41212	57.185, 57.185, 87.586, 90, 90, 90
17	cypD-863_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.24	94.96	P41212	56.917, 56.917, 86.828, 90, 90, 90
18	cypD-864_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.67	97.56	P41212	55.904, 55.904, 79.982, 90, 90, 90
19	cypD-864_1min	mtz003	PROC_1_XDSAPP	cypD-864_1min_w1_1_95_F_reindexed_P41212.mtz	1.36	96.05	P41212	55.835, 55.835, 80.146, 90, 90, 90
20	cypD-865_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.1	97.94	P41212	57.319, 57.319, 87.742, 90, 90, 90
21	cypD-865_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.01	87.2	P41212	57.2763, 57.2763, 87.709, 90, 90, 90
22	cypD-866_6min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05	81.21	P41212	57.231, 57.231, 87.54, 90, 90, 90

- Option example: --autoproc

List only mtz from autoPROC, or if none list mtz with best completeness, for each dataset.


mtz_to_treat_P41212_autoPROC.csv - LibreOffice Calc
Fichier Édition Affichage Insertion Format Styles Feuille Données Outils Fenêtre Aide
Liberation Sans
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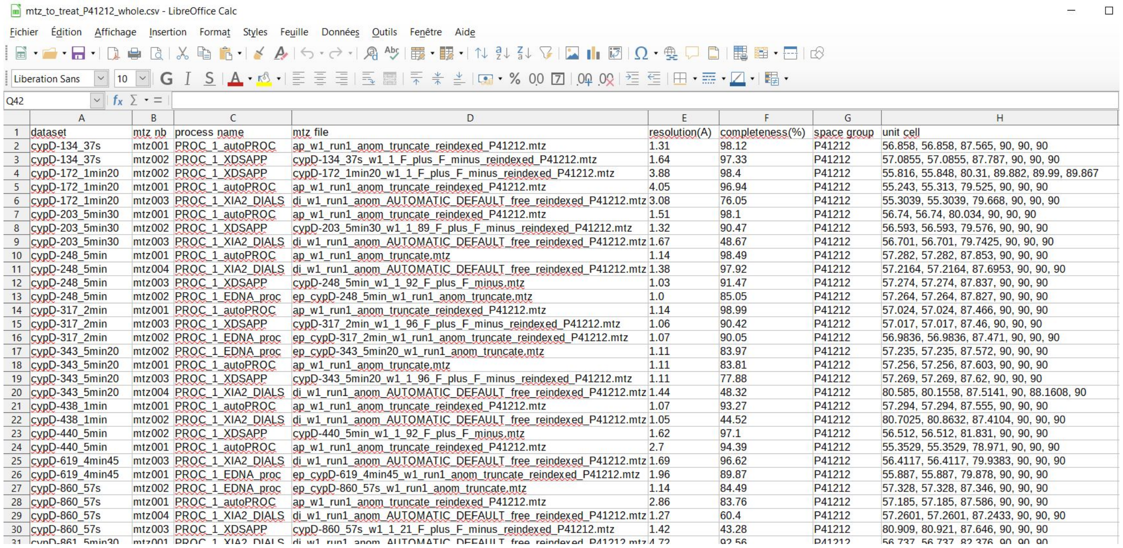
N63

	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12	P41212	56.858, 56.858, 87.565, 90, 9
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1	P41212	56.74, 56.74, 80.034, 90, 90,
4	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 9
5	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99	P41212	57.024, 57.024, 87.466, 90, 9
6	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 9
7	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27	P41212	57.294, 57.294, 87.555, 90, 9
8	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41212	56.512, 56.512, 81.831, 90, 9
9	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	97.29	P41212	56.4117, 56.4117, 79.9383, 9
10	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86	83.76	P41212	57.185, 57.185, 87.586, 90, 9
11	cypD-863_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.24	94.96	P41212	56.917, 56.917, 86.828, 90, 9
12	cypD-864_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.67	97.56	P41212	55.904, 55.904, 79.982, 90, 9
13	cypD-865_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.1	97.94	P41212	57.319, 57.319, 87.742, 90, 9
14	cypD-866_6min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05	81.21	P41212	57.231, 57.231, 87.54, 90, 90
15	cypD-867_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05	94.77	P41212	57.317, 57.317, 87.721, 90, 9
16	cypD-869_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.36	95.66	P41212	56.773, 56.773, 86.916, 90, 9
17	cypD-872_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.34	94.25	P41212	56.569, 56.569, 81.405, 90, 9
18	cypD-877_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.87	98.84	P41212	55.929, 55.929, 80.734, 90, 9
19	cypD-879_3min20	mtz001	PROC_1_EDNA_proc	ep_cypD-879_3min20_w1_run1_anom_truncate.mtz	1.82	98.41	P41212	55.7825, 55.7825, 80.083, 90
20	cypD-880_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.39	98.99	P41212	55.782, 55.782, 79.804, 90, 9
21	cypD-881_2min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.17	98.24	P41212	57.197, 57.197, 87.073, 90, 9
22	cypD-882_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.25	94.38	P41212	56.948, 56.948, 87.535, 90, 9
23	cypD-885_55s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.25	96.67	P41212	57.112, 57.112, 87.45, 90, 90
24	cypD-886_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.35	99.21	P41212	57.094, 57.094, 87.427, 90, 9

- Option example: --whole

Whereas it is not recommended because it is time demanding, for problematic data it could be usefull to treat the whole mtz processed. You also can launch –whole option in *simulate mode*, and choose for processes to be treated or not, before launching again.



	A	B	C	D	E	F	G	H
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	space group	unit cell
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12	P41212	56.858, 56.858, 87.565, 90, 90, 90
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F_plus_F_minus_reindexed_P41212.mtz	1.64	97.33	P41212	57.0855, 57.0855, 87.787, 90, 90, 90
4	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F_plus_F_minus_reindexed_P41212.mtz	3.88	98.4	P41212	55.816, 55.848, 80.31, 89.882, 89.99, 89.867
5	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	4.05	96.94	P41212	55.243, 55.313, 79.525, 90, 90, 90
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	3.08	76.05	P41212	55.3039, 55.3039, 79.668, 90, 90, 90
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1	P41212	56.74, 56.74, 80.034, 90, 90, 90
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_plus_F_minus_reindexed_P41212.mtz	1.32	90.47	P41212	56.593, 56.593, 79.576, 90, 90, 90
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.67	48.67	P41212	56.701, 56.701, 79.7425, 90, 90, 90
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41212	57.282, 57.282, 87.853, 90, 90, 90
11	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.38	97.92	P41212	57.2164, 57.2164, 87.6953, 90, 90, 90
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_92_F_plus_F_minus.mtz	1.03	91.47	P41212	57.274, 57.274, 87.837, 90, 90, 90
13	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41212	57.264, 57.264, 87.827, 90, 90, 90
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99	P41212	57.024, 57.024, 87.466, 90, 90, 90
15	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.06	90.42	P41212	57.017, 57.017, 87.46, 90, 90, 90
16	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	90.05	P41212	56.9836, 56.9836, 87.471, 90, 90, 90
17	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41212	57.235, 57.235, 87.572, 90, 90, 90
18	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41212	57.256, 57.256, 87.603, 90, 90, 90
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.11	77.88	P41212	57.269, 57.269, 87.62, 90, 90, 90
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.44	48.32	P41212	80.585, 80.1558, 87.5141, 90, 88.1608, 90
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27	P41212	57.294, 57.294, 87.555, 90, 90, 90
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.05	44.52	P41212	80.7025, 80.8632, 87.4104, 90, 90, 90
23	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62	97.1	P41212	56.512, 56.512, 81.831, 90, 90, 90
24	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.7	94.39	P41212	55.3529, 55.3529, 78.971, 90, 90, 90
25	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	96.62	P41212	56.4117, 56.4117, 79.9383, 90, 90, 90
26	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	89.87	P41212	55.887, 55.887, 79.878, 90, 90, 90
27	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41212	57.328, 57.328, 87.346, 90, 90, 90
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86	83.76	P41212	57.185, 57.185, 87.586, 90, 90, 90
29	cypD-860_57s	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.27	60.4	P41212	57.2601, 57.2601, 87.2433, 90, 90, 90
30	cypD-860_57s	mtz003	PROC_1_XDSAPP	cypD-860_57s_w1_1_21_F_plus_F_minus_reindexed_P41212.mtz	1.42	43.28	P41212	80.909, 80.921, 87.646, 90, 90, 90
31	cypD-861_5min30	mtz001	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	4.72	92.56	P41212	56.737, 56.737, 82.376, 90, 90, 90

9.2.3 3. List mtz files with mode and ligand information for running Phenix

> **Note**
>
> Phenix options for the different modes are specified *hereafter*.

For each dataset, write in a 'launch csv' file:

- if ligand cif file is present for search when asked
- mode that will be launched depending on mode asked, the presence (or not) of ligand cif file and data quality
- information in case mode is different from mode asked
- result folder name

Limits for poor data: There are minimum limits to process in 'full' or 'allsg' modes. These limits can be modified in config.py file (after what easypipe should be reinstalled).

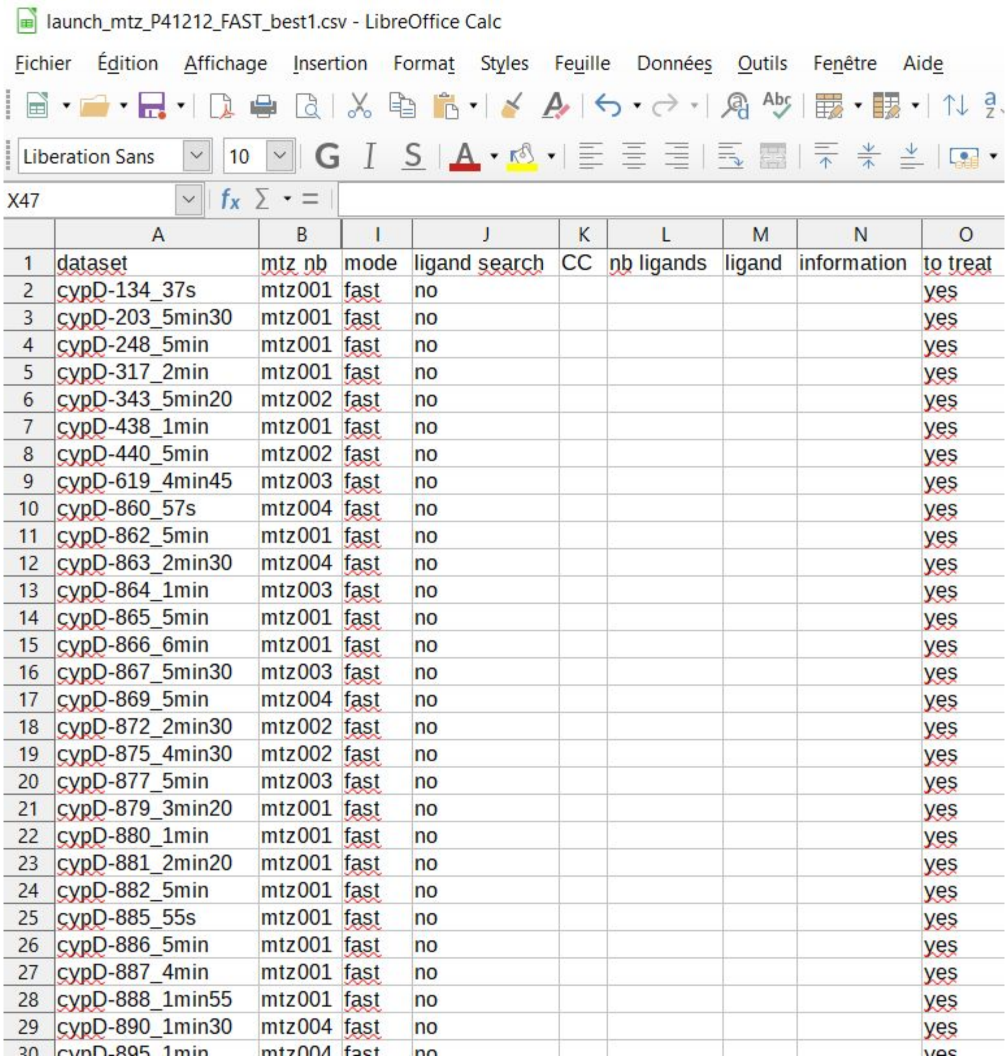
- minimum completeness (default = 70%)
- minimum resolution (default = 3.75)

Poor data will be treated in 'fast' mode.

Option examples:

- Option example: --mode fast (default)

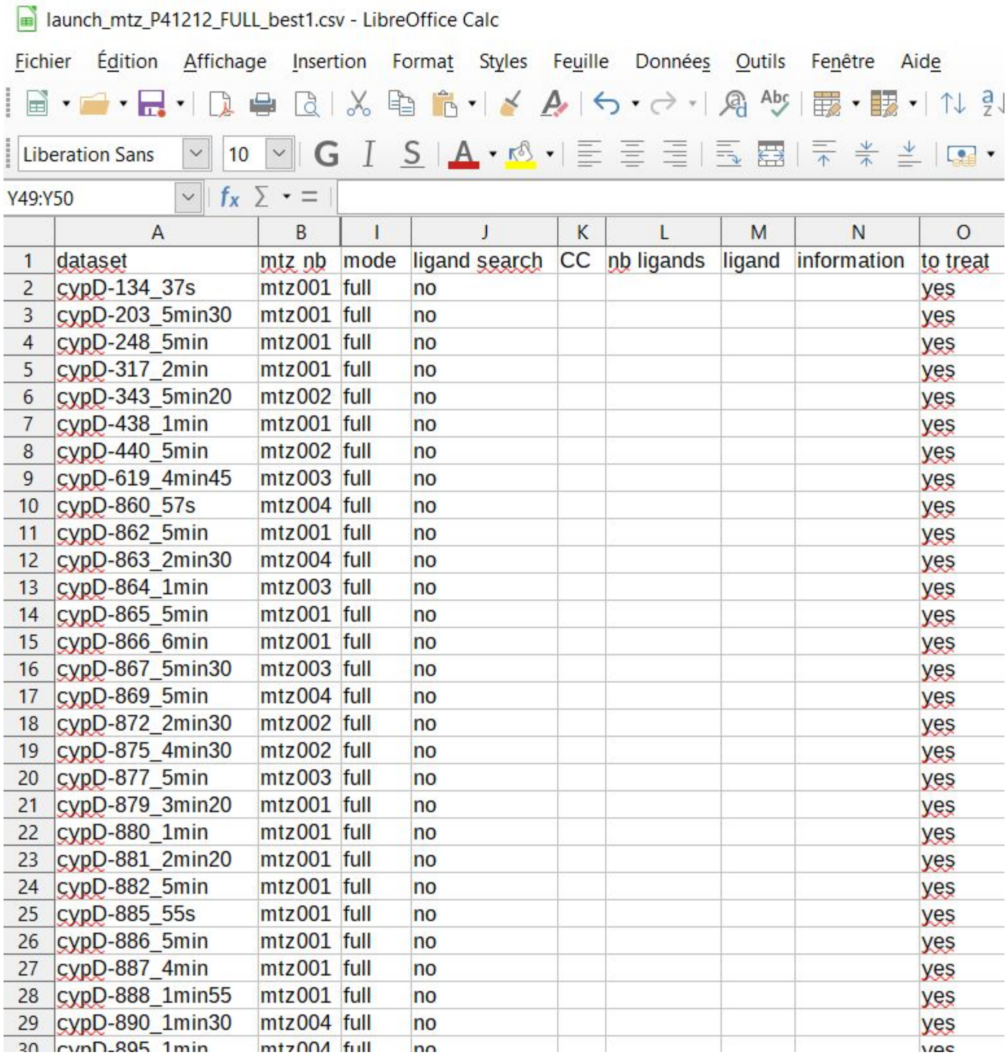
Phenix uses a simple rigid-body refinement for model placement, which is faster and most of the time sufficient if the input model is already close enough to the target structure.


launch_mtz_P41212_FAST_best1.csv - LibreOffice Calc
Fichier Édition Affichage Insertion Format Styles Feuille Données Outils Fenêtre Aide
Liberation Sans
10
X47

	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	fast	no					yes
3	cypD-203_5min30	mtz001	fast	no					yes
4	cypD-248_5min	mtz001	fast	no					yes
5	cypD-317_2min	mtz001	fast	no					yes
6	cypD-343_5min20	mtz002	fast	no					yes
7	cypD-438_1min	mtz001	fast	no					yes
8	cypD-440_5min	mtz002	fast	no					yes
9	cypD-619_4min45	mtz003	fast	no					yes
10	cypD-860_57s	mtz004	fast	no					yes
11	cypD-862_5min	mtz001	fast	no					yes
12	cypD-863_2min30	mtz004	fast	no					yes
13	cypD-864_1min	mtz003	fast	no					yes
14	cypD-865_5min	mtz001	fast	no					yes
15	cypD-866_6min	mtz001	fast	no					yes
16	cypD-867_5min30	mtz003	fast	no					yes
17	cypD-869_5min	mtz004	fast	no					yes
18	cypD-872_2min30	mtz002	fast	no					yes
19	cypD-875_4min30	mtz002	fast	no					yes
20	cypD-877_5min	mtz003	fast	no					yes
21	cypD-879_3min20	mtz001	fast	no					yes
22	cypD-880_1min	mtz001	fast	no					yes
23	cypD-881_2min20	mtz001	fast	no					yes
24	cypD-882_5min	mtz001	fast	no					yes
25	cypD-885_55s	mtz001	fast	no					yes
26	cypD-886_5min	mtz001	fast	no					yes
27	cypD-887_4min	mtz001	fast	no					yes
28	cypD-888_1min55	mtz001	fast	no					yes
29	cypD-890_1min30	mtz004	fast	no					yes
30	cypD-895_1min	mtz004	fast	no					yes

- Option example: --mode full

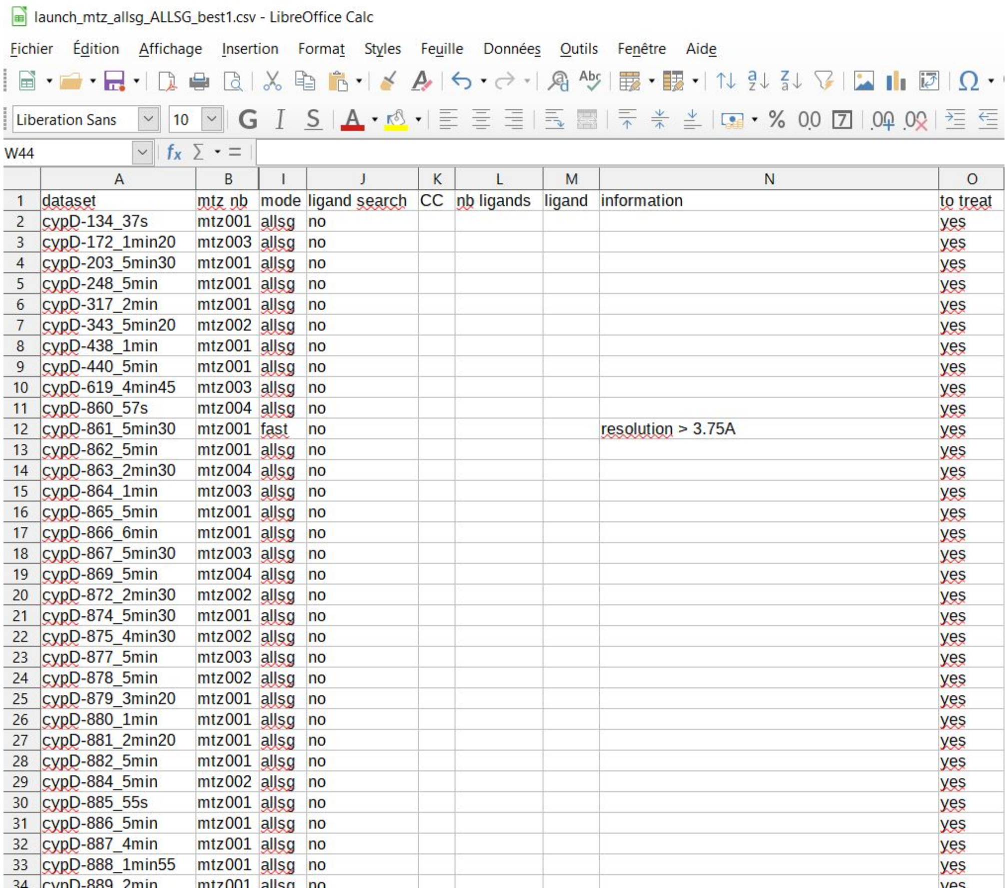
Phenix will try rigid-body refinement first, then run Phaser if the R-free is too high (>0.4), it will run AutoBuild after initial refinement only if R-free is greater than the max_r_free cutoff = 0.3.



	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	full	no					yes
3	cypD-203_5min30	mtz001	full	no					yes
4	cypD-248_5min	mtz001	full	no					yes
5	cypD-317_2min	mtz001	full	no					yes
6	cypD-343_5min20	mtz002	full	no					yes
7	cypD-438_1min	mtz001	full	no					yes
8	cypD-440_5min	mtz002	full	no					yes
9	cypD-619_4min45	mtz003	full	no					yes
10	cypD-860_57s	mtz004	full	no					yes
11	cypD-862_5min	mtz001	full	no					yes
12	cypD-863_2min30	mtz004	full	no					yes
13	cypD-864_1min	mtz003	full	no					yes
14	cypD-865_5min	mtz001	full	no					yes
15	cypD-866_6min	mtz001	full	no					yes
16	cypD-867_5min30	mtz003	full	no					yes
17	cypD-869_5min	mtz004	full	no					yes
18	cypD-872_2min30	mtz002	full	no					yes
19	cypD-875_4min30	mtz002	full	no					yes
20	cypD-877_5min	mtz003	full	no					yes
21	cypD-879_3min20	mtz001	full	no					yes
22	cypD-880_1min	mtz001	full	no					yes
23	cypD-881_2min20	mtz001	full	no					yes
24	cypD-882_5min	mtz001	full	no					yes
25	cypD-885_55s	mtz001	full	no					yes
26	cypD-886_5min	mtz001	full	no					yes
27	cypD-887_4min	mtz001	full	no					yes
28	cypD-888_1min55	mtz001	full	no					yes
29	cypD-890_1min30	mtz004	full	no					yes
30	cypD-895_1min	mtz004	full	no					yes

- Option example: --mode allsg

In this mode, mtz will be treated regardless of the space group. Phenix will run Phaser, then run AutoBuild after initial refinement only if R-free is greater than the max_r_free cutoff = 0.3.



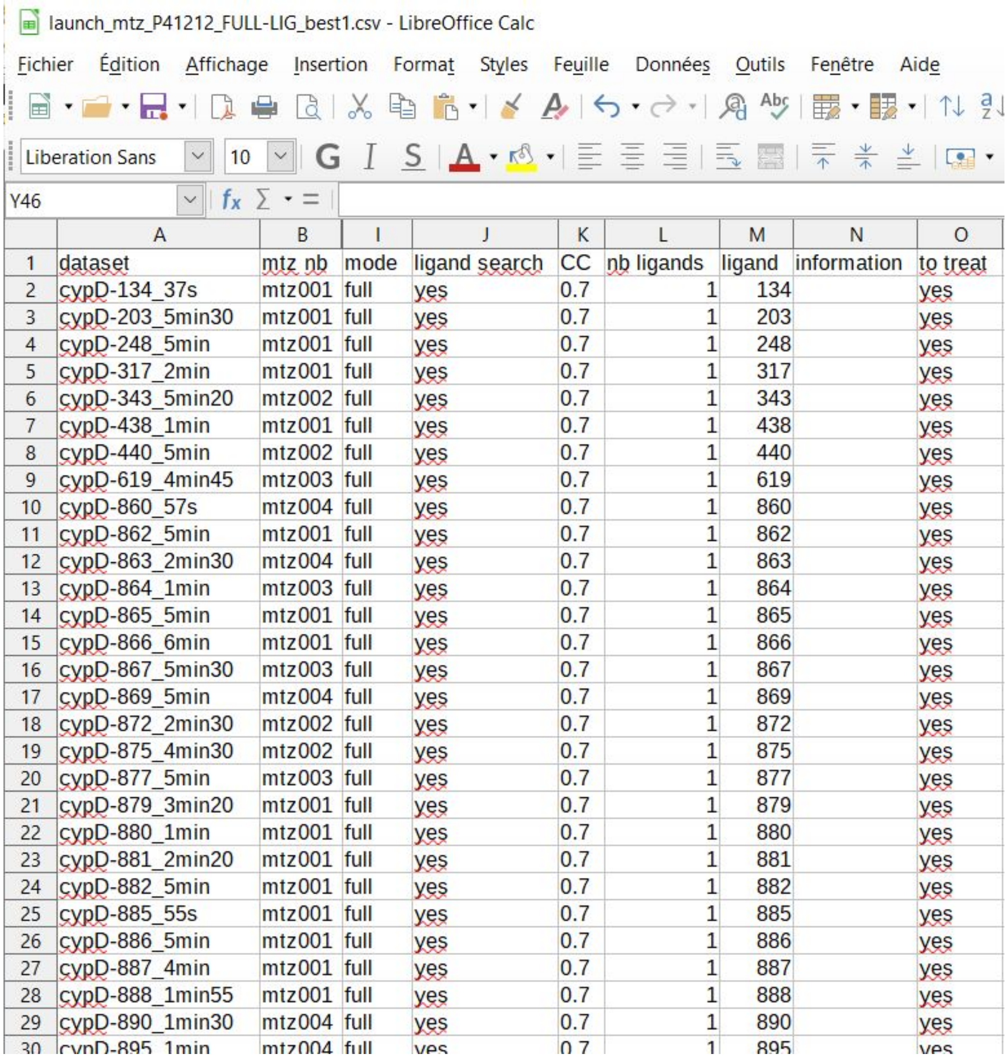
launch_mtz_allsg_ALLSG_best1.csv - LibreOffice Calc

	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	allsg	no					yes
3	cypD-172_1min20	mtz003	allsg	no					yes
4	cypD-203_5min30	mtz001	allsg	no					yes
5	cypD-248_5min	mtz001	allsg	no					yes
6	cypD-317_2min	mtz001	allsg	no					yes
7	cypD-343_5min20	mtz002	allsg	no					yes
8	cypD-438_1min	mtz001	allsg	no					yes
9	cypD-440_5min	mtz001	allsg	no					yes
10	cypD-619_4min45	mtz003	allsg	no					yes
11	cypD-860_57s	mtz004	allsg	no					yes
12	cypD-861_5min30	mtz001	fast	no				resolution > 3.75A	yes
13	cypD-862_5min	mtz001	allsg	no					yes
14	cypD-863_2min30	mtz004	allsg	no					yes
15	cypD-864_1min	mtz003	allsg	no					yes
16	cypD-865_5min	mtz001	allsg	no					yes
17	cypD-866_6min	mtz001	allsg	no					yes
18	cypD-867_5min30	mtz003	allsg	no					yes
19	cypD-869_5min	mtz004	allsg	no					yes
20	cypD-872_2min30	mtz002	allsg	no					yes
21	cypD-874_5min30	mtz001	allsg	no					yes
22	cypD-875_4min30	mtz002	allsg	no					yes
23	cypD-877_5min	mtz003	allsg	no					yes
24	cypD-878_5min	mtz002	allsg	no					yes
25	cypD-879_3min20	mtz001	allsg	no					yes
26	cypD-880_1min	mtz001	allsg	no					yes
27	cypD-881_2min20	mtz001	allsg	no					yes
28	cypD-882_5min	mtz001	allsg	no					yes
29	cypD-884_5min	mtz002	allsg	no					yes
30	cypD-885_55s	mtz001	allsg	no					yes
31	cypD-886_5min	mtz001	allsg	no					yes
32	cypD-887_4min	mtz001	allsg	no					yes
33	cypD-888_1min55	mtz001	allsg	no					yes
34	cypD-889_2min	mtz001	allsg	no					yes

- Option example: --mode full –lig

Phenix will be run in ‘full’ mode. Then ligand will be searched with LigandFit[2] and placed if cutoff model-to-map CC is more than 0.7 (default). This cutoff can be changed with ‘–cclig’ option. The number of ligands to be placed (default=1) can be changed with ‘–nblig’ option.

[2] https://www.phenix-online.org/documentation/reference/ligandfit.html


launch_mtz_P41212_FULL-LIG_best1.csv - LibreOffice Calc

	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	full	yes	0.7	1	134		yes
3	cypD-203_5min30	mtz001	full	yes	0.7	1	203		yes
4	cypD-248_5min	mtz001	full	yes	0.7	1	248		yes
5	cypD-317_2min	mtz001	full	yes	0.7	1	317		yes
6	cypD-343_5min20	mtz002	full	yes	0.7	1	343		yes
7	cypD-438_1min	mtz001	full	yes	0.7	1	438		yes
8	cypD-440_5min	mtz002	full	yes	0.7	1	440		yes
9	cypD-619_4min45	mtz003	full	yes	0.7	1	619		yes
10	cypD-860_57s	mtz004	full	yes	0.7	1	860		yes
11	cypD-862_5min	mtz001	full	yes	0.7	1	862		yes
12	cypD-863_2min30	mtz004	full	yes	0.7	1	863		yes
13	cypD-864_1min	mtz003	full	yes	0.7	1	864		yes
14	cypD-865_5min	mtz001	full	yes	0.7	1	865		yes
15	cypD-866_6min	mtz001	full	yes	0.7	1	866		yes
16	cypD-867_5min30	mtz003	full	yes	0.7	1	867		yes
17	cypD-869_5min	mtz004	full	yes	0.7	1	869		yes
18	cypD-872_2min30	mtz002	full	yes	0.7	1	872		yes
19	cypD-875_4min30	mtz002	full	yes	0.7	1	875		yes
20	cypD-877_5min	mtz003	full	yes	0.7	1	877		yes
21	cypD-879_3min20	mtz001	full	yes	0.7	1	879		yes
22	cypD-880_1min	mtz001	full	yes	0.7	1	880		yes
23	cypD-881_2min20	mtz001	full	yes	0.7	1	881		yes
24	cypD-882_5min	mtz001	full	yes	0.7	1	882		yes
25	cypD-885_55s	mtz001	full	yes	0.7	1	885		yes
26	cypD-886_5min	mtz001	full	yes	0.7	1	886		yes
27	cypD-887_4min	mtz001	full	yes	0.7	1	887		yes
28	cypD-888_1min55	mtz001	full	yes	0.7	1	888		yes
29	cypD-890_1min30	mtz004	full	yes	0.7	1	890		yes
30	cypD-895_1min	mtz004	full	yes	0.7	1	895		yes

9.2.4 4. Launch Phenix according to chosen mode and options - Simulation mode

phenix.ligand_pipeline[Page 37, 1] is launched for each mtz file according to chosen mode and options, as listed in the 'launch csv' file (see 3. above).

If this 'launch csv' exists and you have modified something like adding a ligand cif for example, 'launch' mode should be run again, but in simulation mode so as it generates a new correct launch csv file instead of using existing one. When a new 'launch csv' file has been generated, just run the same command without simulation mode.

Example:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --autoproc --simulate
then:
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --autoproc
```

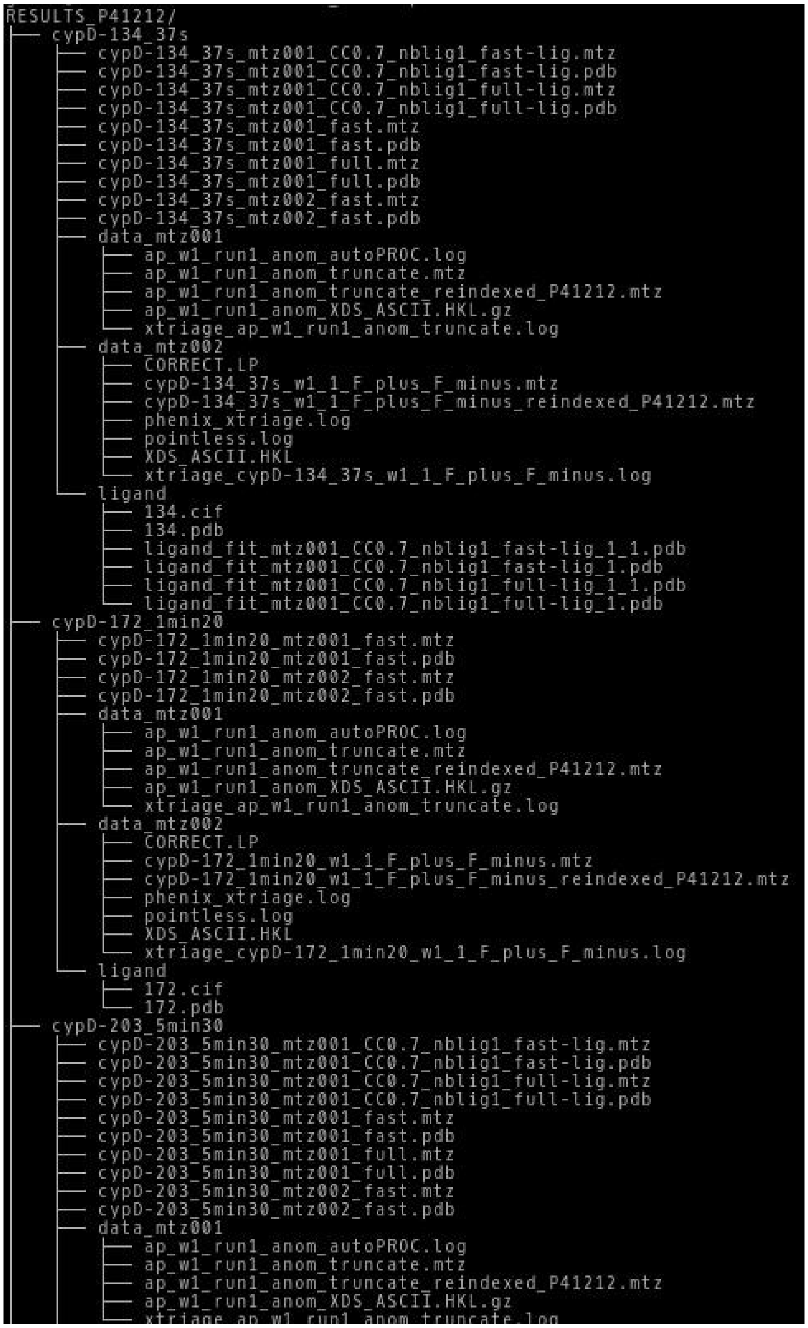
Simulation mode also allows to modify the 'to treat' column of the 'launch csv' file (replacing 'yes' by 'no'). Useful if you want to run some options only on some mtz. Then just run the same command without simulation mode. You can also modify the following columns: 'mode', 'ligand search', 'CC', 'nb ligands', as long as you know what you are doing.

9.2.5 5. Write results

At the end of each ‘launch’ subcommand, results are copied in a ‘RESULTS’ folder.

In datasets folders, copy of:

- corresponding processed data and logs (useful for deposition at the PDB)
- pdb and mtz result files
- phenix cif file if ligand found
- ligand folder, if exists
- pdb of ligand(s) placed by LigandFit (all CC)

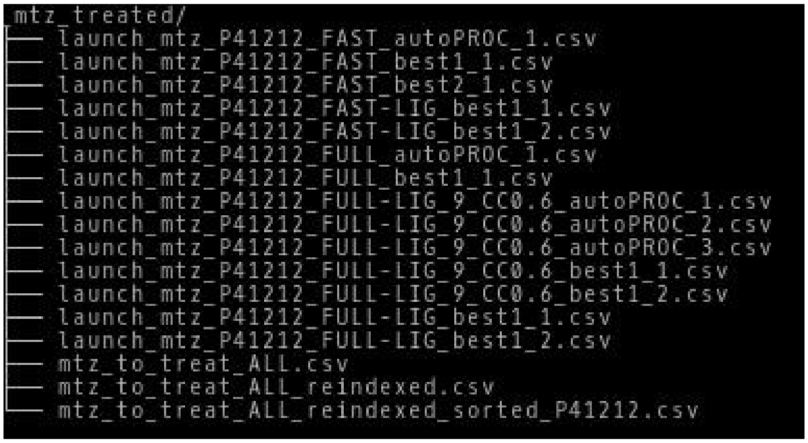


```
RESULTS_P41212/
├── cypD-134_37s
│   ├── cypD-134_37s_mtz001_CC0.7_nblig1_fast-lig.mtz
│   ├── cypD-134_37s_mtz001_CC0.7_nblig1_fast-lig.pdb
│   ├── cypD-134_37s_mtz001_CC0.7_nblig1_full-lig.mtz
│   ├── cypD-134_37s_mtz001_CC0.7_nblig1_full-lig.pdb
│   ├── cypD-134_37s_mtz001_fast.mtz
│   ├── cypD-134_37s_mtz001_fast.pdb
│   ├── cypD-134_37s_mtz001_full.mtz
│   ├── cypD-134_37s_mtz001_full.pdb
│   ├── cypD-134_37s_mtz002_fast.mtz
│   ├── cypD-134_37s_mtz002_fast.pdb
│   ├── data_mtz001
│   │   ├── ap_w1_run1_anom_autoPROC.log
│   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   ├── ap_w1_run1_anom_truncate_reindexed_P41212.mtz
│   │   ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
│   │   └── xtriage_ap_w1_run1_anom_truncate.log
│   ├── data_mtz002
│   │   ├── CORRECT.LP
│   │   ├── cypD-134_37s_w1_1_F_plus_F_minus.mtz
│   │   ├── cypD-134_37s_w1_1_F_plus_F_minus_reindexed_P41212.mtz
│   │   ├── phenix_xtriage.log
│   │   ├── pointless.log
│   │   ├── XDS_ASCII.HKL
│   │   └── xtriage_cypD-134_37s_w1_1_F_plus_F_minus.log
│   └── ligand
│       ├── 134.cif
│       ├── 134.pdb
│       ├── ligand_fit_mtz001_CC0.7_nblig1_fast-lig_1_1.pdb
│       ├── ligand_fit_mtz001_CC0.7_nblig1_fast-lig_1.pdb
│       ├── ligand_fit_mtz001_CC0.7_nblig1_full-lig_1_1.pdb
│       └── ligand_fit_mtz001_CC0.7_nblig1_full-lig_1.pdb
├── cypD-172_1min20
│   ├── cypD-172_1min20_mtz001_fast.mtz
│   ├── cypD-172_1min20_mtz001_fast.pdb
│   ├── cypD-172_1min20_mtz002_fast.mtz
│   ├── cypD-172_1min20_mtz002_fast.pdb
│   ├── data_mtz001
│   │   ├── ap_w1_run1_anom_autoPROC.log
│   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   ├── ap_w1_run1_anom_truncate_reindexed_P41212.mtz
│   │   ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
│   │   └── xtriage_ap_w1_run1_anom_truncate.log
│   ├── data_mtz002
│   │   ├── CORRECT.LP
│   │   ├── cypD-172_1min20_w1_1_F_plus_F_minus.mtz
│   │   ├── cypD-172_1min20_w1_1_F_plus_F_minus_reindexed_P41212.mtz
│   │   ├── phenix_xtriage.log
│   │   ├── pointless.log
│   │   ├── XDS_ASCII.HKL
│   │   └── xtriage_cypD-172_1min20_w1_1_F_plus_F_minus.log
│   └── ligand
│       ├── 172.cif
│       └── 172.pdb
├── cypD-203_5min30
│   ├── cypD-203_5min30_mtz001_CC0.7_nblig1_fast-lig.mtz
│   ├── cypD-203_5min30_mtz001_CC0.7_nblig1_fast-lig.pdb
│   ├── cypD-203_5min30_mtz001_CC0.7_nblig1_full-lig.mtz
│   ├── cypD-203_5min30_mtz001_CC0.7_nblig1_full-lig.pdb
│   ├── cypD-203_5min30_mtz001_fast.mtz
│   ├── cypD-203_5min30_mtz001_fast.pdb
│   ├── cypD-203_5min30_mtz001_full.mtz
│   ├── cypD-203_5min30_mtz001_full.pdb
│   ├── cypD-203_5min30_mtz002_fast.mtz
│   ├── cypD-203_5min30_mtz002_fast.pdb
│   ├── data_mtz001
│   │   ├── ap_w1_run1_anom_autoPROC.log
│   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   ├── ap_w1_run1_anom_truncate_reindexed_P41212.mtz
│   │   ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
│   │   └── xtriage_ap_w1_run1_anom_truncate.log
```

In a 'ALL_pdb_mtz' folder, for a rapid and easier visualization of all results in a same coot session, copy of all the pdb and mtz files of datasets treated in this 'RESULTS' folder.

In a '_mtz_treated' folder, copy of:

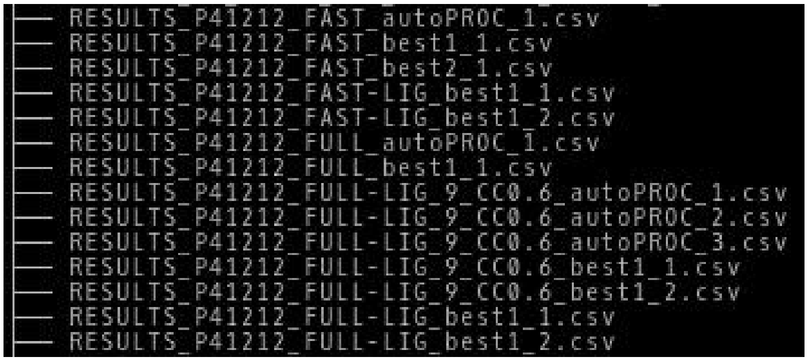
- csv listing datasets without mtz file
- csv with mtz list
- csv with mtz list after reindexing
- csv with mtz list sorted according to reference space group
- all 'launch' csv files, with a counter at the end of the names in case of several launches (with handmade modifications of launch csv file for example)



```
_mtz_treated/
├── launch_mtz_P41212_FAST_autoPROC_1.csv
├── launch_mtz_P41212_FAST_best1_1.csv
├── launch_mtz_P41212_FAST_best2_1.csv
├── launch_mtz_P41212_FAST-LIG_best1_1.csv
├── launch_mtz_P41212_FAST-LIG_best1_2.csv
├── launch_mtz_P41212_FULL_autoPROC_1.csv
├── launch_mtz_P41212_FULL_best1_1.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_autoPROC_1.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_autoPROC_2.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_autoPROC_3.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_best1_1.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_best1_2.csv
├── launch_mtz_P41212_FULL-LIG_best1_1.csv
├── launch_mtz_P41212_FULL-LIG_best1_2.csv
├── mtz_to_treat_ALL.csv
├── mtz_to_treat_ALL_reindexed.csv
└── mtz_to_treat_ALL_reindexed_sorted_P41212.csv
```

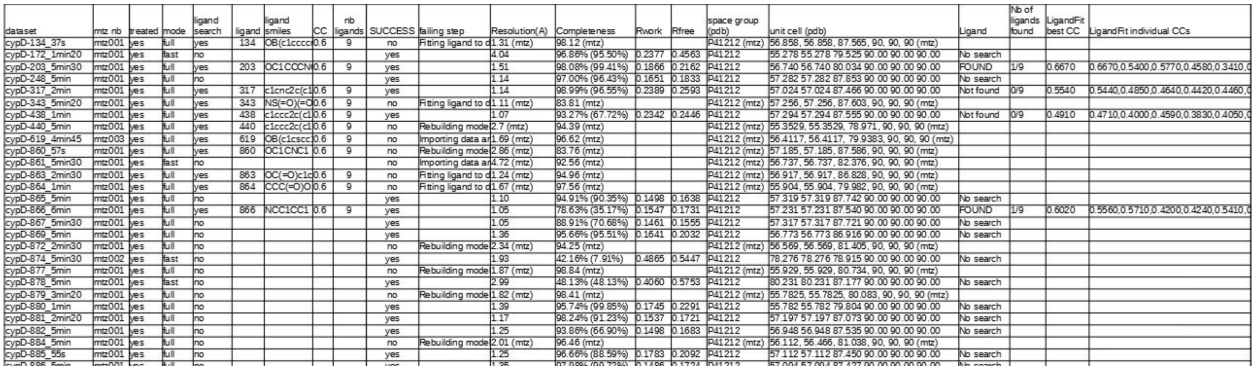
For each 'launch' subcommand, a csv file is created that summarizes the corresponding results for each dataset, with information on:

- success of Phenix
- failing step (in case success = no)
- resolution (from pdb file, if failed from mtz data file)
- completeness (from pdb file, if failed from mtz data file)
- Rwork / Rfree
- space group (from pdb file, if failed from mtz data file)
- unit cell (from pdb file, if failed from mtz data file)
- if ligand has been placed, number of ligands found, corresponding CC



```
│├── RESULTS_P41212_FAST_autoPROC_1.csv
│├── RESULTS_P41212_FAST_best1_1.csv
│├── RESULTS_P41212_FAST_best2_1.csv
│├── RESULTS_P41212_FAST-LIG_best1_1.csv
│├── RESULTS_P41212_FAST-LIG_best1_2.csv
│├── RESULTS_P41212_FULL_autoPROC_1.csv
│├── RESULTS_P41212_FULL_best1_1.csv
│├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_1.csv
│├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_2.csv
│├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_3.csv
│├── RESULTS_P41212_FULL-LIG_9_CC0.6_best1_1.csv
│├── RESULTS_P41212_FULL-LIG_9_CC0.6_best1_2.csv
│├── RESULTS_P41212_FULL-LIG_best1_1.csv
│├── RESULTS_P41212_FULL-LIG_best1_2.csv
```

Option example: -a –mode full –lig –nblig 9 –cclig 0.6



dataset	mtz nb	treated	mode	ligand search	ligand	ligand smiles	CC	nb ligands	SUCCESS	failing step	Resolution(A)	Completeness	Rwork	Rfree	space group (pdb)	unit cell (pdb)	Ligand	Nb of ligands found	LigandFit best CC	LigandFit individual CCs
cypD-134_37s	mtz001	yes	full	yes	134	OB(c1cccc	0.6	9	no	Fitting ligand to d	1.31 (mtz)	98.12 (mtz)			P41212 (mtz)	56.858, 56.858, 87.565, 90, 90, 90 (mtz)				
cypD-172_1min20	mtz001	yes	fast	no					yes		4.04	96.86% (95.50%)	0.2377	0.4563	P41212	55.278 55.278 79.525 90.00 90.00 90.00	No search			
cypD-203_5min30	mtz001	yes	full	yes	203	OC1CCCN	0.6	9	yes		1.51	98.08% (99.41%)	0.1866	0.2162	P41212	56.740 56.740 80.034 90.00 90.00 90.00	FOUND	1/9	0.6670	0.6670,0.5400,0.5770,0.4580,0.3410,0
cypD-248_5min	mtz001	yes	full	no					yes		1.14	97.00% (96.43%)	0.1651	0.1833	P41212	57.282 57.282 87.853 90.00 90.00 90.00	No search			
cypD-317_2min	mtz001	yes	full	yes	317	c1cnc2c(c1	0.6	9	yes		1.14	98.99% (96.55%)	0.2389	0.2593	P41212	57.024 57.024 87.466 90.00 90.00 90.00	Not found	0/9	0.5540	0.5440,0.4850,0.4640,0.4420,0.4460,0
cypD-343_5min20	mtz001	yes	full	yes	343	NS(=O)(=O	0.6	9	no	Fitting ligand to d	1.11 (mtz)	83.81 (mtz)			P41212 (mtz)	57.256, 57.256, 87.603, 90, 90, 90 (mtz)				
cypD-438_1min	mtz001	yes	full	yes	438	c1ccc2c(c1	0.6	9	yes		1.07	93.27% (67.72%)	0.2342	0.2446	P41212	57.294 57.294 87.555 90.00 90.00 90.00	Not found	0/9	0.4910	0.4710,0.4000,0.4590,0.3830,0.4050,0
cypD-440_5min	mtz001	yes	full	yes	440	c1ccc2c(c1	0.6	9	no	Rebuilding mode	2.7 (mtz)	94.39 (mtz)			P41212 (mtz)	55.3529, 55.3529, 78.971, 90, 90, 90 (mtz)				
cypD-619_4min45	mtz003	yes	full	yes	619	OB(c1cscc	0.6	9	no	Importing data ar	1.69 (mtz)	96.62 (mtz)			P41212 (mtz)	56.4117, 56.4117, 79.9383, 90, 90, 90 (mtz)				
cypD-860_57s	mtz001	yes	full	yes	860	OC1CNC1	0.6	9	no	Rebuilding mode	2.86 (mtz)	83.76 (mtz)			P41212 (mtz)	57.185, 57.185, 87.586, 90, 90, 90 (mtz)				
cypD-861_5min30	mtz001	yes	fast	no					no	Importing data ar	4.72 (mtz)	92.56 (mtz)			P41212 (mtz)	56.737, 56.737, 82.376, 90, 90, 90 (mtz)				
cypD-863_2min30	mtz001	yes	full	yes	863	OC(=O)c1c	0.6	9	no	Fitting ligand to d	1.24 (mtz)	94.96 (mtz)			P41212 (mtz)	56.917, 56.917, 86.828, 90, 90, 90 (mtz)				
cypD-864_1min	mtz001	yes	full	yes	864	CCC(=O)O	0.6	9	no	Fitting ligand to d	1.67 (mtz)	97.56 (mtz)			P41212 (mtz)	55.904, 55.904, 79.982, 90, 90, 90 (mtz)				
cypD-865_5min	mtz001	yes	full	no					yes		1.10	94.91% (90.35%)	0.1498	0.1638	P41212	57.319 57.319 87.742 90.00 90.00 90.00	No search			
cypD-866_6min	mtz001	yes	full	yes	866	NCC1CC1	0.6	9	yes		1.05	78.63% (35.17%)	0.1547	0.1731	P41212	57.231 57.231 87.540 90.00 90.00 90.00	FOUND	1/9	0.6020	0.5560,0.5710,0.4200,0.4240,0.5410,0
cypD-867_5min30	mtz001	yes	full	no					yes		1.05	88.91% (70.68%)	0.1461	0.1555	P41212	57.317 57.317 87.721 90.00 90.00 90.00	No search			
cypD-869_5min	mtz001	yes	full	no					yes		1.36	95.66% (95.51%)	0.1641	0.2032	P41212	56.773 56.773 86.916 90.00 90.00 90.00	No search			
cypD-872_2min30	mtz001	yes	full	no					no	Rebuilding mode	2.34 (mtz)	94.25 (mtz)			P41212 (mtz)	56.569, 56.569, 81.405, 90, 90, 90 (mtz)				
cypD-874_5min30	mtz002	yes	fast	no					yes		1.93	42.16% (7.91%)	0.4865	0.5447	P41212	78.276 78.276 78.915 90.00 90.00 90.00	No search			
cypD-877_5min	mtz001	yes	full	no					no	Rebuilding mode	1.87 (mtz)	98.84 (mtz)			P41212 (mtz)	55.929, 55.929, 80.734, 90, 90, 90 (mtz)				
cypD-878_5min	mtz001	yes	fast	no					yes		2.99	48.13% (48.13%)	0.4060	0.5753	P41212	80.231 80.231 87.177 90.00 90.00 90.00	No search			
cypD-879_3min20	mtz001	yes	full	no					no	Rebuilding mode	1.82 (mtz)	98.41 (mtz)			P41212 (mtz)	55.7825, 55.7825, 80.083, 90, 90, 90 (mtz)				
cypD-880_1min	mtz001	yes	full	no					yes		1.39	95.74% (99.85%)	0.1745	0.2291	P41212	55.782 55.782 79.804 90.00 90.00 90.00	No search			
cypD-881_2min20	mtz001	yes	full	no					yes		1.17	98.24% (91.23%)	0.1537	0.1721	P41212	57.197 57.197 87.073 90.00 90.00 90.00	No search			
cypD-882_5min	mtz001	yes	full	no					yes		1.25	93.86% (66.90%)	0.1498	0.1683	P41212	56.948 56.948 87.535 90.00 90.00 90.00	No search			
cypD-884_5min	mtz001	yes	full	no					no	Rebuilding mode	2.01 (mtz)	96.46 (mtz)			P41212 (mtz)	56.112, 56.466, 81.038, 90, 90, 90 (mtz)				
cypD-885_55s	mtz001	yes	full	no					yes		1.25	96.66% (88.59%)	0.1783	0.2092	P41212	57.112 57.112 87.450 90.00 90.00 90.00	No search			
cypD-886_5min	mtz001	yes	full	no					yes		1.35	97.98% (90.73%)	0.1486	0.1724	P41212	57.004 57.004 87.427 90.00 90.00 90.00	No search			

Finally, the results of all 'launch' subcommands you have run are compiled by running automatically the *'summary'* subcommand.

Note

If there are several RESULTS folders (case when launched for several space groups, or different templates), a global SUMMARY file that compiles all SUMMARY files can be created by manually running *'summary'* subcommand.

9.3 Phenix options according to modes (only for information)

phenix.ligand_pipeline[Page 37, 1] options are the following:

- common options:

nproc=Auto

preserve_chain_id=True: Preserves the original chain ID

refine.after_ligand.hydrogens=False: Hydrogen atoms won't be added prior to the final refinement step (else refinement significantly slower)

prune=False: disable Prune the model after refinement to remove residues and sidechains in poor density

keep_hetatms=True: prevent Phaser from resetting HETATMs occupancies to zero

refine.after_mr.update_waters=False: don't add/remove waters automatically

- 'fast' mode:

skip_xtriage=True

mr=False: rigid-body refinement will be used

quick_refine=True: which will shorten both refinement steps from 6 to 3 cycles, and disable weight optimization.

build=False

skip_ligand=True

reference_structure='model.pdb': If specified, phenix.find_alt_orig_sym_mate will be applied to map the solution to the reference structure (not working when Phaser with several monomers)

- 'full' mode:

mr=Auto: the program will try rigid-body refinement first, then run Phaser if the R-free is too high (>0.4)

build=Auto: Run AutoBuild after initial refinement. By default, this will be done if R-free is greater than the max_r_free cutoff = 0.3

autobuild.quick=True: Run AutoBuild in quick mode. Inferior results, but a huge time-saver

quick_refine=True: which will shorten both refinement steps from 6 to 3 cycles, and disable weight optimization.

- ‘allsg’ mode:

mr=True

quick_refine=False

- if ligand search:

ligand_copies=1 (except if option –nblig >1)

keep_input_restraints=True : if the input files include pre-calculated restraints for the target ligand, eLBOW will propagate these restraints instead of generating new ones.

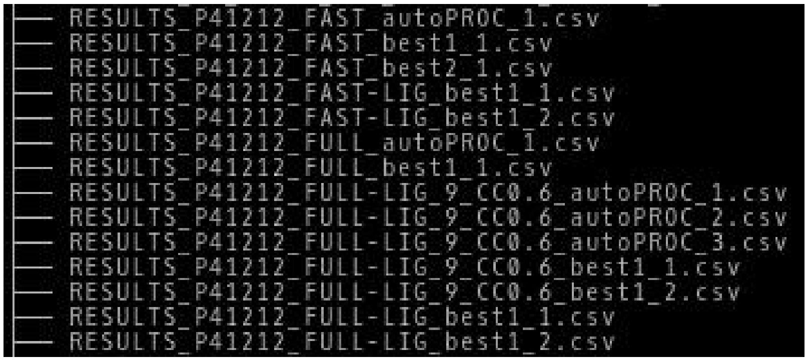
9.4 References

CHAPTER TEN

EASYPIPE 'SUMMARY'

This step can be run after several runs of *'launch'* subcommands.

For each 'launch' subcommand, a 'RESULT' csv file is created that summarizes the corresponding results for each dataset (*see here*). So, if you have tried several options, you will have as many 'RESULTS' csv files.



```
├── RESULTS_P41212_FAST_autoPROC_1.csv
├── RESULTS_P41212_FAST_best1_1.csv
├── RESULTS_P41212_FAST_best2_1.csv
├── RESULTS_P41212_FAST-LIG_best1_1.csv
├── RESULTS_P41212_FAST-LIG_best1_2.csv
├── RESULTS_P41212_FULL_autoPROC_1.csv
├── RESULTS_P41212_FULL_best1_1.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_1.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_2.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_3.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_best1_1.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_best1_2.csv
├── RESULTS_P41212_FULL-LIG_best1_1.csv
├── RESULTS_P41212_FULL-LIG_best1_2.csv
```

Then, you probably want to compile all these results for a better view.

Now, the command 'summary' is automatically run at the end of each 'launch' command, but only for the RESULTS folder of this command (in this example, the 'RESULTS_P41212' folder).

If you have done several 'launch' with different space group for example, that means the RESULTS folders will be different, you will have to run manually the 'summary' command.

Then a global SUMMARY file will be created, that compiles all SUMMARY files present in RESULTS folders if there are several RESULTS folders (case when launched for several space groups, or different templates).

10.1 Usage

easypipe.py data summary [-h]

arguments	description
-h, –help	show this help message and exit
-o, –only_success	generate also a result file with only successfull treatments

Example:

```
$ easypipe.py PROCESSED_DATA summary
```

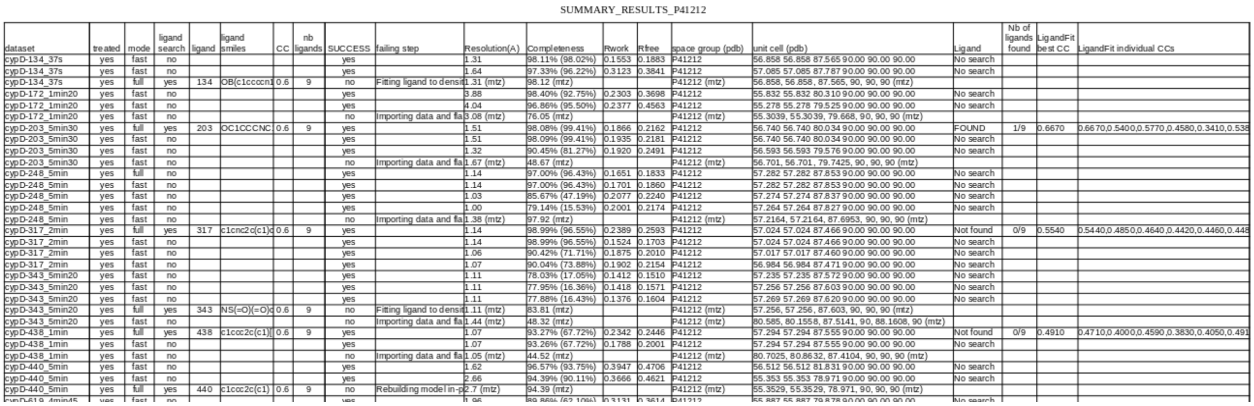
10.2 What does it do ?

In the ‘RESULT’ folder, ‘summary’ subcommand creates a ‘SUMMARY’ csv file where all datasets results are compiled.

With the option ‘–only_success’, unsucessfull treatments are not listed in the summary file, for a better clarity.

For each datasets, redondant results are deleted and the remaining ones are sorted according to:

- ‘dataset’
- ‘SUCCESS’
- ‘ligand search’
- ‘Ligand’ (found or not)
- ‘Completeness’
- ‘Nb of ligands found’
- ‘Rwork’



SUMMARY_RESULTS_P41212

dataset	treated	mode	ligand search	ligand	ligand smiles	CC	nb ligands	SUCCESS	failing step	Resolution(A)	Completeness	Rwork	Rfree	space group (pdb)	unit cell (pdb)	Ligand	Nb of ligands found	LigandFit best CC	LigandFit individual CCs
cypD-134_37s	yes	fast	no					yes		1.31	98.11% (98.02%)	0.1553	0.1883	P41212	56.858 56.858 87.565 90.00 90.00 90.00	No search			
cypD-134_37s	yes	fast	no					yes		1.64	97.33% (96.22%)	0.3123	0.3841	P41212	57.085 57.085 87.787 90.00 90.00 90.00	No search			
cypD-134_37s	yes	full	yes	134	OB(c1ccccn1	0.6	9	no	Fitting ligand to densit	1.31 (mtz)	98.12 (mtz)			P41212 (mtz)	56.858, 56.858, 87.565, 90, 90, 90 (mtz)				
cypD-172_1min20	yes	fast	no					yes		3.88	98.40% (92.75%)	0.2303	0.3698	P41212	55.832 55.832 80.310 90.00 90.00 90.00	No search			
cypD-172_1min20	yes	fast	no					yes		4.04	96.86% (95.50%)	0.2377	0.4563	P41212	55.278 55.278 79.525 90.00 90.00 90.00	No search			
cypD-172_1min20	yes	fast	no					no	Importing data and fla	3.08 (mtz)	76.05 (mtz)			P41212 (mtz)	55.3039, 55.3039, 79.668, 90, 90, 90 (mtz)				
cypD-203_5min30	yes	full	yes	203	OC1CCCNC	0.6	9	yes		1.51	98.08% (99.41%)	0.1866	0.2162	P41212	56.740 56.740 80.034 90.00 90.00 90.00	FOUND	1/9	0.6670	0.6670,0.5400,0.5770,0.4580,0.3410,0.538
cypD-203_5min30	yes	fast	no					yes		1.51	98.09% (99.41%)	0.1935	0.2181	P41212	56.740 56.740 80.034 90.00 90.00 90.00	No search			
cypD-203_5min30	yes	fast	no					yes		1.32	90.45% (81.27%)	0.1920	0.2491	P41212	56.593 56.593 79.576 90.00 90.00 90.00	No search			
cypD-203_5min30	yes	fast	no					no	Importing data and fla	1.67 (mtz)	48.67 (mtz)			P41212 (mtz)	56.701, 56.701, 79.7425, 90, 90, 90 (mtz)				
cypD-248_5min	yes	full	no					yes		1.14	97.00% (96.43%)	0.1651	0.1833	P41212	57.282 57.282 87.853 90.00 90.00 90.00	No search			
cypD-248_5min	yes	fast	no					yes		1.14	97.00% (96.43%)	0.1701	0.1860	P41212	57.282 57.282 87.853 90.00 90.00 90.00	No search			
cypD-248_5min	yes	fast	no					yes		1.03	85.67% (47.19%)	0.2077	0.2240	P41212	57.274 57.274 87.837 90.00 90.00 90.00	No search			
cypD-248_5min	yes	fast	no					yes		1.00	79.14% (15.53%)	0.2001	0.2174	P41212	57.264 57.264 87.827 90.00 90.00 90.00	No search			
cypD-248_5min	yes	fast	no					no	Importing data and fla	1.38 (mtz)	97.92 (mtz)			P41212 (mtz)	57.2164, 57.2164, 87.6953, 90, 90, 90 (mtz)				
cypD-317_2min	yes	full	yes	317	c1cnc2c(c1)c	0.6	9	yes		1.14	98.99% (96.55%)	0.2389	0.2593	P41212	57.024 57.024 87.466 90.00 90.00 90.00	Not found	0/9	0.5540	0.5440,0.4850,0.4640,0.4420,0.4460,0.448
cypD-317_2min	yes	fast	no					yes		1.14	98.99% (96.55%)	0.1524	0.1703	P41212	57.024 57.024 87.466 90.00 90.00 90.00	No search			
cypD-317_2min	yes	fast	no					yes		1.06	90.42% (71.71%)	0.1875	0.2010	P41212	57.017 57.017 87.460 90.00 90.00 90.00	No search			
cypD-317_2min	yes	fast	no					yes		1.07	90.04% (73.88%)	0.1902	0.2154	P41212	56.984 56.984 87.471 90.00 90.00 90.00	No search			
cypD-343_5min20	yes	fast	no					yes		1.11	78.03% (17.05%)	0.1412	0.1510	P41212	57.235 57.235 87.572 90.00 90.00 90.00	No search			
cypD-343_5min20	yes	fast	no					yes		1.11	77.95% (16.36%)	0.1418	0.1571	P41212	57.256 57.256 87.603 90.00 90.00 90.00	No search			
cypD-343_5min20	yes	fast	no					yes		1.11	77.88% (16.43%)	0.1376	0.1604	P41212	57.269 57.269 87.620 90.00 90.00 90.00	No search			
cypD-343_5min20	yes	full	yes	343	NS(=O)(=O)c	0.6	9	no	Fitting ligand to densit	1.11 (mtz)	83.81 (mtz)			P41212 (mtz)	57.256, 57.256, 87.603, 90, 90, 90 (mtz)				
cypD-343_5min20	yes	fast	no					no	Importing data and fla	1.44 (mtz)	48.32 (mtz)			P41212 (mtz)	80.585, 80.1558, 87.5141, 90, 88.1608, 90 (mtz)				
cypD-438_1min	yes	full	yes	438	c1ccc2c(c1)[	0.6	9	yes		1.07	93.27% (67.72%)	0.2342	0.2446	P41212	57.294 57.294 87.555 90.00 90.00 90.00	Not found	0/9	0.4910	0.4710,0.4000,0.4590,0.3830,0.4050,0.491
cypD-438_1min	yes	fast	no					yes		1.07	93.26% (67.72%)	0.1788	0.2001	P41212	57.294 57.294 87.555 90.00 90.00 90.00	No search			
cypD-438_1min	yes	fast	no					no	Importing data and fla	1.05 (mtz)	44.52 (mtz)			P41212 (mtz)	80.7025, 80.8632, 87.4104, 90, 90, 90 (mtz)				
cypD-440_5min	yes	fast	no					yes		1.62	96.57% (93.75%)	0.3947	0.4706	P41212	56.512 56.512 81.831 90.00 90.00 90.00	No search			
cypD-440_5min	yes	fast	no					yes		2.66	94.39% (90.11%)	0.3666	0.4621	P41212	55.353 55.353 78.971 90.00 90.00 90.00	No search			
cypD-440_5min	yes	full	yes	440	c1ccc2c(c1)	0.6	9	no	Rebuilding model in-p	2.7 (mtz)	94.39 (mtz)			P41212 (mtz)	55.3529, 55.3529, 78.971, 90, 90, 90 (mtz)				
cypD-619_4min45	yes	fast	no					yes		1.96	89.86% (62.10%)	0.3131	0.3614	P41212	55.887 55.887 79.878 90.00 90.00 90.00	No search			

This way, the first row of each dataset should be most of the time the best treatment to consider, but is always better to have a critical eye on information like completeness or resolution to be sure …

And, if there are several RESULTS folders (case when launched for several space groups, or different templates), a global SUMMARY file will be created, that compiles all SUMMARY files present in RESULTS folders. Sorting criteria are the same as above.

CHAPTER ELEVEN

EASYPIPE ‘AUTO’

This mode allows to launch main easYPipe steps (prep, reindex, launch, summary) without any intervention. Ligand search is not possible for the moment.

11.1 Usage

easypipe.py data auto [-h] [-m {fast,full,allsg}] ref

arguments	description
ref	folder with fasta file and pdb file for replacement, and cif(s) if ligand(s) in the model

Warning

reference pdb files should include the row starting with ‘CRYST1’ containing information on space group

optional arguments	description
-h, –help	show this help message and exit
-m {fast,full,allsg}, –mode {fast,full,allsg}	running mode: fast, full, or allsg (default = fast)
-b NUMBER, –best NUMBER	launch only for mtz with best completeness, NUMBER indicates how many mtz to treat (default 1), ex: –best 2
-a, –autoproc	launch only for mtz from autoPROC, or if none launch for mtz with best completeness
-w, –whole	launch for the whole mtz processes
-t TEMPLATE, –template TEMPLATE	optional template name for log files and result folders, in case re-launching with different reference pdb of the same space group (else will overwrite).

Example:

```
$ easypipe.py PROCESSED_DATA auto my_ref_folder --best 2 --mode full
equivalent to:
$ easypipe.py PROCESSED_DATA auto my_ref_folder -b 2 -m full
```

11.2 How the data should be organized ?

Processed data should be in datasets folders, all grouped in a folder. More information on how to organize your data *here*.

11.3 What does it do ?

Executes successively, without any intervention, the following steps:

- *prep*
- *reindex*
- *launch*
- *summary*

The options are the same as for *launch*, except for the options concerning the search for ligands which is not enabled at the moment. In the same way, the option “simulate” is not possible because it would imply an intervention. A new ‘launch csv’ file is therefore generated each time.

CHAPTER

TWELVE

EASYPIPE ‘PANDDA’

If you have more than 40 datasets, you can try to use PanDDA[1] which is particularly suitable to the detection of weakly bound ligands such as fragments.

This step can be run after all ‘launch’ subcommands have been executed, and aims at organizing the data processed with easYPipe in order to be able to run PanDDA.

12.1 Usage

easypipe.py data pandda [-h]

Example:

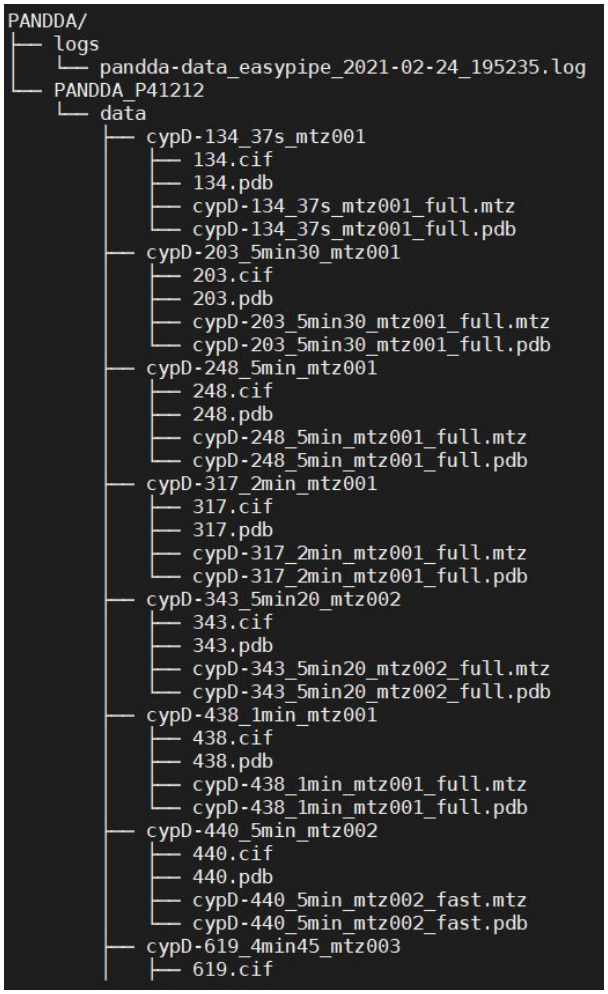
```
$ easypipe.py ./PROCESSED_DATA/ pandda
```

12.2 What does it do ?

For each dataset, ‘pandda’ easYPipe subcommand copies in a dataset folder suitable for PanDDA:

- pdb and mtz files generated with easYPipe,
- cif and pdb files of corresponding ligand,

[1] https://pandda.bitbucket.io/



```
PANDDA/
├── logs
│   └── pandda-data_easypipe_2021-02-24_195235.log
└── PANDDA_P41212
    └── data
        ├── cypD-134_37s_mtz001
        │   ├── 134.cif
        │   ├── 134.pdb
        │   ├── cypD-134_37s_mtz001_full.mtz
        │   └── cypD-134_37s_mtz001_full.pdb
        ├── cypD-203_5min30_mtz001
        │   ├── 203.cif
        │   ├── 203.pdb
        │   ├── cypD-203_5min30_mtz001_full.mtz
        │   └── cypD-203_5min30_mtz001_full.pdb
        ├── cypD-248_5min_mtz001
        │   ├── 248.cif
        │   ├── 248.pdb
        │   ├── cypD-248_5min_mtz001_full.mtz
        │   └── cypD-248_5min_mtz001_full.pdb
        ├── cypD-317_2min_mtz001
        │   ├── 317.cif
        │   ├── 317.pdb
        │   ├── cypD-317_2min_mtz001_full.mtz
        │   └── cypD-317_2min_mtz001_full.pdb
        ├── cypD-343_5min20_mtz002
        │   ├── 343.cif
        │   ├── 343.pdb
        │   ├── cypD-343_5min20_mtz002_full.mtz
        │   └── cypD-343_5min20_mtz002_full.pdb
        ├── cypD-438_1min_mtz001
        │   ├── 438.cif
        │   ├── 438.pdb
        │   ├── cypD-438_1min_mtz001_full.mtz
        │   └── cypD-438_1min_mtz001_full.pdb
        ├── cypD-440_5min_mtz002
        │   ├── 440.cif
        │   ├── 440.pdb
        │   ├── cypD-440_5min_mtz002_fast.mtz
        │   └── cypD-440_5min_mtz002_fast.pdb
        ├── cypD-619_4min45_mtz003
        │   ├── 619.cif
```

12.3 References