

# PEINTS

# -MR for ligand screening -

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KEK IMSS PF SBRC

# Contents in the package

- `peints_gui.py`
  - GUI
- `main.py`
  - A main program
- `peints_main_parent.sh`
  - Pipeline script to process your data.
  - `peints_main_parent.sh` will be edited as your checkboxes, “image capture by coot” or “phenix.refine”, to `peints_main.sh`
- `peints_coot.py`
  - A template text file for coot to capture images
  - `peints_coot.py` will be edited as your input of “Target site”
- `peints_results.py`
  - Module to output your results as HTML file
- `mypool.py`
  - Module to run `peints_main.sh` using multiprocessors

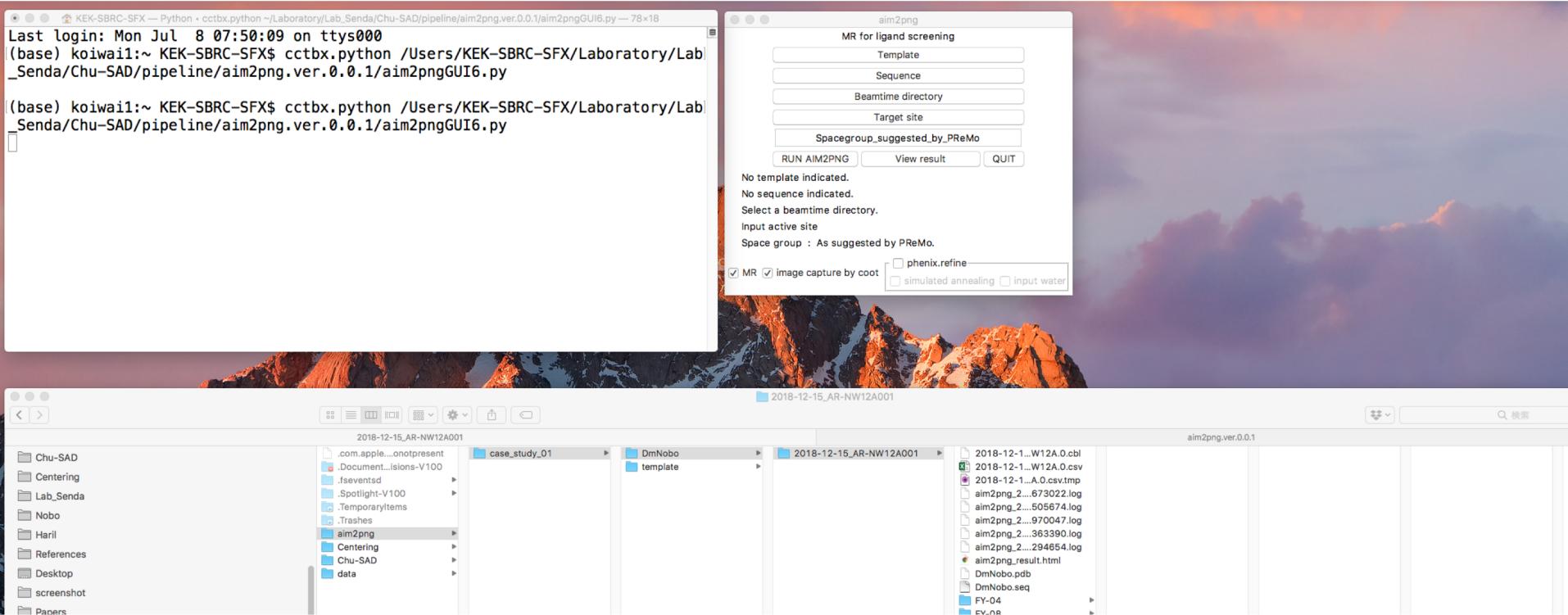
# Requirement to use

- Python2.7~ or python3~ is installed
- CCP4 package is installed
  - Tkinter is necessary
  - If you use CCP4-7.0, you cannot capture images by coot.
- Datasets are output by PReMo
  - aimless.mtz, aimless.log, and XDS\_ASCII.HKL are in sub-directories.
- Option: PHENIX package is installed
- Firefox is installed to watch HTML output file from points\_gui directly.

# How to use -1-

1. peints\_gui run using a command

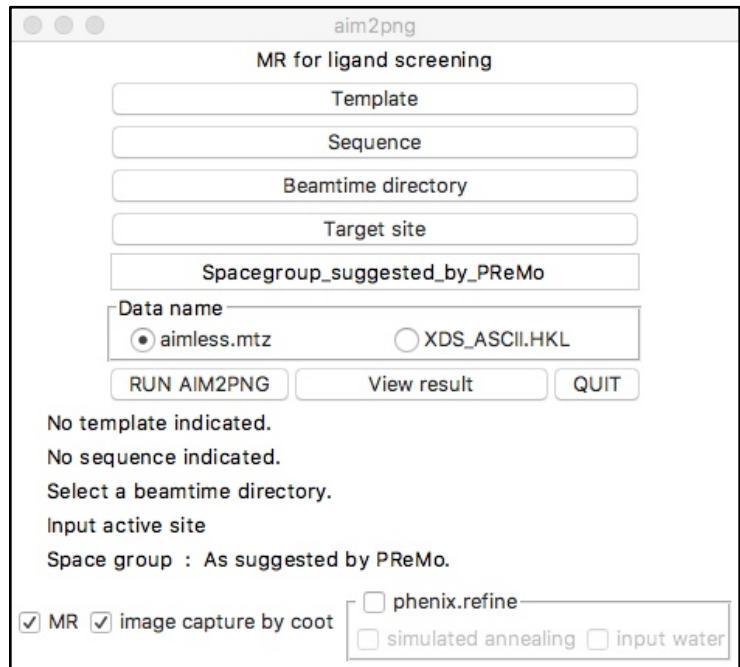
```
$ cctbx.python <peints_directory>/peints_gui.py
```



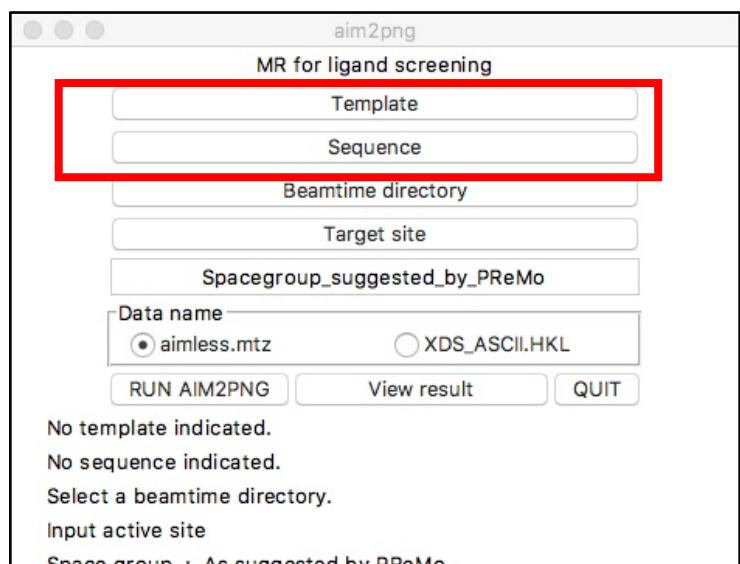
# How to use -2-

3. Select your template pdb file
  - .pdb file is selectable
4. Select your sequence file
  - .txt or .seq file is selectable

## 1. GUI window



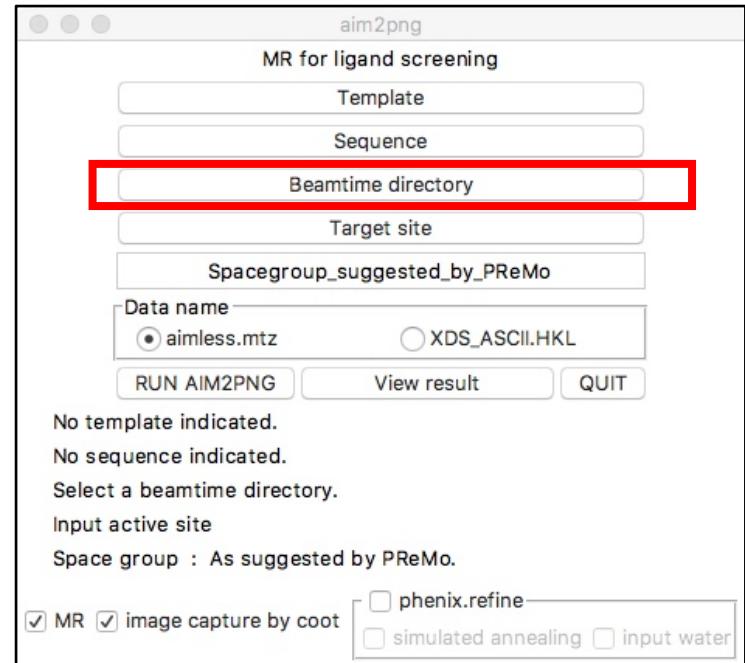
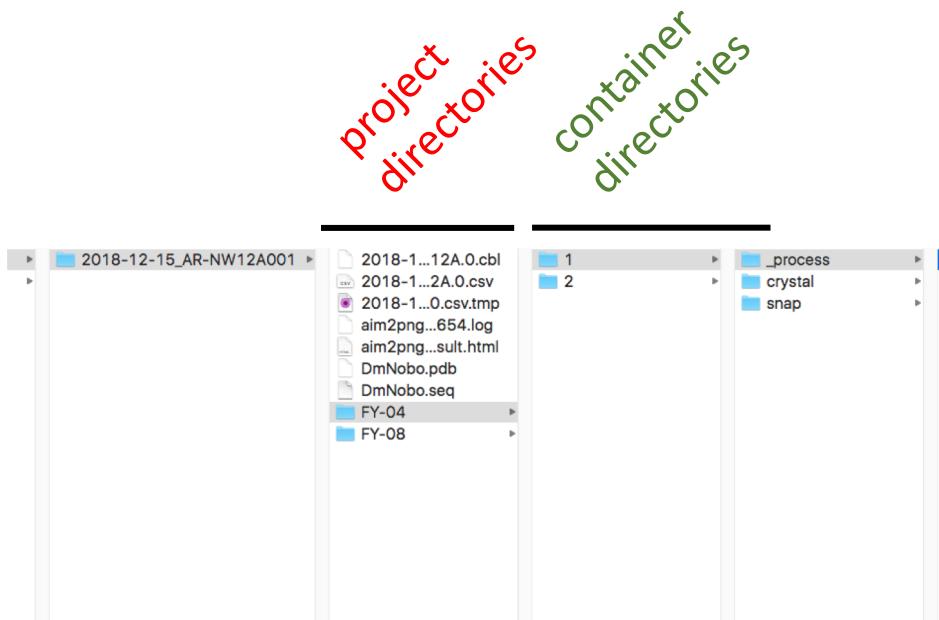
## 2. Template pdb and sequence are selected.



# How to use -3-

## 5. Select a beamtime directory

- A container directory is also selectable  
e.g. 2018-12-15\_AR-NE3A001



xds\_\* directory

- PReMo automatically outputs  
BeamtimeDir/ContainerDir/CrystalDir/\_process/xds\_?/aimless.mtz

# How to use -4-

## 6. Input your target site

Format : <chainID>/<residue No.>/<atomID> or

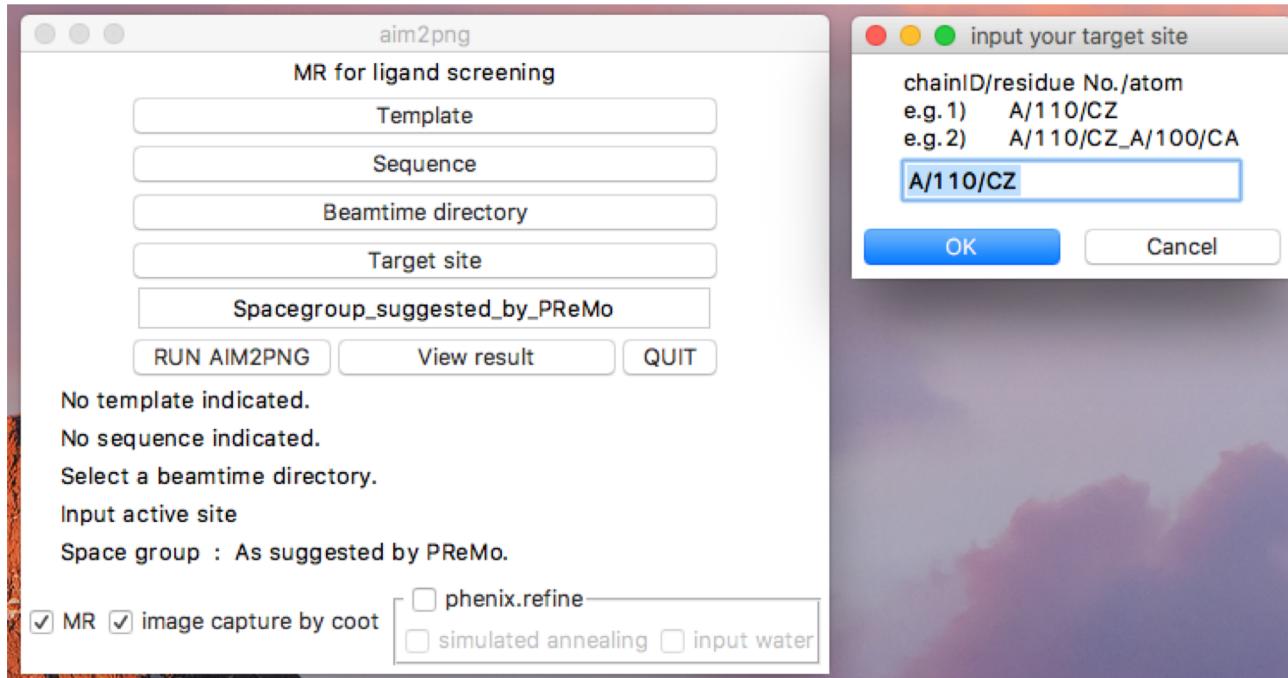
<chainID>/<residue No.>/<atomID>\_<chainID>/<residue No.>/<atomID>

e.g.1) input single <chainID>/<residue No.>/<atomID>

- points will get images focusing the indicated atom

e.g.2) input single <chainID>/<residue No.>/<atomID>\_<chainID>/<residue No.>/<atomID>

- points will place pseudoatom between the indicated atoms, and will get images focusing the pseudoatom



# How to use -5-

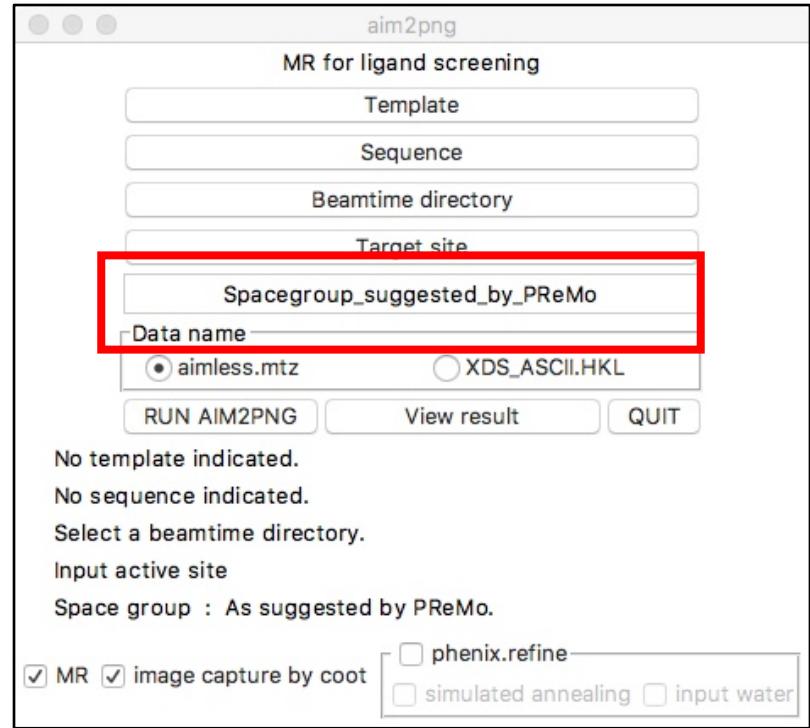
## 7. Input a spacegroup name.

- Default value is

Spacegroup\_suggested\_by\_PReMo

e.g.) P212121

- If the spacegroup is not match with that suggested by PReMo, points re-processes the data with *POINTLESS* and *AIMLESS* using XDS\_ASCII.HKL



# How to use -6-

## 8. Select your options

MR:

ON:      peints do MR with *MOLREP* and refinement with *REFMAC5*

OFF:     peints do only refinement with *REFMAC5*

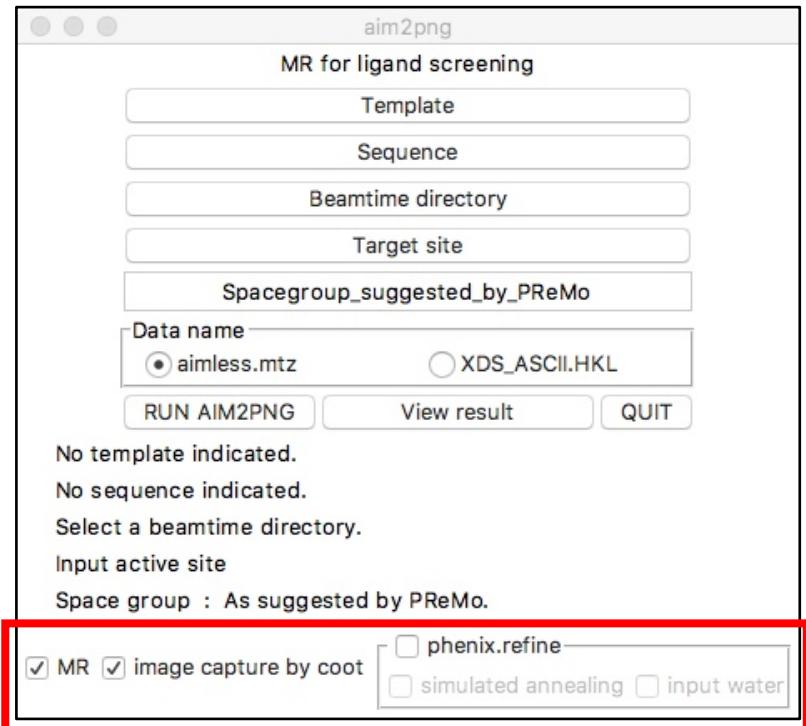
Image capture by coot:

**CAUTION: if you will process many dataset using image-capture by coot, coot will start as the number of the datasets.**

phenix.refine:

ON:      peints do refinement with *PHENIX.REFINE* after *REFMAC5*

## 9. Start by “RUN peints”



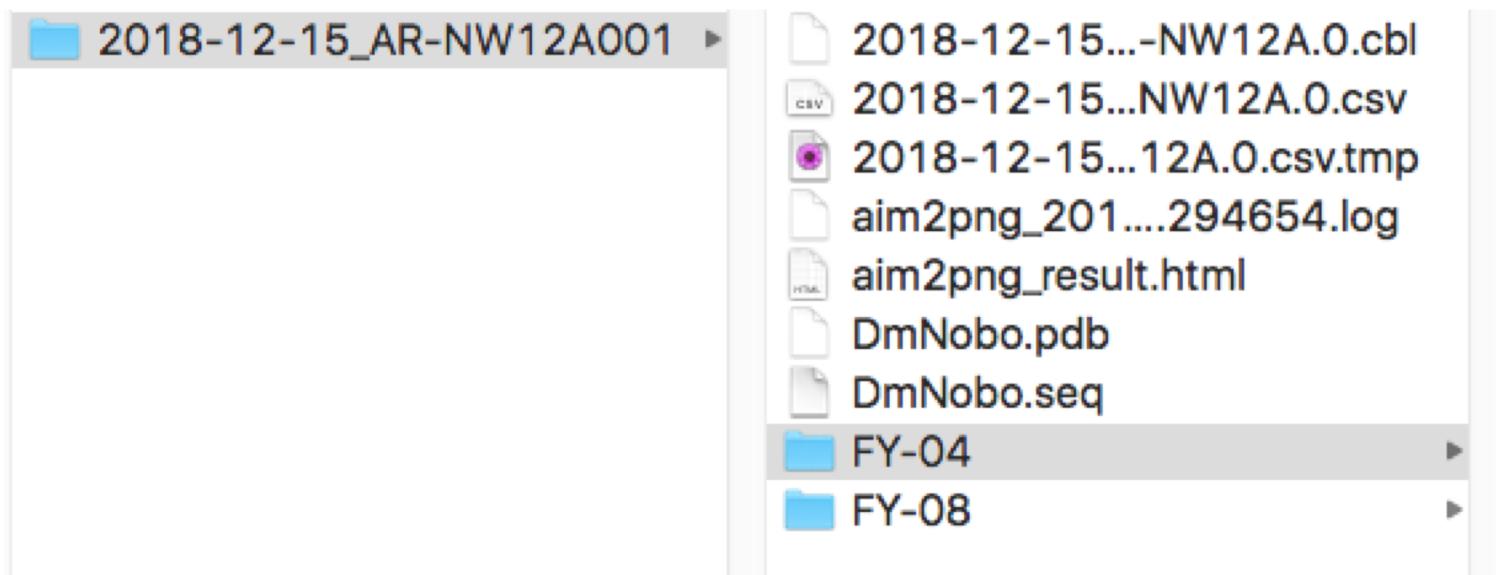
You can cancel peints by [Ctrl] + C on the terminal window.

# How to use -7-

## 10. View your result

Your summarized HTML result is output in project directory as python\_split-results2.html.

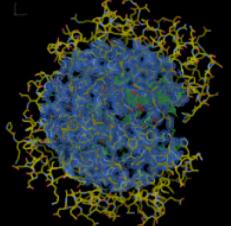
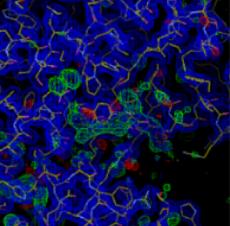
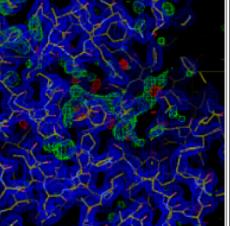
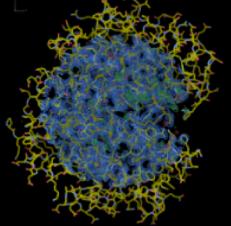
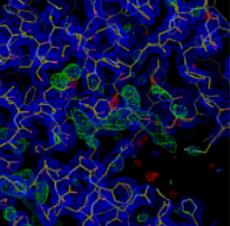
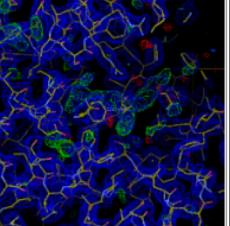
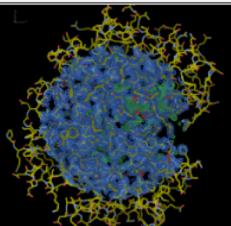
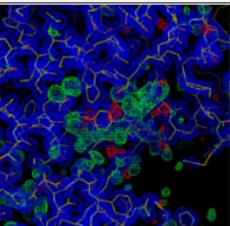
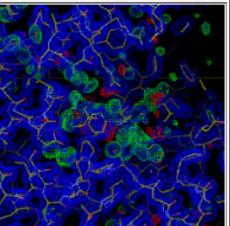
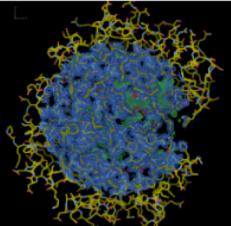
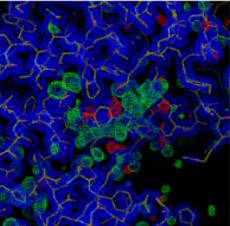
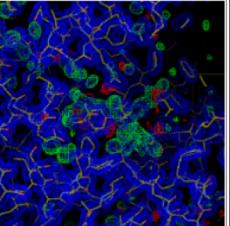
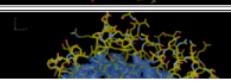
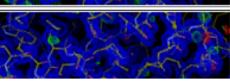
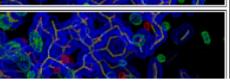
Firefox must be installed.



# peints\_result.html

## Results of AIM2PNG

Project directory: /Volumes/ChuSAD\_02/aim2png/case\_study\_01/DmNobo/2018-12-15\_AR-NW12A001  
Template PDB: /Volumes/ChuSAD\_02/aim2png/case\_study\_01/DmNobo/2018-12-15\_AR-NW12A001/DmNobo.pdb  
Sequence : /Volumes/ChuSAD\_02/aim2png/case\_study\_01/DmNobo/2018-12-15\_AR-NW12A001/DmNobo.seq

unipuck	crystal	spacegroup	unit cell	resolution high	resolution low	Rwork	Rfree	overall	pocket_1	pocket_2
FY-04	1	P212121	58.623 75.496 106.713 90.00 90.00 90.00	1.91	39.49	0.24311	0.27873			
FY-04	2	P212121	58.533 75.436 106.316 90.00 90.00 90.00	2.16	46.29	0.26563	0.29422			
FY-08	1	P212121	58.580 75.312 107.753 90.00 90.00 90.00	1.55	43.86	0.25581	0.27895			
FY-08	1	P212121	58.607 75.316 107.801 90.00 90.00 90.00	1.55	43.87	0.25054	0.27490			
										

# Output files

1. In the beamtime directory:
  1. peints\_results.html
2. In the peints directory:
  1. refmac1.pdb
  2. refmac1.mtz
  3. refmac1\_all.png
  4. refmac1\_targetsite\_1.png
  5. refmac1\_targetsite\_2.png

# References

- POINTLESS
  - Evans P (2006) Scaling and assessment of data quality. *Acta Crystallogr Sect D Biol Crystallogr* 62(1):72–82.
- AIMLESS
  - Evans PR, Murshudov GN (2013) How good are my data and what is the resolution? *Acta Crystallogr Sect D Biol Crystallogr* 69(7):1204–1214.
- MOLREP
  - Vagin A, Teplyakov A (1997) *MOLREP* : an Automated Program for Molecular Replacement. *J Appl Crystallogr* 30(6):1022–1025.
- REFMAC5
  - Murshudov GN, Vagin AA, Dodson EJ (1997) Refinement of Macromolecular Structures by the Maximum-Likelihood Method. *Acta Crystallogr Sect D Biol Crystallogr* 53(3):240–255.
- COOT
  - Emsley P, Lohkamp B, Scott WG, Cowtan K (2010) Features and development of Coot. *Acta Crystallogr Sect D Biol Crystallogr* 66(4):486–501.
- PHENIX.REFINE
  - Afonine P V, et al. (2012) Towards automated crystallographic structure refinement with phenix.refine. *Acta Crystallogr D Biol Crystallogr* 68(Pt 4):352–367.