

PEINTS

-MR for ligand screening -

20190923

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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

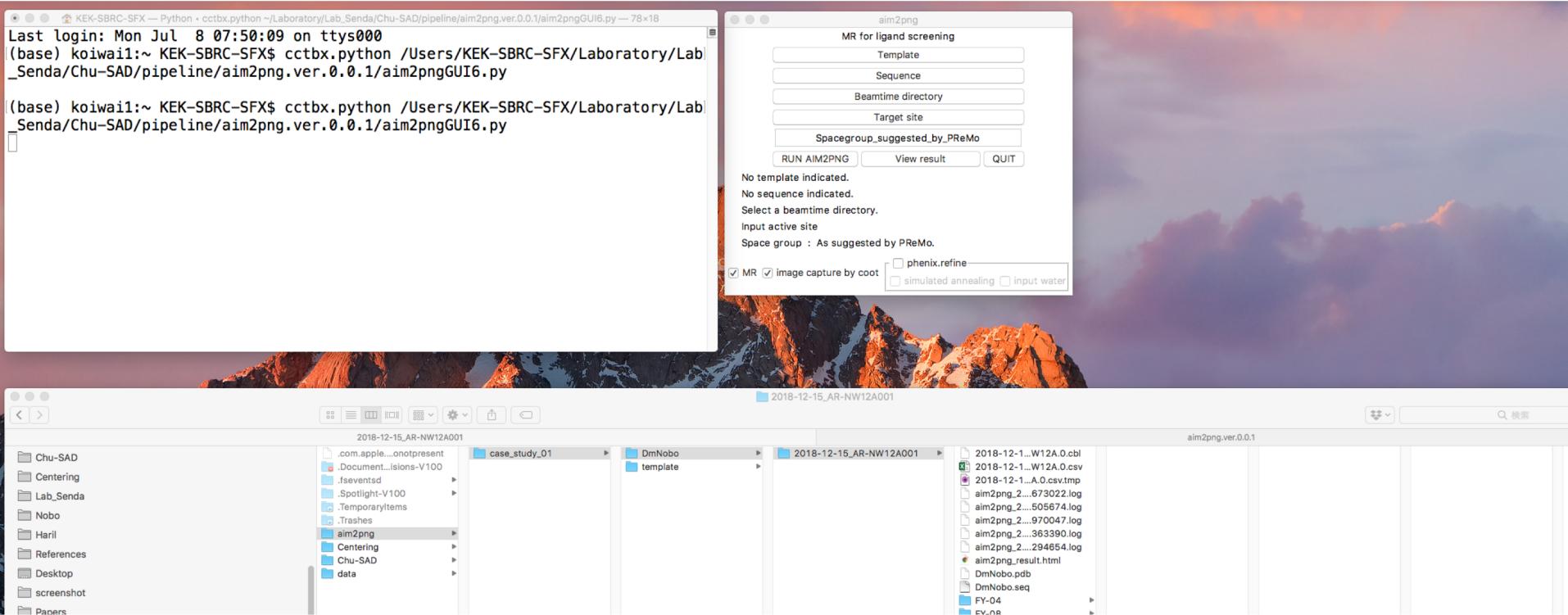
Requirement to use

- 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 pointsGUI6 directly.

How to use -1-

1. peints_gui is run using

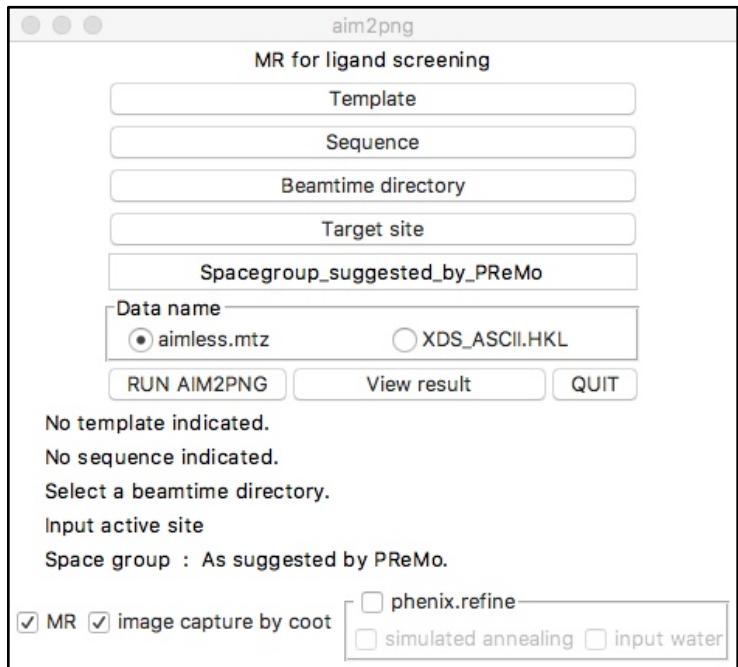
```
$ cctbx.python <peints_directory>/peints_gui.py
```



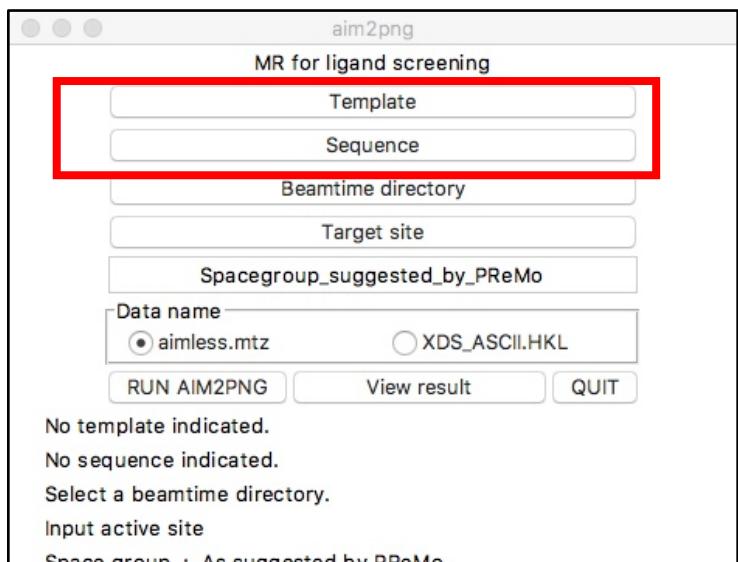
How to use -2-

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

1. GUI window



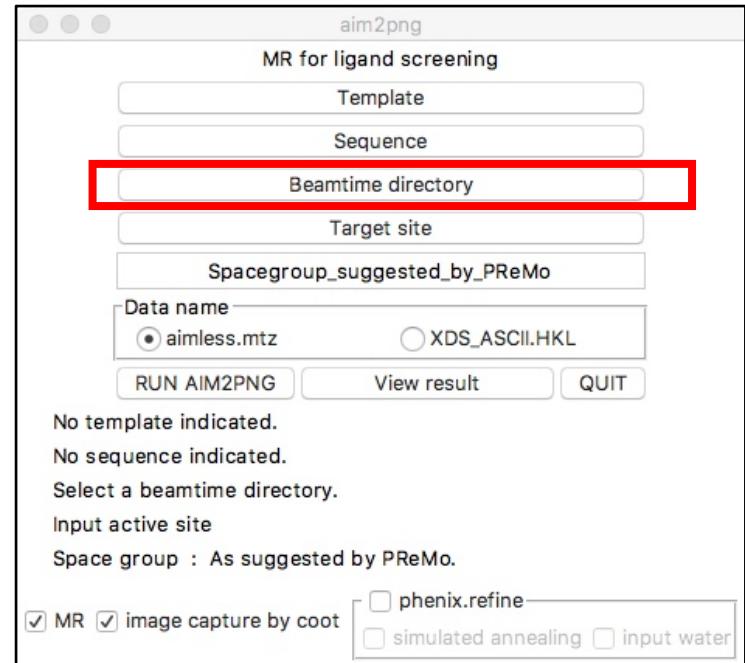
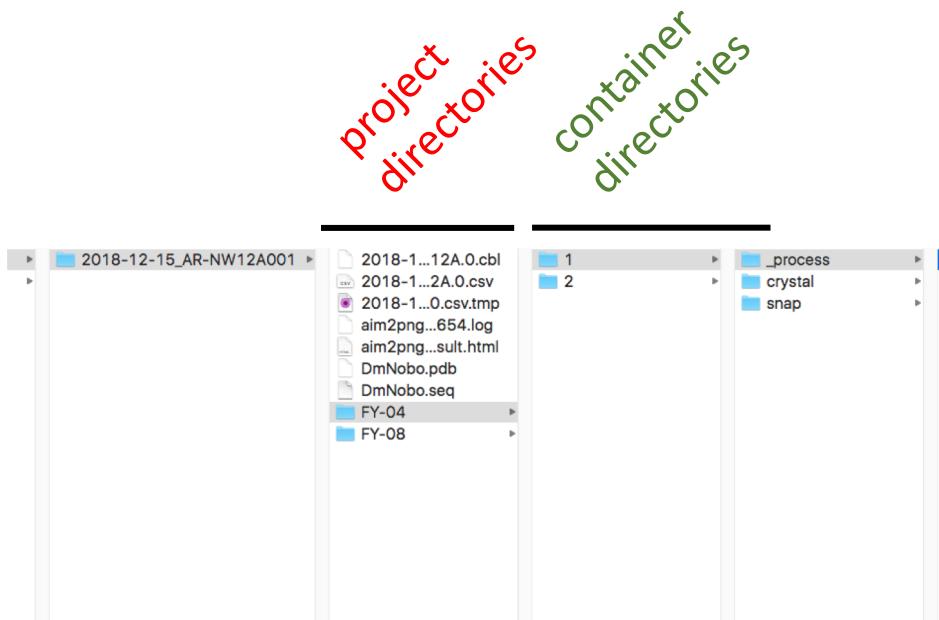
2. Template pdb and sequence are selected.



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

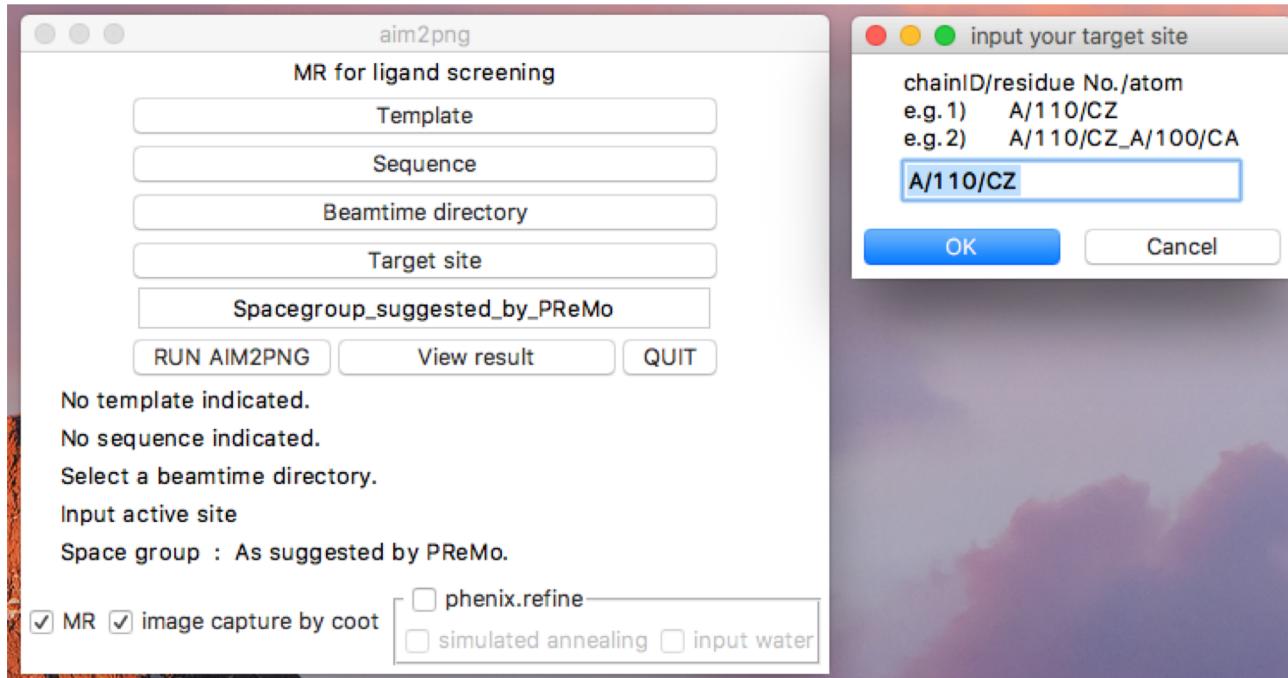
<chainID>/<residue No.>/<atomID>_<chainID>/<residue No.>/<atomID>

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-

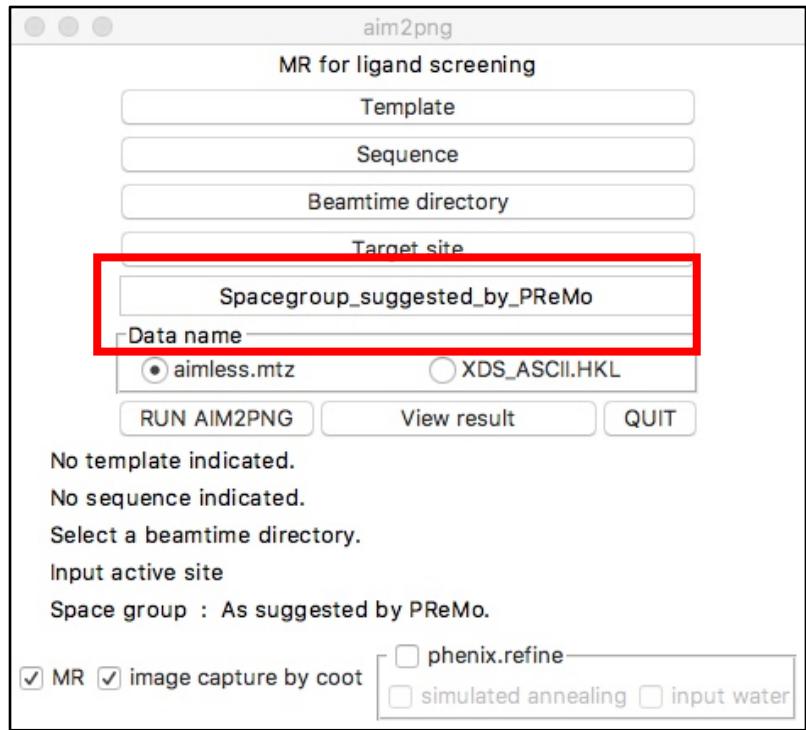
7. Input a spacegroup name.

- 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*

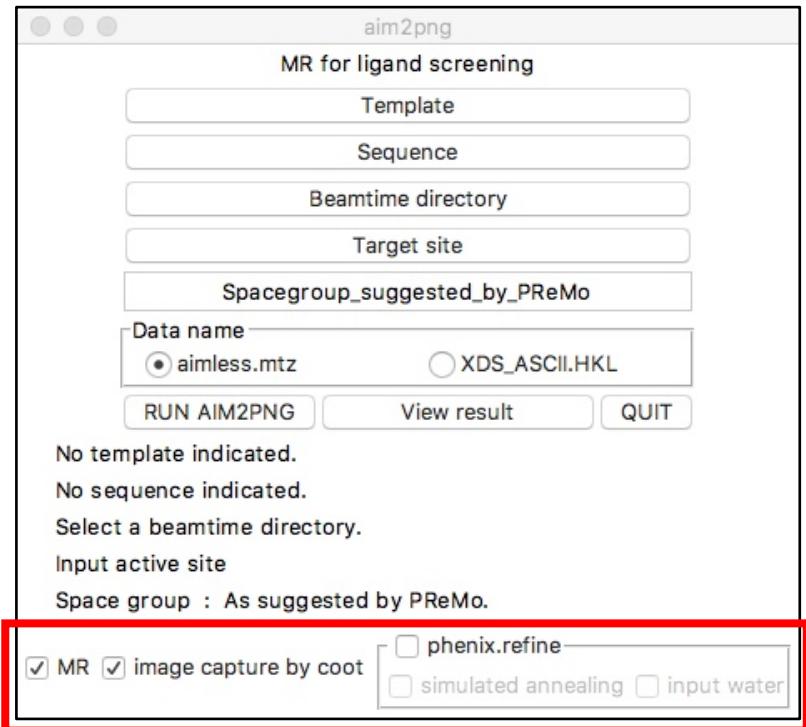
Image capture by coot:

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”



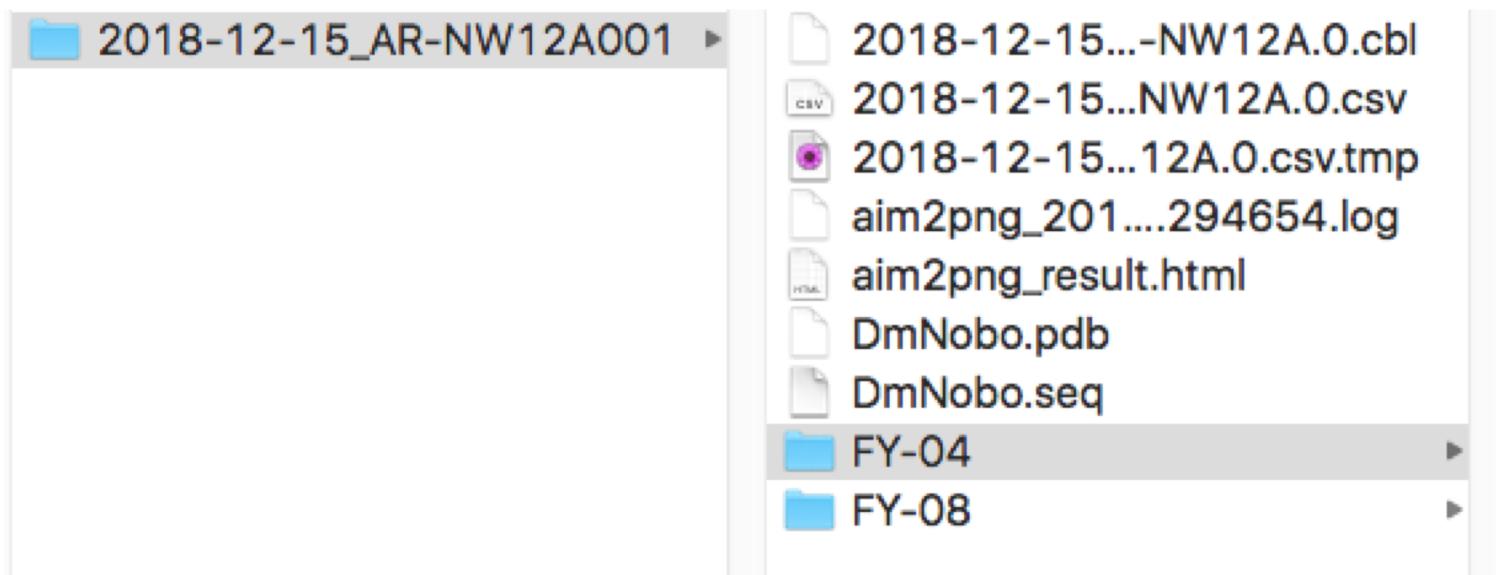
You can cancel peints by [Ctrl] + C on the terminal window.

How to use -7-

10. View your result

Your summarized HTML result is output in project directory as python_split-results2.html.

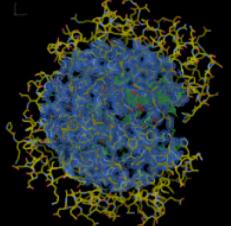
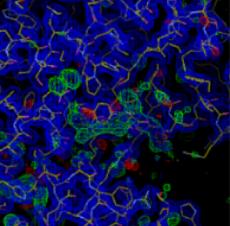
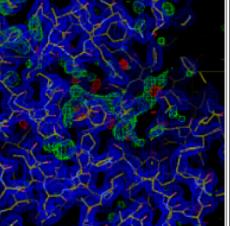
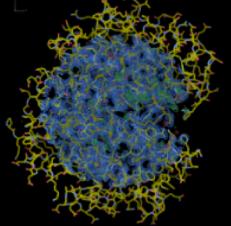
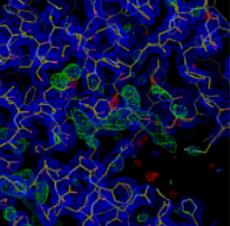
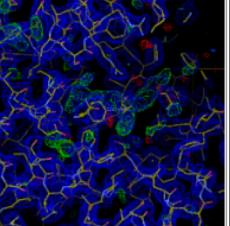
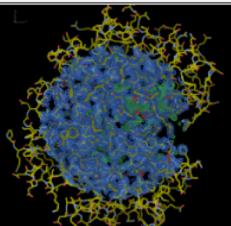
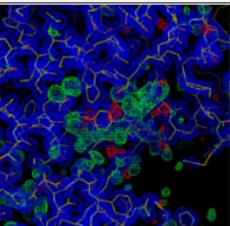
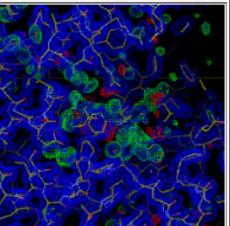
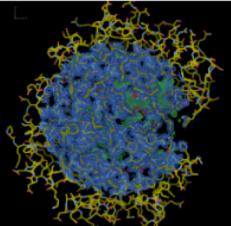
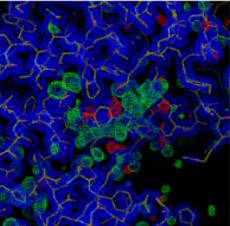
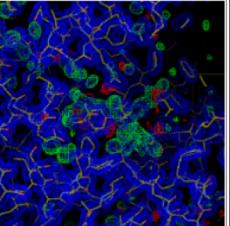
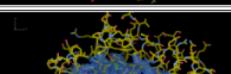
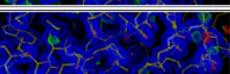
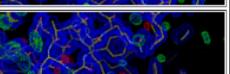
Firefox must be installed.



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