2QVO
2011-03-18

1. Beam center OK, distance OK

2. Index from first image, check predictions on 2-6. They are wrong.
Switch rotation axis direction:
SCAN_ROTATION_AXIS_NAME is Phi
CRYSTAL_GONIO_VECTORS: negate Phi vector

3. Beam mask. Parts of the detector do not get X-rays, especially at the
edges. Mask them out. Seams have problems, but ignore that.

4. Index as P1, integrate, run "dtcell dtprofit.ref" see that spacegroup is
   P4sub2

5. Rescale in P4(2), and select 2.4 as the reso cutoff.

Noticed that the two scans have different crystal orientations.
They seem to have a different goniometer position or
they are different crystals or the crystal was removed and replaced.

One crystal (scan 2) has stronger diffraction than the other. Why?
Exposure time? Radiation damage?

Spacegroup appears to be P4(2).

PDB has resolution of 1.85

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SCRIPTS to do this yourself:

(First edit a_do_all.csh to set the IMAGE_DIR environment variable near the
top of the file. Do the same for b_do_all.csh.)

a+b_do_all.csh runs both
   a_do_all.csh
and
   b_do_all.csh

There are comments in the scripts to help you understand them.

The results from d*TREK are

   a2_dtscale.ref
   b2_dtscale.ref
and
   a+b_dtscale.ref

Example:
   a+b_do_all.csh >&! a+b.log &

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One could do many other things which I may get to later

Jim