Drawing Electron Density Maps with COOT

COOT

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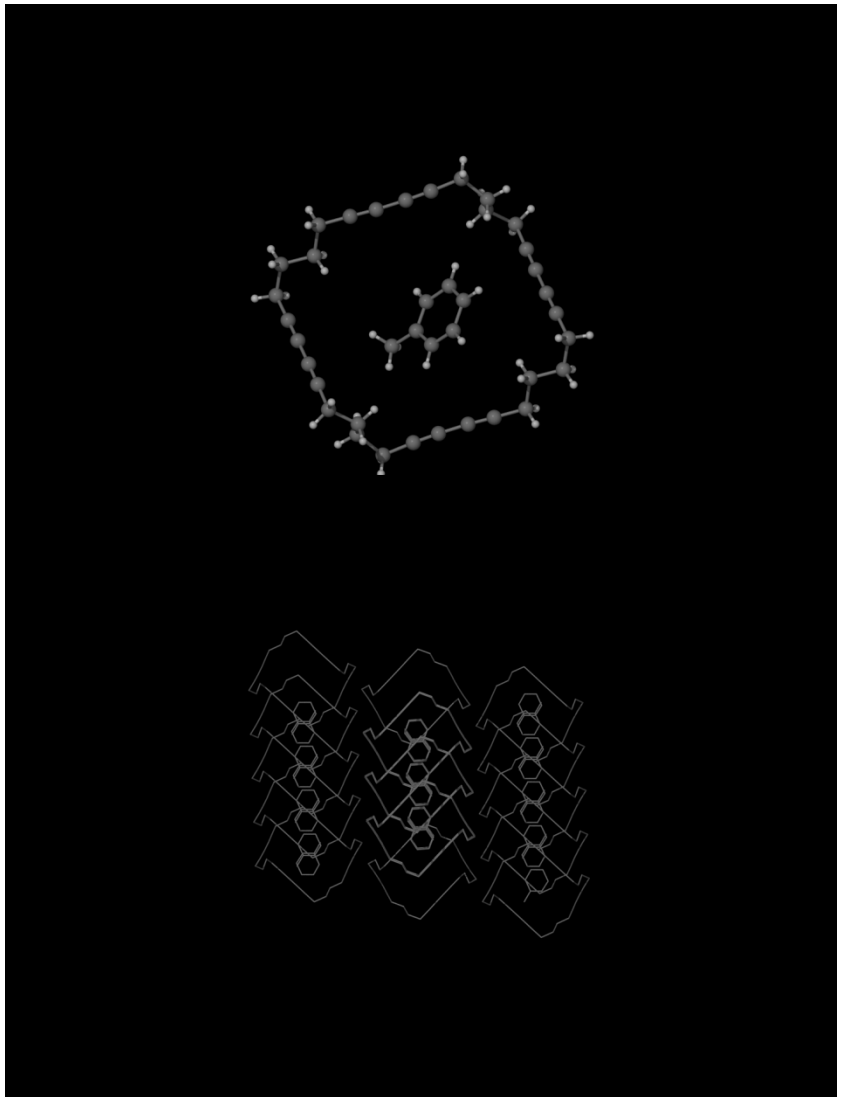
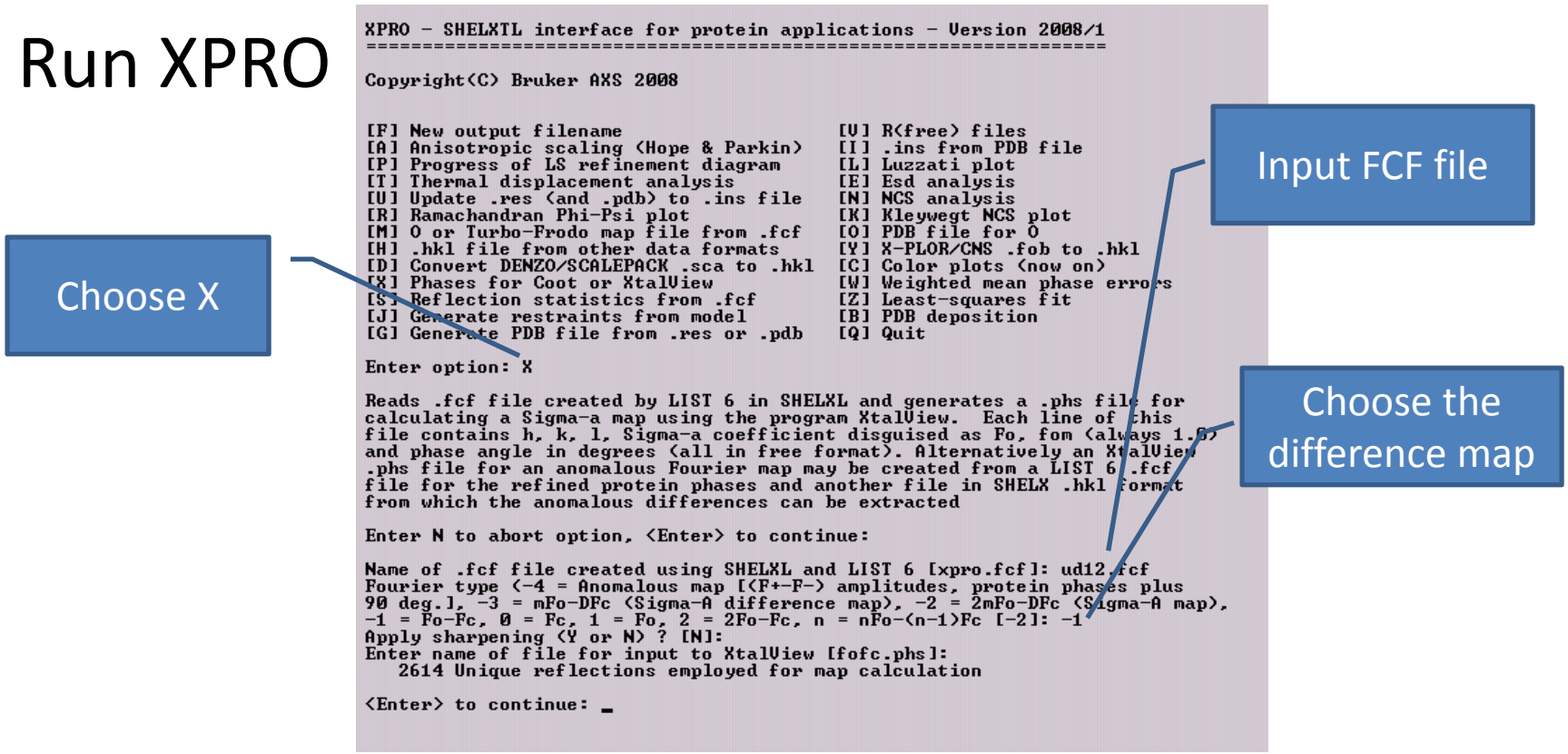
Macrocylic ligand with included solvent

- Problem
  - Disordered Toluene in the macrocyclic ring
  - Draw the electron density in the macocyclic void in order to understand the disorder



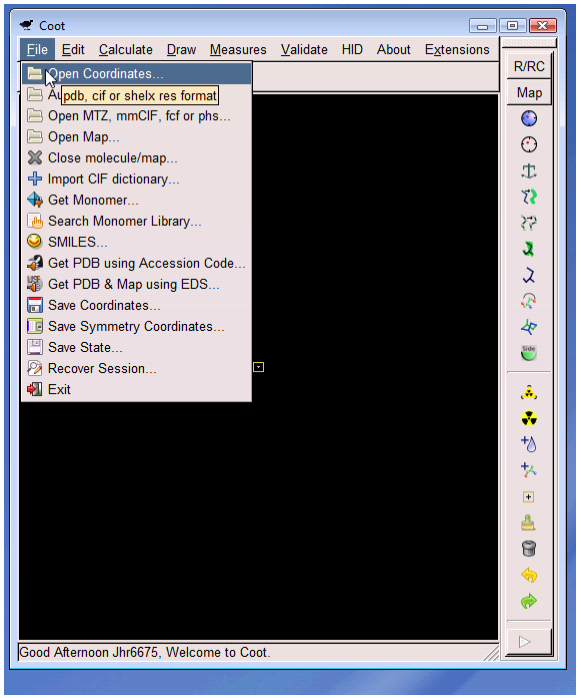
Step one

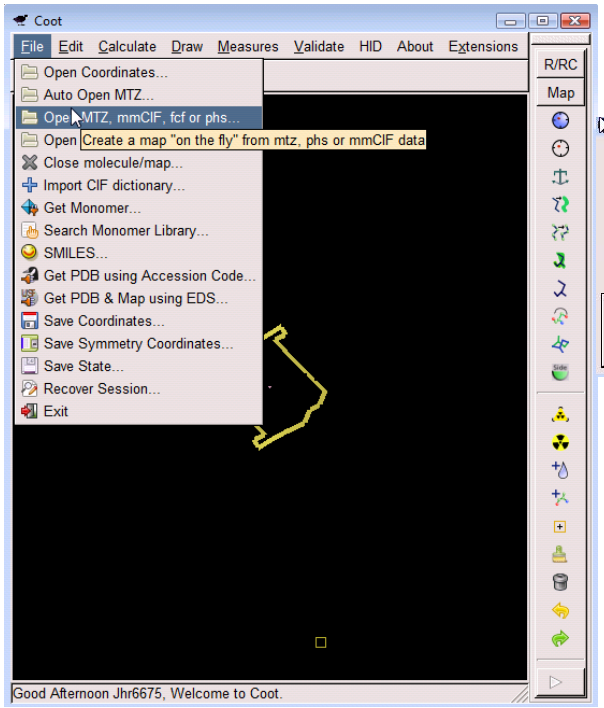
- In the INS file add the LIST 6 command to generate a FCF file (after refinement)
- Run XPRO

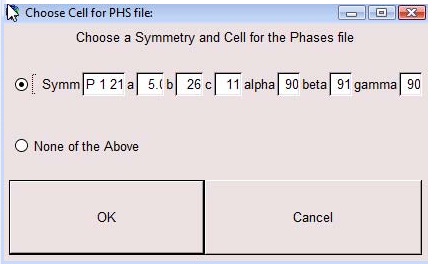


Step 2

- If necessary generate full molecule in XSEED or XP and save as a *.ins or *.pdb file
- Start COOT and read *.ins or *.pdb file
- Read the *.phs file

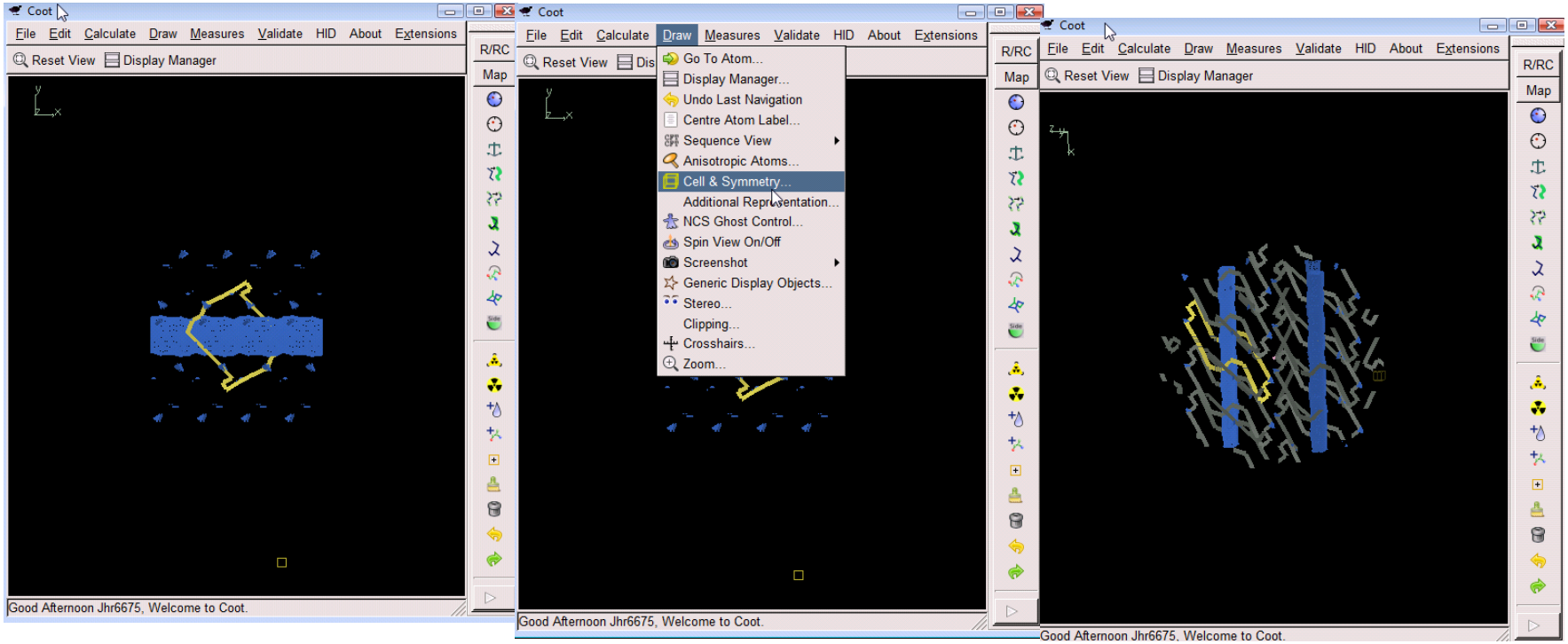






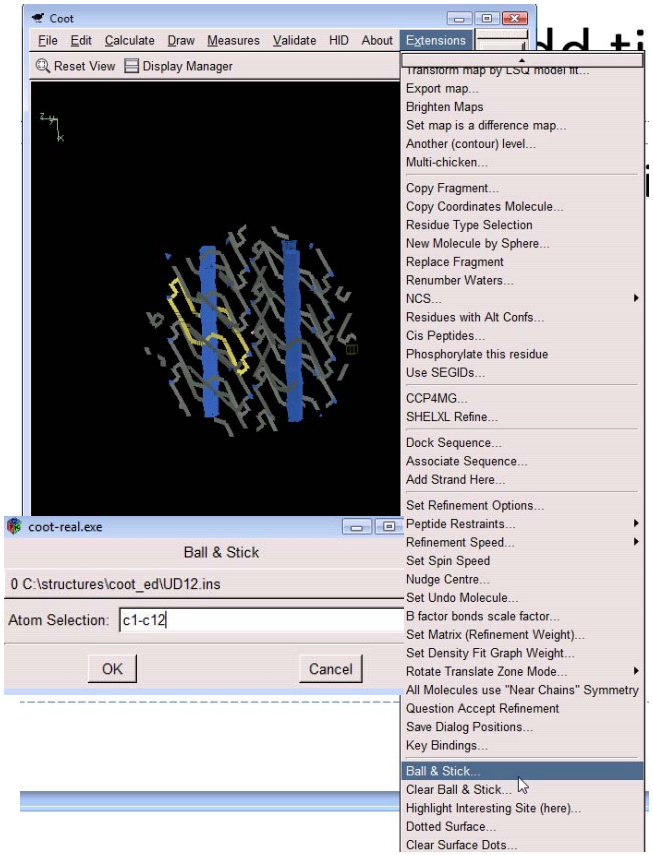
Step 3

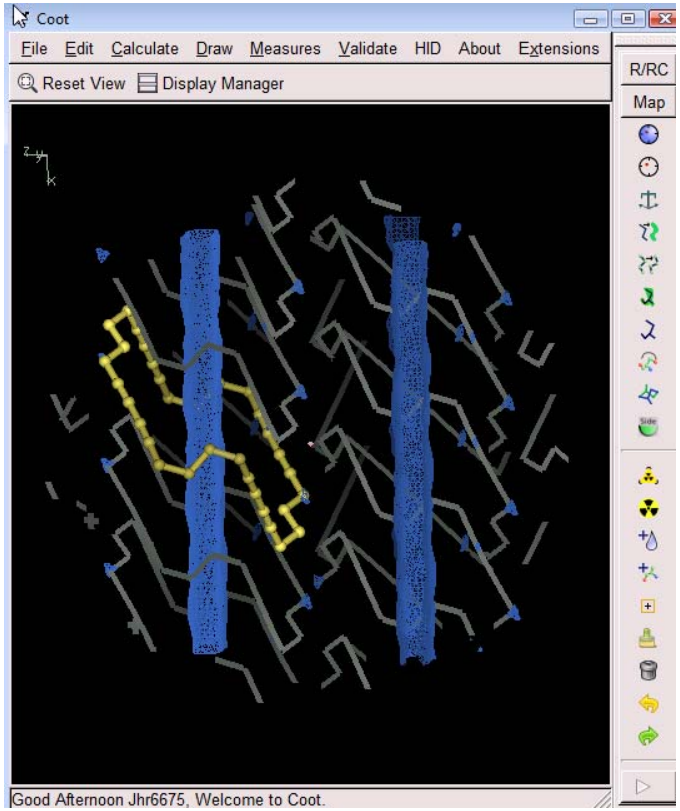
- Basic map has been read and displayed.
- Generate symmetry related molecules
- Rotate view (use shift key to pan)



Step 4

- All ball and stick plot to spice it up

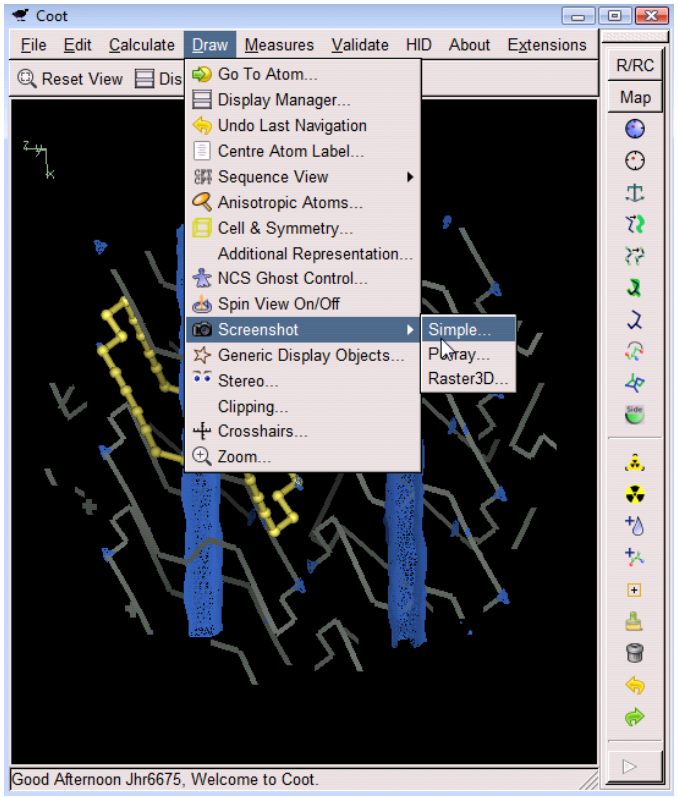


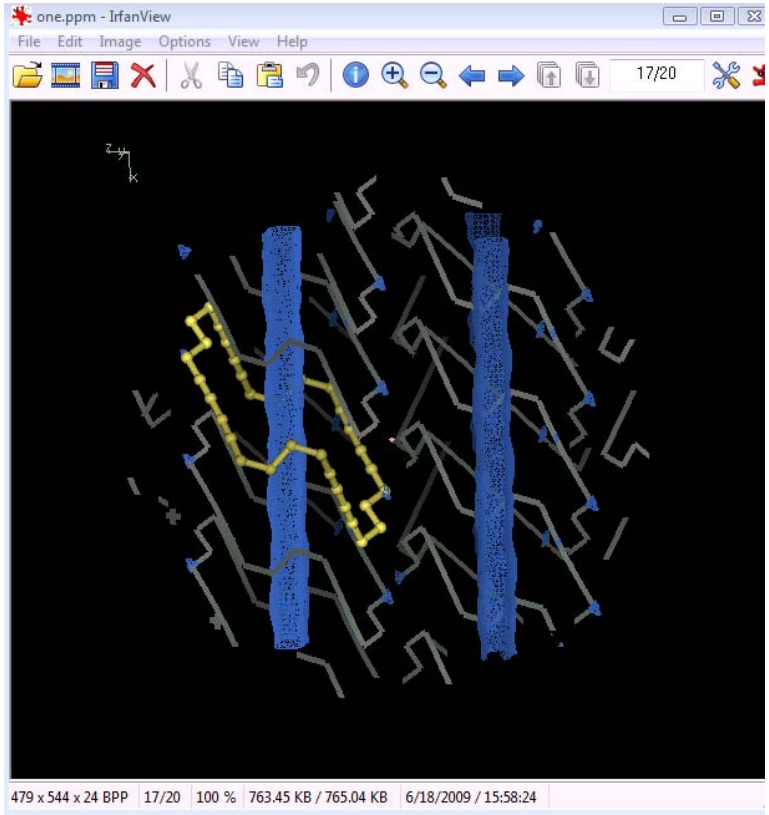


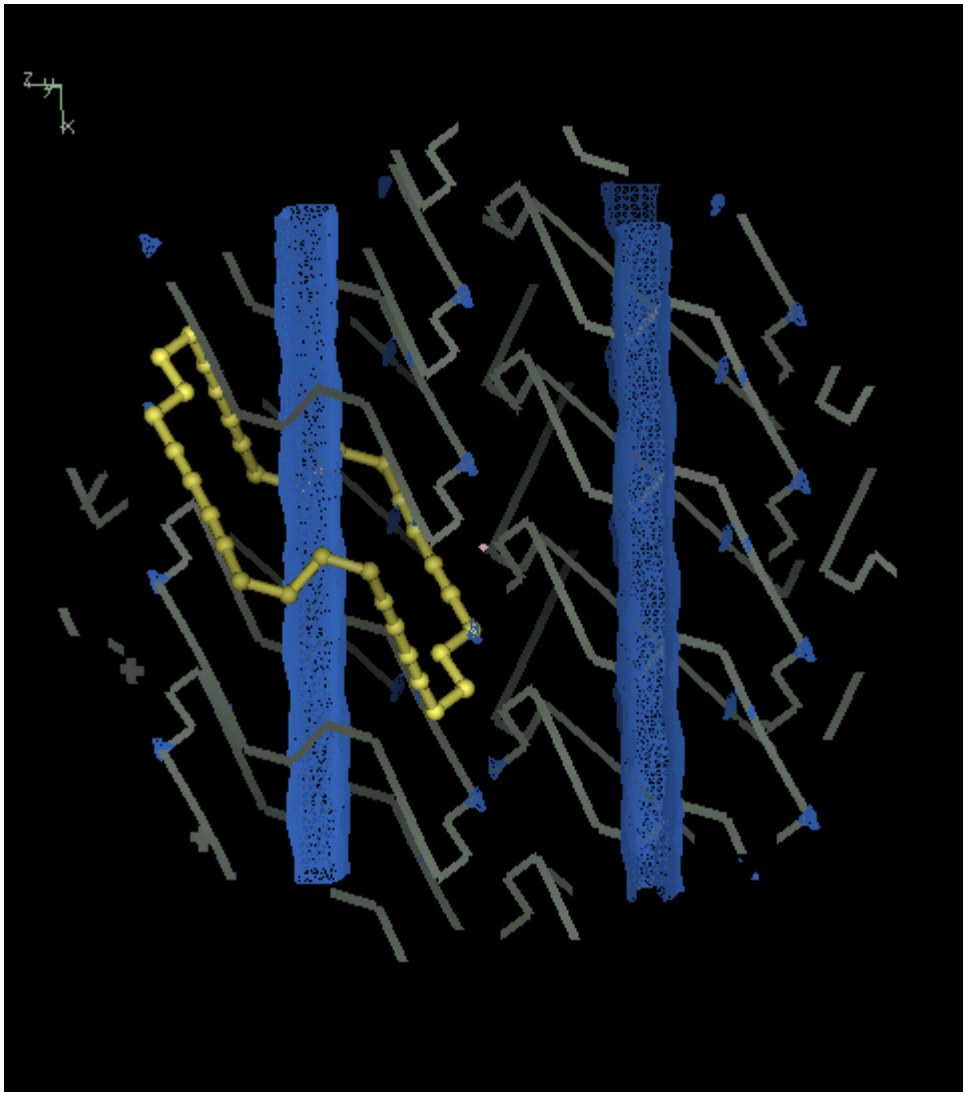
ZOOMED

Step 5

- Save screen shot (simple)
- Use an external program (Irfan) to convert the *.ppm file to a PNG, JPEG etc.






Z
Y
X