

# Drawing Electron Density Maps with COOT

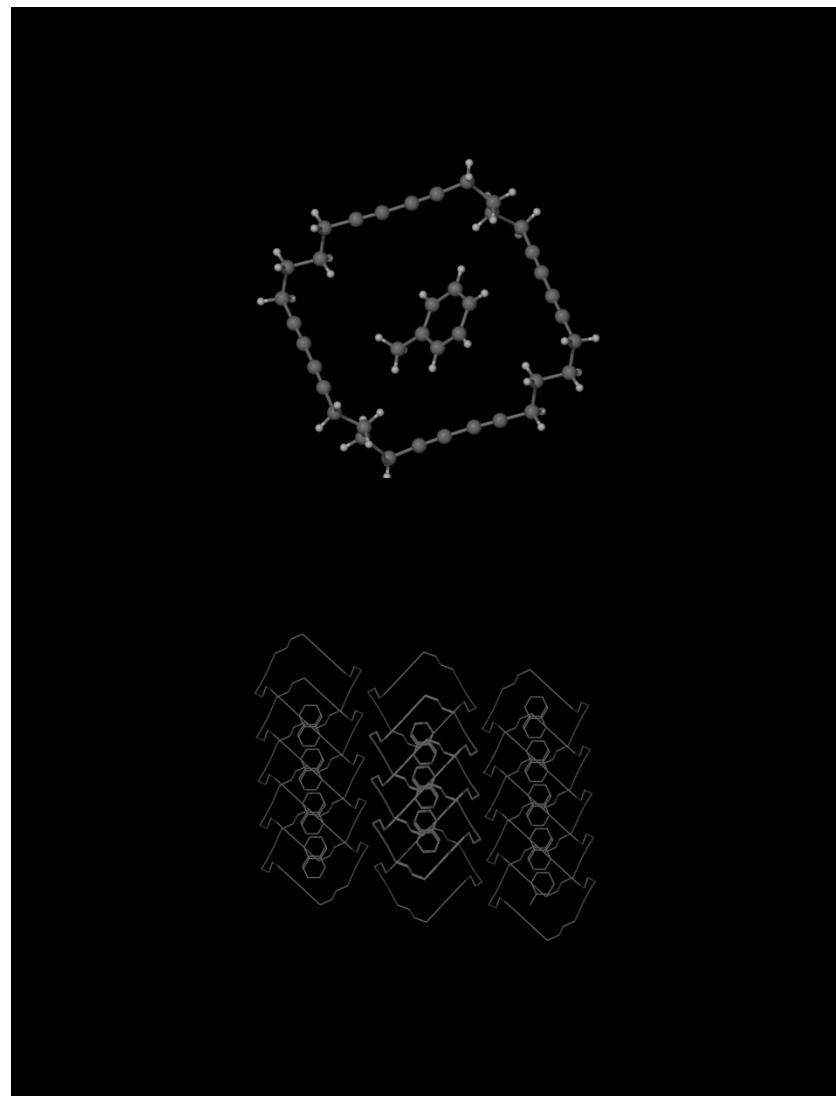
COOT

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# Macrocyclic ligand with included solvent

- Problem
  - Disordered Toluene in the macrocyclic ring
  - Draw the electron density in the macrocyclic 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

```
XPRO - SHELXTL interface for protein applications - Version 2008/1
=====
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```

```
[F] New output filename
[A] Anisotropic scaling (Hope & Parkin)
[P] Progress of LS refinement diagram
[T] Thermal displacement analysis
[U] Update .res (and .pdb) to .ins file
[R] Ramachandran Phi-Psi plot
[M] O or Turbo-Frodo map file from .fcf
[H] .hkl file from other data formats
[D] Convert DENZO/SCALEPACK .sca to .hkl
[X] Phases for Coot or XtalView
[S] Reflection statistics from .fcf
[J] Generate restraints from model
[G] Generate PDB file from .res or .pdb

[U] R(free) files
[I] .ins from PDB file
[L] Luzzati plot
[E] Esd analysis
[N] NCS analysis
[K] Kleywegt NCS plot
[O] PDB file for O
[Y] X-PLOR/CNS .fob to .hkl
[C] Color plots (now on)
[W] Weighted mean phase errors
[Z] Least-squares fit
[B] PDB deposition
[Q] Quit
```

Choose X

Enter option: X

```
Reads .fcf file created by LIST 6 in SHELXL and generates a .phs file for
calculating a Sigma-a map using the program XtalView. Each line of this
file contains h, k, l, Sigma-a coefficient disguised as Fo, fom (always 1.0)
and phase angle in degrees (all in free format). Alternatively an XtalView
.phs file for an anomalous Fourier map may be created from a LIST 6 .fcf
file for the refined protein phases and another file in SHELX .hkl format
from which the anomalous differences can be extracted
```

Enter N to abort option, <Enter> to continue:

```
Name of .fcf file created using SHELXL and LIST 6 [xpro.fcf]: ud12.fcf
Fourier type (-4 = Anomalous map [F+-F-] amplitudes, protein phases plus
90 deg.l, -3 = mFo-DFc (Sigma-A difference map), -2 = 2mFo-DFc (Sigma-A map),
-1 = Fo-Fc, 0 = Fc, 1 = Fo, 2 = 2Fo-Fc, n = nFo-(n-1)Fc [-2]: -1
Apply sharpening (Y or N) ? [N]:
```

```
Enter name of file for input to XtalView [foc.phs]:
2614 Unique reflections employed for map calculation
```

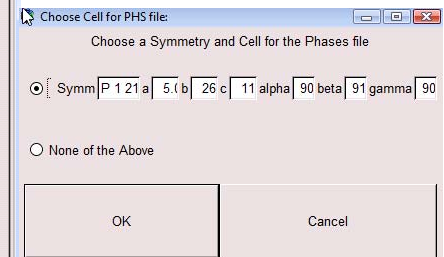
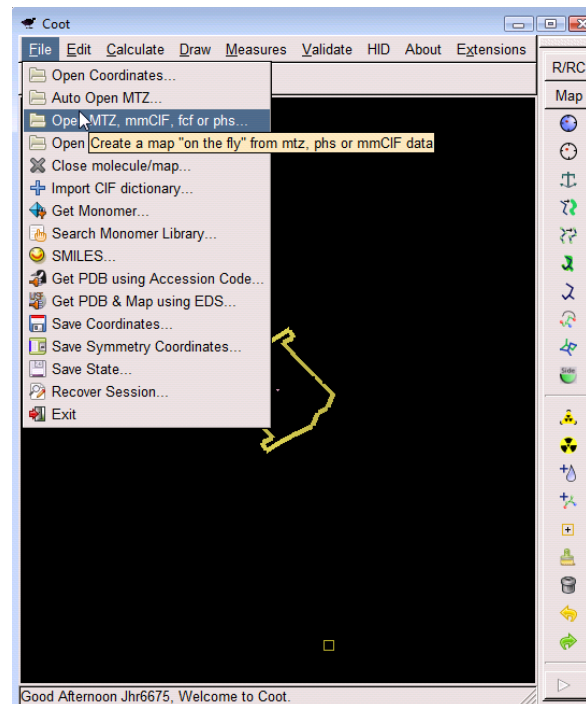
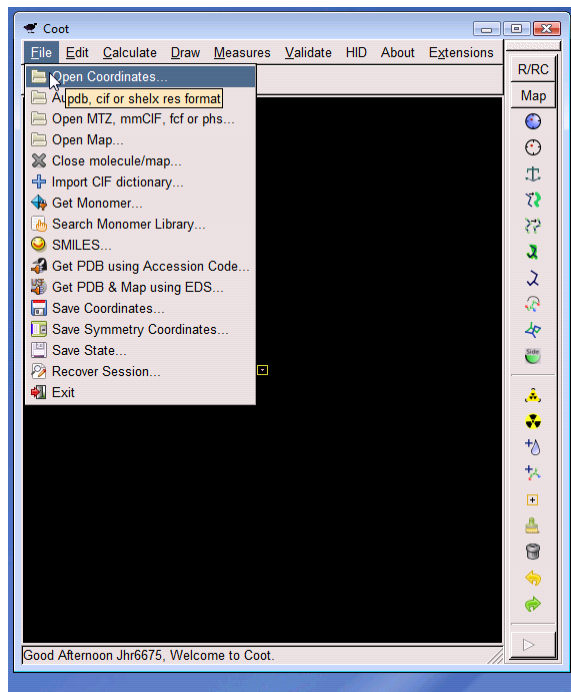
<Enter> to continue: \_

Input FCF file

Choose the  
difference map

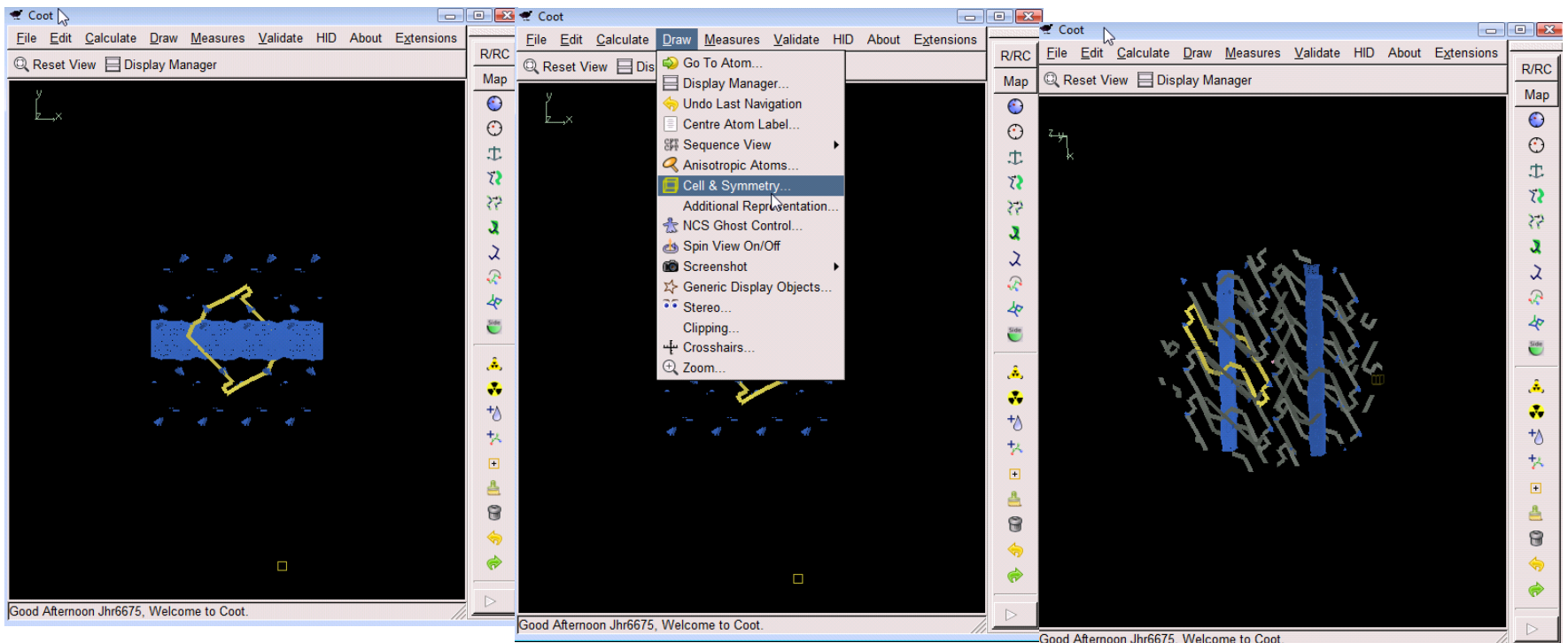
# Step 2

- 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



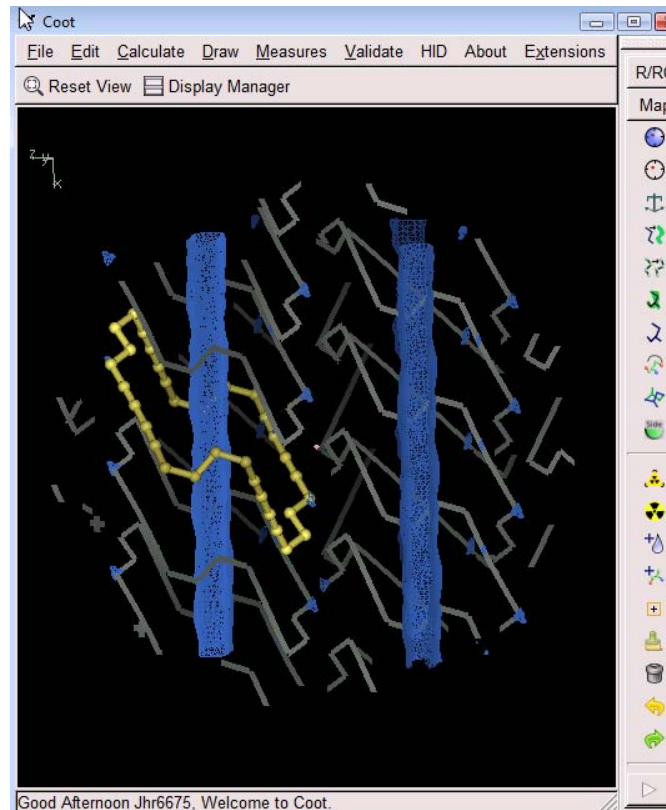
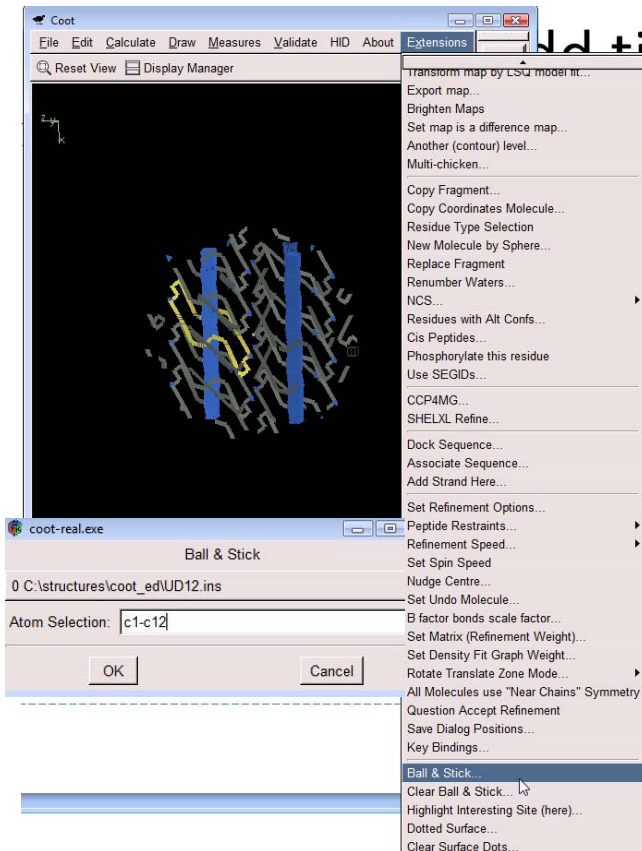
# Step 3

- 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.

