

Drawing Electron Density Maps with COOT

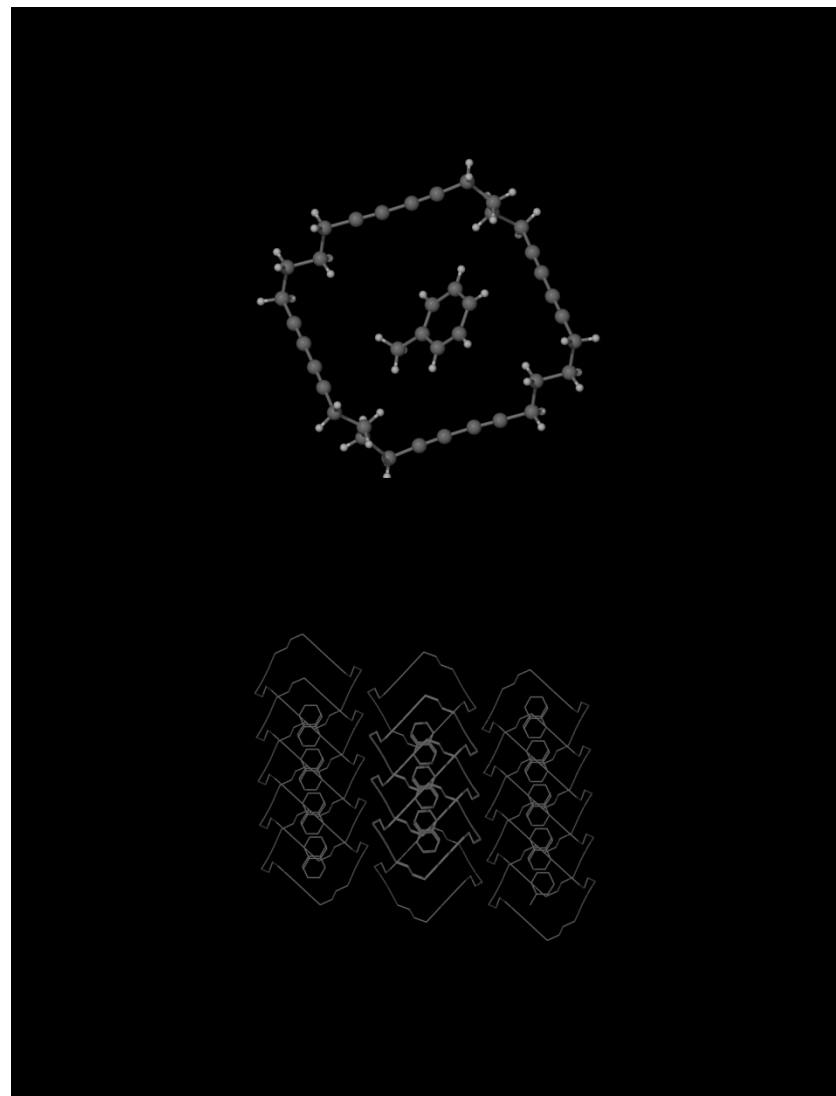
COOT

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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
```

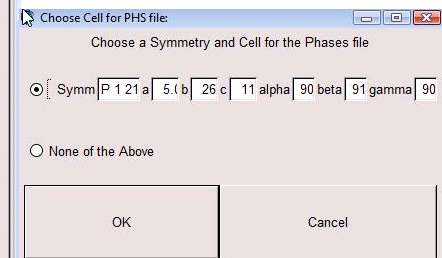
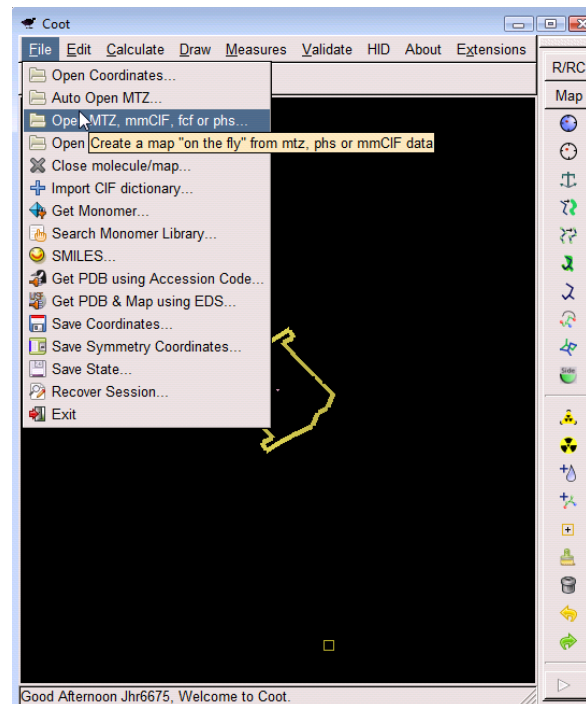
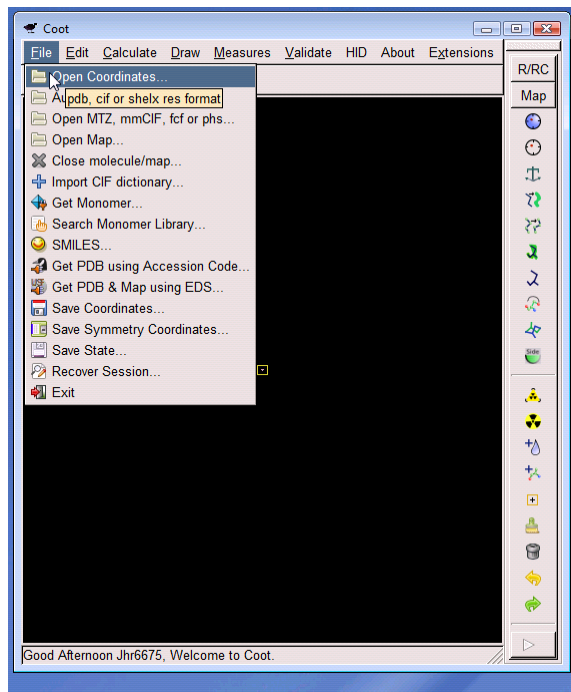
```
<Enter> to continue: _
```

Input FCF file

Choose the
difference map

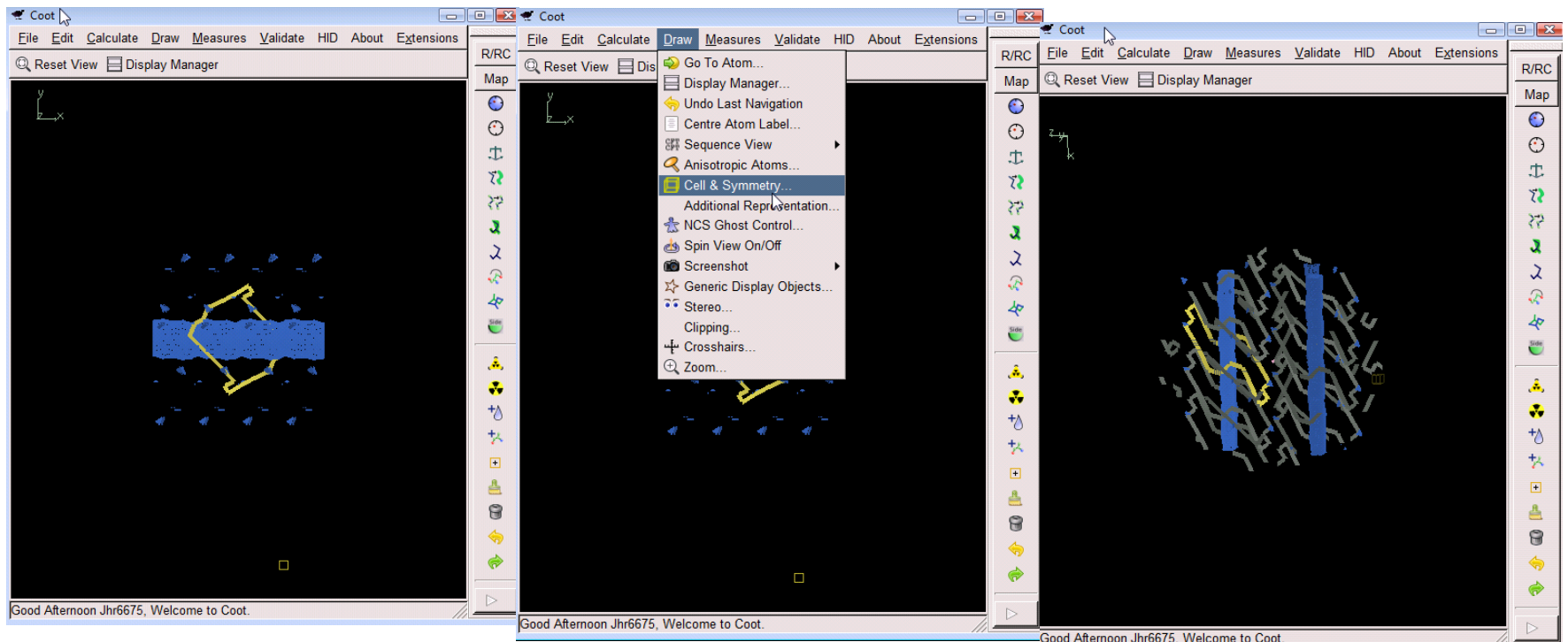
Step 2

- 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



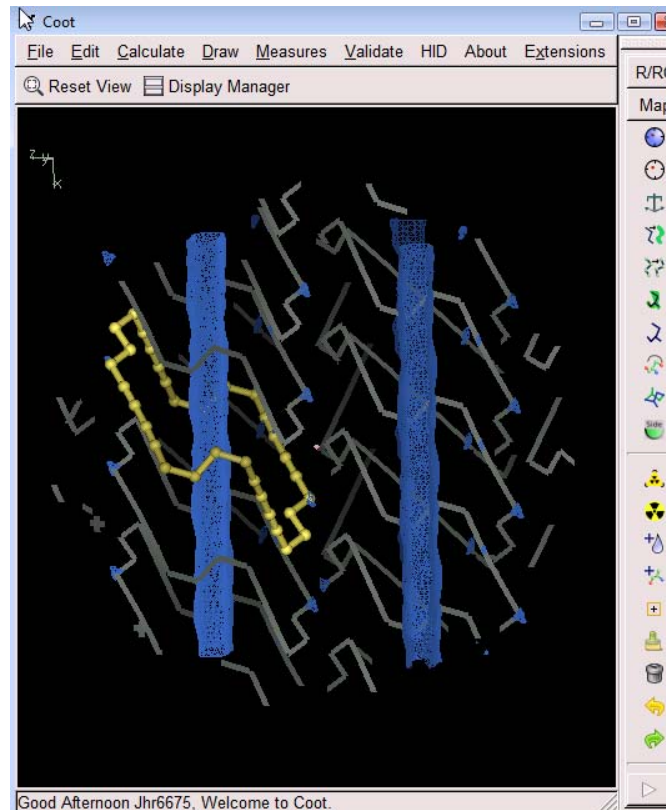
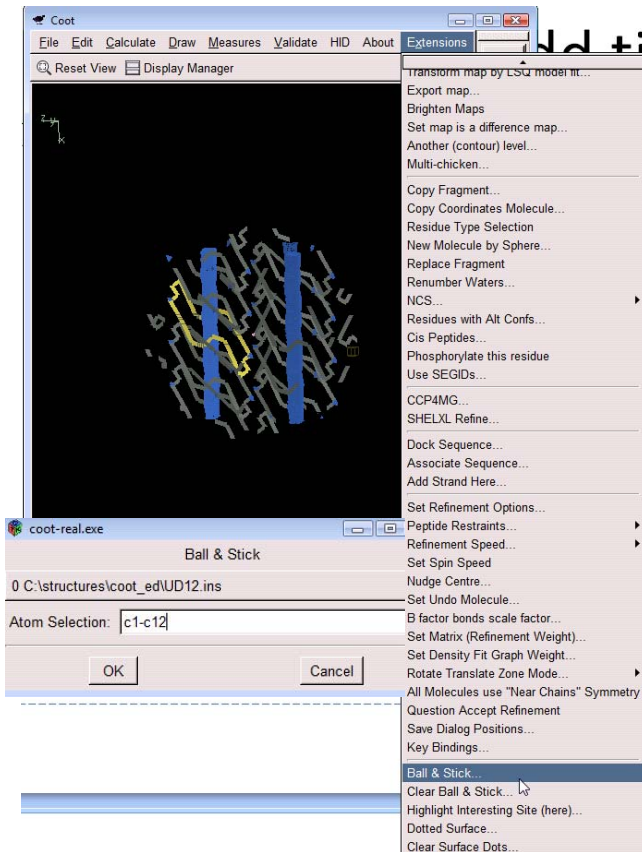
Step 3

- 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.

