CIF's

- CIFs from SHELX
- CIFs from MOLEN
- Working with CIFS
  - ENCIFER
  - PUBLCIF
  - PLATON Validation

CIF from SHEX

- If the command ACTA is included in the SHELX input the program will generate two files.
- One is xl.cif
  - This is a cif with everything SHELX knows
  - It does not know about details of the data collection, structure solution, etc.
- The other is xl.fcf
  - This contains the Fo and Fc data
  - This is not simply .hkl reformated

CIF's from MOLEN

- MOLEN is the old NONIUS software
- Use the local commands endprep or rendprep to go from SHELX to MOLEN
- Program to generate cif is cifgen or rcifgen.
- This program will create a full cif file called ciffile.dat
- This is a full cif ready to go.

Parts of a cif

- Every cif must have a data_name command at the start.
- Name can be either a compound id or global.
- There can only be one global data section and this must be at the start.
- The idea is as follows
  - Global
  - Compound I
  - Compound II
  - etc

To build a Multi-structure CIF

- Use the idfull.cif cif as the first cif part.
- Append the other id.cif's after this.
- Note the global data covers all the compounds included.
- If there is more than one data_global then the cif will fail all format checking and be rejected!

Acta Cryst Submission

- It is possible to submit an entire manuscript in a cif
- In fact this is the only way of submitting to Acta Cryst Journals.
- The Global section will contain the manuscript and other items needed for publication
- Look at a cif.

Bonds and Angles to be published

```
loop_
_geom_angle_atom_site_label_
1
_geom_angle_atom_site_label_
2
_geom_angle_atom_site_label_
3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C4 N3 C2 117.2(3) . . . ?
O91 N9 O92 124.6(3) . . . ?
O91 N9 C9 117.7(3) . . . ?
O92 N9 C9 117.6(3) . . . ?
C2 C1 C10 119.8(3) . . . ?
```

PUBLCIF

- This is a free program that allows you to edit both the cif and the publication data at the same time
- Exists for all operating systems
- Available from the IUCr

ENCIFER

- This is a free cif editor available from the CCDC
- It allows easy changes to the cif.
- It checks the cif format and some basic input
- DOES NOT check for consistency of most numbers
- Also has a display function for molecular graphics

PLATON

- PLATON has the most complete cif checking facility.
- It can be used locally if you have a copy of PLATON or by uploading the cif to the web site http://checkcif.iucr.org/
- To use locally start platon by platon xxx.cif and use the validation function from the menu.