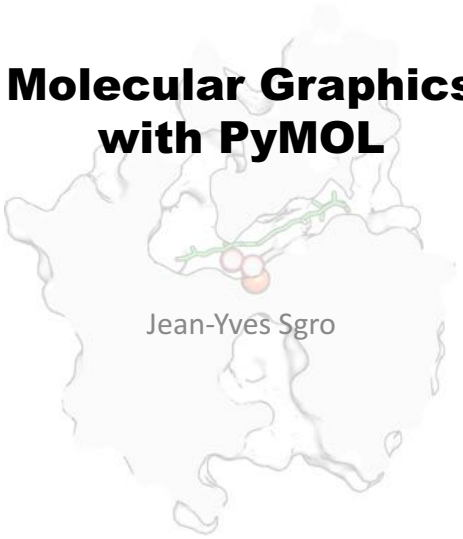
Molecular Graphics with PyMOL



Jean-Yves Sgro

PDB File Format

Plain Text – 80 columns

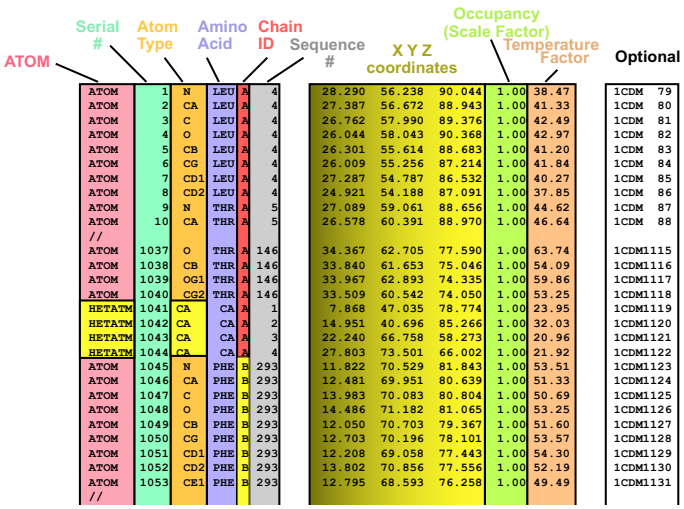
```
1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890
```

Header

3D coordinates

Connectivity
End records

3D Data



PDB files with 2 chains and 2 models

```
1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890
```

Header

MODEL 1
ATOM LINES FOR CHAIN A
TER
ATOM LINES FOR CHAIN B
TER

3D coordinates MODEL 1

ENDMDL

MODEL 2
ATOM LINES FOR CHAIN A
TER
ATOM LINES FOR CHAIN B
TER

3D coordinates MODEL 2

ENDMDL

Connectivity
End records

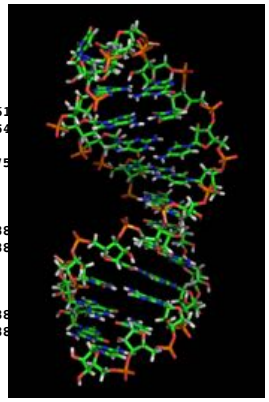
Multiple Models

MODEL & ENDMDL

Record Type

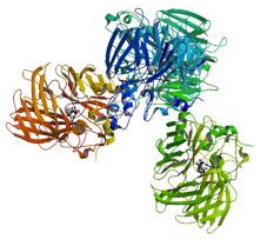
XYZ coordinates

```
MODEL        1
ATOM      1  O5'   G A   1     -11.545 -12.549   4.261
ATOM      2  C5'   G A   1     -12.281 -11.830   5.254
//
ATOM    768  H6    C A  24      -0.402 -19.203   3.575
TER     769        C A  24
ENDMDL
MODEL        2
ATOM      1  O5'   G A   1     -10.937 -10.771   1.038
ATOM      2  C5'   G A   1     -12.150 -10.309   1.638
//
ENDMDL
MODEL        3
ATOM      1  O5'   G A   1     -10.937 -10.771   1.038
ATOM      2  C5'   G A   1     -12.150 -10.309   1.638
//
```

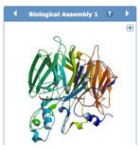


Functional Biological Unit

Example 1: **2biw** APOCAROTENOID CLEAVAGE OXYGENASE



Asymmetric Unit



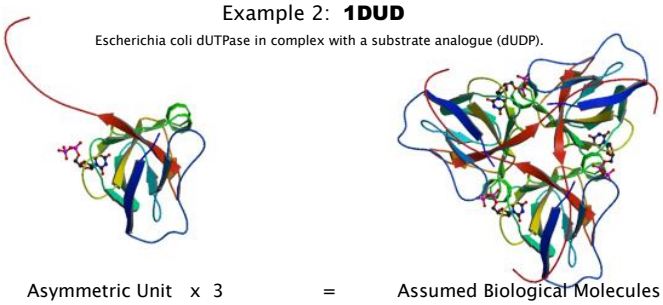
Biological Unit 1 + Biological Unit 2

Biological Unit 3 + Biological Unit 4

Functional Biological Unit

Example 2: **1DUD**

Escherichia coli dUTPase in complex with a substrate analogue (dUDP).



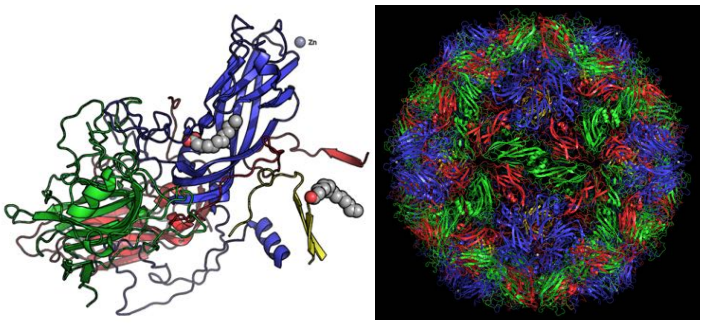
Asymmetric Unit x 3 = Assumed Biological Molecules

```
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   2 -0.500000 -0.866025  0.000000       43.32000
REMARK 350   BIOMT2   2  0.866025 -0.500000  0.000000       75.03244
REMARK 350   BIOMT3   2  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   3 -0.500000  0.866025  0.000000      -43.32000
REMARK 350   BIOMT2   3 -0.866025 -0.500000  0.000000       75.03244
REMARK 350   BIOMT3   3  0.000000  0.000000  1.000000        0.00000
```

Functional Biological Unit

Example 3: **1AYM**

HUMAN RHINOVIRUS 16 COAT PROTEIN AT HIGH RESOLUTION



Asymmetric Unit x 60 = Assumed Biological Molecules

Wizards

Specific functions are handled by calling on wizards

Today we shall visit 2 wizards:

- **Measurement Wizard**
  (to draw a distance line between atoms) and
- **Mutagenesis Wizard**
  (to mutate an amino acid side chain)

Today's menu

- Clipping planes and surfaces (p 79)
- Distances and Labels (p 82) - Wizard
- Extract and modify ligand (p 88)
- Display H-bonds (p 91)
- Electrostatic potential (p 93)
- Side chain mutation (p 98) - Wizard
- Automatic 3D superimposition (p 102)
- Model building (alpha helix; p 106)

Today

- Begin where you left off last week or follow the following suggestions:

PyMol Exercises - start on page - 79-
- end on page - 109-