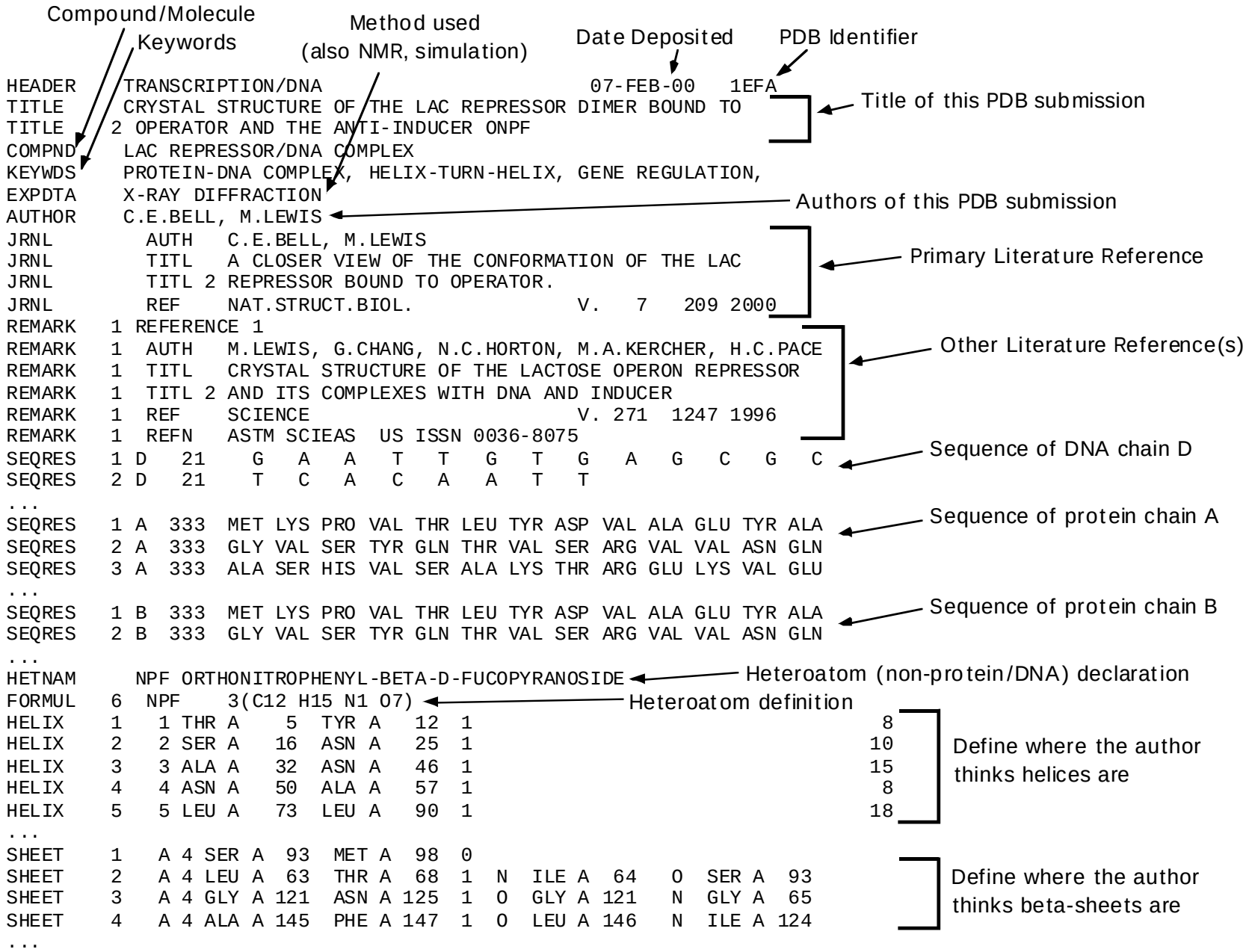
Anatomy of a PDB file



```
CISPEP   1 ILE C  283    PRO C  284          1        -0.51
...
CRYST1  251.438  251.438  204.791  90.00  90.00 120.00 H 3 2        54
ORIGX1      1.000000  0.000000  0.000000        0.00000
...
SCALE1      0.003977  0.002296  0.000000        0.00000
...
ATOM      1  O5*   T D   5      -6.441  91.288 -22.163  1.00136.32           O
ATOM      2  C5*   T D   5      -6.339  92.635 -21.685  1.00136.72           C
...
ATOM     12  N3    T D   5     -11.923  96.235 -21.510  1.00137.53           N
ATOM     13  C4    T D   5     -12.400  95.306 -20.603  1.00137.44           C
...
ATOM     18  P     G D   6      -4.758  96.798 -21.981  1.00137.50           P
ATOM     19  O1P   G D   6      -3.345  96.432 -21.701  1.00137.33           O
...
TER     696        A E  18
ATOM    699  C   LYS A   2       7.988 103.719  -3.783  1.00105.99           C
ATOM    700  O   LYS A   2       8.319 103.402  -4.923  1.00106.22           O
ATOM    701  N   PRO A   3       7.446 102.838  -2.929  1.00106.03           N
ATOM    702  CA  PRO A   3       7.183 101.430  -3.245  1.00106.19           C
ATOM    703  C   PRO A   3       6.592 101.207  -4.633  1.00106.39           C
...
TER    5575       ALA B 331
HETATM 5576  C1  NPF   901     -13.446  87.461  32.376  1.00 58.71           C
HETATM 5577  C2  NPF   901     -12.756  88.680  32.106  1.00 59.04           C
...
HETATM 5616  O   HOH     1       1.628  87.097  33.699  1.00 35.03           O
...
CONECT 5576 5577 5581 5585
CONECT 5577 5576 5578
...
MASTER       30    0    0   36   36    0    0    6 7838    5   40   82
END
```

This molecule has a cis-proline

Crystallographic rotation and scaling matrices

Nucleic acid residue atom coordinates

sugar atoms

base atoms

backbone atoms

Indicates end of a chain

Amino acid residue atom coordinates

(parts of residues 2 and 3 of chain A are shown)

Indicates end of a chain

Heteroatom atom coordinates

Water atom coordinates

Instructions for connecting heteroatom atoms

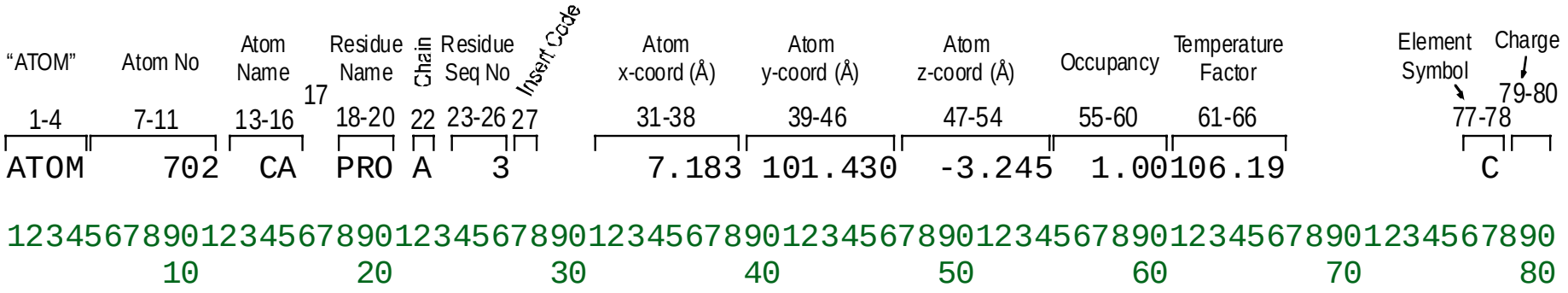
Some wrap-up thing

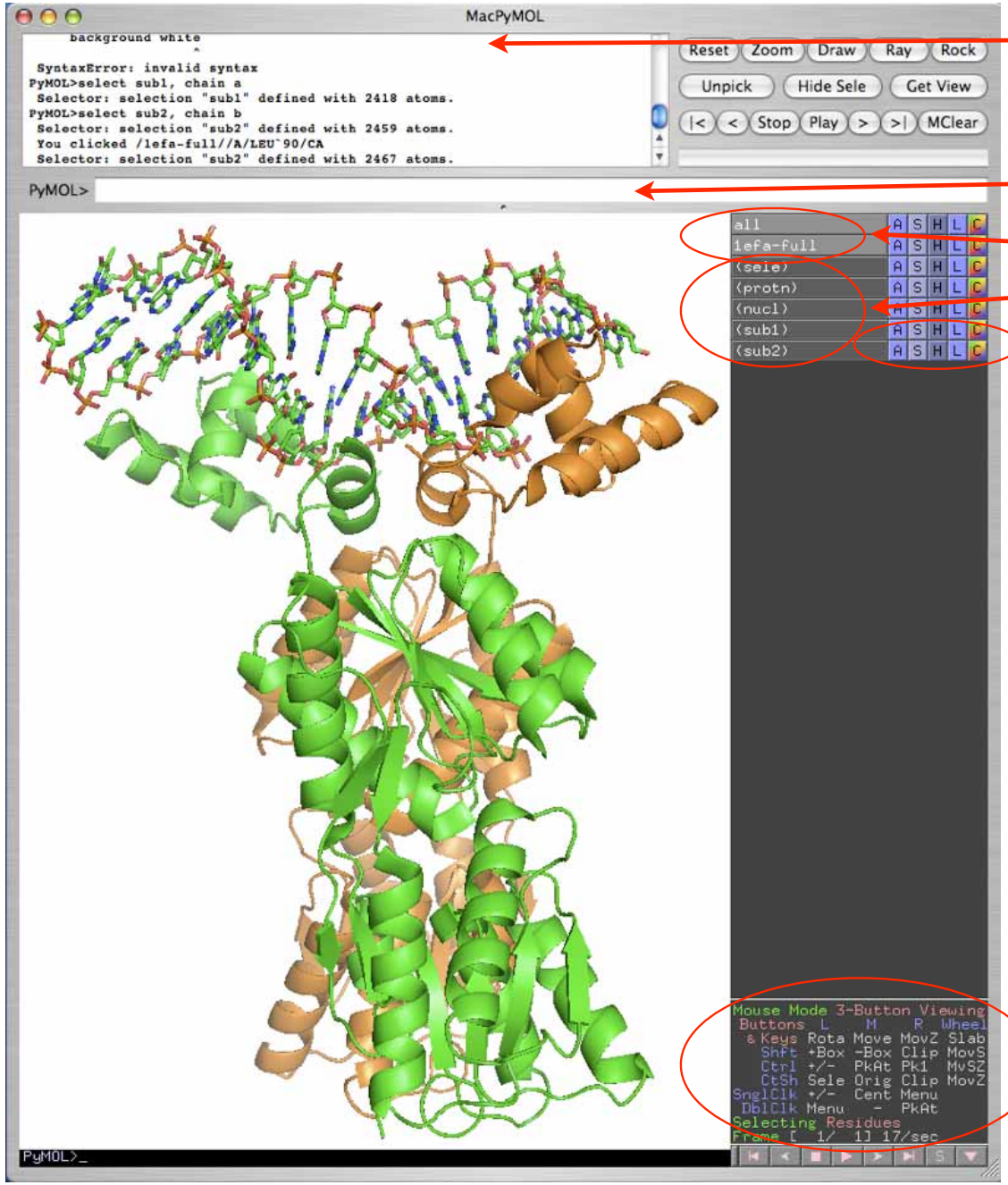
Signals end of the entire file (subsequent lines ignored)

"ATOM"	Atom No	Atom Name	Residue Name	Chain	Residue Seq No	Insert Code	Atom x-coord (Å)	Atom y-coord (Å)	Atom z-coord (Å)	Occupancy	Temperature Factor	Element Symbol	Charge
1-4	7-11	13-16	18-20	22	23-26	27	31-38	39-46	47-54	55-60	61-66	77-78	79-80
ATOM	702	CA	PRO	A	3		7.183	101.430	-3.245	1.00	106.19	C	

```
1234567890123456789012345678901234567890123456789012345678901234567890
        10        20        30        40        50        60        70        80
```

Official Coordinate File Format





Messages show up here
(press <esc> to see more)

Enter your commands here

Objects (not in parenthesis)

Selections (in parenthesis)

Actions (applied to object/selection):

- A: Misc actions
- S: Show
- H: Hide
- L: Label
- C: Color

Mousing reminders

PyMol