ATOMTV:
Protein Data Bank Atomic Coordinate Viewer

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The Protein Data Bank (PDB)

- "An archive of experimentally determined three-dimensional structures of biological macromolecules that serves a global community of researchers, educators, and students."

"Protein Data Bank Contents Guide, Atomic Coordinate Entry Format Description Version 3.2, Document Published by the wwPDB. See www.wwpdb.org"
Records

- Header
- Title
- ATOM
Provides information about molecule such as short title, date uploaded to data bank and id number.
The ATOM records present the atomic coordinates for standard amino acids and nucleotides.
**ATOM Record Format**

- **Record Format**

<table>
<thead>
<tr>
<th>COLUMNS</th>
<th>DATA TYPE</th>
<th>FIELD</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 6</td>
<td>Record name</td>
<td>&quot;ATOM &quot;</td>
<td></td>
</tr>
<tr>
<td>7 - 11</td>
<td>Integer</td>
<td>serial</td>
<td>Atom serial number.</td>
</tr>
<tr>
<td>13 – 16</td>
<td>Atom</td>
<td>name</td>
<td>Atom name.</td>
</tr>
<tr>
<td>17</td>
<td>Character</td>
<td>altLoc</td>
<td>Alternate location indicator.</td>
</tr>
<tr>
<td>18 – 20</td>
<td>Residue name</td>
<td>resName</td>
<td>Residue name.</td>
</tr>
<tr>
<td>22</td>
<td>Character</td>
<td>chainID</td>
<td>Chain identifier.</td>
</tr>
<tr>
<td>23 – 26</td>
<td>Integer</td>
<td>resSeq</td>
<td>Residue sequence number.</td>
</tr>
<tr>
<td>27</td>
<td>AChar</td>
<td>iCode</td>
<td>Code for insertion of residues.</td>
</tr>
<tr>
<td>31 – 38</td>
<td>Real(8.3)</td>
<td>x</td>
<td>Orthogonal coordinates for X in Angstroms.</td>
</tr>
<tr>
<td>39 – 46</td>
<td>Real(8.3)</td>
<td>y</td>
<td>Orthogonal coordinates for Y in Angstroms.</td>
</tr>
<tr>
<td>47 – 54</td>
<td>Real(8.3)</td>
<td>z</td>
<td>Orthogonal coordinates for Z in Angstroms.</td>
</tr>
<tr>
<td>55 – 60</td>
<td>Real(6.2)</td>
<td>occupancy</td>
<td>Occupancy.</td>
</tr>
<tr>
<td>61 – 66</td>
<td>Real(6.2)</td>
<td>tempFactor</td>
<td>Temperature factor.</td>
</tr>
<tr>
<td>77 – 78</td>
<td>LString(2)</td>
<td>element</td>
<td>Element symbol, right-justified.</td>
</tr>
<tr>
<td>79 – 80</td>
<td>LString(2)</td>
<td>charge</td>
<td>Charge on the atom.</td>
</tr>
</tbody>
</table>
main(){
  drawDisk
  createDisk
  DiskFilters
  writePPM
  initPGMCanvasbuf
}
main(){

Animate::animateIT

Animate::Read

x_Rotate::
x_Rotate

y_Rotate::
y_Rotate

Animate::getDiskFile

Animate::getIncrementofRotations

Animate::x_RotationCalculations

Animate::y_RotationCalculations

Animate::x_RotationCalculations

Animate::x_RotationCalculations

Animate::getAxisOfRotation

Animate::Write

Animate::getAxisOfRotation

Animate::getIncrementofRotations
## Animate::x_RotationCalculations

### Rotation Matrix

<table>
<thead>
<tr>
<th></th>
<th>Rx</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>cos</td>
<td>-sin</td>
<td>y</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>sin</td>
<td>-cos</td>
<td>z</td>
<td></td>
</tr>
</tbody>
</table>

### Code

- $y = y \cdot \cos - z \cdot \sin$
- $z = y \cdot \sin + z \cdot \cos$

### Rotation Matrix

<table>
<thead>
<tr>
<th></th>
<th>Ry</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>cos</td>
<td>0</td>
<td>sin</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>y</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-sin</td>
<td>0</td>
<td>-cos</td>
<td>z</td>
<td></td>
</tr>
</tbody>
</table>

### Code

- $x = x \cdot \cos + z \cdot \sin$
- $z = -x \cdot \sin + z \cdot \cos$
fetch[LOC|PDB].csh

- Awk
  - Preprocessing of
    - Title
    - Header
    - Disk Description file records
      - "disk \{x xv y yv z zv size ele ele filter quad operation over\}\", size, color
      - "disk \{x xv y yv z zv size sv ele filter quad operation over \}\", color
      - "disk \{x xv y yv z zv size sv r rv g gv b bv filter quad operation over \}\"
  - Legend
AWK Preprocessing

**Awk**

- **Disk Description file records (size and radii)**
  - cat $repos_Dir"_Sorted" | awk '{printf "disk {x %.3f y %.3f z %.3f size %s %s filter quad operation over}\n", $1,$2,$3,$4,$4 }' > $repos_Dir"_tmpdF"
  - awk 'NR == FNR {a[$1] = "r "$3 " g "$4 " b "$5; next} {$10 = a[$10]1' $misc_Dir"elementColors.txt"
  - $repos_Dir"_tmpdF" > $repos_Dir"_diskFileTmp"
  - awk 'NR == FNR {b[$1] = $6; next} {$9 = b[$9]1' $misc_Dir"elementColors.txt" $repos_Dir"_diskFileTmp" > $repos_Dir"_diskFile"

- **Legend**
  - #Make a legend by eliminating duplicate element names from $repos_Dir"_tmpdF"
    #Based on last field. http://unstableme.blogspot.com/2008/03/remove-duplicates-based-on-fields-awk.html
    
    awk '!
x[$10]++ {printf "%s\n",$10}' $repos_Dir"_tmpdF" > $repos_Dir"_NoDup"
  - #Make color each element for legend
    
    awk 'NR == FNR {a[$1] = "#"$2 " $1 " ; next} {$1 = a[$1]1' $misc_Dir"elementColors.txt"
    $repos_Dir"_NoDup" > $repos_Dir"_Legend"
SW Design Summary

- **PHP**
  - Driver – Makes execute call to C, C++, AWK, Imagemagick

- **C++**
  - X, Y Rotations

- **C**
  - Draws disk using disk description file

- **AWK, csh**
  - Preprocessing
  - Disk description files, heading, legend, sorts
  - Uses associative array for elements’ colors and sizes

- **Imagemagick**
  - Sizes Image, convert ppms to animated gif of X, Y rotations

- **JavaScript, HTML**
  - Client Presentation
## Protein Data Banks

<table>
<thead>
<tr>
<th>URL</th>
<th>PDB</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Viewing Mode**

- **Gif**  
- **Video**
Going LIVE!

Atomic Coordinate Viewer