

ATOMTV:

Protein Data Bank Atomic Coordinate Viewer

E. Anthony T. Allen

University of Tennessee
Knoxville

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

Header, Title

- Provides information about molecule such as short title, date uploaded to data bank and id number.

ATOM

- The ATOM records present the atomic coordinates for standard amino acids and nucleotides.

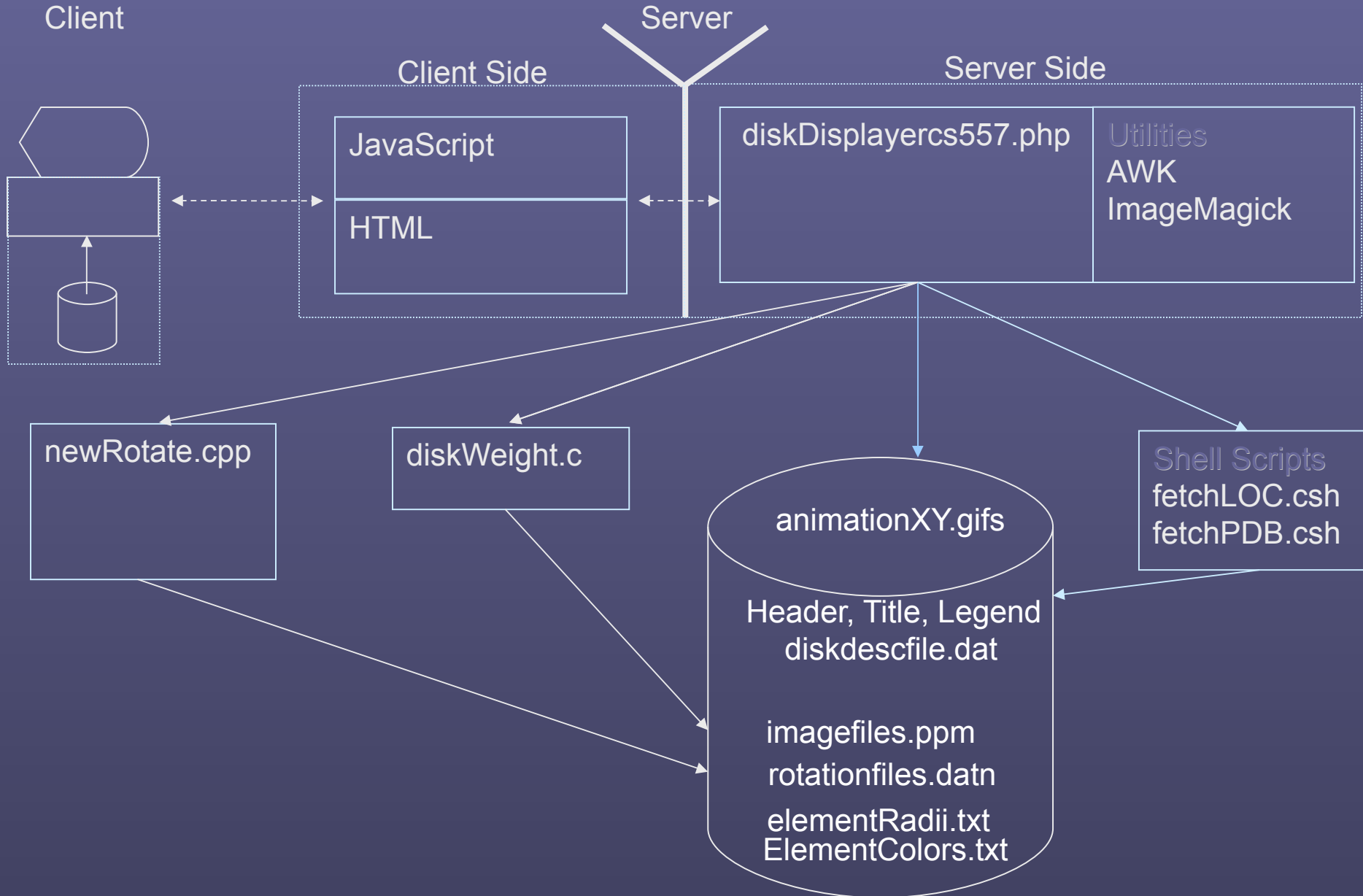
ATOM Record Format

- Record Format

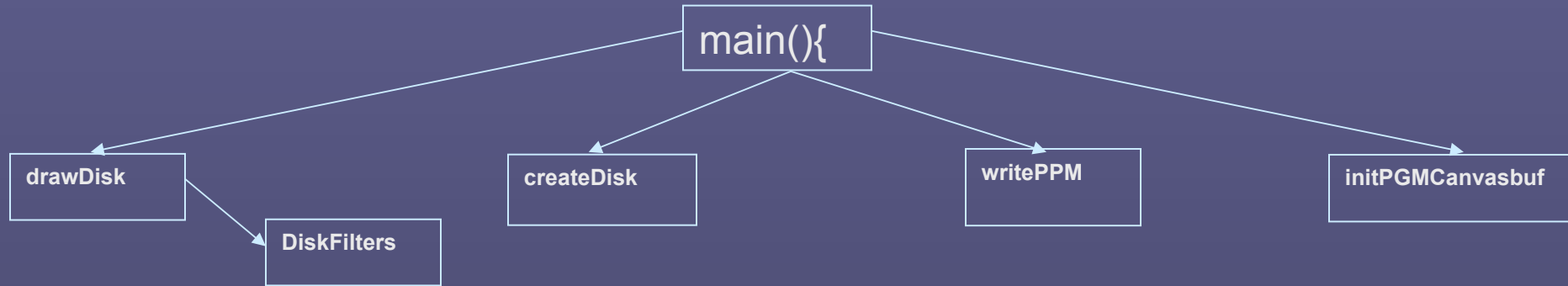
COLUMNS	DATA TYPE	FIELD	DEFINITION
---------	-----------	-------	------------

1 – 6	Record name	"ATOM "	
7 - 11	Integer	serial	Atom serial number.
13 – 16	Atom	name	Atom name.
17	Character	altLoc	Alternate location indicator.
18 – 20	Residue name	resName	Residue name.
22	Character	chainID	Chain identifier.
23 – 26	Integer	resSeq	Residue sequence number.
27	AChar	iCode	Code for insertion of residues.
31 – 38	Real(8.3)	x	Orthogonal coordinates for X in Angstroms.
39 – 46	Real(8.3)	y	Orthogonal coordinates for Y in Angstroms.
47 – 54	Real(8.3)	z	Orthogonal coordinates for Z in Angstroms.
55 – 60	Real(6.2)	occupancy	Occupancy.
61 – 66	Real(6.2)	tempFactor	Temperature factor.
77 – 78	LString(2)	element	Element symbol, right-justified.
79 – 80	LString(2)	charge	Charge on the atom.

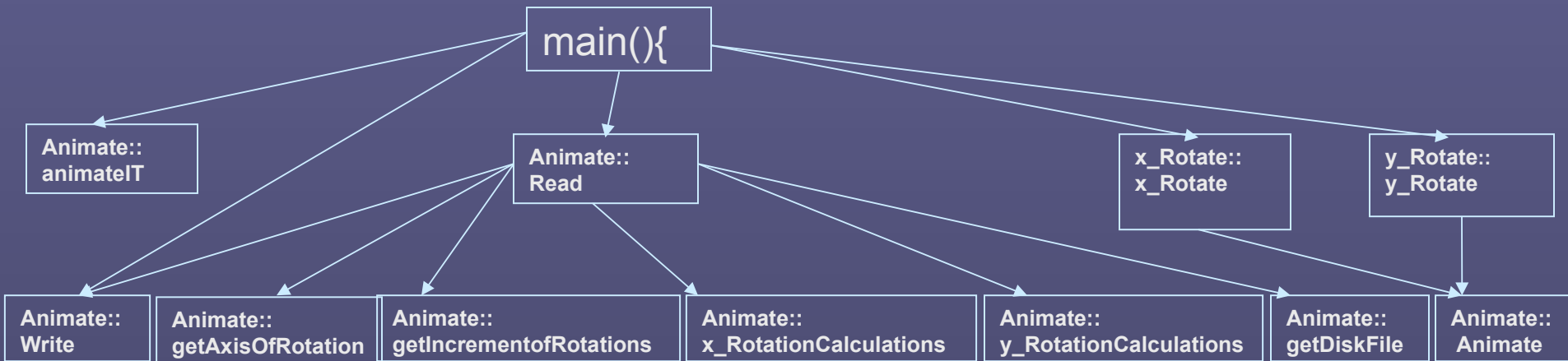
SW Design Overview



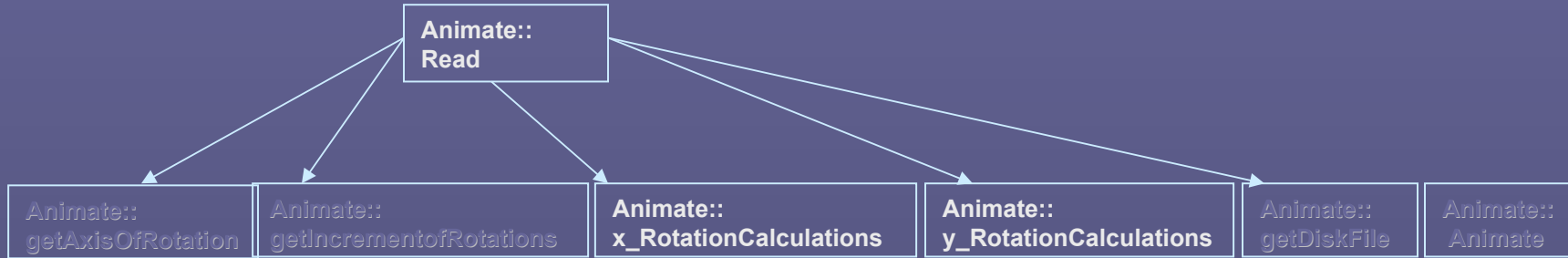
diskWeight.c



newRotate.cpp



Animate::x_RotationCalculations



Rotation Matrix

Rx

1	0	0	x
0	cos	-sin	y
0	sin	-cos	z

Ry

cos	0	sin	x
0	1	0	y
-sin	0	-cos	z

Code

```

y = y * cos - z * sin
z = y * sin + z * cos
    
```

```

x = x * cos + z * sin
z = -x * sin + z * 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

Download

# ATOMTV

Play-list ...

## Channels

Alzheimer's

Human Eye

Laminin

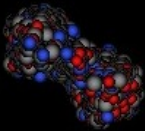
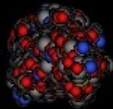
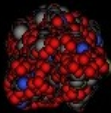
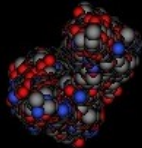
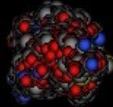
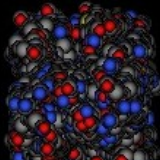
Serotonin

Yellow Fever

PDBs

## Viewing Mode

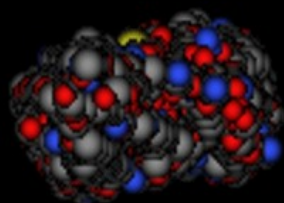
Gif |  Video

|                                                                                                                                                           |                                                                                     |                                                                                                                                                                                     |                                                                                       |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| <p><b>COMPLEX (SERINE PROTEASE/INHIBITOR)   22-DEC-96   1CBW</b></p> <p>BOVINE CHYMOTRYPSIN COMPLEXED TO BPTI</p> <p>&lt;1&gt;</p>                        |    | <p><b>HYDROLASE   21-DEC-99   1DX6</b></p> <p>STRUCTURE OF ACETYLCHOLINESTERASE COMPLEXED WITH (-)-GALANTHAMINE AT 2.3A RESOLUTION</p> <p>&lt;2&gt;</p>                             |    |
| <p><b>HYDROLASE   06-NOV-00   1EA5</b></p> <p>NATIVE ACETYLCHOLINESTERASE (E.C. 3.1.1.7) FROM TORPEDO CALIFORNICA AT 1.8A RESOLUTION</p> <p>&lt;3&gt;</p> |    | <p><b>HYDROLASE/HYDROLASE INHIBITOR   09-AUG-00   1FKN</b></p> <p>STRUCTURE OF BETA-SECRETASE COMPLEXED WITH INHIBITOR</p> <p>&lt;4&gt;</p>                                         |    |
| <p><b>HYDROLASE   07-NOV-01   1GPN</b></p> <p>STRUCTURE OF ACETYLCHOLINESTERASE COMPLEXED WITH HUPERZINE B AT 2.35A RESOLUTION</p> <p>&lt;5&gt;</p>       |    | <p><b>HYDROLASE   30-JUL-02   1HX3</b></p> <p>STRUCTURE OF ACETYLCHOLINESTERASE (E.C. 3.1.1.7) COMPLEXED WITH (S,S)-(-)-BIS(12)-HUPYRIDONE AT 2.15A RESOLUTION</p> <p>&lt;6&gt;</p> |    |
| <p><b>PROTEIN BINDING   06-SEP-02   1IYT</b></p> <p>SOLUTION STRUCTURE OF THE ALZHEIMER'S DISEASE</p>                                                     |  | <p><b>HYDROLASE   01-OCT-02   1MX1</b></p> <p>CRYSTAL STRUCTURE OF HUMAN LIVER CARBOXYL ESTERASE</p>                                                                                |  |

**COMPLEX (SERINE PROTEASE/INHIBITOR) | 22-DEC-96 | 1CBW**

Repository - 19 -

**Legend**

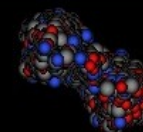
 O ●  
 N ●  
 C ●  
 S ●

**BOVINE CHYMOTRYPSIN COMPLEXED TO BPTI**

 Gif |  Video

[Channels](#) | [Viewing Guide](#)
**COMPLEX (SERINE PROTEASE/INHIBITOR)**  
**| 22-DEC-96 | 1CBW**

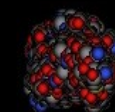
BOVINE CHYMOTRYPSIN COMPLEXED TO BPTI

&lt;1&gt;


**HYDROLASE | 21-DEC-99 | 1DX6**

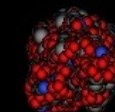
 STRUCTURE OF ACETYLCHOLINESTERASE  
 COMPLEXED WITH (-)-GALANTHAMINE AT 2.3Å  
 RESOLUTION

&lt;2&gt;


**HYDROLASE | 06-NOV-00 | 1EA5**

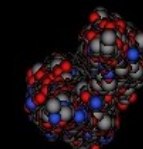
 NATIVE ACETYLCHOLINESTERASE (E.C. 3.1.1.7)  
 FROM TORPEDO CALIFORNICA AT 1.8Å  
 RESOLUTION

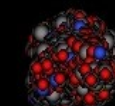
&lt;3&gt;


**HYDROLASE/HYDROLASE INHIBITOR |**  
**09-AUG-00 | 1FKN**

 STRUCTURE OF BETA-SECRETASE COMPLEXED  
 WITH INHIBITOR

&lt;4&gt;


**HYDROLASE | 07-NOV-01 | 1GPN**

 STRUCTURE OF ACETYLCHOLINESTERASE  
 COMPLEXED WITH HUPERZINE B AT 2.35Å


[Download from...](#)

Protein Data Banks

URL

PDB

Watch

Local

Browse...

Watch

Viewing Mode

Gif

Video



# Going LIVE!

## Atomic Coordinate Viewer