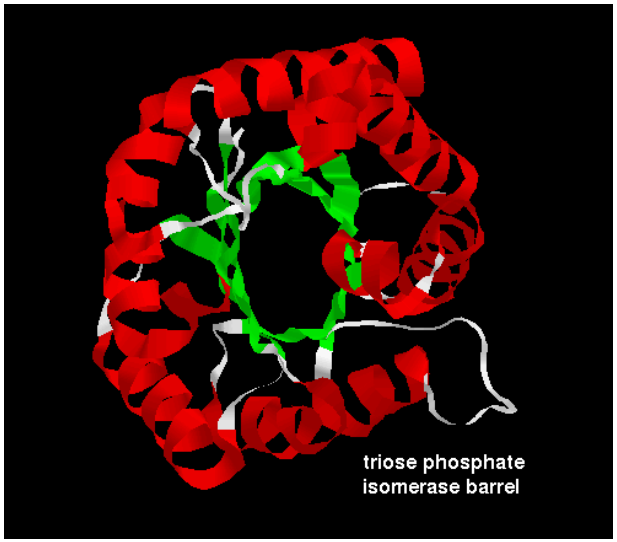
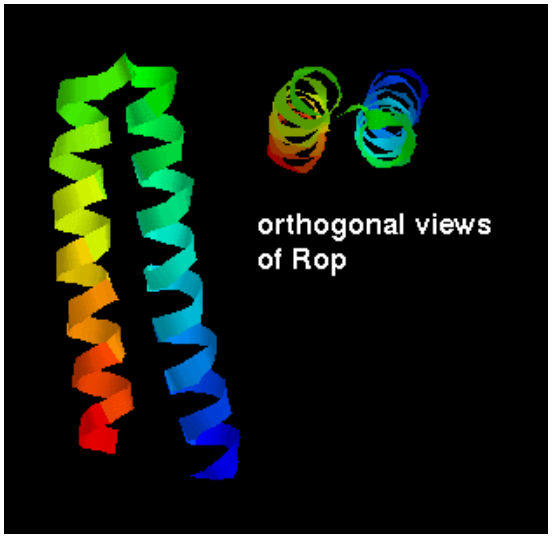
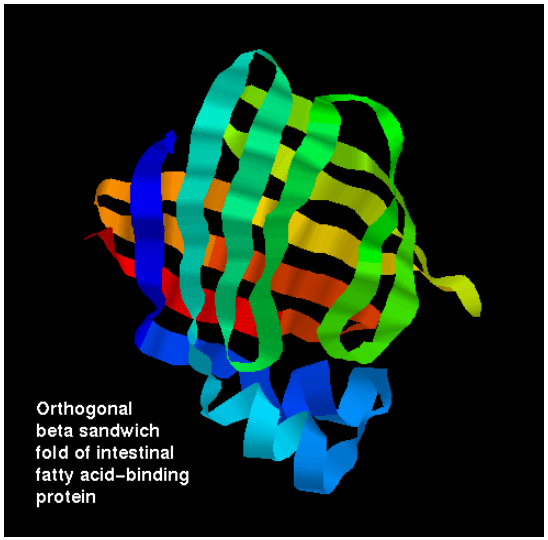
3D Structure

Visualizing, Comparing, Classifying







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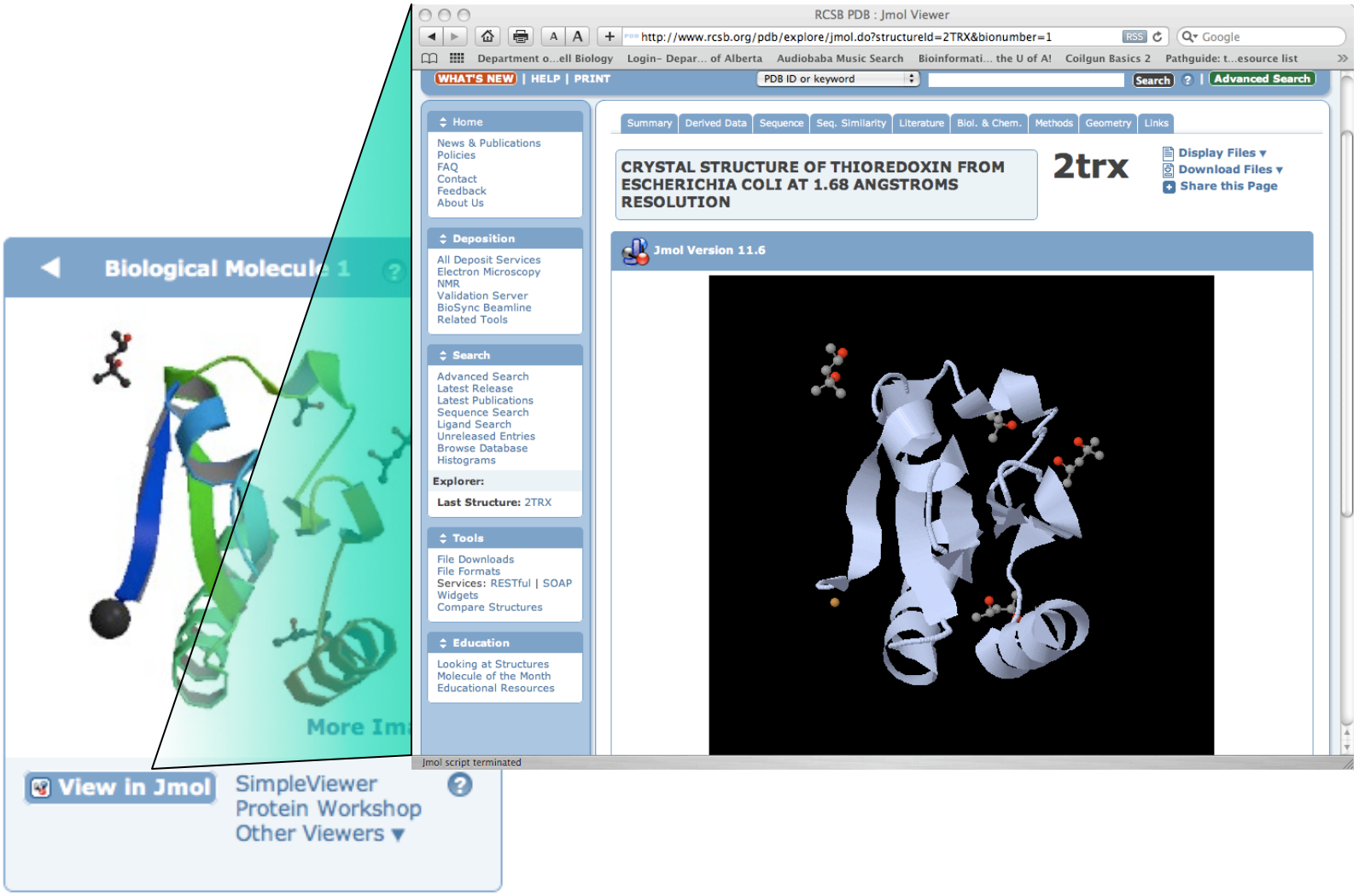
Outline & Objectives*

- Visualization Programs
- Vectors & Matrices
- Difference Distance Matrices
- Molecular Superposition
- Measuring Superposition
- Classifying 3D Structures

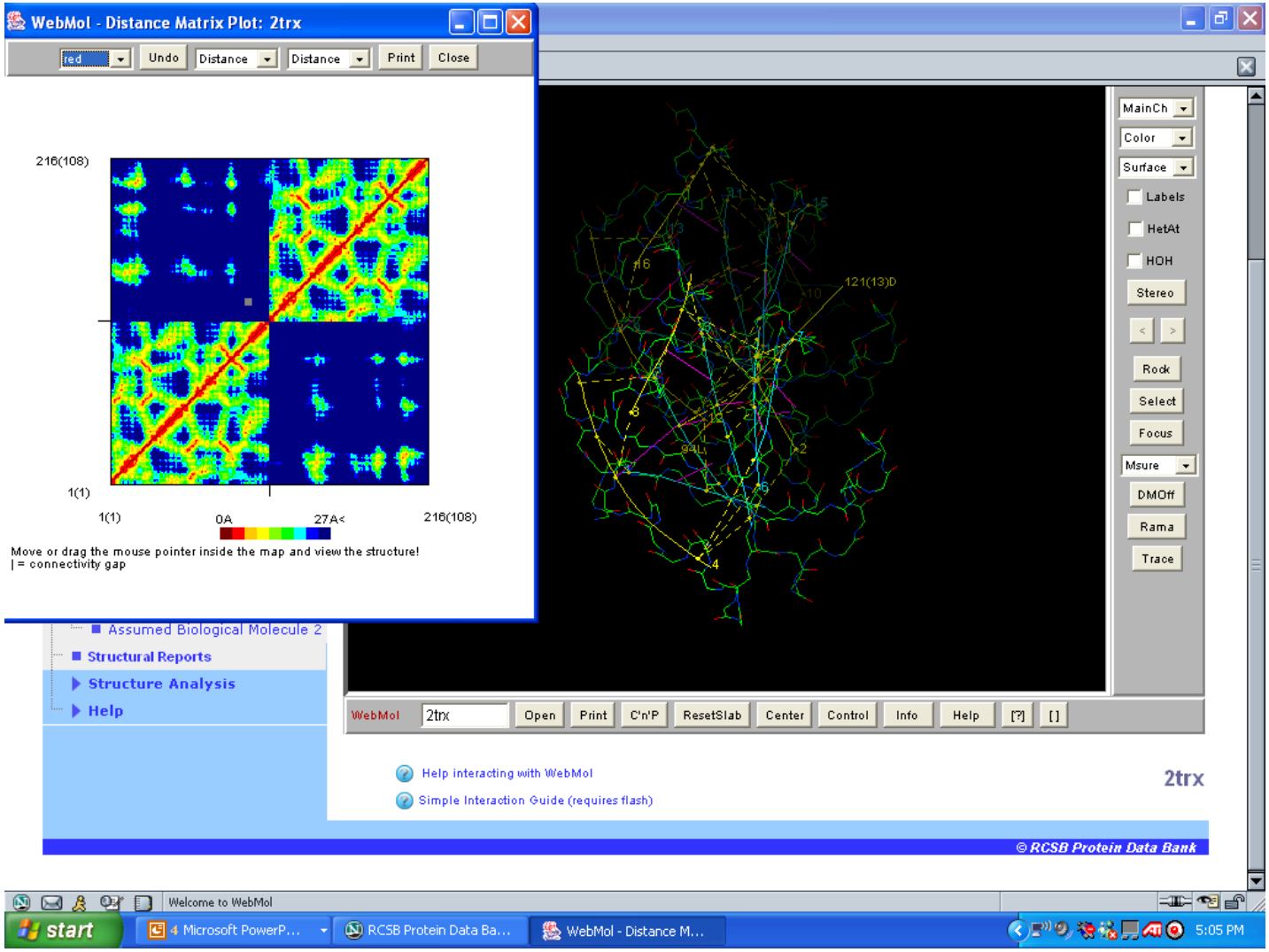
PDB Viewers


RCSB PDB : Jmol Viewer
http://www.rcsb.org/pdb/explore/jmol.do?structureId=2TRX&bionumber=1
WHAT'S NEW | HELP | PRINT
PDB ID or keyword
Search
Advanced Search
Home
News & Publications
Policies
FAQ
Contact
Feedback
About Us
Deposition
All Deposit Services
Electron Microscopy
NMR
Validation Server
BioSync Beamline
Related Tools
Search
Advanced Search
Latest Release
Latest Publications
Sequence Search
Ligand Search
Unreleased Entries
Browse Database
Histograms
Explorer:
Last Structure: 2TRX
Tools
File Downloads
File Formats
Services: RESTful | SOAP
Widgets
Compare Structures
Education
Looking at Structures
Molecule of the Month
Educational Resources
Summary
Derived Data
Sequence
Seq. Similarity
Literature
Biol. & Chem.
Methods
Geometry
Links
CRYSTAL STRUCTURE OF THIOREDOXIN FROM ESCHERICHIA COLI AT 1.68 ANGSTROMS RESOLUTION
2trx
Display Files
Download Files
Share this Page
Jmol Version 11.6
Jmol script terminated
Biological Molecule 1
More Im
View in Jmol
SimpleViewer
Protein Workshop
Other Viewers

Jmol*

- Java-based program
- Open source applet and application
  - Compatible with Linux, MacOS, Windows
- Menus access by clicking on Jmol icon on lower right corner of applet
- Works with all major web browsers
  - Internet Explorer (Win32)
  - Mozilla/Firefox (Win32, OSX, *nix)
  - Safari (Mac OS X) and Opera 7.5.4

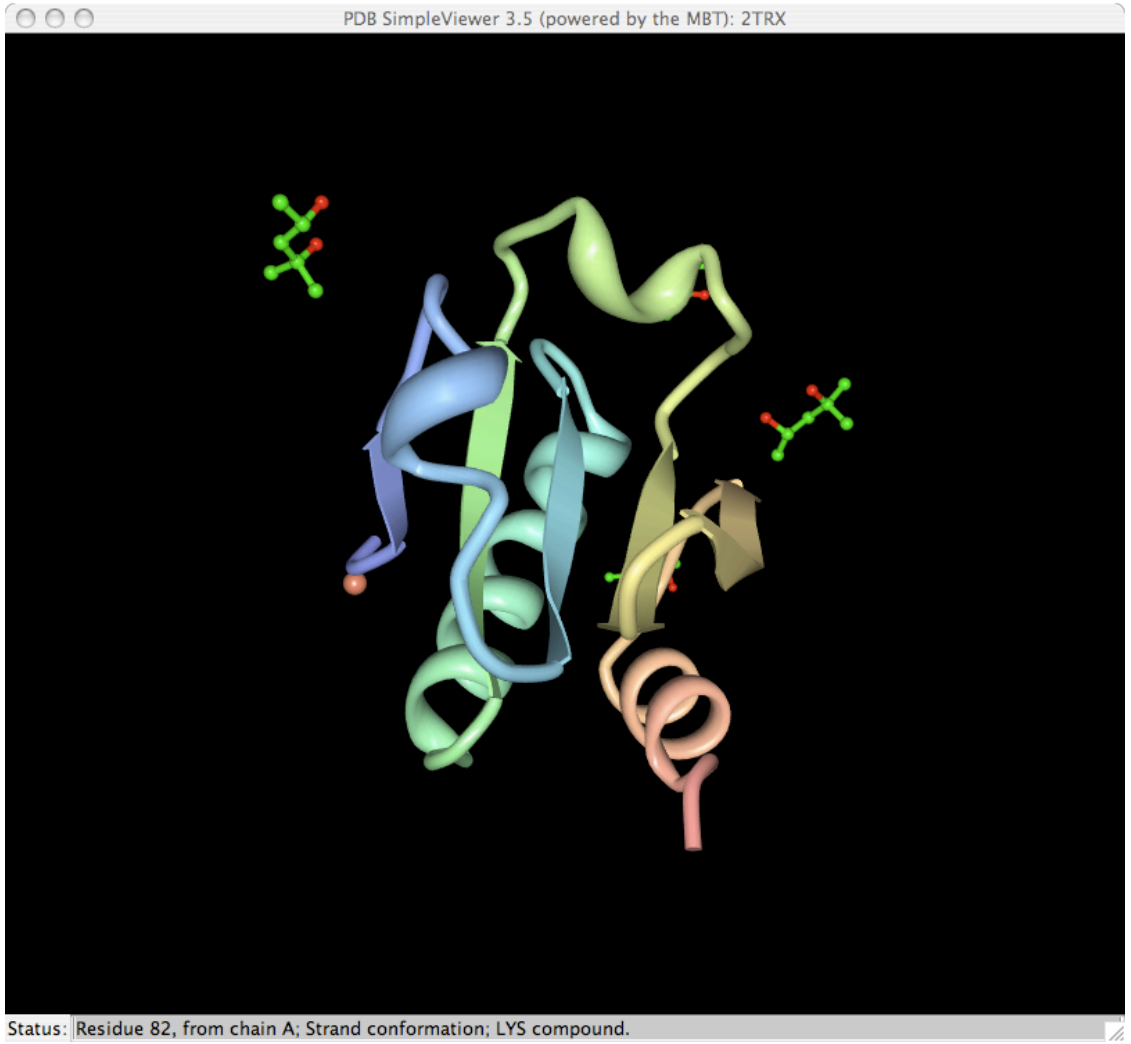
WebMol*


WebMol - Distance Matrix Plot: 2trx
red
Undo
Distance
Distance
Print
Close
216(108)
1(1)
1(1)
0A
27A<
216(108)
Move or drag the mouse pointer inside the map and view the structure!
| = connectivity gap
MainCh
Color
Surface
Labels
HetAt
HOH
Stereo
Rock
Select
Focus
Msure
DMOff
Rama
Trace
121(13)D
Assumed Biological Molecule 2
Structural Reports
Structure Analysis
Help
WebMol
2trx
Open
Print
C'n'P
ResetSlab
Center
Control
Info
Help
[?]
[]
Help interacting with WebMol
Simple Interaction Guide (requires flash)
2trx
© RCSB Protein Data Bank
Welcome to WebMol
start
4 Microsoft PowerP...
RCSB Protein Data Ba...
WebMol - Distance M...
5:05 PM

WebMol*

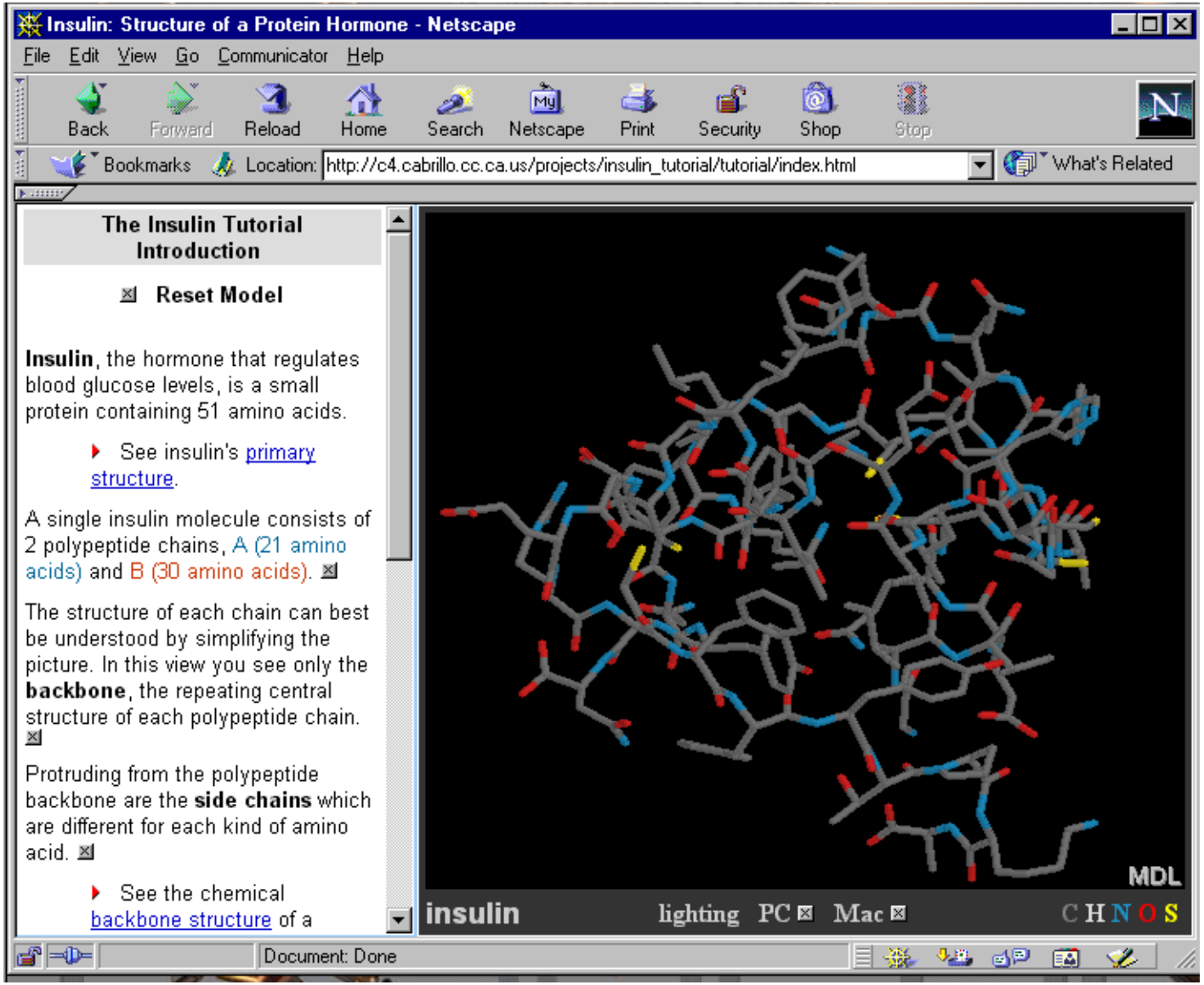
- Both a Java Applet and a downloadable application
- Offers many tools including distance, angle, dihedral angle measurements, detection of steric conflicts, interactive Ramachandran plot, diff. distance plot
- Compatible with most Java (1.3+) enabled browsers including:
  - Internet Explorer
  - Safari on Mac OS
  - Mozilla 1.6/Firefox on Linux (Redhat 8.0)

PDB SimpleViewer



Requires Java WebStart (~30 sec install)

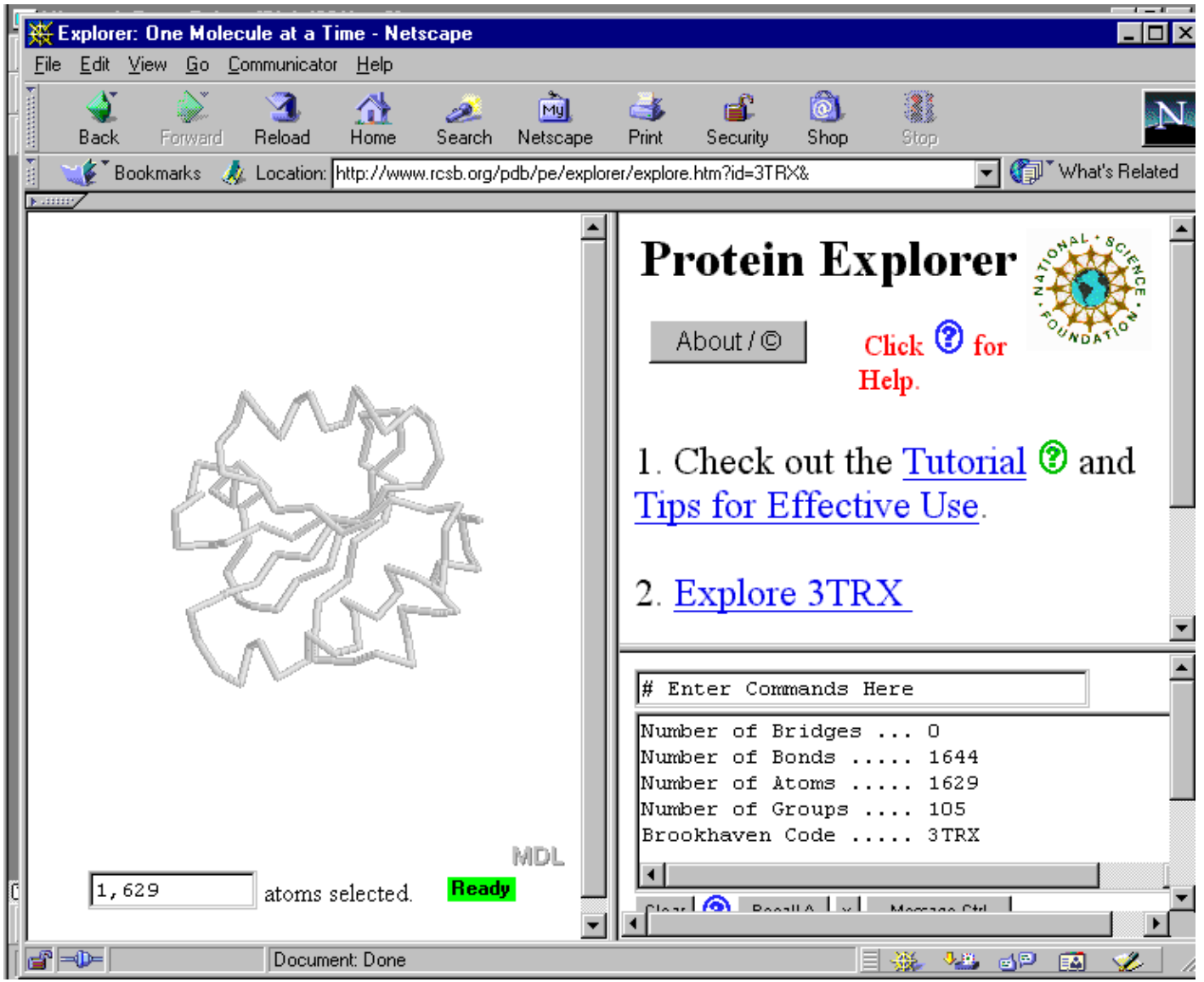
Chime*


Insulin: Structure of a Protein Hormone - Netscape
File Edit View Go Communicator Help
Back Forward Reload Home Search Netscape Print Security Shop Stop
Bookmarks Location: http://c4.cabrillo.cc.ca.us/projects/insulin_tutorial/tutorial/index.html What's Related
The Insulin Tutorial
Introduction
Reset Model
Insulin, the hormone that regulates blood glucose levels, is a small protein containing 51 amino acids.
See insulin's primary structure.
A single insulin molecule consists of 2 polypeptide chains, A (21 amino acids) and B (30 amino acids).
The structure of each chain can best be understood by simplifying the picture. In this view you see only the backbone, the repeating central structure of each polypeptide chain.
Protruding from the polypeptide backbone are the side chains which are different for each kind of amino acid.
See the chemical backbone structure of a
MDL
insulin lighting PC Mac C H N O S
Document: Done

Chime*

- http://www.umass.edu/microbio/chime/neccsoft.htm#download_install
- Among first PDB viewing programs with limited manipulation capacity
- Uses Rasmol for its back end source
- View both large and small molecules
- Browser Plug-in (Like PDF reader)
- Interesting from historical perspective (now mostly phased out)

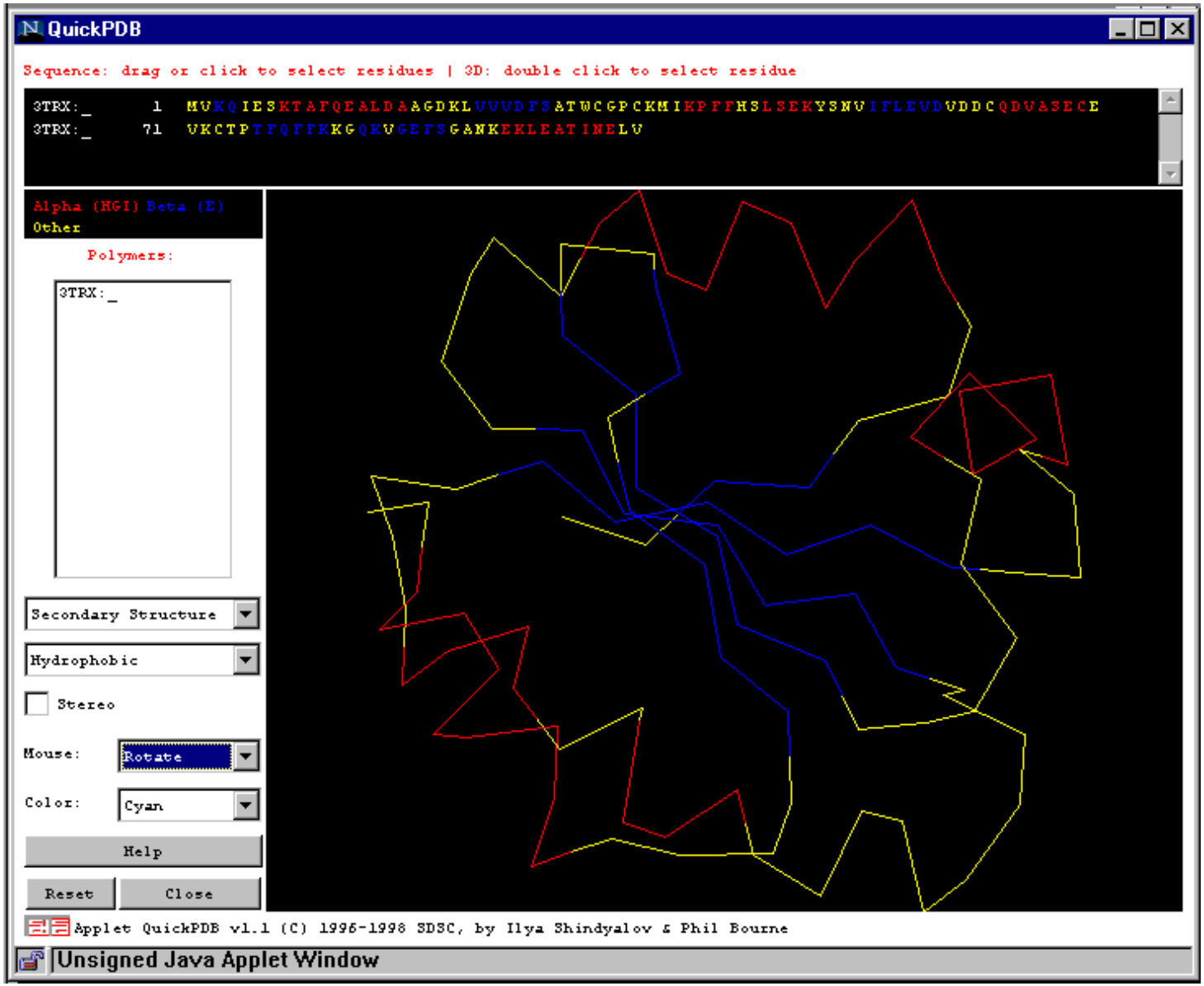
Protein Explorer (Chime)



Protein Explorer*

- http://www.umass.edu/microbio/chime/pe_beta/pe/protexpl/
- Uses Chime or Jmol for its back-end
- Very flexible, user friendly, well documented, offers morphing, sequence structure interface, comparisons, context-dependent help, smart zooming, off-line
- Browser Plug-in (Like PDF reader)
- Compatible with Netscape (Mac & Win)

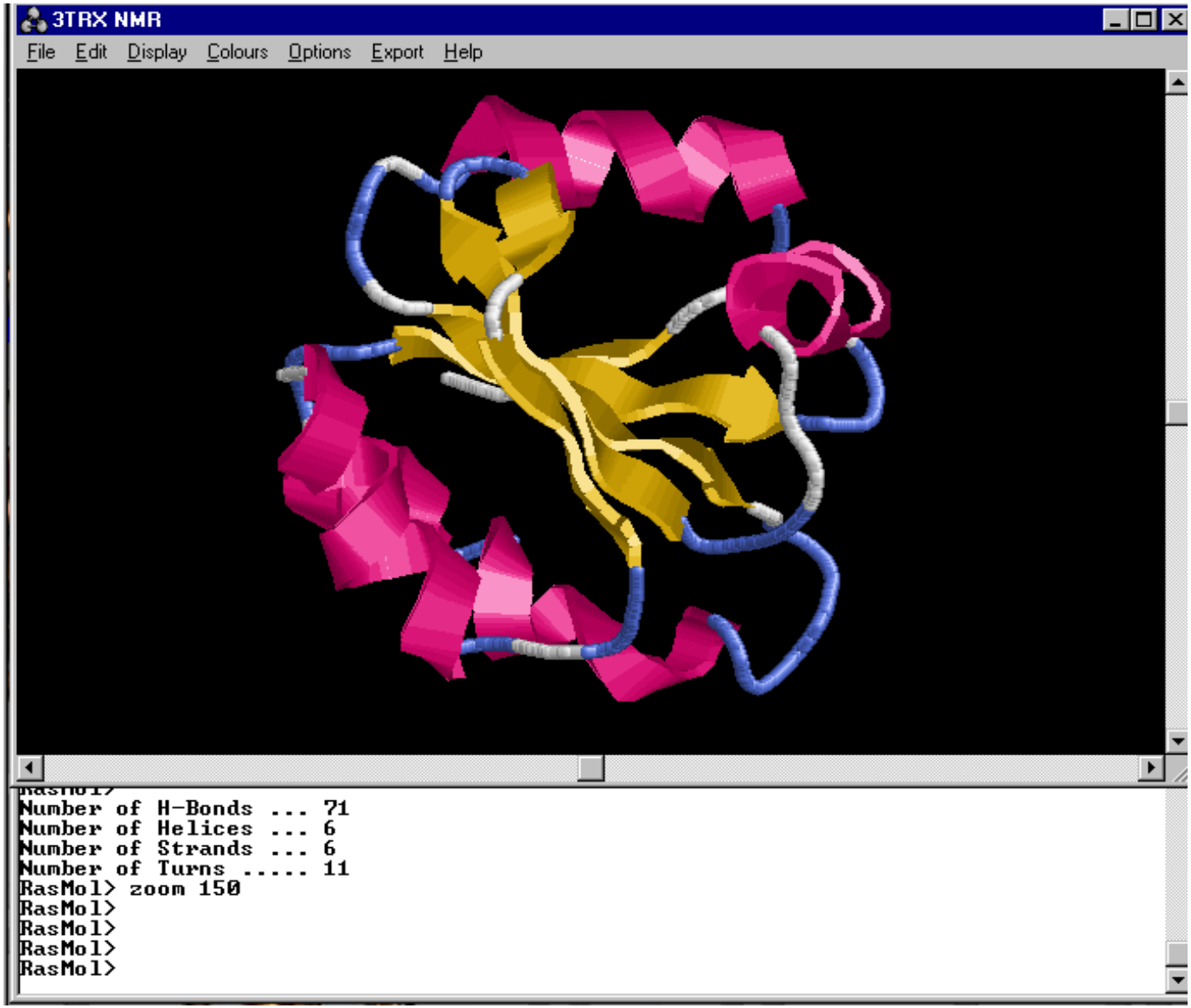
QuickPDB


QuickPDB
Sequence: drag or click to select residues | 3D: double click to select residue
3TRX:_ 1 MVKQIESKTAFQEALDAAGDKLVVVDFSATWCGPCKMIKPFFHSLSEKYSNVIFLEVDVDDCQDVASECE
3TRX:_ 71 VKCTPTFQFFKKGQKVGEFSGANKEKLEATINELV
Alpha (HGI) Beta (E)
Other
Polymers:
3TRX:_
Secondary Structure
Hydrophobic
Stereo
Mouse:
Rotate
Color:
Cyan
Help
Reset
Close
Applet QuickPDB v1.1 (C) 1996-1998 SDSC, by Ilya Shindyalov & Phil Bourne
Unsigned Java Applet Window

Quick PDB*

- http://www.sdsc.edu/pb/Software.html
- Very simple viewing program with limited manipulation and very limited rendering capacity -- Very fast
- Java Applet (Source code available)
- Compatible with most browsers and computer platforms

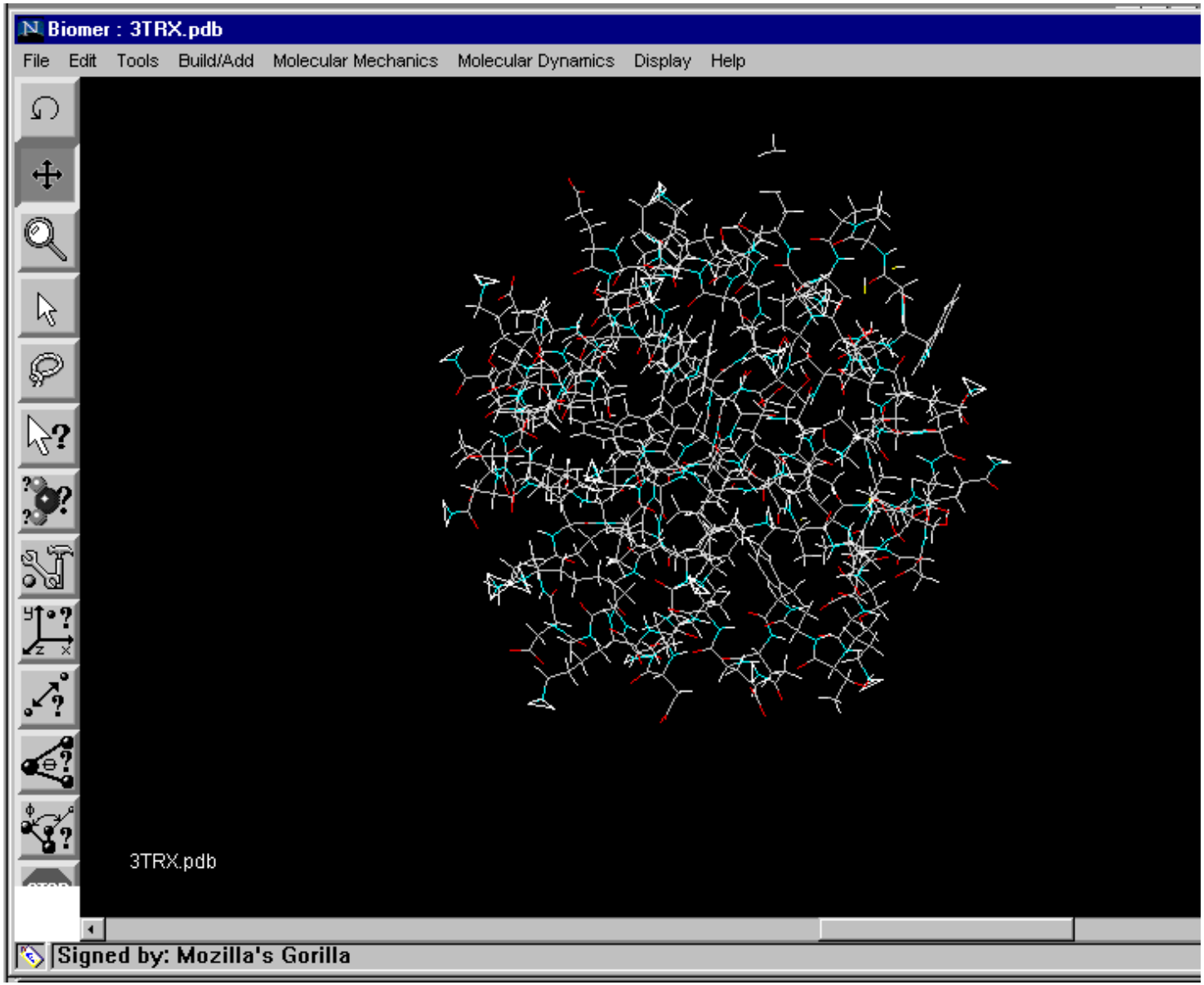
Rasmol


3TRX NMR
File Edit Display Colours Options Export Help
Number of H-Bonds ... 71
Number of Helices ... 6
Number of Strands ... 6
Number of Turns 11
RasMol> zoom 150
RasMol>
RasMol>
RasMol>
RasMol>

Rasmol*

- http://www.umass.edu/microbio/rasmol/
- Very simple viewing program with limited manipulation capacity, easy to use!
- “Grand-daddy” of all visual freeware
- Runs as installed “stand-alone” program
- Source code available
- Runs on Mac, Windows, Linux, SGI and most other UNIX platforms

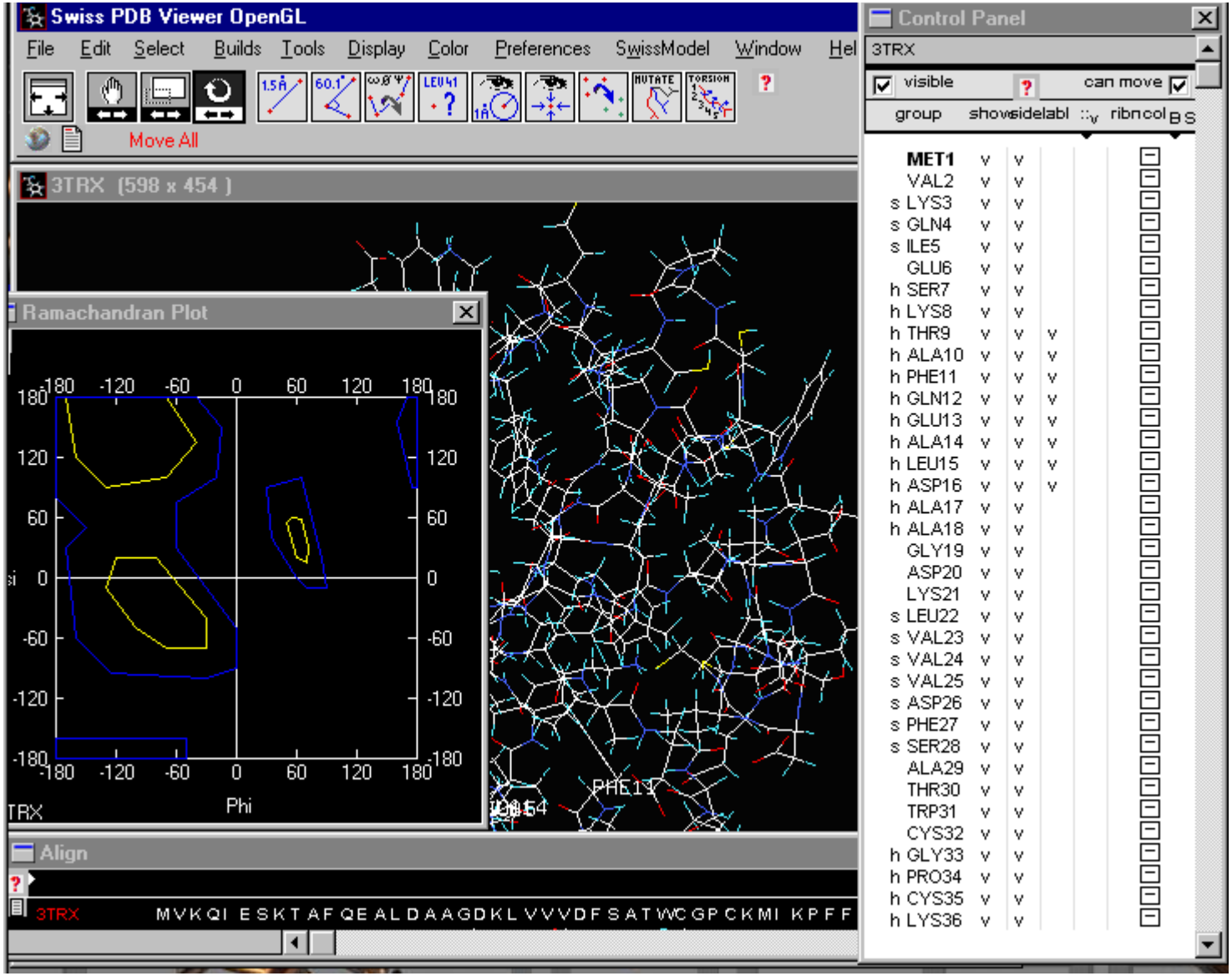
B (Biomer)


Biomer : 3TRX.pdb
File
Edit
Tools
Build/Add
Molecular Mechanics
Molecular Dynamics
Display
Help
3TRX.pdb
Signed by: Mozilla's Gorilla

Biomer (B)

- http://casegroup.rutgers.edu/Biomer/index.html
- Very sophisticated molecular rendering and modelling package for both large and small molecules (kind of rough)
- Supports molecular dynamics & En. min
- Written in Java (source code available)
- Can run as an applet or stand-alone
- Compatible on most platforms

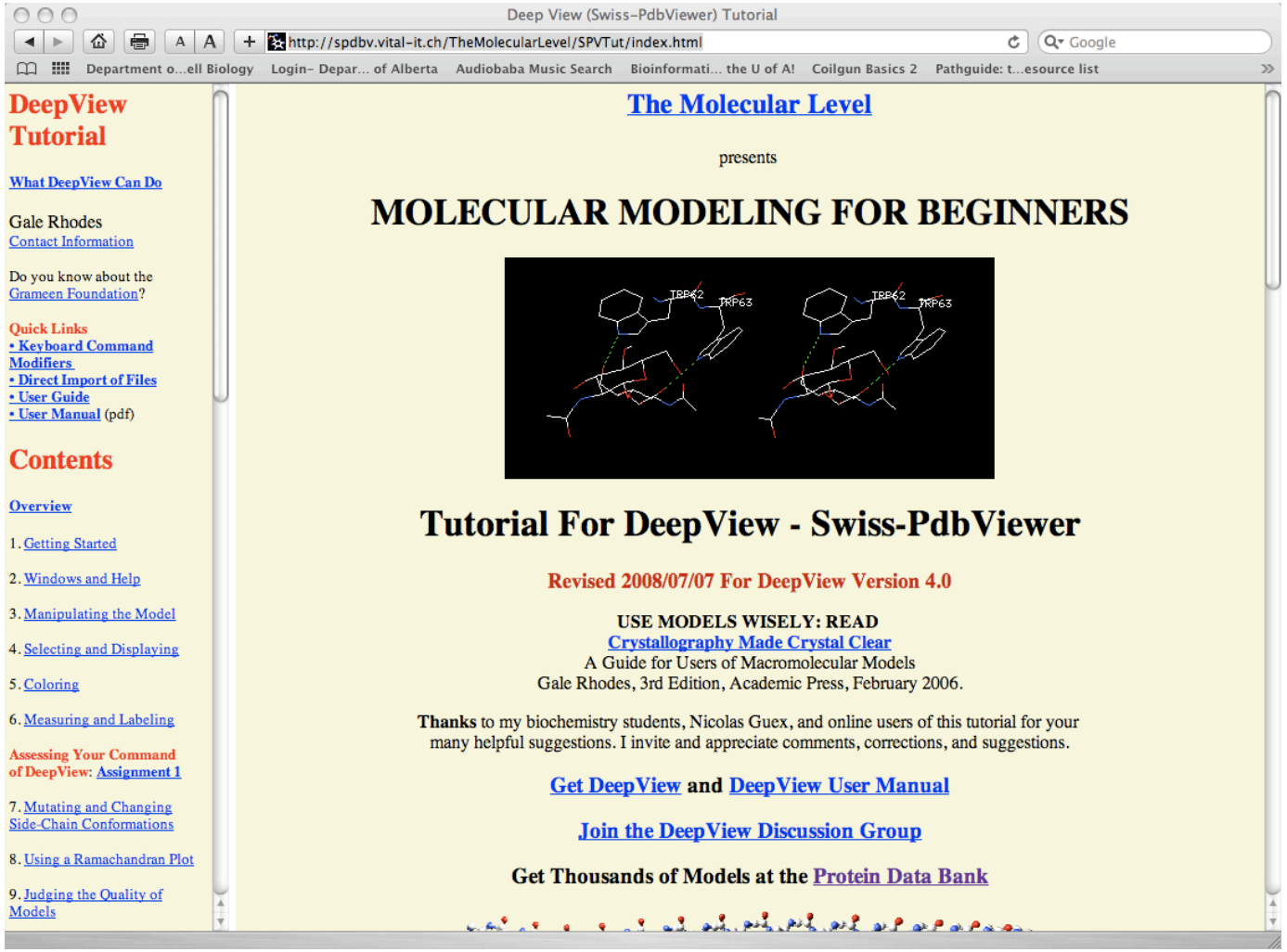
Swiss PDB Viewer



Swiss PDB Viewer*

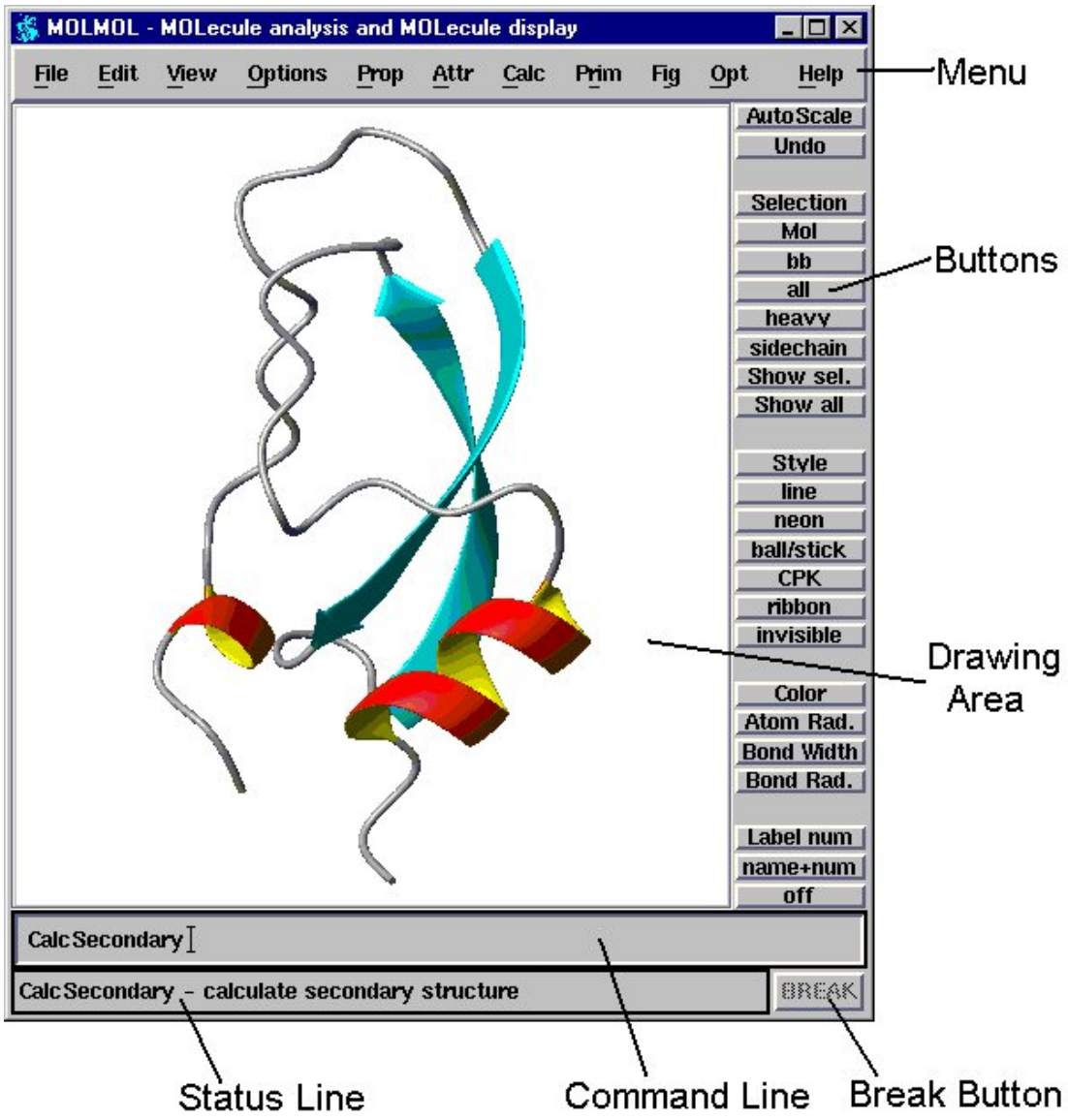
- http://spdbv.vital-it.ch/
- Among most sophisticated molecular rendering, manipulation and modelling packages (commercial or freeware)
- Supports threading, hom. modelling, energy minimization, seq/struc interface
- Stand-alone version only
- Compatible on Mac, Win, Linux, SGI

Swiss PDB Tutorial*



http://spdbv.vital-it.ch/TheMolecularLevel/SPVTut/index.html

MolMol


MOLMOL - MOLecule analysis and MOLecule display
File Edit View Options Prop Attr Calc Prim Fig Opt Help
Menu
AutoScale
Undo
Selection
Mol
bb
all
heavy
sidechain
Show sel.
Show all
Buttons
Style
line
neon
ball/stick
CPK
ribbon
invisible
Drawing Area
Color
Atom Rad.
Bond Width
Bond Rad.
Label num
name+num
off
CalcSecondary
CalcSecondary - calculate secondary structure
BREAK
Status Line
Command Line
Break Button

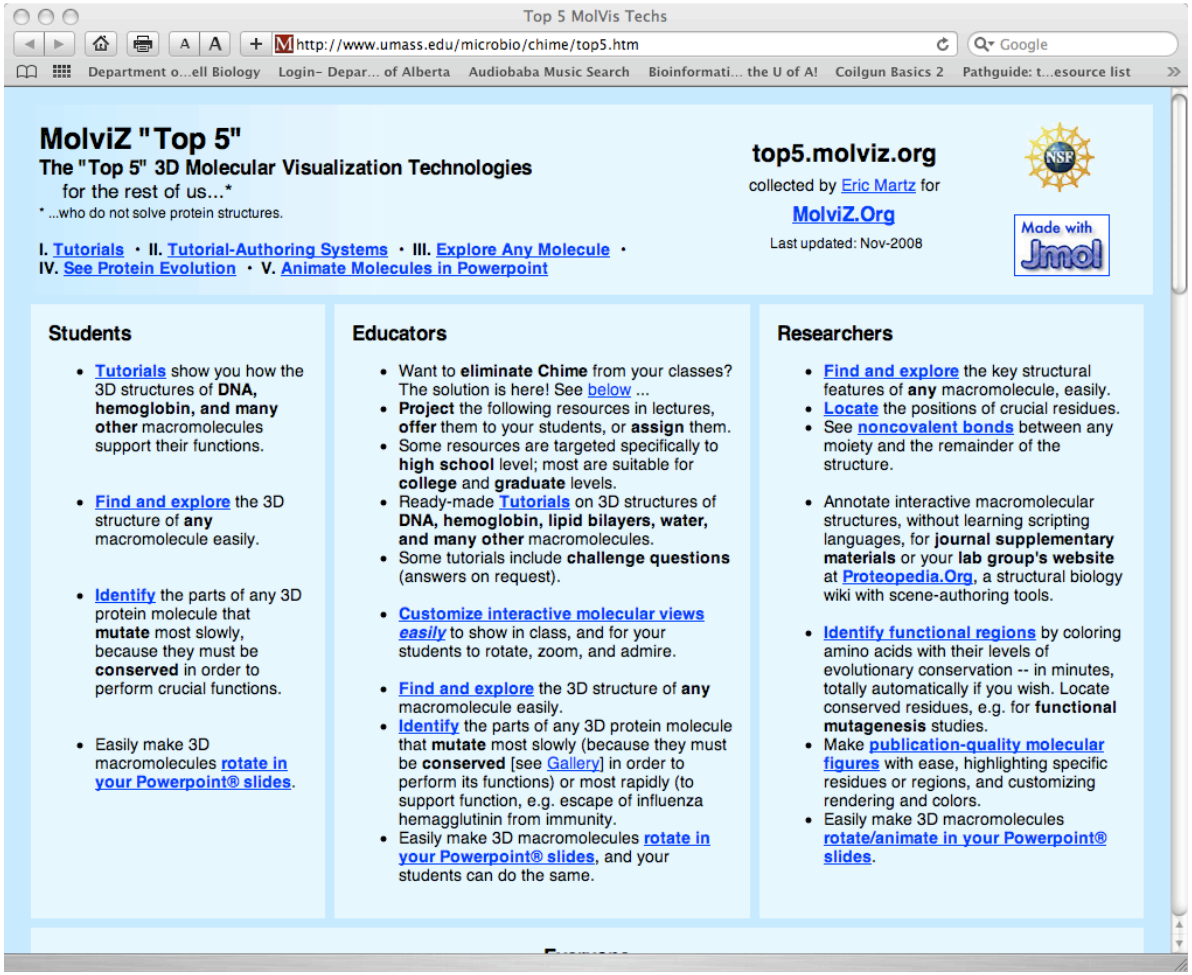
MolMol*

- http://www.mol.biol.ethz.ch/wuthrich/software/molmol/
- **Very sophisticated molecular rendering, and manipulation package (among the best graphics of all freeware)**
- **Special focus on NMR compatibility, supports many calculations/plots**
- **Stand-alone version only**
- **Compatible on Win, Unix (nearly all)**

Summary*

	Mac	Win	Unix	Rendr	SeqView	Super	E Min	Modeling
Rasmol	+	+	+	++	-	-	-	-
Chime	+	+	-	+	-	-	-	-
Prot. Expl.	+	+	-	++	+	+	-	-
Quick PDB	+	+	+	+	+	-	-	-
Biomer	+	+	+	++	-	+	+	+
SwP Viewer	+	+	+	+++	+	+	+	+
MolMol	-	+	+	+++	-	+	-	+

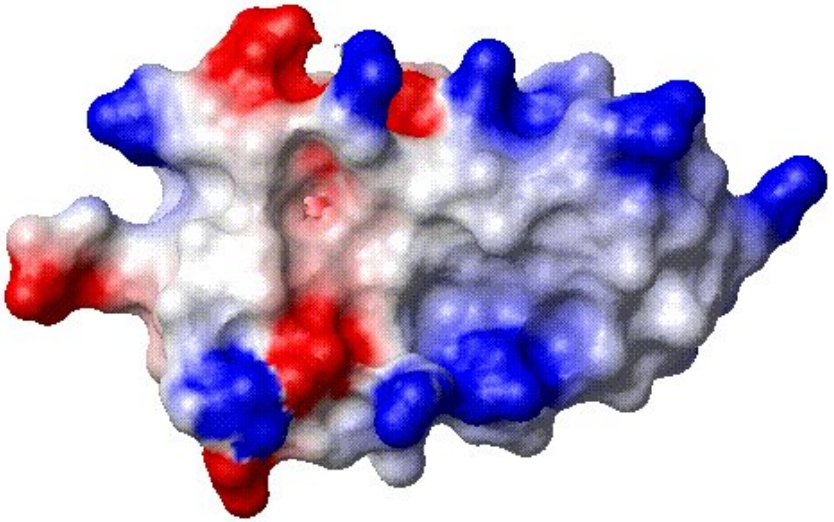
Visualization Hub

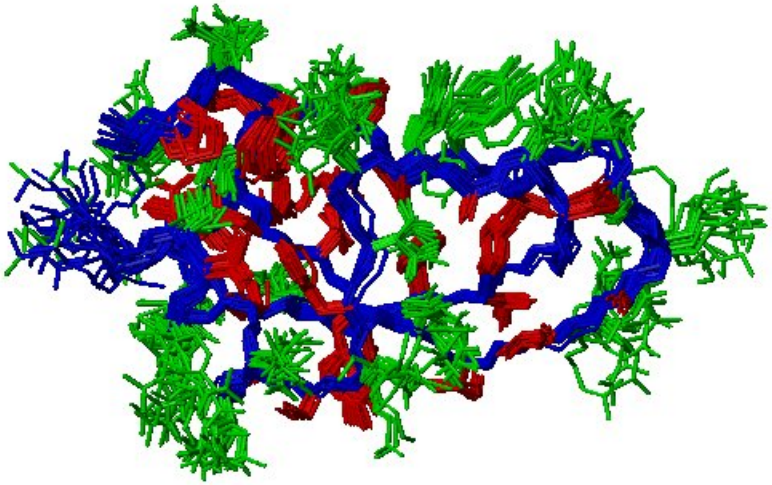


http://www.umass.edu/microbio/chime/top5.htm

Graphics Formats

- GIF
- JPEG
- PNG
- TIFF (Tag Image)
- BMP
- EPS
- PS
- RGP (SGI)





Graphics Formats*

- **GIF (Graphical Interchange Format)**
  - **pronounced "JIF"**
  - **introduced in 1987 by CompuServe**
  - **handles 8 bit colour (256 colours)**
  - **lossy compression (up to 10 X)**
  - **best for drawings, simple B+W or colour diagrams, images with hard edges**
  - **supported by Perl graphics library (GD.pm)**
  - **supports animation & transparency**

Graphics Formats*

- **JPEG (Joint Photographic Experts Group)**
  - **pronounced "JAY-peg"**
  - **exploits eye's poor perception of small changes in colour variation**
  - **handles 24 bit colour (1.6 million colours)**
  - **allows adjustable lossy compression**
  - **best for colour pictures of real objects with varied colour, shadow, fuzzy edges**
  - **among most common web image formats**

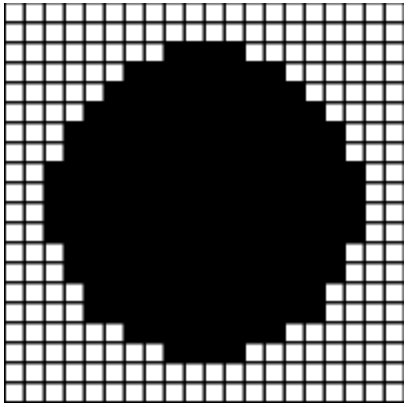
Graphics Formats*

- **PNG (Portable Network Graphics)**
  - designed to replace GIF and TIFF
  - supports lossless compression
  - supports 24 bit, grayscale and 8 bit
  - supports transparency & interlacing
  - offers better compression than GIF (15%)
  - supported by new GD.pm Perl library
  - problems with many early browsers in viewing PNG (now fixed)

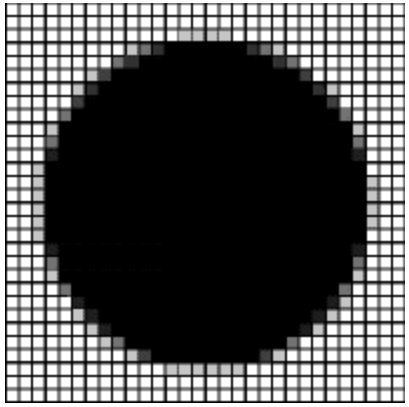
PovRay (www.povray.org)

Aliasing & Antialiasing*

True Image



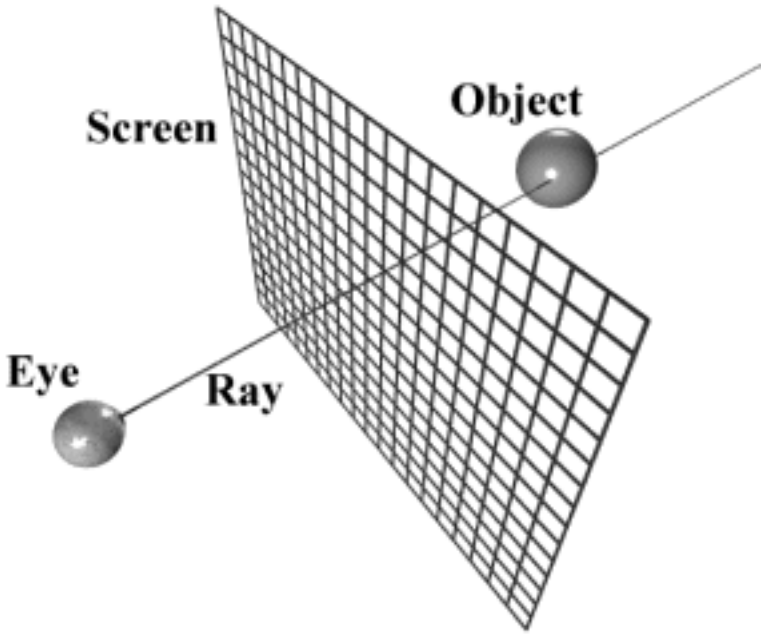
Aliased Image



Anti-aliased Image

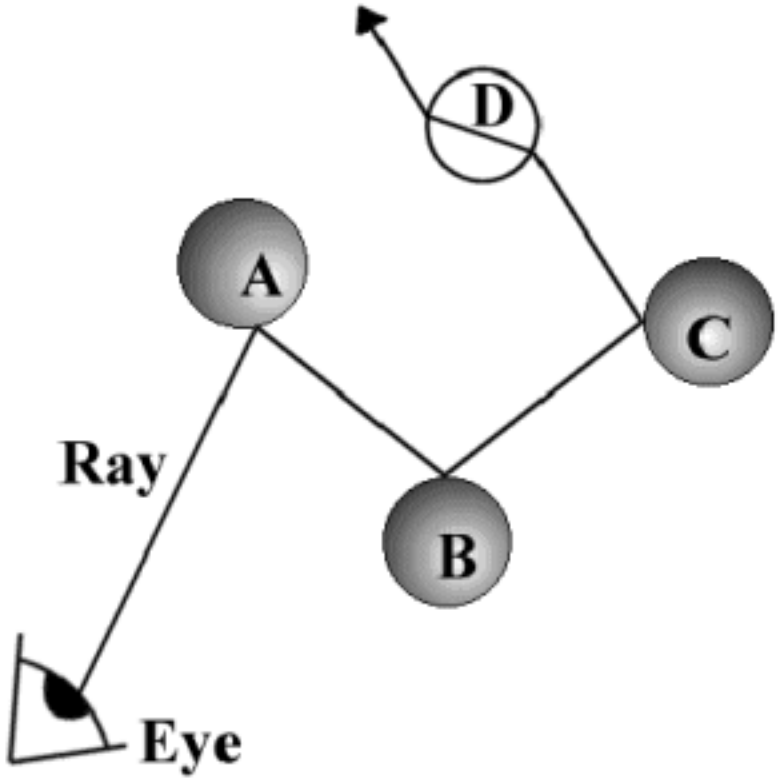
Ray Casting (from 3D to 2D)*

- Ray = beam of light
- For each pixel on screen, cast ray from eye thru pixel
- Test every object in scene to see if ray intersects object
- Each ray intersection nearest to eye is made visible, color pixel



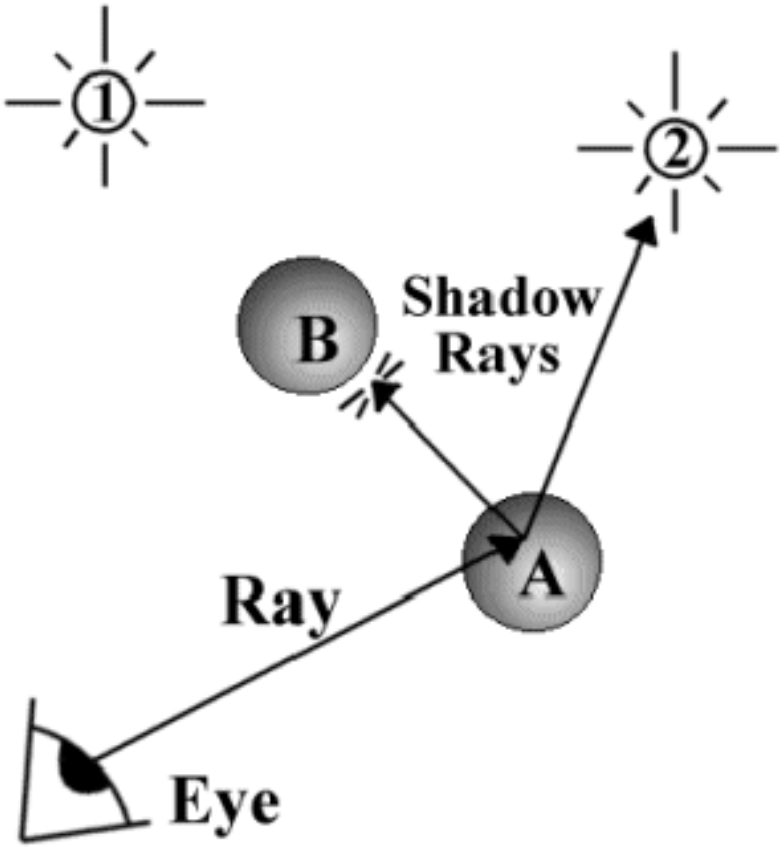
Ray Tracing & Reflection*

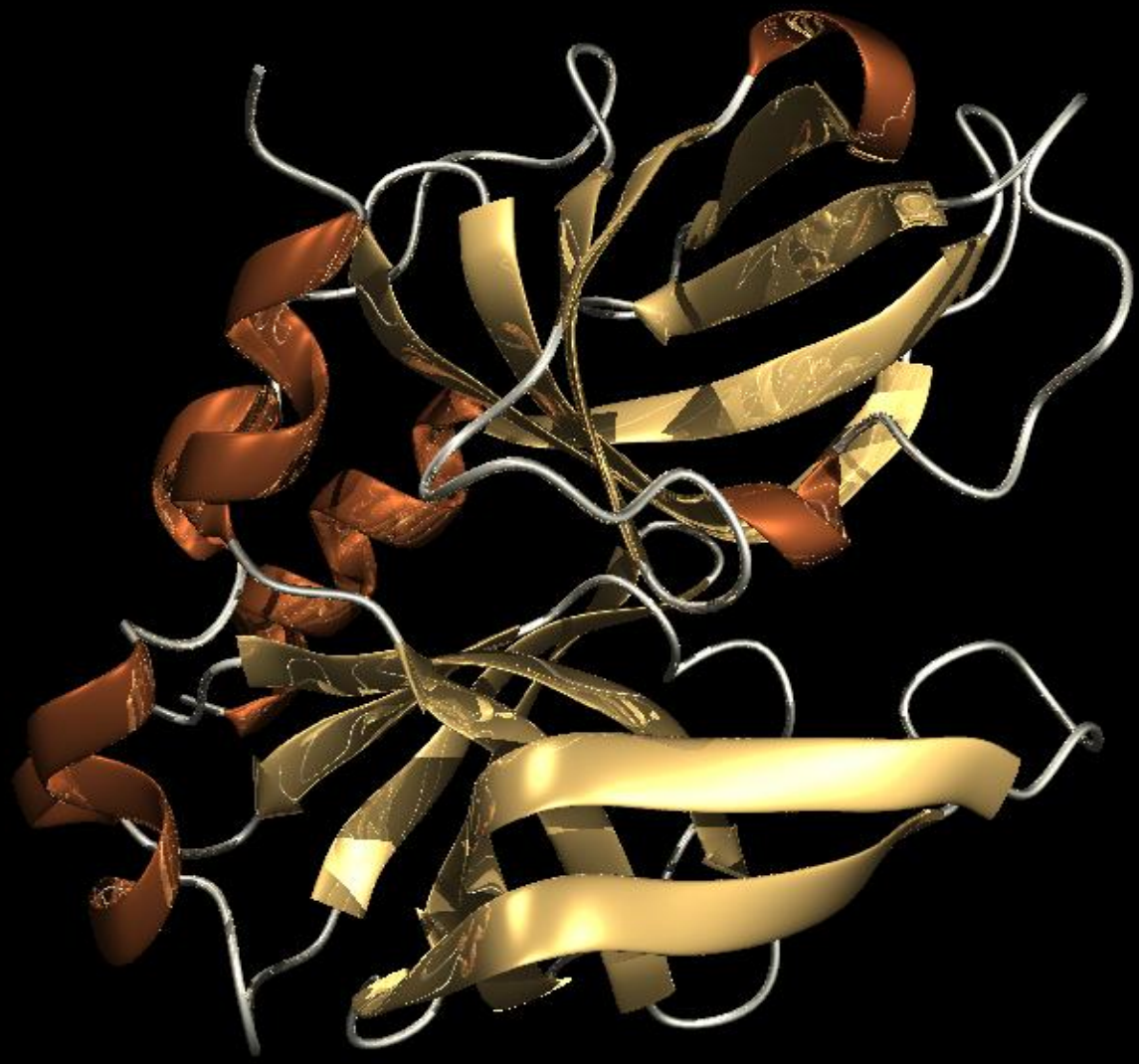
- Used to determine surface appearance
- Begins with ray casting, determine intersects, then recursively sends 2ndary rays to see which objects reflect, which are transparent, which absorb, etc.



Shadowing*

- Uses ray tracing algorithm
- Sends out 2ndary rays towards light sources to see if opaque objects are in the way, if so, then surface is in shadow
- “shadow feelers”



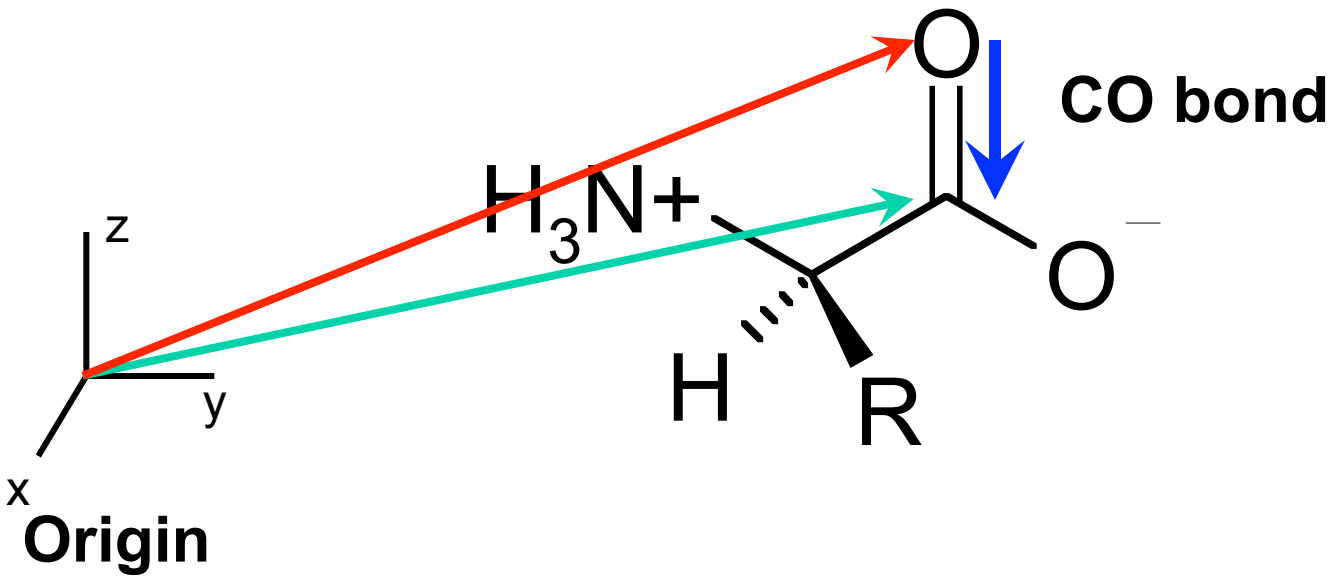


HAV-3C Protease - Alan Gibbs

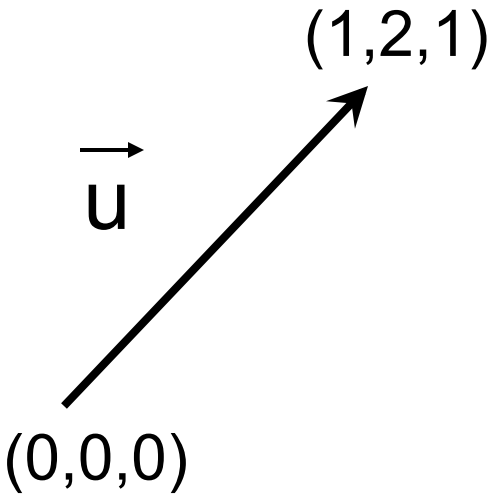
Outline

- Visualization Programs
- Vectors & Matrices
- Difference Distance Matrices
- Molecular Superposition
- Measuring Superposition
- Classifying 3D Structures

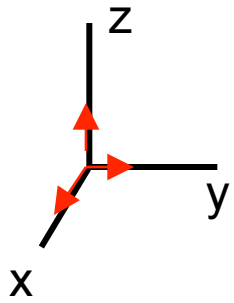
Vectors Define Bonds and Atomic Positions



Review – Vectors*



$$\vec{u} = 1\hat{i} + 2\hat{j} + 1\hat{k}$$



$$\vec{u} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$$

$$\left|\vec{u}\right| = \sqrt{(1-0)^2 + (2-0)^2 + (1-0)^2} = \sqrt{6}$$

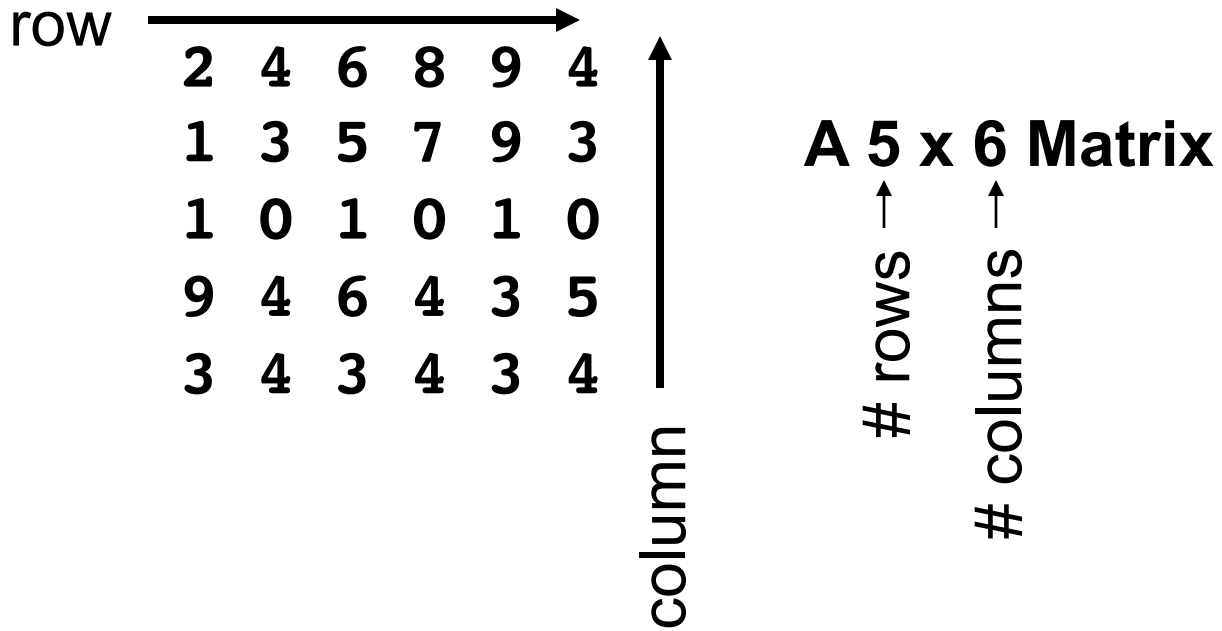
Vectors have a length & a direction

Review - Vectors

- Vectors can be added together
- Vectors can be subtracted
- Vectors can be multiplied (dot or cross or by a matrix)
- Vectors can be transformed (resized)
- Vectors can be translated
- Vectors can be rotated

Matrices*

- A matrix is a table or “array” of characters
- A matrix is also called a tensor of “rank 2”



Different Types of Matrices

$$\begin{bmatrix} 2 & 4 & 6 & 8 & 9 & 4 \\ 1 & 3 & 5 & 7 & 9 & 3 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 9 & 4 & 6 & 4 & 3 & 5 \\ 3 & 4 & 3 & 4 & 3 & 4 \\ 3 & 6 & 7 & 9 & 1 & 0 \end{bmatrix}$$

A square Matrix

$$\begin{bmatrix} 2 & 4 & 6 & 8 & 9 & 4 \\ 4 & 3 & 5 & 7 & 9 & 3 \\ 6 & 5 & 1 & 0 & 1 & 0 \\ 8 & 7 & 0 & 4 & 3 & 5 \\ 9 & 9 & 1 & 3 & 3 & 4 \\ 4 & 3 & 0 & 5 & 4 & 0 \end{bmatrix}$$

A symmetric Matrix

$$\begin{bmatrix} 1 \\ 3 \\ 5 \\ 9 \\ 7 \\ 3 \end{bmatrix}$$

A column Matrix (A vector)

Different Types of Matrices*

$$\begin{bmatrix} A & B & C & D & E & F \\ G & H & I & J & K & L \\ M & N & O & P & Q & R \\ S & T & U & V & W & X \end{bmatrix}$$

A rectangular Matrix

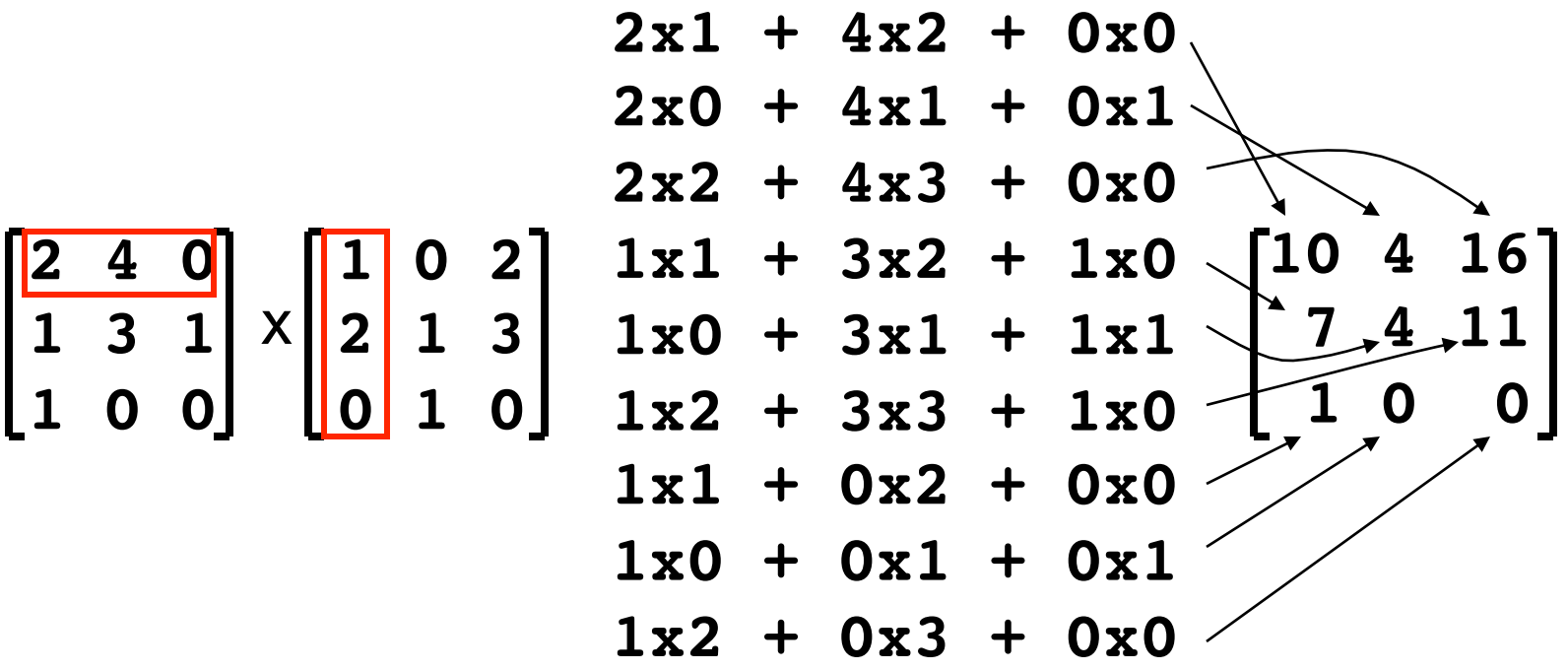
$$\begin{bmatrix} \cos\theta & \sin\theta & 0 \\ \sin\theta & -\cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

A rotation Matrix

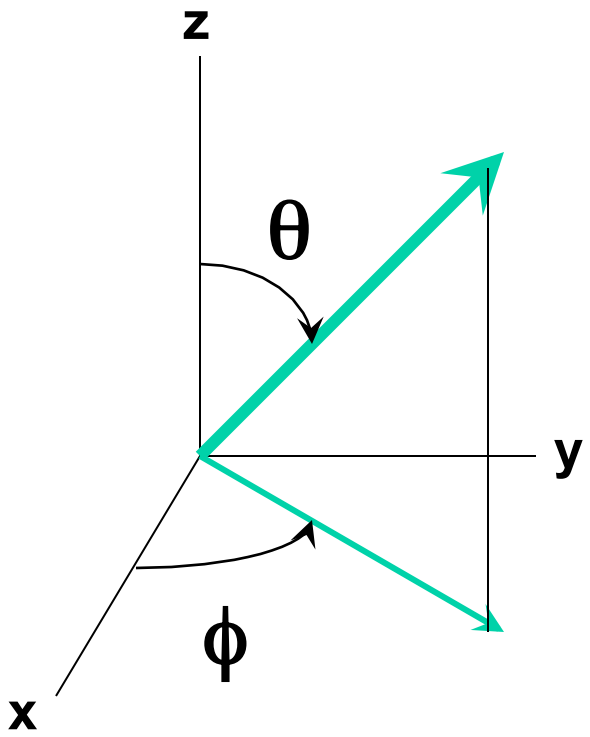
$$\begin{bmatrix} 2 & 4 & 6 & 8 & 9 \end{bmatrix}$$

A row Matrix
(A vector)

Review - Matrix Multiplication



Rotation*



$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}$$

Rotate about x

$$\begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotate about z

Rotation*

Counterclockwise about x

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$$

Counterclockwise about z

$$\begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

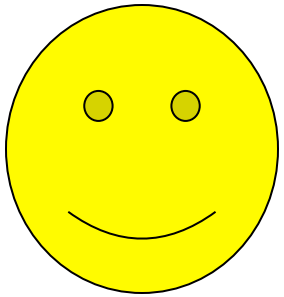
Clockwise about x

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}$$

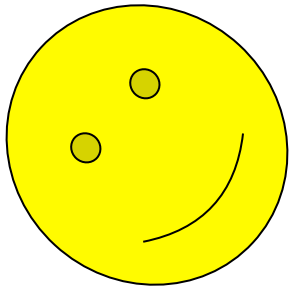
Clockwise about z

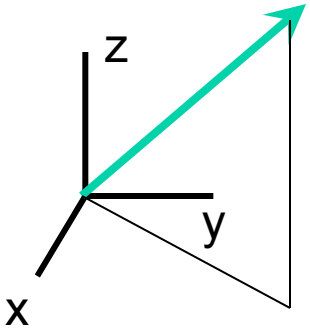
$$\begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotation

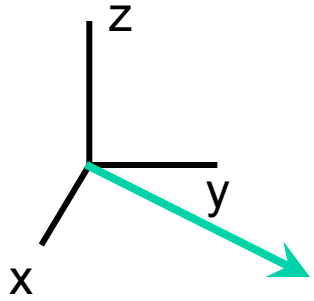


$$\times \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} =$$



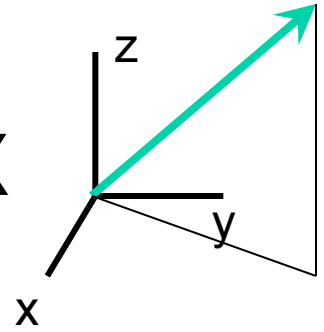


$$\times \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} =$$



Rotation (Detail)*

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \mathbf{X}$$



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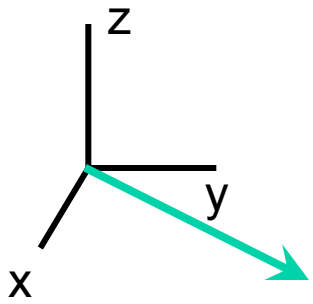
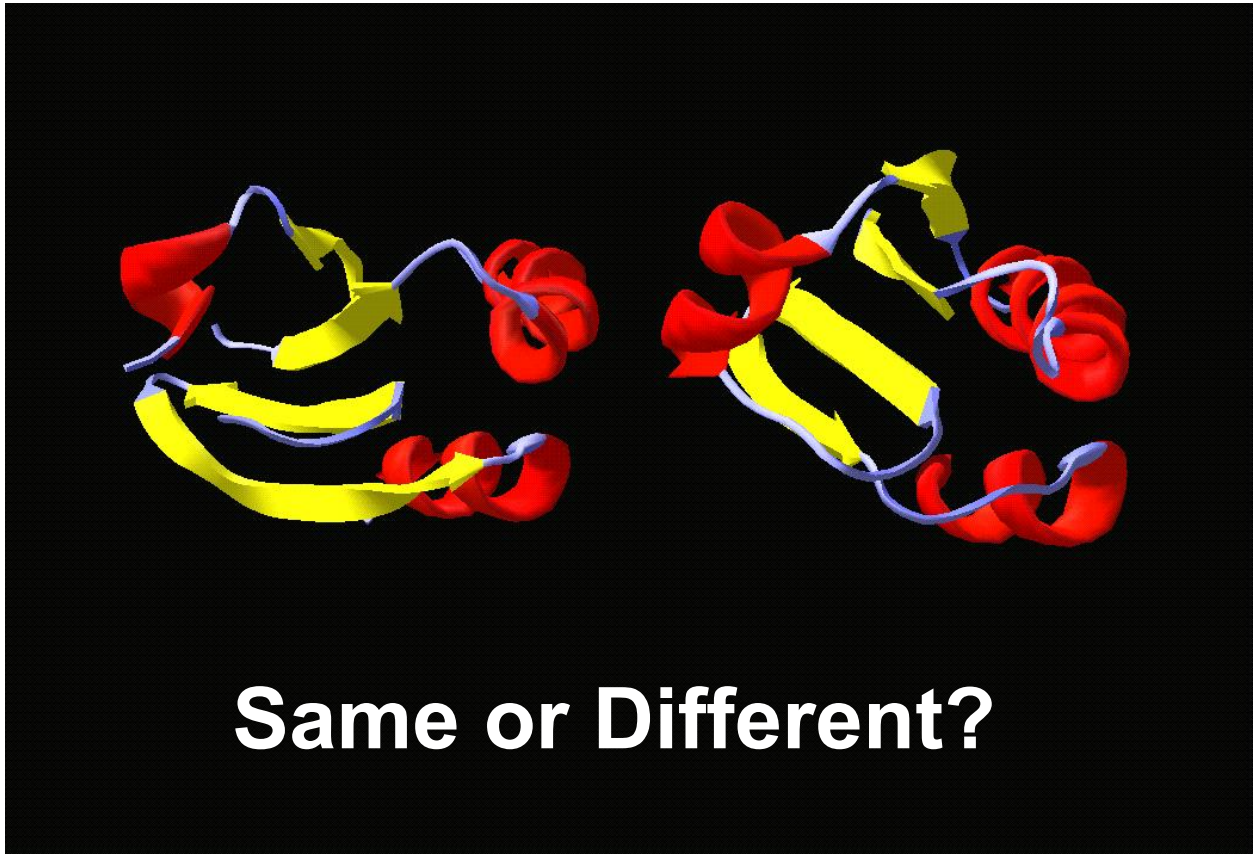


$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ \cos\theta + \sin\theta \\ -\sin\theta + \cos\theta \end{bmatrix}$$

Comparing 3D Structures

- Visual or qualitative comparison
- Difference Distance Matrices
- Superimposition or superposition
- Root mean square deviation (RMSD)
- Subgraph isomorphisms (Ullman's algorithm)
- Combinatorial extension (CE)

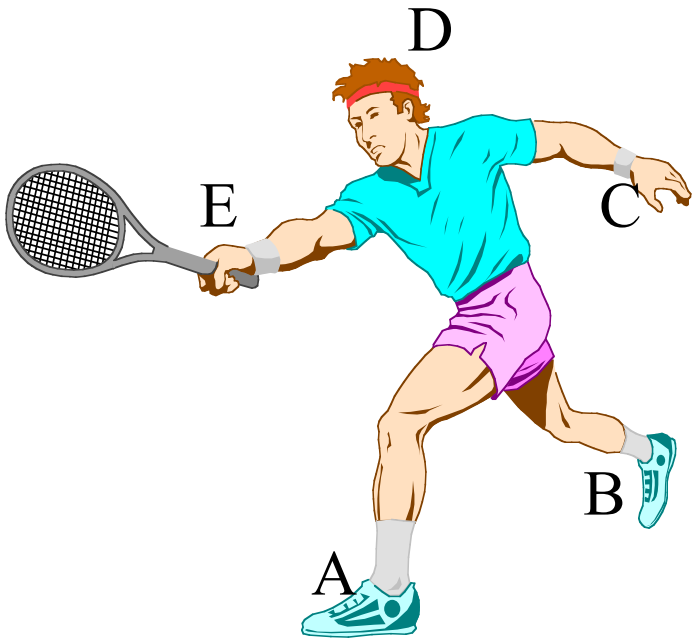
Qualitative Comparison

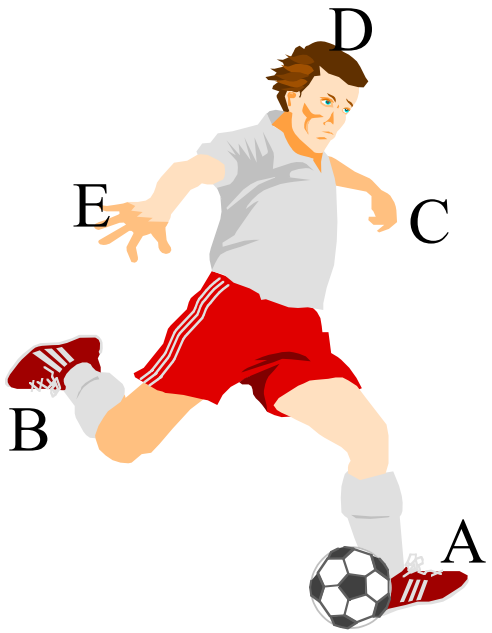


Outline

- Visualization Programs
- Vectors & Matrices
- Difference Distance Matrices
- Molecular Superposition
- Measuring Superposition
- Classifying 3D Structures

Difference Distance Matrix*





Object A **Object B**

Difference Distance Matrix*

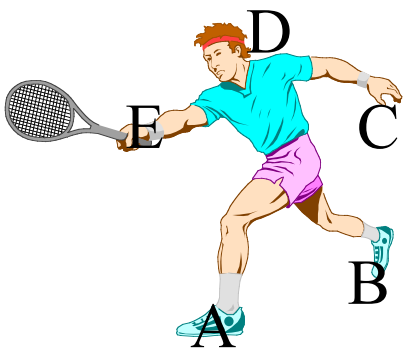
	A	B	C	D	E
A	0	4	5	6	4
B		0	4	6	7
C			0	3	6
D				0	3
E					0

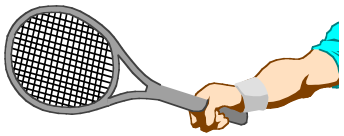
−

	A	B	C	D	E
A	0	4	5	6	4
B		0	4	5	3
C			0	3	5
D				0	3
E					0

=

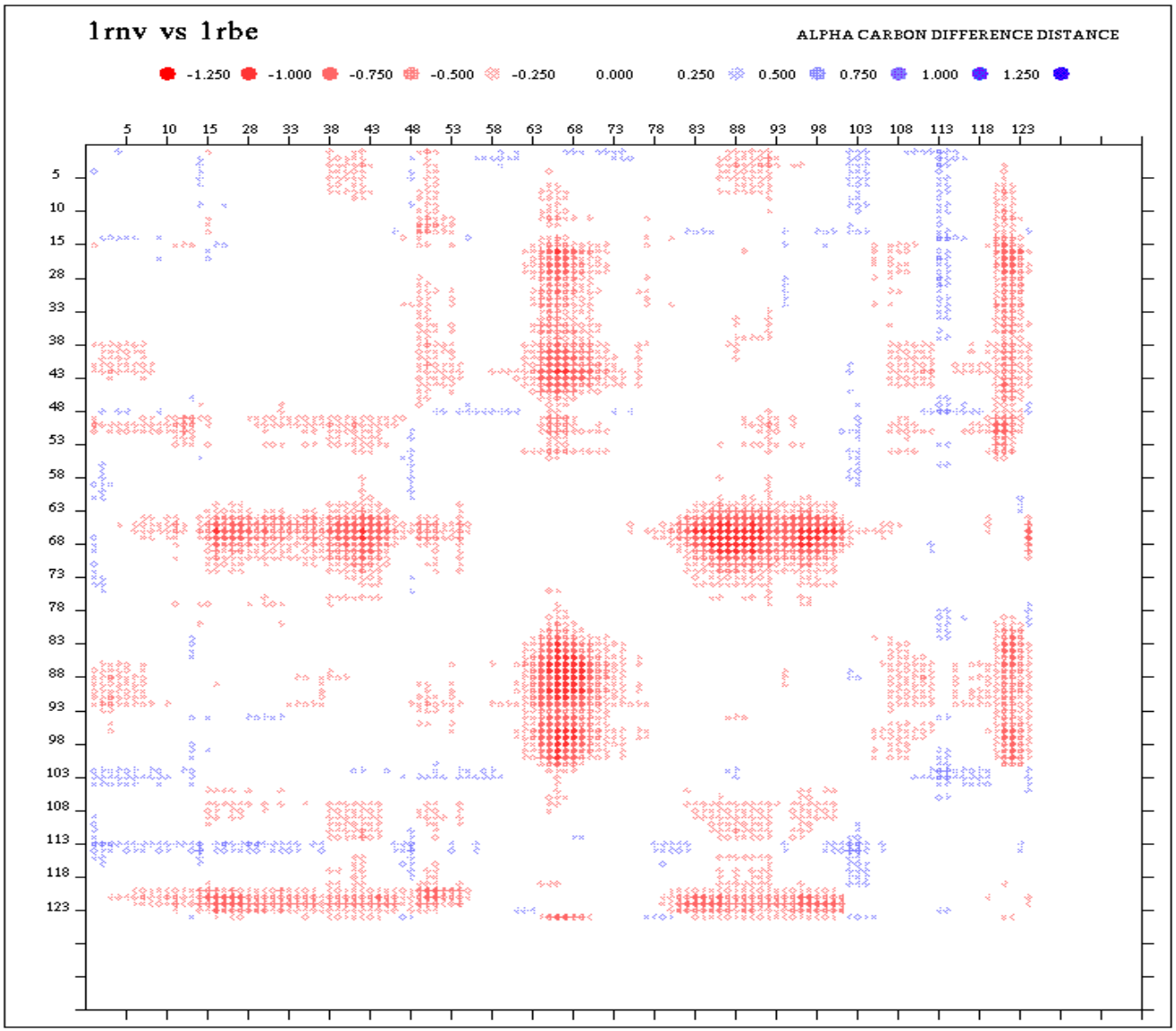
	A	B	C	D	E
A	0	0	0	0	0
B		0	0	1	4
C			0	0	1
D				0	0
E					0





Hinge motion

Difference Distance Matrix



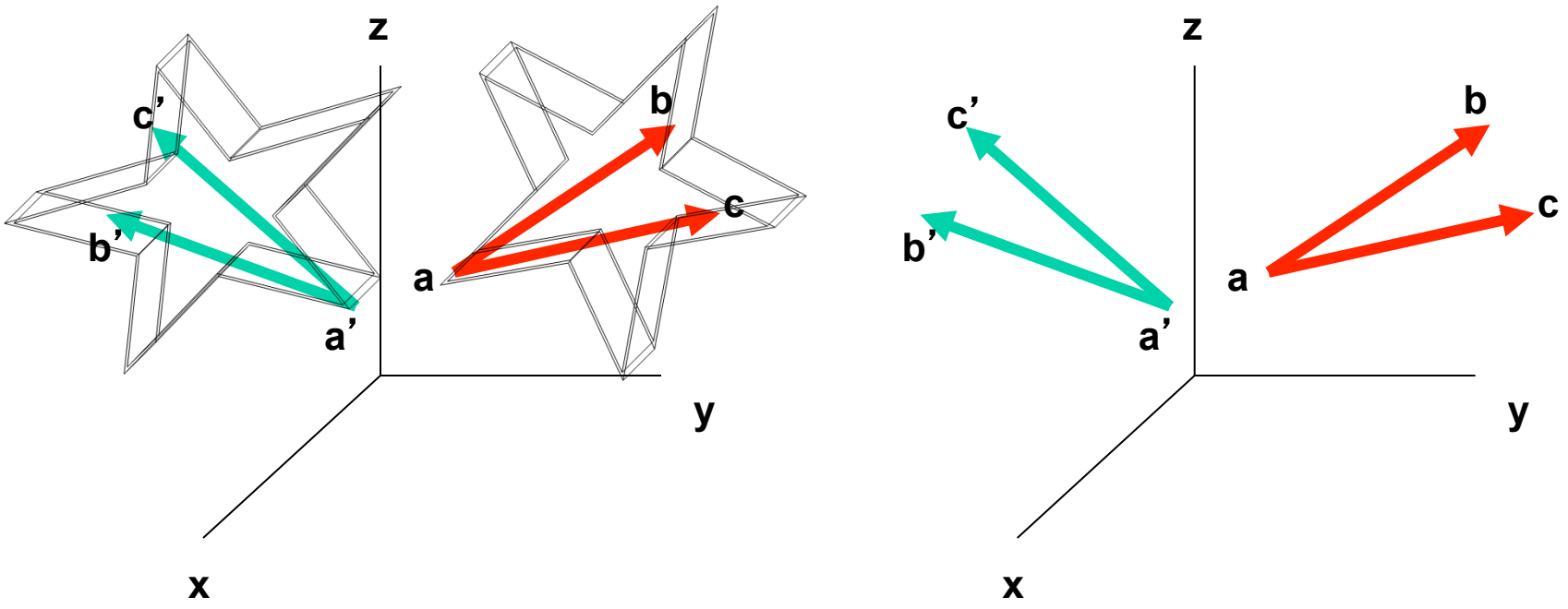
Difference Distance Matrices or DDM's*

- Simplest method to perform structural comparisons
- Requires no transfomations, no rotations or superpositions
- Very effective at identifying "hinge" motions or localized changes
- Produces a visually pleasing, quantitative measure of similarity

Superposition*

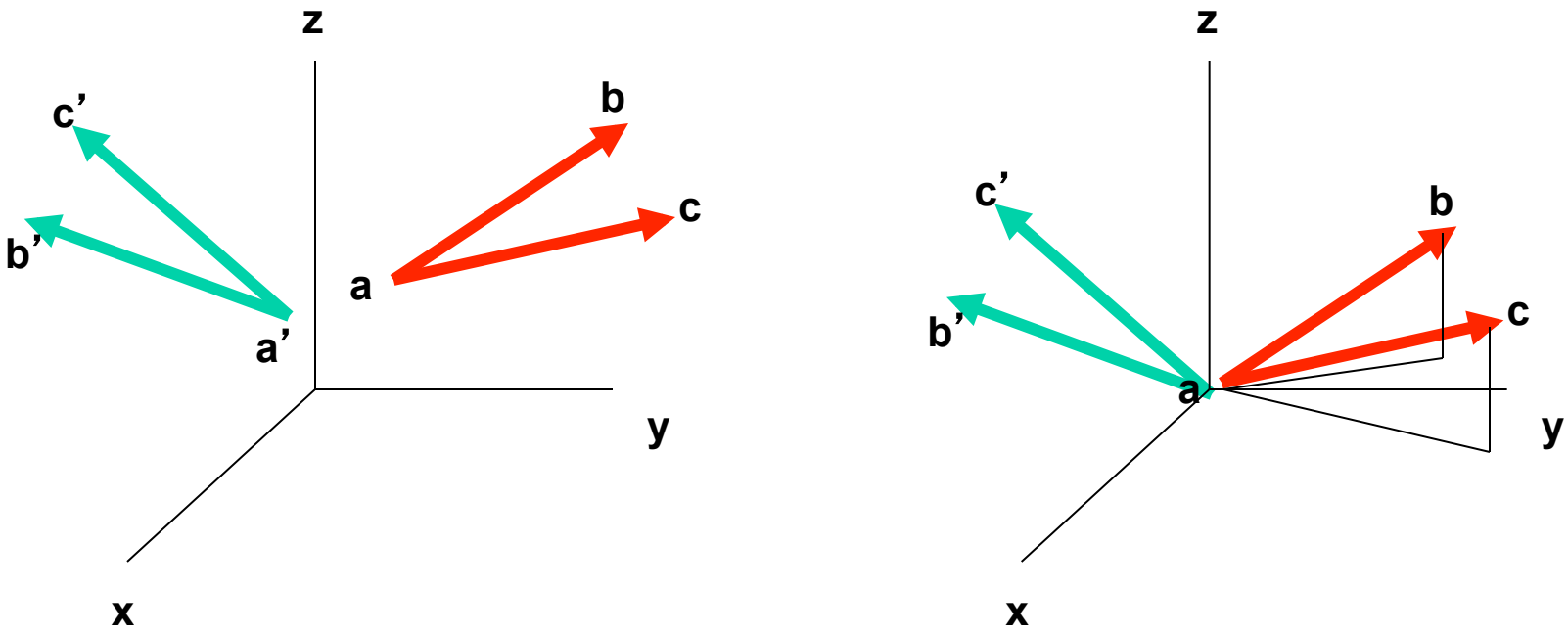
- Objective is to match or overlay 2 or more similar objects
- Requires use of translation and rotation operators (matrices/vectors)
- Recall that very three dimensional object can be represented by a plane defined by 3 points

Superposition*



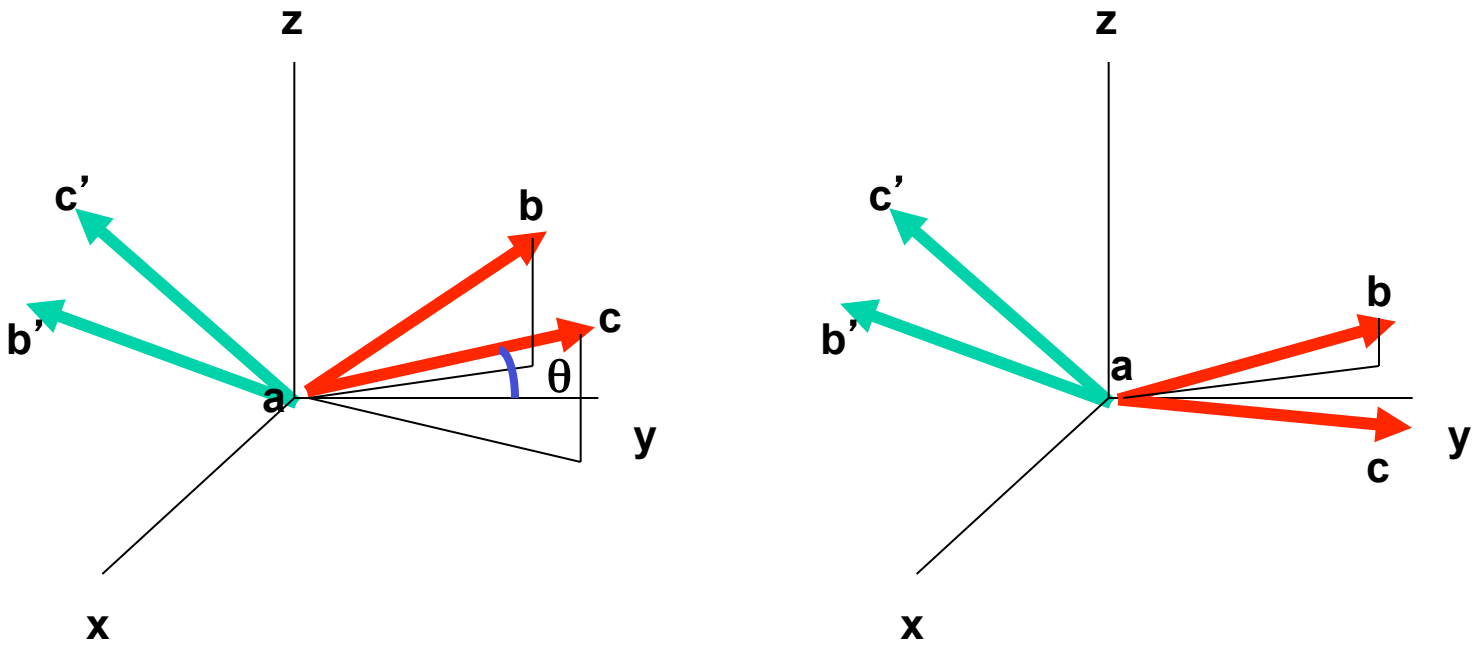
Identify 3 “equivalence” points in objects to be aligned

Superposition



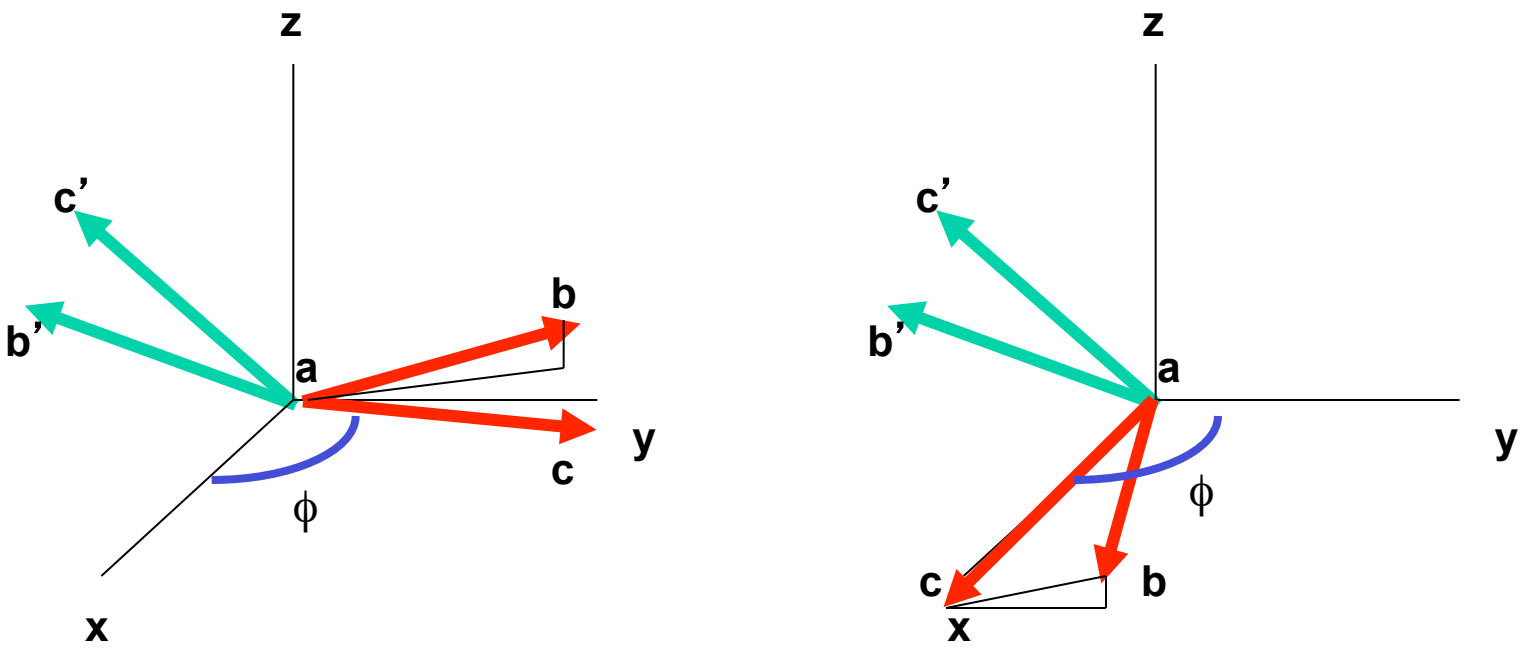
Translate points a,b,c and a’ ,b’ ,c’ to origin

Superposition



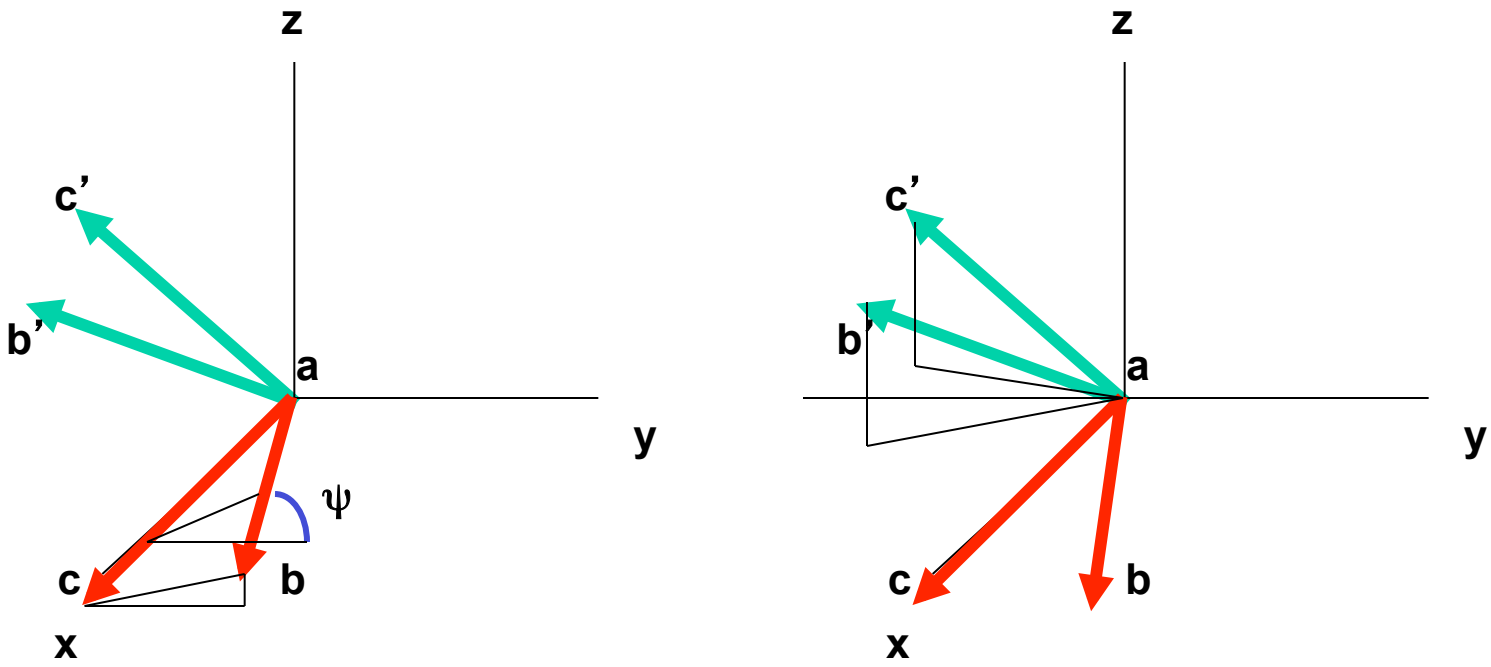
Rotate the a,b,c plane clockwise by θ about x axis

Superposition



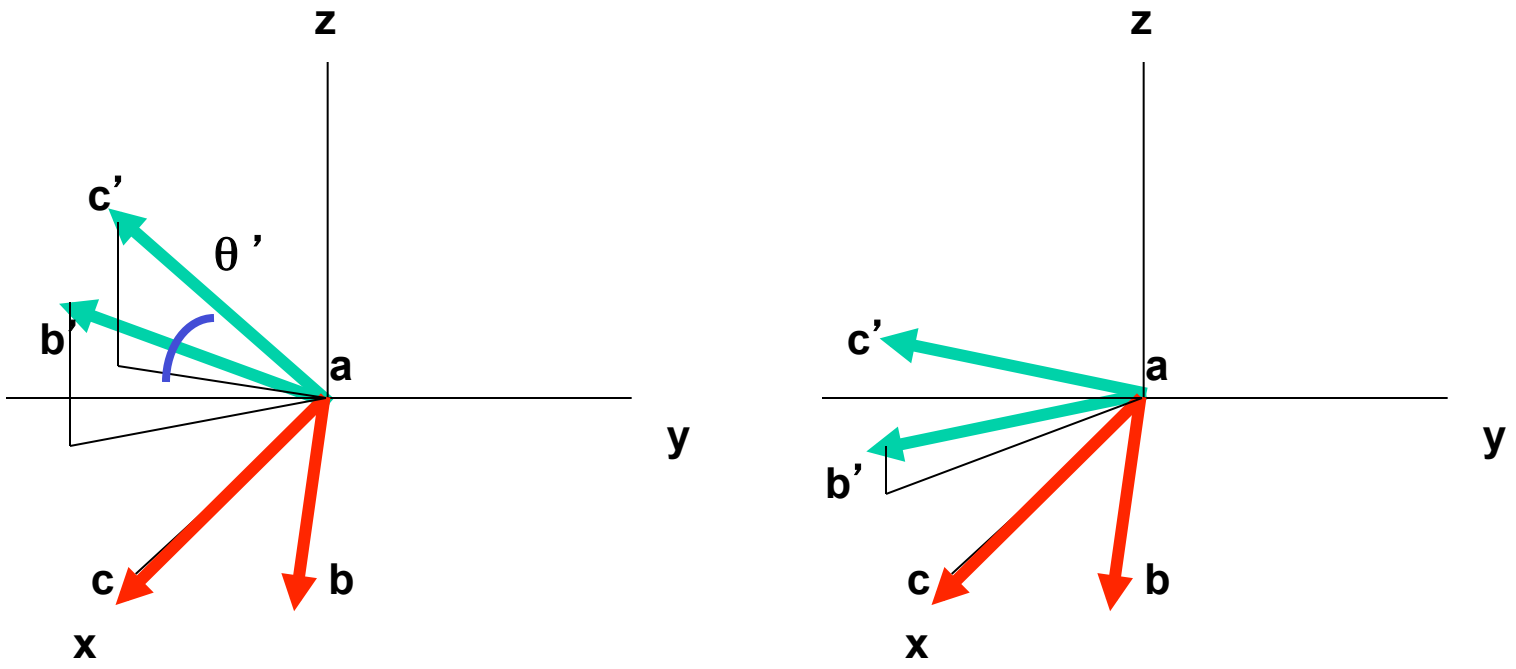
Rotate the a,b,c plane clockwise by ϕ about z axis

Superposition



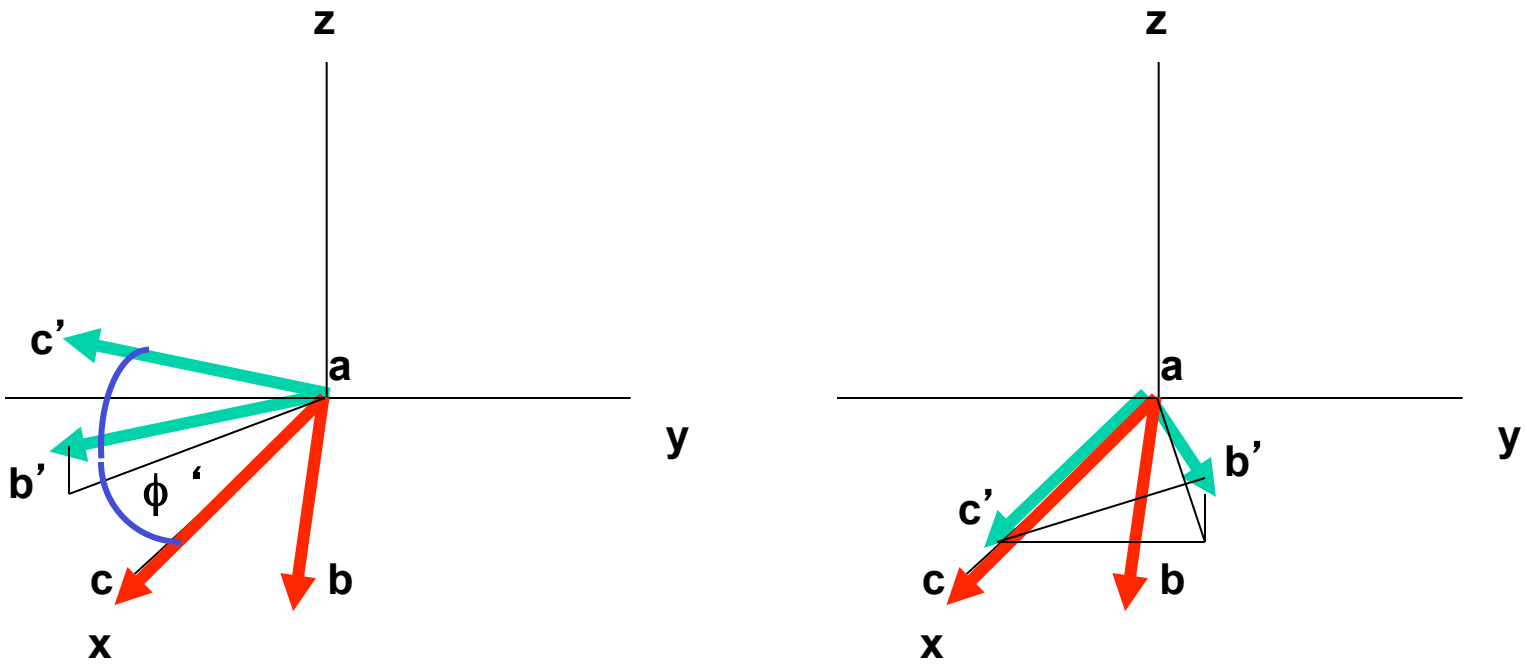
Rotate the a,b,c plane clockwise by ψ about x axis

Superposition



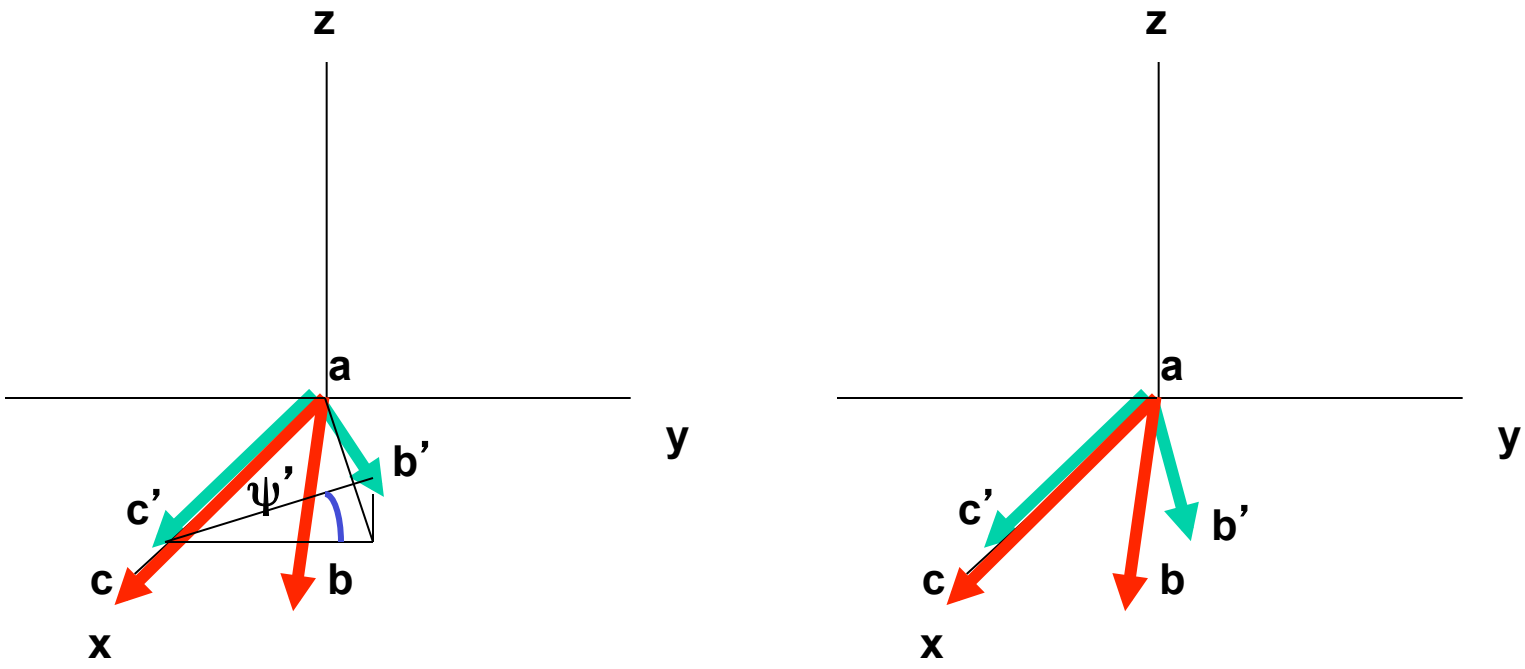
Rotate the a’,b’,c’ plane anticlockwise by θ’ about x axis

Superposition



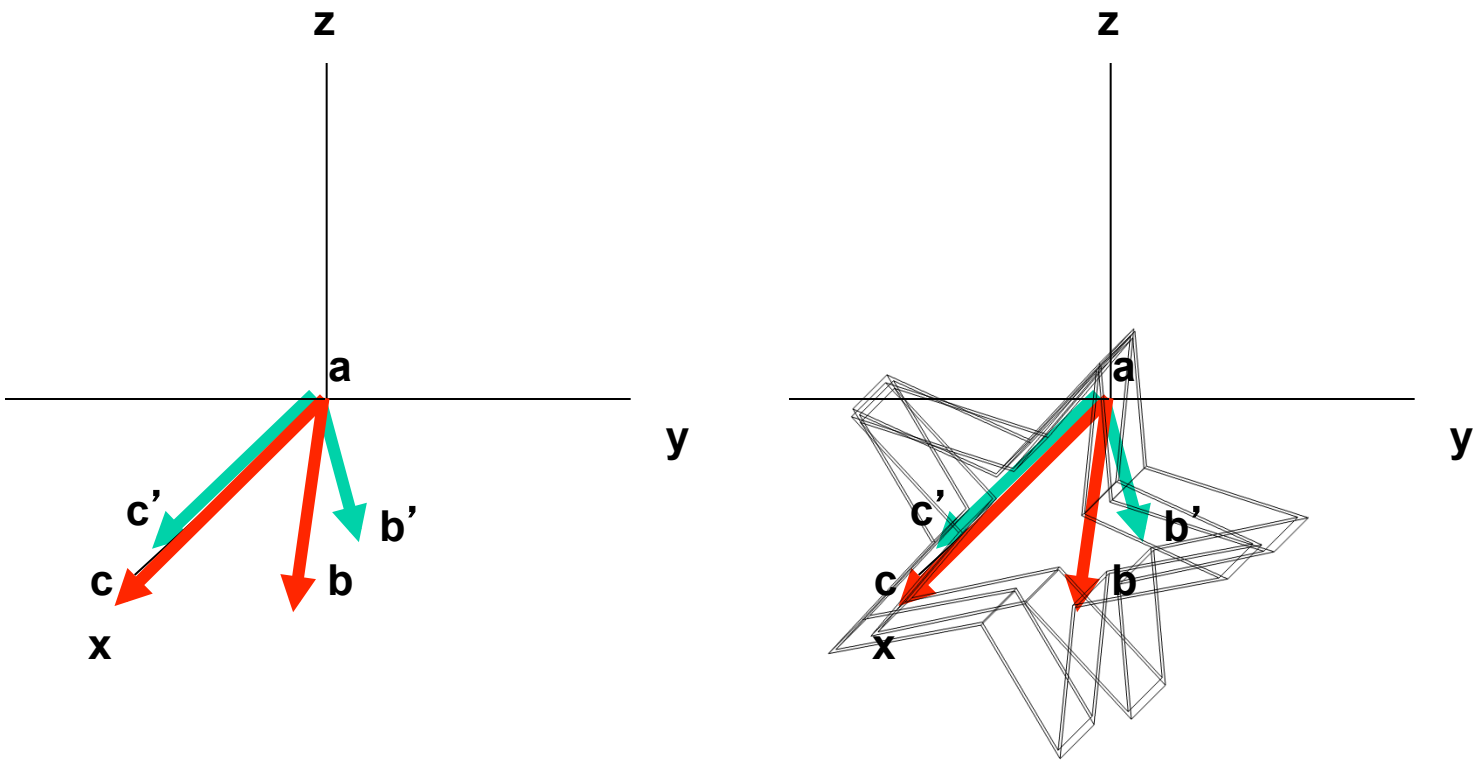
Rotate the a’,b’,c’ plane anticlockwise by ϕ’ about z axis

Superposition



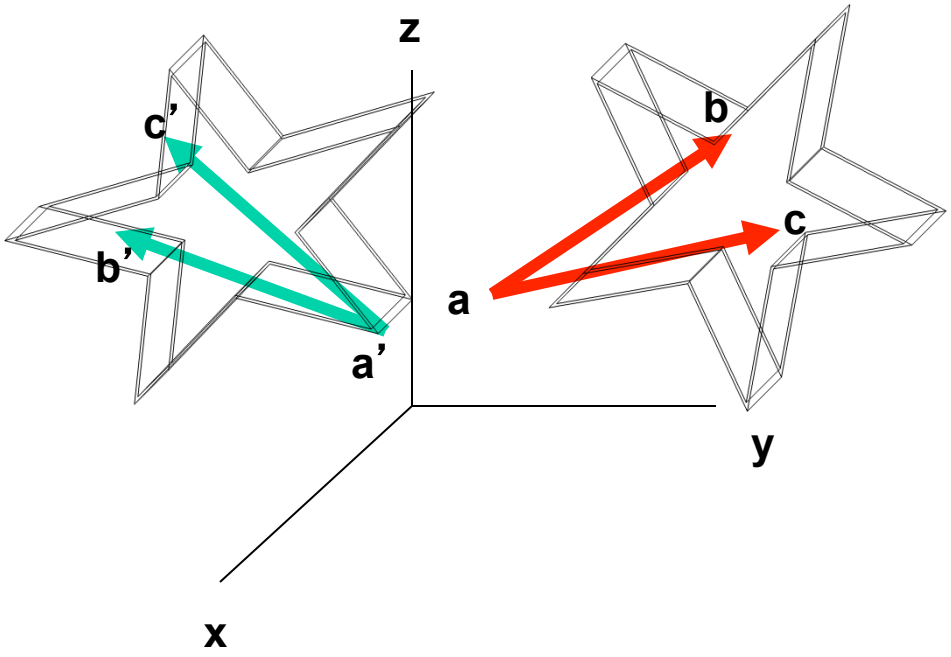
Rotate the a', b', c' plane clockwise by ψ' about x axis

Superposition

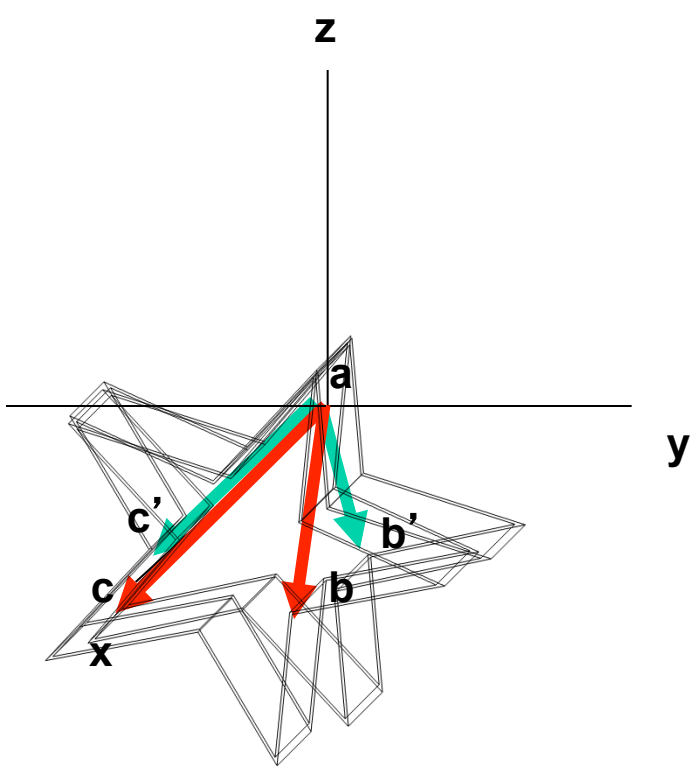


Apply all rotations and translations to remaining points

Superposition

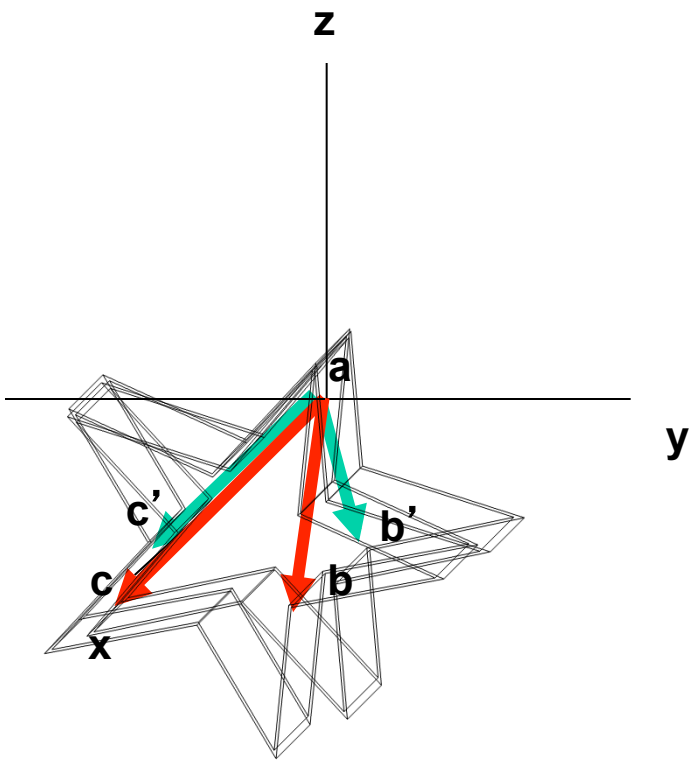


Before

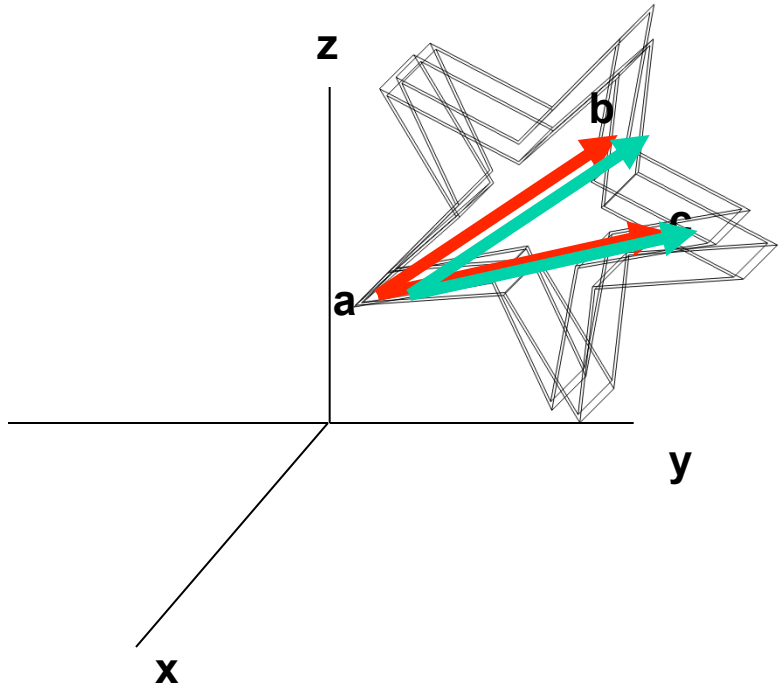


After

Returning to the “red” frame



Before



After

Returning to the "red" frame*

- Begin with the superimposed structures on the x-y plane
- Apply counterclockwise rot. By ψ
- Apply counterclockwise rot. By ϕ
- Apply counterclockwise rot. By θ
- Apply red translation to red origin

Just do things in reverse order!

Shortcomings*

- **Requires some initial assumptions regarding the anchoring points for superposition**
- **Anchoring points can't always *a priori* be known or easily calculated**
- **It "privileges" the first point "a" over "c" which is in turn privileged over "b"**

More General Approaches*

- Monte Carlo or Genetic Algorithms
- Matrix methods using least squares or conjugate gradient minimization (McLachlan/Kabsch)
- Lagrangian multipliers
- Rotation Angle Methods
- Quaternion-based methods (fastest)

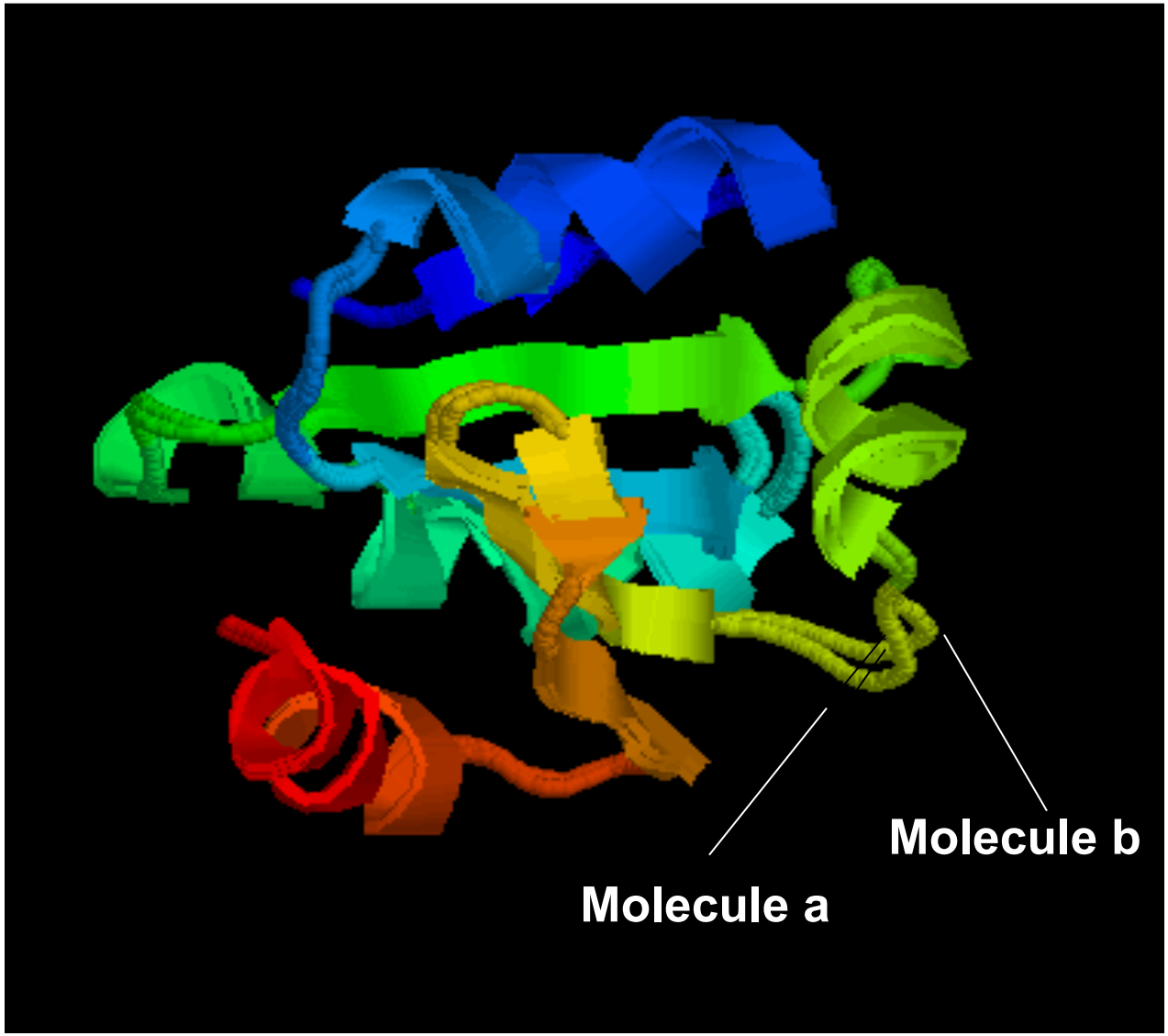
Superposition – Applications*

- **Ideal for comparing or overlaying two or more protein structures**
- **Allows identification of structural homologues (CATH and SCOP)**
- **Allows loops to be inserted or replaced from loop libraries (comparative modelling)**
- **Allows side chains to be replaced or inserted with relative ease**

Outline

- Visualization Programs
- Vectors & Matrices
- Difference Distance Matrices
- Molecular Superposition
- Measuring Superposition
- Classifying 3D Structures

Measuring Superpositions

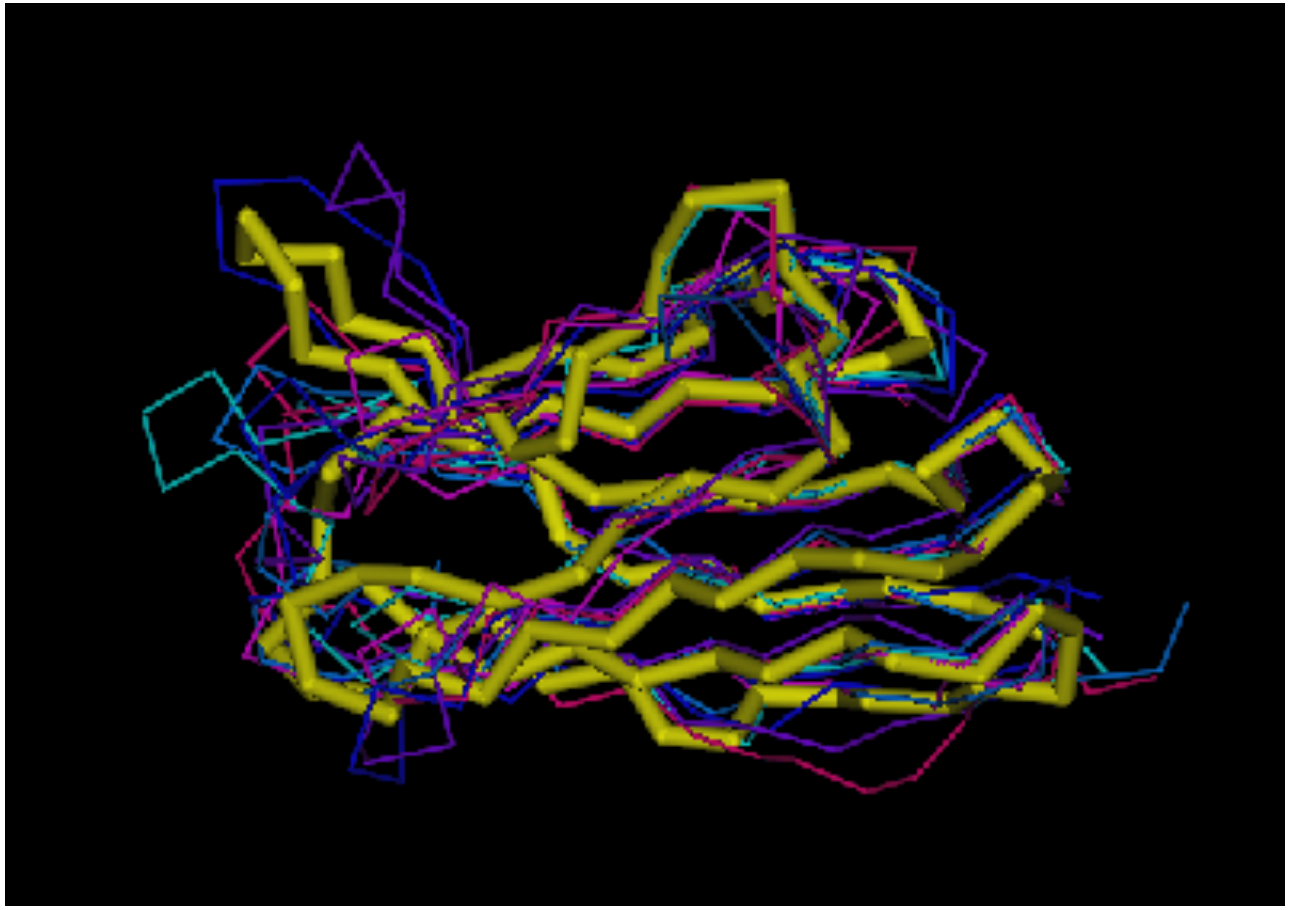


RMSD - Root Mean Square Deviation*

- **Method to quantify structural similarity - same as standard deviation**
- **Requires 2 superimposed structures (designated here as “a” & “b”)**
- **N = number of atoms being compared**

$$RMSD = \frac{\sqrt{\sum_i (x_{ai} - x_{bi})^2 + (y_{ai} - y_{bi})^2 + (z_{ai} - z_{bi})^2}}{\sqrt{N}}$$

Superpositions for Multiple Structures



RMSD - For Multiple Structures*

- Requires multiple superimposed structures over a single "averaged" structure ($\bar{x},\bar{y},\bar{z}$)
- N = number of atoms being compared
- M = number of structures superimposed

$$\text{RMSD} = \sum_{a} \left\{ \frac{\sqrt{\sum_{i} (x_{ai} - \bar{x}_i)^2 + (y_{ai} - \bar{y}_i)^2 + (z_{ai} - \bar{z}_i)^2}}{\sqrt{N}} \right\} \Bigg/ M$$

RMSD without Superposition*

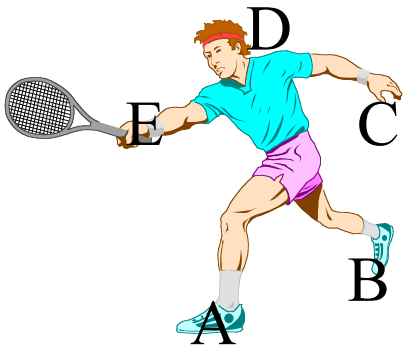
	A	B	C	D	E
A	0	4	5	6	4
B		0	4	6	7
C			0	3	6
D				0	3
E					0

−

	A	B	C	D	E
A	0	4	5	6	4
B		0	4	5	3
C			0	3	5
D				0	3
E					0

=

	A	B	C	D	E
A	0	0	0	0	0
B		0	0	1	4
C			0	0	1
D				0	0
E					0

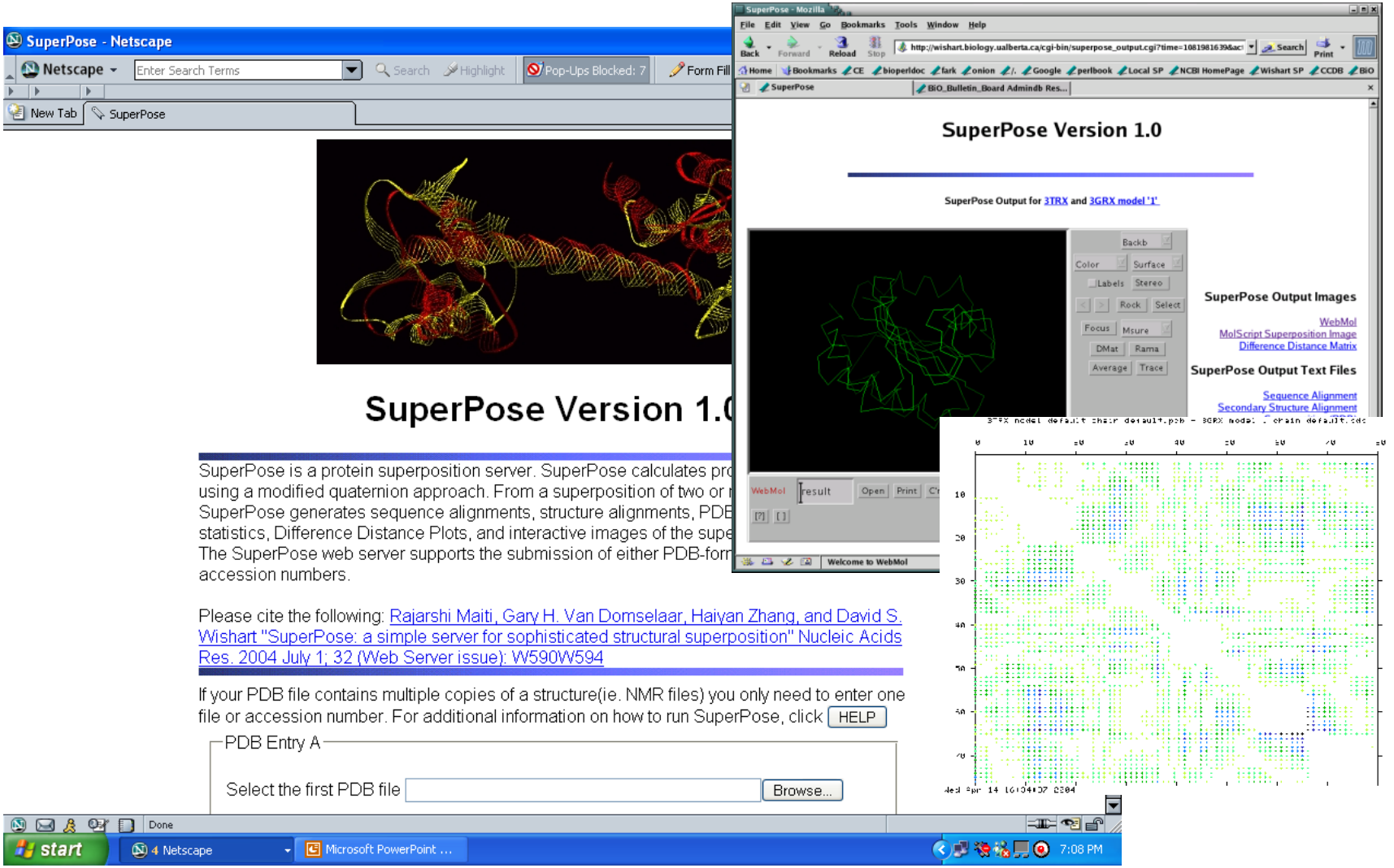


$$\text{RMS} = \frac{1+4+1}{\sqrt{10}} = 1.89$$

RMSD*

- 0.0-0.5 Å → Essentially Identical
- <1.5 Å → Very good fit
- < 5.0 Å → Moderately good fit
- 5.0-7.0 Å → Structurally related
- > 7.0 Å → Dubious relationship
- > 12.0 Å → Completely unrelated

SuperPose Web Server



http://wishart.biology.ualberta.ca/SuperPose/

Outline

- Visualization Programs
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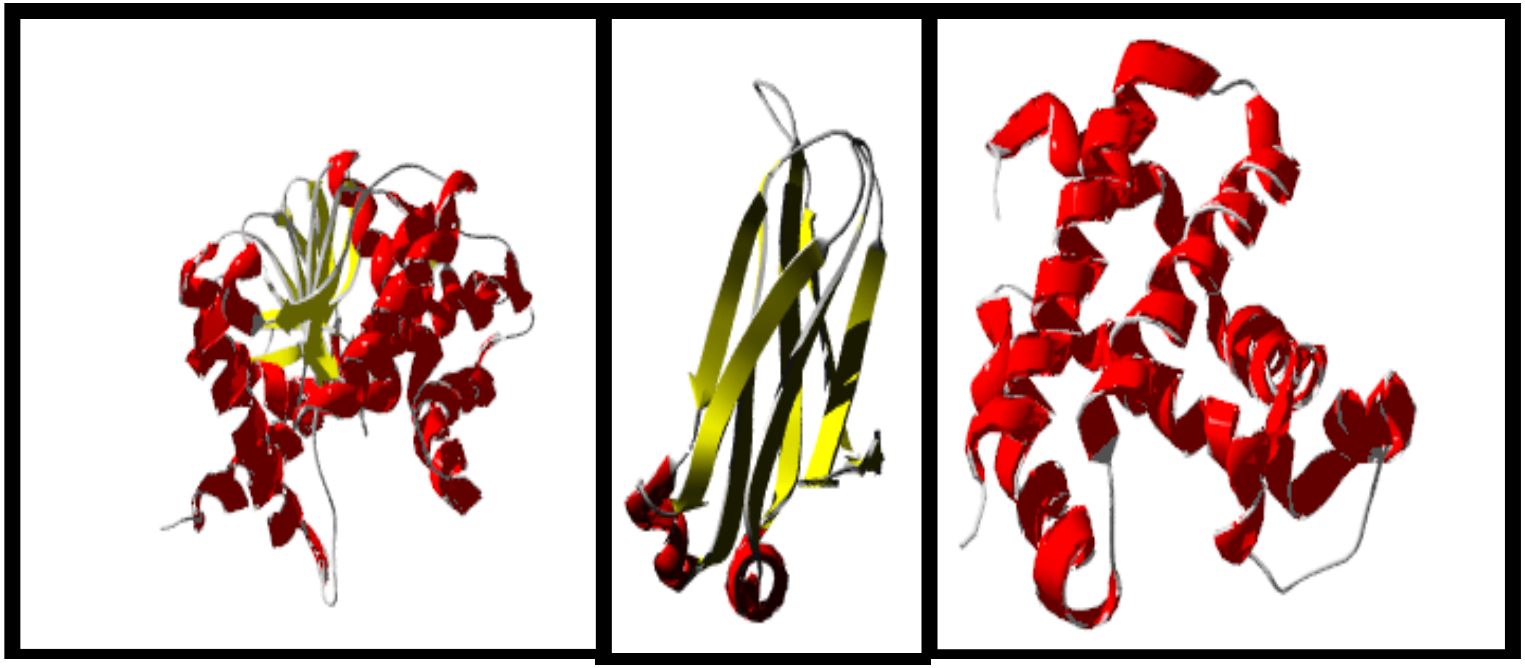
Classifying Protein Folds*

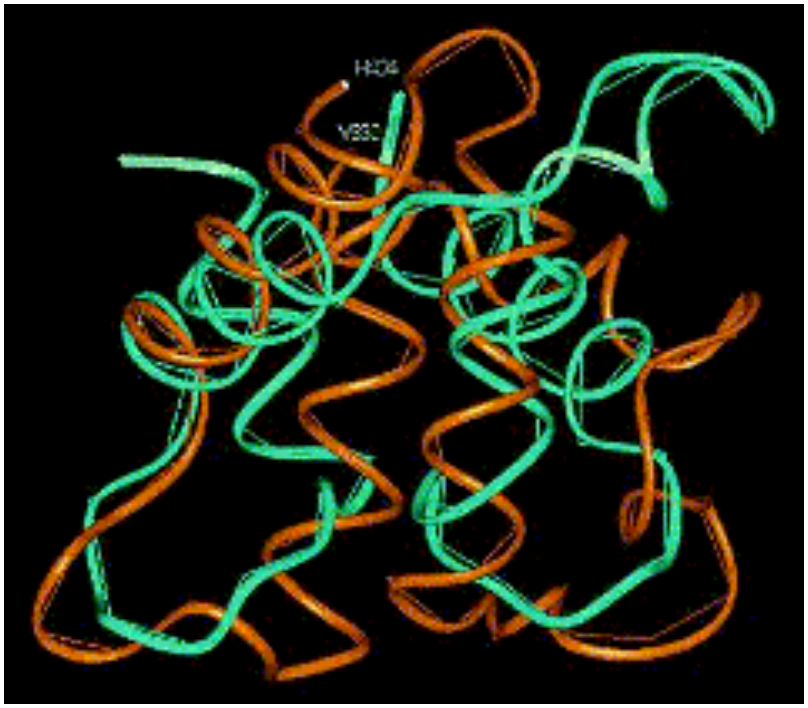


Lactate Dehydrogenase: Mixed α / β

Immunoglobulin Fold: β

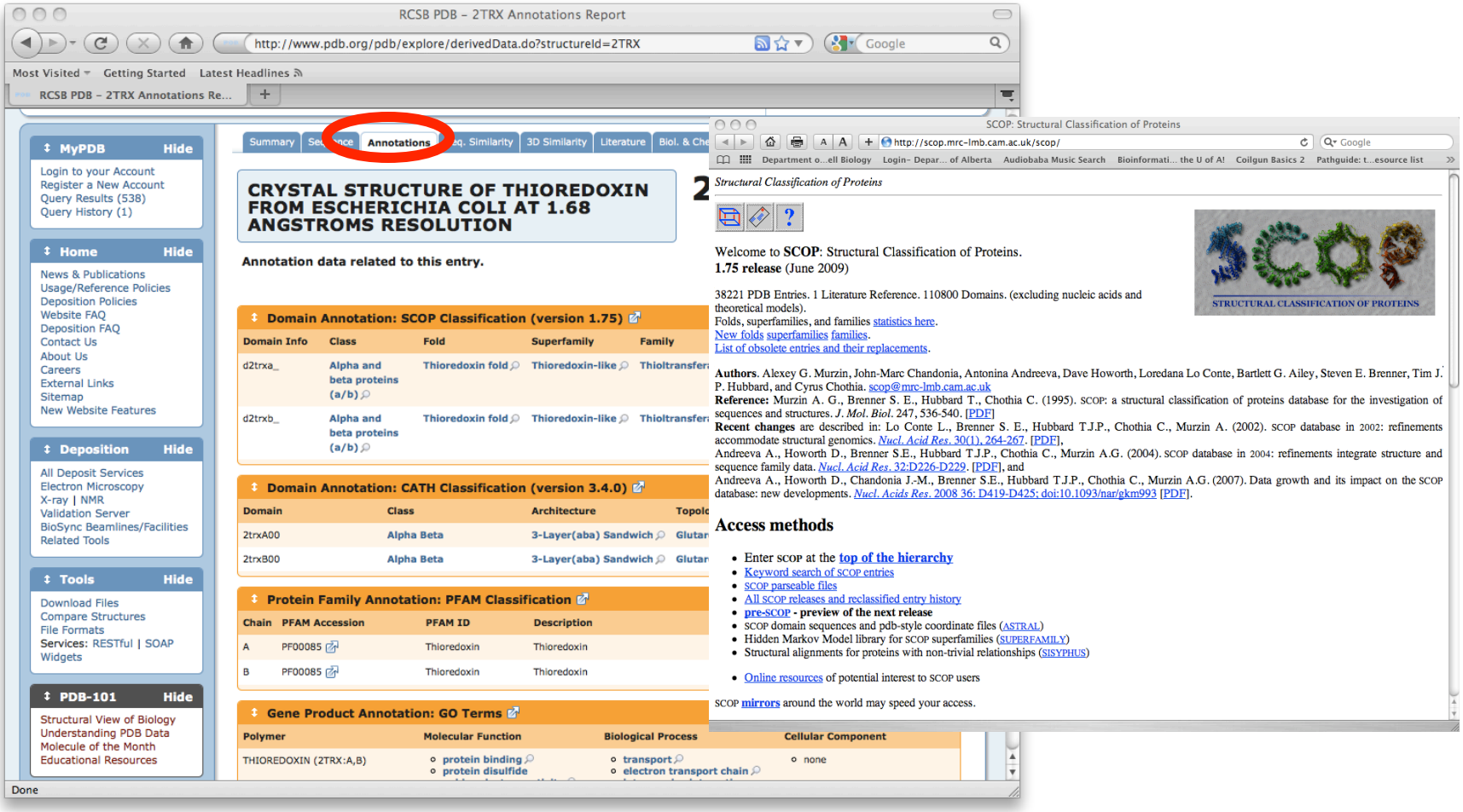
Hemoglobin B Chain: α

Detecting Unusual Relationships

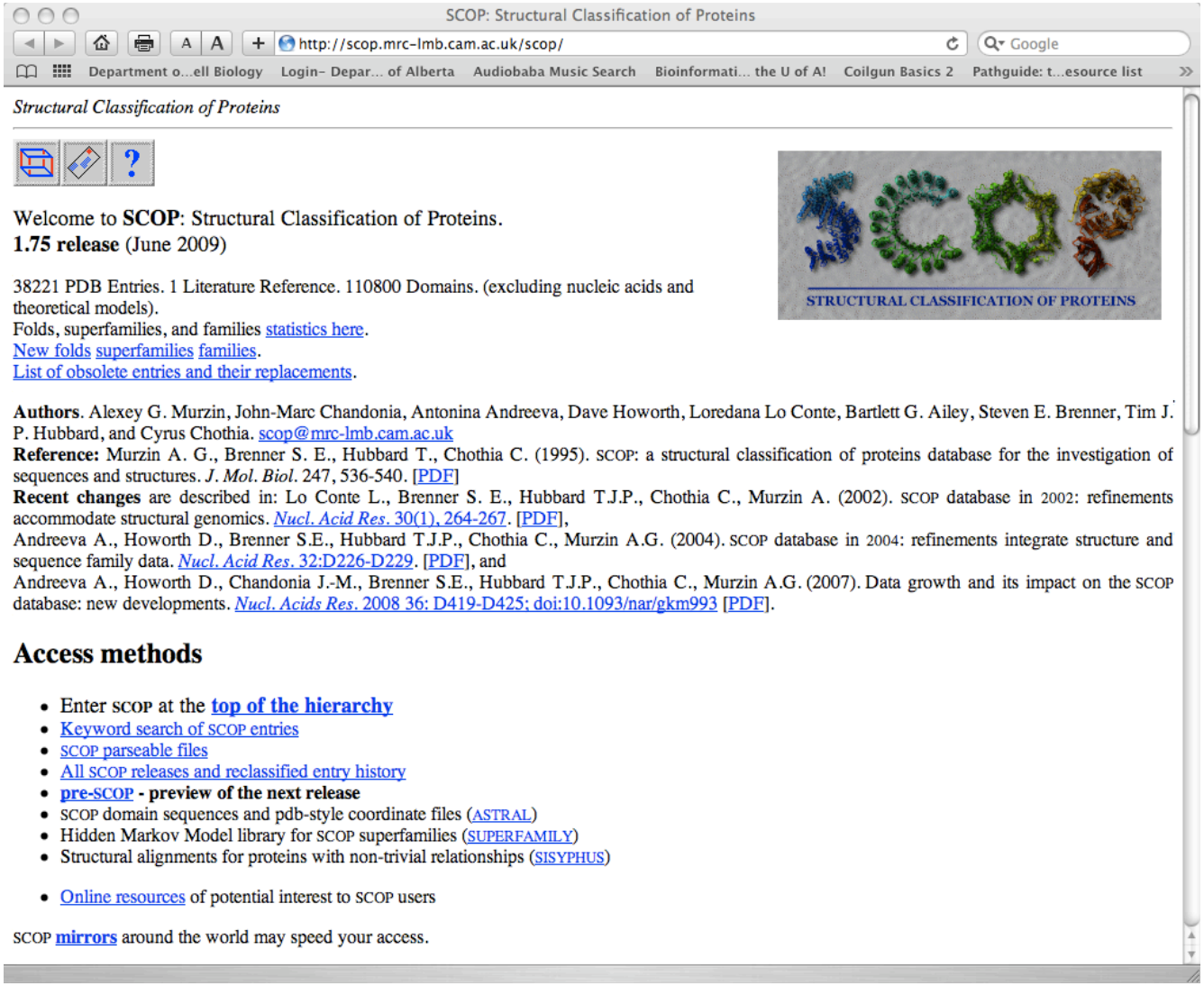


Similarity between Calmodulin and Acetylcholinesterase

Classifying Protein Folds



SCOP Database

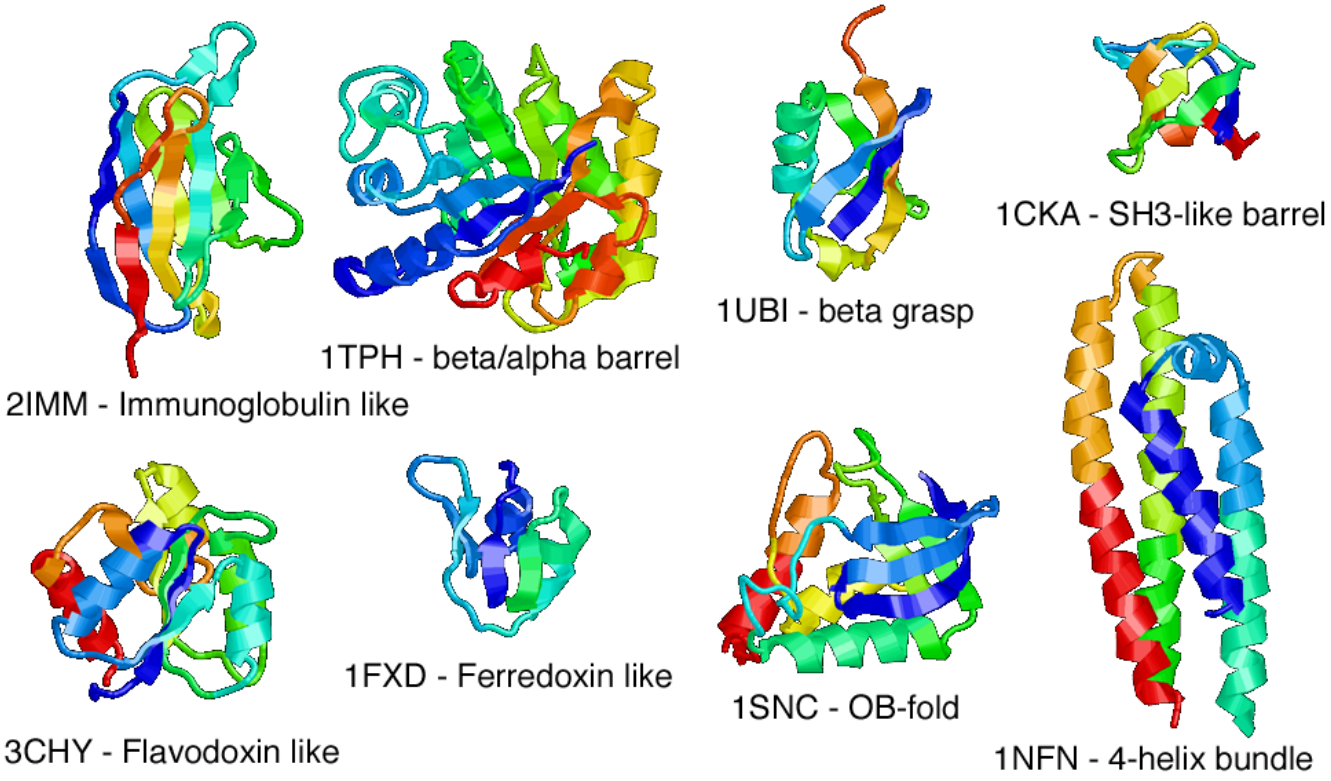


http://scop.mrc-lmb.cam.ac.uk/scop

SCOP

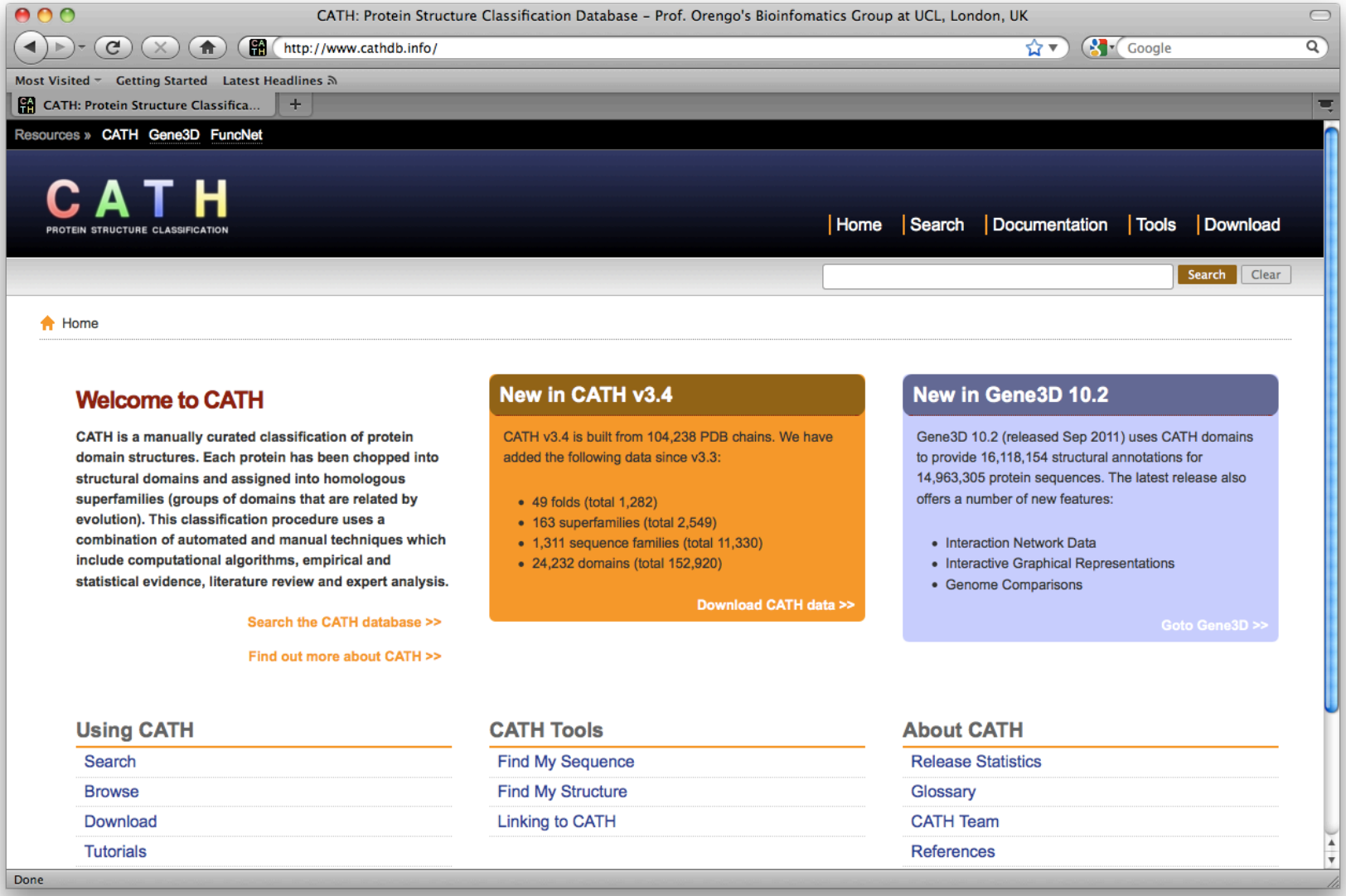
- **Class** folding class derived from secondary structure content
- **Fold** derived from topological connection, orientation, arrangement and # 2° structures
- **Superfamily** clusters of low sequence ID but related structures & functions
- **Family** clusers of proteins with seq ID > 30% with v. similar struct. & function

SCOP Structural Classification



The eight most frequent SCOP superfolds

The CATH Database

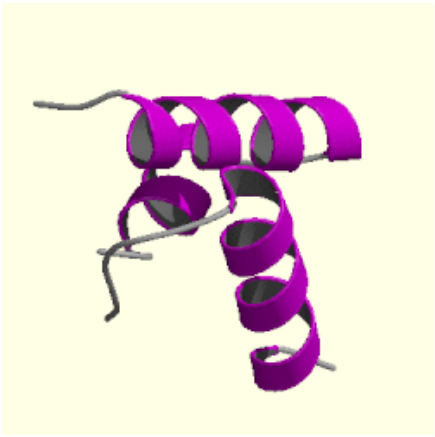


http://www.cathdb.info

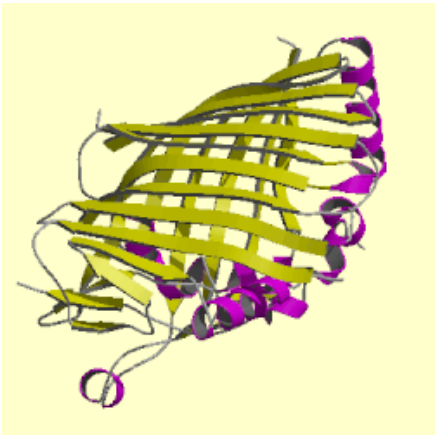
CATH

- **Class** [C] derived from secondary structure content (automatic)
- **Architecture** (A) derived from orientation of 2° structures (manual)
- **Topology** (T) derived from topological connection and # 2° structures
- **Homologous** Superfamily (H) clusters of similar structures & functions

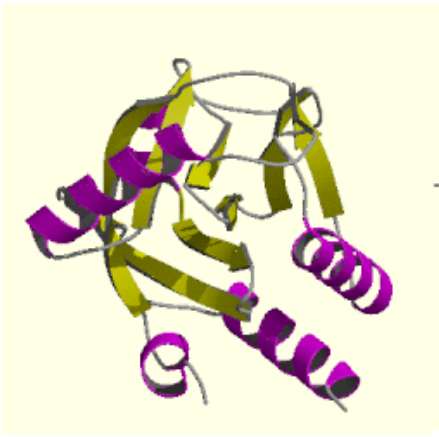
CATH - Class



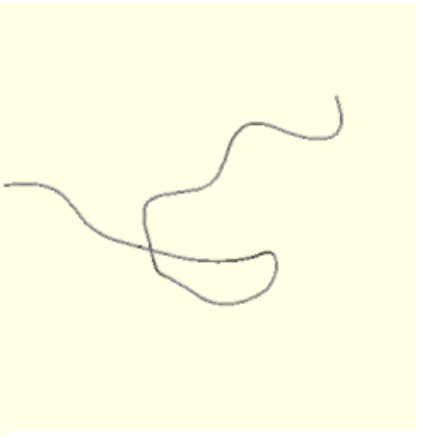
Class 1:
Mainly Alpha



Class 2:
Mainly Beta



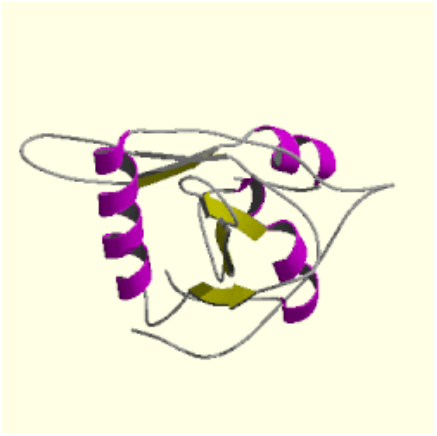
Class 3:
Mixed Alpha/
Beta



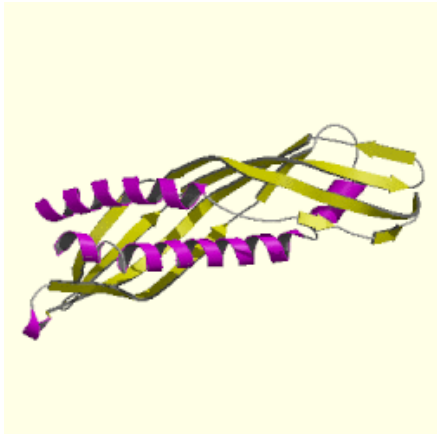
Class 4:
Few Secondary
Structures

Secondary structure content (automatic)

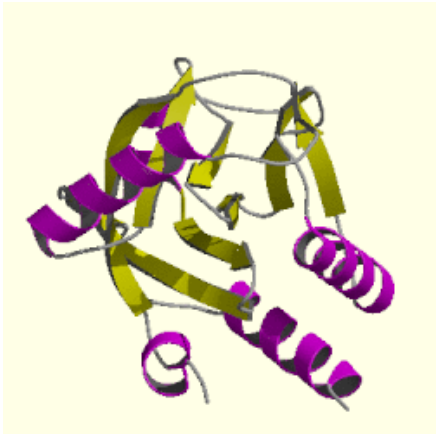
CATH - Architecture



Roll



Super Roll

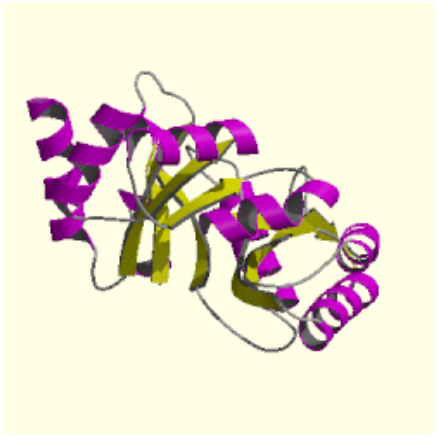


Barrel

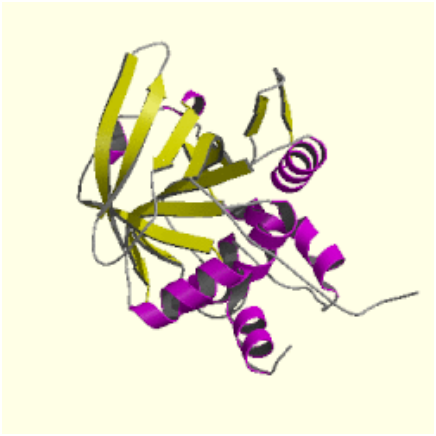
2-Layer Sandwich

Orientation of secondary structures (manual)

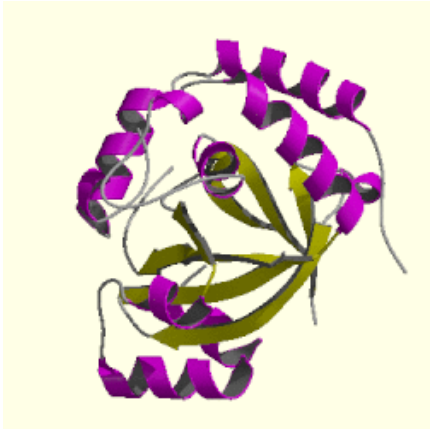
CATH - Topology



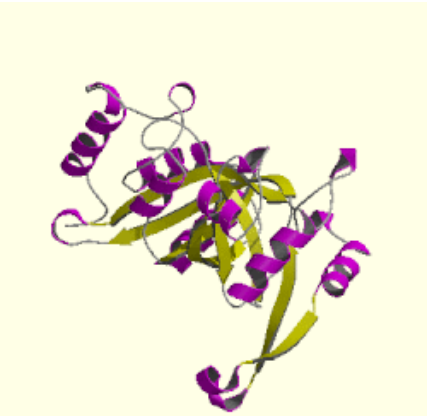
L-fucose Isomerase



Serine Protease



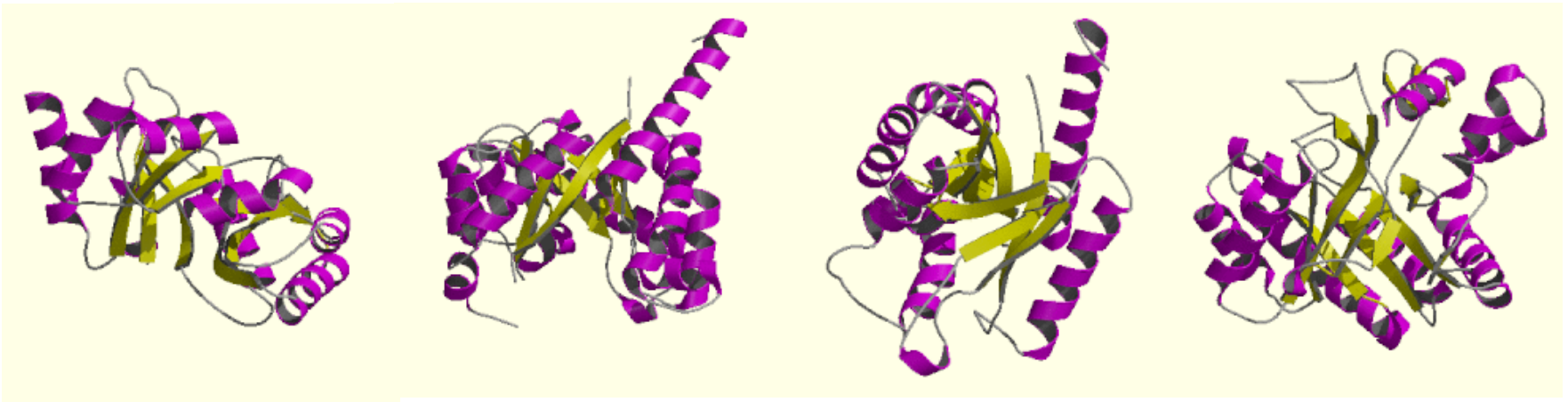
Aconitase, domain 4



TIM Barrel

Topological connection and number of secondary structures

CATH - Homology



Alanine racemase

Dihydropteroate (DHP) synthetase

FMN dependent fluorescent proteins

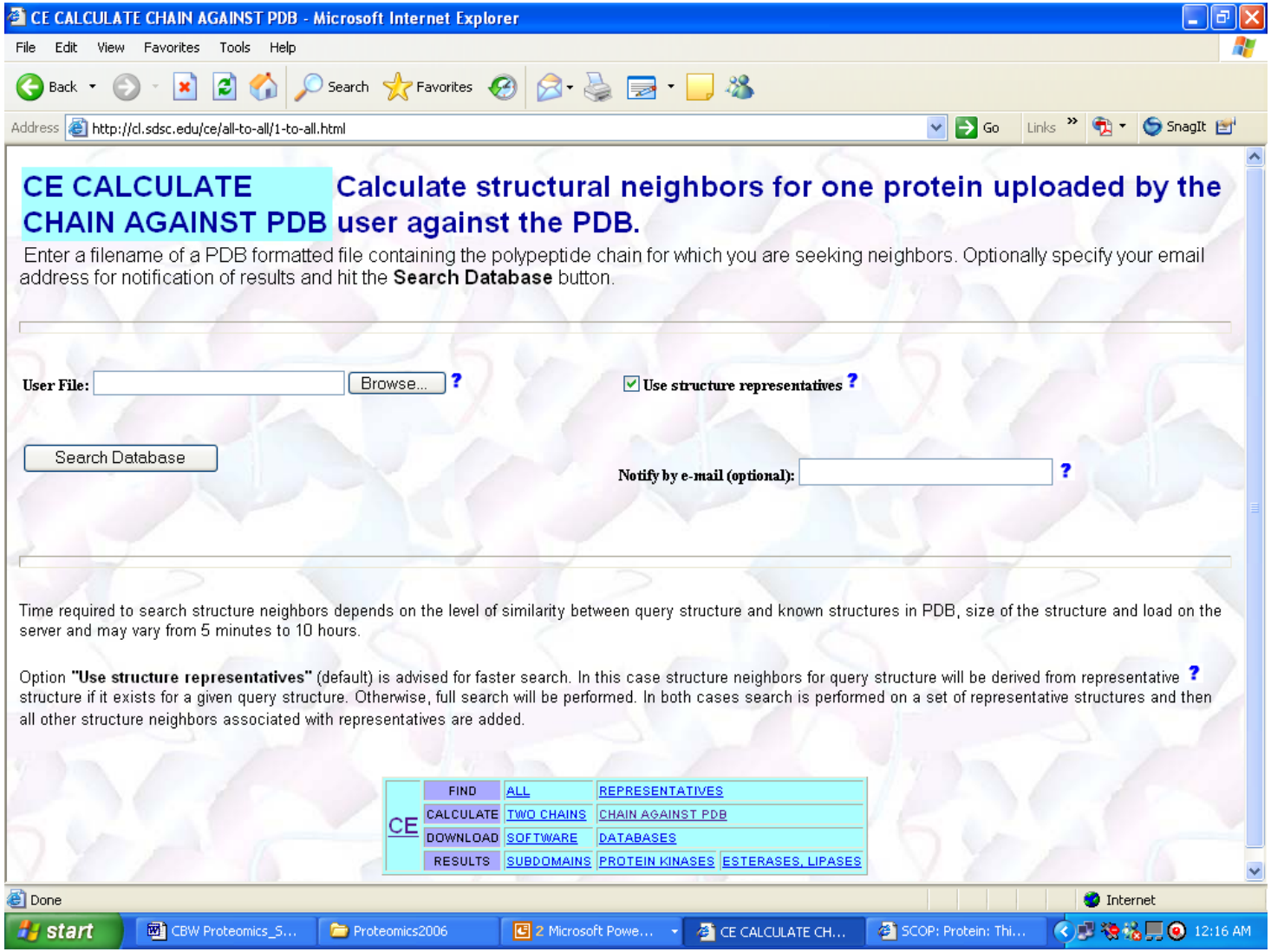
7-stranded glycosidases

Superfamily clusters of similar structures & functions

Other Servers/Databases

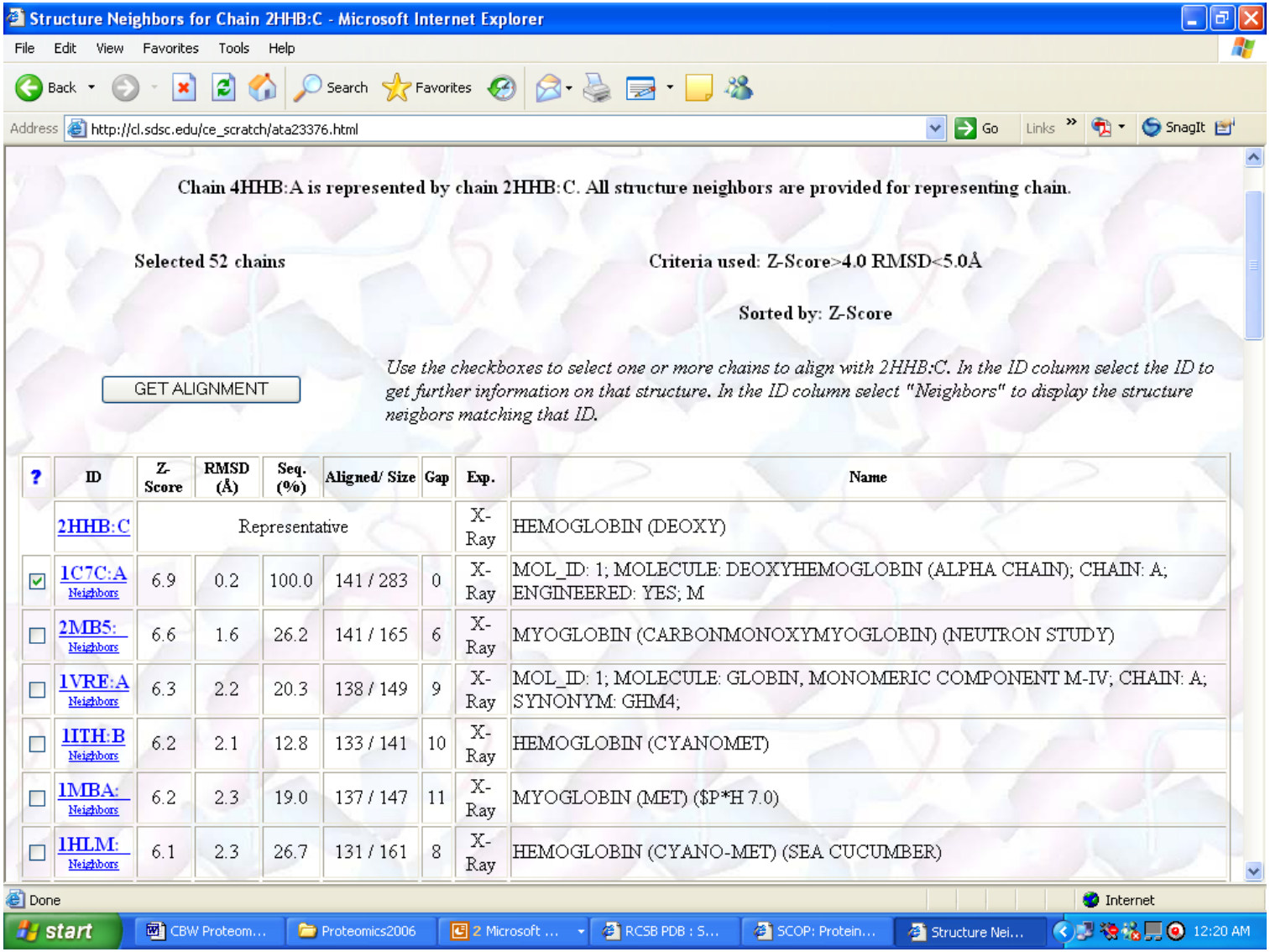
- **Dali -** http://ekhidna.biocenter.helsinki.fi/dali_server/
- **VAST -** http://www.ncbi.nlm.nih.gov/Structure/VAST/vast.shtml
- **Matras -** http://biunit.aist-nara.ac.jp/matras/
- **CE -** http://cl.sdsc.edu/ce.html
- **TopMatch -** http://topmatch.services.came.sbg.ac.at/
- **PDBsum -** http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/

CE Search



http://cl.sdsc.edu/ce/all-to-all/1-to-all.html

CE Search


Structure Neighbors for Chain 2HHB:C - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites
Address http://cl.sdsc.edu/ce_scratch/ata23376.html
Go Links SnagIt
Chain 4HHB:A is represented by chain 2HHB:C. All structure neighbors are provided for representing chain.
Selected 52 chains
Criteria used: Z-Score>4.0 RMSD<5.0Å
Sorted by: Z-Score
GET ALIGNMENT
Use the checkboxes to select one or more chains to align with 2HHB:C. In the ID column select the ID to get further information on that structure. In the ID column select "Neighbors" to display the structure neigbors matching that ID.
? | ID | Z-Score | RMSD (Å) | Seq. (%) | Aligned/ Size | Gap | Exp. | Name
2HHB:C | Representative | X-Ray | HEMOGLOBIN (DEOXY)
1C7C:A Neighbors | 6.9 | 0.2 | 100.0 | 141 / 283 | 0 | X-Ray | MOL_ID: 1; MOLECULE: DEOXYHEMOGLOBIN (ALPHA CHAIN); CHAIN: A; ENGINEERED: YES; M
2MB5: Neighbors | 6.6 | 1.6 | 26.2 | 141 / 165 | 6 | X-Ray | MYOGLOBIN (CARBONMONOXYMYOGLOBIN) (NEUTRON STUDY)
1VRE:A Neighbors | 6.3 | 2.2 | 20.3 | 138 / 149 | 9 | X-Ray | MOL_ID: 1; MOLECULE: GLOBIN, MONOMERIC COMPONENT M-IV; CHAIN: A; SYNONYM: GHM4;
1ITH:B Neighbors | 6.2 | 2.1 | 12.8 | 133 / 141 | 10 | X-Ray | HEMOGLOBIN (CYANOMET)
1MBA: Neighbors | 6.2 | 2.3 | 19.0 | 137 / 147 | 11 | X-Ray | MYOGLOBIN (MET) ($P*H 7.0)
1HLM: Neighbors | 6.1 | 2.3 | 26.7 | 131 / 161 | 8 | X-Ray | HEMOGLOBIN (CYANO-MET) (SEA CUCUMBER)
Done
Internet
start
CBW Proteom...
Proteomics2006
2 Microsoft ...
RCSB PDB : S...
SCOP: Protein...
Structure Nei...
12:20 AM

Summary

- **Many different tools and formats to visualize 3D structure – *learn how to use at least one of them***
- **Visualization on computers is mostly about matrix and vector manipulation**
- **Structure comparison also requires the use of linear algebra**
- **Protein structures can be compared and aligned – just like sequences**