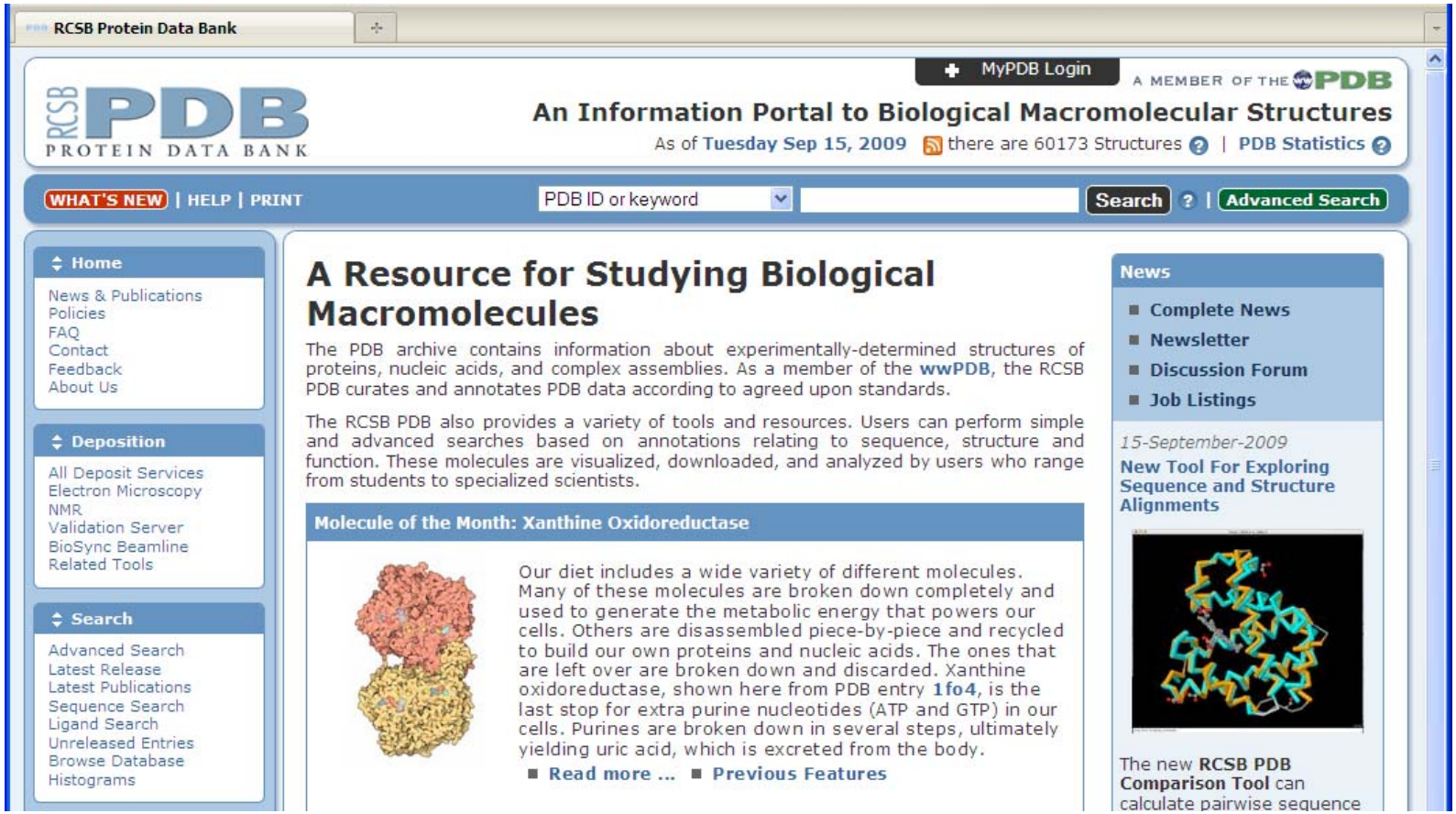
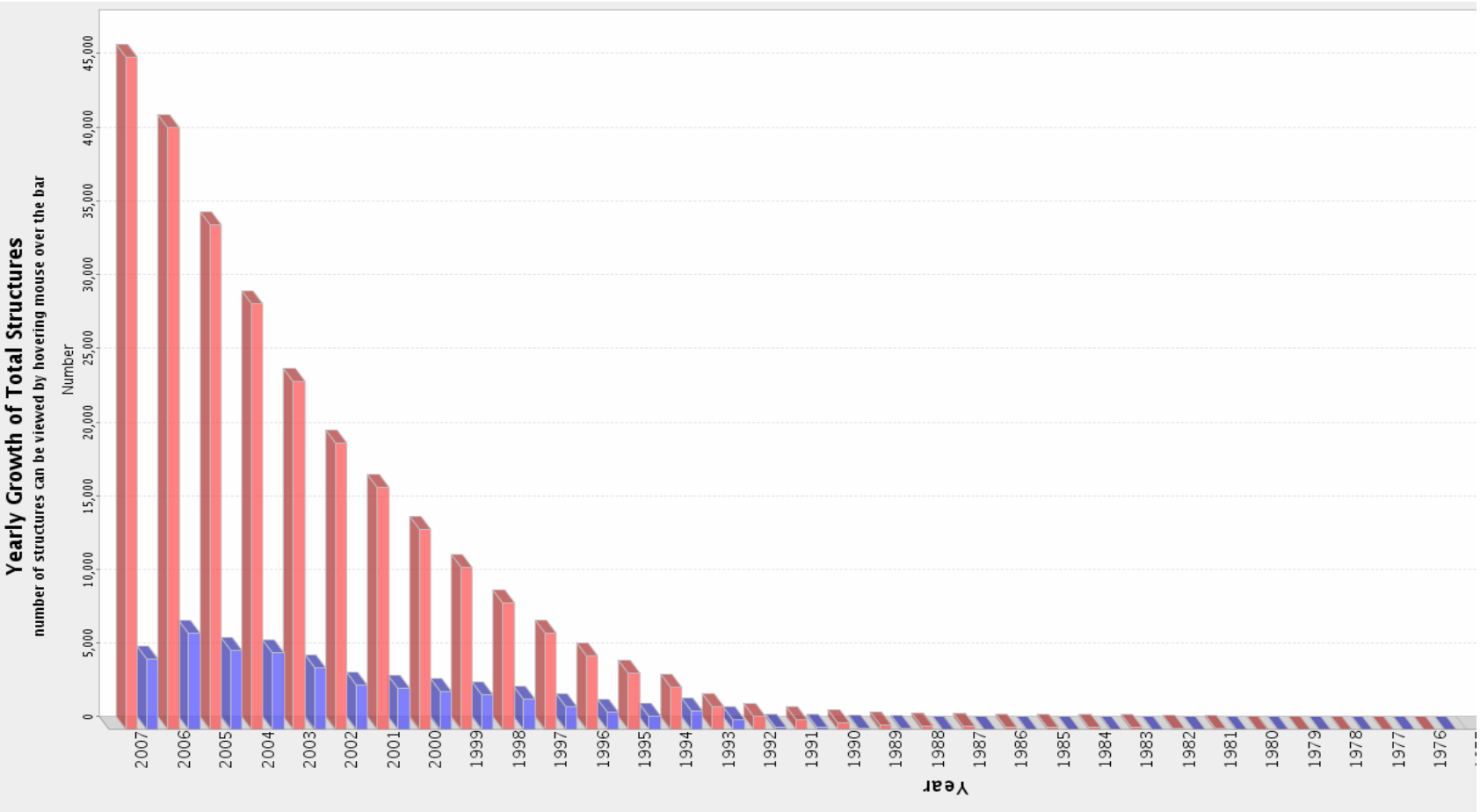
Protein databases

PDB database

- From the class website
- External Links/Structure Databases/PDB database

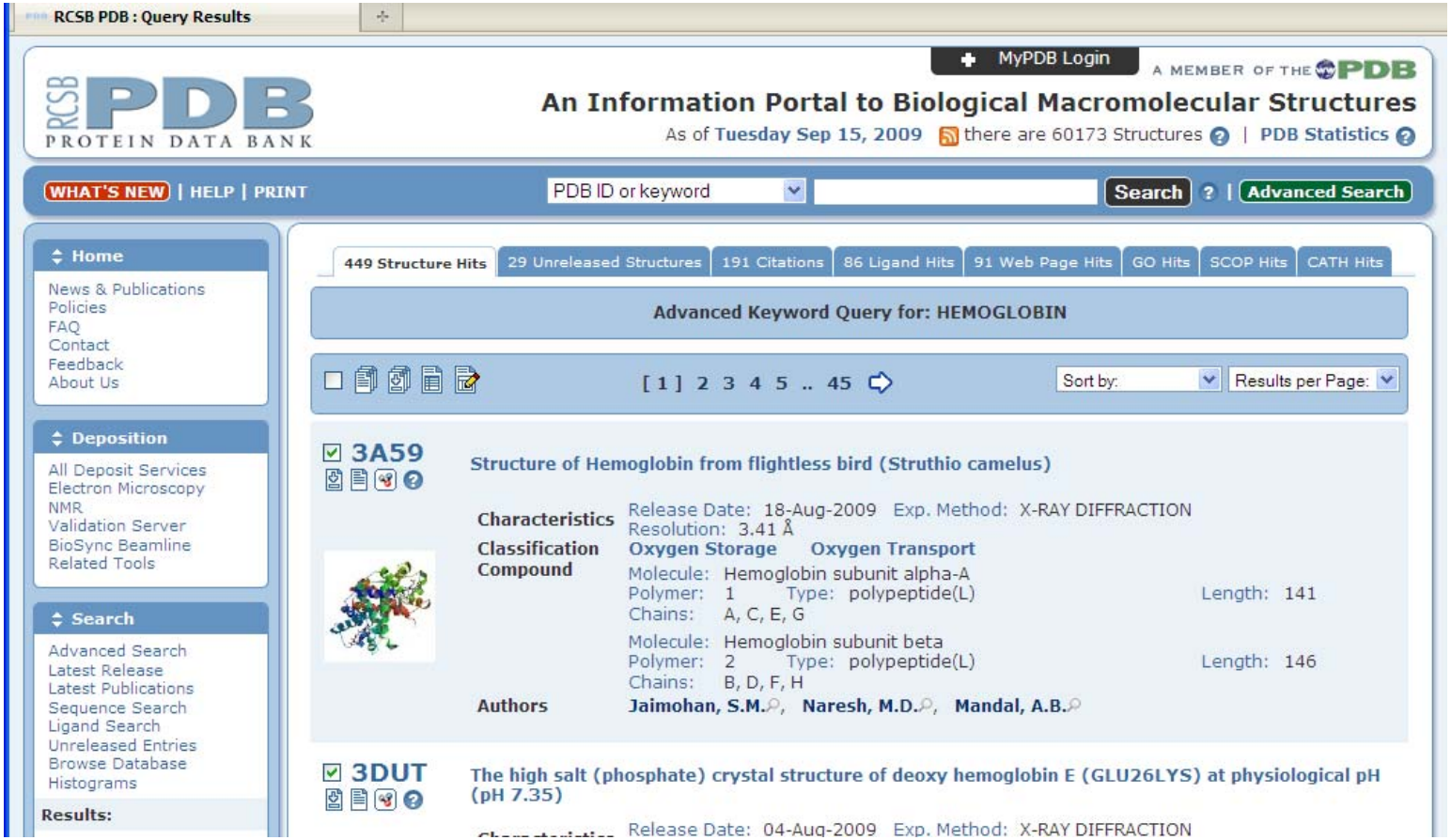


What's in this database



A range of contents

- PDB code (simplest, and most common)
- Advanced search: molecule name
  - Hemoglobin (449 hits)
  - Histone acetylase (7 hits)
- Select one (Click on pdb code)

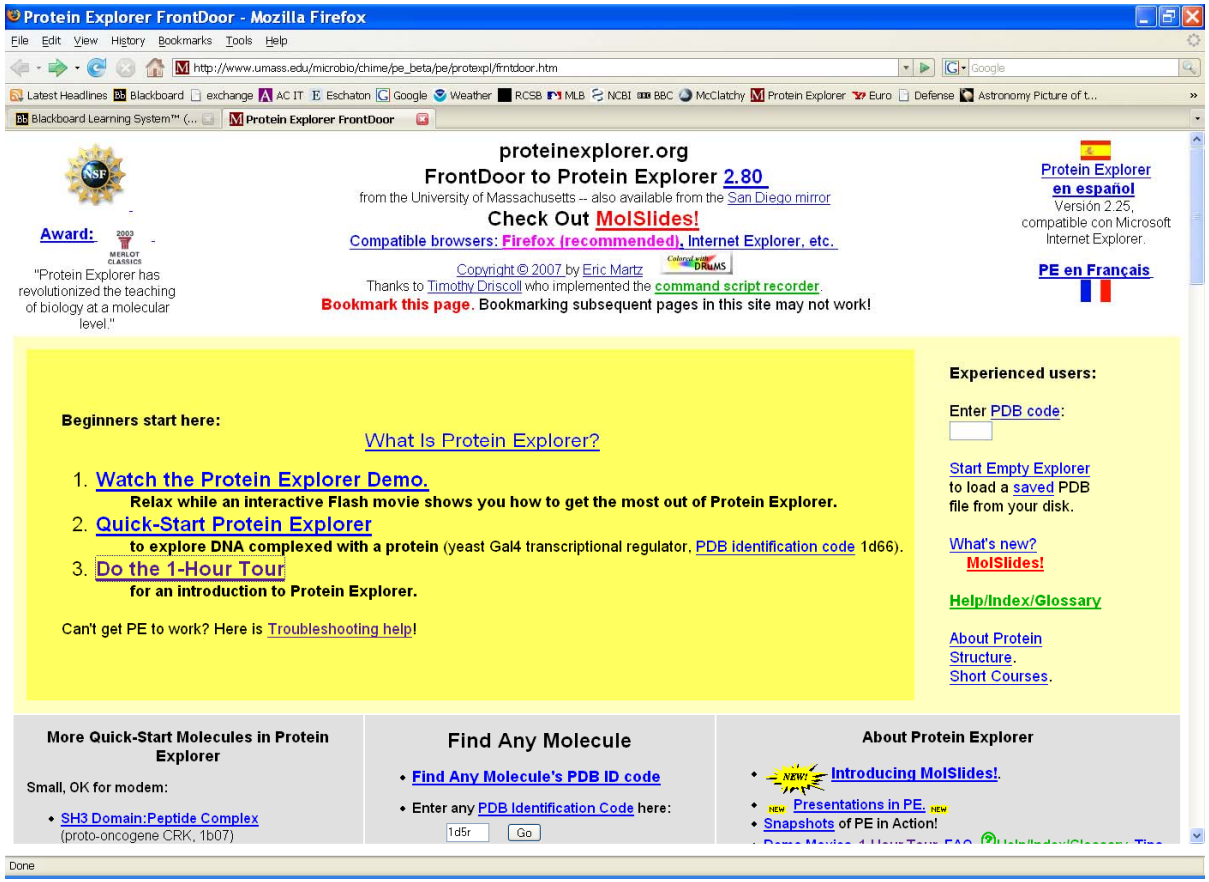


What's to see

- "View in Jmol"
  - (Viewer option, Java based)
- "Display files"
  - PDB file
  - Straight text file with coordinates of lots of atoms
- "Download Files"
  - Bring file to your own computer
  - Note "Biological Unit gz"
    - Zipped file
    - Only one molecule to look at (or one protein with its subunits)

Visualizing pdb files: Protein Explorer

- From Course web site, select “Protein Explorer”
  - Open in new window
  - Requires “Chime”, a free add-in
- Front Door
  - Variety of resources
  - Tutorial (1-hour tour)

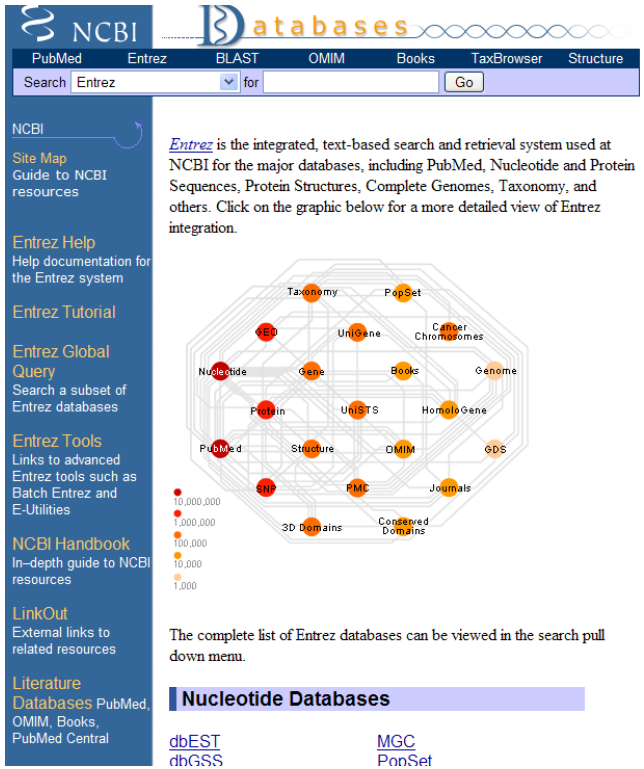


NCBI/Cn3D

- Blackboard
- National Center for Biotechnology Information (NCBI)
- www.ncbi.nlm.nih.gov

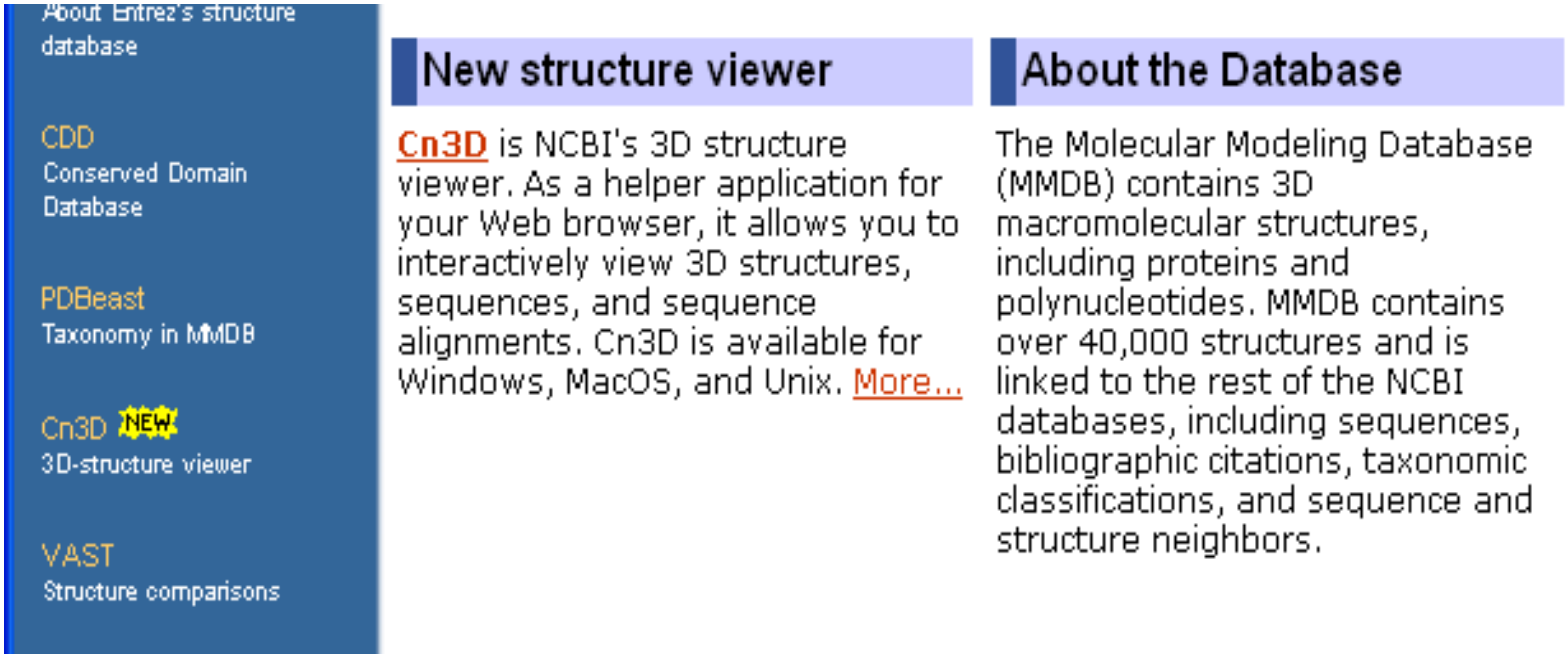
Databases

- Scroll down on main page
- Select Molecular Databases
- Scroll down again
- Select Structure (MMCB)



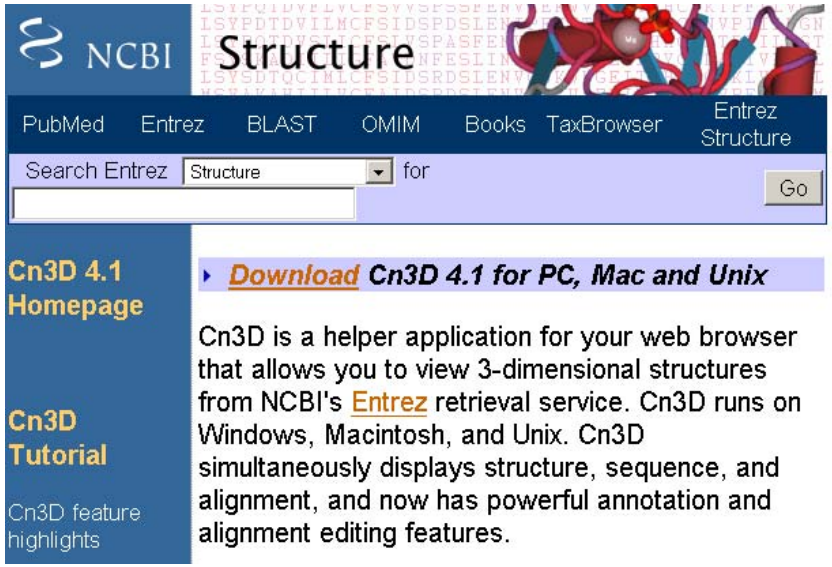
MMDB database

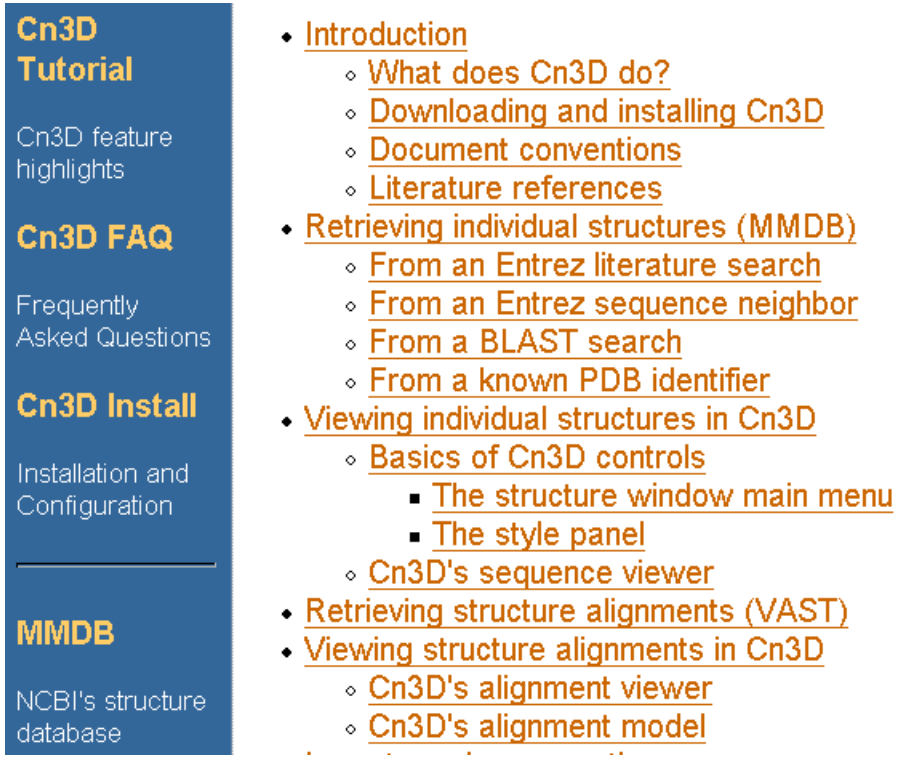
- Scroll down page
- Select Cn3D v4.1 (you could download from here)



Cn3D

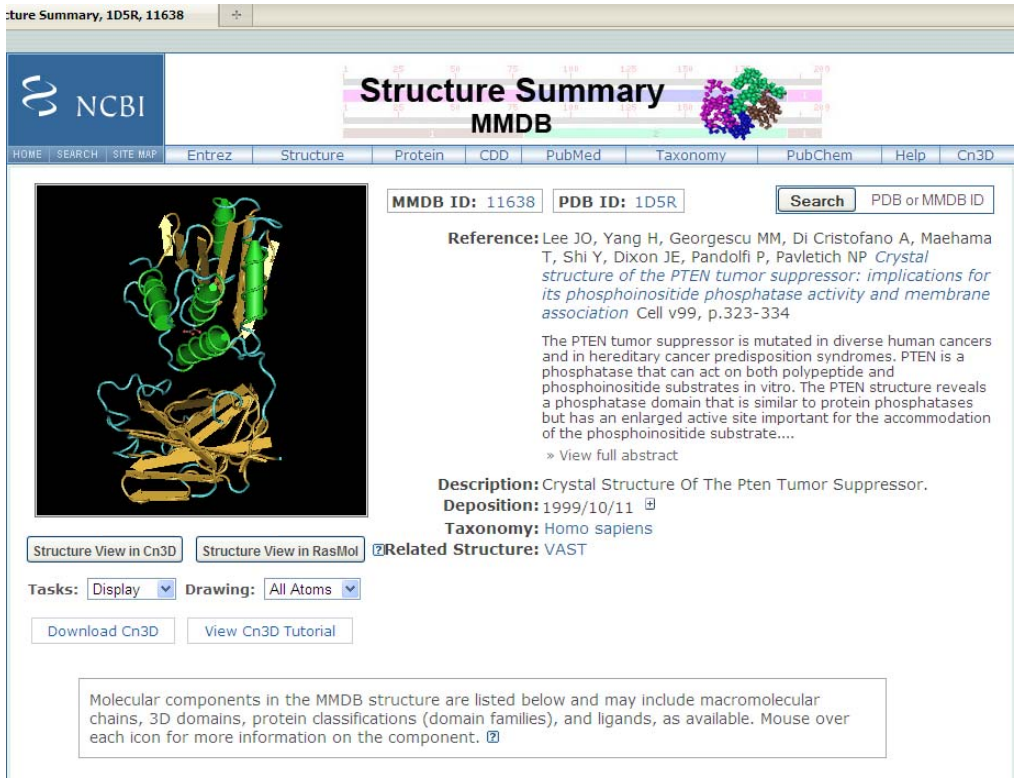
- Note tutorial
- Search for 1d5r





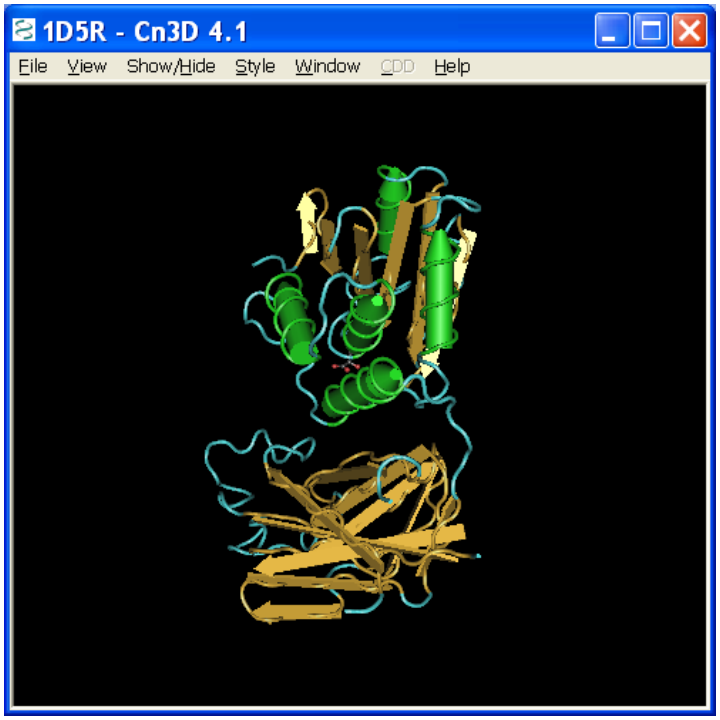
Seeing what's there…

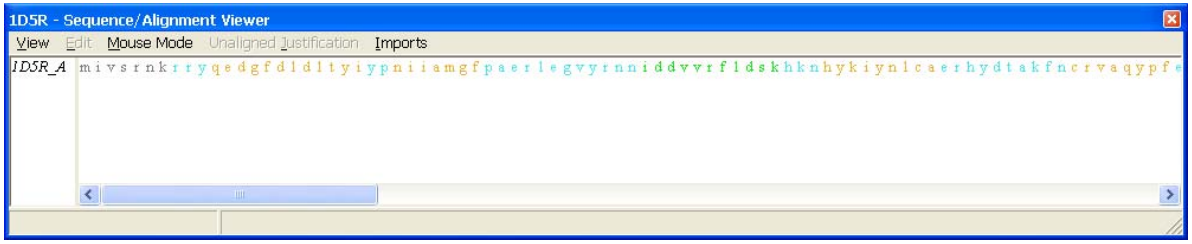
- Note links to other databases (related structures, literature, etc.)
- Click on entry number (1D5R) or thumbnail to get to Structure Summary page



From Structure Summary page…

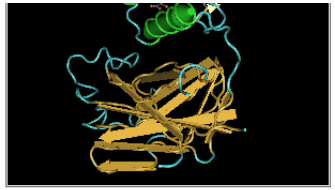
- Click “View 3D structure” to bring up structure in Cn3D viewer
  - Structure window
    - Style menu to modify views
    - Edit Global style for complete control
  - Sequence window!!
    - Highlight amino acids in structure by highlighting in sequence
    - Alignment tool





VAST

- Click “Structure Neighbors: VAST”
- From Related structures page, select “entire chain”
  - List of structural homologs
  - Sequence homologies diagrammed by red bars
  - Note effect of “mouse-over” on the list of PDB codes
- Select a homolog by checking little left hand box
- Hit “View 3D Alignment button



The PTEN tumor suppressor is mutated in diverse human cancers and in hereditary cancer predisposition syndromes. PTEN is a phosphatase that can act on both polypeptide and phosphoinositide substrates in vitro. The PTEN structure reveals a phosphatase domain that is similar to protein phosphatases but has an enlarged active site important for the accommodation of the phosphoinositide substrate....

» View full abstract

Description: Crystal Structure Of The Pten Tumor Suppressor.
Deposition: 1999/10/11
Taxonomy: Homo sapiens

Structure View in Cn3D | Structure View in RasMol

Tasks: Display | Drawing: All Atoms

Download Cn3D | View Cn3D Tutorial

VAST related structures have been calculated separately for individual protein chains and 3d domains present in this structure. To see the related structure list for each choose a chain or 3d domain from the table below.

Chain ID	Domains	Residue Range	No. of Neighbors
[A]	entire chain	1 - 324	399
[A]	domain 1	1 - 182	1502
[A]	domain 2	183 - 324	355

NCBI

Related Structures
VAST

PubMed | BLAST | Structure | Taxonomy | OMIM | Help? | Cn3D

VAST related structures for: **MMDB 11638, 1D5R sequence A**

Overview: There are two main sections to this page. The first section consists of the alignment view controls, the list controls, and the advanced related structure search controls. The second section is the VAST related structure list itself.

View 3D Alignment of All Atoms with Cn3D Display *Download Cn3D!*

View Sequence Alignment using Hypertext for Selected VAST related structures

List Medium redundancy subset, sorted by Aligned Length in Graphics

Advanced related structure search

Move the mouse over the red alignment footprints in the graphics below and click, you will obtain a structure-based sequence alignment.

Total related structures: 399; 14 representatives from the Medium redundancy subset displayed.

Click to: Check All Uncheck All

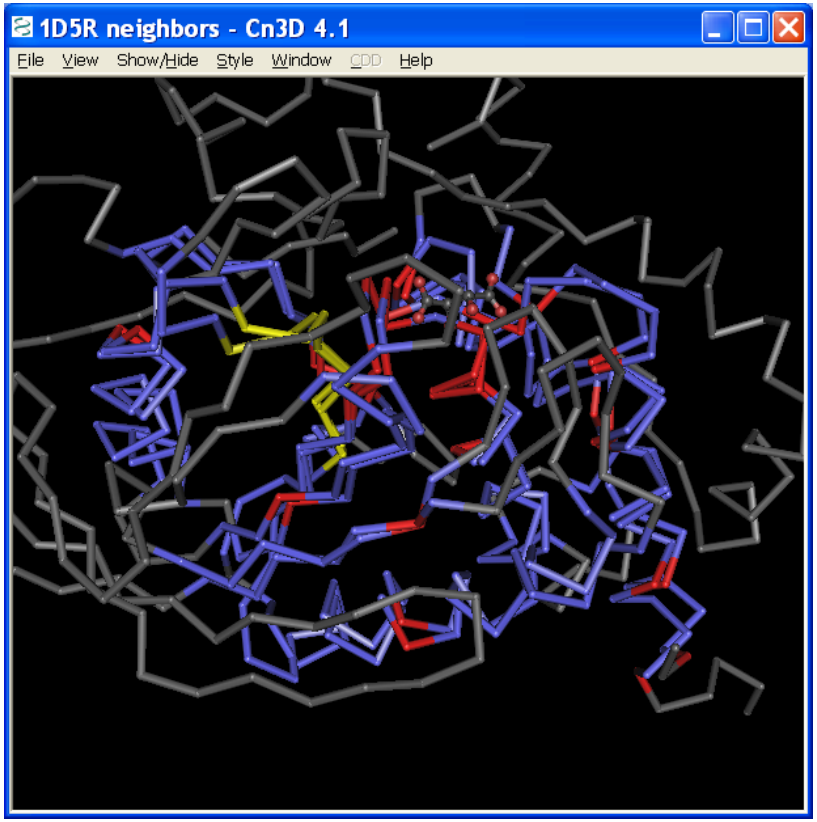
1 75 150 225 300 324 Ali_len

1D5R A
3D Domains
Domain Families
Super Families

Chain A
PTPc superfamily | PTEN_C2 superfamily

1I9T A 147
1PA9 A 141
1QHC A 2 139

Structure alignments



- Structure Window
  - Superimposed backbones
  - Gray backbones with no corresponding structures
  - Edit global style, turning on helix and strand objects
- Sequence Window
  - Both sequences
  - Try highlighting regions of aligned sequence, vs regions of unaligned sequence
  - Note alignment of dissimilar residues (structure based alignment)

One last thing…

- Course website again/External Links
- Theoretical structures