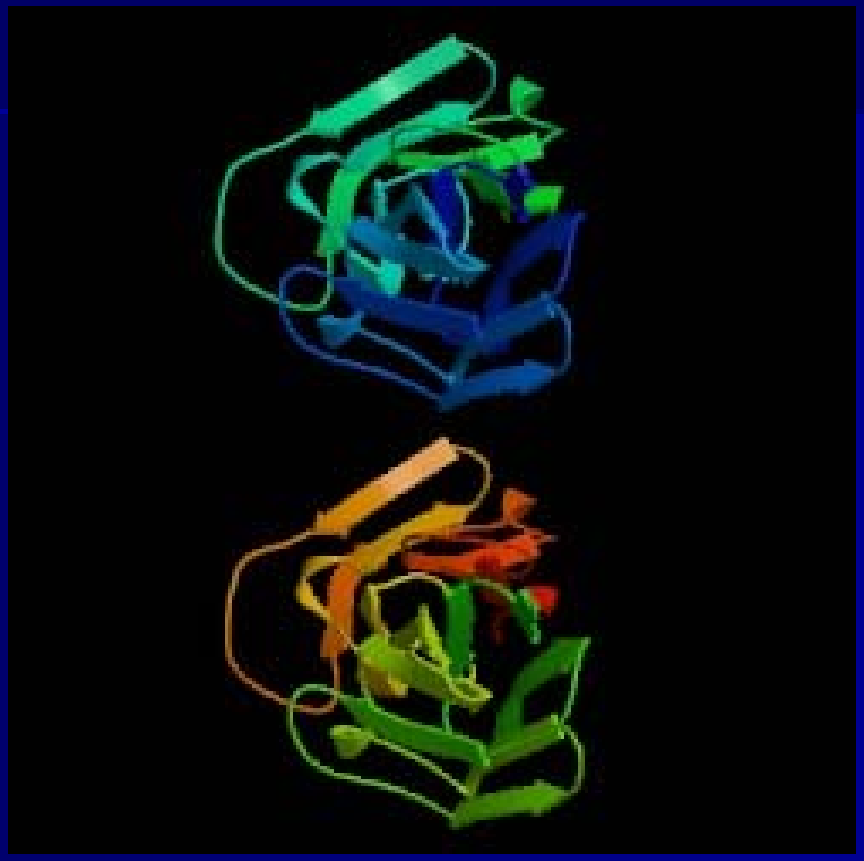
Databases for Protein Structure



C. S. Cheng

Institute of Bioinformatics and Structural Biology

Molecular Biology Database Collection

~ more than 1000 databases

- Nucleotide Sequence Databases
- RNA sequence databases
- Protein sequence databases
- Structure Databases
- Genomics Databases (non-vertebrate)
- Metabolic and Signaling Pathways
- Human and other Vertebrate Genomes
- Human Genes and Diseases
- Microarray Data and other Gene Expression Databases
- Proteomics Resources
- Other Molecular Biology Databases
- Organelle databases
- Plant databases
- Immunological databases

The Molecular Biology Database Collection: 2008 update

Nucleic Acids Research, 2008, Vol. 36, Database issue **D2-D4**

- Structure Databases
  - Small molecules
    - AANT - Amino Acid - Nucleotide interaction database
    - ChEBI - Chemical Entities of Biological Interest
    - ChemBank
    - ChemDB
    - CSD - Cambridge Structural Database
    - DrugBank
    - Het-PDB Navi
    - HIC-Up
    - Klotho
    - LIGAND
    - PDB-Ligand
    - PubChem
    - R.E.DD.B.
    - SuperDrug
    - SuperNatural
  - Carbohydrates
    - BCSDB/Glycoscience
    - CCSD - Complex Carbohydrate Structure Database (CarbBank)
    - CSS - Carbohydrate Structure Suite
    - Glycan
    - Glycoconjugate Data Bank
    - GlycoMapsDB
    - GlycoSuiteDB
    - Monosaccharide Browser
    - SWEET-DB

- Structure Databases
  - Nucleic acid structure
    - Greglist
    - GRSDB
    - ITS2
    - MeRNA
    - NCIR - Non-Canonical Interactions in RNA
    - NDB
    - NTDB
    - QuadBase
    - Rfam
    - RNA FRABASE
    - RNA SSTRAND
    - RNABase
    - RNAJunction
    - SARS-CoV RNA SSS
    - SCOR - Structural Classification Of RNA
    - Vir-Mir db
  - Protein structure
    - 3D-Genomics
    - 3DID - 3D interacting domains
    - ArchDB
    - ASTRAL
    - AutoPSI
    - BANMOKI
    - BioMagResBank
    - CADB - Conformational Angles DataBase of Proteins
    - CATH
    - CE
    - CoC Central
    - ColiSNP

- Structure Databases
  - Protein structure
    - Columba
    - CSA - Catalytic Site Atlas
    - Dali database
    - DBAli
    - Decoys-R-Us
    - DisProt - Database of Protein Disorder
    - DMAPS
    - Dockground
    - DomIns - Database of Domain Insertions
    - DSDBASE - Disulfide Database
    - DSMM - a Database of Simulated Molecular Motions
    - E-MSD - EBI-Macromolecular Structure Database
    - eF-site - Electrostatic surface of Functional site
    - EzCatDB
    - FireDB
    - FSN
    - Gene3D
    - Genomic Threading Database
    - GTOP - Genomes To Protein structures
    - HOMSTRAD - Homologous Structure Alignment Database
    - HotSprint
    - IMB Jena Image Library
    - IMGT/3Dstructure-DB
    - IMOTdb
    - MALISAM
    - LPFC
    - MegaMotifbase
    - MMDB
    - ModBase
    - MolMovDB - Database of Macromolecular Movements
    - PASS2

- Structure Databases
  - Protein structure
    - PDB
    - PDB-REPRDB
    - PDBselect
    - PDBsum
    - PDB_TM
    - PepConfDB
    - PFD - Protein Folding Database
    - Phospho3D
    - PIDD
    - PMDB - Protein Model Database
    - Structure Superposition Database
    - ProSAS
    - PROTCOM
    - PRTAD
    - RESID
    - S4: Structure-based Sequence Alignments of SCOP Superfamilies
    - SCOP - Structural Classification Of Proteins
    - SCOPPI
    - SitesBase
    - SNAPPI
    - SSToSS - Sequence-Structural Templates of Single-member Superfamilies
    - STINGreport
    - SUPERFAMILY
    - SURFACE
    - SWISS-MODEL Repository
    - TargetDB
    - TMBETA-GENOME
    - TOPOFIT-DB
    - TOPS - Topology Of Protein Structures

Protein Data Bank (PDB)

- http://www.rcsb.org/pdb/Welcome.do
- Structure data determined by X-ray crystallography and NMR
- The data include the atom coordinate, reference, sequence, secondary structure, disulfide bond ……etc.

RCSB Protein Data Bank - Microsoft Internet Explorer

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Address http://www.rcsb.org/pdb/home/home.do;jsessionid=18C61D483B9AE4ED6EDF6533F4FE40ED

Go Links

The number of protein structure and the last update date

An Information Portal to Biological Macromolecular Structures

As of Tuesday Jul 15, 2008 there are 51860 Structures | PDB Statistics

Site Search | Advar

PDB Statistics
51860 Structures
Last Update: Jul 15, 2008

Home Search

- Home
- Getting Started
- Download Files
- Deposit and Validate
- Structural Genomics
- Dictionaries & File Formats
- Software Tools
- General Education
- Site Tutorials
- BioSync
- General Information
- Acknowledgements
- Frequently Asked Questions
- Report Bugs/Comments

Quick Tips:

Want to search by sequence? Click here.

Are you missing data updates? The PDB archive has moved to ftp://ftp.w
For more information click here.

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their relationships to sequence, function, and disease.

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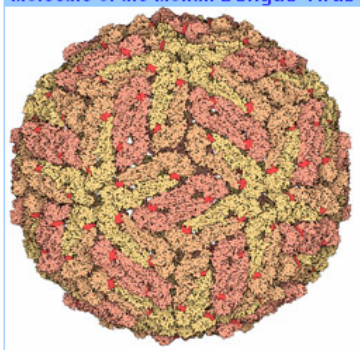
Comments? info@rcsb.org

Molecule of the Month: Dengue Virus



Dengue virus is a major threat to health in tropical countries around the world. It is limited primarily to the tropics because it is transmitted by a tropical mosquito, but even with this limitation, 50-100 million people are infected each year. Most infected people experience dengue fever, with terrible headaches and fever and rashes that last a week or two. In some cases, however, the virus weakens the circulatory system and can lead to deadly hemorrhaging. Researchers are now actively studying the virus to try to develop drugs to cure infection, and vaccines to block infection before it starts.

- More ...
- Previous Features

- mplete News
- ewsletter
- Discussion Forum
- Job Listings

15-July-2008

RCSB PDB at ISMB, Protein Society Meetings

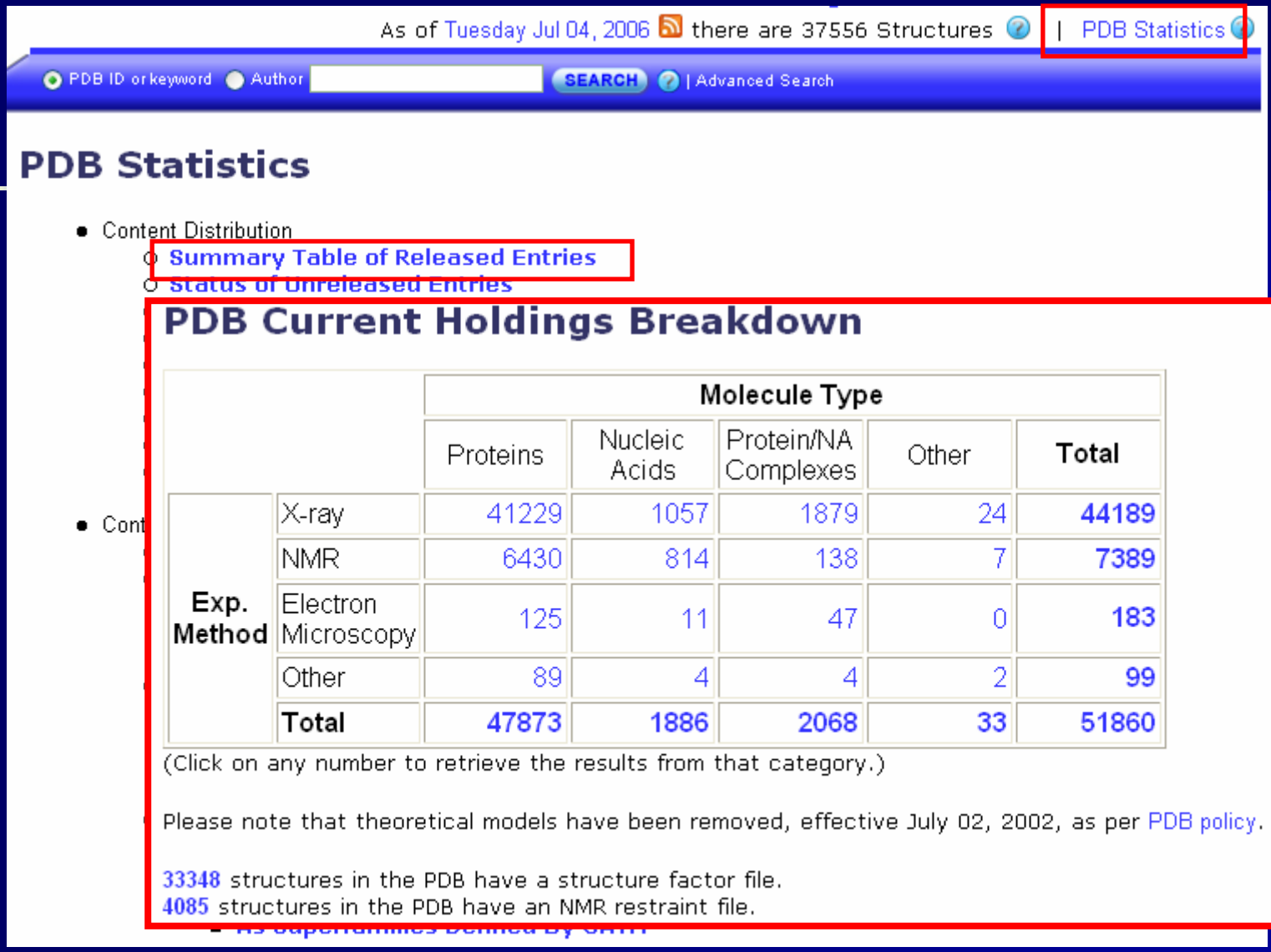
Stop by exhibit booth #19 at the 16th Annual International Conference for Intelligent Systems for Molecular Biology (ISMB) to visit with the RCSB PDB (July 19-23; Toronto, Canada). Also at this meeting, the RCSB PDB Poster Prize will be awarded for the outstanding student poster in the "structure and function prediction" category. Associate Director Phil Bourne will be involved with presentations and discussions, including a 3DSig Keynote Lecture at the Structural Bioinformatics and Computational Biophysics satellite meeting.

- Full article ...

The RCSB PDB is managed by two members of the RCSB: Rutgers, The State University of New Jersey and the San Diego Supercomputer Center

In citing the PDB please refer to:

Done Internet


As of Tuesday Jul 04, 2006 there are 37556 Structures
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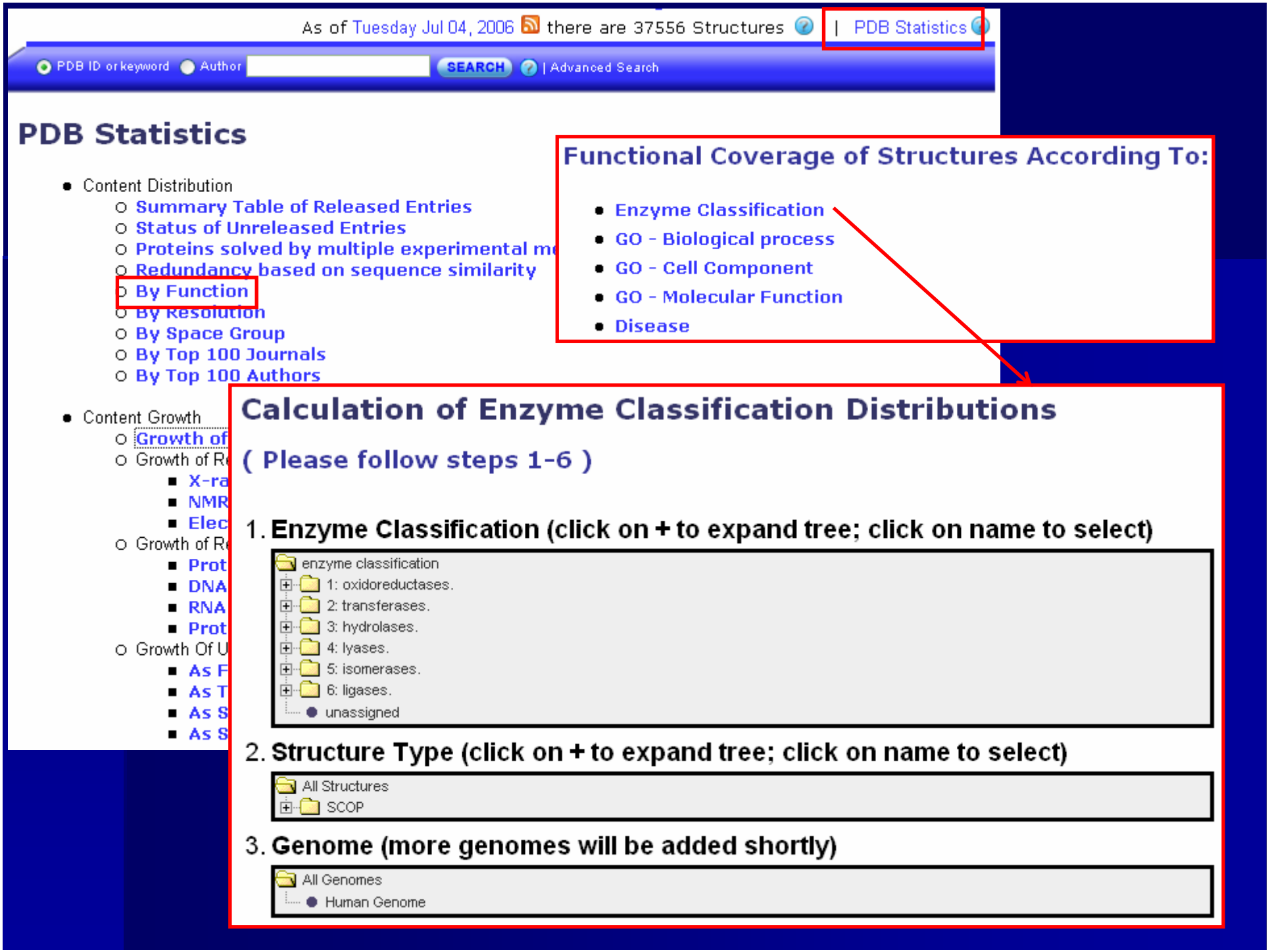
Advanced Search
PDB Statistics
Content Distribution
Summary Table of Released Entries
Status of Unreleased Entries
PDB Current Holdings Breakdown
Molecule Type
Proteins
Nucleic Acids
Protein/NA Complexes
Other
Total
Exp. Method
X-ray 41229 1057 1879 24 44189
NMR 6430 814 138 7 7389
Electron Microscopy 125 11 47 0 183
Other 89 4 4 2 99
Total 47873 1886 2068 33 51860
(Click on any number to retrieve the results from that category.)
Please note that theoretical models have been removed, effective July 02, 2002, as per PDB policy.
33348 structures in the PDB have a structure factor file.
4085 structures in the PDB have an NMR restraint file.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Status of Unreleased Entries
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By Resolution
By Space Group
By Top 100 Journals
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Functional Coverage of Structures According To:
Enzyme Classification
GO - Biological process
GO - Cell Component
GO - Molecular Function
Disease
Calculation of Enzyme Classification Distributions
(Please follow steps 1-6)
1. Enzyme Classification (click on + to expand tree; click on name to select)
enzyme classification
1: oxidoreductases.
2: transferases.
3: hydrolases.
4: lyases.
5: isomerases.
6: ligases.
unassigned
2. Structure Type (click on + to expand tree; click on name to select)
All Structures
SCOP
3. Genome (more genomes will be added shortly)
All Genomes
Human Genome

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PDB Statistics

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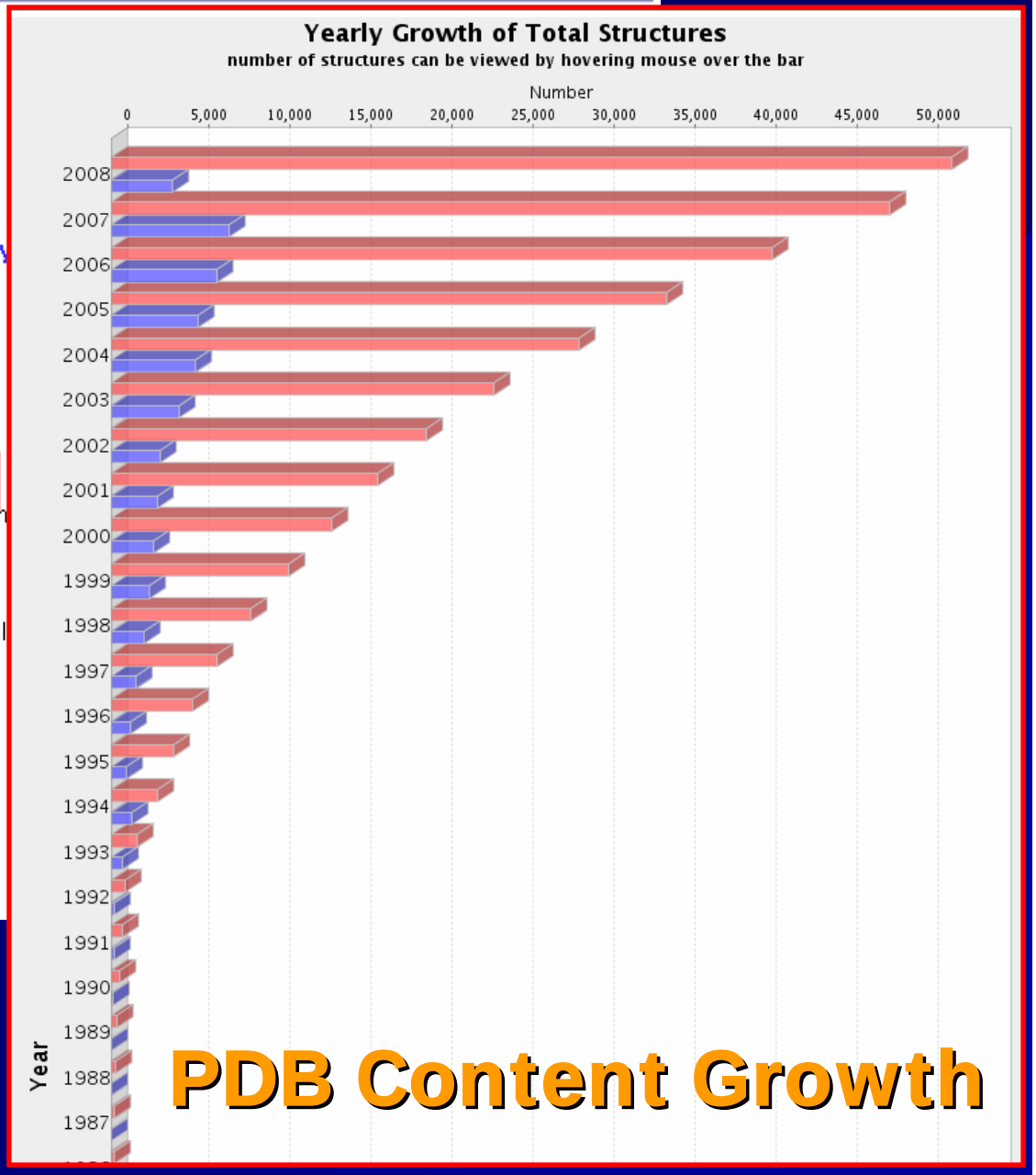
  - Status of Unreleased Entries
  - Proteins solved by multiple experimental
  - Redundancy based on sequence similarity
  - By Function
  - By Resolution
  - By Space Group
  - By Top 100 Journals
  - By Top 100 Authors

- Content Growth
  - Growth of Released Structures Per Year
  - Growth of Released Structures Per Year by Experim
    - X-ray
    - NMR
    - Electron Microscopy
  - Growth of Released Structures Per Year By Molecul
    - Protein Only
    - DNA Only
    - RNA Only
    - Protein Nucleic Acid Complexes
  - Growth Of Unique Protein Classifications Per Year
    - As Folds Defined By SCOP
    - As Topologies Defined By CATH
    - As Superfamilies Defined By SCOP
    - As Superfamilies Defined By CATH



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  - Status of Unreleased Entries
  - Proteins solved by multiple experimental metho
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  - By Resolution
  - By Space Group
  - By Top 100 Journals
  - By Top 100 Authors
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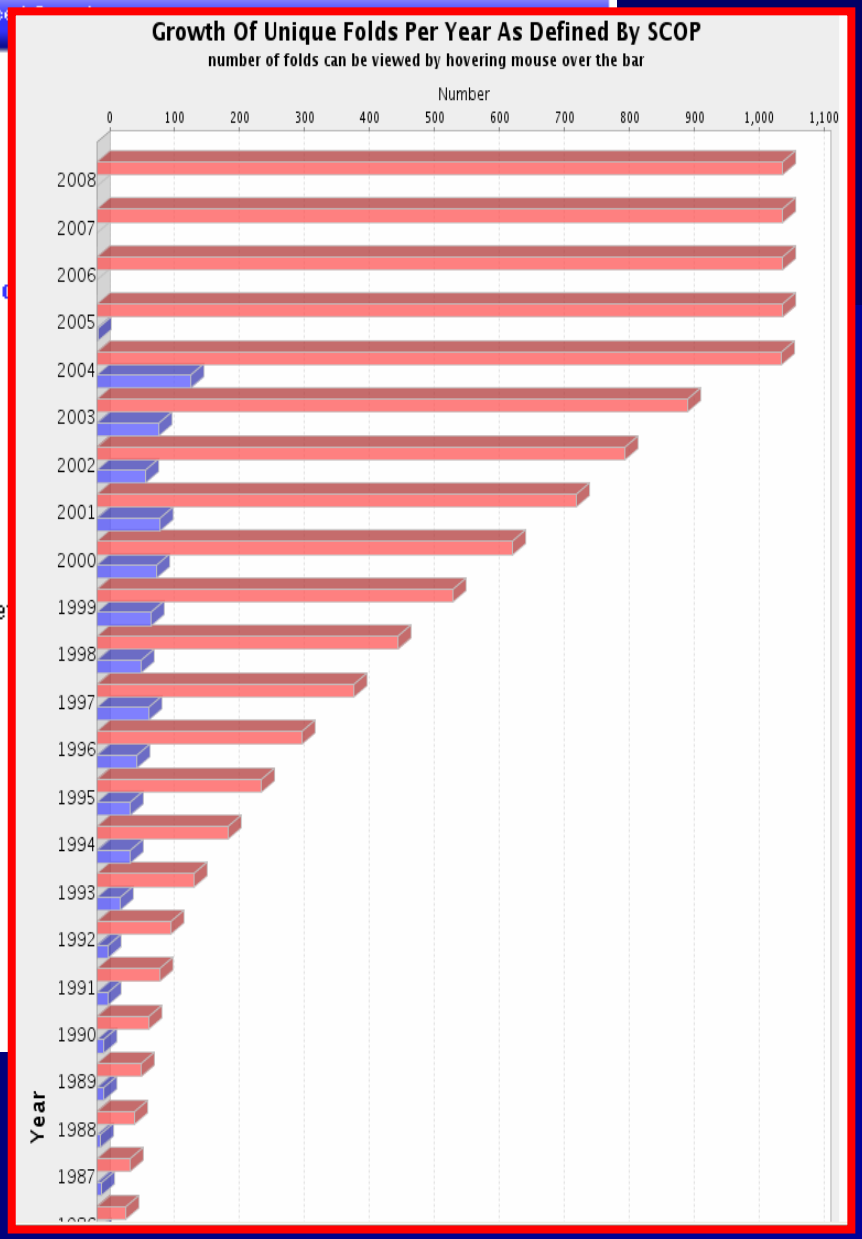
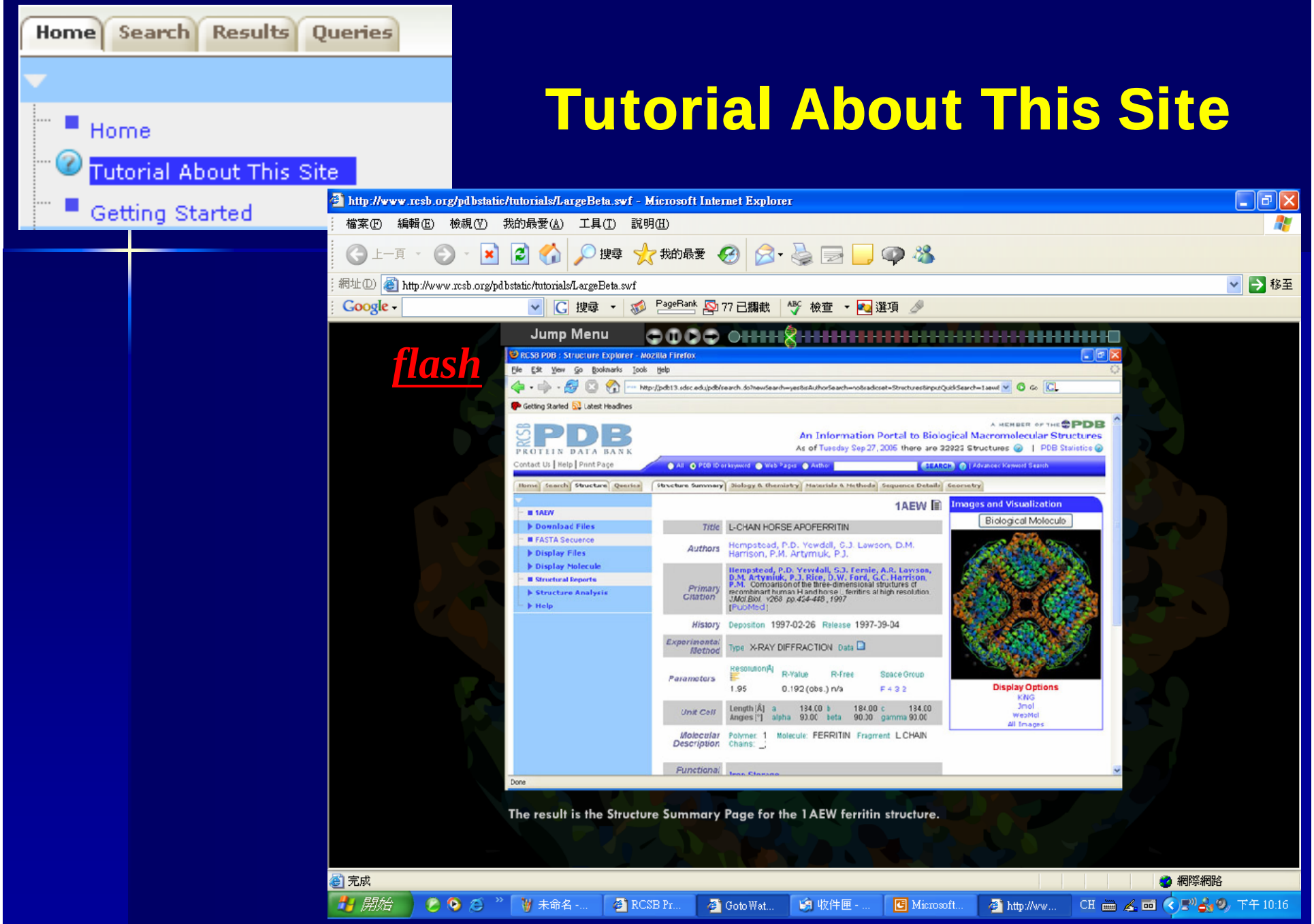
  - Growth of Released Structures Per Year by Experimental Me
    - X-ray
    - NMR
    - Electron Microscopy
  - Growth of Released Structures Per Year By Molecular Type
    - Protein Only
    - DNA Only
    - RNA Only
    - Protein Nucleic Acid Complexes
  - Growth Of Unique Protein Classifications Per Year
    - As Folds Defined By SCOP
    - As Topologies Defined By CATH
    - As Superfamilies Defined By SCOP
    - As Superfamilies Defined By CATH



Growth of Unique Folds Per Year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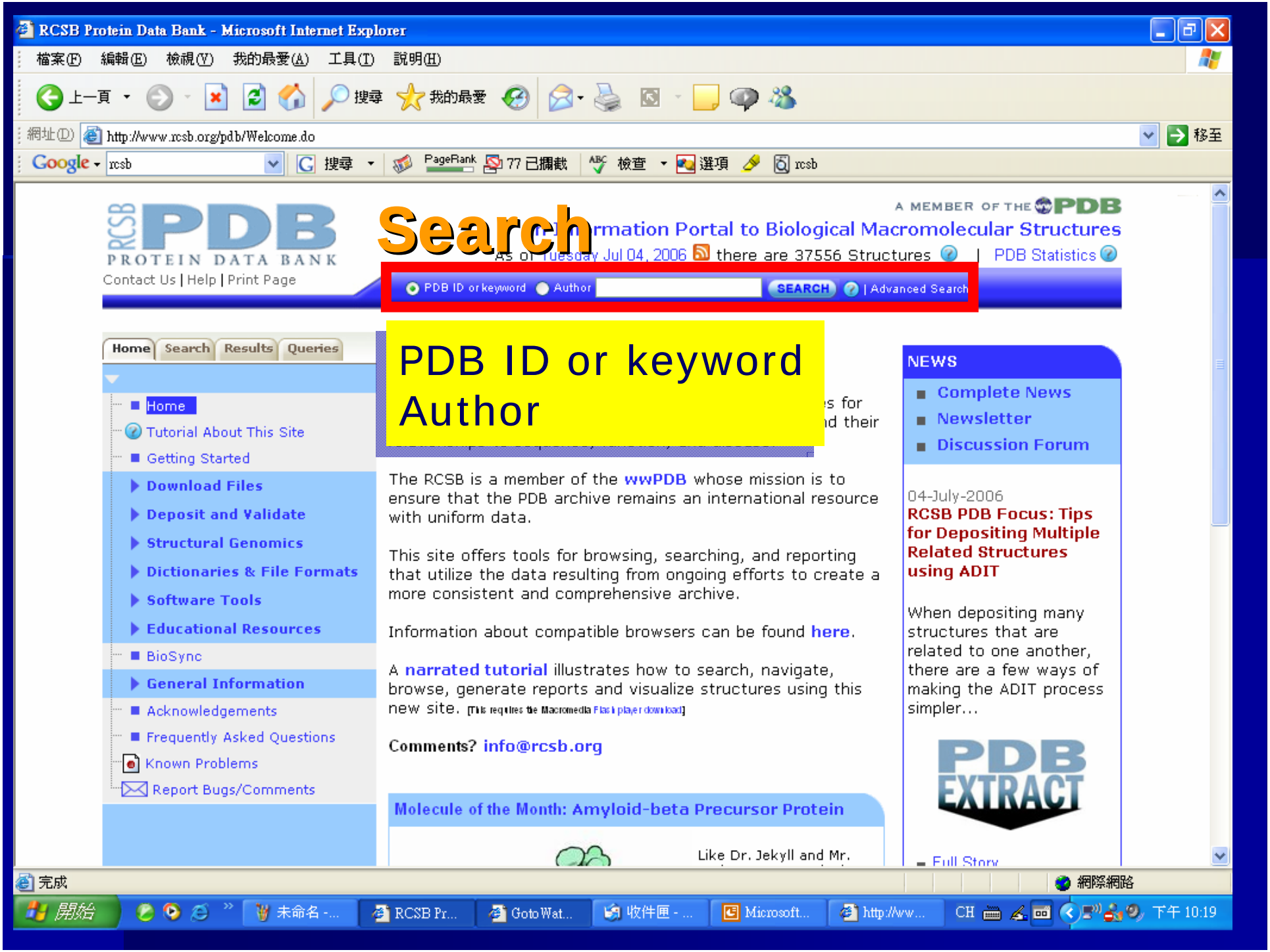
Jump Menu
The result is the Structure Summary Page for the 1AEW ferritin structure.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When depositing many structures that are related to one another, there are a few ways of making the ADIT process simpler...
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Full Story
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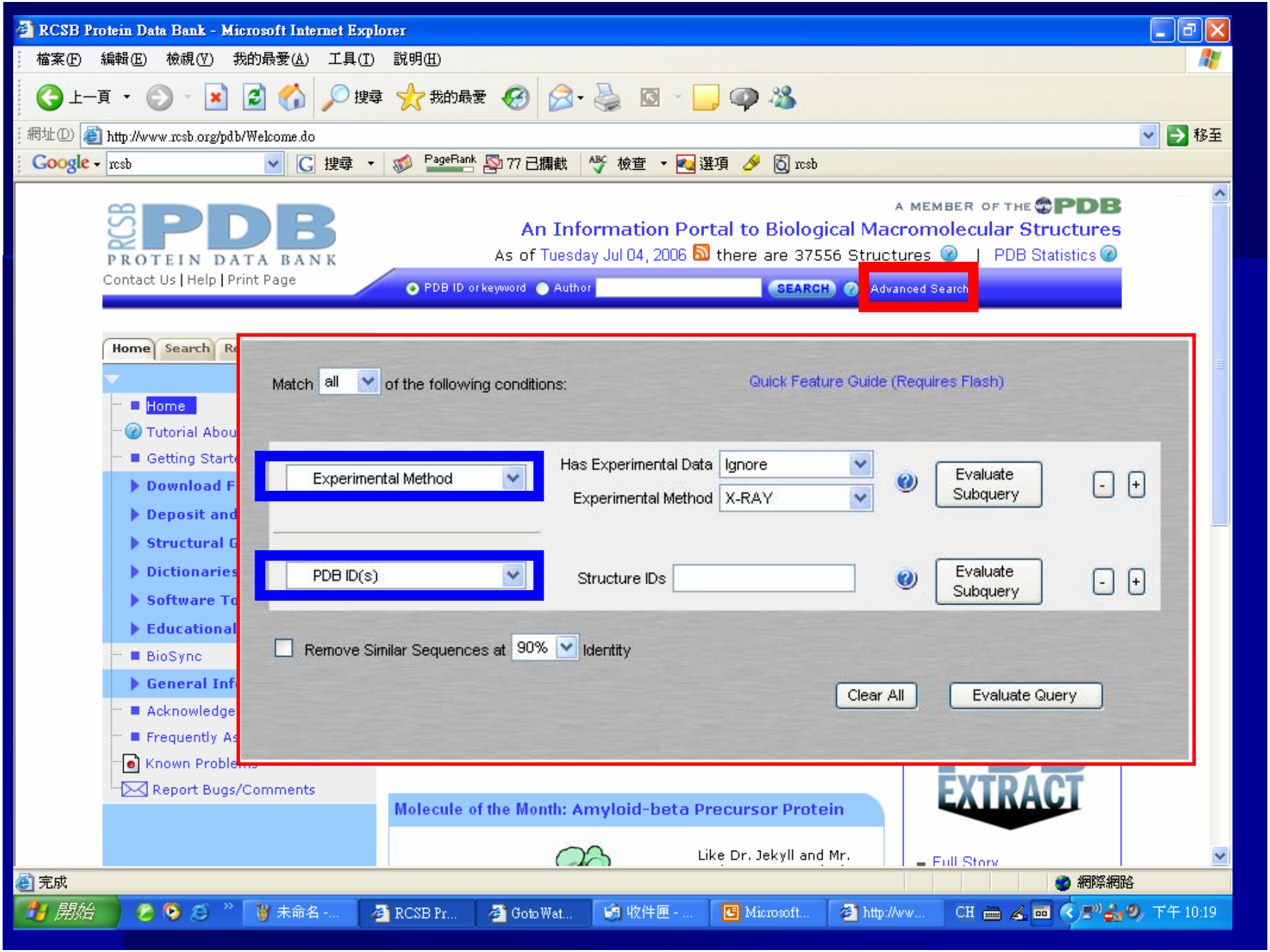
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Experimental Method X-RAY
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PDB ID(s)
Structure IDs
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Evaluate Query
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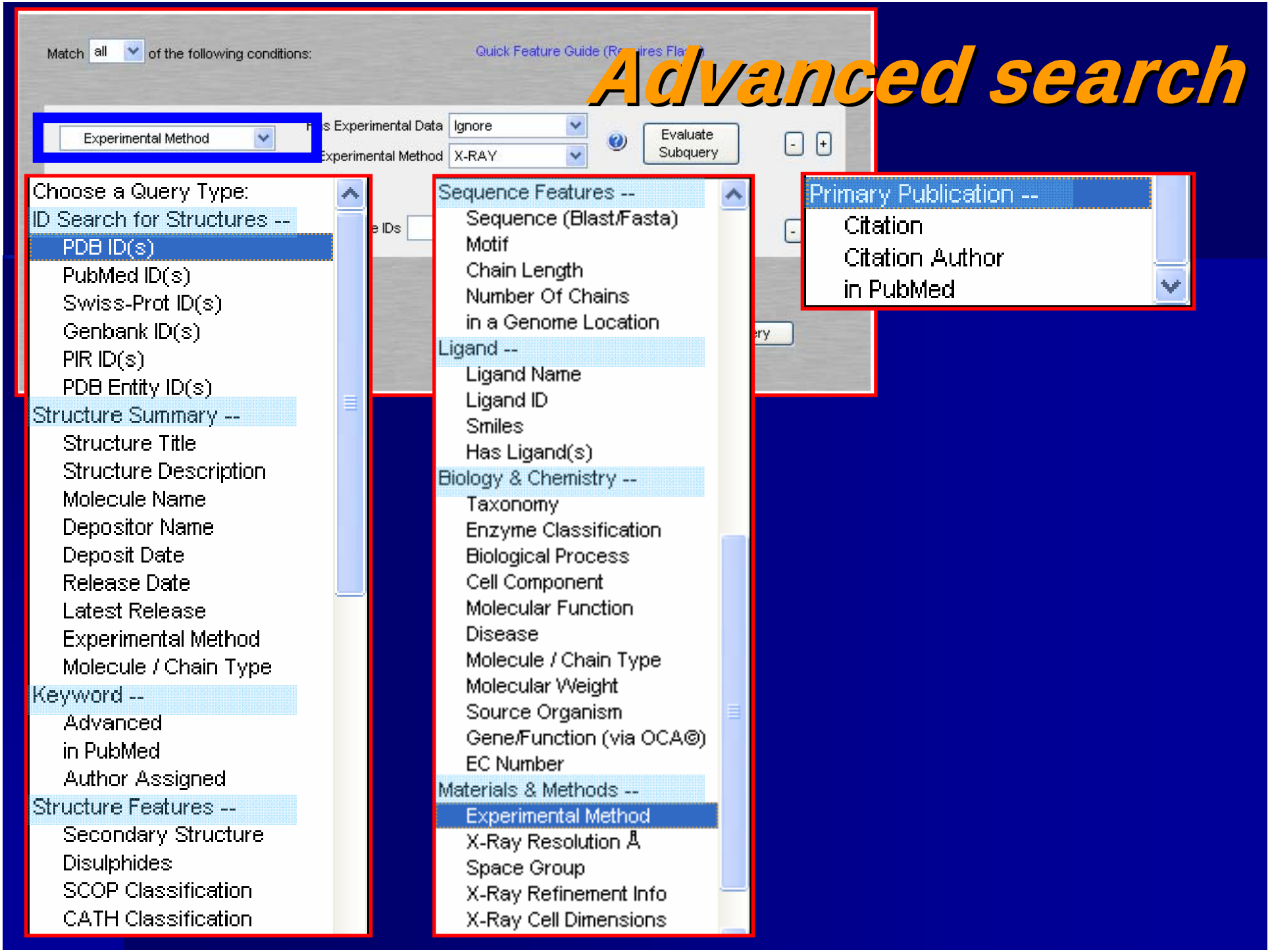
Advanced search
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Swiss-Prot ID(s)
Genbank ID(s)
PIR ID(s)
PDB Entity ID(s)
Structure Summary --
Structure Title
Structure Description
Molecule Name
Depositor Name
Deposit Date
Release Date
Latest Release
Experimental Method
Molecule / Chain Type
Keyword --
Advanced
in PubMed
Author Assigned
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CATH Classification
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Enzyme Classification
Biological Process
Cell Component
Molecular Function
Disease
Molecule / Chain Type
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Materials & Methods --
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X-Ray Refinement Info
X-Ray Cell Dimensions
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Citation
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Structure Summary | Biology & Chemistry | Materials & Methods | Sequence Details | Geometry

- 1L6H
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- Display Files
- Display Molecule
- Structural Reports
- Structure Analysis
- Help

1L6H

PDB ID

Title Solution Structure of Plant nsLTP2 purified from R[illegible]e (oryza Sativa)

Authors Samuel, D., Lyu, P.-C.

Primary Citation **Samuel, D., Liu, Y.J., Cheng, C.S., Lyu, P.C.** Solution structure of plant nonspecific lipid transfer protein-2 from rice (Oryza sativa). *J.Biol.Chem.* *v277* *pp.35267-35273*, *2002* [Abstract]

History Deposition 2002-03-11 Release 2002-10-02

Experimental Method Type NMR, minimized average structure Data N/A

NMR Ensemble Conformers Calculated n/a Conformers Submitted n/a Selection Criteria n/a

NMR Refine Method NMR, minimized average structure

Molecular Description Asymmetric Unit Polymer: 1 Molecule: Non-Specific Lipid Transfer Protein Chains: A

Functional Class **Lipid Transport**

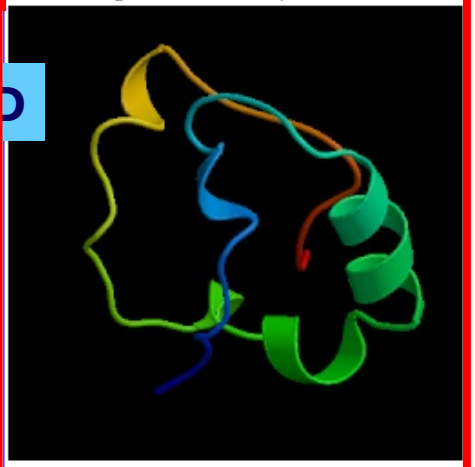
Source Polymer: 1 Scientific Name: **Oryza sativa** Common Name: **Rice** Rice

SCOP Classification (version 1.69)

Domain Info	Class	Fold	Superfamily	Family	Domain	Species
d1l6ha_	All alpha proteins	Bifunctional inhibitor/lipid-transfer protein/seed storage 2S	Bifunctional inhibitor/lipid-transfer protein/seed storage 2S	Plant lipid-transfer and hydrophobic proteins	Non-specific lipid-transfer protein homologue (nc- LTP2)	Rice (Oryza sativa)

Images and Visualization

Biological Molecule / Asymmetric Unit



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WebMol
Protein Workshop
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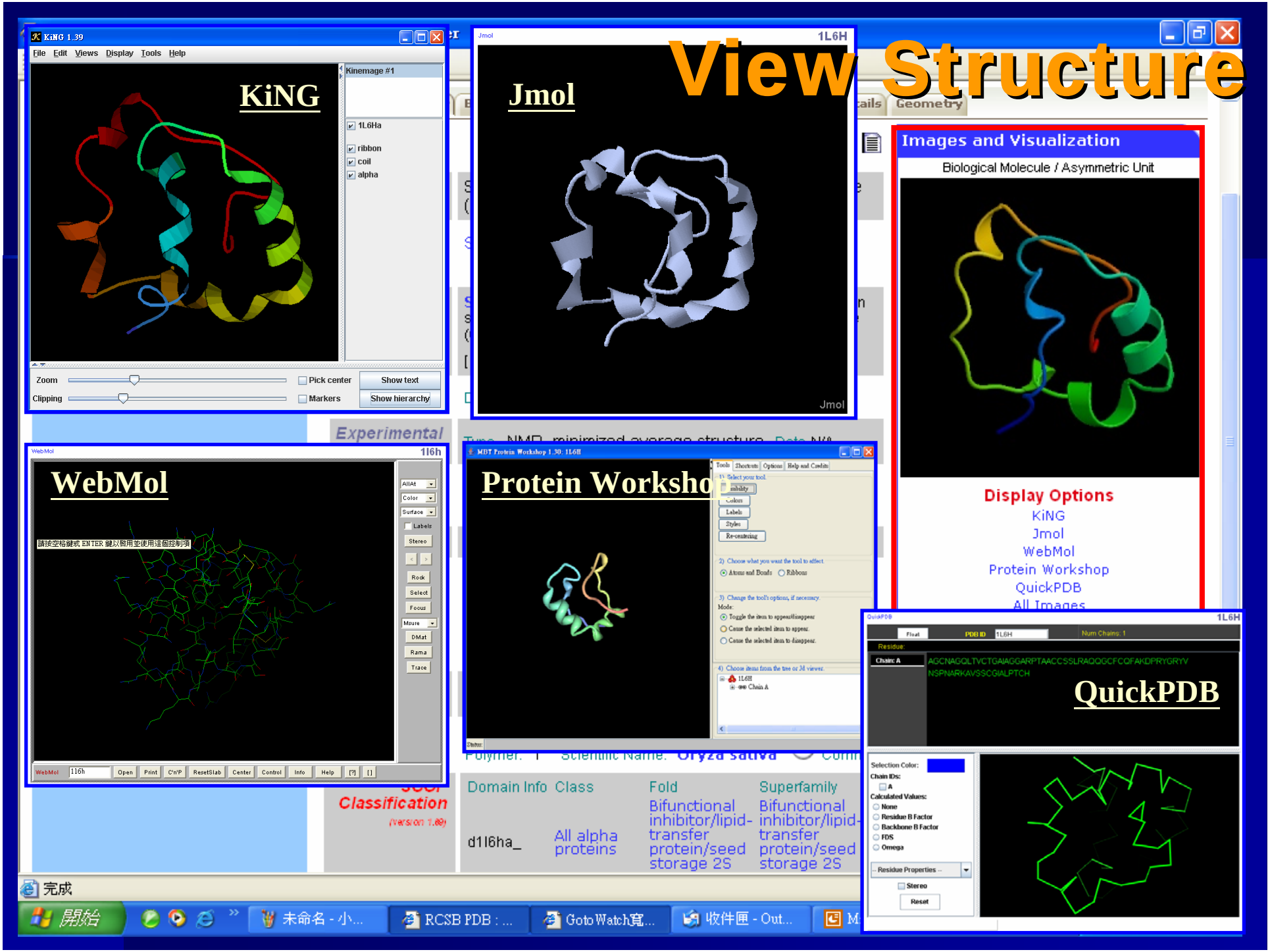
View Structure
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WebMol
Protein Worksho
QuickPDB
Experimental
Classification
Domain Info Class
Fold
Superfamily
d1l6ha_
All alpha proteins
Bifunctional inhibitor/lipid-transfer protein/seed storage 2S
Bifunctional inhibitor/lipid-transfer protein/seed storage 2S

Structure Summary | Biology & Chemistry | Materials & Methods | Sequence Details | Geometry

Biology and Chemistry Report 1L6H

Structural Details

Keywords	LIPID TRANSPORT
Text	nsLTP2, Plant LTP, lipid transfer

Polymeric Molecules

Chain A

Description	Non Specific Lipid Transfer Protein
Fragment	null
Mutation	null
Formula Weight	7021.1
Source Method	nat
Entity Name	LTP2
Entity Name Sys	n/a

Entity Poly

Entity	Chains	Chirality	Linkage	Monomer	# Mon.	Type	Details
1	A	n/a	no	no	n/a	polypeptide(L)	n/a

Source, Chain A

Common Name	Rice
Scientific Name	Oryza sativa

Details | Geometry

equence Details | Geometry

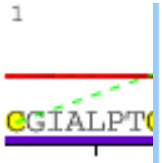
1L6H

lefined as a multiple of the standard deviation for a

4.0 | 5.0 | >5.0

Std Val	Std StdDev	Minimum	Maximum
1.329	0.014	1.30	1.365
1.341	0.016	1.32	1.373
1.231	0.02	1.17	1.232
1.525	0.021	1.46	1.566
1.516	0.018	1.50	1.541
1.53	0.02	1.49	1.565
1.521	0.033	1.51	1.546
1.54	0.027	1.48	1.551
1.458	0.019	1.40	1.472
1.451	0.016	1.44	1.464
1.466	0.015	1.43	1.467

Save Report



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Bond Angle

Bond Angle	Chain Id	Tot Num	Cal Ave	Cal StdDev	Std Val	Std StdDev	Minimum	Maximum
C-N-CA	A	56	120.21	3.335	121.7	1.8	108.97	129.886
C-N-CA(G)	A	8	120.10	3.569	120.6	1.7	115.22	126.594
C-N-CA(P)	A	4	118.81	4.046	122.6	5.0	113.45	124.818

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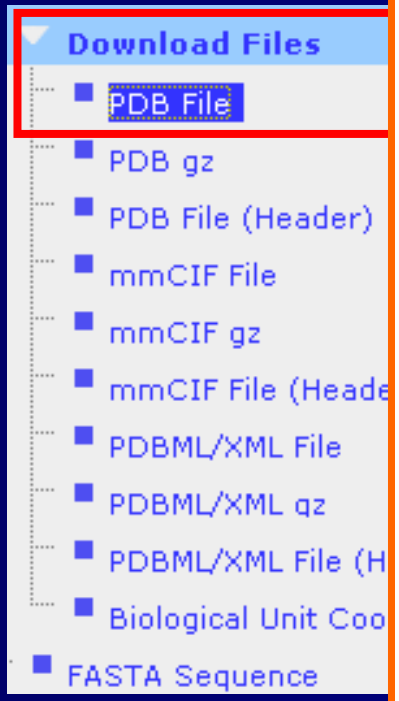

						x	y	z		
ATOM	498	O	GLY	A	76	29.245	33.349	14.558	1.00	15.75
ATOM	499	N	VAL	A	77	29.049	33.359	16.772	1.00	12.83
ATOM	500	CA	VAL	A	77	28.416	34.651	16.814	1.00	16.32
ATOM	501	C	VAL	A	77	29.429	35.571	17.448	1.00	17.48
ATOM	502	O	VAL	A	77	30.141	35.163	18.354	1.00	21.82
ATOM	503	CB	VAL	A	77	27.168	34.597	17.686	1.00	17.72
ATOM	504	CG1	VAL	A	77	26.650	36.016	18.011	1.00	21.68
ATOM	505	CG2	VAL	A	77	26.101	33.790	16.984	1.00	21.25
ATOM	506	N	SER	A	78	29.476	36.812	17.002	1.00	16.53
ATOM	507	CA	SER	A	78	30.421	37.778	17.553	1.00	21.19
ATOM	508	C	SER	A	78	29.660	38.910	18.233	1.00	18.21
ATOM	509	O	SER	A	78	28.835	39.524	17.580	1.00	20.01
ATOM	510	CB	SER	A	78	31.248	38.453	16.434	1.00	24.42
ATOM	511	OG	SER	A	78	32.363	37.685	15.993	1.00	38.73
ATOM	512	N	ILE	A	79	29.822	39.082	19.552	1.00	16.06
ATOM	513	CA	ILE	A	79	29.225	40.227	20.266	1.00	16.26
ATOM	514	C	ILE	A	79	30.433	40.982	20.868	1.00	13.63
ATOM	515	O	ILE	A	79	31.419	40.366	21.263	1.00	12.37
ATOM	516	CB	ILE	A	79	28.128	39.890	21.354	1.00	14.93
ATOM	517	CG1	ILE	A	79	28.544	38.728	22.242	1.00	16.78
ATOM	518	CG2	ILE	A	79	26.779	39.666	20.665	1.00	18.07
ATOM	519	CD1	ILE	A	79	27.710	38.573	23.503	1.00	17.98
ATOM	520	N	PRO	A	80	30.333	42.321	20.970	1.00	13.89
ATOM	521	CA	PRO	A	80	31.444	43.127	21.506	1.00	14.07
ATOM	522	C	PRO	A	80	31.611	43.158	23.014	1.00	12.76
ATOM	523	O	PRO	A	80	32.406	43.939	23.509	1.00	14.46
ATOM	524	CB	PRO	A	80	31.155	44.521	20.933	1.00	13.96
ATOM	525	CG	PRO	A	80	29.626	44.590	20.957	1.00	14.89
ATOM	526	CD	PRO	A	80	29.178	43.161	20.577	1.00	15.92
ATOM	527	N	TYR	A	81	30.817	42.371	23.747	1.00	8.63
ATOM	528	CA	TYR	A	81	30.955	42.338	25.209	1.00	10.23
ATOM	529	C	TYR	A	81	30.712	40.922	25.698	1.00	9.25

PDB File Title Section

HEAD	First line of the entry, contains PDB ID code, classification, and date of deposition.	**HELIX**	Identification of helical substructures.
COMPND	Description of macromolecular contents of the entry.	**CRYST1**	Unit cell parameters, space group, and Z.
SOURCE	Biological source of macromolecules in the entry.	**ORIGXn**	Transformation from orthogonal coordinates to the submitted coordinates (n = 1, 2, or 3).
AUTHOR	List of contributors.	**SCALEn**	Transformation from orthogonal coordinates to fractional crystallographic coordinates (n = 1, 2, or 3).
REVDAT	Revision date and related information.	**MTRIXn**	Transformations expressing non-crystallographic symmetry (n = 1, 2, or 3). There may be multiple sets of these records.
JRNL	Literature citation that defines the coordinate set.	**ATOM**	Atomic coordinate records for standard groups.
REMARK	General remarks, some are structured and some are free form.	**HETATM**	Atomic coordinate records for heterogens.
SEQRES	Primary sequence of backbone residues.	**TER**	Chain terminator.
FORMUL	Chemical formula of non-standard groups.	**END**	Last record in the file.

RCSB PDB : Structure Explorer - Microsoft Internet Explorer

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An Information Portal to Biological Macromolecular Structures

As of Tuesday Jul 04, 2006 there are 37556 Structures | PDB Statistics

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MolProbity Ramachandran analysis

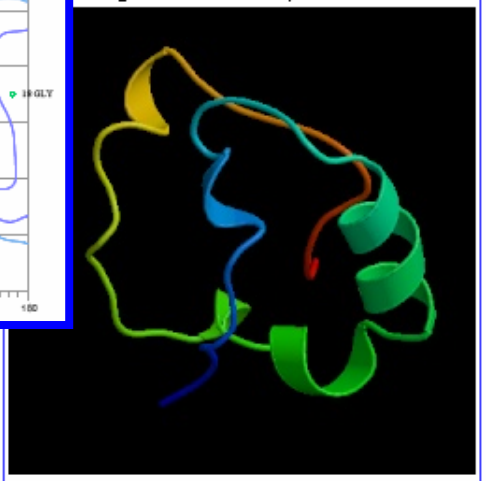
1L6H, model 1

General case Glycine

Psi Phi

ges and Visualization

Biological Molecule / Asymmetric Unit



Display Options

KiNG
Jmol
WebMol
Protein Workshop
QuickPDB
All Images

History	Deposition 2002-03-11 Release 2002-10-02
Experimental Method	Type NMR, minimized average structure Data N/A
NMR Ensemble	Conformers Calculated n/a Conformers Submitted n/a Selection Criteria n/a
NMR Refine	Method NMR, minimized average structure
Molecular Description Asymmetric Unit	Polymer: 1 Molecule: Non-Specific Lipid Transfer Protein Chains: A

完成 網際網路

開始 Microsoft Pow... RCSB PDB : ... 未命名 - 小... 兵役 - Outloo... http://www.rcs... CH 上午 11:42

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    - MMDB
    - OCA
    - CSU Contacts
    - MSD (wwPDB partner)
    - DSSP Secondary Structure
    - Protein Motions
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    - Columbia Surface Picture Gallery
  - Classification

PDBsum

MMDB (Molecular Modeling DataBase

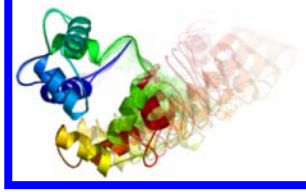
OCA©, a browser-database for protein structure/function.

Analysis of interatomic Contacts of Structural Units in PDB entry:

1L6H

Macromolecular Structure Database

DSSP Secondary Structure



Database of Macromolecular Movements
with Associated Tools for Flexibility and Geometric Analysis
This describes the motions that occur in proteins and other macromolecules, particularly using movies. Associated with it are a variety of free software tools and servers for structural analysis. (Citation info)

Computed Atlas of Surface Topography of proteins

Surface Picture Gallery

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    - FATCAT
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    - CE
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PQS Protein Quaternary Structure Query Form at the EBI

SCOP
STRUCTURAL CLASSIFICATION OF PROTEINS

CATH
Protein Structure Classification

Class(C)
Architecture (A)
Topology (T)
Homologous superfamily (H)

3Dee - Database of Protein Domain Definitions

HSSP HOMOLOGY DERIVED SECONDARY STRUCTURE OF PROTEINS

FATCAT

Flexible structure AlignmenT by Chaining Aligned fragment pairs allowing Twists

VAST
Structure Neighbors

Dali Fold Classification

Databases and Tools for 3-D Protein Structure Comparison and Alignment

Using the Combinatorial Extension (CE) Method

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PDBsum

- http://www.biochem.ucl.ac.uk/bsm/pdbsum
- Summaries and analyses of PDB structures
- To search all TITLE, HEADER, COMPND and SOURCE records in the PDB

PDBsum

A database of the known 3D structures

of proteins and nucleic acids

30 April 2004

PDBSum has moved to the EBI

It can now be found at www.ebi.ac.uk/t

If you are not automatically forwarded

PDBsum home page - Microsoft Internet Explorer

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EMBL-EBI European Bioinformatics Institute

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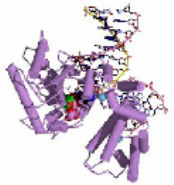

1bpv

PDBsum

PDBsum is a pictorial database providing an at-a-glance overview of every macromolecular structure deposited in the Protein Data Bank (PDB).

It provides schematic diagrams of the molecules in each structure and of the interactions between them. Entries are accessed by their PDB code, by simple text search, or through any of the browse options on the left.

Input the PDB ID

Enter PDB code *(4 characters)* 1L6H Find Reset

Text search Search

The text search scans all TITLE, HEADER, COMPND, SOURCE and AUTHOR records in the PDB (eg to find a given protein by name). For more information on searching, click here.

Note, the **Generate** option on the left lets you submit your own structure and have a password protected PDBsum analysis generated for it.

Latest enhancements

Enzyme structures

EC-PDB

The Enzyme Structures Database contains the known enzyme 3D structures in the Protein Data Bank (PDB), organized by the E.C. numbering hierarchy.

Sequence annotated by structure

SAS

SAS searches a given protein sequence against the sequences of the proteins of known 3D structure in the Protein Data Bank (PDB) and annotates the resultant alignment with structural information.

Function prediction

ProFunc

開始 Microsoft... RCSB P... 未命名 -... 兵役 - O... http://140... PDBsum ... CH 上午 10:59

http://www.ebi.ac.uk - PDBsum entry: 116h - Microsoft Internet Explorer

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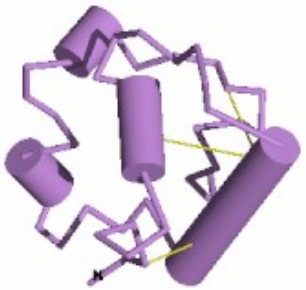
PDBsum

Go to PDB code: 116h go

Top page | Protein | Clefts | Links

Lipid

PDB id: 116h
Name: Lipid tr
Title: Solutio
Structure: Non-sp
Source: Oryza s
UniProt: P8321C
NMR structure: 1 mode
Authors: D.Samu
Key ref: D.Samu rice (Or
Date: 11-Mar-
Release date: 02-Oct-



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* Residue conservation analysis

Tools

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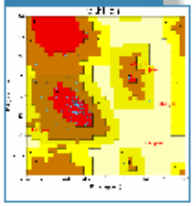
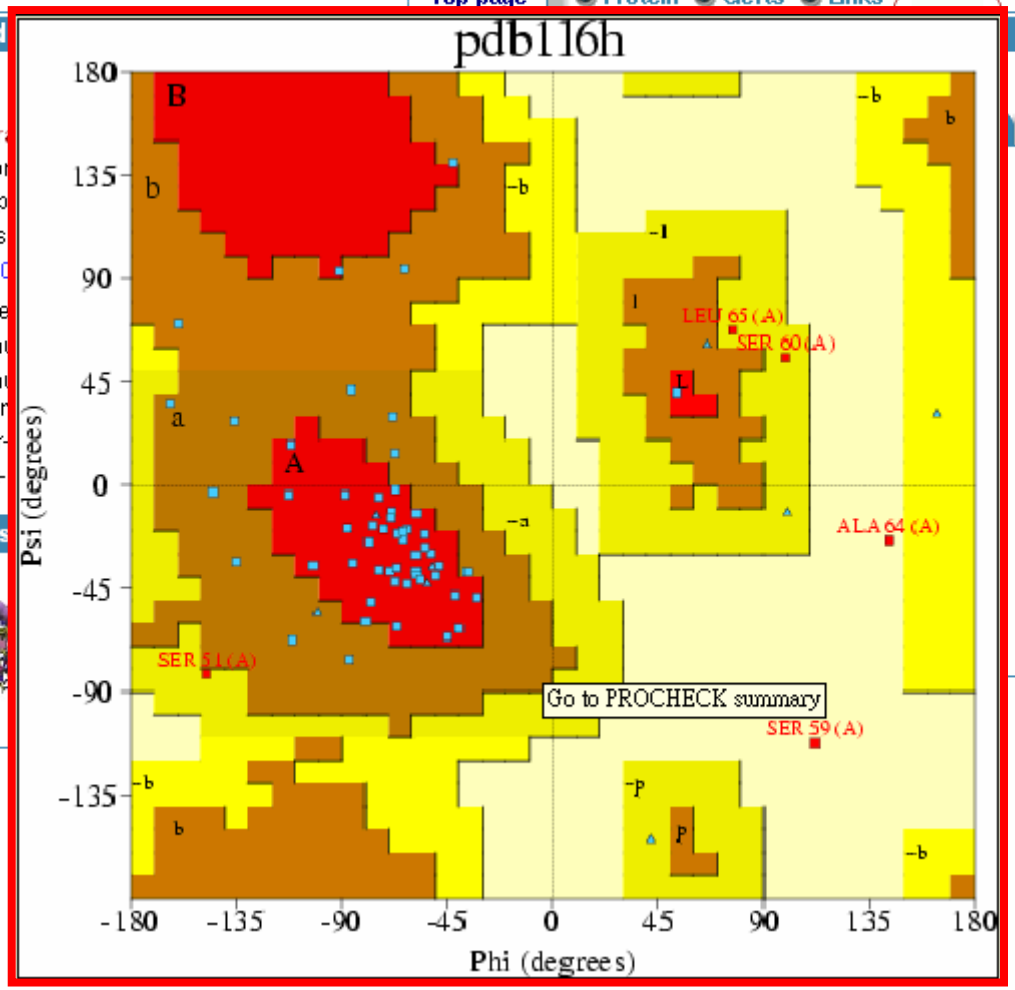
Run PROCHECK

Procheck



Clefts



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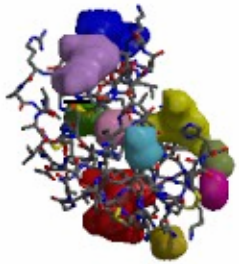
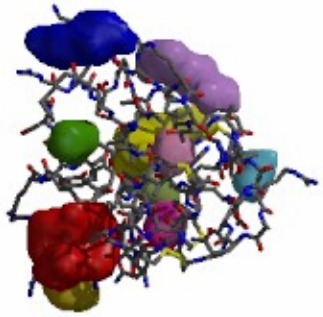
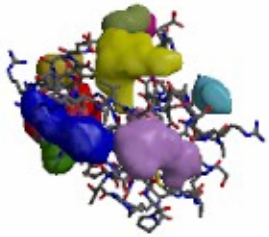
Cleft analysis for: 1l6h — PDB Id: 1l6h







View options

- (•) Binding-site(s) 
- ( ) Binding-surface(s) 

Coloured by

- (•) **cleft** (as in table below)
- ( ) **closest atom type**
- ( ) **residue type**
- ( ) **residue conservation**

Jmol | RasMol

Clefts

	Volume	R1 ratio	Accessible vertices		Buried vertices		Average depth		Residue type								Ligands
1	339.61	1.48	64.96	3	9.46	1	9.07	1	2	0	1	3	3	2	1		
2	229.08	0.00	61.78	5	8.59	2	5.12	4	1	0	3	4	0	2	2		
3	229.08	0.00	64.17	4	2.67	6	5.86	3	1	1	1	6	2	0	0		
4	198.70	0.00	56.78	8	5.31	3	6.21	2	2	0	1	1	0	2	0		
5	84.80	0.00	81.15	2	5.00	4	0.00	6	0	0	1	3	1	1	0		

* Residue conservation analysis

Tools

- Image Generation
- AstexViewer™@MSD-EBI
- Run PROCHECK

http://www.ebi.ac.uk - PDBsum entry: 1l6h - Microsoft Internet Explorer

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PDBsum

Go to PDB code: 1l6h go

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Lipid transport PDB Id: 1l6h

PDB id:	1l6h
Name:	Lipid transport
Title:	Solution structure of plant nsltp2 purified from rice (oryza sativa)
Structure:	Non-specific lipid transfer protein. Chain: a. Synonym: ltp2
Source:	Oryza sativa. Rice
UniProt:	P83210 (NLTPX_ORYSA) [Pfam]
NMR structure:	1 models
Authors:	D.Samuel,P.-C.Lyu
Key ref:	D.Samuel et al. (2002). Solution structure of plant nonspecific lipid transfer protein-2 from rice (Oryza sativa).. *J Biol Chem*, **277**, 35267-35273. [PubMed id: 12011089]
Date:	11-Mar-02
Release date:	02-Oct-02

Quick links: PDB, MSD, SRS, MMDB, Jena, OCA, CATH, SCOP, FSSP, HSSP, ProSAT, GRASS, STING, Whatcheck

Jmol

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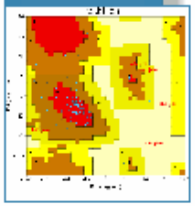
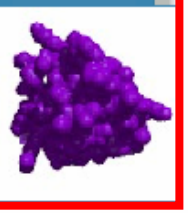
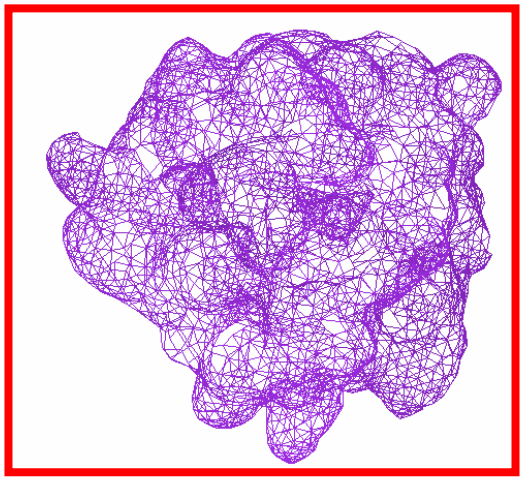
* Residue conservation analysis

Procheck | Clefts | Surface







Tools

Image Generation

AstexViewer™@MSD-EBI

Run PROCHECK

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DSDBASE

- http://caps.ncbs.res.in/dsdbase/dsdbase.html
- A database on disulphide bonds in proteins that provides information on native disulfides and those which are stereochemically possible between pairs of residues in a protein.

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- List of Enzymes
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- Labpage
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DSDBASE

Disulphide database

DSDBASE is a database on disulphide bonds in proteins that provides information on native disulphides and those which are stereochemically possible between pairs of residues in a protein.

One of the potential uses of such a disulphide database is to design site-directed mutants in order to enhance the thermal stability of the protein in question. Another important application is to employ this database for proposing 3D models of disulphide-rich polypeptides like toxins and small proteins by searching for sub-structural motifs which are compatible with the derived disulphide bond connectivity. The user can obtain information about disulphide bonds of a particular protein of interest or probe the database for multiple disulphide bonded systems of particular connectivity. [More...]

---

* *Several new features are added to the database. Click here for more*

Three different datasets are created for modelling purpose:

1. PDB entries (April 2003 release)

2. Non-redundant dataset (25% sequence identity cutoff)

3. Native disulphide bonds from the non-redundant dataset

Click here for previous release statistics

Distribution of Disulphide Bonds in DSBASE

Distribution of Disulphide Bonds in DSDBASE

S.No	Dataset	No. of Proteins	Native Disulphides	Modelled Disulphides	Total Disulphides
1	Non-redundant (April-2003)	2,849	2,170	147,722	149,892
2	Full database (April-2003)	19,612	31,657	2,353,960	2,385,617

* Search is now available on PDB-April 2003 release also.

Native and Modelled disulphide details for 1L6H

PDB code : 1l6h
Resolution(Angstroms) : NOT APPLICABLE
Number of disulphides : 30
Native : 4
Model : 26
A grade : 2
B grade : 5
C grade : 9
D grade : 14

Native : where both the residues are Cysteines

as annotated in the PDB file
as identified by MODIP

CYS Redox active cysteine

Click here for explanation of grade

Native and Modelled disulphide details for 1L6H

No.	Type	Residue i			Residue j			Grade	Retrive PDB file	Rasmol View	Stereo chemistry
		Residue	Chain	Res No	Residue	Chain	Res No				
1	Model	ALA	A	1	PRO	A	43	B	Mutant		
2	Model	ALA	A	1	ARG	A	44	D	Mutant		
3	Native	CYS	A	3	CYS	A	35	C	Wild		
4	Model	ASN	A	4	LEU	A	8	C	Mutant		
5	Model	CYS	A	11	THR	A	22	D	Mutant		
6	Native	CYS	A	11	CYS	A	25	B	Wild		
7	Model	THR	A	12	ALA	A	16	D	Mutant		
8	Model	ALA	A	14	ALA	A	19	C	Mutant		
9	Model	ALA	A	14	SER	A	59	C	Mutant		
10	Model	ALA	A	14	CYS	A	61	B	Mutant		

PDB-Ligand

- **http://www.idrtech.com/PDB-Ligand/**
- **PDB-Ligand** is a three dimensional structure database of small molecular ligands that are bound to larger biolomocules deposited in the **Protein Data Bank (PDB)**.

PDB-Ligand - Microsoft Internet Explorer

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PDB-Ligand

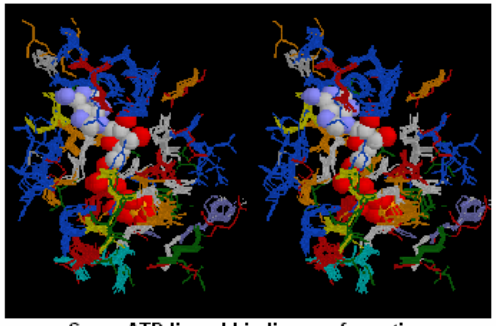
PDB-Ligand is a three dimensional structure database of small molecular ligands that are bound to larger biolomocules deposited in the **Protein Data Bank (PDB)**.

One unique feature of **PDB-Ligand** is that one can browse, classify, superimpose, and visualize the interactions between ligands and proteins.

PDB-Ligand serves as an interactive structural analysis and clustering tool for all the ligand-binding structures in PDB.

PDB-Ligand also provides an easier way to obtain a number of different structure alignments of many related ligand-binding structures based on simple and flexible ligand clustering method.

PDB-Ligand will be a good resource both for the better interpretation of ligand-binding structures and for the development of better scoring functions to be used in many drug discovery applications



Same ATP ligand binding conformation extracted from 10 different PDBs.

Start Browsing

PDB-Ligand News

- **March 3, 2006: New version PDB-Ligand 1.4 has been rele**
  - 6466 ligands types and 190928 models extracted from
- **April 4, 2005: New version PDB-Ligand 1.3 has been relea**
  - 5646 ligands types and 150747 models extracted from
  - 'Greedy Method' by Hobohm and Sander is used in clu
- **November 9, 2004: New version PDB-Ligand 1.2 has been**
  - 5391 ligands types and 138800 models extracted from
- **September 25, 2004: Web interface update**

PDB-Ligand

PDB-Ligand DataBase Statistics

Total Ligand	6466
Total Model	190918
Total PDB	25770

1. Entry Statistics
2. Most Abundant Ligands
3. Largest Ligands
4. Clustering Results for selected ligand

PDB-Ligand

| Home | Browse | Statistics | Help | FAQ |

Search for " serotonin "

HET	Full Name	MW	Formular	Model	PDB
ASE	N-acetyl Serotonin	218.14	C12 H14 N2 O2	1	1

Total 1 Hit(s)

PDB-Ligand - Microsoft Internet Explorer

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Address http://www.idrtech.com/PDB-Ligand/ Go

PDB-Ligand

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Back to search

ASE

N-acetyl Serotonin
(C12 H14 N2 O2)

	PDB	Ligand	Select	Link
1	1nas	ASE 1	☐	RCSB

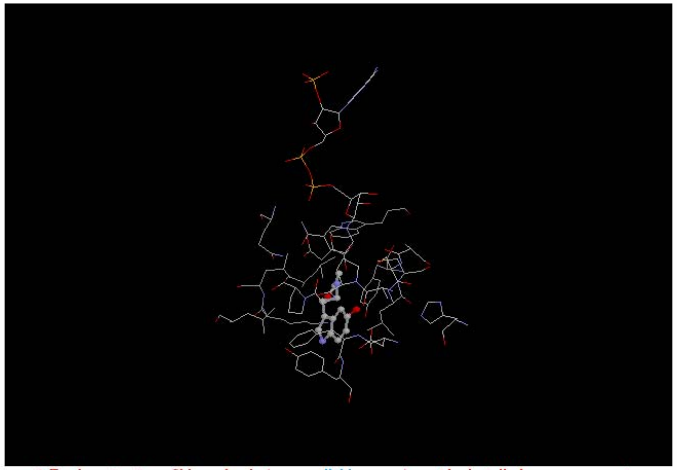
Select Ligands

Select All | View Selected

Color Change

Color Model | Color Atom

ASE Structure View



To view structure, Chime plug-in (www.mdlchime.com) must be installed on your computer

Chime Log (copy atoms to cluster)

```
Chime script completed.
script <exiting>
wireframe 0.1
cpk 0.3
16 atoms selected!
select (ASE)
```

Selected Atoms (paste selected atoms)

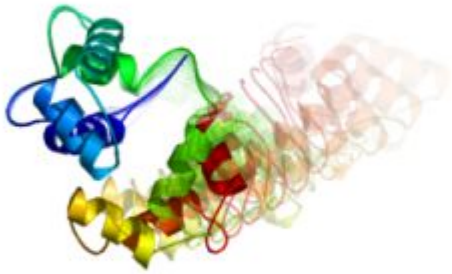
Clear

RMS value 0.5 Cluster Now Clear

Database of Macromolecular Movements

- http://molmovdb.mbb.yale.edu/molmovdb/
- This describes the motions that occur in proteins and other macromolecules, particularly using movies. Associated with it are a variety of free software tools and servers for structural analysis.

molmovdb.org



Database of Macromolecular Movements

with Associated Tools for Geometric Analysis

This describes the motions that occur in proteins and other macromolecules, particularly using movies. Associated with it are a variety of free software tools and servers for structural analysis.

[Citation info | Old front page]

Explore the database

Browse the database through the hierarchy of motions. Entries are organized by type of motion and by CATH classification.

View a sortable list of of all movies. Recent submissions are displayed first. The highlights page showcases some of our best movies.

Select a motion:

16S fragment of small ribosomal subu... [16S]

Search database: Full-text

Use our software

If you want to make your own movies, we have a Morph Server that will interpolate between any two protein conformations. In development is a server for Normal Mode Analysis of protein domains.

Many useful programs for structure analysis produced by members of the lab are available for download.

Other Resources

- General help and information
- Motions in membrane proteins
- Gerstein Lab home page

Email: Mark.Gerstein@yale.edu
This page created by Nat Echols
Last modified Nov. 7, 2002

Database overview - Microsoft Internet Explorer

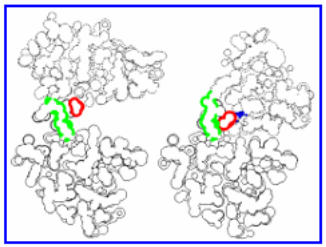
File Edit View Favorites Tools Help

Back Search Favorites

Address http://www.molmovdb.org/cgi-bin/browse.cgi

Go Links

molmovdb.org



Molecular Movements Database

This outline presents the current database classified by any classification scheme for which data has been compiled. The original schema which separates motions by type of movement is defined on the help page. Thumbnail images appear for motions which have available movies, and link to the best morph for that particular protein.

Many more movies can be seen here, including structures not represented on this page. The movies page also allows searches for protein names or specific PDB IDs.

Switch to CATH survey

I. Motions of Fragments Smaller than Domains

A. Motion is predominantly shear

F-s-2. Proteins for which two or more conformations are known

Adenosylcobinamide Kinase [motion] [morph]

Small G-protein Arf6 [motion] [morph]

Bacteriorhodopsin (bR) [motion] [morph]

Calbindin [motion] [morph]

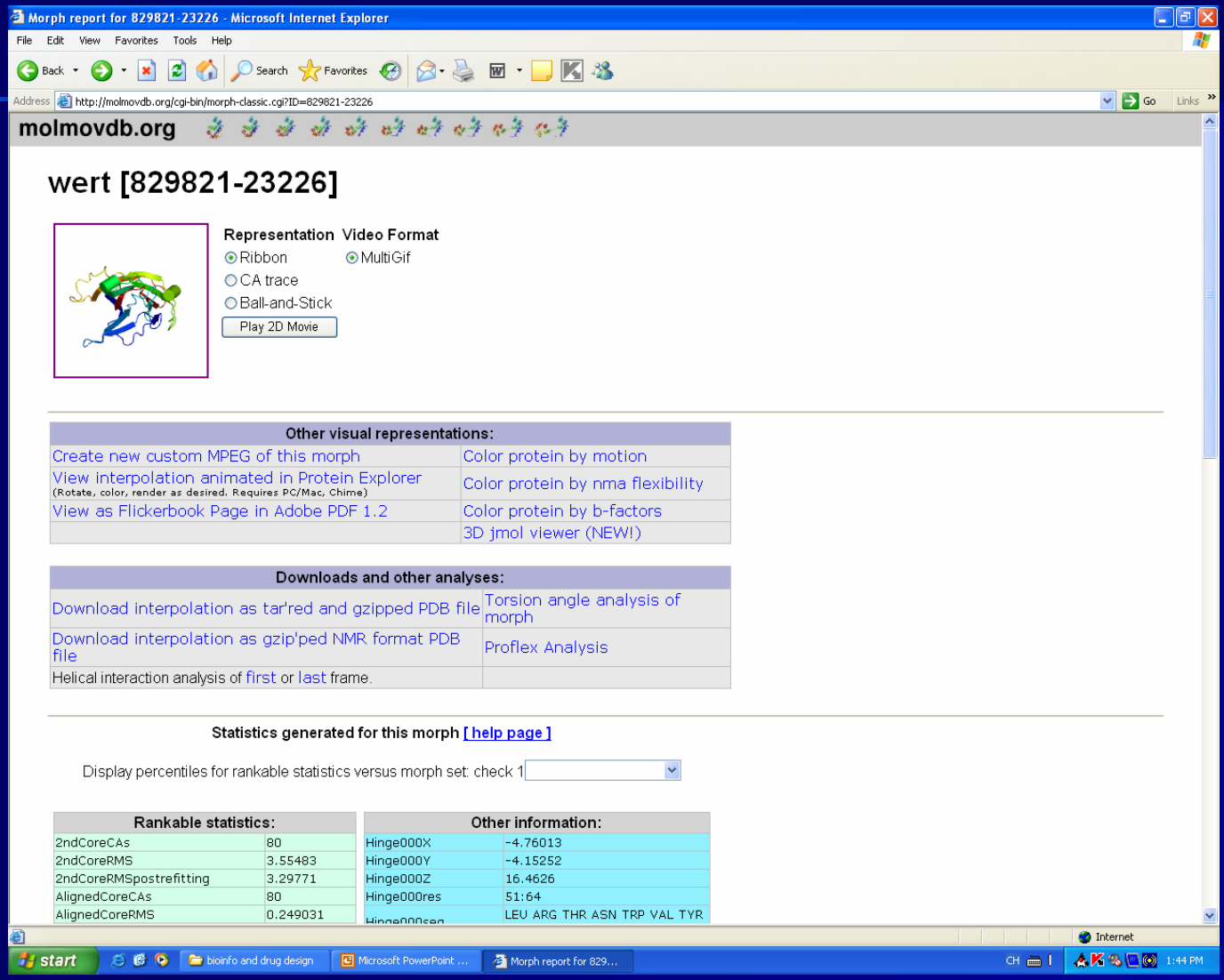
Dihydrofolate Reductase (DHFR) [motion] [morph]

(76 items remaining) Downloading picture http://www.molmovdb.org/uploads/tms/sicon.png...

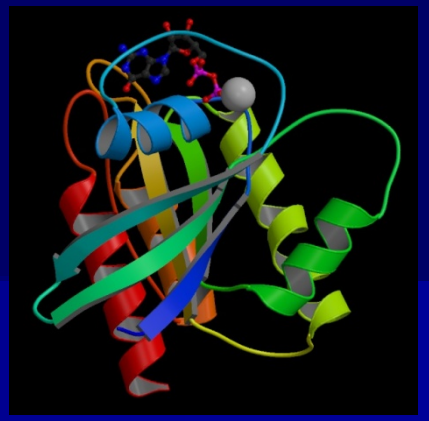
Internet

start bioinfo and drug design Microsoft PowerPoint ... Database overview - ... CH 1:30 PM

http://molmovdb.org/cgi-bin/morph-classic.cgi?ID=829821-23226

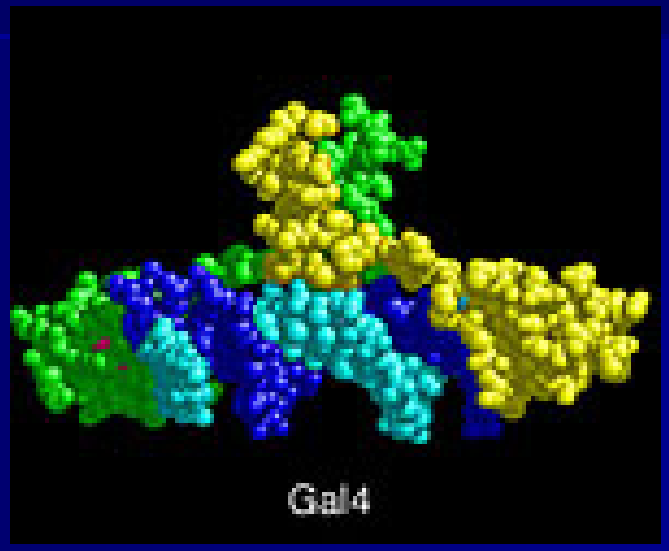


蛋白質結構軟體應用
Software for Protein Structure Visualization



- RasMol http://www.umass.edu/microbio/rasmol/
- Chemscape ChimeTM http://www.mdlchime.com/chime/
- MolPOV http://www.chem.ufl.edu/~der/der_pov2.htm
- MolMol http://www.mol.biol.ethz.ch/wuthrich/software/molmol/
- Ribbons http://www.cmc.uab.edu/ribbons/
- MolScript http://www.avatar.se/molscript/
- WebLab ViewerLite and ViewerPro http://www.accelrys.com/about/msi.html
- Swiss-PDB Viewer http://www.expasy.ch/spdbv/
- XtalView http://www.scripps.edu/pub/dem-web/toc.html
- MolView and MolView Lite http://bilbo.bio.purdue.edu/~tom/
- Pymol
- Chimera

RasMol for Dummies



A Tutorial for the Rasmol Basics

http://mod.life.nthu.edu.tw/bioinfo/rasmol/

The End