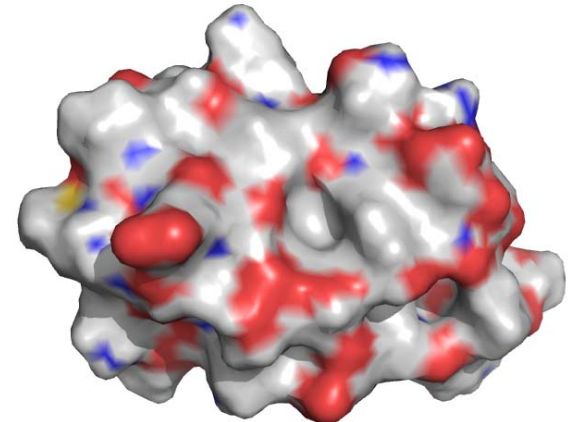
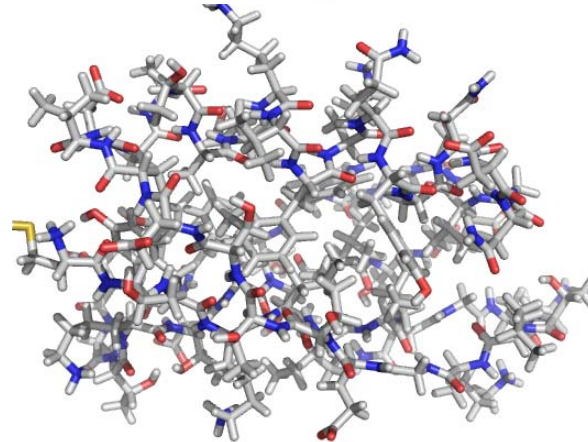
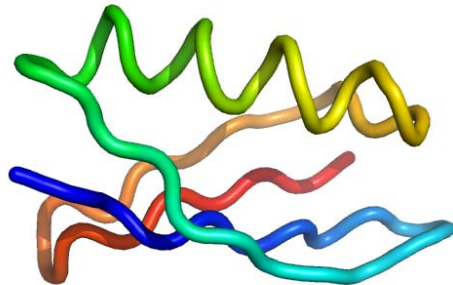
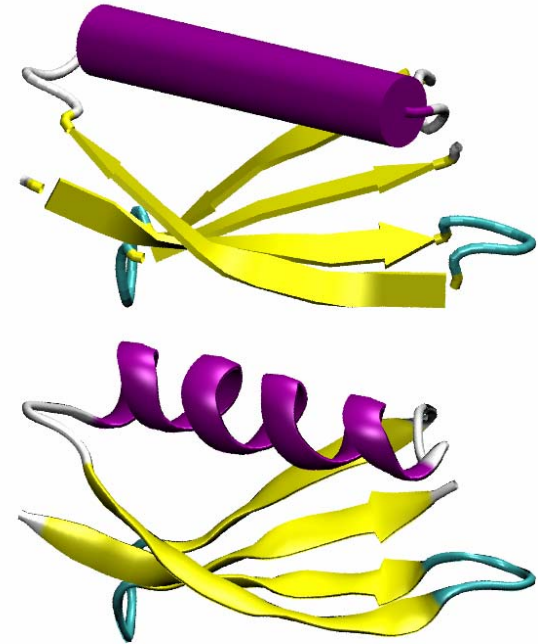
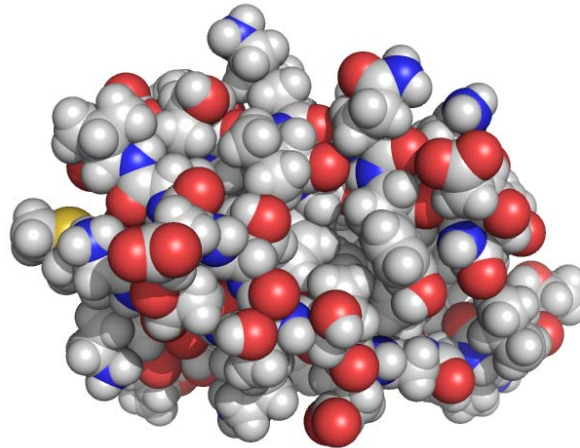
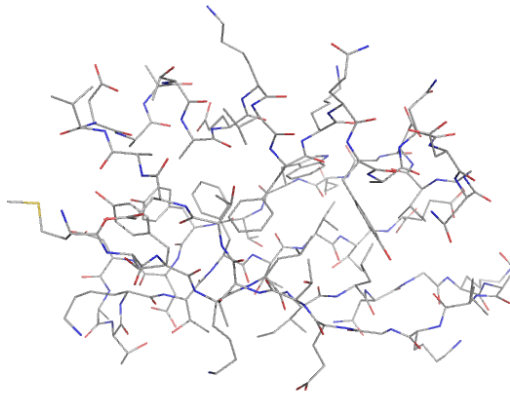


Graphical Representation of Protein

- Line, bond, van der Waals (CPK), trace, cartoon, surface, etc



Experimental Structural Data

Description of the databases

How to explore and query the data

Source of the data

X-ray crystallography, NMR

Quality of the data

How to manipulate 3D data

How to visualize the data

<http://www.rcsb.org/pdb>

RCSB PDB
PROTEIN DATA BANK

Welcome to the PDB, the single worldwide repository for the processing and distribution of 3-D biological macromolecular structure data.

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browse LINKS
BETA TEST new features
BETA PDBML/XML files

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29956 Structures
Last Update: 08-Mar-2005
[PDB Statistics](#)

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RCSB PDB Beta Site

Molecule of the Month:
[T-Cell Receptor](#)

The Protein Data Bank (PDB) is operated by Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the Center for Advanced Research in Biotechnology/UMI/NIST - three members of the [Research Collaboratory for Structural Bioinformatics \(RCSB\)](#).

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08-Mar-2005
[Physical Model of February's Molecule of the Month - Major Histocompatibility Complex - Available on Loan to Educators](#)
As part of a project by Molecule of the Month author David S. Goodsell (The Scripps Institute) and Tim Herman (Center for BioMolecular Modeling), a physical model of Class I MHC is available on loan to educators. [\[MORE...\]](#)

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H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne:
[The Protein Data Bank](#), *Nucleic Acids Research*, 28 pp. 235-242 (2000)

The PDB database is the main repository for the processing and distribution of 3-D biological macromolecular structure data

Anatomy of PDB Files

Protein description

Literature

Data about the experiment

Sequence

Structure (atomic coordinates)

Connectivity

File Format

```
HEADER IMMUNOGLOBULIN 25-OCT-96 1IGT
COMPND MOLECULE: IGG2A INTACT ANTIBODY - MAB231;
SOURCE MOUSE (MUS MUSCULUS, STRAIN BALB/C)
KEYWDS INTACT IMMUNOGLOBULIN V REGION C REGION, IMMUNOGLOBULIN
EXPDTA X-RAY DIFFRACTION
AUTHOR L.J.HARRIS,S.B.LARSON,K.W.HASEL,A.MCPHERSON
REVDAT 1 07-JUL-97 1IGT 0
JRNL AUTH L.J.HARRIS,S.B.LARSON,K.W.HASEL,A.MCPHERSON
JRNL TITL REFINED STRUCTURE OF AN INTACT IGG2A MONOCLONAL
JRNL TITL 2 ANTIBODY
JRNL REF BIOCHEMISTRY V. 36 1581 1997
JRNL REFN ASTM BICHAW US ISSN 0006-2960 0033
***
REMARK 2 RESOLUTION. 2.8 ANGSTROMS.
***
SEQRES 1 A 214 ASP ILE VAL LEU THR GLN SER PRO SER SER LEU SER ALA
SEQRES 2 A 214 SER LEU GLY ASP THR ILE THR ILE THR CYS HIS ALA SER
SEQRES 3 A 214 GLN ASN ILE ASN VAL TRP LEU SER TRP TYR GLN GLN LYS
***
HET NAG D 1 26
HETNAM NAG N-ACETYL-D-GLUCOSAMINE
FORMUL 5 NAG 8(C8 H15 N1 O6)
***
HELIX 1 1 PRO A 80 ASP A 82 5
***
SHEET 1 A 4 LEU A 4 SER A 7 0
SHEET 2 A 4 ILE A 19 HIS A 24 -1 N HIS A 24 0 THR A 5
SHEET 3 A 4 GLY A 70 ILE A 75 -1 N ILE A 75 0 ILE A 19
SHEET 4 A 4 PHE A 62 SER A 67 -1 N SER A 67 0 GLY A 70
***
SSBOND 1 CYS A 23 CYS A 88
***
CRYST1 65.820 76.770 100.640 88.05 92.35 97.23 P 1 2
***
ATOM 1 N ASP A 1 1.600 -85.453 44.624 1.00 43.02 N
ATOM 2 CA ASP A 1 1.649 -84.304 45.569 1.00 38.99 C
ATOM 3 C ASP A 1 0.334 -84.255 46.321 1.00 38.23 C
ATOM 4 O ASP A 1 -0.652 -84.862 45.904 1.00 49.17 O
ATOM 5 CB ASP A 1 1.826 -82.992 44.807 1.00 45.89 C
ATOM 6 CG ASP A 1 3.124 -82.933 44.021 1.00 54.91 C
ATOM 7 OD1 ASP A 1 3.551 -83.966 43.460 1.00 58.03 O
ATOM 8 OD2 ASP A 1 3.713 -81.831 43.950 1.00 61.73 O
ATOM 9 1H ASP A 1 0.744 -85.315 44.045 1.00 15.00 H
ATOM 10 2H ASP A 1 2.453 -85.542 44.045 1.00 15.00 H
ATOM 11 3H ASP A 1 1.443 -86.304 45.196 1.00 15.00 H
ATOM 12 N ILE A 2 0.340 -83.582 47.459 1.00 34.73 N
ATOM 13 CA ILE A 2 -0.861 -83.420 48.270 1.00 29.53 C
***
TER 2034 CYS A 214
HETATM12748 C1 NAG D 1 15.179 2.409 -21.411 1.00138,48 C
HETATM12749 C2 NAG D 1 14.181 1.365 -20.856 1.00137,31 C
HETATM12750 C3 NAG D 1 14.918 0.088 -20.438 1.00133,46 C
***
CONECT 194 193 814
***
END
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Header section

Coordinate section

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HEADER	IMMUNOGLOBULIN				25-OCT-96	1IGT
COMPND	MOLECULE: IGG2A INTACT ANTIBODY - MAB231;					
SOURCE	MOUSE (MUS MUSCULUS, STRAIN BALB/C)					
KEYWDS	INTACT IMMUNOGLOBULIN V REGION C REGION, IMMUNOGLOBULIN					
EXPDTA	X-RAY DIFFRACTION					
AUTHOR	L.J.HARRIS,S.B.LARSON,K.W.HASEL,A.MCPHERSON					
REVDAT	1	07-JUL-97	1IGT	0		

1 2 3 4 5 6
12345678901234567890123456789012345678901234567890123456

JRNL AUTH L.J.HARRIS,S.B.LARSON,K.W.HASEL,A.MCPHERSON
JRNL TITL REFINED STRUCTURE OF AN INTACT IGG2A MONOCLONAL
JRNL TITL 2 ANTIBODY
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JRNL REFN ASTM BICHAW US ISSN 0006-2960 0033

1 2 3 4 5 6
12345678901234567890123456789012345678901234567890123456

REMARK 2 RESOLUTION. 2.8 ANGSTROMS.

1 2 3 4 5 6
123456789012345678901234567890123456789012345678901234567890123456

REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER ;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER ;
REMARK 470 I=INSERTION CODE :(

REMARK 470 M RES CSSEQI ATOMS

REMARK 470 LEU A 6 CG CD1 CD2

REMARK 470 ARG A 8 CG CD NE CZ NH1 NH2

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HELIX 1 1 PRO A 80 ASP A 82 5

SHEET 1 A 4 LEU A 4 SER A 7 0

SHEET 2 A 4 ILE A 19 HIS A 24 -1 N HIS A 24 O THR A

SHEET 3 A 4 GLY A 70 ILE A 75 -1 N ILE A 75 O ILE A

SHEET 4 A 4 PHE A 62 SER A 67 -1 N SER A 67 O GLY A

	1	2	3	4	5	6
1234567890	1234567890	1234567890	1234567890	1234567890	1234567890	123456

SSBOND 1 CYS A 23 CYS A 88

CRYST1 65.820 76.770 100.640 88.05 92.35 97.23 P 12

	1	2	3	4	5	6
	123456789012345678901234567890123456789012345678901234567890123456					
SEQRES	1 A 214	ASP ILE VAL LEU THR GLN SER PRO SER SER LEU SER				
SEQRES	2 A 214	SER LEU GLY ASP THR ILE THR ILE THR CYS HIS ALA				
SEQRES	3 A 214	GLN ASN ILE ASN VAL TRP LEU SER TRP TYR GLN GLN				

	1	2	3	4	5	6
	123456789012345678901234567890123456789012345678901234567890123456					
HET	NAG D 1	26				
HETNAM	NAG N-ACETYL-D-GLUCOSAMINE					
FORMUL	5 NAG	8(C8 H15 N1 O6)				

										1	2		3			4			5			6					
										12345678901	23456789012	34567890123	45678901234	56789012345	67890123456	78901234567	89012345678	90123456789	01234567890	12345678901	23456789012	34567890123	45678901234	56789012345			
										Atom	Atom	Res	Res	X			Y			Z			Occ	B-fact			
										No	name		No														
										-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
ATOM		1	N	ASP	A	1		1.600	-85.453	44.624	1.00	43.02															
ATOM		2	CA	ASP	A	1		1.649	-84.304	45.569	1.00	38.99															

										1	2		3			4			5			6		
										12345678901	23456789012	34567890123	45678901234	56789012345	67890123456	78901234567	89012345678	90123456789	01234567890	12345678901	23456789012	34567890123	45678901234	56789012345
HETATM	3568	CA	CA	0	12.108	-17.156	78.830	1.00	7.31															
HETATM	3569	O	HOH	1	12.160	-19.496	78.042	1.00	33.27															
HETATM	3570	O	HOH	2	23.163	-36.984	67.113	1.00	18.80															
HETATM	3571	O	HOH	3	10.102	-42.843	63.995	1.00	24.28															
HETATM	3572	O	HOH	4	22.311	-19.282	69.877	1.00	27.58															

1 2 3 4 5 6
123456789012345678901234567890123456789012345678901234567890123456

CONNECT 482 480 3568

CONNECT 509 507 3568

CONNECT 3568 482 509 3799

Molecular Viewers

- VMD – versatile, steep learning curve
<http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD>
Windows version available on Ublearns
manual: ublearns
- Swiss-PDB Viewer (DeepView) – light and easy to work with but unstable
download: <http://www.expasy.ch/spdbv/text/getpc.htm>
Windows version available on Ublearns
not supported on Linux
manual: <http://www.usm.maine.edu/~rhodes/SPVTut/>
- PyMol – very nice graphics, very hard to work with
<http://pymol.sourceforge.net/>
Windows version available on Ublearns
- PMV
<http://mgltools.scripps.edu/flash/pmv>
- Jmol, Kinemage (KiNG), RasMol (not recommended)

Pick one and learn it well !!

OpenGL

VMD

Controls display

Main window

The screenshot displays the VMD (Visual Molecular Dynamics) software interface. The main window shows a 3D rendering of a protein structure (1STP) in a yellow ribbon representation, set against a black background. A red arrow points to the 'OpenGL' label in the top-left corner of the window title bar. To the right, the 'Graphical Representations' panel is open, showing settings for the selected molecule (1: 1STP). The 'Style' is set to 'NewCartoon', 'Color' to 'Structure', and 'Selection' to 'all'. Below this, the 'Selected Atoms' field contains 'all'. The 'Draw style' tab is active, showing 'Coloring Method' as 'Structure' and 'Material' as 'Opaque'. The 'Drawing Method' is 'NewCartoon' and 'Spline Style' is 'Catmull-Rom'. The 'Aspect Ratio' is 4.10 and 'Thickness' is 0.30. The 'Resolution' is set to 6. The 'Apply Changes Automatically' checkbox is checked. Below the main window, the 'VMD Main' window is open, displaying a table with the following data:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	T	A	D	F	1STP	1001	1	0

At the bottom, the console window shows the following output:

```
vmd > mol new 1STP
Info> Using plugin wepddb for structure file 1STP
Info> Using plugin wepddb for coordinates from file 1STP
Info> Determining bond structure from distance search ...
Info> Analyzing structure ...
Info> Atoms: 1001
Info> Bonds: 940
Info> Residues: 206
Info> Waters: 84
Info> Segments: 1
Info> Fragments: 86 Protein: 1 Nucleic: 0
1
Info> Finished with coordinate file 1STP.
vmd > Info> In any publication of scientific results based in part or
Info> completely on the use of the program STRIDE, please reference:
Info> Frishman,D & Argos,P. (1995) Knowledge-based secondary structure
Info> assignment. Proteins: structure, function and genetics, 23, 566-579.
```

Swiss-PDB Viewer

The screenshot displays the Swiss-PDB Viewer interface. The main window shows a 3D ribbon representation of a protein structure (1GB1) with orange and green ribbons. The interface includes a menu bar, a toolbar, and several panels:

- Ramachandran Plot:** A plot showing the distribution of Phi and Psi angles for the protein structure. The plot is titled "Ramachandran Plot" and shows the distribution of Phi and Psi angles for the protein structure. The x-axis is labeled "Phi" and the y-axis is labeled "Psi".
- Control Panel:** A panel for controlling the visibility and movement of the protein structure. It lists the amino acid residues and their corresponding checkboxes for visibility and movement.
- Layers Infos:** A table showing the properties of the layers in the viewer.
- Alignment:** A panel showing the sequence alignment of the protein structure.

layer	vis	mov	axis	CA	O	H	Hbond	Hdst	side	HOH	cyc	Sel
1GB1	v	v	v	v	v	v	v	v	v	v	v	57

The alignment panel shows the sequence: MT Y K L I L N G K I L K D E T T T E A V D A A T A E K V F K Q Y A N D N G V D G E W T Y D D A T K T F T V T E

Ramachandran plot

Control panel

Sequence alignment

Layer info

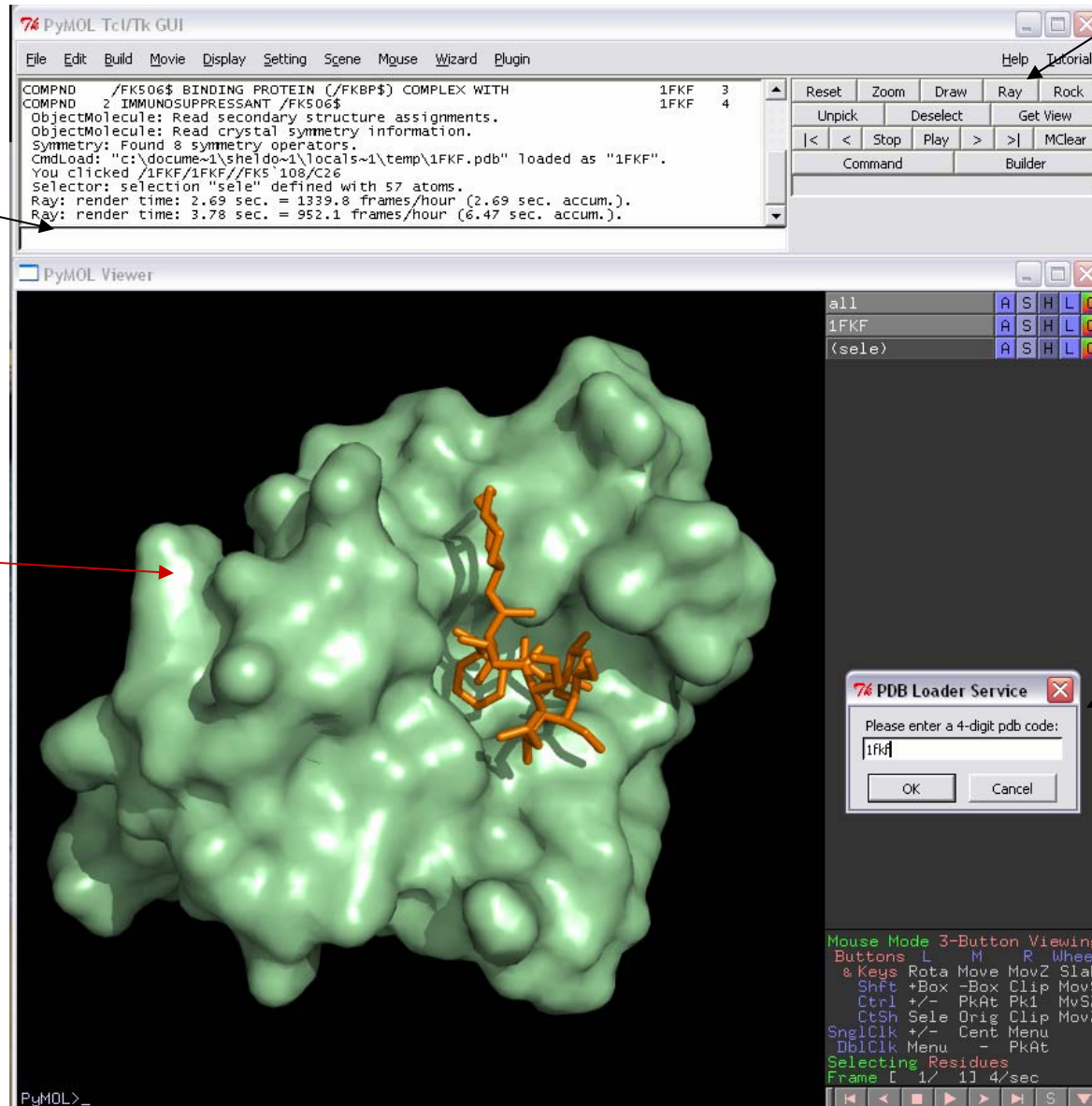
PyMol

Ray tracing

Enter commands

Publication quality graphics

Download structure directly from PDB



Short demo of PMV

file:///D:/CE%20405%20Protein%20Engineering/pmv_demo.html

from

<http://mgltools.scripps.edu/flash/pmv>