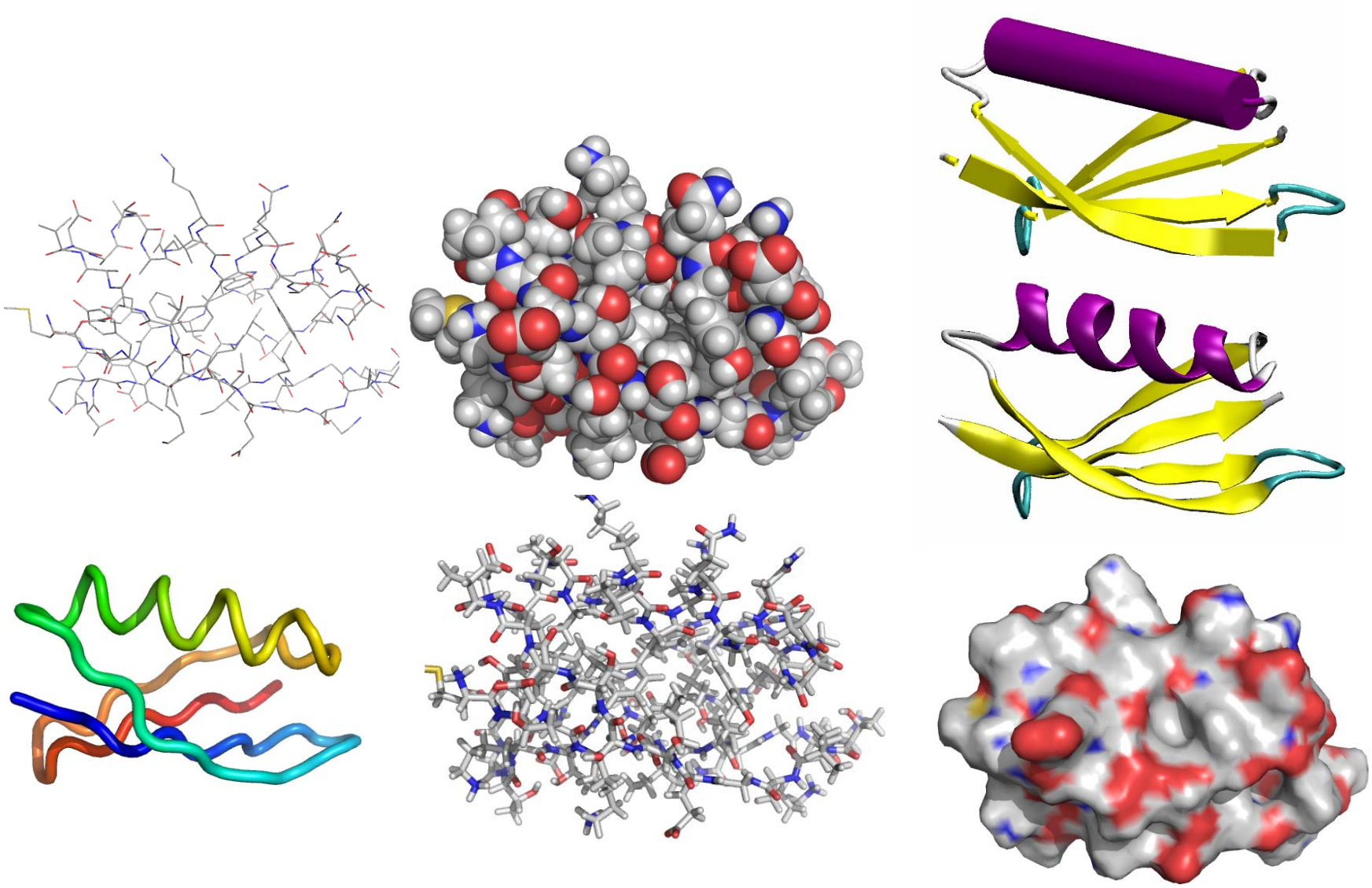
Graphical Representation of Protein

•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

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                                   3
...
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   5
SHEET    3   A 4 GLY A  70  ILE A  75 -1  N  ILE A  75   O  ILE A  19
SHEET    4   A 4 PHE A  62  SER A  67 -1  N  SER A  67   O  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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123456789012345678901234567890123456789012345678901234567890123456

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
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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
```

```
         1         2         3         4         5         6
123456789012345678901234567890123456789012345678901234567890123456

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
```

```
         1         2         3         4         5         6
123456789012345678901234567890123456789012345678901234567890123456

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
123456789012345678901234567890123456789012345678901234567890123456

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
123456789012345678901234567890123456789012345678901234567890123456

       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
123456789012345678901234567890123456789012345678901234567890123456

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
```

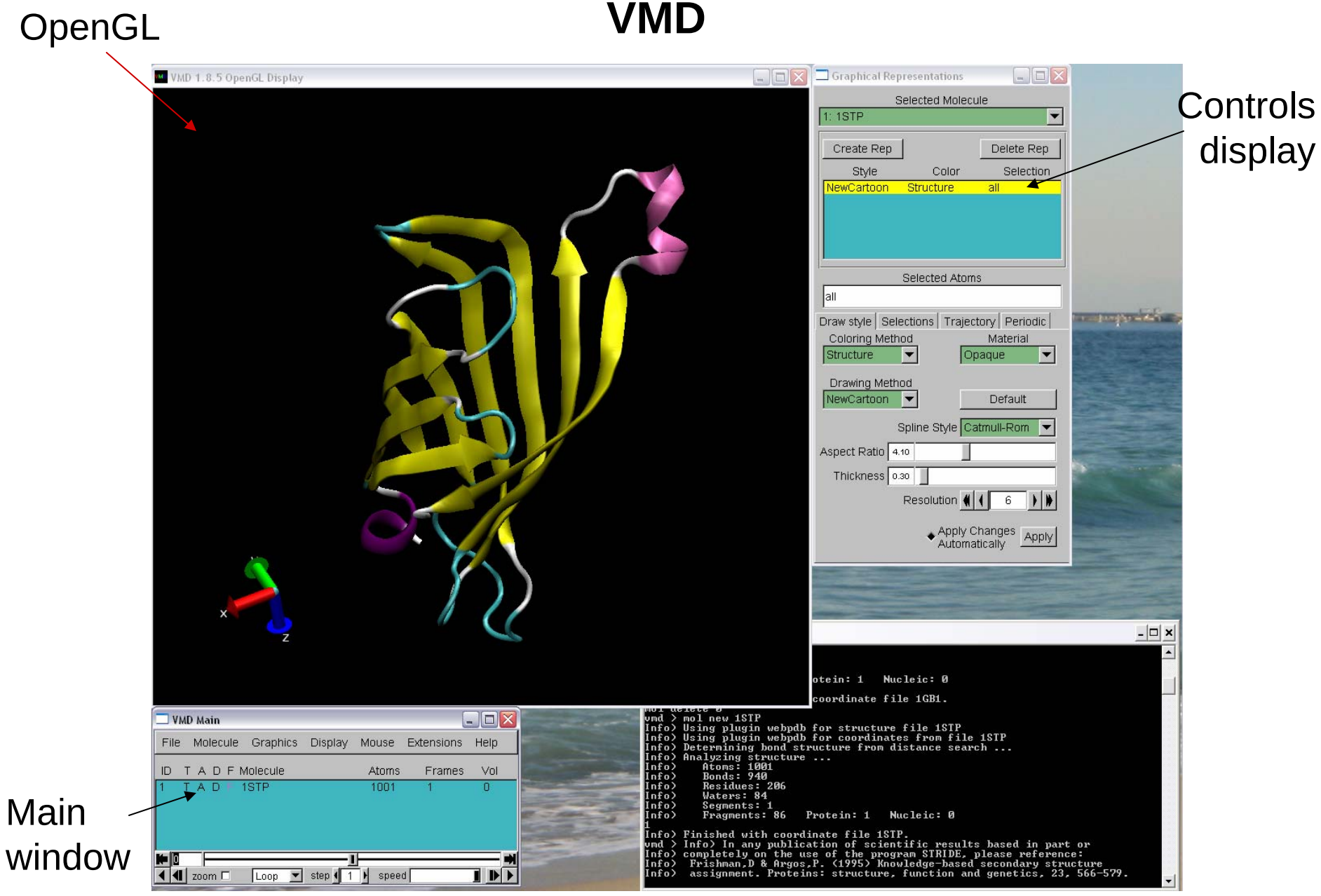
```
         1         2         3         4         5         6
123456789012345678901234567890123456789012345678901234567890123456

CONECT  482  480 3568
CONECT  509  507 3568
CONECT 3568  482  509 3799
```

Molecular Viewers

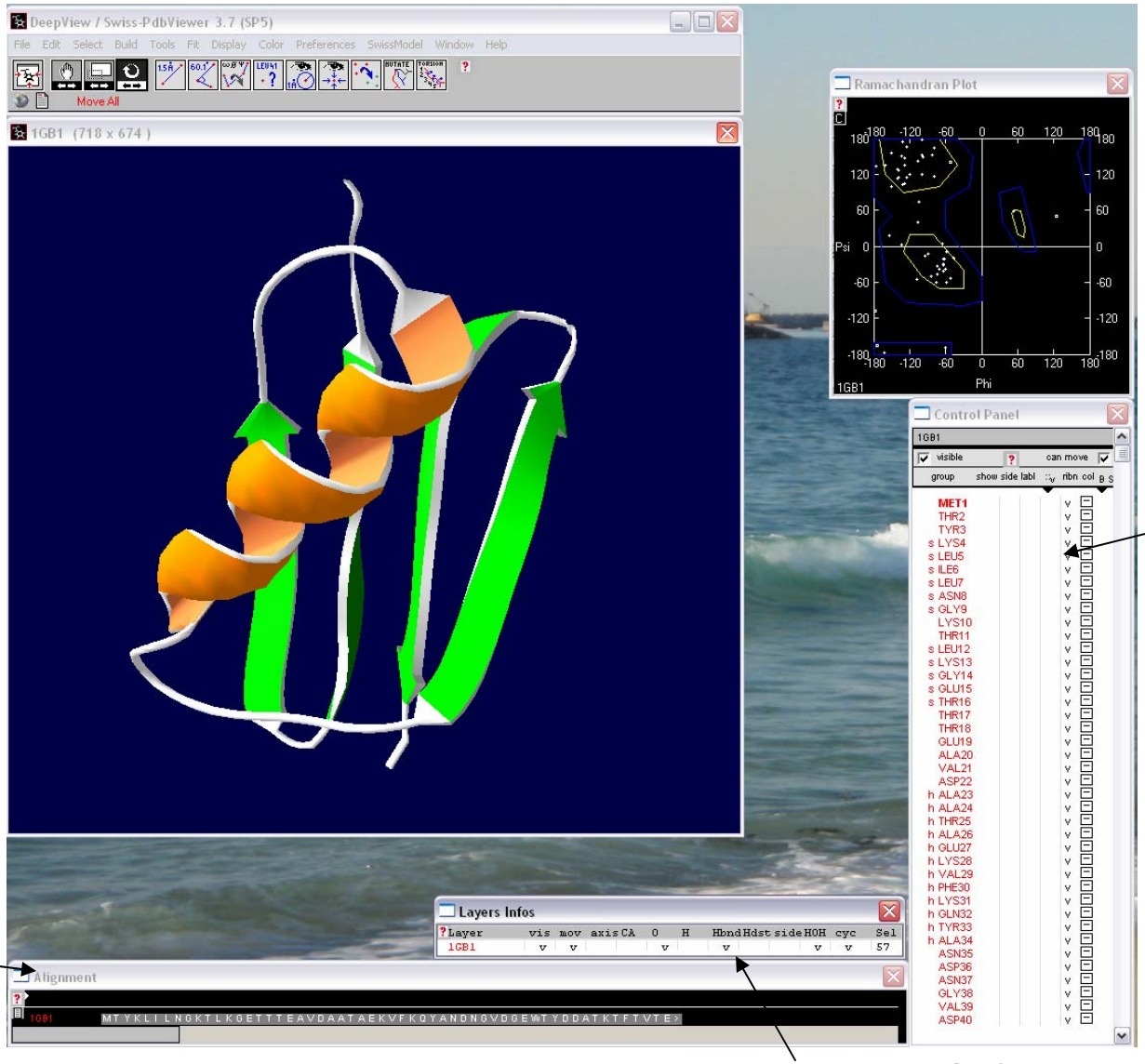
- VMD – versatile, steep learning curve
  - http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD
  - Windows version available on Ublearns
  - manual: ublearns
- Swiss-PDB Viewer (DeepView) – light and easy to work with but unstable
  - download: http://www.expasy.ch/spdbv/text/getpc.htm
  - 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 !!

VMD


OpenGL
Controls display
Main window
VMD 1.8.5 OpenGL Display
Graphical Representations
Selected Molecule
1: 1STP
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Selected Atoms
all
Draw style
Selections
Trajectory
Periodic
Coloring Method
Structure
Material
Opaque
Drawing Method
NewCartoon
Default
Spline Style
Catmull-Rom
Aspect Ratio
4.10
Thickness
0.30
Resolution
6
Apply Changes Automatically
Apply
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Frames
Vol
1 T A D 1STP
1001
1
0
zoom
Loop
step
1
speed
otein: 1 Nucleic: 0
coordinate file 1GB1.
vmd > mol new 1STP
Info) Using plugin webpdb for structure file 1STP
Info) Using plugin webpdb 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
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



Ramachandran plot

Control panel

Sequence alignment

Layer info

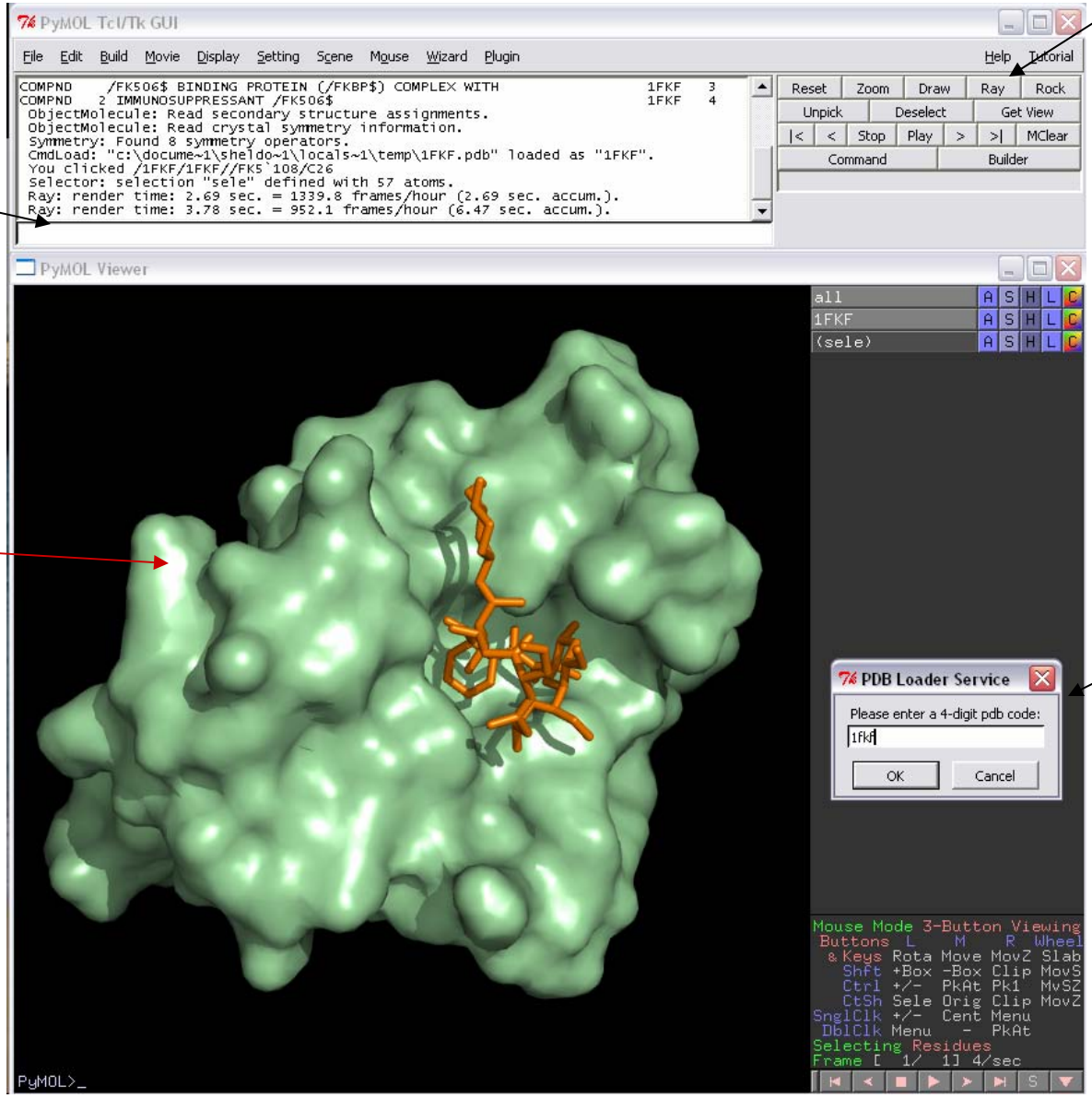
PyMol

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