

# Structure visualization



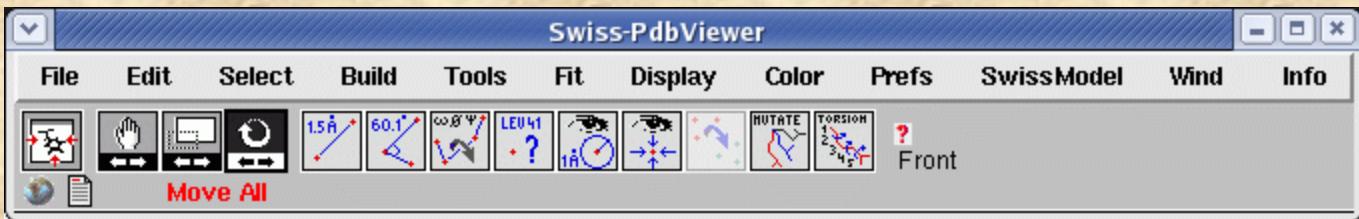
Practical examples

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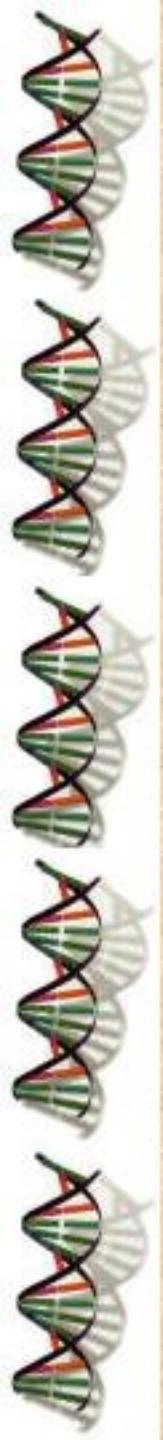
# Open structure

- Start program “SwissPDB View” (spdbv)
- Open structure:
  - File -> Open PDB File...
  - Select file with the structure
  - If file contains more than one model, load only one:
    - Load 1 models
  - Close report window

A terminal-like window titled "/root/SPDBV/temp/inputlog2.txt". It displays a log message about loading a PDB file. The log starts with a note about default behavior, followed by the command "LOAD PDB log file for /u/jc/tmp/pdb1eri.ent", and then a detailed list of missing atoms for residues 1 through 13 of chain B. The log concludes with "done loading layer 0:pdb1eri".

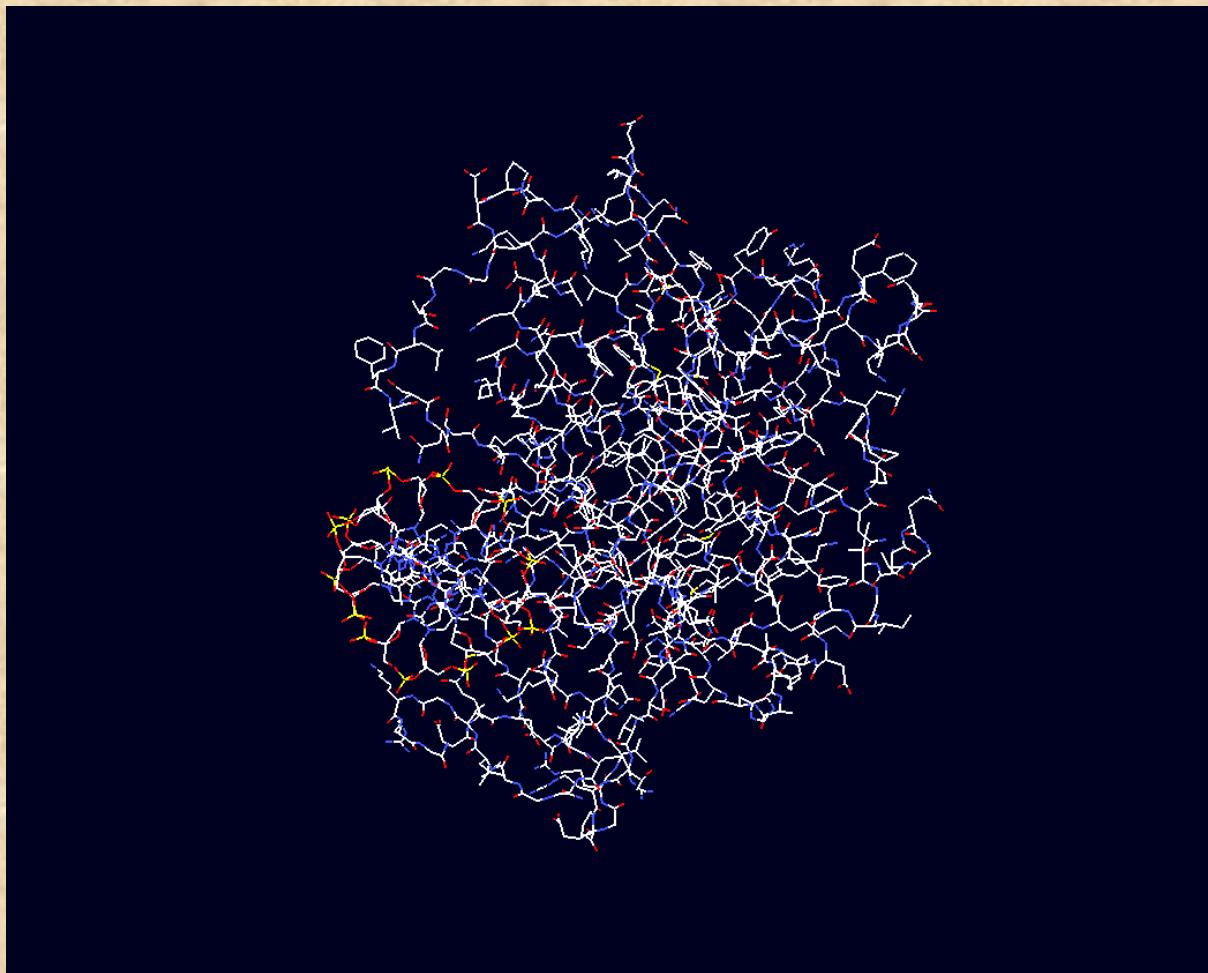
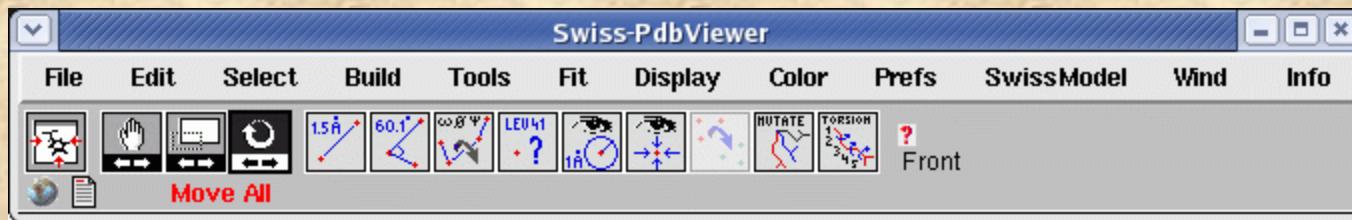
```
By default this log will appear each time a molecule
is loaded. This option can be disabled in
the General Preferences dialog.

LOAD PDB log file for /u/jc/tmp/pdb1eri.ent
=====
loading layer 0
Missing Atom: P    for residue   T    1 of chain 'B'
Missing Atom: O1P   for residue   T    1 of chain 'B'
Missing Atom: O2P   for residue   T    1 of chain 'B'
Missing Atom: O2*   for residue   C    2 of chain 'B'
Missing Atom: O2*   for residue   G    3 of chain 'B'
Missing Atom: O2*   for residue   C    4 of chain 'B'
Missing Atom: O2*   for residue   G    5 of chain 'B'
Missing Atom: O2*   for residue   A    6 of chain 'B'
Missing Atom: O2*   for residue   A    7 of chain 'B'
Missing Atom: O2*   for residue   C    10 of chain 'B'
Missing Atom: O2*  for residue   G    11 of chain 'B'
Missing Atom: O2*   for residue   C    12 of chain 'B'
Missing Atom: O2*   for residue   G    13 of chain 'B'
done loading layer 0:pdb1eri
```



# SwissPDB View

- Composed by various windows:
  - Menus
  - Image (allows molecule manipulation)
  - Control Panel (allows choosing various parts of the molecule)
- To rotate the molecule, press the mouse button and move within the image window.
- To select click on the panel
- To select everything press right button

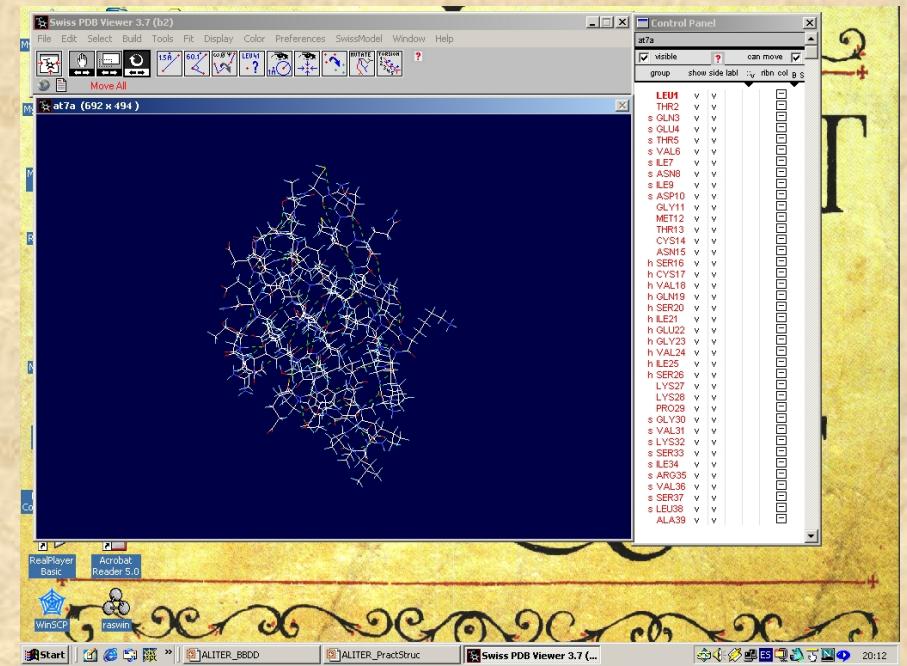


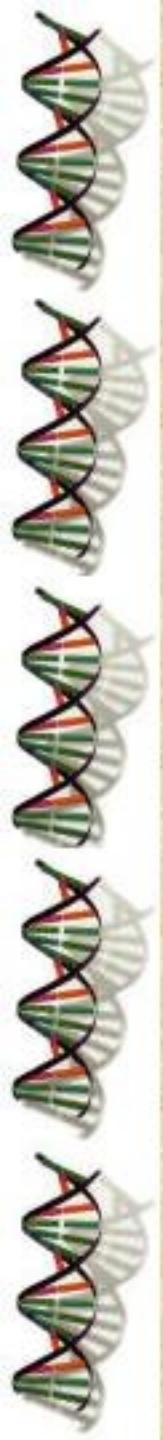
The Control Panel window displays a list of residues from the protein structure. Each row contains the residue name, its group (A or B), and several checkboxes indicating visibility and moveability settings.

		visible	?	can move	?
group	show side labl	?	?	ribn col	BS
A	SER17	✓	✓		
A	GLN18	✓	✓		
A	GLY19	✓	✓		
A	VAL20	✓	✓		
A h	ILE21	✓	✓		
A h	GLY22	✓	✓		
A h	ILE23	✓	✓		
A h	PHE24	✓	✓		
A h	GLY25	✓	✓		
A h	ASP26	✓	✓		
A h	TYR27	✓	✓		
A h	ALA28	✓	✓		
A h	LYS29	✓	✓		
A	ALA30	✓	✓		
A	HIS31	✓	✓		
A	ASP32	✓	✓		
A	LEU33	✓	✓		
A	ALA34	✓	✓		
A h	VAL35	✓	✓		
A h	GLY36	✓	✓		
A h	GLU37	✓	✓		
A h	VAL38	✓	✓		
A h	SER39	✓	✓		
A h	LYS40	✓	✓		
A h	LEU41	✓	✓		
A h	VAL42	✓	✓		
A h	LYS43	✓	✓		

# Add H and H-bonds

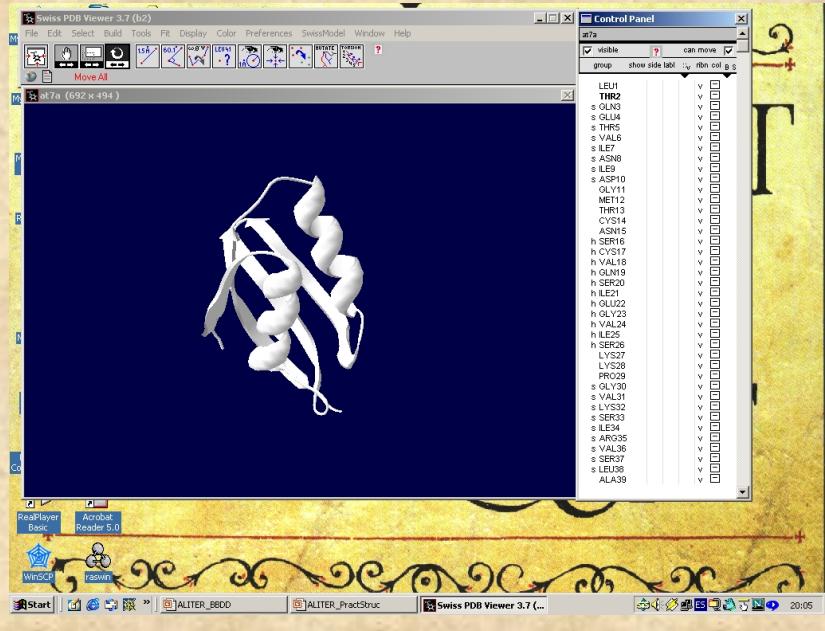
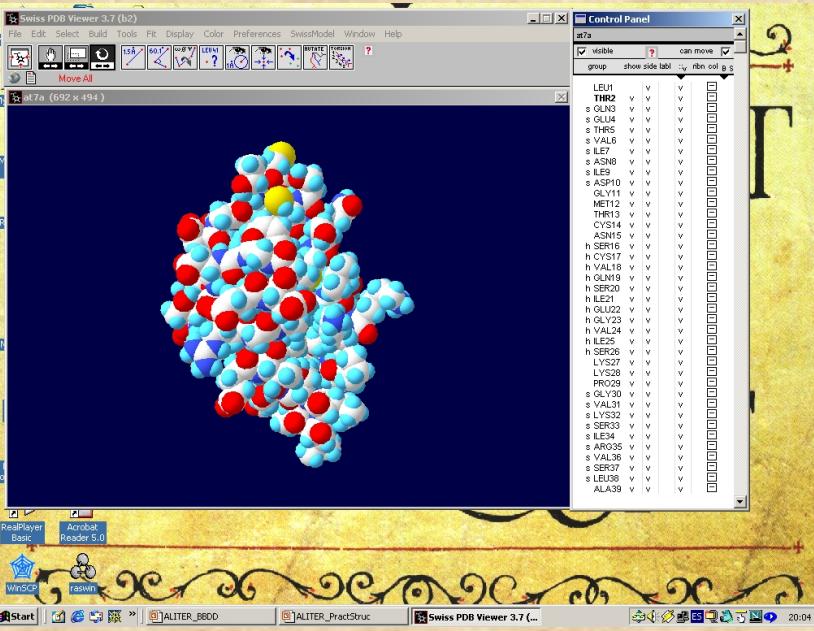
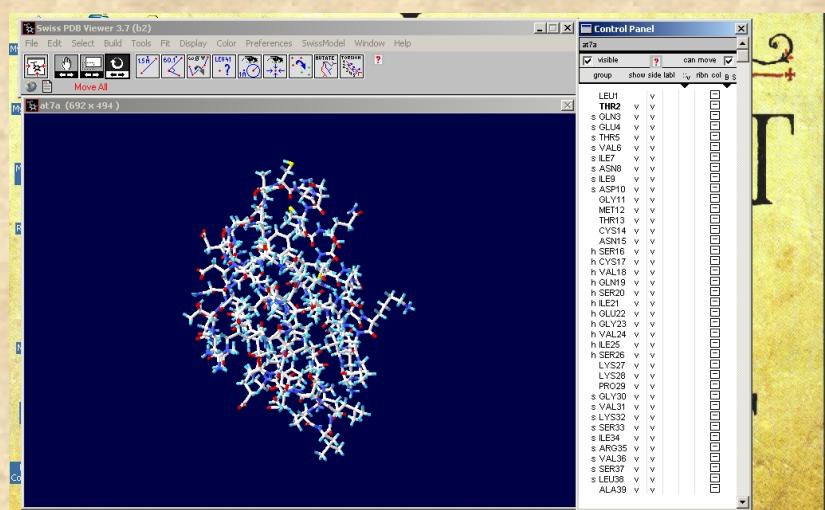
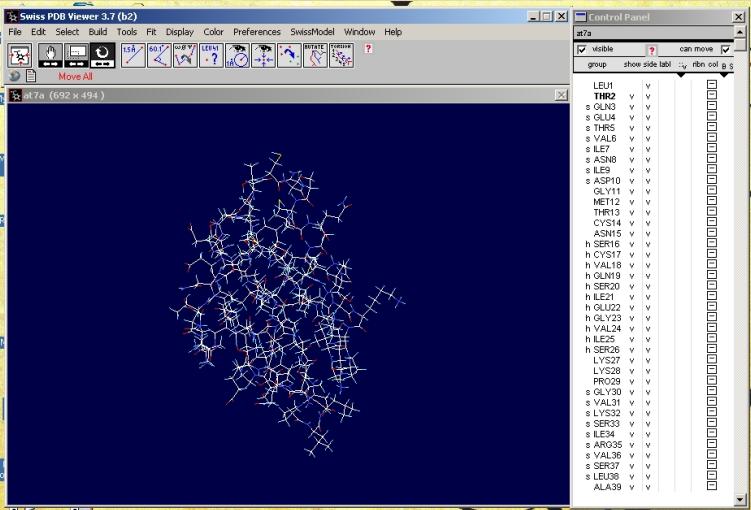
- Hydrogen and hydrogen bonds are often missing from the PDB file
- To add them automatically, choose
  - Build
    - Add hydrogens
  - Tools
    - Compute H-bonds
- To see them select
  - Display
    - Show H-Bonds





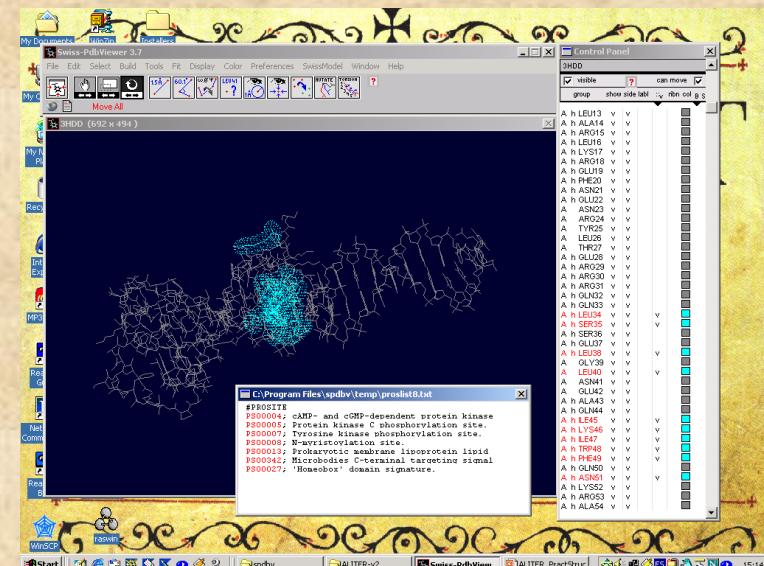
# Various visualization forms

- By default uses a wireframe model: only shows bonds
- Stick: in the “Display” menu select “Use OpenGL” and “Render in solid 3D”
- Balls: on the “Control Panel” activate “:.v” for all the groups using the right button.
- Ribbons: in the “Control panel” deactivate “:.v” and activate “ribn”
- Remove side chains: in “Control panel” deactivate “side” for all groups using the right button.



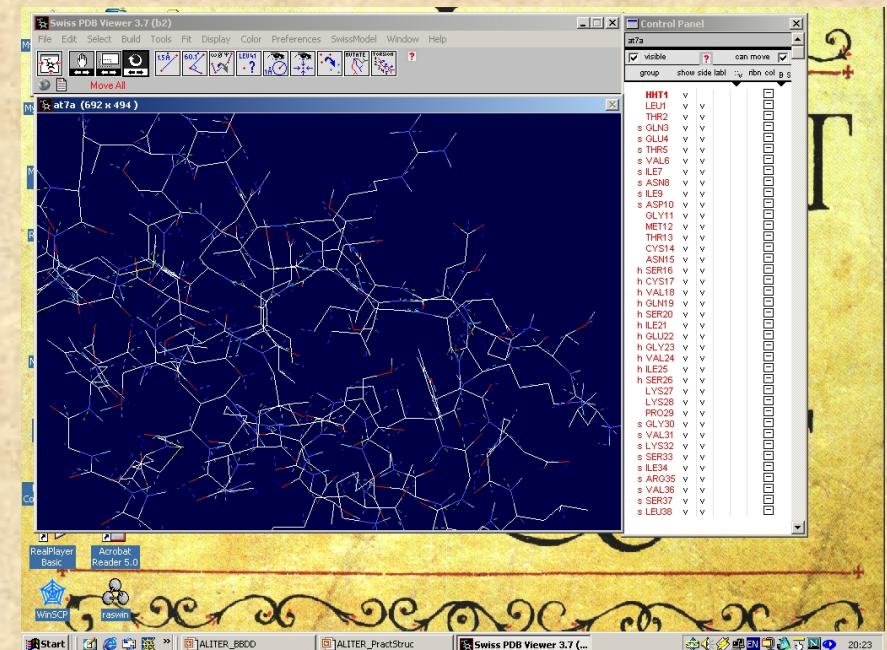
# PROSITE

- Download prosite.dat and prosite.doc from [www.expasy.ch/prosite](http://www.expasy.ch/prosite)
  - Place them in the **usrstuff** folder
- Locate properties
  - Edit
    - Search Prosite Pattern
  - Get a report of sites
    - Press on an element
    - Visualize in image window



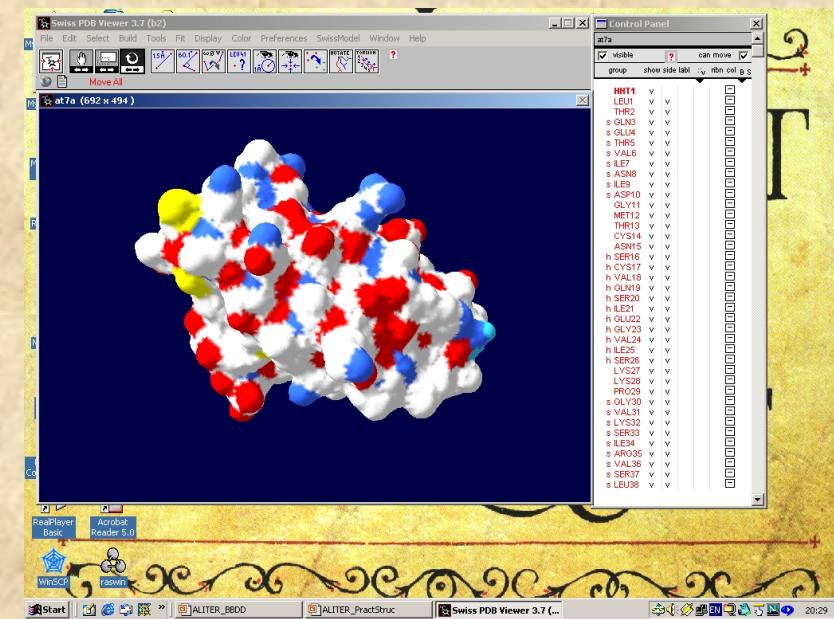
# Molecular stability

- Depends on molecular energy
- Energy is computed from atomic attraction and repulsions and the tensions over the structure
- Select
  - Tools
    - Compute energy  
(force field)
- Close report and select
  - Display
    - Show forces



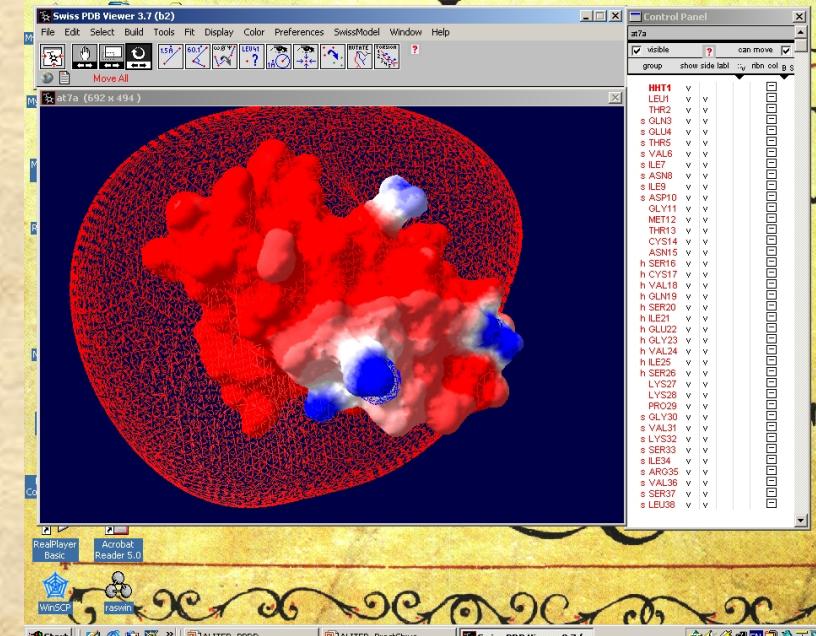
# Molecular surface

- The balls model shows the Van der Waals radii of each atom
- Other molecules cannot access all the cavities due to their radii
- The surface really accessible can be computed with
  - Tools
    - Compute molecular surface
  - Display
    - Show dots surface



# Electrostatic potential

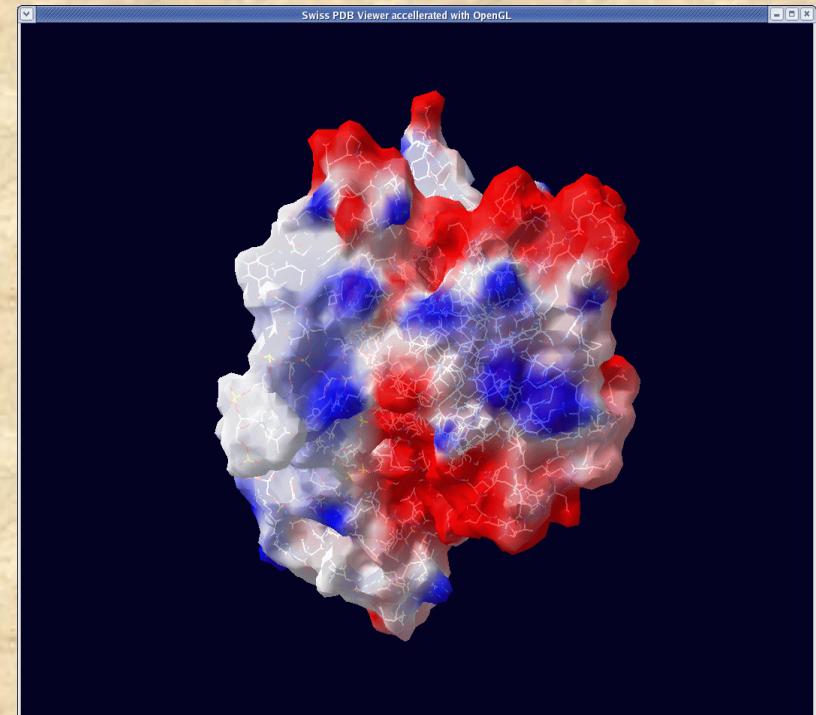
- Depends on the electric charge distribution in the molecule
- Defines the interactions with other molecules
- To compute it
  - Tools
    - Compute electrostatic potential

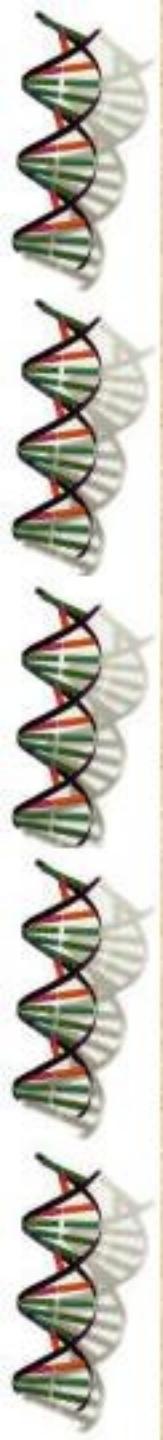


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# Mapping the electrostatic potential

- Go to preferences and select Surfaces...
  - Default surface color
    - Electrostatic potential
- Recompute the surface
  - Tools
    - Compute molecular surface



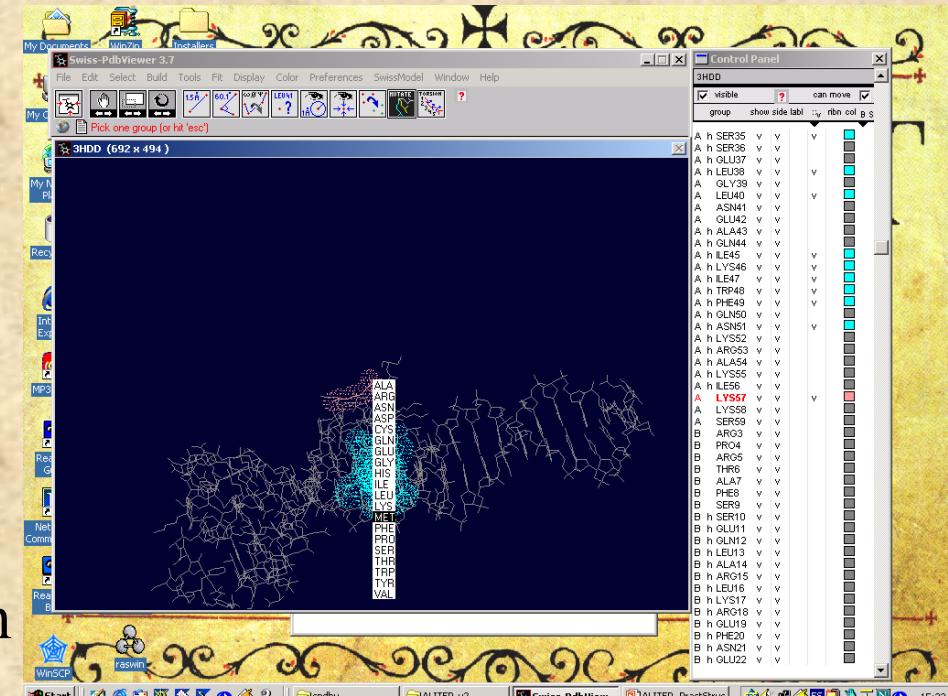


# Getting molecule details

- File
  - Open TEXT file....
    - Select the same PDB file
    - Study properties and details

# Simulating mutants

- DeepView provides basic facilities for mutant analysis
  - Press mutate icon
    - Select amino acid
      - Choose new residue
    - Try totamers <>
      - Check score
    - Minimize energy
      - Energy minimisation
    - Optimize side chains
      - Fix side chains





# Much more...

- DeepView is a window to full homology structure modelling
- And much, much more
  - See the manual and tutorials for details