# Computational Biochemistry

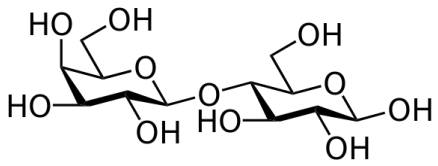
## Lecture 2
## Biomolecular structures & visualization

# Biomolecules

**Biomolecules** or biological molecules are molecules that are present in living organisms.

Small Molecules:

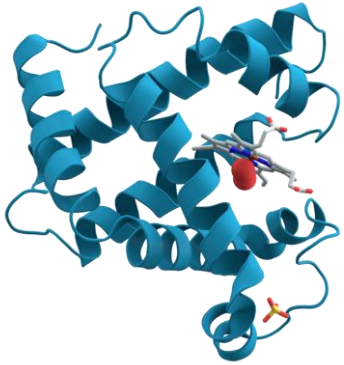
- Water molecules
- Organic/Drug molecules
- Amino acids
- Monosaccharide
- Nucleotides




Lactose

Large Molecules:

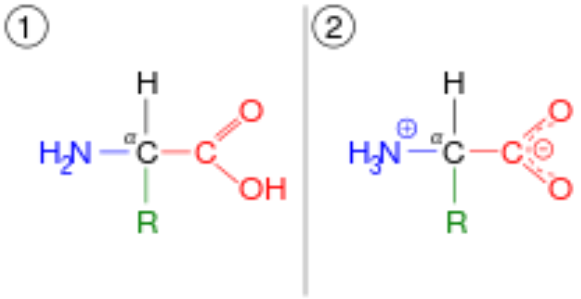
- Protein
- Nucleic acids
- Oligosaccharides
- Lipids
- Nature products



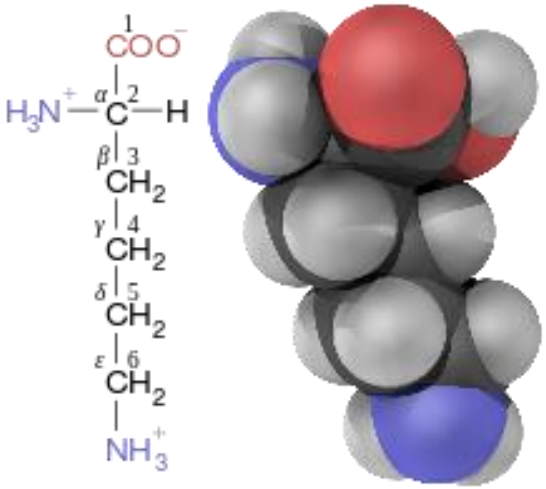
Myoglobin

Cotton

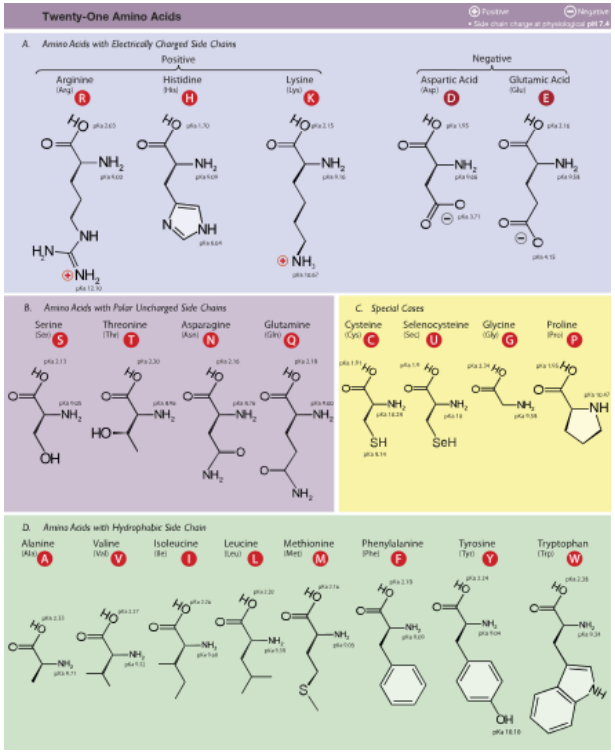
# Amino acids




Backbone

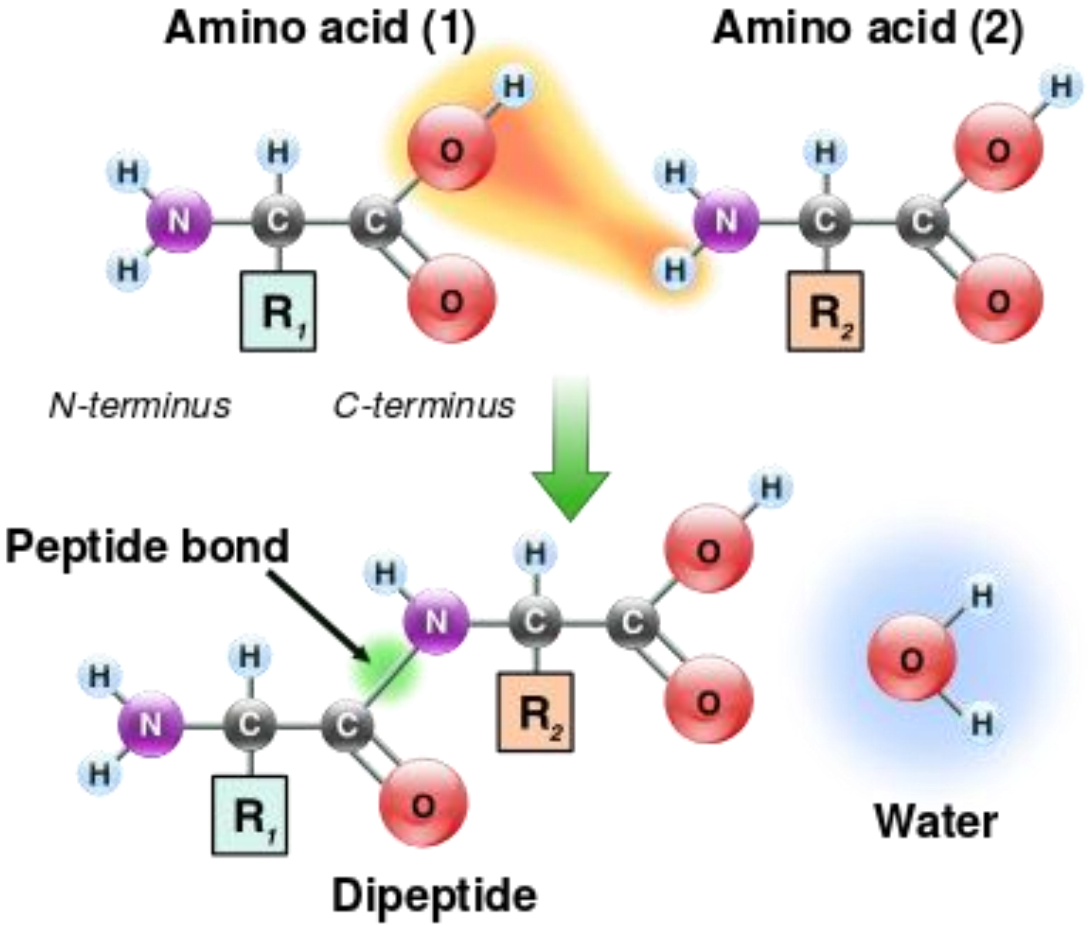



Side chain

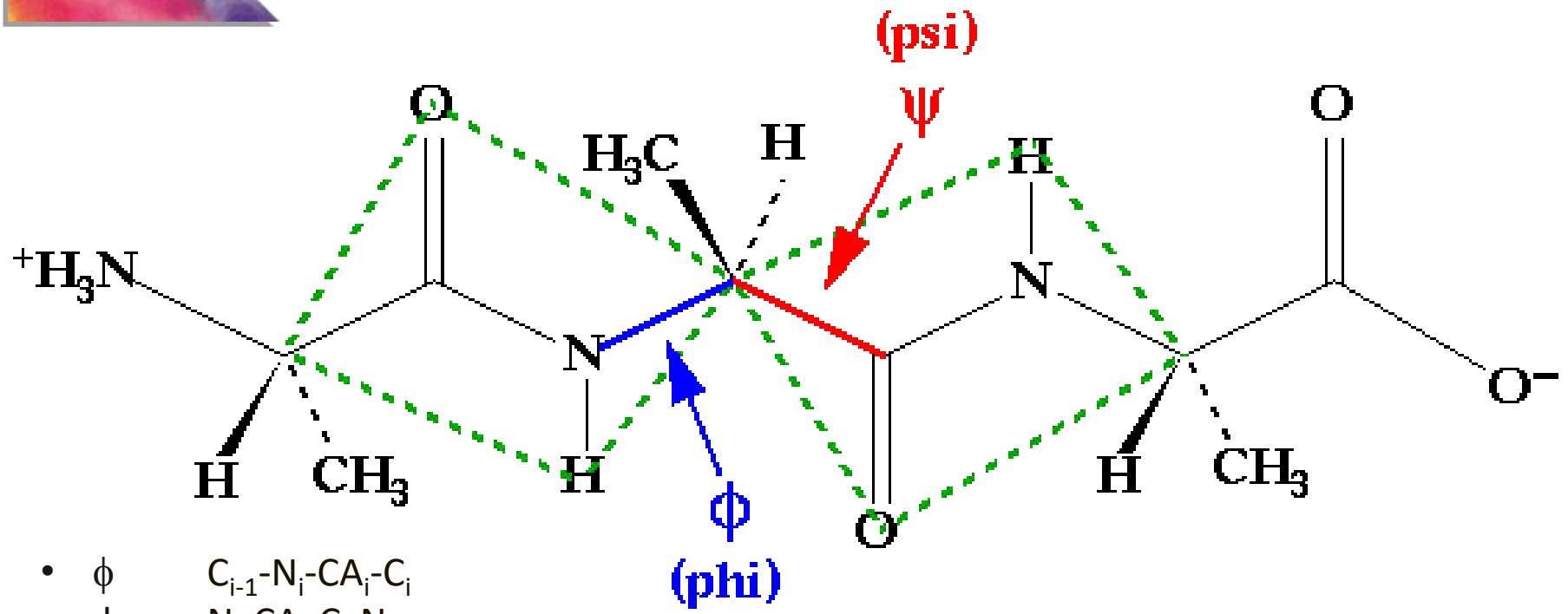


# Amino acids

- Dipeptide



# Amino acids




- ϕ $C_{i-1}$-$N_i$-$CA_i$-$C_i$
- ψ $N_i$-$CA_i$-$C_i$-$N_{i+1}$
- ω $CA_i$-$C_i$-$N_{i+1}$-$CA_{i+1}$

- Due to the peptide bond's partial double-bond character, the ω angle is restrained to values near 0° (*cis*-peptide) and **180°** (*trans*-peptide)

- *Cis*-peptides are relatively rare and usually (but not always) occur if the next residue is a proline.

- The ω angle has little to offer as a validation check, although values outside of the range of ±20 or ±160 degrees should be treated with caution.

# Protein Structure

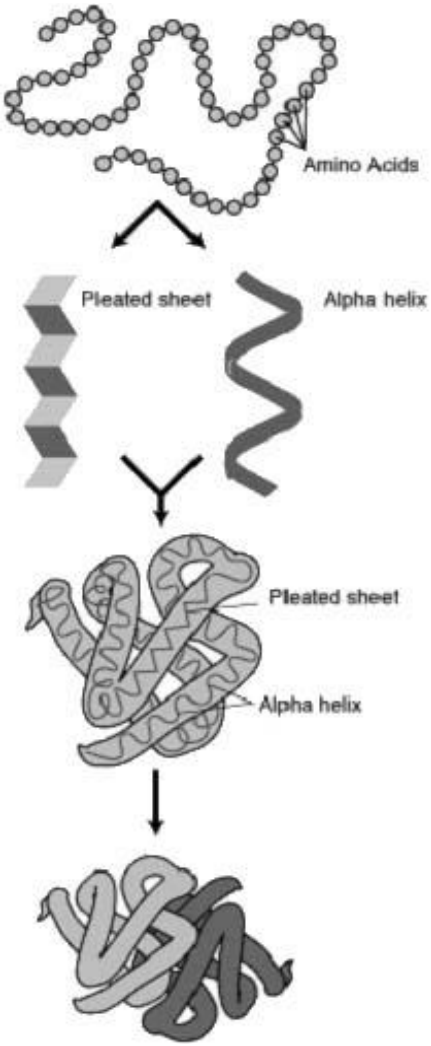
STRUCTURE

Primary

Secondary

Tertiary

Quaternary




Assembly

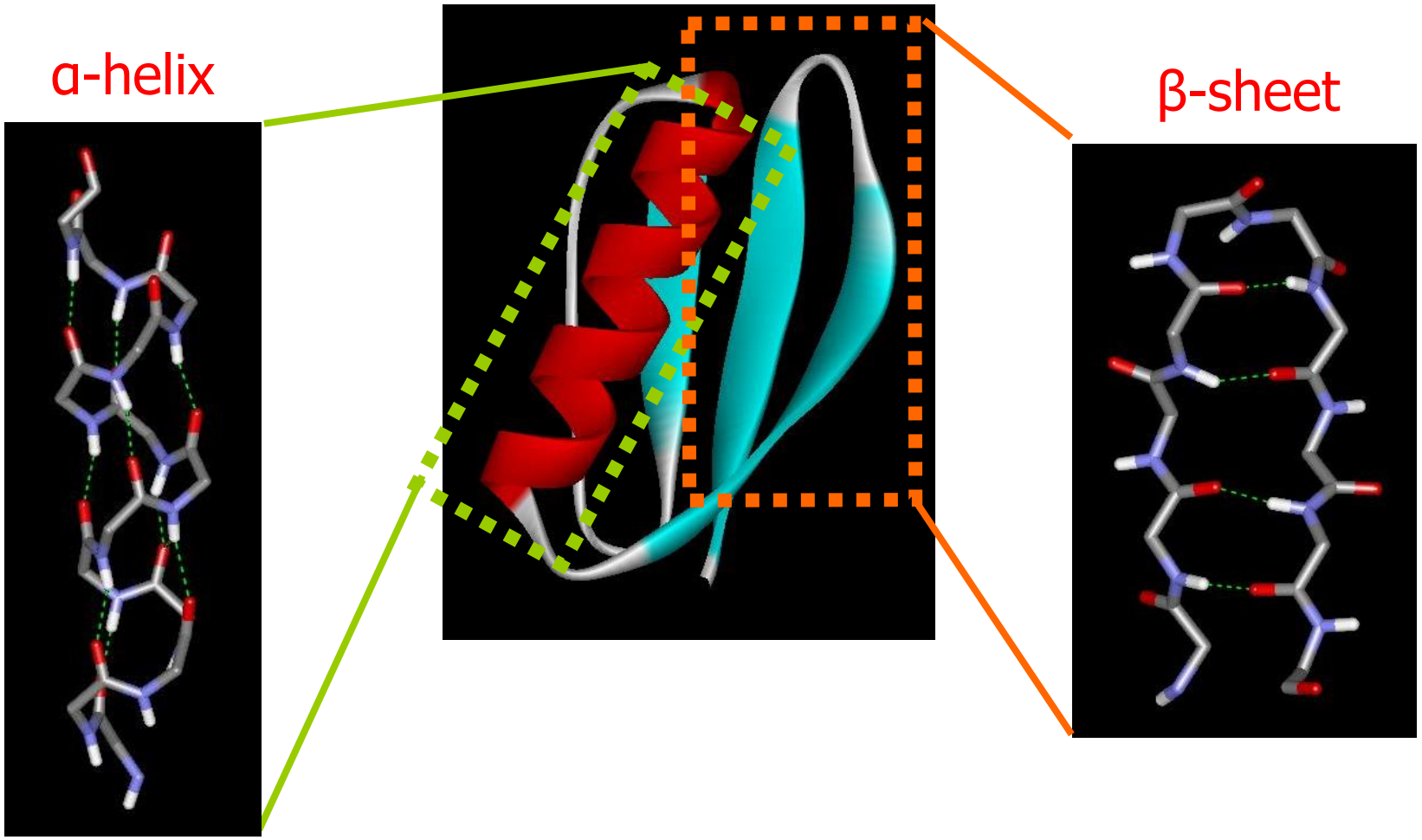
Folding

Packing

Interaction

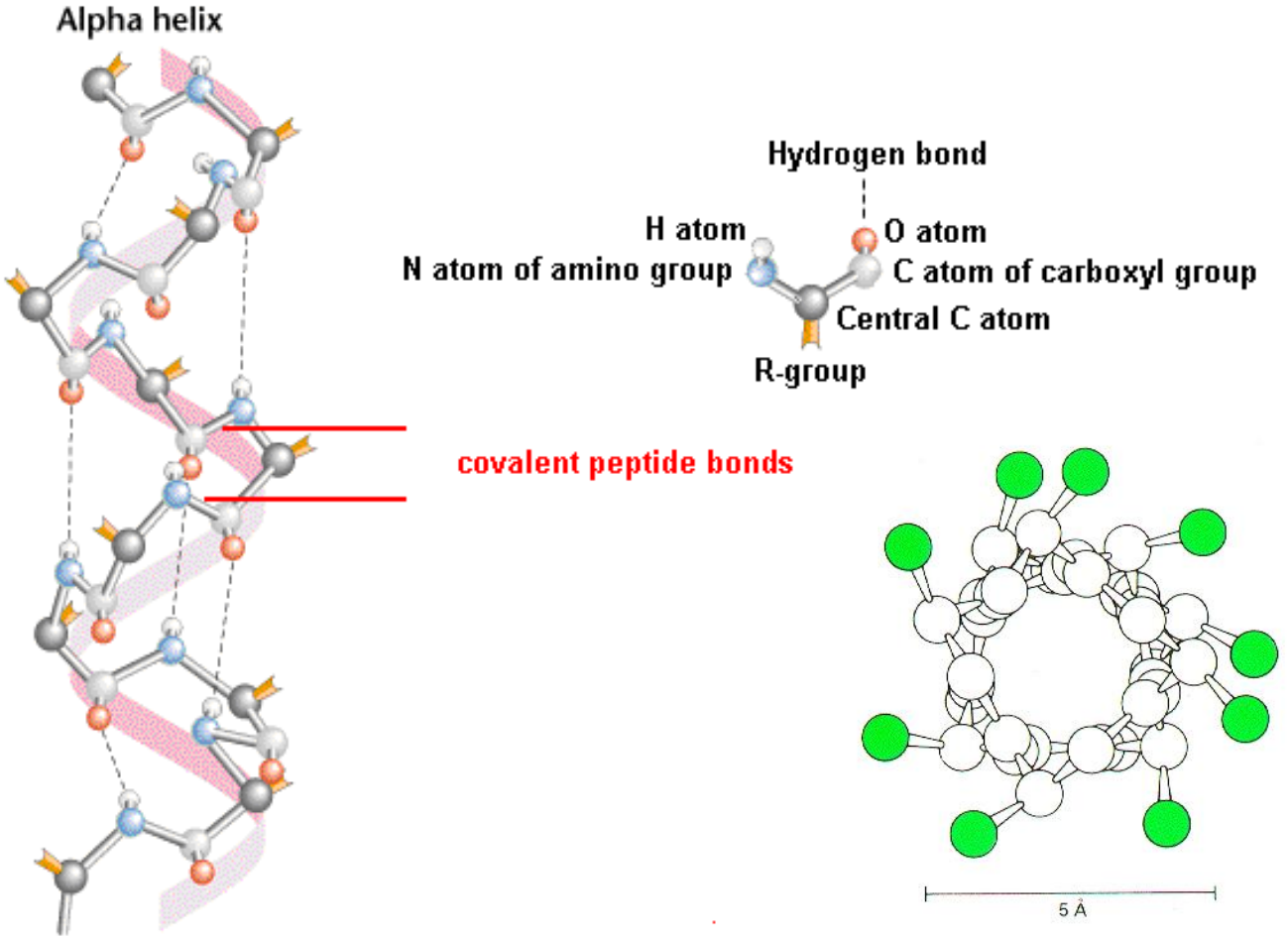
PROCESS

# Secondary Structure




- α-helix and β-sheet, have regular hydrogen-bonding patterns.

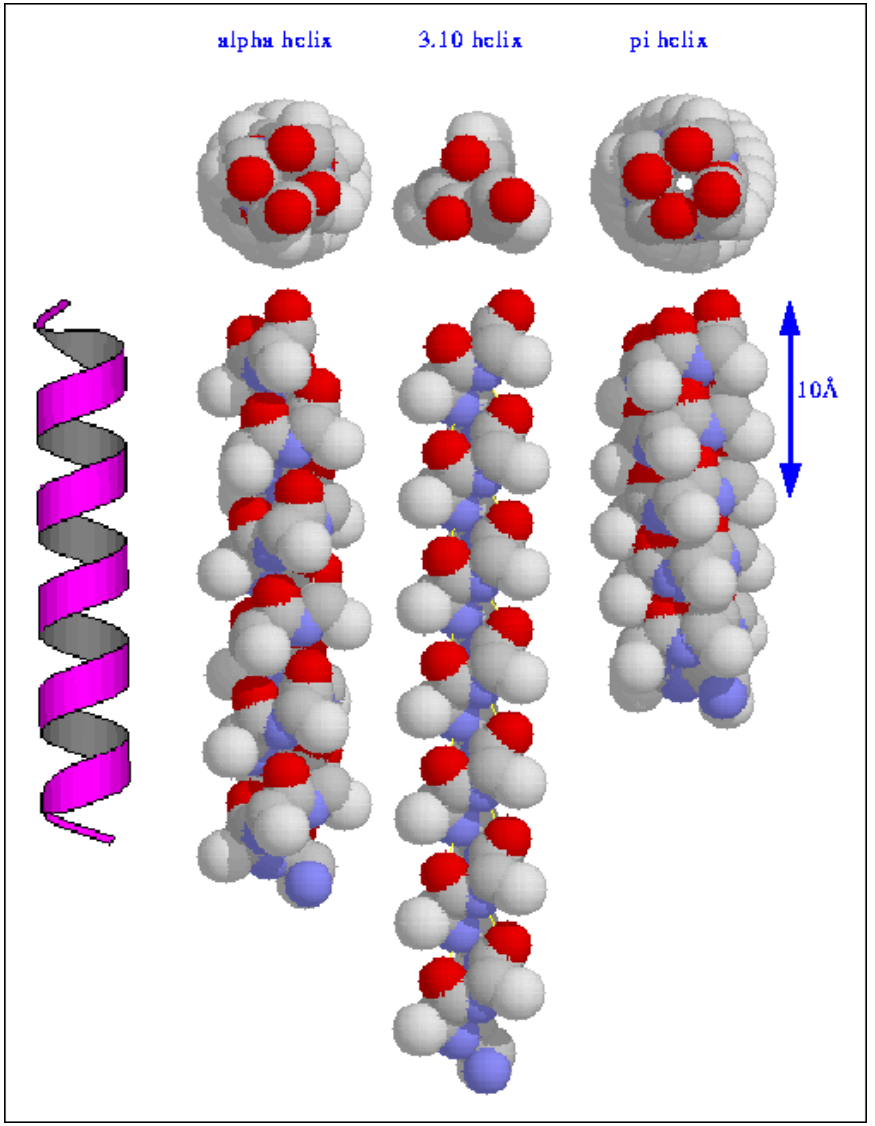
# α-helix




http://cmgm.stanford.edu/biochem/biochem201/Slides/

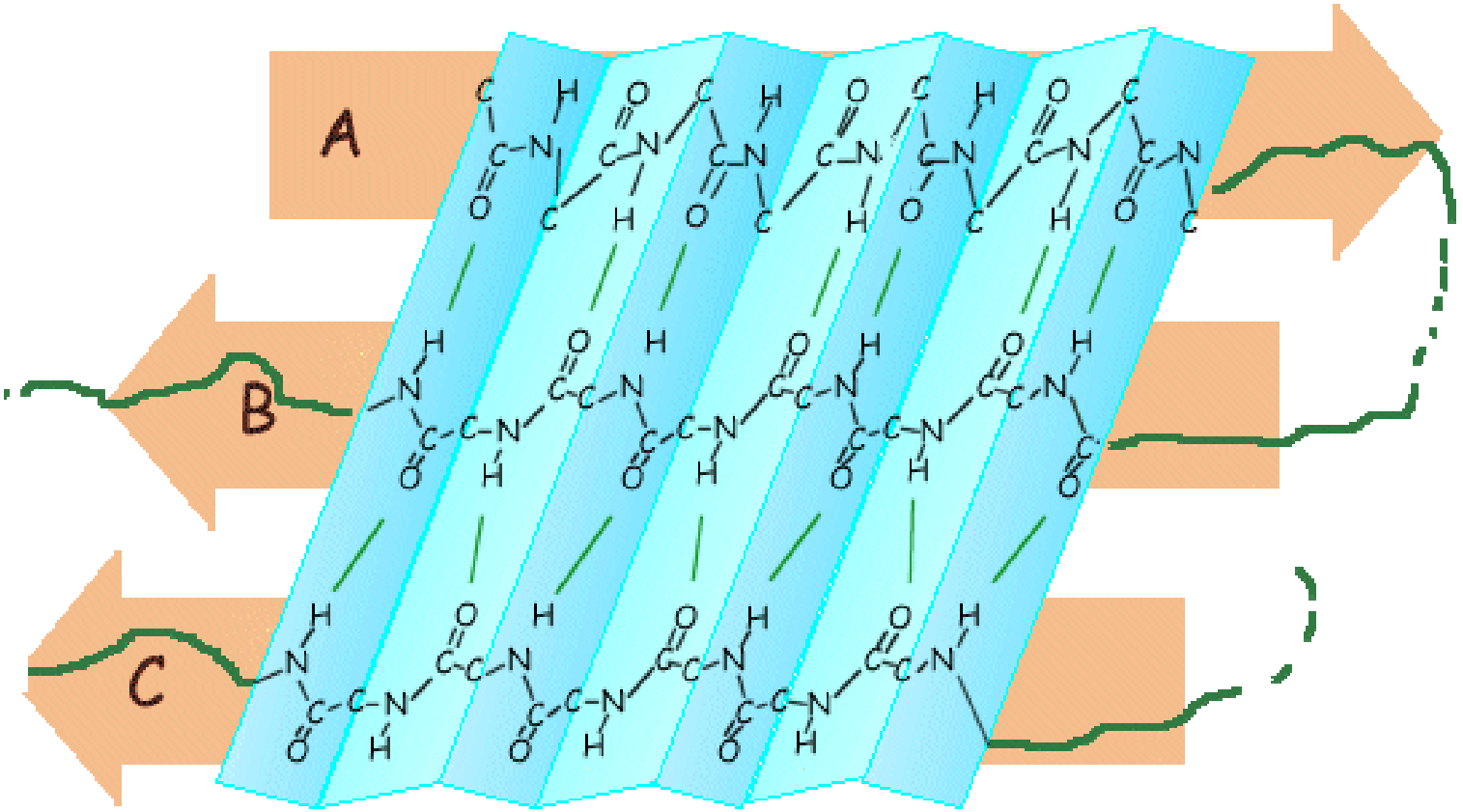
# α-helix

| | Φ | ψ | H Bond | R/t | A/t |
|---|---|---|---|---|---|
| Alpha | -57.8 | -47 | i, i + 4 | 3.6 | 13 |
| 3-10 Helix | -49 | -26 | i, i + 3 | 3.0 | 10 |
| Pi Helix | -57 | -80 | i , i + 5 | 4.4 | 16 |




http://broccoli.mfn.ki.se

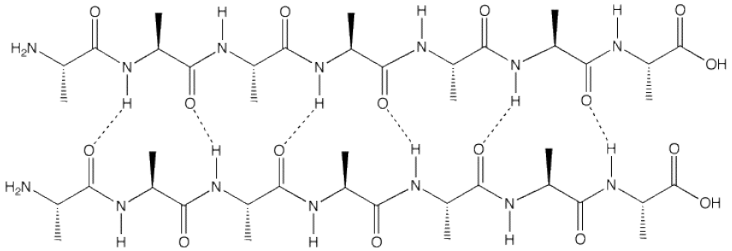
# β-sheet



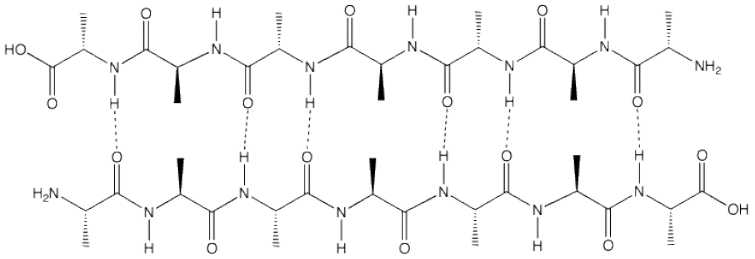

http://www.rothamsted.bbsrc.ac.uk/notebook/courses/guide/images/sheet.gif

# β-sheet

Parallel



Anti-parallel



Features:

- Sheets can be made up of any number of strands.
- Orientation and hydrogen bonding pattern of strands gives rise to flat or twisted sheets
- Parallel sheets buried inside, while Antiparallel sheets occurs on the surface

# Structure Assessment

**Good indicators of stereochemical quality**

- planarity
- chirality
- phi/psi angles
- chi angles
- non-bonded contact distances
- unsatisfied donors and acceptors

# Structure Assessment

## Bond Lengths

In protein structure, internal bond lengths should conform to known values.

Model bond lengths should lie within a few standard deviations of the mean bond length observed in the PDB.

Bond lengths and statistical outliers of the residue bonds N-CA, CA-CB, CA-C, C-O and C-N.

## Bond Angles

Angles are normally distributed about the mean angles observed in the PDB.

Internal bond angles and statistical outliers of the angles C-N-CA, N-CA-C, N-CA-CB, CB-CA-C, CA-C-N, CA-C-O, and O-C-N.

## Dihedral Angles

Internal dihedral angles phi, omega, psi, and chi1 angles.

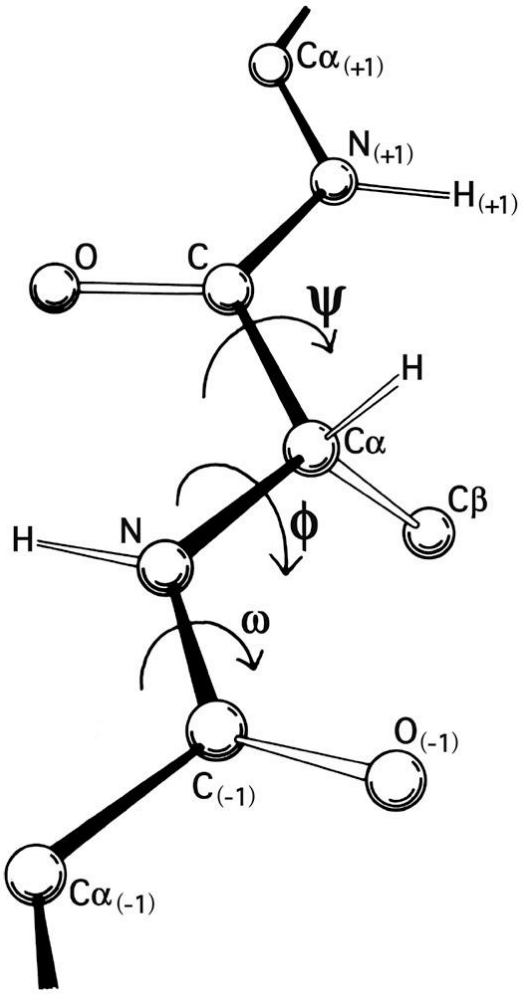
## Non-bonded Contacts

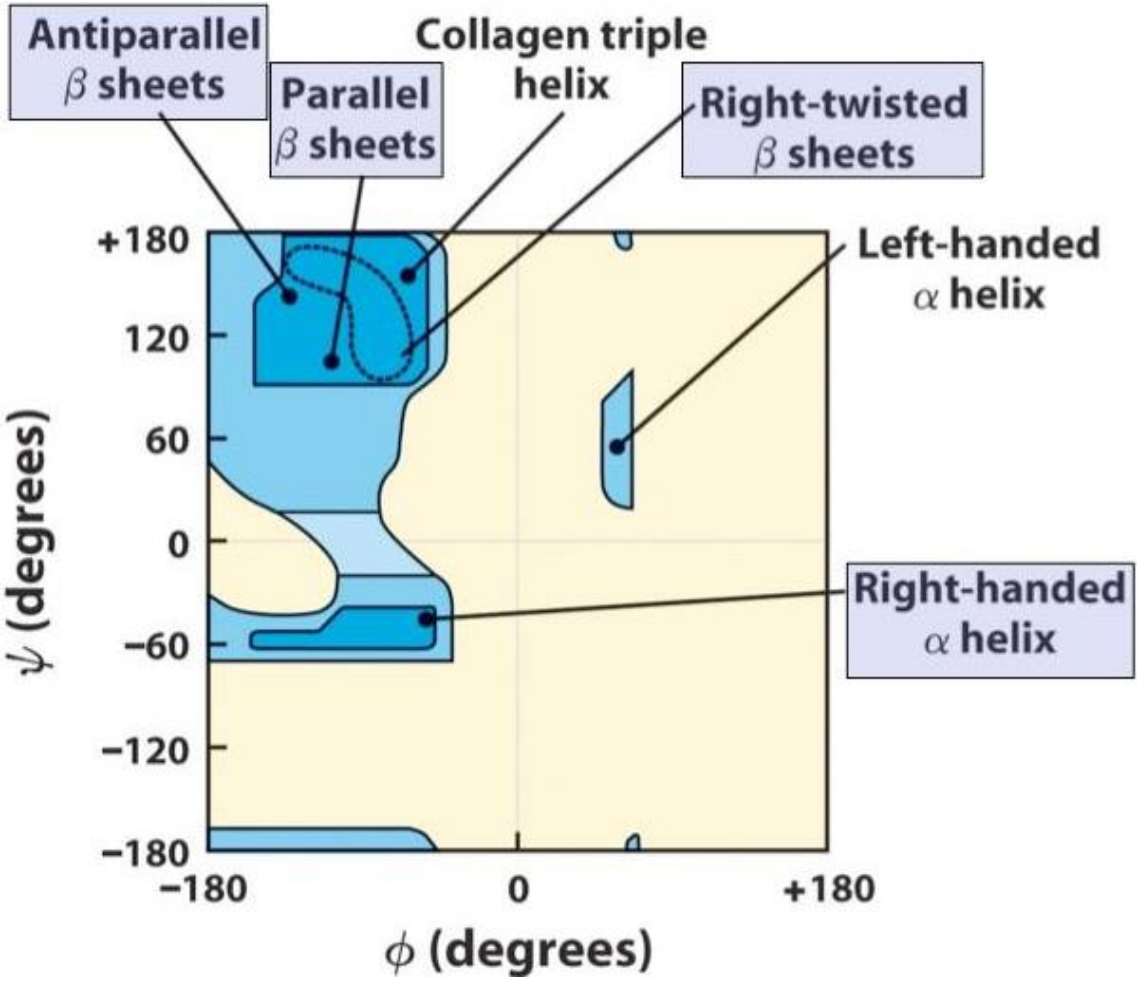
Non-bonded and non-hydrogen bonded contacts where the van der Waals radii overlap by more than a prescribed value

# Structure Assessment

- **Ramachandran plot**

A scatter plot of ϕ and ψ values for all residues in a protein.



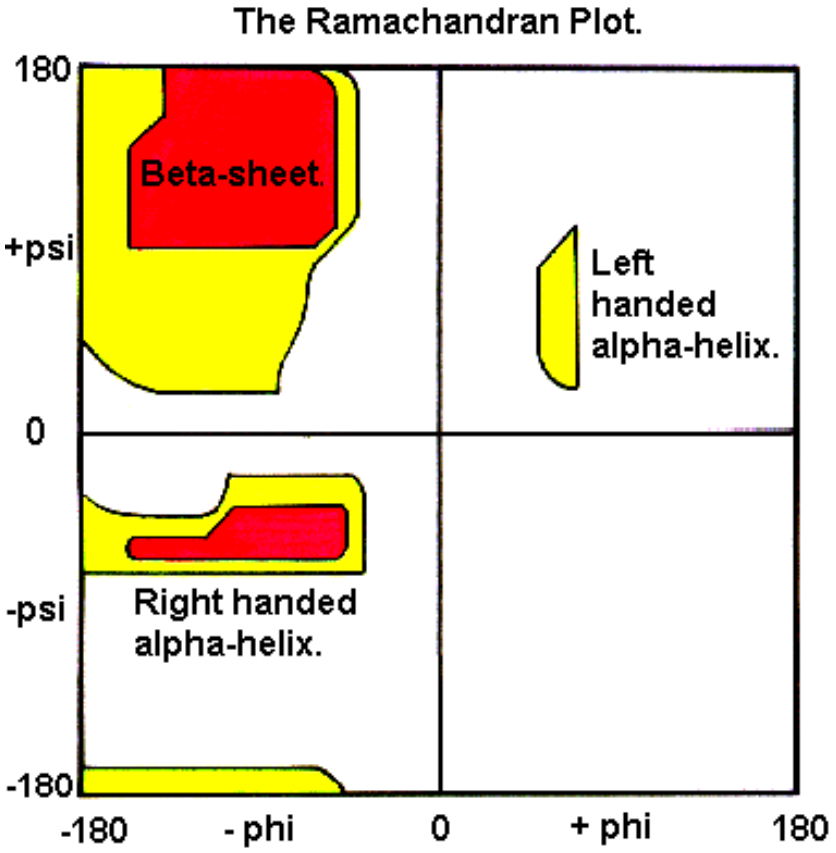



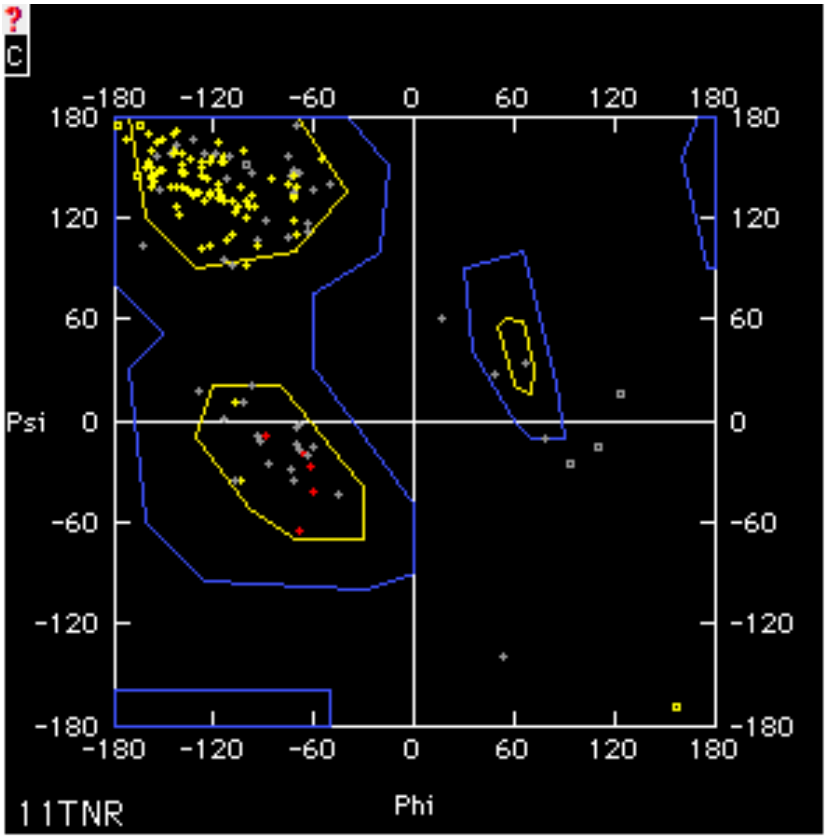
# Ramachandran Plots

- The $\phi$ and $\psi$ torsion angles are less restricted than $\omega$, but due to steric hindrance, there are several preferred combinations of $\phi$ and $\psi$ values.
- Values of $\phi$ are generally limited to the range between -60° and -150°.
- For $\psi$, the range is generally limited to regions centered about -60° and +120°.
- The $\phi$ and $\psi$ distributions for proline and glycine residues, are **atypical**.

  Glycine has no side chain and is very flexible, adopting $\phi$ and $\psi$ angles in all 4 quadrants of Ramachandran plot

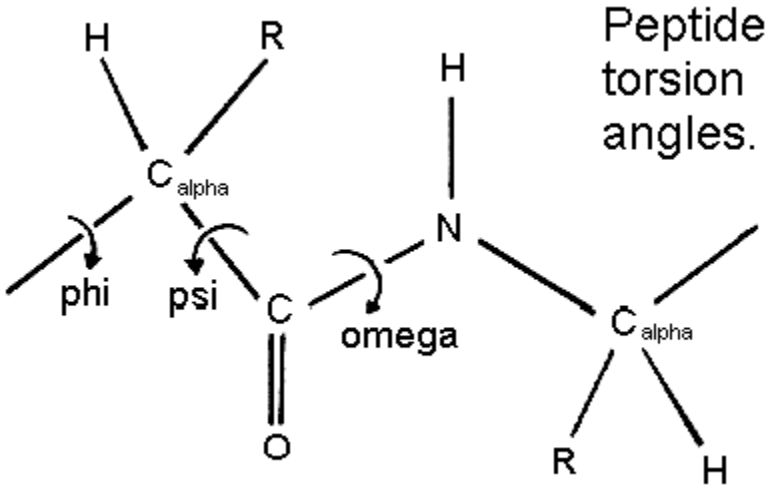
# Ramachandran Plots



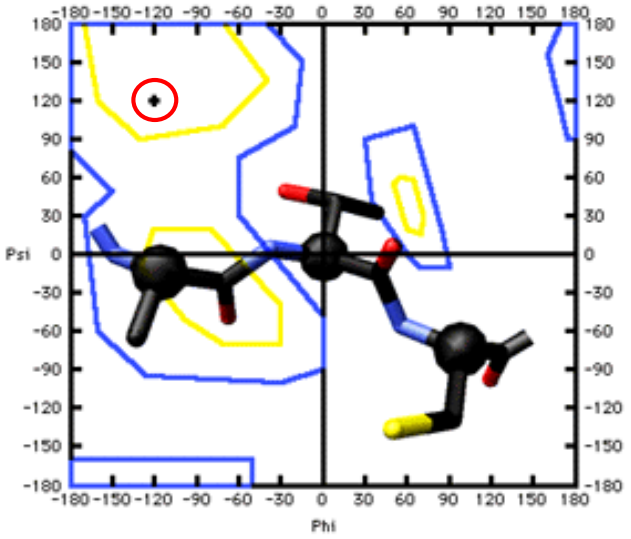



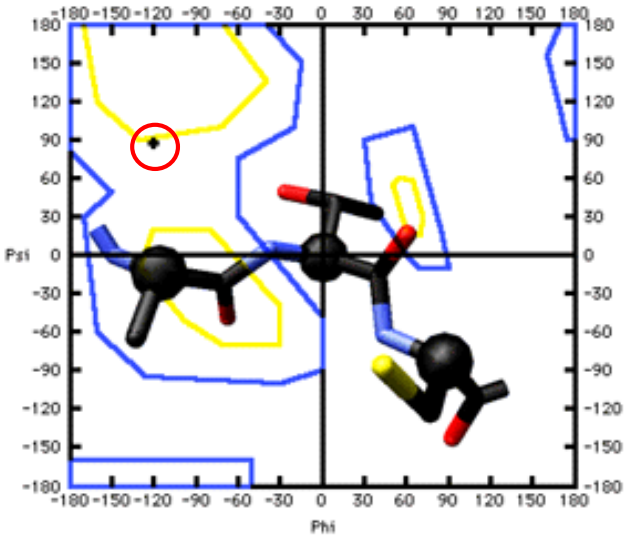

- Good structures have most of the residues clustered tightly in the most-favored regions with very few outliers
- Good, but low-resolution structures, may have less pronounced clustering, but still have few outliers
- Poor models have poor clustering and or many outliers

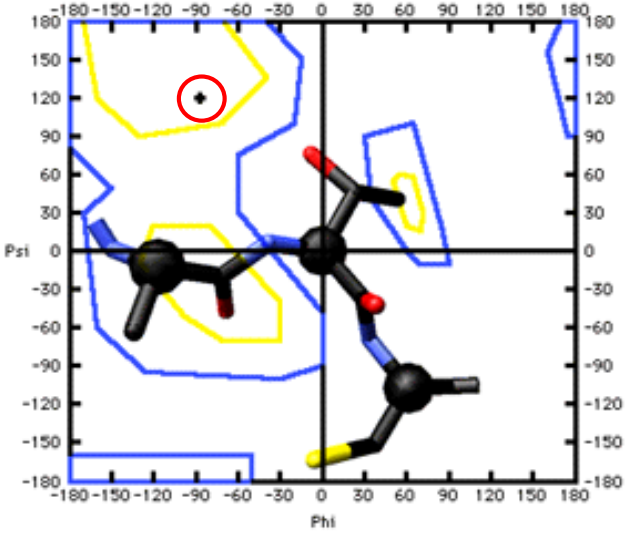
# Ramachandran Plots




- Minor Phi and Psi angle changes can alter the 3D shape



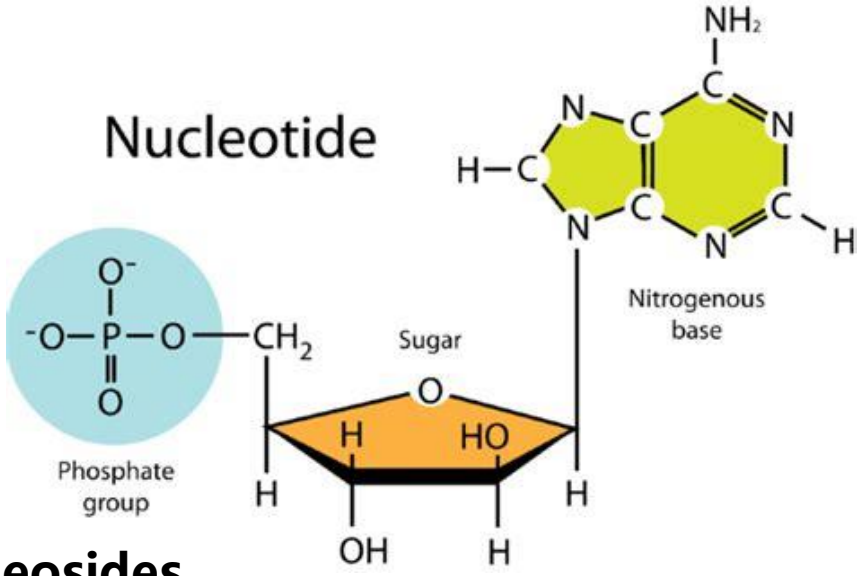



# Nucleotides

**Nucleotides**

- **Nitrogenous bases**
  - Purines
  - Pyrimidines
- **Sugar**
  - Ribose
  - Deoxyribose
- **Phosphates**

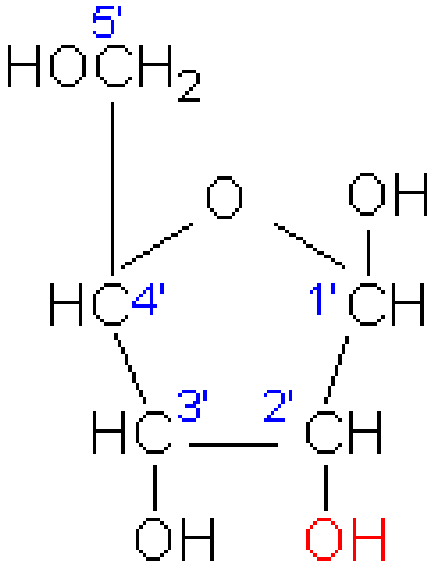
**Nucleosides**



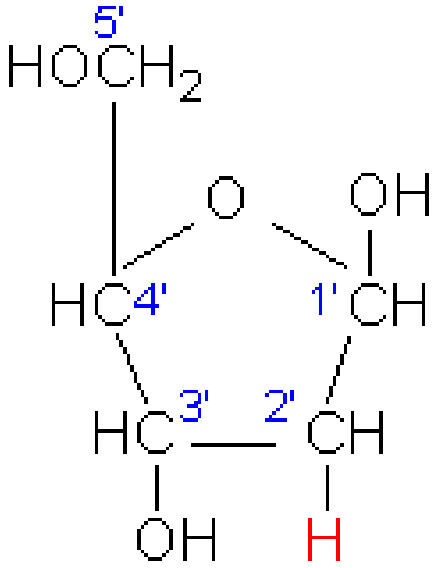

nucleoside + phosphate = nucleotide

**Nucleic acids** are polymers

# Nucleotides - sugars



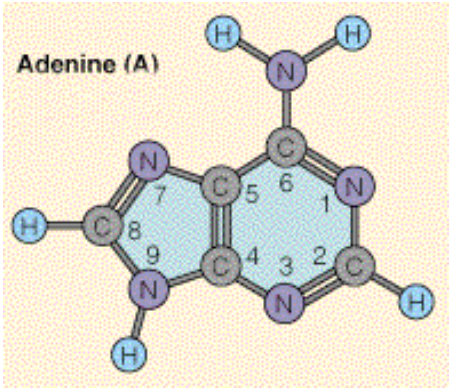

Ribose
(in RNA)

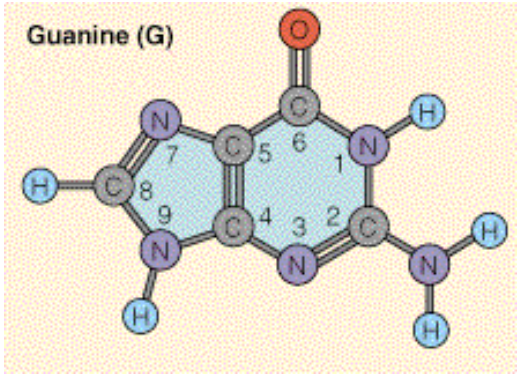



2'-Deoxyribose
(in DNA)

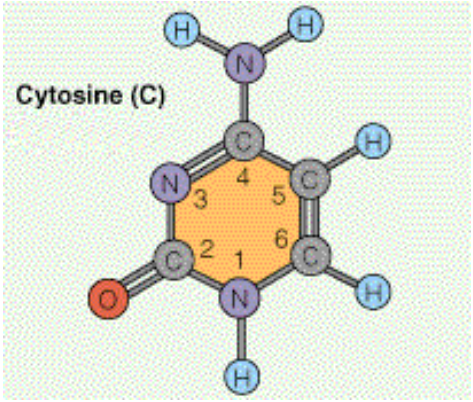
# Nucleotides - bases

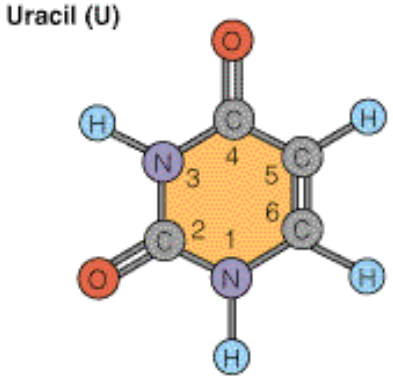
Purines:



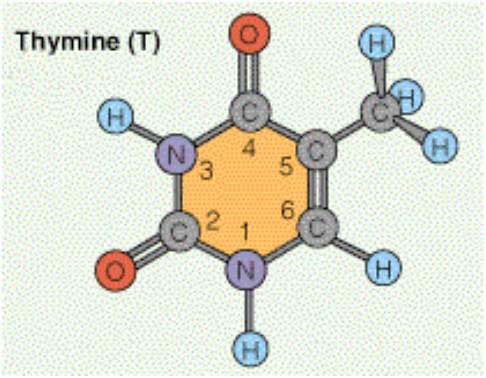




Pyrimidines:




RNA only



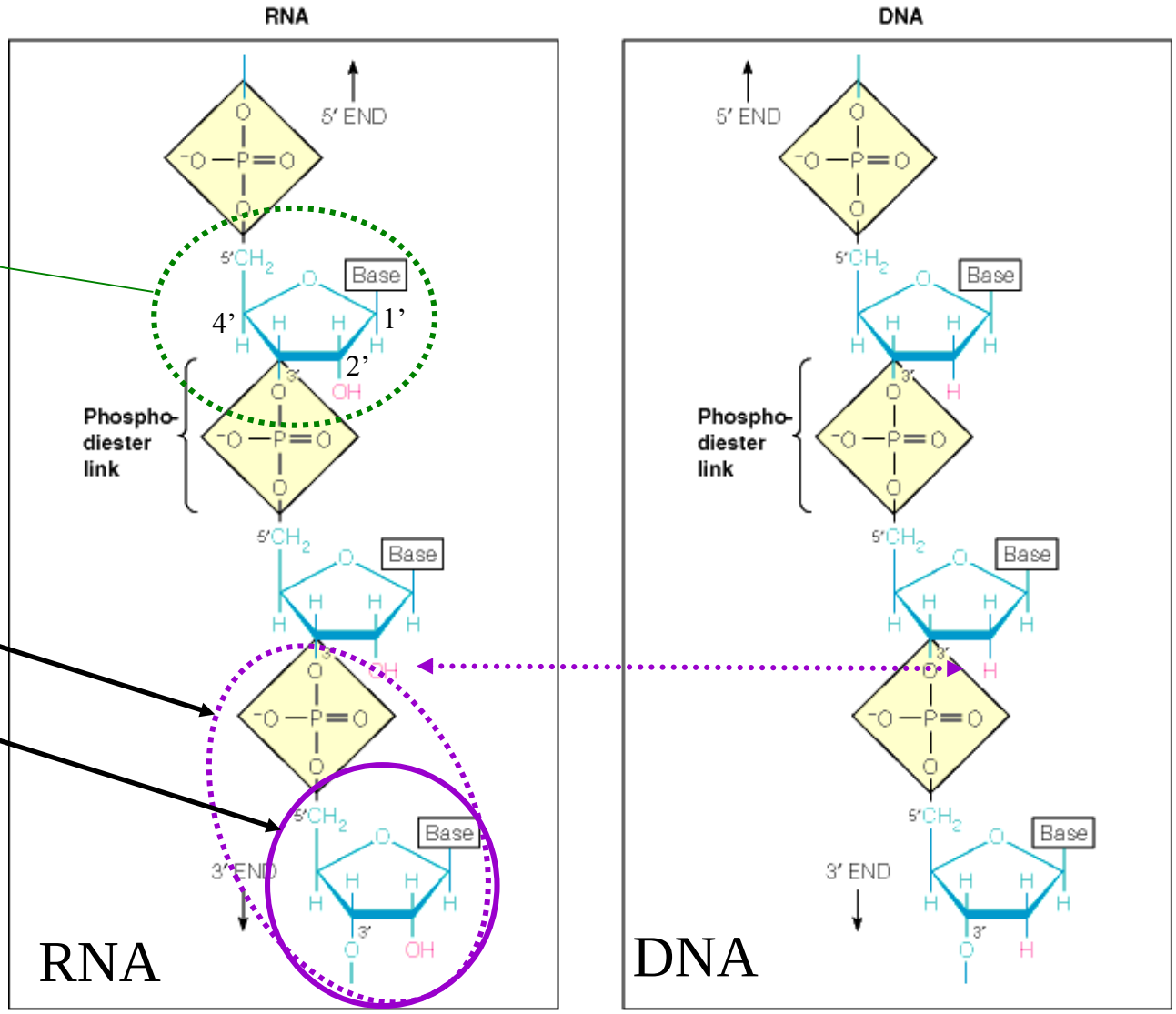

DNA only

# Chemical Structure of DNA and RNA

The C is named 1'-5'

Nucleotide

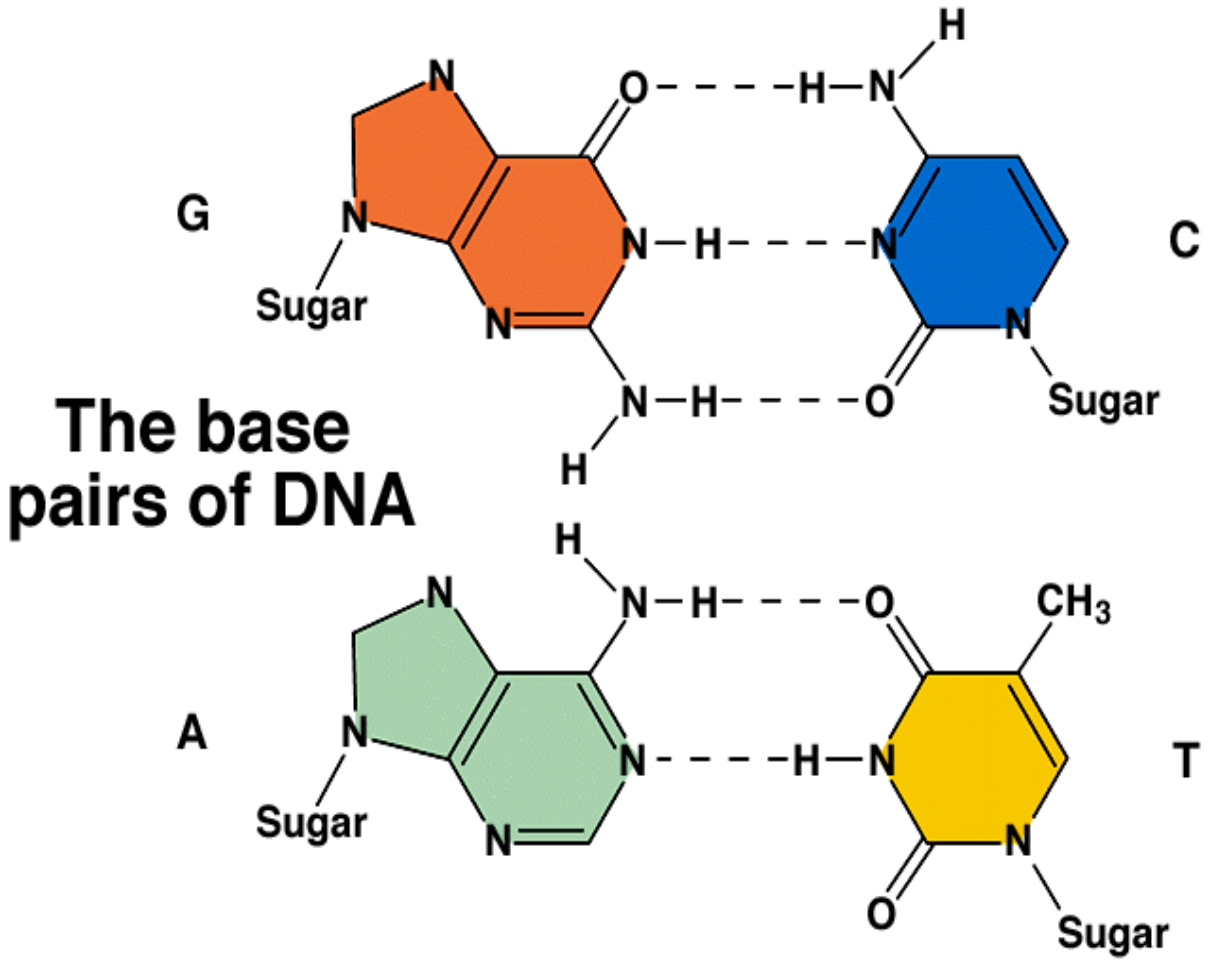
Nucleoside




Resume

# DNA Stabilization– Complementary Base Pairing

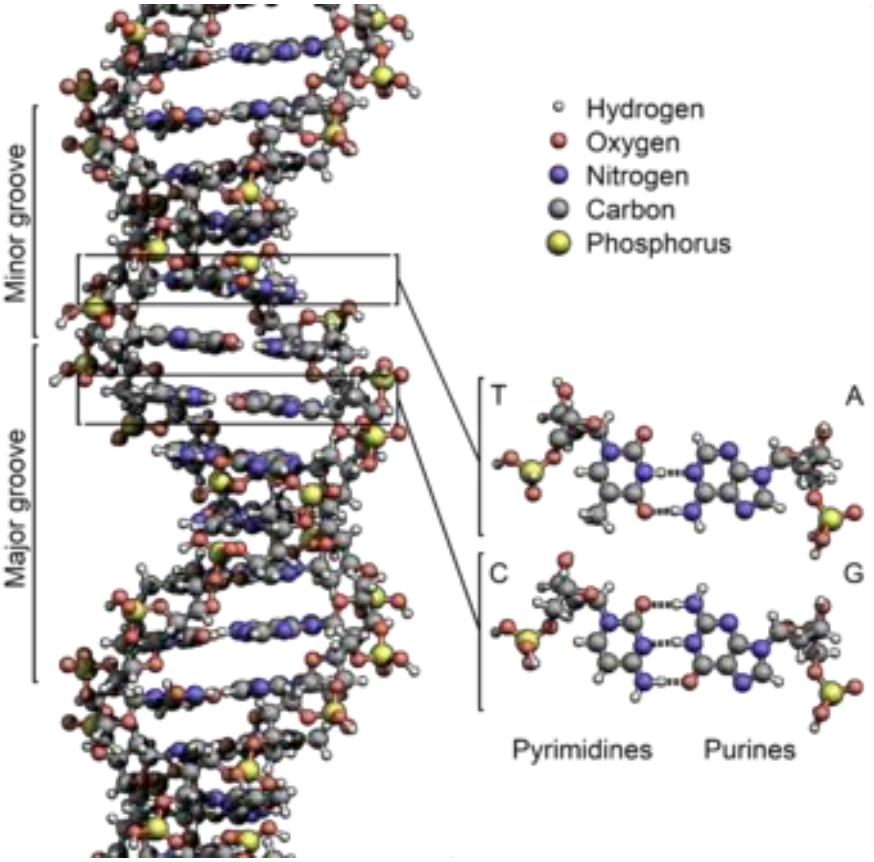


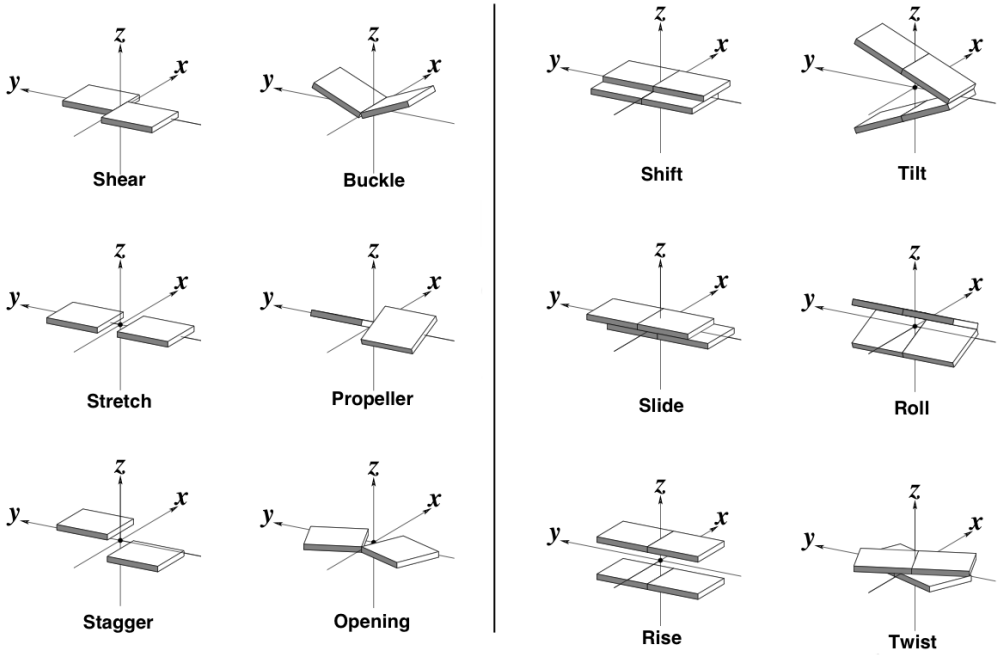



James Watson and Francis Crick(right), co-originators of the double-helix model, with Maclyn McCarty (left).

Watson-Crick base pair

# DNA double helix




http://x3dna.org/

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## A Structural View of Biology

This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

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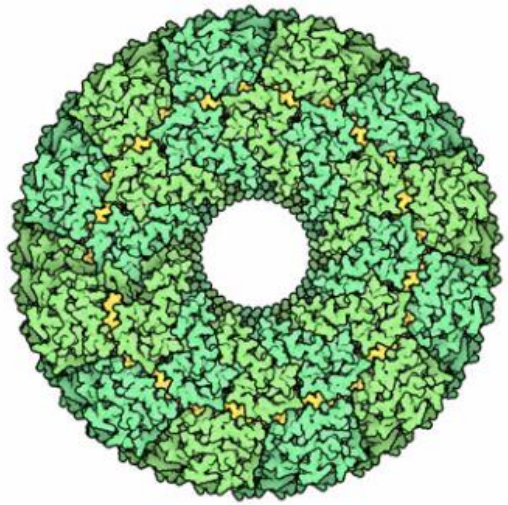
The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

### Superbugs! How Bacteria Evolve Resistance to Antibiotics


## March **Molecule of the Month**



Measles Virus Proteins

# Always read the PDB Header Information

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REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 6.0
REMARK   3   FREE R VALUE TEST SET SELECTION  : NULL
REMARK   3   R VALUE            (WORKING SET) : 0.170
REMARK   3   B VALUES.
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REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 18.25
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REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.0
REMARK 200  RESOLUTION RANGE LOW       (A) : 13.89
REMARK 200  COMPLETENESS FOR RANGE     (%) : 94.7
REMARK 200  DATA REDUNDANCY                : 4.3
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.05
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CISPEP   2 THR L   94    PRO L   95          0        -1.90
CRYST1   90.245   90.245   56.235  90.00  90.00  90.00 P 43 21 2     8
ATOM    818  N   GLN H 201      -7.404  44.620  37.768  1.00 29.62
ATOM    819  CA  GLN H 201      -8.563  43.726  37.825  1.00 25.50
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SSBOND   2 CYS H  222    CYS H  295
CISPEP   2 THR L   94    PRO L   95          0        -1.90
CRYST1   90.245   90.245   56.235  90.00  90.00  90.00 P 43 21 2     8
ATOM    818  N   GLN H 201      -7.404  44.620  37.768  1.00 29.62
ATOM    819  CA  GLN H 201      -8.563  43.726  37.825  1.00 25.50
...
```

# Always read the PDB Header Information

```
HEADER    IMMUNOGLOBULIN                          16-MAR-98   1A7R
TITLE     FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.01
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 6.0
REMARK   3   FREE R VALUE TEST SET SELECTION  : NULL
REMARK   3   R VALUE            (WORKING SET) : 0.170
REMARK   3   B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : 15.94
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 18.25
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 96880
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.0
REMARK 200  RESOLUTION RANGE LOW       (A) : 13.89
REMARK 200  COMPLETENESS FOR RANGE     (%) : 94.7
REMARK 200  DATA REDUNDANCY                : 4.3
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.05
REMARK 200  COMPLETENESS FOR SHELL     (%) : 43.3
SSBOND   2 CYS H  222    CYS H  295
CISPEP   2 THR L   94     PRO L   95          0         -1.90
CRYST1   90.245   90.245   56.235  90.00  90.00  90.00 P 43 21 2      8
ATOM    818  N   GLN H 201      -7.404  44.620  37.768  1.00 29.62
ATOM    819  CA  GLN H 201      -8.563  43.726  37.825  1.00 25.50
...
```

# Always read the PDB Header Information

```
HEADER    LECTIN                                          23-AUG-96   1JBC
TITLE     CONCANAVALIN A
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: CONCANAVALIN A;
COMPND   3 CHAIN: NULL;
COMPND   4 SYNONYM: CONA
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: CANAVALIA ENSIFORMIS;
SOURCE   3 ORGANISM_COMMON: JACK BEAN
KEYWDS    LECTIN, CALCIUM, MANGANESE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    S.PARKIN,B.RUPP,H.HOPE
REVDAT   3   10-MAY-00 1JBC    1       REMARK
REVDAT   2   11-OCT-99 1JBC    1       JRNL
REVDAT   1   12-FEB-97 1JBC    0
JRNL        AUTH   S.PARKIN,B.RUPP,H.HOPE
JRNL        TITL   ATOMIC RESOLUTION STRUCTURE OF CONCANAVALIN A AT
JRNL        TITL 2 120 K
JRNL        REF    ACTA CRYSTALLOGR., SECT.D     V.  52  1161 1996
JRNL        REFN   ASTM ABCRE6  DK ISSN 0907-4449
```

Locate and read the publication related to the crystal structure!

# Atomic Coordinates and B-factors

| | | Atom Name | Residue Name | Residue Number | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | ALA | 1 | 31.897 | 63.988 | 41.605 | 1.00 | 29.47 | N |
| ATOM | 2 | CA | ALA | 1 | 32.746 | 63.458 | 40.564 | 1.00 | 24.39 | C |
| ATOM | 3 | C | ALA | 1 | 33.907 | 62.748 | 41.281 | 1.00 | 19.86 | C |
| ATOM | 4 | O | ALA | 1 | 34.103 | 62.907 | 42.507 | 1.00 | 22.64 | O |
| ATOM | 5 | CB | ALA | 1 | 33.205 | 64.553 | 39.636 | 1.00 | 35.03 | C |
| ATOM | 6 | N | ASP | 2 | 34.538 | 61.829 | 40.586 | 1.00 | 15.91 | N |
| ATOM | 7 | CA | ASP | 2 | 35.750 | 61.159 | 41.003 | 1.00 | 12.36 | C |
| ATOM | 8 | C | ASP | 2 | 36.869 | 62.191 | 41.301 | 1.00 | 11.49 | C |
| ATOM | 9 | O | ASP | 2 | 36.769 | 63.352 | 40.847 | 1.00 | 13.73 | O |
| ATOM | 10 | CB | ASP | 2 | 36.222 | 60.263 | 39.835 | 1.00 | 12.99 | C |
| ATOM | 11 | CG | ASP | 2 | 35.357 | 59.029 | 39.633 | 1.00 | 10.89 | C |
| ATOM | 12 | OD1 | ASP | 2 | 34.554 | 58.662 | 40.569 | 1.00 | 13.84 | O |
| ATOM | 13 | OD2 | ASP | 2 | 35.474 | 58.421 | 38.564 | 1.00 | 12.98 | O |
| ATOM | 14 | N | THR | 3 | 37.956 | 61.748 | 41.961 | 1.00 | 10.35 | N |
| ATOM | 15 | CA | THR | 3 | 39.147 | 62.535 | 42.168 | 1.00 | 10.77 | C |
| ATOM | 16 | C | THR | 3 | 40.259 | 61.858 | 41.370 | 1.00 | 10.78 | C |
| ATOM | 17 | O | THR | 3 | 40.509 | 60.687 | 41.600 | 1.00 | 12.16 | O |
| ATOM | 18 | CB | THR | 3 | 39.555 | 62.604 | 43.644 | 1.00 | 11.80 | C |

# Atomic Coordinates and B-factors

Cartesian Coordinates

| | | | | | X | Y | Z | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | ALA | 1 | 31.897 | 63.988 | 41.605 | 1.00 | 29.47 | N |
| ATOM | 2 | CA | ALA | 1 | 32.746 | 63.458 | 40.564 | 1.00 | 24.39 | C |
| ATOM | 3 | C | ALA | 1 | 33.907 | 62.748 | 41.281 | 1.00 | 19.86 | C |
| ATOM | 4 | O | ALA | 1 | 34.103 | 62.907 | 42.507 | 1.00 | 22.64 | O |
| ATOM | 5 | CB | ALA | 1 | 33.205 | 64.553 | 39.636 | 1.00 | 35.03 | C |
| ATOM | 6 | N | ASP | 2 | 34.538 | 61.829 | 40.586 | 1.00 | 15.91 | N |
| ATOM | 7 | CA | ASP | 2 | 35.750 | 61.159 | 41.003 | 1.00 | 12.36 | C |
| ATOM | 8 | C | ASP | 2 | 36.869 | 62.191 | 41.301 | 1.00 | 11.49 | C |
| ATOM | 9 | O | ASP | 2 | 36.769 | 63.352 | 40.847 | 1.00 | 13.73 | O |
| ATOM | 10 | CB | ASP | 2 | 36.222 | 60.263 | 39.835 | 1.00 | 12.99 | C |
| ATOM | 11 | CG | ASP | 2 | 35.357 | 59.029 | 39.633 | 1.00 | 10.89 | C |
| ATOM | 12 | OD1 | ASP | 2 | 34.554 | 58.662 | 40.569 | 1.00 | 13.84 | O |
| ATOM | 13 | OD2 | ASP | 2 | 35.474 | 58.421 | 38.564 | 1.00 | 12.98 | O |
| ATOM | 14 | N | THR | 3 | 37.956 | 61.748 | 41.961 | 1.00 | 10.35 | N |
| ATOM | 15 | CA | THR | 3 | 39.147 | 62.535 | 42.168 | 1.00 | 10.77 | C |
| ATOM | 16 | C | THR | 3 | 40.259 | 61.858 | 41.370 | 1.00 | 10.78 | C |
| ATOM | 17 | O | THR | 3 | 40.509 | 60.687 | 41.600 | 1.00 | 12.16 | O |
| ATOM | 18 | CB | THR | 3 | 39.555 | 62.604 | 43.644 | 1.00 | 11.80 | C |

# Atomic Coordinates and B-factors

Atomic Occupancy

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | ALA | 1 | 31.897 | 63.988 | 41.605 | 1.00 | 29.47 | N |
| ATOM | 2 | CA | ALA | 1 | 32.746 | 63.458 | 40.564 | 1.00 | 24.39 | C |
| ATOM | 3 | C | ALA | 1 | 33.907 | 62.748 | 41.281 | 1.00 | 19.86 | C |
| ATOM | 4 | O | ALA | 1 | 34.103 | 62.907 | 42.507 | 1.00 | 22.64 | O |
| ATOM | 5 | CB | ALA | 1 | 33.205 | 64.553 | 39.636 | 1.00 | 35.03 | C |
| ATOM | 6 | N | ASP | 2 | 34.538 | 61.829 | 40.586 | 1.00 | 15.91 | N |
| ATOM | 7 | CA | ASP | 2 | 35.750 | 61.159 | 41.003 | 1.00 | 12.36 | C |
| ATOM | 8 | C | ASP | 2 | 36.869 | 62.191 | 41.301 | 1.00 | 11.49 | C |
| ATOM | 9 | O | ASP | 2 | 36.769 | 63.352 | 40.847 | 1.00 | 13.73 | O |
| ATOM | 10 | CB | ASP | 2 | 36.222 | 60.263 | 39.835 | 1.00 | 12.99 | C |
| ATOM | 11 | CG | ASP | 2 | 35.357 | 59.029 | 39.633 | 1.00 | 10.89 | C |
| ATOM | 12 | OD1 | ASP | 2 | 34.554 | 58.662 | 40.569 | 1.00 | 13.84 | O |
| ATOM | 13 | OD2 | ASP | 2 | 35.474 | 58.421 | 38.564 | 1.00 | 12.98 | O |
| ATOM | 14 | N | THR | 3 | 37.956 | 61.748 | 41.961 | 1.00 | 10.35 | N |
| ATOM | 15 | CA | THR | 3 | 39.147 | 62.535 | 42.168 | 1.00 | 10.77 | C |
| ATOM | 16 | C | THR | 3 | 40.259 | 61.858 | 41.370 | 1.00 | 10.78 | C |
| ATOM | 17 | O | THR | 3 | 40.509 | 60.687 | 41.600 | 1.00 | 12.16 | O |
| ATOM | 18 | CB | THR | 3 | 39.555 | 62.604 | 43.644 | 1.00 | 11.80 | C |

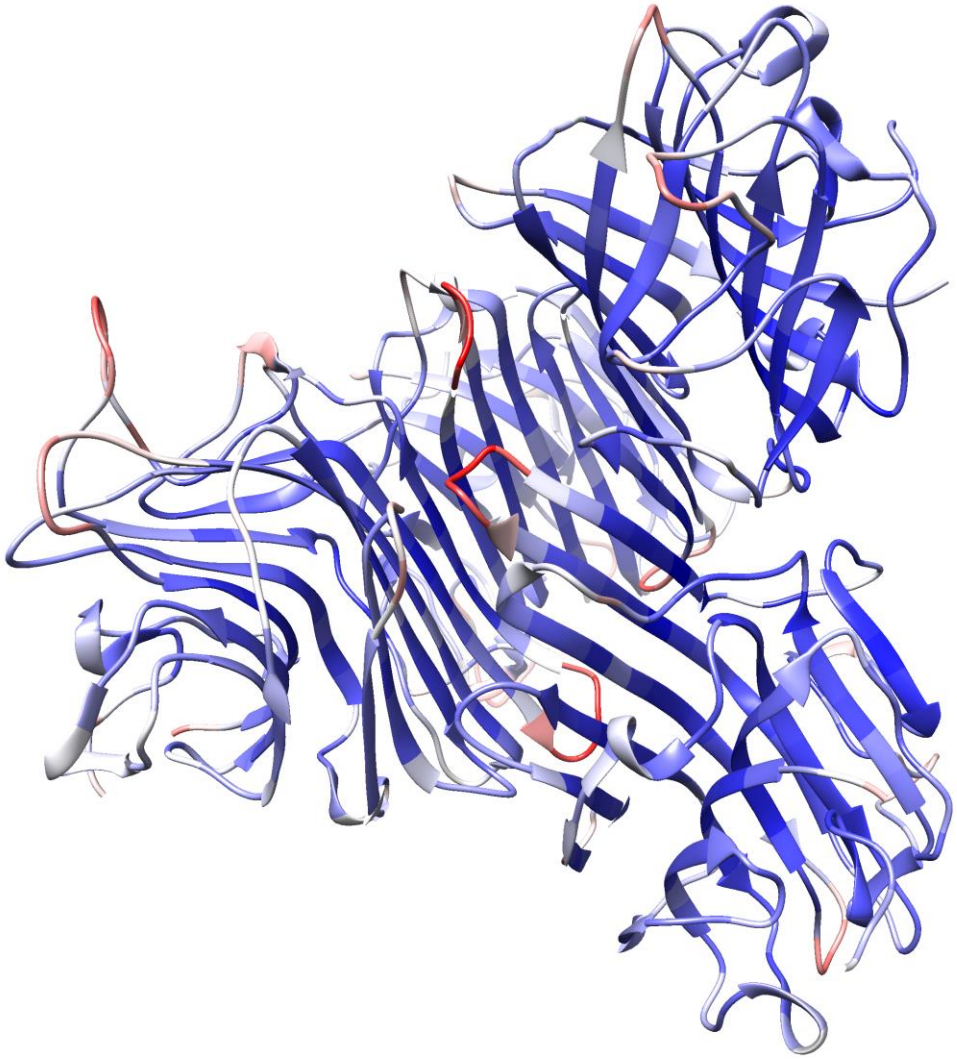
# Atomic Coordinates and B-factors

B Factor

```
ATOM      1  N   ALA     1      31.897  63.988  41.605  1.00 29.47           N
ATOM      2  CA  ALA     1      32.746  63.458  40.564  1.00 24.39           C
ATOM      3  C   ALA     1      33.907  62.748  41.281  1.00 19.86           C
ATOM      4  O   ALA     1      34.103  62.907  42.507  1.00 22.64           O
ATOM      5  CB  ALA     1      33.205  64.553  39.636  1.00 35.03           C
ATOM      6  N   ASP     2      34.538  61.829  40.586  1.00 15.91           N
ATOM      7  CA  ASP     2      35.750  61.159  41.003  1.00 12.36           C
ATOM      8  C   ASP     2      36.869  62.191  41.301  1.00 11.49           C
ATOM      9  O   ASP     2      36.769  63.352  40.847  1.00 13.73           O
ATOM     10  CB  ASP     2      36.222  60.263  39.835  1.00 12.99           C
ATOM     11  CG  ASP     2      35.357  59.029  39.633  1.00 10.89           C
ATOM     12  OD1 ASP     2      34.554  58.662  40.569  1.00 13.84           O
ATOM     13  OD2 ASP     2      35.474  58.421  38.564  1.00 12.98           O
ATOM     14  N   THR     3      37.956  61.748  41.961  1.00 10.35           N
ATOM     15  CA  THR     3      39.147  62.535  42.168  1.00 10.77           C
ATOM     16  C   THR     3      40.259  61.858  41.370  1.00 10.78           C
ATOM     17  O   THR     3      40.509  60.687  41.600  1.00 12.16           O
ATOM     18  CB  THR     3      39.555  62.604  43.644  1.00 11.80           C
```

- Large B-factors reflect uncertainty in the atomic position

# B-factor display for 1VAL



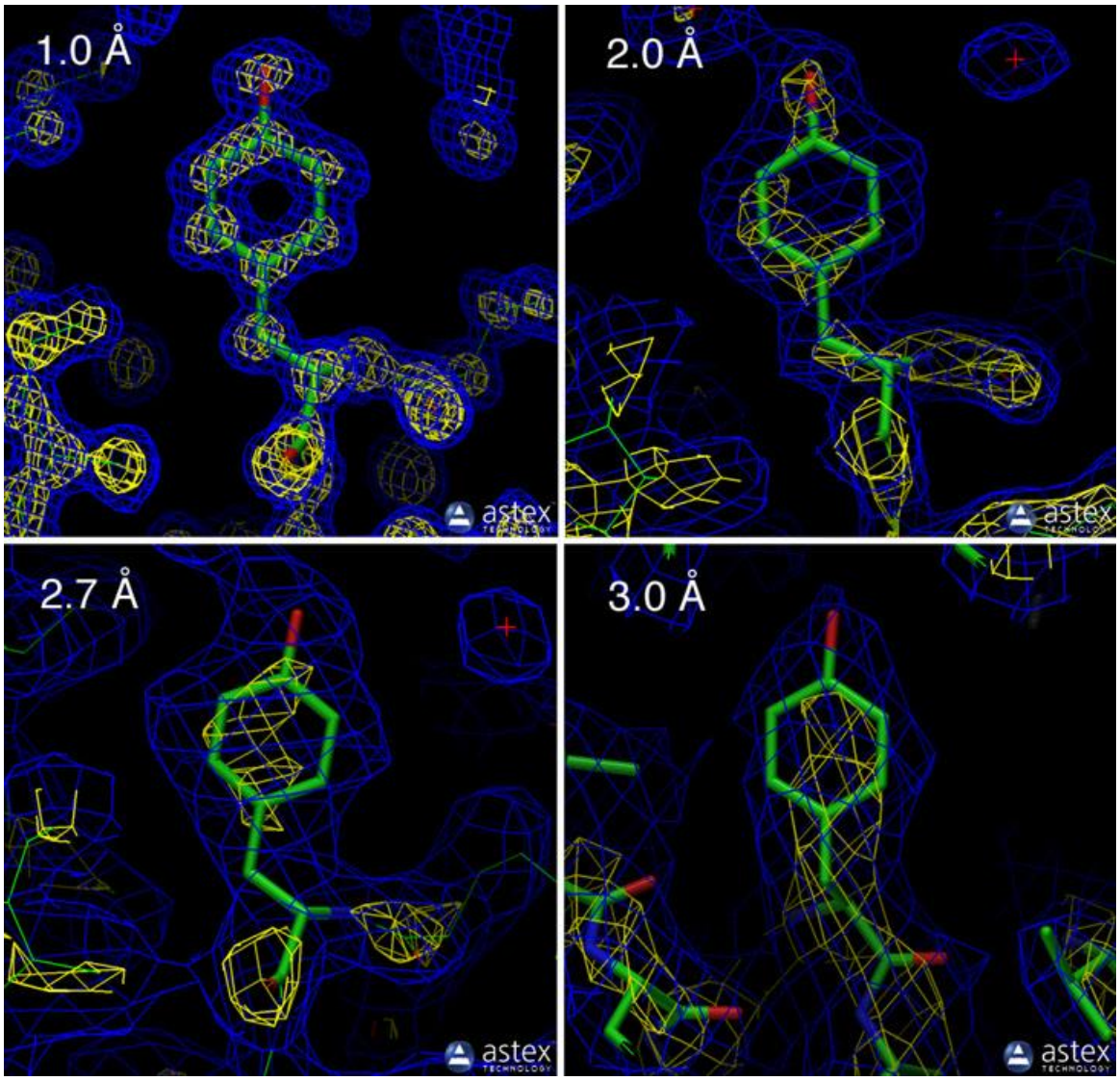
Concanavalin A colored by B-factors on relative scale:

- high **red**
- low **blue**

- B-factors are indicators of relative mobility.

# Experimental resolution and structure accuracy

**Electron density maps for structures with a range of resolutions.**

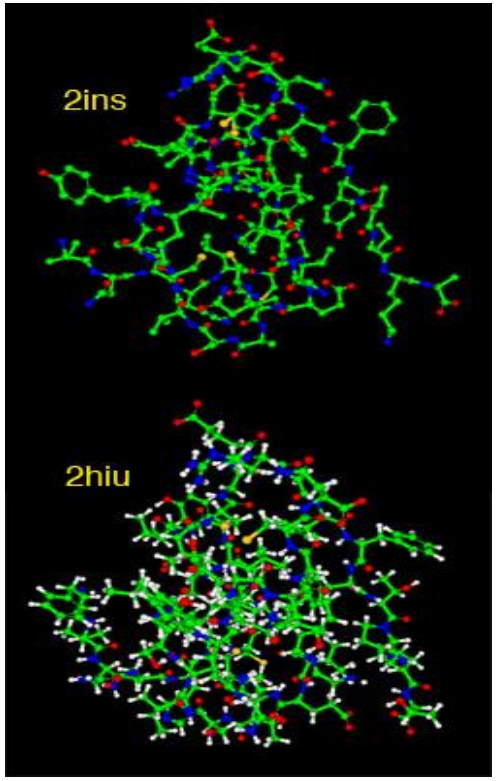



- The first three show tyrosine 103 from myoglobin, from entries 1A6M (1.0 Å resolution), 106M (2.0 Å), and 108M (2.7 Å).
- The final example shows tyrosine 130 from hemoglobin, from entry 1S0H (3.0).
- In the pictures, the blue and yellow contours surround regions of high electron density, and **the atomic model is shown with sticks.**

http://pdb101.rcsb.org

# Hydrogen Atoms

- Most crystallographic experiments do not resolve hydrogen atoms, so most of the crystallographic coordinate files in the PDB archive only include positions for the non-hydrogen atoms.




These two structures of insulin were solved by different experimental techniques.

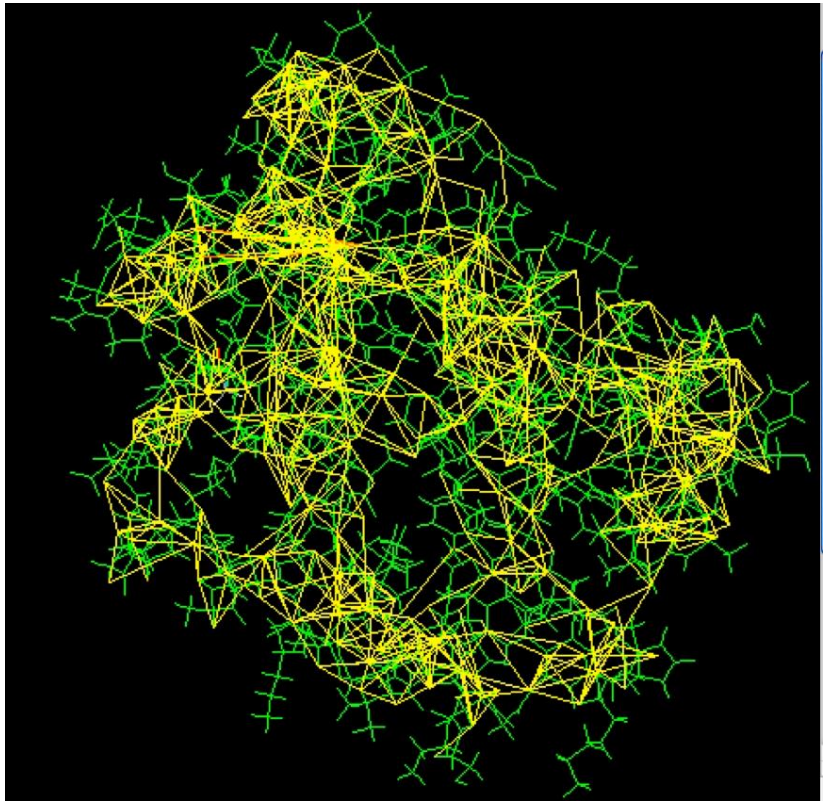
- The top one (PDB entry 2ins) was solved by X-ray crystallography, which does not provide data for the positions of hydrogen atoms.

- The bottom one (PDB entry 2hiu) was solved by NMR spectroscopy and includes hydrogen coordinates.

# NMR Spectroscopy

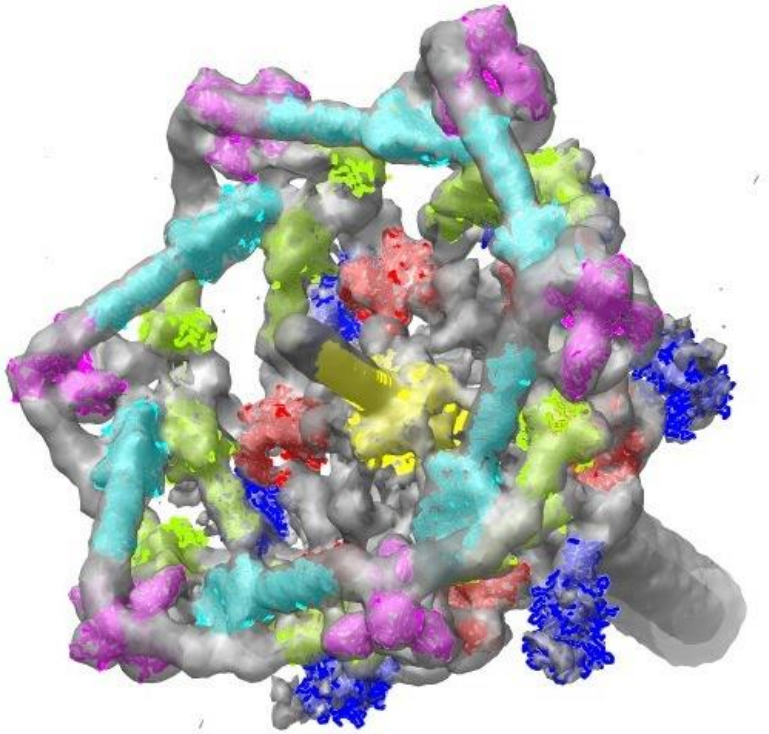
Premier method for studying the atomic structures of flexible proteins.

An ensemble of protein structures.

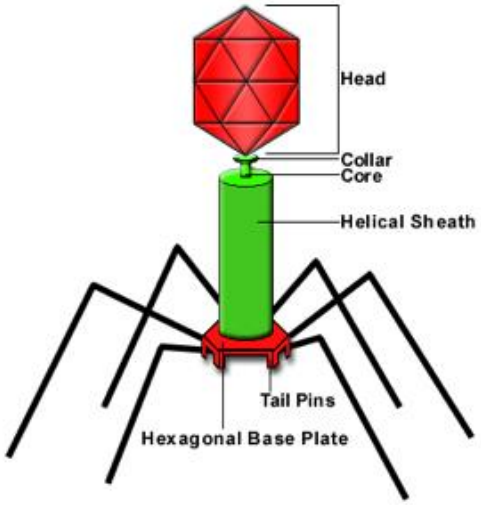


Some of the restraints used to solve the structure of a small monomeric hemoglobin are shown here, using software from the BioMagResBank1. The protein (1vre and 1vrf) is shown in green, and restraints are shown in yellow.

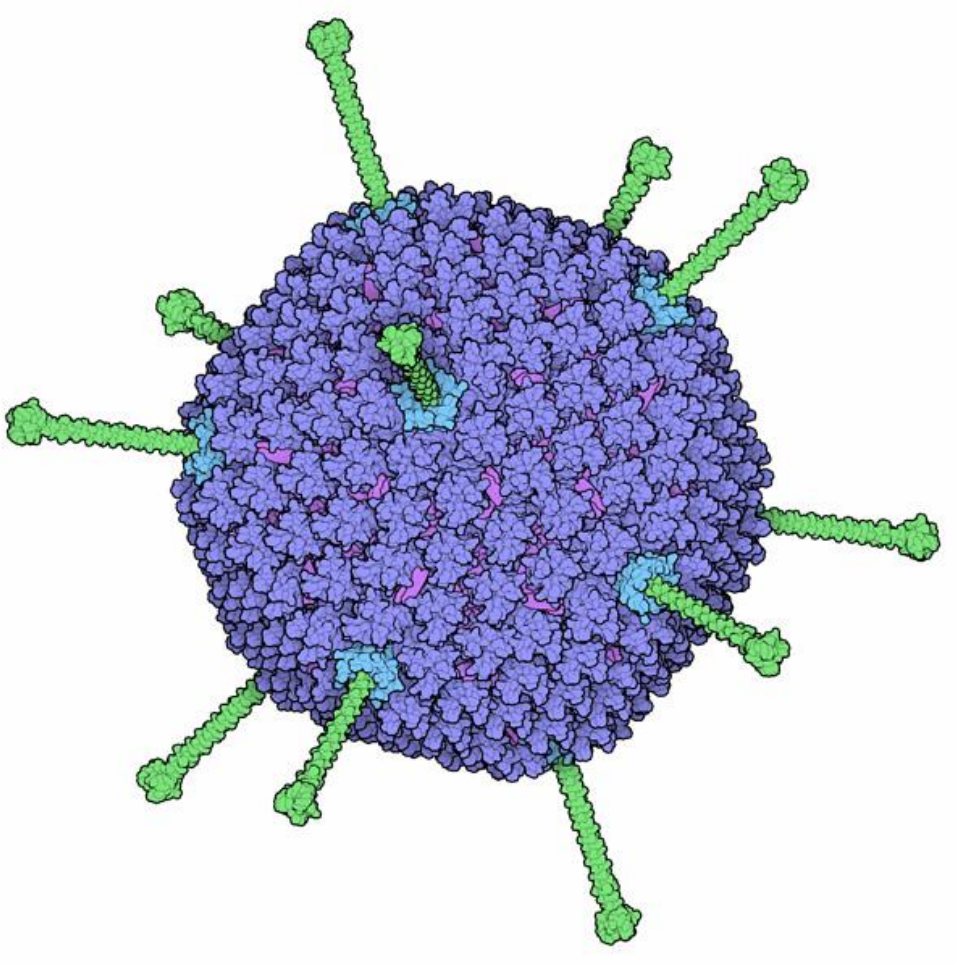
# Electron Microscopy



The tail of the T4 bacteriophage has been examined by combining electron microscopy and atomic structures. The image shows a surface rendering of the EM data (emd-1048) with atomic coordinates from PDB entries 1pdf, 1pdi, 1pdl, 1pdm, 1pdp, and 2fl8.



# Cryo-electron microscopy

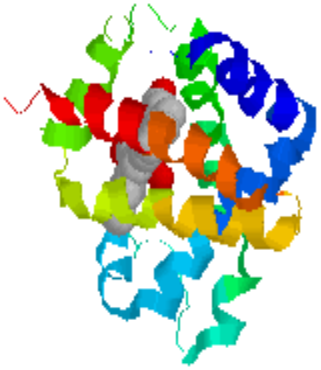


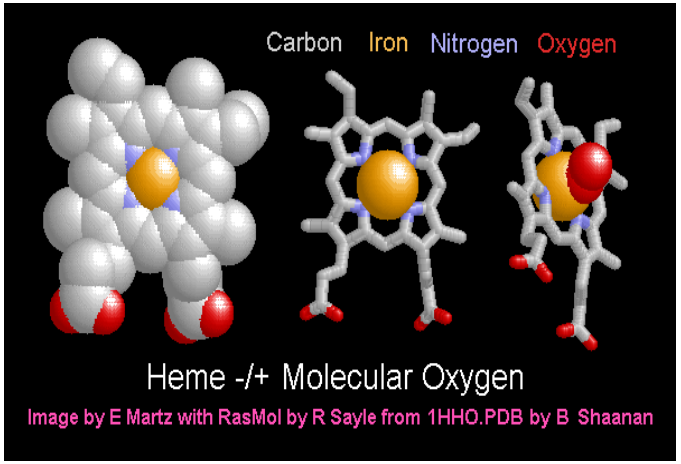
**Adenovirus**

cryo-electron microscopy (PDB entry 3iyn ) and x-ray crystallography (PDB entry 1vsz ).

# Molecular Visualization

- Goal: Clear visualization of molecular structure
- Different visualization modes elucidate different molecular properties
- Some representations include Ribbons, SpaceFill and Backbone





# Demonstration of visualization protein

Use “VMD” as the visualization software.

Use P-selectin/PSGL-1 complex as an example.