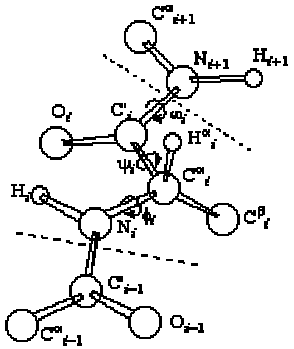
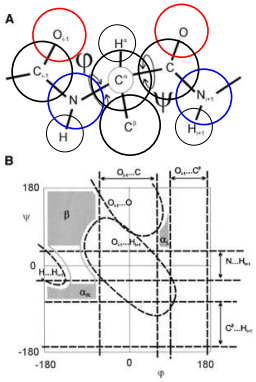
Polypeptide backbone (or the main chain)



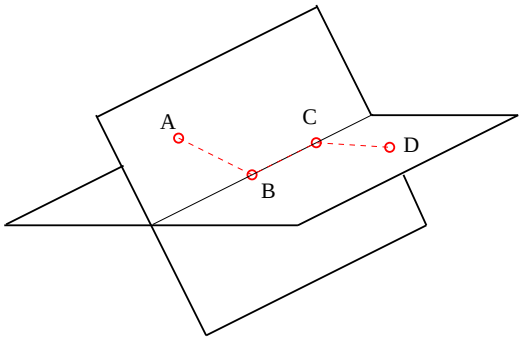
[IUPAC-IUB Commission on Biochemical Nomenclature, Abbreviations and Symbols for the Description of the Conformation of Polypeptide Chains. Eur. J. Biochem., 1969, 17, 193-201]

Ramachandran steric map



[Ho, K.H., Thomas, A. and Brasseur, R., Protein Science, 2003, 12:2508-2522]

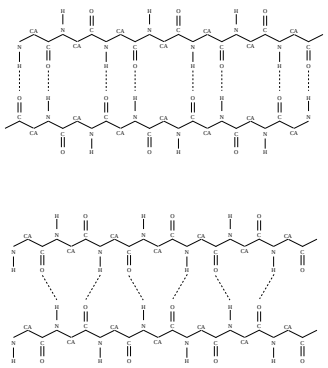
Dihedral angle



Protein Data Bank entry (extract)

```
COMPND    TRIOSE PHOSPHATE ISOMERASE (E.C.5.3.1.1)
SOURCE    CHICKEN (GALLUS GALLUS) BREAST MUSCLE
AUTHOR    D.W.BANNER,A.C.BLOOMER,G.A.PETSKO,D.C.PHILLIPS,
AUTHOR   2 I.A.WILSON
  :
JRNL        AUTH   D.W.BANNER,A.C.BLOOMER,G.A.PETSKO,D.C.PHILLIPS,
JRNL        AUTH 2 I.A.WILSON
JRNL        TITL   ATOMIC COORDINATES FOR TRIOSE PHOSPHATE ISOMERASE
JRNL        TITL 2 FROM CHICKEN MUSCLE
JRNL        REF    BIOCHEM.BIOPHYS.RES.COMM.     V.  72   146 1976
JRNL        REFN   ASTM BBRCA9  US ISSN 0006-291X                146
  :
REMARK   2 RESOLUTION. 2.5 ANGSTROMS.
  :
SEQRES   1 A  247  ALA PRO ARG LYS PHE PHE VAL GLY GLY ASN TRP LYS MET
SEQRES   2 A  247  ASN GLY LYS ARG LYS SER LEU GLY GLU LEU ILE HIS THR
  :
ATOM      1  N   ALA A   1      43.240  11.990  -6.915  1.00  0.00
ATOM      2  CA  ALA A   1      43.888  10.862  -6.231  1.00  0.00
ATOM      3  C   ALA A   1      44.791  11.378  -5.094  1.00  0.00
ATOM      4  O   ALA A   1      44.633  10.992  -3.937  1.00  0.00
ATOM      5  CB  ALA A   1      44.722  10.051  -7.240  1.00  0.00
ATOM      6  N   PRO A   2      45.714  12.244  -5.497  1.00  0.00
ATOM      7  CA  PRO A   2      46.689  12.815  -4.561  1.00  0.00
ATOM      8  C   PRO A   2      46.042  13.601  -3.411  1.00  0.00
ATOM      9  O   PRO A   2      46.030  13.141  -2.267  1.00  0.00
  :
```

Hydrogen bonds in β-sheets



DSSP summary codes

H 4-helix (α-helix)
B residue in isolated β-bridge
E extended strand, participates in β-ladder
G 3-helix
I 5-helix
T H-bonded turn
S bend

Crambin (1CRN)

```
TTCCPSIVARSNFNVCRLPGTPEAICATYTGCIIIPGATCPGDYAN
 EE SSHHHHHHHHHHHHTT  HHHHHHHHS EE SSS   TTS
```


DSSP

Hydrogen bond energy

$$E = q_1 q_2 \left(\frac{1}{d(ON)} + \frac{1}{d(CH)} - \frac{1}{d(OH)} - \frac{1}{d(CN)} \right) \times f$$

Antiparallel bridge:

[hbond(i,j) and hbond(j,i)]
or
[hbond(i-1,j+1) and hbond(j-1,i+1)]

Parallel bridge:

[hbond(i-1,j) and hbond(j,i+1)]
or
hbond(j-1,i) and hbond(i,j+1)]

Protein stability

- good stereochemistry; no steric clashes;
- buried charged atoms must be paired;
- enough hydrophobic surface must be buried, and the interior must be sufficiently densely packed, to provide thermodynamic stability.

Modular proteins

- multi-domain proteins, often with many copies of related domains;
- domains recur in many proteins in different structural contexts.

3D Transformations

Translation

$$T(d_x, d_y, d_z) = \begin{bmatrix} 1 & 0 & 0 & d_x \\ 0 & 1 & 0 & d_y \\ 0 & 0 & 1 & d_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Scaling

$$S(s_x, s_y, s_z) = \begin{bmatrix} s_x & 0 & 0 & 0 \\ 0 & s_y & 0 & 0 \\ 0 & 0 & s_z & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

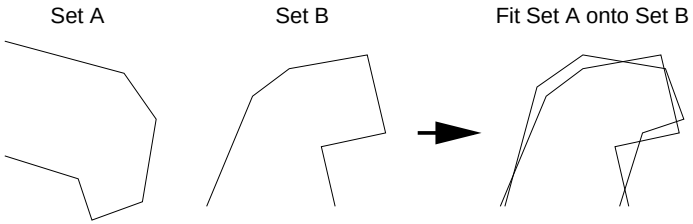
Rotation

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) & 0 \\ 0 & \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R_y(\theta) = \begin{bmatrix} \cos(\theta) & 0 & \sin(\theta) & 0 \\ 0 & 1 & 0 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R_z(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 & 0 \\ \sin(\theta) & \cos(\theta) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Comparing molecular fragments



- 3-D transformation to map Set A onto Set B
- Root Mean Square (RMS) distance