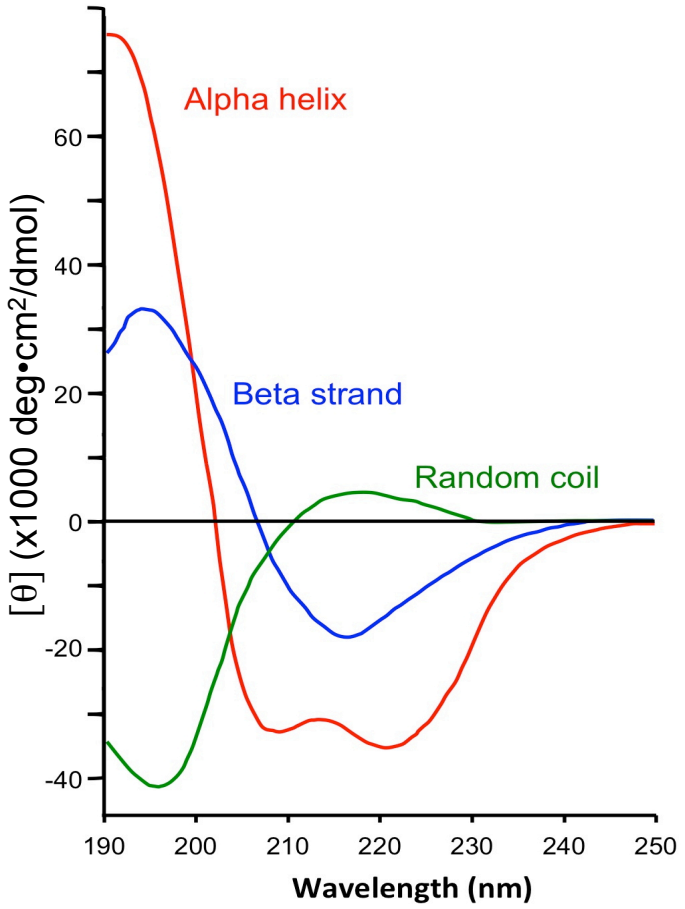
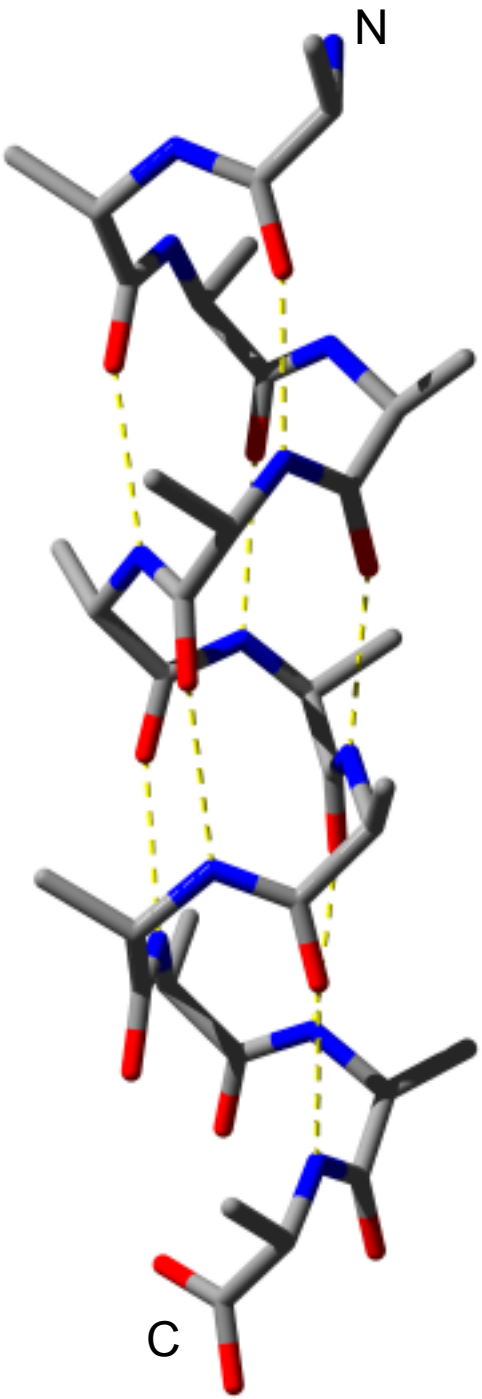
CD Spectra of 2^{o} Structure

θ = ellipticity
$[\theta]$ = mean residue ellipticity
$[\theta] = 3298(\varepsilon_L - \varepsilon_R)$





α-Helix Statistics

Right-handed twist

ϕ, ψ = -47˚, -57˚
3.6 residues/turn

Rise/AA along axis = 1.5 Å
Rise/turn along axis = 5.4 Å

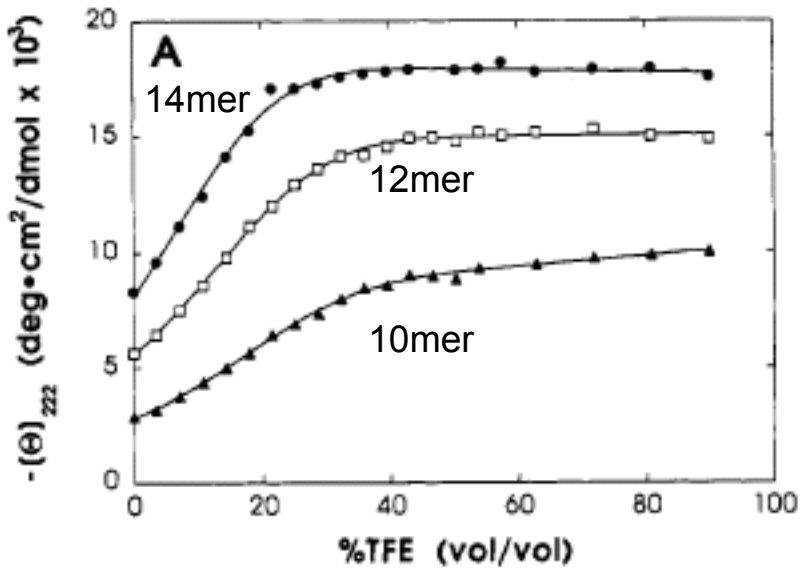
Helix diameter = 4.6 Å

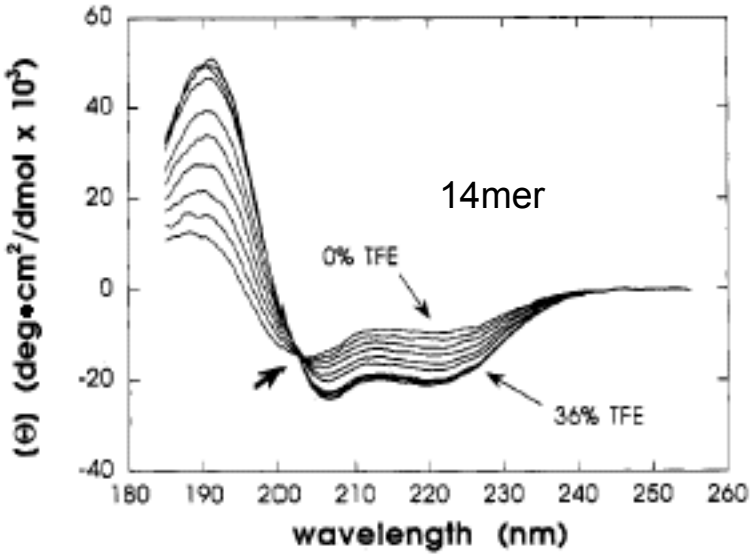
Helix stabilization by TFE

Biochemistry **1994,** *33,* 2129–2135

Quantitative Determination of Helical Propensities from Trifluoroethanol Titration Curves†

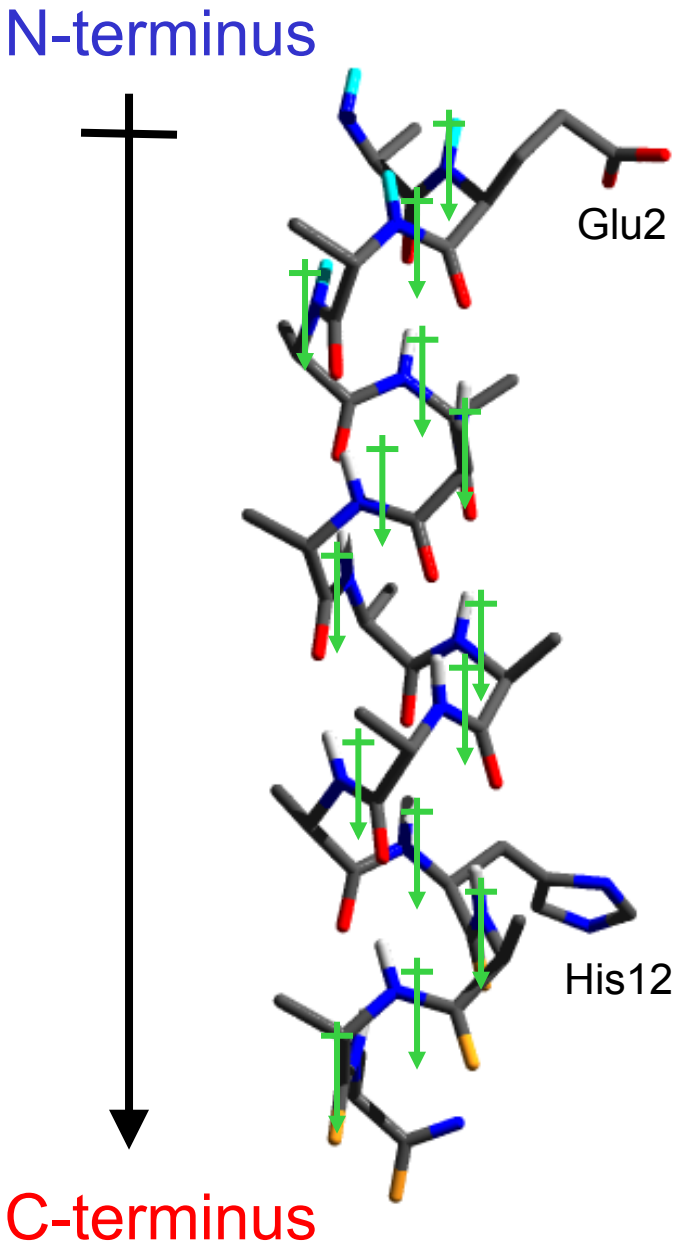
Alan Jasanoff‡ and Alan R. Fersht*





Increased negative ellipticity [θ] at 222 nm indicates greater helix content in increasing concentrations of trifluoroethanol.

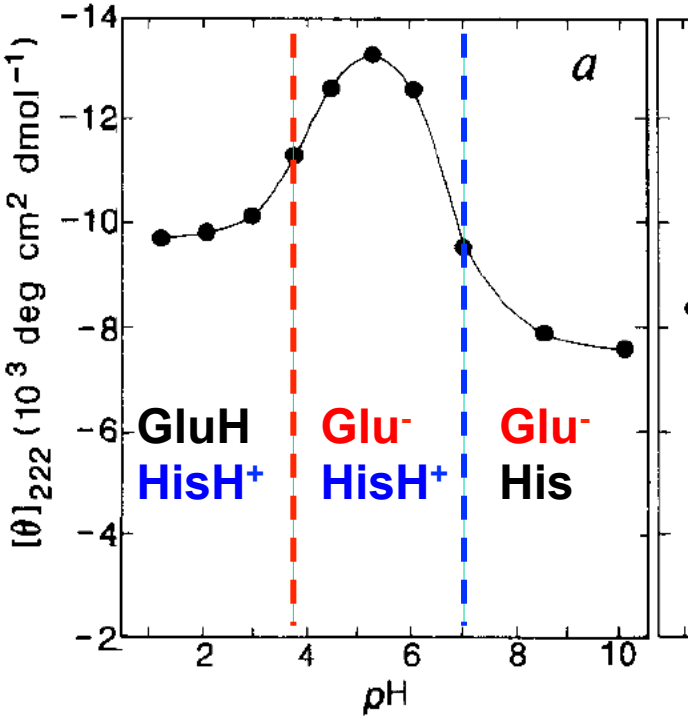
Helix Dipole

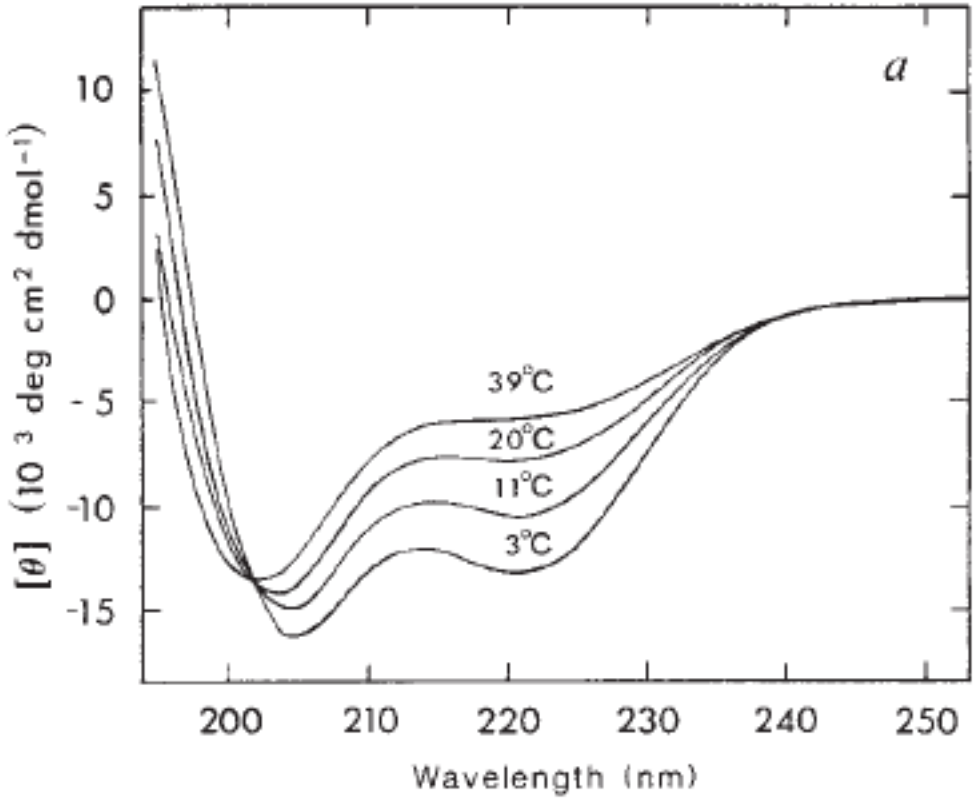


The Helix Dipole, proposed by Wim Hol, predicts that there will be an overall separation of charge related to the alignment of each individual amide group dipole within the helix. The N-terminus will experience the positive end of the dipole, and the C-terminus will experience the negative end.

Test of the Helix Dipole Model

Sequence: Ac-A**E**TAAAKFLRA**H**A-NH_2

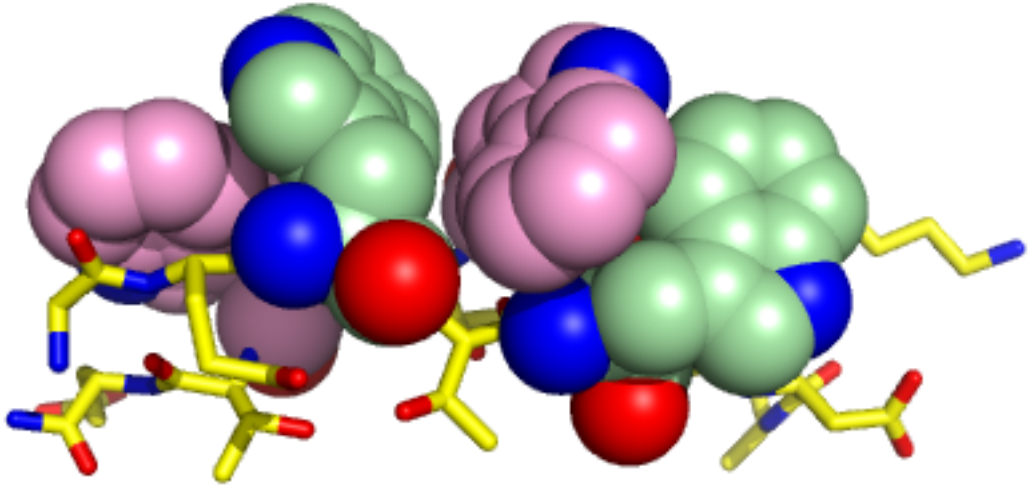


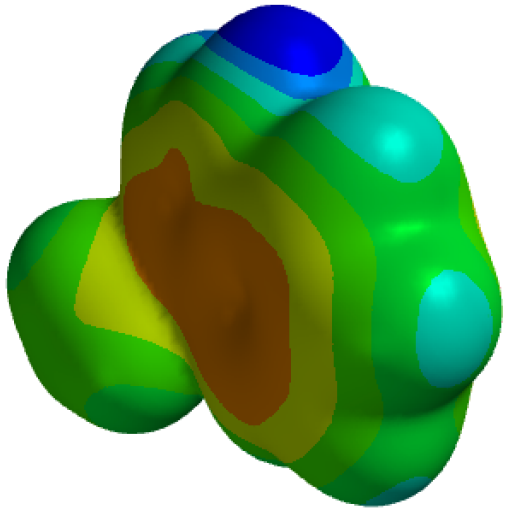


Shoemaker et al. (1987) *Nature* **326**, 563

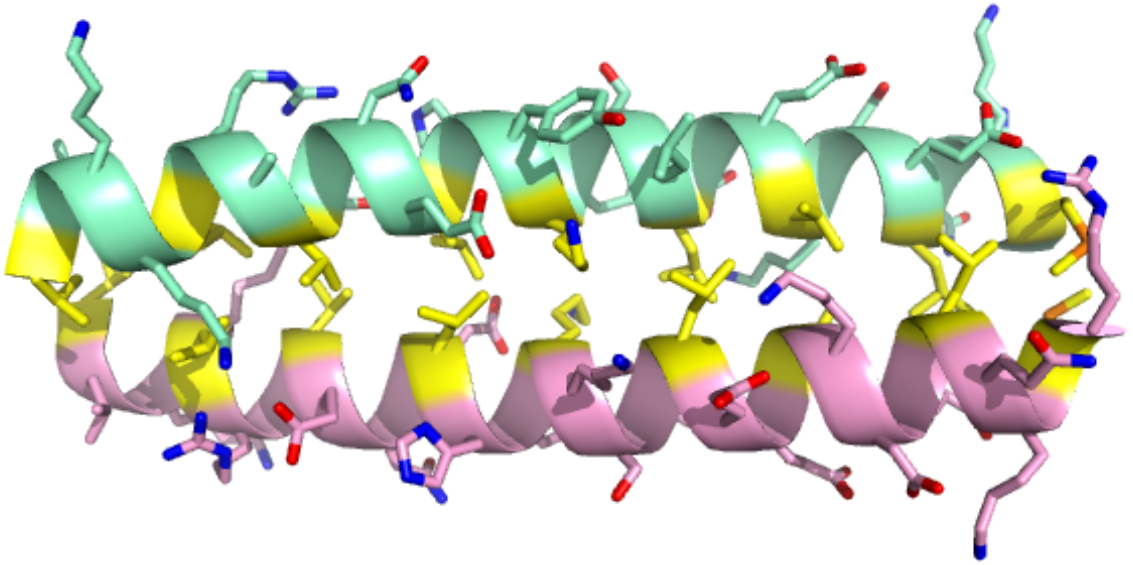
TrpZip: Stable Hairpin Turn

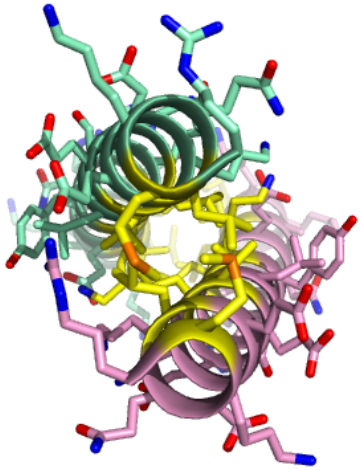
```
gb1     GEWTYDDATKTFTVTE Tm ≈ 0°C
Trpzip GEWTWDDATKTWTWTE Tm = 70°C
```





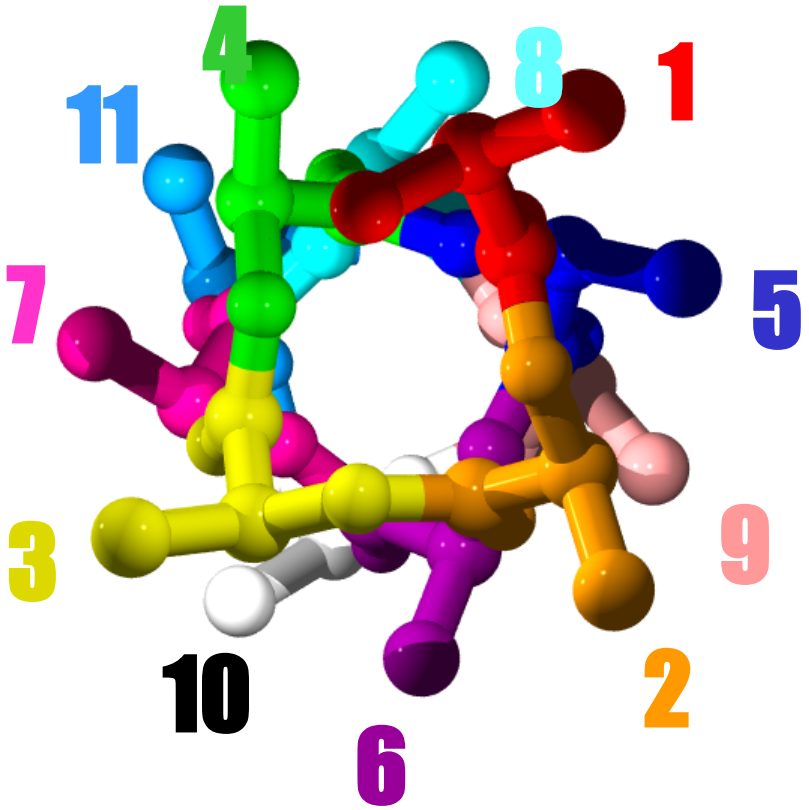
Coiled coil dimer





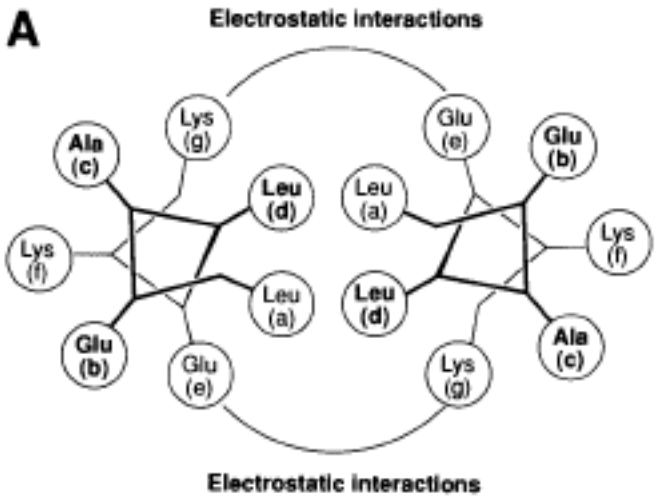
Heptad repeat residues shown in yellow

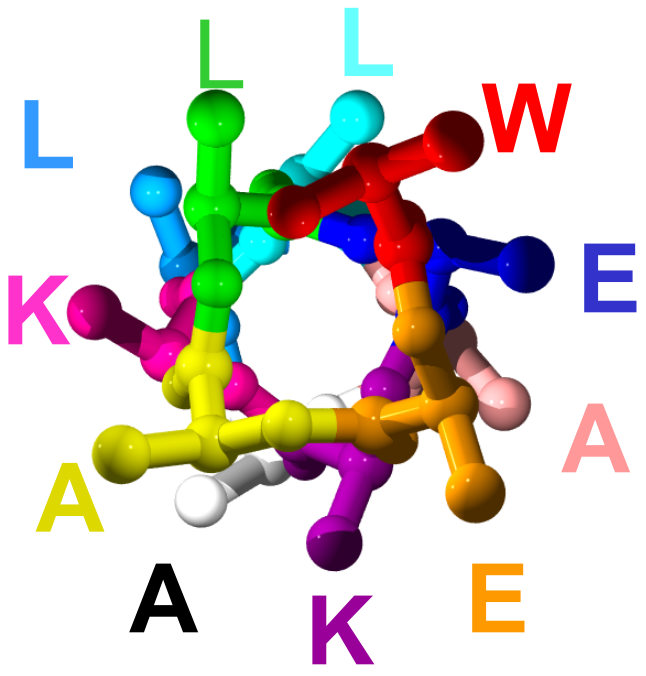
The Helical Wheel



http://www.tcdb.org/progs/helical_wheel.php

O'Neil, K. T. & DeGrado, W. F. (1990). A Thermodynamic Scale for the Helix-Forming Tendencies of the Commonly Occurring Amino Acids. *Science* 250, 646-651.

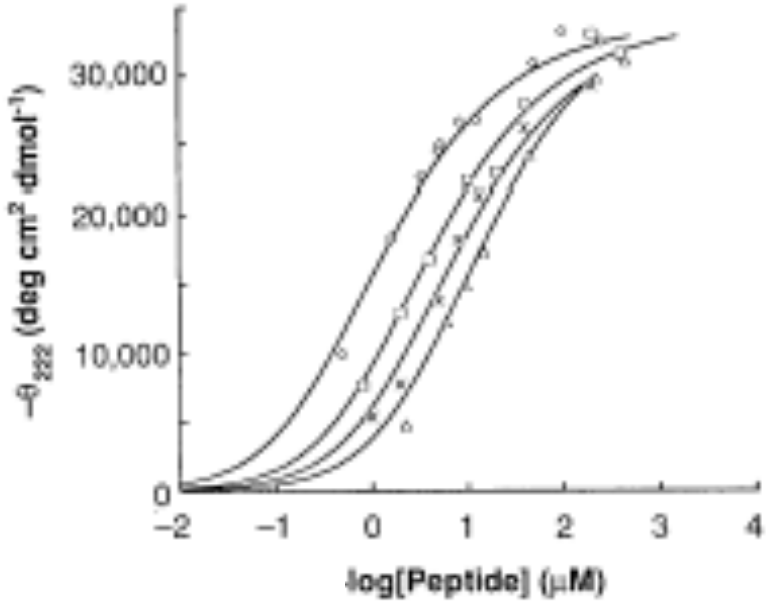




EWEALEKKLAALEXKLQALEKKLEHG

1234567123456712345671EHG

O'Neil, K. T. & DeGrado, W. F. (1990). A Thermodynamic Scale for the Helix-Forming Tendencies of the Commonly Occurring Amino Acids. *Science* 250, 646-651.



2 monomer ⟷ 1 dimer

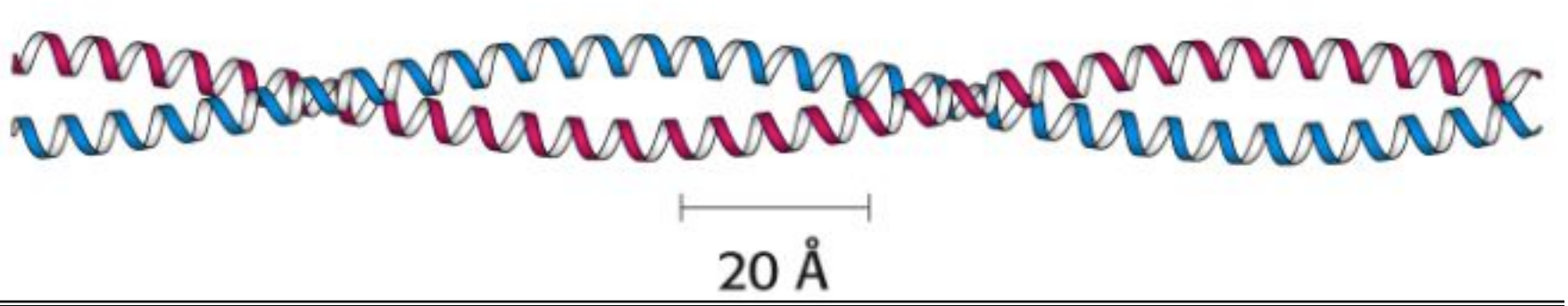
Amino acid	$\Delta\Delta G_\alpha$ (kcal/mol)
Ala	−0.77
Aib	−0.69
Arg	−0.68*
Lys	−0.65*
Leu	−0.62
Met	−0.50
Trp	−0.45
Phe	−0.41
Ser	−0.35
Gln	−0.33
Glu	−0.27*
Cys	−0.23
Ile	−0.23
Tyr	−0.17
Asp	−0.15*
Val	−0.14
Thr	−0.11
Asn	−0.07
His	−0.06*
Gly	0.00
Pro	~3

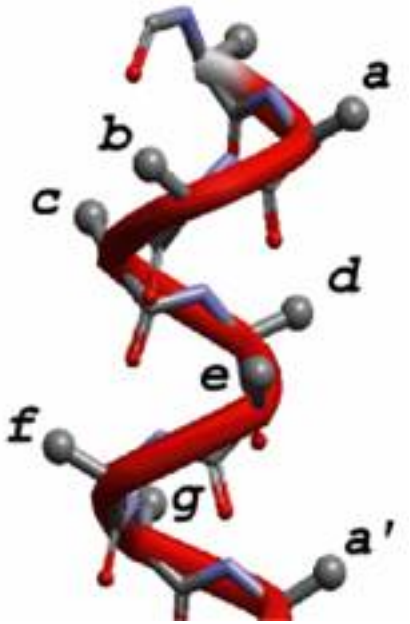
Chou-Fasman Parameters

Amino Acid	P_α	P_β
Alanine	142	83
Arginine	98	93
Aspartic Acid	101	54
Asparagine	67	89
Cysteine	70	119
Glutamic Acid	151	137
Glutamine	111	110
Glycine	**57**	**75**
Histidine	100	87
Isoleucine	108	160
Leucine	121	130
Lysine	114	74
Methionine	145	105
Phenylalanine	113	138
Proline	**57**	**55**
Serine	77	75
Threonine	83	119
Tryptophan	108	137
Tyrosine	69	147
Valine	106	170

The **propensities** (in %)
P_a and P_b are calculated from fraction of residues of each amino acid in that conformation divided by fraction of all residues occupying that conformation.

α-Keratin: A Stable Dimer of Helices



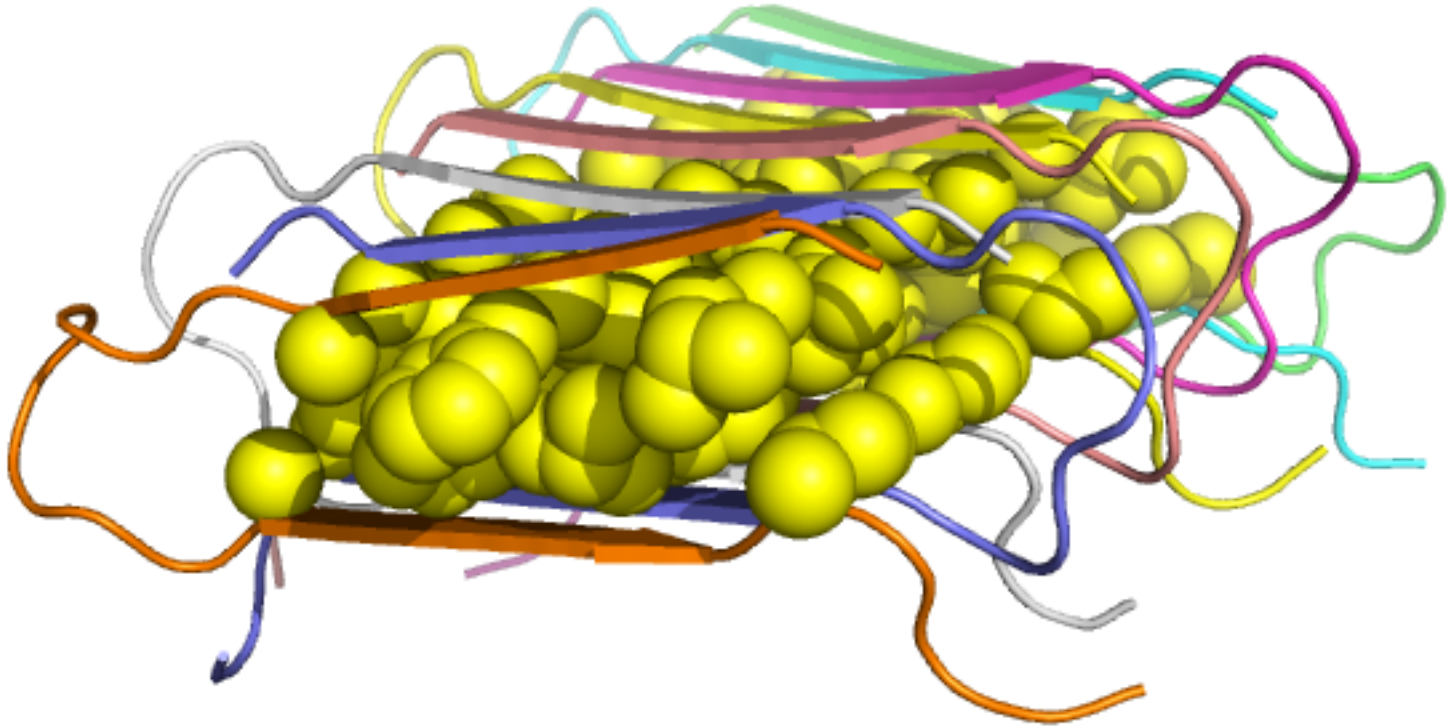


The "Heptad Repeat"

a	Leu
b	Xaa
c	Xaa
d	Leu
e	Xaa
f	Xaa
g	Xaa
a'	Leu

β-Sheet in Amyloid Fibrils

QK**L**V**F**F**A**ENVSNKK**A**I**I**G**L**M**V**GGVV



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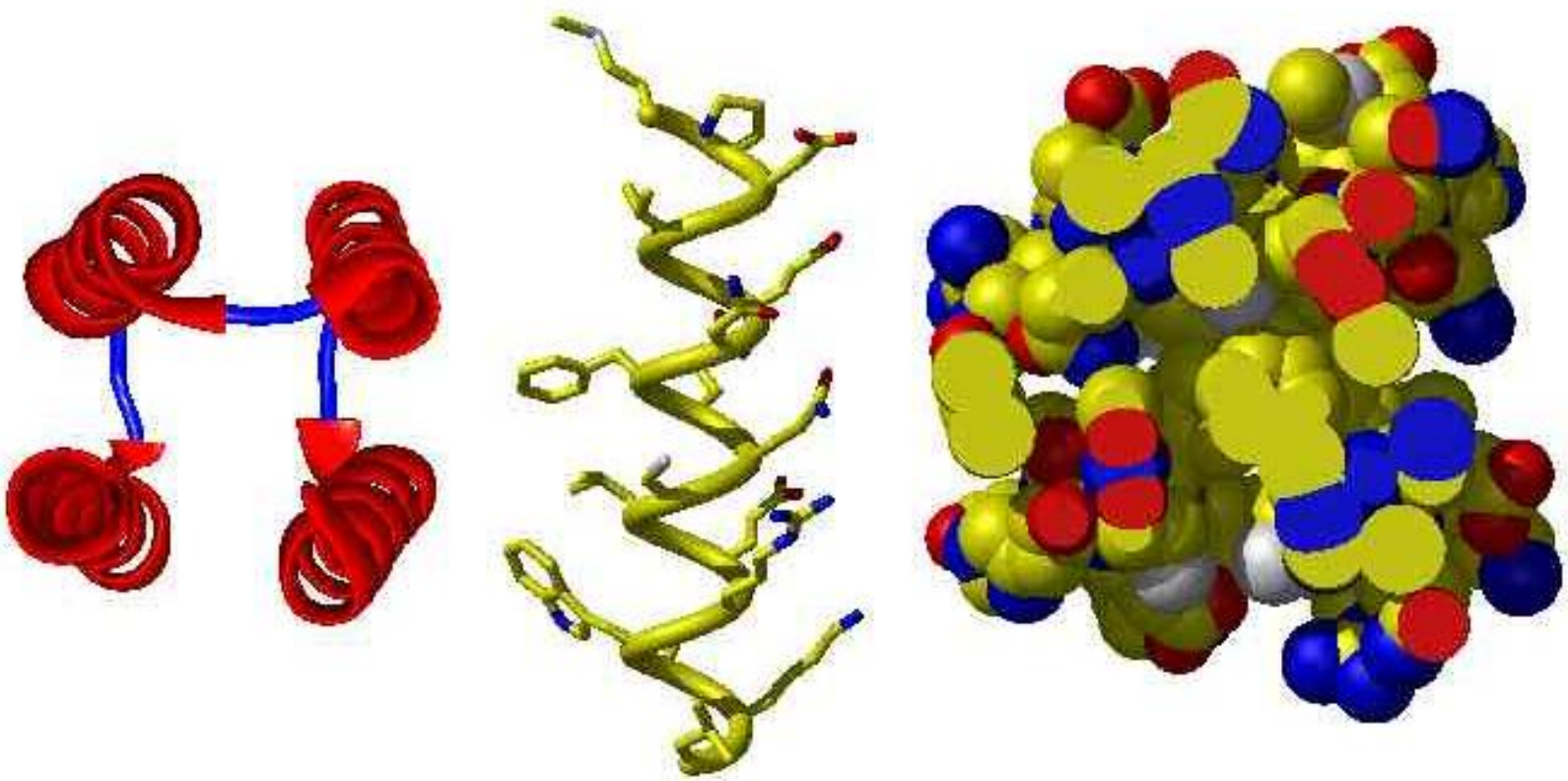
Four Helix Bundle

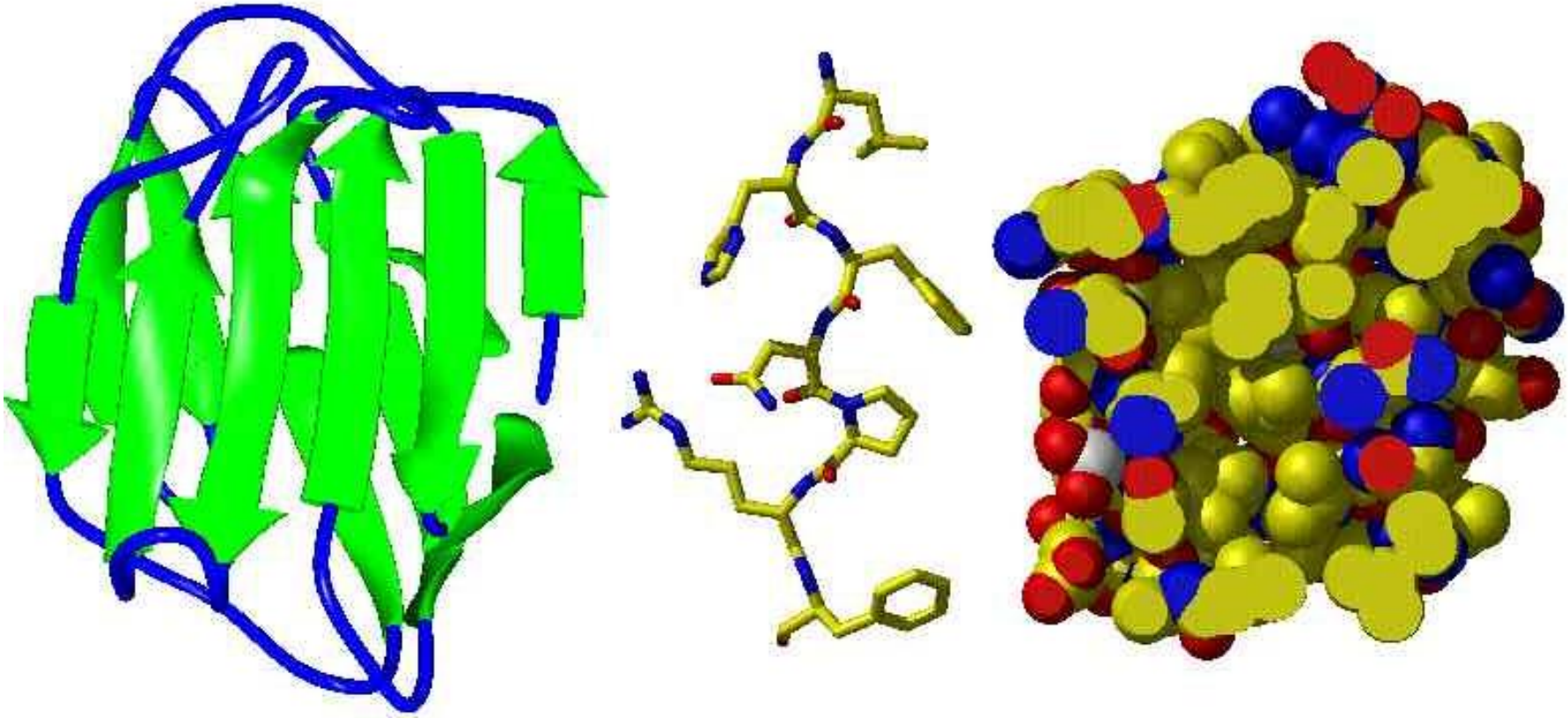
Theoretical model of *de novo* designed protein, felix
Richardson *et al.*, *Science*, **249**, 884(1990) 3flx



amphiphilic
helix

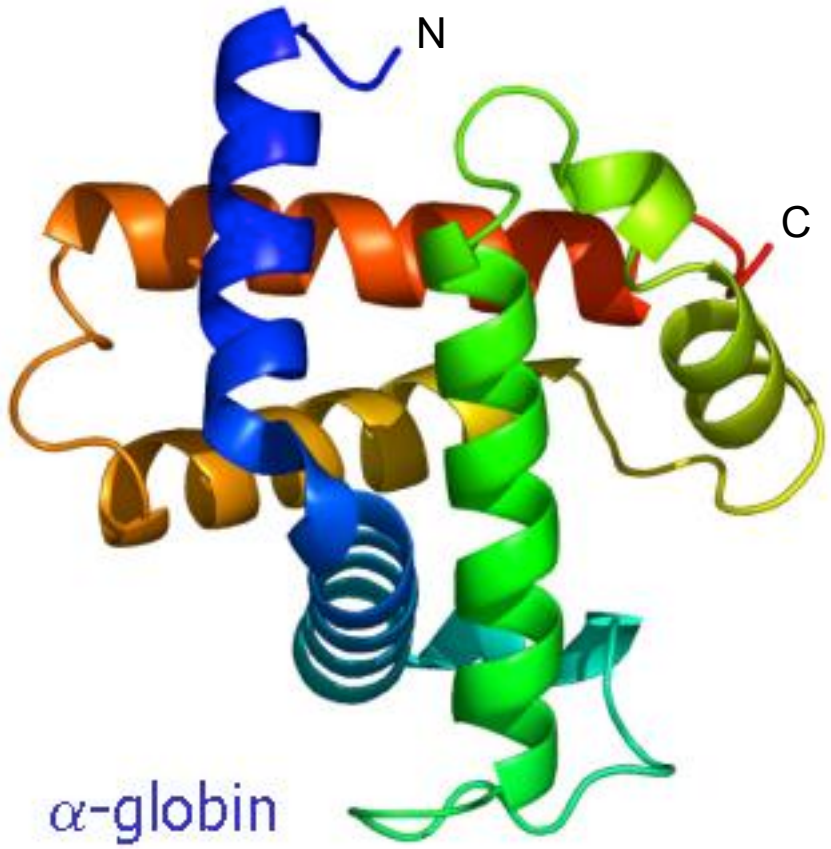
Antiparallel β–Sandwich

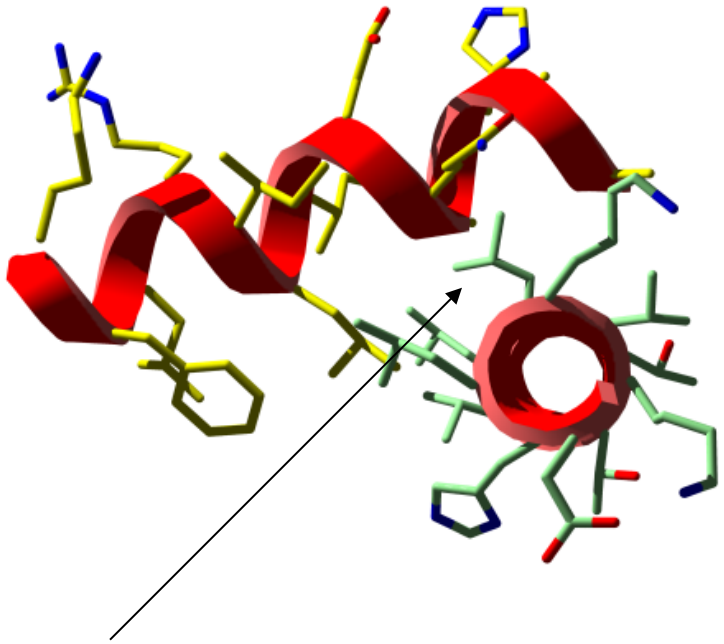
S–Lectin from Bovine Spleen
Liao *et al.*, *PNAS*, **91**, 1429(1994) 1slt



amphiphilic
strand

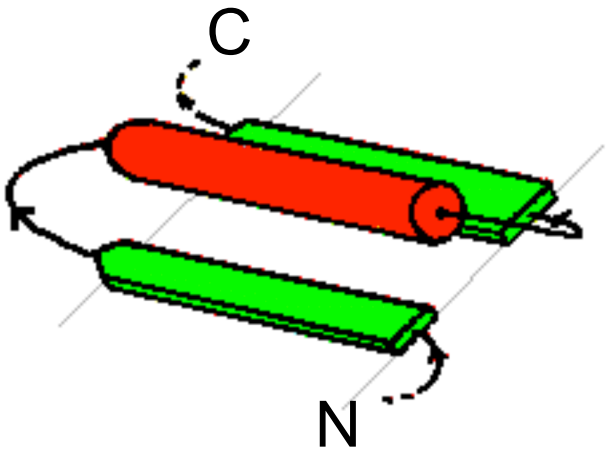
Other All-Helix Topologies



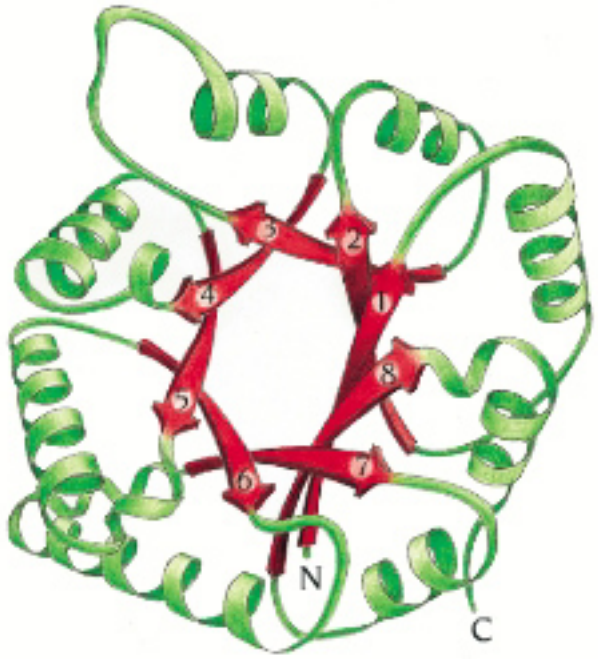


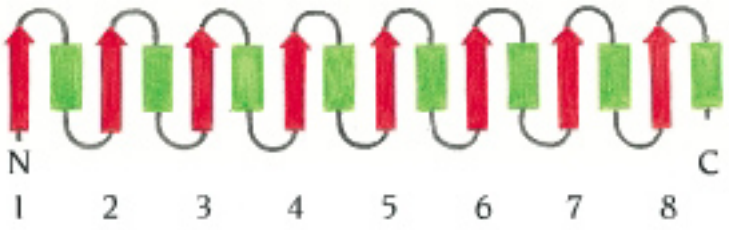
Notch at interface created by two glycines, which allows close orthogonal approach of helices.

Beta-Alpha-Beta Motif



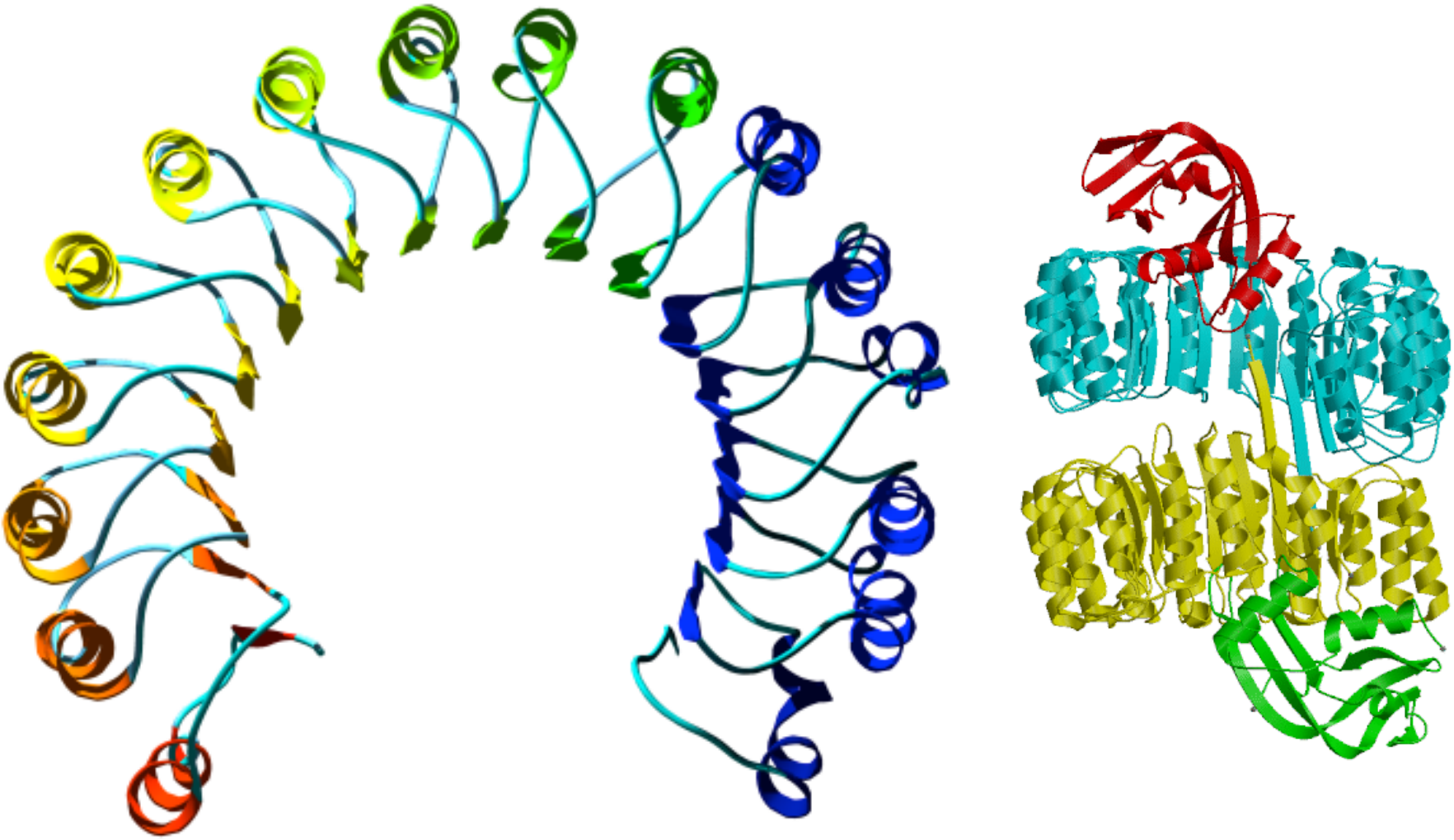
The right–handed beta–alpha–beta unit. The helix lies above the plane of the strands.



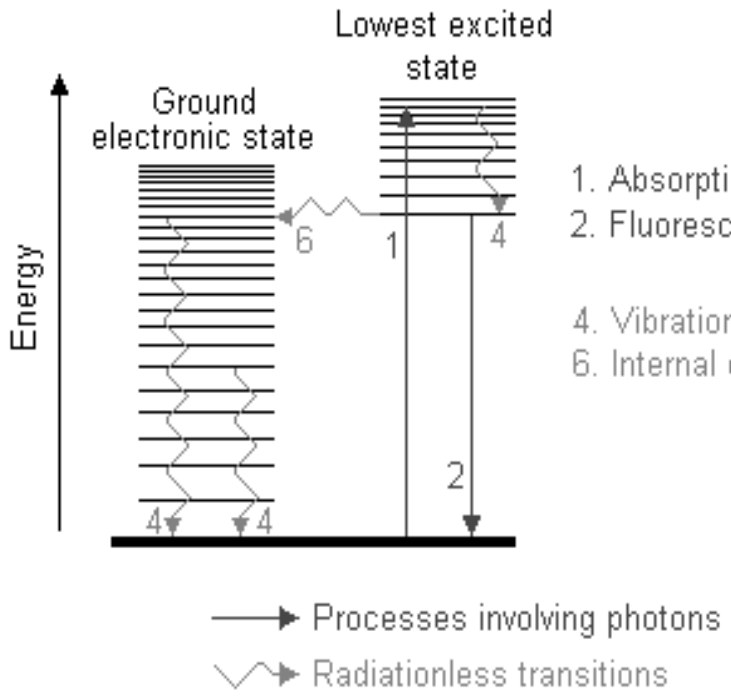


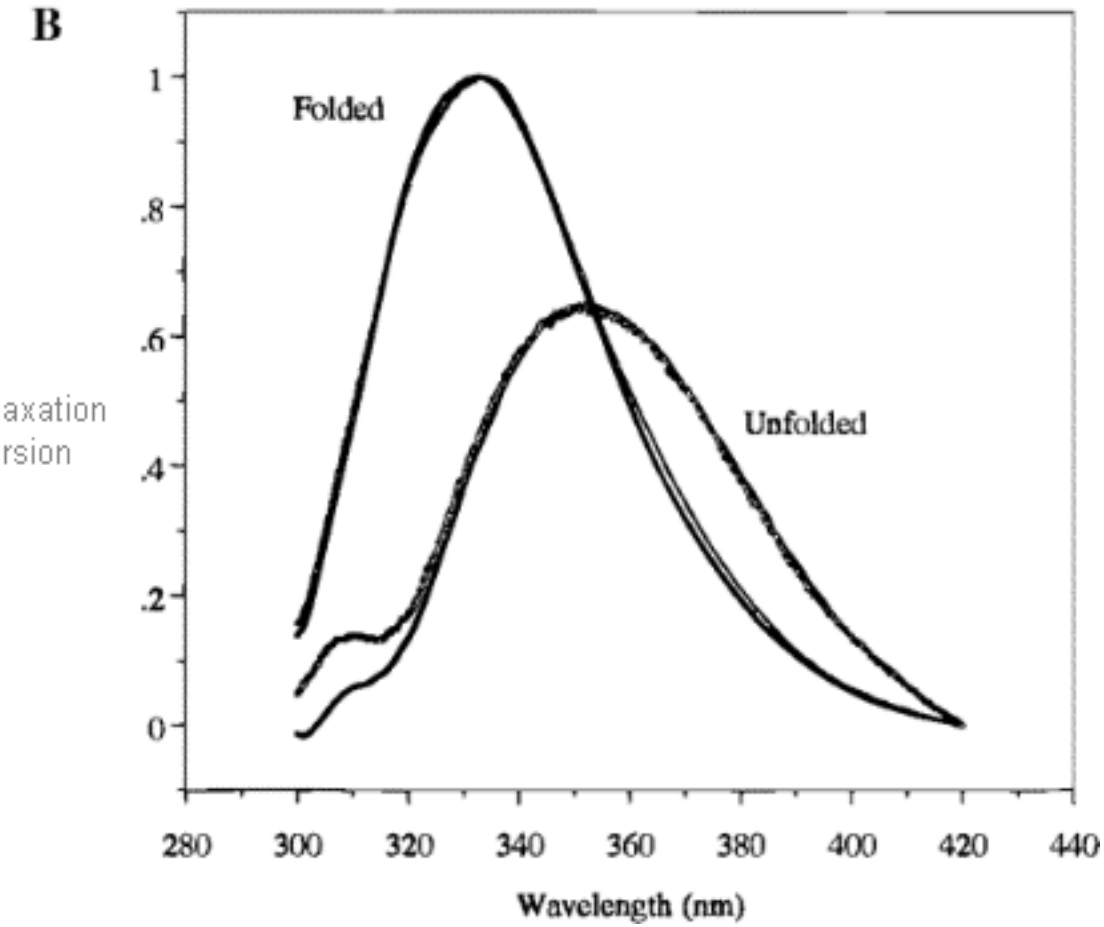
a/b Barrel

Ribonuclease Inhibitor

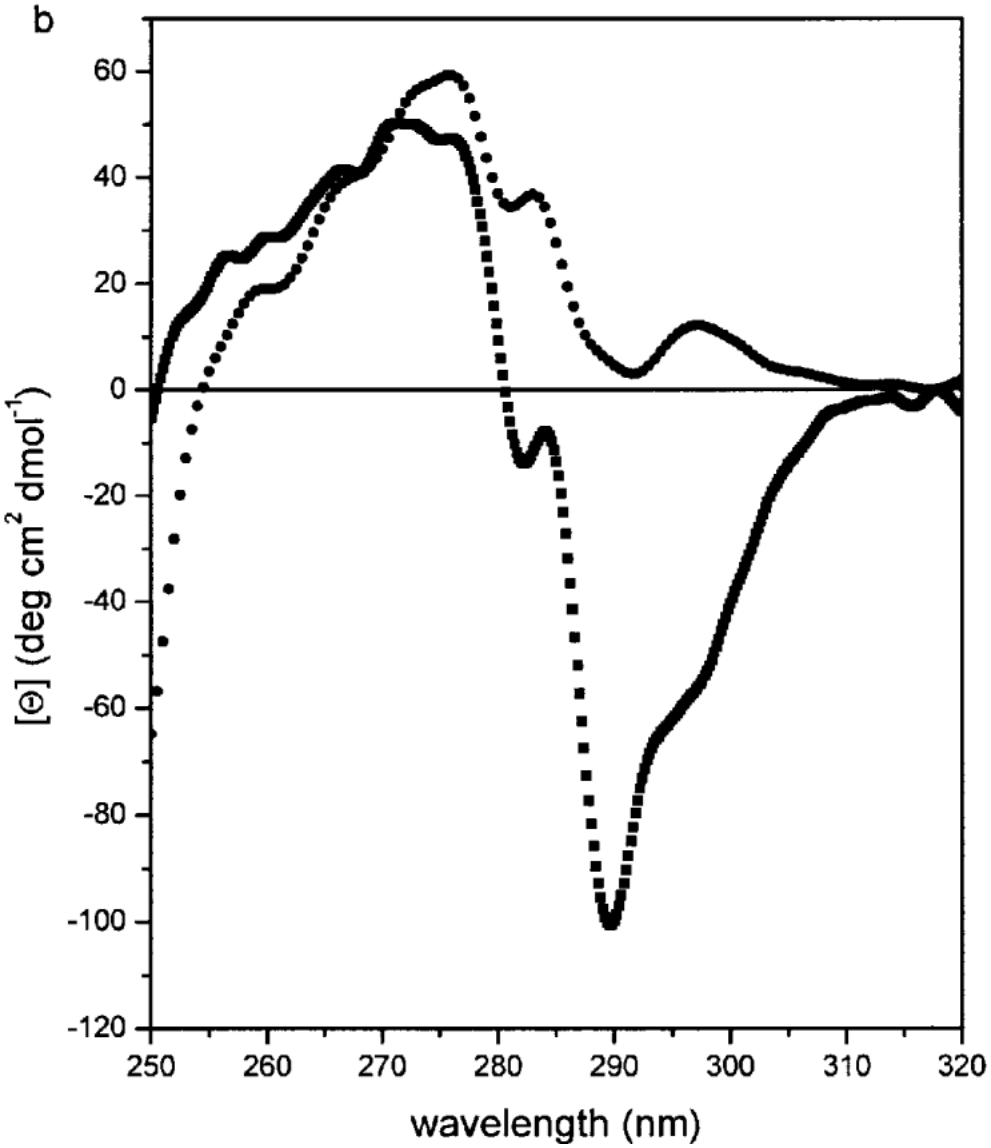


Intrinsic Tryptophan Fluorescence





Near UV Circular Dichroism



Reports on asymmetry in local environment of UV-absorbing side chains

(Tyr and Trp)