**BCH 258 lecture notes**  Mon. Sept 8, 2008

A) **Structure Classification** - continued
   see earlier handout sheet about motifs, domains, and classification

- Assignment: Start thinking about: Coloring Book: due Wednesday Sept. 17.

**Coloring Book**
In the Protein Structure Coloring Book (class hand-out), pick one α/β protein and one All-β protein to color, using any system that interests you and that makes sense relative to the 3D structure; hand in those two. [Note that the coloring book includes All-α and Small Irregular proteins as well.]

Graphics: Coloring Book Slides (shown in class) [slide_archive/ribbons/etc/]
11.GammaCrystallinJane.jpg  barrel fold
12.GammaCrystallinCyrus.jpg  sheet sandwich
13.GammaCrystallinTom.jpg  evolution, gene duplications
22.BPTISSluminated.jpg  β sidedness, SS
31.SODpastel.jpg  depth
32.TIMpastel.jpg  depth and sec. str.
41.IggVLcolorBkice.jpg  simple topol.: connections: GK vs hairpin
43.CAPgreekKeyPair.jpg  simple: GK pair
45.CPAspider_Duncan.jpg  complex: sec. str., sided, ~H-bonds, etc.
Domains, defined in terms of contained motifs

Structural Domain (the unit of tertiary-structure description, or “fold”)
Local region in 3D with presumption of (or better score for) contiguous sequence
(beware alternate definitions: 3D & sequence, or just sequence)
(Note: “domain swap”: part of a domain swapped with a neighbor)
Independently stable; may move as a rigid body
Analogous structure to other entire protein (or plausible as such)

Major categories of tertiary structures (many “folds” in each category)
I. All-α (chap. 3)
II. α/β (chap. 4)
III. All-β (chap. 5)
+. Small irregular; mixtures; miscellaneous

Alternative scheme: “Superfolds”
Commonest “folds” with same topology & shape in “core” part,
Found in >= 3 unrelated protein families

α – motifs: helix-helix contacts; Hphobic patches; pack spiral ridges of sidechains
Helix hairpin: adjacent, ↑↓ pair of α; +15-20°; form helix bundles
EF hands, helix-turn-helix: adjacent pair ~90°; Ca<sup>2+</sup> binding, DNA binding

Small irregular motifs:
Zn finger in metal-rich (several kinds; bind DNA)
SS β cross in SS-rich: 2 crossed SS’s, from β hairpin

α/β motifs: righthanded crossover, or βαβ unit
its alternation of β & α, and its handedness, dominates α/β folds
α/β superfolds:
singly-wound β-barrel, = TIM barrel, or = (βα)<sub>8</sub> barrel
α/β horseshoe
doubly-wound β-sheet, = twisted open sheet, or = nucleotide-binding domain
the commonest protein fold, esp. for enzymes
active or binding site at “switch point”

β motifs:
β hairpin (2 ↑↓ strands)
Greek key +1, -3; long β-hairpin coiled around,
Handed (ccw from outside)
twist of double ribbon (belt) becomes loops around "barrel" ends
axis of barrel along strand direction,
barrel closed by H-bonds of edge strands
some quite round, some flattened:
described as 2-layer "sandwich"

β superfolds:
up & down β-barrel (& β-trefoils)
Greek key β-barrel 6 or 8 strands, & “jellyroll” >8 strands
open-face sheet
β-propeller
parallel β-helix