

BCH 258 lecture notes Wed. Sept 08, 2010 revised Structural Motifs and Domains

Homework:

- Reading Suggestion: Chapters 2 - 5 in Branden & Tooze
- Worksheet5-Structural Classes: (preparation for Coloring Book)
- Coloring Book: due Wed. Sept 16

c2Motifs.kin, c3Alpha.kin, c4Al_Bet.kin, c5Beta.kin

In class:

revisit with Kendrews: Helix N-cap – residue half in & half out of helix: e.g. Asn

Structural Motifs : small, favored clusterings of 2-4 pieces of sec. str.; strong
General preference for contact of near neighbors in sequence

Helix hairpin : successive $\uparrow\downarrow$ helices; pack best at $\sim 15\text{-}20^\circ$ angle
Hydrophobic patches; spiral ridges of sidechains; coiled-coil

$\sim 90^\circ$ helix contacts: “EF hand” Ca^{++} -binding; “helix-turn-helix” DNA-binding

β -hairpin : successive $\uparrow\downarrow$ β strands; shortest with tight turn

crossover or $\beta\alpha\beta$ connection : successive $\uparrow\uparrow$ β -strands
>>99% righthanded; determines architecture of α/β folds

Greek key β :

SS β -cross : 2 touching SS spirals (1L,1R) on adjacent β hairpin strands

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, $\uparrow\downarrow$ pair of α ; +15-20°; form helix bundles
EF hands, helix-turn-helix: adjacent pair $\sim 90^\circ$; Ca^{++} 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 $\beta\alpha\beta$ unit
its alternation of β & α , and its handedness, dominates α/β folds

α/β superfolds :

singly-wound β -barrel, = TIM barrel, or = $(\beta\alpha)_8$ 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”

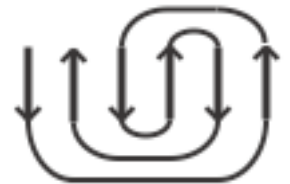
β motifs :

β hairpin (2 $\uparrow\downarrow$ 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



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
21.RubiscoJSRic.jpg	sec. str.
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.