Answers to Problem Set #1:

(1) Types I at 46% of all β–turns and II at 23% are by far the most common of the classical β–turn structures. Much less common are types I' (5.4%) and II' (2.7%) which have phi–psi backbone dihedral angles that are the negative (hence the mirror image) of types I and II respectively. Upon surveying the known protein structures, Sibanda and Thornton (*Nature*, 316, 170–174 '85) found that types I' and II' are much more common than I and II at the corner of β–hairpins. This is thought to be due to the fact that the twist of the I' and II' turns matches the twist of the β–strands of the hairpin.

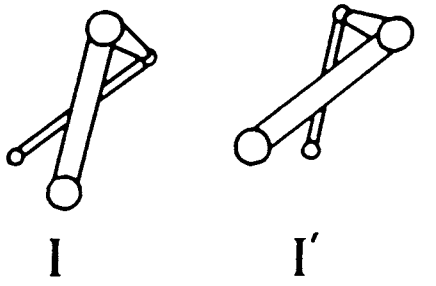
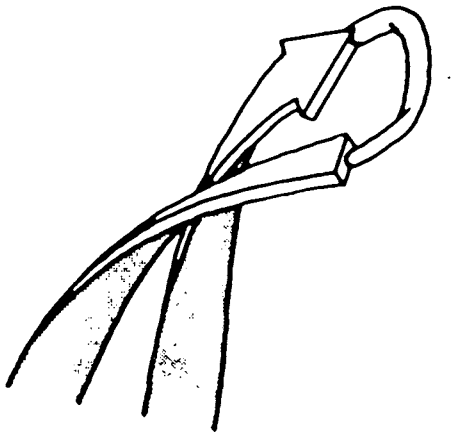
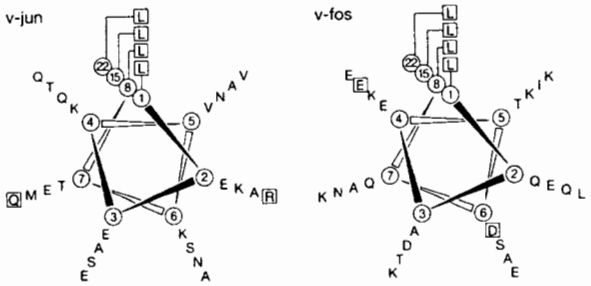


FIGURE 16 Simplified drawings of Type I vs. Type I' tight turns, showing that Type I has a twist incompatible with the twist direction of β hairpins.

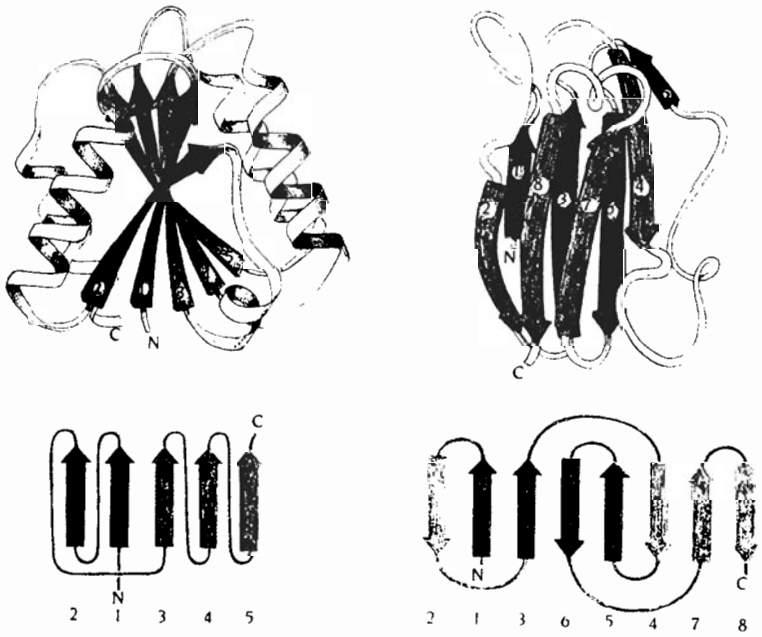


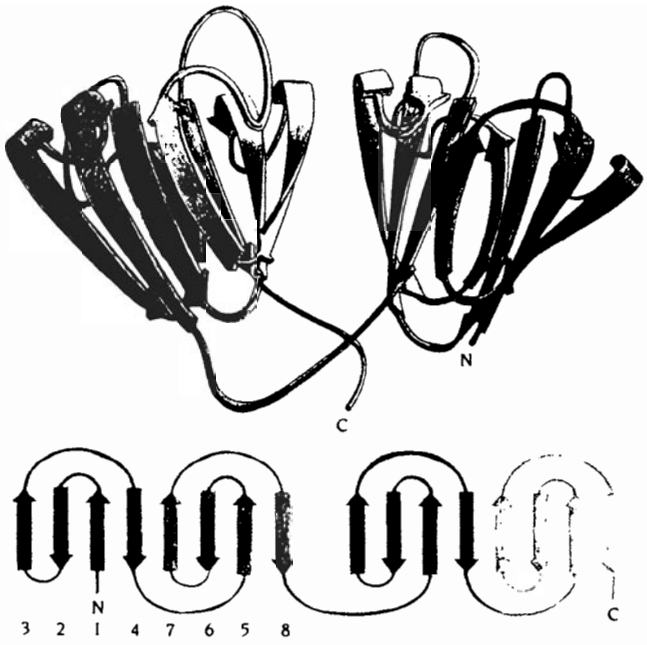
(2) The two structures shown in the problem are just rotated mirror images of each other. The one on the right is the correct structure of natural RNAse A. The correct structure has right–handed twist to both the helices and the antiparallel sheet.

(3) As discussed in class, one of the preferred "knobs–into–holes" packing motifs has a +20 degree angle between the two helices. If we imagine this packing extending for a longer distance and with the two helices wrapping around each other, the result is a "coiled coil" structure with a left–handed supertwist. Helical wheel diagrams for the Fos and Jun partial sequences are shown below. The interface between the helices is formed mostly by the hydrophobic side chains of the 1 (all leucine !!) and 5 positions.



(4) Topological diagrams are shown below for each of the proteins. From left to right, top to bottom they are: (1) flavodoxin, with a five stranded parallel β–sheet and three βαβ units, (2) plastocyanin, an eight stranded antiparallel closed barrel, (3) γ–crystallin, which contains two Greek key motifs connected by a short loop, (4) the ATP–binding domain of hexokinase, an open twisted α/β structure, and (5) phosphoglycerate mutase, another open α/β structure of slightly different topology.




N
C
N
C
3 2 1 4 7 6 5 8


C
N
C
N
5 4 1 2 3
6 5 1 4 2 3

(5) The answer is outlined in the first column of page 1128 and in figure 1 of the Rose, *et. al.* article. Basically, the Schellman motif is preferred when the C1 and Ccap positions are polar and Gly, and when the C" and C3 positions are hydrophobic. This results in a helix cap region that has a polar surface (the C1/Ccap side) and a nonpolar surface (on the C"/C3 side). Glycine is required at the Ccap residue due to the backbone conformation needed at that position of the Schellman structure. Similar arguments can be made for the α_L motif. Helix continuation is the default result observed in the absence of these specific motifs.

(6) The preferred Greek key topology is the one that allows the correct right–handed supertwist of the overall sheet, and places the majority of the side chains between the "short" antiparallel hydrogen bond pairs on the "inner" surface of the sheet structure.