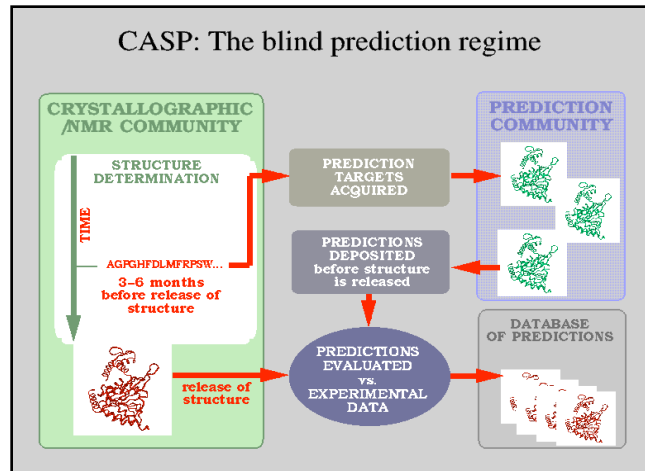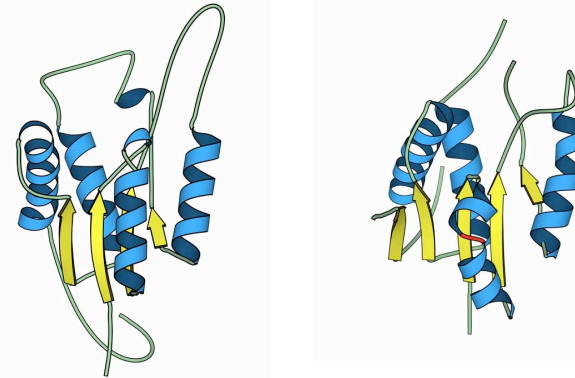# Prediction of Protein Structure

CASP: The blind prediction regime

Very low homology T0173: Mycothiol deacetylase

Goals

- Better understanding of evolutionary relationships
- Characterization of molecular function
- Guiding further experiments

Major challenges

Comparative modeling (homology modeling):

Reliability of sequence alignments

Identification and modeling of structural change

Refinement!

Fold recognition:

Sequence alignments (potentially combinatorial)

Whole genome applications (model quality assessment)

De novo structure prediction:

Still mostly an unsolved problem!

Importance of methods development cannot be underestimated