

Structure Refinement Using RDCs

- Rat apo S100B($\beta\beta$) (Ca²⁺-binding EF-hand)

> 500 RDC restraints, backbone RMSD 1.04 \rightarrow 0.29 Å

Residues in favored regions of Ramachandran 76 \rightarrow 86%

Poorly defined 3rd helix now precise, change in helix 3 to helix 4 angle is 90° upon Ca²⁺ binding, not 116°

Drohatski, Tjandra, Baldisseri and Weber, Protein Sci. 8 (1999), 800-809

- Yeast Splicing Factor Prp40: are the two adjacent WW domains positioned to allow simultaneous binding of poly-proline binding partners?

Backbone RMSD 1.14 \rightarrow 0.55 Å

Each WW domain leans away from the linker region, so the two binding sites face in opposite directions

Wiesner, Stier, Sattler and Macias, J. Mol. Biol. 324 (2002), 807-822