**PROBLEM SET**

NMR Spectroscopy and Protein Structures

CHEM 991A, Fall 2007

1. Using the Solution Structure of the 50S Ribosomal Protein L35AE from Pyrococcus furiosus (PDBID: 1SQR):
   1. Generate an XPLOR PSF file for the 1SQR.

**Required for Remainder of Problem Set**

* 1. Use XPLOR to calculate an average structure for the ten structures in the ensemble.

**Required for Remainder of Problem Set**

* 1. Calculate an RMSD for each structure relative to the average structure using:
     1. Only backbone atoms (C’, C, N)
        1. **0.995**
        2. **1.12**
        3. **1.01**
        4. **1.23**
        5. **1.04**
        6. **1.07**
        7. **1.44**
        8. **1.01**
        9. **1.07**
        10. **1.00**
     2. All atoms
        1. **1.69**
        2. **1.76**
        3. **1.64**
        4. **1.82**
        5. **1.76**
        6. **1.63**
        7. **2.26**
        8. **1.6**
        9. **1.73**
        10. **1.55**
  2. Using the backbone RMSD, identify which structure(s) from the ensemble is the best-representative structure.

**Structure 1 has the lowest RMSD relative to the average structure, so it would be the best representative structure.**

* 1. Identify which amino-acid residues should be assigned to an -helix, -strand or turn based on:
     1. Phi (), psi () dihedral angles (using the best-representative structure from the ensemble)

**Based on PROCHECK analysis of dihedral angles (\*.rin file)**

**-helix:31-39**

**-sheet:3-11, 21-27,41-45,53-61,66-70,82-86**

**Turns:48-51,79-81**

* + 1. Carbon chemical shifts

**-helix:32-37**

**-sheet:9-13, 21-26, 42-47,51-56, 66-71,82-86**



* 1. Identify (if any) which residues are in the generously allowed or disallowed regions of the Ramachandran , plot.

**Generously allowed: His18, Asn19,Gln78**

**Disallowed region: Thr63**

* 1. Use XPLOR to determine the number of proton pairs/groups that are separated by less than 3Å in the best-representative structure.

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* 1. Use XPLOR to predict the C and C chemical shifts for each residue in the best-representative structure.
     1. Plot the per residue Cand Cchemical shifts between the predicted and experimental carbon chemical shift values.

