Protein Structure Analysis

http://binf.gmu.edu/vaisman/binf731/

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Protein Structure Hierarchy

- Primary - the sequence of amino acid residues
- Secondary - ordered regions of primary sequence (helices, beta-sheets, turns)
- Tertiary - the three-dimensional fold of a protein subunit
- Quaternary - the arrangement of subunits in oligomers.

Secondary Structure: Computational Problems

Secondary structure characterization
Secondary structure assignment
Secondary structure prediction
Protein structure classification
Protein representations

Protein backbone

NWVLSTAAAMQGVVDGMASGLDKD

Peptide bond formation

Adopted from Zvelebil, Baum, 2008
Secondary Structures

Adopted from Zvelebil, Baum, 2008

Secondary Structure (Helices)

Helix

Secondary Structure (Beta-sheets)

Antiparallel Beta-Sheet

Can you identify the amine- and carboxy- termini of the strands?
Reverse Turns on a Ramachandran Plot

Beta-hairpin Turns on a Ramachandran Plot

Side-Chain Atom Nomenclature

Reverse turns.

Type I

Type II

The white dots indicate hydrogen bonds.

Two-residue beta-hairpin turns.

Type I'

Type II'

White dots indicate hydrogen bonds.
The main difference between these two turns is the orientation of the peptide group between residues 1 and 2.

Two amino acid side chains to indicate the atom naming convention. Hydration are not shown.
Side-Chain Torsional Angles

Secondary Structure: Computational Problems

Secondary structure characterization
- Secondary structure assignment
- Secondary structure prediction
- Protein structure classification

Secondary Structure Conformations

<table>
<thead>
<tr>
<th>Structural Type</th>
<th>( \phi )</th>
<th>( \psi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>alpha helix</td>
<td>-57</td>
<td>-47</td>
</tr>
<tr>
<td>alpha-L</td>
<td>57</td>
<td>47</td>
</tr>
<tr>
<td>3-10 helix</td>
<td>-49</td>
<td>-26</td>
</tr>
<tr>
<td>( \pi ) helix</td>
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<td>-80</td>
</tr>
<tr>
<td>type II helix</td>
<td>-79</td>
<td>150</td>
</tr>
<tr>
<td>( \beta ) sheet parallel</td>
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<td>113</td>
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<tr>
<td>( \beta ) sheet antiparallel</td>
<td>-139</td>
<td>135</td>
</tr>
</tbody>
</table>

Secondary Structure Assignment

Adopted from Zvelebil, Baum, 2008

### Secondary Structure Assignment

<table>
<thead>
<tr>
<th>RESIDUE AA STRUCTURE</th>
<th>Cx-E(1) distance from DSSP</th>
<th>beta strand</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>8.00</td>
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<tr>
<td>36</td>
<td>9.00</td>
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<td>37</td>
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<td>38</td>
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<td>1.00</td>
</tr>
<tr>
<td>39</td>
<td>11.50</td>
<td>1.00</td>
</tr>
</tbody>
</table>

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