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Geometric Computations in Molecular Biology SS07

Backbone hydrogen bonding patterns determine a protein's helices and sheets:
Of course, computers can't visualize proteins the same way we can, but must perform more laborious coordinate comparisons to determine structure. Most of these are surprisingly geometric – e.g. here is a list of all pairs of backbone N and O atoms with distances in (2.8Å,3.15Å) for one of the proteins from the matching game.
Determine the helix and sheet structure of this protein.
Then see if you can determine its PDB id.

```
N   6 -> O   3    dist  3.05
N   8 -> O  32    dist  2.89
N   9 -> O  53    dist  2.89
N  10 -> O  34    dist  2.89
N  11 -> O  55    dist  2.81
N  12 -> O  36    dist  3.13
N  18 -> O  14    dist  3.09
N  19 -> O  15    dist  2.99
N  20 -> O  16    dist  2.92
N  21 -> O  17    dist  2.93
N  22 -> O  18    dist  2.89
N  23 -> O  19    dist  2.89
N  24 -> O  20    dist  2.88
N  25 -> O  21    dist  2.90
N  26 -> O  22    dist  2.96
N  27 -> O  23    dist  2.99
N  27 -> O  24    dist  3.12
N  28 -> O  25    dist  3.00
N  29 -> O  25    dist  3.14
N  29 -> O  26    dist  2.94
N  30 -> O  25    dist  2.91
N  33 -> O  31    dist  3.14
N  34 -> O   8    dist  2.88
N  36 -> O  10    dist  2.93
N  39 -> O  63    dist  3.02
N  42 -> O  38    dist  2.96
N  43 -> O  39    dist  3.02
N  43 -> O  40    dist  3.15
N  44 -> O  40    dist  2.96
N  45 -> O  41    dist  3.06
N  45 -> O  42    dist  3.11
N  46 -> O  42    dist  2.84
N  47 -> O  43    dist  3.05
N  48 -> O  45    dist  2.96
N  49 -> O  46    dist  3.06
N  54 -> O  82    dist  2.90
N  55 -> O   9    dist  2.90
N  56 -> O  84    dist  2.93
N  57 -> O  11    dist  2.98
N  65 -> O  58    dist  3.03
N  68 -> O  64    dist  2.94
N  69 -> O  65    dist  2.93
N  70 -> O  66    dist  2.88
N  71 -> O  67    dist  3.00
N  72 -> O  68    dist  2.95
N  73 -> O  69    dist  2.97
N  74 -> O  70    dist  2.99
N  80 -> O  78    dist  3.08
N  81 -> O  78    dist  3.05
N  84 -> O  54    dist  2.87
N  85 -> O 105    dist  2.94
N  86 -> O  56    dist  2.84
N  87 -> O 107    dist  2.97
N  93 -> O  91    dist  3.15
N  94 -> O  91    dist  2.97
N  95 -> O  91    dist  2.94
N  96 -> O  92    dist  3.01
N  97 -> O  93    dist  2.96
N  98 -> O  94    dist  2.89
N  99 -> O  95    dist  2.90
N 100 -> O  96    dist  2.85
N 101 -> O  97    dist  3.01
N 102 -> O  98    dist  3.13
N 102 -> O  99    dist  2.94
N 103 -> O  98    dist  2.87
N 109 -> O  87    dist  2.94
N 116 -> O 112    dist  2.96
N 117 -> O 113    dist  2.82
N 118 -> O 114    dist  2.99
N 119 -> O 115    dist  2.98
N 119 -> O 116    dist  3.13
N 120 -> O 116    dist  2.83
N 121 -> O 117    dist  2.85
N 122 -> O 118    dist  2.89
N 123 -> O 119    dist  3.00
N 125 -> O 121    dist  2.87
N 126 -> O 122    dist  2.97
N 127 -> O 123    dist  2.88
N 128 -> O 124    dist  2.92
N 129 -> O 124    dist  2.86
```