Version 2.1

**\*\* ONLY TEXT AND IMAGES APPEARING INSIDE THE RED BOXES WILL BE GRADED\*\***

1. PDB entry 1jb0 is the structure of Photosystem I: the Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria. Photosystem I is a massive structure composed of 12 proteins and 127 cofactors (96 chlorophylls, 2 phylloquinones, 3 Fe4S4 clusters, 22 carotenoids, 4 lipids). For this exercise we’ll focus on one protein, called REACTION CENTRE SUBUNIT II, and draw a topology diagram of REACTION CENTRE SUBUNIT II, which is chain D in pdb entry 1jb0.   
     
   The protein topology diagram was invented by Jane Richardson and is used to classify and simplify protein structures.   
     
   Load REACTION CENTRE SUBUNIT II into PyMol and inspect the structure and construct a topology diagram. To start, copy and paste the following into the PyMol command line.

**PyMOL**>  
 #----------start copy-----

reinitialize

bg\_color white

fetch 1jb0

remove not chain D

remove not backbone

hide everything

show cartoon

label resi 28 and name CA, "1"

label resi 38 and name CA, "2"

label resi 47 and name CA, "3"

label resi 55 and name CA, "4"

label resi 82 and name CA, "5"

label resi 92 and name CA, "6"

label resi 114 and name CA, "ignore this"

label resi 29 and name CA, "1"

label resi 39 and name CA, "2"

label resi 48 and name CA, "3"

label resi 56 and name CA, "4"

label resi 83 and name CA, "5"

label resi 93 and name CA, "6"

label resi 114 and name CA, "ignore this"

label resi 18 and name CA, "N-terminus"

label resi 138 and name CA, "C-terminus"

set label\_size, 20

zoom 1jb0

spectrum count, rainbow, 1jb0

create sheet\_1, ss S

disable sheet\_1

remove resi 1-17

#----------end copy---------------

The ribbon diagram of 1jb0 in this PyMol script is colored from blue on the N terminus to red on the C-terminus. Notice that there are two independent b-sheets. One b-sheet has four strands (strands 1,4,5,6) and the other has 2 strands (strands 2,3). Ignore the tiny b-strand near the C-terminus. I have used a command (create sheet\_1, ss S) to make an object that contains just the b-strands. You can turn this object on to help see the b-sheet connectivity and to assist your work here.

Your topology diagram must be a single chain containing the α-helices and b-strands, with correct N to C directionality in the b-strands. Represent the two b-sheets as arrows by drawing b-strands 1,4,5,6 together, and b-strands 2,3 together. Number each b-strand.

Insert images of the ribbon diagram (2 views) here and resize the images so that both fit on this page.

|  |
| --- |
| INSERT VIEW 1 HERE |

|  |
| --- |
| INSERT VIEW 2 HERE |

Insert your topology diagram.

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| --- |
| INSERT TOPOLOGY DIAGRAM |

1. The topology of pdb entry 1ueb (below, chain A only) is a more complex fold than in the previous question.  There are 4 b-sheets  
     
   Sheet 1 is strands 1,2,3,4  
   Sheet 2 is strands 9,8,5,6,7

Sheet 3 is strands 10,13,14  
Sheet 4 is strands 11,12  
  
Using the commands below, number each of the -strands in pdb entry 1ueb.

**PyMOL>**

#----------start copy-----  
reinitialize  
bg\_color white

fetch 1ueb

remove not chain A

remove not backbone  
remove resi 1-9

hide everything

show cartoon

label resi 14 and name O, "1"

label resi 15 and name CA, "1"  
label resi 19 and name CA, "2"

label resi 25 and name CA, "2"  
label resi 39 and name CA, "3"

label resi 52 and name CA, "4"

label resi 60 and name CA, "ignore this"

label resi 68 and name CA, "5"

label resi 69 and name CA, "5"  
label resi 72 and name CA, "5"  
label resi 82 and name CA, "6"

label resi 83 and name CA, "6"

label resi 92 and name CA, "7"  
label resi 112 and name CA, "8"

label resi 113 and name CA, "8"  
label resi 120 and name CA, "9"  
label resi 130 and name CA, "10"

label resi 150 and name CA, "11"

label resi 159 and name CA, "12"  
label resi 172 and name CA, "13"

label resi 181 and name CA, "14"  
label resi 10 and name N, "N-terminus"  
label resi 184 and name C, "C-terminus"  
set label\_size, 20  
zoom 1ueb

spectrum count, rainbow, 1ueb

create sheet\_1, ss S

disable sheet\_1

#----------end copy---------------

Insert an screen grab image of the ribbon diagram.

|  |
| --- |
| INSERT HERE |

Draw the topology diagram of this protein and insert it into this document.

|  |
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| INSERT HERE |