Version 1.3

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

1. If two α-helices twist around each other at an angle of about 20 degrees, their side chains can interlock (zipper) within the center of the superhelix, with a heptad repeat (…a-b-c-d-e-f-g-a-b-c-d-e-f-g-…). The chemical nature of the sidechains (hydrophobic versus hydrophilic) reflects the heptad repeat (a-b-c-d-e-f-g). Positions a and d are usually hydrophobic, while c and f are usually hydrophilic.

b) Examine the amino acid sidechains in the center of coiled coil of PDB entry 3K29 by copying and pasting the commands below into PyMol. Which amino acids are most common at positions a and d and which amino acids are most common at positions c and f? Hint: Display -> Sequence may be helpful. What type of molecular interactions stabilize the coiled-coil?

|  |
| --- |
| INSERT HERE |

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

reinitialize

bg\_color white

fetch 3K29

hide everything

show cartoon, 3K29  
remove resi 130-200  
remove resi 1-4  
create hydrophobes, resn ala+gly+val+ile+leu+phe+met

hide everything, hydrophobes  
show sticks, hydrophobes

disable hydrophobes

color yellow, name C\* and (hydrophobes)

color red, name O\* and (hydrophobes)

color blue, name N\* and (hydrophobes)  
create hydrophilics, resn arg+lys+his+glu+asp+asn+gln+thr+ser+cys

hide everything, hydrophilics  
show sticks, hydrophilics

disable hydrophilics

color wheat, name C\* and (hydrophilics)

color red, name O\* and (hydrophilics)

color blue, name N\* and (hydrophilics)

color cyan, 3K29  
label resi 6 and name CA, "a"

label resi 7 and name CA, "b"

label resi 8 and name CA, "c"

#------------------- strand 1

label resi 9 and name CA, "d"

label resi 10 and name CA, "e"

label resi 11 and name CA, "f"

label resi 12 and name CA, "g"

#

label resi 13 and name CA, "a"

color red, resi 13 and name CA

label resi 14 and name CA, "b"

label resi 15 and name CA, "c"

label resi 16 and name CA, "d"

label resi 17 and name CA, "e"

label resi 18 and name CA, "f"

label resi 19 and name CA, "g"

#

label resi 20 and name CA, "a"

color red, resi 20 and name CA

label resi 21 and name CA, "b"

label resi 22 and name CA, "c"

label resi 23 and name CA, "d"

label resi 24 and name CA, "e"

label resi 25 and name CA, "f"

label resi 26 and name CA, "g"

#

label resi 27 and name CA, "a"

color red, resi 27 and name CA

label resi 28 and name CA, "b"

label resi 29 and name CA, "c"

label resi 30 and name CA, "d"

label resi 31 and name CA, "e"

label resi 32 and name CA, "f"

label resi 33 and name CA, "g"

#

label resi 34 and name CA, "a"

color red, resi 34 and name CA

label resi 35 and name CA, "b"

label resi 36 and name CA, "c"

label resi 37 and name CA, "d"

label resi 38 and name CA, "e"

label resi 39 and name CA, "f"

label resi 40 and name CA, "g"

#

label resi 41 and name CA, "a"

color red, resi 41 and name CA

label resi 42 and name CA, "b"

label resi 43 and name CA, "c"

label resi 44 and name CA, "d"

label resi 45 and name CA, "e"

label resi 46 and name CA, "f"

label resi 47 and name CA, "g"

#

label resi 48 and name CA, "a"

color red, resi 48 and name CA

label resi 49 and name CA, "b"

label resi 50 and name CA, "c"

label resi 51 and name CA, "d"

label resi 52 and name CA, "e"

label resi 53 and name CA, "f"

label resi 54 and name CA, "g"

#------------------- strand 2

label resi 79 and name CA, "a"

color salmon, resi 79 and name CA

label resi 80 and name CA, "b"

label resi 81 and name CA, "c"

label resi 82 and name CA, "d"

label resi 83 and name CA, "e"

label resi 84 and name CA, "f"

label resi 85 and name CA, "g"

#

label resi 86 and name CA, "a"

color salmon, resi 86 and name CA

label resi 87 and name CA, "b"

label resi 88 and name CA, "c"

label resi 89 and name CA, "d"

label resi 90 and name CA, "e"

label resi 91 and name CA, "f"

label resi 92 and name CA, "g"

#

label resi 93 and name CA, "a"

color salmon, resi 93 and name CA

label resi 94 and name CA, "b"

label resi 95 and name CA, "c"

label resi 96 and name CA, "d"

label resi 97 and name CA, "e"

label resi 98 and name CA, "f"

label resi 99 and name CA, "g"

#

label resi 100 and name CA, "a"

color salmon, resi 100 and name CA

label resi 101 and name CA, "b"

label resi 102 and name CA, "c"

label resi 103 and name CA, "d"

label resi 104 and name CA, "e"

label resi 105 and name CA, "f"

label resi 106 and name CA, "g"

#

label resi 107 and name CA, "a"

color salmon, resi 107 and name CA

label resi 108 and name CA, "b"

label resi 109 and name CA, "c"

label resi 110 and name CA, "d"

label resi 111 and name CA, "e"

label resi 112 and name CA, "f"

label resi 113 and name CA, "g"

#

label resi 114 and name CA, "a"

color salmon, resi 114 and name CA

label resi 115 and name CA, "b"

label resi 116 and name CA, "c"

label resi 117 and name CA, "d"

label resi 118 and name CA, "e"

label resi 119 and name CA, "f"

label resi 120 and name CA, "g"

#

label resi 121 and name CA, "a"

color salmon, resi 121 and name CA

label resi 122 and name CA, "b"

label resi 123 and name CA, "c"

label resi 124 and name CA, "d"

label resi 125 and name CA, "e"

label resi 126 and name CA, "f"

label resi 127 and name CA, "g"

#

label resi 5 and name N, "N-terminus"

label resi 129 and name C, "C-terminus"

set label\_size, 20

set\_view (\

-0.190471858, 0.223753944, -0.955851853,\

-0.964548945, -0.223833114, 0.139809534,\

-0.182667524, 0.948592305, 0.258456707,\

0.000067033, -0.000321766, -167.571792603,\

13.686527252, 10.515285492, 51.354915619,\

111.474594116, 223.674896240, -20.000000000 )

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

c) You previously converted your name and city of birth to a 14 amino acid peptide sequence. Paste the sequence from the previous assignment (Assignment 9) here. Highlight the hydrophobic amino acids yellow.

|  |
| --- |
| INSERT HERE |

d) Retaining the blue highlight of the hydrophobic amino acids, mutate and/or rearrange your sequence to approximate a heptad repeat (i.e., make your sequence amphipathic), where positions a and d are hydrophobic, and c and f are hydrophilic. Omit proline and glycine (they are helix breakers). Insert your new (mutated) sequence here.

|  |
| --- |
| INSERT HERE |