Question 6 HW06 WorkSheet

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Q6 - How would you generalize the original code to work with any set of input protein structures?

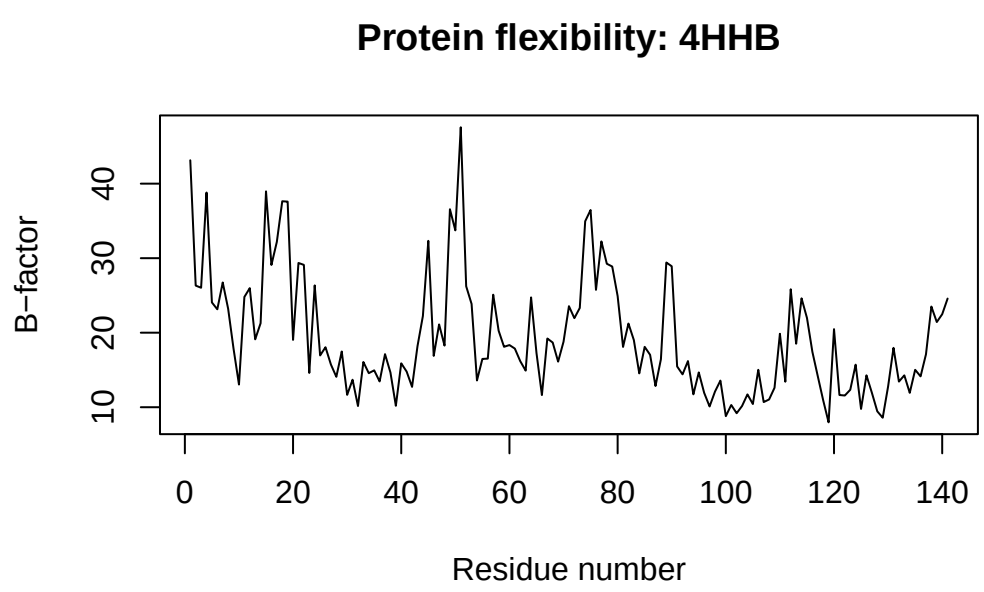
```
library(bio3d)

Protein_Interx <- function(pdb_id,chain = NULL, atom.type = "CA", plot = TRUE)

  {

  pdb <- read.pdb(pdb_id)

  Asel <- atom.select(pdb,
                      chain = chain,
                      elety = atom.type)

  # Annotation: Using the function above, our pdb_id input argument is pdb_id and our chain i


  bfactors <- pdb$atom$b[Asel$atom]
  residues <- pdb$atom$resno[Asel$atom]

  # Annotation: is a vector of B-factors for the chosen atoms. The vector is a numeric one ar
```

```
  result <- data.frame(
    residue = residues,
    bfactor = bfactors
  )

  # Annotation: Creates a data frame as an output. We create the two rows for the outputs of



  if (plot) {
    plot(result$residue,
         result$bfactor,
         type = "l",
         xlab = "Residue number",
         ylab = "B-factor",
         main = paste("Protein flexibility:", pdb_id))
  }



  return(result)
}


# Annotation: First, the 'if' creates a logical statement and serves to produce a line plot.
```

Use the code to inquire about protein structures.

```
Protein_Interx(pdb_id = "4HHB", chain = "A")
```

```
  Note: Accessing on-line PDB file
```



	residue	bfactor
1	1	43.14
2	2	26.32
3	3	26.03
4	4	38.81
5	5	24.06
6	6	23.14
7	7	26.74
8	8	23.21
9	9	17.84
10	10	13.04
11	11	24.80
12	12	25.98
13	13	19.11
14	14	21.27
15	15	38.97
16	16	29.09
17	17	32.19
18	18	37.64
19	19	37.59
20	20	19.03
21	21	29.36
22	22	29.10

23	23	14.60
24	24	26.35
25	25	16.95
26	26	18.05
27	27	15.73
28	28	14.08
29	29	17.48
30	30	11.66
31	31	13.69
32	32	10.16
33	33	16.07
34	34	14.57
35	35	14.95
36	36	13.46
37	37	17.12
38	38	14.66
39	39	10.19
40	40	15.89
41	41	14.78
42	42	12.73
43	43	18.18
44	44	22.24
45	45	32.33
46	46	16.89
47	47	21.11
48	48	18.27
49	49	36.57
50	50	33.73
51	51	47.57
52	52	26.23
53	53	23.86
54	54	13.59
55	55	16.48
56	56	16.52
57	57	25.10
58	58	20.27
59	59	18.11
60	60	18.34
61	61	17.87
62	62	16.18
63	63	14.91
64	64	24.74
65	65	17.27

66	66	11.63
67	67	19.22
68	68	18.68
69	69	16.12
70	70	18.79
71	71	23.56
72	72	21.95
73	73	23.32
74	74	34.95
75	75	36.46
76	76	25.75
77	77	32.25
78	78	29.25
79	79	28.88
80	80	24.91
81	81	18.09
82	82	21.23
83	83	19.01
84	84	14.54
85	85	18.10
86	86	17.03
87	87	12.85
88	88	16.45
89	89	29.42
90	90	28.92
91	91	15.47
92	92	14.41
93	93	16.19
94	94	11.73
95	95	14.67
96	96	11.93
97	97	10.10
98	98	12.10
99	99	13.57
100	100	8.80
101	101	10.30
102	102	9.19
103	103	10.16
104	104	11.72
105	105	10.43
106	106	15.02
107	107	10.69
108	108	11.04

```
109     109   12.61
110     110   19.86
111     111   13.42
112     112   25.83
113     113   18.52
114     114   24.61
115     115   21.98
116     116   17.43
117     117   14.17
118     118   10.93
119     119    7.97
120     120   20.48
121     121   11.64
122     122   11.57
123     123   12.34
124     124   15.71
125     125    9.77
126     126   14.28
127     127   11.94
128     128    9.45
129     129    8.59
130     130   12.80
131     131   17.97
132     132   13.44
133     133   14.28
134     134   11.93
135     135   15.02
136     136   14.14
137     137   17.11
138     138   23.51
139     139   21.43
140     140   22.48
141     141   24.58
```

```
# Annotations: Example uses the Protein Data Bank identifier  for human hemoglobin protein st
```