Homework Question 6

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Can you improve this analysis code?

library(bio3d) s1 <- read.pdb("4AKE") # kinase with drug s2 <- read.pdb("1AKE") # kinase no drug s3 <- read.pdb("1E4Y") # kinase with drug s1.chainA <- trim.pdb(s1, chain="A", elety="CA") s2.chainA <- trim.pdb(s2, chain="A", elety="CA") s3.chainA <- trim.pdb(s1, chain="A", elety="CA") s1.b <- s1.chainA$atom$b s2.b <- s2.chainA$atom$b s3.b <- s3.chainA$atom$b plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor") plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor") plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")

#make a function for this code x <- read.pdb("whatever") x.chainA <- trim.pdb(x, chain="A", elety="CA") x.b <- x.chainA$atom$b plot(x.b, sse=x.chainA, typ="l", ylab="Bfactor")

identify.chain <- function(x) { y<- trim.pdb(x, chain="A", elety="CA") y$atom$b plotb3(y$atom$b, sse=y, typ="l", ylab="Bfactor")}