Class 11

Byanca Lima Valenzuela (A16688058)

db<-read.csv("Data Export Summary.csv", row.names=1)  
head(db)

## X.ray NMR EM Multiple.methods Neutron Other Total  
## Protein (only) 142303 11804 5999 177 70 32 160385  
## Protein/Oligosaccharide 8414 31 979 5 0 0 9429  
## Protein/NA 7491 274 1986 3 0 0 9754  
## Nucleic acid (only) 2368 1372 60 8 2 1 3811  
## Other 149 31 3 0 0 0 183  
## Oligosaccharide (only) 11 6 0 1 0 4 22

Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy?

method.sums<-colSums(db)  
round((method.sums/method.sums["Total"])\*100,2)

## X.ray NMR EM Multiple.methods   
## 87.55 7.36 4.92 0.11   
## Neutron Other Total   
## 0.04 0.02 100.00

Q2: What proportion of structures in the PDB are protein?

round((db$Total/method.sums["Total"])\*100,2)

## [1] 87.36 5.14 5.31 2.08 0.10 0.01

Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB? 1828 Structures

## VMD Structure Visualization Image

Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure? Because they are so small

Q5: There is a conserved water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have (see note below)?



#Section 3 Introduction to Bio3D in R #Using Bio3D

library(bio3d)  
  
pdb<- read.pdb("1HSG")

## Note: Accessing on-line PDB file

pdb

##   
## Call: read.pdb(file = "1HSG")  
##   
## Total Models#: 1  
## Total Atoms#: 1686, XYZs#: 5058 Chains#: 2 (values: A B)  
##   
## Protein Atoms#: 1514 (residues/Calpha atoms#: 198)  
## Nucleic acid Atoms#: 0 (residues/phosphate atoms#: 0)  
##   
## Non-protein/nucleic Atoms#: 172 (residues: 128)  
## Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]  
##   
## Protein sequence:  
## PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD  
## QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE  
## ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP  
## VNIIGRNLLTQIGCTLNF  
##   
## + attr: atom, xyz, seqres, helix, sheet,  
## calpha, remark, call

Q7: How many amino acid residues are there in this pdb object? 198

Q8: Name one of the two non-protein residues? MK1

Q9: How many protein chains are in this structure? 2

pdbseq(pdb)

## 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20   
## "P" "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K"   
## 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40   
## "E" "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G"   
## 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60   
## "R" "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D"   
## 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80   
## "Q" "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T"   
## 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 1   
## "P" "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F" "P"   
## 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21   
## "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K" "E"   
## 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41   
## "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G" "R"   
## 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61   
## "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D" "Q"   
## 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81   
## "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T" "P"   
## 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99   
## "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F"

aa321(pdbseq(pdb))

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: W

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: A

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: A

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: M

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: S

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: W

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: M

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: F

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Y

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: C

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: H

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: A

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: N

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: N

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: C

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: N

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: F

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: W

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: A

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: A

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: M

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: S

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: W

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: M

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: F

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Y

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: D

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: E

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: C

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: H

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: K

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: A

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: P

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: V

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: N

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: R

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: N

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L  
  
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: Q

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: I

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: G

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: C

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: T

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: L

## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: N

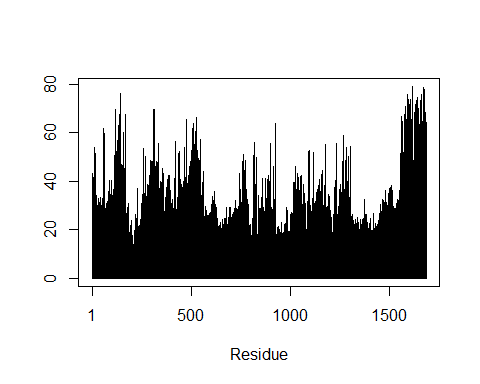
## Warning in FUN(X[[i]], ...): Unknown 3-letters code for aminoacid: F

## [1] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [19] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [37] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [55] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [73] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [91] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [109] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [127] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [145] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [163] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"  
## [181] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"

Plot of B-factor

plot.bio3d(pdb$atom$b, sse=pdb)

## Warning in plotb3(...): Length of input 'sse' does not equal the length of input  
## 'x'; Ignoring 'sse'



The ATOM Records

head(pdb$atom)

## type eleno elety alt resid chain resno insert x y z o b  
## 1 ATOM 1 N <NA> PRO A 1 <NA> 29.361 39.686 5.862 1 38.10  
## 2 ATOM 2 CA <NA> PRO A 1 <NA> 30.307 38.663 5.319 1 40.62  
## 3 ATOM 3 C <NA> PRO A 1 <NA> 29.760 38.071 4.022 1 42.64  
## 4 ATOM 4 O <NA> PRO A 1 <NA> 28.600 38.302 3.676 1 43.40  
## 5 ATOM 5 CB <NA> PRO A 1 <NA> 30.508 37.541 6.342 1 37.87  
## 6 ATOM 6 CG <NA> PRO A 1 <NA> 29.296 37.591 7.162 1 38.40  
## segid elesy charge  
## 1 <NA> N <NA>  
## 2 <NA> C <NA>  
## 3 <NA> C <NA>  
## 4 <NA> O <NA>  
## 5 <NA> C <NA>  
## 6 <NA> C <NA>