lab09

Zijing

```
data <- read.csv("Data Export Summary.csv")
row.names(data) <- data$Molecular.Type
data <- data[-1]
row <- nrow(data)
col <- ncol(data)
for(m in 1:row){
  for(j in 1:col){
    if (grepl(",", data[m,j]) == TRUE){
      bef <- sub(",.*", "", data[m,j])
      aft <- sub(".*,", "", data[m,j])
      num <- paste(bef,aft,sep="")
      data[m,j] <- num}
  }
}
```

Q1

```
x.ray <- 0
total <- 0
em <- 0
for (m in 1:row){
  x.ray <- x.ray + as.numeric(data[m,1])
  em <- em+as.numeric(data[m,3])
  total <- total + as.numeric(data[m,7])
}

perc_xm <- (x.ray+em)/total
perc_xm
```

```
[1] 0.9281395
```

92.8% percent of the structures in the PDB are solved by X.ray or EM.

Q2

```
protein <- 0
tot <- 0
for (m in 1:row){
  if (m<=3){
    protein <- protein+as.numeric(data[m,7])
  }
  tot <- tot+as.numeric(data[m,7])
}

perc_prot <- protein/tot
perc_prot
```

```
[1] 0.9784241
```

97.8% percentage of structures are protein.

Q3

There are 1264 HIV-1 protease structures.

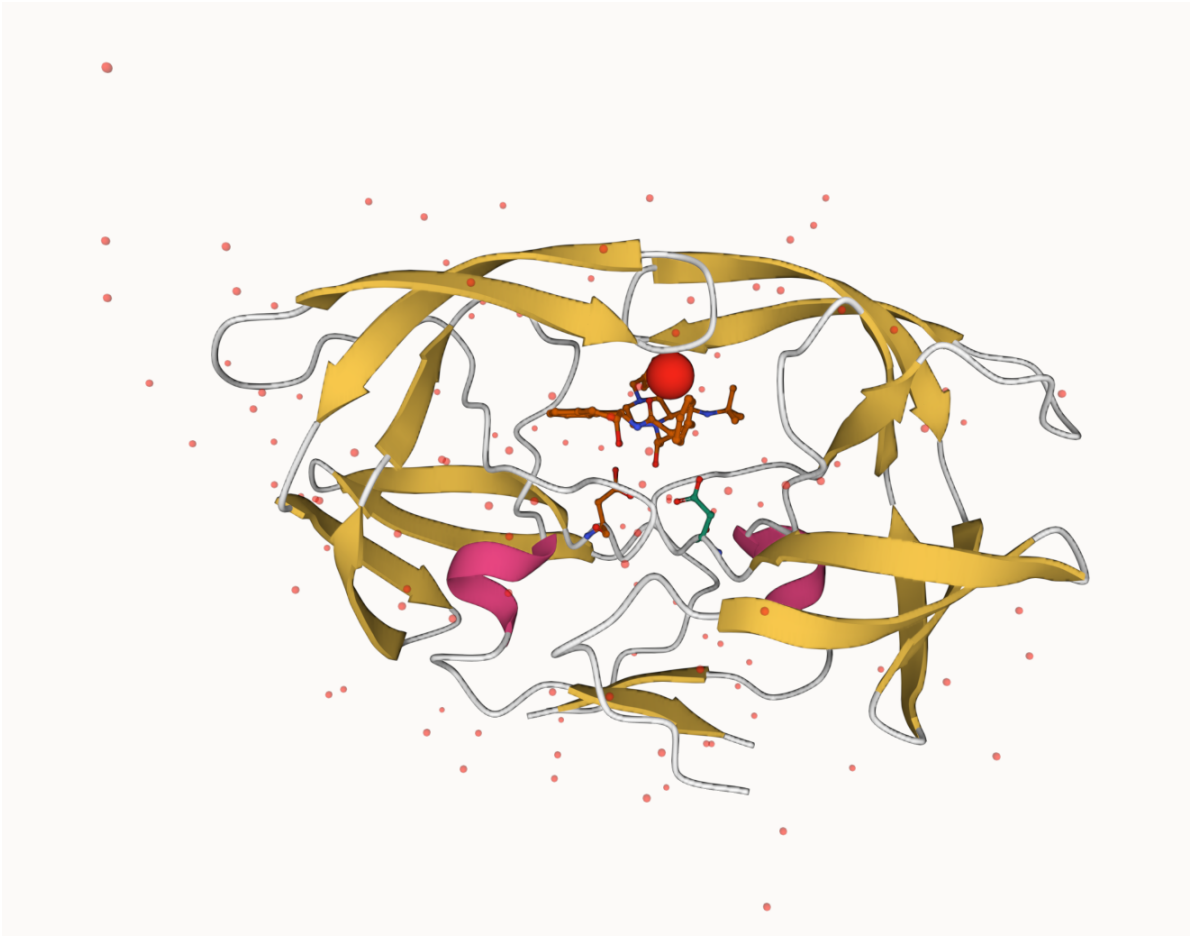
Q4

There is not enough resolution for the hydrogen to be shown.

Q5

The water molecule has residue number HOH 308.

Q6



```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.0.5
```

```
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

There are 198 residues in this pdb object.

Q8

Non-protein residue HOH (127)

Q9

There are two protein chains in this structure.

```
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>
```

```
adk <- read.pdb("6s36")
```

```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

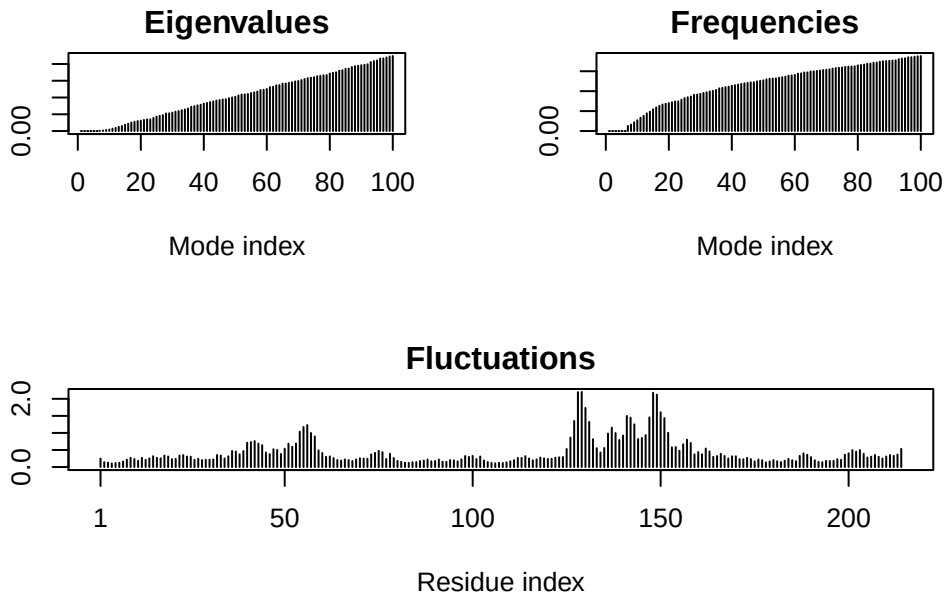
```
adk
```

```
 Call:  read.pdb(file = "6s36")

   Total Models#: 1
     Total Atoms#: 1898,  XYZs#: 5694  Chains#: 1  (values: A)

     Protein Atoms#: 1654  (residues/Calpha atoms#: 214)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 244  (residues: 244)
     Non-protein/nucleic resid values: [ CL (3), HOH (238), MG (2), NA (1) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```
m <- nma(adk)
```

```
Building Hessian...     Done in 0.025 seconds.
Diagonalizing Hessian...   Done in 0.341 seconds.
```

```
plot(m)
```




```
mktrj(m, file="adk_m7.pdb")
```

Q10.

Which of the packages above is found only on BioConductor and not CRAN? msa

Q11.

Which of the above packages is not found on BioConductor or CRAN?: bio3d-view

Q12.

True or False? Functions from the devtools package can be used to install packages from GitHub and BitBucket? TRUE

Comparative Analysis of all ADK structures

```
aa <- get.seq("1ake_a")
```

```
Warning in get.seq("1ake_a"): Removing existing file: seqs.fasta
```

```
Fetching... Please wait. Done.
```

```
aa
```

```
              1        .         .         .         .         .         60
pdb|1AKE|A    MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
              1        .         .         .         .         .         60

             61        .         .         .         .         .         120
pdb|1AKE|A    DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
             61        .         .         .         .         .         120

            121        .         .         .         .         .         180
pdb|1AKE|A    VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
            121        .         .         .         .         .         180

            181        .         .         .   214
pdb|1AKE|A    YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
            181        .         .         .   214

Call:
  read.fasta(file = outfile)

Class:
  fasta
```

```
Alignment dimensions:
  1 sequence rows; 214 position columns (214 non-gap, 0 gap)

+ attr: id, ali, call
```

Q13.

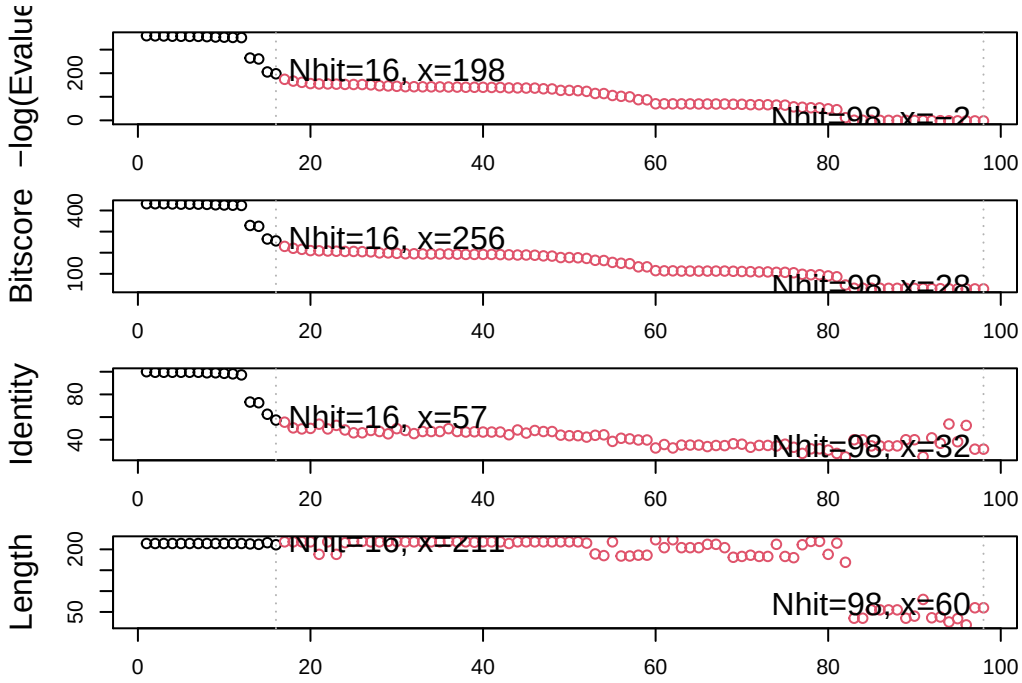
How many amino acids are in this sequence, i.e. how long is this sequence? 214

```
blast <- blast.pdb(aa)
```

```
Searching ... please wait (updates every 5 seconds) RID = NKEJX32K013
.
Reporting 98 hits
```

```
hits <- plot(blast)
```

```
 * Possible cutoff values:    197 -3
           Yielding Nhits:    16 98

 * Chosen cutoff value of:    197
           Yielding Nhits:    16
```




```
pdb.annotate(hits$pdb.id)
```

```
       structureId chainId macromoleculeType chainLength experimentalTechnique
1AKE_A        1AKE       A            Protein         214                 X-ray
4X8M_A        4X8M       A            Protein         214                 X-ray
6S36_A        6S36       A            Protein         214                 X-ray
6RZE_A        6RZE       A            Protein         214                 X-ray
4X8H_A        4X8H       A            Protein         214                 X-ray
3HPR_A        3HPR       A            Protein         214                 X-ray
1E4V_A        1E4V       A            Protein         214                 X-ray
5EJE_A        5EJE       A            Protein         214                 X-ray
1E4Y_A        1E4Y       A            Protein         214                 X-ray
3X2S_A        3X2S       A            Protein         214                 X-ray
6HAP_A        6HAP       A            Protein         214                 X-ray
6HAM_A        6HAM       A            Protein         214                 X-ray
4K46_A        4K46       A            Protein         214                 X-ray
4NP6_A        4NP6       A            Protein         217                 X-ray
3GMT_A        3GMT       A            Protein         230                 X-ray
4PZL_A        4PZL       A            Protein         242                 X-ray
       resolution       scopDomain                                      pfam
1AKE_A      2.000 Adenylate kinase Adenylate kinase, active site lid (ADK_lid)
```

```
4X8M_A      2.600             <NA> Adenylate kinase, active site lid (ADK_lid)
6S36_A      1.600             <NA> Adenylate kinase, active site lid (ADK_lid)
6RZE_A      1.690             <NA> Adenylate kinase, active site lid (ADK_lid)
4X8H_A      2.500             <NA> Adenylate kinase, active site lid (ADK_lid)
3HPR_A      2.000             <NA> Adenylate kinase, active site lid (ADK_lid)
1E4V_A      1.850 Adenylate kinase Adenylate kinase, active site lid (ADK_lid)
5EJE_A      1.900             <NA> Adenylate kinase, active site lid (ADK_lid)
1E4Y_A      1.850 Adenylate kinase Adenylate kinase, active site lid (ADK_lid)
3X2S_A      2.800             <NA> Adenylate kinase, active site lid (ADK_lid)
6HAP_A      2.700             <NA> Adenylate kinase, active site lid (ADK_lid)
6HAM_A      2.550             <NA> Adenylate kinase, active site lid (ADK_lid)
4K46_A      2.010             <NA> Adenylate kinase, active site lid (ADK_lid)
4NP6_A      2.004             <NA> Adenylate kinase, active site lid (ADK_lid)
3GMT_A      2.100             <NA> Adenylate kinase, active site lid (ADK_lid)
4PZL_A      2.100             <NA> Adenylate kinase, active site lid (ADK_lid)
               ligandId
1AKE_A             AP5
4X8M_A            <NA>
6S36_A CL (3),NA,MG (2)
6RZE_A    NA (3),CL (2)
4X8H_A            <NA>
3HPR_A             AP5
1E4V_A             AP5
5EJE_A          AP5,CO
1E4Y_A             AP5
3X2S_A   JPY (2),AP5,MG
6HAP_A             AP5
6HAM_A             AP5
4K46_A      ADP,AMP,PO4
4NP6_A            <NA>
3GMT_A         SO4 (2)
4PZL_A       CA,FMT,GOL
                                                                        ligandName
1AKE_A                                                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
4X8M_A                                                                         <NA>
6S36_A                                  CHLORIDE ION (3),SODIUM ION,MAGNESIUM ION (2)
6RZE_A                                                  SODIUM ION (3),CHLORIDE ION (2)
4X8H_A                                                                         <NA>
3HPR_A                                                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
1E4V_A                                                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
5EJE_A                                BIS(ADENOSINE)-5'-PENTAPHOSPHATE,COBALT (II) ION
1E4Y_A                                                 BIS(ADENOSINE)-5'-PENTAPHOSPHATE
3X2S_A N-(pyren-1-ylmethyl)acetamide (2),BIS(ADENOSINE)-5'-PENTAPHOSPHATE,MAGNESIUM ION
```

```
6HAP_A                                                BIS(ADENOSINE)-5'-PENTAPHOSPHATE
6HAM_A                                                BIS(ADENOSINE)-5'-PENTAPHOSPHATE
4K46_A                  ADENOSINE-5'-DIPHOSPHATE,ADENOSINE MONOPHOSPHATE,PHOSPHATE ION
4NP6_A                                                                              <NA>
3GMT_A                                                                   SULFATE ION (2)
4PZL_A                                              CALCIUM ION,FORMIC ACID,GLYCEROL
                                                 source
1AKE_A                                Escherichia coli
4X8M_A                                Escherichia coli
6S36_A                                Escherichia coli
6RZE_A                                Escherichia coli
4X8H_A                                Escherichia coli
3HPR_A                              Escherichia coli K-12
1E4V_A                                Escherichia coli
5EJE_A            Escherichia coli O139:H28 str. E24377A
1E4Y_A                                Escherichia coli
3X2S_A          Escherichia coli str. K-12 substr. MDS42
6HAP_A            Escherichia coli O139:H28 str. E24377A
6HAM_A                              Escherichia coli K-12
4K46_A                           Photobacterium profundum
4NP6_A       Vibrio cholerae O1 biovar El Tor str. N16961
3GMT_A                    Burkholderia pseudomallei 1710b
4PZL_A Francisella tularensis subsp. tularensis SCHU S4

1AKE_A STRUCTURE OF THE COMPLEX BETWEEN ADENYLATE KINASE FROM ESCHERICHIA COLI AND THE INHIBI
4X8M_A
6S36_A
6RZE_A
4X8H_A
3HPR_A
1E4V_A
5EJE_A                                                                              Cryst
1E4Y_A
3X2S_A
6HAP_A
6HAM_A
4K46_A
4NP6_A
3GMT_A
4PZL_A                                                                  The cryst
                                                    citation rObserved   rFree
1AKE_A                 Muller, C.W., et al. J Mol Biol (1992)   0.19600      NA
4X8M_A                Kovermann, M., et al. Nat Commun (2015)   0.24910 0.30890
```

```
6S36_A                  Rogne, P., et al. Biochemistry (2019)   0.16320 0.23560
6RZE_A                  Rogne, P., et al. Biochemistry (2019)   0.18650 0.23500
4X8H_A                Kovermann, M., et al. Nat Commun (2015)   0.19610 0.28950
3HPR_A  Schrank, T.P., et al. Proc Natl Acad Sci U S A (2009)   0.21000 0.24320
1E4V_A                   Muller, C.W., et al. Proteins (1993)   0.19600      NA
5EJE_A  Kovermann, M., et al. Proc Natl Acad Sci U S A (2017)   0.18890 0.23580
1E4Y_A                   Muller, C.W., et al. Proteins (1993)   0.17800      NA
3X2S_A                Fujii, A., et al. Bioconjug Chem (2015)   0.20700 0.25600
6HAP_A               Kantaev, R., et al. J Phys Chem B (2018)   0.22630 0.27760
6HAM_A               Kantaev, R., et al. J Phys Chem B (2018)   0.20511 0.24325
4K46_A                    Cho, Y.-J., et al. To be published    0.17000 0.22290
4NP6_A                       Kim, Y., et al. To be published    0.18800 0.22200
3GMT_A Buchko, G.W., et al. Biochem Biophys Res Commun (2010)   0.23800 0.29500
4PZL_A                       Tan, K., et al. To be published    0.19360 0.23680
         rWork spaceGroup
1AKE_A 0.19600  P 21 2 21
4X8M_A 0.24630    C 1 2 1
6S36_A 0.15940    C 1 2 1
6RZE_A 0.18190    C 1 2 1
4X8H_A 0.19140    C 1 2 1
3HPR_A 0.20620  P 21 21 2
1E4V_A 0.19600  P 21 2 21
5EJE_A 0.18630  P 21 2 21
1E4Y_A 0.17800   P 1 21 1
3X2S_A 0.20700 P 21 21 21
6HAP_A 0.22370    I 2 2 2
6HAM_A 0.20311       P 43
4K46_A 0.16730 P 21 21 21
4NP6_A 0.18600       P 43
3GMT_A 0.23500   P 1 21 1
4PZL_A 0.19130       P 32
```

```
files <- get.pdb(hits$pdb.id,path="pdbs",split=TRUE, gzip=TRUE)
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
1AKE.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
4X8M.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
6S36.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
6RZE.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
4X8H.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
3HPR.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
1E4V.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
5EJE.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
1E4Y.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
3X2S.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
6HAP.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
6HAM.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
4K46.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
4NP6.pdb.gz exists. Skipping download

Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
3GMT.pdb.gz exists. Skipping download
```

```
Warning in get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE): pdbs/
4PZL.pdb.gz exists. Skipping download


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```

PCA

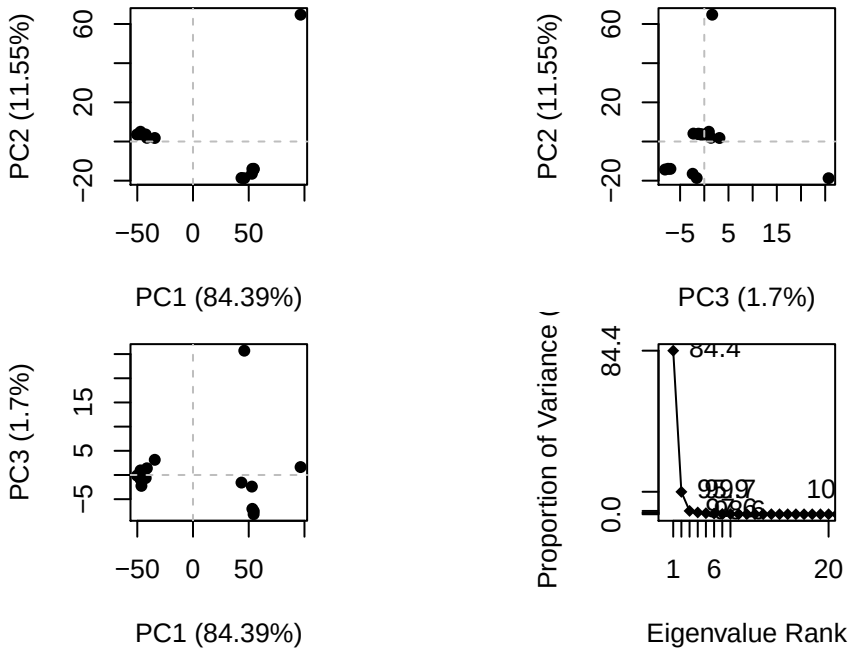
```
pdbs <- pdbaln(files, fit = TRUE, exefile="msa")
```

```
Reading PDB files:
pdbs/split_chain/1AKE_A.pdb
pdbs/split_chain/4X8M_A.pdb
pdbs/split_chain/6S36_A.pdb
pdbs/split_chain/6RZE_A.pdb
pdbs/split_chain/4X8H_A.pdb
pdbs/split_chain/3HPR_A.pdb
pdbs/split_chain/1E4V_A.pdb
pdbs/split_chain/5EJE_A.pdb
pdbs/split_chain/1E4Y_A.pdb
pdbs/split_chain/3X2S_A.pdb
pdbs/split_chain/6HAP_A.pdb
pdbs/split_chain/6HAM_A.pdb
pdbs/split_chain/4K46_A.pdb
pdbs/split_chain/4NP6_A.pdb
pdbs/split_chain/3GMT_A.pdb
pdbs/split_chain/4PZL_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
..   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
..   PDB has ALT records, taking A only, rm.alt=TRUE
..   PDB has ALT records, taking A only, rm.alt=TRUE
....   PDB has ALT records, taking A only, rm.alt=TRUE
.   PDB has ALT records, taking A only, rm.alt=TRUE
....

Extracting sequences

pdb/seq: 1   name: pdbs/split_chain/1AKE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 2   name: pdbs/split_chain/4X8M_A.pdb
pdb/seq: 3   name: pdbs/split_chain/6S36_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 4   name: pdbs/split_chain/6RZE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 5   name: pdbs/split_chain/4X8H_A.pdb
pdb/seq: 6   name: pdbs/split_chain/3HPR_A.pdb
```

```
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 8   name: pdbs/split_chain/5EJE_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 9   name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 10   name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 11   name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 12   name: pdbs/split_chain/6HAM_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 13   name: pdbs/split_chain/4K46_A.pdb
   PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 14   name: pdbs/split_chain/4NP6_A.pdb
pdb/seq: 15   name: pdbs/split_chain/3GMT_A.pdb
pdb/seq: 16   name: pdbs/split_chain/4PZL_A.pdb
```

```
pc.xray <- pca(pdbs)
```

```
plot(pc.xray)
```




```
mktrj(pc.xray, pc=1, file="pc_1.pdb")
```