

comparative structure analysis

Comparative structure analysis

here we run through a complete “pipeline” of structure analysis that begins with a single sequence identifier and ends in a PCA analysis.

```
library(bio3d)
```

step 1. retrieve a sequence for the protein we are interested in . we will take ADK “1ake_A”

```
id <- "1ake_A"  
aa <- get.seq(id)
```

Warning in get.seq(id): Removing existing file: seqs.fasta

Fetching... Please wait. Done.

```
aa
```

```
      1      .      .      .      .      .      60  
pdb|1AKE|A MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAAVKSGSELGKQAKDIMDAGKLV  
      1      .      .      .      .      .      60  
  
      61      .      .      .      .      .      120  
pdb|1AKE|A DELVIALVKERIAQEDCRNGFLLDGFPRTPQADAMKEAGINVDYVLEFDVPDELIVDRI  
      61      .      .      .      .      .      120  
  
      121      .      .      .      .      .      180
```

```

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

              181          .          .          .          214
pdb|1AKE|A    YYSKEAEAGNTKYAKVDGTPVAEVRADLEKILG
              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
```

step 2.

run a BLAST search of the pdb for all the related sequences to our input aa

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

```
Searching ... please wait (updates every 5 seconds) RID = X2ZK4N4B013
```

```
..
```

```
Reporting 87 hits
```

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

```

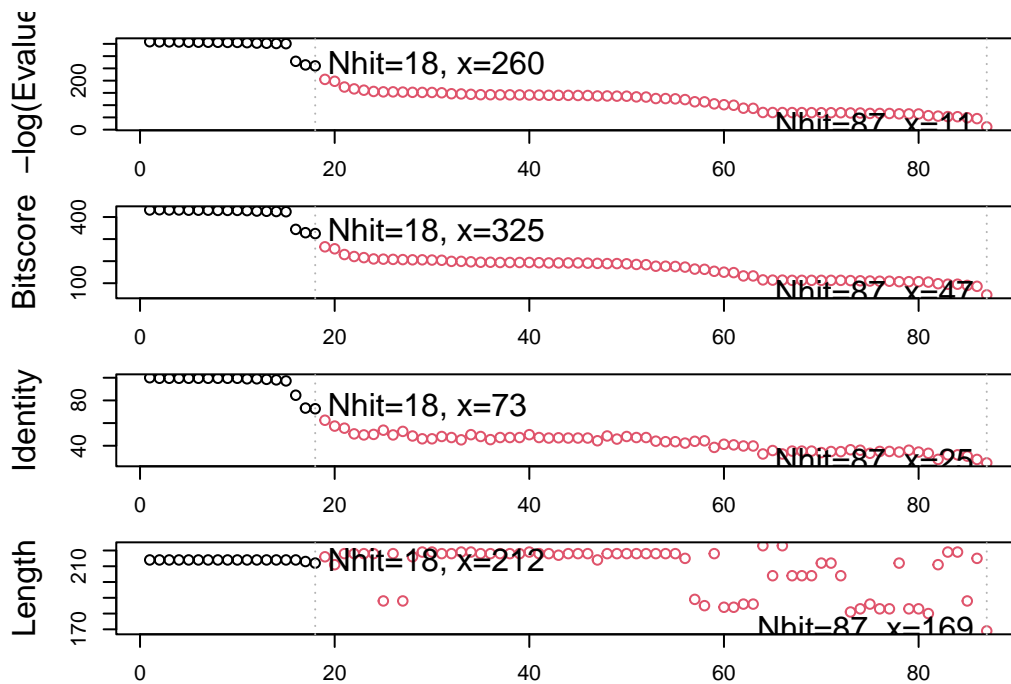
* Possible cutoff values:    260 11
    Yielding Nhits:         18 87

```

```

* Chosen cutoff value of:    260
    Yielding Nhits:          18

```



step3. download structure

these are top hits ie all structures in the pdb data related to our input sequence

```
hits$ pdb.id
```

```
[1] "1AKE_A" "8BQF_A" "4X8M_A" "6S36_A" "8Q2B_A" "8RJ9_A" "6RZE_A" "4X8H_A"
[9] "3HPR_A" "1E4V_A" "5EJE_A" "1E4Y_A" "3X2S_A" "6HAP_A" "6HAM_A" "8PVW_A"
[17] "4K46_A" "4NP6_A"
```

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

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

```
Warning in get.pdb(hits$ pdb.id, path = "pdds", split = TRUE, gzip = TRUE):
pdds/8BQF.pdb exists. Skipping download
```

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

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

Warning in get.pdb(hits\$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8Q2B.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8RJ9.pdb exists. Skipping download

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

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

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

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

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

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

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

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

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

Warning in get.pdb(hits\$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE):
pdbs/8PVW.pdb exists. Skipping download

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

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

	0%
====	6%
=====	11%
=====	17%
=====	22%
=====	28%
=====	33%
=====	39%
=====	44%
=====	50%
=====	56%
=====	61%
=====	67%
=====	72%
=====	78%
=====	83%
=====	89%

```
|=====| 94%  
|  
|=====| 100%
```

setp 4. align the superpose

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

Reading PDB files:

```
pdbbs/split_chain/1AKE_A.pdb  
pdbbs/split_chain/8BQF_A.pdb  
pdbbs/split_chain/4X8M_A.pdb  
pdbbs/split_chain/6S36_A.pdb  
pdbbs/split_chain/8Q2B_A.pdb  
pdbbs/split_chain/8RJ9_A.pdb  
pdbbs/split_chain/6RZE_A.pdb  
pdbbs/split_chain/4X8H_A.pdb  
pdbbs/split_chain/3HPR_A.pdb  
pdbbs/split_chain/1E4V_A.pdb  
pdbbs/split_chain/5EJE_A.pdb  
pdbbs/split_chain/1E4Y_A.pdb  
pdbbs/split_chain/3X2S_A.pdb  
pdbbs/split_chain/6HAP_A.pdb  
pdbbs/split_chain/6HAM_A.pdb  
pdbbs/split_chain/8PVW_A.pdb  
pdbbs/split_chain/4K46_A.pdb  
pdbbs/split_chain/4NP6_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  
..  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/8BQF_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 3   name: pdbs/split_chain/4X8M_A.pdb
pdb/seq: 4   name: pdbs/split_chain/6S36_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 5   name: pdbs/split_chain/8Q2B_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 6   name: pdbs/split_chain/8RJ9_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbs/split_chain/6RZE_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 8   name: pdbs/split_chain/4X8H_A.pdb
pdb/seq: 9   name: pdbs/split_chain/3HPR_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10  name: pdbs/split_chain/1E4V_A.pdb
pdb/seq: 11  name: pdbs/split_chain/5EJE_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12  name: pdbs/split_chain/1E4Y_A.pdb
pdb/seq: 13  name: pdbs/split_chain/3X2S_A.pdb
pdb/seq: 14  name: pdbs/split_chain/6HAP_A.pdb
pdb/seq: 15  name: pdbs/split_chain/6HAM_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 16  name: pdbs/split_chain/8PVW_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 17  name: pdbs/split_chain/4K46_A.pdb
            PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 18  name: pdbs/split_chain/4NP6_A.pdb
```

pdbs

	1	.	.	.	40
[Truncated_Name:1] 1AKE_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				
[Truncated_Name:2] 8BQF_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				
[Truncated_Name:3] 4X8M_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				
[Truncated_Name:4] 6S36_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				
[Truncated_Name:5] 8Q2B_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				
[Truncated_Name:6] 8RJ9_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				
[Truncated_Name:7] 6RZE_A.pdb	--MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLAA				

```
[Truncated_Name:8]4X8H_A.pdb      --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:9]3HPR_A.pdb      --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:10]1E4V_A.pdb     --MRIILLGAPVAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:11]5EJE_A.pdb     --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:12]1E4Y_A.pdb     --MRIILLGALVAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:13]3X2S_A.pdb     --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:14]6HAP_A.pdb     --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:15]6HAM_A.pdb     --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:16]8PVW_A.pdb     --MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGMDMLRAA
[Truncated_Name:17]4K46_A.pdb     --MRIILLGAPGAGKGTQAQFIMAKFGIPQISTGMDMLRAA
[Truncated_Name:18]4NP6_A.pdb     NAMRIILLGAPGAGKGTQAQFIMEKFGIPQISTGMDMLRAA

*****      *****      *~*****
1              .              .              .              40

41              .              .              .              80
[Truncated_Name:1]1AKE_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:2]8BQF_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQE---
[Truncated_Name:3]4X8M_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:4]6S36_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:5]8Q2B_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:6]8RJ9_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:7]6RZE_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:8]4X8H_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:9]3HPR_A.pdb      VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:10]1E4V_A.pdb     VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:11]5EJE_A.pdb     VKSGSELGKQAKDIMDACKLVTDLVIALVKERIAQEDCR
[Truncated_Name:12]1E4Y_A.pdb     VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:13]3X2S_A.pdb     VKSGSELGKQAKDIMDCGKLVTDLVIALVKERIAQEDSR
[Truncated_Name:14]6HAP_A.pdb     VKSGSELGKQAKDIMDAGKLVTDLVIALVRERICQEDSR
[Truncated_Name:15]6HAM_A.pdb     IKSGSELGKQAKDIMDAGKLVTDDEIIIALVKERICQEDSR
[Truncated_Name:16]8PVW_A.pdb     VKSGSELGKQAKDIMDAGKLVTDLVIALVKERIAQEDCR
[Truncated_Name:17]4K46_A.pdb     IKAGTELGKQAKSVIDAGQLVSDDIILGLVKERIAQDDCA
[Truncated_Name:18]4NP6_A.pdb     IKAGTELGKQAKAVIDAGQLVSDDIILGLIKERIAQADCE
~* *~*****  ~*~*  **~*~~~~~*~^*** *
41              .              .              .              80

81              .              .              .              12
[Truncated_Name:1]1AKE_A.pdb      NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:2]8BQF_A.pdb      -GFLLDGFPRTIPQADAMKEAGINVDYVIEFDVPDELIVD
[Truncated_Name:3]4X8M_A.pdb      NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:4]6S36_A.pdb      NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:5]8Q2B_A.pdb      NGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:6]8RJ9_A.pdb      NGFLLAGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVD
```


[Truncated_Name:7] 6RZE_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:8] 4X8H_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:9] 3HPR_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:10] 1E4V_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:11] 5EJE_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:12] 1E4Y_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:13] 3X2S_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:14] 6HAP_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:15] 6HAM_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:16] 8PVW_A.pdb	NGFLLDGFPR TIPQADAMKEAGINVDYVLEFDVPDELIVD
[Truncated_Name:17] 4K46_A.pdb	KGFLLDGFPR TIPQADGLKEVGVVVDYVIEFDVADSVIVE
[Truncated_Name:18] 4NP6_A.pdb	KGFLLDGFPR TIPQADGLKEMGINVDYVIEFDVADDVIVE
	**** *****^~** *^ ***** * ^**^
	81 . . . 120
	121 . . . 160
[Truncated_Name:1] 1AKE_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:2] 8BQF_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:3] 4X8M_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:4] 6S36_A.pdb	KIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:5] 8Q2B_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKA
[Truncated_Name:6] 8RJ9_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:7] 6RZE_A.pdb	AIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:8] 4X8H_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:9] 3HPR_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDGTGEELTTRKD
[Truncated_Name:10] 1E4V_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:11] 5EJE_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:12] 1E4Y_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:13] 3X2S_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:14] 6HAP_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:15] 6HAM_A.pdb	RIVGRRVHAPSGRVYHV KFNPPKVEGKDDVTGEELTTRKD
[Truncated_Name:16] 8PVW_A.pdb	RILKRGE--TSGRV-----D
[Truncated_Name:17] 4K46_A.pdb	RMAGRRAHLASGR TYHNVNPPKVEGKDDVTGEDLVIRE
[Truncated_Name:18] 4NP6_A.pdb	RMAGRRAHLPSGR TYHVVNPPKVEGKDDVTGEDLVIRE
	^ * ***
	121 . . . 160
	161 . . . 200
[Truncated_Name:1] 1AKE_A.pdb	DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:2] 8BQF_A.pdb	DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:3] 4X8M_A.pdb	DQEETVRKRLVEWHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:4] 6S36_A.pdb	DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:5] 8Q2B_A.pdb	DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG

```

[Truncated_Name:6] 8RJ9_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:7] 6RZE_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:8] 4X8H_A.pdb    DQEETVRKRLVEYHQMTAALIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:9] 3HPR_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:10] 1E4V_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:11] 5EJE_A.pdb    DQEECVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:12] 1E4Y_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:13] 3X2S_A.pdb    DQEETVRKRLCEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:14] 6HAP_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:15] 6HAM_A.pdb    DQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:16] 8PVW_A.pdb    DNEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDG
[Truncated_Name:17] 4K46_A.pdb    DKEETVLARLGVYHNQTAPLIAYYGKEAEAGNTQYLKFDG
[Truncated_Name:18] 4NP6_A.pdb    DKEETVRARLNVYHTQTAPLIEYYGKEAAAGKTQYLKFDG
* * * * * ^ * * * * * * * * * *
161 . . . 200

```

```

201 . 216
[Truncated_Name:1] 1AKE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:2] 8BQF_A.pdb    TKPVAEVRADLEKIL-
[Truncated_Name:3] 4X8M_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:4] 6S36_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:5] 8Q2B_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:6] 8RJ9_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:7] 6RZE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:8] 4X8H_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:9] 3HPR_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:10] 1E4V_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:11] 5EJE_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:12] 1E4Y_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:13] 3X2S_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:14] 6HAP_A.pdb    TKPVCEVRADLEKILG
[Truncated_Name:15] 6HAM_A.pdb    TKPVCEVRADLEKILG
[Truncated_Name:16] 8PVW_A.pdb    TKPVAEVRADLEKILG
[Truncated_Name:17] 4K46_A.pdb    TKAVAEVSAELEKALA
[Truncated_Name:18] 4NP6_A.pdb    TKQVSEVSADIAKALA
* * * * * ^ ^ * *
201 . 216

```

Call:

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

Class:

```
pdbs, fasta
```

Alignment dimensions:

18 sequence rows; 216 position columns (182 non-gap, 34 gap)

+ attr: xyz, resno, b, chain, id, ali, resid, sse, call

step 5. PCA

lets use our old friend to make sense of

```
pc <- pca(pdbbs)
plot(pc)
```

