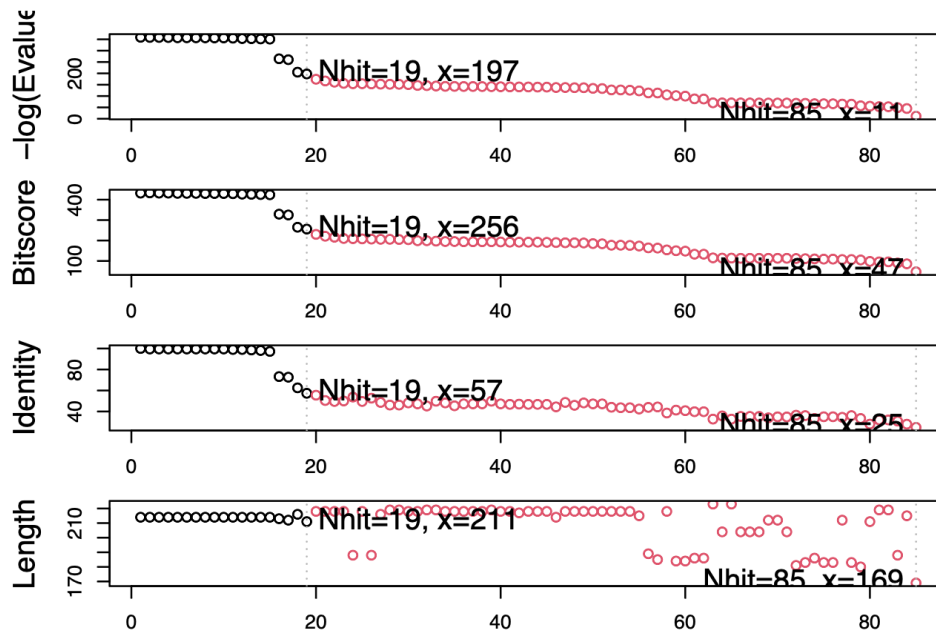


* Chosen cutoff value of: 197
Yielding Nhits: 19



What is inside "hits"

```
attributes(hits)
```

```
$names
[1] "hits" "pdb.id" "acc" "inds"
```

```
$class
[1] "blast"
```

What are the top hits from our blast results

```
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" "4K46_A"
[17] "4NP6_A" "3GMT_A" "4PZL_A"
```

Download PDB files

```
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/8BQF.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/8Q2B.pdb.gz exists. Skipping download
```

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

		0%
====		5%
=====		11%
=====		16%
=====		21%
=====		26%
=====		32%
=====		37%

```

|
|=====| 42%

```

5

```

|
|=====| 47%
|
|=====| 53%
|
|=====| 58%
|
|=====| 63%
|
|=====| 68%
|
|=====| 74%
|
|=====| 79%
|
|=====| 84%
|
|=====| 89%
|
|=====| 95%
|
|=====| 100%

```

I have now found and downloaded all ADK structures in the PDB database. Viewing them is difficult and needs to be aligned and then superimposed. This is evident when we use MolViewer to load up all the structures mentioned before.

Install BiocManager package from CRAN. use `BiocManager::install()` to install any package from bioconductor.

Align related PDBs

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

Reading PDB files:

```
pdb<- readPDB("pdbs/split_chain/1AKE_A.pdb")
```

pdbs/split_chain/8BQF_A.pdb
 pdbs/split_chain/4X8M_A.pdb
 pdbs/split_chain/6S36_A.pdb
 pdbs/split_chain/8Q2B_A.pdb
 pdbs/split_chain/8RJ9_A.pdb
 pdbs/split_chain/6RZE_A.pdb
 pdbs/split_chain/4X8H_A.pdb

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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
 .. 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: pdbc/split_chain/8Q2B_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 6   name: pdbc/split_chain/8RJ9_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7   name: pdbc/split_chain/6RZE_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 8   name: pdbc/split_chain/4X8H_A.pdb
pdb/seq: 9   name: pdbc/split_chain/3HPR_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10  name: pdbc/split_chain/1E4V_A.pdb
pdb/seq: 11  name: pdbc/split_chain/5EJE_A.pdb

```

7

```

PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12  name: pdbc/split_chain/1E4Y_A.pdb
pdb/seq: 13  name: pdbc/split_chain/3X2S_A.pdb
pdb/seq: 14  name: pdbc/split_chain/6HAP_A.pdb
pdb/seq: 15  name: pdbc/split_chain/6HAM_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 16  name: pdbc/split_chain/4K46_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 17  name: pdbc/split_chain/4NP6_A.pdb
pdb/seq: 18  name: pdbc/split_chain/3GMT_A.pdb
pdb/seq: 19  name: pdbc/split_chain/4PZL_A.pdb

```

pdbc

	1	.	.	.	40
[Truncated_Name:1]1AKE_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:2]8BQF_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:3]4X8M_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:4]6S36_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:5]8Q2B_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:6]8RJ9_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:7]6RZE_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:8]4X8H_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:9]3HPR_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:10]1E4V_A.pdb	-----	MRI	ILL	GAP	VAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:11]5EJE_A.pdb	-----	MRI	ILL	GAP	GAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:12]1E4Y_A.pdb	-----	MRI	ILL	GAL	VAGKGTQAQFIMEKYGIPQIS

```

[Truncated_Name:13]3X2S_A.pdb -----MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:14]6HAP_A.pdb -----MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:15]6HAM_A.pdb -----MRIILLGAPGAGKGTQAQFIMEKYGIPQIS
[Truncated_Name:16]4K46_A.pdb -----MRIILLGAPGAGKGTQAQFIMAKFGIPQIS
[Truncated_Name:17]4NP6_A.pdb -----NAMRIILLGAPGAGKGTQAQFIMEKFGIPQIS
[Truncated_Name:18]3GMT_A.pdb -----MRLILLGAPGAGKGTQANFIKEKFGIPQIS
[Truncated_Name:19]4PZL_A.pdb -----TENLYFQSNAMRIILLGAPGAGKGTQAKIIEQKYNIAHIS
                                **^*****  *  *^ *  **
1                                .  .  .  40

41                                .  .  .  80
[Truncated_Name:1]1AKE_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:2]8BQF_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:3]4X8M_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:4]6S36_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE

```

8

```

[Truncated_Name:5]8Q2B_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:6]8RJ9_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:7]6RZE_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:8]4X8H_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:9]3HPR_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:10]1E4V_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:11]5EJE_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDACKLVDELVIALVKE
[Truncated_Name:12]1E4Y_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVKE
[Truncated_Name:13]3X2S_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDCGKLVDELVIALVKE
[Truncated_Name:14]6HAP_A.pdb  TGDMLRAAVKSGSELGKQAKDIMDAGKLVDELVIALVRE
[Truncated_Name:15]6HAM_A.pdb  TGDMLRAAIIKSGSELGKQAKDIMDAGKLVDEIIIALVKE
[Truncated_Name:16]4K46_A.pdb  TGDMLRAAIIKAGTELGKQAKSVIDAGQLVSDDIILGLVKE
[Truncated_Name:17]4NP6_A.pdb  TGDMLRAAIIKAGTELGKQAKAVIDAGQLVSDDIILGLIKE
[Truncated_Name:18]3GMT_A.pdb  TGDMLRAAVKAGTPLGVEAKTYMDEGKLVPSLIIGLVKE
[Truncated_Name:19]4PZL_A.pdb  TGDMIRETIKSGSALGQELKKVLDAGELVSDEFIIVKVD
                                ****^*  ^*  *^ **  *  ^*  **  *  ^^  ^^^^
41                                .  .  .  80

81                                .  .  .  120
[Truncated_Name:1]1AKE_A.pdb  RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:2]8BQF_A.pdb  RIAQE----GFLLDGFPRTIPQADAMKEAGINVDYVIEFD
[Truncated_Name:3]4X8M_A.pdb  RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:4]6S36_A.pdb  RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFD
[Truncated_Name:5]8Q2B_A.pdb  RIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVIEFD

```

```

[Truncated_Name:6]8RJ9_A.pdb
[Truncated_Name:7]6RZE_A.pdb
[Truncated_Name:8]4X8H_A.pdb
[Truncated_Name:9]3HPR_A.pdb
[Truncated_Name:10]1E4V_A.pdb
[Truncated_Name:11]5EJE_A.pdb
[Truncated_Name:12]1E4Y_A.pdb
[Truncated_Name:13]3X2S_A.pdb
[Truncated_Name:14]6HAP_A.pdb
[Truncated_Name:15]6HAM_A.pdb
[Truncated_Name:16]4K46_A.pdb
[Truncated_Name:17]4NP6_A.pdb
[Truncated_Name:18]3GMT_A.pdb
[Truncated_Name:19]4PZL_A.pdb

      RIAQEDCRNGFLLAGFPRTIPQADAMKEAGINVDYVLEFD
      RIAQEDCRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQEDCRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQEDCRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQEDCRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQEDCRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQEDCRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQEDSRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RICQEDSRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RICQEDSRNGFLLDGFPRITIPQADAMKEAGINVDYVLEFD
      RIAQDDCAKGFLDGFPRITIPQADGLKEVGVDYVIEFD
      RIAQADCEKGFLDGFPRITIPQADGLKEMGINVDYVIEFD
      RLKEADCANGYLFDFPRITIPQADAMKEAGVAIDYVLEID
      RISKNDCCNGFLLDGVPRITIPQAQELDKLGVNIDYIVEVD
      *~      *~* * **** *~      *~ ^***~* *
      81      .      .      .      120

121      .      .      .      160
[Truncated_Name:1]1AKE_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG

```

9

```

[Truncated_Name:2]8BQF_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:3]4X8M_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:4]6S36_A.pdb      VPDELIVDKIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:5]8Q2B_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:6]8RJ9_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:7]6RZE_A.pdb      VPDELIVDAIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:8]4X8H_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:9]3HPR_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDGTG
[Truncated_Name:10]1E4V_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:11]5EJE_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:12]1E4Y_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:13]3X2S_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:14]6HAP_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:15]6HAM_A.pdb      VPDELIVDRIVGRRVHAPSGRVYHVKNPPKVEGKDDVTG
[Truncated_Name:16]4K46_A.pdb      VADSVIVERMAGRRAHLASGRTYHNVNPPKVEGKDDVTG
[Truncated_Name:17]4NP6_A.pdb      VADDVIVERMAGRRAHLPSGRTYHVYNPPKVEGKDDVTG
[Truncated_Name:18]3GMT_A.pdb      VPFSEIIERMSGRRTHPASGRTYHVKNPPKVEGKDDVTG
[Truncated_Name:19]4PZL_A.pdb      VADNLLIERITGRRIHPPASGRTYHTKFNPPKVADKDDVTG
      *      ^^^ ^ *** *      *** **      ^*****      *** **

```



```

121 . . . 160
161 . . . 200
[Truncated_Name:1]1AKE_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:2]8BQF_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:3]4X8M_A.pdb EELTTRKDDQEETVRKRLVEWHQMTAPLIGYYSKEAEAGN
[Truncated_Name:4]6S36_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:5]8Q2B_A.pdb EELTTRKADQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:6]8RJ9_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:7]6RZE_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:8]4X8H_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAALIGYYSKEAEAGN
[Truncated_Name:9]3HPR_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:10]1E4V_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:11]5EJE_A.pdb EELTTRKDDQEECVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:12]1E4Y_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:13]3X2S_A.pdb EELTTRKDDQEETVRKRLCEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:14]6HAP_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:15]6HAM_A.pdb EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGN
[Truncated_Name:16]4K46_A.pdb EDLVIREDDKEETVLARLGVYHNQTAPLIAYYGKEAEAGN
[Truncated_Name:17]4NP6_A.pdb EDLVIREDDKEETVRARLNVYHTQTAPLIEYYGKEAAAGK
[Truncated_Name:18]3GMT_A.pdb EPLVQRDDDDKEETVKKRLDVYEAQTKPLITYYGDWARRGA
[Truncated_Name:19]4PZL_A.pdb EPLITRTDDNEDTVKQRLSVYHAQTAKLIDFYRNFSSNT
* * * * ^ * ** ^ * ** ^*
161 . . . 200

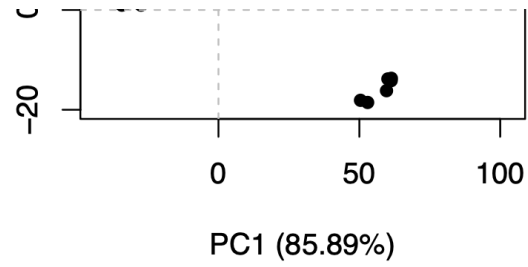
```

10

```

201 . . . 227
[Truncated_Name:1]1AKE_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:2]8BQF_A.pdb T--KYAKVDGTPVAEVRADLEKIL--
[Truncated_Name:3]4X8M_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:4]6S36_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:5]8Q2B_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:6]8RJ9_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:7]6RZE_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:8]4X8H_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:9]3HPR_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:10]1E4V_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:11]5EJE_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:12]1E4Y_A.pdb T--KYAKVDGTPVAEVRADLEKILG-
[Truncated_Name:13]3X2S_A.pdb T--KYAKVDGTPVAEVRADLEKILG-

```

To examine what the PC is capturing, we can plot the loadings or make a movie (trajector) of moving along PC1

```
mktrj(pc, pc=1, file="pc1.pdb")
```