

# AlphaFold Analysis

Jessica Gao PID:A16939806



Figure 1: Superimposed image of HIV monomer

Here we analyze our AlphaFold structure prediction models. The input directory/folder comes from the ColabFold serve:

```
results_dir <- "monomer_94b5b"
```

```
pdb_files <- list.files(path=results_dir,  
                        pattern="*.pdb",  
                        full.names = TRUE)  
basename(pdb_files)
```

```
[1] "monomer_94b5b_unrelaxed_rank_001_alphafold2_ptm_model_5_seed_000.pdb"  
[2] "monomer_94b5b_unrelaxed_rank_002_alphafold2_ptm_model_4_seed_000.pdb"  
[3] "monomer_94b5b_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_000.pdb"  
[4] "monomer_94b5b_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_000.pdb"  
[5] "monomer_94b5b_unrelaxed_rank_005_alphafold2_ptm_model_2_seed_000.pdb"
```

I will use the Bio3D package for analysis

```
library(bio3d)
```

align and superpose

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

Reading PDB files:

```
monomer_94b5b/monomer_94b5b_unrelaxed_rank_001_alphafold2_ptm_model_5_seed_000.pdb  
monomer_94b5b/monomer_94b5b_unrelaxed_rank_002_alphafold2_ptm_model_4_seed_000.pdb  
monomer_94b5b/monomer_94b5b_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_000.pdb  
monomer_94b5b/monomer_94b5b_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_000.pdb  
monomer_94b5b/monomer_94b5b_unrelaxed_rank_005_alphafold2_ptm_model_2_seed_000.pdb  
.....
```

Extracting sequences

```
pdb/seq: 1   name: monomer_94b5b/monomer_94b5b_unrelaxed_rank_001_alphafold2_ptm_model_5_seed_000.pdb  
pdb/seq: 2   name: monomer_94b5b/monomer_94b5b_unrelaxed_rank_002_alphafold2_ptm_model_4_seed_000.pdb  
pdb/seq: 3   name: monomer_94b5b/monomer_94b5b_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_000.pdb  
pdb/seq: 4   name: monomer_94b5b/monomer_94b5b_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_000.pdb  
pdb/seq: 5   name: monomer_94b5b/monomer_94b5b_unrelaxed_rank_005_alphafold2_ptm_model_2_seed_000.pdb
```

pdbs

```

1 . . . . 50
[Truncated_Name:1]monomer_94 PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:2]monomer_94 PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:3]monomer_94 PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:4]monomer_94 PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:5]monomer_94 PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
*****
1 . . . . 50

51 . . . . 99
[Truncated_Name:1]monomer_94 GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:2]monomer_94 GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:3]monomer_94 GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:4]monomer_94 GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:5]monomer_94 GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
*****
51 . . . . 99
```

Call:

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

Class:

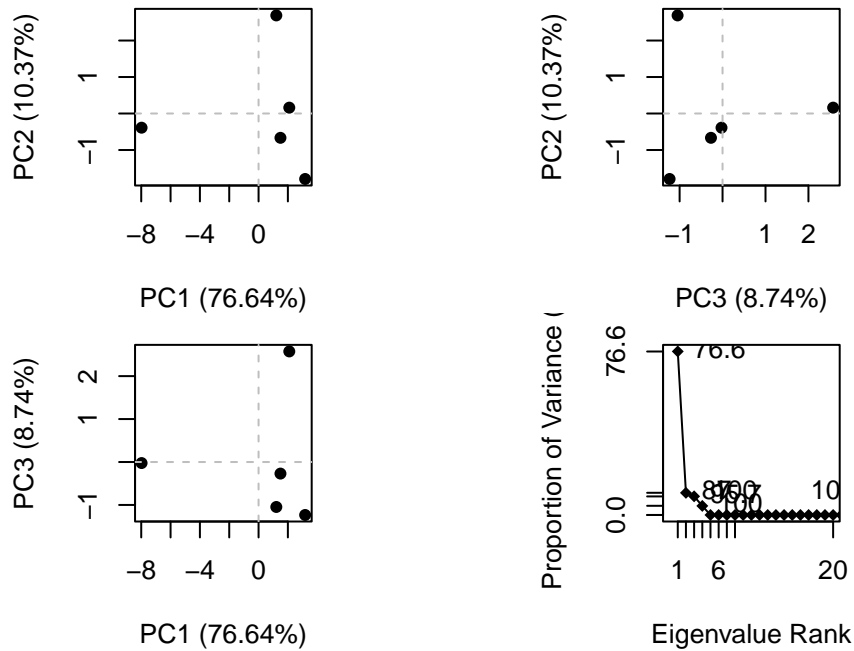
```
pdbs, fasta
```

Alignment dimensions:

```
5 sequence rows; 99 position columns (99 non-gap, 0 gap)
```

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

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



## RMSD analysis

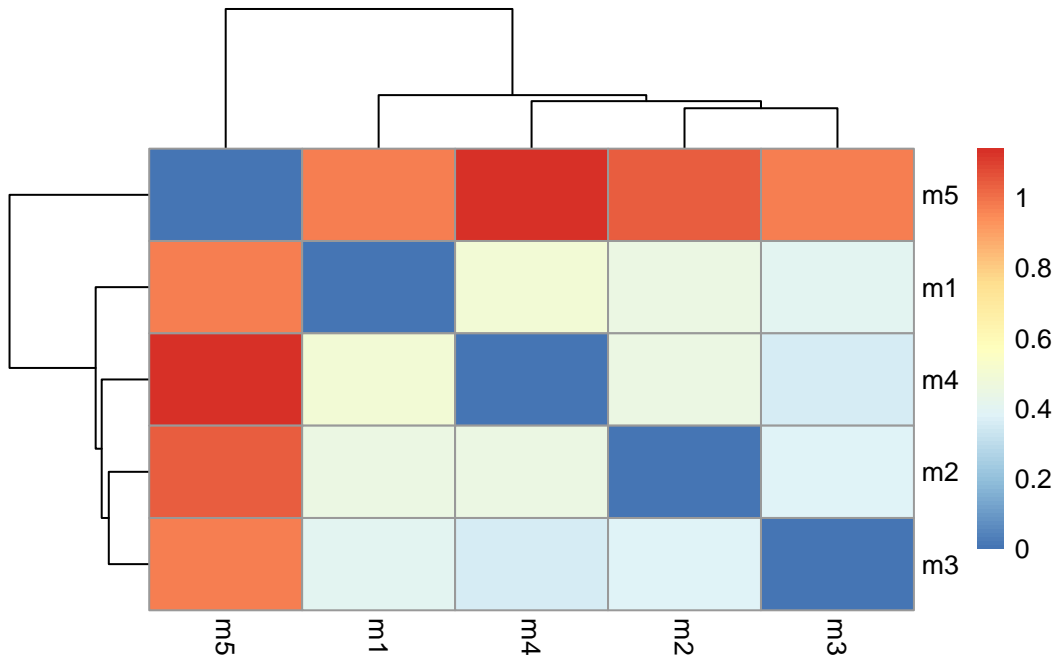
RMSD is a common measure of structural distance used in structural biology

```
rd <- rmsd(pdbbs, fit=T)
```

Warning in rmsd(pdbbs, fit = T): No indices provided, using the 99 non NA positions

```
library(pheatmap)

colnames(rd) <- paste0("m",1:5)
rownames(rd) <- paste0("m",1:5)
pheatmap(rd)
```



**Using my gene of interest: find a gene project gene**

```
gene_int <- "find_a_gene_46bbf"
```

```
pdb_int <- list.files(path=gene_int,
                      pattern="*.pdb",
                      full.names = TRUE)
```

```
basename(pdb_int)
```

```
[1] "find_a_gene_46bbf_unrelaxed_rank_001_alphafold2_ptm_model_3_seed_000.pdb"
[2] "find_a_gene_46bbf_unrelaxed_rank_002_alphafold2_ptm_model_2_seed_000.pdb"
[3] "find_a_gene_46bbf_unrelaxed_rank_003_alphafold2_ptm_model_5_seed_000.pdb"
[4] "find_a_gene_46bbf_unrelaxed_rank_004_alphafold2_ptm_model_1_seed_000.pdb"
[5] "find_a_gene_46bbf_unrelaxed_rank_005_alphafold2_ptm_model_4_seed_000.pdb"
```

```
library(bio3d)
```

```
pdb_find <- pdbaln(pdb_int, fit=TRUE, exefile="msa")
```

Reading PDB files:

find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_001\_alphafold2\_ptm\_model\_3\_seed\_000.pdb  
find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_002\_alphafold2\_ptm\_model\_2\_seed\_000.pdb  
find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_003\_alphafold2\_ptm\_model\_5\_seed\_000.pdb  
find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_004\_alphafold2\_ptm\_model\_1\_seed\_000.pdb  
find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_005\_alphafold2\_ptm\_model\_4\_seed\_000.pdb  
.....

Extracting sequences

pdb/seq: 1 name: find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_001\_alphafold2\_ptm\_model\_3\_seed\_000.pdb  
pdb/seq: 2 name: find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_002\_alphafold2\_ptm\_model\_2\_seed\_000.pdb  
pdb/seq: 3 name: find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_003\_alphafold2\_ptm\_model\_5\_seed\_000.pdb  
pdb/seq: 4 name: find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_004\_alphafold2\_ptm\_model\_1\_seed\_000.pdb  
pdb/seq: 5 name: find\_a\_gene\_46bbf/find\_a\_gene\_46bbf\_unrelaxed\_rank\_005\_alphafold2\_ptm\_model\_4\_seed\_000.pdb

pdb\_find

```

1 . . . . 50
[Truncated_Name:1]find_a_gen MVKGVLKPPQEKNIQVVVRCRPVNSIEKKQNSYSVLDVKPSKKEICVSTE
[Truncated_Name:2]find_a_gen MVKGVLKPPQEKNIQVVVRCRPVNSIEKKQNSYSVLDVKPSKKEICVSTE
[Truncated_Name:3]find_a_gen MVKGVLKPPQEKNIQVVVRCRPVNSIEKKQNSYSVLDVKPSKKEICVSTE
[Truncated_Name:4]find_a_gen MVKGVLKPPQEKNIQVVVRCRPVNSIEKKQNSYSVLDVKPSKKEICVSTE
[Truncated_Name:5]find_a_gen MVKGVLKPPQEKNIQVVVRCRPVNSIEKKQNSYSVLDVKPSKKEICVSTE
*****
1 . . . . 50

51 . . . . 100
[Truncated_Name:1]find_a_gen VAEKASSKIFSFDKVFPGKSPQIEVYKSVVAPILDEVLMGYNCTVFAYGQ
[Truncated_Name:2]find_a_gen VAEKASSKIFSFDKVFPGKSPQIEVYKSVVAPILDEVLMGYNCTVFAYGQ
[Truncated_Name:3]find_a_gen VAEKASSKIFSFDKVFPGKSPQIEVYKSVVAPILDEVLMGYNCTVFAYGQ
[Truncated_Name:4]find_a_gen VAEKASSKIFSFDKVFPGKSPQIEVYKSVVAPILDEVLMGYNCTVFAYGQ
[Truncated_Name:5]find_a_gen VAEKASSKIFSFDKVFPGKSPQIEVYKSVVAPILDEVLMGYNCTVFAYGQ
*****
51 . . . . 100

101 . . . . 150
[Truncated_Name:1]find_a_gen TGTGKTFTMEGERTPDPDLSWEQDPLAGIIPRAMHQIFEKMIGTDIEFSV
[Truncated_Name:2]find_a_gen TGTGKTFTMEGERTPDPDLSWEQDPLAGIIPRAMHQIFEKMIGTDIEFSV
[Truncated_Name:3]find_a_gen TGTGKTFTMEGERTPDPDLSWEQDPLAGIIPRAMHQIFEKMIGTDIEFSV
[Truncated_Name:4]find_a_gen TGTGKTFTMEGERTPDPDLSWEQDPLAGIIPRAMHQIFEKMIGTDIEFSV
[Truncated_Name:5]find_a_gen TGTGKTFTMEGERTPDPDLSWEQDPLAGIIPRAMHQIFEKMIGTDIEFSV
```

```

*****
101      .      .      .      .      150

151      .      .      .      .      200
[Truncated_Name:1]find_a_gen  RVSYLELYNEELFDLLSSQEDTQRLRIFEDSARKGSVVIQGLEEVTVHNK
[Truncated_Name:2]find_a_gen  RVSYLELYNEELFDLLSSQEDTQRLRIFEDSARKGSVVIQGLEEVTVHNK
[Truncated_Name:3]find_a_gen  RVSYLELYNEELFDLLSSQEDTQRLRIFEDSARKGSVVIQGLEEVTVHNK
[Truncated_Name:4]find_a_gen  RVSYLELYNEELFDLLSSQEDTQRLRIFEDSARKGSVVIQGLEEVTVHNK
[Truncated_Name:5]find_a_gen  RVSYLELYNEELFDLLSSQEDTQRLRIFEDSARKGSVVIQGLEEVTVHNK
*****
151      .      .      .      .      200

201      .      .      .      .      250
[Truncated_Name:1]find_a_gen  NEVYAILEKGAARKRTAATLMNAHSSRSRSHSVFSVTIHIKENSIEGDELLK
[Truncated_Name:2]find_a_gen  NEVYAILEKGAARKRTAATLMNAHSSRSRSHSVFSVTIHIKENSIEGDELLK
[Truncated_Name:3]find_a_gen  NEVYAILEKGAARKRTAATLMNAHSSRSRSHSVFSVTIHIKENSIEGDELLK
[Truncated_Name:4]find_a_gen  NEVYAILEKGAARKRTAATLMNAHSSRSRSHSVFSVTIHIKENSIEGDELLK
[Truncated_Name:5]find_a_gen  NEVYAILEKGAARKRTAATLMNAHSSRSRSHSVFSVTIHIKENSIEGDELLK
*****
201      .      .      .      .      250

251      .      .      .      .      300
[Truncated_Name:1]find_a_gen  TGKLNLDLAGSENIGRSGAVDKRAREAGNINQSLTLGRVITALVEHAP
[Truncated_Name:2]find_a_gen  TGKLNLDLAGSENIGRSGAVDKRAREAGNINQSLTLGRVITALVEHAP
[Truncated_Name:3]find_a_gen  TGKLNLDLAGSENIGRSGAVDKRAREAGNINQSLTLGRVITALVEHAP
[Truncated_Name:4]find_a_gen  TGKLNLDLAGSENIGRSGAVDKRAREAGNINQSLTLGRVITALVEHAP
[Truncated_Name:5]find_a_gen  TGKLNLDLAGSENIGRSGAVDKRAREAGNINQSLTLGRVITALVEHAP
*****
251      .      .      .      .      300

301      .      .      .      .      350
[Truncated_Name:1]find_a_gen  HVPYRESKLTRLLQDSLGGRTKTSIIATVSPASINVEETLSTLDYAHRAK
[Truncated_Name:2]find_a_gen  HVPYRESKLTRLLQDSLGGRTKTSIIATVSPASINVEETLSTLDYAHRAK
[Truncated_Name:3]find_a_gen  HVPYRESKLTRLLQDSLGGRTKTSIIATVSPASINVEETLSTLDYAHRAK
[Truncated_Name:4]find_a_gen  HVPYRESKLTRLLQDSLGGRTKTSIIATVSPASINVEETLSTLDYAHRAK
[Truncated_Name:5]find_a_gen  HVPYRESKLTRLLQDSLGGRTKTSIIATVSPASINVEETLSTLDYAHRAK
*****
301      .      .      .      .      350

351      .      .      .      .      400
[Truncated_Name:1]find_a_gen  HITNRPEINQKLTKKALLKEYTEEIEKLRKDLFATREKNGIYLSEEHYKN
[Truncated_Name:2]find_a_gen  HITNRPEINQKLTKKALLKEYTEEIEKLRKDLFATREKNGIYLSEEHYKN
[Truncated_Name:3]find_a_gen  HITNRPEINQKLTKKALLKEYTEEIEKLRKDLFATREKNGIYLSEEHYKN

```



```

[Truncated_Name:4]find_a_gen HITNRPEINQKLTKKALLKEYTEEIEKLRKDLFATREKNGIYLSEEHYKN
[Truncated_Name:5]find_a_gen HITNRPEINQKLTKKALLKEYTEEIEKLRKDLFATREKNGIYLSEEHYKN
*****
351 . . . . 400

401 . . . . 450
[Truncated_Name:1]find_a_gen MEVSIACQRAQIKEMEENIEDLTTQMVKVTELFQKELEERTEEELEVT
[Truncated_Name:2]find_a_gen MEVSIACQRAQIKEMEENIEDLTTQMVKVTELFQKELEERTEEELEVT
[Truncated_Name:3]find_a_gen MEVSIACQRAQIKEMEENIEDLTTQMVKVTELFQKELEERTEEELEVT
[Truncated_Name:4]find_a_gen MEVSIACQRAQIKEMEENIEDLTTQMVKVTELFQKELEERTEEELEVT
[Truncated_Name:5]find_a_gen MEVSIACQRAQIKEMEENIEDLTTQMVKVTELFQKELEERTEEELEVT
*****
401 . . . . 450

451 . . . . 500
[Truncated_Name:1]find_a_gen TKNLEETTETLHVTEKDLRVTTQDRDEQCHLVSEHVKTETQLMSEATQLL
[Truncated_Name:2]find_a_gen TKNLEETTETLHVTEKDLRVTTQDRDEQCHLVSEHVKTETQLMSEATQLL
[Truncated_Name:3]find_a_gen TKNLEETTETLHVTEKDLRVTTQDRDEQCHLVSEHVKTETQLMSEATQLL
[Truncated_Name:4]find_a_gen TKNLEETTETLHVTEKDLRVTTQDRDEQCHLVSEHVKTETQLMSEATQLL
[Truncated_Name:5]find_a_gen TKNLEETTETLHVTEKDLRVTTQDRDEQCHLVSEHVKTETQLMSEATQLL
*****
451 . . . . 500

501 . . . . 550
[Truncated_Name:1]find_a_gen STADSSVTDVGGLHAKLDRKRTVEAHNKSQAEVFAESFHSYTSIDKSSLS
[Truncated_Name:2]find_a_gen STADSSVTDVGGLHAKLDRKRTVEAHNKSQAEVFAESFHSYTSIDKSSLS
[Truncated_Name:3]find_a_gen STADSSVTDVGGLHAKLDRKRTVEAHNKSQAEVFAESFHSYTSIDKSSLS
[Truncated_Name:4]find_a_gen STADSSVTDVGGLHAKLDRKRTVEAHNKSQAEVFAESFHSYTSIDKSSLS
[Truncated_Name:5]find_a_gen STADSSVTDVGGLHAKLDRKRTVEAHNKSQAEVFAESFHSYTSIDKSSLS
*****
501 . . . . 550

551 . . . . 600
[Truncated_Name:1]find_a_gen RLREEQQGKCTSMQQQFEFMISKRTKEAGDLRASLSDMVTSVKGHSAGMM
[Truncated_Name:2]find_a_gen RLREEQQGKCTSMQQQFEFMISKRTKEAGDLRASLSDMVTSVKGHSAGMM
[Truncated_Name:3]find_a_gen RLREEQQGKCTSMQQQFEFMISKRTKEAGDLRASLSDMVTSVKGHSAGMM
[Truncated_Name:4]find_a_gen RLREEQQGKCTSMQQQFEFMISKRTKEAGDLRASLSDMVTSVKGHSAGMM
[Truncated_Name:5]find_a_gen RLREEQQGKCTSMQQQFEFMISKRTKEAGDLRASLSDMVTSVKGHSAGMM
*****
551 . . . . 600

601 . . . . 650
[Truncated_Name:1]find_a_gen EESQRKREEWEKWSNDACAEHSKFEDVIDSMNDFHSNRFLTAMNMLAEK

```

```

[Truncated_Name:2]find_a_gen EESQRKREEWEKWSNDACAEHSKFEDVIDSMNDFHSNRFLTAMNMLAEK
[Truncated_Name:3]find_a_gen EESQRKREEWEKWSNDACAEHSKFEDVIDSMNDFHSNRFLTAMNMLAEK
[Truncated_Name:4]find_a_gen EESQRKREEWEKWSNDACAEHSKFEDVIDSMNDFHSNRFLTAMNMLAEK
[Truncated_Name:5]find_a_gen EESQRKREEWEKWSNDACAEHSKFEDVIDSMNDFHSNRFLTAMNMLAEK
*****
601 . . . . 650

651 . . . . 700
[Truncated_Name:1]find_a_gen LSSLTESLNECRRDIKTQINSQSETVQACIEKQLDQVNVMTTVEKFS DH
[Truncated_Name:2]find_a_gen LSSLTESLNECRRDIKTQINSQSETVQACIEKQLDQVNVMTTVEKFS DH
[Truncated_Name:3]find_a_gen LSSLTESLNECRRDIKTQINSQSETVQACIEKQLDQVNVMTTVEKFS DH
[Truncated_Name:4]find_a_gen LSSLTESLNECRRDIKTQINSQSETVQACIEKQLDQVNVMTTVEKFS DH
[Truncated_Name:5]find_a_gen LSSLTESLNECRRDIKTQINSQSETVQACIEKQLDQVNVMTTVEKFS DH
*****
651 . . . . 700

701 . . . . 750
[Truncated_Name:1]find_a_gen QRSKISDLSGQLDMLKDQERHRNQDMMKSIQGLFAQREESFASETNKLQE
[Truncated_Name:2]find_a_gen QRSKISDLSGQLDMLKDQERHRNQDMMKSIQGLFAQREESFASETNKLQE
[Truncated_Name:3]find_a_gen QRSKISDLSGQLDMLKDQERHRNQDMMKSIQGLFAQREESFASETNKLQE
[Truncated_Name:4]find_a_gen QRSKISDLSGQLDMLKDQERHRNQDMMKSIQGLFAQREESFASETNKLQE
[Truncated_Name:5]find_a_gen QRSKISDLSGQLDMLKDQERHRNQDMMKSIQGLFAQREESFASETNKLQE
*****
701 . . . . 750

751 . . . . 800
[Truncated_Name:1]find_a_gen QLEEASTETERVKTSILSQETSVQESCESFRNVHRESSERLISSADSHHE
[Truncated_Name:2]find_a_gen QLEEASTETERVKTSILSQETSVQESCESFRNVHRESSERLISSADSHHE
[Truncated_Name:3]find_a_gen QLEEASTETERVKTSILSQETSVQESCESFRNVHRESSERLISSADSHHE
[Truncated_Name:4]find_a_gen QLEEASTETERVKTSILSQETSVQESCESFRNVHRESSERLISSADSHHE
[Truncated_Name:5]find_a_gen QLEEASTETERVKTSILSQETSVQESCESFRNVHRESSERLISSADSHHE
*****
751 . . . . 800

801 . . . . 850
[Truncated_Name:1]find_a_gen KTVAQVEDIRQHNTSLEESMTSQTNTQIDRQTHMEQVCENFKGHMEEIS
[Truncated_Name:2]find_a_gen KTVAQVEDIRQHNTSLEESMTSQTNTQIDRQTHMEQVCENFKGHMEEIS
[Truncated_Name:3]find_a_gen KTVAQVEDIRQHNTSLEESMTSQTNTQIDRQTHMEQVCENFKGHMEEIS
[Truncated_Name:4]find_a_gen KTVAQVEDIRQHNTSLEESMTSQTNTQIDRQTHMEQVCENFKGHMEEIS
[Truncated_Name:5]find_a_gen KTVAQVEDIRQHNTSLEESMTSQTNTQIDRQTHMEQVCENFKGHMEEIS
*****
801 . . . . 850

```

```

851 . . . 900
[Truncated_Name:1]find_a_gen QHVTQKQADKEAMTIEHEASDETLSSSTVDKQLTEMTTTVTEWTEDESKARS
[Truncated_Name:2]find_a_gen QHVTQKQADKEAMTIEHEASDETLSSSTVDKQLTEMTTTVTEWTEDESKARS
[Truncated_Name:3]find_a_gen QHVTQKQADKEAMTIEHEASDETLSSSTVDKQLTEMTTTVTEWTEDESKARS
[Truncated_Name:4]find_a_gen QHVTQKQADKEAMTIEHEASDETLSSSTVDKQLTEMTTTVTEWTEDESKARS
[Truncated_Name:5]find_a_gen QHVTQKQADKEAMTIEHEASDETLSSSTVDKQLTEMTTTVTEWTEDESKARS
*****
851 . . . 900

901 . . . 950
[Truncated_Name:1]find_a_gen EDMTSWAEMEETVESGLKRVEGFLTRDLKEDVPTGTTTPQRKHFSYPRDL
[Truncated_Name:2]find_a_gen EDMTSWAEMEETVESGLKRVEGFLTRDLKEDVPTGTTTPQRKHFSYPRDL
[Truncated_Name:3]find_a_gen EDMTSWAEMEETVESGLKRVEGFLTRDLKEDVPTGTTTPQRKHFSYPRDL
[Truncated_Name:4]find_a_gen EDMTSWAEMEETVESGLKRVEGFLTRDLKEDVPTGTTTPQRKHFSYPRDL
[Truncated_Name:5]find_a_gen EDMTSWAEMEETVESGLKRVEGFLTRDLKEDVPTGTTTPQRKHFSYPRDL
*****
901 . . . 950

951 . . . 1000
[Truncated_Name:1]find_a_gen TSTEPHGIIILNRFRQECELNQAADMPLPDDSIASECPSDMSLQSTKEMKI
[Truncated_Name:2]find_a_gen TSTEPHGIIILNRFRQECELNQAADMPLPDDSIASECPSDMSLQSTKEMKI
[Truncated_Name:3]find_a_gen TSTEPHGIIILNRFRQECELNQAADMPLPDDSIASECPSDMSLQSTKEMKI
[Truncated_Name:4]find_a_gen TSTEPHGIIILNRFRQECELNQAADMPLPDDSIASECPSDMSLQSTKEMKI
[Truncated_Name:5]find_a_gen TSTEPHGIIILNRFRQECELNQAADMPLPDDSIASECPSDMSLQSTKEMKI
*****
951 . . . 1000

1001 . . . 1050
[Truncated_Name:1]find_a_gen GQSESFLGDTSTDANESTLSRSQSQSLTSKSIDGDDTKENFVMPKSVTT
[Truncated_Name:2]find_a_gen GQSESFLGDTSTDANESTLSRSQSQSLTSKSIDGDDTKENFVMPKSVTT
[Truncated_Name:3]find_a_gen GQSESFLGDTSTDANESTLSRSQSQSLTSKSIDGDDTKENFVMPKSVTT
[Truncated_Name:4]find_a_gen GQSESFLGDTSTDANESTLSRSQSQSLTSKSIDGDDTKENFVMPKSVTT
[Truncated_Name:5]find_a_gen GQSESFLGDTSTDANESTLSRSQSQSLTSKSIDGDDTKENFVMPKSVTT
*****
1001 . . . 1050

1051 . . . 1081
[Truncated_Name:1]find_a_gen ARGKKLPRDRGKNRTPKTKSRLPLRSANSVN
[Truncated_Name:2]find_a_gen ARGKKLPRDRGKNRTPKTKSRLPLRSANSVN
[Truncated_Name:3]find_a_gen ARGKKLPRDRGKNRTPKTKSRLPLRSANSVN
[Truncated_Name:4]find_a_gen ARGKKLPRDRGKNRTPKTKSRLPLRSANSVN
[Truncated_Name:5]find_a_gen ARGKKLPRDRGKNRTPKTKSRLPLRSANSVN
*****

```

1051 . . .1081

Call:

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

Class:

```
pdb, fasta
```

Alignment dimensions:

```
5 sequence rows; 1081 position columns (1081 non-gap, 0 gap)
```

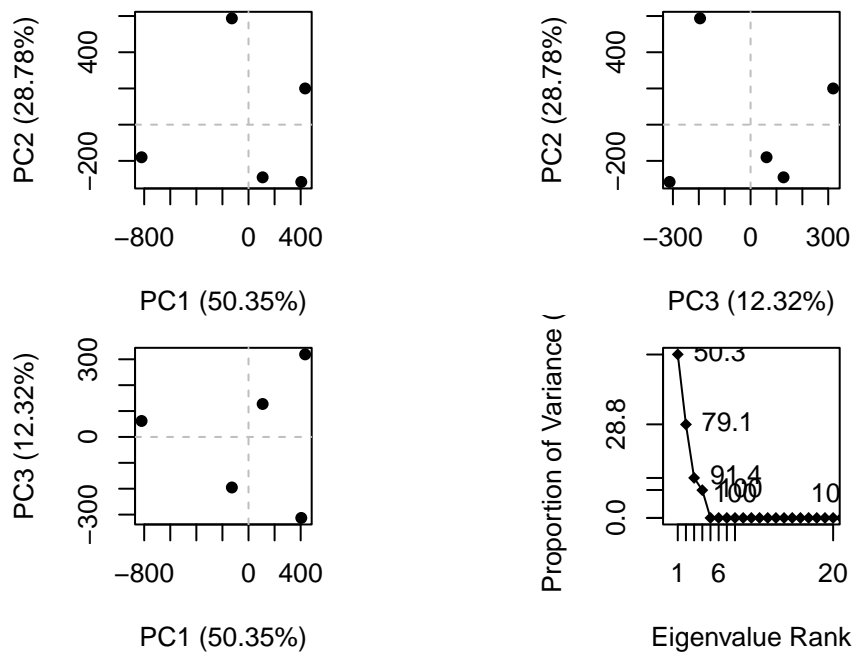
```
+ attr: xyz, resno, b, chain, id, ali, resid, sse, call
```

```
pc_find <- pca(pdb_find)
```

NOTE: In input xyz (MxN),  $N > 3000$  and  $M < N$

Singular Value Decomposition (SVD) approach is faster  
and is recommended (set 'use.svd = TRUE')

```
plot(pc_find)
```

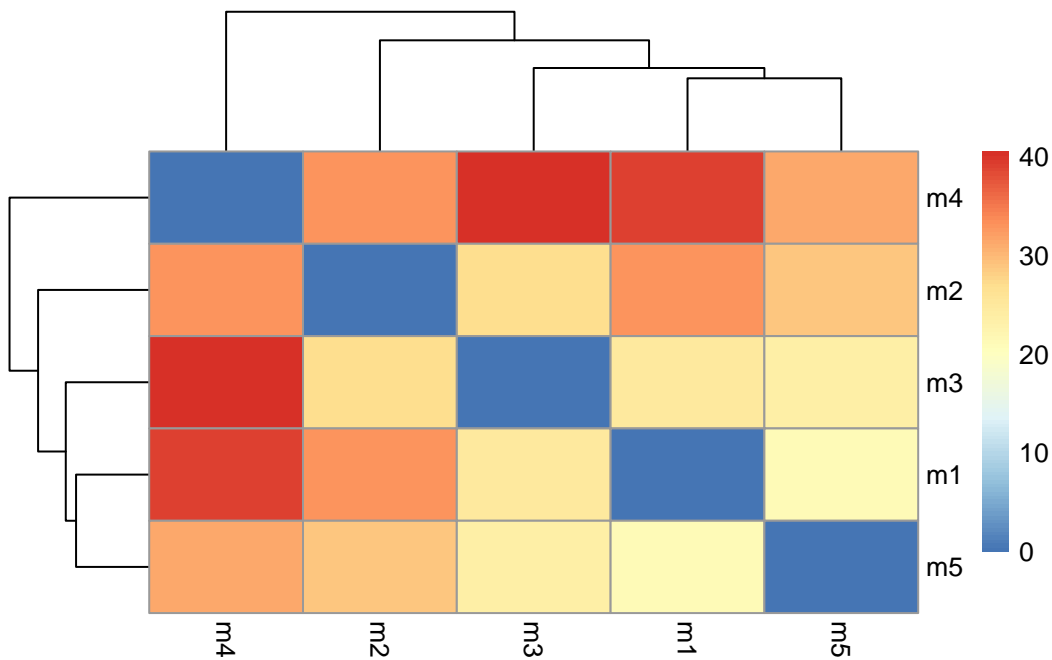


```
rd_find <- rmsd(pdb_find, fit=T)
```

Warning in rmsd(pdb\_find, fit = T): No indices provided, using the 1081 non NA positions

```
library(pheatmap)

colnames(rd_find) <- paste0("m",1:5)
rownames(rd_find) <- paste0("m",1:5)
pheatmap(rd_find)
```



```
# Read a reference PDB structure
pdb_ref <- read.pdb("1hsg")
```

Note: Accessing on-line PDB file

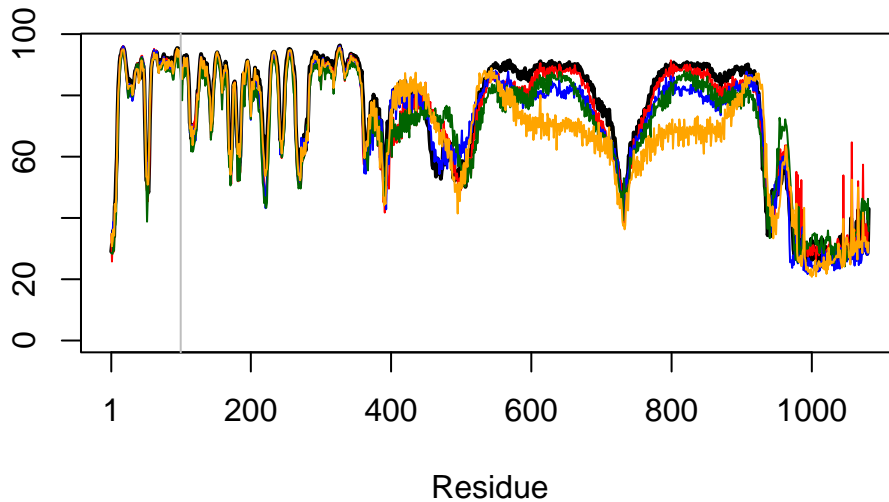
```
plotb3(pdb_find$b[1,], typ="l", lwd=2, sse=pdb_ref)
```

Warning in plotb3(pdb\_find\$b[1, ], typ = "l", lwd = 2, sse = pdb\_ref): Length of input 'sse' does not equal the length of input 'x'; Ignoring 'sse'

```

points(pdb_find$b[2,], typ="l", col="red")
points(pdb_find$b[3,], typ="l", col="blue")
points(pdb_find$b[4,], typ="l", col="darkgreen")
points(pdb_find$b[5,], typ="l", col="orange")
abline(v=100, col="gray")

```



```

core_find <- core.find(pdb_find)

```

```

core size 1080 of 1081  vol = 4368466
core size 1079 of 1081  vol = 4329661
core size 1078 of 1081  vol = 4295830
core size 1077 of 1081  vol = 4263764
core size 1076 of 1081  vol = 4233254
core size 1075 of 1081  vol = 4202631
core size 1074 of 1081  vol = 4172694
core size 1073 of 1081  vol = 4145289
core size 1072 of 1081  vol = 4117877
core size 1071 of 1081  vol = 4089654
core size 1070 of 1081  vol = 4062723
core size 1069 of 1081  vol = 4034424
core size 1068 of 1081  vol = 4009814
core size 1067 of 1081  vol = 3985952

```

core size 1066 of 1081 vol = 3963024  
core size 1065 of 1081 vol = 3939238  
core size 1064 of 1081 vol = 3919327  
core size 1063 of 1081 vol = 3891796  
core size 1062 of 1081 vol = 3870528  
core size 1061 of 1081 vol = 3851310  
core size 1060 of 1081 vol = 3828384  
core size 1059 of 1081 vol = 3803076  
core size 1058 of 1081 vol = 3782663  
core size 1057 of 1081 vol = 3761218  
core size 1056 of 1081 vol = 3742987  
core size 1055 of 1081 vol = 3726411  
core size 1054 of 1081 vol = 3709221  
core size 1053 of 1081 vol = 3691566  
core size 1052 of 1081 vol = 3674462  
core size 1051 of 1081 vol = 3656929  
core size 1050 of 1081 vol = 3640868  
core size 1049 of 1081 vol = 3621317  
core size 1048 of 1081 vol = 3603384  
core size 1047 of 1081 vol = 3588263  
core size 1046 of 1081 vol = 3573197  
core size 1045 of 1081 vol = 3551634  
core size 1044 of 1081 vol = 3532568  
core size 1043 of 1081 vol = 3514068  
core size 1042 of 1081 vol = 3497813  
core size 1041 of 1081 vol = 3477256  
core size 1040 of 1081 vol = 3458985  
core size 1039 of 1081 vol = 3440765  
core size 1038 of 1081 vol = 3424384  
core size 1037 of 1081 vol = 3410176  
core size 1036 of 1081 vol = 3390834  
core size 1035 of 1081 vol = 3371589  
core size 1034 of 1081 vol = 3351958  
core size 1033 of 1081 vol = 3337355  
core size 1032 of 1081 vol = 3324126  
core size 1031 of 1081 vol = 3305369  
core size 1030 of 1081 vol = 3291513  
core size 1029 of 1081 vol = 3272538  
core size 1028 of 1081 vol = 3253718  
core size 1027 of 1081 vol = 3237083  
core size 1026 of 1081 vol = 3218431  
core size 1025 of 1081 vol = 3203202  
core size 1024 of 1081 vol = 3186753

core size 1023 of 1081 vol = 3168768  
core size 1022 of 1081 vol = 3154177  
core size 1021 of 1081 vol = 3136583  
core size 1020 of 1081 vol = 3118887  
core size 1019 of 1081 vol = 3101064  
core size 1018 of 1081 vol = 3083074  
core size 1017 of 1081 vol = 3069362  
core size 1016 of 1081 vol = 3053787  
core size 1015 of 1081 vol = 3038252  
core size 1014 of 1081 vol = 3021293  
core size 1013 of 1081 vol = 3009155  
core size 1012 of 1081 vol = 2997507  
core size 1011 of 1081 vol = 2981509  
core size 1010 of 1081 vol = 2968337  
core size 1009 of 1081 vol = 2953566  
core size 1008 of 1081 vol = 2941738  
core size 1007 of 1081 vol = 2927531  
core size 1006 of 1081 vol = 2914546  
core size 1005 of 1081 vol = 2900039  
core size 1004 of 1081 vol = 2885429  
core size 1003 of 1081 vol = 2871250  
core size 1002 of 1081 vol = 2855758  
core size 1001 of 1081 vol = 2841186  
core size 1000 of 1081 vol = 2828614  
core size 999 of 1081 vol = 2817422  
core size 998 of 1081 vol = 2803381  
core size 997 of 1081 vol = 2789442  
core size 996 of 1081 vol = 2773453  
core size 995 of 1081 vol = 2759127  
core size 994 of 1081 vol = 2746277  
core size 993 of 1081 vol = 2732201  
core size 992 of 1081 vol = 2717923  
core size 991 of 1081 vol = 2703380  
core size 990 of 1081 vol = 2689832  
core size 989 of 1081 vol = 2675892  
core size 988 of 1081 vol = 2661561  
core size 987 of 1081 vol = 2647689  
core size 986 of 1081 vol = 2635976  
core size 985 of 1081 vol = 2620909  
core size 984 of 1081 vol = 2610727  
core size 983 of 1081 vol = 2597279  
core size 982 of 1081 vol = 2586264  
core size 981 of 1081 vol = 2573077



core size 980 of 1081 vol = 2559494  
core size 979 of 1081 vol = 2545751  
core size 978 of 1081 vol = 2532386  
core size 977 of 1081 vol = 2520973  
core size 976 of 1081 vol = 2511516  
core size 975 of 1081 vol = 2498476  
core size 974 of 1081 vol = 2483951  
core size 973 of 1081 vol = 2470868  
core size 972 of 1081 vol = 2458658  
core size 971 of 1081 vol = 2445219  
core size 970 of 1081 vol = 2431748  
core size 969 of 1081 vol = 2418885  
core size 968 of 1081 vol = 2408032  
core size 967 of 1081 vol = 2395315  
core size 966 of 1081 vol = 2385913  
core size 965 of 1081 vol = 2376083  
core size 964 of 1081 vol = 2362713  
core size 963 of 1081 vol = 2349389  
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core size 959 of 1081 vol = 2301848  
core size 958 of 1081 vol = 2287818  
core size 957 of 1081 vol = 2276715  
core size 956 of 1081 vol = 2264994  
core size 955 of 1081 vol = 2252172  
core size 954 of 1081 vol = 2239136  
core size 953 of 1081 vol = 2228078  
core size 952 of 1081 vol = 2215819  
core size 951 of 1081 vol = 2203795  
core size 950 of 1081 vol = 2193170  
core size 949 of 1081 vol = 2181689  
core size 948 of 1081 vol = 2169575  
core size 947 of 1081 vol = 2159317  
core size 946 of 1081 vol = 2148636  
core size 945 of 1081 vol = 2139814  
core size 944 of 1081 vol = 2126528  
core size 943 of 1081 vol = 2115412  
core size 942 of 1081 vol = 2102901  
core size 941 of 1081 vol = 2091955  
core size 940 of 1081 vol = 2079325  
core size 939 of 1081 vol = 2066632  
core size 938 of 1081 vol = 2053950

core size 937 of 1081 vol = 2041361  
core size 936 of 1081 vol = 2028998  
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core size 932 of 1081 vol = 1981867  
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core size 926 of 1081 vol = 1921305  
core size 925 of 1081 vol = 1912954  
core size 924 of 1081 vol = 1905511  
core size 923 of 1081 vol = 1897399  
core size 922 of 1081 vol = 1885553  
core size 921 of 1081 vol = 1874041  
core size 920 of 1081 vol = 1864805  
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core size 917 of 1081 vol = 1839063  
core size 916 of 1081 vol = 1829150  
core size 915 of 1081 vol = 1817923  
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core size 913 of 1081 vol = 1798047  
core size 912 of 1081 vol = 1788113  
core size 911 of 1081 vol = 1776958  
core size 910 of 1081 vol = 1766852  
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core size 873 of 1081 vol = 1435862  
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core size 871 of 1081 vol = 1421127  
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core size 857 of 1081 vol = 1313176  
core size 856 of 1081 vol = 1306655  
core size 855 of 1081 vol = 1301077  
core size 854 of 1081 vol = 1295030  
core size 853 of 1081 vol = 1289051  
core size 852 of 1081 vol = 1283348

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core size 849 of 1081 vol = 1261620  
core size 848 of 1081 vol = 1252256  
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core size 836 of 1081 vol = 1165627  
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core size 823 of 1081 vol = 1073958  
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core size 821 of 1081 vol = 1061039  
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core size 818 of 1081 vol = 1042790  
core size 817 of 1081 vol = 1037824  
core size 816 of 1081 vol = 1031938  
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core size 813 of 1081 vol = 1013126  
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core size 811 of 1081 vol = 1000899  
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core size 806 of 1081 vol = 966226.7  
core size 805 of 1081 vol = 960280.6  
core size 804 of 1081 vol = 954206.9  
core size 803 of 1081 vol = 949517.6  
core size 802 of 1081 vol = 943463.7  
core size 801 of 1081 vol = 937433.1  
core size 800 of 1081 vol = 932243.4  
core size 799 of 1081 vol = 926910.7  
core size 798 of 1081 vol = 922113.9  
core size 797 of 1081 vol = 916947.9  
core size 796 of 1081 vol = 911787.2  
core size 795 of 1081 vol = 905653.2  
core size 794 of 1081 vol = 900000.8  
core size 793 of 1081 vol = 894083.9  
core size 792 of 1081 vol = 889735.1  
core size 791 of 1081 vol = 883900  
core size 790 of 1081 vol = 878111.5  
core size 789 of 1081 vol = 873823.2  
core size 788 of 1081 vol = 867951.1  
core size 787 of 1081 vol = 862014.4  
core size 786 of 1081 vol = 855998.7  
core size 785 of 1081 vol = 851525.7  
core size 784 of 1081 vol = 845679.4  
core size 783 of 1081 vol = 839787.8  
core size 782 of 1081 vol = 833822  
core size 781 of 1081 vol = 827873.1  
core size 780 of 1081 vol = 822986.3  
core size 779 of 1081 vol = 816551.6  
core size 778 of 1081 vol = 810757.6  
core size 777 of 1081 vol = 805122  
core size 776 of 1081 vol = 799599.8  
core size 775 of 1081 vol = 793871  
core size 774 of 1081 vol = 788054.6  
core size 773 of 1081 vol = 782283.4  
core size 772 of 1081 vol = 776406.7  
core size 771 of 1081 vol = 770653.4  
core size 770 of 1081 vol = 764559.8  
core size 769 of 1081 vol = 759707.9  
core size 768 of 1081 vol = 754463  
core size 767 of 1081 vol = 749051.1  
core size 766 of 1081 vol = 743302.1

core size 765 of 1081 vol = 737581.6  
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core size 763 of 1081 vol = 726740.9  
core size 762 of 1081 vol = 720769.4  
core size 761 of 1081 vol = 714930.9  
core size 760 of 1081 vol = 710893  
core size 759 of 1081 vol = 706722.7  
core size 758 of 1081 vol = 702497.4  
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core size 755 of 1081 vol = 687873.2  
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core size 753 of 1081 vol = 678497.6  
core size 752 of 1081 vol = 672791.6  
core size 751 of 1081 vol = 667928.9  
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core size 747 of 1081 vol = 647281.7  
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core size 745 of 1081 vol = 636367.5  
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core size 741 of 1081 vol = 619644.5  
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core size 739 of 1081 vol = 612816.8  
core size 738 of 1081 vol = 607862.3  
core size 737 of 1081 vol = 602873.5  
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core size 735 of 1081 vol = 594339.6  
core size 734 of 1081 vol = 591139.1  
core size 733 of 1081 vol = 587250.3  
core size 732 of 1081 vol = 582286.4  
core size 731 of 1081 vol = 577505.2  
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core size 720 of 1081 vol = 538524.5  
core size 719 of 1081 vol = 534519.2  
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core size 717 of 1081 vol = 526934.3  
core size 716 of 1081 vol = 522400.3  
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core size 712 of 1081 vol = 506690.6  
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core size 709 of 1081 vol = 495736  
core size 708 of 1081 vol = 491397.2  
core size 707 of 1081 vol = 488145.7  
core size 706 of 1081 vol = 484070  
core size 705 of 1081 vol = 479742.3  
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core size 703 of 1081 vol = 472178.4  
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core size 690 of 1081 vol = 423019.3  
core size 689 of 1081 vol = 420205.2  
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core size 684 of 1081 vol = 403339.8  
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core size 674 of 1081 vol = 369771.4  
core size 673 of 1081 vol = 366317.1  
core size 672 of 1081 vol = 363384.5  
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core size 670 of 1081 vol = 357946.8  
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core size 668 of 1081 vol = 352223.7  
core size 667 of 1081 vol = 349648.7  
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core size 665 of 1081 vol = 344436.4  
core size 664 of 1081 vol = 341648.5  
core size 663 of 1081 vol = 339014.3  
core size 662 of 1081 vol = 336659.3  
core size 661 of 1081 vol = 334005.1  
core size 660 of 1081 vol = 331696.4  
core size 659 of 1081 vol = 329338.5  
core size 658 of 1081 vol = 326371.5  
core size 657 of 1081 vol = 323767.9  
core size 656 of 1081 vol = 320760.7  
core size 655 of 1081 vol = 318316.6  
core size 654 of 1081 vol = 315563.9  
core size 653 of 1081 vol = 313134  
core size 652 of 1081 vol = 310509.4  
core size 651 of 1081 vol = 307872.8  
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core size 649 of 1081 vol = 302312.4  
core size 648 of 1081 vol = 299309.1  
core size 647 of 1081 vol = 296409.5  
core size 646 of 1081 vol = 293613.1  
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core size 643 of 1081 vol = 286011.4  
core size 642 of 1081 vol = 283372.8  
core size 641 of 1081 vol = 280523.9  
core size 640 of 1081 vol = 278384.4  
core size 639 of 1081 vol = 275604  
core size 638 of 1081 vol = 272852.2  
core size 637 of 1081 vol = 270052.3



core size 636 of 1081 vol = 267245.1  
core size 635 of 1081 vol = 264553.4  
core size 634 of 1081 vol = 261765.7  
core size 633 of 1081 vol = 259426.7  
core size 632 of 1081 vol = 256768.7  
core size 631 of 1081 vol = 254721.1  
core size 630 of 1081 vol = 252762.1  
core size 629 of 1081 vol = 250286.1  
core size 628 of 1081 vol = 247504.5  
core size 627 of 1081 vol = 244894.5  
core size 626 of 1081 vol = 242521.5  
core size 625 of 1081 vol = 240333.3  
core size 624 of 1081 vol = 237759.2  
core size 623 of 1081 vol = 235921.8  
core size 622 of 1081 vol = 234329.1  
core size 621 of 1081 vol = 232428.4  
core size 620 of 1081 vol = 230455  
core size 619 of 1081 vol = 228385.5  
core size 618 of 1081 vol = 226477.8  
core size 617 of 1081 vol = 224792.2  
core size 616 of 1081 vol = 222730.5  
core size 615 of 1081 vol = 220804  
core size 614 of 1081 vol = 219043.5  
core size 613 of 1081 vol = 217086.2  
core size 612 of 1081 vol = 214900.2  
core size 611 of 1081 vol = 212993.4  
core size 610 of 1081 vol = 210937.6  
core size 609 of 1081 vol = 209293.5  
core size 608 of 1081 vol = 207319.5  
core size 607 of 1081 vol = 205505.7  
core size 606 of 1081 vol = 203929.1  
core size 605 of 1081 vol = 202580  
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core size 52 of 1081 vol = 1.712  
core size 51 of 1081 vol = 1.657  
core size 50 of 1081 vol = 1.518  
core size 49 of 1081 vol = 1.463  
core size 48 of 1081 vol = 1.353  
core size 47 of 1081 vol = 1.259  
core size 46 of 1081 vol = 1.209  
core size 45 of 1081 vol = 1.122  
core size 44 of 1081 vol = 1.071  
core size 43 of 1081 vol = 1.035  
core size 42 of 1081 vol = 0.976  
core size 41 of 1081 vol = 0.907  
core size 40 of 1081 vol = 0.832  
core size 39 of 1081 vol = 0.738  
core size 38 of 1081 vol = 0.652  
core size 37 of 1081 vol = 0.595  
core size 36 of 1081 vol = 0.575  
core size 35 of 1081 vol = 0.542

```
core size 34 of 1081  vol = 0.494  
FINISHED: Min vol ( 0.5 ) reached
```

```
core.inds_find <- print(core_find, vol=0.5)
```

```
# 35 positions (cumulative volume <= 0.5 Angstrom^3)  
  start end length  
1   591 591      1  
2   594 595      2  
3   598 607     10  
4   609 610      2  
5   841 841      1  
6   844 845      2  
7   847 862     16  
8   869 869      1
```

```
abg <- pdbfit(pdb_find, core.inds_find, outputPath="corefit_structures")
```

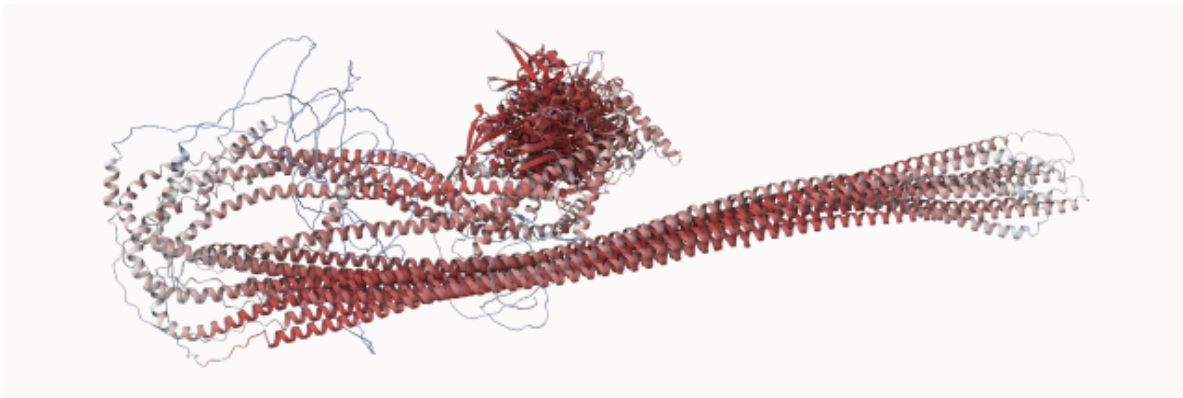
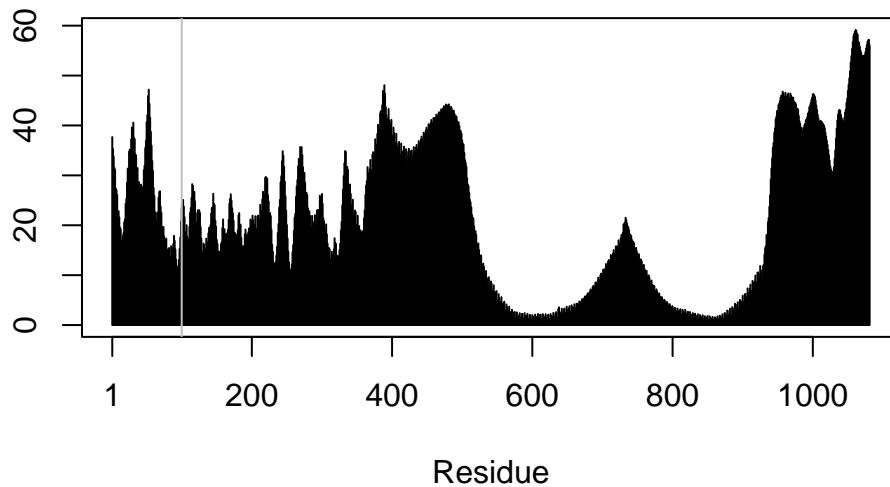


Figure 2: Find a gene sequence view superimposed

```
rf <- rmsf(abg)  
plotb3(rf, sse=pdb_find)
```

Warning in plotb3(rf, sse = pdb\_find): Length of input 'sse' does not equal the length of input 'x'; Ignoring 'sse'

```
abline(v=100, col="gray", ylab="RMSF")
```



```
library(jsonlite)
```

```
# Listing of all PAE JSON files
pae_files_find <- list.files(path=results_dir,
                             pattern=".*model.*\\.json",
                             full.names = TRUE)
```

```
pae2 <- read_json(pae_files_find[2],simplifyVector = TRUE)
pae4 <- read_json(pae_files_find[4],simplifyVector = TRUE)
```

```
attributes(pae2)
```

```
$names
[1] "plddt"    "max_pae" "pae"      "ptm"
```

```
head(pae2$plddt)
```

```
[1] 76.56 85.69 87.06 89.12 88.69 92.19
```



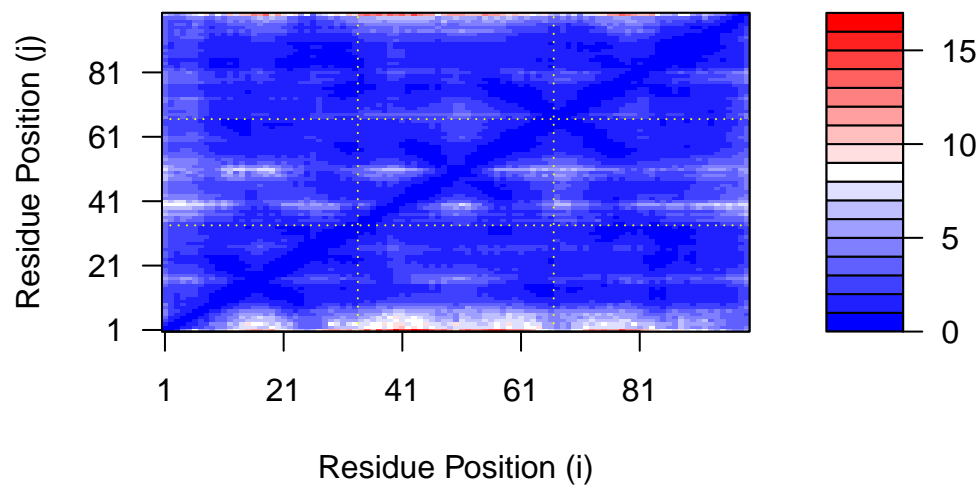
```
pae2$max_pae
```

```
[1] 16.82812
```

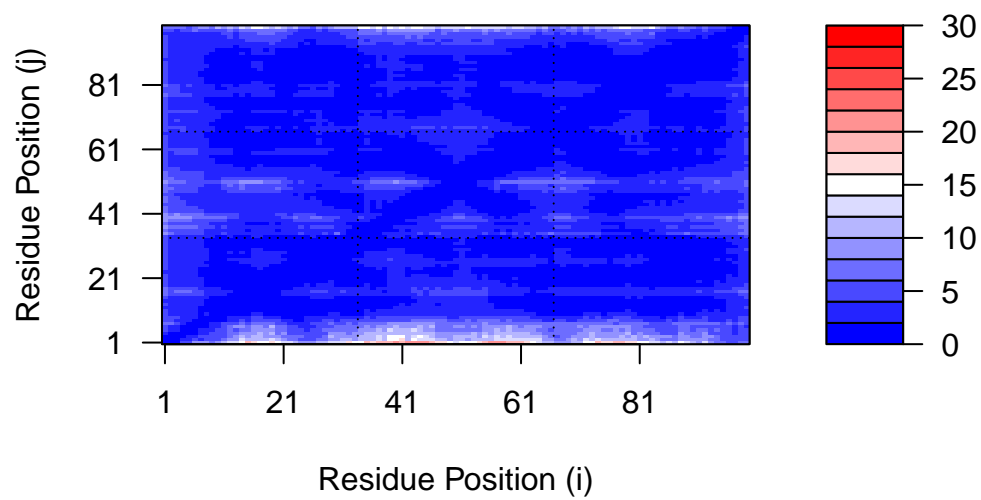
```
pae4$max_pae
```

```
[1] 21.65625
```

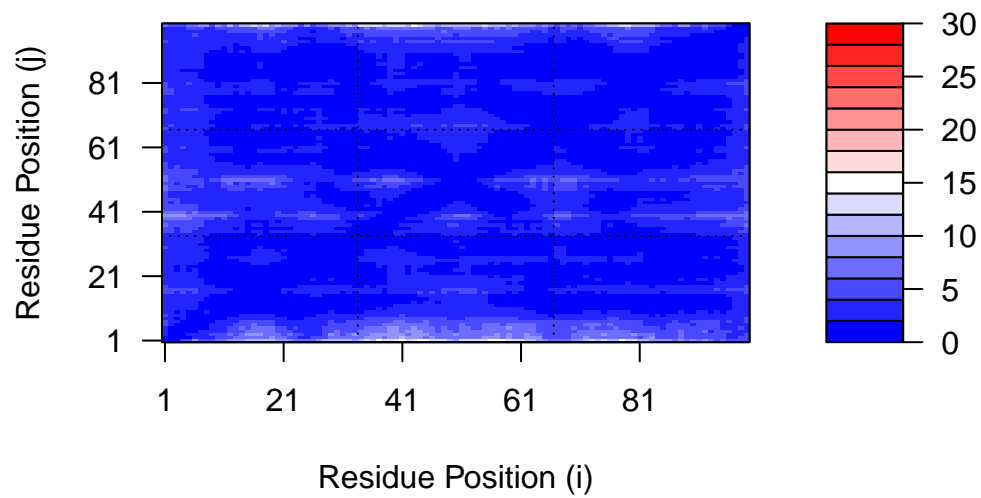
```
plot.dmat(pae2$pae,  
          xlab="Residue Position (i)",  
          ylab="Residue Position (j)")
```



```
plot.dmat(pae4$pae,  
          xlab="Residue Position (i)",  
          ylab="Residue Position (j)",  
          grid.col = "black",  
          zlim=c(0,30))
```



```
plot.dmat(pae2$pae,
  xlab="Residue Position (i)",
  ylab="Residue Position (j)",
  grid.col = "black",
  zlim=c(0,30))
```



```
aln_file <- list.files(path=gene_int,
                       pattern=".a3m$",
                       full.names = TRUE)
aln_file
```

```
[1] "find_a_gene_46bbf/find_a_gene_46bbf.a3m"
```

```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

```
[1] " ** Duplicated sequence id's: 101 **"
```

```
dim(aln$ali)
```

```
[1] 24878 1438
```

## HIV Dimer Analysis

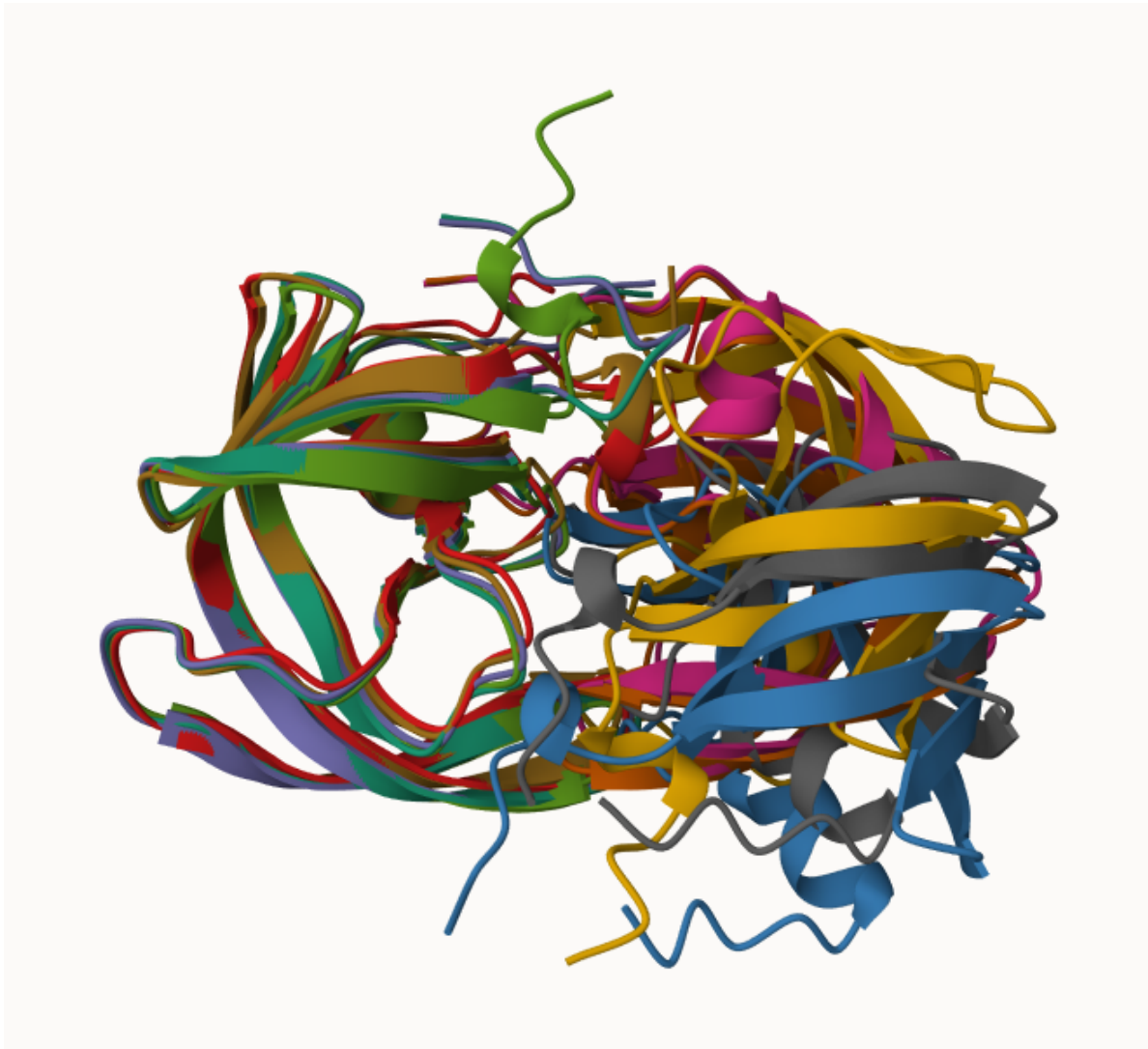


Figure 3: Superimposed image of HIV dimer

```
results_dimer <- "hivpr_dimer_23119"

pdb_dimer <- list.files(path=results_dimer,
                        pattern="*.pdb",
                        full.names = TRUE)

basename(pdb_dimer)
```

```
[1] "hivpr_monomer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb"
[2] "hivpr_monomer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
[3] "hivpr_monomer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[4] "hivpr_monomer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
[5] "hivpr_monomer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

```
library(bio3d)
```

```
pdb_dimer_f <- pdbaln(pdb_dimer, fit=TRUE, exefile="msa")
```

Reading PDB files:

```
hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb
hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb
hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
.....
```

Extracting sequences

```
pdb/seq: 1   name: hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb
pdb/seq: 2   name: hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
pdb/seq: 3   name: hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
pdb/seq: 4   name: hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb
pdb/seq: 5   name: hivpr_dimer_23119/hivpr_monomer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
```

```
pdb_dimer_f
```

```

1                                     .               .               .               .               50
[Truncated_Name:1]hivpr_mono  PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:2]hivpr_mono  PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:3]hivpr_mono  PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:4]hivpr_mono  PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
[Truncated_Name:5]hivpr_mono  PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGI
*****
1                                     .               .               .               .               50

51                                     .               .               .               .               100
[Truncated_Name:1]hivpr_mono  GGFIVKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:2]hivpr_mono  GGFIVKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:3]hivpr_mono  GGFIVKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
```

```

[Truncated_Name:4]hivpr_mono  GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
[Truncated_Name:5]hivpr_mono  GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP
                                *****
                                51                      100

                                101                    150
[Truncated_Name:1]hivpr_mono  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKMIGGIG
[Truncated_Name:2]hivpr_mono  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKMIGGIG
[Truncated_Name:3]hivpr_mono  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKMIGGIG
[Truncated_Name:4]hivpr_mono  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKMIGGIG
[Truncated_Name:5]hivpr_mono  QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKMIGGIG
                                *****
                                101                    150

                                151                    198
[Truncated_Name:1]hivpr_mono  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:2]hivpr_mono  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:3]hivpr_mono  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:4]hivpr_mono  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
[Truncated_Name:5]hivpr_mono  GFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF
                                *****
                                151                    198

```

Call:

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

Class:

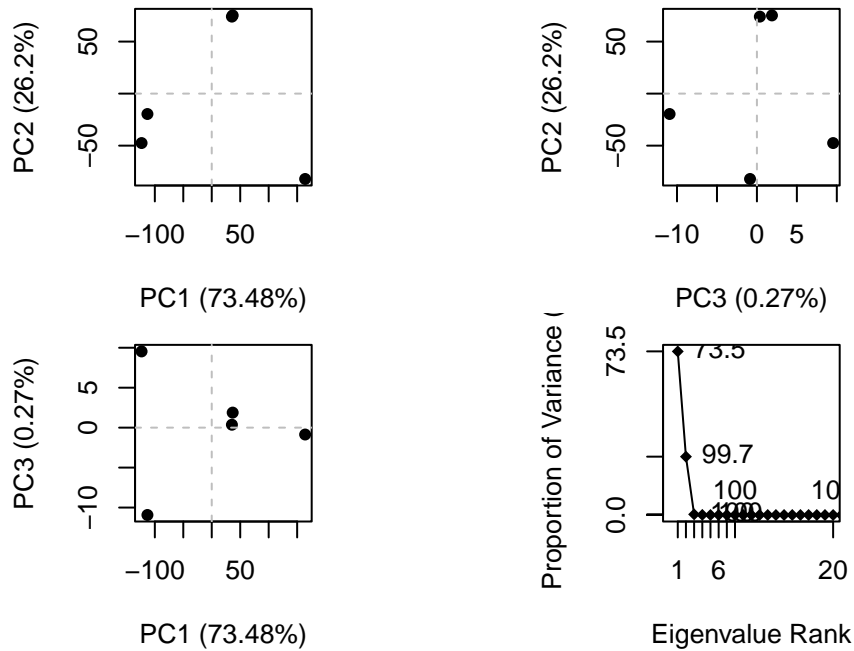
```
pdbs, fasta
```

Alignment dimensions:

```
5 sequence rows; 198 position columns (198 non-gap, 0 gap)
```

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

```
pc_dimer_f <- pca(pdb_dimer_f)
plot(pc_dimer_f)
```



```
rd_dimer <- rmsd(pdb_dimer_f, fit=T)
```

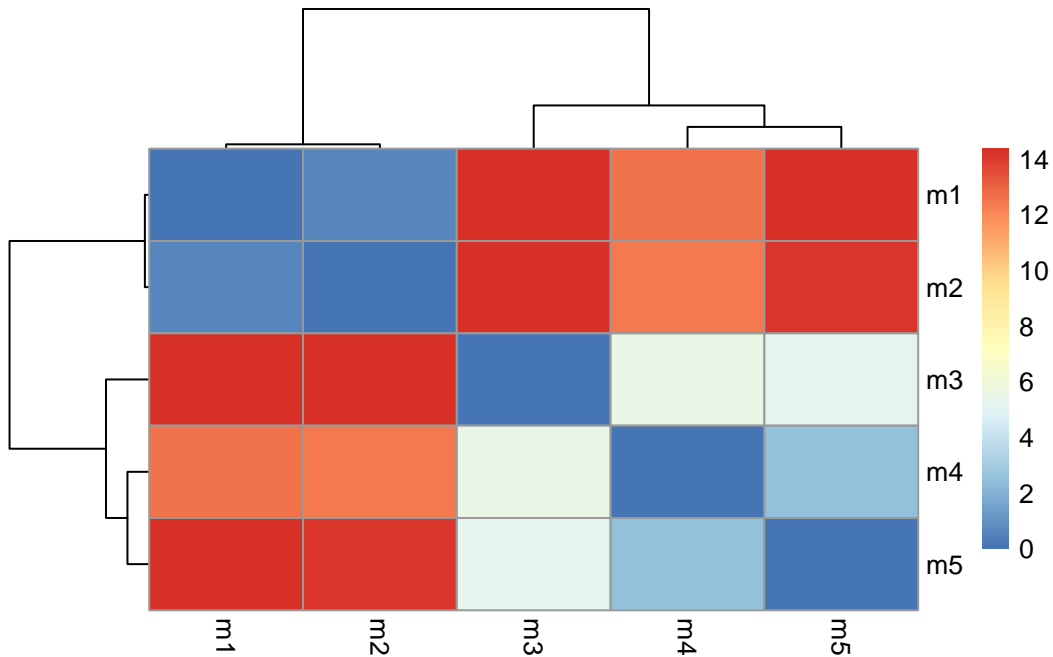
Warning in rmsd(pdb\_dimer\_f, fit = T): No indices provided, using the 198 non NA positions

```
range(rd_dimer)
```

```
[1] 0.000 14.376
```

```
library(pheatmap)
```

```
colnames(rd_dimer) <- paste0("m",1:5)
rownames(rd_dimer) <- paste0("m",1:5)
pheatmap(rd_dimer)
```



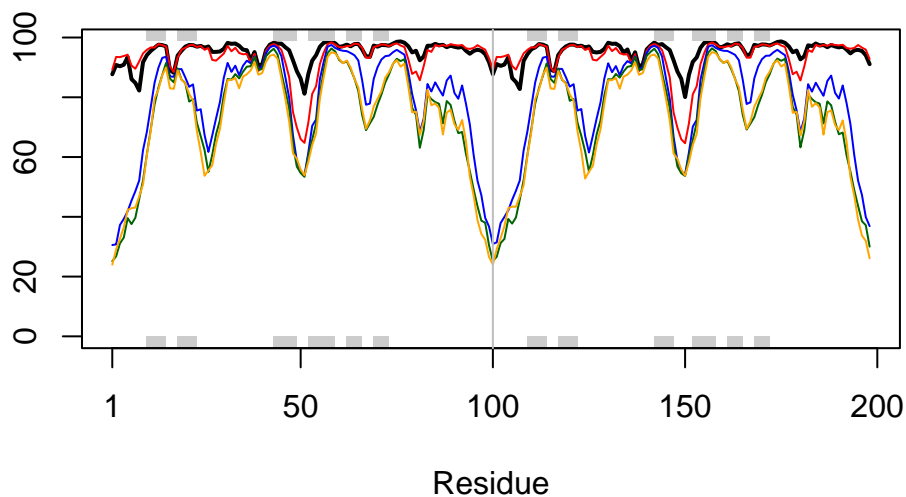
```
pdb_ref <- read.pdb("1hsg")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):  
C:\Users\Jg314\AppData\Local\Temp\RtmpsT3Gxm\1hsg.pdb exists. Skipping download

```
plotb3(pdb_dimer_f$b[1,], typ="l", lwd=2, sse=pdb_ref)
points(pdb_dimer_f$b[2,], typ="l", col="red")
points(pdb_dimer_f$b[3,], typ="l", col="blue")
points(pdb_dimer_f$b[4,], typ="l", col="darkgreen")
points(pdb_dimer_f$b[5,], typ="l", col="orange")
abline(v=100, col="gray")
```





```
core <- core.find(pdb_dimer_f)
```

```
core size 197 of 198 vol = 4916.702
core size 196 of 198 vol = 4311.481
core size 195 of 198 vol = 4101.445
core size 194 of 198 vol = 3907.124
core size 193 of 198 vol = 3711.925
core size 192 of 198 vol = 3546.511
core size 191 of 198 vol = 3440.437
core size 190 of 198 vol = 3317.571
core size 189 of 198 vol = 3220.079
core size 188 of 198 vol = 3142.057
core size 187 of 198 vol = 3066.79
core size 186 of 198 vol = 3015.892
core size 185 of 198 vol = 2959.969
core size 184 of 198 vol = 2913.74
core size 183 of 198 vol = 2880.923
core size 182 of 198 vol = 2848.081
core size 181 of 198 vol = 2857.001
core size 180 of 198 vol = 2871.24
core size 179 of 198 vol = 2905.696
core size 178 of 198 vol = 2953.776
```

core size 177 of 198 vol = 3020.847  
core size 176 of 198 vol = 3087.22  
core size 175 of 198 vol = 3109.99  
core size 174 of 198 vol = 3129.601  
core size 173 of 198 vol = 3135.085  
core size 172 of 198 vol = 3092.283  
core size 171 of 198 vol = 3036.012  
core size 170 of 198 vol = 2947.995  
core size 169 of 198 vol = 2886.897  
core size 168 of 198 vol = 2829.355  
core size 167 of 198 vol = 2746.377  
core size 166 of 198 vol = 2671.189  
core size 165 of 198 vol = 2600.848  
core size 164 of 198 vol = 2534.651  
core size 163 of 198 vol = 2464.3  
core size 162 of 198 vol = 2390.171  
core size 161 of 198 vol = 2322.47  
core size 160 of 198 vol = 2236.698  
core size 159 of 198 vol = 2160.475  
core size 158 of 198 vol = 2077.281  
core size 157 of 198 vol = 2003.596  
core size 156 of 198 vol = 1939.94  
core size 155 of 198 vol = 1859.188  
core size 154 of 198 vol = 1781.083  
core size 153 of 198 vol = 1699.1  
core size 152 of 198 vol = 1622.558  
core size 151 of 198 vol = 1546.319  
core size 150 of 198 vol = 1473.01  
core size 149 of 198 vol = 1414.087  
core size 148 of 198 vol = 1352.547  
core size 147 of 198 vol = 1295.278  
core size 146 of 198 vol = 1246.999  
core size 145 of 198 vol = 1203.962  
core size 144 of 198 vol = 1163.009  
core size 143 of 198 vol = 1110.955  
core size 142 of 198 vol = 1064.672  
core size 141 of 198 vol = 1028.458  
core size 140 of 198 vol = 986.121  
core size 139 of 198 vol = 944.003  
core size 138 of 198 vol = 895.914  
core size 137 of 198 vol = 853.508  
core size 136 of 198 vol = 827.977  
core size 135 of 198 vol = 796.874

core size 134 of 198 vol = 772.763  
core size 133 of 198 vol = 743.108  
core size 132 of 198 vol = 707.65  
core size 131 of 198 vol = 669.172  
core size 130 of 198 vol = 634.655  
core size 129 of 198 vol = 594.035  
core size 128 of 198 vol = 559.154  
core size 127 of 198 vol = 525.971  
core size 126 of 198 vol = 493.19  
core size 125 of 198 vol = 466.473  
core size 124 of 198 vol = 438.433  
core size 123 of 198 vol = 410.725  
core size 122 of 198 vol = 401.38  
core size 121 of 198 vol = 391.76  
core size 120 of 198 vol = 362.084  
core size 119 of 198 vol = 338.183  
core size 118 of 198 vol = 312.338  
core size 117 of 198 vol = 282.176  
core size 116 of 198 vol = 262.215  
core size 115 of 198 vol = 241.577  
core size 114 of 198 vol = 225.151  
core size 113 of 198 vol = 204.137  
core size 112 of 198 vol = 185.038  
core size 111 of 198 vol = 162.728  
core size 110 of 198 vol = 146.181  
core size 109 of 198 vol = 133.352  
core size 108 of 198 vol = 123.207  
core size 107 of 198 vol = 109.228  
core size 106 of 198 vol = 98.824  
core size 105 of 198 vol = 89.735  
core size 104 of 198 vol = 81.206  
core size 103 of 198 vol = 74.188  
core size 102 of 198 vol = 67.042  
core size 101 of 198 vol = 62.043  
core size 100 of 198 vol = 58.432  
core size 99 of 198 vol = 55.149  
core size 98 of 198 vol = 51.114  
core size 97 of 198 vol = 45.798  
core size 96 of 198 vol = 41.161  
core size 95 of 198 vol = 35.619  
core size 94 of 198 vol = 29.784  
core size 93 of 198 vol = 23.233  
core size 92 of 198 vol = 16.669

```

core size 91 of 198  vol = 9.459
core size 90 of 198  vol = 4.595
core size 89 of 198  vol = 3.161
core size 88 of 198  vol = 2.678
core size 87 of 198  vol = 2.293
core size 86 of 198  vol = 1.935
core size 85 of 198  vol = 1.619
core size 84 of 198  vol = 1.367
core size 83 of 198  vol = 1.09
core size 82 of 198  vol = 0.906
core size 81 of 198  vol = 0.764
core size 80 of 198  vol = 0.649
core size 79 of 198  vol = 0.596
core size 78 of 198  vol = 0.53
core size 77 of 198  vol = 0.486
FINISHED: Min vol ( 0.5 ) reached

```

```
core.inds <- print(core, vol=0.5)
```

```

# 78 positions (cumulative volume <= 0.5 Angstrom^3)
  start end length
1    10  25     16
2    28  48     21
3    53  93     41

```

```
xyz <- pdbfit(pdb_dimer_f, core.inds, outpath="corefit_structures")
```

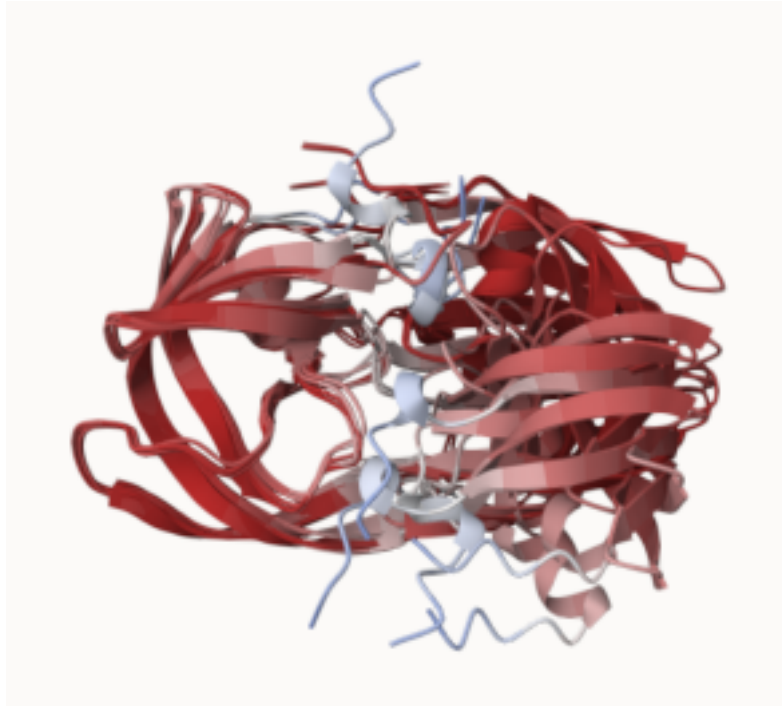
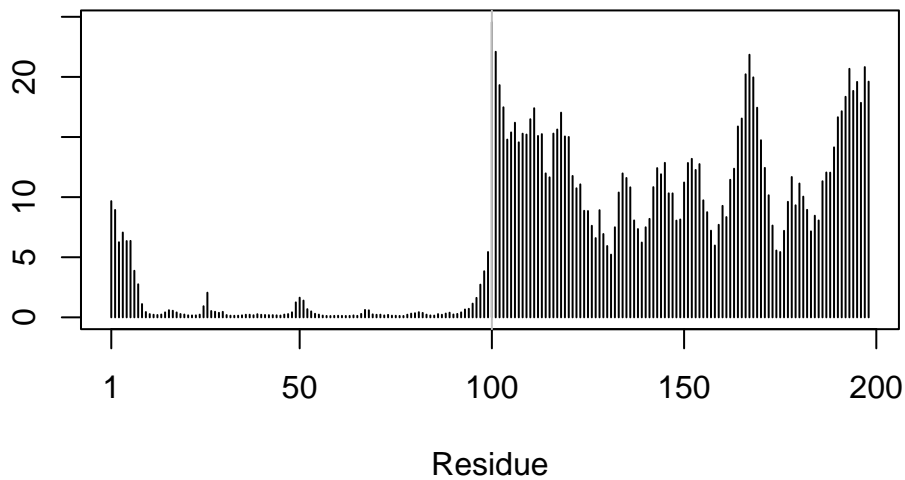


Figure 4: Core superimposed structure of dimer, colored by uncertainty and disorder

```
rf <- rmsf(xyz)
plotb3(rf, sse=pdb_dimer_f)
```

Warning in plotb3(rf, sse = pdb\_dimer\_f): Length of input 'sse' does not equal the length of input 'x'; Ignoring 'sse'

```
abline(v=100, col="gray", ylab="RMSF")
```



### Predicted alignment error for domains

```
library(jsonlite)
```

```
# Listing of all PAE JSON files
```

```
pae_files <- list.files(path=results_dimer,
                        pattern=".*model.*\\.json",
                        full.names = TRUE)
```

```
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
```

```
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)
```

```
attributes(pae1)
```

```
$names
```

```
[1] "plddt" "max_pae" "pae" "ptm" "iptm"
```

```
head(pae1$plddt)
```

```
[1] 87.69 90.81 90.38 90.88 93.44 86.06
```

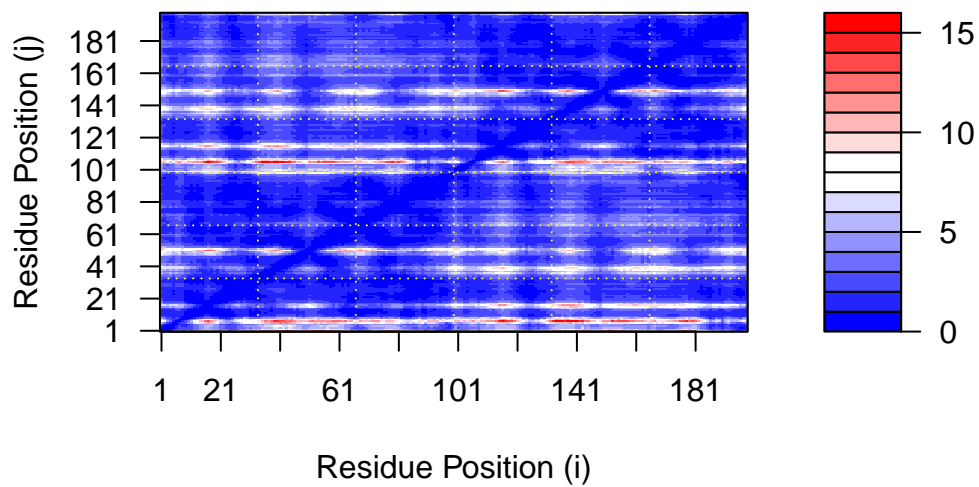
```
pae1$max_pae
```

```
[1] 15.47656
```

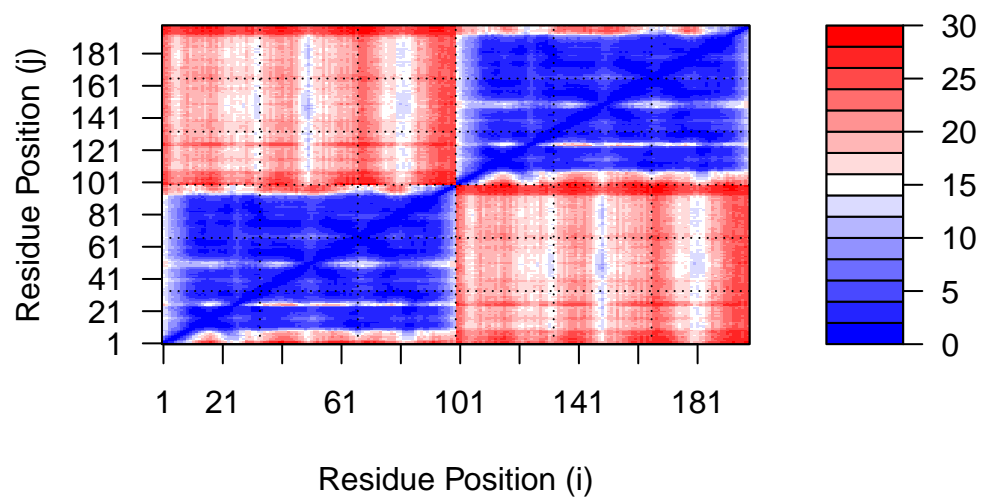
```
pae5$max_pae
```

```
[1] 29.32812
```

```
plot.dmat(pae1$pae,  
          xlab="Residue Position (i)",  
          ylab="Residue Position (j)")
```

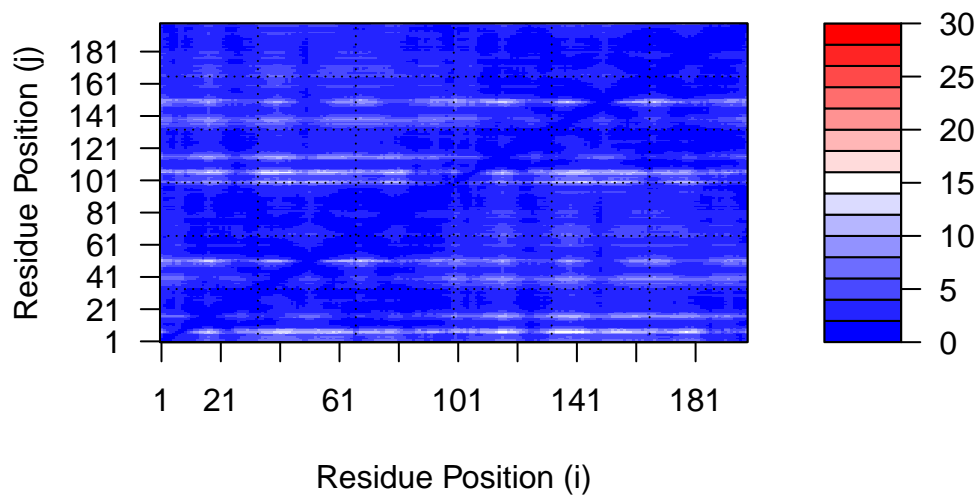


```
plot.dmat(pae5$pae,  
          xlab="Residue Position (i)",  
          ylab="Residue Position (j)",  
          grid.col = "black",  
          zlim=c(0,30))
```



```
plot.dmat(pae1$pae,
  xlab="Residue Position (i)",
  ylab="Residue Position (j)",
  grid.col = "black",
  zlim=c(0,30))
```





### Residue conservaion from alignment file

```
aln_file <- list.files(path=results_dimer,
                      pattern=".a3m$",
                      full.names = TRUE)
aln_file
```

```
[1] "hivpr_dimer_23119/hivpr_monomer_23119.a3m"
```

```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

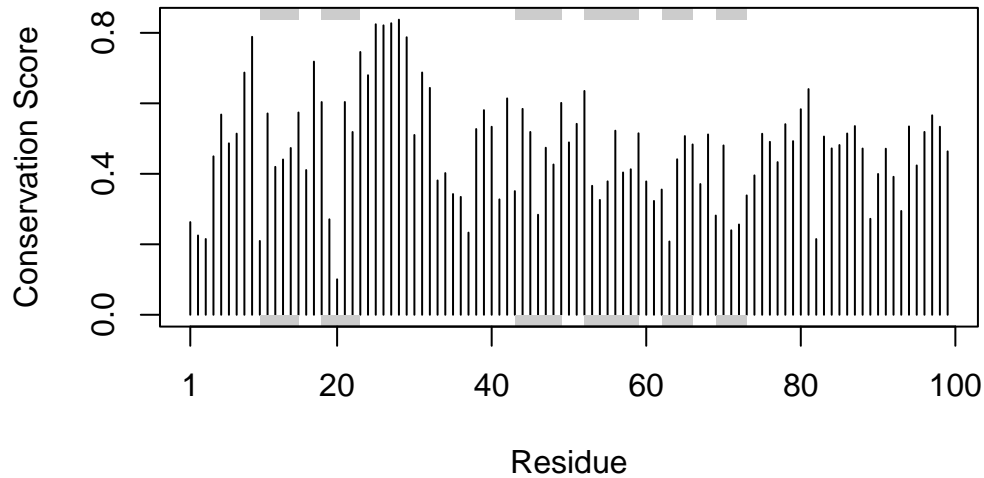
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

```
dim(aln$ali)
```

```
[1] 5378 132
```

```
sim <- conserv(aln)
```

```
plotb3(sim[1:99], sse=trim.pdb(pdb_ref, chain="A"),
       ylab="Conservation Score")
```



```
con <- consensus(aln, cutoff = 0.9)
con$seq
```

```
[1] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[19] "-" "-" "-" "-" "-" "-" "D" "T" "G" "A" "-" "-" "-" "-" "-" "-" "-"
[37] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[55] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[73] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[91] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[109] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[127] "-" "-" "-" "-" "-" "-"
```