

Class 11 - Protein Structure Prediction with AlphaFold

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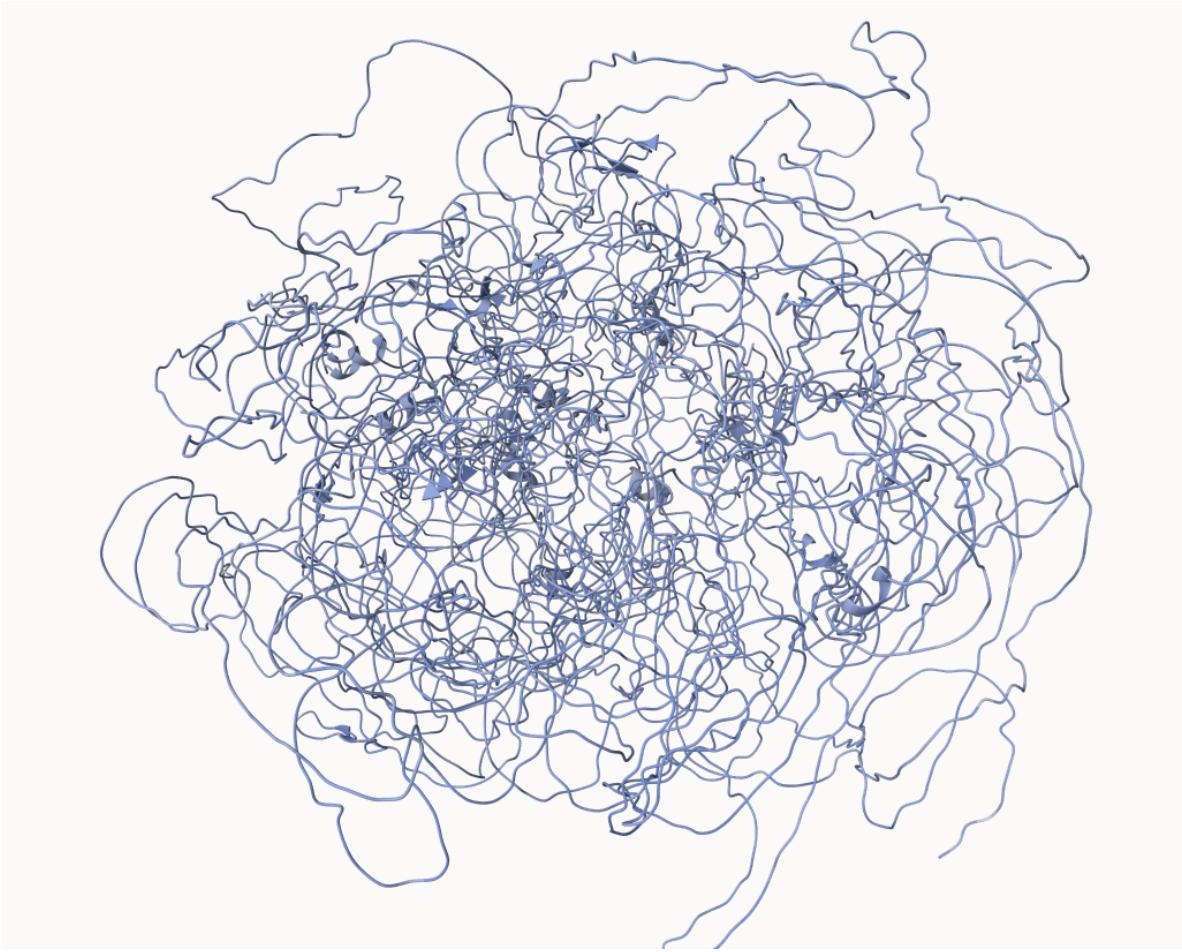
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The following is analysis of my proposed protein of interest for the Find-a-Gene project

The analysis of the HIV-Pr dimer is at the end

Here is the AlphaFold model of the initial set

```
knitr::include_graphics("PROTEINOFINTERESTFROMFASTA_504D5_UNRELAXED_RANK_001_ALPHAFOLD2_PTMs.png")
```



This should really preface what will happen later on in the analysis, because what the heck is this?

```
results_dir <- "ProteinofinterestfromFASTA_504d5"

# File names for all PDB models
pdb_files <- list.files(path=results_dir,
                         pattern="*.pdb",
                         full.names = TRUE)

# Print our PDB file names
basename(pdb_files)
```

```
[1] "ProteinofinterestfromFASTA_504d5_unrelaxed_rank_001_alphaFold2_ptm_model_2_seed_000.pdb"
[2] "ProteinofinterestfromFASTA_504d5_unrelaxed_rank_002_alphaFold2_ptm_model_5_seed_000.pdb"
```

```
[3] "ProteinofinterestfromFASTA_504d5_unrelaxed_rank_003_alphafold2_ptm_model_4_seed_000.pdb"
[4] "ProteinofinterestfromFASTA_504d5_unrelaxed_rank_004_alphafold2_ptm_model_3_seed_000.pdb"
[5] "ProteinofinterestfromFASTA_504d5_unrelaxed_rank_005_alphafold2_ptm_model_1_seed_000.pdb"
```

```
library(bio3d)

# Read all data from Models
# and superpose/fit coords
pdbs <- pdbaln(pdb_files, fit=TRUE, exefile="msa")
```

Reading PDB files:

```
ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelaxed_rank_001_alphafo
ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelaxed_rank_002_alphafo
ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelaxed_rank_003_alphafo
ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelaxed_rank_004_alphafo
ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelaxed_rank_005_alphafo
....
```

Extracting sequences

```
pdb/seq: 1 name: ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelax
pdb/seq: 2 name: ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelax
pdb/seq: 3 name: ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelax
pdb/seq: 4 name: ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelax
pdb/seq: 5 name: ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5_unrelax
```

```
pdbs
```

```
1 . . . 50
[Truncated_Name:1]Proteinofi GGCTGGTGCAGGGGCCGCGGTGAGGAGCTGCTGGTGCAGGGGCCACGC
[Truncated_Name:2]Proteinofi GGCTGGTGCAGGGGCCGCGGTGAGGAGCTGCTGGTGCAGGGGCCACGC
[Truncated_Name:3]Proteinofi GGCTGGTGCAGGGGCCGCGGTGAGGAGCTGCTGGTGCAGGGGCCACGC
[Truncated_Name:4]Proteinofi GGCTGGTGCAGGGGCCGCGGTGAGGAGCTGCTGGTGCAGGGGCCACGC
[Truncated_Name:5]Proteinofi GGCTGGTGCAGGGGCCGCGGTGAGGAGCTGCTGGTGCAGGGGCCACGC
*****
1 . . . 50
51 . . . 100
[Truncated_Name:1]Proteinofi GGGGAGCAGCCTCCTGGCCCTGTCATCTCTGTCAGGAGAAA
[Truncated_Name:2]Proteinofi GGGGAGCAGCCTCCTGGCCCTGTCATCTCTGTCAGGAGAAA
[Truncated_Name:3]Proteinofi GGGGAGCAGCCTCCTGGCCCTGTCATCTCTGTCAGGAGAAA
```

[Truncated_Name:4]Proteinofi	GGGGAGCAGCCTCCTGGCCCTGTCATCTCTGCCCTCCCAGAAA		
[Truncated_Name:5]Proteinofi	GGGGAGCAGCCTCCTGGCCCTGTCATCTCTGCCCTCCCAGAAA		

51	.	.	100
101	.	.	150
[Truncated_Name:1]Proteinofi	ACCTACCAGGGCAGCTACGGTTCCGTCTGGGCTTCTGCATTCTGGGAC		
[Truncated_Name:2]Proteinofi	ACCTACCAGGGCAGCTACGGTTCCGTCTGGGCTTCTGCATTCTGGGAC		
[Truncated_Name:3]Proteinofi	ACCTACCAGGGCAGCTACGGTTCCGTCTGGGCTTCTGCATTCTGGGAC		
[Truncated_Name:4]Proteinofi	ACCTACCAGGGCAGCTACGGTTCCGTCTGGGCTTCTGCATTCTGGGAC		
[Truncated_Name:5]Proteinofi	ACCTACCAGGGCAGCTACGGTTCCGTCTGGGCTTCTGCATTCTGGGAC		

101	.	.	150
151	.	.	200
[Truncated_Name:1]Proteinofi	AGCCAAGTCTGTGACTTGACGTACTCCCCCTGCCCTAACAAAGATGTTT		
[Truncated_Name:2]Proteinofi	AGCCAAGTCTGTGACTTGACGTACTCCCCCTGCCCTAACAAAGATGTTT		
[Truncated_Name:3]Proteinofi	AGCCAAGTCTGTGACTTGACGTACTCCCCCTGCCCTAACAAAGATGTTT		
[Truncated_Name:4]Proteinofi	AGCCAAGTCTGTGACTTGACGTACTCCCCCTGCCCTAACAAAGATGTTT		
[Truncated_Name:5]Proteinofi	AGCCAAGTCTGTGACTTGACGTACTCCCCCTGCCCTAACAAAGATGTTT		

151	.	.	200
201	.	.	250
[Truncated_Name:1]Proteinofi	GCCAAGTGGCAAGACCTGCCCTGTGCAGCTGTGGGTTGATTCCACACCC		
[Truncated_Name:2]Proteinofi	GCCAAGTGGCAAGACCTGCCCTGTGCAGCTGTGGGTTGATTCCACACCC		
[Truncated_Name:3]Proteinofi	GCCAAGTGGCAAGACCTGCCCTGTGCAGCTGTGGGTTGATTCCACACCC		
[Truncated_Name:4]Proteinofi	GCCAAGTGGCAAGACCTGCCCTGTGCAGCTGTGGGTTGATTCCACACCC		
[Truncated_Name:5]Proteinofi	GCCAAGTGGCAAGACCTGCCCTGTGCAGCTGTGGGTTGATTCCACACCC		

201	.	.	250
251	.	.	300
[Truncated_Name:1]Proteinofi	CCGCCCCGGCACCCCGTCCCGGCCATGGCATCTACAAGCAGTCACAGCA		
[Truncated_Name:2]Proteinofi	CCGCCCCGGCACCCCGTCCCGGCCATGGCATCTACAAGCAGTCACAGCA		
[Truncated_Name:3]Proteinofi	CCGCCCCGGCACCCCGTCCCGGCCATGGCATCTACAAGCAGTCACAGCA		
[Truncated_Name:4]Proteinofi	CCGCCCCGGCACCCCGTCCCGGCCATGGCATCTACAAGCAGTCACAGCA		
[Truncated_Name:5]Proteinofi	CCGCCCCGGCACCCCGTCCCGGCCATGGCATCTACAAGCAGTCACAGCA		

251	.	.	300
301	.	.	350
[Truncated_Name:1]Proteinofi	CATGACGGAGGTTGTGAGGCCTGCCACCATGAGCGCTGCTCAGATA		

[Truncated_Name:2]Proteinofi	CATGACGGAGGTTGTGAGGCCTGCCACCCTGAGCGCTGCTCAGATA			
[Truncated_Name:3]Proteinofi	CATGACGGAGGTTGTGAGGCCTGCCACCCTGAGCGCTGCTCAGATA			
[Truncated_Name:4]Proteinofi	CATGACGGAGGTTGTGAGGCCTGCCACCCTGAGCGCTGCTCAGATA			
[Truncated_Name:5]Proteinofi	CATGACGGAGGTTGTGAGGCCTGCCACCCTGAGCGCTGCTCAGATA			

301	.	.	.	350
351	.	.	.	400
[Truncated_Name:1]Proteinofi	GCGATGGTCTGGCCCCTCCTCAGCATCTTATCCGAGTGGAAAGGAATTG			
[Truncated_Name:2]Proteinofi	GCGATGGTCTGGCCCCTCCTCAGCATCTTATCCGAGTGGAAAGGAATTG			
[Truncated_Name:3]Proteinofi	GCGATGGTCTGGCCCCTCCTCAGCATCTTATCCGAGTGGAAAGGAATTG			
[Truncated_Name:4]Proteinofi	GCGATGGTCTGGCCCCTCCTCAGCATCTTATCCGAGTGGAAAGGAATTG			
[Truncated_Name:5]Proteinofi	GCGATGGTCTGGCCCCTCCTCAGCATCTTATCCGAGTGGAAAGGAATTG			

351	.	.	.	400
401	.	.	.	450
[Truncated_Name:1]Proteinofi	CGTGTGGAGTATTGGATGACAGAACACTTTCGACATAGTGTGGTGGT			
[Truncated_Name:2]Proteinofi	CGTGTGGAGTATTGGATGACAGAACACTTTCGACATAGTGTGGTGGT			
[Truncated_Name:3]Proteinofi	CGTGTGGAGTATTGGATGACAGAACACTTTCGACATAGTGTGGTGGT			
[Truncated_Name:4]Proteinofi	CGTGTGGAGTATTGGATGACAGAACACTTTCGACATAGTGTGGTGGT			
[Truncated_Name:5]Proteinofi	CGTGTGGAGTATTGGATGACAGAACACTTTCGACATAGTGTGGTGGT			

401	.	.	.	450
451	.	.	.	500
[Truncated_Name:1]Proteinofi	GCCCTATGAGCCGCTGAGGTTGGCTCTGACTGTACCACCATCCACTACA			
[Truncated_Name:2]Proteinofi	GCCCTATGAGCCGCTGAGGTTGGCTCTGACTGTACCACCATCCACTACA			
[Truncated_Name:3]Proteinofi	GCCCTATGAGCCGCTGAGGTTGGCTCTGACTGTACCACCATCCACTACA			
[Truncated_Name:4]Proteinofi	GCCCTATGAGCCGCTGAGGTTGGCTCTGACTGTACCACCATCCACTACA			
[Truncated_Name:5]Proteinofi	GCCCTATGAGCCGCTGAGGTTGGCTCTGACTGTACCACCATCCACTACA			

451	.	.	.	500
501	.	.	.	550
[Truncated_Name:1]Proteinofi	ACTACATGTGTAACAGTTCTGCATGGCGGCATGAACCGGAGGCCATC			
[Truncated_Name:2]Proteinofi	ACTACATGTGTAACAGTTCTGCATGGCGGCATGAACCGGAGGCCATC			
[Truncated_Name:3]Proteinofi	ACTACATGTGTAACAGTTCTGCATGGCGGCATGAACCGGAGGCCATC			
[Truncated_Name:4]Proteinofi	ACTACATGTGTAACAGTTCTGCATGGCGGCATGAACCGGAGGCCATC			
[Truncated_Name:5]Proteinofi	ACTACATGTGTAACAGTTCTGCATGGCGGCATGAACCGGAGGCCATC			

501	.	.	.	550

	551	.	.	.	600
[Truncated_Name:1]Proteinofi	CTCACCATCATCACACTGGAAGACTCCAGTGGTAATCTACTGGGACGGAA				
[Truncated_Name:2]Proteinofi	CTCACCATCATCACACTGGAAGACTCCAGTGGTAATCTACTGGGACGGAA				
[Truncated_Name:3]Proteinofi	CTCACCATCATCACACTGGAAGACTCCAGTGGTAATCTACTGGGACGGAA				
[Truncated_Name:4]Proteinofi	CTCACCATCATCACACTGGAAGACTCCAGTGGTAATCTACTGGGACGGAA				
[Truncated_Name:5]Proteinofi	CTCACCATCATCACACTGGAAGACTCCAGTGGTAATCTACTGGGACGGAA				

	551	.	.	.	600
	601	.	.	.	650
[Truncated_Name:1]Proteinofi	CAGCTTGAGGTGCGTGTTCGCCTGCCTGGGAGAGACCGGGCGCACAG				
[Truncated_Name:2]Proteinofi	CAGCTTGAGGTGCGTGTTCGCCTGCCTGGGAGAGACCGGGCGCACAG				
[Truncated_Name:3]Proteinofi	CAGCTTGAGGTGCGTGTTCGCCTGCCTGGGAGAGACCGGGCGCACAG				
[Truncated_Name:4]Proteinofi	CAGCTTGAGGTGCGTGTTCGCCTGCCTGGGAGAGACCGGGCGCACAG				
[Truncated_Name:5]Proteinofi	CAGCTTGAGGTGCGTGTTCGCCTGCCTGGGAGAGACCGGGCGCACAG				

	601	.	.	.	650
	651	.	.	.	700
[Truncated_Name:1]Proteinofi	AGGAAGAGAACCTCCGCAAGAAAGGGAGCCTCACACGAGCTGCCCGCA				
[Truncated_Name:2]Proteinofi	AGGAAGAGAACCTCCGCAAGAAAGGGAGCCTCACACGAGCTGCCCGCA				
[Truncated_Name:3]Proteinofi	AGGAAGAGAACCTCCGCAAGAAAGGGAGCCTCACACGAGCTGCCCGCA				
[Truncated_Name:4]Proteinofi	AGGAAGAGAACCTCCGCAAGAAAGGGAGCCTCACACGAGCTGCCCGCA				
[Truncated_Name:5]Proteinofi	AGGAAGAGAACCTCCGCAAGAAAGGGAGCCTCACACGAGCTGCCCGCA				

	651	.	.	.	700
	701	.	.	.	750
[Truncated_Name:1]Proteinofi	GGGAGCACTAAGCGAGCACTGGCAACAAAAACAGCTTCCTTTCCCAGG				
[Truncated_Name:2]Proteinofi	GGGAGCACTAAGCGAGCACTGGCAACAAAAACAGCTTCCTTTCCCAGG				
[Truncated_Name:3]Proteinofi	GGGAGCACTAAGCGAGCACTGGCAACAAAAACAGCTTCCTTTCCCAGG				
[Truncated_Name:4]Proteinofi	GGGAGCACTAAGCGAGCACTGGCAACAAAAACAGCTTCCTTTCCCAGG				
[Truncated_Name:5]Proteinofi	GGGAGCACTAAGCGAGCACTGGCAACAAAAACAGCTTCCTTTCCCAGG				

	701	.	.	.	750
	751	.	.	.	800
[Truncated_Name:1]Proteinofi	CCAAAAAAAACCCCTGGATGGAAAAATATTCCACCCCTTCAAATCC				
[Truncated_Name:2]Proteinofi	CCAAAAAAAACCCCTGGATGGAAAAATATTCCACCCCTTCAAATCC				
[Truncated_Name:3]Proteinofi	CCAAAAAAAACCCCTGGATGGAAAAATATTCCACCCCTTCAAATCC				
[Truncated_Name:4]Proteinofi	CCAAAAAAAACCCCTGGATGGAAAAATATTCCACCCCTTCAAATCC				
[Truncated_Name:5]Proteinofi	CCAAAAAAAACCCCTGGATGGAAAAATATTCCACCCCTTCAAATCC				

```
751 . . . 800
801 . . . 850
[Truncated_Name:1]Proteinofi CGTGGGCCGTGAAACCCCTTCAAAAATGTTCCCACGAATTGAAATGAG
[Truncated_Name:2]Proteinofi CGTGGGCCGTGAAACCCCTTCAAAAATGTTCCCACGAATTGAAATGAG
[Truncated_Name:3]Proteinofi CGTGGGCCGTGAAACCCCTTCAAAAATGTTCCCACGAATTGAAATGAG
[Truncated_Name:4]Proteinofi CGTGGGCCGTGAAACCCCTTCAAAAATGTTCCCACGAATTGAAATGAG
[Truncated_Name:5]Proteinofi CGTGGGCCGTGAAACCCCTTCAAAAATGTTCCCACGAATTGAAATGAG
*****
```

```
801 . . . 850
```

```
851 . 862
[Truncated_Name:1]Proteinofi GGCCTGGAAAC
[Truncated_Name:2]Proteinofi GGCCTGGAAAC
[Truncated_Name:3]Proteinofi GGCCTGGAAAC
[Truncated_Name:4]Proteinofi GGCCTGGAAAC
[Truncated_Name:5]Proteinofi GGCCTGGAAAC
*****
```

```
851 . 862
```

Call:

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

Class:

```
pdb, fasta
```

Alignment dimensions:

```
5 sequence rows; 862 position columns (862 non-gap, 0 gap)
```

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

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

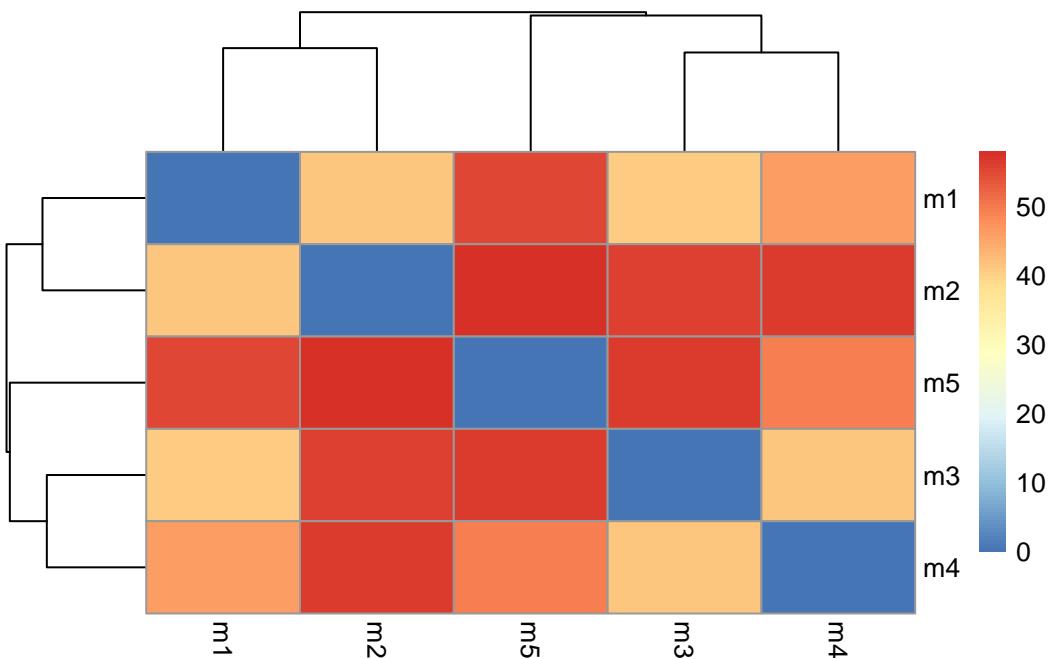
Warning in rmsd(pdb, fit = T): No indices provided, using the 862 non NA positions

```
range(rd)
```

```
[1] 0.00 57.89
```

```
# Drawing a heatmap of RMSD matrix values
## install.packages("pheatmap")
library(pheatmap)

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



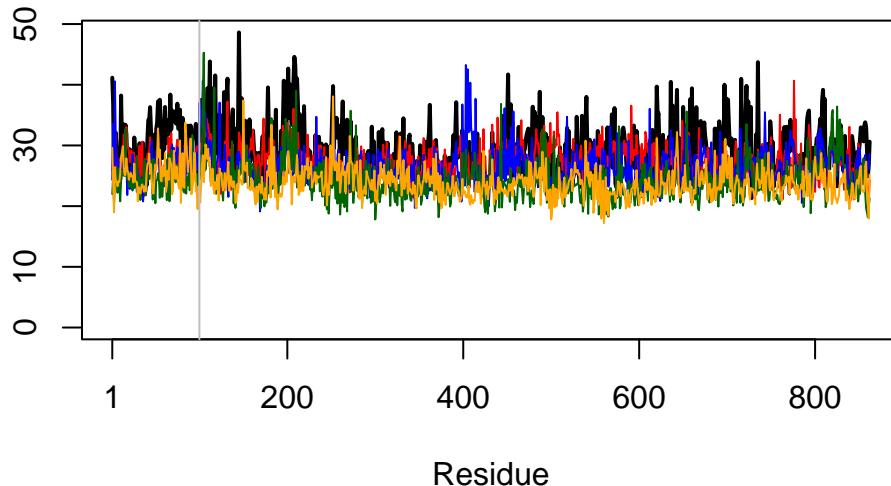
```
# Read a reference PDB structure,
# Reference for protein of interest is "AF-P04637-F1-model_v4.pdb"
pdb <- read.pdb("AF-P04637-F1-model_v4.pdb")
```

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

Warning in pdb2sse(sse): No helix and sheet defined in input 'sse' PDB object:
try using dssp()

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

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



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

```
core size 861 of 862  vol = 14923181
core size 860 of 862  vol = 14673464
core size 859 of 862  vol = 14568144
core size 858 of 862  vol = 14520179
core size 857 of 862  vol = 14493228
core size 856 of 862  vol = 14474476
core size 855 of 862  vol = 14452515
core size 854 of 862  vol = 14429526
core size 853 of 862  vol = 14409548
core size 852 of 862  vol = 14392436
core size 851 of 862  vol = 14373424
core size 850 of 862  vol = 14352818
core size 849 of 862  vol = 14331869
core size 848 of 862  vol = 14300955
```

```
core size 847 of 862 vol = 14275797
core size 846 of 862 vol = 14255099
core size 845 of 862 vol = 14214793
core size 844 of 862 vol = 14187095
core size 843 of 862 vol = 14141020
core size 842 of 862 vol = 14091274
core size 841 of 862 vol = 14041956
core size 840 of 862 vol = 13995535
core size 839 of 862 vol = 13950901
core size 838 of 862 vol = 13904941
core size 837 of 862 vol = 13855340
core size 836 of 862 vol = 13807999
core size 835 of 862 vol = 13760713
core size 834 of 862 vol = 13727660
core size 833 of 862 vol = 13682424
core size 832 of 862 vol = 13633300
core size 831 of 862 vol = 13582504
core size 830 of 862 vol = 13531220
core size 829 of 862 vol = 13492642
core size 828 of 862 vol = 13443079
core size 827 of 862 vol = 13390746
core size 826 of 862 vol = 13348875
core size 825 of 862 vol = 13297786
core size 824 of 862 vol = 13238977
core size 823 of 862 vol = 13191613
core size 822 of 862 vol = 13132779
core size 821 of 862 vol = 13069508
core size 820 of 862 vol = 12999213
core size 819 of 862 vol = 12924853
core size 818 of 862 vol = 12848496
core size 817 of 862 vol = 12769399
core size 816 of 862 vol = 12686326
core size 815 of 862 vol = 12600242
core size 814 of 862 vol = 12514567
core size 813 of 862 vol = 12426439
core size 812 of 862 vol = 12350698
core size 811 of 862 vol = 12265413
core size 810 of 862 vol = 12178551
core size 809 of 862 vol = 12095491
core size 808 of 862 vol = 12007428
core size 807 of 862 vol = 11920955
core size 806 of 862 vol = 11842169
core size 805 of 862 vol = 11757531
```

```
core size 804 of 862  vol = 11674210
core size 803 of 862  vol = 11600281
core size 802 of 862  vol = 11521465
core size 801 of 862  vol = 11445222
core size 800 of 862  vol = 11392486
core size 799 of 862  vol = 11348243
core size 798 of 862  vol = 11296040
core size 797 of 862  vol = 11248381
core size 796 of 862  vol = 11187694
core size 795 of 862  vol = 11121888
core size 794 of 862  vol = 11047021
core size 793 of 862  vol = 11000172
core size 792 of 862  vol = 10935658
core size 791 of 862  vol = 10880623
core size 790 of 862  vol = 10823809
core size 789 of 862  vol = 10766873
core size 788 of 862  vol = 10717160
core size 787 of 862  vol = 10662302
core size 786 of 862  vol = 10624688
core size 785 of 862  vol = 10574737
core size 784 of 862  vol = 10524641
core size 783 of 862  vol = 10473165
core size 782 of 862  vol = 10424635
core size 781 of 862  vol = 10377491
core size 780 of 862  vol = 10327057
core size 779 of 862  vol = 10280775
core size 778 of 862  vol = 10233551
core size 777 of 862  vol = 10210204
core size 776 of 862  vol = 10164409
core size 775 of 862  vol = 10119199
core size 774 of 862  vol = 10075671
core size 773 of 862  vol = 10033163
core size 772 of 862  vol = 9985966
core size 771 of 862  vol = 9965747
core size 770 of 862  vol = 9930488
core size 769 of 862  vol = 9882968
core size 768 of 862  vol = 9864170
core size 767 of 862  vol = 9829496
core size 766 of 862  vol = 9776290
core size 765 of 862  vol = 9720164
core size 764 of 862  vol = 9664144
core size 763 of 862  vol = 9607649
core size 762 of 862  vol = 9552585
```

```
core size 761 of 862 vol = 9531461
core size 760 of 862 vol = 9518049
core size 759 of 862 vol = 9501977
core size 758 of 862 vol = 9487272
core size 757 of 862 vol = 9483685
core size 756 of 862 vol = 9451202
core size 755 of 862 vol = 9417595
core size 754 of 862 vol = 9396444
core size 753 of 862 vol = 9352620
core size 752 of 862 vol = 9319839
core size 751 of 862 vol = 9281408
core size 750 of 862 vol = 9272971
core size 749 of 862 vol = 9236179
core size 748 of 862 vol = 9191092
core size 747 of 862 vol = 9143474
core size 746 of 862 vol = 9094916
core size 745 of 862 vol = 9052822
core size 744 of 862 vol = 9034785
core size 743 of 862 vol = 9001342
core size 742 of 862 vol = 8965272
core size 741 of 862 vol = 8929114
core size 740 of 862 vol = 8892734
core size 739 of 862 vol = 8850543
core size 738 of 862 vol = 8812053
core size 737 of 862 vol = 8771893
core size 736 of 862 vol = 8738074
core size 735 of 862 vol = 8703215
core size 734 of 862 vol = 8666594
core size 733 of 862 vol = 8622725
core size 732 of 862 vol = 8591992
core size 731 of 862 vol = 8561372
core size 730 of 862 vol = 8528534
core size 729 of 862 vol = 8493457
core size 728 of 862 vol = 8472618
core size 727 of 862 vol = 8442702
core size 726 of 862 vol = 8410435
core size 725 of 862 vol = 8375733
core size 724 of 862 vol = 8356425
core size 723 of 862 vol = 8327243
core size 722 of 862 vol = 8294107
core size 721 of 862 vol = 8257450
core size 720 of 862 vol = 8222251
core size 719 of 862 vol = 8183940
```

```
core size 718 of 862 vol = 8145089
core size 717 of 862 vol = 8106774
core size 716 of 862 vol = 8073433
core size 715 of 862 vol = 8037846
core size 714 of 862 vol = 7999003
core size 713 of 862 vol = 7963833
core size 712 of 862 vol = 7932309
core size 711 of 862 vol = 7900398
core size 710 of 862 vol = 7870674
core size 709 of 862 vol = 7840486
core size 708 of 862 vol = 7808737
core size 707 of 862 vol = 7769934
core size 706 of 862 vol = 7731208
core size 705 of 862 vol = 7697256
core size 704 of 862 vol = 7696690
core size 703 of 862 vol = 7670289
core size 702 of 862 vol = 7642634
core size 701 of 862 vol = 7611649
core size 700 of 862 vol = 7582474
core size 699 of 862 vol = 7554222
core size 698 of 862 vol = 7521759
core size 697 of 862 vol = 7478060
core size 696 of 862 vol = 7446830
core size 695 of 862 vol = 7416025
core size 694 of 862 vol = 7380844
core size 693 of 862 vol = 7343536
core size 692 of 862 vol = 7310554
core size 691 of 862 vol = 7273933
core size 690 of 862 vol = 7246554
core size 689 of 862 vol = 7221177
core size 688 of 862 vol = 7195005
core size 687 of 862 vol = 7167932
core size 686 of 862 vol = 7140500
core size 685 of 862 vol = 7101566
core size 684 of 862 vol = 7062665
core size 683 of 862 vol = 7033322
core size 682 of 862 vol = 7005702
core size 681 of 862 vol = 6968319
core size 680 of 862 vol = 6931684
core size 679 of 862 vol = 6895321
core size 678 of 862 vol = 6879871
core size 677 of 862 vol = 6852458
core size 676 of 862 vol = 6840717
```

```
core size 675 of 862 vol = 6818446
core size 674 of 862 vol = 6795657
core size 673 of 862 vol = 6772934
core size 672 of 862 vol = 6763269
core size 671 of 862 vol = 6743959
core size 670 of 862 vol = 6714210
core size 669 of 862 vol = 6684924
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core size 633 of 862 vol = 6068412
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core size 84 of 862 vol = 54503.98
core size 83 of 862 vol = 53191.85
core size 82 of 862 vol = 52391.31
core size 81 of 862 vol = 51816.94
core size 80 of 862 vol = 50969.91
core size 79 of 862 vol = 49259.14
core size 78 of 862 vol = 47073.93
core size 77 of 862 vol = 44928.88
core size 76 of 862 vol = 42546.96
core size 75 of 862 vol = 40226.11
core size 74 of 862 vol = 38369.75
```

```
core size 73 of 862 vol = 36941.94
core size 72 of 862 vol = 35560.57
core size 71 of 862 vol = 34164.78
core size 70 of 862 vol = 32726.81
core size 69 of 862 vol = 31141.15
core size 68 of 862 vol = 29341.24
core size 67 of 862 vol = 27914.21
core size 66 of 862 vol = 26805.26
core size 65 of 862 vol = 25243.14
core size 64 of 862 vol = 24209.74
core size 63 of 862 vol = 22894.54
core size 62 of 862 vol = 21520.08
core size 61 of 862 vol = 20607.21
core size 60 of 862 vol = 19501.14
core size 59 of 862 vol = 18430.33
core size 58 of 862 vol = 17329.81
core size 57 of 862 vol = 16186.36
core size 56 of 862 vol = 15176.47
core size 55 of 862 vol = 14139.51
core size 54 of 862 vol = 13341.23
core size 53 of 862 vol = 12827.74
core size 52 of 862 vol = 12361.62
core size 51 of 862 vol = 11803.36
core size 50 of 862 vol = 11269.89
core size 49 of 862 vol = 10759.38
core size 48 of 862 vol = 10360.41
core size 47 of 862 vol = 9600.398
core size 46 of 862 vol = 9154.469
core size 45 of 862 vol = 8841.7
core size 44 of 862 vol = 8529.917
core size 43 of 862 vol = 8082.282
core size 42 of 862 vol = 7203.198
core size 41 of 862 vol = 6422.092
core size 40 of 862 vol = 5836.059
core size 39 of 862 vol = 5412.672
core size 38 of 862 vol = 5039.886
core size 37 of 862 vol = 4747.069
core size 36 of 862 vol = 4452.278
core size 35 of 862 vol = 4182.016
core size 34 of 862 vol = 4015.358
core size 33 of 862 vol = 3623.023
core size 32 of 862 vol = 3293.066
core size 31 of 862 vol = 3181.074
```

```
core size 30 of 862  vol = 3078.067
core size 29 of 862  vol = 2921.919
core size 28 of 862  vol = 2488.682
core size 27 of 862  vol = 1887.583
core size 26 of 862  vol = 1592.242
core size 25 of 862  vol = 1471.91
core size 24 of 862  vol = 1370.965
core size 23 of 862  vol = 1239.589
core size 22 of 862  vol = 1183.381
core size 21 of 862  vol = 1089.467
core size 20 of 862  vol = 1022.146
core size 19 of 862  vol = 806.567
core size 18 of 862  vol = 639.298
core size 17 of 862  vol = 485.77
core size 16 of 862  vol = 344.517
core size 15 of 862  vol = 286.234
```

```
core inds <- print(core, vol=1000)
```

```
# 20 positions (cumulative volume <= 1000 Angstrom^3)
  start end length
1    252 263     12
2    706 713      8
```

```
#Note, had to adjust threshold to find core positions.
```

```
xyz <- pdbfit(pdbs, core inds, outpath="corefit_structures")
# Notice that for core inds, and from the msa from above, we had no atom, xyz, or resno data

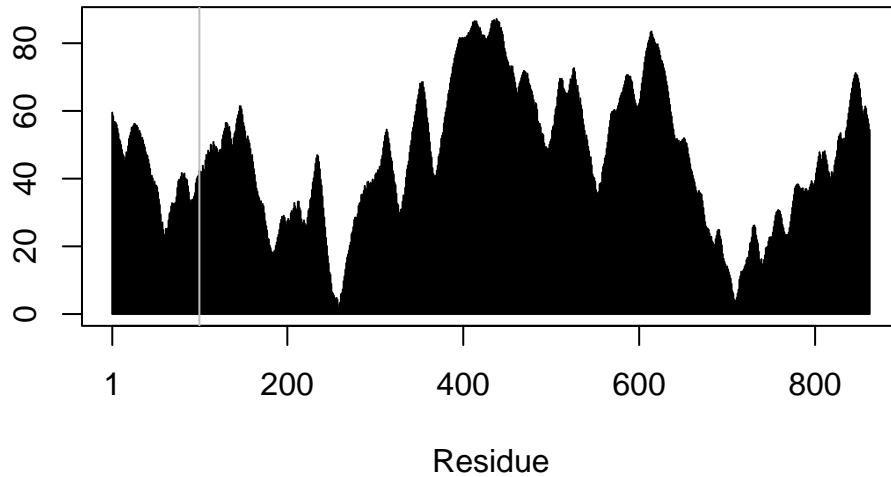
# Now we examine the RMSF b/w positions of the structure to measure conformational variance
rf <- rmsf(xyz)

plotb3(rf, sse=pdb)
```

```
Warning in pdb2sse(sse): No helix and sheet defined in input 'sse' PDB object:
try using dssp()
```

```
Warning in plotb3(rf, sse = pdb): 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 <- list.files(path=results_dir,
                        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"
```

```
# Per-residue pLDDT scores
# same as B-factor of PDB..
head(pae1$plddt)
```

```
[1] 41.16 36.88 23.81 30.98 32.09 29.11
```

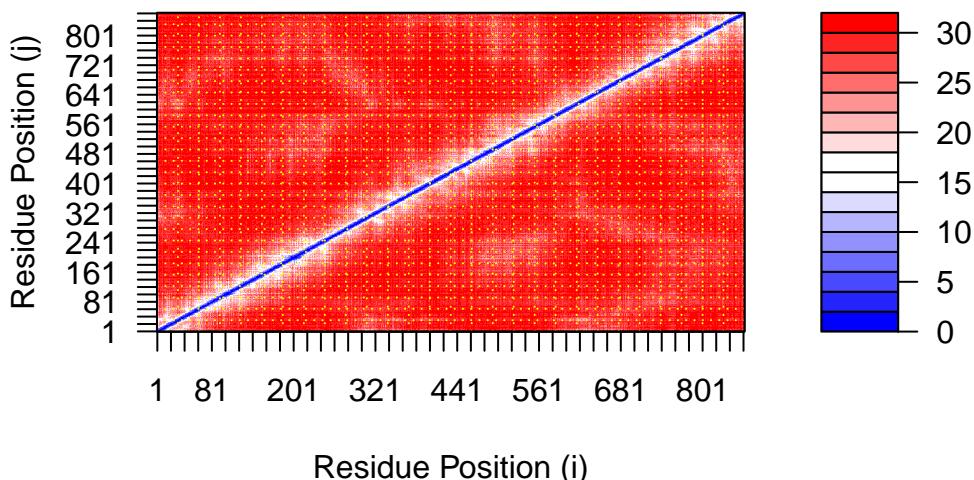
```
pae1$max_pae
```

```
[1] 31.1875
```

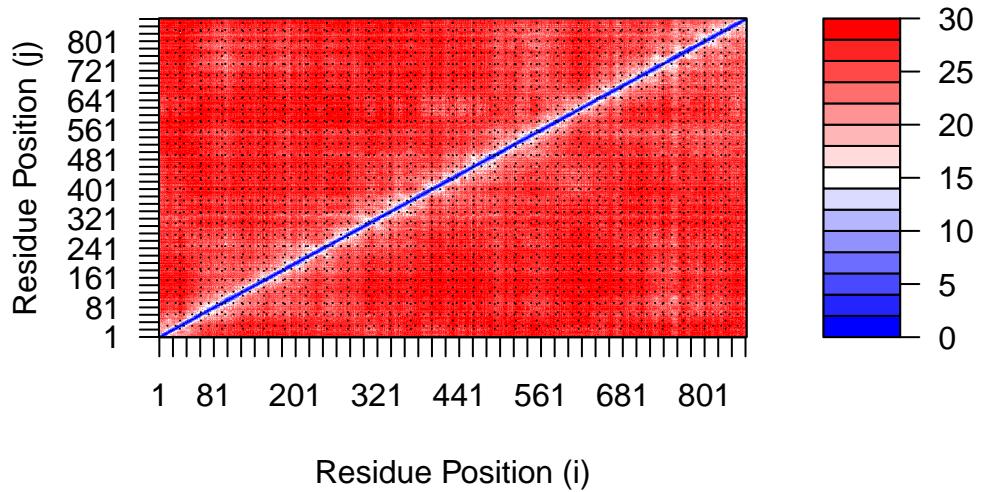
```
pae5$max_pae
```

```
[1] 30.65625
```

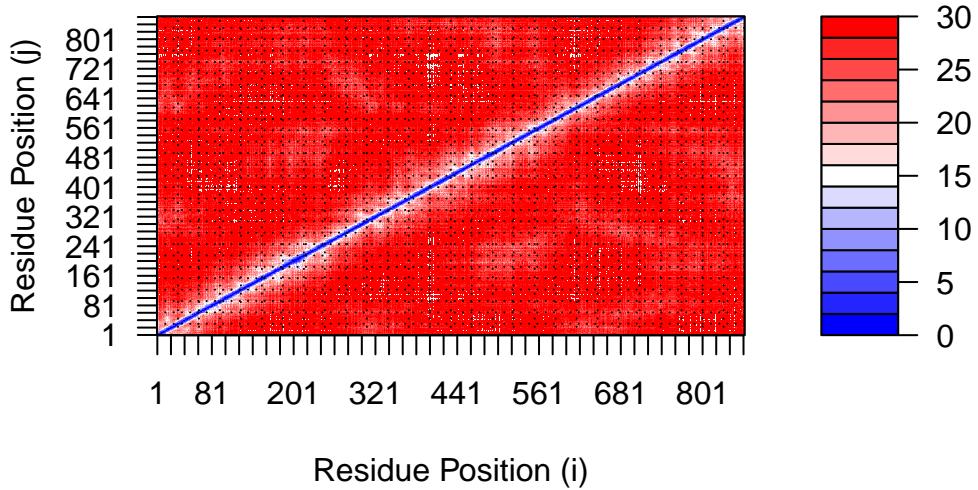
```
plot.dmat(pae1$pae,  
          xlab="Residue Position (i)",  
          ylab="Residue Position (j)")
```



```
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))
```



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

```
[1] "ProteinofinterestfromFASTA_504d5/ProteinofinterestfromFASTA_504d5.a3m"
```

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

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

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

```
NULL
```

```
# Opening the .a3m file, it is just the one sequence duplicated twice, there is no alignment
```

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

```

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

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

#m1.pdb <- read.pdb(pdb_files[1])
#occ <- vec2resno(c(sim[1:99], sim[1:99]), m1.pdb$atom$resno)
#write.pdb(m1.pdb, o=occ, file="m1_conserv.pdb")

```

In summary, because the novel protein of interest is novel, finding core positions for superposing and predicting conservation from the alignment file proved to be difficult. I will be turning it in late after many hours of trying to understand this and I will have to talk to Professor Barry tomorrow...

Here is the analysis for the HIV-Pr dimer AlphaFold2 models.

```
results_dir <- "HIVPRdimer_23119"
```

```

# File names for all PDB models
pdb_files <- list.files(path=results_dir,
                         pattern="*.pdb",
                         full.names = TRUE)

# Print our PDB file names
basename(pdb_files)

```

```
[1] "HIVPRdimer_23119_unrelaxed_rank_001_alphaFold2_multimer_v3_model_1_seed_000.pdb"
[2] "HIVPRdimer_23119_unrelaxed_rank_002_alphaFold2_multimer_v3_model_5_seed_000.pdb"
[3] "HIVPRdimer_23119_unrelaxed_rank_003_alphaFold2_multimer_v3_model_4_seed_000.pdb"
[4] "HIVPRdimer_23119_unrelaxed_rank_004_alphaFold2_multimer_v3_model_2_seed_000.pdb"
[5] "HIVPRdimer_23119_unrelaxed_rank_005_alphaFold2_multimer_v3_model_3_seed_000.pdb"
```

```

library(bio3d)

# Read all data from Models
# and superpose/fit coords
pdbs <- pdbaln(pdb_files, fit=TRUE, exefile="msa")

```

Reading PDB files:

HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
.....

Extracting sequences

pdb/seq: 1 name: HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000
pdb/seq: 2 name: HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
pdb/seq: 3 name: HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
pdb/seq: 4 name: HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000
pdb/seq: 5 name: HIVPRdimer_23119/HIVPRdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000

pdb\$

[Truncated_Name:1] HIVPRdimer	1	50
	PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI					
[Truncated_Name:2] HIVPRdimer	PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI					
[Truncated_Name:3] HIVPRdimer	PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI					
[Truncated_Name:4] HIVPRdimer	PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI					
[Truncated_Name:5] HIVPRdimer	PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGI					

	1	50
[Truncated_Name:1] HIVPRdimer	51	100
	GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP					
[Truncated_Name:2] HIVPRdimer	GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP					
[Truncated_Name:3] HIVPRdimer	GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP					
[Truncated_Name:4] HIVPRdimer	GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP					
[Truncated_Name:5] HIVPRdimer	GGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFP					

	51	100
[Truncated_Name:1] HIVPRdimer	101	150
	QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG					
[Truncated_Name:2] HIVPRdimer	QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG					
[Truncated_Name:3] HIVPRdimer	QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG					
[Truncated_Name:4] HIVPRdimer	QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG					
[Truncated_Name:5] HIVPRdimer	QITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIG					

```

*****
101   .   .   .   .   150

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

```

Call:

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

Class:

```
pdb, fasta
```

Alignment dimensions:

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

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

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

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

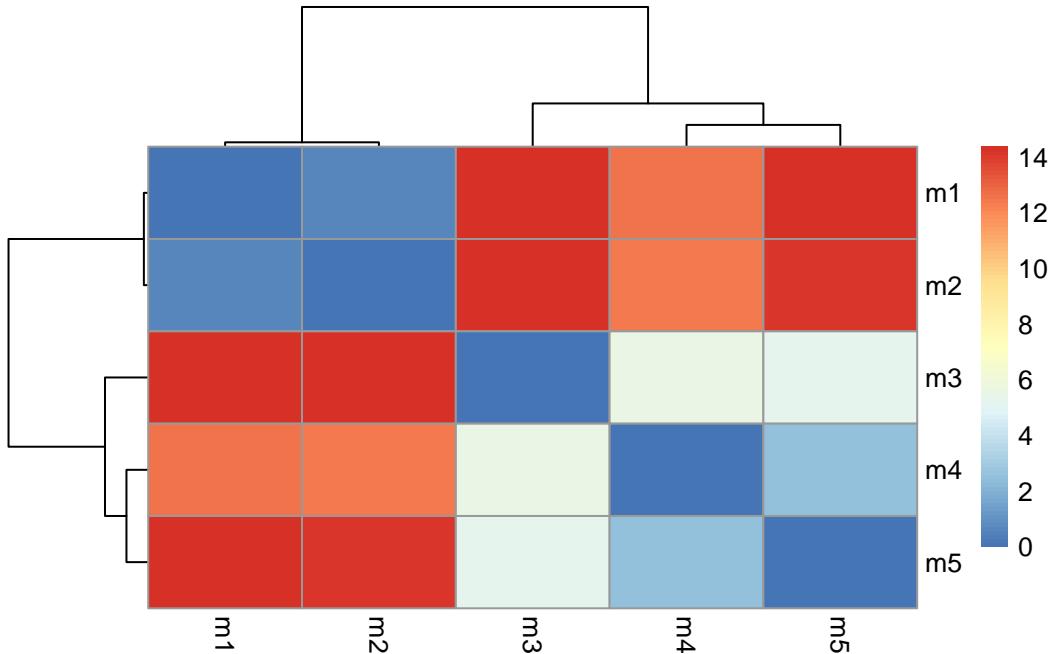
```
range(rd)
```

```
[1] 0.000 14.376
```

Heatmap

```
library(pheatmap)

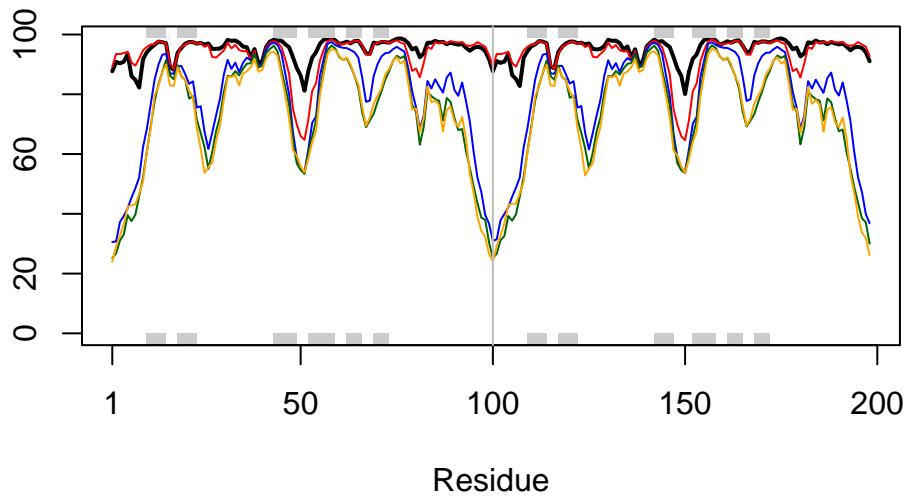
colnames(rd) <- paste0("m", 1:5)
rownames(rd) <- paste0("m", 1:5)
pheatmap(rd)
```



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

Note: Accessing on-line PDB file

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



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

```

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
```

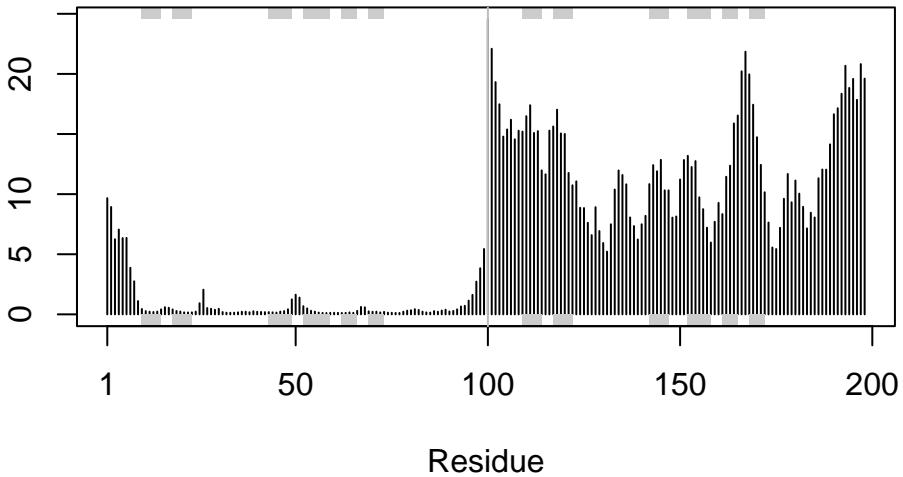
```
core inds <- print(core, vol=0.5)
```

```
# 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, core inds, outpath="corefit_structures")
```

```
rf <- rmsf(xyz)

plotb3(rf, sse=pdb)
abline(v=100, col="gray", ylab="RMSF")
```



Predicted Alignment Error (PAE) for domains

```

library(jsonlite)

# Listing of all PAE JSON files
pae_files <- list.files(path=results_dir,
                         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"

# Per-residue pLDDT scores
# same as B-factor of PDB..
head(pae1$plddt)

[1] 87.69 90.81 90.38 90.88 93.44 86.06

```

```
pae1$max_pae
```

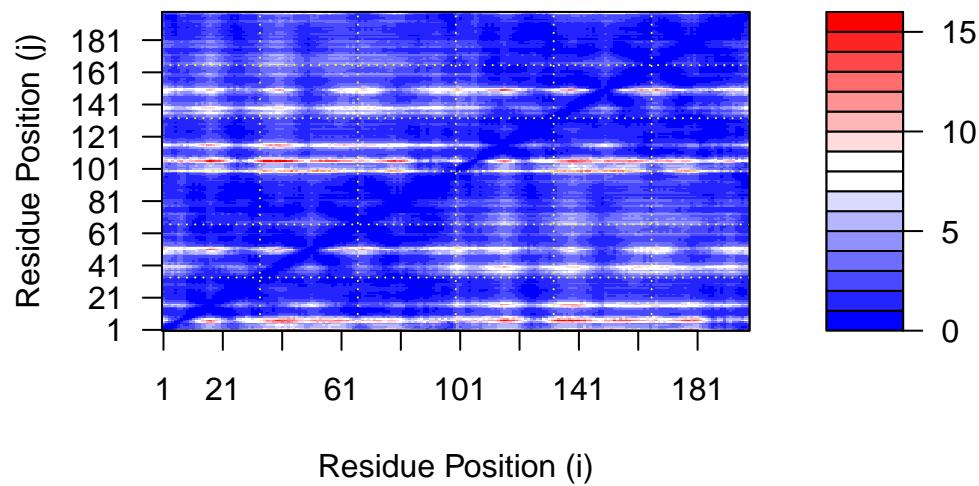
```
[1] 15.47656
```

```
pae5$max_pae
```

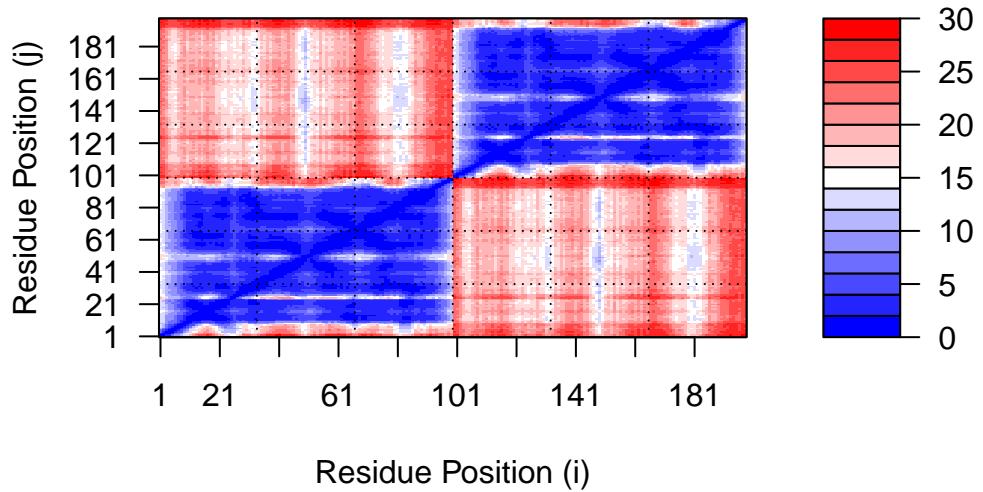
```
[1] 29.32812
```

Plotting N by N PAE scores with Bio3D

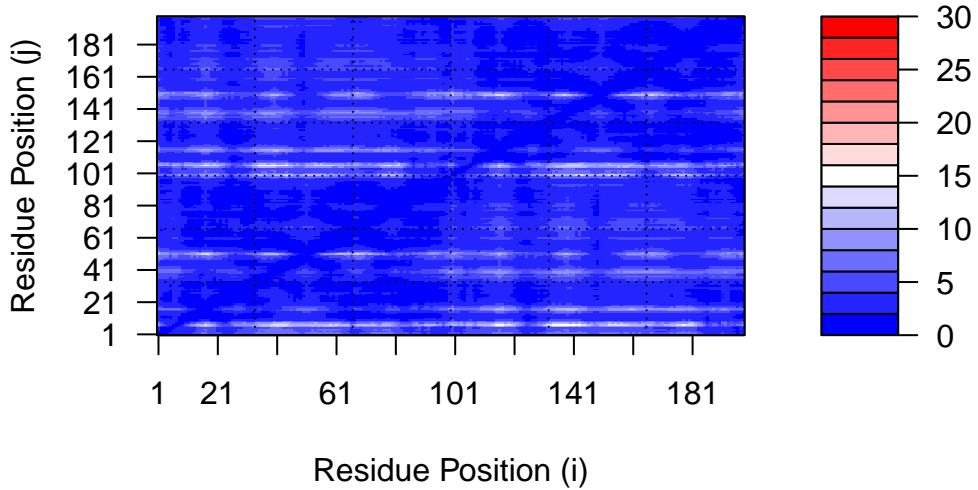
```
plot.dmat(pae1$pae,
           xlab="Residue Position (i)",
           ylab="Residue Position (j)")
```



```
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))
```



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

```
[1] "HIVPRdimer_23119/HIVPRdimer_23119.a3m"
```

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

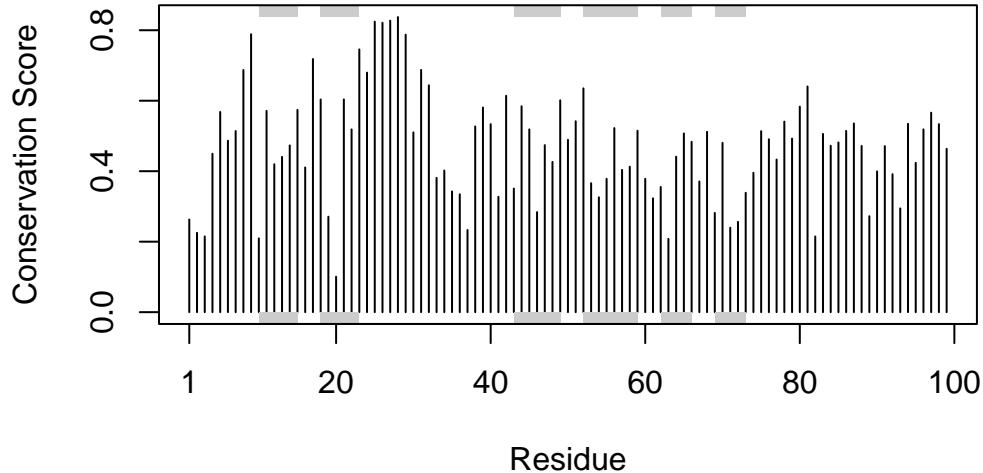
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

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

```
[1] 5378 132
```

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

```
plotb3(sim[1:99], sse=trim.pdb(pdb, 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] "--" "--" "--" "--" "--" "--"
```

```
m1.pdb <- read.pdb(pdb_files[1])
occ <- vec2resno(c(sim[1:99], sim[1:99]), m1.pdb$atom$resno)
write.pdb(m1.pdb, o=occ, file="m1_conserv.pdb")
knitr:::include_graphics("HIVPRDIMER_23119_UNRELAXED_RANK_001_ALPHAfold2_MULTIMER_V3_MODEL_1_S")
```

