class11

Sze Sze Chan

2025-02-19

```r
results_dir <- "smoothie_58941/"
```

```r
pdb_files <- list.files(path=results_dir,
pattern="*.pdb",
full.names = TRUE)
# Print our PDB file names
basename(pdb_files)
```

```
## [1] "smoothie_58941_relaxed_rank_001_alphafold2_ptm_model_3_seed_000.pdb"
## [2] "smoothie_58941_unrelaxed_rank_001_alphafold2_ptm_model_3_seed_000.pdb"
## [3] "smoothie_58941_unrelaxed_rank_002_alphafold2_ptm_model_2_seed_000.pdb"
## [4] "smoothie_58941_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_000.pdb"
## [5] "smoothie_58941_unrelaxed_rank_004_alphafold2_ptm_model_4_seed_000.pdb"
## [6] "smoothie_58941_unrelaxed_rank_005_alphafold2_ptm_model_5_seed_000.pdb"
```

```r
library(bio3d)
```

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

```
## Reading PDB files:
## smoothie_58941//smoothie_58941_relaxed_rank_001_alphafold2_ptm_model_3_seed_000.pdb
## smoothie_58941//smoothie_58941_unrelaxed_rank_001_alphafold2_ptm_model_3_seed_000.pdb
## smoothie_58941//smoothie_58941_unrelaxed_rank_002_alphafold2_ptm_model_2_seed_000.pdb
## smoothie_58941//smoothie_58941_unrelaxed_rank_003_alphafold2_ptm_model_1_seed_000.pdb
## smoothie_58941//smoothie_58941_unrelaxed_rank_004_alphafold2_ptm_model_4_seed_000.pdb
## smoothie_58941//smoothie_58941_unrelaxed_rank_005_alphafold2_ptm_model_5_seed_000.pdb
## ......
##
## Extracting sequences
##
## pdb/seq: 1   name: smoothie_58941//smoothie_58941_relaxed_rank_001_alphafold2_ptm_mod
el_3_seed_000.pdb
## pdb/seq: 2   name: smoothie_58941//smoothie_58941_unrelaxed_rank_001_alphafold2_ptm_m
odel_3_seed_000.pdb
## pdb/seq: 3   name: smoothie_58941//smoothie_58941_unrelaxed_rank_002_alphafold2_ptm_m
odel_2_seed_000.pdb
## pdb/seq: 4   name: smoothie_58941//smoothie_58941_unrelaxed_rank_003_alphafold2_ptm_m
odel_1_seed_000.pdb
## pdb/seq: 5   name: smoothie_58941//smoothie_58941_unrelaxed_rank_004_alphafold2_ptm_m
odel_4_seed_000.pdb
## pdb/seq: 6   name: smoothie_58941//smoothie_58941_unrelaxed_rank_005_alphafold2_ptm_m
odel_5_seed_000.pdb
```

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

```
## Warning in rmsd(pdbs, fit = T): No indices provided, using the 1077 non NA positions
```

```
range(rd)
```
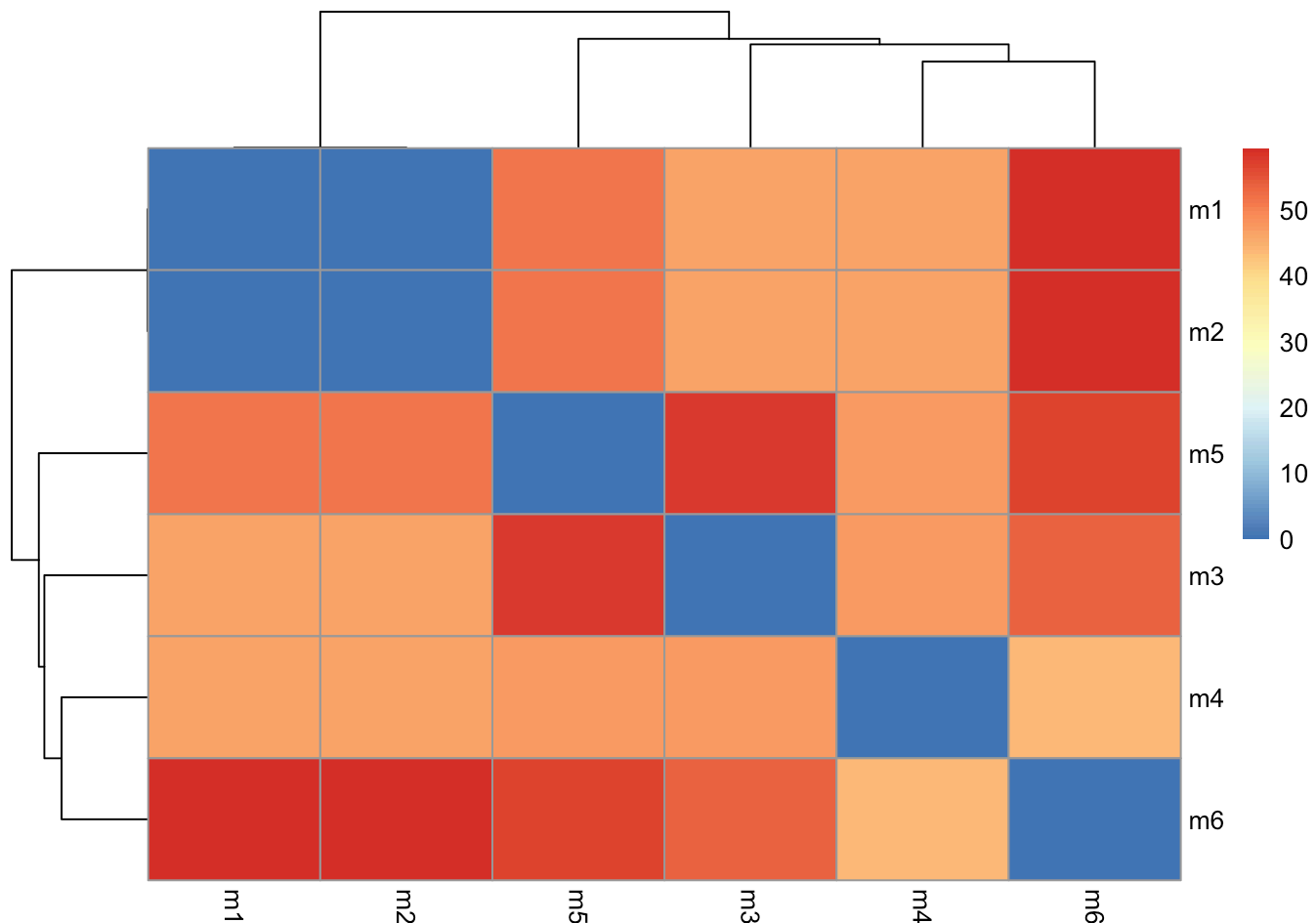
```
## [1]  0.000 59.407
```

```
dim(rd)
```

```
## [1] 6 6
```

```
library(pheatmap)
colnames(rd) <- paste0("m",1:6)
rownames(rd) <- paste0("m",1:6)
pheatmap(rd)
```

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

```
##    Note: Accessing on-line PDB file
```

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

```
## 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'
```

```r
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)
```
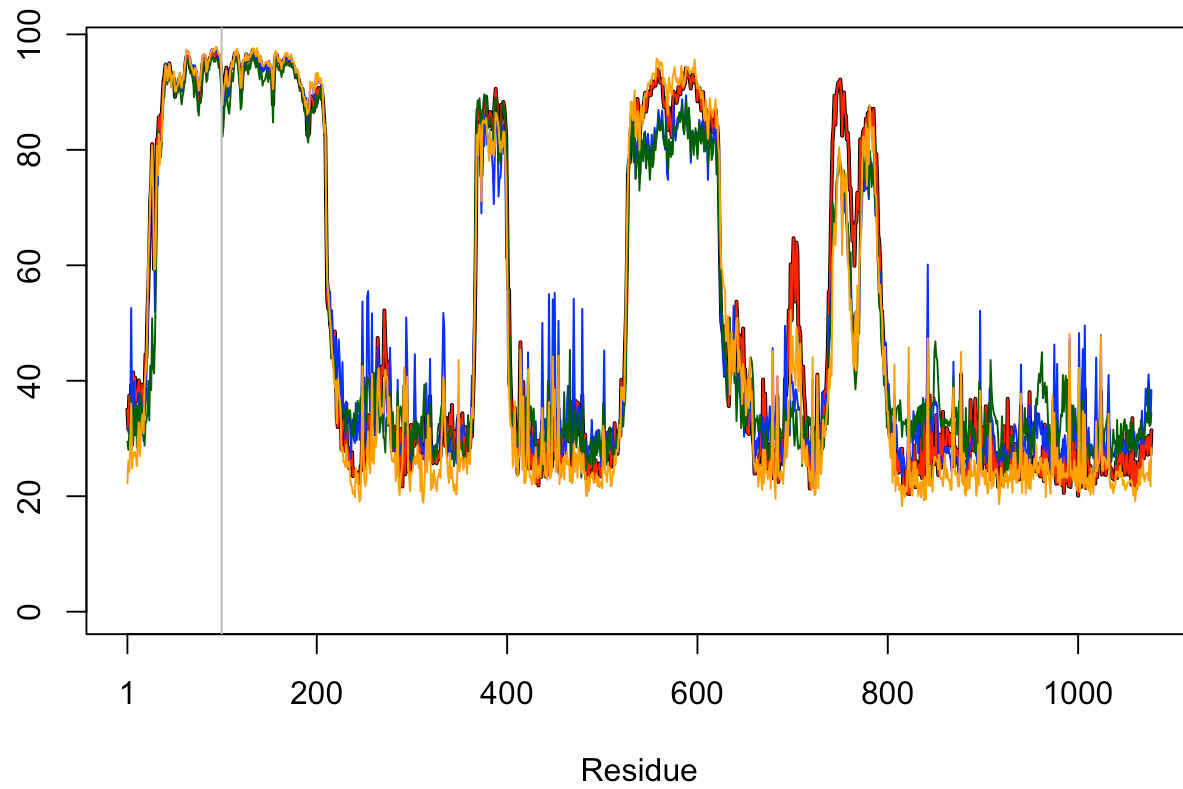
```
##   core size 1076 of 1077   vol = 21226441
##   core size 1075 of 1077   vol = 20974218
##   core size 1074 of 1077   vol = 20739128
##   core size 1073 of 1077   vol = 20512629
##   core size 1072 of 1077   vol = 20288882
##   core size 1071 of 1077   vol = 20070211
##   core size 1070 of 1077   vol = 19848927
##   core size 1069 of 1077   vol = 19631486
##   core size 1068 of 1077   vol = 19411789
##   core size 1067 of 1077   vol = 19192199
##   core size 1066 of 1077   vol = 18974529
##   core size 1065 of 1077   vol = 18755204
##   core size 1064 of 1077   vol = 18535850
##   core size 1063 of 1077   vol = 18316430
##   core size 1062 of 1077   vol = 18098139
##   core size 1061 of 1077   vol = 17878508
##   core size 1060 of 1077   vol = 17663586
##   core size 1059 of 1077   vol = 17453535
##   core size 1058 of 1077   vol = 17253804
##   core size 1057 of 1077   vol = 17059978
##   core size 1056 of 1077   vol = 16876310
##   core size 1055 of 1077   vol = 16696905
##   core size 1054 of 1077   vol = 16529022
##   core size 1053 of 1077   vol = 16360079
##   core size 1052 of 1077   vol = 16209342
##   core size 1051 of 1077   vol = 16066352
##   core size 1050 of 1077   vol = 15924569
##   core size 1049 of 1077   vol = 15800269
##   core size 1048 of 1077   vol = 15676216
##   core size 1047 of 1077   vol = 15559132
##   core size 1046 of 1077   vol = 15465640
##   core size 1045 of 1077   vol = 15372540
##   core size 1044 of 1077   vol = 15278434
##   core size 1043 of 1077   vol = 15185616
##   core size 1042 of 1077   vol = 15093435
##   core size 1041 of 1077   vol = 15002676
##   core size 1040 of 1077   vol = 14892897
##   core size 1039 of 1077   vol = 14801278
##   core size 1038 of 1077   vol = 14712008
##   core size 1037 of 1077   vol = 14621142
##   core size 1036 of 1077   vol = 14515875
##   core size 1035 of 1077   vol = 14428264
##   core size 1034 of 1077   vol = 14326381
##   core size 1033 of 1077   vol = 14240129
##   core size 1032 of 1077   vol = 14145471
##   core size 1031 of 1077   vol = 14051699
##   core size 1030 of 1077   vol = 13968001
##   core size 1029 of 1077   vol = 13876060
##   core size 1028 of 1077   vol = 13782652
##   core size 1027 of 1077   vol = 13691063
##   core size 1026 of 1077   vol = 13591688
##   core size 1025 of 1077   vol = 13505252
```

```
##   core size 1024 of 1077   vol = 13424109
##   core size 1023 of 1077   vol = 13336522
##   core size 1022 of 1077   vol = 13250427
##   core size 1021 of 1077   vol = 13159010
##   core size 1020 of 1077   vol = 13073377
##   core size 1019 of 1077   vol = 12986521
##   core size 1018 of 1077   vol = 12898631
##   core size 1017 of 1077   vol = 12812116
##   core size 1016 of 1077   vol = 12723477
##   core size 1015 of 1077   vol = 12638761
##   core size 1014 of 1077   vol = 12553924
##   core size 1013 of 1077   vol = 12464131
##   core size 1012 of 1077   vol = 12373904
##   core size 1011 of 1077   vol = 12290109
##   core size 1010 of 1077   vol = 12199885
##   core size 1009 of 1077   vol = 12117124
##   core size 1008 of 1077   vol = 12035239
##   core size 1007 of 1077   vol = 11944141
##   core size 1006 of 1077   vol = 11851820
##   core size 1005 of 1077   vol = 11763576
##   core size 1004 of 1077   vol = 11671675
##   core size 1003 of 1077   vol = 11589177
##   core size 1002 of 1077   vol = 11510247
##   core size 1001 of 1077   vol = 11436075
##   core size 1000 of 1077   vol = 11361249
##   core size 999 of 1077   vol = 11285850
##   core size 998 of 1077   vol = 11196999
##   core size 997 of 1077   vol = 11123448
##   core size 996 of 1077   vol = 11052184
##   core size 995 of 1077   vol = 10982106
##   core size 994 of 1077   vol = 10902872
##   core size 993 of 1077   vol = 10817925
##   core size 992 of 1077   vol = 10730571
##   core size 991 of 1077   vol = 10660114
##   core size 990 of 1077   vol = 10583704
##   core size 989 of 1077   vol = 10510383
##   core size 988 of 1077   vol = 10429593
##   core size 987 of 1077   vol = 10364576
##   core size 986 of 1077   vol = 10300992
##   core size 985 of 1077   vol = 10228089
##   core size 984 of 1077   vol = 10148773
##   core size 983 of 1077   vol = 10087467
##   core size 982 of 1077   vol = 10030141
##   core size 981 of 1077   vol = 9973271
##   core size 980 of 1077   vol = 9918022
##   core size 979 of 1077   vol = 9861901
##   core size 978 of 1077   vol = 9805266
##   core size 977 of 1077   vol = 9748817
##   core size 976 of 1077   vol = 9690761
##   core size 975 of 1077   vol = 9635260
##   core size 974 of 1077   vol = 9580533
##   core size 973 of 1077   vol = 9525332
```

```
##   core size 972 of 1077   vol = 9468296
##   core size 971 of 1077   vol = 9413868
##   core size 970 of 1077   vol = 9360267
##   core size 969 of 1077   vol = 9307383
##   core size 968 of 1077   vol = 9252911
##   core size 967 of 1077   vol = 9198919
##   core size 966 of 1077   vol = 9133007
##   core size 965 of 1077   vol = 9076554
##   core size 964 of 1077   vol = 9022754
##   core size 963 of 1077   vol = 8972563
##   core size 962 of 1077   vol = 8919963
##   core size 961 of 1077   vol = 8868483
##   core size 960 of 1077   vol = 8815357
##   core size 959 of 1077   vol = 8761835
##   core size 958 of 1077   vol = 8709785
##   core size 957 of 1077   vol = 8644033
##   core size 956 of 1077   vol = 8588811
##   core size 955 of 1077   vol = 8535814
##   core size 954 of 1077   vol = 8483151
##   core size 953 of 1077   vol = 8430123
##   core size 952 of 1077   vol = 8377442
##   core size 951 of 1077   vol = 8324781
##   core size 950 of 1077   vol = 8272809
##   core size 949 of 1077   vol = 8221542
##   core size 948 of 1077   vol = 8170277
##   core size 947 of 1077   vol = 8118749
##   core size 946 of 1077   vol = 8068370
##   core size 945 of 1077   vol = 8017805
##   core size 944 of 1077   vol = 7966804
##   core size 943 of 1077   vol = 7915803
##   core size 942 of 1077   vol = 7865278
##   core size 941 of 1077   vol = 7815225
##   core size 940 of 1077   vol = 7762653
##   core size 939 of 1077   vol = 7712870
##   core size 938 of 1077   vol = 7651258
##   core size 937 of 1077   vol = 7583210
##   core size 936 of 1077   vol = 7528103
##   core size 935 of 1077   vol = 7476476
##   core size 934 of 1077   vol = 7428159
##   core size 933 of 1077   vol = 7376986
##   core size 932 of 1077   vol = 7328725
##   core size 931 of 1077   vol = 7267103
##   core size 930 of 1077   vol = 7218318
##   core size 929 of 1077   vol = 7170173
##   core size 928 of 1077   vol = 7124024
##   core size 927 of 1077   vol = 7068960
##   core size 926 of 1077   vol = 7011617
##   core size 925 of 1077   vol = 6953639
##   core size 924 of 1077   vol = 6896976
##   core size 923 of 1077   vol = 6841572
##   core size 922 of 1077   vol = 6781529
##   core size 921 of 1077   vol = 6722672
```

```
##   core size 920 of 1077   vol = 6666081
##   core size 919 of 1077   vol = 6608897
##   core size 918 of 1077   vol = 6551633
##   core size 917 of 1077   vol = 6502036
##   core size 916 of 1077   vol = 6462319
##   core size 915 of 1077   vol = 6424652
##   core size 914 of 1077   vol = 6382065
##   core size 913 of 1077   vol = 6340574
##   core size 912 of 1077   vol = 6304894
##   core size 911 of 1077   vol = 6268513
##   core size 910 of 1077   vol = 6231617
##   core size 909 of 1077   vol = 6194155
##   core size 908 of 1077   vol = 6153755
##   core size 907 of 1077   vol = 6113639
##   core size 906 of 1077   vol = 6072734
##   core size 905 of 1077   vol = 6030723
##   core size 904 of 1077   vol = 5991073
##   core size 903 of 1077   vol = 5949353
##   core size 902 of 1077   vol = 5907676
##   core size 901 of 1077   vol = 5867861
##   core size 900 of 1077   vol = 5817685
##   core size 899 of 1077   vol = 5782103
##   core size 898 of 1077   vol = 5742023
##   core size 897 of 1077   vol = 5701583
##   core size 896 of 1077   vol = 5667419
##   core size 895 of 1077   vol = 5628515
##   core size 894 of 1077   vol = 5589673
##   core size 893 of 1077   vol = 5553815
##   core size 892 of 1077   vol = 5515053
##   core size 891 of 1077   vol = 5464728
##   core size 890 of 1077   vol = 5426496
##   core size 889 of 1077   vol = 5388430
##   core size 888 of 1077   vol = 5356139
##   core size 887 of 1077   vol = 5319645
##   core size 886 of 1077   vol = 5284031
##   core size 885 of 1077   vol = 5239839
##   core size 884 of 1077   vol = 5204029
##   core size 883 of 1077   vol = 5169110
##   core size 882 of 1077   vol = 5123007
##   core size 881 of 1077   vol = 5087105
##   core size 880 of 1077   vol = 5044065
##   core size 879 of 1077   vol = 5011904
##   core size 878 of 1077   vol = 4978182
##   core size 877 of 1077   vol = 4944477
##   core size 876 of 1077   vol = 4911464
##   core size 875 of 1077   vol = 4880603
##   core size 874 of 1077   vol = 4848192
##   core size 873 of 1077   vol = 4808154
##   core size 872 of 1077   vol = 4768338
##   core size 871 of 1077   vol = 4734244
##   core size 870 of 1077   vol = 4695519
##   core size 869 of 1077   vol = 4656629
```

```
##   core size 868 of 1077   vol = 4619230
##   core size 867 of 1077   vol = 4585068
##   core size 866 of 1077   vol = 4553226
##   core size 865 of 1077   vol = 4518901
##   core size 864 of 1077   vol = 4489036
##   core size 863 of 1077   vol = 4456791
##   core size 862 of 1077   vol = 4426463
##   core size 861 of 1077   vol = 4393227
##   core size 860 of 1077   vol = 4363898
##   core size 859 of 1077   vol = 4339332
##   core size 858 of 1077   vol = 4312598
##   core size 857 of 1077   vol = 4281713
##   core size 856 of 1077   vol = 4252466
##   core size 855 of 1077   vol = 4226106
##   core size 854 of 1077   vol = 4194685
##   core size 853 of 1077   vol = 4168456
##   core size 852 of 1077   vol = 4134339
##   core size 851 of 1077   vol = 4112731
##   core size 850 of 1077   vol = 4090188
##   core size 849 of 1077   vol = 4067720
##   core size 848 of 1077   vol = 4043925
##   core size 847 of 1077   vol = 4021441
##   core size 846 of 1077   vol = 3993452
##   core size 845 of 1077   vol = 3969436
##   core size 844 of 1077   vol = 3936128
##   core size 843 of 1077   vol = 3907899
##   core size 842 of 1077   vol = 3882002
##   core size 841 of 1077   vol = 3857758
##   core size 840 of 1077   vol = 3831050
##   core size 839 of 1077   vol = 3808183
##   core size 838 of 1077   vol = 3785389
##   core size 837 of 1077   vol = 3762550
##   core size 836 of 1077   vol = 3738540
##   core size 835 of 1077   vol = 3719649
##   core size 834 of 1077   vol = 3694847
##   core size 833 of 1077   vol = 3671775
##   core size 832 of 1077   vol = 3647444
##   core size 831 of 1077   vol = 3622727
##   core size 830 of 1077   vol = 3597923
##   core size 829 of 1077   vol = 3572383
##   core size 828 of 1077   vol = 3541159
##   core size 827 of 1077   vol = 3516556
##   core size 826 of 1077   vol = 3492919
##   core size 825 of 1077   vol = 3467603
##   core size 824 of 1077   vol = 3444121
##   core size 823 of 1077   vol = 3421067
##   core size 822 of 1077   vol = 3399061
##   core size 821 of 1077   vol = 3376377
##   core size 820 of 1077   vol = 3353010
##   core size 819 of 1077   vol = 3328975
##   core size 818 of 1077   vol = 3305235
##   core size 817 of 1077   vol = 3281638
```

```
##   core size 816 of 1077   vol = 3252158
##   core size 815 of 1077   vol = 3227484
##   core size 814 of 1077   vol = 3205371
##   core size 813 of 1077   vol = 3179286
##   core size 812 of 1077   vol = 3157343
##   core size 811 of 1077   vol = 3133929
##   core size 810 of 1077   vol = 3111017
##   core size 809 of 1077   vol = 3088908
##   core size 808 of 1077   vol = 3065718
##   core size 807 of 1077   vol = 3048393
##   core size 806 of 1077   vol = 3027989
##   core size 805 of 1077   vol = 3008856
##   core size 804 of 1077   vol = 2990004
##   core size 803 of 1077   vol = 2971637
##   core size 802 of 1077   vol = 2954192
##   core size 801 of 1077   vol = 2936689
##   core size 800 of 1077   vol = 2917268
##   core size 799 of 1077   vol = 2899126
##   core size 798 of 1077   vol = 2882696
##   core size 797 of 1077   vol = 2864500
##   core size 796 of 1077   vol = 2850198
##   core size 795 of 1077   vol = 2836595
##   core size 794 of 1077   vol = 2823846
##   core size 793 of 1077   vol = 2804897
##   core size 792 of 1077   vol = 2792408
##   core size 791 of 1077   vol = 2780653
##   core size 790 of 1077   vol = 2762746
##   core size 789 of 1077   vol = 2745481
##   core size 788 of 1077   vol = 2729210
##   core size 787 of 1077   vol = 2717870
##   core size 786 of 1077   vol = 2707496
##   core size 785 of 1077   vol = 2691102
##   core size 784 of 1077   vol = 2680654
##   core size 783 of 1077   vol = 2663834
##   core size 782 of 1077   vol = 2655044
##   core size 781 of 1077   vol = 2637927
##   core size 780 of 1077   vol = 2621082
##   core size 779 of 1077   vol = 2603937
##   core size 778 of 1077   vol = 2587165
##   core size 777 of 1077   vol = 2572372
##   core size 776 of 1077   vol = 2562638
##   core size 775 of 1077   vol = 2549352
##   core size 774 of 1077   vol = 2535847
##   core size 773 of 1077   vol = 2520370
##   core size 772 of 1077   vol = 2508503
##   core size 771 of 1077   vol = 2495131
##   core size 770 of 1077   vol = 2481897
##   core size 769 of 1077   vol = 2467751
##   core size 768 of 1077   vol = 2452336
##   core size 767 of 1077   vol = 2437156
##   core size 766 of 1077   vol = 2421514
##   core size 765 of 1077   vol = 2405905
```

```
##   core size 764 of 1077   vol = 2386891
##   core size 763 of 1077   vol = 2370883
##   core size 762 of 1077   vol = 2357540
##   core size 761 of 1077   vol = 2348204
##   core size 760 of 1077   vol = 2332802
##   core size 759 of 1077   vol = 2320169
##   core size 758 of 1077   vol = 2307403
##   core size 757 of 1077   vol = 2300381
##   core size 756 of 1077   vol = 2291088
##   core size 755 of 1077   vol = 2281515
##   core size 754 of 1077   vol = 2270516
##   core size 753 of 1077   vol = 2259254
##   core size 752 of 1077   vol = 2249763
##   core size 751 of 1077   vol = 2235510
##   core size 750 of 1077   vol = 2221267
##   core size 749 of 1077   vol = 2206811
##   core size 748 of 1077   vol = 2195763
##   core size 747 of 1077   vol = 2187978
##   core size 746 of 1077   vol = 2178522
##   core size 745 of 1077   vol = 2168103
##   core size 744 of 1077   vol = 2154001
##   core size 743 of 1077   vol = 2139669
##   core size 742 of 1077   vol = 2127233
##   core size 741 of 1077   vol = 2115098
##   core size 740 of 1077   vol = 2102978
##   core size 739 of 1077   vol = 2090123
##   core size 738 of 1077   vol = 2076305
##   core size 737 of 1077   vol = 2062776
##   core size 736 of 1077   vol = 2054098
##   core size 735 of 1077   vol = 2042998
##   core size 734 of 1077   vol = 2032409
##   core size 733 of 1077   vol = 2023898
##   core size 732 of 1077   vol = 2013701
##   core size 731 of 1077   vol = 2005602
##   core size 730 of 1077   vol = 1992384
##   core size 729 of 1077   vol = 1978238
##   core size 728 of 1077   vol = 1964062
##   core size 727 of 1077   vol = 1952947
##   core size 726 of 1077   vol = 1939861
##   core size 725 of 1077   vol = 1926769
##   core size 724 of 1077   vol = 1919960
##   core size 723 of 1077   vol = 1913836
##   core size 722 of 1077   vol = 1904998
##   core size 721 of 1077   vol = 1897401
##   core size 720 of 1077   vol = 1883705
##   core size 719 of 1077   vol = 1873158
##   core size 718 of 1077   vol = 1865093
##   core size 717 of 1077   vol = 1855091
##   core size 716 of 1077   vol = 1842279
##   core size 715 of 1077   vol = 1836492
##   core size 714 of 1077   vol = 1823797
##   core size 713 of 1077   vol = 1810779
```

```
##   core size 712 of 1077   vol = 1801089
##   core size 711 of 1077   vol = 1791345
##   core size 710 of 1077   vol = 1780121
##   core size 709 of 1077   vol = 1766576
##   core size 708 of 1077   vol = 1754756
##   core size 707 of 1077   vol = 1746900
##   core size 706 of 1077   vol = 1735997
##   core size 705 of 1077   vol = 1723831
##   core size 704 of 1077   vol = 1712000
##   core size 703 of 1077   vol = 1699244
##   core size 702 of 1077   vol = 1687176
##   core size 701 of 1077   vol = 1674525
##   core size 700 of 1077   vol = 1662243
##   core size 699 of 1077   vol = 1652160
##   core size 698 of 1077   vol = 1641285
##   core size 697 of 1077   vol = 1630014
##   core size 696 of 1077   vol = 1619012
##   core size 695 of 1077   vol = 1610429
##   core size 694 of 1077   vol = 1601714
##   core size 693 of 1077   vol = 1592656
##   core size 692 of 1077   vol = 1580452
##   core size 691 of 1077   vol = 1571998
##   core size 690 of 1077   vol = 1562948
##   core size 689 of 1077   vol = 1552971
##   core size 688 of 1077   vol = 1543915
##   core size 687 of 1077   vol = 1532724
##   core size 686 of 1077   vol = 1523299
##   core size 685 of 1077   vol = 1513371
##   core size 684 of 1077   vol = 1500799
##   core size 683 of 1077   vol = 1491094
##   core size 682 of 1077   vol = 1481283
##   core size 681 of 1077   vol = 1471350
##   core size 680 of 1077   vol = 1462777
##   core size 679 of 1077   vol = 1452822
##   core size 678 of 1077   vol = 1443002
##   core size 677 of 1077   vol = 1432575
##   core size 676 of 1077   vol = 1422171
##   core size 675 of 1077   vol = 1412641
##   core size 674 of 1077   vol = 1401484
##   core size 673 of 1077   vol = 1389736
##   core size 672 of 1077   vol = 1380303
##   core size 671 of 1077   vol = 1368772
##   core size 670 of 1077   vol = 1358715
##   core size 669 of 1077   vol = 1347116
##   core size 668 of 1077   vol = 1338287
##   core size 667 of 1077   vol = 1328776
##   core size 666 of 1077   vol = 1320662
##   core size 665 of 1077   vol = 1312663
##   core size 664 of 1077   vol = 1301619
##   core size 663 of 1077   vol = 1291884
##   core size 662 of 1077   vol = 1279982
##   core size 661 of 1077   vol = 1270472
```

```
##   core size 660 of 1077   vol = 1263013
##   core size 659 of 1077   vol = 1253580
##   core size 658 of 1077   vol = 1245053
##   core size 657 of 1077   vol = 1235536
##   core size 656 of 1077   vol = 1227925
##   core size 655 of 1077   vol = 1218406
##   core size 654 of 1077   vol = 1207848
##   core size 653 of 1077   vol = 1197431
##   core size 652 of 1077   vol = 1187645
##   core size 651 of 1077   vol = 1178934
##   core size 650 of 1077   vol = 1170356
##   core size 649 of 1077   vol = 1161426
##   core size 648 of 1077   vol = 1153613
##   core size 647 of 1077   vol = 1146369
##   core size 646 of 1077   vol = 1140087
##   core size 645 of 1077   vol = 1129668
##   core size 644 of 1077   vol = 1119169
##   core size 643 of 1077   vol = 1110700
##   core size 642 of 1077   vol = 1102514
##   core size 641 of 1077   vol = 1092011
##   core size 640 of 1077   vol = 1083872
##   core size 639 of 1077   vol = 1073645
##   core size 638 of 1077   vol = 1065746
##   core size 637 of 1077   vol = 1059365
##   core size 636 of 1077   vol = 1052964
##   core size 635 of 1077   vol = 1047038
##   core size 634 of 1077   vol = 1040457
##   core size 633 of 1077   vol = 1033613
##   core size 632 of 1077   vol = 1027116
##   core size 631 of 1077   vol = 1021778
##   core size 630 of 1077   vol = 1016164
##   core size 629 of 1077   vol = 1010307
##   core size 628 of 1077   vol = 999644.1
##   core size 627 of 1077   vol = 994753.6
##   core size 626 of 1077   vol = 984272.9
##   core size 625 of 1077   vol = 977243.3
##   core size 624 of 1077   vol = 969438.7
##   core size 623 of 1077   vol = 962674.7
##   core size 622 of 1077   vol = 956409.5
##   core size 621 of 1077   vol = 951089.3
##   core size 620 of 1077   vol = 941265.6
##   core size 619 of 1077   vol = 933825.2
##   core size 618 of 1077   vol = 926939.5
##   core size 617 of 1077   vol = 919712.4
##   core size 616 of 1077   vol = 912092.4
##   core size 615 of 1077   vol = 904960.6
##   core size 614 of 1077   vol = 898119.2
##   core size 613 of 1077   vol = 890583.9
##   core size 612 of 1077   vol = 881205
##   core size 611 of 1077   vol = 873715.8
##   core size 610 of 1077   vol = 867590.9
##   core size 609 of 1077   vol = 859944.1
```

```
##   core size 608 of 1077   vol = 852269.6
##   core size 607 of 1077   vol = 843308.9
##   core size 606 of 1077   vol = 836270.1
##   core size 605 of 1077   vol = 828309.9
##   core size 604 of 1077   vol = 820065.2
##   core size 603 of 1077   vol = 811450.4
##   core size 602 of 1077   vol = 804286.6
##   core size 601 of 1077   vol = 797034.4
##   core size 600 of 1077   vol = 790300.7
##   core size 599 of 1077   vol = 783282.9
##   core size 598 of 1077   vol = 776885.9
##   core size 597 of 1077   vol = 771309
##   core size 596 of 1077   vol = 765244
##   core size 595 of 1077   vol = 759145.1
##   core size 594 of 1077   vol = 752775.5
##   core size 593 of 1077   vol = 746598.4
##   core size 592 of 1077   vol = 741133.7
##   core size 591 of 1077   vol = 732815.6
##   core size 590 of 1077   vol = 726902.9
##   core size 589 of 1077   vol = 720751.9
##   core size 588 of 1077   vol = 715364.5
##   core size 587 of 1077   vol = 710053.9
##   core size 586 of 1077   vol = 704806.2
##   core size 585 of 1077   vol = 696603.3
##   core size 584 of 1077   vol = 692592.6
##   core size 583 of 1077   vol = 685801.2
##   core size 582 of 1077   vol = 678637.1
##   core size 581 of 1077   vol = 674283.1
##   core size 580 of 1077   vol = 667735.9
##   core size 579 of 1077   vol = 661286.2
##   core size 578 of 1077   vol = 654926.5
##   core size 577 of 1077   vol = 648819.3
##   core size 576 of 1077   vol = 642505.7
##   core size 575 of 1077   vol = 635518.8
##   core size 574 of 1077   vol = 631275.1
##   core size 573 of 1077   vol = 624459.7
##   core size 572 of 1077   vol = 618341.4
##   core size 571 of 1077   vol = 614002.4
##   core size 570 of 1077   vol = 607686
##   core size 569 of 1077   vol = 601524.3
##   core size 568 of 1077   vol = 594475.3
##   core size 567 of 1077   vol = 587432.5
##   core size 566 of 1077   vol = 582853.8
##   core size 565 of 1077   vol = 576068.6
##   core size 564 of 1077   vol = 569437.9
##   core size 563 of 1077   vol = 563792
##   core size 562 of 1077   vol = 559269.7
##   core size 561 of 1077   vol = 553868.2
##   core size 560 of 1077   vol = 549010.9
##   core size 559 of 1077   vol = 542908.4
##   core size 558 of 1077   vol = 534800.7
##   core size 557 of 1077   vol = 529042.7
```

```
##   core size 556 of 1077   vol = 522925.3
##   core size 555 of 1077   vol = 516581
##   core size 554 of 1077   vol = 510803.4
##   core size 553 of 1077   vol = 504609.8
##   core size 552 of 1077   vol = 501118.3
##   core size 551 of 1077   vol = 495313.4
##   core size 550 of 1077   vol = 489468.6
##   core size 549 of 1077   vol = 483335.2
##   core size 548 of 1077   vol = 476869.5
##   core size 547 of 1077   vol = 470661.6
##   core size 546 of 1077   vol = 464176.6
##   core size 545 of 1077   vol = 457857.5
##   core size 544 of 1077   vol = 451973.1
##   core size 543 of 1077   vol = 447116.6
##   core size 542 of 1077   vol = 441331.4
##   core size 541 of 1077   vol = 436613.4
##   core size 540 of 1077   vol = 430912.6
##   core size 539 of 1077   vol = 426240.1
##   core size 538 of 1077   vol = 421296.3
##   core size 537 of 1077   vol = 415806.5
##   core size 536 of 1077   vol = 411866.3
##   core size 535 of 1077   vol = 407268
##   core size 534 of 1077   vol = 402827.3
##   core size 533 of 1077   vol = 397458
##   core size 532 of 1077   vol = 391911.7
##   core size 531 of 1077   vol = 386646.2
##   core size 530 of 1077   vol = 380978.7
##   core size 529 of 1077   vol = 375727.6
##   core size 528 of 1077   vol = 370930.9
##   core size 527 of 1077   vol = 365852.9
##   core size 526 of 1077   vol = 361888.8
##   core size 525 of 1077   vol = 357175.1
##   core size 524 of 1077   vol = 352311.6
##   core size 523 of 1077   vol = 346609.5
##   core size 522 of 1077   vol = 343089.1
##   core size 521 of 1077   vol = 338672.3
##   core size 520 of 1077   vol = 335672.1
##   core size 519 of 1077   vol = 332861.9
##   core size 518 of 1077   vol = 329877.8
##   core size 517 of 1077   vol = 327192.7
##   core size 516 of 1077   vol = 324237.7
##   core size 515 of 1077   vol = 321612.6
##   core size 514 of 1077   vol = 319087.1
##   core size 513 of 1077   vol = 314911.9
##   core size 512 of 1077   vol = 310454.7
##   core size 511 of 1077   vol = 307176.4
##   core size 510 of 1077   vol = 304607.2
##   core size 509 of 1077   vol = 301144.1
##   core size 508 of 1077   vol = 297902
##   core size 507 of 1077   vol = 295701.8
##   core size 506 of 1077   vol = 293264.5
##   core size 505 of 1077   vol = 290002.1
```

```
##   core size 504 of 1077   vol = 287778.1
##   core size 503 of 1077   vol = 284530.1
##   core size 502 of 1077   vol = 282417.2
##   core size 501 of 1077   vol = 279302.1
##   core size 500 of 1077   vol = 276628.5
##   core size 499 of 1077   vol = 273755
##   core size 498 of 1077   vol = 270786.9
##   core size 497 of 1077   vol = 267678.4
##   core size 496 of 1077   vol = 265503.6
##   core size 495 of 1077   vol = 262259.3
##   core size 494 of 1077   vol = 259084.4
##   core size 493 of 1077   vol = 256505.7
##   core size 492 of 1077   vol = 253378.8
##   core size 491 of 1077   vol = 250260.9
##   core size 490 of 1077   vol = 247898
##   core size 489 of 1077   vol = 244242.2
##   core size 488 of 1077   vol = 241390.5
##   core size 487 of 1077   vol = 237776.3
##   core size 486 of 1077   vol = 235665.1
##   core size 485 of 1077   vol = 233158.3
##   core size 484 of 1077   vol = 231318
##   core size 483 of 1077   vol = 229831.3
##   core size 482 of 1077   vol = 227918.1
##   core size 481 of 1077   vol = 226118.6
##   core size 480 of 1077   vol = 224174.7
##   core size 479 of 1077   vol = 222503.8
##   core size 478 of 1077   vol = 219633.5
##   core size 477 of 1077   vol = 216727.5
##   core size 476 of 1077   vol = 214936
##   core size 475 of 1077   vol = 212312.6
##   core size 474 of 1077   vol = 209715.7
##   core size 473 of 1077   vol = 207218.4
##   core size 472 of 1077   vol = 205194.1
##   core size 471 of 1077   vol = 202605.3
##   core size 470 of 1077   vol = 200389.2
##   core size 469 of 1077   vol = 198467.7
##   core size 468 of 1077   vol = 195887.2
##   core size 467 of 1077   vol = 193545.3
##   core size 466 of 1077   vol = 191170.5
##   core size 465 of 1077   vol = 188932.9
##   core size 464 of 1077   vol = 187171.7
##   core size 463 of 1077   vol = 185009.1
##   core size 462 of 1077   vol = 183054.8
##   core size 461 of 1077   vol = 181570.7
##   core size 460 of 1077   vol = 180309.5
##   core size 459 of 1077   vol = 179366.9
##   core size 458 of 1077   vol = 178522.5
##   core size 457 of 1077   vol = 176731.4
##   core size 456 of 1077   vol = 175120.7
##   core size 455 of 1077   vol = 173856.2
##   core size 454 of 1077   vol = 172206.2
##   core size 453 of 1077   vol = 170711.5
```

```
##   core size 452 of 1077   vol = 169906.1
##   core size 451 of 1077   vol = 168276.2
##   core size 450 of 1077   vol = 166942.9
##   core size 449 of 1077   vol = 165460
##   core size 448 of 1077   vol = 164504.9
##   core size 447 of 1077   vol = 163561
##   core size 446 of 1077   vol = 162345.3
##   core size 445 of 1077   vol = 161266.5
##   core size 444 of 1077   vol = 159908.2
##   core size 443 of 1077   vol = 159302.7
##   core size 442 of 1077   vol = 156765.5
##   core size 441 of 1077   vol = 154958.6
##   core size 440 of 1077   vol = 153633.2
##   core size 439 of 1077   vol = 152775.5
##   core size 438 of 1077   vol = 151943.4
##   core size 437 of 1077   vol = 151174.2
##   core size 436 of 1077   vol = 150438.8
##   core size 435 of 1077   vol = 149554.1
##   core size 434 of 1077   vol = 148773.1
##   core size 433 of 1077   vol = 148066.2
##   core size 432 of 1077   vol = 145511.6
##   core size 431 of 1077   vol = 144733.3
##   core size 430 of 1077   vol = 143884.6
##   core size 429 of 1077   vol = 143165.6
##   core size 428 of 1077   vol = 142430
##   core size 427 of 1077   vol = 141266.8
##   core size 426 of 1077   vol = 140889.5
##   core size 425 of 1077   vol = 138279.6
##   core size 424 of 1077   vol = 135852.2
##   core size 423 of 1077   vol = 134093.6
##   core size 422 of 1077   vol = 131602.5
##   core size 421 of 1077   vol = 130389.5
##   core size 420 of 1077   vol = 129466.5
##   core size 419 of 1077   vol = 128752.5
##   core size 418 of 1077   vol = 128069.5
##   core size 417 of 1077   vol = 127422.1
##   core size 416 of 1077   vol = 126386.2
##   core size 415 of 1077   vol = 125696
##   core size 414 of 1077   vol = 124996.2
##   core size 413 of 1077   vol = 124318.3
##   core size 412 of 1077   vol = 123515.7
##   core size 411 of 1077   vol = 122878.7
##   core size 410 of 1077   vol = 122237.2
##   core size 409 of 1077   vol = 121613.3
##   core size 408 of 1077   vol = 121018
##   core size 407 of 1077   vol = 120515.1
##   core size 406 of 1077   vol = 119707.5
##   core size 405 of 1077   vol = 118878.9
##   core size 404 of 1077   vol = 118302.8
##   core size 403 of 1077   vol = 117522.7
##   core size 402 of 1077   vol = 117024
##   core size 401 of 1077   vol = 116063
```

```
##   core size 400 of 1077   vol = 115530.6
##   core size 399 of 1077   vol = 114982.2
##   core size 398 of 1077   vol = 114477.8
##   core size 397 of 1077   vol = 114082
##   core size 396 of 1077   vol = 113489.1
##   core size 395 of 1077   vol = 112995.8
##   core size 394 of 1077   vol = 112562.4
##   core size 393 of 1077   vol = 112228.4
##   core size 392 of 1077   vol = 111808.4
##   core size 391 of 1077   vol = 111396.7
##   core size 390 of 1077   vol = 110756
##   core size 389 of 1077   vol = 110083.5
##   core size 388 of 1077   vol = 109558.9
##   core size 387 of 1077   vol = 109160.6
##   core size 386 of 1077   vol = 108670.3
##   core size 385 of 1077   vol = 108211
##   core size 384 of 1077   vol = 107814.2
##   core size 383 of 1077   vol = 107351.8
##   core size 382 of 1077   vol = 106876.9
##   core size 381 of 1077   vol = 106455.9
##   core size 380 of 1077   vol = 105959.2
##   core size 379 of 1077   vol = 105382.2
##   core size 378 of 1077   vol = 104824.5
##   core size 377 of 1077   vol = 104327.3
##   core size 376 of 1077   vol = 103865.9
##   core size 375 of 1077   vol = 103532.1
##   core size 374 of 1077   vol = 102972.7
##   core size 373 of 1077   vol = 102492.2
##   core size 372 of 1077   vol = 101963.9
##   core size 371 of 1077   vol = 101427.2
##   core size 370 of 1077   vol = 100883.5
##   core size 369 of 1077   vol = 100292
##   core size 368 of 1077   vol = 99768.76
##   core size 367 of 1077   vol = 99007.44
##   core size 366 of 1077   vol = 98308.28
##   core size 365 of 1077   vol = 97840.52
##   core size 364 of 1077   vol = 96975.75
##   core size 363 of 1077   vol = 96438.97
##   core size 362 of 1077   vol = 95911.91
##   core size 361 of 1077   vol = 95194.64
##   core size 360 of 1077   vol = 94585.24
##   core size 359 of 1077   vol = 93994.37
##   core size 358 of 1077   vol = 93416.96
##   core size 357 of 1077   vol = 92813.64
##   core size 356 of 1077   vol = 92155.87
##   core size 355 of 1077   vol = 91472.35
##   core size 354 of 1077   vol = 90896.05
##   core size 353 of 1077   vol = 90334.25
##   core size 352 of 1077   vol = 89759.69
##   core size 351 of 1077   vol = 89223.81
##   core size 350 of 1077   vol = 88558.57
##   core size 349 of 1077   vol = 88003.71
```

```
##   core size 348 of 1077   vol = 87342.34
##   core size 347 of 1077   vol = 86776.4
##   core size 346 of 1077   vol = 86169.16
##   core size 345 of 1077   vol = 85545.89
##   core size 344 of 1077   vol = 84692.98
##   core size 343 of 1077   vol = 82504.9
##   core size 342 of 1077   vol = 81671.7
##   core size 341 of 1077   vol = 81146.22
##   core size 340 of 1077   vol = 80682.31
##   core size 339 of 1077   vol = 80108.47
##   core size 338 of 1077   vol = 79579.27
##   core size 337 of 1077   vol = 79071.39
##   core size 336 of 1077   vol = 78502.82
##   core size 335 of 1077   vol = 78016.93
##   core size 334 of 1077   vol = 77466.6
##   core size 333 of 1077   vol = 76871.44
##   core size 332 of 1077   vol = 76276.71
##   core size 331 of 1077   vol = 74941.16
##   core size 330 of 1077   vol = 73968.81
##   core size 329 of 1077   vol = 73467.26
##   core size 328 of 1077   vol = 72727.55
##   core size 327 of 1077   vol = 72060.56
##   core size 326 of 1077   vol = 71557.76
##   core size 325 of 1077   vol = 70955.48
##   core size 324 of 1077   vol = 70395.58
##   core size 323 of 1077   vol = 69786.35
##   core size 322 of 1077   vol = 69171.21
##   core size 321 of 1077   vol = 68574.34
##   core size 320 of 1077   vol = 67964.31
##   core size 319 of 1077   vol = 67234.79
##   core size 318 of 1077   vol = 66571.7
##   core size 317 of 1077   vol = 65662.95
##   core size 316 of 1077   vol = 65113.36
##   core size 315 of 1077   vol = 64552.89
##   core size 314 of 1077   vol = 63923.71
##   core size 313 of 1077   vol = 62956.19
##   core size 312 of 1077   vol = 61801.35
##   core size 311 of 1077   vol = 60555.02
##   core size 310 of 1077   vol = 58947.68
##   core size 309 of 1077   vol = 57396.79
##   core size 308 of 1077   vol = 56661.78
##   core size 307 of 1077   vol = 55722.51
##   core size 306 of 1077   vol = 55106.44
##   core size 305 of 1077   vol = 54495.45
##   core size 304 of 1077   vol = 53926.7
##   core size 303 of 1077   vol = 53188.5
##   core size 302 of 1077   vol = 52623.62
##   core size 301 of 1077   vol = 52105.23
##   core size 300 of 1077   vol = 51451.3
##   core size 299 of 1077   vol = 50913.24
##   core size 298 of 1077   vol = 50375.13
##   core size 297 of 1077   vol = 49730.82
```

```
##   core size 296 of 1077   vol = 49205.3
##   core size 295 of 1077   vol = 48621.34
##   core size 294 of 1077   vol = 48094.43
##   core size 293 of 1077   vol = 46781.73
##   core size 292 of 1077   vol = 46099.12
##   core size 291 of 1077   vol = 45564.35
##   core size 290 of 1077   vol = 45070.18
##   core size 289 of 1077   vol = 44542.68
##   core size 288 of 1077   vol = 44046.88
##   core size 287 of 1077   vol = 43543.11
##   core size 286 of 1077   vol = 43053.99
##   core size 285 of 1077   vol = 42392.51
##   core size 284 of 1077   vol = 41859.86
##   core size 283 of 1077   vol = 41249.56
##   core size 282 of 1077   vol = 40653.07
##   core size 281 of 1077   vol = 39587.73
##   core size 280 of 1077   vol = 39060.02
##   core size 279 of 1077   vol = 38505.56
##   core size 278 of 1077   vol = 37952.14
##   core size 277 of 1077   vol = 37227.95
##   core size 276 of 1077   vol = 36723.84
##   core size 275 of 1077   vol = 36261.6
##   core size 274 of 1077   vol = 35784.39
##   core size 273 of 1077   vol = 34811.61
##   core size 272 of 1077   vol = 34198.09
##   core size 271 of 1077   vol = 33576.3
##   core size 270 of 1077   vol = 33048.15
##   core size 269 of 1077   vol = 32540.93
##   core size 268 of 1077   vol = 32011.94
##   core size 267 of 1077   vol = 31427.37
##   core size 266 of 1077   vol = 30933.53
##   core size 265 of 1077   vol = 30432.39
##   core size 264 of 1077   vol = 29954.09
##   core size 263 of 1077   vol = 29570.83
##   core size 262 of 1077   vol = 29238.96
##   core size 261 of 1077   vol = 28779.33
##   core size 260 of 1077   vol = 28302.53
##   core size 259 of 1077   vol = 27820.11
##   core size 258 of 1077   vol = 27311.99
##   core size 257 of 1077   vol = 26848.12
##   core size 256 of 1077   vol = 26411.56
##   core size 255 of 1077   vol = 26018.77
##   core size 254 of 1077   vol = 25646.6
##   core size 253 of 1077   vol = 25297.05
##   core size 252 of 1077   vol = 24874.19
##   core size 251 of 1077   vol = 24472.6
##   core size 250 of 1077   vol = 24111.85
##   core size 249 of 1077   vol = 23707.56
##   core size 248 of 1077   vol = 22964.23
##   core size 247 of 1077   vol = 22564.28
##   core size 246 of 1077   vol = 22113.79
##   core size 245 of 1077   vol = 21695.63
```

```
##   core size 244 of 1077   vol = 21331.9
##   core size 243 of 1077   vol = 21064.81
##   core size 242 of 1077   vol = 20768.14
##   core size 241 of 1077   vol = 20481.68
##   core size 240 of 1077   vol = 20146.41
##   core size 239 of 1077   vol = 19511.95
##   core size 238 of 1077   vol = 19237.95
##   core size 237 of 1077   vol = 19077.95
##   core size 236 of 1077   vol = 18725.03
##   core size 235 of 1077   vol = 18414.85
##   core size 234 of 1077   vol = 18049.48
##   core size 233 of 1077   vol = 17806.39
##   core size 232 of 1077   vol = 17583.63
##   core size 231 of 1077   vol = 17363.07
##   core size 230 of 1077   vol = 16816.93
##   core size 229 of 1077   vol = 16543.74
##   core size 228 of 1077   vol = 16264.25
##   core size 227 of 1077   vol = 16054.95
##   core size 226 of 1077   vol = 15862.02
##   core size 225 of 1077   vol = 15686.72
##   core size 224 of 1077   vol = 15519.77
##   core size 223 of 1077   vol = 15414.64
##   core size 222 of 1077   vol = 15314.65
##   core size 221 of 1077   vol = 15054.91
##   core size 220 of 1077   vol = 14776.25
##   core size 219 of 1077   vol = 14528.69
##   core size 218 of 1077   vol = 14259.97
##   core size 217 of 1077   vol = 14128.63
##   core size 216 of 1077   vol = 13665.92
##   core size 215 of 1077   vol = 13231.62
##   core size 214 of 1077   vol = 13031.37
##   core size 213 of 1077   vol = 12820.51
##   core size 212 of 1077   vol = 12644.99
##   core size 211 of 1077   vol = 12387.02
##   core size 210 of 1077   vol = 12140.74
##   core size 209 of 1077   vol = 11928.41
##   core size 208 of 1077   vol = 11817.7
##   core size 207 of 1077   vol = 11582.43
##   core size 206 of 1077   vol = 11420.71
##   core size 205 of 1077   vol = 11277.19
##   core size 204 of 1077   vol = 11035.52
##   core size 203 of 1077   vol = 10673.77
##   core size 202 of 1077   vol = 10415.89
##   core size 201 of 1077   vol = 10125.48
##   core size 200 of 1077   vol = 9944.149
##   core size 199 of 1077   vol = 9616.276
##   core size 198 of 1077   vol = 9514.812
##   core size 197 of 1077   vol = 9326.08
##   core size 196 of 1077   vol = 8982.881
##   core size 195 of 1077   vol = 8767.197
##   core size 194 of 1077   vol = 8580.543
##   core size 193 of 1077   vol = 8287.347
```

```
##   core size 192 of 1077   vol = 8155.99
##   core size 191 of 1077   vol = 7917.147
##   core size 190 of 1077   vol = 7742.14
##   core size 189 of 1077   vol = 7472.609
##   core size 188 of 1077   vol = 7317.095
##   core size 187 of 1077   vol = 7060.654
##   core size 186 of 1077   vol = 6854.622
##   core size 185 of 1077   vol = 6651.387
##   core size 184 of 1077   vol = 6466.834
##   core size 183 of 1077   vol = 6279.598
##   core size 182 of 1077   vol = 6221.611
##   core size 181 of 1077   vol = 6061.689
##   core size 180 of 1077   vol = 5790.34
##   core size 179 of 1077   vol = 5682.698
##   core size 178 of 1077   vol = 5509.467
##   core size 177 of 1077   vol = 5285.091
##   core size 176 of 1077   vol = 5246.02
##   core size 175 of 1077   vol = 5146.331
##   core size 174 of 1077   vol = 5079.048
##   core size 173 of 1077   vol = 4961.341
##   core size 172 of 1077   vol = 4857.342
##   core size 171 of 1077   vol = 4792.961
##   core size 170 of 1077   vol = 4629.871
##   core size 169 of 1077   vol = 4574.075
##   core size 168 of 1077   vol = 4511.798
##   core size 167 of 1077   vol = 4430.233
##   core size 166 of 1077   vol = 4362.883
##   core size 165 of 1077   vol = 4299.883
##   core size 164 of 1077   vol = 4231.621
##   core size 163 of 1077   vol = 4166.141
##   core size 162 of 1077   vol = 4093.048
##   core size 161 of 1077   vol = 4022.453
##   core size 160 of 1077   vol = 3946.1
##   core size 159 of 1077   vol = 3867.66
##   core size 158 of 1077   vol = 3786.39
##   core size 157 of 1077   vol = 3692.229
##   core size 156 of 1077   vol = 3633.82
##   core size 155 of 1077   vol = 3509.014
##   core size 154 of 1077   vol = 3396.552
##   core size 153 of 1077   vol = 3273.297
##   core size 152 of 1077   vol = 3163.327
##   core size 151 of 1077   vol = 3048.315
##   core size 150 of 1077   vol = 2912.649
##   core size 149 of 1077   vol = 2793.519
##   core size 148 of 1077   vol = 2656.393
##   core size 147 of 1077   vol = 2526.853
##   core size 146 of 1077   vol = 2420.921
##   core size 145 of 1077   vol = 2300.717
##   core size 144 of 1077   vol = 2173.657
##   core size 143 of 1077   vol = 1993.144
##   core size 142 of 1077   vol = 1861.405
##   core size 141 of 1077   vol = 1738.153
```

```
##   core size 140 of 1077   vol = 1607.148
##   core size 139 of 1077   vol = 1529.746
##   core size 138 of 1077   vol = 1411.602
##   core size 137 of 1077   vol = 1315.557
##   core size 136 of 1077   vol = 1218.421
##   core size 135 of 1077   vol = 1152.567
##   core size 134 of 1077   vol = 1079.713
##   core size 133 of 1077   vol = 1022.208
##   core size 132 of 1077   vol = 937.974
##   core size 131 of 1077   vol = 888.936
##   core size 130 of 1077   vol = 835.565
##   core size 129 of 1077   vol = 765.909
##   core size 128 of 1077   vol = 711.329
##   core size 127 of 1077   vol = 657.742
##   core size 126 of 1077   vol = 604.53
##   core size 125 of 1077   vol = 561.353
##   core size 124 of 1077   vol = 522.688
##   core size 123 of 1077   vol = 484.152
##   core size 122 of 1077   vol = 450.032
##   core size 121 of 1077   vol = 414.647
##   core size 120 of 1077   vol = 381.31
##   core size 119 of 1077   vol = 345.365
##   core size 118 of 1077   vol = 305.486
##   core size 117 of 1077   vol = 263.926
##   core size 116 of 1077   vol = 228.664
##   core size 115 of 1077   vol = 194.864
##   core size 114 of 1077   vol = 160.961
##   core size 113 of 1077   vol = 125.613
##   core size 112 of 1077   vol = 91.559
##   core size 111 of 1077   vol = 66.68
##   core size 110 of 1077   vol = 45.203
##   core size 109 of 1077   vol = 28.778
##   core size 108 of 1077   vol = 18.876
##   core size 107 of 1077   vol = 15.91
##   core size 106 of 1077   vol = 12.403
##   core size 105 of 1077   vol = 9.417
##   core size 104 of 1077   vol = 7.77
##   core size 103 of 1077   vol = 6.03
##   core size 102 of 1077   vol = 4.747
##   core size 101 of 1077   vol = 3.718
##   core size 100 of 1077   vol = 3.472
##   core size 99 of 1077   vol = 3.246
##   core size 98 of 1077   vol = 3.068
##   core size 97 of 1077   vol = 2.938
##   core size 96 of 1077   vol = 2.776
##   core size 95 of 1077   vol = 2.651
##   core size 94 of 1077   vol = 2.526
##   core size 93 of 1077   vol = 2.425
##   core size 92 of 1077   vol = 2.286
##   core size 91 of 1077   vol = 2.206
##   core size 90 of 1077   vol = 2.142
##   core size 89 of 1077   vol = 2.083
```

```
##   core size 88 of 1077  vol = 2.022
##   core size 87 of 1077  vol = 1.946
##   core size 86 of 1077  vol = 1.866
##   core size 85 of 1077  vol = 1.797
##   core size 84 of 1077  vol = 1.724
##   core size 83 of 1077  vol = 1.674
##   core size 82 of 1077  vol = 1.606
##   core size 81 of 1077  vol = 1.546
##   core size 80 of 1077  vol = 1.489
##   core size 79 of 1077  vol = 1.407
##   core size 78 of 1077  vol = 1.353
##   core size 77 of 1077  vol = 1.295
##   core size 76 of 1077  vol = 1.255
##   core size 75 of 1077  vol = 1.205
##   core size 74 of 1077  vol = 1.147
##   core size 73 of 1077  vol = 1.103
##   core size 72 of 1077  vol = 1.055
##   core size 71 of 1077  vol = 0.991
##   core size 70 of 1077  vol = 0.93
##   core size 69 of 1077  vol = 0.888
##   core size 68 of 1077  vol = 0.845
##   core size 67 of 1077  vol = 0.812
##   core size 66 of 1077  vol = 0.79
##   core size 65 of 1077  vol = 0.753
##   core size 64 of 1077  vol = 0.716
##   core size 63 of 1077  vol = 0.677
##   core size 62 of 1077  vol = 0.643
##   core size 61 of 1077  vol = 0.6
##   core size 60 of 1077  vol = 0.568
##   core size 59 of 1077  vol = 0.534
##   core size 58 of 1077  vol = 0.503
##   core size 57 of 1077  vol = 0.464
##   FINISHED: Min vol ( 0.5 ) reached
```

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

```
## # 58 positions (cumulative volume <= 0.5 Angstrom^3)
##    start end length
## 1    554 564     11
## 2    566 611     46
## 3    614 614      1
```

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

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

```
## 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")
```
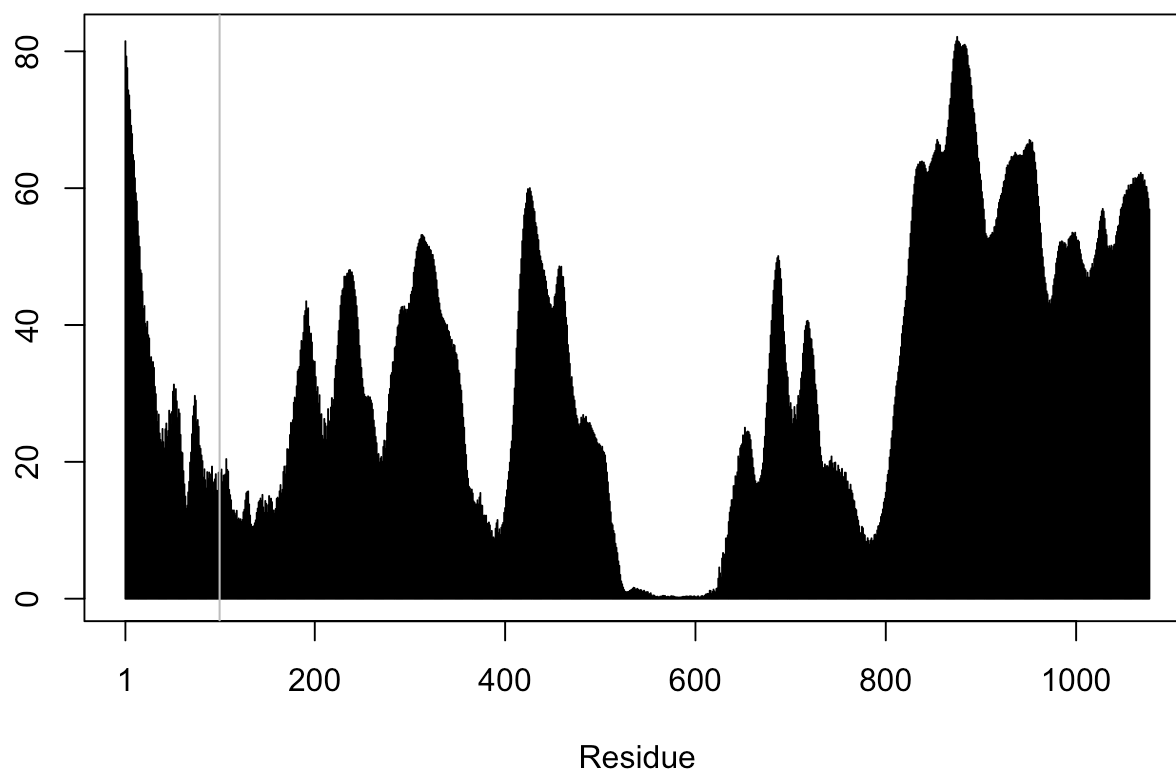


```
library(jsonlite)

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] 35.00 31.70 37.44 33.09 39.28 33.53
```

The maximum PAE values are useful for ranking models. Here we can see that model 5 is much worse than model 1. The lower the PAE score the better. How about the other models, what are thir max PAE scores?

```
pae1$max_pae
```

```
## [1] 31.42188
```

```
pae5$max_pae
```

```
## [1] 31.53125
```

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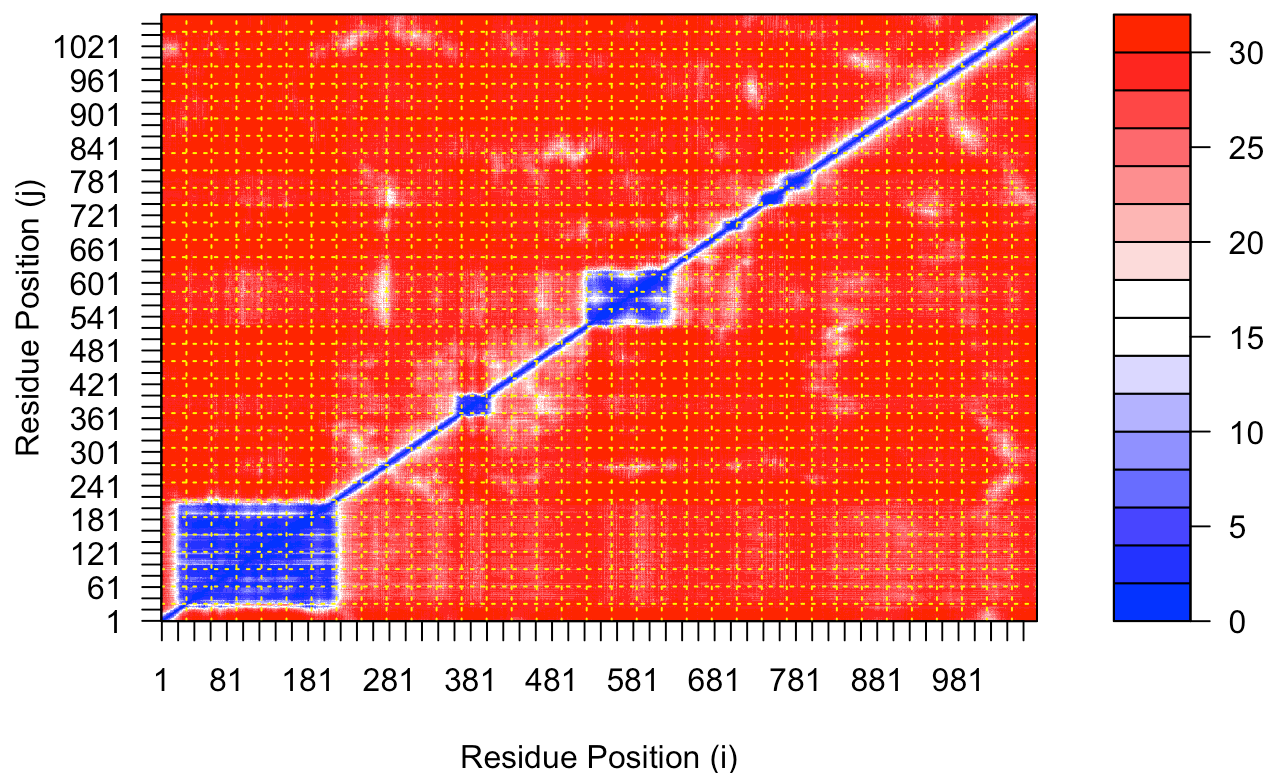


```
plot.dmat(pae5$pae,
xlab="Residue Position (i)",
ylab="Residue Position (j)",
grid.col = "black",
zlim=c(0,30))
```
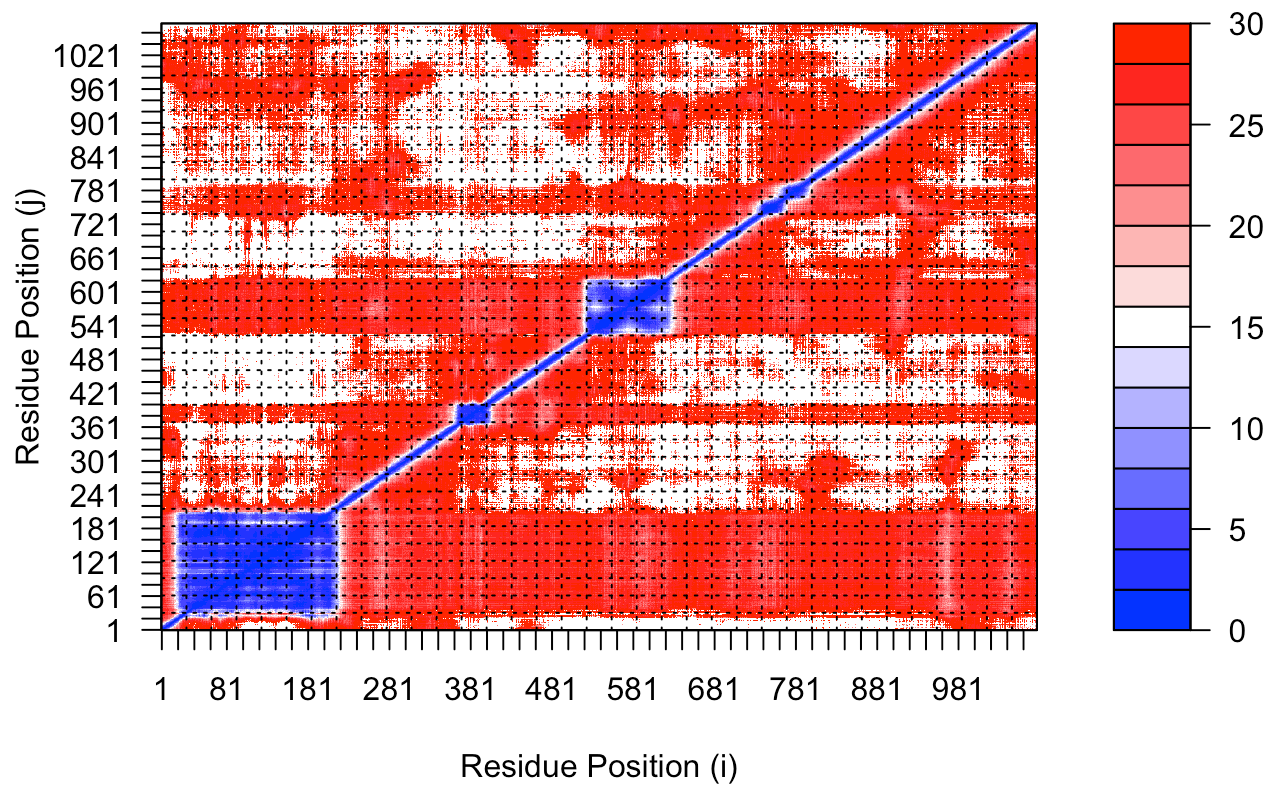
```
plot.dmat(pae1$pae,
xlab="Residue Position (i)",
ylab="Residue Position (j)",
grid.col = "black",
zlim=c(0,30))
```
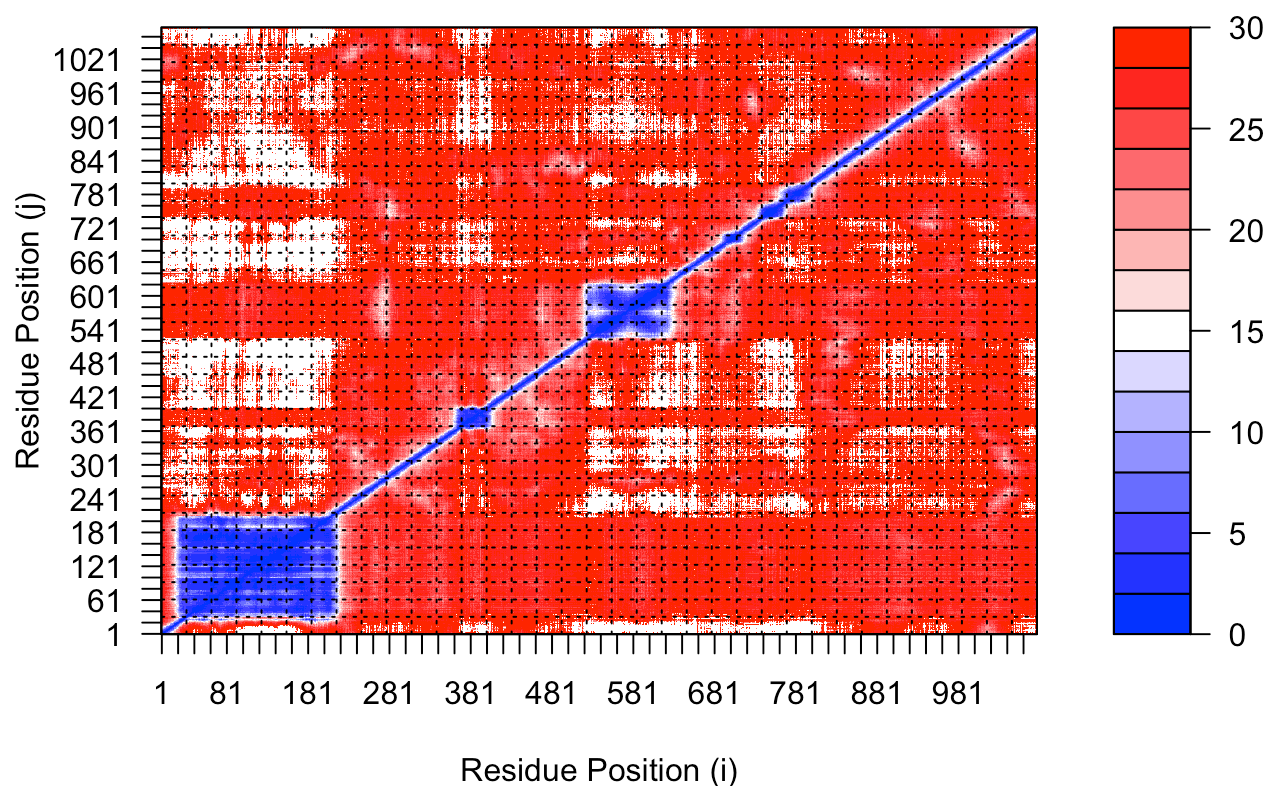
```
aln_file <- list.files(path=results_dir,
pattern=".a3m$",
full.names = TRUE)
aln_file
```

```
## [1] "smoothie_58941//smoothie_58941.a3m"
```

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

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

How many sequences are in this alignment

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

```
## [1] 7407 1645
```

We can score residue conservation in the alignment with the conserv() function.

```
sim <- conserv(aln)
plotb3(sim[1:99], sse=trim.pdb(pdb, chain="A"),
ylab="Conservation Score")
```
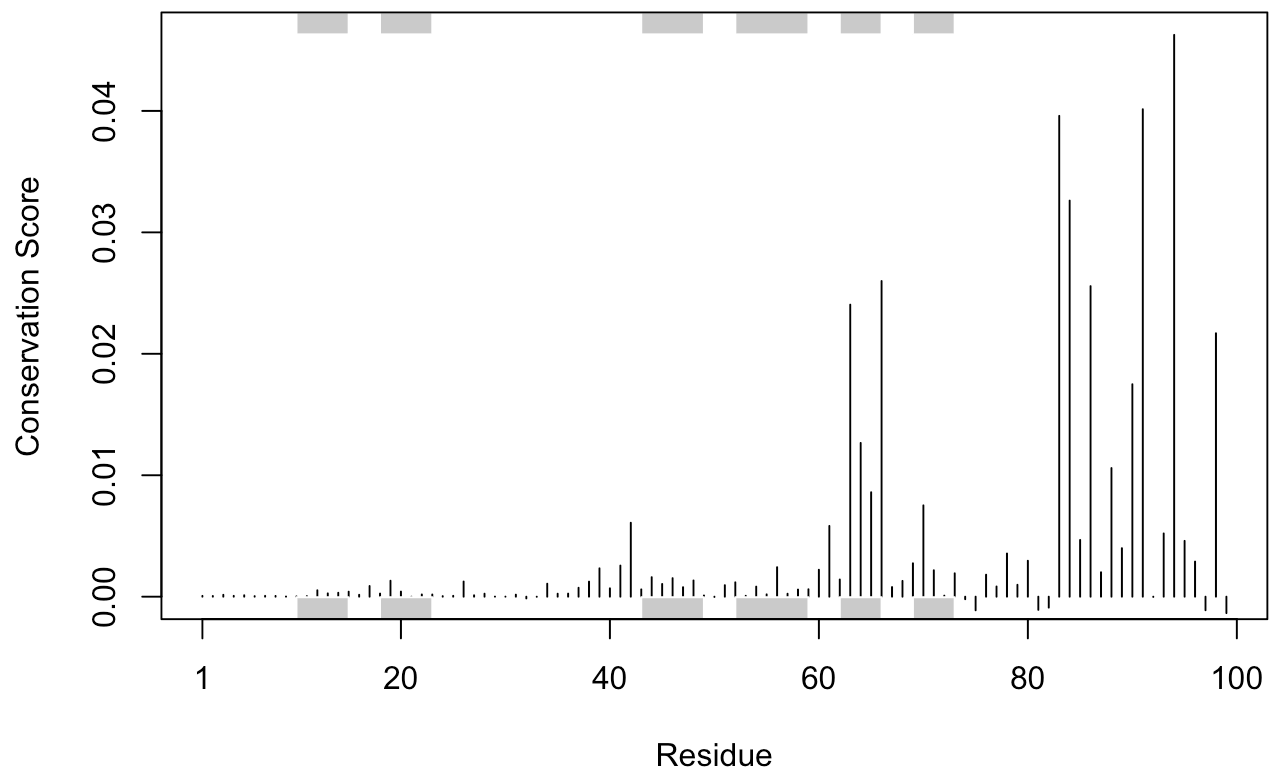
```
con <- consensus(aln, cutoff = 0.9)
con$seq
```

```
##   [1] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
##  [19] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
##  [37] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
##  [55] "_" "BIMM 143 bioinformatics Class11 class11.html" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
##  [73] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
##  [91] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [109] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [127] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [145] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [163] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [181] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [199] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [217] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [235] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [253] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [271] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [289] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [307] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [325] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [343] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [361] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [379] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [397] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [415] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [433] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [451] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [469] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [487] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [505] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [523] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [541] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [559] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [577] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [595] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [613] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [631] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [649] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [667] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [685] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [703] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [721] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [739] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [757] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [775] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [793] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [811] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [829] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [847] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [865] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [883] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [901] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
## [919] "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_" "_"
```

```
##    [937] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
##    [955] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
##    [973] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
##    [991] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1009] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1027] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1045] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1063] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1081] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1099] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1117] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1135] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1153] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1171] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1189] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1207] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1225] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1243] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1261] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1279] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1297] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1315] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1333] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1351] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1369] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1387] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1405] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1423] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1441] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1459] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1477] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1495] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1513] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1531] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1549] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1567] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1585] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1603] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1621] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [1639] "-" "-" "-" "-" "-" "-" "-"
```