

# Class\_11\_021424

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## ALL ABOUT ALPHAFOLD

Link to lab: [https://bioboot.github.io/bggn213\\_W24/class-material/class11\\_alphafold.html#generating-your-own-structure-predictions](https://bioboot.github.io/bggn213_W24/class-material/class11_alphafold.html#generating-your-own-structure-predictions)

To run it, use the GPU notebook to avoid using space on your laptop using the AlphaFold notebooks. There are many other notebooks available: <https://github.com/sokrypton/ColabFold>

**Goal: Find conserved sites by finding conserved AA and the regions using molstar.**

```
pth <- "HIV1dimer_23119"
```

```
list.files(path=pth)
```

```
[1] "cite.bibtex"
[2] "config.json"
[3] "HIV1dimer_23119_coverage.png"
[4] "HIV1dimer_23119_env"
[5] "HIV1dimer_23119_pae.png"
[6] "HIV1dimer_23119_plddt.png"
[7] "HIV1dimer_23119_predicted_aligned_error_v1.json"
[8] "HIV1dimer_23119_scores_rank_001_alphafold2_multimer_v3_model_1_seed_000.json"
[9] "HIV1dimer_23119_scores_rank_002_alphafold2_multimer_v3_model_5_seed_000.json"
[10] "HIV1dimer_23119_scores_rank_003_alphafold2_multimer_v3_model_4_seed_000.json"
[11] "HIV1dimer_23119_scores_rank_004_alphafold2_multimer_v3_model_2_seed_000.json"
[12] "HIV1dimer_23119_scores_rank_005_alphafold2_multimer_v3_model_3_seed_000.json"
[13] "HIV1dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_1_seed_000.pdb"
[14] "HIV1dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb"
```

```
[15] "HIV1dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
[16] "HIV1dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
[17] "HIV1dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
[18] "HIV1dimer_23119.a3m"
[19] "HIV1dimer_23119.csv"
[20] "HIV1dimer_23119.done.txt"
[21] "log.txt"
```

Returning the full file name (i.e with the directory path) of the alignment file (a3m).

```
list.files(path=pth, pattern = ".a3m", full.names = TRUE)
```

```
[1] "HIV1dimer_23119/HIV1dimer_23119.a3m"
```

```
aln.file <- list.files(path=pth, pattern = ".a3m", full.names = TRUE)
```

```
library(bio3d)
aln <- read.fasta(aln.file, to.upper = TRUE)
```

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

Let's look at the alignment.

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

```
[1] 5378 132
```

Let's get some summary of the alignment such as conservation scores.

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

```
[1] 0.2629482 0.2250492 0.2149899 0.4495584 0.5681887 0.4865322
```

The sim file will have scores per column:

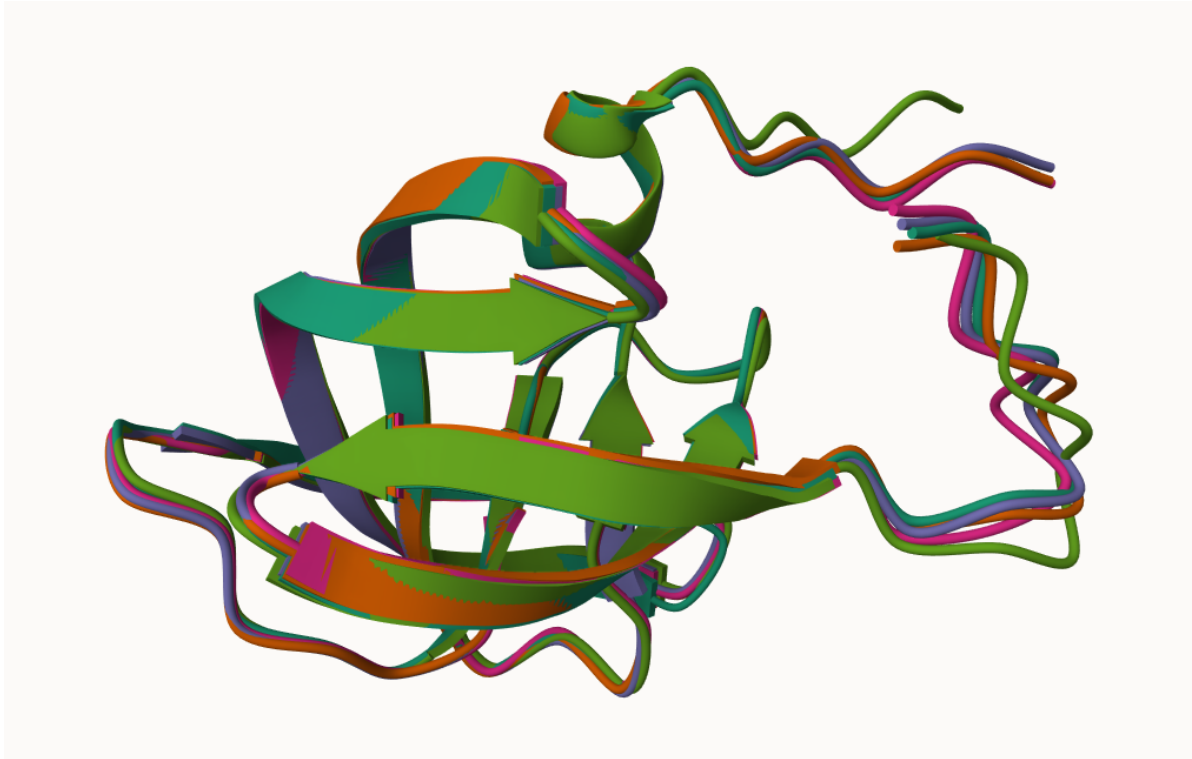
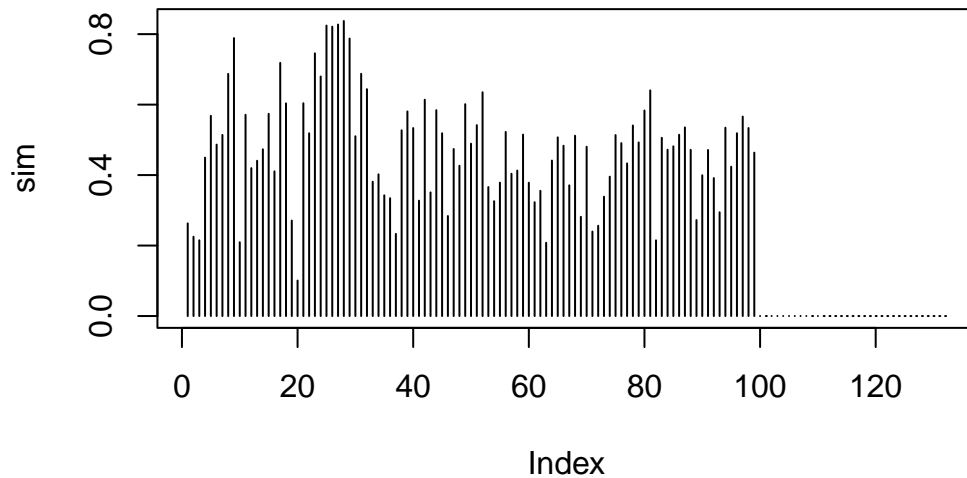


Figure 1: Aligned protein structure of HIV-1 envelope

```
plot(sim, typ="h")
```



We can summarize these conserved columns (the ones with high scores above) via a consensus sequences.

In the result below, AA DTGA are the most conserved (with a threshold of 90%)

```
consensus(aln, cutoff = 0.9)
```

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

$freq
      1          2          3          4          5          6
```

V	0.00000	0.0096690219	0.0092971365	0.0089252510	0.0048345110	0.0009297136
I	0.00000	0.0031610264	0.4631833395	0.0117143920	0.0026031982	0.0001859427
L	0.00000	0.0035329119	0.0040907401	0.0026031982	0.7571587951	0.0039047973
M	0.00000	0.0005578282	0.0001859427	0.0039047973	0.0018594273	0.0000000000
F	0.00000	0.0048345110	0.0336556341	0.0001859427	0.0042766828	0.0016734846
W	0.00000	0.0001859427	0.0000000000	0.0000000000	0.0003718855	0.7314986984
Y	0.00000	0.0078095946	0.0009297136	0.0007437709	0.0009297136	0.0022313128
S	0.00000	0.0007437709	0.0020453700	0.0507623652	0.0016734846	0.0213834139
T	0.00000	0.0000000000	0.0076236519	0.6617701748	0.0100409074	0.0011156564
N	0.00000	0.0000000000	0.0005578282	0.0035329119	0.0003718855	0.0120862774
Q	0.00000	0.4801041279	0.0040907401	0.0000000000	0.0014875418	0.0033469691
H	0.00000	0.0042766828	0.0005578282	0.0011156564	0.0066939383	0.0050204537
K	0.00000	0.0000000000	0.0009297136	0.0003718855	0.0001859427	0.0031610264
R	0.00000	0.0005578282	0.0022313128	0.0011156564	0.0020453700	0.0052063964
D	0.00000	0.0000000000	0.0014875418	0.0195239866	0.0011156564	0.0191521012
E	0.00000	0.0018594273	0.0033469691	0.0005578282	0.0014875418	0.0053923392
A	0.00000	0.0001859427	0.0014875418	0.0048345110	0.0035329119	0.0042766828
G	0.00000	0.0001859427	0.0037188546	0.0003718855	0.0018594273	0.0159910747
P	0.51283	0.0087393083	0.0003718855	0.0185942730	0.0031610264	0.0007437709
C	0.00000	0.0000000000	0.0000000000	0.0001859427	0.0007437709	0.0016734846
-	0.48717	0.4732242469	0.4594644849	0.2062104872	0.1904053552	0.1586091484
X	0.00000	0.0003718855	0.0007437709	0.0029750837	0.0031610264	0.0024172555
		7	8	9	10	11
V	0.0000000000	0.0007437709	0.0048345110	0.1515433247	0.7218296765	0.0094830792
I	0.0001859427	0.0007437709	0.0070658237	0.2973224247	0.0790256601	0.0172926739
L	0.0037188546	0.0040907401	0.0024172555	0.1777612495	0.0511342507	0.0052063964
M	0.0009297136	0.0020453700	0.0024172555	0.0288211231	0.0078095946	0.0044626255
F	0.0003718855	0.0007437709	0.0005578282	0.1320193380	0.0027891409	0.0005578282
W	0.0003718855	0.0000000000	0.0003718855	0.0022313128	0.0011156564	0.0011156564
Y	0.0000000000	0.0001859427	0.0001859427	0.0163629602	0.0005578282	0.0013015991
S	0.0094830792	0.0033469691	0.0011156564	0.0048345110	0.0016734846	0.0502045370
T	0.0126441056	0.0027891409	0.0014875418	0.0213834139	0.0089252510	0.6402008181
N	0.0130159911	0.0011156564	0.0000000000	0.0016734846	0.0001859427	0.0159910747
Q	0.7037932317	0.0096690219	0.0007437709	0.0037188546	0.0031610264	0.0158051320
H	0.0020453700	0.0037188546	0.0005578282	0.0040907401	0.0013015991	0.0022313128
K	0.0340275195	0.0066939383	0.0005578282	0.0200818148	0.0146894756	0.0476013388
R	0.0241725549	0.8281889178	0.0003718855	0.0325399777	0.0105987356	0.0132019338
D	0.0211974712	0.0011156564	0.0005578282	0.0001859427	0.0007437709	0.0122722202
E	0.0206396430	0.0150613611	0.0003718855	0.0076236519	0.0050204537	0.0290070658
A	0.0119003347	0.0037188546	0.0007437709	0.0005578282	0.0042766828	0.0137597620
G	0.0087393083	0.0020453700	0.0011156564	0.0009297136	0.0020453700	0.0013015991
P	0.0027891409	0.0096690219	0.8910375604	0.0027891409	0.0011156564	0.0587579026
C	0.0001859427	0.0018594273	0.0005578282	0.0011156564	0.0130159911	0.0003718855

-	0.1275567125	0.1004090740	0.0821866865	0.0743770919	0.0524358498	0.0500185943
X	0.0022313128	0.0020453700	0.0007437709	0.0180364448	0.0165489029	0.0098549647
	13	14	15	16	17	18
V	0.4025660097	0.0057642246	0.3226106359	0.0022313128	0.0078095946	0.0072517665
I	0.3705838602	0.0117143920	0.5611751581	0.0029750837	0.0020453700	0.0057642246
L	0.0580141316	0.0105987356	0.0364447750	0.0020453700	0.0035329119	0.0094830792
M	0.0094830792	0.0048345110	0.0037188546	0.0011156564	0.0016734846	0.0016734846
F	0.0026031982	0.0052063964	0.0053923392	0.0005578282	0.0039047973	0.0005578282
W	0.0001859427	0.0040907401	0.0000000000	0.0016734846	0.0013015991	0.0001859427
Y	0.0000000000	0.0202677575	0.0000000000	0.0016734846	0.0143175902	0.0007437709
S	0.0009297136	0.0102268501	0.0016734846	0.0066939383	0.0092971365	0.0027891409
T	0.0014875418	0.0262179249	0.0018594273	0.0087393083	0.0053923392	0.0089252510
N	0.0020453700	0.0105987356	0.0011156564	0.0557828189	0.0074377092	0.0085533656
Q	0.0005578282	0.0169207884	0.0016734846	0.0219412421	0.0018594273	0.7510226850
H	0.0000000000	0.0169207884	0.0000000000	0.0014875418	0.0022313128	0.0388620305
K	0.0020453700	0.6468947564	0.0020453700	0.0057642246	0.0026031982	0.0624767572
R	0.0005578282	0.1229081443	0.0016734846	0.0126441056	0.0055782819	0.0251022685
D	0.0024172555	0.0033469691	0.0005578282	0.0148754184	0.0189661584	0.0011156564
E	0.0011156564	0.0230568985	0.0009297136	0.1511714392	0.0135738193	0.0146894756
A	0.0634064708	0.0009297136	0.0003718855	0.0552249907	0.0026031982	0.0031610264
G	0.0033469691	0.0014875418	0.0009297136	0.6015247304	0.8562662700	0.0137597620
P	0.0007437709	0.0011156564	0.0035329119	0.0013015991	0.0005578282	0.0031610264
C	0.0163629602	0.0033469691	0.0003718855	0.0033469691	0.0011156564	0.0013015991
-	0.0466716251	0.0422089996	0.0405355151	0.0384901450	0.0362588323	0.0353291186
X	0.0148754184	0.0113425065	0.0133878765	0.0087393083	0.0016734846	0.0040907401
	19	20	21	22	23	24
V	0.0340275195	0.0925994794	0.0057642246	0.0738192637	0.0111565638	0.0552249907
I	0.1126812942	0.1331349944	0.0027891409	0.0139457047	0.0412792860	0.1020825586
L	0.5251022685	0.0191521012	0.0061361101	0.0247303830	0.8555224991	0.7794719226
M	0.0042766828	0.0375604314	0.0020453700	0.0139457047	0.0158051320	0.0087393083
F	0.0016734846	0.0410933433	0.0029750837	0.0418371142	0.0091111938	0.0217552994
W	0.0048345110	0.0003718855	0.0007437709	0.0009297136	0.0014875418	0.0001859427
Y	0.0009297136	0.0022313128	0.0026031982	0.0007437709	0.0009297136	0.0007437709
S	0.0154332466	0.0031610264	0.0238006694	0.0039047973	0.0057642246	0.0020453700
T	0.0293789513	0.0885087393	0.0336556341	0.0048345110	0.0122722202	0.0009297136
N	0.0070658237	0.0009297136	0.0111565638	0.0005578282	0.0046485682	0.0001859427
Q	0.0288211231	0.0132019338	0.0245444403	0.0026031982	0.0063220528	0.0020453700
H	0.0033469691	0.0042766828	0.0031610264	0.0039047973	0.0016734846	0.0001859427
K	0.0185942730	0.2761249535	0.0304946077	0.0040907401	0.0052063964	0.0009297136
R	0.0102268501	0.1984008925	0.0224990703	0.0052063964	0.0029750837	0.0011156564
D	0.0104127929	0.0011156564	0.0141316475	0.0014875418	0.0003718855	0.0000000000
E	0.0135738193	0.0167348457	0.7751952399	0.0009297136	0.0026031982	0.0009297136
A	0.0078095946	0.0107846783	0.0027891409	0.7214577910	0.0016734846	0.0033469691

G	0.0258460394	0.0033469691	0.0044626255	0.0531796207	0.0009297136	0.0026031982
P	0.0950167348	0.0050204537	0.0048345110	0.0040907401	0.0024172555	0.0014875418
C	0.0033469691	0.0087393083	0.0003718855	0.0022313128	0.0005578282	0.0007437709
-	0.0329118631	0.0267757531	0.0228709557	0.0185942730	0.0145035329	0.0126441056
X	0.0146894756	0.0167348457	0.0029750837	0.0029750837	0.0027891409	0.0026031982
	25	26	27	28	29	30
V	0.0055782819	0.0024172555	0.0011156564	0.0042766828	0.0029750837	0.0476013388
I	0.0037188546	0.0016734846	0.0007437709	0.0001859427	0.0007437709	0.0167348457
L	0.0078095946	0.0053923392	0.0319821495	0.0327259204	0.0029750837	0.0061361101
M	0.0022313128	0.0022313128	0.0026031982	0.0007437709	0.0020453700	0.0042766828
F	0.0009297136	0.0005578282	0.0003718855	0.0000000000	0.0031610264	0.0027891409
W	0.0016734846	0.0005578282	0.0000000000	0.0003718855	0.0007437709	0.0001859427
Y	0.0029750837	0.0000000000	0.0000000000	0.0000000000	0.0020453700	0.0089252510
S	0.0027891409	0.0193380439	0.0013015991	0.0102268501	0.0124581629	0.0074377092
T	0.0072517665	0.9031238379	0.0081814801	0.0061361101	0.0083674228	0.0373744887
N	0.0109706210	0.0009297136	0.0000000000	0.0000000000	0.0094830792	0.0535515061
Q	0.0024172555	0.0013015991	0.0003718855	0.0011156564	0.0169207884	0.0024172555
H	0.0031610264	0.0007437709	0.0001859427	0.0003718855	0.0020453700	0.0158051320
K	0.0052063964	0.0024172555	0.0013015991	0.0001859427	0.0003718855	0.0066939383
R	0.0014875418	0.0016734846	0.0048345110	0.0018594273	0.0001859427	0.0228709557
D	0.9111193752	0.0063220528	0.0052063964	0.0014875418	0.8873187058	0.7322424693
E	0.0096690219	0.0005578282	0.0039047973	0.0016734846	0.0117143920	0.0050204537
A	0.0013015991	0.0119003347	0.0026031982	0.9152101153	0.0109706210	0.0111565638
G	0.0046485682	0.0221271848	0.9224618817	0.0078095946	0.0102268501	0.0035329119
P	0.0007437709	0.0033469691	0.0005578282	0.0029750837	0.0018594273	0.0001859427
C	0.0000000000	0.0005578282	0.0003718855	0.0007437709	0.0005578282	0.0011156564
-	0.0122722202	0.0117143920	0.0113425065	0.0111565638	0.0119003347	0.0120862774
X	0.0020453700	0.0011156564	0.0005578282	0.0007437709	0.0009297136	0.0018594273
	31	32	33	34	35	36
V	0.0026031982	0.7013759762	0.0669393827	0.0208255857	0.002975084	0.0353291186
I	0.0046485682	0.1943101525	0.1379695054	0.0065079955	0.006879881	0.4998140573
L	0.0033469691	0.0165489029	0.4858683525	0.0107846783	0.011900335	0.0630345853
M	0.0014875418	0.0046485682	0.0087393083	0.0005578282	0.001673485	0.1894756415
F	0.0000000000	0.0011156564	0.2300111566	0.0005578282	0.001115656	0.0007437709
W	0.0000000000	0.0000000000	0.0000000000	0.0001859427	0.005578282	0.0001859427
Y	0.0003718855	0.0003718855	0.0014875418	0.0003718855	0.002603198	0.0022313128
S	0.1123094087	0.0061361101	0.0020453700	0.0617329862	0.036258832	0.0158051320
T	0.8092227594	0.0066939383	0.0057642246	0.0330978059	0.020825586	0.0135738193
N	0.0018594273	0.0005578282	0.0018594273	0.0215693566	0.050018594	0.0100409074
Q	0.0001859427	0.0009297136	0.0000000000	0.0602454444	0.019523987	0.0126441056
H	0.0003718855	0.0018594273	0.0007437709	0.0027891409	0.005020454	0.0156191893
K	0.0011156564	0.0001859427	0.0000000000	0.0306805504	0.022870956	0.0187802157
R	0.0044626255	0.0009297136	0.0001859427	0.0178505020	0.010040907	0.0105987356

D	0.0040907401	0.0022313128	0.0308664931	0.0180364448	0.340833023	0.0119003347
E	0.0005578282	0.0013015991	0.0007437709	0.6288583116	0.356266270	0.0174786166
A	0.0050204537	0.0353291186	0.0027891409	0.0489029379	0.011342507	0.0249163258
G	0.0323540350	0.0037188546	0.0005578282	0.0057642246	0.061732986	0.0065079955
P	0.0027891409	0.0001859427	0.0001859427	0.0074377092	0.005392339	0.0145035329
C	0.0001859427	0.0063220528	0.0003718855	0.0018594273	0.001859427	0.0011156564
-	0.0117143920	0.0117143920	0.0119003347	0.0154332466	0.017478617	0.0202677575
X	0.0013015991	0.0035329119	0.0109706210	0.0059501673	0.007809595	0.0154332466
	37	38	39	40	41	42
V	0.024730383	0.0115284492	0.0035329119	0.0044626255	0.0039047973	0.0013015991
I	0.027705467	0.0105987356	0.0022313128	0.0063220528	0.0107846783	0.0016734846
L	0.015247304	0.7601338788	0.0137597620	0.0236147267	0.0234287839	0.0068798810
M	0.004276683	0.0013015991	0.0003718855	0.0050204537	0.0018594273	0.0009297136
F	0.005578282	0.0083674228	0.0003718855	0.0011156564	0.0044626255	0.0011156564
W	0.002789141	0.0723317218	0.0001859427	0.0026031982	0.0003718855	0.8168464113
Y	0.008367423	0.0040907401	0.0011156564	0.0005578282	0.0046485682	0.0317962068
S	0.061175158	0.0182223875	0.0436965415	0.0403495723	0.0332837486	0.0100409074
T	0.030680550	0.0037188546	0.0176645593	0.0065079955	0.0187802157	0.0022313128
N	0.396429900	0.0096690219	0.0055782819	0.0081814801	0.0507623652	0.0042766828
Q	0.019895872	0.0013015991	0.0180364448	0.0122722202	0.0072517665	0.0031610264
H	0.025474154	0.0001859427	0.0022313128	0.0050204537	0.0154332466	0.0011156564
K	0.022127185	0.0018594273	0.0143175902	0.0184083302	0.3205652659	0.0128300483
R	0.002045370	0.0001859427	0.0057642246	0.0211974712	0.3856452213	0.0092971365
D	0.190033470	0.0072517665	0.0070658237	0.0100409074	0.0167348457	0.0066939383
E	0.098177761	0.0024172555	0.0159910747	0.0167348457	0.0102268501	0.0024172555
A	0.013945705	0.0243584976	0.0128300483	0.0104127929	0.0124581629	0.0035329119
G	0.002417255	0.0260319821	0.0317962068	0.7437709186	0.0159910747	0.0241725549
P	0.004090740	0.0078095946	0.7658981034	0.0224990703	0.0072517665	0.0161770175
C	0.005764225	0.0007437709	0.0005578282	0.0027891409	0.0037188546	0.0005578282
-	0.021755299	0.0241725549	0.0314243213	0.0355150614	0.0381182596	0.0414652287
X	0.017292674	0.0037188546	0.0055782819	0.0026031982	0.0143175902	0.0014875418
	43	44	45	46	47	48
V	0.0050204537	0.0065079955	0.0111565638	0.0143175902	0.1524730383	0.0524358498
I	0.0085533656	0.0035329119	0.0132019338	0.3348828561	0.6290442544	0.0182223875
L	0.0130159911	0.0252882112	0.0027891409	0.1156563778	0.0063220528	0.0446262551
M	0.0011156564	0.0013015991	0.0014875418	0.3185198959	0.0061361101	0.0171067311
F	0.0003718855	0.0007437709	0.0003718855	0.0005578282	0.0016734846	0.0009297136
W	0.0098549647	0.0135738193	0.0020453700	0.0457419115	0.0026031982	0.0039047973
Y	0.0026031982	0.0011156564	0.0007437709	0.0005578282	0.0003718855	0.0024172555
S	0.0228709557	0.0206396430	0.0169207884	0.0053923392	0.0178505020	0.0172926739
T	0.1178876906	0.0211974712	0.0223131276	0.0150613611	0.0156191893	0.0105987356
N	0.0079955374	0.0018594273	0.0098549647	0.0031610264	0.0009297136	0.0059501673
Q	0.0072517665	0.0065079955	0.0304946077	0.0040907401	0.0050204537	0.0189661584



H	0.0018594273	0.0050204537	0.0198958721	0.0020453700	0.0003718855	0.0009297136
K	0.6058014132	0.0304946077	0.6991446634	0.0178505020	0.0210115284	0.0076236519
R	0.0286351804	0.0063220528	0.0656377836	0.0059501673	0.0046485682	0.0096690219
D	0.0024172555	0.0016734846	0.0055782819	0.0055782819	0.0007437709	0.0046485682
E	0.0089252510	0.0018594273	0.0078095946	0.0057642246	0.0048345110	0.0076236519
A	0.0105987356	0.0068798810	0.0063220528	0.0094830792	0.0330978059	0.0152473038
G	0.0035329119	0.0137597620	0.0074377092	0.0020453700	0.0022313128	0.6917069543
P	0.0833023429	0.7776124954	0.0159910747	0.0234287839	0.0306805504	0.0078095946
C	0.0003718855	0.0001859427	0.0009297136	0.0003718855	0.0001859427	0.0007437709
-	0.0477872815	0.0522499070	0.0557828189	0.0593157308	0.0591297880	0.0593157308
X	0.0102268501	0.0016734846	0.0040907401	0.0102268501	0.0050204537	0.0022313128
	49	50	51	52	53	54
V	0.0124581629	0.0481591670	0.0150613611	0.0148754184	0.012644106	0.2895128300
I	0.0100409074	0.6957976943	0.0301227222	0.0146894756	0.011528449	0.3657493492
L	0.0068798810	0.0332837486	0.0327259204	0.0053923392	0.110078096	0.0840461138
M	0.0037188546	0.0042766828	0.0040907401	0.0040907401	0.002975084	0.0476013388
F	0.0024172555	0.0022313128	0.0013015991	0.0020453700	0.630531796	0.0081814801
W	0.0024172555	0.0011156564	0.0037188546	0.0011156564	0.001301599	0.0003718855
Y	0.0020453700	0.0020453700	0.0005578282	0.0001859427	0.012644106	0.0001859427
S	0.0098549647	0.0137597620	0.0141316475	0.0143175902	0.005578282	0.0167348457
T	0.0219412421	0.0152473038	0.0267757531	0.0156191893	0.010784678	0.0273335813
N	0.0039047973	0.0065079955	0.0014875418	0.0014875418	0.004276683	0.0005578282
Q	0.0384901450	0.0048345110	0.0033469691	0.0135738193	0.003718855	0.0081814801
H	0.0020453700	0.0085533656	0.0005578282	0.0016734846	0.002789141	0.0065079955
K	0.0046485682	0.0050204537	0.0035329119	0.0033469691	0.003161026	0.0126441056
R	0.0094830792	0.0022313128	0.0111565638	0.0081814801	0.002417255	0.0042766828
D	0.0024172555	0.0066939383	0.0013015991	0.0018594273	0.003904797	0.0007437709
E	0.0065079955	0.0014875418	0.0050204537	0.0040907401	0.003904797	0.0026031982
A	0.0065079955	0.0303086649	0.0154332466	0.0145035329	0.006507996	0.0217552994
G	0.7893268873	0.0392339160	0.7606917070	0.8079211603	0.089996281	0.0234287839
P	0.0029750837	0.0159910747	0.0046485682	0.0050204537	0.002975084	0.0037188546
C	0.0007437709	0.0005578282	0.0014875418	0.0014875418	0.002417255	0.0003718855
-	0.0600595017	0.0604313871	0.0619189290	0.0634064708	0.065265898	0.0648940126
X	0.0011156564	0.0022313128	0.0009297136	0.0011156564	0.010598736	0.0105987356
	55	56	57	58	59	60
V	0.0377463741	0.7394942358	0.0176645593	0.0383042023	0.0052063964	0.0141316475
I	0.0148754184	0.0154332466	0.0055782819	0.0078095946	0.0050204537	0.0039047973
L	0.0096690219	0.0063220528	0.0068798810	0.0024172555	0.0068798810	0.0046485682
M	0.0035329119	0.0018594273	0.0014875418	0.0018594273	0.0026031982	0.0009297136
F	0.0031610264	0.0035329119	0.0007437709	0.0009297136	0.0087393083	0.0018594273
W	0.0027891409	0.0003718855	0.0001859427	0.0139457047	0.0009297136	0.0111565638
Y	0.0009297136	0.0182223875	0.0014875418	0.0013015991	0.7549274823	0.0120862774
S	0.0040907401	0.0066939383	0.0191521012	0.0154332466	0.0100409074	0.0063220528

T	0.0066939383	0.0492748234	0.0107846783	0.0102268501	0.0200818148	0.0236147267
N	0.0455559688	0.0013015991	0.0040907401	0.0046485682	0.0133878765	0.0165489029
Q	0.0122722202	0.0200818148	0.0059501673	0.6117515805	0.0122722202	0.0089252510
H	0.0020453700	0.0026031982	0.0009297136	0.0040907401	0.0022313128	0.0026031982
K	0.5753068055	0.0109706210	0.2469319450	0.0102268501	0.0215693566	0.0306805504
R	0.1279285980	0.0040907401	0.5124581629	0.0119003347	0.0053923392	0.0057642246
D	0.0005578282	0.0013015991	0.0011156564	0.0018594273	0.0040907401	0.5608032726
E	0.0022313128	0.0159910747	0.0039047973	0.1658609148	0.0079955374	0.1509854965
A	0.0050204537	0.0092971365	0.0189661584	0.0065079955	0.0083674228	0.0085533656
G	0.0611751581	0.0213834139	0.0539233916	0.0135738193	0.0342134623	0.0351431759
P	0.0016734846	0.0037188546	0.0037188546	0.0081814801	0.0035329119	0.0206396430
C	0.0003718855	0.0003718855	0.0020453700	0.0005578282	0.0016734846	0.0040907401
-	0.0656377836	0.0652658981	0.0658237263	0.0663815545	0.0686128672	0.0691706954
X	0.0167348457	0.0024172555	0.0161770175	0.0022313128	0.0022313128	0.0074377092
	61	62	63	64	65	66
V	0.0048345110	0.3772777984	0.0332837486	0.1667906285	0.008181480	0.0643361845
I	0.0018594273	0.3726292302	0.0107846783	0.5788397174	0.012458163	0.6840833023
L	0.0249163258	0.0040907401	0.1234659725	0.0330978059	0.014317590	0.0338415768
M	0.0094830792	0.0065079955	0.0009297136	0.0197099293	0.002417255	0.0026031982
F	0.0059501673	0.0018594273	0.0037188546	0.0005578282	0.002789141	0.0366307177
W	0.0005578282	0.0003718855	0.0003718855	0.0001859427	0.001673485	0.0005578282
Y	0.0193380439	0.0009297136	0.0014875418	0.0005578282	0.002975084	0.0033469691
S	0.0052063964	0.0085533656	0.0641502417	0.0247303830	0.015991075	0.0046485682
T	0.0050204537	0.0258460394	0.0769802901	0.0119003347	0.005206396	0.0061361101
N	0.1193752324	0.0068798810	0.0122722202	0.0024172555	0.008925251	0.0033469691
Q	0.5418371142	0.0416511714	0.0213834139	0.0089252510	0.013759762	0.0133878765
H	0.0239866121	0.0022313128	0.0152473038	0.0009297136	0.004462626	0.0022313128
K	0.0210115284	0.0100409074	0.0115284492	0.0072517665	0.042209000	0.0117143920
R	0.0178505020	0.0232428412	0.0124581629	0.0057642246	0.017664559	0.0143175902
D	0.0436965415	0.0065079955	0.0059501673	0.0013015991	0.044998141	0.0027891409
E	0.0580141316	0.0039047973	0.0332837486	0.0061361101	0.705280774	0.0193380439
A	0.0059501673	0.0052063964	0.0217552994	0.0381182596	0.007809595	0.0031610264
G	0.0081814801	0.0048345110	0.0052063964	0.0026031982	0.004090740	0.0039047973
P	0.0031610264	0.0059501673	0.4496095203	0.0091111938	0.005020454	0.0074377092
C	0.0011156564	0.0024172555	0.0139457047	0.0011156564	0.003346969	0.0018594273
-	0.0699144663	0.0697285236	0.0706582373	0.0725176646	0.073261435	0.0730754927
X	0.0087393083	0.0193380439	0.0115284492	0.0074377092	0.003161026	0.0072517665
	67	68	69	70	71	72
V	0.014503533	0.010412793	0.009483079	0.0143175902	0.3315358869	0.1121234660
I	0.013387877	0.011528449	0.008739308	0.0100409074	0.0613611008	0.4685756787
L	0.069170695	0.007251766	0.008553366	0.0165489029	0.0117143920	0.0325399777
M	0.004090740	0.002603198	0.001673485	0.0022313128	0.0016734846	0.0172926739
F	0.019895872	0.002975084	0.001115656	0.0016734846	0.0031610264	0.0022313128

W	0.003346969	0.002789141	0.023428784	0.0011156564	0.0000000000	0.0007437709
Y	0.026031982	0.001301599	0.018408330	0.0007437709	0.0007437709	0.0016734846
S	0.031052436	0.006136110	0.008181480	0.0050204537	0.0059501673	0.0098549647
T	0.011156564	0.019523987	0.007437709	0.0228709557	0.0894384530	0.0989215322
N	0.001673485	0.018222388	0.007437709	0.0039047973	0.0037188546	0.0050204537
Q	0.005578282	0.003346969	0.031982149	0.0161770175	0.0053923392	0.0150613611
H	0.002417255	0.007437709	0.479360357	0.0105987356	0.0037188546	0.0031610264
K	0.006136110	0.021941242	0.191892897	0.6699516549	0.0238006694	0.0219412421
R	0.004462626	0.013573819	0.037932317	0.0777240610	0.0057642246	0.0511342507
D	0.003532912	0.005392339	0.003346969	0.0044626255	0.0230568985	0.0055782819
E	0.030308665	0.017106731	0.011156564	0.0358869468	0.0057642246	0.0260319821
A	0.006136110	0.006136110	0.002975084	0.0031610264	0.3049460766	0.0063220528
G	0.015247304	0.730568985	0.039605801	0.0098549647	0.0154332466	0.0063220528
P	0.002975084	0.017664559	0.005206396	0.0022313128	0.0024172555	0.0124581629
C	0.649683897	0.008925251	0.011714392	0.0024172555	0.0033469691	0.0007437709
-	0.073261435	0.081814801	0.079769431	0.0805132019	0.0805132019	0.0808850874
X	0.005950167	0.003346969	0.010598736	0.0085533656	0.0165489029	0.0213834139
	73	74	75	76	77	78
V	0.0109706210	0.0057642246	0.7207140201	0.0660096690	0.5790256601	0.0317962068
I	0.0197099293	0.0167348457	0.0442543697	0.0146894756	0.1751580513	0.0189661584
L	0.0070658237	0.0044626255	0.0055782819	0.6943101525	0.0275195240	0.0176645593
M	0.0018594273	0.0009297136	0.0011156564	0.0338415768	0.0018594273	0.0013015991
F	0.0013015991	0.0018594273	0.0172926739	0.0081814801	0.0029750837	0.0042766828
W	0.0003718855	0.0001859427	0.0000000000	0.0000000000	0.0001859427	0.0003718855
Y	0.0026031982	0.0035329119	0.0016734846	0.0009297136	0.0018594273	0.0040907401
S	0.0851617702	0.1080327259	0.0055782819	0.0137597620	0.0059501673	0.0055782819
T	0.0412792860	0.5994793604	0.0187802157	0.0145035329	0.0355150614	0.0202677575
N	0.0022313128	0.0072517665	0.0096690219	0.0037188546	0.0009297136	0.0046485682
Q	0.0065079955	0.0020453700	0.0145035329	0.0055782819	0.0066939383	0.0057642246
H	0.0182223875	0.0070658237	0.0094830792	0.0027891409	0.0011156564	0.0033469691
K	0.0120862774	0.0120862774	0.0079955374	0.0100409074	0.0132019338	0.0076236519
R	0.0066939383	0.0061361101	0.0050204537	0.0042766828	0.0033469691	0.0137597620
D	0.0135738193	0.0040907401	0.0111565638	0.0057642246	0.0029750837	0.0013015991
E	0.0310524358	0.0072517665	0.0091111938	0.0115284492	0.0044626255	0.0066939383
A	0.0420230569	0.0314243213	0.0072517665	0.0027891409	0.0081814801	0.0022313128
G	0.5782818892	0.0516920788	0.0206396430	0.0148754184	0.0286351804	0.7595760506
P	0.0033469691	0.0368166605	0.0022313128	0.0076236519	0.0014875418	0.0050204537
C	0.0221271848	0.0011156564	0.0005578282	0.0003718855	0.0013015991	0.0016734846
-	0.0814429156	0.0818148010	0.0823726292	0.0827445147	0.0823726292	0.0825585720
X	0.0120862774	0.0102268501	0.0050204537	0.0016734846	0.0152473038	0.0014875418
	79	80	81	82	83	84
V	0.0252882112	0.0079955374	0.0098549647	0.3625883228	0.0342134623	0.2214577910
I	0.0211974712	0.0052063964	0.0033469691	0.0721457791	0.0226850130	0.5751208628

L	0.0226850130	0.0109706210	0.0057642246	0.0132019338	0.0089252510	0.0210115284
M	0.0016734846	0.0009297136	0.0013015991	0.0139457047	0.0013015991	0.0031610264
F	0.0109706210	0.0014875418	0.0039047973	0.0425808851	0.0078095946	0.0040907401
W	0.0003718855	0.0022313128	0.0000000000	0.0000000000	0.0003718855	0.0001859427
Y	0.0014875418	0.0011156564	0.0022313128	0.0213834139	0.0100409074	0.0014875418
S	0.0104127929	0.0079955374	0.0098549647	0.0334696913	0.0085533656	0.0124581629
T	0.0076236519	0.7664559316	0.0180364448	0.0474153961	0.0074377092	0.0102268501
N	0.0018594273	0.0029750837	0.0009297136	0.0053923392	0.7242469319	0.0113425065
Q	0.0091111938	0.0200818148	0.0089252510	0.0035329119	0.0009297136	0.0011156564
H	0.0029750837	0.0020453700	0.0018594273	0.0024172555	0.0039047973	0.0020453700
K	0.0031610264	0.0072517665	0.0016734846	0.0003718855	0.0016734846	0.0020453700
R	0.0024172555	0.0081814801	0.0026031982	0.0016734846	0.0005578282	0.0063220528
D	0.0360728896	0.0055782819	0.0037188546	0.0014875418	0.0293789513	0.0014875418
E	0.0046485682	0.0126441056	0.0044626255	0.0007437709	0.0005578282	0.0013015991
A	0.0184083302	0.0063220528	0.0145035329	0.2313127557	0.0109706210	0.0111565638
G	0.0135738193	0.0132019338	0.0029750837	0.0026031982	0.0014875418	0.0005578282
P	0.7190405355	0.0293789513	0.8051320193	0.0319821495	0.0371885459	0.0204537003
C	0.0013015991	0.0042766828	0.0163629602	0.0182223875	0.0031610264	0.0033469691
-	0.0821866865	0.0821866865	0.0823726292	0.0831164001	0.0838601711	0.0847898847
X	0.0035329119	0.0014875418	0.0001859427	0.0104127929	0.0007437709	0.0048345110
	85	86	87	88	89	90
V	0.0734473782	0.0267757531	0.0113425065	0.0132019338	0.1080327259	0.0074377092
I	0.6744142804	0.0334696913	0.0111565638	0.0098549647	0.0881368538	0.0091111938
L	0.0301227222	0.0368166605	0.0394198587	0.0245444403	0.4347341019	0.4804760134
M	0.0014875418	0.0014875418	0.0027891409	0.0014875418	0.1297880253	0.3201933804
F	0.0291930086	0.0081814801	0.0026031982	0.0020453700	0.0065079955	0.0024172555
W	0.0005578282	0.0001859427	0.0005578282	0.0003718855	0.0005578282	0.0007437709
Y	0.0001859427	0.0027891409	0.0005578282	0.0011156564	0.0007437709	0.0055782819
S	0.0087393083	0.0009297136	0.0027891409	0.0132019338	0.0046485682	0.0020453700
T	0.0061361101	0.0048345110	0.0046485682	0.0052063964	0.0187802157	0.0016734846
N	0.0137597620	0.0048345110	0.0040907401	0.6874302715	0.0284492376	0.0295648940
Q	0.0013015991	0.0011156564	0.0033469691	0.0033469691	0.0022313128	0.0003718855
H	0.0009297136	0.0026031982	0.0020453700	0.0005578282	0.0014875418	0.0005578282
K	0.0024172555	0.0035329119	0.0078095946	0.0020453700	0.0007437709	0.0014875418
R	0.0022313128	0.0092971365	0.7513945705	0.0258460394	0.0308664931	0.0018594273
D	0.0076236519	0.0027891409	0.0024172555	0.0572703607	0.0202677575	0.0193380439
E	0.0148754184	0.0061361101	0.0016734846	0.0022313128	0.0011156564	0.0016734846
A	0.0037188546	0.0044626255	0.0029750837	0.0037188546	0.0016734846	0.0031610264
G	0.0024172555	0.7525102269	0.0308664931	0.0334696913	0.0029750837	0.0039047973
P	0.0323540350	0.0083674228	0.0273335813	0.0215693566	0.0161770175	0.0119003347
C	0.0009297136	0.0011156564	0.0005578282	0.0013015991	0.0003718855	0.0005578282
-	0.0860914838	0.0866493120	0.0873930829	0.0885087393	0.0886946820	0.0890665675
X	0.0070658237	0.0011156564	0.0022313128	0.0016734846	0.0130159911	0.0068798810

	91	92	93	94	95	96
V	0.005764225	0.0145035329	0.0074377092	0.0081814801	0.0124581629	0.0074377092
I	0.006879881	0.0035329119	0.4124209743	0.0124581629	0.0074377092	0.0230568985
L	0.050948308	0.0230568985	0.3283748605	0.0208255857	0.0476013388	0.0310524358
M	0.007065824	0.0137597620	0.0130159911	0.0044626255	0.0319821495	0.0022313128
F	0.002975084	0.0007437709	0.0026031982	0.0007437709	0.0301227222	0.0007437709
W	0.019523987	0.0163629602	0.0048345110	0.0007437709	0.0020453700	0.0009297136
Y	0.001859427	0.0005578282	0.0001859427	0.0000000000	0.0007437709	0.0003718855
S	0.044254370	0.0107846783	0.0079955374	0.0039047973	0.0031610264	0.0308664931
T	0.690219412	0.0245444403	0.0089252510	0.0007437709	0.0020453700	0.7160654518
N	0.021941242	0.0011156564	0.0016734846	0.0033469691	0.0027891409	0.0035329119
Q	0.001115656	0.6309036817	0.0165489029	0.0055782819	0.0020453700	0.0035329119
H	0.001487542	0.0063220528	0.0014875418	0.0003718855	0.0011156564	0.0014875418
K	0.007065824	0.0693566382	0.0185942730	0.0132019338	0.0014875418	0.0018594273
R	0.003718855	0.0156191893	0.0232428412	0.0282632949	0.0079955374	0.0037188546
D	0.002231313	0.0022313128	0.0039047973	0.0241725549	0.0184083302	0.0048345110
E	0.001859427	0.0094830792	0.0050204537	0.0042766828	0.0011156564	0.0007437709
A	0.018966158	0.0239866121	0.0105987356	0.0050204537	0.0092971365	0.0180364448
G	0.006879881	0.0286351804	0.0217552994	0.7467460022	0.0264038676	0.0316102640
P	0.004648568	0.0035329119	0.0076236519	0.0052063964	0.0016734846	0.0027891409
C	0.002975084	0.0011156564	0.0009297136	0.0109706210	0.6870583860	0.0102268501
-	0.090182224	0.0911119375	0.0974339903	0.0992934176	0.1018966158	0.1037560431
X	0.007437709	0.0087393083	0.0053923392	0.0014875418	0.0011156564	0.0011156564
	97	98	99	100	101	102
V	0.0057642246	0.0033469691	0.0018594273	0.0065079955	0.0065079955	0.0113425065
I	0.0171067311	0.0210115284	0.0154332466	0.0081814801	0.0042766828	0.0035329119
L	0.7658981034	0.0156191893	0.0252882112	0.0094830792	0.0180364448	0.0072517665
M	0.0070658237	0.0027891409	0.0061361101	0.0189661584	0.0039047973	0.0026031982
F	0.0024172555	0.0011156564	0.7015619189	0.0260319821	0.0078095946	0.0009297136
W	0.0009297136	0.0009297136	0.0096690219	0.0014875418	0.0024172555	0.0007437709
Y	0.0001859427	0.0005578282	0.0022313128	0.0003718855	0.0001859427	0.0005578282
S	0.0052063964	0.0135738193	0.0039047973	0.0026031982	0.0031610264	0.0035329119
T	0.0126441056	0.0124581629	0.0037188546	0.0024172555	0.0027891409	0.0068798810
N	0.0000000000	0.7348456675	0.0109706210	0.0081814801	0.0026031982	0.0013015991
Q	0.0211974712	0.0167348457	0.0141316475	0.0055782819	0.0037188546	0.0100409074
H	0.0029750837	0.0024172555	0.0117143920	0.0024172555	0.0003718855	0.0005578282
K	0.0027891409	0.0104127929	0.0029750837	0.0018594273	0.0052063964	0.0013015991
R	0.0079955374	0.0150613611	0.0046485682	0.0029750837	0.0022313128	0.0039047973
D	0.0020453700	0.0102268501	0.0137597620	0.0070658237	0.0026031982	0.0018594273
E	0.0026031982	0.0076236519	0.0020453700	0.0003718855	0.0007437709	0.0042766828
A	0.0137597620	0.0063220528	0.0029750837	0.0013015991	0.0113425065	0.0102268501
G	0.0158051320	0.0072517665	0.0048345110	0.0152473038	0.0111565638	0.0048345110
P	0.0007437709	0.0011156564	0.0007437709	0.0011156564	0.0009297136	0.0000000000

C	0.0024172555	0.0011156564	0.0001859427	0.0011156564	0.0011156564	0.0007437709
-	0.1097062105	0.1137969505	0.1610264039	0.8767199702	0.9088880625	0.9235775381
X	0.0007437709	0.0016734846	0.0001859427	0.0000000000	0.0000000000	0.0000000000
	103	104	105	106	107	108
V	0.0040907401	0.0013015991	0.0061361101	0.0065079955	0.0091111938	0.0018594273
I	0.0083674228	0.0031610264	0.0022313128	0.0029750837	0.0085533656	0.0031610264
L	0.0165489029	0.0161770175	0.0050204537	0.0055782819	0.0024172555	0.0105987356
M	0.0005578282	0.0029750837	0.0007437709	0.0014875418	0.0000000000	0.0000000000
F	0.0009297136	0.0011156564	0.0020453700	0.0005578282	0.0003718855	0.0007437709
W	0.0059501673	0.0027891409	0.0009297136	0.0007437709	0.0000000000	0.0003718855
Y	0.0033469691	0.0001859427	0.0001859427	0.0001859427	0.0000000000	0.0000000000
S	0.0014875418	0.0029750837	0.0009297136	0.0001859427	0.0005578282	0.0003718855
T	0.0011156564	0.0014875418	0.0011156564	0.0018594273	0.0020453700	0.0007437709
N	0.0014875418	0.0026031982	0.0005578282	0.0011156564	0.0005578282	0.0009297136
Q	0.0133878765	0.0042766828	0.0014875418	0.0000000000	0.0001859427	0.0001859427
H	0.0003718855	0.0003718855	0.0001859427	0.0001859427	0.0001859427	0.0000000000
K	0.0013015991	0.0007437709	0.0000000000	0.0042766828	0.0005578282	0.0000000000
R	0.0001859427	0.0005578282	0.0001859427	0.0018594273	0.0013015991	0.0011156564
D	0.0016734846	0.0001859427	0.0011156564	0.0007437709	0.0014875418	0.0050204537
E	0.0005578282	0.0014875418	0.0001859427	0.0000000000	0.0000000000	0.0001859427
A	0.0029750837	0.0016734846	0.0020453700	0.0013015991	0.0001859427	0.0003718855
G	0.0029750837	0.0092971365	0.0156191893	0.0040907401	0.0029750837	0.0011156564
P	0.0000000000	0.0003718855	0.0000000000	0.0000000000	0.0001859427	0.0001859427
C	0.0001859427	0.0000000000	0.0000000000	0.0001859427	0.0000000000	0.0000000000
-	0.9325027891	0.9462625511	0.9592785422	0.9661584232	0.9693194496	0.9730383042
X	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
	109	110	111	112	113	114
V	0.0009297136	0.0005578282	0.0005578282	0.0001859427	0.0000000000	0.0003718855
I	0.0005578282	0.0003718855	0.0001859427	0.0003718855	0.0000000000	0.0005578282
L	0.0035329119	0.0026031982	0.0003718855	0.0003718855	0.0003718855	0.0001859427
M	0.0001859427	0.0003718855	0.0000000000	0.0000000000	0.0001859427	0.0001859427
F	0.0009297136	0.0005578282	0.0005578282	0.0001859427	0.0000000000	0.0001859427
W	0.0000000000	0.0001859427	0.0000000000	0.0009297136	0.0001859427	0.0000000000
Y	0.0003718855	0.0003718855	0.0000000000	0.0000000000	0.0000000000	0.0000000000
S	0.0001859427	0.0001859427	0.0000000000	0.0001859427	0.0000000000	0.0000000000
T	0.0001859427	0.0001859427	0.0001859427	0.0000000000	0.0005578282	0.0000000000
N	0.0001859427	0.0003718855	0.0000000000	0.0001859427	0.0000000000	0.0000000000
Q	0.0001859427	0.0000000000	0.0001859427	0.0001859427	0.0000000000	0.0000000000
H	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
K	0.0000000000	0.0001859427	0.0000000000	0.0001859427	0.0001859427	0.0000000000
R	0.0011156564	0.0001859427	0.0001859427	0.0000000000	0.0001859427	0.0000000000
D	0.0014875418	0.0003718855	0.0007437709	0.0001859427	0.0003718855	0.0003718855
E	0.0001859427	0.0000000000	0.0000000000	0.0001859427	0.0000000000	0.0001859427

A	0.0007437709	0.0009297136	0.0014875418	0.0005578282	0.0001859427	0.0000000000
G	0.0013015991	0.0003718855	0.0009297136	0.0000000000	0.0011156564	0.0009297136
P	0.0000000000	0.0000000000	0.0000000000	0.0003718855	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0001859427
-	0.9877277798	0.9921904054	0.9946076608	0.9959092599	0.9966530309	0.9968389736
X	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
	115	116	117	118	119	120
V	0.0003718855	0.0000000000	0.0000000000	0.0001859427	0.0000000000	0.0000000000
I	0.0000000000	0.0003718855	0.0003718855	0.0000000000	0.0000000000	0.0000000000
L	0.0000000000	0.0011156564	0.0003718855	0.0003718855	0.0000000000	0.0000000000
M	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
F	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0005578282	0.0000000000
W	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
Y	0.0001859427	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000
S	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
T	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000
Q	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
H	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
K	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
R	0.0005578282	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0001859427
D	0.0007437709	0.0001859427	0.0003718855	0.0005578282	0.0001859427	0.0001859427
E	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
A	0.0005578282	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
G	0.0000000000	0.0000000000	0.0007437709	0.0000000000	0.0001859427	0.0000000000
P	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
-	0.9970249163	0.9979546300	0.9981405727	0.9988843436	0.9990702864	0.9996281145
X	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
	121	122	123	124	125	126
V	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
I	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
L	0.0000000000	0.0000000000	0.0001859427	0.0000000000	0.0000000000	0.0000000000
M	0.0000000000	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0001859427
W	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
Y	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
S	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
T	0.0000000000	0.0000000000	0.0000000000	0.0001859427	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
Q	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
H	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
K	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000

R	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0001859427	0.0000000000
D	0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
E	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
A	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
G	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
P	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000
-	0.9998140573	0.9998140573	0.9998140573	0.9998140573	0.9998140573	0.9998140573
X	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000

	127	128	129	130	131	132
V	0.0000000000	0	0	0	0	0
I	0.0000000000	0	0	0	0	0
L	0.0000000000	0	0	0	0	0
M	0.0000000000	0	0	0	0	0
F	0.0000000000	0	0	0	0	0
W	0.0000000000	0	0	0	0	0
Y	0.0000000000	0	0	0	0	0
S	0.0000000000	0	0	0	0	0
T	0.0000000000	0	0	0	0	0
N	0.0000000000	0	0	0	0	0
Q	0.0000000000	0	0	0	0	0
H	0.0000000000	0	0	0	0	0
K	0.0000000000	0	0	0	0	0
R	0.0000000000	0	0	0	0	0
D	0.0000000000	0	0	0	0	0
E	0.0000000000	0	0	0	0	0
A	0.0000000000	0	0	0	0	0
G	0.0001859427	0	0	0	0	0
P	0.0000000000	0	0	0	0	0
C	0.0000000000	0	0	0	0	0
-	0.9998140573	1	1	1	1	1
X	0.0000000000	0	0	0	0	0

\$seq.freq

	1	2	3	4	5	6
0.5128300483	0.4801041279	0.4631833395	0.6617701748	0.7571587951	0.7314986984	
	7	8	9	10	11	12
0.7037932317	0.8281889178	0.8910375604	0.2973224247	0.7218296765	0.6402008181	
	13	14	15	16	17	18
0.4025660097	0.6468947564	0.5611751581	0.6015247304	0.8562662700	0.7510226850	
	19	20	21	22	23	24
0.5251022685	0.2761249535	0.7751952399	0.7214577910	0.8555224991	0.7794719226	
	25	26	27	28	29	30



0.9111193752	0.9031238379	0.9224618817	0.9152101153	0.8873187058	0.7322424693
31	32	33	34	35	36
0.8092227594	0.7013759762	0.4858683525	0.6288583116	0.3562662700	0.4998140573
37	38	39	40	41	42
0.3964298996	0.7601338788	0.7658981034	0.7437709186	0.3856452213	0.8168464113
43	44	45	46	47	48
0.6058014132	0.7776124954	0.6991446634	0.3348828561	0.6290442544	0.6917069543
49	50	51	52	53	54
0.7893268873	0.6957976943	0.7606917070	0.8079211603	0.6305317962	0.3657493492
55	56	57	58	59	60
0.5753068055	0.7394942358	0.5124581629	0.6117515805	0.7549274823	0.5608032726
61	62	63	64	65	66
0.5418371142	0.3772777984	0.4496095203	0.5788397174	0.7052807735	0.6840833023
67	68	69	70	71	72
0.6496838974	0.7305689848	0.4793603570	0.6699516549	0.3315358869	0.4685756787
73	74	75	76	77	78
0.5782818892	0.5994793604	0.7207140201	0.6943101525	0.5790256601	0.7595760506
79	80	81	82	83	84
0.7190405355	0.7664559316	0.8051320193	0.3625883228	0.7242469319	0.5751208628
85	86	87	88	89	90
0.6744142804	0.7525102269	0.7513945705	0.6874302715	0.4347341019	0.4804760134
91	92	93	94	95	96
0.6902194124	0.6309036817	0.4124209743	0.7467460022	0.6870583860	0.7160654518
97	98	99	100	101	102
0.7658981034	0.7348456675	0.7015619189	0.0260319821	0.0180364448	0.0113425065
103	104	105	106	107	108
0.0165489029	0.0161770175	0.0156191893	0.0065079955	0.0091111938	0.0105987356
109	110	111	112	113	114
0.0035329119	0.0026031982	0.0014875418	0.0009297136	0.0011156564	0.0009297136
115	116	117	118	119	120
0.0007437709	0.0011156564	0.0007437709	0.0005578282	0.0005578282	0.0001859427
121	122	123	124	125	126
0.0001859427	0.0001859427	0.0001859427	0.0001859427	0.0001859427	0.0001859427
127	128	129	130	131	132
0.0001859427	0.0000000000	0.0000000000	0.0000000000	0.0000000000	0.0000000000

\$cutoff

[1] 0.9

We will now read the Predicted Alignment Error (PAE) files to make sense of the multichains. These are stored as JSON format.

```
library(jsonlite)

pae_files <- list.files(path=pth,
                        pattern= "000.json",
                        full.names = TRUE)

pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)
```

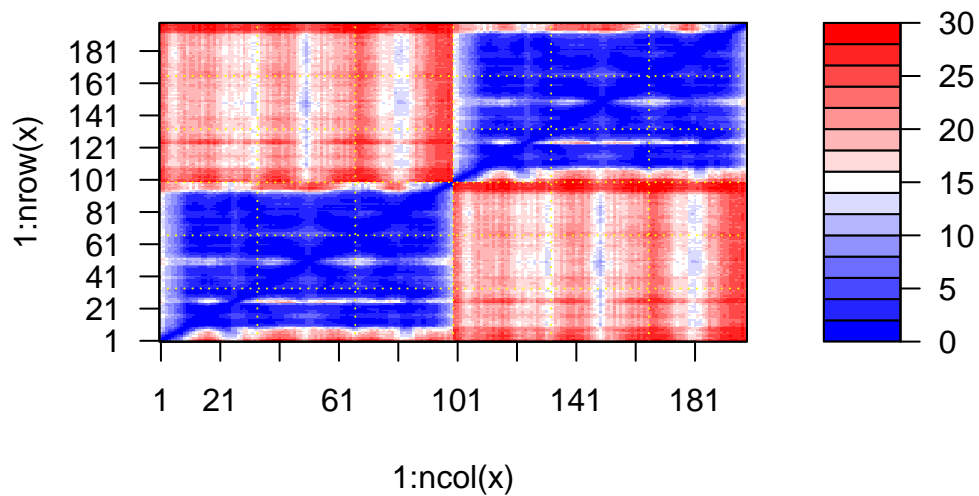
Get an idea of the structure of the data:

```
dim(pae1$pae)
```

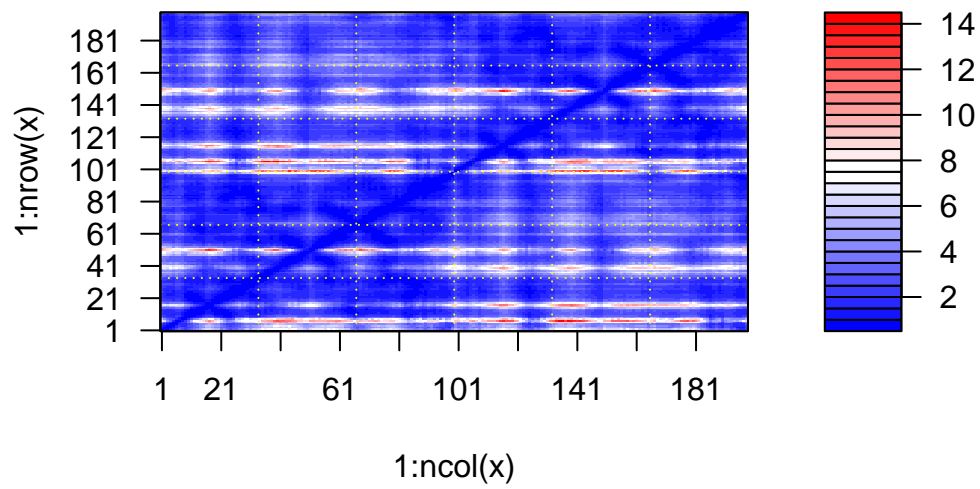
```
[1] 198 198
```

Let's plot this distance matrix:

```
plot.dmat(pae5$pae)
```



```
plot.dmat(pae1$pae)
```



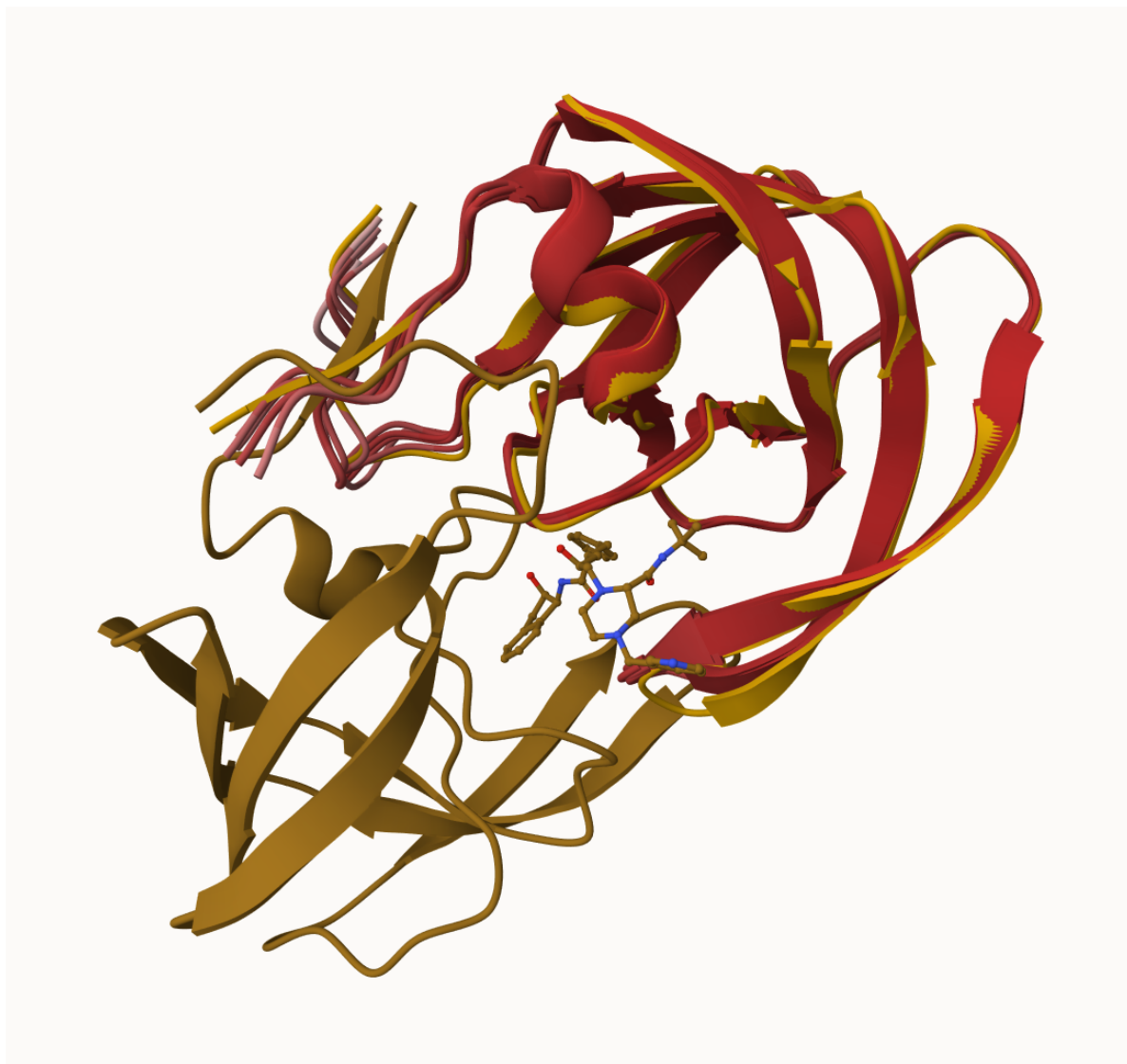


Figure 2: An overlapping image of all structures