Class 09: Structural Bioinformatics

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The PDB Database

The main repository for biomolecular sturcture data is in the Protein Data Bank (PDB): https://www.rcsb.org

Lets have a quick look at the composition of this database:

> Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.

This is annoying, lets try a different import function from the **readr** package.

```
library(readr)

stats <- read_csv("Data Export Summary.csv")
```

```
Rows: 6 Columns: 9
-- Column specification ------------------------------------------------------
Delimiter: ","
chr (1): Molecular Type
dbl (4): Integrative, Multiple methods, Neutron, Other
num (4): X-ray, EM, NMR, Total

i Use `spec()` to retrieve the full column specification for this data.
i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
stats
```

```
# A tibble: 6 x 9
  `Molecular Type`   `X-ray`    EM   NMR Integrative `Multiple methods` Neutron
  <chr>                <dbl> <dbl> <dbl>       <dbl>              <dbl>   <dbl>
1 Protein (only)      176378 20438 12709         342                221      83
```

1

```
2 Protein/Oligosacch~    10284   3396    34           8                    11          1
3 Protein/NA             9007    5931    287          24                   7           0
4 Nucleic acid (only)    3077    200     1554         2                    15          3
5 Other                  174     13      33           3                    0           0
6 Oligosaccharide (o~    11      0       6            0                    1           0
# i 2 more variables: Other <dbl>, Total <dbl>
```

```r
round(sum(stats$`X-ray`)/sum(stats$Total)*100,3)
```

```
[1] 81.432
```

```r
round(sum(stats$EM)/sum(stats$Total)*100,3)
```

```
[1] 12.271
```

Q2: What proportion of structures in the PDB are protein?

```r
total <- sum(stats$Total)
210203/total
```

```
[1] 0.860465
```
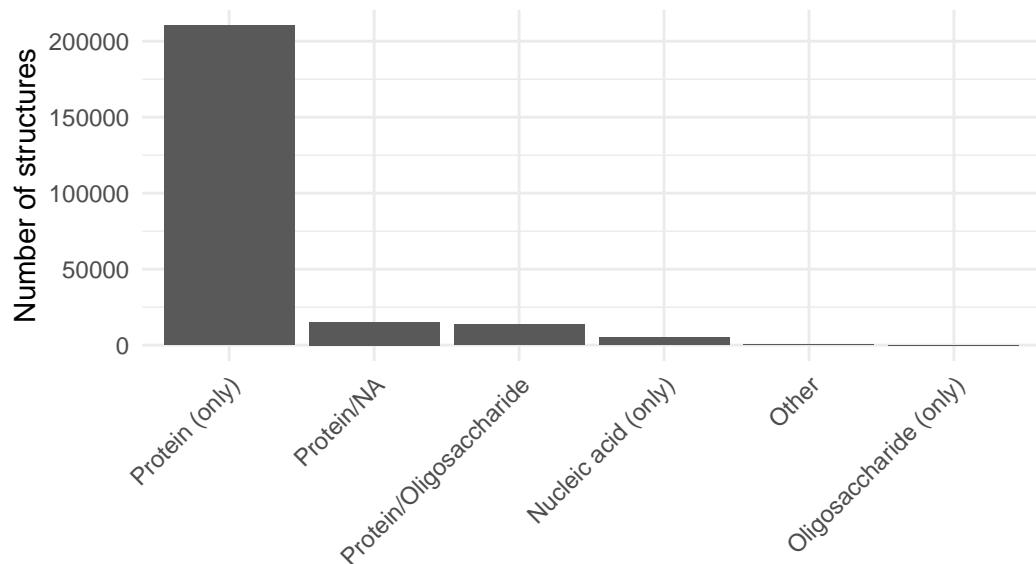
```r
library (ggplot2)

y<- ggplot(stats, aes(reorder(`Molecular Type`, -Total), `Total`))+
  geom_col()+
  labs(title="PDB Database Composition Oct 2025", x="",y= "Number of structures")+
theme_minimal()

y + theme(
  axis.text.x = element_text(angle = 45, hjust = 1)
)
```

PDB Database Composition Oct 2025

Q3.2: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

There are 150 structures.

Visualising structure data

The Mol* viewer is imbedded in many bioinformatics websites. the home page is : https://www.molstar.org

I can insert any figure or file image using the markdown format.
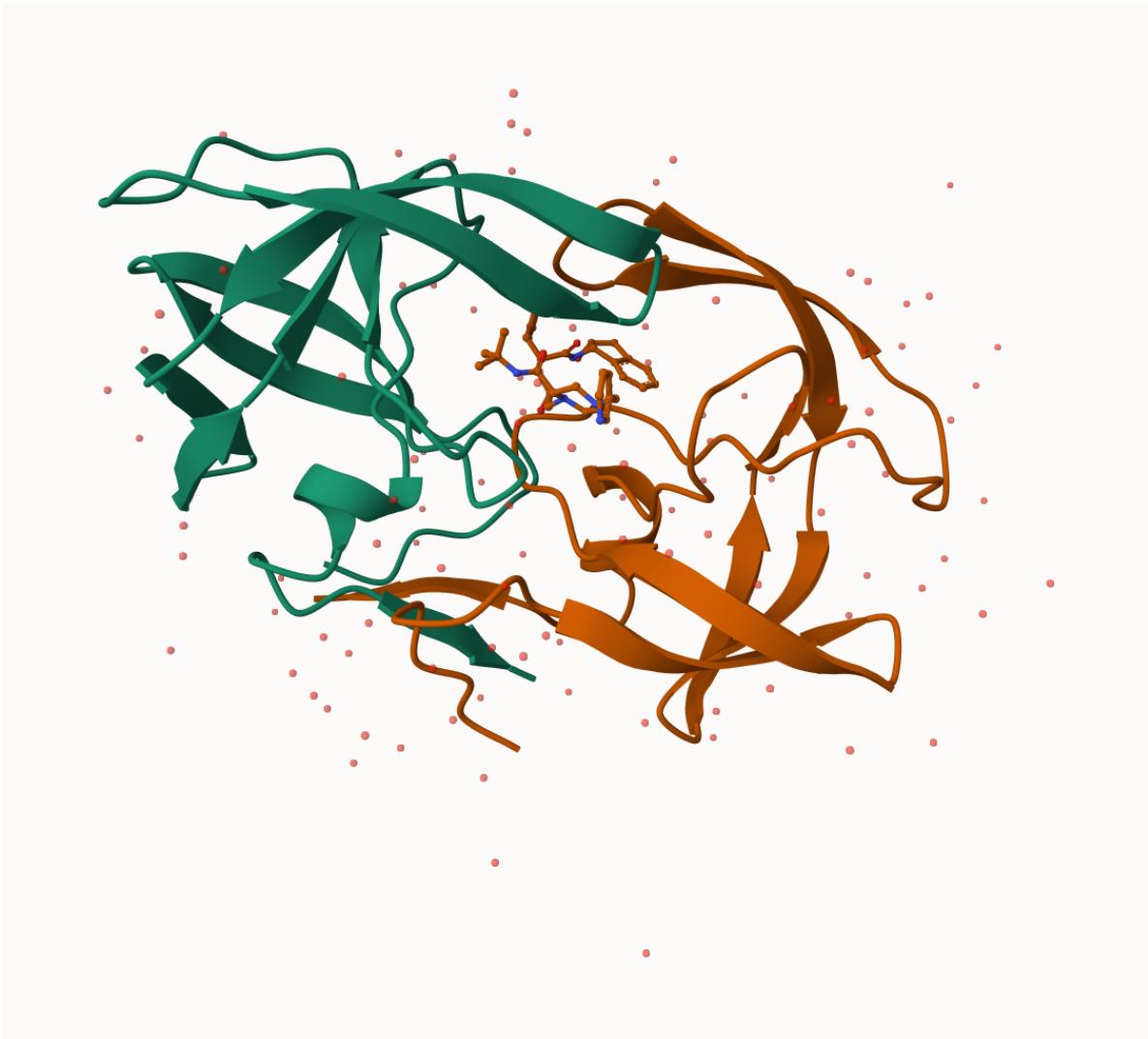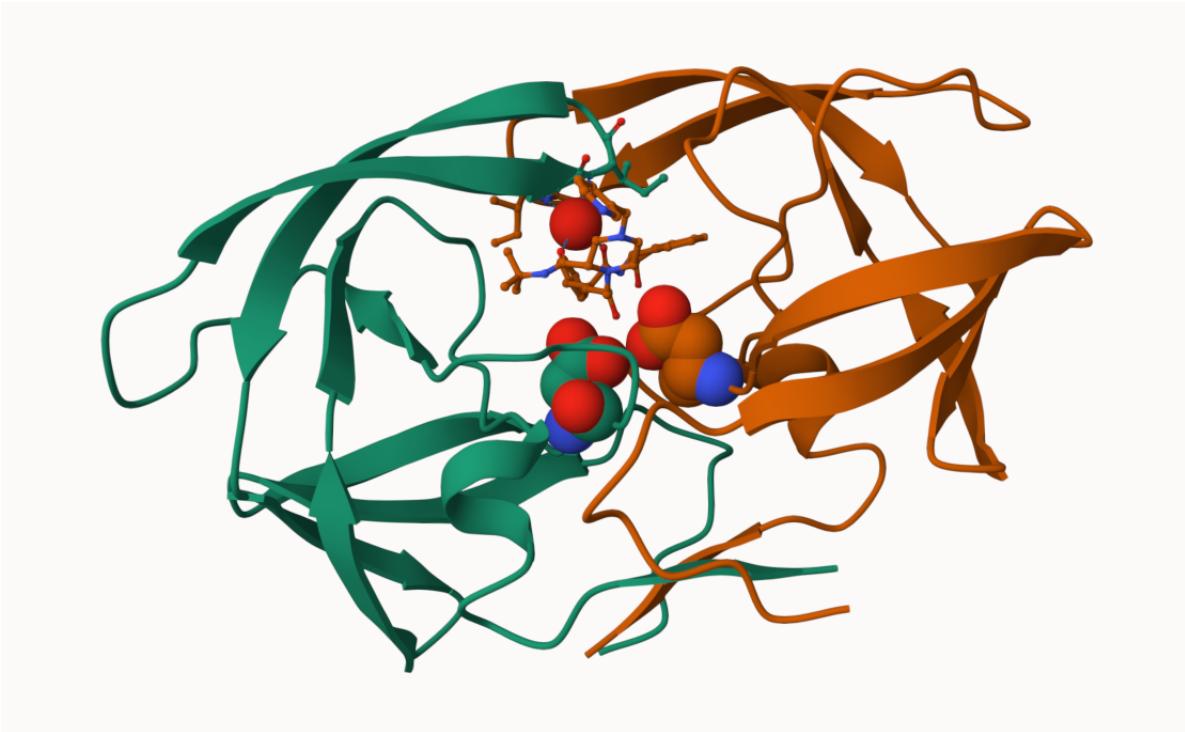
Figure 1: The HIV-Pr dimer with bound inhibitor

Bio3D package for structural bioinformatics

We can used the bio3d package to read and analyze biomolecular data in R:

```
library(bio3d)

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

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

```
hiv
```

```
 Call:  read.pdb(file = "1hsg")

   Total Models#: 1
     Total Atoms#: 1686,  XYZs#: 5058  Chains#: 2  (values: A B)

     Protein Atoms#: 1514  (residues/Calpha atoms#: 198)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
```

```
     Non-protein/nucleic Atoms#: 172   (residues: 128)
     Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]

   Protein sequence:
     PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD
     QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
     ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
     VNIIGRNLLTQIGCTLNF

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```
head(hiv$atom)
```

```
  type eleno elety  alt resid chain resno insert      x      y     z o      b
1 ATOM     1     N <NA>   PRO     A     1   <NA> 29.361 39.686 5.862 1 38.10
2 ATOM     2    CA <NA>   PRO     A     1   <NA> 30.307 38.663 5.319 1 40.62
3 ATOM     3     C <NA>   PRO     A     1   <NA> 29.760 38.071 4.022 1 42.64
4 ATOM     4     O <NA>   PRO     A     1   <NA> 28.600 38.302 3.676 1 43.40
5 ATOM     5    CB <NA>   PRO     A     1   <NA> 30.508 37.541 6.342 1 37.87
6 ATOM     6    CG <NA>   PRO     A     1   <NA> 29.296 37.591 7.162 1 38.40
  segid elesy charge
1 <NA>      N   <NA>
2 <NA>      C   <NA>
3 <NA>      C   <NA>
4 <NA>      O   <NA>
5 <NA>      C   <NA>
6 <NA>      C   <NA>
```

```
pdbseq(hiv)
```

```
   1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
 "P" "Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K"
  21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40
 "E" "A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G"
  41  42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60
 "R" "W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D"
  61  62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80
 "Q" "I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T"
  81  82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99   1
 "P" "V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F" "P"
```

```
  2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20  21
"Q" "I" "T" "L" "W" "Q" "R" "P" "L" "V" "T" "I" "K" "I" "G" "G" "Q" "L" "K" "E"
 22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41
"A" "L" "L" "D" "T" "G" "A" "D" "D" "T" "V" "L" "E" "E" "M" "S" "L" "P" "G" "R"
 42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60  61
"W" "K" "P" "K" "M" "I" "G" "G" "I" "G" "G" "F" "I" "K" "V" "R" "Q" "Y" "D" "Q"
 62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80  81
"I" "L" "I" "E" "I" "C" "G" "H" "K" "A" "I" "G" "T" "V" "L" "V" "G" "P" "T" "P"
 82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99
"V" "N" "I" "I" "G" "R" "N" "L" "L" "T" "Q" "I" "G" "C" "T" "L" "N" "F"
```

Lets trim to chain A and get it's seqeunce:

```
chainA <- trim.pdb(hiv, chain="A")
chainA.seq <-pdbseq(chainA)
```

Let's blast

```
blast<- blast.pdb(chainA.seq)
```

```
 Searching ... please wait (updates every 5 seconds) RID = G56YMRHY014
 .......
 Reporting 249 hits
```

```
head(blast)
```

```
$hit.tbl
         queryid subjectids identity alignmentlength mismatches gapopens
1   Query_7559951     1W5V_A  100.000              99          0        0
2   Query_7559951     2FDE_A  100.000              99          0        0
3   Query_7559951     1AJV_A  100.000              99          0        0
4   Query_7559951     2R38_A   98.990              99          1        0
5   Query_7559951     2R3T_A   98.990              99          1        0
6   Query_7559951     1HXB_A   98.990              99          1        0
7   Query_7559951     1BV9_A   97.980              99          2        0
8   Query_7559951     1AAQ_A   98.990              99          1        0
9   Query_7559951     1AXA_A   98.990              99          1        0
10  Query_7559951     1HVS_A   98.990              99          1        0
11  Query_7559951     1ZP8_A   98.990              99          1        0
12  Query_7559951     2QHC_A   98.990              99          1        0
```

13	Query_7559951	1A8G_A	98.990	99	1	0
14	Query_7559951	2O4L_A	97.980	99	2	0
15	Query_7559951	5COK_A	98.990	99	1	0
16	Query_7559951	1TCX_A	96.970	99	3	0
17	Query_7559951	2Z54_A	97.980	99	2	0
18	Query_7559951	1D4S_A	97.980	99	2	0
19	Query_7559951	1BV7_A	97.980	99	2	0
20	Query_7559951	1BWA_A	96.970	99	3	0
21	Query_7559951	1A9M_A	98.990	99	1	0
22	Query_7559951	2FLE_A	97.980	99	2	0
23	Query_7559951	1ODY_A	97.980	99	2	0
24	Query_7559951	1GNN_A	98.990	99	1	0
25	Query_7559951	1GNM_A	98.990	99	1	0
26	Query_7559951	5YRS_B	97.980	99	2	0
27	Query_7559951	1HEF_E	98.990	99	1	0
28	Query_7559951	1ODX_A	97.980	99	2	0
29	Query_7559951	4QGI_A	97.980	99	2	0
30	Query_7559951	1BVE_A	97.980	99	2	0
31	Query_7559951	2AZ8_A	97.980	99	2	0
32	Query_7559951	1A30_A	96.970	99	3	0
33	Query_7559951	6DH6_A	96.970	99	3	0
34	Query_7559951	6DH0_A	96.970	99	3	0
35	Query_7559951	2I4D_A	98.990	99	1	0
36	Query_7559951	6OOS_A	96.970	99	3	0
37	Query_7559951	1RL8_A	97.980	99	2	0
38	Query_7559951	5YRS_A	97.980	99	2	0
39	Query_7559951	1ZSF_A	98.990	99	1	0
40	Query_7559951	2Q64_A	97.980	99	2	0
41	Query_7559951	6DH3_A	96.970	99	3	0
42	Query_7559951	2NPH_A	97.980	99	2	0
43	Query_7559951	2Q63_A	96.970	99	3	0
44	Query_7559951	1LZQ_A	96.970	99	3	0
45	Query_7559951	1FB7_A	96.970	99	3	0
46	Query_7559951	1G6L_A	98.990	99	1	0
48	Query_7559951	1HIV_A	97.980	99	2	0
49	Query_7559951	6OOU_A	96.970	99	3	0
50	Query_7559951	1HVC_A	100.000	99	0	0
52	Query_7559951	2I4V_A	96.970	99	3	0
53	Query_7559951	2AZ9_A	96.970	99	3	0
54	Query_7559951	6OOT_A	95.960	99	4	0
55	Query_7559951	2P3B_B	97.980	99	2	0
56	Query_7559951	5KAO_A	96.970	99	3	0
57	Query_7559951	2WL0_A	96.970	99	3	0

58	Query_7559951	6OPT_A	95.960	99	4	0
59	Query_7559951	1IZI_A	95.960	99	4	0
60	Query_7559951	1MRX_A	94.949	99	5	0
61	Query_7559951	2PYM_A	96.970	99	3	0
62	Query_7559951	2PYN_A	96.970	99	3	0
63	Query_7559951	1DMP_A	96.970	99	3	0
64	Query_7559951	4K4P_A	96.970	99	3	0
65	Query_7559951	1LV1_A	97.980	99	2	0
67	Query_7559951	1AID_A	94.949	99	5	0
66	Query_7559951	1LV1_A	97.980	99	2	0
68	Query_7559951	1ZBG_A	95.960	99	4	0
69	Query_7559951	3TKG_A	94.949	99	5	0
51	Query_7559951	1HVC_A	96.970	99	3	0
70	Query_7559951	5YOK_A	94.949	99	5	0
47	Query_7559951	1G6L_A	97.980	99	2	0
71	Query_7559951	1FGC_C	94.949	99	5	0
72	Query_7559951	3K4V_A	94.949	99	5	0
73	Query_7559951	3KT5_A	96.970	99	3	0
74	Query_7559951	3KT5_A	96.970	99	3	0
75	Query_7559951	4QLH_A	96.970	99	3	0
76	Query_7559951	4QLH_A	96.970	99	3	0
77	Query_7559951	2F3K_A	94.949	99	5	0
78	Query_7559951	4Q5M_A	96.970	99	3	0
80	Query_7559951	2AOC_A	93.939	99	6	0
81	Query_7559951	3B80_A	93.939	99	6	0
82	Query_7559951	3VF5_A	93.939	99	6	0
83	Query_7559951	2AVQ_A	93.939	99	6	0
84	Query_7559951	1DW6_C	93.939	99	6	0
85	Query_7559951	1KZK_A	93.939	99	6	0
86	Query_7559951	2HS1_A	93.939	99	6	0
87	Query_7559951	1K6C_A	93.939	99	6	0
88	Query_7559951	1MTB_A	93.939	99	6	0
89	Query_7559951	4Q1X_A	93.939	99	6	0
90	Query_7559951	4Q1W_A	93.939	99	6	0
79	Query_7559951	4Q5M_A	96.970	99	3	0
91	Query_7559951	3D1X_A	93.939	99	6	0
92	Query_7559951	2AVM_A	93.939	99	6	0
93	Query_7559951	3PWM_A	93.939	99	6	0
94	Query_7559951	3KT2_A	96.970	99	3	0
95	Query_7559951	3KT2_A	96.970	99	3	0
96	Query_7559951	1SDV_A	93.939	99	6	0
97	Query_7559951	3JVW_A	93.939	99	6	0
98	Query_7559951	3OY4_A	93.939	99	6	0

99	Query_7559951	1A94_A	93.939	99	6	0
100	Query_7559951	2HS2_A	93.939	99	6	0
101	Query_7559951	4EJ8_A	93.939	99	6	0
102	Query_7559951	2FGU_A	92.929	99	7	0
103	Query_7559951	2AVV_A	93.939	99	6	0
104	Query_7559951	3JW2_A	93.939	99	6	0
105	Query_7559951	3BVA_A	93.939	99	6	0
106	Query_7559951	1FFF_C	93.939	99	6	0
107	Query_7559951	3S43_B	91.919	99	8	0
108	Query_7559951	2NXD_A	93.939	99	6	0
109	Query_7559951	1FG6_C	93.939	99	6	0
110	Query_7559951	1EBK_C	93.939	99	6	0
111	Query_7559951	4Q1Y_A	92.929	99	7	0
112	Query_7559951	3EL4_A	92.929	99	7	0
113	Query_7559951	1F7A_A	92.929	99	7	0
114	Query_7559951	1K2B_A	92.929	99	7	0
115	Query_7559951	2FGV_A	92.929	99	7	0
116	Query_7559951	1Z8C_A	94.949	99	5	0
117	Query_7559951	2G69_A	93.939	99	6	0
118	Query_7559951	3EL9_A	91.919	99	8	0
119	Query_7559951	3OXV_A	92.929	99	7	0
120	Query_7559951	1BDR_A	93.939	99	6	0
121	Query_7559951	3N3I_A	96.970	99	3	0
122	Query_7559951	3N3I_A	96.970	99	3	0
123	Query_7559951	3OXW_A	91.919	99	8	0
124	Query_7559951	3S43_A	90.909	99	9	0
125	Query_7559951	3EM3_A	92.929	99	7	0
126	Query_7559951	3CYW_A	93.939	99	6	0
127	Query_7559951	5KQX_A	92.929	99	7	0
128	Query_7559951	2B60_A	91.919	99	8	0
129	Query_7559951	7DOZ_A	95.960	99	4	0
131	Query_7559951	1K2C_A	92.929	99	7	0
132	Query_7559951	1MT7_A	91.919	99	8	0
133	Query_7559951	3EM4_A	91.919	99	8	0
134	Query_7559951	4QJ9_A	92.929	99	7	0
135	Query_7559951	1BDL_A	92.929	99	7	0
136	Query_7559951	3LZS_A	91.919	99	8	0
137	Query_7559951	5T84_A	93.939	99	6	0
138	Query_7559951	4DQB_A	91.919	99	8	0
130	Query_7559951	7DOZ_A	95.960	99	4	0
139	Query_7559951	4QJ2_A	91.919	99	8	0
140	Query_7559951	3LZV_A	91.919	99	8	0
141	Query_7559951	1SGU_A	89.899	99	10	0

142	Query_7559951	2FXE_A	90.909	99	9	0
143	Query_7559951	1BDQ_A	90.909	99	9	0
144	Query_7559951	3U71_A	89.899	99	10	0
145	Query_7559951	2R5P_A	88.889	99	11	0
146	Query_7559951	4OBD_A	91.919	99	8	0
147	Query_7559951	7MAS_A	91.919	99	8	0
148	Query_7559951	3IXO_A	90.909	99	9	0
149	Query_7559951	3D3T_A	90.909	99	9	0
150	Query_7559951	5YOJ_A	88.889	99	11	0
151	Query_7559951	3LZU_A	90.909	99	9	0
152	Query_7559951	4NJS_A	88.889	99	11	0
153	Query_7559951	3EKP_A	90.909	99	9	0
154	Query_7559951	1B6J_A	92.929	99	7	0
155	Query_7559951	3EKQ_A	90.909	99	9	0
156	Query_7559951	2RKF_A	87.879	99	12	0
157	Query_7559951	1C6X_A	90.909	99	9	0
158	Query_7559951	7MAR_A	87.879	99	12	0
159	Query_7559951	4DQF_A	89.899	99	10	0
160	Query_7559951	1RPI_A	87.879	99	12	0
161	Query_7559951	3OU1_B	87.879	99	12	0
162	Query_7559951	3PJ6_A	87.879	99	12	0
163	Query_7559951	2P3A_A	89.899	99	10	0
164	Query_7559951	6OGQ_A	86.869	99	13	0
165	Query_7559951	3OQ7_A	87.879	99	12	0
166	Query_7559951	5KR1_A	88.889	99	11	0
167	Query_7559951	3OQD_A	87.879	99	12	0
168	Query_7559951	4RVI_A	87.879	99	12	0
169	Query_7559951	3OQA_A	87.879	99	12	0
170	Query_7559951	1B6K_A	90.909	99	9	0
171	Query_7559951	3OUD_B	86.869	99	13	0
172	Query_7559951	6MK9_A	84.848	99	15	0
173	Query_7559951	3SO9_A	86.869	99	13	0
174	Query_7559951	1Q9P_A	94.737	95	5	0
175	Query_7559951	6I45_A	85.859	99	14	0
176	Query_7559951	7SEP_A	98.990	99	1	0
177	Query_7559951	4NJT_A	87.879	99	12	0
178	Query_7559951	3BXR_A	89.899	99	10	0
179	Query_7559951	4YOA_A	85.859	99	14	0
180	Query_7559951	4DQC_A	89.899	99	10	0
181	Query_7559951	2FDD_A	85.859	99	14	0
182	Query_7559951	2RKG_A	87.000	100	12	1
183	Query_7559951	4DQH_A	90.909	99	9	0
184	Query_7559951	2P3C_A	85.859	99	14	0

185	Query_7559951	4EP2_A	90.909	99	9	0
186	Query_7559951	4EP2_A	90.909	99	9	0
187	Query_7559951	4EQ0_A	89.899	99	10	0
189	Query_7559951	4NPT_A	82.828	99	17	0
190	Query_7559951	6OPU_A	93.939	99	6	0
191	Query_7559951	4NPU_A	81.818	99	18	0
192	Query_7559951	3U7S_A	79.798	99	20	0
193	Query_7559951	3HAW_A	87.879	99	12	0
194	Query_7559951	2AZB_A	94.949	99	5	0
195	Query_7559951	3TTP_A	79.798	99	20	0
196	Query_7559951	3HBO_A	87.879	99	12	0
197	Query_7559951	3GGU_A	79.798	99	20	0
198	Query_7559951	7N6T_A	80.808	99	19	0
199	Query_7559951	6OPV_A	89.899	99	10	0
188	Query_7559951	4EQ0_A	87.879	99	12	0
200	Query_7559951	6OPX_A	88.889	99	11	0
201	Query_7559951	2O4N_A	92.929	99	7	0
202	Query_7559951	5T2E_A	80.808	99	19	0
203	Query_7559951	3UCB_A	77.778	99	22	0
204	Query_7559951	3KA2_A	87.879	99	12	0
206	Query_7559951	3FSM_A	87.879	99	12	0
208	Query_7559951	6OPW_A	88.889	99	11	0
209	Query_7559951	2AZC_A	91.919	99	8	0
207	Query_7559951	3FSM_A	87.879	99	12	0
210	Query_7559951	3HLO_A	87.879	99	12	0
212	Query_7559951	2P3D_A	78.788	99	21	0
213	Query_7559951	3T3C_A	77.778	99	22	0
214	Query_7559951	7MYP_A	79.798	99	20	0
215	Query_7559951	6O54_X	79.798	99	20	0
216	Query_7559951	6OPY_A	87.879	99	12	0
217	Query_7559951	4Z4X_A	76.768	99	23	0
218	Query_7559951	6OPZ_A	86.869	99	13	0
219	Query_7559951	2JE4_A	89.899	99	10	0
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223	Query_7559951	1K1U_A	92.929	99	7	0
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225	Query_7559951	3MWS_A	78.788	99	21	0
226	Query_7559951	1K1T_A	92.929	99	7	0
227	Query_7559951	8DCH_A	76.768	99	23	0
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229	Query_7559951	6P9A_A	75.758	99	24	0

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230 Query_7559951    2FXD_A   86.869              99          13          0
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246 Query_7559951    3NR6_A   30.108              93          64          1
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248 Query_7559951    8V8F_E  100.000              11           0          0
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4         1    99       1     99 2.50e-67    198.0    100.00 153.3569105 2R38_A
5         1    99       1     99 2.50e-67    198.0    100.00 153.3569105 2R3T_A
6         1    99       1     99 2.50e-67    198.0    100.00 153.3569105 1HXB_A
7         1    99       1     99 3.60e-67    197.0    100.00 152.9922674 1BV9_A
8         1    99       1     99 4.53e-67    197.0    100.00 152.7624793 1AAQ_A
9         1    99       1     99 5.05e-67    197.0    100.00 152.6538130 1AXA_A
10        1    99       1     99 5.22e-67    197.0     98.99 152.6207038 1HVS_A
11        1    99       1     99 6.87e-67    197.0    100.00 152.3460371 1ZP8_A
12        1    99       1     99 7.10e-67    197.0     98.99 152.3131064 2QHC_A
13        1    99       1     99 7.59e-67    197.0    100.00 152.2463696 1A8G_A
14        1    99       1     99 8.65e-67    197.0    100.00 152.1156419 2O4L_A
15        1    99       1     99 8.85e-67    196.0    100.00 152.0927838 5COK_A
16        1    99       1     99 9.45e-67    196.0    100.00 152.0271865 1TCX_A
17        1    99       1     99 1.02e-66    196.0     98.99 151.9508135 2Z54_A
18        1    99       1     99 1.28e-66    196.0     98.99 151.7237561 1D4S_A
19        1    99       1     99 1.28e-66    196.0     98.99 151.7237561 1BV7_A
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21	1	99	1	99	1.67e-66	196.0	98.99	151.4577925	1A9M_A
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23	1	99	1	99	1.75e-66	196.0	98.99	151.4110003	1ODY_A
24	1	99	1	99	1.93e-66	196.0	98.99	151.3130961	1GNN_A
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26	1	99	1	99	2.44e-66	196.0	98.99	151.0786181	5YRS_B
27	1	99	1	99	2.65e-66	195.0	98.99	150.9960565	1HEF_E
28	1	99	1	99	2.80e-66	195.0	97.98	150.9409967	1ODX_A
29	1	99	1	99	2.90e-66	195.0	98.99	150.9059054	4QGI_A
30	1	99	1	99	2.99e-66	195.0	98.99	150.8753428	1BVE_A
31	1	99	1	99	3.09e-66	195.0	100.00	150.8424450	2AZ8_A
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36	1	99	1	99	4.64e-66	195.0	100.00	150.4359018	6OOS_A
37	1	99	1	99	4.69e-66	195.0	97.98	150.4251836	1RL8_A
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39	1	99	1	99	5.36e-66	194.0	98.99	150.2916522	1ZSF_A
40	1	99	1	99	5.60e-66	194.0	98.99	150.2478495	2Q64_A
41	1	99	1	99	5.72e-66	194.0	100.00	150.2266473	6DH3_A
42	1	99	1	99	5.72e-66	194.0	98.99	150.2266473	2NPH_A
43	1	99	1	99	5.98e-66	194.0	98.99	150.1821956	2Q63_A
44	1	99	1	99	6.11e-66	194.0	97.98	150.1606894	1LZQ_A
45	1	99	1	99	6.45e-66	194.0	98.99	150.1065360	1FB7_A
46	1	99	105	203	6.70e-66	198.0	100.00	150.0685086	1G6L_A
48	1	99	1	99	6.74e-66	194.0	98.99	150.0625562	1HIV_A
49	1	99	1	99	7.12e-66	194.0	100.00	150.0077084	6OOU_A
50	1	99	105	203	8.53e-66	198.0	100.00	149.8270268	1HVC_A
52	1	99	1	99	9.17e-66	194.0	98.99	149.7546789	2I4V_A
53	1	99	1	99	9.48e-66	194.0	98.99	149.7214318	2AZ9_A
54	1	99	1	99	1.13e-65	194.0	100.00	149.5458134	6OOT_A
55	1	99	1	99	1.55e-65	193.0	98.99	149.2297761	2P3B_B
56	1	99	1	99	1.68e-65	193.0	97.98	149.1492373	5KAO_A
57	1	99	1	99	1.71e-65	193.0	97.98	149.1315377	2WL0_A
58	1	99	1	99	2.04e-65	193.0	98.99	148.9550812	6OPT_A
59	1	99	1	99	2.36e-65	193.0	97.98	148.8093694	1IZI_A
60	1	99	1	99	2.55e-65	193.0	98.99	148.7319377	1MRX_A
61	1	99	1	99	3.04e-65	192.0	98.99	148.5561735	2PYM_A
62	1	99	1	99	4.13e-65	192.0	97.98	148.2497536	2PYN_A
63	1	99	1	99	4.56e-65	192.0	97.98	148.1507084	1DMP_A
64	1	99	1	99	6.26e-65	192.0	98.99	147.8338509	4K4P_A
65	1	99	105	203	9.79e-65	195.0	98.99	147.3866696	1LV1_A

67	1	99	1	99	1.37e-64	191.0	98.99	147.0506352	1AID_A
66	1	99	1	99	1.60e-64	194.0	98.99	146.8954423	1LV1_A
68	1	99	1	99	1.63e-64	191.0	96.97	146.8768659	1ZBG_A
69	1	99	5	103	2.02e-64	191.0	97.98	146.6623484	3TKG_A
51	1	99	1	99	2.13e-64	194.0	100.00	146.6093240	1HVC_A
70	1	99	2	100	2.36e-64	191.0	97.98	146.5067843	5YOK_A
47	1	99	1	99	2.48e-64	194.0	98.99	146.4571874	1G6L_A
71	1	99	1	99	2.88e-64	190.0	97.98	146.3076557	1FGC_C
72	1	99	2	100	2.97e-64	190.0	97.98	146.2768840	3K4V_A
73	1	99	1	99	3.37e-64	194.0	98.99	146.1505332	3KT5_A
74	1	99	105	203	3.37e-64	194.0	98.99	146.1505332	3KT5_A
75	1	99	1	99	3.48e-64	194.0	97.98	146.1184137	4QLH_A
76	1	99	105	203	3.48e-64	194.0	97.98	146.1184137	4QLH_A
77	1	99	1	99	3.55e-64	190.0	98.99	146.0984983	2F3K_A
78	1	99	105	203	3.76e-64	194.0	98.99	146.0410270	4Q5M_A
80	1	99	1	99	4.37e-64	190.0	97.98	145.8906829	2AOC_A
81	1	99	1	99	4.37e-64	190.0	97.98	145.8906829	3B80_A
82	1	99	1	99	4.37e-64	190.0	97.98	145.8906829	3VF5_A
83	1	99	1	99	4.37e-64	190.0	97.98	145.8906829	2AVQ_A
84	1	99	1	99	4.93e-64	189.0	97.98	145.7701070	1DW6_C
85	1	99	1	99	4.93e-64	189.0	98.99	145.7701070	1KZK_A
86	1	99	1	99	5.21e-64	189.0	97.98	145.7148661	2HS1_A
87	1	99	1	99	5.33e-64	189.0	97.98	145.6920947	1K6C_A
88	1	99	1	99	5.51e-64	189.0	98.99	145.6588813	1MTB_A
89	1	99	1	99	5.69e-64	189.0	98.99	145.6267357	4Q1X_A
90	1	99	1	99	6.01e-64	189.0	98.99	145.5720212	4Q1W_A
79	1	99	1	99	6.22e-64	193.0	98.99	145.5376760	4Q5M_A
91	1	99	1	99	6.64e-64	189.0	97.98	145.4723340	3D1X_A
92	1	99	1	99	7.09e-64	189.0	97.98	145.4067606	2AVM_A
93	1	99	1	99	7.49e-64	189.0	97.98	145.3518772	3PWM_A
94	1	99	1	99	8.18e-64	193.0	98.99	145.2637538	3KT2_A
95	1	99	105	203	8.18e-64	193.0	98.99	145.2637538	3KT2_A
96	1	99	1	99	8.36e-64	189.0	96.97	145.2419875	1SDV_A
97	1	99	1	99	9.03e-64	189.0	96.97	145.1648936	3JVW_A
98	1	99	1	99	9.75e-64	189.0	98.99	145.0881787	3OY4_A
99	1	99	1	99	1.09e-63	189.0	97.98	144.9766832	1A94_A
100	1	99	1	99	1.09e-63	189.0	97.98	144.9766832	2HS2_A
101	1	99	1	99	1.12e-63	189.0	97.98	144.9495322	4EJ8_A
102	1	99	1	99	1.12e-63	189.0	98.99	144.9495322	2FGU_A
103	1	99	1	99	1.20e-63	189.0	96.97	144.8805393	2AVV_A
104	1	99	1	99	1.20e-63	189.0	96.97	144.8805393	3JW2_A
105	1	99	1	99	1.28e-63	189.0	97.98	144.8160008	3BVA_A
106	1	99	1	99	1.28e-63	189.0	97.98	144.8160008	1FFF_C

107	1	99	1	99	1.37e-63	189.0	97.98	144.7480501	3S43_B
108	1	99	1	99	1.38e-63	189.0	98.99	144.7407774	2NXD_A
109	1	99	1	99	1.42e-63	188.0	97.98	144.7122040	1FG6_C
110	1	99	1	99	1.46e-63	188.0	97.98	144.6844244	1EBK_C
111	1	99	1	99	1.46e-63	188.0	97.98	144.6844244	4Q1Y_A
112	1	99	1	99	1.82e-63	188.0	97.98	144.4640244	3EL4_A
113	1	99	1	99	1.90e-63	188.0	98.99	144.4210070	1F7A_A
114	1	99	1	99	2.01e-63	188.0	97.98	144.3647261	1K2B_A
115	1	99	1	99	2.06e-63	188.0	97.98	144.3401549	2FGV_A
116	1	99	1	99	2.15e-63	188.0	95.96	144.2973930	1Z8C_A
117	1	99	1	99	2.27e-63	188.0	96.97	144.2430810	2G69_A
118	1	99	1	99	2.56e-63	188.0	97.98	144.1228536	3EL9_A
119	1	99	1	99	2.65e-63	188.0	97.98	144.0883012	3OXV_A
120	1	99	1	99	3.30e-63	187.0	96.97	143.8689384	1BDR_A
121	1	99	1	99	3.47e-63	191.0	97.98	143.8187063	3N3I_A
122	1	99	105	203	3.47e-63	191.0	97.98	143.8187063	3N3I_A
123	1	99	1	99	3.68e-63	187.0	97.98	143.7599481	3OXW_A
124	1	99	1	99	3.93e-63	187.0	97.98	143.6942214	3S43_A
125	1	99	1	99	3.97e-63	187.0	97.98	143.6840948	3EM3_A
126	1	99	1	99	4.20e-63	187.0	96.97	143.6277763	3CYW_A
127	1	99	1	99	4.74e-63	187.0	97.98	143.5068237	5KQX_A
128	1	99	1	99	5.29e-63	187.0	95.96	143.3970426	2B60_A
129	1	99	105	203	5.49e-63	191.0	97.98	143.3599326	7DOZ_A
131	1	99	1	99	5.58e-63	187.0	96.97	143.3436721	1K2C_A
132	1	99	1	99	5.65e-63	187.0	97.98	143.3312053	1MT7_A
133	1	99	1	99	6.23e-63	187.0	97.98	143.2334845	3EM4_A
134	1	99	1	99	6.23e-63	187.0	97.98	143.2334845	4QJ9_A
135	1	99	1	99	6.30e-63	187.0	96.97	143.2223112	1BDL_A
136	1	99	1	99	6.96e-63	187.0	98.99	143.1226814	3LZS_A
137	1	99	1	99	8.20e-63	186.0	96.97	142.9587267	5T84_A
138	1	99	1	99	8.95e-63	186.0	97.98	142.8712073	4DQB_A
130	1	99	1	99	9.08e-63	190.0	97.98	142.8567867	7DOZ_A
139	1	99	1	99	1.03e-62	186.0	97.98	142.7307170	4QJ2_A
140	1	99	1	99	1.13e-62	186.0	98.99	142.6380581	3LZV_A
141	1	99	1	99	1.18e-62	186.0	95.96	142.5947613	1SGU_A
142	1	99	1	99	1.22e-62	186.0	97.98	142.5614249	2FXE_A
143	1	99	1	99	1.62e-62	186.0	96.97	142.2778496	1BDQ_A
144	1	99	1	99	2.40e-62	185.0	98.99	141.8848070	3U71_A
145	1	99	1	99	2.90e-62	185.0	98.99	141.6955650	2R5P_A
146	1	99	1	99	3.20e-62	185.0	98.99	141.5971250	4OBD_A
147	1	99	1	99	3.23e-62	185.0	95.96	141.5877936	7MAS_A
148	1	99	1	99	3.49e-62	185.0	97.98	141.5103740	3IX0_A
149	1	99	1	99	3.77e-62	185.0	98.99	141.4332008	3D3T_A

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150     1   99       2   100 3.81e-62     185.0        96.97 141.4226466 5YOJ_A
151     1   99       1    99 3.86e-62     185.0        98.99 141.4096086 3LZU_A
152     1   99       1    99 4.55e-62     185.0        95.96 141.2451485 4NJS_A
153     1   99       1    99 5.13e-62     184.0        96.97 141.1251701 3EKP_A
154     1   99       1    99 6.32e-62     184.0        96.97 140.9165566 1B6J_A
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156     1   99       1    99 9.08e-62     184.0        93.94 140.5542016 2RKF_A
157     1   99       1    99 1.28e-61     184.0        94.95 140.2108306 1C6X_A
158     1   99       1    99 1.35e-61     183.0        95.96 140.1575861 7MAR_A
159     1   99       1    99 1.35e-61     183.0        95.96 140.1575861 4DQF_A
160     1   99       1    99 1.75e-61     183.0        96.97 139.8980749 1RPI_A
161     1   99       1    99 1.81e-61     183.0        96.97 139.8643638 3OU1_B
162     1   99       1    99 1.83e-61     183.0        96.97 139.8533747 3PJ6_A
163     1   99       1    99 2.11e-61     183.0        95.96 139.7110027 2P3A_A
164     1   99       1    99 2.18e-61     183.0        97.98 139.6783658 6OGQ_A
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166     1   99       1    99 2.31e-61     183.0        97.98 139.6204431 5KR1_A
167     1   99       1    99 2.63e-61     183.0        96.97 139.4907068 3OQD_A
168     1   99       1    99 2.75e-61     182.0        95.96 139.4460898 4RVI_A
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170     1   99       1    99 4.87e-61     182.0        96.97 138.8745967 1B6K_A
171     1   99       1    99 7.39e-61     182.0        95.96 138.4575629 3OUD_B
172     1   99       1    99 7.81e-61     181.0        97.98 138.4022857 6MK9_A
173     1   99       1    99 7.89e-61     181.0        96.97 138.3920945 3SO9_A
174     1   95       1    95 8.21e-61     181.0        97.89 138.3523377 1Q9P_A
175     1   99       1    99 9.00e-61     181.0        97.98 138.2604661 6I45_A
176     1   99     107   205 1.01e-60     200.0        98.99 138.1451552 7SEP_A
177     1   99       1    99 1.29e-60     181.0        94.95 137.9004634 4NJT_A
178     1   99       1    99 2.07e-60     181.0        96.97 137.4275570 3BXR_A
179     1   99       1    99 2.12e-60     181.0        95.96 137.4036895 4YOA_A
180     1   99       1    99 2.64e-60     180.0        95.96 137.1843267 4DQC_A
181     1   99       2   100 3.91e-60     180.0        95.96 136.7915682 2FDD_A
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134 Query_7559951      4QJ9_A    92.929              99          7          0
135 Query_7559951      1BDL_A    92.929              99          7          0
136 Query_7559951      3LZS_A    91.919              99          8          0
137 Query_7559951      5T84_A    93.939              99          6          0
138 Query_7559951      4DQB_A    91.919              99          8          0
139 Query_7559951      4QJ2_A    91.919              99          8          0
140 Query_7559951      3LZV_A    91.919              99          8          0
141 Query_7559951      1SGU_A    89.899              99          10         0
142 Query_7559951      2FXE_A    90.909              99          9          0
143 Query_7559951      1BDQ_A    90.909              99          9          0
144 Query_7559951      3U71_A    89.899              99          10         0
145 Query_7559951      2R5P_A    88.889              99          11         0
146 Query_7559951      4OBD_A    91.919              99          8          0
147 Query_7559951      7MAS_A    91.919              99          8          0
148 Query_7559951      3IXO_A    90.909              99          9          0
149 Query_7559951      3D3T_A    90.909              99          9          0
150 Query_7559951      5YOJ_A    88.889              99          11         0
151 Query_7559951      3LZU_A    90.909              99          9          0
152 Query_7559951      4NJS_A    88.889              99          11         0
153 Query_7559951      3EKP_A    90.909              99          9          0
154 Query_7559951      1B6J_A    92.929              99          7          0
155 Query_7559951      3EKQ_A    90.909              99          9          0
156 Query_7559951      2RKF_A    87.879              99          12         0
157 Query_7559951      1C6X_A    90.909              99          9          0
158 Query_7559951      7MAR_A    87.879              99          12         0
159 Query_7559951      4DQF_A    89.899              99          10         0
160 Query_7559951      1RPI_A    87.879              99          12         0
161 Query_7559951      3OU1_B    87.879              99          12         0
162 Query_7559951      3PJ6_A    87.879              99          12         0
163 Query_7559951      2P3A_A    89.899              99          10         0
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164	Query_7559951	6OGQ_A	86.869	99	13	0
165	Query_7559951	3OQ7_A	87.879	99	12	0
166	Query_7559951	5KR1_A	88.889	99	11	0
167	Query_7559951	3OQD_A	87.879	99	12	0
168	Query_7559951	4RVI_A	87.879	99	12	0
169	Query_7559951	3OQA_A	87.879	99	12	0
170	Query_7559951	1B6K_A	90.909	99	9	0
171	Query_7559951	3OUD_B	86.869	99	13	0
172	Query_7559951	6MK9_A	84.848	99	15	0
173	Query_7559951	3SO9_A	86.869	99	13	0
174	Query_7559951	1Q9P_A	94.737	95	5	0
175	Query_7559951	6I45_A	85.859	99	14	0
176	Query_7559951	7SEP_A	98.990	99	1	0
177	Query_7559951	4NJT_A	87.879	99	12	0
178	Query_7559951	3BXR_A	89.899	99	10	0
179	Query_7559951	4YOA_A	85.859	99	14	0
180	Query_7559951	4DQC_A	89.899	99	10	0
181	Query_7559951	2FDD_A	85.859	99	14	0
182	Query_7559951	2RKG_A	87.000	100	12	1
183	Query_7559951	4DQH_A	90.909	99	9	0
184	Query_7559951	2P3C_A	85.859	99	14	0
185	Query_7559951	4EP2_A	90.909	99	9	0
186	Query_7559951	4EP2_A	90.909	99	9	0
187	Query_7559951	4EQ0_A	89.899	99	10	0
188	Query_7559951	4EQ0_A	87.879	99	12	0
189	Query_7559951	4NPT_A	82.828	99	17	0
190	Query_7559951	6OPU_A	93.939	99	6	0
191	Query_7559951	4NPU_A	81.818	99	18	0
192	Query_7559951	3U7S_A	79.798	99	20	0
193	Query_7559951	3HAW_A	87.879	99	12	0
194	Query_7559951	2AZB_A	94.949	99	5	0
195	Query_7559951	3TTP_A	79.798	99	20	0
196	Query_7559951	3HB0_A	87.879	99	12	0
197	Query_7559951	3GGU_A	79.798	99	20	0
198	Query_7559951	7N6T_A	80.808	99	19	0
199	Query_7559951	6OPV_A	89.899	99	10	0
200	Query_7559951	6OPX_A	88.889	99	11	0
201	Query_7559951	2O4N_A	92.929	99	7	0
202	Query_7559951	5T2E_A	80.808	99	19	0
203	Query_7559951	3UCB_A	77.778	99	22	0
204	Query_7559951	3KA2_A	87.879	99	12	0
205	Query_7559951	3KA2_A	88.889	99	11	0
206	Query_7559951	3FSM_A	87.879	99	12	0

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207 Query_7559951    3FSM_A    87.879        99       12       0
208 Query_7559951    6OPW_A    88.889        99       11       0
209 Query_7559951    2AZC_A    91.919        99        8       0
210 Query_7559951    3HLO_A    87.879        99       12       0
211 Query_7559951    3HLO_A    88.889        99       11       0
212 Query_7559951    2P3D_A    78.788        99       21       0
213 Query_7559951    3T3C_A    77.778        99       22       0
214 Query_7559951    7MYP_A    79.798        99       20       0
215 Query_7559951    6O54_X    79.798        99       20       0
216 Query_7559951    6OPY_A    87.879        99       12       0
217 Query_7559951    4Z4X_A    76.768        99       23       0
218 Query_7559951    6OPZ_A    86.869        99       13       0
219 Query_7559951    2JE4_A    89.899        99       10       0
220 Query_7559951    1DAZ_C    93.939        99        6       0
221 Query_7559951    7MAP_A    88.889        99       11       0
222 Query_7559951    7MAQ_A    90.909        99        9       0
223 Query_7559951    1K1U_A    92.929        99        7       0
224 Query_7559951    2B7Z_A    89.899        99       10       0
225 Query_7559951    3MWS_A    78.788        99       21       0
226 Query_7559951    1K1T_A    92.929        99        7       0
227 Query_7559951    8DCH_A    76.768        99       23       0
228 Query_7559951    3I2L_A    87.879        99       12       0
229 Query_7559951    6P9A_A    75.758        99       24       0
230 Query_7559951    2FXD_A    86.869        99       13       0
231 Query_7559951    2J9J_A    88.889        99       11       0
232 Query_7559951    3DCK_A    87.879        99       12       0
233 Query_7559951    2J9J_B    87.879        99       12       0
234 Query_7559951    3NXE_A    87.879        99       12       0
235 Query_7559951    3NXE_A    88.889        99       11       0
236 Query_7559951    2O40_A    88.889        99       11       0
237 Query_7559951    2O40_A    88.889        99       11       0
238 Query_7559951    5B18_A    76.768        99       23       0
239 Query_7559951    1SIP_A    51.515        99       48       0
240 Query_7559951    2SAM_A    51.515        99       48       0
241 Query_7559951    1AZ5_A    50.505        99       49       0
242 Query_7559951    1SIV_A    50.505        99       49       0
243 Query_7559951    1HII_A    48.485        99       51       0
244 Query_7559951    1IVP_A    48.485        99       51       0
245 Query_7559951    1BAI_A    43.333        90       35       4
246 Query_7559951    3NR6_A    30.108        93       64       1
247 Query_7559951    2HAH_A    36.792       106       55       3
248 Query_7559951    8V8F_E   100.000        11        0       0
249 Query_7559951    2HRP_P   100.000        10        0       0
```

30

	q.start	q.end	s.start	s.end	evalue	bitscore	positives
1	1	99	12	110	1.38e-67	199.0	100.00
2	1	99	2	100	1.70e-67	198.0	100.00
3	1	99	1	99	1.99e-67	198.0	100.00
4	1	99	1	99	2.50e-67	198.0	100.00
5	1	99	1	99	2.50e-67	198.0	100.00
6	1	99	1	99	2.50e-67	198.0	100.00
7	1	99	1	99	3.60e-67	197.0	100.00
8	1	99	1	99	4.53e-67	197.0	100.00
9	1	99	1	99	5.05e-67	197.0	100.00
10	1	99	1	99	5.22e-67	197.0	98.99
11	1	99	1	99	6.87e-67	197.0	100.00
12	1	99	1	99	7.10e-67	197.0	98.99
13	1	99	1	99	7.59e-67	197.0	100.00
14	1	99	1	99	8.65e-67	197.0	100.00
15	1	99	1	99	8.85e-67	196.0	100.00
16	1	99	1	99	9.45e-67	196.0	100.00
17	1	99	1	99	1.02e-66	196.0	98.99
18	1	99	1	99	1.28e-66	196.0	98.99
19	1	99	1	99	1.28e-66	196.0	98.99
20	1	99	1	99	1.57e-66	196.0	98.99
21	1	99	1	99	1.67e-66	196.0	98.99
22	1	99	1	99	1.67e-66	196.0	98.99
23	1	99	1	99	1.75e-66	196.0	98.99
24	1	99	1	99	1.93e-66	196.0	98.99
25	1	99	1	99	2.13e-66	196.0	98.99
26	1	99	1	99	2.44e-66	196.0	98.99
27	1	99	1	99	2.65e-66	195.0	98.99
28	1	99	1	99	2.80e-66	195.0	97.98
29	1	99	1	99	2.90e-66	195.0	98.99
30	1	99	1	99	2.99e-66	195.0	98.99
31	1	99	1	99	3.09e-66	195.0	100.00
32	1	99	1	99	3.65e-66	195.0	100.00
33	1	99	1	99	3.98e-66	195.0	100.00
34	1	99	1	99	3.98e-66	195.0	100.00
35	1	99	1	99	4.07e-66	195.0	98.99
36	1	99	1	99	4.64e-66	195.0	100.00
37	1	99	1	99	4.69e-66	195.0	97.98
38	1	99	1	99	4.77e-66	195.0	98.99
39	1	99	1	99	5.36e-66	194.0	98.99
40	1	99	1	99	5.60e-66	194.0	98.99
41	1	99	1	99	5.72e-66	194.0	100.00
42	1	99	1	99	5.72e-66	194.0	98.99

43	1	99	1	99	5.98e-66	194.0	98.99
44	1	99	1	99	6.11e-66	194.0	97.98
45	1	99	1	99	6.45e-66	194.0	98.99
46	1	99	105	203	6.70e-66	198.0	100.00
47	1	99	1	99	2.48e-64	194.0	98.99
48	1	99	1	99	6.74e-66	194.0	98.99
49	1	99	1	99	7.12e-66	194.0	100.00
50	1	99	105	203	8.53e-66	198.0	100.00
51	1	99	1	99	2.13e-64	194.0	100.00
52	1	99	1	99	9.17e-66	194.0	98.99
53	1	99	1	99	9.48e-66	194.0	98.99
54	1	99	1	99	1.13e-65	194.0	100.00
55	1	99	1	99	1.55e-65	193.0	98.99
56	1	99	1	99	1.68e-65	193.0	97.98
57	1	99	1	99	1.71e-65	193.0	97.98
58	1	99	1	99	2.04e-65	193.0	98.99
59	1	99	1	99	2.36e-65	193.0	97.98
60	1	99	1	99	2.55e-65	193.0	98.99
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63	1	99	1	99	4.56e-65	192.0	97.98
64	1	99	1	99	6.26e-65	192.0	98.99
65	1	99	105	203	9.79e-65	195.0	98.99
66	1	99	1	99	1.60e-64	194.0	98.99
67	1	99	1	99	1.37e-64	191.0	98.99
68	1	99	1	99	1.63e-64	191.0	96.97
69	1	99	5	103	2.02e-64	191.0	97.98
70	1	99	2	100	2.36e-64	191.0	97.98
71	1	99	1	99	2.88e-64	190.0	97.98
72	1	99	2	100	2.97e-64	190.0	97.98
73	1	99	1	99	3.37e-64	194.0	98.99
74	1	99	105	203	3.37e-64	194.0	98.99
75	1	99	1	99	3.48e-64	194.0	97.98
76	1	99	105	203	3.48e-64	194.0	97.98
77	1	99	1	99	3.55e-64	190.0	98.99
78	1	99	105	203	3.76e-64	194.0	98.99
79	1	99	1	99	6.22e-64	193.0	98.99
80	1	99	1	99	4.37e-64	190.0	97.98
81	1	99	1	99	4.37e-64	190.0	97.98
82	1	99	1	99	4.37e-64	190.0	97.98
83	1	99	1	99	4.37e-64	190.0	97.98
84	1	99	1	99	4.93e-64	189.0	97.98
85	1	99	1	99	4.93e-64	189.0	98.99

86	1	99	1	99	5.21e-64	189.0	97.98
87	1	99	1	99	5.33e-64	189.0	97.98
88	1	99	1	99	5.51e-64	189.0	98.99
89	1	99	1	99	5.69e-64	189.0	98.99
90	1	99	1	99	6.01e-64	189.0	98.99
91	1	99	1	99	6.64e-64	189.0	97.98
92	1	99	1	99	7.09e-64	189.0	97.98
93	1	99	1	99	7.49e-64	189.0	97.98
94	1	99	1	99	8.18e-64	193.0	98.99
95	1	99	105	203	8.18e-64	193.0	98.99
96	1	99	1	99	8.36e-64	189.0	96.97
97	1	99	1	99	9.03e-64	189.0	96.97
98	1	99	1	99	9.75e-64	189.0	98.99
99	1	99	1	99	1.09e-63	189.0	97.98
100	1	99	1	99	1.09e-63	189.0	97.98
101	1	99	1	99	1.12e-63	189.0	97.98
102	1	99	1	99	1.12e-63	189.0	98.99
103	1	99	1	99	1.20e-63	189.0	96.97
104	1	99	1	99	1.20e-63	189.0	96.97
105	1	99	1	99	1.28e-63	189.0	97.98
106	1	99	1	99	1.28e-63	189.0	97.98
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110	1	99	1	99	1.46e-63	188.0	97.98
111	1	99	1	99	1.46e-63	188.0	97.98
112	1	99	1	99	1.82e-63	188.0	97.98
113	1	99	1	99	1.90e-63	188.0	98.99
114	1	99	1	99	2.01e-63	188.0	97.98
115	1	99	1	99	2.06e-63	188.0	97.98
116	1	99	1	99	2.15e-63	188.0	95.96
117	1	99	1	99	2.27e-63	188.0	96.97
118	1	99	1	99	2.56e-63	188.0	97.98
119	1	99	1	99	2.65e-63	188.0	97.98
120	1	99	1	99	3.30e-63	187.0	96.97
121	1	99	1	99	3.47e-63	191.0	97.98
122	1	99	105	203	3.47e-63	191.0	97.98
123	1	99	1	99	3.68e-63	187.0	97.98
124	1	99	1	99	3.93e-63	187.0	97.98
125	1	99	1	99	3.97e-63	187.0	97.98
126	1	99	1	99	4.20e-63	187.0	96.97
127	1	99	1	99	4.74e-63	187.0	97.98
128	1	99	1	99	5.29e-63	187.0	95.96

129	1	99	105	203	5.49e-63	191.0	97.98
130	1	99	1	99	9.08e-63	190.0	97.98
131	1	99	1	99	5.58e-63	187.0	96.97
132	1	99	1	99	5.65e-63	187.0	97.98
133	1	99	1	99	6.23e-63	187.0	97.98
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136	1	99	1	99	6.96e-63	187.0	98.99
137	1	99	1	99	8.20e-63	186.0	96.97
138	1	99	1	99	8.95e-63	186.0	97.98
139	1	99	1	99	1.03e-62	186.0	97.98
140	1	99	1	99	1.13e-62	186.0	98.99
141	1	99	1	99	1.18e-62	186.0	95.96
142	1	99	1	99	1.22e-62	186.0	97.98
143	1	99	1	99	1.62e-62	186.0	96.97
144	1	99	1	99	2.40e-62	185.0	98.99
145	1	99	1	99	2.90e-62	185.0	98.99
146	1	99	1	99	3.20e-62	185.0	98.99
147	1	99	1	99	3.23e-62	185.0	95.96
148	1	99	1	99	3.49e-62	185.0	97.98
149	1	99	1	99	3.77e-62	185.0	98.99
150	1	99	2	100	3.81e-62	185.0	96.97
151	1	99	1	99	3.86e-62	185.0	98.99
152	1	99	1	99	4.55e-62	185.0	95.96
153	1	99	1	99	5.13e-62	184.0	96.97
154	1	99	1	99	6.32e-62	184.0	96.97
155	1	99	1	99	6.46e-62	184.0	96.97
156	1	99	1	99	9.08e-62	184.0	93.94
157	1	99	1	99	1.28e-61	184.0	94.95
158	1	99	1	99	1.35e-61	183.0	95.96
159	1	99	1	99	1.35e-61	183.0	95.96
160	1	99	1	99	1.75e-61	183.0	96.97
161	1	99	1	99	1.81e-61	183.0	96.97
162	1	99	1	99	1.83e-61	183.0	96.97
163	1	99	1	99	2.11e-61	183.0	95.96
164	1	99	1	99	2.18e-61	183.0	97.98
165	1	99	1	99	2.18e-61	183.0	96.97
166	1	99	1	99	2.31e-61	183.0	97.98
167	1	99	1	99	2.63e-61	183.0	96.97
168	1	99	1	99	2.75e-61	182.0	95.96
169	1	99	1	99	3.00e-61	182.0	96.97
170	1	99	1	99	4.87e-61	182.0	96.97
171	1	99	1	99	7.39e-61	182.0	95.96

172	1	99	1	99	7.81e-61	181.0	97.98
173	1	99	1	99	7.89e-61	181.0	96.97
174	1	95	1	95	8.21e-61	181.0	97.89
175	1	99	1	99	9.00e-61	181.0	97.98
176	1	99	107	205	1.01e-60	200.0	98.99
177	1	99	1	99	1.29e-60	181.0	94.95
178	1	99	1	99	2.07e-60	181.0	96.97
179	1	99	1	99	2.12e-60	181.0	95.96
180	1	99	1	99	2.64e-60	180.0	95.96
181	1	99	2	100	3.91e-60	180.0	95.96
182	1	99	1	100	4.98e-60	179.0	93.00
183	1	99	1	99	5.33e-60	179.0	95.96
184	1	99	1	99	9.96e-60	179.0	96.97
185	1	99	1	99	1.35e-59	182.0	96.97
186	1	99	105	203	1.35e-59	182.0	96.97
187	1	99	105	203	2.91e-59	181.0	96.97
188	1	99	1	99	9.97e-57	175.0	94.95
189	1	99	1	99	6.58e-59	177.0	95.96
190	1	99	1	99	1.73e-58	176.0	97.98
191	1	99	1	99	2.40e-58	175.0	95.96
192	1	99	1	99	4.35e-58	174.0	91.92
193	1	99	1	99	6.97e-58	174.0	92.93
194	1	99	1	99	1.03e-57	174.0	97.98
195	1	99	1	99	1.26e-57	173.0	93.94
196	1	99	1	99	1.62e-57	173.0	92.93
197	1	99	1	99	2.28e-57	173.0	92.93
198	1	99	1	99	5.03e-57	172.0	93.94
199	1	99	1	99	6.99e-57	172.0	95.96
200	1	99	1	99	1.84e-56	171.0	95.96
201	1	99	1	99	1.88e-56	171.0	97.98
202	1	99	1	99	2.03e-56	171.0	92.93
203	1	99	1	99	2.72e-56	170.0	92.93
204	1	99	1	99	3.36e-56	173.0	92.93
205	1	99	105	203	1.99e-51	161.0	93.94
206	1	99	1	99	3.43e-56	173.0	92.93
207	1	99	105	203	6.39e-56	173.0	92.93
208	1	99	1	99	4.13e-56	170.0	94.95
209	1	99	1	99	5.50e-56	169.0	96.97
210	1	99	105	203	6.54e-56	173.0	92.93
211	1	99	1	99	2.01e-51	161.0	93.94
212	1	99	1	99	6.63e-56	169.0	93.94
213	1	99	1	99	7.65e-56	169.0	90.91
214	1	99	1	99	7.90e-56	169.0	92.93

```
215        1    99       1    99 9.42e-56    169.0       92.93
216        1    99       1    99 1.16e-55    169.0       94.95
217        1    99       1    99 1.24e-55    168.0       92.93
218        1    99       1    99 2.58e-55    167.0       94.95
219        1    99       1    99 3.25e-55    167.0       95.96
220        1    99       1    99 3.25e-55    167.0       96.97
221        1    99       1    99 4.99e-55    167.0       96.97
222        1    99       1    99 5.22e-55    167.0       95.96
223        1    99       1    99 5.51e-55    167.0       96.97
224        1    99       1    99 9.65e-55    166.0       95.96
225        1    99       1    99 1.34e-54    166.0       90.91
226        1    99       1    99 1.69e-54    166.0       95.96
227        1    99       1    99 3.56e-54    165.0       91.92
228        1    99       1    99 5.46e-54    164.0       92.93
229        1    99       1    99 6.58e-54    164.0       89.90
230        1    99       1    99 1.85e-53    163.0       96.97
231        1    99       1    99 2.46e-53    162.0       93.94
232        1    99       1    99 1.06e-52    161.0       93.94
233        1    99       1    99 1.30e-52    161.0       92.93
234        1    99     105   203 2.82e-52    164.0       92.93
235        1    99       1    99 1.43e-51    162.0       93.94
236        1    99       1    99 1.39e-51    162.0       93.94
237        1    99     105   203 1.39e-51    162.0       93.94
238        1    99       1    99 1.49e-48    150.0       92.93
239        1    99       1    99 2.35e-33    112.0       71.72
240        1    99       1    99 5.91e-33    111.0       70.71
241        1    99       1    99 8.39e-33    111.0       70.71
242        1    99       1    99 2.32e-32    110.0       70.71
243        1    99       1    99 7.92e-32    108.0       68.69
244        1    99       1    99 4.61e-31    106.0       67.68
245       22    97      34   121 1.50e-07     47.4       54.44
246        8    99      22   114 1.30e-05     42.4       49.46
247        4    97       9   114 2.80e-02     33.5       49.06
248       36    46       1    11 5.20e-01     28.5      100.00
249       36    45       1    10 2.90e+00     26.2      100.00
```

$url
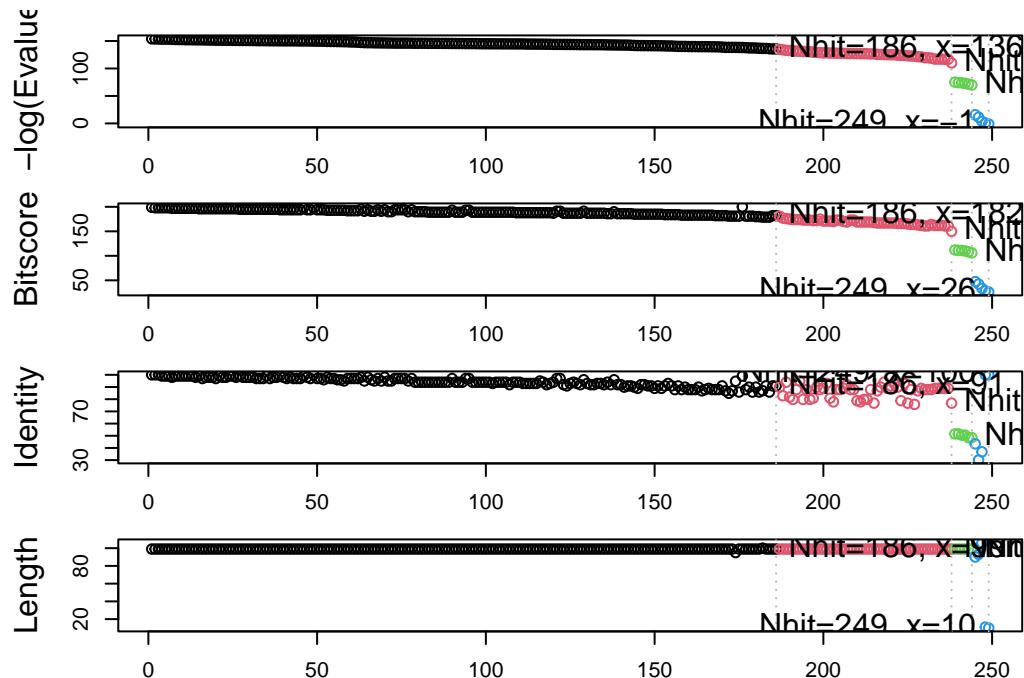
"https://blast.ncbi.nlm.nih.gov/Blast.cgi?CMD=Get&FORMAT_OBJECT=Alignment&ALIGNMENT_VIEW=Tabu

Plot a quick overview of blast results

```
hits<- plot(blast)
```

```
 * Possible cutoff values:    135 110 69 -2
           Yielding Nhits:    186 238 244 249

 * Chosen cutoff value of:    69
           Yielding Nhits:    244
```



```
hits$pdb.id
```

```
  [1] "1W5V_A" "2FDE_A" "1AJV_A" "2R38_A" "2R3T_A" "1HXB_A" "1BV9_A" "1AAQ_A"
  [9] "1AXA_A" "1HVS_A" "1ZP8_A" "2QHC_A" "1A8G_A" "2O4L_A" "5COK_A" "1TCX_A"
 [17] "2Z54_A" "1D4S_A" "1BV7_A" "1BWA_A" "1A9M_A" "2FLE_A" "1ODY_A" "1GNN_A"
 [25] "1GNM_A" "5YRS_B" "1HEF_E" "1ODX_A" "4QGI_A" "1BVE_A" "2AZ8_A" "1A30_A"
 [33] "6DH6_A" "6DH0_A" "2I4D_A" "6OOS_A" "1RL8_A" "5YRS_A" "1ZSF_A" "2Q64_A"
 [41] "6DH3_A" "2NPH_A" "2Q63_A" "1LZQ_A" "1FB7_A" "1G6L_A" "1HIV_A" "6OOU_A"
 [49] "1HVC_A" "2I4V_A" "2AZ9_A" "6OOT_A" "2P3B_B" "5KAO_A" "2WL0_A" "6OPT_A"
 [57] "1IZI_A" "1MRX_A" "2PYM_A" "2PYN_A" "1DMP_A" "4K4P_A" "1LV1_A" "1AID_A"
 [65] "1LV1_A" "1ZBG_A" "3TKG_A" "1HVC_A" "5YOK_A" "1G6L_A" "1FGC_C" "3K4V_A"
 [73] "3KT5_A" "3KT5_A" "4QLH_A" "4QLH_A" "2F3K_A" "4Q5M_A" "2AOC_A" "3B80_A"
 [81] "3VF5_A" "2AVQ_A" "1DW6_C" "1KZK_A" "2HS1_A" "1K6C_A" "1MTB_A" "4Q1X_A"
```

```
 [89] "4Q1W_A" "4Q5M_A" "3D1X_A" "2AVM_A" "3PWM_A" "3KT2_A" "3KT2_A" "1SDV_A"
 [97] "3JVW_A" "3OY4_A" "1A94_A" "2HS2_A" "4EJ8_A" "2FGU_A" "2AVV_A" "3JW2_A"
[105] "3BVA_A" "1FFF_C" "3S43_B" "2NXD_A" "1FG6_C" "1EBK_C" "4Q1Y_A" "3EL4_A"
[113] "1F7A_A" "1K2B_A" "2FGV_A" "1Z8C_A" "2G69_A" "3EL9_A" "3OXV_A" "1BDR_A"
[121] "3N3I_A" "3N3I_A" "3OXW_A" "3S43_A" "3EM3_A" "3CYW_A" "5KQX_A" "2B60_A"
[129] "7DOZ_A" "1K2C_A" "1MT7_A" "3EM4_A" "4QJ9_A" "1BDL_A" "3LZS_A" "5T84_A"
[137] "4DQB_A" "7DOZ_A" "4QJ2_A" "3LZV_A" "1SGU_A" "2FXE_A" "1BDQ_A" "3U71_A"
[145] "2R5P_A" "4OBD_A" "7MAS_A" "3IXO_A" "3D3T_A" "5YOJ_A" "3LZU_A" "4NJS_A"
[153] "3EKP_A" "1B6J_A" "3EKQ_A" "2RKF_A" "1C6X_A" "7MAR_A" "4DQF_A" "1RPI_A"
[161] "3OU1_B" "3PJ6_A" "2P3A_A" "6OGQ_A" "3OQ7_A" "5KR1_A" "3OQD_A" "4RVI_A"
[169] "3OQA_A" "1B6K_A" "3OUD_B" "6MK9_A" "3SO9_A" "1Q9P_A" "6I45_A" "7SEP_A"
[177] "4NJT_A" "3BXR_A" "4YOA_A" "4DQC_A" "2FDD_A" "2RKG_A" "4DQH_A" "2P3C_A"
[185] "4EP2_A" "4EP2_A" "4EQ0_A" "4NPT_A" "6OPU_A" "4NPU_A" "3U7S_A" "3HAW_A"
[193] "2AZB_A" "3TTP_A" "3HBO_A" "3GGU_A" "7N6T_A" "6OPV_A" "4EQ0_A" "6OPX_A"
[201] "2O4N_A" "5T2E_A" "3UCB_A" "3KA2_A" "3FSM_A" "6OPW_A" "2AZC_A" "3FSM_A"
[209] "3HLO_A" "2P3D_A" "3T3C_A" "7MYP_A" "6O54_X" "6OPY_A" "4Z4X_A" "6OPZ_A"
[217] "2JE4_A" "1DAZ_C" "7MAP_A" "7MAQ_A" "1K1U_A" "2B7Z_A" "3MWS_A" "1K1T_A"
[225] "8DCH_A" "3I2L_A" "6P9A_A" "2FXD_A" "2J9J_A" "3DCK_A" "2J9J_B" "3NXE_A"
[233] "2O40_A" "2O40_A" "3NXE_A" "3KA2_A" "3HLO_A" "5B18_A" "1SIP_A" "2SAM_A"
[241] "1AZ5_A" "1SIV_A" "1HII_A" "1IVP_A"
```

Prediction of functional motions

We can run a Normal Mode Analysis (NMA) to predit large scale motions/flexibility/ dynamics
of any biomolecule that we can read into R.

Lets look at ADK

```
adk <- read.pdb("1AKE")
```

```
 Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

```
adk_A<- trim.pdb (adk, chain="A")
adk_A
```

```
 Call:  trim.pdb(pdb = adk, chain = "A")

   Total Models#: 1
     Total Atoms#: 1954,  XYZs#: 5862  Chains#: 1  (values: A)
```

```
    Protein Atoms#: 1656  (residues/Calpha atoms#: 214)
    Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

    Non-protein/nucleic Atoms#: 298  (residues: 242)
    Non-protein/nucleic resid values: [ AP5 (1), HOH (241) ]

  Protein sequence:
     MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
     DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
     VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
     YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, helix, sheet, seqres, xyz,
        calpha, call
```
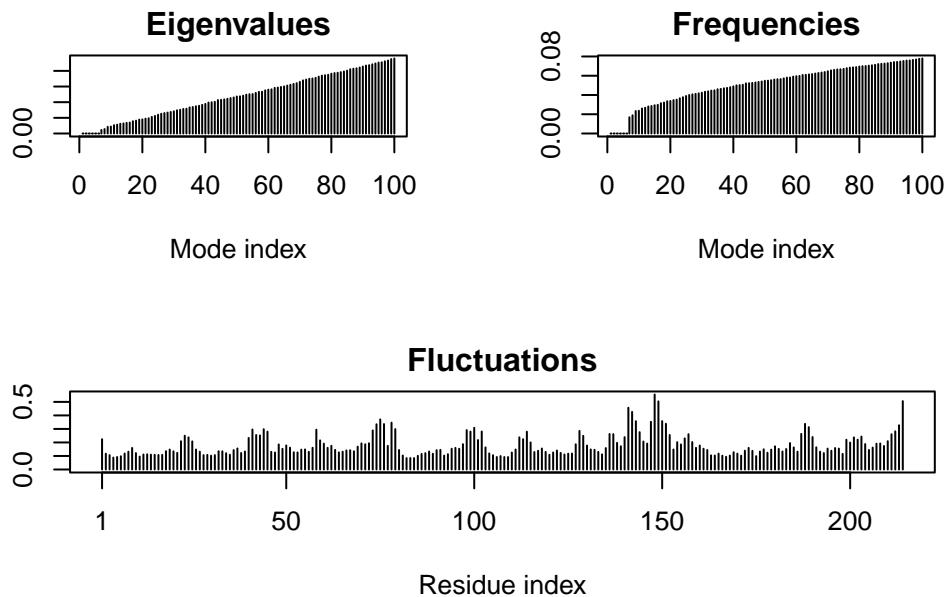
```
m<- nma(adk_A)
```

```
 Building Hessian...        Done in 0.023 seconds.
 Diagonalizing Hessian...   Done in 0.293 seconds.
```

```
plot(m)
```

Eigenvalues

Frequencies

Fluctuations

Let's write out a trajectory of predicted motion

```
mktrj(m, file="adk_nma.pdb")
```

Play with 3D viewing in R

We can use the new **bio3dview** package, which is not yet on CRAN, to render interactive 3D views in R and html quarto output reports.

To install from GitHub we can use the **pak** package

```
library(pak)

#view.pdb(adk)
```