

Class 9

AUTHOR

Kavi (PID: A69046927)

```
stats <- read.csv("PDB_Data_Dis.csv")
as.numeric(sub(",","", stats$X.ray))
```

```
[1] 176378 10284 9007 3077 174 11
```

```
as.numeric(sub(",","", stats$Total))
```

```
[1] 210203 13734 15256 4852 223 22
```

This is annoying. Let's see if we can make it easier with a different package.

```
library(readr)
```

Warning: package 'readr' was built under R version 4.5.2

```
stats <- read_csv("PDB_Data_Dis.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 × 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
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>
```

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

```
n.total <- sum(stats$Total)
n.xray <- sum(stats$`X-ray`)
n.em <- sum(stats$EM)

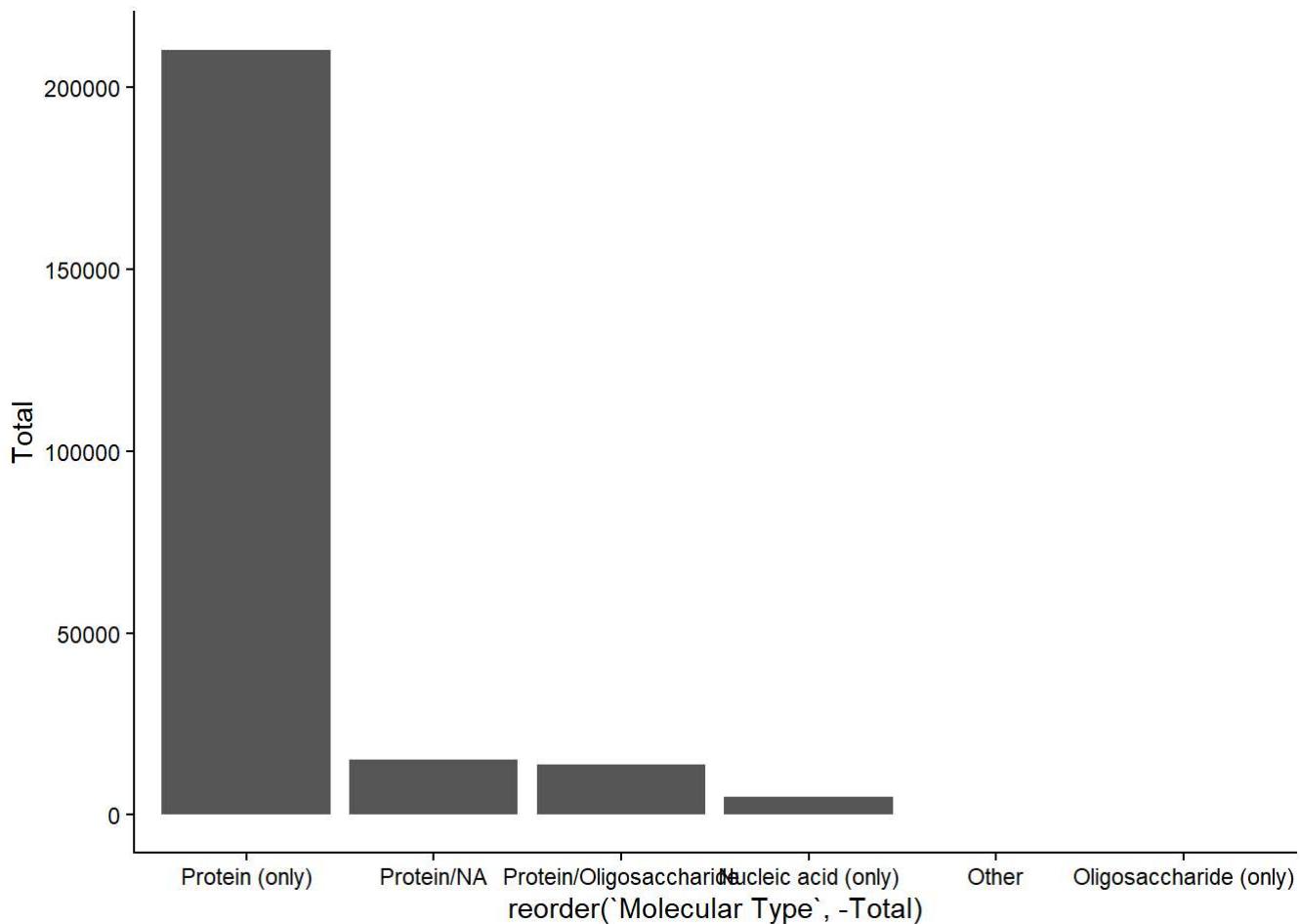
round(n.xray/n.total * 100,2)
```

```
[1] 81.43
```

```
round(n.em/n.total * 100,2)
```

```
[1] 12.27
```

```
library(ggplot2)
ggplot(stats, aes(reorder(`Molecular Type`, -Total), Total)) +
  geom_col() +
  theme_classic()
```



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

```
stats$`Molecular Type` <- trimws(stats$`Molecular Type`)
n.total <- sum(stats$Total)
```

```
n.protein <- sum(stats$Total[grep("Protein", stats$`Molecular Type`, ignore.case = TRUE)])  
prot.por <- round(n.protein / n.total * 100, 2)
```

97.91% of structures in the PDB are protein.

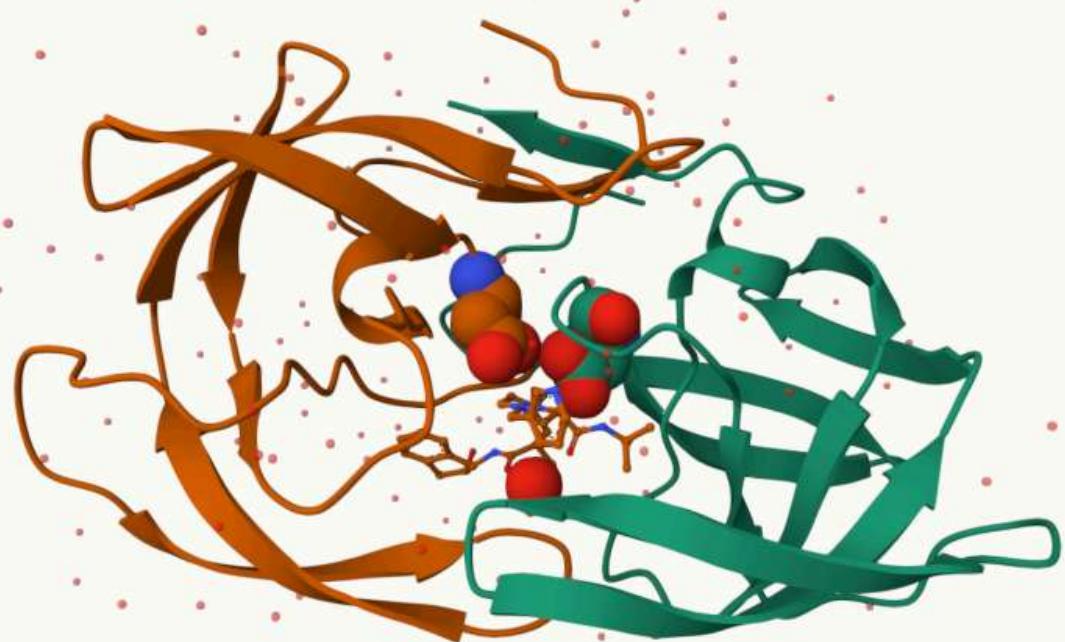
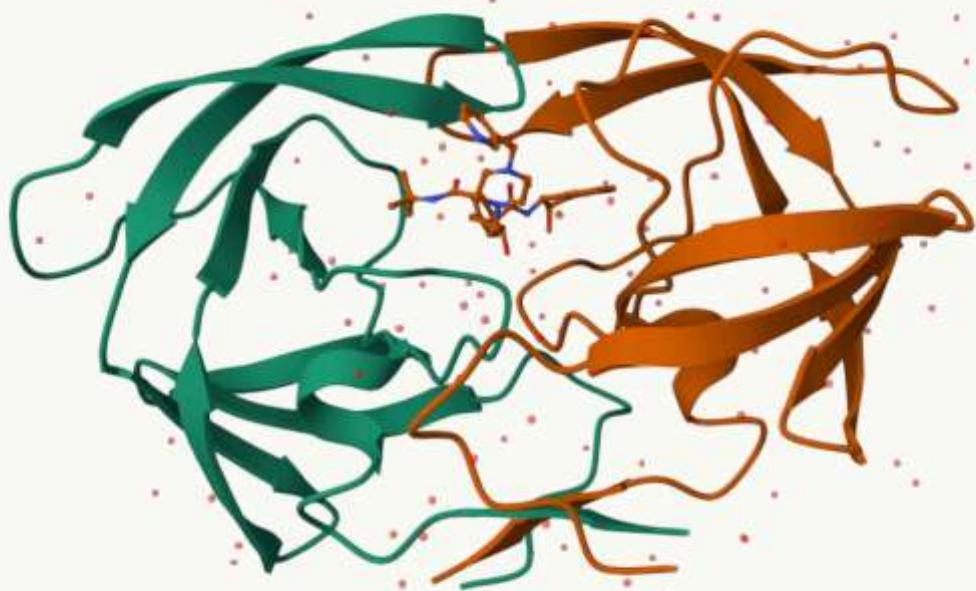
Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

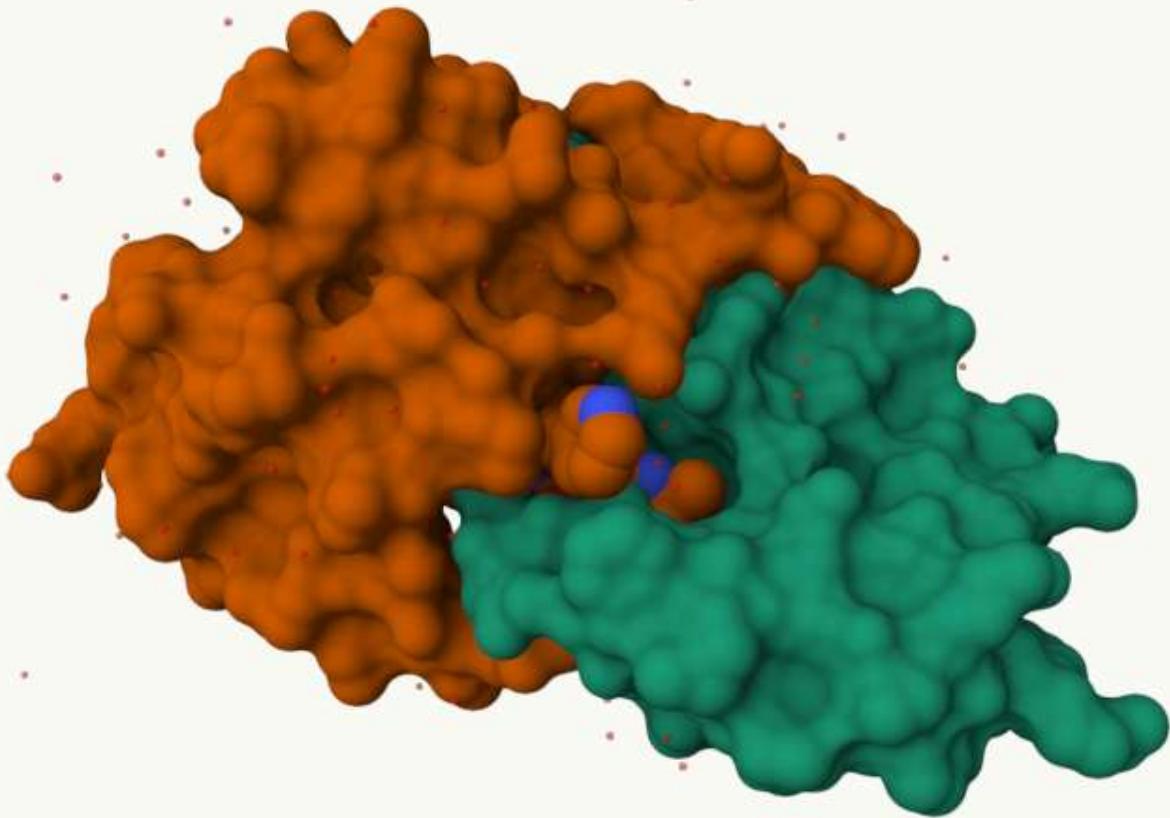
363 structures

Visualizing Structure Data

The Mol* viewer is embedded in many bioinformatics websites. The homepage is <https://molstar.org>

I can insert any figure or image file unsing markdown format





```
## Bio3D package for structural bioinformatics
```

We can use 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:

```
PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWPKPMIGGIGGGFIKVRQYD
QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
ALLDTGADDTVLEEMSLPGRWPKPMIGGIGGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
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>										

Let's get the sequence

```
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"
```

Let's trim to chain A and get just its sequence:

```
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 = GH5ZUHK8016
.
Reporting 249 hits
```

```
head(blast$hit.tbl)
```

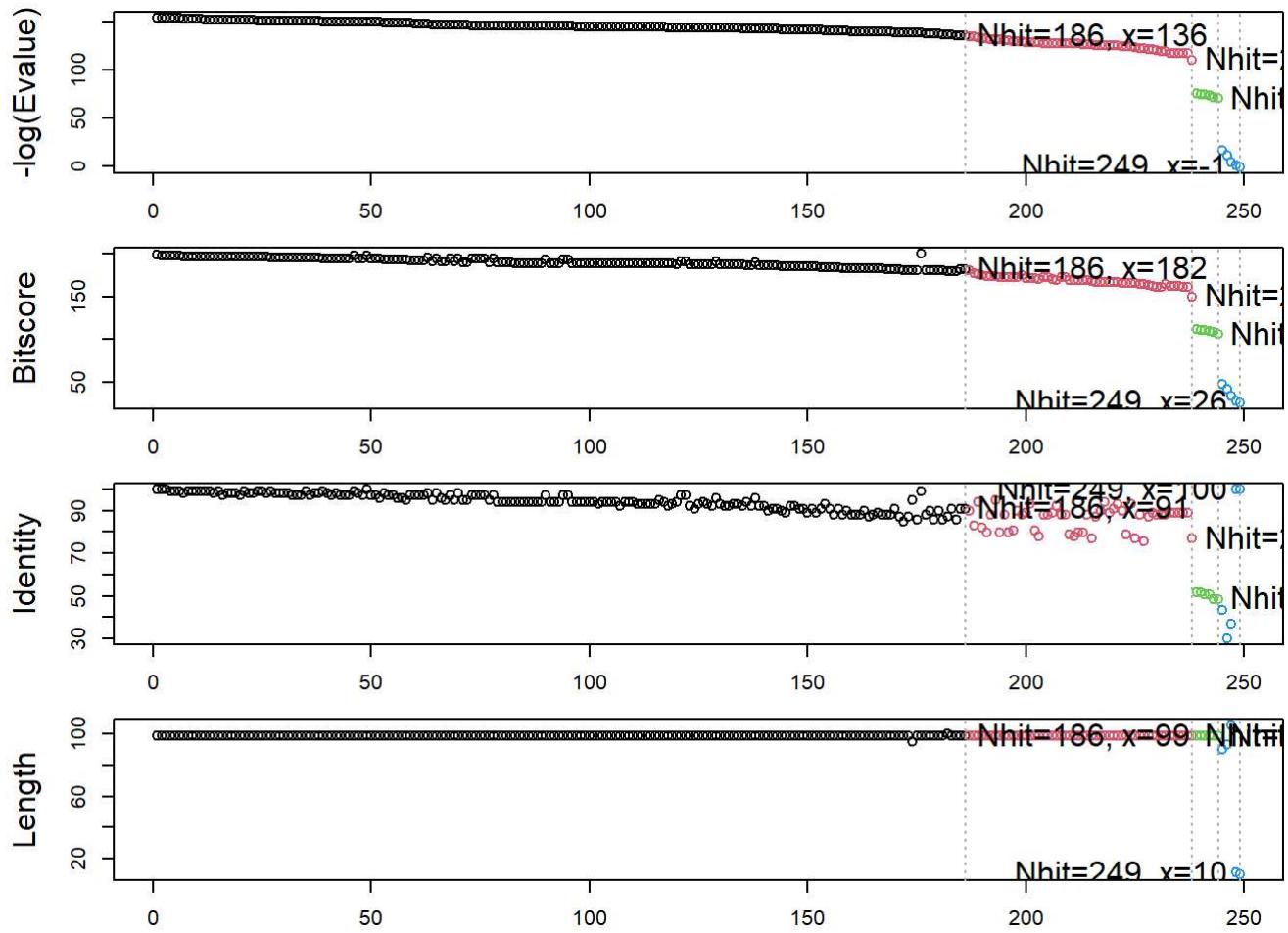
	queryid	subjectids	identity	alignmentlength	mismatches	gapopens	q.start	q.end	s.start	s.end	evalue	bitscore	positives	mlog.evalue	pdb.id	acc
1	Query_3031849	1W5V_A	100.00		99	0	0	1								
2	Query_3031849	2FDE_A	100.00		99	0	0	1								
3	Query_3031849	1AJV_A	100.00		99	0	0	1								
4	Query_3031849	2R38_A	98.99		99	1	0	1								
5	Query_3031849	2R3T_A	98.99		99	1	0	1								
6	Query_3031849	1HXB_A	98.99		99	1	0	1								

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" "204L_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" "10DX_A" "4QGI_A" "1BVE_A" "2AZ8_A" "1A30_A"
[33] "6DH6_A" "6DH0_A" "2I4D_A" "600S_A" "1RL8_A" "5YRS_A" "1ZSF_A" "2Q64_A"
[41] "6DH3_A" "2NPH_A" "2Q63_A" "1LZQ_A" "1FB7_A" "1G6L_A" "1HIV_A" "600U_A"
[49] "1HVC_A" "2I4V_A" "2AZ9_A" "600T_A" "2P3B_B" "5KAO_A" "2WL0_A" "6OPT_A"
[57] "1IZI_A" "1MRX_A" "2PYM_A" "2PYN_A" "1DMMP_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] "3JWV_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" "40BD_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" "60GQ_A" "30Q7_A" "5KR1_A" "3OQD_A" "4RVI_A"
```

```
[169] "30QA_A" "1B6K_A" "3OUD_B" "6MK9_A" "3S09_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] "204N_A" "5T2E_A" "3UCB_A" "3KA2_A" "3FSM_A" "6OPW_A" "2AZC_A" "3FSM_A"
[209] "3HLO_A" "2P3D_A" "3T3C_A" "7MYP_A" "6054_X" "60PY_A" "4Z4X_A" "60PZ_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] "2040_A" "2040_A" "3NXE_A" "3KA2_A" "3HLO_A" "5B18_A" "1SIP_A" "2SAM_A"
[241] "1AZ5_A" "1SIV_A" "1HII_A" "1IVP_A"
```

```
files <- get.pdb(hits$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE)
```

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1W5V.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2FDE.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1AJV.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2R38.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2R3T.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1HXB.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1BV9.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1AAQ.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1AXA.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1HVS.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1ZP8.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2QHC.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip =

TRUE): pdbs/1A8G.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/204L.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/5COK.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1TCX.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2Z54.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1D4S.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1BV7.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1BWA.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1A9M.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2FLE.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1ODY.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1GNN.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1GNM.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/5YRS.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1HEF.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1ODX.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/4QGI.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1BVE.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2AZ8.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1A30.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/6DH6.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/6DH0.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2I4D.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/600S.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1RL8.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1ZSF.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2Q64.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/6DH3.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2NPH.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2Q63.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1LZQ.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1FB7.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1G6L.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1HIV.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/600U.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1HVC.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2I4V.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2AZ9.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/600T.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2P3B.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/5KAO.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2WL0.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/6OPT.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1IZI.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1MRX.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2PYM.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2PYN.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1DMP.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/4K4P.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1LV1.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1AID.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1ZBG.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3TKG.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/5YOK.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1FGC.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3K4V.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3KT5.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/4QLH.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2F3K.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/4Q5M.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2AOC.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3B80.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3VF5.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2AVQ.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1DW6.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1KZK.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2HS1.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1K6C.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1MTB.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/4Q1X.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/4Q1W.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3D1X.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2AVM.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3PWM.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3KT2.pdb exists. Skipping download

Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1SDV.pdb exists. Skipping download

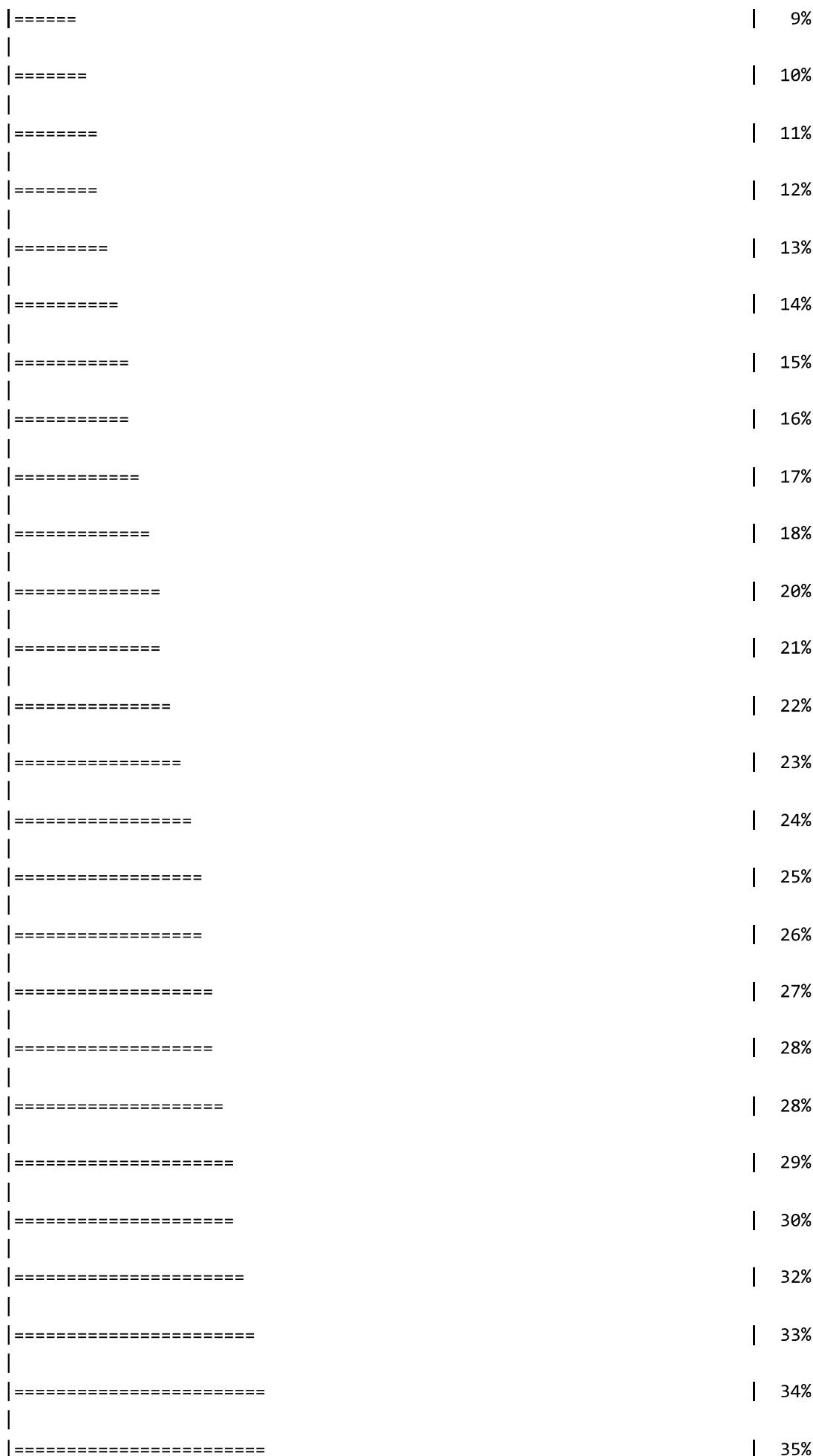
Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3JWW.pdb exists. Skipping download

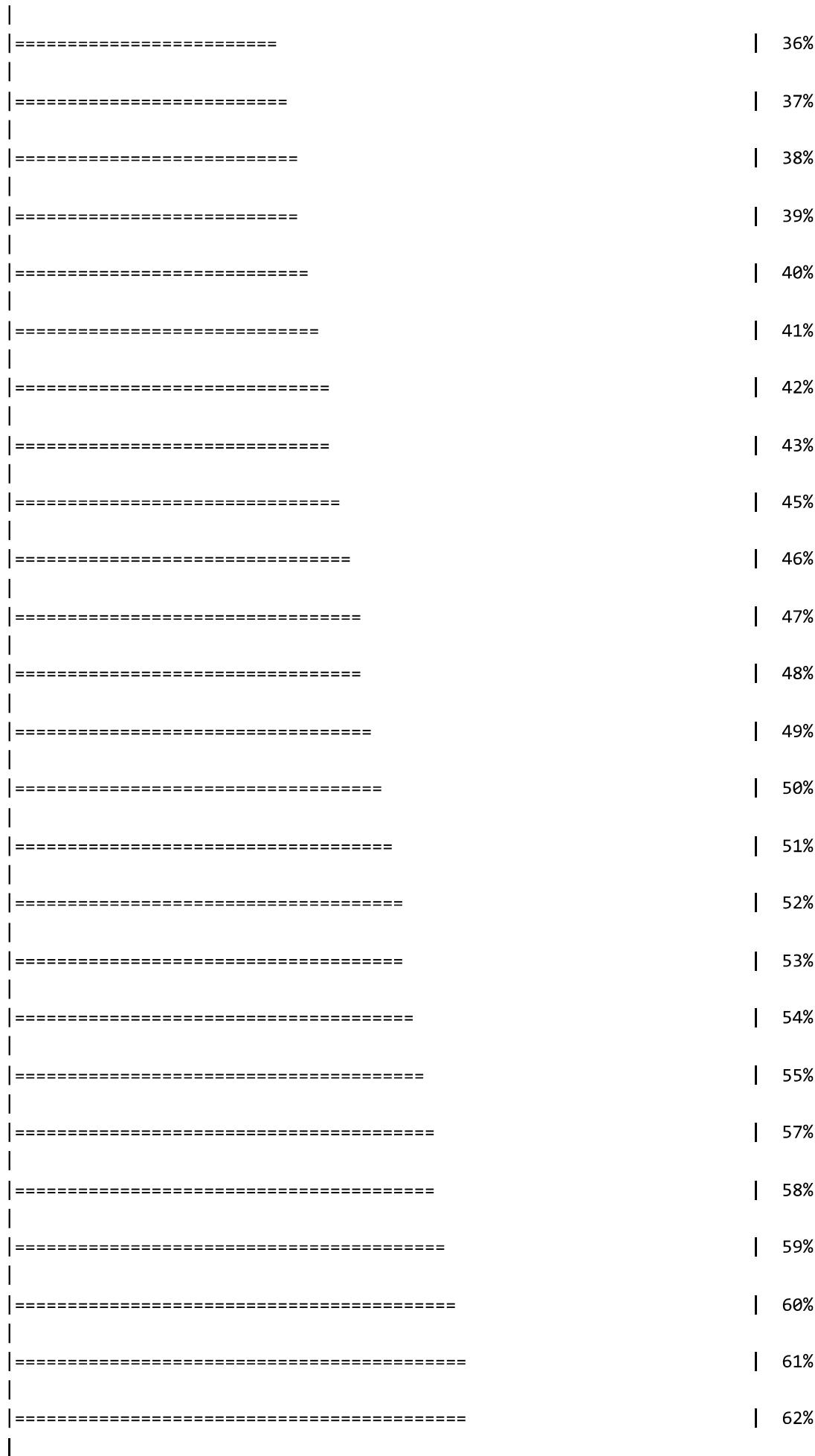
Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/3OY4.pdb exists. Skipping download

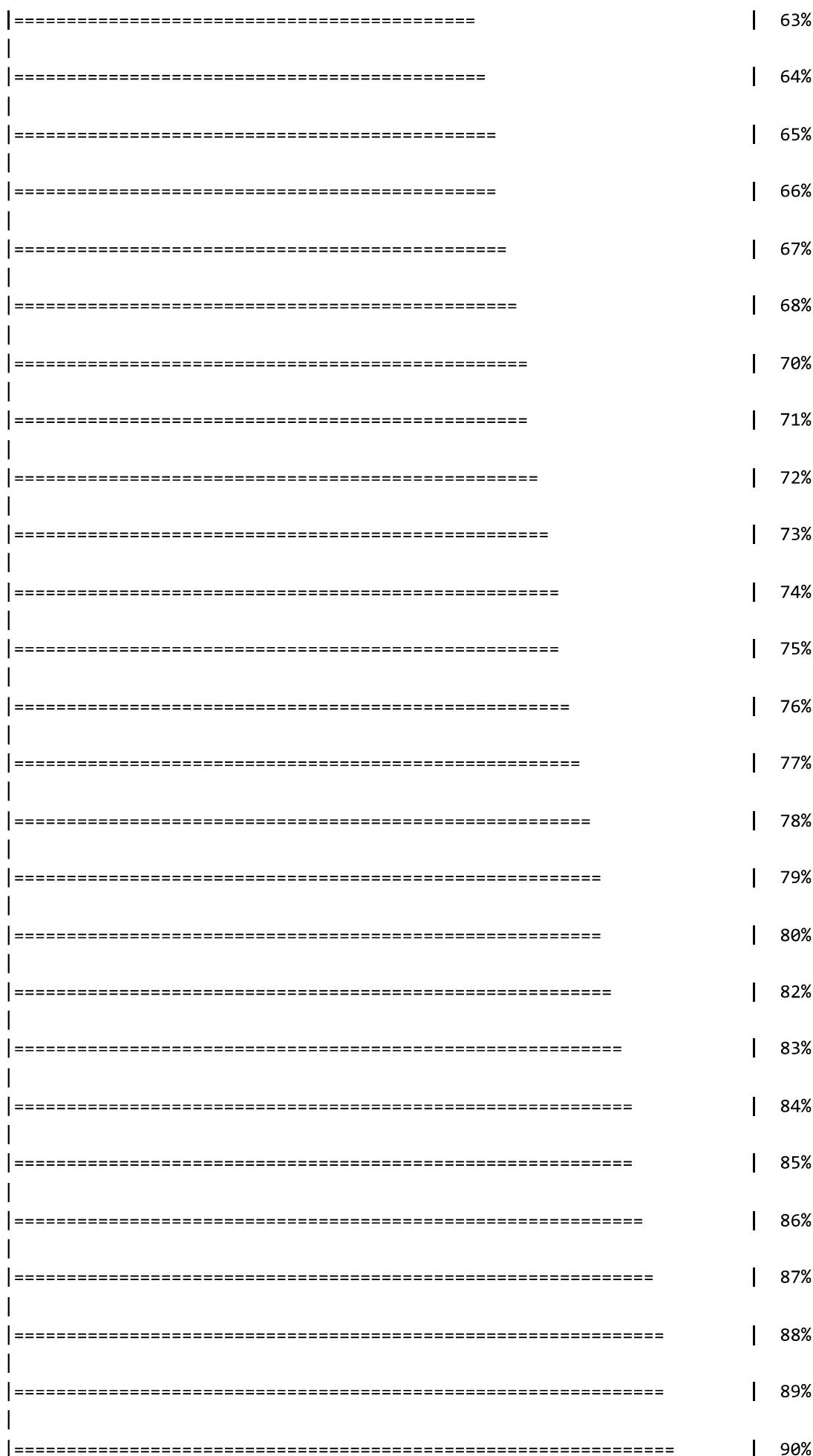
Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/1A94.pdb exists. Skipping download

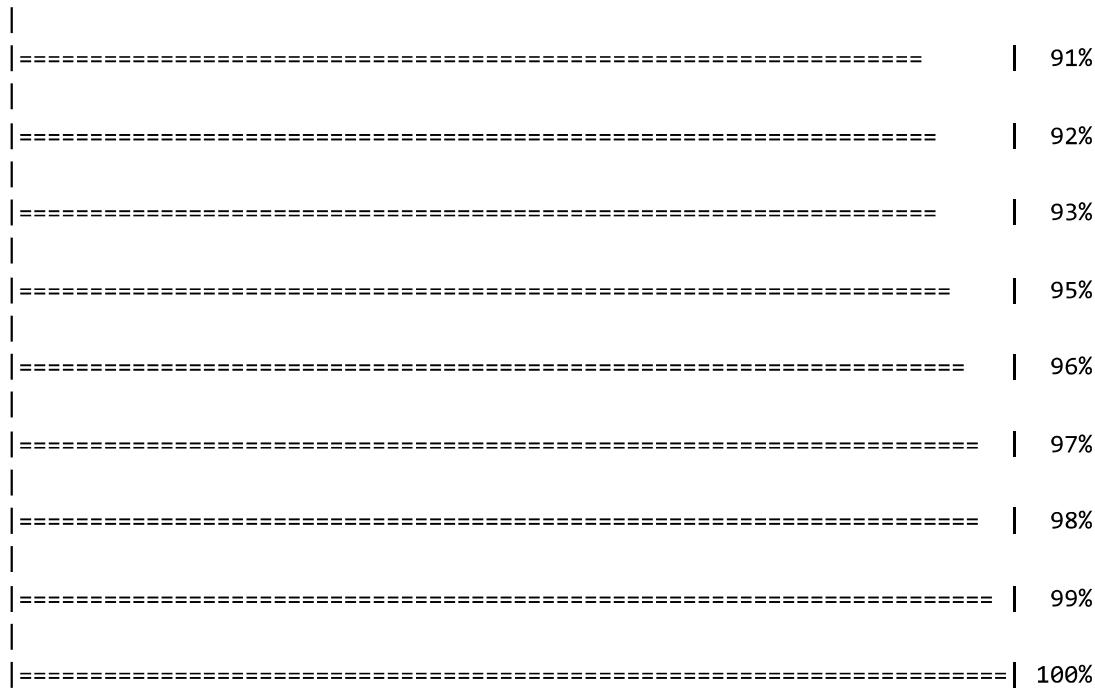
Warning in get.pdb(hits\$pdb.id[1:100], path = "pdbs", split = TRUE, gzip = TRUE): pdbs/2HS2.pdb exists. Skipping download











Align and superpose structures

Next we will use the `pdbaln()` function to align and also optionally fit (i.e. superpose) the identified PDB structures.

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

```
Reading PDB files:  
pdbs/split_chain/1W5V_A.pdb  
pdbs/split_chain/2FDE_A.pdb  
pdbs/split_chain/1AJV_A.pdb  
pdbs/split_chain/2R38_A.pdb  
pdbs/split_chain/2R3T_A.pdb  
pdbs/split_chain/1HXB_A.pdb  
pdbs/split_chain/1BV9_A.pdb  
pdbs/split_chain/1AAQ_A.pdb  
pdbs/split_chain/1AXA_A.pdb  
pdbs/split_chain/1HVS_A.pdb  
pdbs/split_chain/1ZP8_A.pdb  
pdbs/split_chain/2QHC_A.pdb  
pdbs/split_chain/1A8G_A.pdb  
pdbs/split_chain/204L_A.pdb  
pdbs/split_chain/5COK_A.pdb  
pdbs/split_chain/1TCX_A.pdb  
pdbs/split_chain/2Z54_A.pdb  
pdbs/split_chain/1D4S_A.pdb  
pdbs/split_chain/1BV7_A.pdb  
pdbs/split_chain/1BWA_A.pdb  
pdbs/split_chain/1A9M_A.pdb  
pdbs/split_chain/2FLE_A.pdb  
pdbs/split_chain/1ODY_A.pdb
```

pdb/split_chain/1GNN_A.pdb
pdb/split_chain/1GNM_A.pdb
pdb/split_chain/5YRS_B.pdb
pdb/split_chain/5YRS_A.pdb
pdb/split_chain/1HEF_E.pdb
pdb/split_chain/10DX_A.pdb
pdb/split_chain/4QGI_A.pdb
pdb/split_chain/1BVE_A.pdb
pdb/split_chain/2AZ8_A.pdb
pdb/split_chain/1A30_A.pdb
pdb/split_chain/6DH6_A.pdb
pdb/split_chain/6DH0_A.pdb
pdb/split_chain/2I4D_A.pdb
pdb/split_chain/600S_A.pdb
pdb/split_chain/1RL8_A.pdb
pdb/split_chain/1ZSF_A.pdb
pdb/split_chain/2Q64_A.pdb
pdb/split_chain/6DH3_A.pdb
pdb/split_chain/2NPH_A.pdb
pdb/split_chain/2Q63_A.pdb
pdb/split_chain/1LZQ_A.pdb
pdb/split_chain/1FB7_A.pdb
pdb/split_chain/1G6L_A.pdb
pdb/split_chain/1HIV_A.pdb
pdb/split_chain/600U_A.pdb
pdb/split_chain/1HVC_A.pdb
pdb/split_chain/2I4V_A.pdb
pdb/split_chain/2AZ9_A.pdb
pdb/split_chain/600T_A.pdb
pdb/split_chain/2P3B_B.pdb
pdb/split_chain/5KAO_A.pdb
pdb/split_chain/2WL0_A.pdb
pdb/split_chain/6OPT_A.pdb
pdb/split_chain/1IZI_A.pdb
pdb/split_chain/1MRX_A.pdb
pdb/split_chain/2PYM_A.pdb
pdb/split_chain/2PYN_A.pdb
pdb/split_chain/1DMP_A.pdb
pdb/split_chain/4K4P_A.pdb
pdb/split_chain/1LV1_A.pdb
pdb/split_chain/1AID_A.pdb
pdb/split_chain/1ZBG_A.pdb
pdb/split_chain/3TKG_A.pdb
pdb/split_chain/5YOK_A.pdb
pdb/split_chain/1FGC_C.pdb
pdb/split_chain/3K4V_A.pdb
pdb/split_chain/3KT5_A.pdb
pdb/split_chain/4QLH_A.pdb
pdb/split_chain/2F3K_A.pdb
pdb/split_chain/4Q5M_A.pdb
pdb/split_chain/2AOC_A.pdb

pdb/split_chain/3B80_A.pdb
pdb/split_chain/3VF5_A.pdb
pdb/split_chain/2AVQ_A.pdb
pdb/split_chain/1DW6_C.pdb
pdb/split_chain/1KZK_A.pdb
pdb/split_chain/2HS1_A.pdb
pdb/split_chain/1K6C_A.pdb
pdb/split_chain/1MTB_A.pdb
pdb/split_chain/4Q1X_A.pdb
pdb/split_chain/4Q1W_A.pdb
pdb/split_chain/3D1X_A.pdb
pdb/split_chain/2AVM_A.pdb
pdb/split_chain/3PWM_A.pdb
pdb/split_chain/3KT2_A.pdb
pdb/split_chain/1SDV_A.pdb
pdb/split_chain/3JW_A.pdb
pdb/split_chain/3OY4_A.pdb
pdb/split_chain/1A94_A.pdb
pdb/split_chain/2HS2_A.pdb
..... PDB has ALT records, taking A only, rm.alt=TRUE
... PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. PDB has ALT records, taking A only, rm.alt=TRUE
. ... PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. ... PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE
. .. PDB has ALT records, taking A only, rm.alt=TRUE
. . PDB has ALT records, taking A only, rm.alt=TRUE

- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- .. PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking 1 only, rm.alt=TRUE
- .. PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- . PDB has ALT records, taking A only, rm.alt=TRUE
- .. PDB has ALT records, taking A only, rm.alt=TRUE
- .

Extracting sequences

```
pdb/seq: 1  name: pdbs/split_chain/1W5V_A.pdb
pdb/seq: 2  name: pdbs/split_chain/2FDE_A.pdb
pdb/seq: 3  name: pdbs/split_chain/1AJV_A.pdb
pdb/seq: 4  name: pdbs/split_chain/2R38_A.pdb
pdb/seq: 5  name: pdbs/split_chain/2R3T_A.pdb
pdb/seq: 6  name: pdbs/split_chain/1HXB_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 7  name: pdbs/split_chain/1BV9_A.pdb
pdb/seq: 8  name: pdbs/split_chain/1AAQ_A.pdb
pdb/seq: 9  name: pdbs/split_chain/1AXA_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 10 name: pdbs/split_chain/1HVS_A.pdb
pdb/seq: 11 name: pdbs/split_chain/1ZP8_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 12 name: pdbs/split_chain/2QHC_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 13 name: pdbs/split_chain/1A8G_A.pdb
pdb/seq: 14 name: pdbs/split_chain/204L_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 15 name: pdbs/split_chain/5COK_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 16 name: pdbs/split_chain/1TCX_A.pdb
pdb/seq: 17 name: pdbs/split_chain/2Z54_A.pdb
    PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 18 name: pdbs/split_chain/1D4S_A.pdb
pdb/seq: 19 name: pdbs/split_chain/1BV7_A.pdb
pdb/seq: 20 name: pdbs/split_chain/1BWA_A.pdb
pdb/seq: 21 name: pdbs/split_chain/1A9M_A.pdb
pdb/seq: 22 name: pdbs/split_chain/2FLE_A.pdb
pdb/seq: 23 name: pdbs/split_chain/1ODY_A.pdb
```

pdb/seq: 24 name: pdbs/split_chain/1GNN_A.pdb
pdb/seq: 25 name: pdbs/split_chain/1GNM_A.pdb
pdb/seq: 26 name: pdbs/split_chain/5YRS_B.pdb
pdb/seq: 27 name: pdbs/split_chain/5YRS_A.pdb
pdb/seq: 28 name: pdbs/split_chain/1HEF_E.pdb
pdb/seq: 29 name: pdbs/split_chain/10DX_A.pdb
pdb/seq: 30 name: pdbs/split_chain/4QGI_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 31 name: pdbs/split_chain/1BVE_A.pdb
pdb/seq: 32 name: pdbs/split_chain/2AZ8_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 33 name: pdbs/split_chain/1A30_A.pdb
pdb/seq: 34 name: pdbs/split_chain/6DH6_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 35 name: pdbs/split_chain/6DH0_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 36 name: pdbs/split_chain/2I4D_A.pdb
pdb/seq: 37 name: pdbs/split_chain/600S_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 38 name: pdbs/split_chain/1RL8_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 39 name: pdbs/split_chain/1ZSF_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 40 name: pdbs/split_chain/2Q64_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 41 name: pdbs/split_chain/6DH3_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 42 name: pdbs/split_chain/2NPH_A.pdb
pdb/seq: 43 name: pdbs/split_chain/2Q63_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 44 name: pdbs/split_chain/1LZQ_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 45 name: pdbs/split_chain/1FB7_A.pdb
pdb/seq: 46 name: pdbs/split_chain/1G6L_A.pdb
pdb/seq: 47 name: pdbs/split_chain/1HIV_A.pdb
pdb/seq: 48 name: pdbs/split_chain/600U_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 49 name: pdbs/split_chain/1HVC_A.pdb
pdb/seq: 50 name: pdbs/split_chain/2I4V_A.pdb
pdb/seq: 51 name: pdbs/split_chain/2AZ9_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 52 name: pdbs/split_chain/600T_A.pdb
pdb/seq: 53 name: pdbs/split_chain/2P3B_B.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 54 name: pdbs/split_chain/5KAO_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 55 name: pdbs/split_chain/2WL0_A.pdb
pdb/seq: 56 name: pdbs/split_chain/6OPT_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 57 name: pdbs/split_chain/1IZI_A.pdb
pdb/seq: 58 name: pdbs/split_chain/1MRX_A.pdb

pdb/seq: 59 name: pdbs/split_chain/2PYM_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 60 name: pdbs/split_chain/2PYN_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 61 name: pdbs/split_chain/1DMP_A.pdb
pdb/seq: 62 name: pdbs/split_chain/4K4P_A.pdb
pdb/seq: 63 name: pdbs/split_chain/1LV1_A.pdb
pdb/seq: 64 name: pdbs/split_chain/1AID_A.pdb
pdb/seq: 65 name: pdbs/split_chain/1ZBG_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 66 name: pdbs/split_chain/3TKG_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 67 name: pdbs/split_chain/5YOK_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 68 name: pdbs/split_chain/1FGC_C.pdb
pdb/seq: 69 name: pdbs/split_chain/3K4V_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 70 name: pdbs/split_chain/3KT5_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 71 name: pdbs/split_chain/4QLH_A.pdb
pdb/seq: 72 name: pdbs/split_chain/2F3K_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 73 name: pdbs/split_chain/4Q5M_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 74 name: pdbs/split_chain/2AOC_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 75 name: pdbs/split_chain/3B80_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 76 name: pdbs/split_chain/3VF5_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 77 name: pdbs/split_chain/2AVQ_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 78 name: pdbs/split_chain/1DW6_C.pdb
pdb/seq: 79 name: pdbs/split_chain/1KZK_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 80 name: pdbs/split_chain/2HS1_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 81 name: pdbs/split_chain/1K6C_A.pdb
PDB has ALT records, taking 1 only, rm.alt=TRUE
pdb/seq: 82 name: pdbs/split_chain/1MTB_A.pdb
pdb/seq: 83 name: pdbs/split_chain/4Q1X_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 84 name: pdbs/split_chain/4Q1W_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 85 name: pdbs/split_chain/3D1X_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 86 name: pdbs/split_chain/2AVM_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 87 name: pdbs/split_chain/3PWM_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 88 name: pdbs/split_chain/3KT2_A.pdb

```

PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 89 name: pdbs/split_chain/1SDV_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 90 name: pdbs/split_chain/3JW_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 91 name: pdbs/split_chain/3OY4_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE
pdb/seq: 92 name: pdbs/split_chain/1A94_A.pdb
pdb/seq: 93 name: pdbs/split_chain/2HS2_A.pdb
PDB has ALT records, taking A only, rm.alt=TRUE

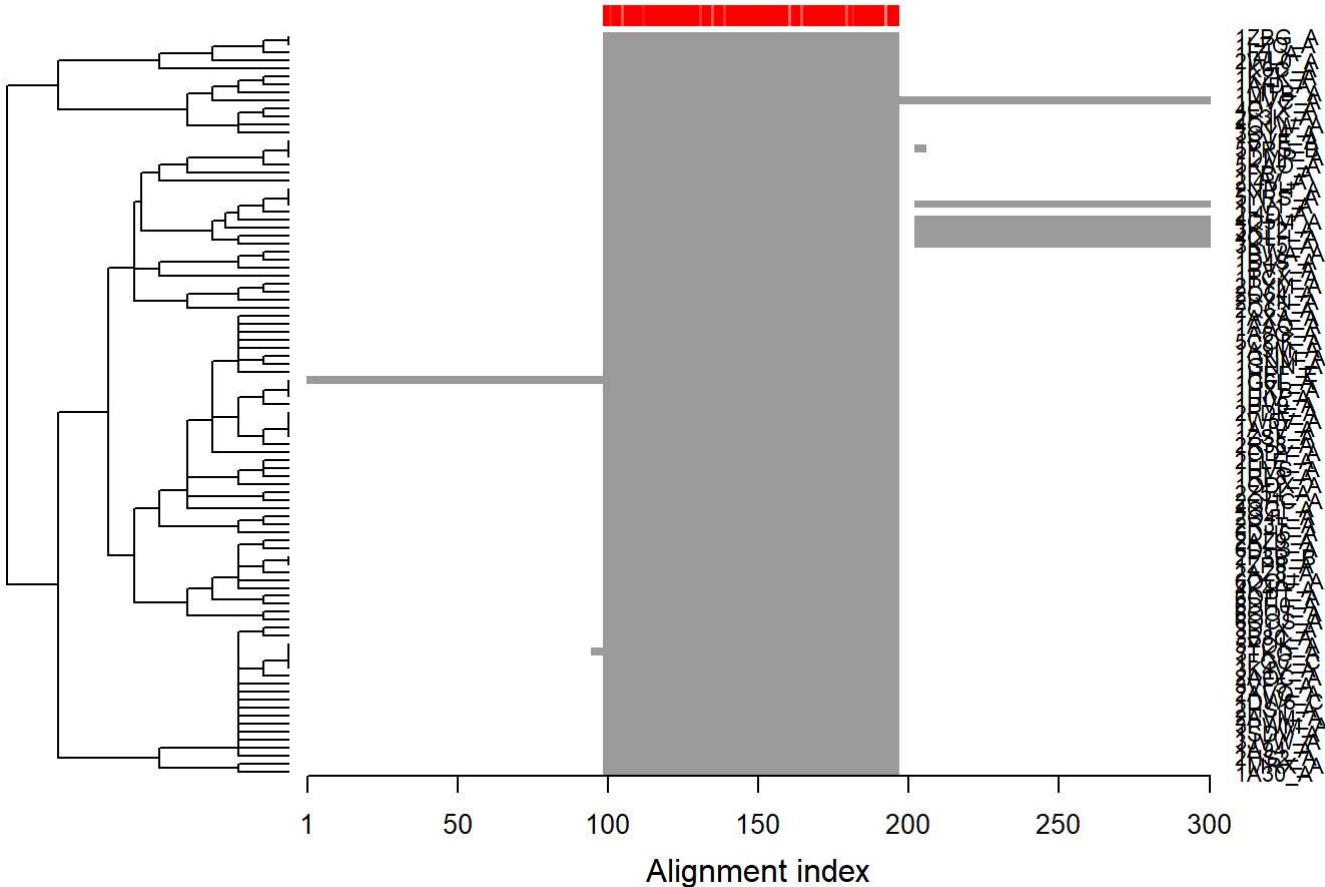
```

```

ids <- basename.pdb(pdbs$id)
plot(pdbs, labels=ids)

```

Sequence Alignment Overview



The function `pdb.annotate()` provides a convenient way of annotating the PDB files we have collected. Below we use the function to annotate each structure to its source species. This will come in handy when annotating plots later on:

```

anno <- pdb.annotate(ids)
unique(anno$source)

```

```

[1] "Human immunodeficiency virus"
[2] "Human immunodeficiency virus 1"

```

- [3] "Human immunodeficiency virus type 1 (CLONE 12)"
- [4] "Human immunodeficiency virus type 1 (BH5 ISOLATE)"
- [5] "HIV-1 M:B_HXB2R"
- [6] "Human immunodeficiency virus type 1 lw12.3 isolate"
- [7] "Human immunodeficiency virus type 1 (Z2/CDC-Z34 ISOLATE)"
- [8] "Human immunodeficiency virus type 1 (BRU ISOLATE)"
- [9] "Human immunodeficiency virus type 1 BH10"
- [10] "Human immunodeficiency virus 1/synthetic construct"
- [11] "NA/Human immunodeficiency virus type 1 group M subtype B (isolate BH5)"
- [12] "HIV-1 M:B_ARV2/SF2"

anno

	structureId	chainId	macromoleculeType	chainLength	experimentalTechnique
1W5V_A	1W5V	A	Protein	110	X-ray
2FDE_A	2FDE	A	Protein	100	X-ray
1AJV_A	1AJV	A	Protein	99	X-ray
2R38_A	2R38	A	Protein	99	X-ray
2R3T_A	2R3T	A	Protein	99	X-ray
1HXB_A	1HXB	A	Protein	99	X-ray
1BV9_A	1BV9	A	Protein	99	X-ray
1AAQ_A	1AAQ	A	Protein	99	X-ray
1AXA_A	1AXA	A	Protein	99	X-ray
1HVS_A	1HVS	A	Protein	99	X-ray
1ZP8_A	1ZP8	A	Protein	99	X-ray
2QHC_A	2QHC	A	Protein	99	X-ray
1A8G_A	1A8G	A	Protein	99	X-ray
204L_A	204L	A	Protein	99	X-ray
5COK_A	5COK	A	Protein	99	X-ray
1TCX_A	1TCX	A	Protein	99	X-ray
2Z54_A	2Z54	A	Protein	99	X-ray
1D4S_A	1D4S	A	Protein	99	X-ray
1BV7_A	1BV7	A	Protein	99	X-ray
1BWA_A	1BWA	A	Protein	99	X-ray
1A9M_A	1A9M	A	Protein	99	X-ray
2FLE_A	2FLE	A	Protein	99	X-ray
1ODY_A	1ODY	A	Protein	99	X-ray
1GNN_A	1GNN	A	Protein	99	X-ray
1GNM_A	1GNM	A	Protein	99	X-ray
5YRS_B	5YRS	B	Protein	104	X-ray
5YRS_A	5YRS	A	Protein	104	X-ray
1HEF_E	1HEF	E	Protein	99	X-ray
10DX_A	10DX	A	Protein	99	X-ray
4QGI_A	4QGI	A	Protein	99	X-ray
1BVE_A	1BVE	A	Protein	99	NMR
2AZ8_A	2AZ8	A	Protein	99	X-ray
1A30_A	1A30	A	Protein	99	X-ray
6DH6_A	6DH6	A	Protein	99	X-ray
6DH0_A	6DH0	A	Protein	99	X-ray
2I4D_A	2I4D	A	Protein	99	X-ray

600S_A	600S	A	Protein	99	X-ray
1RL8_A	1RL8	A	Protein	99	X-ray
1ZSF_A	1ZSF	A	Protein	99	X-ray
2Q64_A	2Q64	A	Protein	99	X-ray
6DH3_A	6DH3	A	Protein	99	X-ray
2NPH_A	2NPH	A	Protein	99	X-ray
2Q63_A	2Q63	A	Protein	99	X-ray
1LZQ_A	1LZQ	A	Protein	99	X-ray
1FB7_A	1FB7	A	Protein	99	X-ray
1G6L_A	1G6L	A	Protein	203	X-ray
1HIV_A	1HIV	A	Protein	99	X-ray
600U_A	600U	A	Protein	99	X-ray
1HVC_A	1HVC	A	Protein	203	X-ray
2I4V_A	2I4V	A	Protein	99	X-ray
2AZ9_A	2AZ9	A	Protein	99	X-ray
600T_A	600T	A	Protein	99	X-ray
2P3B_B	2P3B	B	Protein	99	X-ray
5KAO_A	5KAO	A	Protein	99	X-ray
2WL0_A	2WL0	A	Protein	99	X-ray
6OPT_A	6OPT	A	Protein	99	X-ray
1IZI_A	1IZI	A	Protein	99	X-ray
1MRX_A	1MRX	A	Protein	99	X-ray
2PYM_A	2PYM	A	Protein	99	X-ray
2PYN_A	2PYN	A	Protein	99	X-ray
1DMP_A	1DMP	A	Protein	99	X-ray
4K4P_A	4K4P	A	Protein	99	X-ray
1LV1_A	1LV1	A	Protein	203	X-ray
1AID_A	1AID	A	Protein	99	X-ray
1ZBG_A	1ZBG	A	Protein	99	X-ray
3TKG_A	3TKG	A	Protein	103	X-ray
5YOK_A	5YOK	A	Protein	100	X-ray
1FGC_C	1FGC	C	Protein	99	X-ray
3K4V_A	3K4V	A	Protein	100	X-ray
3KT5_A	3KT5	A	Protein	203	X-ray
4QLH_A	4QLH	A	Protein	203	X-ray
2F3K_A	2F3K	A	Protein	99	X-ray
4Q5M_A	4Q5M	A	Protein	203	X-ray
2AOC_A	2AOC	A	Protein	99	X-ray
3B80_A	3B80	A	Protein	99	X-ray
3VF5_A	3VF5	A	Protein	99	X-ray
2AVQ_A	2AVQ	A	Protein	99	X-ray
1DW6_C	1DW6	C	Protein	99	X-ray
1KZK_A	1KZK	A	Protein	99	X-ray
2HS1_A	2HS1	A	Protein	99	X-ray
1K6C_A	1K6C	A	Protein	99	X-ray
1MTB_A	1MTB	A	Protein	99	X-ray
4Q1X_A	4Q1X	A	Protein	99	X-ray
4Q1W_A	4Q1W	A	Protein	99	X-ray
3D1X_A	3D1X	A	Protein	99	X-ray
2AVM_A	2AVM	A	Protein	99	X-ray
3PWM_A	3PWM	A	Protein	99	X-ray

3KT2_A	3KT2	A	Protein	203	X-ray
1SDV_A	1SDV	A	Protein	99	X-ray
3JVW_A	3JVW	A	Protein	99	X-ray
3OY4_A	3OY4	A	Protein	99	X-ray
1A94_A	1A94	A	Protein	99	X-ray
2HS2_A	2HS2	A	Protein	99	X-ray
resolution		scopDomain			
1W5V_A	1.800	Human immunodeficiency virus type 1 protease			
2FDE_A	2.700	Human immunodeficiency virus type 1 protease			
1AJV_A	2.000	Human immunodeficiency virus type 1 protease			
2R38_A	1.810	Human immunodeficiency virus type 1 protease			
2R3T_A	1.800	Human immunodeficiency virus type 1 protease			
1HXB_A	2.300	Human immunodeficiency virus type 1 protease			
1BV9_A	2.000	Human immunodeficiency virus type 1 protease			
1AAQ_A	2.500	Human immunodeficiency virus type 1 protease			
1AXA_A	2.000	Human immunodeficiency virus type 1 protease			
1HVS_A	2.250	Human immunodeficiency virus type 1 protease			
1ZP8_A	2.020	Human immunodeficiency virus type 1 protease			
2QHC_A	2.802	Human immunodeficiency virus type 1 protease			
1A8G_A	2.500	Human immunodeficiency virus type 1 protease			
204L_A	1.330	Human immunodeficiency virus type 1 protease			
5COK_A	1.801	Human immunodeficiency virus type 1 protease			
1TCX_A	2.300	Human immunodeficiency virus type 1 protease			
2Z54_A	2.310	Human immunodeficiency virus type 1 protease			
1D4S_A	2.500	Human immunodeficiency virus type 1 protease			
1BV7_A	2.000	Human immunodeficiency virus type 1 protease			
1BWA_A	1.900	Human immunodeficiency virus type 1 protease			
1A9M_A	2.300	Human immunodeficiency virus type 1 protease			
2FLE_A	1.900		automated matches		
1ODY_A	2.000	Human immunodeficiency virus type 1 protease			
1GNN_A	2.300	Human immunodeficiency virus type 1 protease			
1GNM_A	2.300	Human immunodeficiency virus type 1 protease			
5YRS_B	1.760		<NA>		
5YRS_A	1.760		<NA>		
1HEF_E	2.200	Human immunodeficiency virus type 1 protease			
10DX_A	2.000	Human immunodeficiency virus type 1 protease			
4QGI_A	1.896	Human immunodeficiency virus type 1 protease			
1BVE_A	NA	Human immunodeficiency virus type 1 protease			
2AZ8_A	2.000	Human immunodeficiency virus type 1 protease			
1A30_A	2.000	Human immunodeficiency virus type 1 protease			
6DH6_A	1.970	Human immunodeficiency virus type 1 protease			
6DH0_A	1.899	Human immunodeficiency virus type 1 protease			
2I4D_A	1.500	Human immunodeficiency virus type 1 protease			
600S_A	1.900	Human immunodeficiency virus type 1 protease			
1RL8_A	2.000	Human immunodeficiency virus type 1 protease			
1ZSF_A	1.980	Human immunodeficiency virus type 1 protease			
2Q64_A	2.500	Human immunodeficiency virus type 1 protease			
6DH3_A	1.908	Human immunodeficiency virus type 1 protease			
2NPH_A	1.650	Human immunodeficiency virus type 1 protease			
2Q63_A	2.200	Human immunodeficiency virus type 1 protease			
1LZQ_A	2.200	Human immunodeficiency virus type 1 protease			

		pfam	ligandId
1FB7_A	2.600 Human immunodeficiency virus type 1 protease		
1G6L_A	1.900 Human immunodeficiency virus type 1 protease		
1HIV_A	2.000 Human immunodeficiency virus type 1 protease		
600U_A	2.127 Human immunodeficiency virus type 1 protease		
1HVC_A	1.800 Human immunodeficiency virus type 1 protease		
2I4V_A	1.500 Human immunodeficiency virus type 1 protease		
2AZ9_A	2.500 Human immunodeficiency virus type 1 protease		
600T_A	1.822 Human immunodeficiency virus type 1 protease		
2P3B_B	2.100 Human immunodeficiency virus type 1 protease		
5KAO_A	1.800 Human immunodeficiency virus type 1 protease		
2WL0_A	1.900 automated matches		
6OPT_A	1.960 Human immunodeficiency virus type 1 protease		
1IZI_A	2.150 Human immunodeficiency virus type 1 protease		
1MRX_A	2.000 Human immunodeficiency virus type 1 protease		
2PYM_A	1.900 Human immunodeficiency virus type 1 protease		
2PYN_A	1.850 Human immunodeficiency virus type 1 protease		
1DMP_A	2.000 Human immunodeficiency virus type 1 protease		
4K4P_A	2.310 Human immunodeficiency virus type 1 protease		
1LV1_A	2.100 Human immunodeficiency virus type 1 protease		
1AID_A	2.200 Human immunodeficiency virus type 1 protease		
1ZBG_A	1.995 Human immunodeficiency virus type 1 protease		
3TKG_A	1.360 Human immunodeficiency virus type 1 protease		
5YOK_A	0.850 Human immunodeficiency virus type 1 protease		
1FGC_C	1.900 Human immunodeficiency virus type 1 protease		
3K4V_A	1.390 Human immunodeficiency virus type 1 protease		
3KT5_A	1.801 Human immunodeficiency virus type 1 protease		
4QLH_A	2.450 <NA>		
2F3K_A	1.599 automated matches		
4Q5M_A	1.795 Human immunodeficiency virus type 1 protease		
2AOC_A	1.300 Human immunodeficiency virus type 1 protease		
3B80_A	1.500 Human immunodeficiency virus type 1 protease		
3VF5_A	1.250 Human immunodeficiency virus type 1 protease		
2AVQ_A	1.300 Human immunodeficiency virus type 1 protease		
1DW6_C	1.880 Human immunodeficiency virus type 1 protease		
1KZK_A	1.090 Human immunodeficiency virus type 1 protease		
2HS1_A	0.840 Human immunodeficiency virus type 1 protease		
1K6C_A	2.200 Human immunodeficiency virus type 1 protease		
1MTB_A	2.500 Human immunodeficiency virus type 1 protease		
4Q1X_A	1.900 Human immunodeficiency virus type 1 protease		
4Q1W_A	1.850 Human immunodeficiency virus type 1 protease		
3D1X_A	1.050 Human immunodeficiency virus type 1 protease		
2AVM_A	1.100 Human immunodeficiency virus type 1 protease		
3PWM_A	1.460 Human immunodeficiency virus type 1 protease		
3KT2_A	1.651 Human immunodeficiency virus type 1 protease		
1SDV_A	1.400 Human immunodeficiency virus type 1 protease		
3JVW_A	1.800 automated matches		
3OY4_A	1.760 Human immunodeficiency virus type 1 protease		
1A94_A	2.000 Human immunodeficiency virus type 1 protease		
2HS2_A	1.220 Human immunodeficiency virus type 1 protease		
1W5V_A	Retroviral aspartyl protease (RVP)		BE3

2FDE_A	Retroviral aspartyl protease (RVP)	K (2),385
1AJV_A	Retroviral aspartyl protease (RVP)	NMB
2R38_A	Retroviral aspartyl protease (RVP)	<NA>
2R3T_A	Retroviral aspartyl protease (RVP)	<NA>
1HXB_A	Retroviral aspartyl protease (RVP)	ROC
1BV9_A	Retroviral aspartyl protease (RVP)	XV6
1AAQ_A	Retroviral aspartyl protease (RVP)	<NA>
1AXA_A	Retroviral aspartyl protease (RVP)	U0E (2)
1HVS_A	Retroviral aspartyl protease (RVP)	A77
1ZP8_A	Retroviral aspartyl protease (RVP)	AB2
2QHC_A	Retroviral aspartyl protease (RVP)	BME
1A8G_A	Retroviral aspartyl protease (RVP)	2Z4
204L_A	Retroviral aspartyl protease (RVP)	CL,TPV,GOL
5COK_A	Retroviral aspartyl protease (RVP)	52U
1TCX_A	Retroviral aspartyl protease (RVP)	IM1
2Z54_A	Retroviral aspartyl protease (RVP)	BME,AB1
1D4S_A	Retroviral aspartyl protease (RVP)	TPV
1BV7_A	Retroviral aspartyl protease (RVP)	XV6
1BWA_A	Retroviral aspartyl protease (RVP)	<NA>
1A9M_A	Retroviral aspartyl protease (RVP)	<NA>
2FLE_A	Retroviral aspartyl protease (RVP)	GOL
10DY_A	Retroviral aspartyl protease (RVP)	LP1
1GNN_A	Retroviral aspartyl protease (RVP)	U0E (2)
1GNM_A	Retroviral aspartyl protease (RVP)	U0E (2)
5YRS_B	Retroviral aspartyl protease (RVP)	<NA>
5YRS_A	Retroviral aspartyl protease (RVP)	<NA>
1HEF_E	Retroviral aspartyl protease (RVP)	<NA>
10DX_A	Retroviral aspartyl protease (RVP)	0E8
4QGI_A	Retroviral aspartyl protease (RVP)	ROC,GOL
1BVE_A	Retroviral aspartyl protease (RVP)	<NA>
2AZ8_A	Retroviral aspartyl protease (RVP)	3TL
1A30_A	Retroviral aspartyl protease (RVP)	<NA>
6DH6_A	Retroviral aspartyl protease (RVP)	S04 (3),017
6DH0_A	Retroviral aspartyl protease (RVP)	017
2I4D_A	Retroviral aspartyl protease (RVP)	<NA>
600S_A	Retroviral aspartyl protease (RVP)	S04 (4),017
1RL8_A	Retroviral aspartyl protease (RVP)	RIT
1ZSF_A	Retroviral aspartyl protease (RVP)	<NA>
2Q64_A	Retroviral aspartyl protease (RVP)	<NA>
6DH3_A	Retroviral aspartyl protease (RVP)	017,S04 (2)
2NPH_A	Retroviral aspartyl protease (RVP)	<NA>
2Q63_A	Retroviral aspartyl protease (RVP)	1UN
1LZQ_A	Retroviral aspartyl protease (RVP)	0ZQ,BME
1FB7_A	Retroviral aspartyl protease (RVP)	ROC
1G6L_A	Retroviral aspartyl protease (RVP)	<NA>
1HIV_A	Retroviral aspartyl protease (RVP)	1ZK
600U_A	Retroviral aspartyl protease (RVP)	017,S04 (2)
1HVC_A	Retroviral aspartyl protease (RVP)	A79
2I4V_A	Retroviral aspartyl protease (RVP)	<NA>
2AZ9_A	Retroviral aspartyl protease (RVP)	3TL
600T_A	Retroviral aspartyl protease (RVP)	S04

2P3B_B	Retroviral aspartyl protease (RVP)	<NA>
5KAO_A	Retroviral aspartyl protease (RVP)	G43
2WL0_A	Retroviral aspartyl protease (RVP)	5AH
6OPT_A	Retroviral aspartyl protease (RVP)	017, S04 (2)
1IZI_A	Retroviral aspartyl protease (RVP)	CL
1MRX_A	Retroviral aspartyl protease (RVP)	<NA>
2PYM_A	Retroviral aspartyl protease (RVP)	1UN
2PYN_A	Retroviral aspartyl protease (RVP)	1UN
1DMP_A	Retroviral aspartyl protease (RVP)	<NA>
4K4P_A	Retroviral aspartyl protease (RVP)	N03
1LV1_A	Retroviral aspartyl protease (RVP)	<NA>
1AID_A	Retroviral aspartyl protease (RVP)	<NA>
1ZBG_A	Retroviral aspartyl protease (RVP)	CL (2)
3TKG_A	Retroviral aspartyl protease (RVP)	CL, GOL
5YOK_A	Retroviral aspartyl protease (RVP)	8Z0
1FGC_C	Retroviral aspartyl protease (RVP)	2NC
3K4V_A	Retroviral aspartyl protease (RVP)	DMS (2)
3KT5_A	Retroviral aspartyl protease (RVP)	<NA>
4QLH_A	Retroviral aspartyl protease (RVP)	<NA>
2F3K_A	Retroviral aspartyl protease (RVP)	P04 (3), R01
4Q5M_A	Retroviral aspartyl protease (RVP)	ROC
2AOC_A	Retroviral aspartyl protease (RVP)	UNX, NA, CL, DMS (3), GOL
3B80_A	Retroviral aspartyl protease (RVP)	NA, CL
3VF5_A	Retroviral aspartyl protease (RVP)	NA, CL (2), ACT (2)
2AVQ_A	Retroviral aspartyl protease (RVP)	DMS, GOL
1DW6_C	Retroviral aspartyl protease (RVP)	<NA>
1KZK_A	Retroviral aspartyl protease (RVP)	JE2, CL (2), EDO (4)
2HS1_A	Retroviral aspartyl protease (RVP)	CL (3), 017
1K6C_A	Retroviral aspartyl protease (RVP)	ACT (2)
1MTB_A	Retroviral aspartyl protease (RVP)	ROC
4Q1X_A	Retroviral aspartyl protease (RVP)	017, GOL
4Q1W_A	Retroviral aspartyl protease (RVP)	P04 (3), 017
3D1X_A	Retroviral aspartyl protease (RVP)	CL, ROC, GOL
2AVM_A	Retroviral aspartyl protease (RVP)	GOL
3PWM_A	Retroviral aspartyl protease (RVP)	CL, ACT (2), NA
3KT2_A	Retroviral aspartyl protease (RVP)	<NA>
1SDV_A	Retroviral aspartyl protease (RVP)	CL
3JWV_A	Retroviral aspartyl protease (RVP)	DMP
3OY4_A	Retroviral aspartyl protease (RVP)	P04 (2), ACT (3)
1A94_A	Retroviral aspartyl protease (RVP)	0Q4
2HS2_A	Retroviral aspartyl protease (RVP)	CL (2), 017

ligandName

1W5V_A

N,N-[2,5-O-DI-3-FLUORO-BENZYL-GLUCARYL]-DI-[1-AMINO-INDAN-2-OL]

2FDE_A POTASSIUM ION (2), (3R, 3AS, 6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL
[(1S, 2R)-3-[(1, 3-BENZODIOXOL-5-YLSULFONYL)(ISOBUTYL)AMINO]-2-HYDROXY-1-{4-[(2-METHYL-1, 3-THIAZOL-4-YL)METHOXY]BENZYL}PROPYL]CARBAMATE

1AJV_A

2,7-DIBENZYL-1,1-DIOXO-3,6-BIS-PHENOXYMETHYL-[1,2,7]THIADIAZEPANE-4,5-DIOL

2R38_A

<NA>
2R3T_A
<NA>
1HXB_A (2S)-N-[(2S,3R)-4-[(2S,3S,4aS,8aS)-3-(tert-butylcarbamoyl)-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinolin-2-yl]-3-hydroxy-1\>n-phenyl-butan-2-yl]-2-(quinolin-2-ylcarbonylamino)butanediamide
1BV9_A [4R-[
(4ALPHA,5ALPHA,6BETA,7BETA)]-3,3'-[[TETRAHYDRO-5,6-DIHYDROXY-2-OXO-4,7-BIS(PHENYLMETHYL)-1H-1,3-DIAZEPINE-1,3(2H)-D\>nIYL] BIS(METHYLENE)]BIS[N-2-TIAZOLYLBENZAMIDE]
1AAQ_A
<NA>
1AXA_A N-[[1-[N-ACETAMIDYL]-[1-CYCLOHEXYL METHYL-2-HYDROXY-4-ISOPROPYL]-BUT-4-YL]-CARBONYL]-GLUTAMINYL-ARGINYL-AMIDE (2)
1HVS_A N-{1-BENZYL-(2R,3S)-2,3-DIHYDROXY-4-[3-METHYL-2-(3-METHYL-3-PYRIDIN-2-YLMETHYL-UREIDO)-BUTYRYLAMINO]-5-PHENYL-PENTYL}-3-METHYL-2-(3-METHYL-3-PYRIDIN-2-YLMETHYL-UREIDO)-BUTYRAMIDE
1ZP8_A [1-((1S,2R)-1-BENZYL-2-HYDROXY-3-{ISOBUTYL[(4-METHOXYPHENYL)SULFONYL]AMINO}PROPYL)-1H-1,2,3-TRIAZOL-4-YL]METHYL (1R,2R)-2-HYDROXY-2,3-DIHYDRO-1H-INDEN-1-YLCARBAMATE
2QHC_A
BETA-MERCAPTOETHANOL
1A8G_A benzyl [(1R)-1-({(1S,2S,3S)-1-benzyl-2-hydroxy-4-[(1S)-1-[(2-hydroxy-4-methoxybenzyl)carbamoyl]-2-methylpropyl]amino)-3-[(4-methoxybenzyl)amino]-4-oxobutyl}carbamoyl)-2,2-dimethylpropyl]carbamate
204L_A CHLORIDE ION,N-(3-{(1R)-1-[(6R)-4-HYDROXY-2-OXO-6-PHENETHYL-6-PROPYL-5,6-DIHYDRO-2H-PYRAN-3-YL]PROPYL}PHENYL)-5-(TRIFLUOROMETHYL)-2-PYRIDINESULFONAMIDE, GLYCEROL
5COK_A (3aS,4S,7aR)-hexahydro-4H-furo[2,3-b]pyran-4-yl\>n[(2S,3R)-3-hydroxy-4-{{(4-methoxyphenyl)sulfonyl}(2-methylpropyl)amino}-1-phenylbutan-2-yl]carbamate
1TCX_A (2R,4S,5S,1'S)-2-PHENYLMETHYL-4-HYDROXY-5-(TERT-BUTOXYCARBONYL)AMINO-6-PHENYL HEXANOYL-N-(1'-IMIDAZO-2-YL)-2'-METHYLPROPANAMIDE
2Z54_A BETA-MERCAPTOETHANOL,N-{1-BENZYL-4-[2-(2,6-DIMETHYL-PHOXY)-ACETYLAMINO]-3-HYDROXY-5-PHENYL-PENTYL}-3-METHYL-2-(2-OXO-TETRAHYDRO-PYRIMIDIN-1-YL)-BUTYRAMIDE
1D4S_A N-(3-{(1R)-1-[(6R)-4-HYDROXY-2-OXO-6-PHENETHYL-6-PROPYL-5,6-DIHYDRO-2H-PYRAN-3-YL]PROPYL}PHENYL)-5-(TRIFLUOROMETHYL)-2-PYRIDINESULFONAMIDE
1BV7_A [4R-[
(4ALPHA,5ALPHA,6BETA,7BETA)]-3,3'-[[TETRAHYDRO-5,6-DIHYDROXY-2-OXO-4,7-BIS(PHENYLMETHYL)-1H-1,3-DIAZEPINE-1,3(2H)-D\>nIYL] BIS(METHYLENE)]BIS[N-2-TIAZOLYLBENZAMIDE]
1BWA_A
<NA>
1A9M_A
<NA>
2FLE_A
GLYCEROL
1ODY_A 4-[2-(2-ACETYLAMINO-3-NAPHTALEN-1-YL-PROPIONYLAMINO)-4-METHYL-PENTANOYLAMINO]-3-HYDROXY-6-METHYL-HEPTANOIC ACID [1-(1-CARBAMOYL-2-

NAPHTHALEN-1-YL-ETHYLCARBAMOYL)-PROPYL]-AMIDE

1GNN_A

N-[[1-[N-ACETAMIDYL]-[1-CYCLOHEXYLMETHYL-2-HYDROXY-4-ISOPROPYL]-BUT-4-YL]-CARBONYL]-GLUTAMINYL-
ARGINYL-AMIDE (2)

1GNM_A

N-[[1-[N-ACETAMIDYL]-[1-CYCLOHEXYLMETHYL-2-HYDROXY-4-ISOPROPYL]-BUT-4-YL]-CARBONYL]-GLUTAMINYL-
ARGINYL-AMIDE (2)

5YRS_B

<NA>

5YRS_A

<NA>

1HEF_E

<NA>

10DX_A

di-tert-butyl {iminobis[(2S,3S)-3-hydroxy-1-phenylbutane-4,2-diyl]}biscarbamate

4QGI_A (2S)-N-[(2S,3R)-4-[(2S,3S,4aS,8aS)-3-(tert-
butylcarbamoyl)-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinolin-2-yl]-3-hydroxy-1\&n-phenyl-butan-2-
yl]-2-(quinolin-2-ylcarbonylamino)butanediamide, GLYCEROL

1BVE_A

<NA>

2AZ8_A

benzyl [(1S,4S,7S,8R,9R,10S,13S,16S)-7,10-

dibenzyl-8,9-dihydroxy-1,16-dimethyl-4,13-bis(1-methylethyl)-2,5,12,15,18-pentaoxo-20-phenyl-19-
oxa-3,6,11,14,17-pentaazaicos-1-yl]carbamate

1A30_A

<NA>

6DH6_A

SULFATE ION

(3),(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL]
(ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE

6DH0_A

(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL]

(ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE

2I4D_A

<NA>

600S_A

SULFATE ION

(4),(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL]
(ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE

1RL8_A

RITONAVIR

1ZSF_A

<NA>

2Q64_A

<NA>

6DH3_A

(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL]
(ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE, SULFATE ION (2)

2NPH_A

<NA>

2Q63_A

2-[2-HYDROXY-3-(3-HYDROXY-2-METHYL-BENZOYLAMINO)-4-PHENYL SULFANYL-BUTYL]-DECAHYDRO-ISOQUINOLINE-
3-CARBOXYLIC ACID TERT-BUTYLAMIDE

1LZQ_A

N-{(3S)-3-[(tert-butoxycarbonyl)amino]-4-phenylbutyl}-L-phenylalanyl-L-alpha-glutamyl-L-phenylalaninamide, BETA-MERCAPTOETHANOL

1FB7_A (2S)-N-[(2S,3R)-4-[(2S,3S,4aS,8aS)-3-(tert-butylcarbamoyl)-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinolin-2-yl]-3-hydroxy-1\|n-phenyl-butan-2-yl]-2-(quinolin-2-ylcarbonylamino)butanediamide

1G6L_A

<NA>

1HIV_A 4-[(2R)-3-{{[(1S,2S,3R,4S)-1-(cyclohexylmethyl)-2,3-dihydroxy-5-methyl-4-((1S,2R)-2-methyl-1-[(pyridin-2-ylmethyl)carba\|nmoyle]butyl)carbamoyl]hexyl}amino}-2-[(naphthalen-1-yloxy)acetyl]amino}-3-oxopropyl]-1H-imidazol-3-ium

600U_A

(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL](ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE, SULFATE ION (2)

1HVC_A N-{1-BENZYL-(2S,3S)-2,3-DIHYDROXY-4-[3-METHYL-2-(3-METHYL-3-PYRIDIN-2-YLMETHYL-UREIDO)-BUTYRYLAMINO]-5-PHENYL-PENTYL}-3-METHYL-2-(3-METHYL-3-PYRIDIN-2-YLMETHYL-UREIDO)-BUTYRAMIDE

2I4V_A

<NA>

2AZ9_A benzyl [(1S,4S,7S,8R,9R,10S,13S,16S)-7,10-dibenzyl-8,9-dihydroxy-1,16-dimethyl-4,13-bis(1-methylethyl)-2,5,12,15,18-pentaoxo-20-phenyl-19-oxa-3,6,11,14,17-pentaazaicos-1-yl]carbamate

600T_A

SULFATE ION

2P3B_B

<NA>

5KAO_A [(3~{a}~{S},4~{R},6~{a}~{R})-2,3,3~{a},4,5,6~{a}-hexahydrofuro[2,3-b]furan-4-yl] ~{N}-[(2~{S},3~{R})-1-(3-chloranyl-4-methoxy-phenyl)-4-[(4-methoxyphenyl)sulfonyl-(2-methylpropyl)amino]-3-oxidanyl-butan-2-yl]carbamate

2WL0_A METHYL [(1S)-1-({2-[(3S)-3-BENZYL-3-HYDROXY-4-[(1S,2R)-2-HYDROXY-2,3-DIHYDRO-1H-INDEN-1-YL]AMINO}-4-OXOBUTYL)-2-(4-PYRIDIN-2-YLBENZYL)HYDRAZINO]CARBONYL)-2,2-DIMETHYLPROPYL]CARBAMATE

6OPT_A

(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL](ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE, SULFATE ION (2)

1IZI_A

CHLORIDE ION

1MRX_A

<NA>

2PYM_A

2-[2-HYDROXY-3-(3-HYDROXY-2-METHYL-BENZOYLAMINO)-4-PHENYL SULFANYL-BUTYL]-DECAHYDRO-ISOQUINOLINE-3-CARBOXYLIC ACID TERT-BUTYLAMIDE

2PYN_A

2-[2-HYDROXY-3-(3-HYDROXY-2-METHYL-BENZOYLAMINO)-4-PHENYL SULFANYL-BUTYL]-DECAHYDRO-ISOQUINOLINE-3-CARBOXYLIC ACID TERT-BUTYLAMIDE

1DMP_A

<NA>

4K4P_A

NITRATE ION

1LV1_A

<NA>

1AID_A

<NA>
1ZBG_A
CHLORIDE ION (2)
3TKG_A
CHLORIDE ION, GLYCEROL
5YOK_A (4R)-N-[(2,6-dimethylphenyl)methyl]-3-[(2S,3S)-3-[(2S)-2-[(7-methoxy-1-benzofuran-2-yl)carbonylamino]-2-[(3R)-oxolan-3\>n-yl]ethanoyl]amino]-2-oxidanyl-4-phenylbutanoyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxamide
1FGC_C
N-{(2S)-2-[(N-acetyl-L-threonyl-L-isoleucyl)amino]hexyl}-L-norleucyl-L-glutaminyl-N~5~-[amino(imino)methyl]-L-ornithinamide
3K4V_A
DIMETHYL SULFOXIDE (2)
3KT5_A
<NA>
4QLH_A
<NA>
2F3K_A PHOSPHATE ION (3), (3S,4AS,8AS)-N-(TERT-BUTYL)-2-[(3S)-3-({3-(METHYLSULFONYL)-N-[(PYRIDIN-3-YLOXY)ACETYL]-L-VALYL}AMINO)-2-OXO-4-PHENYLBUTYL]DECAHYDROISOQUINOLINE-3-CARBOXAMIDE
4Q5M_A (2S)-N-[(2S,3R)-4-[(2S,3S,4aS,8aS)-3-(tert-butylcarbamoyl)-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinolin-2-yl]-3-hydroxy-1\>n-phenyl-butan-2-yl]-2-(quinolin-2-ylcarbonylamino)butanediamide
2AOC_A
UNKNOWN ATOM OR ION, SODIUM ION, CHLORIDE ION, DIMETHYL SULFOXIDE (3), GLYCEROL
3B80_A
SODIUM ION, CHLORIDE ION
3VF5_A
SODIUM ION, CHLORIDE ION (2), ACETATE ION (2)
2AVQ_A
DIMETHYL SULFOXIDE, GLYCEROL
1DW6_C
<NA>
1KZK_A (4R)-3-[(2S,3S)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-phenylbutanoyl]-5,5-dimethyl-N-(2-methylbenzyl)-1,3-thiazolidine-4-carboxamide, CHLORIDE ION (2), 1,2-ETHANEDIOL (4)
2HS1_A CHLORIDE ION (3), (3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[(4-AMINOPHENYL)SULFONYL](ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE
1K6C_A
ACETATE ION (2)
1MTB_A (2S)-N-[(2S,3R)-4-[(2S,3S,4aS,8aS)-3-(tert-butylcarbamoyl)-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinolin-2-yl]-3-hydroxy-1\>n-phenyl-butan-2-yl]-2-(quinolin-2-ylcarbonylamino)butanediamide
4Q1X_A (3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[(4-AMINOPHENYL)SULFONYL](ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE, GLYCEROL
4Q1W_A PHOSPHATE ION (3), (3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[(4-AMINOPHENYL)SULFONYL](ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE
3D1X_A CHLORIDE ION, (2S)-N-[(2S,3R)-4-[(2S,3S,4aS,8aS)-3-(tert-

butylcarbamoyl)-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinolin-2-yl]-3-hydroxy-1\|n-phenyl-butan-2-yl]-2-(quinolin-2-ylcarbonylamino)butanediamide, GLYCEROL

2AVM_A

GLYCEROL

3PWM_A

CHLORIDE ION, ACETATE ION (2), SODIUM ION

3KT2_A

<NA>

1SDV_A

CHLORIDE ION

3JWV_A

[4-R-(-4-ALPHA,5-

ALPHA,6-BETA,7-BETA)]-HEXAHYDRO-5,6-BIS(HYDROXY)-[1,3-BIS([4-HYDROXYMETHYL-PHENYL]METHYL)-4,7-BIS(PHEN\|nYLMETHYL)]-2H-1,3-DIAZEPINONE

3OY4_A

PHOSPHATE ION (2), ACETATE ION (3)

1A94_A

N-

[(2R)-2-(\{N~5~- [amino(imino)methyl]-L-ornithyl-L-valyl}amino)-4-methylpentyl]-L-phenylalananyl-L-alpha-glutamyl-L-alanyl-L-norleucinamide

2HS2_A

CHLORIDE ION

(2),(3R,3AS,6AR)-HEXAHYDROFURO[2,3-B]FURAN-3-YL(1S,2R)-3-[[(4-AMINOPHENYL)SULFONYL](ISOBUTYL)AMINO]-1-BENZYL-2-HYDROXYPROPYLCARBAMATE

source

1W5V_A

Human immunodeficiency virus

2FDE_A

Human immunodeficiency virus 1

1AJV_A

Human immunodeficiency virus 1

2R38_A

Human immunodeficiency virus 1

2R3T_A

Human immunodeficiency virus 1

1HXB_A

Human immunodeficiency virus type 1 (CLONE 12)

1BV9_A

Human immunodeficiency virus 1

1AAQ_A

Human immunodeficiency virus 1

1AXA_A

Human immunodeficiency virus 1

1HVS_A

Human immunodeficiency virus 1

1ZP8_A

Human immunodeficiency virus 1

2QHC_A

Human immunodeficiency virus 1

1A8G_A

Human immunodeficiency virus 1

204L_A

Human immunodeficiency virus 1

5COK_A

Human immunodeficiency virus 1

1TCX_A

Human immunodeficiency virus 1

2Z54_A

Human immunodeficiency virus type 1 (BH5 ISOLATE)

1D4S_A

Human immunodeficiency virus 1

1BV7_A

Human immunodeficiency virus 1

1BWA_A

Human immunodeficiency virus 1

1A9M_A

Human immunodeficiency virus 1

2FLE_A

Human immunodeficiency virus 1

1ODY_A

HIV-1 M:B_HXB2R

1GNN_A

Human immunodeficiency virus 1

1GNM_A

Human immunodeficiency virus 1

5YRS_B

HIV-1 M:B_HXB2R

5YRS_A

HIV-1 M:B_HXB2R

1HEF_E

Human immunodeficiency virus 1

10DX_A

Human immunodeficiency virus 1

4QGI_A Human immunodeficiency virus type 1 lw12.3 isolate
1BVE_A Human immunodeficiency virus 1
2AZ8_A Human immunodeficiency virus 1
1A30_A Human immunodeficiency virus 1
6DH6_A Human immunodeficiency virus 1
6DH0_A Human immunodeficiency virus 1
2I4D_A Human immunodeficiency virus 1
600S_A Human immunodeficiency virus 1
1RL8_A Human immunodeficiency virus 1
1ZSF_A Human immunodeficiency virus 1
2Q64_A Human immunodeficiency virus 1
6DH3_A Human immunodeficiency virus 1
2NPH_A Human immunodeficiency virus 1
2Q63_A Human immunodeficiency virus 1
1LZQ_A Human immunodeficiency virus 1
1FB7_A Human immunodeficiency virus 1
1G6L_A Human immunodeficiency virus 1
1HIV_A Human immunodeficiency virus 1
600U_A Human immunodeficiency virus 1
1HVC_A Human immunodeficiency virus 1
2I4V_A Human immunodeficiency virus 1
2AZ9_A Human immunodeficiency virus 1
600T_A Human immunodeficiency virus 1
2P3B_B Human immunodeficiency virus 1
5KAO_A Human immunodeficiency virus 1
2WL0_A Human immunodeficiency virus type 1 (Z2/CDC-Z34 ISOLATE)
6OPT_A Human immunodeficiency virus 1
1IZI_A Human immunodeficiency virus 1
1MRX_A Human immunodeficiency virus 1
2PYM_A Human immunodeficiency virus 1
2PYN_A Human immunodeficiency virus 1
1DMP_A Human immunodeficiency virus 1
4K4P_A Human immunodeficiency virus type 1 (Z2/CDC-Z34 ISOLATE)
1LV1_A Human immunodeficiency virus 1
1AID_A Human immunodeficiency virus 1
1ZBG_A Human immunodeficiency virus 1
3TKG_A Human immunodeficiency virus type 1 (BRU ISOLATE)
5YOK_A Human immunodeficiency virus 1
1FGC_C Human immunodeficiency virus 1
3K4V_A Human immunodeficiency virus type 1 BH10
3KT5_A HIV-1 M:B_HXB2R
4QLH_A Human immunodeficiency virus 1/synthetic construct
2F3K_A Human immunodeficiency virus 1
4Q5M_A HIV-1 M:B_HXB2R
2AOC_A Human immunodeficiency virus type 1 (BH5 ISOLATE)
3B80_A Human immunodeficiency virus type 1 BH10
3VF5_A Human immunodeficiency virus type 1 (BRU ISOLATE)
2AVQ_A Human immunodeficiency virus type 1 (BH5 ISOLATE)
1DW6_C Human immunodeficiency virus 1
1KZK_A Human immunodeficiency virus 1
2HS1_A Human immunodeficiency virus 1

1K6C_A Human immunodeficiency virus 1
1MTB_A Human immunodeficiency virus 1
4Q1X_A Human immunodeficiency virus 1
4Q1W_A Human immunodeficiency virus 1
3D1X_A NA/Human immunodeficiency virus type 1 group M subtype B (isolate BH5)
2AVM_A Human immunodeficiency virus 1
3PWM_A Human immunodeficiency virus 1
3KT2_A HIV-1 M:B_HXB2R
1SDV_A Human immunodeficiency virus 1
3JWV_A Human immunodeficiency virus type 1 (BRU ISOLATE)
3OY4_A HIV-1 M:B_ARV2/SF2
1A94_A Human immunodeficiency virus 1
2HS2_A Human immunodeficiency virus 1

structureTitle
1W5V_A HIV-1 protease in complex with fluoro substituted diol-based C2-symmetric inhibitor
2FDE_A Wild type HIV protease bound with GW0385
1AJV_A HIV-1 PROTEASE IN COMPLEX WITH THE CYCLIC SULFAMIDE INHIBITOR AHA006
2R38_A I84V HIV-1 protease mutant in complex with a carbamoyl decorated pyrrolidine-based inhibitor
2R3T_A I50V HIV-1 protease mutant in complex with a carbamoyl decorated pyrrolidine-based inhibitor
1HXB_A HIV-1 proteinase complexed with RO 31-8959
1BV9_A HIV-1 PROTEASE (I84V) COMPLEXED WITH XV638 OF DUPONT PHARMACEUTICALS
1AAQ_A HYDROXYETHYLENE ISOSTERE INHIBITORS OF HUMAN IMMUNODEFICIENCY VIRUS-1 PROTEASE: STRUCTURE-ACTIVITY ANALYSIS USING ENZYME KINETICS, X-RAY CRYSTALLOGRAPHY, AND INFECTED T-CELL ASSAYS
1AXA_A ACTIVE-SITE MOBILITY IN HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 PROTEASE AS DEMONSTRATED BY CRYSTAL STRUCTURE OF A28S MUTANT
1HVS_A STRUCTURAL BASIS OF DRUG RESISTANCE FOR THE V82A MUTANT OF HIV-1 PROTEASE: BACKBONE FLEXIBILITY AND SUBSITE REPACKING
1ZP8_A HIV Protease with inhibitor AB-2
2QHC_A The Influence of I47A Mutation on Reduced Susceptibility to the Protease Inhibitor Lopinavir
1A8G_A HIV-1 PROTEASE IN COMPLEX WITH SDZ283-910
204L_A Crystal Structure of HIV-1 Protease (Q7K, I50V) in Complex with Tipranavir
5COK_A X-ray crystal structure of wild type HIV-1 protease in complex with GRL-0476
1TCX_A HIV TRIPLE MUTANT PROTEASE COMPLEXED WITH INHIBITOR SB203386
2Z54_A

The Influence of I47A Mutation on Reduced Susceptibility to the Protease Inhibitor Lopinavir
1D4S_A

HIV-1 PROTEASE V82F/I84V DOUBLE MUTANT/TIPRANAVIR COMPLEX

1BV7_A COUNTERACTING HIV-1 PROTEASE DRUG RESISTANCE:

STRUCTURAL ANALYSIS OF MUTANT PROTEASES COMPLEXED WITH XV638 AND SD146, CYCLIC UREA AMIDES WITH BROAD SPECIFICITIES

1BWA_A

HIV-1 PROTEASE (V82F/I84V) DOUBLE MUTANT COMPLEXED WITH XV638 OF DUPONT PHARMACEUTICALS

1A9M_A

G48H MUTANT OF HIV-1 PROTEASE IN COMPLEX WITH A PEPTIDIC INHIBITOR U-89360E

2FLE_A

Structural analysis of asymmetric inhibitor bound to the HIV-1 Protease V82A mutant

1ODY_A

HIV-1 PROTEASE COMPLEXED WITH AN INHIBITOR LP-130

1GNN_A

HIV-1 PROTEASE MUTANT WITH VAL 82 REPLACED BY ASN (V82N) COMPLEXED WITH U89360E (INHIBITOR)

1GNM_A

HIV-1 PROTEASE MUTANT WITH VAL 82 REPLACED BY ASP (V82D) COMPLEXED WITH U89360E (INHIBITOR)

5YRS_B

X-ray

Snapshot of HIV-1 Protease in Action: Observation of Tetrahedral Intermediate and Its SIHB with Catalytic Aspartate

5YRS_A

X-ray

Snapshot of HIV-1 Protease in Action: Observation of Tetrahedral Intermediate and Its SIHB with Catalytic Aspartate

1HEF_E The crystal structures at 2.2 angstroms resolution of hydroxyethylene-based inhibitors bound to human immunodeficiency virus type 1 protease show that the inhibitors are present in two distinct orientations

10DX_A

HIV-1 Proteinase mutant A71T, V82A

4QGI_A

X-ray crystal structure of HIV-1 protease variant G48T/L89M in complex with Saquinavir

1BVE_A

HIV-1 PROTEASE-DMP323 COMPLEX IN SOLUTION, NMR, 28 STRUCTURES

2AZ8_A

HIV-1 Protease NL4-3 in complex with inhibitor, TL-3

1A30_A

HIV-1 PROTEASE COMPLEXED WITH A TRIPEPTIDE INHIBITOR

6DH6_A

Crystal structure of HIV-1 Protease NL4-3 I50V Mutant in complex with darunavir

6DH0_A

Crystal structure of HIV-1 Protease NL4-3 I84V Mutant in complex with darunavir

2I4D_A

Crystal structure of WT HIV-1 protease with GS-8373

600S_A

HIV-1 Protease NL4-3 L90M Mutant in complex with darunavir

1RL8_A

Crystal structure of the complex of resistant strain of hiv-1 protease(v82a mutant) with ritonavir

1ZSF_A

Crystal Structure of Complex of a Hydroxyethylamine Inhibitor with HIV-1 Protease at 2.0A Resolution

2Q64_A
HIV-1 PR mutant in complex with nelfinavir

6DH3_A
Crystal structure of HIV-1 Protease NL4-3 V82I Mutant in complex with darunavir

2NPH_A
Crystal structure of HIV1 protease in situ product complex

2Q63_A
HIV-1 PR mutant in complex with nelfinavir

1LZQ_A Crystal structure of the complex of mutant HIV-1 protease (A71V, V82T, I84V) with an ethylenamine peptidomimetic inhibitor BOC-PHE-PSI[CH2CH2NH]-PHE-GLU-PHE-NH2

1FB7_A CRYSTAL
STRUCTURE OF AN IN VIVO HIV-1 PROTEASE MUTANT IN COMPLEX WITH SAQUINAVIR: INSIGHTS INTO THE MECHANISMS OF DRUG RESISTANCE

1G6L_A
1.9A CRYSTAL STRUCTURE OF TETHERED HIV-1 PROTEASE

1HIV_A CRYSTAL
STRUCTURE OF A COMPLEX OF HIV-1 PROTEASE WITH A DIHYDROETHYLENE-CONTAINING INHIBITOR: COMPARISONS WITH MOLECULAR MODELING

600U_A
Crystal structure of HIV-1 Protease NL4-3 L89V Mutant in complex with darunavir

1HVC_A
CRYSTAL STRUCTURE OF A TETHERED DIMER OF HIV-1 PROTEASE COMPLEXED WITH AN INHIBITOR

2I4V_A
HIV-1 protease I84V, L90M with TMC126

2AZ9_A
HIV-1 Protease NL4-3 1X mutant

600T_A
HIV-1 Protease NL4-3 L89V, L90M Mutant in complex with darunavir

2P3B_B
Crystal Structure of the subtype B wild type HIV protease complexed with TL-3 inhibitor

5KAO_A
Crystal structure of wild type HIV-1 protease in complex with GRL-10413

2WL0_A HIV-1
Protease Inhibitors Containing a Tertiary Alcohol in the Transition-State Mimic with Improved Cell-Based Antiviral Activity

6OPT_A
HIV-1 Protease NL4-3 V82F, I84V Mutant in complex with darunavir

1IZI_A
Inhibitor of HIV protease with unusual binding mode potently inhibiting multi-resistant protease mutants

1MRX_A
Structure of HIV protease (Mutant Q7K L33I L63I V82F I84V) complexed with KNI-577

2PYM_A
HIV-1 PR mutant in complex with nelfinavir

2PYN_A
HIV-1 PR mutant in complex with nelfinavir

1DMP_A
STRUCTURE OF HIV-1 PROTEASE COMPLEX

4K4P_A
TL-3 inhibited Trp6Ala HIV Protease

1LV1_A

Crystal Structure Analysis of the non-active site mutant of tethered HIV-1 protease to 2.1A resolution

1AID_A

STRUCTURE OF A NON-PEPTIDE INHIBITOR COMPLEXED WITH HIV-1 PROTEASE: DEVELOPING A CYCLE OF STRUCTURE-BASED DRUG DESIGN

1ZBG_A

Crystal structure of a complex of mutant hiv-1 protease (A71V, V82T, I84V) with a hydroxyethylamine peptidomimetic inhibitor BOC-PHE-PSI[R-CH(OH)CH₂NH]-PHE-GLU-PHE-NH₂

3TKG_A

crystal structure of HIV model protease precursor/saquinavir complex

5YOK_A

Structure of HIV-1 Protease in Complex with Inhibitor KNI-1657

1FGC_C

STRUCTURAL IMPLICATIONS OF DRUG

RESISTANT MUTANTS OF HIV-1 PROTEASE: HIGH RESOLUTION CRYSTAL STRUCTURES OF THE MUTANT PROTEASE/SUBSTRATE ANALOG COMPLEXES

3K4V_A

New crystal form of HIV-1 Protease/Saquinavir structure reveals carbamylation of N-terminal proline

3KT5_A

Crystal Structure of N88S mutant HIV-1 Protease

4QLH_A

Crystal structure of drug resistant V82S/V1082S HIV-1 Protease

2F3K_A

Substrate envelope and drug resistance: crystal structure of r01 in complex with wild-type hiv-1 protease

4Q5M_A

D30N tethered HIV-1 protease dimer/saquinavir complex

2AOC_A

Crystal structure analysis of HIV-1 protease mutant I84V with a substrate analog P2-NC

3B80_A

HIV-1 protease mutant I54V complexed with gem-diol-amine intermediate NLLTQI

3VF5_A

Crystal Structure of HIV-1 Protease Mutant I47V with novel P1'-Ligands GRL-02031

2AVQ_A

Kinetics, stability, and

structural changes in high resolution crystal structures of HIV-1 protease with drug resistant mutations L24I, I50V, AND G73S

1DW6_C

Structural and kinetic analysis of drug resistant mutants of HIV-1 protease

1KZK_A

JE-2147-HIV Protease Complex

2HS1_A

Ultra-high resolution X-ray crystal structure of HIV-1 protease V32I mutant with TMC114 (darunavir) inhibitor

1K6C_A

LACK OF SYNERGY FOR INHIBITORS TARGETING A MULTI-DRUG RESISTANT HIV-1 PROTEASE

1MTB_A

Viability of a drug-resistant HIV-1 protease mutant: structural insights for better antiviral therapy

4Q1X_A

Mutations Outside the

Active Site of HIV-1 Protease Alter Enzyme Structure and Dynamic Ensemble of the Active Site to

Confer Drug Resistance

4Q1W_A

Mutations Outside the

Active Site of HIV-1 Protease Alter Enzyme Structure and Dynamic Ensemble of the Active Site to Confer Drug Resistance

3D1X_A

Crystal structure of HIV-1 mutant I54M and inhibitor saquinavir

2AVM_A

Kinetics, stability, and

structural changes in high resolution crystal structures of HIV-1 protease with drug resistant mutations L24I, I50V, AND G73S

3PWM_A

HIV-1 Protease Mutant L76V with Darunavir

3KT2_A

Crystal Structure of N88D mutant HIV-1 Protease

1SDV_A

Crystal structures of HIV protease V82A and L90M mutants reveal changes in indinavir binding site.

3JWV_A

HIV-1 Protease Mutant G86A with symmetric inhibitor DMP323

3OY4_A

Crystal Structure of HIV-1 L76V Protease in Complex with the Protease Inhibitor Darunavir.

1A94_A

STRUCTURAL BASIS FOR SPECIFICITY OF RETROVIRAL PROTEASES

2HS2_A

Crystal structure of M46L mutant of HIV-1 protease complexed with TMC114 (darunavir)

citation nObserved

1W5V_A	Lindberg, J., et al. Eur J Biochem (2004)	0.18900
2FDE_A	Miller, J.F., et al. Bioorg Med Chem Lett (2006)	0.20400
1AJV_A	Backbro, K., et al. J Med Chem (1997)	0.18700
2R38_A	Bottcher, J., et al. J Mol Biology (2008)	0.18280
2R3T_A	Bottcher, J., et al. J Mol Biology (2008)	0.17810
1HXB_A	Krohn, A., et al. J Med Chem (1991)	0.18400
1BV9_A	Ala, P.J., et al. Biochemistry (1998)	0.19800
1AAQ_A	Dreyer, G.B., et al. Biochemistry (1992)	0.19000
1AXA_A	Hong, L., et al. Protein Sci (1998)	NA
1HVS_A	Baldwin, E.T., et al. Nat Struct Biol (1995)	0.15000
1ZP8_A	Brik, A., et al. Chembiochem (2005)	0.19700
2QHC_A	Saskova, K.G., et al. Protein Sci (2008)	0.19277
1A8G_A	Ringhofer, S., et al. J Mol Biology (1999)	0.15000
204L_A	Muzammil, S., et al. J Virol (2007)	0.19300
5COK_A	Aoki, M., et al. J Virol (2015)	0.21220
1TCX_A	Hoog, S.S., et al. Biochemistry (1996)	0.18000
2Z54_A	Saskova, K.G., et al. Protein Sci (2008)	0.20215
1D4S_A	Thaisrivongs, S., et al. J Med Chem (1996)	NA
1BV7_A	Ala, P.J., et al. Biochemistry (1998)	0.19600
1BWA_A	Ala, P.J., et al. Biochemistry (1998)	0.19900
1A9M_A	Hong, L., et al. FEBS Lett (1997)	0.18500
2FLE_A	Clemente, J.C., et al. J Med Chem (2008)	0.20700
1ODY_A	Kervinen, J., et al. Protein Sci (1998)	NA
1GNNA_A	Hong, L., et al. Biochemistry (1996)	NA
1GNM_A	Hong, L., et al. Biochemistry (1996)	NA
5YRS_B	Das, A., et al. J Am Chem Soc (2010)	0.22300

5YRS_A	Das, A., et al. J Am Chem Soc (2010)	0.22300
1HEF_E	Murthy, K.H., et al. J Biological Chem (1992)	0.15900
10DX_A	Kervinen, J., et al. Protein Pept Lett (1996)	NA
4QGI_A	Goldfarb, N.E., et al. Biochemistry (2015)	0.19010
1BVE_A	Yamazaki, T., et al. Protein Sci (1996)	NA
2AZ8_A	Heaslet, H., et al. J Mol Biology (2006)	0.23400
1A30_A	Louis, J.M., et al. Biochemistry (1998)	0.18900
6DH6_A	Lockbaum, G.J., et al. ACS Infect Dis (2019)	0.17740
6DH0_A	Lockbaum, G.J., et al. ACS Infect Dis (2019)	0.18400
2I4D_A	Cihlar, T., et al. J Mol Biology (2006)	NA
600S_A	Henes, M., et al. Biochemistry (2019)	0.16520
1RL8_A	Rezacova, P., et al. To be published (2005)	0.22600
1ZSF_A	Duskova, J., et al. Acta Crystallogr D Biol Crystallogr (2006)	0.22180
2Q64_A	Kozisek, M., et al. J Mol Biology (2007)	0.18280
6DH3_A	Lockbaum, G.J., et al. ACS Infect Dis (2019)	0.17590
2NPH_A	Das, A., et al. Proc Natl Acad Sci U S A (2006)	0.21600
2Q63_A	Kozisek, M., et al. J Mol Biology (2007)	0.19074
1LZQ_A	Skalova, T., et al. J Med Chem (2003)	0.20800
1FB7_A	Hong, L., et al. Protein Sci (2000)	0.18700
1G6L_A	Pillai, B., et al. Proteins (2001)	NA
1HIV_A	Thanki, N., et al. Protein Sci (1992)	0.16900
600U_A	Henes, M., et al. Biochemistry (2019)	0.20640
1HVC_A	Bhat, T.N., et al. Nat Struct Biol (1994)	NA
2I4V_A	Cihlar, T., et al. J Mol Biology (2006)	NA
2AZ9_A	Heaslet, H., et al. J Mol Biology (2006)	0.24800
600T_A	Henes, M., et al. Biochemistry (2019)	0.19690
2P3B_B	Sanches, M., et al. J Mol Biology (2007)	0.16500
5KAO_A	Amano, M., et al. Antimicrob Agents Chemother (2016)	0.18560
2WL0_A	Mahalingam, A.K., et al. J Med Chem (2010)	0.21460
6OPT_A	Henes, M., et al. ACS Chem Biol (2019)	0.18460
1IZI_A	Weber, J., et al. J Mol Biology (2002)	0.19202
1MRX_A	Vega, S., et al. Proteins (2004)	NA
2PYM_A	Kozisek, M., et al. J Mol Biology (2007)	0.19523
2PYN_A	Kozisek, M., et al. J Mol Biology (2007)	0.18993
1DMMP_A	Hodge, C.N., et al. Chem Biol (1996)	0.21000
4K4P_A	Tiefenbrunn, T., et al. Chem Biol Drug Des (2014)	0.18753
1LV1_A	Kumar, M., et al. Biochem Biophys Res Commun (2002)	0.19400
1AID_A	Rutenber, E., et al. J Biological Chem (1993)	0.17400
1ZBG_A	Duskova, J., et al. To be published	0.18498
3TKG_A	Agniswamy, J., et al. Biochemistry (2012)	0.16290
5YOK_A	Hidaka, K., et al. J Med Chem (2018)	NA
1FGC_C	Mahalingam, B., et al. Proteins (2001)	NA
3K4V_A	Olajuyigbe, F.M., et al. ACS Med Chem Lett (2010)	0.15930
3KT5_A	Bihani, S.C., et al. Biochem Biophys Res Commun (2009)	0.18000
4QLH_A	Hosur, M.V. To be published	0.19530
2F3K_A	Prabu-Jeyabalan, M., et al. Antimicrob Agents Chemother (2006)	0.16489
4Q5M_A	Prashar, V., et al. Chem Biol Drug Des (2015)	0.20760
2AOC_A	Tie, Y., et al. FEBS J (2005)	NA
3B80_A	Kovalevsky, A.Y., et al. Biochemistry (2007)	0.15300
3VF5_A	Chang, Y.C., et al. J Med Chem (2012)	0.14680
2AVQ_A	Liu, F., et al. J Mol Biology (2005)	NA

1DW6_C	Mahalingam, B., et al. Eur J Biochem (1999)	NA
1KZK_A	Reiling, K.K., et al. Biochemistry (2002)	0.15200
2HS1_A	Kovalevsky, A.Y., et al. J Mol Biology (2006)	0.12420
1K6C_A	King, N.M., et al. Protein Sci (2002)	0.19400
1MTB_A	Prabu-Jeyabalan, M., et al. J Virol (2003)	0.19100
4Q1X_A	Ragland, D.A., et al. J Am Chem Soc (2014)	0.18289
4Q1W_A	Ragland, D.A., et al. J Am Chem Soc (2014)	0.17454
3D1X_A	Liu, F., et al. J Mol Biology (2008)	0.15470
2AVM_A	Liu, F., et al. J Mol Biology (2005)	0.10400
3PWM_A	Louis, J.M., et al. Biochemistry (2011)	0.14000
3KT2_A	Bihani, S.C., et al. Biochem Biophys Res Commun (2009)	0.18700
1SDV_A	Mahalingam, B., et al. Eur J Biochem (2004)	0.15970
3JVW_A	Ishima, R., et al. Proteins (2009)	0.22560
3OY4_A	Schiffer, C.A., et al. To be published	0.18026
1A94_A	Wu, J., et al. Biochemistry (1998)	0.18200
2HS2_A	Kovalevsky, A.Y., et al. J Mol Biology (2006)	0.13980

rFree rWork spaceGroup

1W5V_A	0.21500	0.18900	P	21	21	2
2FDE_A	0.28000	0.20400		P	61	
1AJV_A	0.24700	0.18700	P	21	21	2
2R38_A	0.23790	0.18110	P	21	21	2
2R3T_A	0.23280	0.17680	P	21	21	2
1HXB_A	NA	0.18400		P	61	
1BV9_A	NA	0.19800		P	61	
1AAQ_A	NA	NA		P	61	
1AXA_A	NA	0.19400		P	61	
1HVS_A	NA	0.15000	P	21	21	21
1ZP8_A	0.32600	0.19700	P	61	2	2
2QHC_A	0.22774	0.19101		P	61	
1A8G_A	0.24400	0.15000		P	61	
204L_A	0.21600	0.19000	P	21	21	2
5COK_A	0.25520	0.21010		P	61	
1TCX_A	NA	0.18000	P	21	21	2
2Z54_A	0.25407	0.19948		P	61	
1D4S_A	0.29400	NA	P	21	21	2
1BV7_A	NA	0.19600		P	61	
1BWA_A	NA	0.19900		P	61	
1A9M_A	NA	0.18500	I	2	2	2
2FLE_A	0.25050	0.19900		P	61	
1ODY_A	NA	0.16700		P	61	
1GNN_A	NA	0.18300		P	61	
1GNM_A	NA	0.17500		P	61	
5YRS_B	0.25000	0.22300		P	61	
5YRS_A	0.25000	0.22300		P	61	
1HEF_E	NA	NA	P	61	2	2
10DX_A	NA	0.16600		P	61	
4QGI_A	0.24570	0.18710	P	21	21	21
1BVE_A	NA	NA	<NA>			
2AZ8_A	0.28600	0.23400	P	61	2	2
1A30_A	0.22700	0.18900	P	21	21	2
6DH6_A	0.22190	0.17500	P	21	21	21

6DH0_A 0.21210 0.18250 P 21 21 21
2I4D_A 0.27400 0.24100 P 21 21 2
600S_A 0.19840 0.16350 P 1 21 1
1RL8_A 0.26900 0.22600 P 61
1ZSF_A 0.27580 0.22100 P 61
2Q64_A 0.25772 0.17924 P 61
6DH3_A 0.20960 0.17410 P 21 21 21
2NPH_A 0.25900 0.21400 P 61
2Q63_A 0.25005 0.18430 P 61
1LZQ_A 0.25200 0.20300 P 61
1FB7_A 0.24300 0.18700 I 21 3
1G6L_A 0.28400 0.19500 P 61
1HIV_A NA NA P 21 21 21
600U_A 0.25490 0.20380 P 21 21 21
1HVC_A NA NA P 21 21 21
2I4V_A 0.25600 0.21900 P 21 21 2
2AZ9_A 0.30200 0.24800 P 61 2 2
600T_A 0.23460 0.19170 P 61
2P3B_B 0.21900 0.15900 P 61
5KAO_A 0.22090 0.18380 P 21 21 21
2WL0_A 0.24400 0.21460 P 21 21 2
6OPT_A 0.22770 0.18240 P 21 21 21
1IZI_A 0.24797 0.18942 P 61
1MRX_A 0.25030 0.20770 P 21 21 2
2PYM_A 0.24378 0.19270 P 61
2PYN_A 0.23809 0.18743 P 61
1DMP_A NA 0.21000 P 61
4K4P_A 0.23400 0.18513 I 41 2 2
1LV1_A 0.26000 0.19400 P 61
1AID_A NA 0.17400 P 41
1ZBG_A 0.23732 0.18665 I 2 2 2
3TKG_A 0.21400 0.16000 P 21 21 21
5YOK_A 0.12500 0.10300 P 21 21 2
1FGC_C 0.26800 0.21200 P 21 21 21
3K4V_A 0.22650 NA P 1 21 1
3KT5_A 0.22500 0.17800 P 61
4QLH_A 0.25597 0.19216 P 61
2F3K_A 0.19667 0.16312 P 21 21 21
4Q5M_A 0.23470 0.20610 P 61
2AOC_A 0.16590 0.12340 P 21 21 2
3B80_A 0.21870 NA P 21 21 2
3VF5_A 0.16860 NA P 21 21 2
2AVQ_A 0.14410 0.11140 P 21 21 2
1DW6_C 0.24900 0.21800 P 21 21 21
1KZK_A 0.18850 0.15060 P 21 21 21
2HS1_A 0.14900 0.12420 P 21 21 21
1K6C_A 0.23100 0.19400 P 21 21 21
1MTB_A 0.25700 0.19100 P 21 21 21
4Q1X_A 0.23410 0.18020 P 21 21 21
4Q1W_A 0.20634 0.17288 P 21 21 21
3D1X_A 0.14700 0.11900 P 21 21 2

```

2AVM_A 0.13200 0.10600 P 21 21 2
3PWM_A 0.18900      NA P 21 21 2
3KT2_A 0.20800 0.18600      P 61
1SDV_A 0.20540 0.15970 P 21 21 2
3JWV_A 0.28880 0.22560 P 21 21 2
3OY4_A 0.21902 0.17814 P 21 21 21
1A94_A 0.28100 0.18200 P 1 1 21
2HS2_A 0.19470 0.13980 P 21 21 21

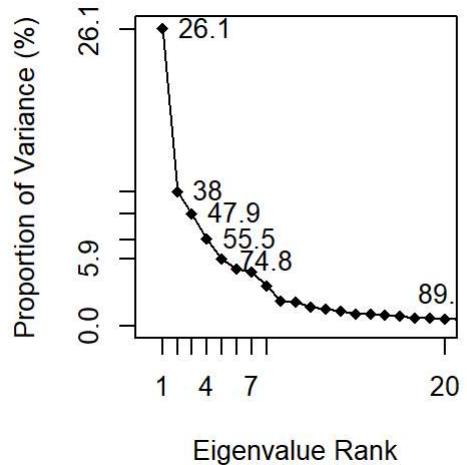
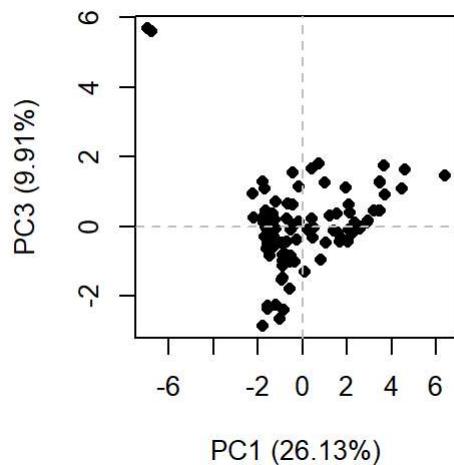
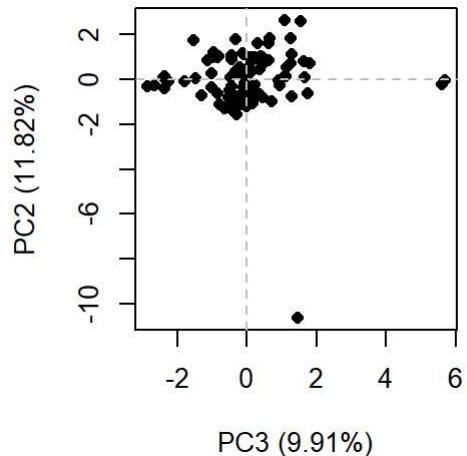
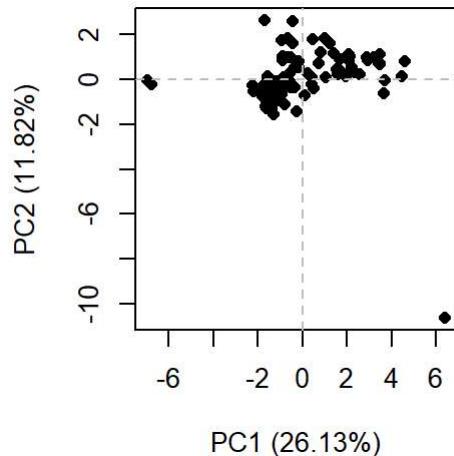
```

Principal component analysis

```

pc.xray <- pca(pdbs)
plot(pc.xray)

```



```

# Calculate RMSD
rd <- rmsd(pdbs)

```

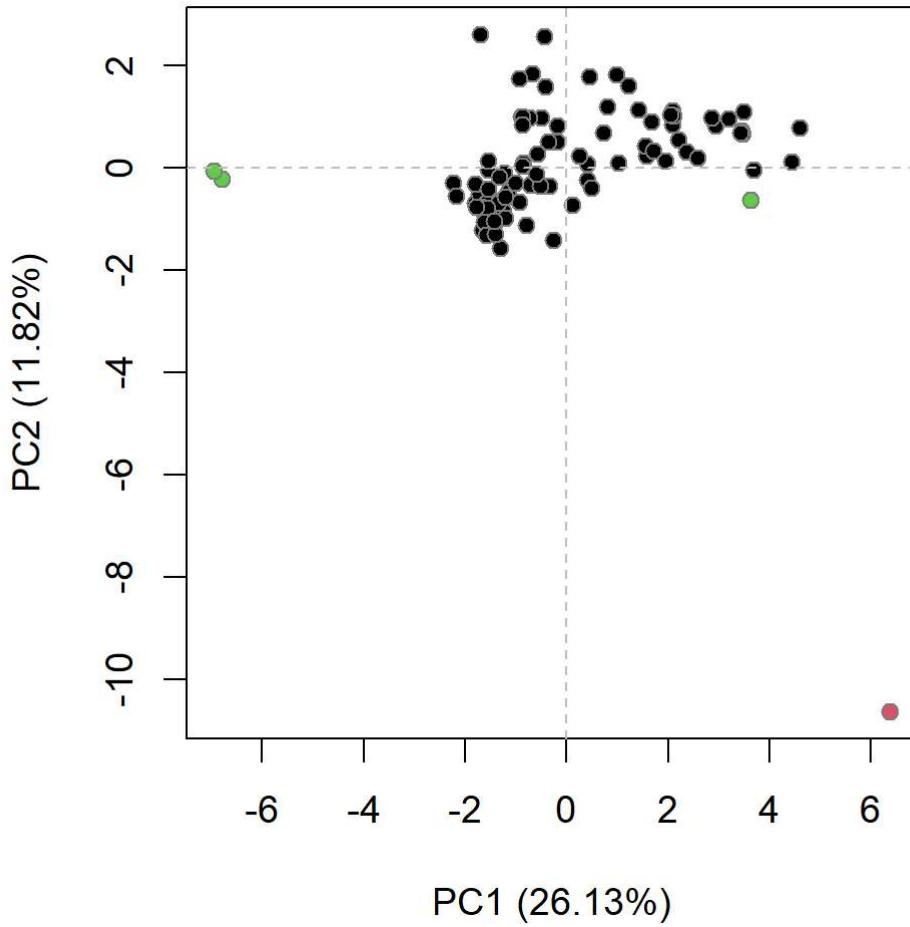
Warning in rmsd(pdbs): No indices provided, using the 99 non NA positions

```

# Structure-based clustering
hc.rd <- hclust(dist(rd))
grps.rd <- cutree(hc.rd, k=3)

```

```
plot(pc.xray, 1:2, col="grey50", bg=grps.rd, pch=21, cex=1)
```



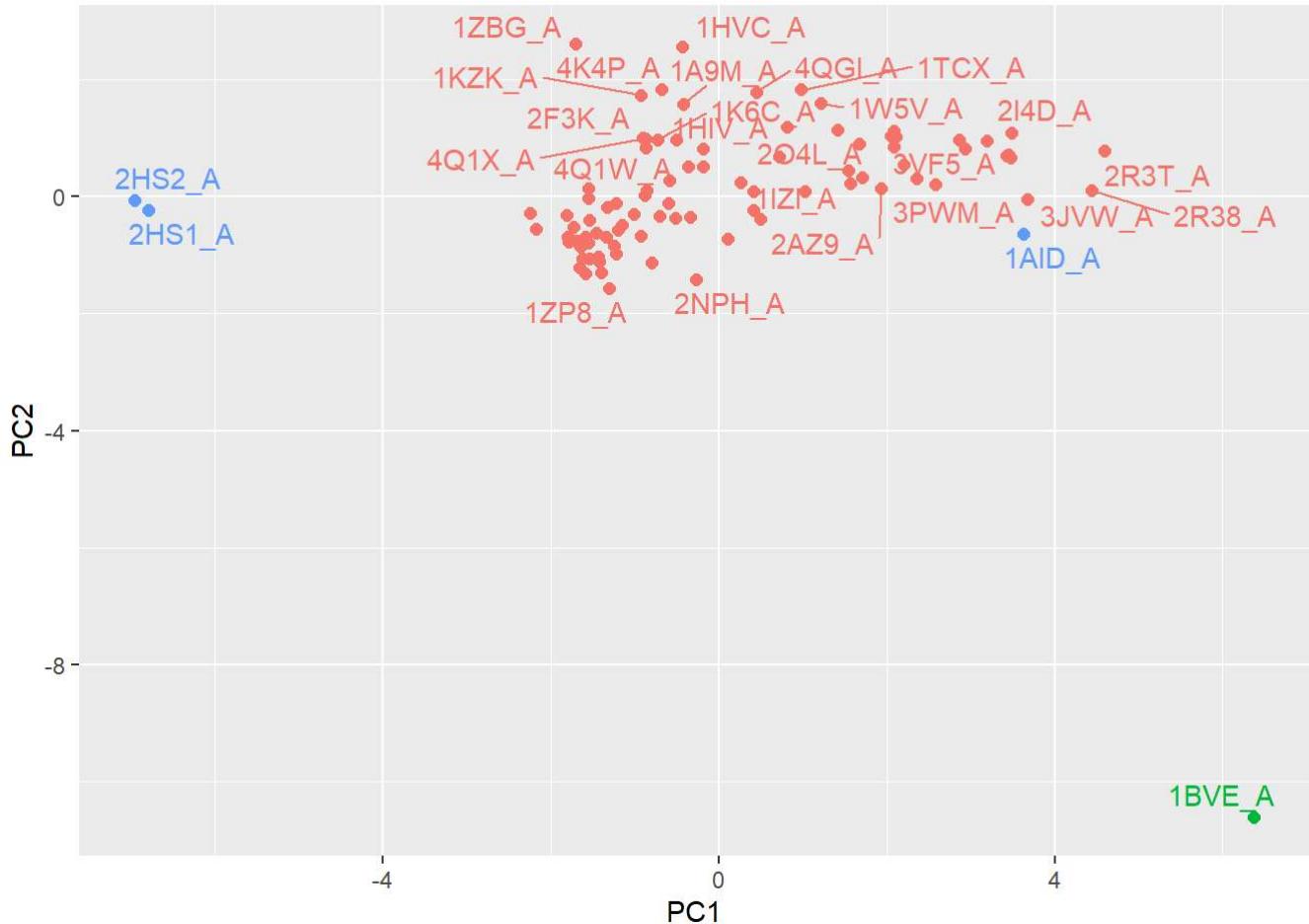
```
pc1 <- mktrj(pc.xray, pc=1, file="pc_1.pdb")
```

```
library(ggplot2)
library(ggrepel)

df <- data.frame(PC1=pc.xray$z[,1],
                  PC2=pc.xray$z[,2],
                  col=as.factor(grps.rd),
                  ids=ids)

p <- ggplot(df) +
  aes(PC1, PC2, col=col, label=ids) +
  geom_point(size=2) +
  geom_text_repel(max.overlaps = 20) +
  theme(legend.position = "none")
p
```

Warning: ggrepel: 65 unlabeled data points (too many overlaps). Consider increasing max.overlaps



```
modes <- nma(pdb)
```

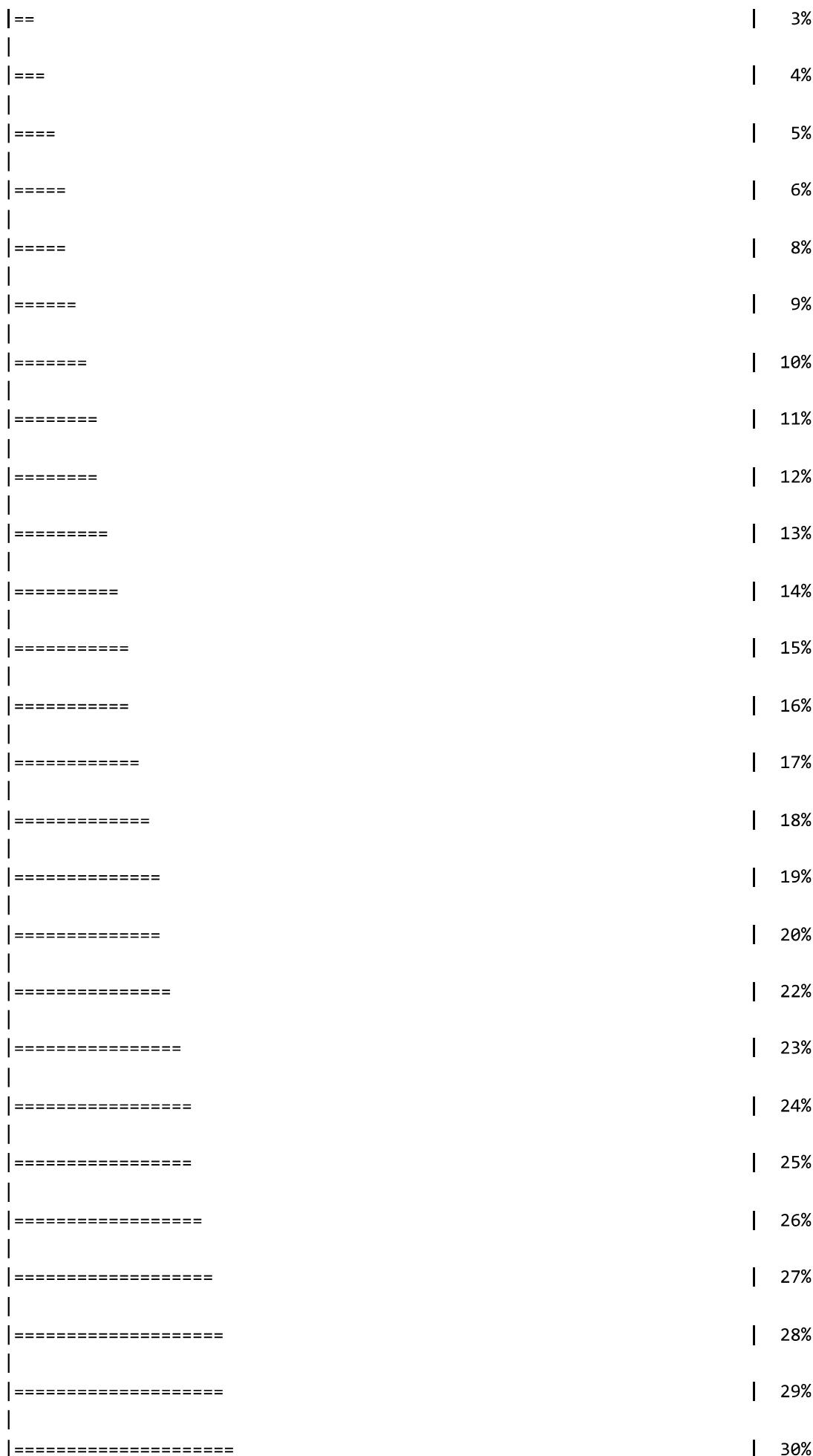
Warning in nma.pdb(pdb): 1G6L_A.pdb, 1LV1_A.pdb, 3KT5_A.pdb, 4QLH_A.pdb, 4Q5M_A.pdb, 3KT2_A.pdb
might have missing residue(s) in structure:

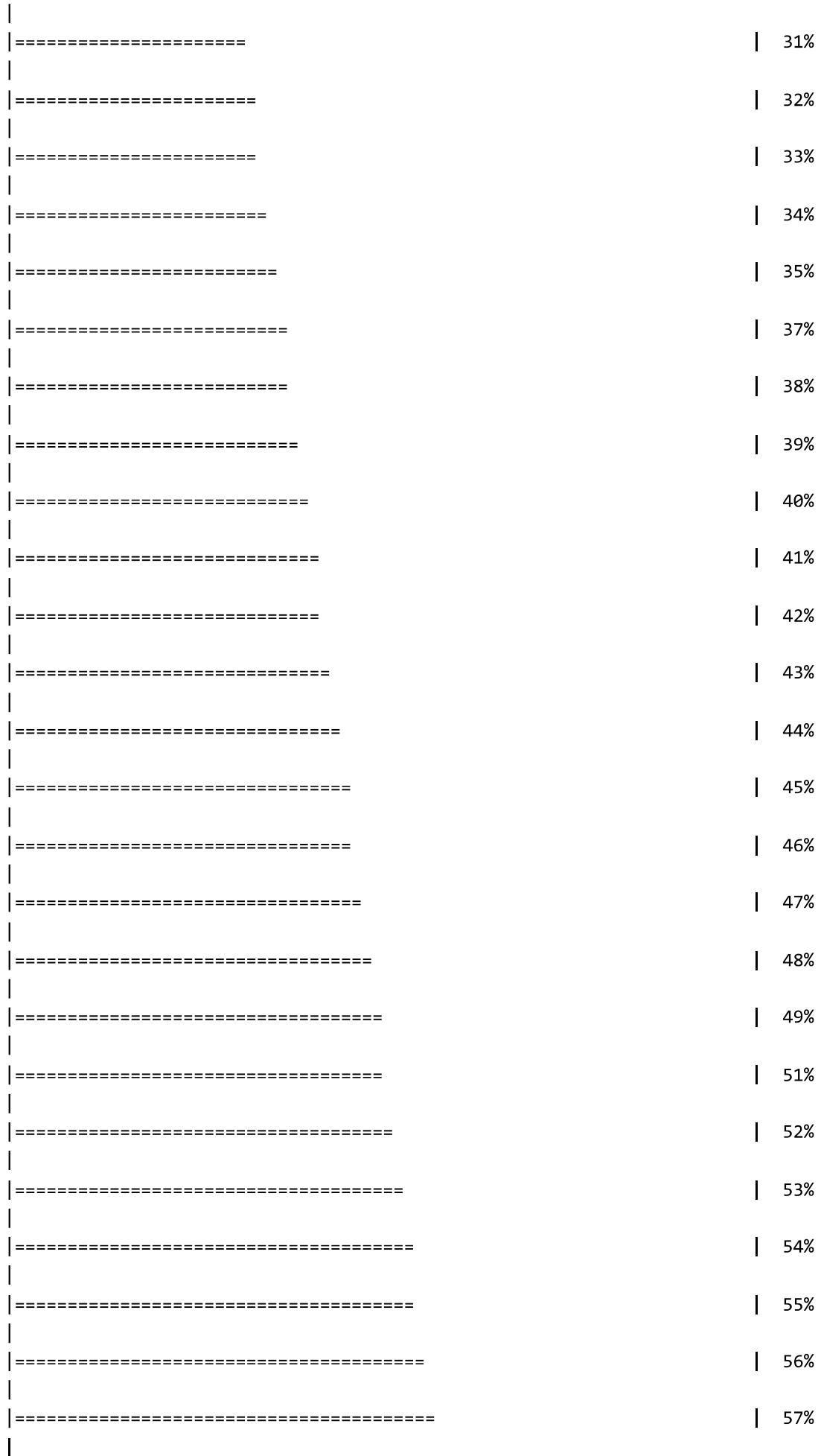
Fluctuations at neighboring positions may be affected.

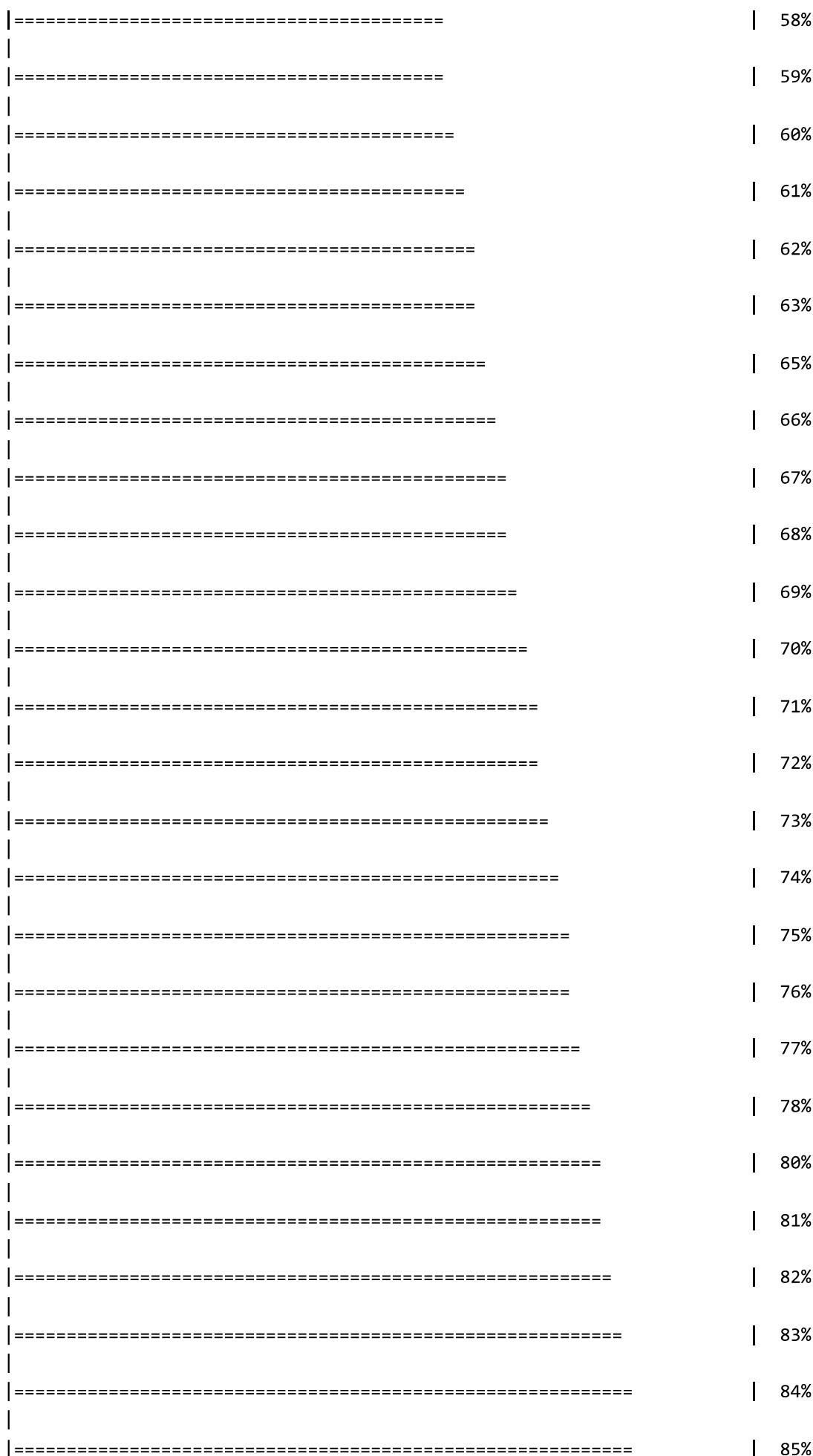
Details of Scheduled Calculation:

- ... 93 input structures
- ... storing 291 eigenvectors for each structure
- ... dimension of x\$U.subspace: (297x291x93)
- ... coordinate superposition prior to NM calculation
- ... aligned eigenvectors (gap containing positions removed)
- ... estimated memory usage of final 'eNMA' object: 61.7 Mb

```
|          | 0%
|          |
|=         | 1%
|
|==        | 2%
```



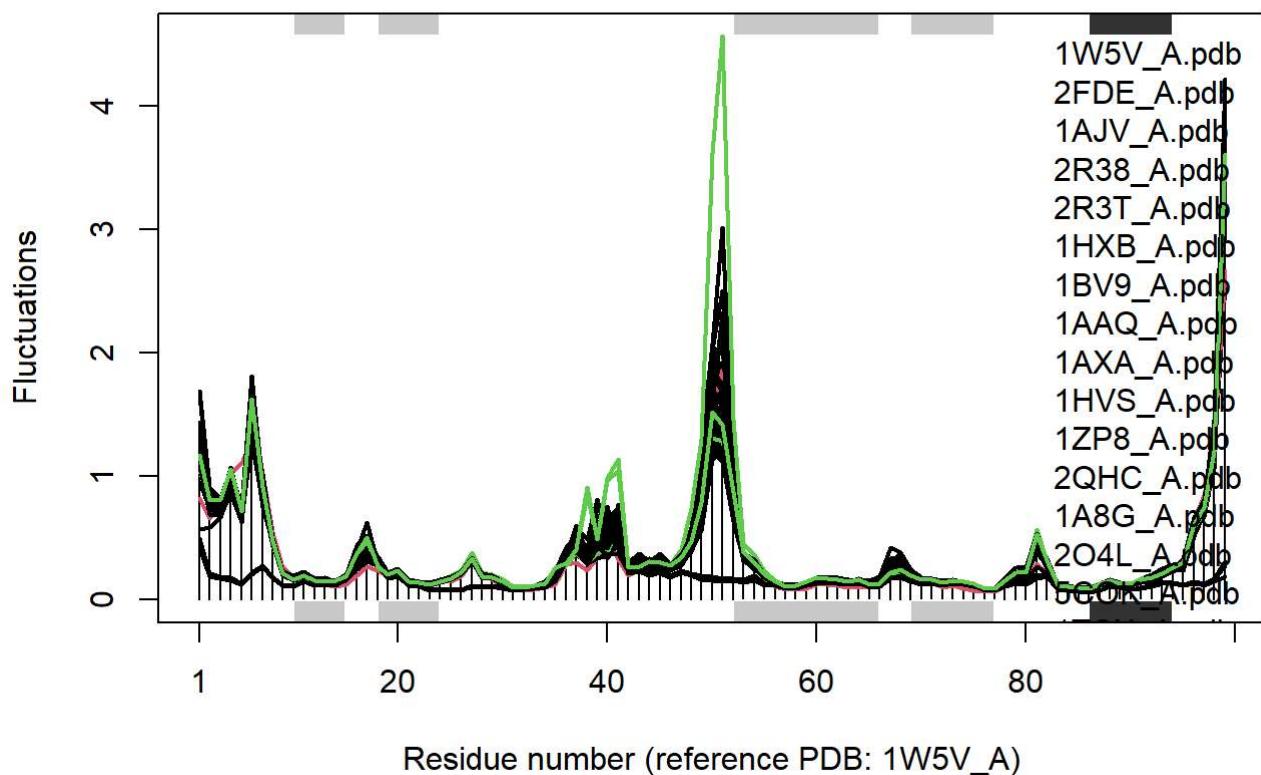




```
|=====| 86%  
|=====| 87%  
|=====| 88%  
|=====| 89%  
|=====| 90%  
|=====| 91%  
|=====| 92%  
|=====| 94%  
|=====| 95%  
|=====| 96%  
|=====| 97%  
|=====| 98%  
|=====| 99%  
|=====| 100%
```

```
plot(modes, pdbs, col=grps.rd)
```

Extracting SSE from pdbs\$sse attribute



Prediction of functional motions

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

Let's 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:

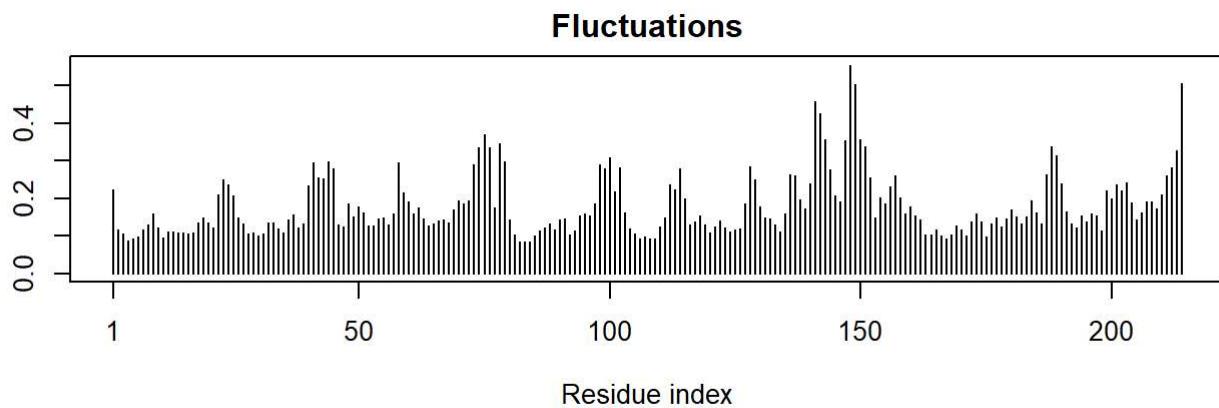
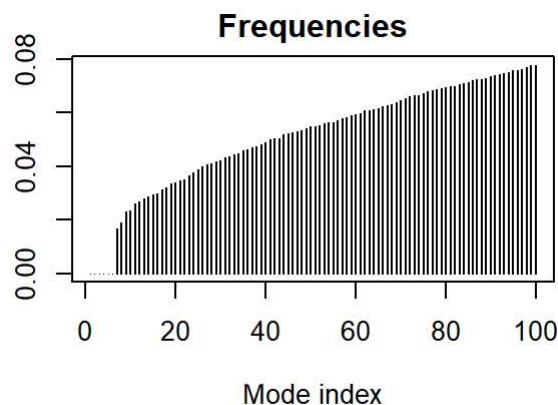
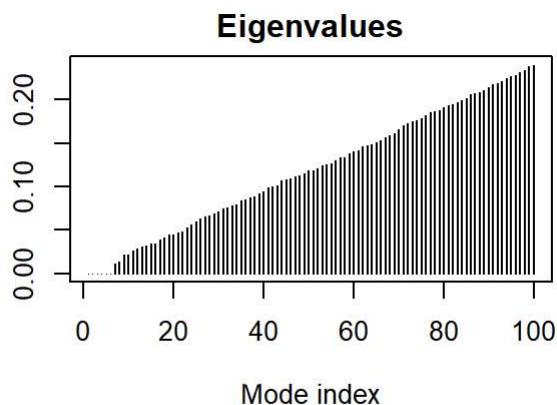
```
MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMRLRAAVKSGSELGKQAKDIMDAGLVT
DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVYLEFDVPDELIVDRI
VGRRVHAPSGRVYHVKNPPKVEGKDDVTGEELLTRKDDQEETVRKRLVEYHQMTAPLIG
YYSKAEAGNTKYAKVDGTPVAEVRADLEKILG
```

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

```
m <- nma(adk_A)
```

```
Building Hessian...      Done in 0.03 seconds.
Diagonalizing Hessian... Done in 0.47 seconds.
```

```
plot(m)
```



Let's write 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)
```

```
Warning: package 'pak' was built under R version 4.5.2
```

```
library(bio3d)
```