

Etude du packing cristallin chez PR1 et PR2

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du Vendredi 18/01/2018 au ..

Objectifs

Etudier la conservation du packing cristallin dans les 11 structures de PR2 et les 15 structures de PR1. Pour cela, on va identifier les résidus qui sont :

- inclus dans le packing cristallin chez toutes (ou la majorité (=80%)) des structures
- inclus dans le packing cristallin chez toutes (ou la majorité (=80%)) des structures de PR1
- inclus dans le packing cristallin chez toutes (ou la majorité (=80%)) des structures de PR2

Données

- 26 fichiers qui contiennent les atomes impliqués dans le packing cristallin pour chaque structure de PR1 et PR2
- le type de PR pour chaque code PDB

PDB code	type	remarque
3s45	PR2	
1hhp	PR1	
1hih	PR1	
1hii	PR2	
1hiv	PR1	
1hvp	PR1	
1hsh	PR2	
1hsi	PR2	
1ivp	PR2	
1sdt	PR1	(peu avoir des pbl de numérotation des résidus)
2hb3	PR1	
2hb4	PR1	(monomère)
2hpe	PR2	
2hpf	PR2	
2ien	PR1	(peu avoir des pbl de numérotation des résidus)
2mip	PR2	
2nph	PR1	(peu avoir des pbl de numérotation des résidus)
3phv	PR1	(monomère)
2z4o	PR1	(peu avoir des pbl de numérotation des résidus)
3ebz	PR2	(peu avoir des pbl de numérotation des résidus)
3ec0	PR2	(peu avoir des pbl de numérotation des résidus)
3ecg	PR2	(peu avoir des pbl de numérotation des résidus)
3ekv	PR1	
3nu3	PR1	(peu avoir des pbl de numérotation des résidus)
4hla	PR1	
4ll3	PR1	
1hsh	PR2	

```
Proteases = c("1hhp", "1hih", "1hii", "1hiv", "1hvp", "1hsh", "1hsi", "1ivp", "1sdt", "2hb3", "2hb4", "2hpe", "2hpf", "2ien", "2mip", "2nph", "3phv", "2z4o", "3ebz", "3ec0", "3ecg", "3ekv", "3nu3", "4hla", "4ll3", "1hsh")
type = c("PR1", "PR1", "PR2", "PR1", "PR1", "PR2", "PR2", "PR2", "PR1", "PR1", "PR1", "PR2", "PR2", "PR1", "PR2", "PR1")
names(type) = Proteases

pos.muT <-c(3,4,7,10,13,14,16,19,20,22,31:37,39:43,55:58,60:62,66:69,71:73,75:77,82,85,89,92:93,95,96,98)
res.muT <-c(paste(pos.muT, "_A", sep=""), paste(pos.muT, "_B", sep=""))
```

Détermination des résidus impliqués dans le packing cristallin chez PR1 et PR2

Création d'une matrice sous R qui contient en lignes les protéines et en colonnes les positions. La case de la matrice contient :

- 1 quand le résidu a au moins 1 atome impliqués dans le packing dans la structure,

- 0 sinon.

Attention,

- certaines structures sont des monomères
- certaines structures ont des mauvaises numérotations des résidus. Normalement les résidus sont numérotés de 1 à 99 pour la chaîne A et la chaîne B. Certaines structures ont les résidus de la chaîne B numérotés de 101 à 109. Ainsi le résidu 101B = 1B

1. Etape 1 : récupération de la liste des fichiers PDB

```
listFile = dir("fileByProt3/")
```

2. Exemple sur le premier fichier

```
filein = listFile[1]
M = read.table(paste("fileByProt3",filein,sep="/"))
listAtom = unique(paste(as.character(M[,6]), as.character(M[,5]), sep="_"))
listAtomSyn = listAtom
listAtomSyn
```

```
[1] "1_A" "2_A" "3_A" "4_A" "5_A" "6_A" "7_A" "8_A" "9_A" "23_A" "24_A" "25_A" "26_A" "27_A"
[43] "98_A" "99_A"
```

3. Récupération de la liste des résidus pour chaque protéine

```
NbProt =(1:26)
NbResidues =(1:159)

for (i in NbProt){
  filein = listFile[i]
  M = read.table(paste("fileByProt3",filein,sep="/"))
  listAtom = unique(paste(as.character(M[,6]), as.character(M[,5]), sep="_"))
  listAtomSyn = unique(c(listAtom,listAtomSyn))
}

length(listAtomSyn)
```

```
[1] 159
```

Dans les 26 structures, il y a 159 atomes qui sont impliqués dans le packing cristallin dans au moins une structure.

4. Création de la matrice

```
matrice <- matrix(0, nrow=length(Proteases), ncol=length(listAtomSyn))
rownames(matrice) <- Proteases
colnames(matrice) <- listAtomSyn

for (i in 1:length(NbProt)) {
  filein = listFile[i]
  M = read.table(paste("fileByProt3",filein,sep="/"))
  Atome <- unique(c(paste(as.character(M[,6]), as.character(M[,5]), sep="_")))
  for (j in 1:length(NbResidues)) {
    for (y in 1:length(Atome)) {
      if ((listAtomSyn[j]) == (Atome[y])){
        matrice[i,j] = 1
      }
    }
  }
}
```

```

    }
}

residue = colnames(matrice)
resA = residue[grepl("_A", residue)]
resA_ssA = as.numeric(gsub("_A","", resA))
names(resA_ssA) = resA

sort.resA = names(sort(resA_ssA))

resB = residue[grepl("_B", residue)]
resB_ssB = as.numeric(gsub("_B","", resB))
names(resB_ssB) = resB

sort.resB = names(sort(resB_ssB))

sort.res = c(sort.resA, sort.resB)
matrice.sort = matrice[,sort.res]

matrice = matrice.sort
dim(matrice)

```

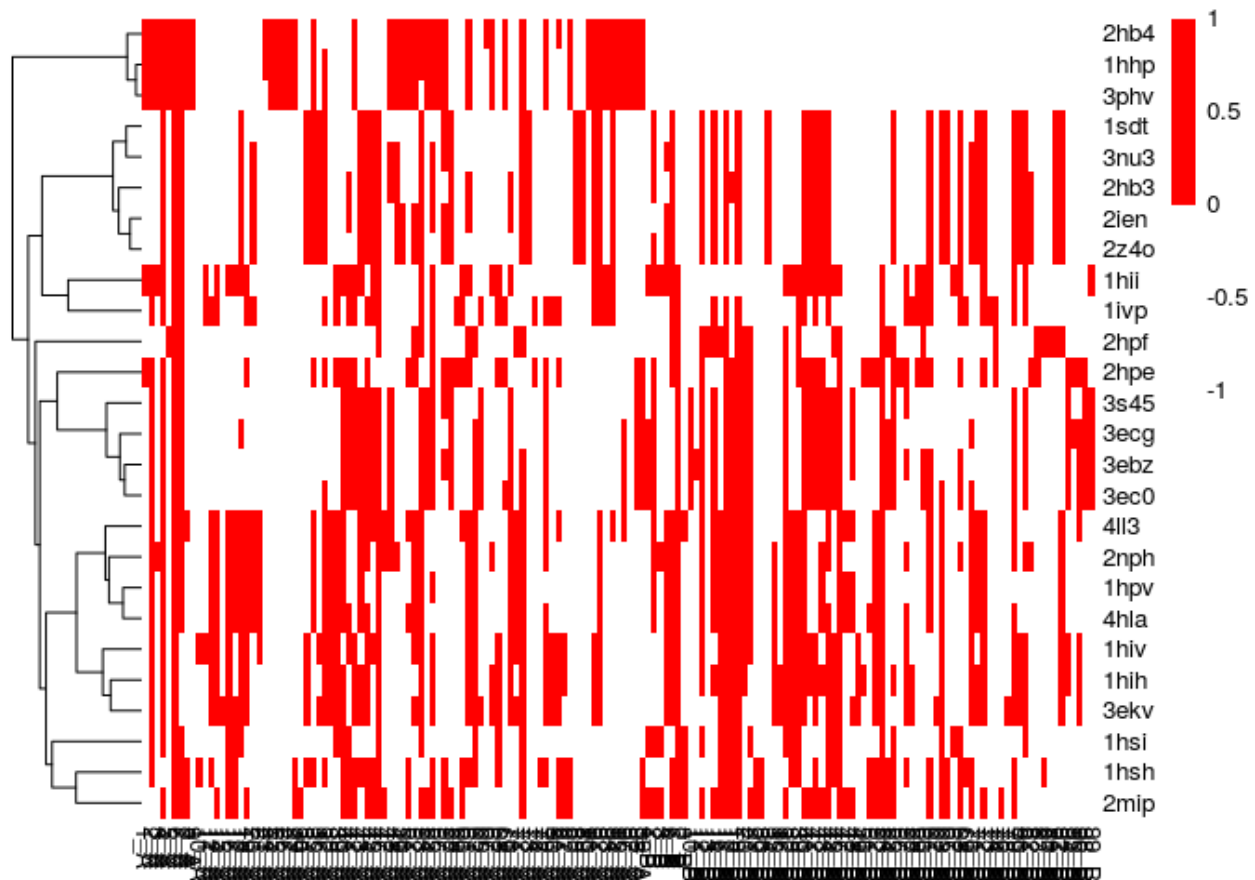
```
[1] 26 159
```

5. Coloration de la matrice b Utilisation la commande `pheatmap` du package `pheatmap`

```

pheatmap(matrice[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1, col=c("white", "red"),
         clustering_distance_rows = "binary")

```



Les protéines sont classées suivant la distance 'binary' (aka asymmetric binary): The vectors are regarded as binary bits, so non-zero elements are 'on' and zero elements are 'off'. The distance is the proportion of bits in which only one is on amongst those in which at least one is on.

Analyse :

On voit tout d'abord :

- les 3 formes non complexées de PR1 sont isolées ce qui s'explique par le fait qu'elles n'ont pas de chaîne B
 - on n'a pas une séparation PR1-PR2
 - On remarque des positions qui sont impliquées dans le packing chez la majorité des structures ex 4, 6A, 7A
6. Représentation sur une structure 3D des résidus impliqués dans packing chez au moins une structure.
→ liste des résidus dans le packing dans au moins une structure de PR2 sous pymol :
7. tous les résidus impliqués dans le packing dans au moins une structure de PR prendre les colnames de la matrice (matrice)
- ouvrir la structure de PR2 complexée avec le darunavir (DRV, code PDB 3EBZ).
 - Représenter la structure en cartoon : couleur ???
 - les résidus impliqués dans le packing en rouge

```
resSelA <- gsub("_A", "", colnames(matrice)[grep("_A", colnames(matrice))])
resSel2A <- paste(resSelA, collapse="+")
paste("select respackA, resid ", resSel2A, " and chain A", sep="")
```

```
[1] "select respackA, resid 1+2+3+4+5+6+7+8+9+10+11+12+14+15+16+17+18+19+20+21+23+24+25+26+27+29+30+34+35+36+37+38+39+40+41+42+43+44+45+46+47+48+49+50+51+52+53+54+55+56+57+58+59+60+61+62+63+64+65+66+67+68+69+70+71+72+73+74+75+76+77+78+79+80+81+82+83+84+85+86+87+88+89+90+91+92+93+94+95+96+97+98+99+100+101+102+103+104+105+106+107+108+109+110+111+112+113+114+115+116+117+118+119+120+121+122+123+124+125+126+127+128+129+130+131+132+133+134+135+136+137+138+139+140+141+142+143+144+145+146+147+148+149+150+151+152+153+154+155+156+157+158+159+160+161+162+163+164+165+166+167+168+169+170+171+172+173+174+175+176+177+178+179+180+181+182+183+184+185+186+187+188+189+190+191+192+193+194+195+196+197+198+199+200+201+202+203+204+205+206+207+208+209+210+211+212+213+214+215+216+217+218+219+220+221+222+223+224+225+226+227+228+229+230+231+232+233+234+235+236+237+238+239+240+241+242+243+244+245+246+247+248+249+250+251+252+253+254+255+256+257+258+259+260+261+262+263+264+265+266+267+268+269+270+271+272+273+274+275+276+277+278+279+280+281+282+283+284+285+286+287+288+289+290+291+292+293+294+295+296+297+298+299+300+301+302+303+304+305+306+307+308+309+310+311+312+313+314+315+316+317+318+319+320+321+322+323+324+325+326+327+328+329+330+331+332+333+334+335+336+337+338+339+340+341+342+343+344+345+346+347+348+349+350+351+352+353+354+355+356+357+358+359+360+361+362+363+364+365+366+367+368+369+370+371+372+373+374+375+376+377+378+379+380+381+382+383+384+385+386+387+388+389+390+391+392+393+394+395+396+397+398+399+400+401+402+403+404+405+406+407+408+409+410+411+412+413+414+415+416+417+418+419+420+421+422+423+424+425+426+427+428+429+430+431+432+433+434+435+436+437+438+439+440+441+442+443+444+445+446+447+448+449+450+451+452+453+454+455+456+457+458+459+460+461+462+463+464+465+466+467+468+469+470+471+472+473+474+475+476+477+478+479+480+481+482+483+484+485+486+487+488+489+490+491+492+493+494+495+496+497+498+499+500+501+502+503+504+505+506+507+508+509+510+511+512+513+514+515+516+517+518+519+520+521+522+523+524+525+526+527+528+529+530+531+532+533+534+535+536+537+538+539+540+541+542+543+544+545+546+547+548+549+550+551+552+553+554+555+556+557+558+559+560+561+562+563+564+565+566+567+568+569+570+571+572+573+574+575+576+577+578+579+580+581+582+583+584+585+586+587+588+589+590+591+592+593+594+595+596+597+598+599+600+601+602+603+604+605+606+607+608+609+610+611+612+613+614+615+616+617+618+619+620+621+622+623+624+625+626+627+628+629+630+631+632+633+634+635+636+637+638+639+640+641+642+643+644+645+646+647+648+649+650+651+652+653+654+655+656+657+658+659+660+661+662+663+664+665+666+667+668+669+670+671+672+673+674+675+676+677+678+679+680+681+682+683+684+685+686+687+688+689+690+691+692+693+694+695+696+697+698+699+700+701+702+703+704+705+706+707+708+709+710+711+712+713+714+715+716+717+718+719+720+721+722+723+724+725+726+727+728+729+730+731+732+733+734+735+736+737+738+739+740+741+742+743+744+745+746+747+748+749+750+751+752+753+754+755+756+757+758+759+760+761+762+763+764+765+766+767+768+769+770+771+772+773+774+775+776+777+778+779+780+781+782+783+784+785+786+787+788+789+790+791+792+793+794+795+796+797+798+799+800+801+802+803+804+805+806+807+808+809+810+811+812+813+814+815+816+817+818+819+820+821+822+823+824+825+826+827+828+829+830+831+832+833+834+835+836+837+838+839+840+841+842+843+844+845+846+847+848+849+850+851+852+853+854+855+856+857+858+859+860+861+862+863+864+865+866+867+868+869+870+871+872+873+874+875+876+877+878+879+880+881+882+883+884+885+886+887+888+889+890+891+892+893+894+895+896+897+898+899+900+901+902+903+904+905+906+907+908+909+910+911+912+913+914+915+916+917+918+919+920+921+922+923+924+925+926+927+928+929+930+931+932+933+934+935+936+937+938+939+940+941+942+943+944+945+946+947+948+949+950+951+952+953+954+955+956+957+958+959+960+961+962+963+964+965+966+967+968+969+970+971+972+973+974+975+976+977+978+979+980+981+982+983+984+985+986+987+988+989+990+991+992+993+994+995+996+997+998+999+1000+1001+1002+1003+1004+1005+1006+1007+1008+1009+1010+1011+1012+1013+1014+1015+1016+1017+1018+1019+1020+1021+1022+1023+1024+1025+1026+1027+1028+1029+1030+1031+1032+1033+1034+1035+1036+1037+1038+1039+1040+1041+1042+1043+1044+1045+1046+1047+1048+1049+1050+1051+1052+1053+1054+1055+1056+1057+1058+1059+1060+1061+1062+1063+1064+1065+1066+1067+1068+1069+1070+1071+1072+1073+1074+1075+1076+1077+1078+1079+1080+1081+1082+1083+1084+1085+1086+1087+1088+1089+1090+1091+1092+1093+1094+1095+1096+1097+1098+1099+1100+1101+1102+1103+1104+1105+1106+1107+1108+1109+1110+1111+1112+1113+1114+1115+1116+1117+1118+1119+1120+1121+1122+1123+1124+1125+1126+1127+1128+1129+1130+1131+1132+1133+1134+1135+1136+1137+1138+1139+1140+1141+1142+1143+1144+1145+1146+1147+1148+1149+1150+1151+1152+1153+1154+1155+1156+1157+1158+1159+1160+1161+1162+1163+1164+1165+1166+1167+1168+1169+1170+1171+1172+1173+1174+1175+1176+1177+1178+1179+1180+1181+1182+1183+1184+1185+1186+1187+1188+1189+1190+1191+1192+1193+1194+1195+1196+1197+1198+1199+1200+1201+1202+1203+1204+1205+1206+1207+1208+1209+1210+1211+1212+1213+1214+1215+1216+1217+1218+1219+1220+1221+1222+1223+1224+1225+1226+1227+1228+1229+1230+1231+1232+1233+1234+1235+1236+1237+1238+1239+1240+1241+1242+1243+1244+1245+1246+1247+1248+1249+1250+1251+1252+1253+1254+1255+1256+1257+1258+1259+1260+1261+1262+1263+1264+1265+1266+1267+1268+1269+1270+1271+1272+1273+1274+1275+1276+1277+1278+1279+1280+1281+1282+1283+1284+1285+1286+1287+1288+1289+1290+1291+1292+1293+1294+1295+1296+1297+1298+1299+1300+1301+1302+1303+1304+1305+1306+1307+1308+1309+1310+1311+1312+1313+1314+1315+1316+1317+1318+1319+1320+1321+1322+1323+1324+1325+1326+1327+1328+1329+1330+1331+1332+1333+1334+1335+1336+1337+1338+1339+1340+1341+1342+1343+1344+1345+1346+1347+1348+1349+1350+1351+1352+1353+1354+1355+1356+1357+1358+1359+1360+1361+1362+1363+1364+1365+1366+1367+1368+1369+1370+1371+1372+1373+1374+1375+1376+1377+1378+1379+1380+1381+1382+1383+1384+1385+1386+1387+1388+1389+1390+1391+1392+1393+1394+1395+1396+1397+1398+1399+1400+1401+1402+1403+1404+1405+1406+1407+1408+1409+1410+1411+1412+1413+1414+1415+1416+1417+1418+1419+1420+1421+1422+1423+1424+1425+1426+1427+1428+1429+1430+1431+1432+1433+1434+1435+1436+1437+1438+1439+1440+1441+1442+1443+1444+1445+1446+1447+1448+1449+1450+1451+1452+1453+1454+1455+1456+1457+1458+1459+1460+1461+1462+1463+1464+1465+1466+1467+1468+1469+1470+1471+1472+1473+1474+1475+1476+1477+1478+1479+1480+1481+1482+1483+1484+1485+1486+1487+1488+1489+1490+1491+1492+1493+1494+1495+1496+1497+1498+1499+1500+1501+1502+1503+1504+1505+1506+1507+1508+1509+1510+1511+1512+1513+1514+1515+1516+1517+1518+1519+1520+1521+1522+1523+1524+1525+1526+1527+1528+1529+1530+1531+1532+1533+1534+1535+1536+1537+1538+1539+1540+1541+1542+1543+1544+1545+1546+1547+1548+1549+1550+1551+1552+1553+1554+1555+1556+1557+1558+1559+1560+1561+1562+1563+1564+1565+1566+1567+1568+1569+1570+1571+1572+1573+1574+1575+1576+1577+1578+1579+1580+1581+1582+1583+1584+1585+1586+1587+1588+1589+1590+1591+1592+1593+1594+1595+1596+1597+1598+1599+1600+1601+1602+1603+1604+1605+1606+1607+1608+1609+1610+1611+1612+1613+1614+1615+1616+1617+1618+1619+1620+1621+1622+1623+1624+1625+1626+1627+1628+1629+1630+1631+1632+1633+1634+1635+1636+1637+1638+1639+1640+1641+1642+1643+1644+1645+1646+1647+1648+1649+1650+1651+1652+1653+1654+1655+1656+1657+1658+1659+1660+1661+1662+1663+1664+1665+1666+1667+1668+1669+1670+1671+1672+1673+1674+1675+1676+1677+1678+1679+1680+1681+1682+1683+1684+1685+1686+1687+1688+1689+1690+1691+1692+1693+1694+1695+1696+1697+1698+1699+1700+1701+1702+1703+1704+1705+1706+1707+1708+1709+1710+1711+1712+1713+1714+1715+1716+1717+1718+1719+1720+1721+1722+1723+1724+1725+1726+1727+1728+1729+1730+1731+1732+1733+1734+1735+1736+1737+1738+1739+1740+1741+1742+1743+1744+1745+1746+1747+1748+1749+1750+1751+1752+1753+1754+1755+1756+1757+1758+1759+1760+1761+1762+1763+1764+1765+1766+1767+1768+1769+1770+1771+1772+1773+1774+1775+1776+1777+1778+1779+1780+1781+1782+1783+1784+1785+1786+1787+1788+1789+1790+1791+1792+1793+1794+1795+1796+1797+1798+1799+1800+1801+1802+1803+1804+1805+1806+1807+1808+1809+1810+1811+1812+1813+1814+1815+1816+1817+1818+1819+1820+1821+1822+1823+1824+1825+1826+1827+1828+1829+1830+1831+1832+1833+1834+1835+1836+1837+1838+1839+1840+1841+1842+1843+1844+1845+1846+1847+1848+1849+1850+1851+1852+1853+1854+1855+1856+1857+1858+1859+1860+1861+1862+1863+1864+1865+1866+1867+1868+1869+1870+1871+1872+1873+1874+1875+1876+1877+1878+1879+1880+1881+1882+1883+1884+1885+1886+1887+1888+1889+1890+1891+1892+1893+1894+1895+1896+1897+1898+1899+1900+1901+1902+1903+1904+1905+1906+1907+1908+1909+1910+1911+1912+1913+1914+1915+1916+1917+1918+1919+1920+1921+1922+1923+1924+1925+1926+1927+1928+1929+1930+1931+1932+1933+1934+1935+1936+1937+1938+1939+1940+1941+1942+1943+1944+1945+1946+1947+1948+1949+1950+1951+1952+1953+1954+1955+1956+1957+1958+1959+1960+1961+1962+1963+1964+1965+1966+1967+1968+1969+1970+1971+1972+1973+1974+1975+1976+1977+1978+1979+1980+1981+1982+1983+1984+1985+1986+1987+1988+1989+1990+1991+1992+1993+1994+1995+1996+1997+1998+1999+2000+2001+2002+2003+2004+2005+2006+2007+2008+2009+2010+2011+2012+2013+2014+2015+2016+2017+2018+2019+2020+2021+2022+2023+2024+2025+2026+2027+2028+2029+2030+2031+2032+2033+2034+2035+2036+2037+2038+2039+2040+2041+2042+2043+2044+2045+2046+2047+2048+2049+2050+2051+2052+2053+2054+2055+2056+2057+2058+2059+2060+2061+2062+2063+2064+2065+2066+2067+2068+2069+2070+2071+2072+2073+2074+2075+2076+2077+2078+2079+2080+2081+2082+2083+2084+2085+2086+2087+2088+2089+2090+2091+2092+2093+2094+2095+2096+2097+2098+2099+2100+2101+2102+2103+2104+2105+2106+2107+2108+2109+2110+2111+2112+2113+2114+2115+2116+2117+2118+2119+2120+2121+2122+2123+2124+2125+2126+2127+2128+2129+2130+2131+2132+2133+2134+2135+2136+2137+2138+2139+2140+2141+2142+2143+2144+2145+2146+2147+2148+2149+2150+2151+2152+2153+2154+2155+2156+2157+2158+2159+2160+2161+2162+2163+2164+2165+2166+2167+2168+2169+2170+2171+2172+2173+2174+2175+2176+2177+2178+2179+2180+2181+2182+2183+2184+2185+2186+2187+2188+2189+2190+2191+2192+2193+2194+2195+2196+2197+2198+2199+2200+2201+2202+2203+2204+2205+2206+2207+2208+2209+2210+2211+2212+2213+2214+2215+2216+2217+2218+2219+2220+2221+2222+2223+2224+2225+2226+2227+2228+2229+2230+2231+2232+2233+2234+2235+2236+2237+2238+2239+2240+2241+2242+2243+2244+2245+2246+2247+2248+2249+2250+2251+2252+2253+2254+2255+2256+2257+2258+2259+2260+2261+2262+2263+2264+2265+2266+2267+2268+2269+2270+2271+2272+2273+2274+2275+2276+2277+2278+2279+2280+2281+2282+2283+2284+2285+2286+2287+2288+2289+2290+2291+2292+2293+2294+2295+2296+2297+2298+2299+2300+2301+2302+2303+2304+2305+2306+2307+2308+2309+2310+2311+2312+2313+2314+2315+2316+2317+2318+2319+2320+2321+2322+2323+2324+2325+2326+2327+2328+2329+2330+2331+2332+2333+2334+2335+2336+2337+2338+2339+2340+2341+2342+2343+2344+2345+2346+2347+2348+2349+2350+2351+2352+2353+2354+2355+2356+2357+2358+2359+2360+2361+2362+2363+2364+2365+2366+2367+2368+2369+2370+2371+2372+2373+2374+2375+2376+2377+2378+2379+2380+2381+2382+2383+2384+2385+2386+2387+2388+2389+2390+2391+2392+2393+2394+2395+2396+2397+2398+2399+2400+2401+2402+2403+2404+2405+2406+2407+2408+2409+2410+2411+2412+2413+2414+2415+2416+2417+2418+2419+2420+2421+2422+2423+2424+2425+2426+2427+2428+2429+2430+2431+2432+2433+2434+2435+2436+2437+2438+2439+2440+2441+2442+2443+2444+2445+2446+2447+2448+2449+2450+2451+2452+2453+2454+2455+2456+2457+2458+2459+2460+2461+2462+2463+2464+2465+2466+2467+2468+2469+2470+2471+2472+2473+2474+2475+2476+2477+2478+2479+2480+2481+2482+2483+2484+2485+2486+2487+2488+2489+2490+2491+2492+2493+2494+2495+2496+2497+2498+2499+2500+2501+2502+2503+2504+2505+2506+2507+2508+2509+2510+2511+2512+2513+2514+2515+2516+2517+2518+2519+2520+2521+2522+2523+2524+2525
```

```
[1] "select respackB, resid 1+2+3+4+6+7+8+10+11+12+13+14+16+17+18+19+20+21+29+30+34+35+36+37+38+39+40+41+42+43+44+45+46+47+48+49+50+51+52+53+54+55+56+57+58+59+60+61+62+63+64+65+66+67+68+69+70+71+72+73+74+75+76+77+78+79+80+81+82+83+84+85+86+87+88+89+90+91+92+93+94+95+96+97+98+99+100+101+102+103+104+105+106+107+108+109+110+111+112+113+114+115+116+117+118+119+120+121+122+123+124+125+126+127+128+129+130+131+132+133+134+135+136+137+138+139+140+141+142+143+144+145+146+147+148+149+150+151+152+153+154+155+156+157+158+159+160+161+162+163+164+165+166+167+168+169+170+171+172+173+174+175+176+177+178+179+180+181+182+183+184+185+186+187+188+189+190+191+192+193+194+195+196+197+198+199+200+201+202+203+204+205+206+207+208+209+210+211+212+213+214+215+216+217+218+219+220+221+222+223+224+225+226+227+228+229+230+231+232+233+234+235+236+237+238+239+240+241+242+243+244+245+246+247+248+249+250+251+252+253+254+255+256+257+258+259+260+261+262+263+264+265+266+267+268+269+270+271+272+273+274+275+276+277+278+279+280+281+282+283+284+285+286+287+288+289+290+291+292+293+294+295+296+297+298+299+300+301+302+303+304+305+306+307+308+309+310+311+312+313+314+315+316+317+318+319+320+321+322+323+324+325+326+327+328+329+330+331+332+333+334+335+336+337+338+339+340+341+342+343+344+345+346+347+348+349+350+351+352+353+354+355+356+357+358+359+360+361+362+363+364+365+366+367+368+369+370+371+372+373+374+375+376+377+378+379+380+381+382+383+384+385+386+387+388+389+390+391+392+393+394+395+396+397+398+399+400+401+402+403+404+405+406+407+408+409+410+411+412+413+414+415+416+417+418+419+420+421+422+423+424+425+426+427+428+429+430+431+432+433+434+435+436+437+438+439+440+441+442+443+444+445+446+447+448+449+450+451+452+453+454+455+456+457+458+459+460+461+462+463+464+465+466+467+468+469+470+471+472+473+474+475+476+477+478+479+480+481+482+483+484+485+486+487+488+489+490+491+492+493+494+495+496+497+498+499+500+501+502+503+504+505+506+507+508+509+510+511+512+513+514+515+516+517+518+519+520+521+522+523+524+525+526+527+528+529+530+531+532+533+534+535+536+537+538+539+540+541+542+543+544+545+546+547+548+549+550+551+552+553+554+555+556+557+558+559+560+561+562+563+564+565+566+567+568+569+570+571+572+573+574+575+576+577+578+579+580+581+582+583+584+585+586+587+588+589+590+591+592+593+594+595+596+597+598+599+600+601+602+603+604+605+606+607+608+609+610+611+612+613+614+615+616+617+618+619+620+621+622+623+624+625+626+627+628+629+630+631+632+633+634+635+636+637+638+639+640+641+642+643+644+645+646+647+648+649+650+651+652+653+654+655+656+657+658+659+660+661+662+663+664+665+666+667+668+669+670+671+672+673+674+675+676+677+678+679+680+681+682+683+684+685+686+687+688+689+690+691+692+693+694+695+696+697+698+699+700+701+702+703+704+705+706+707+708+709+710+711+712+713+714+715+716+717+718+719+720+721+722+723+724+725+726+727+728+729+730+731+732+733+734+735+736+737+738+739+740+741+742+743+744+745+746+747+748+749+750+751+752+753+754+755+756+757+758+759+760+761+762+763+764+765+766+767+768+769+770+771+772+773+774+775+776+777+778+779+780+781+782+783+784+785+786+787+788+789+790+791+792+793+794+795+796+797+798+799+800+801+802+803+804+805+806+807+808+809+810+811+812+813+814+815+816+817+818+819+820+821+822+823+824+825+826+827+828+829+830+831+832+833+834+835+836+837+838+839+840+841+842+843+844+845+846+847+848+849+850+851+852+853+854+855+856+857+858+859+860+861+862+863+864+865+866+867+868+869+870+871+872+873+874+875+876+877+878+879+880+881+882+883+884+885+886+887+888+889+890+891+892+893+894+895+896+897+898+899+900+901+902+903+904+905+906+907+908+909+910+911+912+913+914+915+916+917+918+919+920+921+922+923+924+925+926+927+928+929+930+931+932+933+934+935+936+937+938+939+940+941+942+943+944+945+946+947+948+949+950+951+952+953+954+955+956+957+958+959+960+961+962+963+964+965+966+967+968+969+970+971+972+973+974+975+976+977+978+979+980+981+982+983+984+985+986+987+988+989+990+991+992+993+994+995+996+997+998+999+1000+1001+1002+1003+1004+1005+1006+1007+1008+1009+1010+1011+1012+1013+1014+1015+1016+1017+1018+1019+1020+1021+1022+1023+1024+1025+1026+1027+1028+1029+1030+1031+1032+1033+1034+1035+1036+1037+1038+1039+1040+1041+1042+1043+1044+1045+104
```

7. Représentation sur une structure 3D des résidus impliqués dans packing conservés entre toutes les structures. **To do**

```
list.bk = c("C", "O", "N", "CA")
Localisation = c("Backbone", "ChaineLat")
NbAtomeinPC = 1:6039 ##Il faudrait automatiser ces valeurs

matrice3 <- matrix(0, nrow=length(Localisation), ncol=length(NbResidues))

rownames(matrice3) <- Localisation
colnames(matrice3) <- sort.res

listAtomSyn = c()
for (i in NbProt){
  filein = listFile[i]
  N = read.table(paste("fileByProt3", filein, sep="/"))
  listAtom = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))
  listAtomSyn = (c(listAtom, listAtomSyn))
}

listAtomSyn2 = c()

for (i in NbProt){
  filein = listFile[i]
  N = read.table(paste("fileByProt3", filein, sep="/"))
  listAtom = (paste(as.character(N[,3])))
  listAtomSyn2 = (c(listAtom, listAtomSyn2))
}

names(listAtomSyn) = listAtomSyn2

for (j in 1:length(sort.res)) {
  for (k in 1:length(NbAtomeinPC)) {

    if (sort.res[j] == listAtomSyn[k]){

      #if (((listAtomSyn2[k]) == "C") || ((listAtomSyn2[k]) == "CA") || ((listAtomSyn2[k]) == "O"))
      if (is.element(listAtomSyn2[k], list.bk) == TRUE){
```

```

matrice3[1,sort.res[j]] = matrice3[1,sort.res[j]] + 1
}else{
  matrice3[2,sort.res[j]] = matrice3[2,sort.res[j]] + 1
}
}
}
}
}

```

En moyenne on a :

```

apply(matrice3, 1, mean)

```

```

Backbone ChaîneLat
13.44025  24.54088

```

```

t.test(matrice3[1,],matrice3[2,], var.equal=TRUE, alternative="less")

```

Two Sample t-test

```

data:  matrice3[1, ] and matrice3[2, ]
t = -3.9373, df = 316, p-value = 0.00005071
alternative hypothesis: true difference in means is less than 0
95 percent confidence interval:
    -Inf -6.449546
sample estimates:
mean of x mean of y
 13.44025  24.54088

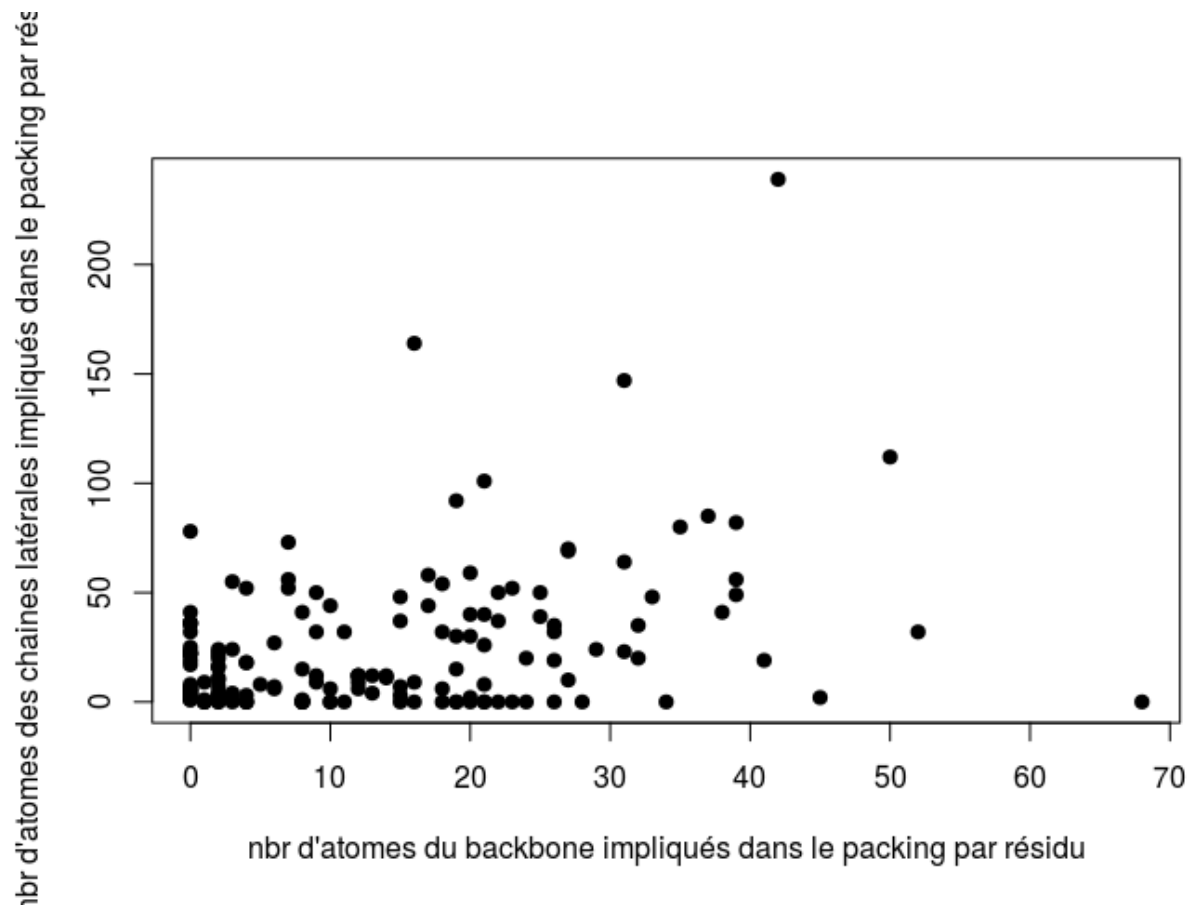
```

On voit qu'en moyenne les résidus ont plus d'atomes des chaînes latérales impliqués dans le packing cristallin que des atomes du backbone (p-value = 5.071e-05).

```

plot(matrice3[1,],matrice3[2,], xlab="nbr d'atomes du backbone impliqués dans le packing par résidu",
      ylab="nbr d'atomes des chaines latérales impliqués dans le packing par résidu", pch=19)

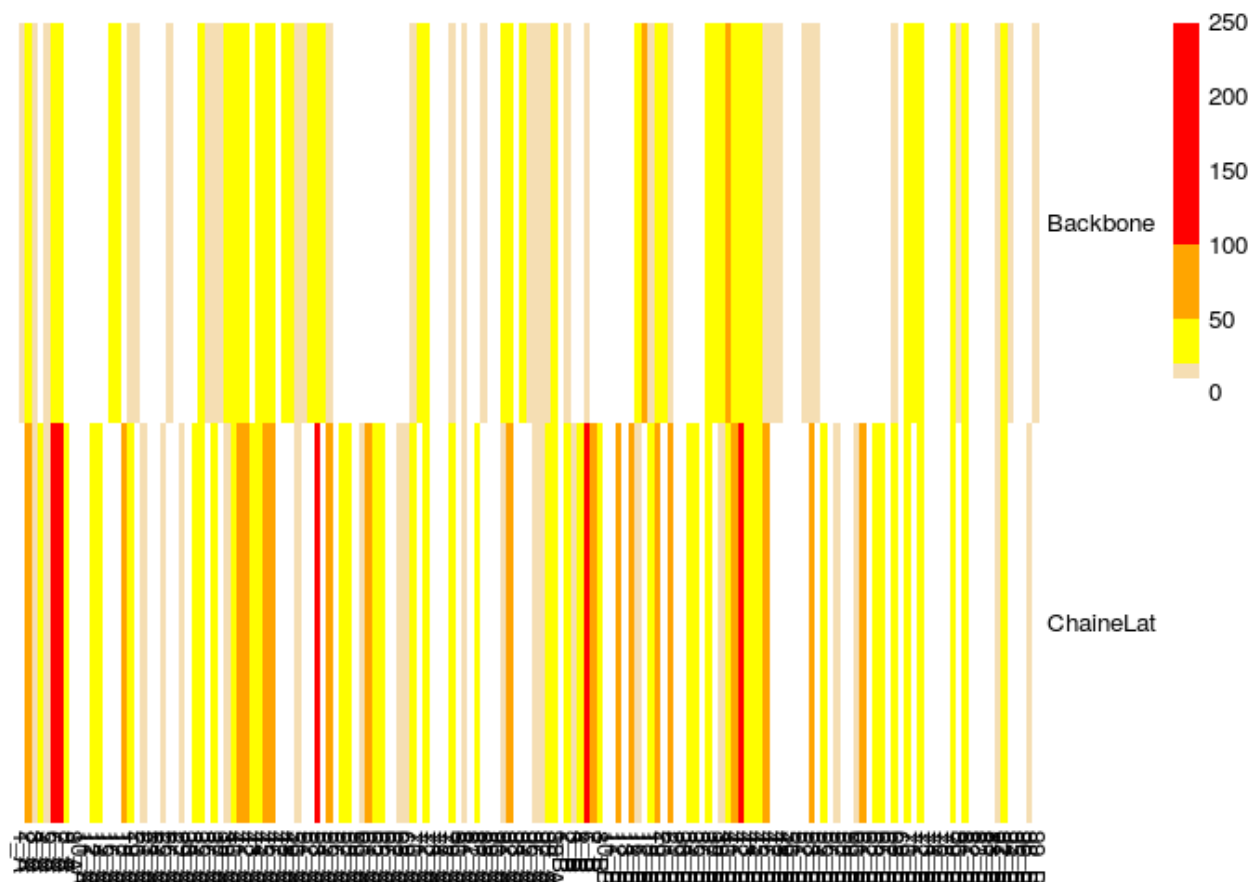
```



On voit qu'il n'y a pas de lien entre le nombre d'atomes du backbone impliqués dans le packing par résidus et le nombre d'atomes des chaînes latérales impliqués dans le packing par résidus. Ce n'est pas parce qu'un résidu a beaucoup d'atomes de sa chaîne latérale impliqués dans le packing, qu'il aura beaucoup d'atomes de son backbone impliqués dans le packing.

Visualisation du type d'atomes impliqués dans le packing cristallin

```
pheatmap(matrice3, cluster_cols = FALSE, cluster_rows = FALSE, breaks = c(-1, 10, 20, 50, 100, 250),
  col = c("white", "wheat", "yellow", "orange", "red"))
```

A refaire pour le nombre de protéine : matrice avec des 0 et 1

```
matriceBackBonePR <- matrix(0, nrow=length(Proteases), ncol=length(NbResidues))

rownames(matriceBackBonePR) <- Proteases
colnames(matriceBackBonePR) <- sort.res

matriceChaineLatPR <- matrix(0, nrow=length(Proteases), ncol=length(NbResidues))

rownames(matriceChaineLatPR) <- Proteases
colnames(matriceChaineLatPR) <- sort.res

NbAtomeinPC = c(1:length(listAtomSyn2))
names(listAtomSyn) = listAtomSyn2
for (i in 1:length(Proteases)) {

  listAtomSyn = NULL
  listAtomSyn2 = NULL

  filein = listFile[i]
  N = read.table(paste("fileByProt3",filein,sep="/"))

  listAtomSyn = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))
```

```

listAtomSyn2 = (paste(as.character(N[,3])))

for (k in 1:length(listAtomSyn)) {
  for (j in 1:length(sort.res)) {

    if (listAtomSyn[k] == sort.res[j]){
      if (is.element(listAtomSyn2[k], list.bk)==TRUE){

        matriceBackBonePR[Proteases[i],sort.res[j]] = 1
      }else{
        matriceChaineLatPR[Proteases[i],sort.res[j]] = 1
      }
    }
  }
}
}

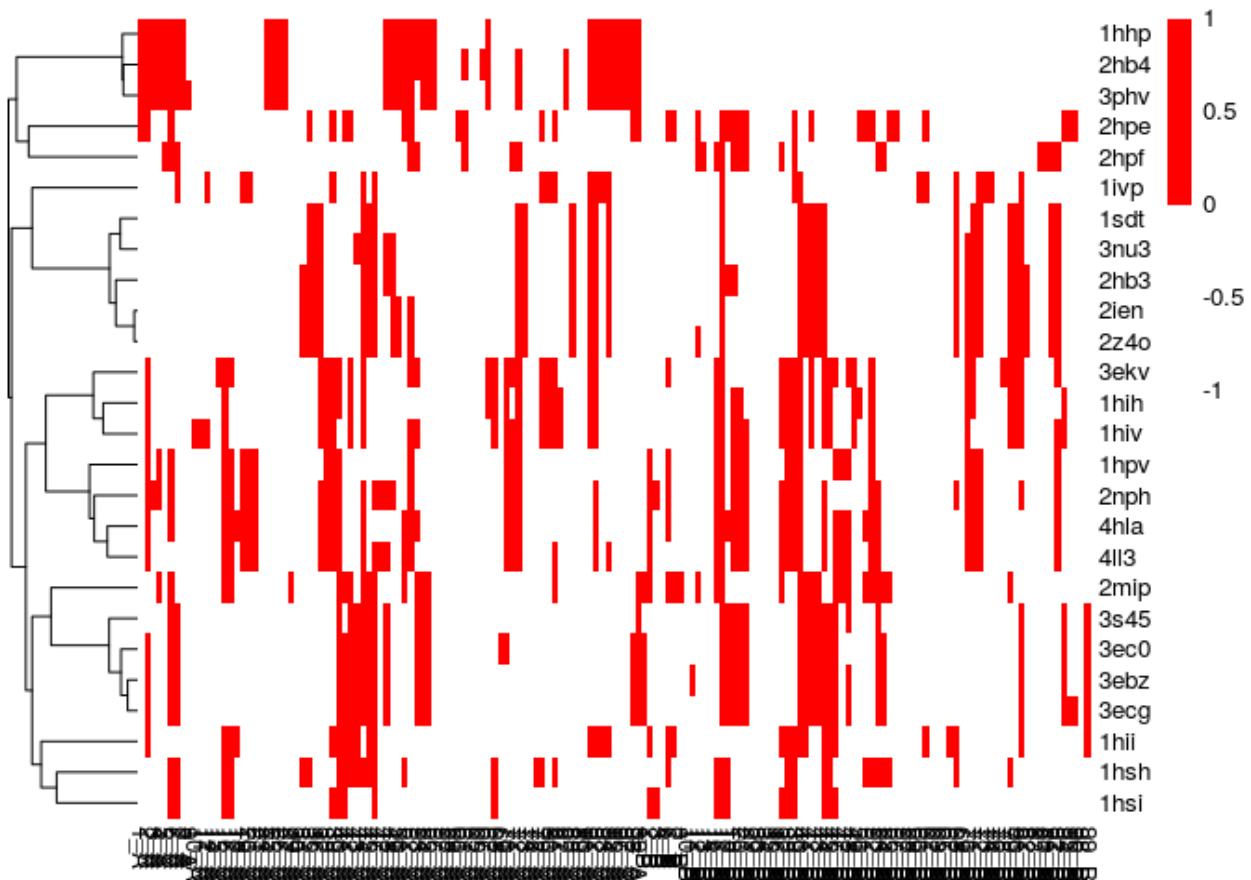
```

Visualisation des résultats

```

pheatmap(matriceBackBonePR[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1,
  col=c("white", "red"), clustering_distance_rows = "binary")

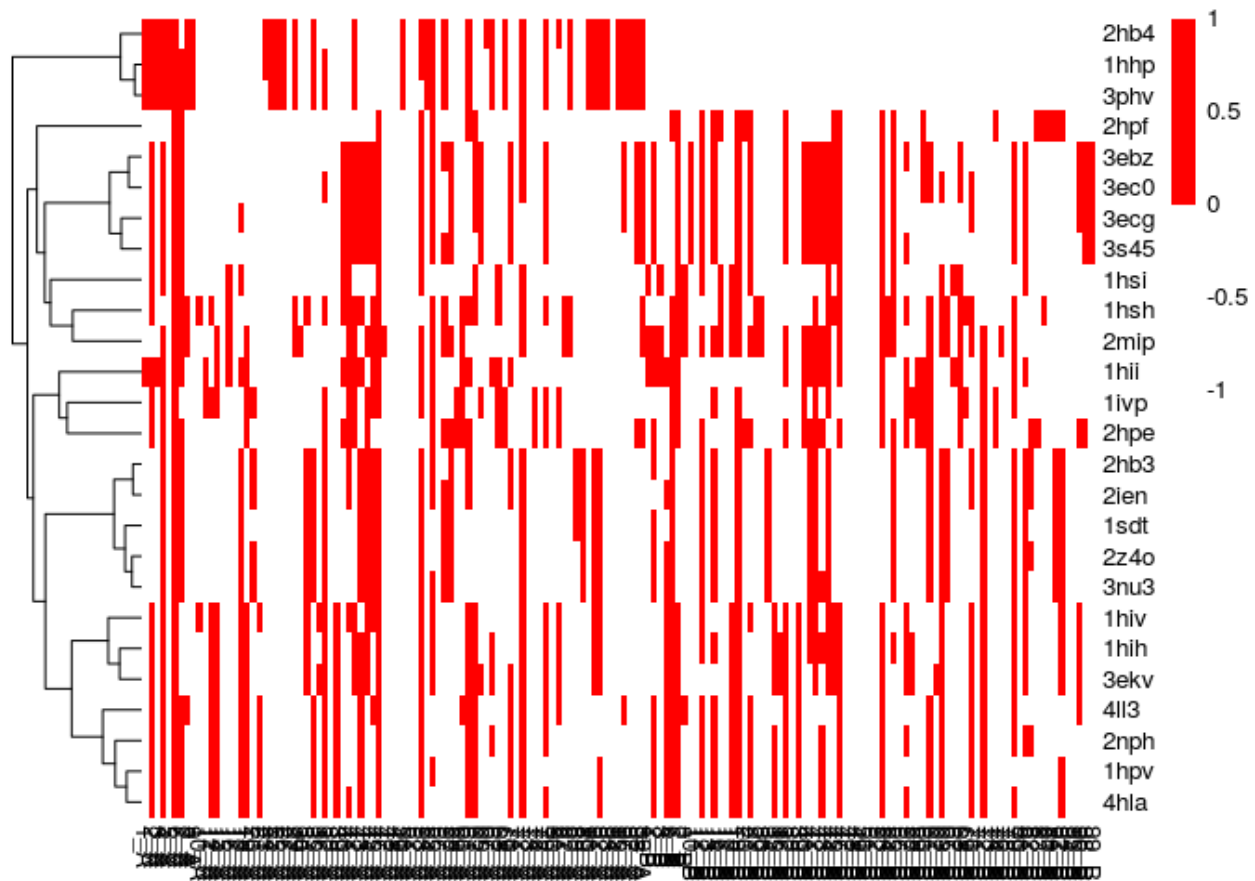
```



```

pheatmap(matriceChaineLatPR[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1,
  col=c("white", "red"), clustering_distance_rows = "binary")

```



Détermination du nombre de structures dans lequel un résidu est impliqué dans le packing cristallin

Le nombre de structure dans lequel un résidu est impliqué dans le packing cristallin = la somme des colonnes de la matrice

1. Calculer le nombre de structure dans lequel un résidu est impliqué dans le packing cristallin

```
StructinPC = c("NbStructinPC", "NbStructinPC.PR1", "NbStructinPC.PR2")

matriceStruct <- matrix(0, nrow=length(StructinPC), ncol=length(sort.res))

rownames(matriceStruct) <- StructinPC
colnames(matriceStruct) <- sort.res

for (i in 1:length(NbResidues)){
  y = 0
  for (j in 1:length(Proteases[1:26])) {
    if (matrice[j,i] == 1){
      y = y+1
      matriceStruct[1,i] = y
    }
  }
}
```

```
}
```

Voir si ces deux lignes de codes sont nécessaires, car le vecteur type existe déjà mais ne contient pas les mêmes données

```
type = matrice[,ncol(matrice)]  
names(type)
```

```
[1] "1hhp" "1hih" "1hii" "1hiv" "1hvp" "1hsh" "1hsi" "1ivp" "1sdt" "2hb3" "2hb4" "2hpe" "2hpf" "2ien"
```

```
#matrice[names(which(type=="PR2")),]
```

```
matrice2 = matrice[, -ncol(matrice)]
```

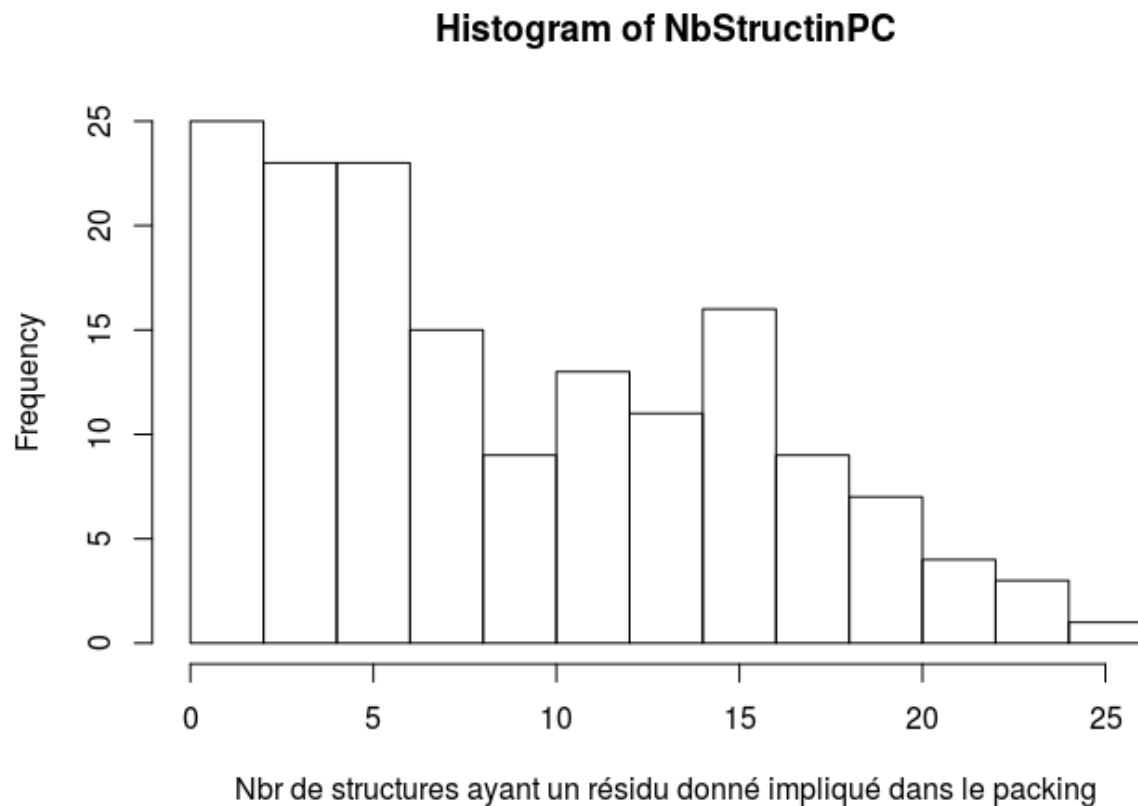
```
NbStructinPC = apply(matrice[1:26,],2,sum)
```

D'après ces résultats on voit que le résidu 6_A est impliqué dans le packing cristallin dans toutes les structures.

D'autres résidus sont retrouvés dans la majorité des structures (>80%) : 4_A, 6_A, 7_A, 46_A, 53_A, 72_A, 17_B, 19_B

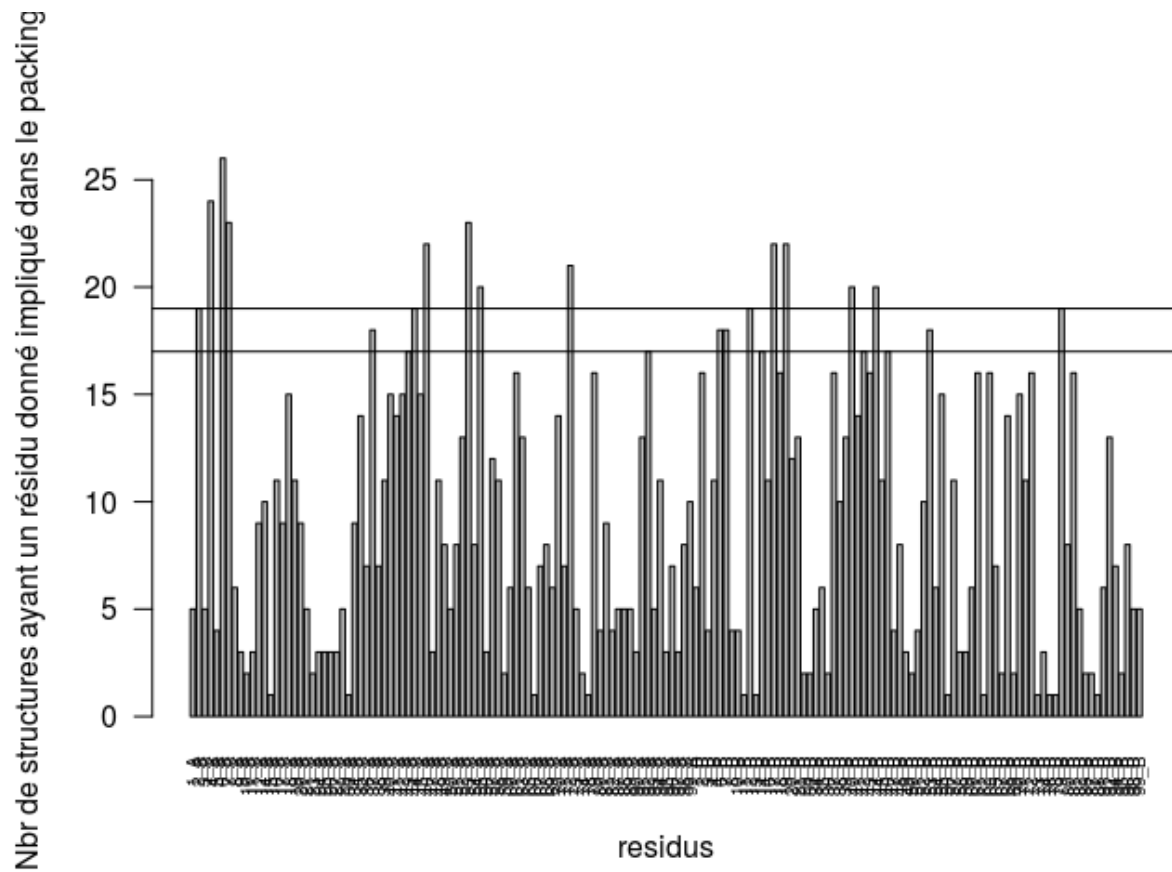
2. Représenter ces valeurs graphiquement

```
hist(NbStructinPC,xlab="Nbr de structures ayant un résidu donné impliqué dans le packing")
```



On va aussi faire un barplot pour voir le nombre pour chaque résidu

```
barplot(NbStructinPC, las = 2, cex.names = 0.6, xlab="residus", ylab="Nbr de structures ayant un résidu",
abline(h=c(19,17))
```



On voit des différences dans les chaînes A et B

3. Calculer la moyenne et écart type de ce nombre

```
mean(matriceStruct[1,])
```

```
[1] 9.157233
```

```
sd(matriceStruct[1,])
```

```
[1] 6.383855
```

On définit un résidu impliqué dans le packing dans la majorité des structures comme étant :

- les résidus de la chaîne A vu dans au moins 70% des structures = 19 structures
- les résidus de la chaîne B vu dans au moins 70% des structures = 17 structures

4. Calcul une p-value pour déterminer si les positions sont conservées

```
f.permut = function(vect){
  return(sample(vect))
}
```

```
occ <- apply(matrice,2,sum)
```

```

resA <- colnames(matrice)[grep("_A", colnames(matrice))]
resB<- colnames(matrice)[grep("_B", colnames(matrice))]

nbrSimul <- 10000

occ.SupbyPos <- rep(0, length = ncol(matrice))
names(occ.SupbyPos) <- colnames(matrice)
for( rep in 1:nbrSimul){
  mat.rand.A <- t(apply(matrice[,resA],1,f.permut))
  mat.rand.B <- t(apply(matrice[,resB],1,f.permut))
  matrice.random <- cbind(mat.rand.A, mat.rand.B)
  colnames(matrice.random) <- c(resA,resB)
  occ.rand <- apply(matrice.random,2,sum)
  diff <- occ.rand-occ
  occ.SupbyPos [names(which(diff > 0))] = occ.SupbyPos[names(which(diff > 0))] +1
}

pval <- occ.SupbyPos/nbrSimul

```

Les positions qui sont sur-représentées sont ($pvalue < 0.05$) 2_A, 4_A, 6_A, 7_A, 18_A, 35_A, 37_A, 40_A, 41_A, 42_A, 43_A, 44_A, 45_A, 46_A, 52_A, 53_A, 55_A, 61_A, 63_A, 70_A, 72_A, 79_A, 91_A, 92_A, 2_B, 6_B, 7_B, 12_B, 14_B, 17_B, 18_B, 19_B, 21_B, 37_B, 39_B, 40_B, 41_B, 42_B, 43_B, 44_B, 46_B, 53_B, 55_B, 61_B, 63_B, 68_B, 70_B, 72_B, 79_B, 81_B, 92_B. Ces positions sont impliquées dans le packing dans la majorité des structures.

Détermination des résidus impliqués dans le packing cristallin chez PR1

Identification des résidus impliqués dans le packing cristallin chez au moins une structure de PR1

1. Matrice ne contenant que des protéines PR1

```

type = c("PR1","PR1","PR2","PR1","PR1","PR2","PR2","PR2","PR1","PR1","PR1","PR2","PR2","PR1","PR2","PR1","PR2","PR1")
names(type) = Proteases

ProtPR1 <- names(which(type=="PR1"))
MatricePR1 <- matrice[ProtPR1,]

```

2. Calcul de la significativité

```

nbrSimul <- 10000

f.computPval <- function(MatricePR1, nbrSimul){
  occ.PR1 <- apply(MatricePR1,2,sum)
  resA <- colnames(MatricePR1)[grep("_A", colnames(MatricePR1))]
  resB <- colnames(MatricePR1)[grep("_B", colnames(MatricePR1))]

  occ.SupbyPos.PR1 <- rep(0, length = ncol(MatricePR1))
  names(occ.SupbyPos.PR1) <- colnames(MatricePR1)

  for( rep in 1:nbrSimul){

```

```

mat.rand.A <- t(apply(MatricePR1[,resA],1,f.permut))
mat.rand.B <- t(apply(MatricePR1[,resB],1,f.permut))
matrice.random <- cbind(mat.rand.A, mat.rand.B)
colnames(matrice.random) <- c(resA,resB)
occ.rand <- apply(matrice.random,2,sum)
diff <- occ.rand-occ.PR1
occ.SupyPos.PR1 [names(which(diff > 0))] = occ.SupyPos.PR1[names(which(diff > 0))] +1
}

pval.PR1 <- occ.SupyPos.PR1/nbrSimul
return(pval.PR1)
}

pval.PR1 <- f.computPval(MatricePR1, nbrSimul=20000)

length(which(pval.PR1 < 0.05/ncol(MatricePR1)))

```

[1] 24

```
res.conserv.PR1 <- names(which(pval.PR1 < 0.05))
```

Chez PR1, il y a 41 résidus qui sont impliqués dans le packing cristallin dans la majorité des PR1.

On regarde dans combien de structures de PR1 ses résidus sont impliqués dans le packing

```
occ.PR1 <- apply(MatricePR1,2,sum)
occ.PR1[res.conserv.PR1]
```

2_A	4_A	6_A	7_A	18_A	35_A	37_A	43_A	44_A	46_A	52_A	53_A	55_A	61_A	70_A	72_A	79_A	91_A	92_A	94_A	2_1
10	15	15	12	12	12	14	11	11	12	11	14	10	12	9	15	9	11	15	9	8

On regarde dans combien de structures de PR1 ses résidus sont impliqués dans le packing Il faut différencier les chaînes A et B, car trois structures de PR1 n'ont pas de chaîne B.

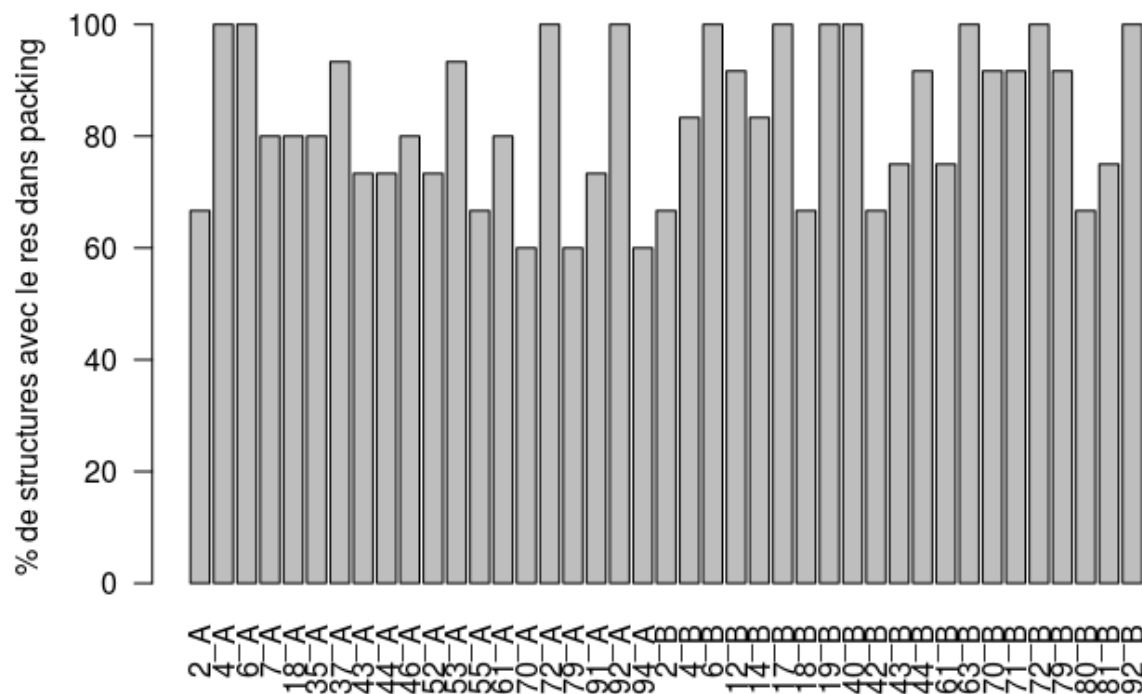
```

resA.1 <- intersect(res.conserv.PR1, colnames(MatricePR1)[grep("_A", colnames(MatricePR1))])
resB.1 <- intersect(res.conserv.PR1, colnames(MatricePR1)[grep("_B", colnames(MatricePR1))])

pourc.PR1 <- round(c(occ.PR1[resA.1] / nrow(MatricePR1),
                    occ.PR1[resB.1] / (nrow(MatricePR1)-3))*100,2)

barplot(pourc.PR1, las=2, ylab="% de structures avec le res dans packing")

```



Ces résidus conservés dans le packing de PR1 sont impliqués dans le packing dans 11.15 (+/- 1.98) structures.

3. Représentation sur une structure 3D des résidus impliqués dans le packing cristallin spécifiques de PR1

- Pour la visualisation utiliser la structure de PR1 complexée au DRV : PDB code : 2ien.
- résidus impliqués dans le packing cristallin spécifiques de PR1 = Résidus ceux qui sont très souvent impliqués dans le packing chez PR1 et très peu voir jamais chez PR2

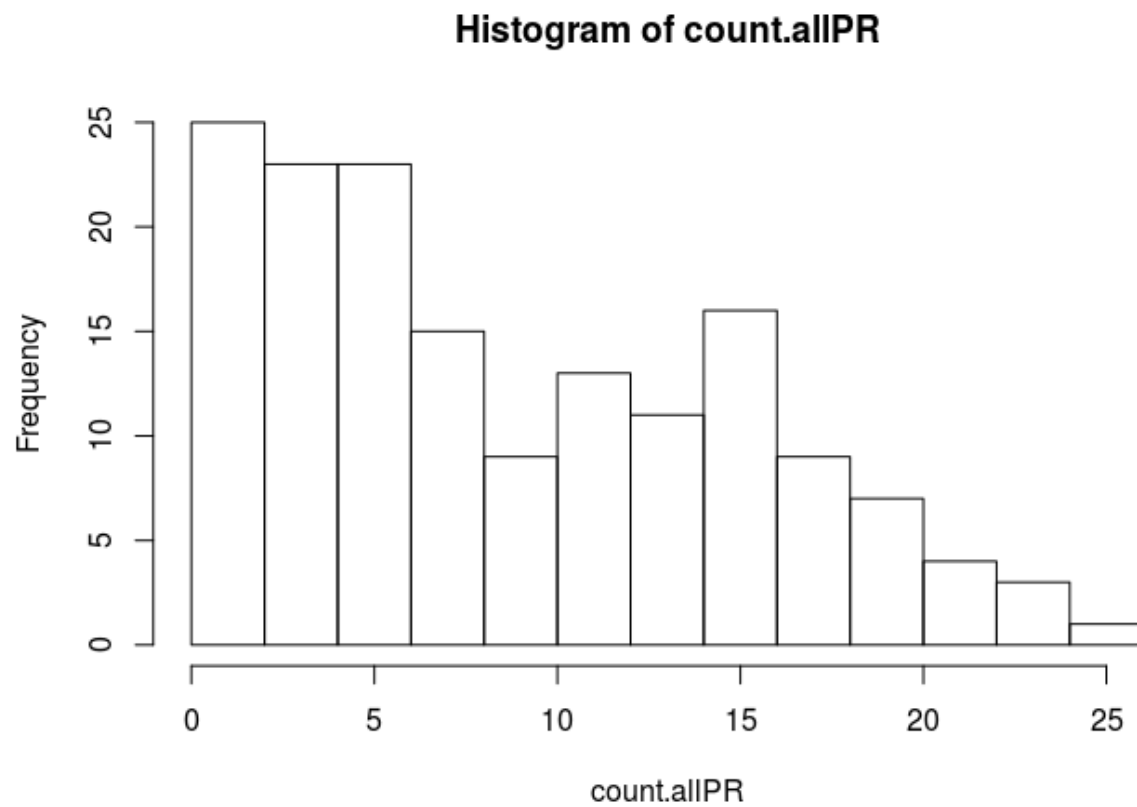
Bien lister les résidus qui ont été colorés et comment ils ont été sélectionnés : quel seuil ?

```
resSel_A_PR1 <- gsub("_A", "", colnames(matrice)[grep("_A", colnames(matrice))])
resSel2_A_PR1 <- paste(resSel_A_PR1, collapse="+")
paste("select respackA, resid ", resSel2_A_PR1, " and chain A", sep="")
```

```
[1] "select respackA, resid 1+2+3+4+5+6+7+8+9+10+11+12+14+15+16+17+18+19+20+21+23+24+25+26+27+29+30+34+35+36+37+38+39+40+41+42+43+44+45+46+47+48+49+50+51+52+53+54+55+56+57+58+59+60+61+62+63+64+65+66+67+68+69+70+71+72+73+74+75+76+77+78+79+80+81+82+83+84+85+86+87+88+89+90+91+92+93+94+95+96+97+98+99+100+101+102+103+104+105+106+107+108+109+110+111+112+113+114+115+116+117+118+119+120+121+122+123+124+125+126+127+128+129+130+131+132+133+134+135+136+137+138+139+140+141+142+143+144+145+146+147+148+149+150+151+152+153+154+155+156+157+158+159+160+161+162+163+164+165+166+167+168+169+170+171+172+173+174+175+176+177+178+179+180+181+182+183+184+185+186+187+188+189+190+191+192+193+194+195+196+197+198+199+200+201+202+203+204+205+206+207+208+209+210+211+212+213+214+215+216+217+218+219+220+221+222+223+224+225+226+227+228+229+230+231+232+233+234+235+236+237+238+239+240+241+242+243+244+245+246+247+248+249+250+251+252+253+254+255+256+257+258+259+260+261+262+263+264+265+266+267+268+269+270+271+272+273+274+275+276+277+278+279+280+281+282+283+284+285+286+287+288+289+290+291+292+293+294+295+296+297+298+299+300+301+302+303+304+305+306+307+308+309+310+311+312+313+314+315+316+317+318+319+320+321+322+323+324+325+326+327+328+329+330+331+332+333+334+335+336+337+338+339+340+341+342+343+344+345+346+347+348+349+350+351+352+353+354+355+356+357+358+359+360+361+362+363+364+365+366+367+368+369+370+371+372+373+374+375+376+377+378+379+380+381+382+383+384+385+386+387+388+389+390+391+392+393+394+395+396+397+398+399+400+401+402+403+404+405+406+407+408+409+410+411+412+413+414+415+416+417+418+419+420+421+422+423+424+425+426+427+428+429+430+431+432+433+434+435+436+437+438+439+440+441+442+443+444+445+446+447+448+449+450+451+452+453+454+455+456+457+458+459+460+461+462+463+464+465+466+467+468+469+470+471+472+473+474+475+476+477+478+479+480+481+482+483+484+485+486+487+488+489+490+491+492+493+494+495+496+497+498+499+500+501+502+503+504+505+506+507+508+509+510+511+512+513+514+515+516+517+518+519+520+521+522+523+524+525+526+527+528+529+530+531+532+533+534+535+536+537+538+539+540+541+542+543+544+545+546+547+548+549+550+551+552+553+554+555+556+557+558+559+560+561+562+563+564+565+566+567+568+569+570+571+572+573+574+575+576+577+578+579+580+581+582+583+584+585+586+587+588+589+590+591+592+593+594+595+596+597+598+599+600+601+602+603+604+605+606+607+608+609+610+611+612+613+614+615+616+617+618+619+620+621+622+623+624+625+626+627+628+629+630+631+632+633+634+635+636+637+638+639+640+641+642+643+644+645+646+647+648+649+650+651+652+653+654+655+656+657+658+659+660+661+662+663+664+665+666+667+668+669+670+671+672+673+674+675+676+677+678+679+680+681+682+683+684+685+686+687+688+689+690+691+692+693+694+695+696+697+698+699+700+701+702+703+704+705+706+707+708+709+710+711+712+713+714+715+716+717+718+719+720+721+722+723+724+725+726+727+728+729+730+731+732+733+734+735+736+737+738+739+740+741+742+743+744+745+746+747+748+749+750+751+752+753+754+755+756+757+758+759+760+761+762+763+764+765+766+767+768+769+770+771+772+773+774+775+776+777+778+779+780+781+782+783+784+785+786+787+788+789+790+791+792+793+794+795+796+797+798+799+800+801+802+803+804+805+806+807+808+809+810+811+812+813+814+815+816+817+818+819+820+821+822+823+824+825+826+827+828+829+830+831+832+833+834+835+836+837+838+839+840+841+842+843+844+845+846+847+848+849+850+851+852+853+854+855+856+857+858+859+860+861+862+863+864+865+866+867+868+869+870+871+872+873+874+875+876+877+878+879+880+881+882+883+884+885+886+887+888+889+890+891+892+893+894+895+896+897+898+899+900+901+902+903+904+905+906+907+908+909+910+911+912+913+914+915+916+917+918+919+920+921+922+923+924+925+926+927+928+929+930+931+932+933+934+935+936+937+938+939+940+941+942+943+944+945+946+947+948+949+950+951+952+953+954+955+956+957+958+959+960+961+962+963+964+965+966+967+968+969+970+971+972+973+974+975+976+977+978+979+980+981+982+983+984+985+986+987+988+989+990+991+992+993+994+995+996+997+998+999+1000+1001+1002+1003+1004+1005+1006+1007+1008+1009+1010+1011+1012+1013+1014+1015+1016+1017+1018+1019+1020+1021+1022+1023+1024+1025+1026+1027+1028+1029+1030+1031+1032+1033+1034+1035+1036+1037+1038+1039+1040+1041+1042
```

```
#type[rownames(matrice)[j]] == "PR1"
```

```
count.allPR <- apply(matrice, 2, sum)
hist(count.allPR)
```

```
dim(matrice)
```

```
[1] 26 159
```

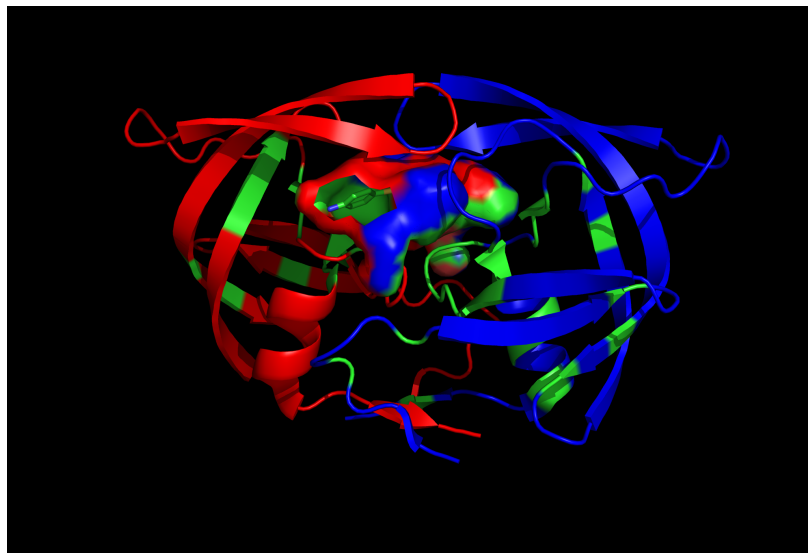


Figure 1: legende

Calcul du nombre de structure dans lequel un résidu est impliqué dans le packing cristallin pour les PR1

1. Calculer le nombre de structure dans lequel un résidu est impliqué dans le packing cristallin pour les PR1

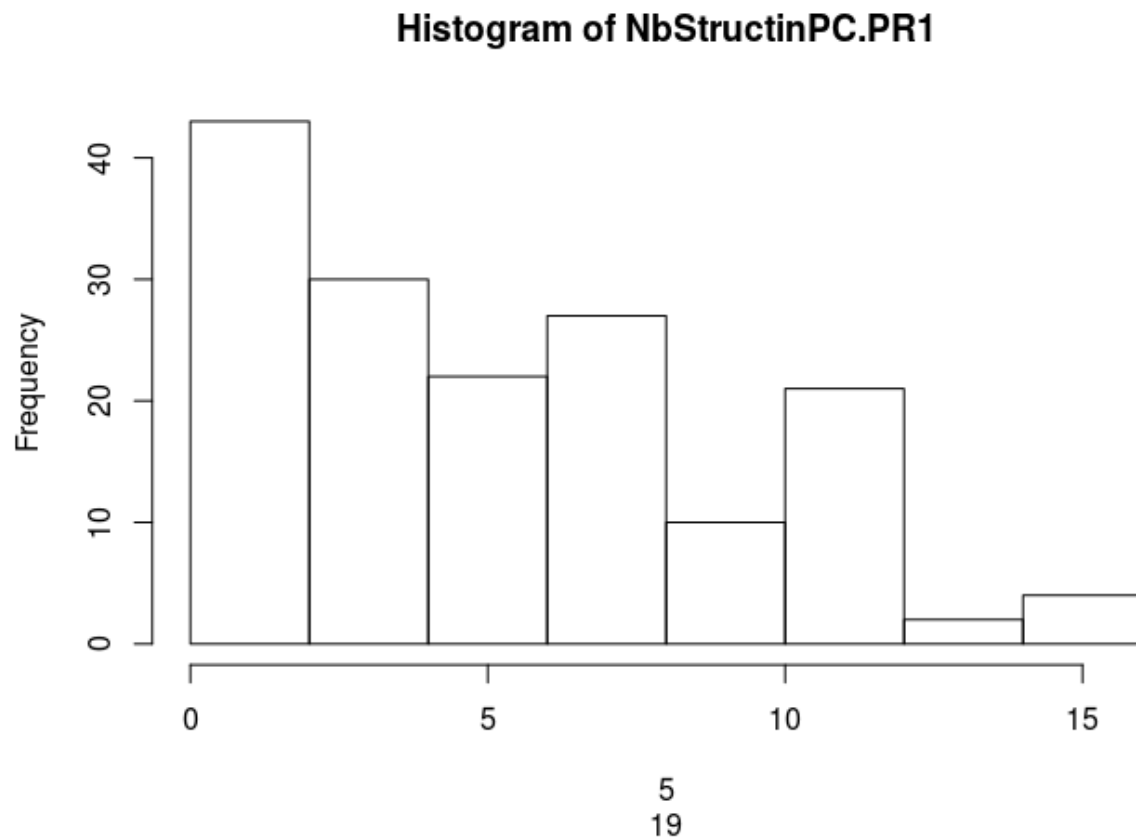
```
##version courte
NbStructinPC = apply(matrice,2,sum)

ind.PR1 = names(which(type == "PR1"))
NbStructinPC.PR1 = apply(matrice[ind.PR1,],2,sum)

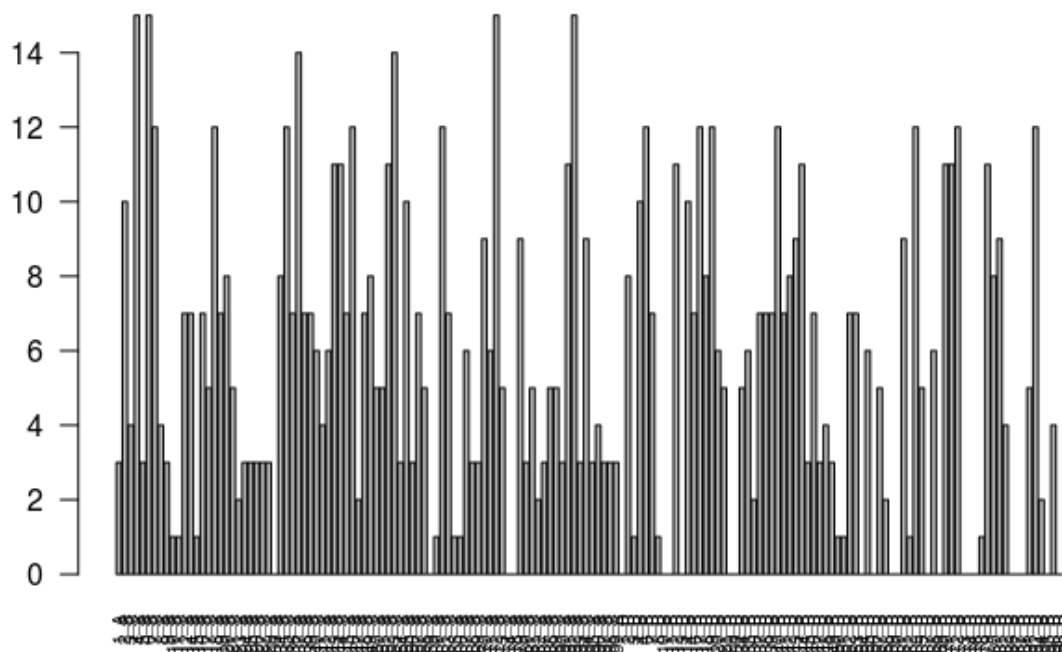
matriceStruct = rbind(NbStructinPC,NbStructinPC.PR1)
```

2. Représenter ces valeurs graphiquement

```
hist(NbStructinPC.PR1, xlab = matriceStruct[1,])
```



```
barplot(NbStructinPC.PR1, las = 2, cex.names = 0.6)
```



3. Calculer la moyenne et écart type de ce nombre

```
mean(matriceStruct["NbStructinPC.PR1",])
```

```
[1] 5.408805
```

```
sd(matriceStruct["NbStructinPC.PR1",])
```

```
[1] 4.182867
```

Etude du type d'atomes impliqués dans le packing cristallin chez PR1

```
Localisation = c("Backbone", "ChaineLat")
```

```
matrice3PR1 <- matrix(0, nrow=length(Localisation), ncol=length(NbResidues))
```

```
rownames(matrice3PR1) <- Localisation
```

```
colnames(matrice3PR1) <- sort.res
```

```
type.file = c("PR1", "PR1", "PR2", "PR1", "PR1", "PR2", "PR2", "PR2", "PR1", "PR1", "PR1", "PR2", "PR2", "PR1", "PR2"
```

```
names(type.file) = c("1hhp_packCryst.pdb", "1hih_packCryst.pdb", "1hii_packCryst.pdb", "1hiv_packCryst.pdb"
```

```
ind.PR1 = names(which(type.file == "PR1"))
```

```

#ici je ne comprends pas pourquoi vous faites une double boucle
listAtomSyn = c()

listAtomSyn = NULL
listAtomSyn2 = NULL

pp =NULL

for (j in NbProt) {
  for (i in 1:length(ind.PR1)){
    filein = listFile[j]
    N = read.table(paste("fileByProt3",filein,sep="/"))
    if((filein) == (ind.PR1[i])){
      pp = c(pp, filein)
      listAtom = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))
      listAtomSyn = (c(listAtom,listAtomSyn))
    }
  }
}

for (j in NbProt){
  for (i in 1:length(ind.PR1)) {
    filein = listFile[j]

    if((filein) == (ind.PR1[i])){
      N = read.table(paste("fileByProt3",filein,sep="/"))
      listAtom = (paste(as.character(N[,3])))
      listAtomSyn2 = (c(listAtom,listAtomSyn2))
    }
  }
}

NbAtomeinPC.1 = c(1:length(listAtomSyn2))
names(listAtomSyn) = listAtomSyn2

for (j in 1:length(sort.res)) {
  for (k in 1:length(NbAtomeinPC.1)) {

    if (sort.res[j] == listAtomSyn[k]){

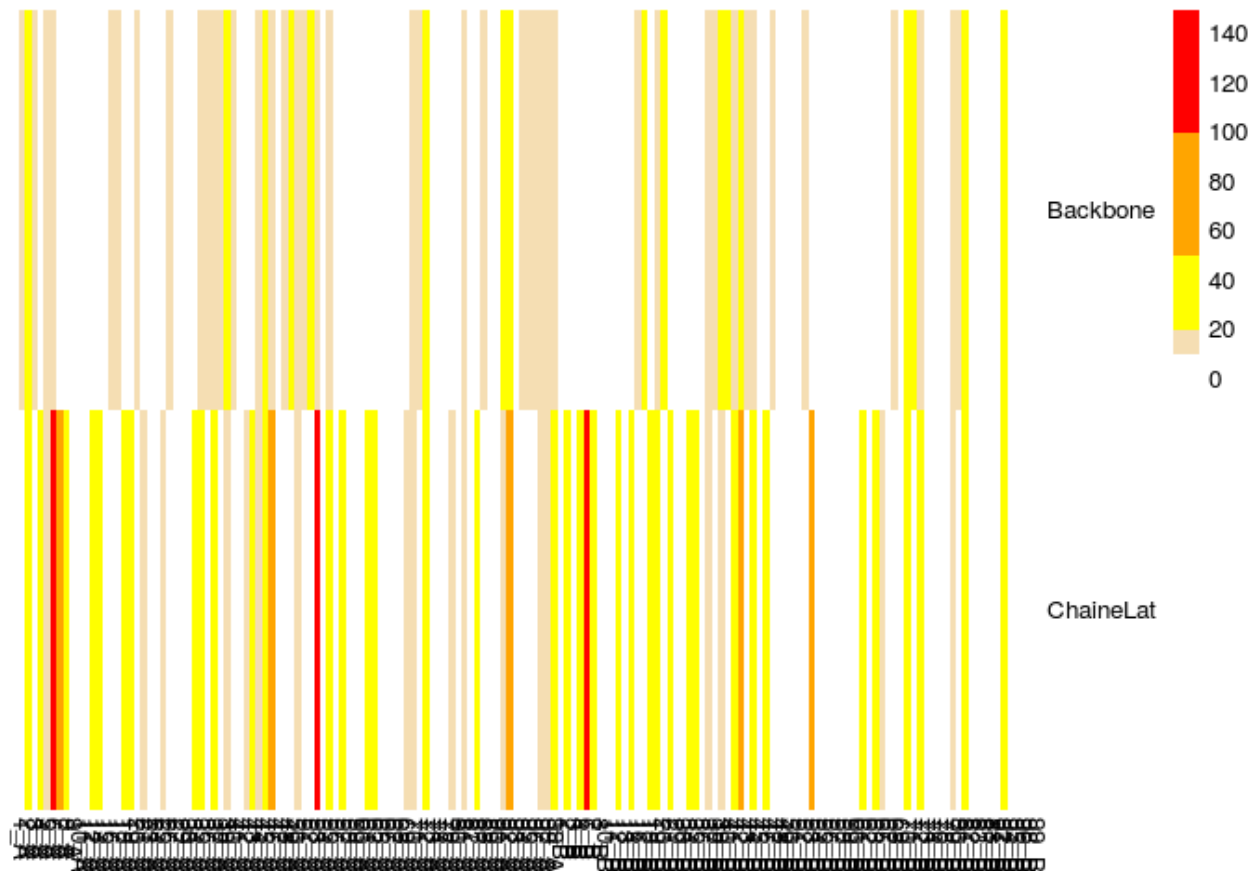
      if (((listAtomSyn2)[k]) == "C") || (((listAtomSyn2)[k]) == "CA") || (((listAtomSyn2)[k]) == "O")

      matrice3PR1[1,sort.res[j]] = matrice3PR1[1,sort.res[j]] + 1
    }else{
      matrice3PR1[2,sort.res[j]] = matrice3PR1[2,sort.res[j]] + 1
    }
  }
}

}

pheatmap(matrice3PR1, cluster_cols = FALSE, cluster_rows = FALSE, breaks = c(-1, 10, 20, 50, 100, 150),

```



A refaire pour le nombre de protéine : matrice avec des 0 et 1 pour PR1

```
ProtPR1 = c("1hhp", "1hih", "1hiv", "1hpv", "1sdt", "2hb3", "2hb4", "2ien", "2nph", "2z4o", "3ekv", "3nu3", "3phv")
list.bk = c("C", "O", "N", "CA")

matriceBackBonePR1 <- matrix(0, nrow=length(ProtPR1), ncol=length(NbResidues))

rownames(matriceBackBonePR1) <- ProtPR1
colnames(matriceBackBonePR1) <- sort.res

matriceChaineLatPR1 <- matrix(0, nrow=length(ProtPR1), ncol=length(NbResidues))

rownames(matriceChaineLatPR1) <- ProtPR1
colnames(matriceChaineLatPR1) <- sort.res

NbAtomeinPC = c(1:length(listAtomSyn2))
names(listAtomSyn) = listAtomSyn2
for (i in 1:length(ind.PR1)) {

  listAtomSyn = NULL
  listAtomSyn2 = NULL

  filein = ind.PR1[i]
```

```
N = read.table(paste("fileByProt3",filein,sep="/"))

listAtomSyn = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))

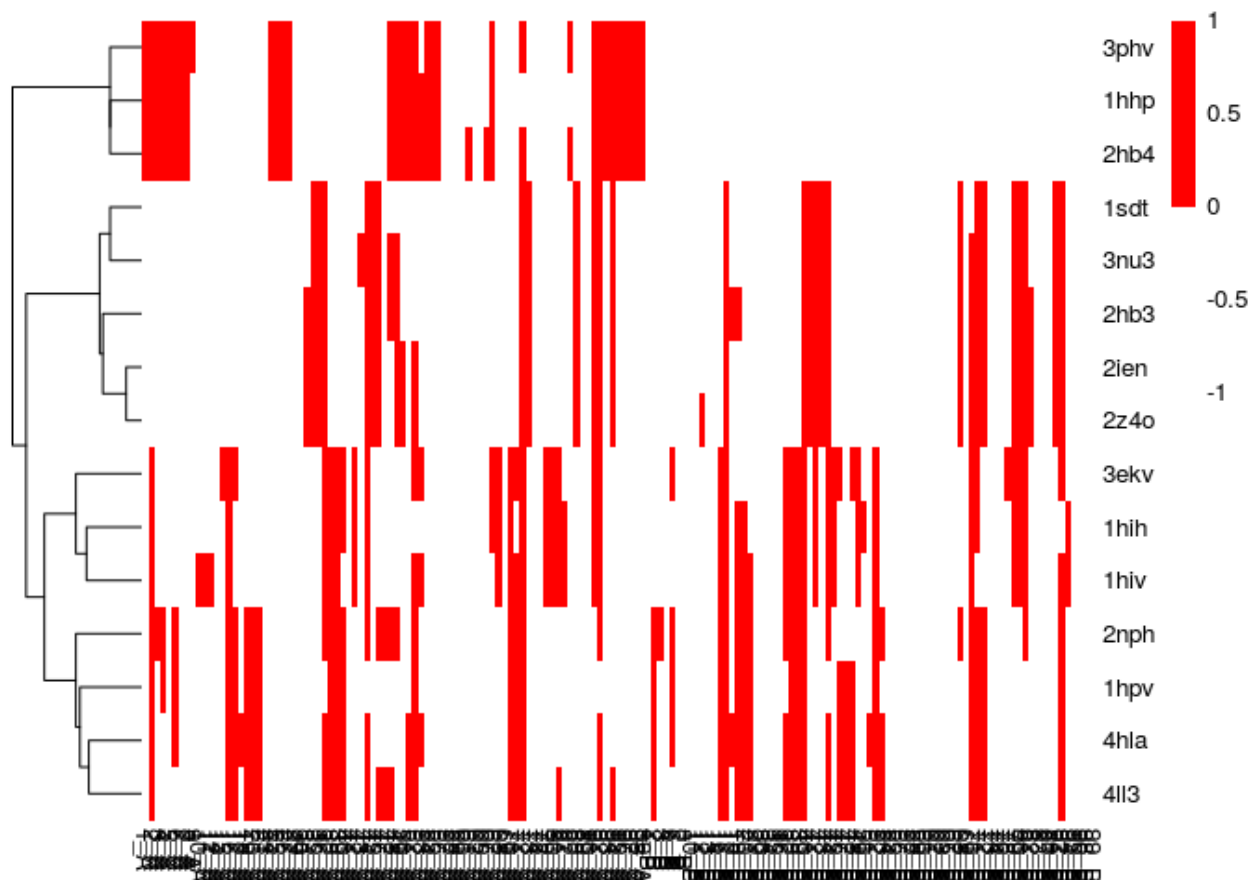
listAtomSyn2 = (paste(as.character(N[,3])))

for (k in 1:length(listAtomSyn)) {
  for (j in 1:length(sort.res)) {

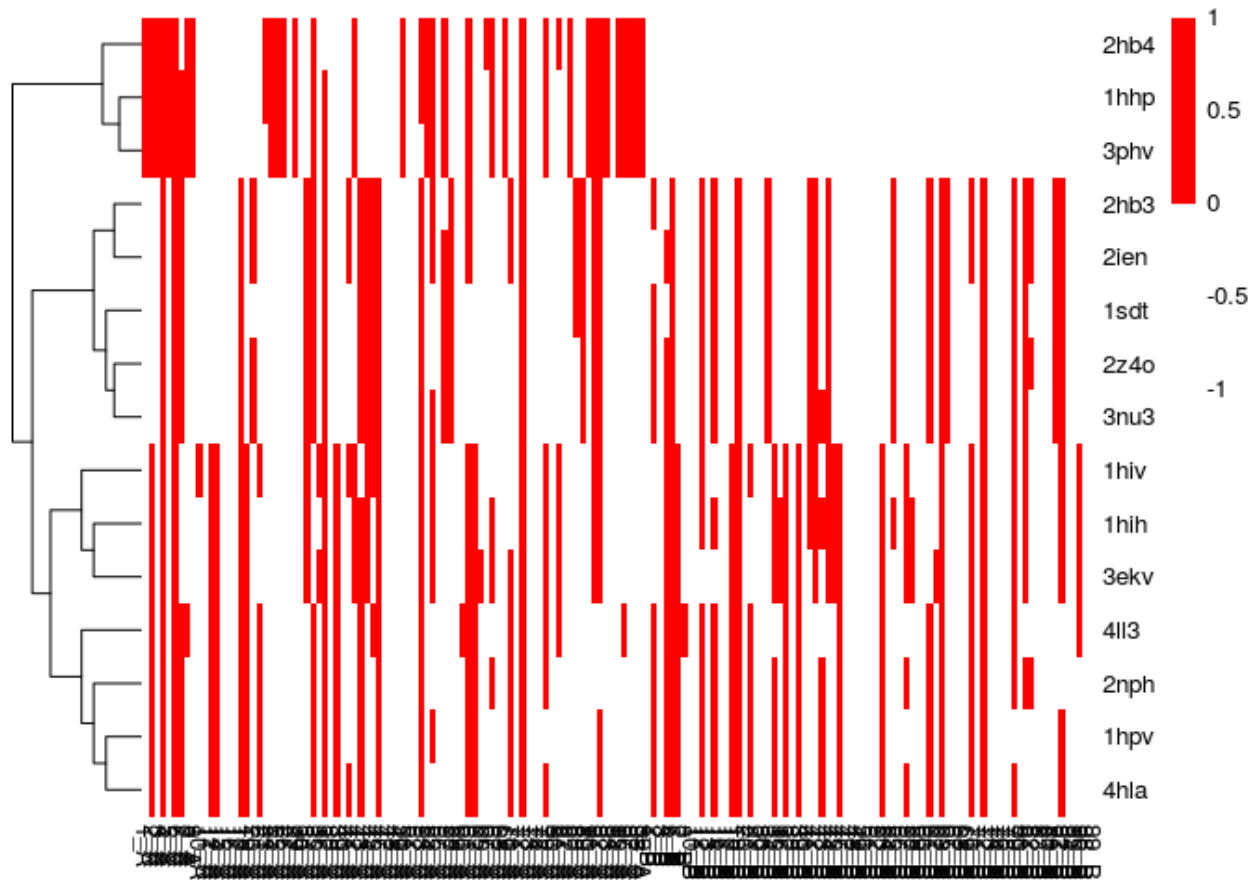
    if (listAtomSyn[k] == sort.res[j]){
      if (is.element(listAtomSyn2[k], list.bk)==TRUE){

        matriceBackBonePR1[ProtPR1[i],sort.res[j]] = 1
      }else{
        matriceChaineLatPR1[ProtPR1[i],sort.res[j]] = 1
      }
    }
  }
}

pheatmap(matriceBackBonePR1[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1, col=c("white"
```



```
heatmap(matriceChaineLatPR1[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1, col=c("white", "red"))
```



Détermination des résidus impliqués dans le packing cristallin chez PR1

Identification des résidus impliqués dans le packing cristallin dans au moins une structure de PR2

1. Calcul de la matrice donnant si le résidu est impliqué dans le packing chez une des structures de PR2

```
type = c("PR1","PR1","PR2","PR1","PR1","PR2","PR2","PR2","PR1","PR1","PR1","PR2","PR2","PR1","PR2","PR1")
names(type) = Proteases

ProtPR2 = names(which(type=="PR2"))

MatricePR2 <- matrice[ProtPR2,]
dim(MatricePR2)
```

```
[1] 11 159
```

2. Calcul de la significativité pour déterminer les résidus conservés

```
pval.PR2 <- f.computPval(MatricePR2, nbrSimul=20000)
res.conserv.PR2 <- names(which(pval.PR2 < 0.05))
```

Chez PR2, il y a 40 résidus qui sont impliqués dans le packing cristallin dans la majorité des PR2.

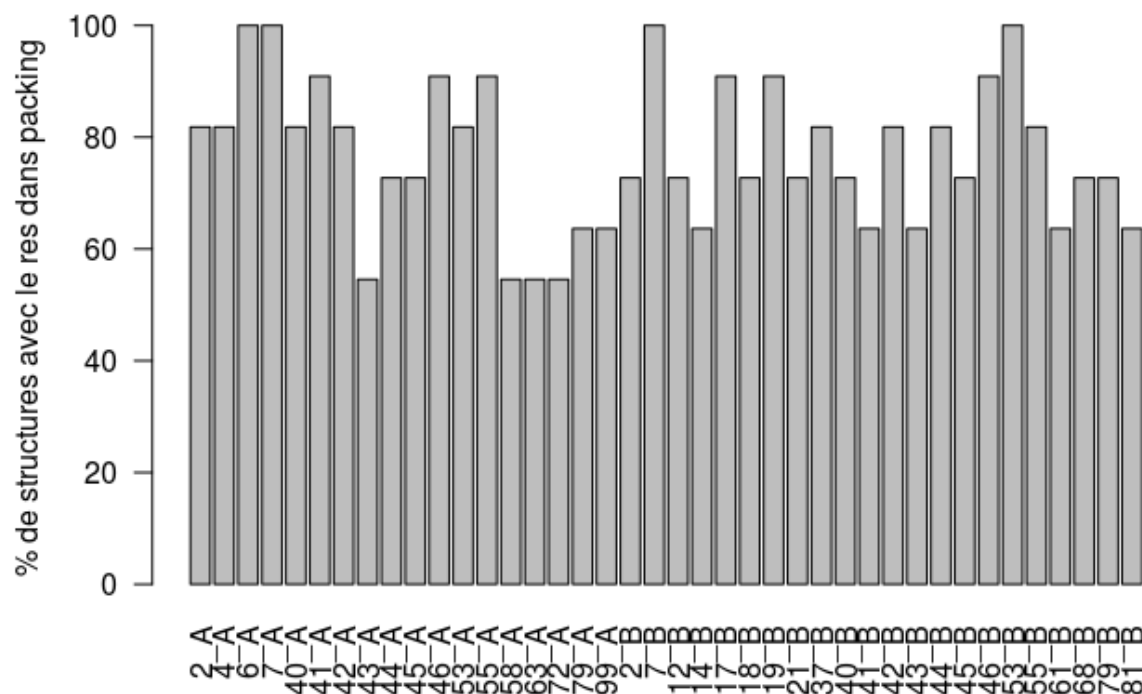
On regarde dans combien de structures de PR1 ses résidus sont impliqués dans le packing

```
occ.PR2 <- apply(MatricePR2,2,sum)
occ.PR2[res.conserv.PR2]
```

```
2_A  4_A  6_A  7_A 40_A 41_A 42_A 43_A 44_A 45_A 46_A 53_A 55_A 58_A 63_A 72_A 79_A 99_A 2_B  7_B 12_B
  9    9   11   11   9   10   9    6    8    8   10    9   10    6    6    6    7    7    8   11    8
```

On calcule le pourcentage de structures de PR2 contenant ces résidus dans le packing

```
pourc.PR2 <- round(occ.PR2[res.conserv.PR2] / nrow(MatricePR2)*100,2)
barplot(pourc.PR2, las=2, ylab="% de structures avec le res dans packing")
```



Ces résidus conservés dans le packing de PR2 sont impliqués dans le packing dans 8.45 (+/- 1.47) structures.

3. Représentation sur une structure 3D des résidus impliqués dans le packing cristallin spécifiques de PR2

- Pour la visualisation utiliser la structure de PR2 complexée au DRV : PDB code : 3EBZ.
- résidus impliqués dans le packing cristallin spécifiques de PR2 = Résidus ceux qui sont très souvent impliqués dans le packing chez PR2 et très peu voir jamais chez PR1

Bien lister les résidus qui ont été colorés et comment ils ont été sélectionnés : quel seuil ?

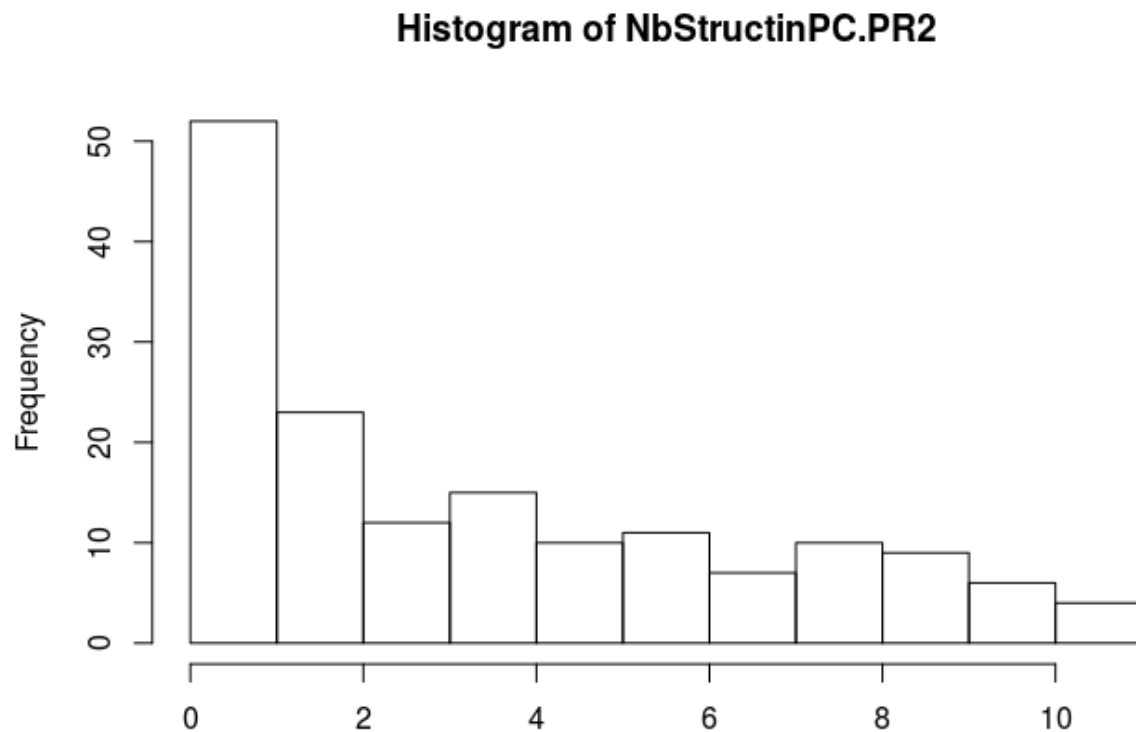
Calcul du nombre de structures de PR2 dans lequel un résidu est impliqué dans le packing cristallin

1. Calculer le nombre de structure dans lequel un résidu est impliqué dans le packing cristallin pour les PR2

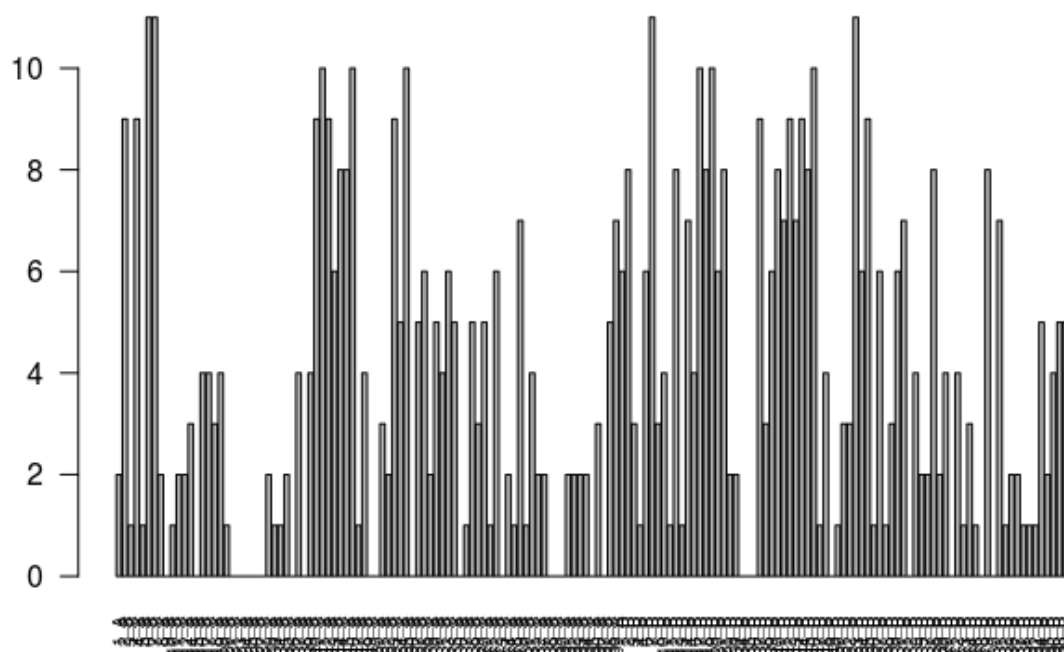
```
ind.PR2 = names(which(type == "PR2"))  
  
NbStructinPC.PR2 = apply(matrice[ind.PR2,], 2, sum)  
  
matriceStruct = rbind(matriceStruct, NbStructinPC.PR2)
```

2. Représenter ces valeurs graphiquement

```
hist(NbStructinPC.PR2, xlab = "")
```



```
barplot(NbStructinPC.PR2, las = 2, cex.names = 0.6)
```



3. Calculer la moyenne et écart type de ce nombre

```
mean(matriceStruct["NbStructinPC.PR2",])
```

```
[1] 3.748428
```

```
sd(matriceStruct["NbStructinPC.PR2",])
```

```
[1] 3.25298
```

Type d'atomes impliqués dans le packing cristallin chez PR2

```
Localisation = c("Backbone", "ChaineLat")

matrice3PR2 <- matrix(0, nrow=length(Localisation), ncol=length(NbResidues))

rownames(matrice3PR2) <- Localisation
colnames(matrice3PR2) <- sort.res

ind.PR2 = names(which(type.file == "PR2"))

listAtomSyn2 = NULL
listAtomSyn = NULL

listAtomSyn = c()
```

```

for (j in NbProt) {
  for (i in 1:length(ind.PR2)){
    filein = listFile[j]
    if((filein) == (ind.PR2[i])){
      N = read.table(paste("fileByProt3",filein,sep="/"))
      listAtom = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))
      listAtomSyn = (c(listAtom,listAtomSyn))
    }
  }
}

for (j in NbProt){
  for (i in 1:length(ind.PR2)) {
    filein = listFile[j]
    if((filein) == (ind.PR2[i])){
      N = read.table(paste("fileByProt3",filein,sep="/"))
      listAtom = (paste(as.character(N[,3])))
      listAtomSyn2 = (c(listAtom,listAtomSyn2))
    }
  }
}

NbAtomeinPC.2 = c(1:length(listAtomSyn2))
list.bk = c("C","CA","N","O")
names(listAtomSyn) = listAtomSyn2

for (j in 1:length(sort.res)) {
  for (k in 1:length(NbAtomeinPC.2)) {

    if (sort.res[j] == listAtomSyn[k]){

      #if (((listAtomSyn2[k]) == "C") || ((listAtomSyn2[k]) == "CA") || ((listAtomSyn2[k]) == "O"))
      if (is.element(listAtomSyn2[k], list.bk)==TRUE){

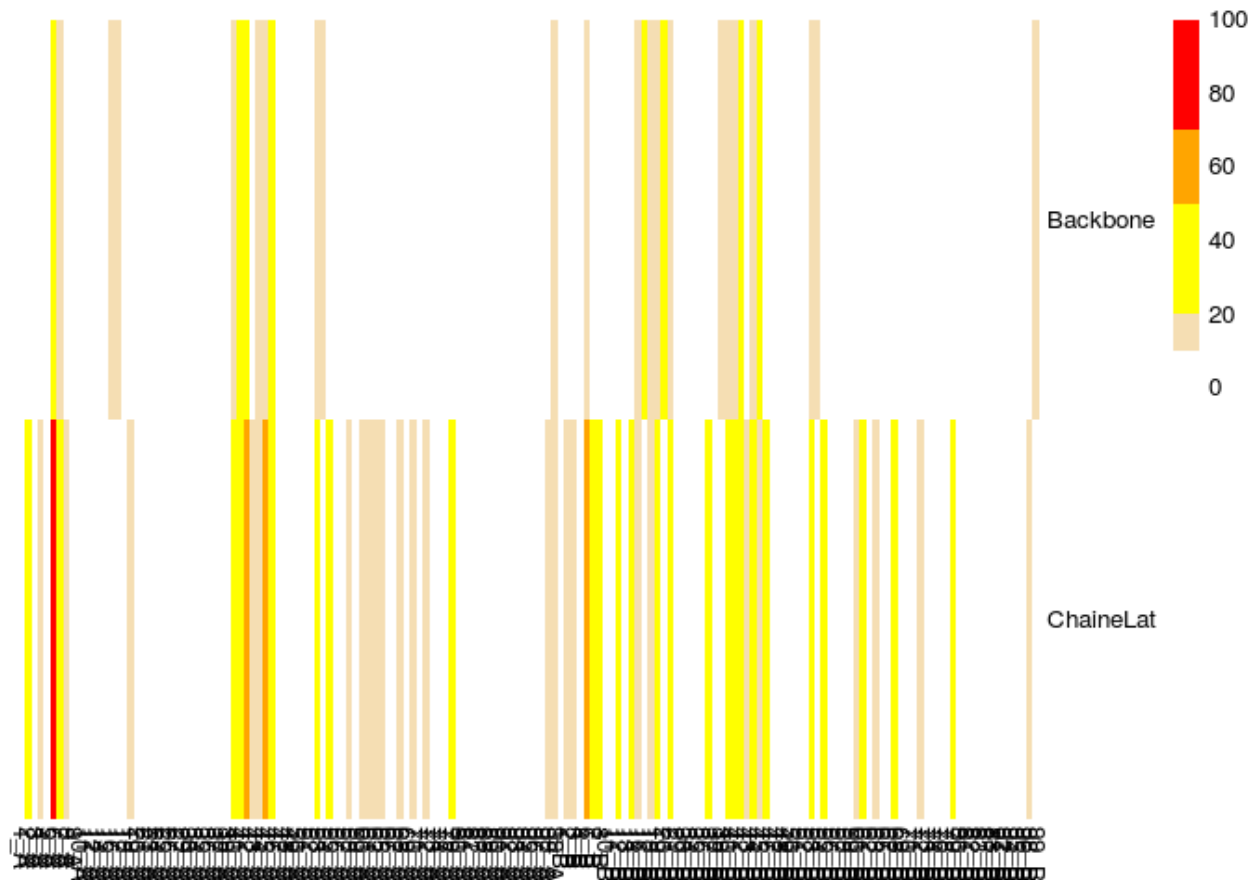
        matrice3PR2[1,sort.res[j]] = matrice3PR2[1,sort.res[j]] + 1
      }else{
        matrice3PR2[2,sort.res[j]] = matrice3PR2[2,sort.res[j]] + 1
      }
    }
  }
}
matrice3PR2

```

	1_A	2_A	3_A	4_A	5_A	6_A	7_A	8_A	9_A	10_A	11_A	12_A	14_A	15_A	16_A	17_A	18_A	19_A	20_A	21_A	23_A
Backbone	4	6	0	1	1	25	12	0	0	0	0	1	0	0	13	18	2	2	2	0	
ChaineLat	2	22	2	19	0	93	46	11	0	1	2	2	10	0	10	0	7	11	2	0	
	68_A	69_A	70_A	71_A	72_A	73_A	74_A	78_A	79_A	80_A	81_A	82_A	87_A	88_A	89_A	90_A	91_A	92_A	93_A		
Backbone	2	2	2	1	2	0	0	2	7	4	6	0	0	0	0	0	2	3	4		
ChaineLat	15	4	18	0	14	0	3	0	22	0	4	3	3	0	0	0	0	0	0		
	48_B	49_B	50_B	51_B	52_B	53_B	54_B	55_B	56_B	57_B	58_B	59_B	60_B	61_B	62_B	63_B	65_B	67_B	68_B		
Backbone	8	0	1	6	8	16	15	8	4	0	0	0	2	4	0	0	0	3	7		
ChaineLat	0	0	0	0	0	39	7	34	0	10	3	3	16	21	0	15	7	4	30		

```
matricetotale = matrice3PR1 + matrice3PR2
```

```
pheatmap(matrice3PR2, cluster_cols = FALSE, cluster_rows = FALSE, breaks = c(-1, 10, 20, 50, 70, 100),
```



A refaire pour le nombre de protéine : matrice avec des 0 et 1 pour PR2

```
ProtPR2 = c("1hii", "1hsh", "1hsi", "1ivp", "2hpe", "2hpf", "2mip", "3ebz", "3ec0", "3ecg", "3s45")
```

```
list.bk = c("C", "O", "N", "CA")
```

```
matriceBackBonePR2 <- matrix(0, nrow=length(ProtPR2), ncol=length(NbResidues))
```

```
rownames(matriceBackBonePR2) <- ProtPR2
```

```
colnames(matriceBackBonePR2) <- sort.res
```

```
matriceChaineLatPR2 <- matrix(0, nrow=length(ProtPR2), ncol=length(NbResidues))
```

```
rownames(matriceChaineLatPR2) <- ProtPR2
```

```
colnames(matriceChaineLatPR2) <- sort.res
```

```
NbAtomeinPC = c(1:length(listAtomSyn2))
```

```
names(listAtomSyn) = listAtomSyn2
```

```
for (i in 1:length(ind.PR2)) {
```

```

listAtomSyn = NULL
listAtomSyn2 = NULL

filein = ind.PR2[i]
N = read.table(paste("fileByProt3",filein,sep="/"))

listAtomSyn = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))

listAtomSyn2 = (paste(as.character(N[,3])))

for (k in 1:length(listAtomSyn)) {
  for (j in 1:length(sort.res)) {

    if (listAtomSyn[k] == sort.res[j]){
      if (is.element(listAtomSyn2[k], list.bk)==TRUE){

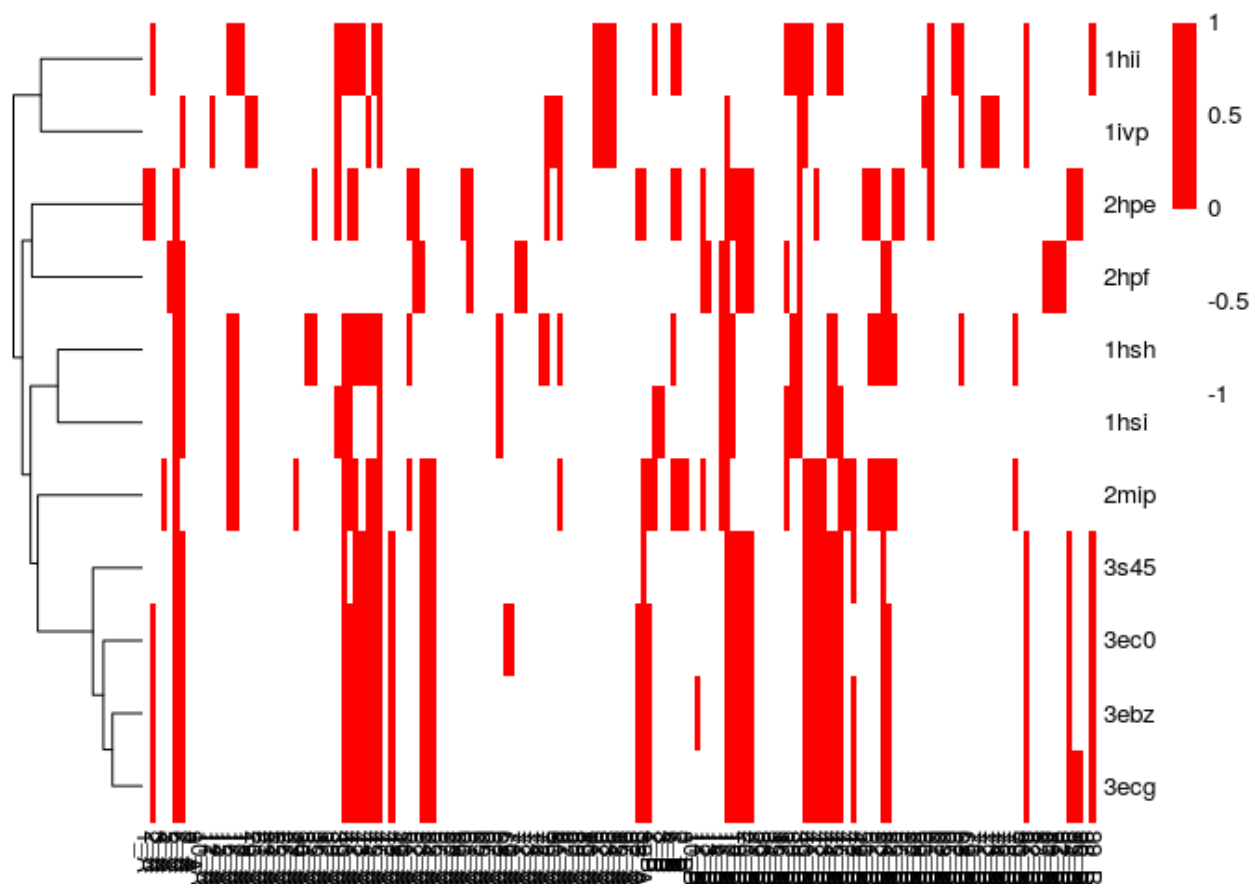
        matriceBackBonePR2[ProtPR2[i],sort.res[j]] = 1
      }else{
        matriceChaineLatPR2[ProtPR2[i],sort.res[j]] = 1
      }
    }
  }
}

}

}

heatmap(matriceBackBonePR2[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1, col=c("white

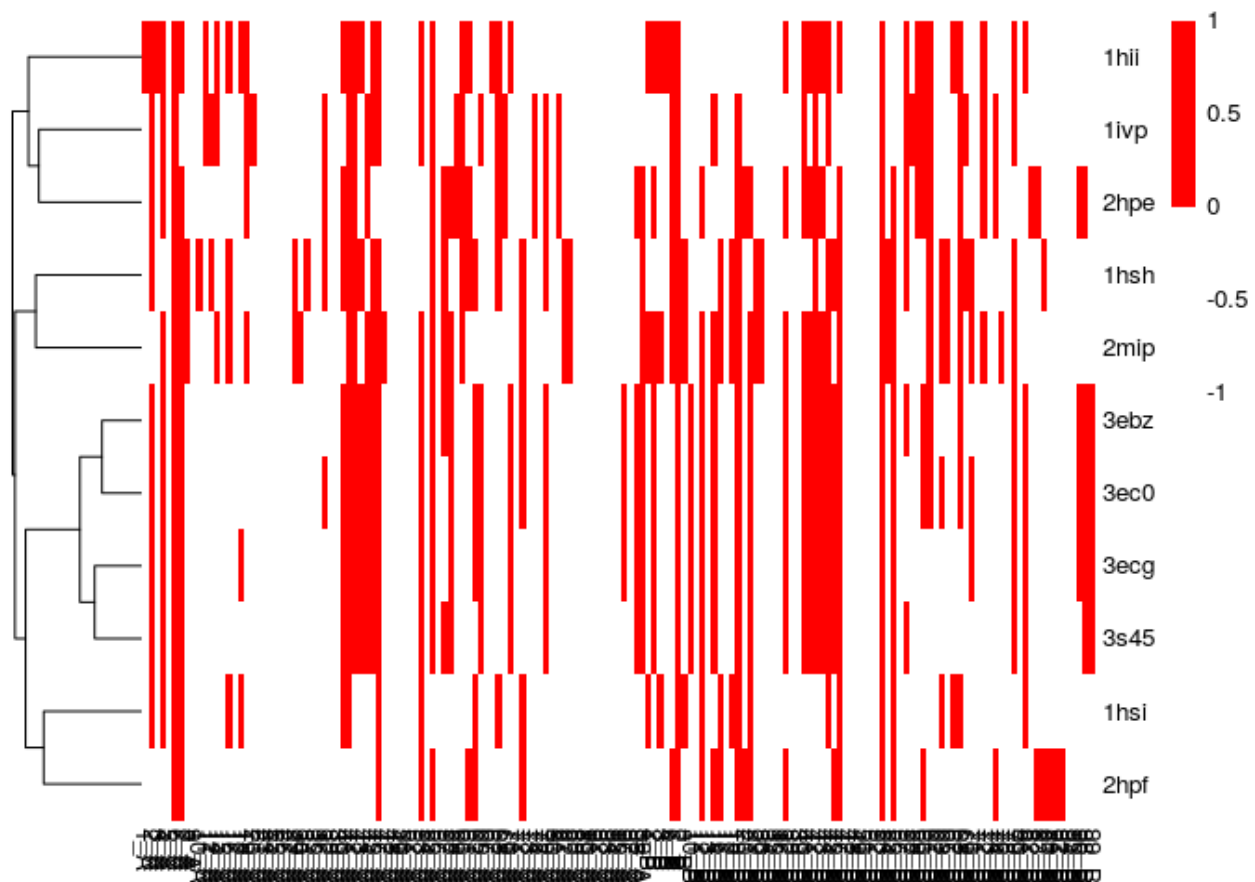
```



```

pheatmap(matriceChaineLatPR2[-27:-29,], cluster_rows = TRUE, cluster_cols = FALSE, br=-1:1, col=c("white", "black", "red", "blue"))

```



Comparaison des résidus impliqués dans le packing cristallin chez PR1 et PR2

différence des résidus impliqués dans le packing chez PR1 et PR2

résidus conservés chez PR1 et pas chez PR2

```
consrvPR1.NotinPR2 <- setdiff(res.conserv.PR1, res.conserv.PR2)
```

Il y a 17 résidus qui sont impliqués dans le packing chez la plupart des PR1 mais pas chez PR2 : 18_A, 35_A, 37_A, 52_A, 61_A, 70_A, 91_A, 92_A, 94_A, 4_B, 6_B, 63_B, 70_B, 71_B, 72_B, 80_B, 92_B.

Pour chaque résidu, on regarde :

- Nombre de structures de PR1 et PR2 avec ces résidus dans le packing
- la localisation de ces résidus dans la structure
- le type d'atomes
- si c'est un résidu muté

```
regionfile <- read.table("description_regions.csv", sep=",")
regionV = c(as.character(regionfile[,2]), as.character(regionfile[,2]))
names(regionV) <- c(paste(as.character(regionfile[,1]), "A", sep="_"),
  paste(as.character(regionfile[,1]), "B", sep="_"))
```

Détermine si les résidus sont mutés

```
mut.diff11 <- rep("no", length = length(consvPR1.NotinPR2))
names(mut.diff11) <- consvPR1.NotinPR2
mut.diff11[intersect(res.muT, consvPR1.NotinPR2)] = "yes"
```

```
tmp.occ <- data.frame(consvPR1.NotinPR2,
                      occ.PR1[consvPR1.NotinPR2],
                      occ.PR2[consvPR1.NotinPR2],
                      regionV[consvPR1.NotinPR2],
                      t(matrice3PR1[,consvPR1.NotinPR2]),
                      t(matrice3PR2[,consvPR1.NotinPR2]),
                      mut.diff11
                      )
colnames(tmp.occ) <- c("residues", "PR1.Occ", "PR2.Occ", "loc",
                      "BB.PR1", "SC.PR1",
                      "BB.PR2", "SC.PR2", "mutation")
tmp.occ
```

	residues	PR1.Occ	PR2.Occ	loc	BB.PR1	SC.PR1	BB.PR2	SC.PR2	mutation
18_A	18_A	12	3	fulcrum	1	48	2	7	no
35_A	35_A	12	2	R2	20	37	2	0	yes
37_A	37_A	14	4	elbow	15	38	0	10	yes
52_A	52_A	11	2	flaps	24	0	2	0	no
61_A	61_A	12	4	cantilever	4	42	3	14	yes
70_A	70_A	9	5	cantilever	16	14	2	18	no
91_A	91_A	11	2	alpha-helix	22	20	2	0	no
92_A	92_A	15	2	alpha-helix	36	56	3	0	yes
94_A	94_A	9	2	alpha-helix	19	0	4	0	no
4_B	4_B	10	1	dimer	0	21	0	2	yes
6_B	6_B	12	6	R1	5	113	11	51	no
63_B	63_B	12	4	cantilever	0	26	0	15	no
70_B	70_B	11	4	cantilever	26	26	0	6	no
71_B	71_B	11	0	cantilever	28	0	0	0	yes
72_B	72_B	12	4	cantilever	20	35	2	15	yes
80_B	80_B	8	0	wall	18	0	0	0	no
92_B	92_B	12	1	alpha-helix	31	47	2	1	yes

résidus conservés chez PR2 et pas chez PR1

```
consvPR2.NotinPR1 <- setdiff(res.conserv.PR2, res.conserv.PR1)
```

Il y a 16 résidus qui sont impliqués dans le packing chez la plupart des PR1 mais pas chez PR2 : 40_A, 41_A, 42_A, 45_A, 58_A, 63_A, 99_A, 7_B, 21_B, 37_B, 41_B, 45_B, 46_B, 53_B, 55_B, 68_B.

Pour chaque résidu, on regarde :

- Nombre de structures de PR1 et PR2 avec ces résidus dans le packing
- la localisation de ces résidus dans la structure
- le type d'atomes
- si c'est un résidu muté

Détermine si les résidus sont mutés

```
mut.diff2 <- rep("no", length = length(consvPR2.NotinPR1))
names(mut.diff2) <- consvPR2.NotinPR1
```



```
mut.diff2[intersect(res.muT, consvPR2.NotinPR1)] = "yes"
```

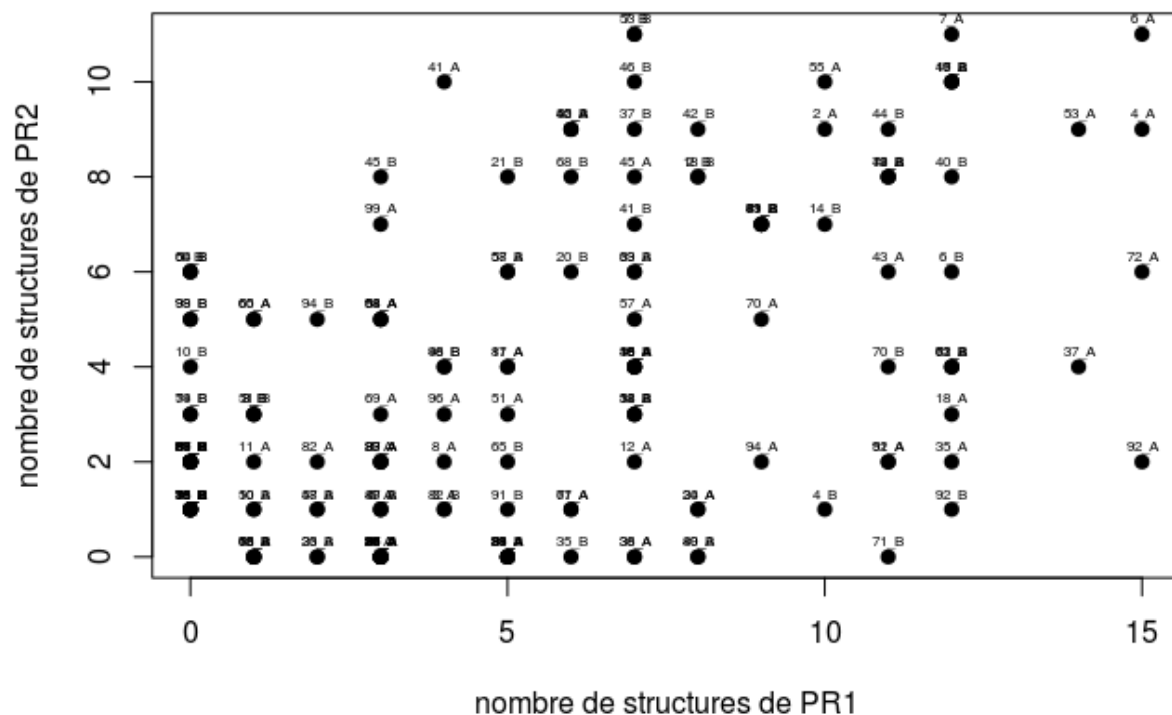
```
tmp.occ <- data.frame(consvPR2.NotinPR1,
                      occ.PR1[consvPR2.NotinPR1],
                      occ.PR2[consvPR2.NotinPR1],
                      regionV[consvPR2.NotinPR1],
                      t(matrice3PR1[,consvPR2.NotinPR1]),
                      t(matrice3PR2[,consvPR2.NotinPR1]),
                      mut.diff2
                      )
colnames(tmp.occ) <- c("residues", "PR1.Occ", "PR2.Occ", "loc",
                      "BB.PR1", "SC.PR1",
                      "BB.PR2", "SC.PR2", "mutation")
tmp.occ
```

	residues	PR1.Occ	PR2.Occ	loc	BB.PR1	SC.PR1	BB.PR2	SC.PR2	mutation
40_A	40_A	6	9	elbow	13	0	18	23	yes
41_A	41_A	4	10	elbow	0	10	23	42	yes
42_A	42_A	6	9	elbow	3	18	24	51	yes
45_A	45_A	7	8	flaps	21	33	16	52	no
58_A	58_A	5	6	flaps	0	10	0	12	yes
63_A	63_A	7	6	cantilever	0	21	0	15	no
99_A	99_A	3	7	dimer	12	24	14	11	yes
7_B	7_B	7	11	R1	0	28	7	45	yes
21_B	21_B	5	8	fulcrum	6	21	14	38	no
37_B	37_B	7	9	elbow	11	15	10	25	yes
41_B	41_B	7	7	elbow	15	46	20	34	yes
45_B	45_B	3	8	flaps	8	10	21	14	no
46_B	46_B	7	10	flaps	9	26	9	28	no
53_B	53_B	7	11	flaps	3	53	16	39	no
55_B	55_B	6	9	flaps	0	7	8	34	yes
68_B	68_B	6	8	cantilever	13	0	7	30	yes

Représentation du nombre de structures de PR1 ayant chaque résidu comme asymétrique en fonction du nombre de structures de PR1 ayant chaque résidu comme asymétrique

Refaire ce graphique en % car nombre PR1 n'est pas le même que le nombre de PR2

```
plot(matriceStruct["NbStructinPC.PR1",], matriceStruct["NbStructinPC.PR2",], pch = 19,
     xlab="nombre de structures de PR1",
     ylab="nombre de structures de PR2")
text(matriceStruct["NbStructinPC.PR1",], matriceStruct["NbStructinPC.PR2",],
     colnames(matriceStruct), pos=3, offset=0.3, cex=0.5 )
```



On calcule ensuite la corrélation entre ces deux variables

```
cor(matriceStruct["NbStructinPC.PR1",], matriceStruct["NbStructinPC.PR2",])
```

```
[1] 0.465773
```

Localisation des résidus impliqués dans le packing cristallin

Pour PR

```
RegionPacking = c("dimer1A","R1A","fulcrumA","catalyticA","R2A","elbowA","flapsA","cantileverA","R3A","")
ResidueTotaux = c("1_A","2_A","3_A","4_A","5_A","6_A","7_A","8_A","9_A","10_A","11_A","12_A","13_A","14_A")

regionfile <- read.table("description_regions.csv", sep=",")
regionV = (paste(as.character(regionfile[,2])))

for (i in 1:99) {
  regionV[i+99]=regionV[i]
}

regionSyn = NULL
for (i in 1:length(ResidueTotaux)) {
  region = (paste(as.character(regionV[i]),as.character(ResidueTotaux[i]), sep="_"))
  regionSyn[i] = region
}
```

```

}
names(ResidueTotaux) = regionSyn

matrice3PR <- matrix(0,nrow=length(Proteases),ncol=length(RegionPacking))
rownames(matrice3PR) <- Proteases
colnames(matrice3PR) <- RegionPacking

listAtomSyn = NULL

for (i in NbProt){
  filein = listFile[i]
  N = read.table(paste("fileByProt3",filein,sep="/"))
  listAtom = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))
  listAtomSyn = (c(listAtom,listAtomSyn))
}

listAtomSyn2 = NULL

for (i in NbProt){
  filein = listFile[i]
  N = read.table(paste("fileByProt3",filein,sep="/"))
  listAtom = (paste(as.character(N[,3])))
  listAtomSyn2 = (c(listAtom,listAtomSyn2))
}

#[grep("_A", colnames(matrice))]

names(listAtomSyn) = listAtomSyn2
for (j in 1:length(RegionPacking)) {
  for (k in 1:length(NbAtomeinPC.2)) {

    if (sort.res[j] == listAtomSyn[k]){

      matrice3PR[i,j] = 1
    }
  }
}
}

```

Pour PR1

Pour PR2

```

region.file <- read.table("description_regions.csv", sep=",")
as.character(region.file[4,2])

```

```
[1] "dimer"
```

```

listAtom = unique(paste(as.character(M[,6]), as.character(M[,5]), sep="_"))
listAtomSyn = unique(c(listAtom,listAtomSyn))

```

```

matrice3PR2 <- matrix(0, nrow=length(Proteases), ncol=length(NbResidues))

rownames(matrice3PR2) <- Proteases
colnames(matrice3PR2) <- sort.res


listAtomSyn = NULL
for (j in NbProt) {
  for (i in 1:length(ind.PR2)){
    filein = listFile[j]
    if((filein) == (ind.PR2[i])){
      N = read.table(paste("fileByProt3",filein,sep="/"))
      listAtom = (paste(as.character(N[,6]), as.character(N[,5]), sep="_"))
      listAtomSyn = (c(listAtom,listAtomSyn))
    }
  }
}
listAtomSyn2 = NULL

for (j in NbProt){
  for (i in 1:length(ind.PR2)) {
    filein = listFile[j]
    if((filein) == (ind.PR2[i])){
      N = read.table(paste("fileByProt3",filein,sep="/"))
      listAtom = (paste(as.character(N[,3])))
      listAtomSyn2 = (c(listAtom,listAtomSyn2))
    }
  }
}

list.bk = c("C","CA","N","O")
names(listAtomSyn) = listAtomSyn2

for (j in 1:length(sort.res)) {
  for (k in 1:length(NbAtomeinPC.2)) {

    if (sort.res[j] == listAtomSyn[k]){

      #if (((listAtomSyn2[k])=="C") || ((listAtomSyn2[k])=="CA") || ((listAtomSyn2[k])=="O"))
      if (is.element(listAtomSyn2[k], list.bk)==TRUE){

        matrice3PR2[1,sort.res[j]] = matrice3PR2[1,sort.res[j]] + 1
      }else{
        matrice3PR2[2,sort.res[j]] = matrice3PR2[2,sort.res[j]] + 1
      }
    }
  }
}

```

```
}
matrice3PR2
```

	1_A	2_A	3_A	4_A	5_A	6_A	7_A	8_A	9_A	10_A	11_A	12_A	14_A	15_A	16_A	17_A	18_A	19_A	20_A	21_A	23_A	24_A
1hhp	4	6	0	1	1	25	12	0	0	0	0	1	0	0	13	18	2	2	2	0	0	
1hih	2	22	2	19	0	93	46	11	0	1	2	2	10	0	10	0	7	11	2	0	0	
1hii	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1hiv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1hvp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1hsh	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1hsi	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1ivp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1sdt	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2hb3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2hb4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2hpe	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2hpf	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2ien	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2mip	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2nph	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2z4o	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3ebz	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3ec0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3ecg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3ekv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3nu3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3phv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3s45	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4hla	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4l13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	69_A	70_A	71_A	72_A	73_A	74_A	78_A	79_A	80_A	81_A	82_A	87_A	88_A	89_A	90_A	91_A	92_A	93_A	94_A	95_A		
1hhp	2	2	1	2	0	0	2	7	4	6	0	0	0	0	0	2	3	4	4			
1hih	4	18	0	14	0	3	0	22	0	4	3	3	0	0	0	0	0	0	0			
1hii	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
1hiv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
1hvp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
1hsh	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
1hsi	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
1ivp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
1sdt	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2hb3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2hb4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2hpe	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2hpf	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2ien	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2mip	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2nph	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
2z4o	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
3ebz	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
3ec0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
3ecg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
3ekv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
3nu3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
3phv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			

3s45	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4hla	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4l13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	50_B	51_B	52_B	53_B	54_B	55_B	56_B	57_B	58_B	59_B	60_B	61_B	62_B	63_B	65_B	67_B	68_B	69_B	70_B	71_B		
1hhp	1	6	8	16	15	8	4	0	0	0	2	4	0	0	0	3	7	0	0	0	0	0
1hih	0	0	0	39	7	34	0	10	3	3	16	21	0	15	7	4	30	8	6	0	0	0
1hii	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1hiv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1hvp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1hsh	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1hsi	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1ivp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1sdt	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2hb3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2hb4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2hpe	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2hpf	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2ien	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2mip	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2nph	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2z4o	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3ebz	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3ec0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3ecg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3ekv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3nu3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3phv	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3s45	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4hla	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4l13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Etudier le lien entre la conservation des résidus impliqués dans le packing cristallin et l'espace cristallo des structures

1. Déterminer l'espace cristallographique de chaque structure en allant sur la site de la PDB (rcsb.org)

#BROUILLON

```

"1_A" "2_A" "3_A" "4_A" "5_A" 5
"6_A" "7_A" "8_A" "9_A" 4
"10_A" "11_A" "12_A" "14_A" "15_A" "16_A" "17_A" "18_A" "19_A" "20_A" "21_A" "23_A" 12
"24_A" "25_A" "26_A" "27_A" "29_A" "30_A" 6
"34_A" "35_A" "36_A" 3
"37_A" "38_A" "39_A" "40_A" "41_A" "42_A" 6
"43_A" "44_A" "45_A" "46_A" "47_A" "48_A" "49_A" "50_A" "51_A" "52_A" "53_A" "54_A" "55_A" "56_A" "57_A"
"59_A" "60_A" "61_A" "63_A" "65_A" "66_A" "67_A" "68_A" "69_A" "70_A" "71_A" "72_A" "73_A"
"74_A" 14
"78_A" "79_A" 2
"80_A" "81_A" "82_A" 3

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"87_A" "88_A" "89_A" "90_A" "91_A" "92_A" "93_A" "94_A" "95_A"          9
"96_A" "97_A" "98_A" "99_A"          4

names (sort.res) = c("dimer","dimer","dimer","dimer","dimer",
                     "R1","R1","R1","R1",
                     "fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum",
                     "catalytic","catalytic","catalytic","catalytic","catalytic","catalytic",
                     "R2","R2","R2",
                     "flapelbow","flapelbow","flapelbow","flapelbow","flapelbow","flapelbow",
                     "flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps",
                     "cantilever","cantilever","cantilever","cantilever","cantilever","cantilever","cantilever","cantilever",
                     "R3","R3",
                     "wall","wall","wall",
                     "alphahelix","alphahelix","alphahelix","alphahelix","alphahelix","alphahelix","alphahelix",
                     "dimer","dimer","dimer","dimer",)

Region2 = c("dimer","R1","fulcrum","catalytic","R2","flapelbow","flaps","cantilever","R3","wall","R4",)

"1_B"  "2_B"  "3_B"  "4_B"          4
"6_B"  "7_B"  "8_B"          3
"10_B" "11_B" "12_B" "13_B" "14_B" "16_B" "17_B" "18_B" "19_B" "20_B" "21_B"          11
"29_B" "30_B"          2
"34_B" "35_B" "36_B"          3
"37_B" "38_B" "39_B" "40_B" "41_B" "42_B"          6
"43_B" "44_B" "45_B" "46_B""47_B" "48_B" "49_B" "50_B" "51_B" "52_B" "53_B" "54_B" "55_B" "56_B" "57_B"
"59_B" "60_B" "61_B" "62_B" "63_B" "65_B" "67_B" "68_B" "69_B" "70_B" "71_B" "72_B" "73_B" "74_B"
                                     10
"76_B" "78_B" "79_B"          3
"80_B" "81_B" "82_B" "83_B"          4
"87_B" "88_B" "91_B" "92_B" "94_B" "95_B"          6
"96_B" "98_B" "99_B"          3

names (sort.res) = c("dimer","dimer","dimer","dimer",
                     "R1","R1","R1",
                     "fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum","fulcrum",
                     "catalytic","catalytic",
                     "R2","R2","R2",
                     "flapelbow","flapelbow","flapelbow","flapelbow","flapelbow","flapelbow",
                     "flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps","flaps",
                     "cantilever","cantilever","cantilever","cantilever","cantilever","cantilever","cantilever","cantilever",
                     "R3","R3","R3",
                     "wall","wall","wall","wall",
                     "alphahelix","alphahelix","alphahelix","alphahelix","alphahelix","alphahelix",
                     "dimer","dimer","dimer",)

test

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```
"1_A" "2_A" "3_A" "4_A" "5_A" 5  
"6_A" "7_A" "8_A" "9_A" 4  
"10_A" "11_A" "12_A" "14_A" "15_A" "16_A" "17_A" "18_A" "19_A" "20_A" "21_A" "23_A" 12  
"24_A" "25_A" "26_A" "27_A" "29_A" "30_A" 6  
"34_A" "35_A" "36_A" 3  
"37_A" "38_A" "39_A" "40_A" "41_A" "42_A" 6  
"43_A" "44_A" "45_A" "46_A" "47_A" "48_A" "49_A" "50_A" "51_A" "52_A" "53_A" "54_A" "55_A" "56_A" "57_A"  
  
"59_A" "60_A" "61_A" "63_A" "65_A" "66_A" "67_A" "68_A" "69_A" "70_A" "71_A" "72_A" "73_A"  
"74_A" 14  
"78_A" "79_A" 2  
"80_A" "81_A" "82_A" 3  
"87_A" "88_A" "89_A" "90_A" "91_A" "92_A" "93_A" "94_A" "95_A" 9  
"96_A" "97_A" "98_A" "99_A" 4  
  
names(sort.res) = c("dimer","dimer","dimer","dimer","dimer","R1","R1","R1","R1","fulcrum","fulcrum","fulcrum")  
test = c("dimer","dimer","dimer","dimer","dimer","R1","R1","R1","R1","fulcrum","fulcrum","fulcrum","fulcrum")  
  
Region2 = c("dimer","R1","fulcrum","catalytic","R2","flapelbow","flaps","cantilever","R3","wall","R4","")  
  
"1_B" "2_B" "3_B" "4_B" 4  
"6_B" "7_B" "8_B" 3  
"10_B" "11_B" "12_B" "13_B" "14_B" "16_B" "17_B" "18_B" "19_B" "20_B" "21_B" 11  
"29_B" "30_B" 2  
"34_B" "35_B" "36_B" 3  
"37_B" "38_B" "39_B" "40_B" "41_B" "42_B" 6  
"43_B" "44_B" "45_B" "46_B""47_B" "48_B" "49_B" "50_B" "51_B" "52_B" "53_B" "54_B" "55_B" "56_B" "57_B"  
  
"59_B" "60_B" "61_B" "62_B" "63_B" "65_B" "67_B" "68_B" "69_B" "70_B" "71_B" "72_B" "73_B" "74_B"  
10  
"76_B" "78_B" "79_B" 3  
"80_B" "81_B" "82_B" "83_B" 4  
"87_B" "88_B" "91_B" "92_B" "94_B" "95_B" 6  
"96_B" "98_B" "99_B" 3
```



```
Region1 = c("dimer","dimer","dimer","dimer","dimer","R1","R1","R1","R1","fulcrum","fulcrum","fulcrum",".")
```